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Analysis of superoscillatory wave functions

Matt S. Calder and Achim Kempf
Department of Applied Mathematics, University of Waterloo, Ontario, Canada N2L 3G1

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Surprisingly, differentiable functions are able to oscillate arbitrarily faster than their highest Fourier component would suggest. The phenomenon is called *superoscillation*. Recently, a practical method for calculating superoscillatory functions was presented and it was shown that superoscillatory quantum mechanical wave functions should exhibit a number of counter-intuitive physical effects. Following up on this work, we here present more general methods which allow the calculation of superoscillatory wave functions with custom-designed physical properties. We give concrete examples and we prove results about the limits to superoscillatory behavior. We also give a simple and intuitive new explanation for the exponential computational cost of superoscillations. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1825076]

I. INTRODUCTION

It used to be believed that a function could not oscillate much faster than its highest Fourier component. Aharonov, Berry and others showed that this is not the case by giving explicit counter-examples which they named superoscillatory functions, see, e.g., Refs. 1–4. In fact, there are functions which on arbitrarily long stretches oscillate arbitrarily faster than their highest frequency Fourier component, see Ref. 5. In other words, the presence of localized fast oscillations in a continuous function need not be visible at all in the function's global Fourier transform. In a function's global Fourier transform, contributions from regions of fast oscillations can be cancelled perfectly by contributions from regions where the wave function is oscillating slowly.

In the context of quantum theory, wave functions that superoscillate are able to cause a number of counter-intuitive effects. Some of these may be of conceptual significance in quantum gravity, see Refs. 6 and 7. But effects of superoscillations also enter in the low energy realm of nonrelativistic quantum mechanics. Among such potentially observable low-energy effects is the counter-intuitive phenomenon that particles with superoscillatory wave functions can be made to accelerate when passing through a neutral slit.

Consider a particle which possesses a bounded momentum range, i.e., its momentum wave function vanishes for momenta that are larger than some $p_{\max}$. As will be explained below, we can arrange that in a certain region in space the particle's wave function superoscillates, i.e., that it oscillates with a much shorter wavelength than $h/p_{\max}$. Now let the wave function be incident onto a screen with a single slit in such a way that it is the superoscillatory part of the wave function which passes through the slit. Upon emerging from the slit the particle's wave function will then oscillate rapidly where the slit is and will be zero elsewhere. The very short wavelengths of the emerging wave function will be visible in its global Fourier transform. This is because the contributions to the global Fourier transform which come from the fast oscillations in the slit interval are no longer cancelled by contributions from outside the slit interval. Therefore, the particle will have gained momentum merely by passing the slit. The momentum gain is determined by the shortness of the wavelength of the superoscillations and, as explained below, there is no limit, in principle, to how short that wavelength can be made.

In order to facilitate the design of experiments that can realize the effects of superoscillatory wave functions it is desirable to possess methods for explicitly calculating superoscillatory wave functions with predetermined properties. In particular, one may wish to calculate those low-

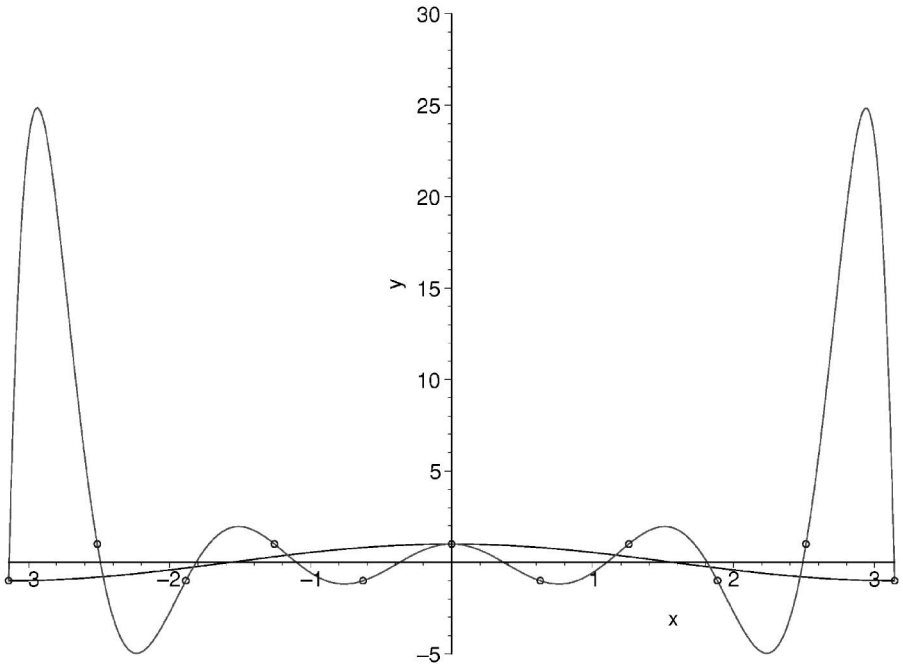

FIG. 1. Example of a superoscillation created by requiring the wave function to pass through certain points. A cosine function of the minimum wavelength/maximum frequency is shown for comparison.

momentum but superoscillatory wave functions which after passing through the slit yield wave functions with a predetermined arbitrarily large momentum and a momentum uncertainty that is as small as is allowed by the uncertainty relation. Our aim here is to develop methods that allow us to solve this and other problems.

Our starting point will be the method for calculating superoscillatory wave functions which was developed in Ref. 6 using results of Refs. 8 and 9. This method allows the construction of wave functions of arbitrarily low fixed frequency content that pass through an arbitrary finite number of prespecified points. Figures 1 and 2 show an example.

Our aim is to develop more general methods for designing superoscillatory functions with generic prespecified properties. We will also ask what the in-principle limits are for the construction of superoscillatory wave functions.

II. SELF-ACCELERATION THROUGH SINGLE SLIT

In order to motivate and formalize the mathematical problem that we will address, let us consider the illustrative example of particles that self-accelerate when passing through a slit.

A. Notation

The Fourier transform of a wave function ψ will be denoted by $\tilde{\psi}$,

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} \, \mathrm{d}x. \tag{1}$$

We will often consider particles whose momentum is bounded by a finite value $p_{\max}$,

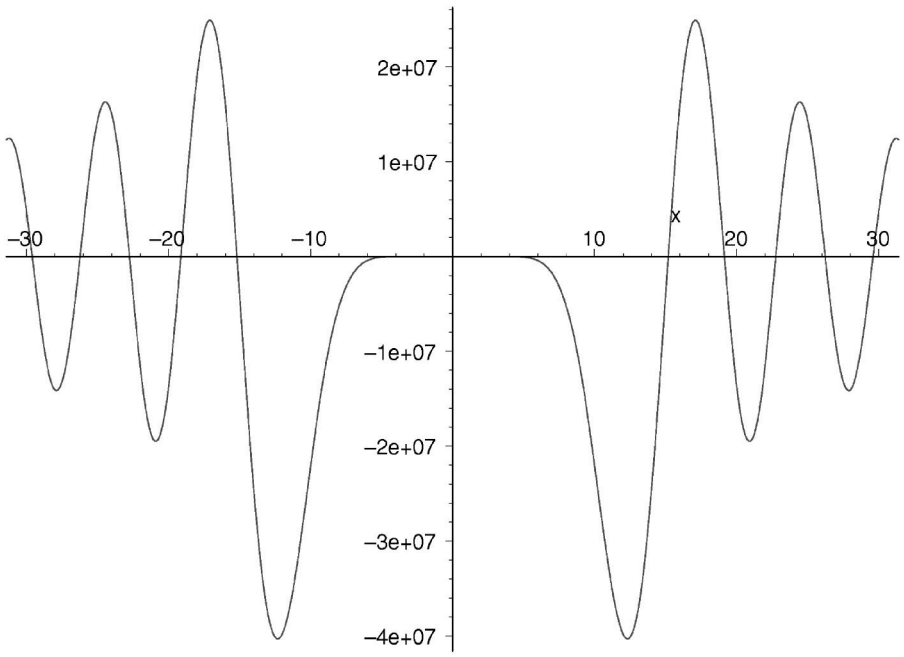

FIG. 2. A zoomed-out Fig. 1. Notice that, as is typical, the amplitudes in the superoscillating region are far smaller (here even unnoticable) than those on either side.

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-p_{\max}}^{p_{\max}} \tilde{\psi}(p) e^{ipx/\hbar}\, \mathrm{d}x. \tag{2}$$

Borrowing terminology from communication engineering and sampling theory, see, e.g., Ref. 10, we will speak of such a function $\psi(x)$ as having bandwidth $p_{\max}$, as being band limited, or in this case as being momentum limited. It will be convenient to define the sinc function as

$$\mathrm{sinc}(x) := \begin{cases} \dfrac{\sin(x)}{x} & \text{if } x \neq 0, \\ 1 \quad \text{if } x = 0. \end{cases} \tag{3}$$

Notice that definitions of the sinc function elsewhere may include a factor of π.

B. Gedanken experiment

Let us consider a particle in two dimensions which travels along the x_1 direction towards a screen which is parallel to the x_2 direction. Assume the particle passes through a slit with x_2-coordinate interval $[-L/2, L/2]$ in the screen. Henceforth, we will assume that the incident particle's momentum parallel to the screen, $\mathbf{p}_2$, has a finite bound $p_{2_{\max}}$,

$$\tilde{\psi}(p_1, p_2, t) = 0 \quad \text{if } p_2 \notin [-p_{2_{\max}}, p_{2_{\max}}]. \tag{4}$$

Our aim is to compare the particle's momentum parallel to the screen before and after the particle passes the slit. For simplicity, we will suppress the variables x_1, p_1, and t. From now on, x_2 is renamed x and p_2 is renamed p. We denote the incident wave function just before passing through the slit by $\psi(x)$ and we denote the wave function which emerges from the slit by $\Psi(x)$. The state $|\Psi\rangle$ is of course given by projection and renormalization,

$$|\Psi\rangle := \frac{P_s|\psi\rangle}{\|P_s|\psi\rangle\|}, \tag{5}$$

where P_s projects onto the slit,

$$P_s\psi(x) := \begin{cases} \psi(x), & \text{if } |x| \leqslant \frac{L}{2}, \\ 0, & \text{otherwise.} \end{cases} \tag{6}$$

Similarly, we define P_b as the projector onto a finite momentum interval,

$$P_b\tilde{\psi}(p) := \begin{cases} \tilde{\psi}(p), & \text{if } |p| \leqslant p_{\max}, \\ 0, & \text{otherwise.} \end{cases} \tag{7}$$

While the incident wave function is momentum limited, $P_b|\psi\rangle = |\psi\rangle$, the emerging wave function is position limited, obeying $P_s|\Psi\rangle = |\Psi\rangle$.

As was shown in Refs. 5 and 6, it is always possible to find incident wave functions $\psi(x)$ which obey the momentum bound $p_{\max}$ and which at any finite number of points in the slit interval take arbitrarily prescribed amplitudes (we will reproduce this result as a special case below). We will be able to arrange, therefore, that the wave function $\psi(x)$ takes, for example, the alternating values $(-1)^n$ at an arbitrarily large number of points in the slit interval—which enforces superoscillations. These $\psi(x)$ will be differentiable and square integrable. Then, if the particle passes the slit, only the superoscillating stretch of the wave function emerges from the slit. Renormalized, we denote it $\Psi(x)$. The Fourier transform $\tilde{\Psi}(p)$ of $\Psi(x)$ will show the presence of small wavelengths, implying that the particle emerges from the slit accelerated to a momentum beyond $p_{\max}$.

C. Template functions

As already mentioned, the results of Refs. 5 and 6 showed that functions of fixed bandwidth can always be found which at arbitrarily but finitely many points possess predetermined amplitudes. Therefore, the width or narrowness of the slit does not limit how short the wavelength of the superoscillations can be. As a consequence, there is no slit-dependent limit to the amount of self-acceleration that can be achieved in this way.

This leads us to ask more generally whether the process of self-acceleration can be designed virtually at will: is it always possible to construct incident wave functions $\psi(x)$ of fixed momentum limit $p_{\max}$ which on the slit interval $[-L/2, L/2]$ match any arbitrarily chosen template function, say $\Phi(x)$? This is of interest because, if true, we can optimize the predictability of the self-acceleration. To this end, we would choose the template function $\Phi(x)$ to be a wave function with a fixed arbitrarily large momentum expectation $\overline{p}$ whose momentum uncertainty Δp is as small as allowed by the uncertainty relation. If the incident superoscillatory wave function matched this template function in the slit interval (up to normalization), then the wave function would merge from the slit with the chosen momentum expectation $\overline{p}$ and lowest possible momentum uncertainty, Δp, for the given width of the slit. For later use, let us calculate these ideal template functions $\Phi(x)$.

1. Ideal template functions

Our aim is to find ideal template functions $\Phi(x)$ defined on the slit interval $[-L/2, L/2]$ which minimize the momentum uncertainty Δp, possess a predetermined momentum expectation $\langle\Phi|\mathbf{p}|\Phi\rangle = \overline{p}$ and are normalized $\langle\Phi|\Phi\rangle = 1$. To this end, we need to solve the constrained variational problem with the functional

$$\mathcal{L} = \langle \Phi|\mathbf{p}^2|\Phi\rangle + \mu_1\langle \Phi|\mathbf{p}|\Phi\rangle + \mu_2\langle \Phi|\Phi\rangle, \tag{8}$$

where μ_1 and μ_2 are Lagrange multipliers. Note that minimizing Δp is equivalent to minimizing $\langle \Phi|\mathbf{p}^2|\Phi\rangle$ because $\overline{p}$ is fixed. Hence the Euler–Lagrange equation in position space is

$$-\hbar^2\Phi''(x) - i\hbar\mu_1\Phi'(x) + \mu_2\Phi(x) = 0. \tag{9}$$

Since any wave function that emerges from the slit vanishes at the slit boundaries, we require $\Phi(\pm L/2)=0$. The solution, which is unique up to a phase, is

$$\Phi(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{\pi}{L}x\right)e^{ix\overline{p}/\hbar}. \tag{10}$$

Its uncertainties are $\Delta x = L((\pi^2-6)/12\pi^2)^{1/2} \approx 0.18L$ and $\Delta p = \pi\hbar/L$. We have $\Delta x\Delta p \approx 0.57\hbar$ which is a little larger than what the uncertainty relation allows because our problem requires template functions $\Phi(x)$ to be zero outside the slit interval.

2. Superoscillatory wave functions cannot match arbitrary templates

Let us now come back to the question whether it is generally possible to find an incident wave function $\psi(x)$ which obeys a momentum bound $p_{\max}$ while in the interval $[-L/2, L/2]$ agreeing completely with an arbitrarily chosen template function $\Phi(x)$, such as the function $\Phi(x)$ just calculated in Sec. II C 1. Strictly speaking, the answer is no.

As is easily verified, all band-limited functions are entire functions. In particular, any momentum-limited incident wave function $\psi(x)$ is entire and it is, therefore, everywhere differentiable. Now choose, for example, a template function $\Phi(x)$ which is not differentiable at some point in the interval $[-L/2, L/2]$. Thus, there cannot exist a momentum-limited incident wave function which obeys $\psi(x)=\Phi(x)$ for all $x \in [-L/2, L/2]$. Nevertheless, a slightly weaker proposition does hold.

3. Convergence towards arbitrary template functions

Let $\Phi(x)$ be a continuous and square integrable template function. Let us ask whether one can always find a sequence of wave functions $\psi_N(x)$ of fixed momentum bound $p_{\max}$ which behave with more and more precision like $\Phi(x)$ over the region of the slit. To be precise, is it possible to find a sequence of momentum-limited incident waves $|\psi_N\rangle$ whose emerging wave functions $|\Psi_N\rangle$ have asymptotically vanishing L^2-distance $\||\Psi_N\rangle - |\Phi\rangle\|$ to an arbitrary template state $|\Phi\rangle$? This is indeed the case.

To see this, consider in the quantum mechanical Hilbert space of states $\mathcal{H}$ with scalar product

$$\langle \xi_1|\xi_2\rangle := \int_{-\infty}^{\infty} \xi_1^*(x)\xi_2(x)\mathrm{d}x, \tag{11}$$

and the following three subspaces:

$$\mathcal{H}_s := P_s\mathcal{H}, \tag{12}$$

$$\mathcal{H}_b := P_b\mathcal{H}, \tag{13}$$

$$\mathcal{H}_{sb} := P_sP_b\mathcal{H}. \tag{14}$$

That is, $\mathcal{H}_s$ is the subspace of states with position limitation to the slit, $\mathcal{H}_b$ is the subspace of states with fixed momentum limitation $p_{\max}$, and $\mathcal{H}_{sb}$ is the subspace of states obtained after passing the momentum-limited wave functions through the slit.

Proposition 1: $\mathcal{H}_{sb}$ is dense in $\mathcal{H}_s$, i.e.,

$$\forall |\Phi\rangle \in \mathcal{H}_s, \varepsilon > 0 \, \exists \, |\Psi\rangle \in \mathcal{H}_{sb} : \| |\Psi\rangle - |\Phi\rangle \| < \varepsilon. \tag{15}$$

Proof: If $|\Phi\rangle = 0$, then take $|\Psi\rangle = 0$. For $|\Phi\rangle \neq 0$ we must show that

$$\nexists |\Phi\rangle \in \mathcal{H}_s \setminus \{0\} : \langle \Psi | \Phi \rangle = 0 \; \forall \, |\Psi\rangle \in \mathcal{H}_{sb}. \tag{16}$$

Since $|\Phi\rangle$ is position limited, this is equivalent to showing that

$$\nexists |\Phi\rangle \in \mathcal{H}_s \setminus \{0\} : \langle \psi | \Phi \rangle = 0 \; \forall \, |\psi\rangle \in \mathcal{H}_b. \tag{17}$$

Assume, for a contradiction, that

$$\exists |\Phi\rangle \in \mathcal{H}_s \setminus \{0\} : \langle \psi | \Phi \rangle = 0 \; \forall \, |\psi\rangle \in \mathcal{H}_b. \tag{18}$$

This implies that $|\Phi\rangle \perp \mathcal{H}_b$. Thus, $\tilde{\Phi}(p) = 0$ on $[-p_{\max}, p_{\max}]$. But, since $\tilde{\Phi}(p)$ is entire and zero over a finite interval, $\tilde{\Phi}(p) = 0$ everywhere on $\mathbb{R}$, i.e., $|\Phi\rangle = 0$. This is a contradiction. Therefore, $\mathcal{H}_{sb}$ is dense in $\mathcal{H}_s$. □

While this result proves the existence of band-limited functions that are arbitrarily close in the L^2 topology to any template function within the window of the slit, the result does not provide explicit methods for constructing such band-limited functions.

III. CONSTRUCTIVE METHOD FOR GENERAL LINEAR CONSTRAINTS

We now focus on practical methods for calculating superoscillatory wave functions that approximate template functions in the slit interval. We begin with the method for constructing superoscillatory functions presented in Ref. 6. This method allows one to specify that the to-be-found superoscillatory function takes arbitrarily chosen amplitudes a_k at any finite number N of arbitrarily chosen points x_k,

$$\psi^{(u)}(x_k) = a_k \quad \text{for } k = 1, \ldots, N. \tag{19}$$

The superscript (u) is to indicate that the fuction will generally be unnormalized. Equation (19) specifies a function which possesses a superoscillating stretch. For example, we may choose the x_k spaced closer than $h/p_{\max}$ and the amplitudes alternating, e.g., $a_k = (-1)^k$. The normalized wave function $\psi(x) = \psi^{(u)}(x)/\|\psi^{(u)}\|$ then possesses superoscillations that are as rapid as those of $\psi^{(u)}$ but with a renormalized amplitude. Thus, in order to obtain the $\psi(x)$ with the most pronounced superoscillations, i.e., the superoscillations of largest possible amplitude, one needs to find that function $\psi^{(u)}(x)$ whose L^2 norm $\|\psi^{(u)}\|$ is minimal. The method of Ref. 6 solves this optimization problem.

We now generalize the method of Ref. 6. To this end, we begin by rewriting the requirement that $\psi^{(u)}(x)$ be band limited by $p_{\max}$ and pass through the points $\{(x_k, a_k)\}_{k=1}^N$, namely (19), in momentum space as

$$\frac{1}{\sqrt{2\pi\hbar}} \int_{-p_{\max}}^{p_{\max}} e^{i(x_k/\hbar)p} \tilde{\psi}^{(u)}(p) \mathrm{d}p = a_k. \tag{20}$$

Our aim is to obtain a method for constructing superoscillatory wave functions which not only pass through predetermined points but which obey also more generic types of constraints. To this end, let us allow constraints on the function $\tilde{\psi}^{(u)}$ which are of the general linear form,

$$a_k = \frac{1}{\sqrt{2\pi\hbar}} \int_{-p_{\max}}^{p_{\max}} \tilde{\chi}_k^*(p) \tilde{\psi}^{(u)}(p) \mathrm{d}p \quad \forall \, k \in \{1, \ldots, N\}. \tag{21}$$

Here, the $\tilde{\chi}_k$ are arbitrary linearly independent differentiable functions. By choosing these, we will be able to prescribe for the superoscillatory wave function not only amplitudes but also arbitrary derivatives, integrals and any other linear constraint. In order to obtain the most pronounced

superoscillations in the normalized function $\tilde{\psi}$ we minimize the norm of $\tilde{\psi}^{(u)}$, subject to the constraints in Eq. (21). The to-be-optimized functional with Lagrange multipliers λ_k reads

$$\mathcal{L} = \int_{-p_{\max}}^{p_{\max}} \tilde{\psi}^{(u)*}(p)\tilde{\psi}^{(u)}(p)\mathrm{d}p - \sum_{k=1}^{N} \frac{\lambda_k^*}{\sqrt{2\pi\hbar}} \int_{-p_{\max}}^{p_{\max}} \tilde{\chi}_k^*(p)\tilde{\psi}^{(u)}(p)\mathrm{d}p + \text{c.c.}, \tag{22}$$

leading to the Euler–Lagrange equation,

$$\tilde{\psi}^{(u)}(p) = \frac{1}{\sqrt{2\pi\hbar}} \sum_{k=1}^{N} \lambda_k \tilde{\chi}_k(p). \tag{23}$$

Recall that $\tilde{\psi}^{(u)}$ is zero outside the interval $[-p_{\max}, p_{\max}]$ by assumption. Thus, using (23) in (21),

$$a_k = \sum_{r=1}^{N} T_{kr}\lambda_r, \tag{24}$$

where the Hermitian matrix T is defined by

$$T_{kr} := \frac{1}{2\pi\hbar} \int_{-p_{\max}}^{p_{\max}} \tilde{\chi}_k^*(p)\tilde{\chi}_r(p)\mathrm{d}p. \tag{25}$$

As we will show below, T is invertible. Thus, $\vec{\lambda} = T^{-1}\vec{a}$, i.e.,

$$\lambda_k = \sum_{r=1}^{N} T_{kr}^{-1} a_r. \tag{26}$$

Thus, using the Fourier transform of the constraint function

$$\chi_k(x) := \frac{1}{\sqrt{2\pi\hbar}} \int_{-p_{\max}}^{p_{\max}} \tilde{\chi}_k(p) e^{ixp/\hbar}\, \mathrm{d}p \tag{27}$$

we obtain from (23) that the desired superoscillatory (still unnormalized) incident wave function in position space is given by

$$\psi^{(u)}(x) = \frac{1}{\sqrt{2\pi\hbar}} \sum_{k=1}^{N} \lambda_k \chi_k(x). \tag{28}$$

Existence of the solution: It remains to be shown that T is indeed invertible. To see this, let $\vec{u}$ be an arbitrary vector. Then

$$\vec{u}^{\dagger} T \vec{u} = \sum_{k,r=1}^{N} u_k^* T_{kr} u_r = \frac{1}{2\pi\hbar} \int_{-p_{\max}}^{p_{\max}} \sum_{k,r=1}^{N} u_k^* \tilde{\chi}_k^*(p)\tilde{\chi}_r(p) u_r \,\mathrm{d}p = \frac{1}{2\pi\hbar} \int_{-p_{\max}}^{p_{\max}} \left| \sum_{m=1}^{N} u_m \tilde{\chi}_m(p) \right|^2 \mathrm{d}p.$$

Since the $\tilde{\chi}_k$ are linearly independent the integrand is positive. Therefore, T is positive definite and hence invertible.

IV. THE COST OF SUPEROSCILLATIONS

As was shown in Ref. 6, one cost of superoscillations is that requiring more or faster superoscillations makes the matrix T increasingly difficult to invert numerically, as its smallest and largest eigenvalues differ by growing orders of magnitude. The condition number was found to increase exponentially with the number of superoscillations.

We here only remark that, in the sense of computational complexity, this makes it computationally hard to calculate superoscillations. Interestingly, this also means that any quantum effect

that naturally produces functions with arbitrarily large superoscillatory stretches constitutes an example of an exponential speed-up in the sense of quantum computing. Physical occurrences of superoscillations, e.g., in the context of evanescent waves, have been discussed, e.g., in Refs. 3 and 4. Also, for example (rather speculatively), the possibility of an unbounded production of superoscillations has been discussed in the context of the trans-Planckian problem of black holes in Refs. 11 and 12.

Here, we will focus on a more immediate cost of superoscillations, namely the need for an increasingly large dynamical range, a function's superoscillations are generally of low amplitude when compared to the function's amplitudes to the left and right of its superoscillatory stretch. To be precise, it was shown in Ref. 6 that the L^2 norm of the function increases polynomially with the frequency of the prescribed superoscillations, for fixed prescribed superoscillating amplitudes. In particular, it was also shown that the norm increases exponentially with the number of imposed superoscillations. Correspondingly, in normalized wave functions the amplitudes of superoscillations decrease exponentially with the number of superoscillations. (Of course, if the superoscillating stretch of the particle's wave function happens to pass through the slit then its wave function, however small, is renormalized whereby the superoscillating amplitudes will be restored to the amplitudes of the template function.)

By making use of the special properties of prolate functions these scaling results were derived for the type of superoscillations produced with the method of Ref. 6. In the following two sections we will show more directly the underlying reason for this exponential behavior of the norm of superoscillatory functions. Our argument will apply more generally to all superoscillatory functions that arise from linear constraints.

A. Derivatives and norms

If a function $\psi^{(u)}(x)$ is band limited, one would expect that there is a bound on its derivatives. Applying the Cauchy–Schwarz inequality, consider

$$\begin{aligned}\left|\frac{\mathrm{d}^n}{\mathrm{d}x^n}\psi^{(u)}(x)\right|^2 &= \frac{1}{2\pi\hbar}\left|\int_{-p_{\max}}^{p_{\max}}\tilde{\psi}^{(u)}(p)\left(\frac{ip}{\hbar}\right)^n e^{ipx/\hbar}\,\mathrm{d}p\right|^2 \\ &\leqslant \frac{1}{2\pi\hbar}\left(\int_{-p_{\max}}^{p_{\max}}\left|\tilde{\psi}^{(u)}(p)\left(\frac{ip}{\hbar}\right)^n\right|^2\mathrm{d}p\right)\left(\int_{-p_{\max}}^{p_{\max}}1\,\mathrm{d}p\right) \\ &\leqslant \frac{1}{2\pi\hbar}\left(\frac{p_{\max}}{\hbar}\right)^{2n}2p_{\max}\|\psi^{(u)}\|^2.\end{aligned}$$

Thus,

$$\left|\frac{\mathrm{d}^n}{\mathrm{d}x^n}\psi^{(u)}(x)\right| \leqslant \left(\frac{p_{\max}}{\hbar}\right)^n\sqrt{\frac{p_{\max}}{\pi\hbar}}\|\psi^{(u)}\|. \tag{29}$$

Thus arbitrarily large derivatives, as they can be produced with superoscillations, are consistent with a finite fixed bandwidth but we see that the cost must be an increase in the norm of the function $\|\psi^{(u)}\|$.

B. The norm of superoscillating functions

A precise expression for the norm $\|\psi^{(u)}\|$ of the superoscillatory functions obtained by our method can be derived,

$$\|\psi^{(u)}\|^2 = \frac{1}{2\pi\hbar}\int_{-p_{\max}}^{p_{\max}}\left|\sum_{k=1}^{N}\lambda_k\tilde{\chi}_k(p)\right|^2\mathrm{d}p = \frac{1}{2\pi\hbar}\int_{-p_{\max}}^{p_{\max}}\sum_{k,r=1}^{N}\lambda_k^*\tilde{\chi}_k^*(p)\tilde{\chi}_r(p)\lambda_r\,\mathrm{d}p = \vec{\lambda}^{\dagger}T\vec{\lambda}. \tag{30}$$

Hence,

$$\|\psi^{(u)}\|^2 = \vec{\lambda}^\dagger \vec{a} = \vec{a}^\dagger \vec{\lambda} = \vec{a}^\dagger T^{-1} \vec{a}. \tag{31}$$

Note that T^{-1} is a positive self-adjoint matrix. We now see that for given constraint functions, χ_k, the most norm-expensive superoscillatory functions are obtained if we choose the constraint parameters a_k such that $\vec{a}$ is the eigenvector of T^{-1} with largest eigenvalue. We will arrive at those extreme superoscillations also from independent momentum space considerations in Sec. VI.

C. Adding successive constraints

Consider a set of constraints, described by a set of functions $\{\tilde{\chi}_k\}_{k=1}^N$ and parameters $\{a_k\}_{k=1}^N$ and suppose that, using our method, the momentum-limited wave function which obeys all those constraints and is of minimum norm has been calculated. Let us ask how the norm of the solution to this problem changes if we add one additional constraint

$$a_{N+1} = \frac{1}{\sqrt{2\pi\hbar}} \int_{-p_{\max}}^{p_{\max}} \tilde{\chi}_{N+1}(p) \tilde{\psi}(p) \mathrm{d}p, \tag{32}$$

where χ_{N+1} and a_{N+1} are chosen arbitrarily. Let us denote the solution to the initial problem of N constraints by $\tilde{\psi}_N$ and let us define,

$$c := \frac{1}{\sqrt{2\pi\hbar}} \int_{-p_{\max}}^{p_{\max}} \tilde{\chi}_{N+1}(p) \tilde{\psi}_N(p) \mathrm{d}p. \tag{33}$$

Clearly, if we choose the $(N+1)$st constraint with $a_{N+1} := c$ then $\tilde{\psi}_N$ is also the function of minimum norm obeying the $N+1$ constraints, i.e., $\tilde{\psi}_{N+1} = \tilde{\psi}_N$, just as if we had not added a new constraint, or as if we had set the $(N+1)$st Lagrange multiplier to zero, $\lambda_{N+1} = 0$.

Now, let us allow the constraint parameter a_{N+1} to vary away from c. Correspondingly, our method will yield a family of functions, $\tilde{\psi}_{N+1}$ $(\neq \tilde{\psi}_N)$, parametrized by a_{N+1}. We observe from (31) (letting the sum run to $N+1$) that the norm squared of these functions is a quadratic (and of course positive) polynomial in a_m. Note that its minimum occurs if we choose the a_{N+1} value,

$$c = a_{N+1} = -\frac{1}{T^{-1}_{(N+1),(N+1)}} \sum_{r \neq (N+1)} T^{-1}_{(N+1),r} a_r, \tag{34}$$

because then $\Sigma_{s \neq (N+1)} T^{-1}_{(N+1),s} a_s = 0$. Using (24) we see that this choice of a_{N+1} leads to the vanishing of the Lagrange multiplier $\lambda_{N+1} = 0$, which is what we expected for if we add a new constraint that is already satisfied, $\tilde{\psi}$ will not change.

Crucially, we now see that as we tune a_{N+1} away from c, say in order to enforce an additional superoscillation twist, the squared norm of the solution increases quadratically. Therefore, if we keep adding new generic constraints, say in order to implement more and more superoscillations, this will generally increase the norm of the solution by a factor in each step. Thus, the norm of the solution will generically scale exponentially with an increase in the number of constraints N.

This finding widely generalizes the result of Ref. 6 which applied only to constraints of the special form (19) and among them only to those with equidistant spacings of the x_k.

V. APPLICATIONS TO AN IDEAL TEMPLATE FUNCTION

In Sec. II C 1, we asked how the wave function $\Psi(x)$ that emerges from the slit would have to look in order to describe a particle with an arbitrarily high predetermined momentum expectation value $\overline{p}$ and a momentum uncertainty Δp which is as small as is allowed by the uncertainty relation. This ideal template function was given in (10).

Let us consider the concrete example, $\hbar = 1$, $L = 2\pi$, $p_{\max} = 1$, and $\overline{p} = 2$. If the emerging wave function Ψ can be arranged to be equal or close to this template function Φ, this clearly exhibits

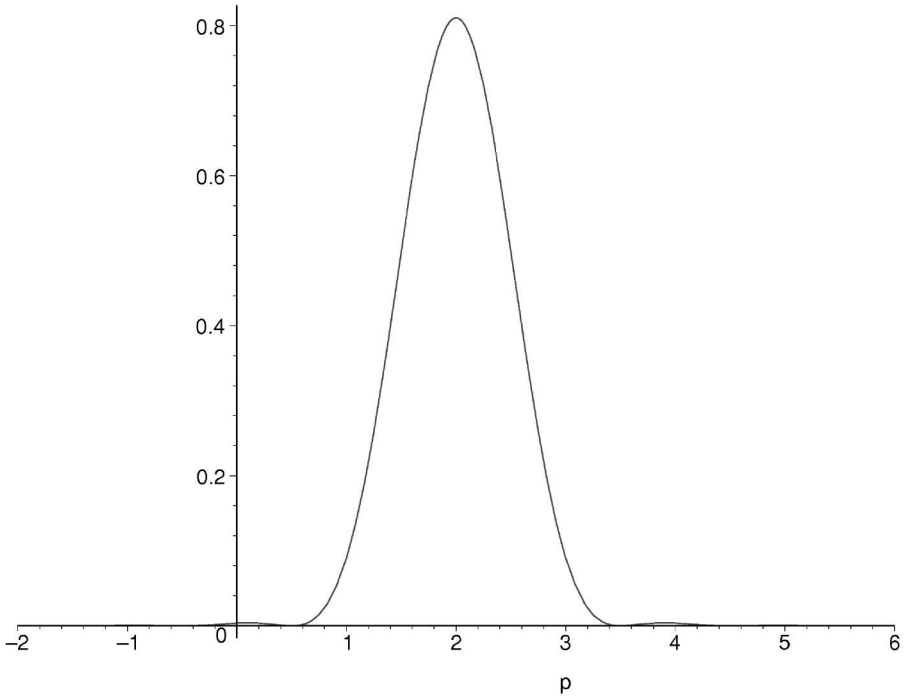

FIG. 3. The ideal template's momentum wave function $|\tilde{\Phi}(p)|^2$. Notice that it is centered well outside the original bandwidth $p_{\max}=1$.

the phenomenon of self-acceleration because the emerging momentum wave function would be peaked at $p \approx \overline{p}=2$, i.e., well outside the original bandwidth of $p_{\max}=1$, see Fig. 3.

We had shown that exact matching, $\Psi(x)=\Phi(x)$, is generally not possible, but we also saw that there always exists a sequence of incident waves ψ_N so that for the emerging waves Ψ_N we have $\Psi_N \to \Phi$ in the L^2 topology, which is here the only physically relevant topology. Thus, there are superoscillatory incident wave functions which achieve the prescribed self-acceleration properties to arbitrary precision. For illustration, let us explicitly calculate such superoscillatory incident wave functions.

A. Method of matching amplitudes

Let us begin by applying the method presented in Ref. 6, which is a special case of our method of general linear constraints. In this special case, we require the momentum-limited incident wave $\psi^{(u)}(x)$ to exactly match the amplitude of the ideal template function at several points x_k of the slit interval $[-L/2, L/2]$. The constraints in the variational problem are then given by the linearly independent constraint functions $\tilde{\chi}_k(p) := e^{-ipx_k/\hbar}$ and constraint parameters $a_k := \Phi(x_k)$. Thus,

$$T_{kr} = \frac{1}{2\pi\hbar}\int_{-p_{\max}}^{p_{\max}} e^{(ip/\hbar)(x_k - x_r)}\, \mathrm{d}p = \frac{p_{\max}}{\pi\hbar}\,\mathrm{sinc}\left(\frac{p_{\max}}{\hbar}[x_k - x_r]\right) \tag{35}$$

which leads to the solution

$$\psi^{(u)}(x) = \frac{1}{\sqrt{2\pi\hbar}}\sum_{k=1}^{N} \lambda_k \chi_k(x), \tag{36}$$

where $\vec{\lambda} = T^{-1}\vec{a}$ and where

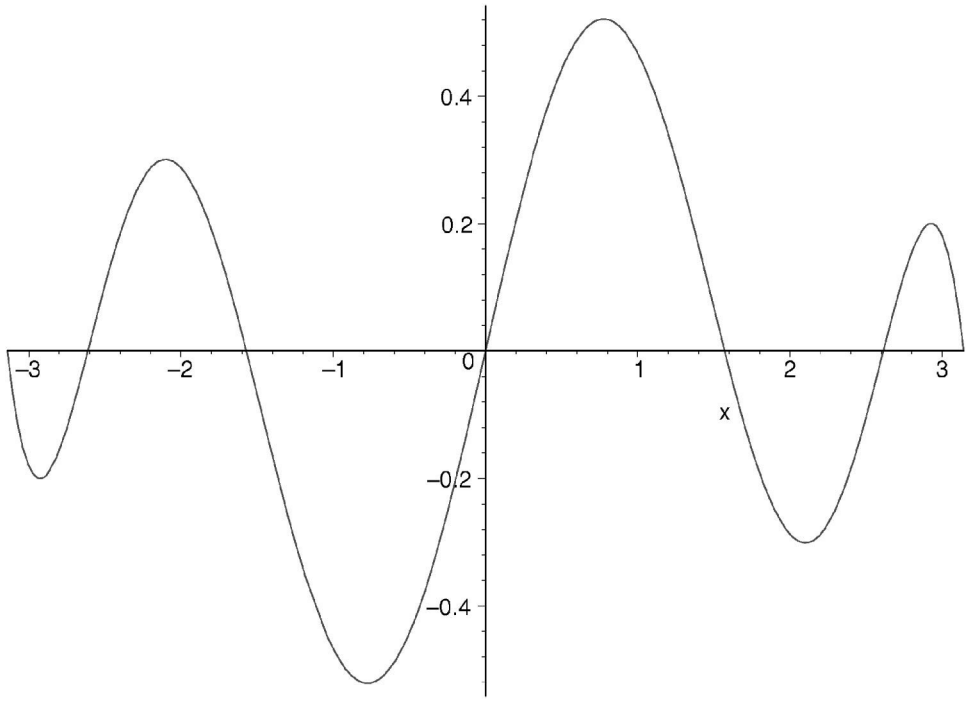

FIG. 4. $\mathrm{Im}(\psi^{(u)}(x))$ over the slit in the example of Sec. V A. The wavelength is about $0.5\lambda_{\min}$.

$$\chi_k(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-p_{\max}}^{p_{\max}} e^{(ip/\hbar)(x-x_k)}\, \mathrm{d}p = p_{\max} \sqrt{\frac{2}{\pi\hbar}}\, \mathrm{sinc}\left(\frac{p_{\max}}{\hbar}[x - x_k] \right). \tag{37}$$

We observe that the wave function $\psi^{(u)}(x)$ is a linear combination of sinc functions centered at the x_k and we note that $\psi(x)$ is square integrable, since the sinc functions are. In general, T is ill conditioned, i.e., care must be taken to invert it with enough numerical precision so as to satisfy the constraints with sufficient accuracy.

We used routines in Maple which calculate $\vec{\lambda} = T^{-1}\vec{a}$ by solving $T\vec{\lambda} = \vec{a}$ using Gaussian elimination. Concretely, we required $\psi^{(u)}(x)$ to match the ideal template function $\Phi(x)$ with $\overline{p} = 2$ at $N = 9$ equidistantly spaced points x_k from slit boundary to slit boundary. For example, Fig. 4 shows the imaginary part of the superoscillatory function $\psi^{(u)}$ over the slit interval. Figure 5 shows a zoomed-out view of $|\psi^{(u)}(x)|^2$, displaying the typical big amplitudes to the left and right of the superoscillating stretch.

The momentum expectation value for the ideal template function that we chose is $\overline{p} = 2p_{\max}$. Numerically, we found that the strictly momentum-limited incident wave function $\psi(x)$ for $N = 9$ yields an emerging wave function $\Psi(x)$ whose momentum expectation value is $\overline{p} \approx 1.92 p_{\max}$. Clearly, the momentum of particles which pass through the slit essentially doubles by self-acceleration, as intended. The momentum uncertainty of the emerging wave function is $\Delta p \approx 1.42 p_{\max}$.

Recall that for this slit size the momentum uncertainty could be significantly smaller, namely $\Delta p = 1/2$, as is precisely realized in the ideal template function. By increasing N, we can achieve that the incident wave function $\psi^{(u)}(x)$ better matches the template, leading to a lowering of Δp towards that limiting value. For example, for $N = 15$ we find $\overline{p} \approx 1.999\,47 p_{\max}$ and $\Delta p \approx 0.500\,25 p_{\max}$. For significantly larger N the exponential computational expense sets in. Our generalized method for linear constraints allows us to use other linear constraints which we found to be numerically more efficient in the sense of allowing us to reach larger values of N. We will discuss the use of these alternative constraints in Sec. V B.

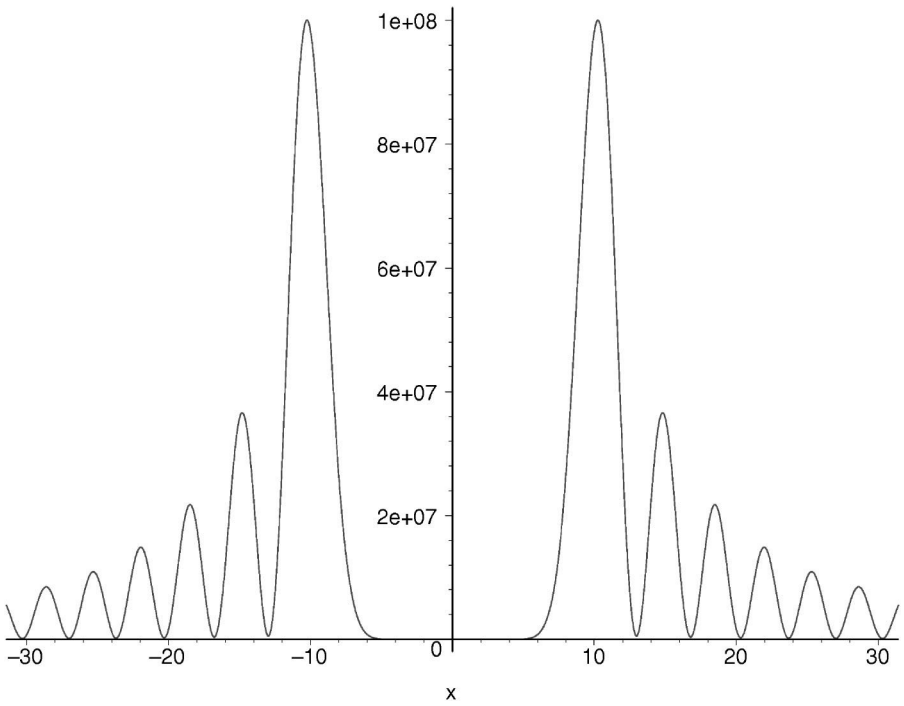

FIG. 5. $|\psi^{(u)}(x)|^2$ over the slit and surrounding regions in the example in Sec. V A.

Figure 6 shows the accuracy with which the $\psi^{(u)}(x)$ obtained by matching $N=9$ amplitudes of $\psi^{(u)}(x)$ to those of $\Phi(x)$ agrees with the ideal template function $\Phi(x)$ for arbitrary x in the slit interval. The behavior is similar for all values of N (that we tested). For general N, there are $N-1$ peaks and the height of the highest peak decreases with N.

B. Method of matching derivatives

In order to illustrate the generality of our new method of Sec. III, let us now construct superoscillatory wave functions by requiring that the wave function matches value and derivatives of the template at one point, instead of requiring, as we did in Sec. V A, that the wave function matches only the value of the template function at several points.

Concretely, let us require that the value and first $N-1$ derivatives of the to-be-found wave function $\psi^{(u)}$ agree at $x=0$ with those of the ideal template function Φ of above. In the equation for general linear constraints (21), we obtain a constraint on the $(k-1)$st derivative by choosing for the constraint function

$$\tilde{\chi}_k(p) = \left(-\frac{ip}{\hbar}\right)^{k-1}. \tag{38}$$

Matching the derivatives to those of the template is to choose the constraint parameters to be $a_k := \Phi^{(k-1)}(0)$, where $\Phi^{(k-1)}$ denotes the $(k-1)$st derivative. Since the $\tilde{\chi}_k$ are linearly independent,

$$T_{kr} = \frac{1}{2\pi\hbar}\int_{-p_{\max}}^{p_{\max}} \left(\frac{ip}{\hbar}\right)^{k-1}\left(-\frac{ip}{\hbar}\right)^{r-1} \mathrm{d}p \tag{39}$$

is invertible, yielding the solution

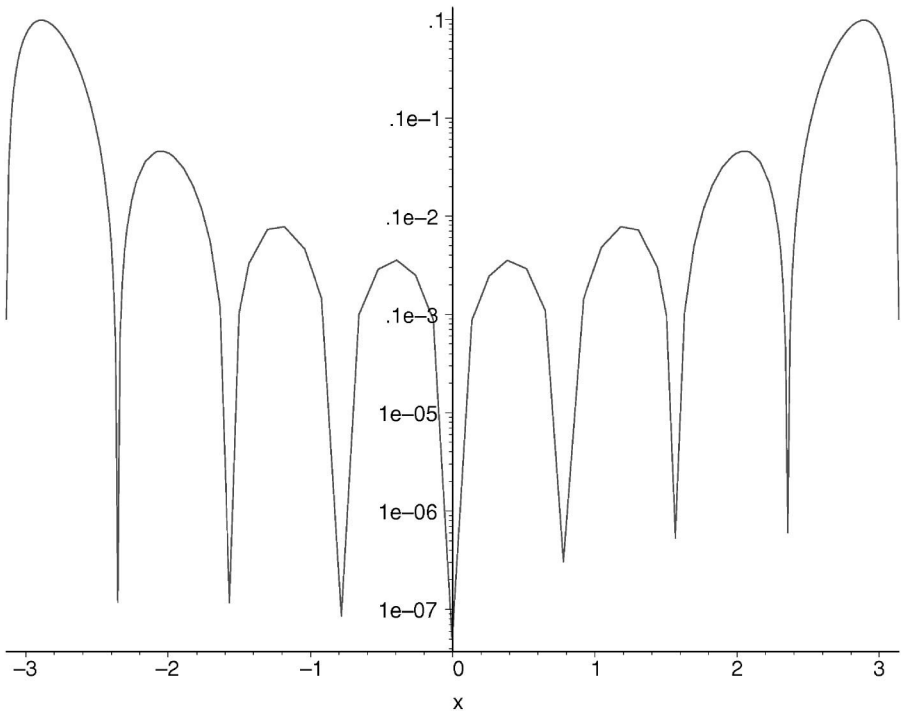

FIG. 6. $|\Psi(x)-\Phi(x)|^2$ over the slit in the example in Sec. V A.

$$\psi^{(u)}(x) = \frac{1}{\sqrt{2\pi\hbar}} \sum_{k=1}^{N} \lambda_k \chi_k(x), \tag{40}$$

where

$$\chi_k(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-p_{\max}}^{p_{\max}} \left(-\frac{ip}{\hbar}\right)^{k-1} e^{ipx/\hbar}\, dp. \tag{41}$$

Note that $\psi(x)$ is a linear combination of derivatives of sinc functions, each of which is band limited. In this case, T is simpler to invert and we can go, for example, to the case $N=23$ before the exponential computational expense sets in. In this case, for large N the coefficients λ_k quickly grow large and hence the subtle cancellations in the Fourier transform require fast increasing numerical precision.

We considered the example where the value of the function and its first 22 derivatives is required to match those of the ideal template function at $x=0$. We found numerically that the momentum-limited superoscillating function, after passing through the slit, then exhibits a momentum expectation value of $\overline{p} \approx 2.0002 p_{\max}$ and momentum uncertainty $\Delta p \approx 0.500\,49$. Thus we reach the targeted momentum-doubling self-acceleration, with a momentum uncertainty which is only marginally above the uncertainty relation limit $\Delta p = 1/2$ for this slit size. Figure 7 displays the accuracy $|\Psi(x)-\Phi(x)|^2$.

VI. A MOMENTUM SPACE METHOD

In position space, superoscillatory wave functions $\psi(x)$ generally possess a characteristic shape: rapid but small oscillations in the superoscillating stretch and a few large long-wavelength amplitudes shortly before and after. Do these states also possess a characteristic shape in momentum space?

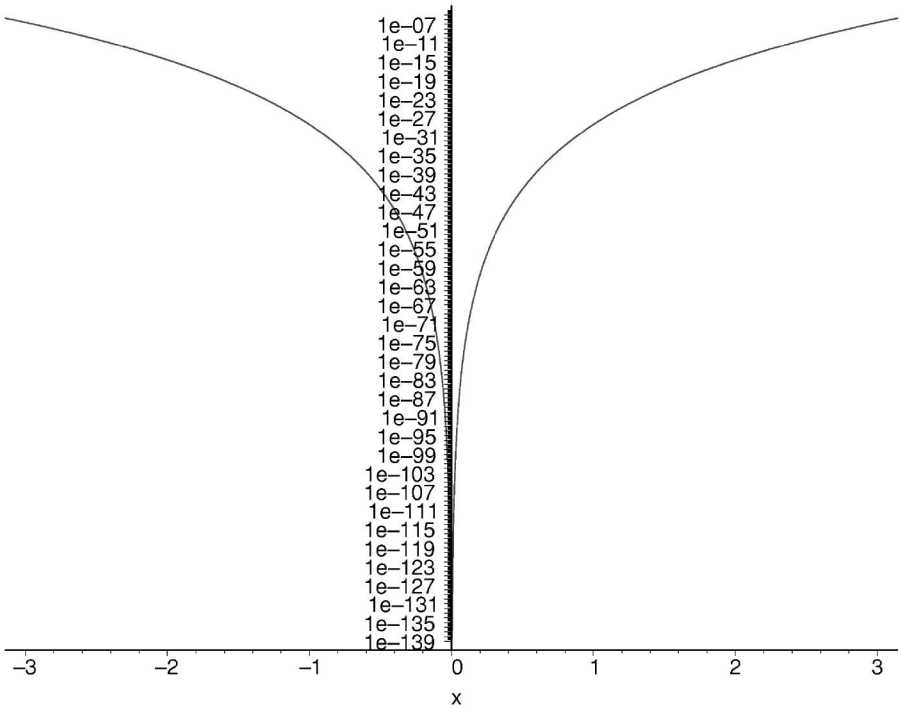

FIG. 7. $|\Psi(x)-\Phi(x)|^2$ over the slit in the example in Sec. V B.

Let us consider, for example, the superoscillations obtained by prescribing oscillating amplitude values a_k at close-by points x_k. We found that, in momentum space, such a state is a linear combination of plane waves $\exp(-ix_kp)$,

$$\tilde{\psi}(p) := \begin{cases} \frac{1}{\sqrt{2\pi\hbar}} \sum_{r=1}^{N} \lambda_r e^{-i(x_r/\hbar)p}, & \text{if } |p| \leqslant p_{\max}, \\ 0, & \text{if } |p| > p_{\max}. \end{cases} \tag{42}$$

It appears, see, e.g., Fig. 8, that these $\tilde{\psi}(p)$ generally possess small amplitudes in most of the momentum interval $[-p_{\max}, p_{\max}]$, except for near the boundaries $\pm p_{\max}$. We calculated the Fourier transforms of a number of superoscillatory wave functions and observed this as a general feature.

Thus, in momentum space, these superoscillations appear to be a linear combination of plane waves whose interference is close to being as strong as it can be, with the effect that the resulting function is of minimized norm.

If this assumption is correct, we should be able to derive superoscillatory wave functions by calculating that linear combination of plane waves in momentum space whose norm is minimal. To this end, let $\{x_r\}_{r=1}^N$ be points in $[-L/2, L/2]$. Our aim is to find a coefficient vector $\{q_r\}_{r=1}^N$ of fixed length, say $\|\vec{q}\|=1$ such that

$$\tilde{\psi}(p) := \begin{cases} \frac{1}{\sqrt{2\pi\hbar}} \sum_{r=1}^{N} q_r e^{-i(x_r/\hbar)p}, & \text{if } |p| \leqslant p_{\max}, \\ 0, & \text{if } |p| > p_{\max}, \end{cases} \tag{43}$$

is of minimum norm. The constrained optimization problem with Lagrange multiplier ν,

$$\mathcal{L} = \|\psi\|^2 + \nu(\|\vec{q}\|^2 - 1) \tag{44}$$

leads to

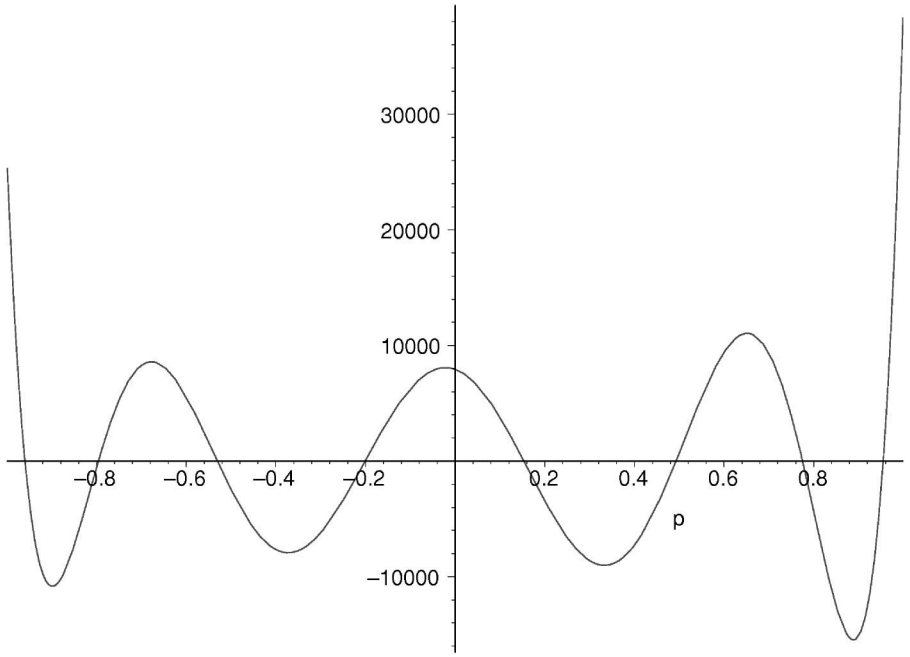

FIG. 8. $\mathrm{Re}(\tilde{\psi}(p))$ of the incident superoscillatory wave in the example in Sec. V A.

$$T\vec{q} = \nu\vec{q}. \tag{45}$$

Thus, the coefficient vector $\vec{q}$ which solves this optimization problem must be eigenvector to T. From Eq. (30), we obtain the general expression for the norm, $\|\psi\|^2 = \vec{q}^{\dagger} T\vec{q}$. Thus, $\vec{q}$ must be that eigenvector of T with the smallest eigenvalue.

Indeed, the position wave function determined by these coefficients $\vec{q}$ is superoscillatory: already in Sec. IV B, we encountered the wave functions whose coefficient vectors λ are the eigenvectors of T^{-1} of largest eigenvalue. There, we found that these are the superoscillatory wave functions which for a given set of constraint points $\{x_k\}$ are most norm expensive and which, therefore, possesses the most pronounced superoscillations.

VII. OPEN PROBLEMS

We know from Sec. II C 3 that it is always possible to find incident wave functions of fixed momentum bound that in the slit interval are matching any given template function arbitrarily closely in the L^2 norm topology. Thus, for all practical purposes, the self-acceleration phenomenon can be tailored at will. Our method of general linear constraints can be used to explicitly construct a sequence of momentum-limited superoscillatory wave functions $\psi_N(x)$ which more and more closely match any given template function Φ. The $\psi_N(x)$ approach $\Phi(x)$ in the slit interval in the sense that they obey more and more linear constraints that tie $\psi_N(x)$ to $\Phi(x)$.

In Sec. V A and Sec. V B we showed that a close approach to a fixed template function can be done numerically efficiently. Clearly, intuition and the easily achieved numerical accuracy lead us to conjecture that our methods for producing superoscillations, as used in Secs. V A and V B, do indeed always lead to convergence in the L^2 topology towards the template function. So far, however, we have no proof that our particular method for producing superoscillatory wave functions from linear constraints does indeed realize the L^2 convergence to generic template functions.

A. Quadratic constraints

Let us ask, therefore, if there is a choice of linear constraints that directly targets the area under the functions and that thereby directly guarantees convergence in the L^2 sense.

One may try, for example, constraints which require that the functions $\psi^{(u)}$ and Φ enclose equal areas on certain subintervals of the slit. This can be set into the form of a linear constraint: Let $\{x_k\}_{k=1}^{N+1}$ be equidistantly spaced points in $[-L/2, L/2]$. We require the linear constraints of (21) with the constraint functions

$$\tilde{\chi}_k(p) = \int_{x_k}^{x_{k+1}} e^{-ipx/\hbar}\, \mathrm{d}x \tag{46}$$

and the constraint parameters

$$a_k = \int_{x_k}^{x_{k+1}} \Phi(x)\mathrm{d}x. \tag{47}$$

While this can easily be carried out, these constraints are not directly guaranteeing L^2 convergence towards the template function by refining the partition of the slit interval into increasingly smaller subintervals: in principle, even functions that enclose equal areas on a very small interval may have very different amplitudes. Let us, therefore, consider to impose constraints which require the area of the function $|\Psi(x)-\Phi(x)|^2$ on small subintervals to be small. It is clear that to this end it would be necessary to implement also constraints that are quadratic in the field $\Psi(x)$. We will here not pursue this strategy to the end. As a preliminary step, however, let us generalize our method for constructing superoscillatory functions to include quadratic constraints.

To this end, we formulate the variational problem of finding the function $\tilde{\psi}^{(u)}$ of smallest norm and with momentum cutoff $p_{\max}$ which satisfies N linear and M quadratic constraints that tie it to a template function Φ,

$$a_k = \frac{1}{\sqrt{2\pi\hbar}} \int_{-p_{\max}}^{p_{\max}} \tilde{\psi}^{(u)}(p)\tilde{\chi}_k^*(p)\mathrm{d}p \quad \text{for } k = 1, \ldots, N, \tag{48}$$

$$b_k = \frac{1}{\sqrt{2\pi\hbar}} \int_{-p_{\max}}^{p_{\max}} \tilde{\psi}^{(u)*}(p)\tilde{\psi}^{(u)}(p)\tilde{\Xi}_k^*(p)\mathrm{d}p \quad \text{for } k = 1, \ldots, M. \tag{49}$$

The to-be-optimized functional with Lagrange multipliers $\{\lambda_k\}_{k=1}^N$ and $\{\mu_k\}_{k=1}^M$, reads

$$\begin{aligned}\mathcal{L} = &\int_{-p_{\max}}^{p_{\max}} \tilde{\psi}^{(u)*}(p)\tilde{\psi}^{(u)}(p)\mathrm{d}p - \sum_{k=1}^{N} \frac{\lambda_k^*}{\sqrt{2\pi\hbar}} \int_{-p_{\max}}^{p_{\max}} \tilde{\psi}^{(u)}(p)\tilde{\chi}_k^*(p)\mathrm{d}p \\ &+ \sum_{k=1}^{N} \frac{\mu_k^*}{\sqrt{2\pi\hbar}} \int_{-p_{\max}}^{p_{\max}} \tilde{\psi}^{(u)*}(p)\tilde{\psi}^{(u)}(p)\tilde{\Xi}_k^*(p)\mathrm{d}p + \text{c.c.}\end{aligned} \tag{50}$$

and the Euler–Lagrange equation reduces to

$$\tilde{\psi}^{(u)}(p) = \frac{\frac{1}{\sqrt{2\pi\hbar}} \sum_{k=1}^{N} \lambda_k \tilde{\chi}_k(p)}{1 + \frac{1}{\sqrt{2\pi\hbar}} \sum_{k=1}^{N} \mu_k \tilde{\Xi}_k(p)}. \tag{51}$$

Although this may be difficult in practice, in principle, the substitution of (51) into (48) and (49) yields sufficient equations to solve for the $\{\lambda_k\}_{k=1}^N$ and $\{\mu_k\}_{k=1}^M$ in terms of the $\{a_k\}_{k=1}^N$ and $\{b_k\}_{k=1}^M$ and this yields the solution $\tilde{\psi}^{(u)}$.

B. A conjecture

Consider the case of a differentiable template function Φ whose derivative is bounded, $|\Phi'(x)| \leqslant K \forall x \in [-L/2, L/2]$, for some finite K. Assume that $\psi_N^{(u)}$ is a sequence of incident wave functions, calculated through the method of Sec. V A with the amplitudes of $\psi_N^{(u)}(x)$ and $\Phi(x)$ matched at N equidistantly spaced points x_k. We conjecture then that the supremum $|\psi_N'(x)|$ for all x and all N is finite as well,

$$|\psi_N'(x)| \leqslant M \quad \forall\, x \in \left[-\frac{L}{2}, \frac{L}{2}\right], \tag{52}$$

for some finite M. This is plausible because, else, $|\psi_N'(x)|$ would have to develop arbitrarily sharp spikes away from the template function in between some two points where its amplitudes are matched to those of the template function. From Sec. IV C, however, we expect large oscillations in the superoscillating stretch to be norm expensive and therefore be prevented from occurring, given that the $\psi_N^{(u)}$ are optimized to possess minimum norm for a given set of constraints.

C. Convergence

Proposition 2: Assume that the conjecture of Sec. VII B holds true. Then, $\{\psi_N(x)\}_N$ *converges uniformly and in the* L^2 *topology over the interval* $[-L/2, L/2]$ *to* $\Phi(x)$ *for* $N \to \infty$.

Proof: Partition the slit into $(N-1)$ equal-length intervals with the N endpoints $x_k^{(N)} := -(L/2) + (k-1)[L/(N-1)]$. Define $\{\alpha_N(x)\}_{N=2}^{\infty}$ by

$$\alpha_N(x) := \max\{x_k^{(N)} | k \in \{1, \ldots, N\}, x_k^{(N)} \leqslant x\}. \tag{53}$$

That is, $\alpha_N(x)$ is the closest point in the partition from the left to x. Then,

$$\begin{aligned} |\psi_N(x) - \Phi(x)| &\leqslant |\psi_N(x) - \Phi(\alpha_N(x))| + |\Phi(\alpha_N(x)) - \Phi(x)| \\ &= |\psi_N(x) - \psi_N(\alpha_N(x))| + |\Phi(\alpha_N(x)) - \Phi(x)| \\ &\leqslant M|x - \alpha_N(x)| + K|\alpha_N(x) - x| \leqslant \frac{(M+K)L}{N-1}, \end{aligned} \tag{54}$$

where we applied the triangle inequality and the mean value theorem. We therefore have uniform and L^2 convergence. □

VIII. SUMMARY

We started with the method for calculating superoscillatory wave functions introduced in Ref. 6 and applied it to concrete examples. We then generalized this method so that it now allows us to construct superoscillatory low-momentum wave functions with a wide range of predetermined properties. Namely, we can impose any arbitrary finite number of linear constraints. We calculated concrete examples.

Further, we addressed the question whether superoscillatory functions can be made to match any arbitrary continuous function on a finite interval. This would correspond to imposing an infinite number of constraints. Generally, the answer is no. However, we were able to prove that there always exists a sequence of superoscillatory wave functions which converges in the physically relevant L^2 topology towards any continuous template function over an arbitrarily large chosen interval.

This is of interest, for example, in the case of the single slit. We proved that the wave function of an incident low-momentum particle can be chosen to arbitrary precision such that, if the particle

passes through the slit, it will emerge with a predetermined arbitrarily large momentum expectation and with a momentum uncertainty that is as small as permitted by the width of the slit.

Our method for constructing superoscillating wave functions allows us to construct superoscillatory wave functions which match any *finite* number N of properties of a given template function (such as the template function's amplitudes or derivatives at specified points). This leads to the question if by letting the number of constraints, N, go to infinity we can obtain one of those sequences of superoscillatory wave functions which converge towards the template function in the L^2 topology.

We proved that such sequences exist but we have not proved that our particular method produces such sequences. The numerical evidence certainly suggests that this is the case. In fact, we found rather fast numerical convergence.

Nevertheless, it would be highly desirable to be able to prove that a given method for producing superoscillations can be used to calculate a sequence of superoscillatory functions that converges in the L^2 topology towards any given template function on an interval. An investigation based on Weierstrass' approximation theorem is in progress.[13]

Last, we found a method for identifying a class of superoscillatory functions by looking at their behavior in momentum space: superoscillatory functions can be viewed as functions which in momentum space are a linear combination of plane waves with coefficients such that their interference is maximal, i.e., such that their norm is minimal.

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Contextual logic for quantum systems

Graciela Domenech[a)]
Instituto de Astronomía y Física del Espacio (IAFE), Casilla de Correo 67, Sucursal 28, 1428 Buenos Aires, Argentina

Hector Freytes[b)]
Escuela de Filosofía - Universidad Nacional de Rosario, Entre Ríos 758, 2000, Rosario, Argentina

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In this work we build a quantum logic that allows us to refer to physical magnitudes pertaining to different contexts from a fixed one without the contradictions with quantum mechanics expressed in no-go theorems. This logic arises from considering a sheaf over a topological space associated with the Boolean sublattices of the ortholattice of closed subspaces of the Hilbert space of the physical system. Different from standard quantum logics, the contextual logic maintains a distributive lattice structure and a good definition of implication as a residue of the conjunction. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1819525]

I. INTRODUCTION

Quantum mechanics has profound conceptual difficulties that may be posed in several ways. Nonetheless, almost every problem in the relation between the mathematical formalism and what may be called "our experience about the behavior of physical objects" can be encoded in the question about the possible meaning of the proposition "the physical magnitude *A* has a value and the value is this or that real number." Already from the first formalizations this point was recognized. For example, Dirac stated in his famous book: "The expression that an observable 'has a particular value' for a particular state is permissible in quantum mechanics in the special case when a measurement of the observable is certain to lead to the particular value, so that the state is an eigenstate of the observable. It may easily be verified from the algebra that, with this restricted meaning for an observable 'having a value,' if two observables have values for a particular state, then for this state the sum of the two observables (if the sum is an observable) has a value equal to the sum of the values of the two observables separately and the product of the two observables (if this product is an observable) has a value equal to the product of the values of the two observables separately."[10] This last point is the requirement of the functional compatibility condition (FUNC), to which we will return later. As long as we limit ourselves to speak about measuring results and avoid being concerned with what happens to nature when she is not measured, quantum mechanics carries out predictions with great accuracy. But, if we naively try to interpret eigenvalues as the possible or actual values of the physical properties of a system, we are faced with all kinds of no-go theorems that preclude this possibility. Most remarkable is the Kochen–Specker (KS) theorem, which rules out the noncontextual assignment of values to physical magnitudes.[17] Of course, to restrict the valuation to a subset of observables—typically to a complete set of commuting observables (CSCO) which constitutes a *context*—and refer to values of physical variables only in the sense allowed by the mathematical formalism, ensures no contradiction. So, a widely accepted position is to abandon seeking to describe what nature at the quantum level is and use the theory as a mere instrument of prediction. But, there are also different

[a)]Fellow of the Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET); Electronic mail: domenech@iafe.uba.ar
[b)]Electronic mail: hfreytes@dm.uba.ar

proposals to investigate how to assign objective and measurable properties to a physical entity, i.e., how far we can refer to physical objects without contradiction with quantum theory. This paper is framed in that search.

Our proposal is to construct a logic to enable not only a Boolean valuation in each fixed context but also that, once chosen, certain set of projectors of the spectral decomposition of the operators (correspondingly, closed subspaces of Hilbert space $\mathcal{H}$) that admits a global Boolean valuation, to make it possible to refer at least partially to projectors pertaining to other contexts with the least arbitrariness.

Let us be concerned here with the simplest cases: pure states of the system are represented by normalized vectors of $\mathcal{H}$ and dynamical variables A by bounded self-adjoint operators $\mathbf{A}$ with discrete spectra. The possible results of the measurement of a (sharp) magnitude A are the eigenvalues a_i pertaining to the spectrum $\sigma(\mathbf{A})$ of its associated operator $\mathbf{A}$. To each of the eigenvalues a_i corresponds a projector $\mathbf{P}_i$ and correspondingly a closed subspace of $\mathcal{H}$. Every $\mathbf{A}$ admits a spectral decomposition

$$\mathbf{A} = \sum_i a_i \mathbf{P}_i,$$

where the equality is considered as a convergence in norm. So, observables may be discomposed to give an exhaustive and exclusive partition of the possible alternatives for the results of measurements. The probability to obtain one of them in an experimental procedure is given by the Born rule.

Now, let us suppose the state of the physical system is an eigenvector of a nondegenerate observable $\mathbf{A}$ (i.e., $\mathbf{A}$ constitutes a CSCO) so we know the eigenvalues of all projectors $\mathbf{P}_1, \mathbf{P}_2, \ldots, \mathbf{P}_n, \ldots$ of $\mathbf{A}$ for the system in this state. If any $\mathbf{P}_i$ lies in the spectral decomposition of another observable $\mathbf{B}$, then this "part" of B can be valued in a Boolean way. It is important to realize that this allows one to refer to observables pertaining to a CSCO from another CSCO. In categorical terms, this will be related to the possible local sections of a sheaf satisfying a certain kind of compatibility with respect to fixed contexts, to be exactly stated in what follows. From this formal analysis in terms of sheaves, we intend to build the mentioned logic, which we will call *contextual logic*. This *contextual logic* will allow us to formalize to what extent we can consider as objective properties of a physical system those properties represented by projectors pertaining to different contexts without facing no-go theorems. We will use a categorial frame to develop this logic, as has been the case during the last years, when applications of category theory tools to logical questions in standard quantum mechanics have begun to appear (for example, Isham and Butterfield,[15,16,13,6] also in the consistent histories approach,[14] in the interpretation of the Sasaki hook as an adjunction[8] and, in general, in the Geneve–Brussels approach[1,2,7]).

In Sec. II we introduce basic notions about lattice theory and topics in categories. We devote Sec. III to the problem of the valuations of physical magnitudes pertaining to different CSCCs. In Sec. IV we face the same problem from the point of view of sheaves, relating it to the dual spectral presheaf introduced in Ref. 15. In Sec. V we develop the contextual logic in a Kripke style and intuitionistic way. Finally, in Sec. VI we outline our conclusions.

II. BASIC NOTIONS

We recall from Refs. 3, 4, 11, and 18 some notions of the lattice theory and categories that will play an important role in what follows.

First, let $(A, \leqslant)$ be a poset and $X \subseteq A$. X is *decreasing set* if and only if for all $x \in X$, if $a \leqslant x$ then $a \in X$. For each $a \in A$ we define the *principal decreasing set* associated with a as $(a] = \{x \in A : x \leqslant a\}$. The set of all decreasing sets in A is denoted by A^+, and it is well known that $(A^+, \subseteq)$ is a complete lattice; thus $\langle A, A^+ \rangle$ is a topological space. We observe that if $G \in A^+$ and $a \in G$, then $(a] \subseteq G$. Therefore, $B = \{(a] : a \in A\}$ is a base of the topology A^+, which we will refer to as the *canonical base*. If $X \subseteq A$, we denote by ∂X the border of X, $C(X)$ the complement of X and X° the interior of X.

Let $\mathcal{A}$ be a category. We denote by $Ob(\mathcal{A})$ the class of objects and by $Ar(\mathcal{A})$ the class of arrows. Given an arrow $f:a\to b$, a is called domain of $f(a=\mathrm{dom}(f))$ and b is called codomain of $f(\mathrm{cod}(f))$. We denote by $[a,b]_{\mathcal{A}}$ the class of all arrows $a\to b$ in the category and by 1_A the identity arrow over the object A. $\mathcal{A}$ is said to be *small category* if and only if $Ob(\mathcal{A})$ is a set. A partially ordered set $(P,\leqslant)$ gives rise to a category with the elements of P as objects, and with precisely one arrow $p\to q$ if and only if $p\leqslant q$. In this case, $(P,\leqslant)$ is a small category. The category whose objects are sets and arrows are functions with the usual composition is denoted by *Ens*.

Let I be a topological space. A *sheaf* over I is a pair (A,p), where A is a topological space and $p:A\to I$ is a local homeomorphism. This means that each $a\in A$ has an open set G_a in A that is mapped homeomorphically by p onto $p(G_a)=\{p(x):x\in G_a\}$, and the latter is open in I. It is clear that p is a continuous and open map. If $p:A\to I$ is a sheaf over I, for each $i\in I$, the set $A_i=\{x\in A:p(x)=i\}$ is called the *fiber* over i. Each fiber has the discrete topology as subspace of A. *Local sections* of the sheaf p are continuous maps $\nu:U\to A$ defined over open proper subsets U of I such that the following diagram is commutative:

$$\begin{array}{ccc} U & \overset{\upsilon}{\longrightarrow} & A \\ & 1_U \searrow \equiv & \downarrow p \\ & & U \end{array}$$

In particular, we use the term *global section* only when $U=I$.

Given the category $\mathcal{A}$, one can form a new category $\mathcal{A}^{op}$, called *dual* category of $\mathcal{A}$, by taking the same objects but reversing the directions of all the arrows and the order of all compositions. $Ens^{\mathcal{A}^{op}}$ or $\hat{\mathcal{A}}$, where $\mathcal{A}$ is a small category, is the category whose objects are functors $F:\mathcal{A}^{op}\to Ens$ (also called *presheaves*) and whose arrows are natural transformations between presheaves. $\hat{\mathcal{A}}$ is a topos, i.e., has terminal object, pullbacks, exponentiation, and subobject classifier. The terminal object in $\hat{\mathcal{A}}$ is the functor $\mathbf{1}:\mathcal{A}^{op}\to Ens$ such that $\mathbf{1}(A)=\{*\}$ (the singleton) for each $A\in\mathcal{A}$ and for each arrow f, $\mathbf{1}(f)=\mathbf{1}_{\{*\}}$. For any presheaf $F:\mathcal{A}^{op}\to Ens$, the unique arrow $F\to\mathbf{1}$ is the natural transformation whose components are the unique functions $F(A)\to\{*\}$ for each object A in $\mathcal{A}$. Pullbacks, limits, and colimits are defined componentwise.

A *local section* of a presheaf $F:\mathcal{A}^{op}\to Ens$ is a natural transformation $\tau:U\to F$ such that U is a subfunctor of the presheaf $\mathbf{1}$. We only refer to *global sections* in the case that $U=\mathbf{1}$.

III. THE QUESTION OF VALUATION

Let $\mathcal{H}$ be the Hilbert space associated with the physical system and $L(\mathcal{H})$ be the set of closed subspaces on $\mathcal{H}$. If we consider the set of these subspaces ordered by inclusion, then $L(\mathcal{H})$ is a complete orthomodular lattice.[19] It is well known that each self-adjoint operator $\mathbf{A}$ has an associated Boolean sublattice W_A of $L(\mathcal{H})$. More precisely, W_A is the Boolean algebra of projectors $\mathbf{P}_i$ of the spectral decomposition $\mathbf{A}=\Sigma_i\, a_i\mathbf{P}_i$. We will refer to W_A as the spectral algebra of the operator $\mathbf{A}$. Any proposition about the system is represented by an element of $L(\mathcal{H})$ which is the algebra of quantum logic introduced by Birkhoff and von Neumann.[5]

Assigning values to a physical quantity A is equivalent to establishing a Boolean homomorphism $\upsilon:W_A\to\mathbf{2}$,[15] 2 being the two-element Boolean algebra. So, it is natural to consider the following definition.

Definition 3.1: Let $(W_i)_{i\in I}$ be the family of Boolean sublattices of $L(\mathcal{H})$. A global valuation over $L(\mathcal{H})$ is a family of Boolean homomorphisms $(\upsilon_i:W_i\to\mathbf{2})_{i\in I}$ such that $\upsilon_i|W_i\cap W_j=\upsilon_j|W_i\cap W_j$ for each $i,j\in I$.

This global valuation would give the values of all magnitudes at the same time maintaining a **compatibility condition** in the sense that whenever two magnitudes shear one or more projectors, the values assigned to those projectors are the same from every context.

But, KS theorem assures that we cannot assign real numbers pertaining to their spectra to operators $\mathbf{A}$ in such a way to satisfy the functional composition principle (FUNC), which is the expression of the "natural" requirement mentioned by Dirac that, for any operator $\mathbf{A}$ representing

a dynamical variable and any real-valued function $f(\mathbf{A})$, the value of $f(\mathbf{A})$ is the corresponding function of the value of $\mathbf{A}$. This is a very restrictive constraint because it does not allow assignment of values to all possible physical quantities or assignment of true–false as truth values to all propositions about the system, nor even noncontextual partial ones. KS theorem means that, if we demand a valuation to satisfy FUNC, then it is forbidden to define it in a noncontextual fashion for subsets of quantities represented by commuting operators. In the algebraic terms of the previous definition, KS theorem reads:

Theorem 3.2: *If $\mathcal{H}$ is a Hilbert space such that $dim(\mathcal{H})>2$, then a global valuation over $L(\mathcal{H})$ is not possible.* □

Of course, contextual valuations allow us to refer to different sets of actual properties of the system which define its state in each case. Algebraically, a *contextual valuation* is a Boolean valuation over one chosen spectral algebra. In classical particle mechanics it is possible to define a Boolean valuation of all propositions, that is to say, it is possible to give a value to all the properties in such a way of satisfying FUNC. This possibility is lost in the quantum case. And, it is not a matter of interpretation, it is the underlying mathematical structure that enables this possibility for classical mechanics and forbids it in the quantum case. The impossibility to assign values to the properties while at the same time satisfying FUNC is a weighty obstacle for almost any interpretation of the formalism as something more than a mere instrument.

IV. SPECTRAL SHEAF

$L(\mathcal{H})$ being the lattice of closed subspaces of the Hilbert space $\mathcal{H}$, we consider the family $\mathcal{W}$ of all Boolean subalgebras of the lattice $L(\mathcal{H})$ ordered by inclusion and the topological space $\langle \mathcal{W}, \mathcal{W}^+ \rangle$. On the set

$$E = \{(W,f): W \in \mathcal{W}, \quad f: W \to \mathbf{2} \text{ is a Boolean homomorphism}\},$$

we define a partial ordering given as

$$(W_1,f_1) \leqslant (W_2,f_2) \Leftrightarrow W_1 \subseteq W_2 \quad \text{and } f_1 = f_2|W_1.$$

Thus, we consider the topological space $\langle E, E^+ \rangle$ whose canonical base is given by the principal decreasing sets $((W,f)] = \{(G, f|G): G \subseteq W\}$. By simplicity $((W,f)]$ is noted as $(W,f]$.

Proposition 4.1: The map $p: E \to \mathcal{W}$ such that $(W,f) \mapsto W$ is a sheaf over $\mathcal{W}$.

Proof: Let $(W,f) \in E$. If we consider the open set $(W,f]$ in E, then $p((W,f]) = (W]$, and as a consequence $p((W,f])$ is an open set in $\mathcal{W}$. If we denote by p' the restriction $p|(W,f]$, then from the definition of p it is clear that $p': (W,f] \to (W]$ is a bijective map that preserves order inclusion. Thus, p' is a continuous map. Finally, p is a local homeomorphism. □

We refer to the sheaf $p: E \to \mathcal{W}$ as the *spectral sheaf*.

Proposition 4.2: Let $\nu: U \to E$ be a local section of the spectral sheaf p. Then, for each $W \in U$ we have

(1) $\nu(W) = (W,f)$ *for some Boolean homomorphism* $f: W \to \mathbf{2}$,
(2) *if* $W_0 \subseteq W$, *then* $\nu(W_0) = (W_0, f|W_0)$.

Proof: Since ν is a local section we consider the following commutative diagram:

$$\begin{array}{ccc} U & \xrightarrow{\upsilon} & E \\ & 1_U \searrow & \equiv \quad \downarrow p \\ & & U \end{array}$$

(1) It follows as an immediate consequence of the commutativity of the diagram.
(2) Since ν is continuous, $\nu^{-1}((W,f])$ is an open set in $\mathcal{W}$ (i.e., a decreasing set). Consequently, $W_0 \in \nu^{-1}((W,f])$ since $W_0 \subseteq W$ and $W \in \nu^{-1}((W,f])$. Thus, $\nu(W_0) \in (W,f]$, resulting in $\nu(W_0) = (W_0, f|W_0)$. □

From the physical perspective, we may state that the spectral sheaf takes into account the whole set of possible ways of assigning truth values to the propositions associated with the projectors of the spectral decomposition $\mathbf{A}=\Sigma_i a_i\mathbf{P}_i$. The continuity of a local section of p guarantees that the truth value of a proposition is maintained when considering the inclusion of subalgebras. In this way, the *compatibility condition* of the Boolean valuation with respect of intersection of pairs of Boolean sublattices of $L(\mathcal{H})$ is maintained.

A global section $\tau:\mathcal{W}\rightarrow E$ of p is interpreted as follows: the map assigns to every $W\in\mathcal{W}$ a fixed Boolean valuation $\tau_w:W\rightarrow\mathbf{2}$, obviously satisfying the compatibility condition. So, KS theorem in terms of the spectral sheaf reads:

Theorem 4.3: *If $\mathcal{H}$ is a Hilbert space such that $dim(\mathcal{H})>2$, then the spectral sheaf p has no global sections.* □

We may build a *contextual valuation* in terms of a local section as follows:

Let A be a physical magnitude with known value, i.e., we have been able to establish a Boolean valuation $f:W_A\rightarrow 2$. It is not very hard to see that the assignment

$$\nu:(W]\rightarrow E \text{ such that for each } W_i\in(W],\nu(W_i)=(W_i,\ f|W_i),$$

is a local section of p.

To extend contextual valuations we turn now to consider local sections. To do this we introduce the following definition:

Definition 4.4: Let ν be a local section of p and W_A the spectral algebra associated with the operator **A**. *Then, an extended valuation over A is given by the set*

$$\overline{\nu}(A)=\{W_B\in dom(\nu):W_B\subseteq W_A\}.$$

Given the previous definition, it is easy to prove the following proposition:

Proposition 4.5: If ν is a local section of p and W_A the spectral algebra associated to the operator **A**, *then*

(1) $\overline{\nu}(A)$ *is a decreasing set,*
(2) *if* $W_A\in U$ *then* $\overline{\nu}(A)=(W_A]$. □

We can start from the spectral sheaf to build a representation as presheaf such that local sections of the former are identifiable to local sections of the latter. When considering the family $\mathcal{W}$ ordered by inclusion, $\mathcal{W}$ can be regarded as a small category. Thus, we can take the topos presheaf $\hat{\mathcal{W}}$. Denoting E_W the fiber of the spectral sheaf p over W for each $W\in\mathcal{W}$, we consider the following presheaf:

$$D:\mathcal{W}^{op}\rightarrow Ens$$

such that

(i) $D(W)=E_W$ for each $W\in Ob(\mathcal{W})$;
(ii) if $i:W_1\subseteq W_2$ lies in $Ar(\mathcal{W})$, then $D_i:D(W_2)\rightarrow D(W_1)$ is such that $D_i(g)=g|W_1$.

It is clear that the presheaf acting over arrows satisfies the compatibility condition. Denoting Sec_p and Sec_D the sets of (global and local) sections of p and D, respectively, we can establish the following proposition:

Proposition 4.6:

$$Sec_p\simeq Sec_D.$$

Proof: Let $\nu:U\rightarrow E\in Sec_p$ and consider the presheaf $\tilde{U}:\mathcal{W}^{op}\rightarrow Ens$, whose action over $Ob(\mathcal{W})$ is given by

$$\widetilde{U}(W) = \begin{cases} \{*\}, & \text{if } W \in U \\ \varnothing, & \text{otherwise,} \end{cases}$$

and whose action over arrows is immediate. It is clear that $\widetilde{U}$ is a subfunctor of the presheaf **1**. From U we construct a natural transformation

$$\begin{array}{ccc} & & D \\ & & \rightarrow \\ \mathcal{W}^{op} & \tau_\nu \uparrow & Ens \\ & & \rightarrow \\ & & \widetilde{U} \end{array},$$

such that, for each $W \in \mathcal{W}$, $\tau_\nu(U(W)) = \nu(W)$. Thus, we have a map $Sec_p \rightarrow Sec_D$ given by $\nu \mapsto \tau_\nu$. It is not hard to see that this is an injective map. To see that it is also a surjective map, we consider a section of the presheaf D, namely $\tau: \widetilde{U} \rightarrow D$, and we prove that there exists a section ν of the spectral sheaf such that $\nu \mapsto \tau_\nu = \tau$. Let $U = \{W \in \mathcal{W}: \widetilde{U}(W) = \{*\}\}$. If $W \in U$ and $W_o \subseteq W$, then $\widetilde{U}(W_o) = \{*\}$, since $\widetilde{U}$ is a contravariant subfunctor of **1**. Thus, W_o lies in U, resulting in U, a decreasing set (i.e., an open set) in $\mathcal{W}$. Now, we consider the map $\nu: U \rightarrow E$ such that, for each $W \in U$, $\nu(W) = (W, \tau(\widetilde{U}(W)))$. It is clear that the following diagram is commutative:

$$\begin{array}{ccc} U & \overset{\upsilon}{\longrightarrow} & E \\ & 1_U \searrow \equiv & \downarrow p \\ & & U \end{array}$$

Now, we prove that ν is a continuous map. Let $(W_1, f]$ be an open set of the canonical base of E, $\nu^{-1}((W_1, f]) = \{W \in \mathcal{W}: \nu(W) \in (W_1, f]\}$, and we assume that $\nu^{-1}((W_1, f])$ is not the empty set. Let $W \in \nu^{-1}((W_1, f])$ and $W_x \subseteq W$. Since τ is a natural transformation, it follows that $\tau(\widetilde{U}(W_x)) = \tau(\widetilde{U}(W))|W_x$. Since $\nu(W) \in (W_1, f]$, it is clear that $\nu(W) = (W, f|W)$, resulting that $\widetilde{U}(W_x) = f|W_x$ and $W_x \in \nu^{-1}((W_1, f])$. This proves the continuity of the map. It is not very hard to see that $\tau = \tau_\nu$, thus it is proved that it is a surjective map. □

Remark 4.7: The presheaf D from the spectral sheaf is the dual spectral presheaf defined in Ref. 15.

Taking into account the last Proposition, we can write KS theorem in terms of presheaves from the spectral sheaf:

Theorem 4.8: *If $\mathcal{H}$ is a Hilbert space such that $dim(\mathcal{H}) > 2$, then the dual spectral presheaf D has no global sections.* □

Possible obstructions to the construction of global sections for the case of finite dimensional $\mathcal{H}$ are shown in Ref. 12.

On the other hand, in terms of a local section $\nu: U \rightarrow D$ of D, extended contextual valuations over an operator A may be defined as

$$\overline{\nu}(A) = \{W_B \subseteq W_A: U(W_B) = \{*\}\}.$$

Valuations are deeply connected to the election of particular local sections of the spectral sheaf. So, we see here once more that we cannot speak of the value of a physical magnitude without specifying this election, which clearly means the election of a particular context. This is in agreement with the statement that contextuality is "endemic" in any attempt to ascribe properties to quantities in quantum theories.[15]

V. CONTEXTUAL LOGIC

We know that if $\mathcal{W}$ is the family of Boolean subalgebras of $L(\mathcal{H})$, to take a local section ν of the spectral sheaf means an assignment of Boolean valuations to algebras in the proper subfamily $Dom(\nu)$ maintaining the compatibility condition. Now, an interesting question is to ask what ν can "tell us" about W when $W \notin Dom(\nu)$. Let us state more accurately this expression to precise our aim in the search of a *contextual logic*.

Definition 5.1: Let ν be a local section of the spectral sheaf. If $W_B \in Dom(\nu)$ and $W_B \subseteq W_A$, then we will say that W_B has *Boolean information* about *W_A*.

Clearly, this means that, in a given state of the system, the complete knowledge of the spectral decomposition of **B** lets us know the eigenvalue of one or more projectors in the spectral decomposition of **A**. *Contextual logic* allows some kind of "paste" among Boolean sublattices of $L(\mathcal{H})$ and so among CSCOs. A valuation in terms of decreasing sets maintains it "downstream" with respect to subalgebras, i.e., when the valuation of a subalgebra is given, all its subalgebras are automatically valuated. This makes it possible to have Boolean information of different contexts from the one chosen in the following sense: once fixed a local section ν, if $W_B \in Dom(\nu)$ and $W_A \notin Dom(\nu)$ then, referring to W_A from W_B takes into account the Boolean information that $W_B \cap W_A$ has about W_A.

We will now construct a propositional language *Self* for contextual logic whose atomic formulas refer to the physical magnitudes represented for bounded self-adjoint operators with discrete spectra. Intuitively, we can consider the set of atomic formulas $\mathcal{P}$ as

$$\mathcal{P} = \{A{:}A \text{ bounded self} - \text{adjoint operator}\}.$$

Then, this language is conformed as follows:

$$Self = \langle \mathcal{P}, \vee, \wedge, \rightarrow, \neg \rangle,$$

and it is clear that the formulas may be obtained in the usual way.

We will now turn to the use of Kripke models built starting from any local section of the spectral sheaf p because it allows us to naturally adapt the idea of Boolean knowledge. Thus, the obtained valuation will result in an extended contextual valuation.

Definition 5.2: We consider the poset $\langle \mathcal{W}, \subseteq \rangle$ as a *frame* for the Kripke model for *Self*. Let ν be a local section of p. Thus, we define the Kripke model $\mathcal{M} = \langle \mathcal{W}, \overline{\nu} \rangle$ with the following forcing:

(1) $\mathcal{M} \Vdash_W A$ if and only if $\mathcal{W} \in \overline{\nu}(\mathbf{A})$ with $A \in \mathcal{P}$;
(2) $\mathcal{M} \Vdash_W \alpha \vee \beta$ if and only if $\mathcal{M} \Vdash_W \alpha$ or $\mathcal{M} \Vdash_W \beta$;
(3) $\mathcal{M} \Vdash_W \alpha \wedge \beta$ if and only if $\mathcal{M} \Vdash_W \alpha$ and $\mathcal{M} \Vdash_W \beta$;
(4) $\mathcal{M} \Vdash_W \alpha \rightarrow \beta$ if and only if $\forall B \subseteq W$, if $\mathcal{M} \Vdash_B \alpha$, then $\mathcal{M} \Vdash_B \beta$;
(5) $\mathcal{M} \Vdash_W \neg \alpha$ if and only if $\forall B \subseteq W\ \mathcal{M} \nVdash_B \alpha$.

Given this forcing we can accurately define the idea of extended contextual valuation over *Self*.

Definition 5.3: Given a local section ν over p, an extended contextual valuation is the map $\overline{\nu}{:}Self \rightarrow \mathcal{W}^+$ defined as

$$\overline{\nu}(\alpha) = \{W{:}\mathcal{M} \Vdash_W \alpha\}.$$

Taking into account that $\mathcal{W}^+$ is a topological space, it is not very hard to see that $\overline{\nu}(\alpha)$ is an open set of $\mathcal{W}$. Now, we can to establish the following proposition:

Proposition 5.4: Let α be a formula in Self and consider the Kripke model $\mathcal{M} = \langle \mathcal{W}, \nu \rangle$. Then

(1) $\mathcal{M} \Vdash_W \neg \alpha$ if and only if $W \in (C\overline{\nu}(\alpha))^\circ$,
(2) $\mathcal{M} \nVdash_W \alpha$ and $\mathcal{M} \nVdash_W \neg \alpha$ if and only if $W \in \partial \overline{\nu}(\alpha)$.

Proof: (1) If $\mathcal{M} \Vdash_W \neg \alpha$, then $\forall B \subseteq W$, $\mathcal{M} \nVdash_B \alpha$ and $\forall B \subseteq W\ B \notin \overline{\nu}(\alpha)$. Thus $(W] \subseteq (C\overline{\nu}(\alpha))^\circ$ and $W \in (C\overline{\nu}(\alpha))^\circ$. On the other hand, if $W \in (C\overline{\nu}(\alpha))^\circ$, then there exists an open set G in $\mathcal{W}$ such

that $W \in G \subseteq C(\overline{\nu}(\alpha))$. Since G is a decreasing set, we have that $(W] \subseteq G \subseteq C(\overline{\nu}(\alpha))$ and $\mathcal{M}\| =_W \neg\alpha$. (2) It follows from (1) and the fact that $\mathcal{W} = \overline{\nu}(\alpha) \cup (C\overline{\nu}(\alpha))^\circ \cup \partial\overline{\nu}(\alpha))$. □

Remark 5.5: Following the usual interpretation of the Kripke model, the frame represents all possible states of knowledge that are preserved forward in time. In our case, the frame $\langle \mathcal{W}, \subseteq \rangle$, $\mathcal{W}$ represents all states of Boolean knowledge in the sense of all possible Boolean valuations of spectral algebras, and the usual notion of "preserving knowledge through time" must be understood in terms of $\subseteq$ as "preserving valuations in spectral subalgebras." The forcing $K\|=_W \alpha$ is interpreted as *the spectral algebra W has Boolean knowledge about* α, i.e., the complete Boolean valuation of W is known and W lies in the decreasing set associated with the formula α. By Proposition 4.5, to know the eigenvalue of $\mathbf{A}$ is expressed in terms of the forcing as $\mathcal{M}\|=_{(W_A]} A$.

$\mathcal{W}^+$ being a topological space, it is a Heyting algebra with meet and join operations, the classical ones and implication and negation defined as follows:

$$S \to T = \{P \in \mathcal{W}: \forall\, X \subseteq P, \textit{if } X \in S \textit{ then } X \in T\},$$

$$\neg S = \{P \in \mathcal{W}: \forall\, X \subseteq P, X \notin S\}.$$

Thus, the extended contextual valuation is a Heyting valuation of *Self* from the Heyting algebra $\mathcal{W}^+$ such that

(1) $\overline{\nu}(\alpha \vee \beta) = \overline{\nu}(\alpha) \cup \overline{\nu}(\beta)$;
(2) $\overline{\nu}(\alpha \wedge \beta) = \overline{\nu}(\alpha) \cap \overline{\nu}(\beta)$;
(3) $\overline{\nu}(\alpha \to \beta) = \overline{\nu}(\alpha) \to \overline{\nu}(\beta)$;
(4) $\overline{\nu}(\neg\alpha) = \neg\,\overline{\nu}(\alpha)$.

Taking into account the restrictions in the valuations imposed by the KS theorem, a Heyting valuation $v: Self \to \mathcal{W}^+$ such that $v(A) = (A]$ for each atomic formula A is not possible. So, it is clear that contextual logic is an intuitionistic logic in which not all of the Heyting valuations are allowed.

VI. CONCLUSIONS

Contextual logic is a formal language to deal with combinations of propositions about physical properties of a quantum system that are well defined in different contexts. These properties are regarded from a fixed context, which guarantees the avoidance of no-go theorems. This means that one can refer to contexts other than the chosen one by building a Kripke model in which each proposition is given a decreasing set as its truth value.

There are different formal languages on the orthomodular lattice of closed subspaces of $\mathcal{H}$ (such as orthologic or orthomodular quantum logic), but these logics give rise to different problems that lack an intuitive understanding, such as the "implication problem" (briefly, eight different connectives may represent the material conditional; see Ref. 9). On the contrary, as contextual logic is an intuitionistic one—with restrictions on the allowed valuations arising from the KS theorem—it has "good" properties as the distributive lattice structure and a nice definition of the implication as a residue of the conjunction. The price paid is it being a contextual language. But, this is not a difficulty, it is a main feature of quantum mechanics.

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Two and three dimensional Hamiltonians with generalized and ordinary shape invariance symmetry

H. Panahi[a)]
Department of Physics, Guilan University, Rasht 41335-1914, Iran and Institute for Studies in Theoretical Physics and Mathematics, Teheran 19395-1795, Iran

M. A. Jafarizadeh[b)]
Department of Theoretical Physics and Astrophysics, Tabriz University, Tabriz 51664, Iran; Institute for Studies in Theoretical Physics and Mathematics, Teheran 19395-1795, Iran; and Research Institute for Fundamental Sciences, Tabriz 51664, Iran

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Two and three dimensional Hamiltonians with generalized and ordinary shape invariance symmetry have been obtained by Fourier transforming over some coordinates of the SU(3) Casimir operator defined on SU(3)/SU(2) symmetric space. It is shown that the generalized shape invariance of the two dimensional Hamiltonian is equivalent to SU(3) symmetry while in the three dimensional one, the ordinary shape invariance is equivalent to contracted SU(3) and there is one to one correspondence between the representations of the generalized shape invariance symmetry of the two (three) dimensional Hamiltonian and SU(3) [contracted SU(3)] Verma bases. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1827325]

I. INTRODUCTION

Exactly solvable potentials are the central and fundamental problems of mathematical physics, consequently they have attracted much interest both in theoretical physics and mathematics. There are many methods of obtaining exactly solvable potentials in quantum mechanics. The most powerful methods are the algebraic method,[1] supersymmetric and shape invariant factorization of the Schrödinger equation in one and two or three dimensional exactly solvable models.[2–5] In all these works it is shown that there is a close connection between the shape invariance symmetry of one or higher dimensional Hamiltonians and some rank one semisimple Lie algebra or higher rank nonsemisimple algebras, where this equivalence between the one dimensional shape invariant and the rank one semisimple Lie algebra has been shown in Ref. 6.

Here in this work we introduce two and three dimensional Hamiltonians with a new kind of shape invariance. It is shown that the shape invariance symmetry of the two dimensional Hamiltonian is equivalent to SU(3) symmetry where we call it generalized shape invariance while the shape invariance associated with the three dimensional Hamiltonian is equivalent to contracted SU(3) ordinary shape invariance and there is one to one correspondence between the representation of the generalized shape invariance symmetry of two (three) dimensional Hamiltonians and SU(3) [contracted SU(3)] Verma bases.

The paper is organized as follows: In Sec. II after introducing the parametrization of SU(3) Lie group we derive its right invariant vector fields and Casimir operator on SU(3)/SU(2). In Sec. III, using the Fourier transformation together with the coset reduction we obtain the two dimensional Hamiltonian $H_l(m_1,m_2)$ of charged particle on S^2 sphere in the presence of an electric field. Section IV is devoted to SU(3) Verma basis,[7] and their connection with eigenspectrum and de-

a)Author to whom correspondence should be addressed. Electronic mail: t-panahi@guilan.ac.ir
b)Electronic mail: jafarizadeh@tabrizu.ac.ir

generacy of the above Hamiltonian. In Sec. V we talk about the generalized shape invariance of this Hamiltonian. In Sec. V, through Inonu–Wigner contraction[8] of SU(3), we obtain three dimensional ordinary shape invariance Hamiltonians. The paper is ended with a conclusion and one appendix.

II. THE RIGHT INVARIANT VECTOR FIELDS AND QUADRATIC CASIMIR OPERATOR OF SU(3) GROUP OVER THE SU(3)/SU(2) COSET MANIFOLD

According to Ref. 9, we can parametrize an arbitrary element of the SU(3)/SU(2) coset manifolds in the following form:

$$U=\begin{pmatrix} \sin(\theta) & 0 & \cos(\theta)e^{i(\eta+\chi_1)} \\ -\cos(\theta)\cos(\varphi)e^{i(\chi_2-\chi_1)} & \sin(\varphi)e^{-i\eta} & \sin(\theta)\cos(\varphi)e^{i(\eta+\chi_2)} \\ -\cos(\theta)\sin(\varphi)e^{-i\chi_1} & -\cos(\varphi)e^{-i(\eta+\chi_2)} & \sin(\theta)\sin(\varphi)e^{i\eta} \end{pmatrix}, \tag{2.1}$$

where $0<\theta, \varphi\leqslant\pi/2$ and $0\leqslant\eta, \chi_1, \chi_2<2\pi$. Now, an arbitrary element of SU(3) group manifold can be obtained by multiplying the coset element given in (2.1) by an arbitrary element h of stability group SU(2) with the parametrization $h=\exp(i\lambda_3\alpha)\exp(i\lambda_2\beta)\exp(i\lambda_3\gamma)$ from left or right, where 3×3 Hermitian Gell–Mann matrices λ_i, $i=1,2,\ldots,8$ are defined as

$$\lambda_1=\begin{pmatrix}0&1&0\\1&0&0\\0&0&0\end{pmatrix},\quad \lambda_2=\begin{pmatrix}0&-i&0\\i&0&0\\0&0&0\end{pmatrix},\quad \lambda_3=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&0\end{pmatrix},$$

$$\lambda_4=\begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix},\quad \lambda_5=\begin{pmatrix}0&0&-i\\0&0&0\\i&0&0\end{pmatrix},\quad \lambda_6=\begin{pmatrix}0&0&0\\0&0&1\\0&1&0\end{pmatrix}, \tag{2.2}$$

$$\lambda_7=\begin{pmatrix}0&0&0\\0&0&-i\\0&i&0\end{pmatrix},\quad \lambda_8=\frac{1}{\sqrt{3}}\begin{pmatrix}1&0&0\\0&1&0\\0&0&-2\end{pmatrix}.$$

Usually the right invariant vector fields of SU(3) group manifold can be obtained from the right invariant su(3) Lie algebra valued one forms $dG\,G^{-1}=e^i_\mu\,d\xi^\mu\,\lambda_i$ with $G=Uh$,[10] where e^i_μ are right invariant fiel-beins and $\xi^\mu=(\theta,\varphi,\eta,\chi_1,\chi_2,\alpha,\beta,\gamma)$ are coordinates of SU(3) group manifold. Then the right invariant vector field can be written as $R_i=e^\mu_i(\partial/\partial\xi^\mu)$, where e^μ_i are the inverse of the right invariant fiel-beins e^i_μ. Now, the SU(3) right invariant vector fields over the SU(3)/SU(2) coset manifold[11,12] can be obtained simply by projecting the SU(3) right invariant vector fields over the principal bundle SU(3) to the base manifold SU(3)/SU(2), where it leads to the vanishing of the components which are tangent to SU(2) fiber manifold (stability group).

Using the above prescription, after some lengthy and tedious calculation via Maple software we get the following expressions for the SU(3) right invariant vector fields over the SU(3)/SU(2) coset manifold:

$$R_\pm=\frac{1}{2}e^{\pm i(\chi_1-\chi_2)}\left[\mp\cos(\varphi)\frac{\partial}{\partial\theta}\pm\cot(\theta)\sin(\varphi)\frac{\partial}{\partial\varphi}+i\tan(\theta)\cos(\varphi)\frac{\partial}{\partial\chi_1}+i\frac{\cot(\theta)}{\cos(\varphi)}\frac{\partial}{\partial\chi_2}\right], \tag{2.3}$$

$$Y_\pm=\frac{1}{2}e^{\pm i\chi_1}\left[\pm\sin(\varphi)\frac{\partial}{\partial\theta}\pm\cot(\theta)\cos(\varphi)\frac{\partial}{\partial\varphi}-i\frac{\cot(\theta)}{\sin(\varphi)}\frac{\partial}{\partial\eta}\right.$$
$$\left.+2i\frac{\cos^2(\theta)-\sin^2(\theta)\sin^2(\varphi)}{\sin(2\theta)\sin(\varphi)}\frac{\partial}{\partial\chi_1}+i\frac{\cot(\theta)}{\sin(\varphi)}\frac{\partial}{\partial\chi_2}\right], \tag{2.4}$$

$$X_{\pm}=\frac{1}{2}e^{\mp i\chi_2}\left[\mp\frac{\partial}{\partial\varphi}-i\cot(\varphi)\left(\frac{\partial}{\partial\eta}-\frac{\partial}{\partial\chi_1}\right)+2i\cot(2\varphi)\frac{\partial}{\partial\chi_2}\right], \tag{2.5}$$

$$R_3=-\frac{i}{2}\left(\frac{\partial}{\partial\chi_1}-\frac{\partial}{\partial\chi_2}\right),\quad R_8=\frac{i\sqrt{3}}{2}\left(\frac{2}{3}\frac{\partial}{\partial\eta}-\frac{\partial}{\partial\chi_1}-\frac{\partial}{\partial\chi_2}\right), \tag{2.6}$$

where $R_{\pm}=\frac{1}{2}(R_1\pm iR_2)$, $Y_{\pm}=\frac{1}{2}(R_4\mp iR_5)$, and $X_{\pm}=\frac{1}{2}(R_6\pm iR_7)$. After some algebraic calculations one can show that, the above generators satisfy su(3) Lie algebra commutation relations. Also it is straightforward to show that the following defined su(3) quadratic Casimir operator commutes with all of the above generators

$$C=\tfrac{1}{2}(R_+R_-+R_-R_+)+\tfrac{1}{2}(Y_+Y_-+Y_-Y_+)+\tfrac{1}{2}(X_+X_-+X_-X_+)+R_3^2+R_8^2, \tag{2.7}$$

where after calculations, we obtain the following expression (by ignoring the factor $\frac{1}{4}$):

$$\begin{aligned}C=-\Bigg[&\frac{\partial^2}{\partial\theta^2}+\frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\varphi^2}+\frac{4-\cos^2(\theta)\sin^2(\varphi)-\cos^2(\varphi)}{3\sin^2(\theta)\sin^2(\varphi)}\frac{\partial^2}{\partial\eta^2}+\frac{1-\sin^2(\theta)\cos^2(\varphi)}{\sin^2(\theta)\cos^2(\theta)\sin^2(\varphi)}\frac{\partial^2}{\partial\chi_1^2}\\&+\frac{1}{\sin^2(\theta)\sin^2(\varphi)\cos^2(\varphi)}\frac{\partial^2}{\partial\chi_2^2}-\frac{2}{\sin^2(\theta)\sin^2(\varphi)}\left(\frac{\partial^2}{\partial\eta\partial\chi_1}+\frac{\partial^2}{\partial\eta\partial\chi_2}-\frac{\partial^2}{\partial\chi_1\partial\chi_2}\right)\\&+\frac{2(4\cos^2(\theta)-1)}{\sin(2\theta)}\frac{\partial}{\partial\theta}+\frac{2\cot(2\varphi)}{\sin^2(\theta)}\frac{\partial}{\partial\varphi}\Bigg].\end{aligned} \tag{2.8}$$

Similarly we can calculate the SU(3) left invariant vector fields, where its structure constant, is minus the right invariant ones but its quadratic Casimir operator is the same as the right one. Here we need only the right invariant vector fields and we do not need to quote the left invariant ones here. Also one can show that the Casimir operator is the same as Laplace–Beltrami operator of adjoint invariant metric.

III. REDUCTION OF THE CASIMIR OPERATOR TO TWO-DIMENSIONAL HAMILTONIAN OF A CHARGED PARTICLE ON S^2 SPHERE

In order to reduce the SU(3) Casimir operator together with its right invariant vector fields defined on SU(3)/SU(2) coset manifold to a two-dimensional operator, first we eliminate the coordinate η by Fourier transforming over the coordinate η by kernel $e^{i\eta l}$, where after similarity transformation $R\to f^{-1}(\theta,\varphi)Rf(\theta,\varphi)$ with similarity function $f^{-1}(\theta,\varphi)=\sin(\theta)\sqrt{\cos(\theta)\sin(2\varphi)}$ the right invariant vector fields and their quadratic Casimir operator take the following form:

$$\begin{aligned}R_{\pm}=\frac{1}{2}e^{\pm i(\chi_1-\chi_2)}\Bigg[&\mp\cos(\varphi)\frac{\partial}{\partial\theta}\pm\cot(\theta)\sin(\varphi)\frac{\partial}{\partial\varphi}+i\tan(\theta)\cos(\varphi)\frac{\partial}{\partial\chi_1}\\&+i\frac{\cot(\theta)}{\cos(\varphi)}\frac{\partial}{\partial\chi_2}\pm\frac{\cos^2(\theta)-\cos^2(\varphi)\sin^2(\theta)}{\sin(2\theta)\cos(\varphi)}\Bigg],\end{aligned} \tag{3.1}$$

$$\begin{aligned}Y_{\pm}=\frac{1}{2}e^{\pm i\chi_1}\Bigg[&\pm\sin(\varphi)\frac{\partial}{\partial\theta}\pm\cot(\theta)\cos(\varphi)\frac{\partial}{\partial\varphi}+2i\frac{\cos^2(\theta)-\sin^2(\theta)\sin^2(\varphi)}{\sin(2\theta)\sin(\varphi)}\frac{\partial}{\partial\chi_1}\\&+i\frac{\cot(\theta)}{\sin(\varphi)}\frac{\partial}{\partial\chi_2}\mp\frac{\cos^2(\theta)-\sin^2(\varphi)\sin^2(\theta)}{\sin(2\theta)\sin(\varphi)}+l\frac{\cot(\theta)}{\sin(\varphi)}\Bigg],\end{aligned} \tag{3.2}$$

$$X_{\pm}=\frac{1}{2}e^{\mp i\chi_2}\left[\mp\frac{\partial}{\partial\varphi}+i\cot(\varphi)\frac{\partial}{\partial\chi_1}+2i\cot(2\varphi)\frac{\partial}{\partial\chi_2}\pm\cot(2\varphi)+l\cot(\varphi)\right], \tag{3.3}$$

$$R_3 = -\frac{i}{2}\left(\frac{\partial}{\partial\chi_1} - \frac{\partial}{\partial\chi_2}\right), \quad R_8 = -\frac{i\sqrt{3}}{2}\left(\frac{\partial}{\partial\chi_1} + \frac{\partial}{\partial\chi_2} - 2i\frac{l}{3}\right). \tag{3.4}$$

One can straightforwardly show that the above generators satisfy su(3) Lie algebra commutation relations

$$[R_3, R_\pm] = \pm R_\pm, \quad [R_3, Y_\pm] = \pm \tfrac{1}{2} Y_\pm, \quad [R_3, X_\pm] = \pm \tfrac{1}{2} X_\pm,$$

$$[R_8, Y_\pm] = \pm \frac{\sqrt{3}}{2} Y_\pm, \quad [R_8, X_\pm] = \mp \frac{\sqrt{3}}{2} X_\pm,$$

$$[R_+, R_-] = 2R_3, \quad [R_\pm, Y_\mp] = \pm X_\pm, \quad [R_\pm, X_\mp] = \mp Y_\pm,$$

$$[Y_+, Y_-] = R_3 + \sqrt{3}R_8, \quad [X_+, X_-] = R_3 - \sqrt{3}R_8, \quad [Y_\pm, X_\pm] = \mp R_\pm. \tag{3.5}$$

Also the Casimir operator reduces to

$$\begin{aligned} C = -\Bigg[& \frac{\partial^2}{\partial\theta^2} + \cot(\theta)\frac{\partial}{\partial\theta} + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin^2(\theta)\sin^2(\varphi)}\Bigg(\frac{1-\sin^2(\theta)\cos^2(\varphi)}{\cos^2(\theta)}\frac{\partial^2}{\partial\chi_1^2} \\ & + \frac{1}{\cos^2(\varphi)}\frac{\partial^2}{\partial\chi_2^2} + 2\frac{\partial^2}{\partial\chi_1\partial\chi_2} - 2il\left(\frac{\partial}{\partial\chi_1} + \frac{\partial}{\partial\chi_2}\right) - \frac{l^2}{3}(4 - \cos^2(\theta)\sin^2(\varphi) - \cos^2(\varphi))\Bigg) \\ & + \frac{1}{4}\tan^2(\theta) + \cot^2(\theta) + \frac{\cot^2(2\varphi)}{\sin^2(\theta)}\Bigg]. \end{aligned} \tag{3.6}$$

For convenience we have denoted the reduced generators with the same notation of the preceding section. Now we eliminate the coordinates χ_1 and χ_2 through Fourier transformation over them with the kernel $e^{i(m_1\chi_1 - m_2\chi_2)}$, then Casimir operator (3.6) reduces to the following Hamiltonian:

$$H_l(m_1, m_2) = -\left(\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\sin(\theta)\frac{\partial}{\partial\theta} + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\varphi^2}\right) + V_{l,m_1,m_2}(\theta,\varphi) \tag{3.7}$$

with

$$\begin{aligned} V_{l,m_1,m_2}(\theta,\varphi) = \frac{1}{\sin^2(\theta)\sin^2(\varphi)}\Bigg(& \frac{m_1^2(1-\sin^2(\theta)\cos^2(\varphi))}{\cos^2(\theta)} + \frac{m_2^2}{\cos^2(\varphi)} - 2m_1m_2 - 2l(m_1 - m_2) \\ & + \frac{l^2}{3}(4 - \cos^2(\theta)\sin^2(\varphi) - \cos^2(\varphi))\Bigg) - \frac{1}{4}\tan^2(\theta) - \cot^2(\theta) - \frac{\cot^2(2\varphi)}{\sin^2(\theta)}. \end{aligned} \tag{3.8}$$

On the other hand, the dynamical symmetric of motion of a charged particle in the presence of an external electromagnetic field on the symmetric spaces can give the following nonrelativistic Hamiltonian for motion of a charged particle on the two dimensional manifold with metric $g_{\mu\nu}$ in the presence of static electromagnetic fields with vector potential $\vec{A}$ and scalar potential V as[13]

$$H = -\frac{1}{\sqrt{g}}(\partial_\mu - iA_\mu)(\sqrt{g}g^{\mu\nu}(\partial_\nu - iA_\nu)) + V, \tag{3.9}$$

where g is the determinant of metric $g_{\mu\nu}$. Therefore, the Hamiltonian (2.8) can be interpreted as the Hamiltonian of a charged particle on S^2 sphere with metric

$$g_{\mu\nu}=\begin{pmatrix}1 & 0\\ 0 & \sin^2(\theta)\end{pmatrix}, \tag{3.10}$$

in the presence of an electric field with scalar potential (3.8).

IV. THE ALGEBRAIC SOLUTION OF THE HAMILTONIAN BY USING VERMA BASES

Here in this section we try to solve our Hamiltonian algebraically, that is we will obtain its eigenspectrum by using the Verma bases of su(3) or A_2 Lie algebra. According to Ref. 7, Verma bases of the irreducible representation space $V(\Lambda)$ of A_2 over C Lie algebra, where $\Lambda=(p,q)$ is the highest weight, consist of all vectors

$$f_1^{a_3}f_2^{a_2}f_1^{a_1}|p,q\rangle, \tag{4.1}$$

such that

$$0\leqslant a_1\leqslant p,\quad 0\leqslant a_2\leqslant q+a_1,\quad 0\leqslant a_3\leqslant \min[q,a_2], \tag{4.2}$$

where e_i, f_i, h_i, $i=1$ and 2 are base of A_2 Lie algebra satisfying the commutation relations

$$[e_i,f_i]=h_i,\quad [h_i,e_i]=2e_i,\quad [h_i,f_i]=-2f_i,\quad i=1,2 \tag{4.3}$$

for each simple root $\alpha_1=(\frac{1}{2},\sqrt{3}/2)$ and $\alpha_2=(\frac{1}{2},-\sqrt{3}/2)$. Now, by comparing the commutation relations

$$[Y_+,Y_-]=R_3+\sqrt{3}R_8,\quad [R_3+\sqrt{3}R_8,Y_\pm]=\pm 2Y_\pm,$$

$$[X_+,X_-]=R_3-\sqrt{3}R_8,\quad [R_3-\sqrt{3}R_8,X_\pm]=\pm 2X_\pm \tag{4.4}$$

with (4.3) we have

$$h_1=R_3+\sqrt{3}R_8,\quad e_1=Y_+,\quad f_1=Y_-,$$

$$h_2=R_3-\sqrt{3}R_8,\quad e_2=X_+,\quad f_2=X_-. \tag{4.5}$$

In an arbitrary representation of A_2 with highest weight $\Lambda(p,q)$, the highest eigenweight satisfies

$$e_i|p,q\rangle=0,\quad i=1,2. \tag{4.6}$$

Therefore, the highest eigenfunction $\psi^{p,q}(\theta,\varphi,\chi_1,\chi_2)=\langle\chi_2,\chi_1,\varphi,\theta|p,q\rangle$ satisfies the following first order linear differential equations:

$$\left[\sin(\varphi)\frac{\partial}{\partial\theta}+\cot(\theta)\cos(\varphi)\frac{\partial}{\partial\varphi}+2i\frac{\cos^2(\theta)-\sin^2(\theta)\sin^2(\varphi)}{\sin(2\theta)\sin(\varphi)}\frac{\partial}{\partial\chi_1}+i\frac{\cot(\theta)}{\sin(\varphi)}\frac{\partial}{\partial\chi_2}\right.$$
$$\left.-\frac{\cos^2(\theta)-\sin^2(\varphi)\sin^2(\theta)}{\sin(2\theta)\sin(\varphi)}+l\frac{\cot(\theta)}{\sin(\varphi)}\right]\psi^{p,q}(\theta,\varphi,\chi_1,\chi_2)=0, \tag{4.7}$$

$$\left[-\frac{\partial}{\partial\varphi}+i\cot(\varphi)\frac{\partial}{\partial\chi_1}+2i\cot(2\varphi)\frac{\partial}{\partial\chi_2}+\cot(2\varphi)+l\cot(\varphi)\right]\psi^{p,q}(\theta,\varphi,\chi_1,\chi_2)=0. \tag{4.8}$$

On the other hand, the highest eigenweight is the eigenstate of the Cartan subalgebra with R_3 and R_8 as its Gell–Mann basis,[14] where the bases h_{α_1} and h_{α_2} are associated with simple roots α_1 and α_2, and they can be written in terms of these bases in the following form:[15]

$$h_{\alpha_1} = R_3 + \sqrt{3}R_8, \quad h_{\alpha_2} = R_3 - \sqrt{3}R_8. \tag{4.9}$$

Writing the highest eigenweight in terms of fundamental weights, that is $\mu = p\mu^1 + q\mu^2$ and considering the following relation between the simple roots and fundamental weights:

$$2\frac{(\mu^i, \alpha_j)}{(\alpha_j, \alpha_j)} = \delta^i_j, \tag{4.10}$$

we can write

$$\begin{aligned}(R_3 + \sqrt{3}R_8)\psi^{p,q}(\theta,\varphi,\chi_1,\chi_2) &= \langle \mu, R_3 + \sqrt{3}R_8\rangle \psi^{p,q}(\theta,\varphi,\chi_1,\chi_2) \\ &= \langle \mu, h_{\alpha_1}\rangle \psi^{p,q}(\theta,\varphi,\chi_1\chi_2) = 2\frac{(\mu,\alpha_1)}{(\alpha_1,\alpha_1)}\psi^{p,q}(\theta,\varphi,\chi_1,\chi_2)\end{aligned}$$

or

$$(R_3 + \sqrt{3}R_8)\psi^{p,q}(\theta,\varphi,\chi_1\chi_2) = p\psi^{p,q}(\theta,\varphi,\chi_1,\chi_2). \tag{4.11}$$

Similarly by acting out the other basis of Cartan subalgebra on highest eigenweight we obtain

$$(R_3 - \sqrt{3}R_8)\psi^{p,q}(\theta,\varphi,\chi_1\chi_2) = q\psi^{p,q}(\theta,\varphi,\chi_1,\chi_2). \tag{4.12}$$

The above eigenvalue equations imply the following χ_1 and χ_2 dependence of highest eigenweight $\psi^{p,q}(\theta,\varphi,\chi_1,\chi_2)$,

$$\psi^{p,q}(\theta,\varphi,\chi_1,\chi_2) = e^{(i/3)(2p+q+l)\chi_1} e^{-(i/3)(p+2q-l)\chi_2} \phi^{p,q}(\theta,\varphi). \tag{4.13}$$

Substituting (4.13) in (4.7) and (4.8), we see that the integrability of the latter equation requires that $p = q + l$, that is for given values of the parameter l, only the representations $(q+l, q)$ are relevant to the eigenspectrum of our Hamiltonian. Hence, integrating Eqs. (4.7) and (4.8) we get the following expression for the highest eigenweight in these particular representations:

$$\psi^{q,l}(\theta,\varphi,\chi_1,\chi_2) = e^{i((q+l)\chi_1 - q\chi_2)}(\cos^q(\varphi)\sin^{q+1}(\theta)\cos^{q+l}(\theta)\sqrt{\cos(\theta)\sin(2\varphi)}). \tag{4.14}$$

Now, using the formula (4.1) we can obtain the lower eigenweights or Verma bases,

$$\psi^{(a_3,a_2,a_1)}(\theta,\varphi,\chi_1,\chi_2) = Y_-^{a_3} X_-^{a_2} Y_-^{a_1} \psi^{q,l}(\theta,\varphi,\chi_1,\chi_2), \tag{4.15}$$

where $0 \leqslant a_1 \leqslant q+l$, $0 \leqslant a_2 \leqslant q + a_1$, $0 \leqslant a_3 \leqslant \min[q, a_2]$. In order to obtain eigenspectrum of the Hamiltonian (3.7), it is sufficient to eliminate χ_1 and χ_2 coordinates dependence of SU(3) Verma basis by Fourier transforming over them. This can be achieved simply by shifting the phase factor $e^{i((q+l)\chi_1 - q\chi_2)}$ to the left-hand side of lowering operators X_- and Y_- in the above relation and integrating over the coordinates χ_1 and χ_2. Hence, we obtain

$$\psi^{(a_3,a_2,a_1)}(\theta,\varphi,\chi_1,\chi_2) = e^{i(q+l-a_1-a_3)\chi_1} e^{-i(q-a_2)\chi_2} \chi^{q,l}_{q+l-a_1-a_3,q-a_2}(\theta,\varphi), \tag{4.16}$$

where

$$\chi^{q,l}_{q+l-a_1-a_3,q-a_2}(\theta,\varphi)=\left(\prod_{i=1}^{a_3}Y_-(q+l-a_1-i+1,q-a_2)\right)\left(\prod_{i=1}^{a_2}X_-(q+l-a_1,q-i+1)\right)$$
$$\times\left(\prod_{i=1}^{a_1}Y_-(q+l-i+1,q)\right)(\cos^q(\varphi)\sin^{q+1}(\theta)\cos^{q+l}(\theta)\sqrt{\cos(\theta)\sin(2\varphi)}), \tag{4.17}$$

and the operators appear in the products as $\Pi_{i=1}^{m}K(i)=K(m)K(m-1)\cdots K(1)$ also the Fourier transformed operators have the following form:

$$R_\pm(m_1,m_2)=\frac{1}{2}\Bigg[\mp\cos(\varphi)\frac{\partial}{\partial\theta}\pm\cot(\theta)\sin(\varphi)\frac{\partial}{\partial\varphi}-m_1\tan(\theta)\cos(\varphi)$$
$$+m_2\frac{\cot(\theta)}{\cos(\varphi)}\pm\frac{\cos^2(\theta)-\cos^2(\varphi)\sin^2(\theta)}{\sin(2\theta)\cos(\varphi)}\Bigg], \tag{4.18}$$

$$Y_\pm(m_1,m_2)=\frac{1}{2}\Bigg[\pm\sin(\varphi)\frac{\partial}{\partial\theta}\pm\cot(\theta)\cos(\varphi)\frac{\partial}{\partial\varphi}-2m_1\frac{\cos^2(\theta)-\sin^2(\theta)\sin^2(\varphi)}{\sin(2\theta)\sin(\varphi)}$$
$$+m_2\frac{\cot(\theta)}{\sin(\varphi)}\mp\frac{\cos^2(\theta)-\sin^2(\varphi)\sin^2(\theta)}{\sin(2\theta)\sin(\varphi)}+l\frac{\cot(\theta)}{\sin(\varphi)}\Bigg], \tag{4.19}$$

$$X_\pm(m_1,m_2)=\frac{1}{2}\Bigg[\mp\frac{\partial}{\partial\varphi}-m_1\cot(\varphi)+2m_2\cot(2\varphi)\pm\cot(2\varphi)+l\cot(\varphi)\Bigg], \tag{4.20}$$

$$R_3(m_1,m_2)=\tfrac{1}{2}(m_1+m_2),\quad R_8(m_1,m_2)=\frac{\sqrt{3}}{2}\left(m_1-m_2-\frac{2}{3}l\right). \tag{4.21}$$

Now, by defining $m_1=q+l-a_1-a_3$ and $m_2=q-a_2$, we see that due to the inequalities (4.2), the parameters m_1 and m_2 must satisfy $-q\leqslant m_1\leqslant q+l$ and $-(q+l)\leqslant m_2\leqslant q$. Also it is straightforward to see that an arbitrary Verma basis is proportional to $e^{i(m_1\chi_1-m_2\chi_2)}$ or we can write

$$\psi^{q,l}_{m_1,m_2}(\theta,\varphi,\chi_1,\chi_2)=e^{i(m_1\chi_1-m_2\chi_2)}\chi^{q,l}_{m_1,m_2}(\theta,\varphi). \tag{4.22}$$

Now, substituting (4.22) in (3.6) and Fourier transforming over the coordinates χ_1 and χ_2, the Casimir operator reduces to the required two dimensional Hamiltonian $H_l(m_1,m_2)$ given in (3.7). Therefore, the general eigenfunctions of the above Hamiltonian with eigenvalue $E(q,l)=\frac{1}{3}((q+l)(2q+l+3)+q(q+3))$ (for the degeneracy of these eigenvalues see the Appendix) can be written as

$$\chi^{q,l}_{m_1,m_2}(\theta,\varphi)=\left(\prod_{i=1}^{a_3}Y_-(m_1+a_3-i+1,m_2)\right)\left(\prod_{i=1}^{q-m_2}X_-(m_1+a_3,q-i+1)\right)$$
$$\times\left(\prod_{i=1}^{q+l-m_1-a_3}Y_-(q+l-i+1,q)\right)\left(\cos^q(\varphi)\sin^{q+1}(\theta)\cos^{q+l}(\theta)\sqrt{\cos(\theta)\sin(2\varphi)}\right). \tag{4.23}$$

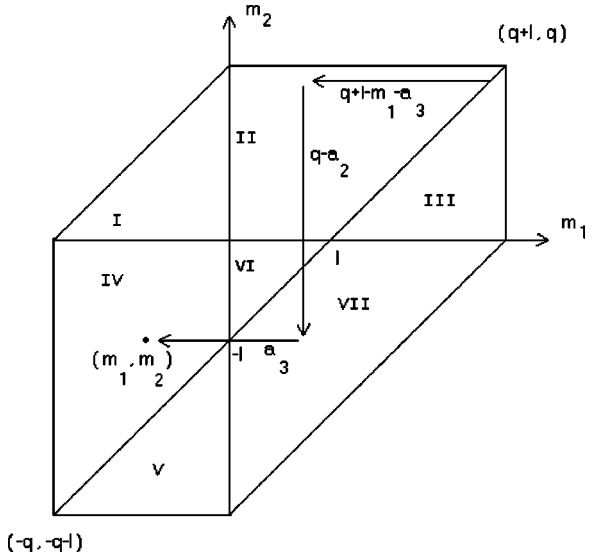

FIG. 1. Diagram of seven possible allowed regions of eigenspectrum of Hamiltonian $H_l(m_1,m_2)$ in the (m_1,m_2) plane for given values of integer parameters q, l, m_1, and m_2 with $l \geqslant 0$. Horizontal lines mean application of the lowering operator Y_- while the vertical line indicates the application of the lowering operator X_-.

V. GENERALIZED SHAPE INVARIANCE SYMMETRY

In this section we show that the Hamiltonian $H_l(m_1,m_2)$ possesses a new kind of shape invariance symmetry, we call it generalized shape invariance. Obviously SU(3) symmetry of the Casimir operator before the reduction generates this special shape invariance symmetry. Using this symmetry we will obtain below the eigenspectrum of Hamiltonian $H_l(m_1,m_2)$, that is the eigenfunctions $\chi^{q,l}_{m_1,m_2}(\theta,\varphi)$ corresponding to eigenvalue $E(q,l)$ by consecutive application of lowering operators over the state with $m_1=q+l$ and $m_2=q$. We will also obtain its degeneracy for given values of $(q+l,q)$, where it is the same as the one that can be obtained by using the inequalities (4.2) corresponding to Figs. 1 and 2.

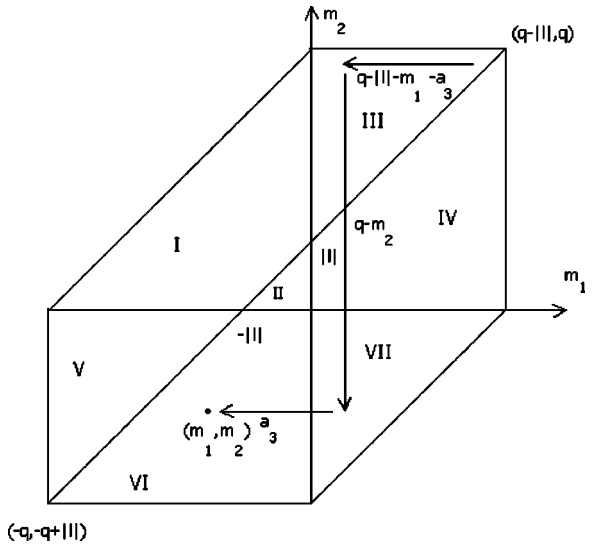

FIG. 2. Diagram of seven possible allowed regions of eigenspectrum of Hamiltonian $H_l(m_1,m_2)$ in the (m_1,m_2) plane for given values of integer parameters q, l, m_1, and m_2 with $l<0$. Horizontal lines mean application of the lowering operator Y_- while the vertical line indicates the application of the lowering operator X_-.

First we write the Hamiltonian $H_l(m_1,m_2)$ operator in terms of the Fourier transformed operators given in (4.18)–(4.21),

$$H_l(m_1,m_2)=\frac{1}{2}[R_+(m_1-1,m_2-1)R_-(m_1,m_2)+R_-(m_1+1,m_2+1)R_+(m_1,m_2)$$
$$+Y_+(m_1-1,m_2)Y_-(m_1,m_2)+Y_-(m_1+1,m_2)Y_+(m_1,m_2)+X_+(m_1,m_2-1)X_-(m_1,m_2)$$
$$+X_-(m_1,m_2+1)X_+(m_1,m_2)]+\frac{(m_1+m_2)^2}{4}+\frac{3\left(m_1-m_2-\frac{2}{3}l\right)^2}{4}. \tag{5.1}$$

Now, using the following commutation relations,

$$[R_3+\sqrt{3}R_8,Y_\pm]=\pm 2Y_\pm,\quad [R_3-\sqrt{3}R_8,Y_\pm]=\mp Y_\pm,$$
$$[R_3-\sqrt{3}R_8,X_\pm]=\pm 2X_\pm,\quad [R_3+\sqrt{3}R_8,X_\pm]=\mp X_\pm, \tag{5.2}$$

we can obtain the following relations:

$$(R_3(m_1\pm 1,m_2)+\sqrt{3}R_8(m_1\pm 1,m_2))Y_\pm(m_1,m_2)-Y_\pm(m_1,m_2)(R_3(m_1,m_2)$$
$$+\sqrt{3}R_8(m_1,m_2))=\pm 2Y_\pm(m_1,m_2),$$

$$(R_3(m_1\pm 1,m_2)-\sqrt{3}R_8(m_1\pm 1,m_2))Y_\pm(m_1,m_2)-Y_\pm(m_1,m_2)(R_3(m_1,m_2)$$
$$-\sqrt{3}R_8(m_1,m_2))=\mp Y_\pm(m_1,m_2),$$

$$(R_3(m_1,m_2\pm 1)-\sqrt{3}R_8(m_1,m_2\pm 1))X_\pm(m_1,m_2)-X_\pm(m_1,m_2)(R_3(m_1,m_2)$$
$$-\sqrt{3}R_8(m_1,m_2))=\pm 2X_\pm(m_1,m_2),$$

$$(R_3(m_1,m_2\pm 1)+\sqrt{3}R_8(m_1,m_2\pm 1))X_\pm(m_1,m_2)-X_\pm(m_1,m_2)(R_3(m_1,m_2)$$
$$+\sqrt{3}R_8(m_1,m_2))=\mp X_\pm(m_1,m_2). \tag{5.3}$$

The above relations imply that the Hamiltonian $H_l(m_1,m_2)$ possesses shape invariance symmetry. Since, through the left action of the operators $Y_\pm(m_1,m_2)$ and $X_\pm(m_1,m_2)$ on both sides of the following eigenvalue equations,

$$H_l(m_1,m_2)\chi^{q,l}_{m_1,m_2}(\theta,\varphi)=E(q,l)\chi^{q,l}_{m_1,m_2}(\theta,\varphi),$$

$$(R_3(m_1,m_2)+\sqrt{3}R_8(m_1,m_2))\chi^{q,l}_{m_1,m_2}(\theta,\varphi)=\left(2m_1-m_2-\frac{l}{2}\right)\chi^{q,l}_{m_1,m_2}(\theta,\varphi), \tag{5.4}$$

$$(R_3(m_1,m_2)-\sqrt{3}R_8(m_1,m_2))\chi^{q,l}_{m_1,m_2}(\theta,\varphi)=\left(-m_1+2m_2+\frac{l}{2}\right)\chi^{q,l}_{m_1,m_2}(\theta,\varphi),$$

we get

$$\chi^{q,l}_{m_1\pm 1,m_2}(\theta,\varphi)=Y_\pm(m_1,m_2)\chi^{q,l}_{m_1,m_2}(\theta,\varphi), \tag{5.5}$$

$$\chi^{q,l}_{m_1,m_2\pm 1}(\theta,\varphi)=X_\pm(m_1,m_2)\chi^{q,l}_{m_1,m_2}(\theta,\varphi). \tag{5.6}$$

Therefore, the operators $Y_\pm(m_1,m_2)$ shift the parameter m_1 by one unit or they push the unrenormalized eigenfunctions horizontally in Figs. 1 and 2, while the operators $X_\pm(m_1,m_2)$ shift the

parameter m_2 by one unit or they push the eigenfunctions vertically in Figs. 1 and 2. Obviously the eigenfunctions vanish in the forbidden regions of Figs. 1 and 2. Using the relations (5.5) and (5.6), we obtain the following relations:

$$Y_+(m_1-1,m_2)Y_-(m_1,m_2)\chi^{q,l}_{m_1,m_2}(\theta,\varphi)\simeq\chi^{q,l}_{m_1,m_2}(\theta,\varphi),$$

$$Y_-(m_1,m_2)Y_+(m_1-1,m_2)\chi^{q,l}_{m_1-1,m_2}(\theta,\varphi)\simeq\chi^{q,l}_{m_1-1,m_2}(\theta,\varphi) \tag{5.7}$$

and

$$X_+(m_1,m_2-1)X_-(m_1,m_2)\chi^{q,l}_{m_1,m_2}(\theta,\varphi)\simeq\chi^{q,l}_{m_1,m_2}(\theta,\varphi),$$

$$X_-(m_1,m_2)X_+(m_1,m_2-1)\chi^{q,l}_{m_1,m_2-1}(\theta,\varphi)\simeq\chi^{q,l}_{m_1,m_2-1}(\theta,\varphi), \tag{5.8}$$

which indicate that the Hamiltonian $H_l(m_1,m_2)$ possesses the shape invariance symmetry. Actually the first pair of equations given in (5.7) imply the horizontal shape invariance while the second pair of equations given in (5.8) imply the vertical shape invariance symmetry in Figs. 1 and 2, respectively. Therefore, using this symmetry we can obtain the eigenfunctions of the isospectral Hamiltonians $H_l(m_1,m_2)$ with the eigenvalue $E(q,l)$ simply by applying the lowering operators X_- and Y_- over the highest weight $\chi^{q,l}_{q+l,q}(\theta,\varphi)$, namely we obtain all the eigenstates for the values of parameters m_1 and m_2 given in the allowed region of Figs. 1 and 2, such that these eigenfunctions vanish for the values of the parameters corresponding to the forbidden region. Also one can show that in this way we obtain exactly the same eigenspectrum that we have obtained in Sec. IV by using the Verma basis.

Therefore, by consecutive application of lowering operators over highest eigenweight $\chi^{q,l}_{q+l,q}(\theta,\varphi)$, we can obtain an arbitrary eigenstate $\chi^{q,l}_{m_1,m_2}(\theta,\varphi)$, where the existence of different ordering of lowering operators or the different paths indicate the degeneracy of the Hamiltonian $H_l(m_1,m_2)$. It is straightforward to show that by this method we get exactly the eigenspectrum of the preceding section. For an illustration we explain below the real representation with $q=1$ and $l=0$ in detail. Using the relation (4.23), we get the following expression for highest eigenweight of (1,1) representation:

$$\chi^{1,0}_{1,1}(\theta,\varphi)=2\sin^2(\theta)\cos(\theta)\cos(\varphi)\sqrt{\cos(\theta)\sin(2\varphi)}, \tag{5.9}$$

then using (5.5) we get

$$\chi^{1,0}_{0,1}(\theta,\varphi)=Y_-(1,1)\chi^{1,0}_{1,1}(\theta,\varphi)=-\sin^3(\theta)\sin(2\varphi)\sqrt{\cos(\theta)\sin(2\varphi)}. \tag{5.10}$$

Now, we cannot lower the above eigenstate by acting the operator Y_- on it, since the function $\chi^{1,0}_{-1,1}(\theta,\varphi)$ corresponds to the values of parameters ($m_1=-1$, $m_2=1$) which is not allowed for $q=1$ and $l=0$. Therefore in order to get lower eigenstates we must act out the operator X_- on it, that is, we have

$$\chi^{1,0}_{0,0}(\theta,\varphi)=X_-(0,1)\chi^{1,0}_{0,1}(\theta,\varphi)=2\sin^3(\theta)\cos(2\varphi)\sqrt{\cos(\theta)\sin(2\varphi)}. \tag{5.11}$$

On the other hand, if we act out the lowering operator X_- on the highest eigenstate, we will obtain

$$\chi^{1,0}_{1,0}(\theta,\varphi)=X_-(1,1)\chi^{1,0}_{1,1}(\theta,\varphi)=-2\sin^2(\theta)\cos(\theta)\sin(\varphi)\sqrt{\cos(\theta)\sin(2\varphi)}, \tag{5.12}$$

where its further action will kill it, since the values of parameters ($m_1=1$, $m_2=-1$) are not allowed, hence we cannot have the eigenstate corresponding to these values of parameters. Similarly the action of Y_- will shift $\chi^{1,0}_{1,0}(\theta,\varphi)$ state to ($m_1=0$, $m_2=0$) or zero weight eigenstate,

$$\tilde{\chi}^{1}_{0,0}(\theta,\varphi) = Y_{-}(1,0)\chi^{1,0}_{1,0}(\theta,\varphi) = 2(\cos^2(\theta) - \sin^2(\varphi)\sin^2(\theta))\sin(\theta)\sqrt{\cos(\theta)\sin(2\varphi)}. \quad (5.13)$$

We see that zero weight is degenerate but other eigenvalues are nondegenerate which is in agreement with the results of the preceding section. With the same procedure we can obtain the remaining part of the spectrum, that is we have

$$\chi^{1,0}_{0,-1}(\theta,\varphi) = X_{-}(0,0)\chi^{1,0}_{0,0}(\theta,\varphi) = -2\sin(2\varphi)\sin^3(\theta)\sqrt{\cos(\theta)\sin(2\varphi)},$$

$$\chi^{1,0}_{-1,0}(\theta,\varphi) = Y_{-}(0,0)\chi^{1,0}_{0,0}(\theta,\varphi) = 2\sin(\varphi)\sin(2\theta)\sin(\theta)\sqrt{\cos(\theta)\sin(2\varphi)}, \quad (5.14)$$

and

$$\chi^{1,0}_{-1,-1}(\theta,\varphi) = Y_{-}(0,-1)\chi^{1,0}_{0,-1}(\theta,\varphi) = X_{-}(-1,0)\chi^{1,0}_{-1,0}(\theta,\varphi) = 2\sin(2\theta)\cos(\varphi)\sin(\theta)\sqrt{\cos(\theta)\sin(2\varphi)}. \quad (5.15)$$

We should remind that all eigenfunctions associated with the forbidden region of (m_1, m_2) plane vanish. For example, the action of the operators $X_{-}^3 Y_{-}$ and $Y_{-}^2 X_{-}^2 Y_{-}$ on highest eigenstate leads to vanishing functions $\chi^{1}_{0,-2}(\theta,\varphi)$ and $\chi^{1}_{-2,-1}(\theta,\varphi)$, respectively. Also one can show that by acting the operators $X_{-}Y_{-}X_{-}Y_{-}$ and $Y_{-}X_{-}Y_{-}X_{-}$ on the highest eigenstate we obtain eigenstates which are both proportional to Verma base $\chi^{1,0}_{-1,-1}(\theta,\varphi) = Y_{-}X_{-}^2 Y_{-}\chi^{1,0}_{1,1}(\theta,\varphi)$.

VI. THREE DIMENSIONAL HAMILTONIAN WITH ORDINARY SHAPE INVARIANCE SYMMETRY

Here in this section we first make Inonu–Wigner contraction[8] over the generators of su(3) Lie algebra given in (2.3)–(2.6), simply by making the change of coordinate $\theta = r/R$ and relating the new contracted generators to the old ones by $R^c_{\pm} = (1/R)R_{\pm}$, $R^c_3 = R_3$, $X^c_{\pm} = X_{\pm}$, $Y^c_{\pm} = (1/R)Y_{\pm}$, $R^c_8 = R_8$. Then in the limit of $R \to \infty$ the set of su (3) bases reduces to

$$R^c_{\pm} = \frac{1}{2}e^{\pm i(\chi_1 - \chi_2)}\left[\mp\cos(\varphi)\frac{\partial}{\partial r} \pm \frac{\sin(\varphi)}{r}\frac{\partial}{\partial\varphi} + \frac{i}{r\cos(\varphi)}\frac{\partial}{\partial\chi_2}\right], \quad (6.1)$$

$$Y^c_{\pm} = \frac{1}{2}e^{\pm i\chi_1}\left[\pm\sin(\varphi)\frac{\partial}{\partial r} \pm \frac{\cos(\varphi)}{r}\frac{\partial}{\partial\varphi} + \frac{i}{r\sin(\varphi)}\left(-\frac{\partial}{\partial\eta} + \frac{\partial}{\partial\chi_1} + \frac{\partial}{\partial\chi_2}\right)\right], \quad (6.2)$$

$$X^c_{\pm} = \frac{1}{2}e^{\mp i\chi_2}\left[\mp\frac{\partial}{\partial\varphi} - i\cot(\varphi)\left(\frac{\partial}{\partial\eta} - \frac{\partial}{\partial\chi_1}\right) + 2i\cot(2\varphi)\frac{\partial}{\partial\chi_2}\right], \quad (6.3)$$

$$R^c_3 = -\frac{i}{2}\left(\frac{\partial}{\partial\chi_1} - \frac{\partial}{\partial\chi_2}\right), \quad R^c_8 = \frac{i\sqrt{3}}{2}\left(\frac{2}{3}\frac{\partial}{\partial\eta} - \frac{\partial}{\partial\chi_1} - \frac{\partial}{\partial\chi_2}\right) \quad (6.4)$$

with the following commutation relations:

$$[R^c_3, R^c_{\pm}] = \pm R^c_{\pm}, \quad [R^c_3, Y^c_{\pm}] = \pm\tfrac{1}{2}Y^c_{\pm}, \quad [R^c_3, X^c_{\pm}] = \pm\tfrac{1}{2}X^c_{\pm},$$

$$[R^c_8, Y^c_{\pm}] = \pm\frac{\sqrt{3}}{2}Y^c_{\pm}, \quad [R^c_8, X^c_{\pm}] = \mp\frac{\sqrt{3}}{2}X^c_{\pm}, \quad (6.5)$$

$$[R^c_{\pm}, X^c_{\mp}] = \mp Y^c_{\pm}, \quad [X^c_{+}, X^c_{-}] = R^c_3 - \sqrt{3}R^c_8, \quad [Y^c_{\pm}, X^c_{\pm}] = \mp R^c_{\pm}.$$

Therefore, the generators R^c_{-}, R^c_{+}, Y^c_{-}, and Y^c_{+} commute with each other. Also the quadratic Casimir operator (2.8) reduces to

$$-C^c=\frac{\partial^2}{\partial r^2}+\frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}+\frac{1}{r^2\sin^2(\varphi)}\frac{\partial^2}{\partial\eta^2}+\frac{3}{r}\frac{\partial}{\partial r}+\frac{2\cot(2\varphi)}{r^2}\frac{\partial}{\partial\varphi}+\frac{1}{r^2\sin^2(\varphi)}$$
$$\times\left(\frac{\partial^2}{\partial\chi_1{}^2}+\frac{1}{\cos^2(\varphi)}\frac{\partial^2}{\partial\chi_2{}^2}+2\frac{\partial^2}{\partial\chi_1\partial\chi_2}-2\frac{\partial^2}{\partial\eta\partial\chi_1}-2\frac{\partial^2}{\partial\eta\partial\chi_2}\right), \tag{6.6}$$

where after the similarity transformation $\tilde{C}^c=f^{-1}(r,\varphi)C^cf(r,\varphi)$ with $f(r,\varphi)=1/\sqrt{r\cos(\varphi)}$ we get

$$-\tilde{C}^c=-\frac{1}{2}(\tilde{R}^c_-\tilde{R}^c_++\tilde{R}^c_+\tilde{R}^c_-+Y^c_-Y^c_++Y^c_+Y^c_-)$$
$$=+\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{1}{r^2\sin(\varphi)}\frac{\partial}{\partial\varphi}\sin(\varphi)\frac{\partial}{\partial\varphi}+\frac{1}{r^2\sin^2(\varphi)}\frac{\partial^2}{\partial\eta^2}+\frac{1}{4r^2\cos^2(\varphi)}$$
$$+\frac{1}{r^2\sin^2(\varphi)}\left(\frac{\partial^2}{\partial\chi_1^2}+\frac{1}{\cos^2(\varphi)}\frac{\partial^2}{\partial\chi_2^2}+2\frac{\partial^2}{\partial\chi_1\chi_2}-2\frac{\partial^2}{\partial\eta\partial\chi_1}-2\frac{\partial^2}{\partial\eta\partial\chi_2}\right), \tag{6.7}$$

where $\tilde{Y}^c_\pm=Y^c_\pm$ and $\tilde{R}^c_\pm=R^c_\pm\pm[1/4r\cos(\varphi)]e^{\pm i(\chi_1-\chi_2)}$. Now, by Fourier transforming over the coordinates χ_1 and χ_2 with the kernel $e^{i(m_1\chi_1-m_2\chi_2)}$, and the similarity transformation with function $e^{i(m_1-m_2)\eta}$, the above Casimir operator reduces to

$$H(m_2)=-\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{1}{r^2\sin(\varphi)}\frac{\partial}{\partial\varphi}\sin(\varphi)\frac{\partial}{\partial\varphi}+\frac{1}{r^2\sin^2(\varphi)}\frac{\partial^2}{\partial\eta^2}-\frac{(m_2^2-\frac{1}{4})}{r^2\cos^2(\varphi)}\right]. \tag{6.8}$$

Also after Inonu–Wigner contraction together with the Fourier transformation, the Casimir eigenvalue equation $(C/R^2)\psi=[E(q,l)/R^2]\psi$ reduces to $H(m_2)\psi^{(k)}_{m_2}=k^2\psi^{(k)}_{m_2}$ provided that for finite l, we let $q\to\infty$, $R\to\infty$ such that $q/R=\text{finite}=k$, therefore, we have a hierarchy of isospectral Hamiltonians labeled by the parameter m_2 and one can show that this isospectral symmetry comes from the shape invariance symmetry of these Hamiltonians. To see this we first write the Hamiltonian $H(m_2)$ in terms of Fourier transformed and similarity transformed lowering and rising operators,

$$A_\pm(m_2)=\frac{1}{2}\left(\mp\cos(\varphi)\frac{\partial}{\partial r}\pm\frac{\sin(\varphi)}{r}\frac{\partial}{\partial\varphi}+\frac{2m_2-1}{2r\cos(\varphi)}\right),$$

$$B_+=\frac{1}{2}\left(\sin(\varphi)\frac{\partial}{\partial r}+\frac{\cos(\varphi)}{r}\frac{\partial}{\partial\varphi}-\frac{i}{r\sin(\varphi)}\frac{\partial}{\partial\eta}+\frac{1}{r\sin(\varphi)}\right), \tag{6.9}$$

$$B_-=\frac{1}{2}\left(-\sin(\varphi)\frac{\partial}{\partial r}-\frac{\cos(\varphi)}{r}\frac{\partial}{\partial\varphi}-\frac{i}{r\sin(\varphi)}\frac{\partial}{\partial\eta}\right),$$

in the following form:

$$H(m_2)=A_+(m_2)A_-(m_2)+B_+B_-, \tag{6.10}$$

$$H(m_2-1)=A_-(m_2)A_+(m_2)+B_+B_-. \tag{6.11}$$

Now, multiplying the eigenvalue equation

$$H(m_2)\psi^{(k)}_{m_2}=(A_+(m_2)A_-(m_2)+B_+B_-)\psi^{(k)}_{m_2} \tag{6.12}$$

from the left-hand side by the operator $A_-(m_2)$ and using the fact that $A_\pm(m_2)$ commute with $B_\pm$, we obtain

$$H(m_2-1)(A_-(m_2)\psi^{(k)}_{m_2}) = k^2(A_-(m_2))\psi^{(k)}_{m_2}), \tag{6.13}$$

therefore, $A_-(m_2)\psi^{(k)}_{m_2}$ is the eigenfunction of $H(m_2-1)$ with the same eigenvalue k^2, hence the operator $A_-(m_2)$ lowers the index m_2 by one unit. The similarity one shows that $A_+(m_2)$ raises m_2 by one unit, respectively. Therefore, the Hamiltonian $H(m_2)$ possesses ordinary shape invariance symmetry with respect to parameter m_2.

For half-integer value of the parameter m_2 we can obtain the continuous eigenspectrum of these Hamiltonians (since these Hamiltonians are positive definite), simply by acting these lowering and raising operators over the eigenfunction of the free particle as follows.

Since for $m_2=\frac{1}{2}$ the Hamiltonian $H(m_2)$ reduces to $H(\frac{1}{2})=-\nabla^2$ with the eigenvalue $E=k^2$ and eigenfunction $\psi^{(\vec{k})}_{1/2}=e^{i\vec{k}.\vec{x}}$ and for Hamiltonian $H(n_2+\frac{1}{2})$ with non-negative integer n_2, we have $H(n_2+\frac{1}{2})\psi^{(\vec{k})}_{n_2}=k^2\psi^{(\vec{k})}_{n_2}$ with

$$\psi^{(\vec{k})}_{n_2}=\prod_{j=1}^{n_2}A_+\left(j+\frac{1}{2}\right)e^{i\vec{k}.\vec{x}}. \tag{6.14}$$

VII. CONCLUSION

Here in this work we have generalized the ordinary exactly solvable shape invariance Hamiltonians to Hamiltonians with non-Abelian type of shape invariance symmetry and an ordinary shape invariance one. Again it is shown that the new kind of shape invariance symmetry has its origin in group theory or better to say, the exact solvability of Hamiltonians are related in some way to Lie algebras or Lie groups.

APPENDIX: DEGENERACY OF HAMILTONIAN $H_l(m_1, m_2)$

In order to determine the degeneracy of Hamiltonian $H_l(m_1,m_2)$ for a given value of integer parameters m_1 and m_2, we should determine the range of variation of integer a_3 by imposing the inequalities (4.2).

For $l\geqslant 0$ and $0\leqslant m_2\leqslant q$ we have the following three different regions for integer parameter m_1:

(I) $-m_1\leqslant a_3\leqslant q-m_2$, $m_2-m_1\leqslant q$, $-q\leqslant m_1<0$, degeneracy$=q-m_2+m_1+1$,
(II) $0\leqslant a_3\leqslant q-m_2$, $0\leqslant m_1<l+m_2$, degeneracy$=q-m_2+1$,
(III) $0\leqslant a_3\leqslant q+l-m_1$, $l+m_2\leqslant m_1\leqslant q+l$, degeneracy$=q+l-m_1+1$,
while for $-q-l\leqslant m_2<0$ there are another four different regions for m_1,
(IV) $-m_1\leqslant a_3\leqslant q$, $-q\leqslant m_1<l+m_2<0$, $-q-l\leqslant m_2<0$, degeneracy$=q+m_1+1$,
(V) $-m_1\leqslant a_3\leqslant q+l-m_1+m_2$, $l+m_2\leqslant m_1<0$, $-q-l\leqslant m_2<-l$, degeneracy$=q+l+m_2+1$,
(VI) $0\leqslant a_3\leqslant q$, $0\leqslant m_1<l+m_2$, $-l\leqslant m_2<0$, degeneracy$=q+1$,
(VII) $0\leqslant a_3\leqslant q+l-m_1+m_2$, $l\leqslant m_1-m_2\leqslant q+l$, $0\leqslant m_1\leqslant q+l$, $-l-q\leqslant m_2<0$, degeneracy $=q+l-m_1+m_2+1$.

For $l<0$ and $0\leqslant m_2\leqslant q$ we have the following four different regions for integer parameter m_1:

(I) $-m_1\leqslant a_3\leqslant q-m_2$, $|l|<m_2-m_1\leqslant q$, $-q\leqslant m_1\leqslant 0$, $0\leqslant m_2\leqslant q$, degeneracy$=q-m_2+m_1+1$,
(II) $-m_1\leqslant a_3\leqslant q-|l|-m_1$, $m_2-|l|\leqslant m_1<0$, $0\leqslant m_2<|l|$, degeneracy$=q-|l|+1$,
(III) $0\leqslant a_3\leqslant q-m_2$, $0\leqslant m_1\leqslant m_2-|l|$, $|l|\leqslant m_2\leqslant q$, degeneracy$=q-m_2+1$,
(IV) $0\leqslant a_3\leqslant q-|l|-m_1$, $0\leqslant m_2-|l|\leqslant m_1\leqslant q-|l|$, $0\leqslant m_2\leqslant q$, degeneracy$=q-|l|-m_1+1$,
while for $-q+|l|\leqslant m_2<0$ there are another three different regions for m_1,
(V) $-m_1\leqslant a_3\leqslant q$, $-q\leqslant m_1<m_2-|l|$, degeneracy$=q+m_1+1$,
(VI) $-m_1\leqslant a_3\leqslant q-|l|-m_1+m_2$, $m_2-|l|\leqslant m_1<0$, degeneracy$=q-|l|+m_2+1$,
(VII) $0\leqslant a_3\leqslant q-|l|-m_1+m_2$, $m_1-m_2\leqslant q-|l|$, $0\leqslant m_1<q-|l|$, degeneracy$=q-|l|-m_1+m_2+1$.

For given values of the integer parameters q, l, m_1, and m_2 the eigenspectrum of Hamiltonian $H_l(m_1,m_2)$ exists in the above seven regions of the (m_1,m_2) plane (see Fig. 1 for $l \geqslant 0$ and Fig. 2 for $l<0$). Therefore for given values of m_1 and m_2 the eigenspectrum can be obtained simply by consecutive application of lowering operators over the highest eigenweight according to the paths shown in Figs. 1 and 2.

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Implementation of group-covariant positive operator valued measures by orthogonal measurements

Thomas Decker[a] and Dominik Janzing[b]
Institut für Algorithmen und Kognitive Systeme, Arbeitsgruppe Quantum Computing, Universität Karlsruhe, Am Fasanengarten 5, D-76 131 Karlsruhe, Germany

Martin Rötteler[c]
Institute for Quantum Computing, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

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We consider group-covariant positive operator valued measures (POVMs) on a finite dimensional quantum system. Following Neumark's theorem a POVM can be implemented by an orthogonal measurement on a larger system. Accordingly, our goal is to find a quantum circuit implementation of a given group-covariant POVM which uses the symmetry of the POVM. Based on representation theory of the symmetry group we develop a general approach for the implementation of group-covariant POVMs which consist of rank-one operators. The construction relies on a method to decompose matrices that intertwine two representations of a finite group. We give several examples for which the resulting quantum circuits are efficient. In particular, we obtain efficient quantum circuits for a class of POVMs generated by Weyl–Heisenberg groups. These circuits allow to implement an approximative simultaneous measurement of the position and crystal momentum of a particle moving on a cyclic chain. © *2005 American Institute of Physics.*
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I. INTRODUCTION

General measurements of quantum systems are described by positive operator-valued measures (POVMs).[1,2] For several optimality criteria the use of POVMs can be advantageous as compared to projector valued measurements. This is true, e.g., for the mean square error, the minimum probability of error,[3] and the mutual information.[4] POVMs are more flexible than orthogonal von Neumann measurements and can consist of finite as well as of an infinite number of elements. An example for the latter is given in Ref. 5 where a POVM for measuring the spin direction is proposed. Here we restrict our attention to the finite case where a POVM is described by a set of positive operators which sum up to the identity. Such a POVM is called group-covariant if the set is invariant under the action of a group. The example of POVMs for the Weyl–Heisenberg groups as well as an example given in Ref. 5 show that POVMs are needed to describe phenomenologically the mesoscopic scale of quantum systems. They allow *approximatively* simultaneous measurements of quantum observables which are actually incompatible. For instance, the classical phase space of a particle can be approximatively reproduced by simultaneous measurements of momentum and position. Descriptions of quantum particles which have strong analogy to the classical phase space are helpful to understand the relations between the classical and the quantum world.[6] Also for several other tasks in quantum information processing the implementation of POVMs is of interest.[7–9]

[a]Electronic mail: decker@ira.uka.de
[b]Electronic mail: janzing@ira.uka.de
[c]Electronic mail: mroetteler@iqc.ca

Neumark's theorem[10,11] states that in principle every POVM can be implemented by an orthogonal measurement of the joint system consisting of the system and an ancilla system. However, the orthogonal measurement required by this construction may not be a "natural" observable of the joint system. One may need an additional unitary transform to obtain a reduction to a more natural observable which henceforth will be called the measurement in the computational basis of the quantum system.

Therefore, the question arises how to actually implement a POVM in terms of a quantum circuit which itself is composed of a sequence of elementary quantum gates.[12] So far, only little is known about the implementation of POVMs even in quantum systems with a small number of dimensions. While some rather specific single-qubit measurements have been studied,[4,13,14] not much is known about the general problem of how to implement a POVM by a unitary transform on the quantum register of a possibly larger space followed by an orthogonal measurement in the computational basis.

When studying quantum circuits for families of POVMs questions about the complexity of the required unitary transforms arise. In some cases we can exploit the fact that they admit some additional symmetry. This leads to the study of group-covariant POVMs which has been studied extensively in the literature.[4,15–17] As a recent example we mention the construction of symmetric informationally complete POVMs by means of suitable finite symmetry groups.[18]

The main contribution of this paper is a general method which computes an embedding of group-covariant POVMs into orthogonal measurements on a larger Hilbert space. A particular feature of the computed embedding is that it uses the symmetry. This in turn allows to apply known techniques for decomposing matrices with symmetry to the unitary matrices obtained by this embedding. For several cases this leads to families of *efficient* quantum circuits implementing the given POVMs.

Outline: In Sec. II we briefly recall the definition of POVMs. In Sec. III we consider the decomposition of matrices that have a symmetry with respect to a group. This type of decomposition is a basic tool for our constructions. We also define group-covariance of POVMs with respect to a symmetry group and a group representation. Furthermore, we explain how POVMs with this group covariance are related to so-called monomial representations of the symmetry group. In Sec. IV we explain the general scheme for the construction of a unitary transform that implements a group-covariant POVM. The basis for this construction is the analysis of the intertwining space between the group representation that is given by the group covariance of the POVM and the monomial representation. This is the starting point for methods using fast quantum Fourier transforms as described in Sec. V. Finally, in Sec. VI we give several examples of implementations of group-covariant POVMs.

Notations: We denote the field of complex numbers by $\mathbb{C}$. The group of invertible $n\times n$ matrices is denoted by $\mathrm{GL}_n(\mathbb{C})$ and the subgroup consisting of the unitary $n\times n$ matrices is denoted by $\mathcal{U}(n)$. We denote the identity matrix in $\mathcal{U}(n)$ by $\mathbf{1}_n$. If not denoted otherwise all matrices are matrices over the complex numbers. The cyclic group of order n is denoted by $\mathbb{Z}_n$. Representations are denoted by small greek letters, e. g., φ, ψ, etc. By abuse of notation we also denote the trivial representation of dimension n (i.e., dimension n) by $\mathbf{1}_n$. The direct sum of matrices and representations is denoted by $A\oplus B$ and $\varphi\oplus\psi$ and the tensor product is denoted by $A\otimes B$ and $\varphi\otimes\psi$, respectively. We make frequent use of the Pauli matrices

$$\sigma_x=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_y=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma_z=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.$$

A diagonal matrix with diagonal entries $\lambda_1,\ldots,\lambda_n$ is abbreviated by $\mathrm{diag}(\lambda_1,\ldots,\lambda_n)$. We denote the symmetric group on n symbols by $\mathcal{S}_n$. To each permutation $\sigma\in\mathcal{S}_n$ naturally corresponds the permutation matrix $\Sigma_i|\sigma(i)\rangle\langle i|$. By abuse of notation we identify σ with the corresponding permutation matrix. We often use the permutation matrix S_m which corresponds to the m-cycle $(1,2,\ldots,m)$ and the matrix$T_m=\mathrm{diag}(1,\omega_m,\ldots,\omega_m^{m-1})$ which contains the eigenvalues of $\mathcal{S}_m$. The basis states of an n-qubit system correspond to binary strings of length n. Quantum circuits are

written from the left to the right, and the qubits are arranged such that the most significant qubit (characterizing the left-most symbol of a binary string) is on top. Throughout the paper a matrix entry "·" stands for zero.

II. POVMs AND ORTHOGONAL MEASUREMENTS

A POVM for a quantum system with Hilbert space $\mathbb{C}^d$ is a set $P=\{A_1,\ldots,A_n\}\subseteq\mathbb{C}^{d\times d}$ of non-negative operators, where $\Sigma_k A_k=\mathbf{1}_d$. For a more general definition for POVMs with an infinite number of operators we refer to Ref. 19. For example, the set of matrices

$$P_2=\left\{\frac{1}{3}\begin{pmatrix}1&1\\1&1\end{pmatrix},\frac{1}{3}\begin{pmatrix}1&\omega\\\omega^2&1\end{pmatrix},\frac{1}{3}\begin{pmatrix}1&\omega^2\\\omega&1\end{pmatrix}\right\}\subseteq\mathbb{C}^{2\times 2},$$

where $\omega=\exp(2\pi i/3)$ is a third root of unity, defines a POVM on a system with corresponding Hilbert space $\mathbb{C}^2$. Suppose that the state of the system is described by the density matrix $\rho\in\mathbb{C}^{d\times d}$. Then for a general POVM the probability p_k for the result k is given by $p_k=\mathrm{tr}(\rho A_k)$. An *orthogonal* measurement is a POVM with mutually orthogonal operators A_k, i. e., we have that $A_kA_l=A_lA_k=0$ for $k\neq l$.

In the following we restrict ourselves to rank-one operators $A_k=|\Psi_k\rangle\langle\Psi_k|$. Note that the POVM vectors $|\Psi_k\rangle$ need not be normalized and that the restriction to operators of rank one is for some applications justified by Davies' theorem.[15] It states that we can always find a POVM with rank-one operators that maximizes the mutual information. The example P_2, which consists of three rank-one operators, can be written as $P_2=\{|\Psi_1\rangle\langle\Psi_1|,|\Psi_2\rangle\langle\Psi_2|,|\Psi_3\rangle\langle\Psi_3|\}$, where

$$|\Psi_1\rangle=\frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\end{pmatrix},\quad |\Psi_2\rangle=\frac{1}{\sqrt{3}}\begin{pmatrix}1\\\omega^2\end{pmatrix},\quad \text{and } |\Psi_3\rangle=\frac{1}{\sqrt{3}}\begin{pmatrix}1\\\omega\end{pmatrix}$$

are the corresponding POVM vectors in $\mathbb{C}^2$. Neumark's theorem[11] states that it is possible to implement a POVM by reducing it to an orthogonal measurement on a larger system. We briefly recall this construction. Let $P=\{A_k\}=\{|\Psi_k\rangle\langle\Psi_k|\}$ be a POVM with n operators that acts on the Hilbert space $\mathbb{C}^d$. For $n>d$ the vectors $|\Psi_k\rangle$ cannot be mutually orthogonal. Consequently, we must extend the system by at least $n-d$ dimensions in order to define an orthogonal measurement with n different measurement outcomes. We want to implement an orthogonal measurement $\tilde{P}=\{\tilde{A}_k\}=\{|\tilde{\Psi}_k\rangle\langle\tilde{\Psi}_k|\}$ on the system with n dimensions such that $\tilde{P}$ corresponds to the POVM P on the subsystem with d dimensions, i.e., $p_k=\mathrm{tr}(\rho A_k)=\mathrm{tr}(\tilde{\rho}\tilde{A}_k)$. Here we have that the embedding of the state into the larger system is $\tilde{\rho}=\rho\oplus 0_{n-d}\in\mathbb{C}^{n\times n}$ where 0_{n-d} denotes the zero matrix of size $n-d$.

We write the POVM vectors $|\Psi_k\rangle$ as columns of the matrix $M=(|\Psi_1\rangle\cdots|\Psi_n\rangle)\in\mathbb{C}^{d\times n}$. In the following we refer to M as the defining matrix for the POVM P. Now, the vectors $|\tilde{\Psi}_k\rangle=|\Psi_k\rangle\oplus|\Phi_k\rangle$ corresponding to $\tilde{A}_k=|\tilde{\Psi}_k\rangle\langle\tilde{\Psi}_k|\in\mathbb{C}^{n\times n}$ are the columns of the matrix

$$\tilde{M}=\begin{pmatrix}|\Psi_1\rangle&\cdots&|\Psi_n\rangle\\|\Phi_1\rangle&\cdots&|\Phi_n\rangle\end{pmatrix}\in\mathcal{U}(n).$$

Note that $\tilde{M}$ can be an arbitrary unitary matrix which contains M as upper part of size $d\times n$. Since P is a POVM we have $MM^\dagger=\Sigma_k|\Psi_k\rangle\langle\Psi_k|=\Sigma_k A_k=\mathbf{1}_d$, i. e., finding a suitable $\tilde{M}$ is always possible. For example, in case of P_2 we obtain the defining matrix

$$M=\frac{1}{\sqrt{3}}\begin{pmatrix}1&1&1\\1&\omega^2&\omega\end{pmatrix}\in\mathbb{C}^{2\times 3}$$

and one possible choice for $\tilde{M}$ is to add the row given by $(1/\sqrt{3})(1,\omega,\omega^2)$. Hence the rank-one projectors corresponding to the orthogonal measurement $\tilde{M}$ are

$$|\tilde{\Psi}_1\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix}, \quad |\tilde{\Psi}_2\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\\omega^2\\\omega\end{pmatrix}, \quad \text{and } |\tilde{\Psi}_3\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\\omega\\\omega^2\end{pmatrix}.$$

The probability distribution $\tilde{p}_k = \mathrm{tr}(\tilde{\rho}\tilde{A}_k)$ of the constructed orthogonal measurement equals the distribution p_k of the original POVM since

$$\tilde{p}_k = \mathrm{tr}(\tilde{\rho}\tilde{A}_k) = \mathrm{tr}\left((\rho \oplus 0_{n-d})\begin{pmatrix}|\Psi_k\rangle\langle\Psi_k| & |\Psi_k\rangle\langle\Phi_k|\\ |\Phi_k\rangle\langle\Psi_k| & |\Phi_k\rangle\langle\Phi_k|\end{pmatrix}\right) = \mathrm{tr}(\rho A_k) = p_k.$$

The embedding into a larger system can be realized by using an ancilla register of a quantum computer. It consists of l qubits such that $2^l \geqslant n-d$. They are initially in the state $|0\cdots0\rangle$. Then the space $\mathbb{C}^d \otimes |0\cdots0\rangle$ is the subspace where the POVM acts on and $\mathbb{C}^d \otimes (\mathbb{C}^2)^{\otimes l}$ is the extension. The density operator $\tilde{\rho}$ acts on an n-dimensional subspace of the joint system consisting of the original system and the ancilla register. In the following we will assume that also the system space $\mathbb{C}^d$ is embedded into the state space of some qubits.

As explained above, we can implement the POVM with corresponding matrix M by applying the unitary transform $\tilde{M}^\dagger$ to the initial state $\tilde{\rho}$ of the joint system followed by a measurement in the computational basis. Note that for the special case where the columns of M are already orthogonal we have that $\tilde{M} = M$. In this case by implementing the matrix $M^\dagger$ followed by a measurement in the computational basis we can perfectly distinguish between the columns of M.

In principle, the construction of an appropriate matrix $\tilde{M}$ is simple since we just have to find mutually orthogonal rows that lead to a unitary matrix. However, k qubits allow POVMs with $n = 2^k$ operators. Hence the size of $\tilde{M}$ is exponential in k. The complexity to implement a unitary matrix on k qubits can be upper bounded[20] by $O(4^k)$ and a generic element of $\mathcal{U}(2^k)$ will indeed require an exponential number of elementary transforms (e.g., one- and two-qubit gates). Therefore we are interested in the construction of a matrix $\tilde{M}$ that can be implemented efficiently, if such a construction exists at all. While finding efficient factorizations is a hard problem in general, the situation becomes easier in some cases where we are given the additional structure of a group-covariant POVM. In the following sections we will give a definition of group covariance and the related notion of symmetry. Later, we exploit the symmetry of the matrix M and give several examples of POVMs that have efficient quantum circuit implementations.

III. GROUP-COVARIANT POVMs AND MATRICES WITH SYMMETRY

In the following we give a precise mathematical definition of the notion of *symmetry* of a matrix $M \in \mathbb{C}^{m\times n}$. Later we define group covariance of a POVM and show that the group covariance in a natural way leads to matrices with symmetry. For the necessary background on finite groups and representations we refer to standard textbooks such as Refs. 21 and 22.

We start with a finite group G and a pair (φ, ψ) of matrix representations of G which are compatible with the size of M, i.e., $\varphi: G \to \mathrm{GL}_m(\mathbb{C})$ and $\psi: G \to \mathrm{GL}_n(\mathbb{C})$. Following Refs. 23 and 24 we call the triple (G, φ, ψ) a symmetry of M if the identity $\varphi(g)M = M\psi(g)$ holds for all $g \in G$. Sometimes we abbreviate this by using the shorthand notation $\varphi M = M\psi$. Note that if M is not a square matrix the representations φ and ψ have different dimensions.

To give an example we let $\omega = \exp(2\pi i/3)$ and let $\alpha, \beta, \gamma \in \mathbb{C}$. Then for all $j \in \{0,1,2\}$ we have that

$$\begin{pmatrix}1&\cdot&\cdot\\ \cdot&\omega&\cdot\\ \cdot&\cdot&\omega^2\end{pmatrix}^j \begin{pmatrix}\alpha&\alpha&\alpha\\ \beta&\beta\omega&\beta\omega^2\\ \gamma&\gamma\omega^2&\gamma\omega\end{pmatrix} = \begin{pmatrix}\alpha&\alpha&\alpha\\ \beta&\beta\omega&\beta\omega^2\\ \gamma&\gamma\omega^2&\gamma\omega\end{pmatrix} \begin{pmatrix}\cdot&\cdot&1\\ 1&\cdot&\cdot\\ \cdot&1&\cdot\end{pmatrix}^j.$$

Hence we obtain a symmetry which is given by the cyclic group $\mathbb{Z}_3 = \{0,1,2\}$ together with the two representations $\varphi, \sigma: \mathbb{Z}_3 \to \mathcal{U}(3)$ given by $\varphi(1) = \mathrm{diag}(1, \omega, \omega^2)$ and $\sigma(1) = (1,3,2)$.

Note that given two representations φ, ψ of a group G the set of all matrices M which fulfill $\varphi(g)M=M\psi(g)$ for all $g\in G$ is a vector space. It turns out that the matrices in this vector space have a special form. Hence we explore its structure in more detail in the following.

Definition 1 (intertwining space): Let G be a group and let φ, ψ be representations of G of dimensions n and m, respectively. Then

$$\mathrm{Int}(\varphi,\psi) := \{M:\varphi(g)M = M\psi(g),\ \textit{for all } g\in G\}$$

with $M\in\mathbb{C}^{n\times m}$ is called the intertwining space of φ and ψ.

In the following we denote by $\varphi_1,\ldots,\varphi_k$ a complete list of pairwise inequivalent irreducible representations of G. Recall that for any representation of a finite group it is always possible to find a base change such that the corresponding representation is a direct sum of irreducible representations.[22] For representations which are completely decomposed into a direct sum of irreducibles the structure of the intertwining space is known. This is the content of the following theorem which follows directly from Schur's lemma (see Ref. 26, Sec. 29).

Theorem 2: *Let G be a finite group and $\varphi=\oplus_{i=1}^{k}(\mathbf{1}_{n_i}\otimes\varphi_i)$ and $\psi=\oplus_{i=1}^{k}(\mathbf{1}_{m_i}\otimes\varphi_i)$ two representations of G which have been completely decomposed into pairwise inequivalent representations φ_i with $i=1,\ldots,k$. Then the intertwining space of φ and ψ has the following structure:*

$$\mathrm{Int}(\varphi,\psi) = (\mathbb{C}^{n_1\times m_1}\otimes\mathbf{1}_{\deg(\varphi_1)})\oplus\cdots\oplus(\mathbb{C}^{n_k\times m_k}\otimes\mathbf{1}_{\deg(\varphi_k)}).$$

A matrix A is called *block permuted* if there are permutation matrices P and Q such that $PAQ=B_1\oplus\cdots\oplus B_k$, where $B_1,\ldots,B_k$ are (rectangular) matrices. For all $n,m,k\in\mathbb{N}$ there exist permutation matrices $P_{n,m,k}$ and $Q_{n,m,k}$ such that for all $A\in\mathbb{C}^{n\times m}$ we have $P_{n,m,k}(A\otimes\mathbf{1}_k)Q_{n,m,k}=\mathbf{1}_k\otimes A$. Hence we have shown that the elements of the intertwining space of completely reduced representations are block permuted.

We continue with an easy observation which turns out to be essential for the approach of extending the symmetry of a given group-covariant POVM to a measurement on a larger space. Suppose that $M\in\mathrm{Int}(\varphi,\psi)$ and that the matrices U and W decompose the representations φ and ψ into the direct sums, i.e., $U\varphi U^\dagger=\varphi_1\oplus\cdots\oplus\varphi_n$ and $V\psi V^\dagger=\psi_1\oplus\cdots\oplus\psi_m$. Then we can rewrite $\varphi M=M\sigma$ as

$$U^\dagger(\varphi_1\oplus\cdots\oplus\varphi_n)UM = MW^\dagger(\psi_1\oplus\cdots\oplus\psi_m)W.$$

Multiplying this from the left by U and from the right by $W^\dagger$ shows that $C:=UMW^\dagger$ is an element of the intertwining space $\mathrm{Int}(\varphi_1\oplus\cdots\oplus\varphi_n,\psi_1\oplus\cdots\oplus\psi_m)$ of two completely reduced representations. In particular, we can apply Theorem 2 to determine the structure of C. In particular we obtain that C is block permuted and the size of the blocks depend on the multiplicities and dimensions of the irreducible representations contained in φ and ψ.

Matrices with symmetry arise naturally in context of group-covariant POVMs. We first give a definition of these POVMs and then establish a connection between the notions of group covariance and symmetry.

Definition 3 (group-covariant POVMs): A POVM $P=\{A_1,\ldots,A_n\}\subseteq\mathbb{C}^{d\times d}$ with $A_k\neq A_l$ for $k\neq l$ is group-covariant with respect to the group G if there exists a projective unitary representation $\varphi:G\to\mathcal{U}(d)$ with $\varphi(g)A_k\varphi(g)^\dagger\in P$ for all $g\in G$ and all k.

Note that a group-covariant POVM is also group covariant for all subgroups $H\leqslant G$ and the restriction of the representation φ to H. As a special case, the choice of the trivial subgroup $H=\{1\}$ means that we do not use the symmetry of the POVM at all.

A minor complication arises due to the fact that while the notion of symmetry of matrices relies on ordinary, i.e., nonprojective representations, the definition of group-covariant POVMs relies on projective representations. Therefore, we need a construction which allows to transform the projective representation of the symmetry group of a group-covariant POVM into a nonprojective representation. This connection is established using so-called *central extensions* which is a method going back to Schur. We briefly recall this construction [see also Ref. 22, Lemma (11.16)]. Let $\varphi:G\to\mathrm{GL}_d(\mathbb{C})$ be a projective representation of the group G. More precisely, we have

$\varphi(gh)=\gamma_{gh}\varphi(g)\varphi(h)$ for $g,h\in G$, where γ_{gh} is a factor system. Let $H=\langle\gamma_{gh}:g,h\in G\rangle$ be the group generated by the γ_{gh}. We consider the group $\hat{G}$ consisting of the elements (g,h) with $g\in G$ and $h\in H$. The multiplication of two elements (g,h) and (g',h') of $\hat{G}$ is defined by $(g,h)(g',h')=(gg',\gamma_{gg'}hh')$. Then the map $\tilde{\varphi}((g,h))=h\varphi(g)$ is a representation with $\tilde{\varphi}((g,1))=\varphi(g)$, i.e., the representation $\tilde{\varphi}$ equals φ on the elements $(g,1)$ and the group $\hat{G}$ is a central extension of the group G.

In the following we always assume φ to be a nonprojective representation of the symmetry group G by this construction. This is justified since the set of POVM operators does not change by switching from G to a central extension $\hat{G}$ because scalar multiples of the identity transform trivially under conjugation.

We now analyze the structure of the matrix M corresponding to the group-covariant POVM $P=\{|\Psi_k\rangle\langle\Psi_k|\}$ with rank-one operators. Note that the phases of the vectors $|\Psi_k\rangle$ can be chosen arbitrarily without changing the POVM. Let $\varphi:G\to\mathcal{U}(d)$ be the representation corresponding to the symmetry of P. We then have the equation

$$\varphi(g)|\Psi_k\rangle\langle\Psi_k|\varphi(g)^\dagger=|\Psi_{\pi(g)k}\rangle\langle\Psi_{\pi(g)k}|,$$

where $\pi:G\to S_n$ denotes a permutation representation of the group G. Indeed, the equation $|\Psi_{\pi(g)j}\rangle\langle\Psi_{\pi(g)j}|=|\Psi_{\pi(g)k}\rangle\langle\Psi_{\pi(g)k}|$ implies $|\Psi_j\rangle\langle\Psi_j|=|\Psi_k\rangle\langle\Psi_k|$ by conjugation with $\varphi(g)^\dagger$ since $A_j\neq A_k$ for $j\neq k$. Therefore, the map $\pi(g)$ is injective for all $g\in G$. Since an injective map on a finite set is also surjective the map $\pi(g)$ defines a permutation.

Next, we consider the action of φ on the columns of the matrix M. As stated above the columns $|\Psi_k\rangle$ of M can have arbitrary phase factors. The action of $\varphi(g)$ on the columns of M can be described by the equation $\varphi(g)|\Psi_k\rangle=e^{i\phi(g,k)}|\Psi_{\pi(g)k}\rangle$ where $\phi(g,k)$ depends on k, g and the fixed phase factors of the vectors $|\Psi_k\rangle$. We identify the columns $|\Psi_k\rangle$ with a basis b_k of the vector space $\mathbb{C}^n$ in order to construct a representation that describes the action of φ on the columns of M. With this identification the action of $\varphi(g)$ corresponds to the map $b_k\mapsto e^{i\phi(g,k)}b_{\pi(g)k}$.

By writing down the matrix corresponding to this map, we see that in each row and each column there is precisely one entry different from zero. Matrices having a structure like this are called *monomial matrices*[25] (Ref. 26, Sec. 43). Whenever the images under a representation consist entirely of monomial matrices, we denote this with a subscript, i.e., we write $\varphi_{\mathrm{mon}}(g)$. Now, the two representations φ and φ_{mon} define the symmetry $\varphi M=M\varphi_{\mathrm{mon}}$ of the matrix M. The monomial representation φ_{mon} acts on the columns of M. For each $g\in G$ it permutes the columns of M and multiplies each column with a phase factor.

Example 4: As an example in two dimensions we consider the following POVM:

$$P=\left\{\begin{pmatrix}|\alpha|^2 & \alpha\overline{\beta}\\ \overline{\alpha}\beta & |\beta|^2\end{pmatrix},\begin{pmatrix}|\alpha|^2 & -\alpha\overline{\beta}\\ -\overline{\alpha}\beta & |\beta|^2\end{pmatrix},\begin{pmatrix}|\beta|^2 & \overline{\alpha}\beta\\ \alpha\overline{\beta} & |\alpha|^2\end{pmatrix},\begin{pmatrix}|\beta|^2 & -\overline{\alpha}\beta\\ -\alpha\overline{\beta} & |\alpha|^2\end{pmatrix}\right\}\subseteq\mathbb{C}^{2\times 2}$$

with $\alpha,\beta\in\mathbb{C}$ and $|\alpha|^2+|\beta|^2=1/2$. Then P is covariant with respect to $\mathbb{Z}_2\times\mathbb{Z}_2$. The corresponding projective representation $\varphi:\mathbb{Z}_2\times\mathbb{Z}_2\to\mathcal{U}(2)$ is defined by the equations

$$\varphi(0,0)=\mathbf{1}_2,\quad \varphi(0,1)=\sigma_z,\quad \varphi(1,0)=\sigma_x,\quad \varphi(1,1)=\sigma_z\sigma_x,$$

where (0,0), (0,1), (1,0), and (1,1) denote the elements of the group $\mathbb{Z}_2\times\mathbb{Z}_2$.

For this projective representation of $\mathbb{Z}_2\times\mathbb{Z}_2$ a simple computation shows that the central extension $\hat{G}$ of $\mathbb{Z}_2\times\mathbb{Z}_2$ is isomorphic to the dihedral group with eight elements. In the following it is sufficient to consider the definition of the representation on the elements ((0,1),1) and ((1,0),1) since these elements generate $\hat{G}=\{(g,h):g\in\mathbb{Z}_2\times\mathbb{Z}_2,h\in\{\pm 1\}\}$. We can choose

$$M = \begin{pmatrix} \alpha & \alpha & \beta & \beta \\ \beta & -\beta & \alpha & -\alpha \end{pmatrix} \in \mathbb{C}^{2\times 4}$$

or a matrix with the same columns (up to an arbitrary phase factor for each column). This leads to a symmetry group given by the monomial representation

$$\varphi_{\mathrm{mon}}((0,1),1) = \begin{pmatrix} \cdot & 1 & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & 1 & \cdot \end{pmatrix} \quad \text{and} \quad \varphi_{\mathrm{mon}}((1,0),1) = \begin{pmatrix} \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & -1 \\ 1 & \cdot & \cdot & \cdot \\ \cdot & -1 & \cdot & \cdot \end{pmatrix}.$$

For a different choice of phase factors we obtain another representation φ_{mon}. The modified pair of representations φ, φ_{mon} also defines a symmetry of M.

An important special case of group-covariant POVMs are *group-generated* POVMs which we describe next. Let G be a group and $\varphi: G \to \mathbb{C}^{d\times d}$ an (ordinary) unitary representation. A group-generated POVM is described by the POVM vectors $\varphi(g)|\Psi\rangle$ for $g \in G$ and an initial vector $|\Psi\rangle \in \mathbb{C}^d$. The corresponding operators of the POVM are given by $A_g = \varphi(g)|\Psi\rangle\langle\Psi|\varphi(g)^\dagger$ for $g \in G$. In other words, all POVM vectors are obtained by the initial vector $|\Psi\rangle$ under the operation of the group G, i.e., they form an orbit. Obviously, a group-generated POVM is a group-covariant POVM with a single orbit under the action of the group. With this construction, the phase factors of the POVM vectors $\varphi(g)|\Psi\rangle$ are fixed by the phase factor of the initial vector $|\Psi\rangle$. The phase factors $e^{i\phi(g,k)}$ of the monomial representation φ_{mon} corresponding to φ equal 1. As a consequence, the monomial representation φ_{mon} equals the regular representation of G with respect to a fixed order of the elements of G.

Note that the operators $\{\varphi(g)|\Psi\rangle\langle\Psi|\varphi(g)^\dagger\}$ in general do not define a POVM for arbitrary representations φ and initial vectors $|\Psi\rangle$. However, if φ acts irreducibly one has (after appropriate normalization) for every vector $|\Psi\rangle$ the equation $\Sigma_{g\in G}\varphi(g)|\Psi\rangle\langle\Psi|\varphi(g)^\dagger = \mathbf{1}_d$.

IV. CONSTRUCTION OF THE ORTHOGONAL MEASUREMENT

Following the preceding section we can arrange the vectors which correspond to the elements of a POVM with rank-one projectors into the columns of a matrix M. We have seen that in case of a group-covariant POVM the matrix $M \in \mathbb{C}^{d\times n}$ always has the symmetry $\varphi M = M\varphi_{\mathrm{mon}}$ where φ is the given representation and φ_{mon} is a monomial representation. Both representations are representations of the symmetry group of the group-covariant POVM. We know that both representations are equivalent to direct sums of irreducible representations. Hence we can find unitary matrices U and W such that $U\varphi U^\dagger = \varphi_1 \oplus \cdots \oplus \varphi_n$ and $W\varphi_{\mathrm{mon}}W^\dagger = \sigma_1 \oplus \cdots \oplus \sigma_m$ where the φ_k and the σ_l denote irreducible representations of the group G. In general, we can write the equation $\varphi M = M\varphi_{\mathrm{mon}}$ as

$$U^\dagger(\varphi_1 \oplus \cdots \oplus \varphi_n)UM = MW^\dagger(\sigma_1 \oplus \cdots \oplus \sigma_m)W.$$

This is equivalent to $C = UMW^\dagger \in T := \mathrm{Int}(\varphi_1 \oplus \cdots \oplus \varphi_n, \sigma_1 \oplus \cdots \oplus \sigma_m)$. Conversely, a matrix C which is contained in this intertwining space and has orthogonal rows defines (up to an appropriate normalization) a group-covariant POVM with corresponding matrix $M = U^\dagger CW$.

For a given matrix $M \in \mathbb{C}^{d\times n}$ we now consider the construction of a unitary matrix $\tilde{M} \in \mathcal{U}(n)$ such that $\tilde{M}$ contains M as the upper part, i.e., we are looking for a matrix $\tilde{M}$ such that

$$\tilde{M} = \begin{pmatrix} M \\ N \end{pmatrix},$$

where $N \in \mathbb{C}^{(n-d)\times n}$. In addition to this we intend to get the symmetry $(\varphi \oplus \varphi')\tilde{M} = \tilde{M}\varphi_{\mathrm{mon}}$ with an appropriate representation $\varphi': G \to \mathcal{U}(n-d)$. If we succeed in constructing an appropriate representation φ' and matrix $\tilde{M}$ then we have the equation $\varphi \oplus \varphi' = \tilde{M}\varphi_{\mathrm{mon}}\tilde{M}^\dagger$, i.e., the representation

$\varphi \oplus \varphi'$ must be equivalent to φ_{mon}. In other words, each irreducible representation of G is contained the same number of times in $\varphi \oplus \varphi'$ and in φ_{mon}. Furthermore, from the decompositions $(U \oplus \mathbf{1}_{n-d})(\varphi \oplus \varphi')(U^\dagger \oplus \mathbf{1}_{n-d}) = \sigma_{\pi(1)} \oplus \cdots \oplus \sigma_{\pi(m)}$ and $W\varphi_{\mathrm{mon}}W^\dagger = \sigma_1 \oplus \cdots \oplus \sigma_m$ we obtain that

$$(U \oplus \mathbf{1})\widetilde{M}W^\dagger \in \widetilde{T} := \mathrm{Int}(\sigma_{\pi(1)} \oplus \cdots \oplus \sigma_{\pi(m)}, \sigma_1 \oplus \cdots \oplus \sigma_m) \subseteq \mathbb{C}^{n\times n}. \tag{1}$$

The permutation τ used in Eq. (1) is a suitable reordering of the irreducible representations. The structure of the intertwining space $\widetilde{T}$ is known from Theorem 2 since we can compute the irreducible representations σ_j from φ_{mon}.

In the following discussion we consider the construction of φ' and $\widetilde{M}$. Our goal is to show that the construction of φ' that makes $U\varphi U^\dagger \oplus \varphi'$ equal to $W\varphi_{\mathrm{mon}}W^\dagger$ up to a permutation τ of the irreducible components is always possible.

Important for the extension of M to $\widetilde{M}$ will be the following theorem which characterizes the relations of two representations in case there is an intertwiner of maximal possible rank. Recall that ψ_1 is a constituent of ψ_2 if and only if there is a base change U such that $U^{-1}\psi_2(g)U = \psi_1(g) \oplus \psi_1'(g)$ where ψ_1' is a representation of G.

Theorem 5: *Let G be a finite group and let ψ_1, ψ_2 be representations of G of dimensions $d_1 = \deg(\psi_1)$ and $d_2 = \deg(\psi_2)$, respectively. Let $M \in \mathbb{C}^{d_1\times d_2}$ be a matrix with $\psi_1(g)M = M\psi_2(g)$ for all $g \in G$ and $\mathrm{rk}(M) = \deg(\psi_1)$. Then ψ_1 is a constituent of ψ_2.*

Proof: Let M be such that $\psi_1(g)M = M\psi_2(g)$ and let $\varphi_1, \ldots, \varphi_k$ be a complete set of pairwise inequivalent irreducible representations of G. Since ψ_1, ψ_2 are representations of a finite group over the field of complex numbers we find unitary matrices U, W such that $U\psi_1 U^\dagger = \oplus_{i=1}^k m_i\varphi_i$ and $W\psi_2 W^\dagger = \oplus_{i=1}^k n_i\varphi_i$, where the multiplicities m_i and n_i are non-negative integers. We must show that actually $m_i \leq n_i$ for all $i = 1, \ldots, k$.

From $\psi_1 M = M\psi_2$ and the choice of U and W we obtain $(\oplus m_i\varphi_i)(UMW^\dagger) = (UMW^\dagger)(\oplus n_i\varphi_i)$, i.e., we have that $UMW^\dagger \in \mathrm{Int}(\oplus_{i=1}^k m_i\varphi_i, \oplus_{i=1}^k n_i\varphi_i)$. By the remarks following Theorem 2 we know that there are permutation matrices P and Q such that $M_0 := P(UMW^\dagger)Q = (\mathbf{1}_{\deg(\varphi_1)} \otimes B_1) \oplus \cdots \oplus (\mathbf{1}_{\deg(\varphi_k)} \otimes B_k)$ where each $B_i \in \mathbb{C}^{m_i\times n_i}$. Multiplication with invertible matrices preserves the property that M and hence also M_0 have full rank [given by $\deg(\psi_1)$]. On the other hand, we know that the rank of a block diagonal matrix is given by the sum of the ranks of the blocks. Hence $\mathrm{rk}(M_0) = \Sigma_{i=1}^k \deg(\varphi_i) \cdot \mathrm{rk}(B_i)$ which shows that each B_i must have full rank. Since B_i is an $m_i \times n_i$ matrix this in particular implies that $m_i \leq n_i$. This shows that ψ_1 is a constituent of ψ_2.

We now use Eq. (1) to construct the matrix $\widetilde{M}$ for the implementation of a group-covariant POVM. Having determined U and W we can compute the matrix $C = UMW^\dagger \in \mathrm{Int}(U\varphi U^\dagger, W\varphi_{\mathrm{mon}}W^\dagger)$. The multiplicity of each irreducible representation in φ' can be computed. Since the structure of the intertwining space $\widetilde{T} = \mathrm{Int}(U\varphi U^\dagger \oplus \varphi', W\varphi_{\mathrm{mon}}W^\dagger)$ is known we can extend C to an arbitrary unitary matrix $\widetilde{C}$ of the intertwining space $\widetilde{T}$. This extension is always possible since both representations $U\varphi U^\dagger \oplus \varphi'$ and $W\varphi_{\mathrm{mon}}W^\dagger$ contain each irreducible representation the same number of times. The matrix C defines some of the rows of A. Since M defines a POVM the rows are mutually orthogonal. Consequently, the matrix components of $\widetilde{C}$ corresponding to an irreducible representation can be chosen under the constraint that they are orthogonal. We now have that for any $V \in \mathcal{U}(n-d)$ the matrix $\widetilde{M} = (U^\dagger \oplus V^\dagger)\widetilde{C}W$ yields a unitary that extends the matrix M and has the symmetry we wanted to construct.

Hence, we obtain the following algorithm to construct an orthogonal measurement which realizes the given POVM and preserves the symmetry.

Algorithm 6: Let $P = \{A_1, \ldots, A_n\} \subseteq \mathbb{C}^{d\times d}$ be a POVM. Then the following steps implement P by a von Neumann measurement on a larger space.

(1) Write the rank-one operators $A_k = |\Psi_k\rangle\langle\Psi_k|$ of the POVM as columns of the matrix $M \in \mathbb{C}^{d\times n}$.
(2) Determine an appropriate symmetry group with corresponding representation $\varphi: G \to \mathcal{U}(d)$.
(3) Compute the monomial representation $\varphi_{\mathrm{mon}}: G \to \mathcal{U}(n)$.

(4) Find a matrix $U \in \mathcal{U}(d)$ that decomposes φ into irreducible representations where equivalent ones are equal.
(5) Find a matrix $W \in \mathcal{U}(n)$ that decomposes φ_{mon} into irreducible representations where equivalent ones are equal.
(6) Construct the representation φ' such that $U\varphi U^\dagger \oplus \varphi'$ is equal to $W\varphi_{\mathrm{mon}}W^\dagger$ up to a permutation τ of the irreducibles.
(7) Construct $\widetilde{C} \in \mathcal{U}(n)$ that contains $C = UMW^\dagger \in \mathbb{C}^{d\times n}$ as upper part and is in the intertwining space $\widetilde{T}$ of $U\varphi U^\dagger \oplus \varphi'$ and $W\varphi_{\mathrm{mon}}W^\dagger$.
(8) Choose an arbitrary unitary matrix $V \in \mathcal{U}(n-d)$.
(9) Compute $\widetilde{M} = (U^\dagger \oplus V^\dagger)\widetilde{C}W \in \mathcal{U}(n)$.

Then $\widetilde{M}^\dagger$ implements the POVM P by a von Neumann measurement on a larger space, i.e., for any state ρ on the original d-dimensional system we have that $p_k = \mathrm{tr}(\widetilde{\rho}\widetilde{A}_k) = \langle \widetilde{\Psi}_k | \widetilde{\rho} | \widetilde{\Psi}_k \rangle$. Here $|\widetilde{\Psi}_k\rangle$ denote the rows of $\widetilde{M}$ and $\widetilde{\rho} = \rho \oplus 0_{n-d}$ is the embedding of ρ to a state of an n-dimensional system.

Example 7: We consider the example of the preceding section with the matrix

$$M = \begin{pmatrix} \alpha & \alpha & \beta & \beta \\ \beta & -\beta & \alpha & -\alpha \end{pmatrix} \in \mathbb{C}^{2\times 4}$$

and the group $G = \{(g,h) : g \in \mathbb{Z}_2 \times \mathbb{Z}_2, h \in \{\pm 1\}\}$ which is isomorphic to the dihedral group of order eight. The representation $\varphi : G \to \mathcal{U}(2)$ is given by $\varphi((0,1),1) = \sigma_z$ and $\varphi((1,0),1) = \sigma_x$. We have $U = \mathbf{1}_2$ and $U\varphi U^\dagger = \varphi$ since the representation φ is already irreducible. An elementary computation shows that the corresponding monomial representation φ_{mon} is given by

$$W\varphi_{\mathrm{mon}}((0,1),1)W^\dagger = \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & -1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & -1 \end{pmatrix}, \quad W\varphi_{\mathrm{mon}}((1,0),1)W^\dagger = \begin{pmatrix} \cdot & 1 & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & 1 & \cdot \end{pmatrix}$$

with the unitary matrix

$$W = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & -1 \\ \cdot & \cdot & 1 & 1 \\ 1 & -1 & \cdot & \cdot \end{pmatrix} \in \mathcal{U}(4).$$

Therefore, φ_{mon} contains the irreducible representation φ twice, i.e., $W\varphi_{\mathrm{mon}}W^\dagger = \varphi \oplus \varphi$.

With the matrices $M \in \mathbb{C}^{2\times 4}$, $U \in \mathcal{U}(2)$ and $W \in \mathcal{U}(4)$ as above we find that $C = UMW^\dagger = \sqrt{2}(\alpha\ \beta) \otimes \mathbf{1}_2 \in \mathbb{C}^{2\times 4}$, which is an element of the intertwining space

$$\mathrm{Int}(\varphi, W\varphi_{\mathrm{mon}}W^\dagger) = \mathrm{Int}(\varphi, \varphi \oplus \varphi).$$

Since we have $W\varphi_{\mathrm{mon}}W^\dagger = \varphi \oplus \varphi$, we must choose $\varphi' = \varphi$. The intertwining space $\widetilde{T}$ is given by

$$\widetilde{T} = \mathrm{Int}(\varphi \oplus \varphi, \varphi \oplus \varphi) = \left\{ \begin{pmatrix} \lambda_{11} & \cdot & \lambda_{12} & \cdot \\ \cdot & \lambda_{11} & \cdot & \lambda_{12} \\ \lambda_{21} & \cdot & \lambda_{22} & \cdot \\ \cdot & \lambda_{21} & \cdot & \lambda_{22} \end{pmatrix} : \lambda_{ij} \in \mathbb{C} \right\} \subseteq \mathbb{C}^{4\times 4}.$$

In our example, the matrix $C = UMW^\dagger$ defines the first two rows of the matrix $\widetilde{C} \in \widetilde{T} = \mathrm{Int}(\varphi \oplus \varphi, \varphi \oplus \varphi)$.

In particular, we have the equations $\lambda_{11} = \sqrt{2}\alpha$ and $\lambda_{12} = \sqrt{2}\beta$. For example, it is possible to choose $\lambda_{21} = \sqrt{2}\overline{\beta}$ and $\lambda_{22} = -\sqrt{2}\overline{\alpha}$ for $\alpha, \beta \in \mathbb{C}$ to obtain the unitary matrix

$$\tilde{C} = \sqrt{2}\begin{pmatrix} \alpha & \cdot & \beta & \cdot \\ \cdot & \alpha & \cdot & \beta \\ \overline{\beta} & \cdot & -\overline{\alpha} & \cdot \\ \cdot & \overline{\beta} & \cdot & -\overline{\alpha} \end{pmatrix} \in \mathcal{U}(4),$$

which has the symmetry $(\varphi \oplus \varphi)\tilde{C} = \tilde{C}(\varphi \oplus \varphi)$. With $\tilde{M} = (U^\dagger \oplus V^\dagger)\tilde{C}W$ and $V = \mathbf{1}_2$ we compute the matrix

$$\tilde{M} = \begin{pmatrix} \alpha & \alpha & \beta & \beta \\ \beta & -\beta & \alpha & -\alpha \\ \overline{\beta} & \overline{\beta} & -\overline{\alpha} & -\overline{\alpha} \\ -\overline{\alpha} & \overline{\alpha} & \overline{\beta} & -\overline{\beta} \end{pmatrix} \in \mathcal{U}(4)$$

that contains M as the upper part and has the symmetry $(\varphi \oplus \varphi)\tilde{M} = \tilde{M}\varphi_{\mathrm{mon}}$. Note that all unitary matrices $V \in \mathcal{U}(2)$ give rise to possible extensions $\tilde{M}$.

V. EFFICIENT IMPLEMENTATIONS OF GROUP-COVARIANT POVMs

From the general construction of a von Neumann measurement which realizes a given POVM using the symmetry of the POVM we now turn to the question of decomposing the unitary $\tilde{M}$ into gates. This can be seen as a first step towards the more general question of how POVMs can be implemented efficiently on a quantum computer.

When speaking about the efficiency, we mean the cost of implementing the POVM as a von Neumann measurement on a larger Hilbert space, i.e., the number of elementary gates we need to actually implement the necessary unitary operation on this bigger space. First note that the discussed construction of $\tilde{M}$ has several degrees of freedom:

(i) The matrix $\tilde{C}$ that contains C as upper part can be chosen arbitrarily. The matrix $\tilde{C}$ has to be a unitary matrix in the intertwining space $\tilde{T}$.
(ii) The matrix $V \in \mathcal{U}(n-d)$ can be an arbitrary unitary matrix.
(iii) The order and phase factors of the POVM vectors in the matrix M can be chosen arbitrarily. However, it must be possible to deduce the applied POVM operator from the result of the orthogonal measurement efficiently.
(iv) The permutation τ of the irreducible representations in $U\varphi U^\dagger \oplus \varphi'$ can be chosen arbitrarily.
(v) The symmetry group G can be restricted to subgroups $H \leqslant G$ which might lead to different realizations of the POVM.

The constructions depend on the symmetry group G we consider for the POVM. Sometimes, we can obtain simple implementations by restricting the symmetry group to a subgroup $H \leqslant G$. If we consider a subgroup H of G and construct the POVM with respect to H we have several changes in the construction compared to the construction with the group G. On the one hand, the number of occurrences of the irreducible representations in φ_{mon} increase. On the other hand, the number of inequivalent irreducible representations of the symmetry group decreases. Consequently, the matrices of the intertwining spaces are more complex since there are more irreducible representations in φ and φ_{mon} that are equivalent. As a tradeoff we have that the complexity of the transform W decreases. The circuits constructed in Ref. 14 show that the restriction of the symmetry group to a cyclic subgroup can lead to efficient algorithms in some cases.

Let G be a finite group and $\{\varphi_1, \ldots, \varphi_k\}$ a system of representatives for the irreducible representations of G. Let the coefficients of these representation be indexed by the list $L' := [(m;i,j), 1 \leqslant m \leqslant k, 1 \leqslant i,j \leqslant \deg(\varphi_m)]$. Furthermore, let the elements of G be indexed by the list L. Then the matrix

$$1/\sqrt{|G|}(\sqrt{\deg(\varphi_m)}\varphi_m(g)_{ij})_{(m;i,j),g}$$

is unitary and is called a Fourier transform (or DFT for short) for G (Refs. 27 and 28) (with respect to L and L').

For several groups it is known how to realize a DFT efficiently on a quantum computer.[29–31] In these cases the symmetry φ_{mon} can be decomposed efficiently whenever we have that (i) φ_{mon} is a regular representation of G and that (ii) the DFT for G can be computed efficiently. Note that the computational complexity of this von Neumann measurement depends essentially on the complexity of implementing DFT_G in terms of elementary quantum gates. Hence we obtain several families of POVMs for which the monomial representation φ_{mon} can be decomposed efficiently. The complexity of the corresponding POVM then depends on the remaining matrices C, U, and W used in Algorithm 6.

VI. EXAMPLES

In this section we apply the methods discussed in the preceding sections to some examples of group-covariant POVMs. We exploit the symmetry of group-covariant POVMs with respect to cyclic groups, dihedral groups, and Weyl–Heisenberg groups in order to construct quantum circuits for the implementation of these POVMs. Quantum circuits for the implementation of group-covariant POVMs on a single qubit with respect to the cyclic and dihedral groups are also discussed in Ref. 14.

A. Cyclic groups

Let $\mathbb{Z}_n=\{0,1,\ldots,n-1\}$ be a cyclic group with n elements and let $\omega=\exp(2\pi i/n)$ be a primitive nth root of unity. On a d-dimensional Hilbert space we consider a group-generated POVM with respect to the representation $\varphi:\mathbb{Z}_n\to\mathcal{U}(d)$ that is defined on the generator by $\varphi(1)=\mathrm{diag}(1,\omega,\omega^2,\ldots,\omega^{d-1})$. With an appropriate initial vector $|\Psi\rangle\in\mathbb{C}^d$ the elements $\varphi(g)|\Psi\rangle$ for $g\in\mathbb{Z}_n$ define a POVM. In the following, we only consider the vector $|\Psi\rangle=1/\sqrt{n}(1,\ldots,1)^T\in\mathbb{C}^d$. This vector leads to the POVM with the defining matrix

$$M=\frac{1}{\sqrt{n}}\begin{pmatrix}1 & 1 & 1 & \ldots & 1\\ 1 & \omega & \omega^2 & \ldots & \omega^{n-1}\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 1 & \omega^{d-1} & \omega^{2(d-1)} & \ldots & \omega^{(n-1)(d-1)}\end{pmatrix}\in\mathbb{C}^{d\times n}. \tag{2}$$

The matrix $M\in\mathbb{C}^{d\times n}$ has the symmetry $\varphi M=M\varphi_{\mathrm{mon}}$ where $\varphi_{\mathrm{mon}}(1)=(1,2,\ldots,n)$. The representation φ_{mon} is the regular representation of the cyclic group where the elements are ordered as $[0,1,\ldots,(n-1)]$. With the Fourier matrix

$$F_n=\frac{1}{\sqrt{n}}(\omega^{jk})_{j,k=0}^{n-1}\in\mathcal{U}(n)$$

we can write $F_n\varphi_{\mathrm{mon}}(1)F_n^\dagger=\mathrm{diag}(1,\omega,\omega^2,\ldots,\omega^{n-1})$. This shows that the Fourier transform decomposes the regular representation of $\mathbb{Z}_n$ into a direct sum of irreducible representations.

According to the preceding discussion (and notation) we have that $U=\mathbf{1}_d$ and $W=F_n$. As a consequence we have the equation $\mathbf{C}=UMW^\dagger=MF_n^\dagger$. More precisely, we have $C=MF_n^\dagger=\mathrm{diag}(1,1,\ldots,1)\in\mathbb{C}^{d\times n}$.

We now consider the construction of the matrices $\tilde{C}$ and $\tilde{M}$. The representation $\varphi:\mathbb{Z}_n\to\mathcal{U}(d)$ with $\varphi(1)=\mathrm{diag}(1,\omega,\omega^2,\ldots,\omega^{d-1})$ contains the irreducible representations $1\mapsto(\omega^k)$ for all $k\in\{0,\ldots,d-1\}$. The representation $F_n\varphi_{\mathrm{mon}}F_n^\dagger:\mathbb{Z}_n\to\mathcal{U}(n)$ with $F_n\varphi_{\mathrm{mon}}(1)F_n^\dagger=\mathrm{diag}(1,\omega,\omega^2,\ldots,\omega^{n-1})$ contains the irreducible representations $1\mapsto(\omega^k)$ for all $k\in\{0,1,\ldots,n-1\}$. Following Algorithm 6 from Sec. IV, we choose φ' with $\varphi'(1)=\mathrm{diag}(\omega^d,\ldots,\omega^{n-1})$ in order

to obtain $\varphi \oplus \varphi' = F_n \varphi_{\mathrm{mon}} F_n^\dagger$. Since each irreducible representation $1 \mapsto (\omega^k)$ with $k \in \{0,1,\ldots,n-1\}$ has dimension one and the irreducible representations defined by $1 \mapsto (\omega^k)$ are inequivalent for different k we have the intertwining space

$$\widetilde{T} = \mathrm{Int}(\varphi \oplus \varphi', F_n \varphi_{\mathrm{mon}} F_n^\dagger) = \{\mathrm{diag}(\lambda_1, \ldots, \lambda_n) : \lambda_j \in \mathbb{C}\} \subseteq \mathbb{C}^{n \times n}.$$

We have to find a matrix $\widetilde{C} \in \mathcal{U}(n)$ in the intertwining space $\widetilde{T}$ that has the matrix $C \in \mathbb{C}^{d \times n}$ as upper part. As stated above, the matrix $M \in \mathbb{C}^{d \times n}$ defines $\lambda_j = 1$ for $j \in \{0,1,\ldots,d-1\}$. Since $\widetilde{C}$ has to be a unitary matrix we must choose λ_j with the absolute value $|\lambda_j| = 1$ for $j \in \{d,\ldots,n-1\}$.

In order to simplify the matrices we set $\lambda_j = 1$ for all $j \in \{d,\ldots,n-1\}$. With these elements λ_j we have the equation $\widetilde{C} = \mathbf{1}_n$. Furthermore, we choose $V = \mathbf{1}_{n-d}$ in Algorithm 6 from Sec. IV leading to $U \oplus V = \mathbf{1}_n$. Consequently, we obtain the equation

$$\widetilde{M}^\dagger = W^\dagger \widetilde{C}^\dagger (U \oplus V) = F_n^\dagger \mathbf{1}_n \mathbf{1}_n = F_n^\dagger.$$

This equation shows that the inverse Fourier transform $\widetilde{M}^\dagger = F_n^\dagger$ is a unitary transform that implements the group-covariant POVM with defining matrix (2). Recall that for $n = 2^k$ where $k \in \mathbb{N}$ the Fourier transform can be implemented efficiently on a qubit register.[32,33]

B. Dihedral groups

Let $D_{2m} = \langle r, s : r^m = 1, s^2 = 1, srs^{-1} = r^{-1} \rangle$ be the dihedral group[34] with $n = 2m = 2^{k+1}$ elements for a fixed $m = 2^k \geqslant 4$. The element r denotes the rotation and s the reflection of the dihedral group. We consider the irreducible representation $\varphi : D_{2m} \to \mathcal{U}(2)$ that is defined by

$$\varphi(r) = \begin{pmatrix} \omega & 0 \\ 0 & \omega^{-1} \end{pmatrix} \quad \text{and} \quad \varphi(s) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The element $\omega = \exp(2\pi i/m)$ is an mth root of unity. For $\alpha, \beta \in \mathbb{C}$ with $|\alpha|^2 + |\beta|^2 = 1/m$ we consider the POVM with the corresponding matrix

$$M = \begin{pmatrix} \alpha & \ldots & \alpha & \beta & \ldots & \beta \\ \beta & \ldots & \beta\omega^{m-1} & \alpha & \ldots & \alpha\omega^{m-1} \end{pmatrix} \in \mathbb{C}^{2 \times n}.$$

The matrix $M \in \mathbb{C}^{2 \times n}$ has the symmetry $\varphi M = M \varphi_{\mathrm{mon}}$ where φ_{mon} is defined by the equations $\varphi_{\mathrm{mon}}(r) = \mathbf{1}_2 \otimes \omega S_m^{-2}$ and $\varphi_{\mathrm{mon}}(s) = \sigma_x \otimes F_m^2 T_m$. The matrices $S_m, T_m \in \mathbb{C}^{m \times m}$ are defined by the equations (indices are taken modulo m)

$$S_m = \sum_{i=0}^{m-1} |i+1\rangle\langle i|, \quad T_m = \sum_{i=0}^{m-1} \omega^i |i\rangle\langle i|,$$

and F_m denotes the discrete Fourier transform defined in the preceding section. In order to decompose φ_{mon} into irreducibles the following permutation Q_k is useful. Denoting by $\overline{x}$ the binary complement of the binary vector x of length k we define $Q_k : |x,0\rangle \mapsto |x,0\rangle$ and $Q_k : |x,1\rangle \mapsto |\overline{x},1\rangle$. Furthermore, we introduce the representations φ_l defined by

$$\varphi_l(r) = \begin{pmatrix} \omega^l & 0 \\ 0 & \omega^{-l} \end{pmatrix} \quad \text{and} \quad \varphi_l(s) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

With this notation we have $\varphi = \varphi_1$. The two-dimensional representations φ_l are irreducible and inequivalent[34] for different $l \in \{1,\ldots,m/2\}$. Now, using the base change $W := Q_m(\mathbf{1}_2 \otimes F_m^\dagger) \in \mathbb{C}^{n \times n}$ we obtain that

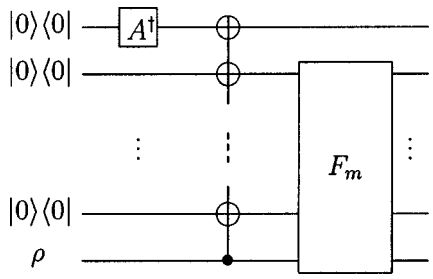

FIG. 1. Quantum circuit for the implementation of the dihedral POVM.

$$W\varphi_{\mathrm{mon}}W^\dagger = \psi \oplus \psi \oplus \psi \oplus \psi,$$

where ψ is a direct sum of all representations φ_j with odd j. The first component of ψ is φ_1, the other components φ_j appear in a specific order which is irrelevant in the sequel. We choose the representation

$$\varphi' = \psi' \oplus \psi \oplus \psi \oplus \psi,$$

where ψ' is obtained from ψ by dropping φ_1. This leads to $\varphi \oplus \varphi' = W\varphi_{\mathrm{mon}}W^\dagger$. The matrix $C = MW^\dagger = (\sqrt{m}\alpha\ 0\cdots 0 \,|\, \sqrt{m}\beta\ 0\cdots 0) \otimes \mathbf{1}_2 \in \mathbb{C}^{2\times n}$ defines the first two rows of the intertwining matrix $\widetilde{C}$ we want to construct according to Algorithm 6 from Sec. IV. A possible extension of the intertwining matrix $C \in \mathbb{C}^{2\times n}$ to a unitary matrix $\widetilde{C} \in \mathcal{U}(n)$ is $\widetilde{C} = A \otimes \mathbf{1}_{m/2}$ with the matrix

$$A = \sqrt{m}\begin{pmatrix} \alpha & \beta \\ \overline{\beta} & -\overline{\alpha} \end{pmatrix} \in \mathcal{U}(2).$$

According to Algorithm 6 from Sec. IV we must define the matrices $U \in \mathcal{U}(2)$ and $V \in \mathcal{U}(n-2)$. The equations $\varphi = \varphi_1$ and $W\varphi_{\mathrm{mon}}W^\dagger = (\varphi_1 \oplus \psi') \oplus \psi \oplus \psi \oplus \psi$ show that $U = \mathbf{1}_2$. Furthermore, we choose $V = \mathbf{1}_{n-2}$. Then we have the matrix $U \oplus V = \mathbf{1}_n$. To summarize, we must implement the matrix

$$\widetilde{M}^\dagger = W^\dagger \widetilde{C}^\dagger = (\mathbf{1}_2 \otimes F_m) Q_k (A^\dagger \otimes \mathbf{1}_4) \in \mathcal{U}(n)$$

in order to measure the POVM corresponding to the dihedral group D_m. The scheme of the circuit corresponding to $\widetilde{M}^\dagger$ is shown in Fig. 1.

C. Weyl–Heisenberg groups

In the following we introduce the finite Weyl–Heisenberg groups which are matrix groups acting on a finite-dimensional vector space. For our purposes we consider vector spaces of dimension $m = 2^k$ only, where $k \geq 2$. Then the Weyl–Heisenberg group G_m is the group generated by the matrices $S_m = (1, 2, \ldots, m)$ and $T_m = \mathrm{diag}(1, \omega, \omega^2, \ldots, \omega^{m-1})$ where $\omega = \exp(2\pi i/m) \in \mathbb{C}$ is a primitive mth root of unity. It is known that G_m contains m^3 elements.[35] POVMs that are covariant with respect to the Weyl–Heisenberg groups have a physical motivation. Since the position and momentum of a particle cannot be measured simultaneously by any projection-valued measurement one must construct POVMs which measure both observables with a certain inaccuracy. This idea has already been described in Ref. 19 starting from a wave packet, i.e., a unit vector $|\psi\rangle \in L^2(\mathbb{R})$ we define a set $\{M_{s,t}\}$ of operators by

$$M_{s,t} := \frac{1}{2\pi} e^{isP+tQ} |\psi\rangle\langle\psi| e^{-isP-tQ},$$

where $s,t \in \mathbb{R}$ and P and Q are the position and momentum operators, respectively. Explicitly, they are defined by $(P\psi)(x) := -i(d/\mathrm{d}x)\psi(x)$ and $(Q\psi)(x) := x\psi(x)$. We then have that

$$\int_{s,t} M_{s,t}\, \mathrm{d}s\, \mathrm{d}t = 1.$$

The POVM $\{M_{s,t}\}$ provides an approximative realization of the classical phase space since the measurement outcome (s,t) can be interpreted as the point (s,t) in the phase space. In the following we are interested in finite-dimensional approximations of this. Assume that we want to measure the position and crystal momentum of a particle on a lattice with m points for $m=2^k$.[36] Furthermore, we assume that it is possible to transfer the state of such a system into k qubits of a quantum register in the sense that one can implement the SWAP operations,

$$|j\rangle \otimes |i\rangle \leftrightarrow |i\rangle \otimes |j\rangle.$$

Here the left-hand vector denotes a joint state of particle and register where the particle is at position j in the lattice and the register is in its ith canonical basis state. The states corresponding to the vectors $\Sigma_{j=0}^{m-1} e^{2\pi i l j/m} |j\rangle$ with $l=0,\ldots,m-1$ are the eigenstates of the crystal momentum. Explicitly, the crystal momentum p can be defined by $p := 2\pi l/m - \pi$. With this definition the values of p are in the interval $[-\pi,\pi]$ that meets the usual physical intuition of the one-dimensional Brillouin zone of an infinite one-dimensional crystal. Here we characterize the position and momentum simply by the integer values j, $l=0,\ldots,m-1$. The cyclic translation of the position is given by the action of S_m and a change of crystal momentum by the action of T_m. Consider a rank-one positive operator $|\psi\rangle\langle\psi|$ with the property that neither the position nor the momentum of the corresponding state is completely undefined. Set

$$M_{j,l} := \frac{1}{m} S_m^j T_m^l |\psi\rangle\langle\psi| T_m^{-l} S_m^{-j}.$$

Due to irreducible group action the equation $\Sigma_{j,l} M_{j,l} = \mathbf{1}_m$ holds and the operators $M_{j,l}$ define a POVM. For large m we can find states with corresponding state vectors $|\psi\rangle$ such that both values j and l are approximately defined. Here the word "approximately" is understood with respect to the cyclic topology, i.e., $m-1$ and 0 are "almost" the same value. A good choice for the POVM will be the following. Set $|\psi\rangle := \Sigma_j c_j |j\rangle$ where the coefficients c_j are chosen such that the function $j \mapsto |c_j|^2$ has a unique maximum at j_0 and the modulus of the values c_j decrease with increasing distance from j_0 in the cyclic topology. If all values c_j are real and they decrease not too quickly the momentum l of the state is around j_0, too. Then the measurement values j,l can directly be interpreted as a good estimation for the position and momentum values. We will show that an efficient implementation of the POVM can be found in the case where $|\Psi\rangle = 1/\sqrt{\kappa}(1,\alpha,\alpha^2,\ldots,\alpha^{m/2-2},\alpha^{m/2-1},\alpha^{m/2-1},\alpha^{m/2-2},\ldots,\alpha^2,\alpha,1)^T \in \mathbb{C}^m$ with $\alpha \in \mathbb{C}$ and an appropriate normalization factor $1/\sqrt{\kappa}$.

In the following we consider the group-generated POVMs with respect to G_m and the natural representation φ defined by $\varphi(g)=g$ for all $g \in G_m$. This representation is irreducible. Therefore, following Algorithm 6 from Sec. IV we can set $U=\mathbf{1}_m$ since $\mathbf{1}_m$ decomposes φ into a direct sum of irreducible representations. The vector $|\Psi\rangle = (v_1,\ldots,v_m)^T \in \mathbb{C}^m$ with the normalization $|v_1|^2 + \cdots + |v_m|^2 = 1/m$ leads to the POVM where the defining matrix $M \in \mathbb{C}^{m\times n}$ is given by

$$\begin{pmatrix} v_1 & v_1 & \cdots & v_1 & v_m & \cdots & v_m & \cdots & v_2 & \cdots & v_2 \\ v_2 & v_2\omega & \cdots & v_2\omega^{m-1} & v_1 & \cdots & v_1\omega^{m-1} & \cdots & v_3 & \cdots & v_3\omega^{m-1} \\ & \vdots & \ddots & & & \ddots & & \ddots & & \ddots & \\ v_m & v_m\omega^{m-1} & \cdots & v_m\omega & v_{m-1} & \cdots & v_{m-1}\omega & \cdots & v_1 & \cdots & v_1\omega \end{pmatrix}.$$

Note that we identify vectors $g|\Psi\rangle$ and $h|\Psi\rangle$ for different $g,h \in G_m$ that are equal up to a global phase factor. Consequently, the POVM consists of at most $n=m^2$ different operators. For example, when $m=4$ the vector $|\Psi\rangle=(v_1,v_2,v_3,v_4)^T \in \mathbb{C}^4$ with $|v_1|^2+|v_2|^2+|v_3|^2+|v_4|^2=1/4$ leads to the POVM with $n=16$ operators and the corresponding matrix $M \in \mathbb{C}^{4\times 16}$ where M is defined by

$$\begin{pmatrix} v_1 & v_1 & v_1 & v_1 & v_4 & v_4 & v_4 & v_4 & \cdots & v_2 & v_2 & v_2 & v_2 \\ v_2 & v_2 i & -v_2 & -v_2 i & v_1 & v_1 i & -v_1 & -v_1 i & \cdots & v_3 & v_3 i & -v_3 & -v_3 i \\ v_3 & -v_3 & v_3 & -v_3 & v_2 & -v_2 & v_2 & -v_2 & \cdots & v_4 & -v_4 & v_4 & -v_4 \\ v_4 & -v_4 i & -v_4 & v_4 i & v_3 & -v_3 i & -v_3 & v_3 i & \cdots & v_1 & -v_1 i & -v_1 & v_1 i \end{pmatrix}.$$

The symmetry of $M \in \mathbb{C}^{m\times n}$ can be described on the generators by the equations $T_m M = M(\mathbf{1}_m \otimes S_m)$ and $S_m M = M(S_m \otimes T_m^\dagger)$. Therefore the representation $\varphi_{\mathrm{mon}}: G_m \to \mathcal{U}(n)$ is defined by $\varphi_{\mathrm{mon}}(T_m)=\mathbf{1}_m \otimes S_m$ and $\varphi_{\mathrm{mon}}(S_m)=S_m \otimes T_m^\dagger$. The symmetry of M can also be written as

$$T_m M = M(\mathbf{1}_m \otimes T_m)^{F_m^\dagger \otimes F_m} \quad \text{and} \quad S_m M = M(T_m^\dagger \otimes S_m)^{F_m^\dagger \otimes F_m},$$

where we use the notation $A^X = X^\dagger A X$ and the Fourier transform F_m as defined in Sec. VI A. We can write $(\mathbf{1}_m \otimes T_m)$ and $(T_m^\dagger \otimes S_m)$ as direct sums

$$(\mathbf{1}_m \otimes T_m) = T_m \oplus T_m \oplus \cdots \oplus T_m \quad \text{and} \quad (T_m^\dagger \otimes S_m) = S_m \oplus \omega^{m-1} S_m \oplus \cdots \oplus \omega S_m.$$

By using the equations $T_m S_m T_m^\dagger = \omega S_m$ and $(\mathbf{1}_m \otimes S_m)^{Z^\dagger} = (T_m^\dagger \otimes S_m)$ we can conjugate these matrices with the diagonal matrix $Z = \mathbf{1}_m \oplus T_m^{m-1} \oplus T_m^{m-2} \oplus \cdots \oplus T_m^2 \oplus T_m$ in order to obtain the equations

$$T_m M = M(\mathbf{1}_m \otimes T_m)^{Z^\dagger (F_m^\dagger \otimes F_m)} \quad \text{and} \quad S_m M = M(\mathbf{1}_m \otimes S_m)^{Z^\dagger (F_m^\dagger \otimes F_m)}.$$

These equations show that we have the decomposition $W \varphi_{\mathrm{mon}} W^\dagger = \varphi \oplus \cdots \oplus \varphi$ with the matrix $W = Z^\dagger (F_m^\dagger \otimes F_m)$. The representation $W \varphi_{\mathrm{mon}} W^\dagger$ contains m components φ. Following Algorithm 6 from Sec. IV we must find a representation φ' that leads to the direct sum $\varphi \oplus \varphi' = \varphi \oplus \cdots \oplus \varphi$ with m components φ. Consequently, we choose $\varphi' = \varphi \oplus \cdots \oplus \varphi$ with $m-1$ components φ. We now consider the extension of the matrix $C = MW^\dagger = M(F_m \otimes F_m^\dagger)Z \in \mathbb{C}^{m\times n}$ to a unitary matrix $\widetilde{C} \in \mathcal{U}(n)$. The matrix C is an element of the intertwining space,

$$\mathrm{Int}(\varphi, \varphi \oplus \cdots \oplus \varphi) = \{(\alpha_1, \ldots, \alpha_n) \otimes \mathbf{1}_m : \alpha_j \in \mathbb{C}\} \subseteq \mathbb{C}^{m\times n}.$$

More precisely, we have $C = ((\sqrt{m}v_1, \ldots, \sqrt{m}v_m)F_m^\dagger) \otimes \mathbf{1}_m \in \mathbb{C}^{m\times n}$. For example, for $m=4$ we obtain the group $G_4 = \langle S_4, T_4 \rangle$ with $S_4 = (1,2,3,4)$ and $T_4 = \mathrm{diag}(1,i,-1,-i)$ that contains 64 elements. In this example we have the equation

$$C = \left((v_1,v_2,v_3,v_4) \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -i & -1 & i \\ 1 & -1 & 1 & -1 \\ 1 & i & -1 & -i \end{pmatrix} \right) \otimes \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 \end{pmatrix} \in \mathbb{C}^{4\times 16}.$$

The matrix $C \in \mathbb{C}^{m\times n}$ determines the first m rows of the matrix $\widetilde{C}$ we want to construct. The matrix $\widetilde{C}$ is a unitary matrix of the intertwining space,

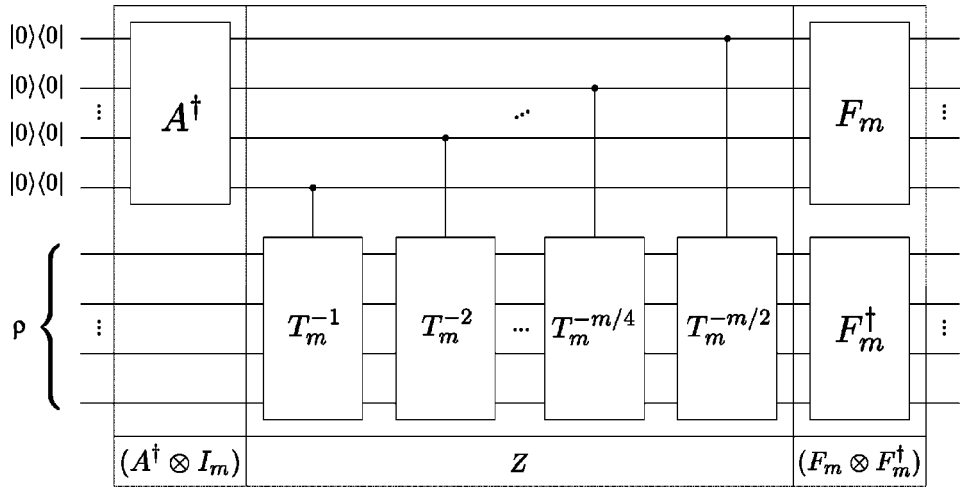

FIG. 2. Circuit for the implementation of the POVM with respect to the Weyl–Heisenberg group and the vector $|\Psi\rangle = (v_1, \ldots, v_m)^T$. The vector $|\Psi\rangle$ determines the matrix $A^\dagger$.

$$\mathrm{Int}(\varphi \oplus \cdots \oplus \varphi, \varphi \oplus \cdots \oplus \varphi) = \{A \otimes \mathbf{1}_m : A \in \mathbb{C}^{m\times m}\} \subseteq \mathbb{C}^{n\times n}.$$

When we write $\tilde{C} = A \otimes \mathbf{1}_m$ then the matrix C determines the first row of A. Explicitly, the first row of A is

$$(\sqrt{m}v_1, \ldots, \sqrt{m}v_m)F_m^\dagger. \tag{3}$$

The operation $\tilde{M}^\dagger$ for the implementation of the POVM is defined by

$$\tilde{M}^\dagger = W^\dagger \tilde{C}^\dagger (U \oplus V) = (F_m \otimes F_m^\dagger) Z (A^\dagger \otimes \mathbf{1}_m) \in \mathcal{U}(n).$$

In this equation we have $V = \mathbf{1}_{n-m}$ leading to $U \oplus V = \mathbf{1}_m \oplus \mathbf{1}_{n-m} = \mathbf{1}_n$. The general scheme for the implementation of the matrix $\tilde{M}^\dagger$ is shown in Fig. 2. For $m = 2^k$ the circuit contains the k controlled operations

$$T_m^{-1}, T_m^{-2}, \ldots, T_m^{-m/4}, T_m^{-m/2}$$

for the implementation of the matrix Z. The matrix $T_m = \mathrm{diag}(1, \omega, \omega^2, \ldots, \omega^{m-1})$ can be written as Kronecker product

$$T_m = \begin{pmatrix} 1 & 0 \\ 0 & \omega^{m/2} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & \omega^{m/4} \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} 1 & 0 \\ 0 & \omega \end{pmatrix} \in \mathcal{U}(m).$$

Therefore, the matrices T_m^j of the circuit in Fig. 2 can be implemented efficiently on a register of qubits.

The circuit in Fig. 2 is efficient if the matrix A that contains the vector (3) as the first row can be implemented efficiently. We can find such a matrix for the POVM with the vector

$$|\Psi\rangle = \frac{1}{\sqrt{\kappa}}(1, \alpha, \alpha^2, \ldots, \alpha^{m/2-2}, \alpha^{m/2-1}, \alpha^{m/2-1}, \alpha^{m/2-2}, \ldots, \alpha^2, \alpha, 1)^T \in \mathbb{C}^m, \tag{4}$$

where we have $\alpha \in \mathbb{C}$ and the normalization $\kappa = 2m(1 + |\alpha|^2 + |\alpha|^4 + \cdots + |\alpha|^{m-2})$. A matrix $A \in \mathcal{U}(m)$ that contains the vector (3) as the first row is given by

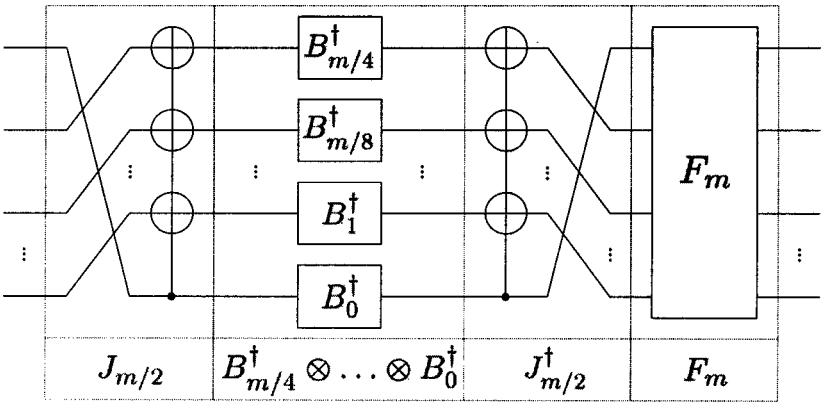

FIG. 3. Implementation of the matrix $A^\dagger$ where A is a matrix that contains the vector (3) as the first row. This matrix is part of the circuit in Fig. 2 for the vectors (4).

$$A = J^\dagger_{m/2}(B_{m/4} \otimes B_{m/8} \otimes \cdots \otimes B_4 \otimes B_2 \otimes B_1 \otimes B_0)J_{m/2}F^\dagger_m,$$

where we use the unitary matrices

$$B_j = \frac{1}{\sqrt{1+|\alpha|^{2j}}}\begin{pmatrix} 1 & \alpha^j \\ \overline{\alpha^j} & -1 \end{pmatrix} \in \mathcal{U}(2).$$

Here J_k is defined to be the permutation matrix which maps $2i \mapsto i$ and $(2i-1) \mapsto -i$ for $i = 0, \ldots, k$. In our example with $m=4$ we have the matrix

$$J^\dagger_2(B_1 \otimes B_0)J_2 = \frac{1}{\sqrt{2+2|\alpha|^2}}\begin{pmatrix} 1 & \alpha & \alpha & 1 \\ \overline{\alpha} & -1 & -1 & \overline{\alpha} \\ \overline{\alpha} & -1 & 1 & -\overline{\alpha} \\ 1 & \alpha & -\alpha & -1 \end{pmatrix}.$$

The circuit scheme for the implementation of the matrix

$$A^\dagger = F_m J^\dagger_{m/2}(B^\dagger_{m/4} \otimes B^\dagger_{m/8} \otimes \cdots \otimes B^\dagger_4 \otimes B^\dagger_2 \otimes B^\dagger_1 \otimes B^\dagger_0)J_{m/2}$$

is shown in Fig. 3.

VII. CONCLUSIONS AND OUTLOOK

We have shown that a group-covariant POVM can be reduced to an orthogonal measurements by a unitary transform which is symmetric in the sense that it intertwines two different group representations. The symmetry of the unitary transform can be used to derive decompositions which in several cases of interest (as the Weyl–Heisenberg group) leads to an efficient quantum circuit for the implementation of the POVM.

We have argued that POVMs are often necessary in order to understand why large quantum systems show typically classical behavior on the phenomenological level. The POVM with Weyl–Heisenberg symmetry as well as the example in Ref. 5 show that the POVMs which appear in this context are often covariant with respect to some group.

Besides the physical motivation to study implementations of POVMs by means of orthogonal measurements in terms of quantum circuits there is also a motivation from computer science. The so-called *hidden subgroup problem*[37] is an attractive generalization of the quantum algorithms for discrete logarithms and factoring.[38] The standard approach for the hidden subgroup problem consists in a Fourier transform for the respective group followed by a suitable post-processing on the Fourier coefficients.[39] For Abelian groups this post-processing consists simply in an orthogo-

nal measurement in the computational basis. However, for non-Abelian group measurements which are in fact POVMs are often more advantageous, see, e.g., Ref. 40. The POVMs which appear to be useful to solve hidden subgroup problems for non-Abelian groups are naturally group covariant. The methods presented in this paper might be useful to find quantum algorithms for the hidden subgroup problem for new classes of non-Abelian groups.

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Remarks on the spectrum of the Neumann problem with magnetic field in the half-space

Abderemane Morame[a)]
Départment de Mathématiques, Université de Nantes, Faculté des Sciences, UMR 6629 du CNRS, B.P. 99208, 44322 Nantes Cedex 3, France

Françoise Truc[b)]
Institut Fourier, Laboratoire de Mathématiques, UMR5582 (UJF-CNRS), B.P. 74, 38402 St. Martin D'Hères Cedex, France

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We consider a Schrödinger operator with a constant magnetic field in a one-half three-dimensional space, with Neumann-type boundary conditions. It is known from the works by Lu–Pan and Helffer–Morame that the lower bound of its spectrum is less than b, the intensity of the magnetic field, provided that the magnetic field is not normal to the boundary. We prove that the spectrum under b is a finite set of eigenvalues (each of infinite multiplicity). In the case when the angle between the magnetic field and the boundary is small, we give a sharp asymptotic expansion of the number of these eigenvalues. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1827922]

I. INTRODUCTION

Let us consider, for (t,x,y) in the half-space $E=\mathbb{R}_+\times\mathbb{R}^2$, the Neumann realization of the operator with magnetic field

$$H=(D_t-A_1)^2+(D_x-A_2)^2+(D_y-A_3)^2,$$

where $D_s=-i(\partial/\partial s)$.

We will assume that the magnetic field $B=\mathrm{d}A$, seen as a three-dimensional vector field, is not tangent to the boundary ∂E, and denote by θ the angle between B and the plane $t=0$ and by b the norm of B.

This implies that a suitable choice for the gauge A is the 1-form,

$$A=b(x\sin\theta-t\cos\theta)\mathrm{d}y$$

(so that $A_1=A_2=0$), since the condition $B=\mathrm{d}A$ leads to the 2-form,

$$B=b\sin\theta\,\mathrm{d}x\wedge\mathrm{d}y-b\cos\theta\,\mathrm{d}t\wedge\mathrm{d}y\quad\left(\theta\in\left[0,\frac{\pi}{2}\right]\right).$$

Now the operator H can be written as

$$H_\theta=D_t^2+D_x^2+(D_y-b(x\sin\theta-t\cos\theta))^2. \tag{1.1}$$

The spectrum of the Neumann operator H_0 (corresponding to the case $\theta=0$) is absolutely continuous, as proved by Lu and Pan.[10–12] More precisely one has

$$\sigma(H_0)=\sigma_{ac}(H_0)=[b\mu_0+\infty[, \tag{1.2}$$

[a)]Electronic mail: morame@math.univ-nantes.fr
[b)]Electronic mail: francoise.truc@ujf-grenoble.fr

$$\mu_0 = \inf_{\xi \in \mathbb{R}} \mu(\xi), \tag{1.3}$$

where $\mu(\xi)$ denotes the first eigenvalue of the Neumann operator $Q_\xi = D_t^2 + (t-\xi)^2$ on $L^2(\mathbb{R}_+)$,

$$\mu(\xi) = \inf \sigma(Q_\xi) = \inf_{\|f\|_{L^2(\mathbb{R}_+)}=1} \int_{\mathbb{R}_+} [|D_t f|^2 + (t-\xi)^2 |f|^2] \mathrm{d}t. \tag{1.4}$$

It is also shown in Refs. 10–12 that, if $\theta = \pi/2$, the spectrum of $H_{\pi/2}$ is absolutely continuous,

$$\sigma(H_{\pi/2}) = \sigma_{ac} = [b, +\infty[. \tag{1.5}$$

When $\theta \in]0, \pi/2[$, the spectrum of H_θ is no longer absolutely continuous (see Refs. 8–12). We are precisely interested in that case,

$$0 < \theta < \frac{\pi}{2}. \tag{1.6}$$

First, performing a partial Fourier transform in the variable y we observe that

$$\sigma(H_\theta) = \bigcup_{\tau \in \mathbb{R}} \sigma(H_{\theta,\tau}), \tag{1.7}$$

where $H_{\theta,\tau}$ denotes the Neumann realization in the half-plane $F = \mathbb{R}_+ \times \mathbb{R}$ of the operator,

$$H_{\theta,\tau} = D_t^2 + D_x^2 + (\tau - b(x \sin\theta - t\cos\theta))^2. \tag{1.8}$$

Furthermore, using for any τ the change of coordinates $x \to x - (\tau/b \sin\theta)$, we see that $\sigma(H_{\theta,\tau}) = \sigma(H_{\theta,0})$, and then the spectrum of H_θ is essential and given by

$$\sigma(H_\theta) = \sigma_{\mathrm{ess}}(H_\theta) = \sigma(H_{\theta,0}) = b \times \sigma(P_\theta), \tag{1.9}$$

if $P_\theta = D_t^2 + D_x^2 + (t\cos\theta - x\sin\theta)^2$ is the Neumann operator on the half-plane $F = \mathbb{R}_+ \times \mathbb{R}$.

In Refs. 9 and 12 it was proved that

$$\inf \sigma(P_\theta) = \nu(\theta) < 1 = \inf \sigma_{\mathrm{ess}}(P_\theta), \tag{1.10}$$

so there exists a countable set of eigenvalues of P_θ, $(\nu_j(\theta))_{j\in I}$, $(I \subset \mathbb{N})$, in $[\nu(\theta), 1[$. Each eigenvalue is of finite multiplicity, so we will assume that each one is repeated according to its multiplicity. The associated orthonormalized sequence of eigenfunctions will be denoted by $(\psi_{\theta,j})_{j\in I}$,

$$P_\theta \psi_{\theta,j} = \nu_j(\theta)\psi_{\theta,j},$$

$$\langle \psi_{\theta,j} | \psi_{\theta,k} \rangle = \delta_{jk},$$

$$E_{]-\infty,1[}(P_\theta) f = \sum_j \langle \psi_{\theta,j} | f \rangle \psi_{\theta,j}$$

[$\langle g | f \rangle = \int_F \overline{g} f \, \mathrm{d}t \, \mathrm{d}x$ and $E_J(P_\theta)$ denotes the spectral projection of P_θ on J]. Coming back to the operator (H_θ) we can write

$$\sigma(H_\theta) \cap \,]-\infty, b[= \{b\nu_1(\theta), b\nu_2(\theta), \ldots, b\nu_j(\theta), b\nu_{j+1}(\theta), \ldots\}, \tag{1.11}$$

where each $b\nu_j(\theta)$ is now an eigenvalue of infinite multiplicity of H_θ.

For any $d \leqslant 1$ let us denote by $N(d, P_\theta)$ the number of eigenvalues of P_θ in $]-\infty, d[$,

$$N(d, P_\theta) = \mathrm{Tr}(E_{]-\infty,d[}(P_\theta) = \#\{j; \nu_j(\theta) < d\}. \tag{1.12}$$

The aim of this work is first to prove that for any $\theta \in]0,\pi/2[$, the number of eigenvalues of P_θ in $]-\infty,1[$ is finite. This is the purpose of Sec. II. Another interesting question is to get the asymptotic behavior of $N(d,P_\theta)$ as θ goes to zero, when $d<1$. This is done in Sec. IV. Section III is devoted to a survey of preliminary results about the function $\mu(\xi)$ defined in (1.4), which are required in the computation of the asymptotics in Sec. IV.

II. FINITENESS OF THE DISCRETE SPECTRUM

The purpose of this section is to prove the following theorem.

Theorem 2.1: *There exists a constant $C \geqslant 1$ such that, for any $\theta \in]0,\pi/2[$,*

$$N(1,P_\theta) \leqslant \frac{C}{\sin\theta}. \tag{2.1}$$

Proof: We have the following conventions.

Convention 2.2: $\theta \in]0,\pi/2[$ is fixed.

Convention 2.3: From now on, any constant depending only on θ will be denoted invariably as C_θ.

If the constant does not depend on θ, it will be denoted invariably as C.

Let us denote by q_θ the quadratic form associated to P_θ,

$$q_\theta(u) = \int_F [|D_t u|^2 + |D_x u|^2 + (t\cos\theta - x\sin\theta)^2 |u|^2]\mathrm{d}t\,\mathrm{d}x, \tag{2.2}$$

$$\forall u \in H^1(F) \cap L^2(F;(t\cos\theta - x\sin\theta)^2\,\mathrm{d}t\,\mathrm{d}x)\ (F = \mathbb{R}_{+,t}\times\mathbb{R}_x).$$

There exists a partition of unity $(\chi_0(t),\chi_1(t))$ satisfying

$$\chi_0(t) = 1 \quad \text{if } t<1,$$

$$\chi_0(t) = 0 \quad \text{if } t>2, \tag{2.3}$$

$$\chi_0^2(t) + \chi_1^2(t) = 1.$$

Let $R>1$ be fixed. We consider the following covering of F:

$$O_{0,R} = \{(t,x) \in \mathbb{R}_+ \times \mathbb{R},\ 0<t<2R\},$$

$$O_{1,R} = \{(t,x) \in \mathbb{R}_+ \times \mathbb{R},\ R<t\}. \tag{2.4}$$

We define the partition of unity $(\chi_{0,R}(t),\chi_{1,R}(t))$ by

$$\chi_{j,R}(t) = \chi_t\left(\frac{t}{R}\right). \tag{2.5}$$

Let us recall that

$$q_\theta(u) = \sum_j q_\theta(\chi_{j,R}u) - \sum_j \|\chi'_{j,R}u\|^2. \tag{2.6}$$

We define the following quadratic forms:

$$q_{\theta,0}(u) = \int_{O_{0,R}} [|D_t u|^2 + |D_x u|^2 + ((t\cos\theta - x\sin\theta)^2 - V_R(t))|u|^2]\mathrm{d}t\,\mathrm{d}x, \tag{2.7}$$

$$\forall u \in H^1(O_{0,R}) \cap L^2(O_{0,R}; x^2\,\mathrm{d}t\,\mathrm{d}x), \quad u/\{t = 2R\} = 0,$$

with $V_R(t) = \Sigma_j |\chi'_{j,R}(t)|^2$, and

$$q_{\theta,1}(u) = \int_{O_{1,R}} [|D_t u|^2 + |D_x u|^2 + ((t\cos\theta - x\sin\theta)^2 - V_R(t))|u|^2]\mathrm{d}t\,\mathrm{d}x, \tag{2.8}$$

$$\forall u \in H^1(O_{1,R}) \cap L^2(O_{1,R}; (t\cos\theta - x\sin\theta)^2\,\mathrm{d}t\,\mathrm{d}x), \quad u/\{t = R\} = 0.$$

By min–max principle, we have

$$N(1, q_\theta) \leqslant N(1, q_{\theta,0}) + N(1, q_{\theta,1}). \tag{2.9}$$

This estimate remains if we change $O_{1,R}$ into $\mathbb{R}^2$ in the definition of $q_{\theta,1}$,

$$q_{\theta,1}(u) = \int_{\mathbb{R}^2} [|D_t u|^2 + |D_x u|^2 + ((t\cos\theta - x\sin\theta)^2 - V_R(t))|u|^2]\mathrm{d}t\,\mathrm{d}x, \tag{2.10}$$

$$\forall u \in H^1(\mathbb{R}^2) \cap L^2(\mathbb{R}^2; (t\cos\theta - x\sin\theta)^2\,\mathrm{d}t\,\mathrm{d}x).$$

The operator $P_{\theta,0}$, associated to $q_{\theta,0}$ has compact resolvent, and

$$q_{\theta,0}(u) \geqslant \int_{O_{0,R}} \left[|D_t u|^2 + |D_x u|^2 + \left(\frac{1}{2}x^2\sin^2\theta - 4R^2\cos^2\theta - \frac{C}{R^2}\right)|u|^2 \right]\mathrm{d}t\,\mathrm{d}x.$$

So, if we denote by ρ_j^0 the eigenvalues of $|D_t u|^2$ on [0,1] with Neumann conditions on 0 and Dirichlet conditions on 1, we have

$$N(1, q_{\theta,0}) \leqslant \#\left\{ (k;j) \in \mathbb{N}^2; \frac{2k+1}{\sqrt{2}}\sin\theta + \frac{\rho_j^0}{4R^2} \leqslant 1 + 4R^2\cos^2\theta + \frac{C}{R^2} \right\}. \tag{2.11}$$

Using that $\rho_j^0 \sim j^2$ as $j \to \infty$, we get easily

$$N(1, q_{\theta,0}) \leqslant \frac{CR}{\sin\theta}[1 + R^2\cos^2\theta]^{3/2}. \tag{2.12}$$

Using the orthonormal change of coordinates, $(t,x) \to (s,y)$ with $s = t\cos\theta - x\sin\theta$, and $y = t\sin\theta + x\cos\theta$, we can take for $q_{\theta,1}$ the following expression:

$$q_{\theta,1}(u) = \int_{\mathbb{R}^2} [|D_s u|^2 + |D_y u|^2 + (s^2 - V_R(s,y))|u|^2]\mathrm{d}s\,\mathrm{d}y, \tag{2.13}$$

$\forall u \in H^1(\mathbb{R}^2) \cap L^2(\mathbb{R}^2;\ s^2\,\mathrm{d}s\,\mathrm{d}y)$, with

$$V_R(s,y) = \frac{1}{R^2}\sum_j \left| \chi'_j\left(\frac{s\cos\theta + y\sin\theta}{R}\right)\right|^2. \tag{2.14}$$

Let us consider the orthogonal projections

$$\Pi_1(u)(s,y) = e^{-s^2/2}\int_{\mathbb{R}} u(\tau,y)e^{-\tau^2/2}\frac{\mathrm{d}\tau}{\sqrt{\pi}},$$

$$\Lambda_1 u = u - \Pi_1 u, \tag{2.15}$$

so that, for any $u \in L^2(\mathbb{R}^2)$, we get $\|u\|^2 = \|\Pi_1 u\|^2 + \|\Lambda_1 u\|^2$.

Writing $\Pi_1 u(s,y) = (e^{-s^2/2}/\pi^{1/4})\psi(y)$ and

$$W_R(y) = \frac{1}{\sqrt{\pi}}\int_{\mathbb{R}} e^{-s^2}V_R(s,y)\mathrm{d}s,$$

we obtain that

$$q_{\theta,1}(\Pi_1 u) = \int_{\mathbb{R}} [|D_y\psi|^2 + (1 - W_R(y))|\psi|^2]\mathrm{d}y. \tag{2.16}$$

We have also

$$q_{\theta,1}(\Lambda_1 u) \geqslant \int_{\mathbb{R}^2}\left[|D_y\Lambda_1 u|^2 + \left(3 - \frac{C}{R^2}\right)|\Lambda_1 u|^2\right]\mathrm{d}s\,\mathrm{d}y. \tag{2.17}$$

But

$$q_{\theta,1}(u) = q_{\theta,1}(\Pi_1 u) + q_{\theta,1}(\Lambda_1 u) - 2\,\mathcal{R}e\int_{\mathbb{R}^2} V_R(s,y)\Pi_1 u \cdot \overline{\Lambda_1 u}\,\mathrm{d}s\,\mathrm{d}y, \tag{2.18}$$

so, for any $\epsilon \in]0,1[$,

$$q_{\theta,1}(u) \geqslant q_{\theta,1}(\Pi_1 u) - \frac{1}{\epsilon}\int_{\mathbb{R}^2} V_R^2(s,y)|\Pi_1 u|^2\,\mathrm{d}s\,\mathrm{d}y + q_{\theta,1}(\Lambda_1 u) - \epsilon\|\Lambda_1 u\|^2. \tag{2.19}$$

Thanks to (2.17), we can take $\epsilon = 1$ and R large enough such that

$$q_{\theta,1}(\Lambda_1 u) - \|\Lambda_1 u\|^2 > \|\Lambda_1 u\|^2, \tag{2.20}$$

for example, R satisfying $2 - (C/R^2) > 1$.

Then, by (2.16), (2.18), and (2.20), we get that

$$N(1, q_{\theta,1}) \leqslant N(0, q_{\theta,1,0}), \tag{2.21}$$

if

$$q_{\theta,1,0}(\psi) = \int_{\mathbb{R}} [|D_y\psi|^2 - W_{R,1}(y)|\psi|^2]\mathrm{d}y, \tag{2.22}$$

$\forall\,\psi \in H^1(\mathbb{R})$, with

$$W_{R,1}(y) = \frac{1}{\sqrt{\pi}}\int_{\mathbb{R}} e^{-s^2}[V_R(s,y) + V_R^2(s,y)]\mathrm{d}s.$$

From (2.3) and the formula (2.14), the following bound holds:

$$0 \leqslant W_{R,1}(y) \leqslant \frac{C}{R^2}\int_{(R-y\sin\theta)/\cos\theta}^{(2R-y\sin\theta)/\cos\theta} e^{-s^2}\,\mathrm{d}s$$

[we used the fact that, for any fixed y, $V_R(s,y)=0$ for s outside the interval defined by $R<s\cos\theta+y\sin\theta<2R$], so

$$0 \leqslant W_{R,1}(y) \leqslant \frac{C}{R^2}\chi_{[R/2\sin\theta,3R/\sin\theta]}(y) + \frac{C}{R\cos\theta}[e^{-[(y\sin\theta-R)^2]/\cos^2\theta} + e^{-[(y\sin\theta-2R)^2]/\cos^2\theta}]. \tag{2.23}$$

As the operators on $L^2(\mathbb{R})$, $\frac{1}{3}D_y^2-(C/R\cos\theta)e^{-[(y\sin\theta-R)^2]/\cos^2\theta}$, $\frac{1}{3}D_y^2-(C/R\cos\theta)\times e^{-[(y\sin\theta-2R)^2]/\cos^2\theta}$, and $(\sin^2\theta/3\cos^4\theta)D_y^2-(C/R\cos\theta)e^{-y^2}$ have the same spectrum, we get from (2.21)–(2.23) that

$$N(1,q_{\theta,1}) \leqslant 2N(0,q_{\theta,1,1}) + N(0,q_{\theta,1,2}), \tag{2.24}$$

if

$$q_{\theta,1,1}(\psi) = \int_{\mathbb{R}}\left[\frac{\sin^2\theta}{3\cos^4\theta}|D_y\psi|^2 - \frac{C}{R\cos\theta}e^{-y^2}|\psi|^2\right]\mathrm{d}y, \tag{2.25}$$

and

$$q_{\theta,1,2}(\psi) = \int_{\mathbb{R}}\left[\frac{1}{3}|D_y\psi|^2 - \frac{C}{R^2}\chi_{[R/2\sin\theta,3R/\sin\theta]}(y)|\psi|^2\right]\mathrm{d}y, \tag{2.26}$$

$\forall\psi\in H^1(\mathbb{R})$, for some $R>1$ independent of $\theta\in\,]0,\pi/2[$.

It is now possible to deduce from Theorem 1 in the work of Egorov and Kondrat'ev[5] the following estimates: $N(0,q_{\theta,1,1})\leqslant C(\cos^{3/2}\theta/\sin\theta)$ and $N(0,q_{\theta,1,2})\leqslant C/\sin\theta$, so

$$N(1,q_{\theta,1}) \leqslant \frac{C}{\sin\theta}. \tag{2.27}$$

We conclude from (2.9), (2.12), and (2.27) that the estimate (2.1) is valid.

III. SOME PROPERTIES OF $\mu(\xi)$

The properties of the first eigenvalue, $\mu(\xi)$, of the Neumann operator on $L^2(\mathbb{R}_+)$, $Q_\xi=D_t^2+(t-\xi)^2$, can be found in Refs. 3, 7, 11, and 13 (also see Refs. 2, 4, and 6).

The main ones are

$$\mu\in C^\infty(\mathbb{R}),$$

$$\mu'(\xi)\neq 0 \quad \text{if } \xi\neq\xi_0,$$

$$\mu(\xi)>1 \quad \text{if } \xi<0, \tag{3.1}$$

$$\mu(\xi)<1 \quad \text{if } \xi>0,$$

$$\lim_{\xi\to-\infty}\mu(\xi)=+\infty, \quad \lim_{\xi\to+\infty}\mu(\xi)=1$$

[$\xi_0>0$ is such that $\xi_0^2=\mu(\xi_0)$].

Let φ_ξ be a normalized eigenfunction associated to $\mu(\xi)$,

$$\|\varphi_\xi\|_{L^2(\mathbb{R}_+)} = 1, \quad \varphi'_\xi(0) = 0, \quad Q_\xi\varphi_\xi = \mu(\xi)\varphi_\xi, \tag{3.2}$$

then

$$\mu'(\xi) = -(\mu(\xi) - \xi^2)\varphi_\xi^2(0). \tag{3.3}$$

It is easy to see that φ_ξ is exponentially decreasing. More precisely we have the following.

Lemma 3.1: There exists $C_0 > 1$ such that

$$1 - C_0 e^{-|\xi|^2/C_0} \leqslant \mu(\xi). \tag{3.4}$$

Moreover, if $\mu_2(\xi)$ is the second eigenvalue of Q_ξ, then we have also

$$3 - C_0 e^{-|\xi|^2/C_0} \leqslant \mu_2(\xi). \tag{3.5}$$

Proof: We proceed as in Ref. 4 to get first the following bound: For any $\xi > 1$ and $\eta \in]0,1[$,

$$\int_{\mathbb{R}_+} [\eta(t-\xi)^2 - \mu(\xi)]_+ e^{(1-\eta)^{1/2}(t-\xi)^2} |\varphi_\xi(t)|^2 \, dt \leqslant \mu(\xi) e^{\mu(\xi)/\eta}. \tag{3.6}$$

For any Lipschitz and real function Φ, with compact support,

$$\|D_t(e^\Phi \varphi_\xi)\|^2_{L^2(\mathbb{R}_+)} = \langle [\mu(\xi) - (t-\xi)^2 + (\Phi')^2] e^\Phi \varphi_\xi | e^\Phi \varphi_\xi \rangle$$

so

$$\langle [(t-\xi)^2 - \mu(\xi) - (\Phi')^2]_+ e^\Phi \varphi_\xi | e^\Phi \varphi_\xi \rangle \leqslant \langle [\mu(\xi) - (t-\xi)^2 + (\Phi')^2]_+ e^\Phi \varphi_\xi | e^\Phi \varphi_\xi \rangle.$$

This estimate is still valid for Φ with noncompact support, provided that the right-hand side of the inequality is finite; so we can take $\Phi(t) = (1-\eta)^{1/2}(t-\xi)^2/2$ to get (3.6). Now, let χ be a smooth cutoff function on $\mathbb{R}$,

$$\begin{gathered} \chi \in C^\infty(\mathbb{R}), \\ \chi(t) = 1 \quad \text{if } -1 < t < 1, \\ \chi(t) = 0 \quad \text{if } |t| > 2, \\ 0 \leqslant \chi \leqslant 1. \end{gathered} \tag{3.7}$$

If $\xi > 1$, we define the function $\tilde{\varphi}_{1,\xi}(t) = \chi(4[(t-\xi)/\xi])\varphi_\xi(t)$.

So,

$$\|D_t\tilde{\varphi}_{1,\xi}\|^2 + \|(t-\xi)\tilde{\varphi}_{1,\xi}\|^2 = \mu(\xi))\|\tilde{\varphi}_{1,\xi}\|^2 + \frac{16}{\xi^2}\left\|\chi'\left(4\frac{t-\xi}{\xi}\right)\tilde{\varphi}_\xi\right\|^2.$$

As $\tilde{\varphi}_{1,\xi}$ is of compact support and the first eigenvalue of $D_t^2 + (t-\xi)^2$ on $L^2(\mathbb{R})$ is 1, then

$$\|\tilde{\varphi}_{1,\xi}\|^2 \leqslant \mu(\xi))\|\tilde{\varphi}_{1,\xi}\|^2 + \frac{16}{\xi^2}\left\|\chi'\left(4\frac{t-\xi}{\xi}\right)\varphi_\xi\right\|^2,$$

then we use the estimate (3.6) to see that, for some constant $C > 1$, $1 \leqslant \mu(\xi) + Ce^{-\xi^2/C}$, the estimate (3.4) follows.

If $\mu_2(\xi)$ is the second eigenvalue of Q_ξ and $\varphi_{2,\xi}$ the associated normalized eigenfunction, then we have in the same way, for any real function Φ,

$$\langle[(t-\xi)^2-\mu_2(\xi)-(\Phi')^2]_+e^{\Phi}\varphi_{2,\xi}|e^{\Phi}\varphi_{2,\xi}\rangle \leqslant \langle[\mu_2(\xi)-(t-\xi)^2+(\Phi')^2]_+e^{\Phi}\varphi_{2,\xi}|e^{\Phi}\varphi_{2,\xi}\rangle,$$

so $\varphi_{2,\xi}$ is exponentially decreasing as φ_{ξ}, and if $\tilde{\varphi}_{2,\xi}(t)=\chi(4[(t-\xi)/\xi])\varphi_{2,\xi}(t)$, then

$$\|D_t\tilde{\varphi}_{2,\xi}\|^2+\|(t-\xi)\tilde{\varphi}_{2,\xi}\|^2 \leqslant \mu_2(\xi)+Ce^{-\xi^2/C}$$

and

$$|\|\tilde{\varphi}_{2,\xi}\|-1| \leqslant Ce^{-\xi^2/C},$$

$$|\langle\tilde{\varphi}_{1,\xi}|\tilde{\varphi}_{2,\xi}\rangle| \leqslant Ce^{-\xi^2/C}. \tag{3.8}$$

Those estimates, (3.4) and the min–max principle show that $\mu_2(\xi)+Ce^{-\xi^2/C}$ is greater than the second eigenvalue of $D_t^2+(t-\xi)^2$ on $L^2(\mathbb{R})$, so $3\leqslant\mu_2(\xi)+Ce^{-\xi^2/C}$. This ends the proof of the lemma.

IV. THE CASE OF SMALL θ

We are still investigating the spectrum of the operator P_θ, defined in the Introduction as follows:

$$P_\theta=D_t^2+D_x^2+(t\cos\theta-x\sin\theta)^2.$$

Performing the scaling $(t,x)\to(t\sqrt{\cos\theta},-x\sin\theta/\sqrt{\cos\theta})$, we observe that this operator has the same spectrum as

$$P_\theta=\cos\theta[D_t^2+(t-x)^2]+\frac{\sin^2\theta}{\cos\theta}D_x^2$$

(we keep on the same notation for simplification).

It has been proved in Ref. 8 that for small values of $\theta>0$ the following asymptotics hold:

$$\inf\sigma(P_\theta)\sim\mu_0+\sum_{j\geqslant 1}c_j\theta^j.$$

Therefore let us consider a set,

$$I_d=\,]-\infty,d[\quad\text{with } d\in\,]\mu_0,1[.$$

The goal of this section is to get information about

$$N(d,P_\theta)=\#\,\sigma(P_\theta)\cap\,]-\infty,d[, \tag{4.1}$$

which denotes the number of eigenvalues of P_θ included in the set I_d.

For a fixed $a>1$ let us consider the following sets:

$$J_0=[-a,+\infty[\,,\quad J_1=\left]-\infty,-\frac{a}{2}\right],$$

and a partition of unity

$$\chi_0^2(x)+\chi_1^2(x)=1,\quad \text{support}\,(\chi_j)\subset J_j,\quad \sum_j|\chi_j'(x)|^2<C.$$

For $j=0,1$ let us denote by Ω_j the domains $\mathbb{R}_+\times J_j$, $\Omega_0=\mathbb{R}_+\times\,]-a,+\infty[$ and $\Omega_1=\mathbb{R}_+\times\,]-\infty,-a/2[$. We take now the realization of the operators P_θ^j on each domain Ω_j, associated to the quadratic form q_{Ω_j}, with Neumann conditions on $\Gamma_N=\{0\}\times J_j$ and Dirichlet conditions on $\Gamma_D=\mathbb{R}_+\times\partial J_j$.

The quadratic forms are defined as follows:

$$q_{\Omega_j}(u) = \int_{\Omega_j} \left\{ \cos\theta\,[|D_t u|^2 + (t-x)^2|u|^2] + \frac{\sin^2\theta}{\cos\theta}|D_x u|^2 - \frac{\sin^2\theta}{\cos\theta}\sum_{j=0}^{1} |\chi_j'(x)|^2|u|^2 \right\} \mathrm{d}t\,\mathrm{d}x.$$

Let us first explain why q_{Ω_1} will not give any contribution to the term $N(d,P_\theta)$.

According to Sec. III we know that $\mu(x)$, the first eigenvalue of $D_t^2+(t-x)^2$ is decreasing on J_1, so we have

$$q_{\Omega_1}(u) \geqslant \left[\mu\left(-\frac{a}{2}\right)\cos\theta - C\frac{\sin^2\theta}{\cos\theta} \right] \|u\|^2_{L^2(\Omega_1)}.$$

But $\mu(-a/2)>1$, so for small θ the preceding minoring ensues

$$q_{\Omega_1}(u) \geqslant \|u\|^2_{L^2(\Omega_1)} \quad \text{if } 0<\theta<\theta_0, \tag{4.2}$$

for some $\theta_0 \in]0,\pi/4[$.

In order to study the form q_{Ω_0}, it is convenient to use the normalized eigenfunction φ_x, associated to $\mu(x)$, in the following way.

Let us denote by $\Pi_0(u)$ the orthogonal projection on the set

$$F_0 = \{\varphi_x(t)\psi(x);\ \psi \in L^2(J_0)\}, \tag{4.3}$$

defined by

$$\Pi_0(u) = \varphi_x(t)\left(\int_{\mathbb{R}_+} u(s,x)\varphi_x(s)\mathrm{d}s \right), \tag{4.4}$$

and by $F_1=(F_0)^\perp$ the orthogonal set of F_0. The corresponding orthogonal projection is

$$\Pi_1 = I - \Pi_0.$$

A direct computation gives

$$\partial_x(\Pi_0 u) = \Pi_0(\partial_x u) + R(u),$$

where R is defined by

$$R(u) = \varphi_x(t)\left(\int_{\mathbb{R}_+} u(s,x)\partial_x\varphi_x(s)\mathrm{d}s \right) + \partial_x\varphi_x(t)\left(\int_{\mathbb{R}_+} u(s,x)\varphi_x(s)\mathrm{d}s \right). \tag{4.5}$$

The additional fact that

$$\partial_x(\Pi_1 u) = \Pi_1(\partial_x u) - R(u)$$

yields the following bounds:

$$(1-\epsilon)[\|\partial_x(\Pi_0 u)\|^2_{L^2(\Omega_0)} + \|\partial_x(\Pi_1 u)\|^2_{L^2(\Omega_0)}] + 2\left(1-\frac{1}{\epsilon}\right)\|R(u)\|^2_{L^2(\Omega_0)}$$

$$\leqslant \|\partial_x u\|^2_{L^2(\Omega_0)} \leqslant (1+\epsilon)[\|\partial_x(\Pi_0 u)\|^2_{L^2(\Omega_0)} + \|\partial_x(\Pi_1 u)\|^2_{L^2(\Omega_0)}] + 2\left(1+\frac{1}{\epsilon}\right)\|R(u)\|^2_{L^2(\Omega_0)}.$$

Let us establish now the following lemma.

Lemma 4.1:

$$\exists C_0>0, \quad s.t.\ \forall\, u \in L^2(\Omega_0), \quad \|R(u)\|_{L^2(\Omega_0)} \leqslant C_0\|u\|_{L^2(\Omega_0)}. \tag{4.6}$$

Taking norms in (4.5) we have

$$\|R(u)\|^2_{L^2(\Omega_0)} \leqslant 2\int_{\Omega_0} |u(s,x)(\partial_x\varphi_x(s))|^2 \,\mathrm{d}s\,\mathrm{d}x + 2\sup_{x\in J_0}\|\partial_x\varphi_x(t)\|^2_{L^2(\mathbb{R}_+)}\|u\|^2_{L^2(\Omega_0)}$$
$$\leqslant 4\sup_{x\in J_0}\|\partial_x\varphi_x(t)\|^2_{L^2(\mathbb{R}_+)}\|u\|^2_{L^2(\Omega_0)}.$$

The lemma will then be proved if we show that $\sup_{x\in J_0}\|\partial_x\varphi_x(t)\|^2_{L^2(\mathbb{R}_+)}\|$ is finite.

We recall that some elementary technique of perturbation shows that

$$\frac{\partial}{\partial x}\varphi_x(t) = 2[Q_x - \mu(x)]^{-1}\psi_x, \tag{4.7}$$

with

$$\psi_x(t) = (t-x)\varphi_x(t) - \langle (t-x)\varphi_x|\varphi_x\rangle\varphi_x(t).$$

Now using

$$\|D_t^2\varphi_x\|^2_{L^2(\mathbb{R}^2_+)} + \|(t-x)\varphi_x\|^2_{L^2(\mathbb{R}^2_+)} = \mu(x)\|\varphi_x\|^2_{L^2(\mathbb{R}^2_+)} = \mu(x),$$

we get that

$$\|(t-x)\varphi_x\|_{L^2(\mathbb{R}^2_+)} \leqslant \sqrt{\mu(x)},$$

and then

$$|\langle (t-x)\varphi_x|\varphi_x\rangle_{L^2(\mathbb{R}^2_+)}| \leqslant \sqrt{\mu(x)},$$

so

$$\|\psi_x\|_{L^2(\mathbb{R}^2_+)} \leqslant 2\sqrt{\mu(x)}.$$

Since ψ_x lives on the orthogonal space of φ_x, let us consider the norm N_x of the restriction of $[Q_x-\mu(x)]^{-1}$ to this orthogonal space. It is given by

$$N_x = \frac{1}{\mu_2(x)-\mu_1(x)} = \frac{1}{\mu_2(x)-\mu(x)},$$

where $(\mu_j(x))_j$ is the increasing sequence of the eigenvalues of Q_x.

According to (3.1) and (3.5), $\mu(x)$ and N_x are uniformly bounded on J_0, so there exists $C_0 > 0$ such that

$$\sup_{x\in J_0}\|\partial_x\varphi_x(t)\|_{L^2(\mathbb{R}^2_+)} \leqslant 2\sup_{x\in J_0}\frac{\sqrt{\mu(x)}}{\mu_2(x)-\mu(x)} \leqslant C_0, \tag{4.8}$$

so the Lemma 4.1 follows.

From Lemma 4.1, we see that we can find a constant $C_1>0$, such that, for any $\epsilon\in\,]0,1[$,

$$(1-\epsilon)[\|\partial_x(\Pi_0 u)\|^2_{L^2(\Omega_0)} + \|\partial_x(\Pi_1 u)\|^2_{L^2(\Omega_0)}] - \frac{C_1}{\epsilon}\|u\|^2_{L^2(\Omega_0)}$$
$$\leqslant \|\partial_x u\|^2_{L^2(\Omega_0)} \leqslant (1+\epsilon)[\|\partial_x(\Pi_0 u)\|^2_{L^2(\Omega_0)} + \|\partial_x(\Pi_1 u)\|^2_{L^2(\Omega_0)}] + \frac{C_1}{\epsilon}\|u\|^2_{L^2(\Omega_0)}.$$

From that we obtain the corresponding bounds on the quadratic form q_{Ω_0},

$$q^{\epsilon,-}_{\Omega_0}(\Pi_0 u) + q^{\epsilon,-}_{\Omega_0}(\Pi_1 u) \leqslant q_{\Omega_0}(u) \leqslant q^{\epsilon,+}_{\Omega_0}(\Pi_0 u) + q^{\epsilon,+}_{\Omega_0}(\Pi_1 u), \tag{4.9}$$

where we used the natural notations

$$q^{\epsilon,-}_{\Omega_0}(u) = \int_{\Omega_0} \left\{ \cos\theta \left[|D_t u|^2 + (t-x)^2 |u|^2 \right] + (1-\epsilon) \frac{\sin^2\theta}{\cos\theta} |D_x u|^2 \right\} \mathrm{d}t\, \mathrm{d}x - \frac{\sin^2\theta}{\cos\theta} \left[C + \frac{C_1}{\epsilon} \right] \|u\|^2_{L^2(\Omega_0)}$$

and

$$q^{\epsilon,+}_{\Omega_0}(u) = \int_{\Omega_0} \left\{ \cos\theta \left[|D_t u|^2 + (t-x)^2 |u|^2 \right] + (1+\epsilon) \frac{\sin^2\theta}{\cos\theta} |D_x u|^2 \right\} \mathrm{d}t\, \mathrm{d}x + \frac{\sin^2\theta}{\cos\theta} \frac{C_1}{\epsilon} \|u\|^2_{L^2(\Omega_0)}.$$

Writing

$$h = \frac{\sin\theta}{\sqrt{\cos\theta}}, \tag{4.10}$$

taking into account (4.3), we define

$$W(x) = \int_{\mathbb{R}_+} \left| \frac{\partial}{\partial x} \varphi_x(t) \right|^2 \mathrm{d}t,$$

and we get, using (4.4) that

$$q^{\epsilon,-}_{\Omega_0}(\Pi_0 u) = q^{\epsilon,-}(\psi) = \int_{J_0} \left\{ \left[\mu(x)\cos\theta + (1-\epsilon) h^2 W(x) \right] |\psi(x)|^2 + (1-\epsilon) h^2 |D_x \psi(x)|^2 - h^2 \left[C + \frac{C_1}{\epsilon} \right] |\psi(x)|^2 \right\} \mathrm{d}x.$$

In the same way we have

$$q^{\epsilon,+}_{\Omega_0}(\Pi_0 u) = q^{\epsilon,+}(\psi) = \int_{J_0} \left\{ \left[\mu(x)\cos\theta + (1+\epsilon) h^2 W(x) \right] |\psi(x)|^2 + (1+\epsilon) h^2 |D_x \psi(x)|^2 + h^2 \frac{C_1}{\epsilon} |\psi(x)|^2 \right\} \mathrm{d}x.$$

Now we must deal with the terms involving the second projection $\Pi_1 u$. But the definition of $\Pi_1 u$, the min–max principle and the estimate $1-\cos\theta \leqslant h^2 C$ give the following lower bound:

$$q^{\epsilon,\pm}_{\Omega_0}(\Pi_1 u) \geqslant \left[\inf_{x \in J_0} \mu_2(x) - h^2 \left(C + \frac{C_1}{\epsilon} \right) \right] \|\Pi_1 u\|_{L^2(\Omega_0)},$$

where $\mu_2(x)$ denotes the second eigenvalue defined in the Lemma 3.1. This eigenvalue must be greater than the first eigenvalue of the corresponding Dirichlet problem, so

$$\mu_2(x) > 1.$$

Let us take $\epsilon = h$. We get that

$$N(d, q^{h,\pm}_{\Omega_0}) = N(d, q^{h,\pm}).$$

Let us take an extension $\tilde{\mu}(x)$ of $\mu(x)$ outside of

$$J_{0,d} = \{x \in J_0,\ \mu(x) < d + (1-d)/2\}, \tag{4.11}$$

such that

$$\tilde{\mu}(x) = \mu(x) \quad \text{if } x \in J_{0,d},$$

$$\tilde{\mu}(x) \geqslant (1+d)/2, \quad \forall\, x \notin J_{0,d}, \tag{4.12}$$

$$\tilde{\mu}(x) = 1 \quad \text{if } |x| > C_d,$$

for some constant $C_d > 0$. Let us define

$$q_0^{h,\pm}(\psi) = \int_{\mathbb{R}} [\tilde{\mu}(x)|\psi(x)|^2 + (1 \pm h)h^2|D_x\psi(x)|^2]\mathrm{d}x.$$

We will need the following lemma.

Lemma 4.2: Let $U(x) \in C^\infty(\mathbb{R};\mathbb{R})$, $E \in \mathbb{R}$ and $\eta > 0$ such that $U^{-1}(]-\infty, E+\eta])$ is bounded.

Then for any interval I of $\mathbb{R}$ satisfying $\mathbb{R}\backslash I \subset [E+(\eta/2), +\infty[$, there exists a constant $C = C_\eta > 0$ such that

$$N(E, q_{h,U,I}) \leqslant N(E, q_{h,U}) \leqslant N(E + h^2C, q_{h,U,I}), \tag{4.13}$$

if

$$q_{h,U}(\psi) = \int_{\mathbb{R}} [h^2|D_x\psi(x)|^2 + U(x)|\psi(x)|^2]\mathrm{d}x, \quad \forall\, \psi \in C_0^\infty(\mathbb{R}),$$

and

$$q_{h,U,I}(\psi) = \int_I [h^2|D_x\psi(x)|^2 + U(x)|\psi(x)|^2]\mathrm{d}x, \ \forall\, \psi \in C_0^\infty(I).$$

From the estimate (4.13) we get

$$N(d - hC, q_0^{\epsilon,\pm}) \leqslant N(d, q^{\epsilon,\pm}) \leqslant N(d + hC, q_0^{\epsilon,\pm}) \tag{4.14}$$

[we have used that $W(x)$ is bounded in J_0, thanks to (4.8), then we apply the left-hand side of (4.13) to $N(d+hC, q_0^{\epsilon,\pm})$ and the right-hand side of (4.13) to $N(d-hC, q_0^{\epsilon,\pm})$, both with $I = J_0$].

Applying a classical estimate of $N(d, q_0^{h,\pm})$ (see, for example, Ref. 13, Theorem V-11, p. 263), we have that, for any $\lambda < (1+d)/2$, there exists $C_\lambda > 0$ such that, for any $h \in]0, 1/2[$,

$$\left| N(\lambda, q_0^{h,\pm}) - \frac{1}{2\pi h\sqrt{1 \pm h}} \int_{\mathbb{R}} [\lambda - \mu(x)]_+^{1/2}\, \mathrm{d}x \right| \leqslant C_\lambda. \tag{4.15}$$

According to the choice of d and (3.1), we can use the fact that $\mu'(x) \neq 0$ for $\mu(x) = d$ and get from (4.9)–(4.12), (4.14), and (4.15) with $\lambda = d \pm hC$, that there exists $C_d > 0$, depending only on d, such that

$$\left| N(d, q_{\Omega_0}) - \frac{1}{2\pi \sin\theta} \int_{\mathbb{R}} [d - \mu(x)]_+^{1/2}\, \mathrm{d}x \right| \leqslant C_d. \tag{4.16}$$

We get easily from the above discussion the following theorem.

Theorem 4.3: *For any $d \in]\mu_0, 1[$, there exists $C_d > 0$ such that*

$$\left| N(d, P_\theta) - \frac{1}{2\pi \sin\theta} \int_{\mathbb{R}} [d - \mu(x)]_+^{1/2}\, \mathrm{d}x \right| \leqslant C_d. \tag{4.17}$$

Sketch of the proof of Lemma 4.2: The min–max principle proves the left-hand side of (4.13). For the right-hand side, take a partition of unity of $\mathbb{R}$, $\chi_0^2(x)+\chi_1^2(x)=1$ such that χ_0 is supported in I and χ_1 supported $J\subset U^{-1}([E+\eta_0,+\infty[)$, for some $\eta_0>0$. Then $q_{h,U}(\psi)=q_{h,U_h}(\chi_0\psi)+q_{h,U_h}(\chi_1\psi)$, with $U_h(x)=U(x)-h^2[(\chi_0'(x))^2+(\chi_1'(x))^2]$. From the min–max principle, we get that

$$N(E,q_{h,U})\leqslant N(E,q_{h,U_h,I})+N(E,q_{h,U_h,J}).$$

If h is small enough, then $N(E,q_{h,U_h,J})=0$ and we get the right-hand side of (4.13).

Remark 4.4: The condition $\theta<\theta_0$ (4.2) *can be removed since* $N(d,P_\theta)$ *is finite for fixed* θ *according to Theorem 2.1.*

Remark 4.5: It should be possible to apply the technique of Balazard–Konlein[1] *to get the asymptotics of* $N(d,P_\theta)$*, but the result would be rough, compared to our result in Theorem 4.3: our remainder is an* $\mathbf{O}(1)$ *and the result of Ref. 1 would give* $\mathbf{O}(\sin^{-\rho}\theta)$ *with* $\rho>1/2$.

Moreover the assumptions in Ref. 1 are not satisfied in our case.

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Wigner–Weyl isomorphism for quantum mechanics on Lie groups

N. Mukunda[a)]
Centre for Theoretical Studies, Indian Institute of Science, Bangalore 560 012, India

G. Marmo[b)] and A. Zampini[c)]
Dipartimento di Scienze Fisiche, Universita di Napoli Federico II and INFN, Via Cinzia, 80126 Napoli, Italy

S. Chaturvedi[d)]
School of Physics, University of Hyderabad, Hyderabad 500 046, India

R. Simon[e)]
The Institute of Mathematical Sciences, C. I. T. Campus, Chennai 600 113, India

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The Wigner–Weyl isomorphism for quantum mechanics on a compact simple Lie group G is developed in detail. Several features are shown to arise which have no counterparts in the familiar Cartesian case. Notable among these is the notion of a semiquantized phase space, a structure on which the Weyl symbols of operators turn out to be naturally defined and, figuratively speaking, located midway between the classical phase space T^*G and the Hilbert space of square integrable functions on G. General expressions for the star product for Weyl symbols are presented and explicitly worked out for the angle-angular momentum case. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1825078]

I. INTRODUCTION

It is well known that the method of Wigner distributions,[1] which describes every state of a quantum mechanical system by a corresponding real quasiprobability density on the classical phase space, is dual to the Weyl mapping[2] of classical dynamical variables to quantum mechanical operators. Together they provide the Wigner–Weyl isomorphism, whereby both states and operators in quantum mechanics can be given c-number descriptions on the classical phase space. The trace of the product of two operators is then calculable as the integral of the product of the two corresponding Weyl symbols or phase space functions. Combined with the work of Moyal,[3] which shows how products and commutators of operators are expressed in phase space language, this entire development may be called the Wigner–Weyl–Moyal or WWM method in quantum mechanics and has been instrumental in giving rise to the fertile subject of deformation quantization.[4] An important feature of the Wigner distribution is that while it is not by itself a phase space probability density, its marginals obtained by, respectively, integrating over momenta or over coordinates do reproduce the quantum mechanical expressions for probability densities in coordinate and in momentum space, respectively.

The WWM method has been studied most extensively in the case of Cartesian systems in quantum mechanics. By this we mean those systems whose configuration space Q is $\mathbb{R}^n$ for some integer $n \geqslant 1$. The classical phase space is then $T^*Q \simeq \mathbb{R}^{2n}$. While Schrödinger wave functions are

[a)]Electronic mail: nmukunda@cts.iisc.ernet.in
[b)]Electronic mail: giuseppe.marmo@na.infn.it
[c)]Electronic mail: alessandro.zampini@na.infn.it
[d)]Electronic mail: scsp@uohyd.ernet.in
[e)]Electronic mail: simon@imsc.res.in

square integrable functions on $\mathbb{R}^n$, both Wigner distributions and Weyl symbols are functions on $\mathbb{R}^{2n}$. Quantum kinematics can be expressed via the Heisenberg canonical commutation relations for Cartesian coordinates and their conjugate momenta, or via the exponentiated Weyl form using families of unitary operators. An important feature in this case is that as far as their eigenvalue spectra are concerned, the momenta do not experience any quantization on their own; they account for the second factor in $T^*Q \simeq \mathbb{R}^{2n} \simeq \mathbb{R}^n \times \mathbb{R}^n$. Furthermore we have in this case the Stone–von Neumann theorem on the uniqueness of the irreducible representation of the Heisenberg commutation relations, and the important roles of the groups $\mathrm{Sp}(2n,R)$ and $\mathrm{Mp}(2n)$ corresponding to linear canonical transformations on coordinates and momenta.

There has been for some time considerable interest in developing the Wigner–Weyl isomorphism for other kinds of quantum systems, that is, for non-Cartesian systems.[5–16] In these cases, typically the underlying quantum kinematics cannot be expressed by Heisenberg-type commutation relations. The situations studied include the quantum mechanics of an angle-angular momentum pair, where the configuration space is $Q=\mathbb{S}^1$,[17,18] and finite state quantum systems corresponding to a finite dimensional Hilbert space.[19,20] More recently, the method of Wigner distributions has been developed for quantum systems whose configuration space is a compact simple Lie group; and in the discrete case when it is a finite group of odd order.[21,22] In all these departures from the Cartesian situation, an important aspect is the occurrence of new features which do not show up at all with Cartesian variables.

The aim of the present work is to develop in detail the Wigner–Weyl isomorphism for quantum mechanics on a compact simple Lie group. Here the configuration space Q is a (compact simple) Lie group G, so the corresponding classical phase space is $T^*G \simeq G \times \underline{G}^*$, where $\underline{G}^*$ is the dual to the Lie algebra $\underline{G}$ of G. In the quantum situation, Schrödinger wave functions are complex square integrable functions on G, and observables or dynamical variables are linear Hermitian operators acting on such functions. The replacements for the canonical Heisenberg commutation relations are best formulated using the (commutative) algebra of suitable smooth functions on G, and (say) the left regular representation of G acting on functions on itself. The natural question that arises in trying to set up a Wigner–Weyl isomorphism in this case is whether quantum states and operators are to be described using suitable functions on the classical phase space T^*G. In Ref. 21 an overcomplete Wigner distribution formalism for quantum states, which transforms in a reasonable way under left and right group actions and also reproduces the natural marginal probability distributions, has been developed. The methods developed there are here exploited to set up a Wigner–Weyl isomorphism in full detail, disclosing many interesting differences compared to the Cartesian case. In particular we find that this isomorphism does not directly utilize c-number functions on T^*G at all, but instead uses a combination of functions on G and operators on a simpler Hilbert space, standing in a sense midway between T^*G and the Hilbert space of the quantum system. This feature is traceable to the non-Abelian nature of G, something which is absent in the Cartesian case when Q is the Abelian group $\mathbb{R}^n$.

The material of this paper is organized as follows. In Sec. II we briefly recapitulate key features of the Wigner–Weyl isomorphism for the Cartesian and angle-angular momentum cases. This sets the stage for Sec. III where we develop the quantum kinematics for situations where the configuration space is a compact Lie group and thus go beyond the Abelian cases discussed in Sec. I. This analysis leads to a proper identification of the analogues of the momenta of the Cartesian case and helps set up the Wigner distribution for such situations possessing properties expected of a Wigner distribution. The Wigner distributions so defined have a certain degree of overcompleteness about them, a circumstance forced by the non-Abelian nature of the underlying group G. A key ingredient in this construction is the notion of the midpoint of two group elements introduced in an earlier work.[21] In Sec. IV a more compact description in terms of Weyl symbols devoid of any redundances is developed and correspondences facilitating transition from the Cartesian case to more general situations are established. The results of Sec. IV are exploited in Sec. V towards defining a star product between Weyl symbols for operators and the general expression for the star product is explicitly worked out for the non-Cartesian, albeit Abelian case of angle-angular momentum. Section VI is devoted to analyzing the minimal structure on which the Weyl symbols for

operators find their natural definition. This leads to the concept of a noncommutative cotangent space or a semiquantized phase space the ramifications of which are examined further towards highlighting the structural similarity between classical phase space functions and the Weyl symbols. A short appendix contains some technical details concerning results used in Sec. V.

II. THE WIGNER–WEYL ISOMORPHISM: CARTESIAN AND ANGLE-ANGULAR MOMENTUM CASES

In this section we recall briefly the relevant structures needed to set up the Wigner–Weyl isomorphism for Cartesian quantum mechanics. This is to facilitate comparison with the Lie group case later on. For simplicity we choose one degree of freedom only, as the extension to $Q=\mathbb{R}^n$ is straightforward. We also recall the angle-angular momentum case, $Q=\mathbb{S}^1$, where we already see significant differences from the Cartesian case; these increase when we go to $Q=G$.

One-dimensional Cartesian quantum mechanics: The canonical Heisenberg commutation relation between Hermitian coordinate and momentum operators $\hat{q}$ and $\hat{p}$, fixing the kinematics, is

$$[\hat{q},\hat{p}] = i. \tag{2.1}$$

In the unitary Weyl form this is expressed as follows:

$$U(p) = \exp(ip\hat{q}), \quad V(q) = \exp(-iq\hat{p}),$$

$$U(p)V(q) = V(q)U(p)e^{iqp}, \quad q,p \in \mathbb{R}. \tag{2.2}$$

In the Cartesian case the exponentials can be combined to define a phase space displacement operator

$$D(q,p) = U(p)V(q)e^{-iqp/2} = V(q)U(p)e^{iqp/2} = \exp(ip\hat{q} - iq\hat{p}). \tag{2.3}$$

However this cannot be done even in the single angle-angular momentum pair case, and also when we treat the Lie group case. We therefore use expressions in which the exponentials are kept separate.

The standard form of the unique irreducible representation of Eqs. (2.1) and (2.2) uses the Hilbert space of square integrable functions $\psi(q)$ on $\mathbb{R}$. Introducing as usual an ideal basis of eigenvectors of $\hat{q}$ we have

$$\mathcal{H} = L^2(\mathbb{R}) = \left\{ \psi(q) \mid \|\psi\|^2 = \int_{\mathbb{R}} \mathrm{d}q |\psi(q)|^2 < \infty \right\},$$

$$\psi(q) = \langle q|\psi\rangle, \quad \hat{q}|q\rangle = q|q\rangle, \tag{2.4}$$

$$\langle q'|q\rangle = \delta(q'-q).$$

On such $\psi(q)$ (subject to relevant domain conditions) the actions of $\hat{q}$, $\hat{p}$, $U(p)$, $V(q)$ are

$$(\hat{q}\psi)(q) = q\psi(q), \quad (\hat{p}\psi)(q) = -i\frac{\mathrm{d}}{\mathrm{d}q}\psi(q),$$

$$(U(p')\psi)(q) = e^{ip'q}\psi(q), \quad (V(q')\psi)(q) = \psi(q-q'). \tag{2.5}$$

The momentum space description of $|\psi\rangle$ uses the Fourier transform of $\psi(q)$; in terms of the ideal eigenstates $|p\rangle$ for $\hat{p}$,

$$\tilde{\psi}(p) = \langle p|\psi\rangle = \int_{\mathbb{R}} \frac{\mathrm{d}q}{\sqrt{2\pi}} \exp(-ipq)\psi(q),$$

$$\|\psi\|^2 = \int_{\mathbb{R}} \mathrm{d}p |\tilde{\psi}(p)|^2. \tag{2.6}$$

The displacement operators (2.2) form a complete trace orthonormal set (in the continuum sense) in the space of operators on $\mathcal{H}$,

$$\mathrm{Tr}((U(p')V(q'))^\dagger U(p)V(q)) = 2\pi\delta(q'-q)\delta(p'-p). \tag{2.7}$$

The completeness property will be used later.

The definitions of the Wigner distribution for a normalized pure state $|\psi\rangle \in \mathcal{H}$, or more generally for a mixed state with density operator $\hat{\rho}$, are

$$W(q,p) = \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}q'\ \psi\left(q - \frac{1}{2}q'\right)\psi\left(q + \frac{1}{2}q'\right)^* \exp(ipq'),$$

$$W(q,p) = \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}q' \left\langle q - \frac{1}{2}q'|\hat{\rho}|q + \frac{1}{2}q'\right\rangle \exp(ipq'). \tag{2.8}$$

(The dependences on $|\psi\rangle$, $\hat{\rho}$ are left implicit.) While $W(q,p)$ is real though not always nonnegative, the recovery of the marginal position and momentum space probability densities is assured by

$$\int_{\mathbb{R}} \mathrm{d}p\ W(q,p) = \langle q|\hat{\rho}|q\rangle, \quad \int_{\mathbb{R}} \mathrm{d}q\ W(q,p) = \langle p|\hat{\rho}|p\rangle. \tag{2.9}$$

It is possible to express $W(q,p)$ in a more compact form by introducing a family of Hermitian operators $\hat{W}(q,p)$ on $\mathcal{H}$ with interesting algebraic properties. They are essentially the double Fourier transforms of the displacement operators (2.2),

$$W(q,p) = \mathrm{Tr}(\hat{\rho}\hat{W}(q,p)),$$

$$\hat{W}(q,p) = \hat{W}(q,p)^\dagger = \frac{1}{(2\pi)^2}\int_{\mathbb{R}}\int_{\mathbb{R}} \mathrm{d}q'\ \mathrm{d}p'\ U(p')V(q')e^{ipq'-ip'(q+(1/2)q')}. \tag{2.10}$$

It has been shown in Ref. 17 that, apart from sharing the trace orthonormality property (2.7) which is preserved by the Fourier transformation,

$$\mathrm{Tr}(\hat{W}(q',p')\hat{W}(q,p)) = \frac{1}{2\pi}\delta(q'-q)\delta(p'-p), \tag{2.11}$$

we have the following behaviors under anticommutation with $\hat{q}$ and $\hat{p}$:

$$\tfrac{1}{2}\{\hat{q}, \hat{W}(q,p)\} = q\hat{W}(q,p), \quad \tfrac{1}{2}\{\hat{p}, \hat{W}(q,p)\} = p\hat{W}(q,p). \tag{2.12}$$

Thus we may regard $\hat{W}(q,p)$ as operator analogues of Dirac delta functions concentrated at individual phase space points. In Ref. 19 they have been called phase point operators.

Turning to the Weyl map, it takes a general classical dynamical variable, a (square integrable) function $a(q,p)$ on the classical phase space, to a corresponding (Hilbert–Schmidt) operator $\hat{A}$ on $\mathcal{H}$:

$$a(q,p) \to \tilde{a}(p',q') = \int_{\mathbb{R}} \int_{\mathbb{R}} \mathrm{d}q\, \mathrm{d}p\, a(q,p) e^{i(pq'-qp')}$$

$$\to \hat{A} = \frac{1}{2\pi} \int_{\mathbb{R}} \int_{\mathbb{R}} \mathrm{d}q'\, \mathrm{d}p'\, \tilde{a}(p',q') U(p') V(q') e^{-iq'p'/2}. \tag{2.13}$$

The important property of this map is that traces of operators on $\mathcal{H}$ go into integrals over phase space,

$$\mathrm{Tr}(\hat{A}^{\dagger}\hat{B}) = \int_{\mathbb{R}} \int_{\mathbb{R}} \mathrm{d}q\, \mathrm{d}p\, a(q,p) * b(q,p). \tag{2.14}$$

One can immediately see that the relation between $a(q,p)$ and $\hat{A}$ is given by

$$\hat{A} = 2\pi \int_{\mathbb{R}} \int_{\mathbb{R}} \mathrm{d}q\, \mathrm{d}p\, a(q,p) \hat{W}(q,p), \tag{2.15}$$

thus establishing that the Wigner and Weyl maps are inverses of one another. Indeed extending the definition of the Wigner distribution (2.10) to a general operator $\hat{A}$ on $\mathcal{H}$, we have

$$a(q,p) = \mathrm{Tr}(\hat{A}\hat{W}(q,p)). \tag{2.16}$$

It is this kind of isomorphism that we wish to develop when $\mathbb{R}$ is replaced by a compact simple Lie group G.

The angle-angular momentum case: We now trace the changes which appear if we replace the Cartesian variable $q \in \mathbb{R}$ by an angle $\theta \in (-\pi, \pi)$. The corresponding Hermitian operator is denoted by $\hat{\theta}$, with eigenvalues θ; its canonical conjugate $\hat{M}$ has integer eigenvalues $m = 0, \pm 1, \pm 2, \ldots$. Thus $m \in \mathbb{Z}$ unlike the Cartesian p, so $\hat{M}$ is already quantized. The replacements for Eqs. (2.4) and (2.6) are

$$\mathcal{H} = L^2(\mathrm{S}^1) = \left\{ \psi(\theta) \,|\, \|\psi\|^2 = \int_{-\pi}^{\pi} \mathrm{d}\theta |\psi(\theta)|^2 < \infty \right\},$$

$$\psi(\theta) = \langle \theta | \psi \rangle, \quad \langle \theta' | \theta \rangle = \delta(\theta' - \theta), \quad \hat{\theta} | \theta \rangle = \theta | \theta \rangle,$$

$$\psi_m = \langle m | \psi \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{d}\theta\, e^{-im\theta} \psi(\theta), \tag{2.17}$$

$$\|\psi\|^2 = \sum_{m \in \mathbb{Z}} |\psi_m|^2,$$

$$\hat{M} | m \rangle = m | m \rangle, \quad \langle \theta | m \rangle = \frac{1}{\sqrt{2\pi}} e^{im\theta}.$$

In place of the Heisenberg commutation relation (2.1), we have only the exponentiated Weyl version,

$$U(m) = \exp(im\hat{\theta}), \quad V(\theta) = \exp(-i\theta\hat{M}),$$

$$U(m)V(\theta) = V(\theta)U(m)e^{im\theta}. \tag{2.18}$$

With the actions

$$(U(m')\psi)(\theta) = e^{im'\theta}\psi(\theta),$$

$$(V(\theta')\psi)(\theta) = \psi([\theta - \theta']), \tag{2.19}$$

$$[\theta - \theta'] = \theta - \theta' \bmod 2\pi,$$

we have an irreducible system on $\mathcal{H}=L^2(\mathbb{S}^1)$. The analogues of the displacement operators (2.3) are now

$$U(m)V(\theta)e^{-im\theta/2} = V(\theta)U(m)e^{im\theta/2}, \tag{2.20}$$

but here the exponents cannot be combined. They do however form a complete trace orthonormal system,

$$\mathrm{Tr}((U(m')V(\theta'))^{\dagger}U(m)V(\theta)) = 2\pi\delta_{mm'}\delta(\theta' - \theta). \tag{2.21}$$

With this preparation we can turn to the definition of the Wigner distribution and the Weyl map. For a given density operator $\hat{\rho}$ on $\mathcal{H}$, the former is

$$W(\theta,m) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}\theta' \left\langle \theta - \frac{1}{2}\theta' \middle| \hat{\rho} \middle| \theta + \frac{1}{2}\theta' \right\rangle \exp(im\theta'). \tag{2.22}$$

We see immediately that this is not a function on the classical phase space $T^*\mathbb{S}^1 \simeq \mathbb{S}^1 \times \mathbb{R}$, which is a cylinder, but on a partially quantized space $\mathbb{S}^1 \times \mathbb{Z}$. We may regard this space as standing somewhere in between $T^*\mathbb{S}^1$ and the fully quantum mechanical Hilbert space and operator setup. The marginals are properly reproduced in the sense that

$$\int_{-\pi}^{\pi} \mathrm{d}\theta\, W(\theta,m) = \langle m|\hat{\rho}|m\rangle,$$

$$\sum_{m\in\mathbb{Z}} W(\theta,m) = \langle \theta|\hat{\rho}|\theta\rangle. \tag{2.23}$$

We can display $W(\theta,m)$ as

$$W(\theta,m) = \mathrm{Tr}(\hat{\rho}\hat{W}(\theta,m)),$$

$$\hat{W}(\theta,m) = \hat{W}(\theta,m)^{\dagger} = \frac{1}{(2\pi)^2}\sum_{m'\in\mathbb{Z}}\int_{-\pi}^{\pi} \mathrm{d}\theta'\; U(m')V(\theta')e^{im\theta' - im'(\theta + 1/2\theta')}, \tag{2.24}$$

and like their Cartesian counterparts these operators form a trace orthonormal system,

$$\mathrm{Tr}(\hat{W}(\theta',m')\hat{W}(\theta,m)) = \frac{1}{2\pi}\delta(\theta' - \theta)\delta_{mm'}. \tag{2.25}$$

In a similar spirit, the Weyl map now takes any classical function $a(\theta,m)$ on $\mathbb{S}^1 \times \mathbb{Z}$ into an operator on $L^2(\mathbb{S}^1)$,

$$a(\theta,m) \to \tilde{a}(m',\theta') = \sum_{m\in\mathbb{Z}} \int_{-\pi}^{\pi} \mathrm{d}\theta\, a(\theta,m) e^{i(m\theta'-m'\theta)}$$

$$\to \hat{A} = \frac{1}{2\pi} \sum_{m'\in\mathbb{Z}} \int_{-\pi}^{\pi} \mathrm{d}\theta'\, \tilde{a}(m',\theta') U(m') V(\theta') e^{-im'\theta'/2}. \tag{2.26}$$

Then the trace operation becomes, as in (2.14),

$$\mathrm{Tr}(\hat{A}^{\dagger}\hat{B}) = \sum_{m\in\mathbb{Z}} \int_{-\pi}^{\pi} \mathrm{d}\theta\, a(\theta,m) * b(\theta,m). \tag{2.27}$$

Combining Eqs. (2.24) and (2.26) we are able to get the analogue to (2.15),

$$\hat{A} = 2\pi \sum_{m\in\mathbb{Z}} \int_{-\pi}^{\pi} \mathrm{d}\theta\, a(\theta,m) \hat{W}(\theta,m). \tag{2.28}$$

In this way the similarities as well as important differences compared to the Cartesian case are easily seen.

III. QUANTUM KINEMATICS IN THE LIE GROUP CASE AND THE WIGNER DISTRIBUTION

Let G be a (non-Abelian) compact simple Lie group of order n, with elements $g, g', \ldots$ and composition law $g', g \to g'g$. To set up the kinematics appropriate for a quantum system with configuration space $Q=G$, it is simplest to begin with the Hilbert space of Schrödinger wave functions. The normalized left and right invariant volume element on G is written as $\mathrm{d}g$. For suitable functions $f(g)$ on G we have the invariances and normalization condition

$$\int_G \mathrm{d}g\, f(g) = \int_G \mathrm{d}g\, (f(g'g) \quad \text{or } f(gg') \text{ or } f(g^{-1})),$$

$$\int_G \mathrm{d}g = 1. \tag{3.1}$$

Correspondingly we can introduce a Dirac delta function on G characterized by

$$\int_G \mathrm{d}g (\delta(g'^{-1}g) \quad \text{or } \delta(gg'^{-1}) \quad \text{or } \delta(g^{-1}g') \quad \text{or } \delta(g'g^{-1})) f(g) = f(g'). \tag{3.2}$$

Thus $\delta(g)$ is a delta function concentrated at the identity element $e \in G$.

We take the Hilbert space $\mathcal{H}$ for the quantum system to be made up of all complex square integrable functions on G:

$$\mathcal{H} = L^2(G) = \left\{ \psi(g) \in C \mid \|\psi\|^2 = \int_G \mathrm{d}g |\psi(g)|^2 < \infty \right\}. \tag{3.3}$$

A convenient basis of ideal vectors $|g\rangle$ can be introduced such that for a general $|\psi\rangle \in \mathcal{H}$ we may write

$$\psi(g) = \langle g|\psi\rangle, \quad \langle g'|g\rangle = \delta(g'g^{-1}). \tag{3.4}$$

The notion of position coordinates is intrinsically captured by the commutative algebra representing real valued smooth functions $f(g)$ on G, i.e., $f \in \mathcal{F}(G)$. To each such function we associate a Hermitian multiplicative operator $\hat{f}$ on $\mathcal{H}$:

$$f \in \mathcal{F}(G) \to \hat{f} = \int_G \mathrm{d}g\, f(g)|g\rangle\langle g|,$$

$$(\hat{f}\psi)(g) = f(g)\psi(g). \tag{3.5}$$

Thus all these operators commute with one another, being diagonal in the position description $\psi(g)$ of $|\psi\rangle$.

To complete the kinematics and to obtain an irreducible system of operators on $\mathcal{H}$ we have to adjoin suitable momenta. Here we have two choices, corresponding to the left and right translations of G on itself by group action. We choose the former, and so define a family of unitary operators $V(g)$ to give the left regular representation of G:

$$(V(g')\psi)(g) = \psi(g'^{-1}g),$$

$$V(g')|g\rangle = |g'g\rangle. \tag{3.6}$$

They obey

$$V(g')V(g) = V(g'g),$$

$$V(g)^\dagger V(g) = I. \tag{3.7}$$

To identify their Hermitian generators, we introduce a basis $\{e_r\}$ in the Lie algebra $\underline{G}$ of G. Using the exponential map $\underline{G} \to G$, we write a general $g \in G$ as

$$g = \exp(\alpha^r e_r), \tag{3.8}$$

the sum on r being from 1 to n. The generators $\hat{J}_r$ of $V(g)$ are then identified by

$$V(\exp(\alpha^r e_r)) = \exp(-i\alpha^r \hat{J}_r). \tag{3.9}$$

These are Hermitian operators on the Hilbert space $\mathcal{H}$, obeying commutation relations involving the structure constants C_{rs}^t of G:

$$[\hat{J}_r, \hat{J}_s] = iC_{rs}{}^t \hat{J}_t. \tag{3.10}$$

On Schrödinger wave functions $\psi(g)$ each $\hat{J}_r$ acts as a first order partial differential operator; indeed if the (right invariant) vector fields generating the left action of G on itself are written as X_r, then we have

$$\hat{J}_r\psi(g) = iX_r\psi(g). \tag{3.11}$$

The commutation relations (3.10) are direct consequences of similar commutation relations among the vector fields X_r.

The analogue of the Cartesian Heisenberg–Weyl system (2.1) and (2.2) is now obtained by setting together the following ingredients:

$$f_1, f_2 \in \mathcal{F}(G) \to \hat{f}_1\hat{f}_2 = \hat{f}_2\hat{f}_1,$$

$$f \in \mathcal{F}(G), \quad g' \in G \to V(g')\hat{f}V(g')^{-1} = \hat{f}', \tag{3.12}$$

$$f'(g) = f(g'^{-1}g),$$

along with the representation property (3.7) for $V(g)$. This is in the spirit of the unitary Weyl system (2.2). In infinitesimal terms we have

$$[\hat{J}_r, \hat{f}] = i\widehat{(X_r f)}, \tag{3.13}$$

combined with (3.10). The space $\mathcal{H}$ is indeed irreducible with respect to the family of operators $\{\hat{f}, V(\cdot)\}$ or equivalently $\{\hat{f}, \hat{J}_r\}$.

We can express functions of position also via unitary operators in the Weyl spirit as follows: for each real $f \in \mathcal{F}(G)$, we define the unitary operator $U(f)$ by

$$U(f) = e^{i\hat{f}}\colon\ (U(f)\psi)(g) = e^{if(g)}\psi(g). \tag{3.14}$$

It is then easy to see that we have the relations

$$\begin{aligned}
(U(f)V(g')\psi)(g) &= e^{if(g)}\psi(g'^{-1}g),\\
(V(g')U(f)\psi)(g) &= e^{if(g'^{-1}g)}\psi(g'^{-1}g),\\
(U(f)V(g')(V(g')U(f))^{\dagger}\psi)(g) &= e^{if(g)-if(g'^{-1}g)}\psi(g),
\end{aligned} \tag{3.15}$$

which is in the spirit of Eqs. (2.2) and (2.18), except that f is not restricted to be linear in any coordinate variables.

We see here that unlike in the n-dimensional Cartesian case the canonical momenta are a noncommutative system. Therefore the analogue or generalization of the single momentum eigenstate $|\underline{p}\rangle$ in the Cartesian situation will turn out to be a generally multidimensional Hermitian irreducible representation of (3.10), namely the generators of some unitary irreducible representation (UIR) of G. We will see this in detail as we proceed.

For completeness we should mention the operators giving the right regular representation of G. These are, say, $\tilde{V}(g)$, defined by and obeying

$$\begin{aligned}
(\tilde{V}(g')\psi)(g) &= \psi(gg'),\\
\tilde{V}(g')|g\rangle &= |gg'^{-1}\rangle,\\
\tilde{V}(g')\tilde{V}(g) &= \tilde{V}(g'g),\\
V(g')\tilde{V}(g) &= \tilde{V}(g)V(g').
\end{aligned} \tag{3.16}$$

However as is well known their generators $\hat{\tilde{J}}_r$ are determined by $\hat{J}_r$ and the matrices $(\mathcal{D}^s_r(g))$ of the adjoint representation of G, by

$$\hat{\tilde{J}}_r = -\mathcal{D}^s_r(g)\hat{J}_s. \tag{3.17}$$

Therefore it suffices to regard the collection of operators $\{\hat{f}, V(\cdot)\}$ as providing the replacement for the Heisenberg–Weyl system in the present case.

Complementary to the position basis $|g\rangle$ for $\mathcal{H}$ is a momentum basis. This can be set up using the Peter–Weyl theorem involving all the UIR's of G. We denote the various UIR's by j, with dimension N_j; we label rows and columns within the jth UIR by magnetic quantum numbers m, n. Thus the unitary matrix representing $g \in G$ in the jth UIR is

$$g \to (D^j_{mn}(g)). \tag{3.18}$$

In general each of j,m,n is a collection of several independent discrete quantum numbers, and there is a freedom of unitary changes in the choice of m,n. In addition to unitarity and the composition law,

$$\sum_n D^j_{mn}(g) * D^j_{m'n}(g) = \delta_{mm'},$$

$$\sum_n D^j_{mn}(g')D^j_{nn'}(g) = D^j_{mn'}(g'g), \tag{3.19}$$

we have orthogonality and completeness properties,

$$\int_G \mathrm{d}g\, D^j_{mn}(g)D^{j'}_{m'n'}(g)\, * \,= \delta_{jj'}\delta_{mm'}\delta_{nn'}/N_j,$$

$$\sum_{jmn} N_j D^j_{mn}(g)D^j_{mn}(g')\, * \,= \delta(g^{-1}g'). \tag{3.20}$$

Then a simultaneous complete reduction of both representations $V(\cdot)$, $\tilde{V}(\cdot)$ of G is achieved by passing to a new orthonormal basis $|jmn\rangle$ for $\mathcal{H}$. Its definition and basic properties are

$$|jmn\rangle = N_j^{1/2}\int_G \mathrm{d}g\, D^j_{mn}(g)|g\rangle,$$

$$\langle j'm'n'|jmn\rangle = \delta_{j'j}\delta_{m'm}\delta_{n'n},$$

$$V(g)|jmn\rangle = \sum_{m'} D^j_{mm'}(g^{-1})|jm'n\rangle, \tag{3.21}$$

$$\tilde{V}(g)|jmn\rangle = \sum_{n'} D^j_{n'n}(g)|jmn'\rangle.$$

Therefore in $|jmn\rangle$ the index n counts the multiplicity of occurrence of the jth UIR in the reduction of $V(\cdot)$ and m performs a similar function in the reduction of $\tilde{V}(\cdot)$.

We now regard the sets of N_j^2 states $\{|jmn\rangle\}$ for each fixed j as momentum eigenstates in the present context. This means that the n-dimensional real momentum eigenvalue $\underline{p}$ in Cartesian quantum mechanics is now replaced by a collection of (discrete) quantum numbers jmn. A vector $|\psi\rangle \in \mathcal{H}$ with wave function $\psi(g)$ is given in the momentum description by a set of expansion coefficients ψ_{jmn},

$$\psi \in \mathcal{H} \to \psi_{jmn} = \langle jmn|\psi\rangle = N_j^{1/2}\int_G \mathrm{d}g\, D^j_{mn}(g) * \psi(g),$$

$$\|\psi\|^2 = \sum_{jmn} |\psi_{jmn}|^2. \tag{3.22}$$

A normalized $|\psi\rangle$ then determines two complementary probability distributions, $|\psi(g)|^2$ on G and $|\psi_{jmn}|^2$ on momentum space.

In this situation a (provisional and overcomplete) Wigner distribution $\tilde{W}(g;jmn\,m'n')$ can be defined for each $|\psi\rangle \in \mathcal{H}$ (or for any mixed state $\hat{\rho}$ as well). (Here we depart slightly from the

notation in Ref. 21, so that our later expressions are more concise.) It transforms in a reasonable manner when $|\psi\rangle$ is acted upon by $V(\cdot)$ or $\tilde{V}(\cdot)$; and it reproduces in a simple and direct way the two probability distributions determined by $|\psi\rangle$, as marginals. We give only the latter property here,

$$\sum_{jmn} \tilde{W}(g;jmn\ mn) = |\psi(g)|^2,$$

$$\int_G \mathrm{d}g\ \tilde{W}(g;jmn\ m'n') = \psi_{jm'n'}\ \psi^*_{jmn}. \tag{3.23}$$

The right-hand side of the second relation is a natural generalization of $|\psi_{jmn}|^2$, to allow for freedom in the choice of labels m,n within each UIR j. The expression for this Wigner distribution involves a function s, $G\times G\to G$ obeying certain conditions and is

$$\tilde{W}(g;jmn\ m'n') = N_j \int_G \mathrm{d}g' \int_G \mathrm{d}g''\ \psi(g'')\psi(g') * D^j_{m'n'}(g'') * D^j_{mn}(g')\,\delta(g^{-1}s(g',g'')). \tag{3.24}$$

Reality in the Cartesian or single angle-angular momentum cases is replaced here by Hermiticity,

$$\tilde{W}(g;jmn\ m'n') * = \tilde{W}(g;jm'n'\ mn). \tag{3.25}$$

The conditions on $s(g',g'')$ to ensure that all the above properties are secured are

$$g',g'' \in G \to s(g',g'') = s(g'',g') \in G,$$

$$s(g_1g'g_2,g_1g''g_2) = g_1\ s(g',g'')g_2, \tag{3.26}$$

$$s(g',g') = g'.$$

We can simplify the problem of constructing such a function by exploiting the second of these relations to write

$$s(g',g'') = g's(e,g'^{-1}g'') = g's_0(g'^{-1}g''), \tag{3.27}$$

so the function $s_0(g)$ of a single group element must satisfy

$$s_0(e) = e,$$

$$s_0(g^{-1}) = g^{-1}s_0(g) = s_0(g)g^{-1}, \tag{3.28}$$

$$s_0(g'gg'^{-1}) = g'\ s_0(g)g'^{-1}.$$

The solution proposed in Ref. 21 is to take $s_0(g)$ to be the midpoint along the geodesic from the identity $e\in G$ to g. These geodesics are determined starting from the invariant Cartan–Killing metric on G, and have the necessary behaviors under left and right group actions to ensure that all of Eqs. (3.26) and (3.28) are obeyed. In the exponential notation of Eq. (3.8) we have

$$s_0(\exp(\alpha^r\ e_r)) = \exp(\tfrac{1}{2}\alpha^r\ e_r), \tag{3.29}$$

since it is true that geodesics passing through the identity are one parameter subgroups. With this explicit construction we have the additional relation

$$s_0(g^{-1}) = s_0(g)^{-1},$$

i.e.,

$$s_0(g)\ s_0(g) = g. \tag{3.30}$$

Thus $s_0(g)$ is the (almost everywhere unique) square root of g and $s(g',g'')$ is a kind of symmetric square root of g' and g''.

We shall explore the properties of $\tilde{W}(g;jmn\,m'n')$ in the next section, especially the sense in which it contains information about $|\psi\rangle\langle\psi|$ in an overcomplete manner. This will then lead to the Wigner–Weyl isomorphism for quantum mechanics on a (compact simple) Lie group.

IV. THE WIGNER–WEYL ISOMORPHISM IN THE LIE GROUP CASE

The definition (3.24) can be immediately extended to associate an object $\tilde{W}_{\hat{A}}(g;jmn\,m'n')$ with every linear operator $\hat{A}$ on $\mathcal{H}$ (of Hilbert–Schmidt class). In terms of the integral kernel $\langle g''|\hat{A}|g'\rangle$ of $\hat{A}$ we have

$$\tilde{W}_{\hat{A}}(g;jmn\,m'n') = N_j \int_G \mathrm{d}g' \int_G \mathrm{d}g'' \langle g''|\hat{A}|g'\rangle D^j_{m'n'}(g'') * D^j_{mn}(g')\,\delta(g^{-1}s(g',g'')). \tag{4.1}$$

It is indeed the case that this expression describes or determines $\hat{A}$ completely, however this happens in an overcomplete manner. There are certain linear relations obeyed by $\tilde{W}_{\hat{A}}(g;jmn\,m'n')$ which have an $\hat{A}$ independent form. We now obtain these relations, then proceed to construct a simpler expression which contains complete information about $\hat{A}$ without redundancy.

The Dirac delta function in the integral on the right-hand side of Eq. (4.1) means that the only contributions to the integral are from the points where

$$s(g',g'') = g. \tag{4.2}$$

Writing this as

$$s_0(g'^{-1}g'') = g'^{-1}g, \tag{4.3}$$

and then using Eq. (3.30), we see that, say, in the g'' integration the delta function picks out the single point determined by

$$g'^{-1}g'' = (g'^{-1}g)^2,$$

i.e.,

$$g'' = gg'^{-1}g. \tag{4.4}$$

This means that $\delta(g^{-1}s(g',g''))$ is some Jacobian factor times $\delta(g''^{-1}gg'^{-1}g)$. We are therefore permitted to use this value for g'' elsewhere in the integrand, so

$$\tilde{W}_{\hat{A}}(g;jmn\,m'n') = N_j \int_G \mathrm{d}g' \int_G \mathrm{d}g'' \langle gg'^{-1}g|\hat{A}|g'\rangle D^j_{m'n'}(gg'^{-1}g) * D^j_{mn}(g')\,\delta(g^{-1}s(g',g'')). \tag{4.5}$$

Transferring the g-dependent representation matrices from the right-hand side to the left-hand side and using unitarity, we get

$$\sum_{m'n'} D^j_{m'm''}(g)D^j_{n''n'}(g)\tilde{W}_{\hat{A}}(g;jmn\ m'n') = N_j \int_G \mathrm{d}g' \int_G \mathrm{d}g''\ \delta(g^{-1}s(g',g'')) \times \langle gg'^{-1}g|\hat{A}|g'\rangle D^j_{n''m''}(g')D^j_{mn}(g'). \tag{4.6}$$

It is now clear we have symmetry of the expression on the left-hand side under the simultaneous interchanges $m \leftrightarrow n''$, $n \leftrightarrow m''$, a statement independent of $\hat{A}$. This is the sense in which $\tilde{W}_{\hat{A}}(g;jmn\ m'n')$ contains information about $\hat{A}$ in an overcomplete manner, and this happens only when G is non-Abelian.

Taking advantage of this, we now associate to $\hat{A}$ the simpler quantity

$$W_{\hat{A}}(g;jmm') = N_j^{-1}\sum_n \tilde{W}_{\hat{A}}(g;jmn\ m'n) = \int_G \mathrm{d}g' \int_G \mathrm{d}g''\langle g''|\hat{A}|g'\rangle D^j_{mm'}(g'g''^{-1})\delta(g^{-1}s(g',g'')). \tag{4.7}$$

We shall call this the Weyl symbol corresponding to the operator $\hat{A}$. The passage $\hat{A} \to \hat{A}^\dagger$ results in

$$W_{\hat{A}^\dagger}(g;jmm') = W_{\hat{A}}(g;jm'm)^*. \tag{4.8}$$

It is easy to obtain the transformation properties of the Weyl symbol under conjugation of $\hat{A}$ by either the left or the right regular representation,

$$\hat{A}' = V(g_0)\hat{A}V(g_0)^{-1},$$

$$W_{\hat{A}'}(g;jmm') = \sum_{m_1m_1'} D^j_{mm_1}(g_0)D^j_{m'm_1'}(g_0)^* W_{\hat{A}}(g_0^{-1}g;jm_1m_1'), \tag{4.9}$$

$$\hat{A}'' = \tilde{V}(g_0)\hat{A}\tilde{V}(g_0)^{-1},$$

$$W_{\hat{A}''}(g;jmm') = W_{\hat{A}}(gg_0;jmm').$$

Next we can verify that if $\hat{A}$ and $\hat{B}$ are any two Hilbert–Schmidt operators on $\mathcal{H}$, then $\mathrm{Tr}(\hat{A}\hat{B})$ can be simply expressed in terms of their Weyl symbols,

$$\mathrm{Tr}(\hat{A}\hat{B}) = \sum_{jmm'} N_j \int_G \mathrm{d}g\ W_{\hat{A}}(g;jmm')W_{\hat{B}}(g;jm'm). \tag{4.10}$$

The proof exploits the completeness relation in (3.20) and the properties (3.26) of $s(g',g'')$. This key result proves that $\hat{A}$ is indeed completely determined by its Weyl symbol: $\hat{A}$ is certainly determined by the values of $\mathrm{Tr}(\hat{A}\hat{B})$ for all $\hat{B}$, and the latter are known once the Weyl symbols are known.

Before expressing the Weyl symbol of $\hat{A}$ in a form analogous to Eq. (2.16), we give examples for some simple choices of $\hat{A}$,

$$\begin{array}{cc} \hat{A} & W_{\hat{A}}(g;jmm') \\ \hline \hat{f}=\int_G \mathrm{d}g\, f(g)|g\rangle\langle g| & f(g)\delta_{mm'} \\ V(g_0) & D^j_{mm'}(g_0^{-1}) \\ \tilde{V}(g_0) & D^j_{mm'}(gg_0g^{-1}) \\ \hat{f}V(g_0) & f(s_0(g_0)g)D^j_{mm'}(g_0^{-1}) \\ V(g_0)\hat{f} & f(s_0(g_0)^{-1}g)D^j_{mm'}(g_0^{-1}) \end{array} \tag{4.11}$$

We shall comment later on the structure of these Weyl symbols. However it is already instructive to compare these results with the Cartesian situation

$$\begin{array}{cc} \hat{A} & W(q,p) \\ \hline \hat{f}=f(\hat{q}) & f(q) \\ V(q') & \exp(-ipq') \\ \hat{f}V(q')=f(\hat{q})V(q') & f(q+q'/2)\exp(-ipq') \\ V(q')f(\hat{q}) & f(q-q'/2)\exp(-ipq') \end{array} \tag{4.12}$$

Now we turn to the problem of expressing the Weyl symbol of $\hat{A}$ in the form

$$W_{\hat{A}}(g;jmm')=\mathrm{Tr}(\hat{A}\hat{W}(g;jmm')) \tag{4.13}$$

for a suitable operator $\hat{W}(g;jmm')$. This would be the analogue of $\hat{W}(q,p)$ in Eq. (2.10). Since the kernel $\langle g''|\hat{A}|g'\rangle$ is quite general, Eq. (4.13) and Eq. (4.7) imply

$$\langle g'|\hat{W}(g;jmm')|g''\rangle = D^j_{mm'}(g'g''^{-1})\,\delta(g^{-1}s(g',g'')) = D^j_{mm'}(g'g''^{-1})\,\delta(g^{-1}s_0(g''g'^{-1})g'). \tag{4.14}$$

We shall synthesize $\hat{W}(g;jmm')$ in steps. We begin by defining a family of commuting operators $U(jmn)$ in the manner of Eq. (3.5), all of them diagonal in the position basis,

$$(U(jmn)\psi)(g)=D^j_{mn}(g)\psi(g). \tag{4.15}$$

These are analogous to the Cartesian $U(p')$, labeled by a momentum eigenvalue jmn, functions of position alone. They are unitary in the matrix sense,

$$\sum_m U(jmn)^\dagger U(jmn')=\sum_m U(jnm)^\dagger U(jn'm)=\delta_{n'n}I. \tag{4.16}$$

These operators allow us to express the map $f\in\mathcal{F}(G)\to\hat{f}$ of Eq. (3.5) more explicitly as follows:

$$f(g)=\sum_{jmn} f_{jmn}D^j_{mn}(g)\Rightarrow \hat{f}=\sum_{jmn} f_{jmn}U(jmn). \tag{4.17}$$

Upon conjugation by $V(g)$ we have

$$V(g)^{-1}U(jmn)V(g)=\sum_{m'} D^j_{mm'}(g)U(jm'n). \tag{4.18}$$

Combining Eqs. (3.16), (3.20), and (4.15) we easily obtain the trace orthonormality property

$$\mathrm{Tr}((U(j'm'n')V(g'))^{\dagger}U(jmn)V(g)) = N_j^{-1}\delta_{j'j}\delta_{m'm}\delta_{n'n}\delta(g^{-1}g'), \tag{4.19}$$

analogous to Eqs. (2.7) and (2.5). The action of $U(j'm'n')$ on the momentum eigenstates $|jmn\rangle$ can be worked out; it involves the Clebsch–Gordan coefficients for the reduction of direct products of two general UIR's of G and reads

$$U(j'm'n')|jmn\rangle = \sum_{j''m''n''\lambda} \sqrt{\frac{N_j}{N_{j''}}} C^{j'jj''\lambda}_{m'mm''} * C^{j'jj''\lambda}_{n'nn''} |j''m''n''\rangle. \tag{4.20}$$

Here λ is a multiplicity index keeping track of the possibly multiple occurrences of the UIR $D^{j''}$ in the reduction of the direct product $D^{j'} \times D^{j}$. The significance of this relation is similar in spirit to the statement in the Cartesian case that $U(p') = \exp(ip'\hat{q})$ generates a translation in $\hat{p}$, in other words that in the momentum description $\hat{q}$ is given by the differential operator $i(\mathrm{d}/\mathrm{d}p)$. The result (4.20) however involves discrete labels since G is compact, unlike continuous Cartesian variables, and incorporates non-Abelianness as well. Therefore translating the momentum jmn by the amount $j'm'n'$ yields several final momenta $j''m''n''$ according to the contents of the direct product $D^{j'} \times D^{j}$ of UIR's of G.

Now multiply both sides of Eq. (4.14) by $D^{j_1}_{m_1m_1'}(g)$ and integrate with respect to g, this is Fourier transformation with respect to g and gives

$$\langle g'| \int_G \mathrm{d}g\, D^{j_1}_{m_1m_1'}(g) \hat{W}(g;jmm')|g''\rangle = D^{j}_{mm'}(g'g''^{-1}) D^{j_1}_{m_1m_1'}(s_0(g''g'^{-1})g'). \tag{4.21}$$

Now perform an inverse Fourier transformation with respect to the momenta jmm' to get

$$\begin{aligned} &\sum_{jmm'} N_j D^{j}_{mm'}(g_1) * \langle g'| \int_G \mathrm{d}g\, D^{j_1}_{m_1m_1'}(g) \hat{W}(g;jmm')|g''\rangle \\ &\quad = D^{j_1}_{m_1m_1'}(s_0(g''g'^{-1})g')\,\delta(g_1g''g'^{-1}) = D^{j_1}_{m_1m_1'}(s_0(g_1^{-1})g')\,\delta(g_1g''g'^{-1}) \\ &\quad = \langle g'|g_1g''\rangle D^{j_1}_{m_1m_1'}(s_0(g_1^{-1})g') = \sum_{m_2} \langle g'|U(j_1m_2m_1')V(g_1)|g''\rangle D^{j_1}_{m_1m_2}(s_0(g_1^{-1})). \end{aligned} \tag{4.22}$$

Comparing the two sides and peeling off $\langle g'|$ and $|g''\rangle$ gives

$$\sum_{jmm'} N_j D^{j}_{mm'}(g_1) * \int_G \mathrm{d}g\, D^{j_1}_{m_1m_1'}(g) \hat{W}(g;jmm') = \sum_{m_2} D^{j_1}_{m_1m_2}(s_0(g_1^{-1})) U(j_1m_2m_1')V(g_1). \tag{4.23}$$

Then Fourier inversion twice yields the result

$$\hat{W}(g;jmm') = \sum_{j_1m_1m_2} N_{j_1} \int_G \mathrm{d}g_1\, U(j_1m_2m_1)V(g_1) D^{j}_{mm'}(g_1) D^{j_1}_{m_1m_2}(g^{-1}s_0(g_1^{-1})). \tag{4.24}$$

This may be compared in every detail with the Cartesian result in Eq. (2.10), the correspondence of arguments and integration/summation variables is (including the factors representing momentum eigenfunctions)

$$q \to g, \quad p \to jmm', \quad q' \to g_1, \quad p' \to j_1m_1m_2,$$

$$e^{ipq'} \to D^{j}_{mm'}(g_1), \quad e^{-ip'(q+q'/2)} \to D^{j_1}_{m_1m_2}(g^{-1}s_0(g_1^{-1})). \tag{4.25}$$

Giving due attention to the new matrix features, the correspondence is quite remarkable.

Combining Eqs. (3.28) and (4.14) we obtain the relation

$$\hat{W}(g;jmn)^{\dagger} = \hat{W}(g;jnm). \tag{4.26}$$

Similarly combining Eqs. (4.24) and (4.19) and carrying out quite elementary operations leads to analogues to the Cartesian relations (2.11) and (2.15) in the forms

$$\mathrm{Tr}(\hat{W}(g';j'm'n')^{\dagger}\hat{W}(g;jmn)) = N_j^{-1}\delta_{jj'}\delta_{mm'}\delta_{nn'}\delta(g^{-1}g'),$$

$$\hat{A} = \sum_{jmn} N_j \int_G \mathrm{d}g\; W_{\hat{A}}(g;jnm)\hat{W}(g;jmn). \tag{4.27}$$

We may thus conclude that we have succeeded in setting up a Wigner–Weyl isomorphism for quantum mechanics on a compact simple Lie group with reasonable properties.

V. THE STAR PRODUCT FOR WEYL SYMBOLS

In this section we sketch the derivation of the expression for noncommutative operator multiplication in terms of the corresponding Weyl symbols, relegating some details to the Appendix. Thus, for two operators $\hat{A}$ and $\hat{B}$ we seek an expression for the Weyl symbol of $\hat{A}\hat{B}$ in terms of those of $\hat{A}$ and $\hat{B}$ in the form

$$W_{\hat{A}\hat{B}}(g;jmn) = (W_{\hat{A}} \star W_{\hat{B}})(g;jmn). \tag{5.1}$$

From Eq. (4.13) we have

$$(W_{\hat{A}} \star W_{\hat{B}})(g;jmn) = \mathrm{Tr}(\hat{A}\hat{B}\hat{W}(g;jmn)), \tag{5.2}$$

so using Eq. (4.27) for $\hat{A}$ as well as for $\hat{B}$ we have

$$(W_{\hat{A}} \star W_{\hat{B}})(g;jmn) = \sum_{\substack{j'm'n' \\ j''m''n''}} N_{j'}N_{j''} \int_G \mathrm{d}g'' \int_G \mathrm{d}g'\; W_{\hat{A}}(g'';j''n''m'')W_{\hat{B}}(g';j'n'm') \times \mathrm{Tr}(\hat{W}(g'';j''m''n'')\hat{W}(g';j'm'n')\hat{W}(g;jmn)). \tag{5.3}$$

We therefore need to compute the trace of the product of three $\hat{W}$'s, which is a nonlocal integral kernel defining the (associative but noncommutative) star product on the left-hand side. The two ingredients for this calculation are expressions for the product $U(jmn)V(g)$ in terms of $\hat{W}(g';j'm'n')$, and for the product $U(j'm'n')V(g')U(jmn)V(g)$ in terms of similar products UV. These are

$$U(jmn)V(g) = \sum_{j'm'n'} N_{j'} D^{j'}_{m'n'}(g) * \int_G \mathrm{d}g'\; D^{j}_{mn}(s_0(g)g')\hat{W}(g';j'm'n'), \tag{5.4a}$$

$$U(j'm'n')V(g')U(jmn)V(g) = \sum_{j''m''n''k} C^{j'\ j\ j''}_{m'n'\ kn\ m''n''} D^{j}_{mk}(g'^{-1})U(j''m''n'')V(g'g). \tag{5.4b}$$

The derivations are given in the Appendix, and the C-symbol on the right-hand side in the second equation is a sum of products of Clebsch–Gordan coefficients of the type occurring in Eq. (4.20).

Starting from Eq. (4.24) and using Eq. (5.4b) we have for the product of two $\hat{W}$'s,

$$\hat{W}(g';j'm'n')\hat{W}(g;jmn)$$

$$= \sum_{\substack{j_0,m_0,n_0\\ j_0'm_0'n_0'}} N_{j_0}N_{j_0'}\int_G \mathrm{d}g_0 \int_G \mathrm{d}g_0'\, D^{j}_{mn}(g_0)D^{j'}_{m'n'}(g_0')$$

$$\times D^{j_0}_{n_0m_0}(g^{-1}s_0(g_0^{-1}))D^{j_0'}_{n_0'm_0'}(g'^{-1}s_0(g_0'^{-1}))U(j_0'm_0'n_0')V(g_0')U(j_0m_0n_0)V(g_0)$$

$$= \sum_{\substack{j_0m_0n_0k_0\\ j_0'm_0'n_0'\\ j_0''m_0''n_0''}} N_{j_0}N_{j_0'}C^{j_0'}_{m_0'n_0'\ k_0n_0}\ {}^{j_0''}_{m_0''n_0''}\int_G \mathrm{d}g_0 \int_G \mathrm{d}g_0'\, D^{j}_{mn}(g_0)D^{j'}_{m'n'}(g_0')$$

$$\times D^{j_0}_{m_0k_0}(g_0'^{-1})D^{j_0}_{n_0m_0}(g^{-1}s_0(g_0^{-1}))D^{j_0'}_{n_0'm_0'}(g'^{-1}s_0(g_0'^{-1}))\times U(j_0''m_0''n_0'')V(g_0'g_0). \tag{5.5}$$

If here we use Eq. (5.4a) and then Eq. (4.27) we obtain for the kernel in Eq. (5.3),

$$\mathrm{Tr}(\hat{W}(g'';j''m''n'')\hat{W}(g';j'm'n')\hat{W}(g;jmn))$$

$$= \sum_{\substack{j_0m_0n_0k_0\\ j_0'm_0'n_0'\\ j_0''m_0''n_0''}} N_{j_0}N_{j_0'}C^{j_0'}_{m_0'n_0'\ k_0n_0}\ {}^{j_0''}_{m_0''n_0''}\int_G \mathrm{d}g_0 \int_G \mathrm{d}g_0'\, D^{j}_{mn}(g_0)D^{j'}_{m'n'}(g_0')D^{j''}_{n''m''}(g_0'g_0)\ *$$

$$\times D^{j_0}_{m_0k_0}(g_0'^{-1})D^{j_0}_{n_0m_0}(g^{-1}s_0(g_0^{-1}))D^{j_0'}_{n_0'm_0'}(g'^{-1}s_0(g_0'^{-1}))D^{j_0''}_{m_0''n_0''}(s_0(g_0'g_0)g''). \tag{5.6}$$

The star product of Eq. (5.3) is then obtained by inserting this integral kernel on the right-hand side.

A slightly simpler expression—which amounts to trading four of the D-functions for Dirac delta functions—results from direct use of Eq. (4.14),

$$\mathrm{Tr}(\hat{W}(g'';j''m''n'')\hat{W}(g';j'm'n')\hat{W}(g;jmn))$$

$$= \int_G \mathrm{d}g_0 \int_G \mathrm{d}g_0' \int_G \mathrm{d}g_0'' \langle g_0|\hat{W}(g'';j''m''n'')|g_0'\rangle\langle g_0'|\hat{W}(g';j'm'n')|g_0''\rangle\langle g_0''|\hat{W}(g;jmn)|g_0\rangle$$

$$= \int_G \mathrm{d}g_0 \int_G \mathrm{d}g_0' \int_G \mathrm{d}g_0''\, D^{j''}_{m''n''}(g_0g_0'^{-1})D^{j'}_{m'n'}(g_0'g_0''^{-1})$$

$$\times D^{j}_{mn}(g_0''g_0^{-1})\,\delta(g''^{-1}s(g_0,g_0'))\,\delta(g'^{-1}s(g_0',g_0''))\,\delta(g^{-1}s(g_0'',g_0)). \tag{5.7}$$

These expressions for the star product show an unavoidable complexity for general compact non-Abelian G. In the one-dimensional Abelian (but non-Cartesian) case $Q=\mathbb{S}^1$, there are some simplifications. Referring to Sec. II, we have the rule for Weyl symbols given by Eq. (2.25) and (2.28),

$$a(\theta;m) = \mathrm{Tr}(\hat{A}\hat{W}(\theta;m)),$$

$$\hat{A} = 2\pi \sum_{m\in\mathbb{Z}} \int_{-\pi}^{\pi} \mathrm{d}\theta\, a(\theta;m)\hat{W}(\theta;m). \tag{5.8}$$

The star product then appears as

$$(a \star b)(\theta;m) = \sum_{m',m'' \in \mathbb{Z}} \int_{-\pi}^{\pi} \mathrm{d}\theta'' \int_{-\pi}^{\pi} \mathrm{d}\theta' \ \mathrm{Tr}(\hat{W}(\theta'';m'')\hat{W}(\theta';m')\hat{W}(\theta;m))a(\theta'';m'')b(\theta';m'),$$

$$\mathrm{Tr}(\hat{W}(\theta'';m'')\hat{W}(\theta';m')\hat{W}(\theta;m)) = \frac{1}{4\pi^2} \sum_{m_0,m_0' \in \mathbb{Z}} \int_{-\pi}^{\pi} d\theta_0' \int_{-\pi}^{\pi} d\theta_0 e^{i/2(m_0'\theta_0 - m_0\theta_0')} \exp[i(m\theta_0 - m_0\theta + m'\theta_0' - m_0'\theta' + (m_0 + m_0')\theta'' - m''(\theta_0 + \theta_0'))]. \tag{5.9}$$

This expression for the kernel results from Eq. (5.6) if we first drop the magnetic quantum numbers $m,n,m',n',m'',n'',m_0,n_0,k_0,m_0',n_0',m_0'',n_0''$; then set the dimensionalities N_{j0}, $N_{j_0'}$ equal to unity; next make the replacements $j \to m, j' \to m', j'' \to m'', j_0 \to m_0, j_0' \to m_0', g_0 \to \theta_0, g_0' \to \theta_0'$, and use for the C coefficient the Kronecker delta $\delta_{j_0'',m_0+m_0'}$. Even with some simplifications, the kernel in Eq. (5.9) remains nonlocal because of (among other things) the occurrence of half-angles in the exponent.

VI. DISCUSSION AND CONCLUDING REMARKS

The characteristic feature revealed by our analysis is that for quantum mechanics on a Lie group G as configuration space, the concept of canonical momentum is a collection of noncommuting operators $\hat{J}_r$, in fact constituting the Lie algebra of the left regular representation of G on $L^2(G)$. This in itself is known, but it results in the analogues of momentum eigenvalue being a set of discrete labels jmn, and the single Cartesian momentum eigenvector $|p\rangle$ being replaced by a multidimensional set of vectors $\{|jmn\rangle\}$. Other consequences of this non-Abelianness should be noted. One needs to work with both overcomplete and with complete nonredundant Weyl symbols for general operators $\hat{A}$: the former are useful for reproducing in a simple manner the two complementary marginal probability distributions associated with a pure or mixed quantum state from its Wigner distribution as shown in Eq. (3.23); while the latter lead to the Wigner–Weyl isomorphism in a reasonable manner.

It is interesting that the Weyl symbols $W_{\hat{A}}(g;jmm')$ are not complex valued functions on the classical phase space T^*G. They may be more compactly viewed as follows. Whereas by the Peter–Weyl theorem the Hilbert space $\mathcal{H}=L^2(G)$ carries each UIR $\mathcal{D}^{(j)}(\cdot)$ of G as often as its dimension N_j, the structure of Eq. (4.7) leads us to define a smaller Hilbert space $\mathcal{H}_0$ carrying each UIR of G exactly once:

$$\mathcal{H}_0 = \sum_j \oplus \mathcal{H}^{(j)},$$

$$\mathcal{H}^{(j)} = \mathrm{Sp}\{|jm)\}, \quad \dim \mathcal{H}^{(j)} = N_j, \tag{6.1}$$

$$(j'm'|jm) = \delta_{j'j}\delta_{m'm},$$

with $\mathcal{H}^{(j)}$ carrying the UIR $\mathcal{D}^{(j)}(\cdot)$ of G. Then the Weyl symbol of a general operator $\hat{A}$, $W_{\hat{A}}(g;jmm')$, may be regarded as a function of $g \in G$ and an operator on $\mathcal{H}_0$. This is evident from the examples of Weyl symbols given in Eq. (4.11); in the Cartesian case in Eq. (4.12) such features are of course absent. This can be understood also from the following point of view. In the normal quantum description an operator $\hat{A}$ on $\mathcal{H}=L^2(G)$ can be given via its kernel $\langle g''|\hat{A}|g'\rangle$, or via its complementary diagonal plus off-diagonal matrix elements $\langle j'm'n'|\hat{A}|jmn\rangle$. If in the latter we trade half of the labels for a dependence on a group element g, we arrive at the Weyl symbol $W_{\hat{A}}(g;jmm')$ viewed as a block diagonal operator on $\mathcal{H}_0$ with simultaneously a dependence on g. Thus while the Wigner–Weyl isomorphism does not work directly with the true classical phase

space T^*G, it seems to use what may be called a noncommutative cotangent space, standing somewhere between T^*G and operators on $L^2(G)$.

Nevertheless the link to functions on the classical phase space T^*G can be established, as we will see below.

We may use the phrase "semiquantized phase space" for the space on which the Weyl symbols $W_{\hat{A}}(g;jmn)$ of operators $\hat{A}$ are defined. It is to be understood that this phrase includes the restriction that only (g-dependent) block-diagonal operators on $\mathcal{H}_0$ are encountered. This may be viewed as a superselection rule. In detail, given an operator $\hat{A}$ on $\mathcal{H}=L^2(G)$, we associate with it the g-dependent block-diagonal operator,

$$\tilde{A}(g) = \sum_j \sum_{m,n} \sqrt{N_j} W_{\hat{A}}(g;jmn)|jm)(jn|, \tag{6.2}$$

acting on $\mathcal{H}_0$, and we then have the connection

$$\mathrm{Tr}_{\mathcal{H}}(\hat{A}\hat{B}) = \int_G \mathrm{d}g\, \mathrm{Tr}_{\mathcal{H}_0}(\tilde{A}(g)\tilde{B}(g)). \tag{6.3}$$

The Weyl symbol $\tilde{A}(g)$ is simpler than $\hat{A}$ both in that it acts on the much smaller Hilbert space $\mathcal{H}_0$, and in that it is block diagonal.

To finally establish the link to suitable functions on the classical phase space T^*G, we exploit both the fact that the representation of G on $\mathcal{H}_0$ has a multiplicity-free reduction into UIR's, and the fact that $\tilde{A}(g)$ is block diagonal. Let us denote the generators of G on $\mathcal{H}_0$ by $\hat{J}^{(0)}_r$, $r=1,2,\ldots,n$. The Weyl symbol $\tilde{A}(g)$ may initially be written as the direct sum of symbols $\tilde{A}_j(g)$ acting within each subspace $\mathcal{H}^{(j)}$ in $\mathcal{H}_0$,

$$\tilde{A}(g) = \sum_j \oplus \tilde{A}_j(g),$$

$$\tilde{A}_j(g) = \sum_{m,n} \sqrt{N_j} W_{\tilde{A}}(g;jmn)|jm)(jn|. \tag{6.4}$$

Next, using the irreducibility of $\{\hat{J}^{(0)}_r\}$ acting on $\mathcal{H}^{(j)}$, we can expand $\tilde{A}_j(g)$ uniquely as a sum of symmetrized polynomials in $\hat{J}^{(0)}_r$,

$$\tilde{A}_j(g) = \sum_{N=0,1,\ldots} \sum_{r_1,r_2,\ldots,r_N} a_{r_1\ldots r_N}(g;j)\{\hat{J}^{(0)}_{r_1}\hat{J}^{(0)}_{r_2}\cdots\hat{J}^{(0)}_{r_N}\}^{(j)}_S,$$

$$\{\hat{J}^{(0)}_{r_1}\hat{J}^{(0)}_{r_2}\cdots\hat{J}^{(0)}_{r_N}\}^{(j)}_S = \frac{1}{N!}\sum_{P\in S_N}(\hat{J}^{(0)}_{r_{P(1)}}\cdots\hat{J}^{(0)}_{r_{P(N)}})^{(j)}. \tag{6.5}$$

Here the upper limit of N is determined by the UIR D^j; S_N is the permutation group on N symbols; and the superscript (j) denotes the restriction to $\mathcal{H}^{(j)}$. The coefficients $a_{r_1,\ldots,r_N}(g;j)$ are c-number quantities symmetric in $r_1,\ldots,r_N$. If we now replace their j dependences by dependences on the independent mutually commuting Casimir operators $\hat{\mathcal{C}}$ of G, themselves symmetric homogeneous polynomials in $\hat{J}^{(0)}_r$, we can use (6.5) in (6.4) and write

$$\tilde{A}(g) = \sum_{N=0}^{\infty} \sum_{r_1,\ldots,r_N} a_{r_1,\ldots,r_N}(g;\hat{\mathcal{C}})\{\hat{J}^{(0)}_{r_1}\cdots\hat{J}^{(0)}_{r_N}\}_S. \tag{6.6}$$

This expression for the Weyl symbol $\tilde{A}(g)$ of $\hat{A}$ can now be set into one-to-one correspondence with the classical phase space function

$$a(g;J) = \sum_{N=0}^{\infty} \sum_{r_1,\ldots,r_N} a_{r_1,\ldots,r_N}(g;\mathcal{C}) J_{r_1} \cdots J_{r_N}, \tag{6.7}$$

where the commuting classical variables J_r are the canonical momentum coordinates of the classical phase space T^*G,[21] while $\mathcal{C}$ are invariant (Casimir) homogeneous polynomials in them. Thus we have the two-stage sequence of correspondences

$$\hat{A} \text{ on } \mathcal{H} = L^2(G) \Leftrightarrow \tilde{A}(g) = \text{block-diagonal operator on } \mathcal{H}_0 \leftrightarrow a(g;J) \in \mathcal{F}(T^*G). \tag{6.8}$$

The importance of the multiplicity-free nature of the representation of G on $\mathcal{H}_0$, and the superselection rule, is evident. In contrast to the Cartesian case in Sec. II, the appearance of the semiquantized phase space as an intermediate step is to be noted. We hope to return to this aspect in a future publication.

APPENDIX

We indicate here the derivations of Eqs. (5.4a) and (5.4b). For Eq. (5.4a), we begin with Eq. (4.23) and use the unitarity of the D-matrices to shift the D-matrix on the right-hand side to the left-hand side. This immediately gives Eq. (5.4a). For Eq. (5.4b) we begin with the decomposition of the product of two U's; from Eq. (4.15), using Eq. (A29) in Ref. 21,

$$U(j'm'n')U(jmn)|g\rangle = D^{j'}_{m'n'}(g)D^{j}_{mn}(g)|g\rangle = \sum_{j''m''n''\lambda} C^{j'\ j\ j''\lambda *}_{m'\ m\ m''} C^{j'\ j\ j''\lambda}_{n'\ n\ n''} D^{j''}_{m''n''}(g)|g\rangle. \tag{A1}$$

Here the C's are the usual Clebsch–Gordan coefficients for the decomposition of the direct product $D^{j'} \times D^{j}$ of two UIR's into UIR's $D^{j''}$, with a multiplicity index λ to keep track of multiple occurrences of a given $D^{j''}$. If we introduce the short-hand notation

$$C^{j'\ \ j\ \ j''}_{m'n'\ mn\ m''n''} = \sum_{\lambda} C^{j'\ j\ j''\lambda *}_{m'\ m\ m''} C^{j'\ j\ j''\lambda}_{n'\ n\ n''}, \tag{A2}$$

we get from (A1):

$$U(j'm'n')U(jmn) = \sum_{j''m''n''} C^{j'\ \ j\ \ j''}_{m'n'\ mn\ m''n''} U(j''m''n''). \tag{A3}$$

We can now tackle the product of four factors in Eq. (5.4b). First using Eqs. (3.7) and (4.18) and then using (A3) above gives

$$\begin{aligned} U(j'm'n')V(g')U(jmn)V(g) &= U(j'm'n') \sum_{k} D^{j}_{mk}(g'^{-1}) U(jkn) V(g'g) \\ &= \sum_{j''m''n''k} D^{j}_{mk}(g'^{-1}) C^{j'\ \ j\ \ j''}_{m'n'\ kn\ m''n''} U(j''m''n'') V(g'g), \end{aligned} \tag{A4}$$

which is Eq. (5.4b).

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Schrödinger problems for surfaces of revolution—the finite cylinder as a test example

Jens Gravesen and Morten Willatzen
Mads Clausen Institute for Product Innovation, University of Southern Denmark, Grundtvigs Allé 150, DK-6400 Sønderborg, Denmark

L. C. Lew Yan Voon
Department of Physics, Worcester Polytechnic Institute, Worcester, Massachusetts 01609

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A set of ordinary differential equations is derived employing the method of differentiable forms so as to describe the quantum mechanics of a particle constrained to move on a general two-dimensional surface of revolution. Eigenvalues and eigenstates are calculated quasianalytically in the case of a finite cylinder (finite along the axis) and compared with the eigenvalues and eigenstates of a full three-dimensional Schrödinger problem corresponding to a hollow cylinder in the limit where the inner and outer radii approach each other. Good agreement between the two models is obtained for a relative difference less than 20% in inner and outer radii. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1829376]

I. INTRODUCTION

With the recent advances in nanotechnology,[1] it is now possible to grow quasi-two-dimensional surfaces of almost arbitrary shape where quantum effects play a major role.[2] Examples include single crystal $NbSe_3$ Möbius strips,[3] spherical CdSe–ZnS core-shell quantum dots,[4] and Si nanowire and nanoribbon transistors.[5] Due to the confinement of the quantum-mechanical particle to a two-dimensional surface, differential geometry methods offer certain advantages above the usual three-dimensional treatment of Schrödinger-equation problems in determining eigenvalues and eigenstates. Several publications have appeared on the constrainment of quantum-mechanical particles (with applications in, e.g., standard Schrödinger equation problems and relativistic Dirac equation problems) to a two-dimensional surface since the original works by Jensen and Koppe, da Costa[6–8] clarified that physical properties of two-dimensional systems in general depend on the surrounding three-dimensional space.

In the present work, we derive the three-dimensional Schrödinger equation in curvilinear coordinates u^1, u^2, u^3 with $u^3=0$ defining the two-dimensional surface to which the particle is confined. The resulting representation of the Schrödinger equation in u^1, u^2, u^3 can be separated into three ordinary differential equations (one for each u^i, $i=1,2,3$) for any surface of revolution. In doing this, simple equations are obtained relevant to the more general case of surfaces than those considered in Ref. 9 where the surface was restricted to obey the relation $z=S(r)$ where z, r are the axial and radial cylinder coordinates, respectively.

Next, we solve the problem of a particle confined to the surface of a finite cylinder and determine eigenvalues and eigenstates analytically. The corresponding eigenvalues and eigenstates of a hollow cylinder in three dimensions is also solved quasianalytically. In particular, we show that three-dimensional results for a thin hollow cylinder agree very well with results obtained by performing a quasi-two-dimensional differential form analysis of the Schrödinger equation.

II. SCHRÖDINGER's EQUATION IN CURVED COORDINATES

Let (u^1,u^2,u^3) be *normal coordinates* in $\mathbb{R}^3$ with respect to a surface Σ embedded in $\mathbb{R}^3$, i.e., u^1,u^2 are coordinates on the surface and u^3 is the distance to the surface. A simple calculation

shows that the volume element in $\mathbb{R}^3$ is $F\sqrt{g}\,\mathrm{d}u^1\,\mathrm{d}u^2\,\mathrm{d}u^3$, where $F=1-2Mu^3+K(u^3)^2$, and M and K denote the mean and Gaussian curvature, respectively. If we let $\chi=\sqrt{F}\phi$, then we can write the Laplacian in $\mathbb{R}^3$ acting on ψ as

$$\sqrt{F}\Delta_{\mathbb{R}^3}\psi=(\Delta_0+u^3\Delta_1+(u^3)^2\Delta_2+\cdots)\chi+\partial_3^2\chi, \tag{1}$$

where Δ_k, $k=0,1,2,\ldots$ are operators on Σ. In particular,

$$\Delta_0=\Delta_\Sigma+(M^2-K), \tag{2}$$

see Ref. 7, where Δ_Σ is the Laplace–Beltrami operator on Σ,

$$\Delta_\Sigma=g^{-1/2}\partial_\beta g^{\alpha\beta}g^{1/2}\partial_\beta=g^{\alpha\beta}\partial_\alpha\partial_\beta+\left(\frac{g^{\alpha\beta}}{2}\frac{\partial_\beta g}{g}+\partial_\beta g^{\alpha\beta}\right)\partial_\alpha, \tag{3}$$

and $\partial_\alpha=\partial/\partial u^\alpha$, $g_{\alpha\beta}$ are the components of the metric tensor, $g=\det[g_{\alpha\beta}]$ and $[g^{\alpha\beta}]=[g_{\alpha\beta}]^{-1}$ (see Ref. 6).

We now specialize to a *surface of revolution*. It can be parametrized as $\mathbf{x}(u^1,u^2)=(r(u^1)\cos u^2, r(u^1)\sin u^2, z(u^1))$, where $(r(u^1),z(u^1))$ is a curve in the xz plane. The metric tensor is given by $g_{11}=r'(u^1)^2+z'(u^1)^2$, $g_{22}=r(u^1)^2$, and $g_{12}=g_{21}=0$, and the principal curvatures are $\kappa_1=\kappa(u^1)=(r'z''-z'r'')/(r'^2+z'^2)^{3/2}$ and $\kappa_2=z'/r\sqrt{r'^2+z'^2}$, see Ref. 10. The mean and Gaussian curvature are $\frac{1}{2}(\kappa_1+\kappa_2)$ and $\kappa_1\kappa_2$, respectively, so $M^2-K=\frac{1}{4}(\kappa_1-\kappa_2)^2$ and

$$\Delta_0=\frac{\partial_1^2}{r'^2+z'^2}+\frac{\partial_2^2}{r^2}+\left(\frac{r'}{r(r'^2+z'^2)}-\frac{r'r''+z'z''}{(r'^2+z'^2)^2}\right)\partial_1+\frac{1}{4}\frac{1}{r'^2+z'^2}\left(\frac{r'z''-z'r''}{r'^2+z'^2}-\frac{z'}{r}\right)^2. \tag{4}$$

If the curve $(r(u^1),z(u^1))$ is parametrized by arc length, i.e., $r'^2+z'^2=1$, the expression simplifies to

$$\Delta_0=\partial_1^2+\frac{\partial_2^2}{r^2}-\frac{r'}{r}\partial_1+\frac{1}{4}\left(r'z''-z'r''-\frac{z'}{r}\right)^2. \tag{5}$$

For the sake of completeness, let us next write the Schrödinger equation in curved coordinates for a particle confined to the surface $(u^1,u^2,u^3=0)$,

$$\frac{-\hbar^2}{2m}(\Delta_0+\partial_3^2)\chi(u^1,u^2,u^3)+V(u^1,u^2,u^3)\chi(u^1,u^2,u^3)=E\chi(u^1,u^2,u^3), \tag{6}$$

where the Laplacian is as given by Eq. (2), and

$$V(u^1,u^2,u^3)=\begin{cases}0 & \text{if } |u^3|\leqslant\epsilon_3,\\ \infty & \text{otherwise.}\end{cases} \tag{7}$$

For a surface of revolution, the Schrödinger equation can be written as three ordinary differential equations using the separation-of-variables method. Hence, assuming $\chi(u^1,u^2,u^3)=\chi_1(u^1)\chi_2(u^2)\chi_3(u^3)$ and inserting into Eq. (6) leads to [by use of the more general expression for Δ_0 given by Eqs. (4) and (7)]

$$\partial_1^2\chi_1+\left(\frac{r'}{r}-\frac{r'r''+z'z''}{r'^2+z'^2}\right)\partial_1\chi_1+\left(\frac{1}{4}\left(\frac{r'z''-z'r''}{r'^2+z'^2}-\frac{z'}{r}\right)^2-\left(c_1+\frac{c_2}{r^2}\right)(r'^2+z'^2)\right)\chi_1=0, \tag{8}$$

$$\partial_2^2\chi_2+c_2\chi_2=0, \tag{9}$$

$$\partial_3^2\chi_3+\left(\frac{2m(E-V(u^3))}{\hbar^2}+c_1\right)\chi_3=0. \tag{10}$$

III. ENERGY SPECTRUM OF A PARTICLE CONFINED TO THE SURFACE OF A FINITE CYLINDER

In the following, the possible energy eigenvalues of a particle obeying Schrödinger's equation confined to the surface of a finite cylinder with radius R and length L will be determined. First, a parametrization of the cylinder surface is defined by

$$(r(u^1),z(u^1)) = (R,u^1), \quad 0 \leqslant u^1 \leqslant L. \tag{11}$$

Inserting this into Eqs. (8)–(10) immediately yields

$$\partial_1^2\chi_1 + \left(\frac{1}{4R^2} - \frac{c_2}{R^2} - c_1\right)\chi_1 = 0, \tag{12}$$

$$\partial_2^2\chi_2 + c_2\chi_2 = 0, \tag{13}$$

$$\partial_3^2\chi_3 + \left(\frac{2m}{\hbar^2}E + c_1\right)\chi_3 = 0, \tag{14}$$

where c_1, c_2 are separation constants and $\chi(u^1,u^2,u^3) \equiv \chi_1(u^1)\chi_2(u^2)\chi_3(u^3)$.

Consider first the equation in u^2. The solution satisfying the periodic condition $\chi_2(2\pi) = \chi_2(0)$, is

$$\chi_2(u^2) = \exp(\pm i\sqrt{c_2}u^2) = \exp(ilu^2), \tag{15}$$

where l is an integer (positive or negative), i.e.,

$$c_2 = l^2. \tag{16}$$

Next, c_1 is determined from Eq. (12) by imposing the boundary conditions

$$\chi_1(u^1 = 0) = \chi_1(u^1 = L) = 0. \tag{17}$$

The corresponding solution is

$$\chi_1(u^1) = \sin\left(\sqrt{-\frac{c_2}{R^2} - c_1 + \frac{1}{4R^2}}u^1\right) = \sin\left(\frac{k\pi}{L}u^1\right), \quad k = 1,2,3,\ldots, \tag{18}$$

i.e.,

$$c_1 = -\left(\frac{k\pi}{L}\right)^2 - \frac{c_2}{R^2} + \frac{1}{4R^2} = -\left(\frac{k\pi}{L}\right)^2 - \frac{l^2}{R^2} + \frac{1}{4R^2}. \tag{19}$$

The remaining equation in u^3 can finally be solved—subject to the boundary conditions $\chi(u^1,u^2,u^3 = \pm\epsilon_3) = 0$,

$$\chi_3(u^3) = \sin\left(\frac{n\pi}{2\epsilon_3}(u^3 - \epsilon_3)\right), \quad n = 1,2,3,\ldots. \tag{20}$$

In other words, the energy spectrum is found from Eqs. (14), (19), and (20) and reads

$$E_{\mathrm{DG}} = \frac{\hbar^2}{2m}\left[\left(\frac{n\pi}{2\epsilon_3}\right)^2 + \left(\frac{k\pi}{L}\right)^2 + \frac{l^2}{R^2} - \frac{1}{4R^2}\right], \tag{21}$$

where $n = 1,2,3,\ldots$, $k = 1,2,3,\ldots$, and $l = 0,1,2,3,\ldots$ are quantum indices.

IV. ENERGY SPECTRUM OF A PARTICLE CONFINED TO A HOLLOW CYLINDER—THREE-DIMENSIONAL TREATMENT

The Schrödinger equation in cylindrical coordinates reads

$$\frac{\partial^2\psi}{\partial r^2}+\frac{1}{r}\frac{\partial\psi}{\partial r}+\frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2}+\frac{\partial^2\psi}{\partial z^2}+\kappa(r)^2\psi=0, \tag{22}$$

where

$$\kappa(r)^2=\frac{2m}{\hbar^2}(E-V(r)), \tag{23}$$

for a potential depending on the radial coordinate r only. Here, $V(r)$ is a step potential confining the particle to the hollow cylinder, i.e.,

$$V(r)=\begin{cases}0 & \text{if } R_i\leqslant r\leqslant R_o,\\ \infty & \text{otherwise,}\end{cases} \tag{24}$$

and R_i (R_o) is the inner (outer) radius of the hollow cylinder. A separable solution in the region $R_i\leqslant r\leqslant R_o$ is sought in the form

$$\psi(r,\theta,z)=\rho(r)\Theta(\theta)Z(z), \tag{25}$$

where

$$\frac{\mathrm{d}^2Z}{\mathrm{d}z^2}=-k_{zk}^2Z, \tag{26}$$

$$\frac{\mathrm{d}^2\Theta}{\mathrm{d}\theta^2}=-l^2\Theta, \tag{27}$$

$$r^2\frac{\mathrm{d}^2\rho}{\mathrm{d}r^2}+r\frac{\mathrm{d}\rho}{\mathrm{d}r}+(k_{ln}^2r^2-l^2)\rho=0, \tag{28}$$

and $\kappa^2=k_{ln}^2+k_{zk}^2$. The potential $V(r)$ in Eq. (24) ensures that the wave function vanishes at the inner and outer radii positions, $\psi(r=R_i,\theta,z)=\psi(r=R_o,\theta,z)=0$. The solution for $Z(z)$ amenable with the boundary conditions $Z(z=0)=Z(z=L)=0$, is

$$Z(z)=\sin(k_{zk}z)=\sin\left(\frac{k\pi}{L}z\right),\quad k=1,2,3,\ldots\ . \tag{29}$$

The general solution to the Bessel equation [Eq. (28)] is

$$\rho(r)=AJ_l(k_{ln}r)+BY_l(k_{ln}r), \tag{30}$$

where A, B are numbers and J_l, Y_l are Bessel functions of order l of the first and second kind, respectively. Hence, the boundary conditions lead to the determinental equation for nontrivial solutions,

$$J_l(k_{ln}R_i)Y_l(k_{ln}R_o)-J_l(k_{ln}R_o)Y_l(k_{ln}R_i)=0. \tag{31}$$

Equation (31) can be easily solved for k_{ln}. Thus, the eigenstates correspond to an energy in the form,

$$E_{\mathrm{HC}}=\frac{\hbar^2(k_{ln}^2+k_{zk}^2)}{2m}=\frac{\hbar^2}{2m}\left(k_{ln}^2+\left(\frac{k\pi}{L}\right)^2\right). \tag{32}$$

TABLE I. Energy gaps ΔE_{DG} and the relative error $\delta(\epsilon)$, for a quantum-mechanical particle with mass m confined to a set of hollow cylinders with $R_i=(1-\epsilon)$ nm and $R_0=(1+\epsilon)$ nm, as calculated employing Eqs. (33) and (35), respectively. Length is measured in nm and other units are chosen such that $\hbar^2/2m\equiv 1$.

n	l	ΔE_{DG}	$\delta(\epsilon=10^{-4})$	$\delta(\epsilon=10^{-3})$	$\delta(\epsilon=10^{-2})$	$\delta(\epsilon=10^{-1})$
	0	−0.250 00	3.9×10^{-9}	3.9×10^{-7}	3.9×10^{-5}	3.9×10^{-3}
	1	0.750 00	3.9×10^{-9}	3.9×10^{-7}	3.9×10^{-5}	3.9×10^{-3}
	2	3.750 00	3.9×10^{-9}	3.9×10^{-7}	3.9×10^{-5}	3.9×10^{-3}
1	3	8.750 00	3.9×10^{-9}	3.9×10^{-7}	3.9×10^{-5}	3.9×10^{-3}
	4	15.750 00	3.9×10^{-9}	3.9×10^{-7}	3.9×10^{-5}	3.8×10^{-3}
	5	24.750 00	3.9×10^{-9}	3.9×10^{-7}	3.9×10^{-5}	3.8×10^{-3}
	6	35.750 00	3.9×10^{-9}	3.9×10^{-7}	3.9×10^{-5}	3.7×10^{-3}
	0	−0.250 00	8.5×10^{-9}	8.5×10^{-7}	8.5×10^{-5}	8.5×10^{-3}
	1	0.750 00	8.5×10^{-9}	8.5×10^{-7}	8.5×10^{-5}	8.5×10^{-3}
	2	3.750 00	8.5×10^{-9}	8.5×10^{-7}	8.5×10^{-5}	8.5×10^{-3}
2	3	8.750 00	8.5×10^{-9}	8.5×10^{-7}	8.5×10^{-5}	8.5×10^{-3}
	4	15.750 00	8.5×10^{-9}	8.5×10^{-7}	8.5×10^{-5}	8.5×10^{-3}
	5	24.750 00	8.5×10^{-9}	8.5×10^{-7}	8.5×10^{-5}	8.5×10^{-3}
	6	35.750 00	8.5×10^{-9}	8.5×10^{-7}	8.5×10^{-5}	8.5×10^{-3}

V. NUMERICAL RESULTS AND DISCUSSIONS

In this section, we compare results for eigenstates of electrons confined to a thin cylindrical shell employing the full three-dimensional Schrödinger equation and the quasi-two-dimensional Schrödinger equation based on differential-form methods using curvilinear coordinates (u^1,u^2,u^3) with u^3 nearly zero in the cylindrical shell. The energies E_{DG} and E_{HC} of the two theories are given by Eqs. (21) and (32), respectively, and we see that they have the term $(\hbar/2m)(k\pi/L)^2$ in common. The dominating term in (21) is $E_n=(\hbar/2m)(n\pi/2\epsilon)^2$ which is order of magnitudes larger than the other terms so in order to compare the two theories we will consider E_n as a reference energy and define the energy gap

$$\Delta E_{\mathrm{DG}} = E_{\mathrm{DG}} - E_n - \frac{\hbar}{2m}\left(\frac{k\pi}{L}\right)^2 = \frac{\hbar}{2m}\frac{4l^2-1}{4R^2}, \tag{33}$$

$$\Delta E_{\mathrm{HC}} = E_{\mathrm{HC}} - E_n - \frac{\hbar}{2m}\left(\frac{k\pi}{L}\right)^2 = \frac{\hbar}{2m}\left(k_{ln}^2 - \left(\frac{n\pi}{2\epsilon}\right)^2\right), \tag{34}$$

and the relative error

$$\delta = \frac{\Delta E_{\mathrm{HC}} - \Delta E_{\mathrm{DG}}}{\Delta E_{\mathrm{DG}}} = \frac{E_{\mathrm{HC}} - E_{\mathrm{DG}}}{\Delta E_{\mathrm{DG}}}. \tag{35}$$

The relative error δ can now be used to rewrite Eq. (32) so as to obtain the form

$$E_{\mathrm{HC}} = \frac{\hbar}{2m}\left[\left(\frac{n\pi}{2\epsilon}\right)^2 + \left(\frac{k\pi}{L}\right)^2 + (1+\delta)\frac{4l^2-1}{4R^2}\right], \tag{36}$$

where $R_o=R+\epsilon$ and $R_i=R-\epsilon$. Except for the term δ, which in most cases can be neglected, this is the same as Eq. (21). In Table I, we list the energy gap ΔE_{DG} and the relative error δ, as obtained for a hollow cylinder with $R=1$ nm and $\epsilon=10^{-4}R$, $10^{-3}R$, $10^{-2}R$, and $10^{-1}R$.

Evidently, the agreement is surprisingly good between the two models even for the case where ϵ is 10% of R. The eigenstates for the full three-dimensional problem are

$$\psi(r,\theta,z) = \sin\left(\frac{k\pi}{L}z\right)\exp(il\theta)\left(J_l(k_{ln}r) - \frac{J_l(k_{ln}R_o)}{Y_l(k_{ln}R_o)}Y_l(k_{ln}r)\right), \tag{37}$$

corresponding to the energy eigenvalues given by Eq. (32). Similarly, the eigenstates for the two-dimensional problem are

$$\chi(r,\theta,z) = \sin\left(\frac{k\pi}{L}u^1\right)\exp(ilu^2)\chi_3(u^3), \tag{38}$$

with

$$\chi_3(u^3) = \sin\left(\frac{n\pi}{2\epsilon_3}(u^3-\epsilon_3)\right), \quad n = 1,2,3,\ldots, \tag{39}$$

corresponding to the energy eigenvalues given by Eq. (21). Note that these eigenstates are exactly the same in their z and θ dependencies (or u^1 and u^2 dependencies) since $u^1 \in [0;L]$, $u^2 \in [0;2\pi[$, $\theta \in [0;2\pi[$, and $z \in [0;L]$ with k, l, and n integers. This could in fact have been seen beforehand. Indeed, for the cylinder we have $u^1=z$, $u^2=\theta$, and $u^3=R-r$. So the equation $\chi = \sqrt{F}\psi = \sqrt{1-u^3/R}\psi$ gives us in the limit $\epsilon^3 \to 0$ that $\chi_1(u^1)=Z(z)$ and $\chi_2(u^2)=\Theta(\theta)$. For the sake of completeness we note that the exact equation for χ is

$$-\frac{\hbar^2}{2m}\left(\partial_1^2 + \frac{1}{(R-u^3)^2}\partial_2^2 + \partial_3^2 - \frac{1}{4(R-u^3)^2}\right)\chi + V(u^3)\chi = E\chi, \tag{40}$$

and in Sec. III the factor $(R-u^3)^{-2}$ in Eq. (40) is replaced with the zeroth order term R^{-2}.

We would like to point out that we obtain the same result for an annulus in $\mathbb{R}^2$ as for the hollow cylinder in $\mathbb{R}^3$, except that in the former case, the u^1 dependence disappears in the eigenstates as does the term $(k\pi/L)^2$ in the corresponding energy eigenvalue expressions. However, the $1/4R^2$ contribution to the energy also appears in the annulus problem as this term reflects radial confinement of the quantum-mechanical particle.

VI. CONCLUSIONS

The Schrödinger equation in curvilinear coordinates (u^1,u^2,u^3) is derived where $(u^1,u^2,u^3=0)$ describes the two-dimensional surface to which a quantum-mechanical particle is confined. In the case of a surface of revolution it is possible to separate the Schrödinger equation in curvilinear coordinates so as to obtain three ordinary differential equations. As an example, energy eigenvalues and eigenstates are determined quasianalytically for the case of confinement to a finite cylindrical surface. Results are in good agreement with corresponding full three-dimensional results of a hollow cylinder in the case where the inner and outer radii approach each other.

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Quantum integrability of bosonic massive Thirring model in continuum

Tanaya Bhattacharyya[a)]
Theory Group, Saha Institute of Nuclear Physics, 1/AF Bidhan Nagar, Kolkata 700 064, India

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By using a variant of the quantum inverse scattering method, commutation relations between all elements of the quantum monodromy matrix of the bosonic massive Thirring (BMT) model are obtained. Using those relations, the quantum integrability of BMT model is established and the *S*-matrix of two-body scattering between the corresponding quasiparticles has been obtained. It is observed that for some special values of the coupling constant, there exists an upper bound on the number of quasiparticles that can form a quantum-soliton state of the BMT model. We also calculate the binding energy for a *N*-soliton state of the quantum BMT model. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1818722]

I. INTRODUCTION

Quantum integrable field models in $1+1$ dimensions are objects of interest due to their close connections with different areas of physics as well as mathematics.[1–10] These integrable theories have played an important role in understanding the basic nonperturbative aspects of physical theories relevant in the realistic $3+1$ dimensional models. Through quantum inverse scattering method (QISM) one can establish the integrability property of these models and obtain the spectrum as well as different correlation functions of the corresponding models.[4]

Massive Thirring model in $1+1$ dimensions has been widely studied as a toy counterpart to low energy QCD, since it does not include many of the complications arising in $3+1$ dimensions. The study of a nonlocal massless Thirring model is relevant, not only from a purely field theoretical point of view but also because of its connection with the physics of strongly correlated systems in one spatial dimension. This model describes an ensemble of nonrelativistic particles coupled through a two-body forward-scattering potential and displays Luttinger-liquid behavior[11] that can play a role in real one-dimensional semiconductors.[12]

Massive Thirring model in $1+1$ dimensions can be treated through QISM for both bosonic and fermionic field operators.[6] In this paper, we shall focus our attention to the bosonic massive Thirring (BMT) model. The classical version of the BMT model is described by the Hamiltonian

$$H=\int_{-\infty}^{\infty}\mathrm{d}x\left[-\frac{i}{2}\left\{\left(\phi_1^*\frac{\partial\phi_1}{\partial x}-\frac{\partial\phi_1^*}{\partial x}\phi_1\right)-\left(\phi_2^*\frac{\partial\phi_2}{\partial x}-\frac{\partial\phi_2^*}{\partial x}\phi_2\right)\right\}-(\phi_1^*\phi_2+\phi_2^*\phi_1)-4\xi\phi_1^*\phi_2^*\phi_2\phi_1\right] \tag{1.1}$$

with the equal time Poisson bracket (PB) relations,

$$\{\phi_1(x),\phi_1(y)\}=\{\phi_1^*(x),\phi_1^*(y)\}=0,\ \ \{\phi_1(x),\phi_1^*(y)\}=-i\delta(x-y),$$

a)Electronic mail: tanaya@theory.saha.ernet.in

$$\{\phi_2(x),\phi_2(y)\}=\{\phi_2^*(x),\phi_2^*(y)\}=0,\ \ \{\phi_2(x),\phi_2^*(y)\}=-i\delta(x-y). \tag{1.2}$$

It is well known that this BMT model is intimately connected with the derivative nonlinear Schrödinger (DNLS) model. In fact, one can generate the Lax operator of the BMT model by "fusing" two Lax operators of DNLS model with different spectral parameters.[13] The integrability of the classical DNLS model, possessing ultralocal PB structure, can be established from the fact that the corresponding monodromy matrix satisfies the classical Yang–Baxter equation.[14] The quantized version of this DNLS model also preserves the integrability property. By applying QISM, the quantum integrability of DNLS model is established and the Bethe eigenstates for all conserved quantities have been constructed.[14,15]

In an earlier work by Kulish and Sklyanin,[6] the Lax operator and the corresponding *R*-matrix for the quantum BMT model has been given, though the detailed calculations are not being explicitly shown. Moreover, the quantum Yang–Baxter equation (QYBE) at the infinite interval limit and hence the corresponding commutation relation between the creation and annihilation operators have not been studied. However, it is evident that taking the infinite interval limit of the monodromy matrix and corresponding QYBE is necessary to get the spectrum for the quantum version of the Hamiltonian (1.1). In this context it may be mentioned that, by applying a variant of the QISM[3] which is directly applicable to field theoretical models, the quantum DNLS model has been shown to be integrable.[15,16] The infinite interval limit of the corresponding QYBE enabled us to obtain the spectrum of all the conserved quantities including the Hamiltonian and also the two-particle *S*-matrix. Therefore, it is interesting to explore the integrability property of the quantum BMT model by using the same variant of QISM that we applied for the DNLS model. It may be noted that the one-dimensional Hubbard model has been treated earlier through algebraic Bethe ansatz in the infinite interval limit. As an advantage of taking this infinite interval limit, the commutation relations among various elements of the corresponding monodromy matrix are obtained in a much simpler form.[17] In this paper our aim is to establish the integrability property of the quantum BMT model and to obtain the spectrum of all conserved quantities including the Hamiltonian by using the QISM at an infinite interval limit.

The arrangement of this paper is as follows. In Sec. II, we consider the classical BMT model and evaluate the PB relations among the various elements of the corresponding monodromy matrix at the infinite interval limit. Using these PB relations, the integrability of the classical BMT model can be established in the Liouville sense. In this section we also derive the expressions for the classical conserved quantities of the BMT model. In Sec. III, we construct the quantum monodromy matrix of the BMT model on a finite interval and derive the corresponding QYBE. In Sec. IV, we consider the infinite interval limit of QYBE and obtain the commutation relations among the various elements of the corresponding quantum monodromy matrix. Such commutation relations allow us to construct exact eigenstates for the quantum conserved quantities of the BMT model by using the prescription of algebraic Bethe ansatz. In particular we are able to obtain the spectrum for the quantum version of the Hamiltonian (1.1). Furthermore we obtain the commutation relation between creation and annihilation operators of quasiparticles associated with the BMT model and find out the *S*-matrix of two-body scattering among such quasiparticles. In this section we also calculate the binding energy for a *N*-soliton state of the quantum BMT model. Section V is the concluding section.

II. INTEGRABILITY OF THE CLASSICAL MASSIVE THIRRING MODEL

The classical version of the BMT model is described by the Lax operator,[6]

$$U(x,\lambda)=i\begin{pmatrix}\xi\{\rho_1(x)-\rho_2(x)\}-\frac{1}{4}\left\{\lambda^2-\frac{1}{\lambda^2}\right\} & \xi\left\{\lambda\phi_1^*(x)-\frac{1}{\lambda}\phi_2^*(x)\right\}\\ \lambda\phi_1(x)-\frac{1}{\lambda}\phi_2(x) & -\xi\{\rho_1(x)-\rho_2(x)\}+\frac{1}{4}\left\{\lambda^2-\frac{1}{\lambda^2}\right\}\end{pmatrix}, \tag{2.1}$$

where $\rho_1(x)=\phi_1^*(x)\phi_1(x)$, $\rho_2(x)=\phi_2^*(x)\phi_2(x)$, λ is the spectral parameter and ξ is the coupling constant of the theory. The bosonic fields $\phi_1(x)$, $\phi_2(x)$ satisfy the PB relations (1.2) and vanish at

$|x| \to \infty$ limit. The monodromy matrix on finite and infinite intervals are defined as

$$T_{x_1}^{x_2}(\lambda) = \mathcal{P} \exp \int_{x_1}^{x_2} U(x,\lambda) \mathrm{d}x \tag{2.2}$$

and

$$T(\lambda) = \lim_{\substack{x_2 \to +\infty \\ x_1 \to -\infty}} e(-x_2,\lambda) \left\{ \mathcal{P} \exp \int_{x_1}^{x_2} U(x,\lambda) \mathrm{d}x \right\} e(x_1,\lambda), \tag{2.3}$$

respectively, where $\mathcal{P}$ denotes the path ordering and $e(x,\lambda) = e^{-(i/4)\{\lambda^2 - (1/\lambda^2)\}\sigma_3 x}$.

First, we want to investigate the symmetry properties of the monodromy matrix (2.3). It is easy to check that, the Lax operator (2.1) satisfies the relations

$$U(x,\lambda)^* = K U(x,\lambda^*) K, \tag{2.4a}$$

$$U(x,-\lambda) = K' U(x,\lambda) K', \tag{2.4b}$$

where $K = \begin{pmatrix} 0 & \sqrt{-\xi} \\ 1/\sqrt{-\xi} & 0 \end{pmatrix}$ and $K' = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. By using these relations, we find that the symmetries of the monodromy matrix $T(\lambda)$ (2.3) are given by

$$T(\lambda)^* = K T(\lambda^*) K, \tag{2.5a}$$

$$T(-\lambda) = K' T(\lambda) K'. \tag{2.5b}$$

Due to the relation (2.5a), $T(\lambda)$ can be expressed in the form

$$T(\lambda) = \begin{pmatrix} a(\lambda) & -\xi b^*(\lambda) \\ b(\lambda) & a^*(\lambda) \end{pmatrix}, \tag{2.6}$$

where λ is taken as a real parameter. Moreover, by using the symmetry relation (2.5b), it is easy to see that $a(-\lambda) = a(\lambda)$ and $b(-\lambda) = -b(\lambda)$. Therefore, it is sufficient to derive the PB relations among the elements of $T(\lambda)$ only for $\lambda \geqslant 0$.

Next, our aim is to calculate the classical conserved quantities of the BMT model by using the approach described in Ref 2. From (2.2), one obtains the differential equation followed by the monodromy matrix $T_{x_1}^{x_2}(\lambda)$ as

$$\frac{\partial}{\partial x_2} T_{x_1}^{x_2}(\lambda) = U(x_2,\lambda) T_{x_1}^{x_2}(\lambda). \tag{2.7}$$

Now, let us decompose the monodromy matrix in the form

$$T_{x_1}^{x_2}(\lambda) = (1 + W(x_2,\lambda)) \exp Z(x_2,x_1,\lambda) (1 + W(x_1,\lambda)), \tag{2.8}$$

where $Z(x_2,x_1,\lambda)$ is a diagonal matrix and $W(x,\lambda)$ is a nondiagonal one. The Lax operator of the classical BMT model can be expressed as $U(x,\lambda) = U_d(x,\lambda) + U_{nd}(x,\lambda)$, where $U_d(x,\lambda)$ is the diagonal part and $U_{nd}(x,\lambda)$ is the nondiagonal part of $U(x,\lambda)$. Using the above expression of the Lax operator $U(x,\lambda)$ (2.1), the differential equation (2.7) can be decomposed into

$$\frac{\mathrm{d}Z}{\mathrm{d}x} = U_d + U_{nd} W, \tag{2.9a}$$

$$\frac{dW}{dx} - 2U_d W - U_{nd} + WU_{nd}W = 0. \tag{2.9b}$$

The structure of the Lax operator (2.1) ensures that $W(x_2,\lambda)$ and $Z(x_2,x_1,\lambda)$ can be written in the form

$$W(x_2,\lambda) = -\xi w^*(x_2,\lambda)\sigma_+ + w(x_2,\lambda)\sigma_-,$$

$$Z(x_2,x_1,\lambda) = z(x_2,x_1,\lambda)\sigma_3.$$

Substituting Eqs. (2.6) and (2.8) in the expression (2.3), and using $W(x,\lambda)\to 0$ at $|x|\to\infty$ limit, one obtains

$$\ln a(\lambda) = \lim_{\substack{x_2\to+\infty \\ x_1\to-\infty}} \left\{ z(x_2,x_1,\lambda) + \frac{i\lambda^2}{4}(x_2 - x_1) \right\}.$$

Substituting the explicit form of $z(x_2,x_1,\lambda)$ [as obtained by integrating Eq. (2.9a)] to the above expression, we get the following form of $\ln a(\lambda)$:

$$\ln a(\lambda) = i\xi \int_{-\infty}^{+\infty} \{\phi_1^*\phi_1 - \phi_2^*\phi_2\}dx + i\xi\lambda \int_{-\infty}^{+\infty} \phi_1^* w dx - \frac{i\xi}{\lambda}\int_{-\infty}^{+\infty} \phi_2^* w dx. \tag{2.10}$$

Next, we expand $w(x,\lambda)$ in inverse powers of λ as

$$w(x,\lambda) = \sum_{j=0}^{\infty} \frac{w_j}{\lambda^{2j+1}}.$$

Using the differential Eq. (2.9b) followed by $W(x,\lambda)$, the expansion coefficient w_j's can be obtained explicitly in a recursive way. The first few nonzero w_j's are given by

$$w_0 = -2\phi_1, \quad w_2 = 4i\phi_{1_x} + 8\xi\phi_1(\phi_2^*\phi_2) + 2\phi_2.$$

Substituting w_j's in the expression of $\ln a(\lambda)$ (2.10), one gets

$$\ln a(\lambda) = \sum_{n=0}^{\infty} \frac{iC_n}{\lambda^{2n}},$$

where C_n's represent an infinite set of conserved quantities. The first two of them are explicitly given by

$$C_0 = -\xi \int_{-\infty}^{+\infty} \{\phi_1^*\phi_1 + \phi_2^*\phi_2\}dx, \tag{2.11a}$$

$$C_1 = 4i\xi \int_{-\infty}^{+\infty} \phi_1^*\phi_{1x}\, dx + 2\xi \int_{-\infty}^{+\infty} \{\phi_1^*\phi_2 + \phi_2^*\phi_1\}dx + 8\xi^2 \int_{-\infty}^{+\infty} (\phi_1^*\phi_1)(\phi_2^*\phi_2)dx. \tag{2.11b}$$

Next we expand $w(x,\lambda)$ in powers of λ as

$$w(x,\lambda) = \sum_{j=0}^{\infty} \tilde{w}_j \lambda^{2j+1}.$$

In a similar way as above, using (2.9b), the first few nonzero $\tilde{w}_j$'s can be obtained as

$$\tilde{w}_0 = -2\phi_2, \quad \tilde{w}_2 = -4i\phi_{2_x} + 8\xi(\phi_1^*\phi_1)\phi_2 + 2\phi_1.$$

Correspondingly, Eq. (2.10) yields

$$\ln a(\lambda) = \sum_{n=0}^{\infty} i\tilde{C}_n\lambda^{2n},$$

where $\tilde{C}_n$'s represent another infinite set of conserved quantities. The first two of them are explicitly given by

$$\tilde{C}_0 = \xi\int_{-\infty}^{+\infty}\{\phi_1^*\phi_1 + \phi_2^*\phi_2\}\mathrm{d}x, \tag{2.12a}$$

$$\tilde{C}_1 = 4i\xi\int_{-\infty}^{+\infty}\phi_2^*\phi_{2_x}\,\mathrm{d}x - 2\xi\int_{-\infty}^{+\infty}\{\phi_1^*\phi_2 + \phi_2^*\phi_1\}\mathrm{d}x - 8\xi^2\int_{-\infty}^{+\infty}(\phi_1^*\phi_1)(\phi_2^*\phi_2)\mathrm{d}x. \tag{2.12b}$$

Now by combining these two sets of conserved quantities, the mass, momentum, and the Hamiltonian of classical BMT model can be expressed in the following way:

$$N = -\frac{1}{2\xi}(C_0 - \tilde{C}_0) = \int_{-\infty}^{+\infty}(\phi_1^*\phi_1 + \phi_2^*\phi_2)\mathrm{d}x,$$

$$P = -\frac{1}{4\xi}(C_1 + \tilde{C}_1) = \int_{-\infty}^{+\infty}(\phi_1^*\phi_{1x} + \phi_2^*\phi_{2x})\mathrm{d}x$$

$$H = -\frac{1}{4\xi}(C_1 - \tilde{C}_1) = \int_{-\infty}^{\infty}[-i(\phi_1^*\phi_{1_x} - \phi_2^*\phi_{2_x}) - \{\phi_1^*\phi_2 + \phi_2^*\phi_1\} - 4\xi\phi_1^*\phi_2^*\phi_2\phi_1]\mathrm{d}x.$$

Next, we want to derive the PB relations among the elements of $T(\lambda)$ (2.6). We apply the equal time PB relations (1.2) between the basic field variables to evaluate the PB relations among the elements of the Lax operator (2.1) and find that

$$\{U(x,\lambda) \overset{\otimes}{,} U(y,\mu)\} = [r(\lambda,\mu), U(x,\lambda)\otimes 1 + 1\otimes U(y,\mu)]\delta(x-y), \tag{2.13}$$

where

$$r(\lambda,\mu) = -\xi\{t^c\sigma_3\otimes\sigma_3 + s^c(\sigma_+\otimes\sigma_- + \sigma_-\otimes\sigma_+)\} \tag{2.14}$$

with

$$t^c = \frac{\lambda^2+\mu^2}{2(\lambda^2-\mu^2)}, \quad s^c = \frac{2\lambda\mu}{\lambda^2-\mu^2}.$$

Now, by using Eqs. (2.13) and (2.3), one obtains

$$\{T(\lambda) \overset{\otimes}{,} T(\mu)\} = r_+(\lambda,\mu)T(\lambda)\otimes T(\mu) - T(\lambda)\otimes T(\mu)r_-(\lambda,\mu), \tag{2.15}$$

where

$$r_\pm = -\xi(t^c\sigma_3\otimes\sigma_3 + s_\pm^c\sigma_+\otimes\sigma_- + s_\mp^c\sigma_-\otimes\sigma_+),$$

with $s_\pm^c = \pm 2i\pi\lambda^2\delta(\lambda^2-\mu^2)$. By substituting the symmetric form of $T(\lambda)$ (2.6) to Eq. (2.15) and comparing the individual elements in both sides, we obtain

$$\{a(\lambda),a(\mu)\}=0, \tag{2.16a}$$

$$\{a(\lambda),a^*(\mu)\}=0, \tag{2.16b}$$

$$\{b(\lambda),b(\mu)\}=0, \tag{2.16c}$$

$$\{a(\lambda),b(\mu)\}=\xi\left(\frac{\lambda^2+\mu^2}{\lambda^2-\mu^2}\right)a(\lambda)b(\mu)-2i\pi\xi\lambda^2\delta(\lambda^2-\mu^2)b(\lambda)a(\mu), \tag{2.16d}$$

$$\{a(\lambda),b^*(\mu)\}=-\xi\left(\frac{\lambda^2+\mu^2}{\lambda^2-\mu^2}\right)a(\lambda)b^*(\mu)+2i\pi\xi\lambda^2\delta(\lambda^2-\mu^2)b^*(\lambda)a(\mu), \tag{2.16e}$$

$$\{b(\lambda),b^*(\mu)\}=-4i\pi\lambda^2\delta(\lambda^2-\mu^2)|a(\lambda)|^2. \tag{2.16f}$$

From Eq. (2.16a) it follows that all expansion coefficients occurring in the expansions of $\ln a(\lambda)$ will have vanishing PB relations among themselves. Hence, the following expressions will hold true

$$\{C_m,C_n\}=\{\tilde{C}_m,\tilde{C}_n\}=\{C_m,\tilde{C}_n\}=0,$$

for all values of m and n. Since the mass, momentum, and the Hamiltonian of the classical BMT model has been expressed in terms of the expansion coefficients C_n and $\tilde{C}_n$'s, all of them will have vanishing PB relations among themselves. Thus the integrability property of the classical BMT model, described by the Hamiltonian (1.1), is established in the Liouville sense.

III. COMMUTATION RELATIONS FOR THE QUANTUM MONODROMY MATRIX ON A FINITE INTERVAL

By using a version of QISM which is directly applicable to field models,[3] in this section we shall show that the quantum monodromy matrix of the BMT model on a finite interval satisfies QYBE. The basic field operators of the quantum BMT model satisfy the following equal time commutation relations:

$$[\phi_1(x),\phi_1(y)]=[\phi_1^\dagger(x),\phi_1^\dagger(y)]=0,\ \ [\phi_1(x),\phi_1^\dagger(y)]=\hbar\delta(x-y),$$

$$[\phi_2(x),\phi_2(y)]=[\phi_2^\dagger(x),\phi_2^\dagger(y)]=0,\ \ [\phi_2(x),\phi_2^\dagger(y)]=\hbar\delta(x-y), \tag{3.1}$$

and the vacuum state is defined through the relations $\phi_1(x)|0\rangle=\phi_2(x)|0\rangle=0$.

In analogy with the classical Lax operator (2.1), we assume that the quantum Lax operator of BMT model is given by

$$\mathcal{U}_q(x,\lambda)=i\begin{pmatrix} f_1\rho_1(x)-f_2\rho_2(x)-\dfrac{\lambda^2}{4}+\dfrac{1}{4\lambda^2} & \xi\lambda\phi_1^\dagger(x)-\dfrac{\xi}{\lambda}\phi_2^\dagger(x) \\ \lambda\phi_1(x)-\dfrac{1}{\lambda}\phi_2(x) & -g_1\rho_1(x)+g_2\rho_2(x)+\dfrac{\lambda^2}{4}-\dfrac{1}{4\lambda^2}\end{pmatrix}, \tag{3.2}$$

where $\rho_1(x)=\phi_1^\dagger(x)\phi_1(x)$, $\rho_2(x)=\phi_2^\dagger(x)\phi_2(x)$ and f_1,f_2,g_1,g_2 are four parameters which will be determined later in this section through QYBE. Using the Lax operator (3.2), the quantum monodromy matrix on a finite interval is defined as

$$\mathcal{T}_{x_1}^{x_2}(\lambda) =: \mathcal{P}\exp\int_{x_1}^{x_2}\mathcal{U}_q(x,\lambda)\mathrm{d}x:, \tag{3.3}$$

where the symbol $::$ denotes the normal ordering of operators. This quantum monodromy matrix (3.3) satisfies a differential equation given by

$$\begin{aligned}\frac{\partial}{\partial x_2}\mathcal{T}_{x_1}^{x_2}(\lambda) =: \mathcal{U}_q(x_2,\lambda)\mathcal{T}_{x_1}^{x_2}(\lambda): = &-\frac{i}{4}\left\{\lambda^2-\frac{1}{\lambda^2}\right\}\sigma_3\mathcal{T}_{x_1}^{x_2}(\lambda)+i\xi\lambda\phi_1^\dagger(x_2)\sigma_+\mathcal{T}_{x_1}^{x_2}(\lambda)\\ &-\frac{i\xi}{\lambda}\phi_2^\dagger(x_2)\sigma_+\mathcal{T}_{x_1}^{x_2}(\lambda)+i\lambda\sigma_-\mathcal{T}_{x_1}^{x_2}(\lambda)\phi_1(x_2)-\frac{i}{\lambda}\sigma_-\mathcal{T}_{x_1}^{x_2}(\lambda)\phi_2(x_2)\\ &+if_1\phi_1^\dagger(x_2)e_{11}\mathcal{T}_{x_1}^{x_2}(\lambda)\phi_1(x_2)-if_2\phi_2^\dagger(x_2)e_{11}\mathcal{T}_{x_1}^{x_2}(\lambda)\phi_2(x_2)\\ &-ig_1\phi_1^\dagger(x_2)e_{22}\mathcal{T}_{x_1}^{x_2}(\lambda)\phi_1(x_2)+ig_2\phi_2^\dagger(x_2)e_{22}\mathcal{T}_{x_1}^{x_2}(\lambda)\phi_2(x_2),\end{aligned} \tag{3.4}$$

where $e_{11}=\frac{1}{2}(1+\sigma_3)$ and $e_{22}=\frac{1}{2}(1-\sigma_3)$. Now, to apply QISM, we must find out the differential equation satisfied by the product $\mathcal{T}_{x_1}^{x_2}(\lambda)\otimes\mathcal{T}_{x_1}^{x_2}(\mu)$. By using the basic commutation relations (3.1) and the method of "extension,"[3] we find that the product of two monodromy matrices satisfies the following differential equation (detail calculations are given in the Appendix):

$$\frac{\partial}{\partial x_2}(\mathcal{T}_{x_1}^{x_2}(\lambda)\otimes\mathcal{T}_{x_1}^{x_2}(\mu)) = \vdots\ \mathcal{L}(x_2;\lambda,\mu)\mathcal{T}_{x_1}^{x_2}(\lambda)\otimes\mathcal{T}_{x_1}^{x_2}(\mu)\ \vdots\ , \tag{3.5}$$

where

$$\mathcal{L}(x;\lambda,\mu)=\mathcal{U}_q(x,\lambda)\otimes\mathbb{1}+\mathbb{1}\otimes\mathcal{U}_q(x,\mu)+\mathcal{L}_\Delta(x;\lambda,\mu), \tag{3.6}$$

with

$$\mathcal{L}_\Delta(x;\lambda,\mu)=\begin{pmatrix}-\hbar f_1^2\rho_1(x) & -\hbar\xi\mu f_1\phi_1^\dagger(x) & 0 & 0\\ -\hbar f_2^2\rho_2(x) & -\dfrac{\hbar\xi}{\mu}f_2\phi_2^\dagger(x) & & \\ 0 & \hbar g_1 f_1\rho_1(x) & 0 & 0\\ & +\hbar g_2 f_2\rho_2(x) & & \\ -\hbar\lambda f_1\phi_1(x) & -\hbar\xi\left\{\lambda\mu+\dfrac{1}{\lambda\mu}\right\} & \hbar g_1 f_1\rho_1(x) & \hbar\xi\mu g_1\phi_1^\dagger(x)\\ -\dfrac{\hbar f_2}{\lambda}\phi_2(x) & & +\hbar g_2 f_2\rho_2(x) & +\dfrac{\hbar\xi g_2}{\mu}\phi_2^\dagger(x)\\ 0 & \hbar\lambda g_1\phi_1(x) & 0 & -\hbar g_1^2\rho_1(x)\\ & +\dfrac{\hbar g_2}{\lambda}\phi_2(x) & & -\hbar g_2^2\rho_2(x)\end{pmatrix}. \tag{3.7}$$

In the expression (3.5), the sign of normal arrangement of operator factors is taken as $\vdots\,\vdots$. The sign $\vdots\,\vdots$, applied to the product of several operator factors (including ϕ_1, ϕ_2, $\phi_1^\dagger$, and $\phi_2^\dagger$), ensures the arrangement of all $\phi_1^\dagger$, $\phi_2^\dagger$ on the left, and all ϕ_1, ϕ_2 on the right, *without altering the order of the remaining factors*. For example,

$$:X\phi_1\phi_2\phi_1^\dagger\phi_2^\dagger Y: = \phi_1^\dagger\phi_2^\dagger XY\phi_1\phi_2,$$

where X and Y may in general be taken as some functions of the basic field operators.

Now one can easily check that $\mathcal{L}(x;\lambda,\mu)$ (3.6) follows an equation given by

$$R(\lambda,\mu)\mathcal{L}(x;\lambda,\mu) = \mathcal{L}(x;\mu,\lambda)R(\lambda,\mu), \tag{3.7}$$

where $R(\lambda,\mu)$ is a (4×4) matrix of the form

$$R(\lambda,\mu) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & s(\lambda,\mu) & t(\lambda,\mu) & 0 \\ 0 & t(\lambda,\mu) & s(\lambda,\mu) & 0 \\ 0 & 0 & 0 & 1, \end{pmatrix}, \tag{3.8}$$

with

$$t(\lambda,\mu) = \frac{\lambda^2-\mu^2}{\lambda^2 q-\mu^2 q^{-1}},\quad s(\lambda,\mu) = \frac{(q-q^{-1})\lambda\mu}{\lambda^2 q-\mu^2 q^{-1}}$$

and $q=e^{-i\alpha}$. The above equation (3.7) enables us to determine the exact expressions of the parameters f_1, f_2, g_1, g_2, α in terms of the coupling constant ξ. We obtain

$$\hbar\xi = -\sin\alpha, \tag{3.9a}$$

$$f_1 = g_2 = \frac{\xi e^{-i\alpha/2}}{\cos\alpha/2}, \tag{3.9b}$$

$$g_1 = f_2 = \frac{\xi e^{i\alpha/2}}{\cos\alpha/2}. \tag{3.9c}$$

Using Eqs. (3.5) and (3.7), we find that the monodromy matrix (3.3) satisfies QYBE given by

$$R(\lambda,\mu)\mathcal{T}_{x_1}^{x_2}(\lambda)\otimes\mathcal{T}_{x_1}^{x_2}(\mu) = \mathcal{T}_{x_1}^{x_2}(\mu)\otimes\mathcal{T}_{x_1}^{x_2}(\lambda)R(\lambda,\mu). \tag{3.10}$$

Using the above QYBE (3.10), the commutation relations among all elements of the quantum monodromy matrix (3.3) can be obtained easily.

Equations (3.9a), (3.9b), and (3.9c), describing the relations between f_1, f_2, g_1, g_2, α and the coupling constant ξ, provide the necessary conditions for the Lax operator (3.2) to satisfy QYBE (3.10). From Eq. (3.9a) we can conclude that, the above method of deriving QYBE for quantum BMT model is applicable only when the coupling constant ξ lies within the range $|\xi|\leqslant 1/\hbar$. The parameter α has a one-to-one correspondence with the coupling constant ξ for $-\pi/2\leqslant\alpha\leqslant\pi/2$. For the purpose of investigating the classical limit of the quantum Lax operator (3.2), we take the $\alpha\to 0$ limit which is equivalent to the $\hbar\to 0$ limit for a fixed value of ξ. From Eqs. (3.9b) and (3.9c), it follows that at this limit $f_1, f_2\to\xi$ and $g_1, g_2\to\xi$. Hence we find that the quantum Lax operator (3.2) correctly reproduces the classical Lax operator (2.1) at $\hbar\to 0$ limit.

IV. ALGEBRAIC BETHE ANSATZ FOR THE QUANTUM MONODROMY MATRIX ON AN INFINITE INTERVAL

The quantum monodromy matrix in an infinite interval is defined as

$$\mathcal{T}(\lambda) = \lim_{\substack{x_2 \to +\infty \\ x_1 \to -\infty}} e(-x_2,\lambda)\mathcal{T}_{x_1}^{x_2}(\lambda)e(x_1,\lambda), \tag{4.1}$$

where $\mathcal{T}_{x_1}^{x_2}(\lambda)$ is given by Eq. (3.3). Just as in the classical case, the quantum Lax operator (3.2) also satisfies the symmetry relations

$$\mathcal{U}_q(x,\lambda)^* = K\mathcal{U}_q(x,\lambda^*)K, \tag{4.2a}$$

$$\mathcal{U}_q(x,-\lambda) = K'\mathcal{U}_q(x,\lambda)K', \tag{4.2b}$$

where K and K' matrices have appeared earlier in Eq. (2.4). Using Eq. (4.2a), the quantum monodromy matrix (4.1) can be expressed in a symmetric form given by

$$\mathcal{T}(\lambda) = \begin{pmatrix} A(\lambda) & -\xi B^\dagger(\lambda) \\ B(\lambda) & A^\dagger(\lambda) \end{pmatrix}, \tag{4.3}$$

where λ is a real parameter. From Eq. (4.2b), it follows that $A(-\lambda)=A(\lambda)$ and $B(-\lambda)=-B(\lambda)$. So it is sufficient to obtain the commutation relations among the elements of the quantum monodromy matrix (4.3) only for $\lambda \geqslant 0$.

Now we aim to obtain the infinite interval limit of the QYBE satisfied by $\mathcal{T}(\lambda)$ (4.3). To this end, we split the $\mathcal{L}(x;\lambda,\mu)$ matrix (3.6) into two parts:

$$\mathcal{L}(x;\lambda,\mu) = \mathcal{L}_0(\lambda,\mu) + \mathcal{L}_1(x;\lambda,\mu),$$

where $\mathcal{L}_0(\lambda,\mu)$ is given by

$$\mathcal{L}_0(\lambda,\mu) = \lim_{|x|\to\infty} \mathcal{L}(x;\lambda,\mu) = \begin{pmatrix} -\frac{i}{4}(\lambda^2+\mu^2) + \frac{i}{4}\left(\frac{1}{\lambda^2}+\frac{1}{\mu^2}\right) & 0 & 0 & 0 \\ 0 & -\frac{i}{4}(\lambda^2-\mu^2) + \frac{i}{4}\left(\frac{1}{\lambda^2}-\frac{1}{\mu^2}\right) & 0 & 0 \\ 0 & -\hbar\xi\lambda\mu - \frac{\hbar\xi}{\lambda\mu} & \frac{i}{4}(\lambda^2-\mu^2) - \frac{i}{4}\left(\frac{1}{\lambda^2}-\frac{1}{\mu^2}\right) & 0 \\ 0 & 0 & 0 & \frac{i}{4}(\lambda^2+\mu^2) - \frac{i}{4}\left(\frac{1}{\lambda^2}+\frac{1}{\mu^2}\right) \end{pmatrix},$$

and $\mathcal{L}_1(x;\lambda,\mu)$ is the field dependent part of $\mathcal{L}(x;\lambda,\mu)$, which vanishes at $x \to \pm\infty$. From Eq. (3.7) we get

$$R(\lambda,\mu)\varepsilon(x;\lambda,\mu) = \varepsilon(x;\mu,\lambda)R(\lambda,\mu), \tag{4.4}$$

where $\varepsilon(x;\lambda,\mu)=e^{\mathcal{L}_0(\lambda,\mu)x}$. By using the above mentioned splitting of $\mathcal{L}(x;\lambda,\mu)$, we derive the integral form of the differential equation (3.5) as

$$\mathcal{T}_{x_1}^{x_2}(\lambda)\otimes\mathcal{T}_{x_1}^{x_2}(\mu)=\varepsilon(x_2-x_1;\lambda,\mu)+\int_{x_1}^{x_2}\mathrm{d}x\,\varepsilon(x_2-x;\lambda,\mu)\,{:}\,\mathcal{L}_1(x,\lambda,\mu)\mathcal{T}_{x_1}^{x}(\lambda)\otimes\mathcal{T}_{x_1}^{x}(\mu)\,{:}\ .$$

From this integral relation it is clear that at the asymptotic limit $x_1,x_2\to\pm\infty$, $\mathcal{T}_{x_1}^{x_2}(\lambda)\otimes\mathcal{T}_{x_1}^{x_2}(\mu)\to\varepsilon(x_2-x_1;\lambda,\mu)$, which is an oscillatory term. To get rid of this problem, we define an operator like

$$W(\lambda,\mu)=\lim_{\substack{x_2\to+\infty\\ x_1\to-\infty}}\varepsilon(-x_2;\lambda,\mu)\mathcal{T}_{x_1}^{x_2}(\lambda)\otimes\mathcal{T}_{x_1}^{x_2}(\mu)\varepsilon(x_1;\lambda,\mu). \tag{4.5}$$

In the above defined operator, the oscillatory nature of $\mathcal{T}_{x_1}^{x_2}(\lambda)\otimes\mathcal{T}_{x_1}^{x_2}(\mu)$ has been removed and $W(\lambda,\mu)$ is perfectly well behaved at the limit $x_1,x_2\to\pm\infty$. By using (3.10) and (4.4), it is easy to verify that the operator $W(\lambda,\mu)$ (4.5) satisfies an equation given by

$$R(\lambda,\mu)W(\lambda,\mu)=W(\mu,\lambda)R(\lambda,\mu). \tag{4.6}$$

The above equation represents the QYBE of the BMT model at an infinite interval limit.

Next, we want to express the QYBE (4.6) directly in terms of the monodromy matrices (4.1) defined in an infinite interval. For this purpose, $W(\lambda,\mu)$ (4.5) can be rewritten as

$$W(\lambda,\mu)=C_+(\lambda,\mu)\mathcal{T}(\lambda)\otimes\mathcal{T}(\mu)C_-(\lambda,\mu), \tag{4.7}$$

where

$$C_+(\lambda,\mu)=\lim_{x\to\infty}\varepsilon(-x;\lambda,\mu)E(x;\lambda,\mu), \tag{4.8a}$$

$$C_-(\lambda,\mu)=\lim_{x\to-\infty}E(-x;\lambda,\mu)\varepsilon(x;\lambda,\mu), \tag{4.8b}$$

with $E(x;\lambda,\mu)=e(x,\lambda)\otimes e(x,\mu)$. Substituting the explicit forms of $E(x;\lambda,\mu)$ and $\varepsilon(x;\lambda,\mu)$ to (4.8a) and (4.8b), and taking the limits in the principal value sense: $\lim_{x\to\pm\infty}P(e^{ikx}/k)=\pm i\pi\delta(k)$, we obtain

$$C_+(\lambda,\mu)=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&\rho_+(\lambda,\mu)&1&0\\0&0&0&1\end{pmatrix},\quad C_-(\lambda,\mu)=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&\rho_-(\lambda,\mu)&1&0\\0&0&0&1\end{pmatrix}, \tag{4.9}$$

where

$$\begin{aligned}\rho_\pm(\lambda,\mu)&=\mp\frac{2i\hbar\xi\left(\lambda\mu+\frac{1}{\lambda\mu}\right)}{\lambda^2-\mu^2-\frac{1}{\lambda^2}+\frac{1}{\mu^2}}+2\pi\hbar\xi\left(\lambda\mu+\frac{1}{\lambda\mu}\right)\delta\left(\lambda^2-\mu^2-\frac{1}{\lambda^2}+\frac{1}{\mu^2}\right)\\&=\mp\frac{2i\hbar\xi\left\{\lambda\mu+\frac{1}{\lambda\mu}\right\}}{\lambda^2-\mu^2-\frac{1}{\lambda^2}+\frac{1}{\mu^2}\mp i\epsilon}.\end{aligned} \tag{4.10}$$

Substituting the expression of $W(\lambda,\mu)$ (4.7) in Eq. (4.6), we can express this QYBE for the infinite interval in the form

$$R(\lambda,\mu)C_+(\lambda,\mu)\mathcal{T}(\lambda)\otimes\mathcal{T}(\mu)C_-(\lambda,\mu)=C_+(\mu,\lambda)\mathcal{T}(\mu)\otimes\mathcal{T}(\lambda)C_-(\mu,\lambda)R(\lambda,\mu). \tag{4.11}$$

By inserting the explicit forms of $R(\lambda,\mu)$ (3.8), $C_{\pm}(\lambda,\mu)$ (4.9), and $\mathcal{T}(\lambda)$ (4.3) to the above QYBE (4.11) and comparing the matrix elements from both sides of this equation, we obtain the following commutation relations:

$$[A(\lambda),A(\mu)]=0, \tag{4.12a}$$

$$[A(\lambda),A^{\dagger}(\mu)]=0, \tag{4.12b}$$

$$[B(\lambda),B(\mu)]=0, \tag{4.12c}$$

$$A(\lambda)B^{\dagger}(\mu)=\frac{\mu^2q-\lambda^2q^{-1}}{\mu^2-\lambda^2-i\epsilon}B^{\dagger}(\mu)A(\lambda)=\frac{\mu^2q-\lambda^2q^{-1}}{\mu^2-\lambda^2}B^{\dagger}(\mu)A(\lambda)-2\pi\hbar\xi\lambda\mu\delta(\lambda^2-\mu^2)B^{\dagger}(\lambda)A(\mu), \tag{4.12d}$$

$$B(\mu)A(\lambda)=\frac{\mu^2q-\lambda^2q^{-1}}{\mu^2-\lambda^2-i\epsilon}A(\lambda)B(\mu)=\frac{\mu^2q-\lambda^2q^{-1}}{\mu^2-\lambda^2}A(\lambda)B(\mu)-2\pi\hbar\xi\lambda\mu\delta(\lambda^2-\mu^2)A(\mu)B(\lambda), \tag{4.12e}$$

$$B(\mu)B^{\dagger}(\lambda)=\tau(\lambda,\mu)B^{\dagger}(\lambda)B(\mu)+4\pi\hbar\xi\lambda\mu\delta(\lambda^2-\mu^2)A^{\dagger}(\lambda)A(\lambda), \tag{4.12f}$$

where

$$\tau(\lambda,\mu)=\left[1+\frac{8\hbar^2\xi^2\lambda^2\mu^2}{(\lambda^2-\mu^2)^2}-\frac{4\hbar^2\xi^2\left\{\lambda\mu+\frac{1}{\lambda\mu}\right\}^2}{\left(\lambda^2-\mu^2-\frac{1}{\lambda^2}+\frac{1}{\mu^2}-i\epsilon\right)\left(\lambda^2-\mu^2-\frac{1}{\lambda^2}+\frac{1}{\mu^2}+i\epsilon\right)}\right].$$

It is interesting to note that, for the case $\lambda\neq\mu$, Eq. (4.12f) gives $[B(\lambda),B^{\dagger}(\mu)]\neq 0$, whereas from Eq. (2.16f), one obtains that $\{b(\lambda),b^{*}(\mu)\}=0$ for $\lambda\neq\mu$. Thus the correspondence principle is not manifest here in a straightforward manner. However the $\hbar\to 0$ limit of $\tau(\lambda,\mu)$, gives the correct classical counterpart of the commutation relation (4.12f).

Due to Eq. (4.12a), all the operator valued coefficients occuring in the expansion of $\ln A(\lambda)$ will commute among themselves. As a consequence the BMT model described by the Lax operator (3.2) turn out to be a quantum integrable system. By applying the method of algebraic Bethe ansatz, one can also construct the exact eigenstates for all commuting operators which are generated through the expansion of $\ln A(\lambda)$. With the help of Eq. (4.1), it is easy to find that $A(\lambda)|0\rangle=|0\rangle$. By using this relation and Eq. (4.12d), it can be shown that

$$A(\lambda)|\mu_1,\mu_2,\ldots,\mu_N\rangle=\prod_{r=1}^{N}\left(\frac{\mu_r^2q-\lambda^2q^{-1}}{\mu_r^2-\lambda^2-i\epsilon}\right)|\mu_1,\mu_2,\ldots,\mu_N\rangle, \tag{4.13}$$

where μ_j's are all distinct real or complex numbers and $|\mu_1,\mu_2,\ldots,\mu_N\rangle \equiv B^{\dagger}(\mu_1)B^{\dagger}(\mu_2)\ldots B^{\dagger}(\mu_N)|0\rangle$ represents a Bethe eigenstate. Using the commutation relation (4.12f) one can also calculate the norm of the eigenstates $B^{\dagger}(\mu_1)B^{\dagger}(\mu_2)\cdots B^{\dagger}(\mu_N)|0\rangle$. However, the commutation relation (4.12f) contains product of singular functions

$$\left(\lambda^2-\mu^2-\frac{1}{\lambda^2}+\frac{1}{\mu^2}-i\epsilon\right)^{-1}\left(\lambda^2-\mu^2-\frac{1}{\lambda^2}+\frac{1}{\mu^2}+i\epsilon\right)^{-1},$$

which is undefined at the limit $\lambda\to\mu$. As a result, eigenstates like $B^{\dagger}(\mu_1)B^{\dagger}(\mu_2)\cdots B^{\dagger}(\mu_N)|0\rangle$ are not normalized on the δ-function. To solve this problem, we consider a reflection operator given by

$$R^{\dagger}(\lambda) = B^{\dagger}(\lambda)(A^{\dagger}(\lambda))^{-1} \tag{4.14}$$

and its adjoint $R(\lambda)$. By using Eqs. (4.12a), (4.12b), (4.12c), (4.12d), (4.12e), and (4.12f), we find that such reflection operators satisfy well-defined commutation relations like

$$R^{\dagger}(\lambda)R^{\dagger}(\mu) = S^{-1}(\lambda,\mu)R^{\dagger}(\mu)R^{\dagger}(\lambda),$$

$$R(\lambda)R(\mu) = S^{-1}(\lambda,\mu)R(\mu)R(\lambda), \tag{4.15}$$

$$R(\lambda)R^{\dagger}(\mu) = S(\lambda,\mu)R^{\dagger}(\mu)R(\lambda) + 4\pi\hbar\lambda^2\delta(\lambda^2-\mu^2),$$

where

$$S(\lambda,\mu) = \frac{\lambda^2 q - \mu^2 q^{-1}}{\lambda^2 q^{-1} - \mu^2 q}. \tag{4.16}$$

The $S(\lambda,\mu)$ defined above represents the nontrivial S-matrix element of two-body scattering among the related quasiparticles. We find that this $S(\lambda,\mu)$ satisfies the following conditions:

$$S^{-1}(\lambda,\mu) = S(\mu,\lambda) = S^{*}(\lambda,\mu), \tag{4.17}$$

and remains nonsingular at the limit $\lambda \to \mu$. Consequently, the action of the operators like $R^{\dagger}(\lambda)$ on the vacuum would produce well-defined states which can be normalized on the δ-function.

The point to be noted here is that in Eq. (4.13), the eigenvalues of $A(\lambda)$ are in general complex. To get real eigenvalues, we define a new operator $\ln \hat{A}(\lambda)$ through the relation $\ln \hat{A}(\lambda) \equiv \ln A(\lambda e^{-i\alpha/2})$ and expand this operator in inverse powers of λ,

$$\ln \hat{A}(\lambda) = \sum_{n=0}^{\infty} \frac{i\mathcal{C}_n}{\lambda^{2n}}. \tag{4.18}$$

Using Eqs. (4.13) and (4.18), it is easy to see that $\mathcal{C}_n$'s satisfy eigenvalue equations like

$$\mathcal{C}_n|\mu_1,\mu_2,\ldots,\mu_N\rangle = \chi_n|\mu_1,\mu_2,\ldots,\mu_N\rangle,$$

where the first few χ_n's are explicitly given by

$$\chi_0 = \alpha N, \quad \chi_1 = 2\sin\alpha\sum_{j=1}^{N}\mu_j^2, \quad \chi_2 = \sin 2\alpha\sum_{j=1}^{N}\mu_j^4. \tag{4.19}$$

It may be noted that these eigenvalues are all real when μ_j's are taken as real numbers. Next we expand the operator $\ln \hat{A}(\lambda)$ in powers of λ as

$$\ln \hat{A}(\lambda) = \sum_{n=0}^{\infty} i\tilde{\mathcal{C}}_n\lambda^{2n}, \tag{4.20}$$

and by using (4.13) we obtain

$$\tilde{\mathcal{C}}_n|\mu_1,\mu_2,\ldots,\mu_N\rangle = \tilde{\chi}_n|\mu_1,\mu_2,\ldots,\mu_N\rangle.$$

The first few $\tilde{\chi}_n$'s are explicitly given by

$$\tilde{\chi}_0 = -\alpha N,\ \ \tilde{\chi}_1 = -2\sin\alpha\sum_{j=1}^{N}\frac{1}{\mu_j^2},\ \ \tilde{\chi}_2 = -\sin 2\alpha\sum_{j=1}^{N}\frac{1}{\mu_j^4}. \tag{4.21}$$

In analogy with the classical case, one can now define the momentum and Hamiltonian of the quantum BMT model as

$$\mathcal{P} = -\frac{1}{4\xi}(C_1 + \tilde{C}_1),\ \ \mathcal{H} = -\frac{1}{4\xi}(C_1 - \tilde{C}_1).$$

By using (4.19) and (4.21), the eigenvalue equations corresponding to the above momentum and Hamiltonian are obtained as

$$\mathcal{P}|\mu_1,\mu_2,\ldots,\mu_N\rangle = \frac{\hbar}{2}\sum_{j=1}^{N}\left(\mu_j^2 - \frac{1}{\mu_j^2}\right)|\mu_1,\mu_2,\ldots,\mu_N\rangle,$$

$$\mathcal{H}|\mu_1,\mu_2,\ldots,\mu_N\rangle = \frac{\hbar}{2}\sum_{j=1}^{N}\left(\mu_j^2 + \frac{1}{\mu_j^2}\right)|\mu_1,\mu_2,\ldots,\mu_N\rangle. \tag{4.22}$$

In the above expressions, μ_j's are taken as real numbers and $|\mu_1,\mu_2,\ldots,\mu_N\rangle$ represents a scattering state. Now to construct quantum N-soliton states of the BMT model, complex values of μ_j can be chosen in such a way so that the eigenvalues corresponding to different expansion coefficients of $\ln\hat{A}(\lambda)$ still remains real. Such a choice is given by

$$\mu_j = \mu\exp\left[-i\alpha\left(\frac{N+1}{2} - j\right)\right], \tag{4.23}$$

where μ is a real parameter and $j \in [1,2,\ldots,N]$. For the above choice of μ_j, Eq. (4.13) takes the form

$$A(\lambda)|\mu_1,\mu_2,\ldots,\mu_N\rangle = q^{-N}\left(\frac{\lambda^2 - \mu^2 q^{N+1}}{\lambda^2 - \mu^2 q^{-N+1}}\right)|\mu_1,\mu_2,\ldots,\mu_N\rangle. \tag{4.24}$$

Consequently, the energy eigenvalue equation corresponding to the quantum N-soliton state can be obtained as $\mathcal{H}|\mu_1,\mu_2,\ldots,\mu_N\rangle = E|\mu_1,\mu_2,\ldots,\mu_N\rangle$, where

$$E = \frac{\hbar}{2}\left(\mu^2 + \frac{1}{\mu^2}\right)\frac{\sin\alpha N}{\sin\alpha}. \tag{4.25}$$

Thus we find that quantum N-soliton states can be constructed for the BMT model for $N > 1$. Now we assume a particular value of the coupling constant ξ given by $\hbar\xi = -\sin\alpha = -\sin(2\pi m/n)$, where m and n are nonzero integers which do not have any common factor. From Eq. (4.23), we obtain $\mu_j = \mu_{j+n}$ for the above choice of ξ. Since all the μ_j's must be distinct, we get $N \leqslant n$ as a restriction on the number of quasiparticles that can form a quantum soliton state for the BMT model when $\xi = -(1/\hbar)\sin(2\pi m/n)$.

Next we aim to calculate the binding energy for a N-soliton state of the quantum BMT model. Substituting the expression of μ_j (4.23) to the first relation in Eq. (4.22), the momentum eigenvalue of a N-soliton state is obtained as

$$P = \frac{\hbar}{2}\left(\mu^2 - \frac{1}{\mu^2}\right)\frac{\sin\alpha N}{\sin\alpha}. \tag{4.26}$$

It is interesting to observe that the energy (4.25) and the momentum eigenvalue (4.26) of a N-soliton state satisfy the dispersion relation $E^2 = P^2 + m^2$, where $m = \hbar\sin\alpha N/\sin\alpha$. To calculate binding energy we assume that the momentum P (4.26) is equally distributed among N number of

single-particle scattering states. The real wave number associated with each of these single particle states is denoted by μ_0. With the help of Eqs. (4.22) and (4.26), we find that

$$\mu_0^2 - \frac{1}{\mu_0^2} = \left(\mu^2 - \frac{1}{\mu^2}\right)\frac{\sin \alpha N}{N \sin \alpha}. \tag{4.27}$$

Using Eq. (4.22), the total energy for N number of such single particle states is obtained as

$$E' = \frac{\hbar N}{2}\left(\mu_0^2 + \frac{1}{\mu_0^2}\right) = \frac{\hbar N}{2}\left\{\left(\mu^2 - \frac{1}{\mu^2}\right)^2 \frac{\sin^2 \alpha N}{N^2 \sin^2 \alpha} + 4\right\}^{1/2}. \tag{4.28}$$

Subtracting E (4.25) from E' (4.28), we obtain the binding energy of the quantum N-soliton state as

$$E_B(\alpha, N) = E' - E = \frac{\hbar N}{2}\left\{\left(\mu^2 - \frac{1}{\mu^2}\right)^2 \frac{\sin^2 \alpha N}{N^2 \sin^2 \alpha} + 4\right\}^{1/2} - \frac{\hbar}{2}\left(\mu^2 + \frac{1}{\mu^2}\right)\frac{\sin \alpha N}{\sin \alpha}. \tag{4.29}$$

Note that the above expression of $E_B(\alpha, N)$ remains invariant under the transformation $\alpha \to -\alpha$. So it is sufficient to analyze the nature of binding energy within the range $0 < \alpha \leqslant \pi/2$. Now, for $E_B(\alpha, N)$ to represent the energy of a real bound state, E' must be greater than E. Since E' (4.28) is always positive, it is evident that $E' > E$ for $E < 0$. So we will restrict our attention only for the case $E > 0$, when the condition $E' > E$ is equivalent to $E'^2 > E^2$. Substituting the explicit expressions for E' (4.28) and E (4.25), the above condition takes the form

$$N \sin \alpha > \sin \alpha N. \tag{4.30}$$

Substituting $N = 2$ in (4.30), we get the trivial inequality $1 > \cos \alpha$ for $\alpha > 0$. So the condition (4.30) is satisfied for the $N = 2$ case within our chosen range of α. By using the method of induction, we can easily prove that the condition (4.30) is valid for arbitrary values of N. Thus we get an N-soliton bound state when α lies in the range $0 < |\alpha| \leqslant \pi/2$.

V. CONCLUDING REMARKS

In this paper we consider the classical Lax operator of the BMT model and obtain the PB relations among various elements of the classical monodromy matrix at the infinite interval limit. By using these PB relations, the classical integrability of the BMT model is established in the Liouville sense. We also calculate the classical conserved quantities of BMT model. Next, we quantize the Lax operator of the BMT model. By using a variant of QISM, that can be directly applied to the field theoretic models, we obtain the QYBE for the quantum monodromy matrix at a finite interval. This QYBE enables us to determine the various parameters of the quantum Lax operator in terms of the coupling constant ξ. Then we take the infinite interval limit of this QYBE and derive all possible commutation relations among the various elements of the corresponding quantum monodromy matrix. These commutation relations enable us to establish the quantum integrability of the BMT model and also to construct the exact eigenstates for the quantum version of the Hamiltonian (1.1) as well as other conserved quantities by using algebraic Bethe ansatz. We also obtain the commutation relation between creation and annihilation operators associated with quasiparticles of the BMT model and find out the S-matrix for two-body scattering.

In this context, we consider the BMT model with some special values of coupling constant given by $\xi = -(1/\hbar)\sin \alpha = -(1/\hbar)\sin(2\pi m/n)$, where m and n are nonzero integers with no common factor. It turns out that the number of quasiparticles, which form a bound state for such quantum BMT model, cannot exceed the value of n. We have also derived the exact expression of binding energy for a N-soliton state of the quantum BMT model. The binding energy turns out to be positive for all allowed values of α.

The commutation relation between creation and annihilation operators will play an important role in the future study, since by using it one might be able to calculate the norm of Bethe eigenstates and various correlation functions of the BMT model. In the future, we would also like

to obtain the quantum conserved quantities of the BMT model in terms of the field operators by using a method which was used earlier in the case of the nonlinear Schrödinger model[18] and DNLS model.[16]

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APPENDIX

Here we give the details of deriving Eq. (3.5). Direct attempt to calculate $(\partial/\partial x_2)(\mathcal{T}_{x_1}^{x_2}(\lambda) \otimes \mathcal{T}_{x_1}^{x_2}(\mu))$ by using Eq. (3.4), leads to indeterminate expressions of the form $[\mathcal{T}_{x_1}^{x_2}(\lambda), \phi_1^\dagger(x_2)]$ and $[\mathcal{T}_{x_1}^{x_2}(\lambda), \phi_2^\dagger(x_2)]$. To avoid this problem by using the method of extension,[3] we shift the upper limit of the monodromy matrix $\mathcal{T}_{x_1}^{x_2}(\lambda)$ by a small amount ϵ and take $\epsilon \to 0$ limit only after differentiating the product $\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda) \otimes \mathcal{T}_{x_1}^{x_2}(\mu)$ with respect to x_2. So, using Eq. (3.4), we obtain

$$\frac{\partial}{\partial x_2}(\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda) \otimes \mathcal{T}_{x_1}^{x_2}(\mu)) = :(\mathcal{U}_q(x_2+\epsilon;\lambda) \otimes \mathbb{1} + \mathbb{1} \otimes \mathcal{U}_q(x_2;\mu))\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda) \otimes \mathcal{T}_{x_1}^{x_2}(\mu):\ + K_+ + K_-, \tag{A1}$$

where

$$\begin{aligned} K_+ = {} & i\xi\mu[\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda), \phi_1^\dagger(x_2)] \otimes \sigma_+ \mathcal{T}_{x_1}^{x_2}(\mu) - \frac{i\xi}{\mu}[\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda), \phi_2^\dagger(x_2)] \otimes \sigma_+ \mathcal{T}_{x_1}^{x_2}(\mu) + if_1[\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda), \phi_1^\dagger(x_2)] \\ & \otimes e_{11}\mathcal{T}_{x_1}^{x_2}(\mu)\phi_1(x_2) - if_2[\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda), \phi_2^\dagger(x_2)] \otimes e_{11}\mathcal{T}_{x_1}^{x_2}(\mu)\phi_2(x_2) - ig_1[\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda), \phi_1^\dagger(x_2)] \\ & \otimes e_{22}\mathcal{T}_{x_1}^{x_2}(\mu)\phi_1(x_2) + ig_2[\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda), \phi_2^\dagger(x_2)] \otimes e_{22}\mathcal{T}_{x_1}^{x_2}(\mu)\phi_2(x_2), \end{aligned}$$

$$\begin{aligned} K_- = {} & i\lambda\sigma_- \mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda) \otimes [\phi_1(x_2+\epsilon), \mathcal{T}_{x_1}^{x_2}(\mu)] - \frac{i}{\lambda}\sigma_- \mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda) \otimes [\phi_2(x_2+\epsilon), \mathcal{T}_{x_1}^{x_2}(\mu)] + if_1\phi_1^\dagger(x_2 \\ & + \epsilon)e_{11}\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda) \otimes [\phi_1(x_2+\epsilon), \mathcal{T}_{x_1}^{x_2}(\mu)] - if_2\phi_2^\dagger(x_2+\epsilon)e_{11}\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda) \otimes [\phi_2(x_2+\epsilon), \mathcal{T}_{x_1}^{x_2}(\mu)] \\ & - ig_1\phi_1^\dagger(x_2+\epsilon)e_{22}\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda) \otimes [\phi_1(x_2+\epsilon), \mathcal{T}_{x_1}^{x_2}(\mu)] + ig_2\phi_2^\dagger(x_2+\epsilon)e_{22}\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda) \otimes [\phi_2(x_2 \\ & + \epsilon), \mathcal{T}_{x_1}^{x_2}(\mu)]. \end{aligned}$$

Now we consider the case, $\epsilon > 0$. Since $\phi_1(x_2+\epsilon)$ and $\phi_2(x_2+\epsilon)$ commute with $\phi_1(x)$, $\phi_1^\dagger(x)$, $\phi_2(x)$, $\phi_2^\dagger(x)$ for all x lying within x_1 and x_2, we get $[\phi_1(x_2+\epsilon), \mathcal{T}_{x_1}^{x_2}(\mu)] = [\phi_2(x_2+\epsilon), \mathcal{T}_{x_1}^{x_2}(\mu)] = 0$. Thus we can conclude that for a positive ϵ, $K_- = 0$. So we must calculate only the nontrivial commutators $[\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda), \phi_1^\dagger(x_2)]$ and $[\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda), \phi_2^\dagger(x_2)]$ appearing in the expression of K_+.

First let us calculate the commutator $[\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda), \phi_1^\dagger(x_2)]$. For this purpose, we consider a "transformation" Ω, which replaces the classical variables $\phi_1(x)$, $\phi_2(x)$, and $\phi_1^*(x)$, $\phi_2^*(x)$ by quantum operators $\phi_1(x)$, $\phi_2(x)$ and $\phi_1^\dagger(x)$, $\phi_2^\dagger(x)$, respectively. Next we use a correspondence principle,[3]

$$[\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda), \phi_1^\dagger(x_2)] = i\hbar :\Omega\{T_{x_1}^{x_2+\epsilon}(q;\lambda), \phi_1^*(x_2)\}: , \tag{A2}$$

where $T_{x_1}^{x_2+\epsilon}(q;\lambda)$ represents a classical monodromy matrix given by

$$T_{x_1}^{x_2+\epsilon}(q;\lambda) = \mathcal{P}\exp\int_{x_1}^{x_2} U_q(x,\lambda)\mathrm{d}x,$$

and $U_q(x,\lambda)=\Omega^{-1}\mathcal{U}_q(x,\lambda)$. By using the fundamental PB relations (1.2), it is easy to find that

$$\begin{aligned}\{T_{x_1}^{x_2+\epsilon}(q;\lambda),\phi_1^*(x_2)\} &= \int_{x_1}^{x_2+\epsilon} \mathrm{d}x\, T_x^{x_2+\epsilon}(q;\lambda)\{U_q(x,\lambda),\phi_1^*(x_2)\}T_{x_1}^{x}(q,\lambda)\\ &= T_{x_2}^{x_2+\epsilon}(q;\lambda)(f_1\phi_1^*(x_2)e_{11} - g_1\phi_1^*(x_2)e_{22} + \lambda\sigma_-)T_{x_1}^{x_2}(q;\lambda).\end{aligned}$$

Taking $\epsilon\to 0$ limit of the above expression and substituting it in (A2), we obtain

$$\lim_{\epsilon\to 0}[\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda),\phi_1^\dagger(x_2)] = i\hbar(f_1\phi_1^\dagger(x_2)e_{11} - g_1\phi_1^\dagger(x_2)e_{22} + \lambda\sigma_-)\mathcal{T}_{x_1}^{x_2}(\lambda). \tag{A3}$$

Next we must calculate the commutator $[\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda),\phi_2^\dagger(x_2)]$. Using the same correspondence principle as before and finally taking the $\epsilon\to 0$ limit one obtains

$$\lim_{\epsilon\to 0}[\mathcal{T}_{x_1}^{x_2+\epsilon}(\lambda),\phi_2^\dagger(x_2)] = i\hbar\left(-f_2\phi_2^\dagger(x_2)e_{11} + g_2\phi_2^\dagger(x_2)e_{22} - \frac{1}{\lambda}\sigma_-\right)\mathcal{T}_{x_1}^{x_2}(\lambda). \tag{A4}$$

Taking the $\epsilon\to 0$ limit of Eq. (A1) and using (A3) and (A4), we finally obtain the differential equation (3.5). Note that, instead of $\epsilon>0$, we could have chosen $\epsilon<0$ in Eq. (A1). In that case only the commutators $[\phi_1(x_2+\epsilon),\mathcal{T}_{x_1}^{x_2}(\mu)]$ and $[\phi_2(x_2+\epsilon),\mathcal{T}_{x_1}^{x_2}(\mu)]$ give nontrivial contributions. However, by repeating similar steps as outlined above and finally taking the $\epsilon\to 0$ limit, we would have obtained the same differential equation (3.5).

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The de Sitter relativistic top theory

J. Armenta
Departamento de Investigación en Física de la Universidad de Sonora, 83000 Hermosillo Sonora, Mexico and Instituto Tecnológico y de Estudios Superiores de Monterrey, Campus Obregón, Apdo. Postal 622, 85000 Cd. Obregón Sonora, Mexico

J. A. Nieto[a)]
Facultad de Ciencias Físico-Matemáticas de la Universidad Autónoma de Sinaloa, 80010 Culiacán Sinaloa, Mexico

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We discuss the relativistic top theory from the point of view of the de Sitter (or anti–de Sitter) group. Our treatment rests on the Hanson–Regge spherical relativistic top Lagrangian formulation. We propose an alternative method for studying spinning objects via Kaluza–Klein theory. In particular, we derive the relativistic top equations of motion starting with the geodesic equation for a point particle in $4+N$ dimensions. We compare our approach with Fukuyama's formulation of spinning objects, which is also based on Kaluza–Klein theory. We also report a generalization of our approach to a $4+N+D$ dimensional theory. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1827923]

I. INTRODUCTION

If one compares Regge's work[1,2] published in 1959 and 1960, respectively, with the Hanson–Regge work of 1974 about the relativistic spherical top theory[3] (see also Ref. 4), one gets the feeling that Regge thought of the trajectory constraint linking mass and the spin of a relativistic spinning object as a deep physical concept of nature. Through the years it has become clear that Regge was right. In fact, such a constraint, now called Regge trajectory, plays a fundamental role not only in the dual string models[5] and the relativistic rotator theory,[6,7] but also in string theory[8] and in the black holes approach.[9] It seems that even Regge is in the sky[10] in connection with the mass and the internal angular momentum of celestial objects.

One of the simplest Regge trajectory for a spherical relativistic top is provided by the expression[3,4]

$$H \equiv P^{\mu}P_{\mu} + \frac{1}{2r^2}\Sigma^{\mu\nu}\Sigma_{\mu\nu} + m_0^2 \approx 0, \tag{1}$$

where P^{μ} and $\Sigma^{\mu\nu}=-\Sigma^{\nu\mu}$ are the linear momentum and the internal angular momentum, respectively, associated with some spinning object. Here, m_0 and r are constants determining the properties of the system and the symbol "≈ 0" means weakly equal zero in the sense of the terminology of Dirac's constraints Hamiltonian formalism.[11] (Here the indices μ,ν run from 0 to 3.)

One of the interesting aspects of (1) is that it resembles one of the Casimir operator's of the de Sitter group,

$$C_1 = \tfrac{1}{2}S^{AB}S_{AB}, \tag{2}$$

where the indices A,B run from 0 to 4. In fact, if classically it is possible to make the identifications

a)Electronic mail: nieto@uas.uasnet.mx

$$S^{4\mu} \to rP^{\mu}, \quad S^{\mu\nu} \to \Sigma^{\mu\nu}, \quad C_1 \to -r^2 m_0^2, \tag{3}$$

then the spherical relativistic top may lead naturally to a de Sitter relativistic top and several properties of the de Sitter group can be applied to such a system. The problem, however, it is not so simple because the momenta P^{μ} and $\Sigma^{\mu\nu}$ are restricted to satisfy the so-called Tulczyjew constraint[12]

$$\Sigma^{\mu\nu} P_{\nu} \approx 0 \tag{4}$$

and it seems that there is not a counterpart in the de Sitter group formalism of this constraint. One of the main goals of this work is to use a Lagrangian analysis of the relativistic top in order to shed some light on this and other related problems.

As soon as we make the identification (3) the parameter r, measuring the "size" of the top, may acquire a particular interesting meaning, namely, it can be identified with the Planck length $l_P=(\hbar G/c^3)^{1/2}$ or with the radius of the universe R. In the first case, the relativistic top may have contact not only with elementary particles through the superstring top theory,[13,14] but also with gravity itself.[15] In fact, it has been shown[15] that extending the Poincaré group to the de Sitter group through a Wigner contraction with l_P as a parameter one can make sense of a gravitational theory as a gauge theory. Similar conclusion is provided by the MacDowell–Mansouri formalism.[16]

In the second case, one may find a connection between the relativistic top with accelerated universe via the de Sitter space–time. In some sense, one may say that Regge is not only in the sky but in the cosmos as well.

The central idea of this work is to develop different aspects of the de Sitter top theory using the spherical relativistic top theory as a guide. For this purpose in Secs. II and III we show explicitly how the first order and second order formalisms of a particular spherical top system are related. In Sec. IV, we show how the Kaluza–Klein formalism may lead to de Sitter top theory. In Sec. V, we make some final remarks. In Appendix B we report a generalization of our formalism to $4+N+D$ dimensions.

II. FROM THE FIRST ORDER TO THE SECOND ORDER LAGRANGIAN

Let us describe the motion of the top by four coordinates $x^{\mu}(\tau)$ and a tetrad $e^{\mu}_{(\alpha)}(\tau)$ where τ is an arbitrary parameter along the world line of the top. Here $x^{\mu}(\tau)$ is used to describe the position of the system, while $e^{\mu}_{(\alpha)}(\tau)$ is attached to the top in order to describe its rotations. We shall assume that the tetrad $e^{\mu}_{(\alpha)}(\tau)$ satisfies the orthonormal relations

$$\eta_{\mu\nu} e^{\mu}_{(\alpha)} e^{\nu}_{(\beta)} = \eta_{(\alpha\beta)},$$

$$\eta^{(\alpha\beta)} e^{\mu}_{(\alpha)} e^{\nu}_{(\beta)} = \eta^{\mu\nu}, \tag{5}$$

where $\eta_{\mu\nu}=\mathrm{diag}(-1,1,1,1)$ is the Minkowski metric. We shall associate the canonical linear momentum P_{μ} to the linear velocity $u^{\mu}=\mathrm{d}x^{\mu}/\mathrm{d}\tau$ and the spin tensor $\Sigma^{\mu\nu}=-\Sigma^{\nu\mu}$ to the angular velocity $\sigma^{\mu\nu}=e^{\mu}_{(\alpha)}(\mathrm{d}e^{\nu}_{(\alpha)}/\mathrm{d}\tau)$.

Consider the first order Lagrangian corresponding to a special type of a relativistic top,[3,4]

$$L = u^{\mu} P_{\mu} + \frac{1}{2}\sigma^{\mu\nu}\Sigma_{\mu\nu} - \frac{\lambda}{2}\left(P^{\mu}P_{\mu} + \frac{1}{2r^2}\Sigma^{\mu\nu}\Sigma_{\mu\nu} + m_0^2\right) + \xi_{\mu}\Sigma^{\mu\nu}P_{\nu}, \tag{6}$$

where λ and ξ_{μ} are Lagrange multipliers. Varying L with respect to P_{μ} gives

$$u^{\mu} = \lambda P^{\mu} + V^{\mu}, \tag{7}$$

where

$$V^{\mu} = \Sigma^{\mu\nu}\xi_{\nu}, \tag{8}$$

while varying L with respect to $\Sigma_{\mu\nu}$ yields

$$\sigma^{\mu\nu} = \frac{\lambda}{r^2}\Sigma^{\mu\nu} + P^{\mu}\xi^{\nu} - P^{\nu}\xi^{\mu}. \tag{9}$$

Similarly varying L with respect to ξ_{μ} leads to the constraint

$$\Sigma^{\mu\nu}P_{\nu} = 0, \tag{10}$$

while varying L with respect to λ one obtains

$$P^{\mu}P_{\mu} + \frac{1}{2r^2}\Sigma^{\mu\nu}\Sigma_{\mu\nu} + m_0^2 = 0. \tag{11}$$

Since $\Sigma^{\mu\nu}$ is antisymmetric, we observe from (6) that if ξ_{μ} is parallel to P_{μ} the last term in (6) vanishes identically. Therefore, we may set

$$\xi^{\mu}P_{\mu} = 0. \tag{12}$$

This condition must be added to the Lagrangian (6) in the form $\eta(\xi^{\mu}P_{\mu})$, where η is another Lagrange multiplier. Varying the resultant extended Lagrangian with respect to η leads to (12). While arbitrary variations with respect to ξ^{μ} leads to the equation $\Sigma^{\mu\nu}P_{\nu} + \eta P^{\mu} = 0$ which, after multiplying it by P_{μ}, gives $\eta = 0$ and therefore one recovers the Lagrangian (6).

Our goal is to derive the second order Lagrangian associated with the Lagrangian (6). Our proof consists of some elementary algebra and for that reason in this section we shall only mention the main results. Nevertheless, since in such an algebra there are some key steps, in Appendix A we present the computation in more detail.

The main idea is to compute from (7)–(12) the combination $u\sigma\sigma u - r^2 \det\sigma$, where

$$u\sigma\sigma u \equiv u_{\mu}\sigma^{\mu\nu}\sigma_{\nu}{}^{\alpha}u_{\alpha} \tag{13}$$

and

$$\det\sigma = \frac{1}{4!}\varepsilon^{\mu\nu\alpha\beta}\varepsilon^{\tau\lambda\sigma\rho}\sigma_{\mu\tau}\sigma_{\nu\lambda}\sigma_{\alpha\sigma}\sigma_{\beta\rho}. \tag{14}$$

One finds the following result (for details see Appendix A):

$$u\sigma\sigma u - r^2 \det\sigma = \frac{m_0^2}{r^2}\left[\left(u^2 + \frac{r^2\sigma^2}{2}\right)\lambda^2 + \frac{1}{r^2}\lambda^4 m_0^2\right], \tag{15}$$

where we used the notation $a^2 = a^{\mu}a_{\mu}$, for any dynamical variable a^{μ}. Using once again the constraint (11) we find that (15) leads to the expression

$$\lambda^4 + \frac{\lambda^2}{m_0^2}\left(u^2 + \frac{1}{2}r^2\sigma^2\right) - \frac{r^2}{m_0^4}(u\sigma\sigma u - r^2 \det\sigma) = 0. \tag{16}$$

This expression can be solved for λ in terms of the Lorentz scalars u^2, σ^2, $u\sigma\sigma u$, and $\det\sigma$. But before solving for λ, let us show that λ and the Lagrangian L are related by the expression

$$L = -m_0^2\lambda. \tag{17}$$

First using the constraints (10) and (11) the Lagrangian (6) becomes

$$L = u^{\mu}P_{\mu} + \tfrac{1}{2}\sigma^{\mu\nu}\Sigma_{\mu\nu}.$$

From (7) and (9) we find the results

$$u^\mu P_\mu = \lambda P^2 \tag{18}$$

and

$$\frac{1}{2}\sigma^{\mu\nu}\Sigma_{\mu\nu} = \lambda\frac{\Sigma^2}{2r^2}. \tag{19}$$

So, we get

$$L = u^\mu P_\mu + \frac{1}{2}\sigma^{\mu\nu}\Sigma_{\mu\nu} = \lambda\left(P^2 + \frac{1}{2r^2}\Sigma^2\right). \tag{20}$$

By using (11) once again, we see that (20) leads to (17).

Thus, (16) and (17) leads to the Lagrangian

$$L = -m_0\left[\frac{-(u^2 + \frac{1}{2}r^2\sigma^2) \pm \sqrt{(u^2 + \frac{1}{2}r^2\sigma^2)^2 + r^2(u\sigma\sigma u - r^2 \det\sigma)}}{2}\right]^{1/2}. \tag{21}$$

Observe that if σ vanishes only the minus sign in the symbol $\pm\sqrt{}$ makes sense. In this case (21) is reduced to

$$L = -m_0[-u^2]^{1/2}, \tag{22}$$

which is the well-known Lagrangian for a relativistic point particle.

Since the Lagrangian (21) is a function of the all Lorentz scalars that can be formed from the velocities u and σ, namely u^2, σ^2, $u\sigma\sigma u$, and $\det\sigma$ we observe that such a Lagrangian has manifest Lorentz invariance. In fact, the Lagrangian (21) has a Poincaré invariance under the infinitesimal transformations $\delta x^\mu = a^\mu + \omega^\mu_\nu x^\nu$ and $\delta e^\mu_{(\alpha)} = \omega^\mu_\nu e^\nu_{(\alpha)}$, for arbitrary $\omega_{\mu\nu} = -\omega_{\nu\mu}$. By explicit computation, one can show by applying Noether's procedure to these transformations that P^μ and $M^{\mu\nu} = x^\mu P^\nu - x^\nu P^\mu + \Sigma^{\mu\nu}$ are conserved generators obeying the Poincaré group algebra (see Refs. 3 and 4 for details).

III. THE CONSTRAINTS FROM THE SECOND ORDER LAGRANGIAN

The central idea in this section is to derive the set of constraints associated with (21) which, of course, should correspond to (10) and (11). Instead of starting with the Lagrangian given in (21) we shall take advantage of the formulas (16) and (17). From this perspective one may assume that $\lambda = \lambda(u, \sigma)$ and define a "linear momentum" p_μ and an "internal angular momentum" $l_{\mu\nu}$ as

$$p_\mu = \frac{\partial\lambda}{\partial u^\mu} \tag{23}$$

and

$$l_{\mu\nu} = \frac{\partial\lambda}{\partial\sigma^{\mu\nu}}, \tag{24}$$

respectively. According to (17) we have the relations: $P_\mu = -m_0^2 p_\mu$ and $\Sigma_{\mu\nu} = -m_0^2 l_{\mu\nu}$. One of the reasons to define p_μ and $l_{\mu\nu}$ is to avoid carrying all the time the factor m_0^2.

Taking the derivative of (16) with respect to u^μ leads to

$$\left[\lambda^3 + \frac{\lambda}{2m_0^2}\left(u^2 + \frac{1}{2}r^2\sigma^2\right)\right]p_\mu = -\frac{\lambda^2}{2m_0^2}u_\mu + \frac{r^2}{2m_0^4}u^\alpha\sigma_{\alpha\beta}\sigma^\beta{}_\mu. \tag{25}$$

Let us define

$$A = \left[\lambda^3 + \frac{\lambda}{2m_0^2}\left(u^2 + \frac{1}{2} r^2 \sigma^2 \right) \right]. \tag{26}$$

We find

$$A^2 p^2 = \frac{\lambda^4 u^2}{4m_0^4} - \frac{\lambda^2 r^2}{2m_0^6} u\sigma\sigma u + \frac{r^4}{4m_0^8} u^\alpha \sigma_{\alpha\beta} \sigma^\beta{}_\mu \sigma^\mu{}_\tau \sigma^\tau{}_\lambda u^\lambda. \tag{27}$$

But the identity (A19) leads to

$$u^\alpha \sigma_{\alpha\beta} \sigma^\beta{}_\mu \sigma^\mu{}_\tau \sigma^\tau{}_\lambda u^\lambda = u^\alpha \sigma_{\alpha\beta} [-\tfrac{1}{2} \sigma^\beta{}_\lambda \sigma^2 - \tfrac{1}{4} \sigma^{*\beta}{}_\lambda (\sigma * \sigma)] u^\lambda \tag{28}$$

and therefore we have

$$A^2 p^2 = \frac{\lambda^4}{4m_0^4} u^2 - \frac{\lambda^2 r^2}{2m_0^6} u\sigma\sigma u - \frac{r^4}{8m_0^8} u\sigma\sigma u \sigma^2 + \frac{1}{64} \frac{r^4}{m_0^8} u^2 (\sigma \cdot \sigma *)^2, \tag{29}$$

where we used the fact that

$$\sigma_{\alpha\beta} \sigma^{*\beta}{}_\lambda = -\tfrac{1}{4} \eta_{\alpha\lambda} (\sigma \cdot \sigma *). \tag{30}$$

Similarly, applying to (16) the derivative with respect to $\sigma^{\mu\nu}$ we obtain

$$\left[\lambda^3 + \frac{\lambda}{2m_0^2}\left(u^2 + \frac{1}{2} r^2 \sigma^2 \right) \right] l_{\mu\nu} = -\frac{\lambda^2 r^2}{2m_0^2} \sigma_{\mu\nu} + \frac{r^2}{2m_0^4} (u^\alpha \sigma_{\alpha\mu} u_\nu - u^\alpha \sigma_{\alpha\nu} u_\mu) + \frac{r^4}{8m_0^4} \sigma^*_{\mu\nu} (\sigma \cdot \sigma *), \tag{31}$$

where we used (A18). This expression yields

$$A^2 l^2 = \frac{\lambda^4 r^4}{4m_0^4} \sigma^2 - \frac{\lambda^2 r^4}{m_0^6} u\sigma\sigma u - \frac{\lambda^2 r^6}{8m_0^6} (\sigma \cdot \sigma *)^2 - \frac{r^4}{2m_0^8} u\sigma\sigma u u^2 - \frac{r^6}{16m_0^8} u^2 (\sigma \cdot \sigma *)^2 - \frac{r^8 \sigma^2}{64 m_0^8} (\sigma \cdot \sigma *)^2, \tag{32}$$

where we used the identities $\sigma^* \sigma^* = -\sigma\sigma$ and (30).

Adding (29) and (32) leads to

$$\begin{aligned} A^2 \left(p^2 + \frac{1}{2r^2} l^2 \right) = {} & \frac{\lambda^4}{4m_0^4} \left(u^2 + \frac{1}{2} r^2 \sigma^2 \right) - \frac{\lambda^2 r^2}{m_0^6} (u\sigma\sigma u - r^2 \det \sigma) \\ & - \frac{r^4}{4m_0^8} \left(u^2 + \frac{1}{2} r^2 \sigma^2 \right) (u\sigma\sigma u - r^2 \det \sigma), \end{aligned} \tag{33}$$

where we used (A18).

Using (16) and (26) we discover that

$$p^2 + \frac{1}{2r^2} l^2 = -\frac{1}{m_0^2}. \tag{34}$$

Since $P_\mu = -m_0^2 p_\mu$ and $\Sigma_{\mu\nu} = -m_0^2 l_{\mu\nu}$ we finally get from (34) the constraint

$$P^2 + \frac{1}{2r^2} \Sigma^2 + m_0^2 = 0. \tag{35}$$

Let us now derive from (25) and (31) the constraint $\Sigma^{\mu\nu} P_\nu = 0$. We have

$$A^2 l^{\mu\nu} p_\nu = \frac{\lambda^4 r^2}{2m_0^2}\sigma^{\mu\nu}u_\nu + \frac{\lambda^2 r^2 u^2}{2m_0^6}\sigma^{\mu\nu}u_\nu - \frac{\lambda^2 r^4}{8m_0^6}(\sigma\cdot\sigma^*)\sigma^{*\mu\nu}u_\nu - \frac{\lambda^2 r^4}{2m_0^6}\sigma^{\mu\nu}\sigma_{\nu\alpha}\sigma^{\alpha\beta}u_\beta - \frac{r^4(u\sigma\sigma u)}{2m_0^8}\sigma^{\mu\nu}u_\nu + \frac{r^4 u^\mu}{2m_0^8}u_\tau\sigma^{\tau\nu}\sigma_{\nu\alpha}\sigma^{\alpha\beta}u_\beta + \frac{r^6}{2m_0^8}(\sigma\cdot\sigma^*)\sigma^{*\mu\nu\tau\nu}\sigma_{\nu\alpha}\sigma^{\alpha\beta}u_\beta. \tag{36}$$

The sixth term on the right-hand side of (36) vanishes due to the identity $u_\tau\sigma^{\tau\nu}\sigma_{\nu\alpha}\sigma^{\alpha\beta}u_\beta \equiv 0$. Using (A19) and (30) it is not difficult to show that (36) is reduced to

$$A^2 l^{\mu\nu} p_\nu = \frac{\lambda^4 r^2}{2m_0^2}\sigma^{\mu\nu}u_\nu + \frac{\lambda^2 r^2}{2m_0^6}\left(u^2 + \frac{r^2}{2}\sigma^2\right)\sigma^{\mu\nu}u_\nu - \frac{r^4}{2m_0^8}(u\sigma\sigma u - r^2\det\sigma)\sigma^{\mu\nu}u_\nu. \tag{37}$$

Solving the factor $(u\sigma\sigma u - r^2\det\sigma)$ in (16) and substituting the result in (37) we finally discover that $l^{\mu\nu}p_\nu = 0$. This leads to the constraint

$$\Sigma^{\mu\nu}P_\nu = 0, \tag{38}$$

which is the Tulczyjew constraint.

Summarizing, we have shown that the Lagrangian (21) leads to the constraints (35) and (38) which were the starting point in the first order formalism of Sec. II.

IV. FROM A POINT PARTICLE IN HIGHER DIMENSIONS TO THE DE SITTER RELATIVISTIC TOP

Let us start writing the higher dimensional metric γ_{MN} in terms of the vielbien field E_M^A,

$$\gamma_{MN} = E_M^A E_N^B \eta_{AB}, \tag{39}$$

where η_{AB} is a *flat metric* in $4+N$ dimensions. Here we are considering the vielbien field E_M^A as a the function of the coordinates x^M.

The Lagrangian of a point particle moving in a background determined by the metric γ_{MN} is

$$L = -M_0(-\gamma_{MN}\dot{x}^M\dot{x}^N)^{1/2}, \tag{40}$$

where M_0 is the analogue of the mass of the object and $\dot{x}^M \equiv \mathrm{d}x^M/\mathrm{d}\tau$. From this Lagrangian one gets the Euler–Lagrange equations of motion

$$\frac{DP^M}{D\tau} \equiv \dot{P}^M + \Gamma_{RS}^M \dot{x}^R P^S = 0, \tag{41}$$

where

$$P_M = \frac{\partial L}{\partial \dot{x}^M} \tag{42}$$

and Γ_{RS}^M are the Christoffel symbols associated with γ_{MN}. We can write E_M^A in the form

$$E_M^A = \begin{pmatrix} E_\mu^a(x,y) & E_\mu^{a'}(x,y) \\ E_i^a(x,y) & E_i^{a'}(x,y) \end{pmatrix}, \tag{43}$$

where we used the notation $x^M = (x^\mu, y^i) = (x, y)$.

Using the Kaluza–Klein mechanism it is well known that E_M^A can be written in the form

$$E_M^A = \begin{pmatrix} e_\mu^a(x) & \omega_\mu^{a'}(x) \\ 0 & e_i^{a'}(y) \end{pmatrix}. \tag{44}$$

Here, for later convenience, we used the notation $\omega_\mu^{a'} \equiv E_\mu^{a'}$, $e_\mu^a \equiv E_\mu^a$, and $e_i^{a'} \equiv E_i^{a'}$.

Using (44) we can brake the metric (39) in the form

$$\gamma_{\mu\nu} = g_{\mu\nu} + \omega_\mu^{a'}\omega_\nu^{b'}\eta_{a'b'},$$

$$\gamma_{\mu i} = \omega_\mu^{a'} e_i^{b'}\eta_{a'b'}, \tag{45}$$

$$\gamma_{ij} = e_i^{a'} e_j^{b'}\eta_{a'b'} = g_{ij}(y),$$

where $g_{\mu\nu}(x) = e_\mu^a(x)e_\nu^b(x)\eta_{ab}$.

The line element ds^2 associated with γ_{MN} is

$$ds^2 = \gamma_{MN}\,dx^M\,dx^N = \gamma_{\mu\nu}\,dx^\mu\,dx^\nu + 2\gamma_{\mu i}\,dx^\mu\,dy^i + \gamma_{ij}\,dy^i\,dy^j. \tag{46}$$

Substituting (45) within (46) one gets

$$ds^2 = (g_{\mu\nu} + \omega_\mu^{a'}\omega_\nu^{b'}\eta_{a'b'})dx^\mu\,dx^\nu + 2(\omega_\mu^{a'}e_i^{b'}\eta_{a'b'})dx^\mu\,dy^i + (e_i^{a'}e_j^{b'}\eta_{a'b'})dy^i\,dy^j. \tag{47}$$

This expression can be rewritten in the following form:

$$ds^2 = g_{\mu\nu}dx^\mu\,dx^\nu + (\omega_\mu^{a'}\,dx^\mu + e_i^{a'}\,dy^i)^2, \tag{48}$$

which is the Fukuyama starting point in the study of spinning particles.[17] If we choose the base[18,19]

$$\theta^\mu = dx^\mu \tag{49a}$$

and

$$\theta^{a'} = \omega_\mu^{a'}\,dx^\mu + e_i^{a'}\,dy^i, \tag{49b}$$

then we have that the line element (48) becomes

$$ds^2 = g_{\mu\nu}\theta^\mu\theta^\nu + \eta_{a'b}\theta^{a'}\theta^{b'}. \tag{50}$$

Therefore, in the base (49) the metric takes the form

$$\hat{\gamma}_{MM} = \begin{pmatrix} g_{\mu\nu} & 0 \\ 0 & \eta_{a'b'} \end{pmatrix}. \tag{51}$$

The dual base is given by

$$D_\mu = \partial_\mu - \omega_\mu^{a'}e_{a'}^i\partial_i \tag{52a}$$

and

$$D_{a'} = e_{a'}^i\partial_i. \tag{52b}$$

In fact, one can verify that

$$\langle\theta^\mu, D_\nu\rangle = \langle dx^\mu, \partial_\nu - \omega_\nu^{a'}e_{a'}^i\partial_i\rangle = \delta_\nu^\mu \tag{53}$$

and

$$\langle\theta^{a'}, D_{b'}\rangle = \langle\omega_\mu^{a'}\,dx^\mu + e_i^{a'}\,dx^i, u_{b'}^j\partial_j\rangle = e_i^{a'}e_{b'}^i = \delta_{b'}^{a'}. \tag{54}$$

Similarly, one can check that

$$\langle \theta^{a'}, D_\nu \rangle = \langle \omega_\mu^{a'}\, \mathrm{d}x^\mu + e_i^{a'}\, \mathrm{d}x^i, \partial_\nu - \omega_\nu^{b'} e_{b''}^j \partial_j \rangle = \omega_\nu^{a'} - e_j^{a'} e^{jb'} \omega_{b'\nu} = \omega_\nu^{a'} - \eta^{a'b'} \omega_{b'\nu} = 0. \quad (55)$$

Let us compute the commutator $[D_\mu, D_\nu]$. From (52a) we have

$$[D_\mu, D_\nu] = [\partial_\mu - \omega_\mu^{a'} e_{a'}^i \partial_i, \partial_\nu - \omega_\nu^{b'} e_{b''}^j \partial_j] = \partial_\mu(\partial_\nu - \omega_\nu^{b'} e_{b''}^j \partial_j) - \omega_\mu^{a'} e_{a'}^i \partial_i(\partial_\nu - \omega_\nu^{b'} e_{b''}^j \partial_j)$$
$$= -\partial_\nu(\partial_\mu - \omega_\mu^{a'} e_{a'}^i \partial_i) + \omega_\nu^{b'} e_{b''}^j \partial_j(\partial_\mu - \omega_\mu^{a'} e_{a'}^i \partial_i). \quad (56)$$

Considering that $[\partial_\mu, \partial_\nu]=0$, $[\partial_i, \partial_j]=0$ and $[\partial_\mu, \partial_i]=0$ we find that the expression (56) reduces to

$$[D_\mu, D_\nu] = (-\partial_\mu \omega_\nu^{b'} + \partial_\nu \omega_\mu^{b'}) e_{b'}^j \partial_j + (\omega_\mu^{a'} e_{a'}^i \omega_\nu^{b'} - \omega_\nu^{c'} e_{c'}^i \omega_\mu^{b'})(\partial_i e_{b'}^j)\partial_j. \quad (57)$$

The second term in (57) can be rewritten as

$$(\omega_\mu^{a'} e_{a'}^i \omega_\nu^{b'} - \omega_\nu^{c'} e_{c'}^i \omega_\mu^{b'})(\partial_i e_{b'}^j)\partial_j = \omega_\mu^{a'} \omega_\nu^{b'} (e_{a'}^i \partial_i e_{b'}^j - e_{b''}^l \partial_l e_{a'}^j). \quad (58)$$

Let us write $e_{a'} \equiv e_{a'}^i \partial_i$, thus we have

$$(e_{a'}^i \partial_i e_{b'}^j - e_{b''}^l \partial_l e_{a'}^j) = [e_{a'}, e_{b'}]. \quad (59)$$

We assume that

$$[e_{a'}, e_{b'}] = -C_{a'b'}^{d'} e_{d'}, \quad (60)$$

where $C_{a'b'}^{d'}$ are the structure constants associated with some group G. Substituting (60) into (57) we find the expression

$$[D_\mu, D_\nu] = (-\partial_\mu \omega_\nu^{b'} + \partial_\nu \omega_\mu^{b'}) e_{b'} - \omega_\mu^{a'} \omega_\nu^{b'} C_{a'b'}^{d'} e_{d'}, \quad (61)$$

which by means of the definition

$$R_{\mu\nu}^{b'} = \partial_\mu \omega_\nu^{b'} - \partial_\nu \omega_\mu^{b'} + C_{c'd'}^{b'} \omega_\mu^{c'} \omega_\nu^{d'} \quad (62)$$

becomes

$$[D_\mu, D_\nu] = -R_{\mu\nu}^{b'} e_{b'}. \quad (63)$$

Following similar procedure we find that

$$[D_\mu, D_{a'}] = 0 \quad (64)$$

and

$$[D_{a'}, D_{b'}] = -C_{a'b'}^{d'} e_{d'}. \quad (65)$$

Thus, from (63)–(65) we see that the only nonvanishing structure constants related to the commutator $[D_M, D_N]$ are $C_{\mu\nu}^{b'} = -R_{\mu\nu}^{b'}$ and $C_{a'b'}^{d'}$.

In general, in a nonbase frame, the connection Γ_{MNP} is given by

$$\Gamma_{MNP} = \tfrac{1}{2}(D_P \hat{\gamma}_{MN} + D_N \hat{\gamma}_{MP} - D_M \hat{\gamma}_{NP}) + \tfrac{1}{2}(C_{MNP} + C_{MPN} - C_{NPM}). \quad (66)$$

Since $C_{\mu\nu\alpha}=0$ and $\hat{\gamma}_{\mu\nu}=g_{\mu\nu}(x)$ we get

$$\Gamma_{\mu\nu\alpha} = \tfrac{1}{2}(D_\alpha \hat{\gamma}_{\mu\nu} + D_\nu \hat{\gamma}_{\nu\alpha} - D_\mu \hat{\gamma}_{\nu\alpha}) = \tfrac{1}{2}(\partial_\alpha g_{\mu\nu} + \partial_\nu g_{\nu\alpha} - \partial_\mu g_{\nu\alpha}) \equiv \{\mu\nu\alpha\}. \quad (67)$$

In the same way, since $C_{\mu\nu a'} = -R_{\mu\nu a'}$ we obtain

$$\Gamma_{\mu\nu a'} = \tfrac{1}{2}(C_{\mu\nu a'} + C_{\mu a'\nu} - C_{\nu a'\mu}) = -\tfrac{1}{2}R_{\mu\nu a'}. \tag{68}$$

We also get

$$\Gamma_{\mu a'b'} = 0 \tag{69}$$

and

$$\Gamma_{a'b'c'} = -\tfrac{1}{2}C_{a'b'c'}. \tag{70}$$

With these results in hand for Γ_{MNP} we shall proceed to see their consequences in the equations of motion (41). Let us start splitting (41) in the following form:

$$\dot{P}^{\mu} + \Gamma^{\mu}_{\nu\alpha}\dot{x}^{\nu}P^{\alpha} + \Gamma^{\mu}_{\nu a'}\dot{x}^{\nu}P^{a'} + \Gamma^{\mu}_{a'\nu}\dot{x}^{a'}P^{\nu} = 0 \tag{71}$$

and

$$\dot{P}^{a'} + \Gamma^{a'}_{b'c'}\dot{x}^{b'}P^{c'} = 0, \tag{72}$$

where we used the fact that the only nonvanishing components of Γ_{MNP} are $\Gamma_{\mu\nu\alpha}$, $\Gamma_{\mu\nu a'}$ and $\Gamma_{a'b'c'}$.

Using (67) and (68) we discover that (71) and (72) yields

$$\frac{\overline{D}P^{\mu}}{\overline{D}\tau} = R^{\mu}_{\nu a'}\dot{x}^{\nu}P^{a'} \tag{73}$$

and

$$\dot{P}^{a'} = 0, \tag{74}$$

respectively, where $\overline{D}/\overline{D}\tau$ means covariant derivative in terms of the Christoffel symbols $\{\mu\nu\alpha\}$. Here we used the fact that

$$P_M = \frac{M_0\gamma_{MN}\dot{x}^N}{(-\gamma_{PQ}\dot{x}^P\dot{x}^Q)^{1/2}}, \tag{75}$$

which means that $P^M = \lambda\dot{x}^M$, with $\lambda = M_0(-\gamma_{PQ}\dot{x}^P\dot{x}^Q)^{-1/2}$.

We shall show now that (73) and (74) are equivalent to the relativistic top equations of motion (RTEM) in a gravitational field.[20–25] For that purpose we shall make the indices identification $a' \to (a,b)$ where the pair (a,b) is antisymmetric. Thus, the equations of motion (73) and (74) become

$$\frac{\overline{D}P^{\mu}}{\overline{D}\tau} = \frac{1}{2}R^{\mu}_{\nu ab}\dot{x}^{\nu}S^{ab} \tag{76}$$

and

$$\dot{S}^{ab} = 0, \tag{77}$$

where we used the notation $S^{ab} \equiv P^{ab}$ and introduced in (76) the quantity $\frac{1}{2}$ in order to avoid counting twice.

The last step is to write $S^{ab} = e^a_{\mu}e^b_{\nu}S^{\mu\nu}$ in order to write (76) and (77) in the form

$$\frac{\overline{D}P^{\mu}}{\overline{D}\tau} = \frac{1}{2}R^{\mu}_{\nu\alpha\beta}\dot{x}^{\nu}S^{\alpha\beta} \tag{78}$$

and

$$\frac{\overline{D}S^{\mu\nu}}{\overline{D}\tau} = 0, \tag{79}$$

which are the traditional forms given to the RTEM in a gravitational field.

It is interesting to clarify the meaning of the constant M_0. From (75) it follows the constraint

$$P^M P^N \hat{\gamma}_{MM} = -M_0^2, \tag{80}$$

which in virtue of the form of the metric $\hat{\gamma}_{MM}$, given in (51), we see that (80) can be written as

$$g_{\mu\nu}P^{\mu}P^{\nu} + \eta_{a'b'}P^{a'}P^{b'} = -M_0^2 \tag{81}$$

or

$$g_{\mu\nu}P^{\mu}P^{\nu} + \frac{1}{2r^2}S^{\mu\nu}S_{\mu\nu} = -m_0^2, \tag{82}$$

where we used the relation $S^{ab}=e^a_{\mu}e^b_{\nu}S^{\mu\nu}$ and redefined P^{μ} as rP^{μ} and M_0 as rm_0 with r a constant of the motion. If we compare the expression (82) with (1) we observe their great similarity. However, they are not exactly the same because the constraint $\Sigma^{\mu\nu}P_{\nu}\approx 0$ given in (4) is not satisfied by P^{μ} and $S^{\mu\nu}$. Instead of the constraint (4) we can define the vector

$$S^{\mu} = \tfrac{1}{2}\epsilon^{\mu\nu\alpha\beta}P_{\nu}S_{\alpha\beta} \tag{83}$$

and, as a consequence of this formula, we have

$$S^{\mu}P_{\mu} = 0. \tag{84}$$

Nevertheless, the relation between $\Sigma^{\mu\nu}$ and $S^{\mu\nu}$ is subtle and requires a careful analysis. First of all, let us write the first order Lagrangian

$$L = \dot{x}^M P_M - \frac{\lambda'}{2}(P^M P_M + M_0^2), \tag{85}$$

corresponding to (40). Using (82) we see that (40) can be written as

$$L = \dot{x}^{\mu}P_{\mu} + \frac{1}{2}\dot{x}^{\mu\nu}S_{\mu\nu} - \frac{\lambda}{2}\left(P^{\mu}P_{\mu} + \frac{1}{2r^2}S^{\mu\nu}S_{\mu\nu} + m_0^2\right), \tag{86}$$

where $\dot{x}^{\mu\nu}=e^{\mu}_a e^{\nu}_b \dot{x}^{ab}$ and $\lambda \equiv r^2\lambda'$. Comparing (86) with (6) one observes the close similarity between both Lagrangians. We can even try to go from (86) to (6) by using the transformation

$$S^{\mu\nu} = \Sigma^{\mu\nu} + \xi^{\mu}P^{\nu} - \xi^{\nu}P^{\mu}. \tag{87}$$

But this implies to redefine the velocities u^{μ} and $\sigma^{\mu\nu}$ in terms of the velocities $\dot{x}^{\mu}$ and $\dot{x}^{\mu\nu}$. This is related to the fact that the motion of a relativistic top can be described, in an equivalent way, by two position vectors, namely, the center of mass and the center of charge. (An extensive discussion about the meaning of these two position vectors of a relativistic top can be found in Ref. 26.) The center of mass can be associated with $\Sigma^{\mu\nu}$ via the constraint $\Sigma^{\mu\nu}P_{\nu}\approx 0$, while the center of charge with $S^{\mu\nu}$. Thus, the transformation (87) suggests to identify the variable ξ^{μ} with the difference between the center of mass and the center of charge. In fact, multiplying (87) by P_{μ} one gets

$$S^{\mu\nu}P_{\nu} = \xi^{\mu}P^{\nu}P_{\nu}, \tag{88}$$

where we assumed $\xi^{\mu}P_{\mu}=0$. Substituting this expression into (87) one discovers that $\Sigma^{\mu\nu}$ can be obtained from $S^{\mu\nu}$ using the projector $\eta^{\mu\alpha}-(1/P^2)P^{\mu}P^{\alpha}$.

Summarizing, we have shown that using the Kaluza–Klein theory it is possible to obtain the relativistic top theory from a point particle in higher dimensions. This is in fact a very interesting result because it means that although the top does not follow geodesics in four dimensions, it does in higher dimensions.

V. FINAL COMMENTS

In this paper we have shown different aspects of a particular relativistic top, namely the top satisfying (1) and (4). First, we showed the equivalence between the first and second order Lagrangians (6) and (21). Then, the form of the Lagrangian (6) motivated us to look for a higher dimensional description of the top, and as a matter of fact we discovered that it is possible to obtain the relativistic top equations of motion starting from a geodesic equation of motion of a point particle in higher dimensions. This is an interesting result that deserves to be analyzed in terms of a fiber bundle scenario.

First we notice that such a result is similar to the case of the Lorentz force associated with a charged particle which can be obtained from a geodesic in five dimensions. More generally, our result is similar to the generalized Lorentz force associated with a Yang–Mills gauge field which can be obtained by a geodesic in $4+D$-dimensions. In this case, the traditional method is to consider a $4+D$-dimensional principle fiber bundle P, which locally looks like $M^4\times B$, where M^4 is a four-dimensional base space and B is a group manifold whose dimension is D. The key object to connect the geodesic in $4+D$-dimensions with the generalized Lorentz force in four dimensions is the one-form in the cotangent space $T^*(P)$,

$$\omega = g^{-1}\,\mathrm{d}g + g^{-1}Ag, \tag{89}$$

where $A=A^{a}_{\mu}T_a\,\mathrm{d}x^{\mu}$ can eventually be identified with the Yang–Mills gauge field. Here, T_a are the generators of some group G acting transitively on B and having the properties

$$[T_a,T_b] = C^{c}_{ab}T_c. \tag{90}$$

In principle, if we consider the fiber space $M^4\times Q$, where Q corresponds also to a four-dimensional manifold, one may apply similar description to the case of a spinning object (see Ref. 17). In this case the connection one-form reads as

$$\omega = g^{-1}\,\mathrm{d}g + g^{-1}\Omega g, \tag{91}$$

where Ω is given by

$$\Omega = \tfrac{1}{2}\omega^{AB}_{\mu}S_{AB}\,\mathrm{d}x^{\mu}. \tag{92}$$

Here, we shall assume that S_{AB} are the generators of the de Sitter group SO(1,4) [or anti–de Sitter group SO(2,3)]. If we compare (49b) with (91) we observe that both expressions are very similar. In fact, since g is an element of SO(1,4) we can write g as a matrix in the form Λ^{A}_{B} and therefore the one-form (91) yields

$$\omega^{AB} = \omega^{AB}_{i}\,\mathrm{d}y^{i} + \omega^{AB}_{\mu}\,\mathrm{d}x^{\mu}, \tag{93}$$

where $\omega^{AB}_{i}=\Lambda^{CA}\partial_i\Lambda^{B}_{C}$. This expression can be written as

$$\omega^{5a} = \omega^{5a}_{i}\,\mathrm{d}y^{i} + \omega^{5a}_{\mu}\,\mathrm{d}x^{\mu} \tag{94}$$

and

$$\omega^{ab} = \omega_i^{ab}\, \mathrm{d}y^i + \omega_\mu^{ab}\, \mathrm{d}x^\mu. \tag{95}$$

The base (49a) and (49b) arises from (94) and (95) by defining $e_i^{a'} \equiv \omega_i^{ab}$, $e_\mu^a \equiv \omega_\mu^{5a}$ and setting ω_i^{5a} equal to zero. This means that we can write (44) in the following form:

$$\omega_M^{AB} = \begin{pmatrix} \omega_\mu^{5a}(x) & \omega_\mu^{ab}(x) \\ 0 & \omega_i^{ab}(y) \end{pmatrix}. \tag{96}$$

Therefore, the metric γ_{MN} in (39) becomes

$$\gamma_{MN} = \tfrac{1}{2}\omega_M^{AB}\omega_{NAB} \tag{97}$$

and consequently the Lagrangian (40) can be written as

$$L = -M_0(-\tfrac{1}{2}\omega_M^{AB}\omega_{NAB}\dot{x}^M\dot{x}^N)^{1/2}. \tag{98}$$

Thus, the corresponding line element is

$$\mathrm{d}s^2 = \tfrac{1}{2}\omega_M^{AB}\omega_{NAB}\, \mathrm{d}x^M\, \mathrm{d}x^N, \tag{99}$$

which is in agreement with the Fukuyama's suggestion.[17] We shall call the system described by the Lagrangian (98) with ω_M^{AB} given by (96) the *de Sitter top*.

There are several observations that one can make from our analysis but perhaps one of the most important is the fact that the top theory leads naturally to consider the de Sitter group SO(1,4) [or anti–de Sitter group SO(2,3)] via the connection ω_M^{AB}. As it is well known, this group structure appears in several fronts of current interest, including Maldacena's conjecture in string theory, accelerated universe, and the gravitational gauge approach of MacDowell–Mansouri. For this reason it turns out to be of particular interest for further research to study the possible connection between the de Sitter top and these lines of research.

On the other hand, since in the Kaluza–Klein $4+N+D$-dimensional space the metric gives gravity, Yang–Mills, and scalar fields, a top moving in this space will be acted on by these fields. It may be interesting to see how the Yang–Mills field, which can be understood as the field which generates rotations in the isospace, affects the motion of the top. In Ref. 27 some computations in this direction were reported. We attach a brief review of such computations as an appendix (see Appendix B). Part of our task, for further research, is to analyze these computations from the point of view of the present work.

Finally, the Regge trajectory (1) which lead us to the de Sitter relativistic top concept is a very particular relation between the mass and the spin of a particle. In general, a singular Lagrangian can lead to more general Regge trajectories of the form (B5). In particular, by using group theoretical methods, Atre and Mukunda[7] have developed a systematic procedure for other possible Regge trajectories. In those cases one should expect generalizations or alternatives of the de Sitter relativistic top which is based in the de Sitter group. From the group theoretical point of view, however, such a generalization or alternative appears as an intriguing possibility motivating further research on the subject.

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APPENDIX A

In this appendix we present the proof of formula (15). From (7) and (10) we get

$$u^2 = \lambda^2 P^2 + V^2. \tag{A1}$$

Similarly, from (9), (10), and (12) we find

$$\sigma^2 = \frac{\lambda^2}{r^4}\Sigma^2 + 2\xi^2 P^2. \tag{A2}$$

Here we also used the notation $b^2 = b^{\mu\nu}b_{\mu\nu}$, for any tensor $b^{\mu\nu}$.

We shall compute

$$\sigma^4 \equiv \sigma_{\mu\nu}\sigma^{\nu}{}_{\alpha}\sigma^{\alpha}{}_{\beta}\sigma^{\beta\mu}. \tag{A3}$$

Observe first that

$$\sigma^{\mu\alpha}\sigma_{\alpha}{}^{\nu} = \frac{\lambda^2}{r^4}\Sigma^{\mu\alpha}\Sigma_{\alpha}{}^{\nu} - \frac{\lambda}{r^2}(V^{\mu}P^{\nu} + V^{\nu}P^{\mu}) - \xi^2 P^{\mu}P^{\nu} - P^2\xi^{\mu}\xi^{\nu}, \tag{A4}$$

where we used (10) and (12). The expression (A4) leads to

$$\sigma^4 = \frac{\lambda^4}{r^8}\Sigma^4 + 4\frac{\lambda^2}{r^4}P^2V^2 + 2\xi^2\xi^2P^2P^2, \tag{A5}$$

where once again we used (10) and (12) and antisymmetric properties, such as $\Sigma^{\mu\nu}\xi_{\mu}\xi_{\nu} \equiv 0$.

We also need to compute

$$u\sigma\sigma u \equiv u_{\mu}\sigma^{\mu\nu}\sigma_{\nu}{}^{\alpha}u_{\alpha}. \tag{A6}$$

From (7), (9), (10), and (12) we find

$$\sigma^{\mu\nu}u_{\nu} = \frac{\lambda}{r^2}\Sigma^{\mu\nu}V_{\nu} - \lambda P^2\xi^{\mu}. \tag{A7}$$

Therefore, we have

$$u\sigma\sigma u = -\lambda^2\left(-\frac{1}{r^4}V_{\mu}\Sigma^{\mu\nu}\Sigma_{\nu}{}^{\alpha}V_{\alpha} + \frac{2}{r^2}P^2V^2 + P^2P^2\xi^2\right) \tag{A8}$$

or

$$u\sigma\sigma u = -\lambda^2\left(\frac{1}{r^4}\xi_{\alpha}\Sigma^{\alpha\nu}\Sigma_{\nu\tau}\Sigma^{\tau\lambda}\Sigma_{\lambda}{}^{\beta}\xi_{\beta} + \frac{2}{r^2}P^2V^2 + P^2P^2\xi^2\right). \tag{A9}$$

Now, let us define the dual of any antisymmetric tensor $A_{\alpha\beta}$ as

$$A^{*\mu\nu} = \tfrac{1}{2}\epsilon^{\mu\nu\alpha\beta}A_{\alpha\beta}, \tag{A10}$$

where $\varepsilon^{\mu\nu\alpha\beta}$ is the completely antisymmetric Levi–Cività tensor.

It turns out that from the constraint (10) it follows

$$\Sigma^{*\mu\nu}\Sigma_{\mu\nu} = 0. \tag{A11}$$

Using (A11) it is not difficult to show that

$$\Sigma^{\mu\nu}\Sigma_{\nu\alpha}\Sigma^{\alpha\tau} = -\tfrac{1}{2}\Sigma^{\mu\tau}(\Sigma^2). \tag{A12}$$

Thus, using (A12) one finds that (A9) becomes

$$u\sigma\sigma u = -\lambda^2\left(\frac{1}{2r^4}V^2\Sigma^2 + \frac{2}{r^2}P^2V^2 + P^2P^2\xi^2\right). \tag{A13}$$

On the other hand, from (A2) we obtain

$$\sigma^2\sigma^2 = \frac{\lambda^4}{r^8}\Sigma^2\Sigma^2 + \frac{4\lambda^2}{r^4}\xi^2P^2\Sigma^2 + 4\xi^2\xi^2P^2P^2. \tag{A14}$$

Therefore, (A5) and (14) imply

$$\sigma^2\sigma^2 - 2\sigma^4 = \frac{4\lambda^2}{r^4}\xi^2P^2\Sigma^2 - \frac{8\lambda^2}{r^4}P^2V^2, \tag{A15}$$

where we used the fact that from (A12) it follows that

$$2\Sigma^4 - \Sigma^2\Sigma^2 = 0. \tag{A16}$$

Now, define

$$\det\sigma = \frac{1}{4!}\varepsilon^{\mu\nu\alpha\beta}\varepsilon^{\tau\lambda\sigma\rho}\sigma_{\mu\lambda}\sigma_{\nu\lambda}\sigma_{\alpha\sigma}\sigma_{\beta\rho}. \tag{A17}$$

It is not difficult to show that

$$\det\sigma = -\tfrac{1}{16}(\sigma * \sigma)^2. \tag{A18}$$

From the identity

$$\sigma^{\mu\alpha}\sigma_{\alpha\beta}\sigma^{\beta\nu} = -\tfrac{1}{2}\sigma^{\mu\nu}(\sigma^2) - \tfrac{1}{4}\sigma^{*\mu\nu}(\sigma * \sigma), \tag{A19}$$

we find

$$\sigma^4 = \tfrac{1}{2}\sigma^2\sigma^2 + \tfrac{1}{4}(\sigma * \sigma)(\sigma * \sigma). \tag{A20}$$

Therefore, by combining (A18) and (A20) we obtain

$$\det\sigma = \tfrac{1}{8}(\sigma^2\sigma^2 - 2\sigma^4). \tag{A21}$$

From (A15) we see that (A21) implies

$$\det\sigma = \frac{\lambda^2}{2r^4}\xi^2P^2\Sigma^2 - \frac{\lambda^2}{r^4}P^2V^2. \tag{A22}$$

Now, from (A13) and (A22) we see that

$$u\sigma\sigma u - r^2\det\sigma = \lambda^2\left[\frac{-1}{2r^4}V^2\Sigma^2 - \frac{2}{r^2}P^2V^2 - \xi^2r^2P^2 - \frac{1}{2r^2}\xi^2P^2\Sigma^2 + \frac{1}{r^2}P^2V^2\right] = \lambda^2\left[\frac{m_0^2}{r^2}V^2 + m_0^2\xi^2P^2\right]. \tag{A23}$$

Using (A1) and (A2) one finally sees that (A23) leads to (15).

APPENDIX B

In $4+N'$ dimensions, with $N'=N+D$, a top can be described by the variables $x^M(\tau)$ and $E_A^M(\tau)$, where x^M are $4+N'$ coordinates, $E_A^M(\tau)$ are $4+N'$ orthonormal vectors, τ is an arbitrary parameter and the index A in parentheses labels the name of the vector. The vectors E_A^M satisfy the condition

$$\gamma_{MN} = E_M^A E_N^B \eta_{AB}, \tag{B1}$$

where $\eta_{AB}=\mathrm{diag}(-1,1,\ldots,1)$ is a scalar matrix and γ_{MN} is the curved metric generalized to $4+N'$ dimensions.

Define the linear velocity u^M and the angular velocity σ^{MN} as follows:

$$u^M \equiv \frac{\mathrm{d}x^M}{\mathrm{d}\tau} = \dot{x}^M, \tag{B2}$$

$$\sigma^{MN} = \eta^{AB} E_A^M \frac{\Delta}{\mathrm{d}\tau} E_B^N = -\sigma^{NM}. \tag{B3}$$

Here, the symbol $\Delta/\mathrm{d}\tau$ means covariant derivative with respect to τ, having the Christoffel symbols Γ_{NP}^M as the connection. One sees that σ^{MN} is again antisymmetric by virtue of the condition (B1).

Consider a top with linear velocity u^M, angular velocity σ^{MN}, linear momentum P^M, and internal angular momentum S^{MN}. We will assume that the dynamics of the system is generated by the Lagrangian

$$L = -u^M P_M - \tfrac{1}{2}\sigma^{MN} S_{MN} + \lambda H + \lambda_M H^M, \tag{B4}$$

where

$$H \equiv P^M P_M - f(\tfrac{1}{2} S^{MN} S_{MN}) \tag{B5}$$

and

$$H^M \equiv S^{MN} P_N \tag{B6}$$

corresponds to the Regge and Tulcyzjew constraints, respectively, generalized to $4+N'$ dimensions. Here, λ and λ_M are Lagrange multipliers.

Using the Lagrangian (B4) and assuming the equivalence principle in $4+N'$ dimensions leads to the RTEM equations of motion generalized to higher dimensions,

$$\frac{\Delta P^M}{\mathrm{d}\tau} = -\frac{1}{2} R^M_{NPQ} u^N S^{PQ} \tag{B7}$$

and

$$\frac{\Delta S^{MN}}{\mathrm{d}\tau} = P^M u^N - P^N u^M. \tag{B8}$$

Here, $\Delta A^M/\mathrm{d}\tau = (\mathrm{d}A^M/\mathrm{d}\tau) + \Gamma^M_{NP} A^N u^P$, where A^M is any vector and R^M_{NPQ} is the Riemann tensor.

Using the constraint $H^M = 0$ one sees from (B8) that $J^2 = \frac{1}{2} S^{MN} S_{MN}$ is a constant of the motion. Using this fact and the constraint $H = 0$ one can show that $P^M P_M = -M^2$ is also a constant of the motion.

We will follow the strategy of doing the computations in the *horizontal lift base* defined by the commutators[18,19]

$$[D_\mu, D_\nu] = -F^a_{\mu\nu} D_a,$$

$$[D_\mu, D_a] = 0, \tag{B9}$$

$$[D_a, D_b] = f^c_{ab} D_c.$$

Therefore the only nonvanishing commutation coefficients are

$$C^c_{\mu\nu} = -F^c_{\mu\nu} \tag{B10}$$

and

$$C_{ab}^{c} = f_{ab}^{c}. \tag{B11}$$

In the base (B9) the metric associated with $M^4 \times N'$ is

$$\hat{\gamma}_{MN} = \begin{pmatrix} g_{\mu\nu} & 0 \\ 0 & g_{ab} \end{pmatrix}, \tag{B12}$$

with

$$D_a g_{\mu\nu} = 0,$$

$$D_c g_{ab} = f_{cab} + f_{cba},$$

$$D_\mu g_{ab} = \partial_\mu g_{ab} - A_\mu^c D_c g_{ab} = g_{\ ab|\mu},$$

$$D_\alpha g_{\mu\nu} = g_{\mu\nu,\alpha}. \tag{B13}$$

The Christoffel symbols are given in a noncoordinate base by

$$\hat{\Gamma}_{MNP} = \tfrac{1}{2}(D_P \hat{\gamma}_{MN} + D_N \hat{\gamma}_{MP} - D_N \hat{\gamma}_{NP}) + \tfrac{1}{2}(C_{MNP} + C_{MPN} - C_{NPM}), \tag{B14}$$

and the Riemann tensor is given by

$$\hat{R}_{NPQ}^{M} = D_P \hat{\Gamma}_{NQ}^{M} - D_Q \hat{\Gamma}_{NQ}^{M} + \hat{\Gamma}_{RP}^{M} \hat{\Gamma}_{NQ}^{R} - \hat{\Gamma}_{RQ}^{M} \Gamma_{NP}^{R} - \hat{\Gamma}_{NR}^{M} C_{PQ}^{R}. \tag{B15}$$

The linear velocity u^M, angular velocity σ^{MN}, linear momentum P^M, and internal angular momentum S^{MN} will be referred to below with respect to the "horizontal lift base" defined in (B9). By using (B12)–(B15) one may reduce the equations of motion (B7) to four dimensions,

$$\frac{D\Pi^\mu}{\mathrm{d}\tau} = -\tfrac{1}{2} R_{\nu\alpha\beta}^{\mu} u^\nu S^{\alpha\beta} + Q_a F_\nu^{\mu a} u^\nu + \tfrac{1}{4} F_{\alpha\beta}^{a}{}^{;\mu} M_a^{\alpha\beta} + Z^\mu. \tag{B16}$$

Here the following definitions were used:

$$\Pi^\mu \equiv P^\mu - \tfrac{1}{2} g_{ab} F_\nu^{\mu a} S^{\nu b}, \tag{B17}$$

$$Q_a \equiv g_{ab} P^b + \tfrac{1}{4} g_{ab} f_{ce}^{b} S^{ce} + \tfrac{1}{4} g_{ab} F_{\alpha\beta}^{b} S^{\alpha\beta} + \tfrac{1}{2} g_{\ ab|\alpha} S^{\alpha b}, \tag{B18}$$

$$M_a^{\alpha\beta} \equiv g_{ab} u^a S^{\alpha\beta} + g_{ab} u^\beta S^{\alpha b} - g_{ab} u^\alpha S^{\beta b}, \tag{B19}$$

and

$$Z^\mu = [(\tfrac{1}{2} u^a P^b - \tfrac{1}{4} F_{\alpha\beta}^{a} u^\alpha S^{\beta b} + \tfrac{1}{4} F_{\alpha\beta}^{a} S^{\alpha\beta} u^b - \tfrac{1}{4} g^{af} g_{\ fe|\alpha} u^e S^{\alpha b}) - \tfrac{1}{4} g^{af} g_{\ fe|\alpha} u^\alpha S^{eb} + (f_{ec}^{a} + f_{ce}^{a} + f_{ec}^{a}) u^e S^{cb}$$
$$- (f_{ec}^{b} u^a S^{ec})] g_{ab}{}^{|\mu} + \tfrac{1}{2} g_{ab}{}^{|\mu}{}_{;\alpha} S^{\alpha b} u^a. \tag{B20}$$

Here, the symbol $g_{ab}{}^{|\mu}{}_{;\alpha}$ means

$$g_{ab}{}^{|\mu}{}_{;\alpha} = g_{ab}{}^{|\mu}{}_{|\alpha} + \begin{Bmatrix} \mu \\ \beta\alpha \end{Bmatrix} g_{ab}{}^{|\beta},$$

where $g_{ab}{}^{|\mu}$ is defined in (B13), while the symbol $F_\alpha^{\mu a}{}_{;\beta}$ means

$$F_\alpha^{\mu a}{}_{;\beta} = F_\alpha^{\mu a}{}_{,\beta} + \begin{Bmatrix} \mu \\ \sigma\beta \end{Bmatrix} F_\alpha^{\sigma a} - \begin{Bmatrix} \sigma \\ \beta\alpha \end{Bmatrix} F_\sigma^{\mu a}.$$

In terms of the definitions (B17) and (B19) the equation of motion (B8) leads to

$$\frac{DS^{\mu\nu}}{d\tau} = \Pi^{\mu}u^{\nu} - \Pi^{\nu}u^{\mu} + \frac{1}{2}(F^{\mu\alpha a}M^{\nu}_{\alpha a} - M^{\mu\alpha}_{a}F^{\nu a}_{\alpha}) + H^{\mu\nu}, \tag{B21}$$

where

$$H^{\mu\nu} = S^{\mu a}u^{b}g_{ab}{}^{|\nu} - S^{\nu a}u^{b}g_{ab}{}^{|\mu}.$$

Clearly, Eqs. (B16) and (B21) are generalizations of the usual four-dimensional case. One can show that the quantity Q_a given in (B18) is a constant of the motion. It turns out that Q_a can be interpreted as charges of the system. For details the reader is referred to Ref. 27.

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No self-interaction for two-column massless fields

Xavier Bekaert[a)]
Dipartimento di Fisica, Universitá degli Studi di Padova, INFN, Sezione di Padova, via F. Marzolo 8, 35131 Padova, Italy

Nicolas Boulanger[b)]
Department of Applied Mathematics and Theoretical Physics, Cambridge CB3 0WA, United Kingdom

Sandrine Cnockaert[c)]
Physique Théorique et Mathématique and International Solvay Institutes, Université Libre de Bruxelles, C.P. 231, Bld. du Triomphe, 1050 Bruxelles, Belgium

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We investigate the problem of introducing consistent self-couplings in free theories for mixed tensor gauge fields whose symmetry properties are characterized by Young diagrams made of two columns of arbitrary (but different) lengths. We prove that, in flat space, these theories admit no local, Poincaré-invariant, smooth, self-interacting deformation with at most two derivatives in the Lagrangian. Relaxing the derivative and Lorentz-invariance assumptions, there still is no deformation that modifies the gauge algebra, and in most cases no deformation that alters the gauge transformations. Our approach is based on a Becchi-Rouet-Stora-Tyutin (BRST) -cohomology deformation procedure. © *2005 American Institute of Physics.*
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I. INTRODUCTION

These last few years, mixed symmetry gauge fields (i.e., that are neither completely symmetric nor antisymmetric) have attracted some renewed attention,[1–10] thereby reviving the efforts made in this direction during the 1980s, under the prompt of string field theory.[11–14] Mixed-symmetry fields appear in a wide variety of higher-dimensional ($D>4$) contexts. Indeed, group theory imposes that first-quantized particles propagating in flat background should provide representations of the Poincaré group. The cases $D=3,4$ are very particular in the sense that each tensor irreducible representation (irrep) of the little groups O(2) and O(3) is equivalent to a completely symmetric tensor irrep (pictured by a one-row Young diagram with S columns for a spin-S particle). When $D>4$, more complicated Young diagrams are allowed. For instance, all critical string theory spectra contain massive fields in mixed symmetry representations of the Lorentz group. In the tensionless limit ($\alpha' \to \infty$) all these massive excitations become massless. Another way to generate various mixed symmetry fields is by dualizing totally symmetric fields in higher dimensions.[3,6]

An irrep of the general linear group $\mathrm{GL}(D,\mathbb{R})$ is denoted by $[c_1,c_2,\ldots,c_L]$, where c_i indicates the number of boxes in the ith column of the Young diagram characterizing the corresponding irrep. We will focus on theories describing gauge fields $\phi_{\mu_1\cdots\mu_p|\nu_1\cdots\nu_q}$ whose symmetries correspond to the Young diagram $[p,q]$ formed by two columns of arbitrary (but different) lengths p and q ($p>q$). The physical degrees of freedom for such theories correspond to a traceless tensor carrying an irrep of the little group $\mathrm{O}(D-2)$ associated with the Young diagram $[p,q]$. Therefore,

a)Electronic mail: xavier.bekaert@pd.infn.it
b)Electronic mail: n.boulanger@damtp.cam.ac.uk
c)Aspirant du F.N.R.S., Belgium. Electronic mail: sandrine.cnockaert@ulb.ac.be

we will work in space–time dimension $D \geqslant p+q+2$ so that the field carries local physical degrees of freedom. Such fields were studied recently at the free level in anti–de Sitter background.[9,10] In the sequel, we will frequently use a loose terminology by referring to a tensor irrep by its Young diagram.

In the present paper, we address the natural problem of switching on consistent self-interactions among $[p,q]$-type tensor gauge fields in flat background, where $p \neq q$. As in Refs. 15–20, we use the BRST-cohomological reformulation of the Noether method for the problem of consistent interactions.[21] For an alternative Hamiltonian-based deformation point of view, see Ref. 22. The question of consistent self-interactions in flat background has already been investigated in the case of vector (i.e., [1,0]) gauge fields in Ref. 15, p-forms (i.e., $[p,0]$-fields) in Ref. 16, Fierz–Pauli [1,1]-fields in Ref. 17, $[p,1]$-fields ($p>1$) in Ref. 18, [2,2]-fields in Ref. 19, and $[p,p]$-fields ($p>1$) in Ref. 20. Here, we extend and strengthen the results of Ref. 18 by relaxing some assumptions on the number of derivatives in the interactions. The present work is thus the completion of the analysis of self-interactions for *arbitrary* $[p,q]$-type tensor gauge fields in flat space.

Our main (no-go) result can be stated as follows, spelling out explicitly our assumptions.

Theorem: *In flat space and under the assumptions of locality and translation-invariance, there is no consistent smooth deformation of the free theory for* $[p,q]$*-type tensor gauge fields with* $p \neq q$ *that modifies the gauge algebra. Furthermore, for* $q>1$*, when there is no positive integer* n *such that* $p+2=(n+1)(q+1)$*, there exists no smooth deformation that alters the gauge transformations either. Finally, if one excludes deformations that involve four derivatives or more in the Lagrangian and that are not Lorentz-invariant, then there is no smooth deformation at all.*

The paper is organized as follows. In Sec. II, we review the free theory of $[p,q]$-type tensor gauge fields. In Sec. III, we introduce the BRST construction for the theory. Sections IV–VII are devoted to the proof of cohomological results. We compute $H(\gamma)$ in Sec. IV, an invariant Poincaré lemma is proved in Sec. V, the cohomologies $H_k^D(\delta|\mathrm{d})$ and $H_k^{D\ \mathrm{inv}}(\delta|\mathrm{d})$ are computed, respectively, in Secs. VI and VII. The self-interaction question is answered in Sec. VIII. A brief concluding section is finally followed by three appendixes containing the proofs of three theorems presented in the core of the paper.

II. FREE THEORY

As stated above, we consider theories for mixed tensor gauge fields $\phi_{\mu_1\cdots\mu_p|\nu_1\cdots\nu_q}$ whose symmetry properties are characterized by two columns of arbitrary (but different) lengths. In other words, the gauge field obeys the conditions

$$\phi_{\mu_1\cdots\mu_p|\nu_1\cdots\nu_q} = \phi_{[\mu_1\cdots\mu_p]|\nu_1\cdots\nu_q} = \phi_{\mu_1\cdots\mu_p|[\nu_1\cdots\nu_q]},$$

$$\phi_{[\mu_1\cdots\mu_p|\nu_1]\nu_2\cdots\nu_q} = 0,$$

where the square brackets denote strength-one complete antisymmetrization.

A. Lagrangian and gauge invariances

The Lagrangian of the free theory is

$$\mathcal{L} = -\frac{1}{2(p+1)!q!}\delta^{[\rho_1\cdots\rho_q\mu_1\cdots\mu_{p+1}]}_{[\nu_1\cdots\nu_q\sigma_1\cdots\sigma_{p+1}]}\partial^{[\sigma_1}\phi^{\ \sigma_2\cdots\sigma_{p+1}]|}_{\rho_1\cdots\rho_q}\partial_{[\mu_1}\phi_{\ \mu_2\cdots\mu_{p+1}]|}^{\ \ \ \ \ \ \nu_1\cdots\nu_q},$$

where the generalized Kronecker delta has strength one. This Lagrangian was obtained for [2,1]-fields in Ref. 11, for $[p,1]$-fields in Ref. 12 and, for the general case of $[p,q]$-fields, in the second paper of Ref. 5.

The quadratic action

$$S_0[\phi] = \int \mathrm{d}^D x\, \mathcal{L}(\partial\phi) \tag{1}$$

is invariant under gauge transformations with gauge parameters $\alpha^{(1,0)}$ and $\alpha^{(0,1)}$ that have respective symmetries $[p-1,q]$ and $[p,q-1]$. In the same manner as p-forms, these gauge transformations are *reducible*, their order of reducibility growing with p. We identify the gauge field ϕ with $\alpha^{(0,0)}$, the zeroth order parameter of reducibility. The gauge transformations and their reducibilities are (we introduce the short notation $\mu_{[p]} \equiv [\mu_1 \cdots \mu_p]$; a comma stands for a derivative, $\alpha_{,\nu} \equiv \partial_\nu \alpha$)

$$\delta\alpha^{(i,j)}_{\mu_{[p-i]}|\nu_{[q-j]}} = \partial_{[\mu_1}\alpha^{(i+1,j)}_{\mu_2\cdots\mu_{p-i}]|\nu_{[q-j]}} + b_{i,j}\left(\alpha^{(i,j+1)}_{\mu_{[p-i]}|[\nu_{[q-j-1]},\nu_{q-j}]} + a_{i,j}\alpha^{(i,j+1)}_{\nu_{[q-j]}[\mu_{q-j+1}\cdots\mu_{p-i}|\mu_{[q-j-1]},\mu_{q-j}]}\right), \tag{2}$$

where $i=0,\ldots,p-q$ and $j=0,\ldots,q$. The coefficients $a_{i,j}$ and $b_{i,j}$ are given by

$$a_{i,j} = \frac{(p-i)!}{(p-i-q+j+1)!(q-j)!}, \quad b_{i,j} = (-)^i \frac{(p-q+j+2)}{(p-i-q+j+2)}.$$

To the above formulas, we must add the convention that, for all j, $\alpha^{(p-q+1,j)} = 0 = \alpha^{(i,q+1)}$. The symmetry properties of the parameters $\alpha^{(i,j)}$ are those of Young diagrams with two columns of lengths $p-i$ and $q-j$. More details on the reducibility parameters $\alpha^{(i,j)}_{\mu_1\cdots\mu_{p-i}|\nu_1\cdots\nu_{q-j}}$ will be given in Sec. III B.

The fundamental gauge-invariant object is the field strength K, the $[p+1,q+1]$-tensor defined as the double curl of the gauge field

$$K_{\mu_1\cdots\mu_{p+1}|\nu_1\cdots\nu_{q+1}} \equiv \partial_{[\mu_1}\phi_{\mu_2\cdots\mu_{p+1}]|[\nu_1\cdots\nu_q,\nu_{q+1}]}.$$

By definition, it satisfies the Bianchi (BII) identities

$$\partial_{[\mu_1}K_{\mu_2\cdots\mu_{p+2}]|\nu_1\cdots\nu_{q+1}} = 0, \quad K_{\mu_1\cdots\mu_{p+1}|[\nu_1\cdots\nu_{q+1},\nu_{q+2}]} = 0. \tag{3}$$

The field strength tensor K plays a crucial role in the determination of the physical degrees of freedom described by the action $S_0[\phi]$.

B. Equations of motion

The equations of motion are expressed in terms of the field strength,

$$G^{\mu_1\cdots\mu_p|}{}_{\nu_1\ldots\nu_q} \equiv \frac{\delta\mathcal{L}}{\delta\phi_{\mu_1\ldots\mu_p|}{}^{\nu_1\ldots\nu_q}} = \frac{1}{(p+1)!q!}\delta^{[\rho_1\cdots\rho_{q+1}\mu_1\cdots\mu_p]}_{[\nu_1\cdots\nu_q\sigma_1\cdots\sigma_{p+1}]}K^{\sigma_1\cdots\sigma_{p+1}|}{}_{\rho_1\cdots\rho_{q+1}} \approx 0,$$

where a weak equality "$\approx$" means "equal on the surface of the solutions of the equations of motion." This is a generalization of vacuum Einstein equations, linearized around the flat background. Taking successive traces of the equations of motion, one can show that they are equivalent to the tracelessness of the field strength,

$$\eta^{\sigma_1\rho_1}K_{\sigma_1\cdots\sigma_{p+1}|\rho_1\cdots\rho_{q+1}} \approx 0. \tag{4}$$

This equation generalizes the vanishing of the Ricci tensor (in the vacuum), and is nontrivial only when $p+q+2 \leqslant D$. Together with the "Ricci equation" (4), the Bianchi identities (3) imply[3]

$$\partial^{\sigma_1}K_{\sigma_1\cdots\sigma_{p+1}|\rho_1\cdots\rho_{q+1}} \approx 0 \approx \partial^{\rho_1}K_{\sigma_1\cdots\sigma_{p+1}|\rho_1\cdots\rho_{q+1}}. \tag{5}$$

The gauge invariance of the action is equivalent to the divergenceless of the tensor $G^{\mu_{[p]}|\nu_{[q]}}$, that is, the latter satisfies the Noether identities

$$\partial^{\sigma_1} G_{\sigma_1 \cdots \sigma_{p+1} | \rho_1 \cdots \rho_{q+1}} = 0 = \partial^{\rho_1} G_{\sigma_1 \cdots \sigma_{p+1} | \rho_1 \cdots \rho_{q+1}} . \tag{6}$$

These identities are a direct consequence of the Bianchi ones (3). The Noether identities (6) ensure that the equations of motion can be written as

$$0 \approx G^{\mu_1 \cdots \mu_p | \nu_1 \cdots \nu_q} = \partial_\alpha H^{\alpha \mu_1 \cdots \mu_p | \nu_1 \cdots \nu_q} ,$$

where

$$H^{\alpha \mu_1 \cdots \mu_p |}{}_{\nu_1 \cdots \nu_q} = \frac{1}{(p+1)! q!} \delta^{[\rho_1 \cdots \rho_q \alpha \mu_1 \cdots \mu_p]}_{[\nu_1 \cdots \nu_q \beta \sigma_1 \cdots \sigma_p]} \partial^{[\beta} \phi^{\sigma_1 \cdots \sigma_p] |}{}_{\rho_1 \cdots \rho_q} .$$

The symmetries of the tensor H correspond to the Young diagram $[p+1,q]$. This property will be useful in the computation of the local BRST cohomology.

C. Physical degrees of freedom

The "Ricci equation" (4) states that, on-shell, the field strength belongs to the irrep $[p+1,q+1]$ of $\mathrm{O}(D-1,1)$. The Bianchi identities together with (5) further imply that the on-shell nonvanishing components of the field strength belong to the unitary irrep $[p,q]$ of the little group $\mathrm{O}(D-2)$. Indeed, on-shell, gauge fields in the light-cone gauge are essentially field strengths,[13] and the "Ricci equation" takes the form

$$\delta^{i_1 j_1} \phi_{i_1 \cdots i_p | j_1 \cdots j_q} \approx 0 ,$$

where i and j denote light-cone indices $(i,j=1,\ldots,D-2)$. As a consistency check, one can note that the latter equation is nontrivial only when $p+q \geqslant D-2$. The theory describes the correct physical degrees of freedom of a first-quantized massless particle propagating in flat space, i.e., the latter particle provides a unitary irrep of the group $\mathrm{IO}(D-1,1)$.

We should stress that the exact analogue of all the previous properties hold for arbitrary mixed symmetry fields. This result was obtained by two of us and was mentioned in Ref. 7 but the detailed proof was not given there. [The proof presented in this paper (Appendix A) provides an indirect proof that the light-cone gauge is reachable (so that the theory describes the correct number of physical degrees of freedom). We would like to underline the fact that Refs. 3 and 5 assume (but do not contain any rigorous proof of) this fact. It would not be straightforward to prove it directly because the tower of ghosts is extremely complicated in the general case.] We take the opportunity to provide this extremely simple proof in Appendix A for the particular case of two-column gauge fields, since it already covers all the features of the general case for arbitrary mixed tensor gauge fields.

III. BRST CONSTRUCTION

A. BRST deformation technique

Once one has a consistent free theory, it is natural to try to deform it into an interacting theory. The traditional Noether deformation procedure assumes that the deformed action can be expressed as a power series in a coupling constant g, the zeroth-order term in the expansion describing the free theory S_0. The procedure is perturbative: one tries to construct the deformations order by order in the deformation parameter g.

Some physical requirements naturally come out.

(i) *Nontriviality:* We reject *trivial* deformations arising from field redefinitions that reduce to the identity at order g^0,

$$\phi \to \phi' = \phi + g\theta(\phi, \partial\phi, \ldots) + \mathcal{O}(g^2) . \tag{7}$$

(ii) *Consistency:* A deformation of a theory is called *consistent* if the deformed theory possesses the same number of (possibly deformed) independent gauge symmetries, reducibility

identities, etc., as the system we started with. In other words, the number of physical degrees of freedom is unchanged.

(iii) *Locality:* The deformed action $S[\phi]$ must be a *local* functional. The deformation of the gauge transformations, etc., must be local functions, as well as the field redefinitions.

We remind the reader that a local function of some set of fields φ^i is a smooth function of the fields φ^i and their derivatives $\partial\varphi^i$, $\partial^2\varphi^i$,… up to some *finite* order, say k, in the number of derivatives. Such a set of variables φ^i, $\partial\varphi^i$, …, $\partial^k\varphi^i$ will be collectively denoted by $[\varphi^i]$. Therefore, a local function of φ^i is denoted by $f([\varphi^i])$. A local p-form $(0\leqslant p\leqslant D)$ is a differential p-form, the components of which are local functions,

$$\omega = \frac{1}{p!}\omega_{\mu_1\cdots\mu_p}(x,[\phi^i])\mathrm{d}x^{\mu_1}\wedge\cdots\wedge\mathrm{d}x^{\mu_p}.$$

A local functional is the integral of a local D-form.

As shown in Ref. 21, the Noether procedure can be reformulated in a BRST-cohomological formalism: the first-order nontrivial consistent local interactions are in one-to-one correspondence with elements of the cohomology $H^{D,0}(s|\mathrm{d})$ of the BRST differential s modulo the total derivative d, in maximum form-degree D and in ghost number 0. That is, one must compute the general solution of the cocycle condition

$$sa^{D,0} + \mathrm{d}b^{D-1,1} = 0, \tag{8}$$

where $a^{D,0}$ is a top-form of ghost number zero and $b^{D-1,1}$ a $(D-1)$-form of ghost number one, with the understanding that two solutions of (8) that differ by a trivial solution should be identified,

$$a^{D,0} \sim a^{D,0} + sm^{D,-1} + \mathrm{d}n^{D-1,0},$$

as they define the same interactions up to field redefinitions (7). The cocycles and coboundaries a, b, m, n,… are local forms of the field variables (including ghosts and antifields).

B. BRST spectrum

In the theories under consideration and according to the general rules of the BRST-antifield formalism, one associates with each gauge parameter $\alpha^{(i,j)}$ a ghost, and then to any field (including ghosts) a corresponding antifield (or antighost) of opposite Grassmann parity. More precisely, the spectrum of fields (including ghosts) and antifields is given by

(i) *the fields*, $A^{(i,j)}_{\mu_{[p-i]}|\nu_{[q-j]}}$, where $A^{(0,0)}$ is identified with ϕ;

(ii) *the antifields*, $A^{*(i,j)\,\mu_{[p-i]}|\nu_{[q-j]}}$,

where $i=0,\ldots,p-q$ and $j=0,\ldots,q$. The symmetry properties of the fields $A^{(i,j)}_{\mu_{[p-i]}|\nu_{[q-j]}}$ and antifields $A^{*(i,j)\,\mu_{[p-i]}|\nu_{[q-j]}}$ are those of Young diagrams with two columns of lengths $p-i$ and $q-j$. To each field and antifield are associated a pure ghost number and an antifield (or antighost) number. The pure ghost number is given by $i+j$ for the fields $A^{(i,j)}$ and 0 for the antifields, while the antifield number is 0 for the fields and $i+j+1$ for the antifields $A^{*(i,j)}$. The Grassmann parity is given by the pure ghost number (or the antighost number) modulo 2. All this is summarized in Table I.

TABLE I. Symmetry, pure ghost and antighost numbers, and parity of the (anti)fields.

	Young	puregh	antigh	Parity
$A^{(i,j)}$	$[p-i,q-j]$	$i+j$	0	$i+j$
$A^{*(i,j)}$	$[p-i,q-j]$	0	$i+j+1$	$i+j+1$

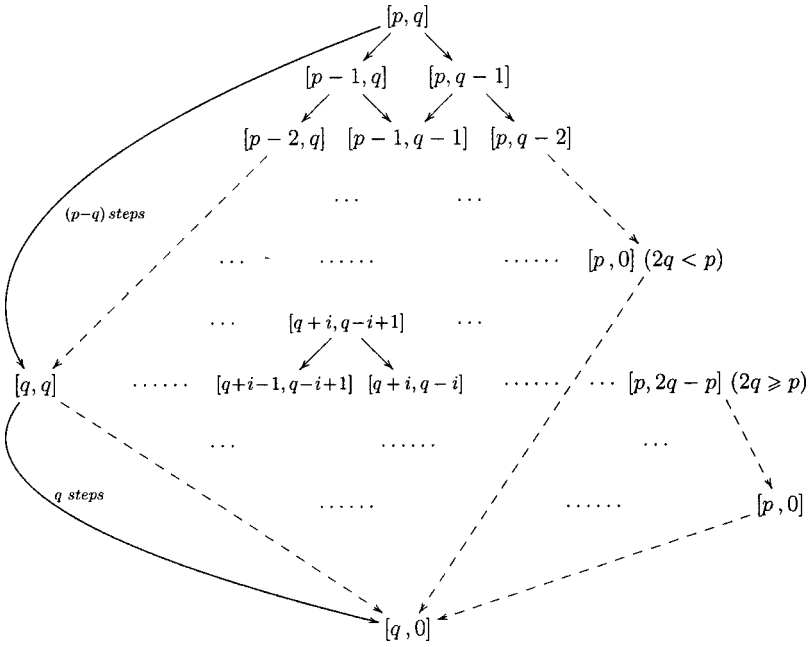

FIG. 1. Antighost-zero BRST spectrum of $[p,q]$-type gauge field.

One can visualize the whole BRST spectrum in vanishing antighost number as well as the procedure that gives all the ghosts starting from $\phi_{\mu_{[p]}|\nu_{[q]}}$ in Fig. 1, where the pure ghost number increases from top down, by one unit at each line.

At the top of Fig. 1 lies the gauge field $\phi_{\mu_{[p]}|\nu_{[q]}}$ with pure ghost number zero. At the level below, one finds the pure ghost number one "gauge parameters" $A^{(1,0)}_{\mu_{[p-1]}|\nu_{[q]}}$ and $A^{(0,1)}_{\mu_{[p]}|\nu_{[q-1]}}$ whose respective symmetries are obtained by removing a box in the first (respectively, second) column of the Young diagram $[p,q]$ corresponding to the gauge field $\phi_{\mu_{[p]}|\nu_{[q]}}$ [the rules that give the $(i+1)$th generation ghosts from the ith generation ones can be found in Refs. 4 and 14],

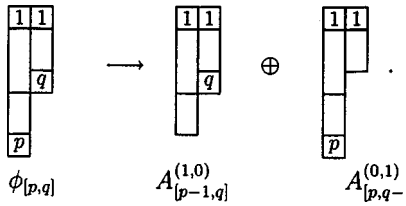

In pure ghost number $p-q$, we obtain a set of ghosts containing $A^{(p-q,0)}_{\mu_{[q]}|\nu_{[q]}} \sim [q,q]$. The Young diagram corresponding to the latter ghost is obtained by removing $p-q$ boxes from the first column of $[p,q]$.

If $q<p-q$, we do not have to reach the pure ghost level $p-q$ to find the p-form ghost $A^{(0,q)}_{\mu_{[p]}} \sim [p,0]$. If $2q \geqslant p$, we must remove additional boxes from the second column of $[p,q]$ in order to empty it completely and obtain the p-form ghost $A^{(0,q)}_{\mu_{[p]}}$. The Young diagrams of the remaining ghosts are obtained by further removing boxes from the Young diagram corresponding to the ghost $A^{(0,q)}_{\mu_{[p]}}$ with puregh$=q$. This procedure will terminate at pure ghost number p with the q-form ghost $A^{(p-q,q)}_{\mu_{[q]}} \sim [q,0]$. It is not possible to find ghosts $A_{\mu_{[r]}|\nu_{[s]}}$ with r and $s<q$, since it would mean that two boxes from a same row would have been removed from $[p,q]$, which is not allowed.[4,14]

The antighost sector has exactly the same structure as the ghost sector in Fig. 1, where each ghost $A^{(i,j)}$ is replaced by its antighost $A^{*(i,j)}$.

C. BRST differential

The BRST differential s of the free theory (1) and (2) is generated by the functional

$$W_0 = S_0[\phi] + \int \mathrm{d}^D x \left[\sum_{i=0}^{p-q} \sum_{j=0}^{q} (-)^{i+j} A^{*(i,j)\mu_1 \cdots \mu_{p-i}|\nu_1 \cdots \nu_{q-j}} \times (\partial_{[\mu_1} A^{(i+1,j)}_{\mu_2 \cdots \mu_{p-i}]|\nu_1 \cdots \nu_{q-j}} - b_{i+1,j} A^{(i,j+1)}_{\mu_1 \cdots \mu_{p-i}|[\nu_1 \cdots \nu_{q-j-1}, \nu_{q-j}]}) \right],$$

with the convention that $A^{(p-q+1,j)} = A^{(i,q+1)} = A^{*(-1,j)} = A^{*(i,-1)} = 0$. More precisely, W_0 is the generator of the BRST differential s of the free theory through

$$sA = (W_0, A)_{a.b.},$$

where the antibracket $(,)_{a.b.}$ is defined by

$$(A,B)_{a.b.} = \frac{\delta^R A}{\delta \Phi^I} \frac{\delta^L B}{\delta \Phi^*_I} - \frac{\delta^R A}{\delta \Phi^*_I} \frac{\delta^L B}{\delta \Phi^I},$$

Φ^I collectively denoting all fields and ghosts, and Φ^*_I the antighosts. The functional W_0 is a solution of the *master equation*

$$(W_0, W_0)_{a.b.} = 0.$$

The BRST-differential s decomposes into $s = \gamma + \delta$. The first piece γ, the differential along the gauge orbits, increases the pure ghost number by one unit, whereas the Koszul–Tate differential δ decreases the antighost (or antifield) number by one unit. A $\mathbb{Z}$-grading called *ghost number* (or gh) corresponds to the differential s. We have

$$\mathrm{gh} = \mathrm{puregh} - \mathrm{antigh}.$$

The action of γ and δ on the BRST variables is zero, except

$$\gamma A^{(i,j)}_{\mu_{[p-i]}|\nu_{[q-j]}} = \partial_{[\mu_1} A^{(i+1,j)}_{\mu_2 \cdots \mu_{p-i}]|\nu_{[q-j]}} + b_{i,j} (A^{(i,j+1)}_{\mu_{[p-i]}|[\nu_{[q-j-1]}, \nu_{q-j}]} + a_{i,j} A^{(i,j+1)}_{\nu_{[q-j]}[\mu_{q-j+1} \cdots \mu_{p-i}|\mu_{[q-j-1]}, \mu_{q-j}]}),$$

$$\delta A^{*(0,0)\mu_{[p]}|\nu_{[q]}} = G^{\mu_{[p]}|\nu_{[q]}},$$

$$\delta A^{*(i,j)\mu_{[p-i]}|\nu_{[q-j]}} = (-)^{i+j} \left(\partial_\sigma A^{*(i-1,j)\sigma\mu_{[p-i]}|\nu_{[q-j]}} - \frac{1}{p-i+1} \partial_\sigma A^{*(i-1,j)\nu_1 \mu_{[p-i]}|\sigma\nu_2 \cdots \nu_{q-j}} \right) + (-)^{i+j+1} b_{i+1,j-1} \partial_\sigma A^{*(i,j-1)\mu_{[p-i]}|\nu_{[q-j]}\sigma},$$

where the last equation holds only for (i,j) different from (0, 0).

For later computations, it is useful to define a unique antifield for each antighost number,

$$C^*_{p+1-j}{}^{\mu_1 \cdots \mu_q|\nu_1 \cdots \nu_j} = \sum_{k=0}^{j} \epsilon_{k,j} A^{*(p-q-j+k,q-k)\mu_1 \cdots \mu_q[\nu_{k+1} \cdots \nu_j|\nu_1 \cdots \nu_k]}$$

for $0 \leqslant j \leqslant p$, and, in antighost zero, the following specific combination of single derivatives of the field:

TABLE II. Young representation, pure ghost and antighost numbers, and parity of C_k^*.

	Young diagram	puregh	antigh	Parity
C_k^*	$[q]\otimes[p+1-k]-[p+1]\otimes[q-k]$	0	k	k

$$C_0^{*\mu_1\cdots\mu_q|\nu_1\cdots\nu_{p+1}} = \epsilon_{q,p+1} H^{\mu_1\cdots\mu_q[\nu_{q+1}\cdots\nu_{p+1}|\nu_1\cdots\nu_q]},$$

where $\epsilon_{k,j}$ vanishes for $k>q$ and for $j-k>p-q$, and is given in the other cases by

$$\epsilon_{k,j} = (-)^{pk+j(k+p+q)+[k(k+1)/2]} \frac{\binom{k}{p+1}\binom{k}{j}}{\binom{k}{q}},$$

where $\binom{m}{n}$ are the binomial coefficients ($n \geqslant m$). Some properties of the new variables C_k^* are summarized in Table II.

The symmetry properties of C_k^* are denoted by

$$[q]\otimes[p+1-k]-[p+1]\otimes[q-k]$$

which means that they have the symmetry properties corresponding to the tensor product of a column $[q]$ by a column $[p+1-k]$ from which one should substract (when $k\leqslant q$) all the Young diagrams appearing in the tensor product $[p+1]\otimes[q-k]$.

The antifields $C_k^{*\mu[q]|\nu[p+1-k]}$ have been defined in order to obey the following relations:

$$\delta C_{p+1-j}^{*\mu_1\cdots\mu_q|\nu_1\cdots\nu_j} = \partial_\sigma C_{p-j}^{*\mu_1\cdots\mu_q|\nu_1\cdots\nu_j\sigma} \quad \text{for } 0\leqslant j\leqslant p,$$

$$\delta C_0^{*\mu_1\cdots\mu_q|\nu_1\cdots\nu_{p+1}} = 0. \tag{9}$$

If we further define the inhomogeneous form

$$\tilde{H}^{\mu_1\cdots\mu_q} \equiv \sum_{j=0}^{p+1} C_{p+1-j}^{*D-j\mu_1\cdots\mu_q},$$

where

$$C_{p+1-j}^{*D-j\mu_1\cdots\mu_q} \equiv (-)^{jp+j(j+1)/2} \frac{1}{j!(D-j)!} C_{p+1-j}^{*\mu_1\cdots\mu_q|\nu_1\cdots\nu_j} \epsilon_{\nu_1\cdots\nu_D}\, \mathrm{d}x^{\nu_{j+1}}\cdots \mathrm{d}x^{\nu_D},$$

then, as a consequence of (9), any polynomial $P(\tilde{H})$ in $\tilde{H}^{\mu_1\cdots\mu_q}$ will satisfy

$$(\delta+d)P(\tilde{H}) = 0. \tag{10}$$

The polynomial $\tilde{H}$ is not invariant under gauge transformations. It is therefore useful to still introduce another polynomial, $\tilde{\mathcal{H}}$, with an explicit x dependence, that *is* invariant. $\tilde{\mathcal{H}}$ is defined by

$$\tilde{\mathcal{H}}_{\mu_{[q]}} \equiv \sum_{j=1}^{p+1} C_{j\mu_{[q]}}^{*D-p-1+j} + \tilde{a}\epsilon_{[\mu_{[q]}\sigma_{[p+1]}\tau_{[D-p-q-1]}]} K^{q+1\sigma_{[p+1]}} x^{\tau_1}\, \mathrm{d}x^{\tau_2}\cdots \mathrm{d}x^{\tau_{D-p-q-1}},$$

where $\tilde{a}=(-)^{[p(p-1)+q(q-1)/2]}[1/q!q!(p+q+1)!(p+1-q)!(D-p-q-1)!]$. One can check that $\tilde{\mathcal{H}}=\tilde{H}+\mathrm{d}m_0^{D-p-2}$. This fact has the consequence that polynomials in $\tilde{\mathcal{H}}$ also satisfy $(\delta+d)P(\tilde{\mathcal{H}})=0$.

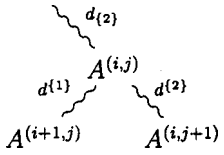

FIG. 2. Ghost $A^{(i,j)}$ appearing in only one reducibility relation.

IV. COHOMOLOGY OF γ

We hereafter give the content of $H(\gamma)$. Subsequently, we explain the procedure that we followed in order to obtain that result.

Theorem 4.1: *The cohomology of* γ *is isomorphic to the space of functions depending on*

(i) *the antifields and their derivatives* $[A^{*(i,j)}]$,
(ii) *the curvature and its derivatives* $[K]$,
(iii) *the pth generation ghost* $A^{(p-q,q)}$, *and*
(iv) *the curl* $D^0_{\mu_1\cdots\mu_{p+1}} \equiv (-)^q \partial_{[\mu_1} A^{(0,q)}_{\mu_2\cdots\mu_{p+1}]}$ *of the qth generation ghost* $A^{(0,q)}$,

$$H(\gamma) \simeq \{f([A^{*(i,j)}],[K],A^{(p-q,q)},D^0_{\mu_1\cdots\mu_{p+1}})\}.$$

Proof: The antifields and all their derivatives are annihilated by γ. Since they carry no pure ghost degree by definition, they cannot be equal to the γ-variation of any quantity. Hence, they obviously belong to the cohomology of γ.

To compute the γ-cohomology in the sector of the field, the ghosts and all their derivatives, we split the variables into three sets of *independent* variables obeying, respectively, $\gamma u^\ell = v^\ell$, $\gamma v^\ell = 0$, and $\gamma w^i = 0$. The variables u^ℓ and v^ℓ form so-called "contractible pairs" and the cohomology of γ is therefore generated by the variables w^i (see, e.g., Ref. 23, Theorem 8.2).

We decompose the spaces spanned by the derivatives $\partial_{\mu_1\cdots\mu_k} A^{(i,j)}$, $k \geqslant 0$, $0 \leqslant i \leqslant p-q$, $0 \leqslant j \leqslant q$, into irreps of $\mathrm{GL}(D,\mathbb{R})$ and use the structure of the reducibility conditions (see Figs. 2 and 3) in order to group the variables into contractible pairs.

We use the differential operators $d^{\{i\}}$, $i=1,2,\ldots$ (see Ref. 4 for a general definition) which act, for instance, on Young-symmetry-type tensor fields $T_{[2,1]}$, as follows:

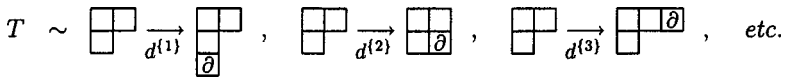

For fixed i and j the set of ghosts $A^{(i,j)}$ and all their derivatives decompose into three types of independent variables,

$$[A^{(i,j)}] \leftrightarrow \mathcal{O}A^{(i,j+1)}, \mathcal{O}d^{\{1\}}A^{(i,j+1)}, \mathcal{O}d^{\{2\}}A^{(i,j+1)}, \mathcal{O}d^{\{1\}}d^{\{2\}}A^{(i,j+1)},$$

where $\mathcal{O}$ denotes any operator of the type $\Pi_{m\geqslant 3} d^{\{m\}}$ or the identity.

Different cases arise depending on the position of the field $A^{(i,j)}$ in Fig. 1. We must consider fields that sit in the interior, on a border or at a corner of the diagram.

Interior: In this case, all the ghosts $A^{(i,j)}$ and their derivatives form u^ℓ or v^ℓ variables. Indeed, we have the relations

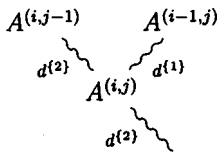

FIG. 3. Ghost $A^{(i,j)}$ the reducibility relation of which involves only one ghost.

$$\gamma A^{(i,j)} \propto [d^{\{1\}}A^{(i+1,j)} - d^{\{2\}}A^{(i,j+1)}],$$

$$\gamma[d^{\{1\}}A^{(i+1,j)} - d^{\{2\}}A^{(i,j+1)}] = 0,$$

$$\gamma[d^{\{1\}}A^{(i+1,j)} + d^{\{2\}}A^{(i,j+1)}] \propto d^{\{1\}}d^{\{2\}}A^{(i+1,j+1)},$$

$$\gamma[d^{\{1\}}d^{\{2\}}A^{(i,j+1)}] = 0,$$

and $\mathcal{O}$ commutes with γ. From which we conclude that one can perform a change of variable from the sets $[A^{(i,j)}]$ to the contractible pairs

$$u^{\ell} \leftrightarrow \mathcal{O}A^{(i,j)}, \mathcal{O}[d^{\{1\}}A^{(i+1,j)} + d^{\{2\}}A^{(i,j+1)}],$$

$$v^{\ell} \leftrightarrow \mathcal{O}[d^{\{1\}}A^{(i+1,j)} - d^{\{2\}}A^{(i,j+1)}], \mathcal{O}d^{\{1\}}d^{\{2\}}A^{(i+1,j+1)},$$

so that the ghosts $A^{(i,j)}$ in the interior and all their derivatives do not appear in $H(\gamma)$.

Border: If a ghost $A^{(i,j)}$ stands on a border of Fig. 1, it means that either (i) its reducibility relation involves only one ghost (see, e.g., Fig. 3), or (ii) there exists only one field whose reducibility relation involves $A^{(i,j)}$ (see, e.g., Fig. 2).

(i) Suppose $A^{(i,j)}$ stands on the left-hand (lower) edge of Fig. 1. We have the relations

$$\gamma A^{(i,j)} \propto d^{\{2\}}A^{(i,j+1)},$$

$$\gamma[d^{\{2\}}A^{(i,j+1)}] = 0,$$

$$\gamma[d^{\{1\}}A^{(i,j)}] \propto d^{\{1\}}d^{\{2\}}A^{(i,j+1)},$$

$$\gamma[d^{\{1\}}d^{\{2\}}A^{(i,j+1)}] = 0,$$

so that the corresponding sets $[A^{(i,j)}]$ on the left-hand edge do not contribute to $H(\gamma)$. We reach similar conclusion if $A^{(i,j)}$ lies on the right-hand (higher) border of Fig. 1, substituting $d^{\{1\}}$ for $d^{\{2\}}$ when necessary.

(ii) Since, by assumption, $A^{(i,j)}$ does not sit in a corner of Fig. 1 (but on the higher left-hand or lower right-hand border), its reducibility transformation involves two ghosts, and we proceed as if it were in the interior. The only difference is that $\mathcal{O}d^{\{1\}}d^{\{2\}}A^{(i,j)}$ will be equal to either $\gamma\mathcal{O}d^{\{1\}}A^{(i,j-1)}$ or $\gamma\mathcal{O}d^{\{2\}}A^{(i-1,j)}$, depending whether the field above $A^{(i,j)}$ is $A^{(i-1,j)}$ or $A^{(i,j-1)}$.

Lower corner: On the one hand, we have $\gamma A^{(p-q,q)}_{[q,0]} = 0$. As the operator γ introduces a derivative, $A^{(p-q,q)}_{[q,0]}$ cannot be γ-exact. As a result, $A^{(p-q,q)}_{[q,0]}$ is a w^i-variable and thence belongs to $H(\gamma)$. On the other hand, we find $\partial_{\nu}A^{(p-q,q)}_{\mu_1\cdots\mu_q} = \gamma[A^{(p-q-1,q)}_{\nu\mu_1\cdots\mu_q} + (-)^{p-q}[q/(p+1)]A^{(p-q,q-1)}_{\mu_1\cdots\mu_q|\nu}]$, which implies that all the derivatives of $A^{(p-q,q)}$ do not appear in $H(\gamma)$.

Left-hand corner: In this case, the ghost $A^{(i,j)}$ is characterized by a squared-shape Young diagram (it is the only one with this property). Its reducibility transformation involves only one ghost and there exists only one field whose reducibility transformation involves $A^{(i,j)}$. Because of its symmetry properties, $d^{\{2\}}A^{(i,j)} \sim d^{\{1\}}A^{(i,j)}$. Better, $d^{\{2\}}$ is not well-defined on $A^{(i,j)}$, it is only well defined on $d^{\{1\}}A^{(i,j)}$. Therefore, the derivatives $\partial_{\mu_1\cdots\mu_k}A^{(i,j)}$ decompose into $\mathcal{O}A^{(i,j)}$, $\mathcal{O}d^{\{1\}}A^{(i,j)}$, and $\mathcal{O}d^{\{1\}}d^{\{2\}}A^{(i,j)}$. The first set $\mathcal{O}A^{(i,j)}$ forms u^{ℓ}-variables associated with $\mathcal{O}d^{\{2\}}A^{(i,j+1)}$. The second set is grouped with $\mathcal{O}d^{\{1\}}d^{\{2\}}A^{(i,j+1)}$, and the third one forms v^{ℓ}-variables with $\mathcal{O}d^{\{2\}}A^{(i-1,j)}$.

Upper corner: In the case where $A^{(i,j)}$ is the gauge field, we proceed exactly as in the "interior" case, except that the variables $\mathcal{O}d^{\{1\}}d^{\{2\}}A^{(0,0)} = 0$ are not grouped with any other variables any

longer. They constitute true w^i-variables and are thus present in $H(\gamma)$. Recalling the definition of the curvature K, we have $\mathcal{O}d^{\{1\}}d^{\{2\}}A^{(0,0)} \propto [K]$.

Right-hand corner: In this case, the field $A^{(i,j)}$ is the p-form ghost $A^{(0,q)}_{[p]}$. We have the (u,v)-pairs $(\mathcal{O}d^{\{2\}}A^{(0,q)}, \mathcal{O}d^{\{1\}}d^{\{2\}}A^{(1,q)})$, $(\mathcal{O}d^{\{1\}}A^{(0,q-1)}, \mathcal{O}d^{\{1\}}d^{\{2\}}A^{(0,q)})$.

The derivative $d^{\{1\}}A^{(0,q)}_{[p]} \propto D^0_{[p+1]}$ is a w^i-variable since it is invariant and no other variable $\partial_{\mu_1 \cdots \mu_k} A^{(i,j)}$ possesses the same symmetry. □

In the sequel, the polynomials $\alpha([K],[A^*])$ in the curvature, the antifields and all their derivatives will be called "invariant polynomials." We will denote by $\mathcal{N}$ the algebra generated by all the ghosts and the noninvariant derivatives of the field ϕ. The entire algebra of the fields and antifields is then generated by the invariant polynomials and the elements of $\mathcal{N}$.

V. INVARIANT POINCARÉ LEMMA

The space of *invariant* local forms is the space of (local) forms that belong to $H(\gamma)$. The algebraic Poincaré lemma tells us that any closed form is exact (except top forms and constants). However, if the form is furthermore invariant, it is not guaranteed that the form is exact in the space of invariant forms. The following lemma tells us more about this important subtlety, in a limited range of form degree.

Lemma 5.1 (invariant Poincaré lemma in form degree $k<p+1$): Let α^k be an invariant local k-form, $k<p+1$,

$$\textit{if } \mathrm{d}\alpha^k = 0, \ \textit{then } \alpha^k = Q(K^{q+1}_{\mu_1 \cdots \mu_{p+1}}) + \mathrm{d}\beta^{k-1},$$

where Q is a polynomial in the $(q+1)$-forms,

$$K^{q+1}_{\mu_1 \cdots \mu_{p+1}} \equiv K_{\mu_1 \cdots \mu_{p+1}|\nu_1 \cdots \nu_{q+1}} \, \mathrm{d}x^{\nu_1} \cdots \mathrm{d}x^{\nu_{q+1}},$$

while β^{k-1} is an invariant local form.

A closed invariant local form of form-degree $k<p+1$ and of strictly positive antighost number is always exact in the space of invariant local forms.

The proof is directly inspired from the one given in Ref. 24 (Theorem 6).

A. Beginning of the proof of the invariant Poincaré lemma

The second statement of the lemma [i.e., the case antigh $(\alpha^k) \neq 0$] is part of a general theorem (see, e.g., Ref. 25) which holds without any restriction on the form degree. It will not be reviewed here.

We will thus assume that antigh$(\alpha^k)=0$, and prove the first part of Lemma 5.1 by induction.

Induction basis: For $k=0$, the invariant Poincaré lemma is trivially satisfied, $\mathrm{d}\alpha^0=0$ implies that α^0 is a constant by the usual Poincaré lemma.

Induction hypothesis: The lemma holds in form degree k' such that $0 \leqslant k' < k < p+1$.

Induction step: We will prove in the sequel that under the induction hypothesis, the lemma holds in form degree k.

Because $\mathrm{d}\alpha^k=0$ and $\gamma\alpha^k=0$, we can build a descent as follows:

$$\mathrm{d}\alpha^k = 0 \Rightarrow \alpha^k = \mathrm{d}a^{k-1,0}, \tag{11}$$

$$0 = \gamma a^{k-1,0} + \mathrm{d}a^{k-2,1}, \ldots, \tag{12}$$

$$0 = \gamma a^{k-j,j-1} + \mathrm{d}a^{k-j-1,j}, \tag{13}$$

$$0 = \gamma a^{k-j-1,j}, \tag{14}$$

where $a^{r,i}$ is a r-form of pure ghost number i. The pure ghost number of $a^{r,i}$ must obey $0 \leqslant i \leqslant k-1$. Of course, since we assume $k < p+1$, we have $i < p$. The descent stops at (14) either because $k-j-1=0$ or because $a^{k-j-1,j}$ is invariant. The case $j=0$ is trivial since it gives immediately $\alpha^k = \mathrm{d}\beta^{k-1}$, where $\beta^{k-1} \equiv a^{k-1,0}$ is invariant. Accordingly, we assume from now on that $j > 0$.

Since we are dealing with a descent, it is helpful to introduce one of its building blocks, which is the purpose of the next section. We will complete the induction step in Sec. V C.

B. A descent of γ modulo d

Let us define the following differential forms built up from the ghosts:

$$D^l_{\mu_1\cdots\mu_{p+1}} \equiv (-)^{l(q+1)+q} \partial_{[\mu_1} A^{(0,q-l)}_{\mu_2\cdots\mu_{p+1}]|\nu_1\cdots\nu_l} \, \mathrm{d}x^{\nu_1} \cdots \mathrm{d}x^{\nu_l},$$

for $0 \leqslant l \leqslant q$. It is easy to show that these fields verify the following descent:

$$\gamma(D^0_{\mu_1\cdots\mu_{p+1}}) = 0, \tag{15}$$

$$\gamma(D^{l+1}_{\mu_1\cdots\mu_{p+1}}) + \mathrm{d}D^l_{\mu_1\cdots\mu_{p+1}} = 0, \quad 0 \leqslant l \leqslant q-1,$$

$$\mathrm{d}D^q_{\mu_1\cdots\mu_{p+1}} = K^{q+1}_{\mu_1\cdots\mu_{p+1}}. \tag{16}$$

It is convenient to introduce the inhomogeneous form

$$D_{\mu_1\cdots\mu_{p+1}} = \sum_{l=0}^{q} D^l_{\mu_1\cdots\mu_{p+1}}$$

because it satisfies a so-called "Russian formula,"

$$(\gamma + \mathrm{d}) D_{\mu_1\cdots\mu_{p+1}} = K^{q+1}_{\mu_1\cdots\mu_{p+1}}, \tag{17}$$

which is a compact way of writing the descent (15) to (16).

Let $\omega_{(n,m)}$ be a homogeneous polynomial of degree m in D and of degree n in K. Its decomposition is

$$\omega_{(n,m)}(K,D) = \omega^{n(q+1)+mq,0} + \cdots + \omega^{n(q+1)+j,mq-j} + \cdots + \omega^{n(q+1),mq},$$

where $\omega^{n(q+1)+j,mq-j}$ has form degree $n(q+1)+j$ and pure ghost number $mq-j$. Due to (17), the polynomial satisfies

$$(\gamma + \mathrm{d})\omega_{(n,m)} = K^{q+1}_{\mu_1\cdots\mu_{p+1}} \frac{\partial^L \omega_{(n,m)}}{\partial D_{\mu_1\cdots\mu_{p+1}}}, \tag{18}$$

the form-degree decomposition of which leads to the descent

$$\gamma(\omega^{n(q+1),mq}) = 0,$$

$$\gamma(\omega^{n(q+1)+j+1,mq-j-1}) + \mathrm{d}\omega^{n(q+1)+j,mq-j} = 0, \quad 0 \leqslant j \leqslant q-1,$$

$$\gamma(\omega^{n(q+1)+q+1,(m-1)q-1}) + \mathrm{d}\omega^{n(q+1)+q,(m-1)q} = K^{q+1}_{\mu_1\cdots\mu_{p+1}}\left[\frac{\partial^L \omega}{\partial D_{\mu_1\cdots\mu_{p+1}}}\right]^{n(q+1),(m-1)q}, \tag{19}$$

where $[\partial\omega/\partial D]^{n(q+1),(m-1)q}$ denotes the component of form degree $n(q+1)$ and pure ghost equal to $(m-1)q$ of the derivative $\partial\omega/\partial D$. This component is the homogeneous polynomial of degree $m-1$ in the variable D^0,

$$\left[\frac{\partial\omega}{\partial D_{\mu_1\cdots\mu_{p+1}}}\right]^{n(q+1),(m-1)q} = \left.\frac{\partial\omega}{\partial D_{\mu_1\cdots\mu_{p+1}}}\right|_{D=D^0}.$$

The right-hand side of (19) vanishes if and only if the right-hand side of (18) does.

Two cases arise depending on whether the right-hand side (rhs) of (18) vanishes or not.

(i) The rhs of (18) vanishes, then the descent is said not to be obstructed in any strictly positive pure ghost number and goes all the way down to the bottom equations

$$\gamma(\omega^{n(q+1)+mq,0}) + \mathrm{d}\omega^{n(q+1)+mq+1,1} = 0, \quad 0 \leqslant j \leqslant q-1,$$

$$\mathrm{d}(\omega^{n(q+1)+mq,0}) = 0.$$

(ii) The rhs of (18) is not zero, then the descent is obstructed after q steps. It is not possible to find an $\tilde{\omega}^{n(q+1)+q+1,(m-1)q-1}$ such that

$$\gamma(\tilde{\omega}^{n(q+1)+q+1,(m-1)q-1}) + \mathrm{d}\omega^{n(q+1)+q,(m-1)q} = 0,$$

because the rhs of (19) is an element of $H(\gamma)$. This element is called the *obstruction* to the descent. One also says that this obstruction cannot be lifted more than q times, and $\omega^{n(q+1),mq}$ is the top of the ladder [in this case it must be an element of $H(\gamma)$].

This covers the general type of ladder (descent as well as lift) that does not contain the pth generation ghost $A^{(p-q,q)}$.

C. End of the proof of the invariant Poincaré lemma

As $j<p$, Theorem 4.1 implies that the equation (14) has nontrivial solutions only when $j=mq$ for some integer m

$$a^{k-mq-1,mq} = \sum_I \alpha_I^{k-mq-1}\omega_I^{0,mq}, \tag{20}$$

up to some γ-exact term. The α_I^{k-mq-1}'s are invariant forms, and $\{\omega_I^{0,mq}\}$ is a basis of polynomials of degree m in the variable D^0. The ghost $A^{(p-q,q)}$ is absent since the pure ghost number is $j=mq<p$.

The equation (13) implies $\mathrm{d}\alpha_I^{k-mq-1}=0$. Together with the induction hypothesis, this implies

$$\alpha_I^{k-mq-1} = P_I(K^{q+1}_{\mu_1\cdots\mu_{p+1}}) + \mathrm{d}\beta_I^{k-mq-2}, \tag{21}$$

where the polynomials P_I of order n are present iff $k-mq-1=n(q+1)$. Inserting (21) into (20) we find that, up to trivial redefinitions, $a^{k-j-1,j}$ is a polynomial in $K^{q+1}_{\mu_1\cdots\mu_{p+1}}$ and $D^0_{\mu_1\cdots\mu_{p+1}}$.

From the analysis performed in Sec. V B, we know that such an $a^{k-j-1,j}$ can be lifted at most q times. Therefore, $a^{k-j-1,j}$ belongs to a descent of type (11)–(14) only if $j=q$. Without loss of generality we can thus take $a^{k-q-1,q}=P(K^{q+1}_{\mu_1\cdots\mu_{p+1}},D^0)$ where P is a homogeneous polynomial with a linear dependence in D^0 (since $m=1$). In such a case, it can be lifted up to (11). Furthermore, because $a^{k-1,0}$ is defined up to an invariant form $\beta^{k-1,0}$ by the equation (12), the term $\mathrm{d}a^{k-1,0}$ of (11) must be equal to the sum

$$\mathrm{d}a^{k-1,0} = \underbrace{P(K^{q+1},K^{q+1})}_{\equiv Q(K^{q+1}_{\mu_1\cdots\mu_{p+1}})} + \mathrm{d}\beta^{k-1,0}$$

of a homogeneous polynomial Q in K^{q+1} (the lift of the bottom) and a form d-exact in the invariants. □

VI. COHOMOLOGY OF δ MODULO d: $H_k^D(\delta|\mathrm{d})$

In this section, we compute the cohomology of δ modulo d in top form degree and antighost number k, for $k \geqslant q$. We will also restrict ourselves to $k>1$. The group $H_1^D(\delta|\mathrm{d})$ describes the infinitely many conserved currents and will not be studied here.

Let us first recall a general theorem (Theorem 9.1 in Ref. 26).

Theorem 6.1: *For a linear gauge theory of reducibility order* $p-1$,

$$H_k^D(\delta|\mathrm{d}) = 0 \quad \text{for } k > p+1.$$

The computation of the cohomology groups $H_k^D(\delta|\mathrm{d})$ for $q \leqslant k \leqslant p+1$ follows closely the procedure used for p-forms in Ref. 24. It relies on the following theorems.

Theorem 6.2: *Any solution of* $\delta a^D + \mathrm{d}b^{D-1} = 0$ *that is at least bilinear in the antifields is necessarily trivial.*

The proof of Theorem 6.2 is similar to the proof of Theorem 11.2 in Ref. 26 and will not be repeated here.

Theorem 6.3: *A complete set of representatives of* $H_{p+1}^D(\delta|\mathrm{d})$ *is given by the antifields* $C^{*D}_{p+1\mu_1\cdots\mu_q}$, *i.e.,*

$$\delta a^D_{p+1} + \mathrm{d}a^{D-1}_p = 0 \Rightarrow a^D_{p+1} = \lambda^{\mu_{[q]}} C^{*D}_{p+1\mu_{[q]}} + \delta b^D_{p+2} + \mathrm{d}b^{D-1}_{p+1},$$

where the $\lambda^{[\mu_1\cdots\mu_q]}$ *are constants.*

Proof: Candidates: any polynomial of antighost number $p+1$ can be written

$$a^D_{p+1} = \Lambda^{[\mu_1\cdots\mu_q]} C^{*D}_{p+1[\mu_1\cdots\mu_q]} + \mu^D_{p+1} + \delta b^D_{p+2} + \mathrm{d}b^{D-1}_{p+1},$$

where Λ does not involve the antifields and where μ^D_{p+1} is at least quadratic in the antifields. The cocycle condition $\delta a^D_{p+1} + \mathrm{d}a^{D-1}_p = 0$ then implies

$$-\Lambda^{[\mu_1\cdots\mu_q]}\,\mathrm{d}C^{*D-1}_{p[\mu_1\cdots\mu_q]} + \delta(\mu^D_{p+1} + \mathrm{d}b^{D-1}_{p+1}) + da^{D-1}_p = 0.$$

By taking the Euler–Lagrange derivative of this equation with respect to $C^*_{p[\mu_1\cdots\mu_q]|\nu}$, one gets the weak equation $\partial^\nu \Lambda^{[\mu_1\cdots\mu_q]} \approx 0$. Considering ν as a form index, one sees that Λ belongs to $H_0^0(\mathrm{d}|\delta)$. The isomorphism $H_0^0(\mathrm{d}|\delta)/\mathbb{R} \cong H_D^D(\delta|\mathrm{d})$ (see Ref. 26) combined with the knowledge of $H_D^D(\delta|\mathrm{d}) \cong 0$ (by Theorem 6.1) implies $\Lambda^{[\mu_1\cdots\mu_q]} = \lambda^{[\mu_1\cdots\mu_q]} + \delta\nu_1^{[\mu_1\cdots\mu_q]}$ where $\lambda^{[\mu_1\cdots\mu_q]}$ is a constant. The term $\delta\nu_1^{[\mu_1\cdots\mu_q]} C^{*D}_{p+1[\mu_1\cdots\mu_q]}$ can be rewritten as a term at least bilinear in the antifields up to a δ-exact term. Inserting $a^D_{p+1} = \lambda^{[\mu_1\cdots\mu_q]} C^{*D}_{p+1\mu_1\cdots\mu_q} + \mu^D_{p+1} + \delta b^D_{p+2} + \mathrm{d}b^{D-1}_{p+1}$ into the cocycle condition, we see that μ^D_{p+1} must be a solution of $\delta\mu^D_{p+1} + \mathrm{d}b^{D-1} = 0$ and is therefore trivial by Theorem 6.2.

Nontriviality: It remains to show that the cocycles $a^D_{p+1} = \lambda C^{*D}_{p+1}$ are nontrivial. Indeed one can prove that $\lambda C^{*D}_{p+1} = \delta u^D_{p+2} + \mathrm{d}v^{D-1}_{p+1}$ implies that λC^{*D}_{p+1} vanishes. It is straightforward when u^D_{p+2} and v^{D-1}_{p+1} do not depend explicitly on x: δ and d bring in a derivative while λC^{*D}_{p+1} does not contain any. If u and v depend explicitly on x, one must expand them and the equation $\lambda C^{*D}_{p+1} = \delta u^D_{p+2} + \mathrm{d}v^{D-1}_{p+1}$ according to the number of derivatives of the fields and antifields to reach the conclusion. Explicitly, $u^D_{p+2} = u^D_{p+2,0} + \cdots + u^D_{p+2,l}$ and $v^{D-1}_{p+1} = v^{D-1}_{p+1,0} + \cdots + v^{D-1}_{p+1,n}$. If $n>l$, the equation in degree $n+1$ reads $0 = \mathrm{d}' v^{D-1}_{p+1,n}$ where d' does not differentiate with respect to the explicit dependence in x. This in turn implies that $v^{D-1}_{p+1,n} = \mathrm{d}'\tilde{v}^{D-1}_{p+1,n-1}$ and can be removed by redefining $v^{D-1}_{p+1}: v^{D-1}_{p+1} \to v^{D-1}_{p+1} - \mathrm{d}\tilde{v}^{D-1}_{p+1,n-1}$. If $l>n$, the equation in degree $l+1$ is $0 = \delta u^D_{p+2,l}$ and implies, together with the acy-

clicity of δ, that one can remove $u^D_{p+2,l}$ by a trivial redefinition of u^D_{p+2}. If $l=n>0$, the equation in degree $l+1$ reads $0=\delta u^D_{p+2,l}+\mathrm{d}' v^{D-1}_{p+1,l}$. Since there is no cohomology in antighost number $p+2$, this implies that $u^D_{p+2,l}=\delta \overline{u}^D_{p+3,l-1}+\mathrm{d}'\overline{u}^{D-1}_{p+2,l-1}$ and can be removed by trivial redefinitions: $u^D_{p+2}\to u^D_{p+2}-\delta\overline{u}^D_{p+3,l-1}$ and $v^{D-1}_{p+1}\to v^{D-1}_{p+1}-\mathrm{d}\tilde{u}^{D-1}_{p+2,l-1}$. Repeating the steps above, one can remove all $u^D_{p+2,l}$ and $v^{D-1}_{p+1,n}$ for $l,n>0$. One is left with $\lambda C^{*D}_{p+1}=\delta u^D_{p+2,0}+\mathrm{d}' v^{D-1}_{p+1,0}$. The derivative argument used in the case without explicit x dependence now leads to the desired conclusion. □

Theorem 6.4: *The cohomology groups $H^D_k(\delta|\mathrm{d})$ $(k>1)$ vanish unless $k=D-r(D-p-1)$ for some strictly positive integer r. Furthermore, for those values of k, $H^D_k(\delta|\mathrm{d})$ has at most one nontrivial class.*

Proof: We already know that $H^D_k(\delta|\mathrm{d})$ vanishes for $k>p+1$ and that $H^D_{p+1}(\delta|\mathrm{d})$ has one nontrivial class. Let us assume that the theorem has been proved for all k's strictly greater than K (with $K<p+1$) and extend it to K. Without loss of generality we can assume that the cocycles of $H^D_K(\delta|\mathrm{d})$ take the form (up to trivial terms) $a^D_K=\lambda^{\mu_1\cdots\mu_{p+1-K}|\nu_1\cdots\nu_q}C^{*D-p-1+K}_{K\ \nu_1\cdots\nu_q|\mu_1\cdots\mu_{p+1-K}}+\mu^D_K$, where λ does not involve the antifields and μ is at least bilinear in the antifields. Taking the Euler–Lagrange derivative of the cocycle condition with respect to C^*_{K-1} implies that $\lambda^{p+1-K}_{\nu_1\cdots\nu_q}\equiv\lambda_{\mu_1\cdots\mu_{p+1-K}|\nu_1\cdots\nu_q}\,\mathrm{d}x^{\mu_1}\cdots\mathrm{d}x^{\mu_{p+1-K}}$ defines an element of $H_0^{p+1-K}(\mathrm{d}|\delta)$. If λ is d-trivial modulo δ, then it is straightforward to check that $\lambda C^{*D-p-1+K}_K$ is trivial or bilinear in the antifields. Using the isomorphism $H_0^{p+1-K}(\mathrm{d}|\delta)\cong H^D_{D-p-1+K}(\delta|\mathrm{d})$, we see that λ must be trivial unless $D-p-1+K=D-r(D-p-1)$, in which case $H^D_{D-p-1+K}(\delta|\mathrm{d})$ has one nontrivial class. Since $K=D-(r+1)(D-p-1)$ is also of the required form, the theorem extends to K. □

Theorem 6.5: *Let r be a strictly positive integer. A complete set of representatives of $H^D_k(\delta|\mathrm{d})$ $[k=D-r(D-p-1)\geqslant q]$ is given by the terms of form-degree D in the expansion of all possible homogeneous polynomials $P(\tilde{H})$ of degree r in $\tilde{H}$ [or equivalently $P(\tilde{\mathcal{H}})$ of degree r in $\tilde{\mathcal{H}}$].*

The proof of this theorem is given in Appendix B.

These theorems give us a complete description of all the cohomology groups $H^D_k(\delta|\mathrm{d})$ for $k\geqslant q$ (with $k>1$).

VII. INVARIANT COHOMOLOGY OF δ MODULO d, $H^{\mathrm{inv}}_k(\delta|\mathrm{d})$

In this section, we compute the set of invariant solutions a^D_k $(k\geqslant q)$ of the equation $\delta a^D_k+\mathrm{d}b^{D-1}_{k-1}=0$, up to trivial terms $a^D_k=\delta b^D_{k+1}+\mathrm{d}c^{D-1}_k$, where b^D_{k+1} and c^{D-1}_k are invariant. This space of solutions is the invariant cohomology of δ modulo d, $H^{\mathrm{inv}}_k(\delta|\mathrm{d})$. We first compute representatives of all the cohomology classes of $H^{\mathrm{inv}}_k(\delta|\mathrm{d})$, then we find out the cocycles without explicit x dependence.

Theorem 7.1: *For $k\geqslant q$, a complete set of invariant solutions of the equation $\delta a^D_k+\mathrm{d}b^{D-1}_{k-1}=0$ is given by the proper component in the expansion of the polynomials in the curvature K^{q+1} and in $\tilde{\mathcal{H}}$ (modulo trivial solutions),*

$$\delta a^D_k+\mathrm{d}b^{D-1}_{k-1}=0\Rightarrow a^D_k=P(K^{q+1},\tilde{\mathcal{H}})|^D_k+\delta\mu^D_{k+1}+\mathrm{d}\nu^{D-1}_k,$$

where μ^D_{k+1} and ν^{D-1}_k are invariant forms.

Proof: From the preceding section, we know that for $k\geqslant q$ the general solution of the equation $\delta a^D_k+\mathrm{d}b^{D-1}_{k-1}=0$ is $a^D_k=Q(\tilde{\mathcal{H}})|^D_k+\delta m^D_{k+1}+\mathrm{d}n^{D-1}_k$ where $Q(\tilde{\mathcal{H}})$ is a homogeneous polynomial of degree r in $\tilde{\mathcal{H}}$ [it exists only when $k=D-r(D-p-1)$]. Note that m^D_{k+1} and n^{D-1}_k are not necessarily invariant. However, one can prove the following theorem (the lengthy proof of which is given in Appendix C).

Theorem 7.2: *Let α^D_k be an invariant polynomial $(k\geqslant q)$. If $\alpha^D_k=\delta m^D_{k+1}+\mathrm{d}n^{D-1}_k$, then*

$$\alpha^D_k=R^{(s,r)}(K^{q+1},\tilde{\mathcal{H}})|^D_k+\delta\mu^D_{k+1}+\mathrm{d}\nu^{D-1}_k,$$

where $R^{(s,r)}(K^{q+1},\tilde{\mathcal{H}})$ is a polynomial of degree s in K^{q+1} and r in $\tilde{\mathcal{H}}$, such that the strictly positive integers s, r satisfy $D=r(D-p-1)+k+s(q+1)$ and μ^D_{k+1} and ν^{D-1}_k are invariant forms.

As a^D_k and $Q(\tilde{\mathcal{H}})|^D_k$ are invariant, this theorem implies that

$$a_k^D = P^{(s,r)}(K^{q+1},\tilde{\mathcal{H}})|_k^D + \delta\mu_{k+1}^D + \mathrm{d}\nu_k^{D-1},$$

where $P^{(s,r)}(K^{q+1},\tilde{\mathcal{H}})$ is a polynomial of non-negative degree s in K^{q+1} and of strictly positive degree r in $\tilde{\mathcal{H}}$. Note that the polynomials of nonvanishing degree in K^{q+1} are trivial in $H_k^D(\delta|\mathrm{d})$ but not necessarily in $H_k^{D\ \mathrm{inv}}(\delta|\mathrm{d})$. □

Part of the solutions found in Theorem 7.1 depend explicitly on the coordinate x, because $\tilde{\mathcal{H}}|_0$ does. Therefore the question arises whether there exist other representatives of the same nontrivial equivalence class $[P^{(s,r)}(K^{q+1},\tilde{\mathcal{H}})|_k^D] \in H_k^{D\ \mathrm{inv}}(\delta|\mathrm{d})$ that *do not* depend explicitly on x. The answer is negative when $r>1$. In other words, we can prove the general theorem.

Theorem 7.3: *When $r>1$, there is no nontrivial invariant cocycle in the equivalence class $[P^{(s,r)}(K^{q+1},\tilde{\mathcal{H}})|_k^D] \in H_k^{D\ \mathrm{inv}}(\delta|\mathrm{d})$ without explicit x* dependence.

To do so, we first prove the following lemma.

Lemma 7.1: Let $P(K^{q+1},\tilde{\mathcal{H}})$ be a homogeneous polynomial of order s in the curvature K^{q+1} and r in $\tilde{\mathcal{H}}$. If $r\geqslant 2$, then the component $P(K^{q+1},\tilde{\mathcal{H}})|_k^D$ always contains terms of order $r-1(\neq 0)$ in $\tilde{\mathcal{H}}|_0$.

Proof: Indeed, $P(K^{q+1},\tilde{\mathcal{H}})$ can be freely expanded in terms of $\tilde{\mathcal{H}}|_0$ and the undifferentiated antighost forms. The Grassmann parity is the same for all terms in the expansion of $\tilde{\mathcal{H}}$, therefore the expansion is the binomial expansion up to the overall coefficient of the homogeneous polynomial and up to relative signs obtained when reordering all terms. Hence, the component $P(K^{q+1},\tilde{\mathcal{H}})|_k^D$ always contains a term that is a product of $(r-1)$ $\tilde{\mathcal{H}}|_0^{D-p-1}$'s, a single antighost $C_k^{*D-p-1+k}$ and s curvatures, which possesses the correct degrees as can be checked straightforwardly. □

Proof of Theorem 7.3: Let us assume that there exists a nonvanishing invariant x-independent representative $\alpha_k^{D,\mathrm{inv}}$ of the equivalence class $[P^{(s,r)}(K^{q+1},\tilde{\mathcal{H}})|_k^D] \in H_k^{D\ \mathrm{inv}}(\delta|\mathrm{d})$, i.e.,

$$P^{(s,r)}(K^{q+1},\tilde{\mathcal{H}})|_k^D + \delta\rho_{k+1}^D + \mathrm{d}\sigma_k^{D-1} = \alpha_k^{D,\mathrm{inv}}, \tag{22}$$

where ρ_{k+1}^D and σ_k^{D-1} are invariant and allowed to depend explicitly on x.

We define the descent map $f:\alpha_m^n \to \alpha_{m-1}^{n-1}$ such that $\delta\alpha_m^n + \mathrm{d}\alpha_{m-1}^{n-1} = 0$, for $n \leqslant D$. This map is well defined on equivalence classes of $H^{\mathrm{inv}}(\delta|\mathrm{d})$ when $m>1$. Hence, going down $k-1$ steps, it is clear that the equation (22) implies

$$P^{(s,r)}(K^{q+1},\tilde{\mathcal{H}})|_1^{D-k+1} + \delta\rho_2^{D-k+1} + \mathrm{d}\sigma_1^{D-k} = \alpha_1^{D-k+1,\mathrm{inv}},$$

with $\alpha_1^{D-k+1,\mathrm{inv}} \neq 0$.

We can decompose this equation in the polynomial degree in the fields, antifields, and all their derivatives. Since δ and d are linear operators, they preserve this degree; therefore

$$P^{(s,r)}(K^{q+1},\tilde{\mathcal{H}})|_{1,r+s}^{D-k+1} + \delta\rho_{2,r+s}^{D-k+1} + \mathrm{d}\sigma_{1,r+s}^{D-k} = \alpha_{1,r+s}^{D-k+1,\mathrm{inv}}, \tag{23}$$

where $r+s$ denotes the polynomial degree. The homogeneous polynomial $\alpha_{1,r+s}^{D-k+1,\mathrm{inv}}$ of polynomial degree $r+s$ is linear in the antifields of antighost number equal to one, and depends on the fields only through the curvature.

Finally, we introduce the number operator N defined by

$$N = r\partial_{\rho_1}\cdots\partial_{\rho_r}\phi_{\mu_1\cdots\mu_p|\nu_1\cdots\nu_q}\frac{\partial}{\partial(\partial_{\rho_1}\cdots\partial_{\rho_r}\phi_{\mu_1\cdots\mu_p|\nu_1\cdots\nu_q})} + (r+1)\partial_{\rho_1}\cdots\partial_{\rho_r}\Phi^*_A\frac{\partial}{\partial(\partial_{\rho_1}\cdots\partial_{\rho_r}\Phi^*_A)} - x^\mu\frac{\partial}{\partial x^\mu},$$

where $\{\Phi^*_A\}$ denotes the set of all antifields. It follows immediately that δ and d are homogeneous of degree one and the degree of $\tilde{\mathcal{H}}$ is also equal to one,

$$N(\delta) = N(d) = 1 = N(\tilde{\mathcal{H}}).$$

Therefore, the decomposition in N-degree of the equation (23) reads in N-degree equal to $n=r+2s$,

$$P^{(s,r)}(K^{q+1},\tilde{\mathcal{H}})|^{D-k+1}_{1,r+s} + \delta\rho^{D-k+1}_{2,r+s,r+2s-1} + \mathrm{d}\sigma^{D-k}_{1,r+s,r+2s-1} = \alpha^{D-k+1,\mathrm{inv}}_{1,r+s,r+2s} \tag{24}$$

and, in N-degree equal to $n>r+2s$,

$$\delta\rho^{D-k+1}_{2,r+s,n-1} + \mathrm{d}\sigma^{D-k}_{1,r+s,n-1} = \alpha^{D-k+1,\mathrm{inv}}_{1,r+s,n}.$$

The component $\alpha^{D-k+1,\mathrm{inv}}_{1,r+s,r+2s}$ of N-degree equal to $r+2s$ is x-independent, depends linearly on the (possibly differentiated) antighost of antifield number 1, and is of order $r+s-1$ in the (possibly differentiated) curvatures. Direct counting shows that there is no polynomial of N-degree equal to $r+2s$ satisfying these requirements when $r\geqslant 2$. Thus for $r\geqslant 2$ the component $\alpha^{D-k+1,\mathrm{inv}}_{1,r+s,r+s}$ vanishes, and then the equation (24) implies that $P^{(s,r)}(K^{q+1},\tilde{\mathcal{H}})|^{D-k+1}_{1,r+s}$ is trivial (and even vanishes when $s=0$, by Theorem 6.5).

In conclusion, if $P(K^{q+1},\tilde{\mathcal{H}})$ is a polynomial that is quadratic or more in $\tilde{\mathcal{H}}$, then there exists no nontrivial invariant representative without explicit x dependence in the cohomology class $[P(K^{q+1},\tilde{\mathcal{H}})]$ of $H^{\mathrm{inv}}(\delta|\mathrm{d})$. □

This leads us to the following theorem.

Theorem 7.4: *The invariant solutions a^D_k $(k\geqslant q)$ of the equation $\delta a^D_k+\mathrm{d}b^{D-1}_{k-1}=0$ without explicit x dependence are all trivial in $H^{\mathrm{inv}}_k(\delta|\mathrm{d})$ unless $k=p+1-s(q+1)$ for some non-negative integer s. For those values of k, the nontrivial representatives are given by polynomials that are linear in $C^{*D-p-1+k}_k$ and of order s in K^{q+1}.*

Proof: By Theorem 7.1, invariant solutions of the equation $\delta a^D_k+\mathrm{d}b^{D-1}_{k-1}=0$ are polynomials in K^{q+1} and $\tilde{\mathcal{H}}$ modulo trivial terms. When the polynomial is quadratic or more in $\tilde{\mathcal{H}}$, then Theorem 7.3 states that there is no representative without explicit x dependence in its cohomology class, which implies that it should be rejected. The remaining solutions are the polynomials linear in $\tilde{\mathcal{H}}|_k=C^{*D-p-1+k}_k$ and of arbitrary order in K^{q+1}. They are invariant and x independent, they thus belong to the set of looked-for solutions. □

VIII. SELF-INTERACTIONS

As explained in Sec. III, the nontrivial first order deformations of the free theory are given by the elements of $H^{D,0}(s|\mathrm{d})$, the cohomological group of the BRST differential s in the space of local forms in top form degree and in ghost number zero. The purpose of this section is to compute this group. As the computation is very similar to the computation of similar groups in the case of p-forms,[16] gravity,[17] dual gravity,[18] and $[p,p]$-fields,[20] we will not reproduce it here entirely and refer to the works just cited (e.g., Ref. 17) for technical details. We just present the main steps of the procedure and the calculations that are specific to the case of $[p,q]$-fields.

The proof is given for a single $[p,q]$-field ϕ but extends trivially to a set $\{\phi^a\}$ containing a finite number n of them (with fixed p and q) by writing some internal index $a=1,\ldots,n$ everywhere.

The group $H(s|\mathrm{d})$ is the group of solutions a of the equation $sa+\mathrm{d}b=0$, modulo trivial solutions of the form $a=sm+\mathrm{d}n$. The basic idea to compute such a group is to use homological perturbation techniques by expanding the quantities and the equations according to the antighost number.

Let $a^{D,0}$ be a solution of $sa^{D,0}+\mathrm{d}b^{D-1,1}=0$ with ghost number zero and top form degree. For convenience, we will frequently omit to write the upper indices. One can expand $a(=a^{D,0})$ as $a=a_0+a_1+\cdots+a_k$ where a_i has antighost number i. The expansion can be assumed to stop at some finite value of the antighost number under the sole hypothesis that the first-order deformation of the Lagrangian has a finite derivative order.[27] Let us recall[21] that (i) the antifield-independent piece a_0 is the deformation of the Lagrangian; (ii) the terms linear in the ghosts contain the information about the deformation of the reducibility conditions; (iii) the other terms give the information about the deformation of the gauge algebra.

Under the assumption of locality, the expansion of b also stops at some finite antighost number. Without loss of generality, one can assume that $b_j=0$ for $j\geqslant k$. Decomposing the BRST differential as $s=\gamma+\delta$, the equation $sa+\mathrm{d}b=0$ is equivalent to

$$\begin{aligned}
&\delta a_1+\gamma a_0+\mathrm{d}b_0=0,\\
&\delta a_2+\gamma a_1+\mathrm{d}b_1=0,\ \ldots,\\
&\delta a_k+\gamma a_{k-1}+\mathrm{d}b_{k-1}=0,\\
&\gamma a_k=0.
\end{aligned}\tag{25}$$

The next step consists in the analysis of the term a_k with highest antighost number and the determination of whether it can be removed by trivial redefinitions or not. We will see in the sequel under which assumptions this can be done.

A. Computation of a_k for $k>1$

The last equation of the descent (25) is $\gamma a_k=0$. It implies that $a_k=\alpha_J\omega^J$ where α_J is an invariant form and ω^J is a polynomial in the ghosts of $H(\gamma)$: $A^{(p-q,q)}_{\mu_{[q]}}$ and $D^0_{\mu_{[p+1]}}$. Inserting this expression for a_k into the second to last equation leads to the result that α_J should be an element of $H^{D,\mathrm{inv}}_k(\delta|\mathrm{d})$. Furthermore, if α_J is trivial in this group, then a_k can be removed by trivial redefinitions. The vanishing of $H^{D,\mathrm{inv}}_k(\delta|\mathrm{d})$ is thus a sufficient condition to remove the component a_k from a. It is however not a necessary condition, as we will see in the sequel.

We showed that nontrivial interactions can arise only if some $H^{D,\mathrm{inv}}_k(\delta|\mathrm{d})$ do not vanish. The requirement that the Lagrangian should not depend explicitly on x implies that we can restrict ourselves to x-independent elements of this group. Indeed, it can be shown[23] that, when a_0 does not depend explicitly on x, the whole cocycle $a=a_0+a_1+\cdots+a_k$ satisfying $sa+\mathrm{d}b=0$ is x independent (modulo trivial redefinitions). By Theorem 7.4, $H^{D,\mathrm{inv}}_k(\delta|\mathrm{d})$ contains nontrivial x-independent elements only if $k=p+1-s(q+1)$ for some non-negative integer s. The form of the nontrivial elements is then $\alpha^D_k=C^{*D-p-1+k}_k(K^{q+1})^s$. In order to be (possibly) nontrivial, a_k must thus be a polynomial linear in $C^{*D-p-1+k}_k$, of order s in the curvature K^{q+1} and of appropriate orders in the ghosts $A^{(p-q,q)}_{\mu_{[q]}}$ and $D^0_{\mu_{[p+1]}}$.

As a_k has ghost number zero, the antighost number of a_k should match its pure ghost number. Consequently, as the ghosts $A^{(p-q,q)}_{\mu_{[q]}}$ and $D^0_{\mu_{[p+1]}}$ have puregh$=p$ and q, respectively, the equation $k=np+mq$ should be satisfied for some positive integers n and m. If there is no couple of integers n, m to match k, then no a_k satisfying the relevant equations of the descent (25) can be constructed and a_k thus vanishes.

In the sequel, we will consider the case where n and m satisfying $k=np+mq$ can be found and classify the different cases according to the following values of n and m: (i) $n\geqslant 2$, (ii) $n=1$, (iii)

$n=0$, $m>1$, and (iv) $n=0$, $m=1$. We will show that the corresponding candidates a_k are either obstructed in the lift to a_0 or that they are trivial, except in the case (iv). In this case, a_k can be lifted but a_0 depends explicitly on x and contains more than two derivatives.

(i) Candidates with $n\geqslant 2$: The constraints $k\leqslant p+1$ and $k=np+mq$ have no solutions. (There is a solution in the case previously considered in Ref. 17, where $p=q=1$, $n=2$. As shown in Ref. 17, this solution gives rise to Einstein's theory of gravity.)

(ii) Candidates with $n=1$: The conditions $k=mq+p\leqslant p+1$ are only satisfied for $q=1=m$. As shown in Ref. 18, the lift of these candidates is obstructed after one step without any additional assumption.

(iii) Candidates with $n=0$, $m>1$: For a nontrivial candidate to exist at $k=mq$, Theorem 7.4 tells us that p and q should satisfy the relation $p+1=mq+s(q+1)$ for some positive or null integer s. The candidate then has the form

$$a^D_{mq}=C^{*D-p-1+mq}_{mq\nu_{[q]}}\omega^{\nu_{[q]}}_{(s,m)}(K,D),$$

where what is meant by a polynomial $\omega_{(s,m)}$ is explained in Sec. V B.

We will show that these candidates are either trivial or that there is an obstruction to lift them up to a^D_0 after q steps.

It is straightforward to check that, for $1\leqslant j\leqslant q$, the terms

$$a^D_{mq-j}=C^{*D-p-1+mq-j}_{mq-j}\omega^{s(q+1)+j,mq-j}$$

satisfy the descent equations, since, as $m>1$, all antifields $C^{*D-p-1+mq-j}_{mq-j}$ are invariant. The set of summed indices $\nu_{[q]}$ is implicit as well as the homogeneity degree of the generating polynomials $\omega_{(s,m)}$. We can thus lift a^D_{mq} up to $a^D_{(m-1)q}$. As $m>1$, this is not yet a_0.

There is however no $a^D_{(m-1)q-1}$ such that

$$\gamma(a^D_{(m-1)q-1})+\delta a^D_{(m-1)q}+\mathrm{d}\beta^{D-1}_{(m-1)q-1}=0. \tag{26}$$

Indeed, we have

$$\delta a^D_{(m-1)q}=-\gamma(C^{*D-(s+1)(q+1)}_{(m-1)q-1}\omega^{(s+1)(q+1),(m-1)q-1})+(-)^{D-mq}C^{*D-(s+1)(q+1)}_{(m-1)q-1}K^{q+1}\left[\frac{\partial^L\omega}{\partial D}\right]^{s(q+1),(m-1)q}.$$

Without loss of generality, we can suppose that

$$a^D_{(m-1)q-1}=C^{*D-(s+1)(q+1)}_{(m-1)q-1}\bar{a}^{(s+1)(q+1)}_0+\bar{a}^D_{(m-1)q-1},$$

where there is an implicit summation over all possible coefficients $\bar{a}^{(s+1)(q+1)}_0$, and most importantly the two $\bar{a}$'s *do not* depend on $C^*_{(m-1)q-1}$. (This is not true in the case—excluded in this paper—where $p=q=1$ and $m=2$: since $C^*_{(m-1)q-1}\equiv C^*_0$ has antighost number zero, the antighost number counting does not forbid that the $\bar{a}$'s depend on C^*_0. Candidates arising in this way are treated in Ref. 28 and give rise to a consistent deformation of the Fierz–Pauli theory in $D=3$.) Taking the Euler–Lagrange derivative of (26) with respect to $C^*_{(m-1)q-1}$ yields

$$\gamma(\bar{a}^{(s+1)(q+1)}_0-\omega^{(s+1)(q+1),(m-1)q-1})\propto K^{q+1}\left[\frac{\partial^L\omega}{\partial D}\right]^{s(q+1),(m-1)q}.$$

The product of nontrivial elements of $H(\gamma)$ in the rhs is not γ-exact and constitutes an obstruction to the lift of the candidate, unless it vanishes. The latter happens only when the polynomial $\omega_{(s,m)}$ can be expressed as

$$\omega^{\nu_{[q]}}_{(s,m)}(K,D) = K^{q+1}\mu_{[p+1]}\frac{\partial^L \widetilde{\omega}^{\nu_{[q]}}_{(s-1,m+1)}(K,D)}{\partial D^{\mu_{[p+1]}}},$$

for some polynomial $\widetilde{\omega}^{\nu_{[q]}}_{(s-1,m+1)}(K,D)$ of order $s-1$ in K^{q+1} and $m+1$ in D. However, in this case, a^D_{mq} can be removed by the trivial redefinition

$$a^D \to a^D + s(\widetilde{H}_{\nu_{[q]}}\widetilde{\omega}^{\nu_{[q]}}_{(s-1,m+1)}|^D).$$

This completes the proof that these candidates are either trivial or that their lift is obstructed. As a consequence, they do not lead to consistent interactions and can be rejected. Let us stress that no extra assumptions are needed to get this result. In the particular case $q=1$, this had already been guessed but not proved in Ref. 18.

(iv) Candidates with $n=0$, $m=1$: These candidates exist only when the condition $p+2=(s+1)(q+1)$ is satisfied, for some strictly positive integer s. It is useful for the analysis to write the indices explicitly,

$$a^D_q = g^{\nu_{[q]}\|\mu^1_{[p+1]}|\cdots|\mu^{s+1}_{[p+1]}}C^{*D-p-1+q}_{q\nu_{[q]}}\left(\prod_{i=1}^{s}K^{q+1}_{\mu^i_{[p+1]}}\right)D^0_{\mu^{s+1}_{[p+1]}},$$

where g is a constant tensor.

We can split the analysis into two cases: (i) $g\to(-)^q g$ under the exchange $\mu^s_{[p+1]}\leftrightarrow\mu^{s+1}_{[p+1]}$, and (ii) $g\to(-)^{q+1}g$ under the same transformation.

In the case (i), a^D_q can be removed by adding the trivial term $s\,m^D$ where $m^D=\Sigma^{2q}_{j=q}m^D_j$ and

$$m^D_j = (-)^{D-q}\frac{1}{2}g^{\nu_{[q]}\|\mu^1_{[p+1]}|\cdots|\mu^{s+1}_{[p+1]}}C^{*D-p-1+j}_{j\nu[q]}\left(\prod_{i=1}^{s-1}K^{q+1}_{\mu^i_{[p+1]}}\right)[D_{\mu^s_{[p+1]}}D_{\mu^{s+1}_{[p+1]}}]^{2q+1-j}.$$

This construction does not work in the case (ii) where the symmetry of g makes m^D vanish.

In the case (ii), the candidate a^D_q can be lifted up to a^D_0,

$$a^D_0 \propto f^{\sigma_{[p+1]}\|\mu^1_{[p+1]}|\cdots|\mu^{s+1}_{[p+1]}}_{\tau_{[D-p-q-1]}}x^{\tau_1}\,\mathrm{d}x^{\tau_2}\cdots\mathrm{d}x^{\tau_{D-p-q-1}}K^{q+1}_{\sigma_{[p+1]}}\left(\prod_{i=1}^{s}K^{q+1}_{\mu^i_{[p+1]}}\right)D^q_{\mu^{s+1}_{[p+1]}},$$

where the constant tensor f is defined by

$$f^{\sigma_{[p+1]}\|\mu^1_{[p+1]}|\cdots|\mu^{s+1}_{[p+1]}}_{\tau_{[D-p-q-1]}} \equiv g^{\nu_{[q]}\|\mu^1_{[p+1]}|\cdots|\mu^{s+1}_{[p+1]}}\epsilon^{\sigma_{[p+1]}}{}_{\nu_{[q]}\tau_{[D-p-q-1]}}.$$

Let us first note that this deformation does not affect the gauge algebra, since it is linear in the ghosts.

The Lagrangian deformation a^D_0 depends explicitly on x, which is not a contradiction with translation invariance of the physical theory if the x dependence of the Lagrangian can be removed by adding a total derivative and/or a δ-exact term. If it were the case, a^D_0 would have the form $a^D_0=xG(\cdots)+x^\alpha\mathrm{d}(\cdots)_\alpha$. We have no complete proof that a^D_0 does not have this form, but we think it very unlikely. In any case, this deformation is ruled out by the requirement that the deformation of the Lagrangian contains at most two derivatives.

To summarize the results obtained in this section, we have proved that, under the hypothesis of translation invariance of the first-order vertex a^D_0, all a^D_k $(k>1)$ can be removed by trivial redefinitions of a, except when $p+2=(s+1)(q+1)$ for some positive integer s. In that case, the supplementary assumption that the deformed Lagrangian contains no more than two derivatives is needed to reach the same conclusion, and the only possible deformation (without the latter assumption) does not modify the gauge algebra.

B. Computation of a_1

The term a_1 vanishes without any further assumption when $q>1$. Indeed, when $q>1$, the vanishing of the cohomology of γ in puregh 1 implies that there is no nontrivial a_1.

This is not true when $q=1$, as there are some nontrivial cocycles with pure ghost number equal to one. However, it can be shown[18] that any nontrivial a_1^D leads to a deformation of the Lagrangian with at least four derivatives.

C. Computation of a_0

This leaves us with the problem of solving the equation $\gamma a_0^D + \mathrm{d} b_0^{D-1} = 0$ for a_0^D. Such solutions correspond to deformations of the Lagrangian that are invariant up to a total derivative. Proceeding as in Ref. 20 and asking for Lorentz invariance and that a_0^D should not contain more than two derivatives leaves only (when $p=q$, there exists also a cosmological-like term,[20] $a_0 = \Lambda \eta_{\mu_1\nu_1} \cdots \eta_{\mu_p\nu_p} \phi^{\mu_1 \cdots \mu_p | \nu_1 \cdots \nu_p}$) the Lagrangian itself. This deformation is of course trivial.

IX. CONCLUSIONS

Assembling the results of the present paper ($p \neq q$) with those previously obtained in Ref. 20 ($p=q \neq 1$), we can state general conclusions for $[p,q]$-tensor gauge fields where p and q are now arbitrary but not both equal to one. Under the hypothesis of locality and translation invariance, there is no smooth deformation of the free theory that modifies the gauge algebra, which remains Abelian. This result strengthens the conclusions of Ref. 18 as no condition on the number of derivative is needed any longer. Furthermore, for $q>1$, when there is no positive integer s such that $p+2=(s+1)(q+1)$, there exists also no smooth deformation that alters the gauge transformations. Finally, if one excludes deformations that involve more than two derivatives in the Lagrangian and are not Lorentz invariant, then the only smooth deformation of the free theory is a cosmological-like term for $p=q$.[20]

These no-go results complete the search for self-interactions of $[p,q]$-tensor gauge fields. It is still an open question whether interactions are possible between N different $[p,q]$-type fields (where "different" means $[p_1,q_1] \neq [p_2,q_2]$ for $N=2$), or with other types of fields.

As a conclusion, one can reformulate the results in more physical terms by saying that no analogue of Yang–Mills nor Einstein theories seems to exist for more exotic fields (at least not in the range of local perturbative theories).

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APPENDIX A: GOING TO THE LIGHT CONE

Theorem A.1: *Let K be a tensor in the irreducible representation $[p+1,q+1]$ of $O(D-1,1)$. The space of such harmonic multiforms K, i.e., solutions of*

$$\left.\begin{aligned} \partial_{[\mu_0} K_{[\mu_1 \cdots \mu_{p+1}]|\nu_1 \cdots \nu_{q+1}} = 0 = K_{\mu_1 \cdots \mu_{p+1}|[\nu_1 \cdots \nu_{q+1}, \nu_0]} \quad \text{(closed)} \\ \partial^{\mu_1} K_{\mu_1 \cdots \mu_{p+1}|\nu_1 \cdots \nu_{q+1}} = 0 = \partial^{\nu_1} K_{\mu_1 \cdots \mu_{p+1}|\nu_1 \cdots \nu_{q+1}} \quad \text{(coclosed)} \end{aligned}\right\} \Rightarrow \Box K = 0$$

is a unitary irreducible module of $O(D-2)$ associated to the Young diagram $[p,q]$.

Proof: Since $\Box K(x)=0$ then, after Fourier transform, $K(p)\neq 0$ iff $p^2=0$. In the light-cone frame, the lightlike momentum p^μ decomposes into

$$p^\mu = (p^+, p^-, \underbrace{0, \cdots, 0}_{D-2}), \quad p^- = 0.$$

(i) The condition that K is closed implies

$$p_\mu \varepsilon^{\mu\nu_1\cdots\nu_{D-p-2}\mu_1\cdots\mu_{p+1}} K_{\mu_1\cdots\mu_{p+1}|\alpha_1\cdots\alpha_{q+1}} = 0,$$

$$p_\mu \varepsilon^{\mu\nu_1\cdots\nu_{D-q-2}\mu_1\cdots\mu_{q+1}} K_{\alpha_1\cdots\alpha_{p+1}|\mu_1\cdots\mu_{q+1}} = 0,$$

i.e.,

$$\varepsilon^{-\nu_1\cdots\nu_{D-p-2}\mu_1\cdots\mu_{p+1}} K_{\mu_1\cdots\mu_{p+1}|\alpha_1\cdots\alpha_{q+1}} = 0,$$

$$\varepsilon^{-\nu_1\cdots\nu_{D-q-2}\mu_1\cdots\mu_{q+1}} K_{\alpha_1\cdots\alpha_{p+1}|\mu_1\cdots\mu_{q+1}} = 0.$$

The italic indices will run over the $D-2$ transverse values. Assigning $\nu_1=+$, $\nu_2=j_2,\ldots,\ \nu_{D-\ell-2}=j_{D-\ell-2}$ (where $\ell=p$ or q, respectively), one finds

$$K_{i_1\cdots i_{p+1}|\alpha_1\cdots\alpha_{q+1}} = 0 = K_{\alpha_1\cdots\alpha_{p+1}|i_1\cdots i_{q+1}}.$$

In other words, K vanishes whenever one of its columns contains only transverse indices.

(ii) The fact that K is coclosed on-shell implies

$$p_{[-} K_{+\mu_2\cdots\mu_{p+1}]|\alpha_1\cdots\alpha_{q+1}} = 0 = K_{\alpha_1\cdots\alpha_{p+1}|[+\mu_2\cdots\mu_{q+1}} p_{-]},$$

i.e.,

$$K_{+\mu_2\cdots\mu_{p+1}|\alpha_1\cdots\alpha_{q+1}} = 0 = K_{\alpha_1\cdots\alpha_{p+1}|+\mu_2\cdots\mu_{q+1}}.$$

In other words, K vanishes whenever one of its columns contains a "+" index.

Once it has been observed that each column of K must contain at least one "−" index and no "+" index, one finds that the tensor

$$\phi_{i_1\cdots i_p|j_1\cdots j_q} \equiv \frac{(p+1)(q+1)}{p_-^2} K_{-i_1\cdots i_p|j_1\cdots j_q-}$$

obeys

$$0 = \frac{p+2}{p_-^2} K_{[-i_1\cdots i_p|j_1]\cdots j_q-} = \phi_{[i_1\cdots i_p|j_1]\cdots j_q},$$

$$0 = \eta^{\mu_1\nu_1} K_{\mu_1\mu_2\cdots\mu_{p+1}|\nu_1\cdots\nu_{q+1}} \Rightarrow 0 = \frac{(p+1)(q+1)}{p_-^2} \delta^{i_1j_1} K_{-i_1i_2\cdots i_p|j_1\cdots j_q-} = \delta^{i_1j_1}\phi_{i_1i_2\cdots i_p|j_1\cdots j_q}.$$

□

APPENDIX B: PROOF OF THEOREM 6.5

In this appendix, we give the proof of Theorem 6.5.

Let r be a strictly positive integer. A complete set of representatives of $H_k^D(\delta|\mathrm{d})$ [$k>1$ and $k=D-r(D-p-1)\geqslant q$] is given by the terms of form-degree D in all homogeneous polynomials

$P^{(r)}(\tilde{H})$ *of degree r in* $\tilde{H}$ [*or equivalently* $P^{(r)}(\tilde{\mathcal{H}})$ *of degree r in* $\tilde{\mathcal{H}}$].

It is obvious from the definition of $\tilde{\mathcal{H}}$ and from Eq. (10) that the term of form-degree D in $P^{(r)}(\tilde{H})$ has the right antighost number and is a cocycle of $H_k^D(\delta|\mathrm{d})$. Furthermore, as $\tilde{\mathcal{H}}=\tilde{H}+d(\cdots)$, $P^{(r)}(\tilde{\mathcal{H}})$ belongs to the same cohomology class as $P^{(r)}(\tilde{H})$ and can as well be chosen as a representative of this class. To prove the theorem, it is then enough, by Theorem 6.4, to prove that the cocycle $P^{(r)}(\tilde{H})|_k^D$ is nontrivial. The proof is by induction: we know the theorem to be true for $r=1$ by Theorem 6.3, supposing that the theorem is true for $r-1$ [i.e., $[P^{(r-1)}(\tilde{H})]_{k+D-p-1}^D$ is not trivial in $H_{k+D-p-1}^D(\delta|\mathrm{d})$] we prove that $[P^{(r)}(\tilde{H})]_k^D$ is not trivial either.

Let us assume that $[P^{(r)}(\tilde{H})]_k^D$ is trivial: $[P^{(r)}(\tilde{H})]_k^D=\delta(u_{k+1}\,\mathrm{d}^Dx)+\mathrm{d}v_k^{D-1}$. We take the Euler–Lagrange derivative of this equation with respect to $C^*_{k,\mu_{[q]}|\nu_{[p+1-k]}}$. For $k>q$, it reads

$$\alpha_{\mu_{[q]}|\nu_{[p+1-k]}}=(-)^k\delta(Z_{1\,\mu_{[q]}|\nu_{[p+1-k]}})-Z_{0\,\mu_{[q]}[\nu_{[p-k]},\nu_{p+1-k}]}, \tag{B1}$$

where

$$\alpha_{\mu_{[q]}|\nu_{[p+1-k]}}\,\mathrm{d}^Dx\equiv\frac{\delta^L[P^{(r)}(\tilde{H})]_k^D}{\delta C_k^{*\,\mu_{[q]}|\nu_{[p+1-k]}}},$$

$$Z_{k+1-j\,\mu_{[q]}|\nu_{[p+1-j]}}\equiv\frac{\delta^L u_{k+1}}{\delta C_j^{*\,\mu_{[q]}|\nu_{[p+1-j]}}}\quad\text{for } j=k,k+1.$$

For $k=q$, there is an additional term,

$$\alpha_{\mu_{[q]}|\nu_{[p+1-q]}}=(-)^q\delta(Z_{1\,\mu_{[q]}|\nu_{[p+1-q]}})-(Z_{0\,\mu_{[q]}[\nu_{[p-q]},\nu_{p+1-q}]}-Z_{0[\,\mu_{[q]}|\nu_{[p-q]},\nu_{p+1-q}]}). \tag{B2}$$

The origin of the additional term lies in the fact that $C_q^{*\mu_{[q]}|\nu_{[p+1-q]}}$ does not possess all the irreducible components of $[q]\otimes[p+1-q]$: the completely antisymmetric component $[p+1]$ is missing. Taking the Euler–Lagrange derivative with respect to this field thus involves projecting out this component.

We will first solve the equation (B1) for $k>q$, then come back to (B2) for $k=q$.

Explicit computation of $\alpha_{\mu_{[q]}|\nu_{[p+1-k]}}$ for $k>q$ yields

$$\alpha_{\mu_{[q]}|\nu_{[p+1-k]}}=[\tilde{H}^{\rho^1_{[q]}}]_{0,\sigma^1_{[D-p-1]}}\cdots[\tilde{H}^{\rho^{r-1}_{[q]}}]_{0,\sigma^{r-1}_{[D-p-1]}}a_{\mu_{[q]}|\rho^1_{[q]}|\cdots|\rho^{r-1}_{[q]}}\delta^{[\sigma^1_{[D-p-1]}\cdots\sigma^{r-1}_{[D-p-1]}]}_{\nu_{[p+1-k]}},$$

where a is a constant tensor and the notation $[A]_{k,\nu_{[p]}}$ means the coefficient $A_{k,\nu_{[p]}}$, with antighost number k, of the p-form component of $A=\Sigma_{k,I}A_{k,\nu_{[I]}}\,\mathrm{d}x^{\nu_1}\cdots\mathrm{d}x^{\nu_I}$. Considering the indices $\nu_{[p+1-k]}$ as form indices, (B1) reads

$$\begin{aligned}\alpha^{p+1-k}_{\mu_{[q]}}&=[\tilde{H}^{\rho^1_{[q]}}]_0^{D-p-1}\cdots[\tilde{H}^{\rho^{r-1}_{[q]}}]_0^{D-p-1}a_{\mu_{[q]}|\rho^1_{[q]}|\cdots|\rho^{r-1}_{[q]}}\\&=\left[\prod_{i=1}^{(r-1)}\tilde{H}^{i\,\rho_{[q]}}\right]_0^{p+1-k}a_{\mu_{[q]}|\rho^1_{[q]}|\cdots|\rho^{r-1}_{[q]}}=(-)^k\delta(Z^{p+1-k}_{1\mu_{[q]}})+(-)^{p-k+1}\,\mathrm{d}Z^{p-k}_{0\mu_{[q]}}.\end{aligned}$$

The latter equation is equivalent to

$$\left[\prod_{i=1}^{(r-1)}\tilde{H}^{i\,\rho_{[q]}}\right]_{D-p-1+k}^{D}a_{\mu_{[q]}|\rho^1_{[q]}|\cdots|\rho^{r-1}_{[q]}}=\delta(\cdots)+\mathrm{d}(\cdots),$$

which contradicts the induction hypothesis. The assumption that $[P^{(r)}(\tilde{H})]_k^D$ is trivial is thus wrong, which proves the theorem for $k>q$.

The philosophy of the resolution of (B2) for $k=q$ is inspired by the proof of Theorem 3.3 in Ref. 20 and goes as follows: first, one must constrain the last term of (B2) in order to get an equation similar to the equation (B1) treated previously, then one solves this equation in the same way as for $k>q$.

Let us constrain the last term of (B2). Equation (B2) and explicit computation of $\alpha_{\mu_{[q]}|\nu_{[p+1-k]}}$ imply

$$\partial_{[\nu_{p+1-q}}\alpha_{\ \mu_{[q]}|\nu_{[p-q]}]\lambda} = (-)^q\delta(\partial_{[\nu_{p+1-q}}Z_{1\ \mu_{[q]}|\nu_{[p-q]}]\lambda}) - b\partial_{[\nu_{p+1-q}}Z_{0\ \mu_{[q]}|\nu_{[p-q]}],\lambda}$$
$$\approx b\partial_\lambda([\tilde{H}^{\rho^1_{[q]}}]_{0,\sigma^1_{[D-p-1]}}\cdots[\tilde{H}^{\rho^{r-1}_{[q]}}]_{0,\sigma^{r-1}_{[D-p-1]}}\delta^{[\sigma^1_{[D-p-1]}\cdots\sigma^{r-1}_{[D-p-1]}]}_{[\nu_{p+1-k}]}a_{[\mu_{[q]}]|\rho^1_{[q]}|\cdots|\rho^{r-1}_{[q]}}),$$

where $b=q/(p+1)(p+1-q)$. By the isomorphism $H_0^0(\mathrm{d}|\delta)/\mathbb{R}\cong H_D^D(\delta|\mathrm{d})\cong 0$, the latter equation implies

$$Z_{0[\mu_{[q]}|\nu_{[p-q]},\nu_{p+1-q}]} \approx -[\tilde{H}^{\rho^1_{[q]}}]_{0,\sigma^1_{[D-p-1]}}\cdots[\tilde{H}^{\rho^{r-1}_{[q]}}]_{0,\sigma^{r-1}_{[D-p-1]}}a_{\mu_{[q]}|\rho^1_{[q]}|\cdots|\rho^{r-1}_{[q]}}\delta^{[\sigma^1_{[D-p-1]}\cdots\sigma^{r-1}_{[D-p-1]}]}_{\nu_{[p+1-k]}}$$

(the constant solutions are removed by considering the equation in polynomial degree $r-1$ in the fields and antifields). Inserting this expression for $Z_{0[\mu_{[q]}|\nu_{[p-q]},\nu_{p+1-q}]}$ into (B2) and redefining Z_1 in a suitable way yields (B1) for $k=q$. The remaining proof is then the same as for $k>q$. □

APPENDIX C: PROOF OF THEOREM 7.2

In this appendix, we give the complete (and lengthy) proof of Theorem 7.2.

Let a_k^D be an invariant polynomial. If $a_k^D=\delta b_{k+1}^D+\mathrm{d}c_k^{D-1}$, then

$$a_k^D = P_{(s,r)}(K^{q+1},\tilde{\mathcal{H}})|_k^D + \delta\mu_{k+1}^D + \mathrm{d}\nu_k^{D-1},$$

where $P_{(s,r)}(K^{q+1},\tilde{\mathcal{H}})$ is a polynomial of degree s in K^{q+1} and r in $\tilde{\mathcal{H}}$, such that the integers $s,r\geqslant 1$ satisfy $D=r(D-p-1)+k+s(q+1)$ and μ_{k+1}^D and ν_k^{D-1} are invariant polynomials.

The proof is by induction and follows closely the steps of the proof of similar theorems in the case of 1-forms,[26,27] p-forms,[24] gravity[17] or $[p,p]$-fields.[20]

There is a general procedure to prove that Theorem 7.2 holds for $k>D$, that can be found, e.g., in Ref. 17 and will not be repeated here. We assume that the theorem has been proved for any $k'>k$, and show that it is still valid for k.

The proof of the induction step is rather lengthy and is decomposed into several steps.

(i) The Euler–Lagrange derivatives of a_k with respect to the fields ϕ and C_j^* $(1\leqslant j\leqslant p+1)$ are computed in terms of the Euler–Lagrange derivatives of b_{k+1} (Appendix C 1).
(ii) It is shown that the Euler–Lagrange derivatives of b_{k+1} can be replaced by invariant quantities in the expression for the Euler–Lagrange derivative of a_k with the lowest antighost number, up to some additional terms (Appendix C 2).
(iii) The preceding step is extended to all the Euler–Lagrange derivatives of a_k (Appendix C 3).
(iv) The Euler–Lagrange derivative of a_k with respect to the field ϕ is re-expressed in terms of invariant quantities (Appendix C 4).
(v) A homotopy formula is used to reconstruct a_k from its Euler–Lagrange derivatives (Appendix C 5).

1. Euler–Lagrange derivatives of a_k

We define

$$Z_{k+1-j\,\mu_{[q]}|\nu_{[p+1-j]}} = \frac{\delta^L b_{k+1}}{\delta C_j^{*\,\mu_{[q]}|\nu_{[p+1-j]}}},\quad 1\leqslant j\leqslant p+1,$$

$$Y_{k+1}^{\mu_{[p]}|\nu_{[q]}} = \frac{\delta^L b_{k+1}}{\delta \phi_{\mu_{[p]}|\nu_{[q]}}}.$$

Then, the Euler–Lagrange derivatives of a_k are given by

$$\frac{\delta^L a_k}{\delta C^{*\mu_{[q]}}_{p+1}} = (-)^{p+1} \delta Z_{k-p\mu_{[q]}}, \tag{C1}$$

$$\frac{\delta^L a_k}{\delta C^{*}_{j\,\mu_{[q]}|\nu_{[p+1-j]}}} = (-)^j \delta Z_{k+1-j\,\mu_{[q]}|\nu_{[p+1-j]}} - Z_{k-j\,\mu_{[q]}[\nu_{[p-j]},\nu_{p+1-j]}}, \quad q < j \leqslant p,$$

$$\frac{\delta^L a_k}{\delta C^{*}_{j\,\mu_{[q]}|\nu_{[p+1-j]}}} = (-)^j \delta Z_{k+1-j\,\mu_{[q]}|\nu_{[p+1-j]}} - Z_{k-j\,\mu_{[q]}[\nu_{[p-j]},\nu_{p+1-j]}}\big|_{\text{sym of } C^*_j}, \quad 1 \leqslant j \leqslant q,$$

$$\frac{\delta^L a_k}{\delta \phi^{\mu_{[p]}|\nu_{[q]}}} = \delta Y_{k+1\,\mu_{[p]}|\nu_{[q]}} + \beta D_{\mu_{[p]}|\nu_{[q]}|\rho_{[p]}|\sigma_{[q]}} Z_k^{\sigma_{[q]}|\rho_{[p]}}, \tag{C2}$$

where

$$\beta \equiv (-)^{(q+1)[p+(q/2)]} \frac{(p+1)!}{q!(p-q+1)!}$$

and

$$D^{\nu_{[q]}|}{}_{\rho_{[p]}|\mu_{[p]}|}{}^{\sigma_{[q]}} \equiv \frac{1}{(p+1)!q!} \delta^{[\sigma_{[q]}\alpha\mu_{[p]}]}_{[\nu_{[q]}\beta\rho_{[p]}]} \partial_\alpha \partial^\beta$$

is the second-order self-adjoint differential operator defined by $G_{\mu_{[p]}|\nu_{[q]}} \equiv D_{\mu_{[p]}|\nu_{[q]}|\rho_{[p]}|\sigma_{[q]}} \times C^{\rho_{[p]}|\sigma_{[q]}}$.

As in Appendix B, the projection on the symmetry of the indices of C_j^* is needed when $j \leqslant q$, since in that case the variables C_j^* do not possess all the irreducible components of $[q] \otimes [p+1-j]$, but only those where the length of the first column is smaller or equal to p. When $j > q$, the projection is trivial.

2. Replacing *Z* by an invariant in the Euler–Lagrange derivative of a_k with the lowest antighost number

We should first note that, when $k < p+1$, some of the Euler–Lagrange derivatives of a_k vanish identically: indeed, as there is no negative antighost-number field, a_k cannot depend on C_j^* if $j > k$. Some terms on the right-hand side of (C1) and (C2) also vanish, Z_{k+1-j} vanishes when $j > k+1$. This implies that the $p+1-k$ top equations of (C1) and (C2) are trivially satisfied, the $p-k$ first equations involve only vanishing terms, and the $(p-k+1)$th involves in addition the δ of an antighost-zero term, which also vanishes trivially. The first nontrivial equation is then

$$\frac{\delta^L a_k}{\delta C^{*}_{k\mu_{[q]}|\nu_{[p+1-k]}}} = (-)^k \delta(Z_{1\mu_{[q]}|\nu_{[p+1-k]}}) - Z_{0\mu_{[q]}[\nu_{[p-k]},\nu_{p+1-k]}}\big|_{\text{sym of } C^*_k}. \tag{C3}$$

Let us now define $[T^q_{\rho_{[p+1]}}]_{\nu_{[q]}} \equiv (-)^q \partial_{[\rho_1} \phi_{\rho_2 \cdots \rho_{p+1}]|\nu_{[q]}}$. We will prove the following lemma for $k \geqslant q$.

Lemma C.1: In the first nontrivial equation of the system (C1) to (C2) [i.e., (C1) when $k \geqslant p+1$ *and (C3) when* $p+1 > k \geqslant q$*], respectively,* Z_{k-p} *or* Z_1 *satisfies*

$$Z_{l\mu_{[q]}|\nu_{[p+l-k]}} = Z'_{l\mu_{[q]}|\nu_{[p+l-k]}} + (-)^{k-l}\delta\beta_{l+1\mu_{[q]}|\nu_{[p+l-k]}} + \beta_{l\mu_{[q]}|[\nu_{[p+l-k-1]},\nu_{p+l-k}]}\Big|_{\text{sym of } C^*_{k-l+1}}$$
$$+ A_l\left[P^{(n)}_{\mu_{[q]}}(\tilde{\mathcal{H}}) + \frac{1}{s}T^q_{\rho_{[p+1]}}\frac{\partial^L R^{(s,r)}_{\mu_{[q]}}(K^{q+1},\tilde{\mathcal{H}})}{\partial K^{q+1}_{\rho_{[p+1]}}}\right]_{l,\nu_{[p+l-k]}}\Bigg|_{\text{sym of } C^*_{k-l+1}}, \tag{C4}$$

where Z'_l is invariant, the β_l's are at least linear in $\mathcal{N}$ and possess the same symmetry of indices as Z_{l-1}, $A_l \equiv (-)^{lp+p+1+[l(l+1)/2]}$, $P^{(n)}$ is a polynomial of degree n in $\tilde{\mathcal{H}}$ and $R^{(s,r)}$ is a polynomial of degree s in K^{q+1} and r in $\tilde{\mathcal{H}}$. The polynomials are present only when $p-k=n(D-p-1)$ or $p+1-k=s(q+1)+r(D-p-1)$, respectively.

Moreover, when $p+1>k\geqslant q$, the first nontrivial equation can be written

$$\frac{\delta^L a_k}{\delta C^*_{k\mu_{[q]}|\nu_{[p+1-k]}}} = (-)^k\delta Z'_{1\mu_{[q]}|\nu_{[p+1-k]}} - Z'_{0\mu_{[q]}|[\nu_{[p-k]},\nu_{p+1-k}]}\Big|_{\text{sym of } C^*_k}$$
$$+ \left([Q^{(m)}_{\mu_{[q]}}(K^{q+1})]_{\nu_{[p+1-k]}} + (-)^k[R^{(s,r)}_{\mu_{[q]}}(K^{q+1},\tilde{\mathcal{H}})]_{0,\nu_{[p+1-k]}}\right)\Big|_{\text{sym of } C^*_k},$$

where Z'_0 is an invariant and $Q^{(m)}_{\mu_{[q]}}(K^{q+1})$ is a polynomial of degree m in K^{q+1}, present only when $p+1-k=m(q+1)$.

The lemma will be proved in this Appendix Secs. C 2 a–C 2 c, respectively, for the cases $k\geqslant p+1$, $q<k<p+1$, and $k=q$.

a. Proof of Lemma C.1 for k⩾p+1

As $k-p>0$, there is no trivially satisfied equation and we start with the top equation of (C1) to (C2).

The Lemma C.1 is a direct consequence of the well-known Lemma C.2 (see, e.g., Ref. 17).

Lemma C.2: Let α be an invariant local form that is δ-exact, i.e., $\alpha=\delta\beta$. Then $\beta=\beta'+\delta\sigma$, where β' is invariant and we can assume without loss of generality that σ is at least linear in the variables of $\mathcal{N}$.

b. Proof of Lemma C.1 for q<k<p+1

The first nontrivial equation is (as $k>q$)

$$\frac{\delta^L a_k}{\delta C^*_{k\mu_{[q]}|\nu_{[p+1-k]}}} = (-)^k\delta(Z_{1\mu_{[q]}|\nu_{[p+1-k]}}) - Z_{0\mu_{[q]}|[\nu_{[p-k]},\nu_{p+1-k}]}. \tag{C5}$$

We will first prove that Z_1 has the required form, then we will prove the first nontrivial equation can indeed be re-expressed as stated in Lemma C.1.

First part: Defining

$$\alpha_{0\mu_{[q]}|\nu_{[p+1-k]}} \equiv \frac{\delta^L a_q}{\delta C^*_{q\mu_{[q]}|\nu_{[p+1-q]}}},$$

the above equation can be written as

$$\alpha_0^{p+1-k} = (-)^k\delta(Z_1^{p+1-k}) + (-)^{p+1-k}\,\mathrm{d}Z_0^{p-k}, \tag{C6}$$

where we consider the indices $\nu_{[p+1-k]}$ as form indices and omit to write the indices $\mu_{[q]}$. Acting with d on this equation yields $\mathrm{d}\alpha_0^{p+1-k}=(-)^{k+1}\delta(\mathrm{d}Z_1^{p+1-k})$. Due to Lemma C.2, this implies that

$$\alpha_1^{p+2-k} = \mathrm{d}Z_1^{p+1-k} + \delta Z_2^{p+2-k}, \tag{C7}$$

for some invariant α_1^{p+2-k} and some Z_2^{p+2-k}. These steps can be reproduced to build a descent of equations ending with

$$\alpha^D_{D-p-1+k} = \mathrm{d}Z^{D-1}_{D-p-1+k} + \delta Z^D_{D-p+k},$$

where $\alpha^D_{D-p-1+k}$ is invariant. As $D-p-1+k>k$, the induction hypothesis can be used and implies

$$\alpha^D_{D-p-1+k} = \mathrm{d}Z'^{D-1}_{D-p-1+k} + \delta Z'^D_{D-p+k} + [R(K^{q+1},\tilde{\mathcal{H}})]^D_{D-p-1+k},$$

where Z'^D_{D-p+k} and $Z'^{D-1}_{D-p-1+k}$ are invariant, and $R(K^{q+1},\tilde{\mathcal{H}})$ is a polynomial of order s in K^{q+1} and r in $\tilde{\mathcal{H}}$ (with $r,s>0$), present when $p+1-k=s(q+1)+r(D-p-1)$. This equation can be lifted and implies that

$$\alpha_1^{p+2-k} = \mathrm{d}Z_1'^{p+1-k} + \delta Z_2'^{p+2-k} + [R(K^{q+1},\tilde{\mathcal{H}})]_1^{p+2-k},$$

for some invariant quantities $Z_1'^{p+1-k}$ and $Z_2'^{p+2-k}$. Substracting the last equation from (C7) yields

$$\mathrm{d}\left(Z_1^{p+1-k} - Z_1'^{p+1-k} - \frac{1}{s}T^q\left[\frac{\partial^L R(K^{q+1},\tilde{\mathcal{H}})}{\partial K^{q+1}}\right]_1^{p+1-k-q}\right) + \delta(\cdots) = 0.$$

As $H_1^{p+1-k}(\mathrm{d}|\delta) \cong H^D_{D-(p-k)}(\delta|\mathrm{d})$, by Theorem 6.5 the solution of this equation is

$$Z_1^{p+1-k} = Z_1'^{p+1-k} + \frac{1}{s}T^q\left[\frac{\partial^L R(K^{q+1},\tilde{\mathcal{H}})}{\partial K^{q+1}}\right]_1^{p+1-k-q} + \mathrm{d}\beta_1^{p-k} + \delta\beta_2^{p+1-k} + [P^{(n)}(\tilde{\mathcal{H}})]_1^{p+1-k},$$

where the last term is present only when $p-k=n(D-p-1)$.

This proves the first part of the induction basis, regarding Z_1.

Second part: We insert the above result for Z_1 into (C6). Knowing that $\delta([P(\tilde{\mathcal{H}})]_1^{p+1-k}) + \mathrm{d}([P(\tilde{\mathcal{H}})]_0^{p-k}) = 0$ and defining

$$W_0^{p-k} = (-)^{k+1}\left((-)^p Z_0^{p-k} + \delta\beta_1^{p-k} + [P^{(n)}(\tilde{\mathcal{H}})]_0^{p-k} + \frac{1}{s}T^q\left[\frac{\partial^L R(K^{q+1},\tilde{\mathcal{H}})}{\partial K^{q+1}}\right]_0^{p-k-q}\right),$$

we get

$$\alpha_0^{p+1-k} = (-)^k\delta(Z_1'^{p+1-k}) + \mathrm{d}(W_0^{p-k}) + (-)^k[R(K^{q+1},\tilde{\mathcal{H}})]_0^{p-k}.$$

Thus $\mathrm{d}(W_0^{p-k})$ is an invariant and the invariant Poincaré Lemma 5.1 then states that

$$\mathrm{d}(W_0^{p-k}) = \mathrm{d}(Z_0'^{p-k}) + Q(K^{q+1})$$

for some invariant $Z_0'^{p-k}$ and some polynomial in K^{q+1}, $Q(K^{q+1})$. This straightforwardly implies

$$\alpha_0^{p+1-k} = (-)^k\delta(Z_1'^{p+1-k}) + \mathrm{d}(Z_0'^{p-k}) + Q(K^{q+1}) + (-)^k[R(K^{q+1},\tilde{\mathcal{H}})]_0^{p-k},$$

which completes the proof of Lemma C.1 for $q<k<p+1$. □

c. Proof of Lemma C.1 for k=q

The first nontrivial equation is

$$\frac{\delta^L a_q}{\delta C^*_{q\mu_{[q]}|\nu_{[p+1-q]}}} = (-)^q \delta(Z_{1\mu_{[q]}|\nu_{[p+1-q]}}) - (Z_{0\mu_{[q]}[\nu_{[p-q]},\nu_{p+1-q}]} - Z_{0[\,\mu_{[q]}|\nu_{[p-q]},\nu_{p+1-q}]}). \tag{C8}$$

This equation is different from the equations treated in the previous cases because the operator acting on Z_0 cannot be seen as a total derivative, since it involves the projection on a specific Young diagram. The latter problem was already faced in the $[p,p]$ case and the philosophy of the resolution goes as follows:[20]

(1) one first constrains the last term of (C8) to get an equation similar to Eq. (C3) treated previously,
(2) one solves it in the same way as for $q<k<p+1$.

We need the useful Lemma C.3, proved in Ref. 20.

Lemma C.3: If α_0^1 is an invariant polynomial of antighost number 0 and form degree 1 that satisfies $\alpha_0^1=\delta Z_1^1+\mathrm{d}W_0^0$, then, for some invariant polynomials $Z_1'^1$ and $W_0'^0$, $Z_1^1=Z_1'^1+\delta\phi_2^1+\mathrm{d}\chi_1^0$ and $W_0^0=W_0'^0+\delta\chi_1^0$

As explained above, we now constrain the last term of (C8). Equation (C8) implies

$$\partial_{[\rho}\,\alpha_{0\mu_{[q]}|\,\nu_{[p-q]}]\nu_{p+1-q}} = (-)^q\delta(\partial_{[\rho}\,Z_{1\mu_{[q]}|\,\nu_{[p-q]}]\nu_{p+1-q}}) - b\partial_{[\rho}\,Z_{0\mu_{[q]}|\,\nu_{[p-q]}],\nu_{p+1-q}},$$

where $b\equiv q/(p+1)(p+1-q)$. Defining

$$\tilde{\alpha}^1_{0[\rho\mu_{[q]}\nu_{[p-q]}]} = \partial_{[\rho}\,\alpha_{0\mu_{[q]}|\,\nu_{[p-q]}]\nu_{p+1-q}}\,\mathrm{d}x^{\nu_{p+1-q}},$$

$$\tilde{Z}^1_{1[\rho\mu_{[q]}\nu_{[p-q]}]} = (-)^q\partial_{[\rho}\,Z_{1\mu_{[q]}|\,\nu_{[p-q]}]\nu_{p+1-q}}\mathrm{d}x^{\nu_{p+1-q}},$$

$$\tilde{W}^0_{0[\rho\mu_{[q]}\nu_{[p-q]}]} = -\,a\partial_{[\rho}Z_{0\mu_{[q]}|\,\nu_{[p-q]}]},$$

and omitting to write the indices $[\rho\mu_{[q]}\nu_{[p-q]}]$, the above equation reads $\tilde{\alpha}_0^1=\delta\tilde{Z}_1^1+\mathrm{d}\tilde{W}_0^0$. Lemma C.3 then implies that $\tilde{W}_0^0=I_0'^0+\delta m_1^0$ for some invariant $I_0'^0$. By the definition of $\tilde{W}_0^0$, this statement is equivalent to

$$\partial_{[\rho}\,Z_{0\mu_{[q]}|\,\nu_{[p-q]}]} = I'_{0[\mu_{[q]}\nu_{[p-q]}\rho]} + \delta m_{1[\mu_{[q]}\nu_{[p-q]}\rho]}.$$

Inserting this result into (C8) yields

$$\alpha_{0\mu_{[q]}|\nu_{[p+1-q]}} - I'_{0[\mu_{[q]}\nu_{[p+1-q]}]} = \delta((-)^q Z_{1\mu_{[q]}|\nu_{[p+1-q]}} + m_{1[\mu_{[q]}\nu_{[p+1-q]}]}) - Z_{0\mu_{[q]}[\nu_{[p-q]},\nu_{p+1-q}]}.$$

This equation has the same form as (C5) and can be solved in the same way to get the following result:

$$Z_{1\mu_{[q]}|\nu_{[p+1-q]}} = (-)^{q+1}m_{1[\mu_{[q]}\nu_{[p+1-q]}]} + Z'_{1\mu_{[q]}|\nu_{[p+1-q]}} + \beta_{1\mu_{[q]}[\nu_{[p-q]},\nu_{p+1-q}]} + \delta\beta_{2\mu_{[q]}|\nu_{[p+1-q]}}$$
$$+\frac{1}{s}\left[T^q_{\rho_{[p+1]}}\frac{\partial^L R_{\mu_{[q]}}(K^{q+1},\tilde{\mathcal{H}})}{\partial K^{q+1}_{\rho_{[p+1]}}}\right]_{1,\nu_{[p+1-q]}} + [P(\tilde{\mathcal{H}})]_{1,\nu_{[p+1-k]}},$$

$$\alpha_{0\mu_{[q]}|\nu_{[p+1-q]}} = I'_{0[\,\mu_{[q]}|\nu_{[p+1-q]}]} + (-)^q\delta(Z'_{1\mu_{[q]}|\nu_{[p+1-q]}}) + Z'_{0\mu_{[q]}[\nu_{[p-q]},\nu_{p+1-q}]} + [Q_{\mu_{[q]}}(K^{q+1})]_{\nu_{[p+1-q]}}$$
$$+(-)^k[R(K^{q+1},\tilde{\mathcal{H}})]_{0,\nu_{[p+1-q]}}.$$

Removing the completely antisymmetric parts of these equations yields the desired result. □

This ends the proof of Lemma C.1 for $k \geqslant q$.

3. Replacing all *Z* and *Y* by invariants

We will now prove the following lemma.

Lemma C.4: The Euler–Lagrange derivatives of a_k can be written

$$\frac{\delta^L a_k}{\delta C^{*\mu_{[q]}}_{p+1}} = (-)^{p+1}\delta(Z'_{k-p\mu_{[q]}}),$$

$$\frac{\delta^L a_k}{\delta C_j^{*\mu_{[q]}|\nu_{[p+1-j]}}} = (-)^j \delta(Z'_{k+1-j\mu_{[q]}|\nu_{[p+1-j]}}) - Z'_{k-j\mu_{[q]}|[\nu_{[p-j]},\nu_{p+1-j}]}, \quad q < j \leqslant p,$$

$$\frac{\delta^L a_k}{\delta C_j^{*\mu_{[q]}|\nu_{[p+1-j]}}} = (-)^j \delta(Z'_{k+1-j\mu_{[q]}|\nu_{[p+1-j]}}) - Z'_{k-j\mu_{[q]}|[\nu_{[p-j]},\nu_{p+1-j}]}\big|_{\text{sym of } C_j^*}, \quad 1 \leqslant j \leqslant q,$$

$$\frac{\delta^L a_k}{\delta \phi^{\mu_{[q]}|\nu_{[q]}}} = \delta(Y'_{k+1\,\mu_{[q]}|\nu_{[q]}}) + \beta D_{\mu_{[q]}|\nu_{[q]}|\rho_{[p]}|\sigma_{[q]}} Z'^{\,\sigma_{[q]}|\rho_{[p]}}_{k},$$

where Z'_l $(k-p \leqslant l \leqslant k)$ and Y'_{k+1} are invariant polynomials, except in the following cases. When $k=p+1-m(q+1)$ for some strictly positive integer m, there is an additional term in the first nontrivial equation,

$$\frac{\delta^L a_k}{\delta C_k^{*\mu_{[q]}|\nu_{[p+1-k]}}} = (-)^k \delta Z'_{1\mu_{[q]}|\nu_{[p+1-k]}} - Z'_{0\mu_{[q]}|[\nu_{[p-k]},\nu_{p+1-k}]} + [Q_{\mu_{[q]}}(K^{q+1})]_{\nu_{[p+1-k]}}\big|_{\text{sym of } C_k^*},$$

where Q is a polynomial of degree m in K^{q+1}. Furthermore, when $k=p+1-r(D-p-1)-s(q+1)$ for a couple of integer $r,s>0$, then there is an additional term in each Euler–Lagrange derivative,

$$\frac{\delta^L a_k}{\delta C_j^{*\mu_{[q]}|\nu_{[p+1-j]}}} = (-)^j \delta(Z'_{k+1-j\mu_{[q]}|\nu_{[p+1-j]}}) - Z'_{k-j\mu_{[q]}|[\nu_{[p-j]},\nu_{p+1-j}]}\big|_{\text{sym of } C_j^*} + (-)^{k+p+1} A_{k-j}\,[R_{\mu_{[q]}}(K^{q+1},\tilde{\mathcal{H}})]_{k-j\nu_{[p+1-j]}}\big|_{\text{sym of } C_j^*},$$

$$\frac{\delta^L a_k}{\delta \phi^{\mu_{[q]}|\nu_{[q]}}} = \delta(Y'_{k+1\mu_{[q]}|\nu_{[q]}}) + \beta D_{\mu_{[q]}|\nu_{[q]}|\rho_{[p]}|\sigma_{[q]}} Z'^{\,\sigma_{[q]}|\rho_{[p]}}_{k} + A\delta^{[\sigma_{[q]}\alpha\mu_{[p]}\xi]}_{[\nu_{[q]}\beta\rho_{[p+1]}]}\partial_\alpha\partial^\beta(x_\xi[R_{\sigma_{[q]}}(K^{q+1},\tilde{\mathcal{H}})]^{\rho_{[p+1]}}_k),$$

where

$$A = \beta\frac{p+q+2}{(D-p-q-1)(p+1)!q!}A_k(-)^{p+k+1}.$$

Proof: By Lemma C.1, we know that the Z's involved in the first nontrivial equation satisfy (C4) and that this equation has the required form. We will proceed by induction and prove that when Z_{k-j} (where $k-j \geqslant 1$) satisfies (C4), then the equation for $\delta^L a_k/\delta C_j^*$ also has the desired form and Z_{k-j+1} also satisfies (C4).

Let us assume that Z_{k-j} satisfies (C4) and consider the following equation:

$$\frac{\delta^L a_k}{\delta C^*_{j\mu_{[q]}|\nu_{[p+1-j]}}} = (-)^j \delta(Z^{\mu_{[q]}|\nu_{[p+1-j]}}_{k+1-j}) - \left. Z^{\mu_{[q]}|[\nu_{[p-j]},\nu_{p+1-j}]}_{k-j}\right|_{\text{sym of } C^*_j}. \tag{C9}$$

Inserting (C4) for Z_{k-j} into this equation yields

$$\begin{aligned}\frac{\delta^L a_k}{\delta C^*_{j\mu_{[q]}|\nu_{[p+1-j]}}} &= (-)^j \delta(Z^{\mu_{[q]}|\nu_{[p+1-j]}}_{k+1-j} - \left.\beta^{\mu_{[q]}|[\nu_{[p-j]},\nu_{p-j+1}]}_{k-j+1}\right|_{\text{sym of } C^*_j}) \\ &\quad + (-)^{k+p} a_{k-j}\delta\left[P^{\mu_{[q]}}(\tilde{\mathcal{H}}) + \frac{1}{s} T^q_{\rho_{[p+1]}} \frac{\partial^L R^{\mu_{[q]}}(K^{q+1},\tilde{\mathcal{H}})}{\partial K^{q+1}_{\rho_{[p+1]}}}\right]^{\nu_{[p+1-j]}}_{k-j+1 \ \text{sym of } C^*_j} \\ &\quad + \left(-Z'^{\mu_{[q]}|[\nu_{[p-j]},\nu_{p+1-j}]}_{k-j} + (-)^{p+k+1} A_{k-j}[R^{\mu_{[q]}}(K^{q+1},\tilde{\mathcal{H}})]^{\nu_{[p+1-j]}}_{k-j}\right)\Big|_{\text{sym of } C^*_j}. \end{aligned} \tag{C10}$$

Note that one can omit to project on the symmetries of C^*_{j+1} when inserting (C4) into (C9). Indeed the Young components that are removed by this projection would be removed later anyway by the projection on the symmetries of C^*_j.

Defining the invariant

$$\begin{aligned} Z'^{\mu_{[q]}|\nu_{[p+1-j]}}_{k+1-j} &\equiv \left. Z^{\mu_{[q]}|\nu_{[p+1-j]}}_{k+1-j}\right|_{\mathcal{N}=0} + (-)^{k+p+j} A_{k-j} \\ &\quad \times \left[P^{\mu_{[q]}}(\tilde{\mathcal{H}}) + \frac{1}{s} T^q_{\rho_{[p+1]}} \frac{\partial^L R^{\mu_{[q]}}(K^{q+1},\tilde{\mathcal{H}})}{\partial K^{q+1}_{\rho_{[p+1]}}}\right]^{\nu_{[p+1-j]}}_{k-j+1} \Bigg|_{\text{sym of } C^*_j} \Bigg|_{\mathcal{N}=0} \end{aligned}$$

and setting $\mathcal{N}=0$ in the last equation yields, as β_{k-j+1} is at least linear in $\mathcal{N}$,

$$\begin{aligned}\frac{\delta^L a_k}{\delta C^*_{j\mu_{[q]}|\nu_{[p+1-j]}}} &= (-)^j \delta(Z'^{\mu_{[q]}|\nu_{[p+1-j]}}_{k+1-j}) - \left. Z'^{\mu_{[q]}|[\nu_{[p-j]},\nu_{p+1-j}]}_{k-j}\right|_{\text{sym of } C^*_j} \\ &\quad + (-)^{p+k+1} A_{k-j} \left. [R^{\mu_{[q]}}(K^{q+1},\tilde{\mathcal{H}})]^{\nu_{[p+1-j]}}_{k-j}\right|_{\text{sym of } C^*_j}. \end{aligned} \tag{C11}$$

This proves the part of the induction regarding the equations for the Euler–Lagrange derivatives. We now prove that Z_{k-j+1} verifies (C4).

Substracting (C11) from (C10), we get

$$\begin{aligned} 0 &= (-)^j \delta\Bigg(\left. Z^{\mu_{[q]}|\nu_{[p+1-j]}}_{k+1-j} - Z'^{\mu_{[q]}|\nu_{[p+1-j]}}_{k+1-j} - \beta^{\mu_{[q]}|[\nu_{[p-j]},\nu_{p+1-j}]}_{k+1-j}\right|_{\text{sym of } C^*_j} \\ &\quad + (-)^{j+k+p} A_{k-j}\left[P^{\mu_{[q]}}(\tilde{\mathcal{H}}) + \frac{1}{s} T^q_{\rho_{[p+1]}} \frac{\partial^L R^{\mu_{[q]}}(K^{q+1},\tilde{\mathcal{H}})}{\partial K^{q+1}_{\rho_{[p+1]}}}\right]^{\nu_{[p+1-j]}}_{k+1-j} \Bigg|_{\text{sym of } C^*_j} \Bigg). \end{aligned}$$

As $k+1-j>0$, this implies

$$\begin{aligned} Z^{\mu_{[q]}|\nu_{[p+1-j]}}_{k+1-j} &= Z'^{\mu_{[q]}|\nu_{[p+1-j]}}_{k+1-j} + (-)^{j-1}\delta\beta^{\mu_{[q]}|\nu_{[p+1-j]}}_{k-j} + \left.\beta^{\mu_{[q]}|[\nu_{[p-j]},\nu_{p+1-j}]}_{k-j+1}\right|_{\text{sym of } C^*_j} \\ &\quad + A_{k+1-j}\left[P^{\mu_{[q]}}(\tilde{\mathcal{H}}) + \frac{1}{s} T^q_{\rho_{[p+1]}} \frac{\partial^L R^{\mu_{[q]}}(K^{q+1},\tilde{\mathcal{H}})}{\partial K^{q+1}_{\rho_{[p+1]}}}\right]^{\nu_{[p+1-j]}}_{k+1-j} \Bigg|_{\text{sym of } C^*_j}, \end{aligned}$$

which is the expression (C4) for Z_{k+1-j}.

Assuming that Z_{k-j} satisfies (C4), we have thus proved that the equation for $\delta^L a_k/\delta C_j^*$ has the desired form and that Z_{k+1-j} also satisfies (C4). Iterating this step, one shows that all Z's satisfy (C4) and that the equations involving only Z's have the desired form.

It remains to be proved that the Euler–Lagrange derivative with respect to the field takes the right form. Inserting the expression (C4) for Z_k into (C2) and some algebra yield

$$\frac{\delta^L a_k}{\delta\phi^{\mu_{[q]}|\nu_{[q]}}} = \delta(\tilde{Y}_{k+1\mu_{[q]}|\nu_{[q]}}|_{\text{sym of }\phi}) + \beta D_{\mu_{[q]}|\nu_{[q]}|\rho_{[p]}|\sigma_{[q]}} Z'^{\sigma_{[q]}|\rho_{[p]}}_{k} + A\delta^{[\sigma_{[q]}\alpha\mu_{[p]}\xi]}_{[\nu_{[q]}\beta\rho_{[p+1]}]}\partial_\alpha\partial^\beta\,(x_\xi[R_{\sigma_{[q]}}(K^{q+1},\tilde{\mathcal{H}})]^{\rho_{[p+1]}}_k)|_{\text{sym of }\phi},$$

where

$$\tilde{Y}_{k+1\mu_{[q]}|\nu_{[q]}} \equiv Y_{k+1\mu_{[q]}|\nu_{[q]}} + \beta D_{\mu_{[q]}|\nu_{[q]}|\rho_{[p]}|\sigma_{[q]}}\beta^{\sigma_{[q]}|\rho_{[p]}}_{k+1} + c\delta^{[\sigma_{[q]}\alpha\mu_{[p]}]}_{[\nu_{[q]}\beta\rho_{[p]}]}\partial_\alpha\left[P_{\sigma_{[q]}}(\tilde{\mathcal{H}}) + \frac{1}{s}T^q_{\lambda_{[p+1]}}\frac{\partial^L R^{\sigma_{[q]}}(K^{q+1},\tilde{\mathcal{H}})}{\partial K^{q+1}_{\lambda_{[p+1]}}}\right]^{[\rho_{[p]}\beta]}_{k+1} + (-)^{k+q+1}A\delta^{[\sigma_{[q]}\alpha\mu_{[p]}\xi]}_{[\nu_{[q]}\beta\rho_{[p+1]}]}\partial_\alpha(x_\xi[R_{\sigma_{[q]}}(K^{q+1},\tilde{\mathcal{H}})]^{[\rho_{[p+1]}\beta]}_{k+1})$$

and $c\equiv\beta[1/(p+1)!q!]A_k(-)^{p+k+1}$. Defining $Y'_{k+1\mu_{[p]}|\nu_{[q]}}\equiv \tilde{Y}_{k+1\mu_{[q]}|\nu_{[q]}}|_{\text{sym of }\phi}|_{\mathcal{N}=0}$ and setting $\mathcal{N}=0$ in the above equation completes the proof of Lemma C.4. □

4. Euler–Lagrange derivative with respect to the field

In this section, we manipulate the Euler–Lagrange derivative of a_k with respect to the field ϕ. We have proved in the preceding section that it can be written in the form

$$\frac{\delta^L a_k}{\delta\phi^{\mu_{[p]}|\nu_{[q]}}} = \delta(Y'_{k+1\mu_{[p]}|\nu_{[q]}}) + \beta D_{\mu_{[p]}|\nu_{[q]}|\rho_{[p]}|\sigma_{[q]}} Z'^{\sigma_{[q]}|\rho_{[p]}}_{k} + A\delta^{[\sigma_{[q]}\alpha\mu_{[p]}\xi]}_{[\nu_{[q]}\beta\rho_{[p+1]}]}\partial_\alpha\partial^\beta\,(x_\xi[R_{\sigma_{[q]}}(K^{q+1},\tilde{\mathcal{H}})]^{\rho_{[p+1]}}_k)|_{\text{sym of }\phi}.$$

As a_k is invariant, it can depend on $\phi_{\mu_{[p]}|\nu_{[q]}}$ only through $K_{\mu_{[p]}\alpha|\nu_{[q]}\beta}$, which implies that $\delta^L a_k/\delta\phi^{\mu_{[p]}|\nu_{[q]}} = \partial^{\alpha\beta}X_{[\mu_{[p]}\alpha][\nu_{[q]}\beta]}$, where X has the symmetry of the curvature. This in turn implies that $\delta(Y'_{k+1\mu_{[p]}|\nu_{[q]}}) = \partial^{\alpha\beta}W_{\mu_{[p]}\alpha|\nu_{[q]}\beta}$ for some W with the Young symmetry $[p+1,q+1]$. Let us consider the indices $\mu_{[p]}$ as form indices. As $H^{D-p}_{k+1}(\delta|\mathrm{d})\cong H^D_{p+1+k}(\delta|\mathrm{d})\cong 0$ for $k>0$, the last equation implies

$$Y'_{k+1\mu_{[p]}|\nu_{[q]}} = \delta A_{k+2\mu_{[p]}|\nu_{[q]}} + \partial^\lambda T_{k+1[\lambda\mu_{[p]}]|\nu_{[q]}}. \tag{C12}$$

By the induction hypothesis for $p+1+k$, we can take A_{k+2} and T_{k+1} invariant. Antisymmetrizing (C12) over the indices $\mu_q\cdots\mu_p\nu_1\cdots\nu_q$ yields

$$0 = \delta A_{k+2\mu_1\cdots\mu_{q-1}[\mu_q\cdots\mu_p|\nu_1\cdots\nu_q]} + \partial^\lambda T_{k+1\lambda\mu_1\cdots\mu_{q-1}[\mu_q\cdots\mu_p|\nu_1\ldots\nu_q]}.$$

The solution of this equation for T_{k+1} is

$$T_{k+1\mu_0\cdots\mu_{q-1}[\mu_q\cdots\mu_p|\nu_1\cdots\nu_q]} = \delta Q_{k+2\mu_0\cdots\mu_{q-1}|[\mu_q\cdots\mu_p\nu_1\cdots\nu_q]} + \partial^\alpha S_{k+1\alpha\mu_0\cdots\mu_{q-1}|[\mu_q\cdots\mu_p\nu_1\cdots\nu_q]} + [U^{(u)}_{[\mu_q\cdots\mu_p\nu_1\cdots\nu_q]}(\tilde{\mathcal{H}})]^{\rho_{[D-q]}}_{k+1}\epsilon_{\mu_0\cdots\mu_{q-1}\rho_{[D-q]}},$$

where $U^{(u)}$ is a polynomial of degree u in $\tilde{\mathcal{H}}$, present when $k+q+1=D-u(D-p-1)$ for some

strictly positive integer u. As T and $U^{(u)}(\tilde{\mathcal{H}})$ are invariant, we can use the induction hypothesis for $k'=k+1+q$. This implies

$$T_{k+1\mu_0\cdots\mu_{q-1}[\mu_q\cdots\mu_p|\nu_1\cdots\nu_q]} = \delta Q'_{k+2\mu_0\cdots\mu_{q-1}|[\mu_q\cdots\mu_p\nu_1\cdots\nu_q]} + \partial^\alpha S'_{k+1\alpha\mu_0\cdots\mu_{q-1}|[\mu_q\cdots\mu_p\nu_1\cdots\nu_q]} + [U^{(u)}_{[\mu_q\cdots\mu_p\nu_1\cdots\nu_q]}(\tilde{\mathcal{H}}) + V^{(v,w)}_{[\mu_q\cdots\mu_p\nu_1\cdots\nu_q]}(K^{q+1},\tilde{\mathcal{H}})]^{\rho_{[D-q]}}_{k+1}\epsilon_{\mu_0\cdots\mu_{q-1}\rho_{[D-q]}}, \tag{C13}$$

where Q'_{k+2} and S'_{k+1} are invariants and $V^{(v,w)}$ is a polynomial of order v and w in K^{q+1} and $\tilde{\mathcal{H}}$, respectively, present when $D-q=v(q+1)+w(D-p-1)+k+1$ for some strictly positive integers v,w.

We define the invariant tensor $E_{\alpha\mu_{[p]}|\beta\nu_{[q]}}$ with Young symmetry $[p+1,q+1]$ by

$$E_{\alpha\mu_{[p]}|\beta\nu_{[q]}} = \sum_{i=0}^{q+1} \alpha_i S'_{k+1\rho_0\cdots\rho_{i-1}[\nu_i\cdots\nu_q|\beta\nu_1\cdots\nu_{i-1}]\rho_i\cdots\rho_p}\delta^{[\rho_0\cdots\rho_p]}_{[\alpha\mu_{[p]}]},$$

where $\alpha_i=\alpha_0[(q+1)!/(q+1-i)!i!]$ and $\alpha_0=(-)^{pq}\{((p+1)!)^2/(p-q)!(q!)^2(p-q+1)(p+2)\Sigma_{j=0}^{q}[(p-j)!/(q-j)!]\}$.

Writing $\partial^{\alpha\beta}E_{k+1\alpha\mu_{[p]}|\beta\nu_{[q]}}$ in terms of S'_{k+1} and using (C13) and (C12) yields

$$Y'_{k+1\mu_{[p]}|\nu_{[q]}} = \partial^{\alpha\beta}E_{k+1\alpha\mu_{[p]}|\beta\nu_{[q]}} + \delta F_{k+2\mu_{[p]}|\nu_{[q]}} + \partial^\alpha\sum_{i=0}^{q}\beta_i[V^{(v,w)}_{[\alpha\nu_{[i]}\mu_{i+1}\cdots\mu_p]}(K^{q+1},\tilde{\mathcal{H}})]^{\rho_{[D-q]}}_{k+1}\epsilon_{\mu_{[i]}\nu_{i+1}\cdots\nu_q\rho_{[D-q]}}, \tag{C14}$$

where F_{k+2} is invariant, $\beta_i\equiv\alpha_0[(p+2)q!/(p+1)i!(q-i)!]$ and v is allowed to take the value $v=0$ to cover also the case of the polynomial $U^{(w)}(\tilde{\mathcal{H}})$.

5. Homotopy formula

We will now use the homotopy formula to reconstruct a_k from its Euler–Lagrange derivatives,

$$a^D_k = \int_0^1 \mathrm{d}t\left[\phi_{\mu_{[p]}|\nu_{[q]}}\frac{\delta^L a_k}{\delta\phi_{\mu_{[p]}|\nu_{[q]}}} + \sum_{j=1}^{p+1} C^*_{j\mu_{[q]}|\nu_{[p+1-j]}}\frac{\delta^L a_k}{\delta C^*_{j\mu_{[q]}|\nu_{[p+1-j]}}}\right]\mathrm{d}^Dx.$$

Inserting the expressions for the Euler–Lagrange derivatives given by Lemma C.4 yields

$$a^D_k = \int_0^1 \mathrm{d}t\left[\delta(\phi_{\mu_{[p]}|\nu_{[q]}}Y'^{\mu_{[p]}|\nu_{[q]}}_{k+1}) + \sum_{j=1}^{p+1}\delta(C^*_{j\mu_{[q]}|\nu_{[p+1-j]}}Z'^{\mu_{[q]}|\nu_{[p+1-j]}}_{k+1-j}) + \sum_{j=1}^{k} C^*_{j\mu_{[q]}|\nu_{[p+1-j]}} \times(-)^{k+p+1}A_{k-j}[R^{\mu_{[q]}}(K^{q+1},\tilde{\mathcal{H}})]^{\nu_{[p+1-j]}}_{k-j} + \phi_{\mu_{[p]}|\nu_{[q]}}A\delta^{[\sigma_{[q]}\alpha\mu_{[p]}\xi]}_{[\nu_{[q]}\beta\rho_{[p+1]}]}\partial_\alpha\partial^\beta(x_\xi[R_{\sigma_{[q]}}(K^{q+1},\tilde{\mathcal{H}})]^{\rho_{[p+1]}}_k) + C^*_{k\mu_{[q]}|\nu_{[p+1-k]}}[Q^{(m)\mu_{[q]}}(K^{q+1})]^{\nu_{[p+1-k]}}\right]\mathrm{d}^Dx + \mathrm{d}n^{D-1}_k.$$

Using the result (C14) for Y'_{k+1} and some algebra, one finds

$$a_k^D = \int_0^1 \mathrm{d}t \Bigg[\delta(K_{\mu_{[p+1]}|\nu_{[q+1]}} E_{k+1}^{\mu_{[p+1]}|\nu_{[q+1]}} \mathrm{d}^D x) + a_v K_{\mu_{[p+1]}}^{q+1} [V^{(v,w)\mu_{[p+1]}}(K^{q+1}, \tilde{\mathcal{H}})]_k^{D-q-1}$$
$$+ \sum_{j=1}^{p+1} \delta(C^*_{j\mu_{[q]}|\nu_{[p+1-j]}} Z'^{\mu_{[q]}|\nu_{[p+1-j]}}_{k+1-j} \mathrm{d}^D x) + a_r [\tilde{\mathcal{H}}^{\sigma_{[q]}} R_{\sigma_{[q]}}(K^{q+1}, \tilde{\mathcal{H}})]_k^D$$
$$+ a_q [\tilde{\mathcal{H}}^{\sigma_{[q]}}]_k^{D-m(q+1)} Q^{(m)}_{\sigma_{[q]}}(K^{q+1}) \Bigg] + \mathrm{d}\bar{n}_k^{D-1},$$

where $a_v = (-)^{k(q+1)} \Sigma_{i=0}^q \beta_i [i!(p-i)!/p!]$, $a_r = (-)^{D(p+k+1)+\{[p(p+1)+k(k+1)]/2\}}$ and $a_q = (-)^k a_r$. In short,

$$a_k^D = [P(K^{q+1}, \tilde{\mathcal{H}})]_k^D + \delta \mu_{k+1}^D + \mathrm{d}\bar{n}_k^{D-1}$$

for some invariant μ_{k+1}^D, and some polynomial P of strictly positive order in K^{q+1} and $\tilde{\mathcal{H}}$.

We must still prove that $\bar{n}_k^{D-1}$ can be taken invariant.

Acting with γ on the last equation yields $\mathrm{d}(\gamma \bar{n}_k^{D-1}) = 0$. By the Poincaré lemma, $\gamma \bar{n}_k^{D-1} = \mathrm{d}(r_k^{D-2})$. Furthermore, a well-known result on $H(\gamma|\mathrm{d})$ for positive antighost number k (see e.g., Appendix A.1 of Ref. 17) states that one can redefine $\bar{n}_k^{D-1}$ in such a way that $\gamma \bar{n}_k^{D-1} = 0$. As the pure ghost number of $\bar{n}_k^{D-1}$ vanishes, the last equation implies that $\bar{n}_k^{D-1}$ is an invariant polynomial.

This completes the proof of Theorem 7.2 for $k \geqslant q$. □

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Critical behavior of the compactified $\lambda\phi^4$ theory

L. M. Abreu and C. de Calan
Centre de Physique Théorique, Ecole Polytechnique, 91128 Palaiseau, France

A. P. C. Malbouisson
CBPF/MCT, Rua Dr. Xavier Sigaud, 150, Rio de Janeiro RJ, Brazil

J. M. C. Malbouisson[a)]
Department of Physics, University of Alberta, Edmonton, AB, Canada, T6G 2J1

A. E. Santana
Instituto de Física, Universidade de Brasília, 70910-900, Brasília-DF, Brazil

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We investigate the critical behavior of the N-component Euclidean $\lambda\phi^4$ model, in the large N limit, in three situations: confined between two parallel planes a distance L apart from one another; confined to an infinitely long cylinder having a square transversal section of area L^2; and to a cubic box of volume L^3. Taking the mass term in the form $m_0^2=\alpha(T-T_0)$, we retrieve Ginzburg–Landau models which are supposed to describe samples of a material undergoing a phase transition, respectively, in the form of a film, a wire and of a grain, whose bulk transition temperature (T_0) is known. We obtain equations for the critical temperature as functions of L and of T_0, and determine the limiting sizes sustaining the transition. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1828589]

I. INTRODUCTION

Models with fields confined in spatial dimensions play important roles both in field theory and in quantum mechanics. Relevant examples are the Casimir effect and superconducting films, where confinement is carried on by appropriate boundary conditions. For Euclidean field theories, imaginary time and the spatial coordinates are treated exactly on the same footing, so that an extended Matsubara formalism can be applied for dealing with the breaking of invariance along any one of the spatial directions.

Relying on this fact, in the present work we discuss the critical behavior of the Euclidean $\lambda\varphi^4$ model compactified in one, two, and three spatial dimensions. We implement the spontaneous symmetry breaking by taking the bare mass coefficient in the Lagrangian parametrized as $m_0^2=\alpha(T-T_0)$, with $\alpha>0$ and the parameter T varying in an interval containing T_0. With this choice, considering the system confined between two parallel planes a distance L apart from one another, in an infinitely long square cylinder with transversal section area $A=L^2$, and in a cube of volume $V=L^3$, in dimension $D=3$, we obtain Ginzburg–Landau models describing phase transitions in samples of a material in the form of a film, a wire and a grain, respectively, T_0 standing for the bulk transition temperature. Such descriptions apply to physical circumstances where no gauge fluctuations need to be considered.

We start recapitulating the general procedure developed in Ref. 1 to treat the massive $(\lambda\varphi^4)_D$ theory in Euclidean space, compactified in a d-dimensional subspace, with $d\leqslant D$. This permits to extend to an arbitrary subspace some results in the literature for finite temperature field theory[2] and for the behavior of field theories in the presence of spatial boundaries.[3,4] We shall consider the vector N-component $(\lambda\varphi^4)_D$ Euclidean theory at leading order in $1/N$, thus allowing for nonper-

[a)]Permanent address: Instituto de Física, Universidade Federal da Bahia, 40210-340, Salvador, BA, Brazil.

turbative results, the system being submitted to the constraint of compactification of a d-dimensional subspace. After describing the general formalism, we readdress the renormalization procedure we use treating the simpler situation of $d=1$, which corresponds to the system confined between parallel planes (a film), analyzed in Ref. 5 for the case of two components, $N=2$. We then focus on two other particularly interesting cases of $d=2$ and $d=3$, in the three-dimensional Euclidean space, corresponding, respectively, to the system confined to an infinitely long cylinder with square transversal section (a wire) and to a finite cubic box (a grain). Extending the investigation to these new cases demands further developments in the subject of multidimensional Epstein functions.

For these situations, in the framework of the Ginzburg–Landau model we derive equations for the critical temperature as a function of the confining dimensions. For a film, we show that the critical temperature decreases linearly with the inverse of the film thickness while, for a square wire and for a cubic grain, we obtain that the critical temperatures decrease linearly with the inverse of the side of the square and with the inverse of the edge of the cube, respectively, but with larger coefficients. In all cases, we are able to calculate the minimal system size (thickness, transversal section area, or volume) below which the phase transition does not take place.

II. THE COMPACTFIED MODEL

In this section we review the analytical methods of compactification of the N-component Euclidean $\lambda\varphi^4$ model developed in Ref. 1 We consider the model described by the Hamiltonian density,

$$\mathcal{H}=\frac{1}{2}\partial_\mu\varphi_a\partial^\mu\varphi_a+\frac{1}{2}\overline{m}_0^2\varphi_a\varphi_a+\frac{\lambda}{N}(\varphi_a\varphi_a)^2, \tag{1}$$

in Euclidean D-dimensional space, confined to a d-dimensional spatial rectangular box of sides L_j, $j=1,2,\ldots,d$. In the above equation λ is the *renormalized* coupling constant, $\overline{m}_0^2$ is a boundary-modified mass parameter depending on $\{L_i\}$ $i=1,2,\ldots,d$, in such a way that

$$\lim_{\{L_i\}\to\infty}\overline{m}_0^2(L_1,\ldots,L_d)=m_0^2(T)\equiv\alpha(T-T_0), \tag{2}$$

$m_0^2(T)$ being the constant mass parameter present in the usual free-space Ginzburg–Landau model. In Eq. (2), T_0 represents the bulk transition temperature. Summation over repeated "color" indices a is assumed. To simplify the notation in the following we drop out the color indices, summation over them being understood in field products. We will work in the approximation of neglecting boundary corrections to the coupling constant. A precise definition of the boundary-modified mass parameter will be given later for the situation of $D=3$ with $d=1$, $d=2$, and $d=3$, corresponding, respectively, to a film of thickness L_1, to a wire of rectangular section $L_1\times L_2$ and to a grain of volume $L_1\times L_2\times L_3$.

We use Cartesian coordinates $\mathbf{r}=(x_1,\ldots,x_d,\mathbf{z})$, where $\mathbf{z}$ is a $(D-d)$-dimensional vector, with corresponding momentum $\mathbf{k}=(k_1,\ldots,k_d,\mathbf{q})$, $\mathbf{q}$ being a $(D-d)$-dimensional vector in momentum space. Then the generating functional of correlation functions has the form

$$\mathcal{Z}=\int\mathcal{D}\varphi^\dagger\,\mathcal{D}\varphi\exp\left(-\int_0^{\mathbf{L}}\mathrm{d}^dr\int\mathrm{d}^{D-d}\mathbf{z}\,\mathcal{H}(\varphi,\nabla\varphi)\right), \tag{3}$$

where $\mathbf{L}=(L_1,\ldots,L_d)$, and we are allowed to introduce a generalized Matsubara prescription, performing the following multiple replacements (compactification of a d-dimensional subspace):

$$\int \frac{\mathrm{d}k_i}{2\pi} \to \frac{1}{L_i} \sum_{n_i=-\infty}^{+\infty}, \quad k_i \to \frac{2n_i\pi}{L_i}, \quad i = 1,2,\ldots,d. \tag{4}$$

A simpler situation is the system confined simultaneously between two parallel planes a distance L_1 apart from one another normal to the x_1 axis and two other parallel planes, normal to the x_2 axis separated by a distance L_2 (a "wire" of rectangular section).

We start from the well-known expression for the one-loop contribution to the zero-temperature effective potential,[6]

$$U_1(\varphi_0) = \sum_{s=1}^{\infty} \frac{(-1)^{s+1}}{2s} [12\lambda\varphi_0^2]^s \int \frac{\mathrm{d}^D k}{(2\pi)^D} \frac{1}{(k^2+m^2)^s}, \tag{5}$$

where m is the physical mass and φ_0 is the normalized vacuum expectation value of the field (the classical field). In the following, to deal with dimensionless quantities in the regularization procedures, we introduce parameters

$$c = \frac{m}{2\pi\mu}, \quad b_i = \frac{1}{L_i\mu}, \quad g = \frac{\lambda}{4\pi^2\mu^{4-D}}, \quad \phi_0^2 = \frac{\varphi_0^2}{\mu^{D-2}}, \tag{6}$$

where μ is a mass scale. In terms of these parameters and performing the replacements (4), the one-loop contribution to the effective potential can be written in the form

$$U_1(\phi_0, b_1, \ldots, b_d) = \mu^D b_1 \cdots b_d \sum_{s=1}^{\infty} \frac{(-1)^s}{2s} [12g\phi_0^2]^s \sum_{n_1,\ldots,n_d=-\infty}^{+\infty} \int \frac{\mathrm{d}^{D-d} q'}{(b_1^2 n_1^2 + \cdots + b_d^2 n_d^2 + c^2 + \mathbf{q}'^2)^s}, \tag{7}$$

where $\mathbf{q}' = \mathbf{q}/2\pi\mu$ is dimensionless. Using a well-known dimensional regularization formula[7] to perform the integration over the $(D-d)$ noncompactified momentum variables, we obtain

$$U_1(\phi_0, b_1, \ldots, b_d) = \mu^D b_1 \cdots b_d \sum_{s=1}^{\infty} f(D,d,s) [12g\phi_0^2]^s A_d^{c^2}\left(s - \frac{D-d}{2}; b_1, \ldots, b_d\right), \tag{8}$$

where

$$f(D,d,s) = \pi^{(D-d)/2} \frac{(-1)^{s+1}}{2s\Gamma(s)} \Gamma\left(s - \frac{D-d}{2}\right) \tag{9}$$

and

$$\begin{aligned} A_d^{c^2}(\nu; b_1, \ldots, b_d) &= \sum_{n_1,\ldots,n_d=-\infty}^{+\infty} (b_1^2 n_1^2 + \cdots + b_d^2 n_d^2 + c^2)^{-\nu} \\ &= \frac{1}{c^{2\nu}} + 2\sum_{i=1}^{d} \sum_{n_i=1}^{\infty} (b_i^2 n_i^2 + c^2)^{-\nu} \\ &\quad + 2^2 \sum_{i<j=1}^{d} \sum_{n_i,n_j=1}^{\infty} (b_i^2 n_i^2 + b_j^2 n_j^2 + c^2)^{-\nu} + \cdots \\ &\quad + 2^d \sum_{n_1,\ldots,n_d=1}^{\infty} (b_1^2 n_1^2 + \cdots + b_d^2 n_d^2 + c^2)^{-\nu}. \end{aligned} \tag{10}$$

Next we can proceed generalizing to several dimensions the mode-sum regularization prescription described in Ref. 8. This generalization has been done in Ref. 1 and we briefly describe here its principal steps. From the identity

$$\frac{1}{\Delta^{\nu}} = \frac{1}{\Gamma(\nu)} \int_0^{\infty} \mathrm{d}t\, t^{\nu-1} e^{-\Delta t}, \tag{11}$$

and using the following representation for Bessel functions of the third kind, K_{ν},

$$2(a/b)^{\nu/2} K_{\nu}(2\sqrt{ab}) = \int_0^{\infty} \mathrm{d}x\, x^{\nu-1} e^{-(a/x)-bx}, \tag{12}$$

we obtain after some rather long but straightforward manipulations,[1]

$$\begin{aligned} A_d^{c^2}(\nu; b_1, \ldots, b_d) = \frac{2^{\nu-(d/2)+1}\pi^{2\nu-(d/2)}}{b_1 \cdots b_d \Gamma(\nu)} \Bigg[& 2^{\nu-(d/2)-1}\Gamma\left(\nu - \frac{d}{2}\right)(2\pi c)^{d-2\nu} \\ & + 2\sum_{i=1}^{d}\sum_{n_i=1}^{\infty} \left(\frac{n_i}{2\pi c b_i}\right)^{\nu-(d/2)} K_{\nu-(d/2)}\left(\frac{2\pi c n_i}{b_i}\right) + \cdots \\ & + 2^d \sum_{n_1,\ldots,n_d=1}^{\infty} \left(\frac{1}{2\pi c}\sqrt{\frac{n_1^2}{b_1^2} + \cdots + \frac{n_d^2}{b_d^2}}\right)^{\nu-(d/2)} K_{\nu-(d/2)}\left(2\pi c \sqrt{\frac{n_1^2}{b_1^2} + \cdots + \frac{n_d^2}{b_d^2}}\right) \Bigg]. \end{aligned} \tag{13}$$

Taking $\nu = s - (D-d)/2$ in Eq. (13) and inserting it in Eq. (8), we obtain the one-loop correction to the effective potential in D dimensions with a compactified d-dimensional subspace in the form (recovering the dimensionful parameters)

$$\begin{aligned} U_1(\varphi_0, L_1, \ldots, L_d) = \sum_{s=1}^{\infty} [12 g \phi_0^2]^s h(D,s) \Bigg[& 2^{s-(D/2)-2}\Gamma\left(s - \frac{D}{2}\right) m^{D-2s} \\ & + \sum_{i=1}^{d}\sum_{n_i=1}^{\infty} \left(\frac{m}{L_i n_i}\right)^{(D/2)-s} K_{(D/2)-s}(m L_i n_i) \\ & + 2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty} \left(\frac{m}{\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}}\right)^{(D/2)-s} K_{(D/2)-s}(m\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}) + \cdots \\ & + 2^{d-1} \sum_{n_1,\ldots,n_d=1}^{\infty} \left(\frac{m}{\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}}\right)^{(D/2)-s} K_{(D/2)-s}(m\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}) \Bigg], \end{aligned} \tag{14}$$

with

$$h(D,s) = \frac{1}{2^{D/2+s-1}\pi^{D/2}} \frac{(-1)^{s+1}}{s\Gamma(s)}. \tag{15}$$

Criticality is attained when the inverse squared correlation length, $\xi^{-2}(L_1, \ldots, L_d, \varphi_0)$, vanishes in the large-$N$ gap equation,

$$\xi^{-2}(L_1,\ldots,L_d,\varphi_0)=\overline{m}_0^2+12\lambda\varphi_0^2+\frac{24\lambda}{L_1\cdots L_d}\sum_{n_1,\ldots,n_d=-\infty}^{\infty}\int\frac{\mathrm{d}^{D-d}q}{(2\pi)^{D-d}}\times\frac{1}{\mathbf{q}^2+\left(\frac{2\pi n_1}{L_1}\right)^2+\cdots+\left(\frac{2\pi n_d}{L_d}\right)^2+\xi^{-2}(L_1,\ldots,L_d,\varphi_0)},\tag{16}$$

where φ_0 is the normalized vacuum expectation value of the field (different from zero in the ordered phase). In the disordered phase, φ_0 vanishes and the inverse correlation length equals the physical mass, given below by Eq. (18). Recalling the condition,

$$\left.\frac{\partial^2}{\partial\varphi_0^2}U(D,L_1,L_2)\right|_{\varphi_0=0}=m^2,\tag{17}$$

where U is the sum of the tree-level and one-loop contributions to the effective potential (remembering that at the large-N limit it is enough to take the one-loop contribution to the mass), we obtain

$$\begin{aligned}m^2(L_1,\ldots,L_d)=\overline{m}_0^2(L_1,\ldots,L_d)+\frac{24\lambda}{(2\pi)^{D/2}}\Bigg[&\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}\left(\frac{m}{L_in_i}\right)^{(D/2)-1}K_{(D/2)-1}(mL_in_i)\\&+2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2n_i^2+L_j^2n_j^2}}\right)^{(D/2)-1}K_{(D/2)-1}(m\sqrt{L_i^2n_i^2+L_j^2n_j^2})+\cdots\\&+2^{d-1}\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}\right)^{(D/2)-1}K_{(D/2)-1}(m\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2})\Bigg].\end{aligned}\tag{18}$$

Notice that, in writing Eq. (18), we have suppressed the parcel $2^{-(D/2)-1}\Gamma[1-(D/2)]m^{D-2}$ from its square brackets, the parcel that emerges from the first term in the square bracket of Eq. (14). This expression, which does not depend explicitly on L_i, diverges for D even due to the poles of the gamma function; in this case, this parcel is subtracted to get a renormalized mass equation. For D odd, $\Gamma[1-(D/2)]$ is finite but we also subtract this term (corresponding to a finite renormalization) for sake of uniformity; besides, for $D\geqslant 3$, the factor m^{D-2} does not contribute in the criticality.

The vanishing of Eq. (18) defines criticality for our compactified system. We claim that, taking $d=1$, $d=2$, and $d=3$ with $D=3$, we are able to describe, respectively, the critical behavior of samples of materials in the form of films, wires, and grains. Notice that the parameter m on the right-hand side of Eq. (18) is the boundary-modified mass $m(L_1,\ldots,L_d)$, which means that Eq. (18) is a self-consistency equation, a very complicated modified Schwinger–Dyson equation for the mass, not soluble by algebraic means. Nevertheless, as we will see in the next sections, a solution is possible at criticality, which allows us to obtain a closed formula for the boundary-dependent critical temperature.

III. CRITICAL BEHAVIOR FOR FILMS

We now consider the simplest particular case of the compactification of only one spatial dimension, with the system confined between two parallel planes a distance L apart from one another. This case, which has already been considered in Ref. 5 concerning with the two-component model, is reanalyzed here to set the required renormalization procedure in the proper large-N grounds and, also, for the sake of completeness. Thus, from Eq. (18), taking $d=1$, we get in the disordered phase

$$m^2(L) = \overline{m}_0^2(L) + \frac{24\lambda}{(2\pi)^{D/2}} \sum_{n=1}^{\infty} \left(\frac{m}{nL}\right)^{(D/2)-1} K_{(D/2)-1}(nLm), \tag{19}$$

where L $(=L_1)$ is the separation between the planes, the film thickness. If we limit ourselves to the neighborhood of criticality $(m^2 \approx 0)$ and consider L finite and sufficiently small, we may use an asymptotic formula for small values of the argument of Bessel functions,

$$K_\nu(z) \approx \frac{1}{2}\Gamma(|\nu|)\left(\frac{z}{2}\right)^{-|\nu|} \quad (z \approx 0), \tag{20}$$

and Eq. (19) reduces, for $D>3$, to

$$m^2(L) \approx \overline{m}_0^2(L) + \frac{6\lambda}{\pi^{D/2} L^{D-2}} \Gamma\left(\frac{D}{2} - 1\right) \zeta(D-2), \tag{21}$$

where $\zeta(D-2)$ is the Riemann *zeta*-function, defined for $\mathrm{Re}\{D-2\}>1$ by the series

$$\zeta(D-2) = \sum_{n=1}^{\infty} \frac{1}{n^{D-2}}. \tag{22}$$

It is worth mentioning that for $D=4$, taking $m^2(L)=0$ and making the appropriate changes $(L \to \beta, \lambda \to \lambda/4!)$, Eq. (21) is *formally identical* to the high-temperature (low values of β) critical equation obtained in Ref. 9, thus providing a check of our calculations.

For $D=3$, Eq. (21) can be made physically meaningful by a regularization procedure as follows. We consider the analytic continuation of the *zeta*-function, leading to a meromorphic function having only one simple pole at $z=1$, which satisfies the reflection formula

$$\zeta(z) = \frac{1}{\Gamma(z/2)} \Gamma\left(\frac{1-z}{2}\right) \pi^{z-1/2} \zeta(1-z). \tag{23}$$

Next, remembering the formula

$$\lim_{z \to 1} \left[\zeta(z) - \frac{1}{z-1} \right] = \gamma, \tag{24}$$

where $\gamma \approx 0.5772$ is the Euler–Mascheroni constant, we define the L-dependent bare mass for $D \approx 3$, in such a way that the pole at $D=3$ in Eq. (21) is suppressed, that is we take

$$\overline{m}_0^2(L) \approx M - \frac{1}{(D-3)} \frac{6\lambda}{\pi L}, \tag{25}$$

where M is independent of D. To fix the finite term, we make the simplest choice satisfying (2),

$$M = m_0^2(T) = \alpha(T - T_0), \tag{26}$$

T_0 being the bulk critical temperature. In this case, using Eq. (25) in Eq. (21) and taking the limit as $D \to 3$, the L-dependent renormalized mass term in the vicinity of criticality becomes

$$m^2(L) \approx \alpha(T - T_c(L)), \tag{27}$$

where the modified, L-dependent, transition temperature is given by

$$T_c(L) = T_0 - C_1 \frac{\lambda}{\alpha L}, \tag{28}$$

L being the thickness of the film, with the constant C_1 given by

$$C_1 = \frac{6\gamma}{\pi} \approx 1.1024. \tag{29}$$

From this equation, we see that for L smaller than

$$L_{\min} = C_1 \frac{\lambda}{\alpha T_0}, \tag{30}$$

$T_c(L)$ becomes negative, meaning that the transition does not occur.[5]

IV. CRITICAL BEHAVIOR FOR WIRES

We now focus on the situation where two spatial dimensions are compactified. From Eq. (18), taking $d=2$, we get (in the disordered phase)

$$\begin{aligned} m^2(L_1,L_2) = \overline{m}_0^2(L_1,L_2) + \frac{24\lambda}{(2\pi)^{D/2}}\Bigg[& \sum_{n=1}^{\infty}\left(\frac{m}{nL_1}\right)^{(D/2)-1} K_{(D/2)-1}(nL_1 m) \\ & + \sum_{n=1}^{\infty}\left(\frac{m}{nL_2}\right)^{(D/2)-1} K_{(D/2)-1}(nL_2 m) \\ & + 2\sum_{n_1,n_2=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2 n_1^2 + L_2^2 n_2^2}}\right)^{(D/2)-1} K_{(D/2)-1}(m\sqrt{L_1^2 n_1^2 + L_2^2 n_2^2})\Bigg]. \end{aligned} \tag{31}$$

If we limit ourselves to the neighborhood of criticality, $m^2 \approx 0$, and taking both L_1 and L_2 finite and sufficiently small, we may use Eq. (20) to rewrite Eq. (31) as

$$m^2(L_1,L_2) \approx \overline{m}_0^2(L_1,L_2) + \frac{6\lambda}{\pi^{D/2}}\Gamma\left(\frac{D}{2}-1\right)\left[\left(\frac{1}{L_1^{D-2}} + \frac{1}{L_2^{D-2}}\right)\zeta(D-2) + 2E_2\left(\frac{D-2}{2};L_1,L_2\right)\right], \tag{32}$$

where $E_2[(D-2)/2;L_1,L_2]$ is the generalized (multidimensional) Epstein *zeta*-function defined by

$$E_2\left(\frac{D-2}{2};L_1,L_2\right) = \sum_{n_1,n_2=1}^{\infty}[L_1^2 n_1^2 + L_2^2 n_2^2]^{-[(D-2)/2]}, \tag{33}$$

for $\mathrm{Re}\{D\} > 3$.

As mentioned before, the Riemann *zeta*-function $\zeta(D-2)$ has an analytical extension to the whole complex D-plane, having a unique simple pole (of residue 1) at $D=3$. One can also construct analytical continuations (and recurrence relations) for the multidimensional Epstein functions which permit to write them in terms of Kelvin and Riemann *zeta*-functions. To start one considers the analytical continuation of the Epstein–Hurwitz *zeta*-function given by[8]

$$\sum_{n=1}^{\infty}(n^2+p^2)^{-\nu} = -\frac{1}{2}p^{-2\nu} + \frac{\sqrt{\pi}}{2p^{2\nu-1}\Gamma(\nu)}\left[\Gamma\left(\nu-\frac{1}{2}\right) + 4\sum_{n=1}^{\infty}(\pi p n)^{\nu-1/2}K_{\nu-1/2}(2\pi p n)\right]. \tag{34}$$

Using this relation to perform one of the sums in (33) leads immediately to the question of which sum is first evaluated. As it is done in Ref. 10, whatever the sum one chooses to perform first, the manifest $L_1 \leftrightarrow L_2$ symmetry of Eq. (33) is lost; to overcome such an obstacle, in order to preserve this symmetry, we adopt here a symmetrized summation generalizing the prescription introduced in Ref. 1 for the case of many variables.

To derive an analytical continuation and symmetrized recurrence relations for the multidimensional Epstein functions, we start by taking these functions defined as the symmetrized summations

$$E_d(\nu;L_1,\ldots,L_d)=\frac{1}{d!}\sum_{\sigma}\sum_{n_1=1}^{\infty}\cdots\sum_{n_d=1}^{\infty}[\sigma_1^2n_1^2+\cdots+\sigma_d^2n_d^2]^{-\nu}, \tag{35}$$

where $\sigma_i=\sigma(L_i)$, with σ running in the set of all permutations of the parameters $L_1,\ldots,L_d$, and the summations over $n_1,\ldots,n_d$ being taken in the given order. Applying (34) to perform the sum over n_d, one gets

$$E_d(\nu;L_1,\ldots,L_d)=-\frac{1}{2d}\sum_{i=1}^{d}E_{d-1}(\nu;\ldots,\widehat{L_i},\ldots)+\frac{\sqrt{\pi}}{2\,\mathrm{d}\Gamma(\nu)}\Gamma\left(\nu-\frac{1}{2}\right)\sum_{i=1}^{d}\frac{1}{L_i}E_{d-1}\left(\nu-\frac{1}{2};\ldots,\widehat{L_i},\ldots\right)$$
$$+\frac{2\sqrt{\pi}}{\mathrm{d}\Gamma(\nu)}W_d\left(\nu-\frac{1}{2},L_1,\ldots,L_d\right), \tag{36}$$

where the hat over the parameter L_i in the functions E_{d-1} means that it is excluded from the set $\{L_1,\ldots,L_d\}$ (the others being the $d-1$ parameters of E_{d-1}), and

$$W_d(\eta;L_1,\ldots,L_d)=\sum_{i=1}^{d}\frac{1}{L_i}\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{\pi n_i}{L_i\sqrt{(\cdots+\widehat{L_i^2n_i^2}+\cdots)}}\right)^{\eta}K_{\eta}\left(\frac{2\pi n_i}{L_i}\sqrt{(\cdots+\widehat{L_i^2n_i^2}+\cdots)}\right), \tag{37}$$

with $(\cdots+\widehat{L_i^2n_i^2}+\cdots)$ representing the sum $\Sigma_{j=1}^{d}L_j^2n_j^2-L_i^2n_i^2$. In particular, noticing that $E_1(\nu;L_j)=L_j^{-2\nu}\zeta(2\nu)$, one finds

$$E_2\left(\frac{D-2}{2};L_1^2,L_2^2\right)=-\frac{1}{4}\left(\frac{1}{L_1^{D-2}}+\frac{1}{L_2^{D-2}}\right)\zeta(D-2)+\frac{\sqrt{\pi}\Gamma\left(\frac{D-3}{2}\right)}{4\Gamma\left(\frac{D-2}{2}\right)}\left(\frac{1}{L_1L_2^{D-3}}+\frac{1}{L_1^{D-3}L_2}\right)\zeta(D-3)$$
$$+\frac{\sqrt{\pi}}{\Gamma\left(\frac{D-2}{2}\right)}W_2\left(\frac{D-3}{2};L_1,L_2\right), \tag{38}$$

which is a meromorphic function of D, symmetric in the parameters L_1 and L_2 as Eq. (33) suggests.

Using the above expression, Eq. (32) can be rewritten as

$$m^2(L_1,L_2)\approx\overline{m}_0^2(L_1,L_2)+\frac{3\lambda}{\pi^{D/2}}\left[\left(\frac{1}{L_1^{D-2}}+\frac{1}{L_2^{D-2}}\right)\Gamma\left(\frac{D-2}{2}\right)\zeta(D-2)\right.$$
$$\left.+\sqrt{\pi}\left(\frac{1}{L_1L_2^{D-3}}+\frac{1}{L_1^{D-3}L_2}\right)\Gamma\left(\frac{D-3}{2}\right)\zeta(D-3)+2\sqrt{\pi}W_2\left(\frac{D-3}{2};L_1,L_2\right)\right]. \tag{39}$$

This equation presents no problems for $3<D<4$ but, for $D=3$, the first and second terms between the square brackets of Eq. (39) are divergent due to the ζ-function and Γ-function, respectively. We can deal with divergences remembering the property in Eq. (24) and using the expansion of $\Gamma[(D-3)/2]$ around $D=3$,

$$\Gamma\left(\frac{D-3}{2}\right)\approx\frac{2}{D-3}+\Gamma'(1), \tag{40}$$

$\Gamma'(z)$ standing for the derivative of the Γ-function with respect to z. For $z=1$ it coincides with the Euler digamma-function $\psi(1)$, which has the particular value $\psi(1)=-\gamma$. We notice however, that differently from the case treated in the preceding section, where a renormalization procedure was

needed, here the two divergent terms generated by the use of formulas (24) and (40) cancel exactly between them. No renormalization is needed. Thus, for $D=3$, taking the bare mass given by $\overline{m}_0^2(L_1,L_2)=\alpha(T-T_0)$, we obtain the renormalized boundary-dependent mass term in the form

$$m^2(L_1,L_2) \approx \alpha(T - T_c(L_1,L_2)), \tag{41}$$

with the boundary-dependent critical temperature given by

$$T_c(L_1,L_2) = T_0 - \frac{9\lambda\gamma}{2\pi\alpha}\left(\frac{1}{L_1}+\frac{1}{L_2}\right) - \frac{6\lambda}{\pi\alpha}W_2(0;L_1,L_2), \tag{42}$$

where

$$W_2(0;L_1,L_2) = \sum_{n_1,n_2=1}^{\infty}\left\{\frac{1}{L_1}K_0\left(2\pi\frac{L_2}{L_1}n_1n_2\right)+\frac{1}{L_2}K_0\left(2\pi\frac{L_1}{L_2}n_1n_2\right)\right\}. \tag{43}$$

The quantity $W_2(0;L_1,L_2)$, appearing in Eq. (42), involves complicated double sums, very difficult to handle for $L_1\neq L_2$; in particular, it is not possible to take limits such as $L_i\to\infty$. For this reason we will restrict ourselves to the case $L_1=L_2$. For a wire with the square transversal section, we have $L_1=L_2=L=\sqrt{A}$ and Eq. (42) reduces to

$$T_c(A) = T_0 - C_2\frac{\lambda}{\alpha\sqrt{A}}, \tag{44}$$

where C_2 is a constant given by

$$C_2 = \frac{9\gamma}{\pi}+\frac{12}{\pi}\sum_{n_1,n_2=1}^{\infty}K_0(2\pi n_1n_2) \approx 1.6571. \tag{45}$$

We see that the critical temperature of the square wire depends on the bulk critical temperature and the Ginzburg–Landau parameters α and λ (which are characteristics of the material constituting the wire), and also on the area of its cross section. Since T_c decreases linearly with the inverse of the side of the square, this suggests that there is a minimal area for which $T_c(A_{\min})=0$,

$$A_{\min} = \left(C_2\frac{\lambda}{\alpha T_0}\right)^2; \tag{46}$$

for square wires of the transversal section areas smaller than this value, in the context of our model the transition should be suppressed. On topological grounds, we expect that (apart from appropriate coefficients) our result should be independent of the transverse section shape of the wire, at least for transversal sectional regular polygons.

V. CRITICAL BEHAVIOR FOR GRAINS

We now turn our attention to the case where all three spatial dimensions are compactified, corresponding to the system confined in a box of sides L_1,L_2,L_3. Taking $d=3$ in Eq. (18) and using Eq. (20), we obtain (for sufficiently small L_1,L_2,L_3 and in the neighborhood of classicality, $m^2\approx 0$)

$$m^2(L_1,L_2,L_3) \approx \overline{m}_0^2(L_1,L_2,L_3) + \frac{6\lambda}{\pi^{D/2}}\Gamma\left(\frac{D-2}{2}\right)\left[\sum_{i=1}^{3}\frac{\zeta(D-2)}{L_i^{D-2}} + 2\sum_{i<j=1}^{3}E_2\left(\frac{D-2}{2};L_i,L_j\right) + 4E_3\left(\frac{D-2}{2};L_1,L_2,L_3\right)\right], \tag{47}$$

where $E_3(\nu;L_1,L_2,L_3)=\Sigma_{n_1,n_2,n_3=1}^{\infty}[L_1^2n_1^2+L_2^2n_2^2+L_3^2n_3^2]^{-\nu}$ and the functions E_2 are given by Eq. (38).

The analytical structure of the function $E_3[(D-2)/2;L_1,L_2,L_3]$ can be obtained from the general symmetrized recurrence relation given by Eqs. (36) and (37); explicitly, one has

$$E_3\left(\frac{D-2}{2};L_1,L_2,L_3\right) = -\frac{1}{6}\sum_{i<j=1}^{3}E_2\left(\frac{D-2}{2};L_i,L_j\right) + \frac{\sqrt{\pi}\Gamma\left(\frac{D-3}{2}\right)}{6\Gamma\left(\frac{D-2}{2}\right)}\sum_{i,j,k=1}^{3}\frac{(1+\varepsilon_{ijk})}{2}\frac{1}{L_i} \times E_2\left(\frac{D-2}{2};L_j,L_k\right) + \frac{2\sqrt{\pi}}{3\Gamma\left(\frac{D-2}{2}\right)}W_3\left(\frac{D-3}{2};L_1,L_2,L_3\right), \tag{48}$$

where ε_{ijk} is the totally antisymmetric symbol and the function W_3 is a particular case of Eq. (37). Using Eqs. (38) and (48), the boundary dependent mass can be written as

$$m^2(L_1,L_2,L_3) \approx \overline{m}_0^2(L_1,L_2,L_3) + \frac{6\lambda}{\pi^{D/2}}\left[\frac{1}{3}\Gamma\left(\frac{D-2}{2}\right)\sum_{i=1}^{3}\frac{1}{L_i^{D-2}}\zeta(D-2) + \frac{\sqrt{\pi}}{6}\zeta(D-3) \times \sum_{i<j=1}^{3}\left(\frac{1}{L_i^{D-3}L_j}+\frac{1}{L_j^{D-3}L_i}\right)\Gamma\left(\frac{D-3}{2}\right) + \frac{4\sqrt{\pi}}{3}\sum_{i<j=1}^{3}W_2\left(\frac{D-3}{2};L_i,L_j\right) + \frac{\pi}{6}\zeta(D-4)\Gamma\left(\frac{D-4}{2}\right)\sum_{i,j,k=1}^{3}\frac{(1+\varepsilon_{ijk})}{2}\frac{1}{L_i}\left(\frac{1}{L_j^{D-4}L_k}+\frac{1}{L_k^{D-4}L_j}\right) + \frac{2\pi}{3}\sum_{i,j,k=1}^{3}\frac{(1+\varepsilon_{ijk})}{2}\frac{1}{L_i}W_2\left(\frac{D-4}{2};L_j,L_k\right) + \frac{8\sqrt{\pi}}{3}W_3\left(\frac{D-3}{2};L_1,L_2,L_3\right)\right]. \tag{49}$$

The first two terms in the square brackets of Eq. (49) diverge as $D\to 3$ due to the poles of the Γ and ζ-functions. However, as it happens in the case of wires, using Eqs. (24) and (40) it can be shown that these divergences cancel exactly one another. After some simplifications, for $D=3$, the boundary dependent mass (49) becomes

$$m^2(L_1,L_2,L_3) \approx \overline{m}_0^2(L_1,L_2,L_3) + \frac{6\lambda}{\pi}\left[\frac{\gamma}{2}\sum_{i=1}^{3}\frac{1}{L_i} + \frac{4}{3}\sum_{i<j=1}^{3}W_2(0;L_i,L_j) + \frac{\pi}{18}\sum_{i,j,k=1}^{3}\frac{(1+\varepsilon_{ijk})}{2}\frac{L_i}{L_jL_k} + \frac{2\sqrt{\pi}}{3}\sum_{i,j,k=1}^{3}\frac{(1+\varepsilon_{ijk})}{2}\frac{1}{L_i}W_2\left(-\frac{1}{2};L_j,L_k\right) + \frac{8}{3}W_3(0;L_1,L_2,L_3)\right]. \tag{50}$$

As before, since no divergences need to be suppressed, we can take the bare mass given by $\overline{m}_0^2(L_1,L_2,L_3)=\alpha(T-T_0)$ and rewrite the renormalized mass as $m^2(L_1,L_2,L_3)\approx\alpha(T-T_c(L_1,L_2,L_3))$. The expression of $T_c(L_1,L_2,L_3)$ can be easily obtained from Eq. (50), but it is a very complicated formula, involving multiple sums, which makes almost impossible a general

analytical study for arbitrary parameters L_1, L_2, L_3; thus, we restrict ourselves to the situation where $L_1=L_2=L_3=L$, corresponding to a cubic box of volume $V=L^3$. In this case, the boundary dependent critical temperature reduces to

$$T_c(V) = T_0 - C_3 \frac{\lambda}{\alpha V^{1/3}}, \tag{51}$$

where the constant C_3 is given by [using that $K_{-1/2}(z)=\sqrt{\pi/2z}e^{-z}$]

$$C_3 = 1 + \frac{9\gamma}{\pi} + \frac{12}{\pi}\sum_{n_1,n_2=1}^{\infty}\frac{e^{-2\pi n_1 n_2}}{n_1} + \frac{48}{\pi}\sum_{n_1,n_2=1}^{\infty} K_0(2\pi n_1 n_2) + \frac{48}{\pi}\sum_{n_1,n_2,n_3=1}^{\infty} K_0(2\pi n_1\sqrt{n_2^2+n_3^2}) \approx 2.7657. \tag{52}$$

One sees that the minimal volume of the cubic grain sustaining the transition is

$$V_{\min} = \left(C_3 \frac{\lambda}{\alpha T_0}\right)^3. \tag{53}$$

VI. CONCLUSIONS

In this paper we have discussed the spontaneous symmetry breaking of the $(\lambda\phi^4)_D$ theory compactified in $d \leqslant D$ Euclidean dimensions, extending some results of Ref. 1. We have parametrized the bare mass term in the form $m_0^2(T-T_0)$, thus placing the analysis within the Ginzburg–Landau framework. We focused on the situations with $D=3$ and $d=1,2,3$, corresponding (in the context of condensed matter systems) to films, wires, and grains, respectively, undergoing phase transitions which may be described by (mean-field) Ginzburg–Landau models. This generalizes to more compactified dimensions of previous investigations on the superconducting transition in films, both without[5] and in the presence of a magnetic field.[11] In all cases studied here, in the absence of gauge fluctuations, we found that the boundary-dependent critical temperature decreases linearly with the inverse of the linear dimension L: $T_c(L)=T_0-C_d\lambda/\alpha L$, where α and λ are the Ginzgurg–Landau parameters, T_0 is the bulk transition temperature, and C_d is a constant equal to 1.1024, 1.6571, and 2.6757 for $d=1$ (film), $d=2$ (square wire), and $d=3$ (cubic grain), respectively. Such behavior suggests the existence of a minimal size of the system below which the transition is suppressed. It is worth mentioning that having the transition temperature scaling with the inverse of the relevant length L for all the cases analyzed (films, wires, and grains) is in accordance with what one learns from finite-size scaling arguments.[12]

These findings seems to be in *qualitative* agreement with results for the existence of a minimal thickness for disappearance of superconductivity in films.[13–16] Experimental investigations in nanowires searching to establish whether there is a limit to how thin a superconducting wire can be, while retaining its superconducting character, have also drawn the attention of researchers; for example, in Ref. 17 the behavior of nanowires has been studied. Similar questions have also been raised concerning the behavior of superconducting nanograins.[18,19] Nevertheless, an important point to be emphasized is that our results are obtained in a field-theoretical framework and do not depend on microscopic details of the material involved nor account for the influence of manufacturing aspects of the sample; in other words, our results emerge solely as a topological effect of the compactification of the Ginzburg–Landau model in a subspace. Detailed microscopic analysis is required if one attempts to account quantitatively for experimental observations which might deviate from our mean field results.

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Uniqueness of the topological multivortex solution in the self-dual Chern–Simons theory

Kwangseok Choe[a)]
Department of Mathematics, Seoul National University, Seoul 151-747, Korea

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We establish a uniqueness result for the topological multivortex solution to the self-dual equations of the Abelian relativistic self-dual Chern–Simons–Higgs model. We prove that the topological multivortex solution is unique if the Chern–Simons coupling parameter $\kappa>0$ is sufficiently small. We also establish a uniqueness result for $\kappa>0$ sufficiently large. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Chern–Simons theories have attracted much attention as they are believed relevant to physical phenomena such as high-temperature superconductivity and anyon physics. In particular, Hong–Kim–Pac[18] and Jackiw–Weinberg[19] proposed an Abelian Chern–Simons–Higgs model whose dynamics is governed only by the Chern–Simons term. This model is given in the $(2+1)$-dimensional Minkowski space with metric $g_{\mu\nu}=\mathrm{diag}(1,-1,-1)$. When a suitable Higgs potential is chosen, this model admits a self-dual structure which enables us to study the static solutions rigorously.

The Lagrangian density[18,19] is given by

$$\mathcal{L}=\frac{\kappa}{4}\varepsilon^{\mu\nu\rho}F_{\mu\nu}A_\rho+g^{\mu\nu}D_\mu\phi\overline{D_\nu\phi}-\frac{1}{\kappa^2}|\phi|^2(1-|\phi|^2)^2,$$

where A_μ $(\mu=0,1,2)$ is a real gauge field on $\mathbb{R}^3$, ϕ is the complex-valued Higgs field, $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$ is the curvature tensor, $D_\mu=\partial_\mu-\sqrt{-1}A_\mu$ is the gauge covariant derivative, $\varepsilon^{\mu\nu\rho}$ is totally skew symmetric tensor with $\varepsilon^{012}=1$, and $\kappa>0$ is the Chern–Simons coupling constant. Hereafter, we let $i=\sqrt{-1}$.

The Euler–Lagrange equations corresponding to $\mathcal{L}$ are given by

$$\begin{aligned}&\frac{\kappa}{2}\varepsilon^{\mu\nu\rho}F_{\mu\nu}=i(\phi\overline{D^\rho\phi}-\overline{\phi}D^\rho\phi),\\&D_\mu D^\mu\phi=-\frac{1}{\kappa^2}(|\phi|^2-1)(3|\phi|^2-1)\phi.\end{aligned}\tag{1.1}$$

We seek the static configuration of (1.1). Then, the $\rho=0$ component of (1.1) yields $\kappa F_{12}=-2A_0|\phi|^2$, which in turn implies that the corresponding static energy density is given by

a)Electronic mail: kschoe@math.snu.ac.kr

$$\mathcal{E} = \frac{\kappa^2 F_{12}^2}{4|\phi|^2} + |D_1\phi|^2 + |D_2\phi|^2 + \frac{1}{\kappa^2}|\phi|^2(1-|\phi|^2)^2$$
$$= \left| \frac{\kappa F_{12}}{2|\phi|} \pm \frac{1}{\kappa}|\phi|(|\phi|^2-1) \right|^2 + |D_1\phi \pm iD_2\phi|^2 \pm F_{12} \mp i\varepsilon^{jk}\partial_j(\bar{\phi}D_k\phi).$$

By taking the conjugate $(\bar{\phi}, -A_\mu)$ of (ϕ, A_μ) if necessary, we may choose the upper sign in the above formula. If $|\phi||D\phi| = o(|x|^{-1})$ as $|x| \to \infty$, then $E = \int_{\mathbb{R}^2} \mathcal{E} dx \geqslant \int_{\mathbb{R}^2} F_{12} dx$, and the minimum is saturated if and only if (ϕ, A_μ) satisfies the following self-dual equations:

$$D_1\phi + iD_2\phi = 0,$$

$$F_{12} + \frac{2}{\kappa^2}|\phi|^2(|\phi|^2-1) = 0, \tag{1.2}$$

$$\kappa F_{12} + 2A_0|\phi|^2 = 0.$$

In order to make the total energy E finite, we impose a suitable boundary condition on ϕ; either $\lim_{|x|\to\infty}|\phi(x)| = 1$ or $\lim_{|x|\to\infty}|\phi(x)| = 0$. The former boundary condition is called topological, the latter one nontopological.

In this paper, we prove that the self-dual equations (1.2) admit a unique topological solution if $\kappa > 0$ is sufficiently small. As (1.2) admits the invariance $A_\mu \to A_\mu + \partial_\mu \eta$ and $\phi \to \phi e^{i\eta}$ for any smooth function $\eta = \eta(x_1, x_2)$, our uniqueness result is established in the sense of equivalence class. (See Main Theorem below.)

It follows from the argument of Jaffe–Taubes[20] that ϕ admits a discrete set of zeros. Then, we can establish existence results for the self-dual equations (1.2) such that ϕ vanishes at any prescribed points $p_1, \ldots, p_m \in \mathbb{R}^2$ with multiplicities $n_1, \ldots, n_m \in \mathbb{Z}_+$, respectively. For this purpose, we follow the argument in Ref. 20 to reduce the self-dual equations (1.2) to a single elliptic equation. Introduce a real-valued function u by

$$\phi = \exp\left[\frac{u}{2} + \sum_{j=1}^{m} i \arg(z - p_j) \right]. \tag{1.3}$$

Then, u satisfies

$$\Delta u = \frac{4}{\kappa^2} e^u (e^u - 1) + 4\pi \sum_{j=1}^{m} n_j \delta_{p_j}, \quad \mathbb{R}^2. \tag{1.4}$$

Once a solution u of (1.4) is found, we can construct a solution (ϕ, A_μ) by (1.3) and

$$A_1 = -\operatorname{Re}(i\partial^* \ln \phi), \quad A_2 = -\operatorname{Im}(i\partial^* \ln \phi) \quad \text{with} \quad \partial^* = \partial_1 + i\partial_2. \tag{1.5}$$

A solution u of (1.4) is topological if $\lim_{|x|\to\infty} u(x) = 0$, and nontopological if $\lim_{|x|\to\infty} u(x) = -\infty$. In both cases, it turns out that $|\phi||D\phi| = o(|x|^{-2})$ as $|x| \to \infty$. In the sequel, we let

$$N = \sum_{j=1}^{m} n_j.$$

Then, it is well known $E = \int_{\mathbb{R}^2} F_{12}\, dx = 2\pi N$ if $u = \ln|\phi|^2$ is topological. However, if u is nontopological, E may take all the values in an interval (see, e.g., Lemma 2.2 below). Moreover, it is also well known that the magnetic flux Φ and electric charge Q are given by $\Phi = \int F_{12}\, dx = E$ and $Q = \kappa \int F_{12}\, dx$, respectively. We refer to the books Refs. 15 and 31 for detailed description of self-dual Chern–Simons theories.

Several existence results are now available for the equation (1.4). The existence result for a topological solution was first established by Wang.[30] Spruck–Yang[28] constructed a topological solution via the iterative method, which is an efficient algorithm for a numerical solution.

For a nontopological solution, Spruck–Yang[27] constructed a radially symmetric solution for the special case $p_1=\cdots=p_m=0$. The result in Ref. 27 was refined by Chen *et al.*[10] and later by Chan *et al.*[8] In Ref. 8, they have established a uniqueness result for radial solutions: If $p_1=\cdots=p_m=0$ and a constant $\beta>2N+4$ is given, (1.4) admits a unique radial solution $u(r)$ such that $u(r)=-\beta \ln r+O(1)$ near ∞. The existence result for the general case where $p_1,\ldots,p_m$ is arbitrary was established by Chae–Imanuvilov.[7] It also turns out in Ref. 7 that if $N>0$, (1.4) admits a one-parameter family of nonradial solutions even if the vortex points p_j's are located at the origin. Hence, we cannot expect the uniqueness of nontopological solutions of (1.4) for $N>0$. It is believed that multiple existence for nontopological solutions depends on the total vortex number N and the location of vortex points p_j. If $N=0$, for instance, it can be proved by the method of moving planes[27] that every nontopological zero-vortex solution is radially symmetric with respect to some point in $\mathbb{R}^2$. If $N>0$, we cannot expect such symmetry any longer. Moreover, Chan *et al.*[8] recently constructed a nontopological solution concentrating at each vortex point $\{p_1,\ldots,p_m\}$ if $\Pi_{j\neq k}|p_j-p_k|$ is independent of k.

Then, it is quite natural to ask if Eq. (1.4) admits a unique topological solution for each $\kappa>0$. The uniqueness of a radial topological solution has been proved in Ref. 10. If $p_1=\cdots=p_m=0$ in (1.4), it has been proved by Han[17] that every topological solution is radially symmetric. Therefore, the uniqueness for the special case $p_1=\cdots=p_m=0$ has been established.

In this paper, we establish uniqueness for a topological solution for $\kappa>0$ sufficiently small.

Theorem 1.1: *Let $p_1,\ldots,p_m\in\mathbb{R}^2$ and $n_1,\ldots,n_m\in\mathbb{Z}_+$ be given. Then, there is a constant $\kappa_0=\kappa_0(p_1,\ldots,p_m,n_1,\ldots,n_m)>0$ such that for $0<\kappa<\kappa_0$, Eq. (1.4) admits a unique topological solution.*

Given $p_1,\ldots,p_m\in\mathbb{R}^2$ and $n_1,\ldots,n_m\in\mathbb{Z}_+$, we also establish a uniqueness result for $\kappa>0$ sufficiently large.

Theorem 1.2: *There is a constant $\kappa_1=\kappa_1(p_1,\ldots,p_m,n_1,\ldots,n_m)>0$ such that for $\kappa>\kappa_1$ Eq. (1.4) admits a unique topological solution.*

Once Theorem 1.1 is proved, we can state the uniqueness result for a solution (ϕ,A_μ) of the self-dual equations (1.2). Assume that (ϕ,A_μ) and $(\hat{\phi},\hat{A}_\mu)$ are two solutions subject to the topological boundary condition $\lim_{|x|\to\infty}|\phi(x)|=\lim_{|x|\to\infty}|\hat{\phi}(x)|=1$. Then, it is obvious that $\hat{A}_0=A_0$. Since $\nabla\times(\hat{A}-A)=0$ with $\hat{A}-A=(\hat{A}_1-A_1,\hat{A}_2-A_2)$, there is a smooth function η such that $\hat{A}-A=\nabla\eta$. Let $\alpha=A_1+iA_2$ and $\hat{\alpha}=\hat{A}_1+i\hat{A}_2$ for simplicity. Then, we can rewrite the first equation of the self-dual equations (1.2) as

$$\partial^*\phi=i\alpha\phi \quad \text{and} \quad \partial^*\hat{\phi}=i\hat{\alpha}\hat{\phi}.$$

Then, we obtain that $\partial^*(\hat{\phi}e^{-i\eta})=i\alpha\hat{\phi}e^{-i\eta}$, which in turn implies that $\partial^*(\hat{\phi}e^{-i\eta}/\phi)=0$. If ϕ and $\hat{\phi}$ have zeros in common, we conclude that $\hat{\phi}=\phi e^{i\eta+h}$ for some holomorphic function h. Due to the topological boundary condition, h must be a constant. Then, we have the uniqueness result for the topological solutions of the self-dual equations (1.2).

Main Theorem: *Given a topological solution u_κ of (1.4), let $(\phi^{(\kappa)},A_\mu^{(\kappa)})$ be given by (1.3) and (1.5) and $A_0^{(\kappa)}=(1/\kappa)|\phi^{(\kappa)}|^2(1-|\phi^{(\kappa)}|^2)$. Then, there are constants $\kappa_0,\kappa_1>0$ such that if $\kappa\in(0,\kappa_0)\cup(\kappa_1,\infty)$ then any topological solution $(\tilde{\phi}^{(\kappa)},\tilde{A}_\mu^{(\kappa)})$ of (1.2) satisfies $\tilde{A}_0^{(\kappa)}=A_0^{(\kappa)}$, $\tilde{A}^{(\kappa)}-A^{(\kappa)}=\nabla\eta_\kappa$ and $\tilde{\phi}^{(\kappa)}=\phi^{(\kappa)}e^{i\eta_\kappa}$ for a real-valued smooth function η_κ.*

We will prove Theorem 1.1 in Sec. III, but we sketch the proof here. We first prove that if $\kappa>0$ is sufficiently small, then any topological solution u_κ is approximated by the sum of rescaled radial topological solutions. More precisely, given $n_j\in\mathbb{Z}_+$, we let ϕ_j be the radial topological solution of $(1.4)_{\kappa=2}$. Then, we will show that if we define z_κ by

$$z_\kappa(x) = \frac{1}{\kappa^3}\left[u_\kappa(x) - \sum_{j=1}^{m} \chi_j(x)\phi_j\left(\frac{2(x-p_j)}{\kappa}\right)\right], \quad x \in \mathbb{R}^2,$$

then $\|z_\kappa\|_{H^2(\mathbb{R}^2)} = o(1)$ as $\kappa \to 0^+$. Here, $\chi_j \in C_0^\infty(\mathbb{R}^2)$ is a cutoff function which is identically 1 near the vortex point p_j. Then, we will construct a functional $\Phi_\kappa : H^2(\mathbb{R}^2) \to H^2(\mathbb{R}^2)$ in such a way that z_κ is a fixed point of Φ_κ for $\kappa > 0$ sufficiently small. Indeed, it will turn out that Φ_κ is a well-defined contraction mapping on a suitable closed subset $\mathcal{B}$ of $H^2(\mathbb{R}^2)$, and $z_\kappa \in \mathcal{B}$ for $\kappa > 0$ sufficiently small. Then, Theorem 1.1 immediately follows from uniqueness of a fixed point in $\mathcal{B}$. Thus, it is a crucial step to obtain the asymptotic behavior of a topological solution u_κ as $\kappa \to 0^+$.

It has been proved by Tarantello[29] that the "maximal" topological solution $\overline{u_\kappa}$ satisfies

$$\frac{4}{\kappa^2} e^{\overline{u}_\kappa}(1 - e^{\overline{u}_\kappa}) \to 4\pi \sum_{j=1}^{m} n_j \delta_{p_j} \quad \text{in the measure sense} \quad \text{as} \quad \kappa \to 0^+.$$

Thus, given any topological solution u_κ, we need to look into the concentration phenomena for u_κ near each p_j for $\kappa > 0$ sufficiently small. For this purpose, we divide $\mathbb{R}^2$ into two disjoint sets, $\Omega_d = \cup_j B_d(p_j)$ and the complement of Ω_d, and apply well-known arguments for uniform estimates and concentration phenomena to u_κ in Ω_d. (See, e.g., Refs. 5, 23, 22, 9, and 3, and references therein.)

Instead of typical topological/nontopological boundary conditions, one may impose the 't Hooft periodic boundary condition on the static configuration of (1.1) and study the equation on a flat torus, $\Omega = \mathbb{R}^2/(a\mathbb{Z} \times b\mathbb{Z})$ with $a, b > 0$. We can also derive self-dual equations (1.2) under the periodic boundary condition, and study the following equation for an unknown $u = \ln|\phi|^2$:

$$\Delta u = \frac{4}{\kappa^2} e^u (e^u - 1) + 4\pi \sum_{j=1}^{m} n_j \delta_{p_j} \quad \text{in} \quad \Omega. \tag{1.6}$$

An existence result for (1.6) was established by Caffarelli–Yang[6] (type I below), and later refined by Tarantello.[29] Tarantello, among other things, established multiple existence results for (1.6). In particular, Tarantello proved that if $N = 1$ then the self-dual equations admit at least two solutions $(\phi^{(\kappa)}, A^{(\kappa)})$ and $(\tilde{\phi}^{(\kappa)}, \tilde{A}^{(\kappa)})$ such that

(a) $|\phi^{(\kappa)}| \to 1$ a.e. as $\kappa \to 0^+$ (type I),

(b) $\forall q \geqslant 0$, $(1/\kappa^2)\|\tilde{\phi}^{(\kappa)}\|_{C^q(\Omega)} \leqslant C_q$ for some constant $C_q > 0$ (type II).
If $N \geqslant 2$, the situation becomes more delicate, and it requires a different approach to establish such multiple existence results. In this case, Eq. (1.4) may admit bubble solutions $\phi^{(\kappa)}$ such that

(c) $F_{12}(\phi^{(\kappa)}, A^{(\kappa)}) \to \Sigma_{k=1}^{l} m_k \delta_{q_k}$ as $\kappa \to 0^+$ in the sense of measure for some $m_k > 0$ and $q_k \in \Omega$. Moreover, $1/\kappa^2 \|\phi^{(\kappa)}\|_{C^0(K)} \to 0$ for any $K \subset\subset \Omega \setminus \{q_1, \ldots, q_l\}$ (type III).

Many experts have pointed out[29,25,12,13] that it is related to the concentration phenomena for a mean-field equation to classify and construct solutions of type II and type III. Recently, it was reported by Nolasco[24] that Eq. (1.4) admits a solution concentrating at the vortex points for $\kappa > 0$ sufficiently small. We also refer to Refs. 5, 23, 22, 9, and 3 for the concentration phenomena for a mean-field equation.

We are interested in the solution of type I. In the following theorem we establish uniqueness result for the solution of type I.

Theorem 1.3: *Let $\Omega = \mathbb{R}^2/(a\mathbb{Z} \times b\mathbb{Z})$ be a flat 2-torus. Then, there exists a constant $\kappa_1 = \kappa_1(p_1, \ldots, p_m, n_1, \ldots, n_m) > 0$ such that for $0 < \kappa < \kappa_1$ Eq. (1.6) admits unique periodic solution $u = \ln|\phi|^2$ which satisfies $u \to 0$ a.e. as $\kappa \to 0^+$.*

From the mathematical point of view, it would be interesting to consider the general situation where Eq. (1.6) is given on a Riemannian 2-manifold (Ω, γ) without boundary. (See Ref. 14.) In

Sec. IV, we will consider such a general situation and establish uniqueness result for $\kappa>0$ sufficiently small. See Theorem 4.1. Theorem 1.3 is indeed a direct consequence of Theorem 4.1. The proof of Theorem 4.1 is similar to that of Theorem 1.1, and we will sketch the proof in Sec. IV.

Theorem 1.3 shows that if $\kappa>0$ is sufficiently small, any solution u_κ of type I is indeed the maximal solution constructed by Caffarelli–Yang.[6] Moreover, the second solution $(\tilde{\phi}^{(\kappa)},\tilde{A}^{(\kappa)})$ found by Tarantello[29] satisfies $|\tilde{\phi}^{(\kappa)}|\to 0$ a.e. as $\kappa\to 0^+$. Theorems 1.1, 1.2, and 1.3 give a partial affirmative answer to the questions raised by Yang[31] and Ding *et al.*[14] The above uniqueness result would also be useful when we classify the solutions of (1.4) or (1.6) for $\kappa>0$ sufficiently small.

This paper is organized as follows. In Sec. II, we collect some well-known results on the solutions of Eq. (1.4). Section III is devoted to the proof of Theorem 1.1 and Theorem 1.2. In Sec. IV, we will sketch the proof of Theorem 1.3.

II. PRELIMINARIES

Hereafter, we let $\epsilon=\kappa/2$ for the sake of simplicity, and rewrite Eq. (1.4) as

$$\Delta u=\frac{1}{\epsilon^2}e^u(e^u-1)+4\pi\sum_{j=1}^{m}n_j\delta_{p_j},\quad \mathbb{R}^2 \tag{2.1}$$

$$u(x)\to 0\quad \text{as}\quad |x|\to\infty. \tag{2.2}$$

We will prove that given $p_1,\ldots,p_m\in\mathbb{R}^2$ and $n_1,\ldots,n_m\in\mathbb{Z}_+$, there is a constant $\epsilon_0=\epsilon_0(p_1,\ldots,p_m,n_1,\ldots,n_m)>0$ such that for $0<\epsilon<\epsilon_0$, Eqs. (2.1) and (2.2) admit a unique solution.

We begin this section by recalling some useful lemmas. Lemma A below is found in Ref. 16.

Lemma A: Given a domain $\Omega\subset\mathbb{R}^2$, let $d_x=\mathrm{dist}(x,\partial\Omega)$ for $x\in\Omega$. Then, $u\in C^2(\Omega)$ satisfies the estimate

$$\sup_\Omega d_x|\nabla u(x)|\leqslant C(\sup_\Omega|u|+\sup_\Omega d_x^2|\Delta u(x)|).$$

In the following two lemmas we collect well-known results for the special case where $p_1=\cdots=p_m=0$ in Eq. (2.1). Instead of the topological boundary condition (2.2), we impose a weaker condition on (2.1).

Lemma 2.1: Let n be a non-negative integer, and u be a solution of the following equation:

$$\begin{cases}\Delta u=e^u(e^u-1)+4\pi n\delta_{p=0}, & \mathbb{R}^2\\ \displaystyle\int_{\mathbb{R}^2}e^u(1-e^u)dx\leqslant C,\end{cases} \tag{2.3}$$

for some constant $C>0$. Then, either

$$\lim_{|x|\to\infty}u(x)=0$$

or

$$\lim_{|x|\to\infty}u(x)=-\infty.$$

Moreover, we have

(i) *if $u\to 0$ near ∞, then u is radially symmetric. Moreover, for each $R>1$ there is a constant $C_R>0$ such that $|u(x)|+|\nabla u(x)|\leqslant C_Re^{-|x|}$ for $|x|>R$.*

(ii) *if $u\to-\infty$ near ∞, then $\int_{\mathbb{R}^2}e^u(1-e^u)dx>8\pi(1+n)$.*

Proof: The proof may be well known to many experts, but we sketch it for completeness. It

follows from the argument of Spruck–Yang[27] that $u<0$ in $\mathbb{R}^2$. Hence, either $\lim_{|x|\to\infty}u(x)=0$ or $\liminf_{|x|\to\infty} u(x)<0$. In the latter case, we claim $\liminf_{|x|\to\infty} u(x)=-\infty$. Otherwise, Lemma A would imply that $\int_{\mathbb{R}^2} e^u(1-e^u)dx=\infty$, which yields a contradiction.

Moreover, it follows from the argument of Chen–Li[11] that there is a constant $\beta=\beta(u)>2$ such that $u(x)=-\beta\ln|x|+O(1)$ near ∞. Therefore, we conclude that if $\liminf_{|x|\to\infty} u(x)<0$ then $u(x)=-\beta\ln|x|+O(1)$ near ∞ for some constant $\beta>2$.

(i) If $\lim_{|x|\to\infty}u(x)=0$, it follows from the method of moving planes that u is radially symmetric.[17] Moreover, it is well known that $u(x)\leqslant C_R e^{-(2/3)|x|}$ for $|x|\geqslant R$, with $R>0$ sufficiently large. Notice that $\Delta u-u=O(u^2)$ near ∞. Comparing u with the comparison function $e^{-|x|}$, we can verify by maximum principle that $|u(x)|\leqslant C_R e^{-|x|}$ for $|x|\geqslant R$ with $R>0$ sufficiently large. The estimate for $|\nabla u(x)|$ follows from Lemma A.

(2) If $\lim_{|x|\to\infty}u(x)=-\infty$, then we have $\int_{\mathbb{R}^2}(e^u-e^{2u})dx=\pi(4n+2\beta)$. The inequality in (ii) follows from the Pohozaev identity. Indeed, multiplying (2.1) by $x\cdot\nabla u$ and integrating by parts on the domain $\Sigma_{\delta,R}=\{x|\delta<|x|<R\}$ with $\delta,R>0$, we obtain

$$\int_{\partial\Sigma_{\delta,R}}\left[\frac{1}{2}(x\cdot\nu)|\nabla u|^2-(x\cdot\nabla u)(\nu\cdot\nabla u)+\frac{1}{2}(x\cdot\nu)e^{2u}-(x\cdot\nu)e^u\right]d\sigma=\int_{\Sigma_{\delta,R}}(e^{2u}-2e^u)dx,$$

where ν is the outward normal vector on $\partial\Sigma_{\delta,R}$. Since $\nabla u(x)=\beta x/|x|^2+o(|x|^{-1})$ near ∞, and $u(x)=2n\ln|x|+v$ near $y=0$ for some smooth function v, we obtain

$$\int_{|x|=\delta}\frac{1}{|x|}(x\cdot\nabla u)^2d\sigma=\frac{1}{\delta}\int_{|x|=\delta}(2n+x\cdot\nabla v)^2d\sigma=8\pi n^2+O(\delta),$$

$$\int_{|x|=\delta}\frac{1}{2}|x||\nabla u|^2d\sigma=\frac{\delta}{2}\int_{|x|=\delta}\left(\frac{4n^2}{\delta^2}+O\left(\frac{1}{\delta}\right)\right)d\sigma=4\pi n^2+O(\delta),$$

as $\delta\to0$, and

$$\int_{|x|=R}\left[\frac{1}{2}(x\cdot\nu)|\nabla u|^2-(x\cdot\nabla u)(\nu\cdot\nabla u)\right]d\sigma=-\pi\beta^2+o(1)\quad\text{as}\quad R\to\infty.$$

Letting $\delta\to0^+$ and $R\to\infty$, we obtain $\pi(4n^2-\beta^2)=\int_{\mathbb{R}^2}(e^{2u}-2e^u)dx$. Then, we have $\int_{\mathbb{R}^2}e^{2u}dx=\pi((\beta-2)^2-4(n+1)^2)>0$. Hence, $\beta>2n+4$ and the desired inequality immediately follows. □

Remark: The Pohozaev identity also implies that if $u\to0$ near ∞ then $\int_{\mathbb{R}^2}(e^u-1)^2dx=4\pi n^2$. Indeed, proceeding as above, we obtain

$$\int_{\partial\Sigma_{\delta,R}}\left(\frac{1}{2}(x\cdot\nu)|\nabla u|^2-(x\cdot\nabla u)(\nu\cdot\nabla u)+\frac{1}{2}(x\cdot\nu)(e^u-1)^2\right)d\sigma=\int_{\partial\Sigma_{\delta,R}}(e^u-1)^2dy.$$

Letting $\delta\to0$ and $R\to\infty$, we obtain the desired result.

Spruck–Yang[27] proved that if $n=0$ then every nontrivial solution of (2.3) is radially symmetric with respect to some point. However, if $n>0$, it has been proved by Chae–Imanuvilov[7] that Eq. (2.3) admits a nonradial solution. If we limit our attention to the radial solutions of (2.3) for $n\geqslant0$, we have the uniqueness result (2.3) established by Chen *et al.*[10] and Chan *et al.*;[8] the topological radial solution is unique. Moreover, given a constant $\beta>2n+4$, (2.3) admits a unique radial solution $u(r)$ such that $u(x)-2n\ln|x|$ is smooth, and $u(r)=-\beta\ln r+O(1)$ as $r\to\infty$. More precisely, we have

Lemma 2.2 (Chen et al.[10]): Given a non-negative integer n, let $u(r;n,s)$ be the radial solution of (2.3) such that $\lim_{r\to0}(u(r;n,s)-2n\ln r)=s$ and $\lim_{r\to0}(u_r(r;n,s)-2n/r)=0$. Then, there is a constant $s_n\in\mathbb{R}$ such that

(i) $u(r;n,s_n)\to0$ *as* $r\to\infty$,

(ii) *If* $s<s_n$, $u(r;n,s_n)\to-\infty$ *as* $r\to\infty$,
(iii) *If* $s>s_n$, $u(r;n,s_n)$ *blows up at some* $r=r(s)$.

Moreover, if we define a function $\beta_n:(-\infty,s_n)\to\mathbb{R}_+=(0,\infty)$ *by*

$$\beta_n(s)=\int_0^\infty e^{u(r;n,s)}(1-e^{u(r;n,s)})r\,dr, \tag{2.4}$$

then $\lim_{s\to s_n}\beta_n(s)=\infty$, $\lim_{s\to-\infty}\beta_n(s)=2n+4$, *and* $\{\beta_n(s)|s<s_n\}=(2n+4,\infty)$.

(Chan et al.[8]*):* β_n *is differentiable and strictly increasing in the interval* $(-\infty,s_n)$.

Remark: It is obvious that $s_n=0$ if $n=0$ in (2.3).

Before proceeding, we fix some notations. For simplicity, we let $\mathcal{Z}=\{p_1,\ldots,p_m\}$ be the set of vortex points. Given a positive constant $r>0$, we let

$$\Omega_r=\bigcup_{j=1}^m B_r(p_j).$$

Hereafter, we denote by χ a cutoff function such that $0\leqslant\chi\leqslant1$, $\chi(x)=1$ for $|x|\leqslant1$, and $\chi(x)=0$ for $|x|\geqslant2$. Given a set Σ, we denote by Σ^c the complement of Σ. $C,c_0,\ldots$ will denote constants independent of ϵ. Throughout this paper, d is a fixed constant such that $0<d<\frac{1}{4}\min\{|p_k-p_j|1\leqslant k<j\leqslant m\}$.

Denote by ϕ_j the radial topological solution of the equation

$$\Delta\phi_j=e^{\phi_j}(e^{\phi_j}-1)+4\pi n_j\delta_{p=0},$$

$$\phi_j\to0\quad\text{near}\quad\infty. \tag{2.5}$$

We will prove in the following section that any solution u_ϵ of (2.1) and (2.2) is "close" to the rescaled radial solution $\phi_j(\epsilon^{-1}(x-p_j)+p_j)$ near each vortex point p_j. Then, we need an estimate for the linearized operator at ϕ_j in order to obtain *a priori* estimates for u_ϵ near $x=p_j$.

Lemma 2.3: Let $L_j:H^2(\mathbb{R}^2)\to L^2(\mathbb{R}^2)$ *be the linearized operator*

$$L_j=\Delta-e^{\phi_j}(2e^{\phi_j}-1).$$

Then, $L_j:H^2(\mathbb{R}^2)\to L^2(\mathbb{R}^2)$ *is one-to-one, and moreover, there is a constant* $c>0$ *such that* $\|L_ju\|_{L^2(\mathbb{R}^2)}\geqslant c\|u\|_{H^2(\mathbb{R}^2)}$ *for all* $u\in H^2(\mathbb{R}^2)$.

Proof: We first show that $L_j:H^2(\mathbb{R}^2)\to L^2(\mathbb{R}^2)$ is one-to-one. Assume that $u\in H^2(\mathbb{R}^2)$ satisfies $L_ju=0$. By Fourier expansion, it suffices to study the following eigenvalue problem:

$$u_k''+\frac{u_k'}{r}-\frac{k^2}{r^2}u_k=e^{\phi_j}(2e^{\phi_j}-1)u_k,$$

$$u_k(r)=r^k(1+O(r))\quad\text{near}\quad r=0,\quad k=0,1,\ldots.$$

We first claim that u_k is positive in $\mathbb{R}_+$ for all $k\geqslant0$. Let $\psi(r)=r\phi_j'(r)$. Then, ψ is positive in $\mathbb{R}_+$, and $\psi(r)=2N+O(r^{2n_j+2})$ near $r=0$. By comparing ψ with u_0, we obtain that $u_0>0$ in $\mathbb{R}_+$. Indeed, it is easily checked that

$$\psi''+\frac{\psi'}{r}=e^{\phi_j}(2e^{\phi_j}-1)\psi+2e^{\phi_j}(e^{\phi_j}-1).$$

Suppose that u_0 has a first zero at $r=r_0>0$, namely, $u_0(r_0)=0$ and $u_0>0$ in the interval $(0,r_0)$. Then, integration by parts gives that

$$0 < \int_0^{r_0} 2e^{\phi_j}(1-e^{\phi_j})u_0\, rdr = [r\psi u_0' - ru_0\psi']_0^{r_0} \leqslant 0,$$

which yields a contradiction. Hence, u_0 is positive in $\mathbb{R}_+$. A comparison lemma also shows that $u_k > 0$ in $\mathbb{R}_+$ for each $k \geqslant 1$. Indeed, if we suppose that u_k has a first zero at $r = r_k > 0$, then we obtain

$$0 < \int_0^{r_k} \frac{k^2}{r} u_0 u_k\, dr = [ru_0 u_k' - ru_k u_0']_0^{r_k} \leqslant 0,$$

which leads to a contradiction. Then, it is easily checked that $\lim_{r\to\infty}[u_k(r)/r] = \infty$. Therefore, we conclude that $ker\ L_j \cap H^2(\mathbb{R}^2) = \{0\}$.

We now prove the second part. We argue by contradiction and suppose that there exists a sequence $\{u_n\} \subset H^2(\mathbb{R}^2)$ such that $\|u_n\|_{H^2(\mathbb{R}^2)} = 1$ while $\|L_j u_n\|_{L^2(\mathbb{R}^2)} = o(1)$ as $n \to \infty$. Passing to a subsequence, we may assume that there exists $u_* \in H^2(\mathbb{R}^2)$ such that $u_n \rightharpoonup u_*$ weakly in $H^2(\mathbb{R}^2)$ and strongly in $W^{1,p}(\Omega)$ for $1 < p < \infty$ and any bounded domain Ω. It is obvious that $L_j u_* = 0$, and hence $u_* \equiv 0$. Consequently, $\|u_n\|_{H^1(\Omega)} = o(1)$ as $n \to \infty$ for each bounded domain $\Omega \subset \mathbb{R}^2$.

Fix a constant $R > 0$ such that $e^{\phi_j(R)} \geqslant 2/3$. Let $B_r^c = \{|x| \geqslant r\}$ and $A_r = \{r \leqslant |x| \leqslant r+1\}$ for a constant $r > 0$. Choose a cutoff function σ such that $0 \leqslant \sigma \leqslant 1$, $\sigma \equiv 1$ in $B_R(0)$, and $\sigma(x) = 0$ for $|x| \geqslant R+1$. Let $u_{1n} = \sigma u_n$ and $u_{2n} = (1-\sigma)u_n$. Then, it is easy to check that

$$L_j u_{2n} = (1-\sigma)L_j u_n - 2\nabla u_n \cdot \nabla \sigma - u_n \Delta\sigma, \tag{2.6}$$

and $\|u_{1n}\|_{H^1(B_{R+1}(0))} = o(1)$ as $n \to \infty$. Multiplying (2.6) by u_{2n}, and integrating by parts, we obtain

$$\|\nabla u_{2n}\|_{L^2(B_R^c)} + \|u_{2n}\|_{L^2(B_R^c)} \leqslant C(\|u_n\|_{H^1(A_R)} + \|L_j u_n\|_{L^2(B_R^c)}) = o(1).$$

In particular, $\|u_n\|_{H^1(B_{R+1}^c)} = o(1)$, which in turn implies that $\|u_n\|_{H^1(\mathbb{R}^2)} = o(1)$ as $n \to \infty$. Consequently, we obtain

$$\|D^2 u_n\|_{L^2(\mathbb{R}^2)} = \|\Delta u_n\|_{L^2(\mathbb{R}^2)} \leqslant \|u_n\|_{L^2(\mathbb{R}^2)} + \|L_j u_n\|_{L^2(\mathbb{R}^2)} = o(1),$$

which yields a contradiction. The proof of Lemma 2.3 is complete. □

Remark: Since $L_j : H^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2)$ is self-adjoint, it follows from Lemma 2.3 that L_j is an isomorphism from $H^2(\mathbb{R}^2)$ onto $L^2(\mathbb{R}^2)$.

III. UNIQUENESS OF A TOPOLOGICAL SOLUTION

We first prove Theorem 1.1. To this end, we first obtain the *a priori* estimates for a solution u_ϵ of (2.1) and (2.2) as $\epsilon \to 0^+$. Those estimates will be given in the following two lemmas.

Lemma 3.1: Let u_ϵ be any topological solution of (2.1). *Then, there is a constant $\epsilon_0 = \epsilon_0(d) > 0$ such that if $0 < \epsilon < \epsilon_0$ then*

$$\|u_\epsilon\|_{H^2(\Omega_d^c)} \leqslant c_0 \exp[-c_1/\epsilon], \tag{3.1}$$

for some positive constants c_0, c_1 depending only on d.

Proof: We divide the proof into three steps.

Step 1: We claim that for each compact subset $K \subset \mathbb{R}^2 \setminus \mathcal{Z}$, there are constants $\epsilon_* > 0$ and $\gamma_0(K) < 0$ such that $\gamma_0(K) \leqslant u_\epsilon < 0$ in K for $0 < \epsilon < \epsilon_*$.

Let

$$u_*(x) = \sum_j 2n_j \ln|x - p_j|,$$

and $v_\epsilon = u_\epsilon - u_*$. Fix a constant $R > \sup_j |p_j|$. Then, it suffices to prove that if $\epsilon > 0$ is sufficiently small then $\inf_{B_R(0)} v_\epsilon \geqslant \gamma_0$ for some constant $\gamma_0(R) < 0$.

We argue by contradiction and suppose that there are sequences $\{\epsilon_n\}$ and $\{x_n\}\subset B_R(0)$ such that $\epsilon_n\to 0^+$ and $v_{\epsilon_n}(x_n)=\inf_{B_R(0)}v_{\epsilon_n}\to-\infty$. For simplicity, we let $v_n:=v_{\epsilon_n}$.

Decompose $v_n=v_{1n}+v_{2n}$, where

$$\begin{cases}\Delta v_{1n}=\dfrac{1}{\epsilon_n^2}e^{u_*+v_n}(e^{u_*+v_n}-1), & B_R(0)\\ v_{1n}=0, & \partial B_R(0)\end{cases}$$

and

$$\begin{cases}\Delta v_{2n}=0, & B_R(0)\\ v_{2n}=v_n, & \partial B_R(0).\end{cases}$$

By the Harnack inequality, we may assume $v_{2n}\to-\infty$ uniformly on $B_R(0)$.

On the other hand, following the argument of Tarantello,[29] we can verify that v_{1n} is bounded in $W_0^{1,q}(B_R(0))$ for each $1<q<2$. By passing to a subsequence, we may assume that $v_{1n}\rightharpoonup v_\infty$ weakly in $W_0^{1,q}(B_R(0))$, and strongly in $L^p(B_R(0))$ for $1\leqslant p<2q/(2-q)$. Consequently, $v_n\to-\infty$ almost everywhere on $B_R(0)$.

Consider the function $\beta_0(s)$ defined in (2.4), and fix a constant $s_0<0$ such that $\beta_0(s_0)>2N$. Let $u_n=v_n+u_*$. For each n, choose $y_n\in\mathbb{R}^2$ such that

$$u_n(y_n)=s_0 \quad\text{and}\quad |y_n|=\sup\{|x|\,|\,u_n(x)=s_0.$$

Notice that $\inf_{|x|\geqslant r}u_n(x)=\inf_{|x|=r}u_n(x)$ for each $r>\sup_j|p_j|$. Since $u_n\to-\infty$ almost everywhere on each compact subset, $|y_n|\to\infty$.

Let $\overline{u_n}(x)=u_n(\epsilon_n x+y_n)$. Then, $\overline{u_n}$ satisfies

$$\begin{cases}\Delta\overline{u_n}=e^{\overline{u_n}}(e^{\overline{u_n}}-1), & \Omega_n:=\{|x|<|y_n|/2\epsilon_n\}\\ \displaystyle\int_{\Omega_n}e^{\overline{u_n}}(1-e^{\overline{u_n}})dx\leqslant 4\pi N.\end{cases}$$

Since $\overline{u_n}(0)=s_0$ and $\overline{u_n}<0$, the argument of Brezis–Merle[5] implies that $\overline{u_n}$ is bounded in $C^0_{loc}(\Omega_n)$. Then, we may assume that $\overline{u_n}$ converges in $C^2_{loc}(\mathbb{R}^2)$ to $\overline{u_*}$ which is a solution of

$$\begin{cases}\Delta\overline{u_*}=e^{\overline{u_*}}(e^{\overline{u_*}}-1), & \mathbb{R}^2,\\ \displaystyle\int_{\mathbb{R}^2}e^{\overline{u_*}}(1-e^{\overline{u_*}})dx\leqslant 4\pi N.\end{cases}$$

Since $\overline{u_*}(0)=s_0<0$, Lemma 2.1 implies that $\overline{u_*}$ is radially symmetric with respect to some point in $\mathbb{R}^2$. Consequently

$$\int_{\mathbb{R}^2}e^{\overline{u_*}}(1-e^{\overline{u_*}})dx\geqslant 2\pi\beta_0(s_0)>4\pi N,$$

which yields a contradiction.

Step 2: Recall that $\Omega_d=\cup_j B_d(p_j)$. We claim that $u_\epsilon\to 0$ in $C^0(\Omega_d^c)$ as $\epsilon\to 0^+$. Moreover, if $\epsilon>0$ is sufficiently small, then

$$\|u_\epsilon\|_{L^\infty(\Omega_d^c)}\leqslant c_2\,\exp[-c_3/\epsilon] \tag{3.2}$$

for some constants $c_2(d),c_3(d)>0$. We note that for each $d>0$, $\|u_\epsilon\|_{L^\infty(\Omega_d^c)}$ is attained on $\partial\Omega_d$. Thus, it suffices to prove $\|u_\epsilon\|_{L^\infty(\partial\Omega_d)}\leqslant\exp[-c_3/\epsilon]$.

The second claim follows from the maximum principle. Indeed, fix two constants $\epsilon_*>0$ and $m<0$ such that $u_\epsilon\geqslant m$ on $\Omega_{d/2}^c$ for $0<\epsilon<\epsilon_*$. Then, it follows that

$$-\epsilon^2\Delta u_\epsilon + e^{2m}u_\epsilon \geqslant 0 \quad \text{on} \quad \Omega^c_{d/2}.$$

For each $x_0 \in \partial\Omega_d$, we define a comparison function w_ϵ by

$$w_\epsilon(x) = (1-m)\exp\left[\frac{e^m}{2d\epsilon}(|x-x_0|^2 - d^2/4)\right] \quad \text{for} \quad |x-x_0| \leqslant d/2.$$

It is easy to check that if $\epsilon > 0$ is sufficiently small

$$-\epsilon^2\Delta(u_\epsilon + w_\epsilon) + e^{2m}(u_\epsilon + w_\epsilon) > 0 \quad \text{on} \quad B_{d/2}(x_0).$$

Then, the maximum principle implies that $(u_\epsilon + w_\epsilon)(x) > (u_\epsilon + w_\epsilon)|_{|x-x_0|=d/2} > 0$ for $|x-x_0| \leqslant d/2$. In particular, there is a constant $c > 0$ such that $u_\epsilon(x) > -\exp[-c/\epsilon]$ for $|x-x_0| \leqslant d/4$. Since the constant c is indepedent of the choice of $x_0 \in \partial\Omega_d$, (3.2) immediately follows.

Step 3: We now prove (3.1). Notice that $\|u_\epsilon\|_{L^\infty(\Omega^c_{d/2})} \leqslant c_2\exp[-c_3/\epsilon]$, and

$$\epsilon^2\Delta u_\epsilon - u_\epsilon = O(1)|u_\epsilon|^2 \quad \text{in} \quad \Omega^c_{d/2}, \tag{3.3}$$

where $O(1)$ denotes a quantity which is uniformly bounded in $C^0(\Omega^c_{d/2})$. Let σ be a smooth function such that $0 \leqslant \sigma \leqslant 1$, $\sigma(x) = 1$ for $x \in \Omega^c_{3d/4}$, and $\sigma(x) = 0$ for $x \in \Omega_{d/2}$. Multiplying (3.3) by σu_ϵ and integrating by parts, we obtain

$$\begin{aligned}\epsilon^2\|\nabla u_\epsilon\|^2_{L^2(\Omega^c_{3d/4})} + \|u_\epsilon\|^2_{L^2(\Omega^c_{3d/4})} &\leqslant C(d)\left[\int_{\Omega_d\setminus\Omega_{d/2}} (\epsilon^2|\Delta\sigma|u_\epsilon^2 + \sigma|u_\epsilon|^3)dx + \int_{\Omega^c_d}|u_\epsilon|^3 dx\right] \\ &\leqslant C(d)[\exp(-c/\epsilon) + \|u_\epsilon\|_{L^\infty(\Omega^c_d)}\|u_\epsilon\|^2_{L^2(\Omega^c_d)}],\end{aligned}$$

which in turn implies that if $\epsilon > 0$ is sufficiently small

$$\epsilon\|\nabla u_\epsilon\|_{L^2(\Omega^c_{3d/4})} + \|u_\epsilon\|_{L^2(\Omega^c_{3d/4})} \leqslant C(d)\epsilon\,\exp[-c_3/\epsilon]. \tag{3.4}$$

Choose a smooth function $\tilde{\sigma}$ such that $0 \leqslant \tilde{\sigma} \leqslant 1$, $\tilde{\sigma}(x) = 1$ for $x \in \Omega^c_d$ and $\tilde{\sigma}(x) = 0$ for $x \in \Omega_{3d/4}$. We note that

$$\|D^2(\tilde{\sigma}u_\epsilon)\|_{L^2(\mathbb{R}^2)} = \|\Delta(\tilde{\sigma}u_\epsilon)\|_{L^2(\mathbb{R}^2)} \leqslant C(\|\Delta u_\epsilon\|_{L^2(\Omega^c_{3d/4})} + \|u_\epsilon\|_{H^1(\Omega^c_{3d/4})}). \tag{3.5}$$

Then, Lemma 3.1 is an immediate consequence of (3.4) and (3.5). □

We now investigate the asymptotic behavior of u_ϵ in each ball $B_d(p_j)$. For each $1 \leqslant j \leqslant m$, let $\hat{u}_{\epsilon,j}(x) = u_\epsilon(\epsilon x + p_j)$ for $|x| \leqslant 2d/\epsilon$. Then, $\hat{u}_{\epsilon,j}$ satisfies

$$\Delta\hat{u}_{\epsilon,j} = e^{\hat{u}_{\epsilon,j}}(e^{\hat{u}_{\epsilon,j}} - 1) + 4\pi n_j\delta_{p=0} \quad \text{for} \quad |x| \leqslant 2d/\epsilon, \tag{3.6}$$

and $|\hat{u}_{\epsilon,j}(x)| = O(e^{-c/\epsilon})$ for $|x| = 2d/\epsilon$. It follows from the Pohozaev identity that

$$\int_{|y|\leqslant 2d/\epsilon} (1 - e^{\hat{u}_{\epsilon,j}})^2 dy = 4\pi n_j^2 + o(e^{-c/\epsilon}), \tag{3.7}$$

for some constant $c > 0$.

The following lemma shows the asymptotic behavior of $\hat{u}_{\epsilon,j}$ in the ball $B_{d/\epsilon}(0)$.

Lemma 3.2: There is a constant $\epsilon_1 = \epsilon_1(d) > 0$ such that if $0 < \epsilon < \epsilon_1$, then

$$\sup_j \|\hat{u}_{\epsilon,j} - \phi_j\|_{H^2(|x|\leqslant d/\epsilon)} \leqslant C_0\,\exp[-C_1/\epsilon], \tag{3.8}$$

for some positive constants C_0 and C_1 depending only on d.

Proof: It follows from Lemma 3.1 that if $\epsilon > 0$ is sufficiently small, then there are positive constants c_0, c_1 such that $\|\hat{u}_{\epsilon,j}\|_{H^2(d/\epsilon\leqslant|x|\leqslant 2d/\epsilon)} \leqslant c_0\,\exp[-c_1/\epsilon]$. The proof of Lemma 3.2 will be given in three steps.

Step 1: We claim that $\hat{u}_{\epsilon,j}-\phi_j\to 0$ in $C^2_{loc}(\mathbb{R}^2)$ as $\epsilon\to 0^+$.

Let $\hat{v}_{\epsilon,j}=\hat{u}_{\epsilon,j}-2n_j\ln|x|$. Then, $\hat{v}_{\epsilon,j}$ satisfies

$$\Delta\hat{v}_{\epsilon,j}=|x|^{2n_j}e^{\hat{v}_{\epsilon,j}}(|x|^{2n_j}e^{\hat{v}_{\epsilon,j}}-1)\quad\text{for}\quad|x|\leqslant 2d/\epsilon,$$

$$\int_{|x|\leqslant 2d/\epsilon}|x|^{2n_j}e^{\hat{v}_{\epsilon,j}}(1-|x|^{2n_j}e^{\hat{v}_{\epsilon,j}})dx=4\pi n_j+o(e^{-c/\epsilon}).$$

We claim that $\hat{v}_{\epsilon,j}$ is bounded in $C^0_{loc}(\mathbb{R}^2)$.

Indeed, since $|x|^{2n_j}e^{\hat{v}_{\epsilon,j}}\leqslant 1$, it follows from the Harnack inequality that either $\hat{v}_{\epsilon,j}$ is bounded in $C_{loc}(\mathbb{R}^2)$, or $\hat{v}_{\epsilon,j}\to-\infty$ uniformly on any compact subset of $\mathbb{R}^2$. If $\hat{v}_{\epsilon,j}\to-\infty$ on any compact subset, then it follows that $\int_{|y|\leqslant R}(1-e^{\hat{u}_{\epsilon,j}})^2dy=\pi R^2+o(1)$ as $\epsilon\to 0^+$ for each $R>0$, which contradicts (3.7). Therefore, $\hat{v}_{\epsilon,j}$ is bounded in $C^0_{loc}(\mathbb{R}^2)$.

By passing to a subsequence, we may assume that $\hat{v}_{\epsilon,j}$ converges uniformly in $C^2_{loc}(\mathbb{R}^2)$ to a function $v_*\in C^2(\mathbb{R}^2)$, which satisfies

$$\Delta v_*=|x|^{2n_j}e^{v_*}(|x|^{2n_j}e^{v_*}-1)\quad\text{in}\quad\mathbb{R}^2,$$

$$\int_{\mathbb{R}^2}|x|^{2n_j}e^{v_*}(1-|x|^{2n_j}e^{v_*})dx\leqslant 4\pi n_j.$$

Let $u_*(x)=v_*(x)+2n_j\ln|x|$. Then, Lemma 2.1 implies that $u_*(x)\to 0$ as $|x|\to\infty$, and hence u_* is radially symmetric. It follows from the uniqueness of radial topological solution[10] that $u_*=\phi_j$.

Step 2: We claim $\sup_{|x|\leqslant 2d/\epsilon}|(\hat{u}_{\epsilon,j}-\phi_j)(x)|\to 0$ as $\epsilon\to 0^+$.

For simplicity, we let

$$\hat{w}_{\epsilon,j}=\hat{u}_{\epsilon,j}-\phi_j,$$

and fix a constant $R_0>0$ such that $e^{\phi_j(R_0)}\geqslant 2/3$. We argue by contradiction and suppose that there exist sequences $\{\epsilon_n\}$ and $\{x_n\}\subset B_{2d/\epsilon_n}(0)$ such that $\epsilon_n\to 0^+$ and

$$|\hat{w}_{\epsilon_n,j}(x_n)|=\sup_{|x|\leqslant 2d/\epsilon_n}|\hat{w}_{\epsilon_n,j}(x)|\geqslant\gamma_0$$

for some constant $\gamma_0>0$. It follows from the previous step that $|x_n|\to\infty$, and we may assume that $R_0<|x_n|<2d/\epsilon_n$. Let $\hat{w}_n=\hat{w}_{\epsilon_n,j}$ for simplicity.

If $\hat{w}_n(x_n)>0$, then we have

$$0\geqslant\Delta\hat{w}_n(x_n)=e^{\phi_j(x_n)+\hat{w}_n(x_n)}(e^{\phi_j(x_n)+\hat{w}_n(x_n)}-1)-e^{\phi_j(x_n)}(e^{\phi_j(x_n)}-1)>0,$$

which yields a contradiction. Consequently, $\hat{w}_n(x_n)<0$. Since $\Delta\hat{w}_n(x_n)\geqslant 0$, we have

$$e^{\phi_j(x_n)+\hat{w}_n(x_n)}+e^{\phi_j(x_n)}\leqslant 1.$$

Then, it follows from Lemma 2.1 that $\hat{w}_n(x_n)\leqslant\ln(e^{-\phi_j(x_n)}-1)\leqslant-|x_n|+C$ for some constant C. In particular, $\hat{w}_n(x_n)\to-\infty$ as $n\to\infty$.

Since $\phi_j<0$ and $\phi_j+w_n<0$, it follows from the Harnack inequality that $\phi_j+\hat{w}_n\to-\infty$ uniformly on $B_R(x_n)$. Then, it follows that $\int_{|x-x_n|<R}(1-e^{\phi_j+\hat{w}_n})^2dx=\pi R^2+o(1)$, which contradicts (3.7).

Step 3: We are now ready to prove the inequality (3.8). Recall that χ is a cutoff function such that $0\leqslant\chi\leqslant 1$, $\chi\equiv 1$ on $B_1(0)$ and $\chi\equiv 0$ outside $B_2(0)$. Let $\sigma_\epsilon(x)=\chi(\epsilon x/d)$.

Since $0\leqslant e^t-1-t\leqslant(t^2/2)e^{\max\{0,t\}}$ for $t\in\mathbb{R}$, we have $L_j\hat{w}_{\epsilon,j}=O(1)|\hat{w}_{\epsilon,j}|^2$ pointwise for $|x|\leqslant 2d/\epsilon$. Then, it is easy to check that

$$L_j(\sigma_\epsilon\hat{w}_{\epsilon,j})=2\nabla\hat{w}_{\epsilon,j}\cdot\nabla\sigma_\epsilon+\hat{w}_{\epsilon,j}\Delta\sigma_\epsilon+O(1)\sigma_\epsilon|\hat{w}_{\epsilon,j}|^2.$$

Let $\hat{A}_\epsilon=\{d/\epsilon\leqslant|x|\leqslant 2d/\epsilon\}$. Then, Lemma 2.3 implies that

$$\|\sigma_\epsilon \hat{w}_{\epsilon,j}\|_{H^2(\mathbb{R}^2)} \leq C(\epsilon\|\nabla \hat{w}_{\epsilon,j}\|_{L^2(\hat{A}_\epsilon)} + \epsilon^2\|\hat{w}_{\epsilon,j}\|_{L^2(\hat{A}_\epsilon)} + \sup_{|x|\leq 2d/\epsilon}|\hat{w}_{\epsilon,j}(x)|\|\sigma_\epsilon \hat{w}_{\epsilon,j}\|_{L^2(\mathbb{R}^2)})$$

for some constant $C=C(d)>0$. Since $\sup_{|x|\leq 2d/\epsilon}|\hat{w}_{\epsilon,j}(x)|=o(1)$ as $\epsilon\to 0^+$, we obtain

$$\begin{aligned}\|\hat{w}_{\epsilon,j}\|_{H^2(|x|\leq d/\epsilon)} \leq \|\sigma_\epsilon \hat{w}_{\epsilon,j}\|_{H^2(\mathbb{R}^2)} &\leq C(\epsilon\|\nabla \hat{w}_{\epsilon,j}\|_{L^2(\hat{A}_\epsilon)} + \epsilon^2\|\hat{w}_{\epsilon,j}\|_{L^2(\hat{A}_\epsilon)}) \\ &\leq C\epsilon\|\hat{w}_{\epsilon,j}\|_{H^2(d/\epsilon\leq|x|\leq 2d/\epsilon)} \leq C_0\exp[-C_1/\epsilon]\end{aligned}$$

for some constants $C_0, C_1>0$ if $\epsilon>0$ is sufficiently small. The proof of Lemma 3.2 is complete.□

For each $1\leq j\leq m$, let $\chi_j(x)=\chi((x-p_j)/d)$. Given a solution u_ϵ of (2.1) and (2.2), let

$$z_\epsilon(x) = \frac{1}{\epsilon^3}\left[u_\epsilon(x) - \sum_{j=1}^m \chi_j(x)\phi_j\left(\frac{x-p_j}{\epsilon}\right)\right], \quad x\in\mathbb{R}^2. \tag{3.9}$$

For the sake of simplicity, we let $\phi_{j,\epsilon}(x)=\phi_j((x-p_j)/\epsilon)$ for $1\leq j\leq m$ and $\epsilon>0$. Then, $z_\epsilon \in H^2(\mathbb{R}^2)$ satisfies

$$\begin{aligned}\Delta z_\epsilon = \frac{1}{\epsilon^5}\exp\left[\sum_j \chi_j\phi_{j,\epsilon} + \epsilon^3 z_\epsilon\right]\left(\exp\left[\sum_j \chi_j\phi_{j,\epsilon} + \epsilon^3 z_\epsilon\right] - 1\right) - \frac{1}{\epsilon^5}\sum_j \chi_j e^{\phi_{j,\epsilon}}(e^{\phi_{j,\epsilon}}-1) \\ - \frac{1}{\epsilon^3}\sum_j [2\nabla\chi_j\cdot\nabla\phi_{j,\epsilon} + \phi_{j,\epsilon}\Delta\chi_j] \quad \text{in} \quad \mathbb{R}^2,\end{aligned} \tag{3.10}$$

and, moreover, it follows from Lemma 3.1 and Lemma 3.2 that $\|z_\epsilon\|_{H^2(\mathbb{R}^2)}=o(1)$ as $\epsilon\to 0^+$.

Given a solution u_ϵ of (2.1) and (2.2), we construct a functional $\Phi_\epsilon: H^2(\mathbb{R}^2)\to H^2(\mathbb{R}^2)$ in such a way that z_ϵ defined in (3.9) is a fixed point of Φ_ϵ. For this purpose, we define an auxiliary functional $F_\epsilon: H^2(\mathbb{R}^2)\to L^2(\mathbb{R}^2)$ by

$$\begin{aligned}F_\epsilon(v) = \Delta v - \frac{1}{\epsilon^5}\exp\left[\sum_j \chi_j\phi_{j,\epsilon} + \epsilon^3 v\right]\left(\exp\left[\sum_j \chi_j\phi_{j,\epsilon} + \epsilon^3 v\right] - 1\right) \\ + \frac{1}{\epsilon^5}\sum_j \chi_j e^{\phi_{j,\epsilon}}(e^{\phi_{j,\epsilon}}-1) + \frac{1}{\epsilon^3}\sum_j [2\nabla\chi_j\cdot\nabla\phi_{j,\epsilon} + \phi_{j,\epsilon}\Delta\chi_j].\end{aligned} \tag{3.11}$$

Indeed, Φ_ϵ will be defined in terms of F_ϵ and $DF_\epsilon(0)$. In order to prove that Φ_ϵ has a unique fixed point in $H^2(\mathbb{R}^2)$, we show that Φ_ϵ is a well-defined contraction mapping on a suitable bounded subset $\mathcal{B}$ of $H^2(\mathbb{R}^2)$. Thus, we need to obtain some estimates for F_ϵ and $DF_\epsilon(0)$. We prove in the following lemma useful properties of F_ϵ for $\epsilon>0$ sufficiently small.

Lemma 3.3: If $\epsilon>0$ is sufficiently small, we have

(a) $\|F_\epsilon(0)\|_{L^2(\mathbb{R}^2)}\leq c_0\exp[-c_1/\epsilon]$ *for some constants* $c_0, c_1>0$.

(b) $DF_\epsilon(0)$ *is an isomophism from* $H^2(\mathbb{R}^2)$ *onto* $L^2(\mathbb{R}^2)$, *and there is a constant* $C>0$ *such that*

$$\|DF_\epsilon(0)h\|_{L^2(\mathbb{R}^2)} \geq C\|h\|_{H^2(\mathbb{R}^2)} \quad \textit{for all} \quad h\in H^2(\mathbb{R}^2). \tag{3.12}$$

(c) $\|DF_\epsilon(z)h - DF_\epsilon(0)h\|_{L^2(\mathbb{R}^2)}\leq C\epsilon\|h\|_{H^2(\mathbb{R}^2)}$ *for* $\|z\|_{H^2(\mathbb{R}^2)}\leq 1$.

Proof:

(a) Estimate for $F_\epsilon(0)$: We note that $F_\epsilon(0)\equiv 0$ both on $\Omega_d=\cup_j B_d(p_j)$ and on Ω_{2d}^c. Moreover, if we set $\Sigma_j=B_{2d}(p_j)\setminus B_d(p_j)$ for each $1\leq j\leq m$, it follows from Lemma 2.1 that

$$\sup_{1\leq j\leq m}(\|\phi_{j,\epsilon}\|_{L^\infty(\Sigma_j)} + \|\nabla\phi_{j,\epsilon}\|_{L^\infty(\Sigma_j)}) \leq c_0\exp[-c_1/\epsilon]$$

for some constants $c_0, c_1>0$. Then (a) follows from the inequality $|e^t-1|\leq|t|e^{|t|}$.

(b) Estimate for $\|DF_\epsilon(0)\|$: Notice that for $h\in H^2(\mathbb{R}^2)$

$$DF_\epsilon(0)h = \Delta h - \frac{1}{\epsilon^2}\exp\left[\sum_j \chi_j \phi_{j,\epsilon}\right]\left(2\,\exp\left[\sum_j \chi_j \phi_{j,\epsilon}\right] - 1\right)h.$$

The proof of (b) is essentially similar to that of Lemma 2.3. We argue by contradiction and suppose there are sequences $\{\epsilon_n\}$ and $\{h_n\} \subset H^2(\mathbb{R}^2)$ such that $\epsilon_n \to 0^+$, $\|h_n\|_{H^2(\mathbb{R}^2)} = 1$, and $\|DF_{\epsilon_n}(0)h_n\|_{L^2(\mathbb{R}^2)} = o(1)$ as $n \to \infty$.

For each $1 \leqslant j \leqslant m$, we let $\tilde{\sigma}_j(x) = \chi(4(x-p_j)/d)$ and $\tilde{h}_n = (1 - \Sigma_j\, \tilde{\sigma}_j)h_n$. Then, $\tilde{h}_n$ satisfies

$$\begin{aligned}\Delta\tilde{h}_n - \frac{1}{\epsilon_n^2}\exp\left[\sum_j \chi_j \phi_{j,\epsilon_n}\right]\left(2\,\exp\left[\sum_j \chi_j \phi_{j,\epsilon_n}\right] - 1\right)\tilde{h}_n \\ = -\sum_j 2\,\nabla h_n \cdot \nabla \tilde{\sigma}_j - \sum_j h_n \Delta\tilde{\sigma}_j + \left(1 - \sum_j \tilde{\sigma}_j\right)DF_{\epsilon_n}(0)h_n. \qquad (3.13)\end{aligned}$$

Recall $\Omega_r^c = [\cup_j B_r(p_j)]^c$ for a constant $r > 0$. Multiplying (3.13) by $\tilde{h}_n$ and integrating by parts, we obtain for n sufficiently large

$$\|\nabla\tilde{h}_n\|^2_{L^2(\Omega^c_{d/4})} + \frac{1}{\epsilon_n^2}\|\tilde{h}_n\|^2_{L^2(\Omega^c_{d/4})} \leqslant C\|\tilde{h}_n\|_{L^2(\Omega^c_{d/4})}(\|h_n\|_{H^1(\Omega^c_{d/4})} + \|DF_{\epsilon_n}(0)h_n\|_{L^2(\Omega^c_{d/4})}) \quad (3.14)$$

for some constant $C = C(d) > 0$. Then, it follows from the assumption that

$$\begin{aligned}\|\nabla h_n\|_{L^2(\Omega^c_{d/2})} + \frac{1}{\epsilon_n}\|h_n\|_{L^2(\Omega^c_{d/2})} &\leqslant \|\nabla\tilde{h}_n\|_{L^2(\Omega^c_{d/4})} + \frac{1}{\epsilon_n}\|\tilde{h}_n\|_{L^2(\Omega^c_{d/4})} \\ &\leqslant C\epsilon_n(\|h_n\|_{H^1(\Omega^c_{d/4})} + \|DF_{\epsilon_n}(0)h_n\|_{L^2(\Omega^c_{d/4})}) \leqslant C\epsilon_n. \qquad (3.15)\end{aligned}$$

Let $\sigma_j^*(x) = \chi(2(x-p_j)/d)$ and $h_n^* = (1 - \Sigma_j\, \sigma_j^*)h_n$. By repeating the above argument (3.13) and (3.14) on $\Omega^c_{d/2}$, we obtain

$$\|\nabla h_n^*\|_{L^2(\Omega^c_{d/2})} + \frac{1}{\epsilon_n}\|h_n^*\|_{L^2(\Omega^c_{d/2})} \leqslant C\epsilon_n(\|h_n\|_{H^1(\Omega^c_{d/2})} + \|DF_{\epsilon_n}(0)h_n\|_{L^2(\Omega^c_{d/2})}) = o(\epsilon_n) \quad \text{as} \quad n \to \infty. \qquad (3.16)$$

Then, it follows that $\|h_n^*\|_{L^2(\Omega^c_{d/2})} = o(\epsilon_n^2)$ and hence $\|\Delta h_n^*\|_{L^2(\Omega^c_{d/2})} = o(1)$. Consequently, $\|h_n\|_{H^2(\Omega_d)} = 1 + o(1)$ as $n \to \infty$.

On the other hand, for each $j = 1, \ldots, m$, let $\chi_j(x) = \chi((x-p_j)/d)$ and $h_{jn} = \chi_j h_n$. Let $\hat{h}_n(x) = h_n(\epsilon_n x + p_j)$, $\hat{\chi}_j(x) = \chi_j(\epsilon_n x + p_j)$, and $\hat{h}_{jn} = \hat{\chi}_j \hat{h}_n$. We also let $\Sigma_j = \{d \leqslant |x - p_j| \leqslant 2d\}$ and $\hat{\Sigma}_0 = \{d/\epsilon_n \leqslant |x| \leqslant 2d/\epsilon_n\}$.

Then it is easily checked that $\hat{h}_{jn}$ satisfies

$$\begin{aligned}L_j\hat{h}_{jn} = 2\,\nabla\hat{h}_n \cdot \nabla\hat{\chi}_j + \hat{h}_n\Delta\hat{\chi}_j + \epsilon_n^2\hat{\chi}_j(x)[DF_{\epsilon_n}(0)h_n](\epsilon_n x + p_j) \\ + [e^{\hat{\chi}_j\phi_j}(2e^{\hat{\chi}_j\phi_j} - 1) - e^{\phi_j}(2e^{\phi_j} - 1)]\hat{h}_{jn} \quad \text{for} \quad |x| \leqslant 2d/\epsilon_n. \qquad (3.17)\end{aligned}$$

Notice that the last term in (3.17) vanishes outside $\hat{\Sigma}_0$. Then, it follows from (3.16) and Lemma 2.3 that

$$\begin{aligned}\|\hat{h}_{jn}\|_{H^2(\mathbb{R}^2)} &\leqslant C(\epsilon_n\|\nabla\hat{h}_n\|_{L^2(\hat{\Sigma}_0)} + \|\hat{h}_n\|_{L^2(\hat{\Sigma}_0)} + \epsilon_n\|DF_{\epsilon_n}(0)h_n\|_{L^2(B_d(p_j))}) \\ &\leqslant C(\epsilon_n\|\nabla h_n\|_{L^2(\Sigma_j)} + \epsilon_n^{-1}\|h_n\|_{L^2(\Sigma_j)} + \epsilon_n\|DF_{\epsilon_n}(0)h_n\|_{L^2(B_d(pj))}) = o(\epsilon_n) \quad \text{as} \quad n \to \infty.\end{aligned}$$

Consequently, $\|h_n\|_{H^2(B_d(pj))} \leqslant \|h_{jn}\|_{H^2(\mathbb{R}^2)} = o(1)$ for each $1 \leqslant j \leqslant m$, which yields a contradiction. Therefore (3.12) is proved.

Since $DF_\epsilon(0): H^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2)$ is self-adjoint (3.12) implies that $DF_\epsilon(0)$ is indeed an iso-

morphism from $H^2(\mathbb{R}^2)$ onto $L^2(\mathbb{R}^2)$, and moreover, $\|[DF_\epsilon(0)]^{-1}\| \leq C$ for $\epsilon > 0$ sufficiently small.

(c) Estimate for $\|DF_\epsilon(z) - DF_\epsilon(0)\|$: Notice that

$$DF_\epsilon(z)h - DF_\epsilon(0)h = -\frac{2}{\epsilon^2}\exp\left[\sum_j 2\chi_j\phi_{j,\epsilon}\right](\exp[2\epsilon^3 z] - 1)h + \frac{1}{\epsilon^2} \times \exp\left[\sum_j \chi_j\phi_{j,\epsilon}\right](\exp[\epsilon^3 z] - 1)h.$$

Then (c) immediately follows from the embedding $H^2(\mathbb{R}^2) \hookrightarrow L^\infty(\mathbb{R}^2)$. □

We are now in a position to prove Theorem 1.1

Proof of Theorem 1.1: Following Ref. 24, we define a functional $\Phi_\epsilon : H^2(\mathbb{R}^2) \to H^2(\mathbb{R}^2)$ by

$$\Phi_\epsilon(v) = v - [DF_\epsilon(0)]^{-1}F_\epsilon(v). \tag{3.18}$$

Then, it suffices to prove that Φ_ϵ admits a unique fixed point in $H^2(\mathbb{R}^2)$ for $\epsilon > 0$ sufficiently small. Let $\mathcal{B} = \{u \in H^2(\mathbb{R}^2) \,|\, \|u\|_{H^2(\mathbb{R}^2)} \leq 1\}$. Then, it follows from Lemma 3.1 and Lemma 3.2 that for each topological solution u_ϵ of (2.1), $z_\epsilon \in H^2(\mathbb{R}^2)$ defined in (3.9) is a fixed point of Φ_ϵ, and moreover, $z_\epsilon \in \mathcal{B}$ for $\epsilon > 0$ sufficiently small.

We claim that $\Phi_\epsilon : \mathcal{B} \to \mathcal{B}$ is a well-defined contraction mapping for $\epsilon > 0$ sufficiently small.

Observe that

$$D\Phi_\epsilon(z)h = -[DF_\epsilon(0)]^{-1}(DF_\epsilon(z) - DF_\epsilon(0))h \quad \text{for} \quad z \in \mathcal{B}, \quad h \in H^2(\mathbb{R}^2).$$

Then, it follows from Lemma 3.3 that if $\epsilon > 0$ is sufficiently small

$$\|D\Phi_\epsilon(z)h\|_{L^2(\mathbb{R}^2)} \leq \|[DF_\epsilon(0)]^{-1}\| \, \|(DF_\epsilon(z) - DF_\epsilon(0))h\|_{L^2(\mathbb{R}^2)} \leq C\epsilon\|h\|_{L^2(\mathbb{R}^2)}$$

for $z \in \mathcal{B}$. Moreover, it also follows from Lemma 3.3 that

$$\|\Phi_\epsilon(0)\|_{H^2(\mathbb{R}^2)} \leq C\|F_\epsilon(0)\|_{L^2(\mathbb{R}^2)} \leq C\exp[-c/\epsilon].$$

Assume that $v, v_1, v_2 \in \mathcal{B}$ are given. If $\epsilon > 0$ is sufficiently small we obtain

$$\begin{aligned}\|\Phi_\epsilon(v)\|_{H^2(\mathbb{R}^2)} &\leq \|\Phi_\epsilon(0)\|_{H^2(\mathbb{R}^2)} + \|\Phi_\epsilon(v) - \Phi_\epsilon(0)\|_{H^2(\mathbb{R}^2)} \\ &\leq \|\Phi_\epsilon(0)\|_{H^2(\mathbb{R}^2)} + (\sup_{z\in\mathcal{B}} \|D\Phi_\epsilon(z)\|)\|v\|_{H^2(\mathbb{R}^2)} \leq C(\exp[-c/\epsilon] + \epsilon),\end{aligned}$$

and

$$\|\Phi_\epsilon(v_1) - \Phi_\epsilon(v_2)\|_{H^2(\mathbb{R}^2)} \leq (\sup_{z\in\mathcal{B}} \|D\Phi_\epsilon(z)\|)\|v_1 - v_2\|_{H^2(\mathbb{R}^2)} \leq C\epsilon\|v_1 - v_2\|_{H^2(\mathbb{R}^2)}.$$

Therefore, if $\epsilon > 0$ is sufficiently small, $\Phi_\epsilon : \mathcal{B} \to \mathcal{B}$ is well-defined contraction mapping, which in turn implies that Φ_ϵ has the unique fixed point $\omega_\epsilon \in \mathcal{B}$.

On the other hand, recall the function z_ϵ defined in (3.9) is also the fixed point of the mapping Φ_ϵ and $\|z_\epsilon\|_{H^2(\mathbb{R}^2)} = o(1)$ as $\epsilon \to 0^+$. Therefore, by the uniqueness of the fixed point, $z_\epsilon = \omega_\epsilon$ for $\epsilon > 0$ sufficiently small.

The proof of Theorem 1.1 is complete. □

We will prove Theorem 1.2 in the rest of this section.

For simplicity, we let $\alpha = 2/\kappa$. Then, it suffices to prove that the following equation:

$$\Delta u = e^u(e^u - 1) + 4\pi\sum_{j=1}^{m} n_j \delta_{\alpha p_j}, \quad \mathbb{R}^2, \tag{3.19}$$

admits a unique topological solution if $\alpha > 0$ is sufficiently small. To this end, we follow the argument in the proof of Theorem 1.1, and show that any topological solution of (3.19) satisfies a specific asymptotic behavior for $\alpha > 0$ sufficiently small. Throughout the rest of this section, $\overline{u}_\alpha$ will denote a topological solution of (3.19).

The following lemma will be very useful when we prove Lemma 3.5.

Lemma 3.4: Let $\alpha > 0$. *There is a constant* $C = C(\{p_j\},\{n_j\}) > 0$ *such that*

$$\int_{\mathbb{R}^2} (e^{\overline{u}_\alpha} - 1)^2 dx \leqslant C.$$

Proof: Let $\overline{v}_{\alpha,j}(x) = \overline{u}_\alpha(x) - 2n_j \ln|x - \alpha p_j|$ for $x \in \mathbb{R}^2$ and $j = 1, \ldots, m$. Then, we claim that

$$\int_{\mathbb{R}^2} (e^{\overline{u}_\alpha} - 1)^2 dx = 4\pi\sum_{j=1}^{m} (n_j^2 + \alpha n_j p_j \cdot \nabla \overline{v}_{\alpha,j}(\alpha p_j)). \tag{3.20}$$

Indeed, (3.20) follows from the Pohozaev identity. Choose a small constant $\varepsilon > 0$ such that $\varepsilon < (1/2)\inf\{|\alpha p_j - \alpha p_k| | j \neq k\}$. Multiplying both sides of (3.19) by $x \cdot \nabla \overline{u}_\alpha$ and integrating on the domain $\mathbb{R}^2 \setminus \cup_j B_\varepsilon(\alpha p_j)$, we obtain

$$\begin{aligned}\sum_{j=1}^{m} \int_{|x-\alpha p_j|=\varepsilon} \left[\frac{1}{\varepsilon}(x \cdot \nabla \overline{u}_\alpha)((x - \alpha p_j) \cdot \nabla \overline{u}_\alpha) - \frac{1}{2\varepsilon}(x \cdot (x - \alpha p_j))|\nabla \overline{u}_\alpha|^2\right] d\sigma \\ = \int_{\mathbb{R}^2 \setminus \cup_j B_\varepsilon(\alpha p_j)} (e^{\overline{u}_\alpha} - 1)^2 dx + \frac{1}{2\varepsilon}\sum_{j=1}^{m} \int_{|x-\alpha p_j|=\varepsilon} (x \cdot (x - \alpha p_j))(e^{\overline{u}_\alpha} - 1)^2 d\sigma. \end{aligned} \tag{3.21}$$

Since $\overline{u}_\alpha(x) = \overline{v}_{\alpha,j}(x) + 2n_j \ln|x - \alpha p_j|$ for each $1 \leqslant j \leqslant m$, it is easily checked that for $|x - \alpha p_j| = \varepsilon$

$$\begin{aligned}&\frac{1}{\varepsilon}(x \cdot \nabla \overline{u}_\alpha)((x - \alpha p_j) \cdot \nabla \overline{u}_\alpha) - \frac{1}{2\varepsilon}(x \cdot (x - \alpha p_j))|\nabla \overline{u}_\alpha|^2 \\ &\quad = \frac{2n_j^2}{\varepsilon} + \frac{2n_j}{\varepsilon}\alpha p_j \cdot \nabla \overline{v}_{\alpha,j}(\alpha p_j) + \frac{2n_j^2}{\varepsilon^3}\alpha p_j \cdot (x - \alpha p_j) + O(1) \quad \text{as} \quad \varepsilon \to 0^+. \end{aligned} \tag{3.22}$$

Then (3.20) is an immediate consequence of (3.21) and (3.22).

Let $\overline{w}_\alpha(x) = \overline{u}_\alpha(x) - \Sigma_{j=1}^m 2n_j \ln|x - \alpha p_j|$. We note that

$$\nabla \overline{w}_\alpha(x) = \frac{1}{2\pi}\int_{\mathbb{R}^2} \frac{x - y}{|x - y|^2} e^{\overline{u}_\alpha(y)}(e^{\overline{u}_\alpha(y)} - 1) dy \quad \text{for} \quad x \in \mathbb{R}^2.$$

If $|x| \leqslant 1$, then we obtain that

$$\begin{aligned}2\pi|\nabla \overline{w}_\alpha(x)| &\leqslant \int_{|y|\leqslant 2} \frac{1}{|x - y|} e^{\overline{u}_\alpha(y)}(1 - e^{\overline{u}_\alpha(y)}) dy + \int_{|y|\geqslant 2} \frac{1}{|x - y|} e^{\overline{u}_\alpha(y)}(1 - e^{\overline{u}_\alpha(y)}) dy \\ &\leqslant \int_{|y|\leqslant 2} \frac{1}{|x - y|} dy + \int_{|y|\geqslant 2} \frac{2}{|y|} e^{\overline{u}_\alpha(y)}(1 - e^{\overline{u}_\alpha(y)}) dy \leqslant C \end{aligned} \tag{3.23}$$

for some constant C depending on $\Sigma_{j=1}^m n_j$. We also note that

$$\nabla \overline{v}_{\alpha,j}(\alpha p_j) = \sum_{k \neq j} \frac{2n_k(p_j - p_k)}{\alpha |p_j - p_k|^2} + \nabla \overline{w}_\alpha(\alpha p_j) \quad \text{for} \quad j = 1, \ldots, m.$$

Then, Lemma 3.4 immediately follows from (3.20) and (3.23). □

Before we proceed, we fix some notations. For $\mu \in \mathbb{R}$, we let

$$f_\mu(x) = \sum_{j=1}^m n_j \ln\left(\frac{|x - \mu p_j|^2}{1 + |x - \mu p_j|^2}\right), \quad g_\mu(x) = \sum_{j=1}^m \frac{4n_j}{(1 + |x - \mu p_j|^2)^2}.$$

Let ϕ be the unique (radial) topological solution of

$$\Delta \phi = e^\phi(e^\phi - 1) + 4\pi\left(\sum_{j=1}^m n_j\right)\delta_{p=0} \quad \text{in} \quad \mathbb{R}^2.$$

Then, it is easily checked that $\overline{u}_\alpha - f_\alpha \in H^2(\mathbb{R}^2)$ and $\phi - f_0 \in H^2(\mathbb{R}^2)$. The following lemma shows the asymptotic behavior of $\overline{u}_\alpha$ for $\alpha > 0$ sufficiently small.

Lemma 3.5: For $\alpha > 0$ sufficiently small, $\overline{u}_\alpha$ can be decomposed as

$$\overline{u}_\alpha = f_\alpha - f_0 + \phi + z_\alpha, \quad z_\alpha \in H^2(\mathbb{R}^2), \tag{3.24}$$

where $\|z_\alpha\|_{H^2(\mathbb{R}^2)} = O(\alpha)$ as $\alpha \to 0^+$.

Proof: The proof of Lemma 3.5 is similar to that of Lemma 3.2, and we just sketch the proof. Let $v_\alpha = \overline{u}_\alpha - f_\alpha$ for simplicity.

Step 1: $v_\alpha \to \phi - f_0$ in $C^2_{loc}(\mathbb{R}^2)$ as $\alpha \to 0^+$.

Indeed, since $e^{\overline{u}_\alpha} \leqslant 1$, it follows from Harnack's inequality (see, e.g., Ref. 5) that either $\{v_\alpha\}$ is bounded in $C^0_{loc}(\mathbb{R}^2)$ or $v_\alpha \to -\infty$ uniformly on any compact subset as $\alpha \to 0^+$. By Lemma 3.4, we conclude that $\{v_\alpha\}$ is bounded in $C^0_{loc}(\mathbb{R}^2)$. Then, the standard diagonal process, Lemma 3.4, and the uniqueness of a radial topological solution imply that $v_\alpha \to \phi - f_0$ in $C^2_{loc}(\mathbb{R}^2)$ as $\alpha \to 0^+$.

Step 2: $\sup_{|x| \geqslant 1} |\overline{u}_\alpha(x) - \phi(x)| \to 0$ as $\alpha \to 0^+$.

Indeed, we note that if $\alpha > 0$ is sufficiently small

$$|f_\alpha(x) - f_0(x)| \leqslant C\alpha(1 + |x|)^{-3} \quad \text{for} \quad |x| \geqslant 1.$$

Consequently, it follows from Step 1 that $\sup_{|x|=1} |\overline{u}_\alpha(x) - \phi(x)| \to 0$ as $\alpha \to 0^+$. Moreover, the maximum principle implies that $\inf_{|x| \geqslant 1} \overline{u}_\alpha$ is bounded below by a fixed constant for $\alpha > 0$ sufficiently small. Therefore, Step 2 follows from Lemma 3.4 and the argument in the proof of Lemma 3.2.

Step 1 and Step 2 imply that $\|v_\alpha - (\phi - f_0)\|_{L^\infty(\mathbb{R}^2)} \to 0$ as $\alpha \to 0^+$. Since

$$|e^{f_\alpha(x)} - e^{f_0(x)}| + |g_\alpha(x) - g_0(x)| \leqslant C\alpha(1 + |x|)^{-3} \quad \text{for} \quad x \in \mathbb{R}^2, \tag{3.25}$$

it follows that

$$|(\Delta - e^\phi(2e^\phi - 1))(v_\alpha - (\phi - f_0))| \leqslant C(|v_\alpha - (\phi - f_0)|^2 + \alpha(1 + |x|)^{-3}).$$

Consequently, Lemma 2.3 implies that

$$\|v_\alpha - (\phi - f_0)\|_{H^2(\mathbb{R}^2)} \leqslant C\alpha$$

for $\alpha > 0$ sufficiently small. Lemma 3.5 is proved. □

We are now in a position to prove Theorem 1.2.

Proof of Theorem 1.2: Fix a small constant $\mu_0 > 0$ and define a mapping $P: H^2(\mathbb{R}^2) \times (-\mu_0, \mu_0) \to L^2(\mathbb{R}^2)$ by

$$P(\psi, \mu) = \Delta\psi - e^{f_\mu - f_0 + \phi + \psi}(e^{f_\mu - f_0 + \phi + \psi} - 1) + e^\phi(e^\phi - 1) - g_\mu + g_0.$$

Then, it is easily checked that (3.19) admits a solution $\overline{u}_\mu$ of the form (3.24) if and only if $P(z_\mu, \mu) = 0$.

Lemma 2.3 implies that $D_\psi P(0,0)$ is an isomorphism from $H^2(\mathbb{R}^2)$ onto $L^2(\mathbb{R}^2)$. Since $P(0,0)=0$, it follows from the implicit function theorem that there is a positive constant $\mu_1 < \mu_0$ such that for each $-\mu_1 < \mu < \mu_1$ the mapping $P(\cdot,\mu)$ admits a unique zero $v=v(\mu)$ in $H^2(\mathbb{R}^2)$. In other words, if $\alpha>0$ is sufficiently small then Eq. (3.19) admits a unique solution which takes the form (3.24) with $\|z_\alpha\|_{H^2(\mathbb{R}^2)} \to 0$ as $\alpha \to 0^+$.

The proof of Theorem 1.2 is complete. □

IV. UNIQUENESS RESULT FOR COMPACT DOMAINS

In the previous section, we obtained *a priori* estimates for the topological solution u_ϵ for $\epsilon > 0$ sufficiently small by dividing $\mathbb{R}^2$ into two disjoint sets, $\Omega_d = U_j B_d(p_j)$ and Ω_d^c. Actually, by making use of the topological boundary condition (2.2), we have proved that u_ϵ is bounded below on Ω_d^c, which is the first step for the proof of Lemma 3.1 and Lemma 3.2.

In this section, we consider a general situation for (2.1), and study (2.1) on a compact Riemannian 2-manifold (Ω, γ) without boundary

$$\Delta_0 u = \frac{1}{\epsilon^2} e^{u_\epsilon}(e^{u_\epsilon} - 1) + 4\pi \sum_{j=1}^{m} n_j \delta_{p_j} \quad \text{in} \quad \Omega, \tag{4.1}$$

where Δ_0 is the Laplace–Beltrami operator on (Ω, γ). In this case, every solution of (4.1) is not bounded below on a compact subset K of $\Omega \backslash \{p_1, \ldots, p_m\}$ because we do not have the topological boundary condition (2.2) anymore. Indeed, it has been proved by Ding *et al.*[14] that for $\epsilon > 0$ sufficiently small (4.1) admits at least two solutions $u_{\epsilon,1}$ and $u_{\epsilon,2}$ such that

(a) $u_{\epsilon,1} \to 0$ a.e. as $\epsilon \to 0^+$ (type I);
(b) $u_{\epsilon,2} \to -\infty$ a.e. as $\epsilon \to 0^+$.

In what follows, we will call u_ϵ a type-I solution if u_ϵ satisfies (4.1) and the above-mentioned asymptotic behavior (a).

Let $G(x,y)$ be the Green function which satisfies

$$\Delta_x G(x,y) = \delta_y - \frac{1}{|\Omega|}, \quad \Omega$$

$$\int_\Omega G(x,y) dV_g(x) = 0.$$

Then, it follows from the arguments in Refs. 29 and 14 that u_ϵ is a type-I solution of (4.1) if and only if $u_\epsilon - \Sigma_j 4\pi n_j G(x,p_j)$ is bounded below by a constant for $\epsilon > 0$ sufficiently small.

We limit our attention to the type-I solutions, and establish a uniqueness result for $\epsilon > 0$ sufficiently small. More precisely, we have

Theorem 4.1: *Fix any constant* $C_* < \inf_{x\in\Omega}(-\Sigma_j 4\pi n_j G(x,p_j))$. *Then, there is a constant* $\epsilon_* > 0$ *such that for each* $0 < \epsilon < \epsilon_*$ (4.1) *admits a unique solution* u_ϵ *which satisfies* $u_\epsilon - \Sigma_j 4\pi n_j G(x,p_j) \geqslant C_*$.

Remark: The constant ϵ_* in Theorem 4.1 depends on C_*, $\{p_j\}$, $\{n_j\}$ and the Riemannian manifold (Ω, γ).

Theorem 1.3 is a direct consequence of Theorem 4.1. We can prove Theorem 4.1 by making use of the argument used in Sec. III. Indeed, every crucial estimate in the previous section is essentially local. We will choose a suitable atlas $\{(U_l, \varphi_l)\}_{l=1}^k$ on Ω, and repeat the proof of Theorem 1.1 on each local chart (U_l, φ_l).

Theorem 4.1 will be proved in several steps, and we will just present the outline of the proof. To this end, we choose an atlas $\{(U_l, x_l)\}_{l=1}^k$ on Ω with the property that

(i) For $1 \leqslant l \leqslant k$, $x_l(U_l)$ is an open neighborhood of the origin in $\mathbb{R}^2$. Moreover, $p_j \in U_j$ and $x_j(p_j) = 0$ for each $1 \leqslant j \leqslant m$.

(ii) For $1 \leqslant l \leqslant k$, (U_l, x_l) is an isothermal coordinate, and there is a smooth function ξ_l such that $\xi_l(0)=0$, $\nabla \xi_l(0)=0$ and $ds^2 = e^{\xi_l(x)}|dx|^2$ on (U_l, x_l).

(iii) For $1 \leqslant j \leqslant m$, there is a constant $0 < d < 1/2$ such that $\{x \in \mathbb{R}^2 | |x| \leqslant 2d\} \subset x_j(U_j)$ and $\|\nabla \xi_j\|_{L^\infty(|x| \leqslant 2d)} \leqslant 1$. Moreover, we assume that $x_j^{-1}(\{|x| \leqslant 2d\}) \cap U_l = \emptyset$ for $l \neq j$.

In what follows, we let

$$V_d = \cup_{j=1}^m x_j^{-1}(\{x \in \mathbb{R}^2 | |x| \leqslant d\}.$$

We first present the following lemma similar to Lemma 3.1.

Lemma 4.1: For $\epsilon > 0$ sufficiently small, there are constants $C, c > 0$ such that

$$\|u_\epsilon\|_{H^2(V_d^c)} \leqslant Ce^{-c/\epsilon}.$$

Proof: On each (U_l, x_l), Eq. (4.1) can be written as

$$\Delta u_\epsilon = \frac{1}{\epsilon^2} e^{\xi_l} e^{u_\epsilon}(e^{u_\epsilon} - 1), \quad |x| \neq 0,$$

where $\Delta = \partial_1^2 + \partial_2^2$ stands for a Laplacian in $\mathbb{R}^2$. Then, the proof is similar to that of Lemma 3.1 (Steps 2, 3). We skip the details. □

We now investigate the asymptotic behavior of u_ϵ near each $p_j \in \Omega$. For each $1 \leqslant j \leqslant m$ (4.1) may be written as

$$\Delta u = \frac{1}{\epsilon^2} e^{\xi_j} e^u (e^u - 1) + 4\pi n_j \delta_{p=0}, \quad \text{for} \quad |x| \leqslant 2d. \tag{4.2}$$

For each $1 \leqslant j \leqslant m$, let $\hat{\xi}_j(x) = \xi_j(\epsilon x)$ for $|x| < 2d/\epsilon$, and

$$\hat{f}_{j,\epsilon}(x) = \begin{cases} e^{\hat{\xi}_j} e^{\phi_j}(2e^{\phi_j} - 1), & |x| \leqslant 2d/\epsilon, \\ e^{\phi_j}(2e^{\phi_j} - 1), & |x| > 2d/\epsilon. \end{cases}$$

The following corollary is the direct consequence of Lemma 2.3.

Corollary 4.1: For $1 \leqslant j \leqslant m$, there are constants $c > 0$ and $\epsilon_1 > 0$ such that

$$\|(\Delta - \hat{f}_{j,\epsilon})v\|_{L^2(\mathbb{R}^2)} \geqslant c\|v\|_{H^2(\mathbb{R}^2)}$$

for all $v \in H^2(\mathbb{R}^2)$ and $0 < \epsilon < \epsilon_1$. Therefore, $\Delta - \hat{f}_{j,\epsilon}$ is an isomorphism from $H^2(\mathbb{R}^2)$ onto $L^2(\mathbb{R}^2)$ for $0 < \epsilon < \epsilon_1$.

For each $1 \leqslant j \leqslant m$ and $0 < \epsilon < \epsilon_1$, let $\hat{\psi}_{j,\epsilon} \in H^2(\mathbb{R}^2)$ be the unique solution of

$$(\Delta - \hat{f}_{j,\epsilon})\hat{\psi}_{j,\epsilon} = g_{j,\epsilon} \quad \text{in} \quad \mathbb{R}^2, \tag{4.3}$$

where $g_{j,\epsilon} \in L^2(\mathbb{R}^2)$ is defined by

$$g_{j,\epsilon}(x) = \begin{cases} (e^{\hat{\xi}_j} - 1)e^{\phi_j}(e^{\phi_j} - 1), & |x| \leqslant 2d/\epsilon \\ 0, & |x| > 2d/\epsilon. \end{cases}$$

Let

$$\alpha_j(\epsilon) = \|g_{j,\epsilon}\|_{L^2(\mathbb{R}^2)}.$$

Since $\xi_j(0) = 0$ and $\nabla \xi_j(0) = 0$, it follows that $\alpha_j(\epsilon) \leqslant C\epsilon^2$ for all $1 \leqslant j \leqslant m$.

Lemma 4.2: There are positive constants C, ϵ_1, and c_1 such that for $0 < \epsilon < \epsilon_1$

$$|\hat{\psi}_{j,\epsilon}(x)| \leqslant C\alpha_j(\epsilon)e^{-c_1|x|}, \quad x \in \mathbb{R}^2. \tag{4.4}$$

Proof: Corollary 4.1 implies that $\|\hat{\psi}_{j,\epsilon}\|_{L^\infty} \leqslant C\|\hat{\psi}_{j,\epsilon}\|_{H^2(\mathbb{R}^2)} \leqslant C\alpha_j(\epsilon)$. Choose two constants R_0 and $0<c_0<1$ such that $\hat{f}_{j,\epsilon}(x) \geqslant 2c_0^2$ for $|x| \geqslant R_0$. Consider a comparison function

$$\varphi(x) = C_0\alpha_j(\epsilon)e^{-c_0|x|}, \quad x \in \mathbb{R}^2.$$

Since $|\phi_j(x)| \leqslant Ce^{-|x|}$ for $x \in \mathbb{R}^2$, there are constants $R>R_0$ and $\epsilon_0>0$ such that

$$(\Delta - \hat{f}_{j,\epsilon})(\hat{\psi}_{j,\epsilon} - \varphi) > 0 \quad \text{for} \quad |x| > R \quad \text{and} \quad 0 < \epsilon < \epsilon_1.$$

Fix a constant $C_0>0$ such that $\hat{\psi}_{j,\epsilon} - \varphi < 0$ for $|x|=R$. Then, the weak maximum principle implies that $\hat{\psi}_{j,\epsilon} \leqslant \varphi$ for $|x|>R$.

Similarly, we can choose positive constants R_1 and C_1 such that $\hat{\psi}_{j,\epsilon} > -C_1\alpha_j(\epsilon)e^{-c_0|x|}$ for $|x| > R_1$ and $0<\epsilon<\epsilon_1$. □

Let $u_{\epsilon,j}$ be a solution of (4.2) such that $\sup_{|x|=2d}|u_{\epsilon,j}(x)| \to 0$ as $\epsilon \to 0^+$. Let $\hat{u}_{\epsilon,j}(x) = u_{\epsilon,j}(\epsilon x)$ for $|x| \leqslant 2d/\epsilon$.

Lemma 4.3: For $\epsilon>0$ sufficiently small, there are constants $C, c>0$ such that

$$\|\hat{u}_{\epsilon,j} - \phi_j - \hat{\psi}_{j,\epsilon}\|_{H^2(|x|\leqslant d/\epsilon)} \leqslant C(e^{-c/\epsilon} + \epsilon^2\alpha_j(\epsilon)). \tag{4.5}$$

Proof: It follows from the Pohozaev identity and the gradient estimate (Lemma A) that

$$\frac{1}{\epsilon^2}\int_{|x|<2d}\left(1 + \frac{1}{2}(x \cdot \nabla \xi_j)\right)e^{\xi_j}(e^{u_{\epsilon,j}} - 1)^2 dx = 4\pi n_j^2 + o(e^{-c/\epsilon})$$

for some constant $c>0$. Since $\|x \cdot \nabla \xi_j\|_{L^\infty(|x|<2d)} \leqslant 1$, it follows that

$$\int_{|x|<2d/\epsilon} e^{\hat{\xi}_j}(e^{\hat{u}_{\epsilon,j}} - 1)^2 dx \leqslant C. \tag{4.6}$$

Step 1: We claim $\sup_{|x|\leqslant 2d/\epsilon}|\hat{u}_{\epsilon,j}(x) - \phi_j(x)| \to 0$ as $\epsilon \to 0^+$.

Indeed, it follows from the argument in Lemma 3.2 (Step 1) and (4.6) that $\hat{u}_{\epsilon,j} - \phi_j \to 0$ in $C^2_{loc}(\mathbb{R}^2)$. For the sake of simplicity, we let $\hat{w}_{\epsilon,j} = \hat{u}_{\epsilon,j} - \phi_j$. Suppose that there are sequences $\{\epsilon_n\}$ and $\{x_n\}$ such that $\epsilon_n \to 0$, $|x_n| < 2d/\epsilon_n$, and

$$|\hat{w}_{\epsilon_n,j}(x_n)| = \sup_{|x|\leqslant 2d/\epsilon_n}|\hat{w}_{\epsilon_n,j}(x)| \geqslant \gamma_0$$

for some constant $\gamma_0>0$. It is easy to check that $|x_n| \to \infty$ and $\epsilon_n|x_n| \to 0$. Since $\hat{\xi}_j(x_n) = o(1)$, we can follow the argument in Lemma 3.2 (Step 2) and conclude that $\hat{w}_{\epsilon_n,j}(x_n) \to -\infty$. Then it follows from the Harnack inequality that $\hat{w}_{\epsilon_n,j} \to -\infty$ uniformly on $B_R(x_n)$ for any constant $R>0$, which contradicts (4.6). Therefore, our claim is proved.

Step 2: We now prove (4.5). Making use of the inequality $0 \leqslant e^t - 1 - t \leqslant t^2 e^{|t|}$, $t \in \mathbb{R}$, we can verify that

$$(\Delta - \hat{f}_{j,\epsilon})(\hat{\psi}_{\epsilon,j} - \hat{\psi}_{j,\epsilon}) = O(1)|\hat{w}_{\epsilon,j}|^2 \quad \text{for} \quad |x| \leqslant 2d/\epsilon. \tag{4.7}$$

Consider a cutoff function $\sigma \in C_0^\infty(\mathbb{R}^2)$ such that $0 \leqslant \sigma \leqslant 1$, $\sigma \equiv 1$ for $|x| \leqslant d$, and $\sigma \equiv 0$ for $|x| \geqslant 2d$. Let $\sigma_\epsilon(x) = \sigma(\epsilon x)$. Then, we obtain

$$(\Delta - \hat{f}_{j,\epsilon})(\sigma_\epsilon(\hat{w}_{\epsilon,j} - \hat{\psi}_{j,\epsilon})) = \sigma_\epsilon((\Delta - \hat{f}_{\epsilon,j})(\hat{w}_{\epsilon,j} - \hat{\psi}_{j,\epsilon})) + [\Delta, \sigma_\epsilon]\hat{w}_{\epsilon,j} - [\Delta, \sigma_\epsilon]\hat{\psi}_{\epsilon,j},$$

where $[\Delta, \sigma_\epsilon]f = f\Delta\sigma_\epsilon + 2\nabla\sigma_\epsilon \cdot \nabla f$. Corollary 4.1 and (4.7) imply that

$$\|\sigma_\epsilon(\hat{w}_{\epsilon,j}-\hat{\psi}_{j,\epsilon})\|_{H^2(\mathbb{R}^2)} \leqslant C(\|[\Delta,\sigma_\epsilon]\hat{w}_{\epsilon,j}\|_{L^2(\mathbb{R}^2)} + \|[\Delta,\sigma_\epsilon]\hat{\psi}_{j,\epsilon}\|_{L^2(\mathbb{R}^2)} + \|\hat{\psi}_{j,\epsilon}\|^2_{L^4(\mathbb{R}^2)}) + C\|\hat{w}_{\epsilon,j}+\hat{\psi}_{j,\epsilon}\|_{L^\infty}\|\sigma_\epsilon(\hat{w}_{\epsilon,j}-\hat{\psi}_{j,\epsilon})\|_{L^2(\mathbb{R}^2)}. \tag{4.8}$$

Moreover, it follows from elliptic estimates that

$$\|\nabla\hat{\psi}_{j,\epsilon}\|_{L^\infty(d/\epsilon\leqslant|x|\leqslant 2d/\epsilon)} \leqslant Ce^{-c/\epsilon}.$$

Then (4.5) is an immediate consequence of (4.4) and (4.8), and Lemma 4.1. □

Recall that ϕ_j is the (unique) radial solution of (2.5). Let $\sigma\in C_0^\infty(\mathbb{R}^2)$ be a cutoff function such that $0\leqslant\sigma\leqslant 1$, $\sigma\equiv 1$ on $B_d(0)$, and $\sigma\equiv 0$ on $B^c_{2d}(0)$. Let $\psi_{j,\epsilon}(x)=\hat{\psi}_{j,\epsilon}(x/\epsilon)$ and $\phi^*_{j,\epsilon}(x)=\phi_j(x/\epsilon)$ for $x\in\mathbb{R}^2$.

For each $1\leqslant j\leqslant m$, we let

$$\overline{\sigma_j}=\sigma\circ x_j,\quad \overline{\phi}_{j,\epsilon}=\phi^*_{j,\epsilon}\circ x_j \quad\text{and}\quad \overline{\psi}_{j,\epsilon}=\psi_{j,\epsilon}\circ x_j.$$

Then, Lemma 4.1 and Lemma 4.3 imply that

Proposition 4.1: Let u_ϵ be a type-I solution of (4.1). *For $\epsilon>0$ sufficiently small, u_ϵ is decomposed as*

$$u_\epsilon=\sum_{j=1}^m \overline{\sigma_j}(\overline{\phi}_{j,\epsilon}+\overline{\psi}_{j,\epsilon})+\epsilon^{5/2}v_\epsilon \tag{4.9}$$

for some $v_\epsilon\in H^2(\Omega)$ such that $\|v_\epsilon\|_{H^2(\Omega)}=o(1)$ as $\epsilon\to 0^+$.

In what follows, we prove that (4.1) admits a unique solution of the form (4.9) if $\epsilon>0$ is sufficiently small.

Construction of a contraction mapping

Define $F_\epsilon: H^2(\Omega)\to L^2(\Omega)$ by

$$F_\epsilon(v)=\Delta_0 v-\frac{1}{\epsilon^{9/2}}\exp\left[\epsilon^{5/2}v+\sum_{j=1}^m\overline{\sigma_j}(\overline{\phi}_{j,\epsilon}+\overline{\psi}_{j,\epsilon})\right]\left(\exp\left[\epsilon^{5/2}v+\sum_{j=1}^m\overline{\sigma_j}(\overline{\phi}_{j,\epsilon}+\overline{\psi}_{j,\epsilon})\right]-1\right) + \frac{1}{\epsilon^{5/2}}\sum_{j=1}^m(\overline{\sigma_j}\Delta_0\overline{\phi}_{j,\epsilon}-4\pi n_j\delta_{p_j})+\frac{1}{\epsilon^{5/2}}\sum_{j=1}^m\overline{\sigma_j}\Delta_0\overline{\psi}_{j,\epsilon}+\frac{1}{\epsilon^{5/2}}\sum_{j=1}^m[\Delta_0,\overline{\sigma_j}](\overline{\phi}_{j,\epsilon}+\overline{\psi}_{j,\epsilon}),$$

where $[\Delta_0,\overline{\sigma_j}]f=f\Delta_0\overline{\sigma_j}+2\nabla f\cdot\nabla\overline{\sigma_j}$. It is easily checked that (4.1) admits a solution u_ϵ of the form (4.9) if and only if $F_\epsilon(v_\epsilon)=0$.

We have the following lemma similar to Lemma 3.3.

Lemma 4.4: There is a constant $\epsilon_1>0$ such that if $0<\epsilon<\epsilon_1$ then we have

(a) $\|F_\epsilon(0)\|_{L^2(\Omega)}\leqslant C(\epsilon^{-3/2}\max_{1\leqslant j\leqslant m}\alpha_j(\epsilon)+e^{-c/\epsilon})$ *for some constants $C,c>0$.*

(b) $DF_\epsilon(0)$ *is an isomophism from $H^2(\Omega)$ onto $L^2(\Omega)$, and there is a constant $C>0$ such that*

$$\|DF_\epsilon(0)h\|_{L^2(\Omega)}\geqslant C\|h\|_{H^2(\Omega)} \quad \textit{for all} \quad h\in H^2(\Omega). \tag{4.10}$$

(c) $\|DF_\epsilon(z)h-DF_\epsilon(0)h\|_{L^2(\Omega)}\leqslant C\epsilon^{1/2}\|h\|_{H^2(\Omega)}$ *for* $\|z\|_{H^2(\Omega)}\leqslant 1$.

Proof: The proof of Lemma 4.4 is similar to that of Lemma 3.3, and we sketch it in brief.

Lemma 4.2 implies that there are some constants $C,c>0$ such that $|F_\epsilon(0)|\leqslant Ce^{-c/\epsilon}$ on V_d^c. For each $1\leqslant j\leqslant m$, it follows that on each local coordinate chart (U_j,x_j)

$$F_\epsilon(0) = -\frac{1}{\epsilon^{9/2}} e^{\phi^*_{j,\epsilon^+}\psi_{j,\epsilon}}(e^{\phi^*_{j,\epsilon^+}\psi_{j,\epsilon}} - 1) + \frac{1}{\epsilon^{9/2}} e^{-\xi_j} e^{\phi^*_{j,\epsilon}}(e^{\phi^*_{j,\epsilon}} - 1) + \frac{1}{\epsilon^{9/2}} e^{\phi^*_{j,\epsilon}}(2e^{\phi^*_{j,\epsilon}} - 1)\psi_{j,\epsilon}$$

$$+ \frac{1}{\epsilon^{9/2}}(1 - e^{-\xi_j}) e^{\phi^*_{j,\epsilon}}(e^{\phi^*_{j,\epsilon}} - 1) = \frac{1}{\epsilon^{9/2}} O(1)|\psi_{j,\epsilon}|^2 \quad \text{for} \quad |x| \leqslant d.$$

Since $\alpha_j(\epsilon) \leqslant C\epsilon^2$, we obtain

$$\|F_\epsilon(0)\|_{L^2(x_j^{-1}(B_d(0)))} \leqslant C\epsilon^{-7/2} \|\hat{\psi}_{j,\epsilon}\|^2_{L^4(B_{d/\epsilon}(0))} \leqslant C\epsilon^{-3/2}\alpha_j(\epsilon).$$

Therefore (a) is proved. In particular, $\|F_\epsilon(0)\|_{L^2(\Omega)} = O(\epsilon^{1/2})$ as $\epsilon \to 0^+$.

Making use of (4.4) and the argument in the proof of Lemma 3.3, we can also prove (b) and (c). We skip the details. See Refs. 1, 2, 4, 21, and 26. □

We are now in a position to prove Theorem 4.1.

Proof of Theorem 4.1: Let $\mathcal{B} = \{v \in H^2(\Omega) | \|v\|_{H^2(\Omega)} \leqslant 1\}$, and define a mapping $\Phi_\epsilon : H^2(\Omega) \to H^2(\Omega)$ by

$$\Phi_\epsilon(v) = v - [DF_\epsilon(0)]^{-1} F_\epsilon(v).$$

It is easily checked that (4.1) admits a solution u_ϵ of the form (4.9) if and only if $v_\epsilon \in H^2(\Omega)$ is a fixed point of Φ_ϵ.

It follows from Lemma 4.4 that Φ_ϵ is a well-defined contraction mapping from $\mathcal{B}$ into $\mathcal{B}$ if $\epsilon > 0$ is sufficiently small. Therefore, if $\epsilon > 0$ is sufficiently small then Φ_ϵ admits a unique fixed point in $\mathcal{B}$.

On the other hand, Proposition 4.1 implies that v_ϵ defined in (4.9) is a fixed point of Φ_ϵ, and moreover, $v_\epsilon \in \mathcal{B}$ if $\epsilon > 0$ is sufficiently small. Therefore, v_ϵ in (4.9) is the unique fixed point of Φ_ϵ for $\epsilon > 0$ sufficiently small.

The proof of Theorem 1.3 is complete. □

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Weak field reduction in teleparallel coframe gravity: Vacuum case

Yakov Itin[a)]
Institute of Mathematics, Hebrew University of Jerusalem, Givat Ram, Jerusalem 91904, Israel

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The teleparallel coframe gravity may be viewed as a generalization of the standard GR. A coframe (a field of four independent 1-forms) is considered, in this approach, to be a basic dynamical variable. The metric tensor is treated as a secondary structure. The general Lagrangian, quadratic in the first order derivatives of the coframe field is not unique. It involves three dimensionless free parameters. We consider a weak field approximation of the general coframe teleparallel model. In the linear approximation, the field variable, the coframe, is covariantly reduced to the superposition of the symmetric and antisymmetric field. We require this reduction to be preserved on the levels of the Lagrangian, of the field equations, and of the conserved currents. This occurs if and only if the pure Yang–Mills-type term is removed from the Lagrangian. The absence of this term is known to be necessary and sufficient for the existence of the viable (Schwarzschild) spherical-symmetric solution. Moreover, the same condition guarantees the absence of ghosts and tachyons in particle content of the theory. The condition above is shown recently to be necessary for a well-defined Hamiltonian formulation of the model. Here we derive the same condition in the Lagrangian formulation by means of the weak field reduction. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1819523]

I. INTRODUCTION

Einstein's general relativity (GR) is very successful in describing the long distance (macroscopic) gravity phenomena. This theory, however, encounters serious difficulties on microscopic distances. So far essential problems appear in all attempts to quantize the standard GR (for recent review, see, e.g., Ref. 1). Also, the Lagrangian structure of GR differs, in principle, from the ordinary microscopic gauge theories. In particular, a covariant conserved energy-momentum tensor for the gravitational field cannot be constructed in the framework of GR. Consequently, the study of alternative models of gravity is justified from the physical as well as from the mathematical point of view. Even in the case when GR is unique true theory of gravity, consideration of close alternative models can shed light on the properties of GR itself.

Among various alternative constructions, the Poincaré gauge theory of gravity, see Refs. 2–11, is of a special interest. This theory proposes a natural bridge between gauge and geometrical theories. Moreover, it has a straightforward generalization to the metric-affine theory of gravity,[5] which involves a wide spectra of space–time geometries. However, it was elucidated recently that even the restriction of the Poincaré gauge theory to the teleparallel model provides a reasonable alternative to GR.

[a)]Electronic mail: itin@math.huji.ac.il

A. Coframe (teleparallel) gravity—basic facts and notations

We start with a brief account of the coframe (teleparallel) model of gravity and establish the notations used in this paper. Details, different approaches, and additional references can be found in Refs. 12–28.

Let a four-dimensional (4D) differential manifold $\mathcal{M}$ be endowed with two smooth fields: a frame field e_a and a coframe field ϑ^a. In a local coordinate chart,

$$e_a = e_a{}^\mu(x)\,\partial/\partial x^\mu, \quad \vartheta^a = \vartheta^a_\mu(x)\mathrm{d}x^\mu, \quad a,\mu = 0,1,2,3. \tag{1.1}$$

These fields allow to compare two vectors (more generally, two tensors) attached to different points of the manifold. It is referred to as the *teleparallel structure* on $\mathcal{M}$. The two basic fields are assumed to fulfill the dual relation: $e_a \rfloor \vartheta^b = \delta^b_a$. We denote by $\rfloor$ the interior product operator $\mathcal{X}\times\Lambda^p \to \Lambda^{p-1}$ that, for an arbitrary vector field $X \in \mathcal{X}$ and a p-form field $w \in \Lambda^p$, $X \rfloor w := w(X,\ldots)$. So only one of the fields, e_a or ϑ^a, is independent. Thus, two alternative (but, principle, equivalent) representations of the teleparallel geometry are possible.

The *frame representation* is based on a complex $\{\mathcal{M}, e_a\}$ and applies the tensorial calculus as the main mathematical tool similar to the Einstein tensorial representation of GR.

The *coframe representation*, which deals with a complex $\{\mathcal{M}, \vartheta^a\}$, applies the exterior form technique. In the present paper, we use this approach and call it the *coframe gravity*, in contrast to the metric gravity of GR.

In a wider context, the coframe field appears as one of the basic dynamical variables in the Poincaré gauge gravity and in the metric-affine gravity. To extract the pure coframe sector, in these theories, one must require vanishing of the curvature. Here, we treat the coframe field as a self-consistent dynamical variable with its own covariant operators: wedge product, Hodge map and exterior derivative. These two approaches (one with a trivial connection and the other without explicit exhibition of a connection) are principally equivalent.

The indices in (1.1) are basically different. The greek indices refer to the coordinate space and describe the behavior of tensors under the group of diffeomorphisms of the manifold $\mathcal{M}$. The italic indices denote different 1-forms of the coframe. The corresponding group of transformations, SO(1,3), comes together with its natural invariant $\eta_{ab} = \mathrm{diag}(1,-1,-1,-1)$.

The metric tensor on $\mathcal{M}$ is expressed via the coframe as

$$g = \eta_{ab}\vartheta^a \otimes \vartheta^b, \tag{1.2}$$

i.e., the coframe is postulated to be pseudo-orthonormal. The coframe field and all the objects constructed from it are assumed to be global (rigid) covariant. In other words, all the constructions are required to be covariant under the global transformations $\vartheta^a \to A^a{}_b\vartheta^b$ with a constant matrix $A^a{}_b \in \mathrm{SO}(1,3)$. The metric tensor (1.2) is invariant under a wider group of transformation: local (pointwise) transformations of the coframe with $A^a{}_b = A^a{}_b(x)$.

Consider a Lagrangian density, which is (i) diffeomorphism invariant, (ii) invariant under global SO(1,3) transformations of the coframe, and (iii) quadratic in the exterior derivatives of the coframe. The most general Lagrangian of this form is a linear combination,[23,26]

$$\mathcal{L} = \frac{1}{2}\sum_{i=1}^{3} \rho_i{}^{(i)}\mathcal{L}, \tag{1.3}$$

where ρ_1, ρ_2, ρ_3 are free dimensionless parameters. The linear independent 4-forms appearing here are expressed via the coframe *field strength*, $\mathcal{C}^a := \mathrm{d}\vartheta^a$,

$${}^{(1)}\mathcal{L} = \mathcal{C}^a \wedge {}^*\,\mathcal{C}_a, \tag{1.4}$$

$${}^{(2)}\mathcal{L} = (\mathcal{C}_a \wedge \vartheta^a) \wedge {}^*\,(\mathcal{C}_b \wedge \vartheta^b), \tag{1.5}$$

$$^{(3)}\mathcal{L} = (\mathcal{C}_a \wedge \vartheta^b) \wedge * (\mathcal{C}_b \wedge \vartheta^a). \tag{1.6}$$

The Hodge dual operator * is defined by the pseudo-orthonormal coframe ϑ^a or, equivalently, by the metric (1.2). One may try to include in the Lagrangian some invariant expressions of the second order (similarly to the Hilbert–Einstein Lagrangian). Such terms, however, are reduced to total derivatives and do not affect the field equations and the Noether conserved currents. So (1.3) is the most general Lagrangian that generates the field equations of the second order.

Let us introduce the notion of the *field strength*

$$\mathcal{F}^a := {}^{(1)}\mathcal{F}^a + {}^{(2)}\mathcal{F}^a + {}^{(3)}\mathcal{F}^a, \tag{1.7}$$

with

$${}^{(1)}\mathcal{F}^a := (\rho_1 + \rho_3)\mathcal{C}^a, \tag{1.8}$$

$${}^{(2)}\mathcal{F}^a := \rho_2\, e^a \rfloor (\vartheta^m \wedge \mathcal{C}_m), \tag{1.9}$$

$${}^{(3)}\mathcal{F}^a := -\rho_3 \vartheta^a \wedge (e_m \rfloor \mathcal{C}^m). \tag{1.10}$$

Such separation of the strength $\mathcal{F}^a$ involves two scalar-valued forms $\vartheta^m \wedge \mathcal{C}_m$ and $e_m \rfloor \mathcal{C}^m$. So some calculations are simplified. For irreducible decomposition of $\mathcal{F}^a$, see Refs. 5 and 23.

In the notations (1.8)–(1.10), the coframe Lagrangian (1.3) takes a form similar to the Maxwell Lagrangian,

$$\mathcal{L} = \tfrac{1}{2}\mathcal{C}^a \wedge * \mathcal{F}_a. \tag{1.11}$$

The free variation of (1.11) relative to the coframe ϑ^a must take into account also the variation of the Hodge dual operator, which implicitly depends on the coframe. It yields the field equation of the form[23]

$$\mathrm{d} * \mathcal{F}^a = \mathcal{T}^a, \tag{1.12}$$

where the 3-form $\mathcal{T}^a$ is the energy-momentum current of the coframe field

$$\mathcal{T}_a = (e_a \rfloor \mathcal{C}_m) \wedge * \mathcal{F}^m - e_a \rfloor \mathcal{L}. \tag{1.13}$$

The conservation law for this 3-form: $\mathrm{d}\mathcal{T}_a = 0$ is a straightforward consequence of (1.12).

B. Viable models—a problem of physical motivation

A general quadratic coframe model, which is global SO(1,3) invariant, involves three parameters,

$$\rho_1, \quad \rho_2, \quad \rho_3 \text{ — free}. \tag{1.14}$$

The ordinary GR is extracted from this family by requiring of the *local* SO(1,3) invariance, which is realized by the following restrictions of the parameters:

$$\rho_1 = 0, \quad 2\rho_2 + \rho_3 = 0. \tag{1.15}$$

The analysis of exact solutions[28] to the field equation (1.12) shows that the Schwarzschild solution appears even for a wider set of parameters (viable set),

$$\rho_1 = 0, \quad \rho_2, \quad \rho_3 \text{ — free}. \tag{1.16}$$

Moreover, for $\rho_1 \neq 0$, spherical-symmetric static solutions to (1.12) do not have the Newtonian behavior at infinity.[28]

So a problem arises: *Which physical motivated requirement extracts the viable set of parameters?*

The quantum-theory solution to this problem is known for a long time. In Refs. 29–33 it was shown that the requirement (1.16) is necessary and sufficient for the absence of ghosts and tachyons in particle content of the theory. Another motivation for (1.16) comes from the requirement that the theory must have a well-defined Hamiltonian formulation (Ref. 34).

In this paper we look for a motivation of (1.16) on a classical Lagrangian level. We deal with linear approximation of the general coframe model. The coframe variable can be treated, in this approximation, as a regular 4×4 matrix. Consequently, it reduced to a composition of two independent variables: the symmetric and the antisymmetric fields.

Our main result is as follows: Only for (1.16), the coframe model is reduced to two independent models, every one with its own Lagrangian, field equation, and conserved current. In other words, the viable model is exactly this one that approaches the *free-field limit*, i.e., any interaction between the approximately independent fields appears only in higher orders.

Linear approximation of coframe models was usually applied for studying the deviation of teleparallel gravity from the standard GR, and for comparison with the observation data, see Refs. 3, 4, 30, and 31. In our approach the reduction of the lower order terms is used as a theoretical device. We show that this condition is enough to distinguish the set of viable models. The relation between these two approaches requires a further consideration.

II. WEAK FIELD REDUCTION

A. Linear approximations

To study the approximate solutions to (1.12), we start with a trivial exact solution, a *holonomic coframe*, for which,

$$\mathrm{d}\vartheta^a = 0. \tag{2.1}$$

Consequently, $\mathcal{F}^a=\mathcal{C}^a=0$, so both sides of Eq. (1.12) vanish. By Poincaré's lemma, the solution of (2.1) can be locally expressed as $\vartheta^a=\mathrm{d}\tilde{x}^a(x)$, where $\tilde{x}^a(x)$ is a set of four smooth functions defined in some neighborhood U of a point $x\in\mathcal{M}$. The functions $\tilde{x}^a(x)$, being treated as the components of a coordinate map $\tilde{x}^a: U\to\mathbb{R}^4$, generate a local coordinate system on U. The metric tensor (1.2) reduces, in this coordinate chart, to the flat Minkowskian metric $g=\eta_{ab}\mathrm{d}\tilde{x}^a\otimes\mathrm{d}\tilde{x}^b$. Thus the holonomic coframe plays, in the teleparallel background, the same role as the Minkowskian metric in the (pseudo-)Riemannian geometry. Moreover, a manifold endowed with a (pseudo-)orthonormal holonomic coframe is flat. The weak perturbations of the basic solution $\vartheta^a=\mathrm{d}x^a$ are

$$\vartheta^a = \mathrm{d}x^a + h^a = (\delta^a_b + h^a{}_b)\mathrm{d}x^b. \tag{2.2}$$

"Weak" means

$$\|h^a{}_b\| = \epsilon = o(1), \quad \|h^a{}_{b,c}\| = O(\epsilon), \quad \|h^a{}_{b,c,d}\| = O(\epsilon), \tag{2.3}$$

where $\|\cdots\|$ denotes the maximal tensor norm. We accept that the coframe ϑ^a and the holonomic coframe $\mathrm{d}x^a$ have the same physical dimension of [*length*]. Thus, the components of the matrix $h^a{}_b$ and the parameter ϵ are dimensionless. Consequently, the approximation conditions (2.3) are invariant under rescaling of the coordinates.

In this paper we will take into account only the first order approximation in the perturbations $h^a{}_b$ and in their derivatives (i.e., in the parameter ϵ). Note that, in this approximation, the difference between coframe and coordinate indices completely disappears. This justifies our choice, in (2.2) and in the sequel, of the same notation for these (basically different) indices.

In accordance with (2.3), only weak coordinate transformations are considered. Under a shift

$$x^a \mapsto x^a + \xi^a(x), \tag{2.4}$$

the components of the coframe are transformed as

$$h^a{}_b \mapsto h^a{}_b - \xi^a{}_{,b}. \tag{2.5}$$

Thus, in order to preserve the weakness of the fluctuation, it is necessary to require $\xi^a{}_{,b}=O(\|h^a{}_b\|)$. We will use the term *approximately covariant*[35] for the expressions which are covariant only to the first order of the perturbations. Observe that this assumption restricts only the amplitudes of the perturbations and of their derivatives. It does not restrict, however, the local freedom to transform the coordinates. An appropriative coordinate system can still be chosen in a small neighborhood of the identity transformation in order to simplify the (local) field equations.

Similarly, in order to be in agreement with the approximation condition (2.3), the global SO(1,3) transformations of the coframe field, $\vartheta^a \mapsto A^a{}_b \vartheta^b$, must also be restricted. It is enough to require the transformations to be in a small neighborhood of the identity

$$A^a{}_b = \delta^a_b + \alpha^a_b, \quad \|\alpha^a_b\| = o(1). \tag{2.6}$$

B. Reduction of the field

In (2.2), $h^a{}_b$ is a perturbation of the flat coframe. Thus we have the following.

(i) To the first order, the holonomic coframe is expressed by the unholonomic one as

$$\mathrm{d}x^a = (\delta^a_b - h^a{}_b)\vartheta^b. \tag{2.7}$$

(ii) The indices in $h^a{}_b$ can be lowered and raised by the Minkowskian metric,

$$h_{ab} := \eta_{am} h^m{}_b, \quad h^{ab} := \eta^{bm} h^a{}_m. \tag{2.8}$$

The first operation is exact (covariant to all orders of approximations), while the second is covariant only to the first order, when $g^{ab} \approx \eta^{ab}$.

(iii) The symmetric and the antisymmetric combinations of the perturbations,

$$\theta_{ab} := h_{(ab)} = \tfrac{1}{2}(h_{ab} + h_{ba}) \quad \text{and} \quad w_{ab} := h_{[ab]} = \tfrac{1}{2}(h_{ab} - h_{ba}) \tag{2.9}$$

as well as the trace $\theta := h^m{}_m = \theta^m{}_m$ are covariant to the first order.

(iv) The components of the metric tensor, in the linear approximation, involve only the symmetric combination of the coframe perturbations,

$$g_{ab} = \eta_{ab} + 2\theta_{ab}. \tag{2.10}$$

(v) Under the transformations (2.4), two covariant pieces of the fluctuation change as

$$\theta_{ab} \mapsto \theta_{ab} - \xi_{(a,b)} \quad \text{and} \quad w_{ab} \mapsto w_{ab} - \xi_{[a,b]}. \tag{2.11}$$

Thus the approximately covariant irreducible decomposition of the dynamical variable

$$h_{ab} = \theta_{ab} + w_{ab} \tag{2.12}$$

is obtained. Thus, instead of one field h_{ab}, we have, in this approximation, two independent fields: a symmetric field θ_{ab} and an antisymmetric field w_{ab}.

C. Gauge conditions

The actual values of the components of the fields θ_{ab} and w_{ab} depend on a choice of a coordinate system. Thus four arbitrary relations between the components (equal to the number of coordinates) may be imposed. We require these relations to be Lorentz invariant, i.e., covariant in the first order approximation. Thus the most general form of constraints (gauge conditions) that involve the first order derivatives is

$$\alpha\theta_{am}{}^{,m} + \beta\theta_{,a} + \gamma w_{am}{}^{,m} = 0, \tag{2.13}$$

where α, β, γ are dimensionless parameters.

Certainly, for some special values of the parameters, these conditions cannot be realized. Indeed, under the coordinate transformations (2.4), Eq. (2.13) changes, in the lowest order, to

$$\alpha\tilde{\theta}_{am}{}^{,m} + \beta\tilde{\theta}_{,a} + \gamma\tilde{w}_{am}{}^{,m} = (\alpha\xi_{(a,m)} + \beta\xi_{m,a} + \gamma\xi_{[a,m]})^{,m}. \tag{2.14}$$

Thus the conditions (2.13) can be realized, by the coordinate transformations (2.4), if and only if the system of PDE (2.14) has a solution $\xi(x)$ for a given left-hand side (LHS).

Let us check the integrability of this system. Equation (2.14) results in

$$(\alpha\xi_{(a,m),b} + \beta\xi_{m,a,b} + \gamma\xi_{[a,m],b})^{,m} = \alpha\tilde{\theta}_{am,b}{}^{,m} + \beta\tilde{\theta}_{,a,b} + \gamma\tilde{w}_{am,b}{}^{,m}. \tag{2.15}$$

Commuting the indices a and b, we obtain

$$(\alpha + \gamma)\,\Box\,\xi_{[a,b]} = 2(\alpha\theta_{m[a,b]} - \gamma w_{m[a,b]})^{,m}. \tag{2.16}$$

Thus, the gauge condition (2.13) with $\alpha = -\gamma \neq 0$ cannot be realized by any change of the coordinate system. Now, take the trace of (2.15),

$$(\alpha + \beta)\,\Box\,\xi_{m}{}^{,m} = \alpha\theta_{mn}{}^{,m,n} + \beta\,\Box\,\theta. \tag{2.17}$$

Thus $\alpha = -\beta \neq 0$ is also forbidden.

We will apply, in the sequel, two separate gauge conditions: for the symmetric field

$$\theta_{am}{}^{,m} - \tfrac{1}{2}\theta_{,a} = 0, \tag{2.18}$$

and for the antisymmetric field

$$w_{am}{}^{,m} = 0. \tag{2.19}$$

Observe, that (2.18) and (2.19) cannot be realized simultaneously by the same coordinate transformation. Indeed, for this, the coordinate functions must satisfy

$$\Box\,\xi_a = 2\theta_{am}{}^{,m} - \theta_{,a} \quad \text{and} \quad \Box\,\xi_a - (\xi_m{}^{,m})_{,a} = w_{am}{}^{,m}. \tag{2.20}$$

The integrability conditions for these equations yield

$$\Box\,\xi_{[a,b]} = 2\theta_{m[a,b]}{}^{,m} = -\,w_{m[a,b]}{}^{,m}. \tag{2.21}$$

For arbitrary independent fields θ_{ab} and w_{ab}, these conditions are not satisfied.

Certainly, the conditions (2.18) and (2.19) can be realized, separately, by transformation of the coordinates.

D. Reduction of the field strengths

By (2.3), let us decompose the field strengths (1.8)–(1.10). The 2-form $\mathcal{C}_a$ is approximated by

$$\mathcal{C}_a = h_{ab,c}\,\mathrm{d}x^c \wedge \mathrm{d}x^b = -\,h_{a[b,c]}\vartheta^b \wedge \vartheta^c = -\,(\theta_{a[b,c]} + w_{a[b,c]})\,\vartheta^b \wedge \vartheta^c. \tag{2.22}$$

Consequently, the first part of the field strength (1.8), takes the form

$${}^{(1)}\mathcal{F}_a = -\,(\rho_1 + \rho_3)(\theta_{a[b,c]} + w_{a[b,c]})\,\vartheta^b \wedge \vartheta^c. \tag{2.23}$$

As for the second part (1.9), it involves only the antisymmetric field,

$${}^{(2)}\mathcal{F}_a = -\,3\rho_2 w_{[ab,c]}\;\vartheta^b \wedge \vartheta^c. \tag{2.24}$$

The third part (1.10), takes the form

$$^{(3)}\mathcal{F}_a = \rho_3 \eta_{ac}(h_{mb}{}^{,m} - h_{,b})\ \vartheta^b \wedge \vartheta^c = \rho_3 \eta_{ac}(\theta_{bm}{}^{,m} - \theta_{,b} - w_{bm}{}^{,m})\vartheta^b \wedge \vartheta^c. \tag{2.25}$$

Therefore, the field strength is reduced to the sum of two independent strengths—one defined by the symmetric field θ_{ab} and the second one defined by the antisymmetric field w_{ab},

$$\mathcal{F}_a(\theta_{mn}, w_{mn}) = {}^{(\mathrm{sym})}\mathcal{F}_a(\theta_{mn}) + {}^{(\mathrm{ant})}\mathcal{F}_a(w_{mn}), \tag{2.26}$$

where

$$^{(\mathrm{sym})}\mathcal{F}_a = -[(\rho_1 + \rho_3)\theta_{a[b,c]} + \rho_3 \eta_{a[b}\ \theta_{c]m}{}^{,m} - \rho_3 \eta_{a[b}\ \theta_{,\,c]}]\vartheta^b \wedge \vartheta^c \tag{2.27}$$

and

$$^{(\mathrm{ant})}\mathcal{F}_a = -[(\rho_1 + \rho_3)w_{a[b,c]} + 3\rho_2 w_{[ab,c]} - \rho_3 \eta_{a[b}\, w_{\,c]m}{}^{,m}]\vartheta^b \wedge \vartheta^c. \tag{2.28}$$

Hence, for arbitrary values of the parameters ρ_i, the field strengths are independent.

E. Reduction of the field equations

The field equation (1.12) includes the second order derivatives of the perturbations on its LHS and the squares of the first order derivatives on both sides. In the linear approximation (2.3), the quadratic terms can be neglected. Thus, (1.12) is approximated by

$$\mathrm{d} * \mathcal{F}^a = 0. \tag{2.29}$$

The covector valued 2-form $\mathcal{F}_a$ can be expressed in the unholonomic basis as $\mathcal{F}_a = \mathcal{F}_{abc}\vartheta^b \wedge \vartheta^c/2$. Accordingly, we derive

$$\mathrm{d} * \mathcal{F}^a = \tfrac{1}{2}F_{abc,m}\ \mathrm{d}x^m \wedge *\,(\vartheta^b \wedge \vartheta^c) = -\tfrac{1}{2}F_{abc}{}^{,m} * [\, e_m \rfloor (\vartheta^b \wedge \vartheta^c) \rfloor = \tfrac{1}{2}F_{a[bc]}{}^{,c} * \vartheta^b.$$

Consequently, Eq. (2.29) reads

$$F_{a[bc]}{}^{,c} = 0. \tag{2.30}$$

Applying the antisymmetrization of the corresponding indices to the expression (2.26) we derive the linearized field equation

$$\begin{aligned}(\rho_1 + \rho_3)(\Box\,\theta_{ab} - \theta_{am,b}{}^{,m}) + \rho_3(-\,\eta_{ab}\,\Box\,\theta - \theta_{mb}{}^{,m}{}_{,a} + \theta_{,a,b} + \eta_{ab}\theta_{mn}{}^{,m,n}) \\ + (\rho_1 + 2\rho_2 + \rho_3)(\Box w_{ab} - w_{am,b}{}^{,m}) + (2\rho_2 + \rho_3)w_{bm,a}{}^{,m} = 0.\end{aligned} \tag{2.31}$$

Proposition 1: For the case $\rho_1 = 0$, *the linearized coframe field equation (2.31), in arbitrary coordinates, splits into two independent systems,*

$$^{(\mathrm{sym})}\mathcal{E}_{(ab)}(\theta_{mn}) = 0 \quad \text{and} \quad {}^{(\mathrm{ant})}\mathcal{E}_{[ab]}(w_{mn}) = 0.$$

If $\rho_1 \neq 0$, *Eq. (2.31) does not split in any coordinate system.*

Proof: The equation (2.31) is tensorial to the first order. Thus, by applying symmetrization and antisymmetrization operations, it is reduced covariantly to a system of two independent tensorial (to the first order) equations. The symmetrization yields a system of 10 independent equations,

$$\Box[(\rho_1 + \rho_3)\theta_{ab} - \rho_3 \eta_{ab}\theta] - (\rho_1 + 2\rho_3)\theta_{m(a,b)}{}^{,m} + \rho_3(\theta_{,a,b} + \eta_{ab}\theta_{mn}{}^{,m,n}) + \rho_1 w_{m(a,b)}{}^{,m} = 0. \tag{2.32}$$

The antisymmetrization yields a system of six independent equations,

$$(\rho_1 + 2\rho_2 + \rho_3)\,\Box\, w_{ab} + (\rho_1 + 4\rho_2 + 2\rho_3) w_{m[a,b]}{}^{,m} - \rho_1 \theta_{m[a,b]}{}^{,m} = 0. \tag{2.33}$$

Evidently, the condition $\rho_1 = 0$ removes the "mixed terms" and yields the separation of the system. Such splitting holds in arbitrary system of coordinates.

Suppose now $\rho_1 \neq 0$. Thus, the "mixed terms" remain in both equations—the w term in (2.32) and the θ term in (2.33). Let us try to remove these terms by an appropriative choice of a coordinate system. For this we must require the equations

$$\theta_{m[a,b]}{}^{,m} = 0 \quad \text{and} \quad w_{m(a,b)}{}^{,m} = 0$$

to hold simultaneously. These equations can be satisfied only if

$$\theta_{ma}{}^{,m} = 0 \quad \text{and} \quad w_{ma}{}^{,m} = 0. \tag{2.34}$$

The actual values of the variables θ_{ab} and w_{ab} depend on a choice of a coordinate system. Recall that the approximation conditions (2.3) do not restrict the freedom to choose the local coordinate transformations. Therefore, by (2.4), four additional conditions (equal to the number of coordinates), can still be applied to the perturbations in order to satisfy (2.34). We need, however, to eliminate eight independent expressions $w_{ma}{}^{,m}$ and $\theta_{ma}{}^{,m}$. This cannot be done by four independent functions of the coordinates. Indeed, under the transformations (2.4),

$$\theta_{ma}{}^{,m} \mapsto \theta_{ma}{}^{,m} - \xi_{(m,a)}{}^{,m}, \tag{2.35}$$

$$w_{ma}{}^{,m} \mapsto w_{ma}{}^{,m} - \xi_{[m,a]}{}^{,m}. \tag{2.36}$$

Hence the coordinate transformations must satisfy

$$\xi_{(m,a)}{}^{,m} = \theta_{ma}{}^{,m} \quad \text{and} \quad \xi_{[m,a]}{}^{,m} = w_{ma}{}^{,m} \tag{2.37}$$

simultaneously. Therefore,

$$\xi_{m,a}{}^{,m} = h_{ma}{}^{,m}. \tag{2.38}$$

The consistency condition for (2.38) is

$$h_{ma,b}{}^{,m} = h_{mb,a}{}^{,m},$$

which it is not satisfied in general. ■

Consequently, for $\rho_1 = 0$ and generic values of the parameters ρ_2, ρ_3, the field equation of the coframe field is reduced to two independent field equations for independent field variables.

(i) The symmetric field θ_{ab} of 10 independent variables satisfies the system of 10 independent equations,

$$^{(\mathrm{sym})}\mathcal{E}_{(ab)}(\theta_{mn}) := \rho_3[\Box(\theta_{ab} - \eta_{ab}\theta) - \theta_{m(a,b)}{}^{,m} + \theta_{,a,b} + \eta_{ab}\theta_{mn}{}^{,m,n}] = 0. \tag{2.39}$$

We rewrite it as

$$\Box(\theta_{ab} - \eta_{ab}\theta) - (\theta_{am}{}^{,m} - \tfrac{1}{2}\theta_{,a})_{,b} - (\theta_{bm}{}^{,m} - \tfrac{1}{2}\theta_{,b})_{,a} + \eta_{ab}\theta_{mn}{}^{,m,n} = 0. \tag{2.40}$$

Substituting here the condition (2.18) and its consequence

$$\theta_{mn}{}^{,m,n} = \tfrac{1}{2}\,\Box\,\theta \tag{2.41}$$

we obtain

$$\Box(\theta^{ab} - \tfrac{1}{2}\eta^{ab}\theta) = 0. \tag{2.42}$$

Equation (2.42) results in $\Box\theta = 0$. Then it is equivalent to

$$\Box\theta_{ab}=0. \tag{2.43}$$

Consequently, in the coordinates associated with (2.18), the symmetric field satisfied the wave equation.

(ii) The antisymmetric system of six independent equations for six independent variables,

$$^{(\mathrm{ant})}\mathcal{E}_{[ab]}(w_{mn}):=(2\rho_2+\rho_3)(\Box w_{ab}+2w_{m[a,b]}{}^{,m})=0. \tag{2.44}$$

In the coordinates associated with (2.19) it is reduced to the wave equation,

$$\Box w_{ab}=0. \tag{2.45}$$

F. Reduction of the Lagrangian

In the sequel of this paper, we consider the models with parameter $\rho_1=0$. Let us examine now the reduction of the Lagrangian (1.3).

Proposition 2: For $\rho_1=0$, the Lagrangian of the coframe field is reduced, up to a total derivative term, to the sum of two independent Lagrangians,

$$\mathcal{L}(\theta_{ab},w_{ab})=^{(\mathrm{sym})}\mathcal{L}(\theta_{ab})+^{(\mathrm{ant})}\mathcal{L}(w_{ab}). \tag{2.46}$$

Proof: With $\rho_1=0$ the term $^{(1)}\mathcal{L}$ does not appear in the Lagrangian. Calculate in the linear approximation (we use the abbreviation $\vartheta^{ab\cdots}=\vartheta^a\wedge\vartheta^b\wedge\cdots$),

$$^{(2)}\mathcal{L}=(\mathrm{d}\vartheta^a\wedge\vartheta_a)\wedge *(\mathrm{d}\vartheta_b\wedge\vartheta^b)=h^{am,n}h_{bp,q}\vartheta_{nma}\wedge *\vartheta^{qpb}. \tag{2.47}$$

Applying the formula

$$\vartheta_{abc}\wedge *\vartheta^{a'b'c'}=6\delta_a^{[a'}\delta_b^{b'}\delta_c^{c']}*1 \tag{2.48}$$

we derive

$$^{(2)}\mathcal{L}=2w^{ab,c}(w_{ab,c}+w_{ca,b}+w_{bc,a})*1. \tag{2.49}$$

So $^{(2)}\mathcal{L}$ depends only on the antisymmetric field. Consider now the linear approximation to the term $^{(3)}\mathcal{L}$,

$$^{(3)}\mathcal{L}=(\mathrm{d}\vartheta_a\wedge\vartheta_b)\wedge *(\mathrm{d}\vartheta^b\wedge\vartheta^a)=h_a{}^{m,n}h^b{}_{p,q}\vartheta_{nmb}\wedge *\vartheta^{qpa}. \tag{2.50}$$

Use (2.48) to get

$$^{(3)}\mathcal{L}=[h_{ab,c}(h^{ab,c}-h^{ac,b})-h_{ab}{}^{,a}h^{cb}{}_{,c}+\theta^a(2h_{ba}{}^{,b}-\theta_{,a})]*1. \tag{2.51}$$

Insert here the splitting (2.12). It follows that the Lagrangian (2.51) is reduced to the sum

$$^{(3)}\mathcal{L}=^{(3)}\mathcal{L}(\theta)+^{(3)}\mathcal{L}(w)+^{(3)}\mathcal{L}(\theta,w), \tag{2.52}$$

where

$$^{(3)}\mathcal{L}(\theta)=[\theta_{ab,c}(\theta^{ab,c}-\theta^{ac,b})-\theta_{ab}{}^{,a}\theta^{cb}{}_{,c}+\theta^a(2\theta_{ba}{}^{,b}-\theta_{,a})]*1, \tag{2.53}$$

$$^{(3)}\mathcal{L}(w)=[w_{ab,c}(w^{ab,c}-w^{ac,b})-w_{ab}{}^{,a}w^{cb}{}_{,c}]*1, \tag{2.54}$$

$$^{(3)}\mathcal{L}(\theta,w)=2[-\theta_{ab,c}w^{ac,b}+\theta^a w_{ba}{}^{,b}-\theta_{ab}{}^{,a}w^{cb}{}_{,c}]*1. \tag{2.55}$$

Extracting the total derivatives in the mixed term (2.55) we obtain

$$^{(3)}\mathcal{L}(\theta,w)=(\theta_{ab}(w^{ac,b}-w^{bc,a})_{,c}-\theta w_{ba}{}^{,a,b})*1+\text{exact terms}. \tag{2.56}$$

The terms in the square brackets vanish identically as a product of symmetric and antisymmetric tensors. Thus the mixed term $^{(3)}\mathcal{L}(\theta,w)$ is a total derivative. Consequently, desired reduction of the Lagrangian is obtained. ■

The Lagrangian of the symmetric field $^{(\text{sym})}\mathcal{L}=^{(3)}\mathcal{L}(\theta)$ may be rewritten in a more compact form. Observing the identity

$$\theta_{ab}{}^{,a}\theta^{cb}{}_{,c}=\theta_{ab}{}^{,c}\theta^{cb}{}_{,a}+\text{exact terms}, \tag{2.57}$$

and extracting the total derivatives, we obtain

$$^{(\text{sym})}\mathcal{L}=\tfrac{1}{2}\rho_3[\theta_{ab,c}(\theta^{ab,c}-2\theta^{ac,b})+\theta^a(2\theta_{ba}{}^{,b}-\theta_{,a})]*1. \tag{2.58}$$

This form of the Lagrangian is acceptable in arbitrary coordinates. In the coordinates associated with the condition (2.18), the last parentheses in (2.58) vanish. In the first parentheses, we extract the total derivatives and use (2.18) to derive (symbol $\approx$ used here for equality up to total derivatives)

$$\theta_{ab,c}\theta^{ac,b}=(\theta_{ab}\theta^{ac,b})_{,c}-\theta_{ab}\theta^{ac,b}{}_{,c}\approx-\tfrac{1}{2}\theta_{ab}\theta^{a,b}\approx\tfrac{1}{2}\theta_{ab}{}^{,b}\theta^a\approx\tfrac{1}{4}\theta_{,a}\theta^a.$$

Consequently the symmetric field Lagrangian (2.53) is reduced to

$$^{(\text{sym})}\mathcal{L}=\tfrac{1}{2}\kappa(\theta_{ab,c}\theta^{ab,c}-\tfrac{1}{2}\theta_{,a}\theta^a)*1. \tag{2.59}$$

Analogously, for the Lagrangian of the antisymmetric field $^{(\text{ant})}\mathcal{L}=^{(2)}\mathcal{L}+^{(3)}\mathcal{L}(w)$, we use the identity

$$w_{ab}{}^{,a}w^{cb}{}_{,c}=w_{ab,c}w^{ac,b}+\text{exact terms} \tag{2.60}$$

and rewrite it, in an arbitrary system of coordinates, as

$$^{(\text{ant})}\mathcal{L}=\tfrac{1}{2}(2\rho_2+\rho_3)[w_{ab,c}(w^{ab,c}-2w^{ac,b})]*1, \tag{2.61}$$

or, equivalently, as

$$\mathcal{L}(w)=\tfrac{1}{2}(2\rho_2+\rho_3)(w_{ab,c}(w^{ab,c}-w^{ac,b})-w_{ab}{}^{,a}w^{cb}{}_{,c})*1.$$

The gauge condition (2.19) removes the last term while the second term is rewritten as

$$w_{ab,c}w^{ac,b}\approx-w_{ab}w^{ac,b}{}_{,c}\approx0.$$

Thus, the Lagrangian of the antisymmetric field is

$$\tilde{\mathcal{L}}(w)=\tfrac{1}{2}(2\rho_2+\rho_3)w_{ab,c}w^{ab,c}*1. \tag{2.62}$$

G. Reduction of the energy-momentum current

The Lagrangian of the coframe field is decomposed, in the first order approximation, to a sum of two independent Lagrangians for two independent fields. The Noether current expression, being derivable from the Lagrangian, must have the same splitting.

Proposition 3: The coframe energy-momentum current is reduced, on shell, in the first order approximation, as

$$\mathcal{T}_a(\theta_{mn},w_{mn})=^{(\text{sym})}\mathcal{T}_a(\theta_{mn})+^{(\text{ant})}\mathcal{T}_a(w_{mn}), \tag{2.63}$$

up to a total derivative.

Proof: The coframe energy-momentum current is of the form

$$\mathcal{T}_a = (e_a \rfloor \mathcal{C}_m) \wedge {}^*\mathcal{F}^m - e_a \rfloor \mathcal{L}. \tag{2.64}$$

Due to Proposition 2, the second term, in the first order approximation, does not contain the mixed terms $\theta' \cdot w'$. Hence, it already has the reduced form. To treat the first term, we write the strengths in the component

$$\mathcal{C}_m = \mathcal{C}_{m[bc]}\vartheta^b \wedge \vartheta^c, \quad \mathcal{F}^m = F^m{}_{[pq]}\vartheta^p \wedge \vartheta^q. \tag{2.65}$$

Thus, the first term of (2.64) is approximated by

$$(e_a \rfloor \mathcal{C}_m) \wedge {}^*\mathcal{F}^m = \mathcal{C}_{m[bc]}F^m{}_{[pq]}(e_a \rfloor \vartheta^{bc}) \wedge {}^*\vartheta^{pq} = 4C_{m[an]}F^{m[bn]} * \vartheta_b = 4h_{m[a,n]}F^{m[bn]} * \vartheta_b. \tag{2.66}$$

The 3-form $*\vartheta_b$, in the lowest order approximation, is an exact form. Thus, it is enough to show that the scalar factor, on the right-hand side (RHS) of (2.66), has the desired splitting. This expression is a sum of two terms. The first one is proportional to

$$h_{ma,n}F^{m[bn]} = -h_{ma}F^{m[bn]}{}_{,n} + \text{total derivatives},$$

i.e., it is, on shell, an exact form. Now we must show that the second term, which is proportional to $h_{ma,n}F^{m[bn]}$, does not involve the mixed products of a type $\theta \cdot w$. The mixed product expression in the latter term is proportional to

$$\theta_{mn,a}(w^{mb,n} + 2\eta^{m[n}w^{b]k}{}_{,k}) + w_{mn,a}(\theta^{mb,n} + \eta^{mb}\theta^{nk}{}_{,k} - \eta^{mb}\theta^{,n}). \tag{2.67}$$

By recollection of the terms, we rewrite this expression as

$$(\theta_{mn,a}w^{mb,n} + \theta_{mn}{}^{,n}w^{bm}{}_{,a}) + (\theta_{,a}w^{bm}{}_{,m} - \theta_{,m}w^{bm}{}_{,a}) + (\theta^{mb,n}w_{mn,a} - \theta^{bm}{}_{,a}w_{mn}{}^{,n}). \tag{2.68}$$

The three brackets above are total derivatives, namely,

$$[(\theta_{mn,a}w^{mb})^{,n} + (\theta_{mn}{}^{,n}w^{bm})_{,a}] + [(\theta w^{bm}{}_{,m})_{,a} - (\theta w^{bm}{}_{,a})_{,m}] + [(\theta^{mb,n}w_{mn})_{,a} - (\theta^{bm}{}_{,a}w_{mn})^{,n}]. \tag{2.69}$$

Thus, (2.66) and, consequently, (2.64) do not involve the mixed terms. The desired splitting is proved. ■

The energy-momentum tensor $T_a{}^b$ can be derived from the Noether current $\mathcal{T}_a$ by applying the relations

$$\mathcal{T}_a = T_a{}^b * \vartheta_b, \quad T_{ab} = e_b \rfloor * \mathcal{T}_a. \tag{2.70}$$

Proposition 4: For the field θ_{ab} in the coordinate system associated with the gauge condition

$$\theta_{am}{}^{,m} - \tfrac{1}{2}\theta_{,a} = 0, \tag{2.71}$$

the energy-momentum tensor is

$$T_{ab} = \tfrac{1}{2}\kappa[(\theta_{mn,a}\theta^{mn}{}_{,b} - \tfrac{1}{4}\eta_{ab}\theta_{lm,n}\theta^{lm,n}) - \tfrac{1}{2}(\theta_{,a}\theta_{,b} - \tfrac{1}{4}\eta_{ab}\theta_{,m}\theta^{,m})]. \tag{2.72}$$

This tensor is symmetric and traceless.

Proof: We start with the energy-momentum current for the coframe field

$$\mathcal{T}_a = (e_a \rfloor \mathcal{C}_m) \wedge {}^*\mathcal{F}^m - e_a \rfloor \mathcal{L}.$$

Due to Proposition 3, in the first order approximation, this current is decomposed to two independent currents. Thus we may assume $w_{ab}=0$ in order to derive the expression for $\mathcal{T}_a(\theta)$.

In the coordinates associated with the gauge condition (2.71), by (2.59),

$$e_a\mathcal{L}=\tfrac{1}{2}\rho_3(\theta_{mn,p}\theta^{mn,p}-\tfrac{1}{2}\theta_{,m}\theta^{m})*\vartheta_a.$$

The first term of $\mathcal{T}_a$ is derived from (2.64),

$$(e_a\rfloor\mathcal{C}_m)\wedge *\mathcal{F}^m=4\theta_{m[a,n]}F^{m[bn]}*\vartheta_b=2(\theta_{ma,n}F^{m[bn]}*\vartheta_b-\theta_{mn,a}F^{m[bn]}*\vartheta_b).$$

Observe that, on shell, up to a total derivative

$$\theta_{ma,n}F^{m[bn]}\approx-\theta_{ma}F^{m[bn]}{}_{,n}=0.$$

Thus,

$$(e_a\rfloor\mathcal{C}_m)\wedge *\mathcal{F}^m=-2\theta_{mn,a}F^{m[bn]}*\vartheta_b.$$

Applying the gauge condition to (2.26) we get

$$\mathcal{F}_a=-\rho_3[\theta_{a[b,c]}+\eta_{a[b}\,(\theta_{\,c]m}{}^{,m}-\theta_{,\,c]})\vartheta^{bc}=-\rho_3(\theta_{a[b,c]}-\tfrac{1}{2}\eta_{a[b}\,\theta_{,\,c]})\vartheta^{bc}.$$

Consequently,

$$(e_a\rfloor\mathcal{C}_m)\wedge *\mathcal{F}^m=2\rho_3\theta_{mn,a}(\theta^{m[b,n]}-\tfrac{1}{2}\eta^{m[b}\,\theta^{\,n]})*\vartheta_b.$$

Extracting the total derivatives

$$\theta_{mn,a}\theta^{mb,n}\approx\theta_{mn}{}^{,n}\theta^{mb}{}_{,a}\approx\tfrac{1}{2}\theta_{,m}\theta^{mb}{}_{,a}\approx\tfrac{1}{4}\theta_{,a}\theta^{b},$$

$$\theta_{mn,a}\eta^{mb}\theta^{n}\approx\theta_{mn}{}^{,n}\theta_{,a}\approx\tfrac{1}{4}\theta_{,a}\theta^{b},$$

it follows that

$$(e_a\rfloor\mathcal{C}_m)\wedge *\mathcal{F}^m=\rho_3(-2\theta_{mn,a}\theta^{mn,b}+\theta_{,a}\theta^{b})*\vartheta_b.$$

Collecting the terms into $\mathcal{T}_a$ and extracting the energy-momentum tensor $T_a{}^b$ from the current $\mathcal{T}_a$ by $T_{ab}=e_b\rfloor*\mathcal{T}_a$ we get the desired expression. It is clear that energy-momentum tensor is symmetric and traceless. ■

In GR, the behavior of small perturbations of the metric tensor is managed by the wave equation. Thus, for a wave propagating in the positive direction of the x axis, only two independent components of the matrix θ_{ab} remain,

$$\theta_{23}=\mu(\tau),\quad \theta_{22}=-\theta_{33}=\nu(\tau),\quad \text{where}\quad \tau=t-x. \tag{2.73}$$

The calculation of the energy-momentum tensor for the symmetric field by use of the tensor (2.72) yields

$$T_{ab}=k(\mu_{,a}\mu_{,b}+\nu_{,a}\nu_{,b}). \tag{2.74}$$

The energy flux reads

$$T_{01}=-\rho_3(\dot{\theta}_{23}^2+\tfrac{1}{4}(\dot{\theta}_{22}-\dot{\theta}_{33})^2). \tag{2.75}$$

Observe that the expressions (2.74) and (2.75) are the same as the expressions obtained in GR from the energy-momentum pseudotensors.

Let us turn now to the antisymmetric field.

Proposition 5: In the coordinate system associated with the gauge condition

$$w_{am}{}^{,m}=0, \tag{2.76}$$

the energy-momentum tensor of the antisymmetric field is

$$T_{ab} = -(2\rho_2 + \rho_3)(w_{mn,a}w^{mn}{}_{,b} - \tfrac{1}{4}\eta_{ab}w_{mn,p}w^{mn,p}). \tag{2.77}$$

This tensor is traceless and symmetric.

Proof: The current of the symmetric and of the antisymmetric fields are decoupled. Thus we may assume $\theta_{ab}=0$. In the coordinates associated with the gauge condition (2.76),

$$e_a \rfloor \mathcal{L} = \tfrac{1}{2}(2\rho_2 + \rho_3)w_{ab,c}w^{ab,c} * \vartheta_b.$$

As for the first term of $\mathcal{T}_a(w)$ we derive from (2.66),

$$(e_a \rfloor \mathcal{C}_m) \wedge * \mathcal{F}^m = 4w_{m[a,n]}F^{m[bn]} * \vartheta_b = 2(w_{ma,n}F^{m[bn]} - w_{mn,a}F^{m[bn]}) * \vartheta_b.$$

The first term vanishes, on shell, up to a total derivative,

$$w_{ma,n}F^{m[bn]} \approx -w_{ma}F^{m[bn]}{}_{,n} = 0.$$

Thus,

$$(e_a \rfloor \mathcal{C}_m) \wedge * \mathcal{F}^m = -2w_{mn,a}F^{m[bn]} * \vartheta_b.$$

Inserting the gauge condition (2.76) into (2.26) we derive

$$\mathcal{F}_a = -(\rho_3 w_{a[b,c]} + 3\rho_2 w_{[ab,c]})\vartheta^{bc}.$$

Hence,

$$(e_a \rfloor \mathcal{C}_m) \wedge * \mathcal{F}^m = 2(\rho_3 w_{ma,n}w^{m[b,n]} + 3\rho_2 w_{ma,n}w^{[mb,n]}) * \vartheta_b.$$

Extract the total derivatives and use the gauge condition to get

$$w_{mn,a}w^{mb,n} \approx w_{mn}{}^{,n}w^{mb}{}_{,a} \approx 0,$$

$$w_{mn,a}w^{bn,m} \approx w_{mn}{}^{,m}w^{bn}{}_{,a} \approx 0.$$

Consequently,

$$(e_a \rfloor \mathcal{C}_m) \wedge * \mathcal{F}^m = -(2\rho_2 + \rho_3)w_{mn,a}w^{mn,b}.$$

The desired expression (2.77) is obtained now by collecting the terms. ■

III. THE ROLE OF THE PARAMETERS ρ_1

The case $\rho_1=0$ is extracted in coframe models by existence of a unique spherical symmetric static solution. Since the exact solution yields the Schwarzschild metric this condition generates a viable subclass of gravity coframe models.

We have involved an independent criteria. Namely, we have shown that only in the case $\rho_1=0$ the weak perturbations of the coframe reduce to two independent fields with their own Lagrangian dynamics. Consequently the models have a free field limit. This effect is correlated to the recently obtained result [34] concerning the Hamiltonian dynamics behavior.

It is interesting to note that in the two-dimensional coframe gravity only one term in the Lagrangian preceded by ρ_1 appears. Thus the corresponding reduction of fields is impossible.

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The wave equation on the Schwarzschild metric II. Local decay for the spin-2 Regge–Wheeler equation

P. Blue
Mathematics Department, Rutgers University, Piscataway, New Jersey 08854

A. Soffer
Mathematics Department, Institute for Advanced Studies, Princeton, New Jersey 08540

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Odd-type spin-2 perturbations of Einstein's equation can be reduced to the scalar Regge–Wheeler equation. We show that the weighted norms of solutions are in L^2 of time and space. This result uses commutator methods and applies uniformly to all relevant spherical harmonics. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Recently, it has been shown that the wave equation for a scalar field on the exterior part of the Schwarzschild manifold satisfies local decay estimates useful for scattering theory and global existence.[2] The extension for the linearized Einstein equation is considered here. In 1957, Regge and Wheeler investigated spin-2 tensor fields on the Schwarzschild manifold.[4] They classified such fields into two types, which they called even and odd. For the odd fields, they were able to reduce the problem to an equation for a scalar field very similar to the wave equation for scalar fields on the Schwarzschild manifold. In 1970, Zerilli extended their results to include the even case; although, the equation for the even case is significantly more complicated and shows less resemblance to the wave equation for a scalar field.[9] Teukolsky has done a related reduction for the rotating Kerr black hole[6] which has been used to investigate the stability of the black holes.[8]

This paper extends the local decay estimate for the scalar wave equation of Ref. 2 to the Regge–Wheeler equation. Many of the proofs used here follow Ref. 2. We obtain the following: for r_* the standard Regge–Wheeler coordinate and $\beta > \frac{3}{2}$, there is a constant C, depending on the initial condition through the energy norm, so that

$$\int_0^\infty \left\| \left(1 + \left(\frac{r_*}{2M}\right)^2\right)^{-\beta/2} u \right\|^2 \mathrm{d}t < C.$$

II. COORDINATES AND EQUATIONS

The Schwarzschild manifold describes a static black hole solution to the Einstein equation. The exterior of the black hole is most easily described by $(t, r, \theta, \phi) \in \mathbf{R} \times (2M, \infty) \times S^2$ with the metric

$$\mathrm{d}s^2 = \left(1 - \frac{2M}{r}\right)\mathrm{d}t^2 - \left(1 - \frac{2M}{r}\right)^{-1} \mathrm{d}r^2 - r^2\, \mathrm{d}s^2_{S^2}. \tag{2.1}$$

To simplify the analysis of linear stability, Regge and Wheeler[4] introduced a new radial coordinate, r_*, satisfying

$$\frac{\partial r}{\partial r_*} = \left(1 - \frac{2M}{r}\right). \tag{2.2}$$

This allows the definition of a spacelike manifold

$$\mathfrak{M} = \mathbf{R} \times S^2. \tag{2.3}$$

The old coordinate r is now treated as a function of r_*.

In these new coordinates, the Regge–Wheeler equation for a scalar field $u: \mathbf{R} \times \mathfrak{M} \to \mathbf{R}$ which determines the behavior of the odd-type tensor fields is

$$\ddot{u} + Hu = 0, \tag{2.4}$$

where

$$H = \sum_{j=1}^{3} H_j, \tag{2.5}$$

$$H_1 = -\frac{\partial^2}{\partial r_*^2}, \tag{2.6}$$

$$H_2 = (1 - s^2)V, \tag{2.7}$$

$$V = \frac{2M}{r^3}\left(1 - \frac{2M}{r}\right), \tag{2.8}$$

$$H_3 = V_L(-\Delta_{S^2}) = V_L \sum_{l=0}^{\infty} l(l+1)P_l, \tag{2.9}$$

$$V_L = \frac{1}{r^2}\left(1 - \frac{2M}{r}\right) \tag{2.10}$$

and where $s=2$ for the case of the tensor field and P_l is projection onto spherical harmonics with total angular momentum l. The case $s=0$ is the scalar field previously considered and $s=1$ is for the odd-type vector (Maxwell) fields.

Because of the way the scalar field u is defined it is not possible for it to have any component with spherical harmonic component $l=0$. It has also been shown that the $l=1$ component corresponds to changing the nonrotating Schwarzschild background to a rotating Kerr solution and to gauge transformations.[3,5] For this reason, we only consider u with no $l=0$ or $l=1$ spherical harmonic component. This provides a lower bound on the spherical Laplace–Beltrami operator,

$$-\Delta_{S^2} \geqslant 2(2+1) = 6. \tag{2.11}$$

For the scalar wave equation, Bachelot and Nicolas have proven global existence[1] in both an energy space and in C^∞. The assumption of global existence in C^∞ greatly simplifies all the following arguments and will be assumed; although, we are not yet aware of a published paper. However, the method of Bachelot and Nicolas should extend to the Regge–Wheeler equation without difficulty. The assumption of global existence in C^∞ means that all solutions are assumed to be $C^\infty(\mathfrak{M}) \cap H^1(\mathfrak{M}, \mathrm{d}r_* \, \mathrm{d}^2\omega_{S^2})$, are infinitely differentiable in t and have time derivative in $C^\infty(\mathfrak{M}) \cap L^2(\mathfrak{M}, \mathrm{d}r_* \, \mathrm{d}^2\omega_{S^2})$. The notation $u(t)$ denotes the function from $\mathfrak{M} \to \mathbf{R}$ corresponding to u evaluated at time t. The measure $\mathrm{d}r_* \, \mathrm{d}^2\omega_{S^2}$ is used for all norms and inner products unless otherwise specified, and the norm $\|\cdot\|$ refers to the L^2 norm.

III. THE HEISENBERG-TYPE RELATION AND PRELIMINARY ESTIMATES

For the Schrödinger equation, the Heisenberg relation describes the time evolution of expectation values for an operator and gives conserved quantities from symmetries of the Hamiltonian. A similar relation exists for the wave equation.[2]

Theorem III.1 (Heisenberg-type relation): *For a time independent operator A and a solution to the linear wave equation* $\ddot{u}+Hu=0$ *such that u and Hu are in the domain of A, and u and Au are in the domain of H,*

$$\frac{\mathrm{d}}{\mathrm{d}t}(\langle u,A\dot{u}\rangle - \langle \dot{u},Au\rangle) = \langle u,[H,A]u\rangle. \tag{3.1}$$

Proof: The proof is found in Theorem 1 of Ref. 2.

The first and most important application of Theorem III.1 is conservation of energy. As usual it is generated by time translation symmetry. This result is already well known.[7]

Theorem III.2 (energy conservation): *The Regge–Wheeler equation, Eq. (2.4), has a conserved quantity* $\|u\|_{\mathcal{H}}^2$ *which we call the energy.*

$$\|u\|_{\mathcal{H}}^2 = \langle \dot{u},\dot{u}\rangle + \langle u',u'\rangle + \langle u,-3Vu\rangle + \sum_{l=2}^{\infty} \langle P_l u, l(l+1)V_L P_l u\rangle. \tag{3.2}$$

This acts as a metric on the space $\mathcal{H}=\{u\in L^2_{\mathrm{loc}}:\|u\|_{\mathcal{H}}<\infty\}$.

Proof: The conservation of energy follows from the Heisenberg-type relation with the multiplier $A=\mathrm{d}/\mathrm{d}t$. This acts as a metric because the $\langle u,(H_2+H_3)u\rangle$ term is positive. The positivity of this potential was known to Regge and Wheeler[4] and is verified here.

Since only functions orthogonal to the spherical harmonics with $l=0$ and $l=1$ are considered

$$\langle u,-3Vu\rangle + \sum_{l=2}^{\infty} \langle P_l u, l(l+1)V_L P_l u\rangle \geqslant \langle u,-3Vu\rangle + \langle u,6V_L u\rangle \geqslant \left\langle u,\left(\frac{-6M}{r^3}+\frac{6}{r^2}\right)\left(1-\frac{2M}{r}\right)u\right\rangle$$
$$\geqslant \left\langle u,\frac{6}{r^2}\left(1-\frac{M}{r}\right)\left(1-\frac{2M}{r}\right)u\right\rangle.$$

Since

$$\frac{6}{r^2}\left(1-\frac{M}{r}\right)\left(1\frac{2M}{r}\right)$$

is always positive, $\langle u,(H_2+H_3)u\rangle$ is positive definite. Since $\langle \dot{u},\dot{u}\rangle$, $\langle u',u'\rangle$, and $\langle u,(H_2+H_3)u\rangle$ are all positive each is defined if $\|u\|_{\mathcal{H}}$ is finite, and $\|u\|_{\mathcal{H}}$ is a metric. □

As stated in the proof of energy conservation, the energy controls certain derivative norms and this can be used to control the growth of the L^2 norm.

Theorem III.3: *If u is a real valued solution of the Regge–Wheeler equation [Eq. (2.4)] and* $\|u(t)\|_{L^2}$ *is the norm of u at time t, then for* $t\geqslant 0$,

$$\|\dot{u}\|_{L^2} \leqslant \|u\|_{\mathcal{H}},$$

$$\|u(t)\| \leqslant t\|u\|_{\mathcal{H}} + \|u(0)\|_{L^2}.$$

Proof: Since $\langle u',u'\rangle$ and $\langle u,(H_2+H_3)u\rangle$ are strictly positive, $\|\dot{u}(t)\|$ is controlled by the energy. This is used to control the growth rate of $\|u(t)\|_{L^2}$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\|u(t)\|_{L^2}^2 = \frac{\mathrm{d}}{\mathrm{d}t}\langle u,u\rangle = 2\langle u,\dot{u}\rangle,$$

$$2\|u\|_{L^2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|_{L^2} \leqslant 2\|u\|_{L^2}\|\dot{u}\|_{L^2},$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\|u\|_{L^2} \leqslant \|\dot{u}\|_{L^2} \leqslant \|u\|_{\mathcal{H}}.$$

□

IV. LOCAL DECAY

For the scalar wave equation, a radial differential operator γ was introduced to prove the local decay estimate.[2] It is used here for the same purpose. This multiplier is centered at the peak of the angular potential V_L. To simplify calculations the standard r_* coordinate is translated to a new one, $\rho_* = r_* - \alpha_*$, so that $\rho_* = 0$ at the peak of V_L. This centrifugal tortoise coordinate satisfies the same differential definition as r_*, Eq. (2.2).

Definition IV.1: The centrifugal origin α, centrifugal tortoise origin α_*, and centrifugal tortoise radius ρ_* are defined by

$$\alpha \equiv 3M, \tag{4.1}$$

$$\alpha_* \equiv r_*|_{r=\alpha=3M}, \tag{4.2}$$

$$\rho_* \equiv r_* - \alpha_*. \tag{4.3}$$

Definition IV.2: Given $\sigma \in (\frac{1}{2}, 1]$, the Morawetz-type multiplier γ_σ is defined by

$$g_\sigma(r_*) \equiv \int_0^{(r_*-\alpha_*)/2M} (1+\tau^2)^{-\sigma}\,\mathrm{d}\tau, \tag{4.4}$$

$$\gamma_\sigma \equiv -\frac{i}{2}\left(g_\sigma\frac{\partial}{\partial r_*} + \frac{\partial}{\partial r_*}g_\sigma\right). \tag{4.5}$$

As before, C^∞ solutions are assumed so that there are no domain issues. In all cases, the value of σ will be fixed and the notation $g = g_\sigma$ and $\gamma = \gamma_\sigma$ will be used.

Theorem IV.3: If $u \in H^1(\mathfrak{M})$ and $\sigma \in (\frac{1}{2}, 1]$, then

$$\langle u, \gamma_\sigma u\rangle = 0 \tag{4.6}$$

and there is a constant $C_\sigma = \lim_{r_*\to\infty} g(r_*)$ such that

$$\|\gamma u\| \leqslant C_\sigma\|u\|_{\mathcal{H}} + \frac{1}{2}\left\|\left(1+\left(\frac{r_*-\alpha_*}{2M}\right)^2\right)^{-\sigma} u\right\|_{L^2}. \tag{4.7}$$

Proof: Equation (4.6) is proven in Theorem 16 of Ref. 2 (the statement of which includes the additional, but unnecessary, assumption that u satisfy the scalar wave equation). For Eq. (4.7), Theorem 17 of Ref. 2 does not directly apply since the space $\mathcal{H}$ defined there involves different potentials. However, the same argument applies. It is first noted that since $\sigma > \frac{1}{2}$ and the integrand in the definition of g is positive and even, $|g|$ is bounded by $C_\sigma = \lim_{r_*\to\infty} g(r_*)$. Now, by direct computation,

$$\|\gamma u\| = \left\|gu' + \frac{1}{2}g'u\right\| \leqslant \|gu'\| + \frac{1}{2}\|g'u\| \leqslant C_\sigma\|u\|_{\mathcal{H}} + \frac{1}{2}\left\|\left(1+\left(\frac{r_*-\alpha_*}{2M}\right)^2\right)^{-\sigma} u\right\|_{L^2}.$$

□

The Heisenberg-type relation will be applied to the multiplier γ. To do this it is necessary to estimate the commutator $[\Sigma_{j=1}^{3} H_j, \gamma]$.

Lemma IV.4: For $\sigma \in (\frac{1}{2}, 1]$,

$$i\left[\frac{-1}{r^2}\left(1-\frac{2M}{r}\right)\Delta_{S^2}, \gamma\right] = -g(r_*)\left[\frac{3M}{r}-1\right]\frac{2}{r^3}\left(1-\frac{2M}{r}\right)\Delta_{S^2} \geqslant 0. \tag{4.8}$$

Proof: The proof is found in Lemma 18 of Ref. 2.

Lemma IV.5: For $\sigma \in (\frac{1}{2}, 1]$ *and u in the domain of* γ *and H,*

$$\left\langle u, i\left[-\frac{\partial^2}{\partial r_*^2}, \gamma\right]u\right\rangle \geqslant \left\langle u, \frac{\sigma}{\left(1+\left(\frac{r_*-\alpha_*}{2M}\right)^2\right)^{\sigma+2}}\frac{1}{(2M)^3}\left[5+(3-2\sigma)\left(\frac{r_*-\alpha_*}{2M}\right)^2\right]u\right\rangle. \tag{4.9}$$

Proof: The proof is found in Lemma 20 of Ref. 2.

Lemma IV.6: For $\sigma \in (\frac{1}{2}, 1]$ *and u in the domain of H and* γ*, there is a constant* c_σ *so that*

$$\left\langle u, i\left[\sum_{i=j}^{3} H_j, \gamma\right]u\right\rangle \geqslant \left\langle u, \frac{c_\sigma}{\left(1+\left(\frac{r_*-\alpha_*}{2M}\right)^2\right)^{\sigma+1}}u\right\rangle. \tag{4.10}$$

Proof: Since $\sigma \leqslant 1$,

$$\frac{\sigma}{\left(1+\left(\frac{r_*-\alpha_*}{2M}\right)^2\right)^{\sigma+2}}\frac{1}{(2M)^3}\left[5+(3-2\sigma)\left(\frac{r_*-\alpha_*}{2M}\right)^2\right] < \frac{\sigma}{\left(1+\left(\frac{r_*-\alpha_*}{2M}\right)^2\right)^{\sigma+1}}.$$

In the proof of Lemma 21 of Ref. 2 it is shown that

$$i[V, \gamma] = g\left(3-\frac{8M}{r}\right)\frac{2M}{r^4}\left(1-\frac{2M}{r}\right). \tag{4.11}$$

Since $g<0$ for $r<3M$ and $g>0$ for $r>3M$, $i[H_2, \gamma]=-3i[V, \gamma]$ is negative for $r<8M/3$, positive for $8M/3<r<3M$, and negative for $3M<r$. In the region $8M/3<r<3M$, all the terms of the form $i[H_j, \gamma]$ are positive so an estimate of the form (4.10) holds. The other r values are now treated.

It is useful to note that a term relating H_2 to H_3 is decreasing since

$$\frac{\mathrm{d}}{\mathrm{d}r}\frac{3-\frac{8M}{r}}{1-\frac{3M}{r}} = -\frac{M}{(r-3M)^2} < 0.$$

At $r=2M$, $3-(8M/r)=-1=2[1-(3M/r)]$. Therefore in $2M<r\leqslant 8M/3$ and for $l \geqslant 2$,

$$\left|3-\frac{8M}{r}\right| < 2\left|1-\frac{3M}{r}\right|,$$

$$\left|g\frac{1}{r^3}\left(1-\frac{2M}{r}\right)\left(\frac{2M}{r}\right)\left(3-\frac{8M}{r}\right)\right| < \left|g\frac{1}{r^3}\left(1-\frac{2M}{r}\right)2\left(1-\frac{3M}{r}\right)\right|,$$

$$|i[H_2,\gamma]| < \frac{3}{6} i[H_3,\gamma].$$

The $\frac{3}{6}$ factor is present due to the restriction that $l \geqslant 2$ and hence that $-\Delta_{S^2} \geqslant 6$ and to the factor of -3 relating V to H_2.

At $r=3.3M$,

$$\left| \frac{2\left(1-\frac{3M}{r}\right)6}{-3\left(3-\frac{8M}{r}\right)} \right| = \frac{12}{19} > \frac{2M}{3.3M}.$$

Therefore for $r>3.3M$ and $l \geqslant 2$

$$\left| -3\left(3-\frac{8M}{r}\right)\frac{2M}{3.3M} \right| < 2\left(1-\frac{3M}{r}\right)6,$$

$$\left| \frac{g}{r^3}\left(1-\frac{2M}{r}\right)(-3)\left(3-\frac{8M}{r}\right)\frac{2M}{r} \right| < \frac{g}{r^3}\left(1-\frac{2M}{r}\right)\left(1-\frac{3M}{r}\right)(-\Delta_{S^2}),$$

$$|i[H_2,\gamma]| < i[H_3,\gamma].$$

Finally for $3M \leqslant r \leqslant 3.3M$, since $i[H_3,\gamma]$ vanishes quadratically in $(r-3M)$ where as $i[H_2,\gamma]$ vanishes only linearly it is necessary to bound $i[H_2,\gamma]$ by $i[H_1,\gamma]$. On this interval $F^{-1}<3$, $\rho_* < 0.9M$, and $g<0.9M$. Again, assuming $l \geqslant 2$,

$$\begin{aligned} |i[H_2,\gamma]| &= 3g\left(3-\frac{8M}{r}\right)\left(\frac{2M}{r}\right)^4 \frac{1}{(2M)^3}\left(1-\frac{2M}{r}\right) \\ &< (3)(0.9)\left(\frac{19}{33}\right)\left(\frac{2}{3}\right)^4\left(\frac{13}{33}\right)\frac{1}{(2M)^3} < 0.121\frac{1}{(2M)^3}, \end{aligned}$$

$$i[H_1,\gamma] > \frac{5\sigma}{\left(1+\left(\frac{\rho_*}{2M}\right)^2\right)^{\sigma+2}}\frac{1}{(2M)^3} > \frac{5\sigma}{(1.2025)^{\sigma+2}}\frac{1}{(2M)^3} > 1.43\frac{1}{(2M)^3}.$$

In summary, for $r<3M$ and for $r>3.3M$, $i[H_2+H_3,\gamma]>0$, and for $3M \leqslant r \leqslant 3.3M$, $i[H_1+H_2,\gamma]$ is strictly positive. Since for $r<3M$ and for $r>3.3M$, $i[H,\gamma]>i[H_1,\gamma]>C(1+(\rho_*/2M)^2)^{-\sigma-1}$ and since for $3M \leqslant r \leqslant 3.3M$, $i[H,\gamma]$ is strictly positive, there is a constant C so that

$$\langle u, i[H,\gamma]u\rangle \geqslant \left\langle u, \frac{C}{\left(1+\left(\frac{r_*-\alpha_*}{2M}\right)^2\right)^{\sigma+1}}u \right\rangle.$$

□

It is now possible to apply the Heisenberg-type relation to γ and integrate the result to prove local decay.

Theorem IV.7 (local decay): *If u is a solution to the Regge–Wheeler equation [Eq. (2.4)], $\|u\|^2_{\mathcal{H}}=E$, $u(0)=f$, and $\beta>\frac{3}{2}$, then there is a constant D_σ such that*

$$\int_0^\infty \left\| \left(1+\left(\frac{r_*}{2M}\right)^2\right)^{-\beta/2} u \right\|^2 \mathrm{d}t \leqslant D_\sigma E^{1/2}(E^{1/2}+\|f\|_{L^2}). \tag{4.12}$$

Proof: Initially the result will be proven with $\beta=\sigma+1$ and $\sigma\in\left(\frac{1}{2},1\right]$ and ρ_* in place of r_*. By integrating Lemma IV.6 and applying the Heisenberg-type relation, Theorem III.1, it is possible to bound the time integral of the local decay term by an inner product evaluated at time T. Despite the explicit factors of i appearing in the following, all terms are real valued:

$$\begin{aligned}\int_0^T\left\|\left(1+\left(\frac{r_*-\alpha_*}{2M}\right)^2\right)^{-(\sigma+1)/2}u\right\|^2\mathrm{d}t &\leqslant \int_0^T\langle u,i[H,\gamma]u\rangle\mathrm{d}t\leqslant\int_0^T\frac{\mathrm{d}}{\mathrm{d}t}(\langle u,i\gamma\dot{u}\rangle-\langle\dot{u},i\gamma u\rangle)\mathrm{d}t\\ &\leqslant\int_0^T i\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathrm{d}}{\mathrm{d}t}\langle u,\gamma u\rangle-2\langle\dot{u},\gamma u\rangle\right)\mathrm{d}t\leqslant\int_0^T-2i\frac{\mathrm{d}}{\mathrm{d}t}\langle\dot{u},\gamma u\rangle\mathrm{d}t\\ &\leqslant 2(\|\dot{u}\|\,\|\gamma u\|)|_{t=T}+2(\|\dot{u}\|\,\|\gamma u\|)|_{t=0}\\ &\leqslant E^{1/2}\left(4C_\sigma E^{1/2}+\left\|\left(1+\left(\frac{r_*-\alpha_*}{2M}\right)^2\right)^{-\sigma}f\right\|\right)\\ &\quad+E^{1/2}\left\|\left(1+\left(\frac{r_*-\alpha_*}{2M}\right)^2\right)^{-\sigma}u(T)\right\|.\end{aligned}\tag{4.13}$$

Since $\sigma>\frac{1}{2}$, q can be chosen so that $(1/2\sigma)+\frac{1}{2}<q<\frac{3}{2}$. If p is the conjugate exponent to q and $\kappa\equiv 2/p$, then

$$\frac{1}{p}<1-\frac{2}{3}=\frac{1}{3},\quad\frac{2-\kappa}{2}q=1,\quad q\sigma>\frac{\sigma+1}{2}.$$

Hölder's inequality can now be applied to the last norm in line (4.13),

$$\begin{aligned}\left\|\left(1+\left(\frac{r_*-\alpha_*}{2M}\right)^2\right)^{-\sigma}u\right\|^2&=\int_{\mathfrak{M}}\frac{|u|^\kappa|u|^{2-\kappa}}{\left(1+\left(\frac{\rho_*}{2M}\right)^2\right)^{2\sigma}}\mathrm{d}r_*\,\mathrm{d}^2\omega_{S^2}\\ &\leqslant\left(\int_{\mathfrak{M}}|u|^{p\kappa}\,\mathrm{d}r_*\,\mathrm{d}^2\omega_{S^2}\right)^{1/p}\left(\int_{\mathfrak{M}}\frac{|u|^{(2-\kappa)q}}{\left(1+\left(\frac{\rho_*}{2M}\right)^2\right)^{2\sigma q}}\mathrm{d}r_*\,\mathrm{d}^2\omega_{S^2}\right)^{1/q},\end{aligned}$$

$$\begin{aligned}\left\|\left(1+\left(\frac{r_*-\alpha_*}{2M}\right)^2\right)^{-\sigma}u\right\|&\leqslant\|u\|^{1/p}\left\|\frac{|u|}{\left(1+\left(\frac{\rho_*}{2M}\right)^2\right)^{\sigma q}}\right\|^{1-(1/p)}\\ &\leqslant(E^{1/2}T+\|f\|)^{1/p}\left\|\frac{u}{\left(1+\left(\frac{\rho_*}{2M}\right)^2\right)^{(\sigma+1)/2}}\right\|^{1-(1/p)}.\end{aligned}$$

For sufficiently large T, there is a constant F so that

$$\begin{aligned}\left\|\left(1+\left(\frac{r_*-\alpha_*}{2M}\right)^2\right)^{-\sigma}u\right\|&\leqslant FT^{1/p}\left\|\frac{u}{\left(1+\left(\frac{\rho_*}{2M}\right)^2\right)^{(\sigma+1)/2}}\right\|^{1-(1/p)},\\ \int_0^T\left\|\left(1+\left(\frac{\rho_*}{2M}\right)^2\right)^{-(\sigma+1)/2}u\right\|^2\mathrm{d}t&\leqslant E^{1/2}(4C_\sigma E^{1/2}+\|f\|)+FT^{1/p}\left\|\frac{u}{\left(1+\left(\frac{\rho_*}{2M}\right)^2\right)^{(\sigma+1)/2}}\right\|^{1-(1/p)}.\end{aligned}\tag{4.14}$$

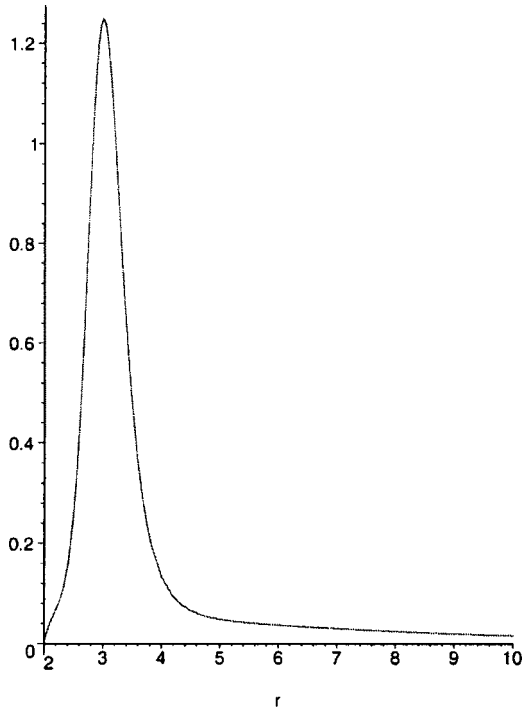

FIG. 1. Plot of a lower bound for $i[H,\gamma]$ as a function of r.

This establishes an integral relation between the local decay norm and its square integral. The local decay norm has bounded derivative since

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\|\frac{u}{\left(1+\left(\frac{\rho_*}{2M}\right)^2\right)^{(\sigma+1)/2}}\right\|^2 = 2\left\langle \frac{u}{\left(1+\left(\frac{\rho_*}{2M}\right)^2\right)^{(\sigma+1)2}}, \frac{\dot{u}}{\left(1+\left(\frac{\rho_*}{2M}\right)^2\right)^{(\sigma+1)2}} \right\rangle$$
$$\leqslant 2\left\|\frac{u}{\left(1+\left(\frac{\rho_*}{2M}\right)^2\right)^{(\sigma+1)/2}}\right\| E^{1/2}. \tag{4.15}$$

These two conditions are sufficient to apply Lemma 25 of Ref. 2. That lemma states that for $\theta:\mathbf{R}\to\mathbf{R}^+$ with uniformly bounded derivative, $\epsilon\in\left(0,\frac{1}{3}\right)$, if $\int_0^t\theta(\tau)^2\,\mathrm{d}\tau\leqslant C_1+C_2t^\epsilon\theta^{1-\epsilon}$ then $t^\epsilon\theta(t)^{1-\epsilon}$ goes to zero sequentially and hence $\int_0^t\theta(\tau)^2\,\mathrm{d}\tau\leqslant C_1$. The lemma can be applied with θ as the local decay norm, $1/p=\epsilon$, and C_1 and C_2 as in (4.14).

This proves the result for $\beta\in\left(\frac{3}{2},2\right]$ and for ρ_* instead of r_*. Since $(1+(\rho_*/2M)^2)^{-\beta}$ is a decreasing function of β, the result holds for all $\beta>\frac{3}{2}$. Finally since for any β there is a constant so that for all r_*, $(1+[(r_*-\alpha_*)/2M]^2)^{-\beta}\leqslant C(1+(r_*/2M)^2)^{-\beta}$ the statement of the theorem holds. □

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APPENDIX: NUMERICAL VERIFICATION OF THE POSITIVITY OF THE COMMUTATOR

The key step in proving the local decay estimate is the lower bound for the commutator $i[H,\gamma]$ proven in Lemma IV.6. From the asymptotics of $i[H_2,\gamma]\approx r^{-4}$ and $i[H_3,\gamma]\approx r^{-3}$ it is clear that the negative contributions from $i[H_2,\gamma]$ will be dominated eventually and it is sufficient to show $i[H,\gamma]$ is positive in some finite domain. To verify positivity of the commutator, the sum of the exact form for $i[H_2,\gamma]$ from Eq. (4.11), the lower bounds for $i[H_1,\gamma]$ from Eq. (4.9), and the lower bound for $i[H_3,\gamma]$ from Eq. (4.8) with $l=2$ is plotted for $M=1$ and $\sigma=1$ in Fig. 1. From the graph it is clear that the total commutator is positive. The graph decays because all the terms involved decay. This provides an alternate, numerical verification of the result proven in Lemma IV.6.

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Necessary and sufficient conditions for *n*-dimensional conformal Einstein spaces via dimensionally dependent identities

S. Brian Edgar[a)]
Matematiska Institutionen, Linköpings Universitet, Linköping S-581 83, Sweden

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Listing has recently extended results of Kozameh, Newman, and Tod for four-dimensional space–times and presented a set of necessary and sufficient conditions for a metric to be locally conformally equivalent to an Einstein metric in all semi-Riemannian spaces of dimension $n \geqslant 4$—subject to a nondegeneracy restriction on the Weyl tensor. By exploiting dimensionally dependent identities we demonstrate how to construct two alternative versions of these necessary and sufficient conditions which we believe will be useful in applications. The four-dimensional case is discussed in detail and examples are also given in five and six dimensions. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1823011]

I. INTRODUCTION

Kozameh, Newman, and Tod[7] have shown that a certain pair of necessary conditions are also sufficient for a *four-dimensional space–time* to be conformal to an Einstein space–time—with the exception of those space–times whose complex Weyl scalar invariant $J=0$. (In the conformal Einstein space with metric g_{ab}, $R^{ab}{}_{cd}$ represents the Riemann tensor, $C^{ab}{}_{cd}$ represents the Weyl conformal tensor, $R^{ab}{}_{cd}$ represents the Ricci tensor, $R=R^{a}{}_{a}$ the Ricci scalar, and $\tilde{R}_{ab}=R_{ab}-Rg_{ab}/n$ the trace-free Ricci tensor where $2\nabla_{[a}\nabla_{b]}V^{c}=-R_{abcd}V^{d}$ for an arbitrary vector V^{a}. I, J are the usual complex Weyl scalar invariants in four dimensions, and $\underset{2}{C}\equiv C^{ab}{}_{cd}C^{cd}{}_{ab}$. More details of the notation are given in the next section.) Implicit in their paper was another result: a *four-dimensional space–time* with metric g_{ab} can be transformed into an Einstein space by a conformal transformation if and only if the vector K^{a} given by

$$K^{a}=4C^{ac}{}_{ij}\nabla^{k}C^{ij}{}_{ck}/\underset{2}{C} \tag{1a}$$

satisfies (the $n=4$ dimension version of)

$$\tilde{R}_{ab}+(n-2)(\nabla_{a}K_{b}-K_{a}K_{b}-(\nabla^{c}K_{c}-K^{c}K_{c})g_{ab}/n)=0 \tag{2a}$$

for the class of space–times where $\underset{2}{C}\neq 0$. The essential ideas in Ref. 7 were to exploit the properties that Einstein spaces are a subset of C spaces (spaces whose Weyl tensor is divergence free, $\nabla_{a}C^{ab}{}_{cd}=0$) and that spaces conformal to C spaces satisfy (the $n=4$ dimension version of)

$$\nabla^{k}C^{ab}{}_{ck}+(n-3)C^{ab}{}_{ck}K^{k}=0 \tag{3}$$

and hence to extract the explicit expression (1a) for K^{a} by using the *four-dimensional* dimensionally dependent identity

a)Electronic mail: bredg@mai.liu.se

$$C^{cj}{}_{ab}C^{ab}{}_{ck} = \delta^{j}_{k}C/4. \tag{4a}$$

The principles underlying the techniques used in Ref. 7 originated in a study of conformal transformations by spinor methods by Szekeres,[12] and although most of the work in Ref. 7 was tensor based, some lemmas were proven by spinor methods; this is probably why Kozameh, Newman, and Tod have commented that their method in Ref. 7 does not seem to be extendible to higher dimensions $n>4$. However, recently Listing[8] has exploited the same principles more generally and shows that the condition that a particular vector $\mathbf{T}^a$ obtained from (3) satisfies (2a) is a necessary and sufficient condition for conformal Einstein spaces in *all semi-Riemannian spaces with dimensions* $n\geqslant 4$—subject to a nondegenerate determinant condition on a matrix representation of the Weyl tensor. On the other hand, when the four-dimensional results from Ref. 8 are compared with Ref. 7, the explicit form of the vector $\mathbf{T}^a$ in Ref. 8 differs considerably from its counterpart K^a used in Ref. 7 and quoted above in (1a); furthermore, the nondegenerate determinant condition in Ref. 8 is not easily translated into a condition on the real Weyl invariant scalars in the n-dimensional case, although Listing states that this condition is equivalent in four dimensions to the complex scalar invariant Weyl scalar $J\neq 0$.

It is well known that we can write $\mathbf{C}^{A}{}_{C}\equiv C^{ab}{}_{cd}$ where $A\equiv[ab]$, $C\equiv[cd]$ so that $A,C=1,2,\ldots,N(=n(n-1)/2)$ and so consider $\mathbf{C}$ as an $N\times N$ trace-free matrix. (Note that we are not making use of the symmetries, $C_{abcd}=C_{cdab}$ and $C_{a[bcd]}=0$, and in fact this construction is valid for any trace-free double 2-form; also, we are not defining a metric for the N-dimensional space, nor even making use of the n-dimensional space metric g_{ab} in this construction.)

Instead of exploiting higher dimensional counterparts of identities such as (4a), Listing's result and proof[8] assumed $\det(\mathbf{C})\neq 0$ and then used the inverse matrix $\mathbf{C}^{-1}$ to solve (3) for K^a; however $\mathbf{C}^{-1}$ cannot be easily interpreted in tensor notation without some translation and, in that form, does not seem to be very useful in practical applications. In the illustrative example in Ref. 8 Listing restricted himself to *four-dimensional Riemann space*, where he followed the technique in Ref. 7 of using the *four-dimensional* identity (4a) to extract K^a, and also used properties dependent on the *positive definite metric*; this avoided having to deal with $\mathbf{C}^{-1}$ directly.

Although the four-dimensional identity (4a) is well known, the existence of higher dimensional analogues (Ref. 2) seems less well known and one purpose of this paper is to draw attention again to the power and usefulness of such dimensionally dependent tensor identities.[2] (See also Refs. 9, 3, and 13.)

We shall show in this paper how to exploit dimensionally dependent identities[2] to obtain results valid in all dimensions $n\geqslant 4$ and automatically in all signatures; in particular we will

(i) reformulate Listing's results in Ref. 8, and in particular, $\det(\mathbf{C})\neq 0$ and the inverse matrix $\mathbf{C}^{-1}$ in the tensor notation of Ref. 7;
(ii) obtain explicit solutions for K^a which avoid the use of $\mathbf{C}^{-1}$ altogether.

We shall also show explicitly how the four-dimensional results implicit in Ref. 7 can be seen as special cases of this formulation of Listing's result, and are valid for all signatures.

To demonstrate the usefulness of our versions, we will consider the four-, five-, and six-dimensional cases, independent of signature. The higher dimensional analogues[2] of the four-dimensional identity (4a) will be the basis for our applications in five and six dimensions.

II. NOTATION

We begin with some notation which we will use to link algebraic and tensor notation, and prove a simple lemma. Let us define, for $p\geqslant 1$ Weyl tensors, a *chain of the zeroth kind*,[13]

$$\underset{p}{C}{}^{ab}{}_{cd} \equiv C^{ab}{}_{i_1j_1}C^{i_1j_1}{}_{i_2j_2}C^{i_2j_2}{}_{i_3j_3}\cdots C^{i_{p-2}j_{p-2}}{}_{i_{p-1}j_{p-1}}C^{i_{p-1}j_{p-1}}{}_{cd},$$

noting that $\underset{1}{C}{}^{ab}{}_{cd}\equiv C^{ab}{}_{cd}$.

A useful relation is

$$\underset{p}{C}{}^{ab}{}_{cd}\underset{q}{C}{}^{cd}{}_{ef} = \underset{p+q}{C}{}^{ab}{}_{ef}$$

and the following scalar invariants arise naturally:

$$\underset{p}{C} \equiv \underset{p}{C}{}^{ab}{}_{ab}.$$

Of course there are other Weyl scalar invariants (e.g., $C^{a}{}_{b}{}^{c}{}_{d}C^{b}{}_{e}{}^{d}{}_{f}C^{e}{}_{a}{}^{f}{}_{c}$) which do not fall into this pattern. The simple obvious identifications which we will exploit are

$$\mathbf{C}^p = \underset{p}{C}{}^{ab}{}_{cd},$$

$$\langle \mathbf{C}^p \rangle = \underset{p}{C}, \tag{5}$$

where $\langle\ \rangle$ denotes the trace of a matrix; but note that expressions like $\underset{2}{C}{}^{cj}{}_{ci}$ have no such obvious identification in the matrix notation.

The Cayley–Hamilton theorem for the trace-free $N\times N$ matrix $\mathbf{C}$ is given by

$$c_0\mathbf{C}^N + c_2\mathbf{C}^{N-2} + c_3\mathbf{C}^{N-3} + \cdots + c_{N-2}\mathbf{C}^2 + c_{N-1}\mathbf{C} + c_N\mathbf{I} = 0, \tag{6}$$

where $\mathbf{I}$ is the $N\times N$ identity matrix, and

$$c_0 = 1,\ \ c_2 = -\tfrac{1}{2}\langle\mathbf{C}^2\rangle,\ \ c_3 = -\tfrac{1}{3}\langle\mathbf{C}^3\rangle,\ \ c_4 = -\tfrac{1}{4}\left(\langle\mathbf{C}^4\rangle - \tfrac{1}{2}\langle\mathbf{C}^2\rangle^2\right),$$

$$c_5 = -\tfrac{1}{5}\left(\langle\mathbf{C}^5\rangle - \tfrac{5}{6}\langle\mathbf{C}^2\rangle\langle\mathbf{C}^3\rangle\right),$$

$$c_6 = -\tfrac{1}{6}\left(\langle\mathbf{C}^6\rangle - \tfrac{3}{4}\langle\mathbf{C}^2\rangle\langle\mathbf{C}^4\rangle - \tfrac{1}{3}\langle\mathbf{C}^3\rangle^2 + \tfrac{1}{8}\langle\mathbf{C}^2\rangle^3\right),\ \ \ldots\ ,$$

$$c_N = -\frac{1}{N}(\langle\mathbf{C}^N\rangle + \cdots + \cdots) \tag{7}$$

are the usual characteristic coefficients; since $\mathbf{C}$ is trace free, $c_1 = 0$. This theorem can easily be rewritten in chain notation as

$$c_0\underset{N}{C}{}^{ab}{}_{cd} + c_2\underset{N-2}{C}{}^{ab}{}_{cd} + c_3\underset{N-3}{C}{}^{ab}{}_{cd} + \cdots + c_{N-2}\underset{2}{C}{}^{ab}{}_{cd} + c_{N-1}\underset{1}{C}{}^{ab}{}_{cd} + c_N\delta^{a}_{[c}\delta^{b}_{d]} = 0, \tag{6′}$$

where the characteristic coefficients are now given in terms of Weyl scalar invariants by

$$c_0 = 1,\ \ c_2 = -\tfrac{1}{2}\underset{2}{C},\ \ c_3 = -\tfrac{1}{3}\underset{3}{C},\ \ c_4 = -\tfrac{1}{4}(\underset{4}{C} - \tfrac{1}{2}\underset{2}{C}{}^2),$$

$$c_5 = -\tfrac{1}{5}(\underset{5}{C} - \tfrac{5}{6}\underset{2}{C}\underset{3}{C}),$$

$$c_6 = -\tfrac{1}{6}(\underset{6}{C} - \tfrac{3}{4}\underset{2}{C}\underset{4}{C} - \tfrac{1}{3}\underset{3}{C}{}^2 + \tfrac{1}{8}\underset{2}{C}{}^3),\ \ \ldots\ ,$$

$$c_N = -\frac{1}{N}(\underset{N}{C} + \cdots + \cdots). \tag{7′}$$

From the well-known result $(-1)^N\det(\mathbf{C}) = c_N$ the required translation of $\det(\mathbf{C}) \neq 0$ into tensor language follows immediately:

$$0 \neq (-1)^{N+1} N \det(\mathbf{C}) = \underset{N}{C} + \cdots + \cdots . \tag{8}$$

Lemma: In n-dimensional spaces, the inhomogeneous algebraic equation for the vector V^d,

$$C^{ab}{}_{cd} V^d = H^{ab}{}_c,$$

has a unique solution when condition (8) holds; the solution is given by

$$V^a = \frac{2}{(n-1)c_N} H^{ij}{}_b (c_0 \underset{N-1}{C}{}^{ab}{}_{ij} + c_2 \underset{N-3}{C}{}^{ab}{}_{ij} + c_3 \underset{N-4}{C}{}^{ab}{}_{ij} + \cdots + c_{N-2} C^{ab}{}_{ij}),$$

where $N = n(-1)/2$ The coefficients $c_0, c_2, c_3, \ldots, c_{N-2}, c_N$ are the usual characteristic coefficients of the Cayley–Hamilton theorem given in (7′).

Proof: We consider the Cayley–Hamilton theorem for the $N \times N$ trace-free matrix $\mathbf{C}$ in tensor notation in (6′), with characteristic coefficients given by (7′).

Multiplying by V_a gives

$$\begin{aligned} 0 &= V_a (c_0 \underset{N}{C}{}^{ab}{}_{cd} + c_2 \underset{N-2}{C}{}^{ab}{}_{cd} + c_3 \underset{N-3}{C}{}^{ab}{}_{cd} + c_4 \underset{N-4}{C}{}^{ab}{}_{cd} + \cdots + c_{N-2} \underset{2}{C}{}^{ab}{}_{cd} + c_{N-1} \underset{1}{C}{}^{ab}{}_{cd}) + c_N V_{[c} \delta^b_{d]} \\ &= V_a \underset{1}{C}{}^{ab}{}_{ij} (c_0 \underset{N-1}{C}{}^{ij}{}_{cd} + c_2 \underset{N-3}{C}{}^{ij}{}_{cd} + c_3 \underset{N-4}{C}{}^{ij}{}_{cd} + c_4 \underset{N-5}{C}{}^{ij}{}_{cd} + \cdots + c_{N-2} \underset{1}{C}{}^{ij}{}_{cd}) + c_{N-1} V_a \underset{1}{C}{}^{ab}{}_{cd} + c_N V_{[c} \delta^b_{d]}. \end{aligned}$$

From which, by taking the trace and remembering $\underset{1}{C}{}^{ab}{}_{cd} \equiv C^{ab}{}_{cd}$ is trace free, we obtain

$$0 = V_a C^{ab}{}_{ij} (c_0 \underset{N-1}{C}{}^{ij}{}_{cb} + c_2 \underset{N-3}{C}{}^{ij}{}_{cb} + c_3 \underset{N-4}{C}{}^{ij}{}_{cb} + c_4 \underset{N-5}{C}{}^{ij}{}_{cb} + \cdots + c_{N-2} C^{ij}{}_{cb}) + \frac{n-1}{2} c_N V_c.$$

Rearranging gives the solution in the lemma. □

For future reference, we note that the *four-dimensional identity* (4a) can be written in the chain notation as

$$\underset{2}{C}{}^{cj}{}_{ck} = \delta^j_k \underset{2}{C}/4$$

and this is actually a special case of the more general identity[13] *in four dimensions only*

$$\underset{p}{C}{}^{cj}{}_{ck} = \delta^j_k \underset{p}{C}/4, \quad p = 2,3,4, \ldots . \tag{4b}$$

We have preferred the notation $\underset{2}{C}, \underset{3}{C}, \ldots, \underset{p}{C}, \ldots$ to the (possibly confusing) notation $C^2, C^3, \ldots, C^p, \ldots$ used in Refs. 7 and 8 and elsewhere for these Weyl scalar invariants.

Finally we note a very useful dimensionally *independent* identity (a direct consequence of the first Bianchi identity),

$$4 C_{a[ij]b} C^{cijd} = C_{abij} C^{cdij}.$$

III. REFORMULATING LISTING's RESULT AND REDERIVING THE IMPLICIT RESULTS IN REF. 7

With this lemma we determine the vector K^a from (3),

$$K^a = \frac{2}{(n-3)(n-1)c_N} \nabla^k C^{ij}{}_{kb} (c_0 \underset{N-1}{C}{}^{ab}{}_{ij} + c_2 \underset{N-3}{C}{}^{ab}{}_{ij} + c_3 \underset{N-4}{C}{}^{ab}{}_{ij} + \cdots + c_{N-2} C^{ab}{}_{ij}) \tag{9}$$

providing restriction (8) holds, where $N = n(n=1)/2$.

Substituting this value for K^a back into (2a) gives necessary and sufficient conditions defined only in terms of the geometry.

We can therefore reformulate Theorem 4.5 in Ref. 8 as follows.

Theorem 1: *A semi-Riemannian manifold, with a Weyl tensor subject to the restriction (8), is locally conformally related to an Einstein space if and only if the vector field K^a given in (9) satisfies (2a).*

Four dimensions: We now will retrieve the four-dimensional results implicit in Ref. 7 from this theorem in a signature independent manner. Instead of substituting for K^a with the expression (1a) as used in Ref. 7, or the four-dimensional version of the expression involving $\mathbf{C}^{-1}$ in Ref. 8, we can now use the $n=4$ version of (9),

$$K^a = \frac{2}{3c_6}\nabla^k C^{ij}{}_{kb}(c_0 \underset{5}{C}{}^{ab}{}_{ij} + c_2 \underset{3}{C}{}^{ab}{}_{ij} + c_3 \underset{2}{C}{}^{ab}{}_{ij} + c_4 C^{ab}{}_{ij}) \tag{10}$$

providing $c_6 \neq 0$ with the characteristic coefficients given by (7′) in terms of Weyl scalars. However, since the solution for K^a is unique we should be able to see precisely the links between these two expressions in (1a) and (10). To retrieve the result (1a) from (10) we simply substitute (3) back into the right-hand side of (a slightly rearranged) (10), for all terms except the last one, and use identity (4a) on each of these terms,

$$\begin{aligned} 3c_6 K^a &= -2K^k C^{ij}{}_{kb}(\underset{5}{C}{}^{ab}{}_{ij} + c_2 \underset{3}{C}{}^{ab}{}_{ij} + c_3 \underset{2}{C}{}^{ab}{}_{ij}) + 2c_4 C^{ab}{}_{ij}\nabla^k C^{ij}{}_{kb} \\ &= -2K^k(\underset{6}{C}{}^{cb}{}_{kb} + c_2 \underset{4}{C}{}^{cb}{}_{kb} + c_3 \underset{3}{C}{}^{cb}{}_{kb}) + 2c_4 C^{ab}{}_{ij}\nabla^k C^{ij}{}_{kb} \\ &= -\tfrac{1}{2}K^a(\underset{6}{C} + c_2 \underset{4}{C} + c_3 \underset{3}{C}) + 2c_4 C^{ij}{}_{cb}\nabla^k C^{ij}{}_{kb} \end{aligned}$$

which rearranges to

$$(6c_6 + \underset{6}{C} + c_2 \underset{4}{C} + c_3 \underset{3}{C})K_c = 4c_4 C^{ij}{}_{cb}\nabla_k C^{kb}{}_{ij}$$

and via (7′) to

$$c_4 \underset{2}{C} K^a = -4c_4 C^{ab}{}_{ij}\nabla^k C^{ij}{}_{kb}$$

and hence to (1a)—providing $\underset{2}{C} \neq 0 \neq \underset{4}{C} - \underset{2}{C}{}^2/2$.

Kozameh, Newman, and Tod[7] have shown that it is possible to obtain three alternative versions to (1a) for K^a consisting of

$$K^a = 4\underset{2}{C}{}^{ac}{}_{ij}\nabla^k C^{ij}{}_{ck}/\underset{3}{C} \quad \text{for } \underset{3}{C} \neq 0$$

together with two other similar expressions with invariants involving the dual of the Weyl tensor. We do not wish to depend on expressions with duals in this work since we wish to generalize the four-dimensional case to all higher dimensions. Instead, from the general identity (4b) we see that we can obtain the various expressions for K^a for all integers $p \geqslant 2$,

$$K^a = 4\,\underset{p-1}{C}{}^{ac}{}_{ij}\nabla^k C^{ij}{}_{ck}/\underset{p}{C} \quad \text{for } \underset{p}{C} \neq 0. \tag{1b}$$

So, in an analogous manner to which we retrieved (1a) from (10), we can also retrieve (1b) for $p=3, 4, 6$; by use of the Cayley–Hamilton theorem we could also retrieve the results for $p=5$ and $p \geqslant 7$, although after $p=6$ these expressions are not independent precisely because of the Cayley–Hamilton theorem. We note that we cannot retrieve the version of (1b) directly with $p=5$ from (10) due to the fact that the relevant term involved the coefficient c_1 which is identically zero, being the trace of $C_{ab}{}^{cd}$.

It is well known that in four dimensions there exist only four algebraically independent Weyl scalar invariants: these are usually given in terms of the well-known complex invariants I and J,

which come naturally from considerations in terms of spinors or complex Weyl tensors (which exploit the very simple and unique structure of the Weyl dual in four dimensions). If we wish to only employ structures which can be exploited in higher dimensions, we would consider instead the four algebraically independent scalars C, C, C, C (or any four from C, C, C, C, C)[10] (see also Refs. 11 and 5); and providing there is at least one Weyl scalar invariant which is nonzero, we can calculate K^a explicitly.

Higher dimensions: Theorem 1 gives an explicit tensor expression for K^a for all dimensions. So, for example, in *five dimensions*, $N=10$ and we obtain

$$K^a = \frac{1}{4c_{10}}\nabla^k C^{ij}{}_{kb}(c_0 C^{ab}{}_{ij} + c_2 C^{ab}{}_{ij} + c_3 C^{ab}{}_{ij} + \cdots + c_7 C^{ab}{}_{ij} + c_8 C^{ab}{}_{ij})$$

providing $c_{10} \neq 0$ with the characteristic coefficients given by (7′) in terms of Weyl scalars. Clearly this expression involves quite high order terms in the Weyl tensor, and we note that in the four-dimensional case, we were able to get lower order expressions for K^a by exploiting the individual dimensionally dependent identities (4b) rather than the Cayley–Hamilton theorem implicit in Theorem 1. So, in higher dimensions, we would also expect to exploit individual dimensional identities, analogous to the four-dimensional identities (4b), in order to obtain alternative lower order forms in the Weyl tensor for K^a in n dimensions.

IV. LOWER ORDER VERSIONS OF K^a IN n-DIMENSIONS

In four dimensions, providing we pay the price that at least one scalar invariant is nonzero, we are able to solve the four-dimensional version of (3), and obtain K^a. The versions from the individual identities (4b) are more concise and manageable than the versions from the Cayley–Hamilton theorem; on the other hand, in four dimensions, the latter include all the simpler results as special cases, and are more general, in the sense of weaker restrictions on the Weyl scalar invariants. Of course also the Cayley–Hamilton approach is applicable in all dimensions. However, we now will show how to obtain alternative simpler versions for K^a in dimensions other than four, by direct application of dimensionally dependent identities analogous to those used in four dimensions in Ref. 7.

The set of identities (4b) are all consequences of the well-known four-dimensional identity [it is interesting to note, in this notation, that the underlying identity for the Cayley–Hamilton theorem for the trace-free 6×6 matrix $\mathbf{C}$ is $\mathbf{C}^{[A}{}_{[P}\delta^{BCDEF]}_{QRSTU]}=0$ (Ref. 2)],[3]

$$C^{[ab}{}_{[cd}\delta^{e]}_{f]} = 0, \tag{11}$$

and we shall now exploit their higher dimensional analogues in the same way as in Ref. 7 for the four-dimensional case. For five dimensions we have

$$C^{[ab}{}_{[cd}\delta^{ef]}_{hi]} = 0, \tag{12}$$

and for six dimensions,

$$C^{[ab}{}_{[cd}\delta^{efg]}_{hij]} = 0, \tag{13}$$

and so on.[2]

These lead to

$$C^{cd}{}_{pe}C^{ph}{}_{ab}C^{[ab}{}_{[cd}\delta^{ef]}_{hi]} = 0 \tag{14}$$

for five dimensions, and

$$C^{cd}{}_{ef}C^{hi}{}_{ab}C^{[ab}{}_{[cd}\delta^{efg]}_{hij]} = 0 \tag{15}$$

for six dimensions, and so on. Of course, these are just representative for each dimension of the various identities that can be created; but it is of interest to note that for the lowest order in Weyl in each dimension—in five dimensions cubic, in six dimensions cubic, in seven dimensions quartic, and so on—there is only one possibility, but as we look at higher orders—in five dimensions quartic, in six dimensions quartic, in seven dimensions quintic, and so on—there will be many more possibilities. Unfortunately, when expanded, such two-index identities in higher dimensions will not have such a simple form as the four-dimensional identities (4b).

In higher dimensions there exist greater numbers of algebraically independent Weyl scalar invariants, and so there will be greater numbers of two-index tensor identities analogous to (4b) for each dimension $n>4$; furthermore, the tensor identities analogous to (4b) will be based on (14) and (15), … and so will also require more Weyl tensors as the dimension increases. Since, in higher dimensions, a product of three or more Weyl tensors yields more than one Weyl scalar algebraically independent of each other and of invariants of lower order (e.g., in general, $\underset{3}{C}$ and $C^{a\ b}_{i\ j}C^{i\ j}_{c\ d}C^{c\ d}_{a\ b}$ are algebraically independent in $n\geqslant 6$ dimensions), and more than one algebraically independent two-index tensor, we expect the higher dimensional analogues of identities (4b) to consist of linear combinations of Weyl tensors on both sides of the identity.

However, it is important to note that, although these higher order two-index identities will have more terms, and higher products, they will have the same crucial structure, which we can represent by

$$\underset{p}{L\{C\}}{}^{j}{}_{k} = \delta^{j}_{k}\underset{p}{L\{C\}}/n, \tag{16}$$

where $\underset{p}{L\{C\}}{}^{j}{}_{k}$ represents a two-index tensor consisting of a linear combination of products of p Weyl tensors, and $\underset{p}{L\{C\}}\equiv\underset{p}{L\{C\}}{}^{i}{}_{i}$ represents a linear combination of scalar products of p Weyl tensors. (Note that each term is unlikely to be just a simple chain.) It follows, for $\underset{p}{L\{C\}}\neq 0$ from (16),

$$K^{j} = n\underset{p}{L\{C\}}{}^{j}{}_{k}K^{k}/\underset{p}{L\{C\}}, \tag{17}$$

and hence all the terms involving the vector K^k on the right-hand side—which will each contain a factor of the form $C^{\cdot\cdot}{}_{.k}K^{k}$—can be replaced using (3) by

$$C^{\cdot\cdot}{}_{.k}K^{k} = -\frac{1}{n-3}\nabla^{k}C^{\cdot\cdot}{}_{.k}. \tag{18}$$

We can summarize these new results as follows.

Theorem 2: *An n-dimensional semi-Riemannian manifold with a nondegenerate Weyl tensor restricted by* $\underset{p}{L\{C\}}\neq 0$ *[where* $\underset{p}{L\{C\}}$ *is associated with an identity of the form (16)] is locally conformally related to an Einstein space if and only if the vector field* K^a *given in (17), with the appropriate substitutions (18), satisfies (2a).*

Clearly from Theorem 2 we will obtain for K^a much lower order expressions in the Weyl tensor than from Theorem 1; for example, in five dimensions using Theorem 1 will require terms involving products of 10 Weyl tensors, whereas if we use Theorem 2 it looks possible to use terms with only three Weyl tensors, from (14).

V. FIVE- AND SIX-DIMENSIONAL SPACES

For higher dimensional spaces we can use Theorem 1 with the respective substitutions $n=5,6,\ldots$ into (9). But for spaces where we know dimensionally dependent identities of the form (14) and (15), etc., we can use Theorem 2.

So for spaces with dimension $n>4$ there is the need to systematically write out explicitly the two-index identities such as (14) and (15), etc., for $n=5,6,\ldots$. In this section we give just a few examples in five and six dimensions as illustrations.

Five dimensions: After a straightforward calculation we find that (14) expands as follows:

$$C^{aj}{}_{bc}C^{bc}{}_{de}C^{de}{}_{ak}-2C^{aj}{}_{bk}C^{bc}{}_{de}C^{de}{}_{ac}-4C^{aj}{}_{bc}C^{bd}{}_{ek}C^{ce}{}_{ad}=\tfrac{1}{5}(C^{ab}{}_{cd}C^{cd}{}_{ef}C^{ef}{}_{ab}-4C^{ab}{}_{cd}C^{ce}{}_{af}C^{df}{}_{be})\delta^{j}_{k}. \tag{19}$$

Although this appears to have the structure of (16), unfortunately when we also consider the scalar identity closely related to (14),

$$C^{cd}{}_{ab}C^{ki}{}_{ej}C^{[ab}{}_{[cd}\delta^{ej]}_{ki]}=0$$

we find

$$C^{ab}{}_{cd}C^{cd}{}_{ef}C^{ef}{}_{ab}=4C^{ab}{}_{cd}C^{ce}{}_{af}C^{df}{}_{be}. \tag{20}$$

(This five-dimensional scalar identity was also noted in Ref. 6, where it was obtained from the *five-dimensional* identity $C^{ab}{}_{[cd}C^{cd}{}_{ef}C^{ef}{}_{ab]}\equiv 0$.) This means that (19) does not have the structure of (16) as we hoped, since its right-hand side is identically zero. However, we do have an interesting two-index *five-dimensional* identity which will be useful in other contexts,

$$C^{aj}{}_{bc}C^{bc}{}_{de}C^{de}{}_{ak}-2C^{aj}{}_{bk}C^{bc}{}_{de}C^{de}{}_{ac}-4C^{aj}{}_{bc}C^{bd}{}_{ek}C^{ce}{}_{ad}=0. \tag{21}$$

On the other hand, if we consider one (of a number of) quartic identity in five dimensions,

$$C^{qg}{}_{ip}C^{ip}{}_{qe}C^{ab}{}_{cd}C^{[cd}{}_{[ab}\delta^{ef]}_{gh]}=0 \tag{22}$$

we obtain

$$\begin{aligned}5C^{qj}{}_{ip}C^{ip}{}_{qk}C^{ab}{}_{cd}C^{cd}{}_{ab}-8C^{qg}{}_{ip}C^{ip}{}_{qk}C^{ab}{}_{cg}C^{cj}{}_{ab}+8C^{qg}{}_{ip}C^{ip}{}_{qe}C^{be}{}_{ag}C^{aj}{}_{bk}-4C^{qg}{}_{ip}C^{ip}{}_{qe}C^{ab}{}_{gk}C^{ej}{}_{ab}\\ -8C^{qg}{}_{ip}C^{ip}{}_{qe}C^{ae}{}_{bk}C^{bj}{}_{ag}=(C^{qg}{}_{ip}C^{ip}{}_{qg}C^{ab}{}_{cd}C^{cd}{}_{ab}-4C^{qg}{}_{ip}C^{ip}{}_{qd}C^{ab}{}_{cg}C^{cd}{}_{ab})\delta^{j}_{k}\end{aligned} \tag{23}$$

which again appears to have the structure of (16). [The use of the identity (21) does not give any simplification.] We need to determine whether the right-hand side of (23) is nonzero. Unlike in the cubic case where there was only one possible scalar identity (20), there will be a number of quartic scalar identities in five dimensions; so although we will return to examine these another time, for now we simply note, via a counterexample, that the right-hand side cannot be identically zero.[14]

Hence, via the substitution (18), we obtain the following form for K^j:

$$\begin{aligned}K^{j}=&-(5C^{qj}{}_{ip}C^{ab}{}_{cd}C^{cd}{}_{ab}\nabla^{k}C^{ip}{}_{qk}-8C^{qg}{}_{ip}C^{ab}{}_{cg}C^{cj}{}_{ab}\nabla^{k}C^{ip}{}_{qk}+8C^{qg}{}_{ip}C^{ip}{}_{qe}C^{be}{}_{ag}\nabla^{k}C^{aj}{}_{bk}\\ &-4C^{qg}{}_{ip}C^{ip}{}_{qe}C^{ej}{}_{ab}\nabla^{k}C^{ab}{}_{gk}-8C^{qg}{}_{ip}C^{ip}{}_{qe}C^{bj}{}_{ag}\nabla^{k}C^{ae}{}_{bk})/2(C^{qg}{}_{ip}C^{ip}{}_{qg}C^{ab}{}_{cd}C^{cd}{}_{ab}\\ &-4C^{qg}{}_{ip}C^{ip}{}_{qe}C^{ab}{}_{cg}C^{ce}{}_{ab}).\end{aligned} \tag{24}$$

We can then substitute this value for K^j into the five-dimension version of (2a),

$$\widetilde{R}_{ab}+3(\nabla_{a}K_{b}-K_{a}K_{b}-(\nabla^{c}K_{c}-K^{c}K_{c})g_{ab}/5)=0 \tag{2b}$$

to obtain the required necessary and sufficient condition.

Six dimensions: When we expand (15) we obtain

$$C_{ak}{}^{bc}C^{aj}{}_{de}C_{bc}{}^{de}-2C_{ak}{}^{bj}C^{ac}{}_{de}C_{bc}{}^{de}-4C_{ak}{}^{bc}C^{dj}{}_{be}C_{cd}{}^{ae}=\tfrac{1}{6}(C_{ab}{}^{cd}C_{cd}{}^{ef}C_{ef}{}^{ab}-4C_{ab}{}^{cd}C^{ae}{}_{cf}C_{de}{}^{bf})\delta^{j}_{k}. \tag{25}$$

Unlike for the case of the five-dimensional two-index identity (19), there is no related scalar identity cubic in Weyl tensors, analogous to (20). So therefore we do not need to worry about the

possibility of the right-hand side of (25) being zero, and so we have an identity which has precisely the structure (16).

Hence, via the substitution (18), we obtain the following form for K^j:

$$K^j = -2(C^{aj}{}_{de}C_{bc}{}^{de}\nabla^k C_{ak}{}^{bc} - 2C^{ac}{}_{de}C_{bc}{}^{de}\nabla^k C_{ak}{}^{bj} - 4C^{dj}{}_{be}C_{cd}{}^{ae}\nabla^k C_{ak}{}^{bc})/(C_{ab}{}^{cd}C_{cd}{}^{ef}C_{ef}{}^{ab} - 4C_{ab}{}^{cd}C^{ae}{}_{cf}C_{de}{}^{bf}). \tag{26}$$

We can then substitute this value for K^j into the six-dimensional version of (2a),

$$\tilde{R}_{ab} + 4(\nabla_a K_b - K_a K_b - (\nabla^c K_c - K^c K_c)g_{ab}/6) = 0, \tag{2c}$$

to obtain the required necessary and sufficient condition.

There do not seem to be many explicit examples of identities for the Weyl tensor in higher dimensions in the literature. However, there does exist a six-dimensional two-index tensor identity quartic in the Weyl tensor which was identified some time ago by Lovelock.[9] A double three-form with the antisymmetric and trace-free properties, respectively,

$$H_{abk}{}^{def} = H_{[abk]}{}^{[def]},$$

$$H_{abi}{}^{dei} = 0 \tag{27}$$

in six dimensions (and lower) satisfies the identity

$$H_{abk}{}^{def}H_{def}{}^{abj} = \tfrac{1}{6}\delta^j_k H_{abc}{}^{def}H_{def}{}^{abc}. \tag{28}$$

This then becomes a quartic identity for Weyl with the choice

$$H_{ijk}{}^{abc} = A_{ijk}{}^{abc} - \tfrac{9}{8}A_{r[jk}{}^{r[bc}\delta_{i]}^{a]} + 3A_{rs[i}{}^{rs[c}\delta_i^a\delta_{k]}^{b]} - \tfrac{1}{4}A_{rst}{}^{rst}\delta^{[a}_{[i}\,\delta^b_j\delta^{c]}_{k]}, \tag{29}$$

where

$$A_{ijk}{}^{abc} = 4C_{[ij}{}^{h[a}C_{k]h}{}^{bc]}. \tag{30}$$

By substituting (29) into (28) we obtain

$$A_{abk}{}^{cde}A_{cde}{}^{abj} + 3A_{abk}{}^{abc}A_{cde}{}^{dej} + 6A_{abk}{}^{acd}A_{cde}{}^{bej} - 3A_{abc}{}^{ade}A_{dek}{}^{bcj} - A_{abc}{}^{abc}A_{dek}{}^{dej} + 6A_{abc}{}^{abd} = \delta^j_k(A_{abc}{}^{abc}A_{def}{}^{def} + 9A_{abc}{}^{ade}A_{def}{}^{bcf} - 9A_{abc}{}^{abd}A_{def}{}^{cef} - A_{abc}{}^{def}A_{def}{}^{abc})/6, \tag{31}$$

which is precisely the structure of (16). Hence, we obtain the following form for K^j,

$$K^j = -6(K^k A_{kab}{}^{cde}A_{cde}{}^{abj} + 3K^k A_{kab}{}^{abc}A_{cde}{}^{dej} + 6K^k A_{kab}{}^{acd}A_{cde}{}^{bej} - 3A_{abc}{}^{ade}K^k A_{kde}{}^{bcj} - A_{abc}{}^{abc}K^k A_{kde}{}^{dej} + 6A_{abc}{}^{abd}K^k A_{kde}{}^{cej})/(A_{abc}{}^{abc}A_{def}{}^{def} + 9A_{abc}{}^{ade}A_{def}{}^{bcf} - 9A_{abc}{}^{abd}A_{def}{}^{cef} - A_{abc}{}^{def}A_{def}{}^{abc}), \tag{32}$$

where all terms involving K^k on the right-hand side are replaced via the substitution

$$K^k A_{kab}{}^{cde} = \nabla^k C_{k[a}{}^{p[c}C_{b]p}{}^{de]} - \nabla^k C_{kp}{}^{[de}C_{ab}{}^{c]p} \tag{33}$$

and all other terms replaced with (30). We then substitute the value for K^j from (32) into (2c) to obtain the required necessary and sufficient condition. It is of course necessary to check that the right-hand side of (32) is not identically zero; this can be confirmed with a simple counterexample.[14]

VI. SUMMARY AND DISCUSSION

We have demonstrated the power of dimensionally dependent identities [either as the Cayley–Hamilton theorem, or as individual identities in specific dimensions such as (4b), (23), (25), and (31)] to translate the existence result of Listing[8] into versions which can be applied directly; furthermore, these applications are completely independent of signature. Theorem 1 gives a general reformulation of Listing's result on the existence of necessary and sufficient conditions in a form which can be directly exploited. So if one wishes to test if a particular metric is conformally Einstein, then it is a simple procedure to find its Weyl and trace-free Ricci tensor and to test directly—for instance, using GRTENSOR II (Ref. 14)—if condition (2a) is satisfied.

We have drawn attention to the higher dimensional analogues (23), (25), and (31), etc., of identities (4b), which are the basis for Theorem 2; for applications, Theorem 2 would seem to provide a simpler and more manageable tool—providing the appropriate identities are known.

A major complication when we move to dimensions $n>4$ is that there are many more Weyl invariant scalars, and of course they cannot all be written in the form C. The same sort of detailed analysis of the Weyl invariant scalars for $n=5,6\ldots$, as has been (partly) carried out for $n=4$, as well as a systematic presentation of two-index identities, is a necessary prerequisite for a systematic examination of all possible versions of the vector K^a. As Bonanos has pointed out,[1] existing detailed studies such as Ref. 4 do not take into account invariants formed from duals, or identities from the Cayley–Hamilton theorem. There are still a number of interesting issues to be investigated further.

There appears to be an important difference between even and odd dimensions: for even dimensions $n=4,6,8,\ldots$ the simplest two-index identity involves products of 2,3,4,… Weyl tensors, respectively, such as (4a) and (25), with a "delta term" on the right-hand side; for odd $n=5,7,\ldots$ the simplest two-index identity involves products of 3, 4,… Weyl tensors, respectively, such as (19), but it would seem likely that as in (21) the "delta term" on the right-hand side disappears because of an identically zero coefficient. For the investigations in this paper we need an identity of the former type, so in general it appears that for even dimensions $n=2m$ we will be able to exploit comparatively simple identities involving products of m Weyl tensors, while for odd dimensions $n=2m-1$ we will only have more complicated identities involving products of $m+1$ Weyl tensors. On the other hand, we anticipate that in other investigations the simple identities such as (21) will be very useful.

Listing[8] has stated that the condition $\det \mathbf{C} \neq 0$ *in four dimensions* is equivalent to the complex Weyl invariant scalar $J \neq 0$; by a little manipulation this can be shown to be equivalent to at least one of C and C being nonzero. It would be useful to know this condition in higher dimensions in terms of the real Weyl invariant scalars, and hence understand it better. The fact that the right-hand side of identity (19) is identically zero should alert us to the possibility of identically zero scalars arising in some situations.

The use of the dual Weyl tensor makes work in four dimensions comparatively easy—for instance there is a basis of four Weyl scalar invariants none of which is higher than cubic in Weyl, compared to having a basis with invariants up to fifth order in Weyl if the dual tensor is not used; in higher dimensions the major advantage (the dual Weyl tensor is also a double two form) does not apply, and work gets more complicated. However, we believe that it is still possible to take advantage of other benefits of the dual tensor, and we will discuss this possibility, together with the other points mentioned here, elsewhere.

Finally, we note that the necessary and sufficient conditions investigated by Listing[8] and in this paper were different from the necessary and sufficient conditions investigated explicitly in Ref. 7 in four dimensions. In Ref. 7 these conditions involved the Bach tensor which of course is only defined in four dimensions. It will be shown elsewhere how the techniques in Ref. 8 and in this paper can be used to investigate these alternative conditions as well as to generate an n-dimensional generalization of the Bach tensor.

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On the eigenvalues of the Chandrasekhar–Page angular equation

Davide Batic[a] and Harald Schmid[b]
NWF I–Mathematik, Universität Regensburg, D-93040 Regensburg, Germany

Monika Winklmeier[c]
FB 3–Mathematik, Universität Bremen, D-28359 Bremen, Germany

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In this paper we study for a given azimuthal quantum number κ the eigenvalues of the Chandrasekhar–Page angular equation with respect to the parameters $\mu := am$ and $\nu := a\omega$, where a is the angular momentum per unit mass of a black hole, m is the rest mass of the Dirac particle and ω is the energy of the particle (as measured at infinity). For this purpose, a self-adjoint holomorphic operator family $A(\kappa;\mu,\nu)$ associated to this eigenvalue problem is considered. At first we prove that for fixed $\kappa \in \mathbb{R}\setminus(-\frac{1}{2},\frac{1}{2})$ the spectrum of $A(\kappa;\mu,\nu)$ is discrete and that its eigenvalues depend analytically on $(\mu,\nu) \in \mathbb{C}^2$. Moreover, it will be shown that the eigenvalues satisfy a first order partial differential equation with respect to μ and ν, whose characteristic equations can be reduced to a Painlevé III equation. In addition, we derive a power series expansion for the eigenvalues in terms of $\nu-\mu$ and $\nu+\mu$, and we give a recurrence relation for their coefficients. Further, it will be proved that for fixed $(\mu,\nu) \in \mathbb{C}^2$ the eigenvalues of $A(\kappa;\mu,\nu)$ are the zeros of a holomorphic function Θ which is defined by a relatively simple limit formula. Finally, we discuss the problem if there exists a closed expression for the eigenvalues of the Chandrasekhar–Page angular equation. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The angular eigenvalue problem of a spin-$\frac{1}{2}$ particle in the Kerr–Newman geometry is given by the Chandrasekhar–Page angular equation

$$\mathcal{L}^{+}_{1/2} S_{+1/2} = (am\cos\theta - \lambda) S_{-1/2}, \tag{1}$$

$$\mathcal{L}^{-}_{1/2} S_{-1/2} = (am\cos\theta + \lambda) S_{+1/2}, \tag{2}$$

see Chandrasekhar (1998, Chap. 10, Sec. 104), where the Kerr parameter a is the angular momentum per unit mass of a black hole and m is the rest mass of the Dirac particle. Moreover, the differential operators $\mathcal{L}^{\pm}_{1/2}$ are defined by

$$\mathcal{L}^{\pm}_{1/2} = \partial_\theta \pm Q(\theta) + \frac{\cot\theta}{2}, \quad Q(\theta) := a\omega\sin\theta + \frac{\kappa}{\sin\theta}, \quad \theta \in (0,\pi),$$

where ω is the energy of the particle (as measured at infinity) and κ is a half-integer, i.e., $\kappa = k - \frac{1}{2}$ with some $k \in \mathbb{Z}$. A parameter $\lambda \in \mathbb{R}$ is called an *eigenvalue* of this spectral problem if the

[a]Electronic mail: davide.batic@mathematik.uni-regensburg.de
[b]Electronic mail: harald.schmid@mathematik.uni-regensburg.de
[c]Electronic mail: winklmeier@math.uni-bremen.de

system given by (1)-(2) has a nontrivial solution which is square-integrable on $(0,\pi)$ with respect to the weight function $\sin\theta$. In this paper we study for fixed κ the eigenvalues of the Chandrasekhar–Page angular equation as a function of the parameters $\mu := am$ and $\nu := a\omega$. As a main result, we will prove that the eigenvalues satisfy a first order quasilinear partial differential equation, and we will derive a power series expansion for the eigenvalues in terms of $\nu-\mu$ and $\nu+\mu$.

For this purpose it is necessary to consider the system (1)-(2) in a more general context where κ is real, $|\kappa| \geqslant \frac{1}{2}$, and μ, ν are complex numbers. At first we rewrite this system for fixed $\kappa \in \mathbb{R}\backslash(-\frac{1}{2},\frac{1}{2})$ as an eigenvalue problem for some self-adjoint holomorphic operator family $A=A(\kappa;\mu,\nu)$ depending on the parameters $(\mu,\nu)\in\mathbb{C}^2$. In the special case where $(\mu,\nu)\in\mathbb{R}^2$ the differential operator $A(\kappa;\mu,\nu)$ is self-adjoint and has purely discrete spectrum. In Sec. II we prove that for a given κ the eigenvalues $\lambda_j(\kappa;\mu,\nu)$ of A are holomorphic functions in (μ,ν), and we derive some basic estimates for them. Furthermore, we transform the system (1)-(2) to a matrix differential equation

$$y'(x) = \left[\frac{1}{x}B_0 + \frac{1}{x-1}B_1 + C\right]y(x) \tag{3}$$

on the interval $(0,1)$ with coefficient matrices

$$B_0 = \begin{pmatrix} -\frac{\kappa}{2}-\frac{1}{4} & \mu-\lambda \\ 0 & \frac{\kappa}{2}+\frac{1}{4} \end{pmatrix}, \quad B_1 = \begin{pmatrix} \frac{\kappa}{2}+\frac{1}{4} & 0 \\ \mu-\lambda & -\frac{\kappa}{2}-\frac{1}{4} \end{pmatrix}, \quad C = \begin{pmatrix} -2\nu & -2\mu \\ 2\mu & 2\nu \end{pmatrix},$$

which can be extended to the complex domain $\mathbb{C}\backslash\{0,1\}$. In this way we obtain a further characterization of the eigenvalues of A and some useful estimates for the corresponding eigenfunctions. Applying analytic perturbation theory, we show in Sec. III that the eigenvalues $\lambda_j(\kappa;\mu,\nu)$ satisfy the partial differential equation

$$(\mu-2\nu\lambda)\frac{\partial\lambda}{\partial\mu} + (\nu-2\mu\lambda)\frac{\partial\lambda}{\partial\nu} + 2\kappa\mu + 2\mu\nu = 0. \tag{4}$$

In particular, this result can be used to obtain a recurrence relation for the coefficients $c_{m,n}$ of a power series expansion

$$\lambda_j(\kappa;\mu,\nu) = \sum_{m,n=0}^{\infty} c_{m,n}(\nu-\mu)^m(\nu+\mu)^n.$$

In Sec. IV we solve the PDE (4) by the method of characteristics. First, we derive an explicit formula for the eigenvalues in the case $|\mu|=|\nu|$. Moreover, in the regions where $|\mu|\neq|\nu|$ we reduce the characteristic equations of (4) to a Painlevé III equation

$$vv' + tvv'' - t(v')^2 - 2\kappa(v^2\pm 1)v - t(v^4-1) = 0$$

with parameters $\alpha=\pm\beta=2\kappa$ and $\gamma=-\delta=1$ according to the notation in Milne *et al.* (1997) and Mansfield and Webster (1998). As this differential equation is in general not solvable in terms of elementary functions, we cannot expect a closed expression for the eigenvalues of the Chandrasekhar–Page angular equation for all $(\mu,\nu)\in\mathbb{R}^2$. However, if κ is a half-integer, i.e., $\kappa=k-\frac{1}{2}$ with some positive integer k, then $\alpha\pm\beta=2(2k-1)$, and there are integrals of polynomial type for the third Painlevé equation in this special case, cf. Milne *et al.* (1997). Hence, if $\kappa=\pm\frac{1}{2},\pm\frac{3}{2},\ldots$, there exist algebraic solutions of the partial differential equation (4), and the question arises if these explicit solutions are in fact eigenvalues of the Chandrasekhar–Page angular equation. It turns out that there is another type of "special values" associated to the operator A, called *monodromy eigenvalues*, which belong to the algebraic solutions of the PDE

(4). For a half-integer κ, the monodromy eigenvalues are introduced in Sec. V by requiring that the system (3) has a fundamental matrix of the form

$$[x(1-x)]^{-(\kappa/2)-1/4}H(x)$$

with an entire matrix function $H:\mathbb{C}\to \mathrm{M}_2(\mathbb{C})$. This property turns out to be equivalent to the existence of special solutions of the form

$$[x(1-x)]^{-(\kappa/2)-1/4}p^{\pm}(x)e^{\pm 2tx},$$

where $p^{\pm}:\mathbb{C}\to\mathbb{C}^2$ are polynomials and $t=\pm\sqrt{\nu^2-\mu^2}$. For comparison purposes, an eigenvalue of A can be characterized by the property that (3) possesses a nontrivial solution of the form

$$[x(1-x)]^{(\kappa/2)+1/4}\eta(x)$$

with some entire vector function $\eta:\mathbb{C}\to\mathbb{C}^2$. We prove that the monodromy eigenvalues are zeros of a polynomial with degree $2k-1$ whose coefficients are polynomials in μ and ν. Moreover, it can be shown that monodromy eigenvalues and "classical" eigenvalues are distinct at least in a neighborhood of $(\mu,\nu)=(0,0)$. Nevertheless, they are both characterized by the fact that certain monodromy data of the system (3) are preserved for all parameters (μ,ν). In fact, λ is a monodromy eigenvalue of A if and only if the monodromy matrices of (3) at the regular-singular points 0 and 1 are diagonal, whereas λ is a classical eigenvalue of A if and only if a certain nondiagonal entry of the connection matrix for the fundamental matrices at 0 and 1 vanishes. Hence, for the Chandrasekhar–Page angular equation the monodromy as well as the classical eigenvalue problem is closely related to the isomonodromy problem for the differential equation (3). Monodromy preserving deformations for such a system were studied by Jimbo *et al.* (1981), but only if the eigenvalues of B_0 and B_1 do not differ by an integer, i.e., $\kappa+\frac{1}{2}\notin\mathbb{Z}$. In Sec. VI we consider the isomonodromy problem for (3) in the case that κ is a half-integer. As a consequence, we show that the monodromy eigenvalues of A satisfy the partial differential equation (4), and we obtain an alternative derivation of (4) for the classical eigenvalues of A. Unlike the proof in Sec. III, which relies on the particular structure of the Chandrasekhar–Page angular equation, the method presented in Sec. V is more general and based on finding suitable deformation equations for parameter-dependent differential equations. Thus, we expect that this technique is applicable to other eigenvalue problems as well.

II. A SELF-ADJOINT HOLOMORPHIC OPERATOR FAMILY ASSOCIATED TO THE CHANDRASEKHAR–PAGE ANGULAR EQUATION

By introducing the notations

$$\mu := am, \quad \nu := a\omega, \quad S(\theta) := \sqrt{\sin\,\theta}\begin{pmatrix} S_{+1/2}(\theta) \\ S_{-1/2}(\theta)\end{pmatrix}, \quad \theta\in(0,\pi),$$

the Chandrasekhar–Page angular equation (1)-(2) takes the form

$$(\mathfrak{A}S)(\theta) := \begin{pmatrix} 0 & 1 \\ -1 & 0\end{pmatrix}S'(\theta) + \begin{pmatrix} -\mu\cos\,\theta & -\dfrac{\kappa}{\sin\,\theta}-\nu\sin\,\theta \\ -\dfrac{\kappa}{\sin\,\theta}-\nu\sin\,\theta & \mu\cos\,\theta\end{pmatrix}S(\theta) = \lambda S(\theta) \tag{5}$$

with fixed $\kappa\in\mathbb{R}\setminus\left(-\frac{1}{2},\frac{1}{2}\right)$ and parameters $(\mu,\nu)\in\mathbb{C}^2$. We can associate the so-called minimal operator A_0 to the formal differential expression $\mathfrak{A}$, which acts in the Hilbert space $\mathcal{H}:=\mathcal{L}^2((0,\pi),\mathbb{C}^2)$ of square integrable vector functions with respect to the scalar product

$$(S_1,S_2) := \int_0^\pi S_2(\theta)^* S_1(\theta)\mathrm{d}\theta, \quad S_1,S_2 \in \mathcal{H}. \tag{6}$$

The operator A_0 given by $\mathcal{D}(A_0)=\mathrm{C}_0^\infty((0,\pi),\mathbb{C}^2)$ and $A_0S:=\mathfrak{A}S$ for $S\in\mathcal{D}(A_0)$ is densely defined and closable. For $|\kappa|\geqslant\frac{1}{2}$ and $(\mu,\nu)\in\mathbb{R}^2$ the formal differential operator in (5) is in the limit point case at 0 and π, hence A_0 is even essentially self-adjoint. In the following we denote the closure of A_0 by $A=A(\kappa;\mu,\nu)$. According to Weidmann (1987, Theorem 5.8) the domain of $A(\kappa;0,0)$ is given by

$$\mathcal{D}(A)=\{S\in\mathcal{H} : S \text{ is absolutely continuous and } A(\kappa;0,0)S\in\mathcal{H}\}.$$

Since $A(\kappa;\mu,\nu)=A(\kappa;0,0)+T(\mu,\nu)$ with the bounded multiplication operator

$$T(\mu,\nu)=\begin{pmatrix} -\mu\cos\theta & -\nu\sin\theta \\ -\nu\sin\theta & \mu\cos\theta \end{pmatrix},$$

its domain of definition $\mathcal{D}(A)$ is independent of $(\mu,\nu)\in\mathbb{C}^2$, see Kato (1966, Chap. IV, §1, Theorem 1.1). Moreover, if $(\mu,\nu)\in\mathbb{R}^2$, then $T(\mu,\nu)$ is a symmetric perturbation of $A(\kappa;0,0)$, and Theorem 4.10 in Kato (1966, Chap. V, §4) yields that $A(\kappa;\mu,\nu)$ is self-adjoint. Thus, according to the classification in Kato (1966, Chap. VII, §3), $A(\kappa;\mu,\nu)$ forms a self-adjoint holomorphic operator family of type (A) in the variables $(\mu,\nu)\in\mathbb{C}^2$. Further, the spectrum of $A(\kappa;0,0)$ is discrete and consists of simple eigenvalues given by

$$\lambda_j(\kappa;0,0)=\mathrm{sgn}(j)(|\kappa|-\tfrac{1}{2}+|j|), \quad j\in\mathbb{Z}\setminus\{0\} \tag{7}$$

(for the details we refer to Appendix A). This means, in particular, that $A(\kappa;0,0)$ has compact resolvent, and from Theorem 2.4 in Kato (1966, Chap. V, §2) it follows that $A(\kappa;\mu,\nu)$ has compact resolvent for all $(\mu,\nu)\in\mathbb{C}^2$. As a consequence, the spectrum of $A(\kappa;\mu,\nu)$, $(\mu,\nu)\in\mathbb{C}^2$, is discrete, and since $A(\kappa;\mu,\nu)$ is in the limit point case at $\theta=0$ and $\theta=\pi$, its spectrum consists of simple eigenvalues for $(\mu,\nu)\in\mathbb{R}^2$. Now, Theorem 3.9 in Kato (1966, Chap. V, §3) implies that the eigenvalues $\lambda_j=\lambda_j(\kappa;\mu,\nu)$, $j\in\mathbb{Z}\setminus\{0\}$, of $A(\kappa;\mu,\nu)$ are simple and depend holomorphically on (μ,ν) in a complex neighborhood of $\mathbb{R}^2$. Moreover, the partial derivatives of A with respect to μ and ν are given by

$$\frac{\partial A}{\partial\mu}=\begin{pmatrix} -\cos\theta & 0 \\ 0 & \cos\theta \end{pmatrix}, \quad \frac{\partial A}{\partial\nu}=\begin{pmatrix} 0 & -\sin\theta \\ -\sin\theta & 0 \end{pmatrix},$$

which yields the following estimates for the growth rate of the eigenvalues, compare Kato (1966, Chap. VII, §3, Sec. 4):

$$\left|\frac{\partial\lambda_j}{\partial\mu}\right|\leqslant\left\|\frac{\partial A}{\partial\mu}\right\|\leqslant 1, \quad \left|\frac{\partial\lambda_j}{\partial\nu}\right|\leqslant\left\|\frac{\partial A}{\partial\nu}\right\|\leqslant 1.$$

Here $\|\cdot\|$ denotes the operator norm of a (2×2) matrix. In addition, by Theorem 4.10 in Kato (1966, Chap. V, §3), we have

$$\min_{j\in\mathbb{Z}\setminus\{0\}}|\lambda-\lambda_j(\kappa;0,0)|\leqslant\|T(\mu,\nu)\|\leqslant\max\{|\mu|,|\nu|\} \tag{8}$$

for each eigenvalue λ of $A(\kappa;\mu,\nu)$. Finally, by interchanging the components of $S(\theta)$, we obtain that a point λ is an eigenvalue of $A(\kappa;\mu,\nu)$ if and only if $-\lambda$ is an eigenvalue of $A(-\kappa;\mu,-\nu)$. Since the eigenvalues depend holomorphically on μ and ν, the identity

$$\lambda_j(\kappa;\mu,\nu) = -\lambda_{-j}(-\kappa;\mu,-\nu)$$

holds for all (μ,ν) in a neighborhood of $\mathbb{R}^2$. Therefore, we restrict our attention to the case $\kappa \in \left[\frac{1}{2},\infty\right)$. Note that $\lambda \in \mathbb{C}$ is an eigenvalue of $A(\kappa;\mu,\nu)$ if and only if the system (5) has a nontrivial solution $S(\theta)$ satisfying

$$\int_0^\pi |S(\theta)|^2 \, \mathrm{d}\theta < \infty. \tag{9}$$

By means of the transformation

$$S(\theta) = \begin{pmatrix} \sqrt{\tan\frac{\theta}{2}} & 0 \\ 0 & \sqrt{\cot\frac{\theta}{2}} \end{pmatrix} y\left(\sin^2\frac{\theta}{2}\right), \quad \theta \in (0,\pi), \tag{10}$$

the differential equation (5) is equivalent to the system

$$y'(x) = \left[\frac{1}{x}B_0 + \frac{1}{x-1}B_1 + C\right] y(x) \tag{11}$$

on the interval $(0,1)$ with coefficient matrices

$$B_0 := \begin{pmatrix} -\frac{\kappa}{2}-\frac{1}{4} & \mu-\lambda \\ 0 & \frac{\kappa}{2}+\frac{1}{4} \end{pmatrix}, \quad B_1 := \begin{pmatrix} \frac{\kappa}{2}+\frac{1}{4} & 0 \\ \mu-\lambda & -\frac{\kappa}{2}-\frac{1}{4} \end{pmatrix}, \quad C := \begin{pmatrix} -2\nu & -2\mu \\ 2\mu & 2\nu \end{pmatrix}, \tag{12}$$

and the normalization condition (9) becomes

$$\int_0^1 y(x)^* \begin{pmatrix} \frac{1}{1-x} & 0 \\ 0 & \frac{1}{x} \end{pmatrix} y(x)\mathrm{d}x < \infty. \tag{13}$$

If we consider the differential equation (11) for a fixed $\kappa \in (0,\infty)$ in the complex plane, then it has two regular singular points, one at $x=0$ and one at $x=1$ with characteristic values $\pm\left[(\kappa/2)+\frac{1}{4}\right]$. From the theory of asymptotic expansions [see Wasow (1965), for example], it follows that for each $\lambda \in \mathbb{C}$ there exists a nontrivial solution

$$y_0(x,\lambda) = x^{(\kappa/2)+1/4} h(x,\lambda), \quad x \in \mathfrak{B}_0 \tag{14}$$

of (11) in the open unit disk $\mathfrak{B}_0 \subset \mathbb{C}$ with center 0, where $h(\cdot,\lambda): \mathfrak{B}_0 \to \mathbb{C}^2$ is a holomorphic function,

$$h(x,\lambda) = \sum_{n=0}^{\infty} x^n h_n(\lambda), \quad h_0(\lambda) := \begin{pmatrix} \mu-\lambda \\ \kappa+\frac{1}{2} \end{pmatrix}. \tag{15}$$

Here $h_0(\lambda)$ is an eigenvector of B_0 for the eigenvalue $(\kappa/2)+\frac{1}{4}$, and the coefficients $h_n(\lambda)$, $n>1$, are uniquely determined by the recurrence relation

$$(B_0 - \alpha - n)h_n(\lambda) = (B_0 + B_1 - C + 1 - \alpha - n)h_{n-1}(\lambda) + C\, h_{n-2}(\lambda) \tag{16}$$

with $\alpha := (\kappa/2)+\frac{1}{4}$ and $h_{-1}(\lambda) := 0$. Since the matrices B_0 and B_1 depend holomorphically on λ, the coefficients $h_n: \mathbb{C} \to \mathbb{C}^2$ are holomorphic functions. By slightly modifying the proof of Theorem 5.3

in Wasow (1965), it can be shown that the series (15) converges uniformly in every compact subset of $\mathfrak{B}_0 \times \mathbb{C}$. Thus, by a theorem of Weierstrass, $h: \mathfrak{B}_0 \times \mathbb{C} \to \mathbb{C}^2$ is a holomorphic vector function in the variables (x, λ). Now, let

$$h\left(\frac{1}{2}, \lambda\right) =: \begin{pmatrix} f(\lambda) \\ g(\lambda) \end{pmatrix},$$

and we define the holomorphic function $\Delta: \mathbb{C} \to \mathbb{C}$ by

$$\Delta(\lambda) := f(\lambda)^2 - g(\lambda)^2, \quad \lambda \in \mathbb{C}. \tag{17}$$

The following lemma provides a connection between the eigenvalues of A and the zeros of Δ.

Lemma 1: For fixed $\kappa \in \left[\frac{1}{2}, \infty\right)$ and $(\mu, \nu) \in \mathbb{C}^2$, a point $\lambda \in \mathbb{C}$ is an eigenvalue of $A(\kappa; \mu, \nu)$ if and only if λ is a zero of the function Δ given by (17). This is equivalent to the statement that the differential equation (11) has a nontrivial solution of the form

$$y(x) = [x(1-x)]^{(\kappa/2)+1/4} \eta(x), \quad x \in \mathbb{C} \setminus \{0, 1\}, \tag{18}$$

where $\eta: \mathbb{C} \to \mathbb{C}^2$ is an entire vector function. As a consequence, if S is an eigenfunction of $A(\kappa; \mu, \nu)$ for some eigenvalue λ, then

$$|S(\theta)| \leqslant C \sin^{\kappa} \theta, \quad \theta \in (0, \pi), \tag{19}$$

with some constant $C > 0$.

Proof: Defining

$$K := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{20}$$

we have $K^{-1} = K$ and $KB_0K = B_1$, $KCK = -C$. Hence, y is a solution of the system (11) if and only if the function $Ky(1-x)$ satisfies (11). In particular, $y_1(x) := Ky_0(1-x)$ is a solution of (11) in the unit disk $\mathfrak{B}_1 \subset \mathbb{C}$ with center 1, and y_1 has the form

$$y_1(x, \lambda) = (1-x)^{(\kappa/2)+1/4} K h(1-x, \lambda), \quad x \in \mathfrak{B}_1.$$

Moreover, by the Levinson theorem, see Eastham (1989, Theorem 1.3.1), any solution of (11) which is linearly independent of y_0 in $(0,1)$ behaves asymptotically like $x^{-(\kappa/2)-1/4}[v_0 + o(1)]$ as $x \to 0$, where v_0 is an eigenvector of B_0 for the eigenvalue $-(\kappa/2) - \frac{1}{4}$. Similarly, any solution of (11) which is linearly independent of y_1 in $(0,1)$ has the asymptotic behavior $(x-1)^{-(\kappa/2)-1/4} \times [v_1 + o(1)]$ as $x \to 1$ with an eigenvector v_1 of B_1 for the eigenvalue $-(\kappa/2) - \frac{1}{4}$. Now, if λ is an eigenvalue of $A(\kappa; \mu, \nu)$, then the system (11) has a nontrivial solution y satisfying (13), and it follows that $y(x) = y_a(x, \lambda) c_a$ holds in $(0,1)$ with some constants $c_a \in \mathbb{C} \setminus \{0\}$, $a \in \{0, 1\}$. Thus, y_0 and y_1 are linearly dependent, and the Wronskian $W(x, \lambda) := \det(y_0(x, \lambda), y_1(x, \lambda))$ vanishes identically for all $x \in (0,1)$. In particular, $0 = W\left(\frac{1}{2}, \lambda\right) = 2^{-\kappa - 1/2} \Delta(\lambda)$. Conversely, if $\Delta(\lambda) = 0$, then $W\left(\frac{1}{2}, \lambda\right) = 0$, which implies that y_0 and y_1 are linearly dependent. Hence, $y_0(x) = y_1(x) c$ with some constant $c \in \mathbb{C} \setminus \{0\}$, and therefore y_0 is a solution of (11) satisfying the condition (13) on the interval $(0,1)$. Moreover, we immediately obtain that y_0 has the form (18) with a holomorphic vector function $\eta: \mathfrak{B}_0 \cup \mathfrak{B}_1 \to \mathbb{C}^2$, and since (11) is regular in $\mathbb{C} \setminus \{0, 1\}$, we can extend $\eta: \mathbb{C} \to \mathbb{C}^2$ to an entire function by the existence and uniqueness theorem. Finally, by means of the transformation (10), an eigenfunction S of $A(\kappa; \mu, \nu)$ has to be a constant multiple of

$$\sin^{\kappa}\theta \begin{pmatrix} \sin\frac{\theta}{2} & 0 \\ 0 & \cos\frac{\theta}{2} \end{pmatrix} \eta\left(\sin^2\frac{\theta}{2}\right), \quad \theta \in (0,\pi),$$

and this yields the estimate (19). □

Lemma 2: For fixed $\kappa \in \left[\frac{1}{2},\infty\right)$ *and* $j \in \mathbb{Z}\backslash\{0\}$*, the jth eigenvalue* $\lambda_j(\kappa;\mu,\nu)$ *of* $A(\kappa;\mu,\nu)$ *has a power series expansion of the form*

$$\lambda_j(\kappa;\mu,\nu) = \sum_{m,n=0}^{\infty} \lambda_{m,n}\mu^m\nu^n, \quad \lambda_{0,0} = \lambda_j(\kappa;0,0), \tag{21}$$

which is uniformly convergent in the polydisc $\mathfrak{C} := \{(\mu,\nu) \in \mathbb{C}^2 : |\mu|,|\nu| \leqslant \frac{1}{2}\}$*. Moreover, for all integers m and n, the following estimate holds:*

$$|\lambda_{m,n}| \leqslant (|\kappa| + |j|)2^{n+m}. \tag{22}$$

Proof: Since the coefficient matrices in (11) depend holomorphically on $(\lambda,\mu,\nu) \in \mathbb{C}^3$, we can modify Theorem 5.3 in Wasow (1965) appropriately in order to obtain that h in (14) and therefore $\Delta = \Delta(\lambda,\mu,\nu)$ as given by (17) are holomorphic functions on $\mathbb{C}^3$. By a similar reasoning as in the proof of Lemma 1, we can show that for fixed $(\mu,\nu) \in \mathbb{C}^2$ the eigenvalues of $A(\kappa;\mu,\nu)$ coincide with the zeros of the function $\lambda \mapsto \Delta(\lambda,\mu,\nu)$. In particular for the case $(\mu,\nu) \in \mathbb{R}^2$ these zeros are simple because $A(\kappa;\mu,\nu)$ has only simple eigenvalues. Hence, by solving the equation $\Delta(\lambda,\mu,\nu)=0$ and using the implicit function theorem, an eigenvalue $\lambda_j(\kappa;\mu,\nu)$ of the operator $A(\kappa;\mu,\nu)$ depends holomorphically on (μ,ν) in a complex neighborhood of $\mathbb{R}^2$. Furthermore, the estimate (8) implies that the set $\{\lambda \in \mathbb{C} : \min_{j\neq 0}|\lambda - \lambda_j(\kappa;0,0)| \geqslant \frac{1}{2}\}$ contains no eigenvalues of $A(\kappa;\mu,\nu)$ for all $(\mu,\nu) \in \mathfrak{C}$. Thus there exists a holomorphic solution $\lambda : \mathfrak{C} \to \mathbb{C}$ of the equation $\Delta(\lambda,\mu,\nu)=0$, which is uniquely determined by $\lambda(0,0) = \lambda_j(\kappa;0,0)$. Consequently, $\lambda_j(\kappa;\mu,\nu)$ is holomorphic in $\mathfrak{C}$, and therefore it has a power series expansion in $\mathfrak{C}$ of the form (21). In addition, by Cauchy's formula,

$$\lambda_{m,n} = -\frac{1}{4\pi^2}\oint_{\partial\mathfrak{C}} \frac{\lambda_j(\kappa;\mu,\nu)}{\mu^{m+1}\nu^{n+1}} \mathrm{d}\mu\, \mathrm{d}\nu,$$

and applying (8) and (7), it follows that

$$|\lambda_j(\kappa;\mu,\nu)| \leqslant |\lambda_j(\kappa;0,0)| + \max\{|\mu|,|\nu|\} \leqslant |\kappa| + |j|,$$

which gives the estimate (22). □

According to Lemma 1, for fixed parameters $(\mu,\nu) \in \mathbb{C}^2$ the eigenvalues of $A(\kappa;\mu,\nu)$ are exactly the zeros of the function $\Delta(\lambda)$ given by (17). In principle, this result can be used for numerical computation of the eigenvalues. However, in order to calculate $\Delta(\lambda)$ at some point $\lambda \in \mathbb{C}$, we first have to determine the coefficients $h_n(\lambda)$ with the help of the recurrence relation (16) and subsequently we need to evaluate $h(x,\lambda)$ at $x=\frac{1}{2}$ by means of the power series expansion (15). Unfortunately, this method requires the calculation of two consecutive limits, making things rather complicated. In the remaining part of this section we show that there is yet another function Θ which encodes the eigenvalues of $A(\kappa;\mu,\nu)$. The main advantage of Θ is, that it can be obtained by only one limit process.

By setting $y(x) := x^{\alpha}(1-x)^{1-\alpha}\hat{y}(x)$ with $\alpha := (\kappa/2) + \frac{1}{4}$, the system (11) becomes

$$\hat{y}'(x) = \left[\frac{1}{x}\hat{B}_0 + \frac{1}{x-1}\hat{B}_1 + C\right]\hat{y}(x) \tag{23}$$

with the coefficient matrices

$$\hat{B}_0 := \begin{pmatrix} -\kappa - \frac{1}{2} & \mu - \lambda \\ 0 & 0 \end{pmatrix}, \quad \hat{B}_1 := \begin{pmatrix} \kappa - \frac{1}{2} & 0 \\ \mu - \lambda & -1 \end{pmatrix}, \quad C = \begin{pmatrix} -2\nu & -2\mu \\ 2\mu & 2\nu \end{pmatrix}.$$

Now, there exists a holomorphic solution of (23) in $\mathfrak{B}_1$ given by

$$\hat{y}(x,\lambda) = \sum_{n=0}^{\infty} x^n d_n(\lambda), \quad d_0(\lambda) := \begin{pmatrix} \mu - \lambda \\ \kappa + \frac{1}{2} \end{pmatrix}, \tag{24}$$

where $d_0(\lambda)$ is an eigenvector of $\hat{B}_0$ for the eigenvalue 0. In addition, the coefficients $d_n(\lambda)$, $n > 1$, are uniquely determined by the recurrence relation

$$d_n(\lambda) = (\hat{B}_0 - n)^{-1}[(E - n)d_{n-1}(\lambda) + Cd_{n-2}(\lambda)]$$

with

$$E := \begin{pmatrix} 2\nu & 3\mu - \lambda \\ -\mu - \lambda & -2\nu \end{pmatrix}, \quad d_{-1}(\lambda) := 0.$$

Finally, we denote by $\Theta_n(\lambda)$ the second component of $d_n(\lambda)$.

Lemma 3: Let $\kappa \in \left[\frac{1}{2}, \infty\right)$ *and* $(\mu, \nu) \in \mathbb{C}^2$ *be fixed. Then, for each* $\lambda \in C$, *the limit*

$$\Theta(\lambda) := \lim_{n \to \infty} \Theta_n(\lambda) \tag{25}$$

exists, and $\Theta : \mathbb{C} \to \mathbb{C}$ *is a holomorphic function. Moreover, a point* $\lambda \in \mathbb{C}$ *is an eigenvalue of* $A(\kappa; \mu, \nu)$ *if and only if* $\Theta(\lambda) = 0$.

Proof: For fixed $\lambda \in \mathbb{C}$, the differential equation (23) has a regular singular point at $x = 1$ with characteristic values -1 and $\kappa - \frac{1}{2}$. First, let us assume that their difference $\kappa + \frac{1}{2}$ is not an integer. In this case the system (23) has a fundamental system of solutions in a complex neighborhood of $x = 1$, which can be written as

$$\hat{y}_1(x,\lambda) = (1-x)^{-1} \sum_{n=0}^{\infty} (1-x)^n d_n^1(\lambda), \quad \hat{y}_2(x,\lambda) = (1-x)^{\kappa - 1/2} \sum_{n=0}^{\infty} (1-x)^n d_n^2(\lambda), \tag{26}$$

where

$$d_0^1(\lambda) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} =: e_2, \quad d_0^2(\lambda) = \begin{pmatrix} \kappa + \frac{1}{2} \\ \mu - \lambda \end{pmatrix}$$

are eigenvectors of $\hat{B}_1$ for the eigenvalues -1 and $\kappa - \frac{1}{2}$, respectively. Now, $\hat{y}$ can be written as a linear combination

$$\hat{y}(x,\lambda) = \gamma_1(\lambda)\hat{y}_1(x,\lambda) + \gamma_2(\lambda)\hat{y}_2(x,\lambda)$$

with connection coefficients $\gamma_1(\lambda), \gamma_2(\lambda) \in \mathbb{C}$. Applying Corollary 1.6 in Schäfke and Schmidt (1980) to the system (23) gives

$$\lim_{n \to \infty} d_n(\lambda) = \gamma_1(\lambda) e_2, \tag{27}$$

and therefore the limit (25) exists. Furthermore, λ is an eigenvalue of $A(\kappa; \mu, \nu)$ if and only if $\gamma_1(\lambda) = 0$, i.e., if and only if $\Theta(\lambda)$ becomes zero. Finally, it can be shown that the functions d_n converge uniformly in every compact subset of $\mathbb{C}$, and Weierstrass' theorem implies that Θ is an entire function.

Now, suppose that $k := \kappa + \frac{1}{2}$ is a positive integer. In this case, a fundamental system of the form (26) may not exist. Nevertheless, it can be proved (see Lemma 6 in Sec. VI) that the system (23) has a fundamental matrix,

$$\hat{Y}(x,\lambda) = G(\lambda)\sum_{n=0}^{\infty} H_n(\lambda)(1-x)^n(1-x)^D(1-x)^{J(\lambda)},$$

in a complex neighborhood of $x=1$, where $D:=\mathrm{diag}(-1,k-1)$, $H_0(\lambda)=I$, and

$$G(\lambda) = \begin{pmatrix} 0 & \kappa+\frac{1}{2} \\ 1 & \mu-\lambda \end{pmatrix}, \quad J(\lambda) = \begin{pmatrix} 0 & 0 \\ q(\lambda) & 0 \end{pmatrix}$$

with some $q(\lambda)\in\mathbb{C}$. In particular, we can write $\hat{Y}$ in the form

$$\hat{Y}(x,\lambda) = \hat{H}(x,\lambda)(1-x)^{\tilde{J}(\lambda)}, \quad \hat{H}(x,\lambda) = \sum_{n=0}^{\infty}(1-x)^n D_n(\lambda),$$

where

$$D_0(\lambda) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \tilde{J}(\lambda) = \begin{pmatrix} -1 & 0 \\ q(\lambda) & -1 \end{pmatrix}.$$

Since $\hat{y}$ solves the system (23), there exists a vector $c(\lambda)\in\mathbb{C}^2$ such that $\hat{y}(x,\lambda)=\hat{Y}(x,\lambda)c(\lambda)$, and Theorem 1.1 in Schäfke (1980) implies

$$d_n(\lambda) = D_0(\lambda)\frac{1}{\Gamma}(-\tilde{J}(\lambda))\Gamma(n+1)\frac{1}{\Gamma}(n-\tilde{J}(\lambda))c(\lambda) + O(n^{\delta-1}) \tag{28}$$

for arbitrary $\delta>0$. For the definition and discussion of the reciprocal gamma function for matrices we refer to the Appendix in Schäfke (1980). Particularly, for the Jordan-type matrices $-\tilde{J}(\lambda)$ and $n-\tilde{J}(\lambda)$ we obtain

$$\frac{1}{\Gamma}(-\tilde{J}(\lambda)) = \begin{pmatrix} 1 & 0 \\ * & 1 \end{pmatrix}, \quad \frac{1}{\Gamma}(n-\tilde{J}(\lambda)) = \begin{pmatrix} \dfrac{1}{\Gamma(n+1)} & 0 \\ * & \dfrac{1}{\Gamma(n+1)} \end{pmatrix}.$$

Now, if $\gamma_1(\lambda)$ denotes the first component of $c(\lambda)$, then (28) implies (27). Since λ is an eigenvalue of $A(\kappa;\mu,\nu)$ if and only if $\gamma_1(\lambda)=0$, the proof of Lemma 3 is complete. □

III. A PARTIAL DIFFERENTIAL EQUATION FOR THE EIGENVALUES

Theorem 1: *For fixed $\kappa\in[\frac{1}{2},\infty)$ and $j\in\mathbb{Z}\backslash\{0\}$, the jth eigenvalue $\lambda=\lambda_j(\kappa;\mu,\nu)$ of A is an analytical function in $(\mu,\nu)\in\mathbb{R}^2$ satisfying the first order quasilinear partial differential equation*

$$(\mu-2\nu\lambda)\frac{\partial\lambda}{\partial\mu} + (\nu-2\mu\lambda)\frac{\partial\lambda}{\partial\nu} + 2\kappa\mu + 2\mu\nu = 0, \tag{29}$$

where $\lambda_j(\kappa;0,0)$ is given by (7).

Proof: Let

$$S(\theta) =: \begin{pmatrix} S_1(\theta) \\ S_2(\theta) \end{pmatrix}, \quad \theta\in(0,\pi),$$

be that eigenfunction of $A(\kappa;\mu,\nu)$ for the eigenvalue $\lambda=\lambda_j(\kappa;\mu,\nu)$ which is normalized by the condition $(S,S)=1$. Introducing the functions

$$U(\theta) := S_1(\theta)^2 + S_2(\theta)^2, \quad V(\theta) := S_2(\theta)^2 - S_1(\theta)^2, \quad W(\theta) := 2S_1(\theta)S_2(\theta),$$

a straightforward calculation shows that U, V, and W are solutions of the system of differential equations

$$U'(\theta) = 2\left(\nu \sin\theta + \frac{\kappa}{\sin\theta}\right)V(\theta) + 2\mu\cos\theta W(\theta), \tag{30}$$

$$V'(\theta) = 2\left(\nu \sin\theta + \frac{\kappa}{\sin\theta}\right)U(\theta) + 2\lambda W(\theta), \tag{31}$$

$$W'(\theta) = 2\mu\cos\theta U(\theta) - 2\lambda V(\theta). \tag{32}$$

Now, from analytic perturbation theory, compare Kato (1966, Chap. VII, §3, Sec. 4), it follows that

$$\frac{\partial\lambda}{\partial\mu} = \left(\frac{\partial A}{\partial\mu}S,S\right) = \int_0^\pi S(\theta)^*\begin{pmatrix}-\cos\theta & 0\\ 0 & \cos\theta\end{pmatrix}S(\theta)\mathrm{d}\theta = \int_0^\pi \cos\theta V(\theta)\mathrm{d}\theta, \tag{33}$$

$$\frac{\partial\lambda}{\partial\nu} = \left(\frac{\partial A}{\partial\nu}S,S\right) = \int_0^\pi S(\theta)^*\begin{pmatrix}0 & -\sin\theta\\ -\sin\theta & 0\end{pmatrix}S(\theta)\mathrm{d}\theta = -\int_0^\pi \sin\theta W(\theta)\mathrm{d}\theta. \tag{34}$$

In addition, from (19) we obtain the estimates

$$|U(\theta)|,|V(\theta)|,|W(\theta)| \leqslant C\sin^{2\kappa}\theta$$

with some constant $C>0$. Since κ is positive, U, V, and W vanish at $\theta=0$ and $\theta=\pi$. If we integrate (33) by parts and replace $V'(\theta)$ with the right-hand side (rhs) of (31), then we get

$$\begin{aligned}\frac{\partial\lambda}{\partial\mu} &= -\int_0^\pi \sin\theta V'(\theta)\mathrm{d}\theta = -\int_0^\pi (2\nu\sin^2\theta + 2\kappa)U(\theta) + 2\lambda\sin\theta W(\theta)\mathrm{d}\theta\\ &= -(2\nu+2\kappa)\int_0^\pi U(\theta)\mathrm{d}\theta - 2\lambda\int_0^\pi \sin\theta W(\theta)\mathrm{d}\theta + 2\nu\int_0^\pi \cos^2\theta U(\theta)\mathrm{d}\theta.\end{aligned}$$

Taking into account that

$$\int_0^\pi U(\theta)\mathrm{d}\theta = (S,S) = 1, \quad \int_0^\pi \sin\theta W(\theta)\mathrm{d}\theta = -\frac{\partial\lambda}{\partial\nu},$$

we have

$$\mu\frac{\partial\lambda}{\partial\mu} = -\mu(2\nu+2\kappa) + 2\mu\lambda\frac{\partial\lambda}{\partial\nu} + 2\mu\nu\int_0^\pi \cos^2\theta U(\theta)\mathrm{d}\theta. \tag{35}$$

Moreover, Eq. (32) implies

$$2\mu\cos^2\theta U(\theta) = \cos\theta W'(\theta) + 2\lambda\cos\theta V(\theta),$$

and integration by parts gives

$$2\mu\nu\int_0^\pi \cos^2\theta U(\theta)\mathrm{d}\theta = \nu\int_0^\pi \cos\theta W'(\theta)\mathrm{d}\theta + 2\nu\lambda\int_0^\pi \cos\theta V(\theta)\mathrm{d}\theta$$

$$= \nu\int_0^\pi \sin\theta W(\theta)\mathrm{d}\theta + 2\nu\lambda\int_0^\pi \cos\theta V(\theta)\mathrm{d}\theta = -\nu\frac{\partial\lambda}{\partial\nu} + 2\nu\lambda\frac{\partial\lambda}{\partial\mu}. \quad (36)$$

Replacing the last term on the rhs of (35) with (36), we obtain exactly the partial differential equation (29). □

The PDE (29) can be used in order to derive a power series expansion for λ_j with respect to μ and ν. For this purpose we introduce the new coordinates,

$$\alpha := \nu - \mu, \quad \beta := \nu + \mu,$$

compare Suffern *et al.* (1983). Then $\hat{\lambda}(\alpha,\beta) := \lambda_j(\kappa;(\beta-\alpha)/2,(\beta+\alpha)/2)$ is a solution of the transformed partial differential equation

$$\alpha(1+2\hat{\lambda})\frac{\partial\hat{\lambda}}{\partial\alpha} + \beta(1-2\hat{\lambda})\frac{\partial\hat{\lambda}}{\partial\beta} = \kappa(\alpha-\beta) + \frac{1}{2}(\alpha^2-\beta^2), \quad (37)$$

where $\hat{\lambda}(0,0)=\lambda_j(\kappa;0,0)$ is given by (7). As $\hat{\lambda}$ depends analytically on (α,β), there exists a series expansion for $\hat{\lambda}$ of the form

$$\hat{\lambda}(\alpha,\beta) = \sum_{m,n=0}^{\infty} c_{m,n}\alpha^m\beta^n \quad (38)$$

(for clarity, the indices κ and j in the coefficients $c_{m,n}$ and in the function $\hat{\lambda}$ have been omitted). Furthermore, (37) is equivalent to

$$\alpha\left(\frac{\partial\hat{\lambda}}{\partial\alpha} + \frac{\partial\hat{\lambda}^2}{\partial\alpha}\right) + \beta\left(\frac{\partial\hat{\lambda}}{\partial\beta} - \frac{\partial\hat{\lambda}^2}{\partial\beta}\right) = \kappa(\alpha-\beta) + \frac{1}{2}(\alpha^2-\beta^2), \quad (39)$$

and since

$$\hat{\lambda}(\alpha,\beta)^2 = \sum_{m,n=0}^{\infty}\left(\sum_{r=0}^{m}\sum_{s=0}^{n} c_{r,s}c_{m-r,n-s}\right)\alpha^m\beta^n,$$

we obtain the identity

$$\sum_{m,n=0}^{\infty}\left((m+n)c_{m,n} + (m-n)\sum_{r=0}^{m}\sum_{s=0}^{n} c_{r,s}c_{m-r,n-s}\right)\alpha^m\beta^n = \kappa(\alpha-\beta) + \frac{1}{2}(\alpha^2-\beta^2).$$

Comparing the terms of equal order in α and β, it follows that

$$c_{0,0} = \lambda_j(\kappa;0,0) =: c_0, \quad c_{1,0} = \frac{\kappa}{2c_0+1}, \quad c_{0,1} = \frac{\kappa}{2c_0-1},$$

$$c_{2,0} = \frac{(2c_0+1)^2-4\kappa^2}{4(2c_0+1)^3}, \quad c_{1,1} = 0, \quad c_{0,2} = \frac{(2c_0-1)^2-4\kappa^2}{4(2c_0-1)^3},$$

and for $m+n>2$ the coefficients $c_{m,n}$ satisfy

$$((m+n)+2c_0(m-n))c_{m,n} = (n-m)\sum_{(r,s)\in[\![m,n]\!]} c_{r,s}c_{m-r,n-s}, \tag{40}$$

where $[\![m,n]\!]$ denotes the set of all pairs $(r,s)\in\mathbb{Z}^2$ with $0\leqslant r\leqslant m$, $0\leqslant s\leqslant n$ and $0<r+s<m+n$. In particular, if $m=n>0$, then we get $2n\ c_{n,n}=0$, which implies

$$c_{n,n}=0 \quad \text{for all } n>0. \tag{41}$$

Moreover, if κ is not a rational number, i.e., $\kappa\in\left[\frac{1}{2},\infty\right)\setminus\mathbb{Q}$, then the initial value c_0 is not a rational number, and we have $(m+n)+2c_0(m-n)\neq 0$ for all $(m,n)\in\mathbb{Z}^2$ with $m+n>2$. In this case (40) gives a recurrence formula for all coefficients of the power series expansion (38).

Now, suppose that $\kappa\in\left[\frac{1}{2},\infty\right)\cap\mathbb{Q}$. Then c_0 is a rational number with $|c_0|\geqslant 1$, and we get $(2c_0-1)/(2c_0+1)=p/q$ with some coprime integers p and q. Now, the prefactor on the left-hand side (lhs) of (40) becomes zero if and only if $m=\ell p$, $n=\ell q$ with some positive integer ℓ, and thus the coefficients $c_{\ell p,\ell q}$ are not determined by (40). However, we can by-pass this problem if we regard κ as an additional parameter in our eigenvalue problem. Since the coefficient matrix of (11) depends holomorphically on $\kappa\in\mathbb{C}^+:=\{z\in\mathbb{C}:\mathrm{Re}\ z>0\}$ and $(\lambda,\mu,\nu)\in\mathbb{C}^3$, we obtain in a similar way as described in Sec. I that h in (14) and therefore $\Delta=\Delta(\kappa;\lambda;\mu,\nu)$ given by (17) is a holomorphic function on $\mathbb{C}^+\times\mathbb{C}^3$. Moreover, in the same way as in the proof of Lemma 1, we can show that for fixed $\kappa\in\left[\frac{1}{2},\infty\right)$ and $(\mu,\nu)\in\mathbb{C}^2$ the eigenvalues of $A(\kappa;\mu,\nu)$ coincide with the zeros of the function $\lambda\mapsto\Delta(\kappa;\lambda;\mu,\nu)$. In the case $(\kappa,\mu,\nu)\in\left[\frac{1}{2},\infty\right)\times\mathbb{R}^2$ these zeros are simple, since $A(\kappa;\mu,\nu)$ has only simple eigenvalues. Hence, by solving the equation $\Delta(\kappa;\lambda;\mu,\nu)=0$, we find that an eigenvalue $\lambda_j(\kappa;\mu,\nu)$ is a holomorphic function in a complex neighborhood of $\left[\frac{1}{2},\infty\right)\times\mathbb{R}^2$. In particular, $\hat{\lambda}$ depends holomorphically on $(\kappa;\alpha,\beta)$, and for a given $\kappa\in\left[\frac{1}{2},\infty\right)$, there exists a power series expansion of the form

$$\hat{\lambda}(\kappa+\varepsilon;\alpha,\beta)=\sum_{l,m,n=0}^{\infty} c_{m,n}^{(l)}\varepsilon^l\alpha^m\beta^n$$

in a neighborhood of $(\kappa,0,0)$. In the following we derive a recurrence relation for the coefficients $c_{m,n}^{(l)}$. Since

$$\hat{\lambda}(\kappa+\varepsilon;\alpha,\beta)^2=\sum_{l,m,n=0}^{\infty}\left(\sum_{t=0}^{l}\sum_{r=0}^{m}\sum_{s=0}^{n} c_{r,s}^{(t)}c_{m-r,n-s}^{(l-t)}\right)\varepsilon^l\alpha^m\beta^n,$$

from (39) it follows that

$$\sum_{l,m,n=0}^{\infty}\left((m+n)c_{m,n}^{(l)}+(m-n)\sum_{t=0}^{l}\sum_{r=0}^{m}\sum_{s=0}^{n} c_{r,s}^{(t)}c_{m-r,n-s}^{(l-t)}\right)\varepsilon^l\alpha^m\beta^n=\kappa(\alpha-\beta)+\varepsilon(\alpha-\beta)+\frac{1}{2}(\alpha^2-\beta^2). \tag{42}$$

Moreover, (7) implies that

$$c_{0,0}^{(l)}=\frac{1}{l!}\frac{\partial^l\lambda}{\partial\kappa^l}(\kappa;0,0)=\begin{cases}\mathrm{sgn}(j)(\kappa-\frac{1}{2}+|j|), & \text{if } l=0,\\ \mathrm{sgn}(j), & \text{if } l=1,\\ 0, & \text{if } l>1.\end{cases}$$

Comparing the terms of equal order in (42), we obtain

$$c_{0,0}^{(0)}=\lambda_j(\kappa;0,0)=:c_0,\quad c_{1,0}^{(0)}=\frac{\kappa}{2c_0+1},\quad c_{0,1}^{(0)}=\frac{\kappa}{2c_0-1},$$

$$c_{2,0}^{(0)} = \frac{(2c_0+1)^2 - 4\,\kappa^2}{4(2c_0+1)^3}, \quad c_{1,1}^{(0)} = 0, \quad c_{0,2}^{(0)} = \frac{(2c_0-1)^2 - 4\,\kappa^2}{4(2c_0-1)^3},$$

$$c_{1,0}^{(1)} = \frac{2c_0+1-2\,\mathrm{sgn}(j)\kappa}{(2c_0+1)^2}, \quad c_{0,1}^{(1)} = \frac{2c_0-1-2\,\mathrm{sgn}(j)\kappa}{(2c_0-1)^2},$$

while the remaining coefficients are determined by the identity

$$((m+n)+2c_0(m-n))c_{m,n}^{(l)} + (m-n)\sum_{(t,r,s)\in[\![l,m,n]\!]} c_{r,s}^{(t)} c_{m-r,n-s}^{(l-t)} = 0, \quad l+m+n>2. \tag{43}$$

Here $[\![l,m,n]\!]$ denotes the set of all triples $(t,r,s)\in\mathbb{Z}^3$ with $0\leqslant t\leqslant l$, $0\leqslant r\leqslant m$, $0\leqslant s\leqslant n$, and $0<t+r+s<l+m+n$. In the case $(m+n)+2c_0(m-n)=0$, the prefactor of $c_{m,n}^{(l)}$ in (43) vanishes, and since $m-n\neq 0$, we get for $l>0$

$$0 = \sum_{(t,r,s)\in[\![l,m,n]\!]} c_{r,s}^{(t)} c_{m-r,n-s}^{(l-t)} = 2c_{0,0}^{(1)} c_{m,n}^{(l-1)} + \sum_{(t,r,s)\in[\![l,m,n]\!]^*} c_{r,s}^{(t)} c_{m-r,n-s}^{(l-t)}, \tag{44}$$

where $[\![l,m,n]\!]^* := [\![l,m,n]\!]\backslash\{(1,0,0),(l-1,m,n)\}$. Now, for all coefficients $c_{m,n}^{(l)}$ with $l+m+n>2$, (43) implies

$$c_{m,n}^{(l)} = \frac{n-m}{(m+n)+2c_0(m-n)} \sum_{(t,r,s)\in[\![l,m,n]\!]} c_{r,s}^{(t)} c_{m-r,n-s}^{(l-t)} \quad \text{if } (m+n)+2c_0(m-n)\neq 0,$$

whereas (44) and $c_{0,0}^{(1)} = \mathrm{sgn}(j)$ yield

$$c_{m,n}^{(l-1)} = -\frac{\mathrm{sgn}(j)}{2} \sum_{(t,r,s)\in[\![l,m,n]\!]^*} c_{r,s}^{(t)} c_{m-r,n-s}^{(l-t)} \quad \text{if } (m+n)+2c_0(m-n)=0 \text{ and } l>1.$$

These recurrence relations can be used to determine all the coefficients $c_{m,n} = c_{m,n}^{(0)}$ of the power series expansion (38) in the case that κ is a rational number.

Remark 1: A series expansion for the eigenvalues $\hat{\lambda}$ with respect to (α,β) has been given by Suffern et al. (1983, Sec. 8), however, only the coefficients $c_{m,n}$ with $m+n\leqslant 5$ have been determined. Furthermore, Kalnins and Miller (1992) studied a series expansion $\lambda = \Sigma_{n=0}^{\infty} \lambda_n a^n$ for the eigenvalues in terms of the Kerr parameter a, but also in this paper only a finite number of coefficients $\lambda_0,\ldots,\lambda_3$ have been explicitly computed. A general recurrence relation for the coefficients of (38) could not be found in the literature. Moreover, the problem of dividing by numbers which may be zero has not been noticed in Suffern et al. (1983) and Kalnins and Miller (1992). Finally, it should be noted that some of the diagonal entries $c_{n,n}$ for $n>0$ in Suffern et al. (1983, Table I) are not equal to zero, in contrast to our result (41).

IV. SOLUTION OF THE PDE BY THE METHOD OF CHARACTERISTICS

In this section the PDE (29) for real parameters $(\mu,\nu)\in\mathbb{R}^2$ and fixed $\kappa\in\left[\frac{1}{2},\infty\right)$ is studied by the method of characteristics. In particular, we obtain an exact formula for the eigenvalues in the case $|\mu|=|\nu|$, and for $|\mu|\neq|\nu|$, it turns out that the characteristic equations can be reduced to the third Painlevé equation.

Theorem 2: *Let $\kappa\in\left[\frac{1}{2},\infty\right)$, $j\in\mathbb{Z}\backslash\{0\}$ and $\tau\in\{-1,+1\}$ be fixed. Then*

$$\lambda_j(\kappa;\mu,\tau\mu) = \frac{\tau}{2} + \mathrm{sgn}(j)\sqrt{\left(\lambda_j(\kappa;0,0)-\frac{\tau}{2}\right)^2 + 2\tau\kappa\mu + \mu^2}, \tag{45}$$

where $\lambda_j(\kappa;0,0) = \mathrm{sgn}(j)\left(\kappa-\frac{1}{2}+|j|\right)$. In particular, if $j=\tau$, then

$$\lambda_j(\kappa;\mu,\tau\mu) = \tau\left(\kappa+\tfrac{1}{2}\right)+\mu.$$

Proof: According to Theorem 1, the function $\lambda(\mu,\nu) := \lambda_j(\kappa;\mu,\nu)$ solves the partial differential equation (29). Defining $w(\mu) := \lambda(\mu,\tau\mu)$, $\mu \in \mathbb{R}$, for some fixed $\tau \in \{-1,+1\}$, we obtain

$$w'(\mu) = \frac{\partial \lambda}{\partial \mu}(\mu,\tau\mu) + \tau \frac{\partial \lambda}{\partial \nu}(\mu,\tau\mu),$$

and with the help of (29) it can be shown that

$$\mu w'(\mu) - 2\tau\mu w(\mu) w'(\mu) = -2\kappa\mu - 2\tau\mu^2.$$

Dividing the above differential equation by $-\tau\mu$ and integrating gives

$$\left(w(\mu) - \frac{\tau}{2}\right)^2 = C + 2\tau\kappa\mu + \mu^2, \quad \mu \in \mathbb{R}, \tag{46}$$

where the constant of integration C is uniquely determined by

$$C = \left(w(0) - \frac{\tau}{2}\right)^2 = \left(\lambda_j(\kappa;0,0) - \frac{\tau}{2}\right)^2.$$

Now, from (46) it follows that

$$w(\mu) = \frac{\tau}{2} + \varepsilon \sqrt{\left(\lambda_j(\kappa;0,0) - \frac{\tau}{2}\right)^2 + 2\tau\kappa\mu + \mu^2} \tag{47}$$

with some $\varepsilon \in \{-1,+1\}$ and the square root assumed to be non-negative. We have to take the sign of ε such that the lhs of (47) is analytic and coincides with $\lambda_j(\kappa;0,0)$ at the point $\mu=0$. If $j=\tau$, then $\lambda_j(\kappa;0,0) = \tau\left(\kappa+\frac{1}{2}\right)$, and (47) implies $w(\mu) = (\tau/2) + \varepsilon(\tau\kappa+\mu)$. Inserting $\mu=0$, it follows that $\varepsilon=\tau$, i.e., $w(\mu) = \tau\left(\kappa+\frac{1}{2}\right)+\mu$. In the case $j \neq \tau$ we have $|\lambda_j(\kappa;0,0) - (\tau/2)| \geqslant \kappa+1$ and thus the radicand in (47) is positive for all $\mu \in \mathbb{R}$. Moreover, by means of

$$\lambda_j(\kappa;0,0) = w(0) = \frac{\tau}{2} + \varepsilon \sqrt{\left(\lambda_j(\kappa;0,0) - \frac{\tau}{2}\right)^2} = \frac{\tau}{2} + \varepsilon \left|\lambda_j(\kappa;0,0) - \frac{\tau}{2}\right|$$

and (7), we get $\varepsilon = \operatorname{sgn}(\lambda_j(\kappa;0,0) - (\tau/2)) = \operatorname{sgn}(j)$, which completes the proof. □

Remark 2: For a given half-integer κ and $\mu=\nu$, this result has been shown by Suffern, Fackerell, and Cosgrove using a power series expansion for the eigenfunctions of (1) and (2) in terms of hypergeometric functions, see Suffern et al. (1983, Secs. 3–5). Here, we obtained the formula for $\lambda_j(\kappa;\mu,\pm\mu)$ as an immediate consequence of the partial differential equation (29). Moreover, it should be noted that the formula (54) in Chakrabarti (1984) is not correct.

Now, let us consider the case $|\mu| \neq |\nu|$. To this purpose, we introduce new coordinates $(t,v) \in (0,\infty) \times (\mathbb{R}\setminus\{0\})$ by

$$\mu(t,v) = \frac{t}{2}\left(v + \frac{\sigma}{v}\right), \quad \nu(t,v) = \frac{t}{2}\left(v - \frac{\sigma}{v}\right) \tag{48}$$

with some fixed $\sigma \in \{-1,+1\}$ [note that $\sigma = \pm 1$ corresponds to the cases $|\mu| > |\nu|$ and $|\mu| < |\nu|$, respectively; moreover, this transformation maps $v=\text{const}$ onto lines in the (μ,ν)-plane starting at the origin, while the curves $t=\text{const}$ are mapped onto hyperboles]. By setting $w(t,v) = \lambda(\mu,\nu)$, we have

$$\frac{\partial w}{\partial t} = \frac{1}{2}\left(v + \frac{\sigma}{v}\right)\frac{\partial \lambda}{\partial \mu} + \frac{1}{2}\left(v - \frac{\sigma}{v}\right)\frac{\partial \lambda}{\partial \nu} = \frac{1}{t}\left(\mu\frac{\partial \lambda}{\partial \mu} + \nu\frac{\partial \lambda}{\partial \nu}\right),$$

$$\frac{\partial w}{\partial v} = \frac{t}{2}\left(1 - \frac{\sigma}{v^2}\right)\frac{\partial \lambda}{\partial \mu} + \frac{t}{2}\left(1 + \frac{\sigma}{v^2}\right)\frac{\partial \lambda}{\partial \nu} = \frac{1}{v}\left(\nu\frac{\partial \lambda}{\partial \mu} + \mu\frac{\partial \lambda}{\partial \nu}\right),$$

and (29) becomes

$$\frac{\partial w}{\partial t} - \frac{2vw}{t}\frac{\partial w}{\partial v} + \kappa\left(v + \frac{\sigma}{v}\right) + \frac{t}{2}\left(v^2 - \frac{1}{v^2}\right) = 0. \tag{49}$$

The characteristic equations of this PDE are given by

$$v'(t) = -\frac{2v(t)w(t)}{t}, \tag{50}$$

$$w'(t) = -\kappa\left(v(t) + \frac{\sigma}{v(t)}\right) - \frac{t}{2}\left(v(t)^2 - \frac{1}{v(t)^2}\right). \tag{51}$$

From (50) we obtain that $w(t) = -tv'(t)/2v(t)$, and (51) implies

$$\frac{v'(t)}{2v(t)} + \frac{tv''(t)}{2v(t)} - \frac{tv'(t)^2}{2v(t)^2} = \kappa\left(v(t) + \frac{\sigma}{v(t)}\right) + \frac{t}{2}\left(v(t)^2 - \frac{1}{v(t)^2}\right).$$

Multiplying the above differential equation with $2v(t)^2$, we get the following third Painlevé equation:

$$tvv'' - t(v')^2 + vv' - 2\kappa(v^2 + \sigma)v - t(v^4 - 1) = 0, \tag{52}$$

with parameters $\alpha = \sigma\beta = 2\kappa$ and $\gamma = -\delta = 1$ [see Milne *et al.* (1997) or Mansfield and Webster (1998), for example]. For further details on the Painlevé III we refer to, e.g., McCoy *et al.* (1977), Widom (2000), and Iwasaki *et al.* (1991).

In general, Painlevé III is not solvable in terms of elementary functions, and therefore we cannot expect a closed expression for the eigenvalues of $A(\kappa;\mu,\nu)$ in the case $|\mu| \neq |\nu|$. On the other hand, for particular values of κ there exist so-called special integrals of polynomial type for this equation, i.e., polynomials Q in t, v, and v' with the property that every solution of the differential equation $Q(t,v,v') = 0$ satisfies (52). As it will be shown below, such special integrals are related to algebraic solutions of the PDE (29), i.e., solutions, which are zeros of a polynomial in λ with rational coefficients in μ and ν. Moreover, taking into account that the eigenvalues $\lambda_j(\kappa;\mu,\tau\mu)$, $\tau \in \{-1,1\}$, of $A(\kappa;\mu,\tau\mu)$ satisfy the quadratic equation

$$\left(\lambda - \frac{\tau}{2}\right)^2 = C + 2\tau\kappa\mu + \mu^2 \quad \text{with} \quad C := \left(\lambda_j(\kappa;0,0) - \frac{\tau}{2}\right)^2,$$

the question arises if such an algebraic expression for the eigenvalues of $A(\kappa;\mu,\nu)$ exists in the case $|\mu| \neq |\nu|$. A first step towards the answer of this problem is given by the next lemma.

Lemma 4: Suppose that there exists a polynomial

$$P(\lambda;\mu,\nu) = \sum_{n=0}^{N} P_n(\mu,\nu)\lambda^n, \quad P_N \equiv 1,$$

of degree $N > 0$ *in* λ *with rational coefficients* P_n *in* μ *and* ν *such that the zeros* $z_j(\mu,\nu)$, $j = 1,\ldots,N$, *of* $P(\cdot;\mu,\nu)$ *are simple, and that the functions* $\lambda = z_j$ *are solutions of the partial differential equation* (29). *Then* κ *is a half-integer. Moreover, if* $N = 1$ *or* $N = 2$, *then* $\kappa = \frac{1}{2}$ *and* $P(\lambda;\mu,\nu) = (\lambda + \mu)^N$.

Proof: Let $Q(t,v,v') = \Sigma_{n=0}^{N} Q_n(t,v)(v')^n$ be the polynomial in v' with coefficients

$$Q_n(t,v) := \left(-\frac{2v}{t}\right)^{N-n} P_n(\mu(t,v),\nu(t,v)), \quad n=0,\ldots,N,$$

where $\mu(t,v)$ and $\nu(t,v)$ are given by (48). Note that the Q_n are again rational functions in t and v. Moreover, let $v:\mathfrak{D}\to\mathbb{R}\setminus\{0\}$ be any solution of the first order ODE $Q(t,v,v')=0$ on some interval $\mathfrak{D}\subset\mathbb{R}\setminus\{0\}$. For the function

$$w(t) = -\frac{tv'(t)}{2v(t)}, \quad t\in\mathfrak{D}, \tag{53}$$

we obtain

$$0 = Q(t,v(t),v'(t)) = \sum_{n=0}^{N} Q_n(t,v(t))\left(-\frac{2v(t)w(t)}{t}\right)^n = \left(-\frac{2v(t)}{t}\right)^N P(w(t);\mu(t,v(t)),\nu(t,v(t))),$$

and thus $w(t)$ is a zero of $P(\cdot;\mu(t,v(t)),\nu(t,v(t)))$ for each $t\in\mathfrak{D}$. Since the zeros of this polynomial depend analytically on the parameter t according to the implicit function theorem, there exists an index $j\in\{1,\ldots,N\}$ such that $w(t)=z_j(\mu(t,v(t)),\nu(t,v(t)))$ for all $t\in\mathfrak{D}$. Furthermore, as z_j solves the PDE (29), it follows that $(t,v(t),w(t))$, $t\in\mathfrak{D}$, is a characteristic curve of (49), and thus v is a solution of (52). Hence, $Q(t,v,v')=0$ implies (52), and therefore Q is a special integral of rational type for this Painlevé III. Multiplying $Q(t,v,v')$ by an appropriate polynomial $r(t,v)$ in t and v, we obtain that the function $\widetilde{Q}(t,v,v') := r(t,v)Q(t,v,v')$ is a special integral of polynomial type of degree N with respect to v'. Now, Theorem 2 in Mansfield and Webster (1998) yields that such a special integral exists if and only if $2\kappa\pm 2\sigma\kappa = 2(2k-1)$ with some integer k, i.e., $\kappa = k-\frac{1}{2}$ is a half-integer. In addition, by Lemma 3 in Mansfield and Webster (1998), the relation $(\sigma q-p)\kappa = N$ must be satisfied for some integers $p,q\in\{-N,-N+2,\ldots,N-2,N\}$. In the case $N=1$ or $N=2$, these conditions imply $\kappa=\frac{1}{2}$, and the corresponding special integrals of polynomial type are explicitly known, namely $r(t)v^s(v'+v^2+\sigma)^N$, where r is some polynomial in t, and s is an integer, compare Sec. II in Mansfield and Webster (1998). Hence, $Q(t,v,v')=(v'+v^2+\sigma)^N$ and

$$P(w(t);\mu(t,v(t)),\nu(t,v(t))) = \left(-\frac{t}{2v(t)}\right)^N Q(t,v(t)) = (w(t)+\mu((t,v(t))))^N, \quad t\in\mathfrak{D},$$

which yields $P(\lambda;\mu,\nu)=(\lambda+\mu)^N$ if $N=1$ or $N=2$. □

As a consequence of this lemma, if a solution $\lambda(\mu,\nu)$ of the PDE (29) is a zero of a linear or quadratic polynomial with rational coefficients in μ and ν, then $\kappa=\frac{1}{2}$ and $\lambda(\mu,\nu)=-\mu$. In fact, the function $\lambda(\mu,\nu)=-\mu$ solves (29) for $\kappa=\frac{1}{2}$, but since $\lambda(0,0)=0$ and the spectrum of $A(\frac{1}{2};0,0)$ is given by $\mathbb{Z}\setminus\{0\}$, it is not an eigenvalue of $A(\frac{1}{2};\mu,\nu)$ for any $(\mu,\nu)\in\mathbb{R}^2$. The following considerations show that this solution is nevertheless of interest.

V. MONODROMY EIGENVALUES

In this section we consider the case that κ is a positive half-integer, i.e., $\kappa=k-\frac{1}{2}$ with some positive integer k, and we assume that the matrix C defined in (12) has distinct eigenvalues, i.e., $\mu^2\neq\nu^2$. For such κ and (μ,ν) there is in addition to the classical eigenvalues of $A(\kappa;\mu,\nu)$ another type of "special values" which we call monodromy eigenvalues. In order to introduce this concept, we first recall the characterization of eigenvalues according to Lemma 1: A point λ is an eigenvalue of $A(\kappa;\mu,\nu)$ if and only if the system (11) has a nontrivial solution of the form

$$y(x) = [x(1-x)]^{(\kappa/2)+1/4}\eta(x), \tag{54}$$

where $\eta:\mathbb{C}\to\mathbb{C}^2$ is an entire vector function. Now, as the difference of the characteristic values $\pm[(\kappa/2)+\frac{1}{4}]$ at 0 and 1 is an integer, the differential equation (11) has a fundamental matrix of the form

$$Y(x) = [x(1-x)]^{-(\kappa/2)-1/4} H(x), \tag{55}$$

where $H(x) = H_a(x)(x-a)^{J_a}$ holds in $\mathfrak{B}_a$, $a \in \{0,1\}$, with some holomorphic function $H_a : \mathfrak{B}_a \to M_2(\mathbb{C})$ and a Jordan matrix J_a, see Theorem 5.6 in Wasow (1965). Hence, the matrix function H is in general not holomorphic in $\mathfrak{B}_0 \cup \mathfrak{B}_1$ since it involves logarithmic terms. In the following, a point $\lambda \in \mathbb{C}$ is called *monodromy eigenvalue* of $A(\kappa;\mu,\nu)$ if and only if the system (11) has a fundamental matrix of the form (55) with the property that $H : \mathbb{C} \to \mathrm{M}_2(\mathbb{C})$ is an entire matrix function. Monodromy eigenvalues are characterized by the following lemma.

Lemma 5: For a given half-integer $\kappa > 0$ and $(\mu,\nu) \in \mathbb{C}^2$ with $\mu^2 \neq \nu^2$, a point $\lambda \in \mathbb{C}$ is a monodromy eigenvalue of $A(\kappa;\mu,\nu)$ if and only if the system (11) has a nontrivial solution of the form

$$[x(1-x)]^{-(\kappa/2)-1/4} p(x) e^{2tx}, \tag{56}$$

where $p : \mathbb{C} \to \mathbb{C}^2$ is a polynomial vector function and $t = \pm\sqrt{\nu^2-\mu^2}$.

Proof: By means of the transformation $y(x) = x^{\alpha}(1-x)^{\alpha}\tilde{y}(x)$ with $\alpha := (\kappa/2) + \frac{1}{4}$, the differential equation (11) is equivalent to the system

$$\tilde{y}'(x) = \left[\frac{1}{x}\tilde{B}_0 + \frac{1}{x-1}\tilde{B}_1 + C\right]\tilde{y}(x), \tag{57}$$

where

$$\tilde{B}_0 = \begin{pmatrix} 0 & \mu-\lambda \\ 0 & k \end{pmatrix}, \quad \tilde{B}_1 = \begin{pmatrix} k & 0 \\ \mu-\lambda & 0 \end{pmatrix}. \tag{58}$$

Now, if λ is a monodromy eigenvalue of $A(\kappa;\mu,\nu)$, then the system (57) has a holomorphic fundamental matrix $H : \mathbb{C} \to \mathrm{M}_2(\mathbb{C})$. Since the coefficient matrix of (57) is a rational matrix function which is bounded at infinity, an extension of Halphen's theorem, see Theorem 2.4 in Gesztesy *et al.* (2000), implies that the system (57) has a fundamental matrix of the form $R(x)e^{Dx}$ with some rational matrix function R and $D := \mathrm{diag}(-2t, 2t)$ (note that $\pm 2t$ are the eigenvalues of C). Moreover, $R(x)e^{Dx} = H(x)Q$ with some invertible matrix Q, and therefore $R(x) = H(x)Qe^{-Dx}$ is an entire matrix function in $\mathbb{C}$. This implies that $R : \mathbb{C} \to \mathrm{M}_2(\mathbb{C})$ is a polynomial. Vice versa, suppose that the system (11) has a nontrivial solution $y(x) = [x(1-x)]^{-\alpha} p(x) e^{2tx}$ with some polynomial vector function $p : \mathbb{C} \to \mathbb{C}^2$. Defining

$$\tilde{y}(x) := e^{-2t} K y(1-x) = [x(1-x)]^{-\alpha} K p(1-x) e^{-2tx}$$

with K given by (20), it follows that $\tilde{y}$ is a solution of (11) which is linearly independent of y. Therefore, (11) has a fundamental matrix of the type (55), where H is the entire matrix function $H(x) = (p(x)e^{2tx}, Kp(1-x)e^{-2tx})$. □

Theorem 3: *For fixed $\kappa = k - \frac{1}{2}$ with a positive integer k there exists a polynomial $P(\kappa;\lambda;\mu,\nu)$ of degree $2k-1$ in λ with polynomial coefficients in μ and ν such that for each $(\mu,\nu) \in \mathbb{C}^2$ with $\mu^2 \neq \nu^2$ a point $\lambda \in \mathbb{C}$ is a monodromy eigenvalue of $A(\kappa;\mu,\nu)$ if and only if λ is a zero of $P(\kappa;\cdot;\mu,\nu)$. Moreover, the integers $1-k, \ldots, k-1$ are the zeros of $P(\kappa;\cdot;0,0)$, and for $\kappa = \frac{1}{2}$ we obtain $P(\frac{1}{2};\lambda;\mu,\nu) = \lambda + \mu$.*

Proof: A point λ is a monodromy eigenvalue of $A(\kappa;\mu,\nu)$ if and only if the differential equation (57) has a nontrivial solution $p(x)e^{2tx}$, where $p(x) = \sum_{n=0}^{N} p_n x^n$, $p_N \neq 0$, is a polynomial vector function, and $t = \pm\sqrt{\nu^2-\mu^2}$. In the following we assume $t = \sqrt{\nu^2-\mu^2}$ (the main branch of the square root) but all considerations remain valid if we replace t with $-t$. If we set $\Lambda := \lambda - \mu$ and $\tilde{C} := C - t$, then the polynomial p satisfies the differential equation

$$p'(x) = \left[\frac{1}{x}\widetilde{B}_0 + \frac{1}{x-1}\widetilde{B}_1 + \widetilde{C}\right]p(x), \tag{59}$$

where the coefficient matrices take the form

$$\widetilde{B}_0 = \begin{pmatrix} 0 & -\Lambda \\ 0 & k \end{pmatrix}, \quad \widetilde{B}_1 = \begin{pmatrix} k & 0 \\ -\Lambda & 0 \end{pmatrix}, \quad \widetilde{C} = \begin{pmatrix} -2\nu - 2t & -2\mu \\ 2\mu & 2\nu - 2t \end{pmatrix}.$$

It is easy to see that the coefficients $p_n \in \mathbb{C}^2$, $n=0,\ldots,N$, form a nontrivial solution of the linear system of equations

$$\widetilde{B}_0 p_0 = 0, \quad (\widetilde{B}_0 - 1)p_1 + \widetilde{S}p_0 = 0, \tag{60}$$

$$(\widetilde{B}_0 - n)p_n + (\widetilde{S} + n - 1)p_{n-1} - \widetilde{C}p_{n-2} = 0 \quad (n = 2, \ldots, N), \tag{61}$$

$$(\widetilde{S} + N)p_N - \widetilde{C}p_{N-1} = 0, \quad -\widetilde{C}p_N = 0, \tag{62}$$

where

$$\widetilde{S} := \widetilde{C} - \widetilde{B}_0 - \widetilde{B}_1 = \begin{pmatrix} -2\nu - 2t - k & -2\mu + \Lambda \\ 2\mu + \Lambda & 2\nu - 2t - k \end{pmatrix}.$$

Multiplying the first equation in (62) from the left with the matrix $\widetilde{C}+4t$ and observing that $(\widetilde{C}+4t)\widetilde{C}=0$, we get

$$0 = (\widetilde{C} + 4t)(\widetilde{S} + N)p_N = \begin{pmatrix} N-k & -\Lambda \\ -\Lambda & N-k \end{pmatrix}\widetilde{C}p_N + 4t(N-k)p_N = 4t(N-k)p_N.$$

Since $t \neq 0$ and $p_N \neq 0$, it follows that $N=k$. Due to technical reasons we must distinguish between the cases $k \geqslant 2$ and $k=1$. We will proceed at first with a detailed proof for the more complicated case $k \geqslant 2$. Adding the second equation in (62) to the first one and then both equations in (62) to (61) for $n=N$, we obtain

$$\widetilde{B}_0 p_0 = 0, \quad (\widetilde{B}_0 - 1)p_1 + \widetilde{S}p_0 = 0, \tag{63}$$

$$(\widetilde{B}_0 - n)p_n + (\widetilde{S} + n - 1)p_{n-1} - \widetilde{C}p_{n-2} = 0 \quad (n = 2, \ldots, k-1), \tag{64}$$

$$-\widetilde{B}_1 p_k + \begin{pmatrix} -1 & \Lambda \\ \Lambda & -1 \end{pmatrix}p_{k-1} - \widetilde{C}p_{k-2} = 0, \tag{65}$$

$$\begin{pmatrix} 0 & \Lambda \\ \Lambda & 0 \end{pmatrix}p_k - \widetilde{C}p_{k-1} = 0, \quad -\widetilde{C}p_k = 0. \tag{66}$$

The system above consists of $2k+6$ linear equations for $2k+2$ unknowns. In the following we prove that only $2k+2$ of these equations are linearly independent. Summation of all equations (60)–(62) yields $-\widetilde{B}_1\Sigma_{n=0}^{k}p_n=0$. Because of rank $(\widetilde{B}_1)=1$, it is possible to eliminate the second line of the first equation in (65) by means of line transformations, and since also rank $(\widetilde{B}_0)=1$, we can delete the first line of the first equation in (63). Thus, the system (63)–(66) consists of at most $2k+4$ linearly independent equations. In order to reduce the equations (66) further, we must consider the cases $\nu - t \neq 0$ and $\nu - t = 0$ separately. First, let us assume that $\nu - t \neq 0$. Multiplying the equations in (66) from the left by the invertible matrix

$$T := \begin{pmatrix} \nu - t & \mu \\ 0 & 1 \end{pmatrix},$$

it follows that (66) is equivalent to

$$\begin{pmatrix} 0 & 0 \\ \Lambda & 0 \end{pmatrix} p_k - \begin{pmatrix} 0 & 0 \\ 2\mu & 2\nu - 2t \end{pmatrix} p_{k-1} = 0, \quad \begin{pmatrix} 0 & 0 \\ 2\mu & 2\nu - 2t \end{pmatrix} p_k = 0. \tag{67}$$

Now, we can represent the system of the linear equations (63)–(65), (67) as a matrix equation $\tilde{\Gamma}\tilde{p}=0$ with $\tilde{p}=(p_0,\ldots,p_k)\in\mathbb{C}^{2k+2}$ and the $(2k+2)\times(2k+2)$ matrix

$$\tilde{\Gamma} := \left(\begin{array}{cc|cc|ccc|cc} 0 & k & 0 & 0 & \cdots & & & \cdots & 0 & 0 \\ \hline \tilde{S} & & \tilde{B}_0 - I & & 0 & & & & 0 & \\ -\tilde{C} & & \tilde{S} + I & & \tilde{B}_0 - 2I & 0 & & & \vdots & \\ 0 & & -\tilde{C} & & \tilde{S} + 2I & \tilde{B}_0 - 3I & 0 & & & \\ \vdots & & \ddots & & \ddots & \ddots & \ddots & \ddots & \vdots & \\ 0 & & \cdots & & 0 & -\tilde{C} & \tilde{S} + (k-2)I & \tilde{B}_0 - (k-1)I & 0 & \\ \hline 0 & 0 & \cdots & & \cdots & 0 & 0 & 2\nu + 2t & 2\mu & -1 & \Lambda & -k & 0 \\ 0 & 0 & \cdots & & \cdots & 0 & 0 & 0 & 0 & -2\mu & 2t - 2\nu & \Lambda & 0 \\ 0 & 0 & \cdots & & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & -2\mu & 2t - 2\nu \end{array}\right).$$

Let $\hat{\Gamma}$ be the $(2k+1)\times(2k+1)$-matrix obtained from $\tilde{\Gamma}$ by deleting the last row and column. Then λ is a monodromy eigenvalue of $A(\kappa;\mu,\nu)$ if and only if $0=\det\tilde{\Gamma}=(2t-2\nu)\det\hat{\Gamma}$, i.e., $\det\hat{\Gamma}=0$ since $\nu-t\neq 0$. Now, suppose that $\nu-t=0$. We will prove that also in this case λ is a monodromy eigenvalue if and only if $\det\hat{\Gamma}=0$. Note that $\nu=t$ implies $\mu=0$, and therefore the equations in (66) are equivalent to

$$\begin{pmatrix} 0 & \Lambda \\ \Lambda & 0 \end{pmatrix} p_k + \begin{pmatrix} 4t & 0 \\ 0 & 0 \end{pmatrix} p_{k-1} = 0, \quad \begin{pmatrix} -4t & 0 \\ 0 & 0 \end{pmatrix} p_k = 0. \tag{68}$$

If λ is a monodromy eigenvalue of $A(\kappa;\mu,\nu)$, then the vector $\tilde{p}=(p_0,\ldots,p_k)$ is a nontrivial solution of the matrix equation $\tilde{\Gamma}\tilde{p}=0$ even though T is not invertible for $\nu-t=0$. If we assume $\det\hat{\Gamma}\neq 0$, it follows that $\Lambda\neq 0$ and the first $2k+1$ components of $\tilde{p}$ must be zero. In particular, $p_1=\cdots=p_{k-1}=0$, and the first equation in (68) yields $p_k=0$. Thus $\tilde{p}=0$, and this contradiction implies $\det\hat{\Gamma}=0$. Conversely, if $\det\hat{\Gamma}=0$, then either $\Lambda=0$, and $\tilde{p}:=(0,\ldots,0,1)\in\mathbb{C}^{2k+2}$ is a nontrivial solution of (63)–(65) and (68), or $\Lambda\neq 0$. In the latter case, there exists a vector $\hat{p}\neq 0$ with components $\hat{p}_1,\ldots,\hat{p}_{2k+1}\in\mathbb{C}$ such that $\hat{\Gamma}\hat{p}=0$. Defining $q:=(4t/\Lambda)\hat{p}_{2k-1}$, then $\tilde{p}:=(\hat{p},q)\in\mathbb{C}^{2k+2}$ is a nontrivial solution of the equations (63)–(65) and (68), i.e., λ is a monodromy eigenvalue. Hence, we have shown that for all $(\mu,\nu)\in\mathbb{C}^2$ with $\mu^2\neq\nu^2$ a point $\lambda\in\mathbb{C}$ is a monodromy eigenvalue of $A(\kappa;\mu,\nu)$ if and only if $\det\hat{\Gamma}=0$. In order to prove that $\det\hat{\Gamma}$ is a polynomial in Λ of degree $2k-1$, we apply once more appropriate line transformations to $\hat{\Gamma}$. Adding successively the second to the fourth line, the fourth to the sixth line and so on up to the $2k$th line, then $\det\hat{\Gamma}=\det\Gamma$ with the $(2k+1)\times(2k+1)$-matrix

$$\Gamma(\kappa;\Lambda;\mu,\nu;t) := \left(\begin{array}{cccccccc}
0 & k & 0 & 0 & \cdots & & & 0 \\
\hline
\widetilde{S}_0 & \widetilde{B}_0 - I & 0 & & & & & \vdots \\
-\widetilde{R} & \widetilde{S}_1 & \widetilde{B}_0 - 2I & 0 & & & & \\
\widetilde{Q} & -\widetilde{R} & \widetilde{S}_2 & \widetilde{B}_0 - 3I & 0 & & & \\
\widetilde{Q} & \widetilde{Q} & -\widetilde{R} & \widetilde{S}_3 & \widetilde{B}_0 - 4I & 0 & & \\
\vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\widetilde{Q} & & & \widetilde{Q} & -\widetilde{R} & \widetilde{S}_{k-2} & \widetilde{B}_0 - (k-1)I & 0 \\
\hline
\widetilde{Q} & \cdots & & & \widetilde{Q} & \widetilde{Q} & -\widetilde{R} & -k \\
 & & & & & & & \Lambda
\end{array}\right)$$

where

$$\widetilde{Q} := \begin{pmatrix} -k & 0 \\ 0 & 0 \end{pmatrix}, \quad \widetilde{R} := \begin{pmatrix} k & 0 \\ 2\mu & 2\nu - 2t \end{pmatrix},$$

$$\widetilde{S}_n := \begin{pmatrix} -2\nu - 2t - k & -2\mu \\ 2\mu + \Lambda & 2\nu - 2t + n - k \end{pmatrix}, \quad n = 0, \ldots, k-2.$$

Now, Λ appears at most once in each row and each column, whereas only the first and the $2k$th line contain no entry involving Λ. It is easy to verify that $\det \Gamma(\Lambda;\mu,\nu;t)$ has the form $\pm k^2 \Lambda^{2k-1} +$ (terms of lower order in Λ), and therefore $\det \Gamma(\Lambda;\mu,\nu;t)$ is a polynomial in Λ with polynomial coefficients in μ, ν, and t. Moreover, for all $(\mu,\nu) \in \mathbb{C}^2$ with $\mu^2 \neq \nu^2$ a point λ is a monodromy eigenvalue of $A(\kappa;\mu,\nu)$ if and only if the determinant of $\Gamma(\kappa;\Lambda;\mu,\nu;t)$ vanishes. As mentioned at the beginning of the proof, this result remains valid if we replace t with $-t$. Hence, the zeros of the polynomials $\det \Gamma(\kappa;\Lambda;\mu,\nu;t)$ and $\det \Gamma(\kappa;\Lambda;\mu,\nu;-t)$ coincide, which implies that $\det \Gamma(\kappa;\Lambda;\mu,\nu;t) = \det \Gamma(\kappa;\Lambda;\mu,\nu;-t)$. Consequently, the polynomial $P(\kappa;\lambda;\mu,\nu) := \det \Gamma(\kappa;\Lambda;\mu,\nu;t)$ contains no terms in t of odd order, and the terms of even order in t depend only on $t^2 = \nu^2 - \mu^2$. It follows that P is a polynomial of degree $2k-1$ in λ with polynomial coefficients in μ and ν, and the zeros of P are exactly the monodromy eigenvalues of $A(\kappa;\mu,\nu)$.

Next, we prove that the integers $1-k, \ldots, k-1$ are the zeros of the polynomial $P(\kappa;\lambda;0,0)$. To this aim, let Γ_0 be the $(2k \times 2k)$ matrix obtained from $\hat{\Gamma}$ for $(\mu,\nu) = (0,0)$ by deleting the last row and column. Then

$$\Gamma_0 = \left(\begin{array}{cccccccc}
0 & k & 0 & 0 & \cdots & & 0 & 0 \\
\hline
Q & \widetilde{B}_0 - I & 0 & \cdots & & & 0 & \\
0 & Q + I & \widetilde{B}_0 - 2I & 0 & & & \vdots & \\
0 & 0 & Q + 2I & \widetilde{B}_0 - 3I & 0 & & & \\
\vdots & & \ddots & \ddots & \ddots & \ddots & \vdots & \\
\vdots & & & 0 & Q + (k-3)I & \widetilde{B}_0 - (k-2)I & 0 & \\
0 & \cdots & & & 0 & Q + (k-2)I & \widetilde{B}_0 - (k-1)I & \\
\hline
0 & 0 & \cdots & & & 0 & 0 & -1 \quad \lambda
\end{array}\right),$$

$$Q := \begin{pmatrix} -k & \lambda \\ \lambda & -k \end{pmatrix},$$

and $\det \hat{\Gamma} = \lambda \det \Gamma_0$. Moreover, $\det \Gamma_0 = 0$ if and only if the equation $\Gamma_0 (p_n)_{n=0}^{k-1} = 0$ has a nontrivial solution. Such a nontrivial solution is a constant multiple of the vector given by the recurrence formula

$$p_0 := \begin{pmatrix} (k-1)! \\ 0 \end{pmatrix},$$

$$p_n = (n - \tilde{B}_0)^{-1}(Q+n-1)p_{n-1} = -\frac{1}{n(k-n)}\begin{pmatrix} (k-n)(k+1-n)-\lambda^2 & \lambda \\ n\lambda & -n(k+1-n) \end{pmatrix} p_{n-1}$$

for $n=1,\ldots,k-1$. By induction, it can be shown that

$$p_n = (-1)^n \frac{(k-n-1)!}{n!}\prod_{j=1}^{n-1}[(k-j)^2-\lambda^2]\begin{pmatrix} k(k-n)-\lambda^2 \\ n\lambda \end{pmatrix}.$$

Multiplying the vector $(p_n)_{n=0}^{k-1}$ from the left by the last line of Γ_0, we get

$$0 = (-1)^{k-1}\frac{1}{(k-1)!}\prod_{j=1}^{k-2}[(k-j)^2-\lambda^2](-k+\lambda^2+(k-1)\lambda^2) = \frac{k(-1)^k}{(k-1)!}\prod_{j=1}^{k-1}[(k-j)^2-\lambda^2].$$

Hence, $\det \Gamma_0 = 0$ if and only if $\lambda^2 \in \{1,\ldots,(k-1)^2\}$, and therefore $1-k,\ldots,k-1$ are the zeros of $P(\kappa;\cdot;0,0)$.

It remains to deal with the case $k=1$, where we must consider only the equations (60) and (62). Adding both equations in (62) to the second equation in (60) gives (65) with $p_{-1} := 0$. Hence, we can replace (60)–(62) with the linear system of equations consisting of the first equation in (63) and Eqs. (65) and (66). Now, by applying a similar reduction procedure as in the case $k \geqslant 2$, we obtain the polynomial

$$P(\tfrac{1}{2};\lambda;\mu,\nu) = \det\begin{pmatrix} 0 & 1 & 0 \\ -1 & \Lambda & -1 \\ -2\mu & 2t-2\nu & \Lambda \end{pmatrix} = \Lambda + 2\mu = \lambda + \mu,$$

whose zero $\lambda = -\mu$ is the uniquely determined monodromy eigenvalue of $A(\frac{1}{2};\mu,\nu)$ for each $(\mu,\nu) \in \mathbb{C}^2$, $\mu^2 \neq \nu^2$. □

Corollary 1: For a fixed half-integer $\kappa = k - \frac{1}{2}$ with a positive integer k, there exists a neighborhood $\mathfrak{U} \subset \mathbb{C}^2$ of $(0,0)$ such that $A(\kappa;\mu,\nu)$ has exactly $2k-1$ many monodromy eigenvalues $\lambda_0^j(\kappa;\mu,\nu)$, $j=1-k,\ldots,k-1$, for all $(\mu,\nu) \in \mathfrak{U}$ with $\mu^2 \neq \nu^2$. Moreover, $\lambda_0^j(\kappa;\mu,\nu)$ depends holomorphically on (μ,ν), and $\lim_{(\mu,\nu)\to(0,0)} \lambda_0^j(\kappa;\mu,\nu) = j$. In particular, monodromy eigenvalues and classical eigenvalues are distinct near $(\mu,\nu)=(0,0)$.

Remark 3: Monodromy eigenvalues also appear in the context of spheroidal wave equations. In Sec. 3.54 in Meixner and Schäfke (1954) they are characterized by a similar property as given in Lemma 5, but they are not specified in detail.

In view of Theorem 3 and Corollary 1 we could alternatively define the monodromy eigenvalues of $A(\kappa;\mu,\nu)$ to be the zeros of the polynomial $P(\kappa;\cdot;\mu,\nu)$ for each $(\mu,\nu) \in \mathbb{C}^2$ (without the restriction $\mu^2 \neq \nu^2$). Then the monodromy eigenvalues $\lambda_0^j(\kappa;0,0) = j$, $j=1-k,\ldots,k-1$, fill in the gap of integers appearing in the spectrum of $A(\kappa;0,0)$. Moreover, $P(\frac{1}{2};\lambda;\mu,\nu) = \lambda+\mu$ is just the polynomial given by Lemma 4 in the case $N=1$, and its zero $\lambda_0^0(\frac{1}{2};\mu,\nu) = -\mu$ satisfies the partial differential equation (29) for $\kappa = \frac{1}{2}$. In the next section we prove that the monodromy eigenvalues of $A(\kappa;\mu,\nu)$ are solutions of the PDE (29) for each half-integer $\kappa \in \{\frac{1}{2},\frac{3}{2},\frac{5}{2},\ldots\}$.

VI. MONODROMY PRESERVING DEFORMATIONS

In Jimbo *et al.* (1981), Jimbo and Miwa (1981a, 1981b), these authors developed a general theory for monodromy preserving deformations of linear ordinary differential equations with rational coefficients. As a main result, they proved that the monodromy data (Stokes multipliers, connection matrices, and exponents of formal monodromy) do not depend on the deformation parameters if and only if certain nonlinear differential equations, the so-called deformation equa-

tions, are satisfied. This result, however, was proved under the restriction that the characteristic values at regular singular points do not differ by an integer. On the other hand, in the theory of special functions and in many physical applications the case where the characteristic values differ by an integer is of great significance. In this section we consider the isomonodromy problem for linear systems with two fixed regular singular points and coefficients which depend on one parameter t. Assuming that the characteristic values at the singular points are distinct and independent of t, we will show that certain components of the monodromy data are constant with respect to t if a deformation equation of the type (1.18) in Jimbo *et al.* (1981) is satisfied. Since the monodromy components in question determine the existence of solutions of the form (54) and (55), they are relevant to monodromy and classical eigenvalue problems. Applying the results to the system (11) with an eigenvalue t of C as deformation parameter, it finally turns out that the deformation equation is in principle the characteristic equation of the partial differential equation (29).

We start with some basic facts about parameter-dependent regular singular systems. At first, let us consider a family of (2×2) systems of differential equations

$$\frac{\partial y}{\partial x}(x,t)=\Phi(x,t)y(x,t),\quad (x,t)\in(\mathfrak{B}\setminus\{0\})\times\mathfrak{D}, \tag{69}$$

in an open disk $\mathfrak{B}\subset\mathbb{C}$ with center 0 that depends on a parameter t varying in some real or complex domain $\mathfrak{D}$. It is assumed that (69) has a regular singular point at 0 for all $t\in\mathfrak{D}$. More precisely, we suppose that the coefficient matrix Φ of (69) has the following properties:

(a) $\Phi(x,t)=(1/x)\Psi(x,t)$, where $\Psi:\mathfrak{B}\times\mathfrak{D}\to \mathrm{M}_2(\mathbb{C})$ is an analytical matrix function.
(b) The eigenvalues α and β of $\Psi(0,t)$ are distinct and independent of $t\in\mathfrak{D}$; $\mathrm{Re}\alpha\leqslant\mathrm{Re}\beta$.
(c) There is an analytical function $G:\mathfrak{D}\to\mathrm{M}_2(\mathbb{C})$ such that $G(t)$ is invertible and

$$G(t)^{-1}\Psi(0,t)G(t)=\mathrm{diag}(\alpha,\beta)=:D,\quad t\in\mathfrak{D},$$

Note that such a matrix function G always exists since the eigenvalues of $\Psi(0,t)$ are distinct, see Theorem 25.1 in Wasow (1965, Chap. VII, Sec. 25).

Lemma 6: If the conditions (a)–(c) are satisfied, then the system (69) has a fundamental matrix of the form

$$Y(x,t)=G(t)H(x,t)x^{D}x^{J(t)},$$

where $H:\mathfrak{B}\times\mathfrak{D}\to\mathrm{M}_2(\mathbb{C})$ *is analytic,* $H(0,t)=I$ *for all* $t\in\mathfrak{D}$, *and*

$$J(t)=\begin{pmatrix}0 & 0\\ p(t) & 0\end{pmatrix} \tag{70}$$

with some analytical function $p:\mathfrak{D}\to\mathbb{C}$. *Moreover, if* $\beta-\alpha$ *is not an integer, then* $p\equiv 0$.

Proof: If $\beta-\alpha$ is not an integer, the existence of such a fundamental matrix with $J\equiv 0$ is well known, cf. Schäfke (1951). Hence, we have to consider only the case that $k:=\beta-\alpha$ is a positive integer. By the transformation

$$y(x,t)=x^{\alpha}G(t)y_0(x,t), \tag{71}$$

the system (69) is equivalent to the differential equation

$$x\frac{\partial y_0}{\partial x}(x,t)=\Psi_0(x,t)y_0(x,t),\quad (x,t)\in(\mathfrak{B}\setminus\{0\})\times\mathfrak{D}, \tag{72}$$

where $\Psi_0(x,t):=G(t)^{-1}\Psi(x,t)G(t)-\alpha$ is an analytical matrix function,

$$\Psi_0(x,t) = \sum_{n=0}^{\infty} x^n \Psi_{0,n}(t), \quad (x,t) \in \mathfrak{B} \times \mathfrak{D},$$

with $\Psi_{0,0}(t) = \mathrm{diag}(0,k)$ for all $t \in \mathfrak{D}$. Now, for $j = 1, \ldots, k-1$ we recursively apply the transformations

$$y_{j-1}(x,t) = \begin{pmatrix} 1 & 0 \\ \dfrac{x}{j-k}\psi_{j-1}(t) & x \end{pmatrix} y_j(x,t), \tag{73}$$

where ψ_{j-1} denotes the (2,1)-coefficient of the matrix $\Psi_{j-1,1}$. At each step, $y_j(x,t)$ is a solution of a system

$$x\frac{\partial y_j}{\partial x}(x,t) = \Psi_j(x,t) y_j(x,t), \quad (x,t) \in (\mathfrak{B} \setminus \{0\}) \times \mathfrak{D}, \tag{74}$$

where the coefficient matrix Ψ_j is analytic in $\mathfrak{B} \times \mathfrak{D}$,

$$\Psi_j(x,t) = \sum_{n=0}^{\infty} x^n \Psi_{j,n}(t), \quad (x,t) \in \mathfrak{B} \times \mathfrak{D},$$

with $\Psi_{j,0}(t) = \mathrm{diag}(0, k-j)$ for all $t \in \mathfrak{D}$, and $\Psi_{j,n}(t), n = 1, \ldots, j-1$, are lower triangular matrix functions [that means, the (1,2) component is identically zero]. Finally, by the shearing transformation

$$y_{k-1}(x,t) = \begin{pmatrix} 1 & 0 \\ 0 & x \end{pmatrix} y_k(x,t), \tag{75}$$

we obtain a differential equation

$$x\frac{\partial y_k}{\partial x}(x,t) = \Psi_k(x,t) y_k(x,t), \quad (x,t) \in (\mathfrak{B} \setminus \{0\}) \times \mathfrak{D}, \tag{76}$$

where $\Psi_k : \mathfrak{B} \times \mathfrak{D} \to \mathrm{M}_2(\mathbb{C})$ is an analytical matrix function,

$$\Psi_k(x,t) = \sum_{n=0}^{\infty} x^n \Psi_{k,n}(t), \quad (x,t) \in \mathfrak{B} \times \mathfrak{D},$$

satisfying

$$\Psi_{k,0}(t) = \begin{pmatrix} 0 & 0 \\ p(t) & 0 \end{pmatrix} =: J(t), \quad t \in \mathfrak{D},$$

with some analytical function $p : \mathfrak{D} \to \mathbb{C}$. Note that p is just the $(2,1)$-component of $\Psi_{k-1,1}$. Moreover, $\Psi_{k,n}(t), n = 0, \ldots, k$, are lower triangular matrices for all $t \in \mathfrak{D}$. Now, the system (76) has a fundamental matrix of the form

$$\tilde{Y}(x,t) = \tilde{H}(x,t) x^{J(t)}$$

provided that $\tilde{H}$ is a solution of the matrix differential equation

$$x\frac{\partial \widetilde{H}}{\partial x}(x,t) = \Psi_k(x,t)\widetilde{H}(x,t) - \widetilde{H}(x,t)J(t), \quad (x,t) \in \mathfrak{B} \times \mathfrak{D}, \tag{77}$$

such that for each $t \in \mathfrak{D}$ the matrix $\widetilde{H}(x,t)$ is invertible for some, and hence all, $x \in \mathfrak{B}$. Obviously, (77) has a formal solution

$$\widetilde{H}(x,t) = \sum_{n=0}^{\infty} x^n \widetilde{H}_n(t), \quad (x,t) \in \mathfrak{B} \times \mathfrak{D}, \tag{78}$$

where $\widetilde{H}_0(t) = I$ and the coefficients $\widetilde{H}_n$, $n > 0$, are uniquely determined by the recurrence relation

$$(J(t) - n)\widetilde{H}_n(t) - \widetilde{H}_n(t)J(t) = -\sum_{j=0}^{n-1} \Psi_{k,n-j}(t)\widetilde{H}_j(t). \tag{79}$$

Following the proof of Theorem 5.3 in the book of Wasow (1965), it can be shown that the series (78) converges uniformly in every compact subset of $\mathfrak{B} \times \mathfrak{D}$. Thus, a Weierstrass theorem implies that $\widetilde{H}$ is analytic in $\mathfrak{B} \times \mathfrak{D}$, and therefore $\widetilde{H}$ is an actual solution of (77). Further, since $J(t)$ has the special form (70) and $\Psi_{k,j}(t), j = 0, \ldots, k$, are lower triangular matrices, it is easy to verify that $\widetilde{H}_j(t)$ are lower triangular matrices for $j = 0, \ldots, k$. Now, by combining the transformations (71), (73), and (75), it follows that the differential equation (69) has a fundamental matrix of the form

$$Y(x,t) = x^{\alpha} G(t) \begin{pmatrix} 1 & 0 \\ xq(x,t) & x^k \end{pmatrix} \widetilde{H}(x,t) x^{J(t)}, \tag{80}$$

where $q(x,t)$ is a polynomial in x of degree $n-1$ with coefficients depending analytically on t, and $\widetilde{H}(x,t)$ is an analytical matrix function of the type

$$\widetilde{H}(x,t) = \begin{pmatrix} h_{11}(x,t) & x^{k+1}h_{12}(x,t) \\ h_{21}(x,t) & h_{22}(x,t) \end{pmatrix}$$

satisfying $h_{11}(0,t) = h_{22}(0,t) = 1$. Now, if we define

$$H(x,t) := \begin{pmatrix} h_{11}(x,t) & xh_{12}(x,t) \\ xq(x,t)h_{11}(x,t) + x^{k+1}h_{21}(t) & x^2 q(x,t)h_{12}(x,t) + h_{22}(x,t) \end{pmatrix},$$

then $H: \mathfrak{B} \times \mathfrak{D} \to \mathrm{M}_2(\mathbb{C})$ is analytic, $H(0,t) = I$ for all $t \in \mathfrak{D}$, and

$$\begin{pmatrix} 1 & 0 \\ xq(x,t) & x^k \end{pmatrix} \widetilde{H}(x,t) = H(x,t) \begin{pmatrix} 1 & 0 \\ 0 & x^k \end{pmatrix}.$$

Hence, we can write the fundamental matrix (80) in the form $Y(x,t) = G(t)H(x,t)x^D x^{J(t)}$, where H has the properties stated in the lemma. □

Now, we consider a family of (2×2) differential systems,

$$\frac{\partial y}{\partial x}(x,t) = \Phi(x,t)y(x,t), \quad (x,t) \in (\mathfrak{G} \setminus \{0,1\}) \times \mathfrak{D}, \tag{81}$$

in a domain $\mathfrak{G}$, $\mathfrak{B}_0 \cup \mathfrak{B}_1 \subset \mathfrak{G} \subset \mathbb{C}$, with regular singular points at $x = 0$ and $x = 1$ and a parameter t varying in some domain $\mathfrak{D} \subset \mathbb{R}$ or $\mathfrak{D} \subset \mathbb{C}$. Further, we assume that the coefficient matrix Φ in (81) has the form

$$\Phi(x,t) = \frac{1}{x(x-1)}\Psi(x,t), \quad (x,t) \in (\mathfrak{G} \setminus \{0,1\}) \times \mathfrak{D},$$

where $\Psi: \mathfrak{G} \times \mathfrak{D} \to \mathrm{M}_2(\mathbb{C})$ is an analytical matrix function with the following properties.

(I) The eigenvalues α, β of $\Psi(a,t)$ are distinct and independent of $t \in \mathfrak{D}$ and $a \in \{0,1\}$; in addition, $\mathrm{Re}\alpha \leqslant \mathrm{Re}\beta$.

(II) There are analytical functions $G_a: \mathfrak{D} \to \mathrm{M}_2(\mathbb{C})$, $a \in \{0,1\}$, such that $G_a(t)$ is invertible for all $t \in \mathfrak{D}$ and

$$G_a(t)^{-1}\Psi(a,t)G_a(t) = (-1)^a \operatorname{diag}(\alpha,\beta).$$

From Lemma 6 it follows that the system (81) possesses a fundamental matrix of the form

$$Y_a(x,t) = G_a(t)H_a(x,t)(x-a)^D(x-a)^{J_a(t)} \tag{82}$$

in the unit disk $\mathfrak{B}_a \subset \mathfrak{G}$ with center $a \in \{0,1\}$, where $H_a: \mathfrak{B}_a \times \mathfrak{D} \to M_2(\mathbb{C})$ is an analytical matrix function satisfying $H_a(0,t)=I$ for all $t \in \mathfrak{D}$, $D=\operatorname{diag}(\alpha,\beta)$, and

$$J_a(t) = \begin{pmatrix} 0 & 0 \\ p_a(t) & 0 \end{pmatrix} \tag{83}$$

with some analytical function $p_a: \mathfrak{D} \to \mathbb{C}$. By analytic continuation along curves, we can assume that Y_a is defined on the universal covering $\mathfrak{R}$ of the set $\mathfrak{G}\setminus\{0,1\}$. Since $Y_a(xe^{2i\pi}+a,t)=Y_a(x+a,t)e^{2i\pi D}[I+2\pi i J_a(t)]$ for all $(x,t) \in (\mathfrak{B}_0\setminus\{0\}) \times \mathfrak{D}$, the diagonal matrix D and the Jordan-type matrix $J_a(t)$ represent the monodromy behavior of Y_a corresponding to a circuit around $a \in \{0,1\}$. Moreover, as Y_0 and Y_1 are both fundamental matrices of the same differential equation (81), there exists an analytical matrix function $Q: \mathfrak{D} \to \mathrm{M}_2(\mathbb{C})$ such that $Y_0(x,t)=Y_1(x,t)Q(t)$ for all $(x,t) \in (\mathfrak{G}\setminus\{0,1\}) \times \mathfrak{D}$, which is called the connection matrix for Y_0 and Y_1. The next result gives a sufficient condition that certain components of the monodromy data J_a and Q are constant in $\mathfrak{D}$. For this reason, we establish in addition to (I) and (II) the following assumptions on the coefficient matrix Φ.

(III) There exists an analytical function $\Omega: \mathfrak{G} \times \mathfrak{D} \to \mathrm{M}_2(\mathbb{C})$ such that

$$\frac{\partial \Phi}{\partial t}(x,t) + \Phi(x,t)\Omega(x,t) = \Omega(x,t)\Phi(x,t) + \frac{\partial \Omega}{\partial x}(x,t), \quad (x,t) \in (\mathfrak{G}\setminus\{0,1\}) \times \mathfrak{D}. \tag{84}$$

(IV) The matrix functions G_a, $a \in \{0,1\}$, satisfy the linear differential equations

$$\frac{\partial G_a}{\partial t}(t) = \Omega(a,t)G_a(t), \quad t \in \mathfrak{D}. \tag{85}$$

Theorem 4: *If the conditions (I)–(IV) are satisfied, then*

$$\frac{\partial J_a}{\partial t} \equiv \frac{\partial Q_{21}}{\partial t} \equiv 0 \text{ in } \mathfrak{D}, \tag{86}$$

where the Jordan matrices J_a, $a \in \{0,1\}$, are given by (83) and $Q_{12}: \mathfrak{D} \to \mathbb{C}$ denotes the (1,2)-component of the connection matrix Q for Y_0 and Y_1.

Proof: Let $\gamma := \beta - \alpha$, and for fixed $a \in \{0,1\}$ we define

$$Z_a(x,t) := \frac{\partial Y_a}{\partial t}(x,t) - \Omega(x,t)Y_a(x,t), \quad (x,t) \in \mathfrak{R} \times \mathfrak{D}.$$

From (81) and the deformation equation (84) it follows that

$$\frac{\partial Z_a}{\partial x} = \frac{\partial^2 Y_a}{\partial x\,\partial t} - \frac{\partial \Omega}{\partial x} Y_a - \Omega \frac{\partial Y_a}{\partial x} = \frac{\partial (\Phi Y_a)}{\partial t} - \frac{\partial \Omega}{\partial x} Y_a - \Omega \Phi Y_a$$
$$= \Phi \frac{\partial Y_a}{\partial t} + \left(\frac{\partial \Phi}{\partial t} - \frac{\partial \Omega}{\partial x} - \Omega \Phi \right) Y_a = \Phi \left(\frac{\partial Y_a}{\partial t} - \Omega Y_a \right) = \Phi Z_a,$$

and therefore Z_a is a matrix solution of the differential equation (81) in $\mathfrak{R}$. Hence, there exists an analytical function $C_a : \mathfrak{D} \to \mathrm{M}_2(\mathbb{C})$ such that

$$Z_a(x,t) = Y_a(x,t) C_a(t), \quad (x,t) \in \mathfrak{R} \times \mathfrak{D}.$$

Now, by means of the differential equation (85), we get

$$\frac{\partial Y_a}{\partial t} = \frac{\partial G_a}{\partial t} H_a (x-a)^D (x-a)^{J_a} + G_a \frac{\partial H_a}{\partial t} (x-a)^D (x-a)^{J_a} + \log(x-a) G_a H_a (x-a)^D \frac{\partial J_a}{\partial t} (x-a)^{J_a}$$
$$= \left(\Omega(a, \cdot) G_a H_a + G_a \frac{\partial H_a}{\partial t} + (x-a)^\gamma \log(x-a) G_a H_a \frac{\partial J_a}{\partial t} \right) (x-a)^D (x-a)^{J_a},$$

and since $C_a = Y_a^{-1} Z_a$, it results that

$$\begin{aligned}
&(x-a)^D (x-a)^{J_a} C_a (x-a)^{-J_a} (x-a)^{-D} \\
&\quad = (x-a)^D (x-a)^{J_a} Y_a^{-1} \left(\frac{\partial Y_a}{\partial t} - \Omega Y_a \right) (x-a)^{-J_a} (x-a)^{-D} \\
&\quad = H_a^{-1} G_a^{-1} (\Omega(a, \cdot) - \Omega) G_a H_a + H_a^{-1} \frac{\partial H_a}{\partial t} + (x-a)^\gamma \log(x-a) \frac{\partial J_a}{\partial t} \\
&\quad = (x-a) F_a + (x-a)^\gamma \log(x-a) \begin{pmatrix} 0 & 0 \\ \dfrac{\partial p_a}{\partial t} & 0 \end{pmatrix}
\end{aligned} \tag{87}$$

with some analytical function $F_a : \mathfrak{G} \times \mathfrak{D} \to \mathrm{M}_2(\mathbb{C})$. Further, by setting

$$C_a(t) =: \begin{pmatrix} C_{11}(t) & C_{12}(t) \\ C_{21}(t) & C_{22}(t) \end{pmatrix}, \quad t \in \mathfrak{D}$$

(for clarity, we omit the index a in the entries of C_a), we have

$$\begin{aligned}
&(x-a)^D (x-a)^{J_a} C_a (x-a)^{-J_a} (x-a)^{-D} \\
&\quad = \begin{pmatrix} 1 & 0 \\ (x-a)^\gamma \log(x-a) p_a & (x-a)^\gamma \end{pmatrix} \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\log(x-a) p_a & (x-a)^{-\gamma} \end{pmatrix} \\
&\quad = \begin{pmatrix} C_{11} - \log(x-a) p_a C_{12} & (x-a)^{-\gamma} C_{12} \\ * & C_{22} + \log(x-a) p_a C_{12} \end{pmatrix}.
\end{aligned} \tag{88}$$

Comparing (87) to (88), it follows that $C_{12} \equiv 0$ in $\mathfrak{D}$ since the function in (87) is bounded at $x=a$. This in turn implies $C_{11} \equiv C_{22} \equiv 0$ as the diagonal entries in (87) have a zero at $x=a$ for all $t \in \mathfrak{D}$. Finally, we obtain that

$$(x-a)^D (x-a)^{J_a} C_a (x-a)^{-J_a} (x-a)^{-D} = \begin{pmatrix} 0 & 0 \\ (x-a)^\gamma C_{21} & 0 \end{pmatrix} \tag{89}$$

has no logarithmic singularity at $x=a$ and therefore the last term (87) vanishes identically. Hence, $\partial J_a / \partial t \equiv 0$ in $\mathfrak{D}$.

Next, we prove that $\partial Q_{12} / \partial t \equiv 0$. Since $Y_0(x,t) = Y_1(x,t) Q(t)$, it follows that

$$\frac{\partial Y_0}{\partial t} = \frac{\partial Y_1}{\partial t} Q + Y_1 \frac{\partial Q}{\partial t}. \tag{90}$$

Further, from $Z_a(x,t) = Y_a(x,t) C_a(t)$ we get

$$\frac{\partial Y_0}{\partial t} Y_0^{-1} - \Omega = Y_0 C_0 Y_0^{-1}, \quad \frac{\partial Y_1}{\partial t} Y_1^{-1} - \Omega = Y_1 C_1 Y_1^{-1}. \tag{91}$$

By means of (90) and $Y_0^{-1} = Q^{-1} Y_1^{-1}$, the first equation in (91) becomes

$$\frac{\partial Y_1}{\partial t} Y_1^{-1} - \Omega = Y_1 Q C_0 Q^{-1} Y_1^{-1} - Y_1 \frac{\partial Q}{\partial t} Q^{-1} Y_1^{-1}. \tag{92}$$

Now, (92) and the second equation in (91) imply

$$Y_1 C_1 Y_1^{-1} = Y_1 Q C_0 Q^{-1} Y_1^{-1} - Y_1 \frac{\partial Q}{\partial t} Q^{-1} Y_1^{-1}$$

and therefore

$$\frac{\partial Q}{\partial t} = Q C_0 - C_1 Q. \tag{93}$$

Note that the matrix function C_a has the form

$$C_a(t) = \begin{pmatrix} 0 & 0 \\ c_a(t) & 0 \end{pmatrix}, \quad a \in \{0,1\}.$$

Hence, if we set

$$Q(t) =: \begin{pmatrix} Q_{11}(t) & Q_{12}(t) \\ Q_{21}(t) & Q_{22}(t) \end{pmatrix}, \quad t \in \mathfrak{D},$$

then (93) is equivalent to the system

$$\frac{\partial}{\partial t} \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} = \begin{pmatrix} c_0 Q_{12} & 0 \\ c_0 Q_{22} - c_1 Q_{11} & c_1 Q_{12} \end{pmatrix},$$

and we immediately obtain that $\partial Q_{12} / \partial t \equiv 0$ in $\mathfrak{D}$. □

In the following we apply the results of Lemma 6 and Theorem 4 to a family of (2×2) differential systems

$$\frac{\partial y}{\partial x}(x,t) = \left[\frac{1}{x} B_0(t) + \frac{1}{x-1} B_1(t) + C(t) \right] y(x,t), \quad (x,t) \in (\mathbb{C} \setminus \{0,1\}) \times \mathfrak{D}, \tag{94}$$

where $t \in \mathfrak{D}$ with some domain $\mathfrak{D} \subset \mathbb{R}$ or $\mathfrak{D} \subset \mathbb{C}$, and we suppose that the coefficients $B_0, B_1, C : \mathfrak{D} \to M_2(\mathbb{C})$ are analytical functions. Further, we assume that the following conditions hold.

(i) The eigenvalues α, β of $B_0(t)$ are distinct and independent of $t \in \mathfrak{D}$. Moreover, they coincide with the eigenvalues of $B_1(t)$, and $\mathrm{Re}\,\alpha \leqslant \mathrm{Re}\,\beta$.

(ii) There are analytical functions $G_a : \mathfrak{D} \to M_2(\mathbb{C})$, $a \in \{0,1\}$, such that $G_a(t)$ is invertible and

$$G_0(t)^{-1} B_0(t) G_0(t) = -G_1(t)^{-1} B_1(t) G_1(t) = \mathrm{diag}(\alpha, \beta) =: D, \quad t \in \mathfrak{D}.$$

Let Y_a, $a \in \{0,1\}$, be fundamental matrices of (94) in the open disk $\mathfrak{B}_a \subset \mathbb{C}$ with center a and radius 1 having the form (82), where $H_a : \mathfrak{B} \times \mathfrak{D} \to \mathrm{M}_2(\mathbb{C})$ is analytical, $H_a(0,t) = I$ for all $t \in \mathfrak{D}$, and $J_a(t)$ is given by (83) with some analytical function $p_a : \mathfrak{D} \to \mathbb{C}$. Again, by analytic continua-

tion, we assume that Y_a is defined on the universal covering $\mathfrak{R}$ of $\mathbb{C}\setminus\{0,1\}$, and we denote by $Q:\mathfrak{D}\to M_2(\mathbb{C})$ the connection matrix for Y_0 and Y_1. In the sequel we are looking for conditions such that for fixed $t\in\mathfrak{D}$ the system (94) has one of the following properties.

(P) There exists a fundamental matrix Y of the form

$$Y(x)=[x(1-x)]^{\alpha}P(x)e^{C(t)x},\quad x\in\mathbb{C}\setminus\{0,1\},\tag{95}$$

where $P:\mathbb{C}\to\mathrm{M}_2(\mathbb{C})$ is a polynomial matrix function.

(H) There exists a nontrivial solution y of the form

$$y(x)=[x(1-x)]^{\beta}h(x),\quad x\in\mathbb{C}\setminus\{0,1\},\tag{96}$$

where $h:\mathbb{C}\to\mathbb{C}^2$ is an entire vector function.

Lemma 7: Suppose that the conditions (i) and (ii) are satisfied, and let $t\in\mathfrak{D}$. Then the system (94) has the property (P) if and only if $\beta-\alpha$ is an integer and $p_0(t)=p_1(t)=0$, and it has the property (H) if and only if $Q_{21}(t)=0$.

Proof: By means of the transformation $y(x)=x^{\alpha}(x-1)^{\alpha}\tilde{y}(x)$, the differential equation (94) is equivalent to the system

$$\frac{\partial\tilde{y}}{\partial x}(x,t)=\left[\frac{1}{x}\tilde{B}_0(t)+\frac{1}{x-1}\tilde{B}_1(t)+C(t)\right]\tilde{y}(x,t),\quad (x,t)\in(\mathbb{C}\setminus\{0,1\})\times\mathfrak{D},\tag{97}$$

where $\tilde{B}_0(t):=B_0(t)-\alpha$ and $\tilde{B}_1(t):=B_1(t)-\alpha$. Moreover,

$$\tilde{Y}_a(x,t)=G_a(t)H_a(x,t)\begin{pmatrix}1&0\\0&(x-a)^{\beta-\alpha}\end{pmatrix}(x-a)^{J_a(t)}\tag{98}$$

are fundamental matrices of (97) in a neighborhood of $a\in\{0,1\}$. First, suppose that $\beta-\alpha$ is an integer and that $p_0(t)=p_1(t)=0$ holds. In this case $J_0(t)=J_1(t)=0$, and the system (97) has a holomorphic fundamental matrix since $(x-a)^{\beta-\alpha}$ is holomorphic and $\tilde{Y}_0(\cdot,t)$, $\tilde{Y}_1(\cdot,t)$ contain no logarithmic terms. Moreover, as the coefficient matrix $\Phi(\cdot,t)$ of (94) is a rational function which is bounded at infinity, the extension of Halphen's theorem, Theorem 2.4 in Gesztesy *et al.* (2000), implies that the system (97) has a fundamental matrix of the form $\tilde{Y}(x)=R(x)e^{C(t)x}$ with some rational (and hence polynomial) matrix function $R:\mathbb{C}\to\mathrm{M}_2(\mathbb{C})$. Conversely, if (94) has a fundamental matrix of the form (95), then $\tilde{Y}_0(\cdot,t)$ and $\tilde{Y}_1(\cdot,t)$ are holomorphic matrix functions, which gives $\beta-\alpha\in\mathbb{Z}$ and $J_0(t)=J_1(t)=0$.

Next, let us assume that $Q_{12}(t)=0$. If we define

$$y(x):=Y_0(x,t)\begin{pmatrix}0\\1\end{pmatrix}=x^{\beta}G_0(t)H_0(x,t)\begin{pmatrix}0\\1\end{pmatrix},$$

then y is a nontrivial solution of (94), and $x^{-\beta}y(x)$ is analytic at $x=0$. Since $Y_0(x,t)=Y_1(x,t)Q(t)$ and $Q_{12}(t)=0$, we obtain

$$y(x)=Y_1(x,t)Q(t)\begin{pmatrix}0\\1\end{pmatrix}=(x-1)^{\beta}G_1(t)H_1(x,t)\begin{pmatrix}0\\Q_{22}(t)\end{pmatrix},$$

and therefore $(1-x)^{-\beta}y(x)$ is analytic in a neighborhood of $x=1$. Now, by the existence and uniqueness theorem, $h(x):=[x(1-x)]^{-\beta}y(x)$ can be extended to an entire vector function. Conversely, suppose that (94) has a nontrivial solution of the form (96). Then

$$y(x)=Y_0(x,t)\begin{pmatrix}0\\c_0\end{pmatrix}=Y_1(x,t)\begin{pmatrix}0\\c_1\end{pmatrix}$$

with some constants $c_0,c_1\in\mathbb{C}\setminus\{0\}$. Since $Y_0(x,t)=Y_1(x,t)Q(t)$, it follows that

$$Q(t)\begin{pmatrix}0\\ c_0\end{pmatrix}=\begin{pmatrix}0\\ c_1\end{pmatrix},$$

which gives $Q_{21}(t)=0$.

Now, in addition to (i) and (ii), we assume that the coefficients of (94) satisfy the following conditions.

(iii) There exists an analytical function $\Omega:\mathbb{C}\times\mathfrak{D}\to M_2(\mathbb{C})$ such that the deformation equation (84) holds in $(\mathbb{C}\setminus\{0,1\})\times\mathfrak{D}$, where Φ is given by

$$\Phi(x,t):=\frac{1}{x}B_0(t)+\frac{1}{x-1}B_1(t)+C(t),\quad (x,t)\in(\mathbb{C}\setminus\{0,1\})\times\mathfrak{D}.$$

(iv) The matrix functions G_a, $a\in\{0,1\}$, satisfy the differential equations

$$\frac{\partial G_a}{\partial t}(t)=\Omega(a,t)G_a(t),\quad t\in\mathfrak{D}.$$

The next result is an immediate consequence of Theorem 4 and Lemma 7.

Corollary 2: Suppose that the conditions (i)–(iv) are satisfied. If (P) holds for one $t_0\in\mathfrak{D}$, then (94) has the property (P) for all $t\in\mathfrak{D}$, and if (H) holds for one $t_0\in\mathfrak{D}$, then (94) has the property (H) for all $t\in\mathfrak{D}$.

Finally, we apply the results of this section to prove that the classical as well as the monodromy eigenvalues of the Chandrasekhar–Page angular equation in dependence of $(\mu,\nu)\in\mathbb{R}^2$ are (locally) solutions of the partial differential equation (29).

Lemma 8: Let $\kappa\in\left[\frac{1}{2},\infty\right)$ and $\sigma\in\{-1,+1\}$ be fixed. Moreover, suppose that the functions $v:\mathfrak{D}\to\mathbb{R}\setminus\{0\}$ and $w:\mathfrak{D}\to\mathbb{R}$ are solutions of the system (50) and (51) on some interval $\mathfrak{D}\subset(0,\infty)$. Finally, let

$$\mu(t):=\frac{t}{2}\left(v(t)+\frac{\sigma}{v(t)}\right),\quad \nu(t):=\frac{t}{2}\left(v(t)-\frac{\sigma}{v(t)}\right),\quad t\in\mathfrak{D},\tag{99}$$

and $t_0\in\mathfrak{D}$. If $w(t_0)$ is an eigenvalue of $A(\kappa;\mu(t_0),\nu(t_0))$, then $w(t)$ is an eigenvalue of $A(\kappa;\mu(t),\nu(t))$ for each $t\in\mathfrak{D}$. Furthermore, if κ is a half-integer and $w(t_0)$ is a monodromy eigenvalue of $A(\kappa;\mu(t_0),\nu(t_0))$, then $w(t)$ is a monodromy eigenvalue of $A(\kappa;\mu(t),\nu(t))$ for each $t\in\mathfrak{D}$.

Proof: In terms of (99) and $\lambda(t):=w(t)$, the coefficient matrices (12) of the system (11) take the form

$$B_0(t)=\begin{pmatrix}-\frac{\kappa}{2}-\frac{1}{4} & \frac{t}{2}\left(v(t)+\frac{\sigma}{v(t)}\right)-w(t)\\ 0 & \frac{\kappa}{2}+\frac{1}{4}\end{pmatrix},$$

$$B_1(t)=\begin{pmatrix}\frac{\kappa}{2}+\frac{1}{4} & 0\\ \frac{t}{2}\left(v(t)+\frac{\sigma}{v(t)}\right)-w(t) & -\frac{\kappa}{2}-\frac{1}{4}\end{pmatrix},$$

$$C(t) = \frac{t}{v(t)} \begin{pmatrix} -(v(t)^2+1) & -(v(t)^2-1) \\ (v(t)^2-1) & (v(t)^2+1) \end{pmatrix},$$

where the condition (i) is satisfied with $\alpha = -(\kappa/2) - \frac{1}{4}$ and $\beta = (\kappa/2) + \frac{1}{4}$. Now, if we define the matrix function

$$\Omega(x,t) := \frac{1}{v(t)} \begin{pmatrix} (v(t)^2-\sigma)\left(\frac{1}{2}-x\right) & (v(t)^2+\sigma)(1-x) \\ (v(t)^2+\sigma)x & (v(t)^2-\sigma)\left(x-\frac{1}{2}\right) \end{pmatrix}, \quad (x,t) \in \mathbb{C} \times \mathfrak{D},$$

then, by a straightforward calculation using the characteristic equations (50) and (51), it follows that the deformation equation in (iii) holds. Finally, by setting

$$G_0(t) := \begin{pmatrix} e^{\phi(t)} & \left[\frac{t}{2}\left(v(t) + \frac{\sigma}{v(t)}\right) - w(t)\right] e^{-\phi(t)} \\ 0 & (\kappa + \frac{1}{2}) e^{-\phi(t)} \end{pmatrix}, \quad G_1(t) := KG_0(t)K,$$

where K is the matrix (20) and

$$\phi(t) := \int_{t_0}^{t} \frac{v(\tau)^2 - \sigma}{2v(\tau)} \mathrm{d}\tau, \quad t \in \mathfrak{D},$$

the conditions (ii), (iv) are satisfied. Since $w(t)$ is a monodromy eigenvalue of $A(\kappa;\mu(t),\nu(t))$ if and only if (11) has the property (P), and $w(t)$ is a classical eigenvalue of $A(\kappa;\mu(t),\nu(t))$ if and only if (11) has the property (H), the assertion follows from Corollary 2. □

Theorem 5: *For a fixed $\kappa = k - \frac{1}{2}$ with a positive integer k, let $(0,0) \in \mathfrak{S} \subset \mathbb{R}^2$ be a simply connected domain such that for each $(\mu,\nu) \in \mathfrak{S}$ all monodromy eigenvalues $\lambda_0^j(\kappa;\mu,\nu)$, $j = 1-k,\ldots,k-1$, of $A(\kappa;\mu,\nu)$ are simple zeros of the polynomial $P(\kappa;\cdot,\mu,\nu)$ given by Theorem 3. Then each function $\lambda = \lambda_0^j$, $j = 1-k,\ldots,k-1$, satisfies the partial differential equation (29) in $\mathfrak{S}$.*

Proof: Let $j \in \{1-k,\ldots,k-1\}$ be fixed. The monodromy eigenvalues of $A(\kappa;\mu,\nu)$ are exactly the zeros of the polynomial $P(\kappa;\cdot;\mu,\nu)$, and since all zeros of $P(\kappa;\cdot;\mu,\nu)$ are simple, the implicit function theorem implies that $\lambda_0^j(\kappa;\mu,\nu)$ depends analytically on (μ,ν) in $\mathfrak{S}$. In order to show that the function $\lambda = \lambda_0^j$ satisfies the PDE (29), we make use of the unique continuation property of analytical functions. That means, it suffices to prove that (29) holds for $\lambda = \lambda_0^j$ in a neighborhood of some point $(\mu,\nu) = (\tau,0) \in \mathfrak{S}$, $\tau > 0$. Now, in view of the coordinate transformation (99), we must verify that the function $\lambda_0^j(\kappa;\mu(t,v),\nu(t,v))$ is a solution of the partial differential equation (49) in a neighborhood of the point $(t,v) = (\tau,1)$. To this end, let us consider the characteristic equations of (49),

$$\frac{\partial v}{\partial t}(t,u) = -\frac{2v(t,u)w(t,u)}{t},$$

$$\frac{\partial w}{\partial t}(t,u) = -\kappa\left(v(t,u) + \frac{1}{v(t,u)}\right) - \frac{t}{2}\left(v(t,u)^2 - \frac{1}{v(t,u)^2}\right)$$

together with the initial values

$$v(\tau,u) = u, \quad w(\tau,u) = \lambda_0^j(\kappa;\mu(\tau,u),\nu(\tau,u)),$$

which depend analytically on the parameter $u \in (0,\infty)$. The solutions $v(t,u)$ and $w(t,u)$ of this initial value problem are analytical functions in a neighborhood of $(\tau,1)$, and since $(\partial v/\partial u)(\tau,u) = 1$, they form locally an integral surface for the PDE (49), compare John (1982, Chap. 1, Sec. 5). More precisely, there exists an analytical function U defined on a neighborhood

$\mathfrak{V}$ of $(t,v)=(\tau,1)$ such that $U(\tau,v)=v$, and $W(t,v):=w(t,U(t,v))$ is a solution of (49) in $\mathfrak{V}$. Now, Lemma 8 implies that $W(t,v)$ is a monodromy eigenvalue of $A(\kappa;\mu(t,v),\nu(t,v))$ for all $(t,v)\in\mathfrak{V}$, and since $W(\tau,v)=\lambda_0^j(\kappa;\mu(\tau,v),\nu(\tau,v))$, it follows that $W(t,v)=\lambda_0^j(\kappa;\mu(t,v),\nu(t,v))$ holds identically on $\mathfrak{V}$. This completes the proof of the theorem. □

In a similar way we can apply Lemma 8 to prove that for fixed $\kappa\in(0,\infty)$ the zeros of the function $\lambda\mapsto\Delta(\kappa;\lambda,\mu,\nu)$ defined in Sec. II and therefore the eigenvalues of $A(\kappa;\mu,\nu)$ satisfy the partial differential equation (29). This alternative proof of Theorem 1 is based on monodromy preserving deformation—a general technique, which should be applicable to other eigenvalue problems as well. Potential candidates and associated Ω-matrices for solving the deformation equations can be found in Jimbo and Miwa (1981a, Appendix C).

Finally, as a consequence of Theorem 5, the zeros of the polynomial $P(\kappa;\cdot;\mu,\nu)$ given by Theorem 3 satisfy the PDE (29) and do not coincide with any eigenvalue of $A(\kappa;\mu,\nu)$ in a neighborhood of $(\mu,\nu)=(0,0)$. Moreover (see the proof of Lemma 4), $P(\kappa;\cdot;\mu,\nu)$ gives rise to a special integral of polynomial type for the Painlevé III (52). Now, the results of Mansfield and Webster (1998) suggest that these special integrals are unique in some sense, which in turn implies that classical eigenvalues of the Chandrasekhar–Page angular equation are not algebraic.

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APPENDIX A: EIGENVALUES AND EIGENFUNCTIONS IN THE CASE $\mu=\nu=0$

For fixed $\kappa\in[\frac{1}{2},\infty)$, a point $\lambda\in\mathbb{C}$ is an eigenvalue of $A(\kappa;0,0)$ if and only if the system (5) with $(\mu,\nu)=(0,0)$ has a nontrivial solution $S(\theta)$ satisfying

$$\int_0^\pi |S(\theta)|^2\,\mathrm{d}\theta<\infty. \tag{A1}$$

Introducing the functions $u,v:(-1,1)\to\mathbb{C}$ by

$$S(\theta) =: \sin^{\kappa+1/2}\theta\begin{pmatrix}\sqrt{\tan\frac{\theta}{2}}\,u(\cos\theta)\\ \sqrt{\cot\frac{\theta}{2}}\,v(\cos\theta)\end{pmatrix}, \tag{A2}$$

then (5) with $(\mu,\nu)=(0,0)$ is transformed into

$$(1-x)u'(x)=(\kappa+\tfrac{1}{2})u(x)+\lambda v(x),\quad (1+x)v'(x)=-\lambda u(x)-(\kappa+\tfrac{1}{2})v(x), \tag{A3}$$

and the normalization condition (A1) is equivalent to

$$\int_{-1}^1 u(x)^2(1-x)^{\kappa+1/2}(1+x)^{\kappa-1/2}\,\mathrm{d}x<\infty,\quad \int_{-1}^1 v(x)^2(1-x)^{\kappa-1/2}(1+x)^{\kappa+1/2}\,\mathrm{d}x<\infty. \tag{A4}$$

If $\lambda=0$, then the differential equations (A3) imply that there are constants $c_1,c_2\in\mathbb{C}$ such that $u(x)=c_1(1-x)^{-\kappa-1/2}$ and $v(x)=c_2(1+x)^{-\kappa-1/2}$, and from the condition (A4) it follows that $c_1=c_2=0$. Hence, $\lambda=0$ is not an eigenvalue of $A(\kappa;0,0)$, and we assume in what follows that $\lambda\neq0$. In this case, the second equation in (A3) gives

$$u(x) = -\frac{1+x}{\lambda}v'(x) - \frac{\kappa+\frac{1}{2}}{\lambda}v(x), \tag{A5}$$

and for v we obtain the second order differential equation

$$(1-x^2)v''(x) + [1-2(\kappa+1)x]v'(x) + \left[\lambda^2 - \left(\kappa+\frac{1}{2}\right)^2\right]v(x) = 0.$$

If we set $\alpha := \kappa - \frac{1}{2}$, $\beta := \kappa + \frac{1}{2}$, and $\Lambda := \lambda - \kappa - \frac{1}{2}$, this differential equation becomes

$$(1-x^2)v''(x) + [\beta - \alpha - (\alpha+\beta+2)x]v'(x) + \Lambda(\Lambda+\alpha+\beta+1)v(x) = 0, \tag{A6}$$

and the second condition in (A4) takes the form

$$\int_{-1}^{1} v(x)^2(1-x)^\alpha(1+x)^\beta \, dx < \infty. \tag{A7}$$

Note that (A6) and (A7) is the eigenvalue problem associated to the Jacobi polynomials. More precisely, the solutions of the differential equation (A6) which are square integrable with respect to the weight function $(1-x)^\alpha(1+x)^\beta$ are constant multiples of the Jacobi polynomials $P_n^{(\alpha,\beta)}$ with some non-negative integer n, and the corresponding eigenvalues $\lambda_n^\pm$ are determined by the equation $\lambda^2 - (\kappa+\frac{1}{2})^2 = n(n+\alpha+\beta+1)$, i.e., $\lambda_n^\pm = \pm(\kappa+\frac{1}{2}+n)$. Now, if we define $v(x) := -P_n^{(\alpha,\beta)}(x)$, $x \in (-1,1)$, then (A5) yields

$$\begin{aligned}
\lambda_n^\pm u(x) &= (1+x)\frac{d}{dx}P_n^{(\alpha,\beta)} + \beta P_n^{(\alpha,\beta)} = \frac{\alpha+\beta+n+1}{2}(1+x)P_{n-1}^{(\alpha+1,\beta+1)} + \beta P_n^{(\alpha,\beta)} \\
&= \frac{\alpha+\beta+n+1}{\alpha+\beta+2n+1}[(\beta+n)P_{n-1}^{(\alpha+1,\beta)} + nP_n^{(\alpha+1,\beta)}] + \beta P_n^{(\alpha,\beta)} \\
&= (\alpha+\beta+n+1)P_n^{(\alpha+1,\beta)} - (\alpha+n+1)P_n^{(\alpha,\beta)} \\
&= (\beta+n)P_n^{(\alpha+1,\beta-1)} = |\lambda_n^\pm| P_n^{(\alpha+1,\beta-1)},
\end{aligned}$$

where we applied the differentiation formulas and contiguous relations for Jacobi polynomials, see Magnus *et al.* (1966, Sec. 5.2). Hence, $u(x) = \pm P_n^{(\alpha+1,\beta-1)}(x)$, $x \in (-1,1)$, and since u satisfies the first condition in (A4), the numbers $\lambda_n^\pm$ are in fact eigenvalues of $A(\kappa;0,0)$. Moreover, the corresponding eigenfunctions are constant multiples of

$$\sin^\kappa\theta \begin{pmatrix} \pm\sqrt{\tan\frac{\theta}{2}}\, P_n^{(\kappa+1/2,\kappa-1/2)}(\cos\theta) \\ -\sqrt{\cot\frac{\theta}{2}}\, P_n^{(\kappa-1/2,\kappa+1/2)}(\cos\theta) \end{pmatrix}, \quad \theta \in (0,\pi),$$

which form a complete orthogonal set in $\mathcal{L}^2((0,\pi),\mathbb{C}^2)$. In particular, the spectrum of $A(\kappa;0,0)$ is given by $\{\lambda_n^\pm : n = 0,1,2,\ldots\}$.

APPENDIX B: A NUMERICAL EXAMPLE

As a numerical example, we have computed the coefficients $c_{m,n}$ of the power series expansion (38) up to and including $m+n=8$ for $\kappa=\frac{1}{2}$ and $j=1$ using the recurrence relation given in Sec. III. The coefficients have been rounded to six significant figures and listed in Table I. It should be noted that they are to some extent different from the coefficients displayed in Suffern *et al.* (1983, Table I). Evaluating the power series expansion (38) at $\alpha=0.01$ and $\beta=0.02$, i.e., $(\mu,\nu) = (0.005, 0.015)$, yields $\tilde{\lambda}_1 = 1.011\,67$ as a numerical approximation for the eigenvalue λ_1, and this result coincides with the value given in Suffern *et al.* (1983, Table II). For a second pair of

TABLE I. The coefficients $c_{m,n}$, $0 \leqslant m+n \leqslant 8$, of the power series expansion (38) in the case $\kappa = \frac{1}{2}$ and $j=1$.

	$m=0$	1	2	3	4	5	6	7	8
$n=0$	1.000 00e+00	5.000 00e−01	0.000 00	0.000 00	0.000 00	0.000 00	0.000 00	0.000 00	0.000 00
1	1.666 67e−01	0.000 00	0.000 00	0.000 00	0.000 00	0.000 00	0.000 00	0.000 00	
2	7.407 41e−02	−1.481 48e−02	0.000 00	0.000 00	0.000 00	0.000 00	0.000 00		
3	−8.230 45e−03	3.292 18e−03	−4.703 12e−04	0.000 00	0.000 00	0.000 00			
4	−9.144 95e−04	5.486 97e−04	−1.222 81e−04	1.358 68e−05	0.000 00				
5	5.080 53e−04	−4.064 42e−04	1.417 90e−04	−2.670 91e−05					
6	−3.387 02e−05	3.387 02e−05	−1.633 51e−05						
7	−2.634 35e−05	3.161 22e−05							
8	7.108 56e−06								

parameters $(\alpha,\beta)=(0.5,1.0)$, i.e., $(\mu,\nu)=(0.25,0.75)$, we obtain $\tilde{\lambda}_1=1.597\,45$, which differs slightly from the value $\hat{\lambda}_1=1.597\,64$ listed in Suffern *et al.* (1983, Table II). In order to test the reliability of our numerical result, we can use the statement of Lemma 3. That means, we approximate $\Theta(\lambda)$ defined in (25) by the second component $\Theta_n(\lambda)$ of $d_n(\lambda)$ for $n=8$, and we compare $\Theta_8(\tilde{\lambda}_1)$ and $\Theta_8(\hat{\lambda}_1)$ with the theoretical result $\Theta(\lambda_1)=0$. As $\Theta_8(\tilde{\lambda}_1)=3.608\,82e-05$ and $\Theta_8(\hat{\lambda}_1)=-2.511\,64e-04$, our result seems to be more trustworthy. Finally, let $(\mu,\nu)=(0.02,0.1)$. The coefficients of the polynomial Θ_8 are given in Table II. For these parameters, our power series approximation gives $\tilde{\lambda}_1=1.073\,79$ which differs significantly from the value $\hat{\lambda}_1=1.061\,04$ given by Chakrabarti (1984, Table I). Despite his claiming of an accuracy of six decimals, the evaluation of Θ_8 at the eigenvalues in question gives $\Theta_8(\tilde{\lambda}_1)=5.688\,99e-12$ and $\Theta_8(\hat{\lambda}_1)=1.527\,70e-02$ in favor of our result. Thus, Chakrabarti's calculations should be taken with some caution.

APPENDIX C: EIGENFUNCTIONS IN THE CASE $|\mu| \neq |\nu|$

Eliminating the second component of y in the system (11), we get a linear second-order differential equation for the first component y_1 given by

$$\frac{\mathrm{d}^2 y_1}{\mathrm{d}x^2}(x) + \left(\frac{1}{x} - \frac{1}{x-b}\right)\frac{\mathrm{d}y_1}{\mathrm{d}x}(x) + \left(\tau_0 + \frac{\tau_1}{x} + \frac{\tau_2}{x^2} + \frac{\tau_3}{x-1} + \frac{\tau_4}{(x-1)^2} + \frac{\tau_5}{x-b}\right) y_1(x) = 0$$

with

$$b := \frac{\mu-\lambda}{2\mu}, \quad \tau_0 := 4(\mu^2-\nu^2),$$

TABLE II. The coefficients δ_n of the polynomial $\Theta_8(\lambda)=\sum_{n=0}^{16}\delta_n\lambda^n$ for $\kappa=\frac{1}{2}$, $\mu=0.02$, $\nu=0.1$.

$n=0$	1.221 51e+00	$n=9$	4.911 51e−06
1	1.443 47e−02	10	−4.220 48e−04
2	−1.705 25e+00	11	−9.466 10e−08
3	−7.922 97e−03	12	1.026 43e−05
4	6.721 14e−01	13	6.889 33e−10
5	1.460 03e−03	14	−1.264 70e−07
6	−1.123 51e−01	15	−1.000 00e−26
7	−1.210 28e−04	16	6.151 19e−10
8	9.396 64e−03		

$$\tau_1 := \lambda^2 - 2\alpha^2 + 2\nu + \alpha - \mu^2 - 4\alpha\nu + \frac{2\alpha\mu}{\mu - \lambda}, \quad \alpha := \frac{\kappa}{2} + \frac{1}{4},$$

$$\tau_2 := -\alpha^2, \quad \tau_3 := \frac{4\alpha\mu^2}{\mu^2 - \lambda^2} + 2\nu - \tau_1, \quad \tau_4 := \alpha(1-\alpha), \quad \tau_5 := \frac{2(\nu\mu^2 + 2\alpha\mu^2 - \nu\lambda^2)}{\lambda^2 - \mu^2}.$$

Now by means of the transformation

$$y_1(x) := x^\alpha (x-1)^\alpha \psi(x) e^{2tx}, \quad t = \pm\sqrt{\nu^2 - \mu^2},$$

we find that $\psi(x)$ satisfies the generalized Heun equation,

$$\frac{d^2\psi(x)}{dx^2} + \left(\frac{1-\mu_0}{x} + \frac{1-\mu_1}{x-1} + \frac{1-\mu_2}{x-b} + 4t\right)\frac{d\psi(x)}{dx} + \frac{\beta_0 + \beta_1 x + \beta_2 x^2}{x(x-1)(x-b)}\psi(x) = 0, \tag{C1}$$

where

$$\mu_0 = -2\alpha, \quad \mu_1 = 1 - 2\alpha, \quad \mu_2 = 2, \quad \beta_2 := 8\alpha t,$$

and

$$\beta_1 = \mu^2 - \lambda^2 - 2t[b + 2\alpha(1+2b)] + 2\alpha(\alpha - 1) + 2\nu(2\alpha - b) - \frac{2\alpha\mu(b-1)}{\lambda + \mu} + \frac{2\alpha\mu b}{\mu - \lambda},$$

$$\beta_0 = b(\lambda^2 - \mu^2) + b[2(\nu + t) - 4\alpha(\nu - t) - 4\alpha^2] + \alpha - \frac{2\mu\alpha b}{\lambda - \mu}.$$

We observe that 0, 1, and b are simple singularities with characteristic exponents $(0, \mu_0)$, $(0, \mu_1)$, and $(0, \mu_2)$, respectively, while ∞ is (at most) an irregular singularity of rank 1. To stress the importance of Eq. (C1), it is sufficient to remark that it contains the ellipsoidal wave equation as well as Heun's equation and thus the Mathieu, spheroidal, Lamé, Whittaker-Hill, and Ince equations as special cases.

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Integrable Hamiltonian systems with vector potentials

Giuseppe Pucacco[a)]
Dipartimento di Fisica, Università di Roma "Tor Vergata," INFN, Sezione di Roma II, Rome, Italy

Kjell Rosquist[b)]
Department of Physics, Stockholm University, Stockholm, Sweden

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We investigate integrable two-dimensional Hamiltonian systems with scalar and vector potentials, admitting second invariants which are linear or quadratic in the momenta. In the case of a linear second invariant, we provide some examples of weakly integrable systems. In the case of a quadratic second invariant, we recover the classical strongly integrable systems in *Cartesian and polar coordinates* and provide some new examples of integrable systems in *parabolic and elliptical coordinates*. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1818721]

I. INTRODUCTION

The direct approach to investigate integrable Hamiltonian systems is a very classical subject.[1,2] It consists in determining the class of potentials supporting additional invariants within some specified family of phase-space functions. This method produced several interesting results in the 1980s, as illustrated in the review by Hietarinta.[3] Recently[4–6] the approach has been applied to treat in a unified way both invariants at arbitrary and fixed energy, where the second possibility is related to the existence of additional "weak" invariants only on given energy hypersurfaces.

Many results are known for natural reversible Hamiltonians. One of the reasons for this is that the search for additional invariants can be restricted to functions with a definite parity in the momenta. This property leads to a substantial reduction in the usually very complicated set of equations. Much less is known in the case of Hamiltonians with vector potentials. For a long time, the only systematic attempt to cope with this case was that of Dorizzi *et al.*[7] providing a set of solutions in Cartesian coordinates. Recently, McSween and Winternitz[8] obtained some new solutions in polar coordinates and Bérubé and Winternitz[9] extended the results to the corresponding quantum problem. In both works the authors also identify the subset of superintegrable systems. In an attempt to extend these results to include weak integrability, we have provided[10] a general solution for linear invariants and analyzed some new classes of weakly integrable systems.

The physical applications of Hamiltonians with terms linear in the momenta are of great relevance. Just to mention one of the most important, we recall the ubiquitous role of rotation in astrophysical problems like those of galactic dynamics. The purpose of the present paper is to reinvestigate Hamiltonian systems with both scalar and vector potentials, trying to identify those admitting the existence of a second invariant which is a quadratic polynomial in the momenta. We state the general approach at arbitrary and fixed value of the first invariant (Jacobi constant) and show that, in the case of strong integrability, it is possible to get a general formal solution. This is valid for every standard coordinate systems which are the same as the separable ones in the purely scalar case. Therefore, in addition to the above-mentioned Cartesian and polar case, solutions in parabolic and elliptical coordinates can be looked for. In all cases, the potentials are defined in terms of a pair of scalar functions for which we get the integrability conditions: solving them

[a)]Electronic mail: pucacco@roma2.infn.it
[b)]Electronic mail: kr@physto.se

determines the vector potential, whereas the scalar potential is subject to an additional linear differential equation. We provide some new examples of integrable systems with a vector potential whose existence can be discovered working in parabolic and elliptical coordinates. The case of quadratic invariants was also addressed by Yehia[11,12] who obtained integrable systems with Riemannian configuration space and applications to rigid body dynamics: the examples with a flat configuration space can be reproduced with the procedure devised here. The issue of separation of the Hamilton–Jacobi equation in presence of a vector potential has been recently faced by Benenti, Chanu, and Rastelli.[13] Their general approach requires an extended configuration space, preventing the application of the approach adopted here which heavily resides on the use of conformal coordinate transformation in two dimensions.

The plan of the paper is as follows: in Sec. II we recall the structure of Hamiltonian systems with terms linear in the velocities; in Sec. III we illustrate a version of the direct approach to find polynomial invariants which is particularly efficient in treating two-dimensional systems; in Sec. IV, for the sake of completeness, we recall systems admitting a second invariant which is a linear polynomial in the momenta; in Sec. V we treat the case of the quadratic second invariant; in Sec. VI we illustrate all known strongly integrable solutions in the quadratic case; and in Sec. VII we conclude.

II. HAMILTONIANS WITH SCALAR AND VECTOR POTENTIALS

We are interested in finding integrable examples of systems generated by a Hamiltonian function of the type

$$\mathcal{H} = \tfrac{1}{2}(p_x^2 + p_y^2) + A_1(x,y)p_x + A_2(x,y)p_y + V(x,y), \tag{1}$$

where the function V is the ordinary "scalar" potential and A_1 and A_2 are the components of a "vector" potential $\mathbf{A}$ in two dimensions. Under the canonical transformation

$$p_x \to p_x + \partial_x F, \quad p_y \to p_y + \partial_y F, \tag{2}$$

where $F(x,y)$ is an arbitrary function, the Hamiltonian remains invariant if $\mathbf{A}$ and V are changed according to

$$\mathbf{A} \to \mathbf{A} + \nabla F, \tag{3}$$

$$V \to V + \mathbf{A} \cdot \nabla F + \tfrac{1}{2}|\nabla F|^2. \tag{4}$$

However, the two quantities

$$\Omega(x,y) = \tfrac{1}{2}(\partial_y A_1 - \partial_x A_2) \tag{5}$$

and

$$W(x,y) = V - \tfrac{1}{2}|\mathbf{A}|^2 \tag{6}$$

are "gauge invariants" and can therefore be used to uniquely characterize the model system. The Hamiltonian to be worked on becomes then

$$\mathcal{H} = \tfrac{1}{2}(p_x + A_1(x,y))^2 + \tfrac{1}{2}(p_y + A_2(x,y))^2 + W(x,y). \tag{7}$$

Ω, the "curl" of the vector potential, has several physical interpretations: in astrophysical and celestial mechanical applications, it usually denotes an angular velocity field; it is a magnetic field in electrodynamics and plasma physics and so on. We remark that in general it is easier to attempt to solve directly for Ω and W. To recover the scalar V, one must have A_1 and A_2 and this can be another difficult problem.[3]

We can first write the canonical equations provided by (1),

$$\dot{x} = p_x + A_1, \tag{8}$$

$$\dot{y} = p_y + A_2, \tag{9}$$

$$\dot{p}_x = -\partial_x A_1 p_x - \partial_x A_2 p_y - \partial_x V, \tag{10}$$

$$\dot{p}_y = -\partial_y A_1 p_x - \partial_y A_2 p_y - \partial_y V, \tag{11}$$

and then simplify them by exploiting the functions introduced above to get the equations of motion

$$\ddot{x} - 2\Omega\dot{y} = -\partial_x W, \tag{12}$$

$$\ddot{y} + 2\Omega\dot{x} = -\partial_y W. \tag{13}$$

It is readily verified that under the phase-space flow generated by (12) and (13), there exists a conserved function that is the first invariant of the system (*Jacobi constant*),

$$J = \tfrac{1}{2}(\dot{x}^2 + \dot{y}^2) + W. \tag{14}$$

In the investigation of the integrability properties of Hamiltonian (7), it turns out to be very helpful to work with complex variables. We perform then the canonical point transformation given by

$$z = x + iy, \quad p_z = p = \tfrac{1}{2}(p_x - ip_y), \tag{15}$$

$$\overline{z} = x - iy, \quad p_{\overline{z}} = \overline{p} = \tfrac{1}{2}(p_x + ip_y), \tag{16}$$

so that Hamiltonian (7) turns out to be

$$\mathcal{H} = 2(p + \Phi)(\overline{p} + \overline{\Phi}) + W(z, \overline{z}), \tag{17}$$

where the complex function

$$\Phi = \tfrac{1}{2}(A_1 - iA_2) \tag{18}$$

has been introduced. In these variables, Ω is given by

$$\Omega = 2\Im\{\partial_z \Phi\}, \tag{19}$$

where $\Im$ denotes the imaginary part. Equations (15) and (16) display a nice space-saving feature of using complex variables: even if an expression is not real, it is enough to write a single relation between complex functions [like, e.g., (15)]. The remaining information is provided by the corresponding complex conjugate expression, which we therefore do not write explicitly. For example, the canonical equations given by (17) are

$$\dot{z} = 2(\overline{p} + \overline{\Phi}), \tag{20}$$

$$\dot{p} = -2(\overline{p} + \overline{\Phi})\partial_z \Phi - 2(p + \Phi)\partial_z \overline{\Phi} - \partial_z W, \tag{21}$$

and the equations of motion corresponding to (12) and (13) are

$$\ddot{z} + 2i\Omega\dot{z} = -2\partial_{\overline{z}} W. \tag{22}$$

The Jacobi constant now is

$$J = \tfrac{1}{2}\dot{z}\dot{\overline{z}} + W. \tag{23}$$

III. POLYNOMIAL INVARIANTS

We are working with a Hamiltonian system with two degrees of freedom of which we already know an invariant, the Jacobi constant. In order to identify integrable systems in the usual Liouville–Arnold sense, we must find a second independent phase-space function conserved along the flow. The standard direct method to solve the problem consists in making a suitable ansatz about this function and trying to solve the system of differential equations ensuing by the conservation condition. For several reasons, the ansatz of a polynomial in the generalized momenta is the most common.[3] It is well suited from the mathematical point of view, since it allows one to get a system of PDEs in the coordinates only and is also well grounded on the basis of experience with already known integrable systems.

Since we are looking for a real function, we make the following assumption:

$$I^{(M)} = \sum_{k=0}^{M} (D_k(p+\Phi)^k + \overline{D}_k(\overline{p}+\overline{\Phi})^k). \tag{24}$$

Although it is common, in the vector potential case, to see the invariant written in terms of the velocities, this is the correct interpretation of $I^{(M)}$ as a phase-space function of the canonical variables. In order to satisfy the conservation of function (24), we impose that its Poisson bracket with the Hamiltonian vanishes,

$$\{I^{(M)}, \mathcal{H}\} = 0, \tag{25}$$

and try to solve for the complex functions $D_k(z,\overline{z})$. In the presentation of the results, for easy comparisons with existing works, we will revert to the usual expressions in terms of the velocities, replacing the momenta in (24) according to (20). In this case, conservation of the invariant can be checked by means of the condition

$$\frac{\mathrm{d}I^{(M)}}{\mathrm{d}t} = 0, \tag{26}$$

along the solution of the equations of motion (22).

Following the approach already used in the scalar case,[4–6] we consistently apply the trick of the energy constraint even in the present case. Here, with energy, we mean the Jacobi constant (23). This method has the advantage of allowing the simultaneous treatment of "strong" invariants (the usual ones which are conserved for arbitrary values of the energy) and "weak" invariants (functions which are conserved only on some energy surfaces). In the papers cited above, we have moreover shown how the energy constraint simplifies the structure of the system of PDEs that must be solved. The essential remark is that, to identify the cases of strong integrability, it is sufficient that in the final results a subset can be isolated which is independent of the energy parameter, in the present situation the given value of the first invariant, let us say C. If we are interested in a "strongly integrable system," in the end we must get a solution independent of C. The procedure may appear more involute, but, at least in the scalar case, it reveals to be very effective.

Formally, the idea of operating with the energy constraint is very simple. It consists first in introducing the "null" Hamiltonian,

$$\mathcal{H}_0 = \mathcal{H} - C \equiv 0, \tag{27}$$

or, on the same footing, the "null" Jacobi invariant,

$$J_0 = J - C = \tfrac{1}{2}\dot{z}\dot{\overline{z}} - G \equiv 0, \tag{28}$$

where C as usual denotes the given fixed value of the Jacobi constant and

$$G = C - W \tag{29}$$

is the so-called "Jacobi potential." Second, using in a consistent way the constraint

$$2(p + \Phi)(\overline{p} + \overline{\Phi}) = G, \tag{30}$$

wherever it appears in the computations. This essentially occurs when, implementing the conservation condition (25), a polynomial relation in the generalized momenta appears and the constraint (30) is used to eliminate powers of the mixed variables $(p+\Phi)(\overline{p}+\overline{\Phi})$ in favor of powers of G. One minor shortcoming of this approach is that, in view of the explicit appearance of the function G, rather than simply the potential W, some of the coefficients of the invariant in general depend on the energy parameter too,

$$D_j = D_j(z, \overline{z}; C), \quad 0 \leqslant j \leqslant M - 2. \tag{31}$$

Therefore, to obtain the standard expression in terms of phase-space coordinates only, in the end we must remember to perform the substitution

$$C \to \mathcal{H}(p, \overline{p}, z, \overline{z}), \tag{32}$$

wherever the parameter C appears. In view of (31), we see that this replacement does not affect the degree of the polynomial in the momenta.

In practice, computing the Poisson bracket (25), using the constraint, collecting the coefficients of the various powers of $p+\Phi$ (they are accompanied by their complex conjugates) and imposing their vanishing, we get the system

$$\partial_{\overline{z}} D_{k-1} + ik\Omega D_k + \frac{1}{2G^k}\partial_z(G^{k+1} D_{k+1}) = 0, \quad k = 0, 1, \ldots, M, \tag{33}$$

where it is implicitly assumed that $D_j = 0$ for $j < 0$ and for $j > M$. The set of equation (33) must be supplemented by the closure equations

$$\partial_{\overline{z}} D_M = 0 \tag{34}$$

and

$$\Re\{\partial_z(G D_1)\} = 0, \tag{35}$$

where $\Re$ denotes the real part. For sake of space, we do not write the expressions of the standard direct approach in real coordinates and without the energy constraint. To compare with, we refer to Sec. IV of Hietarinta[3] and recall the work of Hall,[14] where the study of weak invariants was first addressed and of Sarlet *et al.*,[15] where some wrong deductions contained in Hall's work were corrected. A systematic analysis of the cases with $M = 1$ (linear invariant) and $M = 2$ (quadratic invariant) was started in Ref. 7 and recently taken up again in Ref. 8. A more general version of the problem concerned with quadratic invariants is mentioned in a different context in Ref. 16.

The first result one easily gets with this approach is that Eq. (34) is readily solved as

$$D_M = D_M(z), \tag{36}$$

that is, the leading order coefficient in the invariant is an *arbitrary analytical function*. This result, already known in the inertial case, still holds here. In Ref. 4 it was shown how, in the purely scalar case, the strong conservation condition restricts the form of this function. In what follows we will get analogous results when also a vector potential is present.

One fundamental difference with what happens in the scalar case, is that equations for coefficients with even and odd indexes do not decouple. This fact is due to the Hamiltonian not being reversible in the present instance. System (33) is therefore very awkward to solve in the general case. In the next two sections we present the solutions in the linear and quadratic cases at fixed and arbitrary values of the Jacobi constant.

IV. LINEAR INVARIANTS

We start the investigation looking for systems admitting a second invariant which is a linear function in the momenta. The ansatz is

$$I^{(1)} = S(p + \Phi) + \overline{S}(\overline{p} + \overline{\Phi}) + K, \tag{37}$$

where for the three coefficients we have used a notation which conforms with that in previous works. The system of equations ensuing from the conservation condition is the following:

$$S_{\overline{z}} = 0, \tag{38}$$

$$K_{\overline{z}} + i\Omega S = 0, \tag{39}$$

$$\Re\{(GS)_z\} = 0. \tag{40}$$

In order to compactify formulas, from hereinafter with the subscript we denote the partial derivative with respect to the corresponding variable.

A. The general solution for linear invariants

Equation (38) agrees with (34), confirming that S can be an arbitrary analytic function,

$$S = S(z). \tag{41}$$

To complete the treatment, given an arbitrary $S(z)$, we must solve (39) and (40). This task is more efficiently achieved by performing a coordinate transformation that trivializes the differential equations. Let us consider a conformal transformation $z=F(w)$ to the new complex variable $w=X+iY$ given by

$$\frac{\mathrm{d}z}{\mathrm{d}w} = F'(w) \equiv S(z(w)). \tag{42}$$

The explicit form of the transformation is then

$$w = \int \frac{\mathrm{d}z}{S(z)} \tag{43}$$

and we have the relation between the differential operators

$$\frac{d}{\mathrm{d}w} = F'(w)\frac{d}{\mathrm{d}z} = S\frac{d}{\mathrm{d}z}. \tag{44}$$

Multiplying (40) by the real factor $S\overline{S}$, the content of the curly brackets can be modified in the following way:

$$S\overline{S}(SG)_z = S(S\overline{S}G)_z = (S\overline{S}G)_w. \tag{45}$$

Introducing the "conformal" potential

$$\tilde{G} = |F'|^2 G = |S|^2 G = S\bar{S}G, \tag{46}$$

Eq. (40) reduces to

$$\Re\{\tilde{G}_w\} = 0, \tag{47}$$

which is readily solved in

$$\tilde{G} = g(Y), \tag{48}$$

where g is an arbitrary real function and, according to the definition of the coordinate transformation, Y is the imaginary part of w.

In the new variables w, Eq. (39), together with its complex conjugate, can be rewritten as

$$K_w = i\tilde{\Omega}, \tag{49}$$

$$K_{\bar{w}} = -i\tilde{\Omega}, \tag{50}$$

where the conformal field

$$\tilde{\Omega} = |S|^2 \Omega \tag{51}$$

has been introduced. The integrability condition for the real function K is

$$\Re\{K_w\} = 0, \tag{52}$$

with solution

$$K = k(Y), \tag{53}$$

where k is another arbitrary real function. The conformal vector potential is then given by

$$\tilde{\Omega} = -\frac{k'(Y)}{2}. \tag{54}$$

An inversion of the coordinate transformation allows one to express the solution in the original variables. The second invariant can be expressed as

$$I^{(1)} = \Re\{S\}\dot{x} + \Im\{S\}\dot{y} + K. \tag{55}$$

B. Linear invariants at arbitrary energy

Equation (40), in view of (41) and recalling the definition of G in (29), can be rewritten as

$$\Re\{S'(C - W) - SW_z\} = 0. \tag{56}$$

If we are interested in strong integrability, namely in an invariant which is conserved for arbitrary values of the Jacobi constant, Eq. (56) must be independent of C. Therefore, it decouples in two independent equations: the first is

$$\Re\{S'(z)\} = 0. \tag{57}$$

The second turns out to be

$$\Re\{(SW)_z\} = 0. \tag{58}$$

Equation (57) means that at arbitrary energy, we are no longer free in the choice of the coordinate transformation: we must comply with this condition which actually imposes very strong limitations. It can be integrated to give

$$S(z) = ikz + \alpha, \tag{59}$$

where k is a real constant and α a complex constant. We can prove that it essentially allows only two kinds of new coordinates, (a) polar coordinates, (b) rotated Cartesian coordinates. To show this, we first observe that we can exploit translations and scaling of the complex plane to further reduce the freedom contained in (59). If k is not zero, a translation allows us to set $\alpha=0$. A scaling allows us then to set $k=1$. We have then the two possibilities,

$$\text{(a)} \quad S(z) = iz, \quad F(w) = e^{iw}, \quad x = e^{-Y}\cos X, \quad y = e^{-Y}\sin X, \tag{60}$$

$$\text{(b)} \quad S(z) = \alpha, \quad F(w) = \alpha w, \quad x = aX - bY, \quad y = bX + aY. \tag{61}$$

Case (a) can be recognized as the transformation to *polar* coordinates. In fact, with the usual notation, they are defined as

$$r = e^{-Y}, \quad \theta = X. \tag{62}$$

Solutions (48)–(54), in view of (28), are

$$W = W(r) = \frac{g(r)}{r^2}, \quad K = k(r), \quad \Omega = \frac{k'(r)}{2r}, \tag{63}$$

and the second invariant turns out to be

$$I^{(1)} = i(z\dot{z} - \overline{z\,\dot{z}}) + K = r^2\dot{\theta} + k(r). \tag{64}$$

The problem is rotationally symmetric and the corresponding invariant is a generalization of the angular momentum.

Case (b) can be recognized as the transformation to *rotated Cartesian* coordinates. Solutions (48)–(54), in view of (28), then give

$$W = W(ay - bx), \quad K = k(ay - bx), \quad \Omega = -\frac{k'(ay - bx)}{2}. \tag{65}$$

The second invariant now is

$$I^{(1)} = \dot{z} + \dot{\overline{z}} + K = a\dot{x} + b\dot{y} + k(ay - bx). \tag{66}$$

The problem is invariant under translation along the family of straight lines $ax+by=$const. These two solutions are already well known,[7] and the above procedure can be appreciated in its effectiveness.

C. Examples of weakly integrable systems with linear invariants

We may provide two interesting classes of weakly integrable systems admitting linear invariants.

The first is obtained by the simple observation that, if we choose the level surface $C=0$, it is no longer necessary that condition (57) be satisfied. *Any* analytic function $S=S(z)$ provides a solution through the corresponding conformal transformation. If Y, as above, denotes the new coordinate

$$Y = \Im\left\{\int \frac{dz}{S(z)}\right\}, \tag{67}$$

then the solution is given by

$$W = \frac{g(Y(x,y))}{|S|^2}, \quad K = k(Y(x,y)), \quad \Omega = -\frac{k'(Y(x,y))}{2|S|^2}, \tag{68}$$

with g and k arbitrary real functions.

The second class of weakly integrable systems is obtained with the following trick. Let us consider the analytic function $f(z)$ and consider then the conformal transformation (42) with $S(z)$ given by

$$S = \frac{1}{c + f'(z)}, \tag{69}$$

with c constant. Recalling definition (46), let us consider the "flat" conformal potential $\tilde{G}=1$. In this case, relation (46), using (69), gives

$$G = C - W = \frac{1}{|S|^2} = c^2 + c(f' + \overline{f'}) + |f'|^2. \tag{70}$$

We can therefore interpret c^2 as the fixed value of the Jacobi constant,

$$c^2 \equiv C, \tag{71}$$

and get as a consequence the family of potentials,

$$W(z,\overline{z};c) = -c(f'(z) + \overline{f'}(\overline{z})) - |f'(z)|^2. \tag{72}$$

We remark that the dynamics given by potentials (72) is defined for arbitrary values of C, but it happens to be integrable only on the surface singled out by condition (71).

To complete the solution, we must write explicitly the coordinate transformation generated by (69), that is

$$w = \int \frac{dz}{S(z)} = cz + f(z). \tag{73}$$

Again, an arbitrary function $k(Y)$, with

$$Y = \Im\{cz + f(z)\}, \tag{74}$$

will do the work. For further details on these systems we refer to Ref. 10.

V. QUADRATIC INVARIANTS

We now look for systems admitting a second invariant which is a quadratic function in the momenta. The ansatz is

$$I^{(2)} = S(p + \Phi)^2 + \overline{S}(\overline{p} + \overline{\Phi})^2 + R(p + \Phi) + \overline{R}(\overline{p} + \overline{\Phi}) + K, \tag{75}$$

where, besides S and the real function K, we now must determine the complex function R. The system of equations ensuing from the conservation condition is the following:

$$S_{\overline{z}} = 0, \tag{76}$$

$$R_{\overline{z}} + 2i\Omega S = 0, \tag{77}$$

$$K_{\bar{z}} + SG_z + \tfrac{1}{2}S'G + i\Omega R = 0, \tag{78}$$

$$\Re\{(RG)_z\} = 0, \tag{79}$$

where, in (78) we have already exploited (76), that, as usual, embodies the fact that S is an arbitrary analytic function.

A. Towards a general solution for quadratic invariants

System (76)–(79) is much more difficult to solve than the previous linear case. Indeed we lack a general solution. The main reason for this difficulty is that the coupling between G, R, and Ω produces an integrability condition for K, through Eq. (78) and its complex conjugate, that is a *nonlinear* PDE. However, we can implement the strategy to arrive as close as possible to a general solution and, what is of great importance, we can solve the problem in the strongly integrable case, developing an effective way to construct solutions.

This time we use a conformal transformation to the complex variable $w=X+iY$ given by

$$\frac{\mathrm{d}z}{\mathrm{d}w} = F'(w) \equiv \sqrt{S(z(w))}, \tag{80}$$

so that the explicit form of the transformation is

$$w = \int \frac{\mathrm{d}z}{\sqrt{S(z)}}. \tag{81}$$

Introducing the conformal potential

$$\widetilde{G} = |F'|^2 G = |S|G = \sqrt{S\bar{S}}G, \tag{82}$$

and the new complex function

$$\widetilde{R} = \frac{R}{\sqrt{\bar{S}}}, \tag{83}$$

Eq. (79) keeps its form in the transformed coordinates

$$\Re\{(\widetilde{R}\widetilde{G})_w\} = 0. \tag{84}$$

The solution of this equation is

$$\widetilde{R}\widetilde{G} = i\mathcal{K}_{\bar{w}}, \tag{85}$$

where $\mathcal{K}$ is an arbitrary real function.

Let us now multiply both sides of (77) by

$$\sqrt{\frac{\bar{S}}{S}}. \tag{86}$$

Using (83) and introducing the conformal field

$$\widetilde{\Omega} = |S|\Omega, \tag{87}$$

Eq. (77) transforms into

$$\widetilde{R}_{\bar{w}} + 2i\widetilde{\Omega} = 0. \tag{88}$$

Since the conformal field is real, the solution of (88) is

$$\tilde{R} = -4i\xi_w, \tag{89}$$

where ξ is another arbitrary real function. The factor -4 appears for later convenience. In this way, the conformal field is given by

$$\tilde{\Omega} = 2\xi_{w\bar{w}}. \tag{90}$$

At this point, to get the general solution of the unified treatment of weak and strong integrability, one should try to solve the integrability condition for Eq. (78) in the light of the results (85)–(89). Let us write the integrability condition for K which, computing $K_{z\bar{z}}=K_{\bar{z}z}$ from (78), is

$$\mathfrak{J}\{S''G + 3S'G_z + 2SG_{zz} + 2i(\Omega R)_z\} = 0. \tag{91}$$

In the transformed coordinates, this becomes

$$\mathfrak{J}\{\tilde{G}_{ww}\} + \mathfrak{R}\{(\tilde{R}\tilde{\Omega})_w\} = 0. \tag{92}$$

From (85) and (88) we have

$$\tilde{R}\tilde{\Omega} = \frac{i}{2}\tilde{R}\tilde{R}_{\bar{w}} = \frac{i}{4}(\tilde{R}^2)_{\bar{w}} = -\frac{i}{4}(\tilde{G}^{-2}\mathcal{K}_{\bar{w}}^{-2})_{\bar{w}} \tag{93}$$

so that (92) can be rewritten as

$$\mathfrak{J}\{\tilde{G}_{ww}\} = \tfrac{1}{4}\mathfrak{R}\{i(\tilde{G}^{-2}\mathcal{K}_{\bar{w}})_{\bar{w}w}\}. \tag{94}$$

We can try to solve this equation after specifying $\mathcal{K}$. Unfortunately, the equation is highly nonlinear except in the rather trivial case when $\mathcal{K}$ is constant, so it appears to be very difficult to solve it in the general case. We direct our attention attempting to solve the more limited but fundamental case of strong integrability.

B. Quadratic invariants at arbitrary energy

Starting again with (79), we see that, in view of definition (29), it can be rewritten as

$$\mathfrak{R}\{R_z(C - W) - RW_z\} = 0. \tag{95}$$

If R is independent of C, as is the case under study, in order to satisfy this equation at arbitrary values of the energy, it decouples in two independent equations, the first is

$$\mathfrak{R}\{R_z\} = 0, \tag{96}$$

the second is

$$\mathfrak{R}\{RW_z\} = 0. \tag{97}$$

Equation (96) is solved by introducing the arbitrary real function η so that

$$R = -4i\eta_{\bar{z}}. \tag{98}$$

This allows us to solve equation (97) for W in the form

$$W = W(\eta), \tag{99}$$

that is W is, at this stage, an arbitrary function of the argument.

Comparing (98) with (89) and taking into account definition (83), we get the relation

$$\sqrt{S\bar{S}}\xi_w = |S|\xi_w = \eta_{\bar{w}}. \tag{100}$$

Solving the integrability condition for η with a given form of S allows us to find ξ (and vice versa): Eq. (100) is deceivingly simple; we will see later that it is of some concern. Here we remark that the route followed to treat Eq. (79) reverted to the original physical coordinates z, $\bar{z}$, since they lead to the simple result in (98). However, Eq. (90) is valid in general, it is the simplest way in which we can solve for the vector potential and is expressed in the new coordinates w, $\bar{w}$. This result and the development below show how working in the new coordinates is advantageous in this context too.

In the meantime we must determine the forms of S imposed by strong integrability. Examining the integrability condition (91), the usual condition of independence of the results from C imposes the following constraints on the form of S:

$$\Im\{S''(z)\} = 0. \tag{101}$$

This result, which is valid in the scalar case also, is a natural extension of what was found in the linear case.

Coming back to Eq. (100), we note that, using real coordinates, we have

$$|S|\xi_X = \eta_X, \tag{102}$$

$$|S|\xi_Y = -\eta_Y. \tag{103}$$

It can be proven[17] that condition (101) is equivalent to

$$|S|_{XY} = 0, \tag{104}$$

so that we can also write

$$|S| = A(X) + B(Y), \tag{105}$$

with A and B determined by the specific form of S. Therefore, Eqs. (102) and (103) generate the following differential equations for the functions η and ξ:

$$A'\eta_Y + B'\eta_X - 2(A+B)\eta_{XY} = 0, \tag{106}$$

$$A'\xi_Y + B'\xi_X + 2(A+B)\xi_{XY} = 0. \tag{107}$$

In view of (98), that can be rewritten as

$$|S|\tilde{R} = -4i\eta_{\bar{w}} \tag{108}$$

and of (87), integrability condition (92) can be written in the form

$$\Im\{\tilde{G}_{ww}\} + |S|\Re\{\tilde{R}\Omega_w\} = 0, \tag{109}$$

or, in real coordinates,

$$\tilde{G}_{XY} + 2(\eta_X\Omega_Y - \eta_Y\Omega_X) = 0. \tag{110}$$

If we want to exploit the result established by (99), we must resume the physical potential W through

$$\tilde{G} = |S|(C - W). \tag{111}$$

Using (105) we have

$$\tilde{G}_{XY} = -A'W_Y - B'W_X - (A+B)W_{XY} \tag{112}$$

and so (110) is

$$(A+B)W_{XY} + A'W_Y + B'W_X = 2(\eta_X\Omega_Y - \eta_Y\Omega_X). \tag{113}$$

But (99) tells us that

$$W_X = \eta_X W'(\eta), \quad W_Y = \eta_Y W'(\eta), \quad W_{XY} = \eta_X\eta_Y W'' + \eta_{XY}W', \tag{114}$$

so that (113) becomes

$$W''(\eta) + 3\frac{\eta_{XY}}{\eta_X\eta_Y}W'(\eta) = \frac{2}{A+B}\left(\frac{\Omega_Y}{\eta_Y} - \frac{\Omega_X}{\eta_X}\right). \tag{115}$$

This is the best form we attain to express the integrability condition for the potential: we see that in general it implies that

$$\frac{\eta_{XY}}{\eta_X\eta_Y} = \Phi(\eta), \tag{116}$$

where Φ is arbitrary.

Therefore, the strategy to find strongly integrable systems with scalar and vector potentials supporting quadratic invariants is to choose a suitable S in the class determined by condition (101) (and therefore A and B) and solve (106) and (107) to find $\eta(X,Y)$ and $\xi(X,Y)$; to solve (90) to find

$$\tilde{\Omega} = \tfrac{1}{2}(\xi_{XX} + \xi_{YY}) \tag{117}$$

and use (87) to find

$$\Omega(X,Y) = \frac{\tilde{\Omega}}{A+B} \tag{118}$$

and, finally, try to solve (115) for

$$W = W(\eta(X,Y)) \tag{119}$$

taking into account (116).

C. General form of the quadratic invariant

In the next section we apply the strategy delineated above illustrating how already known and new integrable systems are determined. We end this section with a closer look at the structure of the quadratic invariant.

In the new variables, w, $\overline{w}$, together with the conformal transformation, it is natural to introduce the new time variable τ such that

$$\mathrm{d}\tau = \frac{\mathrm{d}t}{|F'|^2}. \tag{120}$$

We can use the apex to also denote the derivative with respect to τ without risk of confusion with other derivatives with respect to coordinates. Equations of motion (22) then assume the following form:

$$w'' + 2i\tilde{\Omega}w' = 2\tilde{G}_{\overline{w}}. \tag{121}$$

In view of the above positions, the quadratic invariant is most simply expressed as

$$I^{(2)} = \Re\{\tfrac{1}{2}(w')^2 + \widetilde{R}\overline{w'}\} + K, \tag{122}$$

or, in terms of real variables,

$$I^{(2)} = \tfrac{1}{2}[(X')^2 - (Y')^2] - 2(\xi_X Y' + \xi_Y X') + K. \tag{123}$$

We recall that the scalar K, to be found by integrating the transformed version of (78), namely

$$K_{\overline{w}} + \widetilde{G}_w + i\widetilde{\Omega}\widetilde{R} = 0, \tag{124}$$

is a function of the form

$$K = K(w, \overline{w}; C). \tag{125}$$

In the present case of strong integrability, in view of (105), it turns out that this function can be expressed as

$$K = k + C(B - A), \tag{126}$$

and k can be found by integrating the system

$$k_X - \widetilde{W}_X + 4\widetilde{\Omega}\xi_X = 0, \tag{127}$$

$$k_Y + \widetilde{W}_Y - 4\widetilde{\Omega}\xi_Y = 0, \tag{128}$$

where $\widetilde{W} = (A+B)W$. From (123), using (126) and

$$C = \frac{1}{2}\frac{(X')^2 + (Y')^2}{A + B} + W, \tag{129}$$

the general form of the invariant is then

$$I^{(2)} = \frac{1}{A + B}[B(X')^2 - A(Y')^2] - 2(\xi_X Y' + \xi_Y X') + (B - A)W + k. \tag{130}$$

Observing that the relations between velocities in the two gauges are given by

$$X' = \Re\{F'\}\dot{x} + \Im\{F'\}\dot{y}, \tag{131}$$

$$Y' = -\Im\{F'\}\dot{x} + \Re\{F'\}\dot{y}, \tag{132}$$

we can eventually transform the invariant in Cartesian coordinates. Transformation rules automatically account also for the change of the time variable according to (120).

VI. SOLUTIONS WITH QUADRATIC INVARIANTS

Let us recall the coordinate systems given by the condition for the existence of strong quadratic invariants. We observe that the function S we must use is obtained by integrating (101) so that

$$S(z) = cz^2 + \beta z + \alpha, \tag{133}$$

where c is a real constant and β, α complex constants. Exploiting the freedom of making translations, rotations and scaling in the complex plane, we have the following four inequivalent cases (for further details we refer to Refs. 4 and 18):

$$\text{(a)} \quad S(z) = \alpha, \quad F(w) = \alpha w, \quad x = aX - bY, \quad y = bX + aY, \tag{134}$$

$$\text{(b)} \quad S(z) = z^2, \quad F(w) = e^w, \quad x = e^X \cos Y, \quad y = e^X \sin Y, \tag{135}$$

$$\text{(c)} \quad S(z) = 4z, \quad F(w) = w^2, \quad x = X^2 - Y^2, \quad y = 2XY, \tag{136}$$

$$\text{(d)} \quad S(z) = z^2 + \Delta^2, \quad F(w) = \Delta \sinh w, \tag{137}$$

$$x = \Delta \sinh X \cos Y, \quad y = \Delta \cosh X \sin Y. \tag{138}$$

Case (a) gives the rotated Cartesian coordinates (standard Cartesian coordinates if $\alpha=1$). Case (b) gives again the polar coordinates. Case (c) gives the parabolic coordinates which are also referred to as *Levi–Cività* coordinates (the factor 4 in the definition of S appears just for this reason). Finally, case (d) produces the elliptical coordinates. For the sake of completeness, we list, for each of the four cases, the conformal factor and functions A and B introduced in (105):

$$\text{(a)} \quad |S| = 1, \quad A = B = \tfrac{1}{2}, \tag{139}$$

$$\text{(b)} \quad |S| = e^{2X}, \quad A = e^{2X}, \quad B = 0, \tag{140}$$

$$\text{(c)} \quad |S| = 4(X^2 + Y^2), \quad A = 4X^2, \quad B = 4Y^2, \tag{141}$$

$$\text{(d)} \quad |S| = \Delta^2(\sinh^2 X + \cos^2 Y), \tag{142}$$

$$A = \Delta^2 \sinh^2 X, \quad B = \Delta^2 \cos^2 Y. \tag{143}$$

A. Cartesian coordinates

Let us start with the simplest case (a), the Cartesian one. As the structure of the solution will show in the end, there is no need to work with rotated coordinates, therefore we can set $\alpha=1$ and make the trivial identification $X=x$ and $Y=y$. Equations (102) and (103) are

$$\eta_x = \xi_x, \tag{144}$$

$$\eta_y = -\xi_y. \tag{145}$$

The solution is

$$\xi = f(x) + g(y), \tag{146}$$

$$\eta = f(x) - g(y), \tag{147}$$

with f and g arbitrary. From (117) and (118), the vector field is

$$\Omega = \tfrac{1}{2}(f'' + g'') \tag{148}$$

and the R function

$$R = -2(g' + if'). \tag{149}$$

Equation (113) is

$$W_{xy} - (g' f''' + f' g''') = 0. \tag{150}$$

From (99) we have that $W=W(f(x)-g(y))$, so that

$$W_{xy} = -f'g'W'' \tag{151}$$

and (150) becomes

$$W'' + \frac{f'''}{f'} + \frac{g'''}{g'} = 0. \tag{152}$$

A further differentiation by x and y gives

$$\frac{1}{f'}\frac{d}{dx}\frac{f'''}{f'} = -\frac{1}{g'}\frac{d}{dy}\frac{g'''}{g'} = 2a = -W''' \tag{153}$$

with a real constant. We then get two equations for f and g,

$$f'' = af^2 + bf + c, \tag{154}$$

$$g'' = -ag^2 + dg + e, \tag{155}$$

in agreement with the work of Dorizzi *et al.*,[7] that can be integrated for various choices of the constants a, b, c, d, e. The potentials in terms of f and g are

$$W = \frac{a}{3}(g-f)^3 - \frac{b+d}{2}(g-f)^2 + (c-e+m)(g-f), \tag{156}$$

$$2\Omega = a(f^2 - g^2) + bf + dg + c + e, \tag{157}$$

where m is another constant. Integrating Eqs. (127) and (128) gives then

$$K = afg(f+g) + (b-d)fg - a(f^3+g^3) - \tfrac{1}{2}(3b+d)f^2 + \tfrac{1}{2}(3d+b)g^2 - (3c+m+e)f + (c-m+3e)g. \tag{158}$$

The fundamental example of the harmonic oscillator is obtained with the choice

$$a = b = d = 0, \tag{159}$$

so that

$$f = \tfrac{1}{2}cx^2, \tag{160}$$

$$g = \tfrac{1}{2}ey^2, \tag{161}$$

and the potentials are

$$W = \tfrac{1}{2}(c-e+m)(ey^2 - cx^2), \tag{162}$$

$$2\Omega = c + e. \tag{163}$$

We remark that, in this case, the vector field is a *constant angular velocity* and that the isotropic oscillator only exists when the angular velocity vanishes. The second invariant in this case is

$$I^{(2)} = \tfrac{1}{2}(\dot{x}^2 - \dot{y}^2) - 2(cx\dot{y} + ey\dot{x}) + \tfrac{1}{2}[(c-m+3e)ey^2 - (3c+m+e)cx^2]. \tag{164}$$

B. Polar coordinates

In case (b), the polar coordinates, we recall that now

$$r = e^X, \quad \theta = Y \tag{165}$$

and remark the difference of this relation with respect to (62) obtained in the linear case. We have

$$|S| = A = e^{2X} = r^2, \quad B = 0. \tag{166}$$

Equation (106) becomes

$$2e^{2X}(\eta_{XY} - \eta_Y) = 0, \tag{167}$$

which is solved by

$$\eta = e^X g(Y) + f(X), \tag{168}$$

with f and g arbitrary. From (100) we then have

$$\xi = -e^X g + \int e^{-2X} f'(X) \mathrm{d}X. \tag{169}$$

From (117) and (118), the velocity field is

$$2\Omega = e^{-2X}\Delta\xi = e^{-4X}(f'' - 2f') - e^{-3X}(g'' + g). \tag{170}$$

Condition (116) says that

$$\eta_X = e^X g(Y) + f'(X) = \Phi(e^X g(Y) + f(X)). \tag{171}$$

There are two ways in which (171) can be accomplished: the first is $g = \text{const}$ and it is easy to see that in this way we are actually taken back to the spherically symmetric case to which actually a linear invariant is associated. We can take $\eta(X)$ and $W(X)$ arbitrarily whereas, to find the vector field, we observe that

$$\xi'(X) = e^{-2X}\eta'(X), \tag{172}$$

so that

$$2\Omega = e^{-2X}\xi'' = e^{-4X}(\eta'' - 2\eta') = e^{-2X}(e^{-2X}\eta')'. \tag{173}$$

To show that this solution is equivalent to that obtained in the linear case, we compute the scalar k by integrating (127) to get

$$k^{(2)}(X) = e^{2X}W - (e^{-2X}\eta')^2. \tag{174}$$

Observing that, in polar coordinates, relation (120) between old and new time is

$$\mathrm{d}\tau = \frac{\mathrm{d}t}{r^2} \tag{175}$$

and using

$$Y' = r^2\dot{\theta}, \tag{176}$$

expression (130) becomes

$$I^{(2)} = -r^4\dot{\theta}^2 - 2\eta'\dot{\theta} - \frac{(\eta')^2}{r^4}. \tag{177}$$

In the linear case, recalling solution (64), we obtain

$$I^{(1)} = r^2\dot{\theta} + k^{(1)}(r), \tag{178}$$

where, from (63),

$$k^{(1)}(r) = 2\int r\Omega\, \mathrm{d}r = 2\int e^{2X}\Omega\, \mathrm{d}X. \tag{179}$$

Using (173) this becomes

$$k^{(1)}(r) = e^{-2X}\eta' = r^{-2}\eta', \tag{180}$$

so that, comparing (177) with (178), we see that

$$I^{(2)} = -(I^{(1)})^2. \tag{181}$$

The second possibility of satisfying condition (171) is to have $f=\text{const}$ and the constant, without any loss of generality, can be set equal to zero. Therefore, we have

$$\eta = e^X g(Y) \tag{182}$$

and

$$\xi = -e^{-X}g. \tag{183}$$

To find the potential, we must solve (115) which, using (182) and (170), is

$$W''(\eta) + \frac{3}{\eta}W'(\eta) = -\frac{1}{e^{6X}gg'}(g'''g + 3g''g' + 4g'g). \tag{184}$$

The simplest way in which the right-hand side is also a function of η is given by the condition

$$g'''g + 3g''g' + 4g'g = \alpha\frac{g'}{g^5}, \tag{185}$$

with α constant, so that (184) becomes

$$W''(\eta) + \frac{3}{\eta}W'(\eta) + \frac{\alpha}{\eta^6} = 0 \tag{186}$$

with solution

$$W = \frac{\beta}{\eta^2} - \frac{\alpha}{8\eta^4}. \tag{187}$$

To find explicit solution we must determine the possible forms of g which can be obtained by integrating (185) twice,

$$(g')^2 + g^2 + \frac{\alpha}{4g^4} + \frac{\gamma}{g^2} = \delta, \tag{188}$$

with γ and δ constants. All this is in agreement with the results in McSween and Winternitz[8] to which we refer.

Since in the approach with the energy constraint, the coefficients appearing in the invariant must be supplemented by a further substitution in order to get the final physical expression, for the sake of completeness, we work out a specific example. To ease the comparison with the results in Ref. 8, we use explicitly polar coordinates as in (165). The simplest case in the solution above is given by the choice $\alpha=0$. Equation (188) has the solution

$$g(\theta) = \sqrt{a + b\cos 2\theta} \tag{189}$$

with the constants a and b given by

$$\gamma = a^2 - b^2, \quad \delta = 2a. \tag{190}$$

From (187) and (170), the potential and velocity field are given, respectively, by

$$W = \frac{\beta}{r^2(a + b\cos 2\theta)} \tag{191}$$

and

$$\Omega = \frac{b^2 - a^2}{2r^3(a + b\cos 2\theta)^{3/2}}. \tag{192}$$

To find the invariant, we can use (130). Equations (127) and (128) can easily be integrated to get

$$k = -r^2 W - r^{-2} g(g + g''). \tag{193}$$

so that expression (130) becomes

$$I^{(2)} = r^4\dot{\theta}^2 + 2(rg\dot{\theta} - \dot{r}g') + \frac{2\beta}{g^2} + \frac{g(g + g'')}{r^2}. \tag{194}$$

In the specific example of (189) we get

$$I^{(2)} = r^4\dot{\theta}^2 + \frac{2b\sin\theta}{\sqrt{a + b\cos 2\theta}}\dot{r} + 2\sqrt{a + b\cos 2\theta}\, r\dot{\theta} + \frac{1}{a + b\cos 2\theta}\left(\frac{a^2 - b^2}{r^2} + 2\beta\right). \tag{195}$$

We remark that the small discrepancy in (195) with respect to the analogous expression reported in Ref. 8 is due to a difference of a factor of 2 in the definition of Ω as can be seen from Eq. (192).

C. Parabolic coordinates

We use the Levi–Cività representation of the parabolic coordinates introduced in case (c) above and mostly used in celestial mechanical applications. As a first step, the general strategy we depicted at the end of Sec. V B prescribes to determine the functions η and ξ satisfying equations (106) and (107). According to (141), we have

$$A = 4X^2, \quad B = 4Y^2, \tag{196}$$

so that Eq. (106) becomes

$$X\eta_Y + Y\eta_X - (X^2 + Y^2)\eta_{XY} = 0. \tag{197}$$

A fairly general solution of this PDE can be represented in the following form:

$$\eta(X,Y) = \int F(a)\sqrt{(X^2 + a)(Y^2 - a)}\,\mathrm{d}a + \int G(a)\frac{(X^2 + Y^2)^2}{((X^2 + a)(Y^2 - a))^{3/2}}\mathrm{d}a, \tag{198}$$

where a is an arbitrary real parameter and F and G two arbitrary smooth functions.

The subsequent steps should consist in determining the functions ξ and Ω and finally to solve for the potential $W(\eta)$. However, we observe that it is not easy to satisfy the constraint (116) with a too general expression for η: therefore, we first find a suitable form of this function and then proceed as above. A simple but nontrivial possibility is that given by the position

$$F = c\,\delta(a-b), \quad G = 0 \tag{199}$$

in (198), where $\delta(a)$ is the Dirac function. This choice gives the simplest separable solution of the differential equation (197). Therefore, we have

$$\eta(X,Y) = c\sqrt{(X^2+b)(Y^2-b)}, \tag{200}$$

which is easily shown to satisfy condition (116) in the form

$$\frac{\eta_{XY}}{\eta_X \eta_Y} = \frac{1}{\eta}. \tag{201}$$

With solution (200), Eqs. (106) and (107) are readily solved for ξ,

$$\xi(X,Y) = \frac{c}{4}\arctan\sqrt{\frac{X^2+b}{Y^2-b}}, \tag{202}$$

so that, from (117), the conformal vector field is

$$\tilde{\Omega} = \frac{bc}{8}\frac{X^2+Y^2}{((X^2+b)(Y^2-b))^{3/2}}. \tag{203}$$

From this, Eq. (118) gives

$$\Omega = \frac{\tilde{\Omega}}{4(X^2+Y^2)} = \frac{c^4 b}{32}\frac{1}{\eta^3}. \tag{204}$$

This result suggests to set

$$c = 2 \tag{205}$$

in order to simplify formulas and we have the physical vector field from

$$2\Omega = \frac{b}{\eta^3}, \quad \eta(X,Y) = 2\sqrt{(X^2+b)(Y^2-b)}. \tag{206}$$

An important consequence of this result is that, together with W, Ω too depends on the coordinates only through η. This implies that the right-hand side of Eq. (115) for W vanishes, so that, taking into account (201), we get simply

$$W''(\eta) + \frac{3}{\eta}W'(\eta) = 0. \tag{207}$$

The solution for the scalar potential is then

$$W = \frac{\beta}{\eta^2} \tag{208}$$

and we are actually led to a situation analogous to that encountered above in the example examined in polar coordinates. It is interesting to remark that potential (208) is separable if considered in the purely scalar situation, since, using (200), we get

$$W = \frac{\beta}{4(X^2+Y^2)}\left(\frac{1}{X^2+b} + \frac{1}{Y^2-b}\right). \tag{209}$$

Reverting to Cartesian coordinates through

$$X = \sqrt{\frac{r+x}{2}}, \quad Y = \sqrt{\frac{r-x}{2}}, \tag{210}$$

the scalar and vector potentials are, respectively, given by

$$W = \frac{\beta}{y^2 - 4b(x+b)} \tag{211}$$

and

$$\Omega = \frac{b}{2(y^2 - 4b(x+b))^{3/2}}. \tag{212}$$

The second invariant using parabolic coordinates is

$$I^{(2)} = \frac{1}{X^2+Y^2}[Y^2(X')^2 - X^2(Y')^2] + \frac{Y(X^2+b)X' - X(Y^2-b)Y'}{(X^2+Y^2)\sqrt{(X^2+b)(Y^2-b)}} + \frac{b + 8\beta(Y^2 - X^2 - b)}{4(X^2+b)(Y^2-b)}, \tag{213}$$

where the τ time variable is used and, therefore, it is conserved along the solution of the transformed equations of motion of the form (121). Using relations (131) and (132) between velocities in the two gauges,

$$X' = \sqrt{2(r+x)}\dot{x} + \sqrt{2(r-x)}\dot{y}, \tag{214}$$

$$Y' = \sqrt{2(r+x)}\dot{y} - \sqrt{2(r-x)}\dot{x}, \tag{215}$$

we can transform the invariant into Cartesian coordinates,

$$I^{(2)} = (y\dot{x} - x\dot{y})\dot{y} + \frac{y\dot{x} + 2b\dot{y}}{2\sqrt{y^2 - 4b(x+b)}} + \frac{b - 8\beta(x+b)}{4(y^2 - 4b(x+b))}. \tag{216}$$

D. Elliptical coordinates

It turns out that even in elliptical coordinates it is possible to find nontrivial solutions with a structure closely related to that seen in the examples detailed above in polar and parabolic coordinates. In addition, in elliptical coordinates, a solution with a constant vector field also exists (constant angular velocity), whereas this possibility appears to be absent in parabolic coordinates.

A common feature of all these cases is that both the scalar and vector potentials, W and Ω, can be expressed only in terms of η. This implies that the right-hand side of Eq. (115) for W vanishes, so that, taking into account (116), this common feature is embodied in the equation

$$W''(\eta) + \Phi(\eta)W'(\eta) = 0, \tag{217}$$

with suitable Φ. Analogously to what is seen in the polar cases, other solutions may very well exist but they are not so easy to find.

According to (143), we now have

$$A = \Delta^2 \sinh^2 X, \quad B = \Delta^2 \cos^2 Y. \tag{218}$$

In this case Eq. (106) becomes

$$\sinh X \cosh X \eta_Y - \sin Y \cos Y \eta_X - (\sinh^2 X + \cos^2 Y)\eta_{XY} = 0. \tag{219}$$

A simple solution of this PDE is the following:

$$\eta(X,Y) = a\Delta^2(\sinh^2 X - \cos^2 Y) + b\Delta^4(\sinh^2 X + \cos^2 Y)^2, \tag{220}$$

with a and b constants. Using this solution, Eqs. (106) and (107) give for ξ,

$$\xi(X,Y) = a\,\ln[\Delta^2(\sinh^2 X + \cos^2 Y)] + \tfrac{1}{2}b\Delta^2(\cosh 2X - \cos 2Y). \tag{221}$$

Computing the conformal vector potential from (117), we see that the first solution is trivial since its Laplacian vanishes giving a null vector field. We remark that the analogous phenomenon also occurs in the parabolic coordinates case, where it is possible to find several additional solutions of Eq. (197) generating a vanishing vector field.

The second solution appearing in (221) instead gives

$$\tilde{\Omega} = b\Delta^2(\cosh 2X + \cos 2Y) = 2b\Delta^2(\sinh^2 X + \cos^2 Y). \tag{222}$$

We get that the conformal field is proportional to the conformal factor $|S|$ so that, from (118), we have that the vector field is constant

$$\Omega = 2b \equiv \Omega_0. \tag{223}$$

Condition (116) for the nontrivial solution (220) with $a=0$ is

$$\frac{\eta_{XY}}{\eta_X \eta_Y} = \frac{1}{2\eta}, \tag{224}$$

so that Eq. (115) for W is

$$W''(\eta) + \frac{3}{2\eta}W'(\eta) = 0, \tag{225}$$

whose solution is

$$W = \frac{\alpha}{\sqrt{\eta}}, \tag{226}$$

or, using again (220),

$$W(X,Y) = \frac{\beta}{|S|} = \frac{\beta}{\Delta^2(\sinh^2 X + \cos^2 Y)}, \tag{227}$$

where α and β are arbitrary constants. This solution is the simplest separable scalar potential in elliptical coordinates, which is therefore shown to be integrable also in a uniformly rotating system: this result is already known for its application in the modeling of rotating galaxies.[19] The second invariant (130) using elliptical coordinates is

$$I^{(2)} = \frac{1}{\sinh^2 X + \cos^2 Y}[\cos^2 Y(X')^2 - \sinh^2(Y')^2] + \frac{1}{2}\Omega_0(\sin 2YX' - \sinh 2XY') - \beta\frac{\sinh^2 X - \cos^2 Y}{\sinh^2 X + \cos^2 Y} - \Omega_0^2(\sinh^2 X + \cos^2 Y)^2. \tag{228}$$

Reverting to Cartesian coordinates through

$$2\Delta^2 \sinh^2 X = r^2 - \Delta^2 + \sqrt{(r^2+\Delta^2)^2 - 4\Delta^2 y^2}, \tag{229}$$

$$2\Delta^2 \sin^2 Y = r^2 + \Delta^2 - \sqrt{(r^2+\Delta^2)^2 - 4\Delta^2 y^2}, \tag{230}$$

the scalar potential becomes

$$W(x,y) = \frac{\beta}{\sqrt{r^4 + 2\Delta^2(x^2 - y^2) + \Delta^4}} \tag{231}$$

and, using relations (131) and (132) between velocities in the two gauges, we can transform the invariant into Cartesian coordinates,

$$\begin{aligned} I^{(2)} = (y\dot{x} - x\dot{y})^2 - \Delta^2\dot{x}^2 + (\Delta^2 - r^2)(2\Omega_0 y\dot{x} - W(x,y)) \\ + 2\Omega_0(\Delta^2 + r^2)x\dot{y} + \Omega_0^2(r^4 + 2\Delta^2(x^2 - y^2) + \Delta^4). \end{aligned} \tag{232}$$

We pass now to investigate a more complex class of systems. A general solution of Eq. (219) is

$$\begin{aligned} \eta(X,Y) = \int F(a)\sqrt{(\Delta^2 \sinh^2 X + a)(a - \Delta^2 \cos^2 Y)}\mathrm{d}a \\ + \int G(a)\frac{(\Delta^2 \sinh^2 X + \Delta^2 \cos^2 Y)^2}{((\Delta^2 \sinh^2 X + a)(a - \Delta^2 \cos^2 Y))^{3/2}}\mathrm{d}a, \end{aligned} \tag{233}$$

where a is an arbitrary real parameter and F and G are two arbitrary smooth functions. Comparing this solution with that of (198) we can guess analogous developments. Therefore we try with the simple solution

$$F = \delta(a - b), \quad G = 0, \tag{234}$$

which corresponds to the simplest separable solution of the differential equation (219). Therefore, we have

$$\eta(X,Y) = \sqrt{(\Delta^2 \sinh^2 X + b)(b - \Delta^2 \cos^2 Y)}, \tag{235}$$

which satisfies condition (116) in the same form as in (201). With solution (235), Eqs. (106) and (107) give the following expression for ξ:

$$\xi(X,Y) = -\operatorname{arctanh}\sqrt{\frac{b + \Delta^2 \sinh^2 X}{b - \Delta^2 \cos^2 Y}}, \tag{236}$$

so that, from (117), the conformal vector field is

$$\tilde{\Omega} = \frac{b\Delta^2(b - \Delta^2)(\sinh^2 X + \cos^2 Y)}{((\Delta^2 \sinh^2 X + b)(b - \Delta^2 \cos^2 Y))^{3/2}}. \tag{237}$$

From this, Eq. (118) gives

$$\Omega = \frac{\tilde{\Omega}}{\Delta^2(\sinh^2 X + \cos^2 Y)} = \frac{b(b - \Delta^2)}{2\eta^3}. \tag{238}$$

As remarked above, from this result it follows that the right-hand side of Eq. (115) for W vanishes, so that, taking into account (201), we get again (207) so that the solution for the scalar potential is

$$W = \frac{\beta}{\eta^2} = \frac{\beta}{(\Delta^2 \sinh^2 X + b)(b - \Delta^2 \cos^2 Y)}. \tag{239}$$

Even potential (239) is separable if considered in the purely scalar situation, since it can be written in the form

$$W = \frac{\beta}{\Delta^2(\sinh^2 X + \cos^2 Y)}\left(\frac{1}{b - \Delta^2 \cos^2 Y} - \frac{1}{\Delta^2 \sinh^2 X + b}\right). \tag{240}$$

Using the explicit coordinate transformation (229) and (230), the scalar and vector potentials are, respectively, given by

$$W = \frac{\beta}{by^2 + (b - \Delta^2)(x^2 + b)} \tag{241}$$

and

$$\Omega = \frac{b(b - \Delta^2)}{2(by^2 + (b - \Delta^2)(x^2 + b))^{3/2}}. \tag{242}$$

Finally, the second invariant using elliptical coordinates is

$$I^{(2)} = \frac{\cos^2 Y (X')^2 - \sinh^2 (Y')^2}{\sinh^2 X + \cos^2 Y} + \frac{1}{\sinh^2 X + \cos^2 Y}\left(\sin 2Y \sqrt{\frac{b + \Delta^2 \sinh^2 X}{b - \Delta^2 \cos^2 Y}} X' - \sinh 2X \sqrt{\frac{b - \Delta^2 \cos^2 Y}{b + \Delta^2 \sinh^2 X}} Y'\right) + \frac{b(\Delta^2 - b) + 2\beta(\Delta^2(\cos^2 Y - \sinh^2 X) - b)}{(\Delta^2 \sinh^2 X + b)(b - \Delta^2 \cos^2 Y)},$$

whereas using Cartesian coordinates is given by

$$I^{(2)} = (y\dot{x} - x\dot{y})^2 - \Delta^2 \dot{x}^2 + 2\frac{by\dot{x} + (\Delta^2 - b)x\dot{y}}{\sqrt{by^2 + (b - \Delta^2)(x^2 + b)}} + \frac{b(b - \Delta^2) + 2\beta(b - \Delta^2 + x^2 + y^2)}{by^2 + (b - \Delta^2)(x^2 + b)}. \tag{243}$$

VII. CONCLUDING REMARKS

We have investigated Hamiltonian systems with vector potentials admitting a second invariant which is linear or quadratic in the momenta. In our approach, weak and strong invariants are treated in a unified setting where the strong invariants emerge as special cases. As for scalar potentials, the integrable systems can be greatly simplified by introducing certain standardized coordinates, as given in (134)–(138). It is a striking result that these standardized coordinate systems for systems with strong invariants exactly coincide with the classical separable coordinates for scalar potentials.

This work is an extension and improvement of the approach to integrable vector potential Hamiltonians which was proposed in Ref. 10. However, there still remain issues which need clarification. In particular, it should be possible to obtain a better understanding of the integrability conditions, especially the role of the condition (116) for the structure of the strongly invariant case.

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The difficulty of symplectic analysis with second class systems

A. Shirzad[a] and M. Mojiri[b]
Department of Physics, Isfahan University of Technology, Isfahan, Iran and Institute for Studies in Theoretical Physics and Mathematics, P.O. Box 5531, Tehran 19395, Iran

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Using the basic concepts of the chain by chain method we show that the symplectic analysis, which was claimed to be equivalent to the usual Dirac method, fails when second class constraints are present. We propose a modification in symplectic analysis that solves the problem. © *2005 American Institute of Physics.*
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I. INTRODUCTION

There are some attempts to study a constrained system in the framework of first order Lagrangian.[1,2] The coordinates appearing in a first order Lagrangian are in fact the phase space coordinates. The Euler–Lagrange equations of motion of a first order Lagrangian in an ordinary (nonconstrained) system are the same as the canonical equations of motion. The kinetic term in a first order Lagrangian constitutes of a one-form whose exterior derivative appears in the equations of motion. The resulted two-form, called the symplectic tensor, is singular for a constrained system. If the system is not constrained, usually the inverse of the symplectic tensor exists and provides the fundamental Poisson brackets (we exclude degenerate systems discussed in Refs. 3 and 4 in which the symplectic tensor may have a lower rank in some regions of the phase space).

The properties of a constrained system can be determined by trying to overcome the singularity of the symplectic tensor. Faddeev and Jackiw[5] used the Darboux theorem to separate canonical and noncanonical coordinates. They solved the equations of motion for noncanonical coordinates either to decrease the degrees of singularity of the symplectic tensor or to find the next level constraints.

Then using a special system of coordinates, the authors of Ref. 6 showed that the Faddeev–Jackiw approach is essentially equivalent to the usual Dirac method.[7] In a parallel approach, known as symplectic analysis[8–11] one extends the phase space to include the Lagrange multipliers. In this approach the consistency of constraints at each level adds some additional elements to the symplectic tensor. In other words, the kinetic part of the (first order) Lagrangian is responsible to impose the consistency conditions.

The important point in most papers written in the Faddeev–Jackiw method or symplectic analysis is that they often show their results for the constraints in the first level and then *deduce* that the same thing would be repeated at any level. However, the whole procedure of studying the singularities of symplectic tensor, demonstrates some global aspects. For example, some questions that may arise are as follows:

What happens, after all, to the symplectic tensor? Is it ultimately singular? How many degrees of singularity may it have? What is the relation of ultimate singularities with the gauge symmetries of the system and so on? In Ref. 12 we showed that the symplectic analysis gives, at each step, the same results as the traditional Dirac method (in the framework of *the level by level approach*). The

[a]Electronic mail: shirzad@ipm.ir
[b]Electronic mail: mojiri@sepahan.iut.ac.ir

symplectic analysis may also be studied in the framework of *the chain by chain approach*[13] to obtain the Dirac constraints.

Meanwhile, some recent observation[14] shows that in some examples the result of symplectic analysis and the well-established method of Dirac are not the same. This creates serious doubt about the validity of the symplectic analysis. Therefore, it is worth studying the origin of the difference between this approach and that of Dirac.[7] This is the aim of this paper. In the next section we first review the basic concept of symplectic approach as given in Ref. 12. As we will show the symplectic analysis is equivalent to a special procedure in the Dirac approach in which one uses the extended Hamiltonian at each level of consistency. In Sec. III we will show that in the framework of the Dirac method one is not allowed to use an extended Hamiltonian when there exist second class constraints. The important point to be emphasized is that this result can be understood more clearly in the framework of the chain by chain method. In Sec. IV we show that for a one chain system with second class constraints the symplectic analysis as proposed in the literature fails. This result can be simply generalized to the general case of a multichain system. When recognizing the origin of the problem, we give our prescription to solve it in Sec. V. Finally in Sec. VI we give an example.

The last point to be noticed is that the problem would not show itself for systems with two levels of constraints. As we will show, this is the case for second class systems with at least four levels of constraints. That is the reason for the fact that the problem does not appear if one considers just first level constraints.

II. REVIEW OF SYMPLECTIC APPROACH

Consider a phase space with coordinates y^i $(i=1,\ldots,2K)$ specified by the first order Lagrangian,

$$L = a_i(y)\dot{y}^i - H(y), \tag{1}$$

where $H(y)$ is the canonical Hamiltonian of the system. The equations of motion read

$$f_{ij}\dot{y}^j = \partial_i H, \tag{2}$$

where $\partial_i \equiv \partial/\partial y^i$ and the presymplectic tensor f_{ij} is defined as

$$f_{ij} \equiv \partial_i a_j(y) - \partial_j a_i(y). \tag{3}$$

We denote it in matrix notation as f. This matrix is invertible for a regular system. Let f^{ij} be the components of the inverse, f^{-1}. From (2) we have

$$\dot{y}^i = \{y^i, H\}, \tag{4}$$

where the Poisson brackets $\{,\}$ are defined as

$$\{F(y), G(y)\} = f^{ij}\partial_i F \partial_j G. \tag{5}$$

If f is singular, then using the Darboux theorem, as shown in Ref. 5, one can choose the independent coordinates (y'^α, λ^l) such that

$$L = a'_\alpha \dot{y}'^\alpha - \lambda^l \Phi_l(y') - H(y'), \tag{6}$$

where $f'_{\alpha\beta} = \partial_\alpha a'_\beta - \partial_\beta a'_\alpha$ is invertible. This shows that one can consider a system with a singular tensor f_{ij}, as a regular one described by

$$L = a'_\alpha \dot{y}'^\alpha - H(y') \tag{7}$$

together with the primary constraints $\Phi_l(y')$. In other words, without losing the generality one can assume that one is at first given the first order Lagrangian (1) with a regular presymplectic

two-form (3), and then the set of primary constraints $\Phi_\mu^{(1)}$ $(\mu=1,\ldots,M)$ are applied to the system. In this way the system is described by the Lagrangian,

$$L = a_i\dot{y}^i - \lambda^\mu\Phi_\mu^{(1)} - H(y), \tag{8}$$

in the extended space (y^i,λ^μ). The equations of motion (2) should be replaced in matrix form by

$$\begin{pmatrix} f & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \dot{y} \\ \dot{\lambda} \end{pmatrix} = \begin{pmatrix} \partial H \\ \Phi^{(1)} \end{pmatrix}, \tag{9}$$

which is equivalent to Eq. (2) together with the constraint equations $\Phi_\mu^{(1)}=0$ $(\mu=1,\ldots,M)$.

Now one should impose the consistency conditions $\dot{\Phi}_\mu^{(1)}=0$. To do this, one should extend the space to include new variables η^μ and add the term $\eta^\mu\dot{\Phi}_\mu^{(1)}$ (or equivalently $-\dot{\eta}^\mu\Phi_\mu^{(1)}$) to the Lagrangian (8). This leads in the extended space (y,λ,η) to the equations

$$\begin{pmatrix} f & 0 & A \\ 0 & 0 & 0 \\ -\tilde{A} & 0 & 0 \end{pmatrix}\begin{pmatrix} \dot{y} \\ \dot{\lambda} \\ \dot{\eta} \end{pmatrix} = \begin{pmatrix} \partial H \\ \Phi^{(1)} \\ 0 \end{pmatrix}, \tag{10}$$

where the elements of the rectangular matrix A are given by

$$A_{\mu i} = \partial_i\Phi_\mu^{(1)}. \tag{11}$$

However, nothing would be lost if one forgets about the variables λ^μ and reduces the system to the Lagrangian

$$L^{(1)} = a_i\dot{y}^i - \dot{\eta}^\mu\Phi_\mu^{(1)} - H(y). \tag{12}$$

This leads to the symplectic two-form,

$$F = \begin{pmatrix} f & A \\ -\tilde{A} & 0 \end{pmatrix}, \tag{13}$$

in the $(2K+M)$-dimensional space of variables $Y\equiv(y^i,\eta^\mu)$. It should be noted that the Lagrangian $L^{(1)}$ in Eq. (12) is the same as Eq. (8) in which λ^μ is replaced by $\dot{\eta}^\mu$. This means that the derivatives $\dot{\eta}^\mu$ have the same role as Lagrangian multipliers λ^μ corresponding to primary constraints in the total Hamiltonian

$$H_T = H + \lambda^\mu\Phi_\mu^{(1)}. \tag{14}$$

In other words, if some of $\dot{\eta}^\mu$'s are found by the dynamical equations of the system, then the corresponding Lagrange multipliers are obtained. In the Dirac approach[15] this would be the case if there exist some second class constraints.

The equations of motion due to the Lagrangian $L^{(1)}$ can be written in matrix notation as

$$F\dot{Y} = \partial H. \tag{15}$$

Using operations that keep the determinant invariant, it is easy to show that

$$\det F = \det\begin{pmatrix} f & A \\ 0 & \tilde{A}f^{-1}A \end{pmatrix} = (\det f)(\det\tilde{A}f^{-1}A). \tag{16}$$

Since $\det f\neq 0$, F would be singular if $C\equiv\tilde{A}f^{-1}A$ is singular. Using (5) and (11) we have

$$C_{\mu\nu} = \{\Phi^{(1)}_{\mu}, \Phi^{(1)}_{\nu}\}. \tag{17}$$

Suppose rank $(C) = M''$ where $M'' \leqslant M$. This means that F possesses $M' = M - M''$ null-eigenvectors. One can, in principle, divide $\Phi^{(1)}_{\mu}$'s in two sets $\Phi^{(1)}_{\mu'}$ and $\Phi^{(1)}_{\mu''}$ such that

$$\{\Phi^{(1)}_{\mu'}, \Phi^{(1)}_{\nu}\} \approx 0,$$

$$\{\Phi^{(1)}_{\mu''}, \Phi^{(1)}_{\nu''}\} \approx C_{\mu''\nu''}, \quad \det C_{\mu''\nu''} \neq 0, \tag{18}$$

where the weak equality symbol $\approx$ means equality on the surface of the constraints already known (here, the primary constraints). The matrix A can be decomposed to A' and A'' such that

$$A_{\mu' i} = \partial_i \Phi^{(1)}_{\mu'},$$

$$A_{\mu'' i} = \partial_i \Phi^{(1)}_{\mu''}. \tag{19}$$

Accordingly the symplectic tensor F can be written as

$$F = \begin{pmatrix} f & A'' & A' \\ -\tilde{A}'' & 0 & 0 \\ -\tilde{A}' & 0 & 0 \end{pmatrix}. \tag{20}$$

Consider the rectangular matrix

$$(\tilde{A}' f^{-1}, 0, 1), \tag{21}$$

which has M' rows and $2K+M$ columns. Using (18) one can show that its rows are left null-eigenvectors of F. Multiplying (21) with the equations of motion (15) gives the second level constraints as

$$\Phi^{(2)}_{\mu'} \approx \{\Phi^{(1)}_{\mu'}, H\} = 0. \tag{22}$$

On the other hand, F in (20) has an invertible sub-block

$$F_{\text{inv}} = \begin{pmatrix} f & A'' \\ -\tilde{A}'' & 0 \end{pmatrix} \tag{23}$$

with the inverse

$$F^{-1}_{\text{inv}} = \begin{pmatrix} f^{-1} - f^{-1}A''C''^{-1}\tilde{A}''f^{-1} & -f^{-1}A''C''^{-1} \\ C''^{-1}\tilde{A}''f^{-1} & C''^{-1} \end{pmatrix}. \tag{24}$$

This can solve the equations of motion (15) for variables $\dot{\eta}^{\mu''}$ to give

$$\dot{\eta}^{\mu''} = -C^{\mu''\nu''}\{\Phi^{(1)}_{\nu''}, H\}, \tag{25}$$

where $C^{\mu''\nu''}$ is the inverse of $C_{\mu''\nu''}$. Inserting this in the Lagrangian (12) gives

$$L^{(1)} = a_i(y)\dot{y}^i - \dot{\eta}^{\mu'}\Phi^{(1)}_{\mu'} - H^{(1)}(y), \tag{26}$$

where

$$H^{(1)} = H - \{H, \Phi^{(1)}_{\mu''}\}C^{\mu''\nu''}\Phi^{(1)}_{\nu''}. \tag{27}$$

In this way a number of Lagrange multipliers corresponding to the second class constraints are derived whose effect is only replacing the canonical Hamiltonian H with $H^{(1)}$. Now we can forget about them and suppose that we are given the primary constraints $\Phi_\mu^{(1)}$ and the second level constraints $\phi_\mu^{(2)}$. Next, we should consider the consistency of $\Phi_\mu^{(2)}$ and add the term $-\dot{\eta}_2^\mu \Phi_\mu^{(2)}$ to the Lagrangian $L^{(1)}$. Renaming the previous $\eta^{\mu'}$'s as η_1^μ, the new Lagrangian would be

$$L^{(2)} = a_i(y)\dot{y}^i - \dot{\eta}_1^\mu \Phi_\mu^{(1)} - \dot{\eta}_2^\mu \Phi_\mu^{(2)} - H^{(1)}(y) \tag{28}$$

this gives the symplectic two-form

$$F^{(2)} = \begin{pmatrix} f & A^{(1)} & A^{(2)} \\ -\tilde{A}^{(1)} & 0 & 0 \\ -\tilde{A}^{(2)} & 0 & 0 \end{pmatrix} \tag{29}$$

in the space (y, η_1, η_2). Assuming that the composed matrix $A \equiv (A^{(0)}, A^{(1)})$, $F^{(2)}$ has the same form as (13). One should again proceed in the same way to find the null-eigenvectors as well as the invertible sub-block of $F^{(2)}$. The process goes on in this and the subsequent steps as explained in more detail in Ref. 12.

The important point to be emphasized is that the Lagrangian,

$$L^{(n)} = a_i(y)\dot{y}^i - \sum_{k=1}^{n} \dot{\eta}_k^\mu \Phi_\mu^{(k)} - H^{(n)}(y), \tag{30}$$

at the nth level, say, is equivalent to a system with extended Hamiltonian,

$$H_E^{(n)} = H^{(n-1)} + \sum_{k=1}^{n} \lambda_k^\mu \Phi_\mu^{(k)}, \tag{31}$$

at that level. In other words, the symplectic analysis is equivalent to the Dirac approach in the context of the level by level method provided that at each level one adds the new constraints with the corresponding Lagrange multipliers to the Hamiltonian. In fact this slight difference with the standard Dirac method may lead to some difficulties as we will see in the following section.

III. THE PROBLEM WITH EXTENDED HAMILTONIAN

The extended Hamiltonian formalism is well known in the context of first class constraints.[15,16] In fact, it can be shown that the dynamical equation

$$\dot{g} = \{g, H_E\}, \tag{32}$$

leads to the correct equation of motion provided that g is a gauge invariant quantity. In Eq. (32) the extended Hamiltonian H_E is defined as

$$H_E = H + \lambda^m \Phi_m, \tag{33}$$

where Φ_m are only first class constraints (primary or secondary). For a first class system, the extended Hamiltonian can also be used step by step during the process of producing the constraints. In other words, when all of the constraints are first class, there is no difference whether one uses $\dot{\Phi} = \{\Phi, H_T\}$ or $\dot{\Phi} = \{\Phi, H_E\}$.

Now we show that the extended Hamiltonian formalism in the Dirac approach is not suitable when second class constraints are present. We show this point for a system with only one primary constraint, i.e., a one-chain system in the language of chain by chain method. We remember that for such a system level by level and chain by chain methods coincide.

Consider a system with the canonical Hamiltonian $H(y)$ and one primary constraint $\Phi^{(1)}$. The total Hamiltonian reads

$$H_T = H + \lambda\Phi^{(1)}. \tag{34}$$

Suppose the consistency of $\Phi^{(1)}$ leads to $\Phi^{(2)}=\{\Phi^{(1)},H\}$. Then $\Phi^{(3)}$ emerges as $\{\Phi^{(2)},H\}$, and so on. The iterative process that produces the constraints is described by

$$\Phi^{(n+1)} = \{\Phi^{(n)},H\}. \tag{35}$$

The above procedure progresses unless $\{\Phi^{(N)},H_T\}\approx 0$ or $\{\Phi^{(N)},\Phi^{(1)}\}\neq 0$ at the last step N. In the former case the constraints in the chain are first class, i.e., commute with each other;[13] while in the latter all the constraints are second class which means that the matrix

$$C^{nm} = \{\Phi^{(n)},\Phi^{(m)}\} \tag{36}$$

is invertible. In this case the Lagrange multiplier λ would finally be determined as

$$\lambda = \frac{\{\Phi^{(N)},H\}}{\{\Phi^{(N)},\Phi^{(1)}\}}. \tag{37}$$

Using the Jacobi identity, it is shown in Ref. 13 that the matrix C^{nm} in Eq. (36) has the following form:

$$C \approx \begin{pmatrix} 0 & 0 & \cdots & 0 & C^{1N} \\ 0 & 0 & \cdots & C^{2(N-1)} & C^{2N} \\ \vdots & \vdots & & \vdots & \cdots \\ 0 & C^{(N-1)2} & \cdots & C^{(N-1)(N-1)} & C^{(N-1)N} \\ C^{N1} & C^{N2} & \cdots & C^{N(N-1)} & C^{NN} \end{pmatrix}. \tag{38}$$

In other words,

$$\{\Phi^{(i)},\Phi^{(j)}\} \approx 0 \quad \text{if } i+j \leqslant N. \tag{39}$$

Moreover using the Jacobi identity one can show from (35) that

$$\{\Phi^{(1)},\Phi^{(N)}\} \approx -\{\Phi^{(2)},\Phi^{(N-1)}\} \approx \cdots \approx (-1)^{[(N/2)-1]}\{\Phi^{N/2},\Phi^{[(N/2)+1]}\} \neq 0. \tag{40}$$

Remember that N is the number of second class constraints and necessarily should be even.

Now suppose that in order to define the dynamics of the system at some level n, one wishes to use the extended Hamiltonian,

$$H_E^{(n)} = H + \sum_{k=1}^{n} \lambda_k \Phi^{(k)}. \tag{41}$$

If $n \leqslant N/2$ then from (38) the consistency of the constraint $\Phi^{(n)}$ gives

$$\dot{\Phi}^{(n)} = \{\Phi^{(n)},H_E^{(n+1)}\} \approx \{\Phi^{(n)},H\}, \tag{42}$$

which by (35), is the same as $\Phi^{(n+1)}$. However at level $(N/2)+1$ the consistency of $\Phi^{[(N/2)+1]}$, using $H_E^{[(N/2)+1]}$ gives

$$\dot{\Phi}^{[(N/2)+1]} = \{\Phi^{[(N/2)+1]},H\} + \lambda_{N/2}\{\Phi^{[(N/2)+1]},\Phi^{N/2}\}. \tag{43}$$

As is apparent from (40) the above equation solves the Lagrange multiplier $\lambda_{N/2}$. There is no justification to keep $\{\Phi^{[(N/2)+1]},H\}$ as the next constraint $\Phi^{[(N/2)+2]}$. In order to knit the second class chain up to the last element $\Phi^{(N)}$, one is just allowed to use the total Hamiltonian (34). In other words, the second half of the chain can be derived if only the primary constraint $\Phi^{(1)}$ is present in the corresponding Hamiltonian. As explained in the preceding section, using the standard symplectic analysis is equivalent to using the extended Hamiltonian formalism described above. So

one should expect some contradiction in symplectic analysis when second class constraints are present. In the next section we will show the essence of this contradiction for a one chain system and propose a method to resolve it.

IV. SECOND CLASS ONE CHAIN IN SYMPLECTIC ANALYSIS

According to the algorithm given in Sec. II, given the canonical Hamiltonian $H(y)$ and the primary constraint $\Phi_{\mu}^{(1)}$, at the first step of consistency one should consider the Lagrangian (see Ref. 14)

$$L^{(1)} = a_i \dot{y}^i - \dot{\eta}_1 \Phi^{(1)} - H(y). \tag{44}$$

The equations of motion can be written in matrix form as

$$\begin{pmatrix} f & A^{(1)} \\ -\tilde{A}^{(1)} & 0 \end{pmatrix} \begin{pmatrix} \dot{y} \\ \dot{\eta}_1 \end{pmatrix} = \begin{pmatrix} \partial H \\ 0 \end{pmatrix}. \tag{45}$$

It is easy to see that

$$u^1 \equiv (\tilde{A}^{(1)} f^{-1}, 1) \tag{46}$$

is the null-eigenvector of the matrix

$$F = \begin{pmatrix} f & A^{(1)} \\ -\tilde{A}^{(1)} & 0 \end{pmatrix}. \tag{47}$$

Implying u^1 on both sides of (45) and using (5) gives the new constraint

$$\Phi^{(2)} = \{\Phi^{(1)}, H\}. \tag{48}$$

Adding the term $-\dot{\eta}_2 \Phi^{(2)}$ to the Lagrangian (to perform consistency) gives

$$L^{(2)} = a_i \dot{y}^i - \dot{\eta}_1 \Phi^{(1)} - \dot{\eta}_2 \Phi^{(2)} - H(y). \tag{49}$$

The equations of motion are

$$\begin{pmatrix} f & A^{(1)} & A^{(2)} \\ -\tilde{A}^{(1)} & 0 & 0 \\ -\tilde{A}^{(2)} & 0 & 0 \end{pmatrix} \begin{pmatrix} \dot{y} \\ \dot{\eta}_1 \\ \dot{\eta}_2 \end{pmatrix} = \begin{pmatrix} \partial H \\ 0 \\ 0 \end{pmatrix}. \tag{50}$$

Assuming $\{\Phi^{(1)}, \Phi^{(2)}\} \approx 0$, one can find the new null-eigenvector,

$$u^2 \equiv (\tilde{A}^{(2)} f^{-1}, 0, 1). \tag{51}$$

Multiplying u^2 by (50) gives the new constraint $\Phi^{(3)} = \{\Phi^{(2)}, H\}$, and so on.

Suppose one wishes to proceed in this way to find the constraints of the chain discussed in the preceding section, i.e., the second class chain $\Phi^{(1)}, \ldots, \Phi^{(N)}$ with the algebra given in (38)–(40). Suppose the above procedure has been proceeded up to the step $(N/2)+1$ where the equations of motion are

$$\begin{pmatrix} f & A^{(1)} & \cdots & A^{[(N/2)+1]} \\ -\tilde{A}^{(1)} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ -\tilde{A}^{[(N/2)+1]} & 0 & \cdots & 0 \end{pmatrix} \begin{pmatrix} \dot{y} \\ \dot{\eta}_1 \\ \vdots \\ \dot{\eta}_{(N/2)+1} \end{pmatrix} = \begin{pmatrix} \partial H \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{52}$$

Clearly no more null-eigenvector can be found. In fact adding the column and row corresponding to the constraint $\Phi^{[(N/2)+1]}$ has increased the rank of the matrix F by two. This means that the equations of motion can be solved to find $\dot{\eta}^{N/2}$ and $\dot{\eta}^{[(N/2)+1]}$. There is no way in the context of symplectic analysis to proceed further to find the remaining constraints $\Phi^{[(N/2)+1]},\ldots,\Phi^{(N)}$ of the chain. This is really the failure of traditional symplectic analysis. In fact this is the reason why the symplectic analysis has failed in the example given in Ref. 14 (particle in hypersphere). We will discuss this example in Sec. VI.

What we showed here is the failure of symplectic analysis for a second class system with only one primary constraint (i.e., a one chain system). However, one can easily observe that for an arbitrary system with several primary constraints again the symplectic analysis would fail. The reason is that for such a system some of the constraints driven at level n, i.e., $\Phi_{\mu}^{(n)}$, may have nonvanishing Poisson brackets with constraints of previous levels while commuting with primary constraints. As we know from the Dirac approach, in such a case the Poisson brackets of these constraints with Hamiltonian give the next level constraints. Meanwhile, a little care on symplectic analysis shows that in this case a number of Lagrange multipliers corresponding to nonprimary constraints would be determined and there is no way to find the next level constraints. In this way, we conclude that *the symplectic analysis would fail whenever second class constraints emerge at third level or higher*.

V. HOW TO SOLVE THE PROBLEM

In this section we try to find a way to maintain the symplectic analysis by imposing some modifications. The origin of the problem is the fact that $\Phi^{[(N/2)+1]}$ has nonvanishing Poisson brackets with $\Phi^{N/2}$. As a result, the symplectic two-form on the left-hand side of Eq. (52), i.e.,

$$F=\begin{pmatrix} f & A^{(1)} & \cdots & A^{[(N/2)+1]} \\ -\tilde{A}^{(1)} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ -\tilde{A}^{[(N/2)+1]} & 0 & \cdots & 0 \end{pmatrix}, \tag{53}$$

does not possess a new null-eigenvector. If one could consider the vector

$$u^{[(N/2)+1]}\equiv(\tilde{A}^{[(N/2)+1]}f^{-1},0,\ldots,0,1) \tag{54}$$

as a null-eigenvector, then by multiplying $u^{[(N/2)+1]}$ on the right-hand side of (52), one would obtain the next constraint as

$$\Phi^{[(N/2)+2]}=\{\Phi^{[(N/2)+1]},H\}. \tag{55}$$

To reach this goal one should truncate those columns of F which are located after $A^{(1)}$. In other words, instead of F in Eq. (53) one should consider the rectangular matrix

$$\tilde{F}=\begin{pmatrix} f & A^{(1)} \\ -\tilde{A}^{(1)} & 0 \\ \vdots & \vdots \\ -\tilde{A}^{[(N/2)+1]} & 0 \end{pmatrix}. \tag{56}$$

Clearly $u^{[(N/2)+1]}$ in Eq. (54) is the null-eigenvector of $\tilde{F}$. It is obvious that if one does the same thing in the subsequent steps, one can produce all the remaining constraints of the chain, i.e., $\Phi^{[(N/2)+1]},\ldots,\Phi^{(N)}$. In the last step the chain terminates, since $\{\Phi^{(N)},\Phi^{(1)}\}\neq 0$.

But what is the justification to find the null-eigenvectors of $\tilde{F}$, i.e., the *truncated F*. In fact using Eq. (5) the set of equations

$$\begin{pmatrix} f & A^{(1)} \\ -\tilde{A}^{(1)} & 0 \\ \vdots & \vdots \\ -\tilde{A}^{(N)} & 0 \end{pmatrix} \begin{pmatrix} \dot{y} \\ \dot{\eta}_1 \end{pmatrix} = \begin{pmatrix} \partial H \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{57}$$

is equivalent to

$$\dot{y}_i = \{y_i, H + \dot{\eta}_1 \Phi^{(1)}\}, \quad i = 1, \ldots, 2K,$$

$$\dot{\Phi}^{(j)} = 0, \quad j = 1, \ldots, N. \tag{58}$$

Remembering that $\dot{\eta}_1$ has the same role as the Lagrange multiplier λ_1 corresponding to the primary constraint $\Phi^{(1)}$, we see that Eq. (58) is the correct equation of motion

$$\dot{y}_i = \{y_i, H_T\}. \tag{59}$$

On the other hand, it is easy to see that the equations of motion resulting from Eq. (52) can be written as

$$\dot{y}_i = \{y_i, H_E\}, \tag{60}$$

where H_E contains all derived constraints (including second class ones). In fact as we explained before, the correct equations of motion are (58) and not (60).

Therefore, if one wishes to proceed in the context of symplectic analysis, one should consider Eq. (57) instead of Eq. (52).

VI. EXAMPLE

Consider the Lagrangian

$$L = \tfrac{1}{2}\dot{\mathbf{q}}^2 + v(\mathbf{q}^2 - 1), \tag{61}$$

where $\mathbf{q} \equiv (q_1, \ldots, q_n)$. The primary constraint is P_v. The corresponding Hamiltonian is

$$H = \tfrac{1}{2}\mathbf{p}^2 - v(\mathbf{q}^2 - 1), \tag{62}$$

where $\mathbf{p} \equiv (p_1, \ldots, p_n)$. In the usual Dirac approach, using the total Hamiltonian $H_T = H + \lambda P_v$, the consistency of $\Phi^{(1)} = P_v$ gives the following chain of constraints

$$\Phi^{(1)} = P_v,$$

$$\Phi^{(2)} = \mathbf{q}^2 - 1,$$

$$\Phi^{(3)} = 2\mathbf{q} \cdot \mathbf{p},$$

$$\Phi^{(4)} = 2(\mathbf{p}^2 + 2v\mathbf{q}^2). \tag{63}$$

As is apparent, $\Phi^{(4)}$ and $\Phi^{(3)}$ are conjugate to $\Phi^{(1)}$ and $\Phi^{(2)}$, respectively. It is worth remembering that although $\Phi^{(3)}$ is second class, when reaching at third level, the process of consistency should not stop, i.e., it should be proceeded one level more to find $\Phi^{(4)}$ which is conjugate to the primary constraint $\Phi^{(1)}$. In the symplectic approach the corresponding first order Lagrangian is

$$L = \mathbf{p}\dot{\mathbf{q}} + P_v\dot{v} - \tfrac{1}{2}\mathbf{p}^2 + v(\mathbf{q}^2 - 1) - \lambda P_v. \tag{64}$$

This gives the singular presymplectic tensor

$$F=\begin{pmatrix} f & 0 \\ 0 & 0 \end{pmatrix}, \tag{65}$$

where f is the usual $(2n+2)\times(2n+2)$ symplectic tensor,

$$f=\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{66}$$

The equations of motion for $y^i=(\mathbf{q},v,\mathbf{p},P_v,\lambda)$ are $f_{ij}\dot{y}^j=\partial_i H_T$ where $H_T=H+\lambda P_v$. Clearly this gives the canonical equation of motion with Hamiltonian H_T, together with the constraint equation $P_v=0$. Adding the consistency term $-\dot{\eta}_1 P_v$ to the Lagrangian (64), where η_1 is a new variable and forgetting about the term proportional to λ (which just reproduces the primary constraint) one finds

$$L^{(1)}=\mathbf{p}\dot{\mathbf{q}}+P_v\dot{v}-\dot{\eta}_1 P_v-\tfrac{1}{2}\mathbf{p}^2+v(\mathbf{q}^2-1). \tag{67}$$

This gives the equations of motion

$$F^{(1)}_{ij}\dot{Y}^j=\partial_i H, \tag{68}$$

where $Y^i\equiv(\mathbf{q},v,\mathbf{p},P_v,\eta_1)$. In the matrix form we have

$$F^{(1)}=\begin{pmatrix} f & A^{(1)} \\ -\tilde{A}^{(1)} & 0 \end{pmatrix}, \tag{69}$$

where $\tilde{A}^{(1)}=(\mathbf{0},0,\mathbf{0},1)$. Here, bold zero ($\mathbf{0}$) means a row vector with n zero components. Clearly $u^{(1)}=(\mathbf{0},-1,\mathbf{0},0,1)$ is the left null-eigenvector of $F^{(1)}$. Multiplying the equations of motion (68) from the left by $u^{(1)}$ gives the constraint $\Phi^{(2)}=\mathbf{q}^2-1$.

In the next level we have the Lagrangian

$$L^{(2)}=L-\dot{\eta}_1 P_v-\dot{\eta}_2(\mathbf{q}^2-1) \tag{70}$$

written in the space $Y^i\equiv(\mathbf{q},v,\mathbf{p},P_v,\eta_1,\eta_2)$. The corresponding symplectic tensor reads

$$F^{(2)}=\begin{pmatrix} f & A^{(1)} & A^{(2)} \\ -\tilde{A}^{(1)} & 0 & 0 \\ -\tilde{A}^{(2)} & 0 & 0 \end{pmatrix}, \tag{71}$$

where $\tilde{A}^{(2)}=(2\mathbf{q},0,\mathbf{0},0)$. Clearly $u^{(2)}=(\mathbf{0},0,2\mathbf{q},0,0,1)$ is the null-eigenvector of F^2. Multiplying the equations of motion $F^{(2)}_{ij}\dot{Y}^j=\partial_i H_T$ from the left by $u^{(2)}$ gives the next level constraint $\Phi^{(3)}=2\mathbf{q}\cdot\mathbf{p}$. Again considering another variable η_3, the third level Lagrangian would be

$$L^{(3)}=L-\dot{\eta}_1 P_v-\dot{\eta}_2(\mathbf{q}^2-1)-\dot{\eta}_3(2\mathbf{q}\cdot\mathbf{p}). \tag{72}$$

This gives the following symplectic tensor:

$$F^{(3)}=\begin{pmatrix} f & A^{(1)} & A^{(2)} & A^{(3)} \\ -\tilde{A}^{(1)} & 0 & 0 & 0 \\ -\tilde{A}^{(2)} & 0 & 0 & 0 \\ -\tilde{A}^{(3)} & 0 & 0 & 0 \end{pmatrix}, \tag{73}$$

where $\tilde{A}^{(3)}=(2\mathbf{p},0,2\mathbf{q},0)$. Now the crucial point appears. That is, $F^{(3)}$ has no new null-eigenvector. In fact one expects that multiplying $u^{(3)}=(-2\mathbf{q},0,2\mathbf{p},0,0,0,1)$ by the equations of motion due to $L^{(3)}$ gives the next constraint $\Phi^{(4)}=2(\mathbf{p}^2+2v\mathbf{q}^2)$. However, it can be easily checked

that $u^{(3)}F^{(3)}\neq 0$. Moreover, $u^{(2)}$ (with one additional zero as the last element) is no more the null-eigenvector of $F^{(3)}$. This means that adding the $(2n+5)$th row and columns to $F^{(2)}$ has led to increasing the rank of $F^{(3)}$ by two. In other words, the equations of motion for $\dot{\eta}_2$ and $\dot{\eta}_3$ can be solved. Unfortunately without any modification there is no way to find the Lagrangian,

$$L^{(4)}=L-\dot{\eta}_1 P_v-\dot{\eta}_2(\mathbf{q}^2-1)-\dot{\eta}_3(2\mathbf{q}\cdot\mathbf{p})-\dot{\eta}_4(2(\mathbf{p}^2+2v\mathbf{q}^2)). \tag{74}$$

If we could find $L^{(4)}$, then we would be able to have

$$F^{(4)}=\begin{pmatrix} f & A^{(1)} & A^{(2)} & A^{(3)} & A^{(4)} \\ -\tilde{A}^{(1)} & 0 & 0 & 0 & 0 \\ -\tilde{A}^{(2)} & 0 & 0 & 0 & 0 \\ -\tilde{A}^{(3)} & 0 & 0 & 0 & 0 \\ -\tilde{A}^{(4)} & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{75}$$

where $\tilde{A}^{(4)}=(8v\mathbf{q},4\mathbf{q}^2,4\mathbf{p},0)$. If we had somehow derived (74) and (75), then the singularity of symplectic tensor would completely disappear and $\dot{\eta}_1,\ldots,\dot{\eta}_4$ would be obtained. However, using the *truncated symplectic tensor* at the second step as

$$\tilde{F}^{(2)}=\begin{pmatrix} f & A^{(1)} \\ -\tilde{A}^{(1)} & 0 \\ -\tilde{A}^{(2)} & 0 \end{pmatrix} \tag{76}$$

and similarly $\tilde{F}^{(3)}$ at the third level as

$$\tilde{F}^{(3)}=\begin{pmatrix} f & A^{(1)} \\ -\tilde{A}^{(1)} & 0 \\ -\tilde{A}^{(2)} & 0 \\ -\tilde{A}^{(3)} & 0 \end{pmatrix} \tag{77}$$

makes it possible to introduce again $u^{(2)}$ and $u^{(3)}$ as the corresponding left null-eigenvectors of $\tilde{F}^{(2)}$ and $\tilde{F}^{(3)}$, respectively. This makes us able to find $\Phi^{(4)}$ as explained before. It should be noted that one can after all write the complete symplectic tensor $F^{(4)}$.

This example has also been discussed in Ref. 14, where some other reason is proposed as the origin of failure of the symplectic analysis. The same results as what we derived here can be found in every second class system possessing at least four levels of constraints. For example, one can study the simpler Lagrangian $L=\dot{x}\dot{y}-z(x+y)$ as well as the more complicated example of the bosonized Schwinger model in $(1+1)$ dimensions[17,18] given by

$$\mathcal{L}=\tfrac{1}{2}\partial_\mu\phi\partial^\mu\phi+(g^{\mu\nu}-\varepsilon^{\mu\nu})\partial_\mu\phi A_\nu-\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu}+\tfrac{1}{2}A_\mu A^\mu. \tag{78}$$

One can see that the main feature of the above calculations will more or less appear in all such examples.

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A model for Hopfions on the space–time $S^3 \times \mathbb{R}$

E. De Carli
Instituto de Física Teórica, IFT/UNESP, Universidade Estadual Paulista, Rua Pamplona 145, 01405-900, São Paulo–SP, Brazil and Departamento de Engenharia Mecânica, LMPT, Universidade Federal de Santa Catarina, UFSC, Campus Universitário, Trindade, 88040-900, Florianópolis-SC, Brazil

L. A. Ferreira
Instituto de Física de São Carlos, IFSC/USP, Universidade de São Paulo, Caixa Postal 369, CEP 13560-970, São Carlos–SP, Brazil and Instituto de Física Teórica, IFT/UNESP, Universidade Estadual Paulista, Rua Pamplona 145, 01405-900, São Paulo–SP, Brazil

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We construct static and time dependent exact soliton solutions for a theory of scalar fields taking values on a wide class of two dimensional target spaces, and defined on the four dimensional space–time $S^3 \times \mathbb{R}$. The construction is based on an ansatz built out of special coordinates on S^3. The requirement for finite energy introduce boundary conditions that determine an infinite discrete spectrum of frequencies for the oscillating solutions. For the case where the target space is the sphere S^2, we obtain static soliton solutions with nontrivial Hopf topological charges. In addition, such Hopfions can oscillate in time, preserving their topological Hopf charge, with any of the frequencies belonging to that infinite discrete spectrum. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1829911]

I. INTRODUCTION

In this paper we consider a nonlinear theory of a complex scalar field u, on the space–time $S^3 \times \mathbb{R}$. Our considerations apply to a wide class of target spaces, but the case of most interest is that of the sphere S^2, in which case the field u parametrizes a plane corresponding to the stereographic projection of S^2. The action is the integral of the square of the pull-back of the area form on the target space. Therefore, it is quartic in derivatives, but only quadratic in time derivatives. The theory is integrable in the sense that it possesses a generalized zero curvature representation of its equations of motion and an infinite number of local conservation laws.[1,2] The conserved currents are associated to the invariance of the theory under the area preserving diffeomorphisms on the target space.

We construct an infinite number of static and time dependent exact soliton solutions using an ansatz[2,3] that reduces the four dimensional nonlinear equations of motion into linear ordinary differential equations for the profile function. In the case of the target space S^2 the solitons carry nontrivial Hopf topological charges. Although the topology is the same as that of other models possessing Hopfion solutions,[3–5] the Derrick's scaling argument is circumvented in a different manner. The stability of the static three dimensional solutions comes from the fact that the physical space is S^3 and that introduces a length scale given by its radius. A model in Euclidean space where a similar stability mechanism occurs is discussed in Ref. 6.

The requirement for finite energy leads to boundary conditions that determine an infinite discrete set of allowed frequencies for the oscillations of the solutions. Those solutions can be linearly superposed since the profile function satisfies a linear equation. It turns out that the energy of the superposed solution is the sum of the energies of the modes, and in this sense the modes are decoupled. However, the profile function can take values only on some intervals on the real line, which depend on the choice of the target space. Therefore, not all superpositions are allowed and that introduces some sort of coupling among the modes. The allowed superpositions for the case of the target space S^2 are discussed in detail. One of the most interesting superpositions corre-

sponds to oscillating Hopfion solutions. We show that it is possible to superpose to the static Hopfion soliton any number of oscillating modes with any of the frequencies belonging to that infinite discrete spectrum. Although the solution oscillates in time, its topological Hopf charge is preserved. The only constraint on such superposition appears on the intensity of each mode.

The paper is organized as follows: in Sec. II we introduce the model and discuss its integrability properties, in Sec. III we propose the ansatz and construct the exact soliton solutions, in Sec. IV we discuss the energy, boundary conditions and allowed frequencies. The case of the target space S^2 is discussed in Sec. V.

II. THE MODEL

The metric on the space–time $S^3\times\mathbb{R}$ is given by

$$\mathrm{d}s^2 = \mathrm{d}t^2 - r_0^2\left(\frac{\mathrm{d}z^2}{4z(1-z)} + (1-z)\mathrm{d}{\varphi_1}^2 + z\,\mathrm{d}{\varphi_2}^2\right), \tag{1}$$

where t is the time, z, and φ_i, $i=1$, 2, are coordinates on the sphere S^3, and $0\leqslant z\leqslant 1$, $0\leqslant\varphi_i\leqslant 2\pi$, and r_0 is the radius of the sphere S^3. Embedding S^3 on $\mathbb{R}^4$ we get that the Cartesian coordinates of the points of S^3 are

$$x_1 = r_0\sqrt{z}\cos\varphi_2, \quad x_3 = r_0\sqrt{1-z}\cos\varphi_1,$$

$$x_2 = r_0\sqrt{z}\sin\varphi_2, \quad x_4 = r_0\sqrt{1-z}\sin\varphi_1. \tag{2}$$

The model is defined by the action

$$S = \int \mathrm{d}t\int_{S^3}\mathrm{d}\Sigma\,\frac{h_{\mu\nu}^2}{\gamma^2}, \tag{3}$$

where the volume element on S^3 is $\mathrm{d}\Sigma=(r_0^3/2)\mathrm{d}z\,\mathrm{d}\varphi_1\,\mathrm{d}\varphi_2$, and

$$h_{\mu\nu}\equiv\partial_\mu u\partial_\nu u^* - \partial_\nu u\partial_\mu u^*, \tag{4}$$

where ∂_μ denotes partial derivatives with respect to the four coordinates on $S^3\times\mathbb{R}$, namely $\zeta^\mu\equiv(t,z,\varphi_1,\varphi_2)$, u is a complex scalar field, and $\gamma\equiv\gamma(|u|^2)$, is a real functional of the squared modulus of u, and it defines the geometry of the target space. The metric on target space is given by

$$\mathrm{d}\sigma^2 = \frac{\mathrm{d}u\,\mathrm{d}u^*}{\gamma}. \tag{5}$$

Some cases of interest are the following: (a) $\gamma=1$ corresponding to the plane with coordinates being the real and imaginary parts of u, (b) $\gamma=(1-|u|^2)^2$, with $|u|^2<1$, corresponding to the Poincaré hyperbolic disc, and (c) $\gamma=(1+|u|^2)^2$ corresponding to the sphere S^2. In such case, u is related to the three dimensional unit vector $\vec{n}$ ($\vec{n}^2=1$) defining the sphere, through the stereographic projection

$$\vec{n} = \frac{1}{1+|u|^2}(u+u^*,-i(u-u^*),|u|^2-1). \tag{6}$$

Notice that in the case of the target space being S^2, the action (3) corresponds to the quartic term of the Skyrme–Faddeev action[4] which has been studied on the space–time $S^3\times\mathbb{R}$ in Ref. 7.

The Euler–Lagrange equations following from (3) are given by

$$\partial^\mu\left(\frac{K_\mu}{\gamma}\right)=0 \tag{7}$$

together with its complex conjugate, and where

$$K_\mu = h_{\mu\nu}\partial^\nu u = (\partial u\partial u^*)\partial_\mu u - (\partial u)^2\partial_\mu u^*. \tag{8}$$

The model (3) possesses an infinite number of local conserved currents given by

$$J_\mu = \frac{K_\mu}{\gamma}\frac{\delta G}{\delta u} - \frac{K_\mu^*}{\gamma}\frac{\delta G}{\delta u^*}, \tag{9}$$

where G is a function of u and u^* but not of its derivatives. Using the equations of motion (7) and the identities

$$K_\mu\partial^\mu u = 0, \quad K_\mu\partial^\mu u^* - K_\mu^*\partial^\mu u = 0 \tag{10}$$

one can check that (9) is indeed conserved, i.e., $\partial^\mu J_\mu = 0$. The symmetries associated to such conservation laws are the area preserving diffeomorphisms of the target manifold. Indeed, the tensor $h_{\mu\nu}/\gamma$ is the pull-back of the area form on the target space

$$\mathrm{d}A = i\frac{\mathrm{d}u\wedge\mathrm{d}u^*}{\gamma}. \tag{11}$$

Therefore, the action (3) is invariant under diffeomorphisms preserving the area (11) and (9) are the corresponding Noether currents.[2,8]

III. THE ANSATZ

Following Refs. 2 and 3 we introduce the ansatz

$$u = f(t,z)e^{i(m_1\varphi_1+m_2\varphi_2)}, \tag{12}$$

where m_i, $i=1, 2$, are arbitrary integers, and f is a real profile function. Replacing it into the equation of motion (7) one gets

$$\partial_t\left(\frac{\partial_t f^2}{\gamma}\right) - \frac{4z(1-z)}{r_0^2\Omega}\partial_z\left(\Omega\frac{\partial_z f^2}{\gamma}\right) = 0, \tag{13}$$

where

$$\Omega \equiv m_1^2 z + m_2^2(1-z). \tag{14}$$

We now make a change of variable in the profile function, introducing a function g by

$$\mathrm{d}g \sim \frac{\mathrm{d}f^2}{\gamma}. \tag{15}$$

For instance, in the particular cases discussed below (5) we get that (a) for the plane where $\gamma=1$ one has $g=f^2$, and $g\geqslant 0$; (b) for the Poincaré hyperbolic disk where $\gamma=(1-|u|^2)^2$, one has $g=1/(1-f^2)$, and $g\geqslant 1$; (c) for the sphere S^2 where $\gamma=(1+|u|^2)^2$ one has $g=1/(1+f^2)$, and $0\leqslant g\leqslant 1$.

So, with the change (15) one gets that (13) becomes a linear partial differential equation in g

$$\partial_t^2 g - \frac{4z(1-z)}{r_0^2\Omega}\partial_z(\Omega\partial_z g) = 0. \tag{16}$$

The solutions can be obtained by separation of variables introducing

$$g(t,z) = J(t)H(z) \tag{17}$$

and then J and H must satisfy

$$\partial_t^2 J + \omega^2 J = 0 \tag{18}$$

and

$$z(1-z)\partial_z\big[\big(q^2 z + (1-z)\big)\partial_z H\big] + \frac{r_0^2\omega^2}{4}\big(q^2 z + (1-z)\big)H = 0, \tag{19}$$

where ω^2 is the separation of variables constant, and where q is

$$q \equiv \frac{|m_1|}{|m_2|}. \tag{20}$$

Equation (19) is what is called a Heun equation.[9] It is a generalization of Gauss hypergeometric equation in the sense that it has one extra regular singular point. Indeed, (19) reduces to the hypergeometric equation for $q=1$. Notice that (19) is invariant under the joint transformations $q \leftrightarrow 1/q$ and $z \leftrightarrow 1-z$. Therefore, if $H_{q,\omega}(z)$ is a solution of (19) for some value of q, so is

$$H_{1/q,\omega}(z) = H_{q,\omega}(1-z) \tag{21}$$

for the inverse value $1/q$. One can obtain solutions of (19) in powers series around $z=0$ and for $0 \leqslant q \leqslant 1$. The solutions for $q \geqslant 1$, are then obtained from those using the above symmetry. The power series solutions are given by

$$H_{q,\omega}(z) = \frac{1}{v_{q,\omega}}\left(z + \sum_{n=2}^{\infty} c_n z^n\right), \tag{22}$$

where the positive constants $v_{q,\omega}$ are chosen such that the maximum absolute value of $H_{q,\omega}(z)$ in the interval $0 \leqslant z \leqslant 1$, is unity. The coefficients, for $n \geqslant 2$, are determined by the recursion relation (with $c_0=0$, and $c_1=1$)

$$c_n = \frac{-1}{n(n-1)}\left[(q^2-1)\left(\frac{\omega^2 r_0^2}{4} - (n-2)^2\right)c_{n-2} + \left(\frac{\omega^2 r_0^2}{4} - (n-1)(n-2) + (q^2-1)(n-1)^2\right)c_{n-1}\right]. \tag{23}$$

We will be interested in solutions with ω real, and therefore the solutions of (18) are trigonometric functions. Of course, if g is a solution of (16), so is $\alpha g + \beta$, with α and β constants. We will then use the following normalization for the solutions of (16):

$$g_{q,\omega} = \tfrac{1}{2}[\sin(\omega t + \delta)H_{q,\omega}(z) + 1], \quad \omega \neq 0 \tag{24}$$

with $H_{q,\omega}(z)$ given by (22). The advantage of such normalization is that the solutions (24) take values on the real line from zero to unity only. Therefore, they are admissible solutions for the case where the target space is the sphere S^2 [see discussion below (15)].

We normalize the static solutions of (16) as

$$g_{q,0} = \frac{\ln(q^2 z + 1 - z)}{\ln q^2}. \tag{25}$$

So, $g_{q,0}$ is a monotonic function varying from zero at $z=0$ to unity at $z=1$. Notice that $g_{q,0} \to z$ as $q \to 1$. A decreasing function can be obtained by the interchange $g_{q,0} \to 1 - g_{q,0}$. Therefore, (25) are also admissible solutions for the case where the target space is the sphere S^2.

The admissible solutions for the cases of the plane or the Poincaré hyperbolic disk can then be written as

TABLE I. The first three frequencies leading to solutions (22) satisfying the boundary conditions (30) for some chosen values of q. Due to the symmetry (21) the frequencies are invariant under the interchange $q\leftrightarrow 1/q$.

q	$\omega_1^2 r_0^2/4$	$\omega_2^2 r_0^2/4$	$\omega_3^2 r_0^2/4$
1	2	6	12
3/4	1.983 765 266 031	5.987 866 563 654	11.988 820 961 965
1/2	1.913 643 550 920	5.923 271 548 463	11.930 495 946 441
1/4	1.733 644 829 967	5.672 599 570 202	11.668 111 143 086
1/10	1.517 649 738 276	5.238 029 617 258	11.066 608 078 277

$$g_{q,\omega}^{\text{plane}} = \alpha g_{q,\omega}, \quad g_{q,\omega}^{\text{Poinc.disk}} = \alpha g_{q,\omega} + 1 \tag{26}$$

with α being a real and positive constant, and $g_{q,\omega}$ being given either by (24) or (25) (see Tables I–III).

IV. THE ENERGY AND BOUNDARY CONDITIONS

The energy for the solutions obtained through the ansatz (12) and (15) is given by

$$E = \int_{S^3} \mathrm{d}\Sigma\, \mathcal{H} = 16\pi^2 r_0 \int_0^1 \mathrm{d}z\, \Omega\left(\frac{(\partial_t g)^2}{4z(1-z)} + \frac{1}{r_0^2}(\partial_t g)^2\right), \tag{27}$$

where $\mathcal{H}$ is the Hamiltonian density associated to (3). Using the equation of motion (16) one gets that the energy of static configurations is

$$E_{\text{static}} = \frac{16\pi^2}{r_0}(\Omega g \partial_z g)\big|_{z=0}^{z=1}. \tag{28}$$

Therefore, the energy of the static solutions (25) is

$$E(g_{q,0}) = \frac{16\pi^2}{r_0}|m_1 m_2|\frac{(q-1/q)}{\ln q^2}. \tag{29}$$

Notice that the solutions of (19), for $\omega\neq 0$, which do not vanish at $z=0$ or $z=1$, have a logarithmic divergence on its first derivative, at those points. We then observe from (27) that such solutions do not have finite energy. Consequently, we shall impose the following boundary conditions:

$$H_{q,\omega}(0) = H_{q,\omega}(1) = 0 \quad \text{for } \omega \neq 0. \tag{30}$$

In addition, using the equation of motion (16) one obtains that

TABLE II. Numerical values of Λ_{q,ω_i}, as defined in (34), for some chosen values of q and for the three frequencies given in Table I. Due to (21), $\Lambda_{q,\omega}$ is invariant under the interchange $q\leftrightarrow 1/q$.

q	Λ_{q,ω_1}	Λ_{q,ω_2}	Λ_{q,ω_3}
1	4/3	27/5	64/7
3/4	1.362 643	4.693 750	9.501 984
1/2	1.505 658	4.275 566	9.428 440
1/4	2.065 180	4.819 658	8.855 009
1/10	3.739 188	7.930 185	13.004 162

TABLE III. Numerical values of the normalization constant v_{q,ω_i}, as defined in (22), for some chosen values of q and for the three frequencies given in Table I. Due to (21), $v_{q,\omega}$ is invariant under the interchange $q \leftrightarrow 1/q$.

q	v_{q,ω_1}	v_{q,ω_2}	v_{q,ω_3}
1	1/4	$1/6\sqrt{3}$	1/16
3/4	0.285 189 93	0.119 156 83	0.070 789 33
1/2	0.332 611 65	0.152 779 52	0.087 010 28
1/4	0.409 991 03	0.204 149 92	0.126 957 32
1/10	0.502 749 25	0.256 726 47	0.167 310 92

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \frac{32\pi^2}{r_0}\,(\Omega\partial_t g\partial_z g)\big|_{z=0}^{z=1}\,. \tag{31}$$

Therefore, the energy is conserved for the static solutions, and for those solutions (24) satisfying the boundary conditions (30).

Multiplying (19) by $H_{q,\omega}$ and integrating in z, one gets that

$$\int_0^1 \mathrm{d}z \frac{\omega^2\Omega}{4z(1-z)}\,H_{q,\omega}^2 - \frac{1}{r_0^2}\int_0^1 \mathrm{d}z\,\Omega\,(H'_{q,\omega})^2 = -\frac{1}{r_0^2}\,(\Omega H_{q,\omega}\,H'_{q,\omega})\big|_{z=0}^{z=1}. \tag{32}$$

Consequently, the energy (27) for the solutions (24) satisfying (30) is

$$E(g_{q,\omega}) = \frac{16\pi^2}{r_0}\,|m_1\,m_2|\Lambda_{q,\omega}\,, \tag{33}$$

where

$$\Lambda_{q,\omega} = \Lambda_{1/q,\omega} = \frac{\omega^2 r_0^2}{16}\int_0^1 \mathrm{d}z\left(\frac{q}{1-z}+\frac{1}{qz}\right)H_{q,\omega}^2 = \frac{1}{4}\int_0^1 \mathrm{d}z\left(qz+\frac{1-z}{q}\right)(H'_{q,\omega})^2. \tag{34}$$

The fact that $\Lambda_{q,\omega}$ is invariant under $q \leftrightarrow 1/q$, follows from the symmetry (21). In Table II we give the values of $\Lambda_{q,\omega}$ for some chosen values of q and some allowed frequencies ω. So, the energies (29) and (33) do not depend upon the signs of the integers m_1 and m_2 and it is invariant under the interchange $m_1 \leftrightarrow m_2$ [see (20)].

Multiplying (19) by $H_{q,\varpi}$, subtracting from the same relation with ω interchanged with $\overline{\omega}$, and integrating in z, one gets that

$$(\omega^2-\overline{\omega}^2)\int_0^1 \mathrm{d}z\frac{\Omega}{4z(1-z)}H_{q,\omega}H_{q,\varpi} = \frac{1}{r_0^2}\,(\Omega(H_{q,\omega}H'_{q,\varpi} - H'_{q,\omega}H_{q,\varpi}))\big|_{z=0}^{z=1}. \tag{35}$$

Similarly, differentiating (19) with respect to z once, multiplying by $H'_{q,\varpi}$, subtracting from the same relation with ω interchanged with $\overline{\omega}$, and integrating in z, one gets that

$$(\omega^2-\overline{\omega}^2)\int_0^1 \mathrm{d}z\,\Omega H'_{q,\omega}H'_{q,\varpi} = \frac{1}{r_0^2}\,(4z(1-z)\Omega(H'_{q,\omega}H''_{q,\varpi} - H''_{q,\omega}H'_{q,\varpi}))\big|_{z=0}^{z=1}. \tag{36}$$

Consequently, for the solutions (24) satisfying (30), and having finite first and second z-derivatives at $z=0$ and $z=1$, one gets the orthogonality relations

$$\int_0^1 \mathrm{d}z \frac{\Omega}{4z(1-z)} H_{q,\omega} H_{q,\varpi} = \int_0^1 \mathrm{d}z\, \Omega H'_{q,\omega} H'_{q,\varpi} = 0 \quad \text{for } \omega \neq \overline{\omega}. \tag{37}$$

It then follows that the energy (27) of a linear combination of solutions (24) satisfying (30), is just the sum of the energies of each solution, i.e.,

$$E(Ag_{q,\omega} + Bg_{q,\varpi}) = A^2 E(g_{q,\omega}) + B^2 E(g_{q,\varpi}) \quad \text{for } \omega \neq \overline{\omega}. \tag{38}$$

Therefore, in that sense, the modes for the same value of q are decoupled. However, the intensities in which they enter in the superposition are not independent. As discussed below (15) the real values that the profile function g can take depend on the target space under consideration. So, when we take linear combinations of the solutions we have to respect those constraints. In Sec V we discuss those constrained linear combinations in detail in the case where the target space is the sphere S^2.

The boundary conditions (30) lead to a discrete spectrum of allowed frequencies ω. Indeed, for the case where $q=1$ the series (23) truncates whenever

$$\frac{r_0^2\omega^2}{4} = n(\mathrm{n}+1), \quad n = 1,2,3,\ldots, \tag{39}$$

and the corresponding polynomials satisfy the boundary conditions (30). The first four of those polynomials are given by [with the normalization as in (22)]

$$H_{1,2} = 4(z - z^2),$$

$$H_{1,6} = 6\sqrt{3}(z - 3z^2 + 2z^3),$$

$$H_{1,12} = 16(z - 6z^2 + 10z^3 - 5z^4),$$

$$H_{1,20} = \frac{2450(z - 10z^2 + 30z^3 - 35z^4 + 14z^5)}{\sqrt{7}(3\sqrt{5} + 5\sqrt{6})\sqrt{15 - 2\sqrt{30}}}, \tag{40}$$

where the first index refers to $q=1$ and the second to $n(n+1)$ as given by (39).

For $q \neq 1$ the series (22) does not truncate, and the frequencies ω leading to solutions satisfying (30) can be found numerically. We give in Table I the first three frequencies for some chosen values of q. In addition, the same frequencies hold true under the exchange $q \leftrightarrow 1/q$ due to the symmetry (21). Therefore, the frequencies become smaller as q departs from unity, either to smaller or greater values than unity.

In Fig. 1 we exemplify the shape of the functions $H_{q,\omega}$, by plotting the first three modes H_{q,ω_i}, for $q=3/4$ and $q=1/10$ and the frequencies ω_i, $i=1,2,3$, given in Table I. Due to the symmetry (21), $H_{1/q,\omega_i}$ can be obtained by reflecting the plots around $z=1/2$. Notice that the polynomial solutions for $q=1$, given in (40), are invariant under (21). One observes that as q decreases, the functions $H_{q,\omega}$ get deformed in a way that their first derivatives at $z=1$ increase. For $q>1$, it follows, due to (21), that the first derivative of $H_{q,\omega}$ at $z=0$ increases as q increases.

V. THE CASE OF S^2 AS TARGET SPACE

According to the comments below (15), in the case where the target space is the two dimensional sphere S^2, we have that $\gamma=(1+|u|^2)^2$, and so $g=1/(1+f^2)$ and $0\leqslant g\leqslant 1$. The ansatz (12) becomes

$$u = \sqrt{\frac{1-g}{g}}\, e^{i(m_1\varphi_1 + m_2\varphi_2)}. \tag{41}$$

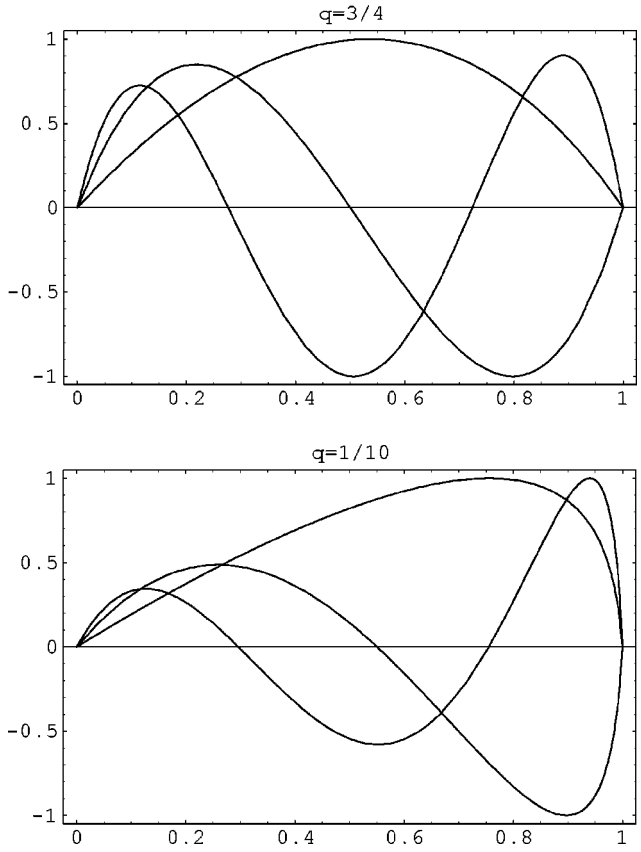

FIG. 1. Plots of $H_{q,\omega_i}(z)$, $i=1, 2, 3$, as normalized in (22), for $q=3/4$ (top) and $q=1/10$ (bottom) and for the three frequencies given in Table I. The number of zeroes increase with the increase of ω_i. The plots of $H_{q,\omega}$ and $H_{1/q,\omega}$ are related by reflection around $z=1/2$ due to the symmetry (21).

As we have discussed, the solutions (24) and (25) are admissible solutions for the case where the target space is S^2. However, one can construct more admissible solutions, i.e., with $0 \leqslant g \leqslant 1$, by taking linear combinations of the solutions (24) and (25). An interesting case corresponds to linear combinations of the static solution $g_{q,0}$ given by (25), with one or more time dependent solutions of the type (24). It leads to oscillating (in time) Hopfion solutions. Let us consider the case $q \leqslant 1$ first. The static solution $g_{q,0}$ vanishes at $z=0$, and has z-derivative equals to $(q^2-1)/\ln q^2$ there. The function $f_q(z) \equiv [(q^2-1)/\ln q^2] v_{q,\omega} H_{q,\omega}(z)$, with $H_{q,\omega}$ given by (23) and satisfying (30), has the same behavior at $z=0$ as $g_{q,0}$. In addition, c_2 given by (23), is negative for the case of $H_{q,\omega}$ satifying (30), and so $f_q(z)$ grows slower than $g_{q,0}$ for small z. We do not have rigorous proof, but by careful direct inspection we found that, as z increases from zero to unity the absolute value of $f_q(z)$ never exceeds the value of $g_{q,0}$, which is a positive monotonic function of z. It then follows that the combination

$$g_{q,0} + \alpha \frac{(q^2-1)}{\ln q^2} v_{q,\omega} \sin(\omega t + \delta) H_{q,\omega}(z) \tag{42}$$

with $0 \leqslant \alpha \leqslant 1$, takes values between zero and unity only, and so it is an admissible time dependent solution for the target space S^2. Therefore, by adding up such types of solutions and dividing by their number, one gets that the time dependent solutions

$$g_q^{(N)}(t,z)=\frac{\ln(q^2z+1-z)}{\ln q^2}+\frac{1}{N}\frac{(q^2-1)}{\ln q^2}\sum_{\omega_i}\alpha_i v_{q,\omega_i}\sin(\omega_i t+\delta_i)H_{q,\omega_i}(z), \tag{43}$$

where N is the number of modes (frequencies) entering into the sum, and α_i's are real coefficients satisfying $0\leqslant\alpha_i\leqslant 1$, are admissible solutions for the target space S^2. The energy of such solutions, according to (24), (25), (29), (33), and (38), is given by

$$E=\frac{16\pi^2}{r_0}|m_1m_2|\frac{(q-1/q)}{\ln q^2}\left(1+4\frac{q^2}{N^2}\frac{(q-1/q)}{\ln q^2}\sum_{\omega_i}\alpha_i^2v_{q,\omega_i}^2\Lambda_{q,\omega_i}\right) \tag{44}$$

with Λ_{q,ω_i} given by (34).

Solutions of the type (43) for $q\geqslant 1$ can be obtained using the symmetry (21), i.e., $g_{1/q}^{(N)}(t,z)=g_q^{(N)}(t,1-z)$. Solutions that decrease from unity at $z=0$ to zero at $z=1$ can be obtained by the symmetry $g_q^{(N)}(t,z)\to 1-g_q^{(N)}(t,z)$. The energy (44) is invariant under those two types of transformations. As we now show, all these solutions correspond to oscillating Hopfions, i.e., solutions that oscillate in time and have a constant (in time) nontrivial Hopf number.

For any fixed time t our solutions define a map from the physical space S^3 to the target space S^2, and so it is a Hopf map.[10] We now show that the Hopf invariant (the linking number) is independent of time for the admissible solutions we have constructed. In order to calculate the Hopf index of the solution we introduce

$$\Phi_1=\sqrt{g}\cos(m_2\varphi_2),\quad \Phi_3=\sqrt{1-g}\cos(m_1\varphi_1),$$

$$\Phi_2=-\sqrt{g}\sin(m_2\varphi_2),\quad \Phi_4=\sqrt{1-g}\sin(m_1\varphi_1), \tag{45}$$

which defines another 3-sphere S^3_Φ, since $\Phi_1^2+\Phi_2^2+\Phi_3^2+\Phi_4^2=1$. The field u in (41) can be written as

$$u=\frac{\Phi_3+i\Phi_4}{\Phi_1+i\Phi_2}. \tag{46}$$

Since u parametrizes the sphere S^2 through the stereographic projection (6), we have that (46) gives the map $S^3_\Phi\to S^2$. So, the Hopf index is in fact evaluated through the map $S^3\to S^3_\Phi\to S^2$, as we now explain. We introduce the potential

$$\vec{A}-\frac{i}{2}(Z^\dagger\vec{\nabla}Z-\vec{\nabla}Z^\dagger Z), \tag{47}$$

where

$$Z=\begin{pmatrix}Z_1\\Z_2\end{pmatrix},\quad Z_1=\Phi_3+i\Phi_4,\quad Z_2=\Phi_1+i\Phi_2 \tag{48}$$

and the differential operator $\vec{\nabla}$ is the gradient on the physical space S^3. The Hopf index is defined by the integral[10]

$$Q_H=\frac{1}{4\pi^2}\int \mathrm{d}\Sigma\,\vec{A}\cdot\mathrm{curl}\,\vec{A}, \tag{49}$$

where $\mathrm{d}\Sigma$ is the volume element on the physical space S^3. Evaluating we get

$$\vec{A}=-m_1\frac{(1-g)}{\sqrt{1-z}}\hat{\mathbf{e}}_{\varphi 1}+m_2\frac{g}{\sqrt{z}}\hat{\mathbf{e}}_{\varphi 2} \tag{50}$$

and

$$\text{curl}\,\vec{A} = 2\partial_z g(-m_2\sqrt{1-z}\hat{\mathbf{e}}_{\varphi 1} + m_1\sqrt{z}\hat{\mathbf{e}}_{\varphi 2}). \tag{51}$$

Consequently we get that

$$Q_H = m_1 m_2[g(t,z=1) - g(t,z=0)]. \tag{52}$$

Therefore, the solutions (25) have Hopf index

$$Q_H(g_{q,0}) = m_1 m_2 \tag{53}$$

and so they are static Hopfion soliton solution. The time dependent solutions (24) are constant at $z=0$ and $z=1$ due to the boundary condition (30), i.e., $g_{q\omega}(t,0)=g_{q\omega}(t,1)=1/2$. Therefore, they carry no Hopf number

$$Q_H(g_{q,\omega}) = 0, \quad \omega \neq 0. \tag{54}$$

The solutions (43) although time dependent, also have contant values at $z=0$ and $z=1$, determined by their static component. It then follows that

$$Q_H\left(g_q^{(N)}\right) = m_1 m_2 \tag{55}$$

and so they do correspond to oscillating Hopfion soliton solutions.

The Hopf index can also be calculated as the linking number of the preimages of two points of S^2.[10] Notice, from (6), that the north pole of S^2, $\vec{n}=(0,0,1)$, corresponds to $u\to\infty$, and so from (41) to $g=0$. On the other hand, the south pole of S^2, $\vec{n}=(0,0,-1)$, corresponds to $u=0$, and so to $g=1$. Therefore, from (45) and (48), we see that the pre-image on S^3_Φ of the north pole of S^2 correponds to $Z_1=e^{im_1\varphi_1}$ and $Z_2=0$, while the preimage of the south pole to $Z_1=0$ and $Z_2=e^{-im_2\varphi_2}$. For the static solution (25) and the time dependent solutions (43), the preimages in the spacial S^3 of these two circles in S^3_Φ are constant in time. In addition, those two circles in S^3_Φ pass through each other m_1m_2 times as φ_1 and φ_2 varies from 0 to 2π in S^3. So their linking number is m_1m_2, and that is the Hopf index. For the time dependent solutions (24) it is not possible to have $g=0$ and $g=1$ on different points on the spatial S^3 at the same time t. Therefore, the preimages of the north and south poles of S^2 never link, and so the Hopf index of such solutions vanishes.

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Dirac-type approach for consistent discretizations of classical constrained theories

Cayetano Di Bartolo
Departamento de Física, Universidad Simón Bolívar, Caracas 1080-A, Venezuela

Rodolfo Gambini
Instituto de Física, Facultad de Ciencias, Iguá 4225, esq. Mataojo, Montevideo, Uruguay

Rafael A. Porto
Department of Physics, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213

Jorge Pullin
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803-4001

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We analyze the canonical treatment of classical constrained mechanical systems formulated with a discrete time. We prove that under very general conditions, it is possible to introduce nonsingular canonical transformations that preserve the constraint surface and the Poisson or Dirac bracket structure. The conditions for the preservation of the constraints are more stringent than in the continuous case and as a consequence some of the continuum constraints become second class upon discretization and need to be solved by fixing their associated Lagrange multipliers. The gauge invariance of the discrete theory is encoded in a set of arbitrary functions that appear in the generating function of the evolution equations. The resulting scheme is general enough to accommodate the treatment of field theories on the lattice. This paper attempts to clarify and put on sounder footing a discretization technique that has already been used to treat a variety of systems, including Yang–Mills theories, BF theory, and general relativity on the lattice. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1823030]

I. INTRODUCTION

We have recently introduced[1,2] a technique for treating the theories that arise when one discretizes (space)–time in a constrained mechanical system or a continuum field theory. We have shown that this technique works for Yang–Mills and BF theories and implemented it for the gravitational case. Previous attempts to studying systems with discrete time had concentrated mostly on systems without constraints or with holonomic constraints only (for a review with a comprehensive reference list see Ref. 3).

The idea consists on starting from a discretized action, constructing discrete Lagrange equations and introducing a symplectic structure in the discrete space. The evolution is implemented via canonical transformations and the consistency of the discrete theory determines in part the Lagrange multipliers. In some totally constrained systems, like general relativity, the resulting discrete theories are constraint-free since the constraints are solved for the Lagrange multipliers. This makes the quantization of the discrete theories considerably simpler than the continuum cases. This was exploited to make progress in solving the problem of time in quantum gravity[4,5] and to implement the Page–Wootters relational time[5,6] and show that a fundamental decoherence arises in quantum mechanics from quantum gravity.

In this paper, we want to address in a more systematic way the issue of the canonical formulation of discrete constrained systems. Up to now, most of the analysis has been made on specific examples, and a canonical analysis, à la Dirac,[7,8] is still lacking. In particular, the technique relied

heavily on defining a canonical transformation that was initially singular (and therefore not a true canonical transformation) and showing that one could eliminate variables and end up with a true canonical transformation. Up to now this was shown in a case by case basis. This paper determines the general conditions needed for the construction of a proper canonical transformation by following a close analogue of the Dirac procedure, adapted to the discrete case. In particular, we note that there are several ways to proceed that yield equivalent results, but that may offer different advantages for particular systems.

In Sec. II we will lay out the framework of how to deal with mechanical systems where time is discrete, including singular and nonsingular systems. In Sec. III we will develop a classification of constraints into first and second class suitable for the discrete context. In Sec. IV we work out a specific example that exhibits the details of the formalism. In Sec. V we discuss an alternative formulation of the formalism and we end with conclusions and discussion.

II. MECHANICS WITH DISCRETE TIME

We start by considering a continuum theory representing a mechanical system. Its Lagrangian will be denoted by $\hat{L}(q^a,\dot{q}^a)$, $a=1,\ldots,M$. This setting is general enough to accommodate, for instance, totally constrained systems. In such case $\dot{q}$ will be the derivative of the canonical variables with respect to the evolution parameter. It is also general enough to include the systems that result from formulating on a discrete space–time lattice a continuum field theory.

We discretize the evolution parameter in intervals (possibly varying upon evolution) $t_{n+1}-t_n=\epsilon_n$ and we label the generalized coordinates evaluated at t_n as q_n. We define the discretized Lagrangian as

$$L(n,n+1)\equiv L(q_n^a,q_{n+1}^a)\equiv \epsilon_n \hat{L}(q^a,\dot{q}^a), \tag{1}$$

where

$$q^a=q_n^a \quad \text{and} \quad \dot{q}^a\equiv \frac{q_{n+1}^a-q_n^a}{\epsilon_n}. \tag{2}$$

Of course, one could have chosen to discretize things in a different fashion, for instance using a different approximation for the derivative, or by choosing to write the continuum Lagrangian in terms of different variables. The resulting discrete theories generically will be different and will approximate the continuum theory in different ways. However, given a discrete theory, the treatment we outline in this paper is unique. For instance, in the method we introduce in order for constraints to be preserved we will fix the values of the Lagrange multipliers. However, if one has constraints that are only function of either the configuration or the momentum variables (but not mixed) the method preserves the constraints automatically. Therefore the determination of the Lagrange multipliers will depend on the particular form chosen for the continuum theory. If one can find a canonical transformation that makes all the constraints only dependent on configuration variables, for example, then the Lagrange multipliers will not be determined and the symmetries implemented by the constraints will be preserved automatically without the need to determine the Lagrange multipliers.

The action can then be written as

$$S=\sum_{n=0}^{N} L(n,n+1). \tag{3}$$

It should be noted that in previous treatments[1,2] we have written the Lagrangian in first order form, i.e., $L=\int \mathrm{d}t(p\dot{q}-H(p,q))$. It should be emphasized that this is contained as a particular case in the treatment we are presenting in this paper. In this case one takes both q and p to be configuration variables, and one is faced with a Lagrangian that involves q_n, p_n, and q_{n+1} as variables, being independent of p_{n+1}. In Sec. IV we discuss an example where in fact we apply the

technique to a Lagrangian of this type. Although in simple examples as these the first order form may appear as a bit of an overkill, since dynamical variables and constraints proliferate, it nevertheless shows that the method is applicable as outlined without problems.

If the continuum theory is invariant under reparametrizations of the evolution parameter, one can show that the information about the intervals ϵ_n may be absorbed in the Lagrange multipliers. In the case of standard mechanical systems it is simpler to use an invariant interval $\epsilon_n = \epsilon$.

The Lagrange equations of motion are obtained by requiring the action to be stationary under variations of the configuration variables q^a fixed at the endpoints of the evolution interval $n=0$, $n=N+1$,

$$\frac{\partial L(n,n+1)}{\partial q_n^a} + \frac{\partial L(n-1,n)}{\partial q_n^a} = 0. \tag{4}$$

These equations define a unique evolution if the determinant is

$$\left| \frac{\partial^2 L(n,n+1)}{\partial q_{n+1}^b \partial q_n^a} \right| \neq 0. \tag{5}$$

We will refer to this case as the nonsingular case. When the determinant vanishes, one must analyze the situation differently. Let us start with the nonsingular case.

A. Nonsingular case

In this case one can solve the Lagrange equations explicitly and the q_{n+1} are uniquely given as a function of q_n and q_{n-1}. This is the equivalent of the Hessian condition for the nonsingular Lagrangian theories in the continuum. The resulting equations are "second order" in the sense that the q_n's are determined provided one knows two previous time levels. One can introduce a "first order" formulation by introducing canonically conjugate variables as is usually done when introducing a Hamiltonian formulation in the continuum theories.

We introduce the following definition of variables that we will later show end up being canonically conjugate momenta of the configuration variables:

$$p_{n+1}^a \equiv \frac{\partial L(n,n+1)}{\partial q_{n+1}^a}, \tag{6}$$

$$p_n^a \equiv \frac{\partial L(n-1,n)}{\partial q_n^a} = -\frac{\partial L(n,n+1)}{\partial q_n^a}, \tag{7}$$

where we have used Eq. (4). Equations (6) and (7) define a canonical transformation for the variables q_n, p_n to q_{n+1}, p_{n+1} with the type 1 generating function $F_1 = -L(q_n^a, q_n^a + 1)$ provided that condition (5) is fulfilled. Notice that the evolution scheme is implicit, one can use the bottom equation (since we are in the nonsingular case) to give an expression for q_{n+1} in terms of q_n, p_n, which in turn can be substituted in the top equation to get an equation for p_{n+1} purely in terms of q_n, p_n.

It should be noted that there are several other possible choices, when going from the set of equations (6) and (7) to an explicit evolution scheme. For example, one can choose to do things in a way that yields a closer analogy with the standard Hamiltonian description in the continuum by introducing type 2 canonical transformations. To do this, we choose to invert Eq. (6) for $q_{n+1}^a \equiv q_{n+1}^a(q_n^b, p_{n+1}^b)$, which is possible only if

$$\left| \frac{\partial^2 L(n,n+1)}{\partial q_{n+1}^a \partial q_{n+1}^b} \right| \neq 0. \tag{8}$$

We can now introduce a Legendre transform and define

$$F_2(q_n,p_{n+1}) \equiv \sum_a q^a_{n+1}p^a_{n+1} - L(q_n,q_{n+1}). \tag{9}$$

From here it is immediate to obtain

$$q^b_{n+1} = \frac{\partial F_2}{\partial p^b_{n+1}}, \tag{10}$$

$$\frac{\partial F_2}{\partial q^b_n} = \frac{-\partial L(n,n+1)}{\partial q^b_n} = p^b_n, \tag{11}$$

where we have used the Lagrange equation in order to obtain the last equality. We easily recognize from here that F_2 behaves as a type 2 generating function of the canonical transformation connecting level n with level $n+1$.

We may define now a sort of "type 2" Hamiltonian [in the sense that it depends on p_{n+1} and q_n, $H_2(p_{n+1},q_n)$] given by

$$H_2(q_n,p_{n+1}) \equiv \sum_a p^a_{n+1}(q^a_{n+1} - q^a_n) - L(q_n,q_{n+1}) = F_2(q_n,p_{n+1}) - \sum_a p^a_{n+1}q^a_n, \tag{12}$$

which leads to the discrete Hamilton equations,

$$q^b_{n+1} = q^b_n + \frac{\partial H_2}{\partial p^b_{n+1}}, \tag{13}$$

$$p^b_n = p^b_{n+1} + \frac{\partial H_2}{\partial q^b_n}. \tag{14}$$

It should be noted that although this formulation has a degree of analogy with the traditional Hamiltonian formulation, there are significant differences due to the fact that the conjugate variables live at different time slices. It would not be possible therefore to use this formulation to attempt to construct a Schrödinger equation starting from the above Hamiltonian.

Provided that the canonical map defined by F_2 is invertible we end up with a discrete evolution implemented by a canonical transformation. It can be easily seen by using the Legendre transform that F_2 will be invertible if and only if

$$\left|\frac{\partial^2 F_2(n,n+1)}{\partial q^a_n p^b_{n+1}}\right| = -\left|\frac{\partial^2 L(n,n+1)}{\partial q^a_n q^b_{n+1}}\right| \times \left|\frac{\partial^2 L(n,n+1)}{\partial q^a_{n+1} q^b_{n+1}}\right|^{-1} \neq 0. \tag{15}$$

Thus, in order to have canonical transformations generated by type 2 functions, the Hessian condition in the continuum time mechanics leads to two independent conditions in the discrete theory given by Eqs. (5) and (8). Notice however that (8) is not necessary for introducing a symplectic structure.

It is clear that when one builds a canonical discrete theory there are four possibilities depending on which pair of variables one chooses to construct the generating functional of the canonical transformation, either q_n,q_{n+1}, q_n,p_{n+1}, p_n,q_{n+1}, p_n,p_{n+1}. In this section we considered only two, but the others can be easily generalized from the discussion here.

B. The singular case

Let us consider as before the generic discrete Lagrangian $L(n,n+1)=L(q^a_n,q^a_{n+1})$ with $a=1,\ldots,M$. It leads to the equations we already discussed,

$$p^a_{n+1} = \frac{\partial L(n,n+1)}{\partial q^a_{n+1}}, \tag{16}$$

$$p_n^a = -\frac{\partial L(n,n+1)}{\partial q_n^a}. \tag{17}$$

If $|\partial^2 L(n,n+1)/\partial q_{n+1}^a \partial q_n^b|$ vanishes and its rank is K, the system is singular and has $M-K$ constraints of the form

$$\Phi_A(q_n^a, p_n^a) = 0 \tag{18}$$

that result from Eq. (17), and $M-K$ constraints,

$$\Psi_A(q_{n+1}^a, p_{n+1}^a) = 0, \tag{19}$$

resulting from Eq. (16). The evolution of the configuration variables from level n to $n+1$ is given by solving for q_{n+1}^a the equation (17). As the system is singular the evolution depends on ($M-K$) arbitrary functions V_n^A,

$$q_{n+1}^a = f^a(q_n^b, p_n^b, V_n^A). \tag{20}$$

We shall follow closely the standard Dirac canonical procedure of continuum mechanics. In this case, the analysis of a constraint system goes through two steps. The first step consists in the definition of a set of evolution equations that weakly preserve the constraints and the Poisson symplectic structure. To do that one defines the total Hamiltonian $H_T = H_0 + V^\alpha \phi_\alpha$, where ϕ_α are the primary constraints, and the V^α are partially determined in order to preserve all the constraints of the system. Even though some of the V's may be arbitrary functions, once they are specified, the evolution generated by H_T preserves the Poisson brackets and the dynamical evolution is consistent at the classical level with the constraint structure. The second step is only required to quantize the system and consists in the identification of the first and second class constraints and the introduction of the Dirac brackets that enforce strongly the second class constraints.

As we shall see, the same procedure may be followed in the discrete case. The main difference is the implementation of the canonical transformation that is not generated by a Hamiltonian but by a canonical transformation of types 2, 3, or 4.

Let us start by completing the evolution equations. We need to add to Eq. (20) an equation for p_{n+1},

$$p_{n+1}^a = \left.\frac{\partial L(q_n, q_{n+1})}{\partial q_{n+1}^a}\right|_{q_{n+1}^a = f^a(q_n^b, p_n^b, V_n^A)}. \tag{21}$$

We now impose the preservation of the constraints

$$\Phi_A(q_{n+1}^a, p_{n+1}^a) = \Phi_A\left(f^a{}_n, \frac{\partial L(q_n, f_n^a)}{\partial q_{n+1}^a}\right) = 0. \tag{22}$$

Furthermore, we need to impose the $n+1$ level constraints at level n, $\Psi_A(q_n^a, p_n^a) = 0$ and impose the consistency conditions

$$\Psi_A\left(f^a{}_n, \frac{\partial L(q_n, f_n^a)}{\partial q_{n+1}^a}\right) = 0. \tag{23}$$

Three different cases may occur.

(a) Equations (22) and (23) vanish automatically, and therefore we are not led to new conditions.
(b) They lead to inconsistencies, and the dynamical system is inconsistent.
(c) New secondary constraints $C(q_n^a, p_n^a)$ appear or/and some of the arbitrary functions V_n^A are determined, that is $V_n^A = V^A(q_n^a, p_n^a, v_n^\alpha)$ with $\alpha = 1, \ldots, R \leqslant (N-K)$, and v_n^α arbitrary functions. The process is repeated until consistency is achieved. That is, until the consistency conditions are automatically satisfied without further constraints and conditions for V.

Substituting V_n^A in (20) and (21) we get the evolution equations that preserve all the constraints: primary, secondary, tertiary, and so on,

$$q_{n+1}^a = f^a(q_n^b, p_n^b, V^A(q,p,v)) = \tilde{f}^a(q_n^b, p_n^b, v^\alpha), \tag{24}$$

$$p_{n+1}^a = g^a(q_n^b, p_n^b, v^\alpha). \tag{25}$$

Initial values need to be restricted by the $n=0$ level constraints,

$$\Phi_A(q_0^a, p_0^a) = \Psi_A(q_0^a, p_0^a) = 0. \tag{26}$$

In order to have a complete analogy with the continuum case, we still need to analyze under what conditions this evolution also preserves the Poisson bracket structure. As in the continuum case we assume that the arbitrary functions v have been fixed. Three different cases may arise depending on if one chooses to implement things in terms of a canonical transformation of types 2, 3 or 4.

Case I: Equation (24) is invertible for q_n^a, that is, $|\partial q_{n+1}^a / \partial q_n^b| \neq 0$ and therefore one can write

$$q_n^a = h^a(q_{n+1}^b, p_n^b). \tag{27}$$

Notice that, under these hypotheses, there are no pseudoconstraints of the form $G(q_{n+1}^a, p_n^a) = 0$. We call these pseudoconstraints because they involve variables at different instants of time.

We may define a type 3 generating function of canonical transformations,

$$F_3(q_{n+1}^b, p_n^b) = [p_n^b q_n^b + L(q_n, q_{n+1})]|_{q_n^b = h^b}. \tag{28}$$

Then we have

$$\frac{\partial F_3(q_{n+1}^a, p_n^a)}{\partial p_n^b} = q_n^b = h^b(q_{n+1}^a, p_n^a) \tag{29}$$

and

$$\frac{\partial F_3(q_{n+1}^a, p_n^a)}{\partial q_{n+1}^b} = \left.\frac{\partial L(q_n^a, q_{n+1}^a)}{\partial q_{n+1}^b}\right|_{q_n = h} = p_{n+1}^b. \tag{30}$$

Notice that in the last equality there are also contributions coming from the dependence on q_{n+1} of the level n variables q_n, but these contributions cancel because of the definition of the canonical momenta. The information about the momenta is completely encoded in the evolution equations $q_{n+1}^a = h^a$ and the constraints. As the first equation is equivalent to (24) one ends up recovering the fundamental evolution equations as a canonical transformation generated by F_3. Furthermore,

$$\left| \frac{\partial F_3(q_{n+1}^a, p_n^a)}{\partial p_n^b \partial q_{n+1}^a} \right| = \left| \frac{\partial q_n^b}{\partial q_{n+1}^a} \right| \neq 0 \tag{31}$$

due to the fact that we have assumed that $|\partial q_{n+1}^b / \partial q_n^a| \neq 0$, and consequently F_3 is a nonsingular generating function and therefore the resulting canonical transformation preserves the Poisson bracket structure.

Case II: Equation (25) is invertible for p_n^a, that is $|\partial p_{n+1}^a / \partial p_n^b| \neq 0$ and therefore one can write

$$p_n^a = g^a(q_n^b, p_{n+1}^b). \tag{32}$$

Notice that, under these hypotheses, there are no pseudoconstraints of the form $G(q_n^a, p_{n+1}^a) = 0$. By substituting (32) in (24), one gets

$$q_{n+1}^a = k^a(q_n^b, p_{n+1}^b), \tag{33}$$

which allows one to introduce a type 2 generating function,

$$F_2(q_n^b, p_{n+1}^b) = [p_{n+1}^b q_{n+1}^b - L(q_n, q_{n+1})]|_{q_{n+1}^b = k^b}. \tag{34}$$

One can now easily check that this generating function reproduces the evolution equations (24) and (25) and defines a nonsingular canonical transformation that preserves the Poisson brackets in the evolution.

Case III: Even when the system has pseudoconstraints of the form $G(q_{n+1}^a, p_n^a)=0$ and $F(q_n^a, p_{n+1}^a)=0$ one may be able to find a canonical transformation provided that the system does not have pseudoconstraints of the form $F(p_n^a, p_{n+1}^a)=0$.

In fact, by using Eq. (25) one can invert for

$$q_n^a = l^a(p_n^b, p_{n+1}^b), \tag{35}$$

and substituting in (24) get

$$q_{n+1}^a = m^a(p_n^b, p_{n+1}^b). \tag{36}$$

A generating function of type 4 that does the same job as the two previous ones may now be introduced,

$$F_4(p_n^b, p_{n+1}^b) = [-p_{n+1}^b q_{n+1}^b + p_n^b q_n^b + L(q_n, q_{n+1})]|_{q_n^b = l^b}^{q_{n+1}^b = m^b}. \tag{37}$$

All of the discrete systems that have been treated up to now in the literature may be analyzed by following this canonical procedure, allowing one to preserve the constraints and the Poisson bracket structure. Later on we will show an example of a system of this type in order to analyze how this procedure works in a concrete case.

It should be noted that there may exist mechanical systems that do not fall into any of the above classifications. For instance, a system could have pseudoconstraints of all the types listed above. In such cases one will need to develop further techniques to treat them. For instance one could introduce canonical transformations of a given type for some of the variables and of a different type for other variables. This would require further study and it does not appear necessary for the systems that have been analyzed up to present.

III. CLASSIFICATION OF THE CONSTRAINTS

At this point we have a set of constraints primary, secondary, tertiary, etc., of the form $\chi_Z(q^a, p^a)=0$ with $Z=1,\ldots,A$ with A the total number of independent constraints, that are preserved under the evolution given by Eqs. (24) and (25) provided part or all of the arbitrary functions V are conveniently fixed.

As in the continuum case it is convenient to introduce the notion of first and second class constraints, in order to quantize the theory. A constraint is of first class if it commutes with all the constraints, if that is not the case it is of second class. As in the continuum case one can define first class functions of the canonical variables $f(q,p)$ that are not necessarily constraints. Such a function will be first class if it commutes with all the constraints. Second class constraints may be imposed strongly by introducing Dirac brackets. As the evolution equations preserve the Poisson structure, they will preserve the Dirac structure because Dirac brackets are defined in terms of Poisson brackets. One ends up with a theory with a set of evolution equations that preserve the symplectic structure of the system, and therefore may be quantized by describing the evolution in terms of unitary operators.

In the discrete case there is not a straightforward relation between the number of first and second class constraints and the number of phase space degrees of freedom. This is due to the fact that now the evolution of the constraints is not directly related with their Poisson brackets with a total Hamiltonian. Thus, the fact that a constraint does not commute with others is not easily

related with the determination of an arbitrary function. It is still very easy to determine the number of phase space degrees of freedom. In fact this number is given by two times the number of configuration variables minus the total number of constraints minus the number of arbitrary functions v.

IV. AN EXAMPLE OF CONSTRAINED SYSTEM WITH SECOND CLASS CONSTRAINTS

To illustrate the techniques elaborated above, we would like to discuss a model that is simple, yet addresses in a nontrivial way the main points we discussed. This example had been treated using ad-hoc techniques in Ref. 4. The model consists of a parametrized free particle in a two-dimensional space–time under the influence of a linear potential. The discrete Lagrangian is given by

$$L_n \equiv L(q_n^a, \pi_n^a, N_n, q_{n+1}^a, \pi_{n+1}^a, N_{n+1}) = \pi_n^a(q_{n+1}^a - q_n^a) - N_n[\pi_n^0 + \tfrac{1}{2}(\pi_n^1)^2 + \alpha q_n^1]. \tag{38}$$

We have chosen a first order formulation for the particle. However, this Lagrangian is of the type we considered in this paper, one simply needs to consider all variables, q^a, π^a, N as configuration variables. The system is clearly singular since the π's and N only appear at level n (or in the continuum Lagrangian, their time derivatives are absent). When considered as a type I generating function, the above Lagrangian leads to the equations

$$p_{\pi,n+1}^a = \frac{\partial L_n}{\partial \pi_{n+1}^a} = 0, \tag{39}$$

$$p_{q,n+1}^a = \frac{\partial L_n}{\partial q_{n+1}^a} = \pi_n^a, \tag{40}$$

$$p_{N,n+1} = \frac{\partial L_n}{\partial N_{n+1}} = 0, \tag{41}$$

and

$$p_{\pi,n}^a = -\frac{\partial L_n}{\partial \pi_n^a} = -(q_{n+1}^a - q_n^a) + \pi_n^1 N_n \delta_1^a + N_n \delta_0^a, \tag{42}$$

$$p_{q,n}^a = -\frac{\partial L_n}{\partial q_n^a} = \pi_n^a + \delta_1^a \alpha N_n, \tag{43}$$

$$p_{N,n} = -\frac{\partial L_n}{\partial N_n} = \pi_n^0 + \frac{1}{2}(\pi_n^1)^2 + \alpha q_n^1. \tag{44}$$

One can easily recognize that the system has six constraints: three at the $n+1$ level, and three at the n level. They are

$$\psi_1^a \equiv p_{\pi,n+1}^a = 0, \tag{45}$$

$$\psi_2 \equiv p_{N,n+1} = 0, \tag{46}$$

$$\Phi_1^a \equiv p_{q,n}^a - (\pi_n^a + \delta_1^a \alpha N_n), \tag{47}$$

$$\Phi_2 \equiv p_{N,n} - [\pi_n^0 + \tfrac{1}{2}(\pi_n^1)^2 + \alpha q_n^1]. \tag{48}$$

Therefore the evolution depends on three arbitrary functions $V_{N,n}, V_{\pi,n}^a$,

$$q_{n+1}^a = q_n^a + \pi_n^1 N_n \delta_1^a + N_n \delta_0^a - p_{\pi,n}^a, \tag{49}$$

$$\pi_{n+1}^a = \pi_n^a + V_{\pi,n}^a, \tag{50}$$

$$N_{n+1} = N_n + V_{N,n}. \tag{51}$$

The preservation of the ψ constraints from level n to level $n+1$ is automatically ensured from (23). Now we impose the preservation of the Φ constraints upon evolution. Let us begin with Φ_1^0,

$$\Phi_{1n+1}^0 \equiv p_{q,n+1}^0 - \pi_{n+1}^0 = p_{q,n}^0 - \pi_n^0 - V_{\pi,n}^0 = 0, \tag{52}$$

which taking into account the constraint Φ_{1n}^0 implies $V_{\pi,n}^0 = 0$.

For the Φ_2 one gets the equation

$$\Phi_{2n+1} = \pi_n^0 + \alpha(q_n^1 + \pi_n^1 N_n) + (\pi_n^1 + V_n^{\pi 1})^2/2 = 0, \tag{53}$$

that taking into account the constraint Φ_{2n} implies that

$$V_{\pi,n}^1 = -\pi_n^1 + \epsilon\sqrt{(\pi_n^1)^2 - 2\pi_n^1 N_n \alpha}, \tag{54}$$

where $\epsilon = \pm 1$.

Finally we have

$$\Phi_{1n+1}^1 = p_{q,n}^1 - N_n\alpha - \pi_n^1 - V_{\pi,n}^1 - \alpha(N_n + V_{N,n}) = 0, \tag{55}$$

that after imposing the constraint at level n leads to

$$V_{N,n} = -\frac{1}{\alpha} V_{\pi,n}^1 - N_n. \tag{56}$$

Thus, the evolution equations for the configuration variables are

$$q_{n+1}^a = q_n^a + \pi_n^1 N_n \delta_1^a + N_n \delta_0^a, \tag{57}$$

$$\pi_{n+1}^0 = \pi_n^0, \tag{58}$$

$$\pi_{n+1}^1 = \epsilon\sqrt{(\pi_n^1)^2 - 2\pi_n^1 N_n \alpha}, \tag{59}$$

$$N_{n+1} = \frac{1}{\alpha}[\pi_n^1 - \epsilon\sqrt{(\pi_n^1)^2 - 2\pi_n^1 N_n \alpha}]. \tag{60}$$

We are now ready to define an invertible canonical transformation with the help of a type 3 generating function. Notice that these evolution equations are invertible for q_n^a, and therefore we are in the case I. The inverse is given by a set of equations of the form $q_n(q_{n+1})$, explicitly given by

$$q_n^1 = q_{n+1}^1 - \pi_{n+1}^1 N_{n+1} - \frac{\alpha}{2}(N_{n+1})^2, \tag{61}$$

$$q_n^0 = q_{n+1}^0 - \frac{\pi_{n+1}^1 N_{n+1} + \frac{\alpha}{2}(N_{n+1})^2}{\pi_{n+1}^1 + \alpha N_{n+1}}, \tag{62}$$

$$\pi_n^0 = \pi_{n+1}^0, \tag{63}$$

$$\pi_n^1 = \pi_{n+1}^1 + \alpha N_{n+1}, \tag{64}$$

$$N_n = \frac{\pi_{n+1}^1 N_{n+1} + \frac{\alpha}{2}(N_{n+1})^2}{\pi_{n+1}^1 + \alpha N_{n+1}}. \tag{65}$$

Recalling that F_3 is given by Eq. (28) we obtain

$$F_3 = p_{\pi,n}^0 \pi_{n+1}^0 + p_{\pi,n}^1(\alpha N_{n+1} + \pi_{n+1}^1) + p_{q,n}^0 q_{n+1}^0 + \frac{1}{2} N_{n+1}[\alpha^2 N_{n+1}^2 + 3\alpha N_{n+1}\pi_{n+1}^1 + 2(\pi_{n+1}^1)^2]$$
$$- \frac{N_{n+1}(\alpha N_{n+1} + 2\pi_{n+1}^1)}{2(\alpha N_{n+1} + \pi_{n+1}^1)}\left[p_{q,n}^0 - p_{N,n} + \frac{1}{2}(\pi_{n+1}^1)^2 + \alpha q_{n+1}^1\right] + p_{q,n}^1\left(q_{n+1}^1 - \frac{\alpha}{2} N_{n+1}^2 - N_{n+1}\pi_{n+1}^1\right). \tag{66}$$

One can check that Eqs. (61)–(65) are easily recovered by taking the partial derivative with respect to p_n^a. By differentiating with respect to q_{n+1}^a one gets

$$p_{q,n+1}^0 = p_{q,n}^0, \tag{67}$$

$$p_{q,n+1}^1 = p_{q,n}^1 - \frac{\alpha}{2} A_n N_{n+1}(\alpha N_{n+1} + 2\pi_{n+1}^1), \tag{68}$$

$$p_{\pi,n+1}^0 = p_{\pi,n}^0, \tag{69}$$

$$p_{\pi,n+1}^1 = p_{\pi,n}^1 + \frac{N_{n+1}}{2}[3\alpha N_{n+1} - 2p_{q,n}^1 + 4\pi_{n+1}^1 + 2B_n A_n - A_n(\pi_{n+1}^1 + B_n A_n)(\alpha N_{n+1} + 2\pi_{n+1}^1)], \tag{70}$$

$$p_{N,n+1} = \tfrac{3}{2}\alpha^2 N_{n+1}^2 + \alpha p_{\pi,n}^1 - p_{q,n}^1 \pi_{n+1}^1 + (\pi_{n+1}^1)^2 + B_n$$
$$+ \alpha N_{n+1}[-p_{q,n}^1 + 3\pi_{n+1}^1 - \tfrac{1}{2} B_n A_n^2(\alpha N_{n+1} + 2\pi_{n+1}^1)], \tag{71}$$

where we have introduced

$$A_n \equiv (\alpha N_{n+1} + \pi_{n+1}^1)^{-1}, \tag{72}$$

$$B_n \equiv p_{N,n} - p_{q,n}^0 - \tfrac{1}{2}(\pi_{n+1}^1)^2 - \alpha q_{n+1}^1. \tag{73}$$

By substituting in Eqs. (67)–(71) the variables q_{n+1} and using the level n constraints one gets Eqs. (39)–(41), which is a canonical transformation that reproduces, on the constraint surface, the evolution equations of the discrete particle.

What remains to be done is to identify the second class constraints and impose them strongly. The complete set of six constraints of this model ψ and Φ are second class and allow one to solve for π^a and N and eliminate completely these variables and their complex conjugates P_π and P_N.

One can proceed in two different ways. The first alternative is to start by observing that P_π and P_N vanish strongly, and then to solve for π and N in terms of the $n+1$ level variables, leading to

$$\pi_n^0 = p_{q,n+1}^0, \tag{74}$$

$$\pi_n^1 = p_{q,n+1}^1, \tag{75}$$

$$N_n = \frac{C_{n+1}}{\alpha p_{q,n+1}^1}, \tag{76}$$

where $C_{n+1}=p_{q,n+1}^0+(p_{q,n+1}^1)^2/2+\alpha q_{n+1}^1$. The relevant evolution equations are obtained from (57), (67), and (68), and are given by

$$q_{n+1}^0 = q_n^0 + N_n = q_n^0 + \frac{C_{n+1}}{\alpha p_{q,n+1}^1}, \tag{77}$$

$$q_{n+1}^1 = q_n^1 + N_n \pi_n^1 = q_n^1 + \frac{C_{n+1}}{\alpha}, \tag{78}$$

$$p_{q,n}^0 = p_{q,n+1}^0, \tag{79}$$

$$p_{q,n}^1 = p_{q,n+1}^1 + \alpha N_n = p_{q,n+1}^1 + \frac{C_{n+1}}{p_{q,n+1}^1}, \tag{80}$$

and we recover the evolution equations obtained in Ref. 4.

The second alternative consists in solving for π and N in terms of the n level variables, leading to

$$\pi_n^0 = p_{q,n}^0, \tag{81}$$

$$\pi_n^1 = \epsilon\sqrt{-2(p_{q,n}^0 + \alpha q_n^1)}, \tag{82}$$

$$N_n = \frac{1}{\alpha}(p_{q,n}^1 - \epsilon\sqrt{-2(p_{q,n}^0 + \alpha q_n^1)}), \tag{83}$$

and from here, computing the evolution equations by using (57), (67), and (68). The two methods yield evolution schemes of different functional form since one propagates "forward" in time and the other "backward." The inequivalence in the functional form stems from the fact that the discretization of the time derivatives chosen in the Lagrangian is not centered. It should be emphasized that if one starts from given initial data and propagates forward with the first system of equations and then backward using the second, one will return to the same initial data.

Notice that we have six second class constraints, and the initial number of phase space degrees of freedom was 10. By noticing that there are no arbitrary functions left, one is left with four degrees of freedom on the constraint surface. The continuum model had two degrees of freedom.

The procedure we have followed here is completely general and may be simplified when one is treating specific cases. For instance, as it happens in the continuum theory[8] it is sometimes possible to implement the canonical analysis by first solving the constraints for the unphysical degrees of freedom N, π, p^N, p^π and then introducing a generating functional on the physical degrees of freedom by following the procedure of the preceding sections. In this particular case it is easy to show that, for $p^{q^1} \neq 0$, $|\partial q_{n+1}^a / \partial q_n^b| \neq 0$, where $q^a \equiv (q^1, q^0)$, and thus it is possible to

construct an F_3 generating functional. In all the models treated up to now in the literature the unphysical degrees of freedom were eliminated before obtaining the canonical transformation for the evolution of the physical degrees of freedom. In order to keep the analysis general in a simple model, here we have kept all the variables involved in this approach.

V. TREATMENT IN TERMS OF TYPE II GENERATING FUNCTIONS

Up to now, we have taken as the starting point a singular type I generating function given by $F_1=-L(q_n^a,q_{n+1}^a)$. It is interesting to analyze how singular systems may be described in terms of other types of generating functions.

Let us assume that neither condition (8) nor condition (5) are fulfilled by the discrete system and, therefore, we are in the singular case. Then, it may be immediately seen, by using (16), and taking into account that the determinant that appears in (8) now vanishes, that singular systems with first order Lagrangians in the continuum lead to the presence of pseudoconstraints $\phi_\alpha(q_n,p_{n+1})=0$, in the theory. Recall that these pseudoconstraints are similar to the constraints that arise in the continuum case, but mixing configuration variables at one level with momenta in the next level. As in the continuum case, one can then introduce the pseudoconstraint surface S_ϕ which we shall assume has well-defined functions,

$$\tilde{\nabla}\phi_\alpha=\left(\cdots\frac{\partial\phi}{\partial q_n^a}\cdots,\cdots\frac{\partial\phi}{\partial p_{n+1}^a}\cdots\right), \tag{84}$$

where a vector $\tilde{\tau}$ in the tangent space of S_ϕ, $T_{(q,p)}S_\phi$, is such that

$$\tilde{\tau}\cdot\tilde{\nabla}\phi_\alpha=0\ \forall\ \alpha. \tag{85}$$

Let us introduce now as before the type 2 Hamiltonian (12),

$$H_2\equiv\sum_a p_{n+1}^a(q_{n+1}^a-q_n^a)-L(q_n,q_{n+1}). \tag{86}$$

It is easy to see, using the pseudoconstraints, that Eq. (86) is a function of q_n,p_{n+1}. Let us consider now an infinitesimal variation of H_2 along the pseudoconstraint surface,

$$\begin{aligned}\mathrm{d}H_2&=\sum_a\left[(q_{n+1}^a-q_n^a)\mathrm{d}p_{n+1}^a+\left(p_{n+1}^a-\frac{\partial L}{\partial q_{n+1}^a}\right)\mathrm{d}q_{n+1}^a-\left(p_{n+1}^a+\frac{\partial L}{\partial q_n^a}\right)\mathrm{d}q_n^a\right]\\&=\sum_a\left[(q_{n+1}^a-q_n^a)\mathrm{d}p_{n+1}^a-\left(p_{n+1}^a+\frac{\partial L}{\partial q_n^a}\right)\mathrm{d}q_n^a\right],\end{aligned} \tag{87}$$

where in the last step we used (6). H_2 is well defined in S_ϕ but can be extended to the whole phase space as it is done in the case of constraints in the continuum theory. In order to obtain the canonical equation of motion we start from the identity,

$$\mathrm{d}H_2(q_n,p_{n+1})=\sum_a\left(\frac{\partial H_2}{\partial q_n^a}\mathrm{d}q_n^a+\frac{\partial H_2}{\partial p_{n+1}^a}\mathrm{d}p_{n+1}^a\right), \tag{88}$$

and evaluating it for an infinitesimal displacement $(\mathrm{d}q,\mathrm{d}p)$ in $T_{(q,p)}S_\phi$, we can use (87) and the Lagrangian equations of motion (7) to obtain

$$\sum_a\left[\left(p_{n+1}^a-p_n^a+\frac{\partial H_2}{\partial q_n^a}\right)\mathrm{d}q_n^a+\left(q_n^a-q_{n+1}^a+\frac{\partial H_2}{\partial p_{n+1}^a}\right)\mathrm{d}p_{n+1}^a\right]=0. \tag{89}$$

Since $(\mathrm{d}q,\mathrm{d}p)$ is an arbitrary tangent vector to S_ϕ, following (85) we obtain that the coefficient must be proportional to the gradient. Introducing therefore the Lagrange multipliers λ^a as the proportionality factors, we will end with the set of equations,

$$q^a_{n+1} = q^a_n + \frac{\partial H_2}{\partial p^a_{n+1}} + \lambda^\alpha_n \frac{\partial \phi_\alpha}{\partial p^a_{n+1}}, \tag{90}$$

$$p^a_{n+1} = p^a_n - \frac{\partial H_2}{\partial q^a_n} - \lambda^\alpha_n \frac{\partial \phi_\alpha}{\partial q^a_n}, \tag{91}$$

$$\phi_\alpha(q_n, p_{n+1}) = 0. \tag{92}$$

This system is similar to the continuum set of equations with the inclusion of pseudoconstraints, which have the same functional form as the continuum constraints, but involve configuration variables at level n and momenta at level $n+1$, instead of n level variables. From this initial evolution equations one may follow a procedure similar to the one developed in the preceding section in order to study the consistency of the (primary) constraints and pseudoconstraints.

VI. DISCUSSION AND CONCLUSIONS

We have provided a canonical procedure for the introduction of a preserved symplectic structure in discrete constrained systems. The analogy with Dirac's procedure in the continuum is quite remarkable. It is possible to define a notion of discrete evolution that weakly preserves constraints and Poisson brackets. The distinction between first and second class constraints is still useful and when second class constraints are imposed strongly the resulting Dirac brackets are preserved.

A feature of the discretized theories is that they may have a smaller number of first class constraints, and consequently more degrees of freedom than the continuum counterparts. The extra degrees of freedom come from the fact that the discrete theories may not necessarily have the same symmetries as the continuum theories. For instance, in the case of homogeneous cosmologies studied in Ref. 9 the extra pair of phase space degrees of freedom are associated with the fact that in the discrete theory different choices of refinements in the discretization in time correspond to different solutions in the discrete theory that nevertheless approximate the same solution in the continuum theory.

An open question at present is if it is possible in cases of interest, like general relativity, to find discretizations in which the symmetries of the continuum are automatically preserved (as is, for instance, the case in discretizations of Yang–Mills theories[1]). At the moment the only way in which this seems possible would be to cast the theory in terms of action-angle variables. There the dynamics simplifies to the point where a discretization preserving the constraints is available. It is not known how to write the theory in this way in general, although one can see this mechanism in action, for instance, in Bianchi models,[9] or in linearized theory.[10]

This is only a first step for a complete understanding of the dynamics of discrete gauge systems. The relation between the number of constraints of first and second class and the number of degrees of freedom, and the connection between the first class constraints and the gauge invariance of the discrete dynamical system need to be further studied. Moreover, as discussed in the body of the paper, if one wishes to consider more pathological systems than the ones considered here, more elaborate canonical transformations may need to be introduced.

The issue of the continuum limit is well understood in the nonsingular case, where there is an external step parameter that controls the approximation. However, it needs further study in the case of singular systems, particularly in the case of totally constrained systems where the step of the approximation is encoded in the additional degrees of freedom of the discrete theory. This issue has been studied in several models[4,9] but a complete characterization of the possible behaviors is still lacking. A similar comment applies to the role of spatial discretizations when one is considering lattice field theories.

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Bifurcation analysis for the construction of a phase diagram of heteropolymer liquids

A. N. Ivanova
Institute of the Problems of Chemical Physics, RAS, Moscow, Russia

S. I. Kuchanov
Institute of Applied Mathematics, RAS, Moscow, Russia

L. I. Manevitch[a)]
Institute of Chemical Physics, RAS, Moscow, Russia

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Rather general mean field theory of heteropolymer liquids developed earlier reduces the problem of the phase diagram construction to the determination of extremals of the free energy functional. These should be subsequently analyzed for their local and global stability. Tackling of this problem traditionally involves the examination of the behavior of the solutions of a set of nonlinear algebraic and partial differential equations at various values of the control parameters. Besides, the necessity arises here to construct in space of these parameters the lines where a polymer system loses the thermodynamic stability. To overcome mathematical difficulties encountered we employed a complex approach that combines analytical and numerical methods. A two-step procedure constitutes the essence of such an approach. First, the bifurcation analysis is invoked to find the asymptotics of the extremals in the vicinity of bifurcation points. Then these asymptotics are used as an initial approximation for the numerical continuation of specific lines, where the stability loss occurs, into regions of the parametric space far removed from bifurcation values. We realized this approach for the melt of linear binary copolymers of various chemical structure with macromolecules having a pattern of arrangement of monomeric units describable by a Markov chain. Bifurcation and phase diagrams for some of these copolymers have been constructed within a wide range of temperatures and volume fractions of a polymer. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1827323]

I. INTRODUCTION

The theoretical physics of polymers in its current state suggests the application of a rather sophisticated mathematical method (see, for instance, Ref. 1). This is because the majority of differential and integral equations which describe polymer systems are nonlinear admitting therefore several physically meaningful solutions.[2] Consequently, problems of nonlinear analysis of these equations based on the approaches of the theory of bifurcations, typical for the mathematical physics, are usually encountered here. One of such nontrivial problems particularly important for the thermodynamics of polymers is attacked in the present paper. The methods of its solution may be of interest for the physicist–theorists dealing with the Landau theory of phase transitions and the statistical physics of disordered systems. The experts in the field of the applied mathematics may also benefit from getting familiar with the solution of this problem, that may prompt them to look for new possible applications of the contemporary methods of the nonlinear analysis in the theoretical physics of polymers.

[a)]Electronic mail: lmanev@chph.ras.ru

The calculation of a phase diagram belongs to the most challenging theoretical problems of the thermodynamics of melts and solutions of polymers.[3] Having constructed such a diagram one might judge about the phase state of a polymer liquid under thermodynamic equilibrium at given values of external parameters. A crucial feature of polymer systems stipulating their qualitative distinction from low-molecular ones is the possibility of the existence of mesophases. Each of them represents such an equilibrium state of the liquid of macromolecules comprising more than one type of elementary units where the density of these latter periodically changes in space at scales lying between atomic and macroscopic length scales. Depending on this density profile dimensionality d a mesophase spatially periodic structures can vary in symmetry. The most investigated among them are lamellar ($d=1$), hexagonal ($d=2$), and body centered cubic ($d=3$) structures. They have been found experimentally and scrutinized theoretically.[4] The type of a heteropolymer equilibrium structure as well as its period and amplitude are controlled along with temperature and pressure also by architecture, composition, and structure of macromolecules. Most theoretical and experimental research addressed monodisperse block copolymers, in which all molecules being identical consist of two or three sufficiently long blocks of elementary units.[5] However, synthetic polymers represent as a rule a mixture of macromolecules markedly distinguishing in the content of various units and in the pattern of their arrangement along polymer chains. Thus the number of types of macromolecules in a real polymer is virtually infinite for any polymer specimen. That is why the description of its chemical structure suggests the recourse to some statistic approach. By the most general of them the set of macromolecules constituting a linear copolymer specimen is presumed to be mapped onto the set of realizations of a stochastic process.[6] It implies the transition from a particular monomeric unit of a macromolecule to the next one at every unit interval of "time." The role of the regular state S_α ($\alpha=1,\ldots,m$) is played here by αth type unit while the transition into absorbing state S_0 corresponds to going out of a macromolecule. Such a stochastic process with discrete time and finite number of states is referred to as a stochastic chain. The best known among them is the Markov chain where the probability to fall into any state at a certain step is exclusively controlled by the type of the state at the preceding step.[7] This absorbing chain is characterized by the matrix of transition probabilities

$$\mathbf{Q}^{ab}=\begin{bmatrix} 1 & \mathbf{0} \\ \boldsymbol{\nu}_0 & \mathbf{Q} \end{bmatrix}.$$

The element $\nu_{\alpha\beta}$ of matrix $\mathbf{Q}$ equals the probability of the transition from regular state S_α into regular state S_β whereas row vector $\mathbf{0}$ and column vector $\boldsymbol{\nu}_0$ have components $\nu_{0\alpha}=0$ and $\nu_{\alpha 0}$, respectively. Probability of the absorption $\nu_{\alpha 0}$ can be expressed through elements of matrix $\mathbf{Q}$ from the normalization condition $\nu_{\alpha 0}=1-(\nu_{\alpha 1}+\cdots+\nu_{\alpha m})$. Hence matrix $\mathbf{Q}$ and vector of initial states $\mathbf{v}$ with components v_α completely specifies a Markov chain.

Nowadays it is established that the chemical structure of many synthetic copolymers is described by a Markov chain. This stipulates practical importance of the investigation of their thermodynamic behavior. Besides, relationships have been derived that express the matrix of transitions $\mathbf{Q}$ and vector $\mathbf{v}$ through kinetic parameters of a reaction system where copolymers are synthesized.[6,8] Because these parameters are reported for a great number of particular copolymerization processes,[8] an opportunity opens up to calculate phase diagrams of real copolymers formed in the course of these processes. In the last decade a number of theoretical works have been published devoted to the description of spatially periodic structures formed in melts of binary Markovian copolymers.[9–16] The approach employed in these papers is a variation of the Landau theory of the phase transitions. This is based on the expansion of a system free energy in powers of the order parameter and on cutting off all terms whose power is more than four. Evidently, such a procedure is correct only in the vicinity of the critical point where the order parameter is sufficiently small. Thus the region of applicability of the phase diagrams presented earlier[9–16] is restricted just to this narrow range of the copolymer melt parameters.

To have phase diagrams constructed within the whole range of external parameters an original approach was put forward which relies on the description of the nuclei of the incipient phase.[17] This approach enabling one to relax the Landau theory restrictions suggests finding nontrivial

solutions of a set of either integral or differential equations with the subsequent analysis of their stability. A major task of this paper is to elucidate the potentialities of the practical implementation of this approach for the construction of the phase diagram of the Markovian copolymer melt using mathematical apparatus of the bifurcation theory. Bifurcation analysis was earlier used for the construction of nonhomogeneous unstable structures occurring in the polymer blends.[18,19]

The efficiency of the bifurcation analysis as applied to the theory of polymer liquids has been demonstrated earlier when describing the dynamics of the phase transitions in a mixture of two homopolymers,[18,19] each consisting of the identical molecules. This system essentially differs from that addressed in the present paper. Qualitative distinction between these two systems lays in the fact that the first of them is a two-component one unlike the second system that comprises virtually infinite number of components. The last circumstance appreciably complicates the thermodynamic description of heteropolymer liquids considered in the present work as compared to the homopolymer ones.

II. PHASE DIAGRAM

We consider the melt of a binary copolymer whose macromolecules have chemical structure described by a Markov chain. This is completely specified by five independent parameters ν_{11}, ν_{12}, ν_{21}, ν_{22}, and v_1 or v_2, through which any statistical characteristic of a copolymer primary structure is expressed. In particular, fractions X_1^0 and X_2^0 of the first and the second type units as well as their average number in a macromolecule, P_N^0, can be calculated by formulas

$$X_1^0 = \frac{\Delta_1}{\Delta}, \quad X_2^0 = \frac{\Delta_2}{\Delta}; \quad \Delta = \Delta_1 + \Delta_2, \quad Y^0 \equiv \frac{1}{P_N^0} = \frac{D}{\Delta}, \tag{1}$$

where the following designations are used:

$$\Delta_1 = \nu_{21} + v_1\nu_{20}, \quad \Delta_2 = \nu_{12} + v_2\nu_{10}, \quad D = \nu_{12}\nu_{20} + \nu_{21}\nu_{10} + \nu_{10}\nu_{20}. \tag{2}$$

Along with "chemical" parameters $\nu_{\alpha\beta}$ and v_α a copolymer melt is characterized by a set of "physical" parameters. Among the latter in the framework of the model in hand are temperature T, pressure P, and parameters $\gamma_{\alpha\beta}$ $(\alpha,\beta=1,2)$ of pair interaction between αth and βth type units. With bifurcation analysis in mind it is more convenient to use parameter $\mathbf{\Phi}^0$, equal to the volume fraction occupied by monomeric units in principal phase, rather than the pressure. This parameter is simply expressed $\mathbf{\Phi}^0 = M^0 v / V$ through volume v of a monomeric unit, their number M^0 in a system and its volume V. Quantity $\mathbf{\Phi}^0$ occurring in most theories of polymer liquid[3,20,21] is uniquely related to P by the equation of state.

Key elements of the phase diagram of such a liquid are two curves, each representing a two-dimensional section of the hypersurface (whose codimension is 1) in the space of external parameters. The first of them, cloud point curve (CPC), is a locus of points where nuclei of incipient phase or mesophase become globally thermodynamically stable. According to which of these cases takes place the CPC branch is said to be trivial or nontrivial. At the second of the above-mentioned curves, termed spinodal, the spatially homogeneous state loses local thermodynamic stability. The spinodal curve (SC) can contain trivial and nontrivial branches depending on the spatial scale (wave vector $\vec{q}=\vec{q}^*$) of the density fluctuations at which the loss of the above stability happens. To a trivial branch there corresponds macroscopic scale ($\vec{q}^* = 0$) while to nontrivial one mesoscopic scale ($\vec{q}^* \neq 0$) conforms. Provided they coexist, these two branches are tangent at the Lifshitz point. A domain of a phase diagram located in between CPC and SC corresponds to the metastable state of the principal phase. The density of each type of units in the incipient phase nuclei has at critical point (where CPC and SC have common tangent) the same value as in the principal phase.

In order to construct the phase diagram of a copolymer melt we will proceed from the general thermodynamic theory of heteropolymer liquids.[17,22] According to this theory the thermodynamic description of a polymer liquid is performed in terms of density functional

$$\Delta\mathcal{F}[\mathbf{\Phi}] \equiv \mathcal{F}[\mathbf{\Phi}] - \mathcal{F}[\mathbf{\Phi}^0] = TM^0\{\mathcal{G}[\mathbf{1}] - \mathcal{G}[\mathbf{s}]\} + \int d\vec{r}\{f^*(\mathbf{\Phi}) - f^*(\mathbf{\Phi}^0)\} + \frac{1}{v}\int d\vec{r}\{\mathbf{H}^0\mathbf{\Phi}^0 - \mathbf{H}\mathbf{\Phi}\}. \tag{3}$$

Each αth component of vectors $\mathbf{\Phi}$,$\mathbf{H}$, and $\mathbf{s}$, entering into the right-hand part of this expression refers to the αth type monomeric unit. So $\mathbf{\Phi}_\alpha$ denotes the volume fraction of these units in nuclei while H_α is the component of external field $\mathbf{H}$ acting upon them. Superscript "$\mathbf{0}$" means that the values of these quantities are taken in the principal phase. As for the argument of generating functional $\mathcal{G}[\mathbf{s}]$ it has components $s_\alpha = \exp\{(H^0_\alpha - H_\alpha)/T\}$. For the case of Markovian copolymers this functional can be presented as follows:

$$\mathcal{G}[\mathbf{s}] = \frac{1}{V}\int d\vec{r}(s_1U_1\nu_{10} + s_2U_2\nu_{20}) = \frac{Y^0}{V}\int d\vec{r}(s_1V_1v_1 + s_2V_2v_2), \tag{4}$$

where dependence of $\mathbf{U}$ and $\mathbf{V}$ on $\mathbf{s}$ is found from the set of four equations,

$$\begin{gathered} KU_\alpha - (U_1s_1\nu_{1\alpha} + U_2s_2\nu_{2\alpha}) = v_\alpha Y^0 \quad (\alpha = 1,2), \\ KV_\alpha - (\nu_{\alpha1}s_1V_1 + \nu_{\alpha2}s_2V_2) = \nu_{\alpha0}. \end{gathered} \tag{5}$$

Linear operator K in the left-hand side of Eqs. (5) is inverse to the integral operator with kernel $\lambda(\vec{r}-\vec{r}')$ which has the sense of the conditional probability for the neighbor of unit situated at point $\vec{r}'$ to be at point $\vec{r}$. Kernel λ is a rapidly decreasing function which vanishes at distance $|\vec{r}-\vec{r}'|$ comparable with a monomeric unit size a. Since essentially larger spatial scales are of actual practical interest, any normalized function satisfying the above condition might be chosen as λ. Its Fourier transform $x \equiv \tilde{\lambda}(q)$ is governed exclusively by the wave vector modulus $q \equiv |\vec{q}|$. Being positive quantity x turns into unity at $q=0$ and vanishes at $q\to\infty$. Function $\tilde{\lambda}(q) = \exp(-a^2q^2/6)$, traditionally employed for numerical calculations, meets these conditions.

Functional (3) is controlled by dimensionless units' densities $\{\mathbf{\Phi}_\alpha\}$ both explicitly and implicitly through field $\mathbf{H}$. Its dependence on Φ is determined from expressions

$$\mathbf{\Phi}_1 = \mathbf{\Phi}^0 s_1U_1V_1, \quad \mathbf{\Phi}_2 = \mathbf{\Phi}^0 s_2U_2V_2, \tag{6}$$

which are obtained from the conditions of vanishing of the first order variational derivatives of functional (3) with respect to H_1 and H_2. As for the explicit dependence of $\Delta\mathcal{F}$ (3) on $\mathbf{\Phi}$, this is specified by function $f^*(\mathbf{\Phi})$ having the following appearance:[17,21]

$$\frac{f^*(\mathbf{\Phi})v}{T} = (1-\Phi)\ln(1-\mathbf{\Phi}) + \mathbf{\Phi} - \frac{1}{T}(\gamma_{11}\mathbf{\Phi}_1^2 + \gamma_{22}\mathbf{\Phi}_2^2 + 2\gamma_{12}\mathbf{\Phi}_1\mathbf{\Phi}_2), \tag{7}$$

where $\mathbf{\Phi} = \mathbf{\Phi}_1 + \mathbf{\Phi}_2$. Hence, expressions (4) and (7) along with equations (5) and (6) completely define density functional (3) defined on the set of smooth functions $\mathbf{\Phi}_1(\vec{r}), \mathbf{\Phi}_2(\vec{r})$ lying within region $0 \leqslant \mathbf{\Phi}_1, \mathbf{\Phi}_2 < 1, \mathbf{\Phi}_1 + \mathbf{\Phi}_2 < 1$.

Equilibrium spatial distributions $\mathbf{\Phi}_1^e(\vec{r})$ and $\mathbf{\Phi}_2^e(\vec{r})$ of the units' volume fractions in nuclei are found by the minimization of the density functional. Necessary conditions of its minimum are

$$\frac{v\,\delta\mathcal{F}[\mathbf{\Phi}]}{\delta\Phi_\alpha(\vec{r})} = -H_\alpha(\vec{r}) + \mu^*_\alpha(\mathbf{\Phi}(\vec{r})) = 0 \quad (\alpha = 1,2), \tag{8}$$

where the following designation is used:

$$\mu_{\alpha}^{*}(\mathbf{\Phi}) \equiv \frac{v\partial f^{*}}{\partial \mathbf{\Phi}_{\alpha}} = -T\ln(1-\mathbf{\Phi}) - 2(\gamma_{\alpha 1}\mathbf{\Phi}_1 + \gamma_{\alpha 2}\mathbf{\Phi}_2). \tag{9}$$

Expression (8) establishes the relation between $\mathbf{H}(\vec{r})$ and $\mathbf{\Phi}(\vec{r})$ taken on functional $\Delta\mathcal{F}$ extremal. With this relation in mind one can find dimensionless equilibrium densities of units in nuclei from the solution $\mathbf{\Phi}_1=\mathbf{\Phi}_1^e, \mathbf{\Phi}_2=\mathbf{\Phi}_2^e$ of equations (5) and (6), where vector $\mathbf{s}$ components read as

$$s_{\alpha} = \exp\{[\mu_{\alpha}^{*}(\mathbf{\Phi}^0) - \mu_{\alpha}^{*}(\mathbf{\Phi})]/T\}. \tag{10}$$

These equations at any values of external parameters have the trivial solution

$$U_{\alpha}(\vec{r}) \equiv U_{\alpha}^0 = X_{\alpha}^0, \quad V_{\alpha}(\vec{r}) \equiv V_{\alpha}^0 = 1, \quad \Phi_{\alpha}(\vec{r}) \equiv \Phi_{\alpha}^0 = X_{\alpha}^0\Phi^0, \quad s_{\alpha}(\vec{r}) \equiv 1 \tag{11}$$

describing spatially homogeneous state of a system. It becomes thermodynamically absolutely unstable on the spinodal, whose mathematical condition is the loss of the positive definiteness by matrix

$$\mathbf{M}^0(x) = [\Phi^0\mathbf{X}^0(x)]^{-1} - \mathbf{C}^0 v^{-1}, \tag{12}$$

where x is a dummy variable laying within the interval between 0 and 1. The right-hand side of this expression comprises copolymer structure matrix $\mathbf{X}^0(x)$ and matrix of direct correlation functions $\mathbf{C}^0 \equiv \mathbf{C}(\Phi^0)$ describing the melt of monomeric units. In the framework of the simplest "lattice liquid" model[21] elements of the latter matrix look as

$$\frac{C_{\alpha\beta}(\mathbf{\Phi})}{v} \equiv -\frac{v\partial^2 f^{*}(\mathbf{\Phi})}{T\partial\mathbf{\Phi}_{\alpha}\partial\mathbf{\Phi}_{\beta}} = -\frac{1}{1-\mathbf{\Phi}} + \frac{2\gamma_{\alpha\beta}}{T}. \tag{13}$$

As for the structure matrix its elements in a simple way[17]

$$X_{\alpha\beta}^0(x) = X_{\alpha}^0\delta_{\alpha\beta} + W_{\alpha\beta}^0(x) + W_{\beta\alpha}^0(x) \tag{14}$$

are related to the elements of matrix $\mathbf{W}^0(x)$ of generating functions of two-point chemical correlators of macromolecules in the principal monophase system. For a Markovian copolymer the following expressions hold:

$$W_{\alpha\beta}^0(x) = X_{\alpha}^0 L_{\alpha\beta}^0(x), \quad \text{where } \mathbf{L}^0(x) = (\mathbf{E} - x\mathbf{Q})^{-1}x\mathbf{Q}, \tag{15}$$

which in combination with expressions (13) and (14) completely define matrix (12). This loses the positive definiteness when its minimal eigenvalue vanishes. If it happens at point $x=1$ or at any other point within interval $0<x<1$ we are dealing with trivial or nontrivial branch of SC, respectively. The explicit equations enabling one to find both branches of the spinodal of a binary Markovian copolymer in terms of the elements of matrices $\mathbf{X}^0(x)$ and $\mathbf{C}^0$ have been presented and analyzed earlier.[9,10]

At some values of the input parameters, the set of equations (5), (6), and (10) can have solutions differing from the trivial one (11). Among these nontrivial solutions $\mathbf{\Phi}=\mathbf{\Phi}^e$ corresponding to the density functional extremals only those have physical meaning on which this functional has a minimum. Just such solutions describe the nuclei of the incipient phase.

A necessary and sufficient condition for a spatially homogeneous nontrivial solution of Eqs. (5), (6), and (10) to provide a minimum of the density functional is the positive definiteness of matrix

$$\mathbf{M}^e(x) = [\Phi^0\mathbf{X}^e(x)]^{-1} - \mathbf{C}^e v^{-1}, \tag{16}$$

where $\mathbf{C}^e \equiv \mathbf{C}(\Phi^e)$ while elements of matrix $\mathbf{X}^e(x)$ are defined by the following expression:

$$X_{\alpha\beta}^e(x) = [\mathbf{\Phi}_{\alpha}^e/\mathbf{\Phi}^0]\delta_{\alpha\beta} + W_{\alpha\beta}^e(x) + W_{\beta\alpha}^e(x) \tag{17}$$

and the designation is employed

$$W^e_{\alpha\beta}(x) = s^e_\alpha s^e_\beta U^e_\alpha L^e_{\alpha\beta}(x) V^e_\beta. \tag{18}$$

Here s^e_α is found by formulas (9) and (10) via substitution of quantities Φ^e_α for Φ_α whereas given $\mathbf{\Phi}^e_\alpha$ values of U^e_α and V^e_α represent the solution of a set of four linear algebraic equations (5). As for matrix $\mathbf{L}^e(x)$ whose elements are $L^e_{\alpha\beta}(x)$ it has the following appearance:

$$\mathbf{L}^e(x) = (\mathbf{E} - x\mathbf{QS})^{-1} x\mathbf{Q}, \tag{19}$$

where $\mathbf{S}$ is the diagonal matrix with elements $s_\alpha \delta_{\alpha\beta}$. Because Eqs. (5), (6), and (10) are nonlinear they can have more than one solution $\mathbf{\Phi}^e$ at the same values of external parameters. Among these extremals only those have physical meaning which provide positive definiteness of matrix (16). Each such solution, $\mathbf{\Phi}^i$, specifies volume fractions $\mathbf{\Phi}^i_1$ and $\mathbf{\Phi}^i_2$ of monomeric units of the ith phase nuclei.

Equations (5), (6), and (10) can have solutions $\Phi^e(\vec{r})$ taking on different values at different points $\vec{r}$ of the Euclidean space. Among these extremals those should be chosen which minimize the density functional. To make this choice it is convenient to consider its second variation represented as a quadratic functional with respect to variations of volume fractions of monomeric units. Such a treatment will be realized in the next section. Having found all local minima of the density functional it is necessary to reveal among them the global one. Equating the value of the above functional in this minimum to its value in the minimum at the trivial solution we will get the condition for finding the cloud point hypersurface. This may be formulated mathematically in terms of the functional

$$R[\mathbf{\Phi}^i] = \int \mathrm{d}\vec{r} \left\{ T\Phi^0 Y^0 \sum_{\alpha=1}^{2} V_\alpha (1 - s^i_\alpha \nu^i_\alpha) + v[P^*(\mathbf{\Phi}^0) - P^*(\mathbf{\Phi}^i)] \right\}, \tag{20}$$

where the following designation is used:

$$vP^*(\mathbf{\Phi}) = -T[\ln(1-\mathbf{\Phi}) + \mathbf{\Phi}] - (\gamma_{11}\mathbf{\Phi}^2_1 + \gamma_{22}\mathbf{\Phi}^2_2 + 2\gamma_{12}\mathbf{\Phi}_1\mathbf{\Phi}_2). \tag{21}$$

Conditions for determining CPC are evident,

$$R[\mathbf{\Phi}^I] = 0, \quad R[\mathbf{\Phi}^i] > 0 \quad \text{at } i \neq I, \tag{22}$$

where superscript I specifies the global minimum of the density functional. Depending on whether $\mathbf{\Phi}^I$ is homogeneous or spatially periodical solution of Eqs. (5), (6), and (10) the conditions (22) refer to the trivial or nontrivial CPC branch, respectively. For the first of them, functional $R[\mathbf{\Phi}^I]$ reduces to function $R(\mathbf{\Phi}^I)$ vanishing when the pressure in nuclei and the principle phase is the same.

All mathematical formulas presented in the foregoing are valid for copolymers whose macromolecules are described by an arbitrary Markov chain. When it is symmetric these formulas become noticeably simpler. The condition of such a symmetry is

$$v_1 \nu_{12} \nu_{20} = v_2 \nu_{21} \nu_{10}. \tag{23}$$

For statistically symmetric Markovian copolymers the following expressions hold:

$$v_1 = \frac{\nu_{21}\nu_{10}}{\nu_{21}\nu_{10} + \nu_{12}\nu_{20}}, \quad v_2 = \frac{\nu_{12}\nu_{20}}{\nu_{21}\nu_{10} + \nu_{12}\nu_{20}}, \tag{24}$$

$$X^0_1 = \frac{\nu_{21}}{\nu_{12} + \nu_{21}}, \quad X^0_2 = \frac{\nu_{12}}{\nu_{12} + \nu_{21}}, \quad Y^0 = X^0_1 \nu_{10} + X^0_2 \nu_{20}. \tag{25}$$

Interestingly, the composition vector $\mathbf{X}^0$ of such copolymers coincides with the stationary vector $\boldsymbol{\pi}$ of the nonabsorbing ergodic Markov chain[7] describing macromolecules of infinite length. From

the symmetry condition (23) there follows the proportionality of the components of vectors **U** and **V**:

$$U_1(\vec{r}) = \pi_1 V_1(\vec{r}), \quad U_2(\vec{r}) = \pi_2 V_2(\vec{r}). \tag{26}$$

Consequently, in case of symmetric Markovian copolymers the first pair of equations (5) may be omitted when finding the density functional extremals. Besides, the matrix of the generating functions of the two-point chemical correlators of such copolymers is symmetric so that equalities $W^0_{\beta\alpha}(x) = W^0_{\alpha\beta}(x)$ and $W^e_{\beta\alpha}(x) = W^e_{\alpha\beta}(x)$ may be taken into account when considering relationships (14) and (17), respectively.

Once the mathematical problem of a phase diagram construction is completely formulated let us address the bifurcation analysis of the above nonlinear equations. Of prime interest here is the behavior of their solutions at scales essentially larger than monomeric unit size a, which is the scale where function λ vanishes. With this in mind the integral operator in Eqs. (5) may be replaced by the differential one as it is customary in statistical physics of polymers.[23] Thus, the first term in the second pair of equations (5) will read

$$KV_\alpha \equiv \int \lambda^{(-1)}(\vec{r} - \vec{r}\,')V_\alpha(\vec{r}\,')\mathrm{d}\vec{r}\,' \to V_\alpha(\vec{r}) - \frac{a^2}{6}\Delta V_\alpha(\vec{r}), \tag{27}$$

where Δ is the Laplace operator. Below, for convenience sake, instead of $\vec{r}$ we will use dimensionless variable $\sqrt{6}\vec{r}/a$.

III. THE BIFURCATION ANALYSIS

Construction of phase diagrams for heteropolymer liquids is a rather complicated global nonlinear problem. It is a reason why only Landau theory of phase transitions has been still applied to this problem, so only the vicinity of critical point could be correctly treated. In order to go beyond the Landau theory we have replaced the solution of global nonlinear problem by subsequent solution of local problems using nonlinear bifurcation analysis and continuation procedure by parameters fixing the temperature and characteristic size of the nonhomogeneous structure.

We start with a determination of nontrivial solutions of the equations (5), (6), and (10) branching from trivial solution in vicinity of the spinodal points. For that we consider the nonlinear operator $\mathbf{A}(\mathbf{U},\mathbf{V},\mathbf{s},\mathbf{\Phi},h)$, which is defined by the left-hand sides of equations (5), (6), and (10) depending on vector functions **U**, **V**, **s**, $\mathbf{\Phi}$ as well as parameter $h = 2\gamma_{12}/T$. Let the vectors $\mathbf{z} = [\mathbf{U}(h),\mathbf{V}(h),\mathbf{s}(h),\mathbf{\Phi}(h)]$ and $\mathbf{z}^0 = [\mathbf{U}^0(h),\mathbf{V}^0(h),\mathbf{s}^0(h),\mathbf{\Phi}^0(h)]$ correspond to the spatially homogeneous solution of these equations and h^* to be a critical value of parameter h, corresponding to spinodal point. Linear operator $\mathbf{L}[\mathbf{z}^0,h]$ being a differential of operator **A** with eigenvalue vanishing at $h = h^*$, may be determined by the following relations [where vectors $\delta\mathbf{z} = (\delta\mathbf{U},\delta\mathbf{V},\delta\mathbf{s},\delta\mathbf{\Phi})$, $\alpha,\beta = \mathbf{1},\mathbf{2},$]:

$$\mathbf{L}(\mathbf{z}^0,h)\delta\mathbf{z}: \begin{bmatrix} \nabla^2\delta U_\alpha - \delta U_\alpha + \sum_\beta Q_{\beta\alpha}(s_\beta\delta U_\beta + U_\beta\delta s_\beta) \\ \nabla^2\delta V_\alpha - \delta V_\alpha + \sum_\beta Q_{\alpha\beta}(s_\beta\delta V_\beta + V_\beta\delta s_\beta) \\ s_\alpha^{-1}\delta s_\alpha - \sum_\beta (-1/(1-\Phi) + h\gamma_{\alpha\beta}/\gamma_{12})\delta\Phi_\beta \\ \delta\Phi_\alpha - \Phi^0(\delta s_\alpha U_\alpha V_\alpha + s_\alpha V_\alpha\delta U_\alpha + s_\alpha U_\alpha\delta V_\alpha) \end{bmatrix}. \tag{28}$$

The components of the vector $\mathbf{z}^0$ determines in particular the trivial solution with relations (11).

The systems of equations (5), (6), and (10) may be represented in the vicinity of $\mathbf{z}^0$ in the following form:

$$\mathbf{A}(\mathbf{z},h) = \mathbf{L}(\mathbf{z}^0,h)(\mathbf{z}-\mathbf{z}^0) + \mathbf{F}(\mathbf{z}^0,\mathbf{z}-\mathbf{z}^0,h), \tag{29}$$

where norm $\mathbf{F}$ $(\mathbf{z}^0,\mathbf{z}-\mathbf{z}^0,h)$ is $O((\mathrm{norm}(\mathbf{z}-\mathbf{z}^0))^2)$. One can introduce matrix $J(q)$,

$$J(q) = \begin{bmatrix} -(q^2+1)E + Q*s & 0 & Q*U & 0 \\ 0 & -(q^2+1)E + Qs & QV & 0 \\ 0 & 0 & s^{-1} & -C \\ -\Phi^0 sV & -\Phi^0 sU & -\Phi^0 UV & E \end{bmatrix} \tag{30}$$

containing the two-dimensional blocks, sU, sV, UV being the products of diagonal matrixes with elements s_α, U_α, V_α. The elements of matrix C are determined by relations (21), E is unit matrix.

The trivial spinodal $h(\Phi^0)$ is determined by the equation $\det J(0)=0$, nontrivial one by two equations, $\det J(q)=0$, $\partial(\det J(q)/\partial q^2 = 0$, and condition $\partial^2 \det J(q)/(\partial q^2)^2 > 0$. In the case of trivial spinodal the eigenfunction $\mathbf{g}(\mathbf{r})$ of the operator L corresponding to vanishing eigenvalue is the eigenvector $\mathbf{g}_1$ of matrix $J(0)$. In the case of nontrivial spinodal similar eigenfunction is the product of eigenvector $\mathbf{g}_1$ of matrix $J(q)$ (with eigenvalue which is equal to zero) and eigenfunction of the Laplace operator under periodic boundary conditions with eigenvalue $-q^2$. This eigenvalue in general is degenerate, i.e., the dimension of proper subspace is greater than 1 and depends on the symmetry of the considered domain. We will consider below the one-dimensional case and denote the first component of vector $\mathbf{r}$ by x. In this case the dimension of proper subspace is 2 and

$$\mathbf{g}(x) = \mathbf{g}_1(a\cos(qx) + b\sin(qx)), \tag{31}$$

where a and b are the arbitrary constants. In this case the degeneracy is the consequence of invariance of the periodic solutions with respect to translation. Later on for the component U_1 we change the periodic conditions from $\partial U_1/\partial x = 0$ to $x=0$ and $x=2\pi/q$. Then it is possible to set $b=0$.

Dealing with bifurcation analysis we introduce the auxiliary parameter ε and represent the solution $\mathbf{z}=(\mathbf{U},\mathbf{V},\mathbf{s},\mathbf{\Phi})$ of the equation

$$\mathbf{A}(\mathbf{U},\mathbf{V},\mathbf{s},\mathbf{\Phi},h) = 0 \tag{32}$$

and parameter h in vicinity of its critical value h^* as asymptotic power series by subsidiary parameter ε, which characterizes the amplitude deviation as the unknown solution from the initial

$$h = h^* + \varepsilon \cdot h^{(1)} + \varepsilon^2 h^{(2)} + \varepsilon^3 h^{(3)} + \cdots,$$

$$\mathbf{z} = \mathbf{z}^{(0)} + \varepsilon \mathbf{z}^{(1)} + \varepsilon^2 \mathbf{z}^{(2)} + \varepsilon^3 \mathbf{z}^{(3)} + \cdots. \tag{33}$$

We present the left-hand side of Eq. (32) as the Taylor series in the vicinity of value $h=h^*$ and vector $\mathbf{z}^{(0)}$,

$$\mathbf{z}^{(0)} = \mathbf{U}^0(h^*), \quad \mathbf{V}^0(h^*), \quad \mathbf{s}^0(h^*), \quad \mathbf{\Phi}^0(h^*).$$

Then we select the terms of identical order with respect to ε and equate them to zero. The equations for $\mathbf{z}^{(1)}$ can be written as follows:

$$\mathbf{L}(\mathbf{z}^{(0)},h^*)\mathbf{z}^{(1)} = 0. \tag{34}$$

Consequently, $\mathbf{z}^{(1)}$ is eigenfunction of operator $\mathbf{L}$ $(\mathbf{z}^{(0)},h^*)$ corresponding to zero eigenvalue. The following equations can be found recursively:

$$\mathbf{L}(\mathbf{z}^{(0)},h^*)\mathbf{z}^{(i)} = \varphi_i(\mathbf{z}^{(1)},\ldots,\mathbf{z}^{(i-1)},h^{(i-1)}). \tag{35}$$

The vector function φ_i on the right-hand side of Eq. (35) is the linear function by $h^{(i-1)}$ and the degree i polynomial of the components of vectors $\mathbf{z}^{(k)}$ $(k<i)$. The function $\varphi_\mathbf{i}$ for $i=2,3$, can be presented as

$$\varphi_2(\mathbf{z}^{(1)},\ldots,\mathbf{z}^{(i-1)},h^{(i-1)}) = -1/2\sum_{k,j}\frac{\partial^2\mathbf{F}}{\partial z_k\partial z_j}z_k^{(1)}z_j^{(1)} - \sum_j\frac{\partial^2\mathbf{F}}{\partial z_j\partial h}z_j^{(1)}h^{(1)}, \tag{36}$$

$$\varphi_3(\mathbf{z}^{(1)},\ldots,\mathbf{z}^{(i-1)},h^{(i-1)}) = -\left(1/2\sum_{k,j}\frac{\partial^2\mathbf{F}}{\partial z_k\partial z_j}(z_k^{(1)}z_j^{(2)}+z_k^{(2)}z_j^{(1)}) + \sum_j\frac{\partial^2\mathbf{F}}{\partial h\partial z_j}(z_j^{(2)}h^{(1)}+z_j^{(1)}h^{(2)}) + 1/6\sum_{j,k,l}\frac{\partial^3\mathbf{F}}{\partial z_j\partial z_k\partial z_l}z_j^{(1)}z_k^{(1)}z_l^{(1)}\right). \tag{37}$$

The operator $\mathbf{L}$ is Fredholm operator of index 0. Therefore the condition of the solution existence for Eq. (35) is the orthogonality of the vector function $\varphi_\mathbf{i}$ to the eigenfunction corresponding to zero eigenvalue of operator conjugate to $\mathbf{L}$ $(\mathbf{z}^{(0)},h^*)$ This condition determines the value of $h^{(i-1)}$. Such a procedure corresponds to Lyapunov–Shmidt method.[24]

In the case of multiple zero eigenvalues, $\mathbf{z}^{(1)}$ is linear combination of linear independent eigenfunctions of operator $\mathbf{L}$. Therefore it is necessary to require the orthogonality $\varphi_\mathbf{i}$ to all independent eigenfunctions corresponding to vanishing eigenvalue of operator conjugate to $\mathbf{L}$ $(\mathbf{z}^{(0)},h^*)$. These conditions determine $h^{(i-1)}$ and the coefficients of the linear combination of independent eigenfunctions.

IV. BIFURCATION OF NONHOMOGENEOUS STRUCTURE FROM HOMOGENEOUS SOLUTIONS

Let $\det J(q^*)=0$ for the function $\mathbf{z}^{(0)}$, which is the trivial or nontrivial homogeneous solution of the equation (32). We consider further the one-dimensional symmetrical case for $m=2$. This case corresponds to the relations (23) and (24) and it is possible to consider the equation for $\mathbf{V}$ only. Then $\mathbf{z}^{(i)}=(\mathbf{V},\mathbf{s},\mathbf{\Phi})$ and in the first approximation $\mathbf{z}^{(1)}=\mathbf{g}\cos(q^*x)$, where $\mathbf{g}$ is the eigenvector corresponding to the zero eigenvalue of the matrix $J(q^*)$. The function φ_2 can be written as follows:

$$\varphi_2 = \begin{bmatrix} Q\mathbf{s}^{(1)}\mathbf{V}^{(1)} \\ -1/2(\mathbf{s}^{(0)})^{-2}(\mathbf{s}^{(1)})^2 - h^{(1)}\gamma\mathbf{\Phi}^{(1)} + \left(\dfrac{\mathbf{\Phi}_1^{(1)}+\mathbf{\Phi}_2^{(1)}}{1-\mathbf{\Phi}^{(0)}}\right)^2 \\ -2\mathbf{\Phi}^{(0)}\mathbf{s}^{(1)}\mathbf{V}^{(0)}\mathbf{V}^{(1)}\Pi - \mathbf{\Phi}^{(0)}\mathbf{s}^{(0)}(\mathbf{V}^{(1)})^2 \end{bmatrix},$$

where the following designations are used:

$$\Pi = \mathrm{diag}[\pi_1,\pi_2], \quad s^{(1)} = \mathrm{diag}[\mathbf{s}_1^{(1)},\mathbf{s}_2^{(1)}], \quad \mathbf{V} = \mathrm{diag}[V_1^{(1)},V_2^{(1)}], \quad \mathbf{\Phi}^{(1)} = \mathrm{diag}[\mathbf{\Phi}_1^{(1)},\mathbf{\Phi}_2^{(2)}].$$

The orthogonality condition leads to the relation $h^{(1)}=0$. The vector $\mathbf{z}^{(2)}$ in the second approximation has the form

$$\mathbf{z}^{(2)} = \mathbf{a} + \mathbf{b}\cos(2q^*x) + \mathbf{a}_h h^{(2)}. \tag{38}$$

The vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{a}_h$ are determined from the following equations:

$$J(0)\mathbf{a} = \mathbf{r}_0, \quad J(2q^*)\mathbf{b} = \mathbf{r}_0, \quad J(0)\mathbf{a}_h = \mathbf{r}_h. \tag{39}$$

The expressions for vectors $\mathbf{r}_0$ and $\mathbf{r}_h$ are presented in Appendix A. The vector $\mathbf{r}_h$ is zero for bifurcation from trivial solution, therefore $\mathbf{a}_h$ also is zero. The value $h^{(2)}$ can be determined from the orthogonality condition φ_3 with respect to the eigenfunction corresponding to the zero eigenvalue of the operator conjugate to $\mathbf{L}$ $(\mathbf{z}^{(0)},h^*)$. Its expression is also presented in Appendix A.

The type of bifurcation is determined by sign $h^{(2)}$. If $h^{(2)}>0$, then the bifurcation is supercritical and pair of nontrivial solutions exists for $h>h^*$. For $h^{(2)}<0$ the bifurcation is subcritical, so that pair of nontrivial solutions exists for $h<h^*$. When dealing with supercritical bifurcation in the point of nontrivial spinodal, nontrivial solution is stable; in the case of subcritical bifurcation

it is unstable. The disposition of the trivial (h_{st}) and nontrivial spinodals (h_{sn}) is determined by the type of bifurcation in the point of trivial spinodal. If $h_{st}<h_{sn}$, a transcritical nontrivial homogeneous solution branches from trivial spinodal. If $h_{st}>h_{sn}$, the equation $J(q)=0$ has two roots q_l and q_r ($q_l<q_r$), between the points $h=h_{sn}$ and $h=h_{st}$ and, respectively, two pairs of branches of nongomogeneous extremals appear. At $h=h_{st}$ is $q_l=0$, and both nontrivial nonhomogeneous and nontrivial homogeneous solutions can branch from trivial spinodal. This case will be considered below.

V. BIFURCATION IN THE SPINODAL POINT

Let $h_{sn}<h_{st}$, then zero is a multiple eigenvalue of the operator $\mathbf{L}$ $(\mathbf{z}^{(0)},h*)$. Simultaneously, $\det J(0)$ and $\det J(q*)$ are equal to zero and $\mathbf{g}^{(0)}$, $\mathbf{g}(q*)$ are eigenvectors of matrixes $J(0)$ and $J(q*)$ corresponding to zero eigenvalues. The first approximation can be expressed as follows:

$$\mathbf{z}^{(1)}=\alpha\mathbf{g}^{(0)}+\beta\mathbf{g}(q*)\cos(q*x).$$

The constants α and β are found from the orthogonality condition of the right-hand side of φ_2 in (35) with respect to two eigenfunctions $\mathbf{g}^{(0)T}$, $\mathbf{g}^{T}(q*)\cos(q*x)$ of operator conjugate to $\mathbf{L}$ $(\mathbf{z}^{(0)},q*)$. The equations for determination of the ratio α/β and $h^{(1)}$ are written as

$$\alpha^2(\mathbf{g}^{(0)T},\mathbf{r}_{00})+\beta^2(\mathbf{g}^{(0)T},\mathbf{r}_{22})=-\alpha h^{(1)}z_{h0},$$

$$\alpha\beta(\mathbf{g}^{T}(q*),\mathbf{r}_{02})=-h^{(1)}z_{h2}\beta.$$

Here $(\mathbf{f}(\mathbf{x}),\mathbf{g}(x))$ is the scalar product vector function in $L^2[0,l]$, the formulas for vectors $\mathbf{r}_{00}$, $\mathbf{r}_{02}$, $\mathbf{r}_{22}$ are presented in Appendix A,

$$z_{h0}=(\gamma\tilde{\mathbf{g}},\tilde{\mathbf{g}}^{T}),\quad z_{h2}=(\gamma\tilde{\mathbf{g}}(q*),\tilde{\mathbf{g}}^{T}(q*)),$$

where

$$\tilde{\mathbf{g}}=[\mathbf{g}^{(0)}[5],\mathbf{g}^{(0)}[6]],\quad \tilde{\mathbf{g}}^{T}=[\mathbf{g}^{(0)T}[3],\mathbf{g}^{(0)T}[4]],$$

$$\tilde{\mathbf{g}}(q*)=[\mathbf{g}(q*)[5],\mathbf{g}(q*)[6]],\quad \tilde{\mathbf{g}}^{T}(q*)=[\mathbf{g}^{T}(q*)[3],\mathbf{g}^{T}(q*)[4]].$$

The system ( ) has several solutions,

(1) $\beta=0$, $h^{(1)}=-\alpha(\mathbf{g}^{(0)T},\mathbf{r}_{00})/z_{h0}$,
(2) $\beta\neq 0$, $h^{(1)}=-(\mathbf{g}^{(0)T},\mathbf{r}_{02})/z_{h2}$,

$$(\beta/\alpha)^2=(z_{ho}/z_{h2}\cdot(\mathbf{g}^{T}(q*),\mathbf{r}_{02})-(\mathbf{g}^{(0)},\mathbf{r}_{00}))/(\mathbf{g}^{(0)T},\mathbf{r}_{22})=c.$$

If $c>0$, then two nonhomogeneous solutions and one homogeneous solution ($\beta=0$) exist in vicinity $h=h*$, otherwise only homogeneous solution exists for $\beta=0$.

If $h_{ns}>h_{st}$ (or if h_{ns} does not exist), only the solution for $\beta=0$ exists. From $h^{(1)}\neq 0$ it follows that the bifurcation is transcritical. The condition $h^{(1)}=0$ in spinodal point corresponds to the critical point in Landau theory.

VI. ANALYSIS OF THE STABILITY

The stability condition for the extremals is positive definiteness of the second variation of the free energy, which is the squared functional with respect to variation $\delta\mathbf{\Phi}_\alpha$, and may be written as

$$\delta^2\mathcal{F}=1\Big/V\int\left(\sum_\alpha\sum_\beta(-\delta H_\alpha+\delta\mu_\alpha^{*})\delta\Phi_\beta\right)d\mathbf{x}. \tag{40}$$

The variations δH_α are coupled with the variations $\delta\mathbf{\Phi}_\alpha$ by the conditions (5) and (6),

$$\delta H_\alpha = T(-\delta\Phi_\alpha/\Phi^e_\alpha + \delta U_\alpha/U^e_\alpha + \delta V_\alpha/V^e_\alpha), \tag{41}$$

$$\begin{aligned}\nabla^2\delta U_\alpha - \delta U_\alpha - \sum_i Q_{i\alpha} s^e_i U^e_i/V^e_i \delta V_i &= -1/\Phi^0 \sum_i Q_{i\alpha}/V^e_i \delta\mathbf{\Phi}_i,\\ \nabla^2\delta V_\alpha - \delta V_\alpha - \sum_i Q_{\alpha i} s^e_i V^e_i/U^e_i \delta U_i &= -1/\Phi^0 \sum_i Q_{\alpha i}/U^e_i \delta\mathbf{\Phi}_i.\end{aligned} \tag{42}$$

The coefficients of the linear equations (41) and (42) are determined on the extremal $(U^e_i, V^e_i, s^e_i\mathbf{\Phi}^e_i)$. It is necessary to convert the operator, which is defined by the left-hand sides of Eqs. (42) for obtaining the explicit form of the functional (40) via $\delta\mathbf{\Phi}_\alpha\ \delta\mathbf{\Phi}_\beta$. Because it is a rather unsolvable problem, for direct calculations we restrict ourselves by the set of periodic fluctuations $\delta\mathbf{\Phi}_\alpha$, $\delta\mathbf{\Phi}_\beta$ with wave numbers q^* and introduce Fourier expansions for $\delta\mathbf{\Phi}_\alpha$, $\delta\mathbf{\Phi}_\beta$,

$$\delta\Phi_\alpha = \sum_k \delta\Phi^{(\alpha c)}_k \cos(kq^* x) + \delta\Phi^{(\alpha s)}_k \sin(kq^* x).$$

The system of Eqs. (41) and (42) is linear with respect to δU, δV, $\delta\mathbf{\Phi}$, therefore its solution can be presented in the form

$$\delta U_\alpha = \sum_{k,i} (U^{ic}_{\alpha k}(x)\delta\mathbf{\Phi}^{(ic)}_k + U^{is}_{\alpha k}(x)\delta\mathbf{\Phi}^{(is)}_k), \tag{43}$$

$$\delta V_\alpha = \sum_{k,i} (V^{ic}_{\alpha k}(x)\delta\mathbf{\Phi}^{(ic)}_k + V^{is}_{\alpha k}(x)\delta\mathbf{\Phi}^{(is)}_k), \tag{44}$$

where the functions $U^{ic}_{\alpha k}(x)$, $V^{ic}_{\alpha k}(x)$ are solutions of the system of nonhomogeneous equations,

$$\begin{aligned}\nabla^2\delta U^{ic}_{\alpha k} - \delta U^{ic}_{\alpha k} - \sum_j Q_{j\alpha} s^e_j U^e_j/V^e_j \delta V^{ic}_{jk} &= -1/\mathbf{\Phi}^0 Q_{\alpha i}/V^e_i \cos(kq^* x),\\ \nabla^2\delta V^{ic}_{\alpha k} - \delta V^{ic}_{\alpha k} - \sum_j Q_{\alpha j} s^e_j V^e_j/U^e_j \delta U^{ic}_{jk} &= -1/\mathbf{\Phi}^0 Q_{\alpha i}/U^e_i \cos(kq^* x),\end{aligned} \tag{45}$$

and the functions $U^{is}_{\alpha k}(x)$, $V^{is}_{\alpha k}(x)$ are solutions of the same systems with substitution $\cos(kq^*x)$ by $\sin(kq^*x)$. Using the relations (41), (43), and (44), the functional (40) may be presented in the matrix form regarding $\delta\mathbf{\Phi}^{(ic)}_k$, $\delta\mathbf{\Phi}^{(is)}_k$ with elements,

$$(\delta^2\mathcal{F})^{cc}_{ij,kl}, (\delta^2\mathcal{F})^{cs}_{ij,kl}, (\delta^2\mathcal{F})^{sc}_{ij,kl}, (\delta^2\mathcal{F})^{ss}_{ij,kl}.$$

Their expressions are presented in Appendix B. Thus, the analysis of stability can be reduced to determination of the spectrum of matrix. When using km harmonics, the dimension of this matrix is $m\cdot(2km+1)$.

VII. NUMERICAL CALCULATIONS

While calculating the phase diagrams, the basic difficulty is the solution of nonlinear systems (5), (6), and (10) for extremals. We used for this goal the iterated Newton method requiring a good starting approximation near bifurcation points if dealing with bifurcation analysis. Then we used a continuation procedure by parameter h with motion along tangent to curve $\mathbf{z}(h)$. Periodic boundary problem for linearized systems on every iteration was solved by the periodic sweep method.[25] Similar procedure was used for the solution of the systems of equation for $\partial\mathbf{z}/\partial h$ by the method of tangents. The operator $\mathbf{L}$ determined by (28) has zero eigenvalue in the turn point of curve $\mathbf{z}(h)$ and method of tangents cannot be used. In this case a change of the sign of step for parameter h

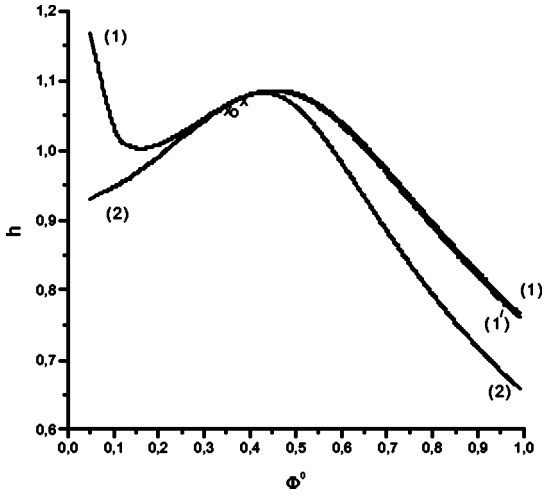

FIG. 1. Phase diagram for system (1). The curves (1), (2) are spinodal and binodal, respectively [for Φ^0 changing from 0 to 0.4 they are trivial ones, for $\Phi^0>0.4$, curve (1′), nontrivial spinodal], $\Phi^0\cong 0.38$ is the critical point (marked by ○), $\Phi^0\cong 0.4$ is the Lifshitz point (marked by ×).

and starting approximation were provided by extrapolation using two previous points. The calculations were performed for different copolymer systems and corresponding phase and bifurcation diagrams are presented in Figs. 1–5.

Melt of diblock copolymers with structural matrix, $Q=\begin{pmatrix}0.9 & 0.1 & 0\\ 0 & 0.95 & 0.05\end{pmatrix}$, and matrix of interaction $\gamma/\gamma_{12}(1;1;1.5)$.

In this system only the trivial spinodal exists for values $\mathbf{\Phi}^0<0.4$, and both the trivial and nontrivial spinodals exist for $\Phi^0>0.4$. The birth of nonhomogeneous structures in all points of nontrivial spinodals is subcritical by parameter h (and they are unstable). The starting appoximation for nonhomogeneous structures was obtained by formulas (38) and (39), and has continued by parameter $h<h^*(\mathbf{\Phi}^0)$ with help of the solutions of Eqs. (5), (6), and (10) up to the coups point $h=h_t$. In this point the operator $\mathbf{L}(\mathbf{U},\mathbf{V},\mathbf{s},\mathbf{\Phi},h_t)$ has vanishing eigenvalue, and couple of structures (stable and unstable) appeared at $h=h^*$ on the nontrivial spinodal disappear. For $h>h_t$ the structures obtained by continuation procedure are stable up to value $h=h_b$ where $R[\Phi^I]=0$. We calculate the spectrum of matrix (40) in every point of the curve $\mathbf{z}(h,\mathbf{\Phi}^0)$. Every branch $\mathbf{z}(h,\mathbf{\Phi}^0)$

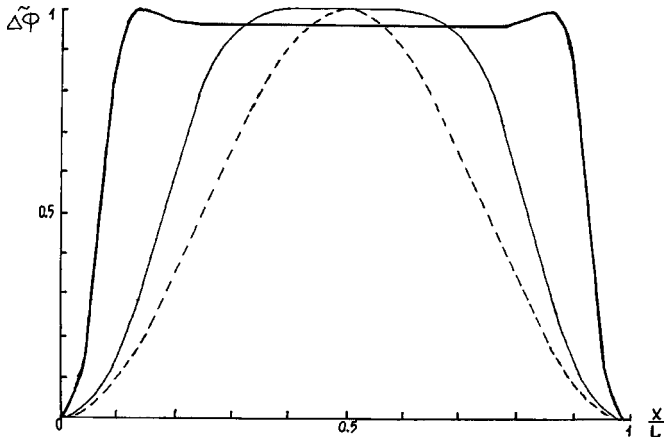

FIG. 2. The spatial distribution $\Phi_2(x/l)$ for $\Phi^0=0.99$ for the system (1) bold curve, for $l=260$; next curve, for $l=2\pi/q^*=78.248$ and value h, corresponding to binodal; dotted line, for $h=h_{sn}$. The curves are plotted in the scale $(\max_x\Phi_2-\min_x\Phi_2)$.

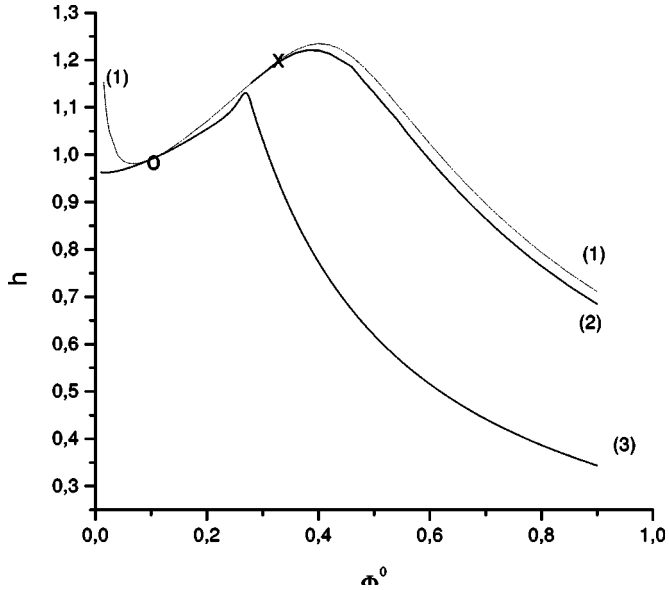

FIG. 3. Phase diagram for system (2). The curve (1), trivial spinodal, the curve (2) is nontrivial spinodal, (3) is the trivial binodal, $\Phi^0 \cong 0.28$ is the Lifshitz point (marked by $\times$), $\Phi^0 \cong 0.099$ is the critical point (marked by $\bigcirc$).

may be continued by parameter q (or $l=2\pi/q$) for $h \neq h^*$. The value of functional $\mathcal{F}[\mathbf{z}]$ and magnitude h_b decrease with increasing l. In these calculations the h_b change was very small. It should be noted that the value h_b for the homogeneous extremal arised transcritically in the spinodal point was practically the same as the value h_b for the branch of nonhomogeneous structures by $l \to \infty$. In Fig. 1 the phase diagrams are plotted, $Q=\begin{pmatrix} 0.99 & 0.01 & 0 \\ 0 & 0.95 & 0.05 \end{pmatrix}$, and the matrix of interaction $\gamma/\gamma_{12}(1.2;1;1.2)$.

The phase and bifurcation (for $\Phi^0=0.5$) diagrams for this system are shown in Figs. 3 and 4. For the nonhomogeneous structures $\Delta\Phi=\max_x \Phi_2-\min_x \Phi_2$, and for the homogeneous solution one deviation from the trivial one.

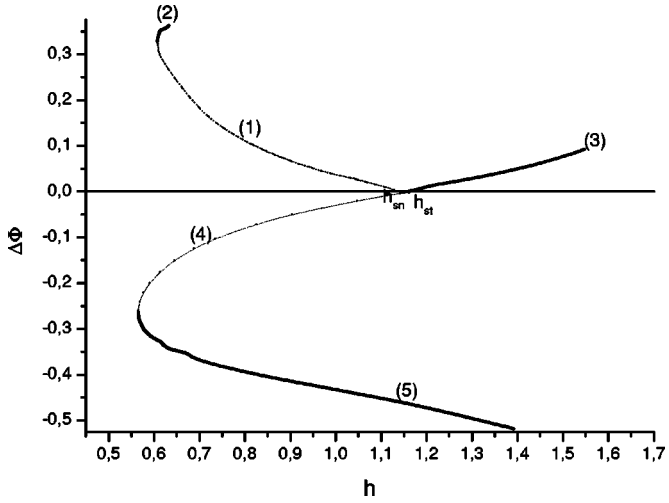

FIG. 4. The bifurcation diagram for the system (2) at $\Phi^0=0.5$. The curve (1) is the unstable nonhomogenous branch, (2) is the stable one, (3) the stable part of the branch appeared transcritically from the spinodal point, (4) is the unstable part of the same branch, (5) is the stable homogeneous nontrivial branch rigidly arising in couple with branch (4).

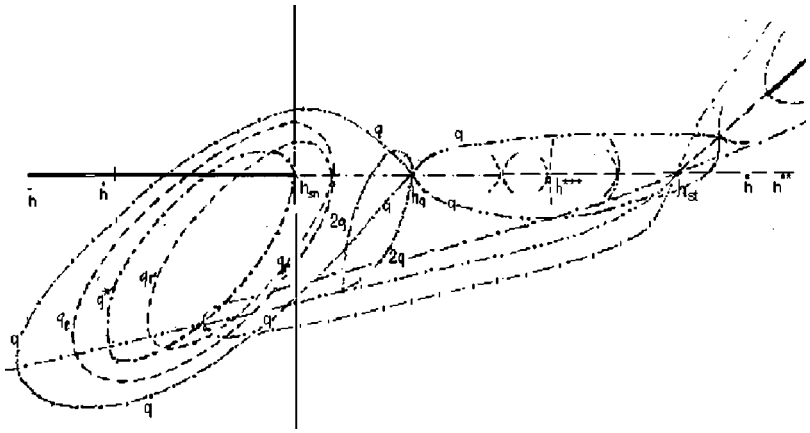

FIG. 5. The bifurcation diagram at $\Phi^0=0.76$ for the system (3).

The nonlinear problem at hand can have far more complicated bifurcation diagrams than those described above. For example, let us consider the system, characterized by a set of input parameters, $Q=\begin{pmatrix}0.15 & 0.84 & 0.01\\ 0.84 & 0.15 & 0.01\end{pmatrix}$, and the matrix of interaction $\gamma/\gamma_{12}(0.08;1;1.5)$.

The bifurcation behavior in the vicinity of the Lifshitz point ($\Phi^0=0.745$, $h=4.0857$) is of particular interest from the physical standpoint. The periodic solutions of the set of equations (5), (6), and (10) have periods substantially exceeding the size of a monomeric unit. To carry out the bifurcation analysis with a single controlled parameter h we have chosen the value $\Phi^0=0.760$ at which the above condition holds. For this value the bifurcation diagram is plotted in Fig. 5.

As depicted in this picture the loss of the thermodynamic stability of the homogeneous state with the temperature decay is observed for the first time at point $h_{sn}=4.3043$ of the nontrivial spinodal. At this point the Turing subcritical bifurcation happens leading to the loss of stability of the nontrivial solution accompanied by the disappearance of the pair of unstable periodic solutions with $q^*=0.5958$. As h subsequently increases the instability interval of wave vectors $q_l<q<q_r$ broadens up to the moment when h attains the value $h_{st}=4.3185$, corresponding to the trivial spinodal.

At point $h=h_{st}$, where $q_l=0$, $q_r=0.986$ the transcritical bifurcation takes place. Then the trivial extremal loses its stability with respect to homogeneous fluctuations whereas the upper part of nontrivial homogeneous extremal acquires it. Both of them, however, are unstable with respect to nonhomogeneous fluctuations in the vicinity of point $h=h_{st}$. Interesting peculiarity of the bifurcation at this specific point is a splitting off from the nontrivial extremal of a pair of periodic ones corresponding to the wave vector q^* unstable with respect to both types of fluctuations. The reason of such bifurcation behavior at point $h=h_{st}$ is that the zero eigenvalue of linear operator at this point has the multiplicity two, corresponding to the two-dimensional proper subspace (this bifurcation was described above).

Apart from the primary bifurcations (points h_{sn}, h_{st}) in Fig. 5 some secondary ones (points h^*, h^{**}) are also depicted which we managed to reveal numerically. When moving from point $h=h_{st}$ along the homogeneous nontrivial extremal the region of unstable wave vectors was found to reduce with the growth of control parameter h to contract to point $q=q^{**}=0.63$ at $h=h^{**}=4.3365$. As the result of this Turing supercritical bifurcation at point h^{**} the nontrivial extremal becomes absolutely stable giving birth to a couple of periodic structures with wave vector q^{**}. The free energy density of homogeneous nuclei described by this extremal turns out to be lower than that in the principal phase.

When moving from point $h=h_{st}$ along the homogeneous nontrivial extremal in the direction of decreasing parameter h the wave vector value q_r, bounding from the right-hand side of the interval of the instability of this extremal gets smaller to reach at point h^* just that value $q=q^*$, at which the stability loss by the trivial extremal happens at point h_{sn}. The amplitude of the pair of periodic

structures with wave vector q^* emerging at point h_{sn} as parameter h decreases, first increases to decay up to zero at the point when $h=h^*$. At this point the Turing subcritical bifurcation occurs resulting in the disappearance of the pair of unstable periodic extremals. Simultaneously, the nontrivial homogeneous extremal, remaining in general unstable, acquires stability with respect to the fluctuations with $q=q^*$. Under further decay of parameter h in the region to the left from the secondary bifurcation point the values $\mathbf{\Phi}_1$ and $\mathbf{\Phi}_2$ tend to zero at this extremal.

Returning to the instability interval one can find, that in every point of the interval $h_{sn}<h<h_{st}$ one can also observe the bifurcations of trivial solution. Type of these bifurcations will be different to the left and to the right of a certain specific point $h^-=4.308$, $q_l=0.393\,362$, where $q_r=2q_l$. To the left of this point both branches corresponding to q_l and q_r arise subcritically, each of them attaining the nontrivial homogeneous branch at corresponding points. To the right of point h^- one branch remains subcritical, while the other becomes supercritical. Such a situation persists under changes of h up to a certain value h^{***}, where coefficients $h^{(2)}$ and $h^{(3)}$ in the expansion (33) vanish. Subcritical branches reach at the bottom part of the nontrivial branch of the homogeneous extremal to the left of point h_{st}, whereas the supercritical ones reach the upper part of this curve. When $h>h^{***}$ bifurcations of both branches again become subcritical and corresponding branches attain the bottom part of the nontrivial extremal. Specific point h^- corresponds to the degenerate case since null space of the operator $\mathbf{L}$ at this point consists of two eigenvectors. Consequently the first approximation reads

$$\mathbf{z}^{(1)} = \alpha \mathbf{g}_l \cos q_l x + \beta \mathbf{g}_r \cos 2q_l x.$$

Constants α and β are determined from the orthogonality conditions for two eigenfunctions $\mathbf{g}_l^T \cos(q_l x)$ and $\mathbf{g}_r^T \cos(2q_l x)$ to the operator conjugate to $\mathbf{L}$. The equations for determination of the ratio α/β and $h^{(1)}$ are written as

$$\begin{aligned} 1/2\alpha^2(\mathbf{g}_r^T, \mathbf{B}_2(\mathbf{g}_l, \mathbf{g}_l)) + \beta h^{(1)}(\mathbf{g}_r^T, \mathbf{B}_2(\mathbf{g}_r, h)) = 0, \\ 1/2\alpha\beta(\mathbf{g}_l^T, \mathbf{B}_2(\mathbf{g}_r, \mathbf{g}_l)) + \alpha h^{(1)}(\mathbf{g}_l^T, \mathbf{B}_2(\mathbf{g}_l, h)) = 0, \end{aligned} \tag{46}$$

where

$$\mathbf{B}_2(\mathbf{y}^1, \mathbf{y}^2) = 1/2 \sum_{i,j} (\partial^2 \mathbf{F}/\partial y_i^1 \partial y_j^2) y_i^1 y_j^2, \quad \mathbf{B}_2(y,h) = \sum_j (\partial^2 \mathbf{F}/\partial y_j \partial h) y_j.$$

This system has several solutions

(1) $\alpha=0$, $h^{(1)}=0$,
(2) $\alpha\neq 0$, $h^{(1)}=-\beta/2(\mathbf{g}_l^T, \mathbf{B}_2(\mathbf{g}_r, \mathbf{g}_l)) / (\mathbf{g}_l^T, \mathbf{B}_2(\mathbf{g}_l, h))$,

$$(\alpha/\beta)^2 = (\mathbf{g}_l^T, \mathbf{B}_2(\mathbf{g}_r, \mathbf{g}_l))/(\mathbf{g}_r^T, \mathbf{B}_2(\mathbf{g}_l, \mathbf{g}_l)) \cdot (\mathbf{g}_r^T, \mathbf{B}_2(\mathbf{g}_r, h)/(\mathbf{g}_l^T, \mathbf{B}_2(\mathbf{g}_l, h)) = c.$$

If $c>0$ (in our case this condition is actually satisfied). The comparison of formulas (46) and (40) leads one to the conclusion that (with substitution α by β) their second equations are identical while the first ones differ by the term proportional to β^2 that is missing in set (46) by virtue of the orthogonality condition of functions $\cos(2q_l x)$ and $\cos^2(2q_l x)$. The solution of set (46) (where $\alpha=0$) describes the subcritical Turing bifurcation with two branches arising at the homogeneous nontrivial branch at $h=h_{2q_l}$. The second solution (where $\alpha\neq 0$) describes the transcritical bifurcation. Two unstable branches with period $2\pi/q_l$ arise when $h^-=2.24$ at the nontrivial homogeneous extremal to the left of point $h=h_{st}$, then one branch transcritically continues when $h=h_{st}$ in the direction of increasing of the parameter h to terminate at $h=4.33$ at the homogeneous extremal.

The bifurcation diagram presented in Fig. 5 is obviously incomplete. This statement is particularly evidenced by the absence in the interval $h_{sn}<h<h^{**}$ of extremals at which the Landau free energy functional has local minimum. Apparently, in this region of parameter h the nuclei of

mesophases with two- or three-dimensional spatial periodicity must be stable. We have in mind to perform a theoretical analysis of the existence and stability of such nuclei in the subsequent publications.[26–28]

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APPENDIX A

The components of vectors $\mathbf{r}_0$ and $\mathbf{r}_h$ in the formulas (39) are

$$\mathbf{r}_0[i] = -1/2\sum_j \nu_{ij}\mathbf{g}[j]\mathbf{g}[j+2],$$

$$\mathbf{r}_0[i+2] = -1/(4)((g[i+2]/s_i)^2 - H_1(g[5]+g[6])^2),$$

$$\mathbf{r}_0[i+4] = 1/2\mathbf{\Phi}^0\pi_i(2V_i\mathbf{g}[i]\mathbf{g}[i+2] + s_i\mathbf{g}[i]^2),$$

$$\mathbf{r}_h[i] = 0, \quad \text{for } i \neq 3,4,$$

$$\mathbf{r}_h[i+2] = -\sum_j \gamma_{ij}(\mathbf{\Phi}^0\pi_j - \mathbf{\Phi}_j),$$

where $(i=1,2)$ the vector $\mathbf{g}$ is the eigenvector of the matrix $J(q^*)$ and

$$H_1 = 1/(1-\Phi_1-\Phi_2)^2, \quad H_2 = 2H_1/(1-\Phi_1-\Phi_2).$$

The expression $h^{(2)}$ in the formulas (31) has the following form: $h^{(2)} = -\Sigma_i P(i)/\Sigma_i P_h(i)$, where the denotations are accepted,

$$ab(i) = a[i] + 1/2b[i], \quad n\mathbf{g}^T[i] = \nu_{i1}\mathbf{g}^T[1] + \nu_{i2}\mathbf{g}^T[2],$$

$$a_h\mathbf{g}[i] = \mathbf{g}[i]\mathbf{a}_h[i+2] + \mathbf{a}_h[i]\mathbf{g}[i+2],$$

$$P(1) = 1/2\sum_1^2 n\mathbf{g}^T[i](ab(i)\mathbf{g}[i+2] + ab(i+2)\mathbf{g}[i]),$$

$$P(2) = 1/2H_1(\mathbf{g}^T[3]+\mathbf{g}^T[4])(\mathbf{g}^T[5]+\mathbf{g}^T[6])(ab(5)+ab(6)),$$

$$P(3) = 1/16H_2(\mathbf{g}^T[3]+\mathbf{g}^T[4])(\mathbf{g}[5]+\mathbf{g}[6])^3,$$

$$P(4) = -1/2\sum_1^{2T} \mathbf{g}[i+2]\mathbf{g}[i+2]/s_i^2(ab(i+2) - 1/(4S_i)\mathbf{g}[i+2]^2),$$

$$P(5) = -\mathbf{\Phi}^0\sum_1^2 \pi_i^T\mathbf{g}[i+4]\mathbf{g}[i]((3/8\mathbf{g}[i+2]\mathbf{g}[i] + ab(i+2)V_i) + ab(i)(V_i\mathbf{g}[i+2] + S_i\mathbf{g}[i])),$$

$$P_h(1) = 1/2\sum_1^2 n\mathbf{g}^T[i]a_h\mathbf{g}[i],$$

$$P_h(2) = H_1/2(a_h[5] + a_h[6])(\mathbf{g}^T[3] + \mathbf{g}^T[4])(\mathbf{g}[5] + \mathbf{g}[6]), \quad P_h(3) = 0,$$

$$P_h(4) = -1/2\sum_1^2 g^T[i+2](1/s_i^{e2}\mathbf{g}[i+2]a_h(i+2) - (\gamma_{i1}\mathbf{g}[5] + \gamma_{i2}\mathbf{g}[6])),$$

$$P_h(5) = -\mathbf{\Phi}^0(\sum_1^2 \pi_i\mathbf{g}^T[i+4]((S_i\mathbf{g}[i] + V_i\mathbf{g}[i+2])\mathbf{a}_h(i) + \mathbf{a}_h(i+2)V_i\mathbf{g}[i])).$$

Let

$$n_0(i) = (\nu_{i1}\mathbf{g}^{(0)}[1]\mathbf{g}^{(0)}[3] + \nu_{i2}\mathbf{g}^{(0)}[2]\mathbf{g}^{(0)}[4]),$$

$$n_2(i) = (\nu_{i1}\mathbf{g}(q*)[1]\mathbf{g}(q*)[3] + \nu_{i2}\mathbf{g}(q*)[2]\mathbf{g}(q*)[4]),$$

$$VS(i) = (2V_i\mathbf{g}^{(0)}[i]\mathbf{g}[i+2] + s_i(\mathbf{g}^{(0)}[i])^2),$$

$$SS(i) = 1/2((\mathbf{g}^{(0)}[i+2])/s_i)^2 - H_1\ (\mathbf{g}^{(0)}[5] + \mathbf{g}^{(0)}[6])^2),$$

$$n_{02}(i) = \sum_1^2 \nu_{ij}(g^{(0)}[j+2]g(q*)[j] + g^{(0)}[j]g(q*)[j+2]),$$

$$S_{02}(i) = 1/2(\mathbf{g}^{(0)}[i+2]\mathbf{g}(q*)[i+2]/s_i^2 - H_1(\mathbf{g}^{(0)}[5] + \mathbf{g}^{(0)}[6])(\mathbf{g}(q*)[5] + \mathbf{g}(q*)[6])),$$

$$VS_{02}(i) = V_i(\mathbf{g}^{(0)}[i+2]\mathbf{g}(q*)[i] + \mathbf{g}^{(0)}[i]\mathbf{g}(q*)[i+2]) + s_i\mathbf{g}^{(0)}[i]\mathbf{g}(q*)[i],$$

$$SS_2(i) = 1/2((g(q*)[i+2]/s_i)^2 - H_1(\mathbf{g}(q*)[5] + \mathbf{g}(q*)[6])^2),$$

$$VS_2(i) = 2V_i(\mathbf{g}(q*)[i+2]\mathbf{g}(q*)[i]) + S_i(\mathbf{g}(q*)[i])^2.$$

Then the vectors $\mathbf{r}_{00}$, $\mathbf{r}_{01}$, $\mathbf{r}_{22}$ have the following form:

$$r_{00} = [-n_0(1), -n_0(2), SS(1), SS(2), \mathbf{\Phi}^0\pi_1 VS(1), \mathbf{\Phi}^0\pi_2 VS(2)],$$

$$r_{02} = [-1/2n_{02}(1), -1/2n_{02}(2), S_{02}(1), S_{02}(2), \mathbf{\Phi}^0\pi_1 VS_{02}(1), \mathbf{\Phi}^0\pi_2 VS_{02}(2)],$$

$$r_{22} = [-1/2n_2(1), -1/2n_2(2), 1/2SS(1), 1/2SS(2), 1/2\mathbf{\Phi}^0\pi_1 VS(1), 1/2\mathbf{\Phi}^0\pi_2 VS(2)].$$

APPENDIX B

The matrix elements of the functional second variation are written as

$$(\delta^2\mathcal{F})_{ij,kl}^{cc} = m_{ij,kl}^{cc} + h_{ij,kl}^{cc}, \quad (\delta^2\mathcal{F})_{ij,kl}^{cs} = m_{ij,kl}^{cs} + h_{ij,kl}^{cs},$$

$$(\delta^2\mathcal{F})_{ij,kl}^{sc} = m_{ij,kl}^{sc} + h_{ij,kl}^{sc}, \quad (\delta^2\mathcal{F})_{ij,kl}^{ss} = m_{ij,kl}^{ss} + h_{ij,kl}^{ss},$$

$$m^{cc}_{ij,kl} = \frac{T}{L}\int_0^L (-c_{ij} + 1/\mathbf{\Phi}_i\delta_{ij})\cos(kqx)\cos(lqx)\mathrm{d}x,$$

$$m^{cs}_{ij,kl} = \frac{T}{L}\int_0^L (-c_{ij} + 1/\mathbf{\Phi}_i\delta_{ij})\cos(kqx)\sin(lqx)\mathrm{d}x,$$

$$m^{sc}_{ij,kl} = \frac{T}{L}\int_0^L (-c_{ij} + 1/\mathbf{\Phi}_i\delta_{ij})\sin(kqx)\cos(lqx)\mathrm{d}x,$$

$$m^{ss}_{ij,kl} = \frac{T}{L}\int_0^L (-c_{ij} + 1/\mathbf{\Phi}_i\delta_{ij})\sin(kqx)\sin(lqx)\mathrm{d}x,$$

$$h^{cc}_{ij,kl} = -\frac{T}{L}\int_0^L (1/U_i(x)\,\delta U^{ic}_{j,k}(x) + 1/V_i(x)\,\delta V^{ic}_{j,k}(x))\cos(lqx)\mathrm{d}x,$$

$$h^{cs}_{ij,kl} = -\frac{T}{L}\int_0^L (1/U_i(x)\,\delta U^{ic}_{j,k}(x) + 1/V_i(x)\,\delta V^{ic}_{j,k}(x))\sin(lqx)\mathrm{d}x,$$

$$h^{sc}_{ij,kl} = -\frac{T}{L}\int_0^L (1/U_i(x)\,\delta U^{is}_{j,k}(x) + 1/V_i(x)\,\delta V^{is}_{j,k}(x))\cos(lqx)\mathrm{d}x,$$

$$h^{ss}_{ij,kl} = -\frac{T}{L}\int_0^L (1/U_i(x)\,\delta U^{is}_{j,k}(x) + 1/V_i(x)\,\delta V^{is}_{j,k}(x))\sin(lqx)\mathrm{d}x.$$

Here the values $U_i(x)$, $V_i(x)$ are given on the extremal, and $\delta U^{is}_{j,k}(x)$, $\delta U^{is}_{j,k}(x)$, $\delta U^{ic}_{j,k}(x)$ $\delta V^{ic}_{j,k}(x)$ are determined by Eq. (45), and $L=2\pi/q^*$.

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Dynamical models of weak scattering

Timothy R. Field
Departments of Electrical and Computer Engineering, Mathematics and Brain Body Institute, McMaster University, 1280 Main Street West, Hamilton, ON, Canada, L8S 4K1

Robert J. A. Tough
TW Research, Harcourt Barn, Harcourt Road, Malvern WR14 4DW, United Kingdom

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We extend a recent diffusion model, in which the continuous time dynamics of the *K*-scattering process have been proposed, to include the effect of the presence of a coherent offset in the scattering amplitude. The weak scattering amplitudes are characterized in terms of continuous time biased random walk models, and the corresponding stochastic dynamics derived. The stochastic differential geometry of the resultant amplitude fluctuations is derived in relation to that of pure *K*-scattering. Asymptotic distributions of amplitude, intensity, and phase are provided, and the condition for detailed balance shown to hold. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1811787]

I. INTRODUCTION

Significant progress has recently been made in our understanding of the dynamics of models of electromagnetic scattering in the context of diffusion processes. Deviations from Rayleigh (Gaussian) scattering have been successfully formulated in the context of *K*-distributed scattering processes (Field and Tough, 2003b) and have formed the basis of an anomaly detection technique that has been successfully applied to maritime radar scattering and laser propagation experiments (Field and Tough, 2003a).

The models considered previously assume a uniform (asymptotic) distribution of phase. In this paper we consider how anisotropic phase distributions can be accommodated within the framework provided by stochastic differential equations (SDEs) that has proved to be useful in *K*-scattering. We have seen how a simple random walk model provides a physically motivated description of the scattering process (Jakeman and Tough, 1988) that at the same time makes useful contact with the SDE formulation of the problem (Field and Tough, 2003a, 2003b). In earlier work, unbiased random walk models have provided useful insight into the Gaussian and non-Gaussian statistics of radiation scattered sufficiently strongly for its phase to be effectively randomized, and to take a uniform asymptotic distribution. A biased random walk model of weak scattering has been discussed in detail in Jakeman and Tough (1987). Their analysis led to the so-called generalized *K*-scattering model. The present paper re-addresses this problem, replacing the static, characteristic function approach with one in which the dynamics is captured by a set of coupled SDEs. A fairly complete analysis is possible that also makes contact with the Rice and homodyned *K* descriptions of weak scattering (Jakeman, 1980). This allows for a detailed description of the geometry of the resultant amplitude fluctuations, which is shown to be different in some significant respects from that encountered in the *K*-distributed case (Field and Tough, 2003b). In addition to developing this SDE description we study the phase distributions implicit in these models in more detail than has been reported previously.

Throughout we shall consistently adopt the notation for the decomposition of a general Ito process q_t into drift and volatility terms, respectively, as $\mathrm{d}q_t = b_t^{(q)}\,\mathrm{d}t + \sigma_t^{(q)}\,\mathrm{d}W_t^{(q)}$, with respect to some (fixed) probability measure on the space of paths, and define the diffusion coefficients $\Sigma^{(\cdot)}$ by $\mathrm{d}q_t\,\mathrm{d}p_t = \Sigma_t^{(q,p)}\,\mathrm{d}t$ and abbreviate via $\mathrm{d}q_t^2 = \Sigma_t^{(q)}\,\mathrm{d}t$. The error surface $\mathcal{S}^q$ of a vector process q^i is then

defined by the (inverse) quadratic form relation $\Sigma^{(q)-1}(\delta q)=1$. We shall adopt the Einstein summation convention throughout (e.g., Penrose and Rindler, 1984), unless explicitly indicated otherwise.

II. *K*-SCATTERING

We review the results of Field and Tough (2003b) that are necessary in the present context for the treatment of weak scattering. The random walk model with step number fluctuations, due to Jakeman (Jakeman, 1980; Jakeman and Tough, 1988), accounts for certain statistical properties of *K*-scattering. The extension to a complete dynamical description, in terms of continuous time diffusion processes, is provided in Field and Tough (2003b), the necessary results of which we review in this section. It is shown in the Rayleigh case of a fixed step number that the amplitude obeys a complex Ornstein–Uhlenbeck equation, and a corresponding SDE in the *K*-distributed case is derived.

(i) *Rayleigh scattering:* In the Rayleigh case consider the random walk model for the scattered electric field (cf. Jakeman, 1980; Tough, 1987; Jakeman and Tough, 1988) with step $s^{(j)}$,

$$\mathcal{E}_t^{(N)}=\sum_{j=1}^{N}\overbrace{\exp[i\varphi_t^{(j)}]}^{s^{(j)}} \tag{2.1}$$

for constant population size N. Since Maxwell's equations for the electromagnetic field possess U(1) gauge invariance with respect to duality rotations, i.e., multiplication by $\exp(i\Lambda)$ for constant Λ (cf. Penrose and Rindler, 1984), the assumption of independence of $\{\varphi^{(j)}\}$ implies that these phases are uniformly distributed. Accordingly in (2.1) the phase factors $\{\exp[i\varphi_t^{(j)}]\}$ are independent and uniformly distributed on the unit circle in $\mathbb{C}$. Our (phase) diffusion model therefore takes $\{\varphi_t^{(j)}\}$ as a collection of (displaced) Wiener processes on a suitable time scale, $\varphi_t^{(j)}=\Delta^{(j)}+\mathcal{B}^{1/2}W_t^{(j)}$, with the random initializations $\{\Delta^{(j)}\}$ a set of independent random variables uniformly distributed on the interval $[0,2\pi)$, and thus $\mathrm{d}\varphi_t^{(j)}=\mathcal{B}^{1/2}\,\mathrm{d}W_t^{(j)}$, $\mathrm{d}\varphi_t^{(j)2}=\mathcal{B}\,\mathrm{d}t$. From Ito's formula (e.g., Oksendal, 1998; Karatzas and Shreve, 1988) the Ito differential of (2.1) is

$$\mathrm{d}\mathcal{E}_t^{(N)}=\sum_{j=1}^{N}\left(i\,\mathrm{d}\varphi_t^{(j)}-\frac{1}{2}\mathrm{d}\varphi_t^{(j)2}\right)\exp[i\varphi_t^{(j)}]. \tag{2.2}$$

The first term $\Sigma_{j=1}^{N}i\,\mathrm{d}\varphi_t^{(j)}\exp[i\varphi_t^{(j)}]$ on the right-hand side of (2.2) consists of a sum of independent randomly phased Wiener processes, with variance equal to $\mathcal{B}N\,\mathrm{d}t$, while the second term is independent of the scatterer label j. Thus from (2.2) we can write

$$\mathrm{d}\mathcal{E}_t^{(N)}=-\tfrac{1}{2}\mathcal{B}\mathcal{E}_t^{(N)}\,\mathrm{d}t+(\mathcal{B}N)^{1/2}\,\mathrm{d}\xi_t, \tag{2.3}$$

where ξ_t is a complex Wiener process satisfying $|\mathrm{d}\xi_t|^2=\mathrm{d}t$, $\mathrm{d}\xi_t^2=0$. The process ξ_t is adapted to the filtration $\mathcal{F}^{(\varphi)}=\cup_j\mathcal{F}^{(j)}$, where $\mathcal{F}^{(j)}$ is the filtration appropriate to the component scatterer phase $\varphi_t^{(j)}$. The (normalized) amplitude process $\mathcal{E}_t$ is then defined by $\mathcal{E}_t=\lim_{N\to\infty}[\mathcal{E}_t^{(N)}/\overline{N^{1/2}}]$ and satisfies the SDE,

$$\mathrm{d}\mathcal{E}_t=-\tfrac{1}{2}\mathcal{B}\mathcal{E}_t\,\mathrm{d}t+(\mathcal{B}x)^{1/2}\,\mathrm{d}\xi_t, \tag{2.4}$$

where the continuous valued random variable x, the average scattering power, arises from an asymptotically large population via $x=\lim_{N\to\infty}[N/\overline{N}]$.

(ii) *K-distributed noise:* In the case of step number fluctuations in the random walk model (2.1), we define the *K*-amplitude ψ_t as a modification to the Rayleigh amplitude, such that we employ a time dependent N_t with $x_t=\lim_{N_t\to\infty}[N_t/\overline{N}]$. Thus

$$\psi_t = \lim_{N_t\to\infty}\left\{\frac{1}{\overline{N}^{1/2}}\sum_{j=1}^{N_t}\exp\left[i\varphi_t^{(j)}\right]\right\} \tag{2.5}$$

$$= \lim_{N_t\to\infty}\left\{\left(\frac{N_t}{\overline{N}}\right)^{1/2}\frac{1}{N_t^{1/2}}\sum_{j=1}^{N_t}\exp\left[i\varphi_t^{(j)}\right]\right\} \tag{2.6}$$

$$= x_t^{1/2}\gamma_t, \tag{2.7}$$

where $\gamma_t = \lim_{N\to\infty}[\mathcal{E}_t^{(N_t)}/N_t^{1/2}]$. Thus the intensity has the compound representation $z_t = x_t u_t$ where $u_t = |\gamma_t|^2$ is the (instantaneous) intensity of the component Rayleigh process. According to the arguments given in the Rayleigh case above, γ_t is a complex Ornstein–Uhlenbeck process which obeys the SDE,

$$\mathrm{d}\gamma_t = -\tfrac{1}{2}\mathcal{B}\gamma_t\,\mathrm{d}t + \mathcal{B}^{1/2}\mathrm{d}\xi_t. \tag{2.8}$$

Observe from (2.4), therefore, that γ_t is a unit power Rayleigh process. The above equation for γ_t can be solved by considering the stochastic differential $\mathrm{d}\left[\exp(\frac{1}{2}\mathcal{B}t)\gamma_t\right]$, which leads to the solution

$$\gamma_t = \exp\left(-\frac{1}{2}\mathcal{B}t\right)\left\{\gamma_0 + \mathcal{B}^{1/2}\int_0^t \exp\left(\frac{1}{2}\mathcal{B}s\right)\mathrm{d}\xi_s\right\}. \tag{2.9}$$

We deduce the expectation formulas,

$$\mathbb{E}[\gamma_t] = \exp\left(-\tfrac{1}{2}\mathcal{B}t\right)\gamma_0, \tag{2.10}$$

$$\mathbb{E}[|\gamma_t|^2] = 1 + \exp\left(-\mathcal{B}t\right)(|\gamma_0|^2 - 1). \tag{2.11}$$

From (2.11) it follows that $\lim_{t\to\infty}\mathbb{E}[|\gamma_t|^2] = 1$ and so from (2.7) we find the intensity process, defined by $z_t = |\psi_t|^2$, satisfies $\mathbb{E}[z_t] = x_t$. The SDE for ψ_t can then be derived by applying the Ito product formula to (2.7). This requires the SDE for the scattering cross section to be specified. In accordance with the birth–death–immigration (BDI) model (Bartlett, 1966), we shall take the rescaled population variate $x \mapsto \alpha x$ to satisfy the SDE,

$$\mathrm{d}x_t = \mathcal{A}(\alpha - x_t)\mathrm{d}t + (2\mathcal{A}x_t)^{1/2}\,\mathrm{d}W_t^{(x)}, \tag{2.12}$$

for an independent Wiener process $W_t^{(x)}$ (Field and Tough, 2003a). (In terms of the underlying population parameters of the BDI model, $\alpha = \nu/\lambda$, the ratio of the immigration to birth rate, the birth and death rates coinciding for an infinite sized population.) Accordingly x_t has an asymptotic Γ-distribution,

$$\Gamma_\alpha(x) = \frac{x^{\alpha-1}\exp(-x)}{\Gamma(\alpha)}, \tag{2.13}$$

with the first two moments $\mathrm{Var}[x] = \langle x\rangle = \alpha$. These preliminaries enable us to provide the dynamics of the amplitude, intensity, and phase of the *K*-scattering process as follows (cf. Field and Tough, 2003b for a detailed treatment).

A. Amplitude

Proposition 2.1: The K-amplitude is governed by the SDE,

$$\frac{\mathrm{d}\psi_t}{\psi_t} = \mathcal{A}\left(\frac{2(\alpha - x_t) - 1}{4x_t}\right)\mathrm{d}t + \left(\frac{\mathcal{A}}{2x_t}\right)^{1/2}\mathrm{d}W_t^{(x)} - \frac{1}{2}\mathcal{B}\,\mathrm{d}t + \frac{\mathcal{B}^{1/2}}{\gamma_t}\mathrm{d}\xi_t. \tag{2.14}$$

This evolution is invariant under the $U(1)$ gauge transformation $\psi_t \mapsto \exp(i\Lambda)\psi_t$, for constant Λ.

B. Intensity

Proposition 2.2: The K-intensity SDE is given by

$$\mathrm{d}z_t = \left[\frac{\mathcal{A}z_t(\alpha - x_t)}{x_t} + \mathcal{B}(x_t - z_t)\right]\mathrm{d}t + \left(\frac{2\mathcal{A}z_t^2}{x_t} + 2\mathcal{B}x_t z_t\right)^{1/2} \mathrm{d}W_t^{(z)} \tag{2.15}$$

in which $W_t^{(z)}$ is correlated with $W_t^{(x)}$ of (2.12), and satisfies

$$\left(\frac{2\mathcal{A}z_t^2}{x_t} + 2\mathcal{B}x_t z_t\right)^{1/2} \mathrm{d}W_t^{(z)} = \left(\frac{2\mathcal{A}}{x_t}\right)^{1/2} z_t\, \mathrm{d}W_t^{(x)} + (2\mathcal{B}x_t z_t)^{1/2}\, \mathrm{d}W_t^{(r)} \tag{2.16}$$

and $W_t^{(r)}$ is a real-valued Wiener process defined by

$$\gamma_t^*\, \mathrm{d}\xi_t + \gamma_t\, \mathrm{d}\xi_t^* \equiv \left(\frac{2z_t}{x_t}\right)^{1/2} \mathrm{d}W_t^{(r)}. \tag{2.17}$$

C. Phase

Proposition 2.3: The resultant phase θ_t of the K-amplitude process satisfies the SDE,

$$\mathrm{d}\theta_t = \left(\frac{\mathcal{B}x_t}{2z_t}\right)^{1/2} \mathrm{d}W_t^{(\theta)}, \tag{2.18}$$

where the distinct (real-valued) Wiener process $W_t^{(\theta)}$ is defined according to

$$\frac{1}{i}(\gamma_t^*\, \mathrm{d}\xi_t - \gamma_t\, \mathrm{d}\xi_t^*) \equiv \left(\frac{2z_t}{x_t}\right)^{1/2} \mathrm{d}W_t^{(\theta)}. \tag{2.19}$$

These various relations allow the K-amplitude dynamics to be recast in terms of $W^{(x)}$, $W^{(\theta)}$, $W^{(r)}$ as follows.

Corollary 2.4: The K-amplitude satisfies the SDE,

$$\frac{\mathrm{d}\psi_t}{\psi_t} = \left[\mathcal{A}\left(\frac{2(\alpha - x_t) - 1}{4x_t}\right) - \frac{1}{2}\mathcal{B}\right]\mathrm{d}t + \left(\frac{\mathcal{A}z_t + \mathcal{B}x_t^2}{2x_t z_t}\right)^{1/2} \mathrm{d}W_t^{(z)} + i\left(\frac{\mathcal{B}x_t}{2z_t}\right)^{1/2} \mathrm{d}W_t^{(\theta)}, \tag{2.20}$$

in which, alternatively, the Wiener terms can be expressed as

$$\left(\frac{\mathcal{A}}{2x_t}\right)^{1/2} \mathrm{d}W_t^{(x)} + \left(\frac{\mathcal{B}x_t}{2z_t}\right)^{1/2} (\mathrm{d}W_t^{(r)} + i\, \mathrm{d}W_t^{(\theta)}). \tag{2.21}$$

The following result, implied by (2.14) and the identities $\mathrm{d}\xi_t^2 = \mathrm{d}\xi_t\, \mathrm{d}W_t^{(x)} = 0$, will be useful in connection with the geometry of fluctuations for weak scattering processes discussed in Sec. V.

Corollary 2.5: The product cross-section/K-amplitude stochastic differentials satisfy

$$\mathrm{d}x_t^2 = 2\mathcal{A}x_t\, \mathrm{d}t, \tag{2.22}$$

$$\mathrm{d}x_t\, \mathrm{d}\psi_t = \mathcal{A}\psi_t\, \mathrm{d}t, \tag{2.23}$$

$$\mathrm{d}\psi_t^2 = \left(\frac{\mathcal{A}\psi_t^2}{2x_t}\right)\mathrm{d}t, \tag{2.24}$$

$$|\mathrm{d}\psi_t|^2 = \left(\frac{\mathcal{A}z_t}{2x_t} + \mathcal{B}x_t\right)\mathrm{d}t. \tag{2.25}$$

D. Geometry of fluctuations

Observe from Propositions 2.2 and 2.3 that $\mathrm{d}W_t^{(z)}\,\mathrm{d}W_t^{(\theta)}=0$, so the fluctuations in R_t, θ_t are statistically independent. The relative magnitude of the radial and orthogonal (phase) fluctuations is determined by

$$\frac{\Sigma_t^{(z)}}{\Sigma_t^{(\theta)}} = 4z_t^2 + \frac{4\mathcal{A}z_t^3}{\mathcal{B}x_t^2}, \tag{2.26}$$

which exceeds the quotient obtained in the Rayleigh case, $\mathcal{A}=0$. These relations can be used to characterize the geometry of the *K*-scattering amplitude fluctuations as follows. We shall refer to the real and imaginary parts of the resultant amplitude *I*, *Q* as the in-phase and quadrature-phase components, respectively (Helmstrom, 1960).

Proposition 2.6: In the K-distributed case, $\mathcal{A}\neq 0$, the amplitude diffusion tensor is nondegenerate, and the fluctuations in the in-phase and quadrature phase components δI_t, δQ_t are correlated. The (comoving) error surface $\mathcal{S}$ of $\delta\psi_t$ is an ellipse whose major axis lies in the instantaneous radial direction defined by ψ_t. Degeneracy occurs in the Rayleigh case $\mathcal{A}=0$, for which $\mathcal{S}$ is a circle, i.e., the fluctuations in ψ_t are isotropic.

For a complete account of the dynamical properties of *K*-scattering see Field and Tough (2003b).

III. WEAK SCATTERING AMPLITUDES

In situations of strong backscattering, such as occur, e.g., in radar applications, the phases of the back-scattered components are taken to be uniformly randomized and correspondingly the dynamics and asymptotic distributions of the resultant amplitude process Ψ_t are invariant under $\Psi_t \mapsto e^{i\Lambda}\Psi_t$. This is no longer the case for weak scattering however, i.e., situations where the Rayleigh component of the scatter is weak in comparison to some coherent offset contribution. In these cases the mean amplitude is offset from zero, and the asymptotic resultant phase distribution is anisotropic. We have seen in the *K*-distributed case that $\psi_t = x_t^{1/2}\gamma_t$ where γ_t describes the (unit-power) Rayleigh process (Field and Tough, 2003b) according to (2.8). When this process lies in superposition with a coherent offset amplitude ϱ_t, the resultant amplitude process Ψ_t depends on the relative scalings of the offset and (modulated) Rayleigh components with respect to population size. There are essentially three cases to consider, each of which can be understood in terms of the random walk model (2.1) by imposing a *bias* on each step $s^{(j)}$, whose physical origin is the coherent offset contribution. We shall describe these cases in the order of Rice, homodyned and generalized *K*-scattering, thus introducing physical features (noise, *K*-noise, fluctuating coherently scattered beam) in a natural order that is mirrored in the increasing complexity of the calculations.

A. Rice model

We assume that the number of scatterers is constant in time, with a constant offset contribution $\varrho_t = a$. Thus modifying the random walk model (2.1) we write

$$\mathcal{E}_t^{(N)} = \sum_{j=1}^{N}\left(\overbrace{a + \exp[i\varphi_t^{(j)}]}^{s^{(j)}}\right). \tag{3.1}$$

Scaling by $1/N$, $1/N^{1/2}$ for the respective terms under the summation, in the x_t-continuum limit ($N\to\infty$) this becomes

$$\Psi_t^{\mathrm{R}} = a + \gamma_t. \tag{3.2}$$

B. Homodyned *K*-scattering

The situation here is the same as for *K*-scattering with the superposition of a constant offset $\varrho_t = a$ that does not fluctuate with N_t. In the continuum limit this amounts to adding a constant to the *K*-amplitude, thus

$$\Psi_t^{\mathrm{HK}} = a + \psi_t. \tag{3.3}$$

C. Generalized *K*-scattering

In a similar fashion (2.1) is modified to become

$$\mathcal{E}_t^{(N_t)} = \sum_{j=1}^{N_t} \left(\overbrace{a + \exp[i\varphi_t^{(j)}]}^{s^{(j)}} \right) \tag{3.4}$$

in which the *t*-dependence of the limit of summation is to be observed, i.e., the step number of the biased random walk has fluctuations. Scaling by the reciprocal mean and root mean populations, respectively, the offset becomes $\varrho_t = a x_t$ and we have

$$\Psi_t^{\mathrm{GK}} = a x_t + \psi_t \tag{3.5}$$

in the continuum limit.

Observe with respect to scaling in the continuum population limit that, in each case, we have divided by the (unique) length scale factors, appropriate to the relevant terms in $s^{(j)}$ separately, that yield finite nonzero resultant amplitudes.

IV. STOCHASTIC DYNAMICS

The stochastic dynamics of the weak scattering amplitudes described above can be calculated from the underlying *K*-scattering dynamics presented in Sec. II. We shall make use of the identities for the (resultant) intensity and phase stochastic differentials in terms of the (resultant) amplitude,

$$\mathrm{d}Z_t \equiv \Psi_t^* \, \mathrm{d}\Psi_t + \Psi_t \, \mathrm{d}\Psi_t^* + |\mathrm{d}\Psi_t|^2,$$

$$\mathrm{d}\Theta_t \equiv \frac{1}{2i}\left[\left(\frac{\mathrm{d}\Psi_t}{\Psi_t} - \frac{1}{2}\left(\frac{\mathrm{d}\Psi_t}{\Psi_t} \right)^2 \right) - \left(\frac{\mathrm{d}\Psi_t^*}{\Psi_t^*} - \frac{1}{2}\left(\frac{\mathrm{d}\Psi_t^*}{\Psi_t^*} \right)^2 \right) \right], \tag{4.1}$$

and their products

$$\Sigma_t^{(Z)} \equiv \Psi_t^2 \Sigma_t^{(\Psi^*)} + \Psi_t^{*2} \Sigma_t^{(\Psi)} + 2 Z_t \Sigma_t^{(\Psi,\Psi^*)},$$

$$\Sigma_t^{(Z,\Theta)} \equiv \Im\left[\left(\frac{\Psi_t^*}{\Psi_t} \right) \Sigma_t^{(\Psi)} \right], \tag{4.2}$$

$$\Sigma_t^{(\Theta)} \equiv \frac{1}{4}\left[\frac{2\Sigma_t^{(\Psi,\Psi^*)}}{Z_t} - \frac{\Sigma_t^{(\Psi)}}{\Psi_t^2} - \frac{\Sigma_t^{(\Psi^*)}}{\Psi_t^{*2}} \right].$$

In combination with (3.2), (3.3), (3.5), and (2.12) and the results of Corollary 2.5 these identities enable us to derive the SDEs satisfied by Z_t, Θ_t in terms of the component Wiener processes $\{W_t^{(r)}, W_t^{(\theta)}, W_t^{(x)}\}$ encountered in Sec. II. The dynamics are the most simple for Rice scattering owing to the differential of (3.2). In the context of radar applications, the Rice model is referred to as a Swerling zero target in Rayleigh clutter, where the target strength is represented by ϱ (assumed constant over the time scale of interest) and the Rayleigh process γ_t represents back-

ground clutter. More care is required in the calculations for the homodyned and generalized *K*-scattering processes owing to certain cross terms that arise. Nevertheless the strategy is the same for each case, and we are led to the dynamical characterizations of the vector scattering process $\mathrm{S}_t=(x_t,Z_t,\Theta_t)^{\mathrm{tr}}$ according to the scheme

$$\mathrm{d}S_t^i = b_t^i\,\mathrm{d}t + \sigma_t^j\,\mathrm{d}W_t^i \tag{4.3}$$

(no summation over i) for a collection of Wiener processes $\{W_t^i|\,\forall\, i\}$ (not necessarily independent) with respective drift and diffusion coefficients b^i, Σ^{ij} determined by

$$b_t^i = \frac{\mathbb{E}[\mathrm{d}S_t^i]}{\mathrm{d}t},$$

$$\mathrm{d}S_t^i\,\mathrm{d}S_t^j = \Sigma_t^{ij}\,\mathrm{d}t. \tag{4.4}$$

The corresponding Fokker–Planck equation (e.g., Risken, 1989) for the joint probability density $\rho_t(x,Z,\Theta)$ is then

$$\partial_t\rho + \partial_i(\rho\mathcal{V}^i) = 0, \tag{4.5}$$

where the vector scattering current $\mathcal{V}^i$ is defined by

$$\mathcal{V}^i = b^i - \tfrac{1}{2}\rho^{-1}\partial_j(\Sigma^{ij}\rho). \tag{4.6}$$

A. Rice

The amplitude dynamics of the Rice process is identical to that of the Rayleigh process and the cross section is constant and equal to unity, as evident from (3.2). We deduce from the identities above that, in terms of the geometry of the underlying Rayleigh process, the resultant intensity satisfies the SDE,

$$\mathrm{d}Z_t = \mathcal{B}[1-u_t-au_t^{1/2}\cos\,\theta_t]\mathrm{d}t + (2\mathcal{B})^{1/2}[(u_t^{1/2}+a\cos\,\theta_t)\mathrm{d}W_t^{(r)} - a\sin\,\theta_t\,\mathrm{d}W_t^{(\theta)}]. \tag{4.7}$$

Likewise the resultant phase satisfies

$$\mathrm{d}\Theta_t = \frac{-\frac{1}{2}\mathcal{B}au_t^{1/2}\sin\,\theta_t\,\mathrm{d}t + \left(\frac{\mathcal{B}}{2}\right)^{1/2}[a\sin\,\theta_t\,\mathrm{d}W_t^{(r)} + (u_t^{1/2}+a\cos\,\theta_t)\mathrm{d}W_t^{(\theta)}]}{(a^2+u_t+2au_t^{1/2}\cos\,\theta_t)}. \tag{4.8}$$

This leads to the following result.

Proposition 4.1: The Rice vector scattering process $\mathbf{S}_t$ *has drift*

$$b^i = \begin{pmatrix} \mathcal{B}[1-Z+aZ^{1/2}\cos\Theta] \\ -(\mathcal{B}a\sin\Theta)/2Z^{1/2} \end{pmatrix}, \tag{4.9}$$

and diffusion tensor

$$\Sigma^{ij} = \begin{pmatrix} 2\mathcal{B}Z & 0 \\ 0 & \mathcal{B}/2Z \end{pmatrix}. \tag{4.10}$$

B. Homodyned *K*

From (3.3) the amplitude dynamics is identical to that of the *K*-process. Thus for the intensity, in terms of the underlying *K*-scattering geometry, we find

$$\begin{aligned} dZ_t = &\left[\frac{\mathcal{A}z_t(\alpha - x_t)}{x_t} + \mathcal{B}(x_t - z_t) + az_t^{1/2}\cos\theta_t\left(\mathcal{A}\left[\frac{\alpha - x_t - \frac{1}{2}}{x_t}\right] - \mathcal{B}\right)\right]dt \\ &+ (2\mathcal{B}x_t)^{1/2}[a\cos\theta_t + z_t^{1/2}]dW_t^{(r)} - (2\mathcal{B}x_t)^{1/2}[a\sin\theta_t]dW_t^{(\theta)} \\ &+ \left(\frac{2\mathcal{A}}{x_t}\right)^{1/2}[az_t^{1/2}\cos\theta_t + z_t]dW_t^{(x)}. \end{aligned} \tag{4.11}$$

Likewise for the resultant phase we find

$$\begin{aligned} d\Theta_t = &\frac{az_t^{1/2}\sin\theta_t}{Z_t}\left\{\mathcal{A}\left[\left(\frac{2(\alpha - x_t) - 1}{4x_t}\right) - \frac{z_t^{1/2}}{2x_tZ_t}(z_t^{1/2} + a\cos\theta_t)\right] - \frac{1}{2}\mathcal{B}\right\}dt + \left(\frac{\mathcal{B}x_t}{2}\right)^{1/2}\frac{a\sin\theta_t}{Z_t}dW_t^{(r)} \\ &+ \left(\frac{\mathcal{B}x_t}{2}\right)^{1/2}\frac{z_t^{1/2} + a\cos\theta_t}{Z_t}dW_t^{(\theta)} + \left(\frac{\mathcal{A}z_t}{2x_t}\right)^{1/2}\frac{a\sin\theta_t}{Z_t}dW_t^{(x)}. \end{aligned} \tag{4.12}$$

Thus in terms of the resultants (Z,Θ) we deduce that the vector homodyned K-process (x_t, Z_t, Θ_t) has the following structure.

Proposition 4.2: The drift vector is given by

$$b^i = \begin{pmatrix} \mathcal{A}(\alpha - x) \\ \dfrac{\mathcal{A}}{x}\left[(\alpha - x)Z + a\left(x - \alpha - \dfrac{1}{2}\right)Z^{1/2}\cos\Theta + \dfrac{1}{2}a^2\right] + \mathcal{B}(x - Z + aZ^{1/2}\cos\Theta) \\ \dfrac{a\sin\Theta}{Z^{1/2}}\left\{\mathcal{A}\left[\left(\dfrac{2(\alpha - x) - 1}{4x}\right) - \dfrac{1}{2xZ^{1/2}}(Z^{1/2} - a\cos\Theta)\right] - \dfrac{1}{2}\mathcal{B}\right\} \end{pmatrix}. \tag{4.13}$$

The (symmetric) diffusion tensor is

$$\Sigma^{ij} = \begin{pmatrix} 2\mathcal{A}x & 2\mathcal{A}(Z - aZ^{1/2}\cos\Theta) & \dfrac{\mathcal{A}a\sin\Theta}{Z^{1/2}} \\ \cdots & 2Z\left[\dfrac{\mathcal{A}(Z^{1/2} - a\cos\Theta)^2}{x} + \mathcal{B}x\right] & (\mathcal{A}a\sin\Theta)(Z^{1/2} - a\cos\Theta)/x \\ \cdots & \cdots & \dfrac{1}{2Z}\left[\dfrac{\mathcal{A}a^2\sin^2\Theta}{x} + \mathcal{B}x\right] \end{pmatrix}. \tag{4.14}$$

C. Generalized *K*

The differential of the amplitude (3.5) contains both a K-scattering component and an explicit fluctuating part from the cross section, i.e., $d\Psi_t = a\,dx_t + d\psi_t$. This leads, in terms of the K-geometry, to the intensity SDE,

$$\begin{aligned} dZ_t = &\mathcal{A}\left[\frac{z_t(\alpha - x_t)}{x_t} + 2a^2x_t(\alpha - x_t + 1) + 3az_t^{1/2}\left(\alpha - x_t + \frac{1}{2}\right)\cos\theta_t\right]dt + \mathcal{B}(x_t - z_t - ax_tz_t^{1/2}\cos\theta_t)dt \\ &+ (2\mathcal{B}x_t)^{1/2}(z_t^{1/2} + ax_t\cos\theta_t)dW_t^{(r)} - (2\mathcal{B}x_t)^{1/2}ax_t\sin\theta_t\,dW_t^{(\theta)} \\ &+ (2\mathcal{A}x_t)^{1/2}\left(\frac{z_t}{x_t} + 2a^2x_t + 3az_t^{1/2}\cos\theta_t\right)dW_t^{(x)}. \end{aligned} \tag{4.15}$$

Likewise for the phase we find

$$\mathrm{d}\Theta_t = \frac{a z_t^{1/2}\sin\theta_t}{2Z_t}\left[\mathcal{A}\left(\frac{z_t + 2a^2x_t^2 + 3ax_t z_t^{1/2}\cos\theta_t}{Z_t} + x_t - \alpha - \frac{1}{2}\right) - \mathcal{B}x_t\right]\mathrm{d}t + \left(\frac{\mathcal{B}x_t}{2}\right)^{1/2}\frac{ax_t\sin\theta_t}{Z_t}\mathrm{d}W_t^{(r)}$$
$$+ \left(\frac{\mathcal{B}x_t}{2}\right)^{1/2}\frac{z_t^{1/2} + ax_t\cos\theta_t}{Z_t}\mathrm{d}W_t^{(\theta)} - \left(\frac{\mathcal{A}x_t z_t}{2}\right)^{1/2}\frac{a\sin\theta_t}{Z_t}\mathrm{d}W_t^{(x)}. \tag{4.16}$$

Combining these results we obtain the following.

Proposition 4.3: The vector generalized K-scattering process has drift

$$b^i = \begin{pmatrix} \mathcal{A}(\alpha - x) \\ \mathcal{A}\left[Z(\alpha/x - 1) + \frac{1}{2}a^2x + aZ^{1/2}\left(\alpha - x + \frac{3}{2}\right)\cos\Theta\right] + \mathcal{B}(x - Z + aZ^{1/2}x\cos\Theta) \\ a\sin\Theta\left\{\mathcal{A}\left[(Z^{1/2} + ax\cos\Theta)/Z^{1/2} - \left(\alpha - x + \frac{1}{2}\right)\right] - \mathcal{B}x\right\} \Big/ 2Z^{1/2} \end{pmatrix} \tag{4.17}$$

and (symmetric) diffusion tensor

$$\Sigma^{ij} = \begin{pmatrix} 2\mathcal{A}x & 2\mathcal{A}(Z + axZ^{1/2}\cos\Theta) & -\mathcal{A}ax\sin\Theta/Z^{1/2} \\ \cdots & 2\mathcal{A}(Z + axZ^{1/2}\cos\Theta)^2/x + 2\mathcal{B}xZ & -\mathcal{A}a(Z^{1/2} + ax\cos\Theta)\sin\Theta \\ \cdots & \cdots & (\mathcal{B} + \mathcal{A}a^2\sin^2\Theta)x/2Z \end{pmatrix}. \tag{4.18}$$

V. GEOMETRY OF AMPLITUDE FLUCTUATIONS

We begin with some purely geometrical results concerning the correlation structure in the amplitude fluctuations. Combining drift terms as quantities of $o(\mathrm{d}t^{1/2})$, we write the amplitude stochastic differential as

$$\mathrm{d}\Psi_t = iR_t\exp(i\Theta_t)\mathrm{d}\Theta_t + \exp(i\Theta_t)\mathrm{d}R_t + o(\mathrm{d}t^{1/2}) = \alpha_t\exp[i(\Theta_t + \phi_t)] + i\beta_t\exp[i(\Theta_t + \phi_t)] + o(\mathrm{d}t^{1/2}), \tag{5.1}$$

where α_t, β_t are real valued Ito differentials and ϕ_t is chosen so that their Ito product $\alpha_t\beta_t$ vanishes, i.e., the Wiener components of α_t, β_t are statistically independent (see, e.g., Karatzas and Shreve, 1988). Comparing the two decompositions of $\mathrm{d}\Psi_t$ above, it follows that [neglecting terms of $o(\mathrm{d}t^{1/2})$]

$$\alpha_t\cos\phi_t - \beta_t\sin\phi_t = dR_t,$$

$$\alpha_t\sin\phi_t + \beta_t\cos\phi_t = R_t\,\mathrm{d}\Theta_t. \tag{5.2}$$

Therefore

$$(\alpha_t^2 - \beta_t^2)\sin 2\phi_t = 2R_t\,\mathrm{d}R_t\,\mathrm{d}\Theta_t,$$

$$(\alpha_t^2 - \beta_t^2)\cos 2\phi_t = \mathrm{d}R_t^2 - R_t^2\mathrm{d}\Theta_t^2 \tag{5.3}$$

up to $o(\mathrm{d}t)$. From (4.1)

$$(\Sigma_t^{(\alpha)} - \Sigma_t^{(\beta)})\sin 2\phi_t = \frac{1}{2i}\left[\left(\frac{\Psi_t^*}{\Psi_t}\right)\Sigma_t^{(\Psi)} - \left(\frac{\Psi_t}{\Psi_t^*}\right)\Sigma_t^{(\Psi^*)}\right],$$

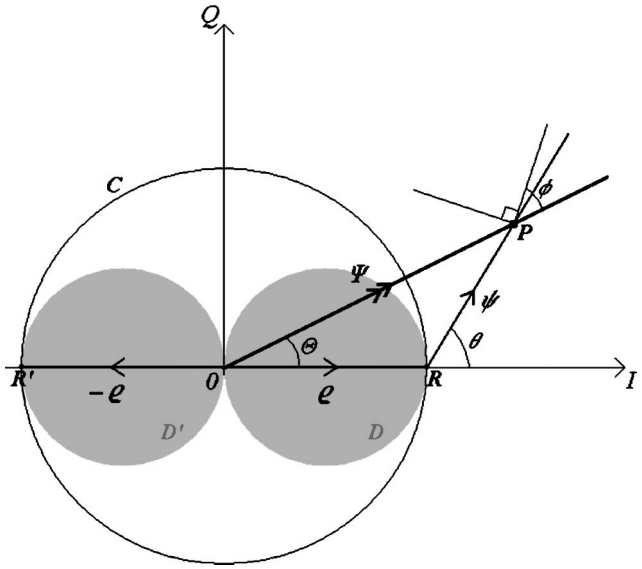

FIG. 1. Geometry of fluctuations for weak scattering processes depicting orthogonal dyad with respect to which resultant amplitude fluctuations decorrelate.

$$(\Sigma_t^{(\alpha)} - \Sigma_t^{(\beta)}) \cos 2\phi_t = \frac{1}{2}\left[\left(\frac{\Psi_t^*}{\Psi_t} \right) \Sigma_t^{(\Psi)} + \left(\frac{\Psi_t}{\Psi_t^*} \right) \Sigma_t^{(\Psi^*)} \right]. \tag{5.4}$$

Also, from (5.2) we find $\alpha_t^2 + \beta_t^2 = \mathrm{d}R_t^2 + R_t^2\, \mathrm{d}\Theta_t^2$ so that

$$\Sigma_t^{(\alpha)} + \Sigma_t^{(\beta)} = \Sigma_t^{(\Psi,\Psi^*)}. \tag{5.5}$$

We deduce from (5.3) that

$$\Sigma_t^{(\alpha)} - \Sigma_t^{(\beta)} = \pm \sqrt{\Sigma_t^{(\Psi)} \Sigma_t^{(\Psi^*)}} \tag{5.6}$$

which, combining with (5.5), yields the following result.

Lemma 5.1:

$$\Sigma_t^{(\alpha)} = \tfrac{1}{2}(\Sigma_t^{(\Psi,\Psi^*)} \pm \sqrt{\Sigma_t^{(\Psi)} \Sigma_t^{(\Psi^*)}}),$$

$$\Sigma_t^{(\beta)} = \tfrac{1}{2}(\Sigma_t^{(\Psi,\Psi^*)} \mp \sqrt{\Sigma_t^{(\Psi)} \Sigma_t^{(\Psi^*)}}). \tag{5.7}$$

with $\pm$ corresponding to the major/minor axes of the error surface of the resultant amplitude, respectively.

Observe that (5.6) and (5.7) have the appropriate symmetry under interchange $\alpha \leftrightarrow \beta$. The angle ϕ_t represents a rotation in the geometry of the resultant amplitude fluctuations relative to the case of pure K-scattering, for which $\phi = 0$. From (5.4) this angle is determined as follows.

Lemma 5.2: The phase rotation ϕ_t, that yields an orthogonal dyad (Fig. 1) associated with independent Wiener increments in the resultant amplitude process Ψ_t, satisfies the geometrical identity

$$\tan 2\phi_t = \frac{4Z_t \Sigma_t^{(Z,\Theta)}}{\Sigma_t^{(Z)} - 4Z_t^2 \Sigma_t^{(\Theta)}}. \tag{5.8}$$

Equivalently, in terms of the resultant complex amplitude process, we have the geometrical identity

$$\tan 2\phi_t = -\frac{\Im[\Psi_t^2\, \mathrm{d}\Psi_t^{*2}]}{\Re[\Psi_t^2\, \mathrm{d}\Psi_t^{*2}]}, \tag{5.9}$$

where $\Re$, $\Im$ *denote the real and imaginary parts, respectively*.

Before applying this geometry to the weak scattering processes described earlier, as a preliminary we give a result which provides the relationship between the structure of the diffusion tensor that arises in the cases of homodyned and generalized *K*-scattering.

Proposition 5.3: The transformation $a \mapsto -ax_t$ *maps the homodyned to the generalized K-scattering diffusion tensor of the vector scattering process* (x_t, Z_t, Θ_t).

Proof: Choose an arbitrary instant of time, labeled $t=0$. Define

$$\Psi_t^{(\mathrm{GK})} = ax_t + \psi_t,$$

$$\Psi_t^{(\mathrm{HK})} = -ax_0 + \psi_t', \tag{5.10}$$

for all $t \geqslant 0$, coincident at $t=0$. Thus $\psi_0' = 2ax_0 + \psi_0$ and otherwise ψ_t, ψ_t' are considered independent *K*-scattering processes. The result is equivalent to the corresponding (complex-valued) vector processes $(x_t, \Psi_t^{(\cdot)})$ having the same diffusion tensor, at the chosen instant. The amplitude components are best computed using the complex polarization, i.e.,

$$\Sigma^{i\,\bar{i}}\mathrm{d}t = \begin{pmatrix} \mathrm{d}\Psi_t^2 & \mathrm{d}\Psi_t\, \mathrm{d}\Psi_t^* \\ \cdots & \mathrm{d}\Psi_t^{*2} \end{pmatrix}. \tag{5.11}$$

The results of Corollary 2.5 and the above relation between ψ_t, ψ_t' at $t=0$ imply that $\mathrm{d}\Psi_0^{(\cdot)2}$ are identical. Likewise the expressions for $|\mathrm{d}\Psi_0^{(\cdot)}|^2$ coincide, by virtue of the cosine rule applied to $\Delta PRR'$ of Fig. 1. The same method shows that $\mathrm{d}x_t\, \mathrm{d}\Psi_t^{(\cdot)}$ are identical at the chosen instant. □

The image point R' has the physical interpretation of a fluctuating cancelling beam, π out of phase with the original $\varrho_t(R)$. A result corresponding to Proposition 5.3 does not hold for the vector scattering drift however, as evident from comparing Propositions 4.2 and 4.3.

A. Rice

The situation here is straightforward since the resultant amplitude dynamics is identical to that of Rayleigh scattering. Thus, as we have seen in Proposition 4.1, the cross term $\Sigma^{(Z,\Theta)}$ vanishes, so that $W_t^{(Z)}$, $W_t^{(\Theta)}$ are independent. The error surface $\mathcal{S}$ at P of Fig. 1 is circular, i.e., the amplitude fluctuations are isotropic and ϕ_t can take any value [both the numerator and denominator in (5.8) are identically zero].

B. Homodyned *K*

Using Lemma 5.2 and (4.14) we find

$$\tan\phi_t = \frac{a\sin\Theta_t}{Z_t^{1/2} - a\cos\Theta_t} \tag{5.12}$$

and minus its reciprocal for the perpendicular $\phi \mapsto \phi + \pi/2$. Thus, in terms of the geometry of Fig. 1 (e.g., by drawing a perpendicular from R to the line OP) we see that $\phi_t = \theta_t - \Theta_t$ $(\hat{OPR})$, i.e., the (major) axis of $\mathcal{S}^{\mathrm{HK}}$ coincides with that of the underlying *K*-scattering process, as anticipated from the differential of (3.3). The radial and angular components of the resultant amplitude fluctuations decorrelate [the diffusion coefficient $\Sigma^{(Z,\Theta)}$ of (4.14) vanishes] if the major/minor axis of the error ellipse of the *K*-amplitude fluctuations is aligned with the resultant amplitude (respectively, the first/second factor in $\Sigma^{(Z,\Theta)}$ vanishes). In the latter case P lies on the boundary ∂D and OP, PR are perpendicular. Inside the domain D the error surface $\mathcal{S}$ rotates (anticlockwise for P shown in the upper half plane in Fig. 1) and $\Sigma^{(Z,\Theta)} \lessgtr 0$ according as P lies in the upper/lower half-plane, while the opposite situation holds for the complement $\bar{D}$.

C. Generalized *K*

Perhaps the most interesting geometrical features emerge for generalized *K*-scattering. In this case the coherent offset (e.g., a fluctuating beam) $\varrho_t = ax_t$ has intrinsic fluctuations, arising from those in the scattering population (cf. in Fig. 1 the boundaries ∂D and $\partial D'$ fluctuate in time). Using Lemma 5.2, Proposition 5.3 and the homodyned result (5.12) it is immediate that, for generalized *K*-scattering,

$$\tan \phi_t = -\frac{ax_t \sin \Theta_t}{Z_t^{1/2} + ax_t \cos \Theta_t} \tag{5.13}$$

(and minus the reciprocal). The above tangent corresponds to an axis of $\mathcal{S}^{\mathrm{GK}}$ along $R'P$ (as seen, e.g., by drawing a perpendicular from R' to the continuation in Fig. 1 of OP). In contrast to homodyned *K*-scattering, the symmetry axes of the error surface $\mathcal{S}^{\mathrm{GK}}$ of the resultant amplitude are no longer aligned to those of the underlying *K*-amplitude. For alignment of the axes of $\mathcal{S}^{\mathrm{GK}}$ and $\mathcal{S}^{\mathrm{K}}$ to occur, we require the above tangent to coincide with $\tan \phi_0 = ax \sin \Theta/(Z^{1/2} - ax \cos \Theta)$, or minus the reciprocal, which occurs if $Z=0$ or $Z^{1/2}=ax$. In the latter case P lies on the circle C shown, consistently on which PR, PR' are perpendicular. The major axis of $\mathcal{S}^{\mathrm{GK}}$ at a general P can be identified by writing

$$d\Psi_t = (A_t + iB_t)\hat{z}_t + o(\mathrm{d}t^{1/2}), \tag{5.14}$$

where A_t, B_t are independent real-valued (Wiener components of) Ito differentials, and $\hat{z}_t = (\Psi_t + ax_t)/|\Psi_t + ax_t|$ corresponding to a unit vector in the axial direction $R'P$. Then we have the squared relation $\mathrm{d}\Psi_t^2 = (A_t^2 - B_t^2)\hat{z}_t^2$. Comparing with the expression for $\mathrm{d}\Psi_t^2$ derived from Corollary 2.5 and (3.5) we find

$$\Sigma_t^{(A)} - \Sigma_t^{(B)} = \frac{\mathcal{A}|\Psi_t + ax_t|^2}{2x_t}, \tag{5.15}$$

so $\Sigma_t^{(A)} \geqslant \Sigma_t^{(B)}$ with equality if and only if $\mathcal{A}=0$ or $\Psi_t + ax_t = 0$, i.e., $P=R'$. Strict inequality implies $R'P$ is the major axis of $\mathcal{S}^{\mathrm{GK}}$ with (circular) degeneracy otherwise. From the expression for $\Sigma_t^{(Z,\Theta)}$ in (4.18), decorrelation of the radial and angular components of Ψ_t occurs if P lies on the I axis or boundary $\partial D'$. In the latter case $R'P$ is the major axis of $\mathcal{S}^{\mathrm{GK}}$ and OP, PR' are perpendicular ($P \neq R'$). Inside D' in the upper/lower half-plane, $\Sigma^{(Z,\Theta)} \gtrless 0$ and $\mathcal{S}$ rotates with a corresponding orientation.

A measure of the total uncertainty ϵ_t in the resultant amplitude Ψ_t is provided by the eigenvalue product $\Sigma_t^{(\alpha)}\Sigma_t^{(\beta)} = \det[\Sigma_t^{ij}]$. For homodyned *K*-scattering, Corollary 2.5 and (5.7) imply

$$\Sigma_t^{(\alpha)} = \begin{cases} \dfrac{1}{2}\left(\dfrac{\mathcal{A}}{x_t}(\overbrace{Z_t - 2aZ_t^{1/2}\cos\Theta_t + a^2}^{z_t}) + \mathcal{B}x_t\right), \\ \dfrac{1}{2}\mathcal{B}x_t, \end{cases} \tag{5.16}$$

so that $\epsilon_t = \frac{1}{4}\mathcal{B}(\mathcal{A}z_t + \mathcal{B}x_t^2)$. Setting $\mathcal{A}=0$, $x_t=1$ for Rice and using Proposition 5.3 and (5.16) for generalized *K*-scattering we deduce the hierarchy of increasing uncertainties (in the sense of the proliferation of terms that arise)

$$\epsilon_t = \begin{cases} \frac{1}{4}\mathcal{B}^2 \quad (\mathrm{Rice}), \\ \frac{1}{4}\mathcal{B}(\mathcal{A}z_t + \mathcal{B}x_t^2) \quad (\mathrm{HK}), \\ \frac{1}{4}\mathcal{B}(\mathcal{A}z_t + \mathcal{B}x_t^2) + \mathcal{A}\mathcal{B}Z_t^{1/2}ax_t\cos\Theta_t \quad (\mathrm{GK}). \end{cases} \tag{5.17}$$

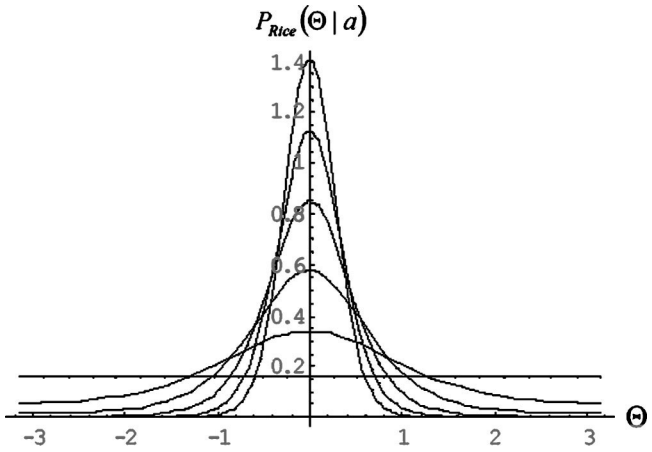

FIG. 2. Phase pdf for the Rice model, $a=0,\frac{1}{2},1,\frac{3}{2},2,\frac{5}{2}$.

We remark that these geometrical properties of the amplitude fluctuations should provide various means for anomaly detection, through the observability of the squared volatilities (cf. Field and Tough, 2003a) and their departure, for $a \neq 0$, from the pure K-scattering values.

VI. ASYMPTOTIC BEHAVIOR

The effect of the offset in the mean amplitude $\langle \Psi \rangle \neq 0$ for $a \neq 0$ is that the resulting (asymptotic) phase distributions are nonuniform. Expressions for these distributions can be calculated for the various processes we have described. We begin by deriving the joint asymptotic probability distribution functions (pdf) for the cross section, modulus amplitude and phase, and from these deduce the marginal pdf's of these quantities by integration.

A. Rice

Noting that ψ_t is a complex Gaussian process, we see that the familiar Rice process (Rice, 1954) emerges as the model for weak scattering. If we write the amplitude and phase of the scattered field as (E,Θ) their joint distribution takes the form

$$P(E,\Theta) = \frac{E \exp(-(E^2 + a^2 - 2Ea\cos\Theta))}{\pi}. \tag{6.1}$$

From this we can derive the familiar result for the marginal pdf of the field amplitude

$$P(E) = 2E \exp(-(E^2 + a^2)) I_0(2Ea), \tag{6.2}$$

where I_0 is the modified Bessel function of the first kind. The phase distribution associated with the Rice model can be obtained from (6.1) by integration over E. The result can be expressed in a reasonable closed form in terms of the error function,

$$\begin{aligned} P(\Theta|a) &= \int_0^\infty P(E,\Theta)\mathrm{d}E = \frac{\exp(-a^2\sin^2\Theta)}{\pi} \int_0^\infty E \exp(-(E - a\cos\Theta)^2)\mathrm{d}E \\ &= \frac{\exp(-a^2\sin^2\Theta)}{\pi} \int_{-a\cos\Theta}^\infty (E + a\cos\Theta)\exp(-E^2)\mathrm{d}E \\ &= \frac{1}{2\pi}\exp(-a^2) + \frac{a\cos\Theta}{2\sqrt{\pi}}(1 + \mathrm{erf}(a\cos\Theta))\exp(-a^2\sin^2\Theta). \end{aligned} \tag{6.3}$$

Figure 2 shows the behavior of this function, for differing values of a, whose square can be

interpreted as a signal to noise power ratio.

B. Homodyned *K*

In the case of the homodyned *K*-scattering process, which can be represented through (3.3), the joint pdf of the cross section, field amplitude and phase is

$$P(x,E,\Theta) = \frac{Eb^{\alpha}}{\pi\Gamma(\alpha)} x^{\alpha-2} \exp(-bx)\exp(-(E^2+a^2)/x) \exp(2Ea\cos\Theta/x). \tag{6.4}$$

The field amplitude pdf associated with the homodyned *K*-scattering model cannot be rendered in a simple closed form for general values of the shape parameter α. Its compound representation takes the form

$$P(E) = \frac{2Eb^{\alpha E}}{\Gamma(\alpha)} \int_0^{\infty} x^{\alpha-2} \exp(-bx) \exp(-(E^2+a^2)/x) I_0(2Ea/x)\mathrm{d}x. \tag{6.5}$$

The asymptotic phase distribution for the homodyned *K*-scattering model cannot be evaluated in closed form. The compound representation of the process indicates that the phase pdf can be written as

$$P(\Theta|a,b,\alpha) = \frac{b^{\alpha}}{\Gamma(\alpha)} \int_0^{\infty} P(\Theta|a,x) \exp(-bx) x^{\alpha-1}\,\mathrm{d}x, \tag{6.6}$$

where we define

$$P(\Theta|a,x) = \frac{1}{2\pi} \exp(-a^2/x) + \frac{a\cos\Theta}{2\sqrt{\pi x}}(1+\mathrm{erf}(a\cos\Theta/\sqrt{x})) \exp(-a^2\sin^2\Theta/x). \tag{6.7}$$

This can be recast in the form

$$\begin{aligned} P(\Theta|a,b,\alpha) = {} & \frac{(a^2b)^{\alpha/2}}{\pi\Gamma(\alpha)} K_{\alpha}(2\sqrt{ba^2}) + \frac{a\cos\Theta b^{(\alpha/2)-1/4}(a^2\sin^2\Theta)^{(\alpha/2)+1/4}}{\sqrt{\pi}\Gamma(\alpha)} K_{\alpha-1/2}(2\sqrt{ba^2\sin^2\Theta}) \\ & + 2\frac{a^{\alpha+1}b^{(\alpha+1)/2}\cos^2\Theta}{\pi\Gamma(\alpha)} \int_0^1 K_{\alpha-1}(2\sqrt{ba^2(\sin^2\Theta + t^2\cos^2\Theta)}) \\ & \times(\sin^2\Theta + t^2\cos^2\Theta)^{(\alpha-1)/2}\,\mathrm{d}t \end{aligned} \tag{6.8}$$

by using the integral representation of the error function

$$\mathrm{erf}(a\sqrt{x}\cos\Theta) = \frac{2a\sqrt{x}\cos\Theta}{\sqrt{\pi}} \int_0^1 \exp(-s^2a^2x\cos^2\Theta)\mathrm{d}s. \tag{6.9}$$

The representation (6.8) while a little arcane appears, when implemented in *Mathematica* (Wolfram, 1999), to be more stable and efficient than a direct numerical integration of (6.6). The corresponding plots of the phase pdf for the homodyned *K*-scattering model are shown in Figs. 3 and 4.

C. Generalized *K*

To generalize the weak scattering model to the non-Gaussian regime we allow the number of steps in the biased random walk to fluctuate according to (3.4). The joint distribution of the cross-section, field amplitude, and phase now takes the form

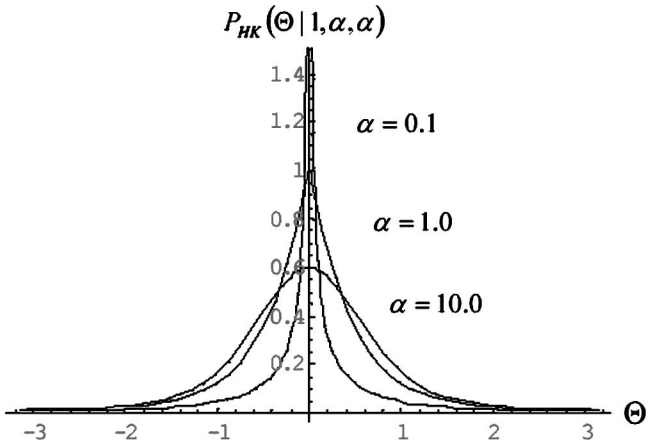

FIG. 3. Phase pdf's derived from the homodyned *K*-scattering model, $\alpha = 0.1, 1.0, 10.0$.

$$P(x,E,\Theta) = \frac{Eb^{\alpha}}{\pi\Gamma(\alpha)} x^{\alpha-2} \exp(-bx) \exp(-(E^2 + a^2x^2)/x) \exp(2Ea\cos\Theta). \tag{6.10}$$

(Here we have introduced the scale parameter b to relax the condition that the power in the complex Ornstein–Uhlenbeck process is taken as unity.) This provides us with the compound representation of the generalized *K*-scattering process in accordance with (2.7). This is to be contrasted with the corresponding result for the homodyned *K*-scattering process above. Thus by integration we have the field amplitude pdf given by

$$P(E) = \frac{4Eb^{\alpha}}{\Gamma(\alpha)(a^2+b)^{(\alpha-1)/2}} I_0(2Ea) K_{\alpha-1}(2E\sqrt{a^2+b}), \tag{6.11}$$

which is essentially the result obtained in Jakeman and Tough (1987) using the method of characteristic functions. The calculation of the asymptotic phase distribution for Rice scattering can be extended straightforwardly to the generalized and homodyned *K*-scattering models, essentially by exploiting the compound representation (2.7). Thus using (6.7) we construct

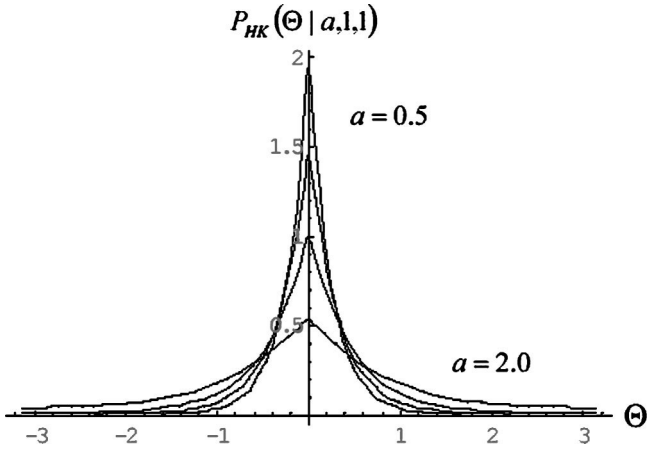

FIG. 4. Phase pdf's derived from the homodyned *K*-scattering model, $a = 0.5, 1.0, 1.5, 2.0$.

$$P(\Theta|a,b,\alpha) = \frac{b^\alpha}{\Gamma(\alpha)} \int_0^\infty P(\Theta|ax,x) \exp(-bx) x^{\alpha-1}\, dx. \tag{6.12}$$

This consists of three terms; two are straightforward while the third can be expressed in terms of a hypergeometric function. To this end we have

$$\begin{aligned} &\frac{b^\alpha}{\Gamma(\alpha)} \frac{1}{2\pi} \int_0^\infty x^{\alpha-1} \exp(-(b+a^2)x) dx = \frac{1}{2\pi} \left(\frac{b}{b+a^2} \right)^\alpha, \\ &\frac{b^\alpha}{\Gamma(\alpha)} \frac{1}{2\sqrt{\pi}} a \cos\Theta \int_0^\infty x^{\alpha-1/2} \exp(-(b+a^2 \sin^2\Theta)x) dx \\ &\quad = \frac{a\cos\Theta}{\sqrt{(b+a^2\sin^2\Theta)}} \frac{\Gamma(\alpha+1/2)}{2\Gamma(\alpha)\sqrt{\pi}} \frac{1}{(1+a^2\sin^2\Theta/b)^\alpha}. \end{aligned} \tag{6.13}$$

The third term can be evaluated by substituting (6.9) and integrating over x, thus

$$\begin{aligned} &\int_0^\infty \exp(-(a^2\sin^2\Theta + b)x) x^{\alpha-1} a\sqrt{x} \cos\Theta \operatorname{erf}(a\sqrt{x}\cos\Theta) dx \\ &\quad = \frac{2\Gamma(\alpha+1)}{\sqrt{\pi}} a^2 \cos^2\Theta \int_0^1 (b + a^2\sin^2\Theta + a^2 s^2 \cos^2\Theta)^{-(\alpha+1)}\, ds \\ &\quad = \frac{2\Gamma(\alpha+1)}{\sqrt{\pi}} \frac{a^2\cos^2\Theta}{(a^2\sin^2\Theta + b)^{\alpha+1}} {}_2F_1(1/2, \alpha+1; 3/2; -a^2\cos^2\Theta/(a^2\sin^2\Theta + b)). \end{aligned} \tag{6.14}$$

On bringing these results together we obtain

$$\begin{aligned} P(\Theta|a,b,\alpha) = {} & \frac{1}{2\pi} \left(\frac{b}{b+a^2} \right)^\alpha + \frac{a\cos\Theta}{\sqrt{(b+a^2\sin^2\Theta)}} \frac{\Gamma(\alpha+1/2)}{2\Gamma(\alpha)\sqrt{\pi}} \frac{1}{(1+a^2\sin^2\Theta/b)^\alpha} + \frac{\alpha}{\pi} \\ & \times \frac{a^2\cos^2\Theta}{(a^2\sin^2\Theta + b)} \frac{1}{(1+a^2\sin^2\Theta/b)^\alpha} {}_2F_1(1/2, \alpha+1; 3/2; -a^2\cos^2\Theta/(a^2\sin^2\Theta + b)). \end{aligned} \tag{6.15}$$

It is interesting to compare this result with that derived in an analysis of the performance of interferometric synthetic aperture radar [Eq. (53) in Tough, 1991], to which the above result reduces when the shape parameter α takes integer values. Figure 5 shows the phase pdf derived from the generalized K-scattering model. We have chosen $a=1$, $\langle x \rangle = 1$, and $\alpha = 0.1$, 1, 10. Spikier noise, associated with lower values of α, results in a broader distribution of phase. In Fig. 6 we show the variation in the phase distribution with the parameter a, keeping the mean noise power $\langle x \rangle = 1$ and $\alpha = 1$. The phase distribution becomes narrower as the parameter a increases. Comparison with Fig. 2 shows that, while the mean noise power is the same in each, the more spiky nature of the noise is manifest in a broader phase distribution.

The most marked difference between the phase pdf's derived from the homodyned and generalized K-scattering models is evident at small values of α (i.e., less than unity), where a singular behavior is observed at the origin. This can be seen quite clearly in Fig. 4. When α takes larger values a behavior more reminiscent of that seen in Fig. 2 emerges, as the noise becomes more Gaussian in character. In the case where $\alpha = 1$, the phase pdf displays a cusp at the origin, irrespective of the value of a; this can be seen in Fig. 4. The differences between the phase pdf's derived from the homodyned and generalized models can be understood qualitatively in terms of the signal fluctuating with x_t in the latter, but remaining constant in the former. Jakeman and Tough (1987) discuss the implications of this difference between the models in some detail, without making explicit reference to the asymptotic phase pdf's.

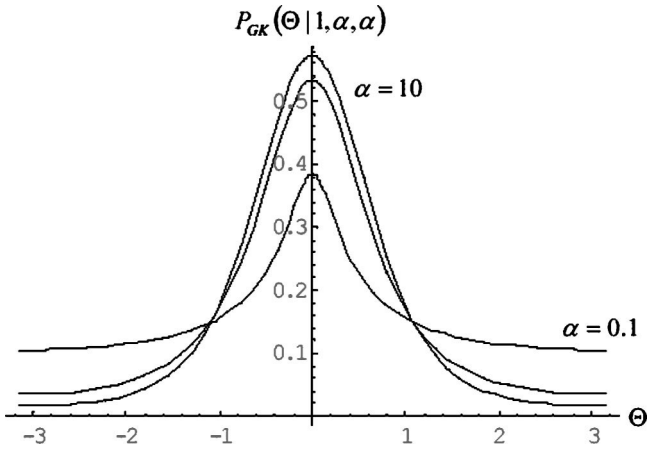

FIG. 5. Phase pdf's derived from the generalized *K*-scattering model, $\alpha = 0.1, 1.0, 10.0$.

D. Detailed balance

The detailed balance condition holds (asymptotically) for each of the weak scattering processes we have described. This result follows essentially from the condition being satisfied in the case of pure *K*-scattering, and the ways in which the weak scattering processes can be represented as functions of an underlying *K*-scattering process. To complete the analysis we shall need the following result.

Lemma 6.1: If a (complex valued/n-dimensional) Ito diffusion process x_t^i *satisfies detailed balance (at time t) then so does the transformed process* $\hat{x}_t^{\hat{i}} = \mathbf{f}(x_t^i)$*, i.e. (in contrast to the drift), if* x_t^i *has vanishing current then so does* $\hat{x}_t^{\hat{i}}$.

Proof: Applying Ito's formula to the components $\hat{x}^{\hat{i}}$ we find

$$b^{\hat{i}} = P_i^{\hat{i}} b^i + \tfrac{1}{2} P_{ij}^{\hat{i}} \Sigma^{ij}, \quad \Sigma^{\hat{i}\hat{j}} = P_i^{\hat{i}} P_j^{\hat{j}} \Sigma^{ij}, \tag{6.16}$$

where $P_i^{\hat{i}}$ denotes the transition matrix of partial derivatives $\partial \hat{x}^{\hat{i}} / \partial x^i$, with a corresponding notation for second derivatives. Attention should be paid to the nontensorial nature of the second term in the drift transformation, which is characteristic of the Ito calculus. The probability density transforms as $\hat{\rho} J = \rho$ where J is the Jacobian of P, i.e., $\varepsilon^{\hat{i}_1 \hat{i}_2 \cdots \hat{i}_n} J = \varepsilon^{i_1 i_2 \cdots i_n} P_{i_1}^{\hat{i}_1} P_{i_2}^{\hat{i}_2} \cdots P_{i_n}^{\hat{i}_n}$. Using the identity

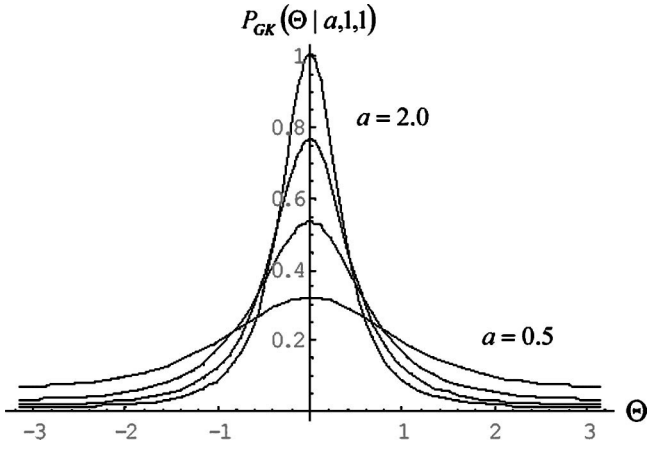

FIG. 6. Phase pdf's derived from the generalized *K*-scattering model, $a = 0.5, 1.0, 1.5, 2.0$.

$\partial_j \log J \equiv P^k_{\hat{j}} P^{\hat{j}}_{jk}$ and the relation (4.6) we deduce the current transformation $\hat{\mathcal{V}^i} = P^{\hat{i}}_i \mathcal{V}^i$, i.e., the current transforms as a vector. The equivalent holomorphic/antiholomorphic representation follows, via a complex change of coordinates. [Compare Field (2003) for an account of the geometrical structure of the transformations in drift and current involved here.] □

It is known that the *K*-scattering amplitude ψ_t (asymptotically) satisfies detailed balance, as evident from the compound representation (2.7) and the equilibrium condition (Field and Tough, 2003b). As a consequence of Lemma 6.1, the relations (3.2), (3.3), (3.5) and the independence of the processes x_t, γ_t we obtain the following result.

Corollary 6.2: The vector scattering processes (x_t, Z_t, Θ_t) *in cases (a)–(c) each satisfy the condition of detailed balance, asymptotically*.

Alternatively, detailed balance can be shown by explicit calculation using (4.6) and the expressions for the asymptotic distributions given above. In the presence of Doppler (Field and Tough, 2003b) detailed balance is no longer satisfied, and the current $\mathcal{V}$ amounts to a (rigid) rotation of the Argand Ψ-plane at a corresponding angular frequency.

VII. DISCUSSION

The *K*-distribution provides a useful model of the non-Gaussian statistics of strongly scattered radiation with a uniform distribution of phase. In recent work (Field and Tough, 2003a, 2003b) a description of the *K*-scattering process in terms of SDEs has been developed that makes direct contact with a simple underlying random walk model of scattering. In this paper we have extended this analysis to models of weak scattering, in which the distribution of phase is nonuniform.

The *K*-scattering process can be derived from an isotropic random walk with a fluctuating number of steps. To incorporate a nonuniform distribution of phase we consider a random walk on which a preferred direction or bias has been imposed. In the case where the random walk has a large, but fixed, number of steps the Rice process emerges as a model for weak scattering. We have analyzed the phase distribution associated with this model, and established the connection between its random walk formulation and a description in terms of SDEs.

The extension of the Rice model to the non-Gaussian regime is effected when we allow the number of steps in the biased random walk to fluctuate. We have shown how this leads to the generalized *K*-scattering process discussed in Jakeman and Tough (1987) and have made contact between this model and the homodyned *K*-scattering process. In each case we have characterized the associated distribution of phase in detail, and have developed a description in terms of SDEs and their equivalent Fokker–Planck equations. This complements the earlier dynamical description of *K*-scattering (Field and Tough, 2003a, 2003b).

The results have implications for detection schemes where the signal behavior (represented by the coherent offset in the resultant amplitude) can, to a reasonable extent, be modeled in the context of ambient *K*-distributed noise (cf. the results reported in Sec. IV of Field and Tough, 2003a). The results of Sec. V indicate a method for anomaly detection based on departures in the geometry of the resultant amplitude fluctuations from that expected in the pure *K*-scattering case. The results should find application in adaptive imaging problems, in the denoising of optical images (signal separation from noise, i.e., extraction of ϱ_t from Ψ_t) and anomaly detection in radar backscatter where a (coherent) reflection contribution is involved (cf. Jakeman and Tough, 1987).

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The generalized Stieltjes transform and its inverse

John H. Schwarz
California Institute of Technology, Pasadena, California 91125

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The generalized Stieltjes transform (GST) is an integral transform that depends on a parameter $\rho>0$. In previous work a convenient form of the inverse transformation was derived for the case $\rho=3/2$. This paper generalizes that result to all $\rho>0$. It is a well-known fact that the GST can be formulated as an iterated Laplace transform, and that therefore its inverse can be expressed as an iterated inverse Laplace transform. The form of the inverse transform derived here is a one-dimensional integral that is considerably simpler. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1825077]

I. INTRODUCTION

In Ref. 1 we encountered the integral equation

$$g(\zeta)=\int_0^\infty (\zeta^2+\mu^2)^{-3/2} f(\mu)\mathrm{d}\mu, \quad |\arg\zeta|<\pi/2, \tag{1}$$

where $g(\zeta)$ was a known function, and we needed to solve for $f(\mu)$. That paper proved that if g has suitable analyticity and asymptotic properties, which were satisfied for the specific function of interest, then

$$f(\mu)=-\frac{i\mu^2}{\pi}\int_0^\pi \cos\theta\, g(-i\mu\cos\theta)\mathrm{d}\theta. \tag{2}$$

This result is reviewed in Ref. 2.

By a change of variables, Eq. (2) can be rewritten in the form

$$f(\mu)=\frac{\mu}{\pi i}\int_{-i\mu}^{i\mu}\frac{\zeta}{\sqrt{\mu^2+\zeta^2}}g(\zeta)\mathrm{d}\zeta. \tag{3}$$

Then letting $y=\mu^2$ and $z=\zeta^2$, as well as $F(y)=(1/2\mu)f(\mu)$ and $G(z)=g(\zeta)$, we obtain

$$G(z)=\int_0^\infty (y+z)^{-3/2}F(y)\mathrm{d}y, \quad |\arg z|<\pi \tag{4}$$

and

$$F(y)=\frac{1}{4\pi i}\int_{\mathcal{C}_y}\frac{G(z)}{\sqrt{y+z}}\mathrm{d}z. \tag{5}$$

The contour $\mathcal{C}_y$ starts and ends at $-y$ and encloses the origin in the counterclockwise sense.

It is convenient to have a y-independent contour, so letting $z=wy$ we obtain

$$F(y) = \frac{1}{4\pi i}\sqrt{y}\int_{\mathcal{C}} \frac{G(yw)}{\sqrt{1+w}}\mathrm{d}w, \tag{6}$$

where $\mathcal{C}$ is a contour that starts and ends at the point $w=-1$ enclosing the origin in the counterclockwise sense. It could be chosen to be the unit circle, for instance. Note that it is not really a closed contour, since $G(z)$ has a branch cut running along the negative real axis. An integration by parts allows this to be rewritten in the form

$$F(y) = -\frac{1}{2\pi i}y^{3/2}\int_{\mathcal{C}} \sqrt{1+w}\,G'(yw)\mathrm{d}w. \tag{7}$$

In this paper, we will formulate and prove a one-parameter generalization of the preceding result. Specifically, we claim that the integral transform

$$G(z) = \int_0^\infty (y+z)^{-\rho}F(y)\mathrm{d}y, \quad |\arg z| < \pi \tag{8}$$

has as its inverse transform

$$F(y) = -\frac{1}{2\pi i}y^{\rho}\int_{\mathcal{C}} (1+w)^{\rho-1}G'(yw)\mathrm{d}w. \tag{9}$$

This integral converges for $\rho>0$. The special case discussed above corresponds to $\rho=3/2$. The counterpart of Eq. (6), obtained by integration by parts, namely

$$F(y) = \frac{1}{2\pi i}(\rho-1)y^{\rho-1}\int_{\mathcal{C}} (1+w)^{\rho-2}G(yw)\mathrm{d}w, \tag{10}$$

is less general, since it is only valid for $\rho>1$. This is allowed in the $\rho=3/2$ case, of course.

We should note for the record what is being assumed about F and G. Specifically, $F(y)$, which is only defined on the positive real axis, is allowed to be an arbitrary distribution (or "generalized function"). We require that there exists a number α with $0<\alpha<\rho$ such that $\left|\int_{y_1}^{y_2} y^{\alpha-\rho}F(y)\,\mathrm{d}y\right|$ is bounded by a number independent of y_1 and y_2 for all $0<y_1<y_2$. The function $G(z)$ is then holomorphic throughout the cut plane $|\arg z|<\pi$, and there exists a positive real number β such that $|z^{\beta}G(z)|$ is bounded at infinity.

The $\rho=1$ case of Eq. (8), known as the Stieltjes transform, is discussed in Widder's classic treatise on the Laplace transform.[3] The only other cases considered by Widder are positive integer values of ρ, which are related to the $\rho=1$ case by differentiation. Following Ref. 4, we refer to the case of arbitrary ρ as the generalized Stieltjes transform (GST). (In Ref. 5 it is called a Stieltjes transform of index ρ.) The formula for the inverse GST in Eq. (9) does not seem to have been found previously. Certainly, it does not appear in Refs. 3–5 or 6.

Much of the literature on the GST is concerned with the asymptotic behavior of $G(z)$ for large $|z|$.[7] We will not address that topic here. As it happens, in Ref. 1 we were interested in deducing the asymptotic behavior of F associated with a given G.

In the special case $\rho=1$ the transform in Eq. (8) reduces to the Stieltjes transform

$$G(z) = S_z[F] = \int_0^\infty \frac{F(y)}{y+z}\mathrm{d}y. \tag{11}$$

Since the Stieltjes transform is well understood, this case provides an instructive test of the proposed inverse transform. Setting $\rho=1$ in Eq. (9) gives an expression that can be integrated explicitly to give

$$F(y) = \lim_{\epsilon \to 0^+} \frac{1}{2\pi i} \big(G(-y - i\epsilon) - G(-y + i\epsilon) \big). \tag{12}$$

Given the stated analytic and asymptotic properties of $G(z)$, it is a simple consequence of Cauchy's theorem that this is the correct solution of Eq. (11) for $y > 0$.

In order to convince oneself that Eqs. (8) and (9) are plausible for all $\rho > 0$, it is instructive to consider a simple example. Specifically, if one chooses

$$F(y) = y^{\nu - 1}, \tag{13}$$

then the integral in Eq. (8) converges for $0 < \nu < \rho$ and gives

$$G(z) = z^{\nu - \rho} B(\nu, \rho - \nu), \tag{14}$$

where $B(u,v)$ is the Euler beta function. It is straightforward to verify that this pair of functions also satisfies Eq. (9).

II. OTHER VERSIONS OF THE INVERSE TRANSFORM

The change of variables $z = wy$ allows us to rewrite Eq. (9) in the alternative form

$$F(y) = -\frac{1}{2\pi i} \int_{\mathcal{C}_y} (y + z)^{\rho - 1} G'(z) \mathrm{d}z. \tag{15}$$

As before, the contour $\mathcal{C}_y$ starts and ends at the point $z = -y$, encircling the origin in the counterclockwise sense. If $\rho > 1$, an integration by parts brings Eq. (15) to the form

$$F(y) = \frac{1}{2\pi i} (\rho - 1) \int_{\mathcal{C}_y} (y + z)^{\rho - 2} G(z) \mathrm{d}z. \tag{16}$$

Since this is only well-defined for $\rho > 1$, Eqs. (9) and (15) are more general than Eq. (16).

Let us define the quantity that appears on the right-hand side of Eq. (12) to be

$$\Delta(t) = \frac{1}{2\pi i} \lim_{\epsilon \to 0^+} \big(G(-t - i\epsilon) - G(-t + i\epsilon) \big), \quad t > 0. \tag{17}$$

We showed that $F(y) = \Delta(y)$ when $\rho = 1$, but this is not the case for other values of ρ. By shrinking the contour $\mathcal{C}_y$ down to the cut, Eq. (16) takes the form

$$F(y) = (\rho - 1) \int_0^y (y - t)^{\rho - 2} \Delta(t) \mathrm{d}t. \tag{18}$$

In similar fashion, Eq. (15) gives rise to

$$F(y) = \int_0^y (y - t)^{\rho - 1} \Delta'(t) \mathrm{d}t. \tag{19}$$

However, these formulas are only correct if the behavior of $G(t)$ near the origin is such that these integrals exist. The contour integral versions of these formulas are more general, since they do not have this restriction.

Equations (18) and (19) have the structure of Abel transforms. The inverse Abel transform is well known and can be used to give a formula for the discontinuity across the cut, $\Delta(t)$, in terms of the original (generalized) function $F(y)$. A version that is suitable if $\rho < 2$ and $F(0) = 0$ is

$$\Delta(t) = \frac{\sin \pi\rho}{\pi(1-\rho)} \int_0^t (t-y)^{1-\rho} F'(y) \mathrm{d}y. \tag{20}$$

This gives the known result for $\rho=1$, namely $\Delta(t)=F(t)$. It can be checked for the simple example $F(y)=y^{\nu-1}$ discussed earlier.

III. PROOF OF THE MAIN RESULT

Let us review how the GST is related to the Laplace transform, for which we use the following notation:

$$\mathcal{L}_x[F] = \int_0^\infty e^{-xy} F(y) \mathrm{d}y. \tag{21}$$

Inserting the identity

$$(y+z)^{-\rho} = \frac{1}{\Gamma(\rho)} \int_0^\infty x^{\rho-1} e^{-x(y+z)}\, \mathrm{d}x \tag{22}$$

into Eq. (8) gives

$$G(z) = \frac{1}{\Gamma(\rho)} \int_0^\infty x^{\rho-1} e^{-xz} \mathcal{L}_x[F] \mathrm{d}x = \frac{1}{\Gamma(\rho)} \mathcal{L}_z[x^{\rho-1} \mathcal{L}_x[F]]. \tag{23}$$

This recasts Eq. (8) as a Laplace transform of a Laplace transform. In particular, setting $\rho=1$, this gives the well-known result that the Stieltjes transform is the square (in the operator sense) of the Laplace transform, i.e., $\mathcal{S}=\mathcal{L}^2$.

Equation (23) implies that

$$\mathcal{L}_x[F] = \Gamma(\rho) x^{1-\rho} \mathcal{L}_x^{-1}[G], \tag{24}$$

where $\mathcal{L}^{-1}$ denotes an inverse Laplace transform. A second inverse Laplace transform gives the formal inversion of Eq. (23),

$$F(y) = \Gamma(\rho) \mathcal{L}_y^{-1}[x^{1-\rho} \mathcal{L}_x^{-1}[G]]. \tag{25}$$

This can be made very explicit by using the standard contour integral realization of the inverse Laplace transformation.[5] The new claim is that Eq. (25) can be simplified to take the form of Eq. (9).

Let us now carry out some similar manipulations of Eq. (9). Substituting

$$G'(yw) = -\int_0^\infty \mathrm{d}t\, e^{-tyw} t \mathcal{L}_t^{-1}[G] \tag{26}$$

into Eq. (9) and taking the Laplace transform of both sides recasts Eq. (9) in the form

$$\mathcal{L}_x[F] = \Gamma(\rho+1) \frac{1}{2\pi i} \int_{\mathcal{C}} \mathrm{d}w (1+w)^{\rho-1} \int_0^\infty \mathrm{d}t (x+tw)^{-\rho-1} t \mathcal{L}_t^{-1}[G]. \tag{27}$$

Comparing Eqs. (24) and (27), we see that their equivalence requires the identity

$$\frac{t\rho}{2\pi i} \int_{\mathcal{C}} \mathrm{d}w (1+w)^{\rho-1} (x+tw)^{-\rho-1} = x^{-1-\rho} \delta(x-t), \tag{28}$$

or equivalently

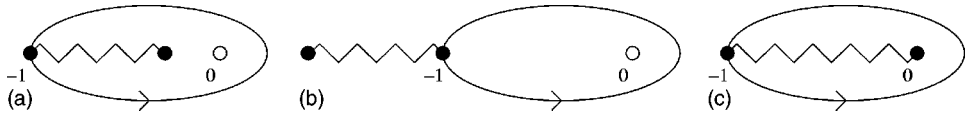

FIG. 1. The contour $\mathcal{C}$ starts and ends at the point $w=-1$ enclosing the origin in the counterclockwise sense. Three possible branch cut configurations are depicted.

$$\frac{\rho}{2\pi i}\int_{\mathcal{C}} \mathrm{d}w(1+w)^{\rho-1}(x+tw)^{-\rho-1} = x^{-\rho}\delta(x-t). \tag{29}$$

Another way of understanding the necessity of Eq. (29) is to consider the special case $F(y) = \delta(y-t)$. In this case the GST is $G(z)=(t+z)^{-\rho}$. The inverse transform Eq. (9) for this choice of $G(z)$ corresponds precisely to Eq. (29). This remarkable equation, which is required to hold for x, $t>0$, is the heart of the matter. Its proof, which is rather nontrivial, is presented in the next section.

IV. REPRESENTATION OF A DELTA FUNCTION

This section proves the key formula, namely Eq. (29). Consider the left-hand side of Eq. (29),

$$\chi_\rho(x,t) = \frac{\rho}{2\pi i}\int_{\mathcal{C}} \mathrm{d}w(1+w)^{\rho-1}(x+tw)^{-\rho-1}, \tag{30}$$

where $x,t>0$ and $\mathcal{C}$ is the contour shown in Fig. 1. By making the change of variables $w\to 1/w$, it is easy to prove that $\chi_\rho(x,t)=\chi_\rho(t,x)$. For $t>x$ the singularity structure is shown in Fig. 1(a), and the contour can be pushed off to infinity, giving zero for the integral. For $t<x$, the contour encloses no singularity [see Fig. 1(b)], so the result is again zero, as required by $x\leftrightarrow t$ symmetry.

Since $\chi_\rho(x,t)$ vanishes for $t\neq x$, it must be some sort of distribution concentrated at $t=x$. If we assume that it is proportional to a delta function, i.e., $f(x)\delta(x-t)$, it is easy to derive $f(x)$. Integrating over t from 0 to y, gives

$$f(x)\theta(y-x) = \frac{1}{2\pi i}\int_{\mathcal{C}} \frac{\mathrm{d}w}{w}(1+w)^{\rho-1}\left[x^{-\rho}-(x+yw)^{-\rho}\right]. \tag{31}$$

The first term on the right-hand side is an elementary contour integral and gives $x^{-\rho}$. The second term is also easily evaluated by Cauchy's theorem. It gives $-x^{-\rho}$ if $x>y$ and zero if $y>x$. Thus we deduce that $f(x)=x^{-\rho}$, and hence

$$\chi_\rho(x,t) = x^{-\rho}\delta(x-t) = t^{-\rho}\delta(x-t). \tag{32}$$

Equation (32) is the correct result, but the derivation given above is not rigorous. It assumes that the distribution is proportional to a delta function, and that it does not involve any derivatives of delta functions. A more careful analysis that is sensitive to such terms if they are present involves checking the proposed answer by integrating both sides against the test function e^{-ty}, i.e., comparing the Laplace transform of both sides of the equation. Thus we need to show that

$$\int_0^\infty \mathrm{d}t\,\chi_\rho(x,t)e^{-ty} = x^{-\rho}e^{-xy}. \tag{33}$$

Evaluating the Laplace transform of Eq. (30) gives (after some simple manipulations)

$$\int_0^\infty \mathrm{d}t\,\chi_\rho(x,t)e^{-ty} = \frac{\rho}{2\pi i}y^\rho\int_{\mathcal{C}} \mathrm{d}w(1+w)^{\rho-1}I(xyw), \tag{34}$$

where

$$I(u) = e^u \int_u^\infty e^{-v} v^{-\rho-1}\, \mathrm{d}v. \tag{35}$$

In order to re-express this function in a more convenient form, we first note that

$$I'(u) = I(u) - u^{-\rho-1}. \tag{36}$$

Let us now assume that ρ is not an integer, which is the case of most interest. This equation is then solved by an expression of the form

$$I(u) = I_1(u) + u^{-\rho} I_2(u), \tag{37}$$

where $I_1(u)$ and $I_2(u)$ are regular at $u=0$. The first term is $I_1(u)=\Gamma(-\rho)e^u$. Its contribution to Eq. (34) is zero, since there is no singularity inside the contour. The function that matters is I_2, which satisfies the differential equation

$$uI_2'(u) - (u+\rho)I_2(u) + 1 = 0. \tag{38}$$

Substituting a power series expansion,

$$I_2(u) = \sum_{n=0}^{\infty} c_n u^n, \tag{39}$$

one obtains the recursion relation $(n+1-\rho)c_{n+1}=c_n$. Thus, since $c_0=I_2(0)=1/\rho$, we conclude that

$$c_n = \frac{\Gamma(1-\rho)}{\rho\Gamma(n+1-\rho)}. \tag{40}$$

To determine the contribution of each term in Eq. (39) to Eq. (34), we need to evaluate

$$\frac{1}{2\pi i}\int_{\mathcal{C}} \mathrm{d}w(1+w)^{\rho-1} w^{n-\rho} = -\frac{\sin\,\pi(n-\rho)}{\pi} B(n-\rho+1,\rho) = \frac{(-1)^n}{\rho c_n n!}. \tag{41}$$

Combining these results, the c_n factors cancel, and we learn that

$$\int_0^\infty \mathrm{d}t\, \chi_\rho(x,t) e^{-ty} = x^{-\rho} \sum_{n=0}^{\infty} \frac{(-xy)^n}{n!} = x^{-\rho} e^{-xy}, \tag{42}$$

which is the result we set out to prove. Even though this derivation needs to be modified when ρ is a positive integer, the result clearly is valid in that case as well. This completes the proof of Eq. (33) and hence of the inverse transform Eq. (9).

The derivation of Eq. (32) (and hence of the inverse GST) can be simplified considerably by using the alternative representation of the inversion formula presented in Eq. (19) together with well-known properties of hypergeometric functions. Specifically, using

$$I(z,\rho,\rho') = \int_{-1}^{0} \mathrm{d}w(1+w)^{\rho-1}(1+zw)^{-p'} = \frac{1}{\rho}(1-z)^{\rho-\rho'}{}_2F_1(\rho,\rho-\rho'+1;\rho+1;z) \tag{43}$$

one can show that

$$\chi_\rho(x,t) = \frac{1}{2\pi i}\rho x^{-\rho-1} \lim_{\epsilon\to 0+}\left[I\left(\rho,\rho+1,\frac{t}{x}+i\epsilon\right) - I\left(\rho,\rho+1,\frac{t}{x}-i\epsilon\right)\right] = \frac{1}{\pi}x^{-\rho}\lim\frac{\epsilon t}{(x-t)^2+(\epsilon t)^2}$$
$$= x^{-\rho}\delta(x-t). \tag{44}$$

The restriction on the behavior of $G(z)$ at the origin mentioned previously can be circumvented by introducing a modified function $G_\delta(z)=G(z+\delta)$, $\delta>0$, and letting $\delta\to 0$ in the final result. The

advantage of this approach is that it is applicable to a wider class of distributions on the real line, namely those that can be written as the difference of the limiting values on the real axis from above and below of two functions, holomorphic in the upper and lower half-plane, respectively.[8,9]

V. AN ALTERNATIVE DERIVATION

In this section we present a simpler, though less general, derivation of the inverse transform. It follows from Cauchy's theorem and the required analytic and asymptotic properties of $G(z)$ that

$$G(z) = \int_0^\infty \frac{\Delta(t)}{z+t} \mathrm{d}t, \tag{45}$$

where $\Delta(t)$ is defined in Eq. (17). The validity of this formula requires that $\Delta(t)$ is not too singular as $t \to 0$, so that the integral exists. This is a significant restriction, since if $F \sim y^{\nu-1}$ with $\nu > 0$ for small y, then $G(z) \sim z^{\nu-\rho}$ for small z. Thus one would need that $\rho < \nu + 1$. No such assumption has been made previously, which is why the derivation in this section is less general.

Equation (45) is precisely a Stieltjes transform, $G = \mathcal{S}[\Delta]$. We noted earlier that this is an iterated Laplace transform, $\mathcal{S} = \mathcal{L}^2$. Therefore,

$$\mathcal{L}_x^{-1}[G] = \mathcal{L}_x[\Delta]. \tag{46}$$

Comparing this with Eq. (24), which we obtained from Eq. (8), we learn that

$$\mathcal{L}_x[F] = \Gamma(\rho) x^{1-\rho} \mathcal{L}_x[\Delta]. \tag{47}$$

Now using $\mathcal{L}_x[t^{\nu-1}] = \Gamma(\nu)\, x^{-\nu}$, this becomes

$$\mathcal{L}_x[F] = (\rho - 1)\mathcal{L}_x[t^{\rho-2}]\mathcal{L}_x[\Delta]. \tag{48}$$

By the convolution theorem, this implies that

$$F(y) = (\rho - 1) \int_0^y (y-t)^{\rho-2} \Delta(t) \mathrm{d}t, \tag{49}$$

which is Eq. (18). The alternative form in Eq. (19) extends the range of validity for ρ, but is even more restricted in its requirements for the behavior of $\Delta(t)$ at the origin. As we pointed out in Sec. II, there is no such issue for the corresponding contour integrals.

VI. CONCLUSION

In this paper we considered the generalized Stieltjes transform

$$G(z) = \int_0^\infty (y+z)^{-\rho} F(y) \mathrm{d}y, \quad |\arg z| < \pi \tag{50}$$

for $\rho > 0$ and proved that it has as its inverse transform

$$F(y) = -\frac{1}{2\pi i} y^\rho \int_{\mathcal{C}} (1+w)^{\rho-1} G'(yw) \mathrm{d}w. \tag{51}$$

The integration contour is described in the text.

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Nonlinear dissipative eigenvalue problems with large initial conditions

Vassilis G. Papanicolaou[a)]
Department of Mathematics, National Technical University of Athens, Zografou Campus, 157 80, Athens, Greece

Paul K. Newton[b)]
Department of Aerospace Engineering and Center for Applied Mathematical Sciences, University of Southern California, Los Angeles, California 90089-1191

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We consider the initial value problem $u''+\phi(t)u'+B^2u^{2p+1}=0,\ t>0,\ u(0)=\gamma,$ $u'(0)=0$, where p is a positive integer, $B,\ \gamma$ are positive parameters, and $\phi(t)$ is a positive function. The differential equation describes a (dissipative) oscillatory system whose amplitude $A(t)$ decreases in time. For a given time $b>0$, our task is to compute the asymptotics of $A(b)$, as $\gamma\to\infty$. In the case where $\phi\in C^1(0,\infty)\cap L_1(0,\varepsilon)$, we give an explicit answer. We also discuss the case where $\phi(t)=2/t$. This case is of particular interest since it is related to the nonlinear Schrödinger equation in three dimensions. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1829154]

I. INTRODUCTION

Before introducing our main problem, let us first consider the system

$$u''(t)+B^2u(t)^{2p+1}=0,\quad t>0, \tag{1.1}$$

$$u(0)=\gamma,\quad u'(0)=0, \tag{1.2}$$

where $p\geqslant 1$ is an integer, and $B,\ \gamma>0$. This is a Hamiltonian system since we have conservation of energy, namely

$$E(t)\overset{\text{def}}{=}u(t)^{2p+2}+\frac{p+1}{B^2}u'(t)^2=\gamma^{2p+2}. \tag{1.3}$$

Hence $u(t)$ oscillates with constant amplitude γ. From (1.3) we get that the period T of oscillation is (notice that $u(T/4)=u(3T/4)=0$ and $u(T/2)=-\gamma$)

$$T=T(\gamma)=\frac{c_p}{B}\frac{1}{\gamma^p}, \tag{1.4}$$

where

[a)]Electronic mail: papanico@math.ntua.gr
[b)]Electronic mail: newton@spock.usc.edu

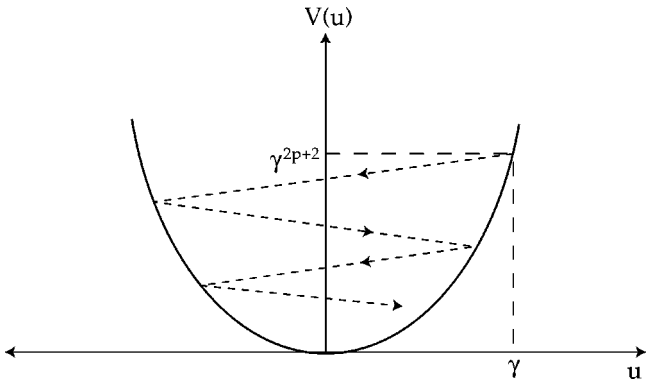

FIG. 1. Energy decay in a single well potential.

$$c_p = 4\sqrt{p+1}\int_0^1 \frac{\mathrm{d}x}{\sqrt{1-x^{2p+2}}} = \frac{2\sqrt{\pi}}{\sqrt{(p+1)}}\frac{\Gamma\left(\frac{1}{2p+2}\right)}{\Gamma\left(\frac{p+2}{2p+2}\right)} \tag{1.5}$$

($\Gamma(\cdot)$ is, of course, the Gamma function). We see that T depends on γ, in contrast to the linear case $p=0$, where $T=2\pi/B$. Here we are interested in

$$u'' + \phi(t)u' + B^2u^{2p+1} = 0, \tag{1.6}$$

where

$$\phi(t) \geqslant 0.$$

Problems of this general type arise when asking about the long time effects of dissipation on Hamiltonian systems. Radially symmetric standing wave solutions to the nonlinear Schrödinger equation arising from hydrodynamic stability theory fall in this category after the time-oscillations are factored out and one is left with a spatial eigenvalue problem with a nonconstant coefficient. In this case, the radial variable plays the role of time. Now (1.3) becomes

$$E(t) = u(t)^{2p+2} + \frac{p+1}{B^2}u'(t)^2 = \gamma^{2p+2} - \frac{2(p+1)}{B^2}\int_0^t \phi(s)u'(s)^2\mathrm{d}s, \tag{1.7}$$

which, of course, implies loss of energy. In fact, one can define the amplitude of oscillation as

$$A(t) = E(t)^{1/(2p+2)}, \tag{1.8}$$

so that we can say that Eq. (1.6) describes an oscillatory system with decreasing amplitude $A(t)$, as shown in Fig. 1 for a symmetric single well potential of the type considered in this paper. Assuming the initial conditions (1.2) (in the sense that $u(0+)=\gamma$, $u'(0+)=0$, since $\phi(t)$ may not be defined at $t=0$), we have

$$E(0) = \gamma^{2p+2}, \quad A(0) = \gamma. \tag{1.9}$$

If $0=t_0'<t_1'<t_2'<\cdots$ are the (positive) zeros of $u'(t)$, then

$$A(t_n') = |u(t_n')| = (-1)^n u(t_n').$$

From the analysis done in the authors' earlier work,[1] it follows that, if N is a fixed integer, then, as $\gamma\to\infty$,

$$|t_n' - nT(\gamma)/2| < C\gamma^{-2p}, \quad n = 0,1,2,\ldots,N, \tag{1.10}$$

where $C>0$ is a constant and $T(\gamma)$ is the period of the conservative case, as given in (1.4) and (1.5). Hence, for a fixed $n \geqslant 0$,

$$t_{n+1}' - t_n' = \frac{c_p}{2B}\frac{1}{\gamma^p} + O(\gamma^{-2p}) \quad \text{as } \gamma \to \infty. \tag{1.11}$$

The problem considered in this article can now be stated. For the system (1.6) and (1.2), if $b>0$ is a given time, determine the (leading) asymptotic behavior of $A(b)$, as $\gamma \to \infty$. In Sec. II we assume that $\phi \in C^1(0,\infty) \cap L_1(0,\varepsilon)$, for $\varepsilon > 0$ (i.e., ϕ is locally integrable), and we show that

$$A(b) = \gamma \exp\left[-\frac{1}{p+2}\int_0^b \phi(t)\mathrm{d}t \right] + o(\gamma) \quad \text{as } \gamma \to \infty.$$

In Sec. III we examine the case of a nonintegrable $\phi(t)$, namely

$$\phi(t) = \frac{2}{t}.$$

Here the formula of Sec. II reduces to $A(b)=o(\gamma)$, as $\gamma \to \infty$. Hence one expects that the analysis of this case, in order to determine the exact asymptotics of $A(b)$, is more challenging than the one needed in Sec. II. Furthermore this case has a particular interest since it is related to the radial nonlinear Schrödinger equation. The results presented in this section are based on the Wentzel–Kramer–Brillouin (WKB) approximation.[2]

II. THE CASE OF A LOCALLY INTEGRABLE $\phi(t)$

As already mentioned, in this section we consider the initial value problem

$$u'' + \phi(t)u' + B^2u^{2p+1} = 0, \quad t > 0, \tag{2.1}$$

$$u(0) = \gamma, \quad u'(0) = 0, \tag{2.2}$$

where $p \geqslant 1$ is an integer, $B>0$, and $\phi(t) \geqslant 0$ is continuously differentiable in $(0, \infty)$ and locally integrable, i.e., integrable near 0. Notice that the (global) existence and uniqueness of $u(t)$ follows easily from (1.7) (see, e.g., Ref. 3).

Differentiating the two sides of the first equation of (1.7) and using (2.1) we obtain

$$E'(t) = \frac{2(p+1)}{B^2}(u'u'' + B^2u^{2p+1}u') = -\frac{2(p+1)}{B^2}\phi(t)(u')^2, \tag{2.3}$$

hence

$$E'(t) \geqslant -\frac{2(p+1)}{B^2}\phi(t)(u')^2 - 2\phi(t)u^{2p+2} = -2\phi(t)E(t),$$

or

$$E'(t) + 2\phi(t)E(t) \geqslant 0.$$

Thus

$$\frac{\mathrm{d}}{\mathrm{d}t}[e^{2\Phi(t)}E(t)] \geqslant 0,$$

where

$$\Phi(t) = \int_0^t \phi(\tau)\mathrm{d}\tau, \tag{2.4}$$

and therefore by integrating and using (1.9)

$$E(t) \geqslant \gamma^{2p+2} e^{-2\Phi(t)}, \tag{2.5}$$

which in view of (1.8) can be also written as

$$A(t) \geqslant \gamma e^{-\Phi(t)/(p+1)} \tag{2.6}$$

(independently of B).

We are now ready for the main result:

Theorem 1: *For the initial value problem (2.1) and (2.2) we have*

$$A(b) = \gamma e^{-\Phi(b)/(p+2)} + o(\gamma) \quad \text{as } \gamma \to \infty, \tag{2.7}$$

where $b>0$ is a fixed number, $A(t)$ is defined in (1.7) and (1.8), and $\Phi(t)$ is defined in (2.4).

Proof: Let $0=t_0'<t_1'<t_2'<\cdots$ be the (positive) zeros of $u'(t)$. For any $\gamma>0$ there is an $n=n(\gamma)\geqslant 0$ such that

$$t_{2n}' \leqslant b < t_{2n+2}',$$

where $t_{2n+2}'\leqslant\infty$ (here the convention is that if t_{2n}' or t_{2n+1}', then we set $t_{2n+2}'=\infty$). If γ is sufficiently large, it follows from (1.10) that $t_{2n+2}'<\infty$. We set

$$b^* = t_{2n}' \tag{2.8}$$

(b^* depends on γ and b; in particular $b^*\leqslant b$). Thus $u(b^*)$ is a local maximum of $u(t)$ and

$$u(b^*) = A(b^*).$$

For the sake of completeness we set $0^*=0$. Notice that (1.11) implies that, as $\gamma\to\infty$,

$$b - b^* = O(\gamma^{-p}), \tag{2.9}$$

which, in turn gives (see (1.7), (1.8), and (2.3))

$$A(b) - A(b^*) = O(\gamma^{1-p}). \tag{2.10}$$

Formula (2.6) suggests that we should look at the limit

$$\lim_{\gamma\to\infty} \frac{u(b^*)}{\gamma}.$$

But, since we do not even know whether this limit exists or not, we start with the upper and lower limits

$$\lambda_{\max}(b) = \limsup_{\gamma\to\infty} \frac{u(b^*)}{\gamma}, \quad \lambda_{\min}(b) = \liminf_{\gamma\to\infty} \frac{u(b^*)}{\gamma}.$$

Of course (since $0^*=0$),

$$\lambda_{\max}(0) = \lambda_{\min}(0) = 1$$

and, furthermore, since $b_1<b_2$ implies $u(b_1^*)\geqslant u(b_2^*)$, we have that $\lambda_{\max}(b), \lambda_{\min}(b)$ are decreasing functions of b. Using (2.6) and (2.9), and the fact that $E(t)$ is decreasing, we get

$$e^{-\Phi(b)/(p+1)} \leqslant \lambda_{\min}(b) \leqslant \lambda_{\max}(b) \leqslant 1.$$

Now let $Q^+ = \{q_1, q_2, q_3, \ldots\}$ be the set of positive rationals. We choose a sequence $\{\gamma_n\}_{n\geqslant 1}$ such that $u(0) = \gamma_n$ (see (2.1) and (2.2)), $\gamma_n \to \infty$, and the limit

$$\lambda(q_1) = \lim_n \frac{u(q_1^*)}{\gamma_n} \tag{2.11}$$

exists. By choosing a subsequence of $\{\gamma_n\}_{n\geqslant 1}$ (which we also denote by γ_n) we can make the limit

$$\lambda(q_2) = \lim_n \frac{u(q_2^*)}{\gamma_n}$$

exist too. We can continue taking subsequences, and finally use a standard diagonal process, to conclude that there is a sequence $\{\gamma_n\}_{n\geqslant 1}$, $\gamma_n \to \infty$, such that the limits

$$\lambda(q) = \lim_n \frac{u(q^*)}{\gamma_n}, \quad q \in Q^+, \tag{2.12}$$

exist.

We, next, want to estimate $u(q_1^*) - u(q_2^*)$, when q_1 and q_2 are given rationals with

$$0 \leqslant q_1 < q_2 \leqslant M \tag{2.13}$$

(without loss of generality M can be assumed rational). Let $t'_{2m}, t'_{2m+1}, t'_{2m+2}$ be consecutive zeros of $u'(t)$ such that

$$q_1^* \leqslant t'_{2m} < t'_{2m+2} \leqslant q_2^*. \tag{2.14}$$

We set

$$T_m = t'_{2m+2} - t'_{2m}$$

(T_m is the temporal duration of the $(m+1)$th "cycle"; in the Hamiltonian case $\phi(t) \equiv 0$, T_m is, of course, the period). We need upper and lower bounds for T_m, valid for large γ. We can consider the solution $v(t) = u(t + t'_{2m})$ of

$$v'' + \phi(t + t'_{2m})v' + B^2 v^{2p+1} = 0,$$

so that $v(0) \in [u(q_2^*), u(q_1^*)]$. Thanks to (2.6), formula (1.11) is valid for $v(t)$. Using these observations we get that

$$T_{\min} \leqslant T_m \leqslant T_{\max}, \tag{2.15}$$

where

$$T_{\min} = \frac{c_p}{B} \frac{1}{u(q_1^*)^p} + O(\gamma_n^{-2p}), \quad T_{\max} = \frac{c_p}{B} \frac{1}{u(q_2^*)^p} + O(\gamma_n^{-2p}). \tag{2.16}$$

We also need to estimate the "drop" of $u(t)$ on each "cycle," namely the quantity

$$\Delta_m = u(t'_{2m}) - u(t'_{2m+2}).$$

A slight adaptation of the analysis done in Ref. 1 gives (since $\phi(t'_{2m+2}) = \phi(t'_{2m}) + \phi'(t'_{2m}) \times (t'_{2m+2} - t'_{2m}) + o(t'_{2m+2} - t'_{2m})$)

$$u(t'_{2m+2}) = u(t'_{2m})\left[1 - \frac{\phi(t'_{2m})A_p}{B}u(t'_{2m})^{-p} + O(u(t'_{2m})^{-2p})\right] \quad \text{as } \gamma \to \infty, \tag{2.17}$$

where

$$A_p = \frac{4}{\sqrt{p+1}}\int_0^1 \sqrt{1-x^{2p+2}}\,dx = \frac{\sqrt{\pi}}{(p+1)^{3/2}} \cdot \frac{\Gamma\left(\frac{1}{2p+2}\right)}{\Gamma\left(\frac{3p+4}{2p+2}\right)}. \tag{2.18}$$

Hence, invoking (2.6), (2.13), (2.14), and (2.17) gives

$$\Delta_m = \frac{\phi(t'_{2m})A_p}{B}u(t'_{2m})^{1-p} + O(\gamma^{1-2p}) \quad \text{as } \gamma \to \infty,$$

and, therefore

$$\Delta_{\min} \leqslant \Delta_m \leqslant \Delta_{\max}, \tag{2.19}$$

where

$$\Delta_{\min} = A_p B^{-1} u(q_1^*)^{1-p} \min_{q_1^* \leqslant t \leqslant q_2^*} \phi(t) + O(\gamma_n^{1-2p}),$$

$$\Delta_{\max} = A_p B^{-1} u(q_2^*)^{1-p} \max_{q_1^* \leqslant t \leqslant q_2^*} \phi(t) + O(\gamma_n^{1-2p}). \tag{2.20}$$

Finally, let $N=N(q_1,q_2)$ be the number of "cycles" from $t=q_1^*$ to $t=q_2^*$. We have

$$\frac{q_2^* - q_1^*}{T_{\max}} \overset{\text{def}}{=} N_{\min} \leqslant N \leqslant N_{\max} \overset{\text{def}}{=} \frac{q_2^* - q_1^*}{T_{\min}}, \tag{2.21}$$

where, by (2.16) and (2.9),

$$N_{\min} = \frac{B(q_2 - q_1)}{c_p}u(q_2^*)^p[1 + O(\gamma_n^{-p})], \quad N_{\max} = \frac{B(q_2 - q_1)}{c_p}u(q_1^*)^p[1 + O(\gamma_n^{-p})]. \tag{2.22}$$

We are now ready to estimate $u(q_1^*) - u(q_2^*)$. We have

$$N_{\min}\Delta_{\min} \leqslant u(q_1^*) - u(q_2^*) \leqslant N_{\max}\Delta_{\max},$$

and thus, by (2.20) and (2.22), and the fact that $A_p/c_p = (p+2)^{-1}$ (this follows from (1.5) and (2.18))

$$\frac{\phi(t'_{2m})(q_2 - q_1)}{p+2}\frac{u(q_2^*)^p}{u(q_1^*)^{p-1}}[1 + O(\gamma_n^{-p})] \leqslant u(q_1^*) - u(q_2^*) \leqslant \frac{\phi(t'_{2m})(q_2 - q_1)}{p+2}\frac{u(q_1^*)^p}{u(q_2^*)^{p-1}}[1 + O(\gamma_n^{-p})]$$

(notice that this estimate is B-free). If we divide the above inequality by γ_n and then take limits, as $n \to \infty$, we obtain (see (2.12))

$$\frac{\min_{q_1 \leqslant t \leqslant q_2}\phi(t)}{p+2}\frac{\lambda(q_2)^p}{\lambda(q_1)^{p-1}}(q_2 - q_1) \leqslant \lambda(q_1) - \lambda(q_2) \leqslant \frac{\max_{q_1 \leqslant t \leqslant q_2}\phi(t)}{p+2}\frac{\lambda(q_1)^p}{\lambda(q_2)^{p-1}}(q_2 - q_1), \tag{2.23}$$

where q_1 and q_2 are rationals in $[0,M]$. Since

$$e^{-\Phi(M)/(p+1)} \leqslant \lambda(q_2) \leqslant \lambda(q_1) \leqslant 1,$$

one consequence of (2.23) is that there is a constant $C>0$ such that

$$|\lambda(q_1) - \lambda(q_2)| \leqslant C|q_1 - q_2|. \tag{2.24}$$

Now let $b \in [0,M]$ be a real number and q_1, q_2 rationals so that $q_1 \leqslant \xi \leqslant q_2$. Then

$$\lambda(q_2) \leqslant \liminf_n \frac{u(b^*)}{\gamma_n} \leqslant \limsup_n \frac{u(b^*)}{\gamma_n} \leqslant \lambda(q_1).$$

But (2.24) implies that $|\lambda(q_1)-\lambda(q_2)|$ can be made as small as we wish. Therefore the limit

$$\lim_n \frac{u(b^*)}{\gamma_n}$$

exists and the function

$$\lambda(b) = \lim_n \frac{u(b^*)}{\gamma_n}$$

is decreasing and continuous for all $b \in (0,\infty)$. Furthermore (2.23) is also valid for irrational numbers $q_1, q_2 > 0$. If we divide all terms of (2.23) by $q_2 - q_1$ and let $q_2 \to q_1$, we obtain the surprising formula

$$\lambda'(b) = -\frac{\phi(b)}{p+2}\lambda(b),$$

and this, together with the equation $\lambda(0)=1$, give

$$\lambda(b) = e^{-\Phi(b)/(p+2)}.$$

In particular,

$$\lambda(q_1) = e^{-\Phi(q_1)/(p+2)}.$$

Since q_1 and $\{\gamma_n\}_{n\geqslant 1}$ of (2.11) are arbitrary, it follows that,

$$\lim_{\gamma\to\infty} \frac{u(b^*)}{\gamma} = e^{-\Phi(b)/(p+2)},$$

and the proof is finished in view of (2.10) and the fact that $A(b^*)=u(b^*)$.

Remarks:

1. The statement of the theorem is quite surprising. Note that the result is independent of B, hence one expects that the theorem should extend to the case

$$u'' + \phi(t)u' + \rho(t)^2 u^{2p+1} = 0, \quad t > 0,$$

$$u(0) = \gamma, \quad u'(0) = 0,$$

where $\rho(t) \geqslant B > 0$. Notice that if $p=0$ (linear case) and $\rho(t)$ is, e.g., periodic, then, even for $\phi(t) \equiv 0$, we have exponential decay if 0 is in the $L_2(R)$-spectrum of the operator L defined by $Lu = -u'' - \rho(t)^2 u$.

2. The theorem remains true if instead of (2.21) we had

$$u'' + \phi(t)u' + B^2 u^{2p+1} + P(u) = 0,$$

where P is a polynomial of degree $\leqslant 2p$.

3. It is interesting to attempt a comparison of the statement of Theorem 1 with the linear case ($p=0$):

$$u'' + \phi(t)u' + B^2\rho(t)^2u = 0, \quad t > 0,$$

$$u(0) = \gamma, \quad u'(0) = 0.$$

Here we assume that $\rho(t) > 0$ and that B is a large (positive) parameter. Then the WKB approximation (see, e.g., Ref. 2 or 4) implies that generically

$$A(b) = \gamma e^{-\Phi(b)/2} + o(1) \quad \text{as } B \to \infty,$$

which mirrors the statement of Theorem 1.[5]

III. A PARTICULAR CASE OF SPECIAL INTEREST

Consider now the initial value problem

$$u'' + \frac{2}{t}u' + B^2u^{2p+1} = 0, \quad t > 0, \tag{3.1}$$

$$u(0) = \gamma, \quad u'(0) = 0, \tag{3.2}$$

where, as before, $p \geqslant 1$ is an integer and $B > 0$ (notice that, $u'' + (2/t)u'$ is the three-dimensional radial Laplacian of u). Again the boundary conditions must be interpreted in the right way, i.e., as limits when $t \to 0^+$. In comparison with (1.6) we have that

$$\phi(t) = \frac{2}{t} \tag{3.3}$$

and, hence

$$\Phi(t) = \int_0^t \phi(\tau)\mathrm{d}\tau = 2\int_0^t \frac{\mathrm{d}\tau}{\tau} = \infty.$$

Proposition 1:The problem (3.1) and (3.2) has a unique solution for all $t > 0$.

Proof: We first notice that (3.1) and (3.2) is equivalent to the integral equation

$$u(t) = \gamma - B^2\int_0^t \tau[1 - (\tau/t)]u(\tau)^{2p+1}\mathrm{d}\tau. \tag{3.4}$$

We must, therefore, look at the map

$$\mathcal{F}[u](t) = \gamma - B^2\int_0^t \tau[1 - (\tau/t)]u(\tau)^{2p+1}\mathrm{d}\tau,$$

mapping $C[0,\varepsilon]$ into itself, for any given $\varepsilon > 0$. It is easy to see that, if ε is chosen sufficiently small, then $\mathcal{F}$ is a contraction, namely

$$\|\mathcal{F}[u] - \mathcal{F}[v]\|_\infty \leqslant c\|u - v\|_\infty,$$

where $c < 1$. Hence $\mathcal{F}$ has a unique fixed point u in $C[0,\varepsilon]$ which is the unique solution of (3.4) in $[0,\varepsilon]$ (and it is automatically smooth). Then the global existence and uniqueness follows by the fact that the energy is decreasing (see (1.7)). ■

In view of Theorem 1 one can infer that, if $b > 0$ is a fixed number, then

$$A(b) = o(\gamma) \quad \text{as } \gamma \to \infty. \tag{3.5}$$

This estimate is somehow vague. Thus, we would like to get a more precise estimate for $A(b)$ or equivalently (see (2.8)) $u(b^*)$. This question requires an approach very different from the one presented in Sec. II.

Let us first look at the linear problem

$$w'' + \frac{2}{t}w' + \Lambda^2\rho(t)^2 w = 0, \quad t > 0, \tag{3.6}$$

$$w(0) = 1, \quad w'(0) = 0, \tag{3.7}$$

where $\rho(t) \geqslant 0$, such that the zeros of $\rho(t)$ form a discrete set and $\rho(0) \neq 0$ (if $\rho(t) \equiv 1$, the solution of the above problem is $\Lambda t^{-1}\sin(\Lambda t)$). We are interested in the behavior of $w(t)$, as $\Lambda \to \infty$.

We set

$$w(t) = \frac{v(t)}{t}, \tag{3.8}$$

so that

$$v'' + \Lambda^2\rho(t)^2 v = 0, \quad t > 0. \tag{3.9}$$

Furthermore the initial conditions (3.7) become

$$v(0) = 0, \quad v'(0) = 1. \tag{3.10}$$

The WKB approximation (see, e.g., Ref. 2 or 4) implies that generically

$$v(t) \sim \frac{\sin\left[\Lambda \int_0^t \rho(\tau)\mathrm{d}\tau\right]}{\Lambda\rho(0)^{1/2}\rho(t)^{1/2}}, \quad \text{as } \Lambda \to \infty, \tag{3.11}$$

hence (see (3.8))

$$w(t) \sim \frac{\sin\left[\Lambda \int_0^t \rho(\tau)\mathrm{d}\tau\right]}{\Lambda\rho(0)^{1/2}\rho(t)^{1/2}t}, \quad \text{as } \Lambda \to \infty, \tag{3.12}$$

where $w(t)$ is the solution of (3.6) and (3.7).

Now, by setting

$$u(t) = \gamma u_1(t), \tag{3.13}$$

(3.1) and (3.2) can be written as

$$u_1'' + \frac{2}{t}u_1' + B^2\gamma^{2p}u_1^{2p+1} = 0, \quad t > 0, \tag{3.14}$$

$$u_1(0) = 1, \quad u'(0) = 0. \tag{3.15}$$

If we apply (3.12) to (3.14) and (3.15), we obtain

$$u_1(t) \sim \frac{\sin\left[B\gamma^p \int_0^t |u_1(\tau)|^p \mathrm{d}\tau\right]}{B\gamma^p |u_1(t)|^{p/2} t}, \quad \text{as } \gamma \to \infty,$$

or, due to (3.13),

$$u(t) \sim \frac{\sin\left[B \int_0^t |u(\tau)|^p \mathrm{d}\tau\right]}{B\gamma^{(p-2)/2} |u(t)|^{p/2} t} \quad \text{as } \gamma \to \infty, \tag{3.16}$$

but it should be kept in mind that (3.16) is valid as long as

$$A(t) \to \infty \quad \text{as } \gamma \to \infty. \tag{3.17}$$

Formula (3.16) implies that, under (3.17),

$$|u(t)|^{(p+2)/2} \sim \frac{\left|\sin\left[B \int_0^t |u(\tau)|^p \mathrm{d}\tau\right]\right|}{B\gamma^{(p-2)/2} t} \quad \text{as } \gamma \to \infty,$$

or

$$|u(t)| \sim \frac{\left|\sin\left[B \int_0^t |u(\tau)| \mathrm{d}\tau\right]\right|^{2/(p+2)}}{B^{2/(p+2)} \gamma^{(p-2)/(p+2)} t^{2/(p+2)}} \quad \text{as } \gamma \to \infty.$$

Therefore

$$A(b) \sim \frac{\gamma^{(2-p)/(2+p)}}{B^{2/(p+2)}} \cdot \frac{1}{b^{2/(p+2)}} \quad \text{as } \gamma \to \infty, \tag{3.18}$$

as long as $A(b) \to \infty$, as $\gamma \to \infty$. We thus have, for example: (a) If $p=1$, then

$$A(b) \sim \frac{\gamma^{1/3}}{B^{2/3}} \cdot \frac{1}{b^{2/3}} \quad \text{as } \gamma \to \infty.$$

(b) If $p \geqslant 2$, then

$$A(b) = O(1) \quad \text{as } \gamma \to \infty.$$

It is worth mentioning that one can arrive at the statement of Theorem 1 by applying the above WKB analysis to (2.1) and (2.2).

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On quasiperiodic boundary condition problem

Y. Charles Li[a)]
Department of Mathematics, University of Missouri, Columbia, Missouri 65211

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The paper raises the question of posing the quasiperiodic boundary condition in the Cauchy problem of partial differential equations. Using the one-dimensional cubic nonlinear Schrödinger as a simple example, we illustrated the various types of questions including global well-posedness, spectra of linear operators, and foliations. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1832754]

I. INTRODUCTION

The quasiperiodic boundary condition problem can be posed for a variety of partial differential equations (PDE) including, e.g., parabolic and hyperbolic equations. Questions that can be asked include local and global well-posedness, dynamics in phase spaces, and asymptotics, etc. Here we take a simple PDE–one-dimensional cubic nonlinear Schrödinger equation (NLS), to study its phase space foliations.

Typical fluid flows are defined on unbounded domain with nondecaying boundary conditions. For example, the Poiseuille flow or the boundary layer flow has nondecaying boundary conditions along the longitudinal direction. In fact, turbulence develops along this longitudinal direction. In many cases, turbulent fluid flows contain both temporal and spatial randomness. Temporal randomness is often caused by temporal chaotic motions. Spatial randomness is often caused by vortex (energy) cascade or inverse cascade. In such cases, periodic boundary conditions put too much constraint. Quasiperiodic or more general boundary conditions are more relevant.

The one-dimensional (1D) cubic NLS under periodic boundary conditions is well understood. It is globally well-posed. Under quasiperiodic boundary conditions, global well-posedness is not known. Under periodic boundary conditions, Stokes wave solution has a finite number of unstable eigenvalues. On the other hand, under quasiperiodic boundary conditions, it has infinitely many unstable eigenvalues dense on an interval. There is no spectral gap. But explicit expressions of the foliation in phase space can be obtained via a Darboux transformation.

II. FORMULATION OF THE PROBLEM

Consider the 1D cubic nonlinear Schrödinger equation

$$iq_t = q_{xx} + 2|q|^2 q, \tag{2.1}$$

where q is a complex-valued function of two real variables (t,x), $i=\sqrt{-1}$. We pose a quasiperiodic boundary condition with two base frequencies β_1 and β_2, β_1/β_2 is irrational. That is,

$$q = q(t,\theta_1,\theta_2), \quad \theta_1 = \beta_1 x, \quad \theta_2 = \beta_2 x,$$

and q is periodic in both θ_1 and θ_2 with period 2π. Thus

[a)]Electronic mail: cli@math.missouri.edu

$$q = q(t,\theta) = \sum_{k\in\mathbb{Z}^2} q_k(t)e^{ik\cdot\theta}, \quad \theta = \begin{pmatrix}\theta_1\\ \theta_2\end{pmatrix}, \quad k = \begin{pmatrix}k_1\\ k_2\end{pmatrix}.$$

It seems that the more natural norm is

$$\|q\|^2_{(s)} = \sum_{k\in\mathbb{Z}^2} (1+|k|^2)^s |q_k|^2,$$

rather than

$$\|q\|^2_{[s]} = \sum_{k\in\mathbb{Z}^2} [1+(k\cdot\beta)^2]^s |q_k|^2, \quad \beta = \begin{pmatrix}\beta_1\\ \beta_2\end{pmatrix}.$$

In terms of Fourier transforms, (2.1) can be rewritten as

$$\begin{aligned} i\frac{dq_k}{dt} &= -\frac{\partial H}{\partial \bar{q}_k},\\ i\frac{d\bar{q}_k}{dt} &= \frac{\partial H}{\partial q_k}, \end{aligned} \tag{2.2}$$

where

$$H = \sum_{k\in\mathbb{Z}^2} (k\cdot\beta)^2 |q_k|^2 - \sum_{k\in\mathbb{Z}^2} \left| \sum_{\hat{k}\in\mathbb{Z}^2} q_{\hat{k}} q_{k-\hat{k}} \right|^2 \tag{2.3}$$

$$= \lim_{a\to+\infty} \frac{1}{2a} \int_{-a}^{a} [|q_x|^2 - |q|^4] dx. \tag{2.4}$$

Using (2.4), the NLS (2.1) can be rewritten as

$$\begin{aligned} iq_t &= -\frac{\delta H}{\delta \bar{q}},\\ i\bar{q}_t &= \frac{\delta H}{\delta q}. \end{aligned} \tag{2.5}$$

Obviously,

$$I = \sum_{k\in\mathbb{Z}^2} |q_k|^2 = \lim_{a\to+\infty} \frac{1}{2a} \int_{-a}^{a} |q|^2 \, dx$$

is an invariant.

III. WELL-POSEDNESS

Explicitly (2.2) can be written as

$$i\dot{q}_k = -(k\cdot\beta)^2 q_k + 2 \sum_{\hat{k},\tilde{k}\in\mathbb{Z}^2} \bar{q}_{\hat{k}} q_{\tilde{k}+\hat{k}} q_{k-\tilde{k}}. \tag{3.1}$$

The method of variation of parameters leads to the integral equation

$$q_k(t) = e^{i(k\cdot\beta)^2 t} q_k(0) - 2i \int_0^t e^{i(k\cdot\beta)^2(t-\tau)} \sum_{\hat{k},\tilde{k}\in\mathbb{Z}^2} \overline{q_{\hat{k}}} q_{\tilde{k}+\hat{k}} q_{k-\tilde{k}}\, d\tau. \tag{3.2}$$

Notice that (3.1) bears more resemblance to two-dimensional (2D), rather than 1D, NLS under the periodic boundary condition. Local well-posedness can be easily established,[1] since the nonlinear term is still locally Lipschitz.

Theorem 3.1 (Local well-posedness): *For any $q_0 \in H_{(s)}$, $s \geqslant 2$, there exists a unique solution $q(t) \in C^0([0,\tau], H_{(s)})$ where $\tau = \tau(\|q_0\|_{(s)})$, to the Cauchy problem of (3.1) with initial condition $q(0) = q_0$. For any fixed $t \in [0,\tau]$, $q(t)$ is C^∞ in q_0.*

The interesting open problem is whether or not (3.1) has global well-posedness. On the one hand, it resembles 2D NLS under periodic boundary condition, therefore, it may not have global well-posedness. In fact, the first term in the Hamiltonian (2.3) is weaker than $\Sigma_{k\in\mathbb{Z}^2}|k|^2|q_k|^2$ of the 2D NLS periodic case. Thus the Hamiltonian cannot bound the $H_{(1)}$ norm. On the other hand, it is still an integrable system, therefore, an infinite sequence of invariants is at one's disposal.

IV. THE SPECTRUM OF A LINEAR NLS OPERATOR

Setting $\partial_x = 0$ in (2.1), one gets an ODE defined on the invariant complex plane

$$iq_t = 2|q|^2 q$$

with all periodic solutions (the so-called Stokes waves)

$$q = ce^{-i[2c^2 t+\gamma]}. \tag{4.1}$$

Linearize the NLS in the manner

$$q = (c + \hat{q})e^{-i[2c^2 t+\gamma]},$$

one has

$$i\hat{q}_t = \hat{q}_{xx} + 2c^2(\hat{q} + \overline{\hat{q}}).$$

Let

$$\hat{q} = \sum_{k\in\mathbb{Z}^2} \hat{q}_k(t) e^{ik\cdot\theta}, \tag{4.2}$$

one gets

$$i\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \hat{q}_k \\ \overline{\hat{q}_{-k}} \end{pmatrix} = \begin{pmatrix} 2c^2 - (k\cdot\beta)^2 & 2c^2 \\ -2c^2 & (k\cdot\beta)^2 - 2c^2 \end{pmatrix}\begin{pmatrix} \hat{q}_k \\ \overline{\hat{q}_{-k}} \end{pmatrix}. \tag{4.3}$$

Let

$$\begin{pmatrix} \hat{q}_k \\ \overline{\hat{q}_{-k}} \end{pmatrix} = e^{\lambda t}\begin{pmatrix} A \\ B \end{pmatrix}, \tag{4.4}$$

where λ, A, and B are complex constants, then

$$\lambda = \pm (k\cdot\beta)\sqrt{(2c)^2 - (k\cdot\beta)^2}. \tag{4.5}$$

Lemma 4.1: *The set $\{k\cdot\beta\}_{k\in\mathbb{Z}^2}$ is dense in $\mathbb{R}$.*

Proof: This proof is furnished by Banks.[2] For any real number z, let $[z]$ denote the greatest integer less than or equal to z, and let $\{z\} = z - [z]$ be the fractional part of z; then $0 \leqslant \{z\} \leqslant 1$. For any irrational number a, it is known that the fractional parts $\{na\}_{n\in\mathbb{Z}}$ are uniformly distributed over

the unit interval [0,1]. For any fixed $b \in \mathbb{R}$, given any $\epsilon > 0$, let k_2 be chosen such that

$$|\{k_2(\beta_2/\beta_1)\} - \{b/\beta_1\}| < \epsilon/\beta_1,$$

and choose $k_1 = [b/\beta_1] - [k_2(\beta_2/\beta_1)]$, then

$$|k_1 + k_2(\beta_2/\beta_1) - b/\beta_1| = |k_1 + [k_2(\beta_2/\beta_1)] - [b/\beta_1] + \{k_2(\beta_2/\beta_1)\} - \{b/\beta_1\}| = |\{k_2(\beta_2/\beta_1)\} - \{b/\beta_1\}| < \epsilon/\beta_1.$$

Multiplying by β_1, one obtains $|k \cdot \beta| < \epsilon$. This proves the lemma. ■

Theorem 4.2: *The spectrum of the linear NLS operator in* $H_{(s)}$, $s \geqslant 0$ *is*

$$\sigma = \sigma_p \cup \sigma_c = [-2c^2, 2c^2] \cup i\mathbb{R}$$

where σ_p *is given by (4.5) and is everywhere dense in* σ.

Proof: The maximum of the function

$$z^2((2c)^2 - z^2), \quad z \in \mathbb{R}$$

is $4c^2$. By Lemma 4.1 and the fact that the spectrum σ is a closed set, we have that

$$[-2c^2, 2c^2] \cup i\mathbb{R} \subset \sigma.$$

In terms of the Fourier transform (4.2), the linear NLS operator has the representation given by (4.3),

$$L_k = -i \begin{pmatrix} 2c^2 - (k \cdot \beta)^2 & 2c^2 \\ -2c^2 & (k \cdot \beta)^2 - 2c^2 \end{pmatrix}.$$

If $\lambda \notin [-2c^2, 2c^2] \cup i\mathbb{R}$, then there is an absolute constant C such that

$$\|(L_k - \lambda)^{-1}\| \leqslant C, \quad \forall\, k$$

and this is true even for some k, $(k \cdot \beta)^2$ might be equal to $(2c)^2$. Thus such λ belongs to the resolvent set, and

$$\sigma = [-2c^2, 2c^2] \cup i\mathbb{R}.$$

Let $\lambda \in \sigma / \sigma_p$ where σ_p is the point spectrum given by (4.5), then there is a sequence $\lambda_j \in \sigma_p$ such that $\lambda_j \to \lambda$, and

$$\|(L_{k_j} - \lambda)^{-1}\| \geqslant 1/|\lambda_j - \lambda| \to +\infty;$$

thus $\lambda \in \sigma_c$ is the continuous spectrum. This proves the theorem. ■

Remark 4.3: For NLS under periodic boundary condition, the spectrum of the linear NLS operator consists of only discrete point spectrum given by

$$\lambda = \pm k\beta\sqrt{(2c)^2 - (k\beta)^2},$$

where $k \in \mathbb{Z}$, and β is a positive constant. For any fixed $c > 0$, there is a finite number of unstable modes. There are gaps among the unstable, center, and stable spectra. As shown above, under quasiperiodic boundary condition, the point spectrum is dense, and there is also a continuous spectrum. For any fixed $c > 0$, there are infinitely many unstable modes. There is no gap among the unstable, center, and stable spectra.

V. FOLIATIONS

Although there is no spectral gap in this quasiperiodic setting, foliations can still be established via explicit expressions. The tool used is the so-called Darboux transformation. The NLS (2.1) has the Lax pair,

$$\psi_x = U\psi, \quad \psi_t = V\psi,$$

where

$$U = i\begin{pmatrix} \lambda & q \\ \bar{q} & -\lambda \end{pmatrix},$$

$$V = i\begin{pmatrix} 2\lambda^2 - |q|^2 & 2\lambda q - iq_x \\ 2\lambda\bar{q} + i\bar{q}_x & -2\lambda^2 + |q|^2 \end{pmatrix}.$$

Theorem 5.1: *Let $q(t,x)$ be a solution, and let ϕ be an eigenfunction of the Lax pair at $\lambda = \nu$ for any $\nu \in \mathbb{C}$. Use ϕ to define a matrix,*

$$G = \Gamma\begin{pmatrix} \lambda - \nu & 0 \\ 0 & \lambda - \bar{\nu} \end{pmatrix}\Gamma^{-1},$$

where

$$\Gamma = \begin{pmatrix} \phi_1 & -\overline{\phi_2} \\ \phi_2 & \overline{\phi_1} \end{pmatrix}.$$

We define Q and Ψ by

$$Q = q + 2(\nu - \bar{\nu})\frac{\phi_1\overline{\phi_2}}{|\phi_1|^2 + |\phi_2|^2}, \quad \Psi = G\psi, \tag{5.1}$$

where ψ solves the Lax pair at (q,λ). Then Ψ solves the Lax pair at (Q,λ) and Q solves the NLS.

This is a well-known theorem in the integrable theory, see, e.g., Ref. 3. The transformation (5.1) is called a Darboux transformation.

For example, let

$$q = ae^{i\theta(t)}, \quad \theta(t) = -[2a^2t + \gamma],$$

where a is the amplitude and γ is the phase. The eigenfunctions of the Lax pair are

$$\phi^{\pm} = \begin{pmatrix} ae^{i\theta(t)/2} \\ (\pm\beta - \lambda)e^{-i\theta(t)/2} \end{pmatrix}e^{\pm i2\lambda\beta t \pm i\beta x}, \quad \lambda = \sqrt{\beta^2 - a^2}.$$

In order to have temporal growth, $\beta^2 < a^2$. For $\beta = \beta_1$, $\lambda = \nu = i\sigma$, let

$$\phi = c^+\phi^+ + c^-\phi^-,$$

where $c^{\pm}$ are two arbitrary complex constants. For $\beta = \beta_2$, $\lambda = \hat{\nu} = i\hat{\sigma}$, let

$$\hat{\phi} = \hat{c}^+\phi^+ + \hat{c}^-\phi^-,$$

where $\hat{c}^{\pm}$ are two arbitrary complex constants. By iterating the Darboux transformation (5.1) at ν and $\hat{\nu}$, one gets

$$Q = q + 2(\nu - \overline{\nu})\frac{\phi_1\overline{\phi_2}}{|\phi_1|^2 + |\phi_2|^2} + 2(\hat{\nu} - \overline{\hat{\nu}})\frac{\hat{\Phi}_1\overline{\hat{\Phi}_2}}{|\hat{\Phi}_1|^2 + |\hat{\Phi}_2|^2},$$

where

$$\hat{\Phi}_1 = \frac{1}{|\phi_1|^2 + |\phi_2|^2}\{[(\hat{\nu} - \nu)|\phi_1|^2 + (\hat{\nu} - \overline{\nu})|\phi_2|^2]\hat{\phi}_1 + (\overline{\nu} - \nu)\phi_1\overline{\phi_2}\hat{\phi}_2\},$$

$$\hat{\Phi}_2 = \frac{1}{|\phi_1|^2 + |\phi_2|^2}\{(\overline{\nu} - \nu)\overline{\phi_1}\phi_2\hat{\phi}_1 + [(\hat{\nu} - \overline{\nu})|\phi_1|^2 + (\hat{\nu} - \nu)|\phi_2|^2]\hat{\phi}_2\}.$$

Explicitly, one has

$$Q = \tilde{Q} + q \sin\hat{\vartheta}_0 \prod_2 \Big/ \prod_1, \tag{5.2}$$

where

$$\tilde{Q} = q[1 + \sin\vartheta_0 \operatorname{sech}\tau\cos X]^{-1}[\cos 2\vartheta_0 - i\sin 2\vartheta_0 \tanh\tau - \sin\vartheta_0 \operatorname{sech}\tau\cos X],$$

$$\begin{aligned}\prod_1 = {} & \left[(\sin\hat{\vartheta}_0)^2(1 + \sin\vartheta_0 \operatorname{sech}\tau\cos X)^2 + \frac{1}{8}(\sin 2\vartheta_0)^2(\operatorname{sech}\tau)^2(1 - \cos 2X)\right] \\ & \times(1 + \sin\hat{\vartheta}_0 \operatorname{sech}\hat{\tau}\cos\hat{X}) - \frac{1}{2}\sin 2\vartheta_0 \sin 2\hat{\vartheta}_0 \operatorname{sech}\tau \operatorname{sech}\hat{\tau}(1 + \sin\vartheta_0 \operatorname{sech}\tau\cos X) \\ & \times\sin X \sin\hat{X} + (\sin\vartheta_0)^2[1 + 2\sin\vartheta_0 \operatorname{sech}\tau\cos X + [(\cos X)^2 - (\cos\vartheta_0)^2](\operatorname{sech}\tau)^2] \\ & \times(1 + \sin\hat{\vartheta}_0 \operatorname{sech}\hat{\tau}\cos\hat{X}) - 2\sin\hat{\vartheta}_0 \sin\vartheta_0[\cos\hat{\vartheta}_0 \cos\vartheta_0 \tanh\hat{\tau}\tanh\tau \\ & + (\sin\vartheta_0 + \operatorname{sech}\tau\cos X)(\sin\hat{\vartheta}_0 + \operatorname{sech}\hat{\tau}\cos\hat{X})](1 + \sin\vartheta_0 \operatorname{sech}\tau\cos X),\end{aligned}$$

$$\begin{aligned}\prod_2 = {} & \left[-2(\sin\hat{\vartheta}_0)^2(1 + \sin\vartheta_0 \operatorname{sech}\tau\cos X)^2 + \frac{1}{4}(\sin 2\vartheta_0)^2(\operatorname{sech}\tau)^2(1 - \cos 2X)\right] \\ & \times(\sin\hat{\vartheta}_0 + \operatorname{sech}\hat{\tau}\cos\hat{X} + i\cos\hat{\vartheta}_0\tanh\hat{\tau}) + 2(\sin\vartheta_0)^2(-\cos\vartheta_0\tanh\tau + i\sin\vartheta_0 \\ & + i\operatorname{sech}\tau\cos X)^2(\sin\hat{\vartheta}_0 + \operatorname{sech}\hat{\tau}\cos\hat{X} - i\cos\hat{\vartheta}_0\tanh\hat{\tau}) + 2\sin\vartheta_0(\sin\vartheta_0 + \operatorname{sech}\tau\cos X \\ & + i\cos\vartheta_0\tanh\tau)[2\sin\hat{\vartheta}_0(1 + \sin\vartheta_0 \operatorname{sech}\tau\cos X)(1 + \sin\hat{\vartheta}_0 \operatorname{sech}\hat{\tau}\cos\hat{X}) \\ & - \sin 2\vartheta_0 \cos\hat{\vartheta}_0 \operatorname{sech}\tau \operatorname{sech}\hat{\tau}\sin X \sin\hat{X}],\end{aligned}$$

and

$$\beta_1 + \nu = ae^{i\vartheta_0}, \quad \beta_2 + \hat{\nu} = ae^{i\hat{\vartheta}_0},$$

$$c^+/c^- = e^{\rho + i\vartheta}, \quad \hat{c}^+/\hat{c}^- = e^{\hat{\rho} + i\hat{\vartheta}},$$

$$\tau = 4\sigma\beta_1 t - \rho, \quad \hat{\tau} = 4\hat{\sigma}\beta_2 t - \hat{\rho},$$

$$X = 2\beta_1 x + \vartheta - \vartheta_0 + \pi/2, \quad \hat{X} = 2\beta_2 x + \hat{\vartheta} - \hat{\vartheta}_0 + \pi/2.$$

The foliation here is with respect to the two linear unstable modes $(2\beta_1,0)$ and $(0,2\beta_2)$ in (4.5). The temporal growth condition $\beta_1^2 < a^2$ or $\beta_2^2 < a^2$ is in agreement with (4.5). Thus (5.2) represents a class of solutions with quasiperiodic boundary condition. For fixed a, β_1, and β_2, the parameters are γ, ρ, $\hat{\rho}$, ϑ, and $\hat{\vartheta}$. As $t \to \pm\infty$, e.g., β_1, β_2, σ, and $\hat{\sigma}$ are all positive,

$$Q \to qe^{\mp i2(\vartheta_0+\hat{\vartheta}_0)}.$$

VI. CONCLUSION AND DISCUSSION

From the presentation in this paper, one can see that the first interesting question on such quasiperiodic boundary condition problem is the global well-posedness. In terms of Fourier transforms, one can see that the integrable NLS resembles the 2D more than the 1D periodic problem. I tend to believe that it may have finite-time blow-up solutions, which will be truly interesting. Also linearization in the quasiperiodic case often leads to a linear operator with continuous spectrum and with no spectral gap. Therefore, the phase space foliation is a challenging and interesting problem. In this paper, through Darboux transformation, such foliation can still be established.

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Time- and space-fractional partial differential equations

Jun-Sheng Duan
Department of Basic Sciences, Tianjin University of Commerce, Tianjin 300134, People's Republic of China

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The fundamental solution for time- and space-fractional partial differential operator $D_t^\lambda + a^2(-\triangle)^{\gamma/2}(\lambda, \gamma > 0)$ is given in terms of the Fox's H-function. Here the time-fractional derivative in the sense of generalized functions (distributions) D_t^λ is defined by the convolution $D_t^\lambda f(t) = \Phi_{-\lambda}(t) * f(t)$, where $\Phi_\lambda(t) = t_+^{\lambda-1}/\Gamma(\lambda)$ and $f(t) \equiv 0$ as $t < 0$, and the fractional n-dimensional Laplace operator $(-\triangle)^{\gamma/2}$ is defined by its Fourier transform with respect to spatial variable $\mathcal{F}[(-\triangle)^{\gamma/2} g(x)] = |\omega|^\gamma \mathcal{F}[g(x)]$. The solutions for initial value problems for time- and space-fractional partial differential equation in the sense of Caputo and Riemann–Liouville time-fractional derivatives, respectively, are obtained by the fundamental solution. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1819524]

I. INTRODUCTION

In recent years interest of some scholars has been shown in research on the problems involving the fractional integrodifferential equations applied to physics, mechanics, and other disciplines. For example, Schneider and Wyss,[20] Rangarajan and Ding,[19] and Fujita[7] have studied the integrodifferential equations with time-fractional integral; the partial differential equations with time-fractional derivative have been treated by Wyss,[23] Metzler *et al.*,[17] Buckwar and Luchko,[2] Gorenflo *et al.*,[10] Henry and Wearne,[12] Mainardi,[14,15] Hilfer,[13] and Podlubny.[18]

Compte[4] and West *et al.*[22] derived a hyperdiffusion (Lévy-flight diffusion) equation $\partial P/\partial t = D(-\triangle)^{\gamma/2} P$, where the fractional n-dimensional Laplace operator $(-\triangle)^{\gamma/2}$ is defined by its Fourier transform with respect to spatial variable $\mathcal{F}[(-\triangle)^{\gamma/2} g(x)] = |\omega|^\gamma \mathcal{F}[g(x)]$, and West *et al.*[22] gave the solution in the one-dimensional case.

In this paper the fundamental solution for the time- and space-fractional partial differential operator $D_t^\lambda + a^2(-\triangle)^{\gamma/2}(\lambda, \gamma > 0)$ is considered and is given in terms of Fox's H-function. Here the time-fractional derivative in the sense of generalized functions[8,18] (distributions) D_t^λ is defined by the convolution $D_t^\lambda f(t) := \Phi_{-\lambda}(t) * f(t)$, where $\Phi_\lambda(t) := t_+^{\lambda-1}/\Gamma(\lambda)$, $\Gamma(z)$ is the gamma function, and $f(t) \equiv 0$ as $t < 0$. The solutions for initial value problems for time- and space-fractional partial differential equation in the sense of Caputo and Riemann–Liouville, respectively, time-fractional derivatives are obtained by the fundamental solution.

Throughout this paper functions of time t are assumed to be causal, i.e., vanishing for $t < 0$. In Sec. II the time-fractional derivatives in the sense of generalized functions are adopted and we do not bother to give descriptions of sets of admissible functions and use, when necessary, formal expressions of generalized functions. In Sec. III the time-fractional derivatives in the Caputo and the Riemann–Liouville sense are defined within the framework of classical functions.

II. FUNDAMENTAL SOLUTION FOR TIME- AND SPACE-FRACTIONAL PARTIAL DIFFERENTIAL OPERATOR

We consider the time- and space-fractional partial differential equation

$$(D_t^{\lambda} + a^2(-\triangle)^{\gamma/2})G = \delta(x)\delta(t) \quad (\lambda, \gamma > 0), \tag{1}$$

where δ is the Dirac delta function, a is a positive constant, and the time-fractional derivative operator D_t^{λ} and the fractional n-dimensional Laplace operator $(-\triangle)^{\gamma/2}$ are defined as in Sec. I. The solution $G=G(x,t;\gamma,\lambda)$ of Eq. (1) is said to be a fundamental solution for the operator $D_t^{\lambda} + a^2(-\triangle)^{\gamma/2}$.

If $\lambda=1$ and $\gamma=2$ the operator in (1) becomes the diffusion operator, while it is a wave operator if $\lambda=2$ and $\gamma=2$.

Applying the Fourier transform with respect to spatial variable x and the Laplace transform with respect to time t (Fourier–Laplace transform) to Eq. (1) yields

$$\overline{G}(\omega,p;\gamma,\lambda) = \frac{1}{p^{\lambda} + a^2|\omega|^{\gamma}}. \tag{2}$$

Here the Fourier transform is defined by

$$\mathcal{F}[g(x),\omega] = \int g(x)e^{i\omega\cdot x}\, \mathrm{d}^n x, \tag{3}$$

whose inverse transform reads

$$\mathcal{F}^{-1}[g(x),\omega] = \frac{1}{(2\pi)^n}\int g(x)e^{-i\omega\cdot x}\, \mathrm{d}^n x, \tag{4}$$

and the Laplace transform is

$$\mathcal{L}[f(t),p] = \int_0^{\infty} f(t)e^{-pt}\, \mathrm{d}t. \tag{5}$$

Using the Mellin transform

$$\hat{f}(s) = \mathcal{M}[f(t),s] = \int_0^{\infty} f(t)t^{s-1}\, \mathrm{d}t \tag{6}$$

and the relation

$$\mathcal{M}[f(t),s] = \frac{1}{\Gamma(1-s)}\mathcal{M}[\mathcal{L}[f(t),p],1-s] \tag{7}$$

connecting Laplace and Mellin transforms we obtain the Fourier–Mellin transform of $G(x,t;\gamma,\lambda)$,

$$\tilde{G}(\omega,s;\gamma,\lambda) = \frac{1}{\lambda\Gamma(1-s)}(a^2|\omega|^{\gamma})^{[(1-s)/\lambda]-1}B\left(\frac{1-s}{\lambda},\frac{\lambda-1+s}{\lambda}\right), \tag{8}$$

where $B(u,v)$ is the beta function.

In order to obtain inverse Fourier transform to (8) introducing n-dimensional spherical coordinates in the inverse Fourier integral to (8) leads to the Mellin transform of $G(x,t;\gamma,\lambda)$ with respect to t,

$$\hat{G}(x,s;\gamma,\lambda) = \frac{|x|^{1-(n/2)}B\left(\frac{1-s}{\lambda},\frac{\lambda-1+s}{\lambda}\right)}{\lambda(2\pi)^{n/2}\Gamma(1-s)a^{[2(s-1)/\lambda]+2}}\int_0^{\infty} \rho^{(n/2)+[\gamma(1-s)/\lambda]-\gamma}J_{(n/2)-1}(\rho|x|)\mathrm{d}\rho, \tag{9}$$

where $\rho=|\omega|$ and $J_{\mu}(z)$ is the Bessel function of the first kind. Using the Mellin transform of the Bessel function,[5]

$$\mathcal{M}[J_\mu(z),s] = \frac{2^{s-1}\Gamma\left(\frac{\mu+s}{2}\right)}{\Gamma\left(\frac{\mu-s}{2}+1\right)}, \quad -\mu < \Re(s) < \mu+2, \tag{10}$$

we obtain

$$\hat{G}(x,s;\gamma,\lambda) = \frac{|x|^{[\gamma(s-1)/\lambda]+\gamma-n}}{\lambda 2^{[\gamma(s-1)/\lambda]+\gamma}\pi^{n/2}a^{2(\lambda+s-1)/\lambda}}\Theta(s), \tag{11}$$

where

$$\Theta(s) = \frac{\Gamma\left(\frac{n\lambda-\gamma\lambda+\gamma-\gamma s}{2\lambda}\right)\Gamma\left(\frac{1-s}{\lambda}\right)\Gamma\left(\frac{\lambda-1+s}{\lambda}\right)}{\Gamma\left(\frac{\gamma\lambda-\gamma+\gamma s}{2\lambda}\right)\Gamma(1-s)}. \tag{12}$$

Taking the inverse Mellin transform yields $G(x,t;\gamma,\lambda)$ in terms of the H-function, and by its properties we have

$$G(x,t;\gamma,\lambda) = \frac{t^{\lambda-1}}{\pi^{n/2}|x|^n}H_{2,3}^{2,1}\left(\frac{|x|^\gamma}{2^\gamma a^2 t^\lambda}\middle|\begin{matrix}(1,1);(\lambda,\lambda)\\(1,1),(n/2,\gamma/2);(1,\gamma/2)\end{matrix}\right). \tag{13}$$

If $\gamma=2$ and $\lambda=1$, (13) degenerates to the Gaussian distribution[16,21]

$$G(x,t;2,1) = \frac{1}{(4\pi a^2 t)^{n/2}}\exp\left(-\frac{|x|^2}{4a^2 t}\right). \tag{14}$$

If $\gamma=\lambda=1$ using the definition and properties of the H-function and the relation

$$\sqrt{\pi}\Gamma(2z) = 2^{2z-1}\Gamma(z)\Gamma(z+\tfrac{1}{2}), \tag{15}$$

(13) is simplified to

$$G(x,t;1,1) = \frac{a^2 t}{\pi^{(n+1)/2}|x|^{n+1}}H_{1,1}^{1,1}\left(\frac{a^4t^2}{|x|^2}\middle|\begin{matrix}(1/2-(n/2),1)\\(0,1)\end{matrix}\right). \tag{16}$$

Expanding the H-function in (16) into the series according to (A4) and (A5), respectively, we obtain the Cauchy distribution

$$G(x,t;1,1) = \frac{\Gamma\left(\frac{n+1}{2}\right)}{\pi^{(n+1)/2}}\frac{a^2 t}{((a^2t)^2+|x|^2)^{(n+1)/2}}. \tag{17}$$

Similarly if $\gamma=\lambda=2$ (13) is simplified to

$$G(x,t;2,2) = \frac{t}{2\pi^{(n-1)/2}(at)^n}H_{1,1}^{1,0}\left(\frac{|x|^2}{a^2t^2}\middle|\begin{matrix}((3-n)/2,1)\\(0,1)\end{matrix}\right). \tag{18}$$

According to (A4) we expand the H-function in (18) and obtain

$$G(x,t;2,2) = \frac{1}{2a\pi^{(n-1)/2}\Gamma\left(\frac{3-n}{2}\right)(a^2t^2 - |x|^2)^{(n-1)/2}}, \quad |x| < at. \tag{19}$$

If n is odd and more than 1 the right-hand side of (19) equals zero while if n is even $(n=2k)$ (19) becomes

$$G(x,t;2,2) = \frac{(-1)^{k-1}1\cdot 3\cdot 5\cdot\cdots\cdot(2k-1)}{a(2k-1)(2\pi)^k(a^2t^2 - |x|^2)^{(n-1)/2}}, \quad |x| < at, \tag{20}$$

which corresponds to the results of the wave equation.[3]

The solution of the equation

$$(D_t^\lambda + a^2(-\triangle)^{\gamma/2})u(x,t;\gamma,\lambda) = h(x,t) \tag{21}$$

may be expressed formally by the fundamental solution

$$u(x,t;\gamma,\lambda) = \int \mathrm{d}^n\xi \int_0^t G(x-\xi,t-\tau;\gamma,\lambda)h(\xi,\tau)\mathrm{d}\tau. \tag{22}$$

III. SOLUTION FOR INITIAL VALUE PROBLEM FOR TIME- AND SPACE-FRACTIONAL PARTIAL DIFFERENTIAL EQUATION IN THE CAPUTO AND THE RIEMANN–LIOUVILLE SENSE

In this section we assume the functions appeared to be locally absolutely integrable at least with respect to time t. The function $\Phi_\beta(t) := t_+^{\beta-1}/\Gamma(\beta)$ is locally integrable as $\beta > 0$ and thus the fractional integral of order $\beta(\beta > 0)$,

$$I_t^\beta f(t) = D_t^{-\beta} f(t) := \Phi_\beta(t) * f(t) = \int_0^t \frac{(t-\tau)^{\beta-1}}{\Gamma(\beta)} f(\tau)\mathrm{d}\tau \tag{23}$$

makes sense in the framework of classical functions. We supplement $I_t^0 f(t) = f(t)$ reasonably.[11,18]

The fractional derivatives of order $\lambda(\lambda > 0)$ in the Caputo and the Riemann–Liouville sense, respectively, are defined by

$${}^C D_t^\lambda f(t) := I_t^{m-\lambda}(f^{(m)}(t)), \quad t \neq 0,\ m-1 < \lambda \leqslant m \tag{24}$$

and

$${}^R D_t^\lambda f(t) := \frac{d^m}{\mathrm{d}t^m}(I_t^{m-\lambda} f(t)), \quad t \neq 0,\ m-1 < \lambda \leqslant m, \tag{25}$$

where m is positive integer and the derivatives of order m on the right-hand side of (24) and (25) are classical ones, and we always assume that the two kinds of fractional derivatives that occurred make sense in the framework of classical functions.

A. Solution in the caputo sense

The initial value problem for time- and space-fractional partial differential equation in the Caputo sense reads

$$({}^C D_t^\lambda + a^2(-\triangle)^{\gamma/2})u(x,t;\gamma,\lambda) = 0, \quad t > 0,\ \gamma > 0,\ 0 \leqslant m-1 < \lambda \leqslant m, \tag{26}$$

$$\frac{\partial^k u}{\partial t^k}(x,0+;\gamma,\lambda) = f_k(x), \quad k = 0,1,\ldots,m-1. \tag{27}$$

The relation between the derivative of order m in the sense of distributions, $D_t^m u$, and the one in the classical sense, $\partial^m u/\partial t^m$, is

$$D_t^m u = \frac{\partial^m u}{\partial t^m} + \sum_{k=0}^{m-1} f_k(x)\,\delta^{(m-1-k)}(t). \tag{28}$$

Inserting $D_t^\lambda u = D_t^{\lambda-m}(D_t^m u)$ and using the fractional integrals of Dirac delta function and its derivatives[18] $I_t^\mu \delta^{(k)}(t) = \Phi_{\mu-k}(t)$ we obtain

$$D_t^\lambda u = {}^C D_t^\lambda u + \sum_{k=0}^{m-1} f_k(x)\Phi_{1-\lambda+k}(t). \tag{29}$$

Thus in the sense of distributions u satisfies the equation

$$(D_t^\lambda + a^2(-\triangle)^{\gamma/2})u(x,t;\gamma,\lambda) = \sum_{k=0}^{m-1} f_k(x)\Phi_{1-\lambda+k}(t). \tag{30}$$

Utilizing (22) we obtain

$$u(x,t;\gamma,\lambda) = \sum_{k=0}^{m-1} \int f_k(\xi) G_k^C(x-\xi,t;\gamma,\lambda)\mathrm{d}^n\xi, \tag{31}$$

where $G_k^C(x,t;\gamma,\lambda) = D_t^{\lambda-1-k} G(x,t;\gamma,\lambda)$.

With the Mellin transform we may verify the fractional derivative of the H-function[9,16,21] (in the sense of distributions),

$$D_z^\nu[z^\alpha H_{p,q}^{m,n}(\,(az)^\beta\big|_{(b_j,\beta_j)}^{(a_j,\alpha_j)})] = z^{\alpha-\nu} H_{p+1,q+1}^{m,n+1}(\,(az)^\beta\big|_{(b_j,\beta_j),(\nu-\alpha,\beta)}^{(-\alpha,\beta),(a_j,\alpha_j)}), \tag{32}$$

where $a>0$, $\beta>0$ and $\alpha+\beta\,\min_{1\leqslant j\leqslant m}\Re(b_j/\beta_j)>-1$. Calculating the fractional derivative of the H-function we have

$$G_k^C(x,t;\gamma,\lambda) = \frac{t^k}{\pi^{n/2}|x|^n} H_{3,2}^{1,2}\left(\frac{2^\gamma a^2 t^\lambda}{|x|^\gamma}\,\middle|\,{}^{(0,1),(1-(n/2),\gamma/2);(0,\gamma/2)}_{(0,1);(-k,\lambda)}\right). \tag{33}$$

If $\gamma=2$ (33) is simplified to Schneider's result,[20]

$$G_k^C(x,t;2,\lambda) = \frac{|x|^{(2k/\lambda)-n}}{2\pi^{n/2}(2a)^{2k/\lambda}} H_{1,2}^{2,0}\left(\frac{|x|}{2at^{\lambda/2}}\,\middle|\,{}^{(1,\lambda/2)}_{(1-(k/\lambda),1/2),((n/2)-(k/\lambda),1/2)}\right), \tag{34}$$

where we confine $\lambda\leqslant 2$ in order to ensure the H-function makes sense. When $n=1$ by the definition of H-function and the relation (15) we may rewrite (34) to

$$G_k^C(x,t;2,\lambda)\big|_{n=1} = \frac{1}{2|x|}\left(\frac{|x|}{a}\right)^{2k/\lambda} H_{1,1}^{1,0}\left(\frac{|x|}{at^{\lambda/2}}\,\middle|\,{}^{(1,\lambda/2)}_{(1-(2k/\lambda),1)}\right), \tag{35}$$

which is proved, with the series expression of the H-function, to be a Wright function[10] also,

$$G_k^C(x,t;2,\lambda)\big|_{n=1} = \frac{1}{2at^{(\lambda/2)-k}} W_{-\lambda/2,1-(\lambda/2)+k}\left(-\frac{|x|}{at^{\lambda/2}}\right). \tag{36}$$

When $k=0$ the result is consistent with Mainardi.[14,15]

If $\lambda=1$ (thus $m=1$), $n=1$ and $u(x,+0;\gamma,1)=f_0(x)=\delta(x)$ the solution of problems (26) and (27) is $G_0^C(x,t;\gamma,1)$ and by the equality (15) and definition and properties of the H-function it can be rewritten as

$$G_0^C(x,t;\gamma,1)=\frac{1}{\gamma|x|}H_{2,2}^{1,1}\left(\frac{|x|}{(a^2t)^{1/\gamma}}\middle|\begin{matrix}(1,1/\gamma),(1,1/2)\\(1,1),(1,1/2)\end{matrix}\right), \tag{37}$$

which is obtained by West *et al.*[22] (where factor π is superfluous).

B. Solution in the Riemann–Liouville sense

The initial value problem for time- and space-fractional partial differential equation in the Riemann–Liouville sense reads

$$({}^RD_t^\lambda + a^2(-\triangle)^{\gamma/2})u(x,t;\gamma,\lambda)=0,\quad t>0,\quad \gamma>0,\quad 0\leqslant m-1<\lambda\leqslant m, \tag{38}$$

$${}^RD_t^{\lambda-k}u(x,0+;\gamma,\lambda)=g_k(x),\quad k=1,2,\ldots,m, \tag{39}$$

where ${}^RD_t^{\lambda-m}u=D_t^{\lambda-m}u$. We consider the derivative of order λ in the sense of generalized functions $D_t^\lambda u$. It can be decomposed to $D_t^\lambda u=D_t^m(D_t^{\lambda-m}u)$, where D_t^m denotes the generalized derivative of order m. Using the relation between generalized derivatives and classical derivatives we obtain

$$D_t^\lambda u={}^RD_t^\lambda u+\sum_{k=1}^m g_k(x)\,\delta^{(k-1)}(t). \tag{40}$$

Inserting (38) yields the equation in the sense of generalized functions,

$$(D_t^\lambda + a^2(-\triangle)^{\gamma/2})u(x,t;\gamma,\lambda)=\sum_{k=1}^m g_k(x)\,\delta^{(k-1)}(t). \tag{41}$$

Utilizing (22) we obtain

$$u(x,t;\gamma,\lambda)=\sum_{k=1}^m\int g_k(\xi)G_k^R(x-\xi,t;\gamma,\lambda)\mathrm{d}^n\xi, \tag{42}$$

where $G_k^R(x,t;\gamma,\lambda)=D_t^{k-1}G(x,t;\gamma,\lambda)$. Calculating the derivative of the H-function we have

$$G_k^R(x,t;\gamma,\lambda)=\frac{t^{\lambda-k}}{\pi^{n/2}|x|^n}H_{3,2}^{1,2}\left(\frac{2^\gamma a^2t^\lambda}{|x|^\gamma}\middle|\begin{matrix}(0,1),(1-(n/2),\gamma/2);(0,\gamma/2)\\(0,1);(k-\lambda,\lambda)\end{matrix}\right). \tag{43}$$

As $\gamma=2$, $m=1$, and $g_1(x)=A\delta(x)$ the solution of the problems (38) and (39) may be simplified as Hilfer's result,[13]

$$G_1^R(x,t;2,\lambda)=\frac{At^{\lambda-1}}{\pi^{n/2}|x|^n}H_{1,2}^{2,0}\left(\frac{|x|^2}{4a^2t^\lambda}\middle|\begin{matrix}(\lambda,\lambda)\\(1,1),(n/2,1)\end{matrix}\right). \tag{44}$$

We note that directly calculating the Laplace transforms of the Caputo and the Riemann–Liouville derivatives also involves the initial values of integer-order derivatives and fractional-order derivatives, respectively.[18] Here we reveal it in the distribution sense.

IV. CONCLUSIONS

The partial differential equation with both the time-fractional derivative and the space-fractional Laplace operator is considered and solved in terms of the Fox H-function. The time-fractional derivatives in the sense of generalized functions, Caputo and Riemann–Liouville are considered, respectively. The initial value problems in the Caputo sense and the Riemann–Liouville sense have unified form in the sense of generalized functions although Caputo's frac-

tional derivatives involve the initial values of derivatives of integer order while the Riemann–Liouville involve the initial values of derivatives and integral of fractional order. Some previous results are contained in our results.

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APPENDIX: FOX'S *H*-FUNCTION

Fox's H-function is defined by the contour integral,[1,6,16,21]

$$H_{p,q}^{m,n}(z) = H_{p,q}^{m,n}\left(z\Big|_{(b_1,\beta_1),\ldots,(b_q,\beta_q)}^{(a_1,\alpha_1),\ldots,(a_p,\alpha_p)}\right) := \frac{1}{2\pi i}\int_L h(s)z^s \mathrm{d}s, \tag{A1}$$

where $h(s)$ is given by

$$h(s) = \frac{\prod_{j=1}^{m}\Gamma(b_j-\beta_j s)\prod_{j=1}^{n}\Gamma(1-a_j+\alpha_j s)}{\prod_{j=m+1}^{q}\Gamma(1-b_j+\beta_j s)\prod_{j=n+1}^{p}\Gamma(a_j-\alpha_j s)}. \tag{A2}$$

Here m,n,p,q are integers satisfying $m^2+n^2\neq 0$, $0\leqslant n\leqslant p, 0\leqslant m\leqslant q$ and empty products are interpreted as unity. The parameters $a_j (j=1,\ldots,p)$ and $b_j (j=1,\ldots,q)$ are complex numbers and $\alpha_j (j=1,\ldots,p)$ and $\beta_j (j=1,\ldots,q)$ are positive numbers satisfying $P_a \cap P_b = \varnothing$, where $P_a=\{s=(b_j+k)/\beta_j, j=1,2,\ldots,m; k=0,1,2,\ldots\}$ and $P_b=\{s=(a_j-1-k)/\alpha_j, j=1,2,\ldots,n; k=0,1,2,\ldots\}$. The integration contour L runs from $s=c-i\infty$ to $s=c+i\infty$ such that P_a lies to the right of L and P_b to the left of L.

Let

$$\mu = \sum_{j=1}^{q}\beta_j - \sum_{j=1}^{p}\alpha_j, \quad \beta = \prod_{j=1}^{p}\alpha_j^{\alpha_j}\prod_{j=1}^{q}\beta_j^{-\beta_j}. \tag{A3}$$

When $\mu\geqslant 0$ and $m\geqslant 1$, the H-function can be expanded to

$$H_{p,q}^{m,n}(z) = -\sum_{s\in P_a}\mathrm{Res}(h(s)z^s), \tag{A4}$$

which exists for all $z\neq 0$ if $\mu>0$ and for $0<|z|<\beta^{-1}$ if $\mu=0$.

When $\mu\leqslant 0$ and $n\geqslant 1$, the H-function can be expanded to

$$H_{p,q}^{m,n}(z) = \sum_{s\in P_b}\mathrm{Res}(h(s)z^s), \tag{A5}$$

which exists for all $z\neq 0$ if $\mu<0$ and for $|z|>\beta^{-1}$ if $\mu=0$.

We list some properties of the H-function,

$$H_{p,q}^{m,n}\left(z\Big|_{(b_1,\beta_1),\ldots,(b_q,\beta_q)}^{(a_1,\alpha_1),\ldots,(a_p,\alpha_p)}\right) = H_{q,p}^{n,m}\left(\frac{1}{z}\,\Bigg|\,{}^{(1-b_1,\beta_1),\ldots,(1-b_q,\beta_q)}_{(1-a_1,\alpha_1),\ldots,(1-a_p,\alpha_p)}\right). \tag{A6}$$

$$H_{p,q}^{m,n}\left(z\Big|_{(b_1,\beta_1),\cdots,(b_{q-1},\beta_{q-1}),(a_1,\alpha_1)}^{(a_1,\alpha_1),\cdots,(a_p,\alpha_p)}\right) = H_{p-1,q-1}^{m,n-1}\left(z\Big|_{(b_1,\beta_1),\cdots,(b_{q-1},\beta_{q-1})}^{(a_2,\alpha_2),\cdots,(a_p,\alpha_p)}\right), \quad n>0, \quad q>m, \tag{A7}$$

$$\frac{1}{k}H_{p,q}^{m,n}\left(z\Big|_{(b_1,\beta_1),\ldots,(b_q,\beta_q)}^{(a_1,\alpha_1),\ldots,(a_p,\alpha_p)}\right)=H_{p,q}^{m,n}\left(z^k\Big|_{(b_1,k\beta_1),\ldots,(b_q,k\beta_q)}^{(a_1,k\alpha_1),\ldots,(a_p,k\alpha_p)}\right),\quad k>0, \tag{A8}$$

$$z^{\sigma}H_{p,q}^{m,n}\left(z\Big|_{(b_1,\beta_1),\ldots,(b_q,\beta_q)}^{(a_1,\alpha_1),\ldots,(a_p,\alpha_p)}\right)=H_{p,q}^{m,n}\left(z\Big|_{(b_1+\sigma\beta_1,\beta_1),\ldots,(b_q+\sigma\beta_q,\beta_q)}^{(a_1+\sigma\alpha_1,\alpha_1),\ldots,(a_p+\sigma\alpha_p,\alpha_p)}\right). \tag{A9}$$

Property (A6) enables us to transform an H-function with $\mu=\Sigma_{j=1}^{q}\beta_j-\Sigma_{j=1}^{p}\alpha_j<0$ to one with $\mu>0$ and vice versa.

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A unified and complete construction of all finite dimensional irreducible representations of gl(2|2)

Yao-Zhong Zhang and Mark D. Gould
Department of Mathematics, University of Queensland, Brisbane, Qld 4072, Australia

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Representations of the non-semisimple superalgebra gl(2|2) in the standard basis are investigated by means of the vector coherent state method and boson-fermion realization. All finite-dimensional irreducible typical and atypical representations and lowest weight (indecomposable) Kac modules of gl(2|2) are constructed explicitly through the explicit construction of all $gl(2)\oplus gl(2)$ particle states (multiplets) in terms of boson and fermion creation operators in the super-Fock space. This gives a unified and complete treatment of finite-dimensional representations of gl(2|2) in explicit form, essential for the construction of primary fields of the corresponding current superalgebra at arbitrary level. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1812829]

I. INTRODUCTION

Recently there is much research interest in superalgebras and their corresponding nonunitary conformal field theories (CFTs), because of their applications in high energy and condensed matter physics including topological field theory,[1,2] logarithmic CFTs (see, e.g., Ref. 3, and references therein), disordered systems, and the integer quantum Hall effects.[4–11] In such contexts, the vanishing of superdimensions and Virasoro central charges and the existence of primary fields with negative dimensions are crucial.[5,6] The most interesting algebras with such properties are osp($n|n$) and gl($n|n$).

In most physical applications, one needs the explicit construction of finite-dimensional representations of a superalgebra. This is particularly the case in superalgebra CFTs. To construct primary fields of such CFTs in terms of free fields, one has to construct the finite-dimensional representations of the superalgebras explicitly. The explicit construction of the primary fields is essential in the investigation of disordered systems by the supersymmetric method.

Unlike ordinary bosonic algebras, there are two types of representations for most superalgebras. They are the so-called typical and atypical representations. The typical representations are irreducible and are similar to the usual representations that appear in ordinary bosonic algebras. The atypical representations have no counterpart in the bosonic algebra setting. They can be irreducible or not fully reducible (i.e., reducible or indecomposable). This makes the study of representations of superalgebras very difficult.

Representations of osp(2|2) were investigated in Refs. 12 and 13. A unified construction of finite-dimensional typical and atypical representations of osp(2|2) were given in Refs. 14 and 15 by means of the vector coherent state method. This enabled the explicit construction of all primary fields of the osp(2|2) CFT[16,14] in terms of free fields.[17,18]

In this paper we investigate finite-dimensional representations of the non-semisimple superalgebra gl(2|2). All finite-dimensional irreducible typical and atypical representations and lowest weight (indecomposable) Kac modules of gl(2|2) are constructed explicitly through the explicit construction of all $gl(2)\oplus gl(2)$ particle states (multiplets) in terms of the boson and fermion creation operators in the super-Fock space. This we believe gives a unified and complete treatment of all finite-dimensional irreducible representations of gl(2|2) in explicit form.

Let us point out that the finite-dimensional representations of gl(2|2) have also been investigated in Refs. 19,20 using the GT basis. Our method is completely different from and in our

opinion is simpler than the method used in these two references. Moreover, our results can be used to construct primary fields of the corresponding gl(2|2) CFTs at arbitrary level, which is the subject of a separate work.

This paper is organized as follows. In Sec. II, we introduce our notations and derive a free boson-fermion realization of gl(2|2) by means of the vector coherent state method. In Sec. III, we describe the explict construction of independent $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$ particle states in the super-Fock space. We derive the actions of odd simple generators of gl(2|2) on these multiplets. The 16 independent multiplets constructed span all finite-dimensional irreducible typical representations of gl(2|2). In Sec. IV, we deduce and construct all four types of finite-dimensional irreducible atypical representations and lowest weight (indecomposable) Kac modules of gl(2|2).

II. BOSON-FERMION REALIZATION OF gl(2|2)

In this section, we obtain a boson-fermion realization of the superalgebra gl(2|2) in the standard basis.

This superalgebra is non-semisimple and can be written as $\mathrm{gl}(2|2)=\mathrm{gl}(2|2)^{\mathrm{even}}\oplus\mathrm{gl}(2|2)^{\mathrm{odd}}$, where

$$\mathrm{gl}(2|2)^{\mathrm{even}}=\mathrm{gl}(2)\oplus\mathrm{gl}(2)=\{I\}\oplus\{\{E_{12},E_{21},H_1\}\oplus\{E_{34},E_{43},H_2\},N\},$$

$$\mathrm{gl}(2|2)^{\mathrm{odd}}=\{E_{13},E_{31},E_{23},E_{32},E_{24},E_{42},E_{14},E_{41}\}. \tag{2.1}$$

In the standard basis, E_{12},E_{34},E_{23} (E_{21},E_{43},E_{32}) are simple raising (lowering) generators, E_{13},E_{14},E_{24} (E_{31},E_{41},E_{42}) are non-simple raising (lowering) generators and H_1,H_2,I,N are elements of the Cartan subalgebra. We have

$$H_1=E_{11}-E_{22},\quad H_2=E_{33}-E_{44},$$

$$I=E_{11}+E_{22}+E_{33}+E_{44}, \tag{2.2}$$

$$N=E_{11}+E_{22}-E_{33}-E_{44}+\beta I$$

with β being an arbitrary parameter. That N is not uniquely determined is a consequence of the fact that gl(2|2) is non-semisimple. The generators obey the following (anti)commutation relations:

$$[E_{ij},E_{kl}]=\delta_{jk}E_{il}-(-1)^{([i]+[j])([k]+[l])}\delta_{il}E_{kj}, \tag{2.3}$$

where $[E_{ij},E_{kl}]\equiv E_{ij}E_{kl}-(-1)^{([i]+[j])([k]+[l])}E_{kl}E_{ij}$ is a commutator or an anticommutator, $[1]=[2]=0$, $[3]=[4]=1$, and E_{ii}, $i=1,2,3,4$ are related to H_1,H_2,I,N via (2.2). The quadratic Casimir of the algebra is given by $C_2=\Sigma_{AB}(-1)^{[B]}E_{AB}E_{BA}$.

Let $|hw\rangle$ be the highest weight state of highest weight (J_1,J_2,q,p) of gl(2|2) defined by

$$H_1|hw\rangle=2J_1|hw\rangle,\quad H_2|hw\rangle=2J_2|hw\rangle,$$

$$I|hw\rangle=2q|hw\rangle,\quad N|hw\rangle=2p|hw\rangle, \tag{2.4}$$

$$E_{12}|hw\rangle=E_{34}|hw\rangle=E_{23}|hw\rangle=E_{13}|hw\rangle=E_{14}|hw\rangle=E_{24}|hw\rangle=0.$$

Here J_1,J_2 are positive integers and half-integers and q,p are arbitrary complex numbers. Define the coherent state[21,22]

$$e^{E_{21}a_{12}+E_{43}a_{34}+E_{31}\alpha_{13}+E_{32}\alpha_{23}+E_{42}\alpha_{24}+E_{41}\alpha_{14}}|hw\rangle.$$

Then state vectors are mapped into functions

$$\psi_{J_1,J_2,q,p} = \langle hw|e^{\alpha_{13}^\dagger E_{13}+\alpha_{23}^\dagger E_{23}+\alpha_{24}^\dagger E_{24}+\alpha_{14}^\dagger E_{14}+a_{12}^\dagger E_{12}+a_{34}^\dagger E_{34}}|\psi\rangle|0\rangle, \tag{2.5}$$

and operators A are mapped as follows

$$A|\psi\rangle \to \Gamma(A)\psi_{J_1,J_2,q,p} = \langle hw|e^{\alpha_{13}^\dagger E_{13}+\alpha_{23}^\dagger E_{23}+\alpha_{24}^\dagger E_{24}+\alpha_{14}^\dagger E_{14}+a_{12}^\dagger E_{12}+a_{34}^\dagger E_{34}}A|\psi\rangle|0\rangle. \tag{2.6}$$

Here $\alpha_{ij}^\dagger$ (α_{ij}) are fermion operators with number operators $N_{\alpha_{ij}}$ and $a_{ij}^\dagger$ (a_{ij}) are boson operators with number operators $N_{a_{ij}}$. They obey relations

$$\{\alpha_{ij},\alpha_{kl}^\dagger\} = \delta_{ik}\delta_{jl}, \quad (\alpha_{ij})^2 = (\alpha_{ij}^\dagger)^2 = 0,$$

$$[N_{\alpha_{ij}},\alpha_{kl}] = -\delta_{ik}\delta_{jl}\alpha_{kl}, \quad [N_{\alpha_{ij}},\alpha_{kl}^\dagger] = \delta_{ik}\delta_{jl}\alpha_{kl}^\dagger,$$

$$[a_{ij},a_{kl}^\dagger] = \delta_{ik}\delta_{jl},$$

$$[N_{a_{ij}},a_{kl}] = -\delta_{ik}\delta_{jl}a_{kl}, \quad [N_{a_{ij}},a_{kl}^\dagger] = \delta_{ik}\delta_{jl}a_{kl}^\dagger, \tag{2.7}$$

and all other (anti-)commutators vanish. Moreover, $a_{12}|0\rangle = a_{34}|0\rangle = \alpha_{23}|0\rangle = \alpha_{13}|0\rangle = \alpha_{14}|0\rangle = \alpha_{24}|0\rangle = 0$.

Taking E_{12}, E_{34}, etc. in turn and after long algebraic computations, we find the following representation of simple generators in terms of the boson and fermion operators:

$$\begin{aligned}
\Gamma(E_{12}) &= a_{12} - \tfrac{1}{2}\alpha_{23}^\dagger\alpha_{13} + \tfrac{1}{2}(\tfrac{1}{6}a_{34}^\dagger\alpha_{23}^\dagger - \alpha_{24}^\dagger)\alpha_{14},\\
\Gamma(E_{34}) &= a_{34} + \tfrac{1}{2}\alpha_{23}^\dagger\alpha_{24} + \tfrac{1}{2}(\tfrac{1}{6}a_{12}^\dagger\alpha_{23}^\dagger + \alpha_{13}^\dagger)\alpha_{14},\\
\Gamma(E_{23}) &= \alpha_{23} + \tfrac{1}{2}a_{12}^\dagger\alpha_{13} - \tfrac{1}{2}a_{34}^\dagger(\alpha_{24} + \tfrac{1}{3}a_{12}^\dagger\alpha_{14}),\\
\Gamma(H_1) &= 2J_1 - 2N_{a_{12}} + N_{\alpha_{23}} - N_{\alpha_{13}} + N_{\alpha_{24}} - N_{\alpha_{14}},\\
\Gamma(H_2) &= 2J_2 - 2N_{a_{34}} + N_{\alpha_{23}} + N_{\alpha_{13}} - N_{\alpha_{24}} - N_{\alpha_{14}},\\
\Gamma(I) &= 2q,\\
\Gamma(N) &= 2p - 2(N_{\alpha_{23}} + N_{\alpha_{13}} + N_{\alpha_{24}} + N_{\alpha_{14}}),
\end{aligned} \tag{2.8}$$

$$\begin{aligned}
\Gamma(E_{21}) &= a_{12}^\dagger[2J_1 - N_{a_{12}} + \tfrac{1}{2}(N_{\alpha_{23}} - N_{\alpha_{13}} + N_{\alpha_{24}} - N_{\alpha_{14}})] - \alpha_{13}^\dagger\alpha_{23} - \alpha_{14}^\dagger\alpha_{24} - \tfrac{1}{4}(a_{12}^\dagger)^2\alpha_{23}^\dagger\alpha_{13}\\
&\quad + \tfrac{1}{12}a_{12}^\dagger a_{34}^\dagger\alpha_{23}^\dagger\alpha_{24} - \tfrac{1}{4}a_{12}^\dagger(a_{12}^\dagger\alpha_{24}^\dagger + \tfrac{1}{3}a_{34}^\dagger\alpha_{13}^\dagger)\alpha_{14},
\end{aligned}$$

$$\begin{aligned}
\Gamma(E_{43}) &= a_{34}^\dagger[2J_2 - N_{a_{34}} + \tfrac{1}{2}(N_{\alpha_{23}} + N_{\alpha_{13}} - N_{\alpha_{24}} - N_{\alpha_{14}})] + \alpha_{24}^\dagger\alpha_{23} + \alpha_{14}^\dagger\alpha_{13} + \tfrac{1}{4}(a_{34}^\dagger)^2\alpha_{23}^\dagger\alpha_{24}\\
&\quad - \tfrac{1}{12}a_{12}^\dagger a_{34}^\dagger\alpha_{23}^\dagger\alpha_{13} + \tfrac{1}{4}(a_{34}^\dagger\alpha_{12}^\dagger + \tfrac{1}{3}a_{12}^\dagger\alpha_{24}^\dagger)a_{34}^\dagger\alpha_{14},
\end{aligned}$$

$$\begin{aligned}
\Gamma(E_{32}) &= \alpha_{23}^\dagger[q - J_1 + J_2 + \tfrac{1}{2}(N_{a_{12}} - N_{a_{34}} + N_{\alpha_{13}} - N_{\alpha_{24}})] + \alpha_{13}^\dagger a_{12} + \alpha_{24}^\dagger a_{34}\\
&\quad + \tfrac{1}{6}\alpha_{23}^\dagger(a_{12}^\dagger\alpha_{24}^\dagger + a_{34}^\dagger\alpha_{13}^\dagger)\alpha_{14},
\end{aligned}$$

and the representation for non-simple generators is easily obtained from that of simple generators above by means of the commutation relations. Equation (2.8) gives a boson-fermion realization of

the non-semisimple superalgebra gl(2|2) in the standard basis. In this realization, the Casimir takes a constant value: $C_2=2[(J_1-J_2)(J_1+J_2+1)+q(p-2)]$.

III. TYPICAL REPRESENTATIONS OF gl(2|2)

Representations of gl(2|2) are labeled by (J_1,J_2,q,p) with J_1,J_2 being positive integers or half-integers and q,p being arbitrary complex numbers. Consider a particle state in the super-Fock space, obtained by acting the creation operators on the vacuum vector $|0\rangle$. We call such a state a level-x state if $\Gamma(H_1),\Gamma(H_2),\Gamma(I),\Gamma(N)$ have eigenvalues $2(m_1+x),2(m_2+x),2q,2(p-x)$, respectively. Obviously, a level-x state is a product of x number of fermion creation operators and boson creation operators of the form $(a_{12}^\dagger)^{J_1-m_1-y}(a_{34}^\dagger)^{J_2-m_2-\bar{y}}$ acting on $|0\rangle$, where $y,\bar{y}$ are certain integers or half-integers, depending on the values of x. It is easy to see that there are 16 independent such states obtained from 16 independent combinations of the creation operators. This includes one level-0 state, four level-1 states, six level-2 states, four level-3 states and one level-4 state. Thus each gl(2|2) representation decomposes into at most 16 representations of the even subalgebra $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$. Let us construct representations for $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$ out of the above states. First the level-0 and level-4 states are already representations of $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$ with highest weights (J_1,J_2,q,p) and $(J_1,J_2,q,p-4)$, respectively. We denote these two multiplets by $|J_1,m_1,J_2,m_2,q;p\rangle$ and $|J_1,m_1,J_2,m_2,q;p-4\rangle$, respectively. So

$$
\begin{aligned}
&|J_1,m_1,J_2,m_2,q;p\rangle=(a_{12}^\dagger)^{J_1-m_1}(a_{34}^\dagger)^{J_2-m_2}|0\rangle,\\
&m_1=J_1,J_1-1,\ldots,-J_1,\quad m_2=J_2,J_2-1,\ldots,-J_2,\\
&|J_1,m_1,J_2,m_2,q;p-4\rangle=\alpha_{23}^\dagger\alpha_{13}^\dagger\alpha_{24}^\dagger\alpha_{14}^\dagger(a_{12}^\dagger)^{J_1-m_1-4}(a_{34}^\dagger)^{J_2-m_2-4}|0\rangle,\\
&m_1=J_1-4,J_1-5,\ldots,-(J_1+4),\quad m_2=J_2-4,J_2-5,\ldots,-(J_2+4).
\end{aligned}
\tag{3.1}
$$

Both multiplets have dimension $(2J_1+1)(2J_2+1)$.

It can be shown that other level-x states can be combined into independent level-x multiplets of $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$ with certain highest weights. The procedure is the following. For a given level x, one considers a combination Ψ_{J_1,m_1,J_2,m_2} of all level-x states. The combination coefficients are in general functions of J_1,m_1,J_2,m_2. We require that Ψ_{J_1,m_1,J_2,m_2} be a representation of $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$. In order for the representation to be finite-dimensional, the actions of the $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$ generators on Ψ_{J_1,m_1,J_2,m_2} must have the following form:

$$
\begin{aligned}
&\Gamma(E_{12})\Psi_{J_1,m_1,J_2,m_2}=(J_1-m_1-z)\Psi_{J_1,m_1+1,J_2,m_2},\\
&\Gamma(E_{21})\Psi_{J_1,m_1,J_2,m_2}=(J_1+m_1+\bar{z})\Psi_{J_1,m_1-1,J_2,m_2},\\
&\Gamma(E_{34})\Psi_{J_1,m_1,J_2,m_2}=(J_2-m_2-u)\Psi_{J_1,m_1,J_2,m_2+1},\\
&\Gamma(E_{43})\Psi_{J_1,m_1,J_2,m_2}=(J_2+m_2+\bar{u})\Psi_{J_1,m_1,J_2,m_2-1},
\end{aligned}
\tag{3.2}
$$

where $z,\bar{z},u,\bar{u}$ are some integers or half-integers to be determined together with the combination coefficients. These requirements give rise to difference equations for the combination coefficients. Solving these difference equations simutaneously for each level x, we determine the combination coefficients and $z,\bar{z},u,\bar{u}$. The procedure of solving the difference equations for each level x is nontrivial and requires long algebraic manipulations. Here we omit the details and only list the results as follows.

The four level-1 states can be combined into four independent multiplets of $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$ with highest weights $(J_1-\frac{1}{2},J_2-\frac{1}{2},q,p-1),(J_1+\frac{1}{2},J_2-\frac{1}{2},q,p-1),(J_1+\frac{1}{2},J_2+\frac{1}{2},q,p-1)$ and $(J_1-\frac{1}{2},J_2+\frac{1}{2},q,p-1)$, respectively:

$$|J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-1\rangle=(\alpha_{14}^\dagger+\tfrac{1}{2}a_{12}^\dagger\alpha_{24}^\dagger-\tfrac{1}{2}\alpha_{13}^\dagger a_{34}^\dagger-\tfrac{1}{3}a_{12}^\dagger\alpha_{23}^\dagger a_{34}^\dagger)\times(a_{12}^\dagger)^{J_1-m_1-3/2}(a_{34}^\dagger)^{J_2-m_2-3/2}|0\rangle,\quad J_1,J_2\geqslant\tfrac{1}{2},$$

$$m_1=J_1-\tfrac{3}{2},J_1-\tfrac{5}{2},\ldots,-(J_1+\tfrac{1}{2}),\quad m_2=J_2-\tfrac{3}{2},J_2-\tfrac{5}{2},\ldots,-(J_2+\tfrac{1}{2}),$$

$$|J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-1\rangle=[\tfrac{1}{2}(3J_1+m_1+\tfrac{5}{2})a_{12}^\dagger\alpha_{24}^\dagger-\tfrac{1}{3}(2J_1+m_1+2)a_{12}^\dagger\alpha_{23}^\dagger a_{34}^\dagger-(J_1-m_1-\tfrac{1}{2})\times(\alpha_{14}^\dagger-\tfrac{1}{2}\alpha_{13}^\dagger a_{34}^\dagger)](a_{12}^\dagger)^{J_1-m_1-3/2}(a_{34}^\dagger)^{J_2-m_2-3/2}|0\rangle,\quad J_2\geqslant\tfrac{1}{2},$$

$$m_1=J_1-\tfrac{1}{2},J_1-\tfrac{3}{2},\ldots,-(J_1+\tfrac{3}{2}),\quad m_2=J_2-\tfrac{3}{2},J_2-\tfrac{5}{2},\ldots,-(J_2+\tfrac{1}{2}),$$

$$\begin{aligned}|J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-1\rangle=[&-\tfrac{1}{4}((3J_1+m_1+\tfrac{5}{2})(3J_2+m_2+\tfrac{5}{2})+\tfrac{1}{3}(J_1-m_1-\tfrac{1}{2})(J_2-m_2-\tfrac{1}{2}))\\&\times a_{12}^\dagger\alpha_{23}^\dagger a_{34}^\dagger+\tfrac{1}{2}(J_1-m_1-\tfrac{1}{2})(3J_2+m_2+\tfrac{5}{2})\alpha_{13}^\dagger a_{34}^\dagger\\&-\tfrac{1}{2}(3J_1+m_1+\tfrac{5}{2})\\&\times(J_2-m_2-\tfrac{1}{2})a_{12}^\dagger\alpha_{24}^\dagger+(J_1-m_1-\tfrac{1}{2})(J_2-m_2-\tfrac{1}{2})\alpha_{14}^\dagger]\\&\times(a_{12}^\dagger)^{J_1-m_1-3/2}(a_{34}^\dagger)^{J_2-m_2-3/2}|0\rangle,\end{aligned}\tag{3.3}$$

$$m_1=J_1-\tfrac{1}{2},J_1-\tfrac{3}{2},\ldots,-(J_1+\tfrac{3}{2}),\quad m_2=J_2-\tfrac{1}{2},J_2-\tfrac{3}{2},\ldots,-(J_2+\tfrac{3}{2}),$$

$$|J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-1\rangle=[\tfrac{1}{2}(3J_2+m_2+\tfrac{5}{2})\alpha_{13}^\dagger a_{34}^\dagger+\tfrac{1}{3}(2J_2+m_2+2)a_{12}^\dagger\alpha_{23}^\dagger a_{34}^\dagger+(J_2-m_2-\tfrac{1}{2})\times(\alpha_{14}^\dagger-\tfrac{1}{2}a_{12}^\dagger\alpha_{24}^\dagger)](a_{12}^\dagger)^{J_1-m_1-3/2}(a_{34}^\dagger)^{J_2-m_2-3/2}|0\rangle,\quad J_1\geqslant\tfrac{1}{2},$$

$$m_1=J_1-\tfrac{3}{2},J_1-\tfrac{5}{2},\ldots,-(J_1+\tfrac{1}{2}),\quad m_2=J_2-\tfrac{1}{2},J_2-\tfrac{3}{2},\ldots,-(J_2+\tfrac{3}{2}).$$

The dimensions for these multiplets are $(2J_1)(2J_2),(2J_1+2)(2J_2),(2J_1+2)(2J_2+2)$ and $(2J_1)(2J_2+2)$, respectively.

The six level-2 states can be combined into six independent multiplets of $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$ with highest weights $(J_1,J_2-1,q,p-2),(J_1-1,J_2,q,p-2),(J_1+1,J_2,q,p-2),(J_1,J_2+1,q,p-2),(J_1,J_2,q,p-2)$ and $(J_1,J_2,q,p-2)$, respectively:

$$|J_1,m_1,J_2-1,m_2,q;p-2\rangle=\alpha_{24}^\dagger\alpha_{14}^\dagger(a_{12}^\dagger)^{J_1-m_1-2}(a_{34}^\dagger)^{J_2-m_2-3}|0\rangle+\tfrac{1}{2}[-\alpha_{23}^\dagger\alpha_{14}^\dagger+\tfrac{1}{6}\alpha_{23}^\dagger\alpha_{24}^\dagger a_{12}^\dagger+\alpha_{13}^\dagger\alpha_{24}^\dagger+\tfrac{1}{2}\alpha_{23}^\dagger\alpha_{13}^\dagger a_{34}^\dagger](a_{12}^\dagger)^{J_1-m_1-2}(a_{34}^\dagger)^{J_2-m_2-2}|0\rangle,$$

$$J_2\geqslant1,\quad m_1=J_1-2,J_1-3,\ldots,-(J_1+2),\quad m_2=J_2-3,J_2-4,\ldots,-(J_2+1),$$

$$|J_1-1,m_1,J_2,m_2,q;p-2\rangle=\alpha_{13}^\dagger\alpha_{14}^\dagger(a_{12}^\dagger)^{J_1-m_1-3}(a_{34}^\dagger)^{J_2-m_2-2}|0\rangle+\tfrac{1}{2}[\alpha_{23}^\dagger\alpha_{14}^\dagger+\tfrac{1}{6}\alpha_{23}^\dagger\alpha_{13}^\dagger a_{34}^\dagger+\alpha_{13}^\dagger\alpha_{24}^\dagger+\tfrac{1}{2}\alpha_{23}^\dagger\alpha_{24}^\dagger a_{12}^\dagger](a_{12}^\dagger)^{J_1-m_1-2}(a_{34}^\dagger)^{J_2-m_2-2}|0\rangle,$$

$$J_1\geqslant1,\quad m_1=J_1-3,J_1-4,\ldots,-(J_1+1),\quad m_2=J_2-2,J_2-3,\ldots,-(J_2+2),$$

$$
\begin{aligned}
|J_1+1,m_1,J_2,m_2,q;p-2\rangle = &[\tfrac{1}{2}[J_1-m_1-1+(3J_1+m_1+3)(3J_1+m_1+5)]\alpha_{23}^\dagger\alpha_{24}^\dagger(a_{12}^\dagger)^2\\
&+(J_1-m_1-1)(J_1-m_1-2)(\alpha_{13}^\dagger\alpha_{14}^\dagger+\tfrac{1}{12}a_{12}^\dagger\alpha_{23}^\dagger\alpha_{13}^\dagger a_{34}^\dagger)-\tfrac{1}{2}(J_1-m_1-1)\\
&\times(3J_1+m_1+4)a_{12}^\dagger(\alpha_{13}^\dagger\alpha_{24}^\dagger+\alpha_{23}^\dagger\alpha_{14}^\dagger)](a_{12}^\dagger)^{J_1-m_1-3}(a_{34}^\dagger)^{J_2-m_2-2}|0\rangle,
\end{aligned}
$$

$$
m_1=J_1-1,J_1-2,\ldots,-(J_1+3),\quad m_2=J_2-2,J_2-3,\ldots,-(J_2+2),
\tag{3.4}
$$

$$
\begin{aligned}
|J_1,m_1,J_2+1,m_2,q;p-2\rangle = &[\tfrac{1}{4}[J_2-m_2-1+(3J_2+m_2+3)(3J_2+m_2+5)]\alpha_{23}^\dagger\alpha_{13}^\dagger(a_{34}^\dagger)^2\\
&+\tfrac{1}{2}(J_2-m_2-1)(3J_2+m_2+4)(\alpha_{23}^\dagger\alpha_{14}^\dagger-\alpha_{13}^\dagger\alpha_{24}^\dagger)a_{34}^\dagger+(J_2-m_2-1)\\
&\times(J_2-m_2-2)(\alpha_{24}^\dagger\alpha_{14}^\dagger+\tfrac{1}{12}\alpha_{23}^\dagger\alpha_{24}^\dagger a_{12}^\dagger a_{34}^\dagger)](a_{12}^\dagger)^{J_1-m_1-2}(a_{34}^\dagger)^{J_2-m_2-3}|0\rangle,
\end{aligned}
$$

$$
m_1=J_1-2,J_1-3,\ldots,-(J_1+2),\quad m_2=J_2-1,J_2-2,\ldots,-(J_2+3),
$$

$$
\begin{aligned}
[J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathbf{I}} = &(J_2-m_2-2)\alpha_{24}^\dagger\alpha_{14}^\dagger(a_{12}^\dagger)^{J_1-m_1-2}(a_{34}^\dagger)^{J_2-m_2-3}|0\rangle\\
&+[\tfrac{1}{2}(J_2+m_2+2)(\alpha_{23}^\dagger\alpha_{14}^\dagger-\alpha_{13}^\dagger\alpha_{24}^\dagger)+\tfrac{1}{12}(J_2-m_2-2)\alpha_{23}^\dagger\alpha_{24}^\dagger a_{12}^\dagger\\
&-\tfrac{1}{4}(3J_2+m_2+2)\alpha_{23}^\dagger\alpha_{13}^\dagger a_{34}^\dagger](a_{\mathbf{34}}^\dagger)^{J_1-m_1-2}(a_{34}^\dagger)^{J_2-m_2-2}|0\rangle,
\end{aligned}
$$

$$
m_1=J_1-2,J_1-3,\ldots,-(J_1+2),\quad m_2=J_2-1,J_2-2,\ldots,-(J_2+2),
$$

$$
\begin{aligned}
[J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathbf{II}} = &(J_1-m_1-2)\alpha_{13}^\dagger\alpha_{14}^\dagger(a_{12}^\dagger)^{J_1-m_1-3}(a_{34}^\dagger)^{J_2-m_2-2}|0\rangle\\
&+[-\tfrac{1}{2}(J_1+m_1+2)(\alpha_{13}^\dagger\alpha_{24}^\dagger+\alpha_{23}^\dagger\alpha_{14}^\dagger)+\tfrac{1}{12}(J_1-m_1-2)\alpha_{23}^\dagger\alpha_{13}^\dagger a_{34}^\dagger\\
&-\tfrac{1}{4}(3J_1+m_1+2)\alpha_{23}^\dagger\alpha_{24}^\dagger a_{12}^\dagger](a_{12}^\dagger)^{J_1-m_1-2}(a_{34}^\dagger)^{J_2-m_2-2}|0\rangle,
\end{aligned}
$$

$$
m_1=J_1-2,J_1-3,\ldots,-(J_1+2),\quad m_2=J_2-1,J_2-2,\ldots,-(J_2+2).
$$

Notice that the last two multiplets, which have been denoted above by $|J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathbf{I}}$ and $|J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathbf{II}}$, respectively, have the same highest weight $(J_1,J_2,q,p-2)$. This means that multiplicity will in general appear in the $\mathrm{gl}(2|2)\downarrow\mathrm{gl}(2)\oplus\mathrm{gl}(2)$ branching rule. It is easy to see from the above expressions that $|J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathbf{I}}\equiv 0$ when $J_2=0$ and $|J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathbf{II}}\equiv 0$ when $J_1=0$.

The dimensions for the first four multiplets are $(2J_1+1)(2J_2-1),(2J_1-1)(2J_2+1),(2J_1+3)\times(2J_2+1)$ and $(2J_1+1)(2J_2+3)$, respectively. The dimension for $|J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathbf{I}}$ is $(2J_1+1)(2J_2+1)$ if $J_2\neq 0$ and zero if $J_2=0$. Similarly, the dimension for $|J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathbf{II}}$ is $(2J_1+1)(2J_2+1)$ if $J_1\neq 0$ and zero if $J_1=0$.

Finally, the four level-3 states are combined into four independent multiplets of $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$ with highest weights $\left(J_1-\frac{1}{2},J_2-\frac{1}{2},q,p-3\right),\left(J_1+\frac{1}{2},J_2-\frac{1}{2},q,p-3\right),\left(J_1-\frac{1}{2},J_2+\frac{1}{2},q,p-3\right)$ and $\left(J_1+\frac{1}{2},J_2+\frac{1}{2},q,p-3\right)$, respectively:

$$
\begin{aligned}
|J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-3\rangle = &[(\alpha_{13}^\dagger+\tfrac{1}{2}a_{12}^\dagger\alpha_{23}^\dagger)\alpha_{24}^\dagger\alpha_{14}^\dagger+\tfrac{1}{2}\alpha_{23}^\dagger\alpha_{13}^\dagger(\alpha_{14}^\dagger a_{34}^\dagger+\tfrac{1}{3}a_{12}^\dagger\alpha_{24}^\dagger a_{34}^\dagger)]\\
&\times(a_{12}^\dagger)^{J_1-m_1-7/2}(a_{34}^\dagger)^{J_2-m_2-7/2}|0\rangle,
\end{aligned}
$$

$$
J_1,J_2\geqslant\tfrac{1}{2},\quad m_1=J_1-\tfrac{7}{2},\ldots,-(J_1+\tfrac{5}{2}),\quad m_2=J_2-\tfrac{7}{2},\ldots,-(J_2+\tfrac{5}{2}),
$$

$$|J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-3\rangle=[-\tfrac{1}{2}(3J_1+m_1+\tfrac{9}{2})\alpha_{23}^{\dagger}\alpha_{24}^{\dagger}\alpha_{14}^{\dagger}a_{12}^{\dagger}+(J_1-m_1-\tfrac{5}{2})(-\alpha_{24}^{\dagger}+\tfrac{1}{2}\alpha_{23}^{\dagger}a_{34}^{\dagger})$$
$$\times\alpha_{13}^{\dagger}\alpha_{14}^{\dagger}-\tfrac{1}{6}(5J_1+m_1+\tfrac{11}{2})\alpha_{23}^{\dagger}\alpha_{13}^{\dagger}\alpha_{24}^{\dagger}a_{12}^{\dagger}a_{34}^{\dagger}]$$
$$\times(a_{12}^{\dagger})^{J_1-m_1-7/2}(a_{34}^{\dagger})^{J_2-m_2-7/2}|0\rangle,$$

$$J_2\geqslant\tfrac{1}{2},\quad m_1=J_1-\tfrac{5}{2},\ldots,-(J_1+\tfrac{7}{2}),\quad m_2=J_2-\tfrac{7}{2},\ldots,-(J_2+\tfrac{5}{2}),$$

$$|J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-3\rangle=[-\tfrac{1}{2}(3J_2+m_2+\tfrac{9}{2})\alpha_{23}^{\dagger}\alpha_{13}^{\dagger}\alpha_{14}^{\dagger}a_{34}^{\dagger}+(J_2-m_2-\tfrac{5}{2})(\alpha_{13}^{\dagger}+\tfrac{1}{2}\alpha_{23}^{\dagger}a_{12}^{\dagger})$$
$$\times\alpha_{24}^{\dagger}\alpha_{14}^{\dagger}-\tfrac{1}{6}(5J_2+m_2+\tfrac{11}{2})\alpha_{23}^{\dagger}\alpha_{13}^{\dagger}\alpha_{24}^{\dagger}a_{12}^{\dagger}a_{34}^{\dagger}]$$
$$\times(a_{12}^{\dagger})^{J_1-m_1-7/2}(a_{34}^{\dagger})^{J_2-m_2-7/2}|0\rangle, \tag{3.5}$$

$$J_1\geqslant\tfrac{1}{2},\quad m_1=J_1-\tfrac{7}{2},\ldots,-(J_1+\tfrac{5}{2}),\quad m_2=J_2-\tfrac{5}{2},\ldots,-(J_2+\tfrac{7}{2}),$$

$$|J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-3\rangle=[\tfrac{1}{4}((3J_1+m_1+\tfrac{9}{2})(3J_2+m_2+\tfrac{9}{2})-\tfrac{1}{3}(J_1-m_1-\tfrac{5}{2})(J_2-m_2-\tfrac{5}{2}))$$
$$\times a_{12}^{\dagger}\alpha_{23}^{\dagger}\alpha_{13}^{\dagger}\alpha_{24}^{\dagger}a_{34}^{\dagger}-\tfrac{1}{2}(J_1-m_1-\tfrac{5}{2})(3J_2+m_2+\tfrac{9}{2})\alpha_{23}^{\dagger}\alpha_{13}^{\dagger}\alpha_{14}^{\dagger}a_{34}^{\dagger}$$
$$-\tfrac{1}{2}(3J_1+m_1+\tfrac{9}{2})(J_2-m_2-\tfrac{5}{2})a_{12}^{\dagger}\alpha_{23}^{\dagger}\alpha_{24}^{\dagger}\alpha_{14}^{\dagger}+(J_1-m_1-\tfrac{5}{2})$$
$$\times(J_2-m_2-\tfrac{5}{2})\alpha_{13}^{\dagger}\alpha_{24}^{\dagger}\alpha_{14}^{\dagger}](a_{12}^{\dagger})^{J_1-m_1-7/2}(a_{34}^{\dagger})^{J_2-m_2-7/2}|0\rangle,$$

$$m_1=J_1-\tfrac{5}{2},\ldots,-(J_1+\tfrac{7}{2}),\quad m_2=J_2-\tfrac{5}{2},\ldots,-(J_2+\tfrac{7}{2}).$$

The dimensions for these multiplets are $(2J_1)(2J_2)$, $(2J_1+2)(2J_2)$, $(2J_1)(2J_2+2)$ and $(2J_1+2)(2J_2+2)$, respectively.

The actions of the odd generators of $\mathrm{gl}(2|2)$ on the $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$ multiplets (3.1) and (3.3)–(3.5) can be computed by means of the free boson-fermion realization of the generators. In the following we list the actions of the odd simple generators. The actions of odd non-simple generators can be easily obtained using the commutation relations.

First for the level-0 multiplet, we have the actions of the odd simple generators

$$\Gamma(E_{23})|J_1,m_1,J_2,m_2,q;p\rangle=0,$$

$$\Gamma(E_{32})|J_1,m_1,J_2,m_2,q;p\rangle=\frac{1}{(2J_1+1)(2J_2+1)}$$
$$\times[-(q+J_1-J_2)(J_1-m_1)(J_2-m_2)|J_1-\tfrac{1}{2},m_1-\tfrac{1}{2},J_2-\tfrac{1}{2},$$
$$m_2-\tfrac{1}{2},q;p-1\rangle$$
$$-(q-J_1-J_2-1)(J_2-m_2)|J_1+\tfrac{1}{2},m_1-\tfrac{1}{2},J_2-\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-1\rangle$$
$$-(q-J_1+J_2)|J_1+\tfrac{1}{2},m_1-\tfrac{1}{2},J_2+\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-1\rangle$$
$$+(q+J_1+J_2+1)(J_1-m_1)|J_1-\tfrac{1}{2},m_1-\tfrac{1}{2},J_2+\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-1\rangle]. \tag{3.6}$$

From (3.6) we see that when $q=J_1-J_2$ (resp., $-J_1+J_2$) the third (resp., first) term vanishes and, if $q=J_1+J_2+1$ (resp., $-J_1-J_2-1$), then the second (resp., fourth) term disappears. This indicates that when $q=\pm(J_1-J_2),\pm(J_1+J_2+1)$ atypical representations arise (see the next section for details).

For the four level-1 multiplets, we obtain the following actions of the odd simple generators, after long algebraic manipulations,

$$\Gamma(E_{23})|J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q,p-1\rangle=-|J_1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p\rangle,$$

$$\Gamma(E_{23})|J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q,p-1\rangle=-(J_1+m_1+\tfrac{3}{2})|J_1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p\rangle,$$

$$\Gamma(E_{23})|J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q,p-1\rangle=-(J_1+m_1+\tfrac{3}{2})(J_2+m_2+\tfrac{3}{2})|J_1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p\rangle,$$

$$\Gamma(E_{23})|J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q,p-1\rangle=-(J_2+m_2+\tfrac{3}{2})|J_1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p\rangle,$$

$$\begin{aligned}
&\Gamma(E_{32})|J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q,p-1\rangle\\
&\quad=-\frac{J_2-m_2-3/2}{2J_2}(q-J_1-J_2-1)|J_1,m_1-\tfrac{1}{2},J_2-1,m_2-\tfrac{1}{2},q;p-2\rangle\\
&\qquad+\frac{q-J_1+J_2-1}{2J_2}|J_1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-2\rangle_{\mathbf{I}}\\
&\qquad-\frac{q-J_1+J_2+1}{2J_2}|J_1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-2\rangle_{\mathbf{II}}\\
&\qquad+\frac{J_1-m_1-3/2}{2J_1}(q+J_1+J_2+1)|J_1-1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-2\rangle,
\end{aligned}\tag{3.7}$$

$$\begin{aligned}
&\Gamma(E_{32})|J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q,p-1\rangle\\
&\quad=\frac{(J_1-m_1-1/2)(J_2-m_2-3/2)}{2J_2}(q+J_1-J_2)|J_1,m_1-\tfrac{1}{2},J_2-1,m_2-\tfrac{1}{2},q;p-2\rangle\\
&\qquad-\frac{J_1-m_1-1/2}{2J_2}(q+J_1+J_2)|J_1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-2\rangle_{\mathbf{I}}\\
&\qquad-\frac{(J_1-m_1-1/2}{2(J_1+1)}(q+J_1+J_2+2)|J_1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-2\rangle_{\mathbf{II}}\\
&\qquad+\frac{q-J_1+J_2}{2(J_1+1)}|J_1+1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-2\rangle,
\end{aligned}$$

$$\begin{aligned}
&\Gamma(E_{32})|J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q,p-1\rangle\\
&\quad=-\frac{(J_1-m_1-1/2)(J_2-m_2-1/2)}{2(J_2+1)}(q+J_1-J_2-1)|J_1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-2\rangle_{\mathbf{I}}\\
&\qquad+\frac{(J_1-m_1-1/2)(J_2-m_2-1/2)}{2(J_1+1)}(q+J_1-J_2+1)|J_1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-2\rangle_{\mathbf{II}}\\
&\qquad-\frac{(J_2-m_2-1/2}{2(J_1+1)}(q-J_1-J_2-1)|J_1+1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-2\rangle\\
&\qquad+\frac{J_1-m_1-1/2}{2(J_2+1)}(q+J_1+J_2+1)|J_1,m_1-\tfrac{1}{2},J_2+1,m_2-\tfrac{1}{2},q;p-2\rangle,
\end{aligned}$$

$$\Gamma(E_{32})|J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q,p-1\rangle$$
$$=-\frac{J_2-m_2-1/2}{2(J_2+1)}(q-J_1-J_2-2)|J_1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-2\rangle_{\mathbf{I}}$$
$$-\frac{J_2-m_2-1/2}{2J_1}(q-J_1-J_2)|J_1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-2\rangle_{\mathbf{II}}$$
$$+\frac{(J_1-m_1-3/2)(J_2-m_2-1/2)}{2J_1}(q+J_1-J_2)|J_1-1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-2\rangle$$
$$+\frac{q-J_1+J_2}{2(J_2+1)}|J_1,m_1-\tfrac{1}{2},J_2+1,m_2-\tfrac{1}{2},q;p-2\rangle.$$

Similar to the level-1 case, we find after long algebraic computations that the actions of the odd simple generators on the six level-2 multiplets are given by

$$\Gamma(E_{23})|J_1,m_1,J_2-1,m_2,q;p-2\rangle=-\frac{J_1+m_1+2}{2J_1+1}|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle$$
$$+\frac{1}{2J_1+1}|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle,$$

$$\Gamma(E_{23})|J_1-1,m_1,J_2,m_2,q;p-2\rangle=\frac{J_2+m_2+2}{2J_2+1}|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle$$
$$+\frac{1}{2J_1+1}|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle,$$

$$\Gamma(E_{23})|J_1+1,m_1,J_2,m_2,q;p-2\rangle=\frac{(J_1+m_1+3)(J_2+m_2+2)}{2J_2+1}|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle$$
$$-\frac{J_1+m_1+3}{2J_2+1}|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle,$$

$$\Gamma(E_{23})|J_1,m_1,J_2+1,m_2,q;p-2\rangle=\frac{J_2+m_2+3}{2J_1+1}|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle$$
$$+\frac{(J_1+m_1+2)(J_2+m_2+3)}{2J_1+1}$$
$$\times|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle,$$

$$\Gamma(E_{23})|J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathbf{I}}=\frac{1}{(2J_1+1)(2J_2+1)}[(J_2+1)(J_1+m_1+2)(J_2+m_2+2)$$
$$\times|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle$$
$$-(J_2+1)(J_2+m_2+2)|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle$$
$$-J_2|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle-J_2(J_1+m_1+2)|J_1$$
$$-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle],\qquad(3.8)$$

$$\Gamma(E_{23})|J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathbf{II}} = \frac{1}{(2J_1+1)(2J_2+1)}[-(J_1+1)(J_1+m_1+2)(J_2+m_2+2)$$
$$\times|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle$$
$$-J_1(J_2+m_2+2)|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle$$
$$+J_1|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle$$
$$-(J_1+1)(J_1+m_1+2)|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-1\rangle,$$

$$\Gamma(E_{32})|J_1,m_1,J_2-1,m_2,q;p-2\rangle = \frac{J_1-m_1-2}{2J_1+1}(q+J_1+J_2+1)$$
$$\times|J_1-\tfrac{1}{2},m_1-\tfrac{1}{2},J_2-\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle$$
$$-\frac{q-J_1+J_2}{2J_1+1}|J_1+\tfrac{1}{2},m_1-\tfrac{1}{2},J_2-\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle,$$

$$\Gamma(E_{32})|J_1-1,m_1,J_2,m_2,q;p-2\rangle = \frac{J_2-m_2-2}{2J_2+1}(q-J_1-J_2-1)$$
$$\times|J_1-\tfrac{1}{2},m_1-\tfrac{1}{2},J_2-\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle$$
$$-\frac{q-J_1+J_2}{2J_2+1}|J_1-\tfrac{1}{2},m_1-\tfrac{1}{2},J_2+\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle,$$

$$\Gamma(E_{32})|J_1+1,m_1,J_2,m_2,q;p-2\rangle = \frac{(J_1-m_1-1)(J_2-m_2-2)}{2J_2+1}(q+J_1-J_2)$$
$$\times|J_1+\tfrac{1}{2},m_1-\tfrac{1}{2},J_2-\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle$$
$$-\frac{J_1-m_1-1}{2J_2+1}(q+J_1+J_2+1)$$
$$\times|J_1+\tfrac{1}{2},m_1-\tfrac{1}{2},J_2+\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle,$$

$$\Gamma(E_{32})|J_1,m_1,J_2+1,m_2,q;p-2\rangle = \frac{(J_1-m_1-2)(J_2-m_2-1)}{2J_1+1}(q+J_1-J_2)|J_1-\tfrac{1}{2},m_1-\tfrac{1}{2},J_2+\tfrac{1}{2},m_2$$
$$-\tfrac{1}{2},q;p-3\rangle-\frac{J_2-m_2-1}{2J_1+1}(q-J_1-J_2-1)|J_1+\tfrac{1}{2},m_1-\tfrac{1}{2},J_2$$
$$+\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle,$$

$$\Gamma(E_{32})|J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathrm{I}} = \frac{1}{(2J_1+1)(2J_2+1)}[(J_2+1)(J_1-m_1-2)(J_2-m_2-2)$$
$$\times(q+J_1-J_2+1)|J_1-\tfrac{1}{2},m_1-\tfrac{1}{2},J_2-\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle-(J_2+1)$$
$$\times(J_2-m_2-2)(q-J_1-J_2)|J_1+\tfrac{1}{2},m_1-\tfrac{1}{2},J_2-\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle$$
$$+J_2(J_1-m_1-2)(q+J_1+J_2+2)|J_1-\tfrac{1}{2},m_1-\tfrac{1}{2},J_2+\tfrac{1}{2},$$
$$m_2-\tfrac{1}{2},q;p-3\rangle$$
$$-J_2(q-J_1+J_2+1)|J_1+\tfrac{1}{2},m_1-\tfrac{1}{2},J_2+\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle],$$

$$\Gamma(E_{32})|J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathrm{II}} = \frac{1}{(2J_1+1)(2J_2+1)}[(J_1+1)(J_1-m_1-2)(J_2-m_2-2)$$
$$\times(q+J_1-J_2-1)|J_1-\tfrac{1}{2},m_1-\tfrac{1}{2},J_2-\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle$$
$$+J_1(J_2-m_2-2)$$
$$\times(q-J_1-J_2-2)|J_1+\tfrac{1}{2},m_1-\tfrac{1}{2},J_2-\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle-(J_1+1)$$
$$\times(J_1-m_1-2)(q+J_1+J_2)|J_1-\tfrac{1}{2},m_1-\tfrac{1}{2},J_2+\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle$$
$$-J_1(q-J_1+J_2-1)|J_1+\tfrac{1}{2},m_1-\tfrac{1}{2},J_2+\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle].$$

The actions of the odd simple generators on the four level-3 multiplets can be obtained in a similar way. We list the results as follows:

$$\Gamma(E_{23})|J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q,p-3\rangle = \frac{J_2+m_2+5/2}{2J_2}|J_1,m_1+\tfrac{1}{2},J_2-1,m_2+\tfrac{1}{2},q;p-2\rangle$$
$$+\frac{1}{2J_2}|J_1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p-2\rangle_{\mathbf{I}}$$
$$+\frac{1}{2J_1}|J_1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p-2\rangle_{\mathbf{II}}$$
$$+\frac{J_1+m_1+5/2}{2J_1}|J_1-1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p-2\rangle,$$

$$\Gamma(E_{23})|J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q,p-3\rangle = -\frac{(J_1+m_1+7/2)(J_2+m_2+5/2)}{2J_2}$$
$$\times|J_1,m_1+\tfrac{1}{2},J_2-1,m_2+\tfrac{1}{2},q;p-2\rangle$$
$$+(J_1+m_1+\tfrac{7}{2})\left[-\frac{1}{2J_2}|J_1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p-2\rangle_{\mathbf{I}}\right.$$
$$\left.+\frac{1}{2(J_1+1)}|J_1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p-2\rangle_{\mathbf{II}}\right]$$
$$+\frac{1}{2(J_1+1)}|J_1+1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p-2\rangle,$$

$$\Gamma(E_{23})|J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q,p-3\rangle = (J_2+m_2+\tfrac{7}{2})\left[\frac{1}{2(J_2+1)}|J_1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p-2\rangle_{\mathbf{I}}\right.$$
$$\left.-\frac{1}{2J_1}|J_1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p-2\rangle_{\mathbf{II}}\right]$$
$$-\frac{(J_1+m_1+5/2)(J_2+m_2+7/2)}{2J_1}$$
$$\times|J_1-1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p-2\rangle$$
$$+\frac{1}{2(J_2+1)}|J_1,m_1+\tfrac{1}{2},J_2+1,m_2+\tfrac{1}{2},q;p-2\rangle,$$

$$\begin{aligned}\Gamma(E_{23})|J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q,p-3\rangle = &-(J_1+m_1+\tfrac{7}{2})(J_2+m_2+\tfrac{7}{2})\\ &\times\Bigg[\frac{1}{2(J_2+1)}|J_1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p-2\rangle_{\mathbf{I}}\\ &+\frac{1}{2(J_1+1)}|J_1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p-2\rangle_{\mathbf{II}}\Bigg]\\ &-\frac{J_2+m_2+7/2}{2(J_1+1)}|J_1+1,m_1+\tfrac{1}{2},J_2,m_2+\tfrac{1}{2},q;p-2\rangle\\ &-\frac{J_1+m_1+7/2}{2(J_2+1)}|J_1,m_1+\tfrac{1}{2},J_2+1,m_2+\tfrac{1}{2},q;p-2\rangle,\end{aligned} \tag{3.9}$$

$$\Gamma(E_{32})|J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q,p-3\rangle=(q-J_1+J_2)|J_1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-4\rangle,$$

$$\Gamma(E_{32})|J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q,p-3\rangle=(q+J_1+J_2+1)(J_1-m_1-\tfrac{5}{2})|J_1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-4\rangle,$$

$$\Gamma(E_{32})|J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q,p-3\rangle=(q-J_1-J_2-1)(J_2-m_2-\tfrac{5}{2})|J_1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-4\rangle,$$

$$\begin{aligned}\Gamma(E_{32})|J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q,p-3\rangle=&(q+J_1-J_2)(J_1-m_1-\tfrac{5}{2})(J_2-m_2-\tfrac{5}{2})\\ &\times|J_1,m_1-\tfrac{1}{2},J_2,m_2-\tfrac{1}{2},q;p-4\rangle.\end{aligned}$$

Finally, the actions of the odd simple generators on the level-4 multiplet are

$$\begin{aligned}\Gamma(E_{23})|J_1,m_1,J_2,m_2,q;p-4\rangle=&\frac{1}{(2J_1+1)(2J_2+1)}[(J_1+m_1+4)(J_2+m_2+4)\\ &\times|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-3\rangle\\ &+(J_2+m_2+4)|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-3\rangle\\ &+(J_1+m_1+4)|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-3\rangle\\ &+|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q,p-3\rangle],\end{aligned}$$

$$\Gamma(E_{32})|J_1,m_1,J_2,m_2,q;p-4\rangle=0. \tag{3.10}$$

Summarizing, we have obtained 16 independent multiplets, (3.1), (3.3), and (3.4), of gl(2) $\oplus$ gl(2) which span finite-dimensional representations of gl(2|2). For generic q, these multiplets span irreducible typical representations of gl(2|2) of dimension $16(2J_1+1)(2J_2+1)$. Denote by $\pi_{(J_1,J_2,q,p)}$ and $\sigma_{(J_1,J_2,q,p)}$ the gl(2|2) and gl(2) $\oplus$ gl(2) representations with highest weight (J_1,J_2,q,p), respectively. Then the gl(2|2) $\downarrow$ gl(2) $\oplus$ gl(2) branching rule for generic q is given by

$$\begin{aligned}\pi_{(J_1,J_2,q,p)}=&\sigma_{(J_1,J_2,q,p)}\oplus\sigma_{(J_1-1/2,J_2-1/2,q,p-1)}\oplus\sigma_{(J_1+1/2,J_2-1/2,q,p-1)}\oplus\sigma_{(J_1+1/2,J_2+1/2,q,p-1)}\\ &\oplus\sigma_{(J_1-1/2,J_2+1/2,q,p-1)}\oplus\sigma_{(J_1,J_2-1,q,p-2)}\oplus\sigma_{(J_1-1,J_2,q,p-2)}\oplus\sigma_{(J_1+1,J_2,q,p-2)}\oplus\sigma_{(J_1,J_2+1,q,p-2)}\\ &\oplus 2\times\sigma_{(J_1,J_2,q,p-2)}\oplus\sigma_{(J_1-1/2,J_2-1/2,q,p-3)}\oplus\sigma_{(J_1+1/2,J_2-1/2,q,p-3)}\oplus\sigma_{(J_1-1/2,J_2+1/2,q,p-3)}\\ &\oplus\sigma_{(J_1+1/2,J_2+1/2,q,p-3)}\oplus\sigma_{(J_1,J_2,q,p-4)}.\end{aligned} \tag{3.11}$$

Some remarks are in order. First, irreducible representations are obtained as submodules (not subquotients) of the super-Fock space generated by $\{a_{ij},a_{ij}^\dagger,\alpha_{ij},\alpha_{ij}^\dagger\}$. This is because the gl(2|2)-module structure of the super-Fock space is the contragredient dual of the Verma model over gl(2|2). Second, as $|J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathbf{I}}\equiv 0$ when $J_2=0$ and $|J_1,m_1,J_2,m_2,q;p-2\rangle_{\mathbf{II}}\equiv 0$

when $J_1=0$, thus if $J_1=0$ or $J_2=0$ only one copy of $\sigma_{(J_1,J_2,q,p-2)}$ remains in the above branching rule. In particular, when $J_1=0=J_2$ which corresponds to the 16-dimensional typical representation of gl$(2|2)$, $\sigma_{(J_1,J_2,q,p-2)}$ disappears and the branching rule becomes

$$\pi_{(0,0,q,p)} = \sigma_{(0,0,q,p)} \oplus \sigma_{(1/2,1/2,q,p-1)} \oplus \sigma_{(1,0,q,p-2)} \oplus \sigma_{(0,1,q,p-2)} \oplus \sigma_{(1/2,1/2,q,p-3)} \oplus \sigma_{(0,0,q,p-4)} \tag{3.12}$$

or $\underline{16}=\underline{1}\oplus\underline{4}\oplus\underline{3}\oplus\underline{3}\oplus\underline{4}\oplus\underline{1}$.

IV. ATYPICAL REPRESENTATIONS OF gl(2|2)

We have different types of atypical representations of gl$(2|2)$. From the actions of the odd generators on the gl$(2)\oplus$gl(2) multiplets, we see that when $q=\pm(J_1-J_2),\pm(J_1+J_2+1)$, the representations become atypical. The Casimir for such representations vanishes, and yet they are not the trivial one-dimensional representation.

A. Atypical representation corresponding to $q=J_1-J_2$

Case 1. $q=J_1-J_2$, $J_1\neq J_2$: Let us introduce the following independent combinations:

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym1}} = J_1|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}} + J_2|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}},$$

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym1}} = J_1|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}} - J_2|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}} \tag{4.1}$$

for $J_1\neq 0, J_2\neq 0$. When $J_1=0$ or $J_2=0$, we let $|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym1}}\equiv 0$ and

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym1}} = \begin{cases} |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}} & \text{if } J_1=0, \\ |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}} & \text{if } J_2=0. \end{cases} \tag{4.2}$$

It can be shown from the actions of odd generators that when $q=J_1-J_2$,

$$\begin{aligned}\Gamma(E_{23})|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym1}} = {} & \frac{1}{(2J_1+1)(2J_2+1)} \\ & \times[(J_1-J_2)(J_1+m_1+2)(J_2+m_2+2) \\ & \times|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q;p-1\rangle \\ & -J_1(2J_2+1)(J_2+m_2+2)|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q;p-1\rangle \\ & -(2J_1+1)J_2(J_1+m_1+2)|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2}, \\ & J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q;p-1\rangle],\end{aligned} \tag{4.3}$$

which does not contain the multiplet $|J_1+\frac{1}{2},m_1,J_2+\frac{1}{2},m_2,q;p-1\rangle$, and

$$\begin{aligned}\Gamma(E_{32})|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym1}} = {} & \frac{(J_1-J_2)(4J_1J_2+2J_1+2J_2+1)}{(2J_1+1)(2J_2+1)}(J_1-m_1-2)(J_2-m_2-2) \\ & \times|J_1-\tfrac{1}{2},m_1-\tfrac{1}{2},J_2-\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle.\end{aligned} \tag{4.4}$$

Thus when $q=J_1-J_2$, if one starts with the level-0 state $|J_1,m_1,J_2,m_2,q;p\rangle$ then we find using the actions (3.6)–(3.10) that the following gl$(2)\oplus$gl(2) multiplets,

$$|J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-1\rangle,$$

$$|J_1+1,m_1,J_2,m_2,q,p-2\rangle, \quad |J_1,m_1,J_2+1,m_2,q,p-2\rangle,$$

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym1}},\quad |J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-3\rangle, \tag{4.5}$$

$$|J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-3\rangle,\quad |J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-3\rangle,$$

$$|J_1,m_1,J_2,m_2,q,p-4\rangle$$

disappear, and only the following multiplets

$$|J_1,m_1,J_2,m_2,q,p\rangle,$$

$$|J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-1\rangle,\quad |J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-1\rangle,$$

$$|J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-1\rangle,$$

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym1}},\quad |J_1-1,m_1,J_2,m_2,q,p-2\rangle,$$

$$|J_1,m_1,J_2-1,m_2,q,p-2\rangle,\quad |J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-3\rangle \tag{4.6}$$

remain. They form irreducible atypical representations of $\mathrm{gl}(2|2)$ of dimension $8[(2J_1+1)J_2+J_1(2J_2+1)]$. So the $\mathrm{gl}(2|2)\downarrow \mathrm{gl}(2)\oplus\mathrm{gl}(2)$ branching rule for $q=J_1-J_2$ is given by

$$\pi_{(J_1,J_2,q,p)} = \sigma_{(J_1,J_2,q,p)} \oplus \sigma_{(J_1-1/2,J_2-1/2,q,p-1)} \oplus \sigma_{(J_1+1/2,J_2+1/2,q,p-1)} \oplus \sigma_{(J_1-1/2,J_2+1/2,q,p-1)} \oplus \sigma_{(J_1,J_2,q,p-2)}$$
$$\oplus \sigma_{(J_1-1,J_2,q,p-2)} \oplus \sigma_{(J_1,J_2-1,q,p-2)} \oplus \sigma_{(J_1-1/2,J_2-1/2,q,p-3)}. \tag{4.7}$$

It should be understood here that $\sigma_{(J_1,J_2,q,p-2)}$ disappears when $J_1=0$ or $J_2=0$.

Case 2. $q=J_1-J_2, J_1=J_2$ so that $q=0$: In this case, we define the independent combinations:

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym1}'} = |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}} + |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}},$$

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym1}'} = |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}} - |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}}. \tag{4.8}$$

Both $|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym1}'}$ and $|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym1}'}$ vanish if $J_1=0=J_2$. Then it is easily shown that $\Gamma(E_{23})|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym1}'}$ does not contain $|J_1-\frac{1}{2},m_1,J_2-\frac{1}{2},m_2,q;p-1\rangle$ and $|J_1+\frac{1}{2},m_1,J_2+\frac{1}{2},m_2,q;p-1\rangle$, and $\Gamma(E_{32})|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym1}'}=0$. Thus only the following multiplets

$$|J_1,m_1,J_2,m_2,q,p\rangle,$$

$$|J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-1\rangle,\quad |J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-1\rangle, \tag{4.9}$$

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym1}'},$$

survive, and they give irreducible atypical representations of dimension $4\left[(2J_1+1)(2J_2+1)-\frac{1}{2}\right]$ if $J_1=J_2\neq 0$ and the trivial one-dimensional representation if $J_1=0=J_2$ [for which the last three multiplets in (4.9) disappear].

Case 3. Lowest weight (indecomposable) Kac modules: Other types of atypical representations when $q=J_1-J_2$ are not irreducible. One such type of representation is obtained by starting with the level-4 state $|J_1,m_1,J_2,m_2,q;p-4\rangle$. These representations contain all 16 multiplets and a nonseparable invariant subspace provided by the multiplets (4.6) [or (4.9) when $J_1=J_2$]. These representations are not fully reducible (i.e., indecomposable) and have dimension $16(2J_1+1)(2J_2+1)$.

B. Atypical representations corresponding to $q=-J_1+J_2$

The case where $J_1=J_2$ so that $q=0$ is the same as case 2 of the last subsection. So in this subsection we only consider the $J_1\neq J_2$ case.

1. Irreducible representations

Let us introduce the following independent combinations:

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym2}}=(J_1+1)|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}}+(J_2+1)|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}},$$

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym2}}=(J_1+1)|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}}-(J_2+1)|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}} \tag{4.10}$$

for $J_1\neq 0, J_2\neq 0$, and let

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym2}}=\begin{cases}|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}} & \text{if } J_1=0,\\ |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}} & \text{if } J_2=0,\end{cases} \tag{4.11}$$

and $|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym2}}=0$ if $J_1=0$ or $J_2=0$.

Similar to the $q=J_1-J_2$ case, we may show that when $q=-J_1+J_2$,

$$\begin{aligned}\Gamma(E_{23})|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym2}}=\frac{1}{(2J_1+1)(2J_2+1)}[&-(2J_1+1)(J_2+1)(J_2+m_2+2)\\ &\times|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q;p-1\rangle+(J_1-J_2)\\ &\times|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q;p-1\rangle-(J_1+1)(2J_2+1)\\ &\times(J_1+m_1+2)|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q;p-1\rangle],\end{aligned} \tag{4.12}$$

which is independent of $|J_1-\frac{1}{2},m_1,J_2-\frac{1}{2},m_2,q;p-1\rangle$ and

$$\begin{aligned}\Gamma(E_{32})|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym2}}=&\frac{(J_1-J_2)(4J_1J_2+2J_1+2J_2+1)}{(2J_1+1)(2J_2+1)}(J_1-m_1-2)(J_2-m_2-2)\\ &\times|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q;p-3\rangle.\end{aligned} \tag{4.13}$$

Thus when $q=-J_1+J_2$, if one starts with the level-0 state, then by the actions (3.6)–(3.10) one finds that the following $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$ multiplets,

$$\begin{gathered}|J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-1\rangle,\\ |J_1,m_1,J_2-1,m_2,q,p-2\rangle,\quad |J_1-1,m_1,J_2,m_2,q,p-2\rangle,\\ |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym2}},\quad |J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-3\rangle,\\ |J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-3\rangle,\quad |J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-3\rangle,\\ |J_1,m_1,J_2,m_2,q,p-4\rangle,\end{gathered} \tag{4.14}$$

drop out of the basis, and only the following multiplets,

$$|J_1,m_1,J_2,m_2,q,p\rangle,$$

$$|J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-1\rangle,\quad |J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-1\rangle,$$

$$|J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-1\rangle, \tag{4.15}$$

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym2}},\quad |J_1+1,m_1,J_2,m_2,q,p-2\rangle,$$

$$|J_1,m_1,J_2+1,m_2,q,p-2\rangle,\quad |J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-3\rangle,$$

survive. They form irreducible atypical representations of gl(2|2) of dimension $8[(J_1+1)(2J_2+1)+(2J_1+1)(J_2+1)]$. The branching rule in this case (i.e., $q=-J_1+J_2$) becomes

$$\begin{aligned}\pi_{(J_1,J_2,q,p)} = {} & \sigma_{(J_1,J_2,q,p)} \otimes \sigma_{(J_1+1/2,J_2+1/2,q,p-1)} \otimes \sigma_{(J_1+1/2,J_2-1/2,q,p-1)} \otimes \sigma_{(J_1-1/2,J_2+1/2,q,p-1)} \\ & \otimes \sigma_{(J_1,J_2,q,p-2)} \otimes \sigma_{(J_1+1,J_2,q,p-2)} \otimes \sigma_{(J_1,J_2+1,q,p-2)} \otimes \sigma_{(J_1+1/2,J_2+1/2,q,p-3)}.\end{aligned} \tag{4.16}$$

2. Lowest weight (indecomposable) Kac modules

If one starts with the level-4 state, then one gets atypical representations which are not irreducible. In such representations, all 16 multiplets appear but there exists a nonseparable invariant superspace generated by multiplets (4.15). These representations are indecomposable and have dimension $16(2J_1+1)(2J_2+1)$.

C. Atypical representations corresponding to $q=J_1+J_2+1$

1. Irreducible representations

Let us introduce the following independent combinations for $J_1\neq 0, J_2\neq 0$,

$$\begin{aligned}|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym3}} &= J_1|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}} + (J_2+1)|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}},\\ |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym3}} &= J_1|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}} - (J_2+1)|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}}.\end{aligned} \tag{4.17}$$

We let

$$\begin{aligned}|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym3}} &= \begin{cases}|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}} & \text{if } J_1=0,\\ 0 & \text{if } J_2=0,\end{cases}\\ |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym3}} &= \begin{cases}0 & \text{if } J_1=0,\\ |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}} & \text{if } J_2=0.\end{cases}\end{aligned} \tag{4.18}$$

It can be seen from the actions of odd generators that when $q=J_1+J_2+1$,

$$\begin{aligned}\Gamma(E_{23})|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym3}} = {} & \frac{1}{(2J_1+1)(2J_2+1)}[(2J_1+1)(J_2+1)(J_2+m_2+2)(J_2+m_2+2)\\ & \times|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q;p-1\rangle - J_1(2J_2+1)\\ & \times|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q;p-1\rangle\\ & +(J_1+J_2+1)(J_1+m_1+2)\\ & \times|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q;p-1\rangle],\end{aligned} \tag{4.19}$$

which does not contain the multiplet $|J_1+\frac{1}{2},m_1,J_2-\frac{1}{2},m_2,q;p-1\rangle$ and

$$\Gamma(E_{32})|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym3}}=\frac{(J_1+J_2+1)(4J_1J_2+J_1+J_2)+(J_1+J_2)^2}{(2J_1+1)(2J_2+1)}\times(J_1-m_1-2)|J_1-\tfrac{1}{2},m_1-\tfrac{1}{2},J_2+\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle. \tag{4.20}$$

Then similar to previous cases, when $q=J_1+J_2+1$, the following $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$ multiplets,

$$|J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-1\rangle,$$

$$|J_1,m_1,J_2-1,m_2,q,p-2\rangle,\quad |J_1+1,m_1,J_2,m_2,q,p-2\rangle,$$

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym3}},\quad |J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-3\rangle, \tag{4.21}$$

$$|J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-3\rangle,\quad |J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-3\rangle,$$

$$|J_1,m_1,J_2,m_2,q,p-4\rangle$$

disappear, and only the following multiplets,

$$|J_1,m_1,J_2,m_2,q,p\rangle,$$

$$|J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-1\rangle,\quad |J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-1\rangle,$$

$$|J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-1\rangle, \tag{4.22}$$

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym3}},\quad |J_1-1,m_1,J_2,m_2,q,p-2\rangle,$$

$$|J_1,m_1,J_2+1,m_2,q,p-2\rangle,\quad |J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-3\rangle$$

remain. They constitute irreducible atypical representations of $\mathrm{gl}(2|2)$ of dimension $8[(2J_1+1)\times(J_2+1)+J_1(2J_2+1)]$. The branching rule in this case (i.e., $q=J_1+J_2+1$) reads

$$\pi_{(J_1,J_2,q,p)}=\sigma_{(J_1,J_2,q,p)}\oplus\sigma_{(J_1-1/2,J_2-1/2,q,p-1)}\oplus\sigma_{(J_1+1/2,J_2+1/2,q,p-1)}\oplus\sigma_{(J_1-1/2,J_2+1/2,q,p-1)}\oplus\sigma_{(J_1,J_2,q,p-2)}\oplus\sigma_{(J_1-1,J_2,q,p-2)}\oplus\sigma_{(J_1,J_2+1,q,p-2)}\oplus\sigma_{(J_1-1/2,J_2+1/2,q,p-3)}. \tag{4.23}$$

Here one should keep in mind that $\sigma_{(J_1,J_2,q,p-2)}$ disappears if $J_1=0$.

2. Lowest weight (indecomposable) Kac representations

Similar to the previous cases, if one retains all 16 multiplets, then one gets lowest weight (indecomposable) Kac representations of $16(2J_1+1)(2J_2+1)$ which contain an invariant but non-separable subspace provided by multiplets (4.22).

D. Atypical representations corresponding to $q=-J_1-J_2-1$

1. Irreducible representations

In this case, we introduce the following independent combinations for $J_1\neq 0, J_2\neq 0$,

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym4}}=(J_1+1)|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}}+J_2|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}},$$

$$|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym4}} = (J_1+1)|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}} - J_2|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}} \tag{4.24}$$

and let

$$\begin{aligned} |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym4}} &= \begin{cases} 0 & \text{if } J_1=0, \\ |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{II}} & \text{if } J_2=0, \end{cases} \\ |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym4}} &= \begin{cases} |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{I}} & \text{if } J_1=0, \\ 0 & \text{if } J_2=0. \end{cases} \end{aligned} \tag{4.25}$$

It can be seen from the actions of odd generators that when $q=-J_1-J_2-1$,

$$\begin{aligned} \Gamma(E_{23})|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym4}} = \frac{1}{(2J_1+1)(2J_2+1)}[&(J_1+1)(2J_2+1)(J_2+m_2+2)(J_2+m_2+2) \\ &\times|J_1-\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q;p-1\rangle - (J_1+J_2+1) \\ &\times(J_2+m_2+2)|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2-\tfrac{1}{2},m_2+\tfrac{1}{2},q;p-1\rangle \\ &-(2J_1+1)J_2|J_1+\tfrac{1}{2},m_1+\tfrac{1}{2},J_2+\tfrac{1}{2},m_2+\tfrac{1}{2},q;p-1\rangle], \end{aligned} \tag{4.26}$$

which has no dependence on the multiplet $|J_1-\frac{1}{2},m_1,J_2+\frac{1}{2},m_2,q;p-1\rangle$ and

$$\begin{aligned} \Gamma(E_{32})|J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym4}} = &-\frac{(J_1+J_2+1)(4J_1J_2+J_1+J_2)+(J_1+J_2)^2}{(2J_1+1)(2J_2+1)} \\ &\times(J_2-m_2-2)|J_1+\tfrac{1}{2},m_1-\tfrac{1}{2},J_2-\tfrac{1}{2},m_2-\tfrac{1}{2},q;p-3\rangle. \end{aligned} \tag{4.27}$$

Thus when $q=-J_1-J_2-1$, the following $\mathrm{gl}(2)\oplus\mathrm{gl}(2)$ multiplets

$$\begin{gathered} |J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-1\rangle, \\ |J_1-1,m_1,J_2,m_2,q,p-2\rangle, \quad |J_1,m_1,J_2+1,m_2,q,p-2\rangle, \\ |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{sym4}}, \quad |J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-3\rangle, \\ |J_1-\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-3\rangle, \quad |J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-3\rangle, \\ |J_1,m_1,J_2,m_2,q,p-4\rangle \end{gathered} \tag{4.28}$$

drop out, and only the following multiplets

$$\begin{gathered} |J_1,m_1,J_2,m_2,q,p\rangle, \\ |J_1-\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-1\rangle, \quad |J_1+\tfrac{1}{2},m_1,J_2+\tfrac{1}{2},m_2,q;p-1\rangle, \\ |J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-1\rangle, \\ |J_1,m_1,J_2,m_2,q,p-2\rangle_{\mathbf{asym4}}, \quad |J_1,m_1,J_2-1,m_2,q,p-2\rangle, \end{gathered} \tag{4.29}$$

$$|J_1+1,m_1,J_2,m_2,q,p-2\rangle, \quad |J_1+\tfrac{1}{2},m_1,J_2-\tfrac{1}{2},m_2,q;p-3\rangle$$

remain. They give irreducible atypical representations of gl(2|2) of dimension $8[(J_1+1)(2J_2+1)+(2J_1+1)J_2]$. In this case the branching rule becomes

$$\pi_{(J_1,J_2,q,p)} = \sigma_{(J_1,J_2,q,p)} \oplus \sigma_{(J_1-1/2,J_2-1/2,q,p-1)} \oplus \sigma_{(J_1+1/2,J_2+1/2,q,p-1)} \oplus \sigma_{(J_1+1/2,J_2-1/2,q,p-1)} \oplus \sigma_{(J_1,J_2,q,p-2)} \oplus \sigma_{(J_1,J_2-1,q,p-2)} \oplus \sigma_{(J_1+1,J_2,q,p-2)} \oplus \sigma_{(J_1+1/2,J_2-1/2,q,p-3)}. \tag{4.30}$$

Here it should be understood that $\sigma_{(J_1,J_2,q,p-2)}$ is not in the branching rule if $J_2=0$.

2. Lowest weight (indecomposable) Kac representations

As before, other types of atypical representations are not irreducible. These representations contain all 16 multiplets which contain a nonseparable invariant subspace generated by multiplets (4.29). They are lowest weight (indecomposable) Kac representations of dimension $16(2J_1+1)\times(2J_2+1)$.

V. CONCLUSIONS AND DISCUSSIONS

In this article we have applied the supercoherent state method to the construction of the free boson-fermion realization and representations of the non-semisimple superalgebra gl(2|2) in the standard basis. The representations are constructed out of the $gl(2)\oplus gl(2)$ particle states in the super-Fock space.

As mentioned in the Introduction, superalgebras and their corresponding nonunitary CFTs emerge in the supersymmetric treatment to disordered systems and the integer quantum Hall plateaus. In such a treatment, primary fields play an important role in the computation of critical properties of the disordered systems. The results obtained in this paper now make possible the construction of all primary fields of the gl(2|2) nonunitary CFT in terms of free fields.[23] This is under investigation and results will be presented elsewhere.

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E_6 unification model building. III. Clebsch–Gordan coefficients in E_6 tensor products of the 27 with higher dimensional representations

Gregory W. Anderson[a)]
Department of Physics and Astronomy, Northwestern University, 2145 Sheridan Road, Evanston, Illinois 60208

Tomáš Blažek[b)]
Department of Physics and Astronomy, University of Southampton, Highfield, Southampton SO17 1BJ, United Kingdom

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E_6 is an attractive group for unification model building. However, the complexity of a rank 6 group makes it nontrivial to write down the structure of higher dimensional operators in an E_6 theory in terms of the states labeled by quantum numbers of the standard model gauge group. In this paper, we show the results of our computation of the Clebsch–Gordan coefficients for the products of the **27** with irreducible representations of higher dimensionality: **78**, **351**, **351′**, $\overline{\mathbf{351}}$, and $\overline{\mathbf{351}}'$. Application of these results to E_6 model building involving higher dimensional operators is straightforward. © *2005 American Institute of Physics.*
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I. INTRODUCTION

E_6 is the minimal simple gauge group which could accommodate one family of the observed fermions, *and* a family of Higgs states, into a single gauge multiplet.[1] Therefore, unification models based on E_6 can provide relationships for the measured charged fermion masses and quark mixing angles: 13 unrelated independent parameters of the standard model of elementary particles, and at the same time a small set of E_6 symmetric operators may relate the charged fermion data both to the masses and mixings in the neutrino sector and to the parameters of the Higgs sector. In this respect, E_6 provides a framework for the most economic unified supersymmetric theories.

As is well known the key feature among the observed masses of the three generations of fermions is the intergenerational hierarchy. Any unified model has to explain the origin of the hierarchy in terms of the dynamics of the underlying theory. In E_6 models, the hierarchy can follow from the pattern of the symmetry breaking as the rank 6 group is broken down to the standard model gauge group, possibly in a succession of steps. The hierarchy may be explicitly realized in terms of higher dimensional operators containing the light states after the superheavy degrees of freedom are integrated out of the effective theory generated below the E_6 breaking scale M_6.[2] From the technical point of view, the construction of higher dimensional E_6 symmetric operators and their structure in terms of the standard model states is a nontrivial task. Assuming that the light states occupy the fundamental 27-dimensional irreducible representation (irrep), a complete knowledge of the tensor products of the **27** irrep with larger irreps is required. For instance, the E_6 symmetry allows for a higher dimensional operator containing the product of three **27**'s and a **78**, suppressed by some heavy scale $M_H \geqslant M_6$. If the **78** acquires a vacuum expectation value (vev) $v_6 \approx M_6$ and all three **27**'s contain light states, such an operator contributes to the generation of fermion mass matrices. In particular, for the first two families it may generate

[a)]Electronic mail: anderson@susy.phys.nwu.edu
[b)]On leave of absence from the Dept. of Theoretical Physics, Comenius Univ., Bratislava, Slovakia; electronic mail: blazek@soton.ac.uk

entries suppressed by v_6/M_H. Yet, the predictivity of E_6 can only be utilized if the exact form of the singlet in $\mathbf{27}\otimes\mathbf{27}\otimes\mathbf{27}\otimes\mathbf{78}$ in terms of the standard model states is known. If two of the **27**'s are contracted antisymmetrically, one needs to know the Clebsch–Gordan decomposition of the **351** in the tensor product $\mathbf{27}\otimes\mathbf{78}$, then the decomposition of the $\overline{\mathbf{27}}$ in the product $\mathbf{27}\otimes\mathbf{351}$, and, lastly, the decomposition of the singlet in the product $\mathbf{27}\otimes\overline{\mathbf{27}}$. However, complete information on general tensor products of the exceptional group E_6 is difficult to obtain.[3] As for particular computations, to our knowledge only the Clebsch–Gordan decompositions of $\mathbf{27}\otimes\mathbf{27}$, $\mathbf{27}\otimes\overline{\mathbf{27}}$, and $\mathbf{78}\otimes\mathbf{78}$ are presently available in the literature.[4–6]. (We note in passing that a separate paper[7] obtains a subset of the results needed for the operator $\mathbf{27}^3\mathbf{78}$ by studying a branching chain of E_6. The results presented in this paper are relevant for the case when the vev is acquired by a zero weight state of the **78**.)

In this paper, we continue in our earlier work[5,6] and provide basic group-theoretical tools for a construction of higher-dimensional E_6 symmetric operators. In particular, we present the results of our computation of the Clebsch–Gordan coefficients (CGCs) for the tensor products involving 27-, 78-, and 351-dimensional representations, the lowest dimensional irreps in E_6. Section II contains some necessary mathematical background for our study, mostly concerned with lowering in the weight system of these irreps. Our main results can be found in Sec. III, where we also comment on the construction and properties of the weight systems of the resulting irreps. Section IV contains the summary, while the appendix provides details on the lowering relations in the presence of degenerate weights.

II. MATHEMATICAL PRELIMINARIES

In this work we consider tensor products of the fundamental 27-dimensional irrep with higher dimensional 78- and 351-dimensional representations of E_6. In particular, we compute the Clebsch–Gordan coefficients for the products

$$\mathbf{27}\otimes\mathbf{78}=\mathbf{1728}\oplus\mathbf{351}\oplus\mathbf{27}, \tag{1a}$$

$$\mathbf{27}\otimes\mathbf{351}=\overline{\mathbf{7371}}\oplus\overline{\mathbf{1728}}\oplus\overline{\mathbf{351}}\oplus\overline{\mathbf{27}}, \tag{1b}$$

$$\mathbf{27}\otimes\mathbf{351}'=\overline{\mathbf{7722}}\oplus\overline{\mathbf{1728}}\oplus\overline{\mathbf{27}}, \tag{1c}$$

$$\mathbf{27}\otimes\overline{\mathbf{351}}=\overline{\mathbf{5824}}\oplus\mathbf{2925}\oplus\mathbf{650}\oplus\mathbf{78}, \tag{1d}$$

$$\mathbf{27}\otimes\overline{\mathbf{351}'}=\mathbf{3003}\oplus\overline{\mathbf{5824}}\oplus\mathbf{650}. \tag{1e}$$

Before we discuss the construction of the weight systems of the irreps on the right-hand side of these relations let us start first with the rules for the construction of the irreps on the left.

The key ingredient of our procedure is the lowering operation which is used to construct a complete weight system by successive application of generators $E_{-\alpha_1},\ldots,E_{-\alpha_6}$. These are the generators which lie outside of the diagonal Cartan subalgebra and correspond to the six simple roots of E_6. (Our choice of generators is described in more detail in Ref. 6, and basically follows the standard conventions of Ref. 8.) The six generators act as ladder operators—at each level the weight of the new state is obtained from the weight at the previous level by subtracting (in the weight space) the respective simple root:

$$E_{-\alpha_i}|w\rangle=N_{-\alpha_i,w}|w-\alpha_i\rangle. \tag{2}$$

For the weight systems of the **27** and **78** constants $N_{-\alpha_i,w}$ satisfy [see Eq. (12) in Ref. 6]

$$|N_{-\alpha_i,(w)_j}|^2=\langle\alpha_i|w\rangle+|\langle(w)_j|(w)_i\rangle|^2|N_{-\alpha_i,w+\alpha_i}|^2. \tag{3}$$

It is understood that the new state $|w-\alpha_i\rangle$ does not exist if $N_{-\alpha_i,w}=0$ or the right-hand side of (3) turns out to be negative. The subscript on the weight (w) is only relevant for the six degenerate zero weight states of the **78** and is to be ignored for nondegenerate weights. In fact, the second term on the right-hand side of (3) never contributes when one constructs the weight system of the **27** as there are no higher multiplets than doublets for any SU(2) subgroup.

We remark that throughout this work, and consistent with our previous studies,[5,6] the lowering phase convention which always fixes constants N to be real and non-negative

$$N_{-\alpha_i,w}\geqslant 0 \tag{4}$$

is adopted for any simple root α_i and any weight system. Then for the zero weight states of the **78** the inner product in (3) can be expressed as

$$\langle (w)_i|(w)_j\rangle = |A_{ij}|/2, \tag{5}$$

where $A_{ij}\equiv\langle\alpha_i|\alpha_j\rangle$ are the elements of the Cartan matrix of E_6.[8,6] This result follows from the decomposition of the **78** weight states into the states of the fundamental representations in the tensor product $\mathbf{27}\otimes\overline{\mathbf{27}}$.[5]

In the appendix, we derive a generalized relation for $N_{-\alpha_i,w}$ for a weight system with multiple degenerate weights at different levels. We now discuss how to apply general formula (A8) to the weight systems of the 351-dimensional representations which appear on the left in Eqs. 1(b)–1(e). These irreps, although already rather large, are still special because for each weight subspace a basis can be defined such that the application of a lowering ladder operator results in a single basis state, as indicated in Eq. (2). (For larger irreps, there are lowerings which lead to a linear combination of the basis states regardless of the basis definition.) Moreover, if weight (w) is degenerate and a state with weight $(w-\alpha)$ exists, then the $(w+\alpha)$ weight state is either nondegenerate or does not exist at all. Thus for the weight system of the **351′** or **351**, Eq. (A8) reduces to a simple form

$$|N_{-\alpha,(w)_a\to(w-\alpha)_{A_a}}|^2=\langle\alpha|w\rangle+|\langle(w)_a|(w)_c\rangle|^2|N_{-\alpha,(w+\alpha)\to(w)_c}|^2, \tag{6}$$

where, formally, the summation over c is assumed in the last term, but no more than one state actually contributes. Concrete applications of this formula are provided at the end of the section.

Compared to Eq. (3) both weights (w) and $(w-\alpha)$ can now be degenerate. We find, however, that in the **351′** or **351** the $(w+\alpha)$ weight state does not exist if $(w-\alpha)$ is a degenerate weight. Hence if both (w) and $(w-\alpha)$ are degenerate, A_a can be set to a by definition and (6) can be simplified even further:

$$|N_{-\alpha,(w)_a\to(w-\alpha)_a}|^2=\langle\alpha|w\rangle, \quad \text{for both } (w) \text{ and } (w-\alpha) \text{ degenerate.} \tag{7}$$

This shows that the definition of the basis states (and their subscript labeling) in the degenerate subspaces of the **351′** or **351** can be induced from the basis states at the previous level. However, once (w) is found degenerate, how do we know if $(w-\alpha)$ is going to be degenerate and what the dimensionality of this subspace is going to be? Similar to the case of the **78** weight system[6] the decomposition of the 351-dimensional irreps into the states of the fundamental representations can be recalled. The product $\overline{\mathbf{27}}\otimes\overline{\mathbf{27}}=\mathbf{351}'\oplus\mathbf{351}\oplus\mathbf{27}$ is conjugated to the product studied in Ref. 4. We refer to this work to claim that all degenerate weight subspaces in the **351′** (or **351**) are of the same dimensionality and that the degenerate weights follow the weight system of the **27**. In the end it thus turns out that complete bases in the degenerate weight subspaces of the **351′** can be obtained starting from the four (100000) weight states at level 8 of the **351′**:[9]

$$|(100000)_3\rangle = E_{-\alpha_3}|(1\bar{1}2\bar{1}0\bar{1})\rangle/\sqrt{2},$$

$$
\begin{aligned}
|(100000)_4\rangle &= E_{-\alpha_4}|(10\bar{1}2\bar{1}0)\rangle/\sqrt{2},\\
|(100000)_5\rangle &= E_{-\alpha_5}|(100\bar{1}20)\rangle/\sqrt{2},\\
|(100000)_6\rangle &= E_{-\alpha_6}|(10\bar{1}002)\rangle/\sqrt{2}.
\end{aligned}
\tag{8}
$$

With lowering convention (4) the remaining 26 degenerate weight subspaces at lower levels can be specified as $|(w)_a\rangle = E_{-\alpha_A}\cdots E_{-\alpha_B}|(100000)_a\rangle$, $a=3,4,5,6$, where $E_{-\alpha_A}\cdots E_{-\alpha_B}$ is the lowering path leading to state $|(w)\rangle$ in the **27**. For the **351** the only difference is that the degenerate weight subspaces are five-dimensional and the relations analogous to (8) also include

$$
|(100000)_2\rangle = E_{-\alpha_2}|(02\bar{1}000)\rangle/\sqrt{2} \tag{9}
$$

when computing the (100000) states at level 7 of this irrep. We note that with this notation the inner product in any degenerate weight subspace of both the **351′** and **351** satisfies

$$
\langle (w)_a|(w)_b\rangle = |A_{ab}|/2, \tag{10}
$$

(where $a,b=3,4,5,6$ for the **351′**, and $a,b=2,3,4,5,6$ for the **351**), in a close similarity to the degenerate zero weight subspace of the **78**, Eq. (5).

As an example of the application of formula (6) consider all possible lowerings of the state $|F_5\rangle$ in the **351′** where, for brevity, F stands for the (100000) weight. Three different states at the next level can be obtained: $E_{-\alpha_1}|F_5\rangle = N_1\,|(\bar{1}10000)_5\rangle$, $E_{-\alpha_4}|F_5\rangle = N_4\,|101\bar{2}10\rangle$, and $E_{-\alpha_5}|F_5\rangle = N_5\,|100\bar{1}20\rangle$. Based on (6) the constants are

$$
|N_1|^2 = 1+0=1,
$$

$$
|N_4|^2 = 0+\left(\frac{1}{2}\right)^2(\sqrt{2})^2=\frac{1}{2},
$$

$$
|N_5|^2 = 0+1^2(\sqrt{2})^2=2,
$$

as we have already shown in the second and third equations of (8) that

$$
N_{-\alpha_4,(F+\alpha_4)\to(F)_4} = N_{-\alpha_5,(F+\alpha_5)\to(F)_5} = \sqrt{2}.
$$

Implicitly, we also used the fact that (8) represents the only way the (100000) weight states can be obtained from the states at the previous level. Note that (7) could be used to compute N_1 since both (100000) and $(\bar{1}10000)$ are degenerate weights.

Finally, we remark that the properties of the $\overline{\mathbf{351}}'$ and $\overline{\mathbf{351}}$ are easily derived from the properties of the **351′** and **351** after the Dynkin coordinates [and any other indices in Dynkin formalism, like e.g., the labeling of states in Eq. (8)] 1 and 2 are exchanged with 5 and 4, respectively.

III. CONSTRUCTION OF CLEBSCH–GORDAN COEFFICIENTS

Tensor products in Eq. (1) can be expressed in terms of the highest weights as

$$
(100000)\otimes(000001)=(100001)\oplus(000100)\oplus(100000), \tag{11a}
$$

$$
(100000)\otimes(000100)=(100100)\oplus(000011)\oplus(010000)\oplus(000010), \tag{11b}
$$

$$
(100000)\otimes(000020)=(100020)\oplus(000011)\oplus(000010), \tag{11c}
$$

TABLE I. Bases in the dominant weight subspaces of the 1728-dimensional (100001) irrep.

Weight state	Lowering path	Weight state	Lowering path
$\|000100_6\rangle$	6321	$\|100000_6\rangle$	65324436321
$\|000100_3\rangle$	3621	$\|100000_7\rangle$	64534236321
$\|000100_2\rangle$	2361	$\|100000_8\rangle$	63214534236
$\|000100_1\rangle$	1236	$\|100000_9\rangle$	63243654321
		$\|100000_{10}\rangle$	53624436321
		$\|100000_{11}\rangle$	54321634236
$\|100000_1\rangle$	12364534236	$\|100000_{12}\rangle$	32164534236
$\|100000_2\rangle$	21364534236	$\|100000_{13}\rangle$	32643654321
$\|100000_3\rangle$	25364436321	$\|100000_{14}\rangle$	32643254361
$\|100000_4\rangle$	24534636321	$\|100000_{15}\rangle$	45346236321
$\|100000_5\rangle$	23643254361	$\|100000_{16}\rangle$	45321634236

$$(100000)\otimes(010000)=(110000)\oplus(001000)\oplus(100010)\oplus(000001), \tag{11d}$$

$$(100000)\otimes(200000)=(300000)\oplus(110000)\oplus(100010). \tag{11e}$$

For each product we start with the construction of the weight system of the first irrep on the right-hand side. The highest weight state of this irrep is nondegenerate and can always be ex-

TABLE II. Bases in the dominant weight subspaces of the (100100) irrep, the $\overline{\mathbf{7371}}$. $|000010_n\rangle$ states are marked $|\bar{F}_n\rangle$ for brevity.

Weight state	Lowering path	Lowering paths to (000010) weight states			
$\|000011_4\rangle$	4321	$\|\bar{F}_1\rangle$	514362236434321	$\|\bar{F}_{23}\rangle$	645342136234321
$\|000011_3\rangle$	3421	$\|\bar{F}_2\rangle$	563214436234321	$\|\bar{F}_{24}\rangle$	643452136234321
$\|000011_2\rangle$	2341	$\|\bar{F}_3\rangle$	536214436234321	$\|\bar{F}_{25}\rangle$	643621345234321
$\|000011_1\rangle$	1234	$\|\bar{F}_4\rangle$	523614436234321	$\|\bar{F}_{26}\rangle$	636231245434321
		$\|\bar{F}_5\rangle$	145362236434321	$\|\bar{F}_{27}\rangle$	633221143645234
		$\|\bar{F}_6\rangle$	146234536234321	$\|\bar{F}_{28}\rangle$	632145364234321
$\|200000_6\rangle$	6345234	$\|\bar{F}_7\rangle$	143621236345234	$\|\bar{F}_{29}\rangle$	344523126634321
$\|200000_3\rangle$	3645234	$\|\bar{F}_8\rangle$	143622336435421	$\|\bar{F}_{30}\rangle$	343221166345234
$\|200000_4\rangle$	4365234	$\|\bar{F}_9\rangle$	162363245434321	$\|\bar{F}_{31}\rangle$	345234126634321
$\|200000_5\rangle$	5436234	$\|\bar{F}_{10}\rangle$	162332143645234	$\|\bar{F}_{32}\rangle$	345216321436234
$\|200000_2\rangle$	2364534	$\|\bar{F}_{11}\rangle$	162332435644321	$\|\bar{F}_{33}\rangle$	342231166345234
		$\|\bar{F}_{12}\rangle$	134562236434321	$\|\bar{F}_{34}\rangle$	342345126634321
		$\|\bar{F}_{13}\rangle$	134632364523421	$\|\bar{F}_{35}\rangle$	342312632645341
$\|010000_1\rangle$	23645341	$\|\bar{F}_{14}\rangle$	134621236345234	$\|\bar{F}_{36}\rangle$	342163423546321
$\|010000_2\rangle$	32645341	$\|\bar{F}_{15}\rangle$	134622336435421	$\|\bar{F}_{37}\rangle$	245134326634321
$\|010000_3\rangle$	31645234	$\|\bar{F}_{16}\rangle$	121364236345234	$\|\bar{F}_{38}\rangle$	241345326634321
$\|010000_4\rangle$	35644321	$\|\bar{F}_{17}\rangle$	122334546634321	$\|\bar{F}_{39}\rangle$	241332166345234
$\|010000_5\rangle$	36435421	$\|\bar{F}_{18}\rangle$	123456321436234	$\|\bar{F}_{40}\rangle$	213245346634321
$\|010000_6\rangle$	61345234	$\|\bar{F}_{19}\rangle$	624134536234321	$\|\bar{F}_{41}\rangle$	213243632645341
$\|010000_7\rangle$	65434321	$\|\bar{F}_{20}\rangle$	621363245434321	$\|\bar{F}_{42}\rangle$	213456321436234
$\|010000_8\rangle$	64534321	$\|\bar{F}_{21}\rangle$	621332143645234	$\|\bar{F}_{43}\rangle$	453423126634321
$\|010000_9\rangle$	63245341	$\|\bar{F}_{22}\rangle$	621332435644321	$\|\bar{F}_{44}\rangle$	432163423546321
$\|010000_{10}\rangle$	41365234				
$\|010000_{11}\rangle$	43265341				
$\|010000_{12}\rangle$	43546321				
$\|010000_{13}\rangle$	51436234				
$\|010000_{14}\rangle$	54326341				
$\|010000_{15}\rangle$	12364534				

TABLE III. Bases in the dominant weight subspaces of the (100020) irrep, the $\overline{\mathbf{7722}}$. (100100) weight is left out as trivial. $|000010_n\rangle$ states are marked $|\overline{F}_n\rangle$ for brevity.

Weight state	Lowering path	Lowering paths to (000010) weight states			
$\|000011_5\rangle$	54321	$\|\overline{F}_1\rangle$	5632144362345321	$\|\overline{F}_{21}\rangle$	3164213623452345
$\|000011_4\rangle$	45321	$\|\overline{F}_2\rangle$	5362144362345321	$\|\overline{F}_{22}\rangle$	3164223645345321
$\|000011_3\rangle$	34521	$\|\overline{F}_3\rangle$	5236144362345321	$\|\overline{F}_{23}\rangle$	3445231266345321
$\|000011_2\rangle$	23451	$\|\overline{F}_4\rangle$	5123644362345321	$\|\overline{F}_{24}\rangle$	3452341266345321
$\|000011_1\rangle$	12345	$\|\overline{F}_5\rangle$	5432163452364321	$\|\overline{F}_{25}\rangle$	3452163452364321
		$\|\overline{F}_6\rangle$	6421345362345321	$\|\overline{F}_{26}\rangle$	3452163421362345
		$\|\overline{F}_7\rangle$	6412345362345321	$\|\overline{F}_{27}\rangle$	3422636345123451
$\|200000_6\rangle$	63452345	$\|\overline{F}_8\rangle$	6453421362345321	$\|\overline{F}_{28}\rangle$	3423451266345321
$\|200000_3\rangle$	36452345	$\|\overline{F}_9\rangle$	6434521362345321	$\|\overline{F}_{29}\rangle$	3423126633454521
$\|200000_4\rangle$	43652345	$\|\overline{F}_{10}\rangle$	6212363343454521	$\|\overline{F}_{30}\rangle$	2451343266345321
$\|200000_5\rangle$	54362345	$\|\overline{F}_{11}\rangle$	6213632343454521	$\|\overline{F}_{31}\rangle$	2411363623452345
		$\|\overline{F}_{12}\rangle$	6213321436452345	$\|\overline{F}_{32}\rangle$	2413453266345321
		$\|\overline{F}_{13}\rangle$	6213324356454321	$\|\overline{F}_{33}\rangle$	2413322663453451
$\|010000_1\rangle$	263453451	$\|\overline{F}_{14}\rangle$	6136232343454521	$\|\overline{F}_{34}\rangle$	2132453466345321
$\|010000_2\rangle$	163452345	$\|\overline{F}_{15}\rangle$	6134522363454321	$\|\overline{F}_{35}\rangle$	2136453421362345
$\|010000_3\rangle$	136452345	$\|\overline{F}_{16}\rangle$	6134213623452345	$\|\overline{F}_{36}\rangle$	1453622363454321
$\|010000_4\rangle$	143652345	$\|\overline{F}_{17}\rangle$	6334542361234521	$\|\overline{F}_{37}\rangle$	1423453266345321
$\|010000_5\rangle$	154362345	$\|\overline{F}_{18}\rangle$	6321453623454321	$\|\overline{F}_{38}\rangle$	1236453421362345
$\|010000_6\rangle$	653454321	$\|\overline{F}_{19}\rangle$	3164362123452345	$\|\overline{F}_{39}\rangle$	4534231266345321
$\|010000_7\rangle$	645345321	$\|\overline{F}_{20}\rangle$	3164522363454321	$\|\overline{F}_{40}\rangle$	4532163452364321
$\|010000_8\rangle$	633454521				
$\|010000_9\rangle$	326453451				
$\|010000_{10}\rangle$	356454321				
$\|010000_{11}\rangle$	344655321				
$\|010000_{12}\rangle$	455364321				
$\|010000_{13}\rangle$	453263451				
$\|010000_{14}\rangle$	543263451				

pressed as a trivial combination of the highest weight states of the two irreps on the left-hand side, with the CGC being equal to $+1$. In the absence of a simple method to determine the bases in the degenerate weight subspaces which follow at lower levels for each of these irreps, we compute directly the complete weight system in each case. However, note that simple lowering (2) does not necessarily hold for weights with multiple degeneracies, as discussed in the appendix. States at lower levels are then computed by successive lowerings applied to the states of the **27**, and **78** in case (a) or one of the 351-dimensional irreps in cases (b)–(e). These lowerings were described in detail in Sec. II. The computed state is accepted and kept as a new basis state if it cannot be expressed as a linear combination of the previously obtained basis states with the same weight.

It is not necessary to show the Clebsch–Gordan coefficients for every linearly independent state, since there are many states with the same CGCs. Instead, we present the results just for the dominant weight states. Dominant weights are weights with all Dynkin coordinates non-negative. The CGCs for the remaining states can then be determined using the charge conjugation operators,[10,11] or in a straightforward way by direct lowering. In Tables I–V we present lowering paths for the dominant weight states of the **1728**, $\overline{\mathbf{7371}}$, $\overline{\mathbf{7722}}$, $\overline{\mathbf{5824}}$, and **3003** irreps. In our abbreviated notation, lowering path, let's say, 3421 stands for $E_{-\alpha_3}E_{-\alpha_4}E_{-\alpha_2}E_{-\alpha_1}$ applied (from the right) to the highest weight state. The lowering paths in Tables I–V actually specify our choice of bases for particular dominant weight subspaces. Explicit Clebsch–Gordan decomposition of the dominant weight states is important because, typically, the multiplicity of degeneracy (i.e., the dimensionality of the weight subspace) changes compared to the degeneracy at the previous level. Clearly, that is why these states cannot be obtained by generalized charge conjugation from the

TABLE IV. Bases in the dominant weight subspaces of the (110000) irrep, the $\overline{\mathbf{5824}}$.

Weight state	Lowering path	Lowering paths to zero weight states			
$\|001000_2\rangle$	21	$\|0_1\rangle$	65241364345236342133221	$\|0_{33}\rangle$	51453643212233664433221
$\|001000_1\rangle$	12	$\|0_2\rangle$	6524136334452132236 4321	$\|0_{34}\rangle$	5143621345223366 4433221
		$\|0_3\rangle$	65142364345236342133221	$\|0_{35}\rangle$	51436213422334566321432
		$\|0_4\rangle$	6514236334452132236 4321	$\|0_{36}\rangle$	53623124536436214433221
$\|100010_1\rangle$	1236432	$\|0_5\rangle$	65362312453436214433221	$\|0_{37}\rangle$	53621453623436214433221
$\|100010_2\rangle$	2136432	$\|0_6\rangle$	65321453623436214433221	$\|0_{38}\rangle$	536214436323145212 36432
$\|100010_3\rangle$	2364321	$\|0_7\rangle$	653214436323145212 36432	$\|0_{39}\rangle$	53621443632314522364321
$\|100010_4\rangle$	6433221	$\|0_8\rangle$	65321443632314522364321	$\|0_{40}\rangle$	54433221166345322364321
$\|100010_5\rangle$	6321432	$\|0_9\rangle$	62451364345236342133221	$\|0_{41}\rangle$	24512345632133664433221
$\|100010_6\rangle$	4321632	$\|0_{10}\rangle$	6245136334452132236 4321	$\|0_{42}\rangle$	24513245632133664433221
$\|100010_7\rangle$	3216432	$\|0_{11}\rangle$	6211344223366554433221	$\|0_{43}\rangle$	24513246321334566321432
$\|100010_8\rangle$	3264321	$\|0_{12}\rangle$	6213632443632155 4433221	$\|0_{44}\rangle$	24513213466345321236432
		$\|0_{13}\rangle$	6213322144336655 4433221	$\|0_{45}\rangle$	24513213466345322364321
		$\|0_{14}\rangle$	62133214432635544321632	$\|0_{46}\rangle$	23312435454634216633221
$\|000001_1\rangle$	653214433221	$\|0_{15}\rangle$	64152364345236342133221	$\|0_{47}\rangle$	23245341166345321236432
$\|000001_2\rangle$	645342133221	$\|0_{16}\rangle$	6415236334452132236 4321	$\|0_{48}\rangle$	2324534116634532236 4321
$\|000001_3\rangle$	536214433221	$\|0_{17}\rangle$	64536421345236342133221	$\|0_{49}\rangle$	23611345422334566321432
$\|000001_4\rangle$	532144321632	$\|0_{18}\rangle$	6453621334452132236 4321	$\|0_{50}\rangle$	23612344321635544321632
$\|000001_5\rangle$	523614433221	$\|0_{19}\rangle$	64534532364312364232121	$\|0_{51}\rangle$	41534563212233664433221
$\|000001_6\rangle$	523144321632	$\|0_{20}\rangle$	61236324436321554433221	$\|0_{52}\rangle$	41534632122334566321432
$\|000001_7\rangle$	512364433221	$\|0_{21}\rangle$	61233221443366554433221	$\|0_{53}\rangle$	41536213452233664433221
$\|000001_8\rangle$	512344321632	$\|0_{22}\rangle$	61233214432635544321632	$\|0_{54}\rangle$	41536213422334566321432
$\|000001_9\rangle$	544362133221	$\|0_{23}\rangle$	63623124436321554433221	$\|0_{55}\rangle$	45334221166345321236432
$\|000001_{10}\rangle$	415321236432	$\|0_{24}\rangle$	63322114432635544321632	$\|0_{56}\rangle$	45334221166345322364321
$\|000001_{11}\rangle$	415322364321	$\|0_{25}\rangle$	52331266453436214433221	$\|0_{57}\rangle$	45345632364312364232121
$\|000001_{12}\rangle$	425132136432	$\|0_{26}\rangle$	52361236453436214433221	$\|0_{58}\rangle$	45346323465121322364321
$\|000001_{13}\rangle$	425132364321	$\|0_{27}\rangle$	52361234536436214433221	$\|0_{59}\rangle$	13456342122334566321432
$\|000001_{14}\rangle$	433654232121	$\|0_{28}\rangle$	52361453623436214433221	$\|0_{60}\rangle$	13456213452233664433221
$\|000001_{15}\rangle$	436542133221	$\|0_{29}\rangle$	523614436323145212 36432	$\|0_{61}\rangle$	13456213422334566321432
$\|000001_{16}\rangle$	364354232121	$\|0_{30}\rangle$	52361443632314522364321	$\|0_{62}\rangle$	13456223645363214433221
$\|000001_{17}\rangle$	314521236432	$\|0_{31}\rangle$	51362362453436214433221	$\|0_{63}\rangle$	36231244332166554433221
$\|000001_{18}\rangle$	314522364321	$\|0_{32}\rangle$	51362324536436214433221	$\|0_{64}\rangle$	36231244321635544321632
$\|000001_{19}\rangle$	322436543121				
$\|000001_{20}\rangle$	321432654321				
$\|000001_{21}\rangle$	211342365432				
$\|000001_{22}\rangle$	213243654321				
$\|000001_{23}\rangle$	213645321432				
$\|000001_{24}\rangle$	123645321432				

states at the previous levels. Moreover, it is important to check the completeness of a reducible dominant weight subspace. If it is impossible to complete its basis by lowering the states at the previous level, new weight systems open up and the remaining basis vectors are their highest weight states. This is what happens for every dominant weight in the tensor products $\mathbf{78}\otimes\mathbf{78}$,[6] $\mathbf{27}\otimes\overline{\mathbf{27}}$,[5] or $\mathbf{27}\otimes\mathbf{27}$[5] studied in the earlier work. However, this property of the dominant weights is no longer true for the products studied here. We now briefly discuss the dominant weights in each of the products in (11).

(a) ***(100000)*** $\otimes$ ***(000001)*** $=$ ***(100001)*** $\oplus$ ***(000100)*** $\oplus$ ***(100000)***. At level 4 of the 1728-dimensional (**100001**) irrep we find four states with weight (000 100). This weight space, however, is five-dimensional, and the computation of the state orthogonal to the previous four yields the highest weight state of the **351** irrep. (See Table VI.) Similarly, at level 11 we find 16-fold degenerate weight (100000), while this reducible subspace unfolds to be 22-dimensional. Since there are five distinct states of the same weight in the **351**, there is room for one extra state. Once computed as orthogonal to all the other 21 states it becomes the highest weight state of the fundamental 27-dimensional (**100000**) irrep. Because the subsequent tables of CG coefficients become too unwieldy to print, we have deposited electronic versions with the electronic Physics Auxiliary

TABLE V. Bases in the dominant weight subspaces of the 3003-dimensional (300000) irrep. (110000) weight is left out as trivial.

Weight state	Lowering path	Weight state	Lowering path
$\|001000\rangle$	211	$\|000000_1\rangle$	652413643453323643222111
		$\|000000_2\rangle$	651423643453323643222111
		$\|000000_3\rangle$	653623124536444333222111
$\|100010_6\rangle$	64332211	$\|000000_4\rangle$	653214436323145236432211
$\|100010_3\rangle$	36432211	$\|000000_5\rangle$	624513643453323643222111
$\|100010_2\rangle$	23643211	$\|000000_6\rangle$	621134342362365544332211
$\|100010_1\rangle$	12364321	$\|000000_7\rangle$	621332243643655443322111
		$\|000000_8\rangle$	641523643453323643222111
		$\|000000_9\rangle$	645364332345221236432111
$\|000001_1\rangle$	6544333222111	$\|000000_{10}\rangle$	612332243643655443322111
$\|000001_2\rangle$	5364433222111	$\|000000_{11}\rangle$	524536361236444333222111
$\|000001_3\rangle$	5236443322111	$\|000000_{12}\rangle$	524133214663452364332211
$\|000001_4\rangle$	5123644332211	$\|000000_{13}\rangle$	524133245434666333222111
$\|000001_5\rangle$	4251364332211	$\|000000_{14}\rangle$	513645236236444333222111
$\|000001_6\rangle$	4152364332211	$\|000000_{15}\rangle$	514362134523623644332211
$\|000001_7\rangle$	4536433222111	$\|000000_{16}\rangle$	536214436323145236432211
$\|000001_8\rangle$	3145236432211	$\|000000_{17}\rangle$	245133214663452364332211
$\|000001_9\rangle$	3452364322111	$\|000000_{18}\rangle$	245133245434666333222111
$\|000001_{10}\rangle$	2345123643211	$\|000000_{19}\rangle$	213216324364365544332211
		$\|000000_{20}\rangle$	415345234234666333222111
		$\|000000_{21}\rangle$	415362134523623644332211
		$\|000000_{22}\rangle$	453342211663452364332211
		$\|000000_{23}\rangle$	134562134523623644332211
		$\|000000_{24}\rangle$	345634234653221236432111

Publication Service.[14] Note that in Table VII[14] we keep the labeling of the five (100000) states of the **351** consistent with the notation introduced in Eqs. (8) and (9).

(b) ***(100000)*⊗*(000100)*=*(100100)*⊕*(000011)*⊕*(010000)*⊕*(000010)***. Lowering down to level 4 of the 7371-dimensional (**100100**) irrep we obtain four distinct (000011) weight states spanned over a five-dimensional reducible subspace. The last basis state in this subspace, orthogonal to the four from the $\overline{\mathbf{7371}}$, becomes the highest weight state of the $\overline{\mathbf{1728}}$. (See Table VIII.) This is a conjugate irrep to the **1728** described in (a). The lowering paths to the dominant weights in its weight system can be obtained from Table I (replacing 1 and 2 with 5 and 4, and *vice versa*. Proceeding to level 7 a fivefold degenerate (200000) dominant weight is found:

$$|200000_a\rangle = |100000\rangle|100000_a\rangle, \quad a = 2,\ldots,6 \tag{12}$$

TABLE VI. CG coefficients for (**000100**) dominant weight in (**100000**)⊗(**000001**). Each entry should be divided by the respective number in the last row to keep the states normalized to 1.

	(100001)				*(000100)*
	$\|000100_6\rangle$	$\|000100_3\rangle$	$\|000100_2\rangle$	$\|000100_1\rangle$	$\|000100\rangle$
$\|000101\overline{\rangle}\|000001\rangle$	1				1
$\|001\overline{1}01\rangle\|001001\overline{\rangle}$	1	1			−1
$\|0\overline{1}1000\rangle\|01\overline{1}100)$		1	1		1
$\|\overline{1}10000\rangle\|1\overline{1}0100\rangle$			1	1	−1
$\|100000\rangle\|\overline{1}00100\rangle$				1	1
	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{5}$

TABLE VIII. CG coefficients for (**000011**) dominant weight in (**100000**)⊗(**000100**). Each entry should be divided by the respective number in the last row to keep the states normalized to 1.

	(100100)				*(000011)*
	$\|000011_4\rangle$	$\|000011_3\rangle$	$\|000011_2\rangle$	$\|000011_1\rangle$	$\|000011\rangle$
$\|000\bar{1}\bar{1}1\rangle\|000100\rangle$	1				1
$\|00\bar{1}\bar{1}01\rangle\|00\bar{1}\bar{1}10\rangle$	1	1			−1
$\|0\bar{1}\bar{1}000\rangle\|01\bar{1}\bar{0}11\rangle$		1	1		1
$\|\bar{1}\bar{1}0000\rangle\|1\bar{1}\bar{0}011\rangle$			1	1	−1
$\|100000\rangle\|\bar{1}\bar{0}0011\rangle$				1	1
	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{5}$

which, obviously, does not leave any extra space for states outside of the $\overline{\mathbf{7371}}$. This is consistent with no observation in (a) of a dominant weight (000020) in the weight system of the **1728**, and also with the fact that there is no (**200000**) irrep on the right-hand side of (11b). The charge conjugation operators can be used to show that a fivefold degenerate weight subspace with CGCs equal to 1 is then present at odd levels of the $\overline{\mathbf{7371}}$ from this level down until subspace $(000\bar{2}\bar{0})$ emerges at level 39. Next, at level 8 fifteen linearly independent (010000) weight states are present, while the weight subspace turns out to be 20-dimensional (Table IX).[14] Not surprisingly there are four states which belong to the weight system of the $\overline{\mathbf{1728}}$ [compare with (a)], and the remaining basis state, orthogonal to the previous 19, represents the highest weight state of the $\overline{\mathbf{351}}$. Last, at level 15 we get the reducible (000010) weight subspace, which is 66-dimensional. That makes room for the highest weight of the $\overline{\mathbf{27}}$, since there are 44 basis states present in the $\overline{\mathbf{7371}}$ together with 16 states of the $\overline{\mathbf{1728}}$. An additional five states of the $\overline{\mathbf{351}}$ should be expected based on Eqs. (8) and (9). The CGCs for this subspace are presented in Tables X and XI.[14]

(c) ***(100000)⊗(000020)=(100020)⊕(000011)⊕(000010)***. In the construction of the 7722-dimensional (**100020**) irrep one finds a dominant weight already at level 1,

$$|100100\rangle = |100000\rangle|000100\rangle. \tag{13}$$

It occupies a one-dimensional subspace, which is consistent with the absence of the (**100100**) irrep in product (11c). The first degenerate dominant weight is obtained at level 5. There, a six-dimensional (000011) weight subspace contains five linearly independent states of the $\overline{\mathbf{7722}}$. The basis in this reducible subspace is completed by the highest weight state of the $\overline{\mathbf{1728}}$ (Table XII). Proceeding further, there is no room for the highest weight state of a new irrep when dominant weights (200000) and (010000) are encountered at levels 8 and 9, respectively. The (200000)

TABLE XII. CG coefficients for (**000011**) dominant weight in (**100000**)⊗(**000020**). Each entry should be divided by the respective number in the last row to keep the states normalized to 1.

	(100020)					*(000011)*
	$\|000011_5\rangle$	$\|000011_4\rangle$	$\|000011_3\rangle$	$\|000011_2\rangle$	$\|000011_1\rangle$	$\|000011\rangle$
$\|000\bar{0}\bar{1}1\rangle\|000020\rangle$	1					$-\sqrt{2}$
$\|000\bar{1}\bar{1}1\rangle\|000100\rangle$	$\sqrt{2}$	1				1
$\|00\bar{1}\bar{1}01\rangle\|00\bar{1}\bar{1}10\rangle$		1	1			−1
$\|0\bar{1}\bar{1}000\rangle\|01\bar{1}\bar{0}11\rangle$			1	1		1
$\|\bar{1}\bar{1}0000\rangle\|1\bar{1}\bar{0}011\rangle$				1	1	−1
$\|100000\rangle\|\bar{1}\bar{0}0011\rangle$					1	1
	$\sqrt{3}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{7}$

TABLE XVI. CG coefficients for (**001000**) dominant weight in (**100000**)⊗(**010000**). Each entry should be divided by the respective number in the last row to keep the states normalized to 1.

	(110000)		*(001000)*
	$\|001000_1\rangle$	$\|001000_2\rangle$	$\|001000\rangle$
$\|0\bar{1}1000\rangle\|010000\rangle$		1	1
$\|\bar{1}10000\rangle\|1\bar{1}1000\rangle$	1	1	−1
$\|100000\rangle\|\bar{1}01000\rangle$	1		1
	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{3}$

subspace is four-dimensional and its basis can be specified as in Eq. (12). (The states are now numbered as $a=3,4,5,6$.) The CGC decomposition of the (010000) subspace can be found in Table XIII.[14] Finally, at level 16 the last dominant weight in this product is unveiled. The reducible (000010) weight subspace turns out to be 57-dimensional, with 40 basis states coming from the $\overline{\mathbf{7722}}$ and 16 states from the $\overline{\mathbf{1728}}$. The remaining state, orthogonal to them, becomes the highest weight state of the $\overline{\mathbf{27}}$ (see Tables XIV and XV).[14]

(d) ***(100000)***⊗***(010000)***=***(110000)***⊕***(001000)***⊕***(100010)***⊕***(000001)***. In this product, we find the dominant weight states encountered already in the decomposition of **78**⊗**78** and **27**⊗$\overline{\mathbf{27}}$. At level 2 of the (**110000**) weight system (i.e., the $\overline{\mathbf{5824}}$ irrep) we reach the three-dimensional (001000) subspace, with two states in the **5824** and the third one being the highest weight state of the **2925**, as shown in Table XVI. Then following the lowering paths in Table IV, Table II in Ref. 6, and Table I in Ref. 5 the dominant weights (100010), (000001), and (000000) follow at levels 7, 12, and 23, respectively. The CGCs for these dominant weights can be found in Tables XVII–XXIII.[14] The reducible (000000) subspace is 135-dimensional and represents the most (technically) involved computation in this study. Obviously, it cannot (and does not) leave any room for the singlet since the two representations in the product are not conjugate to each other.

(e) ***(100000)***⊗***(200000)***=***(300000)***⊕***(110000)***⊕***(100010)***. The 3003-dimensional (**300000**) irrep contains a dominant weight already at level 1:

$$|110000\rangle=(|\bar{1}10000\rangle|200000\rangle+\sqrt{2}|100000\rangle|010000\rangle)/\sqrt{3}. \tag{14}$$

The orthogonal combination

$$|110000\rangle=(\sqrt{2}|\bar{1}10000\rangle|200000\rangle-|100000\rangle|010000\rangle)/\sqrt{3} \tag{15}$$

forms the highest weight state of the $\overline{\mathbf{5824}}$. Since then, the same dominant weights occur as in the weight system of the $\overline{\mathbf{5824}}$ described under (d). There are, however, no **2925** and **78** irreps in this product (see Tables XXIV–XXVI[14]), just the highest weight state of the **650** completes the 13-dimensional (100010) subspace at level 8 (Table XXVII[14]). The reducible (000000) weight subspace is 108-dimensional and its decomposition can be found in Tables XXVIII–XXXI.[14]

IV. SUMMARY

We have presented the Clebsch–Gordan decomposition of the E_6 tensor products of the fundamental **27** irrep with the 78- and 351-dimensional irreps. Analogous products involving the $\overline{\mathbf{27}}$ instead of the **27** can now be obtained trivially by charge conjugation. It is straightforward to apply these results to the construction of higher dimension operators in E_6 model building.[12]

APPENDIX THE PROBLEM OF DEGENERATE WEIGHTS

Rules (2,3) are insufficient for representations with degenerate weights at successive levels. For degenerate weights we must first identify a particular basis. Label the degenerate basis states of weights $(w+\alpha)$, (w), and $(w-\alpha)$ as

$$|(w+\alpha)_\Gamma\rangle, \quad \text{where} \quad \Gamma=1,\ldots D_{w+\alpha},$$

$$|w_c\rangle, \quad \text{where} \quad c=1,\ldots D_w,$$

and

$$|(w-\alpha)_C\rangle, \quad \text{where} \quad C=1,\ldots D_{w-\alpha}.$$

D_w stands for the degeneracy of (w). The basis states are in general nonorthogonal. In our notation, they are always normalized to unity: $\langle w_c|w_c\rangle=1$. The identity operator in the degenerate subspace is

$$\begin{aligned} I&=G_{ab}|w_a\rangle\langle w_b|,\\ G_{ab}&=(M^{-1})_{ab}, \quad \text{where} \quad M_{ab}=\langle w_a|w_b\rangle. \end{aligned} \tag{A1}$$

Although the basis is nonorthogonal, we can construct state vectors which are orthogonal to any state except the state we are interested in

$$\begin{aligned} |\hat{w}_b\rangle&=|w_a\rangle G_{ab},\\ \langle\hat{w}_a|&=G_{ab}\ \langle w_b|, \end{aligned} \tag{A2}$$

which satisfy

$$\langle w_c|\hat{w}_a\rangle=\langle\hat{w}_a|w_c\rangle=\delta_{ac}. \tag{A3}$$

A general raising or lowering of a degenerate weight state can be written as

$$E_{\alpha_i}|w_c\rangle=N_{\alpha_i,w_c\to(w+\alpha_i)_\Gamma}|(w+\alpha_i)_\Gamma\rangle, \tag{A4}$$

$$E_{-\alpha_i}|w_c\rangle=N_{-\alpha_i,w_c\to(w-\alpha_i)_C}|(w-\alpha_i)_C\rangle, \tag{A5}$$

where there is a possible sum over the states on the right-hand side [compare (A5) with (2)]. The lowering normalization constant can then be expressed only as a sum of matrix elements $N_{-\alpha_i,w_a\to(w-\alpha_i)_A}=G_{AB}^{(w-\alpha_i)}\langle(w-\alpha_i)_B|E_{-\alpha_i}|w_a\rangle$.[13] Using $E_\alpha=E_{-\alpha}^\dagger$ and the defining relation (A5) we derive

$$\begin{aligned} &N_{-\alpha,w_a\to(w-\alpha)_A}N^*_{-\alpha,w_b\to(w-\alpha)_B}\langle(w-\alpha)_B|(w-\alpha)_A\rangle\\ &\quad=\langle w_b|E_\alpha E_{-\alpha}|w_a\rangle\\ &\quad=\langle w_b|[E_\alpha,E_{-\alpha}]+E_{-\alpha}E_\alpha|w_a\rangle\\ &\quad=\langle w_b|w_a\rangle\langle\alpha,w\rangle+G_{\Gamma\Delta}^{w+\alpha}\langle w_b|E_{-\alpha}|(w+\alpha)_\Gamma\rangle\langle(w+\alpha)_\Delta|E_\alpha|w_a\rangle\\ &\quad=\langle w_b|w_a\rangle\langle\alpha,w\rangle+G_{\Gamma\Delta}^{w+\alpha}N_{-\alpha,(w+\alpha)_\Gamma\to w_c}\langle w_b|w_c\rangle N^*_{-\alpha,(w+\alpha)_\Delta\to w_d}\langle w_d|w_a\rangle. \end{aligned} \tag{A6}$$

Hence

$$(G^{w-\alpha})^{-1}_{AB} N_{-\alpha,w_a\to(w-\alpha)_A} N^{*}_{-\alpha,w_b\to(w-\alpha)_B}$$
$$= (G^{w})^{-1}_{ab}\langle\alpha,w\rangle + G^{w+\alpha}_{\Gamma\Delta}(G^{w})^{-1}_{bc}(G^{w})^{-1}_{da} N_{-\alpha,(w+\alpha)_\Gamma\to w_c} N^{*}_{-\alpha,(w+\alpha)_\Delta\to w_d}. \quad \text{(A7)}$$

For $a=b$ we get

$$(G^{w-\alpha})^{-1}_{AB} N_{-\alpha,w_a\to(w-\alpha)_A} N^{*}_{-\alpha,w_a\to(w-\alpha)_B}$$
$$= \langle\alpha,w\rangle + G^{w+\alpha}_{\Gamma\Delta}(G^{w})^{-1}_{ac}(G^{w})^{-1}_{ad} N_{-\alpha,(w+\alpha)_\Gamma\to w_c} N^{*}_{-\alpha,(w+\alpha)_\Delta\to w_d}. \quad \text{(A8)}$$

Another useful expression can be found by contracting relation (A7) with G^{w}_{ab}:

$$(G^{w})_{ab}(G^{w-\alpha})^{-1}_{AB} N_{-\alpha,w_a\to(w-\alpha)_A} N^{*}_{-\alpha,w_b\to(w-\alpha)_B}$$
$$= \langle\alpha,w\rangle D_w + G^{w+\alpha}_{\Gamma\Delta}(G^{w})^{-1}_{cd} N_{-\alpha,(w+\alpha)_\Gamma\to w_c} N^{*}_{-\alpha,(w-\alpha)_\Delta\to w_d}. \quad \text{(A9)}$$

This expression is easily iterated along a sequence of lowerings with the same ladder operator:

$$(G^{w})_{ab}(G^{w-\alpha})^{-1}_{AB} N_{-\alpha,w_a\to(w-\alpha)_A} N^{*}_{-\alpha,w_b\to(w-\alpha)_B}$$
$$= \langle\alpha,w\rangle D_w + \langle\alpha,w+\alpha\rangle D_{w+\alpha} + G^{w+2\alpha}_{\gamma\delta}(G^{w+\alpha})^{-1}_{\Gamma\Delta} N_{-\alpha,(w+2\alpha)_\gamma\to(w+\alpha)_\Gamma} N^{*}_{-\alpha,(w+2\alpha)_\delta\to(w+\alpha)_\Delta}$$
$$= \langle\alpha,w\rangle D_w + \langle\alpha,w+\alpha\rangle D_{w+\alpha} + \cdots + \langle\alpha,w+k\alpha\rangle D_{w+k\alpha}, \quad \text{(A10)}$$

where $(w+k\alpha)$ is the highest weight in the SU(2) subgroup chain (w), $(w+\alpha)$, $(w+2\alpha)$,... present in the weight system.

Finally, for completeness, when raising operators are applied, Eq. (A8) can be written as

$$(G^{w+\alpha})^{-1}_{\Gamma\Delta} N_{\alpha,w_a\to(w+\alpha)_\Gamma} N^{*}_{\alpha,w_a\to(w+\alpha)_\Delta}$$
$$= -\langle\alpha,w\rangle + G^{w-\alpha}_{CD}(G^{w})^{-1}_{ac}(G^{w})^{-1}_{ad} N_{\alpha,(w-\alpha)_C\to w_c} N^{*}_{\alpha,(w-\alpha)_D\to w_d}. \quad \text{(A11)}$$

Special Cases: Lowering within basis states. Consider a series of states connected by repeated application of the same lowering operator $E_{-\alpha}$. Choose any states with degenerate weights obtained in this series as part of the basis for the degenerate weights and label these states by i. For the sequence: $\ldots,(w+\alpha)_i, w_i, (w-\alpha)_i,\ldots$ the generalized recursion relation (A8) reduces to

$$|N_{-\alpha,w_i\to(w-\alpha)_i}|^2 = \langle\alpha,w\rangle + G^{w+\alpha}_{\Gamma\Delta}(G^{w})^{-1}_{ic}(G^{w})^{-1}_{id} N_{-\alpha,(w+\alpha)_\Gamma\to w_c} N^{*}_{-\alpha,(w+\alpha)_\Delta\to w_d}. \quad \text{(A12)}$$

When $(w+\alpha)_i$ is the only state which can be lowered by $E_{-\alpha}$ to obtain a state of weight w we get

$$|N_{-\alpha,w_i\to(w-\alpha)_i}|^2 = \langle\alpha,w\rangle + G^{(w+\alpha)}_{ii}|N_{-\alpha,(w+\alpha)_i\to w_i}|^2. \quad \text{(A13)}$$

This includes the case of a nondegenerate $(w+\alpha)$ weight subspace. When $(w+\alpha)$ is nondegenerate $G^{(w+\alpha)}_{ii}=1$, which further simplifies the above-given relation.

A special case of interest is lowering the degenerate zero weight states of the adjoint representation which correspond to the Cartan subalgebra. These degenerate weight states can be labeled $|(0)_i\rangle$ where the ith degenerate weight is obtained by $E_{-\alpha_i}|\alpha_i\rangle \propto |(0)_i\rangle$. This basis, however, is not orthogonal. When lowering such a basis state the general formula (A8) reduces to

$$|N_{-\alpha_i,(0)_j\to(-\alpha_i)}|^2 = [(G^{(0)})^{-1}_{ji}]^2 |N_{-\alpha_i,(\alpha_i)\to(0)_i}|^2 = \langle(0)_j|(0)_i\rangle^2 |N_{-\alpha_i,(\alpha_i)\to(0)_i}|^2. \quad \text{(A14)}$$

This result is consistent with formula (3) in Sec. II when applied to the zero weight states of the **78** in E_6.

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[14] See EPAPS Document No. E-JMAPAQ-44-021203 for all 31 tables. A direct link to this document may be found in the online article's HTML reference section. This document may also be reached via the EPAPS home page (http://www.aip.org/pubservs/epaps.html) or from ftp.aip.org in the directory /epaps/. See the EPAPS homepage for more information.

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Erratum: Inequalities for quantum entropy: A review with conditions for equality [J. Math. Phys. 43, 4358 (2002)]

Mary Beth Ruskai[a)]
Department of Mathematics, Tufts University, Medford, Massachusetts 02155

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There is a subtle error in the sketch of Epstein's proof[1] as presented in the Appendix of this paper. This can be corrected by replacing each inequality for $\Im\omega(C)$ in the chain of implications between (A2) and (A3) by an analogous operator inequality for $\Im C$ where C is one of the operators that appears in these expressions. However, as this paper was intended to be expository, we give a fuller explanation of the difficulty and its resolution.

Any bounded operator C can be written in the form $C=\Re C+i\Im C$ where $\Re C=\frac{1}{2}(C+C^\dagger)$ and $\Im C=-i(\frac{1}{2})(C-C^\dagger)$ are both self-adjoint. Since we are interested in operators on a finite dimensional Hilbert space, we can assume that $\Im C$ has only discrete spectrum and define $\omega_{\max}$ and $\omega_{\min}$ to be, respectively, the largest and smallest eigenvalues of $\Im C$. Then $\omega_{\min}I\leqslant\Im C\leqslant\omega_{\max}I$. Let $\mathrm{UHP}=\{z:\Im z>0\}$ denote the upper half plane.

Now consider the example $C=\left(\begin{smallmatrix}0&2\\0&0\end{smallmatrix}\right)=\sigma_x+i\sigma_y$. Then $\Im C=\sigma_y$ satisfies $-I\leqslant\Im C\leqslant I$. Since 0 is the only eigenvalue of C, its spectrum is $\{0\}$ which lies in the closure of the UHP. But $C-\sigma_x=i\sigma_y$ has eigenvalues $\pm i$ so that its spectrum contains a point $-i$ that is not even close to the UHP. By perturbing this example slightly so that $C=i\epsilon I+\sigma_x+i\sigma_y$ with $\epsilon>0$, we find that the spectrum of $C\subset\mathrm{UHP}$, but the spectrum of $C+K$ does not lie in the UHP when $K=K^\dagger=-\sigma_x$. This shows that the third implication in the sequence need not necessarily hold.

However, in this proof, $C=\log(zA+B)$ is not arbitrary, but satisfies $0<\Im C<\pi I$. If $K=K^\dagger$, then $\Im C=\Im(K+C)$ so that $0<\Im(K+C)<\pi I$.

Therefore, the sequence of implications between (A2) and (A3) should be replaced by the following valid implications:

$$\Im z>0\Rightarrow\Im(zA+B)>0$$

$$\Rightarrow\pi I>\Im\log(zA+B)>0$$

$$\Rightarrow\pi I>\Im[K+\log(zA+B)]>0 \text{ for } K=K^\dagger$$

$$\Rightarrow\Im(e^{K+\log(zA+B)})>0$$

$$\Rightarrow\Im\mathrm{Tr}e^{K+\log(zA+B)}>0.$$

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[a)]Electronic address: marybeth.ruskai@tufts.edu

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Masayuki Tanimoto[a)]
Max-Planck-Institut für Gravitationphysik (Albert-Einstein-Institut), Am Mühlenberg 1, Golm 14476, Germany

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Due to a miscommunication at the proof stage, the article was originally published without three references. AIP apologizes for this error. All online versions of the article have been corrected. The added references appear below:

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[a)]Electronic mail: masayuki.tanimoto@aei.mpg.de.

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Exact solutions of the isoholonomic problem and the optimal control problem in holonomic quantum computation

Shogo Tanimura[a)]
Graduate School of Engineering, Osaka City University, Osaka 558-8585, Japan

Mikio Nakahara[b)]
Department of Physics, Kinki University, Higashi-Osaka 577-8502, Japan

Daisuke Hayashi[c)]
Department of Engineering Physics and Mechanics, Kyoto University, Kyoto 606-8501, Japan

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The isoholonomic problem in a homogeneous bundle is formulated and solved exactly. The problem takes a form of a boundary value problem of a variational equation. The solution is applied to the optimal control problem in holonomic quantum computer. We provide a prescription to construct an optimal controller for an arbitrary unitary gate and apply it to a k-dimensional unitary gate which operates on an N-dimensional Hilbert space with $N \geqslant 2k$. Our construction is applied to several important unitary gates such as the Hadamard gate, the CNOT gate, and the two-qubit discrete Fourier transformation gate. Controllers for these gates are explicitly constructed. © *2005 American Institute of Physics.*
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I. INTRODUCTION

In this paper we solve the isoholonomic problem in a homogeneous bundle and apply this result to the optimal control problem in holonomic quantum computation. In other words, this paper has two purposes; first, we solve a mathematical problem which has been unsolved for more than a decade since it was initially proposed by Montgomery.[1] Second, we provide a scheme to construct explicitly an optimal controller for arbitrary unitary gate in holonomic quantum computation.[2,3]

The isoholonomic problem is one of generalizations of the isoperimetric problem. The isoperimetric problem, also known as Dido's problem, is originally proposed in the context of plane geometry; what is the shape of a domain with the largest area surrounded by a string of a fixed length? The solution is a circle. The isoperimetric problem has a long history and various generalizations thereof have been proposed.

The isoholonomic problem is formulated as follows. Assume that we have a principal fiber bundle (P, M, π, G) with a connection. The base space M is assumed to be a Riemannian manifold. The isoholonomic problem asks to find the shortest possible piecewise smooth loop in M with a given base point $x_0 \in M$, that produces a given element g_0 of the structure group G as its associated holonomy.

Holonomic structures naturally appear in a mechanical system and have been studied from various interests.[4–8] Montgomery faced this problem when physical chemists attempted to observe

[a)]Author to whom correspondence should be addressed; electronic mail: tanimura@mech.eng.osaka-cu.ac.jp
[b)]Electronic mail: nakahara@math.kindai.ac.jp
[c)]Present address: Fuji Photo Film Co. Ltd., Asaka Technology Development Center, Asaka, Saitama 351-8585, Japan; electronic mail: daisuke_hayashi_0102@nifty.com

the non-Abelian Berry phase (the Wilczek–Zee holonomy)[9–12] by nuclear magnetic resonance (NMR) experiment. Montgomery[1] presented various formulations of the problem, clarified their relations, and gave partial answers. However, even in such an idealized case like a homogeneous bundle, it was difficult to obtain a complete solution to the problem, which remained as an open problem to date.

A decade later after Montgomery's work, the notion of holonomic quantum computation was proposed by Zanardi, Rasetti, and Pachos,[2,3] in which the Wilczek–Zee holonomy is utilized to implement unitary gates necessary to execute a quantum algorithm. Since then, a large number of researchers[13–16] have been interested in finding control parameters that implement a desired gate. Optimization of the control has been an active area of research in view of the decoherence issue. The problem to find the optimal control is nothing but a typical isoholonomic problem and its solution for an arbitrary gate must be urgently provided.

Let us briefly review the idea of quantum computation. Quantum computation, roughly speaking, consists of the following three ingredients: (1) an n-qubit register to store information, (2) a unitary matrix $U \in \mathrm{U}(2^n)$ which implements a quantum algorithm, and (3) measurements to extract information from the register. In an ordinary implementation of a quantum algorithm, we take a system whose Hamiltonian $H(\lambda)$ depends on external control parameters $\lambda = (\lambda^1, \ldots, \lambda^m)$. We then properly arrange the parameter sequence $\lambda(t)$ as a function of time t so that the desired unitary matrix U is generated as a time-evolution operator

$$U = \mathcal{T} \exp\left[-\frac{i}{\hbar} \int_0^T H(\lambda(t)) \mathrm{d}t \right], \tag{1.1}$$

where $\mathcal{T}$ stands for the time-ordered product.

Holonomic quantum computing,[2] in contrast, makes use of the holonomy associated with a loop $\lambda(t)$ in the parameter space. It has been demonstrated[17] that an arbitrary unitary matrix can be implemented as a holonomy by choosing an appropriate loop in the parameter space. In fact, there are infinitely many loops that produce a given unitary matrix. Here we consider the isoholonomic problem, namely, to find the shortest possible loop in the parameter space that yields the given holonomy. This problem has been already analyzed previously in Ref. 18, where various penalty functions useful for numerical search for the optimal loop have been employed. Our strategy here is purely geometrical in nature and no intense numerical computations are required. In the previous work[19] we found exact optimal loops to produce several unitary gates. In the present paper we extend the method of optimal loop construction to implement arbitrary gates.

This paper is organized as follows. In Sec. II we briefly review the Wilczek–Zee holonomy to make this paper self-contained and to establish notation conventions. In Sec. III we introduce the geometrical setting for the problem and use it to formulate the isoholonomic problem in a variational form. We derive the associated Euler–Lagrange equation and solve it explicitly. The solution thus obtained (3.37), which we call the horizontal extremal curve, is one of the main results in the first half of the paper. The remaining problem is to adjust the solution to satisfy the boundary conditions, namely the closed loop condition (4.1) and the holonomy condition (4.2). This problem is solved in Sec. IV explicitly and we obtain a set of equations (4.19)–(4.22), which we call the constructing equations of the controller. These are the main results of this paper and are machinery to construct a controller for an arbitrary unitary gate. In Sec. V this machinery is applied to several well-known important unitary gates to demonstrate its power. Section VI is devoted to summary and discussions.

II. WILCZEK–ZEE HOLONOMY AS A UNITARY GATE

A. Wilczek–Zee holonomy

Here we briefly review the Wilczek–Zee (WZ) holonomy[10] associated with an adiabatic change of the control parameters along a loop in the control manifold. We consider a quantum

system that has a finite number N of states. Let $\{H(\lambda)\}$ be a family of Hamiltonians parametrized smoothly by $\lambda=(\lambda^1,\ldots,\lambda^m)\in M$, where the set of control parameters M is called a control manifold. Eignevalues and eigenstates of $H(\lambda)$ are labeled as

$$H(\lambda)|l,\alpha;\lambda\rangle=\varepsilon_l(\lambda)|l,\alpha;\lambda\rangle \quad (l=1,\ldots,L;\ \alpha=1,\ldots,k_l), \tag{2.1}$$

where the lth eigenvalue $\varepsilon_l(\lambda)$ is k_l-fold degenerate. Assume that no level crossings take place, namely, $\varepsilon_l(\lambda)\neq\varepsilon_{l'}(\lambda)$ for arbitrary λ if $l\neq l'$. Then it follows that $\Sigma_{l=1}^{L}k_l=N$. The eigenvectors satisfy the orthonormal condition, $\langle l,\alpha;\lambda|l',\beta;\lambda\rangle=\delta_{ll'}\delta_{\alpha\beta}$. It is important to note that there is $\mathrm{U}(k_l)$ *gauge* freedom in the choice of $\{|l,\alpha;\lambda\rangle|\alpha=1,\ldots,k_l\}$ at each λ and l. Namely, we may redefine the eigenvectors by any unitary matrix $h\in\mathrm{U}(k_l)$ as

$$|l,\alpha;\lambda\rangle\mapsto\sum_{\beta=1}^{k_l}|l,\beta;\lambda\rangle h_{\beta\alpha}(\lambda) \tag{2.2}$$

without violating the orthonormal condition.

We adiabatically change the parameters $\lambda(t)$ as a function of time t along a closed loop in the control manifold so that $\lambda(T)=\lambda(0)$. It is assumed that the *adiabaticity* is satisfied, namely,

$$\{\varepsilon_l(\lambda(t))-\varepsilon_{l'}(\lambda(t))\}T\gg 2\pi\hbar \tag{2.3}$$

is satisfied for $l\neq l'$ during $0\leq t\leq T$. In other words, we change the parameters so slowly that no resonant transitions take place between different energy levels.[20]

We will concentrate exclusively on the ground state of the system and drop the index l (=1) in the following. Accordingly, the basis vectors that span the ground state eigenspace are written as $|\alpha;\lambda\rangle$, $(\alpha=1,\ldots,k)$ and arranged in an $N\times k$ matrix form as

$$V(\lambda)=(|1;\lambda\rangle,|2;\lambda\rangle,\ldots,|k;\lambda\rangle), \tag{2.4}$$

which is called an orthonormal k frame at $\lambda\in M$. The system evolves, with a given $\lambda(t)$, according to the Schrödinger equation

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi_\alpha(t)\rangle=H(\lambda(t))|\psi_\alpha(t)\rangle. \tag{2.5}$$

Suppose the initial condition is $\lambda(0)=\lambda_0$ and $|\psi_\alpha(0)\rangle=|\alpha;\lambda_0\rangle$. The adiabatic theorem[20] tells us that the state $|\psi_\alpha(t)\rangle$ remains in the ground state eigenspace during the time evolution. Therefore $|\psi_\alpha(t)\rangle$ is expanded as

$$|\psi_\alpha(t)\rangle=\sum_{\beta=1}^{k}|\beta;\lambda(t)\rangle c_{\beta\alpha}(t). \tag{2.6}$$

By substituting (2.6) into (2.5), we find

$$\frac{\mathrm{d}}{\mathrm{d}t}c_{\beta\alpha}(t)=-\frac{i}{\hbar}\varepsilon(\gamma(t))c_{\beta\alpha}(t)-\sum_{\gamma=1}^{k}\left\langle\beta;\lambda(t)\left|\frac{\mathrm{d}}{\mathrm{d}t}\right|\gamma;\lambda(t)\right\rangle c_{\gamma\alpha}(t), \tag{2.7}$$

whose formal solution is

$$c_{\beta\alpha}(t)=\exp\left(-\frac{i}{\hbar}\int_0^t\varepsilon(s)\mathrm{d}s\right)\mathcal{T}\exp\left(-\int_0^t\mathcal{A}(s)\mathrm{d}s\right)_{\beta\alpha} \tag{2.8}$$

with the matrix-valued function

$$\mathcal{A}_{\beta\alpha}(t) = \left\langle \beta;\lambda(t) \left| \frac{\mathrm{d}}{\mathrm{d}t} \right| \alpha;\lambda(t) \right\rangle = \sum_{\mu=1}^{k} \left\langle \beta;\lambda \left| \frac{\partial}{\partial\lambda^{\mu}} \right| \alpha;\lambda \right\rangle \frac{\mathrm{d}\lambda^{\mu}}{\mathrm{d}t}. \tag{2.9}$$

It is easily verified that $\mathcal{A}^{*}_{\beta\alpha} = -\mathcal{A}_{\alpha\beta}$ since $\{|\alpha;\lambda(t)\rangle\}$ is orthonormal. We introduce a $\mathfrak{u}(k)$-valued one-form [we denote the Lie algebra of the Lie group $\mathrm{U}(k)$ by $\mathfrak{u}(k)$, which is the set of k-dimensional skew-Hermite matrices]

$$\mathcal{A}_{\beta\alpha}(\lambda) = \sum_{\mu=1}^{k} \left\langle \beta;\lambda \left| \frac{\partial}{\partial\lambda^{\mu}} \right| \alpha;\lambda \right\rangle \mathrm{d}\lambda^{\mu}, \tag{2.10}$$

which is called the Wilczek–Zee (WZ) connection. Then the unitary matrix appearing in (2.8) is rewritten as

$$\Gamma(t) = \mathcal{P} \exp\left(- \int_{\lambda(0)}^{\lambda(t)} \mathcal{A} \right), \tag{2.11}$$

where $\mathcal{P}$ stands for the path-ordered product. As noted in (2.2) the frame (2.4) can be redefined by a family of unitary matrices $h(\lambda) \in \mathrm{U}(k)$. The WZ connection transforms under the change of frame as

$$\mathcal{A} \mapsto \mathcal{A}' = h^{\dagger}\mathcal{A}h + h^{\dagger}\,\mathrm{d}h. \tag{2.12}$$

This is nothing but the gauge transformation rule of a non-Abelian gauge potential.[21]

We assumed that the control parameter $\lambda(t)$ comes back to the initial point $\lambda(T) = \lambda(0) = \lambda_0$. However, the state $|\psi_{\alpha}(T)\rangle$ fails to assume the initial state and is subject to a unitary rotation as

$$|\psi_{\alpha}(T)\rangle = \exp\left(- \frac{i}{\hbar} \int_0^T \varepsilon(s)\mathrm{d}s \right) \sum_{\beta=1}^{k} |\psi_{\beta}(0)\rangle \Gamma_{\beta\alpha}(T). \tag{2.13}$$

The unitary matrix

$$\Gamma[\lambda] \coloneqq \Gamma(T) = \mathcal{P} \exp\left(- \oint_{\lambda} \mathcal{A} \right) \in \mathrm{U}(k) \tag{2.14}$$

is called the holonomy matrix associated with the loop $\lambda(t)$. It is important to realize that $\Gamma[\lambda]$ is independent of the parametrization of the loop $\lambda(t)$, namely, it is independent of how fast the loop λ is traversed, so long as the adiabaticity is observed, and that it depends only on the geometrical image of λ in M.

B. Quantum computation with holonomy

In quantum computation one implements a quantum algorithm by a product of various unitary gates. It is a natural idea to use the WZ holonomy to produce unitary gates necessary for quantum computation. Zanardi and Rasetti[2] were the first who proposed this holonomic quantum computation (HQC). To implement an n-qubit resistor we take a quantum system whose ground state is k-fold degenerate where $k = 2^n$. We call the N-dimensional Hilbert space a working space and call the k-dimensional subspace a qubit space. Then by changing the control parameter adiabatically we will obtain any unitary gate as a resultant holonomy (2.14). Of course we need to design an appropriate control loop λ to implement a particular unitary gate. It is easy, in principle, to compute the holonomy for a given loop. In contrast, to find a loop λ which produces a specified unitary matrix Γ as its holonomy is far from trivial. Moreover, to build a working quantum computer it is strongly desired to reduce the time required to manipulate the computer since a sequence of operations should be carried out before decoherence extinguishes quantum information from the system. At the same time, the control parameter must be changed as slowly as possible to keep adiabaticity intact. Therefore our task is to find a control loop as short as possible

to fulfill these seemingly opposed conditions. This is a typical example of the so-called isoholonomic problem, which is first formulated by Montgomery.[1] In the next section we introduce a geometric setting in a form suitable for our expositions.

III. FORMULATION OF THE PROBLEM AND ITS SOLUTION

A. Geometrical setting

The WZ connection is identified with the canonical connection[22] of the homogenous bundle, as pointed out by Fujii.[23] While precise definitions of these terms can be found in Refs. 21 and 22, we outline the geometrical setting of the problem here to make this paper self-contained.

Suppose that the system has a family of Hamiltonians acting on the Hilbert space $\mathbb{C}^N$ and that the ground state of each Hamiltonian is k-fold degenerate ($k<N$). The most natural mathematical setting to describe this system is the principal bundle $(S_{N,k}(\mathbb{C}), G_{N,k}(\mathbb{C}), \pi, \mathrm{U}(k))$, which consists of the Stiefel manifold $S_{N,k}(\mathbb{C})$, the Grassmann manifolds $G_{N,k}(\mathbb{C})$, the projection map $\pi: S_{N,k}(\mathbb{C}) \to G_{N,k}(\mathbb{C})$, and the unitary group $\mathrm{U}(k)$ as explained below.

The Stiefel manifold is the set of orthonormal k frames in $\mathbb{C}^N$,

$$S_{N,k}(\mathbb{C}) = \{V \in M(N,k;\mathbb{C}) | V^\dagger V = I_k\}, \tag{3.1}$$

where $M(N,k;\mathbb{C})$ is the set of $N \times k$ complex matrices and I_k is the k-dimensional unit matrix. The unitary group $\mathrm{U}(k)$ acts on $S_{N,k}(\mathbb{C})$ from the right,

$$S_{N,k}(\mathbb{C}) \times \mathrm{U}(k) \to S_{N,k}(\mathbb{C}), \quad (V,h) \mapsto Vh \tag{3.2}$$

by means of matrix product. It should be noted that this action is free. In other words, $h=I_k$ if there exists a point $V \in S_{N,k}(\mathbb{C})$ such that $Vh=V$.

The Grassmann manifold is defined as the set of k-dimensional hyperplanes in $\mathbb{C}^N$,

$$G_{N,k}(\mathbb{C}) = \{P \in M(N,N;\mathbb{C}) | P^2 = P,\ P^\dagger = P,\ \mathrm{tr}\ P = k\}, \tag{3.3}$$

where P is a projection operator to a hyperplane in $\mathbb{C}^N$ and the condition $\mathrm{tr}\ P=k$ guarantees that the hyperplane is indeed k dimensional.

The projection map $\pi: S_{N,k}(\mathbb{C}) \to G_{N,k}(\mathbb{C})$ is defined as

$$\pi: V \mapsto P := VV^\dagger. \tag{3.4}$$

It is easily proved that the map π is surjective. Namely, for any $P \in G_{N,k}(\mathbb{C})$, there is $V \in S_{N,k}(\mathbb{C})$ such that $\pi(V)=P$. The right action of $h \in \mathrm{U}(k)$ sends a point $V \in S_{N,k}(\mathbb{C})$ to a point Vh on the same fiber since

$$\pi(Vh) = (Vh)(Vh)^\dagger = Vhh^\dagger V^\dagger = VV^\dagger = \pi(V). \tag{3.5}$$

Thus the Stiefel manifold $S_{N,k}(\mathbb{C})$ becomes a principal bundle over $G_{N,k}(\mathbb{C})$ with the structure group $\mathrm{U}(k)$.

Moreover, the group $\mathrm{U}(N)$ acts on both $S_{N,k}(\mathbb{C})$ and $G_{N,k}(\mathbb{C})$ as

$$\mathrm{U}(N) \times S_{N,k}(\mathbb{C}) \to S_{N,k}(\mathbb{C}), \quad (g,V) \mapsto gV, \tag{3.6}$$

$$\mathrm{U}(N) \times G_{N,k}(\mathbb{C}) \to G_{N,k}(\mathbb{C}), \quad (g,P) \mapsto gPg^\dagger \tag{3.7}$$

by matrix product. It is easily verified that $\pi(gV)=g\pi(V)g^\dagger$. This action is transitive, namely, there is $g \in \mathrm{U}(N)$ for any $V, V' \in S_{N,k}(\mathbb{C})$ such that $V'=gV$. There is also $g \in \mathrm{U}(N)$ for any $P, P' \in G_{N,k}(\mathbb{C})$ such that $P'=gPg^\dagger$. The stabilizer group of each point in $S_{N,k}(\mathbb{C})$ is isomorphic to $\mathrm{U}(N-k)$ while that of each point in $G_{N,k}(\mathbb{C})$ is isomorphic to $\mathrm{U}(k) \times \mathrm{U}(N-k)$. Thus, they are homogeneous spaces and the fiber bundle

$$\pi: S_{N,k}(\mathbb{C}) \cong \mathrm{U}(N)/\mathrm{U}(N-k) \to G_{N,k}(\mathbb{C}) \cong \mathrm{U}(N)/(\mathrm{U}(k) \times \mathrm{U}(N-k)) \tag{3.8}$$

is called a homogeneous bundle.

The canonical connection form on $S_{N,k}(\mathbb{C})$ is defined as a $\mathfrak{u}(k)$-valued one-form,

$$A = V^\dagger \, \mathrm{d}V, \tag{3.9}$$

which is a generalization of the WZ connection (2.10). This is characterized as the unique connection that is invariant under the action (3.6). The associated curvature two-form is then defined as

$$F = \mathrm{d}A + A \wedge A = \mathrm{d}V^\dagger \wedge \mathrm{d}V + V^\dagger \mathrm{d}V \wedge V^\dagger \, \mathrm{d}V = \mathrm{d}V^\dagger \wedge (I_N - VV^\dagger)\mathrm{d}V. \tag{3.10}$$

These manifolds are equipped with Riemannian metrics. We define a metric

$$\|\mathrm{d}V\|^2 = \mathrm{tr}(\mathrm{d}V^\dagger \, \mathrm{d}V) \tag{3.11}$$

for the Stiefel manifold and

$$\|\mathrm{d}P\|^2 = \mathrm{tr}(\mathrm{d}P \, \mathrm{d}P) \tag{3.12}$$

for the Grassmann manifold.

B. The isoholonomic problem

Here we reformulate the WZ holonomy in terms of the geometric terminology introduced above. The state vector $\psi(t) \in \mathbb{C}^N$ evolves according to the Schrödinger equation,

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = H(t)\psi(t). \tag{3.13}$$

The Hamiltonian admits a spectral decomposition,

$$H(t) = \sum_{l=1}^{L} \varepsilon_l(t) P_l(t), \tag{3.14}$$

with projection operators $P_l(t)$. Therefore, the set of energy eigenvalues $(\varepsilon_1, \ldots, \varepsilon_L)$ and orthogonal projectors $(P_1, \ldots, P_L)$ constitutes a complete set of control parameters of the system. Now we concentrate on the eigenspace associated with the lowest energy, which is assumed to be identically zero, $\varepsilon_1 \equiv 0$. We write $P_1(t)$ as $P(t)$ for simplicity. Suppose that the degree of degeneracy $k = \mathrm{tr}\, P(t)$ is constant. For each t, there exists $V(t) \in S_{N,k}(\mathbb{C})$ such that $P(t) = V(t)V^\dagger(t)$. By adiabatic approximation we mean substitution of $\psi(t) \in \mathbb{C}^N$ by a reduced state vector $\phi(t) \in \mathbb{C}^k$ as

$$\psi(t) = V(t)\phi(t). \tag{3.15}$$

Since $H(t)\psi(t) = \varepsilon_1 \psi(t) = 0$, the Schrödinger equation (3.13) becomes

$$\frac{\mathrm{d}\phi}{\mathrm{d}t} + V^\dagger \frac{\mathrm{d}V}{\mathrm{d}t}\phi(t) = 0 \tag{3.16}$$

and its formal solution is written as

$$\phi(t) = \mathcal{P} \exp\left(- \int V^\dagger \, \mathrm{d}V \right) \phi(0). \tag{3.17}$$

Therefore $\psi(t)$ is written as

$$\psi(t) = V(t)\mathcal{P}\exp\left(-\int V^{\dagger}\,\mathrm{d}V\right)V^{\dagger}(0)\psi(0). \tag{3.18}$$

In particular, when the control parameter comes back to the initial point as $P(T)=P(0)$, the holonomy $\Gamma \in \mathrm{U}(k)$ is defined via

$$\psi(T) = V(0)\Gamma\phi(0) \tag{3.19}$$

and it is given explicitly as

$$\Gamma = V(0)^{\dagger}V(T)\mathcal{P}\exp\left(-\int V^{\dagger}\,\mathrm{d}V\right). \tag{3.20}$$

(The definition of the holonomy presented here is slightly different from the one given in the previous Letter.[19] To make correct sense as a unitary gate the holonomy is to be defined in the present form.) If the condition

$$V^{\dagger}\frac{\mathrm{d}V}{\mathrm{d}t} = 0 \tag{3.21}$$

is satisfied, the curve $V(t)$ in $S_{N,k}(\mathbb{C})$ is called a horizontal lift of the curve $P(t)=\pi(V(t))$ in $G_{N,k}(\mathbb{C})$. Then the holonomy (3.20) is reduced to

$$\Gamma = V^{\dagger}(0)V(T) \in \mathrm{U}(k). \tag{3.22}$$

Now we are ready to state the isoholonomic problem in the present context; given a specified unitary gate $U_{\mathrm{gate}} \in \mathrm{U}(k)$ and a fixed point $P_0 \in G_{N,k}(\mathbb{C})$, find the shortest loop $P(t)$ in $G_{N,k}(\mathbb{C})$ with the base points $P(0)=P(T)=P_0$ whose horizontal lift $V(t)$ in $S_{N,k}(\mathbb{C})$ produces a holonomy Γ that coincides with U_{gate}. This problem was first motivated from experimental study of geometric phase and investigated in detail from a mathematician's viewpoint by Montgomery.[1]

We now formulate the isoholonomic problem as a variational problem. The length of the horizontal curve $V(t)$ is evaluated by the functional

$$S[V,\Omega] = \int_0^T \left\{ \mathrm{tr}\left(\frac{\mathrm{d}V^{\dagger}}{\mathrm{d}t}\frac{\mathrm{d}V}{\mathrm{d}t}\right) - \mathrm{tr}\left(\Omega V^{\dagger}\frac{\mathrm{d}V}{\mathrm{d}t}\right)\right\}\mathrm{d}t, \tag{3.23}$$

where $\Omega(t) \in \mathfrak{u}(k)$ is a Lagrange multiplier to impose the horizontal condition (3.21) on the curve $V(t)$. Note that the value of the functional S is equal to the length of the projected curve $P(t)=\pi(V(t))$,

$$S = \int_0^T \frac{1}{2}\mathrm{tr}\left(\frac{\mathrm{d}P}{\mathrm{d}t}\frac{\mathrm{d}P}{\mathrm{d}t}\right)\mathrm{d}t. \tag{3.24}$$

Thus the problem is formulated as follows; find a curve $V(t)$ that attains an extremal value of the functional (3.23) and satisfies the boundary condition (3.22).

C. The solution: horizontal extremal curve

Our task is to find a solution of the variational problem of the functional (3.23). Now we derive the associated Euler–Lagrange equation and solve it explicitly. A variation of the curve $V(t)$ is defined by an arbitrary smooth function $\eta(t) \in \mathfrak{u}(N)$ such that $\eta(0)=\eta(T)=0$ and an infinitesimal parameter $\epsilon \in \mathbb{R}$ as

$$V_{\epsilon}(t) = (1+\epsilon\eta(t))V(t). \tag{3.25}$$

By substituting $V_{\epsilon}(t)$ into (3.23) and differentiating with respect to ϵ, the extremal condition yields

$$0 = \left.\frac{dS}{d\epsilon}\right|_{\epsilon=0} = \int_0^T \mathrm{tr}\{\dot{\eta}(V\dot{V}^\dagger - \dot{V}V^\dagger - V\Omega V^\dagger)\}dt$$
$$= [\mathrm{tr}\{\eta(V\dot{V}^\dagger - \dot{V}V^\dagger - V\Omega V^\dagger)\}]_{t=0}^{t=T} - \int_0^1 \mathrm{tr}\left\{\eta\frac{d}{dt}(V\dot{V}^\dagger - \dot{V}V^\dagger - V\Omega V^\dagger)\right\}dt. \tag{3.26}$$

Thus we obtain the Euler–Lagrange equation

$$\frac{d}{dt}(\dot{V}V^\dagger - V\dot{V}^\dagger + V\Omega V^\dagger) = 0. \tag{3.27}$$

We reproduce the horizontal equation $V^\dagger\dot{V}=0$ from the extremal condition with respect to $\Omega(t)$. Finally, the isoholonomic problem is reduced to the set of equations (3.21) and (3.27), which we call a horizontal extremal equation. It may be regarded as a homogeneous-space version of the Wong equation.[24]

Next, we solve the equations (3.21) and (3.27). The equation (3.27) is integrated to yield

$$\dot{V}V^\dagger - V\dot{V}^\dagger + V\Omega V^\dagger = \mathrm{const} = X \in u(N). \tag{3.28}$$

Conjugation of the horizontal condition (3.21) yields $\dot{V}^\dagger V=0$. Then, by multiplying V on (3.28) from the right we obtain

$$\dot{V} + V\Omega = XV. \tag{3.29}$$

By multiplying $V^\dagger$ on (3.29) from the left we obtain

$$\Omega = V^\dagger XV. \tag{3.30}$$

The equation (3.29) implies $\dot{V}=XV-V\Omega$, and hence the time derivative of $\Omega(t)$ becomes

$$\dot{\Omega} = V^\dagger X\dot{V} + \dot{V}^\dagger XV = V^\dagger X(XV - V\Omega) + (-V^\dagger X + \Omega V^\dagger)XV = [\Omega,\Omega] = 0. \tag{3.31}$$

Therefore, $\Omega(t)$ is actually a constant. Thus the solution of (3.29) and (3.30) is

$$V(t) = e^{tX}V_0e^{-t\Omega}, \quad \Omega = V_0^\dagger XV_0. \tag{3.32}$$

We call this solution the horizontal extremal curve. Then (3.28) becomes

$$(XV - V\Omega)V^\dagger - V(-V^\dagger X + \Omega V^\dagger) + V\Omega V^\dagger = X,$$

which is arranged as

$$X - (VV^\dagger X + XVV^\dagger - VV^\dagger XVV^\dagger) = 0, \tag{3.33}$$

where we used (3.30). We may take, without loss of generality,

$$V_0 = \begin{pmatrix} I_k \\ 0 \end{pmatrix} \in S_{N,k}(\mathbb{C}) \tag{3.34}$$

as the initial point. We can parametrize $X \in \mathfrak{u}(N)$, which satisfies (3.30), as

$$X = \begin{pmatrix} \Omega & W \\ -W^\dagger & Z \end{pmatrix} \tag{3.35}$$

with $W \in M(k,N-k;\mathbb{C})$ and $Z \in \mathfrak{u}(N-k)$. Then the constraint equation (3.33) forces us to choose

$$Z = 0. \tag{3.36}$$

Finally, we obtained a complete set of solution (3.32) of the horizontal extremal equations (3.21) and (3.27). When we take the initial point V_0 as (3.34), the solutions are parametrized by constant matrices $\Omega \in \mathfrak{u}(k)$ and $W \in M(k, N-k; \mathbb{C})$. For definiteness we write down the complete solution

$$V(t) = e^{tX} V_0 e^{-t\Omega}, \quad X = \begin{pmatrix} \Omega & W \\ -W^\dagger & 0 \end{pmatrix}. \tag{3.37}$$

This is one of our main results. We call the matrix X a controller. At this time the holonomy (3.22) is expressed as

$$\Gamma = V^\dagger(0)V(T) = V_0^\dagger e^{TX} V_0 e^{-T\Omega} \in \mathrm{U}(k). \tag{3.38}$$

These results (3.37) and (3.38) have been also given in Montgomery's paper. (In this paper[1] Montgomery cited Bär's theorem to complete the proof. However, Bär's paper being a diploma thesis, it is not widely available. Therefore we took a more direct approach to justify them.) In the present paper we took a different approach from his. Here we wrote down the Euler–Lagrange equation and solved it directly.

We evaluate the length of the extremal curve for later convenience by substituting (3.37) into (3.24) as

$$S = \int_0^T \frac{1}{2} \mathrm{tr}\left(\frac{\mathrm{d}P}{\mathrm{d}t} \frac{\mathrm{d}P}{\mathrm{d}t} \right) \mathrm{d}t = \mathrm{tr}(W^\dagger W) T. \tag{3.39}$$

IV. SOLUTION TO THE INVERSE PROBLEM

Once the solution (3.37) of the horizontal extremal equation is obtained, the remaining problem is to find the matrices Ω and W that satisfy the closed loop condition

$$V(T)V^\dagger(T) = e^{TX} V_0 V_0^\dagger e^{-TX} = V_0 V_0^\dagger \tag{4.1}$$

and the holonomy condition

$$V_0^\dagger V(T) = V_0^\dagger e^{TX} V_0 e^{-T\Omega} = U_{\mathrm{gate}} \tag{4.2}$$

for a specific unitary gate $U_{\mathrm{gate}} \in \mathrm{U}(k)$. Montgomery[1] presented this inverse problem as an open problem. In this section we give a scheme to construct systematically a series of solutions to this problem and in the next section we will apply it to implement various important unitary gates.

A. Equivalence class

There is a class of equivalent solutions with a given initial condition V_0 and a given final condition $V(T) = V_0 U_{\mathrm{gate}}$. Here we clarify the equivalence relation among solutions $\{V(t)\}$ that have the form (3.37) and satisfy (4.1) and (4.2).

We say that two solutions $V(t)$ and $V'(t)$ are equivalent if there are elements $g \in \mathrm{U}(N)$ and $h \in \mathrm{U}(k)$ such that $V(t)$ and

$$V'(t) = gV(t)h^\dagger \tag{4.3}$$

satisfy the same boundary conditions

$$gV_0 h^\dagger = V_0 \tag{4.4}$$

and

$$hU_{\text{gate}}h^{\dagger} = U_{\text{gate}}. \tag{4.5}$$

For the initial point (3.34), the condition (4.4) states that $g \in \mathrm{U}(N)$ must have a block-diagonal form

$$g = \begin{pmatrix} h_1 & 0 \\ 0 & h_2 \end{pmatrix}, \quad h = h_1 \in \mathrm{U}(k), \quad h_2 \in \mathrm{U}(N-k). \tag{4.6}$$

The controller X' of $V'(t)$ are then found from

$$V'(t) = gV(t)h^{\dagger} = ge^{tX}g^{\dagger}gV_0h^{\dagger}he^{-t\Omega}h^{\dagger} = e^{tgXg^{\dagger}}gV_0h^{\dagger}e^{-th\Omega h^{\dagger}} = e^{tgXg^{\dagger}}V_0e^{-th\Omega h^{\dagger}}. \tag{4.7}$$

In summary, two controllers X and X' are equivalent if and only if there are unitary matrices $h_1 \in \mathrm{U}(k)$ and $h_2 \in \mathrm{U}(N-k)$ such that

$$X = \begin{pmatrix} \Omega & W \\ -W^{\dagger} & 0 \end{pmatrix}, \quad X' = \begin{pmatrix} h_1\Omega h_1^{\dagger} & h_1Wh_2^{\dagger} \\ -h_2W^{\dagger}h_1^{\dagger} & 0 \end{pmatrix}, \quad h_1U_{\text{gate}}h_1^{\dagger} = U_{\text{gate}}. \tag{4.8}$$

B. U(1) holonomy

Here we calculate the holonomy for the case $N=2$ and $k=1$. In this case the homogeneous bundle $\pi: S_{2,1}(\mathbb{C}) \to G_{2,1}(\mathbb{C})$ is the Hopf bundle $\pi: S^3 \to S^2$ with the structure group U(1) and the WZ holonomy reduces to the Berry phase. In the subsequent section we will generalize this result to a non-Abelian holonomy. We normalize the cycle time as $T=1$ in the following. Using real numbers $w_1, w_2, w_3 \in \mathbb{R}$ we parametrize the controller as

$$X = \begin{pmatrix} 2iw_3 & iw_1 + w_2 \\ iw_1 - w_2 & 0 \end{pmatrix} = iw_3 I + iw_1\sigma_1 + iw_2\sigma_2 + iw_3\sigma_3, \tag{4.9}$$

where $\{\sigma_j\}$ are the Pauli matrices. Its exponentiation is

$$e^{tX} = e^{itw_3}(I\cos\rho t + i\mathbf{n}\cdot\boldsymbol{\sigma}\sin\rho t), \tag{4.10}$$

where ρ and $\mathbf{n}$ are defined as

$$\rho := \|\mathbf{w}\| = \sqrt{(w_1)^2 + (w_2)^2 + (w_3)^2}, \quad \mathbf{w} = \|\mathbf{w}\|\mathbf{n}. \tag{4.11}$$

The associated horizontal extremal curve (3.32) then becomes

$$V(t) = e^{tX}V_0e^{-t\Omega} = e^{-itw_3}\begin{pmatrix} \cos\rho t + in_3\sin\rho t \\ (in_1 - n_2)\sin\rho t \end{pmatrix} \tag{4.12}$$

and the projected curve in S^2 becomes

$$P(t) = V(t)V^{\dagger}(t) = \tfrac{1}{2}I + \tfrac{1}{2}\boldsymbol{\sigma}\cdot[\mathbf{n}(\mathbf{n}\cdot\mathbf{e}_3) + (\mathbf{e}_3 - \mathbf{n}(\mathbf{n}\cdot\mathbf{e}_3))\cos 2\rho t - (\mathbf{n}\times\mathbf{e}_3)\sin 2\rho t], \tag{4.13}$$

where $\mathbf{e}_3 = (0,0,1)$. We see from (4.13) that the point $P(t)$ in S^2 starts at the north pole $\mathbf{e}_3$ of the sphere and moves along a small circle with the axis $\mathbf{n}$ in the clockwise sense by the angle $2\rho t$. The point $P(t)$ comes back to the north pole when t satisfies $2\rho t = 2\pi n$ with an integer n. To make a closed loop, namely, to satisfy the loop condition (4.1) at $t=T=1$, the control parameters must satisfy

$$\rho = \|\mathbf{w}\| = n\pi \quad (n = \pm 1, \pm 2, \dots). \tag{4.14}$$

Then, the point $P(t)$ travels the same small circle n times during $0 \leqslant t \leqslant 1$. Therefore, the integer n counts the winding number of the loop. At $t=1$, $\cos\rho = (-1)^n$ and the holonomy (4.2) is evaluated as

$$V_0^\dagger e^X V_0 e^{-\Omega} = e^{iw_3}(-1)^n e^{-2iw_3} = e^{-i(w_3 - n\pi)} = U_{\text{gate}} = e^{i\gamma}. \tag{4.15}$$

Thus, to generate the holonomy $U_{\text{gate}} = e^{i\gamma}$, the controller parameters are fixed as

$$w_3 = n\pi - \gamma, \quad w_1 + iw_2 = e^{-i\phi}\sqrt{(n\pi)^2 - (n\pi - \gamma)^2}. \tag{4.16}$$

This is the solution to the inverse problem defined by (4.1) and (4.2). Here the nonvanishing integer n must satisfy $(n\pi)^2 - (n\pi - \gamma)^2 > 0$. The real parameter ϕ is not fixed by the loop condition and the holonomy condition. The phase $h_2 = e^{i\phi}$ parametrizes solutions in an equivalence class as observed in (4.8). The integer n classifies inequivalent classes.

The length of the loop, (3.39), is now evaluated as

$$S = \text{tr}(W^\dagger W)T = (n\pi)^2 - (n\pi - \gamma)^2. \tag{4.17}$$

For a fixed γ in the range $0 \leqslant \gamma < 2\pi$, the simple loop with $n = 1$ is the shortest one among the extremal loops. Thus, we conclude that the controller of $U_{\text{gate}} = e^{i\gamma}$ is

$$X = \begin{pmatrix} 2i(\pi - \gamma) & ie^{i\phi}\sqrt{\pi^2 - (\pi - \gamma)^2} \\ ie^{-i\phi}\sqrt{\pi^2 - (\pi - \gamma)^2} & 0 \end{pmatrix}. \tag{4.18}$$

We call this solution a small circle solution because of its geometric picture mentioned above.

C. U(k) holonomy

Here we give a prescription to construct a controller matrix X that generates a specific unitary gate U_{gate}. In other words, we give a systematic method to solve the inverse problem (4.2). It turns out that the working space should have a dimension $N \geqslant 2k$ to apply our method. In the following we assume that $N = 2k$. The time interval is normalized as $T = 1$ as before.

Our method consists of the following three steps: first, diagonalize the unitary matrix U_{gate} to be implemented; second, construct a diagonal controller matrix by combining small circle solutions; third, undo diagonalization of the controller.

In the first step, we diagonalize a given unitary matrix $U_{\text{gate}} \in \text{U}(k)$ as

$$R^\dagger U_{\text{gate}} R = U_{\text{diag}} = \text{diag}(e^{i\gamma_1}, \ldots, e^{i\gamma_k}) \tag{4.19}$$

with $R \in \text{U}(k)$. Each eigenvalue γ_j is taken in the range $0 \leqslant \gamma_j < 2\pi$. In the second step, we combine single loop solutions associated with the Berry phase to construct two $k \times k$ matrices

$$\Omega_{\text{diag}} = \text{diag}(i\omega_1, \ldots, i\omega_k), \quad \omega_j = 2(\pi - \gamma_j), \tag{4.20}$$

$$W_{\text{diag}} = \text{diag}(i\tau_1, \ldots, i\tau_k), \quad \tau_j = e^{i\phi_j}\sqrt{\pi^2 - (\pi - \gamma_j)^2}. \tag{4.21}$$

Then we obtain a diagonal controller

$$X_{\text{diag}} = \begin{pmatrix} \Omega_{\text{diag}} & W_{\text{diag}} \\ -W_{\text{diag}}^\dagger & 0 \end{pmatrix}.$$

In the third step, we construct the controller X as

$$X = \begin{pmatrix} R & 0 \\ 0 & I_k \end{pmatrix}\begin{pmatrix} \Omega_{\text{diag}} & W_{\text{diag}} \\ -W_{\text{diag}}^\dagger & 0 \end{pmatrix}\begin{pmatrix} R^\dagger & 0 \\ 0 & I_k \end{pmatrix} = \begin{pmatrix} R\Omega_{\text{diag}}R^\dagger & RW_{\text{diag}} \\ -W_{\text{diag}}^\dagger R^\dagger & 0 \end{pmatrix}, \tag{4.22}$$

which is a $2k \times 2k$ matrix. We call the set of equations, (4.19)–(4.22), constructing equations of the controller. This is the main result of this paper.

It is easily verified that the controller X constructed above satisfies the holonomy condition (4.2). The diagonal controller X_{diag} is actually a direct sum of controllers (4.18), which generate Berry phases $\{e^{i\gamma_j}\}$. Hence, its holonomy is also a direct sum of the Berry phases (4.15) as

$$V_0^\dagger e^{X_{\mathrm{diag}}} V_0 e^{-\Omega_{\mathrm{diag}}} = U_{\mathrm{diag}}$$

and hence we have

$$V_0^\dagger e^X V_0 e^{-\Omega} = R V_0^\dagger e^{X_{\mathrm{diag}}} V_0 R^\dagger R e^{-\Omega_{\mathrm{diag}}} R^\dagger = R U_{\mathrm{diag}} R^\dagger = U_{\mathrm{gate}}.$$

V. OPTIMIZING HOLONOMIC QUANTUM COMPUTATION

Now we apply the prescription developed so far to construct controllers of several specific unitary gates, which are fundamental ingredients of quantum computation. Our examples are the Hadamard gate, the CNOT gate, and the two-qubit discrete Fourier transformation (DFT) gate. For each unitary gate U_{gate}, we need to calculate the diagonalizing matrix R. Then the constructing equations of the controller, (4.19)–(4.22), provide the desired optimal controller matrices.

A. Hadamard gate

The Hadamard gate is a one-qubit gate defined as

$$U_{\mathrm{Had}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{5.1}$$

It is diagonalized by

$$R = \begin{pmatrix} \cos\dfrac{\pi}{8} & -\sin\dfrac{\pi}{8} \\ \sin\dfrac{\pi}{8} & \cos\dfrac{\pi}{8} \end{pmatrix} \tag{5.2}$$

as

$$R^\dagger U_{\mathrm{Had}} R = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.3}$$

Needless to say,

$$\cos\frac{\pi}{8} = \frac{\sqrt{2+\sqrt{2}}}{2}, \quad \sin\frac{\pi}{8} = \frac{\sqrt{2-\sqrt{2}}}{2}. \tag{5.4}$$

Therefore, we have $\gamma_1 = 0$ and $\gamma_2 = \pi$. We may set $\phi_1 = \phi_2 = 0$. The ingredients of the constructing equations of the controller, (4.19)–(4.22), are calculated as

$$\Omega_{\mathrm{diag}} = \mathrm{diag}(2i\pi, 0), \quad W_{\mathrm{diag}} = \mathrm{diag}(0, i\pi), \tag{5.5}$$

and hence

$$R\Omega_{\mathrm{diag}} R^\dagger = \frac{i\pi}{\sqrt{2}} \begin{pmatrix} \sqrt{2}+1 & 1 \\ 1 & \sqrt{2}-1 \end{pmatrix}, \quad RW_{\mathrm{diag}} = \frac{i\pi}{2} \begin{pmatrix} 0 & -\sqrt{2-\sqrt{2}} \\ 0 & \sqrt{2+\sqrt{2}} \end{pmatrix}. \tag{5.6}$$

Substituting these into (4.22), we obtain the optimal controller of the Hadamard gate.

B. CNOT gate

One of the most important 2-qubit gates is the CNOT gate defined as

$$U_{\mathrm{CNOT}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{5.7}$$

It is diagonalized by

$$R = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 1 \end{pmatrix} \tag{5.8}$$

as

$$R^{\dagger} U_{\mathrm{CNOT}} R = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{5.9}$$

Therefore, we have $\gamma_1 = \gamma_2 = \gamma_3 = 0$ and $\gamma_4 = \pi$. The ingredients of the controller are

$$\Omega_{\mathrm{diag}} = \mathrm{diag}(2i\pi, 2i\pi, 2i\pi, 0), \quad W_{\mathrm{diag}} = \mathrm{diag}(0, 0, 0, i\pi), \tag{5.10}$$

and hence

$$R\Omega_{\mathrm{diag}}R^{\dagger} = i\pi \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}, \quad RW_{\mathrm{diag}} = \frac{i\pi}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{5.11}$$

Substituting these into (4.22), we obtain the optimal controller of the CNOT gate.

C. DFT2 gate

Discrete Fourier transformation (DFT) gates are important in many quantum algorithms including Shor's algorithm for integer factorization. The two-qubit DFT (DFT2) is a unitary transformation

$$U_{\mathrm{DFT2}} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix}. \tag{5.12}$$

It is diagonalized by

$$R = \frac{1}{2} \begin{pmatrix} 1 & \sqrt{2} & -1 & 0 \\ 1 & 0 & 1 & -\sqrt{2} \\ -1 & \sqrt{2} & 1 & 0 \\ 1 & 0 & 1 & \sqrt{2} \end{pmatrix} \tag{5.13}$$

as

$$R^{\dagger}U_{\mathrm{DFT2}}R=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&i\end{pmatrix}. \tag{5.14}$$

Therefore, we have $\gamma_1=\gamma_2=0$, $\gamma_3=\pi$, and $\gamma_4=\pi/2$. Thus the ingredients of the controller are

$$\Omega_{\mathrm{diag}}=\mathrm{diag}(2i\pi,2i\pi,0,i\pi),\quad W_{\mathrm{diag}}=\mathrm{diag}(0,0,i\pi,i\pi\sqrt{3}/2), \tag{5.15}$$

and hence

$$R\Omega_{\mathrm{diag}}R^{\dagger}=\frac{i\pi}{2}\begin{pmatrix}3&1&1&1\\1&2&-1&0\\1&-1&3&-1\\1&0&-1&2\end{pmatrix},\quad RW_{\mathrm{diag}}=\frac{i\pi}{2}\begin{pmatrix}0&0&-1&0\\0&0&1&-\sqrt{3/2}\\0&0&1&0\\0&0&1&\sqrt{3/2}\end{pmatrix}. \tag{5.16}$$

Substituting these into (4.22), we finally obtain the optimal controller of the DFT2 gate.

VI. SUMMARY AND DISCUSSIONS

Let us summarize our argument. We briefly reviewed the WZ holonomy and discussed that it may be utilizable for implementation of quantum computation. The WZ holonomy is neatly described in terms of differential geometry of a homogeneous bundle, which consists of Stiefel and Grassmann manifolds and is equipped with the canonical connection. We formulated the optimization problem of control in holonomic quantum computation in a form of the isoholonomic problem in the homogenous bundle. We would like to emphasize that it had been left unsolved for more than a decade after the first proposal. We derived a set of equations, (3.21) and (3.27), that characterizes the optimal control and solved it to obtain the horizontal extremal curve (3.37). The curve must satisfy two boundary conditions, (4.1) and (4.2), to be a closed loop in the control manifold and to produce a specified unitary gate as a holonomy. We solved this inverse problem by combining small circle solutions (4.18) to U(1) holonomy into a direct sum. We provided a prescription (4.19)–(4.22) to construct exactly an optimal controller for any unitary gate. Finally we applied our prescription to several important quantum gates.

We would like to discuss prospective development of the results presented above. Although our prescription is applicable to arbitrarily large qubit gates, the homogeneous bundle seems rather over-idealized for practical applications. A realistic quantum system may have smaller control manifold M than the Grassmann manifold. The restricted control manifold M is embedded in the Grassmann manifold by an embedding map $f:M\to G_{N,k}(\mathbb{C})$ and we need to study the isoholonomic problem in the pullbacked bundle $f^{*}S_{N,k}(\mathbb{C})$. Furthermore, the available working Hilbert space in a realistic system may not have dimensions as large as $N\geqslant 2k$. Actually, even when $N<2k$, sequential operations of single loop solutions can generate any unitary gate. However, such a patched solution could not be optimal. These problems will be treated separately in our future publications.

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Universal collective rotation channels and quantum error correction

Marius Junge[a)]
Department of Mathematics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801-2975

Peter T. Kim[b)]
Department of Mathematics and Statistics, University of Guelph, Guelph, ON, Canada N1G 2W1

David W. Kribs[c)]
Department of Mathematics and Statistics, University of Guelph, Guelph, ON, Canada N1G 2WI; Institute for Quantum Computing, University of Waterloo, Waterloo, ON, Canada N2L 3G1; and Perimeter Institute for Theoretical Physics, Waterloo, ON, Canada N2J 2W9

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We present and investigate a new class of quantum channels, what we call "universal collective rotation channels," that includes the class of collective rotation channels as a special case. The fixed point set and noise commutant coincide for a channel in this class. Computing the precise structure of this C^*-algebra is a core problem in a particular noiseless subsystem method of quantum error correction. We prove that there is an abundance of noiseless subsystems for every channel in this class and that the Young tableaux combinatorial machine may be used to explicitly compute these subsystems. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The study of quantum channels is a central theme in quantum computing and quantum information theory.[27] A fundamental class of quantum channels is known as the class of *collective rotation channels*.[3–5,11,12,15,16,18,20,29–35,37] This class has its roots in the postulates of quantum mechanics and has recently played a key role in experimental efforts towards realizing certain quantum error correction methods.[12,33] Of particular interest in the current study is the *noise commutant method of noiseless subsystems*. This is a recently developed paradigm for passive quantum error correction.[10,12,16,19,20,26,36] In this method, the noise commutant is used as a vehicle for encoding states that are left immune to the noise of a given channel. The operator algebras generated by such states are called noiseless subsystems.

In this paper, we present a new class of quantum channels and investigate them in the context of quantum error correction, with specific reference to the noiseless subsystem method. This class is a generalization of the collective rotation class, which arises as an important special case, hence we use the appellation universal collective rotation channels to describe this class. We prove that the noise commutant for every channel in this class has rich structure and hence contains an abundance of noiseless subsystems. To accomplish this, we use operator algebra techniques to make an explicit connection with representation theory of the symmetric group and, as a consequence, the Young tableaux combinatorial machine[13,17] may be used to explicitly compute these noiseless subsystems.

[a)]Electronic mail: junge@math.uiuc.edu
[b)]Electronic mail: pkim@uoguelph.ca
[c)]Electronic mail: dkribs@uoguelph.ca

The paper is organized as follows. Section II contains introductory material on quantum channels and quantum error correction. In Sec. III we define and establish basic properties of the class of universal collective rotation (UCR) channels. We make the connection with representation theory of the symmetric group in Sec. IV and show that the noise commutant for UCR channels is determined by a particular representation of the symmetric group. In Secs. V and VI we collect well-known facts from representation theory of the symmetric group, with emphasis on Young tableaux combinatorics, and work through some low-dimensional examples. We finish with a concluding remark in Sec. VII and discuss possible avenues of further research.

II. QUANTUM CHANNELS AND NOISELESS SUBSYSTEMS

Let $\mathcal{H}$ be a (complex) Hilbert space and let $\mathcal{B}(\mathcal{H})$ be the set of bounded operators on $\mathcal{H}$. When a basis for $\mathcal{H}$ is fixed and $\dim \mathcal{H}=k<\infty$, the algebra $\mathcal{B}(\mathcal{H})$ may be identified with the set of all complex $k\times k$ matrices $\mathbb{M}_k=\mathbb{M}_k(\mathbb{C})$. Throughout the paper, if we are given positive integers $n \geqslant 1$ and $d\geqslant 2$, we let $\{|0\rangle,|1\rangle,\ldots,|d-1\rangle\}$ be a fixed orthonormal basis for d-dimensional Hilbert space $\mathcal{H}_d=\mathbb{C}^d$ and let $\{|i_1 i_2\cdots i_n\rangle: i_j\in\mathbb{Z}_d\}$ be the corresponding orthonormal basis for $\mathcal{H}_{d^n}=(\mathbb{C}^d)^{\otimes n}$.

A linear map $\mathcal{E}:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{H})$ is *completely positive* if for all $k\geqslant 1$ the ampliation maps $\mathbb{1}_k\otimes\mathcal{E}:\mathbb{M}_k\otimes\mathcal{B}(\mathcal{H})\to\mathbb{M}_k\otimes\mathcal{B}(\mathcal{H})$ are positive. See Refs. 21 and 28 for introductions to the study of completely positive maps from different perspectives. A *quantum channel* is a map $\mathcal{E}:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{H})$ that is completely positive and trace preserving. Given $\mathcal{E}$, there is (Refs. 7 and 22) a set of *noise operators*, or *errors*, $\{E_k\}$ on $\mathcal{H}$ such that

$$\mathcal{E}(\rho)=\sum_k E_k\rho E_k^\dagger \quad \text{for } \rho\in\mathcal{B}(\mathcal{H}). \tag{1}$$

Trace preservation means that the noise operators satisfy

$$\sum_k E_k^\dagger E_k=\mathbb{1},$$

where $\mathbb{1}$ is the identity operator on $\mathcal{H}$. The channel is unital if also,

$$\mathcal{E}(\mathbb{1})=\sum_k E_k E_k^\dagger=\mathbb{1}.$$

We will denote the fixed point set for $\mathcal{E}$ by

$$\mathrm{Fix}(\mathcal{E})=\{\rho\in\mathcal{B}(\mathcal{H}):\mathcal{E}(\rho)=\rho\}.$$

Further let $\mathcal{A}$ be the algebra generated by $\{E_k\}$ from (1). This is called the *interaction algebra* in quantum computing.[20] It is a relic of the channel in the sense that the same algebra is obtained whatever the choice of noise operators in (1). This is most succinctly seen in the case of a unital channel. In general, $\mathrm{Fix}(\mathcal{E})$ is just a †-closed subspace of $\mathcal{B}(\mathcal{H})$, but in the case of a unital channel $\mathcal{E}$, the so-called *noise commutant*

$$\mathcal{A}'=\{\rho\in\mathcal{B}(\mathcal{H}):\rho E_k=E_k\rho,\ \forall\ k\}$$

coincides with the fixed point set[6,24]

$$\mathrm{Fix}(\mathcal{E})=\mathcal{A}'.$$

In particular, $\mathrm{Fix}(\mathcal{E})=\mathcal{A}'$ is a †-closed operator algebra (a finite dimensional C^*-algebra[1,9,31]). In this case the von Neumann double commutant theorem from operator algebras shows how the algebra $\mathcal{A}=\mathcal{A}''=\mathrm{Fix}(\mathcal{E})'$ only depends on the channel.

Every finite dimensional C^*-algebra is unitarily equivalent to an orthogonal direct sum of ampliated full matrix algebras; i.e., there is a unitary operator U such that

$$U\mathcal{A}U^{\dagger} = \bigoplus_{k=1}^{r} (\mathbb{1}_{m_k} \otimes \mathbb{M}_{n_k}).$$

From the representation theory perspective, a factor $\mathbb{1}_{m_k} \otimes \mathbb{M}_{n_k}$ corresponds to an n_k-dimensional irreducible representation appearing with multiplicity m_k. With this form for $\mathcal{A}$ given, the structure of the commutant up to unitary equivalence is easily computed by

$$U\,\mathrm{Fix}(\mathcal{E})U^{\dagger} = U\mathcal{A}'U^{\dagger} = \bigoplus_{k=1}^{r} (\mathbb{M}_{m_k} \otimes \mathbb{1}_{n_k}). \tag{2}$$

(See Refs. 12,16,18,23,32,34,35 for more detailed discussions in connection with quantum information theory.)

Given a quantum channel $\mathcal{E}$ with noise operators $\{E_k\}$, the structure of the noise commutant $\mathcal{A}'$ can be used to prepare density operators for use in the noiseless subsystem method of error correction. This is a passive method of quantum error correction, in the sense that such operators will remain immune to the effects of the noise of the channel, without active intervention. Thus, computing the precise structure of $\mathcal{A}'$ as in (2) is of fundamental importance in this method. We mention that for experimental reasons,[25] only one matrix algebra $\mathbb{M}_{m_k} \otimes \mathbb{1}_{n_k}$ may be used at a time in this manner. Hence it is also desirable to find the largest full matrix algebra which is a subalgebra of the noise commutant.

III. UNIVERSAL COLLECTIVE ROTATION CHANNELS

For the rest of the paper, given a positive integer $d \geqslant 2$ we write $\mathbb{M}_d$ for the operator algebra $\mathcal{B}(\mathbb{C}^d)$ represented as $d \times d$ complex matrices with respect to the standard basis $\{|0\rangle, \ldots, |d-1\rangle\}$ for $\mathbb{C}^d$. Further let $\mathbb{M}_{d,sa}$ be the subset of self-adjoint matrices inside $\mathbb{M}_d$.

Fix $n \geqslant 1$. Given $1 \leqslant k \leqslant n$ we define a representation of $\mathbb{M}_d$ on $\mathcal{H}_{d^n}$ by

$$\omega_k(x) = \mathbb{1}_d \otimes \cdots \otimes \mathbb{1}_d \otimes \underbrace{x}_{k\text{-th position}} \otimes \mathbb{1}_d \otimes \cdots \otimes \mathbb{1}_d$$

for all $x \in \mathbb{M}_d$. Then we may define sums of independent copies of x by

$$u_n(x) = \sum_{k=1}^{n} \omega_k(x) \quad \text{for } x \in \mathbb{M}_d.$$

Definition 3.1: Given a finite subset $\mathcal{S} \subset \mathbb{M}_{d,sa}$, we define a *universal collective rotation (UCR) channel* $\mathcal{E}_{\mathcal{S}}$ by

$$\mathcal{E}_{\mathcal{S}}(\rho) = \frac{1}{|\mathcal{S}|} \sum_{x \in \mathcal{S}} e^{i\theta_x u_n(x)} \rho\, e^{-i\theta_x u_n(x)} \quad \text{for } \rho \in \mathcal{B}(\mathcal{H}_{d^n}),$$

where $\{\theta_x : x \in \mathcal{S}\}$ are nonzero angles.

Given a set of operators $\mathcal{R}$, define $\mathrm{Alg}\,\mathcal{R}$ to be the operator algebra generated by $\mathcal{R}$. This is the set of all polynomials in the elements of $\mathcal{R}$. When $\mathcal{R}$ is a self-adjoint set, $\mathrm{Alg}\,\mathcal{R}$ is a C^*-algebra. Through a standard functional calculus argument from operator theory, it follows that the interaction algebra $\mathcal{A}_{\mathcal{S}}$ for $\mathcal{E}_{\mathcal{S}}$ is obtained as $\mathcal{A}_{\mathcal{S}} \equiv \mathrm{Alg}\{e^{i\theta_x u_n(x)} : x \in \mathcal{S}\} = \mathrm{Alg}\{u_n(x) : x \in \mathcal{S}\}$. Thus by von Neumann's double-commutant identity we have

$$\mathcal{A}_{\mathcal{S}} = \{e^{i\theta_x u_n(x)} : x \in \mathcal{S}\}'' = \{u_n(x) : x \in \mathcal{S}\}''.$$

Notice that $\mathcal{A}_{\mathcal{S}}$ is independent of the choice of (nonzero) angles θ_x. As an application of the fixed point theorem from Refs. 6 and 24 we obtain the following.

Theorem 3.2: *If $\mathcal{S}$ is a finite subset of $\mathbb{M}_{d,sa}$, then the UCR-channel $\mathcal{E}_{\mathcal{S}}$ satisfies*

$$\mathrm{Fix}(\mathcal{E}_{\mathcal{S}}) = \mathcal{A}_{\mathcal{S}}'.$$

Observe that $\mathbb{1}_d$ belongs to $\mathcal{A}_\mathcal{S}$ from its characterization as a bicommutant. Since $u_n(\mathbb{1}_d) = n\mathbb{1}_{d^n}$, we may always add $\mathbb{1}_d$ to $\mathcal{S}$ without changing the properties of $\mathrm{Fix}(\mathcal{E}_\mathcal{S})$. This motivates the following definition.

Definition 3.3: We will say that $\mathcal{S}$ is *maximal* if $\mathrm{span}\{x : x \in \mathcal{S}\}$ contains all matrices $x \in \mathbb{M}_d$ with $\mathrm{tr}(x) = 0$.

It turns out that for maximal $\mathcal{S}$ the algebra $\mathcal{A}_\mathcal{S}$ is a well-known object in representation theory.

Remark 3.4: To place the class of UCR-channels in context, we note that the UCR-channels for $d=2$ and general n are the class of two-level collective rotation channels from quantum computing.[3–5,11,12,15,16,18,20,32–35,37] The noise operators in this case are also denoted by J_x, J_y, J_z and they arise in quantum mechanics as the canonical representation of the angular momentum relations.[8] From the noiseless subsystem/quantum error correction perspective, the algebra $\mathrm{Fix}(\mathcal{E}_\mathcal{S}) = \mathcal{A}'_\mathcal{S}$ for this subclass of UCR-channels, and natural d-dimensional representations of the J_k operators, has been analyzed in Ref. 16 from an operator theory quantum mechanics point of view.

IV. REPRESENTATION THEORY AND THE NOISE COMMUTANT

In this section we identify the structure of the noise commutant in terms of representation theory for the symmetric group. We begin with some notation. We shall denote the n-fold tensor product of $\mathbb{M}_d$ by

$$\mathbb{M}_d^{\otimes n} = \underbrace{\mathbb{M}_d \otimes \cdots \otimes \mathbb{M}_d}_{n\text{-times}} \cong \mathbb{M}_{d^n}$$

Let $\mathrm{Sym}^n\mathbb{M}_d$ be the subalgebra of $\mathbb{M}_{d^n}$ generated by the symmetric tensor products; that is, $\mathrm{Sym}^n\mathbb{M}_d$ is the algebra generated by the operators

$$\Phi_n(x_1 \otimes \cdots \otimes x_n) = \frac{1}{n!}\sum_{\pi \in S_n} x_{\pi(1)} \otimes \cdots \otimes x_{\pi(n)},$$

where each $x_i \in \mathbb{M}_d$ and S_n is the permutation group on n letters.

In terms of representation theory, we may equally well consider the representation π, $GL(d) \to GL(d^n)$ given by $\pi(u) = u \otimes \cdots \otimes u$, and then we have

$$\mathrm{Sym}^n\mathbb{M}_d = \pi(GL(d))'',$$

where $GL(d)$ is the group of $d \times d$ nonsingular complex matrices. This tensor product representation of $GL(d)$ is in duality with the representation of the symmetric group S_n defined on vector tensors by

$$\pi(\sigma)(h_1 \otimes \cdots \otimes h_n) = h_{\sigma(1)} \otimes \cdots \otimes h_{\sigma(n)},$$

for $\sigma \in S_n$ and $h_1, \ldots, h_n \in \mathcal{H}_d$. In this context, Schur's classical duality theorem reads as follows.

Theorem 4.1: $\pi(S_n)' = \mathrm{Sym}^n\mathbb{M}_d$.

We use the following characterization of $\mathrm{Sym}^n\mathbb{M}_d$ below.

Lemma 4.2: For positive integers d and n, we have

$$\mathrm{Sym}^n\mathbb{M}_d = \{x^{\otimes n} : x \in \mathbb{M}_d\}'' = \{u_n(x) : x \in \mathbb{M}_d\}''.$$

Proof: It is clear that $\mathrm{Sym}^n\mathbb{M}_d$ contains the C^*-algebra,

$$\mathcal{B} = \{x^{\otimes n} : x \in \mathbb{M}_d\}'' = \mathrm{span}\{x^{\otimes n} : x \in \mathbb{M}_d\} = \mathrm{Alg}\{x^{\otimes n} : x \in \mathbb{M}_d\}$$

as a subalgebra. For the converse inclusion, let $x_1, \ldots, x_n \in \mathbb{M}_d$ and consider the complex matrix integral

$$\int_{z_1,\ldots,z_n\in\mathbb{T}} \left(\sum_{j=1}^{n} z_j x_j\right)^{\otimes n} \frac{dz_1}{z_1}\cdots\frac{dz_n}{z_n} = \sum_{j_1,\ldots,j_n=1}^{n} \left(\int_{z_1,\ldots,z_n\in\mathbb{T}} \prod_{r=1}^{n} z_{j_r}\frac{dz_1}{z_1}\cdots\frac{dz_n}{z_n}\right)(x_{j_1}\otimes\cdots\otimes x_{j_n})$$

$$= \sum_{j_1,\ldots,j_n=1}^{n} \left(\prod_{s=1}^{n}\int_{z\in\mathbb{T}} z^{|\{r:j_r=s\}|}\frac{dz}{z}\right)(x_{j_1}\otimes\cdots\otimes x_{j_n})$$

$$= (2\pi i)^n \sum_{\pi\in S_n} x_{\pi(1)}\otimes\cdots\otimes x_{\pi(n)},$$

where $\mathbb{T}$ denotes the unit circle in the complex plane. It follows that $\Phi_n(x_1\otimes\cdots\otimes x_n)$ belongs to $\mathcal{B}$ for any choice of $x_1,\ldots,x_n$, and hence $\mathcal{B}$ coincides with $\mathrm{Sym}^n\mathbb{M}_d$.

On the other hand, it is clear by definition that $\mathrm{Sym}^n\mathbb{M}_d$ contains the algebra $\{u_n(x):x\in\mathbb{M}_d\}''$ generated by the $u_n(x)$. Moreover, a consideration of the expansion for $u_n(x)^n$ shows that $x^{\otimes n}$ belongs to this double commutant for all $x\in\mathbb{M}_d$. For the sake of brevity let us observe this fact for $n=2$ and $n=3$,

$$x\otimes x = \frac{1}{2!}(u_2(x)^2 - u_2(x^2)),$$

$$x\otimes x\otimes x = \frac{1}{3!}(u_3(x)^3 - 3u_3(x^2)u_3(x) - 2u_3(x^3)).$$

In fact, for all $x\in\mathbb{M}_d$, the tensor product $x^{\otimes n}$ belongs to the algebra $\mathrm{Alg}\{u_n(x^p):1\leqslant p\leqslant n\}$. Thus the second characterization of $\mathrm{Sym}^n\mathbb{M}_d$ follows. □

Observe that as a consequence of this proof, we also have $\mathrm{Sym}^n\mathbb{M}_d=\{u_n(x):x\in\mathbb{M}_{d,sa}\}''$. We can now explicitly link the noise commutant for these channels with representation theory of the symmetric group.

Theorem 4.3: *Let $\mathcal{S}\subset\mathbb{M}_{d,sa}$ be a maximal system, then*

$$\mathrm{Fix}(\mathcal{E}_{\mathcal{S}}) = \mathcal{A}_{\mathcal{S}}' = \pi(S_n)''.$$

Moreover, for an arbitrary finite set $\mathcal{S}\subset\mathbb{M}_{d,sa}$, we have

$$\mathrm{Fix}(\mathcal{E}_{\mathcal{S}}) \supseteq \pi(S_n)''.$$

Proof: If $\mathcal{S}$ is maximal, then the interaction algebra $\mathrm{Fix}(\mathcal{E}_{\mathcal{S}})'=\mathcal{A}_{\mathcal{S}}=\{u_n(x):x\in\mathcal{S}\}''=\{u_n(x):x\in\mathbb{M}_d\}''$ coincides with $\pi(S_n)'$ by Lemma 4.2. For the second assertion, a given finite subset $\mathcal{S}\subset\mathbb{M}_{d,sa}$ is contained inside a maximal system $\mathcal{S}_{\max}$. Hence $\mathcal{A}_{\mathcal{S}}\subseteq\mathcal{A}_{\mathcal{S}_{\max}}$ and

$$\mathrm{Fix}(\mathcal{E}_{\mathcal{S}}) = \mathcal{A}_{\mathcal{S}}' \supseteq \mathcal{A}_{\mathcal{S}_{\max}}' = \pi(S_n)''.$$

□

V. COMPUTING NOISELESS SUBSYSTEMS VIA YOUNG TABLEAUX

In this section, we collect well-known facts from the representation theory of S_n that allow us to describe $\mathrm{Fix}(\mathcal{E}_{\mathcal{S}})=\pi(S_n)''$ in an explicit manner. Recall that this is imperative for using the structure of the noise commutant to produce noiseless subsystems.

For the discussion in this section, we shall fix positive integers $d\geqslant 2$ and $n\geqslant 2$. Let $\{|0\rangle,\ldots,|d-1\rangle\}$ be the orthonormal basis for $\mathcal{H}_d$ corresponding to a given d-level quantum system, and let

$$\{|i_1 \cdots i_n\rangle : 0 \leqslant i_j < d, 1 \leqslant j \leqslant n\}$$

be the corresponding basis for $\mathcal{H}_{d^n}$. Observe that the set of n-tuples $\{i_1, \ldots, i_n\}$ is in one-to-one correspondence with the set of functions $f:\{1, \ldots, n\} \to \{0, \ldots, d-1\}$. So we may define functions k_l for $0 \leqslant l < d$ by

$$k_l(i_1, \ldots, i_n) = \#\{1 \leqslant j \leqslant n | i_j = l\} \quad \text{for } 0 \leqslant i_j < d,$$

and we have $\Sigma_{l=0}^{d-1} k_l(i_1, \ldots, i_n) = n$.

Now, given positive integers $k_0, \ldots, k_{d-1}$ with each $0 \leqslant k_l \leqslant n$, we define a corresponding subspace of $\mathcal{H}_{d^n}$ by

$$\mathcal{H}_{k_0,\ldots,k_{d-1}} = \text{span}\{|i_1 \cdots i_n\rangle : k_l(i_1, \ldots, i_n) = k_l, 0 \leqslant l < d\}.$$

Notice that $\mathcal{H}_{d^n} = \oplus \mathcal{H}_{k_0,\ldots,k_{d-1}}$, where the direct sum runs over all choices of $k_0, \ldots, k_{d-1}$. Clearly, $\mathcal{H}_{k_0,\ldots,k_{d-1}}$ is an invariant (hence reducing) subspace for the action of the symmetric group S_n. More importantly, the irreducible subspaces, or equivalently the decomposition factors of $\mathcal{H}_{k_0,\ldots,k_{d-1}}$ are completely characterized. The key ingredient in this characterization is the notion of Young tableaux.

Given $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_r$, a nonincreasing sequence of positive integers with $\Sigma_i \lambda_i = n$, set $\lambda = (\lambda_1, \ldots, \lambda_r)$. Then the associated λ-*diagram* is defined as

$$[\lambda] = \{c_{ij} : 1 \leqslant i \leqslant r, 1 \leqslant j \leqslant \lambda_i\},$$

where c_{ij} denotes a cell in $[\lambda]$. Simply put, $[\lambda]$ is a diagram with d rows of cells which are left justified and λ_i cells in the ith row. A λ-*tableau* is a bijective function $t:[\lambda] \to \{1, \ldots, n\}$. Clearly, S_n acts by composition $\sigma t = \sigma \circ t$ on λ-tableaux. Given a λ-tableau, the *column stabilizer* C_t is the subgroup of S_n which leaves the columns of λ setwise fixed. Similarly, the *row stabilizer* R_t is the subgroup of S_n which leaves the rows of λ setwise fixed. Two tableaux t_1 and t_2 are *equivalent* if there exists a permutation $\sigma \in R_{t_1}$ such that $\sigma t_1 = t_2$. In particular, this means that the set of *tabloids* $\text{Tab}_\lambda = \{\{t\} : t \text{ a } \lambda\text{-tableau}\}$ of equivalence classes is indexed by all partitions $(A_1, \ldots, A_r)$ of $\{1, \ldots, n\}$ such that the cardinalities $|A_1| = \lambda_1, \ldots, |A_r| = \lambda_r$. Given a λ-diagram $[\lambda]$, consider the (i,j)-cell c_{ij} in $[\lambda]$. The *hook length* $h(i,j)$ for c_{ij} is the number of cells directly below c_{ij} in the ith column of $[\lambda]$ plus the number of cells to the right of c_{ij} in the ith row of $[\lambda]$ plus one (for the cell c_{ij} itself). Formally,

$$h(i,j) = \lambda_i + \lambda'_j + 1 - i - j,$$

where λ'_j is the number of elements in the jth column. Also recall that a tableau $t:[\lambda] \to \{1, \ldots, n\}$ is *standard* if the numbers increase along rows and increase down columns. The abstract S_n-module that has an orthonormal basis in bijective correspondence with elements of Tab_λ is denoted by M^λ, so that

$$M^\lambda = \text{span}\{e_{\{t\}} : \{t\} \in \text{Tab}_\lambda\}.$$

The *Specht module* $\mathcal{S}^\lambda$ is the submodule of M^λ generated by the polytabloids

$$e_t \equiv \sum_{\sigma \in C_t} (\text{sin } \sigma) e_{\sigma\{t\}} \in M^\lambda.$$

Let us summarize the following facts (see Chap. 7 in Ref. 17).

Theorem 5.1: *Let $k_0, \ldots, k_{d-1}$ be positive integers and consider a partition of $\{1, \ldots, n\}$ into sets $A_0, \ldots, A_{d-1}$ with $|A_l| = k_l$. Let λ be the nonincreasing rearrangement of $(k_0, \ldots, k_{d-1})$. Then $\mathcal{H}_{k_0,\ldots,k_{d-1}}$ is isomorphic as an S_n-module to M^λ.*

Every polytabloid e_t is a cyclic vector for the irreducible module $\mathcal{S}^\lambda$. The dimension of $\mathcal{S}^\lambda$ is given by the hook length formula

$$\dim \mathcal{S}^{\lambda} = \frac{n!}{\prod \text{hook lengths in } |\lambda|},$$

and a basis for $\mathcal{S}^{\lambda}$ *is given by*

$$\{e_t : t \text{ standard } \lambda\text{-tableau}\}.$$

Finally, every finite-dimensional irreducible representation of S_n *is unitarily equivalent to a Specht module representation* π_λ*, where* π_λ *is the representation of* S_n *on* $\mathcal{S}^{\lambda}$ *defined by* $\pi_\lambda(\sigma)e_t \equiv e_{\sigma t}$.

For the next discussion let us fix numbers $(k_0,\ldots,k_{d-1})$ and let us denote by $\mu = (\mu_0,\ldots,\mu_{d-1})$ the nonincreasing rearrangement of $(k_0,\ldots,k_{d-1})$. The S_n-module $\mathcal{H}_{k_0,\ldots,k_{d-1}}$ decomposes into a direct sum of irreducible submodules. Fortunately, these submodules and their multiplicity are completely characterized by Young's rule. Moreover, below we shall describe how the decomposition into irreducible submodules of $\mathcal{H}_{k_0,\ldots,k_{d-1}}$ is related to, and determined by, the decomposition of $\mathcal{H}_\mu \equiv \mathcal{H}_{\mu_0,\ldots,\mu_{d-1}}$. (This allows us to explicitly identify links between irreducible subspaces for the representation π.) Here the key combinatorial tool is the notion of a semistandard tableau.

We generalize the notion of λ-tableau, by saying that $T:[\lambda]\to\mathbb{N}$ is a λ-*tableau of type* $\mu = (\mu_0,\ldots,\mu_{d-1})$ if

$$\#\{c_{ij} : T(c_{ij}) = l\} = \mu_l \quad \text{for } l = 0,\ldots,d-1.$$

Then T is called *semistandard* if the numbers that T assigns to the cells of the diagram determined by λ are nondecreasing along rows and strictly increasing down columns. Let us fix a bijection $t_0:[\lambda]\to\{1,\ldots,n\}$. Then S_n acts on the sets $I(\lambda,\mu)$, the set of λ-tableau of type μ, via

$$\sigma(T) = T\, t_0^{-1}\sigma t_0 \quad \text{for } \sigma \in S_n.$$

Given t_0, we will say that T_1 and T_2 are *row* (*column*) equivalent, and write $T_1 \sim^r_{t_0} T_2$, if $\sigma T_1 = \sigma T_2$ holds for all permutations σ in the row (respectively, column) stabilizer of t_0. In particular, this means that T_1 and T_2 are row equivalent if and only if T_2 is obtained from T_1 by permuting the entries in each row accordingly.

In order to define the linking module maps we first need an appropriate bijection. We denote by $\mathcal{P}_{\mu_0,\ldots,\mu_{d-1}}$ the set of partitions $(A_0,\ldots,A_{d-1})$ of $\{1,\ldots,n\}$ such that $|A_l| = \mu_l$. Then $\mathcal{P}_{\mu_0,\ldots,\mu_{d-1}}$ induces a natural relabeling of the standard basis for $\mathcal{H}_\mu$ by

$$f_{A_0,\ldots,A_{d-1}} = |i_1 \cdots i_n\rangle, \tag{3}$$

where $A_l = \{1 \leqslant j \leqslant n \,|\, i_j = l\}$ for $0 \leqslant l < d$. [Every n-tuple $(i_1,\ldots,i_n)$ is associated with a unique d-tuple of sets $(A_0,\ldots,A_{d-1})$ defined in this way.]

Next we define $\gamma_{t_0}: I(\lambda,\mu) \to \mathcal{P}_{\mu_0,\ldots,\mu_{d-1}}$ by

$$\gamma_{t_0}(T) = (A_0,\ldots,A_{d-1}),$$

where

$$A_l = \{1 \leqslant j \leqslant n \,|\, T\, t_0^{-1}(j) = l\} \quad \text{for } 0 \leqslant l < d.$$

Every λ-tableau T of type μ induces an S_n-module map $\Theta_T: M^\lambda \to M^\mu$ by

$$\Theta_T(e_{\{t_0\}}) = \sum_{T' \sim^r_{t_0} T,\, \gamma_{t_0}(T') = (A_0,\ldots,A_{d-1})} f_{A_0,\ldots,A_{d-1}}.$$

Clearly this extends to an S_n-module homomorphism by defining

$$\Theta_T(e_{\{\sigma(t_0)\}}) = \sigma(\Theta_T(e_{\{t_0\}})).$$

This rather abstract description is in fact very concrete. Given indices $i_1,\ldots,i_n \in \{0,\ldots,d-1\}$ and a λ-tableau $t:|\lambda| \to \{1,\ldots,n\}$ we form the generalized tableau $t_{|i_1\cdots i_n\rangle}:[\lambda] \to \{0,\ldots,d-1\}$ by

$$t_{|i_1\cdots i_n\rangle}(c_{ij}) = i_{t_0(c_{ij})}.$$

This means we write the entries $i_1,\ldots,i_n$ into λ following the order given by t_0. Then we say that

$$(i_1,\ldots,i_n) \sim_{t_0} (i_l',\ldots,i_n')$$

if there exists a permutation $\sigma \in S_n$ such that $i_j' = i_{\sigma(j)}$ for $1 \leqslant j \leqslant n$ and $t_0^{-1}\sigma t_0$ leaves the rows of λ invariant. Therefore, we obtain

$$\Theta_T(e_{\{t_0\}}) = \sum_{(i_1,\ldots,i_n)\sim_{t_0}\gamma_{t_0}(T)} |i_1\cdots i_n\rangle,$$

where here we identify $\gamma_{t_0}(T)$ with the n-tuple determined by the partition $\gamma_{t_0}(T) = (A_0,\ldots,A_{d-1})$ as in (3).

For example, let $d=3, n=5$ and let $t_0:[\lambda] \to \{1,\ldots,5\}$ be given by

$$t_0 = \begin{array}{|c|c|c|c|}\hline 1 & 3 & 2 & 4 \\ \hline 5 \\ \cline{1-1}\end{array}$$

and $T:[\lambda] \to \{0,1,2\}$ be given by

$$T = \begin{array}{|c|c|c|c|}\hline 0 & 0 & 1 & 1 \\ \hline 2 \\ \cline{1-1}\end{array}.$$

This yields, by reading off the entries from the corresponding position in the diagram,

$$\gamma_{t_0}(T) = (A_0,A_1,A_2) = (\{1,3\},\{2,4\},\{5\}).$$

Following (3), $\gamma_{t_0}(T)$ is identified with $(i_1,i_2,i_3,i_4,i_5) = (0,1,0,1,2)$. Moreover, the list of equivalent indices is

$$\{(0,1,0,1,2),(0,1,1,0,2),(0,0,1,1,2),(1,0,0,1,2),(1,0,1,0,2),(1,1,0,0,2)\}.$$

Indeed, according to t_0 we have to fix the fifth coordinate and the other four vary in all possible ways. Thus we have

$$\Theta_T(e_{\{t\}}) = \sum_{(i_1,\ldots,i_n)\sim_t\gamma_t(T)} |i_1\cdots i_n\rangle \quad \text{for } e_{\{t\}} \in M^\lambda.$$

Following Young's rule (see Chap. 2, Ref. 17) we obtain the following.

Theorem 5.2: *Let* $\mu = (k_0^*,\ldots,k_{d-1}^*)$ *be the nonincreasing rearrangement of* $(k_0,\ldots,k_{d-1})$. *Let* $\lambda = (\lambda_1,\ldots,\lambda_r)$ *be such that* $\lambda_1 \geqslant \cdots \geqslant \lambda_r$ *and* $\Sigma_i \lambda_i = n$. *Then*

$$\mathcal{H}^\lambda_{k_0,\ldots,k_{d-1}} \equiv \text{span}\left\{\Theta_T\left(\sum_{\sigma\in C_t}(\text{sgn}\,\sigma)e_{\sigma\{t\}}\right): T \in I(\lambda,\mu), t\ \lambda\text{-tableau}\right\}$$

is an irreducible S_n*-submodule. The restriction of the representation* π *to* $\mathcal{H}^\lambda_{k_0,\ldots,k_{d-1}}$ *is equivalent to the irreducible representation* π_μ *of* S_n *on* S^μ *and has-multiplicity*

$$m = \#\{T: T \text{ semistandard } \lambda\text{-tableau of type } \mu\}.$$

If we collect all this information for all $(k_0,\ldots,k_{d-1})$, we can describe the full representation π of $\mathbb{C}[S_n]$:

Corollary 5.3: Let $\lambda=(\lambda_1,\ldots,\lambda_r)$ *be such that* $\lambda_1\geqslant\cdots\geqslant\lambda_r$ *and* $\Sigma_i\lambda_i=n$, *and let* P_λ *be the projection of* $\mathcal{H}_{d^n}$ *onto*

$$\mathcal{H}^\lambda \equiv \bigoplus_{k_0,\ldots,k_{d-1}} \mathcal{H}^\lambda_{k_0,\ldots,k_{d-1}},$$

where the sum indexes over all $k_0,\ldots,k_{d-1}$ *such that* $\Sigma_{l=0}^{d-1}k_l=n$.

Then P_λ *is the minimal central projection for* $\pi(S_n)''$ *which supports the irreducible submodule* $\mathcal{S}^\lambda$. *Moreover,* $P_\lambda\pi P_\lambda$ *is equivalent to the representation* π_λ *on* $\mathcal{S}^\lambda$ *with multiplicity*

$$m_{\lambda,d}=\sum_{\mu_0\geqslant\cdots\geqslant\mu_{d-1}} \mathrm{Arr}(\mu)\mathrm{SST}(\mu),$$

where

$$\mathrm{Arr}(\mu)=\#\{(k_0,\ldots,k_{d-1}):(k_0^*,\ldots,k_{d-1}^*)=(\mu_0,\ldots,\mu_{d-1})\}$$

and

$$\mathrm{SST}(\mu)=\#\{T:[\lambda]\to\{0,\ldots,d-1\}|T \text{ semistandard } \lambda\text{-tableau of type } \mu\}.$$

In particular, for a maximal system $\mathcal{S}$,

$$\mathrm{Fix}(\mathcal{E}_\mathcal{S})=\mathcal{A}'_\mathcal{S}=\pi(S_n)''\cong\sum_{m_{\lambda,d}\neq 0}\mathbb{M}_{\dim(\mathcal{S}^\lambda)}\otimes\mathbb{1}_{m_{\lambda,d}}$$

describes the representation in irreducible parts with multiplicity.

Corollary 5.4: Let $\mathcal{S}$ *be a maximal system, them* $\mathcal{A}_\mathcal{S}$ *is isomorphic to*

$$\mathcal{A}_\mathcal{S}\cong\sum_{m_{\lambda,d}\neq 0}\mathbb{M}_{m_{\lambda,d}}\otimes\mathbb{1}_{\dim\mathcal{S}^\lambda}$$

and the multiplicity of the component $\mathbb{M}_{m_{\lambda,d}}$ *is given by* $\dim\mathcal{S}^\lambda$.

Let us mention that $\mathcal{H}^\lambda$ may also be described by the so-called Garnier relations. Given $\lambda=(\lambda_1,\ldots,\lambda_r)$, we fix the tableau T_λ such that $T_\lambda(c_{kj})=k$ for all cells c_{kj} in $[\lambda]$. It follows that every index $i=(i_1,\ldots,i_n)$ defines a tableau $T_i:[\lambda]\to\{0,\ldots,d-1\}$ given by $T_i(c_{kj})=i_{T_\lambda(c_{kj})}$. Let $G(J)$ be the collection of coset representatives $\{\nu X:\nu\in Y\}$, where Y is the subgroup of S_n which fixes every element outside both $C_h(T_\lambda)\cup J$ and $Y=X\cap C(T)$. Then as is proved in Ref. 14 (p. 66, 5.2b), $|\psi\rangle\in\mathcal{H}^\lambda$ if and only if

(1) $\langle\psi\|i\rangle=0$ for all i such that T_i has equal entries in two distinct places in the same column,
(2) $\pi(\sigma)(|\psi\rangle)=\mathrm{sgn}(\sigma)|\psi\rangle$ for all σ in the column stabilizer of T_λ,
(3) $\Sigma_{\nu\in G(J)}\mathrm{sgn}(\nu)\pi(\nu^{-1})|\psi\rangle=0$ for any nonempty set in the column stabilizer of $C_{h+1}(T_\lambda)$.

VI. EXAMPLES

A. The case *d*=2 and general *n*

As mentioned above, the case of $d=2$ and general n was extensively examined in Ref. 15. Let us indicate how this can be accomplished with Young tableaux.

When $d=2$, we have the pairs (k_1,k_2) given by $(n-k,k)$ where $k=0,\ldots,n$. In terms of λ-tableau we have to calculate $m_{\lambda,2}$. In terms of types we must only consider diagrams $\mu_k=(n-k,k)$ where $0\leqslant k\leqslant 2n$. But we must be aware that every type allows combinations $(n-k,k)$ and $(k,n-k)$. Given $\lambda=(\lambda_1,\ldots,\lambda_r)$, we observe that to obtain a semistandard tableau, we must have $r=2$. Indeed, we are forced to set 0's in the first row on the first λ_2 positions and 1's in the second

row. Thus for fixed k,j with $2k\leqslant n$ and $2j\leqslant n$, we need $k\leqslant j$ in order to produce a λ-tableau of type μ. Since, we also know that there are $n-k$ 0's, we do not have a choice and we have to put them all in the first row one after another. Thus for a fixed λ, we find

$$m_{(n-j,j),2}=\sum_{k\leqslant j}^{\lfloor n/2\rfloor}2+1=2(\lfloor n/2\rfloor-j)+1$$

if n is even and

$$m_{(n-j,j),2}=2(\lfloor n/2\rfloor-j)$$

if n is odd, where $\lfloor\cdot\rfloor$ denotes the greatest integer part of some number.

We also have to understand $\dim(\mathcal{S}^{\lambda})$. If $\lambda=0$, we get $\dim(\mathcal{S}^{(n,0)})=1$. If $1\leqslant j<n/2$, we see for cells c_{1l} with $l\leqslant j$ the hook length is $1+(n-j+1-i)$. This yields $n(n-2j+1)/j!(n-j+1)!$ and hence

$$\dim(\mathcal{S}^{(n-j,j)})=\begin{cases}1 & \text{if } j=0,\\ \dfrac{n-2j+1}{n+1}\binom{n+1}{j} & \text{if } 1<j\leqslant\dfrac{n}{2}.\end{cases}$$

Let us consider the examples $n=4$ and $n=5$. Then

$$\dim\mathcal{S}^{(4,0)}=1,\quad \dim\mathcal{S}^{(3,1)}=3,\quad \dim\mathcal{S}^{(2,2)}=2$$

and

$$m_{(4,0),2}=5,\quad m_{(3,1),2}=3,\quad m_{(2,2),2}=1.$$

In the case $n=5$, we have

$$\dim\mathcal{S}^{(5,0)}=1,\quad \dim\mathcal{S}^{(4,1)}=4,\quad \dim\mathcal{S}^{(3,2)}=5$$

and

$$m_{(5,0),2}=6,\quad m_{(4,1),2}=4,\quad m_{(3,2),2}=2.$$

Bases for $\mathcal{H}_{2^n}$ which yield the associated algebra decompositions may be computed as well. Below we do this for a more intricate example.

B. The case $d=3$ and $n=4$

If $d=3$ and $n=4$, then the set of λ-diagrams which admit semistandard tableaux is given by

$$\left\{(4)=\begin{array}{|c|c|c|c|}\hline x&x&x&x\\\hline\end{array}\quad (3,1)=\begin{array}{|c|c|c|}\hline x&x&x\\\hline x\\\cline{1-1}\end{array}\quad (2,2)=\begin{array}{|c|c|}\hline x&x\\\hline x&x\\\hline\end{array}\quad (2,1,1)=\begin{array}{|c|c|}\hline x&x\\\hline x\\\cline{1-1}x\\\cline{1-1}\end{array}\right\}.$$

In this case, $(3)\pi(S_4)$ acts on $\mathcal{H}_{d^n}=\mathcal{H}_{81}$. As in Theorem 5.1, $M^{(4)}$ is isomorphic to $\mathcal{H}_{4,0,0},\mathcal{H}_{0,4,0}$, and $\mathcal{H}_{0,0,4}$;$M^{(2,2)}$ is isomorphic to $\mathcal{H}_{2,2,0},\mathcal{H}_{2,0,2}$, and $\mathcal{H}_{0,2,2}$; $M^{(2,1,1)}$ is isomorphic to $\mathcal{H}_{2,1,1},\mathcal{H}_{1,2,1}$, and $\mathcal{H}_{1,1,2}$ etc., so that the multiplicities for the M^{λ} are 3 for $M^{(4)},M^{(2,2)}$ and $M^{(2,1,1)}$ and 6 for $M^{(3,1)}$. The dimensions of the Specht modules $\mathcal{S}^{\lambda}$ using the hook length formula are given by

$$\dim\mathcal{S}^{(4)}=1,\quad \dim\mathcal{S}^{(3,1)}=3,\quad \dim\mathcal{S}^{(2,2)}=2,\quad \dim\mathcal{S}^{(2,1,1)}=3.$$

Now, we have to compute the multiplicities of $\mathcal{S}^{\lambda}$ in M^{μ}. If $\mu=(4)[=(4,0,0)]$, then the only semistandard tableau of type μ is $\lambda=(4)$ with 0 in each cell. Thus $M^{(4)}\cong\mathcal{S}^{(4)}$. Further, every M^{μ}

supports a single copy of $\mathcal{S}^{(4)}$ *via* the $\lambda=(4)$-tableau with cell entries given by μ. For $\mu=(3,1)$, the possible semistandard tableaux are

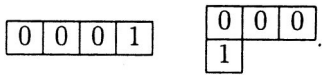

This gives

$$M^{(3,1)} \cong \mathcal{S}^{(4)} \oplus \mathcal{S}^{(3,1)}.$$

For $\mu=(2,2)$, we have

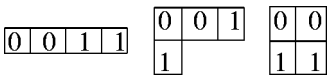

Thus we obtain

$$M^{(2,2)} \cong \mathcal{S}^{(4)} \oplus \mathcal{S}^{(3,1)} \oplus \mathcal{S}^{(2,2)}.$$

Finally, for $\mu=(2,1,1)$ we find

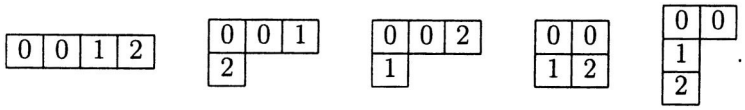

This means

$$M^{(2,1,1)} \cong \mathcal{S}^{(4)} \oplus (\mathcal{S}^{(3,1)} \otimes \mathbb{1}_2) \oplus \mathcal{S}^{(2,2)} \oplus \mathcal{S}^{(2,1,1)}.$$

Setting this all together, we find the module decomposition of $\pi(S_4)$ is given by

$$\begin{aligned}\pi(S_4) &= (M^{(4)} \otimes \mathbb{1}_3) \oplus (M^{(3,1)} \otimes \mathbb{1}_6) \oplus (M^{(2,2)} \otimes \mathbb{1}_3) \oplus (M^{(2,1,1)} \otimes \mathbb{1}_3) \\ &= (\mathcal{S}^{(4)} \otimes \mathbb{1}_3) \oplus ((\mathcal{S}^{(4)} \oplus \mathcal{S}^{(3,1)}) \otimes \mathbb{1}_6) \qquad (4)\end{aligned}$$

$$\oplus ((\mathcal{S}^{(4)} \oplus \mathcal{S}^{(3,1)} \oplus \mathcal{S}^{(2,2)}) \otimes \mathbb{1}_3) \qquad (5)$$

$$\oplus ((\mathcal{S}^{(4)} \oplus (\mathcal{S}^{(3,1)} \otimes \mathbb{1}_2) \oplus \mathcal{S}^{(2,2)} \oplus \mathcal{S}^{(2,1,1)}) \otimes \mathbb{1}_3) \qquad (6)$$

$$= (\mathcal{S}^{(4)} \otimes \mathbb{1}_{15}) \oplus (\mathcal{S}^{(3,1)} \otimes \mathbb{1}_{15}) \oplus (\mathcal{S}^{(2,2)} \otimes \mathbb{1}_6) \oplus (\mathcal{S}^{(2,1,1)} \otimes \mathbb{1}_3). \qquad (7)$$

The direct sums in (4)–(6) are understood to be linked, as reflected in (7). It now follows that

$$\mathrm{Fix}(\mathcal{E}_{\mathcal{S}}) = \pi(S_4)'' \cong (\mathbb{C} \otimes \mathbb{1}_{15}) \oplus (\mathbb{M}_3 \otimes \mathbb{1}_{15}) \oplus (\mathbb{M}_2 \otimes \mathbb{1}_6) \oplus (\mathbb{M}_3 \otimes \mathbb{1}_3). \qquad (8)$$

Notice also that $\mathbb{M}_3$ is the largest full matrix algebra which can be injected into $\mathrm{Fix}(\mathcal{E}_{\mathcal{S}})$ as a subalgebra.

Let us now describe the bases for the decomposition

$$\begin{aligned}\mathcal{H}_{3^4} = &(\mathcal{H}_{4,0,0} \oplus \mathcal{H}_{0,4,0} \oplus \mathcal{H}_{0,0,4}) \oplus (\mathcal{H}_{2,1,1} \oplus \mathcal{H}_{1,2,1} \oplus \mathcal{H}_{1,1,2}) \\ &\oplus (\mathcal{H}_{3,1,0} \oplus \mathcal{H}_{3,0,1} \oplus \mathcal{H}_{0,3,1} \oplus \mathcal{H}_{1,3,0} \oplus \mathcal{H}_{0,1,3} \oplus \mathcal{H}_{1,0,3})\end{aligned}$$

which yields this algebra decomposition. This is easy for $\lambda=(4)$. Indeed, for every $\mathcal{H}_{k_0,k_1,k_2}$ this is given by the invariant average vector

$$h^{(4)} = \sum_{k_0(i_1,i_2,i_3,i_4)=k_0,\ldots,k_2(i_1,i_2,i_3,i_4)=k_2} |i_1 i_2 i_3 i_4\rangle.$$

In the following we will only discuss the case where $k_0 \geqslant k_1 \geqslant k_2$ (i.e., $\mathcal{H}_{4,0,0}, \mathcal{H}_{3,1,0}, \mathcal{H}_{2,1,1}$). For $\lambda = \mu$, we have a natural embedding $\mathcal{S}^\lambda \subseteq M^\lambda \cong \mathcal{H}_{k_0,k_1,k_2}$ given by

$$h_t = \sum_{\sigma \in C_t} \operatorname{sgn}(\sigma) \sum_{(i_1,\ldots,i_4) \sim_t (i_1^t,\ldots,i_4^t)} |i_1 i_2 i_3 i_4\rangle, \tag{9}$$

for all λ-tableau t of type μ. Let us illustrate this in our examples. If $\lambda = (3,1)$, we have three standard tableaux

$$t_0 = \begin{array}{|c|c|c|}\hline 1 & 2 & 3 \\ \hline 4 \\ \cline{1-1}\end{array} \quad t_1 = \begin{array}{|c|c|c|}\hline 1 & 2 & 4 \\ \hline 3 \\ \cline{1-1}\end{array} \quad t_2 = \begin{array}{|c|c|c|}\hline 1 & 3 & 4 \\ \hline 2 \\ \cline{1-1}\end{array}.$$

The column stabilizer of t_0, t_1, t_2 is $C_{t_0} = \{1, (14)\}, C_{t_1} = \{1, (13)\}, C_{t_2} = \{1, (12)\}$. The space $\mathcal{H}_{(3,1)}$ has the basis

$$|0001\rangle, \quad |0010\rangle, \quad |0100\rangle, \quad |1000\rangle.$$

Now, we define on $\mathcal{H}_{(3,1)}$

$$A_{t_i} = \sum_{\sigma \in C_{t_i}} \operatorname{sgn}(\sigma) \pi(\sigma).$$

The range of A_{t_i} is given by the vectors

$$h_{t_0} = |0001\rangle - |1000\rangle,$$

$$h_{t_1} = |0010\rangle - |1000\rangle,$$

$$h_{t_2} = |0100\rangle - |1000\rangle.$$

This provides us with the basis for

$$M^{(3,1)} \cong \mathcal{H}_{(3,1)} = \operatorname{span}\{h^{(4)}\} \oplus \operatorname{span}\{h_{t_0}, h_{t_1}, h_{t_2}\}.$$

Now, we consider $\mathcal{H}_{(2,2,0)}$ spanned by

$$|0011\rangle, \quad |0110\rangle, \quad |0101\rangle, \quad |1100\rangle, \quad |1010\rangle, \quad |1001\rangle.$$

For $\lambda = (3,1)$ we have the following list of λ-tableaux of type $(2,2)$:

$$\begin{array}{|c|c|c|}\hline 0 & 0 & 1 \\ \hline 1 \\ \cline{1-1}\end{array} \quad \begin{array}{|c|c|c|}\hline 0 & 1 & 1 \\ \hline 0 \\ \cline{1-1}\end{array} \quad \begin{array}{|c|c|c|}\hline 0 & 1 & 0 \\ \hline 1 \\ \cline{1-1}\end{array} \quad \begin{array}{|c|c|c|}\hline 1 & 1 & 0 \\ \hline 0 \\ \cline{1-1}\end{array} \quad \begin{array}{|c|c|c|}\hline 1 & 0 & 1 \\ \hline 0 \\ \cline{1-1}\end{array} \quad \begin{array}{|c|c|c|}\hline 1 & 0 & 0 \\ \hline 1 \\ \cline{1-1}\end{array}.$$

Here we used $t_0 = \begin{array}{|c|c|c|}\hline 1 & 2 & 3 \\ \hline 4 \\ \cline{1-1}\end{array}$. Only the first tableaux is semistandard and yields an injection

$$\Theta \equiv \Theta_{\begin{array}{|c|c|c|}\hline 0 & 0 & 1 \\ \hline 1 \\ \cline{1-1}\end{array}} : \mathcal{S}^{(3,1)} \to \mathcal{H}_{(2,2)}$$

with

$$\Theta(e_{\{t_0\}}) = \sum_{(i_1,\ldots,i_4)\sim_{t_0}(0,0,1,1)} |i_1 i_2 i_3 i_4\rangle.$$

This means

$$\Theta(e_{\{t_0\}}) = |0011\rangle + |0101\rangle + |1001\rangle.$$

(See the example in the last section for $n=5$.) Further, this vector is a cyclic vector for the image of $\mathcal{S}^{(3,1)}$ in $\mathcal{H}_{(2,2)}$. The polytabloid is

$$e_{t_0} = \sum_{\sigma\in C_{t_0}} \mathrm{sgn}(\sigma)\sigma e_{\{t_0\}} = e_{\{t_0\}} - (14)e_{\{t_0\}}.$$

Therefore $\Theta(\mathcal{S}^{(3,1)})$ is the module generated by

$$\Theta(e_{t_0}) = h_{t_0} = |0011\rangle - |1010\rangle + |0101\rangle - |1100\rangle.$$

Equivalently,

$$\Theta(\mathcal{S}^{(3,1)}) = \mathrm{span}\{h_{t_0},(12)h_{t_0},(13)h_{t_0}\} = \mathrm{span}\{|0011\rangle - |1010\rangle + |0101\rangle - |1100\rangle, |1100\rangle - |1001\rangle + |0110\rangle - |0011\rangle, |0110\rangle - |0101\rangle + |1010\rangle - |1001\rangle\}.$$

Another way to find a basis is to consider $t_1=\begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3\\\cline{1-1}\end{array}$. In this case, $C_{t1}=\{1,(13)\}$,

$$\Theta(e_{\{t_1\}}) = |0011\rangle + |0110\rangle + |1010\rangle$$

and

$$h_{t_1} = \Theta(e_{\{t_1\}}) - (13)\Theta(e_{\{t_1\}}) = |0011\rangle - |1001\rangle + |0110\rangle - |1100\rangle.$$

Similarly for $t_2=\begin{array}{|c|c|c|}\hline 1&3&4\\\hline 2\\\cline{1-1}\end{array}$, we have $C_{t1}=\{1,(12)\}$ and

$$\Theta(e_{\{t_2\}}) = |0101\rangle + |0110\rangle + |1100\rangle$$

and

$$h_{t_2} = \Theta(e_{\{t_2\}}) - (12)\Theta(e_{\{t_2\}}) = |0101\rangle - |1001\rangle + |0110\rangle - |1010\rangle.$$

The copy of $\mathcal{S}^{(2,2)}$ in $\mathcal{H}_{(2,2)}$ is again easy to find. We recall that $\mathcal{S}^{(2,2)}$ is spanned by the standard tableaux $\{e_{s_0}, e_{s_1}\}$ where

$$s_0 = \begin{array}{|c|c|}\hline 1&2\\\hline 3&4\\\hline\end{array} \quad s_1 = \begin{array}{|c|c|}\hline 1&3\\\hline 2&4\\\hline\end{array}.$$

The column stabilizers are given by $C_{s_0}=\{1,(13),(24),(13)(24)\}$ and by $C_{s_1}=\{1,(12),(34),(12)\times(34)\}$. This yields operators on $\mathcal{H}_{(2,2)}$,

$$A_{s_0} = 1 - \pi((13)) - \pi((24)) + \pi((13)(24))$$

and

$$A_{s_1} = 1 - \pi((12)) - \pi((34)) + \pi((12)(34)).$$

Applied to the unit vectors, we find the ranges

$$\mathrm{Ran}(A_{s_0}) = |0110\rangle - |1010\rangle - |0101\rangle + |1001\rangle$$

and

$$\mathrm{Ran}(A_{s_1}) = |0011\rangle - |1001\rangle - |0110\rangle + |1100\rangle.$$

Finally, we consider $\mathcal{H}_{(2,1,1)}$ with basis

$$\{|0012\rangle,|0021\rangle,|0102\rangle,|0120\rangle,|0201\rangle,|0210\rangle,|1002\rangle,|1020\rangle,|1200\rangle,|2001\rangle,|2010\rangle,|2100\rangle\}.$$

The representation of $\mathcal{S}^{(4)}$ is one-dimensional, given by the average of all these vectors. There are two copies of $\mathcal{S}^{(3,1)}$ corresponding to the two $(3,1)$-tableaux of type $(2,1,1)$,

$$T = \begin{array}{|c|c|c|}\hline 0 & 0 & 1 \\ \hline 2 \\ \cline{1-1}\end{array} \qquad T' = \begin{array}{|c|c|c|}\hline 0 & 0 & 2 \\ \hline 1 \\ \cline{1-1}\end{array}.$$

The basis for $\mathcal{S}^{(3,1)}$ is given by $\{e_{t_0}, e_{t_1}, e_{t_2}\}$ where

$$t_0 = \begin{array}{|c|c|c|}\hline 1 & 2 & 3 \\ \hline 4 \\ \cline{1-1}\end{array} \quad t_1 = \begin{array}{|c|c|c|}\hline 1 & 2 & 4 \\ \hline 3 \\ \cline{1-1}\end{array} \quad t_2 = \begin{array}{|c|c|c|}\hline 1 & 3 & 4 \\ \hline 2 \\ \cline{1-1}\end{array}.$$

Following the definition of $\Theta_T(e_{t_j})$, we get

$$\gamma_{t_0}(T) = (0,0,1,2), \quad \gamma_{t_1}(T) = (0,0,2,1), \quad \gamma_{t_2}(T) = (0,2,0,1).$$

Using row equivalence, we are allowed to permute the entries $\{1,2,3\}$ for t_0, the entries $\{1,2,4\}$ for t_1 and $\{1,3,4\}$ for t_2 and thus

$$\Theta_T(e_{\{t_0\}}) = |0012\rangle + |0102\rangle + |1002\rangle,$$

$$\Theta_T(e_{\{t_1\}}) = |0021\rangle + |0120\rangle + |1020\rangle,$$

$$\Theta_T(e_{\{t_2\}}) = |0201\rangle + |0210\rangle + |1200\rangle.$$

For t_0, t_1, t_2 we have to apply, respectively, $A_{T,t_0} = \mathbb{1} - \pi(14)$, $A_{T,t_1} = \mathbb{1} - \pi(13)$ and $A_{T,t_2} = \mathbb{1} - \pi(12)$ in order to obtain the image of the polytabloids,

$$h_{T,t_0} = |0012\rangle - |2010\rangle + |0102\rangle - |2100\rangle + |1002\rangle - |2001\rangle,$$

$$h_{T,t_1} = |0021\rangle - |2001\rangle + |0120\rangle - |2100\rangle + |1020\rangle - |2010\rangle,$$

$$h_{T,t_2} = |0201\rangle - |2001\rangle + |0210\rangle - |2010\rangle + |1200\rangle - |2100\rangle.$$

This is our first copy of $\mathcal{S}^{(3,1)}$. For the second, we exercise the same procedure in the case of T',

$$\Theta_{T'}(e_{\{t_0\}}) = |0021\rangle + |0201\rangle + |2001\rangle,$$

$$\Theta_{T'}(e_{\{t_1\}}) = |0012\rangle + |0210\rangle + |2010\rangle,$$

$$\Theta_{T'}(e_{\{t_2\}}) = |0102\rangle + |0120\rangle + |2100\rangle.$$

This provides us with

$$h_{T',t_0} = |0021\rangle - |1020\rangle + |0201\rangle - |1200\rangle + |2001\rangle - |1002\rangle,$$

$$h_{T',t_1} = |0012\rangle - |1002\rangle + |0210\rangle - |1200\rangle + |2010\rangle - |1020\rangle,$$

$$h_{T',t_2} = |0102\rangle - |1002\rangle + |0120\rangle - |1020\rangle + |2100\rangle - |1200\rangle.$$

We have one copy of $\mathcal{S}^{(2,2)}$ which is spanned by

$$s_0 = \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & 4 \\ \hline \end{array} \quad s_1 = \begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 & 4 \\ \hline \end{array}$$

Our $(2,2)$ tableau of type $(2,1,1)$ is given by $T = \begin{array}{|c|c|}\hline 0 & 0 \\ \hline 1 & 2 \\ \hline \end{array}$. This gives

$$\Theta(e_{\{s_0\}}) = |0012\rangle + |0021\rangle \quad \text{and } \Theta(e_{\{s_1\}}) = |0102\rangle + |0201\rangle.$$

The operator is $1 - \pi(13) - \pi(24) + \pi((13)(24))$, determined by $C_{s_0} = \{1, (13), (24), (13)(24)\}$, and thus

$$h_{s_0} = |0012\rangle - |1002\rangle - |0210\rangle + |1200\rangle + |0021\rangle - |2001\rangle - |0120\rangle + |2100\rangle$$

and similarly for s_1 we apply $1 - \pi(12) - \pi(34) + \pi((12)(34))$ to obtain

$$h_{s_1} = |0102\rangle - |1002\rangle - |0120\rangle + |1020\rangle + |0201\rangle - |2001\rangle - |0210\rangle + |2010\rangle.$$

Finally we consider the copy of $\mathcal{S}^{(2,1,1)}$, which has basis $\{e_{r_0}, e_{r_1}, e_{r_2}\}$ where

$$r_0 = \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 \\ \cline{1-1} 4 \\ \cline{1-1} \end{array} \quad r_1 = \begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 \\ \cline{1-1} 4 \\ \cline{1-1} \end{array} \quad r_2 = \begin{array}{|c|c|}\hline 1 & 4 \\ \hline 2 \\ \cline{1-1} 3 \\ \cline{1-1} \end{array}.$$

Here $T = \begin{array}{|c|c|}\hline 0 & 0 \\ \hline 1 \\ \cline{1-1} 2 \\ \cline{1-1} \end{array}$. This yields

$$\Theta_T(e_{\{r_0\}}) = |0012\rangle, \quad \Theta_T(e_{\{r_1\}}) = |0102\rangle, \quad \Theta_T(e_{\{r_2\}}) = |0120\rangle.$$

The column stabilizer of r_2 is given by all permutations which leave $\{1,2,3\}$ invariant. This yields

$$h_{r_2} = |0120\rangle - |0210\rangle - |1020\rangle + |1200\rangle + |2010\rangle - |2100\rangle.$$

Similarly, we must look for all permutations of $\{1,3,4\}$ in the column stabilizer of r_0 and we obtain

$$h_{r_0} = |0012\rangle - |0021\rangle - |1002\rangle + |1020\rangle + |2001\rangle - |2010\rangle.$$

For the column stabilizer of r_1, we may permute $\{1,2,4\}$ and hence

$$h_{r_1} = |0102\rangle - |0201\rangle - |1002\rangle + |1200\rangle + |2001\rangle - |2100\rangle.$$

By Eq. (8), the largest full matrix algebra $\mathbb{M}_k$ that can be injected into the noise commutant here is $\mathbb{M}_3$, identified with the subalgebras of $\mathcal{A}'_{\mathcal{S}}$ unitarily equivalent to either $\mathbb{1}_{15} \otimes \mathbb{M}_3$ or $\mathbb{1}_3 \otimes \mathbb{M}_3$. Let us explicitly identify the copy of $\mathbb{1}_3 \otimes \mathbb{M}_3$. The set $\{h_{r_0}, h_{r_1}, h_{r_2}\}$ yields the copy of $S^{(2,1,1)}$ inside $\mathcal{H}^{(2,1,1)}$. A similar analysis yields the basis for the copy of $S^{(2,1,1)}$ inside $\mathcal{H}^{(1,2,1)}$. It is generated by $T' = \begin{array}{|c|c|}\hline 0 & 1 \\ \hline 1 \\ \cline{1-1} 2 \\ \cline{1-1} \end{array}$ and in this case

$$\Theta_{T'}(e_{\{r_0\}}) = |0112\rangle + |1012\rangle,$$

$$\Theta_{T'}(e_{\{r_1\}}) = |0112\rangle + |1102\rangle,$$

$$\Theta_{T'}(e_{\{r_2\}}) = |0121\rangle + |1120\rangle.$$

Thus we have

$$h'_{r_0} = |0112\rangle - |0121\rangle - |1102\rangle + |1120\rangle + |2101\rangle - |2110\rangle,$$

$$h'_{r_1} = |0112\rangle - |0211\rangle - |1012\rangle + |1210\rangle + |2011\rangle - |2110\rangle,$$

$$h'_{r_2} = |0121\rangle - |0211\rangle - |1021\rangle + |1201\rangle + |2011\rangle - |2101\rangle.$$

Further, the basis for the copy of $S^{(2,1,1)}$ inside $\mathcal{H}^{(1,1,2)}$ is generated by $T'' = \begin{array}{|c|c|}\hline 0 & 2 \\ \hline 1 \\ \cline{1-1} 2 \\ \cline{1-1} \end{array}$ and in this case

$$\Theta_{T''}(e_{\{r_0\}}) = |0212\rangle + |2012\rangle,$$

$$\Theta_{T''}(e_{\{r_1\}}) = |0122\rangle + |2102\rangle,$$

$$\Theta_{T''}(e_{\{r_2\}}) = |0122\rangle + |2120\rangle.$$

Thus we have

$$h''_{r_0} = |0212\rangle - |0221\rangle - |1202\rangle + |1220\rangle + |2201\rangle - |2210\rangle,$$

$$h''_{r_1} = |0122\rangle - |0221\rangle - |1022\rangle + |1220\rangle + |2021\rangle - |2120\rangle,$$

$$h''_{r_2} = |0122\rangle - |0212\rangle - |1022\rangle + |1202\rangle + |2012\rangle - |2102\rangle.$$

Let $P_{(2,1,1)}$ be the projection of $\mathcal{H}$ onto the span of $\{h_{r_i}, h'_{r_j}, h''_{r_k} : 0 \leqslant i, j, k \leqslant 2\}$. Then $P_{(2,1,1)}$ is a minimal central projection for $\mathcal{A}'_{\mathcal{S}}$ and the compression subalgebra $P_{(2,1,1)}\mathcal{A}'_{\mathcal{S}}P_{(2,1,1)} = \mathcal{A}'_{\mathcal{S}}P_{(2,1,1)} \subset \mathcal{A}'_{\mathcal{S}}$ is unitarily equivalent to $\mathbb{1}_3 \otimes \mathbb{M}_3$. In fact, with respect to the ordered basis

$$\{h_{r_0}, h_{r_1}, h_{r_2}, h'_{r_0}, h'_{r_1}, h'_{r_2}, h''_{r_0}, h''_{r_1}, h''_{r_2}\}$$

for $P_{(2,1,1)}\mathcal{H}$, we have the matrix representations

$$\mathcal{A}'_{\mathcal{S}}P_{(2,1,1)} = \left\{ \begin{pmatrix} A & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & A \end{pmatrix} : A \in \mathbb{A}_3 \right\}.$$

Note that the subspaces spanned by the sets $\{h_{r_i}\}, \{h'_{r_i}\}$, and $\{h''_{r_i}\}$ are perpendicular, but the vectors within each of these sets do not form an orthogonal basis for the corresponding subspace.

VII. CONCLUSION

We have investigated the operator algebras of fixed points for a class of quantum channels we call universal collective rotation channels $\mathcal{E}_{\mathcal{S}}$. This class includes as a subclass the well-known class of collective rotation channels. We showed that such channels always have an abundance of noiseless subsystems and gave a method for explicitly computing them. In particular, the Young tableaux machine gives a clean approach for this process. In lower dimensional cases (e.g., when $d=2$), our approach is more technical when compared to others in the literature (for instance, Ref. 15). However, an important advantage of the Young tableaux approach for higher dimensional cases is that it is particularly amenable to computations.

An issue we have not pursued here concerns the channels generated by nonmaximal sets $\mathcal{S}$. The d^n-dimensional representations of J_x, J_y, J_z considered in Ref. 15 provide such an example, but we would expect there to be other interesting nontrivial examples of channels $\mathcal{E}_{\mathcal{S}}$ for nonmaximal $\mathcal{S}$. We emphasize that even for nonmaximal $\mathcal{S}$ there is an abundance of noiseless subsystems because $\mathrm{Fix}(\mathcal{E}_{\mathcal{S}})$ contains $\pi(S_n)''$.

We also wonder what other representations of S_n correspond to physically meaningful unital channels, beyond π and its subrepresentations (which correspond to the compressions of UCR-channels). The recent paper[2] of Bacon *et al.*, appears to present further insights into this topic, and also shows how the unitary base change from the standard basis to the basis given by the Young tableaux can be efficiently computed using quantum circuits.

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Path integral for the radial Dirac equation

Takashi Ichinose[a)]
Department of Mathematics, Faculty of Science, Kanazawa University, Kanazawa, 920-1192, Japan

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For the radial Dirac equation, a countably additive path space measure on the space of continuous paths living on the real half-line is constructed to give a path integral representation of its Green function. © *2005 American Institute of Physics.*
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I. INTRODUCTION

In this paper we want to make a mathematical rigorous approach to the path integral for the radial Dirac equation, namely, the radial part of the Dirac equation in spherical coordinates. The equation is given, for $\mathbf{C}^2$-valued functions $\psi(r,t)={}^t(\psi_1(r,t),\psi_2(r,t))$, by

$$\frac{\partial}{\partial t}\psi(r,t) = -i[\tau_k + V(r)]\psi(r,t), \tag{1.1}$$

with a real-valued spherically symmetric potential $V=V(r)$, i.e., a function in the real half-line $\mathbf{R}_+:=(0,\infty)$, where the variables (r,t) lie in radial space–time $\mathbf{R}_+\times\mathbf{R}$. Here τ_k is the free radial Dirac operator with mass m defined for $k=\pm1, \pm2,\ldots$, by

$$\tau_k: f \mapsto \left[\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\frac{\partial}{\partial r} + \begin{pmatrix} m & -k/r \\ -k/r & -m \end{pmatrix}\right]\begin{pmatrix} f_1(r) \\ f_2(r) \end{pmatrix} \tag{1.2a}$$

for suitably smooth $\mathbf{C}^2$-valued functions $f={}^t(f_1,f_2)$ in $\mathbf{R}_+$, in short,

$$\tau_k = -i\sigma_2\frac{\partial}{\partial r} - \sigma_1\frac{k}{r} + m\sigma_3, \tag{1.2b}$$

with the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The free radial Dirac operator τ_k arises from the spin-angular momentum decomposition of the free Dirac operator in three space dimensions. The nonzero integer k represents an eigenvalue of the "spin–orbit operator" [see Bjorken and Drell (1964), Thaller (1992), Weidmann (1987)].

The operator τ_k is a symmetric operator with domain $D[\tau_k]=C_0^\infty(\mathbf{R}_+;\mathbf{C}^2)$ in $L^2(\mathbf{R}_+;\mathbf{C}^2)$. Here $L^2(\mathbf{R}_+;\mathbf{C}^2)$ is the Hilbert space of the $\mathbf{C}^2$-valued square-integrable functions in $\mathbf{R}_+$ with respect to the Lebesgue measure dr, and $C_0^\infty(\mathbf{R}_+;\mathbf{C}^2)$ the locally convex space of the $\mathbf{C}^2$-valued C^∞ functions in $\mathbf{R}_+$ with compact support. It has a singularity at $r=0$ as in (1.2a) and (1.2b). This is indeed harmless if we consider it as an operator in the L^2 space, but is a problem to construct a path space measure, for we need to consider it as an operator in the L^∞ space [for this see Ichinose and Tamura (1984, 1987, 1988)]. In this context, in Ichinose and Jefferies (2002), we have made an explicit construction of the free propagator, namely, the integral kernel $\mathcal{K}_t(r,\rho)$ of $e^{-it\tau_k}$ for $k=1$,

a)Electronic mail: ichinose@kappa.s.kanazawa-u.ac.jp

and shown that, though it turns out to be a distribution *of order zero* in the variables $(r,\rho)\in\mathbf{R}_+\times\mathbf{R}_+=\mathbf{R}_+^{\,2}$, there exists no countably additive path space measure to give a path integral representation to the solution of the Cauchy problem for the radial Dirac equation (1.1).

The aim of this paper is to construct a countably additive path space measure to represent by path integral, though not the propagator, the Green function for the radial Dirac equation (1.1). The main idea is to combine our method of constructing a path space measure developed for the one-dimensional Dirac equation in the papers [Ichinose (1982, 1984), Ichinose and Tamura (1984, 1987, 1988)], in particular, in their a little more refined review [Ichinose (1993)], with the following simple but intriguing procedure of dealing with the singularity, which was invented by Duru and Kleinert (1979) and has since been employed by many physicists [see Kleinert (1995, Chaps. 12 and 14), Inomata, Katsuraji, and Gerry (1992, p. 6), Grosche and Steiner (1998, pp. 77–83)] to perform space–time transformations in path integrals.

The free radial Dirac operator τ_k has a singularity at $r=0$. However, if we multiply this operator τ_k by some (non-negative) functions $a(r)$ and $b(r)$ from the left and right sides, respectively, then $a(r)\tau_k b(r)$ becomes no more singular. Let us take $a(r)=b(r)=r^{1/2}$, and set $T_k=r^{1/2}\tau_k r^{1/2}$. Then $-iT_k$ becomes

$$\begin{aligned}-iT_k=-ir^{1/2}\tau_k r^{1/2}&=-\sigma_2 r^{1/2}\left(\frac{\partial}{\partial r}\right)r^{1/2}+i(k\sigma_1-mr\sigma_3)\\&=-i\begin{pmatrix}0&-1\\1&0\end{pmatrix}r^{1/2}\left(\frac{\partial}{\partial r}\right)r^{1/2}+i\begin{pmatrix}-mr&k\\k&mr\end{pmatrix}=:-iT_{k0}-iT_{k1}.\end{aligned}\tag{1.3}$$

We also consider the operator

$$H(k,rV):=T_k+rV(r),\tag{1.4}$$

relevant to the radial Dirac operator in (1.2a) and (1.2b). Then T_k is a symmetric operator with domain $D[T_k]=C_0^\infty(\mathbf{R}_+;\mathbf{C}^2)$ in $L^2(\mathbf{R}_+;\mathbf{C}^2)$. For the potentials $V(r)$ we are concerned with, we can show $H(k,rV)$ is essentially self-adjoint on $C_0^\infty(\mathbf{R}_+;\mathbf{C}^2)$, as well as T_k. We shall denote their closures or unique selfadjoint extensions again by the same $H(k,rV)$ and T_k.

Then consider, for $H(k,rV)$ instead of $\tau_k+V(r)$, the Cauchy problem

$$\frac{\partial}{\partial t}u(r,t)=-iH(k,rV)u(r,t),\quad u(r,0)=g(r)={}^t(g_1(r),g_2(r))\tag{1.5}$$

for $t\in\mathbf{R}$ or the solution $u(r,t)=(e^{-itH(k,rV)}g)(r)$. Since T_k has no more singularity at $r=0$, we expect to be able to construct a path space measure associated with the semigroup $e^{-itH(k,rV)}$. Since the resolvent is expressed by the Laplace transform of the semigroup, we shall find the following relation between the desired resolvent kernel of τ_k+V and the semigroup $e^{-itH(k,rV)}$, though a little formally expressed:

$$[(\tau_k+V-\lambda)^{-1}](r,\rho)=r^{1/2}[(H(k,rV)-\lambda r)^{-1}](r,\rho)\rho^{1/2}=i\int_0^\infty r^{1/2}e^{-it(H(k,rV)-\lambda r)}\rho^{1/2}\,\mathrm{d}t,$$

for suitable real or complex numbers λ. In this way, we might get, for the original radial Dirac operator $\tau_k+V(r)$, a path integral representation of the resolvent kernel and the Green function if λ might be taken to be zero, though we were unable to find such a representation for the propagator $e^{-it(\tau_k+V)}$ itself.

For the potential $V(x)$, we assume that it is a real-valued function in $\mathbf{R}_+$ such that $V(r)=V_1(r)+V_2(r)$, where $V_1(r)=e/r$ with a real constant e satisfying $|e|\leqslant\sqrt{k^2-\frac{1}{4}}$ and $V_2(r)$ is a locally square-integrable function in $\mathbf{R}_+$ which is bounded near $r=0$.

Note that this class of potentials $V(r)$ contains the Coulomb potential.

In this case it can be shown that the radial Dirac operator τ_k+V in (1.1) is essentially self-adjoint on $C_0^\infty(\mathbf{R}_+;\mathbf{C}^2)$. We denote its unique self-adjoint extension in $L^2(\mathbf{R}_+;\mathbf{C}^2)$ also by the same

τ_k+V. Thus this operator has a real spectrum. Further, as to its spectrum, for instance, the following results are known [Weidmann (1987), Thaller (1992, Theorems 4.18, 4.19)]. If $V_2(r):=V_{21}(r)+V_{22}(r)$ satisfies for some $r_0>0$ that $V_{21}\in L^1((r_0,\infty))$ and V_{22} is of bounded variation in $[r_0,\infty)$ with $\lim_{r\to\infty}V_{22}(r)=0$, then the operator τ_k+V has a purely absolutely continuous spectrum in the real line $\mathbf{R}$ outside the closed interval $[-m,m]$. If $V_1(r)$ is absent (i.e., $e=0$) and if $\lim_{r\to\infty}|V_2(r)|=\infty$ and $\int_{r_0}^{\infty}|V_2'(r)/V_2(r)^2|\mathrm{d}r<\infty$ for some $r_0>0$, then τ_k+V has the whole real line $\mathbf{R}$ as a purely absolutely continuous spectrum.

We will show the following path integral representation for the resolvent kernel $[(\tau_k+V\mp i\varepsilon)^{-1}](r,\rho)$ for $\varepsilon>0$ and the Green function for the radial Dirac operator $\tau_k+V(r)$ in (1.1).

The set of all complex 2×2-matrices is denoted by $M_2(\mathbf{C})=\mathbf{C}^2\otimes(\mathbf{C}^2)'$. With $[0,\infty)=\overline{\mathbf{R}_+}$ being the closed real half-line, let $C_{00}^{\infty}([0,\infty)^2;M_2(\mathbf{C}))$ be the locally convex space of the $M_2(\mathbf{C})$-valued C^{∞} functions $M(r,\rho)$ in $[0,\infty)\times[0,\infty)$ which have compact support and whose derivatives $\partial r^m\partial\rho^n M(r,\rho)$, for all non-negative integers m and n, vanish at $(r,0)$ and $(0,\rho)$ for all $r\geqslant0$ and $\rho\geqslant0$. Let $C_{00}^{\infty}([0,\infty)^2;M_2(\mathbf{C}))'$ be its dual space. As $C_0^{\infty}(\mathbf{R}_+{}^2;M_2(\mathbf{C}))$ is a subspace of $C_{00}^{\infty}([0,\infty)^2;M_2(\mathbf{C}))$, so $C_{00}^{\infty}([0,\infty)^2;M_2(\mathbf{C}))'$ is a subspace of the space $\mathcal{D}'(\mathbf{R}_+{}^2;M_2(\mathbf{C}))$ of the $M_2(\mathbf{C})$-valued distributions in $\mathbf{R}_+\times\mathbf{R}_+$. By $(\cdot,\cdot)$ and $\langle\cdot,\cdot\rangle$ we denote, respectively, the sesquilinear and bilinear inner products of a dual pairing.

The main result of this note is the following theorems. The notation $|0,t|$ stands for the interval $0\leqslant s\leqslant t$ or $0\geqslant s\geqslant t$ according as $t>0$ or $t<0$.

Theorem 1.1: *Let $V(r)$ be a potential mentioned above.*

(i) *For every $\varepsilon>0$, there exists a 2×2-matrix distribution-valued, precisely speaking, $C_{00}^{\infty}([0,\infty)^2;M_2(\mathbf{C}))'$-valued, countably additive path space measure $\mu_{t,0}$ on the Banach space $C(|0,t|\to[0,\infty))$ of the continuous paths $R:|0,t|\to[0,\infty)$ such that the resolvent kernel $[(\tau_k+V\mp i\varepsilon)^{-1}](r,\rho)$ for the radial Dirac operator τ_k+V in (1.1) admits a path integral representation: for every pair $(f,g)\in C_{00}^{\infty}([0,\infty);\mathbf{C}^2)\times C_{00}^{\infty}([0,\infty);\mathbf{C}^2)$,*

$$\begin{aligned}(f,(\tau_k+V\mp i\varepsilon)^{-1}g)&=\int_0^{\infty}\int_0^{\infty}{}^t\overline{f(r)}[(\tau_k+V\mp i\varepsilon)^{-1}](r,\rho)g(\rho)\mathrm{d}r\,\mathrm{d}\rho\\&=i\int_0^{\pm\infty}\mathrm{d}t\int_{C(|0,t|\to[0,\infty))}\left\langle{}^t\overline{f(R(t))},\mathrm{d}\mu_{t,0}(R)g(R(0))\right\rangle R(t)^{1/2}R(0)^{1/2}\\&\quad\times\exp\left[-\int_0^t(iV(R(s))R(s)\pm\varepsilon R(s))\mathrm{d}s\right].\end{aligned}\tag{1.6}$$

In particular, the resolvent kernel $[(\tau_k+V\mp i\varepsilon)^{-1}](r,\rho)$ is a distribution of order zero in $\mathbf{R}_+\times\mathbf{R}_+$.

(ii) *The measure $\mu_{t,0}$ is concentrated on the set of the continuous paths $R:|0,t|\to[0,\infty)$ for which there exists a finite partition: $0=t_0\leqq t_1\leqq\cdots\leqq t_{n+1}=t$ of the interval $|0,t|$ such that for $t_{h-1}\leqq s\leqq t_h$, $1\leqslant h\leqslant n+1$,*

$$R(s)=R(0)e^{\pm[\sum_{p=1}^{h-1}(-1)^{p-1}(t_p-t_{p-1})+(-1)^{h-1}(s-t_{h-1})]}.\tag{1.7}$$

Therefore each of these continuous paths $R(\cdot)$ is, for some finite n, an n-vertex piecewise smooth curve in radial space–time, starting from $R(0)$ at time 0 and reaching $R(t)$ at time t, and exponentially growing or decreasing in each partioned short time interval.

We denote by $G_{\pm}(r,\rho)$ the Green function for the radial Dirac operator τ_k+V to be given as the limit of the integral kernel of the resolvent $(\tau_k+V\mp i\varepsilon)^{-1}$ as $\varepsilon\to+0$, if this limit exists.

Theorem 1.2: *For the same potential $V(r)$ as in Theorem 1.1, suppose that 0 is not an eigenvalue of the radial Dirac operator τ_k+V. Suppose that the Green function $G_{\pm}(r,\rho)$ for the radial Dirac operator τ_k+V in (1.1) exists. Then it is a distribution of order zero in $(r,\rho)\in\mathbf{R}_+\times\mathbf{R}_+$, and admits a path integral representation: for every pair $(f,g)\in C_{00}^{\infty}([0,\infty);\mathbf{C}^2)\times C_{00}^{\infty}([0,\infty);\mathbf{C}^2)$,*

(i)

$$\int_0^\infty \int_0^\infty {}^t\overline{f(r)} G_\pm(r,\rho) g(\rho) \mathrm{d}r\, \mathrm{d}\rho = i \lim_{\varepsilon \to +0} \int_0^{\pm\infty} \mathrm{d}t \int_{C(|0,t| \to [0,\infty))} \left\langle {}^t\overline{f(R(t))}, \mathrm{d}\mu_{t,0}(R) g(R(0)) \right\rangle \times R(t)^{1/2} R(0)^{1/2} \exp\left[- \int_0^t (iV(R(s))R(s) \pm \varepsilon R(s)) \mathrm{d}s \right]; \tag{1.8}$$

(ii)

$$\int_0^\infty \int_0^\infty {}^t\overline{f(r)} G_\pm(r,\rho) g(\rho) \mathrm{d}r\, \mathrm{d}\rho = i \lim_{\varepsilon \to +0} \int_0^{\pm\infty} \mathrm{d}t \int_{C(|0,t| \to [0,\infty))} \left\langle {}^t\overline{f(R(t))}, \mathrm{d}\mu_{t,0}(R) g(R(0)) \right\rangle \times R(t)^{1/2} R(0)^{1/2} \exp\left[- i \int_0^t V(R(s))R(s) \mathrm{d}s \mp \varepsilon t \right]. \tag{1.9}$$

If we formally take the delta functions at the two points $r>0$ and $\rho>0$, respectively, for f and g, the formula (1.8)/(1.9) looks like

$$G_\pm(r,\rho) = i \int_0^{\pm\infty} \mathrm{d}t \int_{C(|0,t| \to [0,\infty)), R(0)=\rho, R(t)=r} r^{1/2} \rho^{1/2} \exp\left[- i \int_0^t V(R(s))R(s) \mathrm{d}s \right] \mathrm{d}\mu_{t,0}(R). \tag{1.10}$$

It should be emphasized that our path integral concerns the three-dimensional Dirac equation, though in the spherical coordinates. For the Dirac equation in the one-dimensional space, i.e., the whole real line **R**, a path integral measure to represent the propagator was constructed first in Ichinose (1982, 1984), Ichinose and Tamura (1984) and then further studied in Ichinose and Tamura (1987, 1988) and Ichinose (1993). The problem was treated in Blanchard *et al.* (1985) from a different point of view based on Poisson process, and there are further related works Gaveau (1984), Gaveau *et al.* (1984), Combe, Sirugue, and Sirugue-Collin (1987), and Zastawniak (1988) on the subject. The method used in the present paper is also connected with the Poisson process, though we do not explicitly appeal to it. This paper is only to give the first step to describe the idea, and application to some problem in quantum field theory will be discussed elsewhere.

To prove the theorems, we investigate, in Sec. II, the Cauchy problem (1.5) in the L^∞ norm for the relevant operator to our radial Dirac operator, and also show essential self-adjointness of both the radial Dirac operator (1.2a) and (1.2b) and its relevant operator (1.4). In Sec. III, we construct, by means of the Riesz representation theorem, a countably additive path space measure associated with the semigroup for the Cauchy problem (1.5), on a big space of paths living on the closed real half-line over each finite time interval $[0,t]$. Then it is shown that this measure is in fact concentrated on the set of continuous, piecewise smooth paths with a finite number of vertices in radial space–time. In Sec. IV, we shall show, together with this measure constructed, a path integral representation of Feynman–Kac type first for this semigroup associated with (1.5) and then through the procedure mentioned for the resolvent kernel and the Green function for the radial Dirac operator we are concerned with.

II. THE RADIAL DIRAC OPERATOR AND ITS RELEVANT OPERATOR

To construct our path measure, we need to investigate the Cauchy problems (1.1) for the radial Dirac operator $\tau_k + V$ and (1.5) for its relevant operator $H(k,rV) = r^{1/2}(\tau_k + V)r^{1/2} = T_k + rV$ in (1.4).

For the potential $V(r)$, it is assumed throughout this section that $V(r)$ is a real-valued function in $\mathbf{R}_+$ such that $V(r) = V_1(r) + V_2(r)$, where $V_1(r) = e/r$ with $|e| \leqslant \sqrt{k^2 - \frac{1}{4}}$ and $V_2(r)$ is a function in $L^2_{\mathrm{loc}}(\mathbf{R}_+)$ which is bounded near $r=0$.

We have so far taken for granted that the radial Dirac operator τ_k+V in (1.1) and its relevant operator $H(k,rV)$ in (1.4) are essentially selfadjoint on $C_0^\infty(\mathbf{R}_+;\mathbf{C}^2)$. We will confirm these facts here. For some related results on the former τ_k+V, we refer also to Weidmann (1987) and Arnold, Kalf, and Schneider (1997). The L^2-norm in $L^2(\mathbf{R}_+;\mathbf{C}^2)$ is denoted by $\|\cdot\|_2$.

First consider the radial Dirac operator τ_k+V in (1.1). There exists a unique solution of the Cauchy problem (1.1).

Proposition 2.1: The operator τ_k+V is essentially self-adjoint on $C_0^\infty(\mathbf{R}_+;\mathbf{C}^2)$.

Proof: Set $D_1:=\tau_k+V_1$, so that $\tau_k+V=D_1+V_2$. It is known by Weidmann (1987), D_1 is essentially self-adjoint on $C_0^\infty(\mathbf{R}_+;\mathbf{C}^2)$. So we consider V_2 is a perturbation from D_1. We are going to use the method by Jörgens (1972, Theorem 5.6). To show essential self-adjointness of D_1+V_2, we need to show the following conditions.

(i) For each $\varphi\in C_0^\infty(\mathbf{R}_+)$, the commutator $[D_1,\varphi]=D_1\varphi-\varphi D_1$ is a bounded operator on $L^2(\mathbf{R}_+;\mathbf{C}^2)$.

(ii) For every nonempty bounded open interval $(r_1,r_2)\subseteq\mathbf{R}_+$, there exist constants $a>0$ and $0\leqslant b<1$ such that

$$\|V_2v\|_{L^2((r_1,r_2);\mathbf{C}^2)}\leqslant a\|v\|_2+b\|D_1v\|_2,\quad v\in C_0^\infty(\mathbf{R}_+;\mathbf{C}^2).$$

(iii) Let $\chi(r)$ be a C^∞-function in $\mathbf{R}_+$ with $0\leqslant\chi(r)\leqslant 1$ such that $\chi(r)=1$, $0<r\leqslant 1$ and $\chi(r)=0$, $r\geqslant 2$. Set $\varphi_n(r)=\chi(r/n)$, so that $\varphi_n(r)$ converges to 1 pointwise as $n\to\infty$. Then $\|[D_1,\varphi_n]v+[V_2,\varphi_n]v\|_2$ is bounded for every $v\in D[(D_1+V_2)^*]$.

But these conditions can be checked as follows.

Indeed, (i) is clear because $[D_1,\varphi]=-i\sigma_2\varphi'(r)$.

To see (ii), let (r_1,r_2) be a bounded open interval in $\mathbf{R}_+$. By assumption, $V_2(r)$ is bounded for $r\leqslant r_0$ for some $r_0>0$. First suppose that $r_1\geqslant r_0$, so that $(r_1,r_2)\subseteq(r_0,r_2)$, and V_2 is in $L^2((r_0,r_2))$ as well as in $L^2((r_1,r_2))$. Then for $v\in C_0^\infty(\mathbf{R}_+;\mathbf{C}^2)$, we have by the Schwarz inequality

$$\|V_2v\|_{L^2((r_1,r_2);\mathbf{C}^2)}\leqslant\|V_2v\|_{L^2((r_0,r_2);\mathbf{C}^2)}\leqslant\|V_2\|_{L^2((r_0,r_2)}\sup_{r_0\leqslant r\leqslant r_2}|v(r)|.$$

On the other hand, for every $\varepsilon>0$ there exists a constant $C(\varepsilon)>0$ such that

$$\sup_{r_0\leqslant r\leqslant r_2}|v(r)|\leqslant\varepsilon\|v'\|_{L^2((r_0,\infty);\mathbf{C}^2)}+C(\varepsilon)\|v\|_{L^2((r_0,r_2);\mathbf{C}^2)}.$$

Moreover we have with (1.2b),

$$\begin{aligned}\|v'\|_{L^2((r_0,\infty);\mathbf{C}^2)}&=\left\|-i\sigma_2\frac{\partial}{\partial r}v\right\|_{L^2((r_0,\infty);\mathbf{C}^2)}\\&=\left\|\left[\tau_k+\left(\sigma_1\frac{k}{r}-m\sigma_3\right)\right]v\right\|_{L^2((r_0,\infty);\mathbf{C}^2)}\\&=\left\|\left[D_1+\left(\sigma_1\frac{k}{r}-m\sigma_3\right)-V_1\right]v\right\|_{L^2((r_0,\infty);\mathbf{C}^2)}\\&\leqslant\|D_1v\|_{L^2((r_0,\infty);\mathbf{C}^2)}+\left\|\left(\sigma_1\frac{k}{r}-m\sigma_3\right)v\right\|_{L^2((r_0,\infty);\mathbf{C}^2)}\\&\quad+\|V_1v\|_{L^2((r_0,\infty);\mathbf{C}^2)}\leqslant\|D_1v\|_2+\left(m+\frac{|k|+|e|}{r_0}\right)\|v\|_2.\end{aligned}$$

It follows that

$$\|V_2 v\|_{L^2((r_1,r_2);\mathbf{C}^2)} \leqslant \varepsilon \|V_2\|_{L^2((r_0,r_2))} \|D_1 v\|_2 + \left[\varepsilon \left(m + \frac{|k|+|e|}{r_0} \right) + C(\varepsilon) \right] \|V_2\|_{L^2((r_0,r_2))} \|v\|_2.$$

So choose ε so small that

$$b =: \varepsilon \|V_2\|_{L^2((r_0,r_2))} < 1$$

and then set

$$a := \left[\varepsilon \left(m + \frac{|k|+|e|}{r_0} \right) + C(\varepsilon) \right] \|V_2\|_{L^2((r_0,r_2))}$$

to get (ii). Next suppose $r_1 \leqslant r_0$, so that $(r_1,r_2)=(r_1,r_0] \cup (r_0,r_2)$, though (r_0,r_2) is empty if $r_0 \geqslant r_2$. We need to see (ii) on $(r_1,r_0]$, since we can see similarly to the above on (r_0,r_2). On the interval $(r_1,r_0]$, we have $\|V_2 v\|_{L^2((r_1,r_2);\mathbf{C}^2)} \leqslant \sup_{r_1 \leqslant r \leqslant r_2} |V_2(r)| \|v\|_2$. Thus in either case we have shown (ii).

(iii) holds because $[V_2, \varphi_n]=0$ and

$$\|[D_1, \varphi_n] v\|_2 = \|-i\sigma_2 \varphi_n' v\|_2 \leqslant \frac{1}{n} \sup_{1 \leqslant r \leqslant 2} |\chi'(r)| \|v\|_2$$

for every $v \in L^2(\mathbf{R}_+;\mathbf{C}^2)$. This proves Proposition 2.1.

Next, consider the Cauchy problem for (1.5) with T_k in (1.3) and $V(r) \equiv 0$,

$$\frac{\partial}{\partial t} u(r,t) = -iT_k u(r,t) = \left[-\sigma_2 \left(r \frac{\partial}{\partial r} + \frac{1}{2} \right) + i(k\sigma_1 - mr\sigma_3) \right] u(r,t), \quad u(r,0) = g(r), \tag{2.1}$$

where the initial data $g={}^t(g_1,g_2)$ is a $\mathbf{C}^2$-valued continuous function in $[0,\infty)$ with compact support. This equation is a hyperbolic system with local propagation speed $c(r)=r$. We can easily show that the solution $u(\cdot,t)$ satisfies for every $t \in \mathbf{R}$,

$$\|u(\cdot,t)\|_2 = \|g\|_2. \tag{2.2}$$

Moreover, this Cauchy problem is L^∞ well-posed with the estimate to be given below. It is this fact that plays a crucial role in this paper.

To describe it, set

$$N := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} = \frac{1}{\sqrt{2}} (\sigma_0 + i\sigma_1),$$

where σ_0 is the 2×2-identity matrix. N is a unitary matrix such that $N\sigma_2 N^{-1} = -\sigma_3$. Note also that $N\sigma_1 N^{-1} = \sigma_1$ and $N\sigma_3 N^{-1} = \sigma_2$. Then there exists a unique solution $u(r,t)$ of (2.1), which is given as the solution of the integral equation

$$u(r,t) = (e^{-itT_{k0}} g)(r,t) - i \int_0^t (e^{-i(t-s)T_{k0}} (T_{k1} u)(\cdot,s))(r) \mathrm{d}s. \tag{2.3}$$

Solving the equation (2.3), we shall show the following proposition.

Proposition 2.2: If $g={}^t(g_1,g_2)$ is a $\mathbf{C}^2$-valued continuous function in $[0,\infty)$ with compact support, e.g., support in a bounded closed interval $[0,S]$ for $S>0$, then the solution $u(\cdot,t)$ has support in the bounded interval $[e^{-|t|} \inf \operatorname{supp} g, e^{|t|} \sup \operatorname{supp} g]$, and satisfies

$$\|Nu(\cdot,t)\|_\infty = \|\exp[-itT_k] Ng\|_\infty \leqslant e^{|t|(mSe^{|t|} + |k| + 1/2)} \|Ng\|_\infty. \tag{2.4}$$

Proof: We may assume that $t>0$. With (1.3) in mind, set for notational simplicity

$$A := -iNT_{k0}N^{-1} = \sigma_3 r^{1/2}\left(\frac{\partial}{\partial r}\right)r^{1/2},$$

$$B := -iNT_{k1}N^{-1} = ik\sigma_1 + (-imr)\sigma_2 =: B_1 + B_2, \tag{2.5}$$

$$C := -iNT_kN^{-1} = \sigma_3 r^{1/2}\left(\frac{\partial}{\partial r}\right)r^{1/2} + (ik\sigma_1 - imr\sigma_2) = A + B.$$

Here and in the following, keep in mind that B_2 and hence B are matrices dependent on the variable r.

Then we have $Nu(r,t)=(e^{tC}Ng)(r)$, and (2.3) becomes

$$e^{tC} = e^{tA} + \int_0^t e^{(t-s)A}Be^{sC}\,\mathrm{d}s, \tag{2.6}$$

these operators being applied to Ng. Then for the first term on the right-hand side of (2.6), it is easy to see that, for a $\mathbf{C}^2$-valued continuous $f={}^t(f_1,f_2)$ on $[0,\infty)$ with support in the bounded closed interval $[0,S]$,

$$(e^{tA}f)(r) = E(t/2)\begin{pmatrix} f_1(re^t) \\ f_2(re^{-t}) \end{pmatrix}, \quad E(t) = \begin{pmatrix} e^t & 0 \\ 0 & e^{-t} \end{pmatrix}, \tag{2.7}$$

so that $e^{tA}f$ has support in $[0,e^tS]$. We shall have with $f=Ng$

$$\|e^{tA}Ng\|_\infty \leqslant e^{t/2}\|Ng\|_\infty,$$

$$\|e^{tC}Ng\|_\infty \leqslant e^{t(mSe^t+|k|+1/2)}\|Ng\|_\infty, \tag{2.8}$$

if g is continuous in $[0,\infty)$ and has support in the bounded closed interval $[0,S]$ for $S>0$.

We have only to prove the latter of (2.8), which amounts to the same thing as (2.4). It will be seen from the integral equation (2.6) for e^{tC}. Iteration of the equation (2.6) yields the Dyson series expansion

$$e^{tC} = e^{tA} + \sum_{n=1}^{\infty}\int_0^t \mathrm{d}t_n \int_0^{t_n}\mathrm{d}t_{n-1}\cdots\int_0^{t_2} e^{(t-t_n)A}Be^{(t_n-t_{n-1})A}B\cdots Be^{t_1A}\,\mathrm{d}t_1. \tag{2.9}$$

We shall see below that this expansion, if applied to a $\mathbf{C}^2$-valued bounded continuous function f with support in the bounded interval $[0,S]$, is convegent in the L^∞ norm.

We want to rewrite the integrand of the above n-ple integral in (2.9).

First we observe that, since the Pauli matrices σ_1, σ_2, and σ_3 anticommute with one another, namely, $\sigma_j\sigma_k+\sigma_k\sigma_j=2\delta_{jk}$ for $j,k=1,2,3$, we have with $E(t)$ in (2.7),

$$e^{tA}B_1 = B_1e^{-tA}, \quad e^{tA}B_2 = B_2E(-t)e^{-tA}. \tag{2.10}$$

It follows that

$$e^{tA}B = e^{tA}(B_1+B_2) = [B_1 + B_2E(-t)]e^{-tA}. \tag{2.11}$$

Here we show (2.10). The first equation is seen because $e^{tA}\sigma_1=\sigma_1e^{-tA}$. The second one is because by (2.7),

$$
\begin{aligned}
(e^{tA}B_2f)(r) &= -im(e^{tA}(r\sigma_2 f))(r)\\
&= -im\sigma_2(e^{-tA}(\rho f))(r)\\
&= -im\int_0^\infty \begin{pmatrix} e^{-t/2}\delta(\rho - re^{-t}) & 0\\ 0 & e^{t/2}\delta(\rho - re^{t})\end{pmatrix}\rho\begin{pmatrix} f_1(\rho)\\ f_2(\rho)\end{pmatrix}\mathrm{d}\rho\\
&= -imr\sigma_2\begin{pmatrix} e^{-3t/2}f_1(re^{-t})\\ e^{3t/2}f_2(re^{t})\end{pmatrix} = \left[B_2\begin{pmatrix} e^{-t} & 0\\ 0 & e^{t}\end{pmatrix}e^{-tA}f\right](r) = [B_2E(-t)e^{-tA}f](r).
\end{aligned}
$$

To treat the integrand of the n-ple integral on the right-hand side of (2.9), we set $\Delta t_j = t_j - t_{j-1}$ with $t_{n+1}=t$ and $t_0=0$. Then we have

$$
\begin{aligned}
e^{\Delta t_{n+1}A}Be^{\Delta t_nA}B\cdots Be^{\Delta t_1A} &= [B_1 + B_2E(-\Delta t_{n+1})]e^{-\Delta t_{n+1}A}e^{\Delta t_nA}B\cdots Be^{\Delta t_1A}\\
&= [B_1 + B_2E(-\Delta t_{n+1})]e^{-(\Delta t_{n+1}-\Delta t_n)A}B\cdots Be^{\Delta t_1A}\\
&= [B_1 + B_2E(-\Delta t_{n+1})][B_1 + B_2E(\Delta t_{n+1}-\Delta t_n)]e^{(\Delta t_{n+1}-\Delta t_n+\Delta t_{n-1})A}B\cdots Be^{\Delta t_1A}\\
&= \prod_{p=2}^{\overleftarrow{n+1}}\left[B_1 + B_2E\left((-1)^p\sum_{q=p}^{n+1}(-1)^{q-1}\Delta t_q\right)\right]e^{\sum_{h=1}^{n+1}(-1)^{h-1}\Delta t_hA}, \qquad (2.12)
\end{aligned}
$$

where $\overleftarrow{\prod}_{p=2}^{n+1}M_p = M_{n+1}M_n\cdots M_2$. Hence the expansion (2.9) becomes

$$
\begin{aligned}
e^{tC} = e^{tA} + \sum_{n=1}^{\infty}\int_0^t \mathrm{d}t_n\int_0^{t_n}\mathrm{d}t_{n-1}\cdots\int_0^{t_2}\mathrm{d}t_1 \times \prod_{p=2}^{\overleftarrow{n+1}}\left[B_1 + B_2E\left((-1)^p\sum_{q=p}^{n+1}(-1)^{q-1}\Delta t_q\right)\right]\\
\times\exp\left[\left(\sum_{h=1}^{n+1}(-1)^{h-1}\Delta t_h\right)A\right] =: \sum_{n=0}^{\infty}C_n(t). \qquad (2.13)
\end{aligned}
$$

For $C_n(t)$ in the expansion (2.13) we have the following lemma.

Lemma 2.3: (i) *The integral kernel* $C_n(t)(r,\rho)$ *of* $C_n(t)$ *has support on the set of* $(r,\rho)\in[0,\infty)\times[0,\infty)$ *with* $\rho = re^{\pm[\sum_{h=1}^{n+1}(-1)^{h-1}\Delta t_h]}$.

(ii) *If* $f(r) = {}^t(f_1(r), f_2(r))$ *is continuous in* $[0,\infty)$ *and has support in* $[0,S]$, *each* $C_n(t)f$ *has support in the bounded interval* $[e^{-|t|}\inf\mathrm{supp}\, f, e^{|t|}\sup\mathrm{supp}\, f]$. *It holds that*

$$
\|C_n(t)f\|_\infty \leqslant \frac{(mSe^{|t|}+|k|)^n}{n!}|t|^n e^{|t|/2}\|f\|_\infty. \qquad (2.14)
$$

Proof of Lemma 2.3: We may assume that $t>0$. Note by (2.7) that the integral kernel of e^{tA} is given by

$$
e^{tA}(r,\rho) = \begin{pmatrix} e^{t/2}\delta(\rho - re^{t}) & 0\\ 0 & e^{-t/2}\delta(\rho - re^{-t})\end{pmatrix} = E(t/2)\begin{pmatrix} \delta(\rho - re^{t}) & 0\\ 0 & \delta(\rho - re^{-t})\end{pmatrix}, \qquad (2.15)
$$

so that the integral kernel of $e^{-itT_{k0}} \equiv N^{-1}e^{tA}N$ becomes

$$
K_0(t;r,\rho) = N^{-1}\begin{pmatrix} e^{t/2}\delta(\rho - re^{t}) & 0\\ 0 & e^{-t/2}\delta(\rho - re^{-t})\end{pmatrix}N = N^{-1}E(t/2)\begin{pmatrix} \delta(\rho - re^{t}) & 0\\ 0 & \delta(\rho - re^{-t})\end{pmatrix}N. \qquad (2.16)
$$

By (2.15) with the expression of $C_n(t)$ in (2.13), we have the assertion (i) and the first half of (ii), because $|\Sigma_{h=1}^{n+1}(-1)^{h-1}\Delta t_h| \leqslant \Sigma_{h=1}^{n+1}(t_h - t_{h-1}) = t$.

Now we show the second half of (ii). We can show for $n\geqslant 1$,

$$\|C_n(t)f\|_\infty \leqslant \int_0^t \mathrm{d}t_n \int_0^{t_n} \mathrm{d}t_{n-1} \cdots \int_0^{t_2} \mathrm{d}t_1 \left\| \overleftarrow{\prod_{p=2}^{n+1}} \left[B_1 + B_2 E\left((-1)^p \sum_{q=p}^{n+1} (-1)^{q-1} \Delta t_q \right) \right] \right.$$
$$\left. \times \exp\left[\left(\sum_{h=1}^{n+1} (-1)^{h-1} \Delta t_h \right) A \right] f \right\|_\infty$$
$$= \int_0^t \mathrm{d}t_n \int_0^{t_n} \mathrm{d}t_{n-1} \cdots \int_0^{t_2} \mathrm{d}t_1 \sup_{r>0} \left\| \overleftarrow{\prod_{p=2}^{n+1}} \left[B_1 + B_2(r) E\left((-1)^p \sum_{q=p}^{n+1} (-1)^{q-1} \Delta t_q \right) \right] \right.$$
$$\left. \times E\left(\frac{1}{2} \sum_{h=1}^{n+1} (-1)^{h-1} \Delta t_h \right) \begin{pmatrix} f_1(re^{\sum_{h=1}^{n+1}(-1)^{h-1}\Delta t_h}) \\ f_2(re^{-\sum_{h=1}^{n+1}(-1)^{h-1}\Delta t_h}) \end{pmatrix} \right\|_{\ell^\infty} \leqslant \frac{(mSe^t + |k|)^n}{n!} t^n e^{t/2} \|f\|_\infty. \tag{2.17}$$

Here the ℓ^∞-norm of a vector $z = {}^t(z_1, z_2) \in \mathbf{C}^2$ is denoted by $\|z\|_{\ell^\infty} = \max\{|z_1|, |z_2|\}$, and we have used

$$\left\| \overleftarrow{\prod_{p=2}^{n+1}} \left[B_1 + B_2 E\left((-1)^p \sum_{q=p}^{n+1} (-1)^{q-1} \Delta t_q \right) \right] \right\| \leqslant (|k| + mre^t)^n, \tag{2.18}$$

and $|\Sigma_{h=1}^{n+1}(-1)^{h-1}\Delta t_h| \leqslant t$ and $\|B_1 + B_2 E((-1)^p \Sigma_{q=p}^{n+1}(-1)^{q-1}\Delta t_q)\| \leqslant |k| + mre^t$. This proves (2.14), ending the proof of Lemma 2.3.

Now we are in a position to finish the proof of Proposition 2.2. By Lemma 2.3, (2.14), we can conclude the expansion (2.9) or (2.13) is convergent in L^∞ norm, which yields the latter half of (2.8) or the estimate (2.4), as well as the support property of the solution $u(\cdot, t)$. This completes the proof of Proposition 2.2.

Proposition 2.4: Let $W(r) = rV(r)$ with $V(r)$ as in Proposition 2.1. Then the operator $H(k, W) = T_k + W(r)$ in (1.4) *(as well as T_k alone) is essentially self-adjoint on $C_0^\infty(\mathbf{R}_+; \mathbf{C}^2)$.*

Proof: We use the method of "invariance of domain" by Chernoff (1973, 1977).

In order to make the notations clearer, inside this proof, we denote the closure of the symmetric operator $H(k, W)$ with domain $C_0^\infty(\mathbf{R}_+; \mathbf{C}^2)$ by $\widetilde{H}(k, W)$. $\widetilde{H}(k, W)$ is also symmetric, and evidently its domain $D[\widetilde{H}(k, W)]$ includes the space $C_0^\infty(\mathbf{R}_+; \mathbf{C}^2)$.

To show that $H(k, W)$ is essentially selfadjoint on $C_0^\infty(\mathbf{R}_+; \mathbf{C}^2)$ or its closure $\widetilde{H}(k, W)$ is self-adjoint, we need to prove that if $\phi \in D[H(k, W)^*]$ satisfies $H(k, W)^* \phi = \pm i\phi$, then $\phi = 0$. Consider the case $H(k, W)^* \phi = -i\phi$. This means that ϕ is in $L^2(\mathbf{R}_+; \mathbf{C}^2)$ and, in view of (1.3), as a distribution

$$0 = H(k, W)^* \phi + i\phi = -i\sigma_2 \left(r\frac{\partial}{\partial r} + \frac{1}{2} \right) \phi + T_{k1}\phi + W(r)\phi + i\phi.$$

Let $\mathcal{D}$ be the subspace of the members of $D[\widetilde{H}(k, W)]$ with compact support in $\mathbf{R}_+$, so that $C_0^\infty(\mathbf{R}_+; \mathbf{C}^2) \subseteq \mathcal{D}$. Take any g in $\mathcal{D}$ and consider the Cauchy problem for $\widetilde{H}(k, W)$,

$$\frac{\partial}{\partial t} u(r, t) = -i\widetilde{H}(k, W) u(r, t), \quad u(r, 0) = g(r). \tag{2.19}$$

Taken into account that $\widetilde{H}(k, W) \subseteq H(k, W)^* = \widetilde{H}(k, W)^*$, this means in view of (1.2b) and (1.3) that the solution $u(r, t)$ in $D[\widetilde{H}(k, W)]$ and so in $L^2(\mathbf{R}_+; \mathbf{C}^2)$ satisfies, as a distribution, the differential equation

$$\frac{\partial}{\partial t}u(r,t) = -i\left[-i\sigma_2\left(r\frac{\partial}{\partial r}+\frac{1}{2}\right)+(-k\sigma_1+mr\sigma_3)+W(r)\right)u(r,t).$$

Then by the analogous arguments used to prove Lemma 2.3, we can see that there exists a unique solution $u(\cdot,t)$ of (2.19), which belongs to the space $\mathcal{D}$. In the same reason as we saw (2.2), we also have $\|u(\cdot,t)\|_2=\|g\|_2$ in L^2-norm.

Set $F(t)=(\phi,u(\cdot,t))$. Then $F(t)$ is bounded in $t\in\mathbf{R}$, because

$$|F(t)|\leqslant\|\phi\|_2\|u(\cdot,t)\|_2=\|\phi\|_2\|g\|_2.$$

Since $H(k,W)^*=\tilde{H}(k,W)^*$, we find by differentiating in t,

$$F'(t)=(\phi,-i\tilde{H}(k,W)u(\cdot,t))=(H(k,W)^*\phi,-iu(\cdot,t))=(\phi,u(\cdot,t))=F(t).$$

It follows that $F(t)=F(0)e^t$. Since $F(t)$ is bounded, we must have $F(0)=0$, that is, $(\phi,g)=0$. Since $\mathcal{D}$ is dense, we can conclude that $\phi=0$. A similar argument can be made for the case $H(k,W)^*\phi=i\phi$. This proves Proposition 2.4.

III. CONSTRUCTION OF THE PATH SPACE MEASURE

We consider only the case $t>0$; the case $t<0$ will be treated similarly. We want to construct our path space measure $\mu_{t,0}$ on the space of the one-dimensional continuous paths $R:[0,t]\to[0,\infty)$ living on the closed half-line $[0,\infty)=\overline{\mathbf{R}_+}$, by modifying the method Nelson (1964) used to construct the Wiener measure. The argument will go analogously with that employed in Ichinose and Tamura (1987, 1988), in particular, in Ichinose (1993) for the Dirac equation in one-dimensional space $\mathbf{R}$.

We write the integral kernel of the unitary group $e^{-itT_k}\equiv N^{-1}e^{tC}N$ with generator (1.3) or (2.5) as $K(t;r,\rho):=e^{-itT_k}(r,\rho)$.

Though in this paper we have meant $\mathbf{R}_+=(0,\infty)$, the open real half-line, we will denote by $\dot{\mathbf{R}}_+=[0,\infty)\cup\{\infty\}$ the one-point compactification of the closed half-line $[0,\infty)$. For each fixed $t>0$ let $\mathcal{R}_{t,0}=\Pi_{[0,t]}\dot{\mathbf{R}}_+=(\dot{\mathbf{R}}_+)^{[0,t]}$ be the uncountably many copies of $\dot{\mathbf{R}}_+$. By the Tychonoff theorem $\mathcal{R}_{t,0}$ is a compact Hausdorff space in the product topology. It may be regarded as the space of all paths $R:[0,t]\to\dot{\mathbf{R}}_+$, possibly discontinuous and possibly passing through zero and/or the infinity ∞. Let $C(\mathcal{R}_{t,0})$ be the Banach space of the complex-valued continuous functions on $\mathcal{R}_{t,0}$ with the maximum norm $\|\cdot\|$, and $C_{\mathrm{fin}}(\mathcal{R}_{t,0})$ the subspace of those Ψ in $C(\mathcal{R}_{t,0})$ for which there exist a finite partition of the interval $[0,t]$,

$$0=s_0<s_1<\cdots<s_\ell=t, \tag{3.1}$$

and a complex-valued bounded continuous function $F(x_0,x_1,\ldots,x_\ell)$ on $(\dot{\mathbf{R}}_+)^{\ell+1}$ such that

$$\Psi(R)=F(R(s_0),R(s_1),\ldots,R(s_\ell)). \tag{3.2}$$

Define, for each fixed $t>0$, a functional $L_{t,0}(\Psi;f,g)$ which is linear in $\Psi\in C_{\mathrm{fin}}(\mathcal{R}_{t,0})$ and sesquilinear in $(f,g)\in C_{00}^\infty([0,\infty);\mathbf{C}^2)\times C_{00}^\infty([0,\infty);\mathbf{C}^2)$, $f={}^t(f_1,f_2)$, $g={}^t(g_1,g_2)$, by

$$\begin{aligned}L_{t,0}(\Psi;f,g)=&\int_0^\infty dr_\ell\int_0^\infty dr_{\ell-1}\cdots\int_0^\infty dr_0\,{}^t\overline{f(r_\ell)}K(s_\ell-s_{\ell-1};r_\ell,r_{\ell-1})\\&\times K(s_{\ell-1}-s_{\ell-2};r_{\ell-1},r_{\ell-2})\cdots K(s_1-s_0;r_1,r_0)F(r_0,r_1,\ldots,r_\ell)g(r_0).\end{aligned} \tag{3.3}$$

The integral on the right-hand side of this equation is equal to

$$\int_0^\infty \mathrm{d}r_\ell \int_0^\infty \mathrm{d}r_{\ell-1} \cdots \int_0^\infty \mathrm{d}r_0 \, {}^t\overline{Nf(r_\ell)}(NK(s_\ell - s_{\ell-1}; r_\ell, r_{\ell-1})N^{-1})$$
$$\times (NK(s_{\ell-1} - s_{\ell-2}; r_{\ell-1}, r_{\ell-2})N^{-1}) \cdots (NK(s_1 - s_0; r_1, r_0)N^{-1})$$
$$\times F(r_0, r_1, \ldots, r_\ell) N g(r_0).$$

Therefore (3.3) can also be written by definition of e^{tC} as

$$L_{t,0}(\Psi; f, g) = \int_0^\infty \int_0^\infty {}^t\overline{Nf(r_\ell)} e^{\Delta s_\ell C} e^{\Delta s_{\ell-1} C} \cdots e^{\Delta s_1 C} F(r_0, \ldots, r_{\ell-1}, r_\ell) N g(r_0) \mathrm{d}r_\ell \, \mathrm{d}r_0, \tag{3.4}$$
$$\Delta s_j = s_j - s_{j-1}, \quad 1 \leqslant j \leqslant \ell,$$

where $e^{\Delta s_j C}$ is a linear operator with kernel $NK(s_j - s_{j-1}; r_j, r_{j-1})N^{-1}$ transforming functions of r_{j-1} to functions of r_j. Substituting e^{tC} in (2.13) with t replaced by Δs_j into (3.4), we get

$$L_{t,0}(\Psi; f, g) = \sum_{n=0}^\infty \sum_{n_1 + \cdots + n_\ell = n} \int_0^\infty \int_0^\infty {}^t\overline{Nf(r_\ell)} C_{n_\ell}(\Delta s_\ell) \cdots C_{n_2}(\Delta s_2) C_{n_1}(\Delta s_1)$$
$$\times [F(r_0, r_1, \ldots, r_\ell) N g(r_0)] \mathrm{d}r_\ell \, \mathrm{d}r_0 =: \sum_{n=0}^\infty L_{t,0}^n(\Psi; f, g). \tag{3.5}$$

To construct the measure $\mu_{t,0}$ on $\mathcal{R}_{t,0}$, the following lemma is of crucial importance.

Lemma 3.1: (i) *For each* $t > 0$, $L_{t,0}(\Psi; f, g)$ *and* $L_{t,0}^n(\Psi; f, g)$ *are independent of the choice of* F *corresponding to* $\Psi \in C_{\mathrm{fin}}(\mathcal{R}_{t,0})$.

(ii) *If one of* f *and* g *in* $C_{00}^\infty([0, \infty); \mathbf{C}^2)$ *has support in the bounded interval* $[0, S]$, *then the following inequalities hold*:

$$|L_{t,0}(\Psi; f, g)| \leqslant \|N\|_1 \|N\|_\infty e^{t(mSe^t + |k| + 1/2)} \|\Psi\| \|f\|_1 \|g\|_\infty, \tag{3.6}$$

$$|L_{t,0}^n(\Psi; f, g)| \leqslant \|N\|_1 \|N\|_\infty \frac{(mSe^t + |k|)^n}{n!} t^n e^{t/2} \|\Psi\| \|f\|_1 \|g\|_\infty, \tag{3.7}$$

for all $n = 0, 1, 2 \ldots$. *Here* $\|N\|_1$ *and* $\|N\|_\infty$ *are the norms of the unitary matrix* N, *respectively, as a linear operator on* $\mathbf{C}^2$ *with* ℓ^1*-norm and* ℓ^∞*-norm, which are less than or equal to* $\sqrt{2}$.

Proof: The first assertion (i) is due to the semigroup property of e^{-itT_k} or e^{tC}. The proof of the second one (ii) will make use of the inequality for $C_{n_j}(\Delta s_j)$ to be obtained from (2.14) with n_j, Δs_j in place of n, t to get

$$|L_{t,0}^n(\Psi; f, g)| \leqslant \sum_{n_1 + \cdots + n_\ell = n} \prod_{p=1}^\ell \left[\frac{(mSe^{\Delta s_p} + |k|)^{n_p}}{n_p!} (\Delta s_p)^{n_p} e^{\Delta s_p / 2} \right] \|F\|_\infty \|Nf\|_1 \|Ng\|_\infty$$
$$\leqslant (mSe^t + |k|)^n \frac{\left(\sum_{p=1}^\ell \Delta s_p \right)^n}{n!} e^{(1/2) \Sigma_{q=1}^\ell \Delta s_q} \|F\|_\infty \|Nf\|_1 \|Ng\|_\infty$$
$$= \frac{(mSe^t + |k|)^n}{n!} t^n e^{t/2} \|\Psi\| \|Nf\|_1 \|Ng\|_\infty.$$

Here we have used that for $1 \leqslant j \leqslant \ell$, $\Delta s_j \leqslant \Sigma_{p=1}^\ell \Delta s_p = t$, and that

$$\sum_{n_1+\cdots+n_\ell=n} \frac{(\Delta s_1)^{n_1}(\Delta s_2)^{n_2}\cdots(\Delta s_\ell)^{n_\ell}}{n_1!n_2!\cdots n_\ell!} = \frac{\left(\sum_{p=1}^{\ell}\Delta s_p\right)^n}{n!} = \frac{t^n}{n!}.$$

Since $\|Nf\|_1 \leqq \|N\|_1\|f\|_1$ and $\|Ng\|_\infty \leqq \|N\|_\infty\|g\|_\infty$, this yields (3.7). Hence by summing up, we also obtain (3.6) from (3.5). This proves Lemma 3.1.

A consequence of this lemma is the following. Since $C_{\mathrm{fin}}(\mathcal{R}_{t,0})$ is dense in $C(\mathcal{R}_{t,0})$ by the Stone–Weierstrass theorem, the inequalities (3.6) and (3.7) are also valid for all $\Psi \in C(\mathcal{R}_{t,0})$. This means that for each fixed pair (f,g), $L_{t,0}(\cdot;f,g)$ and $L^n_{t,0}(\cdot;f,g)$ are complex-valued continuous linear functional on $C(\mathcal{R}_{t,0})$. By the Riesz representation theorem, there exist complex-valued regular Borel measures $\mu_{t,0;f,g}$ and $\mu^n_{t,0;f,g}$ on $\mathcal{R}_{t,0}$ for all $n=0,1,2,\ldots$, such that for all $\Psi \in C(\mathcal{R}_{t,0})$,

$$L_{t,0}(\Psi;f,g) = \int_{\mathcal{R}_{t,0}} \mathrm{d}\mu_{t,0;f,g}(R)\Psi(R), \tag{3.8}$$

$$L^n_{t,0}(\Psi;f,g) = \int_{\mathcal{R}_{t,0}} \mathrm{d}\mu^n_{t,0;f,g}(R)\Psi(R). \tag{3.9}$$

Hence, since the left-hand sides of (3.8) and (3.9) are continuous sesquilinear forms in (f,g) in the product space $C^\infty_{00}([0,\infty);\mathbf{C}^2)\times C^\infty_{00}([0,\infty);\mathbf{C}^2)$, we can also see, with $M_2(\mathbf{C})$ being the set of all 2×2-matrices, that there exist 2×2-matrix distribution-valued, precisely, $C^\infty_{00}([0,\infty)^2;M_2(\mathbf{C}))'$-valued, regular Borel measures $\mu_{t,0}(\cdot)$ and $\mu^n_{t,0}(\cdot)$ on $\mathcal{R}_{t,0}$ such that for every pair $(f,g)\in C^\infty_{00}([0,\infty);\mathbf{C}^2)\times C^\infty_{00}([0,\infty);\mathbf{C}^2)$,

$$\langle \overline{{}^t f}, \mu_{t,0}(\cdot)g\rangle = \mu_{t,0;f,g}(\cdot), \tag{3.10}$$

$$\langle \overline{{}^t f}, \mu^n_{t,0}(\cdot)g\rangle = \mu^n_{t,0;f,g}(\cdot). \tag{3.11}$$

Here we note that we have

$$C^\infty_{00}([0,\infty)^2;M_2(\mathbf{C})) = C^\infty_{00}([0,\infty);\mathbf{C}^2)\hat{\otimes} C^\infty_{00}([0,\infty);\mathbf{C}^2),$$

and the space of the continuous sesquilinear forms on the product space $C^\infty_{00}([0,\infty);\mathbf{C}^2)\times C^\infty_{00}([0,\infty);\mathbf{C}^2)$ coincides with the dual space

$$C^\infty_{00}([0,\infty)^2;M_2(\mathbf{C}))' = C^\infty_{00}([0,\infty);\mathbf{C}^2)'\hat{\otimes} C^\infty_{00}([0,\infty);\mathbf{C}^2)'.$$

Here the tensor products on the right-hand side are completed in the π- or ε-tensor product topology, because $C^\infty_{00}([0,\infty);\mathbf{C}^2)$ and $C^\infty_{00}([0,\infty);\mathbf{C}^2)'$ are nuclear spaces, since they are subspaces of the nuclear spaces $C^\infty_0(\mathbf{R};\mathbf{C}^2)$ and $\mathcal{D}'(\mathbf{R};\mathbf{C}^2)$, respectively [e.g., Pietsch (1970, Chaps. 5, 6), Trèves (1967, Chap. 50)].

It follows from the expansion (3.5) that

$$\mu_{t,0;f,g}(\cdot) = \sum_{n=0}^{\infty} \mu^n_{t,0;f,g}(\cdot) \tag{3.12}$$

in the sense of the expansion of the measure or

$$\mu_{t,0}(\cdot) = \sum_{n=0}^{\infty} \mu^n_{t,0}(\cdot) \tag{3.13}$$

in the sense of the expansion of the 2×2-matrix distribution-valued measure.

Finally we shall observe on which set of the paths the measures $\mu_{t,0}$ and $\mu^n_{t,0}$ are concentrated.

Lemma 3.2: For each $n=0,1,2,\ldots$, *the measure* $\mu^n_{t,0}$ *is concentrated on the set of the continuous, exactly n-vertex piecewise smooth paths* $R:[0,t]\to[0,\infty)$, *in fact, with each of their segments being a particular smooth curve such that for an n-partition:* $0=t_0<t_1<\cdots<t_{n+1}=t$ *of the interval* $[0,t]$ *and for* $t_{h-1}\leqslant s\leqslant t_h$, $1\leqslant h\leqslant n+1$,

$$R(s)=R(0)e^{\pm[\Sigma_{p=1}^{h-1}(-1)^{p-1}(t_p-t_{p-1})+(-1)^{h-1}(s-t_{h-1})]}.$$

Therefore in each n-partitioned short interval (t_{p-1},t_p) *each segement is exponentially growing or decreasing.*

Consequently, the measure $\mu_{t,0}$ *is concentrated on the union of these sets of paths on which the* $\mu^n_{t,0}$ *are concentrated.*

Proof: This basically follows from the very expression (2.15) and (2.16) that the integral kernel of e^{tA} or $e^{-itT_{k0}}$ has. Inspecting through the expression of $C_{n_j}(\Delta s_j)$ in (2.13) with n_j, Δs_j in place of n, t what is the support of the integral kernel of $C_{n_j}(\Delta s_j)$, we shall be able to see through $L^n_{t,0}(\Psi;f,g)$ and $L_{t,0}(\Psi;f,g)$ in (3.5) the statement of this lemma.

We will sketch how it goes. We must investigate what the product operator

$$C_{n_\ell}(\Delta s_\ell)\cdots C_{n_2}(\Delta s_2)C_{n_1}(\Delta s_1)$$

in the integrand in the second member of (3.5) is. This operator corresponds to the partition (3.1) of the interval $[0,t]$. Each factor $C_{n_j}(\Delta s_j)$, $1\leqslant j\leqslant\ell$, is, as seen from the nth term the expansion (2.9)/(2.13), an n_j-ple integral with n_j, Δs_j in place of n, t, and with n_j integration variables $t_{j,q}$ (in place of t_q), moving in the n_j-plex,

$$s_{j-1}\equiv t_{j,0}\leqslant t_{j,1}\leqslant\cdots\leqslant t_{j,n_j}\leqslant t_{j,n_j+1}\equiv s_j. \tag{3.14}$$

Then we have from (2.13), with $\Delta t_{j,q}:=t_{j,q}-t_{j,q-1}$, $1\leqslant q\leqslant n_j+1$,

$$\begin{aligned}
&C_{n_\ell}(\Delta s_\ell)\cdots C_{n_2}(\Delta s_2)C_{n_1}(\Delta s_1)\\
&=\int_{s_{\ell-1}}^{s_\ell}\int_{s_{\ell-1}}^{t_{\ell,n_\ell}}\cdots\int_{s_{\ell-1}}^{t_{\ell,2}}\mathrm{d}t_{\ell,n_\ell}\,\mathrm{d}t_{\ell,n_\ell-1}\cdots\mathrm{d}t_{\ell,1}\int_{s_{\ell-2}}^{s_{\ell-1}}\int_{s_{\ell-2}}^{t_{\ell-1,n_{\ell-1}-1}}\cdots\\
&\quad\times\int_{s_{\ell-2}}^{t_{\ell-1,2}}\mathrm{d}t_{\ell-1,n_{\ell-1}}\,\mathrm{d}t_{\ell-1,n_{\ell-1}-1}\cdots\mathrm{d}t_{\ell-1,1}\cdots\times\int_{s_1}^{s_2}\int_{s_1}^{t_{2,n_2}}\cdots\\
&\quad\times\int_{s_1}^{t_{2,2}}\mathrm{d}t_{2,n_2}\,\mathrm{d}t_{2,n_2-1}\cdots\mathrm{d}t_{2,1}\int_{s_0}^{s_1}\int_{s_0}^{t_{1,n_1}}\cdots\int_{s_0}^{t_{2,2}}\mathrm{d}t_{1,n_1}\,\mathrm{d}t_{1,n_1-1}\cdots\mathrm{d}t_{1,1}\\
&\quad\times\overleftarrow{\prod_{p_\ell=2}^{n_\ell+1}}\left[B_1+B_2E\left((-1)^{p_\ell}\sum_{q=p_\ell}^{n_\ell+1}(-1)^{q-1}\Delta t_{\ell,q}\right)\right]\exp\left[\left(\sum_{h=1}^{n_\ell+1}(-1)^{h-1}\Delta t_{\ell,h}\right)A\right]\\
&\quad\times\overleftarrow{\prod_{p_{\ell-1}=2}^{n_{\ell-1}+1}}\left[B_1+B_2E\left((-1)^{p_{\ell-1}}\sum_{q=p_{\ell-1}}^{n_{\ell-1}+1}(-1)^{q-1}\Delta t_{\ell-1,q}\right)\right]\exp\left[\left(\sum_{h=1}^{n_{\ell-1}+1}(-1)^{h-1}\Delta t_{\ell-1,h}\right)A\right]\times\cdots\\
&\quad\times\overleftarrow{\prod_{p_2=2}^{n_2+1}}\left[B_1+B_2E\left((-1)^{p_2}\sum_{q=p_2}^{n_2+1}(-1)^{q-1}\Delta t_{2,q}\right)\right]\exp\left[\left(\sum_{h=1}^{n_2+1}(-1)^{h-1}\Delta t_{2,h}\right)A\right]\\
&\quad\times\overleftarrow{\prod_{p_1=2}^{n_1+1}}\left[B_1+B_2E\left((-1)^{p_1}\sum_{q=p_1}^{n_1+1}(-1)^{q-1}\Delta t_{1,q}\right)\right]\exp\left[\left(\sum_{h=1}^{n_1+1}(-1)^{h-1}\Delta t_{1,h}\right)A\right].
\end{aligned}\tag{3.15}$$

Here note that this integral (3.15) is a just n-ple integral with $n=n_1+\cdots+n_\ell$, and there are no integrations in the variables

$$s_{\ell-1}\equiv t_{\ell,0}\equiv t_{\ell-1,n_{\ell-1}+1},\quad s_{\ell-2}\equiv t_{\ell-1,0}\equiv t_{\ell-2,n_{\ell-2}+1},\ \ldots,s_1\equiv t_{1,0}\equiv t_{0,n_1+1}.$$

Applying the formula (2.11) to the first product of the integrand on the right-hand side of this equation (3.15), we see the integrand on the right-hand side of (3.15) is equal to

$$\begin{aligned}
&\overset{n_\ell+1}{\underset{p_\ell=2}{\overleftarrow{\prod}}}\left[B_1+B_2E\left((-1)^{p_\ell}\sum_{q=p_\ell}^{n_\ell+1}(-1)^{q-1}\Delta t_{\ell,q}\right)\right]\overset{n_{\ell-1}+1}{\underset{p_{\ell-1}=2}{\overleftarrow{\prod}}}\left[B_1+B_2E\right.\\
&\quad\left.\times\left((-1)^{n_{\ell-1}+2-p_{\ell-1}}\sum_{h=1}^{n_\ell+1}(-1)^{h-1}\Delta t_{\ell,h}+(-1)^{p_{\ell-1}}\sum_{q=p_{\ell-1}}^{n_{\ell-1}+1}(-1)^{q-1}\Delta t_{\ell-1,q}\right)\right]\\
&\quad\times\exp\left[\left((-1)^{n_{\ell-1}}\sum_{h=1}^{n_\ell+1}(-1)^{h-1}\Delta t_{\ell,h}+\sum_{h=1}^{n_{\ell-1}+1}(-1)^{h-1}\Delta t_{\ell-1,h}\right)A\right]\times\cdots\\
&\quad\times\overset{n_2+1}{\underset{p_2=2}{\overleftarrow{\prod}}}\left[B_1+B_2E\left((-1)^{p_2}\sum_{q=p_2}^{n_2+1}(-1)^{q-1}\Delta t_{2,q}\right)\right]\exp\left[\left(\sum_{h=1}^{n_2+1}(-1)^{h-1}\Delta t_{2,h}\right)A\right]\\
&\quad\times\overset{n_1+1}{\underset{p_1=2}{\overleftarrow{\prod}}}\left[B_1+B_2E\left((-1)^{p_1}\sum_{q=p_1}^{n_1+1}(-1)^{q-1}\Delta t_{1,q}\right)\right]\exp\left[\left(\sum_{h=1}^{n_1+1}(-1)^{h-1}\Delta t_{1,h}\right)A\right].
\end{aligned}$$

Then by repeated use of (2.11) we reach

$$\begin{aligned}
&C_{n_\ell}(\Delta s_\ell)\cdots C_{n_2}(\Delta s_2)C_{n_1}(\Delta s_1)\\
&\quad=\int_{s_{\ell-1}}^{s_\ell}\int_{s_{\ell-1}}^{t_{\ell,n_\ell}}\cdots\int_{s_{\ell-1}}^{t_{\ell,2}}\int_{s_{\ell-2}}^{s_{\ell-1}}\int_{s_{\ell-2}}^{t_{\ell-1,n_{\ell-1}-1}}\cdots\int_{s_{\ell-2}}^{t_{\ell-1,2}}\times\cdots\times\int_{s_1}^{s_2}\int_{s_1}^{t_{2,n_2}}\cdots\int_{s_1}^{t_{2,2}}\int_{s_0}^{s_1}\int_{s_0}^{t_{1,n_1}}\cdots\\
&\qquad\times\int_{s_0}^{t_{1,2}}\mathrm{d}t_{\ell,n_\ell}\,\mathrm{d}t_{\ell,n_\ell-1}\cdots\mathrm{d}t_{\ell,1}\,\mathrm{d}t_{\ell-1,n_{\ell-1}}\,\mathrm{d}t_{\ell-1,n_{\ell-1}-1}\cdots\mathrm{d}t_{\ell-1,1}\times\cdots\times\mathrm{d}t_{2,n_2}\,\mathrm{d}t_{2,n_2-1}\cdots\\
&\qquad\times\mathrm{d}t_{2,1}\,\mathrm{d}t_{1,n_1}\,\mathrm{d}t_{1,n_1-1}\cdots\mathrm{d}t_{1,1}B(t;n_1,n_2,\ldots,n_\ell)\\
&\qquad\times\exp\left[\left((-1)^{n_1+n_2+\cdots+n_{\ell-1}}\sum_{h=1}^{n_\ell+1}(-1)^{h-1}\Delta t_{\ell,h}+(-1)^{n_1+n_2+\cdots+n_{\ell-2}}\right.\right.\\
&\qquad\times\sum_{h=1}^{n_{\ell-1}+1}(-1)^{h-1}\Delta t_{\ell-1,h}+\cdots+(-1)^{n_1+n_2}\sum_{h=1}^{n_3+1}(-1)^{h-1}\Delta t_{3,h}+(-1)^{n_1}\\
&\qquad\left.\left.\times\sum_{h=1}^{n_2+1}(-1)^{h-1}\Delta t_{2,h}+\sum_{h=1}^{n_1+1}(-1)^{h-1}\Delta t_{1,h}\right)A\right],
\end{aligned}\tag{3.16}$$

where

$$
\begin{aligned}
&B(t;n_1,n_2,\ldots,n_\ell)\\
&=\overleftarrow{\prod_{p_\ell=2}^{n_\ell+1}}\left[B_1+B_2E\left((-1)^{p_\ell}\sum_{q=p_\ell}^{n_\ell+1}(-1)^{q-1}\Delta t_{\ell,q}\right)\right]\\
&\times\overleftarrow{\prod_{p_{\ell-1}=2}^{n_{\ell-1}+1}}\left[B_1+B_2E\left((-1)^{n_{\ell-1}+2-p_{\ell-1}}\sum_{h=1}^{n_\ell+1}(-1)^{h-1}\Delta t_{\ell,h}+(-1)^{p_{\ell-1}}\sum_{q=p_{\ell-1}}^{n_{\ell-1}+1}(-1)^{q-1}\Delta t_{\ell-1,q}\right)\right]\\
&\times\overleftarrow{\prod_{p_{\ell-2}=2}^{n_{\ell-2}+1}}\left[B_1+B_2E\left((-1)^{n_{\ell-2}+2-p_{\ell-2}+n_{\ell-1}}\sum_{h=1}^{n_\ell+1}(-1)^{h-1}\Delta t_{\ell,h}+(-1)^{n_{\ell-2}+2-p_{\ell-2}}\right.\right.\\
&\left.\left.\times\sum_{h=1}^{n_{\ell-1}+1}(-1)^{h-1}\Delta t_{\ell-1,h}+(-1)^{p_{\ell-2}}\sum_{q=p_{\ell-2}}^{n_{\ell-1}+1}(-1)^{q-1}\Delta t_{\ell-2,q}\right)\right]\times\cdots\\
&\times\overleftarrow{\prod_{p_1=2}^{n_1+1}}\left[B_1+B_2E\left((-1)^{n_1+2-p_1+n_2+\cdots+n_{\ell-1}}\sum_{h=1}^{n_\ell+1}(-1)^{h-1}\Delta t_{\ell,h}+(-1)^{n_1+2-p_1+n_2+\cdots+n_{\ell-2}}\right.\right.\\
&\times\sum_{h=1}^{n_{\ell-1}+1}(-1)^{h-1}\Delta t_{\ell-1,h}+\cdots+(-1)^{n_1+2-p_1+n_2}\sum_{h=1}^{n_3+1}(-1)^{h-1}\Delta t_{3,h}+(-1)^{n_1+2-p_1}\\
&\left.\left.\times\sum_{h=1}^{n_2+1}(-1)^{h-1}\Delta t_{2,h}+(-1)^{p_1}\sum_{q=p_1}^{n_1+1}(-1)^{q-1}\Delta t_{1,q}\right)\right].
\end{aligned}
\tag{3.17}
$$

In the exponential power of the second factor on the right-hand side of (3.16) above, observe the neighboring summations to find the first term in each summation and the last term in its next summation have the same sign, so that for each j with $1\leqslant j\leqslant \ell$,

$$
\begin{aligned}
&(-1)^{n_1+\cdots+n_{j-1}}\Delta t_{j,1}+(-1)^{n_1+\cdots+n_{j-2}}(-1)^{n_{j-1}}\Delta t_{j-1,n_{j-1}+1}\\
&\quad=(-1)^{n_1+\cdots+n_{j-1}}(\Delta t_{j,1}+\Delta t_{j-1,n_{j-1}+1})\\
&\quad=(-1)^{n_1+\cdots+n_{j-1}}((t_{j,1}-t_{j,0})+(t_{j-1,n_{j-1}+1}-t_{j-1,n_{j-1}}))\\
&\quad=(-1)^{n_1+\cdots+n_{j-1}}(t_{j,1}-t_{j-1,n_{j-1}}),
\end{aligned}
$$

because $t_{j,0}=t_{j-1,n_{j-1}+1}=s_j$. The same is true for the neighboring summations in the variables of the matrix $E(\cdot)$ on the right-hand side of (3.17). We see by the partition (3.1) with (3.14) the $n=n_1+\cdots+n_\ell$ integration variables move in the set of ℓ n_j-pleces:

$$
\begin{aligned}
\Delta(s_1,s_2,\ldots,s_\ell):\quad &0\equiv s_0\equiv t_{1,0}\leqslant t_{1,1}\leqslant t_{1,2}\leqslant\cdots\leqslant t_{1,n_1}\leqslant t_{1,n_1+1}\equiv s_1\equiv t_{2,0}\leqslant t_{2,1}\leqslant t_{2,2}\\
&\leqslant\cdots\leqslant t_{2,n_2}\leqslant t_{2,n_2+1}\equiv s_2\equiv t_{3,0}\leqslant t_{3,1}\leqslant\cdots\leqslant t_{\ell-1,n_{\ell-1}}<t_{\ell-1,n_{\ell-1}+1}\equiv s_{\ell-1}\\
&\equiv t_{\ell,0}\leqslant t_{\ell,1}\leqslant t_{\ell,2}\leqslant\cdots\leqslant t_{\ell,n_\ell}\leqslant t_{\ell,n_\ell+1}\equiv s_\ell\equiv t.
\end{aligned}
\tag{3.18}
$$

So, we change the n integration variables $\{t_{j,q}; 1 \leqslant q \leqslant n_j, 1 \leqslant j \leqslant \ell\}$ to $\{t_1, t_2, \ldots, t_n\}$, namely, set $0 \leqslant h \leqslant n_1 + n_2 + \cdots + n_\ell + 1 = n + 1$,

$$t_h = \begin{cases} t_{1,0} = s_0 = 0, \quad h = 0, \\ t_{1,h}, \quad 1 \leqslant h \leqslant n_1, \\ t_{2,h-n_1}, \quad n_1 + 1 \leqslant h \leqslant n_1 + n_2, \\ t_{3,h-(n_1+n_2)}, \quad n_1 + n_2 + 1 \leqslant h \leqslant n_1 + n_2 + n_3, \\ \ldots, \\ t_{j,h-(n_1+n_2+\cdots+n_{j-1})}, \quad n_1 + n_2 + \cdots + n_{j-1} + 1 \leqslant h \leqslant n_1 + n_2 + \cdots + n_j, \\ \ldots, \\ t_{\ell-1,h-(n_1+n_2+\cdots+n_{\ell-2})}, \quad n_1 + n_2 + \cdots + n_{\ell-2} + 1 \leqslant h \leqslant n_1 + n_2 + \cdots + n_{\ell-1}, \\ t_{\ell,h-(n_1+n_2+\cdots+n_{\ell-1})}, \quad n_1 + n_2 + \cdots + n_{\ell-1} + 1 \leqslant h \leqslant n_1 + n_2 + \cdots + n_\ell, \\ t_{\ell,n_\ell+1} = s_\ell = t, \quad h = n_1 + n_2 + \cdots + n_\ell + 1 = n + 1. \end{cases} \tag{3.19}$$

Then we see from (3.18) the new integration variables $t_1, t_2, \ldots, t_n$ move in the set

$$\begin{aligned} \Delta(s_1, s_2, \ldots, s_\ell): \quad & 0 \equiv s_0 \equiv t_0 \leqslant t_1 \leqslant t_2 \leqslant \cdots \leqslant t_{n_1} \leqslant s_1 \leqslant t_{n_1+1} \leqslant \cdots \leqslant t_{n_1+n_2} \leqslant s_2 \leqslant t_{n_1+n_2+1} \\ & \leqslant \cdots \leqslant t_{n_1+\cdots+n_{\ell-1}} \leqslant s_{\ell-1} \leqslant t_{n_1+\cdots+n_{\ell-1}+1} \leqslant \cdots \leqslant t_n \leqslant s_\ell \equiv t. \end{aligned} \tag{3.20}$$

Thus

$$\begin{aligned} C_{n_\ell}(\Delta s_\ell) \cdots C_{n_2}(\Delta s_2) C_{n_1}(\Delta s_1) = \int \cdots \int_{\Delta(s_1, s_2, \ldots, s_\ell)} & \mathrm{d}t_n \, \mathrm{d}t_{n-1} \cdots \mathrm{d}t_2 \, \mathrm{d}t_1 \\ & \times B(t; n_1, n_2, \ldots, n_\ell) \exp\left[\left(\sum_{h=1}^{n+1} (-1)^{h-1} (t_h - t_{h-1}) \right) A \right], \end{aligned} \tag{3.21}$$

where (3.17) turns out to be, with $\Delta t_h := t_h - t_{h-1}$,

$$\begin{aligned} B(t; n_1, n_2, \ldots, n_\ell) = & \overleftarrow{\prod_{p_\ell=2}^{n_\ell+1}} \left[B_1 + B_2 E\left((-1)^{n_1+\cdots+n_{\ell-1}+p_\ell} \sum_{h=n_1+\cdots+n_{\ell-1}+p_\ell}^{n+1} (-1)^{h-1} \Delta t_h \right) \right] \\ & \times \overleftarrow{\prod_{p_{\ell-1}=2}^{n_{\ell-1}+1}} \left[B_1 + B_2 E\left((-1)^{n_1+\cdots+n_{\ell-2}+p_{\ell-1}} \sum_{h=n_1+\cdots+n_{\ell-2}+p_{\ell-1}}^{n+1} (-1)^{h-1} \Delta t_h \right) \right] \\ & \times \overleftarrow{\prod_{p_{\ell-2}=2}^{n_{\ell-2}+1}} \left[B_1 + B_2 E\left((-1)^{n_1+\cdots+n_{\ell-3}+p_{\ell-2}} \sum_{h=n_1+\cdots+n_{\ell-3}+p_{\ell-2}}^{n+1} (-1)^{h-1} \Delta t_h \right) \right] \times \cdots \\ & \times \overleftarrow{\prod_{p_1=2}^{n_1+1}} \left[B_1 + B_2 E\left((-1)^{p_1} \sum_{h=p_1}^{n+1} (-1)^{h-1} \Delta t_h \right) \right]. \end{aligned} \tag{3.22}$$

We can see by this expression (3.21) with (3.22) through (3.5) that the measure $\mu_{t,0}^n$ is concentrated on those paths mentioned in the statement of Lemma 3.2. This ends the proof of this lemma.

IV. PATH INTEGRAL REPRESENTATION

We first establish the path integral representation to the solution $u(r,t)$ of the Cauchy problem (1.5) for the operator $H(k,rV)$ in (1.4), and next give the proof of Theorems 1.1 and 1.2.

We begin with showing the following path integral representation of Feynman–Kac type for the semigroup $e^{-itH(k,rV)}$.

Theorem 4.1: *For $e^{-itH(k,rV)}$ it holds that*

$$(f,e^{-itH(k,rV)}g)=\int_{C([0,t]\to[0,\infty))}\langle {}^t\overline{f(R(t))},\mathrm{d}\mu_{t,0}(R)g(R(0))\rangle\exp\left[-i\int_0^t V(R(s))R(s)\mathrm{d}s\right]. \quad (4.1)$$

Proof: For $s>0$, define a linear operator $\mathrm{U}(s)$ by

$$(U(s)g)(r)=(e^{-isT_k}e^{-isW}g)(r)=\int_0^\infty K(s;r,\rho)e^{-isV(\rho)\rho}g(\rho)\mathrm{d}\rho \quad (4.2)$$

with $W(r)=V(r)r$ for $g\in C_{00}^\infty([0,\infty);\mathbf{C}^2)$; recall $K(s;r,\rho)$ is the integral kernel of the semigroup $e^{-isT_k}\equiv N^{-1}e^{sC}N$ for T_k in (1.3). $U(s)$ is a contraction operator on $L^2(\mathbf{R}_+;\mathbf{C}^2)$ because e^{-isT_k} is a unitary operator, and also bounded in L^∞ operator norm because of (2.4)/(2.8).

Let n be an arbitrary positive integer and set $t_{h-1}=(h-1)t/n$, $h=1,2,\ldots,n+1$. Then we find, with $r_n=r$

$$[U(t/n)^n g](r)=\overbrace{\int_0^\infty\cdots\int_0^\infty}^{n\text{ times}}\prod_{h=1}^{\infty\leftarrow n}K(t/n;r_h-r_{h-1})e^{-i\sum_{h=1}^n V(r_{h-1})r_{h-1}(t/n)}g(r_0)\mathrm{d}r_0\cdots\mathrm{d}r_{n-1}. \quad (4.3)$$

Then the left-hand side converges, by the Trotter product formula [e.g., Reed and Simon (1980)], to $e^{-itH(k,rV)}g$ in $L^2(\mathbf{R}_+;\mathbf{C}^2)$, since we have seen in Proposition 2.4 that $H(k,rV)=T_k+rV$ is essentially self-adjoint. For the right-hand side, we find by (3.3) and (3.8) that taking the sesquilinear inner product of (4.3) with $f\in C_{00}^\infty([0,\infty);\mathbf{C}^2)$ yields

$$(f,U(t/n)^n g)=\int_{C([0,t]\to[0,\infty))}\langle {}^t\overline{f(R(t))},\mathrm{d}\mu_{t,0}(R)g(R(0))\rangle\exp\left[-i\sum_{h=1}^n V(R(t_{h-1}))R(t_{h-1})(t/n)\right], \quad (4.4)$$

the right-hand side of which converges by the Lebesgue bounded convergence theorem, as $n\to\infty$, to

$$\int_{C([0,t]\to[0,\infty))}\langle {}^t\overline{f(R(t))},\mathrm{d}\mu_{t,0}(R)g(R(0))\rangle\exp\left[-i\int_0^t V(R(s))R(s)\mathrm{d}s\right].$$

Thus we have shown Theorem 4.1.

Now, we prove Theorems 1.1 and 1.2.

Proof of Theorem 1.1: In Theorem 4.1, considering, instead of $e^{-itH(h,rV)}$, $e^{-it(H(k,rV)-\lambda r)}$, where $\lambda=\pm i\varepsilon$ with ε being a nonzero real number, so that λ is not in the spectrum of the operator τ_k+V, we can get by Theorem 4.1 the expression (4.1) corresponding to this case. Then taking into account the relation between the radial Dirac operator $\tau_k+V(r)$ concerned and $H(k,rV)$ in (1.4), we have only to take the Laplace transform of both sides to get (1.6) in Theorem 1.1.

Proof of Theorem 1.2: The case (i), (1.8), is an immediate consequence of Theorem 1.1. As for the case (ii), multiply both sides of Eq. (4.1) by $e^{\mp\varepsilon t}$ with the same ε as above. Then we find the expression for $e^{-itH(k,rV)\mp\varepsilon t}$. Note that $H(k,rV)$ has also a real spectrum, since by Proposition 2.4, it is a self-adjoint operator. Then taking the Laplace transform and letting $\varepsilon\to 0$, we have the formula (1.9).

This completes the proof of the main theorems in Sec. I.

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Study of anharmonic singular potentials

Nasser Saad
Department of Mathematics and Statistics, University of Prince Edward Island, 550 University Avenue, Charlottetown, PEI, Canada C1A 4P3

Richard L. Hall
Department of Mathematics and Statistics, Concordia University, 1455 de Maisonneuve Boulevard West, Montréal, Québec, Canada H3G 1M8

Qutaibeh D. Katatbeh
Department of Mathematics and Statistics, Faculty of Science and Arts, Jordan University of Science and Technology, Irbid 22110, Jordan

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A simple and efficient variational method is introduced to accelerate the convergence of the eigenenergy computations for a Hamiltonian H with singular potentials. Closed-form analytic expressions in N dimensions are obtained for the matrix elements of H with respect to the eigenfunctions of a soluble singular problem with two free parameters A and B. The matrix eigenvalues are then optimized with respect to A and B for a given N. Applications, convergence rates, and comparisons with earlier work are discussed in detail. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1836014]

I. INTRODUCTION

Sources of ongoing interest[1–66] in the study of singular potentials are at least threefold, (i) regular Rayleigh–Schrödinger perturbation theory can fail badly for such potentials, (ii) in physics, it is quite common to encounter phenomenological potentials that are strongly singular at the origin, and (iii) because of the intrinsically interesting mathematical problems that arise in their study. A specific family of singular quantum Hamiltonians that has found widespread application in many areas of atomic, molecular, nuclear physics, are the so-called anharmonic singular Hamiltonians given by

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + r^2 + \sum_{n=0}^{N} \frac{\lambda_n}{r^{\alpha_n}}, \tag{1.1}$$

where $r \in (0,\infty)$ and α_n and λ_n are positive real numbers. A particular and important special subclass of (1.1) that has been a subject of intensive studies is the set of spiked harmonic oscillator Hamiltonians[9]

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + r^2 + \frac{\lambda}{r^{\alpha}}, \quad \alpha > 0,\ \lambda > 0 \tag{1.2}$$

acting in the Hilbert space $L_2(0,\infty)$ with eigenfunctions $\psi \in L_2(0,\infty)$ of H satisfying the Schrödinger equation $-\psi'' + (r^2 + \lambda r^{-\alpha})\psi = E\psi$ with $\psi(0) = 0$. The function ψ is an eigenfunction corresponding to the eigenvalue E and the condition $\psi(0) = 0$ is the *Dirichlet boundary condition* we impose. The coupling parameter λ determines the strength of the perturbative potential and the positive constant α represents the type of singularity at the origin. Thanks to the pioneering work of Detwiler and Klauder[8] and of Harrell,[9] remarkable progress has been made over the past three decades in the field of spectral calculations for the spiked harmonic oscillator Hamiltonian (1.2). Other interesting subclasses of (1.1) which have been used in atomic, molecular, and nuclear physics are the anharmonic singular Hamiltonians[47–61]

$$H = -\frac{d^2}{dr^2} + ar^2 + br^{-4} + cr^{-6}, \quad a > 0,\ b > 0,\ c > 0, \tag{1.3}$$

and the positive-parameter singular even-power Hamiltonians[62–66]

$$H = -\frac{d^2}{dr^2} + a_1 r^2 + \frac{a_2}{r^2} + \frac{a_3}{r^4} + \frac{a_4}{r^6}. \tag{1.4}$$

Several numerical and analytical (both variational and perturbative) techniques are avaliable in the literature for the exact and approximate eigenvalue calculations for these families of Hamiltonians. Some of these techniques were devoted to particular classes of singular Hamiltonians and some others were restricted to specific values of the potential parameters. It is of great interest to have a successful method valid for the study all of these classes without the need for major adjustment as one goes from class to class. The purpose of this paper is to provide such technique and to present a rigorous variational approach for the accurate calculation of the energy levels of the singular Hamiltonians (1.1). Our method is very simple and yet accurate enough to determine the entire spectrum in arbitrary dimensions of anharmonic singular Hamiltonians (1.1). It can be viewed as an extension of the earlier variational approach to the study of the spiked Harmonic oscillator potentials.[44] The principal ingredients are (a) the use of a special basis comprising the exact solutions of a singular problem, (b) the determination of exact analytical expressions for the matrix elements with respect to this basis, and (c) the retention of two parameters from the basis problem that can be used as additional variational parameters. These optimizations are made possible because of the progress in the establishment and simplification of closed-form analytic expressions for the matrix elements.

The paper is organized as follows. In Sec. II, we introduce our variational technique: the method is discussed in a general setting with no reference to particular application. In Sec. III, we introduce the Gol'dman and Krivchenkov Hamiltonian as a solvable model. Thereafter, we use its eigensolutions to compute the matrix elements for more general singular operators $r^{-\alpha}, \alpha > 0$. Closed analytical expressions in terms of single finite sums are obtained for the matrix elements of the power-law potentials $r^q, q = 2, 4, 6, \ldots$. In Sec. IV, the applications to singular potentials are discussed. Special attention is paid to spiked harmonic oscillator (1.2) where we compared our results with other techniques avaliable in the literature. Thereafter, we study various higher-order anharmonic singular potentials, such as (1.3) and (1.4), using the approach discussed in Sec. II. The convergence problem of the variational approach is studied in some detail. Comparisons with different methods for special classes of anharmonic singular potentials are also studied.

II. METHODOLOGY

In this section, we develop a detailed variational method for studying the family of Hamiltonians (1.1). The variational function is taken as a linear combination of orthonormal functions of an exactly solvable model which itself has a singular potential. Let $\{E_n(\Omega), \psi_n^\Omega\}$ be the eigenvalues and the eigenfunctions of an exactly solvable Hamiltonian $H^\Omega = -\Delta + v^\Omega(r)$ acting on separable Hilbert space $L_2(D, d\mu)$ such that

$$\begin{aligned} H^\Omega \psi_n^\Omega &= E_n(\Omega)\psi_n^\Omega, \\ \|\psi_n^\Omega\|_D^2 &= \langle \psi_n^\Omega | \psi_n^\Omega \rangle = \int_D |\psi_n^\Omega(r)|^2 \, d\mu(r) = 1. \end{aligned} \tag{2.1}$$

Here $v^\Omega(r)$ is taken as a function of r and depends on the parameters in the set Ω. Let $H^\Lambda = -\Delta + V^\Lambda(r)$ be the quantum Hamiltonian under investigation, where Λ is a fixed set of parameters, and we let $\epsilon(\Lambda)$ be the associated exact eigenvalues of H^Λ. By writing the Hamiltonian H^Λ in the extended form

$$H^{\Lambda} = H^{\Omega} + V^{\Lambda}(r) - v^{\Omega}(r), \tag{2.2}$$

we have that if the integrals

$$\langle \psi_n^{\Omega} | V^{\Lambda}(\cdot) | \psi_n^{\Omega} \rangle = \int_D \overline{\psi_n^{\Omega}} V^{\Lambda} \psi_n^{\Omega} \, \mathrm{d}\mu \quad \text{are finite}, \tag{2.3}$$

then the matrix elements of the Hamiltonian H^{Λ} can be written, for $m,n=0,1,2,\ldots$ as

$$H_{mn}^{\Lambda} \equiv \langle \psi_m^{\Omega} | H | \psi_n^{\Omega} \rangle = E_{mn}(\Omega)\,\delta_{mn} + \langle \psi_m^{\Omega} | V^{\Lambda}(\cdot) | \psi_n^{\Omega} \rangle - \langle \psi_m^{\Omega} | v^{\Omega}(\cdot) | \psi_n^{\Omega} \rangle, \tag{2.4}$$

or in compact form as

$$H_{mn}^{\Lambda} = \langle \psi_n^{\Omega} | -\Delta | \psi_n^{\Omega} \rangle + \langle \psi_n^{\Omega} | V^{\Lambda}(\cdot) | \psi_n^{\Omega} \rangle. \tag{2.5}$$

Our variational technique is based on forming trial wave functions from a linear combination of D-orthonormal functions $\psi_n^{\Omega}(r)$, $n=0,1,2,\ldots,D-1$,

$$\Psi(r) = \sum_{n=0}^{D-1} c_n \psi_n^{\Omega}(r). \tag{2.6}$$

The linear parameters c_n that optimize the energy are determined by the following system of equations:

$$\sum_{n=0}^{D-1} (H_{mn}^{\Lambda} - \epsilon(\Lambda)\,\delta_{mn}) c_n = 0, \quad m = 0,1,2,\ldots,D-1. \tag{2.7}$$

The necessary and sufficient condition for a nontrivial solution of (2.7) is the vanishing of the secular determinant

$$\det | H_{mn}^{\Lambda} - \epsilon(\Lambda)\,\delta_{mn} | = 0. \tag{2.8}$$

The condition (2.8) yields upper bounds to the exact eigenvalues $\epsilon(\Lambda)$ by means of the inequality

$$\epsilon(\Lambda) \leqslant \min_{\Omega} \mathrm{diag} \begin{pmatrix} H_{00}^{\Lambda} & H_{01}^{\Lambda} & \cdots & H_{0D-1}^{\Lambda} \\ H_{10}^{\Lambda} & H_{11}^{\Lambda} & \cdots & H_{1D-1}^{\Lambda} \\ \cdots & \cdots & \cdots & \cdots \\ H_{D-10}^{\Lambda} & H_{D-11}^{\Lambda} & \cdots & H_{D-1D-1}^{\Lambda} \end{pmatrix}, \tag{2.9}$$

where $H_{mn}^{\Lambda} = \langle \psi_m^{\Omega} | H^{\Lambda} | \psi_n^{\Omega} \rangle = H_{mn}^{\Omega} + V_{mn}^{\Lambda}(r) - v_{mn}^{\Omega}(r)$, for fixed Λ, are functions of the parameter set Ω. Note that the equality in (2.9) holds if $V^{\Lambda}(r) = v^{\Omega}(r)$, for all r. The computation of the right-hand side of (2.9) requires a diagonalization of the matrix over the D-dimensional subspace spanned by orthonormal functions ψ_n^{Ω} followed subsequently by a minimization over the parameters Ω. The advantages of this method are (i) only a few matrix elements are needed to achieve accurate bounds to the eigenvalues; (ii) the exact eigenvalues are approached monotonically as D is increased; (iii) the minimization over a set of parameters Ω accelerates the convergence of the energy bounds more rapidly than any standard minimization over a single variable; (iv) the optimization of (2.9) for $D \times D$ matrix gives upper bounds to the energy eigenvalues of the lowest D states; (v) the diagonalization of such a matrix also produces the coefficients required for the corresponding eigenvectors determined variationally.

III. EXACTLY SOLVABLE MODEL AND ASSOCIATED MATRIX ELEMENTS

The accuracy and the computational simplicity of the variational method depends greatly on the analytic structure of the wave functions that we use, in particular, their behavior in the neighborhood of the singularity. Many different forms of trial wave function have been explored

in the literature to solve the spiked harmonic oscillator problem (1.2). The rate of convergence for a variational calculation depends on the ability of the basis functions used in the variational calculation to approximate the behavior of the exact wave function in the neighborhood of the singularity. Recently, Hall *et al.* have pointed out the advantages of basing the variational analysis of singular potentials on an exact soluble model which itself has a singular potential term. They have suggested and used trial wave functions constructed by means of the superposition of the orthonormal functions of the exact solutions of the Gol'dman and Krivchenkov Hamiltonian,

$$H_0 = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + Br^2 + \frac{A}{r^2}. \tag{3.1}$$

It was shown that this orthonormal basis serves as an effective starting point for the variational analysis of the Hamiltonian (1.2). In this paper we use these solutions of H_0 to provide systematic variational solutions for the singular Hamiltonians (1.1). The Gol'dman and Krivchenkov Hamiltonian (3.1) is one of the few that admit exact analytical solutions. The Hamiltonian is the generalization of the familiar harmonic oscillator in three-dimensional $-\mathrm{d}^2/\mathrm{d}r^2+Br^2+l(l+1)/r^2$ where the generalization lies in the parameter A ranging over $[0,\infty)$ instead of only values determined by the angular momentum quantum numbers $l=0,1,2,\ldots$. The background on Gol'dman and Krivchenkov potential $V(r)=Br^2+Ar^{-2}$ relevant to the following discussion can be found in Ref. 44. In particular, the energy spectrum of the Schrödinger Hamiltonian H_0 is given, in terms of parameters A and B, by

$$E_n = 2\beta(2n+\gamma), \quad n = 0,1,2,\ldots, \tag{3.2}$$

in which $\beta=\sqrt{B}$ and $\gamma=1+\sqrt{A+\frac{1}{4}}$ and the normalized wave functions are

$$\psi_n(r) = (-1)^n \sqrt{\frac{2\beta^{\gamma}(\gamma)_n}{n!\,\Gamma(\gamma)}} r^{\gamma-1/2} e^{-(1/2)\beta r^2} F_1(-n;\gamma;\beta r^2). \tag{3.3}$$

Here ${}_1F_1$ is the confluent hypergeometric function

$${}_1F_1(-n;b;z) = \sum_{k=0}^{n} \frac{(-n)_k z^k}{(b)_k k!} \quad (n\text{-degree polynomial in } z) \tag{3.4}$$

and the shifted factorial $(a)_n$ defined by

$$(a)_0 = 1, \quad (a)_n = a(a+1)(a+2)\cdots(a+n-1), \quad \text{for } n = 1,2,3,\ldots \tag{3.5}$$

may be expressed in terms of the gamma function by $(a)_n=\Gamma(a+n)/\Gamma(a)$, when a is not a negative integer $-m$, and, in these exceptional cases, $(-m)_n=0$ if $n>m$ and otherwise $(-m)_n=(-1)^n m!/(m-n)!$.

An important observation regarding the solvable model H_0 is the existence of the A term which has the dimensions of kinetic energy such as the term that appears in higher-dimensional systems. This observation allows us to extend (3.2) and (3.3) to the exact solutions of N-dimensional Gol'dman and Krivchenkov Hamiltonian, namely,

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\Lambda(\Lambda+1)+A}{r^2} + Br^2 \quad (A \geqslant 0, B > 0), \tag{3.6}$$

where $\Lambda=\frac{1}{2}(M-3)$, and $M=N+2l$. The exact solution of (3.6) can be easily found by replacing A in (3.2) and (3.3) with

$$A \to \Lambda(\Lambda+1)+A. \tag{3.7}$$

This particular observation can be extended to any three-dimensional exact solvable quantum model. Indeed, if Schrödinger's equation can be solved for arbitrary angular momentum number l,

then the extension to the N-dimensional case can be obtained by replacing l with Λ. It should be also noted that N and l enter into the Hamiltonian (3.6) in the form of combination $N+2l$. Hence, the energy for a spherically symmetric potential $V(r)$ are the same as long as M is not altered. We now summarize the exact eigenvalues of N-dimensional Schrödinger equation with the Gol'dman and Krivchenkov potential as

$$E_{nl}^{N} = 2\beta(2n + \gamma_N), \quad n,l = 0,1,2, \ldots , \tag{3.8}$$

where $\beta=\sqrt{B}$ and $\gamma_N=1+\sqrt{A+(\Lambda+\frac{1}{2})^2}$, while the exact eigenfunctions are given explicitly by

$$\psi_{nl}^{N}(r) = (-1)^n \sqrt{\frac{2\beta^{\gamma_N}(\gamma_N)_n}{n!\,\Gamma(\gamma_N)}} r^{\gamma_N-1/2} e^{-(1/2)\beta r^2} {}_1F_1\left(\begin{matrix} -n \\ \gamma_N \end{matrix} \middle| \beta r^2 \right) \quad (n,l = 0,1,2, \ldots, N \geqslant 1). \tag{3.9}$$

In the next section all our results are formulated in arbitrary dimension $N \geqslant 1$.

A. Matrix elements of the singular operator $r^{-\alpha}$

The effectiveness of the variational method relies on finding a basis that allows for easy calculation of the matrix elements of the given Hamiltonian. An important advantage of the orthonormal wave functions (3.3) is the existence of closed-form formulas for the singular potential integrals $\langle \psi_m | r^{-\alpha} | \psi_n \rangle$. These closed form expressions are achieved by means of the following identity: For m and n non-negative integers and $2\gamma > \alpha$,

$$\begin{aligned} &\int_0^\infty r^{2\gamma-\alpha-1} e^{-\beta r^2} {}_1F_1\left(\begin{matrix} -n \\ \gamma \end{matrix} \middle| \beta r^2 \right) {}_1F_1\left(\begin{matrix} -m \\ \gamma \end{matrix} \middle| \beta r^2 \right) \mathrm{d}r \\ &\quad = \frac{\left(\frac{\alpha}{2}\right)_n \Gamma\left(\gamma - \frac{\alpha}{2}\right)}{2\beta^{\gamma-(\alpha/2)}(\gamma)_n} {}_3F_2\left(\begin{matrix} -m, \gamma - \frac{\alpha}{2}, 1 - \frac{\alpha}{2} \\ \gamma, 1 - \frac{\alpha}{2} - n \end{matrix} \middle| 1 \right), \end{aligned} \tag{3.10}$$

where the Clausen hypergeometric function ${}_3F_2$ is defined by the series representation

$${}_3F_2\left(\begin{matrix} -m, a, b \\ c, d \end{matrix} \middle| 1 \right) = \sum_{k=0}^{m} \frac{(-m)_k (a)_k (b)_k}{(c)_k (d)_k k!} \quad (m\text{-degree polynomial}).$$

The proof of this identity and some relevant integrals can be found in Ref. 44. Thus the matrix elements $r_{mn}^{-\alpha} = \langle \psi_n | r^{-\alpha} | \psi_n \rangle$ of the singular operator $r^{-\alpha}$ have the explicit forms

$$r_{mn}^{-\alpha} = (-1)^{n+m} \beta^{\alpha/2} \frac{\left(\frac{\alpha}{2}\right)_n}{(\gamma)_n} \frac{\Gamma\left(\gamma - \frac{\alpha}{2}\right)}{\Gamma(\gamma)} \sqrt{\frac{(\gamma)_n (\gamma)_m}{n!\,m!}} {}_3F_2\left(\begin{matrix} -m, \gamma - \frac{\alpha}{2}, 1 - \frac{\alpha}{2} \\ \gamma, 1 - \frac{\alpha}{2} - n \end{matrix} \middle| 1 \right). \tag{3.11}$$

In the case of α being a non-negative even number ($\alpha=2,4,6,\ldots$), the Clausen hypergeometric function ${}_3F_2$ in (3.11) may be looked upon as a polynomial of degree $(\alpha/2)-1$ instead of an m-degree polynomial. This is, of course, not the case for $0<\alpha\neq 2,4,6,\ldots$ in which case the numerical computation would have to be done directly using the expression (3.11). For $n \geqslant m$ and $\alpha=2,4,6,\ldots$ we have by means of the series representation of the hypergeometric function ${}_3F_2$ that

$$ {}_3F_2\left(\begin{matrix} -\left(\frac{\alpha}{2}-1\right), \gamma-\frac{\alpha}{2}, -m \\ \gamma, 1-\frac{\alpha}{2}-n \end{matrix}\middle| 1\right) = \sum_{s=0}^{(\alpha/2)-1} \frac{(-m)_s \left(\gamma-\frac{\alpha}{2}\right)_s \left(1-\frac{\alpha}{2}\right)_s}{s!\,(\gamma)_s \left(1-\frac{\alpha}{2}-n\right)_s}. \tag{3.12} $$

As a result, the matrix elements (3.11) further simplify into the closed form expressions immediately appearing. These are most suitable for computational purposes as for the case of $\gamma>1$ and $\alpha=2$, we indeed have

$$ r_{mn}^{-2} = \begin{cases} (-1)^{m+n} \dfrac{\beta}{\gamma-1} \sqrt{\dfrac{n!\,(\gamma)_m}{m!\,(\gamma)_n}} & \text{if } n>m, \\ \dfrac{\beta}{\gamma-1} & \text{if } n=m, \\ (-1)^{m+n} \dfrac{\beta}{\gamma-1} \sqrt{\dfrac{m!\,(\gamma)_n}{n!\,(\gamma)_m}} & \text{if } n<m. \end{cases} \tag{3.13} $$

On the other hand, for $\gamma>2$ and $\alpha=4$, we have from (3.11) and (3.12) that

$$ r_{mn}^{-4} = \begin{cases} \dfrac{(-1)^{m+n}\beta^2}{\gamma(\gamma-1)(\gamma-2)} \sqrt{\dfrac{n!\,(\gamma)_m}{m!\,(\gamma)_n}} [\gamma(n-m+1)+2m] & \text{if } n>m, \\ \dfrac{\beta^2}{\gamma(\gamma-1)(\gamma-2)} [\gamma+2n] & \text{if } n=m, \\ \dfrac{(-1)^{m+n}\beta^2}{\gamma(\gamma-1)(\gamma-2)} \sqrt{\dfrac{m!\,(\gamma)_n}{n!\,(\gamma)_m}} [\gamma(m-n+1)+2n] & \text{if } n<m. \end{cases} \tag{3.14} $$

We also point out, for $\gamma>3$ and $\alpha=6$, Eq. (3.12) lets us deduce

$$ r_{mn}^{-6} = \begin{cases} \dfrac{(-1)^{m+n}\beta^3}{2(\gamma+1)\gamma(\gamma-1)(\gamma-2)(\gamma-3)} \sqrt{\dfrac{n!\,(\gamma)_m}{m!\,(\gamma)_n}} [(2+n)(1+n)\gamma(\gamma+1) & \\ \quad -2m(1+n)(\gamma-3)(\gamma+1)-m(1-m)(\gamma-2)(\gamma-3)] & \text{if } n>m, \\ \dfrac{\beta^3}{(\gamma+1)\gamma(\gamma-1)(\gamma-2)(\gamma-3)} (\gamma+\gamma^2+6\gamma n+6n^2) & \text{if } n=m, \\ \dfrac{(-1)^{m+n}\beta^3}{2(\gamma+1)\gamma(\gamma-1)(\gamma-2)(\gamma-3)} \sqrt{\dfrac{m!\,(\gamma)_n}{n!\,(\gamma)_m}} [(2+m)(1+m)\gamma(\gamma+1) & \\ \quad -2n(1+m)(\gamma-3)(\gamma+1)-n(1-n)(\gamma-2)(\gamma-3)] & \text{if } n<m. \end{cases} \tag{3.15} $$

We can derive similar expressions for all even integers beyond 6, i.e., $\alpha=8,10,\ldots$, where we have, for $n\geqslant m$, that

$$ r_{mn}^{-\alpha} = (-1)^{n+m}\beta^{\alpha/2} \frac{\left(\frac{\alpha}{2}\right)_n}{(\gamma)_n} \frac{\Gamma\left(\gamma-\frac{\alpha}{2}\right)}{\Gamma(\gamma)} \sqrt{\frac{(\gamma)_n(\gamma)_m}{n!\,m!}} \sum_{s=0}^{(\alpha/2)-1} \frac{(-m)_s \left(\gamma-\frac{\alpha}{2}\right)_s \left(1-\frac{\alpha}{2}\right)_s}{s!\,(\gamma)_s \left(1-\frac{\alpha}{2}-n\right)_s}, \tag{3.16} $$

and the matrix elements with $0\leqslant n<m$ are incorporated by using the symmetry property, i.e., $r_{mn}^{-\alpha}=r_{nm}^{-\alpha}$. For the N-dimensional case, the matrix elements of the singular operator $r^{-\alpha}$ can be easily found in analogy with (3.10),

$$r_{mn}^{-\alpha}=(-1)^{n+m}\beta^{\alpha/2}\frac{\left(\frac{\alpha}{2}\right)_n}{(\gamma)_n}\frac{\Gamma\left(\gamma_N-\frac{\alpha}{2}\right)}{\Gamma(\gamma_N)}\sqrt{\frac{(\gamma_N)_n(\gamma_N)_m}{n!\,m!}}\,{}_3F_2\left(\begin{matrix}-m,\gamma_N-\frac{\alpha}{2},1-\frac{\alpha}{2}\\ \gamma_N,1-n-\frac{\alpha}{2}\end{matrix}\middle|\,1\right). \tag{3.17}$$

The results for the special cases $\alpha=2,4,6,\ldots$ can be obtained in a similar fashion to (3.14)–(3.16) through the substitution of γ by $\gamma_N=1+\sqrt{A+[l+(N/2)-1]^2}$.

B. Matrix elements of the power-law potentials r^q

We now use the orthonormal eigenfunctions (3.3) to compute the matrix elements for the power-law potential operators r^q, $q=2,4,6,\ldots$. In analogy with (3.10), this can be achieved by means of the identity, for m and n non-negative integers and $2\gamma+q>0$,

$$\int_0^\infty r^{2\gamma+q-1}e^{-\beta r^2}\,{}_1F_1\left(\begin{matrix}-n\\ \gamma\end{matrix}\middle|\,\beta r^2\right){}_1F_1\left(\begin{matrix}-m\\ \gamma\end{matrix}\middle|\,\beta r^2\right)\mathrm{d}r$$
$$=\frac{\left(-\frac{q}{2}\right)_n\Gamma\left(\gamma+\frac{q}{2}\right)}{2\beta^{\gamma+(q/2)}(\gamma)_n}\,{}_3F_2\left(\begin{matrix}-m,\gamma+\frac{q}{2},1+\frac{q}{2}\\ \gamma,1+\frac{q}{2}-n\end{matrix}\middle|\,1\right). \tag{3.18}$$

In the case of q being a positive even number ($q=2,4,6,\ldots$), the Clausen hypergeometric function ${}_3F_2$ in (3.18) can be further simplified. Indeed in this case, we prove the following result.

Theorem 1: For $t=0,1,2,\ldots,q/2$ and $q=2,4,6,\ldots$, the matrix elements of the power-law potential r^q, $q=2,4,6,\ldots$ in terms of the orthonormal functions (3.3) are

$$r_{mn}^q=0 \quad \text{if } n>m+\frac{q}{2},$$

$$=\frac{(-1)^q}{\beta^{q/2}}\sqrt{\frac{\left(\gamma+\frac{\alpha}{2}\right)_m\Gamma\left(\gamma+\frac{q}{2}\right)\left(m+\frac{q}{2}\right)!}{(\gamma)_m\Gamma(\gamma)m!}} \quad \text{if } n=m+\frac{q}{2},$$

$$=\frac{\Gamma\left(\gamma+\frac{q}{2}\right)(\gamma+m-t)_{q/2}(m-t+1)_{q/2}}{(-1)^{t-q}\beta^{q/2}t!\,\Gamma(\gamma)(\gamma)_{q/2}}\sqrt{\frac{m!\,(\gamma)_m}{(\gamma)_{m+(q/2)-t}[m+(q/2)-t]!}}$$
$$\times\sum_{j=0}^{t}\frac{(-t)_j\left(\gamma+m+\frac{q}{2}-t\right)_j\left(\frac{q}{2}+m-t+1\right)_j}{(\gamma+m-t)_j(m+1-t)_j j!} \quad \text{if } n=m+\frac{q}{2}-t,$$

$$=\frac{\Gamma\left(\gamma+\frac{q}{2}\right)(1-\gamma-m)_{q/2}(-m)_{q/2}}{(-\beta)^{q/2}\Gamma(\gamma)\frac{q}{2}!\,(\gamma)_{q/2}}\sum_{j=0}^{q/2}\frac{\left(-\frac{q}{2}\right)_j(\gamma+m)_j(m+1)_j}{\left(\gamma+m-\frac{q}{2}\right)_j\left(m+1-\frac{q}{2}\right)_j j!} \quad \text{if } m=n,$$

$$= \frac{\Gamma\left(\gamma+\frac{q}{2}\right)(\gamma+n-t)_{q/2}(n-t+1)_{q/2}}{(-1)^{t-q}\beta^{q/2}t!\,\Gamma(\gamma)(\gamma)_{q/2}} \sqrt{\frac{n!\,(\gamma)_n}{(\gamma)_{n+(q/2)-t}\left(n+\frac{q}{2}-t\right)!}}$$

$$\times \sum_{j=0}^{t} \frac{(-t)_j\left(\gamma+n+\frac{q}{2}-t\right)_j\left(\frac{q}{2}+n-t+1\right)_j}{(\gamma+n-t)_j(n+1-t)_j j!} \quad \text{if } m = n+\frac{q}{2}-t,$$

$$= \frac{(-1)^q}{\beta^{q/2}} \sqrt{\frac{\left(\gamma+\frac{\alpha}{2}\right)_n \Gamma\left(\gamma+\frac{q}{2}\right)\left(n+\frac{q}{2}\right)!}{(\gamma)_n\Gamma(\gamma)n!}} \quad \text{if } m = n+\frac{q}{2},$$

$$= 0 \quad \text{if } m > n+\frac{q}{2}. \tag{3.19}$$

Proof: From (3.18), we have

$$r_{mn}^{q} = (-1)^{m+n}\beta^{-q/2}\frac{\Gamma\left(\gamma+\frac{q}{2}\right)}{\Gamma(\gamma)(\gamma)_n}\sqrt{\frac{(\gamma)_n(\gamma)_m}{n!\,m!}}\left(-\frac{q}{2}\right)_n {}_3F_2\left(\begin{matrix} -m, \gamma+\frac{q}{2}, 1+\frac{q}{2} \\ \gamma, 1+\frac{q}{2}-n \end{matrix}\middle| 1\right)$$

and the problem is now reduced to the simplification of the product

$$\left(-\frac{q}{2}\right)_n {}_3F_2\left(\begin{matrix} -m, \gamma+\frac{q}{2}, 1+\frac{q}{2} \\ \gamma, 1+\frac{q}{2}-n \end{matrix}\middle| 1\right).$$

Using the series representation for ${}_3F_2$, we can write

$$I = \left(-\frac{q}{2}\right)_n {}_3F_2\left(\begin{matrix} -m, \gamma+\frac{q}{2}, 1+\frac{q}{2} \\ \gamma, 1+\frac{q}{2}-n \end{matrix}\middle| 1\right) = \sum_{k=0}^{m} \frac{(-m)_k\left(\gamma+\frac{q}{2}\right)_k\left(-\frac{q}{2}-k\right)_n}{(\gamma)_k k!},$$

where we have used the identity $(a-n)_k=(1-a)_n(a)_k/(1-a-k)_n$. From the definition of the Pochhammer symbol $(-(q/2)-k)_n$ we have that $I=0$ for $n>m+(q/2)$ and for $n=(q/2)+m$ we have

$$I = \frac{(-1)^{q/2}\left(\gamma+\frac{q}{2}\right)_m\left(m+\frac{q}{2}\right)!}{(\gamma)_m}.$$

Finally, for $n=m+(q/2)-t$, $t=0,1,2,\ldots,q/2$,

$$I = \sum_{k=0}^{m} \frac{(-m)_k\left(\gamma+\frac{q}{2}\right)_k\left(-\frac{q}{2}-k\right)_{m+(q/2)-t}}{(\gamma)_k k!} = \sum_{k=m-t}^{m} \frac{(-m)_k\left(\gamma+\frac{q}{2}\right)_k\left(-\frac{q}{2}-k\right)_{m+(q/2)-t}}{(\gamma)_k k!}.$$

The completion of the proof then follows by shifting the index $j=k-m+t$ of the finite sum. □

As consequence of Theorem 1, for $q=2$ and $\gamma>-1$ we have that

$$r_{mn}^2=\begin{cases}0 & \text{if } n>m+1,\\ \beta^{-1}\sqrt{(m+1)(\gamma+m)} & \text{if } n=m+1,\\ \beta^{-1}(\gamma+2n) & \text{if } n=m,\\ \beta^{-1}\sqrt{(n+1)(\gamma+n)} & \text{if } m=n+1,\\ 0 & \text{if } m>n+1.\end{cases} \tag{3.20}$$

Furthermore, the explicit formula for the matrix elements of the operator r^4 now reads

$$r_{mn}^4=\begin{cases}0 & \text{if } n>m+2,\\ \beta^{-2}\sqrt{(m+1)(m+2)(\gamma+m)(\gamma+m+1)} & \text{if } n=m+2,\\ 2\beta^{-2}(\gamma+2m+1)\sqrt{(m+1)(\gamma+m)} & \text{if } n=m+1,\\ \beta^{-2}(\gamma+6m^2+6\gamma m+\gamma^2) & \text{if } n=m,\\ 2\beta^{-2}(\gamma+2n+1)\sqrt{(n+1)(\gamma+n)} & \text{if } m=n+1,\\ \beta^{-2}\sqrt{(n+1)(n+2)(\gamma+n)(\gamma+n+1)} & \text{if } m=n+2,\\ 0 & \text{if } m>n+1.\end{cases} \tag{3.21}$$

IV. APPLICATIONS AND NUMERICAL RESULTS

A. Spiked harmonic oscillator Hamiltonians

There are several reasons for the interest in the spiked harmonic oscillator Hamiltonian (1.2) and its extension, the so-called generalized spiked harmonic oscillator,

$$H=-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+Br^2+\frac{A}{r^2}+\frac{\lambda}{r^\alpha}. \tag{4.1}$$

First, it represents the simplest model of certain realistic interaction potentials in atomic, molecular, and nuclear physics, and second, its interesting intrinsic properties from the viewpoint of mathematical physics are as follows: (1) an eigenvalue of the perturbed operator may not converge to the original one as $\lambda\to 0$ (the Klauder phenomenon) and (2) the perturbation series is ordered in fractional powers of λ, and in the cases $\alpha>5/2$ the regular Rayleigh–Schrödinger perturbation theory fails badly.

We shall consider the problem initially in $N=3$ spatial dimensions. It was proven earlier[44] that the set of $L_2[0,\infty)$-functions $\{\psi_n(r)\}_{n=0}^{\infty}$ as defined by (3.3), is a complete orthonormal basis for the Hilbert space $L_2[0,\infty)$. This basis was the starting point for perturbative expansions and variational analysis of the Hamiltonians (1.2) and (4.1). The main approach of the earlier variational investigation of (1.2) was the rewriting of the Hamiltonian as

$$H\equiv-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+r^2+\frac{A}{r^2}+\left(\frac{\lambda}{r^\alpha}-\frac{A}{r^2}\right). \tag{4.2}$$

The parameter A serves as an extra degree of freedom that can be used to accelerate the convergence to the exact eigenvalues through the minimization of the eigenvalues of the diagonalizable $D\times D$ symmetric matrix. Straightforward calculations using (3.11) and (3.13) show that the matrix elements H_{mn} of the Hamiltonian (4.2) are $(m,n=0,1,2,\ldots,D-1,\ n\geqslant m)$

$$H_{mn} = 2(2n+\gamma)\delta_{nm} + (-1)^{n+m}\lambda \frac{\left(\frac{\alpha}{2}\right)_n}{(\gamma)_n} \frac{\Gamma\left(\gamma - \frac{\alpha}{2}\right)}{\Gamma(\gamma)} \sqrt{\frac{(\gamma)_n(\gamma)_m}{n!m!}}\, {}_3F_2\left(\begin{matrix} -m, \gamma - \frac{\alpha}{2}, 1 - \frac{\alpha}{2} \\ \gamma, 1 - n - \frac{\alpha}{2} \end{matrix} \middle| 1 \right)$$

$$- (-1)^{m+n} \frac{(\gamma - \frac{3}{2})(\gamma - \frac{1}{2})}{\gamma - 1} \sqrt{\frac{n!(\gamma)_m}{m!(\gamma)_n}}, \tag{4.3}$$

where $2\gamma > \alpha$ and the matrix elements with $0 \leqslant n < m$ are incorporated by using the symmetry property of the matrix. In order to apply the method discussed in Sec. II, we write (1.2) in more extended form,

$$H \equiv -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + Br^2 + \frac{A}{r^2} + (1-B)r^2 + \left(\frac{\lambda}{r^\alpha} - \frac{A}{r^2}\right). \tag{4.4}$$

In this case, the matrix elements of the Hamiltonian (4.4) assume the form

$$H_{mn} = 2\beta(2n+\gamma)\delta_{mn} + (1-\beta^2)r^2_{mn} + \lambda r^{-\alpha}_{mn} - A r^{-2}_{mn} \quad (\beta = \sqrt{B}, m, n = 0,1,2,\ldots,D-1), \tag{4.5}$$

where r^2_{mn} is given by (3.20), $r^{-\alpha}_{mn}$ is given by (3.11), and r^{-2}_{mn} is given by (3.13). In order to illustrate the difference between using the expressions (4.3) and (4.5), we restrict our calculation to $\alpha = 4$. The first variational approximation (subspace of dimension 1) of the ground-state eigenvalues of the spiked harmonic oscillator Hamiltonian yields by means of (4.3) the approximation

$$\epsilon_0 = \min_{A > 0.75} \left\{ \gamma + 1 + \frac{\lambda}{(\gamma-1)(\gamma-2)} + \frac{1}{4(\gamma-1)} \right\} \quad \left(\gamma = 1 + \frac{1}{2}\sqrt{1+4A} > 2 \right) \tag{4.6}$$

while the matrix elements (4.5) yield the approximation

$$\epsilon_0 = \min_{A > 0.75, B > 0} \left\{ \frac{\gamma}{\beta} + \beta + \frac{\lambda\beta^2}{(\gamma-1)(\gamma-2)} + \frac{\beta}{4(\gamma-1)} \right\} \quad \left(\gamma = 1 + \frac{1}{2}\sqrt{1+4A} > 2, \beta = \sqrt{B} \right). \tag{4.7}$$

The minimization of (4.6) over the parameter A yields

$$\epsilon_0 = \tfrac{5}{2} + \tfrac{3}{2}(8\lambda - 1 + 4\sqrt{4\lambda^2 - \lambda})^{1/3} + (6\lambda - \tfrac{3}{4} - 3\sqrt{4\lambda^2 - \lambda})(8\lambda - 1 + 4\sqrt{4\lambda^2 - \lambda})^{2/3}$$

which implies the upper bound $\epsilon_0 = 21.427\,793$ for $\lambda = 1000$; while the minimization of (4.7) over A and B yields $\epsilon_0 = 21.374\,087$ with first decimal place exact. In Table I, we present a comparison between eigenvalues computation using (4.6) and (4.7) for $\lambda = 0.1$ to illustrate the increase in the rate of convergence obtained when using our new approach. It should be noted that the optimization over the parameter A of the 1000×1000-diagonalizable matrix yields an upper bound of $E^A = 3.575\,557$ with $A \approx 6.076$, while the minimization and diagonalization of the symmetric matrix over the parameters A and B greatly reduce the number of the matrix elements needed by a ratio of approximately 10:1. As shown in Table I, 100×100 matrix is sufficient to achieve an exact eigenvalue of $E^{A,B} = 3.575\,552$. Because we have established simple formulas for the matrix elements in the cases $\alpha = 4$ and $\alpha = 6$ [given by (3.14) and (3.15), respectively], the determination of the energy values to any desired accuracy reduced to an easy task as indicated in Table II where we report our eigenvalue computation for the case $\alpha = 6$ and for different values of the parameter λ. A heuristic scheme for ascertaining the eigenvalues to any required number of digits is as follows. The eigenvalues obtained from successive levels, such as $(1 \times 1, 2 \times 2, \ldots)$, of the truncated matrix are compared, and the calculation ceases when the successive eigenvalues agree with each other up to the prescribed decimal place. Further advantage of the variational approach presented here is the amount of information that we get about the spectrum of the Hamiltonian

TABLE I. Upper bounds E^A for $H=-\Delta+r^2+(1/10r^4)$ are obtained by diagonalization then minimization of the $D\times D$ matrix, only over the parameter A. $E^{A,B}$ are the corresponding values minimized over both A and B. The eigenvalue 3.575 552 (exact to seven places) can be easily verified by direct numerical integration of Schrödinger's equation.

$D\times D$	E^A	$E^{A,B}$
1×1	3.745 811	3.664 281
	$(A\approx 1.52)$	$(A\approx 1.92, B\approx 1.62)$
10×10	3.602 189	3.582 194
	$(A\approx 2.84)$	$(A\approx 4.75, B\approx 11.66)$
20×20	3.588 143	3.576 773
	$(A\approx 3.68)$	$(A\approx 8.14, B\approx 32.22)$
100×100	3.577 007	3.575 552
	$(A\approx 7.44)$	$(A\approx 9.73, B\approx 297.23)$
200×200	3.576 015	3.575 552
	$(A\approx 10.39)$	$(A\approx 3.76, B\approx 873.58)$

every time we compute the eigenvalues via the diagonalization and minimization. Indeed, we obtain, for $D\times D$-matrix, a set of upper bounds for the eigenvalues $E_0, E_1, \ldots, E_{D-1}$. Each can be improved by either an increase in the dimension of the matrix, or by extracting the desired level through the diagonalization and subsequent minimization with respect to parameters A and B. For the N-dimensional case, the matrix elements of the singular operator $r^{-\alpha}$ turn out to be

$$\langle \psi_{ml}^N | r^{-\alpha} | \psi_{nl}^N \rangle = (-1)^{n+m} \beta^{\alpha/2} \frac{\left(\frac{\alpha}{2}\right)_n}{(\gamma)_n} \frac{\Gamma\left(\gamma_N - \frac{\alpha}{2}\right)}{\Gamma(\gamma_N)} \sqrt{\frac{(\gamma_N)_n (\gamma_N)_m}{n!m!}} {}_3F_2\left(\begin{matrix} -m, \gamma_N - \frac{\alpha}{2}, 1 - \frac{\alpha}{2} \\ \gamma_N, 1 - \frac{q}{2} - n \end{matrix} \middle| 1 \right). \tag{4.8}$$

Matrix elements for the special cases of $\alpha=2,4,6,\ldots$ are obtained by substituting in Eqs. (3.13)–(3.15) for γ the expression γ_N, where $\gamma_N=1+\sqrt{A+(\Lambda+\frac{1}{2})^2}$. The matrix elements of the

TABLE II. Upper bounds E^A for $H=-\Delta+r^2+(\lambda/r^6)$ obtained by diagonalization followed by minimization of the $D\times D$ matrix, only over the parameter A. $E^{A,B}$ are the corresponding values minimized over both A and B. The results are displayed for different values of the potential coupling λ. The eigenvalues are correct for the seven digits, as can be easily verified by direct numerical integration of Schrödinger's equation.

λ	E^A	$E^{A,B}$
1000	12.718 617	12.718 617
	$(32\times 32, A\approx 20.52)$	$(15\times 15, A\approx 54.41, B\approx 4.51)$
100	8.413 358	8.413 358
	$(65\times 65, A\approx 19.61)$	$(22\times 22, A\approx 8.88, B\approx 9.76)$
10	6.003 209	6.003 209
	$(150\times 150, A\approx 9.71)$	$(30\times 30, A\approx 9.66, B\approx 21.41)$
1	4.659 940	4.659 940
	$(350\times 350, A\approx 17.79)$	$(45\times 45, A\approx 18.34, B\approx 56.77)$
0.1	3.915 665	3.915 665
	(1000×1000)	$(80\times 80, A\approx 4.47, B\approx 176.63)$
0.01	3.505 492	3.505 455
	(1000×1000)	$(100\times 100, A\approx 20.88, B\approx 348.92)$

TABLE III. Upper bounds E_{00}^{N} for $H=-(\mathrm{d}^2/\mathrm{d}r^2)+[\Lambda(\Lambda+1)/r^2]+r^2+(1000/r^4)$ for dimension $N=2-10$, obtained by diagonalization then minimization of the 10×10 matrix over A and B.

N	E_{00}^{N}
2	21.350 246 ($A\approx71.44, B\approx1.775$)
3	21.369 463 ($A\approx71.27, B\approx1.774$)
4	21.427 056 ($A\approx70.79, B\approx1.772$)
5	21.522 860 ($A\approx69.96, B\approx1.769$)
6	21.656 596 ($A\approx68.82, B\approx1.764$)
7	21.827 883 ($A\approx67.34, B\approx1.757$)
8	22.036 232 ($A\approx65.45, B\approx1.749$)
9	22.281 057 ($A\approx63.35, B\approx1.740$)
10	22.561 680 ($A\approx60.81, B\approx1.726$)

spiked harmonic oscillator Hamiltonian now turn out to be very similar to those in Eq. (4.5), namely

$$H_{mn}=2\beta(2n+\gamma_N)\delta_{mn}+(1-B)r_{mn}^2+\lambda r_{mn}^{-\alpha}-Ar_{mn}^{-2}. \tag{4.9}$$

In Table III, upper bounds E_{00}^{N}, obtained by the optimization of the eigenvalues of a 10×10-matrix over the parameters A and B, are shown. The results are reported for the Hamiltonian

$$H=-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{\Lambda(\Lambda+1)}{r^2}+r^2+\frac{1000}{r^4}$$

where $\Lambda=\frac{1}{2}(N+2l-3)$ for dimension $N=2-10$ with the angular momentum $l=0$.

B. Anharmonic singular Hamiltonian

The higher-order anharmonic singular Hamiltonians (1.3) have attracted much attention recently.[47–66] This is in part because the study of the relevant Schrödinger equation with anharmonic potentials provides understanding and insight for the corresponding physical problems, and also because the determination of its energy is itself a challenging problem. In three-dimensional space, there are two main methods for dealing with the anharmonic potentials $V(r)=ar^2+br^{-4}+cr^{-6}$. A method due to Varshni[56] is based on an ansatz for the eigenfunctions, sufficient conditions on parameters to yield exact solutions, and a limit from initial box confinement. The other method, mainly proposed by Znojil,[47,48] relies on a Laurent series ansatz for the eigenfunctions, which converts the Schrödinger equation into a difference equation which is solved by the use of continued fractions. An interesting study related to Varshni's idea[56] for the potential $V(r)$ in two dimensions was proposed recently by Dong and Ma.[60]

The method discussed in Sec. II of the present paper provides a uniformly simple, straightforward and very efficient way of yielding accurate energies of the entire spectrum of the anharmonic potentials $V(r)$ not only in one or two dimensions but actually in arbitrary dimensions with arbitrary angular momentum number $l=0,1,2,\ldots$. We start with a wider class of anharmonic singular Hamiltonian given by

$$H=-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{\Lambda(\Lambda+1)}{r^2}+a_1r^2+\frac{a_2}{r^2}+\frac{a_3}{r^4}+\frac{a_4}{r^6}, \tag{4.10}$$

where $\Lambda=\frac{1}{2}(M-3)$, and $M=N+2l$. Clearly, the case $V(r)=a_1r^2+a_3r^{-4}+a_4r^{-6}$ appears as special case with $a_2=0$. Following the procedure discussed in Sec. II, we write the Hamiltonian as

TABLE IV. Upper bounds for the Hamiltonian $V(r)=ar^2+br^{-4}+cr^{-6}$ for different values of the parameters a, b, and c. The eigenvalues are exact for the seven digits shown, as confirmed numerically (or, for the first row, known exactly).

a	b	c	E^U
1	1	1	5.000 000 $(50\times 50, A\approx 25.51, B\approx 54.35)$
1	10	1	6.679 054 $(50\times 50, A\approx 9.65, B\approx 32.24)$
1	1	10	6.140 123 $(50\times 50, A\approx 5.56, B\approx 38.67)$
1	10	10	7.138 261 $(50\times 50, A\approx 7.83, B\approx 31.94)$
1	100	100	11.791 771 $(50\times 50, A\approx 5.15, B\approx 5.00)$
1	1000	1000	21.885 192 $(50\times 50, A\approx 19.42, B\approx 5.00)$

$$H=-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+Br^2+\frac{\Lambda(\Lambda+1)+A}{r^2}+(a_1-B)r^2+\frac{(a_2-A)}{r^2}+\frac{a_3}{r^4}+\frac{a_4}{r^6}. \tag{4.11}$$

The matrix elements of the Hamiltonian (4.11) take the form $(m,n=0,1,2,\ldots)$

$$H_{mn}=2\sqrt{B}(2n+\gamma_N)\delta_{mn}+(a_1-B)r_{mn}^2+(a_2-A)r_{mn}^{-2}+a_3r_{mn}^{-4}+a_4r_{mn}^{-6} \tag{4.12}$$

for $\gamma>3$. To analyze the precision of the method proposed here, we compare our results with some special cases for which the exact eigenvalues are known. The case of $a_1=a_3=a_4=1$, $a_2=0$, which yields the ground-state energy $E=5$ has been analyzed by Znojil,[49] Guardiola and Ros,[54] and Buendía *et al.*[51] by different techniques. Table IV shows the exact eigenvalues of $E=5$ can be reached with the diagonalization of 50×50 matrix. It should be noted however that we have fixed the dimension of the matrix to 50×50, but the particular value $E=5$ can be reached with far fewer matrix elements, indeed a 30×30 matrix is sufficient to achieve such accuracy. Further, the exact energies of 7,7,11 corresponding to $(a_1,a_3,a_4)=(1,9,9),(1,-7,49)$, and (1, 45, 225), respectively, follow simply with the optimization of the diagonalizable 40×40 matrix with $(A,B)=(17.47, 5.69)$, (18.86, 5.53), and (17.92, 5.40). These results simply indicate the generality and the efficiency of our approach. Note, the case of $(a_1,a_3,a_4)=(1,-7,49)$ also demonstrates the applicability of the method in the case of the parameter a_3 is negative. It is quite clear from Tables IV and V the generality of the method proposed here. In Table V, we illustrate the applicability of the method to the problem of obtaining the energies in different dimensions.

TABLE V. Upper bounds E^N for $H=-(\mathrm{d}^2/\mathrm{d}r^2)+[\Lambda(\Lambda+1)/r^2]+r^2+(1/r^4)+(1000/r^6)$ for dimension $N=2-10$, obtained by diagonalization then minimization with respect to A and B of a 30×30 matrix.

N	E^N
2	12.704 404 $(A\approx 5.05, B\approx 5.53)$
3	12.735 264 $(A\approx 11.73, B\approx 6.40)$
4	12.827 666 $(A\approx 5.05, B\approx 7.82)$
5	12.981 081 $(A\approx 5.97, B\approx 7.26)$
6	13.194 635 $(A\approx 6.25, B\approx 7.28)$
7	13.467 115 $(A\approx 6.12, B\approx 7.35)$
8	13.796 990 $(A\approx 6.16, B\approx 7.46)$
9	14.182 423 $(A\approx 6.31, B\approx 7.32)$
10	14.621 300 $(A\approx 3.11, B\approx 7.23)$

Similar results for different excited states can be easily reproduced. All the eigenvalues quoted in Tables I–V agree with the numerical solutions of the corresponding Schrödinger equation. Generally speaking, the precision of the energies to any number of decimal places can be easily achieved by increasing the dimension of the matrix.

V. CONCLUSION

We have developed an effective variational method to study a large family of singular Hamiltonians. A key feature of this work is the establishment and simplification of closed-form analytical expressions for the matrix elements with respect to a basis derived from a soluble singular problem. These formulas are general in the sense that they include two parameters from the basis which can then be used to optimize the matrix eigenvalues obtained for the problem at hand. The improved variational approach yields faster energy convergence than was possible earlier.

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Perturbative and nonperturbative master equations for open quantum systems

Wusheng Zhu and Herschel Rabitz
Department of Chemistry, Princeton University, Princeton, New Jersey 08544-1009

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This paper develops perturbative and nonperturbative master equations for open quantum systems based on time-dependent variational functionals. The perturbative equations are more concise and suitable for dealing with cases of weak system-environment coupling for short evolution time scales. The nonperturbative equations are valid for all time and appropriate to treat cases of strong system-environment coupling. When a system contains an external control field, both the perturbative and nonperturbative master equations reveal the embedded control field dependence upon the system decoherence, which provides a basis for decoherence management. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Open quantum systems have been the focus of extensive studies with many applications ranging from quantum control to quantum computing.[1–4] To describe the dynamics of the reduced system of interest, a master equation based on second order perturbation theory with respect to the environmental interaction is the conventional approach.[5] However, in some cases the coupling between the reduced system and the environment is quite strong, and the equations based on perturbative dynamics are no longer appropriate. Some nonperturbative work has been done to treat specific strong coupling cases, for example, spin-boson problems,[6] high-Q cavities,[7] and coupled linear systems.[8] The purpose of this paper is to develop a nonperturbative framework to treat general open quantum systems.

The Liouville equation describes the dynamics of an arbitrary quantum system in terms of the density operator $\rho(t)$:

$$i\frac{\partial \rho(t)}{\partial t} = [H(t), \rho(t)], \tag{1}$$

where $H(t)$ is the Hamiltonian, and $[H(t), \rho(t)] \equiv H(t)\rho(t) - \rho(t)H(t)$. Solving Eq. (1) generally is not an easy task for complicated Hamiltonians with added difficulty arising from the commutative structure of the operator equation. A polynomial basis function expansion of the propagator is a common method employed in practice.[9,10] Variational tools provide an attractive means to treat Eq. (1) and they have been applied in various contexts such as laser cooling and quantum control.[11–13] One of the earliest examples was put forward by Balian and Veneroni[14] for evaluating the expectation value of an observable A utilizing the following variational functional:

$$\bar{\mathcal{A}}(t) = \mathrm{Tr}\{A\tilde{\rho}(t)\} - \int_0^t \mathrm{Tr}\left\{\tilde{\Lambda}(\tau)\left(\frac{\partial \tilde{\rho}(\tau)}{\partial \tau} + i[H(\tau), \tilde{\rho}(\tau)]\right)\right\} \mathrm{d}\tau, \tag{2}$$

where $\mathrm{Tr}\{\cdot\}$ denotes the trace operation, and $\tilde{\Lambda}(t) = A$, $\tilde{\rho}(0) = \rho_0$ are imposed conditions. Throughout the paper, operators with the tilde symbol represent trials in a variational functional. With respect to the first order variations $\tilde{\rho}(t) = \rho(t) + \delta\rho(t)$ and $\tilde{\Lambda}(t) = \Lambda(t) + \delta\Lambda(t)$, where both $\rho(t)$ and $\Lambda(t)$ satisfy the Liouville equation in Eq. (1), the expectation value $\bar{\mathcal{A}}(t)$ is stationary up to the first order variations such that $\delta\bar{\mathcal{A}} = 0$.

II. TIME-DEPENDENT OPERATOR VARIATIONAL PRINCIPLE

In open quantum systems, partial trace operations often emerge in considering system dynamics in the presence of an environment. The variational principle of the expectation value of the complete trace of an observable [e.g., $\overline{A}(t)$ in Eq. (2)] is not convenient in the analysis of the reduced system dynamics. Therefore, it is worthwhile to develop a variational principle for the operator itself. For the evolution operator associated with Eq. (1),

$$U(t) = \overrightarrow{\exp}\left(- i \int_0^t H(\tau) \mathrm{d}\tau \right), \tag{3}$$

where the symbol $\rightarrow$ indicates the time ordering operation, the following operator functional,

$$\mathcal{U}(t) = \tilde{U}(t) \left[\mathbf{1} - \int_0^t \tilde{U}^{\dagger}(\tau) \left(\frac{\partial}{\partial \tau} + i\, H(\tau) \right) \tilde{U}(\tau) \mathrm{d}\tau \right] \tag{4}$$

forms a variational principle. In Eq. (4), $\mathbf{1}$ is the unit operator and $\dagger$ denotes the adjoint operation. With respect to the first order variation $\tilde{U}(t) = U(t) + \delta U(t)$, where $U(t)$ is defined in Eq. (3), it can be verified that

$$\delta \mathcal{U}(t) = \delta U(t) - \tilde{U}(t) \int_0^t \tilde{U}^{\dagger}(\tau) \left(\frac{\partial}{\partial \tau} + i\, H(\tau) \right) \delta U(\tau) \mathrm{d}\tau = \delta U(t) - \delta U(t) = 0. \tag{5}$$

Here integration by parts has been applied; it is assumed that the Hamiltonian is Hermitian and the trial evolution operator always satisfies $\tilde{U}(t)\tilde{U}^{\dagger}(t) = \mathbf{1}$. The variational evolution operator in Eq. (4) forms the basis for a number of functionals in the framework of the Schrödinger equation in terms of the wave function and the Liouville equation in terms of the density operator. Below we construct a variational functional for the density operator.

Based on Eq. (1), the density operator $\rho(t)$ can be written as

$$\rho(t) = U(t) \rho(0) U^{\dagger}(t). \tag{6}$$

When $U(t)$ is replaced by its variational form in Eq. (4), Eq. (6) will also become a variational form for the density operator,

$$\varrho(t) = \mathcal{U}(t) \rho(0) \mathcal{U}^{\dagger}(t). \tag{7}$$

Namely, inserting Eq. (4) into Eq. (6), and retaining terms up to second order produces the final variational functional for the density operator as

$$\begin{aligned} \varrho(t) &= \tilde{\rho}(t) - \tilde{U}(t) \int_0^t \tilde{U}^{\dagger}(\tau) \left(\frac{\partial \tilde{\rho}(\tau)}{\partial \tau} + i[H(\tau), \tilde{\rho}(\tau)] \right) \tilde{U}(\tau) \mathrm{d}\tau\, \tilde{U}^{\dagger}(t) \\ &= \tilde{\rho}(t) - \int_0^t \tilde{U}(t,\tau) \left(\frac{\partial \tilde{\rho}(\tau)}{\partial \tau} + i[H(\tau), \tilde{\rho}(\tau)] \right) \tilde{U}(\tau,t) \mathrm{d}\tau, \end{aligned} \tag{8}$$

where $\tilde{U}(t,\tau) \equiv \tilde{U}(t)\tilde{U}^{\dagger}(\tau)$. With respect to the first order variations $\tilde{U}(t) = U(t) + \delta U(t)$ and $\tilde{\rho}(t) = \rho(t) + \delta\rho(t)$ where $U(t)$ is defined in Eq. (3) and $\rho(t)$ satisfies Eq. (1), it can be verified from Eq. (8) that

$$\begin{aligned} \delta\varrho(t) &= \delta\rho(t) - \int_0^t \tilde{U}(t,\tau) \left(\frac{\partial\, \delta\rho(\tau)}{\partial \tau} + i[H(\tau), \delta\rho(\tau)] \right) \tilde{U}(\tau,t) \mathrm{d}\tau \\ &= \delta\rho(t) - \int_0^t \frac{\partial}{\partial \tau} [\tilde{U}(t,\tau)\, \delta\rho(\tau) \tilde{U}(\tau,t)] \mathrm{d}\tau = 0. \end{aligned} \tag{9}$$

The variational functional in Eq. (8) for the density operator itself will straightforwardly lead to

the variational functional in Eq. (2) for an expectation value of an observable. But, the former functional is more basic and is more suitable for partial trace processes.

A feature of the variational density operator $\varrho(t)$ in Eq. (8) is that the trace of $\varrho(t)$ is invariant,

$$\mathrm{Tr}\{\varrho(t)\} = \mathrm{Tr}\left\{\tilde{\rho}(t) - \int_0^t U(t,\tau)\left(\frac{\partial\tilde{\rho}(\tau)}{\partial\tau} + i[H(\tau),\tilde{\rho}(\tau)]\right)U(\tau,t)\mathrm{d}\tau\right\} = \mathrm{Tr}\{\rho(0)\} = 1, \tag{10}$$

regardless of the trial density operator $\tilde{\rho}(t)$ chosen in Eq. (8) as long as it satisfies the initial condition. Unlike the preservation property $\mathrm{Tr}\{\varrho(t)\}=1$ of the variational functional in Eq. (8), the variational evolution operator $\mathcal{U}(t)$ in Eq. (4) usually is not unitary, as a second order term survives

$$\begin{aligned}\mathcal{U}(t)\mathcal{U}^{\dagger}(t) = &\left(\mathbf{1} - \int_0^t \tilde{U}(t,\tau)\left(\frac{\partial\tilde{U}(\tau,t)}{\partial\tau} + iH(\tau)\tilde{U}(\tau,t)\right)\mathrm{d}\tau\right)\\ &\times\left(\mathbf{1} - \int_0^t \left(\frac{\partial\tilde{U}^{\dagger}(\tau,t)}{\partial\tau} - i\tilde{U}^{\dagger}(\tau,t)H(\tau)\right)\tilde{U}(\tau,t)\mathrm{d}\tau\right) = \mathbf{1} + \tilde{W}^2(t),\end{aligned} \tag{11}$$

where $\tilde{W}(t)$ is a Hermitian operator defined by

$$\tilde{W}(t) = \tilde{W}^{\dagger}(t) = \int_0^t \tilde{U}(t,\tau)\left(i\frac{\partial}{\partial\tau} - H(\tau)\right)\tilde{U}(\tau,t)\mathrm{d}\tau. \tag{12}$$

Thus, if necessary, a further step is needed to assure complete unitarity of $\mathcal{U}(t)$. For example, when an eigendecomposition is applied to $\mathcal{U}(t)$, and a renormalization condition on each eigenvalue is imposed (i.e., replacing λ_i by $\lambda_i' = \lambda_i/|\lambda_i|$), then a unitary evolution operator $\mathcal{U}'(t)$ will be obtained. It might be also important to preserve the positivity of the density operator as

$$\langle\psi|\varrho(t)|\psi\rangle \geqslant 0, \tag{13}$$

where ψ is an arbitrary function in the full space. Assuring positivity calls for retaining the second order term when inserting Eq. (4) into Eq. (6). In this case the variational functional for the density operator becomes

$$\begin{aligned}\varrho'(t) = &\left(\mathbf{1} - \int_0^t \tilde{U}(t,\tau)\left(\frac{\partial\tilde{U}(\tau,t)}{\partial\tau} + iH(\tau)\tilde{U}(\tau,t)\right)\mathrm{d}\tau\right)\tilde{U}(t)\rho(0)\tilde{U}^{\dagger}(t)\\ &\times\left(\mathbf{1} - \int_0^t \left(\frac{\partial\tilde{U}^{\dagger}(\tau,t)}{\partial\tau} - i\tilde{U}^{\dagger}(\tau,t)H(\tau)\right)\tilde{U}(\tau,t)\mathrm{d}\tau\right)\\ &= \tilde{\rho}(t) + i[\tilde{W}(t),\tilde{\rho}(t)] + \tilde{W}(t)\tilde{\rho}(t)\tilde{W}(t),\end{aligned} \tag{14}$$

where the operator $\tilde{W}(t)$ is defined in Eq. (12). The positivity of $\varrho'(t)$ can be verified as

$$\langle\psi|\varrho'(t)|\psi\rangle = \langle\psi|(\mathbf{1} + i\tilde{W}(t))\tilde{U}(t)\rho(0)\tilde{U}^{\dagger}(t)(\mathbf{1} - i\tilde{W}(t))|\psi\rangle = \langle\psi'|\rho(0)|\psi'\rangle \geqslant 0, \tag{15}$$

where $\psi' = \tilde{U}^{\dagger}(t)(\mathbf{1} - i\tilde{W}(t))\psi$, and the initial density operator is defined to be positive. However, due to the nonunitary feature of the variational evolution operator $\mathcal{U}(t)$, the variational density operator $\varrho'(t)$ in Eq. (14) generally will not preserve the unit trace property. If both positivity and unit trace invariance are required, then the following variational functional can be employed:

$$\varrho''(t) = \frac{\tilde{\rho}(t) + i[\tilde{W}(t),\tilde{\rho}(t)] + \tilde{W}(t)\tilde{\rho}(t)\tilde{W}(t)}{\mathrm{Tr}\{\tilde{\rho}(t)[\mathbf{1} + \tilde{W}^2(t)]\}}. \tag{16}$$

The above considerations about the unit trace invariance and positivity could be important when the ultimate goal is to evaluate the density operator itself. However, if the variational density operator is only utilized for a partial or full trace with some other operators, a small deviation from unit trace invariance or positivity of the density operator might not be significant for the ultimate goal.

III. DYNAMICS OF AN OPEN QUANTUM SYSTEM

An open quantum system generally refers to one which is of primary interest while being coupled to the environment. The dynamics of the environment is not fully or explicitly treated due to the extreme complexity of describing the dynamical details of the environment. The validity of such a treatment rests on the fact that the environment is assumed to be very large and has many degrees of freedom. Thus, the dynamics of the quantum system of interest can be described by isolated unitary evolution along with a dissipative part resulting from the interaction with the environment. In general, the Hamiltonian for the full system (i.e., the open quantum system plus the environment) can be written as

$$H(t) = H'_S(t) + H_E + H'_I(t), \tag{17}$$

where $H'_S(t)$, H_E, and $H'_I(t)$ describe the system, the environment, and their interaction, respectively. As the environment is assumed to be a large reservoir, its Hamiltonian H_E is treated as time independent. In some quantum control systems, the control field may also explicitly couple with the environment, for example, through an environmental dipole interaction,

$$H'_E(t) = H_E - \vec{\mu}_E \cdot \vec{\varepsilon}(t). \tag{18}$$

When the situation in Eq. (18) occurs, it is convenient to treat the stationary part H_E as the environmental Hamiltonian, while the coupling part is included in the interaction Hamiltonian,

$$H'_I(t,\{\vec{\varepsilon}(t)\}) = H'_I(t) - \vec{\mu}_E \cdot \vec{\varepsilon}(t). \tag{19}$$

Thus the time dependence of the Hamiltonians $H'_S(t)$ and $H'_I(t)$ in Eq. (17) can be viewed as general, including the presence of the control field (as a function of time) in both pieces, which could be important in the treatment of control issues. Throughout the paper, no coupling is assumed between the system and environment at the initial time,

$$\rho(0) = \rho_S(0) \otimes \rho_E, \tag{20}$$

where the initial system density operator $\rho_S(0)$ is considered to be a pure state, and the initial environmental density operator ρ_E is a mixed state. As long as no confusion arises, the tensor product symbol $\otimes$ will be omitted afterwards. The reduced density operator $\rho_S(t)$ associated with the system is defined as the trace of the full density operator over the environmental variables or states,

$$\rho_S(t) = \mathrm{Tr}_E\{\rho(t)\}. \tag{21}$$

Since it is reasonable to treat the environment as being in statistical equilibrium, the environmental density operator may be approximated as time independent. Therefore it is rational to repartition the entire Hamiltonian in Eq. (17) as

$$H(t) = H'_S(t) + \mathrm{Tr}_E\{H'_I(t)\rho_E\} + H_E + H'_I(t) - \mathrm{Tr}_E\{H'_I(t)\rho_E\} = H_S(t) + H_E + H_I(t), \tag{22}$$

where $H_S(t) \equiv H'_S(t) + \mathrm{Tr}_E\{H'_I(t)\rho_E\}$ and $H_I(t) \equiv H'_I(t) - \mathrm{Tr}_E\{H'_I(t)\rho_E\}$. Equation (22) implies that the repartitioned interaction Hamiltonian satisfies

$$\mathrm{Tr}_E\{H_I(t)\rho_E\} = 0. \tag{23}$$

The repartitioned system Hamiltonian is assumed to have the following form:

$$H_S(t) = H_S^0 - \vec{\mu} \cdot \vec{\varepsilon}(t), \tag{24}$$

where H_S^0 represents the field-free system Hamiltonian, $\vec{\mu}$ is the system electric dipole moment vector, and $\vec{\varepsilon}(t)$ is the control electric field vector.

Taking a partial trace over the environmental variables on both sides of Eq. (1) will produce the reduced system dynamical equation

$$i\frac{\partial \rho_S(t)}{\partial t} = \mathrm{Tr}_E\{[H(t),\rho(t)]\} = [H_S(t),\rho_S(t)] + \mathrm{Tr}_E\{[H_I(t),\rho(t)]\}. \tag{25}$$

Equation (25) is an exact expression, but it is not in closed form for the reduced system. Various approximations could be applied to the last term in Eq. (25) to achieve a closed form master equation. The treatment below will start with this equation.

IV. VARIATIONAL FUNCTIONALS FOR AN OPEN QUANTUM SYSTEM

The dynamical equation of the reduced density operator in Eq. (25) contains the full density operator $\rho(t)$. Since in practice obtaining $\rho(t)$ from solving Eq. (1) is not feasible, a variational approach provides an attractive means to deal with this problem. When the variational functional $\varrho(t)$ in Eq. (8) is introduced into Eq. (25), we obtain

$$i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t),\rho_S(t)] + \mathrm{Tr}_E\left\{\left[H_I(t),\tilde{\rho}(t) - \int_0^t \tilde{U}(t,\tau)\left(\frac{\partial \tilde{\rho}(\tau)}{\partial \tau} + i[H(\tau),\tilde{\rho}(\tau)]\right)\tilde{U}(\tau,t)\mathrm{d}\tau\right]\right\}. \tag{26}$$

Besides the differential form for $\rho_S(t)$ in Eq. (26), an integral variational functional form for $\rho_S(t)$ also can be constructed. The system density operator $\rho_S(t)$ in Eq. (25) can be formally solved for as

$$\rho_S(t) = U_S(t)\rho_S(0)U_S^\dagger(t) - i\int_0^t U_S(t,\tau)\mathrm{Tr}_E\{[H_I(\tau),\rho(\tau)]\}U_S(\tau,t)\mathrm{d}\tau, \tag{27}$$

where $U_S(t)$ is the system evolution operator. Then the following variational functional can be introduced to evaluate $\rho_S(t)$:

$$\begin{aligned}
\rho_S(t) &= U_S(t)\rho_S(0)U_S^\dagger(t) - i\int_0^t U_S(t,\tau)\mathrm{Tr}_E\{[H_I(\tau),\tilde{\rho}(\tau)]\}U_S(\tau,t)\mathrm{d}\tau \\
&\quad + \int_0^t \mathrm{Tr}_E\left\{U_S(t,\tau)\left(\frac{\partial \tilde{\rho}(\tau)}{\partial \tau} + i[H(\tau),\tilde{\rho}(\tau)]\right)U_S(\tau,t)\right\}\mathrm{d}\tau \\
&\quad - \int_0^t \mathrm{Tr}_E\left\{\tilde{U}(t,\tau)\left(\frac{\partial \tilde{\rho}(\tau)}{\partial \tau} + i[H(\tau),\tilde{\rho}(\tau)]\right)\tilde{U}(\tau,t)\right\}\mathrm{d}\tau \\
&= U_S(t)\rho_S(0)U_S^\dagger(t) + \int_0^t \mathrm{Tr}_E\left\{U_S(t,\tau)\left(\frac{\partial \tilde{\rho}(\tau)}{\partial \tau} + i[H_S(\tau),\tilde{\rho}(\tau)]\right)U_S(\tau,t)\right\}\mathrm{d}\tau \\
&\quad - \int_0^t \mathrm{Tr}_E\left\{\tilde{U}(t,\tau)\left(\frac{\partial \tilde{\rho}(\tau)}{\partial \tau} + i[H(\tau),\tilde{\rho}(\tau)]\right)\tilde{U}(\tau,t)\right\}\mathrm{d}\tau.
\end{aligned} \tag{28}$$

Equation (28) will reduce to Eq. (27) when the trial density operator is exact. Also we can verify that the first order variation $\delta\rho_S$ vanishes with respect to considering $\tilde{\rho}=\rho+\delta\rho$. As a variational functional, Eq. (28) is suitable for numerical implementation by basis expansion or proper parametrization of the trial inputs which will not be explored further in this paper. Equation (26) is

especially suitable for theoretical analysis, as will be evident in the following sections which derive suitable master equations.

V. PERTURBATIVE MASTER EQUATIONS FROM VARIATIONAL FUNCTIONALS

The conventional master equation readily can be obtained starting from Eq. (25) and applying a perturbation expansion (or a weak coupling assumption).[5] Briefly, from Eq. (1), we have the following exact expression:

$$\rho(t) = U_S(t)\rho_S(0)U_S^\dagger(t)\rho_E - i\int_0^t U_{SE}^\dagger(\tau,t)[H_I(\tau),\rho(\tau)]U_{SE}(\tau,t)\mathrm{d}\tau, \tag{29}$$

where $U_{SE}(\tau,t)\equiv U_S(\tau,t)U_E(\tau,t)$ and U_E is the environmental evolution operator. Applying the perturbation approximation $\rho(\tau)\approx\rho_S(\tau)\rho_E$ on the right-hand side of Eq. (29) leads to

$$\rho(t) = U_S(t)\rho_S(0)U_S^\dagger(t)\rho_E - i\int_0^t U_{SE}^\dagger(\tau,t)[H_I(\tau),\rho_S(\tau)\rho_E]U_{SE}(\tau,t)\mathrm{d}\tau. \tag{30}$$

Inserting Eq. (30) into Eq. (25) yields

$$i\frac{\partial\rho_S(t)}{\partial t} = [H_S(t),\rho_S(t)] - i\int_0^t \mathrm{Tr}_E\{[H_I(t),U_{SE}^\dagger(\tau,t)[H_I(\tau),\rho_S(\tau)\rho_E]U_{SE}(\tau,t)]\}\mathrm{d}\tau. \tag{31}$$

Equation (31) is a premaster equation which finally will lead to the conventional master equation by proper expansion of the interaction Hamiltonian and tracing out the environmental variables. In this paper the pre-master equation will be simply called the master equation without confusion.

For the variational functional involving reduced density operator dynamics in Eq. (26), if the trial evolution operator is exact, then Eq. (26) becomes exact no matter what trial density operator $\tilde{\rho}(t)$ is chosen as long as the initial condition is satisfied. Thus, the following equation,

$$i\frac{\partial\rho_S(t)}{\partial t} = [H_S(t),\rho_S(t)] + \mathrm{Tr}_E\left\{\left[H_I(t),\tilde{\rho}(t) - \int_0^t U^\dagger(\tau,t)\left(\frac{\partial\tilde{\rho}(\tau)}{\partial\tau} + i[H(\tau),\tilde{\rho}(\tau)]\right)U(\tau,t)\mathrm{d}\tau\right]\right\}, \tag{32}$$

exactly holds for any $\tilde{\rho}(t)$ with $\tilde{\rho}(0)=\rho(0)$. Since the full evolution operator appears in Eq. (32), it is suggestive to start with the simpler equation,

$$i\frac{\partial\rho_S(t)}{\partial t} = [H_S(t),\rho_S(t)] + \mathrm{Tr}_E\{[H_I(t),U(t)\rho(0)U^\dagger(t)]\}, \tag{33}$$

which can be obtained by directly inserting Eq. (6) into Eq. (25). However, Eq. (33) is only formally useful. Eventually the full evolution operator needs to be introduced with some suitable approximation. The variational principle in Eq. (32) will result an automatic correction for small deviations on the full evolution operator, while there is no such benefit from using Eq. (33). As an illustration, upon applying the approximation

$$U(\tau,t)\approx U_{SE}(\tau,t), \tag{34}$$

Eq. (33) becomes

$$i\frac{\partial\rho_S(t)}{\partial t} = [H_S(t),\rho_S(t)] \tag{35}$$

whose form is unacceptable, as no decoherence is retained. But under the same approximation, generally decoherence is properly retained using Eq. (32), which will be shown below.

As a first example, consider the trial full density operator of the form $\tilde{\rho}(\tau) = U_S(\tau)\rho_S(0)U_S^\dagger(\tau)\rho_E$ (where $\tau \in [0,t]$). Then Eq. (32) becomes

$$i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t),\rho_S(t)] - i\int_0^t \mathrm{Tr}_E\{[H_I(t),U^\dagger(\tau,t)[H_I(\tau),U_S(\tau)\rho_S(0)U_S^\dagger(\tau)\rho_E]U(\tau,t)]\}\mathrm{d}\tau. \tag{36}$$

Equation (36) is exact and can be used as a basis for further approximation to solve for $\rho_S(t)$. However, it is often more useful to have a "homogeneous" differential equation for $\rho_S(t)$ without explicitly involving its initial condition $\rho_S(0)$. This can be done by replacing $\rho_S(0)$ as a functional of $\rho_S(t)$ as follows.

Inserting the same trial density operator $\tilde{\rho}(\tau) = U_S(\tau)\rho_S(0)U_S^\dagger(\tau)\rho_E$ into Eq. (28) will yield another exact formula:

$$U_S(\tau)\rho_S(0)U_S^\dagger(\tau) = \rho_S(\tau) + i\int_0^\tau \mathrm{Tr}_E\{U^\dagger(\tau',\tau)[H_I(\tau'),U_S(\tau')\rho_S(0)U_S^\dagger(\tau')\rho_E]U(\tau',\tau)\}\mathrm{d}\tau'. \tag{37}$$

Recursively inserting Eq. (37) into Eq. (36) will generate a hierarchical series,

$$\begin{aligned} i\frac{\partial \rho_S(t)}{\partial t} = {} & [H_S(t),\rho_S(t)] - i\int_0^t \mathrm{Tr}_E\{[H_I(t),U^\dagger(\tau,t)[H_I(\tau),\rho_S(\tau)\rho_E]U(\tau,t)]\}d\tau \\ & + \int_0^t\int_0^\tau \mathrm{Tr}_E\{[H_I(t),U^\dagger(\tau,t)[H_I(\tau),\mathrm{Tr}_E\{U^\dagger(\tau',\tau) \\ & \times[H_I(\tau'),\rho_S(\tau')\rho_E]U(\tau',\tau)\}\rho_E]U(\tau,t)]\}\mathrm{d}\tau'\mathrm{d}\tau + \cdots. \end{aligned} \tag{38}$$

This series will converge under the weak coupling assumption [i.e., the norm of $H_I(t)$ is sufficiently small]. If only the leading term of the hierarchical series is kept, Eq. (38) will be

$$i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t),\rho_S(t)] - i\int_0^t \mathrm{Tr}_E\{[H_I(t),U^\dagger(\tau,t)[H_I(\tau),\rho_S(\tau)\rho_E]U(\tau,t)]\}\mathrm{d}\tau. \tag{39}$$

Equation (39) is similar, but not identical, to the well-known perturbation result in Eq. (31). Equation (31) can be obtained from Eq. (39) by using the approximation in Eq. (34). Equation (39) is more flexible than Eq. (31), as the full evolution operator can be approximated in various ways other than Eq. (34), even by basis set expansion via a variational procedure.

Like the conventional non-Markovian master equation in Eq. (31), Equation (39) is also an integro-differential equation for $\rho_S(t)$. It is worthwhile to search for a perturbative master equation for $\rho_S(t)$ only involving a differential form. With this goal in mind, Eq. (37) also can be written as

$$\rho_S(0) = U_S^\dagger(t)\rho_S(t)U_S(t) + i\int_0^t \mathrm{Tr}_E\{U_S^\dagger(t)U^\dagger(\tau,t)[H_I(\tau),U_S(\tau)\rho_S(0)U_S^\dagger(\tau)\rho_E]U(\tau,t)U_S(t)\}\mathrm{d}\tau. \tag{40}$$

Recursively inserting Eq. (40) into Eq. (36) will generate the hierarchical series,

$$i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t), \rho_S(t)] - i\int_0^t \mathrm{Tr}_E\{[H_I(t), U^\dagger(\tau,t)[H_I(\tau), U_S(\tau,t)\rho_S(t)U_S^\dagger(\tau,t)\rho_E]U(\tau,t)]\}\mathrm{d}\tau$$
$$+ \int_0^t \int_0^t \mathrm{Tr}_E\{[H_I(t), U^\dagger(\tau,t)[H_I(\tau), \mathrm{Tr}_E\{U_S(\tau,t)U^\dagger(\tau',t)$$
$$\times [H_I(\tau'), U_S(\tau',t)\rho_S(t)U_S^\dagger(\tau',t)\rho_E]U(\tau',t)U_S^\dagger(\tau',t)\}\rho_E]U(\tau,t)]\}\mathrm{d}\tau'\mathrm{d}\tau + \cdots. \quad (41)$$

The leading term in Eq. (41) is

$$i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t), \rho_S(t)] - i\int_0^t \mathrm{Tr}_E\{[H_I(t), U^\dagger(\tau,t)[H_I(\tau), U_S(\tau,t)\rho_S(t)U_S^\dagger(\tau,t)\rho_E]U(\tau,t)]\}\mathrm{d}\tau. \quad (42)$$

The structure of Eq. (42) is distinct from that of the conventional result in Eq. (31), as the former one only involves the differential form of $\rho_S(t)$ and no longer has time integration over the system density operator. Equation (42) can be further expanded into

$$i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t), \rho_S(t)] - i\int_0^t (\mathrm{Tr}_E\{H_I(t)U^\dagger(\tau,t)H_I(\tau)U_S(\tau,t)\rho_E\rho_S(t)U_S^\dagger(\tau,t)U(\tau,t)\}$$
$$+ \mathrm{Tr}_E\{U^\dagger(\tau,t)U_S(\tau,t)\rho_S(t)\rho_E U_S^\dagger(\tau,t)H_I(\tau)U(\tau,t)H_I(t)\}$$
$$- \mathrm{Tr}_E\{H_I(t)U^\dagger(\tau,t)U_S(\tau,t)\rho_S(t)\rho_E U_S^\dagger(\tau,t)H_I(\tau)U(\tau,t)\}$$
$$- \mathrm{Tr}_E\{U^\dagger(\tau,t)H_I(\tau)U_S(\tau,t)\rho_E\rho_S(t)U_S^\dagger(\tau,t)U(\tau,t)H_I(t)\})\mathrm{d}\tau. \quad (43)$$

Equation (43) has the following form of a general master equation:

$$i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t), \rho_S(t)] - \int_0^t \sum_{jk} (A_{jk}(\tau,t)\rho_S(t)B_{jk}^\dagger(\tau,t) - B_{jk}(\tau,t)\rho_S(t)A_{jk}^\dagger(\tau,t) + C_{jk}(\tau,t)\rho_S(t)D_{jk}^\dagger(\tau,t)$$
$$- D_{jk}(\tau,t)\rho_S(t)C_{jk}^\dagger(\tau,t))\mathrm{d}\tau. \quad (44)$$

The operators $A_{jk}, B_{jk}, C_{jk}, D_{jk}$ in Eq. (44) are defined as follows:

$$A_{jk}(\tau,t) = i\sqrt{w_k}\,\langle\phi_j|H_I(t)U^\dagger(\tau,t)H_I(\tau)|\Phi_k\rangle U_S(\tau,t), \quad (45)$$

$$B_{jk}(\tau,t) = \sqrt{w_k}\,\langle\phi_j|U^\dagger(\tau,t)|\Phi_k\rangle U_S(\tau,t), \quad (46)$$

$$C_{jk}(\tau,t) = \sqrt{w_k}\,\langle\phi_j|H_I(t)U^\dagger(\tau,t)|\Phi_k\rangle U_S(\tau,t), \quad (47)$$

$$D_{jk}(\tau,t) = i\sqrt{w_k}\,\langle\phi_j|U^\dagger(\tau,t)H_I(\tau)|\Phi_k\rangle U_S(\tau,t), \quad (48)$$

where $\{\phi_j\}$ is the basis of the environment space, and a general initial environmental density operator,

$$\rho_E = \sum_k w_k|\Phi_k\rangle\langle\Phi_k|, \quad (49)$$

is applied. It can be verified that an identity exists among the operators $A_{jk}, B_{jk}, C_{jk}, D_{jk}$ in Eq. (44),

$$\sum_j B_{jk}^\dagger(\tau,t)A_{jk}(\tau,t) = \sum_j C_{jk}^\dagger(\tau,t)D_{jk}(\tau,t). \quad (50)$$

If necessary, the time integration in Eq. (44) can be removed by expanding the operators $A_{jk}, B_{jk}, C_{jk}, D_{jk}$ in shifted Legendre polynomial[15] $\{P_\ell(\tau/t), \tau/t \in [0,1]\}$, and utilizing the orthogonality relationship

$$\int_0^1 P_\ell(\tau/t) P_{\ell'}(\tau/t) \mathrm{d}\tau/t = \frac{1}{2\ell+1} \delta_{\ell\ell'}. \tag{51}$$

As an illustration, the operator A_{jk} can be expanded into

$$A_{jk}(\tau,t) = \sum_{\ell=0}^{\infty} \left(\frac{2\ell+1}{t}\right)^{1/2} A'_{jk\ell}(t) P_\ell(\tau/t), \tag{52}$$

where the operator $A'_{jk\ell}(t)$ is determined by

$$A'_{jk\ell}(t) = \sqrt{(2\ell+1)t} \int_0^1 A_{jk}(\tau,t) P_\ell(\tau/t) \mathrm{d}\tau/t \tag{53}$$

for all $t \neq 0$, and for $t=0$ it is simply that $A'_{jk\ell}(0)=0$. For the other operators B_{jk}, C_{jk}, D_{jk}, similar expansions can be produced. Thus, Eq. (44) can be expressed as

$$\begin{aligned} i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t), \rho_S(t)] - \sum_{jk\ell} (&A'_{jk\ell}(t)\rho_S(t)B'^{\dagger}_{jk\ell}(t) - B'_{jk\ell}(t)\rho_S(t)A'^{\dagger}_{jk\ell}(t) + C'_{jk\ell}(t)\rho_S(t)D'^{\dagger}_{jk\ell}(t) \\ &- D'_{jk\ell}(t)\rho_S(t)C'^{\dagger}_{jk\ell}(t)), \end{aligned} \tag{54}$$

where the operators $B'_{jk\ell}(t), C'_{jk\ell}(t), D'_{jk\ell}(t)$ are defined similarly to $A'_{jk\ell}(t)$ in Eq. (53).

Equation (44) is fully general, yet somewhat complex to deal with. Below a further simplified version is presented. From the relation

$$i\frac{\partial}{\partial \tau}(U^\dagger(\tau,t)U_S(\tau,t)\rho_S(t)U_S^\dagger(\tau,t)U(\tau,t)) = [-U^\dagger(\tau,t)H_I(\tau)U(\tau,t), U^\dagger(\tau,t)U_S(\tau,t)\rho_S(t)U_S^\dagger(\tau,t)U(\tau,t)] \tag{55}$$

we have the formal solution

$$\begin{aligned} U^\dagger(\tau,t)U_S(\tau,t)\rho_S(t)U_S^\dagger(\tau,t)U(\tau,t) &= \overrightarrow{\exp}\left(i\int_t^\tau U^\dagger(t',t)H_I(t')U(t',t)\mathrm{d}t'\right)\rho_S(t) \\ &\quad \times \overrightarrow{\exp}\left(-i\int_t^\tau U^\dagger(t',t)H_I(t')U(t',t)\mathrm{d}t'\right) \\ &= \rho_S(t) + i\left[\int_t^\tau U^\dagger(t',t)H_I(t')U(t',t)\mathrm{d}t', \rho_S(t)\right] + \cdots, \end{aligned} \tag{56}$$

where the generalized Baker-Hausdorff formula[16] is applied to produce the expansion in the last step. Inserting Eq. (56) into Eq. (43) and taking the leading term yields

$$i\frac{\partial\rho_S(t)}{\partial t}=[H_S(t),\rho_S(t)]-i\Bigg(\mathrm{Tr}_E\Bigg\{H_I(t)\int_0^t U^\dagger(\tau,t)H_I(\tau)\rho_E U(\tau,t)\mathrm{d}\tau\Bigg\}\rho_S(t)$$
$$+\rho_S(t)\ \mathrm{Tr}_E\Bigg\{\int_0^t U^\dagger(\tau,t)\rho_E H_I(\tau)U(\tau,t)\mathrm{d}\tau\, H_I(t)\Bigg\}$$
$$-\mathrm{Tr}_E\Bigg\{H_I(t)\rho_S(t)\int_0^t U^\dagger(\tau,t)\rho_E H_I(\tau)U(\tau,t)\mathrm{d}\tau\Bigg\}$$
$$-\mathrm{Tr}_E\Bigg\{\int_0^t U^\dagger(\tau,t)H_I(\tau)\rho_E U(\tau,t)\mathrm{d}\tau\,\rho_S(t)H_I(t)\Bigg\}\Bigg). \tag{57}$$

Similar to Eq. (8), we have

$$U^\dagger(\tau,t)\rho_E U(\tau,t)=\rho_E-i\int_\tau^t U^\dagger(t',t)[H_I(t'),\rho_E]U(t',t)\mathrm{d}t'. \tag{58}$$

Inserting Eq. (58) into Eq. (57) and taking the leading term produces

$$i\frac{\partial\rho_S(t)}{\partial t}=[H_S(t),\rho_S(t)]-i\Bigg(\mathrm{Tr}_E\Bigg\{H_I(t)\int_0^t U^\dagger(\tau,t)H_I(\tau)U(\tau,t)\mathrm{d}\tau\,\rho_E\Bigg\}\rho_S(t)$$
$$+\rho_S(t)\ \mathrm{Tr}_E\Bigg\{\rho_E\int_0^t U^\dagger(\tau,t)H_I(\tau)U(\tau,t)\mathrm{d}\tau\, H_I(t)\Bigg\}$$
$$-\mathrm{Tr}_E\Bigg\{H_I(t)\rho_S(t)\rho_E\int_0^t U^\dagger(\tau,t)H_I(\tau)U(\tau,t)\mathrm{d}\tau\Bigg\}$$
$$-\mathrm{Tr}_E\Bigg\{\int_0^t U^\dagger(\tau,t)H_I(\tau)U(\tau,t)\mathrm{d}\tau\,\rho_E\rho_S(t)H_I(t)\Bigg\}\Bigg). \tag{59}$$

Defining

$$\overline{H_I}(t)=\int_0^t U^\dagger(\tau,t)H_I(\tau)U(\tau,t)\mathrm{d}\tau, \tag{60}$$

Eq. (59) can be simplified into the master equation

$$i\frac{\partial\rho_S(t)}{\partial t}=[H_S(t),\rho_S(t)]-i\{\mathrm{Tr}_E(H_I(t)\overline{H_I}(t)\rho_E)\rho_S(t)+\rho_S(t)\ \mathrm{Tr}_E(\rho_E\overline{H_I}(t)H_I(t))$$
$$-\mathrm{Tr}_E(H_I(t)\rho_S(t)\rho_E\overline{H_I}(t))-\mathrm{Tr}_E(\overline{H_I}(t)\rho_E\rho_S(t)H_I(t))\}. \tag{61}$$

Equation (61) has a similar but not identical structure as the Lindblad equation,[17]

$$i\frac{\partial\rho_S(t)}{\partial t}=[H_S(t),\rho_S(t)]-i\sum_{\{n\}}\left(\frac{1}{2}\mathcal{L}_{\{n\}}^\dagger\mathcal{L}_{\{n\}}\rho_S(t)+\frac{1}{2}\rho_S(t)\mathcal{L}_{\{n\}}^\dagger\mathcal{L}_{\{n\}}-\mathcal{L}_{\{n\}}\rho_S(t)\mathcal{L}_{\{n\}}^\dagger\right). \tag{62}$$

In fact, the Lindblad version of Eq. (61) can be derived by further approximation. A simple way to reveal the connection between Eqs. (61) and (62) is evident at small time or for the interaction Hamiltonian having a slowly varying profile. Then Eq. (60) can be expressed as

$$\overline{H_I}(t) = \int_0^t U^\dagger(\tau,t)H_I(\tau)U(\tau,t)\mathrm{d}\tau = \int_0^t \left(H_I(\tau) + i\left[\int_t^\tau H(t')\mathrm{d}t', H_I(\tau) \right] + \cdots \right)\mathrm{d}\tau \approx \alpha(t)H_I(t), \tag{63}$$

where $\alpha(t)$ is an appropriate function of time. Inserting Eq. (63) into Eq. (61) will result in

$$i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t),\rho_S(t)] - i\alpha^2(t)\{\mathrm{Tr}_E(H_I^2(t)\rho_E)\rho_S(t) + \rho_S(t)\ \mathrm{Tr}_E(\rho_E H_I^2(t)) - 2\ \mathrm{Tr}_E(H_I(t)\rho_S(t)\rho_E H_I(t))\}. \tag{64}$$

By comparing Eq. (64) to the standard Lindblad equation in Eq. (62) the equivalent Lindblad operator in Eq. (64) can be identified as

$$L_{jk} = \alpha(t)\sqrt{2w_k}\langle\phi_j|H_I(t)|\Phi_k\rangle, \tag{65}$$

where w_k, ϕ_j, and Φ_k are defined before in Eqs. (45)–(49).

Unlike the Lindblad operator in Eq. (62) which usually can only be assigned phenomenologically, Eq. (61) fully specifies each operator involved, which provides the means to map out a deeper relationship between the action of a control field and the system decoherence. In particular, the linear entropy measure of decoherence[18]

$$S_L(t) = 1 - \mathrm{Tr}_S\{\rho_S^2(t)\} \tag{66}$$

can be evaluated through Eq. (61) as

$$S_L(t) = 2\int_0^t \mathrm{Tr}\{(\rho_S^2(\tau)H_I(\tau)\overline{H_I}(\tau) + \rho_S^2(\tau)\overline{H_I}(\tau)H_I(\tau) - \rho_S(\tau)\overline{H_I}(\tau)\rho_S(\tau)H_I(\tau) - \rho_S(\tau)H_I(\tau)\rho_S(\tau)\overline{H_I}(\tau))\rho_E\}, \tag{67}$$

where both $\rho_S(\tau)$ and $\overline{H_I}(\tau)$ depend on the control field. In contrast, the similar formula through the Lindblad equation is

$$S_L(t) = 2\int_0^t \mathrm{Tr}_S\left\{ \sum_k (\rho_S^2(\tau)\mathcal{L}_k^\dagger\mathcal{L}_k - \rho_S(\tau)\mathcal{L}_k\rho_S(\tau)\mathcal{L}_k^\dagger) \right\}, \tag{68}$$

in which only $\rho_S(\tau)$ shows an explicit dependence on the control field.

VI. A VARIATIONALLY BASED NONPERTURBATIVE MASTER EQUATION

The master equation in Eq. (42) arises from the leading term in a hierarchical perturbation expansion. Its validity is based on the assumption of a weak coupling approximation in terms of H_I. If the coupling is sufficiently strong, the hierarchical series expansion in Eq. (41) may not converge. If the coupling is relatively weak but acting for a sufficiently long time, then truncation of the expansion in Eq. (41) to low order can produce significant discrepancies in the decoherent aspects of the system dynamics. In the case of a convergent hierarchical expansion, including higher order terms in Eq. (41) in principle will produce better results, but the complex nature of the higher order terms will prevent any practical implementation. Therefore, a perturbation expansion is likely not the best foundation for developing an ultimate master equation that is valid for all time. In the following material, a nonperturbative formulation of decoherent dynamics will be explored.

Consider once again Eq. (32) as a variational formulation involving the full density operator. In order to derive a nonperturbative master equation, a trial for the full density operator has to be introduced in a nonperturbative fashion. There are many possible choices, and a convenient one is

$$\tilde{\rho}(\tau) = U_S(\tau,t)\rho_S(t)U_S^{\dagger}(\tau,t)\rho_E(1-e^{-c\tau}) + \rho_S(\tau)\rho_E e^{-c\tau}, \tag{69}$$

where $\tau \in [0,t]$, and c is a large positive constant. It is evident that $\tilde{\rho}(\tau)$ in Eq. (69) satisfies the initial condition as $\tilde{\rho}(0)=\rho_S(0)\rho_E$. Inserting Eq. (69) into Eq. (32) will yield

$$\begin{aligned} i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t),\rho_S(t)] - \int_0^t \mathrm{Tr}_E\{[H_I(t),U^{\dagger}(\tau,t)(i[H_I(\tau),\underbrace{U_S(\tau,t)\rho_S(t)U_S^{\dagger}(\tau,t)\rho_E(1-e^{-c\tau})}_{\text{(i)}} \\ + \underbrace{\rho_S(\tau)\rho_E e^{-c\tau}}_{\text{(ii)}}] + \underbrace{U_S(\tau,t)\rho_S(t)U_S^{\dagger}(\tau,t)\rho_E c e^{-c\tau} - \rho_S(\tau)\rho_E c e^{-c\tau}}_{\text{(iii)}} \\ \underbrace{- i\,\mathrm{Tr}_E\{[H_I(\tau),\rho(\tau)]\}\rho_E e^{-c\tau}}_{\text{(iv)}})U(\tau,t)]\}\mathrm{d}\tau. \end{aligned} \tag{70}$$

In Eq. (70), the term (i) will have its major contribution at longer times, while the terms (ii) and (iii) will dominate at short times. But, the contribution of the term (iv) can be neglected for all the time. The reason is that at longer times, the exponential $e^{-c\tau}$ quickly decreases toward zero, while at short times, the full density operator can be well approximated as a tensor product of the uncoupling system and environmental density operators, and $\mathrm{Tr}_E\{[H_I(\tau),\rho_S(\tau)\rho_E]\}=0$. Thus, the dynamical equation reduces to

$$\begin{aligned} i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t),\rho_S(t)] - \int_0^t \mathrm{Tr}_E\{[H_I(t),U^{\dagger}(\tau,t)(i[H_I(\tau),U_S(\tau,t)\rho_S(t)U_S^{\dagger}(\tau,t)\rho_E(1-e^{-c\tau}) \\ + \rho_S(\tau)\rho_E e^{-c\tau}] + U_S(\tau,t)\rho_S(t)U_S^{\dagger}(\tau,t)\rho_E c e^{-c\tau} - \rho_S(\tau)\rho_E c e^{-c\tau})U(\tau,t)]\}\mathrm{d}\tau. \end{aligned} \tag{71}$$

Equation (71) can be expanded into

$$\begin{aligned} i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t),\rho_S(t)] - i\int_0^t (\mathrm{Tr}_E\{H_I(t)U^{\dagger}(\tau,t)H_I(\tau)U_S(\tau,t)\rho_E\rho_S(t)U_S^{\dagger}(\tau,t)U(\tau,t) \\ + U^{\dagger}(\tau,t)U_S(\tau,t)\rho_S(t)\rho_E U_S^{\dagger}(\tau,t)H_I(\tau)U(\tau,t)H_I(t) \\ - H_I(t)U^{\dagger}(\tau,t)U_S(\tau,t)\rho_S(t)\rho_E U_S^{\dagger}(\tau,t)H_I(\tau)U(\tau,t) \\ - U^{\dagger}(\tau,t)H_I(\tau)U_S(\tau,t)\rho_E\rho_S(t)U_S^{\dagger}(\tau,t)U(\tau,t)H_I(t)\})(1-e^{-c\tau})\mathrm{d}\tau \\ - i\int_0^t (\mathrm{Tr}_E\{H_I(t)U^{\dagger}(\tau,t)H_I(\tau)\rho_E\rho_S(\tau)U(\tau,t) + U^{\dagger}(\tau,t)\rho_S(\tau)\rho_E H_I(\tau)U(\tau,t)H_I(t) \\ - H_I(t)U^{\dagger}(\tau,t)\rho_S(\tau)\rho_E H_I(\tau)U(\tau,t) - U^{\dagger}(\tau,t)H_I(\tau)\rho_E\rho_S(\tau)U(\tau,t)H_I(t)\})e^{-c\tau}\,\mathrm{d}\tau \\ - \int_0^t (\mathrm{Tr}_E\{H_I(t)U^{\dagger}(\tau,t)U_S(\tau,t)\rho_S(t)\rho_E U_S^{\dagger}(\tau,t)U(\tau,t) \\ - U^{\dagger}(\tau,t)U_S(\tau,t)\rho_S(t)\rho_E U_S^{\dagger}(\tau,t)U(\tau,t)H_I(t)\})ce^{-c\tau}\,\mathrm{d}\tau \\ + \int_0^t (\mathrm{Tr}_E\{H_I(t)U^{\dagger}(\tau,t)\rho_S(\tau)\rho_E U(\tau,t) - U^{\dagger}(\tau,t)\rho_S(\tau)\rho_E U(\tau,t)H_I(t)\})ce^{-c\tau}\,\mathrm{d}\tau. \end{aligned} \tag{72}$$

Evaluating the trace over the environmental variables, Eq. (72) can be written as

$$
\begin{aligned}
i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t),\rho_S(t)] - \int_0^t \sum_{jk} \{&(A_{jk}(\tau,t)\rho_S(t)B_{jk}^\dagger(\tau,t) - B_{jk}(\tau,t)\rho_S(t)A_{jk}^\dagger(\tau,t) + C_{jk}(\tau,t)\rho_S(t)D_{jk}^\dagger(\tau,t)\\
&- D_{jk}(\tau,t)\rho_S(t)C_{jk}^\dagger(\tau,t))(1-e^{-c\tau}) + (A_{jk}(\tau,t)U_S^\dagger(\tau,t)\rho_S(\tau)U_S(\tau,t)B_{jk}^\dagger(\tau,t)\\
&- B_{jk}(\tau,t)U_S^\dagger(\tau,t)\rho_S(\tau)U_S(\tau,t)A_{jk}^\dagger(\tau,t) + C_{jk}(\tau,t)U_S^\dagger(\tau,t)\rho_S(\tau)U_S(\tau,t)D_{jk}^\dagger(\tau,t)\\
&- D_{jk}(\tau,t)U_S^\dagger(\tau,t)\rho_S(\tau)U_S(\tau,t)C_{jk}^\dagger(\tau,t))e^{-c\tau} + (B_{jk}(\tau,t)U_S^\dagger(\tau,t)\rho_S(\tau)U_S(\tau,t)C_{jk}^\dagger(\tau,t)\\
&- C_{jk}(\tau,t)U_S^\dagger(\tau,t)\rho_S(\tau)U_S(\tau,t)B_{jk}^\dagger(\tau,t))ce^{-c\tau} + (C_{jk}(\tau,t)\rho_S(t)B_{jk}^\dagger(\tau,t)\\
&- B_{jk}(\tau,t)\rho_S(t)C_{jk}^\dagger(\tau,t))ce^{-c\tau}\}\mathrm{d}\tau. \qquad (73)
\end{aligned}
$$

The operators $A_{jk},B_{jk},C_{jk},D_{jk}$ in Eq. (73) are defined in Eqs. (45)–(48). Compared to the perturbative counterpart in Eq. (44), the general nonperturbative master equation in Eq. (73) is valid for all time. If the time t is small, or if the system is in the weak coupling regime, then all terms associated with the exponential $e^{-c\tau}$ will cancel each other under the perturbation approximation of

$$\rho_S(t) \approx U_S^\dagger(\tau,t)\rho_S(\tau)U_S(\tau,t), \qquad (74)$$

and Eq. (73) will become identical to the nonperturbative version in Eq. (44). If the time t is quite large, usually the perturbation approximation in Eq. (74) is not satisfied so that Eq. (73) will be different from Eq. (44).

It should be pointed out that the trial full density operator in Eq. (69) is just one choice, and therefore the nonperturbative formulation in Eq. (73) is not unique. There is much freedom to choose $\tilde{\rho}(t)$, and another simple form is

$$\tilde{\rho}(\tau) = \rho_S(\tau)\rho_E e^{-c\tau}. \qquad (75)$$

Following a procedure similar to that above, with this choice the resultant non-perturbative master equation is

$$
\begin{aligned}
i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t),\rho_S(t)] - i\int_0^t \mathrm{Tr}_E\{[H_I(t),U^\dagger(\tau,t)[H_I(\tau),\rho_S(\tau)\rho_E]U(\tau,t)]\}e^{-c\tau}\,\mathrm{d}\tau\\
+ \int_0^t \mathrm{Tr}_E\{[H_I(t),U^\dagger(\tau,t)\rho_S(\tau)\rho_E U(\tau,t)]\}ce^{-c\tau}\,d\tau. \qquad (76)
\end{aligned}
$$

Each variationally derived nonperturbative equation has second order error, but a different choice of trial density operator in practice will produce distinct levels of error. For example, in practice the implementation of Eq. (76) likely will be less favorable than Eq. (71), since the trial density operator in Eq. (75) will have significant deviations from the exact one at longer times. In contrast, the trial density operator in Eq. (69) is more likely to remain in the vicinity of the true density operator thereby improving the reliability of the variational estimate for ρ_S coming from Eq. (71). A suitable approximation is necessary for evaluating the operators $A_{jk},B_{jk},C_{jk},D_{jk}$ to solve the master equation, and additional approximation can be employed to simplify the time integration in Eqs. (73) based on the rapidly decaying factor $e^{-c\tau}$. Further implementation details will not be explored here.

VII. MODEL ANALYSIS

The purpose of developing nonperturbative master equations is for better treatment of problems with strong system-environment coupling. In such cases, the resultant system dynamics using the perturbative approach may produce significant distortion. To obtain proper physical conclusions, the nonperturbative approach is necessary. This point will be evident from a model analysis below.

The model system is defined to initially be in a pure state,

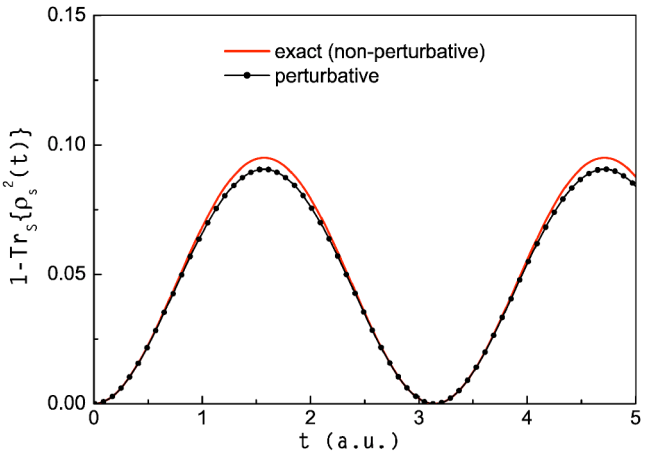

FIG. 1. Comparison of the decoherence degrees from perturbative and nonperturbative approaches. It is a weak coupling case such that $w_0+w_1=0.05$ where w_0, w_1 are defined in Eq. (78).

$$\rho_S(0) = |\psi_0\rangle\langle\psi_0|, \tag{77}$$

where ψ_0 is the ground eigenstate of the system. The environment is in a mixed state as

$$\rho_E = \sum_k w_k |\Phi_k\rangle\langle\Phi_k|, \tag{78}$$

where $\{\Phi_k\}$ is a set of orthonormal states (not necessary being the environment eigenstates), and the unit trace of ρ_E implies that $\Sigma_k\, w_k=1$. The system Hamiltonian $H_S'(t)$ and the environmental Hamiltonian H_E are treated implicitly. The coupling Hamiltonian $H_I'(t)$ is modeled as

$$H_I'(t) = i(|\psi_1\rangle\langle\psi_0| - |\psi_0\rangle\langle\psi_1|) \otimes (|\Phi_1\rangle\langle\Phi_0| + |\Phi_0\rangle\langle\Phi_1|) - H_S(t) \otimes \mathbf{1}_E - \mathbf{1}_S \otimes H_E, \tag{79}$$

where $\mathbf{1}_S$ and $\mathbf{1}_E$ are the unit operators of the system and environment spaces, respectively. The coupling Hamiltonian in Eq. (79) indicates that the total Hamiltonian would be

$$H = i(|\psi_1\rangle\langle\psi_0| - |\psi_0\rangle\langle\psi_1|) \otimes (|\Phi_1\rangle\langle\Phi_0| + |\Phi_0\rangle\langle\Phi_1|), \tag{80}$$

which might be considered as two coupled spin or multilevel systems. The model system shown here is for the purpose demonstrating the failure of the perturbative master equations when dealing with cases of strong system-environment coupling. No control field is present in the Hamiltonians.

Before implementing the dynamical equation, we first perform the repartitioning of the system and coupling Hamiltonians following the procedure described in Sec. III. The repartitioned Hamiltonians become

$$H_I(t) = H_I'(t) - \mathrm{Tr}_E\{H_I'(t)\rho_E\}, \tag{81}$$

$$H_S(t) = H_S'(t) + \mathrm{Tr}_E\{H_I'(t)\rho_E\}. \tag{82}$$

In order to obtain the nonperturbative results, we can evaluate the operators $A_{jk}, B_{jk}, C_{jk}, D_{jk}$ in Eq. (73) by their definitions in Eqs. (45)–(48), and numerically solve the nonperturbative master equation in Eq. (73); this would be a very tedious task. For this model, an alternative can be employed. Since the nonperturbative master equation in Eq. (73) is very close to the exact dynamical equation, the exact solution can represent the nonperturbative result very well. From the exact dynamical equation in Eq. (25), the system density operator can be obtained as

$$\rho_S(t) = |\psi_0\rangle\langle\psi_0| + (|\psi_1\rangle\langle\psi_1| - |\psi_0\rangle\langle\psi_0|)(w_0 + w_1)\sin^2 t. \tag{83}$$

The linear entropy measure of decoherence then becomes

$$1 - \mathrm{Tr}_S\{\rho_S^2(t)\} = 2(w_0 + w_1)\sin^2 t - 2(w_0 + w_1)^2 \sin^4 t. \tag{84}$$

For comparison, a perturbative approach will be analyzed. All the aforementioned perturbative master equations in Eqs. (31), (39), and (44) are truncated to second order in terms of the coupling Hamiltonian. We pick Eq. (44) as it is a natural perturbative version of the nonperturbative master equation in Eq. (73). Once again, we can go back to Eqs. (45)–(48) and map out the operators $A_{jk}, B_{jk}, C_{jk}, D_{jk}$ explicitly. Then the perturbative master equation in Eq. (44) can be solved numerically. Fortunately, for this model, numerical implementation is not necessary since Eq. (44) has an analytic solution for the density operator $\rho_S(t)$.

As an equivalence to Eq. (44), Eq. (42) can be further rewritten,

$$i\frac{\partial \rho_S(t)}{\partial t} = [H_S(t), \rho_S(t)] + \mathrm{Tr}_E\{[H_I(t), U(t)U_S^\dagger(t)\rho_S(t)U_S(t)\rho_E U^\dagger(t)]\}, \tag{85}$$

as long as the assumption of a near equilibrium environment is valid such that $[H_E, \rho_E]=0$. Specifically for the current model, Eq. (85) reduces to

$$i\frac{\partial \rho_S(t)}{\partial t} = \mathrm{Tr}_E\{[H_I(t), U(t)\rho_S(t)\rho_E U^\dagger(t)]\}. \tag{86}$$

Comparing to the exact dynamics equation for this model,

$$i\frac{\partial \rho_S(t)}{\partial t} = \mathrm{Tr}_E\{[H_I(t), U(t)\rho_S(0)\rho_E U^\dagger(t)]\}, \tag{87}$$

we can solve for the analytic perturbative system density operator [denoted as $\overline{\rho_s}(t)$ afterwards to distinguish from the exact one] from Eq. (86) as

$$\overline{\rho_S}(t) = |\psi_0\rangle\langle\psi_0| + (|\psi_1\rangle\langle\psi_1| - |\psi_0\rangle\langle\psi_0|)\tfrac{1}{2}(1 - \exp[-2(w_0 + w_1)\sin^2 t]). \tag{88}$$

The corresponding linear entropy measure of decoherence then becomes

$$1 - \mathrm{Tr}_S\{\overline{\rho}_S^2(t)\} = 1 - \exp[-2(w_0 + w_1)\sin^2 t] + \frac{1}{2}(1 - \exp[-2(w_0 + w_1)\sin^2 t])^2. \tag{89}$$

For comparison of the perturbative and nonperturbative results, the decoherences in Eqs. (84) and (89) give a simple and clear picture. Figure 1 displays the results for a weak coupling case, $w_0+w_1=0.05$. The perturbative decoherence degree follows the nonperturbative result quite well. Figure 2 shows the results for a strong coupling case, $w_0+w_1=0.95$. Overall, in the latter case the perturbative decoherence is very different from the nonperturbative result. Thus, the illustration shows how conclusions drawn from a perturbative treatment could be misleading or distorted. This example clearly demonstrates that nonperturbative approaches are necessary for cases with strong coupling.

VIII. SUMMARY

In this paper, new variational functionals to evaluate the system density operator in the presence of an environment are developed. Both perturbative and nonperturbative master equations for the open quantum system are derived. The perturbative master equation is similar to the conventional one, but without introducing an explicit Markovian approximation. The nonperturbative master equation is attractive because it is valid for all time. What lies ahead are explicit numerical applications of these formulations.

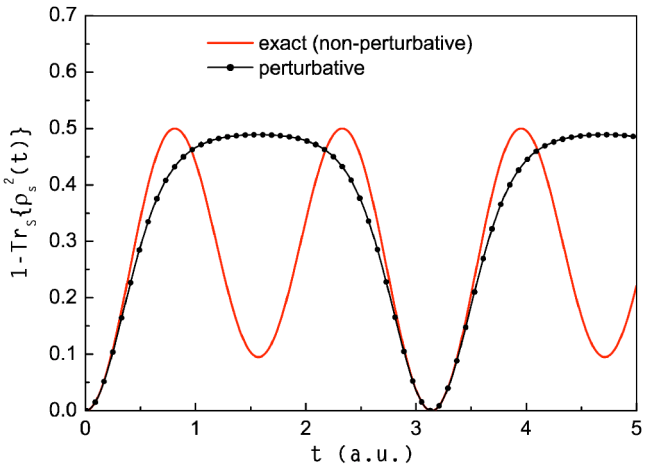

FIG. 2. Comparison of the decoherence degrees from perturbative and nonperturbative approaches. It is a strong coupling case such that $w_0+w_1=0.95$ where w_0, w_1 are defined in Eq. (78).

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There is no generalization of known formulas for mutually unbiased bases

Claude Archer[a)]
Université Libre de Bruxelles, C.P.165/11-Physique et Mathématique,
Faculté des Sciences Appliquées, avenue F.D. Roosevelt 50, 1050 Bruxelles, Belgium

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In a quantum system having a finite number N of orthogonal states, two orthonormal bases $\{a_i\}$ and $\{b_j\}$ are called mutually unbiased if all inner products $\langle a_i|b_j\rangle$ have the same modulus $1/\sqrt{N}$. This concept appears in several quantum information problems. The number of pairwise mutually unbiased bases is at most $N+1$ and various constructions of such $N+1$ bases have been found when N is a power of a prime number. We study families of formulas that generalize these constructions to arbitrary dimensions using finite rings. We then prove that there exists a set of $N+1$ mutually unbiased bases described by such formulas, if and only if N is a power of a prime number. © *2005 American Institute of Physics.*
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I. INTRODUCTION

A. Definitions and previous results

In the N-dimensional Hilbert space $\mathbb{C}^N$, two orthonormal bases $\{a_i\}_{1\leqslant i\leqslant N}$ and $\{b_j\}_{1\leqslant j\leqslant N}$ are called *mutually unbiased* if all inner products $\langle a_i|b_j\rangle$ have the same modulus $|\langle a_i|b_j\rangle|=1/\sqrt{N}$. A set of mutually unbiased bases is a set of orthonormal bases which are pairwise mutually unbiased. In various physical situations (see Sec. I B), the problem is to find the maximal number of mutually unbiased bases. The following result is due to Wootters and Fields but it has been obtained independently by Calderbank *et al.*

Theorem 1.1 (Refs. 16 and 4):

- *In dimension $N\geqslant 2$, the number of mutually unbiased bases is at most $N+1$.*
- *If N is a power of a prime number then there exist $N+1$ mutually unbiased bases.*

In dimension N, a set of mutually unbiased bases is called *complete* if it contains $N+1$ bases. If N is not a prime power, it is not known whether such a complete set exists, even for $N=6$. Originally, constructions of $N+1$ mutually unbiased bases in dimension N were based on the arithmetic of a field, where addition and multiplication are invertible.[16] There exists a field with N elements if and only if N is a power of a prime number. Nevertheless, new constructions have been recently obtained (see Ref. 8) using the arithmetic of rings, where multiplication is not invertible. Since there exist rings of N elements for any N, is it possible to use finite rings to construct $N+1$ mutually unbiased bases for arbitrary dimensions? We will address this issue here. First we will generalize known constructions from Refs. 16 and 8 to any finite ring. Then we will prove that for dimensions N that are not prime powers, there does not exist a complete set of mutually unbiased bases described by this generalization.

[a)]Electronic mail: carcher@ulb.ac.be

B. Applications to quantum information

Mutually unbiased bases (MUBs) have recently been considered with increasing interest because of the central role they play in specific quantum information tasks such as state estimation or Quantum Key Distribution.

1. State estimation

Mutually unbiased bases play an important role in state estimation. Consider a (relatively) large ensemble of N-dimensional quantum systems identically prepared in some unknown state ρ. How can one estimate ρ using projective individual measurements? Since ρ is a trace one Hermitian matrice, it is specified by N^2-1 real parameters. Now imagine performing a nondegenerate measurement on a subensemble of the quantum systems. Such a measurement will yield $N-1$ independent real numbers, i.e., the probabilities associated to $N-1$ of the possible outcomes. So, in order to reconstuct the state ρ, we need at least $N+1$ different sorts of measurements. As argued in Ref. 7, $N+1$ measurements are sufficient when they correspond to MUBs. The reason is that if the basis are MUBs, then the information gained about ρ when performing a measurement in a basis B_i is independent of the information gained when performing a measurement in another basis B_j, for all couple of bases B_i, B_j. So, pooling the data obtained by each of these $N+1$ measurements, one indeed gets information about $(N+1)(N-1)$ independent parameters characterizing the state ρ, and full reconstruction thus becomes possible (we note however that it is not always necessary to invoke MUBs to fully reconstruct a state ρ with $N+1$ different measurements). An explicit formula to estimate the state from these mutually unbiased measurements is given in Ref. 7. Other optimality properties of MUBs with respect to state estimation are described in Ref. 16.

2. Quantum cryptography

The concept of MUBs is also relevant to Quantum Key Distribution (QKD). In the BB84 QKD protocol,[3] two authorized parties, Alice and Bob, use two 2-dimensional MUBs to generate a secret key. MUBs are the basic algebraic structure underlying d-dimensional generalizations of the BB84 protocol.[5] It is precisely the use of such bases which allows these protocols to make the intervention of a potential eavesdropper detectable. Wiesner[14] also introduced several ideas that later grew into quantum cryptography. Assessing the security of the BB84 protocol and its generalizations is a highly nontrivial matter.[13,10] However, considering the simple intercept and resend eavesdropping strategy, it is possible to give a heuristic argument of why the use of MUBs makes such protocols secure. In the d-dimensional generalization, Alice prepares each random key element as follows. She chooses randomly a value $i \in 1, \ldots, d$, chooses randomly a basis A taken among t MUBs, prepares the ith state of A, $|a_i\rangle$, and sends it to Bob. Bob chooses a basis among the t MUBs to measure the state $|a_i\rangle$, and get the value of the key element. With probability $1/t$, Bob will choose the basis A and should then get the measurement outcome i. Now suppose that a potential eavesdropper, Eve, applies a strategy where she also measures the key element sent by Alice in either of the t MUBs and sends Bob a state corresponding to her measurement outcome (intercept and resend attack). With probablity $1/t$, Eve's and Bob's choice of basis will not match. Thus, in those events where Bob happens to choose his measurement basis correctly, Eve will with probability $(t-1)/t$, produce a state that will give Bob a wrong result with probability $(d-1)/d$, i.e., the use of MUBs allows one to make the intervention of a potential eavesdropper detectable. It is also known that a protocol using a larger number of mutually unbiased bases can tolerate a higher error level in the channel (see Ref. 5).

3. MUBs and some discrete Wigner functions

Pure or mixed quantum states are usually represented by the density matrix. However, there is an alternative description in terms of the Wigner function. Several authors have proposed to define a Wigner function for discrete systems having N degrees of freedom.[12,9,15] It turns out that the discrete Wigner function defined in Ref. 15 requires the existence of $N+1$ mutually unbiased bases.

Finally, MUBs have also been shown to be relevant to the mean king's problem, see Ref. 1 and references therein. An interested reader will find recent results and further references on MUBs in Ref. 17, the problem page in Quantum Information at TU Braunschweig.

II. FORMULAS FOR MUTUALLY UNBIASED BASES

A unitary transformation maps a set of MUBs to a set of MUBs. Hence, it is not restrictive to consider only sets X of MUBs containing the standard basis $\{e_k\}_{1\leqslant k\leqslant N}$ since it is always possible to choose a unitary transformation U that maps a given orthonormal basis in X to $\{e_k\}$ so that $U(X)$ is a set of MUBs containing $\{e_k\}$. If a basis $\{v_k\}$ is unbiased with respect to the standard basis $\{e_k\}$ (i.e., $|\langle e_i|v_j\rangle|=1/\sqrt{N}$) then $|(v_k)_l|=|\langle e_l|v_k\rangle|=1/\sqrt{N}$. Hence the coordinates of its vectors must be expressed as $(v_k)_l=(e^{i\Theta(k,l)})/\sqrt{N}$ where $\Theta(k,l)$ belongs to $[0,2\pi]$.

For $N=p^n$ where p is a prime number and n a positive integer, there always exist $N+1$ mutually unbiased bases. We describe here the constructions from Refs. 16 and 8 for these dimensions.

A. Odd prime powers dimensions

Let the superscript r denote the basis, k the vector in the basis, and l the component. The standard basis is $(v_k^{(0)})_l=\delta_{kl}$ for $k,l=0,1,\ldots,N-1$. If $N=p^n$ for a prime number $p\neq 2$, the other such $N=p^n$ bases given in Ref. 16 are

$$(v_k^{(r)})_l=\frac{1}{\sqrt{N}}e^{(2\pi i/p)\mathrm{Tr}(rl^2+kl)},\quad r,k,l\in\mathbb{F}_{p^n}, \tag{1}$$

where $\mathbb{F}_{p^n}$ is the finite field with p^n elements and where Tr denote the trace map from $\mathbb{F}_{p^n}$ into the prime field $\mathbb{F}_p$. For $p\geqslant 5$ odd, a new formula has been proposed in Ref. 8 where the polynomial rl^2+kl is replaced by $(l+r)^3+k(l+r)$. The trace map is a linear map from $\mathbb{F}_{p^n}$, regarded as a vector space, into $\mathbb{F}_p$. In the language of group theory, linear maps are group homomorphisms (i.e., maps that preserve sums). The trace map induces a homomorphism from the additive group of $\mathbb{F}_{p^n}$ into the multiplicative group $\mathbb{C}^*$ of complex numbers, defined by $x\rightarrow e^{(2\pi i/p)\mathrm{Tr}(x)}$.

B. Even prime powers dimensions

For $N=2^n$, Wootters and Fields[16] have used an *ad hoc* construction that may be reformulated in a finite ring R whose 4^n elements are sequences $(x_1,\ldots,x_n)$ with $x_i\in\mathbb{Z}_4$. A much easier construction has been found recently by Klappenecker and Roetteler[8] using the Galois ring $R=GR(4,n)$. Let Tr denotes the trace map from $GR(4,n)$ into $\mathbb{Z}_4$. Once again $T:x\rightarrow e^{(2\pi i/4)\mathrm{Tr}(x)}$ is a group homomorphism from $GR(4,n),+$ into $\mathbb{C}^*$. The 2^n indexes are the elements of T_n, the *Teichmüller* set of $GR(4,n)$ and the 2^n bases described by

$$(v_k^{(r)})_l=\frac{1}{\sqrt{2^n}}e^{(2\pi i/4)\mathrm{Tr}((r+2k)l)},\quad r,k,l\in T_n\subset GR(4,n) \tag{2}$$

together with the standard basis, form a complete set of mutually unbiased bases of $\mathbb{C}^{2^n}$ (see Ref. 8).

C. How to generalize these formulas?

Formulas (1) and (2) as well as others in Ref. 8, share many common characteristics. First of all, the indexes l, k, r, respectively, for components, vectors, and bases are taken in a finite ring R. Both formulas link the indexes in R to complex coordinates by a function $f:(r,k,l)\rightarrow T(P(r,k,l))$ where P is a polynomial and T is a homomorphism from $R,+$ into $\mathbb{C}^*$. We will generalize these characteristics as follows:

1. *The functions* $f:(r,k,l)\to T(P(r,k,l))$. We consider a much larger class of functions that we call *functions preserving a direct sum decomposition of R* (see Sec. IV).
2. *The set S of indexes*. For formula (1) the set of indexes is the whole R while for formula (2), it is a remarkable subset of R. We will see in Sec. II E that these subsets may be defined for every ring R as sets closed under multiplication and transversal to a nilpotent ideal of R.
3. *Distinguish the index r*. In formulas (1) and (2), the nonstandard bases are indexed by r that takes all possible values of a set of size N. This can only be done for dimensions N for which there exist $N+1$ mutually unbiased bases. However, there is, up to now, no result showing that this is true if N is not a prime power. Therefore, we propose to give up formulas that are uniform with respect to r and to consider that each basis r may be described by a different formula. This means that for each r, we choose a different function $f_r:(k,l)\to f_r(k,l)$ into $\mathbb{C}^*$ such that the vectors in basis r are described by

$$(v_k^{(r)})_l = f_r(k,l), \quad k,l \in S, \tag{3}$$

where each f_r preserves a given decomposition $R_1\oplus R_2$ and $S\subset$ is as described in the previous paragraph. For the case of polynomials P and homomorphisms T, it amounts to choosing for each r, different polynomials P_r and homomorphism T_r.

D. Properties of rings

In the following we recall various properties of rings that are needed for this paper.

1. Direct sums of rings

Let R_+ be a ring where addition is commutative but where multiplication is not necessarily commutative. If the additive group R_+ is the direct sum $R_1\oplus R_2$ of two subgroups then every element r of R can be written in a unique way as $r=r_1+r_2$ where $r_i\in R_i$ and $R_1\cap R_2$ is reduced to the zero element. An element $r\in R$ may be represented as a couple (r_1,r_2) and addition in R corresponds to componentwise addition of couples. If, moreover, R_1 and R_2 are two-sided ideals of R (i.e., $r\cdot R_i=R_i=R_i\cdot r$ for every r in R), then multiplication in R is also reduced to componentwise multiplication of couples. Indeed, for $r_i\in R_i$, $r_1.r_2$ belongs to both R_1 and R_2 since these are two-sided ideals and thus $r_1.r_2=0=R_1\cap R_2$. For two ring elements x and y, we obtain for their product $x.y=(x_1+x_2).(y_1+y_2)=x_1.y_1+x_1.y_2+x_2.y_1+x_2.y_2$ and since $x_i.y_j=0$ for $i\neq j$, we get $x.y=x_1.y_1+x_2.y_2$. Thus $(x.y)_i=x_i.y_i$ as expected. Observe also that $a.x_1=(a_1+a_2).x_1=a_1.x_1$ for every $a\in R$. We say that the ring R is the direct sum of its ideals R_1 and R_2. These properties also hold when R is the direct sum of more than two ideals.

2. Polynomial functions in a ring

If a ring is a direct sum, then let us show that polynomial functions in R may be evaluated componentwise. A monomial on the set of variables $\{x,y,\ldots\}$ is a finite product of elements of this set. In a commutative ring R, a polynomial $P(x,y,\ldots)+r_0$ is defined as a linear combination P of monomials (on $\{x,y,\ldots\}$) with coefficients in R and of $r_0\in R$. A polynomial $P+r_0$ defines a polynomial function $(x,y,\ldots)\to P(x,y,\ldots)+r_0$ that maps n-uples of R^n to elements of R. In the noncommutative case, this definition is not very convenient since generally $x.r.y\neq r.x.y$, so that products of polynomials would not in general be polynomials. Hence we define more generally a noncommutative polynomial function as $P:(x,y,\ldots)\to r_0+\Sigma_k m_k(x,y,\ldots)$, where $m_k(x,y,\ldots)=w_k(x,y,\ldots;a,b,\ldots)$ is a finite product of noncommuting variables in $\{x,y,\ldots\}$ and of coefficients from a set $\{a,b,\ldots\}\subset R$.

Assume now that the ring R is a direct sum $R=R_1\oplus R_2$ and for $r\in R$, let $r=r_1+r_2$ be the corresponding decomposition. We have shown in the previous paragraph that products in R may be performed componentwise. Thus, for each term w_k of a polynomial function $w_k(x,y,\ldots;a,b,\ldots)$ is equal to $w_k(x_1,y_1,\ldots;a_1,b_1,\ldots)+w_k(x_2,y_2,\ldots;a_2,b_2,\ldots)$. As $x_1.a_1=x_1.a$ and $a_1.x_1=a.x_1$ for $a,x\in R$ we may conclude that $w_k(x_i,y_i,\ldots;a_i,b_i,\ldots)$ is equal to

$w_k(x_i,y_i,\ldots;a,b,\ldots)$, for $i=1,2$, so that $m_k(x,y,\ldots)=m_k(x_1,y_1,\ldots)+m_k(x_2,y_2,\ldots)$. Hence, for a polynomial function $\overline{P}=P+r_0$ on $R_1\oplus R_2$, we have $P(x,y,\ldots)=P(x_1,y_1,\ldots)+P(x_2,y_2,\ldots)$ and thus for $\lambda=-r_0=\overline{P}(0,0,\ldots)$,

$$\overline{P}(x,y,\ldots)=\lambda+\overline{P}(x_1,y_1,\ldots)+\overline{P}(x_2,y_2,\ldots).$$

3. The Sylow decomposition of a finite ring

Let R be a finite ring and let $|R|=\Pi_i p_i^{e_i}$ be the factorization of its order into powers of distinct prime numbers. The additive group $R,+$ is a finite commutative group. Hence, it is equal to the direct product $\oplus_i \mathrm{Syl}(p_i)$ of its Sylow subgroups and thus every element r of $R,+$ can be written in a unique way as $r=\Sigma r_i$ where $r_i\in S_{p_i}:=\mathrm{Syl}(p_i)$. We call the element r_i, *the p_i-component of r* and it is the unique element contained in the intersection $S_{p_i}\cap\{r+(\oplus_{j\neq i}S_{p_j})\}$ (see Ref. 6, Chap. 3). These subgroups may be defined as $S_{p_i}:=\{x:p_i^{e_i}x=0\}$ where $p_i^{e_i}x$ is the repeated sum of $p_i^{e_i}$ terms x. The subgroups S_{p_i} are two-sided ideals of the ring R, i.e., $r.S_{p_i}=S_{p_i}.r=S_{p_i}$ for every $r\in R$. This is due to the right and left distributive property of a ring since

$$p_i^{e_i}(r.x)=\underbrace{r.x+\ldots+r.x}_{p_i^{e_i}\ terms}=\underbrace{r(x+\ldots+x)}_{p_i^{e_i}\ \mathrm{terms}}=r.(p_i^{e_i}x)=r.0=0$$

if $x\in S_{p_i}$ so that $r.x\in S_{p_i}$ and similarly $x.r\in S_{p_i}$. Hence every finite ring is the direct sum of its Sylow ideals and a finite ring that is not decomposable as a nontrivial direct sum must be of prime power order. Moreover, if $|R|=d_1.d_2$ is the product of two coprime numbers ($\geqslant 2$) then $R=R_1\oplus R_2$ where $R_i:=\oplus_{p|d_i}\mathrm{Syl}(p)$.

4. Ring with unity

From now on, we mainly consider rings R containing a multiplicative unity 1 such that $x.1=x=1.x$ for every $x\in R$. If $R=\oplus_{i\in I}R_i$ has a unity 1 and $R_i\neq\{0\}$ then 1_i is the unity of R_i. An element x has a left inverse x_L (respectively, right inverse x_R) if $x_L.x=1$ (respectively $x.x_R=1$). An element that has both a left and a right inverse is called a *unit*. If x is a unit, then the inverse x^{-1} is unique since $x_L=x_L.(x.x_R)=(x_L.x).x_R=x_R$. The set $U(R)$ of all units of R is a multiplicative group and by the componentwise multiplication $U(R_1\oplus R_2)=U(R_1)\oplus U(R_2)$. A *field* is a ring where every nonzero element is a unit.

5. Nilpotency

An element n of a ring R is called nilpotent if $n^t=0$ for some positive integer t. The set $\mathrm{Nil}(R)$ of all nilpotent elements of R is called the *Nilpotent radical* of R. Once again, by the componentwise multiplication $\mathrm{Nil}(R_1\oplus R_2)=\mathrm{Nil}(R_1)\oplus\mathrm{Nil}(R_2)$. We say that an ideal N is nilpotent provided that every $n\in N$ is nilpotent. For every $r\in R$, if we have $(r.n)^t=0$ then $(n.r)^{t+1}=n.(r.n)^t.r=0$ and thus every nilpotent ideal is two-sided. In every ring with unity, a nilpotent element cannot be a unit but if n is nilpotent ($n^t=0$) then $1+n$ is a unit. To show this, consider $u_t(n)=1+n+\ldots+n^{t-1}$; then since $1=1-n^t=(1-n)u_t(n)=u_t(n)(1-n)$, the element $u_t(-n)$ is the inverse of $1+n=1-(-n)$.

Let us show that in a commutative ring, $\mathrm{Nil}(R)$ is an ideal. If $x^n=0$ then $(r.x)^n=r^n.x^n=0$ and if moreover $y^m=0$ then $(x+y)^{n+m}=0$ since $(x+y)^{n+m}$ is a sum of terms $x^{n+m-k}.y^k$ which are zero for $k\leqslant m$ and for $k\geqslant m$. In a noncommutative ring R, $\mathrm{Nil}(R)$ is not necessarily an ideal. For instance, a sum of nilpotent matrices may be invertible (and thus non-nilpotent) as shown by

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

Thus for the ring $M_2(R)$ of 2×2 matrices over a ring R with unity, the nilpotent radical is not an ideal. However, the subring of upper triangular matrices is also noncommutative but it contains the nilpotent ideal

$$\left\{ \begin{pmatrix} 0 & r \\ 0 & 0 \end{pmatrix} : r \in R \right\}.$$

E. Generalizing *Teichmüller* sets

For every ring R we would like to define a subset $S_R \subset R$ for the indexes k, l of vectors and components, in such a way that for a Galois ring $R=GR(4,n)$, the set S_R is the *Teichmüller* set T_n as in formula (2), while for a finite field $R=\mathbb{F}_{p^n}$ we have $S_R=R$ as in formula (1).

The set $T_n \subset GR(4,n)$ has remarkable properties that are used over and over to compute easily in $GR(4,n)$ (see Ref. 11).

(1) The ideal $N:=\{2t_1 : t_1 \in T_n\}$ is the nilpotent radical of $GR(4,n)$ ($N^2=0$).
(2) Every $r \in GR(4,n)$ can be written in a unique way as $r=t_0+2t_1$ for some t_0, t_1 in T_n. Thus T_n contains exactly one representative of each coset $\{r+N\}_{r\in R}$ of N in R; it is a transversal to the ideal N.
(3) T_n is closed under multiplication. Therefore a product of elements written as $t+n$ for $t \in T_n$ and $n \in N$ is still written in this way since

$$(t_1+n_1)(t_2+n_2) = \underbrace{t_1 t_2}_{\in T_n} + \underbrace{(t_1 n_2 + n_1 t_2 + n_1 n_2)}_{\in N}.$$

This may be generalized to every ring R as follows. We require that the set of indexes S_R is closed under multiplication and that it is a transversal to a nilpotent ideal N. Trivially, if R is a field (as in formula (1)) or even a division ring, then $N=\{0\}$ is the only nilpotent ideal, $S_R=R$ is the only transversal to N and it is closed under multiplication.

A commutative local ring is a ring that has a unique maximal ideal M and the Galois ring $R=GR(4,n)$ is local. In a finite commutative local ring R, the unique maximal ideal is $\mathrm{Nil}(R)$ and the units of R are exactly the non-nilpotent elements (see Ref. 2). Hence in a local ring every ideal ($\neq R$) is nilpotent. Every finite commutative ring with unity is a direct sum of local rings (see Ref. 2, Proposition 8.7).

F. Functions preserving a direct sum decomposition

Let $R=R_1 \oplus R_2$ be a direct sum decomposition of a ring R and let $r=r_1+r_2$ be the corresponding decomposition for $r \in R$. Let $G_{,\star}$ be a commutative group with an operation $\star$ (either "$+$" or "$\cdot$" in this paper). For a finite set of variables $\{x,y,\ldots\}$ belonging to R, we say that a function $f:(x,y,\ldots)\to f(x,y,\ldots)\in G_{,\star}$ *preserves the decomposition* $R_1 \oplus R_2$ if for a constant $\lambda \in R$,

$$f(x,y,\ldots) = \lambda \star f(x_1,y_1,\ldots) \star f(x_2,y_2,\ldots) \quad \text{for every } x,y,\ldots \in R. \tag{4}$$

Observe that $\lambda=(f(0,0,\ldots))^{-1}$ because $(x_1)_2=(y_1)_2=\ldots=0$ implies $f(x_1,y_1,\ldots)=f(x_1+0,y_1+0,\ldots)=\lambda\star f(x_1,y_1,\ldots)\star f(0,0,\ldots)$. If f_i is the restriction of f to R_i then $f(x,y,\ldots)=\lambda\star f_1(x_1,y_1,\ldots)\star f_2(x_2,y_2,\ldots)$. Conversely, for arbitrary functions f_i from R_i into G and $\lambda \in G$, this last equation defines a function that preserves $R_1 \oplus R_2$. It may happen that f preserves $R_1 \oplus R_2$ but does not preserve another decomposition of R.

We have seen in Sec. II D that polynomial functions P on a ring R preserves every direct sum decomposition of R (and in this case $\lambda=-P(0,0,\ldots)$). Thus, since group homomorphisms preserve sums, if T is a group homomorphism from R_+ into a commutative group $G_\star$ and if

$P(x,y,\ldots)$ is a polynomial function on R, then $(x,y,\ldots)\to T(P(x,y,\ldots))$ preserves every direct sum decomposition of R. Hence, these functions generalize formulas (1) and (2) for mutually unbiased bases since those rely on expressions of type $(1/\sqrt{N})T(P(k,l))$ for $k,l\in R$ where $G_\star$ is the multiplicative group of unitary complex number. This is also true for the other formulas proposed in Ref. 8.

More such sophisticated functions may be constructed by products. If $f\cdot g$ is a product of functions into a commutative group G that both preserve a direct sum decomposition $R=R_1\oplus R_2$ then it is easy to show that $f\cdot g$ also preserves $R_1\oplus R_2$. We have $(f\cdot g)(x,y,\ldots)=\lambda_f\cdot\Pi_{i=1,2}f(x_i,y_i,\ldots)\cdot\lambda_g\Pi_{i=1,2}g(x_i,y_i,\ldots)$ and since the elements of G commute, we may rearrange the factors as $(f\cdot g)(x,y,\ldots)=\lambda_f\cdot\lambda_g\Pi_{i=1,2}(f\cdot g)(x_i,y_i,\ldots)$.

III. SUCH SETS OF MUB CANNOT BE COMPLETE

In this section we prove that even with all these generalizations, it is not possible to construct complete sets of $N+1$ mutually unbiased bases for $N\neq p^n$.

Theorem 3.1: *Let $R=R_1\oplus R_2$ be a decomposition of a ring R. For $i=1,2$ let S_i be a nonempty subset of R_i and let $N=|S_1||S_2|$. For each $1\leqslant c\leqslant m$, let $f_c:R_+\to\mathbb{C}^*,\cdot$ be a two variable function that preserves the decomposition $R_1\oplus R_2$ and let us define N vectors $\{v_k^{(c)}\}$ of $\mathbb{C}^N$ as*

$$(v_k^{(c)})_l=f_c(k,l)\quad k,l\in S_1\oplus S_2.$$

Assume that, together with the standard basis, the sets of vectors $\{v_k^{(c)}\}_{1\leqslant c\leqslant m}$ form a set X of $m+1$ mutually unbiased bases. If $|S_i|_{i=1,2}\neq 1$, then

$$m\leqslant\min_i|S_i|<N \text{ and the set } X \text{ is not complete}.$$

Proof: The function f_c preserves the decomposition $R_1\oplus R_2$ so there is a constant λ_c such that $f_c(k,l)=\lambda_c f_c(k_1,l_1)f_c(k_2,l_2)$. For each c, let us define $|S_1|$ vectors $\{a_{k_1}^{(c)}\}_{k_1\in S_1}$ of $\mathbb{C}^{|S_1|}$ and $|S_2|$ vectors $\{b_{k_2}^{(c)}\}_{k_2\in S_2}$ of $\mathbb{C}^{|S_2|}$ as

$$(a_{k_1}^{(c)})_{l_1}=\lambda_c\, f_c(k_1,l_1),\quad (b_{k_2}^{(c)})_{l_2}=f_c(k_2,l_2)\quad \text{for}\quad k_i,l_i\in S_i(i=1,2).$$

Hence $(v_k^{(c)})_l=f_c(k,l)=\lambda_c(a_{k_1}^{(c)})_{l_1}(b_{k_2}^{(c)})_{l_2}$ and since l takes all value in $S_1\oplus S_2$, the vector $v_k^{(c)}=v_{(k_1,k_2)}^{(c)}$ is equal to the tensor product $a_{k_1}^{(c)}\otimes b_{k_2}^{(c)}\in\mathbb{C}^{|S_1||S_2|}$. If we denote by $\{v_k^{(0)}\}_{k\in S_1\oplus S_2}$, $\{a_{k_1}^{(0)}\}_{k_1\in S_1}$, $\{b_{k_2}^{(0)}\}_{k_2\in S_2}$ the standard bases, respectively, in $\mathbb{C}^N$, $\mathbb{C}^{|S_1|}$, and $\mathbb{C}^{|S_2|}$ then also $v_k^{(0)}=v_{(k_1,k_2)}^{(0)}=a_{k_1}^{(0)}\otimes b_{k_2}^{(0)}$.

Therefore if the sets $\{v_k^{(c)}\}_{0\leqslant c\leqslant m}$ form a set X of $m+1$ mutually unbiased bases in $\mathbb{C}^N=\mathbb{C}^{|S_1||S_2|}$, then by Proposition A.1 in the Appendix, there exist $m+1$ mutually unbiased bases in both $\mathbb{C}^{|S_1|}$ and $\mathbb{C}^{|S_2|}$. By Theorem 1.1, if each $|S_i|_{i=1,2}$ is at least 2 then $m+1\leqslant|S_i|+1$ and $m\leqslant\min_i|S_i|<|S_1||S_2|=N$ thus $|X|=m+1<N+1$ and X is not complete. □

Theorem 3.1 requires that the index set S is a product of two subsets. We now prove that this is always the case if $S\subset R$ is closed under multiplication and is transversal to a nilpotent ideal N of R.

Proposition 3.1: In a ring R with 1, let $S\subset R$ be a set closed under multiplication that is a transversal to a nilpotent ideal N of R.

1. *If $R=R_1\oplus R_2$ is a sum of rings with 1 then*

$$S=(S\cap R_1)\oplus(S\cap R_2)$$

and for $i=1,2$, each R_i, $S\cap R_i$ is closed under multiplication and is a transversal to $N\cap R_i$.

2. *If $|S|$ is a product $d_1 \cdot d_2$ of two coprime numbers $\geqslant 2$ and if R is finite, then R is a sum $R_1 \oplus R_2$ of rings with 1 such that $|S \cap R_1| = d_1$ and $|S \cap R_2| = d_2$.*

Proof: (1) $R = R_1 \oplus R_2$ has unity $(1_1, 1_2)$. Every ideal I of R is equal to $I_1 \oplus I_2$ where I_j is an ideal of R_j and N is the sum $N_1 \oplus N_2$ of two nilpotent ideals (see Ref. 2). Let $\tilde{x} = (1_1, 0) + N$. Since S is a transversal to N, it contains a unique element $x \in \tilde{x} \cap S$ where $x = (1_1 + n_1, n_2)$ for some $(n_1, n_2) \in N_1 \oplus N_2$. Since N is a nilpotent ideal, it is two-sided and we may consider the quotient ring R/N where multiplication of cosets is defined as $(x+N)(y+N) = x \cdot y + N$. Thus, in R/N we have $\tilde{x}^2 = \tilde{x}$ whence $x^2 \in \tilde{x}$. Also, $x^2 \in S$ because S is closed under multiplication. Therefore we have $x^2 = S \cap \tilde{x} = x$ and we have

$$(1_1 + n_1)^2 = (1_1 + n_1)\ (1), \quad n_2^2 = n_2\ (2).$$

By nilpotency $n_2^t = 0$ for some positive integer t and by (2), $n_2^t = n_2$ whence $n_2 = 0$. By nilpotency of n_1, $(1 + n_1)$ has an inverse $(1_1 + n_1)^{-1}$ in R_1. Multiplying both sides of (1) by $(1_1 + n_1)^{-1}$ gives $(1_1 + n_1) = 1$ whence $n_1 = 0$. Finally $x = (1_1, 0) \in S$ and the symmetric argument for $S \cap \{(0, 1_2) + N\}$ shows that $(0, 1_2)$ also belongs to S.

As $\{(1_1, 0), (0, 1_2)\} \in S$, for every $(s_1, s_2) \in S$, $(s_1, 0) = s \cdot (1_1, 0) \in S \cap R_1$ and $(0, s_2) = s \cdot (0, 1_2) \in S \cap R_2$. Conversely, it remains to show that for every $(s_1, 0) \in S \cap R_1$ and $(0, s_2) \in S \cap R_2$ we also have $(s_1, s_2) \in S$. Since S is a transversal to N, it contains a unique element $y = (s_1 + n_1, s_2 + n_2) \in S \cap \{(s_1, s_2) + N\}$ and $y \cdot (1_1, 0) = (s_1 + n_1, 0)$ in S. As $(s_1 + n_1, 0)$ and $(s_1, 0)$ are in S and belong to the same coset of N, these must be equal and $n_1 = 0$. Similarly $n_2 = 0$ so that $y = (s_1, s_2) \in S$ whence $S = (S \cap R_1) \oplus (S \cap R_2)$. Finally, let us show that $(S \cap R_i)$ is a transversal to $N_i = N \cap R_i$ in R_i. Every coset $(r_1, 0) + N_1$ is embedded in $(r_1, 0) + N$ which contains a unique element $s = (r_1 + n_1, n_2)$ of S. Then $s \cdot (1_1, 0) = (r_1 + n_1, 0)$ is in $S \cap R_1$ and in $(r_1, 0) + N_1$ and so, $S \cap R_1$ contains at least one representative of each coset. If two elements of $S \cap R_1$ belong to the same coset of N_1 then these belong to the same coset of $N \supset N_1$ and thus are equal. The proof is similar for $(S \cap R_2)$.

(2) Let $\pi(d)$ denote the set of prime divisors of an integer d. For a finite ring R and a divisor d of $|R|$, let us define $\mathrm{Syl}(\pi(d)) := \oplus_{p \in \pi(d)} \mathrm{Syl}(p)$. Since S is a transversal to the ideal N in R then $d_1 \cdot d_2 = |S| = |R| / |N|$ is a divisor of $|R|$. If $\pi_1 = \pi(d_1)$ and $\pi_2 = \pi(|R|) \setminus \pi(d_1)$, we know from Sec. II D that $R = \mathrm{Syl}(\pi_1) \oplus \mathrm{Syl}(\pi_2)$ and since R has unity 1, $\mathrm{Syl}(\pi_i)$ has unity 1_i. Thus, as proven in (1), $S = (S \cap \mathrm{Syl}(\pi_1)) \oplus (S \cap \mathrm{Syl}(\pi_2))$ and

$$d_1 \cdot d_2 = |S| = |S \cap \mathrm{Syl}(\pi_1)| \cdot |S \cap \mathrm{Syl}(\pi_2)|. \tag{5}$$

As $S \cap \mathrm{Syl}(\pi_i)$ is a transversal to the ideal $N \cap \mathrm{Syl}(\pi_i)$ then $|S \cap \mathrm{Syl}(\pi_i)|$ divides $\mathrm{Syl}(\pi_i)$ and so is coprime to d_j $(j \neq i)$. Thus, by equality (5), $|S \cap \mathrm{Syl}(\pi_i)|$ must divide d_i and symmetrically d_i divides $|S \cap \mathrm{Syl}(\pi_i)|$ so that $d_i = |S \cap \mathrm{Syl}(\pi_i)|$. □

Finally, we obtain our main result: complete sets of MUBs described by generalizations of known formulas only exist for prime power dimensions. Moreover, we provide an upper bound for the number of MUBs described by such formulas.

Theorem 3.2: *Let R be a finite ring with unity. Let $S \subset R$ be a subset of N elements that is closed under multiplication and transversal to a nilpotent ideal. For $1 \leqslant c \leqslant N$, let $T_c : R_+ \to \mathbb{C}^*, \cdot$ be a group homomorphism and let $P_c : R^2 \to R$ be a two variables polynomial function. Let us define N sets of vectors $\{v_k^{(c)}\}_{1 \leqslant c \leqslant N}$ in $\mathbb{C}^N$ by*

$$(v_k^{(c)})_l = \frac{1}{\sqrt{N}} T_c(P_c(k, l)), \quad k, l \in S,$$

and let the set $X_{\{T_c\}\{P_c\}}$ be the union of the standard basis with $\{v_k^{(c)}\}_{1 \leqslant c \leqslant N}$.

1. *A set $X_{\{T_c\}\{P_c\}}$ contains at most $1 + \min_i\{p_i^{e_i}\}$ mutually unbiased bases where $N = \Pi_i p_i^{e_i}$ is the factorization of N into powers of distinct prime numbers.*
2. *There exists a complete set $X_{\{T_c\}\{P_c\}}$ of $N+1$ mutually unbiased bases if and only if N is a power of a prime number.*

Proof:

1. We prove that the conditions of Theorem 3.1 apply here. First we show that every vector $v_k^{(c)}$ is unbiased with the standard basis $\{e_k\}$. Every $r \in R$ has finite additive order n_r ($n_r \cdot r = 0$). By the homomorphism property

$$T_c(n \,.\, r) = T_c(\underbrace{r + \ldots + r}_{n \text{ terms}}) = (T_c(r))^n$$

and as $T_c(0) = 1$ we must have $|T_c(r)|^n = 1$ whence $|T_c(r)| = 1$ for every r in R. Thus for every vector $v_k^{(c)}$ we obtain $|\langle e_l | v_k^{(c)} \rangle| = |(v_k^{(c)})_l| = |T_c(P_c(k,l))| / \sqrt{N} = 1/\sqrt{N}$ as announced. Let $m+1$ be the maximal number of mutually unbiased bases contained in $X_{\{T_c\}\{P_c\}}$ and let $Y \subset X_{\{T_c\}\{P_c\}}$ be a set of $m+1$ mutually unbiased bases. Since we have shown that $Y \cup \{\{e_k\}\}$ is also a set of MUBs, the standard basis $\{e_k\}$ must be in Y.
As $|S| = N = \Pi_i p_i^{e_i}$ we may use Proposition 3.1 (2) to show that there is a ring decomposition $R = \oplus_i R_i$ such that $S = \oplus_i S \cap R_i$ and $|S \cap R_i| = p_i^{e_i}$. Finally, since the functions $(k,l) \to T_c(P_c(k,l))$ preserve every direct sum decomposition of R (see Sec. II D), we may apply Theorem 3.1 to Y to show that for every i we must have $m \leqslant p_i^{e_i}$. Hence $1+m \leqslant 1 + \min_i\{p_i^{e_i}\}$.
2. If we have $N+1$ such MUBs, then by (1), $\Pi_i p_i^{e_i} = N \leqslant \min_i\{p_i^{e_i}\}$, which implies that $N = \min_i\{p_i^{e_i}\}$ and thus N is a prime power. Conversely if $N = p_i^{e_i}$, we have shown in Sec. II that the sets of $N+1$ MUBs given by formulas (1) and (2) may be described as sets $X_{\{T_c\}\{P_c\}}$. □

The bound $1 + \min_i\{p_i^{e_i}\}$ can be easily reached for dimension $N = \Pi_i p_i^{e_i}$. It suffices to view $\mathbb{C}^N$ as $\otimes_i \mathbb{C}^{p_i^{e_i}}$. As $\langle b_i \otimes c_k | b_j \otimes c_l \rangle = \langle b_i | b_j \rangle . \langle c_k | c_l \rangle$ we may conclude that a tensor product of two sets with t MUBs is a set of t MUBs in the product space. Since there exist at least $1 + \min_i\{p_i^{e_i}\}$ MUBs in each $\mathbb{C}^{p_i^{e_i}}$ we may construct by tensor product of these, a set of $1 + \min_i\{p_i^{e_i}\}$ MUBs in the product space C^N.

IV. DISCUSSION ON LARGER GENERALIZATIONS AND CONCLUSION

In order to further generalize formula (3) it could be tempting to allow the index set S to be any subset of a finite ring. Unfortunately, this leads to a situation where any set of vectors could be described by such a formula. To see this, let us recall that functions f that preserve a decomposition of a ring R are arbitrary functions on each component R_i. If we choose a ring R that has no decomposition (a field, for instance) then such an f is arbitrary on R. If S is a subset $\{s_1, \ldots, s_N\}$ of N elements, then we may associate an arbitrary set of vectors $\{v_k\}_{1 \leqslant k \leqslant N}$ in $\mathbb{C}^N$ to the couples in $S \times S$ by $(s_k, s_l) \to (v_k)_l$.

This may be extended (in many ways) to a two variable function from $R \times R$ into $\mathbb{C}$ that preserves every decomposition of R (since R cannot be decomposed). One cannot expect to reach algebraic conclusions that are valid for all $N \times N$ arrays with arbitrary complex entries $(v_k)_l$.

For these reasons, it is difficult to generalize formula (3) much more. It indicates that for dimensions that are not prime powers, algebraic formulas providing complete sets of MUBs should have a radically new structure. However, do these complete sets exist for any dimension? Mathematicians are used to properties that behave differently for some particular dimensions but such an answer is unsatisfactory from a physical point of view. Wooters has shown that the absence of $N+1$ MUBs for a dimension N would be problematic for defining his discrete Wigner function in systems having N degrees of freedom (see Ref. 15).

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APPENDIX

In what follows, $\langle|\rangle$ denotes the classical Hermitian product $\langle a,b\rangle=\Sigma_i(a_i)^* b_i$. The tensor product $v\otimes w$ is defined by $(v\otimes w)_{(i,j)}=a_i.b_j$ and thus $\langle v_1\otimes w_1|v_2\otimes w_2\rangle=\langle v_1|v_2\rangle.\langle w_1|w_2\rangle$.

Proposition A.1: Let $N=N_1.N_2$ be a product of positive integers and let $\{v_{i,j}^{(1)}\}\cdots\{v_{i,j}^{(r)}\}$ be r mutually unbiased bases of $\mathbb{C}^N\cong\mathbb{C}^{N_1}\otimes\mathbb{C}^{N_2}$ (for $(i,j)\in\overline{N}:=\{1\cdots N_1\}\times\{1\cdots N_2\}$). Assume that for each $1\leqslant t\leqslant r$ there are N_1 vectors $\{a_i^{(t)}\}$ and N_2 vectors $\{b_j^{(t)}\}$ such that

$$v_{i,j}^{(t)}=a_i^{(t)}\otimes b_j^{(t)}$$

for every $(i,j)\in\overline{N}$, then for $1\leqslant t\leqslant r$, $\{a_i^{(t)}/\|a_i^{(t)}\|\}$ and $\{b_j^{(t)}/\|b_j^{(t)}\|\}$ are r mutually unbiased bases, respectively, in $\mathbb{C}^{N_1}$ and $\mathbb{C}^{N_2}$.

Proof: First we show that $\{a_i^{(t)}\}$ and $\{b_j^{(t)}\}$ are orthogonal bases. Since othonormality of $\{v_{i,j}^{(t)}\}$ implies $\langle v_{i,j}^{(t)}|v_{\underline{k,l}}^{(t)}\rangle=\delta_{\{(i,j),(k,l)\}}=\delta_{ik}\delta_{jl}$, we have $\delta_{ik}\delta_{jl}=\langle a_i^{(t)}\otimes b_j^{(t)}|a_k^{(t)}\otimes b_l^{(t)}\rangle=\langle a_i^{(t)}|a_k^{(t)}\rangle\langle b_j^{(t)}|b_l^{(t)}\rangle$. For every j, $b_j^{(t)}\neq 0$ (otherwise $v_{i,j}^{(t)}=\overline{0}$) so that $\langle a_i^{(t)}|a_k^{(t)}\rangle\langle b_j^{(t)}|b_j^{(t)}\rangle=\delta_{ik}\delta_{jj}=\delta_{ik}$ implies that $\langle a_i^{(t)}|a_k^{(t)}\rangle=0$ for $i\neq k$. Hence $\{a_i^{(t)}\}$ is a set of N_1 mutually orthogonal vectors, thus an orthogonal basis (not necessarily orthonormal) of $\mathbb{C}^{N_1}$. Permuting the role of a and b gives the same result for $\{b_j^{(t)}\}$ in $\mathbb{C}^{N_2}$. Furthermore if we fix $1\leqslant j\leqslant N_2$, the equalities $1=\langle v_{i,j}^{(t)}|v_{i,j}^{(t)}\rangle=\langle a_i^{(t)}|a_i^{(t)}\rangle\langle b_j^{(t)}|b_j^{(t)}\rangle$ may be divided by the constant $\langle b_j^{(t)}|b_j^{(t)}\rangle$ so that for every $1\leqslant i\leqslant N_1$, $L_{a^{(t)}}:=\langle a_i^{(t)}|a_i^{(t)}\rangle$ is constant with respect to i and equal to $1/\langle b_j^{(t)}|b_j^{(t)}\rangle$. Symmetrically, $L_{b^{(t)}}:=\langle b_j^{(t)}|b_j^{(t)}\rangle$ is also constant for every $1\leqslant j\leqslant N_2$ and

$$L_{a^{(t)}}:=\langle a_i^{(t)}|a_i^{(t)}\rangle=\frac{1}{\langle b_j^{(t)}|b_j^{(t)}\rangle}=\frac{1}{L_{b^{(t)}}}\quad\text{for every}\quad(i,j)\in\overline{N}. \tag{A1}$$

Now, it is sufficient to prove the MUB property for each couple of bases among the r, in $\mathbb{C}^{N_1}$ and $\mathbb{C}^{N_1}$. For instance let us consider $\{v_{i,j}^{(1)}\}$ and $\{v_{k,l}^{(2)}\}$. We define $A_{i,k}:=|\langle a_i^{(1)}|a_k^{(2)}\rangle|$ and $B_{j,l}:=|\langle b_j^{(1)}|b_l^{(2)}\rangle|$. The equality

$$1/\sqrt{N}=|\langle\underbrace{v_{i,j}^{(1)}}_{a_i^{(1)}\otimes b_j^{(1)}}\mid\underbrace{v_{k,l}^{(2)}}_{a_k^{(2)}\otimes b_l^{(2)}}\rangle|=A_{i,k}B_{j,l}\text{ for every }(i,j),(k,l)\in\bar{N} \tag{A2}$$

implies that $A_{i,k}$ and $B_{j,l}$ are nonzero. Therefore if (i,k) is fixed and (j,l) varies, $A_{i,k}$ can be simplified and all the $B_{j,l}$ are equal to a common value K_B. Symmetrically, the $A_{i,k}$ are equal to a common value K_A.

In basis $\{a_i^{(1)}\}$ we have $a_k^{(2)}=\Sigma_i\lambda_i a_i^{(1)}$ for $\lambda_i=\langle a_i^{(1)}|a_k^{(2)}\rangle/\langle a_i^{(1)}|a_i^{(1)}\rangle$. Now, equalities (A1) and (A2) prove that $|\lambda_i|=K_A/L_{a^{(1)}}$ whence it is constant for every (i,k). Therefore

$$\begin{aligned}L_{a^{(2)}}=|\langle a_k^{(2)}|a_k^{(2)}\rangle|&=\left|\left\langle\sum_i\lambda_i a_i^{(1)}\middle|\sum_{i'}\right\rangle\right|\\&=\sum_i^{N_1}|\lambda_i|^2|\langle a_i^{(1)}|a_i^{(1)}\rangle|=N_1|\lambda_i|^2L_{a^{(1)}}=N_1\left(\frac{K_A}{L_{a^{(1)}}}\right)^2L_{a^{(1)}}=\frac{N_1(K_A)^2}{L_{a^{(1)}}},\end{aligned} \tag{A3}$$

that is $L_{a^{(1)}}L_{a^{(2)}}=N_1(K_A)^2$.

Finally, we show that $\{a_i^{(1)}/\|a_i^{(1)}\|\}$ and $\{a_k^{(2)}/\|a_k^{(2)}\|\}$ are mutually unbiased bases in $\mathbb{C}^{N_1}$. Indeed

$$\left|\left\langle\frac{a_i^{(1)}}{\|a_i^{(1)}\|}\middle|\frac{a_k^{(2)}}{\|a_k^{(2)}\|}\right\rangle\right|^2=\frac{|\langle a_i^{(1)}|a_k^{(2)}\rangle|^2}{\|a_i^{(1)}\|^2\|a_k^{(2)}\|^2}=\frac{(K_A)^2}{L_{a^{(1)}}L_{a^{(2)}}}=\frac{1}{N_1}$$

(by Eq. (A3)).

The result for $\mathbb{C}^{N_2}$ is obtained in the same way, using $b_l^{(2)}=\Sigma_j\mu_j b_j^{(1)}$ for $\mu_j=\langle b_j^{(1)}|b_l^{(2)}\rangle/\langle b_j^{(1)}|b_j^{(1)}\rangle$, to give $L_{b^{(1)}}L_{b^{(2)}}=N_2(K_B)^2$. □

This proposition can immediately be extended as follows to $\mathbb{C}^N \cong \mathbb{C}^{N_1} \otimes \cdots \otimes C^{N_s}$ for dimension $N = N_1 \ldots N_s$. Under assumption that each of the k bases is a tensor product, we may use induction to conclude to the existence of k mutually unbiased bases in each $\mathbb{C}^{N_i}$.

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Second quantization method in the presence of bound states of particles

Sergey V. Peletminskii[a] and Yuriy V. Slyusarenko[b]
National Science Center, "Kharkov Institute of Physics and Technology," Akademicheskaya Str.,1, Kharkov, 61108, Ukraine

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We develop an approximate second quantization method for describing the many-particle systems in the presence of bound states of particles at low energies (the kinetic energy of particles is small in comparison to the binding energy of compound particles). In this approximation the compound and elementary particles are considered on an equal basis. This means that creation and annihilation operators of compound particles can be introduced. The Hamiltonians, which specify the interactions between compound and elementary particles and between compound particles themselves, are found in terms of the interaction amplitudes for elementary particles. The nonrelativistic quantum electrodynamics is developed for systems containing both elementary and compound particles. Some applications of this theory are considered. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The second quantization is the effective method, which is used for description of physical processes in quantum theory of many-particle systems. The key role of this method consists in introduction of creation and annihilation operators of particles in a certain quantum state. The operators of physical quantities are constructed in terms of creation and annihilation operators. Such a description of quantum many-particle systems implies the particles to be elementary (not consisting of other particles). Moreover, it is absolutely accurate despite of the possible existence of compound particles. Since the interactions between particles may lead to formation of bound states, the standard second quantization method becomes too cumbersome. For this reason the construction of approximate quantum-mechanical theory for many-particle systems consisting of elementary particles and their bound states represents an actual problem. In this theory it is necessary to introduce the creation and annihilation operators of bound states as the operators of elementary objects (not compound). In addition we should preserve the required information concerning internal degrees of freedom for bound states. Such an approach may be actually realized in the approximation in which the binding energy of compound particles is much greater in comparison to their kinetic energy.

The problems leading to the necessity of accounting for compound particles along with elementary ones are typical in studying of the interaction of irradiation with matter (the matter consists of neutral atoms or molecules). The atoms or molecules may be both in the ground and excited states when it is necessary to take into account their internal structure retaining the convenience and simplicity of the second quantization method. Such a situation should take place in describing the experiments on laser cooling of atoms[1–3] or experiments on observation of Bose–Einstein condensates in magnetic traps, where a condensate temperature is reached by laser cooling of gases of alkali atoms.[4] The similar problem of accounting for the bound states occurs also in quantum chemistry, for example, in studying of chemical reactions.

[a]Electronic mail: spelet@kipt.kharkov.ua
[b]Electronic mail: slusarenko@kipt.kharkov.ua

Thus, the construction of the quantum theory of many-particle systems in the presence of bound states of particles within the second quantization method represents not only academic but also applied interest. The formulation of the quantum theory itself is to be done so that the operators of physical quantities are constructed through the creation and annihilation operators of elementary particles and their bound states.

In this paper we demonstrate a possibility of construction of the above-mentioned quantum-mechanical theory by considering a system of two kinds of charged fermions. In this theory the compound particles (atoms) consist of two fermions of various kinds. The choice of such model is not associated with principle difficulties and makes it possible to simplify calculations and to obtain the visual results.

As applications of the developed theory we study a spontaneous radiation of two-component excited atom and obtain the expression for its probability (see, e.g., Ref. 5). We also investigate the attractive forces acting between neutral atoms at long distances (the van der Waals forces) and derive the expression for the potential of the van der Waals forces.[6] Finally we consider a question concerning the scattering of photons and elementary particles by bound states.[7]

II. CREATION AND ANNIHILATION OPERATORS OF BOUND STATES OF PARTICLES

Consider a system consisting of two kinds of fermions with masses m_1 and m_2. As was mentioned in the Introduction this case is more visual in order to demonstrate the procedure for obtaining the operators of basic physical quantities within the second quantization method in the presence of bound states of particles. We shall see that the developed methodology does not contain any difficulties for its generalization (the bound states of more than two particles, the presence of bosons in the system, the bound states of bosons and boson–fermion bound states). For simplicity we do not take into account a spin variable (this can be done without any difficulties).

Let $\hat{\psi}_1(\mathbf{x})$, $\hat{\psi}_2(\mathbf{x})$ be the annihilation operators of two kinds of fermions at the point $\mathbf{x}$,

$$\hat{\psi}_1(\mathbf{x})|0\rangle = \hat{\psi}_2(\mathbf{x})|0\rangle = 0,$$

where $|0\rangle$ is a vacuum state vector. Then the state vectors

$$|\mathbf{x}_1, \ldots, \mathbf{x}_n, \mathbf{y}_1, \ldots, \mathbf{y}_m\rangle = \hat{\psi}_1^+(\mathbf{x}_1) \cdots \hat{\psi}_1^+(\mathbf{x}_n)\hat{\psi}_2^+(\mathbf{y}_1) \cdots \hat{\psi}_2^+(\mathbf{y}_m)|0\rangle \tag{1}$$

$(n, m = 0, 1, 2, \ldots)$ form a basis in the space of states H. In these states the particles are at the certain points $\mathbf{x}_1, \ldots, \mathbf{x}_n; \mathbf{y}_1, \ldots, \mathbf{y}_m \in R$ of the coordinate space. The state vectors (1) satisfy the orthogonality and normalization relations and form a complete set of state vectors.

We assume that the particles of two different kinds form a bound state specified by the wave function

$$\varphi_\alpha(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}) = \varphi_\alpha(\mathbf{x}_1 - \mathbf{x}_2)\delta(\mathbf{x} - \mathbf{X}), \quad \mathbf{X} = \frac{m_1\mathbf{x}_1 + m_2\mathbf{x}_2}{m_1 + m_2}, \tag{2}$$

where $\mathbf{x}$ is the space coordinate and α are the quantum numbers of the bound state (atom) (we suppose that the particles of the same kind do not form the bound states). The corresponding state vector has the form

$$|\alpha, \mathbf{x}\rangle = \int \mathrm{d}\mathbf{x}_1\, \mathrm{d}\mathbf{x}_2\, \varphi_\alpha(\mathbf{x}_1 - \mathbf{x}_2)\delta(\mathbf{x} - \mathbf{X})\hat{\psi}_1^+(\mathbf{x}_1)\hat{\psi}_2^+(\mathbf{x}_2)|0\rangle.$$

For this reason the operators

$$\hat{\varphi}_\alpha^+(\mathbf{x}) = \int \mathrm{d}\mathbf{x}_1\, \mathrm{d}\mathbf{x}_2\, \varphi_\alpha(\mathbf{x}_1 - \mathbf{x}_2)\delta(\mathbf{x} - \mathbf{X})\hat{\psi}_1^+(\mathbf{x}_1)\hat{\psi}_2^+(\mathbf{x}_2) \tag{3}$$

we shall call as the creation operators of the bound states (atoms), so that

$$\hat{\varphi}_\alpha^+(\mathbf{x})|0\rangle = |\alpha,\mathbf{x}\rangle, \quad \hat{\varphi}_\alpha(\mathbf{x})|0\rangle = 0.$$

If the atom has a certain momentum, then its state vector is given by

$$|\alpha,\mathbf{p}\rangle = \frac{1}{\sqrt{\mathcal{V}}}\int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2\,\varphi_\alpha(\mathbf{x}_1-\mathbf{x}_2)e^{i\mathbf{p}\mathbf{X}}\hat{\psi}_1^+(\mathbf{x}_1)\hat{\psi}_2^+(\mathbf{x}_2)|0\rangle,$$

where $\mathcal{V}$ is the volume of the system. The corresponding creation operator $\hat{\varphi}_\alpha^+(\mathbf{p})$ of the atom in the state with momentum $\mathbf{p}$ is defined by

$$|\alpha,\mathbf{p}\rangle = \hat{\varphi}_\alpha^+(\mathbf{p})|0\rangle, \quad \hat{\varphi}_\alpha^+(\mathbf{x}) = \frac{1}{\sqrt{\mathcal{V}}}\sum_{\mathbf{p}} \hat{\varphi}_\alpha^+(\mathbf{p})e^{-i\mathbf{p}\mathbf{x}}.$$

Taking into account that

$$\int \mathrm{d}\mathbf{y}_1\,\varphi_\alpha^*(\mathbf{y}_1-\mathbf{y}_2)\varphi_\beta(\mathbf{y}_1-\mathbf{y}_2) = \delta_{\alpha\beta},$$

it is easy to find the following commutation relations:

$$[\hat{\varphi}_\alpha(\mathbf{x}),\hat{\varphi}_{\alpha'}^+(\mathbf{x}')] = \delta_{\alpha\alpha'}\delta(\mathbf{x}-\mathbf{x}') + \hat{\chi}_{\alpha\alpha'}(\mathbf{x},\mathbf{x}'), \quad [\hat{\varphi}_\alpha(\mathbf{x}),\hat{\varphi}_{\alpha'}(\mathbf{x}')] = 0,$$

where

$$\hat{\chi}_{\alpha\alpha'}(\mathbf{x},\mathbf{x}') = \int \mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{y}'\,\varphi_\alpha^*(\mathbf{y})\varphi_{\alpha'}(\mathbf{y}')\left\{\hat{\psi}_1^+\left(\mathbf{x}+\frac{m_2}{M}\mathbf{y}\right)\hat{\psi}_1\left(\mathbf{x}'+\frac{m_2}{M}\mathbf{y}'\right)\delta\left(\mathbf{y}-\mathbf{y}'-\frac{m_1}{M}(\mathbf{x}-\mathbf{x}')\right)\right.$$
$$\left. + \hat{\psi}_2^+\left(\mathbf{x}'-\frac{m_1}{M}\mathbf{y}'\right)\hat{\psi}_2\left(\mathbf{x}-\frac{m_1}{M}\mathbf{y}\right)\delta\left(\mathbf{y}-\mathbf{y}'+\frac{m_2}{M}(\mathbf{x}-\mathbf{x}')\right)\right\}, \quad M = m_1+m_2,$$

moreover, $\hat{\chi}_{\alpha\alpha'}(\mathbf{x},\mathbf{x}')|0\rangle = 0$. The vectors

$$|\underbrace{\mathbf{x}_1,\ldots}_{n},\underbrace{\mathbf{y}_1,\ldots}_{m},\underbrace{\mathbf{z}_1,\ldots}_{l}\rangle \equiv \prod_{i=1}^{n}\hat{\psi}_1^+(\mathbf{x}_i)\prod_{k=1}^{m}\hat{\psi}_2^+(\mathbf{y}_k)\prod_{j=1}^{l}\hat{\varphi}_{\alpha_j}^+(\mathbf{z}_j)|0\rangle \tag{4}$$

have an obvious physical meaning under the following conditions:

$$|\mathbf{x}_i-\mathbf{x}_j| \gtrsim a, \quad |\mathbf{y}_i-\mathbf{y}_j| \gtrsim a, \quad |\mathbf{z}_i-\mathbf{z}_j| \gtrsim a,$$
$$|\mathbf{x}_i-\mathbf{y}_j| \gtrsim a, \quad |\mathbf{x}_i-\mathbf{z}_j| \gtrsim a, \quad |\mathbf{y}_i-\mathbf{z}_j| \gtrsim a \tag{5}$$

($\mathbf{x},\mathbf{y},\mathbf{z} \in R_a$, $a \gg r_0$, r_0 is the radius of the bound state; the definition of a see below). In this case the elementary particles and their bound states are at the certain space points.

Notice that the state vectors (4) do not form a basis in the Gilbert space H if (5) are valid. However, their linear span, which is a totality of the following vectors:

$$\sum_{n,m,l}\underbrace{\int \mathrm{d}\mathbf{x}_1\cdots\int \mathrm{d}\mathbf{y}_1\cdots\int \mathrm{d}\mathbf{z}_1\cdots}_{R_a} C(\underbrace{\mathbf{x}_1,\ldots}_{n},\underbrace{\mathbf{y}_1,\ldots}_{m},\underbrace{\mathbf{z}_1,\ldots}_{l})|\underbrace{\mathbf{x}_1,\ldots}_{n},\underbrace{\mathbf{y}_1,\ldots}_{m},\underbrace{\mathbf{z}_1,\ldots}_{l}\rangle, \tag{6}$$

form a subspace H_a of the space H. Let us show that the state vectors (4) [with conditions (5)] form an orthonormalized basis in the subspace H_a. To this end it is necessary to take into account that in calculating of the following vacuum averages:

$$\langle 0|\hat{\psi}_1(\mathbf{x}_1)\cdots\hat{\psi}_2(\mathbf{x}_2)\cdots\hat{\varphi}_\alpha(\mathbf{x})\hat{\varphi}_{\alpha'}^+(\mathbf{x}')\cdots\hat{\psi}_2^+(\mathbf{x}_2')\cdots\hat{\psi}_1^+(\mathbf{x}_1')\cdots|0\rangle$$

we can use the Wick theorem with the following contractions:

$$\underset{a}{\hat{\psi}_i}(\mathbf{x})\underset{a}{\hat{\psi}^+_{i'}}(\mathbf{x}') = \langle 0|\hat{\psi}_i(\mathbf{x})\hat{\psi}^+_{i'}(\mathbf{x}')|0\rangle = \delta_{ii'}\delta(\mathbf{x}-\mathbf{x}'),\quad \underset{a}{\hat{\psi}_i}(\mathbf{x})\underset{a}{\hat{\psi}_{i'}}(\mathbf{x}') = 0,$$

if to consider the operators $\hat{\psi}_1$, $\hat{\psi}_2$, $\hat{\varphi}$ referred to the moment of time +0, and operators $\hat{\varphi}^+$, $\hat{\psi}^+_2$, $\hat{\psi}^+_1$ to the moment of time −0. In addition, we should remember that the creation and annihilation operators $\hat{\varphi}_\alpha$, $\hat{\varphi}^+_{\alpha'}$ depend on $\hat{\psi}_i$, $\hat{\psi}_{i'}$ [see (3)]. We also assume that the wave function (2) of the atom differs from zero for $|\mathbf{x}_1-\mathbf{x}_2|<r_0$. Taking into account (3) and noting that for $|\mathbf{x}'_1-\mathbf{x}'_2|>a$,

$$\underset{ab}{\hat{\varphi}_\alpha}(\mathbf{z})\underset{b}{\hat{\psi}^+_2}(\mathbf{x}'_2)\underset{a}{\hat{\psi}^+_1}(\mathbf{x}'_1) = \int \mathrm{d}\mathbf{z}_1\,\mathrm{d}\mathbf{z}_2\varphi^*_\alpha(\mathbf{z}_1-\mathbf{z}_2)\delta(\mathbf{z}-\mathbf{Z})\underset{a}{\hat{\psi}_1}(\mathbf{z}_1)\underset{b}{\hat{\psi}_2}(\mathbf{z}_2)\underset{b}{\hat{\psi}^+_2}(\mathbf{x}'_2)\underset{a}{\hat{\psi}^+_1}(\mathbf{x}'_1)$$
$$= \varphi^*_\alpha(\mathbf{x}'_1-\mathbf{x}_2{}')\delta(\mathbf{z}-\mathbf{X}') = 0,$$

$$\mathbf{X}' = \frac{m_1\mathbf{x}'_1+m_2\mathbf{x}'_2}{m_1+m_2}$$

and also

$$\underset{ab}{\hat{\varphi}_\alpha}(\mathbf{z})\underset{ba}{\hat{\varphi}^+_{\alpha'}}(\mathbf{z}') = \int \mathrm{d}\mathbf{z}_1\mathrm{d}\mathbf{z}_2\mathrm{d}\mathbf{z}'_1\mathrm{d}\mathbf{z}'_2\varphi^*_\alpha(\mathbf{z}_1-\mathbf{z}_2)\delta(\mathbf{z}-\mathbf{Z})\varphi_{\alpha'}(\mathbf{z}'_1-\mathbf{z}_2{}')\delta(\mathbf{z}'$$
$$-\mathbf{Z}')\underset{a}{\hat{\psi}_1}(\mathbf{z}_1)\underset{b}{\hat{\psi}_2}(\mathbf{z}_2)\underset{b}{\hat{\psi}^+_2}(\mathbf{z}'_2)\underset{a}{\hat{\psi}^+_1}(\mathbf{z}'_1)$$
$$= \int \mathrm{d}\mathbf{z}_1\,\mathrm{d}\mathbf{z}_2\varphi^*_\alpha(\mathbf{z}_1-\mathbf{z}_2)\delta(\mathbf{z}-\mathbf{Z})\varphi_{\alpha'}(\mathbf{z}_1-\mathbf{z}_2)\delta(\mathbf{z}'-\mathbf{Z}) = \delta_{\alpha\alpha'}\delta(\mathbf{z}-\mathbf{z}')$$

(the double contractions correspond to the operators $\hat{\varphi}_\alpha$, $\hat{\varphi}^+_\alpha$) we get

$$\langle 0|\underbrace{\hat{\psi}_1(\mathbf{x}_1)\cdots}_{n}\underbrace{\hat{\psi}_2(\mathbf{y}_1)\cdots}_{m}\underbrace{\hat{\varphi}_{\alpha_1}(\mathbf{z}_1)\cdots}_{l}\underbrace{\hat{\varphi}^+_{\alpha'_1}(\mathbf{z}'_1)\cdots}_{l'}\underbrace{\hat{\psi}^+_2(\mathbf{y}'_1)\cdots}_{m'}\underbrace{\hat{\psi}_1(\mathbf{x}'_1)\cdots}_{n'}|0\rangle$$
$$= \delta_{nn'}\delta_{mm'}\delta_{ll'}\sum\mathcal{P}_{x'}\mathcal{P}_{y'}\underbrace{\delta(\mathbf{x}_1-\mathbf{x}'_1)\cdots}_{n}\underbrace{\delta(\mathbf{y}_1-\mathbf{y}'_1)\cdots}_{m}\underbrace{\delta(\mathbf{z}_1-\mathbf{z}'_1)\delta_{\alpha_1\alpha'_1}\cdots}_{l}. \tag{7}$$

This relation shows that the vectors (6) form the orthonormalized basis in the subspace H_a if to consider the creation and annihilation operators $\hat{\varphi}^+_\alpha(\mathbf{z})$, $\hat{\varphi}_\alpha(\mathbf{z})$ as the Bose operators, which commute with $\hat{\psi}_i(\mathbf{x})$, $\hat{\psi}^+_i(\mathbf{x})$. The quantity $\mathcal{P}_{x'}$ in (7) is equal to +1 if the number of permutations of the arguments $\mathbf{x}'_1\cdots\mathbf{x}'_n$ is even and it is equal to −1 if the number of these permutations is odd. The quantity $\mathcal{P}_{y'}$ is defined similarly. However, the case when it is necessary to take into account a more complicated arrangement of the contractions between $\hat{\varphi}_\alpha$, $\hat{\varphi}^+_\alpha$:

$$\underset{a}{\mathbf{x}_4}\underset{b}{\mathbf{x}'_4}\cdots\underset{c}{\mathbf{x}_2}\underset{d}{\mathbf{x}'_2}\cdots\underset{e}{\mathbf{x}_1}\underset{e}{\mathbf{x}'_1}\cdots\underset{c}{\mathbf{x}_3}\underset{b}{\mathbf{x}'_3}\cdots\underset{a}{}$$

can take place (the odd indices correspond to the creation operators and even to annihilation operators). Since $\mathbf{x}'_1=\mathbf{x}'_2$, $\mathbf{x}_2=\mathbf{x}_3$, $\mathbf{x}'_4=\mathbf{x}'_3$,

$$|\mathbf{x}_1-\mathbf{x}'_1|\lesssim r_0,\ |\mathbf{x}'_1-\mathbf{x}_2|\lesssim r_0,\ |\mathbf{x}'_3-\mathbf{x}_2|\lesssim r_0,\ |\mathbf{x}_4-\mathbf{x}'_3|\lesssim r_0,$$

whence $|\mathbf{x}_4-\mathbf{x}_1|\lesssim 4r_0$. Therefore, if $a\leqslant 4r_0$, then the above contractions are to be taken into account. If however, we consider the n-particle states, then the discussed arrangements of the contractions are not to be taken into account for $n\lesssim a/r_0$ [we emphasize that r_0/a is a small parameter in our problem, see (11)]. The above mentioned concerns the majority of problems in nonrelativistic quantum theory, where a finite number of particles is usually studied (see Secs. V and VI).

With the use of (7) it is easy to find the projection operator $\mathcal{P}_{H_a}$ onto the subspace H_a,

$$\mathcal{P}_{H_a} = \sum_{k+m+l\leqslant n} \frac{1}{k!}\frac{1}{m!}\frac{1}{l!} \underbrace{\int \mathbf{dx}_1 \cdots \int \mathbf{dy}_1 \cdots \int \mathbf{dz}_1 \cdots}_{R_a} |\underbrace{\mathbf{x}_1 \cdots}_{k} \underbrace{\mathbf{y}_1 \cdots}_{m} \underbrace{\mathbf{z}_1 \cdots}_{l}\rangle \times \langle \underbrace{\mathbf{x}_1 \cdots}_{k} \underbrace{\mathbf{y}_1 \cdots}_{m} \underbrace{\mathbf{z}_1 \cdots}_{l}|,$$

such that the operators $\underline{A}$ acting in the subspace $H_a \in H$ correspond to the operators of physical quantities A that act in H (hereinafter the sums of $1,2,\ldots,n$-particle subspaces over the bound states are considered; $n \approx a/r_0 \gg 1$),

$$\underline{A} = \mathcal{P}_{H_a} A \mathcal{P}_{H_a}. \tag{8}$$

Let us introduce now an auxiliary space $\tilde{H}$ with the Fermi creation and annihilation operators $\hat{\chi}_1^+(\mathbf{x})$, $\hat{\chi}_2^+(\mathbf{x})$, $\hat{\chi}_1(\mathbf{x})$, $\hat{\chi}_2(\mathbf{x})$ and Bose creation and annihilation operators $\hat{\eta}_\alpha^+(\mathbf{x})$, $\hat{\eta}_\alpha(\mathbf{x})$ and take the vectors

$$|\mathbf{x}_1, \ldots, \mathbf{y}_1, \ldots, \mathbf{z}_1, \ldots) = \hat{\chi}_1^+(\mathbf{x}_1) \cdots \hat{\chi}_2^+(\mathbf{y}_1) \cdots \hat{\eta}_\alpha^+(\mathbf{z}_1) \cdots |0),$$

as a basis of this space, where $|0)$ is a vacuum vector in $\tilde{H}$. Then the linear span of the vectors

$$|\mathbf{x}_1, \ldots, \mathbf{y}_1, \ldots, \mathbf{z}_1, \ldots) \in \tilde{H}_a, \quad \mathbf{x},\mathbf{y},\mathbf{z} \in R_a$$

determines the subspace $\tilde{H}_a$ of the space $\tilde{H}$.

Now we can easily establish the isomorphic correspondence between H_a and $\tilde{H}_a$:

$$|\mathbf{x}_1, \ldots, \mathbf{y}_1, \ldots, \mathbf{z}_1, \ldots\rangle \Leftrightarrow |\mathbf{x}_1, \ldots, \mathbf{y}_1, \ldots, \mathbf{z}_1, \ldots),$$

which preserves the scalar product

$$\langle \mathbf{x}', \ldots, \mathbf{y}', \ldots, \mathbf{z}', \ldots |\mathbf{x}, \ldots, \mathbf{y}, \ldots, \mathbf{z} \ldots\rangle = (\mathbf{x}', \ldots, \mathbf{y}', \ldots, \mathbf{z}', \ldots |\mathbf{x}, \ldots, \mathbf{y}, \ldots, \mathbf{z} \ldots), \quad \mathbf{x},\mathbf{y},\mathbf{z};\mathbf{x}',\mathbf{y}',\mathbf{z}' \in R_a.$$

We can also establish the isomorphism between the operators $\underline{A} \Leftrightarrow \tilde{A}$, acting in the spaces H_a and $\tilde{H}_a$ according to the formula:

$$(\mathbf{x}', \ldots, \mathbf{y}', \ldots, \mathbf{z}', \ldots |\underline{A}|\mathbf{x}, \ldots, \mathbf{y}, \ldots, \mathbf{z} \ldots) = \langle \mathbf{x}', \ldots, \mathbf{y}', \ldots, \mathbf{z}', \ldots |\tilde{A}|\mathbf{x}, \ldots, \mathbf{y}, \ldots, \mathbf{z} \ldots\rangle. \tag{9}$$

This isomorphic correspondence is remained after the multiplication of the operator by a number, after addition of operators, and after multiplication of operators:

$$\lambda\underline{A} \Leftrightarrow \lambda\tilde{A}, \quad \underline{A} + \underline{B} \Leftrightarrow \tilde{A} + \tilde{B}, \quad \underline{A}\underline{B} \Leftrightarrow \tilde{A}\tilde{B}.$$

The formulas (8) and (9) lead to

$$(\mathbf{x}', \ldots, \mathbf{y}', \ldots, \mathbf{z}', \ldots |\tilde{A}|\mathbf{x}, \ldots, \mathbf{y}, \ldots, \mathbf{z} \ldots) = \langle \mathbf{x}', \ldots, \mathbf{y}', \ldots, \mathbf{z}', \ldots |A|\mathbf{x}, \ldots, \mathbf{y}, \ldots, \mathbf{z} \ldots\rangle. \tag{10}$$

This relation determines the operators of various physical quantities $\tilde{A}$ acting in $\tilde{H}_a$ and, hence, transfers the quantum theory in which the compound (the bound states) and elementary particles exist on an equal basis from the space of states H onto the space of states $\tilde{H}_a$. We would like to remind here that $\hat{\varphi}_\alpha^+$ entering (4) is determined by (3).

The relation (10) defines the operator $\tilde{A}$ in $\tilde{H}_a$ uniquely, but it does not define it uniquely in $\tilde{H}$. It is evident that the operator $\tilde{A}$ acting in $\tilde{H}$ (continued from $\tilde{H}_a$ to the whole space $\tilde{H}$) is determined up to the term $\tilde{A}'$, the matrix elements of which are zero in the space $\tilde{H}_a(\tilde{A}=\tilde{A}'+\tilde{A}'')$. If to introduce the projection operator $\mathcal{P}_{\tilde{H}_a}$ onto the subspace $\tilde{H}_a$ and to require that the operator $\tilde{A}$ has no nonzero matrix elements in the orthogonal subspace, then the operator $\tilde{A}$ will be defined in $\tilde{H}$ uniquely, $\tilde{A}=\mathcal{P}_{\tilde{H}_a}\tilde{A}''\mathcal{P}_{\tilde{H}_a}$. We will omit the projection operator $\mathcal{P}_{\tilde{H}_a}$ when constructing the operator $\tilde{A}$ acting in $\tilde{H}$. The reason for this is the assumption that the matrix elements of the operators (in the position space), corresponding to a quite large external parameter $R\sim|\mathbf{x}_i-\mathbf{x}_j|$ give a dominant contribution to the quantum-mechanical processes. Further we will assume that $R\gg r_0$ (usually in case of particle collisions $R^{-1}\sim\sqrt{m\mathcal{E}}$, where $\mathcal{E}$ is the particle kinetic energy). The latter inequality makes it possible to choose parameter a [see (5)] as follows:[8]

$$R\gg a\gg r_0. \tag{11}$$

The matrix elements of the operators should not depend on parameter a chosen by this way. Let us mentally decrease the radius of a bound state, $r_0\to 0$. Then the whole written scheme, as we have already noted, does not depend on a up to the values $a=r_0$. Therefore, the subspace $\tilde{H}_a$ can be identified with $\tilde{H}$ due to the inequality $R\gg a$. In other words, one can consider that $\mathcal{P}_{\tilde{H}_a}\to 1$ for $a\to 0$. At the same time we do not break the quantum-mechanical description of bound states in virtue of the inequality $a\gg r_0$. From the physical point of view the inequality $r_0\ll R$ gives the stability domain for the bound states considered as elementary particles. The calculation of the following approximation is to be associated with accounting of the difference of the subspace H_a from the space H.

Finally we note that for an arbitrary vector $|\ )\in\tilde{H}_a$ the following evident relations are valid:

$$\hat{\zeta}(\mathbf{x})\hat{\xi}(\mathbf{x}')|\ )=0,\ \ (\ |\hat{\zeta}^+(\mathbf{x})\hat{\xi}^+(\mathbf{x}')=0,\ \ |\mathbf{x}-\mathbf{x}'|<a, \tag{12}$$

or

$$\hat{\zeta}(\mathbf{x})\hat{\xi}(\mathbf{x}')\tilde{H}_a=0,\ \ \tilde{H}_a\hat{\zeta}^+(\mathbf{x})\hat{\xi}^+(\mathbf{x}')=0,\ \ |\mathbf{x}-\mathbf{x}'|<a,$$

where $\hat{\zeta}$ and $\hat{\xi}$ are any of the annihilation operators $\hat{\chi}_1$, $\hat{\chi}_2$, $\hat{\eta}$.

III. THE STRUCTURE OF $\tilde{\hat{A}}(\mathbf{u},\mathbf{v})$ OPERATORS

Here we consider the method for obtaining the operators $\tilde{\hat{A}}$. Let the operator $\hat{A}$ represent a normal-ordered production of $\hat{\psi}_i(\mathbf{v})$, $\hat{\psi}_i^+(\mathbf{u})$ $(i=1,2)$,

$$\hat{A}(\mathbf{u},\mathbf{v})=\hat{\psi}_1^+(\mathbf{u}_1)\cdots\hat{\psi}_2^+(\mathbf{u}_2)\hat{\psi}_1(\mathbf{v}_1)\cdots\hat{\psi}_2(\mathbf{v}_2)\cdots\ . \tag{13}$$

The operators of such type are the particle density operator $\hat{\rho}_i(\mathbf{x})$,

$$\hat{\rho}_i(\mathbf{x})=\hat{\psi}_i^+(\mathbf{x})\hat{\psi}_i(\mathbf{x}),$$

the momentum density operator $\hat{\pi}_i(\mathbf{x})$,

$$\hat{\pi}_i(\mathbf{x})=-\frac{i}{2}\left(\hat{\psi}_i^+(\mathbf{x})\frac{\partial\hat{\psi}_i(\mathbf{x})}{\partial\mathbf{x}}-\frac{\partial\hat{\psi}_i^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\psi}_i(\mathbf{x})\right),$$

a Hamiltonian of the system, etc.

The matrix element on the right-hand side of (10) may be written as the following vacuum average:

$$\langle 0|\hat{\psi}_1(\mathbf{x}_1)\cdots\hat{\psi}_2(\mathbf{x}_2)\cdots\hat{\varphi}_\alpha(\mathbf{x})\cdots\hat{A}(\mathbf{u},\mathbf{v})\hat{\varphi}^+_{\alpha'}(\mathbf{x})\cdots\hat{\psi}_2(\mathbf{x}'_2)\cdots\hat{\psi}_1(\mathbf{x}'_1)\cdots|0\rangle.$$

Let us note that when calculating this average by using Wick's theorem, the quantity, which is averaged over the vacuum state has the meaning of a mixed T-product if to consider the operators $\hat{\psi}_1,\ldots,\hat{\psi}_2,\ldots,\hat{\varphi},\ldots$ referring to the moment of time +0, the operators $\hat{\psi}^+_1,\ldots,\hat{\psi}^+_2,\hat{\varphi}^+,\ldots$ to −0, and the normal-ordered operator $\hat{A}(\mathbf{u},\mathbf{v})$ referring to the moment of time 0. Thus, there is no need to place the contractions inside the expression for $\hat{A}(\mathbf{u},\mathbf{v})$. Let

$$A_b(\mathbf{y};\mathbf{y}';\mathbf{u},\mathbf{v}) \equiv A_b(\mathbf{y}_1,\ldots,\mathbf{y}_2,\ldots,\mathbf{y},\ldots;\mathbf{y}'_1,\ldots,\mathbf{y}'_2,\ldots,\mathbf{y}',\ldots;\mathbf{u},\mathbf{v}) \tag{14}$$

be the analytic expression that corresponds to the diagram "b." For this diagram the operators with the arguments $\mathbf{u}$ are related to the operators with the arguments $\mathbf{y}_1,\ldots,\mathbf{y}_2,\ldots,\mathbf{y},\ldots$. In addition, the latter arguments are spaced apart by the distances greater than a and coincide with some of the arguments $\mathbf{x}_1,\ldots,\mathbf{x}_2,\ldots,\mathbf{x},\ldots$. The similar statement should be also made concerning the arguments $\mathbf{y}'_1,\ldots,\mathbf{y}'_2,\ldots,\mathbf{y}',\ldots$. Then, the operator $\tilde{\hat{A}}(\mathbf{u},\mathbf{v})$ acting in $\tilde{H}$ is given, according to (5), by

$$\tilde{\hat{A}}(\mathbf{u},\mathbf{v}) = \sum_b \int \hat{R}_1\hat{R}_2\hat{R}A_b(\mathbf{y};\mathbf{y}';\mathbf{u},\mathbf{v})\hat{R}'_1\hat{R}'_2\hat{R}', \tag{15}$$

where

$$\hat{R}_1 = \prod \hat{\chi}^+(\mathbf{y}_1)d\mathbf{y}_1,\ \ \hat{R}_2 = \prod \hat{\chi}^+(\mathbf{y}_2)d\mathbf{y}_2,\ \ \hat{R} = \prod \hat{\eta}^+(\mathbf{y})d\mathbf{y},$$

$$\hat{R}'_1 = \prod \hat{\chi}(\mathbf{y}'_1)d\mathbf{y}'_1,\ \ \hat{R}'_2 = \prod \hat{\chi}(\mathbf{y}'_2)d\mathbf{y}'_2,\ \ \hat{R}' = \prod \hat{\eta}(\mathbf{y}')d\mathbf{y}'.$$

Here the summation is taken over all diagrams of the described type.

If $\hat{A}(\mathbf{v})=1$ [see the proof of (7)], then $\tilde{\hat{A}}(\mathbf{v})=1$ on the subspace $\tilde{H}_a$. Let now $\hat{A}(\mathbf{u},\mathbf{v})=\hat{\psi}_1(\mathbf{v})$. Then the only diagrams of the described type for the vacuum average $\langle 0|\cdots\hat{\psi}_1(\mathbf{v})\cdots|0\rangle$ are the following diagrams:

$$A_{b_1} = \underset{a}{\hat{\psi}_1}(\mathbf{v})\ldots\underset{a}{\hat{\psi}^+_1}(\mathbf{y}'),\ \ A_{b_2} = \underset{a}{\hat{\psi}_2}(\mathbf{y}_2)\cdots\underset{b}{\hat{\psi}_1}(\mathbf{v})\cdots\underset{ba}{\hat{\varphi}^+_\alpha}(\mathbf{y}').$$

The expressions

$$A_{b_1}(\mathbf{y}'_1;\mathbf{v}) = \delta(\mathbf{v}-\mathbf{y}'_1),$$

$$A_{b_2}(\mathbf{y}_2;\mathbf{y}',\mathbf{v}) = \int d\mathbf{x}_1\, d\mathbf{x}_2\, \varphi_\alpha(\mathbf{x}_1-\mathbf{x}_2)\delta(\mathbf{y}'-\mathbf{X})\delta(\mathbf{v}-\mathbf{x}_1)\delta(\mathbf{x}_2-\mathbf{y}_2) = \varphi_\alpha(\mathbf{v},\mathbf{y}_2,\mathbf{y}'),$$

correspond to the above-mentioned diagrams. Here $\varphi_\alpha(\mathbf{v},\mathbf{y}_2,\mathbf{y}')$ is defined in accordance with (2). Therefore, according to (15) we have

$$\tilde{\hat{\psi}}_1(\mathbf{v}) = \int d\mathbf{y}'_1\, A_{b_1}(\mathbf{y}'_1,\mathbf{v})\hat{\chi}_1(\mathbf{y}'_1) + \int d\mathbf{y}_2\, d\mathbf{y}'\, A_{b_2}(\mathbf{y}_2;\mathbf{y}',\mathbf{v})\hat{\chi}^+_2(\mathbf{y}_2)\hat{\eta}(\mathbf{y}') = \hat{\chi}_1(\mathbf{v}) + \hat{O}_1(\mathbf{v}), \tag{16}$$

where

$$\hat{O}_1(\mathbf{v}) = \int d\mathbf{y}\ \hat{\varphi}(\mathbf{v},\mathbf{y})\hat{\chi}^+_2(\mathbf{y}),\ \ \hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2) = \varphi_\alpha(\mathbf{x})\hat{\eta}_\alpha(\mathbf{X}) \tag{17}$$

and $\mathbf{X}$ is given by (2), $\mathbf{x}=\mathbf{x}_1-\mathbf{x}_2$. Similarly, one finds

$$\tilde{\hat{\psi}}_2(\mathbf{v}) = \hat{\chi}_2(\mathbf{v}) + \hat{O}_2(\mathbf{v}), \tag{18}$$

where

$$\hat{O}_2(\mathbf{v}) = \int \mathrm{d}\mathbf{y}\, \hat{\chi}_1^+(\mathbf{y})\hat{\varphi}(\mathbf{y},\mathbf{v}).$$

When deriving (16) and (18), we have essentially used the inequalities (5).

Now let us consider $\hat{A}(\mathbf{u},\mathbf{v}) = \hat{\psi}_1^+(\mathbf{u})\hat{\psi}_1(\mathbf{v})$. In this case the following five diagrams

$$A_1 = \underset{a}{\hat{\psi}} \cdots \underset{a}{\hat{\psi}_1^+}(\mathbf{u}) \underset{b}{\hat{\psi}_1}(\mathbf{v}) \cdots \underset{b}{\hat{\psi}^+}, \quad A_2 = \underset{a}{\hat{\psi}} \cdots \underset{b}{\hat{\psi}} \cdots \underset{b}{\hat{\psi}_1^+}(\mathbf{u}) \underset{c}{\hat{\psi}_1}(\mathbf{v}) \cdots \underset{ca}{\hat{\varphi}^+},$$

$$A_3 = \underset{ab}{\hat{\varphi}} \cdots \underset{b}{\hat{\psi}_1^+}(\mathbf{u}) \underset{c}{\hat{\psi}_1}(\mathbf{v}) \cdots \underset{c}{\hat{\psi}^+} \cdots \underset{a}{\hat{\psi}^+},$$

$$A_4 = \underset{ab}{\hat{\varphi}} \cdots \underset{b}{\hat{\psi}_1^+}(\mathbf{u}) \underset{c}{\hat{\psi}_1}(\mathbf{v}) \cdots \underset{ca}{\hat{\varphi}^+}, \quad A_5 = \underset{a}{\hat{\psi}} \cdots \underset{bd}{\hat{\varphi}} \cdots \underset{d}{\hat{\psi}_1^+}(\mathbf{u}) \underset{c}{\hat{\psi}_1}(\mathbf{v}) \cdots \underset{ca}{\hat{\varphi}^+} \cdots \underset{b}{\hat{\psi}^+}$$

correspond to this operator (the indices 1 and 2 for $\hat{\psi}$ and $\hat{\psi}^+$ can be easily restored if we take into account (3) and the definition of contractions). The analytic expressions for these diagrams have the form

$$\tilde{\hat{A}}_1 = \hat{\chi}_1^+(\mathbf{u}_1)\hat{\chi}_1(\mathbf{v}_1), \quad \tilde{\hat{A}}_2 = \int \mathrm{d}\mathbf{z}_1\, \mathrm{d}\mathbf{z}_2\, \hat{\varphi}(\mathbf{z}_1,\mathbf{z}_2)\delta(\mathbf{z}_1 - \mathbf{v}_1)\hat{\chi}_1^+(\mathbf{u}_1)\hat{\chi}_2^+(\mathbf{z}_2) = \int \mathrm{d}\mathbf{z}_2\, \hat{\varphi}(\mathbf{v}_1,\mathbf{z}_2)\hat{\chi}_1^+(\mathbf{u}_1)\hat{\chi}_2^+(\mathbf{z}_2),$$

$$\tilde{\hat{A}}_3 = \int \mathrm{d}\mathbf{z}_1\, \mathrm{d}\mathbf{z}_2\, \hat{\varphi}^+(\mathbf{z}_1,\mathbf{z}_2)\delta(\mathbf{z}_1 - \mathbf{u}_1)\hat{\chi}_2(\mathbf{z}_2)\hat{\chi}_1(\mathbf{v}_1) = \int \mathrm{d}\mathbf{z}_2\, \hat{\varphi}^+(\mathbf{u}_1,\mathbf{z}_2)\hat{\chi}_2(\mathbf{z}_2)\hat{\chi}_1(\mathbf{v}_1),$$

$$\tilde{\hat{A}}_4 = \int \mathrm{d}\mathbf{z}_1\, \mathrm{d}\mathbf{z}_2\, \mathrm{d}\mathbf{z}_1'\, \mathrm{d}\mathbf{z}_2'\, \hat{\varphi}^+(\mathbf{z}_1,\mathbf{z}_2)\hat{\varphi}(\mathbf{z}_1',\mathbf{z}_2')\delta(\mathbf{z}_1 - \mathbf{u}_1)\delta(\mathbf{v}_1 - \mathbf{z}_1')\delta(\mathbf{z}_2 - \mathbf{z}_2') = \int \mathrm{d}\mathbf{z}_2\, \hat{\varphi}^+(\mathbf{u}_1,\mathbf{z}_2)\hat{\varphi}(\mathbf{v}_1,\mathbf{z}_2),$$

$$\begin{aligned}\tilde{\hat{A}}_5 &= -\int \mathrm{d}\mathbf{z}_1\, \mathrm{d}\mathbf{z}_2\, \mathrm{d}\mathbf{z}_1'\, \mathrm{d}\mathbf{z}_2'\, \hat{\varphi}^+(\mathbf{z}_1,\mathbf{z}_2)\hat{\varphi}(\mathbf{z}_1',\mathbf{z}_2')\delta(\mathbf{z}_1 - \mathbf{u}_1)\delta(\mathbf{v}_1 - \mathbf{z}_1')\hat{\chi}_2^+(\mathbf{z}_2')\hat{\chi}_2(\mathbf{z}_2) \\ &= -\int \mathrm{d}\mathbf{z}_2\, \mathrm{d}\mathbf{z}_2'\, \hat{\varphi}^+(\mathbf{u}_1,\mathbf{z}_2)\hat{\varphi}(\mathbf{v}_1,\mathbf{z}_2')\hat{\chi}_2^+(\mathbf{z}_2')\hat{\chi}_2(\mathbf{z}_2),\end{aligned}$$

whence, we find the operators (15) corresponding to the diagrams (14),

$$\tilde{\hat{A}}_1 = \hat{\chi}_1^+(\mathbf{u}_1)\hat{\chi}_1(\mathbf{v}_1), \quad \tilde{\hat{A}}_2 = \hat{\chi}_1^+(\mathbf{u}_1)\hat{O}_1(\mathbf{v}_1), \quad \tilde{\hat{A}}_3 = \hat{O}_1^+(\mathbf{u}_1)\hat{\chi}_1(\mathbf{v}_1), \quad \tilde{\hat{A}}_4 + \tilde{\hat{A}}_5 = \hat{O}_1^+(\mathbf{u}_1)\hat{O}_1(\mathbf{v}_1).$$

In obtaining the latter expression, we have taken into account the anticommutative relations for $\hat{\chi}$, $\hat{\chi}^+$. Next bearing in mind (16) and (18) we obtain the final expression for $\tilde{\hat{A}}(\mathbf{u},\mathbf{v}) = \hat{\psi}_1^+(\widetilde{\mathbf{u}_1})\hat{\psi}_1(\mathbf{v}_1)$ that corresponds to $\hat{A}(\mathbf{u},\mathbf{v}) = \hat{\psi}_1^+(\mathbf{u}_1)\hat{\psi}_1(\mathbf{v}_1)$:

$$\hat{\psi}_1^+(\mathbf{u}_1)\hat{\psi}_1(\mathbf{v}_1) \to \hat{\psi}_1^+(\widetilde{\mathbf{u}_1})\hat{\psi}_1(\mathbf{v}_1) = \tilde{\hat{\psi}}_1^+(\mathbf{u}_1)\tilde{\hat{\psi}}_1(\mathbf{v}_1). \tag{19}$$

Similarly, one gets

$$\hat{\psi}_1(\mathbf{u}_1)\hat{\psi}_1(\mathbf{v}_1) \to \hat{\psi}_1(\widetilde{\mathbf{u}_1})\hat{\psi}_1(\mathbf{v}_1) = \tilde{\hat{\psi}}_1(\mathbf{u}_1)\tilde{\hat{\psi}}_1(\mathbf{v}_1),$$
$$\hat{\psi}_1^+(\mathbf{u}_1)\hat{\psi}_2(\mathbf{v}_1) \to \hat{\psi}_1^+(\widetilde{\mathbf{u}_1})\hat{\psi}_2(\mathbf{v}_1) = \tilde{\hat{\psi}}_1^+(\mathbf{u}_1)\tilde{\hat{\psi}}_2(\mathbf{v}_1), \quad \ldots . \tag{20}$$

In the general case the following formula is valid:

$$\hat{\psi}_{i_1}^+(\mathbf{u}_{i_1})\cdots\hat{\psi}_{i_n}^+(\mathbf{u}_{i_n})\hat{\psi}_{j_1}(\mathbf{v}_{j_1})\cdots\hat{\psi}_{j_m}(\mathbf{v}_{j_m}) \to \hat{\psi}_{i_1}^+(\mathbf{u}_{i_1})\cdot\widetilde{\cdots\psi}_{j_m}(\mathbf{v}_{j_m}) = \tilde{\hat{\psi}}_{i_1}^+(\mathbf{u}_1)\cdots\tilde{\hat{\psi}}_{j_m}(\mathbf{v}_{j_m}). \tag{21}$$

To explain this formula we note that each of $\hat{\psi}_j(\mathbf{v}_j)$ [or $\hat{\psi}_i^+(\mathbf{u}_i)$] entering $\hat{A}(\mathbf{u},\mathbf{v})$ [see (13)] is related to other operators $\hat{\psi}^+$ (or $\hat{\psi}$) not entering $\hat{A}(\mathbf{u},\mathbf{v})$ only by unique way, which leads to the binary relations (19) and (20). Therefore, we come to (21) by sorting out all the operators $\hat{\psi}_i$, $\hat{\psi}_{i'}$ contained in $\hat{A}(\mathbf{u},\mathbf{v})$.

The operators $\hat{\psi}_i(\mathbf{x})$, $\hat{\psi}_j(\mathbf{x}')$ are anticommutative. For this reason there is a question concerning the consistency of (20) and (21). The anticommutativity of $\tilde{\hat{\psi}}_i(\mathbf{x})$, $\tilde{\hat{\psi}}_j(\mathbf{x}')$ [and also $\tilde{\hat{\psi}}_i^+(\mathbf{x})$, $\tilde{\hat{\psi}}_j^+(\mathbf{x}')$] represents the consistency condition of these formulas,

$$\{\tilde{\hat{\psi}}_i(\mathbf{x}), \tilde{\hat{\psi}}_j(\mathbf{x}')\} = \{\tilde{\hat{\psi}}_i^+(\mathbf{x}), \tilde{\hat{\psi}}_j^+(\mathbf{x}')\} = 0.$$

The validity of these anticommutative relations can be easily proved if to use the definitions (16)–(18) for $\tilde{\hat{\psi}}$, $\tilde{\hat{\psi}}^+$ and the commutative relations for $\hat{\chi}$, $\hat{\chi}^+$ and $\hat{\eta}_\alpha$, $\hat{\eta}_\alpha^+$.

IV. THE OPERATORS OF BASIC PHYSICAL QUANTITIES

In this section we consider the operators of basic physical quantities, which act in the Hilbert space $\tilde{H}$. Let us start from the density operator for particles of the first kind. The corresponding operator acting in the original Hilbert space H is of the form

$$\hat{\rho}_1(\mathbf{x}) = \hat{\psi}_1^+(\mathbf{x})\hat{\psi}_1(\mathbf{x}).$$

Hence, in accordance with (20), one finds

$$\tilde{\hat{\rho}}_1(\mathbf{x}) = \tilde{\hat{\psi}}_1^+(\mathbf{x})\tilde{\hat{\psi}}_1(\mathbf{x}) = \hat{\chi}_1^+(\mathbf{x})\hat{\chi}_1(\mathbf{x}) + \hat{O}_1^+(\mathbf{x})\hat{\chi}_1(\mathbf{x}) + \hat{\chi}_1^+(\mathbf{x})\hat{O}_1(\mathbf{x}) + \hat{O}_1^+(\mathbf{x})\hat{O}_1(\mathbf{x}).$$

Note that the operators with zero matrix elements in the subspace $\tilde{H}_a$ appear on the right-hand side of (19) because of points $\mathbf{u}_1$ and $\mathbf{v}_1$ are close to each other. Since

$$\hat{O}_1^+(\mathbf{x})\hat{\chi}_1(\mathbf{x}) = \int d\mathbf{y}\ \hat{\varphi}^+(\mathbf{x},\mathbf{y})\hat{\chi}_2(\mathbf{y})\hat{\chi}_1(\mathbf{x}), \quad \hat{\chi}_1^+(\mathbf{x})\hat{O}_1(\mathbf{x}) = \int d\mathbf{y}\ \hat{\chi}_1^+(\mathbf{x})\hat{\chi}_2^+(\mathbf{y})\hat{\varphi}(\mathbf{x},\mathbf{y})$$

and $\hat{\varphi}(\mathbf{x},\mathbf{y})$ differs from zero only for $|\mathbf{x}-\mathbf{y}| \lesssim a$, these operators according to (12) do not have the matrix elements in the subspace $\tilde{H}_a$ and therefore can be omitted. Using the permutation relation $\{\hat{\chi}_2^+(\mathbf{z}_1), \hat{\chi}_2(\mathbf{z}_2)\} = \delta(\mathbf{z}_1-\mathbf{z}_2)$ the operator $\hat{O}_1^+(\mathbf{x})\hat{O}_1(\mathbf{x})$ is written as

$$\hat{O}_1^+(\mathbf{x})\hat{O}_1(\mathbf{x}) = \int d\mathbf{z}\ \hat{\varphi}^+(\mathbf{x},\mathbf{z})\hat{\varphi}(\mathbf{x},\mathbf{z}) + \int d\mathbf{z}_1\, d\mathbf{z}_2\ \hat{\varphi}^+(\mathbf{x},\mathbf{z}_2)\hat{\varphi}(\mathbf{x},\mathbf{z}_1)\hat{\chi}_2^+(\mathbf{z}_1)\hat{\chi}_2(\mathbf{z}_2).$$

The matrix element of the second term is zero in the subspace $\tilde{H}_a$ because of $\mathbf{z}_1 \approx \mathbf{z}_2 \approx \mathbf{x}$ [see (12)]. For this reason this term can be omitted. Thus, with the use of the method that was described in preceding section we have

$$\tilde{\hat{\rho}}_1(\mathbf{x}) = \hat{\chi}_1^+(\mathbf{x})\hat{\chi}_1(\mathbf{x}) + \int \mathrm{d}\mathbf{z}\ \hat{\varphi}^+(\mathbf{x},\mathbf{z})\hat{\varphi}(\mathbf{x},\mathbf{z}). \tag{22}$$

Similarly, if $\hat{\rho}_2(\mathbf{x}) = \hat{\psi}_2^+(\mathbf{x})\hat{\psi}_2(\mathbf{x})$ represents the density operator for particles of the second kind, then $\hat{\rho}_2(\mathbf{x}) \to \tilde{\hat{\rho}}_2(\mathbf{x})$, where

$$\tilde{\hat{\rho}}_2(\mathbf{x}) = \hat{\chi}_2^+(\mathbf{x})\hat{\chi}_2(\mathbf{x}) + \int \mathrm{d}\mathbf{z}\ \hat{\varphi}^+(\mathbf{z},\mathbf{x})\hat{\varphi}(\mathbf{z},\mathbf{x}). \tag{23}$$

Bearing in mind (16) and the assumption concerning the "small radius" of the bound state, one gets the following formulas:

$$\int \mathrm{d}\mathbf{z}\ \hat{\varphi}^+(\mathbf{x},\mathbf{z})\hat{\varphi}(\mathbf{x},\mathbf{z}) \approx \hat{\eta}_\alpha^+(\mathbf{x})\hat{\eta}_\alpha(\mathbf{x}), \quad \int \mathrm{d}\mathbf{z}\ \hat{\varphi}^+(\mathbf{z},\mathbf{x})\hat{\varphi}(\mathbf{z},\mathbf{x}) \approx \hat{\eta}_\alpha^+(\mathbf{x})\hat{\eta}_\alpha(\mathbf{x}),$$

which allow us to obtain the densities operators for particles of the first and second kinds,

$$\tilde{\hat{\rho}}_1(\mathbf{x}) = \hat{\chi}_1^+(\mathbf{x})\hat{\chi}_1(\mathbf{x}) + \hat{\eta}_\alpha^+(\mathbf{x})\hat{\eta}_\alpha(\mathbf{x}), \quad \tilde{\hat{\rho}}_2(\mathbf{x}) = \hat{\chi}_2^+(\mathbf{x})\hat{\chi}_2(\mathbf{x}) + \hat{\eta}_\alpha^+(\mathbf{x})\hat{\eta}_\alpha(\mathbf{x}). \tag{24}$$

Thus, the operators $\hat{\eta}_\alpha^+(\mathbf{x})$, $\hat{\eta}_\alpha(\mathbf{x})$ can be interpreted as the creation and annihilation operators of the bound states with quantum numbers α at the point $\mathbf{x}$, and $\hat{\eta}_\alpha^+(\mathbf{x})\hat{\eta}_\alpha(\mathbf{x})$ as the density operator of the bound states. For example, the first formula from (24) has a simple physical meaning: the density of particles of the first kind is equal to the sum of densities for free particles of the same kind and bound states (each bound state contains one particle of the first kind).

Consider a state vector $\Phi(\mathbf{X}) = \hat{\eta}_\alpha^+(\mathbf{X})|0\rangle$, which specifies a compound particle at the point $\mathbf{X}$ (this state vector corresponds to continuous spectrum). Then, in accordance with (24), we have

$$(\Phi(\mathbf{X}), \hat{\rho}_1(\mathbf{x}_1)\Phi(\mathbf{X}')) = \delta(\mathbf{X}-\mathbf{X}')\left(\frac{M}{m_2}\right)^3 \left|\varphi_\alpha\left(\frac{M}{m_2}(\mathbf{x}_1-\mathbf{X})\right)\right|^2.$$

For a wave packet

$$\Psi_{\mathbf{X}_0} = \int \mathrm{d}\mathbf{X}\ f_{\mathbf{X}_0}(\mathbf{X})\Phi(\mathbf{X}), \quad \int \mathrm{d}\mathbf{X}|f_{\mathbf{X}_0}(\mathbf{X})|^2 = 1$$

the quantity

$$(\Psi_{\mathbf{X}_0}, \hat{\rho}_1(\mathbf{x}_1)\Psi_{\mathbf{X}_0}) = \left(\frac{M}{m_2}\right)^3 \int \mathrm{d}\mathbf{X}|f_{\mathbf{X}_0}(\mathbf{X})|^2 \left|\varphi_\alpha\left(\frac{M}{m_2}(\mathbf{x}_1-\mathbf{X})\right)\right|^2$$

should be treated as the probability density to find the first particle at the point $\mathbf{x}_1$ if the atom is in a state $\Psi_{\mathbf{X}_0}$. If the bound state is localized near a point $\mathbf{X}_0$ (i.e., $|f\mathbf{x}_0(\mathbf{X})|^2 \to \delta(\mathbf{X}-\mathbf{X}_0)$), then

$$(\Psi_{\mathbf{X}_0}, \hat{\rho}_1(\mathbf{x}_1)\Psi_{\mathbf{X}_0}) \to \left(\frac{M}{m_2}\right)^3 \left|\varphi_\alpha\left(\frac{M}{m_2}(\mathbf{x}_1-\mathbf{X}_0)\right)\right|^2.$$

Since $(M/m_2)(\mathbf{x}_1-\mathbf{X}_0) = \mathbf{x} = \mathbf{x}_1-\mathbf{x}_2$, we come (as it should be) to the probability distribution for the space coordinate of the first particle in the atom (the atom is at the point $\mathbf{X}_0$).

Let us find now the momentum density operator in the space $\tilde{H}$. In original Hilbert space, the momentum density operator $\hat{\boldsymbol{\pi}}_1(\mathbf{x})$ for particles of the first kind is defined as

$$\hat{\boldsymbol{\pi}}_1(\mathbf{x}) = -\frac{i}{2}\left(\hat{\psi}_1^+(\mathbf{x})\frac{\partial\hat{\psi}_1(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\psi}_1^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\psi}_1(\mathbf{x})\right).$$

Then according to (20),

$$\hat{\boldsymbol{\pi}}_1(\mathbf{x}) \to \tilde{\hat{\pi}}_1(\mathbf{x}) = -\frac{i}{2}\left(\tilde{\hat{\psi}}_1^+(\mathbf{x})\frac{\partial\tilde{\hat{\psi}}_1(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\tilde{\hat{\psi}}_1^+(\mathbf{x})}{\partial\mathbf{x}}\tilde{\hat{\psi}}_1(\mathbf{x})\right).$$

Following the derivation of (22) and (23) for $\tilde{\hat{\rho}}_1(\mathbf{x})$ and $\tilde{\hat{\rho}}_2(\mathbf{x})$ we obtain

$$\tilde{\hat{\pi}}_1(\mathbf{x}) = -\frac{i}{2}\left(\hat{\chi}_1^+(\mathbf{x})\frac{\partial\hat{\chi}_1(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\chi}_1^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\chi}_1(\mathbf{x})\right) - \frac{i}{2}\int d\mathbf{y}\left(\hat{\varphi}^+(\mathbf{x},\mathbf{y})\frac{\partial\hat{\varphi}(\mathbf{x},\mathbf{y})}{\partial\mathbf{x}} - \frac{\partial\hat{\varphi}^+(\mathbf{x},\mathbf{y})}{\partial\mathbf{x}}\hat{\varphi}(\mathbf{x},\mathbf{y})\right), \tag{25}$$

$$\tilde{\hat{\pi}}_2(\mathbf{x}) = -\frac{i}{2}\left(\hat{\chi}_2^+(\mathbf{x})\frac{\partial\hat{\chi}_2(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\chi}_2^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\chi}_2(\mathbf{x})\right) - \frac{i}{2}\int d\mathbf{y}\left(\hat{\varphi}^+(\mathbf{y},\mathbf{x})\frac{\partial\hat{\varphi}(\mathbf{y},\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\varphi}^+(\mathbf{y},\mathbf{x})}{\partial\mathbf{x}}\hat{\varphi}(\mathbf{y},\mathbf{x})\right). \tag{26}$$

It is convenient for our further consideration to rewrite (25) and (26) in terms of the center of mass variables $\mathbf{y}=\mathbf{y}_1-\mathbf{y}_2$ and $\mathbf{Y}=(m_1\mathbf{y}_1+m_2\mathbf{y}_2)/(m_1+m_2)$,

$$\begin{aligned}\tilde{\hat{\boldsymbol{\pi}}}_1(\mathbf{x}) = &-\frac{i}{2}\left(\hat{\chi}_1^+(\mathbf{x})\frac{\partial\hat{\chi}_1(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\chi}_1^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\chi}_1(\mathbf{x})\right) - \frac{i}{2}\int d\mathbf{y}\, d\mathbf{Y}\ \delta\left(\mathbf{x}-\mathbf{Y}-\frac{m_2}{M}\mathbf{y}\right)\left\{\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\frac{\partial\hat{\varphi}(\mathbf{y},\mathbf{Y})}{\partial\mathbf{y}}\right.\\ &\left.-\frac{\partial\hat{\varphi}^+(\mathbf{y},\mathbf{Y})}{\partial\mathbf{y}}\hat{\varphi}(\mathbf{y},\mathbf{Y}) + \frac{m_1}{M}\left(\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\frac{\partial\hat{\varphi}(\mathbf{y},\mathbf{Y})}{\partial\mathbf{Y}} - \frac{\partial\hat{\varphi}^+(\mathbf{y},\mathbf{Y})}{\partial\mathbf{Y}}\hat{\varphi}(\mathbf{y},\mathbf{Y})\right)\right\},\end{aligned}$$

$$\begin{aligned}\tilde{\hat{\boldsymbol{\pi}}}_2(\mathbf{x}) = &-\frac{i}{2}\left(\hat{\chi}_2^+(\mathbf{x})\frac{\partial\hat{\chi}_2(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\chi}_2^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\chi}_2(\mathbf{x})\right) - \frac{i}{2}\int d\mathbf{y}\, d\mathbf{Y}\ \delta\left(\mathbf{x}-\mathbf{Y}+\frac{m_1}{M}\mathbf{y}\right)\left\{-\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\frac{\partial\hat{\varphi}(\mathbf{y},\mathbf{Y})}{\partial\mathbf{y}}\right.\\ &\left.+\frac{\partial\hat{\varphi}^+(\mathbf{y},\mathbf{Y})}{\partial\mathbf{y}}\hat{\varphi}(\mathbf{y},\mathbf{Y}) + \frac{m_2}{M}\left(\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\frac{\partial\hat{\varphi}(\mathbf{y},\mathbf{Y})}{\partial\mathbf{Y}} - \frac{\partial\hat{\varphi}^+(\mathbf{y},\mathbf{Y})}{\partial\mathbf{Y}}\hat{\varphi}(\mathbf{y},\mathbf{Y})\right)\right\},\end{aligned} \tag{27}$$

where $\hat{\varphi}(\mathbf{y}_1,\mathbf{y}_2)\equiv\hat{\varphi}(\mathbf{y},\mathbf{Y})$. Note that in terms of these variables the operators $\tilde{\hat{\rho}}_1(\mathbf{x})$ and $\tilde{\hat{\rho}}_2(\mathbf{x})$ have the form

$$\begin{aligned}\tilde{\hat{\rho}}_1(\mathbf{x}) &= \hat{\chi}_1^+(\mathbf{x})\hat{\chi}_1(\mathbf{x}) + \int d\mathbf{y}\, d\mathbf{Y}\ \delta\left(\mathbf{x}-\mathbf{Y}-\frac{m_2}{M}\mathbf{y}\right)\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\hat{\varphi}(\mathbf{y},\mathbf{Y}),\\ \tilde{\hat{\rho}}_2(\mathbf{x}) &= \hat{\chi}_2^+(\mathbf{x})\hat{\chi}_2(\mathbf{x}) + \int d\mathbf{y}\, d\mathbf{Y}\ \delta\left(\mathbf{x}-\mathbf{Y}+\frac{m_1}{M}\mathbf{y}\right)\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\hat{\varphi}(\mathbf{y},\mathbf{Y}).\end{aligned} \tag{28}$$

It is clear that (27) and (28) can be expressed through the creation and annihilation operators $\hat{\eta}_\alpha^+(\mathbf{x})$, $\hat{\eta}_\alpha(\mathbf{x})$ of atoms if to employ (17). Taking into account (27) it is easy to find the operator $\tilde{\hat{\boldsymbol{\pi}}}=\tilde{\hat{\pi}}_1(\mathbf{x})+\tilde{\hat{\pi}}_2(\mathbf{x})$ of the total momentum density of the system in the approximation, where the radius of bound state is small,

$$\begin{aligned}\tilde{\hat{\boldsymbol{\pi}}} = &-\frac{i}{2}\left(\hat{\chi}_1^+(\mathbf{x})\frac{\partial\hat{\chi}_1(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\chi}_1^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\chi}_1(\mathbf{x})\right) - \frac{i}{2}\left(\hat{\chi}_2^+(\mathbf{x})\frac{\partial\hat{\chi}_2(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\chi}_2^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\chi}_2(\mathbf{x})\right)\\ &-\frac{i}{2}\left(\hat{\eta}_\alpha^+(\mathbf{x})\frac{\partial\hat{\eta}_\alpha(\mathbf{x})}{\partial\mathbf{x}} - \frac{\partial\hat{\eta}_\alpha^+(\mathbf{x})}{\partial\mathbf{x}}\hat{\eta}_\alpha(\mathbf{x})\right).\end{aligned}$$

The third term in this formula is in accordance with interpretation of $\hat{\eta}_\alpha^+(\mathbf{x})$, $\hat{\eta}_\alpha(\mathbf{x})$ as the creation and annihilation operators of the bound state with quantum numbers α at the point $\mathbf{x}$.

Finally let us consider a Hamiltonian in the space $\tilde{H}$. We suppose that this Hamiltonian has a standard form in the Hilbert space H and can be written as

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{V},$$

where $\hat{\mathcal{H}}_0$ and $\hat{V}$ are the operators of kinetic energy and potential energy given by

$$\hat{\mathcal{H}}_0 = \sum_{i=1}^{2} \frac{1}{2m_i} \int \mathrm{d}\mathbf{x} \frac{\partial \hat{\psi}_i^+(\mathbf{x})}{\partial \mathbf{x}} \frac{\partial \hat{\psi}_i(\mathbf{x})}{\partial \mathbf{x}},$$

$$\hat{V} = \frac{1}{2} \sum_{i,j=1}^{2} \int \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{x}'\ \hat{\psi}_i^+(\mathbf{x}) \hat{\psi}_j^+(\mathbf{x}') \nu_{ij}(\mathbf{x}-\mathbf{x}') \hat{\psi}_j(\mathbf{x}') \hat{\psi}_i(\mathbf{x}), \tag{29}$$

and $\nu_{ij}(\mathbf{x}-\mathbf{x}')$ is a potential energy of interaction for particles of the kinds i and j. After the similar calculations that led us to the expressions for $\tilde{\tilde{\rho}}$, $\tilde{\tilde{\boldsymbol{\pi}}}$, we obtain

$$\hat{\mathcal{H}}_0 \to \tilde{\tilde{\mathcal{H}}}_0 = \sum_{i=1}^{2} \frac{1}{2m_i} \left(\int \mathrm{d}\mathbf{x} \frac{\partial \hat{\chi}_i^+(\mathbf{x})}{\partial \mathbf{x}} \frac{\partial \hat{\chi}_i(\mathbf{x})}{\partial \mathbf{x}} + \int \mathrm{d}\mathbf{x}_1\, \mathrm{d}\mathbf{x}_2 \frac{\partial \hat{\varphi}^+(\mathbf{x}_1,\mathbf{x}_2)}{\partial \mathbf{x}_i} \frac{\partial \hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2)}{\partial \mathbf{x}_i} \right). \tag{30}$$

Next changing to the center of mass variables [see (17)] and noting that

$$\frac{\partial}{\partial \mathbf{x}_1} = \frac{\partial}{\partial \mathbf{x}} + \frac{m_1}{M} \frac{\partial}{\partial \mathbf{X}}, \quad \frac{\partial}{\partial \mathbf{x}_2} = -\frac{\partial}{\partial \mathbf{x}} + \frac{m_2}{M} \frac{\partial}{\partial \mathbf{X}},$$

one gets

$$\tilde{\tilde{\mathcal{H}}}_0 = \sum_{i=1}^{2} \frac{1}{2m_i} \int \mathrm{d}\mathbf{x} \frac{\partial \hat{\chi}_i^+(\mathbf{x})}{\partial \mathbf{x}} \frac{\partial \hat{\chi}_i(\mathbf{x})}{\partial \mathbf{x}} - \frac{1}{2\mu} \int \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{X}\, \hat{\eta}_\alpha^+(\mathbf{X}) \hat{\eta}_\beta(\mathbf{X}) \frac{\partial \varphi_\alpha^*(\mathbf{x})}{\partial \mathbf{x}} \frac{\partial \varphi_\beta(\mathbf{x})}{\partial \mathbf{x}}$$
$$+ \frac{1}{2M} \int \mathrm{d}\mathbf{X} \frac{\partial \hat{\eta}_\alpha^+(\mathbf{X})}{\partial \mathbf{X}} \frac{\partial \hat{\eta}_\alpha(\mathbf{X})}{\partial \mathbf{X}}, \tag{31}$$

where $\mu = m_1 m_2/(m_1+m_2)$ is a reduced mass.

Let us find now $\tilde{\tilde{V}}$ ($\hat{V} \to \tilde{\tilde{V}}$). According to (20) we have

$$\tilde{\tilde{V}} = \frac{1}{2} \sum_{i,j=1}^{2} \int \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{x}' \tilde{\tilde{\psi}}_i^+(\mathbf{x}) \tilde{\tilde{\psi}}_j^+(\mathbf{x}') \nu_{ij}(\mathbf{x}-\mathbf{x}') \tilde{\tilde{\psi}}_j(\mathbf{x}') \tilde{\tilde{\psi}}_i(\mathbf{x}),$$

where $\tilde{\tilde{\psi}}_i(\mathbf{x}) = \hat{\chi}_i(\mathbf{x}) + \hat{O}_i(\mathbf{x})$ [see (20)]. Thus, $\tilde{\tilde{V}}$ can be represented in the form

$$\tilde{\tilde{V}} = \tilde{\tilde{V}}_0 + \tilde{\tilde{V}}_1 + \tilde{\tilde{V}}_2 + \tilde{\tilde{V}}_3 + \tilde{\tilde{V}}_4,$$

where $\tilde{\tilde{V}}_k$ ($k=0,\ldots,4$) contains k multipliers of type $\hat{\chi}$ and $4-k$ multipliers of type $\hat{O}$. The operators $\hat{O}_i(\mathbf{x})$ have, according to (16) and (18), the form

$$\hat{O}_i(\mathbf{x}) = \int \mathrm{d}\mathbf{y}\ \hat{\varphi}_i(\mathbf{x},\mathbf{y}) \hat{\chi}_{i'}^+(\mathbf{y}),$$

$$\hat{\varphi}_1(\mathbf{x},\mathbf{y}) = \hat{\varphi}(\mathbf{x},\mathbf{y}), \quad \hat{\varphi}_2(\mathbf{x},\mathbf{y}) = \hat{\varphi}(\mathbf{y},\mathbf{x}), \tag{32}$$

where index i' is defined as $1'=2$, $2'=1$. Then $\tilde{\tilde{V}}_0$ is of the form

$$\tilde{\hat{V}}_0 = \frac{1}{2}\sum_{i,j=1}^{2} \int d\mathbf{x}_1\, d\mathbf{x}_2\, \nu_{ij}(\mathbf{x}_1 - \mathbf{x}_2)$$
$$\times \int d\mathbf{y}_1\, d\mathbf{y}_2\, d\mathbf{y}_3\, d\mathbf{y}_4\, \hat{\varphi}_i^+(\mathbf{x}_1,\mathbf{y}_1)\hat{\varphi}_j^+(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}_j(\mathbf{x}_2,\mathbf{y}_3)\hat{\varphi}_i(\mathbf{x}_1,\mathbf{y}_4)\hat{\chi}_{i'}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\hat{\chi}_{j'}^+(\mathbf{y}_3)\hat{\chi}_{i'}^+(\mathbf{y}_4). \tag{33}$$

Note that the operators $\hat{\varphi}$ and $\hat{\varphi}^+$ in (33) are normally ordered, whereas $\hat{\chi}$ and $\hat{\chi}^+$ are not normally ordered. Therefore, we put them in order using Wick's theorem,

$$\begin{aligned}
&\hat{\chi}_{i'}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\hat{\chi}_{j'}^+(\mathbf{y}_3)\hat{\chi}_{i'}^+(\mathbf{y}_4)\\
&\quad =: \hat{\chi}_{i'}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\hat{\chi}_{j'}^+(\mathbf{y}_3)\hat{\chi}_{i'}^+(\mathbf{y}_4): + :\overset{}{\underset{a}{\hat{\chi}_{i'}}}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\overset{}{\underset{a}{\hat{\chi}_{j'}^+}}(\mathbf{y}_3)\hat{\chi}_{i'}^+(\mathbf{y}_4):\\
&\qquad + :\overset{}{\underset{a}{\hat{\chi}_{i'}}}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\hat{\chi}_{j'}^+(\mathbf{y}_3)\overset{}{\underset{a}{\hat{\chi}_{i'}^+}}(\mathbf{y}_4): + :\hat{\chi}_{i'}(\mathbf{y}_1)\overset{}{\underset{a}{\hat{\chi}_{j'}}}(\mathbf{y}_2)\overset{}{\underset{a}{\hat{\chi}_{j'}^+}}(\mathbf{y}_3)\hat{\chi}_{i'}^+(\mathbf{y}_4):\\
&\qquad + :\hat{\chi}_{i'}(\mathbf{y}_1)\overset{}{\underset{a}{\hat{\chi}_{j'}}}(\mathbf{y}_2)\hat{\chi}_{j'}^+(\mathbf{y}_3)\overset{}{\underset{a}{\hat{\chi}_{i'}^+}}(\mathbf{y}_4): + :\overset{}{\underset{a}{\hat{\chi}_{i'}}}(\mathbf{y}_1)\overset{}{\underset{b}{\hat{\chi}_{j'}}}(\mathbf{y}_2)\overset{}{\underset{a}{\hat{\chi}_{j'}^+}}(\mathbf{y}_3)\overset{}{\underset{b}{\hat{\chi}_{i'}^+}}(\mathbf{y}_4):\\
&\qquad + :\overset{}{\underset{a}{\hat{\chi}_{i'}}}(\mathbf{y}_1)\overset{}{\underset{b}{\hat{\chi}_{j'}}}(\mathbf{y}_2)\overset{}{\underset{b}{\hat{\chi}_{j'}^+}}(\mathbf{y}_3)\overset{}{\underset{a}{\hat{\chi}_{i'}^+}}(\mathbf{y}_4): .
\end{aligned} \tag{34}$$

The operator $\hat{\varphi}(\mathbf{x},\mathbf{y}) \equiv \varphi_\alpha(\mathbf{x}-\mathbf{y})\,\hat{\eta}_\alpha[(m_1\mathbf{x}+m_2\mathbf{y})/(m_1+m_2)]$ differs from zero only for $\mathbf{x}\approx\mathbf{y}$ ($|\mathbf{x}-\mathbf{y}|<a$). Thus, only those of $\hat{\varphi}_i$, for which $|\mathbf{y}_1-\mathbf{y}_4|<a$ contribute to the integral over $\mathbf{y}$ in (33). This means that the first term in (34) in virtue of (12) does not contribute to the matrix element of $\tilde{\hat{V}}_0$ taken between the states belonging to $\tilde{H}_a$ because of $\hat{\varphi}_i(\mathbf{x}_1,\mathbf{y}_4)\hat{\chi}_i(\mathbf{y}_1)\Phi=0$. Similarly, one can prove that the terms, which contain the single contractions in (34) do not give a contribution to the matrix element of $\tilde{\hat{V}}_0$ taken between the states in $\tilde{H}_a$. The penultimate term in (34) containing the double contractions does not also contribute to the above-mentioned matrix element. Indeed, the penultimate term in (34) equals $\delta(\mathbf{y}_1-\mathbf{y}_3)\delta(\mathbf{y}_2-\mathbf{y}_4)$. In this case the nonzero matrix element exists for $\mathbf{x}_1\approx\mathbf{x}_2$ and $\hat{\varphi}_j(\mathbf{x}_2,\mathbf{y}_3)\hat{\varphi}_i(\mathbf{x}_1,\mathbf{y}_4)\Phi=0$ in virtue of (12). Thus, only the latter term in (34) equal to $\delta(\mathbf{y}_2-\mathbf{y}_3)\delta(\mathbf{y}_1-\mathbf{y}_4)$ can give the contribution to the matrix element of $\tilde{\hat{V}}_0$. Therefore, not changing the matrix elements in $\tilde{H}_a$, the operator $\tilde{\hat{V}}_0$ can be represented in the form

$$\tilde{\hat{V}}_0 = \frac{1}{2}\sum_{i,j=1}^{2} \int d\mathbf{x}_1\, d\mathbf{x}_2\, d\mathbf{y}_1\, d\mathbf{y}_2\, \hat{\varphi}_i^+(\mathbf{x}_1,\mathbf{y}_1)\hat{\varphi}_j^+(\mathbf{x}_2,\mathbf{y}_2)\nu_{ij}(\mathbf{x}_1-\mathbf{x}_2)\hat{\varphi}_j(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}_i(\mathbf{x}_1,\mathbf{y}_1),$$

or, according to (32),

$$\tilde{\hat{V}}_0 = \frac{1}{2}\int d\mathbf{x}_1\, d\mathbf{x}_2\, d\mathbf{y}_1\, d\mathbf{y}_2\, \hat{\varphi}^+(\mathbf{x}_1,\mathbf{y}_1)\hat{\varphi}^+(\mathbf{x}_2,\mathbf{y}_2)$$
$$\times\{\nu_{11}(\mathbf{x}_1-\mathbf{x}_2)+\nu_{22}(\mathbf{y}_1-\mathbf{y}_2)+\nu_{12}(\mathbf{x}_1-\mathbf{y}_2)+\nu_{21}(\mathbf{y}_1-\mathbf{x}_2)\}\hat{\varphi}(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}(\mathbf{x}_1,\mathbf{y}_1).$$

Similarly, noting that

$$\tilde{\hat{V}}_1 = \frac{1}{2}\sum_{i,j=1}^{2} \int d\mathbf{x}_1\, d\mathbf{x}_2\, d\mathbf{y}\ \nu_{ij}(\mathbf{x}_1-\mathbf{x}_2)\{\hat{\varphi}_i^+(\mathbf{x}_1,\mathbf{y})\hat{\chi}_{i'}(\mathbf{y})\hat{\chi}_j^+(\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2)\hat{\chi}_i(\mathbf{x}_1)$$
$$+\hat{\varphi}_j^+(\mathbf{x}_2,\mathbf{y})\hat{\chi}_i(\mathbf{x}_1)\hat{\chi}_{j'}^+(\mathbf{y})\hat{\chi}_j(\mathbf{x}_2)\hat{\chi}_i(\mathbf{x}_1)+\text{H.c.}\},$$

$$\tilde{\tilde{V}}_3 = \frac{1}{2}\sum_{i,j=1}^{2}\int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2\,\mathrm{d}\mathbf{y}_1\,\mathrm{d}\mathbf{y}_2\,\mathrm{d}\mathbf{y}_3\;\nu_{ij}(\mathbf{x}_1-\mathbf{x}_2)$$
$$\times\{\hat{\varphi}_i^+(\mathbf{x}_1,\mathbf{y}_1)\hat{\varphi}_j^+(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}_j(\mathbf{x}_2,\mathbf{y}_3)\hat{\chi}_{i'}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\hat{\chi}_{j'}^+(\mathbf{y}_3)\hat{\chi}_i(\mathbf{x}_1)$$
$$+\,\hat{\varphi}_i^+(\mathbf{x}_1,\mathbf{y}_1)\hat{\varphi}_j^+(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}_i(\mathbf{x}_1,\mathbf{y}_3)\hat{\chi}_{i'}(\mathbf{y}_1)\hat{\chi}_{j'}(\mathbf{y}_2)\hat{\chi}_j(\mathbf{x}_2)\hat{\chi}_{i'}^+(\mathbf{y}_3)+\mathrm{H.c.}\}$$

and performing the same derivation as for $\tilde{\tilde{V}}_0$, it is easy to verify [using the anticommutative relations for $\hat{\chi}$, $\hat{\chi}^+$ and (34)] that we can consider $\tilde{\tilde{V}}_1=\tilde{\tilde{V}}_3=0$ not changing the matrix elements of $\tilde{\tilde{V}}_1$ and $\tilde{\tilde{V}}_3$ in the subspace $\tilde{H}_a$. Next it is evident that the following formula is valid:

$$\tilde{\tilde{V}}_4 = \frac{1}{2}\sum_{i,j=1}^{2}\int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2\;\hat{\chi}_i^+(\mathbf{x}_1)\hat{\chi}_j^+(\mathbf{x}_2)\nu_{ij}(\mathbf{x}_1-\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2)\hat{\chi}_i(\mathbf{x}_1). \tag{35}$$

Finally let us find $\tilde{\tilde{V}}_2$,

$$\tilde{\tilde{V}}_2 = \frac{1}{2}\sum_{i,j=1}^{2}\int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2\;\nu_{ij}(\mathbf{x}_1-\mathbf{x}_2)\{\hat{O}_i^+(\mathbf{x}_1)\hat{O}_j^+(\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2)\hat{\chi}_i(\mathbf{x}_1)+\hat{O}_i^+(\mathbf{x}_1)\hat{\chi}_j^+(\mathbf{x}_2)\hat{O}_j(\mathbf{x}_2)\hat{\chi}_i(\mathbf{x}_1)+\mathrm{h.c.}$$
$$+\,\hat{O}_i^+(\mathbf{x}_1)\hat{\chi}_j^+(\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2)\hat{O}_i(\mathbf{x}_1)+\hat{\chi}_i^+(\mathbf{x}_1)\hat{O}_j^+(\mathbf{x}_2)\hat{O}_j(\mathbf{x}_2)\hat{\chi}_i(\mathbf{x}_1)\}.$$

It can be easily seen that the first two terms and the corresponding Hermitian conjugate terms do not give a contribution to the matrix element of $\tilde{\tilde{V}}_2$ in the subspace $\tilde{H}_a$. Therefore, we can consider

$$\tilde{\tilde{V}}_2 = \frac{1}{2}\sum_{i,j=1}^{2}\int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2\,\mathrm{d}\mathbf{y}_1\,\mathrm{d}\mathbf{y}_2\;\nu_{ij}(\mathbf{x}_1-\mathbf{x}_2)\{\hat{\varphi}_i^+(\mathbf{x}_1,\mathbf{y}_1)\hat{\varphi}_i(\mathbf{x}_1,\mathbf{y}_2)\hat{\chi}_{i'}(\mathbf{y}_1)\hat{\chi}_j^+(\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2)\hat{\chi}_{i'}^+(\mathbf{y}_2)$$
$$+\,\hat{\varphi}_j^+(\mathbf{x}_2,\mathbf{y}_1)\hat{\varphi}_j(\mathbf{x}_2,\mathbf{y}_2)\hat{\chi}_i^+(\mathbf{x}_1)\hat{\chi}_{j'}(\mathbf{y}_1)\hat{\chi}_{j'}^+(\mathbf{y}_2)\hat{\chi}_i(\mathbf{x}_1)\}.$$

The first and second terms in this expression contribute to the matrix element of $\tilde{\tilde{V}}_2$ in $\tilde{H}_a$ under the following arrangements of contractions:

$$:\overset{a}{\hat{\chi}_{i'}}(\mathbf{y}_1)\overset{a}{\hat{\chi}_j^+}(\mathbf{x}_2)\overset{b}{\hat{\chi}_j}(\mathbf{x}_2)\overset{b}{\hat{\chi}_{i'}^+}(\mathbf{y}_2):+:\overset{a}{\hat{\chi}_{i'}}(\mathbf{y}_1)\hat{\chi}_j^+(\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2)\overset{a}{\hat{\chi}_{i'}^+}(\mathbf{y}_2):$$
$$=\delta_{ji'}\delta(\mathbf{y}_1-\mathbf{x}_2)\delta(\mathbf{y}_2-\mathbf{x}_2)+\delta(\mathbf{y}_1-\mathbf{y}_2)\hat{\chi}_j^+(\mathbf{x}_2)\hat{\chi}_j(\mathbf{x}_2),$$

$$:\hat{\chi}_i^+(\mathbf{x}_1)\overset{a}{\hat{\chi}_{j'}}(\mathbf{y}_1)\overset{a}{\hat{\chi}_{j'}^+}(\mathbf{y}_2)\hat{\chi}_i(\mathbf{x}_1):=\delta(\mathbf{y}_1-\mathbf{y}_2)\hat{\chi}_i^+(\mathbf{x}_1)\hat{\chi}_i(\mathbf{x}_1).$$

Thus, we have

$$\tilde{\tilde{V}}_2 = \int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2\;\nu_{12}(\mathbf{x}_1-\mathbf{x}_2)\hat{\varphi}^+(\mathbf{x}_1,\mathbf{x}_2)\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2)+\int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2\;\hat{\varphi}^+(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}(\mathbf{x}_2,\mathbf{y}_2)\{\nu_{11}(\mathbf{x}_1$$
$$-\mathbf{x}_2)\hat{\chi}_1^+(\mathbf{x}_1)\hat{\chi}_1(\mathbf{x}_1)+\nu_{21}(\mathbf{x}_1-\mathbf{y}_2)\hat{\chi}_1^+(\mathbf{x}_1)\hat{\chi}_1(\mathbf{x}_1)+\nu_{22}(\mathbf{x}_1-\mathbf{y}_2)\hat{\chi}_2^+(\mathbf{x}_1)\hat{\chi}_2(\mathbf{x}_1)+\nu_{12}(\mathbf{x}_1$$
$$-\mathbf{x}_2)\hat{\chi}_2^+(\mathbf{x}_1)\hat{\chi}_2(\mathbf{x}_1)\}. \tag{36}$$

The first term in this formula quadratic in field operators can be combined with the latter term in (31). As a result we obtain

$$\int d\mathbf{x}_1\, d\mathbf{x}_2\, \nu_{12}(\mathbf{x}_1-\mathbf{x}_2)\hat{\varphi}^+(\mathbf{x}_1,\mathbf{x}_2)\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2) - \frac{1}{2\mu}\int d\mathbf{x}\, d\mathbf{X}\ \hat{\eta}^+_\alpha(\mathbf{X})\hat{\eta}_\alpha(\mathbf{X})\frac{\partial\varphi^*_\alpha(\mathbf{x})}{\partial\mathbf{x}}\frac{\partial\varphi_\alpha(\mathbf{x})}{\partial\mathbf{x}}$$
$$= \int d\mathbf{x}\, d\mathbf{X}\ \hat{\eta}^+_\alpha(\mathbf{X})\hat{\eta}_\beta(\mathbf{X})\varphi^*_\alpha(\mathbf{x})\left\{-\frac{1}{2\mu}\Delta_{\mathbf{x}} + \nu_{12}(\mathbf{x})\right\}\varphi_\beta(\mathbf{x}).$$

Since $\varphi_\beta(\mathbf{x})$ satisfies the Schrödinger equation

$$\left\{-\frac{1}{2\mu}\Delta_{\mathbf{x}} + \nu_{12}(\mathbf{x})\right\}\varphi_\beta(\mathbf{x}) = \varepsilon_\beta\varphi_\beta(\mathbf{x}),$$

where ε_β are the atomic energy levels, the latter formula takes the form

$$\int d\mathbf{X}\sum_\alpha \varepsilon_\alpha\hat{\eta}^+_\alpha(\mathbf{X})\hat{\eta}_\alpha(\mathbf{X}).$$

Hence, taking into account (30), (31), and (36), the Hamiltonian of the system $\tilde{\tilde{\mathcal{H}}}$ is of the form

$$\tilde{\tilde{\mathcal{H}}} = \tilde{\tilde{\mathcal{H}}}_0 + \tilde{\tilde{\mathcal{H}}}^1_{\text{int}} + \tilde{\tilde{\mathcal{H}}}^2_{\text{int}} + \tilde{\tilde{\mathcal{H}}}^3_{\text{int}},$$

where

$$\tilde{\tilde{\mathcal{H}}}_0 = \sum_{j=1}^{2}\frac{1}{2m_j}\int d\mathbf{x}\frac{\partial\hat{\chi}^+_j(\mathbf{x})}{\partial\mathbf{x}}\frac{\partial\hat{\chi}_j(\mathbf{x})}{\partial\mathbf{x}} + \sum_\alpha\int d\mathbf{X}\left\{\frac{1}{2M}\frac{\partial\hat{\eta}^+_\alpha(\mathbf{X})}{\partial\mathbf{X}}\frac{\partial\hat{\eta}_\alpha(\mathbf{X})}{\partial\mathbf{X}} + \varepsilon_\alpha\hat{\eta}^+_\alpha(\mathbf{X})\hat{\eta}_\alpha(\mathbf{X})\right\} \tag{37}$$

is the Hamiltonian for free particles and bound states, and

$$\tilde{\tilde{\mathcal{H}}}^1_{\text{int}} = \int d\mathbf{x}_1\, d\mathbf{x}_2\, d\mathbf{y}_2\ \hat{\varphi}^+(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}(\mathbf{x}_2,\mathbf{y}_2)\{(\nu_{11}(\mathbf{x}_1-\mathbf{x}_2)+\nu_{21}(\mathbf{x}_1-\mathbf{y}_2))\hat{\chi}^+_1(\mathbf{x}_1)\hat{\chi}_1(\mathbf{x}_1) + (\nu_{22}(\mathbf{x}_1-\mathbf{y}_2)$$
$$+\nu_{12}(\mathbf{x}_1-\mathbf{x}_2))\hat{\chi}^+_2(\mathbf{x}_1)\hat{\chi}_2(\mathbf{x}_1)\}, \tag{38}$$

$$\tilde{\tilde{\mathcal{H}}}^2_{\text{int}} = \frac{1}{2}\int d\mathbf{x}_1\, d\mathbf{x}_2\, d\mathbf{y}_1\, d\mathbf{y}_2\ \hat{\varphi}^+(\mathbf{x}_1,\mathbf{y}_1)\hat{\varphi}^+(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}(\mathbf{x}_2,\mathbf{y}_2)\hat{\varphi}(\mathbf{x}_1,\mathbf{y}_1)\{\nu_{11}(\mathbf{x}_1-\mathbf{x}_2)+\nu_{22}(\mathbf{y}_1-\mathbf{y}_2)$$
$$+\nu_{12}(\mathbf{x}_1-\mathbf{y}_2)+\nu_{21}(\mathbf{y}_1-\mathbf{x}_2)\}, \tag{39}$$

$$\tilde{\tilde{\mathcal{H}}}^3_{\text{int}} = \frac{1}{2}\int d\mathbf{x}_1\, d\mathbf{x}_2\{\nu_{11}(\mathbf{x}_1-\mathbf{x}_2)\hat{\chi}^+_1(\mathbf{x}_1)\hat{\chi}^+_1(\mathbf{x}_2)\hat{\chi}_1(\mathbf{x}_2)\hat{\chi}_1(\mathbf{x}_1) + \nu_{22}(\mathbf{x}_1-\mathbf{x}_2)\hat{\chi}^+_2(\mathbf{x}_1)\hat{\chi}^+_2(\mathbf{x}_2)\hat{\chi}_2(\mathbf{x}_2)\hat{\chi}_2(\mathbf{x}_1)$$
$$+2\nu_{12}(\mathbf{x}_1-\mathbf{x}_2)\hat{\chi}^+_1(\mathbf{x}_1)\hat{\chi}_1(\mathbf{x}_1)\hat{\chi}^+_2(\mathbf{x}_2)\hat{\chi}_2(\mathbf{x}_2)\} \tag{40}$$

are the Hamiltonians of interaction. The Hamiltonian $\tilde{\tilde{\mathcal{H}}}^1_{\text{int}}$ corresponds to scattering of particles of the first and second kinds by bound states; the Hamiltonian $\tilde{\tilde{\mathcal{H}}}^2_{\text{int}}$ corresponds to scattering of bound states by bound states; finally, the Hamiltonian $\tilde{\tilde{\mathcal{H}}}^3_{\text{int}}$ corresponds to scattering of particles of the first and second kinds by particles of the same kinds. The Hamiltonians of interaction (38) and (39) may be written through the creation $\hat{\eta}^+_\alpha(\mathbf{x})$ and annihilation $\hat{\eta}_\alpha(\mathbf{x})$ operators of atoms by using (17). We emphasize that the obtained Hamiltonians of interaction do not lead to decay processes and formation of compound particles as it should be in the low-energy approximation. This fact reflects that atoms are absolutely stable in the main approximation.

In conclusion of this section we address to the Galilean invariance of the developed theory. We suppose that the initial theory based only on the field operators $\hat{\psi}_i(\mathbf{x}), \hat{\psi}_i^+(\mathbf{x})$ $(i=1,2)$ is Galilean invariant. This means that under the following transformations:

$$\hat{\psi}_i(\mathbf{x}) \to \hat{\psi}_i'(\mathbf{x}) = e^{im_i\mathbf{v}\mathbf{x}}\hat{\psi}_i(\mathbf{x})$$

the operators for particles number $\hat{N}_i$, momentum $\hat{\mathcal{P}}_k$, and energy $\hat{\mathcal{H}}$ transform as follows:

$$\hat{N}_i \to \hat{N}_i' = \hat{N}_i, \quad i = 1,2,$$

$$\hat{\mathcal{P}}_k \to \hat{\mathcal{P}}_k' = \hat{\mathcal{P}}_k + v_k(\hat{N}_1 + \hat{N}_2), \quad \hat{\mathcal{H}} \to \hat{\mathcal{H}}' = \hat{\mathcal{H}} + v_k\hat{\mathcal{P}}_k + \tfrac{1}{2}m_1v^2\hat{N}_1 + \tfrac{1}{2}m_2\hat{N}_2v^2.$$

Since $\hat{\psi}_i(\mathbf{x})$ and $\hat{\psi}_i'(\mathbf{x})$ meet the same commutation relations, they are related to each other by the unitary transformation

$$\hat{\psi}_i'(\mathbf{x}) = U_v\hat{\psi}_i(\mathbf{x})U_v^+,$$

where the unitary operator U_v, is defined by[9]

$$U_v = \exp\left(-i\mathbf{v}m_1\int \mathrm{d}\mathbf{x}\,\mathbf{x}\hat{\rho}_1(\mathbf{x}) - i\mathbf{v}m_2\int \mathrm{d}\mathbf{x}\,\mathbf{x}\hat{\rho}_2(\mathbf{x})\right). \tag{41}$$

Let us show that

$$\widetilde{U}_v = \exp\left(-i\mathbf{v}m_1\int \mathrm{d}\mathbf{x}\,\mathbf{x}\widetilde{\hat{\rho}}_1(\mathbf{x}) - i\mathbf{v}m_2\int \mathrm{d}\mathbf{x}\,\mathbf{x}\widetilde{\hat{\rho}}_2(\mathbf{x})\right)$$

defines the Galilei transformations in the presence of bound states of particles [compare to (41)]. To this end we note that this operator can be written, according to (28), in the form

$$\widetilde{U}_v = \exp\left(-i\mathbf{v}\sum_{i=1}^{2} m_i\int \mathrm{d}\mathbf{x}\,\hat{\chi}_i^+(\mathbf{x})\hat{\chi}_i(\mathbf{x}) - i\mathbf{v}\hat{\mathbf{s}}\right),$$

where

$$\hat{\mathbf{s}} = m_1\int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2\,\mathbf{x}_1\hat{\varphi}^+(\mathbf{x}_1,\mathbf{x}_2)\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2) + m_2\int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2\,\mathbf{x}_1\hat{\varphi}^+(\mathbf{x}_2,\mathbf{x}_1)\hat{\varphi}(\mathbf{x}_2,\mathbf{x}_1)$$

$$= \int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2(m_1\mathbf{x}_1 + m_2\mathbf{x}_2)\hat{\varphi}^+(\mathbf{x}_1,\mathbf{x}_2)\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2).$$

Since

$$\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2) = \varphi_\alpha(\mathbf{x})\,\hat{\eta}_\alpha(\mathbf{X}), \quad \int \mathrm{d}\mathbf{x}\,\varphi_\alpha^*(\mathbf{x})\varphi_\beta(\mathbf{x}) = \delta_{\alpha\beta},$$

changing to the center of mass variables one finds

$$\hat{\mathbf{s}} = (m_1 + m_2)\int \mathrm{d}\mathbf{X}\,\mathbf{X}\sum_\alpha \hat{\eta}_\alpha^+(\mathbf{X})\,\hat{\eta}_\alpha(\mathbf{X}).$$

Therefore, just as we expected

$$\tilde{U}_v = \exp\left(- i\mathbf{v}\sum_{i=1}^{2} m_i \int \mathrm{d}\mathbf{x}\, \hat{\chi}_i^+(\mathbf{x})\hat{\chi}_i(\mathbf{x}) - i\mathbf{v}(m_1+m_2)\int \mathrm{d}\mathbf{X}\, \mathbf{X}\sum_{\alpha} \hat{\eta}_\alpha^+(\mathbf{X})\hat{\eta}_\alpha(\mathbf{X})\right).$$

The employment of this formula and the canonic permutation relations result in

$$\tilde{U}_v\hat{\chi}_i(\mathbf{x})\tilde{U}_v^+ = e^{im_i\mathbf{v}\mathbf{x}}\hat{\chi}_i(\mathbf{x}) \equiv \hat{\chi}_i'(\mathbf{x}),\ \ \tilde{U}_v\hat{\eta}_\alpha(\mathbf{X})\tilde{U}_v^+ = e^{i(m_1+m_2)\mathbf{v}\mathbf{X}}\hat{\eta}_\alpha(\mathbf{X}) \equiv \hat{\eta}_\alpha'(\mathbf{X}). \tag{42}$$

Since the quantity $\hat{\varphi}^+(\mathbf{x},\mathbf{X})\hat{\varphi}(\mathbf{x},\mathbf{X})$ is not changed under such transformation, the Hamiltonians of interaction $\tilde{\hat{\mathcal{H}}}_{\mathrm{int}}^1$, $\tilde{\hat{\mathcal{H}}}_{\mathrm{int}}^2$, $\tilde{\hat{\mathcal{H}}}_{\mathrm{int}}^3$ [see (38)–(40)] are invariant with respect to (42). It is easy to verify that the Hamiltonian $\tilde{\hat{\mathcal{H}}}_0$ for free particles and bound states transforms according to the law

$$\tilde{U}_v\tilde{\hat{\mathcal{H}}}_0\tilde{U}_v^+ = \tilde{\hat{H}}_0 + \mathbf{v}\tilde{\hat{\boldsymbol{\mathcal{P}}}} + \frac{m_1v^2}{2}\tilde{\hat{N}}_1 + \frac{m_2v^2}{2}\tilde{\hat{N}}_2 + \frac{(m_1+m_2)v^2}{2}\tilde{\hat{N}}_b.$$

Hence,

$$\tilde{U}_v\tilde{\hat{\mathcal{H}}}\tilde{U}_v^+ = \tilde{\hat{\mathcal{H}}} + \mathbf{v}\tilde{\hat{\boldsymbol{\mathcal{P}}}} + \frac{m_1v^2}{2}\tilde{\hat{N}}_1 + \frac{m_2v^2}{2}\tilde{\hat{N}}_2 + \frac{(m_1+m_2)v^2}{2}\tilde{\hat{N}}_b,$$

$$\tilde{U}_v\tilde{\hat{\boldsymbol{\mathcal{P}}}}\tilde{U}_v^+ = \tilde{\hat{\boldsymbol{\mathcal{P}}}} + m_1\mathbf{v}\tilde{\hat{N}}_1 + m_2\mathbf{v}\tilde{\hat{N}}_2 + (m_1+m_2)\mathbf{v}\tilde{\hat{N}}_b,$$

where $\tilde{\hat{\boldsymbol{\mathcal{P}}}}$, $\tilde{\hat{N}}_1$, $\tilde{\hat{N}}_2$, $\tilde{\hat{N}}_b$ are the momentum operator and the particle number operators (for free particles of the first and second kinds and their bound states). These formulas prove the Galilean invariance of the developed theory. Finally we note the validity of the following formula:

$$\tilde{U}_v\tilde{\hat{\boldsymbol{\pi}}}_i(\mathbf{x})\tilde{U}_v^+ = \tilde{\hat{\boldsymbol{\pi}}}_i(\mathbf{x}) + m_i\mathbf{v}\tilde{\hat{\rho}}_i(\mathbf{x}),$$

which follows from (27) and (28) by using (42).

V. ELECTROMAGNETIC INTERACTION

Here we consider the electromagnetic interaction assuming that the formation of bound states of particles is caused by Coulomb's (electromagnetic) forces. Therefore, the potential energy $\nu_{ij}(\mathbf{x}-\mathbf{x}')$ entering (38)–(40) should be written as

$$\nu_{ij}(\mathbf{x}-\mathbf{x}') = \frac{e_ie_j}{|\mathbf{x}-\mathbf{x}'|}, \quad i,j = 1,2. \tag{43}$$

We also introduce the additional interactions of particles (see below) with an external electromagnetic field $\mathbf{A}^{(e)}(\mathbf{x},t)$, $\varphi^{(e)}(\mathbf{x},t)$ and quantized electromagnetic field specified by a potential $\hat{\mathbf{a}}(\mathbf{x})$ (Coulomb's gauge)

$$\hat{\mathbf{A}}(\mathbf{x},t) = \hat{\mathbf{a}}(\mathbf{x}) + \mathbf{A}^{(e)}(\mathbf{x},t),$$

where[9]

$$\hat{\mathbf{a}}(\mathbf{x}) = \sum_{\mathbf{k}}\sum_{\lambda=1}^{2}\left(\frac{2\pi}{\mathcal{V}\omega_k}\right)^{1/2}(\mathbf{e}_{\mathbf{k}\lambda}\hat{C}_{\mathbf{k}\lambda}e^{i\mathbf{k}\mathbf{x}} + \mathrm{H.c.})$$

($\hat{C}_{\mathbf{k}\lambda}$ is the annihilation operator of a photon with momentum k and polarization $\mathbf{e}_{\mathbf{k}\lambda}$). As in Sec. II, we identify the subspace $\tilde{H}_a$ to $\tilde{H}$ assuming that the matrix elements of the operators in coordinate representation give the main contribution to the quantum electrodynamics processes and correspond to the space scale $\Delta x \gtrsim a$ ($a \to 0$, $a \gg r_0$).

The density $\hat{\varepsilon}(\mathbf{x})$ of a Hamiltonian in the second quantization representation has the well-known form

$$\hat{\varepsilon}(\mathbf{x}) = \hat{\varepsilon}_f(\mathbf{x}) + \hat{\varepsilon}_C(\mathbf{x}) + \sum_{i=1}^{2} e_i \hat{\psi}_i^+(\mathbf{x})\hat{\psi}_i(\mathbf{x})\varphi^{(e)}(\mathbf{x},t)$$
$$+ \sum_{i=1}^{2} \frac{1}{2m_i}\left(\frac{\partial}{\partial \mathbf{x}} - ie_i\hat{\mathbf{A}}(\mathbf{x},t)\right)\hat{\psi}_i^+(\mathbf{x})\left(\frac{\partial}{\partial \mathbf{x}} + ie_i\hat{\mathbf{A}}(\mathbf{x},t)\right)\hat{\psi}_i(\mathbf{x}),$$

where $\hat{\varepsilon}_f(\mathbf{x})$ is the energy density of a free electromagnetic field, $\hat{\varepsilon}_C(\mathbf{x})$ is the energy density of Coulomb's interaction, the third term describes the interaction between the particles and external scalar potential. This formula leads to the following Hamiltonian of the system:

$$\hat{\mathcal{H}}(t) = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}} + \hat{V}(t), \quad \hat{\mathcal{H}}_0 = \hat{\mathcal{H}}_f + \hat{\mathcal{H}}_p, \tag{44}$$

where

$$\hat{\mathcal{H}}_f \equiv \int \mathrm{d}\mathbf{x}\, \hat{\varepsilon}_f(\mathbf{x}) = \sum_{\mathbf{k},\lambda} \omega_k \hat{C}^+_{\mathbf{k}\lambda}\hat{C}_{\mathbf{k}\lambda}, \tag{45}$$

$$\hat{\mathcal{H}}_p = \sum_{i=1}^{2} \frac{1}{2m_i} \int \mathrm{d}\mathbf{x} \frac{\partial \hat{\psi}_i^+(\mathbf{x})}{\partial \mathbf{x}} \frac{\partial \hat{\psi}_i(\mathbf{x})}{\partial \mathbf{x}}, \tag{46}$$

$$\hat{\mathcal{H}}_{\text{int}} = \int \mathrm{d}\mathbf{x}\, \hat{\varepsilon}_C(\mathbf{x}) \tag{47}$$

are the Hamiltonians for free photons, free particles, and Coulomb's interaction, respectively. The operator $\hat{V}(t)$ represents a Hamiltonian that describes the interaction of particles with the electromagnetic fields $\hat{\mathbf{A}}(\mathbf{x},t)$, $\varphi^{(e)}(\mathbf{x},t)$

$$\hat{V}(t) = -\int \mathrm{d}\mathbf{x}\, \hat{\mathbf{A}}(\mathbf{x},t)\hat{\mathbf{J}}(\mathbf{x},t) - \frac{1}{2}\int \mathrm{d}\mathbf{x}\, \hat{\mathbf{A}}^2(\mathbf{x},t)\sum_{i=1}^{2}\frac{e_i}{m_i}\hat{\sigma}_i(\mathbf{x}) + \int \mathrm{d}\mathbf{x}\, \varphi^{(e)}(\mathbf{x},t)\hat{\sigma}, \tag{48}$$

$$\hat{\mathbf{J}}(\mathbf{x},t) = -\hat{\mathbf{A}}(\mathbf{x},t)\sum_{i=1}^{2}\frac{e_i}{m_i}\hat{\sigma}_i(\mathbf{x}) + \hat{\mathbf{j}}_0(\mathbf{x}), \quad \hat{\mathbf{j}}_0(\mathbf{x}) = \sum_{i=1}^{2}\frac{e_i}{m_i}\hat{\boldsymbol{\pi}}_i(\mathbf{x}), \tag{49}$$

where $\hat{\sigma}_i(x) = e_i\hat{\rho}_i(x)$ is the charge density for particles of the kind i, $\hat{\sigma} = \hat{\sigma}_1 + \hat{\sigma}_2$. This Hamiltonian is exact and describes (in this sense) the processes in which the bound states of particles are involved. Since $\hat{\mathbf{a}}(\mathbf{x})$ commute among themselves and with $\hat{\psi}_i(\mathbf{x})$, $\hat{\psi}_i^+(\mathbf{x})$, in order to find the effective Hamiltonian $\tilde{\hat{\mathcal{H}}}(t)$ that describes electrodynamic processes at low energies in the presence of bound states of particles we need, in accordance with Sec. IV, to replace the operators $\hat{\psi}_i$, $\hat{\psi}_i^+$, $\hat{\mathbf{a}}$ by $\tilde{\hat{\psi}}_i$, $\tilde{\hat{\psi}}_i^+$, $\tilde{\hat{\mathbf{a}}}$:

$$\tilde{\hat{\mathcal{H}}}(t) = \hat{\mathcal{H}}(t)|_{\hat{\psi}_1 \to \tilde{\hat{\psi}}_1, \hat{\psi}_2 \to \tilde{\hat{\psi}}_2, \hat{\mathbf{a}} \to \tilde{\hat{\mathbf{a}}}},$$

where

$$\tilde{\hat{\psi}}_1(\mathbf{x}) = \hat{\chi}_1(\mathbf{x}) + \int d\mathbf{y}\ \hat{\varphi}(\mathbf{x},\mathbf{y})\hat{\chi}_2^+(\mathbf{y}),\ \ \tilde{\hat{\psi}}_2(\mathbf{x}) = \hat{\chi}_2(\mathbf{x}) + \int d\mathbf{y}\ \hat{\varphi}(\mathbf{y},\mathbf{x})\hat{\chi}_1^+(\mathbf{y}),\ \ \tilde{\hat{\mathbf{a}}} = \hat{\mathbf{a}}$$

[$\tilde{\hat{\mathbf{a}}}(\mathbf{x})$ coincides with $\hat{\mathbf{a}}(\mathbf{x})$ and acts in the space $\tilde{H}$]. As a result the effective Hamiltonian is defined by (44)–(49), in which

$$\hat{\sigma}_i(\mathbf{x}) \to \tilde{\hat{\sigma}}_i(\mathbf{x}) = e_i\tilde{\hat{\rho}}_i(\mathbf{x}),\ \ \hat{\boldsymbol{\pi}}_i(\mathbf{x}) \to \tilde{\hat{\boldsymbol{\pi}}}_i(\mathbf{x}),\ \ \hat{\psi}_i(\mathbf{x}) \to \tilde{\hat{\psi}}_i(\mathbf{x}), \tag{50}$$

moreover, the operators $\tilde{\hat{\rho}}_i(\mathbf{x})$, $\tilde{\hat{\pi}}_i(\mathbf{x})$, $\tilde{\hat{\psi}}_i(\mathbf{x})$ containing the creation $\hat{\eta}_\alpha^+$ and annihilation $\hat{\eta}_\alpha$ operators of bound states are determined by (27), (28), and (16)–(18).

Let us define the operator of magnetic field

$$\hat{\mathbf{H}}(\mathbf{x},t) = \hat{\mathbf{h}}(\mathbf{x}) + \mathbf{H}^{(e)}(\mathbf{x},t), \tag{51}$$

where

$$\hat{\mathbf{h}}(\mathbf{x}) = \mathrm{rot}\,\hat{\mathbf{a}}(\mathbf{x}),\ \ \mathbf{H}^{(e)}(\mathbf{x},t) = \mathrm{rot}\,\mathbf{A}^{(e)}(\mathbf{x},t),$$

and the operator of electric field

$$\hat{\mathbf{E}}(\mathbf{x},t) = \hat{\mathbf{e}}(\mathbf{x}) + \mathbf{E}^{(e)}(\mathbf{x},t),$$

where

$$\hat{\mathbf{e}}(\mathbf{x}) = \hat{\mathbf{e}}^t(\mathbf{x}) + \hat{\mathbf{e}}^l(\mathbf{x}),\ \ \mathbf{E}^{(e)}(\mathbf{x},t) = -\frac{\partial}{\partial t}\mathbf{A}^{(e)}(\mathbf{x},t) - \frac{\partial}{\partial \mathbf{x}}\varphi^{(e)}(\mathbf{x},t).$$

The transverse $\hat{\mathbf{e}}^t(\mathbf{x})$ and longitudinal $\hat{\mathbf{e}}^l(\mathbf{x})$ components of the electric field created by particles are defined as follows:

$$\hat{\mathbf{e}}^l(\mathbf{x}) = -\frac{\partial}{\partial \mathbf{x}}\hat{\mathbf{a}}_0(\mathbf{x}),\ \ \hat{\mathbf{e}}^t(\mathbf{x}) = -\dot{\hat{\mathbf{a}}}(\mathbf{x}) \equiv -i[\tilde{\hat{\mathcal{H}}}(t),\hat{\mathbf{a}}(\mathbf{x})]. \tag{52}$$

Here $\hat{\mathbf{a}}_0(\mathbf{x})$ represents the operator of the scalar potential,

$$\hat{\mathbf{a}}_0(\mathbf{x}) = \int d\mathbf{x}'\frac{\tilde{\hat{\sigma}}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}. \tag{53}$$

Next it is easy to verify that

$$[\hat{\eta}_\alpha(\mathbf{X}),\hat{\eta}_\beta^+(\mathbf{X}')] = \delta_{\alpha\beta}\delta(\mathbf{X}-\mathbf{X}'),\ \ \sum_\alpha \varphi_\alpha^*(\mathbf{x})\varphi_\alpha(\mathbf{x}') = \delta(\mathbf{x}-\mathbf{x}')$$

lead to the following commutation relation:

$$[\hat{\varphi}(\mathbf{x},\mathbf{X}),\hat{\varphi}^+(\mathbf{x}',\mathbf{X}')] = \delta(\mathbf{x}-\mathbf{x}')\delta(\mathbf{X}-\mathbf{X}'), \tag{54}$$

where $\hat{\varphi}(\mathbf{x},\mathbf{X}) \equiv \hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2)$ is determined by (17). Hereinafter we assume that a set of wave functions $\varphi_\alpha(\mathbf{x}')$ is complete. Therefore this set accounts for the wave functions of continuous spectrum. In addition, if we introduce the operator

$$\hat{n}(\mathbf{x},\mathbf{X}) = \hat{\varphi}^+(\mathbf{x},\mathbf{X})\hat{\varphi}(\mathbf{x},\mathbf{X}),$$

then

$$[\hat{n}(\mathbf{x},\mathbf{X}),\hat{n}(\mathbf{x}',\mathbf{X}')]=0.$$

Thus, it is clear that the Hamiltonian $\tilde{\hat{\mathcal{H}}}_{\text{int}}$, which describes the Coulomb interaction between particles and bound states meets the commutation relation

$$[\tilde{\hat{\mathcal{H}}}_{\text{int}},\tilde{\hat{\rho}}_i(\mathbf{x})]=0.$$

Let us find now a commutator $[\tilde{\hat{\rho}}_i(\mathbf{x}),\tilde{\hat{\mathcal{H}}}_0]$ $(i=1,2)$, where $\tilde{\hat{\rho}}_i(\mathbf{x})$ and $\tilde{\hat{\mathcal{H}}}_0$ are defined by (28), (45), and (46). In order to do this we consider $\tilde{\hat{\rho}}_1(\mathbf{x})$ in the form

$$\tilde{\hat{\rho}}_1(\mathbf{x})=\tilde{\hat{\rho}}_1'(\mathbf{x})+\tilde{\hat{\rho}}_1''(\mathbf{x}),$$

where

$$\tilde{\hat{\rho}}_1'(\mathbf{x})=\hat{\chi}_1^+(\mathbf{x})\hat{\chi}_1(\mathbf{x}),\quad \tilde{\hat{\rho}}_1''(\mathbf{x})=\int \mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{Y}\,\delta\left(\mathbf{x}-\mathbf{Y}-\frac{m_2}{M}\mathbf{y}\right)\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\hat{\varphi}(\mathbf{y},\mathbf{Y}).$$

Then in accordance with the commutation relations for the field operators $\hat{\chi}_i(\mathbf{x})$,

$$[\hat{\chi}_i(\mathbf{x}),\hat{\chi}_j^+(\mathbf{x}')]=\delta_{ij}\delta(\mathbf{x}-\mathbf{x}'),$$

one gets

$$\left[\tilde{\hat{\rho}}_1'(\mathbf{x}),\int \mathrm{d}\mathbf{x}'\sum_{j=1}^{2}\frac{1}{2m_j}\frac{\partial\hat{\chi}_j^+(\mathbf{x}')}{\partial\mathbf{x}'}\frac{\partial\hat{\chi}_j(\mathbf{x}')}{\partial\mathbf{x}'}\right]=-\frac{i}{2m_1}\frac{\partial}{\partial x_k}\left(\hat{\chi}_1^+(\mathbf{x})\frac{\partial\hat{\chi}_1(\mathbf{x})}{\partial x_k}-\frac{\partial\hat{\chi}_1^+(\mathbf{x})}{\partial x_k}\hat{\chi}_1(\mathbf{x})\right).$$

Next according to (30) we have

$$\begin{aligned}i[\tilde{\hat{\rho}}_1''(\mathbf{x}),\tilde{\hat{\mathcal{H}}}_0]=&\frac{1}{2\mu}\int \mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{Y}\,\delta\left(\mathbf{x}-\mathbf{Y}-\frac{m_2}{M}\mathbf{y}\right)\frac{\partial}{\partial y_k}\left(-\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\frac{\partial\hat{\varphi}(\mathbf{y},\mathbf{Y})}{\partial y_k}+\frac{\partial\hat{\varphi}^+(\mathbf{y},\mathbf{Y})}{\partial y_k}\hat{\varphi}(\mathbf{y},\mathbf{Y})\right)\\&+\frac{1}{2M}\int \mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{Y}\,\delta\left(\mathbf{x}-\mathbf{Y}-\frac{m_2}{M}\mathbf{y}\right)\frac{\partial}{\partial Y_k}\left(-\hat{\varphi}^+(\mathbf{y},\mathbf{Y})\frac{\partial\hat{\varphi}(\mathbf{y},\mathbf{Y})}{\partial Y_k}+\frac{\partial\hat{\varphi}^+(\mathbf{y},\mathbf{Y})}{\partial Y_k}\hat{\varphi}(\mathbf{y},\mathbf{Y})\right).\end{aligned}$$

Bearing in mind

$$-\frac{\partial}{\partial y_k}\delta\left(\mathbf{x}-\mathbf{Y}-\frac{m_2}{M}\mathbf{y}\right)=\frac{m_2}{M}\frac{\partial}{\partial x_k}\delta\left(\mathbf{x}-\mathbf{Y}-\frac{m_2}{M}\mathbf{y}\right),\quad -\frac{\partial}{\partial Y_k}\delta\left(\mathbf{x}-\mathbf{Y}-\frac{m_2}{M}\mathbf{y}\right)=\frac{\partial}{\partial x_k}\delta\left(\mathbf{x}-\mathbf{Y}-\frac{m_2}{M}\mathbf{y}\right)$$

and taking into account the definitions of $\tilde{\hat{\rho}}_i$, $\tilde{\hat{\boldsymbol{\pi}}}_i$ $(i=1,2)$, one finds

$$i[\tilde{\hat{\rho}}_1(\mathbf{x}),\tilde{\hat{\mathcal{H}}}_0+\tilde{\hat{\mathcal{H}}}_{\text{int}}]=\frac{1}{m_1}\,\text{div}\,\tilde{\hat{\boldsymbol{\pi}}}_1(\mathbf{x}).\tag{55}$$

Similarly,

$$i[\tilde{\hat{\rho}}_2(\mathbf{x}),\tilde{\hat{\mathcal{H}}}_0+\tilde{\hat{\mathcal{H}}}_{\text{int}}]=\frac{1}{m_2}\,\text{div}\,\tilde{\hat{\boldsymbol{\pi}}}_2(\mathbf{x}).\tag{56}$$

Let us find now a commutator $[\tilde{\hat{\rho}}_i(\mathbf{x}'),\tilde{\hat{\pi}}_k(\mathbf{x})]$ $(i,k=1,2)$. With the use of (27) we have

$$[\tilde{\hat{\rho}}_i''(\mathbf{x}'),\tilde{\hat{\boldsymbol{\pi}}}_k(\mathbf{x})]=i\delta_{ik}\tilde{\hat{\rho}}_i''(\mathbf{x})\frac{\partial}{\partial\mathbf{x}}\delta(\mathbf{x}-\mathbf{x}').$$

Noting also that

$$[\tilde{\hat{\rho}}_i'(\mathbf{x}'), \tilde{\hat{\boldsymbol{\pi}}}_k(\mathbf{x})] = i\delta_{ik}\tilde{\hat{\rho}}_i'(\mathbf{x})\frac{\partial}{\partial \mathbf{x}}\delta(\mathbf{x}-\mathbf{x}'),$$

we get finally

$$[\tilde{\hat{\rho}}_i(\mathbf{x}'), \tilde{\hat{\boldsymbol{\pi}}}_k(\mathbf{x})] = i\delta_{ik}\tilde{\hat{\rho}}_i(\mathbf{x})\frac{\partial}{\partial \mathbf{x}}\delta(\mathbf{x}-\mathbf{x}').$$

These commutation relations along with (49) result in

$$[\tilde{\hat{\mathbf{j}}}_0(\mathbf{x}), \tilde{\hat{\sigma}}(\mathbf{x}')] = -i\sum_{i=1}^{2}\frac{e_i}{m_i}\tilde{\hat{\sigma}}_i(\mathbf{x}')\frac{\partial}{\partial \mathbf{x}}\delta(\mathbf{x}-\mathbf{x}').$$

Thus, according to (52), (55), and (56) we have

$$\dot{\tilde{\hat{\sigma}}}(\mathbf{x}) = i[\tilde{\hat{\mathcal{H}}}(t), \tilde{\hat{\sigma}}(\mathbf{x})] = \operatorname{div}\tilde{\hat{\mathbf{J}}}(\mathbf{x},t).$$

The definitions (52) and (53) of the longitudinal component of the electric field along with the above formula give

$$\dot{\hat{\mathbf{e}}}^l(\mathbf{x}) \equiv i[\tilde{\hat{\mathcal{H}}}(t), \hat{\mathbf{e}}^l(\mathbf{x})] = \frac{\partial}{\partial \mathbf{x}}\operatorname{div}\int d\mathbf{x}'\frac{\tilde{\hat{\mathbf{J}}}(\mathbf{x}',t)}{|\mathbf{x}-\mathbf{x}'|}. \tag{57}$$

Let us find the equation of motion for $\hat{\mathbf{e}}^t$. The use of commutation relations for creation $\hat{C}^+_{\mathbf{k}\lambda}$ and annihilation $\hat{C}_{\mathbf{k}\lambda}$ operators of photons,

$$[\hat{C}_{\mathbf{k}\lambda}, \hat{C}^+_{\mathbf{k}'\lambda'}] = \delta_{\mathbf{k}k'}\delta_{\lambda\lambda'}$$

lead to

$$\hat{\mathbf{e}}^t(\mathbf{x}) = -i[\tilde{\hat{\mathcal{H}}}(t), \hat{\mathbf{a}}(\mathbf{x})] = i\sum_{\mathbf{k}}\sum_{\lambda=1}^{2}\left(\frac{2\pi\omega_k}{\mathcal{V}}\right)^{1/2}(\mathbf{e}^{(\lambda)}_{\mathbf{k}}\hat{C}_{\mathbf{k}\lambda}e^{i\mathbf{k}\mathbf{x}} - \text{H.c.}), \tag{58}$$

$$\dot{\hat{\mathbf{e}}}^t(\mathbf{x}) = -i[\tilde{\hat{\mathcal{H}}}(t), \hat{\mathbf{e}}^t(\mathbf{x})] = \operatorname{rot}\hat{\mathbf{h}}(\mathbf{x}) + i[\tilde{\hat{V}}(t), \hat{\mathbf{e}}^t(\mathbf{x})],$$

and also

$$[\hat{a}_i(\mathbf{x}), \hat{e}^t_s(\mathbf{x}')] = -4\pi i\delta_{is}\delta(\mathbf{x}-\mathbf{x}') - i\frac{\partial^2}{\partial x_i \partial x_s}\frac{1}{|\mathbf{x}-\mathbf{x}'|}.$$

This formula and the definition of $\tilde{\hat{V}}(t)$ allows us to find the commutator:

$$i[\tilde{\hat{V}}(t), \hat{\mathbf{e}}^t(\mathbf{x})] = -4\pi\tilde{\hat{\mathbf{J}}}(\mathbf{x},t) - \frac{\partial}{\partial \mathbf{x}}\operatorname{div}\int d\mathbf{x}'\frac{\tilde{\hat{\mathbf{J}}}(\mathbf{x}',t)}{|\mathbf{x}-\mathbf{x}'|}.$$

Therefore, it follows from (57) and (58) that

$$\dot{\hat{\mathbf{e}}}(\mathbf{x}) = \operatorname{rot}\hat{\mathbf{h}}(\mathbf{x}) - 4\pi\tilde{\hat{\mathbf{J}}}(\mathbf{x},t), \quad \dot{\hat{\mathbf{h}}}(\mathbf{x}) \equiv i[\tilde{\hat{\mathcal{H}}}(t), \hat{\mathbf{h}}(\mathbf{x})] = i[\hat{\mathcal{H}}_f, \hat{\mathbf{h}}(\mathbf{x})]. \tag{59}$$

Upon calculating this commutator with the use of (51), one obtains

$$\dot{\hat{\mathbf{h}}}(\mathbf{x}) = -\operatorname{rot}\hat{\mathbf{e}}(\mathbf{x}). \tag{60}$$

In addition, (51) and (52) give $\operatorname{div}\hat{\mathbf{h}}(\mathbf{x})=0$, $\operatorname{div}\hat{\mathbf{e}}(\mathbf{x})=4\pi\tilde{\tilde{\sigma}}(\mathbf{x})$. These equations along with (59) and (60) represent the Maxwell–Lorentz equations for the operators of electromagnetic field

$$2\dot{\hat{\mathbf{e}}}(\mathbf{x}) = \operatorname{rot}\hat{\mathbf{h}}(\mathbf{x}) - 4\pi\tilde{\tilde{\mathbf{J}}}(\mathbf{x},t), \quad \operatorname{div}\hat{\mathbf{e}}(\mathbf{x}) = 4\pi\tilde{\tilde{\sigma}}(\mathbf{x}),$$

$$\dot{\hat{\mathbf{h}}}(\mathbf{x}) = -\operatorname{rot}\hat{\mathbf{e}}(\mathbf{x}), \quad \operatorname{div}\hat{\mathbf{h}}(\mathbf{x}) = 0.$$

Notice that (46), (51), and (58) result in

$$\hat{\mathcal{H}}_f = \sum_{\mathbf{k}}\sum_{\lambda=1}^{2}\omega_k\hat{C}^{+}_{\mathbf{k}\lambda}\hat{C}_{\mathbf{k}\lambda} = \frac{1}{8\pi}\int d\mathbf{x}(\mathbf{e}^{t_2}+\mathbf{h}^2),$$

where we neglect the unessential term $\Sigma_{\mathbf{k}\lambda}\frac{1}{2}\omega_k$.

Up to now we used the Schrödinger representation, in which the Schrödinger equation has the form

$$i\frac{\partial\Phi(t)}{\partial t} = \tilde{\tilde{\mathcal{H}}}(t)\Phi(t).$$

In this representation a dot above the certain operator $\dot{\hat{b}}(\mathbf{x})$ [see (52)] does not mean the differentiation with respect to time. It means the following:

$$\dot{\hat{b}}(\mathbf{x}) = i[\tilde{\tilde{H}}(\underline{\hat{\chi}}(\mathbf{x}'),t),\hat{b}(\mathbf{x})]. \tag{61}$$

Here the Hamiltonian $\tilde{\tilde{\mathcal{H}}}$ depends on dynamic variables $\underline{\hat{\chi}}(\mathbf{x}')$ (these variables unite $\hat{\chi}$ and $\hat{\eta}$) and time t. Introducing the unitary operator $\hat{S}(t,0)$,

$$i\frac{\partial\hat{S}(t,0)}{\partial t} = \tilde{\tilde{H}}(\underline{\hat{\chi}}(\mathbf{x}'),t)\hat{S}(t,0), \quad \hat{S}(0,0)=1,$$

we can write the solution of the equation for $\Phi(t)$ in the form,

$$\Phi(t) = \hat{S}(t,0)\Phi(0).$$

In the Heisenberg representation the vector $\Phi(0)=\Psi$ is taken as a time-independent state vector. Then, the time-dependent Heisenberg operators

$$\underline{\hat{\chi}}(\mathbf{x},t) \equiv \underline{\hat{\chi}}(x) = \hat{S}^{+}(t,0)\underline{\hat{\chi}}(\mathbf{x})\hat{S}(t,0)$$

satisfy the equation

$$i\frac{\partial\underline{\hat{\chi}}(x)}{\partial t} = [\underline{\hat{\chi}}(x),\tilde{\tilde{\mathcal{H}}}(\underline{\hat{\chi}}(x),t)]. \tag{62}$$

Since the external fields $\mathbf{H}^{(e)},\mathbf{E}^{(e)}$ satisfy the Maxwell equations,

$$\frac{\partial\mathbf{H}^{(e)}}{\partial t} = -\operatorname{rot}\mathbf{E}^{(e)}, \quad \operatorname{div}\mathbf{H}^{(e)}=0,$$

$$\frac{\partial \mathbf{E}^{(e)}}{\partial t} = \operatorname{rot} \mathbf{H}^{(e)} - 4\pi \mathbf{J}^{(e)}, \quad \operatorname{div} \mathbf{E}^{(e)} = 4\pi\sigma^{(e)},$$

the operators of total fields $\hat{\mathbf{E}}, \hat{\mathbf{H}}$ in the Heisenberg representation satisfy, in accordance with (62), the equations

$$\frac{\partial \hat{\mathbf{H}}}{\partial t} = -\operatorname{rot} \hat{\mathbf{E}}, \quad \operatorname{div} \hat{\mathbf{H}} = 0,$$

$$\frac{\partial \hat{\mathbf{E}}}{\partial t} = \operatorname{rot} \hat{\mathbf{H}} - 4\pi(\tilde{\hat{\mathbf{J}}} + \mathbf{J}^{(e)}), \quad \operatorname{div} \hat{\mathbf{E}} = 4\pi(\tilde{\hat{\sigma}} + \sigma^{(e)}), \tag{63}$$

where $\mathbf{J}^{(e)}$ and $\sigma^{(e)}$ are the extrinsic current and charge densities.

Let us write out the expressions for the charge density operator $\tilde{\hat{\sigma}}$ and current density operator $\tilde{\hat{\mathbf{J}}}$ in terms of creation and annihilation operators of particles and bound states. Bearing in mind (50) we have

$$\begin{aligned} \tilde{\hat{\sigma}}(\mathbf{x}) &= \sum_{i=1}^{2} e_i \tilde{\hat{\rho}}_i(\mathbf{x}), \\ \tilde{\hat{\mathbf{J}}}(\mathbf{x}) &= -\hat{\mathbf{A}}(\mathbf{x}) \sum_{i=1}^{2} \frac{e_i^2}{m_i} \tilde{\hat{\rho}}_i(\mathbf{x}) + \sum_{i=1}^{2} \frac{e_i}{m_i} \tilde{\hat{\boldsymbol{\pi}}}_i(\mathbf{x}), \end{aligned} \tag{64}$$

where the particle density operators $\tilde{\hat{\rho}}_i(\mathbf{x})$ are defined by (28) and the momentum density operators $\tilde{\hat{\boldsymbol{\pi}}}_i(\mathbf{x})$ by (27). The first terms in expressions for $\tilde{\hat{\rho}}_i(\mathbf{x})$ and $\tilde{\hat{\boldsymbol{\pi}}}_i(\mathbf{x})$ define the contribution of particles, whereas the second terms define the contribution of bound states [see (27) and (28)].

Let us find now the equations of motion for the field operators of particles $\hat{\chi}_i(\mathbf{x})$ and bound states $\hat{\varphi}(\mathbf{x},\mathbf{y})$. In the Heisenberg representation these equations are obtained from the general formulas (62). Indeed, it follows from (38)–(40) that

$$[\hat{\chi}_1(\mathbf{x}), \tilde{\hat{\mathcal{H}}}_{\text{int}}(\hat{\chi}(\mathbf{x}'))] = \left\{ \int d\mathbf{x}_2 \, \nu_{11}(\mathbf{x}-\mathbf{x}_2) \tilde{\hat{\rho}}_1(\mathbf{x}_2) + \int d\mathbf{x}_2 \, \nu_{12}(\mathbf{x}-\mathbf{x}_2) \tilde{\hat{\rho}}_2(\mathbf{x}_2) \right\} \hat{\chi}_1(\mathbf{x}),$$

$$[\hat{\chi}_2(\mathbf{x}), \tilde{\hat{\mathcal{H}}}_{\text{int}}(\hat{\chi}(\mathbf{x}'))] = \left\{ \int d\mathbf{x}_1 \, \nu_{22}(\mathbf{x}-\mathbf{x}_1) \tilde{\hat{\rho}}_2(\mathbf{x}_1) + \int d\mathbf{x}_2 \, \nu_{21}(\mathbf{x}-\mathbf{x}_1) \tilde{\hat{\rho}}_1(\mathbf{x}_1) \right\} \hat{\chi}_2(\mathbf{x}),$$

$$\begin{aligned} [\hat{\varphi}(\mathbf{x},\mathbf{y}), \tilde{\hat{\mathcal{H}}}_{\text{int}}(\hat{\chi}(\mathbf{x}'))] = \Bigg\{ & \int d\mathbf{x}_2 (\nu_{11}(\mathbf{x}-\mathbf{x}_2) + \nu_{12}(\mathbf{y}-\mathbf{x}_2)) \tilde{\hat{\rho}}_1(\mathbf{x}_2) + \int d\mathbf{x}_2 (\nu_{22}(\mathbf{y}-\mathbf{x}_2) \\ & + \nu_{21}(\mathbf{x}-\mathbf{x}_2)) \tilde{\hat{\rho}}_2(\mathbf{x}_2) \Bigg\} \hat{\varphi}(\mathbf{x},\mathbf{y}). \end{aligned}$$

These formulas allow us to find the equations of motion (62) for $\hat{\chi}_1(\mathbf{x})$, $\hat{\chi}_2(\mathbf{x})$ in the Heisenberg representation,

$$i\dot{\hat{\chi}}_1(\mathbf{x},t) = \left\{ -\frac{1}{2m_1} \left(\frac{\partial}{\partial \mathbf{x}} - ie_1 \hat{\mathbf{A}}(\mathbf{x},t) \right)^2 + e_1 \varphi^{(e)}(\mathbf{x},t) + \hat{v}_1(\mathbf{x},t) \right\} \hat{\chi}_1(\mathbf{x},t),$$

$$i\dot{\hat{\chi}}_2(\mathbf{x},t)=\left\{-\frac{1}{2m_2}\left(\frac{\partial}{\partial\mathbf{x}}-ie_2\hat{\mathbf{A}}(\mathbf{x},t)\right)^2+e_2\varphi^{(e)}(\mathbf{x},t)+\hat{\upsilon}_2(\mathbf{x},t)\right\}\hat{\chi}_2(\mathbf{x},t).$$

It is easy to find also the equation of motion for the field operators $\hat{\varphi}(\mathbf{x},\mathbf{y})$ of bound states,

$$i\dot{\hat{\varphi}}(\mathbf{x}_1,\mathbf{x}_2,t)=\sum_\alpha\varepsilon_\alpha\hat{\eta}_\alpha(\mathbf{X},t)\varphi_\alpha(\mathbf{x})+\left\{-\frac{1}{2m_1}\left(\frac{\partial}{\partial\mathbf{x}_1}-ie_1\hat{\mathbf{A}}(\mathbf{x}_1,t)\right)^2-\frac{1}{2m_2}\left(\frac{\partial}{\partial\mathbf{x}_2}-ie_2\hat{\mathbf{A}}(\mathbf{x}_2,t)\right)^2\right.$$
$$\left.+e_1\varphi^{(e)}(\mathbf{x}_1,t)+e_2\varphi^{(e)}(\mathbf{x}_2,t)+\hat{\upsilon}(\mathbf{x}_1,\mathbf{x}_2,t)\right\}\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2,t). \tag{65}$$

Here

$$\hat{\upsilon}_1(\mathbf{x},t)=\int d\mathbf{x}_2\ \nu_{11}(\mathbf{x}-\mathbf{x}_2)\tilde{\hat{\rho}}_1(\mathbf{x}_2,t)+\int d\mathbf{x}_2\ \nu_{12}(\mathbf{x}-\mathbf{x}_2)\tilde{\hat{\rho}}_2(\mathbf{x}_2,t),$$

$$\hat{\upsilon}_2(\mathbf{x},t)=\int d\mathbf{x}_1\ \nu_{22}(\mathbf{x}-\mathbf{x}_1)\tilde{\hat{\rho}}_2(\mathbf{x}_1,t)+\int d\mathbf{x}_1\ \nu_{21}(\mathbf{x}-\mathbf{x}_1)\tilde{\hat{\rho}}_1(\mathbf{x}_1,t),$$

$$\hat{\upsilon}(\mathbf{x}_1,\mathbf{x}_2,t)=\int d\mathbf{x}'(\nu_{11}(\mathbf{x}_1-\mathbf{x}')+\nu_{12}(\mathbf{x}_2-\mathbf{x}'))\tilde{\hat{\rho}}_1(\mathbf{x}',t)+\int d\mathbf{x}'(\nu_{22}(\mathbf{x}_2-\mathbf{x}')+\nu_{21}(\mathbf{x}_1-\mathbf{x}'))\tilde{\hat{\rho}}_2(\mathbf{x}',t).$$

The operators $\hat{\eta}_\alpha(\mathbf{X},t)$ related to $\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2,t)$ by $\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2,t)=\varphi_\beta(\mathbf{x})\hat{\eta}_\beta(\mathbf{X},t)$.

The equations of motion (63) and (65) are gauge invariant. Indeed, under the following transformations of fields $\hat{\chi}_i$, $\hat{\varphi}$:

$$\hat{\chi}_1(\mathbf{x},t)\to\hat{\chi}_1'(\mathbf{x},t)=e^{ie_1\alpha(\mathbf{x},t)}\hat{\chi}_1(\mathbf{x},t),\quad\hat{\chi}_2(\mathbf{x},t)\to\hat{\chi}_2'(\mathbf{x},t)=e^{ie_2\alpha(\mathbf{x},t)}\hat{\chi}_2(\mathbf{x},t),$$

$$\hat{\varphi}(\mathbf{x},\mathbf{y},t)\to\hat{\varphi}'(\mathbf{x},\mathbf{y},t)=e^{ie_1\alpha(\mathbf{x},t)+ie_2\alpha(\mathbf{y},t)}\hat{\varphi}(\mathbf{x},\mathbf{y},t), \tag{66}$$

and electromagnetic field,

$$\hat{\mathbf{A}}(\mathbf{x},t)\to\hat{\mathbf{A}}'(\mathbf{x},t)=\hat{\mathbf{A}}(\mathbf{x},t)-\frac{\partial}{\partial\mathbf{x}}\alpha(\mathbf{x},t),\quad\varphi^{(e)}(\mathbf{x},t)\to\varphi^{(e)'}(\mathbf{x},t)=\varphi^{(e)}(\mathbf{x})-\frac{\partial\alpha(\mathbf{x},t)}{\partial t}$$

the operators $\tilde{\hat{\rho}}_i(\mathbf{x})$ are invariant,

$$\tilde{\hat{\rho}}_i(\mathbf{x},t)\to\tilde{\hat{\rho}}_i'(\mathbf{x},t)=\tilde{\hat{\rho}}_i(\mathbf{x},t),$$

whereas $\tilde{\hat{\boldsymbol{\pi}}}_i(\mathbf{x})$ transform [see (65)], by the law

$$\tilde{\hat{\boldsymbol{\pi}}}_i(\mathbf{x},t)\to\tilde{\hat{\boldsymbol{\pi}}}_i'(\mathbf{x},t)=\tilde{\hat{\boldsymbol{\pi}}}_i(\mathbf{x},t)+e_i\tilde{\hat{\rho}}_i(\mathbf{x},t)\frac{\partial}{\partial\mathbf{x}}\alpha(\mathbf{x},t).$$

As a result we have [see (64)]

$$\tilde{\hat{\mathbf{J}}}(\mathbf{x},t)\to\tilde{\hat{\mathbf{J}}}'(\mathbf{x},t)=\tilde{\hat{\mathbf{J}}}(\mathbf{x},t),\quad\tilde{\hat{\mathcal{H}}}\to\tilde{\hat{\mathcal{H}}}'=\tilde{\hat{\mathcal{H}}}$$

that provides a gauge invariance of the Maxwell–Lorentz equations (63). Next noting that

$$\left(\frac{\partial}{\partial\mathbf{x}}-ie_i\hat{\mathbf{A}}(\mathbf{x},t)\right)\hat{\chi}_i(\mathbf{x},t)\to\left(\frac{\partial}{\partial\mathbf{x}}-ie_i\hat{\mathbf{A}}'(\mathbf{x},t)\right)\hat{\chi}_i'(\mathbf{x},t)=e^{ie_i\alpha(\mathbf{x},t)}\left(\frac{\partial}{\partial\mathbf{x}}-ie_i\hat{\mathbf{A}}(\mathbf{x},t)\right)\hat{\chi}_i(\mathbf{x},t),$$

we make sure of gauge invariance of the equations of motion for the field operators of particles $\hat{\chi}_i(\mathbf{x})$. Taking into account the transformation law for the field operators of bound states $\hat{\varphi}(\mathbf{x},\mathbf{y})$, it

is easy to prove a gauge invariance of the equation of motion for $\hat{\varphi}(\mathbf{x},\mathbf{y})$.

Since $\hat{\varphi}(\mathbf{x}_1,\mathbf{x}_2,t)=\varphi_\alpha(\mathbf{x})\,\hat{\eta}_\alpha(\mathbf{X},t)$, we have under the gauge transformation (66),

$$\hat{\varphi}'(\mathbf{x}_1,\mathbf{x}_2,t)=\varphi_\alpha(\mathbf{x})\,\hat{\eta}'_\alpha(\mathbf{X},t),$$

where $\mathbf{x}_1=\mathbf{X}+(m_2/M)\mathbf{x}$, $\mathbf{x}_2=\mathbf{X}-(m_1/M)\mathbf{x}$. Hence, we come to the transformation law for the operators $\hat{\eta}_\alpha(\mathbf{X})$:

$$\hat{\eta}_\alpha(\mathbf{X},t)\rightarrow\hat{\eta}'_\alpha(\mathbf{X},t)=\sum_\beta L_{\alpha\beta}(\mathbf{X},t)\,\hat{\eta}_\beta(\mathbf{X},t),$$

$$L_{\alpha\beta}(\mathbf{X},t)=\int \mathrm{d}\mathbf{x}\;\varphi^*_\alpha(\mathbf{x})e^{ie_1\alpha[\mathbf{X}+(m_2/M)\mathbf{x},t]+ie_2\alpha[\mathbf{X}-(m_1/M)\mathbf{x},t]}\varphi_\beta(\mathbf{x}).$$

In conclusion of this section let us note that $\tilde{\tilde{\psi}}_i(\mathbf{x})$ transform under the gauge transformation as well as $\hat{\chi}_i(\mathbf{x})$:

$$\tilde{\tilde{\psi}}_i(\mathbf{x},t)\rightarrow\tilde{\tilde{\psi}}'_i(\mathbf{x},t)=e^{ie_i\alpha(\mathbf{x},t)}\tilde{\tilde{\psi}}_i(\mathbf{x},t).$$

VI. THE PROCESS OF SPONTANEOUS RADIATION BY ATOM

In this section we employ the obtained formulas in order to find the probability distribution of spontaneous radiation of an excited atom. To this end we use the general formulas for the scattering matrix $\hat{S}$ in terms of the T operator,

$$\hat{S}=1-2\pi i\int_{-\infty}^{\infty}\mathrm{d}E\;\delta(E-\hat{\mathcal{H}}_0)\hat{T}^{(+)}(E)\,\delta(E-\hat{\mathcal{H}}_0),$$

$$\hat{T}^{(+)}(E)=\lim_{\eta\rightarrow+0}\hat{T}(E+i\eta), \tag{67}$$

where $\hat{T}(z)$ is found from the equation

$$\hat{T}(z)=\hat{V}+\hat{V}\hat{R}_0\hat{T}(z),\quad \hat{R}_0=\frac{1}{z-\hat{\mathcal{H}}_0}. \tag{68}$$

In the first order of the perturbative approach over charge we have

$$\langle f|\hat{T}(z)|i\rangle\approx\langle f|\hat{V}|i\rangle,$$

where

$$|i\rangle=\hat{\eta}^+_{\alpha\mathbf{p}}|0\rangle,\quad |f\rangle=\hat{C}^+_{\mathbf{k}\lambda}\hat{\eta}^+_{\alpha\mathbf{p}}|0\rangle.$$

Here $|i\rangle$ is the initial state (in which atom is in the state α, $\mathbf{p}$) and $|f\rangle$ is the final state (in which atom is in the state α', $\mathbf{p}'$ and photon is in the state λ, $\mathbf{k}$). According to (48) and (50) we can take $\hat{V}$ in the following form:

$$\tilde{\tilde{V}}=-\int \mathrm{d}\mathbf{x}\;\hat{\mathbf{a}}(\mathbf{x})\tilde{\tilde{\mathbf{j}}}(\mathbf{x}),$$

where the current of bound states is defined by

$$\tilde{\hat{\mathbf{j}}}(\mathbf{x}) = \frac{e_1}{m_1}\tilde{\hat{\boldsymbol{\pi}}}_1(\mathbf{x}) + \frac{e_2}{m_2}\tilde{\hat{\boldsymbol{\pi}}}_2(\mathbf{x}). \tag{69}$$

By using (48) and (50) we find

$$\langle f|\tilde{\hat{V}}|i\rangle = -\left(\frac{2\pi}{\mathcal{V}\omega_k}\right)^{1/2}\mathbf{e}_{\mathbf{k}}^{(\lambda)*}\int \mathrm{d}\mathbf{x}\, e^{-i\mathbf{k}\mathbf{x}}\langle\alpha'\mathbf{p}'|\tilde{\hat{\mathbf{j}}}(\mathbf{x})|\alpha\mathbf{p}\rangle.$$

The formulas (69) and (27) lead to

$$\tilde{\hat{\mathbf{j}}}(\mathbf{k}) \equiv \int \mathrm{d}\mathbf{x}\, e^{-i\mathbf{k}\mathbf{x}}\tilde{\hat{\mathbf{j}}}(\mathbf{x}) = \sum_{\mathbf{p}_1,\mathbf{p}_2}\sum_{\alpha_1,\alpha_2}\hat{\eta}^+_{\alpha_1\mathbf{p}_1}\hat{\eta}_{\alpha_2\mathbf{p}_2}\left(\mathbf{g}_{\alpha_1\alpha_2}(\mathbf{k}) + \frac{\mathbf{p}_1+\mathbf{p}_2}{2M}g_{\alpha_1\alpha_2}(\mathbf{k})\right)\Delta(\mathbf{p}_1-\mathbf{p}_2+\mathbf{k})$$

and, consequently,

$$\langle f|\tilde{\hat{V}}|i\rangle = -\left(\frac{2\pi}{\mathcal{V}\omega_k}\right)^{1/2}\mathbf{e}_{\mathbf{k}}^{(\lambda)*}\left(\mathbf{g}_{\alpha\alpha'}(\mathbf{k}) + \frac{\mathbf{p}+\mathbf{p}'}{2M}g_{\alpha\alpha'}(\mathbf{k})\right)\Delta(\mathbf{p}-\mathbf{p}'-\mathbf{k}),\ \ \mathbf{k}=\mathbf{p}-\mathbf{p}',$$

where $\Delta(\mathbf{p}) = \delta_{\mathbf{p}0}$, and

$$g_{\alpha\beta}(\mathbf{k}) = \int \mathrm{d}\mathbf{y}(e_1 e^{i\mathbf{k}\mathbf{y}(m_2/M)} + e_2 e^{-i\mathbf{k}\mathbf{y}(m_1/M)})\varphi^*_\alpha(\mathbf{y})\varphi_\beta(\mathbf{y}),$$

$$\mathbf{g}_{\alpha\beta}(\mathbf{k}) = -\frac{i}{2}\int \mathrm{d}\mathbf{y}\left(\frac{e_1}{m_1}e^{i\mathbf{k}\mathbf{y}(m_2/M)} - \frac{e_2}{m_2}e^{-i\mathbf{k}\mathbf{y}(m_1/M)}\right)\left(\varphi^*_\alpha(\mathbf{y})\frac{\partial\varphi_\beta(\mathbf{y})}{\partial\mathbf{y}} - \frac{\partial\varphi^*_\alpha(\mathbf{y})}{\partial\mathbf{y}}\varphi_\beta(\mathbf{y})\right). \tag{70}$$

The matrix element of $\hat{S}$-matrix is defined, in accordance with (67), by

$$\langle f|\hat{S}|i\rangle = -2\pi i\langle f|\tilde{\hat{V}}|i\rangle\delta(\varepsilon(\mathbf{p}) - \varepsilon(\mathbf{p}') - \omega_k).$$

Next using the standard method we obtain the following expression for the probability of transition per unit time from the initial state $\hat{\eta}^+_{\alpha\mathbf{p}}|0\rangle$ into the final state $\hat{\eta}^+_{\beta\mathbf{p}'}\hat{C}^+_{\mathbf{k}\lambda}|0\rangle$:

$$\mathrm{d}w_{i\to f} = \frac{2\pi}{\omega_k}\left|\mathbf{e}_{\mathbf{k}}^{(\lambda)}\left(\mathbf{g}_{\alpha\beta}(\mathbf{k}) + \frac{\mathbf{p}+\mathbf{p}'}{2M}g_{\alpha\beta}(\mathbf{k})\right)\right|^2\delta(\omega_k + \varepsilon_\beta(\mathbf{p}') - \varepsilon_\alpha(\mathbf{p}))\mathrm{d}\mathbf{k}.$$

In the domain of small $\mathbf{k}$ ($kr_0 \ll 1$, see Sec. II) the Fourier-components of $\mathbf{g}_{\alpha\beta}(\mathbf{x})$, $g_{\alpha\beta}(\mathbf{x})$ can be written in the form

$$\mathbf{g}_{\alpha\beta}(0) = \left(\frac{e_1}{m_1} - \frac{e_2}{m_2}\right)\int \mathrm{d}\mathbf{y}\ \varphi^*_\alpha(\mathbf{y})\hat{\mathbf{p}}\varphi_\beta(\mathbf{y}) = \left(\frac{e_1}{m_1} - \frac{e_2}{m_2}\right)\langle\alpha|\hat{\mathbf{p}}|\beta\rangle,\ \ g_{\alpha\beta}(0) = (e_1+e_2)\delta_{\alpha\beta}. \tag{71}$$

If $e_2 = -e_1 = -e$ (this case corresponds to the hydrogen atom), then $g_{\alpha\beta}(0) = 0$, $\mathbf{g}_{\alpha\beta}(0) = (e/\mu)\times\langle\alpha|\hat{\mathbf{p}}|\beta\rangle$. The Schrödinger equation for the wave function $\varphi_\alpha(\mathbf{y})$ gives

$$\langle\alpha|\hat{\mathbf{p}}|\beta\rangle = i\mu(\varepsilon_\alpha - \varepsilon_\beta)\int \mathrm{d}\mathbf{y}\ \varphi^*_\alpha(\mathbf{y})\mathbf{y}\varphi_\beta(\mathbf{y}).$$

Therefore,

$$\mathbf{g}_{\alpha\beta}(0) = i(\varepsilon_\alpha - \varepsilon_\beta)\langle\alpha|\hat{\mathbf{d}}|\beta\rangle,$$

where $\hat{\mathbf{d}} = e\hat{\mathbf{y}}$ is the dipole moment of the atom. Hence,

$$dw_{i\to f} = 2\pi\omega_k \left|\langle\alpha|\mathbf{e}_{\mathbf{k}}^{(\lambda)}\hat{\mathbf{d}}|\beta\rangle\right|^2 \delta(\omega_k + \varepsilon_\beta(\mathbf{p}') - \varepsilon_\alpha(\mathbf{p}))d\mathbf{k}.$$

Since $\varepsilon_\alpha(\mathbf{p}) = \varepsilon_\alpha + p^2/2M$, we have for the atom of infinite mass ($m_2 \to \infty$, $M \to \infty$),[5]

$$dw_{i\to f} = \frac{2\pi}{\omega_k}|\mathbf{e}_{\mathbf{k}}^{(\lambda)}\mathbf{g}_{\alpha\beta}(\mathbf{k})|^2 \delta(\omega_k + \varepsilon_\beta - \varepsilon_\alpha)d\mathbf{k},$$

where

$$\mathbf{g}_{\alpha\beta}(\mathbf{k}) = -\frac{ie}{2m_1}\int d\mathbf{y}\, e^{i\mathbf{k}\mathbf{y}}\left(\varphi_\alpha^*(\mathbf{y})\frac{\partial\varphi_\beta(\mathbf{y})}{\partial\mathbf{y}} - \frac{\partial\varphi_\alpha^*(\mathbf{y})}{\partial\mathbf{y}}\varphi_\beta(\mathbf{y})\right)$$

(m_1 is the mass of light fermion).

VII. SCATTERING OF PHOTONS AND FERMIONS BY ATOMS

Here we study the scattering process of long-wave photons by atoms. For this purpose let us use the general formulas (67) and (68), where the Hamiltonian of free particles is defined by

$$\tilde{\tilde{\mathcal{H}}}_0 = \sum_{i=1}^{2}\int d\mathbf{x}\ \nabla\hat{\chi}_i^+(\mathbf{x})\nabla\hat{\chi}_i(\mathbf{x}) + \sum_{\mathbf{k}}\sum_{\lambda=1}^{2}\omega_k\hat{C}_{\mathbf{k}\lambda}^+\hat{C}_{\mathbf{k}\lambda}$$
$$+\sum_\alpha\int d\mathbf{x}\left(\frac{1}{2m}\nabla\hat{\eta}_\alpha^+(\mathbf{x})\nabla\hat{\eta}_\alpha(\mathbf{x}) + \varepsilon_\alpha\hat{\eta}_\alpha^+(\mathbf{x})\hat{\eta}_\alpha(\mathbf{x})\right),$$

and the Hamiltonian associated with electromagnetic interaction by

$$\tilde{\tilde{V}} = \tilde{\tilde{V}}' + \tilde{\tilde{V}}''.$$

In accordance with (48) and (50),

$$\tilde{\tilde{V}}' = \frac{1}{2}\int d\mathbf{x}\,\hat{\mathbf{a}}^2(\mathbf{x})\left(\frac{e^2}{m_1}\tilde{\tilde{\rho}}_1(\mathbf{x}) + \frac{e^2}{m_2}\tilde{\tilde{\rho}}_2(\mathbf{x})\right),\quad \tilde{\tilde{V}}'' = -\int d\mathbf{x}\,\hat{\mathbf{a}}(\mathbf{x})\tilde{\tilde{\mathbf{j}}}(\mathbf{x}),$$

$$\tilde{\tilde{\mathbf{j}}}(\mathbf{x}) = \frac{e}{m_1}\tilde{\tilde{\pi}}_1(\mathbf{x}) + \frac{e}{m_2}\tilde{\tilde{\pi}}_2(\mathbf{x}) \tag{72}$$

(further we assume $e_1 = -e_2 = e$). Since $\tilde{\tilde{V}}' \sim e^2$, $\tilde{\tilde{V}}'' \sim e$, in the second order in charge e, the T-matrix can be written as

$$\hat{T}(z) = \tilde{\tilde{V}}' + \tilde{\tilde{V}}''\hat{R}_0(z)\tilde{\tilde{V}}'',\quad \hat{R}_0 = \frac{1}{z - \tilde{\tilde{\mathcal{H}}}_0}$$

(within the considered approximation it is not necessary to take into account the fields $\hat{\chi}_i(\mathbf{x})$). Bearing in mind (72) and (28), the operator $\tilde{\tilde{V}}'$ can be written as

$$\tilde{\tilde{V}}' = \frac{1}{2\mathcal{V}}\sum_{\mathbf{p}_1,\mathbf{p}_2}\hat{\eta}_\alpha^+(\mathbf{p}_1)\hat{\eta}_\beta(\mathbf{p}_2)q_{\alpha\beta}(\mathbf{p}_1 - \mathbf{p}_2)\int d\mathbf{x}\,\hat{\mathbf{a}}^2(\mathbf{x})e^{i\mathbf{x}(\mathbf{p}_2 - \mathbf{p}_1)},$$

where

$$q_{\alpha\beta}(\mathbf{k}) = \int \mathrm{d}\mathbf{y}\left\{\frac{e^2}{m_1}e^{i\mathbf{k}\mathbf{y}(m_2/M)} + \frac{e^2}{m_2}e^{-i\mathbf{k}\mathbf{y}(m_1/M)}\right\}\varphi^*_\alpha(\mathbf{y})\varphi_\beta(\mathbf{y}).$$

Similarly,

$$\tilde{\hat{V}}'' = -\frac{1}{\mathcal{V}}\sum_{\mathbf{p}_1,\mathbf{p}_2}\hat{\eta}^+_\alpha(\mathbf{p}_1)\hat{\eta}_\beta(\mathbf{p}_2)\mathbf{I}_{\alpha\beta}(\mathbf{p}_1+\mathbf{p}_2,\mathbf{p}_1-\mathbf{p}_2)\int \mathrm{d}\mathbf{x}\,\hat{\mathbf{a}}(\mathbf{x})e^{i\mathbf{x}(\mathbf{p}_2-\mathbf{p}_1)},$$

where

$$\mathbf{I}_{\alpha\beta}(\mathbf{p}_1+\mathbf{p}_2,\mathbf{p}_1-\mathbf{p}_2) = \mathbf{g}_{\alpha\beta}(\mathbf{p}_1-\mathbf{p}_2) + \frac{\mathbf{p}_1+\mathbf{p}_2}{2M}g_{\alpha\beta}(\mathbf{p}_1-\mathbf{p}_2),\ \ \mathbf{p}_1-\mathbf{p}_2=\mathbf{k},\ \ \mathbf{p}_1+\mathbf{p}_2=\mathbf{p},$$

moreover, $\mathbf{g}_{\alpha\beta}(\mathbf{k})$, $g_{\alpha\beta}(\mathbf{k})$ are defined by (70).

Let $\hat{C}^+_{\mathbf{k}\lambda}\hat{\eta}^+_\alpha(\mathbf{p})|0\rangle$ and $\hat{C}^+_{\mathbf{k}'\lambda'}\hat{\eta}^+_{\alpha'}(\mathbf{p}')|0\rangle$ be the initial and final states of the system,

$$|i\rangle = \hat{C}^+_{\mathbf{k}\lambda}\hat{\eta}^+_\alpha(\mathbf{p})|0\rangle,\ \ |i\rangle = \hat{C}^+_{\mathbf{k}'\lambda'}\hat{\eta}^+_{\alpha'}(\mathbf{p}')|0\rangle.$$

Then the matrix element $\langle f|\hat{T}(z)|i\rangle$ can be represented in the form

$$\langle f|\hat{T}(z)|i\rangle = \langle f|\tilde{\hat{V}}'|i\rangle + \langle f|\tilde{\hat{V}}''\hat{R}_0(z)\tilde{\hat{V}}''|i\rangle,$$

where

$$\langle f|\tilde{\hat{V}}'|i\rangle = -\frac{4\pi^2 i}{\mathcal{V}}\frac{1}{\sqrt{\omega\omega'}}R'_{\alpha'\alpha}\Delta(\mathbf{p}+\mathbf{k}-\mathbf{p}'-\mathbf{k}'),$$

$$\langle f|\tilde{\hat{V}}''\hat{R}_0(z)\tilde{\hat{V}}''|i\rangle = -\frac{4\pi^2 i}{\mathcal{V}}\frac{1}{\sqrt{\omega\omega'}}R''_{\alpha'\alpha}\Delta(\mathbf{p}+\mathbf{k}-\mathbf{p}'-\mathbf{k}'),\ \ \Delta(\mathbf{k})=\delta_{\mathbf{k}0},$$

and the matrices $R'_{\alpha'\alpha}$, $R''_{\alpha'\alpha}$ are given by

$$R'_{\alpha'\alpha} = \mathbf{e}^{(\lambda)}_{\mathbf{k}}\mathbf{e}^{(\lambda)*}_{\mathbf{k}}q_{\alpha\alpha'}(\mathbf{k}),\ \ \mathbf{k}=\mathbf{p}'-\mathbf{p},$$

$$R''_{\alpha'\alpha} = \sum_\beta\left\{\frac{(\mathbf{e}'\mathbf{I}_{\beta\alpha'}(\mathbf{p}',\mathbf{k}'))*(\mathbf{e}\mathbf{I}_{\beta\alpha}(\mathbf{p},\mathbf{k}))}{\omega+\varepsilon_\alpha(\mathbf{p})-\varepsilon_\beta(\mathbf{p}+\mathbf{k})} + \frac{(\mathbf{e}'\mathbf{I}_{\alpha\beta}(\mathbf{p},-\mathbf{k}'))*(\mathbf{e}\mathbf{I}_{\alpha'\beta}(\mathbf{p}',-\mathbf{k}))}{-\omega'+\varepsilon_\alpha(\mathbf{p})-\varepsilon_\beta(\mathbf{p}-\mathbf{k}')}\right\}.$$

Here we have taken into account that $\omega+\varepsilon_\alpha(\mathbf{p})=\omega'+\varepsilon_\beta(\mathbf{p}')$ is a consequence of (67) and assumed $E=\omega+\varepsilon_\alpha(\mathbf{p})$. According to our approximation $kr_0\ll 1$ ($\lambda\gg r_0$) we have

$$q_{\alpha\beta}(\mathbf{k}) \approx \frac{e^2}{\mu}\delta_{\alpha\beta},\ \ g_{\alpha\beta}\approx 0,$$

$$\mathbf{g}_{\alpha\beta}(\mathbf{k}) \approx -\frac{ie}{\mu}\int \mathrm{d}\mathbf{y}\,\varphi^*_\alpha(\mathbf{y})\frac{\partial\varphi_\beta(\mathbf{y})}{\partial\mathbf{y}} = \frac{e}{\mu}\langle\alpha|\hat{\mathbf{p}}|\beta\rangle,$$

whence

$$R'_{\alpha'\alpha} \approx \frac{e^2}{\mu}\mathbf{e}_{\mathbf{k}}^{(\lambda)}\mathbf{e}_{\mathbf{k}'}^{(\lambda')*}\delta_{\alpha\alpha'},\ \ \mathbf{I}_{\alpha\beta}(\mathbf{p},\mathbf{k}) \approx \mathbf{g}_{\alpha\beta}(\mathbf{k}) \approx \frac{e}{\mu}\langle\alpha|\hat{\mathbf{p}}|\beta\rangle, \tag{73}$$

where $\hat{\mathbf{p}}=-i\nabla$ is the momentum operator. Noting that $\varepsilon_\alpha(\mathbf{p})=\varepsilon_\alpha+(p^2/2M)$ we neglect the kinetic energy in denominators of $R''_{\alpha'\alpha}$ (the kinetic energy is small in comparison to binding energy of bound states; see Sec. II). The result is

$$R''_{\alpha'\alpha} = \frac{e^2}{\mu^2}\sum_\beta \left\{ \frac{\langle\alpha'|\mathbf{e}'^*\hat{\mathbf{p}}|\beta\rangle\langle\beta|\mathbf{e}\hat{\mathbf{p}}|\alpha\rangle}{\omega+\varepsilon_\alpha-\varepsilon_\beta} + \frac{\langle\alpha'|\mathbf{e}\hat{\mathbf{p}}|\beta\rangle\langle\beta|\mathbf{e}'^*\hat{\mathbf{p}}|\alpha\rangle}{-\omega'+\varepsilon_\alpha-\varepsilon_\beta} \right\}.$$

Let us express this formula through the matrix elements of the dipole moment of the atom. It is easy to verify [by using of Eq. (71)] that

$$\frac{\langle\alpha'|\mathbf{e}'^*\hat{\mathbf{p}}|\beta\rangle\langle\beta|\mathbf{e}\hat{\mathbf{p}}|\alpha\rangle}{\omega+\varepsilon_\alpha-\varepsilon_\beta} = \mu^2\left(\varepsilon_\alpha-\varepsilon_\beta-\omega'+\frac{\omega\omega'}{\omega+\varepsilon_\alpha-\varepsilon_\beta}\right)\langle\alpha'|\mathbf{e}'^*\hat{\mathbf{y}}|\beta\rangle\langle\beta|\mathbf{e}\hat{\mathbf{y}}|\alpha\rangle,$$

$$\frac{\langle\alpha'|\mathbf{e}\hat{\mathbf{p}}|\beta\rangle\langle\beta|\mathbf{e}'^*\hat{\mathbf{p}}|\alpha\rangle}{-\omega'+\varepsilon_\alpha-\varepsilon_\beta} = \mu^2\left(\varepsilon_{\alpha'}-\varepsilon_\beta+\omega'+\frac{\omega\omega'}{-\omega'+\varepsilon_\alpha-\varepsilon_\beta}\right)\langle\alpha'|\mathbf{e}\hat{\mathbf{y}}|\beta\rangle\langle\beta|\mathbf{e}'^*\hat{\mathbf{y}}|\alpha\rangle.$$

Therefore, the quantity $R''_{\alpha'\alpha}$ is of the form

$$R''_{\alpha'\alpha} = Q_{\alpha'\alpha} + \omega\omega'\sum_\beta \left\{ \frac{\langle\alpha'|\mathbf{e}\hat{\mathbf{d}}|\beta\rangle\langle\beta|\mathbf{e}'^*\hat{\mathbf{d}}|\alpha\rangle}{-\omega'+\varepsilon_\alpha-\varepsilon_\beta} + \frac{\langle\alpha'|\mathbf{e}'^*\hat{\mathbf{d}}|\beta\rangle\langle\beta|\mathbf{e}\hat{\mathbf{d}}|\alpha\rangle}{\omega+\varepsilon_\alpha-\varepsilon_\beta} \right\},$$

where $\hat{\mathbf{d}}=e\hat{\mathbf{y}}$ is the dipole moment of the atom, and

$$Q_{\alpha'\alpha} = \mu^2\sum_\beta \{(\varepsilon_\alpha-\varepsilon_\beta-\omega')\langle\alpha'|\mathbf{e}'^*\hat{\mathbf{y}}|\beta\rangle\langle\beta|\mathbf{e}\hat{\mathbf{y}}|\alpha\rangle + (\omega'+\varepsilon_{\alpha'}-\varepsilon_\beta)\langle\alpha'|\mathbf{e}\hat{\mathbf{y}}|\beta\rangle\langle\beta|\mathbf{e}'^*\hat{\mathbf{y}}|\alpha\rangle\}.$$

Next, using that

$$\left[\hat{\mathbf{y}}\mathbf{e}, \frac{p^2}{2\mu}+\hat{V}\right] = \left[\hat{\mathbf{y}}\mathbf{e}, \frac{p^2}{2\mu}\right] = \frac{i}{\mu}\mathbf{e}\hat{\mathbf{p}},$$

one finds

$$Q_{\alpha'\alpha} = -\frac{e^2}{\mu}\mathbf{e}'^*\mathbf{e}\delta_{\alpha\alpha'}.$$

According to (73), the quantity $R'_{\alpha'\alpha}$ is equal to $R'_{\alpha'\alpha}=(e^2/\mu)\mathbf{e}'^*\mathbf{e}\delta_{\alpha\alpha'}$. Thus, the matrix $R=R'+R''$ takes the form

$$R_{\alpha'\alpha} = \omega\omega'\sum_\beta \left\{ \frac{\langle\alpha'|\mathbf{e}\hat{\mathbf{d}}|\beta\rangle\langle\beta|\mathbf{e}'^*\hat{\mathbf{d}}|\alpha\rangle}{-\omega'+\varepsilon_\alpha-\varepsilon_\beta} + \frac{\langle\alpha'|\mathbf{e}'^*\hat{\mathbf{d}}|\beta\rangle\langle\beta|\mathbf{e}\hat{\mathbf{d}}|\alpha\rangle}{\omega+\varepsilon_\alpha-\varepsilon_\beta} \right\}$$

and the amplitude of transition from the initial state into the final state is given by (see Ref. 5)

$$S_{i\to f} = -\frac{4\pi^2 i}{\mathcal{V}}\frac{1}{\sqrt{\omega\omega'}}R_{\alpha'\alpha}\delta(\varepsilon_\alpha(\mathbf{p})+\omega-\varepsilon_{\alpha'}(\mathbf{p}')-\omega')\Delta(\mathbf{p}+\mathbf{k}-\mathbf{p}'-\mathbf{k}').$$

The differential scattering cross section is of the form

$$\mathrm{d}\sigma_{i\to f} = \frac{1}{\omega\omega'}|R_{\alpha'\alpha}|^2\delta(\varepsilon_\alpha(\mathbf{p})+\omega-\varepsilon_{\alpha'}(\mathbf{p}')-\omega')\mathrm{d}\mathbf{k}'.$$

Let us consider the scattering of an elementary particle by compound particle (the scattering of an electron by atom). Due to the structure of the Hamiltonian of interaction (38) it is sufficient to study the scattering of particle of the first kind by bound state. The matrix element of the $\hat{S}$-matrix in the first nonvanishing approximation over interaction is defined by

$$S_{i\to f} = -2\pi i\langle f|\tilde{\tilde{\mathcal{H}}}^1_{\text{int}}|i\rangle\,\delta(\varepsilon_i - \varepsilon_f),$$

where $\tilde{\tilde{\mathcal{H}}}^1_{\text{int}}$ is given by (38) and consequently,

$$\langle f|\tilde{\tilde{\mathcal{H}}}^1_{\text{int}}|i\rangle = \frac{1}{\mathcal{V}^2}\int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2\,\mathrm{d}\mathbf{y}\;\varphi_\alpha(\mathbf{x}_2-\mathbf{y})e^{i\mathbf{p}\mathbf{X}}\varphi_{\alpha'}(\mathbf{x}_2-\mathbf{y})e^{-i\mathbf{p}'\mathbf{X}}(\nu_{11}(\mathbf{x}_1-\mathbf{x}_2)-\nu_{21}(\mathbf{x}_1-\mathbf{y}))e^{i\mathbf{x}_1(\mathbf{k}_1-\mathbf{k}_1')}.$$

Here $\langle f| = \langle 0|\,\hat{\eta}_{\alpha'}(\mathbf{p}')\hat{\chi}_1(\mathbf{k}_1')$ and $|i\rangle = \hat{\chi}_1^+(\mathbf{k}_1)\,\hat{\eta}_\alpha^+(\mathbf{p})|0\rangle$. The simple calculations lead to

$$\langle f|\tilde{\tilde{\mathcal{H}}}^1_{\text{int}}|i\rangle = \frac{1}{\mathcal{V}}\Delta(\mathbf{p}+\mathbf{k}-\mathbf{p}'-\mathbf{k}')\int \mathrm{d}\mathbf{x}\;\varphi^*_{\alpha'}(\mathbf{x})\varphi_\alpha(\mathbf{x})\{\nu_{11}(\mathbf{q})e^{-i\mathbf{q}\mathbf{x}(m_2/M)}$$
$$+\,\nu_{21}(\mathbf{q})e^{i\mathbf{q}\mathbf{x}(m_1/M)}\},\quad \mathbf{q}=\mathbf{k}'-\mathbf{k}.$$

For Coulomb's interaction of particles we have

$$\nu_{11}(\mathbf{q}) = -\,\nu_{21}(\mathbf{q}) \equiv \nu(\mathbf{q}) = \frac{4\pi e^2}{q^2}.$$

Therefore, in the long-wave approximation ($qr_0 \ll 1$), one gets

$$\langle f|\tilde{\tilde{\mathcal{H}}}^1_{\text{int}}|i\rangle = 4\pi i e\frac{1}{\mathcal{V}}\Delta(\mathbf{p}+\mathbf{k}-\mathbf{p}'-\mathbf{k}')\frac{1}{q^2}\mathbf{q}\mathbf{d}_{\alpha'\alpha}, \tag{74}$$

where $\hat{\mathbf{d}} = e\hat{\mathbf{x}}$ is the dipole moment of atom [$\mathbf{d}_{\alpha'\alpha} = \int \mathrm{d}\mathbf{x}\;\varphi^*_{\alpha'}(\mathbf{x})\mathbf{x}\varphi_\alpha(\mathbf{x})$]. Note that the Hamiltonian

$$\tilde{\tilde{V}} = \int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2\;\hat{\chi}^+(\mathbf{x}_1)\hat{\chi}(\mathbf{x}_1)v_{\alpha'\alpha}(\mathbf{x}_1-\mathbf{x}_2)\,\hat{\eta}^+_{\alpha'}(\mathbf{x}_2)\,\hat{\eta}_\alpha(\mathbf{x}_2),$$

which describes the interaction between particles and bound states leads to the same result. Here $\hat{\chi}$, $\hat{\eta}_\alpha$ are the field operators of particles and bound states, respectively, and $v_{\alpha'\alpha}(\mathbf{x}) = (e/x^3)\mathbf{x}\mathbf{d}_{\alpha'\alpha}$. The relation (74) defines the interaction energy of the dipole moment $\mathbf{d}$ and electric charge e, which are at the distance $\mathbf{x}$ from each other.

VIII. THE VAN DER WAALS FORCES

In this section we investigate the forces acting between neutral atoms being in the ground state (the van der Waals forces) on the basis of the developed formalism. In order to solve this problem let us address the Schrödinger equation that determines the energy spectrum of the system,

$$\tilde{\tilde{\mathcal{H}}}\Phi = E\Phi,\quad \tilde{\tilde{\mathcal{H}}} = \tilde{\tilde{\mathcal{H}}}_0 + \tilde{\tilde{V}}. \tag{75}$$

Here $\tilde{\tilde{\mathcal{H}}}_0$ and $\tilde{\tilde{V}} = \tilde{\tilde{\mathcal{H}}}^1_{\text{int}} + \tilde{\tilde{\mathcal{H}}}^2_{\text{int}} + \tilde{\tilde{\mathcal{H}}}^3_{\text{int}}$ are defined by (37)–(40). Since the system in question consists of two atoms, we should seek the solution of (75) in the form

$$\Phi_{\alpha\beta}(\mathbf{X},\mathbf{X}') = \sum_{\lambda\rho}\int \mathrm{d}\mathbf{Y}\,\mathrm{d}\mathbf{Y}'\;K_{\alpha\beta;\lambda\rho}(\mathbf{X},\mathbf{X}';\mathbf{Y},\mathbf{Y}')\,\hat{\eta}^+_\lambda(\mathbf{Y})\,\hat{\eta}^+_\rho(\mathbf{Y}')\Phi_0. \tag{76}$$

The Hamiltonian of interaction $\tilde{\tilde{V}}$ is equal, in accordance with (38)–(40), to

$$\tilde{\tilde{V}} = \frac{1}{2}\int \mathrm{d}\mathbf{X}\,\mathrm{d}\mathbf{Y}\,\hat{\eta}^{+}_{\alpha}(\mathbf{X})\,\hat{\eta}^{+}_{\beta}(\mathbf{Y})\,\hat{\eta}_{\gamma}(\mathbf{Y})\,\hat{\eta}_{\delta}(\mathbf{X})G_{\delta\gamma;\alpha\beta}(\mathbf{X}-\mathbf{Y}), \tag{77}$$

where

$$G_{\delta\gamma;\alpha\beta}(\mathbf{X}-\mathbf{Y}) = \int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y}\;\varphi^{*}_{\alpha}(\mathbf{x})\varphi^{*}_{\beta}(\mathbf{y})\varphi_{\gamma}(\mathbf{y})\varphi_{\delta}(\mathbf{x})\left\{\nu_{12}\left(\mathbf{X}-\mathbf{Y}-\frac{m_1\mathbf{x}+m_2\mathbf{y}}{M}\right)+\nu_{21}\left(\mathbf{X}-\mathbf{Y}+\frac{m_1\mathbf{y}+m_2\mathbf{x}}{M}\right)+\nu_{11}\left(\mathbf{X}-\mathbf{Y}+\frac{m_2}{M}(\mathbf{x}-\mathbf{y})\right)+\nu_{22}\left(\mathbf{X}-\mathbf{Y}-\frac{m_1}{M}(\mathbf{x}-\mathbf{y})\right)\right\}.$$

We suppose that the kinetic energy of atoms is small in comparison to the energy levels $|\varepsilon_\alpha|$ ($\varepsilon_\alpha<0$). In this case, according to (37), the operator $\tilde{\tilde{\mathcal{H}}}_0$ can be represented in the form

$$\tilde{\tilde{\mathcal{H}}}_0 = \sum_{\alpha}\int \mathrm{d}\mathbf{X}\;\varepsilon_\alpha\hat{\eta}^{+}_{\alpha}(\mathbf{X})\,\hat{\eta}_{\alpha}(\mathbf{X}).$$

It can be easily seen that

$$\begin{aligned}\tilde{\tilde{\mathcal{H}}}_0\,\hat{\eta}^{+}_{\lambda}(\mathbf{Z})\,\hat{\eta}^{+}_{\rho}(\mathbf{Z}')\Phi_0 &= (\varepsilon_\lambda+\varepsilon_\rho)\,\hat{\eta}^{+}_{\lambda}(\mathbf{Z})\,\hat{\eta}^{+}_{\rho}(\mathbf{Z}')\Phi_0,\\ \tilde{\tilde{V}}\hat{\eta}^{+}_{\lambda}(\mathbf{Z})\,\hat{\eta}^{+}_{\rho}(\mathbf{Z}')\Phi_0 &= \sum_{\alpha\beta}G_{\lambda\rho;\alpha\beta}(\mathbf{Z}-\mathbf{Z}')\,\hat{\eta}^{+}_{\alpha}(\mathbf{Z})\,\hat{\eta}^{+}_{\beta}(\mathbf{Z}')\Phi_0.\end{aligned} \tag{78}$$

These formulas show that we can seek the solution of (75) in a more simple, rather than (76), form

$$\Phi_{\alpha\beta}(\mathbf{X},\mathbf{X}') = \sum_{\lambda\rho}K_{\alpha\beta;\lambda\rho}(\mathbf{X},\mathbf{X}')\,\hat{\eta}^{+}_{\lambda}(\mathbf{X})\,\hat{\eta}^{+}_{\rho}(\mathbf{X}')\Phi_0,$$

so that the coordinates of atoms have the definite values in the state $\Phi_{\alpha\beta}(\mathbf{X},\mathbf{X}')$. Upon substituting this expression into (75) and using (78), one finds

$$K_{\alpha\beta;\gamma\delta}(\varepsilon_\gamma+\varepsilon_\delta)+\sum_{\lambda\rho}K_{\alpha\beta;\lambda\rho}G_{\lambda\rho;\gamma\delta}(\mathbf{Z}-\mathbf{Z}') = E_{\alpha\beta}K_{\alpha\beta;\gamma\delta}.$$

A perturbative approach for this equation can be easily developed in the domain of great $|\mathbf{Z}-\mathbf{Z}'|$ when the quantity $G_{\lambda\rho;\gamma\delta}(\mathbf{Z}-\mathbf{Z}')$ becomes small [see (77)]. Expanding $K_{\alpha\beta;\gamma\delta}$ in G,

$$K_{\alpha\beta;\gamma\delta} = K^{0}_{\alpha\beta;\gamma\delta}+K^{1}_{\alpha\beta;\gamma\delta}+K^{2}_{\alpha\beta;\gamma\delta}+\cdots,$$

$$E_{\alpha\beta} = E^{0}_{\alpha\beta}+E^{1}_{\alpha\beta}+E^{2}_{\alpha\beta}+\cdots,$$

one obtains in the zeroth order

$$K^{0}_{\alpha\beta;\gamma\delta}(\varepsilon_\gamma+\varepsilon_\delta) = E^{0}_{\alpha\beta}K^{0}_{\alpha\beta;\gamma\delta},$$

whence

$$K^{0}_{\alpha\beta;\gamma\delta} = K^{0}_{\alpha\beta}\delta_{\alpha\gamma}\delta_{\beta\delta},\quad E^{0}_{\alpha\beta} = \varepsilon_\alpha+\varepsilon_\beta.$$

Taking into account this result we have in the first approximation,

$$K^{1}_{\alpha\beta;\gamma\delta}(\varepsilon_\gamma+\varepsilon_\delta)+K^{0}_{\alpha\beta}G_{\alpha\beta;\gamma\delta}(\mathbf{Z}-\mathbf{Z}') = (\varepsilon_\alpha+\varepsilon_\beta)K^{1}_{\alpha\beta;\gamma\delta}+E^{1}_{\alpha\beta}K^{0}_{\alpha\beta}\delta_{\alpha\gamma}\delta_{\beta\delta}.$$

By setting here $\alpha=\gamma$, $\beta=\delta$, one gets

$$E^1_{\alpha\beta} = G_{\alpha\beta;\alpha\beta}(\mathbf{Z}-\mathbf{Z}'), \tag{79}$$

and for $\alpha,\beta \neq \gamma,\delta$,

$$K^1_{\alpha\beta;\gamma\delta} = K^0_{\alpha\beta}\frac{G_{\alpha\beta;\gamma\delta}(\mathbf{Z}-\mathbf{Z}')}{(\varepsilon_\alpha+\varepsilon_\beta-\varepsilon_\gamma-\varepsilon_\delta)}, \quad \alpha,\beta \neq \gamma,\delta. \tag{80}$$

The second order of the perturbative approach gives

$$K^2_{\alpha\beta;\gamma\delta}(\varepsilon_\gamma+\varepsilon_\delta) + \sum_{\lambda\rho} K^1_{\alpha\beta;\lambda\rho}G_{\lambda\rho;\gamma\delta}(\mathbf{Z}-\mathbf{Z}') = (\varepsilon_\alpha+\varepsilon_\beta)K^2_{\alpha\beta;\gamma\delta} + E^1_{\alpha\beta}K^1_{\alpha\beta;\gamma\delta} + E^2_{\alpha\beta}K^0_{\alpha\beta;\gamma\delta}.$$

Taking here $\alpha=\gamma$, $\beta=\delta$, one finds

$$\sum_{\lambda\rho} K^1_{\alpha\beta;\lambda\rho}G_{\lambda\rho;\alpha\beta}(\mathbf{Z}-\mathbf{Z}') = E^1_{\alpha\beta}K_{\alpha\beta;\alpha\beta} + K^0_{\alpha\beta}E^2_{\alpha\beta},$$

whence, according to (79) and (80), we have

$$E^2_{\alpha\beta} = \sum_{\lambda\rho}{}' \frac{G_{\alpha\beta;\lambda\rho}(\mathbf{Z}-\mathbf{Z}')G_{\lambda\rho;\alpha\beta}(\mathbf{Z}-\mathbf{Z}')}{(\varepsilon_\alpha+\varepsilon_\beta-\varepsilon_\lambda-\varepsilon_\rho)}. \tag{81}$$

The prime above the sum means that the terms with $\lambda=\alpha$, $\rho=\beta$ are omitted. The state vector $\Phi_{\alpha\beta}(\mathbf{X},\mathbf{X}')$ in the main approximation of the perturbative approach is determined by

$$\Phi_{\alpha\beta}(\mathbf{X},\mathbf{X}') = K^0_{\alpha\beta}\hat{\eta}^+_\alpha(\mathbf{X})\,\hat{\eta}^+_\beta(\mathbf{X}')\Phi_0 + \cdots$$

[the constant $K^0_{\alpha\beta}$ may be found from the normalization relation, $(\Phi_{\alpha\beta},\Phi_{\alpha\beta})=1$]. Formulas (79) and (81) for $E^1_{\alpha\beta}$ and $E^2_{\alpha\beta}$ give us the corrections to the energy levels $E^0_{\alpha\beta}=\varepsilon_\alpha+\varepsilon_\beta$. It follows from the obtained formulas that the energy of two atoms being in the ground state α and spaced apart for sufficiently long distances is defined by

$$E_{\alpha\alpha} = 2\varepsilon_\alpha + G_{\alpha\alpha;\alpha\alpha}(\mathbf{Z}-\mathbf{Z}') + \sum_{\lambda\rho}{}' \frac{G_{\alpha\alpha;\lambda\rho}(\mathbf{Z}-\mathbf{Z}')G_{\lambda\rho;\alpha\alpha}(\mathbf{Z}-\mathbf{Z}')}{(2\varepsilon_\alpha-\varepsilon_\lambda-\varepsilon_\rho)} + \cdots . \tag{82}$$

Let us prove now that $G_{\alpha\alpha;\alpha\alpha}(\mathbf{Z}-\mathbf{Z}')\equiv 0$. In doing so we use the following formula:[10]

$$\frac{1}{\sqrt{R^2-2R\rho x+\rho^2}} = \frac{1}{|\mathbf{R}-\boldsymbol{\rho}|} = \frac{1}{R} + \sum_{n=1}^{\infty}\left(\frac{\rho}{R}\right)^n \mathcal{P}_n(x),$$

where $x=\cos\vartheta$, ϑ is the angle between vectors $\mathbf{R}$ and $\boldsymbol{\rho}$, and $\mathcal{P}_n(x)$ are the Legendre polynomials. Noting that [see (77)]

$$G_{\alpha\alpha;\alpha\alpha}(\mathbf{Z}-\mathbf{Z}') = \int d\mathbf{x}\,d\mathbf{y}|\varphi_\alpha(\mathbf{x})|^2|\varphi_\alpha(\mathbf{y})|^2\Bigg\{\nu_{12}\left(\mathbf{Z}-\mathbf{Z}'-\frac{m_1\mathbf{x}+m_2\mathbf{y}}{M}\right) + \nu_{21}\left(\mathbf{Z}-\mathbf{Z}'+\frac{m_1\mathbf{y}+m_2\mathbf{x}}{M}\right)$$
$$+ \nu_{11}\left(\mathbf{Z}-\mathbf{Z}'+\frac{m_2}{M}(\mathbf{x}-\mathbf{y})\right) + \nu_{22}\left(\mathbf{Z}-\mathbf{Z}'-\frac{m_1}{M}(\mathbf{x}-\mathbf{y})\right)\Bigg\},$$

we come, taking into account the spherical symmetry of $|\varphi_\alpha(\mathbf{x})|^2$, to

$$G_{\alpha\alpha;\alpha\alpha}(\mathbf{Z}-\mathbf{Z}') = 0. \tag{83}$$

We have also employed here that according to (43),

$$\nu_{ab}(\mathbf{Z}-\mathbf{Z}')=\frac{e_a e_b}{|\mathbf{Z}-\mathbf{Z}'|},\quad e_1=-e_2=e.$$

Let us find now $G_{\alpha\alpha;\lambda\rho}(\mathbf{Z}-\mathbf{Z}')$,

$$G_{\alpha\alpha;\lambda\rho}(\mathbf{Z}-\mathbf{Z}')=\int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y}\;\varphi_\rho^*(\mathbf{x})\varphi_\lambda^*(\mathbf{y})\varphi_\alpha(\mathbf{y})\varphi_\alpha(\mathbf{x})\left\{\nu_{12}\left(\mathbf{Z}-\mathbf{Z}'-\frac{m_1\mathbf{x}+m_2\mathbf{y}}{M}\right)+\nu_{21}\left(\mathbf{Z}-\mathbf{Z}'+\frac{m_1\mathbf{y}+m_2\mathbf{x}}{M}\right)+\nu_{11}\left(\mathbf{Z}-\mathbf{Z}'+\frac{m_2}{M}(\mathbf{x}-\mathbf{y})\right)+\nu_{22}\left(\mathbf{Z}-\mathbf{Z}'-\frac{m_1}{M}(\mathbf{x}-\mathbf{y})\right)\right\}.$$

The presence of multipliers $\varphi_\alpha(\mathbf{y})$ and $\varphi_\alpha(\mathbf{x})$ makes it possible to expand the expression in braces in powers of $\mathbf{x}$, $\mathbf{y}$. As a result we have

$$G_{\alpha\alpha;\beta\lambda}(\mathbf{Z}-\mathbf{Z}')=\frac{1}{|\mathbf{Z}-\mathbf{Z}'|^3}(-3(\mathbf{n}\mathbf{d}_{\beta\alpha})(\mathbf{n}\mathbf{d}_{\lambda\alpha})+(\mathbf{d}_{\beta\alpha}\mathbf{d}_{\lambda\alpha})),$$

where

$$\mathbf{n}=\frac{\mathbf{Z}-\mathbf{Z}'}{|\mathbf{Z}-\mathbf{Z}'|},\quad \mathbf{d}_{\beta\alpha}=e\int \mathrm{d}\mathbf{x}\,\mathbf{x}\varphi_\beta^*(\mathbf{x})\varphi_\alpha(\mathbf{x})$$

($\mathbf{d}_{\beta\alpha}$ are the matrix elements of the dipole moment of atom). Thus, the potential energy of interaction between atoms, $V(\mathbf{Z}-\mathbf{Z}')$ is defined by[6]

$$V(\mathbf{Z}-\mathbf{Z}')\equiv E_{\alpha\alpha}^2-2\varepsilon_\alpha=\frac{1}{|\mathbf{Z}-\mathbf{Z}'|^6}\sum_{\beta\lambda}{}'\frac{|-3(\mathbf{n}\mathbf{d}_{\beta\alpha})(\mathbf{n}\mathbf{d}_{\lambda\alpha})+(\mathbf{d}_{\beta\alpha}\mathbf{d}_{\lambda\alpha})|^2}{2\varepsilon_\alpha-\varepsilon_\beta-\varepsilon_\lambda}<0.$$

Since $\varepsilon_\beta,\varepsilon_\lambda>\varepsilon_\alpha$, $V(\mathbf{Z}-\mathbf{Z}')<0$. Therefore, the attractive forces (the van der Waals forces) act between the neutral atoms at long distances.

Consider now the scattering of a compound particle by compound particle, which are in the ground state. We start from the scattering matrix representation in terms of T-operators (67). Accurate to the terms, which are of the second order in interaction $\tilde{\tilde{V}}$ between the atoms [see (68)], one gets

$$\hat{S}=1-2\pi i\int_{-\infty}^{\infty}\mathrm{d}E\;\delta(E-\tilde{\tilde{\mathcal{H}}}_0)\tilde{\tilde{V}}\delta(E-\tilde{\tilde{\mathcal{H}}}_0)-2\pi i\int_{-\infty}^{\infty}\mathrm{d}E\;\delta(E-\tilde{\tilde{\mathcal{H}}}_0)\tilde{\tilde{V}}\frac{1}{E-\tilde{\tilde{\mathcal{H}}}_0+i\eta}\tilde{\tilde{V}}\delta(E-\tilde{\tilde{\mathcal{H}}}_0).\tag{84}$$

Neglecting the kinetic energy of atoms we replace in the resolvent $(E-\tilde{\tilde{\mathcal{H}}}_0+i\eta)^{-1}$ the Hamiltonian of free particles $\tilde{\tilde{\mathcal{H}}}_0$ by the Hamiltonian $\tilde{\tilde{H}}_0$ of atoms in the rest [see (37)],

$$\tilde{\tilde{\mathcal{H}}}_0\to\tilde{\tilde{H}}_0=\sum_\alpha\int \mathrm{d}\mathbf{x}\;\varepsilon_\alpha\hat{\eta}_\alpha^+(\mathbf{x})\,\hat{\eta}_\alpha(\mathbf{x})$$

(in the low-energy limit we cannot do this under the argument of the δ-function).

Since we study the collision of two atoms and the number of atoms is conserved during the process of collision, we can restrict ourselves by considering this process in the two-particle subspace with the following completeness condition:

$$\frac{1}{2}\int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2 \sum_{\alpha_1,\alpha_2} \hat{\eta}^+_{\alpha_1}(\mathbf{x}_1)\,\hat{\eta}^+_{\alpha_2}(\mathbf{x}_2)|0\rangle\langle 0|\,\hat{\eta}_{\alpha_2}(\mathbf{x}_2)\,\hat{\eta}_{\alpha_1}(\mathbf{x}_1) = 1. \tag{85}$$

In this case formulas (78) are true. Since the atoms are in the ground state, (83) is also valid and, therefore, the matrix element of $\hat{S}$-matrix turns to zero in the first approximation of the perturbation theory.

The second approximation of the perturbation theory is defined, according to (84) and (85), by the formula

$$\tilde{\hat{V}}\frac{1}{E-\tilde{\hat{H}}_0+i\eta}\tilde{\hat{V}} = \frac{1}{2}\sum_{\alpha_1,\alpha_2}\sum_{\beta_1,\beta_2}\sum_{\gamma_1,\gamma_2}\int \mathrm{d}\mathbf{x}_1\mathrm{d}\mathbf{x}_2 \frac{1}{E-\varepsilon_{\alpha_1}-\varepsilon_{\alpha_2}+i\eta} G_{\alpha_1\alpha_2;\beta_1\beta_2}(\mathbf{x}_1-\mathbf{x}_2)\,\hat{\eta}^+_{\beta_1}(\mathbf{x}_1)\,\hat{\eta}^+_{\beta_2}(\mathbf{x}_2)|0\rangle$$
$$\times\langle 0|\,\hat{\eta}_{\gamma_1}(\mathbf{x}_1)\,\hat{\eta}_{\gamma_2}(\mathbf{x}_2) G^+_{\gamma_1\gamma_2;\alpha_1\alpha_2}(\mathbf{x}_1-\mathbf{x}_2).$$

In the two-particle subspace this formula is equivalent to

$$\tilde{\hat{V}}\frac{1}{E-\tilde{\hat{H}}_0+i\eta}\tilde{\hat{V}} = \int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2 \sum_{\beta_1,\beta_2}\sum_{\gamma_1,\gamma_2} \hat{\eta}^+_{\beta_1}(\mathbf{x}_1)\,\hat{\eta}^+_{\beta_2}(\mathbf{x}_2) V_{\beta_1\beta_2;\gamma_1\gamma_2}(\mathbf{x}_1-\mathbf{x}_2;E)\,\hat{\eta}_{\gamma_1}(\mathbf{x}_1)\,\hat{\eta}_{\gamma_2}(\mathbf{x}_2),$$

where

$$V_{\beta_1\beta_2;\gamma_1\gamma_2}(\mathbf{x}_1-\mathbf{x}_2;E) = \sum_{\alpha_1\alpha_2}\frac{1}{E-\varepsilon_{\alpha_1}-\varepsilon_{\alpha_2}+i\eta} G^+_{\gamma_1\gamma_2;\alpha_1\alpha_2}(\mathbf{x}_1-\mathbf{x}_2) G_{\alpha_1\alpha_2;\beta_1\beta_2}(\mathbf{x}_1-\mathbf{x}_2).$$

Since the initial and final states of a particle are the ground states, the scattering matrix in the two-particle subspace can be represented in the form

$$\hat{S} = -2\pi i\int_{-\infty}^{\infty}\mathrm{d}E\;\delta(E-\tilde{\hat{\mathcal{H}}}_0)\hat{V}_{\mathrm{eff}}\delta(E-\tilde{\hat{\mathcal{H}}}_0),$$

where

$$\hat{V}_{\mathrm{eff}} = \frac{1}{2}\int \mathrm{d}\mathbf{x}_1\int \mathrm{d}\mathbf{x}_2\;\hat{\eta}^+_{\alpha_1}(\mathbf{x}_1)\,\hat{\eta}^+_{\alpha_2}(\mathbf{x}_2) V_{\mathrm{eff}}(\mathbf{x}_1-\mathbf{x}_2)\,\hat{\eta}_{\alpha_2}(\mathbf{x}_2)\,\hat{\eta}_{\alpha_1}(\mathbf{x}_1),$$

$$V_{\mathrm{eff}}(\mathbf{x}_1-\mathbf{x}_2) = \sum_{\beta_1\beta_2}\frac{G^+_{\alpha\alpha;\beta_1\beta_2}(\mathbf{x}_1-\mathbf{x}_2)G_{\beta_1\beta_2;\alpha\alpha}(\mathbf{x}_1-\mathbf{x}_2)}{2\varepsilon_\alpha-\varepsilon_{\beta_1}-\varepsilon_{\beta_2}}.$$

We can see that the second order in $\tilde{\hat{V}}$ of perturbation theory for $\hat{S}$-matrix is equivalent to the first order of perturbation theory over effective interaction $\hat{V}_{\mathrm{eff}}$. This effective interaction is determined by van der Waals forces [see formula (82)].

It follows from (39), that the Hamiltonian of interaction of atoms at low energies is defined by

$$\tilde{\hat{V}} = \int \mathrm{d}\mathbf{x}_1\,d\mathbf{x}_2\,v_{\alpha\beta;\gamma\delta}(\mathbf{x}_1-\mathbf{x}_2)\,\hat{\eta}^+_\alpha(\mathbf{x}_1)\,\hat{\eta}^+_\beta(\mathbf{x}_2)\,\hat{\eta}_\gamma(\mathbf{x}_2)\,\hat{\eta}_\delta(\mathbf{x}_1),$$

where

$$v_{\alpha\beta;\gamma\delta}(\mathbf{x}) = \frac{1}{x^5}(x^2(\mathbf{d}_{\alpha\delta}\mathbf{d}_{\beta\gamma}) - 3(\mathbf{x}\mathbf{d}_{\alpha\delta})(\mathbf{x}\mathbf{d}_{\delta\gamma})).$$

This Hamiltonian corresponds to the dipole–dipole interaction of atoms.

IX. CONCLUSION

The goal of this paper was to develop a microscopic approach for describing the physical processes in many-particle systems in the presence of bound states of particles. To achieve this goal we developed an approximate second quantization method for systems with bound states of particles.

The basic results obtained in this paper are the following:

(1) The Fock space was introduced in the second quantization formalism. In this space the creation and annihilation operators of elementary particles $\hat{\chi}^+$, $\hat{\chi}$ and their bound states $\hat{\eta}^+$, $\hat{\eta}$ were introduced on an equal status.

(2) The operators of basic physical quantities acting in this space were constructed. These operators include the Hamiltonians of interaction between elementary particles and their bound states.

(3) It was shown that in the approximation when the radius of interaction is small the above-mentioned Hamiltonians transform into the well-known Hamiltonians for Coulomb's and dipole interactions between the particles of various kinds.

(4) The nonrelativistic quantum electrodynamics of charged and neutral (the bound states) particles was constructed.

(5) The various physical effects including the theory of the van der Waals forces acting between atoms were considered as the approbation of the developed formalism. The description of such effects within the usual formalism requires more considerable efforts associated with introduction of the interaction between neutral currents of bound states and electromagnetic field.

(6) More detailed calculations, which fall out of the limits of our approximation should result in appearance of three- and many-body interactions between unbound particles and two-body bound states. These many-body interactions should be consistent with pair interaction of original particles. The appearance of these many-body terms is analogous to the origin of the terms with photon–photon scattering in transition from the usual standard Lagrangian to the effective low-energy Euler–Heisenberg Lagrangian of quantum electrodynamics.

Especially we would like to emphasize a role of the obtained Hamiltonians, which describe the interaction of quasineutral particles (the bound states of charged fermions) with electromagnetic field, the elementary particles with bound states, and also the bound states with bound states. On the basis of these Hamiltonians one can study such phenomena as Bose–Einstein condensation in a gas of excited atoms, the interaction of condensates with an electromagnetic field in Bose and Fermi systems. These Hamiltonians can be also the basis of the kinetic theory for systems with bound states of particles.

Finally we would like to stress that the developed method can be easily generalized to the case of bound states consisting of more than two particles. The generalization of the offered method for describing the systems with bound states of bosons and also of bosons and fermions taking into account the spin of particles can be also performed without principal difficulties.

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Algebraic geometry realization of quantum Hall soliton

R. Abounasr, M. Ait Ben Haddou,[a] A. El Rhalami, and E. H. Saidi[b]
Lab/UFR-Physique des Hautes Energies, Faculté des Sciences de Rabat, Morocco and Groupement National de Physique des Hautes Energies, GNPHE; Siege focal, Rabat, Morocco

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Using the Iqbal–Netzike–Vafa dictionary giving the correspondence between the H_2 homology of del Pezzo surfaces and *p*-branes, we develop a way to approach the system of brane bounds in M-theory on $\mathbb{S}^1$. We first review the structure of 10-dimensional quantum Hall soliton (QHS) from the view of M-theory on $\mathbb{S}^1$. Then, we show how the *D*0 dissolution in *D*2-brane is realized in M-theory language and derive the *p*-brane constraint equations used to define appropriately the QHS. Finally, we build an algebraic geometry realization of the QHS in type IIA superstring and show how to get its type IIB dual. Other aspects are also discussed. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1834695]

I. INTRODUCTION

A few years ago, it has been conjectured in Ref. 1, see also Ref. 2, that a specific assembly of a system of *KD*0, *D*2 and *N D*6 branes and *N* fundamental *F*1 strings, stretching between *D*2 and *D*6, has a low energy dynamics similar to the fundamental state of fractional quantum Hall (FQH) systems. There, the boundary states of the *F*1 strings ending on the *D*2 brane are interpreted as the FQH particles moving in the *D*2-brane world volume. The external strong magnetic field *B* is represented by a large number of *D*0 branes dissolved in *D*2 and the dynamics of these particles is modeled by a noncommutative Chern–Simons (NCCS) U(1) gauge field theory.[3] Soon after this proposal, several constructions were considered pushing forward this analogy. [4–12] Susskind *et al.* idea was also extended to quantum Hall solitons that are not of Laughlin type,[13] in particular the quantum Hall solitons modeling Haldane hierarchy and multilayer systems as proposed in Ref. 14.

On the other hand, it has been observed recently by Iqbal–Neitzke–Vafa (INV)[15] that there is remarkable correspondence between *p*-branes in M-theory on torii and holomorphic curves in del Pezzo surfaces. A dictionary characterizing this correspondence was given. The result of this work was particularly focused on the study of a mysterious duality in the toroidal compactification of M-theory, for other applications see also Refs. 16 and 17. But here we will use differently the INV link between del Pezzo and M-theory by developing a new method to approach brane systems. The originality of our construction rests on the fact that INV correspondence can be also used to study geometric aspects of brane physics using the power of algebraic geometry and homology. Among our results, we quote the derivation of new representations of *p*-brane systems using the H_2 homology of algebraic curves in del Pezzo surfaces.

To fix the idea on the way we will be doing things, we focus, in a first step, on a special system of branes and show how new representations can be built. The system we will be dealing with here concerns mainly the usual quantum Hall soliton (QHS) we have introduced in the beginning of this introduction. But in the discussion section, we will also draw the lines of other constructions, in particular the way QHS is realized in type IIB superstring on $\mathbb{S}^1$ as well as higher dimensional extensions.

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[a]Also at Department de Mathématiques and Informatique, Faculté des Sciences, Meknes, Morocco.
[b]Electronic mail: h-saidi@fsr.ac.ma

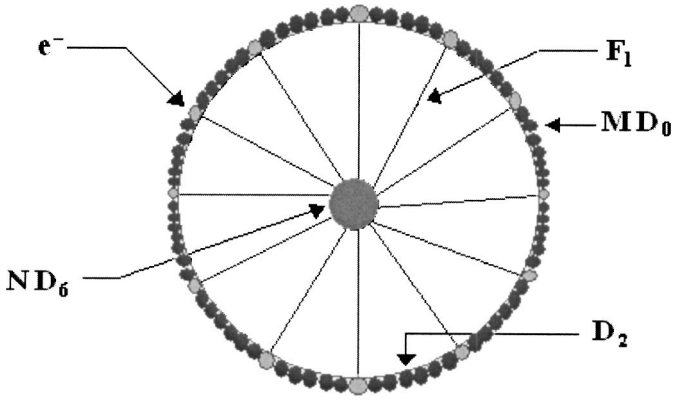

FIG. 1. This figure represents the type IIA stringy representation of a fractional quantum Hall soliton.

The principal aim of this work is then to use results on 10-dimensional QHS, the INV correspondence as well as string theory and mathematical results to develop new realizations of quantum Hall solitons using algebraic geometry curves in del Pezzo surfaces. For simplicity, we will give here the main lines of the method on Susskind *et al.* QHS. A detailed analysis and applications dealing with other types of brane systems will be given in Ref. 18.

The presentation of this paper is as follows. In Sec. II, we describe briefly the quantum Hall soliton in type IIA superstring. We first review the structure of the 10-dimensional QHS as formulated in the literature and then give its representation in the language of the 11-dimensional M-theory on $\mathbb{S}^1$. This change from type IIA to M-theory allows us to reach the two remarkable points: (i) give a geometric realization of the standard idea of dissolution $D0$ branes in $D2$ and (ii) derive the appropriate geometric constraint equations that define QHS. In Sec. III, we review the homology of del Pezzo surfaces as it is one of the basic tools in construction and in Sec. IV we describe the INV correspondence. In Sec. V we first identify the constraint equations for QHS using the H_2 homology of del Pezzo. Then we develop a realization of the Hall soliton using intersecting classes of complex curves in del Pezzo. In Sec. VI, we give our conclusion and make a discussion.

II. QUANTUM HALL SOLITONS

One remarkable observation of Susskind and collaborators in the derivation of the quantum Hall soliton is that the usual $(1+2)$ dimensional condensed matter fractional quantum Hall (FQH) phase has a striking similarity with a specific p-brane configuration in type IIA superstring theory. Following Refs. 1 and 2, see also Ref. 19, there is a one to one correspondence between the three-dimensional (3D) FQH systems of condensed matter physics and the low energy dynamics of brane bounds involving $D0, D2$, and $D6$ branes of the 10-dimensional uncompactified type IIA superstring. There is also $F1$ strings stretching between $D2$ and $D6$ branes, $F1$ ends on $D2$ have an interpretation in terms of FQH particles (Hall electrons). Let us comment briefly on this configuration to which we shall refer hereafter as the type IIA stringy representation of the quantum Hall soliton. Denoting the usual IIA string (bosonic) coordinate field variables $X^\mu(\tau,\sigma)$ by the following equivalent and appropriate ones

$$\{t(\tau), \quad \varrho(\tau,\sigma), \quad \vartheta(\tau,\sigma), \quad \varphi(\tau,\sigma), \quad \{y^i(\tau,\sigma)\}_{4\leqslant i\leqslant 9;}\}, \tag{2.1}$$

where τ and σ are the usual string world sheet variables, the above mentioned p-brane bound system, called also quantum Hall soliton (QHS), is built as follows, see Fig. 1 for illustration.

A. Brane configuration

If forgetting about edge excitations which may be modeled by *NS*5 branes, the simplest structure of QHS is parametrized in terms of the above 10-dimensional string coordinates as follows.

(a) One two space dimensional spherical *D*2 brane; it plays a role of the world volume in FQH systems of condensed matter physics and is parametrized by the spherical coordinates,

$$\{t, \quad \varrho = R; \quad 0 \leqslant \vartheta \leqslant \pi; \quad 0 \leqslant \varphi \leqslant 2\pi; \quad \mathbf{0_6}\}. \tag{2.2}$$

At fixed time, this *D*2 brane is embedded in $R^3 \sim R^+ \times S^2$ and for large values of the radius, *D*2 may be thought of locally as $R^{1,2}$ which is also interpreted as the space–time of the three-dimensional Chern–Simons gauge theory.

(b) *N* coincident flat six-dimensional space *D*6 branes located at the origin of *D*2 and parametrized collectively by the y^i internal Euclidean coordinates as

$$\{t, \quad \mathbf{0_3}, \quad (y^4, \ldots, y^9)\}. \tag{2.3}$$

It can be thought of as an external source of charge density $J^0 \propto N\delta^3(x)$ at the origin $(x^1, x^2, x^3) = (0,0,0)$ of the spherical *D*2 brane.

(c) *N* fundamental strings *F*1 stretching between *D*2 and *D*6 branes and parametrized by

$$\{t, \quad 0 \leqslant \varrho \leqslant R, \quad \mathbf{0_2}, \quad \mathbf{0_6}\}. \tag{2.4}$$

The *F*1 string ends on the *D*2 brane are associated to the electrons of the three-dimensional condensed matter FQH fluids.

(d) *K D*0 branes dissolved into the *D*2 brane; they define the flux quanta associated to the external magnetic field *B* of FQH systems. Recall also that *D*0 and *D*6 are the electric–magnetic dual.

B. Methods

Since the original work linking fractional quantum Hall fluids and NC Chern–Simons gauge theory,[3] several methods have been developed to deal with such kinds of systems.[5,9–20] Matrix model approach from Polychronakos[21] is one of these methods which has been getting a particular interest in the literature. In this matrix model formulation, the FQH particles in the Laughlin state are described by two $N \times N$ Hermitian matrices $X^1_{ij}(t)$ and $X^2_{ij}(t)$ [in our coordinate choice $X^1_{ij}(t) \sim R \sin \vartheta_{ij}(t) \cos \varphi_{ij}(t)$ and $X^2(t) \sim R \sin \vartheta_{ij}(t) \sin \varphi_{ij}(t)$]. For large radius *R*, the two spheres can be locally approximated by a flat patch of the $\mathbb{R}^2$ plane and so one can neglect, in a leading approximation, the curvature effect. In the infinite limit of *N* and *M* (strong external magnetic field), the one-dimensional matrix fields $X^1_{ij}(t)$ and $X^2(t)$ are mapped to the usual $(2+1)$ fields, a behavior which is nicely given by the Susskind map,

$$X^i(t,y) = y^i + \theta \varepsilon^{ij} A_j(t,y) \tag{2.5}$$

as discussed in Refs. 3 and 10. In this relation, one recognizes the $(1+2)$ Chern–Simons gauge field $A_j(t,y)$ and the noncommutativity parameter θ induced by the presence of external *B*.

In our present work, we will use a completely different approach to deal with the QHS. This method is based on algebraic geometry of del Pezzo surfaces and too particularly on their H_2 homology. In our way, one may naturally define all physical quantities one encounters in type IIA stringy representation of QHS and condensed matter FQH fluids. For the present presentation however and for the purpose of illustration of the technique, we will simplify the construction. We skip unnecessary details and essentially focus on the path towards the algebraic geometry realization of QHS.

To proceed, let us say some words on our strategy towards the algebraic geometry realization of QHS. This will be done in four principal steps: (i) In step one, we reformulate the type IIA stringy representation of QHS as a constrained system of *p* branes. Here we show that the

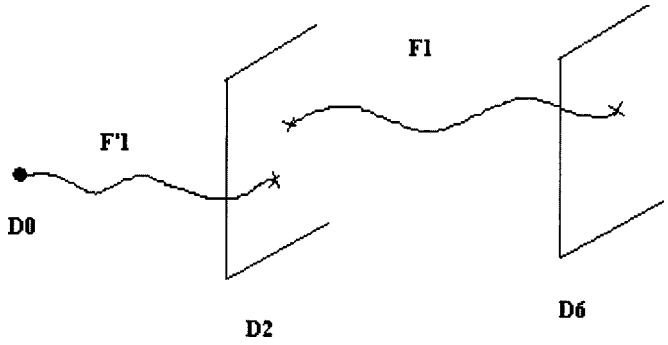

FIG. 2. This figure represents the type IIA stringy representation of a fractional quantum Hall soliton. The ends of $F'1$ strings on $D2$ are the $D0$ branes appearing in the Susskind *et al.* QHS. They are in one to one with the K $D0$'s associated with the eleventh (compact) dimension.

appropriate way to do it is in fact from the view of M-theory on $\mathbb{S}^1$. In this case, we give a geometric realization of the idea of dissolution of $D0$ branes in $D2$ and show that QHS particles, namely electrons and flux quanta, can be treated in a quite similar manner. This step permits us to identify the appropriate geometric constraint equations that define QHS. (ii) In step two, we review the INV correspondence and describe how p branes are represented in algebraic geometry of del Pezzo surfaces. We take this opportunity to draw the main lines of a method of representing homology classes in the del Pezzo surface $\mathbb{B}_1$ by using $F1$ strings and $D2$ branes. This method uses triangulation property of surfaces and is also motivated from formal similarities with Feynman rules in quantum Φ^3 theory. (iii) In step three, we reformulate the structure of the stringy QHS into the language of homology of del Pezzo surfaces. We first give the translation of constraint equations in terms of H_2 homology of $\mathbb{B}_1$, then we study necessary conditions for their solutions. (iv) In the last step, we develop a class of solutions of the homological constraint equations giving an algebraic geometry realization of QHS.

We begin by noting that p branes involved in the above QHS may, roughly speaking, be thought of as sets of points in $p+1$ dimensions. As far as brane links are concerned, we clearly see that intersections between the QHS branes may be naively defined as set intersections as follows:

$$D2 \cap F1 = 1, \quad D2 \cap D6 = 0, \quad D6 \cap F1 = 1. \tag{2.6}$$

For the case of N fundamental strings, the first equation of the above relations extends as $D2 \cap (NF1) = N$ and so on. In 10-dimensional type IIA stringy representation, these relations are natural identities that characterize the QHS and so they should be fulfilled in any other representation of QHS including the algebraic geometry one we are after. However to have a consistent description, we still need information about the K $D0$ branes of the QHS and which have no reference in Eq. (2.6). This brings us to our first comment regarding this special property, which to our knowledge have not been sufficiently explored in the literature. The idea of $D0$ dissolution in $D2$ is in fact strongly related with type IIA representation of QHS requiring that the total space–time dimension of the soliton should be equal to 10. However in 11-dimension M-theory on $\mathbb{S}^1$, we have an extra (compact) dimension which allows us to engineer in a nice geometric way the $D0$ branes in perfect agreement with INV correspondence. The key idea of our representation is summarized as follows: The $D0$ branes (flux quanta) dissolved in $D2$ are treated in M-theory on $\mathbb{S}^1$ on equal footing as the electrons in the sense that they will be also viewed as ends of $F1'$ strings, but this time, stretching between $D2$ and K $D0$ branes, see Fig. 2 for illustration. From this representation, one can clearly see that the total space–time dimension of the QHS is as in the M-theory on $\mathbb{S}^1$. One can also see that $D0$ particles in QHS are associated with the compact direction $\mathbb{S}^1$ and moreover has much to do with the homological class of curve E_M in del Pezzo surface $\mathbb{B}_1$ considered in Ref. 15. As such we have, in addition to Eq. (2.6), the following constraint equations of QHS formulated in the language of M-theory on circle $\mathbb{S}^1$,

$$F'1 \cap D2 = 1, \quad F'1 \cap D6 = 0,$$

$$D0 \cap F'1 = 1, \quad F'1 \cap F1 = 0,$$

$$D0 \cap D2 = 0, \quad D0 \cap D6 = 0, \tag{2.7}$$

where, leaving apart the brane dimension and their charge, there is a quite similar analogy between the role of $D0$ and $D6$ branes. With this reformulation of QHS in M-theory on $\mathbb{S}^1$ and to which we shall continue to refer to it as type IIA stringy representation, we end step one and are now in position to go ahead by following the drawn path. In the second step, we describe briefly some useful tools on the H_2 homology of del Pezzo surfaces and the INV correspondence between p branes and complex curves.

III. DEL PEZZO SURFACES

In this section, we focus on two basic aspects. First we give some useful tools on del Pezzo surfaces $\mathbb{B}_k$, $k=1,2,\ldots$, and particularly on the H_2 homology of their class of curves. Then we consider the main lines of the toric representation of $\mathbb{B}_1$ as this will be also relevant for later analysis.

A. General on $\mathbb{B}_k$

del Pezzo surfaces $\mathbb{B}_k$ are complex dimension two compact manifolds that are obtained by blowing up to eight points ($k \leqslant 8$) in complex projective space $\mathbb{P}^2$.[22,23] These $\mathbb{B}_k$ complex surfaces are simply laced manifolds and their homology $H_2(\mathbb{B}_k, Z)$ is generated by the line class H of $\mathbb{P}^2$ and the exceptional curves E_i generating the k blow ups of $\mathbb{P}^2$. The use of this line's homology turns out to be very helpful in the present study. It offers a powerful tool to study holomorphic curves in del Pezzo and has the advantage of giving a quite complete characterization of analytic curves without the need to specify the explicit form of complex algebraic geometry equations.

Recall that on a compact algebraic and projective variety X, a generic divisor $\mathcal{D}=\Sigma_i n_i \mathcal{D}_i$ is a finite formal linear combination of complex codimension one analytic subvarieties $\mathcal{D}_i$. An instructive illustration of this construction is given by the special case of a holomorphic function $F=F(x_1,x_2,\ldots)$ on X,

$$F = \prod_{j=1}^{s} F_j^{n_j} \tag{3.1}$$

with $F_j=F_j(x_1,x_2,\ldots)$ being the irreducible components of F, they are holomorphic polynomials. Here the above $\mathcal{D}_j$'s are the prime divisors associated with the zeros of F_j. The divisor $\mathcal{D}$, which is called principal, reads as $(F)=\Sigma_j n_j(F_j)$ with n_j positive integers. The support of the divisor is the variety $V(F)=\mathcal{D}_1 \cup \mathcal{D}_2 \cup \cdots \cup \mathcal{D}_s$. Similar relations are also valid for meromorphic functions with zeros and poles. Now, we turn to del Pezzo surfaces and their homology.

In a given del Pezzo surface $\mathbb{B}_k$, each E_i is associated with a $\mathbb{P}^1$ holomorphic curve and the class system $\{H,E_i\}$ satisfies the following pairing:

$$H^2 = 1, \quad H \cdot E_i = 0, \quad E_i \cdot E_j = -\delta_{ij}, \quad i,j = 1, \ldots, k. \tag{3.2}$$

In terms of these basic classes of curves, one defines all the tools we need for the present study. First, note that the generic class of holomorphic curves in $\mathbb{B}_k$ are given by the linear combination type,

$$C_a = n_a H - \sum_{i=1}^{k} m_{ai} E_i, \tag{3.3}$$

with n_a and m_a as integers. These classes of curves are characterized by two basic parameters (a) The self-intersection number C_a^2, which by help of Eq. (3.2) is given by

$$C_a^2 = n_a^2 - \sum_{i=1}^{k} m_{ai}^2, \tag{3.4}$$

and (b) the degree d_{C_a} which, as we shall see, is linked to the space–time dimension of the p branes. Since the C_a^2 and the degree play a crucial role in the algebraic geometry realization of QHS we are considering in this paper, it is interesting to note that among the above classes of curves, there is a particular class of curves with a special property. This concerns the canonical class Ω_k of the $\mathbb{B}_k$ surface which is given by minus the first Chern class $c_1(\mathbb{B}_k)$ of the tangent bundle. It reads as

$$\Omega_k = -\left(3H - \sum_{i=1}^{k} E_i\right), \tag{3.5}$$

and has a self-intersection number $\Omega_k^2 = 9-k$ whose positivity requires $k \leqslant 9$. Obviously $k=0$ corresponds just to the case where we have no blow up; i.e., the $\mathbb{P}^2$ complex surface. With the above relation, we are now in position to define the degree d_C of a given curve class $C = nH - \Sigma_{i=1}^{k} m_i E_i$ in $\mathbb{B}_k$. It is the intersection number between the class C with the anticanonical class $(-\Omega_k)$,

$$d_C = -C \cdot \Omega_k = 3n - \sum_{i=1}^{k} m_i. \tag{3.6}$$

Positivity of this integer puts a constraint equation on the allowed values of the n and m_i integers which should be like $\Sigma_{i=1}^{k} m_i \leqslant 3n$. Note that there is a relation between the self-intersection number C^2 of the classes of holomorphic curves and their degrees d_C. This relation, which is known as the adjunction formula, is given by

$$C^2 = 2g - 2 + d_C, \tag{3.7}$$

it allows us to define the genus g of the curve class C as $g = (2 + n(n-3) - \Sigma_{i=1}^{k} m_i(m_i - 1))/2$ where we have also used the expansion $C = nH - \Sigma_{i=1}^{k} m_i E_i$. Fixing the genus g to given positive number puts then a second constraint equation on n and m_i integers. For the interesting example of rational curves with $g=0$, we have then $C^2 = d_C - 2$ or equivalently

$$\sum_{i=1}^{k} m_i(m_i - 1) = 2 + n(n-3). \tag{3.8}$$

For $k=1$, this relation reduces to $m(m-1) = 2 + n(n-3)$, its leading solutions $n=1, m=0$ and $n=0, m=-1$ give just the classes H and E, respectively. Typical solutions for this constraint equation are given by the generic class $C_{n,n-1} = nH - (n-1)E$ which is more convenient to rewrite it as follows:

$$C_{n,n-1} = H + (n-1)(H - E). \tag{3.9}$$

In this case the degree of these rational curves in $\mathbb{B}_1$ is equal to $d_C = 2n+1$, it deals then with p branes in type IIA strings. However along with the above solution, there is also configurations with even degree. These solutions concerns *NS* branes given by the classes $C_{n,2-n} = C = nH - (2$

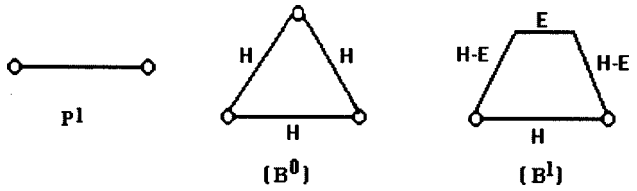

FIG. 3. Three toric diagrams: (a) Diagram of $\mathbb{P}^1$ with two $\mathbb{S}^1$ singularities on borders of the interval. (b) Toric graph of $\mathbb{P}^2$ with three $\mathbb{T}^2$ toric singularities at the vertices, and (c) toric diagram of $\mathbb{B}_1$ with two toric singularities and a blown one.

$-n)E$ with $n=1,2$ and wrapped p branes in type IIB representation. The second issue will be discussed later on.

B. Toric representation of $\mathbb{B}_1$

We need this toric representation to draw pictures for realizations of QHS in terms of classes of curves in $\mathbb{B}_1$. To that purpose recall first that toric representation is a tricky graphic representation that concerns complex manifolds.[24,25] The latter can be usually imagined as given by a real base $\mathcal{B}$ with toric fibers on it. The simplest examples of toric manifolds are naturally the complex projective spaces $\mathbb{P}^n$ where the real dimension n bases $\mathcal{B}_n$ are given by the usual n-simplex and fibers are n-dimensional torii $\mathbb{T}^n$. Therefore in toric representation $\mathbb{P}^1$ is an interval of a straight line with a $\mathbb{S}^1$ circle on top and shrinking at the boundaries. Similarly $\mathbb{P}^2$ is a triangle with three vertices capturing toric singularities. The blow up of one of these three toric singularities of $\mathbb{P}^2$ is just $\mathbb{B}_1$ and is given by a rectangle with four vertices but only two toric singularities. The corresponding toric pictures of these three kinds of toric varieties are shown in Fig. 3. In the H_2 homology of del Pezzo surfaces where line classes in $\mathbb{B}_1$ are of two types, the H standard hyperline and the E exceptional one, we have a nice description of these figures. Figures 3(b) and 3(c) are, respectively, given by the following canonical lines of $\mathbb{P}^2$ and $\mathbb{B}_1$:

$$-3H; \quad -(3H-E) = -[H+2(H-E)+E]. \tag{3.10}$$

Naively, these canonical classes may be thought of as representing the boundaries of these complex surfaces, the triangle for $\mathbb{P}^2$ and rectangle for $\mathbb{B}_1$. Viewed in that way, these boundary lines are genus one classes having degrees $d_{-3H}=9$ and $d_{-3H+E}=8$, respectively, see Eq. (3.7). Moreover, the three edges of $\mathbb{P}^2$ (respectively, four for the case of $\mathbb{B}_1$) correspond just to the number of replication (multiplicity) of the class H (respectively, H and E for $\mathbb{B}_1$) of the basis of the $H_2(\mathbb{B}_k,\mathbb{Z})$ homology. In other words the three (respectively, four) edges for the toric graph of $\mathbb{P}^2$ (respectively, $\mathbb{B}_1$) correspond to the splitting the multiplicity $-3H$ as $-H-H-H$. The same is also valid for the three (four) vertices of the triangle (rectangle), they correspond to the intersection points of the classes of curves.

Along with these figures, one may also draw the pictures associated with the rational curve classes of Eq. (3.9) inside the complex surfaces. Let us give some illustrating examples which will be used later on.

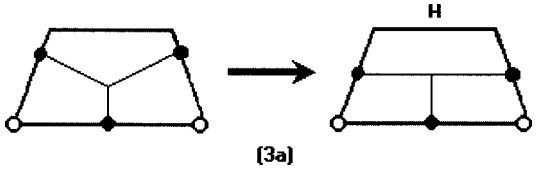

FIG. 4. The graph of the class H in $\mathbb{B}_1$, it looks like the italic letter Y. But as the 3-vertex can be everywhere $\mathbb{B}_1$, it can have different representations. In what follows, we will use the block representation given on right-hand side.

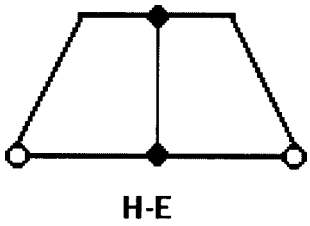

FIG. 5. The internal line crossing the surface of rectangle defines the class $H-E$. It may be viewed as a string stretching between two boundary points on $\mathbb{B}_1$.

1. Graphs of the classes H and E in $\mathbb{B}_1$ *(Fig. 4)*

The hyperline class H has a self-intersection one ($H^2=1$) and a degree $d_H=3$ giving the number of points on the boundary of $\mathbb{B}_1$. It looks like a three point Feynman diagram with three external legs and a three point vertex. The unique self-intersection point we have here belongs to the interior of the $\mathbb{B}_1$ surface and may be interpreted as a signature of the H class in $\mathbb{B}_1$, it is the 3-vertex of the triangulation of the surface. For the exceptional curve E, one may be interested to do the same as H. However, this is not possible in H homological representation since E has a negative self-interaction ($E^2=-1$). This means that E cannot be drawn inside of the rectangle. This is why we will avoid this behavior by changing the orthogonal basis $\{H,E\}$ of the $H_2(\mathbb{B}_1,\mathbb{Z})$ homology into the following equivalent one:

$$H, \quad H-E, \tag{3.11}$$

where the previous difficulty $E^2=-1$ is now solved as $(H-E)^2=0$. The class of $H-E$ is a line in $\mathbb{B}_1$ with its two ends on the boundary. Note that contrary to the old basis $\{H,E\}$ which involves $D0$ and $D2$ branes, the new one implies instead $F1$ strings and $D2$ branes. Note in passing that $\mathbb{B}_1$ may be also defined using the following basis:

$$l_i \cdot l_j = 1 - \delta_{ij}, \quad i,j = 1,2. \tag{3.12}$$

In this basis, the canonical class reads as $-2l_1-2l_2$ and genus zero curves of degree $2n+2$ are given by $C_{n,1}=nl_1+l_2$ or $C_{1,n}=l_1+nl_2$. They will be used later on when we consider type IIB stringy representation of QHS.

2. Graph of the class H−E in $\mathbb{B}_1$ *(Fig. 5)*

In the new basis Eq. (3.11) and thinking about the canonical class Ω_{-3H+E} of $\mathbb{B}_1$ as $-H-2(H-E)-E$, the class $H-E$ inside of $\mathbb{B}_1$ is given by a line stretching between the basic H and E classes of Ω_{-3H+E}. This goes in the same manner as do the two boundary (external) lines $2(H-E)$ of the "line frontier" class Ω_{-3H+E}. The $H-E$ class has no self-intersection (no vertex).

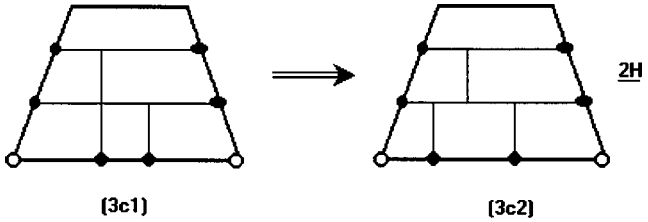

FIG. 6. Graph representing the class $2H=H+H$. The diagrams on the left- and right-hand sides describe, respectively, the class $2H$ before and after triangulation. In type IIA string language, this corresponds to $NS5$.

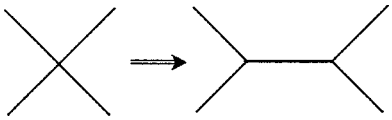

FIG. 7. These figures show the triangulation of four vertex A into two three vertices A1 and A2.

3. Graph of the class 2H in $\mathbb{B}_1$ (Fig. 6)

This is a genus zero class and has a degree equal to 6 and four self-interaction points, its picture is immediately obtained by summing the graphs of two classes as $2H=H+H$. By superposition, we get in a first step the Fig. 6 (left), which involves two kinds of internal vertices, a three vertex and a four one. However splitting the four vertex into two three-vertices using the following triangulation rule, we get the figure on the right-hand side with the appropriate number of internal three-vertices. This property, which is general, is also valid for any sum of class of curves.

4. Graph of the class 2H−E in $\mathbb{B}_1$ (Fig. 7)

Thinking about $2H-E$ as $H+(H-E)$ and following the same lines as before, it is not difficult to show that Fig. 8 represents five external legs and the three self-intersection points.

5. Graph of the class 3H−2E in $\mathbb{B}_1$ (Fig. 8)

Repeating the same process, we get for this class of curve, thought of as the superposition of the following three basic curves $H+(H-E)+(H-E)$, the graph of Fig. 9. Such a procedure is general and applies for all classes of the H_2 homology of del Pezzo. Details will be given in Ref. 18.

IV. BRANES AND HOLOMORPHIC CURVES

Following Ref. 15, there is a remarkable correspondence between del Pezzo surfaces $\mathbb{B}_k$ and M-theory on $\mathbb{T}^k$. Generally speaking an element ω of the real cohomology of del Pezzo associates the basic classes $(H,E_1,\ldots,E_k)$ of the surface $\mathbb{B}_k$ with the point $(l_p,R_1,\ldots,R_k)$, in the moduli space of M-theory on $\mathbb{T}^k$. In practice, this means that ω is a kind of generalized (ω has an indefinite sign) Kahler acting as

$$\omega(H) = -3\ln l_p, \quad \omega(E_i) = -\ln(2\pi R_i), \tag{4.1}$$

where l_p is the Planck scale and where R_i's are the torus radii. Equation (4.1) is in fact a special one, it happens that INV correspondence is more general than given in Eq. (4.1). We have also the following correspondences: (a) Global diffeomorphisms preserving the canonical class Ω_k of the del Pezzo surfaces corresponds precisely to the U duality group of the M-theory on $\mathbb{T}^k$. (b) Rational curves (real two spheres) C with volume $V_C=\omega(C)$ and degree $d_C=(p+1)$ are in one to one with $\frac{1}{2}$BPS p-brane states with tension $T_p=2\pi \exp V_C$. (c) Two classes of rational curves C_1 and C_2 related as $C_1+C_2=-\Omega_k$ corresponds just to the usual electric-magnetic duality linking Dp_1 and Dp_2 with $p_1+p_2=6$.

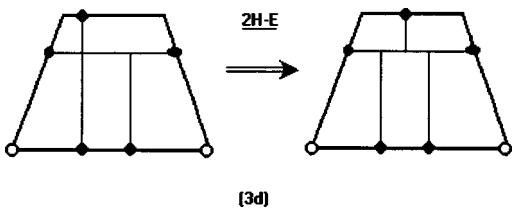

FIG. 8. Building block of the homology class $2H-E$. It represents a $D4$ brane in type IIA stringy description.

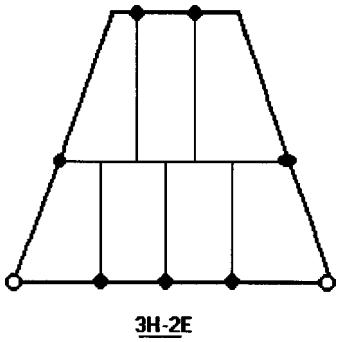

FIG. 9. Building block of the complex curve $3H-2E$ where one recognizes the five self-intersection points. It represents a $D6$ brane in type IIA stringy description.

Therefore p branes of 10-dimensional IIA superstring can be realized as $H_2(\mathbb{B}_k,\mathbb{Z})$ homology classes of holomorphic rational curves in $\mathbb{B}_k$. Of particular interest for our present study is the realization of p branes in terms of $H_2(\mathbb{B}_1,\mathbb{Z})$ classes. More precisely, given a generic $\mathbb{B}_1$ rational curve $C_{n,m}=nH-mE$ with a positive degree $3n-m$ and integers n and m constrained as $m(m-1)=2+n(n-3)$, we can work out all p branes of type IIA superstring with space dimension p equal to $3n-m-1$. The result is reported in the following table:

Classes	$C_0=E$	$C_1=H-E$	$C_2=H$	$C_4=2H-E$	$C_5=2H$	$C_6=3H-2E$	$C_8=4H-3E$
Branes	$D0$	$F1$	$D2$	$D4$	$NS5$	$D6$	$D8$

(4.2)

where now on the subindex carried by the C_p's refers to the real space dimension of the p branes. From this correspondence, one sees that previous figures we have drawn give indeed an algebraic geometry realization of p-branes in terms of classes of holomorphic rational curves in $\mathbb{B}_1$. With these tools in mind, we are now ready to consider the main topic of this paper.

V. REALIZATION OF QHS

To build a QHS representation using homology cycles of $\mathbb{B}_1$, we start by recalling that from the type IIA string representation of QHS we have the following first result:

p-branes	$D0$	$F'1$	$D2$	$F1$	$D6$
Their realization in terms of classes	C_0	C_1'	C_2	C_1	C_6

(5.1)

It gives the p branes involved in QHS and their realization in terms of classes of holomorphic curves in del Pezzo $\mathbb{B}_1$. Here C_1' refers to the class associated with fundamental strings stretching between $D0$ and $D2$ and C_1 to those $F1$ strings stretching between $D2$ and $D6$.

The next thing is to note that the problem of building algebraic geometry realizations of QHS reduces then to the finding of explicit forms of these C_p class of curves in terms of the H and $H-E$ fundamental classes,

$$C_p = C_p(H,E). \tag{5.2}$$

To do so, we first must derive the appropriate constraint equations that should be obeyed by these C_p's, then solve them. We will see that a solution of the form, Eq. (5.2), that satisfies the QHS constraint equations is not possible, one needs many more ingredients to which we describe at the proper time.

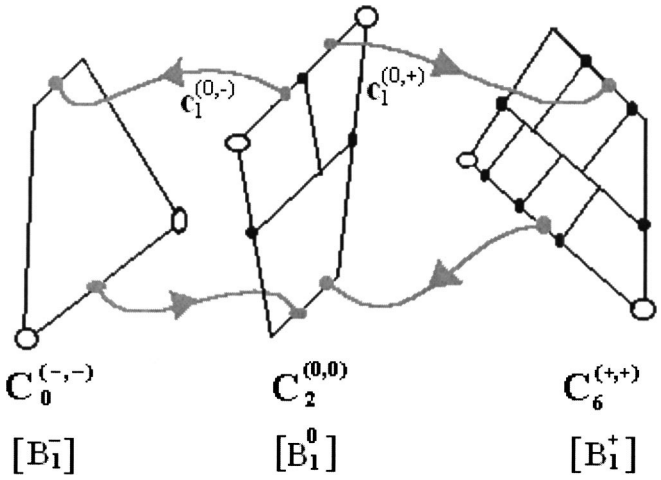

FIG. 10. In this figure, we give a configuration of the homological representation of the QHS involving classes C_0, C_2, and C_6, respectively, associated with one $D0$, one $D2$, and one $D6$ branes. We also represent the curves C_1 illustrating strings stretching between the branes.

A. Constraint equations and solution

By identifying the notion of a set intersection in real geometry with the usual intersection of classes in H_2 homology of $\mathbb{B}_1$, the constraint relations (2.6) and (2.7) of type IIA string representation of QHS translate in $H_2(\mathbb{B}_1,\mathbb{Z})$ homology language as follows:

$$C_0\cdot C_2=0,\quad C_0\cdot C_6=0,\quad C_2\cdot C_6=0,$$

$$C_0\cdot C_1'=1,\quad C_1'\cdot C_2=1,\quad C_1'\cdot C_6=0,$$

$$C_2\cdot C_1=1,\quad C_2\cdot C_6=0,\quad C_1\cdot C_6=1,$$

$$C_0\cdot C_1=0,\quad C_1'\cdot C_1=0,\quad C_2\cdot C_1=1. \tag{5.3}$$

At first sight, solving these constraint equations for rational curves in del Pezzo $\mathbb{B}_1$ seems a simple matter. However, this is not so trivial. While the intersection of classes type $C_2\cdot C_1=1$ or $C_6\cdot C_1=1$ do not cause a problem, the situation is not so obvious for the constraint equations $C_2\cdot C_6=0$, $C_0\cdot C_2=0$, and $C_0\cdot C_6=0$. The point is that there are no class of curves in $\mathbb{B}_1$ with such a feature. This is easily seen by directly computing the corresponding products. For instance the product between $C_2=H$ and $C_6=3H-2E$, using Eqs. (3.2), gives

$$C_2\cdot C_6=3, \tag{5.4}$$

and the same thing for the other relations, which are not as required by the structure of the QHS we are after. A way to overcome this difficulty is to think about the three classes C_0, C_2, and C_6 as belonging to three independent del Pezzo surfaces $\mathbb{B}_1^{(-1)}$, $\mathbb{B}_1^{(0)}$, and $\mathbb{B}_1^{(1)}$ as

$$C_0^{(-1)}=E_{-1},\quad C_2^{(0)}=H_0,\quad C_6^{(1)}=3H_1-2E_1, \tag{5.5}$$

where in addition to Eq. (3.2), we also have $H_0\cdot H_{\pm1}=H_0\cdot E_{\pm1}=H_{\pm1}\cdot E_0=0$, see also Fig. 10. In this case, it is not difficult to check that the intersection products $C_0^{(-1)}\cdot C_2^{(0)}$, $C_0^{(-)}\cdot C_6^{(1)}$, and $C_2^{(0)}\cdot C_6^{(1)}$ are identically zero. The introduction of the $\mathbb{B}_1^{(-1)}$, $\mathbb{B}_1^{(0)}$, and $\mathbb{B}_1^{(1)}$ surfaces is the price one should pay for getting solutions of QHS constraint equations. As such one can think about these three surfaces as three special submanifolds of the blown up of three different $\mathbb{P}^2$'s embedded in $\mathbb{P}^8$. The two extra dimensions in $\mathbb{P}^8$ deal with the curves C_1' and C_1 associated with $F'1$ and $F1$ strings

stretching between the two pairs $\mathbb{B}_1^{(-1)}-\mathbb{B}_1^{(0)}$ and $\mathbb{B}_1^{(0)}-\mathbb{B}_1^{(1)}$, respectively. Therefore a simple solution for the constraint equations (5.3) reads as follows:

$$C_0^{(-1-1)} = E_{-1},$$

$$C_1^{(-10)} = H_{-1} - E_0, \quad C_1^{(0-1)} = H_0 - E_{-1},$$

$$C_2^{(00)} = H_0,$$

$$C_1^{(01)} = H_0 - E_1, \quad C_1^{(10)} = H_1 - E_0,$$

$$C_6^{(11)} = 3H_1 - 2E_1, \tag{5.6}$$

where the upper index (ij) refers to the (i,j) pair of the involved del Pezzo. The couple (00) [respectively, $(\pm 1 \pm 1)$] means that we are dealing with classes of curves in $\mathbb{B}_1^{(0)}$ (respectively, $\mathbb{B}_1^{(\pm 1)}$) and (0 ± 1) or (± 10) with rational curves stretching between $\mathbb{B}_1^{(0)}$ and $\mathbb{B}_1^{(\pm 1)}$. Naturally, the full solution for stretched $F1$ strings is given by the sum $C_1^{(0\pm 1)}+C_1^{(\pm 10)}$ which is equal to $(H_0-E_{\pm 1})+(H_{\pm 1}-E_0)$.

In the above solution (5.6) of the constraint equations for QHS we have considered one $D6$ brane and one $D0$ brane and the same for the $F1$ string stretching between $D0-D2$ and $D2-D6$. These p branes are represented by $H_2(\mathbb{B}_1^{(0,\pm 1)},\mathbb{Z})$ classes describing rational holomorphic curves. In what follows, we derive the general solution of Eqs. (5.3) involving $ND6$ branes and $KD0$ ones, N and K are arbitrary positive integers.

B. Quantum Hall soliton

The algebraic geometry realization of QHS built in terms of a system of intersecting curves is as follows: see Fig. 10 for illustration.

(1) A simple rational curve class $C_2^{(00)}=H_0$ belonging to a basic of del Pezzo copy denoted as $\mathbb{B}_1^{(0)}$ and generated by H_0 and E_0 basic classes with the same properties as above. This class of curve is associated with the $D2$ brane in type IIA stringy representation.

(2) A class of curve with a multiplicity N given by the class $C_6'=N(3H_1-2E_1)$. This is a nonzero genus class $[2g=N(5N-7)+2]$ that corresponds to the N coincident $D6$ branes in the IIA string representation of QHS. To see where this result comes from, it is interesting to recall that in the case where the N $D6$ branes are not coincident, the previous degenerate class split into N simple classes of curves $C_6^{(ii)}$ given by

$$C_6^{(ii)} = 3H_i - 2E_i, \quad i = 1, \ldots, N. \tag{5.7}$$

Each one of these N $C_6^{(ii)}$'s belongs to one of the N del Pezzo copies $\mathbb{B}_1^{(i)}$. The latter have basis $\{H_i,E_i\}$ with the same properties as before but orthogonal to the $\{H_j,E_j\}$ whenever $i\neq j$. This means that in H_2 homology, the N $D6$ branes involve N copies of del Pezzo surfaces $\mathbb{B}_1^{(1)},\ldots,\mathbb{B}_1^{(N)}$ and so requires a larger embedding projective space. To have an idea on the dimension of this space, note that, in addition to $F1$ string loops $C_1^{(ii)}=(H_i-E_i)$ emanating and ending on the same $C_6^{(ii)}$ copy, we have moreover other $F1$ strings stretching between the D6 branes. In H_2 homology, this corresponds to curves $C_1^{(ij)}$ and $C_1^{(ji)}$ stretching between $\mathbb{B}_1^{(i)}$ and $\mathbb{B}_1^{(j)}$. The explicit expression of these classes is given by

$$C_1^{(ij)} = (H_i - E_j), \quad C_6^{(ii)} \cdot C_1^{(ij)} = 1, \quad C_1^{(ij)} \cdot C_6^{(jj)} = 1,$$

$$C_1^{(ji)} = (H_j - E_i), \quad C_1^{(ji)} \cdot C_6^{(ii)} = 1, \quad C_6^{(jj)} \cdot C_1^{(ji)} = 1. \tag{5.8}$$

From these relations, one can clearly see that the $C_1^{(ij)}$ and $C_1^{(ji)}$ classes are stretching between the $C_6^{(ii)}$ and $C_6^{(jj)}$. Since these $C_1^{(ij)}$ and $C_1^{(ji)}$ classes require at least one complex dimension, the embedding projective space should be at least $\mathbb{P}^{3N-1}$. In type IIA stringy representation, this situation describes the case where the gauge symmetry is $\mathrm{U}(1)^N$. For the case of $\mathrm{U}(N)$ gauge symmetry, the $D6$ branes should be coincident and so the corresponding curve classes $C_6^{(ii)}$ must be degenerate curves in $\mathbb{B}_1$. This corresponds to

$$NC_6 = C_6' = N(3H_1 - 2E_1), \tag{5.9}$$

where H_1 and E_1 stand for the basic classes of the del Pezzo surface $\mathbb{B}_1$ where the degenerate NC_6 live.

(3) N holomorphic curves $C_1^{(0i)} + C_1^{(i0)}$ solved as $(H_0 - E_i) + (H_i - E_0)$ and stretching between $C_2^{(00)}$ and $C_6^{(ii)}$. For the case of N coincident $D6$ branes Eq. (5.9), the N classes $C_1^{(0i)} + C_1^{(i0)}$ fuse and give

$$C_1^{(01)} = NH_0 - E_1,$$

$$C_1^{(10)} = H_1 - NE_0, \tag{5.10}$$

where obviously the $F1$ strings stretching between $C_2^{(00)}$ and the $NC_6^{(ii)}$ are collectively described by the sum $(NH_0 - E_1) + (H_1 - NE_0)$. From these solutions, it not difficult to check that the constraint equations (5.10) are exactly fulfilled.

(4) Finally for the K $D0$ branes describing the quantum flux, the construction is quite similar to what we have done for the case of coincident $D6$ branes. The homology class describing the K $D0$ branes is $C_0^{(-1-1)} = kE_{-1}$ and the $F'1$ strings stretching between the $kD0$ and $D2$ realized as $C_0^{(-1-1)}$ and $C_2^{(00)}$ are given by

$$C_1^{(-10)} = (kH_0 - E_{-1}) + (H_{-1} - kE_0), \tag{5.11}$$

The quantum fluxes are naturally given by the ends of the $F'1$ strings on $C_2^{(00)}$ and so are associated with the intersection number $C_1^{(-10)} \cdot C_2^{(00)} = k$ in agreement with the constraint equations.

VI. CONCLUSION AND DISCUSSION

Using a recent result linking p branes and holomorphic curves in del Pezzo surfaces, we have developed a new way to deal with brane bounds of M-theory on $\mathbb{S}^1$. To illustrate our idea in an explicit manner, we have considered the usual type IIA stringy representation of the quantum Hall soliton (QHS) and derived its realization by using the H_2 homology of del Pezzo surfaces. In our representation, QHS is described by a system of intersecting classes of holomorphic curves as given by Eqs. (5.7)–(5.11), see also Fig. 10.

The idea developed here can be used to derive new solutions for QHS but also for studying general branes systems. The development of these issues seems to us important, it offers another way to approach p-brane bounds and uses the powerful tools of homology groups and algebraic geometry that may allow to open new horizons. In particular, one may derive new representations of higher dimensional quantum Hall solitons involving two $D4$ branes and $F1$ strings stretching between them in the same spirit as in Refs. 26–28. One may also consider QHS using p branes of type IIB superstring that are dual to the previous type IIA ones. In the algebraic geometry of QHS we have been considering, this configuration can be obtained without major difficulty. It consists of the system $D3/S^1$, $D7/S^1$, $F1$, $D1$, and $D1/S^1$ and satisfy similar constraint equations to relations (5.3). The correspondence between the two representations is as follows:

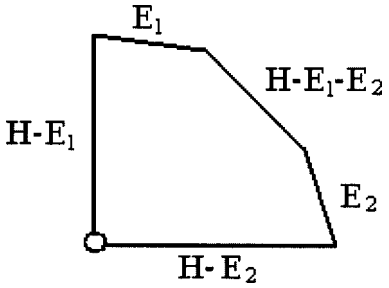

FIG. 11. This graph represents the toric diagram of the del Pezzo surface $\mathbb{B}_2$.

Type IIA	$D2$	$F1$	$D0$	$D4$	$D6$
Curves in $\mathbb{B}_1$	H	$H-E$	E	$2H-E$	$3H-2E$
Type IIB	$D3/S^1$	$F1$, $D1$	$F1/S^1$, $D1/S^1$	$D5/S^1$	$D7/S^1$
Curves in $\mathbb{B}_2$	l_1+l_2-e	l_1, l_2	l_1-e, l_2-e	$2l_1+l_2-e$	$3l_1+l_2-e$

(6.1)

where $l_i \cdot l_j = 1-\delta_{ij}$, $l_i \cdot e = 0$ and $e \cdot e = -1$. In order to algebraic geometry engineer the corresponding QHS dual to the type IIA one, all one must do is, instead of the surface $\mathbb{B}_1$ generated by l_1 and l_2, consider rather the del Pezzo surface $\mathbb{B}_2$, see Fig. 11.

The extra blow up described by the exceptional class e deals with the brane wrapping cycle $\mathbb{S}^1$. The solution to the constraint equations may be obtained without difficulty by using the mapping

$$e = H - E_1 - E_2, \quad l_1 = H - E_1, \quad l_2 = H - E_2. \tag{6.2}$$

Applying the rules we have used in elaborating the type IIA stringy realization of the quantum Hall soliton, we can draw here also the graphs of the $F1$, $D1$ strings and the wrapped D-branes $D3/S^1$ and $D7/S^1$ involved in the type IIB stringy representation of QHS.

Using these graphs, one can also build the QHS diagram similar to that given by Fig. 12. Details on this issue as well as other aspects dealing with the derivation of new solitons including higher dimensional QHS with a configuration type $D4-F1-D4-D0$ will be presented elsewhere.

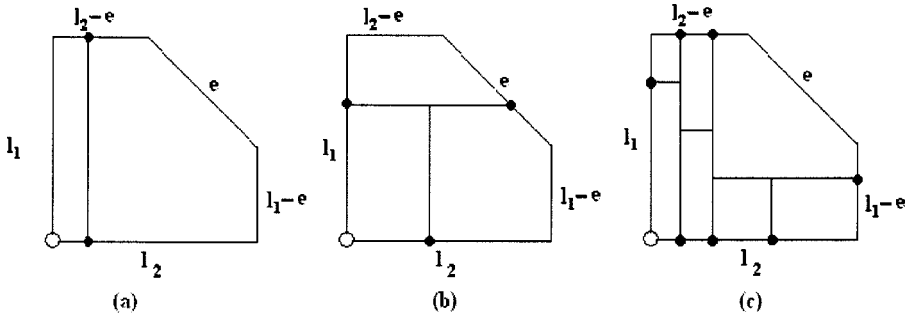

FIG. 12. These are three graphs of curves in the del Pezzo surface B_2, they are involved in the type IIB stringy representation of QHS. These classes are associated with branes in type IIB string on S^1. (a) gives a representation of the $F1$ string. (b) represents a wrapped $D3$ brane on a circle and (c) describes a wrapped $D7$ brane on a circle.

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Casimir energy for a wedge with three surfaces and for a pyramidal cavity

H. Ahmedov[a] and I. H. Duru[b]
Feza Gürsey Institute, P.O. Box 6, 81220, Çengelköy, Istanbul, Turkey

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Casimir energy calculations for the conformally coupled massless scalar field for a wedge defined by three intersecting planes and for a pyramid with four triangular surfaces are presented. The group generated by reflections are employed in the formulation of the required Green functions and the wave functions. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1835546]

I. INTRODUCTION

Having new geometries in hand for which we can evaluate the Casimir energies is of interest: We learn more about the phenomena itself, and hope that experimentalists may realize some of the geometries to measure the effect. At this point we like to emphasize that all experiments so far performed are of two body ones, a single cavity measurement has not been done.[1]

For geometries with planar boundaries, if the planes are parallel or perpendicular to each other, the method of images is easily applicable. The parallel plates and in general rectangular prisms of any dimensions are of that type.[2] For these geometries the groups generated by reflections are Abelian. If the walls of the cavity are not perpendicularly intersecting, the reflection groups are not commutative. This was the case for a previously studied triangular region.[3] If the reflections in the geometry we consider generate a non-Abelian group, one must study the structure of this group, for it is essential in the construction of the required Green functions and wave functions. For example, in the present study the octahedral group provides the basic tools for the calculations.

In the coming section we first calculate the Casimir energy density for the massless scalar field for a wedge with three boundary surfaces.

Section III is devoted to the calculation of the Casimir energy in a pyramidal cavity with four triangular surfaces. We get a positive result.

The corresponding groups generated (related to the octahedral group) by reflections play a vital role in the construction of the Green function and the wave functions. The required group theoretical details are given in the appendixes.

II. PYRAMIDAL WEDGE

Consider the region in the first quadrant ($x_1>0$, $x_2>0$ $x_3>0$) inside the following three planes (Fig. 1):

$$P_1{:}x_1 = x_3, \quad P_2{:}x_2 = 0, \quad P_3{:}x_1 = x_2. \tag{1}$$

Reflection operators with respect to these planes are

[a]Electronic mail: hagi@gursey.gov.tr
[b]Electronic mail: duru@gursey.gov.tr

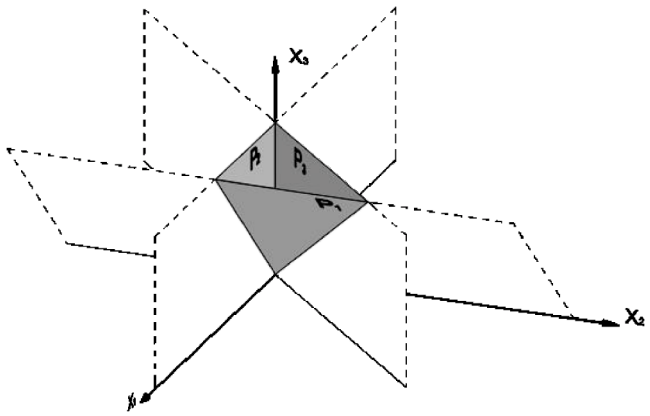

FIG. 1. Planes of Eq. (1).

$$q_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad q_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad q_3 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{2}$$

A group G of order 48 is generated by the above reflections. It's elements are g_j and ig_j; $j=0,\ldots,23$. Here 24 elements of g_j form the octahedral group (see Appendix A) and $i=-1$ is the generator of the inversion group.

Consider the function

$$K(x,y) = \sum_{j=0}^{23} [G(g_j x,y) - G(ig_j x,y)], \tag{3}$$

where $G(x,y)$ is the Green function for the massless scalar field in the Minkowski space,

$$G(x,y) = \frac{1}{4\pi^2}\frac{1}{|x-y|^2}. \tag{4}$$

Here x and y are four vectors with interval $|x-y|^2=|\vec{x}-\vec{y}|^2-(x_0-y_0)^2$; and, g_j act only on the spatial components. To check the boundary conditions let us consider (with $q_1=ig_{21}$)

$$K(q_1 x,y) = \sum_{j=0}^{23} [G(ig_j g_{21} x,y) - G(g_j g_{21} x,y)]. \tag{5}$$

Since for any j we have the element $g_k=g_j g_{21}$ in G, (5) is equal to

$$K(q_1 x,y) = \sum_{k=0}^{23} [G(ig_k x,y) - G(g_k x,y)], \tag{6}$$

which implies

$$K(q_1 x,y) = -K(x,y). \tag{7}$$

In a similar fashion one can verify the antisymmetry property for the elements q_2 and q_3. Therefore the function $K(x,y)$ satisfies Dirichlet boundary conditions on the planes of (1).

Note that in order the equation [with $\eta=\mathrm{diag}(-1,1,1,1)$]

$$\eta^{\mu\nu}\frac{\partial^2}{\partial x^\mu \partial x^\nu}K(x,y) = \delta(x-y) \tag{8}$$

to be satisfied by (3), every point in the region between the planes P_1, P_2, and P_3 must represent different orbits under the action of the group G, which is indeed the case. In other words the region we consider is the fundamental domain of the group G (see Appendix B).

To obtain the energy momentum tensor for the conformally coupled massless scalar field we employ the well-known coincidence limit formula[4]

$$T_{\mu\nu} = \lim_{x\to y}\left[\frac{2}{3}\partial^y_\mu\partial^x_\nu - \frac{1}{6}(\partial^x_\mu\partial^x_\nu + \partial^y_\mu\partial^y_\nu) - \frac{\eta_{\mu\nu}}{6}\eta^{\sigma\rho}\partial^y_\sigma\partial^x_\rho + \frac{\eta_{\mu\nu}}{24}\eta^{\sigma\rho}(\partial^x_\sigma\partial^x_\rho + \partial^y_\sigma\partial^y_\rho)\right]K(x,y). \tag{9}$$

The energy density $T(x) = T_{00}$ is given by

$$T(x) = \frac{1}{12\pi^2}\sum_{j=1}^{23}[T(g_j) - T(ig_j)], \tag{10}$$

where

$$T(g) = \left(\frac{\mathrm{tr}(g)-1}{|\vec{\eta}|^4} - 2\frac{|((1+g)\vec{\eta}\,|^2}{|\vec{\eta}|^6}\right) \tag{11}$$

and

$$\vec{\eta} = (1-g)\vec{x} \tag{12}$$

with g standing for g_j and ig_j.

Using the invariance of $T(g)$ under the $g \to g^{-1}$ we have

$$\begin{aligned} T(g_1) &= T(g_3), \\ T(g_4) &= T(g_6), \\ T(g_7) &= T(g_9), \\ T(g_{10}) &= T(g_{11}), \\ T(g_{12}) &= T(g_{13}), \\ T(g_{14}) &= T(g_{15}), \\ T(g_{16}) &= T(g_{17}). \end{aligned} \tag{13}$$

The same is true for elements ig_j, with j running the same values as (13).

(i) For g_1 which is rotation by angle $\pi/2$ around the x_2 axis we have

$$T(g_1) = -\frac{1}{(x_1^2 + x_3^2)^2}, \tag{14}$$

$$T(ig_1) = -\frac{3(x_1^2 + x_3^2) + 2x_2^2}{2(x_1^2 + x_3^2 + 2x_2^2)^3}. \tag{15}$$

g_4 and g_6 are the rotations by the same angle around the x_1 axis and x_3 axis, respectively. Therefore, $T(g_4)$, $T(ig_4)$ and $T(g_6)$, $T(ig_4)$ are obtained from (14) and (15) with the cyclic replacements of coordinates $(x_1,x_2,x_3)\to(x_3,x_1,x_2)$ and $(x_1,x_2,x_3)\to(x_2,x_3,x_1)$, respectively.

(ii) For the rotation g_{12} by angle $2\pi/3$ around the line passing through the origin and the point $(1,-1,1)$ we have

$$T(g_{12}) = -\frac{3}{((x_1 + x_2)^2 + (x_2 + x_3)^2 + (x_3 - x_1)^2)^2}, \tag{16}$$

$$T(ig_{12}) = -\frac{6|\vec{x}|^2 + 2(x_1x_3 - x_1x_2 - x_2x_3)}{((x_1 - x_2)^2 + (x_2 - x_3)^2 + (x_3 + x_1)^2)^3}. \tag{17}$$

Since g_{14} and g_{16} are rotation matrices by the same angle around the axis passing through the origin and the points $(-1,1,1)$ and $(1,1,-1)$ we conclude that $T(g_{14})$, $T(ig_{14})$ and $T(g_{16})$, $T(ig_{16})$ are given by (16) and (17) with the cyclic replacements of coordinates $(x_1,x_2,x_3)\to(x_3,x_1,x_2)$ and $(x_1,x_2,x_3)\to(x_2,x_3,x_1)$, respectively.

(iii) We also have

$$T(g_{10}) = -\frac{3}{((x_1 - x_2)^2 + (x_2 - x_3)^2 + (x_3 - x_1)^2)^2}, \tag{18}$$

$$T(ig_{10}) = -\frac{6|\vec{x}|^2 - 2(x_1x_2 + x_1x_3 + x_2x_3)}{((x_1 + x_2)^2 + (x_1 + x_3)^2 + (x_2 + x_3)^2)^3}. \tag{19}$$

(iv) For elements satisfying the condition $g^2=1$ the second expression in (11) vanishes. These are the elements g_j, $j=2,5,8$, and $18,\ldots,23$. Since $\mathrm{tr}(ig_j)=1$ we have $T(ig_j)=0$. Nonzero one is

$$T(i) = -\frac{1}{4|\vec{x}|^4}. \tag{20}$$

For rotations g_{20}, g_{21}, and g_2 we get

$$T(g_{20}) = -\frac{1}{2((x_1 - x_3)^2 + 2x_2^2)^2}, \tag{21}$$

$$T(g_{21}) = -\frac{1}{2((x_1 + x_3)^2 + 2x_2^2)^2}, \tag{22}$$

and

$$T(g_2) = -\frac{1}{8(x_1^2 + x_3^2)^2}. \tag{23}$$

Remaining six terms $T(g_{18})$, $T(g_{19})$, $T(g_{22})$, $T(g_{23})$, $T(g_5)$, and $T(g_8)$ are obtained from the above three equations by the cyclic replacements of coordinates.

Energy density (10) is given by

$$T(x) = \frac{1}{12\pi^2}[T(g_{10}) - T(ig_{10}) - T(i)] + \frac{1}{12\pi^2}\Bigg[\frac{17}{8}T(g_1) - 2T(ig_1) + 2T(g_{12}) - 2T(ig_{12}) + T(g_{20}) + T(g_{21}) + \text{c.p.}\Bigg], \tag{24}$$

where c.p. stands for cyclic permutations of coordinates. The system we consider is the intersection region of three wedges (P_1,P_2), (P_2,P_3), and (P_1,P_3). For $x_3 \gg 1$ and $\sqrt{x_1^2+x_2^2} \ll x_3$ our result should reduce to the wedge problem (P_2,P_3). Recall, that energy density in the wedge between two inclined planes is[5]

$$T_W = -\frac{1}{1440\pi^2 r^4}\left(\frac{\pi^4}{\alpha^4} - 1\right), \tag{25}$$

where α is the angle between two planes and r is the minimal distance to the axis which is the intersection of two planes. For the system (P_2,P_3) we have $\alpha = \pi/4$ and $r^2 = x_1^2 + x_2^2$, that is (25) takes the form

$$T_{P_2P_3} = -\frac{255}{1440\pi^2(x_1^2+x_2^2)^2}. \tag{26}$$

Coming to our density (24) for $x_3 \gg 1$ and $\sqrt{x_1^2+x_2^2} \ll x_3$ all terms except the one with $T(g_6)$ are negligibly small; thus, we have

$$T(x) \simeq -\frac{17}{12\pi^2 \cdot 8}T(g_6) = -\frac{17}{96\pi^2(x_1^2+x_2^2)^2}, \tag{27}$$

which is the same as (26). In a similar fashion, terms $T(g_{20})$ and $T(g_{10})$ correspond in the suitable limits to the wedge problems (P_1P_2) and (P_1P_3).

III. PYRAMID

We add to the planes P_1,P_2,P_3 the fourth one $P_4: x_3 = a$. Reflection with respect to the P_4 plane is given by

$$q_4\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ 2 - x_3 \end{pmatrix}. \tag{28}$$

The group generated by q_j, $j=1,2,3,4$ is the semidirect product of the group G defined in the preceding section and the translation group Z^3. The Green function vanishing on the planes P_a, $=1,\ldots,4$ is given by

$$K(x,y) = \sum_{n,m,k=-\infty}^{\infty} \sum_{j=1}^{23} [G(g_j x + \xi, y) - G(ig_j x + \xi, y)], \tag{29}$$

where

$$\xi = \begin{pmatrix} 0 \\ 2na \\ 2ma \\ 2ka \end{pmatrix}. \tag{30}$$

The energy momentum density is

$$T(x) = \frac{1}{6\pi^2} \sum_{n,m,k=-\infty}^{\infty} \sum_{j=1}^{23} [T(g_j) - T(ig_j)], \tag{31}$$

where $T(g)$ is given by (14) with the replacement $\vec{\eta} \to \vec{\eta} + \vec{\xi}$, where $\vec{\xi}$ is the spatial part of the four-dimensional vector ξ. We calculate explicitly the total vacuum energy of the pyramid. For the geometry in hand it is reasonable to use another representation for the Green function related to the wave function and the spectra of the quantum mechanical system inside the pyramid. The wave function which vanishes on the planes P_1, P_2, and P_3 can be obtained in a similar fashion as the Green function,

$$\Psi(\vec{x}) = \Omega \sum_{j=1}^{23} [e^{i(\vec{p}, g_j \vec{x})} - e^{i(\vec{p}, ig_j \vec{x})}] \tag{32}$$

or

$$\Psi_{\vec{p}}(\vec{x}) = -8i\Omega[\sin p_1 x_1 \sin p_2 x_2 \sin p_3 x_3 - \sin p_1 x_1 \sin p_2 x_3 \sin p_3 x_2 + \text{c.p.}], \tag{33}$$

where Ω is the normalization.

The condition $\Psi_{\vec{p}}(\vec{x})|_{P_4} = 0$ implies that the components p_j are proportional to the nonzero positive integers

$$p_1 = \frac{\pi}{a} n, \quad p_2 = \frac{\pi}{a} m, \quad p_3 = \frac{\pi}{a} k. \tag{34}$$

The properties

$$\Psi_{g_j \vec{p}}(\vec{x}) = \Psi_{\vec{p}}(\vec{x}), \quad \Psi_{i\vec{p}}(\vec{x}) = \Psi_{\vec{p}}(\vec{x}) \tag{35}$$

imply that the spectrum takes its values in the quotient space

$$Z^3/G = \{\vec{n} \in Z^3 : k \geqslant n \geqslant m \geqslant 0\} \tag{36}$$

which is the discrete analog of the pyramidal region considered in the preceding section. The wave function (33) vanishes on the boundary B of $A = Z^3/G$. The boundary of A is the union of three regions, $k \geqslant n \geqslant m = 0$, $k \geqslant n = m \geqslant 0$, and $k = n \geqslant m \geqslant 0$. We must drop these values from the spectra. Physical spectra is given by (34) with $k > n > m > 0$ or $\vec{n} \in A/B$.

The Green function can be written as

$$G(x,y) = \sum_{k=3}^{\infty} \sum_{n=2}^{k-1} \sum_{m=1}^{n-1} \frac{e^{i\pi|\vec{p}|(x_0 - y_0)}}{2|\vec{p}|} \Psi_{\vec{p}}(\vec{x}) \Psi_{\vec{p}}(\vec{y}), \tag{37}$$

which implies

$$T(x) = \frac{\pi}{2a} \sum_{k=3}^{\infty} \sum_{n=2}^{k-1} \sum_{m=1}^{n-1} \sqrt{n^2 + m^2 + k^2} |\Psi_{\vec{p}}(\vec{x})|^2. \tag{38}$$

After integration $\int_0^a dx_3 \int_0^{x_3} dx_1 \int_0^{x_1} dx_2$ we have [with $\vec{n} = (n, m, k)$]

$$E = \frac{\pi}{2a} \sum_{\vec{n} \in A/B} |\vec{n}| = \frac{\pi}{96a} \sum_{\vec{n} \in A/B} \sum_{g \in G} |g\vec{n}| = \frac{\pi}{96a} \sum_{\vec{n} \in \cup g(A/B)} |\vec{n}|. \tag{39}$$

Since A is the quotient space Z^3/G we have

$$\bigcup_{g\in G} g(A/B) = Z^3/C, \quad C = \bigcup_{g\in G} gB, \tag{40}$$

which implies

$$E = \frac{\pi}{96a}\left(\sum_{\vec{n}\in Z^3} |\vec{n}| - \sum_{\vec{n}\in C} |\vec{n}|\right). \tag{41}$$

C is the union of nine planes, $m=0$, $n=m$, $n=k$, and six other planes are obtained by cyclic permutations of n, m, and k,

$$\sum_{\vec{n}\in C} |\vec{n}| = 3\sum_{n,m\in Z} \sqrt{n^2+m^2} + 6\sum_{n,m\in Z} \sqrt{2n^2+m^2}. \tag{42}$$

The Casimir energy is

$$E = \frac{1}{6}E_1 - \frac{1}{2}E_2 - \frac{6+4\sqrt{2}}{16}E_3 \simeq \frac{0.069}{a}. \tag{43}$$

Here E_1, E_2, and E_3 are the Casimir energies for the cube with sides a, for the rectangle with sides a, $a/\sqrt{2}$ and for the one dimensional system of length a (see Ref. 2 and references therein),

$$E_1 = \frac{\pi}{2a}\sum_{n,m,k=1}^{\infty} \sqrt{n^2+m^2+k^2} \simeq -\frac{0.015}{a}, \tag{44}$$

$$E_2 = \frac{\pi}{2a}\sum_{n,m=1}^{\infty} \sqrt{n^2+2m^2} \simeq \frac{0.045}{a}, \tag{45}$$

$$E_3 = \frac{\pi}{2a}\sum_{n=1}^{\infty} n \simeq -\frac{0.131}{a}. \tag{46}$$

The positive result of (43) is about the same magnitude as the other well known positive Casimir energy example of the spherical cavity with radius a,[6]

$$E_{\text{ball}} \simeq \frac{0.045}{a}. \tag{47}$$

For nanometer size, that is for $a=10^{-7}$ cm, the energy (43) is (in $\hbar=c=1$ unit, 1 eV$\cong 0.5 \otimes 10^5$ cm^{-1}) $E \simeq 35$ eV which is of considerable magnitude.

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APPENDIX A

Octahedral group O is the group of transformations which transforms the cube into itself. The order of this group is 24. We denote the identity element by g_0. g_1, g_2, and g_3 are rotations on $\pi/2$, π, and $3\pi/2$ around the y axis,

$$g_1=\begin{pmatrix}0&0&-1\\0&1&0\\1&0&0\end{pmatrix},\quad g_2=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix},\quad g_3=\begin{pmatrix}0&0&1\\0&1&0\\-1&0&0\end{pmatrix}. \tag{A1}$$

g_4, g_5, and g_6 are rotations by $\pi/2$, π, and $3\pi/2$ around the x axis,

$$g_4=\begin{pmatrix}1&0&0\\0&0&-1\\0&1&0\end{pmatrix},\quad g_5=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&-1\end{pmatrix},\quad g_6=\begin{pmatrix}1&0&0\\0&0&1\\0&-1&0\end{pmatrix}. \tag{A2}$$

g_7, g_8, and g_9 are rotations by $\pi/2$, π, and $3\pi/2$ around the z axis,

$$g_7=\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix},\quad g_8=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix},\quad g_9=\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix}. \tag{A3}$$

g_{10} and g_{11} are rotations by $2\pi/3$ and $4\pi/3$ around the axis passing through the origin and the point (1,1,1),

$$g_{10}=\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix},\quad g_{11}=\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}. \tag{A4}$$

g_{12} and g_{14} are rotations by $2\pi/3$ and $4\pi/3$ around the axis passing through the origin and the point $(1,-1,1)$,

$$g_{12}=\begin{pmatrix}0&0&1\\-1&0&0\\0&-1&0\end{pmatrix},\quad g_{13}=\begin{pmatrix}0&-1&0\\0&0&-1\\1&0&0\end{pmatrix}. \tag{A5}$$

g_{14} and g_{15} are rotations by $2\pi/3$ and $4\pi/3$ around the axis passing through the origin and the point $(-1,1,1)$,

$$g_{14}=\begin{pmatrix}0&0&-1\\-1&0&0\\0&1&0\end{pmatrix},\quad g_{15}=\begin{pmatrix}0&-1&0\\0&0&1\\-1&0&0\end{pmatrix}. \tag{A6}$$

g_{16} and g_{17} are rotations by $2\pi/3$ and $4\pi/3$ around the axis passing through the origin and the point $(1,1,-1)$,

$$g_{16}=\begin{pmatrix}0&0&-1\\1&0&0\\0&-1&0\end{pmatrix},\quad g_{17}=\begin{pmatrix}0&1&0\\0&0&-1\\-1&0&0\end{pmatrix}. \tag{A7}$$

g_{18} and g_{19} are rotations by π around the axis passing through the origin and the points (1,1,0) and $(1,-1,0)$, respectively,

$$g_{18}=\begin{pmatrix}0&1&0\\1&0&0\\0&0&-1\end{pmatrix},\quad g_{19}=\begin{pmatrix}0&-1&0\\-1&0&0\\0&0&-1\end{pmatrix}. \tag{A8}$$

g_{20} and g_{21} are rotations by π around the axis passing through the origin and the points (1,0,1) and $(1,0,-1)$, respectively,

$$g_{20}=\begin{pmatrix}0&0&1\\0&-1&0\\1&0&0\end{pmatrix},\quad g_{21}=\begin{pmatrix}0&0&-1\\0&-1&0\\-1&0&0\end{pmatrix}. \tag{A9}$$

g_{22} and g_{23} are rotations by π around the axis passing through the origin and the points $(0,1,1)$ and $(0,1,-1)$, respectively,

$$g_{22}=\begin{pmatrix}-1&0&0\\0&0&1\\0&1&0\end{pmatrix},\quad g_{23}=\begin{pmatrix}-1&0&0\\0&0&-1\\0&-1&0\end{pmatrix}. \tag{A10}$$

The tetrahedral group T is the subgroup of O of order 12 with elements $g_0.g_2$, g_5, g_8, and $g_{10},\ldots,g_{17}$. For more details we refer to Ref. 7.

APPENDIX B

Let G be a point group acting in the Euclidean space R^3. A closed subset S of R^3 is called a fundamental domain of G if R^3 is the union of conjugates of S, i.e.,

$$R^3=\bigcup_{g\in G} gS \tag{B1}$$

and the intersection of any two conjugates has no interior.

The fundamental domain of the group generated by the reflections ig_2, ig_5, and ig_8 with respect to $y=0$, $x=0$, and $z=0$ planes is the first quadrant in R^3. This is group of order 8 and divides R^3 into eight equal parts. If one adds to this group the element g_{10} we arrive at the group of order 24 which is the direct product of the tetrahedral group T and inversion one I generated by i. Rotation g_{10} is threefold rotation. It divides the first quadrant into three equal parts. Therefore the fundamental domain for $T\times I$ is the region in the first quadrant between three planes P_2, P_3, and $P_5=\{x_2=x_3\}$. In $T\times I$ there is the reflection operator ig_2 with respect to the P_2 plane. The Green function constructed from the group $T\times I$ will vanish on P_2. For P_3 and P_5 there is no reflection operators. g_{10} rotates P_3 into P_5. If we add to $T\times C$ the reflection operator with respect to the P_3 plane we arrive at the group $O\times I$ which is of order 48. The corresponding fundamental domain can be obtained from that of $T\times C$ by dividing it into two equal parts, that is the region between three planes P_2, P_3, and P_1. There are reflections with respect to these planes. The Green function will vanish on these planes.

[1] For a very short review of the experimental situation see, for example, the book by K. A. Milton, *Physical Manifestations of Zero-Point Energy, the Casimir Effect* (World Scientific, Singapore, 2001).
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Casimir energy in a conical wedge and a conical cavity

H. Ahmedov[a] and I. H. Duru[b]
Feza Gürsey Institute, P.O. Box 6, 81220, Çengelköy, Istanbul, Turkey

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Casimir energies for a massless scalar field for a conical wedge and a conical cavity are calculated. The group generated by the images is employed in deriving the Green function as well as the wave functions and the energy spectrum. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1835547]

I. INTRODUCTION

Image method is one of the best tools in the calculation of the Casimir energies for the polygonal regions. One can use discrete group generated by the reflections with respect to the boundaries of the polygon under consideration to obtain the Green function, wave functions, and spectra of the system. The method is trivially applicable to the cavities or the given regions of space if the following conditions are fulfilled: Surfaces of the region are planar; and, they are parallel or perpendicular to each other. The discrete groups generated by reflections with respect to the planar boundaries appears to be the direct product of the translation Z and the cyclic C_2 groups. The number of copies of Z and C_2 depend on the dimension of the rectangle. For the parallel plate system and two dimensional rectangle we have the groups $C_2 \times Z$ and $(C_2 \times Z)^2$, respectively. (For a Casimir calculation in rectangular region we refer to the monograph[1] and references therein.)

Recently we tried to extend the image method to a set of geometries with planar boundaries without rectangular angles. (To our knowledge, the only previous example without rectangular angles was the wedge problem.[2]) For a class of cavities with triangular cross sections, making use of the tools of the group of reflections from the walls one can obtain the Green function satisfying the Dirichlet boundary conditions, then calculate the Casimir energy.[3] Point groups and crystallographic point groups play important roles in constructing the Green functions and the wave functions if the region we consider is the fundamental domain of the one of those groups. In other words, if every point in the region represents different orbits of the group, the satisfaction of the required wave equation by the Green function is achieved.[3,4]

In this work the example we present is the application of the image method to a geometry with nonplanar boundary. The surface of the cone we deal with is obtained from a geometry with planar surfaces, by identifying two of these surfaces. In fact if there is an element of the point group which maps one planar boundary onto another one, we can obtain volumes with nonplanar boundaries. The simple example we can think of is the wedge in R^2 with the angle $2\pi/N$. By identifying two lines which are the boundaries of the wedge we arrive at the conic surface with the opening angle $2 \arcsin(1/N)$. The corresponding point group is the cyclic one C_N, that is generated by the element q which identifies two boundaries of the wedge. It is clear that $q^N=1$.

In the next section we first consider a conical wedge in R^3 with the opening angle $2 \arcsin \frac{1}{3}$. The region is the fundamental domain of the tetrahedral group which has C_3 as a subgroup. We construct the Green function, then calculate the Casimir energy density for the massless scalar field.

[a]Electronic mail: hagi@gursey.gov.tr
[b]Electronic mail: duru@gursey.gov.tr

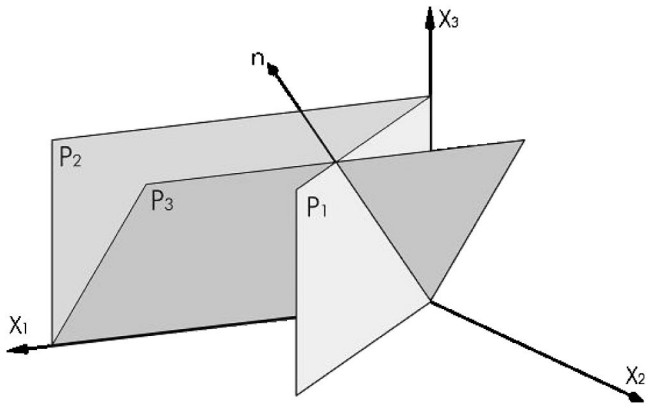

FIG. 1. Planes defined by (1).

In Sec. III making use of the group of the preceding section we construct the wave function and calculate the energy spectrum for the conical wedge.

Section IV is devoted to the closed cone, i.e., conical cavity for which we calculate the Casimir energy which is positive.

In the last section we briefly review the known Casimir energy results for three-dimensional cavities.

The required group theoretical details are given in the Appendix.

II. GREEN FUNCTION AND CASIMIR ENERGY IN A CONICAL WEDGE

Consider the following three planes in the first quadrant ($x_1>0$, $x_2>0$, $x_3>0$) (Fig. 1)

$$P_1{:}x_1 = x_2, \quad P_2{:}x_2 = 0, \quad P_3{:}x_2 = x_3. \tag{1}$$

We are interested in the Green function for the massless scalar field satisfying the boundary conditions

$$K(x,y)\big|_{\vec{x}\in P_2} = 0 \tag{2}$$

and

$$K(x,y)\big|_{\vec{x}\in P_1} = K(x,y)\big|_{g\vec{x}\in P_3}, \tag{3}$$

where

$$g = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \tag{4}$$

is the rotation matrix around $\vec{n}=(1,1,1)$; i.e., the intersection of P_1 and P_3, by angle $2\pi/3$. It transforms P_1 into P_3. The region under consideration

$$S = \{x_1 \geqslant x_2 \geqslant 0,\ x_3 \geqslant x_2 \geqslant 0\} \tag{5}$$

is the fundamental domain $S=R^3/G$ of the group $G=T\times I$, where T is the tetrahedral group and I is the inversion group generated by $i=-1$ (see the Appendix). Identifying planes P_1 and P_3 in the manner described in (3) we arrive at the space which is topologically equivalent to a cone with the plane P_2 being the boundary (Fig. 2). Bringing $\vec{x}_1$ onto $\vec{x}_3$ axis requires a rotation by the angle $2\pi/3$ around $\vec{n}$. Thus the cone we obtained has an opening angle $2\beta=2\arcsin\frac{1}{3}\cong 39°$. Therefore the problem in hand is equivalent to the study of the cone with the Dirichlet boundary condition.

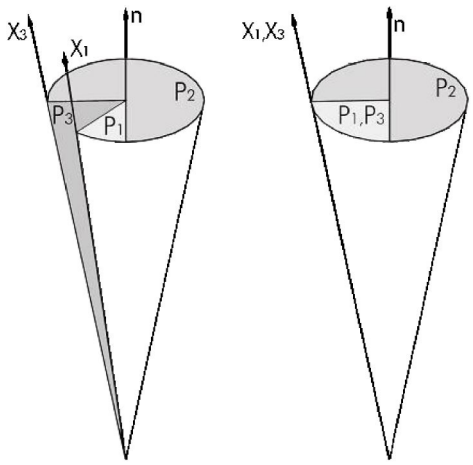

FIG. 2. Cone corresponding to the boundary condition (3).

The desired Green function is of the form

$$K(x,y) = \sum_{j=0}^{11} [G(g_j x,y) - G(ig_j x,y)], \tag{6}$$

where summation runs over the 12 elements of the tetrahedral group. Here $G(x,y)$ is the free Green function for the massless scalar field in the Minkowski space (in $\hbar = c = 1$ units)

$$G(x,y) = \frac{1}{4\pi^2} \frac{1}{|x-y|^2}. \tag{7}$$

To check the boundary conditions, we observe that for any element $g_j \in T$ there exists an element $g_a \in T$ such that $g_a = g_j g$. Therefore

$$K(gx,y) = K(x,y), \tag{8}$$

which implies that the boundary condition (3) is fulfilled. To show the boundary condition (2) we first define the reflection operator with respect to P_2,

$$q = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{9}$$

For any element $g_j \in T$ there exists an element $g_b \in T$ such that $ig_b = g_j q$. Therefore

$$K(qx,y) = -K(x,y), \tag{10}$$

which implies that the boundary condition (2) is fulfilled.

To obtain the energy momentum tensor for the conformally coupled massless scalar field we employ the well-known coincidence limit formula[5]

$$T_{\mu\nu} = \lim_{x \to y} \left[\frac{2}{3} \partial^y_\mu \partial^x_\nu - \frac{1}{6} (\partial^x_\mu \partial^x_\nu + \partial^y_\mu \partial^y_\nu) - \frac{\eta_{\mu\nu}}{6} \eta^{\sigma\rho} \partial^y_\sigma \partial^x_\rho + \frac{\eta_{\mu\nu}}{24} \eta^{\sigma\rho} (\partial^x_\sigma \partial^x_\rho + \partial^y_\sigma \partial^y_\rho) \right] K(x,y). \tag{11}$$

The energy density $T(x) = T_{00}$ is given by

$$T(x) = \frac{1}{12\pi^2}\sum_{j=1}^{11}[T(g_j) - T(ig_j)], \tag{12}$$

where

$$T(g) = \left(\frac{\mathrm{tr}(g) - 1}{|\vec{\eta}|^4} - 2\frac{|((1+g)\vec{\eta})|^2}{|\vec{\eta}|^6}\right) \tag{13}$$

and

$$\vec{\eta} = (1 - g)\vec{x} \tag{14}$$

with g standing for g_j and ig_j.

Using the invariance of $T(g)$ under $g \to g^{-1}$ we have

$$\begin{aligned} T(g_4) &= T(g_5), \\ T(g_6) &= T(g_7), \\ T(g_8) &= T(g_9), \\ T(g_{10}) &= T(g_{11}). \end{aligned} \tag{15}$$

The same equalities are true for elements ig_j, with j running the same values as (15).

(i) For the rotation g_6 by angle $2\pi/3$ around the line passing through the origin and the point $(1,-1,1)$ we have

$$T(g_6) = -\frac{3}{((x_1+x_2)^2 + (x_2+x_3)^2 + (x_3-x_1)^2)^2}, \tag{16}$$

$$T(ig_6) = -\frac{6|\vec{x}|^2 + 2(x_1x_3 - x_1x_2 - x_2x_3)}{((x_1-x_2)^2 + (x_2-x_3)^2 + (x_3+x_1)^2)^3}. \tag{17}$$

Since g_8 and g_{10} are rotation matrices by the same angle around the axis passing through the origin and the points $(-1,1,1)$ and $(1,1,-1)$ we conclude that $T(g_8)$, $T(ig_8)$ and $T(g_{10})$, $T(ig_{10})$ are given by (16) and (17) with the cyclic replacements of coordinates $(x_1,x_2,x_3) \to (x_3,x_1,x_2)$ and $(x_1,x_2,x_3) \to (x_2,x_3,x_1)$, respectively.

(ii) We also have

$$T(g_4) = -\frac{3}{((x_1-x_2)^2 + (x_2-x_3)^2 + (x_3-x_1)^2)^2}, \tag{18}$$

$$T(ig_4) = -\frac{6|\vec{x}|^2 - 2(x_1x_2 + x_1x_3 + x_2x_3)}{((x_1+x_2)^2 + (x_1+x_3)^2 + (x_2+x_3)^2)^3}. \tag{19}$$

(iii) For elements satisfying the condition $g^2 = 1$ the second expression in (13) vanishes. These are the elements g_j, $j = 1,2,3$. Since $\mathrm{tr}(ig_j) = 1$ we have $T(ig_j) = 0$. Nonzero ones are then

$$T(i) = -\frac{1}{4|\vec{x}|^4} \tag{20}$$

and

$$T(g_1) = -\frac{1}{8(x_2^2 + x_3^2)^2}. \tag{21}$$

The remaining two terms $T(g_2)$, $T(g_3)$ are obtained from the above equation by the cyclic replacements of coordinates.

Inserting the results from (16) to (21) into (12) we arrive at the energy density

$$T(x) = \frac{1}{12\pi^2}[T(g_4) - T(ig_4) - T(i)] + \frac{1}{12\pi^2}\left[\frac{1}{8}T(g_1) + 2T(g_6) - 2T(ig_6) + \text{c.p.}\right]. \tag{22}$$

Here c.p. stands for cyclic permutations of coordinates.

III. WAVE FUNCTION AND THE SPECTRUM IN THE CONICAL WEDGE

In this section we briefly present the derivation of the wave function and the spectrum. We write the wave function in a similar fashion as the Green function as

$$\Psi_{\vec{p}}(\vec{x}) = \Omega \sum_{j=0}^{11} [e^{i(\vec{p}, g_j\vec{x})} - e^{i(\vec{p}, ig_j\vec{x})}] \tag{23}$$

or

$$\Psi_{\vec{p}}(\vec{x}) = -8i\Omega[\sin p_1x_1 \sin p_2x_2 \sin p_3x_3 + \text{c.p.}] \tag{24}$$

with Ω being the normalization. To obtain the spectrum we first observe that

$$\Psi_{g_j\vec{p}}(\vec{x}) = \Psi_{\vec{p}}(\vec{x}), \quad \Psi_{i\vec{p}}(\vec{x}) = -\Psi_{\vec{p}}(\vec{x}), \tag{25}$$

which imply that the momentum $\vec{p}$ takes its values in the quotient space R^3/G which is exactly the region S of (5). In other words, the geometry in the momentum space is the replica of the geometry in the configuration space, the fact that can be used in deriving the spectra. Since

$$\Psi_{\vec{p}}(\vec{x})|_{\vec{p}\in P_2} = 0 \tag{26}$$

we must drop the values of $\vec{p}$ on the plane P_2 ($p_2=0$). The condition

$$\Psi_{\vec{p}}(\vec{x})|_{\vec{p}\in P_1} = \Psi_{\vec{p}}(\vec{x})|_{g\vec{p}\in P_3} \tag{27}$$

implies that momenta on the plane P_1 ($p_1=p_2$) are equivalent to the ones on the plane P_3 ($p_2=p_3$). It is sufficient to take into account momenta on one of these planes (take, for example, values on P_1) and drop the ones on the other. Therefore the spectrum in the conical wedge is

$$\Sigma_0 = S \setminus (A \cup B) = \{p_1 \geqslant p_2 > 0,\ p_3 > p_2 > 0\}, \tag{28}$$

where A and B are the boundaries of S corresponding to P_2 and P_3 planes,

$$A = \{p_1 \geqslant 0,\ p_2 = 0\ p_3 \geqslant 0\}, \tag{29}$$

$$B = \{p_1 \geqslant p_2 \geqslant 0,\ p_3 = p_2 \geqslant 0\}. \tag{30}$$

IV. CONICAL CAVITY

In addition to the planes of (1) consider two additional ones,

$$P_4{:}x_1 = a, \quad P_5{:}x_3 = a. \tag{31}$$

The region we consider is then given by

$$H=\{a\geqslant x_1\geqslant x_2\geqslant 0,\ a\geqslant x_3\geqslant x_2\geqslant 0\}. \tag{32}$$

Boundary conditions (26) and (27) and the new Dirichlet conditions on P_4 and P_5,

$$\Psi_{\vec{p}}(\vec{x})\big|_{\vec{p}\in P_4}=\ \Psi_{\vec{p}}(\vec{x})\big|_{\vec{p}\in P_5}=0, \tag{33}$$

imply that the geometry in hand is a conical cavity with the opening angle $\beta=\arcsin\frac{1}{3}$ and height $h=a\cos\beta=(2\sqrt{2}/3)a$. The Dirichlet boundary conditions (33) quantize the momenta,

$$p_1=\frac{\pi}{a}n,\quad p_2=\frac{\pi}{a}m,\quad p_3=\frac{\pi}{a}k, \tag{34}$$

where n, m, and k are integers which subject to the condition (28) [with $\vec{n}=(n,m,k)$]

$$\Sigma=\Sigma_0\cap Z^3=\left\{\vec{p}=\frac{\pi}{a}\vec{n}\colon\ n\geqslant m>0,\ k>m>0\right\}. \tag{35}$$

The Green function can be written as

$$G(x,y)=\sum_{m=1}^{\infty}\sum_{k=m+1}^{\infty}\sum_{n=m}^{\infty}\frac{e^{i\pi|\vec{p}|(x_0-y_0)}}{2|\vec{p}|}\Psi_{\vec{p}}(\vec{x})\Psi_{\vec{p}}(\vec{y}). \tag{36}$$

The energy density we obtain is

$$T(x)=\frac{\pi}{2a}\sum_{m=1}^{\infty}\sum_{k=m+1}^{\infty}\sum_{n=m}^{\infty}\sqrt{n^2+m^2+k^2}\,|\Psi_{\vec{p}}(\vec{x})|^2. \tag{37}$$

After integration $\int_0^a dx_2\int_{x_2}^a dx_3\int_{x_2}^a dx_1$ over the conical cavity H we get the total energy

$$E=\frac{\pi}{2a}\sum_{\vec{n}\in\Sigma}|\vec{n}|=\frac{\pi}{48a}\sum_{\vec{n}\in\Sigma}\sum_{g\in G}|g\vec{n}|=\frac{\pi}{48a}\sum_{\vec{n}\in\cup g\Sigma}|\vec{n}|. \tag{38}$$

Since $\Sigma=\ S\backslash(A\cup B))\cap Z^3$ and $S=R^3/G$ we have

$$\bigcup_{g\in G}g\Sigma=Z^3\backslash C, \tag{39}$$

where

$$C=(\ \bigcup_{g\in G}g(A\cup B))\cap Z^3 \tag{40}$$

is the union of six planes in Z^3: $m=0$, $k=m$ and other four planes are obtained by cyclic permutations of n, m, and k,

$$\sum_{\vec{n}\in C}|\vec{n}|=3\sum_{n,m\in Z}\sqrt{n^2+m^2}+3\sum_{n,m\in Z}\sqrt{2n^2+m^2}, \tag{41}$$

(38) and (39) imply

$$E=\frac{\pi}{48a}\left(\sum_{\vec{n}\in Z^3}|\vec{n}|-\sum_{\vec{n}\in C}|\vec{n}|\right) \tag{42}$$

or

$$E = \frac{1}{3}E_1 - \frac{1}{2}E_2 - \frac{2+\sqrt{2}}{4}E_3 \simeq \frac{0.085}{a}. \tag{43}$$

Here E_1, E_2, and E_3 are the Casimir energies for the cube with sides a, for the rectangle with sides a and $a/\sqrt{2}$; and, for the one-dimensional system of length a, respectively,[6]

$$E_1 = \frac{\pi}{2a}\sum_{n,m,k=1}^{\infty}\sqrt{n^2+m^2+k^2} \simeq -\frac{0.015}{a}, \tag{44}$$

$$E_2 = \frac{\pi}{2a}\sum_{n,m=1}^{\infty}\sqrt{n^2+2m^2} \simeq \frac{0.045}{a}, \tag{45}$$

$$E_3 = \frac{\pi}{2a}\sum_{n=1}^{\infty} n \simeq -\frac{0.131}{a}. \tag{46}$$

V. DISCUSSION

Examples of the Casimir energy calculations for three-dimensional cavities are not plenty. The cubical[1,6] and the spherical[7] cavities have been studied rather extensively. In this work we have studied a conical cavity with a particular opening angle. Similar restriction is true for the recently studied pyramidal geometry for which the angles at the vertices are not arbitrary.[4] We do not have results in hand for the last two kinds of geometries with arbitrary angles. Nevertheless, it may be of interest to briefly review the known Casimir energy calculations (for the massless scalar fields) for the above-mentioned geometries. To have a better idea of the magnitudes we consider the cavities of comparable sizes.

For cube of sides $2b$, we have negative value for the energy: $E_{\text{cub}} \simeq -0.007/b$.[1,6]

For spherical cavity of radius b the Casimir energy is positive $E_{\text{sph}} \simeq 0.046/b$.[7]

Coming to the recently studied pyramidal cavity, let us first describe its position with respect to the above cube. One of the four vertices is located at the center of the cube, the remaining three at the center of a surface, and at the closest vertex and at the middle of the closest edge to this vertex.[4] The volume of this cavity is $b^3/6$ and the Casimir energy is again positive, $E_{\text{pyr}} \simeq 0.069/b$.

For the present conical cavity of opening angle $2\beta = 2\arcsin\frac{1}{3}$ and height b [i.e., $b = (2\sqrt{2}/3)a$] which has the positive energy of (43) is $E_{\text{con}} \simeq 0.080/b$.

To see the dependence of the magnitudes of the positive Casimir energies on the "shapes" of the cavities, let us compare the last three results for the "equal" volumes. If we consider the spherical, pyramidal, and conical cavities with equal volumes we have the following ratios:

$$E_{\text{con}} \simeq 0,54E_{\text{sph}}, \tag{47}$$

$$E_{\text{pyr}} \simeq 0,51E_{\text{sph}}. \tag{48}$$

It is not surprising that the conical and pyramidal geometries are very close to each other.

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APPENDIX

Tetrahedral group T is the group of transformations which transforms cube into itself. The order of this group is 12. We denote the identity element by g_0. g_1, g_2, and g_3 are rotations on π around x, y, and z axis,

$$g_1=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&-1\end{pmatrix},\quad g_2=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix},\quad g_3=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}. \tag{A1}$$

g_4 and g_5 are rotations by $2\pi/3$ and $4\pi/3$ around the axis passing through the origin and the point (1,1,1),

$$g_4=\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix},\quad g_5=\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}. \tag{A2}$$

g_6 and g_7 are rotations by $2\pi/3$ and $4\pi/3$ around the axis passing through the origin and the point $(1,-1,1)$,

$$g_6=\begin{pmatrix}0&0&1\\-1&0&0\\0&-1&0\end{pmatrix},\quad g_7=\begin{pmatrix}0&-1&0\\0&0&-1\\1&0&0\end{pmatrix}. \tag{A3}$$

g_8 and g_9 are rotations by $2\pi/3$ and $4\pi/3$ around the axis passing through the origin and the point $(-1,1,1)$,

$$g_8=\begin{pmatrix}0&0&-1\\-1&0&0\\0&1&0\end{pmatrix},\quad g_9=\begin{pmatrix}0&-1&0\\0&0&1\\-1&0&0\end{pmatrix}. \tag{A4}$$

g_{10} and g_{11} are rotations by $2\pi/3$ and $4\pi/3$ around the axis passing through the origin and the point $(1,1,-1)$,

$$g_{10}=\begin{pmatrix}0&0&-1\\1&0&0\\0&-1&0\end{pmatrix},\quad g_{11}=\begin{pmatrix}0&1&0\\0&0&-1\\-1&0&0\end{pmatrix}. \tag{A5}$$

Let G be a point group acting in the Euclidean space R^3. A closed subset S of R^3 is called a fundamental domain of G if R^3 is the union of conjugates of S, i.e.,

$$R^3=\bigcup_{g\in G} gS \tag{A6}$$

and the intersection of any two conjugates has no interior.

The fundamental domain of the group generated by the reflections ig_1, ig_2, and ig_3 with respect to $x_1=0$, $x_2=0$, and $x_3=0$ planes is the first quadrant in R^3. This is group of order 8 and divides R^3 into eight equal parts. If one adds to this group the element g_4 we arrive at the group of order 24 which is the direct product of the tetrahedral group T and inversion one I generated by i. Rotation g_4 is threefold rotation. It divides the first quadrant into three equal parts. Therefore the fundamental domain for $T\times I$ is the region in the first quadrant between three planes (1).

For more details concerning finite groups we refer to Ref. 8.

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Some remarks on locally conformally flat static space–times

Miguel Brozos-Vázquez,[a] Eduardo García-Río,[b] and Ramón Vázquez-Lorenzo[c]
Department of Geometry and Topology, Faculty of Mathematics, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain

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Necessary and sufficient conditions for a static space–time to be locally conformally flat are obtained, showing some significant restrictions on the possible warping functions of the space–times. This occurs in opposition to cosmological models, where Robertson–Walker space–times are locally conformally flat for any warping function. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1832755]

I. INTRODUCTION

For many years a considerable interest has been shown to the study of physical properties of space–times which are conformal to certain well-known gravitational fields. In locally conformally flat space–times the number of unknown functions is reduced in contrast with general space–times and thus locally conformally flat metrics are of particular interest. A number of locally conformally flat physically significant space–times are known among cosmological models and stationary axisymmetric space–times. Indeed, conformally flat stationary metrics have been recently studied in Refs. 1 and 9 (see also Ref. 10). Summarizing those results it follows that conformally flat stationary circular axisymmetric space–times are necessarily static. (Also, all conformally flat pure radiation metrics are determined in Refs. 6 and 7.) We refer to Ref. 14 for some partial results on locally conformally flat static space–times with perfect fluid energy momentum tensor. However locally conformally flat static space–times are rare in the literature besides the Einstein static Universe or the Schwarzschild interior solution.[3,22]

A Lorentzian manifold (M, g) is called a space–time if there exists a timelike vector field on (M, g). Moreover a future directed unit timelike vector field U is called an observer field. Whenever it is possible to integrate the infinitesimal rest spaces of U to obtain a rest space, U is called *irrotational*. A space–time M is *static* relative to an observer field U if U is irrotational and there is a smooth function $h>0$ on M such that hU is a Killing vector field. (U is called stationary if there is $h>0$ such that hU is Killing, but not necessarily irrotational.) If M is a static space–time with static reference frame U, then M is locally a warped product $N\times_h I$, where $I\subset\mathbb{R}$ is an interval and N is a Riemannian manifold. Thus, in opposition to cosmological space–times, space remains the same but time is warped in static space–times. The fact that only space is warped in Robertson–Walker space–times has important implications as concerns conformal flatness, for instance Robertson–Walker space–times are locally conformally flat for any possible warping function.

By using the warped product structure of static space–times, a direct approach to investigate their conformal properties was based on the fact that the local geometry of the warped product is entirely expressible in terms of the geometry of the rest space and some equations involving the warping functions.[11,12,20] Unfortunately such approach led to some PDE's on the warping function which are difficult to analyze and their geometrical significance remains somehow obscure.

[a]Electronic mail: mbrozos@usc.es
[b]Electronic mail: xtedugr@usc.es
[c]Electronic mail: ravazlor@usc.es

The approach we have followed in investigating locally conformally flatness of warped product metrics essentially differs from previous ones, since it relies on the fact that any warped product metric is in the conformal class of a suitable direct product metric. This presents a main advantage with respect to previous studies: the necessary and sufficient conditions for a warped product metric to be locally conformally flat become more tractable and it is possible to investigate the existence of suitable warping functions which make a standard static space–time locally conformally flat. This is due to the fact that the geometrical significance of the warping function of the product $B\times_f F$ is clearer, since it expresses analytically that $(1/f^2)g_B$ is a metric of constant sectional curvature on the base B. Furthermore, the local existence of solutions of the PDE's defining the warping function for any locally conformally flat base (B, g_B) and any fiber (F, g_F) of constant sectional curvature is guaranteed by the existence of local Möbius transformations among the different spaces of constant sectional curvature, thus showing the richness of the local structure of locally conformally flat warped product metrics. Up to our knowledge, the fact that any warped product metric is in the conformal class of a suitable product metric has not been exploited previously. Since many important properties of space–times like causality conditions, null pregeodesics, null cut points, etc., are conformally invariant, it seems the approach we have followed in investigating conformally flat structures is susceptible to be applied in some other problems.

The paper is organized as follows. Since the geometric construction beside static space–times are warped products, we first obtain a criteria (cf. Theorem 1) for locally conformal flatness of such manifolds in Sec. II. As a consequence, the local structure of locally conformally flat warped product metrics is easily obtained. A commonly used generalization of warped product metrics is that of twisted product metrics, which is investigated in Sec. III, showing that locally conformally flat twisted product metrics are warped product metrics in most cases. In Sec. IV, we study the existence and uniqueness of warping functions in locally conformally flat warped products. All warping functions over a base of constant sectional curvature making $B\times_f\mathbb{R}$ locally conformally flat are determined (Theorem 10), which is a consequence of the fact that all such warping functions define Möbius transformations on the base (B,g_B) (cf. Lemma 9). As a uniqueness result on the warping function we show that the existence of two warping functions making $B\times_{f_1} F_1$ and $B\times_{f_2} F_2$ locally conformally flat for a compact base (B,g_B) forces it to be conformal to the Euclidean sphere S^n (Theorem 13). Finally, some remarks on Riemannian warped products of negative curvature are given in Sec. V.

II. CONFORMALLY FLAT WARPED PRODUCT METRICS

Let (B,g_B) and (F,g_F) be semi-Riemannian manifolds and let $\pi:B\times F\to B$ and $\sigma:B\times F\to F$ be the canonical projections. Also let $f:B\to\mathbb{R}^+$ be a smooth function. Then the *warped product* $B\times_f F$ of (B,g_B) and (F,g_F) with *warping function* f is defined to be the product manifold $M=B\times F$ with the metric tensor $g=\pi^*g_B\oplus(f\circ\pi)^2\sigma^*g_F$. For simplicity g will be denoted by $g=g_B\oplus f^2g_F$ from now on, and we refer to (B,g_B) and (F,g_F) as the *base* and the *fiber* of the product, respectively.[2]

Recall that a semi-Riemannian manifold (M,g) is locally conformally flat if and only if every point in M admits a coordinate neighborhood $\mathfrak{U}$ which is conformal to the semi-Euclidean space $\mathbb{R}^n_\nu$, i.e., there is a diffeomorphism $\Phi:V\subset\mathbb{R}^n_\nu\to\mathfrak{U}$ such that $\Phi^*g=\Psi^2g_{\mathbb{R}^n_\nu}$ for some positive function Ψ. Note that any surface is locally conformally flat, but not every higher dimensional semi-Riemannian manifold admits a locally conformally flat structure. Necessary and sufficient conditions for the existence of such a structure are given by the nullity of the Weyl tensor (if $\dim M\geqslant 4$) and the fact that the Schouten tensor is a Codazzi tensor in dimension three. Locally conformally flat warped product spaces have been investigated by several authors (see, for example, Refs. 11, 12, and 20) who obtained necessary and sufficient conditions for $M=B\times_f F$ to be locally conformally flat in terms of both the curvatures of the base (B,g_B) and the fiber (F,g_F) and some PDE's involving the warping function f. Those results have been obtained as the necessary and sufficient conditions for the vanishing of the Weyl tensor on $B\times_f F$.

The next theorem is a fundamental observation for our purposes since it gives a criterion for

locally conformally flatness of a warped product which enables us to understand the geometrical meaning of the PDE's involving the warping function in Refs. 11 and 20.

Theorem 1: *Let $M=B\times_f F$ be a semi-Riemannian warped product. Then the following hold*:

(i) *If dim $B=1$, then $M=B\times_f F$ is locally conformally flat if and only if (F, g_F) is a space of constant curvature.*

(ii) *If dim $B>1$ and dim $F>1$, then $M=B\times_f F$ is locally conformally flat if and only if*

  (iia) *(F, g_F) is a space of constant curvature c_F.*

  (iib) *The function $f:B\to\mathbb{R}^+$ defines a global conformal deformation on B such that $(B, (1/f^2)g_B)$ is a space of constant curvature $\tilde{c}_B=-c_F$.*

(iii) *If dim $F=1$, then $M=B\times_f F$ is locally conformally flat if and only if the function $f:B\to\mathbb{R}^+$ defines a conformal deformation on B such that $(B, (1/f^2)g_B)$ is a space of constant curvature.*

Proof: Let $g=g_B+f^2g_F$ be the warped product metric on $M=B\times F$ and set $g=f^2(1/f^2g_B+g_F)$. Since locally conformally flatness is a conformally invariant property, g is a locally conformally flat metric on M if and only if so is $\tilde{g}=(1/f^2)g_B+g_F$. Now, after observing that $\tilde{g}$ is nothing but the product metric of $(B, (1/f^2)g_B)$ and (F, g_F), the result follows from Ref. 25, Theorem 4. [Note that the warping function of a warped product is only defined on the base, and thus $(1/f^2)g_B$ is a conformal deformation of g_B.] ■

Note here that for a given fiber (F, g_F) there is no restriction for the warping function f if the base B is one dimensional. Thus, Robertson–Walker space–times are locally conformally flat independently of the warping function, since previous theorem reduces to (i) if dim $B=1$. However as soon as dim $B>1$, there are strong limitations on the possible warping functions, as shown in the next section.

Corollary 2: Let $M=B\times_f F$ be a locally conformally flat semi-Riemannian warped product. Then (B, g_B) is locally conformally flat and (F, g_F) is of constant sectional curvature.

Remark 3: Now, as a consequence of previous results, the local structure of locally conformally flat warped product metrics can be given as follows as a local converse to Corollary 2. *Let (B, g_B) be a locally conformally flat manifold and (F, g_F) a space of constant sectional curvature. Then there exist locally defined warping functions $f_{\mathfrak{U}}:\mathfrak{U}\subset B\to\mathbb{R}^+$ such that the warped product manifold $\mathfrak{U}\times_{f_{\mathfrak{U}}} F$ is locally conformally flat.* Indeed, note that $f_{\mathfrak{U}}$ is defined in terms of the local conformal factor and some appropriate Möbius transformations in order to adjust the sectional curvatures of (F, g_F) and $(\mathfrak{U}, \tilde{g})$.

Note that the vanishing of the Weyl tensor is a local property. Indeed, $M=B\times_f F$ is locally conformally flat if and only if for each point $p\in M$ there exist functions Ψ defined in a neighborhood of p such that the restriction of $\Psi^2\cdot g$ to the defining neighborhood is flat. Since all spaces of constant curvature are locally conformally flat, we have plenty of functions Ψ as before in any locally conformally flat manifold.

However, the implication in Theorem 1 is on the whole base B, since the warping function is globally defined. Therefore, two basic problems arise from the above, when is it possible to extend the locally defined warping functions to the whole base B and, in such case, is there any kind of uniqueness on the warping functions?

Remark 4: As an application of Theorem 1 (iii), a four-dimensional static space–time $B\times_f\mathbb{R}$ is locally conformally flat if and only if $(B,(1/f^2)g_B)$ is Einstein. Therefore, any conformal Einstein 3-manifold gives rise to a suitable defined locally conformally flat static space–time. (See Refs. 15 and 17 and the references therein for more information on conformal Einstein equations.)

Remark 5: As a generalization of the warped product structure, a *doubly warped product* $B_b\times_f F$ of (B, g_B) and (F, g_F) with warping functions f and b is the product manifold $M=B\times F$ with metric tensor $g=b^2g_B\oplus f^2g_F$, where f and b only depend on the points of B and F, respectively. Now, proceeding as above, one can express the double warped metric g as

$$g = b^2 g_B + f^2 g_F = b^2\left(g_B + f^2\left(\frac{1}{b^2}g_F\right)\right) = f^2\left(b^2\left(\frac{1}{f^2}g_B\right) + g_F\right) = b^2 f^2\left(\left(\frac{1}{f^2}g_B\right) + \left(\frac{1}{b^2}g_F\right)\right),$$

which shows that the doubly warped product is in the conformal class of a certain warped product (indeed the conformal class of a direct product). Thus previous Theorem 1 applies to show that $B_b\times_f F$ is locally conformally flat if and only if $(B,\ (1/f^2)g_B)$ and $(F,\ (1/b^2)g_F)$ have constant sectional curvatures, which are necessarily of opposite sign if both B and F have dimension greater than one, thus giving a geometrical meaning to the PDE's systems in Ref. 12.

III. CONFORMALLY FLAT TWISTED PRODUCT METRICS

The *twisted product* $B\times_f F$ of (B,g_B) and (F,g_F) with twisting function f is the product manifold $B\times F$ with metric tensor $g=g_B\oplus f^2 g_F$, where f depends both on the points of B and F, i.e., $f:B\times F\to\mathbb{R}^+$.

A curvature condition, called the mixed Ricci flatness was stated in terms of the product manifold structure in Ref. 8 in order to relate the twisted and warped product structures. Such condition (which essentially means that the Ricci tensor vanishes when it is applied to vector fields on the base and the fiber simultaneously) is satisfied in most physically realistic space–times, such as Kruskal and Robertson–Walker space–times, because of the physical requirements induced by the stress-energy tensor on these space–times. Observing that these space–times are warped products, roughly speaking, the main result in Ref. 8, Theorem 1 allows us to observe that this is the maximal generality for these space–times since they cannot be further generalized to twisted products in a nontrivial way. As an application of such criteria, we have the following theorem.

Theorem 6: *Let* $M=B\times_f F$ *be a semi-Riemannian twisted product with* $\dim B\geqslant 2$ *and* $\dim F\geqslant 2$. *If* M *is locally conformally flat then it can be expressed as a warped product.*

Proof: First of all, recall that a $(n\geqslant 4)$-dimensional semi-Riemannian manifold is locally conformally flat if and only if its Weyl tensor W vanishes, where W is defined as follows:

$$W(X,Y,Z,T) = R(X,Y,Z,T) + \frac{\mathrm{Sc}}{(n-1)(n-2)}\{\langle X,Z\rangle\langle Y,T\rangle - \langle Y,Z\rangle\langle X,T\rangle\}$$
$$- \frac{1}{n-2}\{\mathrm{Ric}(X,Z)\langle Y,T\rangle - \mathrm{Ric}(Y,Z)\langle X,T\rangle + \langle X,Z\rangle\mathrm{Ric}(Y,T) - \langle Y,Z\rangle\mathrm{Ric}(X,T)\}$$

for all vector fields X,Y,Z,T on M. Further the curvature tensor R is the (1,3)-tensor field on M defined by $R(X,Y)Z=\nabla_{[X,Y]}Z-[\nabla_X,\nabla_Y]Z$, for all vector fields X, Y, $Z\in\mathfrak{X}(M)$. The Ricci tensor is the contraction of the curvature tensor given by $\mathrm{Ric}(X,Y)=\mathrm{trace}\{U\rightsquigarrow R(X,U)Y\}$, for all X, $Y\in\mathfrak{X}(M)$, and the scalar curvature is obtained by contracting the Ricci tensor, $\mathrm{Sc}=\mathrm{trace}(\mathrm{Ric})$.

Let X and V denote two non-null vector fields on B and F, respectively. Since $\dim B\geqslant 2$, choose Y a non-null vector field on B in the orthogonal space to X; $Y\in<X>^{\perp}$. After some straightforward calculations, it follows that the Weyl tensor of $M=B\times_f F$ satisfies (cf. see, for example, Ref. 8, Proposition 2, 3, 4 for the expressions of the curvature tensor, the Ricci and scalar curvature of a twisted product)

$$W(Y,X,Y,V) = -\frac{1}{n-2}g(Y,Y)\mathrm{Ric}(X,V).$$

Therefore, if $M=B\times_f F$ is locally conformally flat, then $\mathrm{Ric}(X,V)=0$ for all vector fields X and V on the base and the fiber, which shows that $M=B\times_f F$ is mixed Ricci flat, and thus a warped product if $\dim F\geqslant 2$. ■

Remark 7: Following the same idea behind Theorem 1, for the metric tensor of any twisted product $B\times_f F$, set

$$g_B + f^2 g_F = f^2\left(\frac{1}{f^2} g_B + g_F\right).$$

This shows that $B\times_f F$ is locally conformally flat if and only if so is $F\times_{1/f} B$. But this time $g_F + (1/f^2)g_B$ is still a twisted product metric, since the twisting function f depends both on B and F. However previous relation preserves the (possible) reduction of the twisted product to a warped one, since f decomposes as a product of two functions f_B and f_F defined on B and F, respectively, if and only if so does $1/f$, just observing that $XU(\log f) = -XU[\log(1/f)]$ for all vector fields X, U on B and F, respectively. (See Ref. 8 for more details on the condition for a twisted product to be a warped product.)

Remark 8: The duality condition in the previous remark justifies the symmetry on the conditions $\dim B \geqslant 2$, $\dim F \geqslant 2$ in Theorem 6.

In order to show the necessity of those restrictions, we construct some simple examples showing the necessity of the assumptions on $\dim B \geqslant 2$, $\dim F \geqslant 2$ as follows. Let $I \subset \mathbb{R}$ be an open interval and take $U \subset \mathbb{R}^3$ an open set such that $f(t,x,y,z) = 1/(t+z)$ is positive on $I \times U$. Then the twisted product manifold $I\times_f U$ is locally conformally flat. (The vanishing of the Weyl tensor is obtained after some tedious calculations that we omit.) Furthermore, note that $I\times_f U$ cannot be reduced to a warped product structure since $\mathrm{Ric}(\partial/\partial t, \partial/\partial z) = -2/(t+z)^2$, which shows that it is not mixed Ricci flat.

Locally conformally flat twisted product metrics with one-dimensional fiber are easily obtained from Remark 7 just considering $U\times_{1/f} I$.

IV. LOCALLY CONFORMALLY FLAT STATIC SPACE–TIMES

Since static space–times are locally warped products with one-dimensional fiber, from now on we will restrict to standard static space–times, thus assuming the structure of a warped product $B\times_f \mathbb{R}$ for some positive function f on B.

As a consequence of Theorem 1, a product manifold $B\times\mathbb{R}$ is locally conformally flat if and only if (B, g_B) is a space of constant curvature. This occurs, for instance in the Einstein static universe $\mathbb{S}^n\times\mathbb{R}$. It is obvious that for any constant function f on B, the warped product $B\times_f \mathbb{R}$ is also locally conformally flat. Therefore, it seems natural to wonder whether there are nonconstant warping functions on B defining a locally conformally flat static space–time.

In order to understand the question above, we first introduce some notation as follows. Let ∇ denote both the Levi–Cività connection associated to the given metric and the *gradient operator* on a generic semi-Riemannian manifold (M, g). The *Hessian tensor* h_f of a real-valued function $f: M \to \mathbb{R}$ is defined by $h_f(X) = \nabla_X \nabla f$, where X is a vector field on M. Also the symmetric (0,2)-tensor field H_f defined on (M, g) by $H_f(X,Y) = g(h_f(X), Y)$ is called the *Hessian form* of f. We define the *Laplacian* Δf of a function f on (M, g) by $\Delta f = \mathrm{trace}\, h_f$ $(=\mathrm{div}\, \nabla f)$, where div is the divergence.

It follows from Remark 3 the local existence of warping functions making $(\mathfrak{U}\subset B)\times_{f_{\mathfrak{U}}} \mathbb{R}$ locally conformally flat. However, global existence of such functions is not clear. Next, in order to understand the simplest cases, we consider static space–times with base (B, g_B) of constant sectional curvature and $\dim B = n$. Then we have the following analytical characterization of the warping function.

Lemma 9: Let $M = B\times_f \mathbb{R}$ be a locally conformally flat static space–time. Then (B, g_B) is of constant sectional curvature if and only if the warping function f defines a solution $\phi = -\ln f$ of the Möbius equation $B_{g_B}(\phi) = 0$, where

$$B_{g_B}(\phi) = H_\phi - \mathrm{d}\phi \otimes \mathrm{d}\phi - \frac{1}{n}\{\Delta\phi - \|\nabla\phi\|^2\} g_B. \tag{1}$$

Moreover, for any base (B, g_B) of constant sectional curvature and any positive solution ϕ of (1)*, the warped product $B\times_f \mathbb{R}$ is locally conformally flat.*

Proof: Since (B, g_B) is locally conformally flat by Corollary 2, then it is of constant sectional

curvature if and only if it is Einstein. On the other hand, $(B, (1/f^2)g_B)$ is a space of constant sectional curvature by Theorem 1, and thus Einstein. Therefore (B,g_B) is of constant sectional curvature if and only if the conformal deformation $g_B \mapsto (1/f^2)g_B$ preserves the Einstein property, which occurs if and only if f is a solution of the Möbius equation.[21] Now, the second part of the lemma follows from Theorem 1 and the above considerations. ■

It is shown in Ref. 21 that, if $\phi: B \to \mathbb{R}$ satisfies the Möbius equation on (B,g_B) then the function $\psi = \exp(-\phi)$ satisfies $H_\psi = (1/n)\Delta\psi g_B$ on (B,g_B), since $H_{\exp(\phi)} = \exp(\phi)\{H_\phi + \mathrm{d}\phi \otimes \mathrm{d}\phi\}$. In what follows we will refer to $H_\psi = (1/n)\Delta\psi g_B$ as the linearized Möbius equation on (B,g_B).

From the previous lemma, the following description of the possible warping functions on a locally conformally flat static space–time with base a (complete and simply connected) space of constant sectional curvature is obtained.

Theorem 10: *Let (B, g_B) be a complete and simply connected Riemannian manifold of constant sectional curvature. Then the static space–time $B \times_f \mathbb{R}$ is locally conformally flat if and only if one of the following occurs*:

(i) *If $B \equiv \mathbb{R}^n$, where $\mathbb{R}^n$ denotes the Euclidean space, then all possible warping functions are given by*

$$f(\vec{\mathbf{x}}) = a\|\vec{\mathbf{x}}\|^2 + \langle \vec{\mathbf{b}}, \vec{\mathbf{x}} \rangle + c, \quad \vec{\mathbf{b}} \in \mathbb{R}^n,\ a,c \in \mathbb{R}, \tag{2}$$

where the coefficients a, $\vec{\mathbf{b}}$ and c satisfy $4ac - \|\vec{\mathbf{b}}\|^2 > 0$, $a > 0$ and $\langle , \rangle$ is the Euclidean inner product in $\mathbb{R}^n$.

(ii) *If $B \equiv \mathbb{H}^n$, where $\mathbb{H}^n$ denotes the Poincaré half-space model of the hyperbolic geometry, then all possible warping functions are given by*

$$f(\vec{\mathbf{x}}) = \frac{a\|\vec{\mathbf{x}}\|^2 + \langle \vec{\mathbf{b}}, \vec{\mathbf{x}} \rangle + c}{x_n}, \quad \vec{\mathbf{b}} \in \mathbb{R}^n, a,c \in \mathbb{R}, \tag{3}$$

where the coefficients $a > 0$, $\vec{\mathbf{b}}$ and c satisfy either of

(1) $4ac - \|\vec{\mathbf{b}}\|^2 > 0$, *or*
(2) $4ac - (b_1^2 + b_2^2 + \cdots + b_{n-1}^2) \geqslant 0$ *and* $b_n \geqslant 0$.

(iii) *If $B \equiv \mathbb{S}^n$, where $\mathbb{S}^n$ denotes the Euclidean sphere, then all possible warping functions are given by*

$$f = -\frac{n-1}{\mathrm{Sc}}\psi + \kappa, \tag{4}$$

where ψ is an eigenfunction for the largest eigenvalue of the Laplacian, $\Delta\psi = -[\mathrm{Sc}/(n-1)]\psi$, and κ is a real constant making f positive.

Proof: We analyze each case above separately.

(i) It follows from Lemma 9 that a function $f: \mathbb{R}^n \to \mathbb{R}$ defines a locally conformally flat static space–time $\mathbb{R}^n \times_f \mathbb{R}$ if and only if $\phi = -\ln f$ is a solution of the Möbius equation on $(\mathbb{R}^n, g_0)$. By considering $u = \exp(-\phi)$, one gets that f is indeed a positive solution of the linearized Möbius equation $H_f = (1/n)\Delta f g_0$. Now it follows easily from the linearized Möbius equation that any such function f must be of the form

$$f(\vec{\mathbf{x}}) = a\|\vec{\mathbf{x}}\|^2 + \langle \vec{\mathbf{b}}, \vec{\mathbf{x}} \rangle + c, \quad a,c \in \mathbb{R}, \vec{\mathbf{b}} \in \mathbb{R}^n.$$

Moreover, since f is required to be strictly positive in order to be a warping function, we have the following. First observe that $a > 0$, otherwise f is negative outside a compact set. Now, assuming $a > 0$, $f(\vec{\mathbf{x}}) = a\|\vec{\mathbf{x}}\|^2 + \langle \vec{\mathbf{b}}, \vec{\mathbf{x}} \rangle + c$ attains its minimum at $\vec{\mathbf{x}} = -(1/2a)\vec{\mathbf{b}}$ and $f[-(1/2a)\vec{\mathbf{b}}] = -(1/4a)\|\vec{\mathbf{b}}\|^2 + c$, which must be positive, from where (i) is obtained.

(ii) Let $(\mathfrak{U}^n, g_0)$ denote the Euclidean upper-half-space and consider the Poincarè half-space model $(\mathbb{H}^n, g_{\mathbb{H}})$ as a conformal deformation $g_{\mathbb{H}}=\vartheta^* g_0=(1/x_n^2)g_0$ of the Euclidean metric. Let φ be a Möbius transformation from the hyperbolic space $(\mathbb{H}^n, g_{\mathbb{H}})$ into $(\mathfrak{U}^n,(1/f^2)g_{\mathbb{H}})$ and consider the following diagram:

$$\begin{array}{ccc} & & \varphi \\ \left(\mathbb{H}^n,\, g_{\mathbb{H}}=\dfrac{1}{x_n^2}\, g_0\right) & \to & \left(\mathfrak{U}^n,\, \dfrac{1}{f^2}\, g_{\mathbb{H}}\right) \\ & \vartheta \downarrow & \nearrow \\ & (\mathfrak{U}^n,\, g_0) & \end{array}$$

Note that the set of conformal transformations forms a group with composition and moreover that the Möbius transformations is a proper subgroup.[21] Further, since ϑ is a Möbius transformation, then φ is a Möbius transformation if and only if so is $\varphi\circ\vartheta^{-1}$, which is defined in $(\mathfrak{U}^n, g_0)$. Now, it follows from (i) that $(1/f^2)g_{\mathbb{H}}=[1/(a\|\vec{\mathbf{x}}\|^2+\langle\vec{\mathbf{b}},\vec{\mathbf{x}}\rangle+c)]^2 g_0$ from where it follows that

$$f(\vec{\mathbf{x}})=\frac{a\|\vec{\mathbf{x}}\|^2+\langle\vec{\mathbf{b}},\vec{\mathbf{x}}\rangle+c}{x_n}.$$

Since $x_n>0$ we only have to consider the numerator in the above definition of f in order to analyze its positivity. Now note that $a\|\vec{\mathbf{x}}\|^2+\langle\vec{\mathbf{b}},\vec{\mathbf{x}}\rangle+c$ defines a convex paraboloid (considered as a function in $\mathbb{R}^n$) which is positive on $\mathfrak{U}$ if and only if $a>0$ and it does not intersect the domain $\mathfrak{U}$. Thus two different possibilities may occur. The minimum of the paraboloid is positive and the required condition is $4ac-\|\vec{\mathbf{b}}\|^2>0$, which shows (ii) (1) as in the previous case (i). The other possibility occurs if the minimum is nonpositive but it is realized on the down-half-space [i.e., $(-b_n/2a)\leqslant 0$]. In this case the desired condition is obtained by the positivity of the intersection of the paraboloid defined by $a\|\vec{\mathbf{x}}\|^2+\langle\vec{\mathbf{b}},\vec{\mathbf{x}}\rangle+c$ and the hyperplane $x_n=0$, which gives $4ac-(b_1^2+b_2^2+\cdots+b_{n-1}^2)\geqslant 0$, thus showing (ii) (2).

(iii) As in the previous cases, it follows from Lemma 9 that a function $f:\mathbb{S}^n\to\mathbb{R}$ defines a locally conformally flat static space–time $\mathbb{S}^n\times_f\mathbb{R}$ if and only if $\phi=-\ln f$ is a solution of the Möbius equation on $(\mathbb{S}^n, g_{\mathbb{S}^n})$. By considering $u=\exp(-\phi)$, one gets that f is indeed a positive solution of the linearized Möbius equation and thus $H_f=(1/n)\Delta f g_{\mathbb{S}^n}$.

Next, consider the gradient vector field ∇f on $\mathbb{S}^n$. Since $(\mathcal{L}_{\nabla f}g)(Y,Z)=2H_f(Y,Z)$, it follows from the linearized Möbius equation that ∇f is a conformal vector field on $\mathbb{S}^n$, and then

$$-\Delta(\operatorname{div}\ \nabla f)=\frac{\mathrm{Sc}}{n-1}\operatorname{div}(\nabla f), \tag{5}$$

where Sc denotes the scalar curvature of $(\mathbb{S}^n, g_{\mathbb{S}^n})$ (cf. Ref. 24). Hence $\Delta(\Delta f)=-[\mathrm{Sc}/(n-1)]\Delta f$, which shows that Δf is an eigenfunction for the largest eigenvalue $\lambda_1=-[\mathrm{Sc}/(n-1)]$ of the Laplacian in $(\mathbb{S}^n, g_{\mathbb{S}^n})$. Further, it also follows from (5) that $\Delta(\Delta f+[\mathrm{Sc}/(n-1)]f)=0$ and thus that $\Delta f+[\mathrm{Sc}/(n-1)]f$ is a constant function. Therefore, if ψ denotes a λ_1-eigenfunction for the Laplacian in $(\mathbb{S}^n, g_{\mathbb{S}^n})$, then the desired warping functions are given by $f=[-(n-1)/\mathrm{Sc}]\psi+\kappa$, for some constant κ which makes f positive. ■

Remark 11: Note that the eigenspace corresponding to the largest eigenvalue $\lambda_1=-\mathrm{Sc}/(n-1)$ of the Laplacian in $\mathbb{S}^n$ is generated by the restriction to $\mathbb{S}^n$ of the homogeneous polynomials of degree one in $\mathbb{R}^{n+1}$ (see, for example, Ref. 4, Chap. 3). Thus any such λ_1-eigenfunction is the restriction to $\mathbb{S}^n$ of some Ψ defined on $\mathbb{R}^{n+1}$ by $\Psi(\vec{\mathbf{x}})=\langle\vec{\mathbf{a}},\vec{\mathbf{x}}\rangle$ for $\mathbf{0}\neq\vec{\mathbf{a}}\in\mathbb{R}^{n+1}$.

Remark 12: The conformal deformations of the model spaces defined by the different functions (2)–(4) in the previous theorem affect the sectional curvature as follows:

(i) The sectional curvature of $(\mathbb{R}^n, (1/f^2)g_0)$ is constant $4ac-\|\vec{\mathbf{b}}\|^2>0$, where f is defined by (2).

(ii) The sectional curvature of $(\mathbb{H}^n, (1/f^2)g_{\mathbb{H}^n})$ is constant $4ac-\|\vec{\mathbf{b}}\|^2$, where f is given by (3).

Note that the metrics $(1/f^2)g_0$ and $(1/f^2)g_{\mathbb{H}^n}$ above need not be complete, since otherwise $(\mathbb{R}^n, (1/f^2)g_0)$ and $(\mathbb{H}^n, (1/f^2)g_{\mathbb{H}^n})$ should be compact by Bonnet-Myers' theorem.[18] (This lies on the fact that completeness is not a topological property, but a uniform one.)

(iii) The sectional curvature of $(\mathbb{S}^n, (1/f^2)g_{\mathbb{S}^n})$ is constant $(\kappa^2-[(n-1)^2/\mathrm{Sc}^2]\|\vec{\mathbf{a}}\|^2)$, where f is given by (4) and $\psi=\Psi|_{\mathbb{S}^n}$ is the restriction to $\mathbb{S}^n$ of $\Psi(\vec{\mathbf{x}})=\langle\vec{\mathbf{a}},\vec{\mathbf{x}}\rangle$. Note here that $\kappa^2-[(n-1)^2/\mathrm{Sc}^2]\|\vec{\mathbf{a}}\|^2$ is positive, since κ is greater than $[(n-1)/\mathrm{Sc}]\|\vec{\mathbf{a}}\|$ in order to make f positive.

For a given manifold (B, g_B), to be the base of two different locally conformally flat warped products is a very restrictive fact, as shown in the next results, which give some partial answers on the uniqueness of the warping function of a locally conformally flat warped product.

Theorem 13: *Let (B, g_B) be a compact Riemannian manifold admitting two-distinct (i.e., $f\neq c\hat{f}$) warping functions such that both $B\times_f\mathbb{R}$ and $B\times_{\hat{f}}\mathbb{R}$ are locally conformally flat static space–times. Then (B, g_B) is conformal to the Euclidean sphere by means of the conformal deformation $(1/f^2)g_B$ and $\hat{f}/f$ is one of the functions in Theorem 1: (iii).*

Proof: Let f and $\hat{f}$ be warping functions such that $B\times_f\mathbb{R}$ and $B\times_{\hat{f}}\mathbb{R}$ are locally conformally flat static space–times. Then id: $(B,(1/f^2)g_B)\to(B,(1/\hat{f}^2)g_B)$ is a conformal transformation between two compact spaces of constant sectional curvature. Proceeding as in case (iii) of the previous theorem, it follows that $\hat{f}/f$ is a solution of the linearized Möbius equation on $(B, (1/f^2)g_B)$

$$H_{\hat{f}/f}=\frac{1}{n}\Delta(\hat{f}/f)g$$

and thus $\nabla(\hat{f}/f)$ is a conformal vector field on $(B, (1/f^2)g_B)$. Then it follows from (5) that $\Delta(\Delta(\hat{f}/f)+[\mathrm{Sc}/(n-1)]\hat{f}/f)=0$ and thus $\Delta(\hat{f}/f)+[\mathrm{Sc}/(n-1)]\hat{f}/f$ is a constant function on $(B, (1/f^2)g_B)$.

Next, using the linearized Möbius equation, compute the Hessian of $\Delta(\hat{f}/f)$ to obtain

$$H_{\Delta(\hat{f}/f)}+\frac{\mathrm{Sc}}{n(n-1)}\Delta(\hat{f}/f)g=0. \tag{6}$$

Now, if $\mathrm{Sc}>0$, then (6) is Obata's equation for $\Delta(\hat{f}/f)$. Since $f\neq c\hat{f}$ and for some constant C, $\Delta(\hat{f}/f)=-[\mathrm{Sc}/(n-1)]\hat{f}/f+C$, then it follows that $\Delta(\hat{f}/f)$ is not constant and hence $(B,(1/f^2)g_B)$ is isometric to an Euclidean sphere.[19]

Finally note that $\mathrm{Sc}\leqslant 0$ leads to some contradiction as follows. Indeed, if $\mathrm{Sc}<0$, then the existence of a nonconstant solution $\Delta(\hat{f}/f)$ of (6) is characteristic of warped product structures $\mathbb{R}\times_\xi N$, where N is a complete Riemannian manifold and the warping function satisfies $\xi''+[\mathrm{Sc}/n(n-1)]\xi=0$, $\xi>0$ among complete Riemannian manifolds (Ref. 13, Theorems C, D). This is clearly a contradiction with the compactness of B. The case $\mathrm{Sc}=0$ implies $\Delta(\hat{f}/f)$ is constant and thus it follows from the linearized Möbius equation that $H_{\hat{f}/f}=(\sigma/n)g$ for some constant σ. This shows that $\hat{f}/f$ is a special concircular function on $(B, (1/f^2)g_B)$ and hence it follows from Ref. 23, Theorem 2 that $(B, (1/f^2)g_B)$ is isometric to the Euclidean space, which is also a contradiction. ■

Remark 14: The previous theorem shows the nonexistence of nonconstant globally defined warping functions on flat tori $\mathbb{T}^n$ which make the static space–time $\mathbb{T}^n\times_f\mathbb{R}$ locally conformally flat. However note that such warping functions always exist locally (cf. Remark 3).

The result of Theorem 13 can be extended to static space–times with noncompact base under some completeness assumptions as follows.

Theorem 15: *Let $M=B\times_f\mathbb{R}$ be a locally conformally flat static space–time with $(B, (1/f^2)g_B)$ geodesically complete. If there exists a warping function $\hat{f}\neq cf$ on B such that $B\times_{\hat{f}}\mathbb{R}$ is also locally conformally flat, then one of the following holds:*

(1) *$(B, (1/f^2)g_B)$ is a complete and simply connected space of constant sectional curvature and the warping functions $\hat{f}/f$ are given by Theorem 10, or otherwise.*
(2) *$(B, (1/f^2)g_B)$ is a warped product $\mathbb{R}\times_{\alpha\exp(\alpha t+\beta)}N$, where (N, g_N) is a complete flat Riemannian manifold and the warping functions satisfy*

$$\hat{f}/f=\exp(\alpha t+\beta)+\kappa$$

for some real constants $\alpha>0$, β, $\kappa\geqslant 0$, where $\alpha^2=-[\mathrm{Sc}/n(n-1)]$ and Sc *denotes the scalar curvature of $(B, (1/f^2)g_B)$.*

Proof: Let $f\neq c\hat{f}$ be two warping functions on B such that $B\times_{\hat{f}}\mathbb{R}$ and $B\times_f\mathbb{R}$ are locally conformally flat. Then, by Theorem 1 it follows that $(1/\hat{f}^2)g_B$ and $(1/f^2)g_B$ are constant sectional curvature metrics on B and thus the identity is a conformal diffeomorphism between two Einstein metrics on B. Since $(B, (1/f^2)g_B)$ is assumed to be complete and $\hat{f}\neq cf$, then either $(B, (1/f^2)g_B)$ is a complete and simply connected space of constant sectional curvature, and thus isometric to one of the model spaces in Theorem 10, or otherwise $(B, (1/f^2)g_B)$ is a warped product $\mathbb{R}\times_{\alpha\exp(\alpha t+\beta)}N$, where (N, g_N) is a complete Ricci flat $(n-1)$-dimensional Riemannian manifold and the warping functions satisfy $\hat{f}/f=\exp(\alpha t+\beta)+\kappa$, for some constants α, β, κ.[16] Next, by Corollary 2 it follows that $\mathbb{R}\times_{\alpha\exp(\alpha t+\beta)}N$ is locally conformally flat and thus (N, g_N) is of constant sectional curvature by Theorem 1, which shows that (N, g_N) is flat. Moreover, it follows after some standard calculations that the scalar curvature of $(B, (1/f^2)g_B)$ is $\mathrm{Sc}=-n(n-1)\alpha^2$, which proves the result. ■

V. COMPLETE LOCALLY CONFORMALLY FLAT RIEMANNIAN MANIFOLDS OF NONPOSITIVE CURVATURE

Recall here that the universal cover of a complete locally conformally flat Riemannian manifold with non-negative Ricci curvatures is conformally equivalent to $\mathbb{S}^n$, $\mathbb{R}^n$ or $\mathbb{R}\times\mathbb{S}^{n-1}$, where $\mathbb{S}^n$ and $\mathbb{S}^{n-1}$ are spheres of constant sectional curvature.[26] Henceforth we will pay special attention to the construction of complete locally conformally flat manifolds with nonpositive Ricci curvatures. Also note that warped products are a basic tool in constructing manifolds of nonpositive curvature, which are complete if and only if both factors are complete Riemannian manifolds.[5] For our purposes in this section, write the sectional curvature of a warped product $B\times_f F$ as follows:[5,18]

$$\begin{aligned} K_{XY}&=K^{\mathrm{B}}_{XY},\\ K_{XU}&=-\frac{H_f(X,X)}{f\|X\|^2},\\ K_{UV}&=\frac{1}{f^2}K^F_{UV}-\frac{\|\nabla f\|^2}{f^2}, \end{aligned} \tag{7}$$

where K^B and K^F denote the sectional curvatures on the base B and the fiber F, respectively.

Observe that all the results in the preceding section remain true in the Riemannian setting, since the base of a static space–time has induced positive definite metric, and the fiber plays only a very limited role in the construction of locally conformally flat warped products (cf. Theorem 1).

Let $M=B\times_f F$ be a locally conformally flat Riemannian warped product with base B a model space $\mathbb{R}^s$, $\mathbb{S}^s$ or $\mathbb{H}^s$. If M is assumed to be complete, we have the following consequences of previous results:

(i) If $B \equiv \mathbb{R}^s$, then $\mathbb{R}^s \times_f F$ is of nonpositive sectional curvature for any warping function f as in Theorem 10.

(ii) If $B \equiv \mathbb{S}^s$, then no locally conformally flat warped product $\mathbb{S}^s \times_f F$ may be of nonpositive sectional curvature. Indeed, no locally conformally flat warped product with compact base may have nonpositive sectional curvature, unless it is a direct product since it follows from (7) that the warping function of a warped product $B \times_f F$ of nonpositive sectional curvature satisfies $H_f \geqslant 0$, and thus $\Delta f \geqslant 0$. Now, since B is compact without boundary and $\dim B \geqslant 2$, it follows that $\Delta f = 0$, and thus f is constant.

(iii) If $B \equiv \mathbb{H}^s$, then the necessary and sufficient condition for a locally conformally flat warped product $\mathbb{H}^s \times_f F$ to be of nonpositive sectional curvature is given in terms of the warping function $f(\vec{\mathbf{x}}) = (a\|\vec{\mathbf{x}}\|^2 + \langle \vec{\mathbf{b}}, \vec{\mathbf{x}} \rangle + c)/x_s$ by $f \geqslant 2b_s$, whenever $\dim F \geqslant 2$.

We finish with some simple examples which illustrate the previous situation.

(a) Let M be the product manifold $M = \mathbb{H}^2 \times \mathbb{H}^2$ equipped with the warped metric defined by the warping function

$$f(\vec{\mathbf{x}}) = \frac{\frac{1}{2}\|\vec{\mathbf{x}}\|^2 + x_2 + 1}{x_2}.$$

(b) Let M be the product manifold $M = \mathbb{H}^2 \times \mathbb{R}^2$ equipped with the warped metric defined by the warping function

$$f(\vec{\mathbf{x}}) = \frac{\frac{1}{4}\|\vec{\mathbf{x}}\|^2 + x_1 + 1}{x_2}.$$

After some straightforward calculations we get that the sectional curvature is nonpositive in any of these particular examples.

Next, note that simplest examples of complete locally conformally flat Riemannian manifolds with nonpositive Ricci curvature are warped products as follows:

(1) $\mathbb{H}^2 \times_f \mathbb{H}^2$ with warping function

$$f(\vec{\mathbf{x}}) = \frac{\frac{3}{2}\|\vec{\mathbf{x}}\|^2 + x_1 + 4x_2 + 3}{x_2}.$$

(2) $\mathbb{H}^2 \times_f \mathbb{S}^2$ with warping function

$$f(\vec{\mathbf{x}}) = \frac{\|\vec{\mathbf{x}}\|^2 + 3x_2 + 2}{x_2}.$$

A long but straightforward calculation shows that the Ricci curvatures are nonpositive in previous examples. Moreover, note that the sectional curvature of $\mathbb{H}^2 \times_f \mathbb{S}^2$ has no sign.

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Topological quantization of gravitational fields

Leonardo Patiño[a)]
Department of Mathematical Sciences, University of Durham, Durham DH1 3LE, United Kingdom

Hernando Quevedo[b)]
Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, A.P. 70-543, México D.F. 04510, Mexico, and Department of Physics, University of California, Davis, California 95616

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We introduce the method of topological quantization for gravitational fields in a systematic manner. First we show that any vacuum solution of Einstein's equations can be represented in a principal fiber bundle with a connection that takes values in the Lie algebra of the Lorentz group. This result is generalized to include the case of gauge matter fields in multiple principal fiber bundles. We present several examples of gravitational configurations that include a gravitomagnetic monopole in linearized gravity, the C-energy of cylindrically symmetric fields, the Reissner–Nordström and the Kerr–Newman black holes. As a result of the application of the topological quantization procedure, in all the analyzed examples we obtain conditions implying that the parameters entering the metric in each case satisfy certain discretization relationships. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Dirac's original idea[1] of determining the phase acquired by a charge when moving along a closed path in the field of a magnetic monopole gave as a result that the product of the electric charge times the monopole charge is an integer. Today, this result is known as Dirac's quantization of the electric charge. In a previous work,[2] we introduced a phaselike object which depends on the field strength so that it can be used to investigate any field theory based on a connection. In the special case of the Levi–Cività connection, the field strength is given by the Riemann tensor and the phaselike object can formally be used to investigate the properties of gravitational configurations that satisfy Einstein's equations. Using only the symmetry properties of the Riemann tensor and assuming a quite general symmetry property for the gravitational field, we have shown that this phaselike object for vacuum gravitational configurations behaves under rotations either as a bosonic or a fermionic phase. It was also shown that a certain combination of the eigenvalues of the Riemann tensor can become "quantized" in a fashion similar to that obtained from Dirac's quantization procedure in the system composed of an electric charge and a magnetic monopole.

From the geometric point of view,[3] Dirac's quantization is interpreted as a consequence of the existence of a nontrivial principal fiber bundle of U(1) over the sphere S^2, with a u(1) connection, for the system composed of an electric charge q and a magnetic monopole with magnetic charge g. The Chern numbers associated with this nontrivial fiber bundle turn out to be given as the product qg which, therefore, becomes quantized.

In this work, we introduce the method of topological quantization which can be applied to any field configuration whose geometrical structure allows the existence of a principal fiber bundle. We show that any solution of Einstein's equations minimally coupled to any gauge matter field can

[a)]Electronic mail: e.l.patino-jaidar@durham.ac.uk
[b)]Electronic mail: quevedo@physics.ucdavis.edu

be represented geometrically as a principal fiber bundle with space–time as the base space. The structure group (isomorphic to the standard fiber) follows from the invariance of the orthonormal frame with respect to Lorentz transformations, in the case of a vacuum solution, or with respect to a transformation of the gauge group, in the case of a gauge matter field. If the bundle turns out to be (globally) nontrivial, the conditions under which this construction becomes well defined in all the points where the field configuration exists, manifest themselves in the transition functions between different but intersecting open subsets of the base manifold of the bundle. These conditions on the transition functions turn out to depend on the parameters which determine the physical structure of the field configuration. Consequently, the conditions that arise in the construction of a fiber bundle lead to conditions on the physical parameters which, in turn, implies that a particular combination of those parameters can take only *discrete* values. This discretization can be derived also from the topological invariants of the corresponding nontrivial fiber bundle. This is what we call the *quantization conditions* for a given field configuration. Furthermore, we will see that even in the case of a globally trivial principal fiber bundle certain quantization conditions may appear as a result of demanding regularity of the connection.

In Sec. II, we introduce the method of topological quantization in a systematic manner and briefly discuss the general cases in which nontrivial quantization conditions may appear. In Sec. III we analyze the so(1,3) connection of cylindrically symmetric gravitational fields and show that the corresponding C-energy can take only discrete values. In Sec. IV we present the example of a gravitomagnetic monopole in linearized Einstein's theory which can be investigated by means of a u(1) connection. Section V contains the topological quantization with respect to the electromagnetic connection of gravitational fields which represent electrovacuum black holes. Section VI is devoted to discussions and remarks about future investigations.

II. THE METHOD OF TOPOLOGICAL QUANTIZATION

Consider a Riemannian manifold (M,g), where M is a four-dimensional differential manifold and g is a bilinear form, the metric, on M. For the purpose of analyzing field equations we choose in M a set of local orthonormal 1-forms e^a, $a=0,1,2,3$. The orthonormality condition can be expressed in terms of the local Minkowski metric as $g(e^a,e^b)=\eta^{ab}$, where $\eta^{ab}=\mathrm{diag}(+,-,-,-)$. On a torsion free manifold we can introduce a connection 1-form ω by means of the Cartan first structure equation

$$De^a := de^a + \omega^a{}_b \wedge e^b = 0, \tag{1}$$

where d is the exterior derivative and D the covariant exterior derivative. We demand that ω be a metric connection, i.e., locally $D\eta_{ab}=d\eta_{ab}+\omega_{ab}+\omega_{ba}=0$, a condition which implies the antisymmetry of the connection components. Furthermore, we use the Cartan second structure equation to introduce the curvature 2-form Ω as

$$D\omega^a{}_b := \Omega^a{}_b = d\omega^a{}_b + \omega^a{}_c \wedge \omega^c{}_b, \tag{2}$$

whose components in terms of the local orthonormal frame, $\Omega^a{}_b=(1/2)R^a{}_{bcd}e^c\wedge e^d$, determine the Riemann curvature tensor $R^a{}_{bcd}$. Einstein's gravity theory follows from the variation, with respect to the orthonormal frame e^a of the action

$$S = -\frac{1}{32\pi G}\int_M \Omega^{ab}\wedge e^c \wedge e^d \epsilon_{abcd} + \int_M \mathcal{L}_m, \tag{3}$$

where $\epsilon_{0123}=1$ and $\mathcal{L}_m$ is the matter Lagrangian which depends on e, ω, and the matter fields. The field equations are $\Omega^{ab}\wedge e^c\epsilon_{abcd}=-16\pi G T_c$, where T_c is the energy-momentum 3-form which follows from the variation of the matter action.

The advantage of using a local orthonormal frame e is that the gauge character (at the level of the connection and curvature) of Einstein's theory becomes more plausible (see, for instance, Refs. 3 and 4 for a more detailed discussion). Indeed, the diffeomorphism invariance of the theory is

now reduced to the invariance with respect to the Lorentz group SO(1,3). The change to a different frame $e' = \Lambda e$ is represented by means of a matrix $\Lambda \in \mathrm{SO}(1,3)$. The connection 1-form and the curvature 2-form take values in the corresponding Lorentz algebra so(1,3), and under a change of frame they transform as

$$\omega' = \Lambda \omega \Lambda^{-1} + \Lambda \, \mathrm{d}\Lambda^{-1}, \quad \Omega' = \Lambda \Omega \Lambda^{-1}, \tag{4}$$

respectively. It is in this sense that Einstein's theory can be considered as a gauge theory with respect to the Lorentz group. However, it is at the level of the action that Einstein's theory tremendously differs from pure Yang–Mills gauge theories.

Let us now consider the matter action. As we have mentioned before the matter Lagrangian can depend on the frame e, the connection ω, and the matter fields. We will assume that the matter fields are gauge fields, that is, there exists a connection 1-form A, with values in the Lie algebra of a Lie group G, which generates the gauge field strength F in the standard manner, $F = \mathrm{d}A + A \wedge A$. Under a gauge transformation $\gamma \in G$, these quantities behave as (we assume that the gauge group is a matrix group)

$$A \to A' = \gamma A \gamma^{-1} + \gamma \, \mathrm{d}\gamma^{-1}, \quad F \to F' = \gamma F \gamma^{-1}. \tag{5}$$

A vacuum space–time in general relativity is a solution of Einstein's vacuum equations, represented by an orthonormal frame e. Since we assume that the compatibility condition between the local metric and the connection is satisfied, we can use the connection ω, instead of the orthonormal frame. Moreover, if we adopt the Palatini approach, the connection ω can be considered as the "primary" variable, whereas the orthonormal frame e can be derived from the metricity condition. In the presence of a matter field, one needs additionally the "matter" connection A which satisfies Einstein's equations, with the corresponding energy-momentum 3-form, and the matter field equations that follow from the variation of the matter action with respect to the connection A. For a particular space–time to be well defined we must guarantee that ω and A are well defined everywhere in M. This is a nontrivial remark for the analysis of gravitational fields we want to perform. Indeed, the fact that the connection is demanded to be well defined everywhere in M implies in general certain conditions that we will investigate for explicit fields and which are the fundamental of what we will call topological quantization.

Let us be more specific. The idea behind the introduction of a differentiable manifold as the underlying geometric structure of space–time is that in this way one can guarantee the existence of coordinate sets which cover the entire manifold. For the approach we are using here, this is equivalent to having a finite number of sets of orthonormal frames covering the manifold. Let $\{U_\alpha\}$ be an open covering of M, i.e., $\cup_\alpha U_\alpha = M$. By definition, a differential manifold of dimension n is equipped with an atlas (U_α, ϕ_α), where ϕ_α is a homeomorphism from U_α onto an open subset of the Euclidean space $\mathbf{R}^n$. If we consider two arbitrary open subsets $U_i, U_j \in \{U_\alpha\}$ such that $U_i \cap U_j \neq \emptyset$, then in the intersection region the map $\phi_i \circ \phi_j^{-1}$ is a C^∞ homeomorphism of (open subsets of) $\mathbf{R}^n$. Let $\tilde{\phi}_i$ be the map from U_i into the vector space of 1-forms $\Lambda^1(U_i, \mathrm{so}(1,3))$ that allows us to introduce the orthonormal frame e_i in U_i. Notice that the index i labels different sets of orthonormal frames and does not refer to any specific component of the frame. The orthonormal frame e_j attached to U_j by means of $\tilde{\phi}_j$, is related to e_i through an SO(1,3) matrix, $e_i = \Lambda_{ij} e_j$. It is clear that in the intersection region the compatibility condition $\tilde{\phi}_i \circ \tilde{\phi}_j^{-1} = \Lambda_{ij}$ must be satisfied. On U_i we can also introduce a spin connection 1-form ω_i and a curvature 2-form Ω_i, according to Eqs. (1) and (2), respectively. These are related to the connection and curvature in U_j by means of (no summation over repeated indices)

$$\omega_i = \Lambda_{ij} \omega_j \Lambda_{ij}^{-1} + \Lambda_{ij} \, \mathrm{d}\Lambda_{ij}^{-1}, \quad \Omega_i = \Lambda_{ij} \Omega_j \Lambda_{ij}^{-1}. \tag{6}$$

Consider now a third open subset $U_k \in \{U_\alpha\}$ such that $U_i \cap U_j \cap U_k \neq \emptyset$. Accordingly, in the intersection region we have that $\tilde{\phi}_i \circ \tilde{\phi}_k^{-1} = \Lambda_{ik}$ and $\tilde{\phi}_j \circ \tilde{\phi}_k^{-1} = \Lambda_{jk}$. Then, it follows that

$$\Lambda_{ij}\Lambda_{jk} = \Lambda_{ik}. \tag{7}$$

This allows us to formulate the following.

Theorem 1: A solution of Einstein's vacuum field equations can be represented by a unique 10-dimensional principal fiber bundle P with the space–time M as the base space, the Lorentz group as the structure group (isomorphic to the standard fiber) and a connection with values in the Lie algebra of the Lorentz group.

Proof: A standard theorem (the reconstruction theorem) in differential geometry[5,6] states that a fiber bundle is uniquely specified by the base space, the standard fiber, a structure group which is effectively represented on the fiber and a family of transition functions, with values in the structure group, satisfying the cocycle condition. In the case of a principal fiber bundle P, the fiber is isomorphic to the structure group which is naturally represented on itself by left translations. For a solution of the vacuum field equations, given by an orthonormal frame e, we can take the space–time manifold M described above as the base space. The structure group is identified as SO(1,3). The transition functions are given by the elements $\Lambda_{ij}: U_i \cap U_j \to \mathrm{SO}(1,3)$ and satisfy the cocycle condition which is given above in Eq. (7). Finally, one can show that it is possible to construct the projection $\pi: P \to M$[6], once the transition functions are given. This shows that all the elements of a principle fiber bundle exist and they can be "glued" together to form the desired bundle by means of the transition functions and the projection π.

Finally, we must show that there exists a connection $\boldsymbol{\omega}$ in P. By construction, we do have a connection 1-form ω on M, which is the connection associated with the vacuum solution. We will see that it determines a unique connection in P. To this end, we use the following theorem[4] valid for principal fiber bundles.

Theorem 2: Given an open covering $\{U_\alpha\}$ of M, a structure Lie group G with Lie algebra $\mathbf{g}$, a family of local $\mathbf{g}$-valued 1-forms $\omega_i \in \Lambda^1(U_i, \mathbf{g})$ which fulfill the compatibility condition

$$\omega_i = g_{ji}^{-1}\omega_j g_{ji} + g_{ji}^{-1}\, \mathrm{d}g_{ji}, \tag{8}$$

where $g_{ji}: U_i \cap U_j \to G$ are elements of G, and a set of local sections $\sigma_i: U_i \to \pi^{-1}(U_i)$ satisfying $\sigma_j = \sigma_i g_{ij}$ on $U_i \cap U_j$, then there is a unique connection $\boldsymbol{\omega}$ on P such that $\omega_i = \sigma_i^* \boldsymbol{\omega}$, where σ_i^* is the pull-back induced by σ_i.

In the case we are considering, the structure group is SO(1,3), the family of 1-forms ω_i is determined by the connection ω defined on each $U_i \in \{U_\alpha\}$. The compatibility condition (8) coincides with the transformation property (6), once g_{ji}^{-1} is identified with Λ_{ij}. It remains to show the existence of local sections. Since any fiber bundle accepts a local trivialization which can be defined as $\Psi_i: \pi^{-1}(U_i) \to U_i \times G$, we can introduce a local canonical section on U_i by transferring back to $\pi^{-1}(U_i)$ the section of $U_i \times G$, i.e., by defining $\sigma_i: U_i \to \pi^{-1}(U_i)$ by $\sigma(x) = \Psi_i^{-1}(x, e)$, where $x \in U_i$ and $e = g_{ii}(x)$ is the identity element of G. It is then possible to show[6] that this canonical section satisfies $\sigma_j = \sigma_i g_{ij}$ as required. Thus, according to Theorem 2, there exists a unique connection $\boldsymbol{\omega}$ on P. This ends the proof of Theorem 1.

We have shown that a vacuum solution can naturally be represented as a principal fiber bundle. In all steps of the proof, the local connection ω_i plays an important role and we have assumed that it satisfies the continuity and differentiability conditions on U_i. The question arises whether this assumption can be realized in concrete examples of gravitational configurations. This is exactly the question that we want to address in this work by constructing explicitly the elements of the principal fiber bundles that correspond to given solutions of Einstein's equations. This is what we call the method of "topological quantization." This concept has been used before in the context of diverse monopole configurations.[7] We will see that in the process of constructing a suitable covering $\{U_\alpha\}$ of M, certain "quantization" conditions appear that imply restrictions on the parameters entering the components of the connection.

If it turns out that the constructed principal fiber bundle admits a global section, the bundle is globally trivial and a single connection can be defined everywhere on P. This could happen, for instance, when the base space (space–time manifold) is contractible. We will see that even in this simple case nontrivial conditions arise from the requirement that the connection is regular on all

points of the base space. More general cases can be obtained from noncontractible manifolds which are very common in general relativity. Explicit solutions of Einstein's equations are usually characterized by the existence of singularities, i.e., regions that cannot be described within the formalism of general relativity. In order to properly describe the space–time manifold we need to "remove" those singular regions from the manifold. This procedure can be used to obtain noncontractible base spaces for which we can expect that nontrivial conditions arise from the application of the method of topological quantization. In fact, noncontractible base spaces can give rise to globally nontrivial principal fiber bundles. In this case one needs more than one open subset to cover the base space and, consequently, transition functions appear that turn out to generate nontrivial "quantization" conditions.

Thus, topological quantization is closely related to the problem of determining whether a principal fiber bundle is globally trivial or not. This is a task that involves the relation between the global topological structure of the base space and the fiber, an issue that is used to perform the classification of bundles and is related to the theory of characteristic classes and topological invariants. Consequently, the method of topological quantization is closely related to the study of the topological structure of the underlying bundle.

From the discussion above it follows that one has (at least) two ways to perform the topological quantization of a given solution of Einstein's equations. The first one consists in using Theorem 1 to construct the corresponding principal fiber bundle P and the connection $\boldsymbol{\omega}$. Then, one can analyze the topological invariants of the bundle. The second method consists in constructing explicitly the covering $\{U_\alpha\}$ of M and the family of connection 1-forms $\{\omega_\alpha\}$ on M for the given solution and extracting from there the quantization conditions. Obviously, both methods must yield the same results. When analyzing explicit examples, however, it is not always easy to construct the unknown principal fiber bundle, whereas the second method is straightforward because we know the connection ω explicitly. For this reason, in this work we will apply mainly the second approach for explicit calculations.

All of the above discussion involves only the so(1,3) connection associated to the gravitational action. If an additional matter action is considered, the results can be formulated in the following form.

Theorem 3: A solution of Einstein's field equations coupled to a matter gauge field can be represented by a unique principal fiber bundle with the space–time M as the base space, the gauge group as the structure group (isomorphic to the standard fiber) and a connection with values in the Lie algebra of the gauge group.

The proof of this theorem is similar to that of Theorem 1. Indeed, for each open subset $U_i \in \{U_\alpha\}$ we can calculate the corresponding gauge connection A_i with values in the Lie algebra of G. The proof can then be carried out in a similar manner with ω_i replaced by A_i, Λ_{ij} replaced by $\gamma_{ij} \in G$, and $g_{ji}^{-1} = \gamma_{ij}$. Consequently, in the case of additional matter gauge fields we can construct on M a principal fiber bundle for each additional gauge connection. So we are lead to the concept of "multiple" principal fiber bundles that can be constructed on the same base space M. Since the method of topological quantization can be applied to each bundle separately, one could expect different sets of quantization conditions from each bundle. The compatibility of these sets is an issue that can be treated at the level of explicit gravitational configurations.

In the following sections we will apply Theorems 1 and 3 to different gravitational configurations.

III. CYLINDRICALLY SYMMETRIC GRAVITATIONAL FIELDS

Cylindrically symmetric vacuum gravitational configurations can be described by means of the Einstein–Rosen line element which in an orthormal frame can be written as[8]

$$e^0 = \exp(\gamma - \psi)\mathrm{d}t, \quad e^1 = \exp(\gamma - \psi)\mathrm{d}\rho, \quad e^2 = \exp(\psi)\mathrm{d}z, \quad e^3 = \rho \exp(-\psi)\mathrm{d}\varphi, \tag{9}$$

where t, ρ, z, and φ are cylindrical coordinates and the functions ψ and γ depend on t and ρ only. For the sake of simplicity, here we restrict ourselves to the case in which the Killing vector fields

∂_z and ∂_φ are hypersurface orthogonal. The corresponding vacuum field equations can be reduced to a second-order differential equation for the function ψ,

$$\psi'' + \frac{1}{\rho}\psi' - \ddot{\psi} = 0, \tag{10}$$

and two first-order differential equations for γ,

$$\gamma' = \rho(\dot{\psi}^2 + \psi'^2), \quad \dot{\gamma} = 2\rho\dot{\psi}\psi', \tag{11}$$

where $\dot{\psi} = \partial\psi/\partial t$, $\psi' = \partial\psi/\partial\rho$, etc. The orthonormal frame (9) is defined up to an arbitrary transformation of the Lie group SO(1,3). If we envision the space–time as the four-dimensional base manifold and attach a copy of SO(1,3) at each point of the base manifold, we obtain the 10-dimensional principal fiber bundle considered in Theorem 1. Using the first structure equation (1) it is straightforward to calculate the components of the connection 1-form $\omega^a{}_b$ which can be decomposed as $\omega^a{}_b = \omega^a{}_{b\mu}\, dx^\mu$. It is in this decomposition that the endomorphic character of the connection [a 1-form with values in the Lie algebra so(1,3)] becomes plausible.[9] From Eq. (9) we obtain

$$\omega^0{}_{1t} = \gamma' - \psi', \quad \omega^0{}_{1\rho} = \dot{\gamma} - \dot{\psi},$$

$$\omega^0{}_{2z} = \dot{\psi}\exp(2\psi - \gamma), \quad \omega^1{}_{2z} = -\psi'\exp(2\psi - \gamma), \tag{12}$$

$$\omega^0{}_{3\varphi} = -\rho\dot{\psi}\exp(-\gamma), \quad \omega^1{}_{3\varphi} = -(1 - \rho\psi')\exp(-\gamma).$$

As described in the last section, we must demand the regularity of this connection as a condition for constructing the corresponding principal fiber bundle. It is well known[8] that solutions to the field equations can be generated which are everywhere regular with the symmetry axis ($\rho = 0$) as the only possible hypersurface where curvature singularities may appear. Let us suppose that the symmetry axis is free of curvature singularities. Then, there must exist an atlas where the connection is also regular. The field equations (11) imply that at the axis $\dot{\gamma}(\rho \to 0) = \dot{\gamma}_0 = 0$ and $\gamma'(\rho \to 0) = \gamma'_0 = 0$, if $\dot{\psi}(\rho \to 0) = \dot{\psi}_0$ and $\psi'(\rho \to 0) = \psi'_0$ do not diverge. On the other hand, Eq. (10) implies that near the axis $\psi' \propto \rho^\alpha$ with $\alpha > 1$, i.e., $\psi'_0 = 0$, and, consequently, $\ddot{\psi}(\rho \to 0) \propto \rho^{\alpha-1}$. Then, $\dot{\psi}_0$ is at most a constant that can be set equal to zero by means of a coordinate transformation. Thus we have that the regularity condition at the axis implies that $\dot{\gamma}_0 = \gamma'_0 = \dot{\psi}_0 = \psi'_0 = 0$. The same result can be obtained by analyzing the behavior of the curvature Kretschman scalar near the axis. Hence, from Eq. (13) it follows that at the axis $\omega^a{}_b|_{\rho=0} = \omega^a{}_{b\varphi}|_{\rho=0}\, d\varphi$ with

$$\omega^a{}_{b\varphi}|_{\rho=0} = \exp(-\gamma_0)T_\varphi, \tag{13}$$

where T_φ is one of the generators of the Lie algebra so(1,3),

$$T_\varphi = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{14}$$

If we demand that $\exp(-\gamma_0)$ does not diverge, the components $\omega^a{}_{b\varphi}|_{\rho=0}$ are regular, but we still have a singularity in the 1-form $d\varphi = (\exp(\psi)/\rho)e^0$. Therefore, the only possibility to get rid of this singularity is to find a gauge transformation such that the new components $\omega'^a{}_{b\varphi}|_{\rho=0}$ vanish identically on the axis. To this end, let us consider the SO(1,3) transformation

$$\Lambda = \exp(\tilde{\varphi} T_{\varphi}), \quad \tilde{\varphi} = \exp(-\gamma_0)\varphi. \tag{15}$$

From Eq. (4) we have that the gauge-transformed 1-form connection is given by

$$\omega' = \exp(\tilde{\varphi} T_{\varphi})\omega \exp(-\tilde{\varphi} T_{\varphi}) - \exp(-\gamma_0) T_{\varphi}\, \mathrm{d}\varphi, \tag{16}$$

where

$$\exp(\pm \tilde{\varphi} T_{\varphi}) = 1_{4\times 4} \pm \sin \tilde{\varphi} T_{\varphi} + (1 - \cos \tilde{\varphi}) T_{\varphi}^2, \tag{17}$$

where $1_{4\times4}$ is the 4×4 unit matrix. The explicit calculation of the components can be carried out in a straightforward manner and leads to

$$\omega'^{0}{}_{1t} = (\gamma' - \psi')\cos \tilde{\varphi}, \quad \omega'^{0}{}_{3t} = (\gamma' - \psi')\sin \tilde{\varphi},$$

$$\omega'^{0}{}_{1\rho} = (\dot{\gamma} - \dot{\psi})\cos \tilde{\varphi}, \quad \omega'^{0}{}_{3\rho} = (\dot{\gamma} - \dot{\psi})\sin \tilde{\varphi},$$

$$\omega'^{0}{}_{2z} = \dot{\psi} \exp(2\psi - \gamma), \quad \omega'^{1}{}_{2z} = -\psi' \exp(2\psi - \gamma)\cos \tilde{\varphi}, \tag{18}$$

$$\omega'^{2}{}_{3z} = \psi' \exp(2\psi - \gamma)\sin \tilde{\varphi}, \quad \omega'^{0}{}_{1\varphi} = \rho\dot{\psi} \exp(-\gamma)\sin \tilde{\varphi},$$

$$\omega'^{0}{}_{3\varphi} = -\rho\dot{\psi} \exp(-\gamma)\cos \tilde{\varphi}, \quad \omega'^{1}{}_{3\varphi} = \exp(-\gamma_0)[1 - (1 - \rho\psi')\exp(\gamma_0 - \gamma)].$$

From the last expression it can easily be seen that the gauge-transformed connection vanishes identically on the symmetry axis and no new singularities appear. This has been achieved by means of the gauge transformation (15) which is single-valued only if $\exp(-\gamma_0) = n$, where n is an integer. This, in turn, implies that the gauge-transformed connection is single valued. Consequently, the condition $\exp(-\gamma_0) = n$ needs to be satisfied for the connection to be well defined. This is an interesting result that can be interpreted as a "quantization" of the energy of cylindrically symmetric gravitational fields. Indeed, the concept of C-energy was introduced by Thorne[10] for gravitational fields described by the Einstein–Rosen line element (9). The quantity $E_c = \gamma_0$ has been shown to represent the (normalized) C-energy density per length unit along the symmetry axis at a given time. In terms of the "quantization" derived above this means that $E_c = -\ln n$, i.e., the C-energy is a discrete quantity. The fact that it is a negative quantity is interpreted by Thorne as an indication of its "nonclassical" origin. A second expression that can be considered as a (normalized) C-energy density has been introduced by Thorne as $E_c = 1 - \exp(-2\gamma_0)$. In this case, the quantization condition leads to $E_c = 1 - n^2$, an expression that again indicates the discrete character of the C-energy.

We have shown that it is possible to define just one single connection 1-form on the entire Einstein–Rosen space–time. This means that the base manifold of the principal fiber bundle can be covered by a single open set U and, therefore, can be considered as $\mathbf{R}^4$ which is a contractible manifold. This implies that the corresponding 10-dimensional principal fiber bundle is globally trivial. This is so because we have demanded that the gravitational field be regular at all points of space–time, including the symmetry axis. If, instead, we would allow singularities on the axis, it would be necessary to "remove" the axis from the base manifold. This would open the possibility of obtaining a nontrivial bundle, an issue that would require an analysis different from the one presented in this section.

IV. THE WEAK GRAVITATIONAL FIELD

Consider the following line element in spherical coordinates t, r, θ, φ:

$$ds^2 = (1-2\phi)dt^2 - 2\chi\, dt\, d\varphi - (1+2\phi)[dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)], \tag{19}$$

where ϕ and χ are functions of the spatial coordinates. We assume that $\phi \ll 1$ and $\chi \ll 1$ and consider the weak field limit of Einstein's equations in vacuum. An orthonormal frame appropriate for the line element (19) can be written as

$$e^0 = (1-\phi)dt + \chi\, d\varphi, \quad e^1 = (1+\phi)dr, \quad e^2 = (1+\phi)d\theta, \quad e^3 = (1+\phi)r\sin\theta, \tag{20}$$

where we have neglected all the second order perturbations in ψ and χ.

It is well known[11] that the weak field equations in the Lorentz gauge can be expressed as the Maxwell equations $\tilde{A}_{\mu,\nu}{}^{\nu} = 0$ for the Maxwell potential

$$\tilde{A}_\mu = -\tfrac{1}{4}(4\phi, \chi), \tag{21}$$

which is invariant with respect to the transformation $\tilde{A} \to \tilde{A}' = \tilde{A} + df(x^\mu)$, where $f(x^\mu)$ is an arbitrary smooth function. This indicates that the weak field approximation can be interpreted as U(1)-gauge theory. To see this explicitly, we introduce the u(1) connection 1-form $A = -i\tilde{A}$. Then, the transformation law (5) is identically satisfied for the U(1)-gauge transformation $\gamma = \exp(if(x^\mu))$.

From the Maxwell equations for this case we see that the functions ϕ and χ are decoupled. Let us consider the following special solution:

$$A = i\left[\phi\, dt + \frac{g}{2}(1+\cos\theta)d\varphi\right], \tag{22}$$

where ϕ satisfies the differential equation $\phi_{,j}{}^{j} = 0$ $(j = 1,2,3)$, and g is a constant. This is the connection defined on the base manifold. To investigate the singularities of the connection (22), it is convenient to represent it in the orthonormal frame (20). Neglecting all the second order perturbations we obtain

$$A_1 = i\left[\phi e^0 + \frac{g}{2}\frac{(1+\cos\theta)}{r\sin\theta}e^3\right], \tag{23}$$

where we have introduced the subscript "1" to identify it as the connection on the open subset U_1 that will be determined below. We can see that there is a first singularity at $r = 0$ which, however, is a true curvature singularity as can be seen by analyzing the corresponding curvature. A second singularity is situated at $\theta = 0$ which does not appear at the level of the curvature. We "eliminate" the true curvature singularity by removing the origin $r = 0$ from the space–time. Hence, the base manifold M^4 becomes $M^4 = \mathbf{R}^4 - \{\text{world line of 0}\}$. The second singularity at $\theta = 0$, which corresponds to the positive sector, z_+, of the axis z, implies that the connection A_1 is regular on $U_1 = M^4 - \{z_+\}$. This apparent singularity can be eliminated by means of the gauge transformation $\gamma = \exp(ig\varphi)$ which leads to the new connection (up to first order in the perturbation)

$$A_2 = i\left[\phi e^0 + \frac{g}{2}\frac{(-1+\cos\theta)}{r\sin\theta}e^3\right]. \tag{24}$$

In fact, the singularity at $\theta = 0$ has been removed, but a new singularity has appeared at $\theta = \pi$. Consequently, the connection A_2 is regular only in the open subset $U_2 = M^4 - \{z_-\}$, where $\{z_-\}$ denotes the negative z axis.

The subsets U_1 and U_2 define a covering of the base manifold. In the intersection region $U_1 \cap U_2$ the two connections are related by means of the transition function $g_{12} = \exp(ig\varphi)$ which is single valued only if $g = n$, where n is an integer. To interpret this result we must find out the physical significance of the parameter g. This can be done, for instance, by calculating the multipole moments of this solution.[12] To do this, it is necessary to specify the function ϕ and we chose the simple solution $\phi = m/r$, where m is a constant. Then, it can be shown that the parameter m

represents the monopole moment of a mass distribution and gm corresponds to the monopole moment of an angular momentum distribution. This implies that g represents the gravitomagnetic monopole per mass unit which, according to the quantization condition obtained above, can take only discrete values.

This example reminds us of the case of a magnetic monopole in electrodynamics. Indeed, we have chosen the function χ in the connection (22) as the Maxwell potential for Dirac's magnetic monopole. The rest of the analysis is then carried out in a similar way as in standard electrodynamics, due to the analogy between the field equations for the weak field approximation and the Maxwell equations. The result obtained here by analyzing the behavior of the u(1) connection can be reproduced in terms of the topological invariants. The corresponding principal fiber bundle is a five-dimensional U(1) bundle for which the Chern invariants can be calculated. The result is again that the constant g becomes quantized.

V. THE REISSNER–NORDSTROM BLACK HOLE

Let us consider the following orthonormal frame for the Reissner–Nordstrom metric:

$$e^0 = \frac{[(r-r_-)(r-r_+)]^{1/2}}{r}\mathrm{d}t, \quad e^1 = \frac{r}{[(r-r_-)(r-r_+)]^{1/2}}\mathrm{d}r, \quad e^2 = r\,\mathrm{d}\theta, \quad e^3 = r\sin\theta\,\mathrm{d}\varphi, \tag{25}$$

with

$$r_\pm = m \pm \sqrt{m^2 - e^2}, \tag{26}$$

where m is the mass, e is the net electric charge of the source, and the radial values $r_\pm$ correspond to the horizons of the Reissner–Nordstrom black hole. This is a solution of the Einstein–Maxwell equations with the potential $\tilde{A}=-(e/r)\mathrm{d}t$. The corresponding u(1) connection $A=-i\tilde{A}$ behaves under a gauge transformation as in Eq. (5). According to the discussion of Sec. II and Theorem 3, there exists a principal fiber bundle which can be constructed by attaching at each point of the space–time the fiber U(1).

In this section we will explore the conditions that must be satisfied on the base manifold for constructing that bundle. To investigate the critical points of the connection 1-form we represent it in the orthonormal frame (25). Then

$$A = ie[(r-r_-)(r-r_+)]^{-1/2}e^0. \tag{27}$$

This connection diverges at $r=r_-$ and $r=r_+$, whereas the corresponding field strength is regular at those hypersurfaces. To remove these singularities, we first apply the gauge transformation $\gamma_1 = \exp(iet/r_-)$ on (27) and obtain

$$A_1 = -i\frac{e}{r_-}\left(\frac{r-r_-}{r-r_+}\right)^{1/2}e^0, \tag{28}$$

a u(1) connection which is regular at $r=r_-$, but diverges at $r=r_+$. On the other hand, we can also apply the transformation $\gamma_2=\exp(iet/r_+)$ on (27). The resulting connection

$$A_2 = -i\frac{e}{r_+}\left(\frac{r-r_+}{r-r_-}\right)^{1/2}e^0 \tag{29}$$

is regular at $r=r_+$, but diverges at $r=r_-$. Thus, we have obtained two different connections with different divergences. Let us choose the open subsets $U_1=(0,r_+)$ and $U_2=(r_-,\infty)$. This set of open subsets covers the radial coordinate r completely so that the subsets $U_1\times\mathbf{R}^3$ and $U_2\times\mathbf{R}^3$ are a covering of the base manifold M^4. Then, the connections A_1 and A_2 are well defined on U_1 and U_2, respectively. In the intersection region $U_1\cap U_2=(r_-,r_+)$, the connections A_1 and A_2 must be related by means of the transition function $g_{12}\in\mathrm{U}(1)$ which can easily be calculated as

$$g_{12} = \exp\left[ie\left(\frac{1}{r_-} - \frac{1}{r_+}\right)t \right]. \tag{30}$$

The important point about this transition function is that it depends only on the time coordinate t and is defined only on the region contained between the horizons r_- and r_+. On the other hand, it is well known[13] that in this region the coordinate t is not timelike but spacelike. Indeed, one of the interesting aspects of the region (r_-, r_+) is that the coordinates t and r interchange their role: what was the radial direction becomes timelike, and the timelike direction becomes spacelike. Therefore, we are allowed to consider t as an angle coordinate $0 \leqslant t \leqslant 2\pi$ inside the horizons. This is a consistent procedure that can be carried out explicitly for all black hole vacuum stationary solutions[14,15] and can easily be generalized to the case of electrovacuum stationary axisymmetric solutions. Therefore, if t is a compact and periodic coordinate inside the horizons, the transition function (30) is single-valued only if the coefficient in front of t is an integer, i.e.,

$$e\left(\frac{1}{r_-} - \frac{1}{r_+}\right) = \frac{2}{e}\sqrt{m^2 - e^2} = n. \tag{31}$$

This represents a relationship between the physical parameters which describe the black hole. This specific combination of m and e can take only discrete values. Notice that in the special case of an extreme black hole, $e=m$, the only allowed value is $n=0$. Moreover, the limiting case $e \to 0$ is not allowed. This is due to the fact that in order to perform this "quantization" we have used the u(1)-electromagnetic connection which does not exist in the case $e=0$.

Since the space–time possesses a curvature singularity at $r=0$, we must remove the world line of this event from the base space. This implies that the corresponding principal fiber bundle is not globally trivial. This can be seen explicitly by calculating the topological invariant, which in this case is given in terms of the Chern form $c = -(e/r^2)\mathrm{d}t \wedge \mathrm{d}r$. The Chern number is obtained by integrating the Chern form inside the horizon. As expected, we get the value of $4\pi n$, where n is an integer related to the parameters of the Reissner–Nordstrom black hole as given in (31). This represents an alternative derivation of the quantization condition. To verify that this result is also independent of the coordinates, we have performed a similar analysis of the Reissner–Nordstrom metric in Kruskal-type coordinates. As expected, the quantization condition (31) appears in a similar manner.

To conclude this section, it is worth mentioning that a similar analysis can be performed for the Kerr–Newman black hole. It turns out that in this case it is necessary to introduce again two open subsets in order to cover the entire space–time manifold. The transition function is defined in the region contained between the horizons, where the coordinate t is spacelike, and the quantization condition can be written as

$$\frac{2e^3\sqrt{m^2 - a^2 - e^2}}{e^4 + 4a^2m^2} = n, \tag{32}$$

where a represents the angular moment per unit mass of the black hole. As expected, in the limiting case $a=0$ we recover the expression (31) for the Reissner–Nordstrom black hole.

VI. CONCLUSIONS

In this paper we have developed the method of topological quantization for gravitational field configurations. First, we have shown that for any vacuum solution of Einstein's field equations there exists a natural unique principal fiber bundle with an so(1,3) connection. If the gravitational field is minimally coupled to a gauge matter field, there exists also a principal fiber bundle with a matter connection.

This procedure has been carried out explicitly for the gravitational configurations described by cylindrically symmetric space–times, the gravitomagnetic monopole in linearized gravity and electrovacuum black holes. In all the cases we have analyzed, the result of the topological quantization is a relationship that indicates the discretization of the parameters entering the correspond-

ing metrics. We have shown that the quantization conditions arise as the result of demanding a regular behavior of the connection on the base manifold. Quantization conditions can appear in globally trivial and nontrivial principal fiber bundles. In the latter case, equivalent results can be obtained from the analysis of the corresponding topological invariants.

In this work, we do not analyze the physical significance of the resulting discretization. In particular, it would be interesting to perform the topological quantization of black holes with respect to the so(1,3) connection which would complement the result of the u(1) connection analyzed here. Preliminary calculations show that the complete quantization of black holes metrics leads to a discretization of the horizon area. This task is currently under investigation.[16]

Moreover, in all the examples analyzed in this work we have restricted ourselves to the investigation of the regularity conditions of the connection on the base manifolds. Nevertheless, Theorems 1 and 3 show that there exists an additional connection on the bundle which reduces to the connection on the base manifold, when projected by means of the pull-back of local trivializations. It would be interesting to construct explicitly the connection on the bundle and investigate its properties.

Finally, we should mention that although the term "topological quantization" could be very suggestive, it is by no means a procedure that pretends to compete with already existing and well-developed procedures like canonical quantization. Nevertheless, it is interesting to see that the mere existence of relatively simple geometric structures in gravitational field configurations leads to a discretization of physical parameters, a property that is usually associated with quantization. A much more detailed and deep investigation is necessary in order to establish if topological quantization could be an alternative method to obtain at least partial "quantum" information from a physical system.

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Asymptotic flatness and Bondi energy in higher dimensional gravity

Stefan Hollands[a)]
Enrico Fermi Institute, Department of Physics, University of Chicago, Chicago, Ilinois 60637

Akihiro Ishibashi[b)]
Department of Applied Mathematics and Theoretical Physics, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom

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We give a general geometric definition of asymptotic flatness at null infinity in d-dimensional general relativity (d even) within the framework of conformal infinity. Our definition is arrived at via an analysis of linear perturbations near null infinity and shown to be stable under such perturbations. The detailed falloff properties of the perturbations, as well as the gauge conditions that need to be imposed to make the perturbations regular at infinity, are qualitatively different in higher dimensions; in particular, the decay rate of a radiating solution at null infinity differs from that of a static solution in higher dimensions. The definition of asymptotic flatness in higher dimensions consequently also differs qualitatively from that in $d=4$. We then derive an expression for the generator conjugate to an asymptotic time translation symmetry for asymptotically flat space–times in d-dimensional general relativity (d even) within the Hamiltonian framework, making use especially of a formalism developed by Wald and Zoupas. This generator is given by an integral over a cross section at null infinity of a certain local expression and is taken to be the definition of the Bondi energy in d dimensions. Our definition yields a manifestly positive flux of radiated energy. Our definitions and constructions fail in odd space–time dimensions, essentially because the regularity properties of the metric at null infinity seem to be insufficient in that case. We also find that there is no direct analog of the well-known infinite set of angle dependent translational symmetries in more than four dimensions. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1829152]

I. INTRODUCTION

Theories attempting to unify the forces often require a higher dimensional space–time, and accordingly have different properties than four-dimensional theories. Still important and fundamental even in higher dimensional theories are the notion of an isolated system and associated conserved quantities, such as the total energy of the system.

In four-dimensional general relativity, there exist two satisfactory notions of the total energy of a space–time representing an isolated system, namely the "Arnowitt–Deser–Misner" (ADM) energy[1] and the "Bondi" energy.[2–4] The ADM energy represents the energy of the system "once and for all" and is mathematically given by an integral of a quantity associated with the gravitational field, over a sphere at spatial infinity. The Bondi energy measures the total energy of the system "at an instant of time," and is mathematically given by an integral over a spacelike cross section at null infinity. Thus, while the ADM energy is just a number, the Bondi energy is in

a)Electronic mail: stefan@bert.uchicago.edu
b)Electronic mail: a.ishibashi@damtp.cam.ac.uk

general a function of time in the sense that it depends on the chosen cross section at null infinity. The difference between the Bondi energies at two different times represents the flux of gravitational radiation through the portion of null infinity bounded by the corresponding two cross sections.

While the expression for the ADM energy of a space–time is readily generalized to an arbitrary number of space–time dimensions, this is not so for the Bondi energy. To our knowledge, no expression for the Bondi energy or other quantities associated with the group of asymptotic symmetries has been given in the literature for more than four dimensions, let alone a systematic derivation.[21] This is maybe not so surprising since constructions associated with null infinity tend to be more complicated in nature than corresponding constructions at spatial infinity, which may, e.g., be appreciated from the fact that a completely satisfactory definition of quantities associated with asymptotic symmetries in four dimensions was not given as late as the early 1980s.[6] The purpose of the present paper is to derive an expression for the Bondi energy and momentum (Bondi energy, for short) in space–times of arbitrary (even) dimension.

The basic issue that needs to be settled in order to even get started on a definition of Bondi energy in higher dimensions is to specify what exactly one means by the statement that a space–time represents an "isolated system." Roughly speaking, an isolated system is a space–time that looks like Minkowski space "far away." (Other, less restrictive notions of an isolated system may also be considered, for example, systems that look like a Kaluza–Klein space far out in the "noncompact directions." However, the analysis of such metrics and of the associated conserved quantities would be substantially different from the ones studied in the present paper.) Of course, one must explain exactly what one means by "far away," and one must determine the precise asymptotics that should reasonably be imposed on the gravitational field at null infinity. What are the asymptotics for the gravitational field in d dimensions? For the sake of definiteness, suppose one would attempt to define an isolated system to be a space–time whose metric has the form of the Schwarzschild metric (in suitable coordinates), plus higher order terms in $1/r$ as one goes off to infinity along a null direction. In other words, suppose one were to define asymptotic flatness at null infinity in the same way which works at spatial infinity. Then one would effectively eliminate from consideration all space–times that contain gravitational radiation through null infinity, which are of course precisely the space–times that one wants to describe in the first place. On the other hand, if one imposes drop off conditions that are too weak, then it will in general be impossible to define a notion of radiated energy of such a space–time in a meaningful way. Thus, the task is to find a definition of asymptotic flatness that is both general enough so as to allow sufficiently many physically interesting radiating space–times, and stringent enough so as to allow one to derive meaningful expressions for the energy, as well as possibly other quantities associated with asymptotic symmetries.

The original definition of asymptotic flatness in four dimensions proposed by Bondi and collaborators[2,4] was formulated in terms of detailed conditions on the metric components in a preferred coordinate frame and was arrived at via a study of gravitational waves near infinity. Their definition was later elegantly recast into the language of "conformal infinity" following the work of Penrose.[7–11] In this language, a space–time is said to be asymptotically flat, if it can be conformally embedded into a smooth "unphysical" space–time via a conformal transformation with conformal factor Ω, so that the points at infinity are at the "finite" location $\Omega=0$ in the unphysical space–time, and so that the gradient of the conformal factor Ω is null there. The main arguments that have been advanced in favor of this definition are that it covers the known exact solutions of Einstein's equation that one intuitively thinks of as representing isolated systems, and that the definition can be proven to be stable under linear perturbations,[12] in the sense that any compactly generated solution to the linearized equations of motion around an asymptotically flat solution satisfies the linearized version of the above definition of asymptotic flatness in a suitable gauge. (By contrast, if one were to adopt the, e.g., same definition of asymptotic flatness at null infinity as one has at spatial infinity, then such a definition would not be stable under linear perturbations.)

Thus, the first task of our paper is to obtain an appropriate generalization of asymptotic

flatness to higher dimensions. This definition will be motivated as in four dimensions by a detailed analysis of the decay properties of linear perturbations at null infinity. We show that perturbations typically drop off as $1/r^{(d-2)/2}$ as one approaches null infinity, which, as we note, differs from the drop off rate of the Schwarzschild metric, $1/r^{d-3}$, when the space–time dimensions are greater than 4. The appearance of half-odd integer powers of $1/r$ in the tail of the metric at null infinity in odd d implies in particular that the unphysical metric will not be smooth at null infinity. It turns out that, for this reason, a geometrical definition of null infinity as given above for $d=4$ does not appear to be possible in odd space–time dimensions. We will therefore restrict our attention to space–times of even dimension in this paper. We will also see that the detailed behavior of the perturbations near null infinity differs qualitatively from that in four dimensions in that the trace of the metric perturbation drops off one power in $1/r$ faster than the perturbation itself. (As we will show, this phenomenon is closely related to the fact that the transverse traceless gauge is regular at null infinity in $d>4$, whereas this is not the case in $d=4$, where the so-called "Geroch–Xanthopoulos" gauge has this property.) Consequently, our definition of asymptotic flatness in $d>4$ dimensions also differs qualitatively from that in four dimensions in that it involves, for example, additional conditions on the metric volume element as one approaches null infinity.

The mathematical expression for the ADM energy, including the correct normalization, can be derived (in arbitrary dimension) in a simple and straightforward manner within the Hamiltonian framework of general relativity where it is seen to represent the "charge" conjugate to an infinitesimal asymptotic time translation at spatial infinity.[13] It was shown by Wald and Zoupas[14] (based on earlier work by Ashtekar and Streubel,[11] see also Ref. 15) that an expression for the Bondi energy in four-dimensional general relativity can also be arrived at within a Hamiltonian framework as the quantity conjugate to an asymptotic time translation at null infinity, although the situation is certainly considerably more complicated compared to spatial infinity. This expression was shown to be unique under some natural assumptions and agrees with the previously known one.[10,6] The formalism of Ref. 14 is in fact capable of dealing with arbitrary diffeomorphism covariant theories of gravity (in arbitrary dimension) in the presence of boundary conditions at null surfaces. We employ it here to establish the existence and uniqueness of a generator conjugate to an asymptotic time translation in d-dimensional vacuum general relativity (d an even number) within the context of our asymptotic flatness condition, and we take this generator as the definition of the Bondi energy in d dimensions. The algorithm by Wald and Zoupas specifies this generator only indirectly via its variation under a suitable variation of the space–time metric, so further work is required to actually find a local expression for this quantity. Such an expression is provided in Eq. (100). As in four dimensions, our definition of the Bondi energy has the property that it yields a manifestly positive flux of energy given by the square of a suitably defined "news tensor."

We emphasize that the issue of existence of a generator conjugate to an asymptotic time translation symmetry (or a more general other asymptotic symmetry) is by no means automatic but rather depends crucially on the nature of the boundary conditions. As a rule, boundary conditions that are "too weak" will prohibit the existence of a generator. In our case, the boundary conditions are independently determined by a perturbation analysis, and therefore not put in "by hand" in order to guarantee the existence of a generator. That we find existence of a generator is therefore a consistency check.

The case $d=4$ seems to be "exceptional" with regard to many of our constructions from the point of view of general d. For example, the definition of the news tensor differs in dimensions greater than 4. Also, while the unphysical Weyl tensor can be proven to vanish one order faster than the unphysical Ricci tensor in $d=4$, this does not appear to be the case in higher dimensions. On the other hand, the unphysical Ricci scalar vanishes one order faster than the unphysical Ricci tensor itself in $d>4$, while both quantities generically have the same drop off behavior in $d=4$. In $d=4$, it is well known that the asymptotic symmetries form an infinite dimensional group which comprises, besides the transformations corresponding to the usual symmetries of Minkowski space–time, an additional infinite set of (mutually commuting) "angle dependent translations," sometimes called "supertranslations." (There is no relation with supersymmetry.) We find that there is no direct analog of the supertranslations in $d>4$. Another curious feature, which is of a

more technical nature but nevertheless seems to underlie many of the differences between $d=4$ and higher dimensions is that, while linear perturbations can be proven to be regular at null infinity in the transverse traceless gauge in $d>4$, this is not so in $d=4$, where one must choose the (somewhat complicated) Geroch–Xanthopoulos gauge.[12]

The contents and main results of this paper may now be summarized. In Sec. II we present our definition of asymptotic flatness in arbitrary dimension and define the notion of an asymptotic symmetry. In Sec. III we show that our definition of asymptotic flatness is stable under linear perturbations, provided that the perturbations are in a suitable gauge. In Sec. IV we recall the general formalism of Ref. 14 for defining generators associated with asymptotic symmetries, and in Sec. V we derive our formula for the Bondi energy. We also verify that our expression for the Bondi energy agrees with the expected one (i.e., the ADM energy) in the d-dimensional analogue of the Schwarzschild metric. We draw our conclusions in Sec. VI. For simplicity, we restrict attention to the case of vacuum general relativity throughout this paper. Some remarks concerning the incorporation of matter fields are also given in Sec. VI.

Our conventions are the same as in Ref. 16: The signature of the metric is $(-+++\cdots)$, the convention for the Riemann tensor is $\nabla_{[a}\nabla_{b]}k_c=(1/2)R_{abc}{}^d k_d$ and $R_{ab}=R_{acb}{}^c$ for the Ricci tensor. Indices in parentheses are symmetrized and indices in square brackets are antisymmetrized.

II. ASYMPTOTIC FLATNESS IN *d* DIMENSIONS

Asymptotic conditions in field theory require the specification of a background configuration and the precise rate at which this background is approached. In the case of asymptotic flatness in higher dimensional general relativity, the background is the Minkowski metric. (Other asymptotic conditions would of course require a different background.) In order to specify the precise rate at which Minkowski space–time is approached at null infinity, it is of great technical advantage to work within a framework in which "infinity" is attached as additional points to the space–time manifold, $\tilde{M}$ (thereby obtaining an "unphysical" space–time manifold M), and in which these points are brought metrically to a finite distance by rescaling the physical metric, $\tilde{g}_{ab}$, by a conformal factor Ω^2 with suitable properties. The asymptotic flatness conditions are then formulated in terms of this rescaled "unphysical metric,"

$$g_{ab}=\Omega^2\tilde{g}_{ab}, \tag{1}$$

and its relation to the likewise conformally rescaled version of Minkowski space–time,

$$\bar{g}_{ab}=\Omega^2\tilde{\eta}_{ab}. \tag{2}$$

We will refer to $(\bar{M},\bar{g}_{ab})$ as the "background geometry." As it is well known, Eq. (2) can be realized, e.g., by conformally embedding Minkowski space–time into a patch of the Einstein static universe $\mathbb{R}\times S^{d-1}$ with line element $\mathrm{d}\bar{s}^2=-\mathrm{d}T^2+\mathrm{d}\psi^2+\sin^2\psi\,\mathrm{d}\sigma^2$. Here, $\mathrm{d}\sigma^2$ is the line element of a round $(d-2)$-dimensional sphere, and ψ is the azimuthal angle of S^{d-1}. In these coordinates, Minkowski space–time corresponds to the region $\bar{M}=\{-\pi<T\pm\psi<\pi,\psi>0\}$ of $\mathbb{R}\times S^{d-1}$, see Appendix B for further details of this conformal embedding, as well as the specific form of Ω.

The conformal infinity of Minkowski space–time is the boundary of the region $\bar{M}$ in the Einstein static universe. It is divided into the following five parts: (1) future timelike infinity (the point $T=\pi,\psi=0$), (2) past timelike infinity (the point $T=-\pi,\psi=0$), (3) spacelike infinity (the point $\psi=\pi,T=0$), (4) past null-infinity (the points $T=-\pi+\psi$ for $0<\psi<\pi$), and (5) future null infinity (the points $T=\pi-\psi$ for $0<\psi<\pi$). The conformal factor Ω is smooth in a neighborhood of null infinity and vanishes there, and the gradient of Ω is nonvanishing and null there.

Our definition of asymptotic flatness consists in specifying the precise rate at which g_{ab} approaches $\bar{g}_{ab}$ as one approaches the boundary $\partial\bar{M}$. To quantify how various tensors behave at that boundary, we introduce the following notion: We will say that a tensor field, $L_{ab\cdots c}$, is "of

order Ω^s" with $s \in \mathbb{R}$, written $L_{ab\cdots c} = O(\Omega^s)$, if the tensor field $\Omega^{-s} L_{ab\cdots c}$ is smooth at the boundary. It is a consequence of this definition that if $L_{ab\cdots c}$ is of order s then $\Omega^r L_{ab\cdots c}$ is of order $s+r$, and that $\overline{\nabla}_{d_1} \cdots \overline{\nabla}_{d_k} L_{ab\cdots c}$ is of order $s-k$.

We now state our definition of asymptotic flatness in even space–time dimensions $d > 4$. (From now on, d is taken to be an even number unless stated otherwise.) Let $(\overline{M}, \overline{g}_{ab})$ be the background geometry described above. A d-dimensional space–time $(\tilde{M}, \tilde{g}_{ab})$ will be said to be *weakly asymptotically simple at null infinity* if the following is true:

(1) It is possible to attach a boundary $\mathscr{I}$ to $\tilde{M}$ such that $M = \tilde{M} \cup \mathscr{I}$ is locally diffeomorphic to the manifold $\overline{M}$ near its boundary.
(2) One has, relative to our background metric $\overline{g}_{ab}$, that

$$\overline{g}_{ab} - g_{ab} = O(\Omega^{(d-2)/2}), \quad \overline{\epsilon}_{ab\cdots c} - \epsilon_{ab\cdots c} = O(\Omega^{d/2}), \tag{3}$$

where $\overline{\epsilon}_{ab\cdots c}$ and $\epsilon_{ab\cdots c}$ denote the volume element (viewed as d-forms) associated with the metrics $\overline{g}_{ab}$, respectively, g_{ab}, as well as

$$(\overline{g}^{ab} - g^{ab})(\mathrm{d}\Omega)_a = O(\Omega^{d/2}), \quad (\overline{g}^{ab} - g^{ab})(\mathrm{d}\Omega)_a(\mathrm{d}\Omega)_b = O(\Omega^{(d+2)/2}), \tag{4}$$

where g^{ab} is the inverse of g_{ab} and where $\overline{g}^{ab}$ is the inverse of $\overline{g}_{ab}$.

It is important to note that, while our definition of an asymptotically flat space–time is formulated relative to a specific background geometry, our definition is actually independent of the precise way in which the Minkowski metric $\tilde{\eta}_{ab}$ is written as $\Omega^{-2}\overline{g}_{ab}$ in terms of a background metric (smooth at $\mathscr{I}$), and correspondingly the way in which the physical metric $\tilde{g}_{ab}$ is written as $\Omega^{-2} g_{ab}$ in terms of an auxiliary unphysical metric. In other words, if k is a smooth function defined in a neighborhood of the boundary of $\overline{M}$ such that $k \neq 0$ at null infinity, then our definition of an asymptotically flat metric is unchanged if we change the conformal factor to $\Omega' = k\Omega$, the background metric to $\overline{g}'_{ab} = k^2 \overline{g}_{ab}$, and the unphysical metric to $g'_{ab} = k^2 g_{ab}$.

As in four space–time dimensions, the notion of weak asymptotic simplicity can be strengthened by requiring in addition that every inextendible null geodesic in $(\tilde{M}, \tilde{g}_{ab})$ has precisely two end points on $\mathscr{I}$. Such a space–time is then simply called *asymptotically simple*. This additional condition, combined with the fact that $\mathscr{I}$ is null, makes it possible to divide $\mathscr{I}$ into disjoint sets, $\mathscr{I}^+$ and $\mathscr{I}^-$, on which future, respectively, past directed null geodesics have their end points. These sets are referred to as future, respectively, past null infinity. This condition also implies that $(\tilde{M}, \tilde{g}_{ab})$ necessarily must be globally hyperbolic, by a straightforward generalization of Proposition 6.9.2 of Ref. 17 to d dimensions. (We also note that, by a straightforward generalization of Proposition 6.9.4 of Ref. 17 to d dimensions, the additional condition is in fact only consistent with $\mathscr{I}$ having topology $\mathbb{R} \times S^{d-2}$. This agrees with the topology of the boundary of our background geometry.)

Item (1) of our definition is essentially the statement that, as a manifold, M looks near $\mathscr{I}$ like the background manifold $\overline{M}$ looks near its null boundary. Item (2) of the definition involves three different metrics: The physical $\tilde{g}_{ab}$, unphysical g_{ab}, and the background metric $\overline{g}_{ab}$. The physical and unphysical metric are related by the conformal factor, Ω, which makes the unphysical metric smooth and at the same time brings null infinity, $\mathscr{I}$, to a "finite location," and the background metric is likewise related to Minkowski space–time. The relation between the unphysical and background metric is given by the above set of equations in item (2), which specify the precise manner in which the unphysical metric approaches the background metric, and thus the precise sense in which our space–time is required to flatten out at null infinity. Since $\nabla_a \Omega$ is null relative to the background metric, it is also null relative to the metric g_{ab}, showing that $\mathscr{I}$ is a null surface in the unphysical space–time (M, g_{ab}). Since Ω^2 times Minkowski space–time is isometric to $(\overline{M}, \overline{g}_{ab})$, our definition of asymptotic flatness trivially covers Minkowski space–time.

Since we will be working with different metrics in this paper—physical and unphysical—it is necessary to specify a rule for raising and lowering indices of tensors. Our rule is that indices on tensor fields on M without a "tilde" are raised and lowered with the unphysical metric, g_{ab} and its inverse, whereas indices on tensor fields on $\tilde{M}$ with a "tilde" are raised and lowered with the physical metric, $\tilde{g}_{ab}$, and its inverse. (Note that this rule is consistent with our notation g^{ab} and $\tilde{g}^{ab}$ for the inverse of the metrics g_{ab} and $\tilde{g}_{ab}$.)

Let us compare the above definition of asymptotic flatness with the behavior of the d-dimensional analog of the Schwarzschild metric, given by the line element

$$d\tilde{s}^2 = -(1 - cr^{-(d-3)})dt^2 + (1 - cr^{-(d-3)})^{-1}\, dr^2 + r^2\, d\sigma^2, \quad c > 0, \tag{5}$$

where $d\sigma^2$ is the line element of a round $(d-2)$-dimensional sphere. Introducing a coordinate u by the relation $du = dt - (1 - cr^{-(d-3)})^{-1}\, dr$, the line element takes the form

$$d\tilde{s}^2 = -2\, du\, dr - du^2 + r^2\, d\sigma^2 + cr^{-(d-3)}\, du^2, \tag{6}$$

where the first three terms on the right-hand side are recognized as the Minkowski line element. Multiplying by our conformal factor Ω^2, using $r^{-1} = O(\Omega)$, and using that Ω^2 times the Minkowski metric is equal to our background metric $d\bar{s}^2$ by construction, it follows that the unphysical Schwarzschild metric can be written as $ds^2 = d\bar{s}^2 + O(\Omega^{d-1})du^2$ (noting that u is a good coordinate at infinity). It follows that Schwarzschild space–time is asymptotically flat in the sense of our definition, but it becomes flat at null infinity at a faster rate than that specified above in Eqs. (3) and (4) in $d > 4$. [In $d = 4$, the relevant components drop off at the same rate, as specified in Eqs. (3) and (4).]

The above definition of asymptotic flatness in even dimensions $d > 4$ is not appropriate in odd space–time dimension, since condition (3) in item (2) now says that the unphysical metric g_{ab} differs from the smooth background metric $\bar{g}_{ab}$ by a half-odd integer power of Ω, and thereby manifestly contradicts the assumption in item (1) that g_{ab} is smooth at the boundary. The powers of Ω appearing in Eqs. (3) and (4) reflect the drop off behavior of a linearized perturbation (see Sec. III), and it is hard to see how these powers could be essentially different from the ones in the full nonlinear theory. It therefore appears that the unphysical metric is generically at most $(d-3)/2$ times differentiable at the boundary in odd dimensions. We note that it is also inconsistent in odd dimensions to postulate that the quantity $\Omega^{-(d-2)/2}(g_{ab} - \bar{g}_{ab})$ is smooth at the boundary as we did above in Eq. (3) of item (2) in the even dimensional case, because the unphysical Schwarzschild metric g_{ab} differs from the background $\bar{g}_{ab}$ by terms of order Ω^{d-1}, i.e., by an even power of Ω. Therefore, Eq. (3) is definitely false for the Schwarzschild metric in odd dimensions. For the Schwarzschild metric, $\Omega^{-(d-1)}(g_{ab} - \bar{g}_{ab})$ is smooth at the boundary (in even and odd dimensions), so one might be tempted to try this condition, together with suitable other conditions, as the definition of asymptotic flatness. However, this would eliminate from consideration all radiating space–times and is therefore not acceptable. One may try to bypass these problems by requiring appropriate lower differentiability properties of the corresponding quantities, but these seem neither to lead to a definition of asymptotic flatness that is stable under perturbations, as we briefly discuss in Sec. III, nor do those weaker conditions seem to be able to guarantee the existence of conserved quantities such as Bondi energy. Thus, it seems that a sensible definition of asymptotic simplicity at conformal infinity in odd space–time dimensions would have to differ substantially from the one given above for even dimensions, and it is doubtful that such a definition can be cast into the framework of conformal infinity. For the rest of this paper, we will restrict attention to even space–time dimensions.

We finally comment on how the above definition of asymptotic flatness in even space–time dimensions $d > 4$ compares to the usual definition[10] in four dimensions. In this definition, one simply demands that there exists *some* conformal factor, Ω, such that the corresponding unphysical metric is smooth at $\mathscr{I}$ and such that $\nabla_a\Omega$ is nonvanishing and null there. (The nullness of $\nabla_a\Omega$ follows from the first condition if Einstein's equations with vanishing stress energy at null infinity are assumed.) This definition is different in appearance from that given above and avoids in

particular the introduction of a background geometry. Nevertheless, the definition of asymptotic flatness in $d=4$ as just stated can be brought into a form that is very similar (but not identical) to the one given above for $d>4$. (We emphasize, however, that an analogous statement is not true in $d>4$. Namely, it is not true that our definition of asymptotic flatness in higher dimensions is equivalent to the statement that there exists some conformal factor, Ω, such that the corresponding unphysical metric is smooth at $\mathscr{I}$ and such that $\nabla_a\Omega$ is nonvanishing and null there.) To see this in more detail, we recall that the usual definition of asymptotic flatness in four dimensions is equivalent[18] to the statement that the physical metric can be cast into "Bondi form" [it is assumed in the derivation of Eq. (7) that the vacuum Einstein equations are satisfied], see Eqs. (14) and (31)–(34) of Ref. 2,

$$d\tilde{s}^2 = -2\,du\,dr - du^2 + r^2\,d\sigma^2 + O(r)\mathrm{d(angles)}^2 + O(1)du\,\mathrm{d(angles)} + O(r^{-1})du^2 + O(r^{-2})du\,dr \tag{7}$$

in suitable coordinates near null infinity, where the first line is recognized as the Minkowski line element, and where "angles" stands for the usual polar angles of S^2. In $d>4$ space–time dimensions our asymptotic flatness conditions Eqs. (3) and (4) in effect state that the physical line element can be written in the form

$$\begin{aligned} d\tilde{s}^2 = &-2\,du\,dr - du^2 + r^2\,d\sigma^2 + O(r^{-(d-4)/2})\mathrm{d(angles)}^2 + O(r^{-(d-4)/2})du\,\mathrm{d(angles)} \\ &+ O(r^{-(d-2)/2})du^2 + O(r^{-d/2})du\,dr, \end{aligned} \tag{8}$$

where "angles" now stands for the polar angles of S^{d-2}. One notices that the Bondi form (8) in $d>4$ does not reduce to Eq. (7) when d is set to 4. The difference between the two expressions arises from the $\mathrm{d(angles)}^2$ term, which quantifies the perturbations in the size of the cross sections of a light cone relative to Minkowski space–time. According to Eq. (7), this term is of order $O(1)$ in $d=4$ for a radiating metric, whereas Eq. (8) would say that it should be of order $O(r^{-1})$. The latter is simply wrong for a radiating metric in four dimensions. This difference can be traced back to the last of conditions (3) in $d>4$ dimensions, which therefore does not hold in $d=4$. This special feature of four dimensions will be reflected in corresponding differences in our discussion of the Bondi energy in dimensions $d>4$. We will therefore, for the rest of this paper, keep the case $d=4$ separate and assume throughout that $d>4$ (and even). Our formulas will not be valid in $d=4$ unless stated otherwise.

A diffeomorphism ϕ such that $\phi^*\tilde{g}_{ab}$ is asymptotically flat whenever $\tilde{g}_{ab}$ is asymptotically flat is called an *asymptotic symmetry*. It is clear that the asymptotic symmetries form a group under the composition of two diffeomorphisms. Clearly, the property of being an asymptotic symmetry is only related to the behavior of ϕ near the boundary. An infinitesimal asymptotic symmetry is a smooth vector field ξ^a on $\tilde{M}$ that has a smooth extension (denoted by the same symbol) to the unphysical manifold, M, and which generates a one-parameter group of asymptotic symmetries. It is a direct consequence of our definitions that the quantity

$$\chi_{ab} = \Omega^{-(d-6)/2}\pounds_\xi\tilde{g}_{ab} = 2\Omega^{-(d-2)/2}(\nabla_{(a}\,\xi_{b)} - \Omega^{-1}n^c\xi_c g_{ab}) \tag{9}$$

then must satisfy

$$\chi_{ab} = O(1), \quad \chi_a{}^a = O(\Omega), \quad \chi_{ab}n^a = O(\Omega), \quad \chi_{ab}n^an^b = O(\Omega^2), \quad \xi^a n_a = O(\Omega), \tag{10}$$

where here and in the following we are using the abbreviation

$$n_a = \nabla_a\Omega. \tag{11}$$

Conversely, if the above relations are satisfied for *some* asymptotically flat space–time, then ξ^a is an infinitesimal asymptotic symmetry. The classification of asymptotic symmetries in $d>4$ differs from that in four dimensions. We will discuss this issue in some detail below in Sec. V and in Appendix C, as well as in a forthcoming paper.[19]

III. STABILITY OF ASYMPTOTIC FLATNESS TO LINEAR ORDER

In this section we justify the definition of asymptotic flatness for even d given in the preceding section by showing that it is stable under linear perturbations. What we mean by this is the following. Suppose that $(\tilde{M},\tilde{g}_{ab})$ is an asymptotically flat space–time that is also a solution to the vacuum Einstein equation, $\tilde{R}_{ab}=0$. Consider a solution, $\delta\tilde{g}_{ab}$, to the linearized equations of motion around this background,

$$0=\delta\tilde{R}_{ab}=\tfrac{1}{2}(-\tilde{\nabla}^m\tilde{\nabla}_m\delta\tilde{g}_{ab}-\tilde{\nabla}_a\tilde{\nabla}_b\delta\tilde{g}_m{}^m+2\tilde{\nabla}^m\tilde{\nabla}_{(a}\,\delta\tilde{g}_{\,b)m}), \tag{12}$$

which has the property that the restriction of $\delta\tilde{g}_{ab}$ to a Cauchy surface has compact support. [In this section, by "background" we mean the "unperturbed" physical space–time $(\tilde{M},\tilde{g}_{ab})$, unless otherwise stated. This should not be confused with the background (2), which is our reference space–time for defining asymptotic flatness.] We will show in this section that there exists a gauge (the transverse traceless gauge works) such that, setting $\delta g_{ab}=\Omega^2\delta\tilde{g}_{ab}$,

$$\delta g_{ab}=O(\Omega^{(d-2)/2}),\quad \delta g_{ab}n^a=O(\Omega^{d/2}),\quad \delta g_{ab}n^an^b=O(\Omega^{(d+2)/2}),\quad g^{ab}\delta g_{ab}=O(\Omega^{d/2}), \tag{13}$$

at $\mathscr{I}$ for all even $d>4$. These conditions are recognized as the linearized version of our definition of asymptotic flatness, Eqs. (3) and (4), about an asymptotically flat background. Our definition of asymptotic flatness is therefore stable to linear order.

We have emphasized above that our decay properties of the metric perturbations are valid only in a particular gauge. Indeed, since the linearized equations of motion, $\delta\tilde{R}_{ab}=0$, are invariant under a gauge transformation $\delta\tilde{g}_{ab}\to\delta\tilde{g}_{ab}+\pounds_\xi\tilde{g}_{ab}$ with ξ^a an arbitrary smooth vector field on $\tilde{M}$, Eq. (13) cannot possibly be true in an arbitrary gauge. For if it were to hold in one gauge, it would certainly not hold in a gauge with a ξ^a that is very badly behaved at $\mathscr{I}$. Thus, the specification of an admissible gauge choice for the metric perturbation is an important part of the demonstration of Eq. (13).

A proof that asymptotic flatness is stable to linear order in four dimensions was given by Geroch and Xanthopoulos.[12] Their argument consists of the following two steps: One first writes the linearized equations of motions (12) in terms of the unphysical metric and derivative operator and introduces new field variables such that Eq. (12) is transformed into a hyperbolic system of partial differential equations whose coefficients are either manifestly regular functions as one approaches $\mathscr{I}$ or can be made to vanish by a suitable gauge choice. One then argues, using standard existence and uniqueness results for solutions of hyperbolic partial differential equations, that the new variables therefore have a smooth extension to the unphysical space–time. (Here one needs to use that the perturbation has compactly supported initial data.) Translating this statement about the new variables back into a statement about the metric perturbation, one finds the decay properties of the metric perturbation at $\mathscr{I}$.

We here use this basic strategy to analyze the decay at $\mathscr{I}$ of metric perturbations in even dimensions $d>4$. The second step does not depend on the dimension of the space–time, since it only involves general properties of hyperbolic differential equations. By contrast, the first step, i.e., the actual choice of variables and gauge conditions, is different in nature in $d>4$ dimensions as compared to $d=4$. Finding the appropriate variables and gauge conditions that do the job is, of course, the hard part of the analysis. It needs to be done before writing down any decay properties of the perturbations, which are then supposed to follow from the precise form of the new variables and gauge conditions. We here present things in the opposite order in order to simplify the exposition. (Throughout the rest of this section, $d>4$ and even will be assumed.)

Concerning the proper choice of gauge, we consider the 1-form

$$\tilde{v}_a = \tilde{g}^{bc}\tilde{\nabla}_c\delta\tilde{g}_{ab} - \tilde{g}^{bc}\tilde{\nabla}_a\delta\tilde{g}_{bc}, \tag{14}$$

which is equal to (dual of) the integrand of the surface term arising when varying the Einstein–Hilbert action. Under a gauge transformation, $\delta\tilde{g}_{ab} \to \delta\tilde{g}_{ab} + \pounds_\xi \tilde{g}_{ab}$, this quantity is seen to transform as

$$\tilde{v}^a \to \tilde{v}^a + 2\tilde{\nabla}_b\tilde{\nabla}^{[b}\,\xi^{a]}, \tag{15}$$

where the vacuum Einstein equations $\tilde{R}_{ab}=0$ have been used. On the other hand, the variation of the Ricci tensor can be seen to satisfy

$$\tilde{g}^{ab}\delta\tilde{R}_{ab} = \tilde{\nabla}^a\tilde{v}_a, \tag{16}$$

so that we have $\tilde{\nabla}^a\tilde{v}_a=0$ when the linearized Einstein equations hold. Thus, by Eq. (15), we can set $\tilde{v}_a=0$ throughout $\tilde{M}$ by a choice of gauge transformation when the linearized Einstein equations hold. (Note that $0=\tilde{v}^a+2\tilde{\nabla}_b\tilde{\nabla}^{[b}\,\xi^{a]}$ has the same form as Maxwell's equation for a vector potential, with a divergence free source. A solution therefore exists by the same arguments as for Maxwell's equations.) This gauge choice is invariant under further gauge transformations of the form $\delta\tilde{g}_{ab} \to \delta\tilde{g}_{ab} + \pounds_\xi\tilde{g}_{ab}$, with $\xi^a = \tilde{\nabla}^a\xi$ and ξ as any smooth function on $\tilde{M}$, which can be used, for example, to impose a gauge condition on the trace of the perturbation. We impose

$$\delta\tilde{g}_a{}^a = 0, \tag{17}$$

which can always be realized since the trace transforms as

$$\delta\tilde{g}_a{}^a \to \delta\tilde{g}_a{}^a + 2\tilde{\nabla}^a\tilde{\nabla}_a\xi \tag{18}$$

under the remaining gauge transformations. Thus, our gauge conditions are Eq. (17) and $\tilde{v}_a=0$. Together, they are equivalent to the transverse traceless gauge condition, $\tilde{\nabla}^a\delta\tilde{g}_{ab} = \delta\tilde{g}_m{}^m = 0$.

Concerning the proper choice of field variables when $d>4$, we consider

$$\tau_{ab} \equiv \Omega^{-(d-2)/2}\delta g_{ab}, \quad \tau_a \equiv \Omega^{-1}\tau_{ab}n^b, \quad u \equiv \nabla^a\tau_a. \tag{19}$$

We substitute the definitions (19) into the linearized Einstein equation, and use the background Einstein equation, $\tilde{R}_{ab}=0$, as well as the well-known relations between the physical and unphysical derivative operator and Ricci tensor,

$$\tilde{\nabla}_a k_b = \nabla_a k_b + \Omega^{-1}(2\delta^c_{(a}\,n_{\,b)} - g_{ab}n^c)k_c, \tag{20}$$

$$\tilde{R}_{ab} = R_{ab} + \Omega^{-1}[(d-2)\nabla_a n_b + (\nabla_m n^m)g_{ab} - (d-1)f g_{ab}]. \tag{21}$$

A lengthy calculation shows that the result can be written in the form

$$\begin{aligned} 0 = 2\Omega^{-(d-2)/2}\delta\tilde{R}_{ab} = &-\nabla^c\nabla_c\tau_{ab} + \nabla_a\nabla_b\tau + 4\nabla_{(a}\,\tau_{\,b)} + 2\nabla_{(a}\,y_{\,b)} - 2u g_{ab} - 2R_{acbd}\tau^{cd} - \frac{(d-6)}{2(d-2)}R_{ab}\tau \\ &+ \frac{(d-2)}{4(d-1)}R\tau_{ab} + \frac{(d-6)}{4(d-1)(d-2)}g_{ab}R\tau + \Omega^{-1}(d-2)n_{(a}\,y_{\,b)} \\ &+ \Omega^{-1}g_{ab}\left((d-2)n_c\tau^c + n^c\nabla_c\tau + \frac{(3d-10)}{4}f\tau\right) + (d-4)\Omega^{-1}n_{(a}\,\nabla_{\,b)}\tau \\ &+ \frac{(d-6)(d-4)}{4}\Omega^{-2}n_a n_b\tau, \end{aligned} \tag{22}$$

where we have used the shorthand notation

$$\tau = \tau^a{}_a, \quad y_a = \Omega^{-(d-2)/2}\tilde{v}_a = \nabla^c \tau_{ca} - \nabla_a \tau - \frac{(d+2)}{2}\tau_a - \frac{(d-4)}{2}\Omega^{-1} n_a \tau, \tag{23}$$

as well as

$$f = \Omega^{-1} n_a n^a. \tag{24}$$

We now substitute our gauge conditions, $y_a = \tau = 0$, using in particular that

$$0 = n^a y_a = \frac{1}{2}\left(u + \frac{1}{(d-2)} R^{ab}\tau_{ab}\right) - \frac{d}{4}\Omega^{-1} n^a \tau_a, \tag{25}$$

which follows by combining our gauge condition with the background Einstein equation, to get rid of the $\Omega^{-1} n^a \tau_a$ term in Eq. (22). Then Eq. (22) reduces to

$$\nabla^c \nabla_c \tau_{ab} = 4\nabla_{(a}\,\tau_{b)} - \frac{4}{d} u g_{ab} + \frac{(d-2)}{4(d-1)} R \tau_{ab} + \frac{2}{d} R^{cd}\tau_{cd} g_{ab} - 2R_{acbd}\tau^{cd}, \tag{26}$$

where all singular terms now have dropped out due to our choice of variables and gauge condition. We are, however, not done yet since we also need appropriate equations for the remaining variables, τ_a, u.

In order to get an equation for τ_a, we take the divergence of Eq. (26) with respect to the unphysical metric and use again the transverse traceless gauge condition, $y_a = \tau = 0$. This gives

$$\begin{aligned}(d-2)\nabla^c \nabla_c \tau_a = {} & \frac{4(d-2)}{d}\nabla_a u + \frac{4}{d} R^{bc}\nabla_a \tau_{bc} - 2R^{bc}\nabla_b \tau_{ca} + \left(\frac{(d+2)(d-2)}{4(d-1)} R g_{ab} + 4R_{ab}\right)\tau^b \\ & + 2\left(\nabla_b R_{ca} - \frac{(d-2)}{d}\nabla_a R_{bc} - \frac{d}{4(d-1)}(\nabla_c R) g_{ab}\right)\tau^{bc}.\end{aligned} \tag{27}$$

Finally, in order to get an equation for u, we take a further divergence of Eq. (27). We use Eq. (26) and the divergence of the transverse traceless gauge condition $\nabla^a y_a = \tau = 0$ to eliminate second derivatives of τ_{ab}, giving

$$\begin{aligned}(d-2)(d-4)\nabla^c \nabla_c u = {} & -2(d+2)(d-4) R_{ab}\nabla^a \tau^b - 2(d-4)\nabla^a R^{bc}\nabla_a \tau_{bc} \\ & + \frac{(d-4)(d^3+4d^2+12d-16)}{4d(d-1)} R u - \frac{d(d-2)(d-4)}{2(d-1)}(\nabla_c R)\tau^c \\ & + \left(\frac{d(d-2)}{2(d-1)}\nabla_a \nabla_b R - 2(d-2)\nabla^c \nabla_c R_{ab} - 8R^{cd}R_{acbd} + \frac{d^2+6d-8}{d(d-1)} R R_{ab}\right)\tau^{ab}.\end{aligned} \tag{28}$$

Equations (26), (27), and (28) form a system of linear partial differential equations for the variables τ_{ab}, τ_a, u in the unphysical space–time M, with coefficients that are given in terms of the unphysical Riemann and Ricci tensor and its first and second derivatives. No terms containing explicitly inverse powers of Ω appear due to our particular choice of variables and gauge conditions. Introducing the shorthand notation $\phi_\alpha = (\tau_{ab}, \tau_a, u)$, this system can be rewritten more compactly as

$$g^{ab}\nabla_a \nabla_b \phi_\alpha = A_\alpha{}^{\beta a}\nabla_a \phi_\beta + B_\alpha{}^\beta \phi_\beta. \tag{29}$$

It follows from our definition of an asymptotically flat space–time that the coefficients $A_\alpha{}^{\beta a}$, $B_\alpha{}^\beta$ in this system are smooth tensor fields up to and on the boundary. Equation (29) therefore forms a hyperbolic system of partial differential equations with coefficients that are smooth functions up to and on $\mathscr{I}$. (Meaning, roughly speaking, that it does not contain any second derivatives other than the wave operator. Such terms could have arisen via expressions such as $R^{abcd}\nabla_a \nabla_c \tau_{bd}$ which, as

we note, could not be eliminated in favor of first derivative terms via our gauge condition, $\nabla^m y_m = 0$. Fortunately, these terms happen to cancel.) Hence, this system possesses a well-posed initial value formulation[17] in the unphysical space–time. If ϕ_α has compactly supported initial data as we have assumed, then we conclude by the general argument given in Ref. 12 that ϕ_α and hence τ_{ab}, τ_a and u, extend to smooth tensor fields at $\mathscr{I}$. In combination with Eq. (25), this implies moreover that $\Omega^{-1} n^a \tau_a$ is smooth at $\mathscr{I}$ in the transverse traceless gauge, and hence that $n^a \tau_a = O(\Omega)$. Substituting back the definition (19) of τ_{ab} and τ_a and the gauge condition $\tau = 0$ in terms of δg_{ab}, we altogether find that the desired drop off properties (13) hold for the linearized perturbation at $\mathscr{I}$. Thus, we have shown that our definition of asymptotic simplicity given in the preceding section is stable under linear perturbations when $d > 4$ and even.

For completeness, we now comment upon the status of the above argument in the case when $d > 4$ and odd. In that case, the algebra leading to Eq. (29) is identical as in the case $d > 4$ and even, but the coefficients g^{ab}, $A_\alpha{}^{\beta\alpha}$, $B_\alpha{}^\beta$ in this system now cannot be assumed to be smooth at the boundary, since the unphysical metric g_{ab} itself does not have this property (see the discussion in Sec. II). Instead, since g_{ab} can at best be expected to be of differentiability class C^s, $s = (d-2)/2$ at the boundary, we can at best expect that $A_\alpha{}^{\beta\alpha} \in C^{s-3}$, $B_\alpha{}^\beta \in C^{s-4}$ at the boundary. On the other hand, the standard existence and uniqueness results for linear hyperbolic equations of the form (29) require a higher degree of regularity for the coefficients and therefore do not guarantee the existence of a solution to (29). [In order to guarantee existence and uniqueness of a solution in the class $\phi_\alpha \in W^{d/2+2+A}$, $A \geqslant 0$ (we mean the Sobolev space), one needs $g_{ab} \in W^{d/2+2+A}$, $A_\alpha{}^{\beta\alpha} \in W^{d/2+1+A}$, and $B_\alpha{}^\beta \in W^{d/2+1+A}$. This is stronger than what we know.] Thus, unlike in the case of even $d > 4$, we now cannot conclude that ϕ_α and hence τ_{ab}, τ_a and u, extend to, say continuous, tensor fields at $\mathscr{I}$, and we therefore also cannot conclude that, e.g., δg_{ab} is given by $\Omega^{(d-2)/2}$ times a continuous function. Thus, our stability proof breaks down in odd dimensions. We believe that this is an indication that a geometric definition of asymptotic simplicity that is stable against perturbations is not possible in odd dimensions.

In $d = 4$ space–time dimensions, the above system of equations for τ_{ab}, τ_a, u fails to be even hyperbolic, since the "box term" drops out in Eq. (28) for u. Thus, the above choice of variables and gauge does not work in $d = 4$. A set of variables and gauge conditions that works in four dimensions has been found by Geroch and Xanthopoulos:[12] These variables are τ_{ab}, τ_b and $\sigma = \Omega^{-1}\left(n^a \nabla_a \tau + \frac{1}{2} n^a \tau_a + \frac{1}{4} f \tau\right)$. The gauge condition is chosen to be $y_a = 0$, together with a certain complicated gauge condition on the trace of the perturbation instead of $\tau = 0$. With this choice of variables and gauge conditions in place, it is then shown that τ_{ab}, τ_b, σ satisfy a system of hyperbolic equations with coefficients that are smooth at $\mathscr{I}$ (assuming that the unphysical metric is smooth at $\mathscr{I}$). It follows now that the metric perturbation has the fall-off rate

$$\delta g_{ab} = O(\Omega), \quad \delta g_{ab} n^b = O(\Omega^2), \quad \delta g_{ab} n^a n^b = O(\Omega^3), \quad g^{ab} \delta g_{ab} = O(\Omega) \tag{30}$$

in this gauge. This differs from the corresponding result Eq. (13) $d > 4$ in that the trace of the perturbation is now only falling off as fast as the metric perturbation itself, $\delta g_m{}^m = O(\Omega)$, rather than one power faster as in $d > 4$. This confirms the observation already made in the preceding section that we cannot impose the second of Eqs. (4) in four dimensions, which, as we note, would be the nonlinear analog of the condition $\delta g_m{}^m = O(\Omega^2)$. Hence, it is seen that the definition of asymptotic flatness is qualitatively different in $d > 4$ dimensions. As we will see, this has consequences for our analysis of the Bondi energy in $d > 4$ dimensions.

IV. GENERAL STRATEGY FOR DEFINING "CONSERVED" QUANTITIES AT INFINITY

In this section, we review the general algorithm given by Wald and Zoupas[14] for defining "charges" associated with symmetries preserving a given set of "boundary conditions" in the context of theories derived from a diffeomorphism covariant Lagrangian. This will then be used to define the Bondi energy in d-dimensional general relativity as the generator conjugate to a time translation symmetry.

The algorithm[14] applies to arbitrary theories derived from a diffeomorphism covariant Lagrangian. We will focus here on vacuum general relativity in d dimensions, defined by the Lagrangian density (viewed as a d-form)

$$L = \frac{1}{16\pi G}\tilde{R}\tilde{\epsilon}, \tag{31}$$

and the boundary conditions specified in our definition of asymptotic flatness.

One considers the variation of L, which can always be written in the form

$$\delta L = E + \mathrm{d}\theta, \tag{32}$$

where E are the equations of motion; in our case

$$E_{a_1\cdots a_d} = \frac{1}{16\pi G}\left(\tilde{R}_{bc} - \frac{1}{2}\tilde{R}\tilde{g}_{bc}\right)\delta\tilde{g}^{bc}\tilde{\epsilon}_{a_1\cdots a_d}; \tag{33}$$

and where $\mathrm{d}\theta$ is the exterior differential of a $(d-1)$-form θ, given in our case by

$$\theta_{a_1\cdots a_{d-1}} = \frac{1}{16\pi G}\tilde{v}^c\tilde{\epsilon}_{ca_1\cdots a_{d-1}}, \tag{34}$$

where $\tilde{v}_a$ is given in terms of $\delta\tilde{g}_{ab}$ by Eq. (14). The antisymmetrized second variation ω of θ defines the (dualized) symplectic current,

$$\omega(\tilde{g};\delta_1\tilde{g},\delta_2\tilde{g}) = \delta_1\theta(\tilde{g};\delta_2\tilde{g}) - \delta_2\theta(\tilde{g};\delta_1\tilde{g}), \tag{35}$$

so that ω depends on the unperturbed metric and is skew in the pair of perturbations $(\delta_1\tilde{g}_{ab},\delta_2\tilde{g}_{ab})$ [here, and in similar other formulas involving second variations, we assume without loss of generality that the variations commute, i.e., that $\delta_1(\delta_2\tilde{g})-\delta_2(\delta_1\tilde{g})=0$]. It is given in our case by

$$\omega_{a_1\cdots a_{d-1}} = \frac{1}{16\pi G}\tilde{w}^c\tilde{\epsilon}_{ca_1\cdots a_{d-1}}, \tag{36}$$

where $\tilde{w}^c$ is the symplectic current vector

$$\tilde{w}^a = \tilde{P}^{abcdef}(\delta_1\tilde{g}_{bc}\tilde{\nabla}_d\delta_2\tilde{g}_{ef} - \delta_2\tilde{g}_{bc}\tilde{\nabla}_d\delta_1\tilde{g}_{ef}) \tag{37}$$

with

$$\tilde{P}^{abcdef} = \tilde{g}^{ae}\tilde{g}^{fb}\tilde{g}^{cd} - \tfrac{1}{2}\tilde{g}^{ad}\tilde{g}^{be}\tilde{g}^{fc} - \tfrac{1}{2}\tilde{g}^{ab}\tilde{g}^{cd}\tilde{g}^{ef} - \tfrac{1}{2}\tilde{g}^{bc}\tilde{g}^{ae}\tilde{g}^{fd} + \tfrac{1}{2}\tilde{g}^{bc}\tilde{g}^{ad}\tilde{g}^{ef}. \tag{38}$$

The integral of the symplectic current over an achronal $(d-1)$-dimensional submanifold $\tilde{\Sigma}$ of $\tilde{M}$ defines the symplectic structure, σ, of general relativity

$$\sigma(\tilde{g};\delta_1\tilde{g},\delta_2\tilde{g}) = \int_{\tilde{\Sigma}}\omega. \tag{39}$$

It can be shown that, when both $\delta_1\tilde{g}_{ab}$ and $\delta_2\tilde{g}_{ab}$ satisfy the linearized equations of motion (12), then $\mathrm{d}\omega=0$, or, what is the same thing, that the symplectic current (37) is conserved, $\tilde{\nabla}^a\tilde{w}_a=0$. Consequently, the symplectic structure σ does not depend on the choice of Σ, when $\delta_1\tilde{g}_{ab}$ and $\delta_2\tilde{g}_{ab}$ satisfy the linearized equations of motion with compactly supported initial data.

The algorithm[14] for defining generators associated with asymptotic symmetries now consists of the following steps. First, check whether the symplectic current form $\omega(\tilde{g};\delta_1\tilde{g},\delta_2\tilde{g})$ has a well-defined (i.e., finite) extension to $\mathscr{I}$ for all asymptotically flat metrics satisfying Einstein's equation and all metric perturbations preserving asymptotic flatness to first order, i.e., for all linear perturbations satisfying the linearized equations of motion and Eqs. (13). If this is the case, one

secondly seeks a $(d-1)$-form $\Theta(\tilde{g};\delta\tilde{g})$ on $\mathscr{I}$ which is linear in the perturbation, $\delta\tilde{g}_{ab}$, which is locally constructed out of the metric $\tilde{g}_{ab}$ and its derivatives at the boundary and any further quantities arising in the specification of the boundary condition, and which has the property that the pull back of the symplectic current ω to $\mathscr{I}$ can be written as the antisymmetrized variation of Θ,

$$\omega(\tilde{g};\delta_1\tilde{g},\delta_2\tilde{g}) = \delta_1\Theta(\tilde{g};\delta_2\tilde{g}) - \delta_2\Theta(\tilde{g};\delta_1\tilde{g}). \tag{40}$$

If such a symplectic potential Θ exists (which is by no means guaranteed and depends crucially on the precise form of the boundary conditions under consideration), then a generator conjugate to an asymptotic symmetry can be defined as follows: If ξ^a is a vector field on $\tilde{M}$ representing an infinitesimal asymptotic symmetry, define the associated charge $\mathcal{H}_\xi$ by the formula

$$\delta\mathcal{H}_\xi = \int_B (\delta Q_\xi - \xi\cdot\theta) + \int_B \xi\cdot\Theta, \tag{41}$$

where B is the cross section of $\mathscr{I}$ at which the generator is to be evaluated and where Q_ξ is the Noether-charge $(d-2)$-form, given in the present case by

$$Q_{a_1\cdots a_{d-2}} = -\frac{1}{16\pi G}(\tilde{\nabla}^b\xi^c)\tilde{\epsilon}_{bca_1\cdots a_{d-2}}. \tag{42}$$

In these formulas, the notation "$\xi\cdot A$" means that the vector field ξ^a is contracted into the first index of a differential form A.

It is not immediately evident from what we have said so far that Eq. (41) actually defines a generator (up to an arbitrary constant), i.e., that the right-hand side of Eq. (41) is indeed the "δ" of some quantity $\mathcal{H}_\xi$. To see this, one first verifies that the right-hand side of Eq. (41) has a vanishing antisymmetrized second variation. (This would not be so if we had not added the Θ-term to the expression for $\delta\mathcal{H}_\xi$!) This is certainly a necessary condition for it to arise as the "δ" of some quantity $\mathcal{H}_\xi$, for we always have $(\delta_1\delta_2-\delta_2\delta_1)\mathcal{H}_\xi=0$. As argued in Ref. 14, this is also a sufficient condition if one assumes that the space of asymptotically flat metrics is simply connected. (Note the analogy to "Poincare's lemma" which says that every closed 1-form on a simply connected space is exact, i.e., the "d" of some scalar function.) For the cases considered in this paper, we will prove existence of an $\mathcal{H}_\xi$ and provide an explicit expression solving Eq. (41). The arbitrary constant is fixed by setting $\mathcal{H}_\xi$ equal to 0 on Minkowski space–time.

The "flux" through a segment $\mathcal{S}$ of $\mathscr{I}$ bounded by two cross sections B_1 and B_2 associated with the infinitesimal symmetry ξ^a is defined to be the difference

$$F_\xi = \mathcal{H}_\xi(B_2) - \mathcal{H}_\xi(B_1). \tag{43}$$

One finds the simple formula[14]

$$F_\xi = \int_{\mathcal{S}} \Theta(\tilde{g};\pounds_\xi\tilde{g}). \tag{44}$$

We finally comment on the meaning of the integrals in Eq. (41). The second integral on the right-hand side of (41) has a straightforward meaning since it has been assumed that the integrand, Θ, is well defined and smooth on $\mathscr{I}$. This is, however, not so for the first integral on the right-hand side of (41), because the integrand is defined only in the interior of the space–time. This integral is to be understood instead as the limit of the corresponding integrals for a sequence of closed, smooth $(d-2)$-surfaces B_i in the interior of the physical space–time $\tilde{M}$ that smoothly approach the cross section B of $\mathscr{I}$ as $i\to\infty$. The following argument[14] shows that this limit indeed exists under the assumptions that have been made: Let $I_i=\int_{B_i}[\delta Q_\xi-\xi\cdot\theta]$. Then, since

$$\mathrm{d}[\delta Q_\xi(\tilde{g},\delta\tilde{g}) - \xi\cdot\theta(\tilde{g};\delta\tilde{g})] = \omega(\tilde{g};\delta\tilde{g},\pounds_\xi\tilde{g}), \tag{45}$$

we have, by Stoke's theorem

$$I_i - I_j = \int_{\tilde{\Sigma}_{ij}} \omega(\tilde{g};\delta\tilde{g},\pounds_\xi\tilde{g}), \tag{46}$$

where $\tilde{\Sigma}_{ij}$ is a smooth spacelike $(d-1)$-surface bounded by B_i and B_j. But ω has a smooth extension to $\mathscr{I}$ by assumption, so the right-hand side of this equation goes to 0 as $i,j\to\infty$.

V. THE BONDI ENERGY FORMULA

The aim of this section is to implement the strategy of the preceding section for an asymptotic translation symmetry in even space–time dimensions $d>4$, i.e., to show that a generator $\mathcal{H}_\xi$ exists for such a symmetry, and to derive an expression for this generator. We will take this $\mathcal{H}_\xi$ as the definition of the Bondi energy momentum (Bondi energy, for short) in space–times of even dimension $d>4$.

The crucial issue regarding the existence of a generator conjugate to asymptotic symmetries is whether the symplectic current ω has a (finite) restriction to $\mathscr{I}$and whether there exists, under our choice of boundary conditions, a potential Θ for the pull-back (50) of the symplectic current density to $\mathscr{I}$, i.e., a Θ satisfying (40). We now examine these issues.

We fix the conformal factor Ω once and for all, so that, if $(\tilde{M},\tilde{g}_{ab})$ is an asymptotically flat space–time, then $g_{ab}=\Omega^2\tilde{g}_{ab}$ satisfies Eqs. (69) with this fixed choice of Ω. Consider a solution $\delta\tilde{g}_{ab}$ of the linearized field equations that preserves asymptotic flatness to first order. Then the quantities $\tau_{ab}=\Omega^{-(d-6)/2}\delta\tilde{g}_{ab}$, $\tau_a=\Omega^{-1}\tau_{ab}n^b$ are finite and smooth at $\mathscr{I}$and $\tau_a{}^a$ and $n^a\tau_a$ vanish at $\mathscr{I}$. We substitute these relations into the definition of the symplectic current, use the relation (20) between the physical and unphysical derivative, the relation

$$\tilde{\epsilon}_{s_1\cdots s_d} = \Omega^{-d}\epsilon_{s_1\cdots s_d} \tag{47}$$

between the physical and unphysical volume element, and evaluate at $\mathscr{I}$. After some algebra, we find the simple result

$$\omega_{s_1\cdots s_d} = \frac{1}{32\pi G}(\tau_1^{bc}\nabla^m\tau_{2bc} - \tau_2^{bc}\nabla^m\tau_{1bc})\epsilon_{ma_1\cdots a_{d-1}} + O(\Omega), \tag{48}$$

noticing that this is finite at $\mathscr{I}$ (this formula is valid only in $d>4$). This expression can be rewritten somewhat more conveniently introducing a $(d-1)$-form ${}^{(d-1)}\boldsymbol{\epsilon}$ by the formula

$${}^{(d)}\boldsymbol{\epsilon}_{ma_1\cdots a_{d-1}} = d\cdot n_{[m}\,{}^{(d-1)}\boldsymbol{\epsilon}_{a_1\cdots a_{d-1}]} = (n\wedge{}^{(d-1)}\boldsymbol{\epsilon})_{ma_1\cdots a_{d-1}}, \tag{49}$$

where we have set a superscript on the quantities in order to indicate the degree of the form. [Note that ${}^{(d-1)}\boldsymbol{\epsilon}$ is only defined up to the addition of a $(d-1)$-form of the form $n\wedge{}^{(d-2)}\phi$, where ${}^{(d-2)}\phi$ is arbitrary. The addition of such a form does however not make any difference in the formulas given above.] The pull-back to $\mathscr{I}$ of the symplectic current $(d-1)$-form ω can then be written as

$$\zeta^*\,\omega_{a_1\cdots a_{d-1}} = \frac{1}{32\pi G}(\tau_1^{bc}n^m\nabla_m\tau_{2bc} - \tau_2^{bc}n^m\nabla_m\tau_{1bc})\epsilon_{a_1\cdots a_{d-1}}, \tag{50}$$

where ζ^* denotes the pull-back of a covariant tensor field to $\mathscr{I}$. Thus, it follows from this expression that the pull-back of the symplectic current form to $\mathscr{I}$ is finite and smooth for any linear perturbation preserving our asymptotic flatness condition.

We next look for a potential Θ for (50). The subsequent calculations are somewhat simplified using the tensor S_{ab} defined by the equation

$$R_{abcd} = C_{abcd} + g_{a[c} S_{d]b} - g_{b[c} S_{d]a} \tag{51}$$

in terms of the unphysical Riemann tensor and Weyl tensor. It can be expressed in terms of the unphysical Ricci tensor by

$$S_{ab} = \frac{2}{(d-2)} R_{ab} - \frac{1}{(d-1)(d-2)} R g_{ab}. \tag{52}$$

Using the relation (21) between the physical and unphysical Ricci tensor, we find that Einstein's equation for the physical Ricci tensor takes the form

$$\Omega S_{ab} + 2\nabla_a n_b - f g_{ab} = 0 \tag{53}$$

in terms of the tensor S_{ab}, where we remember the shorthand $f = \Omega^{-1} n^a n_a = O(1)$. We now take the variation of Eq. (53) with respect to a linearized solution of the field equations that preserves asymptotic flatness to first order (remembering $\delta\Omega = 0$ since Ω is rigidly fixed) and substitute the definition of τ_{ab} and τ_b. Using the formulas

$$\delta f = -\Omega^{(d-2)/2} \tau_a n^a, \tag{54}$$

$$\delta(\nabla_a n_b) = \Omega^{(d-2)/2} \left(-\frac{d}{2} n_{(a} \tau_{b)} + \frac{d}{4} f \tau_{ab} + \frac{1}{2} n^c \nabla_c \tau_{ab} - \Omega \nabla_{(a} \tau_{b)} - \frac{1}{2} \Omega S_{c(a} \tau_{b)}{}^{c} \right), \tag{55}$$

we find the result

$$\Omega^{-(d-4)/2} \delta S_{ab} = d \cdot n_{(a} \tau_{b)} - n^c \nabla_c \tau_{ab} - \frac{(d-2)}{2} f \tau_{ab} + \Omega (2\nabla_{(a} \tau_{b)} + S_{c(a} \tau_{b)}{}^{c} - \Omega^{-1} \tau_c n^c g_{ab}), \tag{56}$$

and we note that the right-hand side of this equation is manifestly finite at $\mathscr{I}$ and that the fourth term on the right side is of order Ω. It follows from this relation, together with the relation $\tau_{ab} n^b = O(\Omega)$, that the pull-back of the symplectic current density at $\mathscr{I}$, Eq. (50), can be written as

$$\zeta * \omega_{a_1 \cdots a_{d-1}} = \frac{1}{32\pi G} \Omega^{-(d-4)/2} (\tau_2^{cd} \delta_1 S_{cd} - \tau_1^{cd} \delta_2 S_{cd}) \epsilon_{a_1 \cdots a_{d-1}}. \tag{57}$$

To construct the desired potential, Θ, for Eq. (57), we note that our asymptotic flatness conditions (3) and (4) imply that (we note that the second relation is in general false in $d = 4$)

$$S_{ab} - \overline{S}_{ab} = O(\Omega^{(d-4)/2}), \quad S_m{}^m - \overline{S}_m{}^m = O(\Omega^{(d-2)/2}), \quad f - \overline{f} = O(\Omega^{d/2}). \tag{58}$$

By construction, the restriction of the symplectic form to $\mathscr{I}$, Eq. (57), only depends on the physical metric $\tilde{g}_{ab}$ and its variations, but not on how we have chosen to write them in terms of an unphysical metric g_{ab} and a conformal factor Ω, as long as g_{ab} and $\overline{g}_{ab}$ are smooth at $\mathscr{I}$. We now take advantage of this fact by choosing a conformal factor so that the background metric (2) is flat in a neighborhood of $\mathscr{I}$, i.e., $\overline{S}_{ab} = 0$, and such that $\overline{f} = \text{const}$ there. This is possible, at least locally in a neighborhood of any open subset of $\mathscr{I}^+$, respectively, $\mathscr{I}^-$ with compact closure not intersecting spatial infinity (see Appendix B for details). Consequently, by Eq. (58), in such a gauge we have

$$S_{ab} = O(\Omega^{(d-4)/2}), \quad S_m{}^m = O(\Omega^{(d-2)/2}), \quad f = \text{const} + O(\Omega^{d/2}). \tag{59}$$

Choose any smooth covector field l_a on M with the property that $l_a l^a = 0$, $n^a l_a = +1$ at $\mathscr{I}$, set

$$q_{ab} = g_{ab} - 2 n_{(a} l_{b)} \tag{60}$$

and define the "news tensor" by

$$N_{ab} = \zeta^* (\Omega^{-(d-4)/2} q^m{}_a q^n{}_b S_{mn}) \quad (\text{assuming } d > 4), \tag{61}$$

where ζ^* denotes the pull-back to $\mathscr{I}$. By definition, N_{ab} is a well-defined smooth tensor field at $\mathscr{I}$ with vanishing trace. Using the identity

$$S_{ab} n^b + \nabla_a f = 0, \tag{62}$$

one sees that N_{ab} is independent of the particular choice of l^a. A symplectic potential Θ at $\mathscr{I}$ with the desired properties is now given by

$$\Theta_{a_1 \cdots a_{d-1}} \equiv \frac{1}{32\pi G} \tau^{cd} N_{cd} \epsilon_{a_1 \cdots a_{d-1}}. \tag{63}$$

While the restriction of the symplectic form ω to $\mathscr{I}$ [see Eq. (57)] only depends on the physical metric and its perturbation, but not on the particular choice of the conformal factor Ω and unphysical metric (although the latter were used to obtain a convenient form for ω), this need not be the case for Θ, as the latter is a potential for ω and therefore only unique up to a "total variation" $\delta\Pi$. We therefore must investigate the behavior of Θ under "conformal gauge changes." If we change the conformal factor to $\Omega' = k\Omega$ with some smooth k, then, since the physical metric is to remain unchanged, the unphysical metric changes by $g'_{ab} = k^2 g_{ab}$, and likewise the background metric changes as $\overline{g}'_{ab} = k^2 \overline{g}_{ab}$. The quantities S_{ab}, n^a, f change in the following way:

$$n^{a\prime} = k^{-1} n^a + k^{-2} \Omega \nabla^a k,$$

$$S'_{ab} = S_{ab} + 2k^{-1} \nabla_a \nabla_b k - k^{-2} g_{ab} (\nabla_m k) \nabla^m k, \tag{64}$$

$$f' = k^{-1} f + 2k^{-2} n^a \nabla_a k + k^{-3} (\nabla^a k) \nabla_a k \tag{65}$$

with similar formulas for the background quantities $\overline{S}_{ab}$, $\overline{n}^a$, $\overline{f}$. In order to arrive at the above formula for Θ, we assumed that we were in a gauge such that $S_{ab} = 0$, and such that $\overline{f} = \text{const}$. Since we have thereby already partially fixed the gauge, we need to demand that k be such that $\overline{S}'_{ab} = 0$ and such that $\overline{f}' = \text{const}$. Inserting these formulas, we find that for such k,

$$\Theta' = \Theta + \delta\Pi, \tag{66}$$

where Π is the $(d-1)$-form on $\mathscr{I}$ defined by

$$\Pi_{a_1 \cdots a_{d-1}} = \frac{(d-2)}{2^6 \pi G} \Omega^{-(d-2)} k^{-1} n^b (\nabla_b k) (g - \overline{g})_{cd} q^{ce} q^{df} (g - \overline{g})_{ef} \epsilon_{a_1 \cdots a_{d-1}}. \tag{67}$$

Since $\delta\Pi$ is not vanishing at $\mathscr{I}$, this means that the definition of Θ is not completely independent upon how the physical metric is written as $\Omega^2 \tilde{g}_{ab} = g_{ab}$, respectively, how the Minkowski metric is written as $\Omega^2 \tilde{\eta}_{ab} = \overline{g}_{ab}$ in terms of a conformal background metric, with $\overline{S}_{ab} = 0$ and $\overline{f} = \text{const}$. We resolve this gauge ambiguity by choosing a representer $\overline{g}_{ab}$ in the conformal class of the Einstein static universe which has

$$\overline{f} = 0, \quad \overline{\nabla}_a \overline{n}^b = 0, \quad \overline{S}_{ab} = 0 \quad \text{near } \mathscr{I}, \tag{68}$$

where $\overline{\nabla}_a$ denotes the derivative operator associated with $\overline{g}_{ab}$. It can be seen that $\Pi = 0$ for any further gauge change preserving this gauge condition, i.e., that Θ is now defined in a gauge invariant way. We will stick with this gauge choice for the remainder of the paper. It follows from these gauge conditions that

$$f = O(\Omega^{d/2}), \quad \nabla_a n_b = O(\Omega^{(d-2)/2}). \tag{69}$$

Some further explanations concerning this gauge choice are provided in Appendix B.

By the general analysis reviewed in the last section we infer that generators $\mathcal{H}_\xi$ associated with asymptotic symmetries ξ^a exist in d-dimensional general relativity with our choice of asymptotic flatness conditions, and that analysis instructs us to define $\mathcal{H}_\xi$ by

$$\delta\mathcal{H}_\xi = \int_B (\delta Q_\xi - \xi \cdot \theta) + \frac{1}{32\pi G}\int_B \tau^{ab} N_{ab} \xi \cdot {}^{(d-1)}\boldsymbol{\epsilon}, \tag{70}$$

where Q_ξ and θ were defined in Eqs. (42) and (34).

Formulas (70) and (63) are also correct in $d=4$ (for a derivation, see Ref. 14), provided that N_{ab} is given by the usual definition of the news tensor in four dimensions, $N_{ab}=\zeta^*(q^m{}_a q^n{}_b S_{mn}) - \rho_{ab}$, instead of Eq. (61). Here, ρ_{ab} is the uniquely determined symmetric tensor on $\mathscr{I}$ provided by Theorem 5 of Ref. 10, whose precise form depends on the chosen gauge.

Plugging the expression (63) for the symplectic potential into the flux formula, Eq. (44), and setting as above $\chi_{ab}=\Omega^{-(d-6)/2}\pounds_{\tilde{\xi}}\tilde{g}_{ab}$ we get the following expression for the flux associated with an asymptotic symmetry ξ^a through a segment $\mathcal{S}$ of $\mathscr{I}$:

$$F_\xi = \frac{1}{32\pi G}\int_{\mathcal{S}} \chi^{cd} N_{cd}{}^{(d-1)}\boldsymbol{\epsilon}, \tag{71}$$

noting that this is finite on account of our definition of an asymptotic symmetry, see Eqs. (10).

Having established the existence of a generator $\mathcal{H}_\xi$, we now discuss its uniqueness. The definition of $\mathcal{H}_\xi$ depends on the choice of Θ, which is itself only unique up to the addition of a $(d-1)$-form on $\mathscr{I}$ of the form δW, where W is an arbitrary $(d-1)$-form on $\mathscr{I}$ that is locally constructed out of the physical metric, the physical Riemann tensor and its derivatives, and Ω. The change $\Omega \to \lambda\Omega$ and $g_{ab} \to \lambda^2 g_{ab}$ with λ a constant will keep the physical metric fixed and preserve (69), so gauge invariance requires that $W \to W$ under this change of the unphysical metric and the conformal factor. [This requirement is met by our definition (63) of Θ.] Moreover, the symplectic potential Θ defined in (63) has the property that it vanishes whenever the news tensor, N_{ab}, vanishes. A vanishing news tensor indicates the absence of radiation (at least in four dimensions), and our definition (63) for Θ has the property that it vanishes when $N_{ab}=0$, thereby implying by Eq. (44) that the flux also vanishes whenever the news vanishes. It is natural to demand that any reasonable definition of Θ, and hence the flux, vanishes when the news is zero, which in turn leads to the requirement that $W=0$ whenever $N_{ab}=0$. If W has furthermore an analytic dependence on the (physical) metric, then we claim that these requirements imply that $W=0$, and hence that Θ is unique.

In order to see that this is indeed true, it is useful to introduce the "scaling dimension"[10] of a tensor $L^{a\cdots b}{}_{c\cdots d}$ with u upper indices and l lower indices that is constructed out of the unphysical metric and Ω. We say that such a tensor has scaling dimension s if $L^{a\cdots b}{}_{c\cdots d} \to \lambda^{s-u+l} L^{a\cdots b}{}_{c\cdots d}$ under a change $\Omega \to \lambda\Omega$ and $g_{ab} \to \lambda^2 g_{ab}$. It follows from this definition that the scaling dimension does not depend on the position of the indices and is additive under the tensor product. The dimension of g_{ab} is 0, the dimension of Ω is +1, the dimension of the Riemann tensor is −2 and each derivative decreases the dimension by 1, which implies that the dimension of n_a is 0. By assumption, the $(d-1)$ form

$$W_{ab\cdots c} = Y(\Omega, g_{ab}, n_a, \ldots, (\nabla_m)^r n_a, R_{abcd}, \ldots, (\nabla_m)^t R_{abcd})^{(d-1)}\boldsymbol{\epsilon}_{ab\cdots c} \tag{72}$$

has scaling dimension $-(d-1)$. Therefore, since ${}^{(d-1)}\boldsymbol{\epsilon}$ has scaling dimension 0, Y must have scaling dimension $-(d-1)$. Using Einstein's equation to eliminate covariant derivatives of n_a in terms of covariant derivatives or S_{ab}, and using Eq. (51) to eliminate the Riemann tensor in favor of C_{abcd} and S_{ab}, we can write a term in Y schematically in the form

$$\Omega^v (n_a)^l \prod_{i=1}^{r} (\nabla_m)^{s_i} (\Omega^{-(d-4)/2} S_{ab}) \prod_{j=1}^{u} (\nabla_m)^{t_j} (\Omega^{-(d-6)/2} C_{abcd}), \tag{73}$$

where we have suppressed contractions with the metric g_{ab} to lighten the notation. The scaling dimension of this term must be equal to $-(d-1)$, which implies that

$$\sum_i s_i + \frac{d}{2} r + \sum_j t_j + \frac{(d-2)}{2} u - v = d - 1. \tag{74}$$

Since the expressions $\Omega^{-(d-4)/2} S_{ab}$ and $\Omega^{-(d-6)/2} C_{abcd}$ are smooth at $\mathscr{I}$ as a consequence of our definition of asymptotic flatness, the expression (73) can be nonvanishing at $\mathscr{I}$ if and only if $v \leqslant 0$ (note that $v < 0$ is allowed, since the other terms appearing in the above expression could vanish at $\mathscr{I}$). Furthermore, $\Omega^{-(d-4)/2} S_{ab}$ vanishes at $\mathscr{I}$ if and only if the news vanishes at $\mathscr{I}$. Therefore, since we want Y to vanish whenever $N_{ab} = 0$, we must have $r > 0$. On the other hand, Eq. (74) implies that $r \leqslant 1$, so $r = 1$. We now analyze the remaining cases: When $r = 1$ and $u = 0$, then the term (73) looks schematically like

$$\Omega^v (n_a)^l (\nabla_m)^s (\Omega^{-(d-4)/2} S_{ab}), \tag{75}$$

with $s - v = (d-2)/2$. This term must vanish when the news vanishes and hence when $\Omega^{-(d-4)/2} S_{ab}$, but not necessarily its derivatives, vanishes at $\mathscr{I}$. This implies $s = 0$ and hence $v = -(d-2)/2$, so we need contractions of n_a with itself to get a term that is finite at $\mathscr{I}$. But contractions of n_a with itself give a power of at least $\Omega^{(d+2)/2}$, therefore terms of the form Eq. (75) cannot occur. The only remaining nontrivial case is $r = 1$ and $u = 1$. In this case, we must have $s_i = t_j = v = 0$ and the term (73) must take the form $\Omega^{-(d-5)} C_{abcd} S^{ac} n^b n^d$. But this term vanishes at $\mathscr{I}$, by Eq. (A14) in the appendix. We have therefore shown that $W = 0$ and hence that the symplectic potential Θ given by Eq. (63) is unique under the above assumptions.

We now consider the flux for the special case of "translational" asymptotic symmetries ξ^a. These are distinguished by the fact that the restriction of ξ^a to $\mathscr{I}$ is proportional to n^a, i.e., $\xi^a = \alpha n^a + \Omega k^a$, for some k^a, smooth at $\mathscr{I}$. A vector field ξ^a is an asymptotic symmetry if and only if the tensor $\chi_{ab} = \Omega^{-(d-6)/2} \pounds_\xi \tilde{g}_{ab}$ satisfies Eqs. (10). If we substitute this form of ξ^a into Eqs. (10), we see that $k^a = -\nabla^a \alpha$ at $\mathscr{I}$. Let us therefore make the ansatz

$$\xi^a = \alpha n^a - \Omega \nabla^a \alpha. \tag{76}$$

For which α is this an asymptotic symmetry? Inserting (76) into χ_{ab}, we find that

$$\chi_{ab} = 2\Omega^{-(d-4)/2} (-\nabla_a \nabla_b \alpha + \Omega^{-1} \alpha \nabla_a n_b + \Omega^{-1} g_{ab} n^c \nabla_c \alpha). \tag{77}$$

Using that $\nabla_a n_b = O(\Omega^{(d-2)/2})$ in our gauge choice [see Eq. (69)] we see that χ_{ab} is finite at $\mathscr{I}$ if and only if α satisfies

$$\nabla_a \nabla_b \alpha - \Omega^{-1} g_{ab} n^c \nabla_c \alpha = O(\Omega^{(d-4)/2}). \tag{78}$$

Dotting n^a into Eq. (77), and using that $f = O(\Omega^{d/2})$ in our gauge choice, we see that $\chi_{ab} n^b = O(\Omega)$ if and only if

$$\nabla^b (\Omega^{-1} n^a \nabla_a \alpha) = O(\Omega^{(d-4)/2}). \tag{79}$$

Contracting this once more into n^a, we see that $\chi_{ab} n^a n^b = O(\Omega^2)$ if

$$\Omega^{-1} n^b \nabla_b (\Omega^{-1} n^a \nabla_a \alpha) = O(\Omega^{(d-4)/2}). \tag{80}$$

In $d > 4$, an asymptotic symmetry must furthermore satisfy $\chi^a{}_a = O(\Omega)$. However, this condition actually automatically follows for any asymptotic symmetry ξ^a once $\chi_{ab} = O(1)$, $\chi_{ab} n^b = O(\Omega)$, $\chi_{ab} n^a n^b = O(\Omega^2)$ are satisfied. To see this, we note that since $\delta \tilde{g}_{ab} = \pounds_\xi \tilde{g}_{ab}$ satisfies the linearized Einstein equation, the tensor χ_{ab} satisfies Eq. (22) (with $\tau_{ab} = \chi_{ab}$ in that equation).

Multiplying Eq. (22) by Ω, we see that the only remaining singular term on the right-hand side is given by a constant that is nonzero for $d \neq 4$, times $\Omega^{-1} n_a n_b \chi_c{}^c$, which implies that $\chi_a{}^a = O(\Omega)$ when $d > 4$. Thus, if Eqs. (78), (79), and (80) hold, then the vector field $\xi^a = \alpha n^a - \Omega \nabla^a \alpha$ is an symptotic symmetry.

The above conditions on α can be understood as follows. In $d=4$ dimensions, conditions (78) and (79) together imply that α must be constant along the null generators of $\mathscr{I}$, whereas condition (80) gives a restriction on how α is defined off of $\mathscr{I}$. Hence, α is essentially an arbitrary function on a given cross section of $\mathscr{I}$, which is propagated along the null generator to the other cross sections. The corresponding symmetries are commonly referred to as "supertranslations." They comprise the ordinary "pure" translations, as well as an additional infinite set of mutually commuting so-called "angle dependent" translations. In $d > 4$, the above conditions are more restrictive than in $d=4$ and are analyzed in Appendix C. There are now only d linearly independent admissible functions α up to correction terms which essentially do not affect the restriction of χ_{ab} to $\mathscr{I}$, in the sense that the correction terms do not make a contribution to the flux. The translational asymptotic symmetries associated with these choices of α correspond to the d translational Killing fields in Minkowski space–time. There is no direct analog of the angle dependent translations in higher dimensions. The asymptotic translations with $\alpha \geqslant 0$ correspond precisely to the future directed ($\alpha \geqslant 0$ means that $\xi^a = \alpha n^a$ is the future pointing near $\mathscr{I}^+$) timelike or null translational Killing fields in Minkowski space–time.

Let us calculate the flux when $\xi^a = \alpha n^a - \Omega \nabla^a \alpha$ is an asymptotic future directed time translation, i.e., $\alpha \geqslant 0$. Using Einstein's equation (53) to eliminate the term proportional to $\nabla_a n_b$ in Eq. (77) in favor of S_{ab}, we can bring χ_{ab} into the form

$$\chi_{ab} = -\Omega^{-(d-4)/2}(2\nabla_a \nabla_b \alpha + \alpha S_{ab} - 2\Omega^{-1} g_{ab} n^c \nabla_c \alpha - \alpha \Omega^{-1} f g_{ab}). \tag{81}$$

Substituting it into the flux formula, Eq. (71), one finds

$$F_\xi = -\frac{1}{32\pi G}\int_{\mathcal{S}} \alpha N^{cd} N_{cd}{}^{(d-1)} \boldsymbol{\epsilon} \leqslant 0. \tag{82}$$

This shows that the flux of energy (defined via *any* future directed asymptotic time translation) through $\mathscr{I}$ is always negative, i.e., that the energy radiated away by the system is always positive.

The generators $\mathcal{H}_\xi$ are determined, in principle, by the defining relation Eq. (70) and the requirement that $\mathcal{H}_\xi = 0$ on Minkowski space–time. If ξ^a is not a translation, i.e., if ξ^a is tangent to some cross section B of $\mathscr{I}$, then the term involving Θ vanishes in the expression for the variation of $\mathcal{H}_\xi$, Eq. (70), and an explicit expression for $\mathcal{H}_\xi$ can be derived in basically the same manner as in four dimensions, see Ref. 14. We will not discuss this case here but focus on the case when ξ^a is a translation for the rest of this section.

In that case, the defining relation (70) is not useful to actually find the expression for the generators $\mathcal{H}_\xi$, although the right-hand side of that equation is, of course, explicitly known. Indeed, in Ref. 14, an explicit expression for $\mathcal{H}_\xi$ in $d=4$ was found by verifying that relation (70) is satisfied by a known expression for the Bondi energy previously given by Geroch.[10] Such a candidate expression is, of course, not available in $d > 4$, since this is precisely what we are actually looking for in the first place. We therefore proceed by a different route, restricting ourselves for simplicity first to the case of the asymptotic translation $\xi^a = \alpha n^a$, with α a constant.

Consider the $(d-1)$-form $\Theta(\tilde{g}; \pounds_{\alpha n}\tilde{g})$ on $\mathscr{I}$ that is given by the integrand of the flux integral, Eq. (82). We extend this to a $(d-1)$-form that is defined on the entire unphysical space–time M by setting

$$\Theta_{s_1 \cdots s_{d-1}} = \frac{1}{32\pi G}\alpha \Omega^{-(d-4)}(S_{ab} S_{cd} q^{ac} q^{bd}) \boldsymbol{\epsilon}_{s_1 \cdots s_{d-1}}. \tag{83}$$

Define the vector field

$$P^a \equiv \frac{\alpha}{8(d-3)\pi G}\Omega^{-(d-4)}(S_{de}q^{ce}q^{d[b}\,n^{\,a]}\nabla_b l_c - \Omega^{-1}C^{abcd}n_b l_c n_d), \tag{84}$$

in the interior of the space–time, where l_a is any smooth vector field such that $l_a l^a = 0$ and $n^a l_a = 1$ on $\mathscr{I}$ and such that relations (A2) are satisfied. We show in the Appendix that

$$\nabla^a P_a = \frac{1}{32\pi G}\alpha\Omega^{-(d-4)}S_{ab}S_{cd}q^{ac}q^{bd} + O(\Omega), \tag{85}$$

and it can be verified directly from the definition of P^a that $P^a n_a = O(\Omega^2)$. Next, define the $(d-2)$-form μ by[22]

$$\mu_{a_1\cdots a_{d-2}} = \epsilon_{a_1\cdots a_{d-2}cd}l^c P^d = \tfrac{1}{2}[*(l\wedge P)]_{a_1\cdots a_{d-2}}. \tag{86}$$

Then it follows that

$$\begin{aligned}(\mathrm{d}\mu)_{a_1\cdots a_{d-1}} &= 2\nabla_m(P^{[m}\,l^{\,n]})\epsilon_{na_1\cdots a_{d-1}}\\ &= 2n_n\nabla_m(P^{[m}\,l^{\,n]})\epsilon_{a_1\cdots a_{d-1}} - 2(d-1)\nabla_m(P^{[m}\,l^{\,n]})n_{[a_1}\,\epsilon_{\,|n|a_2\cdots a_{d-1}]}\\ &= (\nabla_m P^m)\epsilon_{a_1\cdots a_{d-1}} - 2(d-1)\nabla_m(P^{[m}\,l^{\,n]})n_{[a_1}\,\epsilon_{\,|n|a_2\cdots a_{d-1}]} + O(\Omega)\\ &= (\Theta + \mathrm{d}\Omega\wedge\varphi)_{a_1\cdots a_{d-1}} + O(\Omega),\end{aligned} \tag{87}$$

where $\epsilon_{a_1\cdots a_{d-1}}$ is as in Eq. (49), where it has been used that $P^a n_a = O(\Omega^2)$, and where we have set $\varphi_{a_1\cdots a_{d-2}} = 2\nabla_m(P^{[m}\,l^{\,n]})\epsilon_{na_1\cdots a_{d-2}}$.

Consider now a segment $\mathcal{S}$ of $\mathscr{I}$ bounded by cross sections B_1 and B_2, and a sequence of smooth $(d-1)$-surfaces $\mathcal{S}_i$ of constant Ω that approach $\mathcal{S}$. Using Eqs. (44) and (87), we can write the flux through the segment $\mathcal{S}$ as follows:

$$F_{\alpha n} = \lim_{i\to\infty}\int_{\mathcal{S}_i}\Theta(\tilde{g},\pounds_{\alpha n}\tilde{g}) = \lim_{i\to\infty}\int_{\mathcal{S}_i}(\mathrm{d}\mu - \mathrm{d}\Omega\wedge\varphi) = \lim_{i\to\infty}\left(\int_{(\partial\mathcal{S}_i)_2}\mu - \int_{(\partial\mathcal{S}_i)_1}\mu\right), \tag{88}$$

where we have used Stoke's theorem and where we have written $(\partial\mathcal{S}_i)_1$ for the connected component of the boundary approaching B_1 and $(\partial\mathcal{S}_i)_2$ for the connected component of the boundary approaching B_2. **(**A subtlety arises from the fact that the gauge that we are working in [chosen such that Eq. (69) holds] is actually not defined on all of $\mathscr{I}$, but only on $\mathscr{I}$ minus a single generator, see Appendix B. Therefore, there also should appear another "boundary term" in Eq. (88) corresponding to that single generator. However, it can be seen that this term does not make a contribution by passing to a suitable gauge which is defined on all of $\mathscr{I}$, and by transforming the expression for μ accordingly using formulas very similar to those given on pp. 50 and 51 of Ref. 9. An example is worked out in Appendix B. Similar remarks apply to other formulas below.**)** Now take the variation of this equation and substitute the variation of the flux formula (43), $\delta F_{\alpha n} = \delta\mathcal{H}_{\alpha n}(B_1) - \delta\mathcal{H}_{\alpha n}(B_2)$. This gives

$$\delta\mathcal{H}_{\alpha n}(B_1) - \delta\mathcal{H}_{\alpha n}(B_2) = \lim_{i\to\infty}\left(\delta\int_{(\partial\mathcal{S}_i)_2}\mu - \delta\int_{(\partial\mathcal{S}_i)_1}\mu\right). \tag{89}$$

Consider a variation of the metric that vanishes in a neighborhood of *some* cross section of $\mathscr{I}$, in addition to satisfying the linearized equations of motion and the linearized conditions of asymptotic flatness. Then it follows from Eq. (89) that for such a variation,

$$\delta\mathcal{H}_{\alpha n}(B) = \delta\int_B\mu \tag{90}$$

for *any* cross section B of $\mathscr{I}$, where the integral on the right-hand side is defined by the limit of the

corresponding integrals over $(d-2)$-surfaces of constant Ω that smoothly approach B from the interior of the space–time. [This shows in particular that the right-hand side of Eq. (90) (defined via this limiting procedure) is actually finite. This is not obvious from the definition since P^a as well as its variation is *not* manifestly finite at $\mathscr{I}$ in $d>4$. Indeed, the Weyl term in the definition of P^a can only be shown to make a contribution of order $O(\Omega^{-(d-4)/2})$ using our asymptotic flatness conditions.] Next, consider a variation that is pure gauge, $\delta\tilde{g}_{ab}=\pounds_\eta\tilde{g}_{ab}$, for some asymptotic symmetry η^a. For such a variation, we have

$$\delta\int_B \mu=\int_B \pounds_\eta\mu=\int_B [\mathrm{d}(\eta\cdot\mu)+\eta\cdot \mathrm{d}\mu]=\int_B \eta\cdot\Theta(\tilde{g};\pounds_{\alpha n}\tilde{g}), \tag{91}$$

where the integrals are defined by a limiting procedure as above. We now show that $\delta\mathcal{H}_{\alpha n}(B)$ for this variation is also given by the right-hand side of the above equation. For this, we consider the one-parameter family of diffeomorphisms Φ_t generated by η^a which maps points in $\mathscr{I}$ to points in $\mathscr{I}$. If $\Phi_t^* B$ is the cross section of $\mathscr{I}$ obtained from B by applying this diffeomorphism, and if $\mathcal{S}_t$ is the segment of $\mathscr{I}$ bounded by these two cross sections, then we have

$$\delta\mathcal{H}_{\alpha n}(B)=\lim_{t\to 0}\frac{1}{t}[\mathcal{H}_{\alpha n}(B)-\mathcal{H}_{\alpha n}(\Phi_t^* B)]=\lim_{t\to 0}\frac{1}{t}\int_{\mathcal{S}_t}\Theta(\tilde{g};\pounds_{\alpha n}\tilde{g})=\int_B \eta\cdot\Theta(\tilde{g};\pounds_{\alpha n}\tilde{g}), \tag{92}$$

for the variation $\delta\tilde{g}_{ab}=\pounds_\eta\tilde{g}_{ab}$, where we have used the flux formula Eq. (44) in the second line, and where we have used that $\Theta(\tilde{g};\pounds_{\alpha n}\tilde{g})$ is smooth at $\mathscr{I}$ in the third line. Hence, we conclude that Eq. (90) also holds for any variation of the form $\delta\tilde{g}_{ab}=\pounds_\eta\tilde{g}_{ab}$. Consider now a variation with compact support K on some Cauchy surface which satisfies the linearized field equations and the linearized conditions of asymptotic flatness. Then it follows from the arguments given in Sec. III that such a variation can be written as a sum $\delta\tilde{g}_{ab}+\pounds_\eta\tilde{g}_{ab}$, where η^a is some asymptotic symmetry and where $\delta\tilde{g}_{ab}$ has support in $J^+(K)\cup J^-(K)$. It follows that there exist cross sections B^+ of $\mathscr{I}^+$ and B^- of $\mathscr{I}^-$ such that $\delta\tilde{g}_{ab}$ vanishes in a neighborhood of B^+ and B^-. By the arguments already given, Eq. (90) therefore holds for any variation which has compact support on some Cauchy surface. Consequently, Eq. (90) will also hold for any variation such that the corresponding fields τ_{ab}, τ_a and their first (unphysical) derivatives can be approximated near B by the corresponding fields for a sequence of variations that have compact support on a Cauchy surface. We believe that all variations that satisfy the linearized equations of motion and the linearized conditions of asymptotic flatness can be approximated in this way. Assuming that this is true, it follows that Eq. (90) holds for all variations.

We have $\int_B\overline{\mu}=0$ for our background geometry, since we are in a gauge in which $\overline{g}_{ab}$ is flat in a neighborhood of $\mathscr{I}$, therefore $\overline{\mu}=0$ in a neighborhood of $\mathscr{I}$. Therefore, modulo the proof of the approximation property mentioned in the last paragraph, we have shown that

$$\mathcal{H}_\xi=\int_B \mu=\frac{1}{2}\int_B *(l\wedge P) \tag{93}$$

for asymptotic time translations, $\xi^a=\alpha n^a$, where P^a is given by Eq. (84). This is our expression for the Bondi energy of an asymptotically flat space–time in d dimensions.

Our expression for the Bondi energy is independent of the particular choice of l_a with the properties (A2): Consider another l'_a with the same properties as l_a, and set $x_a=l_a-l'_a$. Then x_a satisfies the relations $\nabla_b x_a=O(\Omega^{(d-4)/2})$, $n_a x^a=O(\Omega^{d/2})$, and $l^a x_a=O(\Omega^{(d-2)/2})$. Consider the antisymmetric tensor field X^{ab} defined by

$$X^{ab}=\frac{1}{8(d-3)\pi G}\alpha\Omega^{-(d-4)}S_{ef}q^{ed}q^{f[a}n^{b]}x_d. \tag{94}$$

Then it can be seen, using formulas (A2), (69), and (A6), that $X^{ab}n_b=O(\Omega)$, and

$$P'^a = P^a + \nabla_b X^{ab} + O(\Omega). \tag{95}$$

Consider now a sequence of embedded $(d-2)$-surfaces that are smoothly embedded into M and which approach a cross section B of $\mathscr{I}$ as $i \to \infty$. Without loss of generality we may assume that $\Omega = \text{const}$ on each of these surfaces, so that n^a is one of the normals to the surfaces. Let u^a be another normal so that the field $n^{[a} u^{b]}$ is a binormal, meaning that $\epsilon_{a_1 \cdots a_{d-2}} = \zeta_i^*(n^{[m} u^{n]} \epsilon_{mna_1 \cdots a_{d-2}})$ is equal to the $(d-2)$-volume form induced by g_{ab} on each of these surfaces, where ζ_i^* denotes the pull-back to B_i. Then from Eq. (95), we get

$$\begin{aligned}\zeta_i^*(\mu - \mu')_{a_1 \cdots a_{d-2}} = {} & \tfrac{3}{2}\zeta_i^* \nabla_q (X^{[qm} l^{n]}) \epsilon_{mna_2 \cdots a_{d-2}} - \zeta_i^*(\tfrac{3}{2} X^{[mq} \nabla_q l^{n]} + \tfrac{1}{2} l^q \nabla_q X^{mn} \\ & + P'^{[m} x^{n]}) n_m u_n \epsilon_{a_1 \cdots a_{d-2}}.\end{aligned} \tag{96}$$

But the terms in the last line are all of $O(\Omega)$, since $X^{ab} = O(\Omega^{(d-4)/2})$, $X^{ab} n_b = O(\Omega^2)$, $P^a n_a = O(\Omega^2)$, and since $x^a n_a = O(\Omega^{d/2})$, $n^b \nabla_a l_b = O(\Omega^{(d-2)/2})$ by Eqs. (A2). This shows that, in differential forms notation,

$$\zeta_i^*(\mu - \mu') = -\tfrac{1}{3}\zeta_i^*\{\mathrm{d}[*(X \wedge l)]\} + O(\Omega), \tag{97}$$

and therefore, by Stoke's theorem, that

$$\int_B \mu - \int_B \mu' = \lim_{i \to \infty} \int_{B_i} (-\tfrac{1}{3}\mathrm{d}[*(X \wedge l)] + O(\Omega)) = 0, \tag{98}$$

since B_i has no boundary. Thus, our definition (93) of the Bondi energy does not depend on our choice of l_a.

Substituting our expression (84) for P^a into Eq. (93), using the definition of S_{ab} together with the fact that $S_m{}^m = O(\Omega^{(d-2)/2})$, we can express $\mathcal{H}_\xi$ by the final formula

$$\mathcal{H}_\xi = \frac{1}{8(d-3)\pi G} \int_B \alpha \Omega^{-(d-4)} \left(\frac{1}{(d-2)} R_{ab} q^{ac} q^{bd} (\nabla_c l_d) n^e l^f - \Omega^{-1} l^{[e} C^{f]bcd} n_b l_c n_d \right) \epsilon_{efa_1 \cdots a_{d-2}}. \tag{99}$$

This formula holds for the special translation $\xi^a = \alpha n^a$, with $\alpha = \text{const}$. The above arguments and calculations can be generalized to arbitrary (null) translations, $\xi^a = \alpha n^a - \Omega \nabla^a \alpha$. One now finds the formula

$$\begin{aligned}\mathcal{H}_\xi = {} & \frac{1}{8(d-3)\pi G} \int_B \Omega^{-(d-4)} \left(\frac{1}{(d-2)} R_{ab} q^{ac} q^{bd} (\nabla_c l_d) \xi^e l^f \right. \\ & \left. - \Omega^{-1} \alpha^{-1} (l^{[e} - v \alpha^{-1} \nabla^{[e} \alpha) C^{f]bcd} \xi_b (l_c - v \alpha^{-1} \nabla_c \alpha) \xi_d \right) \epsilon_{efa_1 \cdots a_{d-2}},\end{aligned} \tag{100}$$

where v is a function such that $\nabla_a v = l_a$. It can be verified again that this expression does not depend on the particular choice of l_a. Formula (100) can alternatively be derived by noting that any null translation ξ^a can be obtained from n^a by applying an asymptotic symmetry ϕ to the latter, $\xi^a = \phi * n^a$. Since the Bondi energy for the vector field ξ^a and metric $\tilde{g}_{ab}$ evaluated at B is equal to the Bondi energy for $n^a = \xi^{a\prime} = \phi^{-1} * \xi^a$ and metric $\tilde{g}'_{ab} = \phi^{-1} * \tilde{g}_{ab}$ evaluated at the cross section $B' = \phi(B)$, one can obtain the Bondi energy for ξ^a by applying Eq. (99) to the metric $\tilde{g}'_{ab}$ and the cross section B'. The above expression (100) is then obtained using the formulas $\phi * g'_{ab} = \alpha^{-2} g_{ab}$, $\phi * \Omega = \alpha^{-1}\Omega$, $\phi * l^{a\prime} = \alpha l^a - v \nabla^a \alpha$, $\phi * n^{a\prime} = \alpha n^a - \Omega \nabla^a \alpha$, as well as our asymptotic flatness conditions.

Equation (100) is the main result of our paper. It holds in the gauge defined in (68). The corresponding formula for other choices of the background geometry $\bar{g}_{ab}$ can be obtained by applying the corresponding gauge transformation to our formula. In the case $d=4$, formula (100)

is not correct. An expression in $d=4$ has been given by Geroch.[10] It involves, among other things, the news tensor (given by $N_{ab}=S_{ab}-\rho_{ab}$ in $d=4$), instead of the unphysical Ricci tensor.

The first and second term in the integrand of (100) can be roughly interpreted as follows: the second term is the "Coulomb part" of the Weyl tensor (multiplied by suitable powers of Ω), and represents the "pure Coulomb contribution" to the Bondi energy. The first term represents contributions from gravitational radiation; it follows from Eq. (A2) given in Appendix A that it vanishes if and only if the news tensor, N_{ab}, and hence the flux, vanishes. In four dimensions, it can be proven[10] that the news tensor, and hence the radiative contribution to the Bondi energy, always vanishes in stationary space–times. It would be interesting to see whether an analog of this result holds in d dimensions.

In the d-dimensional analog of Schwarzschild space–time given by the line element (5), the Bondi energy is evaluated as follows. The term involving R_{ab} in our expression (100) for the Bondi energy does not contribute, showing that there is no radiative contribution to the Bondi energy. The Coulomb contribution is found to be $\Omega^{-(d-3)}C^{abcd}l_a n_b l_c n_d = c(d-2)(d-3)/4$ at $\mathscr{I}$. Normalizing α so that $\alpha n^a - \Omega\nabla^a\alpha$ is equal to the timelike Killing field t^a of the metric (5) at infinity gives

$$\mathcal{H}_{\alpha n} = \frac{c(d-2)A_{d-2}}{16\pi G} \quad \left(= \frac{c}{2G} \text{ in four dimensions}\right), \tag{101}$$

where A_{d-2} is the area of the unit sphere S^{d-2}. This coincides with the ADM mass of the space–time (5) (given, e.g., in Ref. 20), as we expect.

VI. CONCLUSIONS

We have given a geometrical definition of the asymptotic flatness at null infinity in space–times of even dimension d greater than four within the framework of conformal infinity. Our definition was shown to be stable against perturbations to linear order and was shown to be stringent enough to allow one to define the total energy of the system viewed from null infinity as the generator conjugate to an asymptotic time translation. We proposed to take this notion of energy as the natural generalization of the Bondi energy to higher dimensions. Our definitions of asymptotic flatness and the Bondi energy differ qualitatively from the corresponding definitions in $d=4$; although the asymptotic structure of null infinity in higher dimensions parallels that in four dimensions in some ways, the latter seems to be a rather special case on the whole compared to general $d>4$.

Our definitions and constructions related to asymptotic flatness and Bondi energy do not work in odd space–time dimensions, essentially because the unphysical metric seems to have insufficient regularity properties at null infinity in that case. The case of odd dimensional theories of gravity therefore remains open. Apart from this issue, the analysis given in this paper could be generalized in two obvious ways: (1) by including matter fields, and (2) by admitting higher derivative terms such as the square of the scalar curvature in the gravitational action.

With regard to the first possibility, one would first have to formulate appropriate asymptotic conditions on the matter fields, which in practice would presumably be found by performing a perturbation analysis. We expect the analysis given in Sec. III of this paper to generalize straightforwardly to include conformally invariant fields such as a conformally coupled scalar field, or an Abelian p-form gauge field A [with Lagrangian density $L=\mathrm{d}A\wedge *(\mathrm{d}A)$] in $d=2p+2$ space–time dimensions. This kind of analysis should also still work for other (nonconformally invariant) massless fields. For massive fields a different kind of analysis is probably needed, although we expect on physical grounds that these fields have the best (i.e., exponential) drop off behavior at null infinity. Altogether, we expect that the asymptotic conditions for the combined metric and matter fields are given by the conditions given in Sec. II for the metric, plus a condition of the form $T_{ab}=O(\Omega^s)$ for the stress energy of the matter fields, where s is a suitable number. With these conditions in place, a derivation of the Bondi energy can presumably be given in close parallel to our analysis in Sec. V.

With regard to the second possibility, it is much less clear to us what the likely asymptotic conditions on the gravitational fields might be in that case, or even how they depend on the actual form of the Lagrangian. In fact, it is not even clear to us that there will generically be *any* reasonable definition of asymptotic flatness that is stable under linear perturbations. Moreover, the linearized equations will now have more derivatives and are therefore presumably harder to analyze than the linearized Einstein's equations. One may ignore the issue of stability and simply try to repeat the analysis of this paper and Ref. 14 using the asymptotic flatness conditions of Sec. II which have been shown to work for general relativity. However, even though an expression for the Bondi energy might be found in this way, its physical significance would be far from clear under these circumstances.

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APPENDIX A: DERIVATION OF EQUATION (84)

In this appendix we derive expression (84) for P^a as a solution to the equation

$$\nabla^a P_a = \frac{1}{32\pi G}\alpha\Omega^{-(d-4)} S_{ab}S_{cd}q^{ac}q^{bd} + O(\Omega). \tag{A1}$$

It follows from Eqs. (3) and (4) that the covector l_a can be chosen in such a way that the following conditions are satisfied:

$$\nabla_a l_b = O(\Omega^{(d-4)/2}), \quad l^a l_a = O(\Omega^{(d-2)/2}), \quad l_a n^a = 1 + O(\Omega^{d/2}) \tag{A2}$$

[for example, take $l_a = g_{ab}\overline{l^b}$, where $\overline{l^a}$ is a vector field on $\overline{M}$ such that $\overline{g_{ab}}\,\overline{l^a}\,\overline{l^b} = \overline{\nabla_a}\,\overline{l^b} = 0$ and $\overline{l^a}(\mathrm{d}\Omega)_a = 1$ in a neighborhood of $\partial\overline{M}$]. We assume from now on that l_a has been chosen in this way.

From the defining relation for S_{ab}, together with Eq. (62), we have

$$2n^a\nabla_{[a}\nabla_{b]}l_c = R_{abcd}n^a l^d = C_{abcd}n^a l^d + \tfrac{1}{2}S_{db}n_c l^d - \tfrac{1}{2}S_{cb} - \tfrac{1}{2}l_b\nabla_c f + \tfrac{1}{2}g_{bc}l^d\nabla_d f. \tag{A3}$$

Contracting this equation with $S_{de}q^{bd}q^{ce}$, and making use of the relations $S_{ab}n^b = -\nabla_a f$, $\nabla_a f = \kappa n_a$, $\kappa = O(\Omega^{(d-2)/2})$ and Eq. (A2), gives

$$\Omega^{-(d-4)}S_{ab}S_{cd}q^{ac}q^{bd} = -4\Omega^{-(d-4)}n^a(\nabla_{[a}\nabla_{b]}l_c)S_{de}q^{bd}q^{ce} + 2\Omega^{-(d-4)}C_{abcf}n^a l^f S_{de}q^{bd}q^{ce} + O(\Omega). \tag{A4}$$

Thus, the task is to show that the right-hand side of this equation can be written as a constant times the divergence of P^a, plus terms of order Ω.

We now evaluate the right-hand side of Eq. (A4) up to order Ω, proceeding term by term and make heavy use of the drop-off conditions, Eq. (A2) and (69). For the second term in Eq. (A4) containing the Weyl tensor, we have, using the symmetry of the Weyl tensor $C_{abcd} = C_{cdab}$,

$$
\begin{aligned}
2\Omega^{-(d-4)}C_{abcf}n^a l^f S_{de}q^{bd}q^{ce} &= 2\Omega^{-(d-4)+1}(\nabla_{[c}S_{f]b})l^f S_{de}q^{bd}q^{ce} \\
&= 2\Omega\nabla_{[c}(\Omega^{-(d-4)/2}S_{f]b})l^f q^{cd}q^{be}(\Omega^{-(d-4)/2}S_{de}) \\
&\quad + (d-4)\Omega^{-(d-4)}n_{[c}S_{f]b}l^f q^{cd}q^{be}S_{de} \\
&= -\frac{(d-4)}{2}\Omega^{-(d-4)}S_{ab}S_{cd}q^{ac}q^{bd} + O(\Omega),
\end{aligned} \tag{A5}
$$

where the identity [compare Eq. (9) of Ref. 10]

$$
\Omega\nabla_{[a}S_{b]c} + C_{abcd}n^d = 0 \tag{A6}
$$

has been used in the first line. Note that the term (A5) is of order Ω in four dimensions, in accordance with the fact that by Theorem 11 of Ref. 10, the unphysical Weyl tensor vanishes at $\mathscr{I}$ in four dimensions. We next turn to the first term on the right-hand side of Eq. (A4). This can be written as

$$
\begin{aligned}
-4\Omega^{-(d-4)}n^a(\nabla_{[a}\nabla_{b]}l_c)S_{de}q^{bd}q^{ce} &= -4\nabla_a(\Omega^{-(d-4)}S_{de}q^{ce}q^{d[b}n^{a]}\nabla_b l_c) \\
&\quad + 4\Omega^{-(d-4)}(\nabla_a S_{de})q^{ce}q^{d[b}n^{a]}\nabla_b l_c + O(\Omega).
\end{aligned} \tag{A7}
$$

In the second term on the right-hand side, we may replace $\nabla_a S_{ed}$ by the expression $2\nabla_{[a}S_{e]d}$, because

$$
\begin{aligned}
\Omega^{-(d-4)}(\nabla_e S_{ad})q^{ce}q^{d[b}n^{a]}\nabla_b l_c &= \tfrac{1}{2}\Omega^{-(d-4)}[(\nabla_e\nabla_d f)q^{db}q^{ce} - (\nabla_e S_m{}^m)q^{ce}n^b \\
&\quad - 2\nabla_e(l^a\nabla_a f)q^{ce}n^b]\nabla_b l_c + O(\Omega) = O(\Omega),
\end{aligned} \tag{A8}
$$

where we have used that

$$
\nabla_a S_m{}^m = \nabla_m S_a{}^m \tag{A9}
$$

by the Bianchi identities, that $S_m{}^m = O(\Omega^{(d-2)/2})$ and that $\nabla_a f = \kappa n_a$, $\kappa = O(\Omega^{(d-2)/2})$. We can now apply the identity (A6) to write the right-hand side of Eq. (A7) as

$$
\begin{aligned}
&= -4\nabla_a(\Omega^{-(d-4)}S_{de}q^{ce}q^{d[b}n^{a]}\nabla_b l_c) - 8\Omega^{-(d-3)}C_{aedf}q^{ce}q^{d[b}n^{a]}n^f\nabla_b l_c + O(\Omega) \\
&= -4\nabla_a(\Omega^{-(d-4)}S_{de}q^{ce}q^{d[b}n^{a]}\nabla_b l_c) - 4\Omega^{-(d-3)}C_{aedf}n^a n^f\nabla^d l^e \\
&\quad + 4\Omega^{-(d-3)}C_{aedf}n^a n^f l^e n^c\nabla^d l_c + O(\Omega) \\
&= -4\nabla_a(\Omega^{-(d-4)}S_{de}q^{ce}q^{d[b}n^{a]}\nabla_b l_c) \\
&\quad + 4\nabla^d(\Omega^{-(d-3)}C_{dfea}n^f l^e n^a) + 4\Omega^{-(d-3)}C_{aedf}n^a n^f l^e n^c\nabla^d l_c \\
&\quad + 4\Omega^{-(d-3)}C_{aedf}l^e n^f\nabla^d n^a + O(\Omega),
\end{aligned} \tag{A10}
$$

where we have used the tracelessness and symmetries of the Weyl tensor and Eqs. (A2) and (69) in the second line, and where we have used [compare Eq. (12) of Ref. 10]

$$
\Omega\nabla^d C_{abcd} + C_{abcd}n^d = 0 \tag{A11}
$$

in the third line. Using Einstein's equation (53), the last term in the last line of Eq. (A10) is seen to be equal to $+2\Omega^{-(d-4)}C_{adef}n^a l^f S^{de}$, up to terms of order Ω. Using Eqs. (A5) and (A6), this term can be further rewritten as

$$
\begin{aligned}
2\Omega^{-(d-4)}C_{adef}n^a l^f S^{de} &= 2\Omega^{-(d-4)}C_{adef}n^a l^f S_{bc}q^{bd}q^{ec} + 2\Omega^{-(d-4)+1}(\nabla_{[e}S_{f]d})l^f n^e l^c q^{bd}S_{bc} \\
&\quad - 2\Omega^{-(d-4)+1}(\nabla_{[e}S_{f]d})l^f l^d q^{ec}\nabla_c f \\
&= -\frac{(d-4)}{2}\Omega^{-(d-4)}S_{ab}S_{cd}q^{ac}q^{bd} + \Omega^{-(d-4)+1}(n^e\nabla_e S_{df})l^f l^c q^{bd}S_{bc} \\
&\quad - \Omega^{-(d-4)+1}(\nabla_f S_{de})n^e l^f l^c q^{bd}S_{bc} + O(\Omega) \\
&= -\frac{(d-4)}{2}\Omega^{-(d-4)}S_{ab}S_{cd}q^{ac}q^{bd} + \Omega^{-(d-4)+1}(\nabla_f\nabla_d f + S_{de}\nabla_f n^e)l^f l^c q^{bd}S_{bc} + O(\Omega) \\
&= -\frac{(d-4)}{2}\Omega^{-(d-4)}S_{ab}S_{cd}q^{ac}q^{bd} + O(\Omega). \qquad \text{(A12)}
\end{aligned}
$$

The term $+4\Omega^{-(d-3)}C_{aedf}n^a n^f l^e n^c \nabla^d l_c$ on the right-hand side of Eq. (A10) can be seen to be of order Ω by using the identities

$$
n^c\nabla^d l_c = \nabla^d(n^c l_c) - (\nabla^d n^c)l_c = O(\Omega^{(d-2)/2}), \qquad \text{(A13)}
$$

$$
C_{aedf}n^a n^f = -\frac{\Omega}{2}(n^a\nabla_a S_{ed} + \nabla_e\nabla_d f + (\nabla_e n^a)S_{ad}) = O(\Omega^{(d-2)/2}). \qquad \text{(A14)}
$$

Substituting now Eqs. (A10) and (A5) back into Eq. (A4), we obtain

$$
-(d-3)\Omega^{-(d-4)}S_{ab}S_{cd}q^{ac}q^{bd} = 4\nabla_a[\Omega^{-(d-4)}(S_{de}q^{ce}q^{d[b}n^{a]}\nabla_b l_c - \Omega^{-1}C^{abcd}n_b l_c n_d)] + O(\Omega), \qquad \text{(A15)}
$$

from which Eq. (A1) follows immedliately.

APPENDIX B: CONFORMAL GAUGE CHOICES

In this appendix we review transformations related to the conformal completion of Minkowski space–time, thereby eludicating our gauge choice (68) for the background geometry. Let us denote by x^μ the usual Cartesian coordinates of Minkowski space–time $(\mathbb{R}^d, \tilde{\eta}_{ab})$. Introducing the radial coordinate

$$
r = \sqrt{\sum_{\mu=1}^{d-1}(x^\mu)^2} \qquad \text{(B1)}
$$

and $t = x^0$, the Minkowski metric can be rewritten as

$$
\mathrm{d}\tilde{s}^2 = -\mathrm{d}t^2 + \mathrm{d}r^2 + r^2\,\mathrm{d}\sigma^2 = \Omega^{-2}\{-\mathrm{d}T^2 + \mathrm{d}\psi^2 + \sin^2\psi\,\mathrm{d}\sigma^2\}, \qquad \text{(B2)}
$$

where $\mathrm{d}\sigma^2$ is the line element of the unit sphere S^{d-2}, and where

$$
\Omega = 2\cos\frac{T+\psi}{2}\cos\frac{T-\psi}{2}. \qquad \text{(B3)}
$$

The coordinates T, ψ are defined by

$$
\frac{T+\psi}{2} = \tan^{-1}(t+r), \quad \frac{T-\psi}{2} = \tan^{-1}(t-r). \qquad \text{(B4)}
$$

We view these relations as a map λ from the portion $\bar{M} = \{-\pi < T \pm \psi < \pi, \psi \geqslant 0\}$ of the Einstein static universe $\mathbb{R}\times S^{d-1}$ to Minkowski space–time $\mathbb{R}^d$. In other words,

$$\overline{g}_{ab} = \Omega^2 \lambda * \tilde{\eta}_{ab}, \tag{B5}$$

where $\overline{g}_{ab}$ is the metric of the Einstein static universe. The boundary of $\overline{M}$ corresponds to the conformal infinity of Minkowski space–time. It is naturally divided into future/past timelike infinity, future/past null infinity $\mathscr{I}^{\pm}$, and spatial infinity. The conformal factor Ω is well defined and smooth in a neighborhood of the null infinities $\mathscr{I}$, and vanishes there. The metric $\overline{g}_{ab}$ is conformally flat (implying $\overline{C}_{abcd}=0$), but not flat, $\overline{S}_{ab} \neq 0$.

If we change

$$\overline{g}_{ab} \to k^2 \overline{g}_{ab}, \quad \Omega \to k\Omega, \tag{B6}$$

with k a nonvanishing smooth scalar function defined in a neighborhood of $\overline{M}$ in the Einstein static universe which does not vanish at $\mathscr{I}$, then the physical metric remains unchanged, and the unphysical metric and the conformal factor remain smooth at $\mathscr{I}$. One may use this gauge freedom to make suitable "gauge choices" for the unphysical metric, and we will now discuss some of the choices that are being made in the main part of the paper. Let B be a cross section of, say future, null infinity which does not intersect spatial infinity. Then it is possible to choose Ω so that $\overline{g}_{ab}$ is Minkowskian in an open neighborhood of B not intersecting spatial infinity. This can be seen as follows.

Any neighborhood of the indicated form is contained in the causal future of some point in the interior of the space–time, which of course, corresponds to the interior of a future directed light cone V^+, whose apex we may assume to be at the origin,

$$V^+ = \{x^\mu | x^\mu x_\mu < 0, x^0 > 0\}. \tag{B7}$$

A conformal factor, Ω, defined on V^+ such that $\overline{g}_{ab}$ is flat and Minkowskian and such that the gauge condition (68) is satisfied can be constructed as follows. Consider the map ϕ,

$$\phi: x^\mu \to x'^\mu = \frac{a^\mu + b^\mu x^\lambda x_\lambda + 2q^{\mu\nu} x_\nu}{2b^\nu x_\nu},$$

$$a^\mu = (1,-1,0,\ldots,0), \quad b^\mu = (1,1,0,\ldots,0), \quad q^{\mu\nu} = \eta^{\mu\nu} + a^{(\mu} b^{\nu)}, \tag{B8}$$

which maps points of the interior of V^+ bijectively into points in the "right wedge" W of Minkowski space–time

$$W = \{x^\mu | x^1 \geqslant |x^0|\}. \tag{B9}$$

The portion of $\mathscr{I}^+$ lying in the causal future of V^+ corresponds, under the map ϕ, to the "upper horizon" of W, defined by $\partial W^+ = \{x^\mu | b^\mu x_\mu = 0, x^0 > 0\}$. The cross section of $\mathscr{I}^+$ corresponding to the light rays outgoing from the apex of V_+ corresponds to the "edge" $(x^0=0=x^1)$ of the wedge, whereas the light rays themselves are represented by the null curves generated by $a^\mu(\partial/\partial x^\mu)^a$ on the "lower horizon" of W, given by $\partial W^- = \{x^\mu | a^\mu x_\mu = 0, x^0 < 0\}$. We find that this map ϕ is a conformal isometry of Minkowski space–time with conformal factor

$$\Omega = b_\mu x^\mu, \tag{B10}$$

i.e., the background metric $\overline{g}_{ab} = \Omega^2 \phi * \tilde{\eta}_{ab}$ is Minkowskian. The quantities $\overline{f}, \overline{n}^a$ associated with this choice of conformal factor are

$$\overline{f} = 0, \quad \overline{n}^a = b^\mu \left(\frac{\partial}{\partial x^\mu} \right)^a, \quad \overline{\nabla}_a \overline{n}^b = 0. \tag{B11}$$

Thus, the conformal transformation (B8) with conformal factor (B10) satisifies our gauge condition (68).

An awkward feature of the map ϕ is that it is not globally defined on the boundary of V^+, for the single null generator corresponding to $x'^\mu = \lambda b^\mu$, $\lambda > 0$ of the boundary of V^+ is mapped to infinity. Consequently, there is also a single corresponding generator of $\mathscr{I}^+$ which is not represented as a corresponding generator of ∂W^+, or, stated differently, is mapped to the null generator at infinity of the upper horizon ∂W^+ (corresponding to $b_\mu x^\mu = 0$, $x^0 > 0$ but $x^{\mu=2,\ldots,d-1} \to \pm\infty$). Consequently, the cross sections of $\mathscr{I}^+$ within the causal future of V^+ now correspond to noncompact cross sections of the upper horizon of W (of topolgy $\mathbb{R}^{d-2}$). This feature of the conformal embedding ϕ has the undesirable consequence that the integrals in Sec. V over cross sections of $\mathscr{I}^+$ inside V^+ are now integrals over a noncompact set and therefore the convergence issue must be addressed. An example of such an integral is $\int_{\mathcal{S}} \Theta$, where Θ is the symplectic potential $(d-1)$-form introduced in Eq. (63), and where $\mathcal{S}$ is a segment of $\mathscr{I}^+$. We will now explain how the convergence issue is dealt with in this example.

For this purpose, it is useful to introduce another conformal transformation:

$$\psi: x^\mu \to x'^\mu = \frac{(x+t)^\nu (x+t)_\nu t^\mu + 2(x+t)^\mu}{(x-t)^\lambda (x-t)_\lambda}, \quad t^\mu = (1,0,0,\ldots,0), \tag{B12}$$

which maps points in V^+ into points of the interior of a double cone K of Minkowski space–time,

$$K = \{ x^\mu \,|\, |x^0| + r \leqslant 1 \}. \tag{B13}$$

This map also provides a conformal isometry of Minkowski space–time with conformal factor

$$\Omega' = -(x-t)^\mu (x-t)_\mu, \tag{B14}$$

rendering the metric $\overline{g'}_{ab} = \Omega'^2 \psi^* \tilde{\eta}_{ab}$ Minkowskian in the portion of space–time corresponding to the interior of the future light cone V^+. The derivative operator $\overline{\nabla'}_a$ compatible with $\overline{g'}_{ab} = \Omega'^2 \psi^* \tilde{\eta}_{ab}$ is simply equal to the coordinate derivative operator $\partial/\partial x^\mu$ associated with Cartesian coordinates. The portion of $\mathscr{I}^+$ that can be reached from within V^+ corresponds precisely to the points x^μ in K such that $\Omega' = 0$, i.e., the "upper cap" of the double cone K, defined by $\partial K^+ = \{x^\mu \,|\, x^0 + r = 1, x^0 > 0\}$. Future timelike infinity corresponds to the apex $x^\mu = t^\mu$ of the upper cap. The apex of V^+ corresponds to the apex of the lower cap of K given by $x^\mu = -t^\mu$, and the light rays going out from the apex of V_+ correspond to the null generators of the lower cap, ∂K^-, of K. We should note that this choice of conformal factor Ω' does not satisfy our gauge condition (68), as the quantities $\overline{n'}^a, \overline{f'}$ associated with Ω' satisfy

$$\overline{f'} = 4, \quad \overline{n'}^a = -2(x-t)^\mu \left(\frac{\partial}{\partial x^\mu}\right)^a, \quad \overline{\nabla'}_a \overline{n'}^b = -2\delta_a{}^b. \tag{B15}$$

The advantage of the conformal transformation (B12) with conformal factor Ω' is however that it preserves the compactness of cross sections of $\mathscr{I}^+$. In fact, the cross section of $\mathscr{I}^+$ corresponding to the outgoing light rays from the apex of V^+ is represented by the "belt" of K ($x^0 = 0, r = 1$), and all other cross sections to the future of this particular one are given by cross sections of the upper cap, and are therefore topological spheres.

We compose the two maps ϕ and ψ to the map $\sigma = \phi \circ \psi^{-1}: K \to W$. Under the map σ the set ∂W^+ is identified with the upper cap ∂K^+ of the double cone K. If we denote $\overline{g}_{ab}$ the Minkowskian metric of W, then under this map, $\overline{g}_{ab}$ gets mapped to the metric $k^{-2}\overline{g'}_{ab}$, where $\overline{g'}_{ab}$ is the Minkowskian metric on K, and where k is calculated to be

$$k = (x - t + b)^\mu (x - t + b)_\mu. \tag{B16}$$

The conformal factor k vanishes on the single null generator emanating from future timelike infinity (represented by the point $x^\mu = t^\mu$ of ∂K^+) parallel to b^μ. This generator corresponds to the generator at infinity in ∂W^+ under the map σ, and the vanishing of k on this generator is a reflection of this fact. (In other words, ∂K^+ is the comactification of ∂W^+).

Returning to the example integral, let $\mathcal{S}$ be a segment of $\mathscr{I}^+$, viewed as a subset of the upper horizon ∂W^+ of W, with noncompact cross sections, i.e., $\mathcal{S}$ has topology $\mathbb{R}^{d-2}\times I$, where I is a compact interval. Let $\mathcal{S}'$ be the segment of ∂K^+ corresponding to $\mathcal{S}$ under σ, i.e., $\sigma(\mathcal{S}')=\mathcal{S}$. Then $\mathcal{S}'$ has compact cross sections homeomorphic to $\mathcal{S}^{d-2}$ as ∂K^+ does. By Eq. (66) the symplectic form satisfies

$$\int_{\mathcal{S}} \Theta = \int_{\mathcal{S}'} \Theta' + \delta \int_{\mathcal{S}'} \Pi', \tag{B17}$$

where Θ' is given in terms of $\Omega' = k^{-1}\sigma^*\Omega$, $g'_{ab} = k^2\sigma^* g_{ab}$, and $\tau'_{ab} = k^{(d-2)/2}\sigma^*\tau_{ab}$ by a formula analogous to (63), and where Π' is given by Eq. (67). Using that $n'^a = -2(x^\mu - t^\mu)(\partial/\partial x^\mu)^a$ by Eq. (B15), as well as the above expression (B16) for the conformal factor k, one immediately finds that

$$k^{-1} n'^a \nabla'_a k = -2 \tag{B18}$$

at points of ∂K^+. Inserting this into the definition of Π', one gets

$$\Pi' = \frac{(d-2)}{2^5 \pi G} \Omega'^{-(d-2)} (g' - \overline{g}')_{cd} q'^{ce} q'^{df} (g' - \overline{g}')_{ef}{}^{(d-1)} \boldsymbol{\epsilon}'. \tag{B19}$$

Now Π' and Θ' are finite at $\mathscr{I}$ as a result of our asymptotic flatness conditions, and the integrals on the right-hand side of Eq. (B17) are over a compact set, $\mathcal{S}'$ of $\mathscr{I}$ (viewed as a subset of the upper cap ∂K^+ via the map σ). This shows that the integral of the symplectic potential over $\mathcal{S}$ appearing on the left-hand side of Eq. (B17) is convergent. The same kind of argument can be made for other integrals appearing in Sec. V.

APPENDIX C: ASYMPTOTIC TRANSLATIONS

We finally discuss the space of translational asymptotic symmetries ξ^a of the form $\xi^a = \alpha n^a - \Omega \nabla^a \alpha$ in $d>4$ dimensions. As discussed in Sec. V, in order for such a vector field to be an asymptotic symmetry, we must satisfy Eqs. (78), (79), and (80) which we here repeat for convenience,

$$\nabla_a \nabla_b \alpha - \Omega^{-1} g_{ab} n^c \nabla_c \alpha = O(\Omega^{(d-4)/2}), \tag{C1}$$

$$\nabla^b (\Omega^{-1} n^a \nabla_a \alpha) = O(\Omega^{(d-4)/2}), \tag{C2}$$

$$\Omega^{-1} n^b \nabla_b (\Omega^{-1} n^a \nabla_a \alpha) = O(\Omega^{(d-4)/2}). \tag{C3}$$

These equations hold in any conformal gauge choice satisfying Eq. (68). Actually, by our asymptotic flatness conditions, if these conditions are satisfied for one given asymptotically flat metric, they are satsified for any asymptotically flat metric [satisfying our gauge choice (68)]. In order to analyze these equations, we may therefore choose g_{ab} to be equal to our Minkowskian background metric $\overline{g}_{ab} = \Omega^2 \phi^* \tilde{\eta}_{ab}$, where ϕ is the conformal map $V_+ \to W$ defined in Eq. (B8), and where the conformal factor is defined in Eq. (B10). The derivative operator $\overline{\nabla}_a$ is then given by the coordinate derivative operator $\partial/\partial x^\mu$, and the associated quantity $\overline{n^a}$ is given by b^μ in Cartesian coordinates. Inserting these expressions and going to Cartesian coordinates, Eqs. (C1), (C2), and (C3) become, respectively,

$$\partial_\mu \partial_\nu \alpha + 2\eta_{\mu\nu} w^{-1} \partial_v \alpha = O(w^{(d-4)/2}), \tag{C4}$$

$$\partial_\mu (w^{-1} \partial_v \alpha) = O(w^{(d-4)/2}), \tag{C5}$$

$$w^{-1}\partial_v(w^{-1}\partial_v\alpha) = O(w^{(d-4)/2}), \tag{C6}$$

where we have now set $w=x^0-x^1$ and $v=x^0+x^1$, and where we remember that the location of null infinity corresponds to $\Omega=-w=0$ in our gauge.

Let us first check that the timelike translational Killing vector fields

$$\tau^a = \tau^\mu\left(\frac{\partial}{\partial x^\mu}\right)^a, \quad \tau^\mu = (\tau^0, \tau^1, \ldots, \tau^{d-1}) = \text{const} \tag{C7}$$

in Minkowski space–time give rise to solutions of Eqs. (C4). Under the identification provided by the map ϕ, these vector fields correspond to

$$\xi^a = \phi * \tau^a = (\alpha b^\mu - \Omega\partial^\mu\alpha)\left(\frac{\partial}{\partial x^\mu}\right)^a = \alpha\overline{n}^a - \Omega\overline{\nabla}^a\alpha, \tag{C8}$$

where

$$\alpha = \tfrac{1}{2}(b^\lambda\tau_\lambda x^\mu x_\mu + 2q_{\mu\nu}\tau^\mu x^\nu + a^\mu\tau_\mu). \tag{C9}$$

By construction, since ϕ is a conformal isometry of Minkowski space–time, we must have

$$\partial_\mu\partial_\nu\alpha + 2\eta_{\mu\nu}w^{-1}\partial_v\alpha = 0, \tag{C10}$$

which can also be verified explicitly. This shows Eq. (C4), and the other equations (C5) and (C6) follow by dotting b^μ into this equation. It is not difficult to see that (in $d>4$), any other solution α to Eqs. (C4), (C5), and (C6) is given by

$$\alpha = \alpha_0 + O(\Omega^{d/2}), \tag{C11}$$

where α_0 is given by Eq. (C9). Inserting this into the definition of χ_{ab}, Eq. (77), we see that

$$\chi_{ab} = \chi_{0ab} + O(1)n_a n_b + O(\Omega), \tag{C12}$$

where χ_{0ab} is defined by Eq. (77), with α replaced by α_0. Now the integrand of the flux associated with an asymptotic symmetry is given by [see Eq. (71)] $N_{ab}\chi^{ab}$ up to numerical factors, and $N_{ab}n^b=0$. Thus, the second term in Eq. (C12) does not contribute to the flux. This shows that the α_0 given by Eq. (C9) are essentially the only solutions to Eqs. (C4), in the sense that any other solution will give rise to the same flux. Hence, the vector space of infinitesimal asymptotic translations is d dimensional in $d>4$, consists of the vector fields $\xi^a=\alpha n^a-\Omega\nabla^a\alpha$, with α given by Eq. (C9) in the gauge that we are working in.

Let us finally characterize the α corresponding to a future directed timelike translational Killing fields τ^μ of Minkowski space–time. A point x^μ of $\mathscr{I}^+$ corresponds to a point on ∂W^+ under the map ϕ, so we have $b^\mu x_\mu=0$ and $x^\lambda x_\lambda = q_{\mu\nu}x^\mu x^\nu$ for such points. Also, since τ^μ is future pointing timelike, we have $a^\mu\tau_\mu b^\nu\tau_\nu > q_{\mu\nu}\tau^\mu\tau^\nu$. Using this, and the inequality obtained by expanding out the relation

$$0 \leqslant q_{\mu\nu}[(b^\lambda\tau_\lambda)^{-1/2}\tau^\mu + (b^\lambda\tau_\lambda)^{1/2}x^\mu][(b^\sigma\tau_\sigma)^{-1/2}\tau^\nu + (b^\sigma\tau_\sigma)^{1/2}x^\nu], \tag{C13}$$

one easily finds that $\alpha>0$ on ∂W^+. Conversely, if τ^μ is such that $\alpha>0$ on ∂W^+, then one sees by the same argument that it must be future directed timelike. Thus, future directed timelike translational Killing fields correspond to asymptotic symmetries ξ^a with $\alpha>0$ on $\mathscr{I}^+$.

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[21] A generalization of the Bondi–Metzner–Sachs group to higher dimensions has been discussed in the context of supergravity (Ref. 5). The definition of asymptotic flatness given in that paper differs from the definition given in the present paper.
[22] Note that throughout this paper, our convention for the $*$ operation of a p-form is $(*A)_{a_1\cdots a_{d-p}} = \epsilon_{a_1\cdots a_{d-p}}{}^{b_1\cdots b_p} A_{b_1\cdots b_p}$.

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Path description of conserved quantities of generalized periodic box-ball systems

Jun Mada[a)]
Graduate School of Mathematical Sciences, University of Tokyo, 3-8-1 Komaba, Tokyo 153-8914, Japan

Makoto Idzumi[b)]
Department of Mathematics, Faculty of Education, Shimane University, Matsue 690-8504, Japan

Tetsuji Tokihiro[c)]
Graduate School of Mathematical Sciences, University of Tokyo, 3-8-1 Komaba, Tokyo 153-8914, Japan

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We investigate conserved quantities of periodic box-ball systems (PBBS) with arbitrary kinds of balls and box capacity greater than or equal to 1. We introduce the notion of nonintersecting paths on the two dimensional array of boxes, and give a combinatorial formula for the conserved quantities of the generalized PBBS using these paths. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1842354]

I. INTRODUCTION

The box-ball system (BBS) is a reinterpretation of a soliton cellular automaton proposed by Takahashi–Satsuma[1] as a dynamical system of balls in a one dimensional array of boxes.[2] Hence, the BBS shows both a feature of cellular automata (CA) and that of solitons.

CAs are mathematical idealizations of physical systems in which space and time are discrete, and physical quantities take on a finite set of discrete values. The CAs were originally introduced by von Neumann and Ulam as a possible idealization of biological systems, with the particular purpose of modeling biological self-reproduction. Physical systems containing many discrete elements with local interactions are often conveniently modeled as the CAs. Many biological systems have been modeled by the CAs. The CAs have also been used to study problems in number theory and their applications to tapestry design. The CAs play an important role in various fields like these.

On the other hand, the notion of a soliton arose from a peculiar solution of partial differential equations.[3,4] Actually, the system in which solitons exist has continuous and smooth mathematical structures, such as an inverse scattering method, a pseudodifferential operator, an algebraic manifold, an infinite-dimensional Lie group and so on. Because of these rich structures, the soliton systems play an important role in various fields of mathematics and physics.

The reason why the BBS has these two completely different features is well explained by the notion of ultradiscretization.[5] Ultradiscretization is a limiting procedure through which we can construct piecewise linear equations or CAs from continuous equations. By taking the ultradiscrete limit, the rich mathematical structures of soliton systems are introduced to the CAs. On the other hand, the useful properties of the CAs for computer simulation are introduced to the continuous systems by inverse ultradiscretization. Using this limiting procedure, the BBSs are obtained from

[a)]Electronic mail: mada@ms.u-tokyo.ac.jp
[b)]Electronic mail: idzumi@edu.shimane-u.ac.jp
[c)]Electronic mail: toki@poisson.ms.u-tokyo.ac.jp

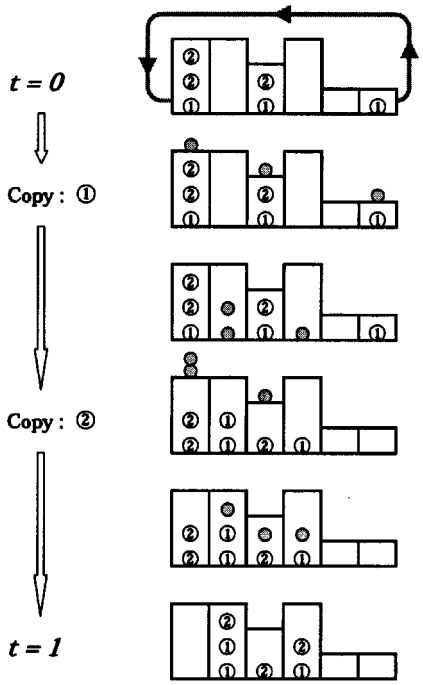

$$N = 6,\ M = 2,\ \theta_1 = \theta_2 = \theta_4 = 3,\ \theta_3 = 2,\ \theta_5 = \theta_6 = 1.$$

FIG. 1. Time evolution rule for the PBBS.

the soliton equations (the KdV equation and the Toda equation).[6,7] Thus the BBS has N soliton solutions and an infinite number of conserved quantities and the BBS is called an "integrable" CA.

The periodic box-ball system (PBBS) is the BBS in which the updating rule is extended to be compatible with a periodic boundary condition.[8] Let us consider a one-dimensional array of N boxes. A periodic boundary condition is imposed by assuming that the Nth box is adjacent to the first one. (We may imagine that the boxes are arranged in a circle.) In the generalized PBBS (gPBBS), the capacity of the nth ($1 \leqslant n \leqslant N$) box is denoted by a positive integer θ_n, and we suppose that there are M kinds of balls distinguished by an integer index j ($1 \leqslant j \leqslant M$). When ${}^{\forall}n\,\theta_n = 1$ and $M = 1$, the gPBBS coincides with the PBBS. Then, the rule for the time evolution of the gPBBS from time step t to $t+1$ is given as follows:

(1) At each box, create the same number of copies of the balls with index 1.
(2) Choose one of the copies arbitrarily and move it to the nearest box with an available space to the right of it.
(3) Choose one of the remaining copies and move it to the nearest available box on the right of it.
(4) Repeat the above procedure until all the copies have been moved.
(5) Delete all the original balls with index 1.
(6) Perform the same procedure for the balls with index 2.
(7) Repeat this procedure successively until all of the balls are moved.

An example of the time evolution of the gPBBS according to this rule is shown in Fig. 1.

In Ref. 9, we have established an algorithm to construct the conserved quantities of the gPBBS by means of the ultradiscretization of the nonautonomous discrete KP (ndKP) equation.[10] Using this algorithm, we obtain an expression for the conserved quantities of the gPBBS in the

case of one kind of balls ($M=1$). We have also proved that, when box capacities are all one, our conserved quantities for $M=1$ coincide with those described by the Young diagram.[11]

In this paper, using a path description and the results obtained in Ref. 9, we investigate the conserved quantities of the gPBBS for arbitrary M. In Sec. II, we derive the path description of the characteristic polynomial of a particular matrix. In Sec. III, we briefly summarize the results of Ref. 9, which we will use in the subsequent sections. In Sec. IV, we treat the ndKP equation which corresponds to the gPBBS. We shall obtain an explicit expression for the conserved quantities of the ndKP equation. Using the results in Sec. IV, we construct the conserved quantities of the gPBBS in Sec. V. In Sec. VI, we discuss algebraic aspects of the gPBBS with respect to the affine Weyl group and the crystals of quantum affine algebra. Section VII is devoted to concluding remarks.

II. PATH DESCRIPTION OF CHARACTERISTIC POLYNOMIAL FOR A PARTICULAR MATRIX

For a particular matrix A which contains a parameter μ in the upper half elements, we give a combinatorial description for coefficients of the characteristic polynomial $\det(\lambda I-A)$ in λ and μ in terms of nonintersecting paths (Theorem II.1). The result will be used in the subsequent sections to obtain a combinatorial formula for conserved quantities of the gPBBS.

We denote by S_X the set of all permutations of elements in $X\subset\{1,2,\ldots,N\}$. Let A be an arbitrary $N\times N$ matrix, and $A_{n,m}$ denote the (n,m) element of A. The characteristic polynomial of A is

$$\begin{aligned}\det(\lambda I-A) &= \sum_{\sigma\in S_{\{1,2,\ldots,N\}}} \operatorname{sgn}(\sigma)\prod_{i=1}^{N}(\lambda\delta_{i,\sigma(i)}-A_{i,\sigma(i)})\\ &= \sum_{k=0}^{N}(-1)^{N-k}\lambda^{k}\sum_{\substack{X\subset\{1,2,\ldots,N\}\\ \sharp X=N-k}}\sum_{\sigma\in S_X}\operatorname{sgn}(\sigma)\prod_{i\in X}A_{i,\sigma(i)},\end{aligned}$$

where $\delta_{n,m}$ is Kronecker's delta. For $J\subset X$, we set

$$S_X^J := \left\{\sigma\in S_X \,\middle|\, \begin{array}{ll} i<\sigma(i) & (i\in J),\\ i\geqslant\sigma(i) & (i\in X-J).\end{array}\right\}.$$

Since

$$S_X=\bigcup_{j=0}^{N}\bigcup_{\substack{J\subset X\\ \sharp J=j}} S_X^J \quad \text{(disjoint)},$$

we have

$$\begin{aligned}\det(\lambda I-A) &= \sum_{k=0}^{N}(-1)^{N-k}\lambda^{k}\sum_{\substack{X\subset\{1,2,\ldots,N\}\\ \sharp X=N-k}}\sum_{j=0}^{N-k}\sum_{\substack{J\subset X\\ \sharp J=j}}\sum_{\sigma\in S_X^J}\operatorname{sgn}(\sigma)\prod_{i\in X}A_{i,\sigma(i)}\\ &= \sum_{k=0}^{N}(-1)^{N-k}\lambda^{k}\sum_{j=0}^{N-k}\sum_{\substack{X\subset\{1,2,\ldots,N\}\\ \sharp X=N-k}}\sum_{\substack{J\subset X\\ \sharp J=j}}\sum_{\sigma\in S_X^J}\operatorname{sgn}(\sigma)\left(\prod_{i\in J}A_{i,\sigma(i)}\right)\left(\prod_{i\in X-J}A_{i,\sigma(i)}\right). \qquad (1)\end{aligned}$$

Now we assume

$$A = (D_0 - \Upsilon)(D_1 - \Upsilon)\cdots(D_M - \Upsilon), \tag{2}$$

where $D_i = \mathrm{diag}(x_{1,i}, x_{2,i}, \ldots, x_{N,i})$ $(i = 0, 1, \ldots, M)$ and

$$\Upsilon := \begin{bmatrix} & & & & \mu \\ 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \end{bmatrix}.$$

If we set $D_i^{(0)} := D_i$ and $D_i^{(r)} := \mathrm{diag}(x_{N-r+1,i}, x_{N-r+2,i}, \ldots, x_{N,i}, x_{1,i}, \ldots, x_{N-r,i})$ for $0 < r < N$, we have $D_i^{(r+1)}\Upsilon = \Upsilon D_i^{(r)}$. Hereafter, for $i = 0$, we define $\Sigma_{c_1<c_2<\cdots<c_i}\cdots := 1$. Then

$$A = \sum_{\ell=0}^{M+1} (-1)^\ell \left(\sum_{\substack{0\le h_1<h_2<\cdots \\ \cdots<h_{M-\ell+1}\le M}} D_{h_1}^{(h_1)} D_{h_2}^{(h_2-1)} \cdots D_{h_{M-\ell+1}}^{(h_{M-\ell+1}-M+\ell)} \right) \Upsilon^\ell.$$

We assume $M+1 < N$. The (n,m) element of A is the following.

(i) if $m = n$, $x_{n,0}x_{n,1}\cdots x_{n,M}$;
(ii) if $m = N+n-\ell$ $(\ell = 1, 2, \ldots, M)$,

$$(-1)^\ell \mu \sum_{\substack{0\le h_1<h_2<\cdots \\ \cdots<h_{M-\ell+1}\le M}} \prod_{i=1}^{M-\ell+1} x_{n-h_i+i-1,h_i};$$

(ii′) if $m = n-\ell$ $(\ell = 1, 2, \ldots, M)$,

$$(-1)^\ell \sum_{\substack{0\le h_1<h_2<\cdots \\ \cdots<h_{M-\ell+1}\le M}} \prod_{i=1}^{M-\ell+1} x_{n-h_i+i-1,h_i};$$

(iii) if $m = N+n-M-1$, $(-1)^{M+1}\mu$;
(iii′) if $m = n-M-1$, $(-1)^{M+1}$;
(iv) otherwise, 0.

Hence, from (1), we have

$$\begin{aligned} \det(\lambda I - A) = \sum_{k=0}^{N} (-1)^{N-k} \lambda^k \sum_{j=0}^{N-k} \mu^j \sum_{\substack{X\subset\{1,2,\ldots,N\} \\ \sharp X = N-k}} \sum_{\substack{J\subset X \\ \sharp J = j}} \sum_{\sigma\in S_X^J} \mathrm{sgn}(\sigma) \\ \times \left(\prod_{n\in J} \left(\sum_{\substack{0\le h_1<h_2<\cdots \\ \cdots<h_{M-N-n+\sigma(n)+1}\le M}} \prod_{i=1}^{M-N-n+\sigma(n)+1} x_{n-h_i+i-1,h_i} \right) \right) \\ \times \left(\prod_{n\in X-J} \left(\sum_{\substack{0\le h_1<h_2<\cdots \\ \cdots<h_{M-n+\sigma(n)+1}\le M}} \prod_{i=1}^{M-n+\sigma(n)+1} x_{n-h_i+i-1,h_i} \right) \right). \end{aligned} \tag{3}$$

A combinatorial description of the coefficients is possible.

By $C_{N,M+1}$ we denote the $N\times(M+1)$ boxes in Fig. 2 and by (n,m)-box the box at the nth column in the $(m+1)$th row. We assume that the Nth column is adjacent to the first one.

Let a and b be column indices $(a, b = 1, 2, \ldots, N)$. A *path* connecting the *initial point a* and the

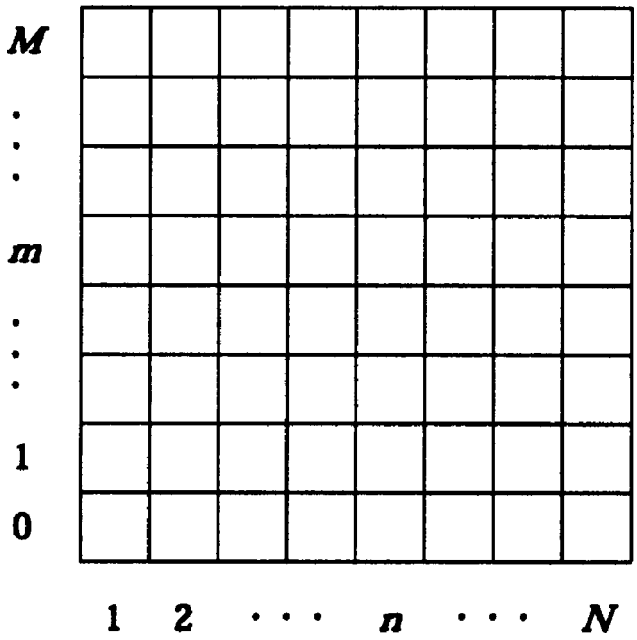

FIG. 2. $N\times(M+1)$ boxes.

end point b is a (continuous) polygonal line from the initial point *a* to the end point *b* which consists of (i), (ii) or (iii) in Fig. 3 locally; here by the initial point *a* we mean the middle point of the south edge of $(a,0)$-box and by the end point *b* the middle point of the north edge of (b,M)-box. For example, the left-hand part in Fig. 4 shows a path connecting the initial point 1 and the end point 1, and the right-hand part shows a path from 5 to 2.

There is a natural correspondence between $\Pi_{i=1}^{M-\ell+1}x_{n-h_i+i-1,h_i}$ $(0\leqslant h_1<h_2<\cdots<h_{M-\ell+1}\leqslant M)$ and a path on $C_{N,M+1}$. To put it concretely, we draw the line (i) on $(n-h_i+i-1,h_i)$-box $(i=1,2,\ldots,M-\ell+1)$; for each r, $h_i<r<h_{i+1}$, we draw the line (ii) on $(n+i-r,r)$-box and the line (iii) on $(n+i-r-1,r)$-box where $h_0=-1$ and $h_{M-\ell+2}=M+1$; then we obtain a path. For example, for $N=8$ and $M=5$, $x_{1,0}x_{1,1}x_{1,2}x_{1,3}x_{1,4}x_{1,5}$ and $x_{5,0}x_{4,2}x_{2,5}$ correspond to paths in Fig. 4, respectively.

Let $X=\{d_1,d_2,\ldots,d_{N-k}\}$ $(1\leqslant d_1<d_2<\cdots<d_{N-k}\leqslant N)$; we denote by $\mathcal{P}(d;\sigma)$ the set of all paths which connect the initial point d and the end point $\sigma(d)$ $(d\in X,\ \sigma\in S_X$; cf. Fig. 5). Define $\xi_{n,m}:\mathcal{P}(d;\sigma)\to\{x_{n,m},1\}$ as

$$\xi_{n,m}(P):=\begin{cases}x_{n,m} & (P \text{ has the vertical line on the}(n,m)\text{-box of } C_{N,M+1}),\\ 1 & (\text{otherwise}),\end{cases} \tag{4}$$

where $P\in\mathcal{P}(d;\sigma)$. Then, we obtain

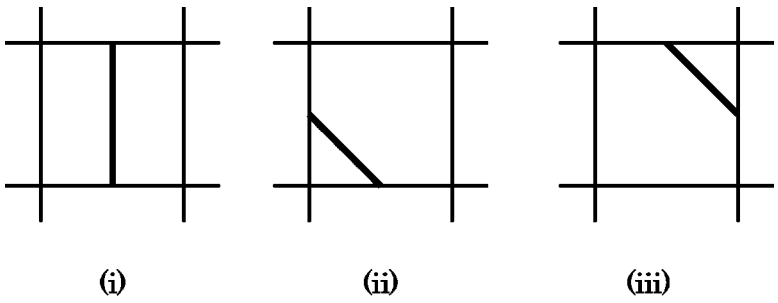

FIG. 3. A line can pass through a box in three possible ways.

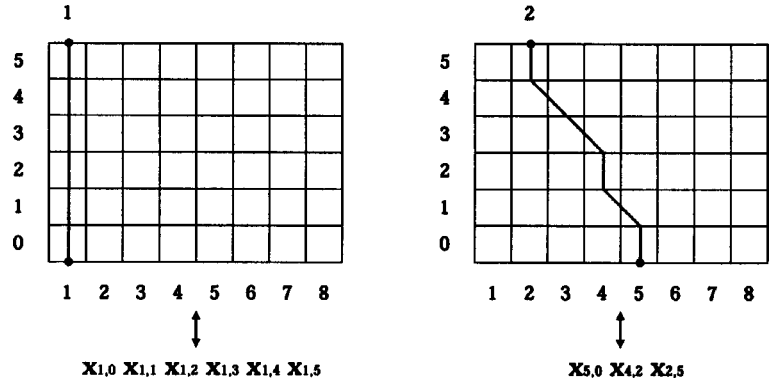

FIG. 4. Paths corresponding to $x_{1,0}x_{1,1}x_{1,2}x_{1,3}x_{1,4}x_{1,5}$ and $x_{5,0}x_{4,2}x_{2,5}$.

$$\sum_{\substack{X\subset\{1,2,\ldots,N\}\\ \sharp X=N-k}}\sum_{\substack{J\subset X\\ \sharp J=j}}\sum_{\sigma\in S_X^J}\operatorname{sgn}(\sigma)\left(\prod_{n\in J}\left(\sum_{\substack{0\leqslant h_1<h_2<\cdots\\ \cdots<h_{M-N-n+\sigma(n)+1}\leqslant M}}\prod_{i=1}^{M-N-n+\sigma(n)+1}x_{n-h_i+i-1,h_i}\right)\right)$$
$$\times\left(\prod_{n\in X-J}\left(\sum_{\substack{0\leqslant h_1<h_2<\cdots\\ \cdots<h_{M-n+\sigma(n)+1}\leqslant M}}\prod_{i=1}^{M-n+\sigma(n)+1}x_{n-h_i+i-1,h_i}\right)\right)$$
$$=\sum_{\substack{1\leqslant d_1<d_2<\cdots\\ \cdots<d_{N-k}\leqslant N}}\sum_{\substack{J\subset X\\ \sharp J=j}}\sum_{\sigma\in S_X^J}\sum_{P_1\in\mathcal{P}(d_1;\sigma)}\cdots\sum_{P_{N-k}\in\mathcal{P}(d_{N-k};\sigma)}\operatorname{sgn}(\sigma)\prod_{i=1}^{N-k}\prod_{n=1}^{N}\prod_{m=0}^{M}\xi_{n,m}(P_i). \tag{5}$$

If we draw $N-k$ paths $P_1\in\mathcal{P}(d_1;\sigma),\ldots,P_{N-k}\in\mathcal{P}(d_{N-k};\sigma)$ on $C_{N,M+1}$, some paths may go

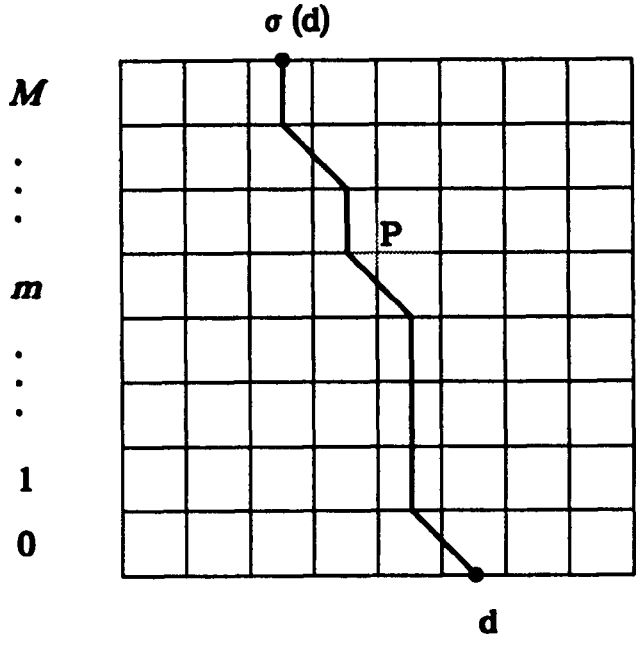

FIG. 5. A path $P\in\mathcal{P}(d;\sigma)$.

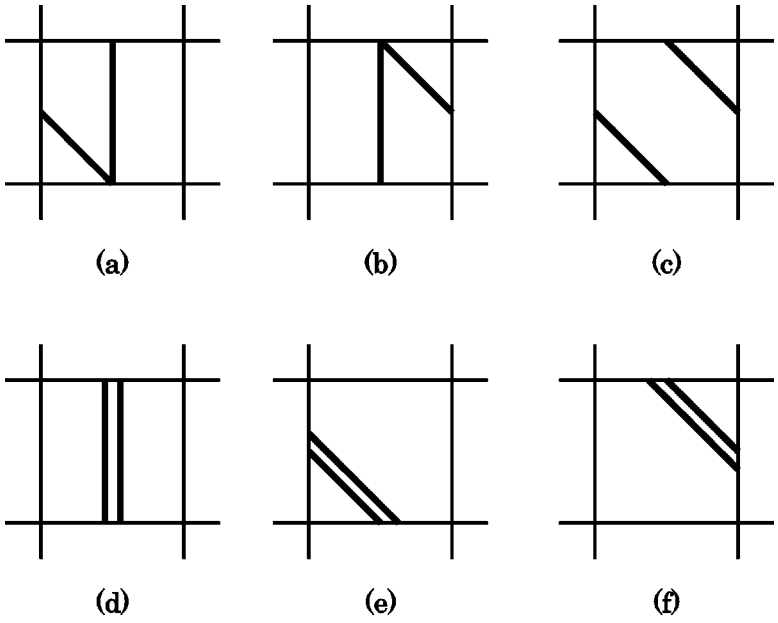

FIG. 6. Two lines can pass through a box in six possible ways.

through the same box (cf. Fig. 6). When two paths pass through a single box, there are six possible states as shown in Fig. 6. Except for the state (c) in Fig. 6, the lines touch each other. When the lines touch each other, we say that the lines *intersect*.

Now we show that, in (5), terms corresponding to intersecting paths cancel out. Let $P_{i_1} \in \mathcal{P}(d_{i_1};\sigma)$ and $P_{i_2} \in \mathcal{P}(d_{i_2};\sigma)$ be paths which intersect $(i_1 < i_2)$. Then at some box, the state (a) occurs as in the left-hand part of Fig. 7. Let P'_{i_1} and P'_{i_2} denote new paths constructed from P_{i_1} and P_{i_2} by exchanging lines in the box as shown in Fig. 7, where $P'_{i_1} \in \mathcal{P}(d_{i_1};\sigma')$, $P'_{i_2} \in \mathcal{P}(d_{i_2};\sigma')$ and

$$\sigma' = \begin{pmatrix} d_1 & \cdots & d_{i_1} & \cdots & d_{i_2} & \cdots & d_{N-k} \\ \sigma(d_1) & \cdots & \sigma(d_{i_2}) & \cdots & \sigma(d_{i_1}) & \cdots & \sigma(d_{N-k}) \end{pmatrix}.$$

Since $\mathrm{sgn}(\sigma) = -\mathrm{sgn}(\sigma')$ and $\xi_{n,m}(P'_{i_1})\xi_{n,m}(P'_{i_2}) = \xi_{n,m}(P_{i_1})\xi_{n,m}(P_{i_2})$ for any $P_i \in \mathcal{P}(d_i;\sigma)$ $(i \neq i_1, i_2)$, the terms corresponding to $(P_1, \ldots, P_{i_1}, \ldots, P_{i_2}, \ldots, P_{N-k})$ and $(P_1, \ldots, P'_{i_1}, \ldots, P'_{i_2}, \ldots, P_{N-k})$ cancel each other out in (5).

If any two of $P_1, \ldots, P_{N-k}$ do not intersect, we say that the paths are nonintersecting. Hence only terms corresponding to nonintersecting paths contribute to (5).

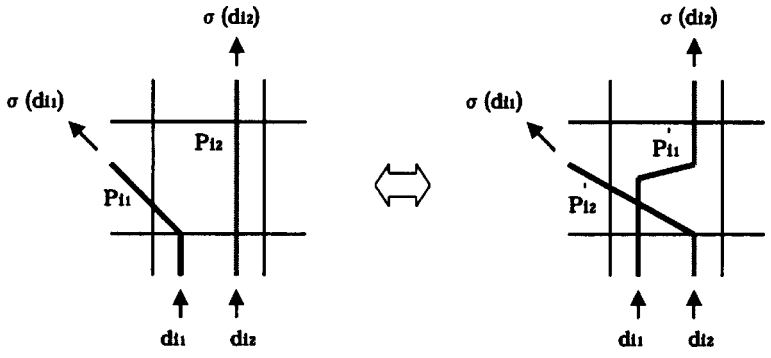

FIG. 7. Definition of P'_{i_1} and P'_{i_2}.

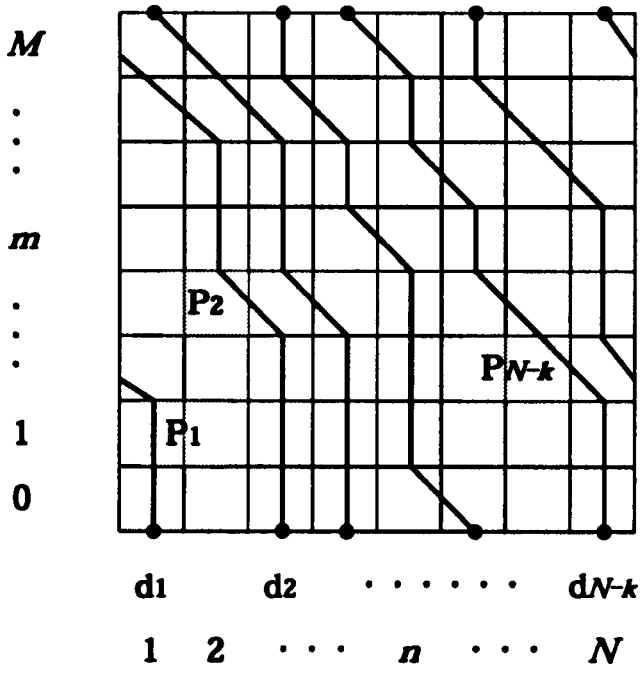

FIG. 8. Nonintersecting paths $P_1, \ldots, P_{N-k}$.

When $P_1, \ldots, P_{N-k}$ are nonintersecting $[P_1 \in \mathcal{P}(d_1;\sigma), \ldots, P_{N-k} \in \mathcal{P}(d_{N-k};\sigma)$ and $\sigma \in S_X^J, \sharp J = j]$,

$$\sigma(d_i) = \begin{cases} d_{i-j} & (i-j \geqslant 1), \\ d_{N+i-j} & (i-j \leqslant 0) \end{cases}$$

(cf. Fig. 8 and Fig. 9), and therefore $\mathrm{sgn}(\sigma) = (-1)^{j(N-k-1)}$.

In (3), the upper bound of the summation over j is $\{[(N-k)/N](M+1)\}$ where $[\ell]$ denotes the largest integer which does not exceed ℓ.

From (3) and (5), we obtain the following theorem.

Theorem II.1: *For A defined in (2), it holds that*

$$\det(\lambda I - A) = \sum_{k=0}^{N} (-1)^{N-k} \lambda^k \sum_{j=0}^{[(N-k)(M+1)/N]} (-1)^{j(N-k-1)} \mu^j \sum_{\substack{1 \leqslant d_1 < d_2 < \cdots \\ \cdots < d_{N-k} \leqslant N}} \sum_{\substack{(P_1,\ldots,P_{N-k}) \\ \in \mathcal{P}^{(j)}(d_1,\ldots,d_{N-k})}} \prod_{i=1}^{N-k} \prod_{n=1}^{N} \prod_{m=0}^{M} \xi_{n,m}(P_i),$$

where $\xi_{n,m}$ *are defined in (4) and*

$$\mathcal{P}^{(j)}(d_1, \ldots, d_{N-k}) := \left\{ (P_1, \ldots, P_{N-k}) \;\middle|\; \begin{array}{l} P_i \text{ connects the initial point } d_i \text{ and the} \\ \text{end point } d_{N+i-j} (1 \leqslant i \leqslant j); P_i \\ \text{connects } d_i \text{ and } d_{i-j} (j < i \leqslant N-k). \\ \text{Any two of them are nonintersecting} \end{array} \right\}. \tag{6}$$

■

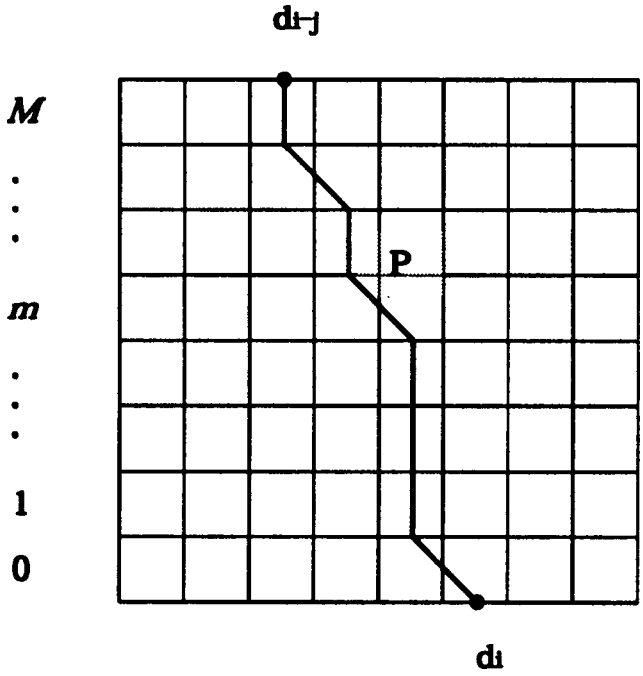

FIG. 9. A path $P \in \mathcal{P}(d_i;\sigma)$, $\sigma \in S_X^J$, $\sharp J=j$, which connects d_i and $\sigma(d_i)=d_{i-j}$.

III. gPBBS AND ndKP EQUATION

We briefly summarize the results obtained in Ref. 9 to fix the notations used in the subsequent sections.

A. gPBBS and its equation of motion

In order to describe the dynamics of the gPBBS, we introduce a new independent variable s ($s \in \mathbb{Z}$). As any integer s can be uniquely expressed as $s=Mt+j$ ($t \in \mathbb{Z}, 1 \leqslant j \leqslant M$), we denote by u_n^s the number of balls with index $j \equiv s \bmod M$ in the nth box at time step $t=[(s-1)/M]$, where $[x]$ denotes the largest integer which does not exceed x. In other words, the new *time* variable s is a refinement of the original time, indicating explicitly when balls with index j move.

We assume that θ_n and u_n^s satisfy the relation

$$\sum_{n=1}^{N} \theta_n - \sum_{j=1}^{M} \sum_{n=1}^{N} u_n^j \geqslant \sum_{n=1}^{N} u_n^k \quad (k=1,2,\ldots,M). \tag{7}$$

The first and second terms of the left-hand side of (7) represent the number of spaces and the number of balls in the gPBBS, respectively, hence the left-hand side is the total number of free spaces of the gPBBS. The right-hand side of (7) is the number of balls with index k. Thus (7) requires the total number of free spaces of the gPBBS to be larger than the number of copies of any type of ball in the time evolution process.

Let us consider the process at time s, i.e., the movement of the balls with index j at time step t where $s=Mt+j$; we often use s instead of j, i.e., we treat the indices modulo M. If we define κ_n^s, which denotes the number of spaces of the nth box at s, by

$$\kappa_n^s := \theta_n - (u_n^s + u_n^{s-1} + \cdots + u_n^{s-M+1}),$$

condition (7) is rewritten as

$$\sum_{n=1}^{N} \kappa_n^s \geqslant \sum_{n=1}^{N} u_n^{s-M+k} \quad (k=1,2,\ldots,M).$$

Theorem III.1 (Ref. 9): *The time evolution of the gPBBS is described by an ultradiscrete equation,*

$$u_n^{s+1} - \kappa_n^s = \max_{k=1,\ldots,N}\left[\sum_{j=1}^{k} u_{n-j}^{s-M+1} - \kappa_{n-j+1}^s\right] - \max\left[0, \max_{k=1,\ldots,N-1}\left[\sum_{j=1}^{k} u_{n-j}^{s-M+1} - \kappa_{n-j+1}^s\right]\right]. \tag{8}$$

■

B. From ndKP equation to gPBBS

The ndKP equation is obtained from the generating formula of the KP hierarchy.[12,13] It is given as

$$(b(m)-c(n))\tau(l+1,m,n)\tau(l,m+1,n+1) + (c(n)-a(l))\tau(l,m+1,n)\tau(l+1,m,n+1) + (a(l) - b(m))\tau(l,m,n+1)\tau(l+1,m+1,n) = 0, \tag{9}$$

where l, m, $n \in \mathbb{Z}$ are independent variables, the tau function $\tau: \mathbb{Z}\times\mathbb{Z}\times\mathbb{Z}\to\mathbb{R}$ (or $\mathbb{C}$) is dependent variable and the coefficients $a(l)$, $b(m)$, $c(n)$ are arbitrary functions which depend on the independent variables l, m, n, respectively.

In order to relate the ndKP equation to the gPBBS, we take $a(l)=0$, $b(m)=1$, $c(n)=1+\delta_n$ and impose the following constraint on $\tau(l,m,n)$:

$$\tau(l,m,n) = \tau(l-M, m-1, n).$$

If we define $\sigma_n^s := \tau(s-1,0,n)$, (9) turns into

$$\frac{\sigma_{n+1}^{s+M-1}\sigma_{n+1}^{s}}{\sigma_{n+1}^{s+M}\sigma_{n+1}^{s-1}} - (1+\delta_{n+1})\frac{\sigma_n^{s-1}\sigma_{n+1}^{s}}{\sigma_{n+1}^{s-1}\sigma_n^s} = -\delta_{n+1}\frac{\sigma_n^{s+M}\sigma_{n+1}^{s}}{\sigma_n^s\sigma_{n+1}^{s+M}}. \tag{10}$$

Furthermore, we define U_n^s and K_n^s as

$$U_n^s := \frac{\sigma_{n+1}^s\sigma_n^{s+1}}{(1+\delta_{n+1})\sigma_n^s\sigma_{n+1}^{s+1}}, \quad \frac{1}{K_n^s} = \delta_{n+1}\cdot\prod_{j=1}^{M} U_n^{s-j+1}$$

and impose the following periodic condition on U_n^s:

$$U_n^s = U_{n+N}^s. \tag{11}$$

Then, from (10), we have

$$\frac{U_n^{s+1}}{K_n^s} = \frac{\displaystyle\sum_{k=1}^{N}\prod_{j=1}^{k}\frac{U_{n-j}^{s-M+1}}{K_{n-j+1}^s}}{\displaystyle 1+\sum_{k=1}^{N-1}\prod_{j=1}^{k}\frac{U_{n-j}^{s-M+1}}{K_{n-j+1}^s}}. \tag{12}$$

To take the ultradiscrete limit, we set $U_n^s = e^{u_n^s/\epsilon}$, $K_n^s = e^{\kappa_n^s/\epsilon}$, $1/\delta_{n+1} = e^{\theta_n/\epsilon}$. Then, we found the following.

Theorem III.2 (Ref. 9): *The ultradiscrete limit of the constrained ndKP equation with the periodic boundary condition [i.e., (11) and (12)] coincides with the time evolution equation of the gPBBS (8).* ■

IV. CONSERVED QUANTITIES OF ndKP EQUATION

In Ref. 9 we derived the Lax representation for the ndKP equation when it has period N in the spatial variable n. In short, the equation (12) is equivalent to the matrix equation

$$\tilde{M}(s)L(M;s) = L(M;s-1)\tilde{M}(s),$$

where $\tilde{M}(s) = G_{U;s} - \tilde{\Upsilon}$,

$$L(M;s) = (-G_{K;s} + \tilde{\Upsilon})(G_{U;s-M+1} - \tilde{\Upsilon})(G_{U;s-M+2} - \tilde{\Upsilon}) \cdots (G_{U;s} - \tilde{\Upsilon}), \tag{13}$$

$G_{K;s} = \mathrm{diag}(1/K_1^s, 1/K_2^s, \ldots, 1/K_N^s)$, $G_{U;s} = \mathrm{diag}(1/U_1^s, 1/U_2^s, \ldots, 1/U_N^s)$, and

$$\tilde{\Upsilon} := \begin{bmatrix} & & & & (1+\delta_N)\cdot\eta \\ 1+\delta_1 & & & & \\ & 1+\delta_2 & & & \\ & & \ddots & & \\ & & & 1+\delta_{N-1} & \end{bmatrix};$$

here, η is an arbitrary parameter.

This means

$$\det(\lambda I + L(M;s)) = \det(\lambda I + L(M;s-1));$$

therefore, the coefficients e_k of the characteristic polynomial

$$\det(\lambda I + L(M;s)) = \lambda^N + e_{N-1}\lambda^{N-1} + e_{N-2}\lambda^{N-2} + \cdots + e_1\lambda + e_0$$

are conserved in time s. Furthermore, since η is arbitrary and e_k contain η, if we define $e_k^{[j]}$ by

$$e_k = \sum_j e_k^{[j]} \eta^j, \tag{14}$$

then $e_k^{[j]}$ are also conserved.

Let $\Delta := \Pi_{i=1}^N (1+\delta_i)$,

$$\Upsilon := \begin{bmatrix} & & & & \eta\Delta \\ 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \end{bmatrix},$$

and $D_\delta := \mathrm{diag}(1, 1+\delta_1, (1+\delta_1)(1+\delta_2), \ldots, \Pi_{i=1}^{N-1}(1+\delta_i))$. Since $\Upsilon = (D_\delta)^{-1}\tilde{\Upsilon}D_\delta$ we have (Ref. 9)

$$\det(\lambda I + L(M;s)) = \det(\lambda I + L_0(M;s)), \tag{15}$$

where

$$L_0(M;s) := (-G_{K;s} + \Upsilon)(G_{U;s-M+1} - \Upsilon)(G_{U;s-M+2} - \Upsilon) \cdots (G_{U;s} - \Upsilon).$$

From Theorem II.1, we obtain a combinatorial formula for $e_k^{[j]}$ immediately.

Theorem IV.1: *Set*

$$x_{n,0} = \frac{1}{K_n^s}, \quad x_{n,m} = \frac{1}{U_n^{s-M+m}} \quad (m \neq 0)$$

in (4) and set $\mu = \eta\Delta$. *Then, for* $k = 0, 1, \ldots, N$ *and* $j = 0, 1, \ldots, [(N-k)(M+1)/N]$, *it holds that*

$$e_k^{[j]} = (-1)^{\ell(k,j)}\Delta^j \sum_{\substack{1\leqslant d_1<d_2<\cdots \\ \cdots<d_{N-k}\leqslant N}} \sum_{(P_1,\ldots,P_{N-k}) \atop \in \mathcal{P}^{(j)}(d_1,\ldots,d_{N-k})} \prod_{i=1}^{N-k}\prod_{n=1}^{N}\prod_{m=0}^{M} \xi_{n,m}(P_i),$$

where $\ell(k,j) := (j+1)N-(k+j+kj)$. ■

V. CONSERVED QUANTITIES OF gPBBS

Using the results in Sec. IV, we construct the conserved quantities of the gPBBS.

For $k=0,1,\ldots,N$ and $j=0,1,\ldots,[(N-k)(M+1)/N]$, the ultradiscrete limit of $e_k^{[j]}$ is

$$ue_k^{[j]} := -\lim_{\epsilon\to+0}\epsilon\log((-1)^{\ell(k,j)}e_k^{[j]}) = -\lim_{\epsilon\to+0}\epsilon\log\left(\Delta^j \sum_{\substack{1\leqslant d_1<d_2<\cdots \\ \cdots<d_{N-k}\leqslant N}} \sum_{(P_1,\ldots,P_{N-k}) \atop \in \mathcal{P}^{(j)}(d_1,\ldots,d_{N-k})} \prod_{i=1}^{N-k}\prod_{n=1}^{N}\prod_{m=0}^{M} \xi_{n,m}(P_i)\right).$$

Since θ_n is the capacity of the nth box,

$$\lim_{\epsilon\to+0}\epsilon\log\Delta^j = j\cdot\lim_{\epsilon\to+0}\epsilon\log\prod_{j=1}^{N}(1+e^{-\theta_j/\epsilon}) = j\cdot\sum_{j=1}^{N}\max[0,-\theta_j] = 0.$$

Therefore, from Theorem IV.1, $ue_k^{[j]}$ is given by the following.

Theorem V.1: *Set*

$$x_{n,0} = \kappa_n^s, \quad x_{n,m} = u_n^{s-M+m}\ (m\neq 0)$$

in (4). Then, for $k=0,1,\ldots,N$ *and* $j=0,1,\ldots,[(N-k)(M+1)/N]$, *it holds that*

$$ue_k^{[j]} = \min_{\substack{1\leqslant d_1<d_2<\cdots \\ \cdots<d_{N-k}\leqslant N}}\left[\min_{(P_1,\ldots,P_{N-k}) \atop \in \mathcal{P}^{(j)}(d_1,\ldots,d_{N-k})}\left[\sum_{i=1}^{N-k}\sum_{n=1}^{N}\sum_{m=0}^{M}\xi_{n,m}(P_i)\right]\right].$$

■

Remark V.1: The conserved quantity $ue_k^{[0]}$ $(0\leqslant k\leqslant N)$ *is trivial. Since* $j=0$, *all paths are vertical lines. Hence we have*

$$ue_k^{[0]} = \min_{\substack{1\leqslant d_1<d_2<\cdots \\ \cdots<d_{N-k}\leqslant N}}\left[\sum_{i=1}^{N-k}\left(\kappa_{d_i}^s + \sum_{m=1}^{M}u_{d_i}^{s-M+m}\right)\right] = \min_{\substack{1\leqslant d_1<d_2<\cdots \\ \cdots<d_{N-k}\leqslant N}}\left[\sum_{i=1}^{N-k}\theta_{d_i}\right].$$

As θ_n *is the capacity of the nth box,* $ue_k^{[0]}$ *does not depend on the time steps. So we are not interested in them.*

Remark V.2: Once we obtain all quantities that are conserved in variable s, we are to have all quantities that are conserved in the original time variable t. The reasoning is as follows: Assume that A_1 *is a conserved quantity of the gPBBS; this means* $A_1=A_1(s)$ *has period M in s.* [*Since equation of motion (8) is Mth order in s,* $A_1(s)$ *is written as*

$$A_1(s) = F(u_1^s,\ldots,u_N^s,u_1^{s-1},\ldots,u_N^{s-1},\ldots,u_1^{s-M+1},\ldots,u_N^{s-M+1})$$

by some function F.] *Let* $A_j(s)=A_1(s+j-1)$ $(j=2,3,\ldots)$; *they all have period M in s. By definition* $A_j(s+1)=A_{j+1}(s)$ $(j=1,2,\ldots)$, *and, since* $A_1(s)$ *has period M,* $A_M(s+1)=A_1((s+1)+M-1)=A_1(s+M)=A_1(s)$; *hence, symmetric polynomials of* $A_1(s),\ldots,A_M(s)$ *are conserved in s. More explicitly, let* $S_k(s)$ *be the kth elementary symmetric polynomial of* $A_1(s),\ldots,A_M(s)$; *then, we have M quantities* $S_1(s),\ldots,S_M(s)$ *that are conserved in s. Conversely, once we know the elementary symmetric polynomials* $S_1(s),\ldots,S_M(s)$ *of* $A_1(s),\ldots,A_M(s)$, *we can obtain* $A_1(s),\ldots,A_M(s)$. *Therefore, the statement follows.*

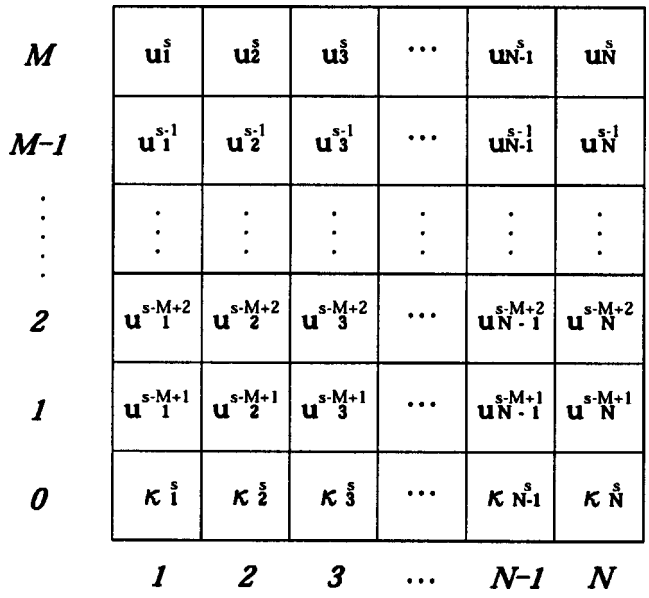

FIG. 10. Associate values κ_n^s, $u_n^s, \ldots, u_n^{s-M+1}$ with boxes of $C_{N,M+1}$.

An easy way to read off $\Sigma_{i=1}^{N-k}\Sigma_{n=1}^{N}\Sigma_{m=0}^{M}\xi_{n,m}(P_i)$ is as follows: Associate values κ_n^s, $u_n^s, \ldots, u_n^{s-M+1}$ with boxes of $C_{N,M+1}$ as shown in Fig. 10. For $(P_1, \ldots, P_{N-k}) \in \mathcal{P}^{(j)}(d_1, \ldots, d_{N-k})$, summing up the values corresponding to the vertical lines of the paths, we get the value $\Sigma_{i=1}^{N-k}\Sigma_{n=1}^{N}\Sigma_{m=0}^{M}\xi_{n,m}(P_i)$.

Example V.1: For a state in Fig. 11 $(N=10, M=5)$*, we obtain a table in Fig. 12. For paths shown in Fig. 13,*

$$\sum_{i=1}^{N-k}\sum_{n=1}^{N}\sum_{m=0}^{M}\xi_{n,m}(P_i) = (0+0+1)+(0+1+0+0)+(0+0+0+0)+(0+1+0)+(0+0+1)$$
$$+(0+1+0)+(1+0)=6.$$

Occasionally these paths minimize $\Sigma_{i=1}^{N-k}\Sigma_{n=1}^{N}\Sigma_{m=0}^{M}\xi_{n,m}(P_i)$*; thus,* $ue_3^{[2]}$ *is* 6.

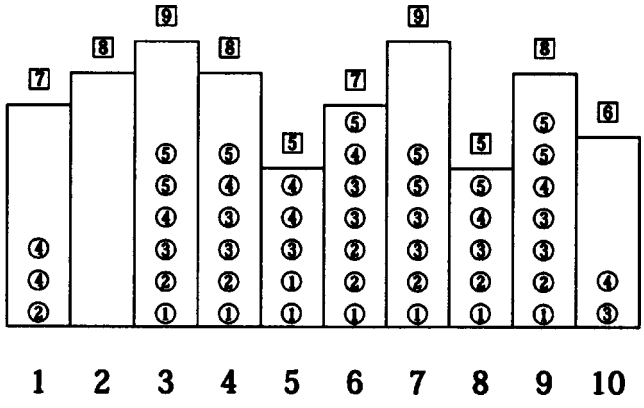

FIG. 11. A state of the gPBBS.

5	0	0	2	1	0	1	2	1	2	0
4	2	0	1	1	2	1	0	1	1	1
3	0	0	1	2	1	2	2	1	2	1
2	1	0	1	1	0	2	1	1	1	0
1	0	0	1	1	2	1	1	1	1	0
0	4	8	3	2	0	0	3	0	1	4
	1	2	3	4	5	6	7	8	9	10

FIG. 12. A table obtained for a state in Fig. 11 ($N=10, M=5$).

VI. DISCUSSION

In this section we discuss some algebraic aspects of the gPBBS. The time evolution of the gPBBS is decomposed into a product of transformations, each of which is a representation of the generators of the affine Weyl group $\widetilde{W}(A_M^{(1)})$. Furthermore a state of the gPBBS is naturally identified with a vector of a tensor product of the crystals $U_q'(A_M^{(1)})$, and a time evolution pattern is interpreted as twisted lattices of the crystals $U_q'(A_{N-1}^{(1)})$ whose Boltzmann weights are determined by the combinatorial R matrices.

A. Affine Weyl group and gPBBS

Let $\mathcal{T}$ be the set of $N\times(M+1)$ rectangular tableaux with integer entries, and $s_\ell(\ell\in\mathbb{Z}/(M+1)\mathbb{Z})$ and π be mappings: $\mathcal{T}\to\mathcal{T}$. For a tableau

$$Y=\begin{array}{|c|c|c|c|}\hline y_{1,M} & y_{2,M} & \cdots & y_{N,M}\\ \hline \vdots & \vdots & \cdots & \vdots\\ \hline y_{1,1} & y_{2,1} & \cdots & y_{N,1}\\ \hline y_{1,0} & y_{2,0} & \cdots & y_{N,0}\\ \hline\end{array},$$

these mappings are given as

$$s_\ell(Y)=\begin{array}{|c|c|c|c|}\hline s_\ell(y_{1,M}) & s_\ell(y_{2,M}) & \cdots & s_\ell(y_{N,M})\\ \hline \vdots & \vdots & \cdots & \vdots\\ \hline s_\ell(y_{1,1}) & s_\ell(y_{2,1}) & \cdots & s_\ell(y_{N,1})\\ \hline s_\ell(y_{1,0}) & s_\ell(y_{2,0}) & \cdots & s_\ell(y_{N,0})\\ \hline\end{array},$$

$$\pi(Y)=\begin{array}{|c|c|c|c|}\hline \pi(y_{1,M}) & \pi(y_{2,M}) & \cdots & \pi(y_{N,M})\\ \hline \vdots & \vdots & \cdots & \vdots\\ \hline \pi(y_{1,1}) & \pi(y_{2,1}) & \cdots & \pi(y_{N,1})\\ \hline \pi(y_{1,0}) & \pi(y_{2,0}) & \cdots & \pi(y_{N,0})\\ \hline\end{array},$$

where

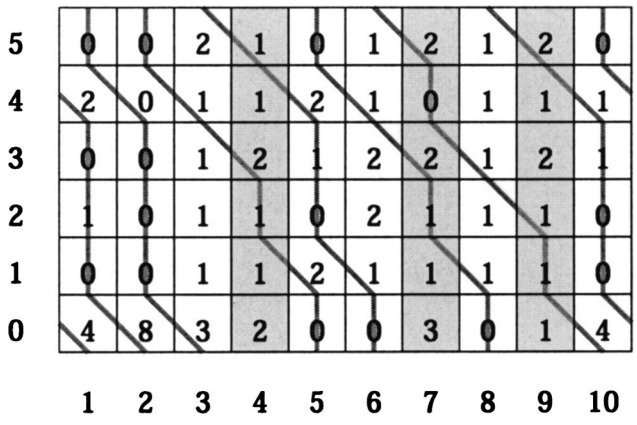

FIG. 13. Paths (see text).

$$s_\ell(y_{n,m}) = y_{n,m+1} + Q_{n,m} - Q_{n-1,m} \quad (m \equiv \ell \bmod M+1),$$

$$s_\ell(y_{n,m+1}) = y_{n,m} + Q_{n-1,m} - Q_{n,m} \quad (m \equiv \ell \bmod M+1),$$

$$s_\ell(y_{n,m}) = y_{n,m} \quad (m \neq \ell, \ell+1 \bmod M+1),$$

$$\pi(y_{n,m}) = y_{n,m+1},$$

and

$$Q_{n,m} = \max_{1 \leqslant h \leqslant N} \left[\sum_{k=1}^{h-1} y_{n+k,m+1} + \sum_{k=h+1}^{N} y_{n+k,m} \right].$$

Here we extend the indices n,m of $y_{n,m}$ for $n,m \in \mathbb{Z}$ by the condition $y_{n+N,m}=y_{n,m+M+1}=y_{n,m}$.

The following theorem is proved by direct calculations.

Theorem VI.1 (Refs. 14 and 15): *The mappings* s_ℓ $(\ell \in \mathbb{Z}/(M+1)\mathbb{Z})$ *and* π *defined as above give a realization of the affine Weyl group* $\tilde{W}(A_M^{(1)})$. ■

Remark VI.1: The affine Weyl group $\tilde{W}(A_{n-1}^{(1)})$ *is defined as the group generated by the simple reflections* $s_0, s_1, \ldots, s_{n-1}$ *and diagram rotation* π *subject to the fundamental relations*

$$s_i^2 = 1,$$

$$s_i s_j = s_j s_i \quad (j \neq i, i \pm 1 \bmod n),$$

$$s_i s_j s_i = s_j s_i s_j \quad (j \equiv i \pm 1 \bmod n),$$

$$\pi s_i = s_{i+1} \pi,$$

where we understand the indices for s_i *as elements of* $\mathbb{Z}/(M+1)\mathbb{Z}$.

When we set

$$y_{n,0} = \kappa_n^s, \quad y_{n,m} = u_n^{s-M+m} \quad (m \neq 0), \tag{16}$$

we get the following theorem which gives a relation between the gPBBS and the affine Weyl group.

Theorem VI.2: $\pi s_{M-1} s_{M-2} \cdots s_0$ *gives the time evolution which concerns the original time*

variable t, i.e.,

$$\pi s_{M-1}s_{M-2}\cdots s_0 \begin{pmatrix} u_1^s & u_2^s & \cdots & u_N^s \\ \vdots & \vdots & \cdots & \vdots \\ u_1^{s-M+1} & u_2^{s-M+1} & \cdots & u_N^{s-M+1} \\ \kappa_1^s & \kappa_2^s & \cdots & \kappa_N^s \end{pmatrix} = \begin{pmatrix} u_1^{s+M} & u_2^{s+M} & \cdots & u_N^{s+M} \\ \vdots & \vdots & \cdots & \vdots \\ u_1^{s+1} & u_2^{s+1} & \cdots & u_N^{s+1} \\ \kappa_1^{s+M} & \kappa_2^{s+M} & \cdots & \kappa_N^{s+M} \end{pmatrix}$$

. ■

The proof goes as follows.

The equation of motion (8) is

$$u_n^{s+1} = u_n^{s-M+1} + Q_{n-1,0} - Q_{n,0}.$$

This means

$$s_0(\kappa_n^s) = u_n^{s+1},$$

and

$$s_0(u_n^{s-M+1}) = \kappa_n^s + Q_{n-1,0} - Q_{n,0} = \kappa_n^s + u_n^{s+1} - u_n^{s-M+1};$$

in the gPBBS, κ_n^s denotes the number of spaces of the nth box at s, and u_n^{s+1}, u_n^{s-M+1} denote the numbers of balls which come in the nth box and get out the nth box from time step s to $s+1$, respectively; hence

$$s_0(u_n^{s-M+1}) = \kappa_n^{s+1}.$$

Therefore

$$s_0 \begin{pmatrix} u_1^s & u_2^s & \cdots & u_N^s \\ \vdots & \vdots & \cdots & \vdots \\ u_1^{s-M+1} & u_2^{s-M+1} & \cdots & u_N^{s-M+1} \\ \kappa_1^s & \kappa_2^s & \cdots & \kappa_N^s \end{pmatrix} = \begin{pmatrix} u_1^s & u_2^s & \cdots & u_N^s \\ \vdots & \vdots & \cdots & \vdots \\ s_0(u_1^{s-M+1}) & s_0(u_2^{s-M+1}) & \cdots & s_0(u_N^{s-M+1}) \\ s_0(\kappa_1^s) & s_0(\kappa_2^s) & \cdots & s_0(\kappa_N^s) \end{pmatrix}$$

$$= \begin{pmatrix} u_1^s & u_2^s & \cdots & u_N^s \\ \vdots & \vdots & \cdots & \vdots \\ \kappa_1^{s+1} & \kappa_2^{s+1} & \cdots & \kappa_N^{s+1} \\ u_1^{s+1} & u_2^{s+1} & \cdots & u_N^{s+1} \end{pmatrix}.$$

Repeating the above procedure, we obtain

$$s_{M-1}s_{M-2}\cdots s_0 \begin{pmatrix} u_1^s & u_2^s & \cdots & u_N^s \\ \vdots & \vdots & \cdots & \vdots \\ u_1^{s-M+1} & u_2^{s-M+1} & \cdots & u_N^{s-M+1} \\ \kappa_1^s & \kappa_2^s & \cdots & \kappa_N^s \end{pmatrix} = \begin{pmatrix} \kappa_1^{s+M} & \kappa_2^{s+M} & \cdots & \kappa_N^{s+M} \\ u_1^{s+M} & u_2^{s+M} & \cdots & u_N^{s+M} \\ \vdots & \vdots & \cdots & \vdots \\ u_1^{s+1} & u_2^{s+1} & \cdots & u_N^{s+1} \end{pmatrix}.$$

Finally, applying π upon it immediately gives Theorem VI.2.

B. gPBBS as twisted crystal lattice

The BBSs can be reformulated as integrable lattice models at temperature zero from viewpoint of the crystal theory and the combinatorial R matrix.[16,17] The PBBS with one kind of ball and box capacity one has also been reformulated into two types of lattice models, a periodic $A_1^{(1)}$ crystal lattice and a twisted $A_{N-1}^{(1)}$ crystal chain, where N denotes the number of the boxes in the system.[8] It is straightforward to extend this result to the case of the gPBBS. In this section, we will briefly show how the gPBBS is reinterpreted as some integrable lattice systems. Since the proofs for the statements below are almost the same as those in Ref. 8, we will omit them here.

Let B_k be the classical crystal of $U_q'(A_M^{(1)})$ corresponding to the k-fold symmetric tensor representation of $U_q(A_M)$. As a set it consists of the single row semistandard tableaux of length k on letters $\{1,2,\ldots,M+1\}$,

$$B_k := \left\{ \boxed{i_1}\boxed{i_2}\boxed{\cdots}\boxed{i_k} \;\middle|\; 1 \le i_1 \le i_2 \le \cdots \le i_k \le M+1 \right\}.$$

An element b

$$b = \boxed{i_1}\boxed{i_2}\boxed{\cdots}\boxed{i_k} \in B_k$$

is also denoted as a series of $M+1$ integers $b \equiv (x^{(M+1)}, x^{(M)}, \ldots, x^{(2)}, x^{(1)})$, where $x^{(j)}$ is the number of letters j in b. A state $|\psi\rangle_t$ of the gPBBS is naturally identified with

$$|\psi\rangle_t \cong b_1^t \otimes b_2^t \otimes \cdots \otimes b_N^t \in B_{\theta_1} \otimes B_{\theta_2} \otimes \cdots \otimes B_{\theta_N},$$

where

$$b_n^t = (\kappa_n^s, u_n^{s-M+1}, u_n^{s-M+2}, \ldots, u_n^s) \quad (n = 1,2,\ldots,N).$$

For the BBS without the periodic boundary condition, time evolution is given by the isomorphism induced by the combinatorial R matrices,

$$\mathcal{T}: B_\infty \otimes (B_{\theta_1} \otimes B_{\theta_2} \otimes \cdots \otimes B_{\theta_N}) \to (B_{\theta_1} \otimes B_{\theta_2} \otimes \cdots \otimes B_{\theta_N}) \otimes B_\infty,$$

$$\mathcal{T}: |\{0\}\rangle \otimes |\psi\rangle_t \to |\psi\rangle_{t+1} \otimes |\{0\}\rangle,$$

where $|\{0\}\rangle$ is the highest weight vector of B_∞. For the gPBBS, by taking the trace of the auxiliary state in B_∞, $T := \mathrm{Tr}_{B\infty}\,\mathcal{T}$, we have the time evolution

$$T: B_{\theta_1} \otimes B_{\theta_2} \otimes \cdots \otimes B_{\theta_N} \to B_{\theta_1} \otimes B_{\theta_2} \otimes \cdots \otimes B_{\theta_N},$$

$$T: |\psi\rangle_t \to |\psi\rangle_{t+1}.$$

As the $A_1^{(1)}$ crystal, the operator T maps $|\psi\rangle_t$ to the unique tensor product of $A_M^{(1)}$ crystal that exactly corresponds to the state of the gPBBS at $t+1$.

The gPBBS is also reformulated as a twisted lattice of M vertical axes in terms of $A_{N-1}^{(1)}$ crystals. In this case, a state $|\psi\rangle_t$ is identified

$$|\psi\rangle_t \cong b_\kappa^t \otimes (b_{u_1}^t \otimes b_{u_2}^t \otimes \cdots \otimes b_{u_M}^t) \in B_k \otimes (B_{n_1} \otimes B_{n_2} \otimes \cdots \otimes B_{n_M}),$$

where

$$b_\kappa^t = (\kappa_N^s, \kappa_{N-1}^s, \ldots, \kappa_1^s),$$

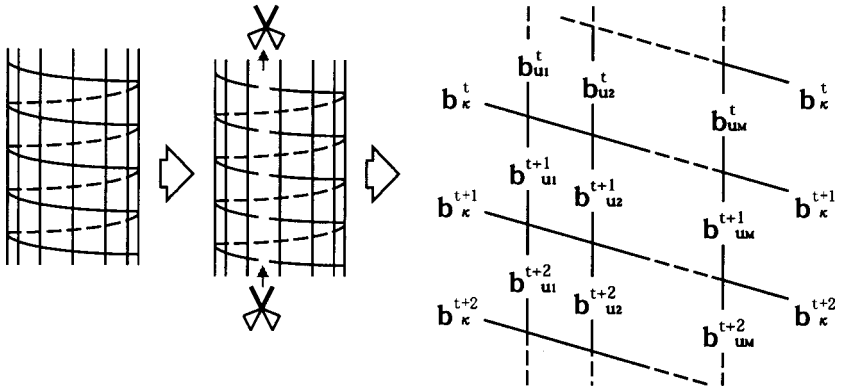

FIG. 14. The twisted crystal lattice associated with the gPBBS.

$$b^t_{u_j} = (u_N^{s-M+j}, u_{N-1}^{s-M+j}, \ldots, u_1^{s-M+j}) \quad (j = 1,2, \ldots, M),$$

$k := \Sigma_{n=1}^N \kappa_n^s$ and $n_j := \Sigma_{n=1}^N u_n^{s-M+j}$. The time evolution is determined by the isomorphism induced by the combinatorial R-matrix for $A_{N-1}^{(1)}$ crystal,

$$b^t_\kappa \otimes (b^t_{u_1} \otimes b^t_{u_2} \otimes \cdots \otimes b^t_{u_M}) \cong (b^{t+1}_{u_1} \otimes b^{t+1}_{u_2} \otimes \cdots \otimes b^{t+1}_{u_M}) \otimes b^{t+1}_\kappa.$$

In Fig. 14, we schematically show the twisted crystal lattice associated with the gPBBS.

VII. CONCLUDING REMARKS

In this paper, using a path description of the characteristic polynomial of particular matrices and an algorithm to construct the conserved quantities using the Lax representation of the ndKP equation, we showed explicit form of the conserved quantities of the gPBBS. Relations to the affine Weyl group action and the crystal theory were also clarified. An advantage to reformulate the PBBS as crystal lattices is that we can extend it to the crystals associated with other root systems.

Since the gPBBS is composed of a finite number of boxes and balls, it can only take on a finite number of patterns. Hence its trajectory is always periodic and a fundamental cycle, i.e., the shortest period of the periodic motion, exists for any given initial state. In the case where the box capacity is one everywhere and only one kind of ball exists, the formula used to calculate the fundamental cycle is explicitly obtained using the conserved quantities and some rescaling properties of the states.[18] Hence, using the results in this paper, we may get the formula to calculate the fundamental cycle for the gPBBS, which is a problem we wish to address in the future.

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A revised model for diffusion induced segregation processes

T. Blesgen[a)]
Max-Planck-Institute for Mathematics in the Sciences, Inselstraße 22-26, 04103 Leipzig, Germany

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A mathematical model for chalcopyrite disease within sphalerite is developed. As one main result, by analyzing the system enthalpy, correct expressions for the reaction terms in a system undergoing phase transitions are worked out. For the resulting equations, the thermodynamical validity is shown and the existence of a unique solution is proved. © *2005 American Institute of Physics.*
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I. INTRODUCTION

In the present work we are concerned with diffusion-induced segregation (DIS) phenomena. This class is characterized by segregation processes that can only take place after a sufficient amount of a diffusor has penetrated the crystal. We will exemplary study the so-called chalcopyrite disease within sphalerite, which is a well-known and extensively discussed problem arising in geology and a particular example of DIS, but the techniques developed here apply as well for other DIS phenomena.

In Ref. 3 a first model for chalcopyrite disease has been developed, Ref. 4 discusses related ternary systems. Reference 3 also provides references to the mineralogical experiments and illuminates the physical background. But as a deeper thermodynamical analysis in this paper reveals, the reaction terms chosen in this first model are only approximately true and will in general depend on the phase parameter (the function χ introduced later on). The principles worked out are quite general and will apply whenever reactions and phase transitions take place simultaneously. The presentation is completed by showing existence and uniqueness of the solutions.

II. DERIVATION OF THE REVISED MODEL

Let us consider the following reaction diffusion equations:

$$\partial_t c_i = \mathrm{div}(J_i) + r_i = \left(\sum_l \frac{\partial}{\partial x_l} J_{i,l} \right) + r_i, \quad i = 1, \ldots, 4. \tag{1}$$

In (1), $c_i = c_i(x,t)$ denotes the relative number of species i, $i = 1, \ldots, 4$ per available lattice point at time t and space point $x \in \Omega$, Ω a (time-independent) domain in $\mathbb{R}^D$, $1 \leqslant D \leqslant 3$. By $T_0 > 0$ we denote a stop time and by $\Omega_{T_0} := \Omega \times (0, T_0)$ a cylinder in space–time.

We introduce the notations

$$c_1 \approx \mathrm{Fe}^{3+}, \quad c_2 \approx \mathrm{Fe}^{2+}, \quad c_3 \approx \mathrm{Cu}^{+}, \quad c_4 \approx \mathrm{Zn}^{2+}, \quad c_5 \approx \text{vacancies}.$$

c_1 satisfies $c_1 = N_{\mathrm{Fe}}^{3+} / N_{\mathrm{Me}}$, where $N_{\mathrm{Fe}^{3+}}$ is the number of Fe^{3+} atoms and N_{Me} is the number of metal ion sites. Similar relationships hold for c_2, c_3, and c_4. It is an essential property of this formulation that there is no equation for c_5, but the vacancy concentration is obtained implicitly by the conservation of mass

a)Electronic mail: blesgen@mis.mpg.de

$$c_5 = 1 - \sum_{i=1}^{4} c_i.$$

In (1), r_i denote the reaction terms and J_i the fluxes of metal ions of species i. The reaction terms model the jumps of the electrons. A first ansatz is $r=(r_1,-r_1,0,0)$ and [see (22) below for explanation]

$$r_1 = k(c_2^2 - \kappa c_1 c_e),$$

where $k>0$ and $k\kappa>0$ are the reaction rates and c_e denotes the electron concentration. If we assume that all sulfur places are occupied by S^{2-}, by the condition of electric neutrality we can compute

$$c_e = 2 - 3c_1 - 2c_2 - c_3 - 2c_4 = 2 - 2(c_1 + c_2 + c_3 + c_4) - c_1 + c_3 = 2c_5 - c_1 + c_3. \tag{2}$$

In the presence of phase transitions the reaction rates may not be chosen to be constants, as we shall see below.

Onsager's postulate,[11,12] states that each thermodynamic flux is linearly related to every thermodynamic force. Since in our case the thermodynamic forces are the negative chemical potential gradients, we obtain the phenomenological equations, see Ref. 9, p. 137,

$$J_i = \sum_{j=1}^{4} L_{ij} \nabla \mu_j, \quad 1 \leqslant i \leqslant 4, \tag{3}$$

with a constant mobility matrix L. The Onsager reciprocity law,[9,11,12] states that L must be symmetric which we assume in the following. To simplify the existence theory we will further assume in the sequel that L is positive definite. By

$$\mu_j = \frac{\partial f}{\partial c_j}$$

we denote the chemical potential.

In this work the temperature T is held constant reflecting the situation of the mineralogical experiments. Let f denote the Helmholtz free energy density of the system, which is the convex hull of the free energy density of f_1, f_2 with f_1 for chalcopyrite, f_2 for sphalerite. Hence, the two different phases or lattice orders are characterized by two different free energies, and f is the convex hull of f_1 and f_2.

For order-disorder phase transitions, we make the first ansatz

$$f_l = f_l(c) = k_B T \sum_{i=1}^{5} \beta_i^l c_i \ln c_i + \sum_{i=1}^{3} E_i c_i + \left(\sum_{i=1}^{4} \alpha_i c_i \right)^2, \quad l = 1,2. \tag{4}$$

The elastic coefficients α_i do not change for both phases, only the β_i^l differ. The convex terms $c_i \ln c_i$ are motivated by considerations from statistical mechanics on the system entropy by counting the different configurations. The term $\Sigma_{i=1}^{3} E_i c_i$ refers to the system enthalpy and is a consequence of the presence of the Fe reaction. It will be discussed in the subsequent section.

The expression $(\Sigma_{i=1}^{4} \alpha_i c_i)^2$ is a consequence of Hooke's law. The constants α_i correspond to the ion radii and measure the volume response when replacing Zn^{2+} by other metal ions. In (4), the β_i^1, β_i^2 are positive constants and k_B is the Boltzmann constant.

Equation (4) is a very reasonable term for a numerical computation, since (4) implies infinite slope of Df_l if one component c_j approaches 0 or 1. This guarantees, see Ref. 13,

$$c_j \in (0,1) \quad \text{in } \Omega, t > 0 \tag{5}$$

and c_j has physical meaning. As there is no maximum principle for systems of equations, without the logarithmic terms in (4), Condition (5) may be violated even if $c_j \in (0,1)$ holds for $t=0$.

At this stage, a control mechanism for the segregation process is introduced. The following principle is well known. Let $\chi = \chi(x,t) \in [0,1]$ be a function that measures the volume fraction of the chalcopyrite phase; e.g., $\chi(x_0,t_0)=0$ means that for $t=t_0$ in $x_0 \in \Omega$ only the sphalerite phase is present, $\chi(x_0,t_0)=\frac{1}{2}$ that the system is in x_0 in an intermediate state with no dominant phase.

Let $\gamma > 0$ be a small constant, denoting the square of the thickness of the interface between the sphalerite and chalcopyrite phase. We define the density of the mixing entropy s_M by

$$s_M(\chi) = W(\chi) + \frac{\gamma}{2}|\nabla \chi|^2, \tag{6}$$

with the double-well potential

$$W(\chi) := \chi \ln \chi + (1-\chi)\ln(1-\chi). \tag{7}$$

Since $f := \mathrm{conv}(f_1, f_2)$, we will consider f as the convex combination of f_1 and f_2. Because s_M is subtracted from the entropy density s, the thermodynamic relation $f=e-Ts$ thus implies

$$f(c,\chi) := \chi f_1(c) + (1-\chi) f_2(c) + T s_M(\chi). \tag{8}$$

The phase parameter χ is governed by the modified Allen–Cahn equation

$$\tau \partial_t \chi = -\partial_\chi \left(\frac{f}{T}\right) = \gamma \Delta \chi - \omega(c,\chi), \tag{9}$$

where $\gamma\Delta\chi$ comes from the first variation of $-\int_\Omega (\gamma/2)|\nabla\chi|^2$ with respect to χ and τ is a scaling parameter to adjust the different time scales between mass diffusion and growing of the chalcopyrite phase. The driving force ω in (9) is given by

$$\omega(c,\chi) := \ln\left(\frac{\chi}{1-\chi}\right) + m(c). \tag{10}$$

The value $m(c)$ accounts for the growing of chalcopyrite in copper rich regions and is gained implicitly by $\tau\partial_t\chi = -\partial_\chi(f/T)$. Since so far the final formula for f has not been derived, we will postpone the discussion of this term and of the mechanism responsible for the growing of chalcopyrite in copper rich regions. The final definition of ω is given in (29).

III. AN ENTHALPY PRINCIPLE FOR A PURELY REACTIVE SYSTEM

We want to incorporate the electron jumps by including reaction terms in the model. The reactions are represented in the free energy by enthalpic terms. To understand the nature of these enthalpic terms, we consider a purely reactive system without diffusion and derive general properties of reactive systems.

Let the domain Ω comprise of substances A, B, C, and D subject to the reactions

$$A + B \overset{r_+}{\rightarrow} C + D,$$

$$A + B \overset{r_-}{\leftarrow} C + D.$$

Let $\tilde{c}_1$, $\tilde{c}_2$, $\tilde{c}_3$, and $\tilde{c}_4$ denote the concentration of substances A, B, C, and D where we assume

$$\sum_{i=1}^{4} \tilde{c}_i = 1. \tag{11}$$

In the language of partial differential equations, these reactions can be written as, see Ref. 8,

$$\partial_t \tilde{c}_1 = \partial_t \tilde{c}_2 = - r_+ \tilde{c}_1 \tilde{c}_2 + r_- \tilde{c}_3 \tilde{c}_4,$$

$$\partial_t \tilde{c}_3 = \partial_t \tilde{c}_4 = + r_+ \tilde{c}_1 \tilde{c}_2 - r_- \tilde{c}_3 \tilde{c}_4. \tag{12}$$

From statistical mechanics we infer

$$r_+ = \exp\left(\frac{\tilde{E}_1 + \tilde{E}_2 - \tilde{E}_S}{k_B T} \right),$$

$$r_- = \exp\left(\frac{\tilde{E}_3 + \tilde{E}_4 - \tilde{E}_S}{k_B T} \right), \tag{13}$$

where $\tilde{E}_1 + \tilde{E}_2$ is the energy level before the reaction $A + B \to C + D$, $\tilde{E}_3 + \tilde{E}_4$ the energy level after the reaction. $\tilde{E}_S$ is the activation energy or sattle point energy that must be exceeded to start the reaction.

For the free energy we make the ansatz

$$\tilde{F}(\tilde{c}) = \int_\Omega k_B T \sum_{i=1}^{4} \tilde{c}_i \left(\ln \tilde{c}_i + \frac{\tilde{E}_i}{k_B T} \right). \tag{14}$$

Now we will show the following properties of $\tilde{F}$:

$$\partial_t \tilde{F}(\tilde{c}(t)) = 0 \quad \text{iff } \partial_t \tilde{c}_i = 0,\ 1 \leqslant i \leqslant 4, \tag{15}$$

$$\partial_t \tilde{F}(\tilde{c}(t)) \leqslant 0, \tag{16}$$

$$\tilde{F}(\tilde{c}(t)) \text{ is critical} \quad \text{iff } \partial_t \tilde{c}(t) = 0. \tag{17}$$

In order to show (15) and (16), after setting

$$R := - r_+ \tilde{c}_1 \tilde{c}_2 + r_- \tilde{c}_3 \tilde{c}_4 = \partial_t \tilde{c}_1 = \partial_t \tilde{c}_2 = - \partial_t \tilde{c}_3 = - \partial_t \tilde{c}_4,$$

elementary computations yield

$$\partial_t \tilde{F}(\tilde{c}) = \int_\Omega k_B T R \left[\ln\left(\frac{\tilde{c}_1 \tilde{c}_2}{\tilde{c}_3 \tilde{c}_4} \right) + \frac{\tilde{E}_1 + \tilde{E}_2 - \tilde{E}_S}{k_B T} - \frac{\tilde{E}_3 + \tilde{E}_4 - \tilde{E}_S}{k_B T} \right] = \int_\Omega k_B T R \ln\left[\left(\frac{\tilde{c}_1 \tilde{c}_2}{\tilde{c}_3 \tilde{c}_4} \right) \left(\frac{r_+}{r_-} \right) \right]. \tag{18}$$

We observe

$$\ln\left(\frac{\tilde{c}_1 \tilde{c}_2 r_+}{\tilde{c}_3 \tilde{c}_4 r_-} \right) = 0 \quad \text{iff } \tilde{c}_1 \tilde{c}_2 r_+ = \tilde{c}_3 \tilde{c}_4 r_-$$

and together with (18) we find (15). Equation (18) directly implies the free energy inequality (16). To see this, let us consider the following two mutual exclusive cases:

$$\text{(A)} \quad R \geqslant 0 \Leftrightarrow \tilde{c}_3\tilde{c}_4 r_- \geqslant \tilde{c}_1\tilde{c}_2 r_+ \Leftrightarrow \ln\left(\frac{\tilde{c}_1\tilde{c}_2 r_+}{\tilde{c}_3\tilde{c}_4 r_-}\right) \leqslant 0,$$

$$\text{(B)} \quad R < 0 \Leftrightarrow \tilde{c}_3\tilde{c}_4 r_- < \tilde{c}_1\tilde{c}_2 r_+ \Leftrightarrow \ln\left(\frac{\tilde{c}_1\tilde{c}_2 r_+}{\tilde{c}_3\tilde{c}_4 r_-}\right) > 0.$$

This discussion reveals the natural structure of the problem,

$$[\ln(\tilde{c}_1\tilde{c}_2 r_+) - \ln(\tilde{c}_3\tilde{c}_4 r_-)](\tilde{c}_3\tilde{c}_4 r_- - \tilde{c}_1\tilde{c}_2 r_+) \leqslant 0, \tag{19}$$

from which we unconditionally infer $\partial_t \tilde{F}(\tilde{c}(t)) \leqslant 0$. We see that the canonical structure of the problem goes along with the ansatz of the free energy.

A critical point $\tilde{c}$ of $\tilde{F}$ is characterized by

$$\ln \tilde{c}_l + \frac{\tilde{E}_l}{k_B T} + 1 = 0 \quad \text{for } 1 \leqslant l \leqslant 4. \tag{20}$$

This implies $\partial_t \tilde{c}_i = 0$, $1 \leqslant i \leqslant 4$ because from (20) it follows with (13)

$$\ln(\tilde{c}_1\tilde{c}_2 r_+) = -2,$$

$$\ln(\tilde{c}_3\tilde{c}_4 r_-) = -2,$$

and when subtracting the last two identities we find

$$\ln\left(\frac{\tilde{c}_1\tilde{c}_2 r_+}{\tilde{c}_3\tilde{c}_4 r_-}\right) = 0.$$

This implies at once $\partial_t \tilde{c}_i = 0$, $1 \leqslant i \leqslant 4$. The other implication in (17) is shown similarly.

IV. DERIVATION OF THE COMPLETE MODEL

Equation (19) reveals the underlying structure of reaction–diffusion equations which allows to discuss the reaction terms and give a complete description of the model. The swift jumps of the electrons are integrated into the model by two reactions,

$$\mathrm{Fe}^{2+} \overset{k}{\rightarrow} \mathrm{Fe}^{3+} + e^-,$$

$$\mathrm{Fe}^{2+} \overset{\kappa k}{\leftarrow} \mathrm{Fe}^{3+} + e^-. \tag{21}$$

Here, e^- is a free lattice electron and k, κk are reaction rates. A formula for c_e has already been found with (2).

The standard approach to model reactions (21) analogous to Eq. (12) is

$$r_1 = k(c_2^2 - \kappa c_1 c_e). \tag{22}$$

The principles leading to (22) are carefully explained in Ref. 8. But as we will show, (22) is wrong in our case as the rates will depend on χ! With the knowledge of (19) we can obtain a consistent formulation of r that generalizes (22). In this generalization, the rates will depend on χ.

To perfectly adjust the model, we first remind that the oxidation of Fe is caused by swift shifts of the electrons and occurs thus much faster than any other process, i.e., faster than diffusion. Hence, it is reasonable to assume that this oxidation is instantaneous. Thus we will replace the equation for c_1 by a stationary elliptic equation.

Second, due to electric neutrality, we postulate

$$c_5 = \tfrac{1}{2} c_1. \tag{23}$$

This condition was found experimentally in Ref. 2 long before a mathematical model had been developed. Equation (23) is the key to finding a consistent formulation for the reaction term. There is one difficulty here because (23) tells us that the movement of the vacancies is on the same fast time scale as the movement of the free electrons. We will bypass this problem by demanding $\partial_t c_5 = 0$ in the derivation of the reaction term in (27). All crystallographic measurements verify relation (23), but the quick electron jumps are beyond the resolution horizon of todays methods

As the main consequence of (2) and (23) we find

$$c_e = c_3. \tag{24}$$

To end up with the reaction terms having the structure of (19), the logarithms must have the same factors. Hence we assume

$$\beta_1^l + \frac{\beta_5^l}{2} = \beta_2^l = \beta_3^l = \beta_4^l =: b^l, \quad l = 1,2.$$

The final form of the free energy (4) is thus

$$f_l(c) = k_B T b^l \sum_{i=1}^{4} c_i \ln c_i + \sum_{i=1}^{3} c_i E_i + \left(\sum_{i=1}^{4} \alpha_i c_i \right)^2, \quad l = 1,2. \tag{25}$$

Combined, (8) and (25) define the free energy,

$$F(c,\chi) = \int_\Omega f(c,\chi) = \int_\Omega \left[k_B T b_\chi \left(\sum_{i=1}^{4} c_i \ln c_i \right) + \sum_{i=1}^{3} c_i E_i + \left(\sum_{i=1}^{4} \alpha_i c_i \right)^2 + \frac{\gamma T}{2} |\nabla \chi|^2 + TW(\chi) \right]. \tag{26}$$

Here we introduced the abbreviation $b_\chi := \chi b^1 + (1-\chi) b^2$. The rates fulfill

$$r_+ = k\kappa = \exp\left(\frac{E_1 + E_3 + E_S}{k_B T} \right), \quad r_- = k = \exp\left(\frac{2E_2 - E_S}{k_B T} \right).$$

We can give a quick motivation for the correct reaction term by considering again a purely reactive system, this time with phase changes. If we consider the oxidation process alone (without diffusion) we have

$$\partial_t c_4 = \partial_t c_5 = 0 \tag{27}$$

and from $\partial_t c_1 = \partial_t c_3$ and $\Sigma_{i=1}^5 c_i = 1$ we infer $\partial_t c_2 = -2\partial_t c_1$. With these constraints we compute $\partial_t F(c(t), \chi(t))$ for the free energy (26), where we can drop $(\Sigma_{i=1}^4 \alpha_i c_i)^2$ (the estimation of this term is possible as in Sec. V). We find

$$\begin{aligned} \partial_t F(c(t),\chi(t)) &= \int_\Omega \left[k_B T b_\chi \partial_t c_1 \ln\left(\frac{c_1 c_3}{c_2^2} \right) + \frac{E_1 + E_3 - E_S}{k_B T} - \frac{2E_2 - E_S}{k_B T} - (\partial_t \chi)^2 \right] \\ &= \int_\Omega \left[k_B T b_\chi \partial_t c_1 \ln\left(\frac{c_1 c_3 (r_+)^{1/b_\chi}}{c_2^2 (r_-)^{1/b_\chi}} \right) - (\partial_t \chi)^2 \right]. \end{aligned}$$

The consistent form of the reaction term that replaces (22) is hence

$$r_1 = r_3 = -\tfrac{1}{2} r_2 = (k)^{1/b_\chi} (c_2^2 - \kappa^{1/b_\chi} c_1 c_3), \quad r_4 = 0. \tag{28}$$

b^1 and b^2 should be in the magnitude of 1 and for $b^1 = b^2$ there would be no χ dependence. For $b^1 = b^2 = 1$ we fall back to standard formulas of r.

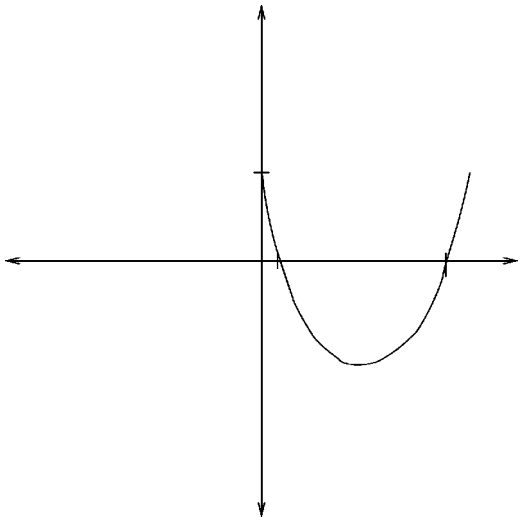

FIG. 1. Plot of $m(c_3)$.

It remains to discuss the control mechanism for the chalcopyrite phase. Equation (26) together with $\tau\partial_t\chi = -\partial_\chi(f/T) = \gamma\Delta\chi - \omega(c,\chi)$ gives rise to setting

$$\omega(c,\chi) = W'(\chi) + k_B(b^2 - b^1)\left(\sum_{i=1}^{4} c_i \ln c_i + \overline{\alpha}\right). \tag{29}$$

Here, $\overline{\alpha} > 0$ is a temperature-dependent constant. Additive constants occur in (26) because one can only measure the change δF of F when varying a quantity q, commonly temperature or volume, within some interval (q_0, q_1), finding the expression $\int_{q_0}^{q_1}\delta F$ for F. Frequently, we will set $\overline{\alpha} := \ln 3$.

To understand the principle of the control mechanism, we first freeze c_1, c_2, and c_4 and consider for constants $\alpha > 0$, $\beta > 0$, see Fig. 1,

$$\omega(c_3,\chi) = W'(\chi) + m(c_3),$$

$$m(c_3) = \beta c_3 \ln c_3 + \alpha.$$

The mechanism thus obtained is similar to the one commonly used in phase field models, where c_3 plays the role of temperature. From convexity of $m(c_3)$ and from the magnitude of α and β, we get the existence of $x_1, x_2 \in (0,1)$, $x_1 < x_2$ with $m(c_3) > 0$ for $c_3 \in (0,x_1) \cup (x_2,1)$ and $m(c_3) < 0$ for $c_3 \in (x_1,x_2)$. Consequently for $c_3 < x_1$, the sphalerite phase is preferred, whereas for $x_1 < c_3 < x_2$, chalcopyrite can form. In practice, the branch $c_3 > x_2$ is never reached, and the chalcopyrite phase once it has formed does not destabilize at a later time.

Expression (29) is symmetric with respect to the variables $c_1, \ldots, c_4$ and so the mechanism just explained also applies for the other variables. Yet there is unsymmetry which comes from the initial values for c. If we consider Fig. 1 again, this time imagining it as a function of c_1, then due to $c_1(t=0)$ one will stay in the part $(0,x_1)$. Hence, the reason why c_3 is mainly responsible for controlling the chalcopyrite disease is caused by the size of initial values $c(t=0)$. Now, the derivation of the model is complete.

Find for $t \geqslant 0$ the vector (c_1,c_2,c_3,c_4), χ such that in $\Omega \subset \mathbb{R}^D$ for $t > 0$,

$$0 = \operatorname{div}\left(\sum_{j=1}^{4} L_{1j}\nabla\mu_j\right) + k^{1/b_\chi}(c_2^2 - (\kappa)^{1/b_\chi}c_1c_3),$$

$$\partial_t c_i = \operatorname{div}\left(\sum_{j=1}^{4} L_{ij} \nabla \mu_j\right) + r_i(c,\chi), \quad i = 2,3,4,$$

$$\mu_i = \frac{\partial f}{\partial c_i}(c,\chi), \quad 1 \leqslant i \leqslant 4,$$

$$\tau \partial_t \chi = \gamma \Delta \chi - \omega(c,\chi),$$

and for $t=0$, $x \in \Omega$,

$$c_i(x,0) = c_{0i}(x), \quad i = 2,3,4,$$

$$\chi(x,0) = \chi_0(x),$$

and for $t>0$, $x \in \partial\Omega$,

$$c_i = g_i, \quad 1 \leqslant i \leqslant 4,$$

$$\mu_i = h_i, \quad 1 \leqslant i \leqslant 4 \tag{30}$$

with given Dirichlet data $g=(g_1,\ldots,g_4)$ *and* $h=(h_1,\ldots,h_4)$ *defined on* $\partial\Omega$.

V. THE FREE ENERGY INEQUALITY

We will show the thermodynamical correctness of system (30) under isothermal conditions, where the approximating elliptic equation is replaced by the original time-dependent formulation. It is suitable to reformulate (30),

$$\partial_t c + \operatorname{div}(J) = r, \tag{31}$$

$$\tau \partial_t \chi = -\frac{\partial f}{\partial \chi}, \tag{32}$$

where

$$J = -L \nabla \mu$$

and r is defined by (28). An application of the chain rule yields

$$\frac{d}{dt} f(c,\chi) = \sum_{j=1}^{4} \frac{\partial f}{\partial c_j} \partial_t c_j + \frac{\partial f}{\partial \chi} \partial_t \chi. \tag{33}$$

From (33) we learn that we must test the equation for c_i with $\partial f/\partial c_i = \mu_i$, $1 \leqslant i \leqslant 4$ and Eq. (32) with $\partial f/\partial \chi$. After integrating over Ω, one integration by parts we obtain

$$\frac{d}{dt}\int_\Omega f(c,\chi) - \int_\Omega \left(\sum_{j=1}^{4} \mu_j r_j + \sum_{j=1}^{4} \nabla \mu_j \cdot J_j + \frac{\partial f}{\partial \chi}\partial_t \chi\right) + \int_{\partial\Omega} \sum_{j=1}^{4} \mu_j J_j \cdot \vec{\nu} = 0. \tag{34}$$

This is the constitutive equality for the Helmholtz free energy density f.

To recast (34) as an inequality, we have that the matrix L is positive definite,

$$\sum_{j=1}^{4} \nabla \mu_j \cdot J_j = -L \nabla \mu : \nabla \mu \leqslant 0. \tag{35}$$

Additionally, by (32), we have $(\partial f/\partial \chi)\partial_t \chi = -\tau(\partial_t \chi)^2 \leqslant 0$. It remains to show

$$\int_\Omega \sum_{j=1}^{4} \mu_j r_j \leqslant 0. \tag{36}$$

We exploit the particular form of r and f and structure (19). Let $Q(c) := \Sigma_{i=1}^{4} \alpha_i c_i$. Since $r_1 = r_3 = -\frac{1}{2} r_2$, $r_4 = 0$ we have

$$\begin{aligned}
\int_\Omega \sum_{j=1}^{4} \mu_j r_j &= \int_\Omega (\mu_1 - 2\mu_2 + \mu_3) r_1 \\
&= \int_\Omega \left\{ k_B T b_\chi \left[\ln\left(\frac{c_1 c_3}{c_2^2} \right) + \frac{E_1 + E_3 - E_S}{k_B T b_\chi} - \frac{2E_2 - E_S}{k_B T b_\chi} \right] + 2(\alpha_1 - 2\alpha_2 + \alpha_3) Q(c) \right\} r_1 \\
&= \int_\Omega \left[k_B T b_\chi \ln\left(\frac{c_1 c_3 (r_+)^{1/b_\chi}}{c_2^2 (r_-)^{1/b_\chi}} \right) + 2(\alpha_1 - \alpha_2 + \alpha_3) Q(c) \right] r_1.
\end{aligned}$$

The first term can be estimated analogous to (19),

$$\int_\Omega k_B T b_\chi \ln\left(\frac{c_1 c_3 (r_+)^{1/b_\chi}}{c_2^2 (r_-)^{1/b_\chi}} \right) r_1 \leqslant 0 \tag{37}$$

but to estimate $\int_\Omega 2(\alpha_1 - 2\alpha_2 + \alpha_3) Q(c) r_1$ additional considerations are necessary. The logarithmic form (26) of the free energy guarantees $c_i > 0$ in Ω_{T_0} for $t > 0$ if this is true for $t = 0$. In Sec. VI a rigorous proof of this statement will be given. Hence we obtain $Q(c) > 0$ in Ω_{T_0}. Let

$$\sigma_1 := \sup_{x \in \Omega} c_1(x,0), \quad \sigma_2 := \inf_{x \in \Omega} c_{02}(x), \quad \sigma_3 := \sup_{x \in \Omega} c_{03}(x), \tag{38}$$

where σ_1, σ_2, σ_3 are positive constants. By the parabolic maximum principle,[13] as for fixed c_2, c_3, χ the mapping $c_1 \mapsto r_1(c, \chi)$ decreases as c_1 increases, and (now for fixed c_1, c_3, χ) $c_2 \mapsto r_1(c, \chi)$ increases and finally $c_3 \mapsto r_1(c, \chi)$ decreases, we have $\sigma_1 = \sup_{\overline{\Omega_{T_0}}} c_1$, $\sigma_2 = \inf_{\overline{\Omega_{T_0}}} c_2$, and $\sigma_3 = \sup_{\overline{\Omega_{T_0}}} c_3$.

Now a sufficient condition for $r_1 > 0$ in Ω_{T_0} is

$$\kappa^{1/b_\chi} < \frac{\sigma_2^2}{\sigma_1 \sigma_3}. \tag{39}$$

We remark that in the crystallographic measurements, the ratio constant κ never exceeded a value of 0.07 (otherwise the matrix becomes unstable). For an estimate of the volume term we require

$$\alpha_1 - 2\alpha_2 + \alpha_3 < 0. \tag{40}$$

This is a condition on the ion radii of Fe^{3+}, Fe^{2+}, and Cu^{+} and fulfilled in nature, see Table I.

Together with $r_1 > 0$ and the above estimate this shows $\int_\Omega 2(\alpha_1 - 2\alpha_2 + \alpha_3) Q(c) r_1 < 0$. Hence, (36) is proved and we have shown the *constitutive free energy inequality*

$$\frac{d}{dt} \int_\Omega f(c(t), \chi(t)) + \int_{\partial\Omega} \sum_{j=1}^{4} \mu_j J_j \cdot \vec{\nu} \leqslant 0. \tag{41}$$

In a thermodynamically closed system the fluxes on $\partial\Omega$ disappear. Hence we impose as condition on the Dirichlet data,

TABLE I. Values of sulfide crystal radii taken from Ref. 10.

Symbol	Species	Ion radius
α_1	Fe^{3+}	0.555 Å
α_2	Fe^{2+}	0.660 Å
α_3	Cu^{+}	0.635 Å
α_4	Zn^{2+}	0.640 Å

$$h_i = 0, \quad 1 \leqslant i \leqslant 4.$$

Instead we could impose the Neumann boundary conditions $\partial_\nu \mu_j = 0$, $1 \leqslant j \leqslant 4$ on $\partial\Omega$.

VI. EXISTENCE OF WEAK SOLUTIONS FOR POLYNOMIAL FREE ENERGY

The rest of the paper is devoted to the proof of global existence and uniqueness of a solution to the sharp interface model (30) with classical Dirichlet boundary conditions, i.e., $g=h=0$, and with the elliptic equation in (30) replaced by the original parabolic equation. The proof of existence is done in three steps. An additional (and artificial) surface energy term $\int_\Omega (\lambda/2)|\nabla c|^2$ is added to the free energy functional leading to a diffuse interface model. This term is necessary to guarantee the existence of a minimizer (Lemma 1). The first part is contained in Secs. VII–XIII and discusses the case of polynomial free energies for this diffuse interface model. Then we generalize to logarithmic free energies and finally the limit $\lambda \searrow 0$ is carried out. Some of the techniques used in the following sections were developed for the Cahn–Hilliard model, we mainly refer to Refs. 5, 6, and 1, and in particular Ref. 7.

VII. PRELIMINARIES

In what follows, $f = f(c,\chi)$ denotes the free energy density without the surface energy terms $(\gamma/2)|\nabla \chi|^2 + (\lambda/2)|\nabla c|^2$. C will denote generic constants that can change from estimate to estimate. With the additional surface term the model is the following.

Find for $t \geqslant 0$ the vector (c,μ,χ) such that in $\Omega_{T_0} := \Omega \times (0,T_0)$,

$$\partial_t c = \operatorname{div}(L \nabla \mu) + r(c,\chi),$$

$$\mu(c,\chi) = \frac{\partial f}{\partial c}(c,\chi) - \lambda \Delta c,$$

$$\tau \partial_t \chi = \gamma \Delta \chi - \omega(c,\chi)$$

and for $t=0$ in Ω,

$$c(\cdot,0) = c_0(\cdot), \quad \chi(\cdot,0) = \chi_0(\cdot)$$

and for $t>0$ in $\partial\Omega$,

$$c_i = \mu_i = 0, \quad 1 \leqslant i \leqslant 4. \tag{42}$$

$T_0 > 0$ denotes the stop time, $\omega = \partial_\chi f$, and $r(c,\chi)$ is given by (28).

Now, let us collect general properties of the model and some necessary tools that will be needed in the sequel. As a consequence of the assumed relation (23) the concentration vector c lies in the simplex

$$c \in \Sigma := \{d = (d_1, \ldots, d_4) \in \mathbb{R}^4 | \tfrac{3}{2} d_1 + d_2 + d_3 + d_4 = 1\}. \tag{43}$$

We do not propose $0 \leqslant c_i \leqslant 1$ in Ω because for the polynomial free energies considered here this is simply not true. This is one of the reasons why logarithmic free energies are introduced later on. Let

$$X_1 := \{c \in H_0^{1,2}(\Omega;\mathbb{R}^4) \| c \in \Sigma \text{ almost everywhere}\},$$

$$X_2 := H^{1,2}(\Omega;\mathbb{R}).$$

Since we have (classical) Dirichlet boundary conditions for the equations of conservation of mass, we consider the space of test functions,

$$Y := H_0^{1,2}(\Omega;\mathbb{R}^4)$$

and its dual

$$\mathcal{D} := (H_0^{1,2}(\Omega;\mathbb{R}^4))' = H^{-1,2}(\Omega;\mathbb{R}^4).$$

Let us now consider the mapping $\mathcal{L}(\mu): Y \to \mathcal{D}$ corresponding to $\mu \mapsto -\mathrm{div}(L \nabla \mu)$ with Dirichlet boundary conditions, defined by

$$\mathcal{L}(\mu)(\zeta) := \int_\Omega L \nabla \mu : \nabla \zeta.$$

To simplify the argumentation later we will need the inverse $\mathcal{G}$ of $\mathcal{L}$. The existence of $\mathcal{G}$ is derived from the Poincaré inequality and the Lax-Milgram theorem, since L is positive definite. From this we find that $\mathcal{G}$ is positive definite, self-adjoint, injective, and compact. Hence we have

$$(L \nabla \mathcal{G} v, \nabla \zeta)_{L^2} = (\zeta, v) \quad \text{for all } \zeta \in Y \text{ and } v \in \mathcal{D}.$$

We define for $v_1, v_2 \in \mathcal{D}$ the L scalar product by

$$(v_1, v_2)_L := (L \nabla \mathcal{G} v_1, L \nabla \mathcal{G} v_2)_{L^2}$$

with the corresponding norm

$$\|v\|_L := \sqrt{(v,v)_L}.$$

Functions $v \in Y$ canonically define an element in Y and consequently $(\cdot,\cdot)_L$ and $\|\cdot\|_L$ are as well defined for elements in Y.

With the help of Young's inequality we find for $\delta > 0$ and all $d \in Y$,

$$\|d\|_{L^2} = (L \nabla \mathcal{G} d, \nabla d)_{L^2} \leqslant \|L^{1/2} \nabla \mathcal{G} d\|_{L^2} \|L^{1/2} \nabla d\|_{L^2} \leqslant \frac{C_L}{\delta} \|d\|_L^2 + \delta \|\nabla d\|_{L^2}^2, \tag{44}$$

where C_L is a positive constant depending on L.

The Green's function $\mathcal{G}$ allows to rewrite the conservation of mass equations as

$$\mathcal{G}(\partial_t c - r(c,\chi)) = \mu := \left(\frac{\partial f}{\partial c_j}\right)_{1 \leqslant j \leqslant 4}. \tag{45}$$

VIII. THE WEAK FORMULATION OF THE PROBLEM

We call a triple $(c,\mu,\chi) \in L^2(0,T_0;H_0^{1,2}(\Omega;\mathbb{R}^4)) \times L^2(0,T_0;H_0^{1,2}(\Omega;\mathbb{R}^4)) \times L^2(0,T_0;H^{1,2}(\Omega;\mathbb{R}))$ with $r(c,\chi)$, $\omega(c,\chi) \in L^1(\Omega_{T_0})$ a *weak solution* of (42) if

$$-\int_{\Omega_{T_0}} \partial_t \xi \cdot (c - c_0) + \int_{\Omega_{T_0}} L \nabla \mu : \nabla \xi - \int_{\Omega_{T_0}} r(c,\chi)\xi = 0 \tag{46}$$

for all $\xi \in L^2(0,T_0;H_0^1(\Omega;\mathbb{R}^4))$ with $\partial_t \xi \in L^2(\Omega_{T_0})$, $\xi(T_0)=0$, and

$$\int_{\Omega_{T_0}} \mu \cdot \eta = \int_{\Omega_{T_0}} \left(\frac{\partial f}{\partial c}(c) \cdot \eta + \lambda \nabla c \cdot \nabla \eta \right) \tag{47}$$

for all $\eta \in L^2(0,T_0;H_0^1(\Omega;\mathbb{R}^4)) \cap L^\infty(\Omega_{T_0};\mathbb{R}^4)$, and

$$-\int_{\Omega_{T_0}} \tau \partial_t \zeta (\chi - \chi_0) + \int_{\Omega_{T_0}} \gamma \nabla \chi \cdot \nabla \zeta - \int_{\Omega_{T_0}} \omega(c,\chi)\zeta = 0 \tag{48}$$

for all $\zeta \in L^2(0,T_0;H^1(\Omega;\mathbb{R}))$ with $\partial_t \zeta \in L^2(\Omega_{T_0})$, $\zeta(T_0)=0$.

IX. A SEMI-IMPLICIT TIME DISCRETIZATION

We fix an $M \in \mathbb{N}$ and set $h := T_0/M$. For $m \geqslant 1$ and given $(c^{m-1},\mu^{m-1},\chi^{m-1}) \in H_0^{1,2}(\Omega;\mathbb{R}^4) \times H_0^{1,2}(\Omega,\mathbb{R}^4) \times H^{1,2}(\Omega;\mathbb{R})$,

$$\frac{c^m - c^{m-1}}{h} = \operatorname{div}(L \nabla \mu^m) + r(c^{m-1},\chi^{m-1}),$$

$$\mu^m = \frac{\partial f}{\partial c}(c^m,\chi^m) - \lambda \Delta c^m, \tag{49}$$

$$\tau \frac{\chi^m - \chi^{m-1}}{h} = \gamma \Delta \chi^m + \omega(c^m,\chi^m)$$

defines the implicit time discretization of system (42) except for the reaction term r that has been treated explicitly. Therefore, we call the resulting scheme semi-implicit. In (49), $\omega(c,\chi) = \partial_\chi f(c,\chi)$ and for the subsequent sections, let $r^{m-1} := r(c^{m-1},\chi^{m-1})$.

X. STRUCTURAL ASSUMPTIONS

In order to be able to establish the existence of weak solutions in the sense of Sec. VIII, the following assumptions are made.

(A1) $\Omega \subset \mathbb{R}^D$ is a bounded domain with Lipschitz boundary.

(A2) The free energy density f can be written as

$$f(c,\chi) = f^1(c,\chi) + f^2(c,\chi) \quad \text{for all } c \in \mathbb{R}^4, \quad \chi \in \mathbb{R}$$

with f^1, $f^2 \in C^1(\mathbb{R}^4 \times \mathbb{R};\mathbb{R})$ and $f^1(\cdot,\chi)$ convex for every $\chi \in \mathbb{R}$, $f^1(c,\cdot)$ convex for every $c \in \mathbb{R}^4$. Furthermore, we have the following:

(A2.1) $f^1 \geqslant 0$.

(A2.2) There exists a constant $C_1 > 0$ such that

$$|\partial_c f^2(c,\chi)| \leqslant C_1(|c| + 1) \quad \text{for all } c \in \Sigma, \chi \in \mathbb{R},$$

$$|\partial_\chi f^2(c,\chi)| \leqslant C_1(|\chi| + 1) \quad \text{for all } c \in \Sigma, \chi \in \mathbb{R}.$$

(A2.3) For all $\delta > 0$ there exists a constant $C_\delta > 0$ such that

$$|\partial_c f^1(c,\chi)| + |\partial_\chi f^1(c,\chi)| \leqslant \delta f^1(c,\chi) + C_\delta \quad \text{for all } c \in \Sigma,\ \chi \in \mathbb{R}.$$

(A3) The initial data (c_0,χ_0) fulfills

$$f(c_0,\chi_0)<\infty,\quad \omega(c_0,\chi_0)<\infty.$$

(A4.1) The diffusion tensor L is symmetric and positive definite.

(A4.2) $\gamma>0$ is a constant, $0<\lambda<\lambda_0$ where λ_0 is a small constant such that the estimate $\partial_t F\leqslant 0$ is valid.

(A5) The reaction term r is chosen in correspondence to f such that

$$\int_\Omega \mu\cdot r\leqslant 0. \tag{50}$$

(A6) The coefficients $\alpha_i>0$ satisfy condition (40). Furthermore $0<\kappa\leqslant 1$, $k>0$ and $0<b^1$, $b^2\leqslant 1$. The initial values c_0 of c and κ, b^1, b^2 fulfill [compare with (39)].

$$\kappa^{1/\max(b^1,b^2)}<\frac{\sigma_2^2}{\sigma_1\sigma_3}. \tag{51}$$

By assumption (A2) any polynomial growth is allowed for f^1, whereas exponential growth is not. For the nonconvex part, sublinear growth of $\partial_c f^2$ in c and $\partial_\chi f^2$ in χ is prescribed.

If we approximate a logarithmic free energy function f by a polynomial, we also must replace the reaction term by a suitable approximation. This is the gist of (A5). In Sec. XV it is shown how a suitable r can be constructed for approximations f^δ of f.

If one chooses $\lambda>0$ small enough, one can guarantee $\partial_t F(c(t),\chi(t))\leqslant 0$ because then the term with the possibly wrong sign $\lambda\Delta c r_1$ can be compensated by $(\alpha_1-2\alpha_2+\alpha_3)Q(c)r_1(c)<0$. From now on we assume without further stating that the assumptions (A1)–(A6) hold.

XI. EXISTENCE OF SOLUTIONS TO THE TIME DISCRETE SCHEME

For the treatment of the diffuse interface model we introduce the energy functional

$$F(c,\chi):=\int_\Omega\left(f(c,\chi)+\frac{\lambda}{2}|\nabla c|^2+\frac{\gamma}{2}|\nabla\chi|^2\right). \tag{52}$$

Additionally, for each time step m in the semi-implicit time discretization (49), given step size $h>0$ and given (c^{m-1},χ^{m-1}) we define the discrete energy functional

$$F^{m,h}(c,\chi):=F(c,\chi)+\frac{1}{2h}\|c-c^{m-1}-hr^{m-1}\|_L^2+\frac{\tau}{2h}\|\chi-\chi^{m-1}\|_{L^2}^2. \tag{53}$$

Lemma 1: Let $(c^{m-1},\chi^{m-1})\in X_1\times X_2$ *be given. Then for* $0<h<\min\{\tau/2C_1,\lambda/8C_1^2C_L\}$ *the functional* $F^{m,h}$ *possesses a minimizer in* $X_1\times X_2$.

Proof: We will show that $F^{m,h}$ is coercive and weakly lower semicontinuous. Using assumptions (A2.1) and (A2.2) we find

$$\begin{aligned}
&F^{m,h}(c,\chi)\\
&\quad\geqslant\frac{\lambda}{2}\|\nabla c\|_{L^2}^2+\frac{\gamma}{2}\|\nabla\chi\|_{L^2}^2-C_1(\|c\|_{L^2}^2+\|\chi\|_{L^2}^2)-C+\frac{1}{2h}(\|c-c^{m-1}-hr^{m-1}\|_L^2+\tau\|\chi-\chi^{m-1}\|_{L^2}^2)\\
&\quad\geqslant\left(\frac{\lambda}{2}-\delta C_1\right)\|\nabla c\|_{L^2}^2+\left(\frac{1}{2h}-\frac{C_1C_L}{\delta}\right)\|c-c^{m-1}-hr^{m-1}\|_L^2+\frac{\gamma}{2}\|\nabla\chi\|_{L^2}^2\\
&\qquad\times\left(\frac{\tau}{2h}-C_1\right)\|\chi-\chi^{m-1}\|_{L^2}^2-C,
\end{aligned}$$

where in the second estimate (44) was used and $C=C(c^{m-1},\chi^{m-1},r)$. Now, for $0<h$

$<\min\{\tau/2C_1, \lambda/8C_1^2C_L\}$ by choosing $\delta=\lambda/4C_1$, we conclude with the help of the Poincaré inequality that $F^{m,h}$ is coercive on $X_1\times X_2$. Let

$$d := \inf\{F^{m,h}(c,\chi)|c \in X_1,\ \chi \in X_2\}, \quad d<\infty.$$

If we now consider a minimizing sequence $(c_l,\chi_l)_{l\in\mathbb{N}}\subset X_1\times X_2$ with $F^{m,h}(c_l,\chi_l)\to d$, the coercivity of $F^{m,h}$ implies the boundedness of (c_l,χ_l) uniformly in l. Passing to a subsequence if necessary, by the reflexivity of $X_1\times X_2$ we may assume

$$(c_l,\chi_l)\to(c,\chi)\in X_1\times X_2 \quad \text{for } l\to\infty$$

and by Rellich's theorem or Sobolev's imbedding theorem,

$$(c_l,\chi_l)\to(c,\chi)\in L^2(\Omega,\mathbb{R}^4)\times L^2(\Omega,\mathbb{R}) \quad \text{for } l\to\infty$$

and $(c_l,\chi_l)\to(c,\chi)$ a.e. in Ω.

To verify the weak lower semicontinuity of $F^{m,h}$ in $X_1\times X_2$ we first remark that this is true for all convex terms. For $\int_\Omega f^1(c,\chi)$ this follows from assumption (A2) and for $\int_\Omega f^2(c,\chi)$ from (A2.2) and the dominated convergence theorem of Lebesgue. This implies $F^{m,h}(c,\chi)\leqslant\liminf_{l\to\infty}F^{m,h}(c_l,\chi_l)$. ■

Lemma 2: The minimizer (c^m,χ^m) *of* $F^{m,h}$ *fulfills*

$$\int_\Omega \frac{c^m-c^{m-1}}{h}\cdot\xi+\int_\Omega L\nabla\mu^m:\nabla\xi=\int_\Omega r^{m-1}\xi \quad \textit{for all } \xi\in Y, \tag{54}$$

$$\int_\Omega(\lambda\nabla c^m\cdot\nabla\eta+\partial_c f(c^m,\chi^m)\cdot\eta)=\int_\Omega\mu^m\cdot\eta \quad \textit{for } \eta\in Y\cap L^\infty(\Omega;\mathbb{R}^4), \tag{55}$$

$$\int_\Omega\left[\tau\frac{\chi^m-\chi^{m-1}}{h}+\omega(c^m,\chi^m)\right]\zeta+\int_\Omega\gamma\nabla\chi^m\cdot\nabla\zeta=0 \quad \textit{for } \zeta\in H^1(\Omega). \tag{56}$$

Here,

$$\mu^m=\mathcal{G}\left(\frac{c^m-c^{m-1}}{h}-r^{m-1}\right).$$

Proof: We choose directions $\xi\in Y\cap L^\infty(\Omega;\mathbb{R}^4)$, $\zeta\in X_2\cap L^\infty(\Omega;\mathbb{R})$ and determine the variations of $F^{m,h}(c,\chi)$ with respect to c and χ for ξ, ζ. We start with the variation with respect to c, i.e.,

$$\lim_{s\to0}((F^{m,h}(c^m+s\xi,\chi^m)-F^{m,h}(c^m,\chi^m))s^{-1}). \tag{57}$$

Since f^1 is convex in c, we have

$$f^1(c^m,\chi^m)\geqslant f^1(c^m+s\xi,\chi^m)-s\partial_c f^1(c^m+s\xi,\chi^m)\cdot\xi.$$

This implies

$$f^1(c^m+s\xi,\chi^m)\leqslant f^1(c^m,\chi^m)+|s\partial_c f^1(c^m+s\xi,\chi^m)|\|\xi\|_{L^\infty}\leqslant f^1(c^m,\chi^m)+|s|f^1(c^m+s\xi,\chi^m)\|\xi\|_{L^\infty}+C|s|.$$

The last is by assumption (A2.3) with $\delta=1$. Hence, for s small enough,

$$\left|\frac{f^1(c^m+s\xi,\chi^m)-f^1(c^m,\chi^m)}{s}\right|\leqslant C(f^1(c^m,\chi^m)+1).$$

Assumption (A2.2) and Lebesgue's dominated convergence theorem imply

$$\lim_{s\to 0}\frac{1}{s}\left(\int_\Omega f(c^m+s\xi,\chi^m)-f(c^m,\chi^m)\right)=\int_\Omega \partial_c f(c^m,\chi^m)\cdot\xi.$$

The variation of the quadratic form $c\mapsto(1/2h)\|c^m-c^{m-1}-hr^{m-1}\|_L^2$ yields

$$\lim_{s\to 0}[s^{-1}(2h)^{-1}(\|c^m+s\xi-c^{m-1}-hr^{m-1}\|_L^2-\|c^m-c^{m-1}-hr^{m-1}\|_L^2)]$$
$$=\left(\frac{c^m-c^{m-1}-hr^{m-1}}{h},\xi\right)_L=\left(\mathcal{G}\left(\frac{c^m-c^{m-1}}{h}-r^{m-1}\right),\xi\right)_{L^2}=(\mu^m,\xi)_{L^2}$$

and finally

$$\frac{\lambda}{2}\lim_{s\to 0}\{s^{-1}[(\nabla(c+s\xi),\nabla(c+s\xi))_{L^2}-(\nabla c,\nabla c)_{L^2}]\}=\lambda(\nabla c,\nabla\xi)_{L^2}=-\lambda(\Delta c,\xi)_{L^2}.$$

Hence we obtain (54). The equality (55) follows because (c^m,χ^m) is a minimizer and thus the variation in (57) is 0. To derive (56), we consider the variation of $F^{m,h}(c^m,\chi^m)$ with respect to χ. As before,

$$\lim_{s\to 0}[\tau s^{-1}(2h)^{-1}(\|\chi^m+s\zeta-\chi^{m-1}\|_{L^2}^2-\|\chi^m-\chi^{m-1}\|_{L^2}^2)]=\left(\tau\frac{\chi^m-\chi^{m-1}}{h},\zeta\right)_{L^2}.$$

It remains to prove

$$\lim_{s\to 0}\int_\Omega (f(c^m,\chi^m+s\zeta)-f(c^m,\chi^m))=\int_\Omega \partial_\chi f(c^m,\chi^m)\zeta.$$

This limit can be justified in the same way as (57) and identity (56) follows. ■

XII. UNIFORM ESTIMATES

In the preceding sections we proved the existence of a discrete solution (c^m,μ^m,χ^m) for $1\leqslant m\leqslant M$ and arbitrary $M\in\mathbb{N}$. We define the piecewise constant extension (c_M,μ_M,χ_M) of $(c^m,\mu^m,\chi^m)_{1\leqslant m\leqslant M}$ by

$$(c_M(t),\mu_M(t),\chi_M(t)):=(c_M^m,\mu_M^m,\chi_M^m):=(c^m,\mu^m,\chi^m)\quad\text{for } t\in((m-1)h,mh)$$

and $c_M(0)=c_0$, $\chi_M(0)=\chi_0$, $\mu_M(0)$ obtained from Eq. (55).

The piecewise linear extension $(\overline{c_M},\overline{\mu_M},\overline{\chi_M})$ for $t=[\beta m+(1-\beta)(m-1)]h$ with appropriate $\beta\in[0,1]$ is given by the interpolation

$$(\overline{c_M},\overline{\mu_M},\overline{\chi_M})(t):=\beta(c_M^m,\mu_M^m,\chi_M^m)+(1-\beta)(c_M^{m-1},\mu_M^{m-1},\chi_M^{m-1}).$$

Lemma 3: For sufficiently small h the following a priori estimates are valid.

(a) *For all $M\in\mathbb{N}$ and all $t\in[0,T_0]$ we have the dissipation inequality*

$$F(c_M,\chi_M)(t)+\frac{1}{2}\int_{\Omega_t}(L\nabla\mu_M:\nabla\mu_M+|\partial_t\chi_M|^2)\leqslant F(c_0,\chi_0).$$

(b) *There exists a constant $C>0$ such that*

$$\sup_{0\leqslant t\leqslant T_0}\{\|c_M(t)\|_{H^1}+\|\chi_M(t)\|_{H^1}\}\leqslant C, \tag{58}$$

$$\sup_{0\leqslant t\leqslant T_0}\int_\Omega f^1(c_M(t),\chi_M(t))+\|\nabla\mu_M\|_{L^2(\Omega_{T_0})}+\|\partial_t\chi_M\|_{L^2(\Omega_{T_0})}\leqslant C. \tag{59}$$

Proof: The idea of the proof is to use the decay of $t \mapsto F(c(t),\chi(t))$. Here, a modification of the standard proof becomes necessary which reveals that the treatment of the reaction term in (49) is natural.

As (c^m,χ^m) is minimizer of $F^{m,h}$,

$$F(c^m,\chi^m)+\frac{1}{2h}\|c^m-c^{m-1}-hr^{m-1}\|_L^2+\frac{\tau}{2h}\|\chi^m-\chi^{m-1}\|_{L^2}^2 \leqslant F(c^{m-1}+hr^{m-1},\chi^{m-1}). \tag{60}$$

A direct calculation yields

$$\frac{1}{2h}\|c^m-c^{m-1}-hr^{m-1}\|_L^2=\frac{h}{2}(\nabla\mu^m,L\,\nabla\,\mu^m)_{L^2}.$$

To bring the right-hand side of (60) in a form suitable for recursion, we remark that for sufficiently small h,

$$F(c^{m-1}+hr^{m-1},\chi^{m-1}) \leqslant F(c^{m-1},\chi^{m-1}).$$

This is equivalent to

$$\frac{F(c^{m-1}+hr^{m-1},\chi^{m-1})-F(c^{m-1},\chi^{m-1})}{h} \leqslant 0 \quad \text{for all } h>0.$$

By Lebesgue's dominated convergence theorem, a sufficient condition for the last inequality is $\partial_c F(c^{m-1},\chi^{m-1})\cdot r^{m-1} \leqslant 0$ which holds due to (A5).

By iterating (60) with the estimated right-hand side, we find

$$F(c_M^m,\chi_M^m)+\frac{1}{2}\int_0^{mh}((\nabla\mu_M^m,L\,\nabla\,\mu_M^m)_{L^2}+(\partial_t\chi_M^m,\partial_t\chi_M^m)_{L^2})\mathrm{d}t \leqslant F(c_0,\chi_0).$$

Using the assumptions and with the help of the Poincaré inequality this proves the lemma. ■

We extend c_M by the initial value c_0 of c for $t\in(-h,0]$. Now, for the linear interpolation $\overline{c_M}$ of c_M^m, the Euler–Lagrange equation (54) can be rewritten as

$$\int_\Omega \partial_t\overline{c_M}(t)\cdot\xi+\int_\Omega L\,\nabla\,\mu_M(t):\nabla\,\xi=\int_\Omega r(c_M(t-h),\chi_M(t-h))\cdot\xi \quad \text{for all } \xi\in Y \tag{61}$$

which holds for almost all $t\in(0,T_0)$. Together with the uniform estimates of Lemma 3, (61) allows to show compactness in time.

Lemma 4: There exists a constant $C>0$ such that for all t_1, $t_2\in[0,T_0]$,

$$\|\overline{c_M}(t_2)-\overline{c_M}(t_1)\|_{L^2} \leqslant C|t_2-t_1|^{1/4}.$$

Furthermore, there is a subsequence $(c_M)_{M\in\mathcal{N}}$ and a subsequence $(\mu_M)_{M\in\mathcal{N}}$ with $\mathcal{N}\subset\mathbb{N}$ and there are $c\in L^\infty(0,T_0;Y)$, $\mu\in L^2(0,T_0;Y)$ such that

(i) $\overline{c_M}\to c$ *in* $C^{0,\alpha}([0,T_0];L^2(\Omega;\mathbb{R}^4))$ *for all* $\alpha\in(0,\frac{1}{4})$,
(ii) $c_M\to c$ *in* $L^\infty(0,T_0;L^2(\Omega;\mathbb{R}^4))$,
(iii) $c_M\to c$ *almost everywhere in* Ω_{T_0},
(iv) $c_M\overset{*}{\rightharpoonup}c$ *in* $L^\infty(0,T_0;H_0^1(\Omega;\mathbb{R}^4))$,
(v) $\mu_M\rightharpoonup\mu$ *in* $L^2(0,T_0;H_0^1(\Omega;\mathbb{R}^4))$

as $M\in\mathcal{N}$ *tends to infinity*.

Proof: We test Eq. (61) with $\xi:=\overline{c_M}(t_2)-\overline{c_M}(t_1)$, where t_1, $t_2\in[0,T_0]$ with $t_1<t_2$. After integration in time from t_1 to t_2, we obtain

$$\|\overline{c_M}(t_2)-\overline{c_M}(t_1)\|_{L^2}^2+\int_{t_1}^{t_2}\int_\Omega L\,\nabla\,\mu_M(t):\nabla\,(\overline{c_M}(t_2)-\overline{c_M}(t_1))\mathrm{d}t$$
$$=\int_{t_1}^{t_2}\int_\Omega r(c_M(t-h),\chi_M(t-h))(\overline{c_M}(t_2)-\overline{c_M}(t_1))\mathrm{d}t.$$

The c_M^m are uniformly bounded in Y, therefore the linear interpolants $\overline{c_M}$ are uniformly bounded in $L^\infty(0,T_0;Y)$. Thus we obtain

$$\|\overline{c_M}(t_2)-\overline{c_M}(t_1)\|_{L^2}^2\leqslant C\|\overline{c_M}\|_{L^\infty(H^1)}\int_{t_1}^{t_2}(\|\nabla\,\mu_M(t)\|_{L^2}+\|r(c_M(t-h),\chi_M(t-h))\|_{L^2})\mathrm{d}t$$
$$\leqslant C\|\overline{c_M}\|_{L^\infty(H^1)}[(t_2-t_1)^{1/2}\|\nabla\,\mu\|_{L^2(\Omega_{T_0})}+(t_2-t_1)\|r(c_M,\chi_M)\|_{L^\infty(L^2)}].$$

Employing the *a priori* estimates (58) and (59) we have shown

$$\|\overline{c_M}(t_2)-\overline{c_M}(t_1)\|_{L^2}\leqslant C|t_2-t_1|^{1/4}\quad\text{for all } t_1,t_2\in[0,T_0]$$

for a positive constant C. This is the equicontinuity of $(\overline{c_M})_{M\in\mathbb{N}}$. The boundedness of $(\overline{c_M})$ in $L^\infty(0,T_0;H_0^{1,2}(\Omega))$ and the fact that H^1 is compactly imbedded in L^2 yields (i) as a consequence of the Arzelà–Ascoli theorem. The claims (ii), (iii), and (iv) follow exactly as in Ref. 7. We choose for $t\in[0,T_0]$ values $m\in\{1,\ldots,M\}$ and $\beta\in[0,1]$ such that $t=[\beta m+(1-\beta)(m-1)]h$. From the definition of $\overline{c}$ we get at once

$$\|\overline{c_M}(t)-c_M(t)\|_{L^2}=\|\beta c_M^m+(1-\beta)c_M^{m-1}-c_M^m\|_{L^2}=(1-\beta)\|c_M^m-c_M^{m-1}\|_{L^2}\leqslant Ch^{1/4}.$$

This tends to zero as M becomes infinite. With the help of (i), this proves (ii). Since for a subsequence we have convergence almost everywhere, (iii) is proved, too. Claim (iv) is a direct consequence of estimate (58) which gives the boundedness of c_M in $L^\infty(0,T_0;Y)$.

For the proof of (v) we notice that due to estimate (59), the $(\nabla\mu_M)$ are uniformly bounded in $L^2(\Omega_{T_0})$. By the Poincaré inequality the (μ_M) are uniformly bounded in $L^2(0,T_0;H_0^1(\Omega))$. With the Banach–Alaoglu theorem (v) follows. ■

Lemma 5: For a suitable subsequence $\mathcal{N}\subset\mathbb{N}$, we have

(i) $\overline{\chi_M}\to\chi$ *in* $C^{0,\alpha}([0,T_0];L^2(\Omega))$ *for all* $\alpha\in(0,\frac{1}{2})$,
(ii) $\chi_M\to\chi$ *in* $L^\infty(0,T_0;L^2(\Omega))$,
(iii) $\chi_M\to\chi$ *almost everywhere in* Ω_{T_0},
(iv) $\chi_M\overset{*}{\rightharpoonup}\chi$ *in* $L^\infty(0,T_0;H^1(\Omega))$,
(v) $\partial_c f(c_M,\chi_M)\to\partial_c f(c,\chi)$ *in* $L^1(\Omega_{T_0})$,
(vi) $\partial_\chi f(c_M,\chi_M)\to\partial_\chi f(c,\chi)$ *in* $L^1(\Omega_{T_0})$

as $M\in\mathcal{N}$ tends to infinity.

Proof: Similar to Eq. (61) we can reformulate identity (56) to

$$\tau\int_\Omega\partial_t\overline{\chi_M}(t)\zeta+\int_\Omega\gamma\nabla\,\chi_M(t)\cdot\nabla\,\zeta+\int_\Omega\omega(c_M(t),\chi_M(t))\zeta=0\quad\text{for all }\zeta\in H^1(\Omega)\qquad(62)$$

which holds for almost all $t\in[0,T_0]$.

We test (62) with $\zeta:=\overline{\chi_M}(t_2)-\overline{\chi_M}(t_1)$, where t_1, $t_2\in[0,T_0]$, $t_2>t_1$. After integration in time from t_1 to t_2 we get

$$\tau\|\overline{\chi}_M(t_2)-\overline{\chi}_M(t_1)\|_{L^2}^2+\int_{t_1}^{t_2}\int_\Omega \gamma\nabla\chi_M(t)\cdot\nabla(\overline{\chi}_M(t_2)-\overline{\chi}_M(t_1))\mathrm{d}t+\int_{t_1}^{t_2}\omega(c_M(t),\chi_M(t))(\overline{\chi}_M(t_2)-\overline{\chi}_M(t_1))\mathrm{d}t=0.$$

From the uniform boundedness of $\overline{\chi}_M$ in $L^\infty(0,T_0;H^1(\Omega))$ and in $L^\infty(\Omega_{T_0})$ we obtain

$$\int_{t_1}^{t_2}\int_\Omega \gamma\nabla\chi_M(t)\cdot\nabla(\overline{\chi}_M(t_2)-\overline{\chi}_M(t_1))\mathrm{d}t\leqslant c\|\overline{\chi}_M\|_{L^\infty(H^1)}\int_{t_1}^{t_2}\|\nabla\chi_M(t)\|_{L^2}\mathrm{d}t,$$

$$\int_{t_1}^{t_2}\omega(c_M(t),\chi_M(t))(\overline{\chi}_M(t_2)-\overline{\chi}_M(t_1))\mathrm{d}t\leqslant c\|\overline{\chi}_M\|_{L^\infty(\Omega_{T_0})}\int_{t_1}^{t_2}\omega(c_M(t),\chi_M(t))\mathrm{d}t.$$

With the continuity of ω, these estimates imply

$$\|\overline{\chi}_M(t_2)-\overline{\chi}_M(t_1)\|_{L^2}\leqslant C|t_2-t_1|^{1/2}\quad\text{for all } t_1,t_2\in[0,T_0]$$

and exactly as in Lemma 4 this yields statements (i)–(iv).

In order to prove (v) and (vi), we first notice that by assumption (A2), $\partial_c f$ and $\partial_\chi f$ are continuous functions. Hence, by (iii) and Lemma 4(iii),

$$\partial_c f(c_M,\chi_M)\to\partial_c f(c,\chi)\quad\text{almost everywhere in }\Omega_{T_0},$$

$$\partial_\chi f(c_M,\chi_M)\to\partial_\chi f(c,\chi)\quad\text{almost everywhere in }\Omega_{T_0}.$$

The growth condition of assumption (A2.3) on f^1 now yields that for arbitrary $\delta>0$ and all measurable $E\subset\Omega$,

$$\int_E|\partial_c f^1(c_M,\chi_M)|\leqslant\delta\int_E f^1(c_M,\chi_M)+C_\delta|E|\leqslant\delta C+C_\delta|E|.$$

Therefore, $\int_E|\partial_c f^1(c_M,\chi_M)|\to 0$ as $|E|\to 0$ uniformly in M and by Vitali's theorem, $f^1(c_M,\chi_M)\to f^1(c,\chi)$ in $L^1(\Omega_{T_0})$ as $M\in\mathcal{N}$ tends to infinity. The same result for f^2 follows directly from (A2.2) and the dominated convergence theorem of Lebesgue. The proof of $\partial_\chi f(c_M,\chi_M)\to\partial_\chi f(c,\chi)$ exploiting (A2.3) and (A2.2) is similar. ■

XIII. GLOBAL EXISTENCE OF SOLUTIONS FOR POLYNOMIAL FREE ENERGY

We are now in the position to state one of the main results.

Theorem 1: *Let the assumptions of Sec. X hold. Then, there exists a weak solution* (c,μ,χ) *of the diffuse interface equations in the sense of (46)–(48) such that*

(i) $c\in C^{0,1/4}([0,T_0];L^2(\Omega;\mathbb{R}^4))$,
(ii) $\partial_t c\in L^2(0,T_0;(H_0^1(\Omega;\mathbb{R}^4))')$,
(iii) $\chi\in C^{0,1/2}([0,T_0];L^2(\Omega))$,
(iv) $\partial_t\chi\in L^2(0,T_0;(H_0^1(\Omega))')$.

Proof: We are going to prove that (c,μ,χ) introduced in Lemmata 4 and 5 is the desired weak solution in the sense of (46)–(48). From Eq. (61) we learn

$$-\int_{\Omega_{T_0}}\partial_t\xi(\overline{c_M}-c_0)+\int_{\Omega_{T_0}}L\nabla\mu_M:\nabla\xi+\int_{\Omega_{T_0}}r(c_M,\chi_M)=0$$

for all $\xi\in L^2(0,T_0;Y)$ with $\partial_t\xi\in L^2(\Omega_{T_0})$ and $\xi(T_0)=0$. Passing to the limit $M\to\infty$ together with Lemma 4 this implies (46). Now we show (47). From (55) we see

$$\int_\Omega \lambda \nabla c_M \cdot \nabla \eta + \partial_c f(c_M, \chi_M) \cdot \eta = \int_\Omega \mu_M \cdot \eta \quad \text{for all } \eta \in Y \cap L^\infty(\Omega; \mathbb{R}^4).$$

The convergence of

$$\int_\Omega \lambda c_M \cdot \nabla \eta \to \int_\Omega \lambda c \cdot \nabla \eta$$

as $M \to \infty$ is clear by linearity and the convergence

$$\int_\Omega \partial_c f(c_M, \chi_M) \cdot \eta \to \int_\Omega \partial_c f(c, \chi) \cdot \eta$$

is again evident by Vitali's theorem similar to the proof of Lemma 5 by using the almost everywhere convergence of c_M and χ_M, the growth condition (A2.3), estimate (59) on f^1 and the boundedness of η.

In the same way, we obtain (48) from (62). ■

XIV. UNIQUENESS OF THE DIFFUSE INTERFACE MODEL

To show uniqueness of (42), we use an integration in time method. The proof requires the validity of the free energy inequality and the validity of (A6).

Theorem 2: *The solution (c, μ, χ) of the diffuse interface equations obtained in Theorem 1 is unique in the spaces stated in this theorem.*

Proof: Assume that (c^i, χ^i, μ^i), $i = 1, 2$ are two solutions of system (42). Now, let $c := c^2 - c^1$, $\chi := \chi^2 - \chi^1$, $\mu := \mu^2 - \mu^1$, $r := r(c^2, \chi^2) - r(c^1, \chi^1)$, $\omega := \partial_\chi f(c^2, \chi^2) - \partial_\chi f(c^1, \chi^1)$. The difference (c, χ, μ) solves the weak formulation

$$-\int_{\Omega_{T_0}} \partial_t \xi \cdot c + \int_{\Omega_{T_0}} L \nabla \mu : \nabla \xi - \int_{\Omega_{T_0}} r \cdot \xi = 0, \tag{63}$$

$$\int_{\Omega_{T_0}} [(\partial_c f(c^2, \chi^2) - \partial_c f(c^1, \chi^1)) \cdot \eta + \lambda \nabla c \cdot \nabla \eta] = \int_{\Omega_{T_0}} \mu \cdot \eta, \tag{64}$$

$$-\int_{\Omega_{T_0}} \tau \partial_t \zeta \chi + \int_{\Omega_{T_0}} \gamma \nabla \chi \cdot \nabla \zeta - \int_{\Omega_{T_0}} \omega \cdot \zeta = 0. \tag{65}$$

For given $\eta \in L^2(0, T_0; H_0^1(\Omega, \mathbb{R}^4))$ and $t_0 \in (0, T_0)$ we define

$$\xi(\cdot, t) := \begin{cases} \displaystyle\int_t^{t_0} \eta(\cdot, s)\mathrm{d}s & \text{if } t \leqslant t_0, \\ 0 & \text{if } t > t_0. \end{cases} \tag{66}$$

Using this test function in (63) we find after integration by parts in time

$$\begin{aligned} 0 &= \int_{\Omega_{t_0}} c \cdot \eta + \int_{\Omega_{t_0}} L \nabla \mu : \nabla \left(\int_t^{t_0} \eta(s)\mathrm{d}s \right) - \int_{\Omega_{t_0}} r \cdot \left(\int_t^{t_0} \eta(s)\mathrm{d}s \right) \\ &= \int_{\Omega_{t_0}} c \cdot \eta + \int_{\Omega_{t_0}} L \nabla \left(\int_0^t \mu(s)\mathrm{d}s \right) : \nabla \eta - \int_{\Omega_{t_0}} \left(\int_0^t r(s)\mathrm{d}s \right) \cdot \eta. \end{aligned} \tag{67}$$

This implies

$$\mathcal{G}\left(c-\int_0^t r(s)\mathrm{d}s\right)=-\int_0^t \mu(s)\mathrm{d}s \quad \text{and } \partial_t\mathcal{G}\left(c-\int_0^t r(s)\mathrm{d}s\right)=-\mu.$$

By choosing $\eta:=\mu$ in (67) we obtain

$$0=\int_{\Omega_{t_0}} c\cdot\mu+\int_{\Omega_{t_0}} L\,\nabla\left(\mathcal{G}\left(\int_0^t r(s)\mathrm{d}s-c\right)\right):\nabla\left(\partial_t\mathcal{G}\left(\int_0^t r(s)\mathrm{d}s-c\right)\right)-\int_{\Omega_{t_0}}\left(\int_0^t r(s)\mathrm{d}s\right)\cdot\mu$$

and consequently

$$0=\int_{\Omega_{t_0}} c\cdot\mu+\int_{\Omega} L\,\nabla\,\mathcal{G}\left(\int_0^{t_0} r(s)\mathrm{d}s-c(t_0)\right):\nabla\,\mathcal{G}\left(\int_0^{t_0} r(s)\mathrm{d}s-c(t_0)\right)-\int_{\Omega_{t_0}}\left(\int_0^t r(s)\mathrm{d}s\right)\cdot\mu. \tag{68}$$

In Eq. (64) we test with $\eta:=\chi_{[0,t_0]}c$. Hence we have

$$\int_{\Omega_{t_0}} c\cdot\mu=\int_{\Omega_{t_0}}\lambda|\nabla c|^2+(\partial_c f(c^2,\chi^2)-\partial_c f(c^1,\chi^1))\cdot c. \tag{69}$$

From (68) and (69) we learn

$$\left\|\left(\int_0^{t_0} r\right)-c(t_0)\right\|_L^2+\int_{\Omega_{t_0}}\lambda|\lambda c|^2-\int_{\Omega_{t_0}}\left(\int_0^t r(s)\mathrm{d}s\right)\cdot\mu=-\int_{\Omega_{t_0}}(\partial_c f(c^2,\chi^2)-\partial_c f(c^1,\chi^1))\cdot c. \tag{70}$$

From the free energy estimate we infer that if conditions (40) and (51) and (A4.2) hold (i.e., if $\lambda<\lambda_0$), then

$$\int_{\Omega_{t_0}}\left(\int_0^t r(s)\mathrm{d}s\right)\cdot\mu\leqslant 0. \tag{71}$$

This holds because $r(t)\cdot\mu(t)=r_1(t)(\mu_1(t)-2\mu_2(t)+\mu_3(t))$ and $(\mu_1(t)-2\mu_2(t)+\mu_3(t))<0$, $\int_0^L r(s)\mathrm{d}s\geqslant r_1(t)>0$ for almost every $t\in\Omega_{T_0}$, see Sec. V. Therefore we obtain as a consequence of (70)

$$\lambda\int_{\Omega_{t_0}}|\nabla c|^2\leqslant-\int_{\Omega_{t_0}}(\partial_c f(c^2,\chi^2)-\partial_c f(c^1,\chi^1))\cdot c. \tag{72}$$

In (65) we choose the test function $\mathrm{X}_{[0,t_0]}\chi$ analogous to (66). This leads to

$$\frac{\tau}{\gamma}\int_{\Omega_{t_0}}\chi\eta+\int_{\Omega_{t_0}}\nabla\left(\int_0^t\chi(s)\mathrm{d}s\right):\nabla\,\eta(t)-\frac{1}{\gamma}\int_{\Omega_{t_0}}\eta(t)\int_0^t\omega(s)\mathrm{d}s=0. \tag{73}$$

This implies because of $\chi(0)=0$,

$$(-\Delta)^{-1}\left(\frac{\tau}{\gamma}\chi-\frac{1}{\gamma}\int_0^t\omega(s)\mathrm{d}s\right)=-\int_0^t\chi(s)\mathrm{d}s,$$

$$\partial_t(-\Delta)^{-1}\left(\frac{\tau}{\gamma}\chi-\frac{1}{\gamma}\int_0^t\omega(s)\mathrm{d}s\right)=-\chi(t).$$

We set $\eta:=\chi$ in (73). As in the treatment of Eq. (63) this yields

$$0 = \gamma\tau\int_{\Omega_{t_0}} |\chi|^2 + \left\| \tau\chi(t_0) - \left(\int_0^{t_0} \omega(s) \right) \right\|_{L^2}^2 - \gamma \int_{\Omega_{t_0}} \chi(t) \int_0^t \omega(s)\mathrm{d}s$$

and consequently with Young's inequality

$$\tau\int_{\Omega_{t_0}} |\chi|^2 \leqslant \delta\int_{\Omega_{t_0}} |\chi|^2 + \frac{C}{\delta}\int_{\Omega_{t_0}} \left(\int_0^t \omega(s)\mathrm{d}s \right)^2. \tag{74}$$

Now we add (72) and (74) and find

$$\lambda\int_{\Omega_{t_0}} |\nabla c|^2 + \tau\int_{\Omega_{t_0}} |\chi|^2 \leqslant \delta C\int_{\Omega_{t_0}} (|c|^2 + |\chi|^2) + \frac{C}{\delta}\int_{\Omega_{t_0}} \left(\int_0^t \omega(s)\mathrm{d}s \right)^2 + |\partial_c f(c^2,\chi^2) - \partial_c f(c^1,\chi^1)|^2.$$

For δ small the first integral on the right-hand side can be absorbed on the left. As

$$|\partial_c f(c^2,\chi^2) - \partial_c f(c^1,\chi^1)|^2 + |\partial_\chi f(c^2,\chi^2) - \partial_\chi f(c^1,\chi^1)|^2 \leqslant C_0(|c|^2 + |\chi|^2),$$

where C_0 depends on the Lipschitz constant of $\partial_c f$ and $\partial_\chi f$, we find at last by exploiting the Poincaré inequality

$$\int_{\Omega_{t_0}} (|\nabla c|^2 + |\chi|^2) \leqslant C\int_{\Omega_{t_0}} (|\nabla c|^2 + |\chi|^2) + \int_0^t \int_{\Omega_{t_0}} (|\nabla c|^2 + |\chi|^2).$$

With Gronwall's inequality this finally means $c=\chi=0$ in Ω_{t_0} and with (64) $\mu=0$ in Ω_{t_0}. By repeating the argument, as $t_0>0$, this holds in the whole of Ω_{T_0}. ■

XV. LOGARITHMIC FREE ENERGY

In the following four sections we are going to extend Theorem 1 to logarithmic free energies. The results will in particular be taylor made for the free energy functional considered in definition (8),

$$f(c,\chi) = \chi b^1 \sum_{j=1}^4 c_j \ln c_j + (1-\chi) b^2 \sum_{j=1}^4 c_j \ln c_j + \sum_{i=1}^3 c_i E_i + \left(\sum_{j=1}^4 \alpha_j c_j \right)^2 + TW(\chi). \tag{75}$$

We will use the statements proved for polynomial free energies that can be regarded as a Taylor expansion.

For the proof of $0<c_j<1$, $1\leqslant j\leqslant 4$, we approximate f for $\delta>0$ by some f^δ that fulfills the requirements of Sec. X and find suitable *a priori* estimates that put us in the position to pass to the limit $\delta\to 0$.

The logarithmic form of the free energy guarantees that the concentration vector c lies inside the transformed Gibbs simplex,

$$G := \Sigma \cap \{c \in \mathbb{R}^4 | c_j \geqslant 0 \text{ for } 1 \leqslant j \leqslant 4\}$$

and that $\chi \in (0,1)$. Therefore (c,χ) is physically meaningful.

The assumptions (A2) and (A3) of Sec. X are replaced by the following:

(A2′) f is of the form (75) with constants $\alpha_j>0$, $b^1>0$, $b^2>0$, $T>0$.

(A3′) The initial values $c_0 \in X_1$, $\chi_0 \in X_2$ fulfill $c_0 \in G$, $\chi \in [0,1]$ almost everywhere and

$$\int_\Omega c_{0l} > 0 \quad \text{for } 1 \leqslant l \leqslant 4, \quad \int_\Omega \chi > 0, \quad \int_\Omega (1-\chi) > 0.$$

(A6′) Additional to the conditions in (A6) we demand

$$\kappa^{1/\max(b^1,b^2)} < \frac{1}{e^2}. \tag{76}$$

The assumptions (A1) and (A4) remain unchanged and continue to hold.

To proceed, we define for $d>0$ the convex function

$$\psi(d) := d \ln d$$

and for $\delta>0$ its regularization (defined for $d \in \mathbb{R}$)

$$\psi^\delta(d) := \begin{cases} d \ln d & \text{for } d \geqslant \delta, \\ d \ln \delta - \dfrac{\delta}{2} + \dfrac{d^2}{2\delta} & \text{for } d < \delta. \end{cases}$$

The regularized free energy functional is defined such that $\psi^\delta \in C^2$ and the derivative $(\psi^\delta)'$ is monotone increasing. This ansatz goes back to Ref. 5.

The free energy of the regularized δ-problem is found by replacing $\Sigma_i c_i \ln c_i$ by $\Sigma_i \psi^\delta(c_i)$ in (26). Since the convex combination

$$\overline{f}(c,\chi) := \chi f_1(c) + (1-\chi) f_2(c)$$

would define a nonconvex functional in c if $\chi \notin [0,1]$, we consider the following penalization [$f^\delta = f^{1,\delta} + f^2$, see assumption (A2)]:

$$f^{1,\delta}(c,\chi) := \begin{cases} \chi b^1 \sum\limits_j \psi^\delta(c_j) + (1-\chi) b^2 \sum\limits_j \psi^\delta(c_j) + T[\psi^\delta(\chi) + \psi^\delta(1-\chi)] & \text{if } \chi \in (0,1), \\ +\infty \quad \text{else}, \end{cases}$$

$$f^2(c,\chi) := \left(\sum_{j=1}^4 \alpha_j c_j \right)^2.$$

Due to the expression $\psi^\delta(\chi)+\psi^\delta(1-\chi)$ in the definition of f^δ it is obvious that every minimizer χ fulfills $0<\chi<1$. This is proved rigorously in Lemma 8.

It can be easily checked that the functional $F^{m,h}$ of Sec. XI still has a minimizer (c^m,χ^m) for every m and sufficiently small h. For $\chi \in (0,1)$, $f^{1,\delta}$ is still continuously differentiable. Since $f^{1,\delta}$, f^2 fulfill the assumptions of Sec. X the earlier existence results can be carried over.

The regularization f^δ of f also implies that $\omega(c^\delta,\chi^\delta) = \partial_\chi f^\delta(c^\delta,\chi^\delta)$ depends on δ and therefore we will replace $\omega(c^m,\chi^m)$ in the implicit time discretization (49) by $\omega^\delta(c^m,\chi^m)$ and the weak formulation (48) by

$$-\int_{\Omega_{T_0}} \tau \partial_t \zeta (\chi^\delta - \chi_0) + \int_{\Omega_{T_0}} \gamma \nabla \chi^\delta \cdot \nabla \zeta - \int_{\Omega_{T_0}} \omega^\delta(c^\delta,\chi^\delta)\zeta = 0 \tag{77}$$

for all $\zeta \in L^2(0,T_0;H^1(\Omega;\mathbb{R}))$ with $\partial_t \zeta \in L^2(\Omega_{T_0})$, $\zeta(T_0)=0$. Later we will show that $\omega^\delta(c^\delta,\chi^\delta) \to \omega(c,\chi)$ in $L^1(\Omega_{T_0})$ as $\delta \searrow 0$.

The only assumption that needs further clarification is (A5). In order to verify (50), we must construct an approximation $r^\delta = (r_1^\delta, -r_1^\delta, r_1^\delta, 0)$ of r and must check that

$$\int_\Omega k_B T b_\chi \left[(\psi^\delta)'(c_1) - 2(\psi^\delta)'(c_2) + (\psi^\delta)'(c_3) + \frac{E_1 - 2E_2 + E_3}{k_B T b_\chi} \right] r_1^\delta \leqslant 0.$$

We claim that a good choice for r_1^δ is

$$r_1^\delta(c,\chi) := k^{1/b_\chi}(\max(c_2,\delta)^2 - \kappa^{1/b_\chi}\max(c_1,\delta)\max(c_3,\delta)). \tag{78}$$

To illustrate (78), let us consider three characteristic cases.

Case 1: $c_1 \geqslant \delta$, $c_2 \geqslant \delta$, $c_3 \geqslant \delta$. Apparently $r^\delta = r$, and (50) follows verbatim as in the proof of the free energy inequality in Sec. V.

Case 2: $c_1 < \delta$, $c_2 \geqslant \delta$, $c_3 \geqslant \delta$. From the definition of ψ^δ we find that we must estimate

$$\int_\Omega k_B T b_\chi \left(\ln \delta + \frac{c_1}{\delta} - 2\ln c_2 - 2 + \ln c_3 + 1 + \frac{E_1 + E_3 - 2E_2}{k_B T b_\chi} \right) r_1^\delta$$
$$= \int_\Omega k_B T b_\chi \left[\ln\left(\frac{\delta c_3 \kappa^{1/b_\chi}}{c_2^2} \right) + \frac{c_1}{\delta} - 1 \right] r_1^\delta.$$

The estimate follows now from $[\ln(\delta c_3 \kappa^{1/b_\chi}) - \ln(c_2^2)] r_1^\delta < 0$ and because of $(c_1/\delta) - 1 < 0$ and $r_1^\delta = k^{1/b_\chi}(c_2^2 - \kappa^{1/b_\chi}\delta c_3) > 0$ for δ sufficiently small. We emphasize that we need $r_1^\delta > 0$ in order to have $\int_\Omega (\alpha_1 - 2\alpha_2 + \alpha_3) Q(c^\delta) r_1^\delta < 0$ which allows to compensate the surface energy term for sufficiently small λ.

Case 3: $c_1 < \delta$, $c_2 < \delta$, $c_3 < \delta$. Here we must estimate

$$\int_\Omega k_B T b_\chi \left[\ln\left(\frac{\delta^2}{\delta^2} \right) + \frac{c_1}{\delta} - 2\frac{c_2}{\delta} + \frac{c_3}{\delta} + \frac{E_1 - 2E_2 + E_3}{k_B T b_\chi} \right] r_1^\delta.$$

We observe $r_1^\delta = k^{1/b_\chi}\delta^2(1 - \kappa^{1/b_\chi}) > 0$ due to assumption (A6). Finally

$$\int_\Omega \left(\frac{E_1 - 2E_2 + E_3}{k_B T b_\chi} + \frac{c_1 - 2c_2 + c_3}{\delta} \right) \leqslant \int_\Omega [\ln(\kappa^{1/b_\chi}) + 2] < 0$$

if κ satisfies (76). The remaining cases can be treated similar to case 2.

XVI. UNIFORM ESTIMATES

The following lemma was first stated and proved in Elliott and Luckhaus[5] for logarithmic free energies typical for the Cahn–Hilliard system.

Lemma 6: For $\delta_0 = 1/e$ there exists a $K > 0$ such that for all $\delta \in (0, \delta_0)$,

$$f^\delta(c,\chi) \geqslant -K \text{ for all } c \in \Sigma,\ \chi \in [0,1].$$

Proof: For $\delta_0 < 1/e$ one has $\psi^\delta(d) \geqslant -1/e$ for all $\delta < \delta_0$. As b^l, $T > 0$, the proof is complete.■

Lemma 7: (a) For $\delta \in (0, \delta_0)$ there exists a weak solution $(c^\delta, \mu^\delta, \chi^\delta)$ of (42) with a logarithmic free energy that satisfies (A2′)–(A6′) in the sense of Sec. VIII with (48) replaced by (77).

(b) There exists a constant $C > 0$ independent of δ such that for all $\delta \in (0, \delta_1)$ with some constant $\delta_1 \leqslant \delta_0$

$$\sup_{t \in [0,T_0]} \{ \|c^\delta(t)\|_{H^1} + \|\chi^\delta(t)\|_{H^1} \} \leqslant C,$$

$$\sup_{t \in [0,T_0]} \int_\Omega f^{1,\delta}(c^\delta(t), \chi^\delta(t)) + \|\nabla \mu^\delta\|_{L^2(\Omega_{T_0})} \leqslant C$$

and

$$\|c^\delta(t_2) - c^\delta(t_1)\|_{L^2} \leqslant C|t_2 - t_1|^{1/4},$$

$$\|\chi^\delta(t_2) - \chi^\delta(t_1)\|_{L^2} \leqslant C|t_2 - t_1|^{1/2}$$

for all t_1, $t_2 \in [0, T_0]$.

(c) One can extract subsequences $(c^\delta)_{\delta\in\mathcal{R}}$, $(\mu^\delta)_{\delta\in\mathcal{R}}$ *and* $(\chi^\delta)_{\delta\in\mathcal{R}}$ *where* $\mathcal{R}\subset(0,\delta_1)$ *is a countable set with zero as the only accumulation point such that*

(i) $c^\delta\to c$ *in* $C^{0,\alpha}([0,T_0];L^2(\Omega;\mathbb{R}^4))$ *for all* $\alpha\in\left(0,\frac{1}{4}\right)$,
(ii) $c^\delta\to c$ *almost everywhere in* Ω_{T_0},
(iii) $c^\delta\overset{*}{\rightharpoonup}c$ *in* $L^\infty(0,T_0;H_0^1(\Omega;\mathbb{R}^4))$,
(iv) $\chi^\delta\to\chi$ *in* $C^{0,\alpha}([0,T_0];L^2(\Omega))$ *for all* $\alpha\in\left(0,\frac{1}{2}\right)$,
(v) $\chi^\delta\to\chi$ *almost everywhere in* Ω_{T_0} *and* $0\leqslant\chi^\delta,\ \chi\leqslant 1$ *a.e. in* Ω_{T_0},
(vi) $\chi^\delta\overset{*}{\rightharpoonup}\chi$ *in* $L^\infty(0,T_0;H^1(\Omega))$,
(vii) $\mu^\delta\rightharpoonup\mu$ *in* $L^2(0,T_0;H_0^1(\Omega;\mathbb{R}^4))$

as $\delta\in\mathcal{R}$ *tends to zero.*

Proof: Using Lemma 6, the regularized problem satisfies the assumptions of Sec. X and by Theorem 1, a weak solution for fixed $\delta\in(0,\delta_0)$ exists. This proves (a). The estimates in (b) are a direct consequence of Lemma 3 and Lemma 4, where due to assumption (A4.2) we must choose δ small enough for Lemma 3 to hold. From Lemma 3, it follows that $F^\delta(c_0,\chi_0)$ does not depend on δ, hence the constant on the right-hand side does not depend on δ. (c) is proved by Lemmata 4 and 5. ■

XVII. HIGHER INTEGRABILITY FOR THE LOGARITHMIC FREE ENERGY

Since $\varphi^\delta:=(\psi^\delta)'$ will be singular as $\delta\to 0$ we introduce for $r>0$

$$\varphi_r^\delta(d):=\begin{cases}\varphi^\delta(d)|\varphi^\delta(d)|^{r-1} & \text{if } \varphi^\delta(d)\neq 0,\\ 0 & \text{if } \varphi^\delta(d)=0.\end{cases}$$

By definition, $\varphi_r^\delta\in C^0(\mathbb{R})$.

For $0<r<1$, φ_r^δ is not differentiable at the zero point of φ^δ. To overcome this difficulty, for $\varrho>0$ introduce the function $\varphi_r^{\delta,\varrho}$ with $\varphi_r^{\delta,\varrho}=\varphi_r^\delta$ in $\mathbb{R}\backslash[0,1]$ and define $\varphi_r^{\delta,\varrho}$ in [0, 1] such that $\varphi_r^{\delta,\varrho}$ is a C^1 function, monotone increasing and $\varphi_r^{\delta,\varrho}\to\varphi_r^\delta$ in $C^0(\mathbb{R})$ as $\varrho\searrow 0$.

For the approximation of $\varphi^\delta(\chi^\delta)$ in the modified Allen–Cahn equation it is more suitable to introduce the Dirac sequence

$$\varphi^{\delta,\varepsilon}(x):=(\varphi^\delta * J_\varepsilon)(x):=\varepsilon^{-D}\int_{\mathbb{R}^D}\varphi^\delta(x)J((x-y)/\varepsilon)\mathrm{d}y,$$

where the kernal $J\in C^\infty(B^1(0))$ is a positive smooth polynomial [see assumption (A2)]. As is well known, $\varphi^{\delta,\varepsilon}\in C^\infty$ and $\varphi^{\delta,\varepsilon}\to\varphi^\delta$ in $L^p(\Omega)$ as $\varepsilon\searrow 0$ for any $p\geqslant 1$.

Even though by construction $0<\chi^\delta<1$ almost everywhere, it might still happen that for the limit the sets $\{x\in\Omega\,|\,\chi(x)=0\}$ and $\{x\in\Omega\,|\,\chi(x)=1\}$ have nonzero Lebesgue measure and that the entropic terms in the free energy density become singular. Now we will show that this is not the case.

Lemma 8: There exists a constant $C>0$ *such that for all* $\delta\in(0,\delta_0)$,

(i) $\|\varphi^\delta(c_l^\delta)\|_{L^q(\Omega_{T_0})}\leqslant C$ *for a suitable* $q>1$ *and all* $1\leqslant l\leqslant 4$,
(ii) $\|\varphi^\delta(\chi^\delta)+\varphi^\delta(1-\chi^\delta)\|_{L^2(\Omega_{T_0})}\leqslant C$.

Proof: The weak formulation (47) for the generalized chemical potential is

$$\int_{\Omega_{T_0}} \mu^\delta \cdot \eta = \int_{\Omega_{T_0}} \left\{ \lambda \sum_{l=1}^{4} \nabla c_l^\delta \cdot \nabla \eta_l + 2 \left[\alpha_l \sum_{j=1}^{4} \alpha_j c_j^\delta \right]_{1\leqslant l\leqslant 4} \cdot \eta + \sum_{l=1}^{3} E_l \eta_l \right\}$$
$$+ \int_{\Omega_{T_0}} (\chi^\delta b^1 + (1-\chi^\delta) b^2)[\varphi^\delta(c_l^\delta)]_{1\leqslant l\leqslant 4} \cdot \eta \tag{79}$$

for all $\eta \in L^2(0,T_0;H^1(\Omega;\mathbb{R}^4)) \cap L^\infty(\Omega_{T_0},\mathbb{R}^4)$. We choose $\eta := [\varphi_r^{\delta,\varrho}(c_l^\delta)]_{1\leqslant l\leqslant 4}$ in (79) which is an admissible test function because of the Sobolev imbedding theorem and because $\varphi_r^{\delta,\varrho} \in C^1$. We obtain

$$\int_{\Omega_{T_0}} \sum_{l=1}^{4} \mu_l^\delta \varphi_r^{\delta,\varrho}(c_l^\delta) = + \int_{\Omega_{T_0}} \sum_{l=1}^{4} \varphi_r^{\delta,\varrho}(c_l^\delta) \left(2\alpha_l \sum_{j=1}^{4} \alpha_j c_j^\delta + E_l \right) + \int_{\Omega_{T_0}} \lambda \sum_{l=1}^{4} \nabla c_l^\delta \cdot \nabla \varphi_r^{\delta,\varrho}(c_l^\delta)$$
$$+ \int_{\Omega_{T_0}} \sum_{l=1}^{4} (\chi^\delta b^1 + (1-\chi^\delta) b^2) \varphi^\delta(c_l^\delta) \varphi_r^{\delta,\varrho}(c_l^\delta).$$

In the last formula we set for simplicity $E_4 := 0$. Due to $(\varphi_r^{\delta,\varrho})' \geqslant 0$ we find

$$\int_{\Omega_{T_0}} \lambda \sum_{l=1}^{4} \nabla c_l^\delta \cdot \nabla \varphi_r^{\delta,\varrho}(c_l^\delta) \geqslant 0.$$

This implies

$$\int_{\Omega_{T_0}} \sum_{l=1}^{4} (\chi^\delta b^1 + (1-\chi^\delta) b^2) \ \varphi^\delta(c_l^\delta)) \varphi_r^{\delta,\varrho}(c_l^\delta)$$
$$\leqslant \int_{\Omega_{T_0}} \sum_{l=1}^{4} \mu_l^\delta \varphi_r^{\delta,\varrho}(c_l^\delta) - \int_{\Omega_{T_0}} \sum_{l=1}^{4} \varphi_r^{\delta,\varrho}(c_l^\delta) \left(2\alpha_l \sum_{j=1}^{4} \alpha_j c_j + E_l \right)$$
$$\leqslant C \max_{1\leqslant l\leqslant 4} \|\varphi_r^{\delta,\varrho}(c_l^\delta)\|_{L^2(\Omega_{T_0})} (\|\mu^\delta\|_{L^2(\Omega_{T_0})} + \|c^\delta\|_{L^2(\Omega_{T_0})})$$

where the constant C in the last line depends on $\alpha_1,\ldots,\alpha_4$ and on $E_1,\ldots,E_3$. For $\varrho \searrow 0$ employing Lemma 6 and Lemma 7 this proves

$$\int_{\Omega_{T_0}} \sum_{l=1}^{4} (\chi^\delta b^1 + (1-\chi^\delta) b^2) \varphi^\delta(c_l^\delta) \varphi_r^\delta(c_l^\delta) \leqslant C. \tag{80}$$

A direct computation finally yields

$$\int_{\Omega_{T_0}} \sum_{l=1}^{4} (\chi^\delta b^1 + (1-\chi^\delta) b^2) \ \varphi^\delta(c_l^\delta)) \varphi_r^\delta(c_l^\delta) \geqslant \int_{\Omega_{T_0}} \max_{1\leqslant l\leqslant 4} (\chi^\delta b^1 + (1-\chi^\delta) b^2) |\varphi^\delta(c_l^\delta)|^{r+1}$$
$$\geqslant \int_{\Omega_{T_0}} C \max_{1\leqslant l\leqslant 4} |\varphi^\delta(c_l^\delta)|^{r+1}$$

for a constant $C = C(b^1,b^2)$. The last is possible because $\chi^\delta b^1 + (1-\chi^\delta) b^2 > 0$ almost everywhere in Ω_{T_0}. Together with (80) this proves (i).

Next we consider the weak formulation (77),

$$-\int_{\Omega_{T_0}} \tau\partial_t\zeta(\chi^\delta-\chi_0)+\int_{\Omega_{T_0}}\gamma\nabla\chi^\delta\cdot\nabla\zeta-\int_{\Omega_{T_0}}(b^2-b^1)\sum_{j=1}^{4}\psi^\delta(c_j^\delta)\zeta+\int_{\Omega_{T_0}}T(\varphi^\delta(\chi^\delta)+\varphi^\delta(1-\chi^\delta))\zeta$$
$$=0 \tag{81}$$

of the Allen–Cahn equation. We want to test Eq. (81) with $\zeta:=\varphi^{\delta,\varepsilon}(\chi)+\varphi^{\delta,\varepsilon}(1-\chi)$. Since by Theorem 1 $\chi^\delta\in C^{0,1/2}(0,T_0;L^2(\Omega_{T_0}))$, we can use Fourier theory to formally shift a half-time derivative from ζ to $\chi^\delta-\chi_0$. After this procedure we find with Lemma 7,

$$\int_{\Omega_{T_0}}\tau\partial_t^{1/2}(\varphi^{\delta,\varepsilon}(\chi^\delta)+\varphi^{\delta,\varepsilon}(1-\chi^\delta))\partial_t^{1/2}(\chi^\delta-\chi_0)\leqslant C.$$

To estimate the second integral in (81), we notice

$$\int_{\Omega_{T_0}}\gamma\nabla\chi^\delta\cdot\nabla(\varphi^{\delta,\varepsilon}(\chi^\delta)+\varphi^{\delta,\varepsilon}(1-\chi^\delta))=\int_{\Omega_{T_0}}\gamma|\nabla\chi^\delta|^2[(\varphi^{\delta,\varepsilon})'(\chi^\delta)-(\varphi^{\delta,\varepsilon})'(1-\chi^\delta)].$$

By Lemma 7, χ^δ is bounded in $L^\infty(0,T_0;H^1(\Omega))$ which implies the boundedness of the integral.

If we choose δ sufficiently small in (i) we find $c_j\in(0,1)$ for $1\leqslant j\leqslant 4$, see also the proof of Theorem 3. This guarantees that $\psi^\delta(c_j)$ does not become singular and thus proves the boundedness of the third integral in (81) independently of δ. Finally, we have

$$0\leqslant\int_{\Omega_{T_0}}(\varphi^\delta(\chi^\delta)+\varphi^\delta(1-\chi^\delta))(\varphi^{\delta,\varepsilon}(\chi^\delta)+\varphi^{\delta,\varepsilon}(1-\chi^\delta))\to\|\varphi^\delta(\chi^\delta)+\varphi^\delta(1-\chi^\delta)\|_{L^2(\Omega_{T_0})}\quad\text{as }\varepsilon\searrow 0.$$

By combining these results, (ii) follows. ■

XVIII. GLOBAL EXISTENCE OF SOLUTIONS FOR LOGARITHMIC FREE ENERGIES

Theorem 3: *Let the assumptions of Sec. XV hold. Then there exists a weak solution* (c,μ,χ) *in the sense of Sec. VIII of the diffuse interface equations (42) with logarithmic free energy such that*

(i) $c\in C^{0,1/4}([0,T_0];L^2(\Omega;\mathbb{R}^4))$,
(ii) $\partial_t c\in L^2(0,T_0;(H_0^1(\Omega;\mathbb{R}^4))')$,
(iii) $\chi\in C^{0,1/2}([0,T_0];L^2(\Omega))$,
(iv) $\partial_t\chi\in L^2(0,T_0;(H_0^1(\Omega))')$,
(v) *there exists a* $q>1$ *such that* $\ln c_j\in L^q(\Omega_{T_0})$ *for* $1\leqslant j\leqslant 4$, $\ln\chi$, $\ln(1-\chi)\in L^2(\Omega_{T_0})$ *and in particular* $0<\chi$, $c_j<1$ *a.e.*

Proof: We pass to the limit $\delta\searrow 0$ in the weak formulation (46)–(48) with f defined by (75) and must show that (c,μ,χ) found in Lemma 7 is a solution.

For the limit in (47), the argumentation is an extension to Ref. 7. In particular we must take care of the term

$$\chi^\delta b^1\sum_{j=1}^{4}\varphi^\delta(c_j^\delta)+(1-\chi^\delta)b^2\sum_{j=1}^{4}\varphi^\delta(c_j^\delta). \tag{82}$$

From the almost everywhere convergence of c_l^δ to c_l, Lemma 8(i) and the Lemma of Fatou we find

$$\int_{\Omega_{T_0}}\liminf_{\delta\searrow 0}|\varphi^\delta(c_l^\delta)|^q\leqslant\liminf_{\delta\searrow 0}\int_{\Omega_{T_0}}|\varphi^\delta(c_l^\delta)|^q\leqslant C.$$

Next we will show that

$$\lim_{\delta\searrow 0}\varphi^{\delta}(c_l^{\delta})=\begin{cases}\varphi(c_l) & \text{if } \lim_{\delta\searrow 0} c_l^{\delta}=c_l>0\\ \infty & \text{if } \lim_{\delta\searrow 0} c_l^{\delta}=c_l\leqslant 0\end{cases}, \tag{83}$$

almost everywhere in Ω_{T_0}. For a point $(x,t)\in\Omega_{T_0}$ with $\lim_{\delta\searrow 0} c_l^{\delta}(x,t)=c_l(x,t)>0$, we obtain from $\varphi^{\delta}(d)=\varphi(d)$ for $d\geqslant\delta$ that $\varphi^{\delta}(c^{\delta}(x,t))\to\varphi(c(x,t))$. In the second case of a point $(x,t)\in\Omega_{T_0}$ with $\lim_{\delta\searrow 0} c_l^{\delta}(x,t)=c_l(x,t)\leqslant 0$, we have for δ small enough

$$|\varphi^{\delta}(c_l^{\delta}(x,t))|\geqslant\varphi(\max\{\delta,c_l^{\delta}(x,t)\})\to\infty \quad \text{for } \delta\searrow 0.$$

This proves (83). A similar statement holds for $\psi^{\delta}(\chi^{\delta})$.

From (83) and Lemma 8(i) we deduce $0<c_l<1$ a.e., $\int_{\Omega_{T_0}}|\varphi(c_l)|^q\leqslant C$ and $\varphi^{\delta}(c_l^{\delta})\to\varphi(c_l)$ a.e. With Vitali's theorem we find

$$\varphi^{\delta}(c_l^{\delta})\to\varphi(c_l) \quad \text{in } L^1(\Omega_{T_0}).$$

This allows to pass to the limit in (47).

Let us now consider the limit in (77). The relation $0<c_j<1$ almost everywhere implies $b^l\Sigma_{j=1}^4\psi^{\delta}(c_j^{\delta})\to b^l\Sigma_{j=1}^4\psi(c_j)$, $l=1,2$ almost everywhere in Ω_{T_0} like in the first case of (83). From $\varphi^{\delta}(c_j^{\delta})\in L^q(\Omega_{T_0})$, the uniform boundedness of χ^{δ} and Vitali's theorem we obtain

$$\chi^{\delta}b^1\sum_{j=1}^{4}\psi^{\delta}(c_j^{\delta})\to\chi^{b^1}\sum_{j=1}^{4}\psi(c_j),\quad (1-\chi^{\delta})b^2\sum_{j=1}^{4}\psi^{\delta}(c_j^{\delta})\to(1-\chi)b^2\sum_{j=1}^{4}\psi(c_j)$$

in $L^1(\Omega_{T_0})$ such that

$$\omega^{\delta}(c^{\delta},\chi^{\delta})\to\omega(c,\chi) \quad \text{in } L^1(\Omega_{T_0}) \text{ for } \delta\searrow 0.$$

By repeating the argumentation from above for $\varphi^{\delta}(\chi^{\delta})+\varphi^{\delta}(1-\chi^{\delta})$ we deduce $0<\chi<1$ almost everywhere in Ω_{T_0} which again with the help of Vitali's theorem and Lemma 8(ii) yields

$$\varphi^{\delta}(\chi^{\delta})+\varphi^{\delta}(1-\chi^{\delta})\to\varphi(\chi)+\varphi(1-\chi) \quad \text{in } L^1(\Omega_{T_0}).$$

So we can also pass to the limit in (77). The limit for (46) can be justified in the same way as in the proof of Theorem 1 if we additionally show

$$r^{\delta}(c^{\delta},\chi^{\delta})\to r(c,\chi) \quad \text{in } L^1(\Omega_{T_0}). \tag{84}$$

From the almost everywhere convergence of c_l^{δ} to c_l and $c_l>0$ almost everywhere in Ω_{T_0} we obtain

$$\max(c_l^{\delta},\delta)\to c_l \quad \text{almost everywhere in } \Omega_{T_0},\ \delta\searrow 0,\quad 1\leqslant l\leqslant 3.$$

Since the functions $\chi\mapsto k^{1/b\chi}$ and $\chi\mapsto\kappa^{1/b\chi}$ are in C^1, we find

$$k^{1/b\chi^{\delta}}(\max(c_2^{\delta},\delta)^2-\kappa^{1/b\chi^{\delta}}\max(c_1,\delta)\max(c_3,\delta))\to k^{1/b\chi}(c_2^2-\kappa^{1/b\chi}c_1c_3)$$

almost everywhere in Ω_{T_0} as $\delta\searrow 0$. By Lebesgue's dominated convergence theorem we find (84), because $k^{1/b\chi^{\delta}}\leqslant k^{1/\min(b^1,b^2)}$ almost everywhere in Ω_{T_0} if $k\geqslant 1$, respectively, $k^{1/b\chi^{\delta}}\leqslant k^{1/\max(b^1,b^2)}$ almost everywhere if $k<1$ and the analogous estimate for the κ-term, hence

$$\int_{\Omega_{T_0}}|r_1^{\delta}|\leqslant C\int_{\Omega_{T_0}}(|c_2^2|+|c_1c_3|)$$

for a constant C that depends on κ and k. ■

Uniqueness of the solution to Theorem 3 can be obtained in exactly the same way as in Theorem 2 if we replace (A6) by (A6′).

XIX. THE SHARP INTERFACE MODEL

It remains to perform the limit $\lambda \to 0$. This limit is carried out in the same way as before by showing *a priori* estimates and compactness results.

Lemma 9: (a) For $\lambda \in (0,\lambda_0)$ *there exists a weak solution* $(c^\lambda, \mu^\lambda, \chi^\lambda)$ *of (42) with a logarithmic free energy that satisfies (A2′)–(A6′).*

(b) There is a constant $C>0$ *independent of* λ *such that for all* $\lambda \in (0,\lambda_0)$,

$$\sup_{t\in[0,T_0]} \{\|c^\lambda(t)\|_{H^1} + \|\chi^\lambda(t)\|_{H^1}\} \leqslant C,$$

$$\sup_{t\in[0,T_0]} \int_\Omega f^1(c^\lambda(t),\chi^\lambda(t)) + \|\nabla \mu^\lambda\|_{L^2(\Omega_{T_0})} \leqslant C$$

and for all $t_1, t_2 \in [0,T_0]$

$$\|c^\lambda(t_2) - c^\lambda(t_1)\|_{L^2} \leqslant C|t_2 - t_1|^{1/4},$$

$$\|\chi^\lambda(t_2) - \chi^\lambda(t_1)\|_{L^2} \leqslant C|t_2 - t_1|^{1/2}.$$

(c) One can extract subsequences $(c^\lambda)_{\lambda\in\mathcal{R}}$, $(\mu^\lambda)_{\lambda\in\mathcal{R}}$, *and* $(\chi^\lambda)_{\lambda\in\mathcal{R}}$ *where* $\mathcal{R}\subset(0,\lambda_0)$ *is a countable set with zero as the only accumulation point such that*

(i) $c^\lambda \to c$ *in* $C^{0,\alpha}([0,T_0];L^2(\Omega;\mathbb{R}^4))$ *for all* $\alpha \in (0,\frac{1}{4})$,
(ii) $c^\lambda \to c$ *almost everywhere in* Ω_{T_0},
(iii) $c^\lambda \overset{*}{\rightharpoonup} c$ *in* $L^\infty(0,T_0;H_0^1(\Omega;\mathbb{R}^4))$,
(iv) $\chi^\lambda \to \chi$ *in* $C^{0,\alpha}([0,T_0];L^2(\Omega))$ *for all* $\alpha \in (0,\frac{1}{2})$,
(v) $\chi^\lambda \to \chi$ *almost everywhere in* Ω_{T_0} *and* $0 \leqslant \chi^\lambda$, $\chi \leqslant 1$ *a.e. in* Ω_{T_0},
(vi) $\chi^\lambda \overset{*}{\rightharpoonup} \chi$ *in* $L^\infty(0,T_0;H^1(\Omega))$,
(vii) $\mu^\lambda \rightharpoonup \mu$ *in* $L^2(0,T_0;H_0^1(\Omega;\mathbb{R}^4))$

as $\lambda \in \mathcal{R}$ *tends to zero.*

Proof: By Theorem 3, a weak solution for fixed $\lambda \in (0,\lambda_0)$ exists. This proves (a). The estimates in (b) are a direct consequence of Lemma 7, where due to assumption (A4.2) we must choose $\lambda < \lambda_0$ for Lemma 3 to hold. Since $F^\lambda(c_0,\chi_0)$ can be estimated independently of λ, the constant C on the right-hand side does not depend on λ. (c) is proved by Lemma 7. ■

We make precise what we mean by a weak solution to the sharp interface model. We call a triple $(c,\mu,\chi) \in L^2(0,T_0;H_0^{1,2}(\Omega;\mathbb{R}^4)) \times L^2(0,T_0;H_0^{1,2}(\Omega;\mathbb{R}^4)) \times L^2(0,T_0;H^{1,2}(\Omega;\mathbb{R}))$ with $r(c,\chi)$, $\omega(c,\chi) \in L^1(\Omega_{T_0})$ a *weak solution* of the sharp interface model (30) if

$$-\int_{\Omega_{T_0}} \partial_t \xi \cdot (c - c_0) + \int_{\Omega_{T_0}} L\nabla\mu : \nabla\xi - \int_{\Omega_{T_0}} r(c,\chi)\xi = 0 \tag{85}$$

for all $\xi \in L^2(0,T_0;H_0^1(\Omega;\mathbb{R}^4))$ with $\partial_t\xi \in L^2(\Omega_{T_0})$, $\xi(T_0)=0$, and

$$\int_{\Omega_{T_0}} \mu\cdot\eta = \int_{\Omega_{T_0}} \frac{\partial f}{\partial c}(c)\cdot\eta \tag{86}$$

for all $\eta \in L^2(0,T_0;H_0^1(\Omega;\mathbb{R}^4)) \cap L^\infty(\Omega_{T_0};\mathbb{R}^4)$, and

$$-\int_{\Omega_{T_0}} \tau\partial_t\zeta(\chi-\chi_0) + \int_{\Omega_{T_0}} \gamma\nabla\chi\cdot\nabla\zeta - \int_{\Omega_{T_0}} \omega(c,\chi)\zeta = 0 \tag{87}$$

for all $\zeta \in L^2(0,T_0;H^1(\Omega;\mathbb{R}))$ with $\partial_t\zeta \in L^2(\Omega_{T_0})$, $\zeta(T_0)=0$.

Theorem 4: *Let the assumptions of Sec. XV hold. Then, there exists a weak solution* (c,μ,χ) *in the sense of (85) of the sharp interface equations (30) with a logarithmic free energy that satisfies (A2′)–(A6′) such that*

(i) $c \in C^{0,1/4}([0,T_0];L^2(\Omega;\mathbb{R}^4))$,
(ii) $\partial_t c \in L^2(0,T_0;(H_0^1(\Omega;\mathbb{R}^4))')$,
(iii) $\chi \in C^{0,1/2}([0,T_0];L^2(\Omega))$,
(iv) $\partial_t \chi \in L^2(0,T_0;(H_0^1(\Omega))')$,
(v) *there exists a* $q>1$ *such that* $\ln c_j \in L^q(\Omega_{T_0})$ *for* $1 \leqslant j \leqslant 4$, $\ln \chi$, $\ln(1-\chi) \in L^2(\Omega_{T_0})$ *and in particular* $0<\chi,c_j<1$ *a.e.*

Proof: We pass to the limit $\lambda \searrow 0$ in the weak formulation. In order to show that the limit (c,μ,χ) found in Lemma 9 is a solution we must only observe that in (47) $\lambda\Delta\mu \to 0$ in $H_0^{1,2}(\Omega)$ as $\lambda \searrow 0$. ■

Theorem 5: *If* $\partial_c f$, $\partial_\chi f$ *are Lipschitz continuous, the solution* (c,μ,χ) *of the sharp interface equations obtained in Theorem 4 is unique in the spaces stated in this theorem.*

Proof: The proof of Theorem 2 can be reused after sharpening estimate (71). We have according to (A4.2),

$$-\int_{\Omega_{t_0}} \left(\int_0^t r(s)\mathrm{d}s \right) \cdot \mu \geqslant \int_{\Omega_{t_0}} r_1(t)(\mu_1(t) - 2\mu_2(t) + \mu_3(t))$$

$$\geqslant \int_{\Omega_{t_0}} (\alpha_1 - 2\alpha_2 + \alpha_3) Q(c) r_1 \geqslant \lambda \int_{\Omega_{t_0}} |\nabla c|^2$$

for an arbitrary constant $\lambda < \lambda_0$. Then one can proceed with the proof. ■

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Shock waves in the Tamm problem and the possibility of their experimental observation

G. N. Afanasiev[a] and V. M. Shilov
Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, Moscow District, 141980, Russia

Yu. P. Stepanovsky
Institute of Physics and Technology, Kharkov, Ukraine

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The position of the singular electromagnetic shock waves arising in the smooth Tamm problem is found. They consist of the Cherenkov shock wave and shock waves arising when the charge velocity coincides with the velocity of light in medium. In the limit of small intervals of accelerated and decelerated motion they are not transformed into the singular electromagnetic shock waves of the original Tamm problem. The reasons for this and the relation of the arising electromagnetic shock waves to the experimental situation are discussed. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1836013]

I. INTRODUCTION

Usually, the radiation of a charge moving uniformly in medium, in a finite space interval is described in the framework of the so-called Tamm problem.[1] In it, a charge being initially at rest exhibits instantaneous acceleration acquiring the velocity v with which it moves uniformly in a finite space interval. Later, a charge exhibits instantaneous deceleration coming to the permanent state of rest. Using some approximations Tamm obtained a remarkably simple formula having a sharp maximum at the Cherenkov angle θ_c defined by $\cos\theta_c = 1/\beta n$ ($\beta = v/c$, n is the medium refractive index). This formula is frequently used for identification of the charge velocity.[2,3] Analytic formulas and numerical results presented in Ref. 4 demonstrate that in realistic conditions the Tamm formula does not work properly. The radiation intensity has a form of plateau [Fig. 1(a)] with intensity bursts at the ends of this plateau [Fig. 1(b)]. It was shown in Ref. 4 that this plateau is the Cherenkov shock wave of finite extension while the intensity bursts were *ad hoc* associated with the shock waves arising when the charge velocity coincides with the velocity of light $c_n = c/n$ in medium. On the other hand, the experimental intensity presented in Ref. 4 had a triangle form (Fig. 2). When evaluating the radiation intensities in the spectral representation (Figs. 1, 5, and 7) we omit the overall factor $(Ze)^2/c$. Thus obtained intensities have the dimension cm^{-1}. The Tamm approximate radiation intensities are highly oscillating functions. To make them more visible, we draw them through their maxima.

The goal of this consideration is to analyze the following questions: (1) how are the shock waves distributed in the original and smooth Tamm problems; (2) how are they manifested in experimental data.

The plan of our exposition is as follows. The mathematical preliminaries are collected in Sec. II. For the pedagogical purposes the derivation of the position of the electromagnetic shock waves in the original Tamm problem is presented in Sec. III. The method for finding the electromagnetic field singularities accompanying the moving charge is exposed in Sec. IV. In Sec. V, the electromagnetic field (EMF) singularities arising in the smooth Tamm problem are found. To our surprise, in the limit of small acceleration and deceleration intervals, the resulted configuration of the

[a]Author to whom correspondence should be addressed. Electronic mail: afanasev@thsun1.jinr.ru

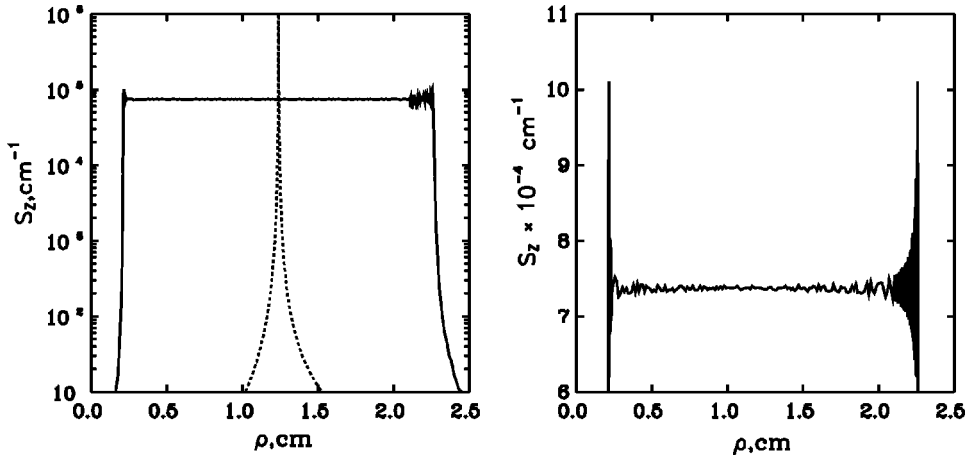

FIG. 1. Spectral radiation intensities corresponding to the charge motion in a finite spatial interval $L=2z_0=2.95$ cm in the plane perpendicular to the motion axis in logarithmic (a) and linear (b) scales. The distance from the end point of the motion interval to the observation plane is 0.3 cm. The dotted curve passes through the peaks of the Tamm approximate intensity. The refractive index of the medium is 1.505, the observed wavelength $\lambda=4\times10^{-5}$ cm, the charge velocity $\beta \approx 0.81$. The plateau corresponds to the Cherenkov shock wave, the intensity bursts at its ends correspond to the shock waves arising at the beginning (right peak) and the end (left peak) of the charge motion.

electromagnetic shock waves does not coincide with that of the original Tamm problem. The reason for this and the relation of the arising electromagnetic shock waves to the experimental radiation intensities are presented in Sec. VI. In the same section, the physical meaning of the smooth Tamm problem and the recommendations for the experimental search of the shock waves associated with the overcoming the light velocity barrier are given. A short resume of the results obtained is given in Sec. VII.

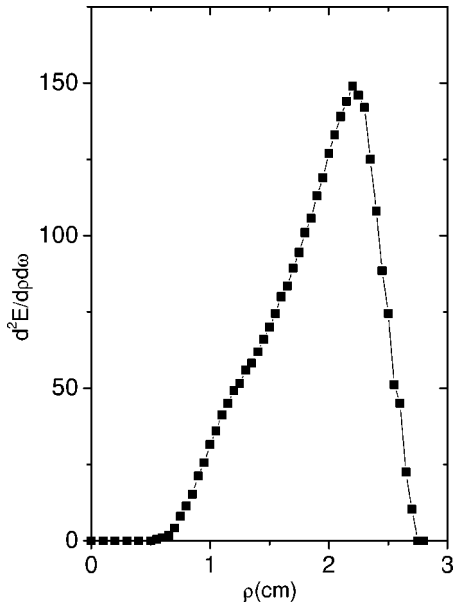

FIG. 2. The experimental radiation intensity (in arbitrary units) for the same parameters as in Fig. 1. One observes the increment of the radiation intensity at $\rho \approx 2.25$ cm which corresponds to the Cherenkov ray emitted from the initial point of the charge motion. No frequency filters were used in this experiment.

II. MATHEMATICAL PRELIMINARIES

Let a pointlike charge move inside the nondispersive medium with polarizabilities ϵ and μ along the given trajectory $\vec{\xi}(t)$. Then its EMF potentials at the observational point (ρ,z) are given by

$$\Phi(\vec{r},t)=\frac{e}{\epsilon}\frac{1}{|R|},\qquad \vec{A}(\vec{r},t)=\frac{e\mu}{c}\frac{\vec{v}}{|R|},\quad \operatorname{div}\vec{A}+\frac{\epsilon\mu}{c}\dot{\Phi}=0,\quad c_n=c/n. \tag{2.1}$$

Here

$$\vec{v}=\left(\frac{\mathrm{d}\vec{\xi}}{\mathrm{d}t}\right)\Bigg|_{t=t'},\quad R=|\vec{r}-\vec{\xi}(t')|-\vec{v}_i(\vec{r}-\vec{\xi}(t'))/c_n.$$

The proper or retarded time t' satisfies the equation

$$c_n(t-t')=|\vec{r}-\vec{\xi}(t')|. \tag{2.2}$$

To preserve the causality, the time t' of the radiation should be smaller than the observational time t. Obviously, t' depends on the coordinates $\vec{r}$, t of the point P at which the EMF is observed. If there are few t' satisfying (2.2), the electromagnetic potentials (2.1) should involve the sum over all these t'.

III. PEDAGOGICAL EXAMPLE: THE ORIGINAL TAMM PROBLEM IN THE ABSENCE OF DISPERSION

In this problem, a charge is at rest at the point $z=-z_0$ of the motion axis up to $t'=-t_0$ ($t_0=z_0/v$). At this instant it exhibits instantaneous acceleration acquiring the velocity v_0. With this velocity the charge moves uniformly up to reaching the point $z=z_0$ at $t'=t_0$. At this instant it exhibits instant deceleration coming to the permanent state of rest. For $t'<-t_0$ and $t'>t_0$ a charge is at rest at the $z=\mp z_0$ points, respectively. The corresponding electric scalar potentials are given by

$$\Phi_1=\frac{e}{r_1}\Theta[r_1-c_n(t+t_0)],\quad \Phi_2=\frac{e}{r_2}\Theta[c_n\ (t-t_0)-r_2)]. \tag{3.1}$$

Here $r_{1,2}=\sqrt{\rho^2+(z\pm z_0)^2}$. It is seen that Φ_1 describes the electrostatic field of charge at rest at $z=-z_0$. It differs from zero outside the sphere BS_1 defined by $r_1\equiv\sqrt{\rho^2+(z+z_0)^2}=c_n(t+t_0)$. Information on the beginning of motion does not reach the points lying outside BS_1. Correspondingly, Φ_2 describes the electrostatic field of charge at rest at $z=z_0$. It differs from zero inside the sphere BS_2 defined by $r_2\equiv\sqrt{\rho^2+(z-z_0)^2}=c_n(t-t_0)$. Information on the end of the charge motion does not reach the points lying inside BS_2.

There are two roots of (2.2) for $-t_0<t'<t_0$,

$$t'_{1,2}=\frac{1}{c_n(\beta_{0n}^2-1)}(\beta_{0n}z-c_nt\pm r_m), \tag{3.2}$$

where $r_m=\sqrt{(z-v_0t)^2+(1-\beta_{0n}^2)\rho^2}$ ($\beta_{0n}=\beta_0n$, $\beta_0=v_0/c$). Imposing the condition $-t_0<t'<t_0$ one finds space–time regions where t'_1 and t'_2 exist. However, at first we define the straight lines L_1 ($z=-z_0+\rho\gamma_{0n}$, $\gamma_{0n}=1/\sqrt{\beta_{0n}^2-1}$) and L_2 ($z=z_0+\rho\gamma_{0n}$) [Fig. 3(a)]. They originate from the $\mp z_0$ points and are inclined at the angle θ_c ($\cos\theta_c=1/\beta_0n$) towards the motion axis. Then, to the left of L_1 ($z<-z_0+\rho\gamma_{0n}$), t'_1 exists between BS_1 and BS_2 ($-t_0+r_1/c_n<t<t_0+r_2/c_n$). Between L_1 and L_2 ($-z_0+\rho\gamma_{0n}<z<z_0+\rho\gamma_{0n}$), t'_1 exists in the space–time region $(z+\rho/\gamma_{0n})/v<t<t_0+r_2/c_n$ which lies between BS_2 and the straight-line segment $z+\rho/\gamma_{0n}=vt$ enclosed between L_1 and L_2 and perpendicular to them. Its normal is inclined at the angle θ_c towards the motion axis. This segment is a piece of the Cherenkov shock wave enclosed between L_1 and L_2.[4,5] We refer to it as CSW. It

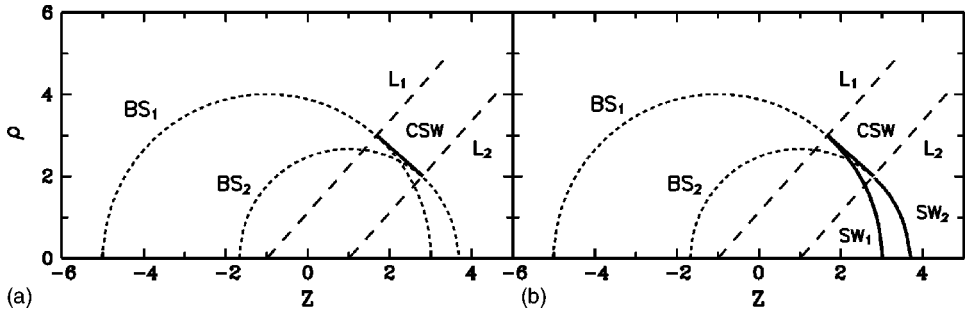

FIG. 3. (a) The position of the shock waves in the original Tamm problem. BS_1 and BS_2 are the bremsstrahlung shock waves emitted at the beginning and the end of motion; CSW (straight thick line) is the finite Cherenkov shock wave; (b) the position of the shock waves in the limiting case of the smooth Tamm problem (see Fig. 4) when the lengths of accelerated and decelerated parts of the charge trajectory tend to zero. The thick curves SW_1 and SW_2 are the shock waves arising at the accelerated and decelerated parts of the charge trajectory, respectively. Due to the instantaneous velocity jumps, SW_1 and SW_2 partly coincide with the BS_1 and BS_2 shock waves, respectively.

corresponds to the plateau shown in Fig. 1. As to t_2', it exists between BS_1 and BS_2 $(t_0+r_2/c_n < t < -t_0+r_1/c_n)$ to the right of L_2 $(z>z_0+\rho\gamma_{0n})$. Between L_1 and L_2 $(-z_0+\rho\gamma_{0n}<z<z_0+\rho\gamma_{0n})$, t_2' differs from zero in the space–time $(z+\rho/\gamma_{0n})/v<t<-t_0+r_1/c_n$ region surrounded by BS_1 and CSW. The space–time region where both t_1' and t_2' differ from zero lies between L_1 and L_2, outside BS_1 and BS_2 and below the CSW. Substituting either t_1' or t_2' into the denominator R entering into (3.1) one finds that $|R|=r_m$. With the account of all this, one finds for the electromagnetic potentials

$$\Phi=\Phi_1+\Phi_2+\Phi_3, \quad A_z=\mu\beta\epsilon\Phi_3, \tag{3.3}$$

$$\begin{aligned}\Phi_3=\frac{e}{\epsilon r_m}\{&\Theta(\rho\gamma_{0n}-z-z_0)\Theta[c_n(t+t_0)-r_1]\Theta[r_2-c_n(t-t_0)]+\Theta(z-z_0-\rho\gamma_{0n})\\&\times\Theta[c_n(t-t_0)-r_2]\Theta[r_1-c_n(t+t_0)]+\Theta(z+z_0-\rho\gamma_{0n})\\&\times\Theta(z_0+\rho\gamma_{0n}-z)\Theta(vt-z-\rho/\gamma_{0n})\times[\Theta(r_2-c_n(t-t_0))+\Theta(r_1-c_n(t+t_0))]\}.\end{aligned}$$

It is seen that $r_m=0$ on the CSW defined by $z+\rho/\gamma_{0n}=vt$ while the electromagnetic potentials are infinite there. There are no other singularities of electromagnetic potentials. However, the EMF strengths have additional delta-type singularities. They are due to the discontinuities of electromagnetic potentials at the boundaries of the BS_1, BS_2, and CSW surfaces.

IV. MOVING SINGULARITIES OF THE ELECTROMAGNETIC FIELD

With the account of (2.2) one finds for R

$$R=c_n(t-t')-\vec{v}(\vec{r}-\vec{\xi}(t'))/c_n. \tag{4.1}$$

We seek the singularities of the EMF potentials for which the denominators R entering into (3.1) disappear,

$$c_n(t-t')-\vec{v}(\vec{r}-\vec{\xi}(t'))/c_n=0.$$

In what follows we limit ourselves to the one-dimensional motion in the positive direction of the z axis. Then

$$c_n(t-t')=v(z-\xi(t'))/c_n=0. \tag{4.2}$$

For this motion $z-\xi(t')>0$. We rewrite (4.1) and (4.2) in the following form:

$$z = \xi(t') + \frac{c_n^2}{v}(t - t'), \quad \rho = \frac{c_n^2(t - t')}{v\gamma_n}. \tag{4.3}$$

Here $\gamma_n = 1/\sqrt{\beta^2 n^2 - 1}$, $\beta = v(t')/c$.

Our procedure reduces to the following one. For the fixed observation time t, we vary t' over the motion interval, evaluate $z(t')$ and $\rho(t')$ and draw the dependence $\rho(z)$ for the fixed t. Due to the axial symmetry of the problem, this curve is in fact the surface on which the electromagnetic potentials are singular. It follows from (4.3) that these singular surfaces exist only if $v > c/n$, that is if the charge velocity is greater than the light velocity in medium. There are other surfaces on which the EMF strengths are singular and which are not described by (4.3). For example, on the surfaces of the bremsstrahlung (BS) shock waves arising at the start or the end of motion, the electromagnetic potentials exhibit finite jumps. The corresponding EMF strengths have δ singularities on these surfaces. In the next section, we demonstrate that for the Tamm problem thus obtained singularities coincide with those found in Sec. III.

Moving singularity of the original Tamm problem: In the time interval $-t_0 < t' < t_0$, $(t_0 = z_0/v_0)$ where a charge moves uniformly with the velocity v_0 equations (4.3) look like

$$\rho = \frac{c_n^2}{v_0\gamma_{0n}}(t - t'), \quad z = v_0 t' + \frac{c_n^2}{v_0}(t - t'). \tag{4.4}$$

Here $\gamma_{0n} = 1/\sqrt{v_0^2/c_n^2 - 1}$. Excluding t' from these equations one finds

$$\rho = (v_0 t - z)\gamma_{0n}, \tag{4.5}$$

where ρ and z are changed in the intervals

$$z_1^0 < z < v_0 t, \quad 0 < \rho < \frac{c_n^2}{v_0\gamma_{0n}}(t + t_0)$$

for $-t_0 < t < t_0$ and

$$z_1^0 < z < z_2^0, \quad \rho_2 < \rho < \rho_1$$

for $t > t_0$. Here

$$z_1^0 = \frac{c^2}{v_0 n^2}(t + t_0) - z_0, \quad \rho_1 = \frac{c^2}{v_0 n^2 \gamma_{0n}}(t + t_0),$$

$$z_2^0 = \frac{c_n^2}{v_0}(t - t_0) + z_0, \quad \rho_2 = \frac{c_n^2}{v_0\gamma_{0n}}(t - t_0).$$

It is seen that for each $t > t_0$ the singular segment (4.5) enclosed between the straight lines L_1 and L_2 is perpendicular to both of them and coincides with the CSW defined in Sec. III. Its normal is inclined at the angle θ_c towards the motion axis. As time goes, it propagates between L_1 and L_2. For $-t_0 < t < t_0$ the CSW is enclosed between the moving charge and the straight line L_1.

V. SMOOTH TAMM PROBLEM

A. Motivation for the smooth Tamm problem

Usually the measurements of the Cherenkov radiation are made in the plane perpendicular to the motion axis. Numerical and analytical calculations[4] made in the framework of the original Tamm problem showed that the spectral radiation intensity has a plateau $\rho_2 < \rho < \rho_1$ with sharp bursts at the end of this plateau. They were *ad hoc* associated with the shock waves arising when the charge velocity coincides with the velocity of light c_n in medium. Since in the original Tamm problem the charge velocity changes instantaneously at the start and the end of motion, the above

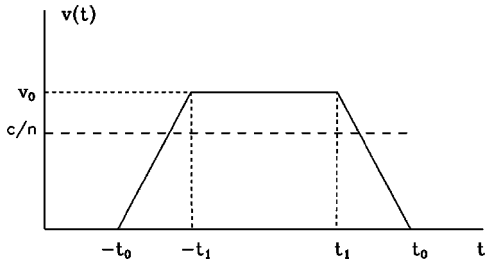

FIG. 4. Schematic presentation of the smooth Tamm problem.

shock waves coincide with bremsstrahlung (BS) shock waves arising at the start and the end of motion. Because of this, we consider the smooth Tamm problem (Fig. 4) in which a charge is at rest up to some instant of time ($t<-t_0$), moves with constant acceleration up to reaching some velocity v_0 ($-t_0<t<-t_1$), moves with this velocity ($-t_1<t<t_1$) and, finally, decelerates down ($t_1<t<t_0$) to reaching the permanent state of rest ($t>t_0$). Since the points where these shock waves are created are separated in space and time, the space–time separation of the resulting shock waves is also to be expected. It was shown in Ref. 6 analytically and numerically that for the semi-infinite accelerated charge motion the resulting configuration of shock waves consists of the BS shock wave and of the indivisible complex consisting of the finite Cherenkov cone and the shock wave closing this cone. Time evolution of the shock waves in the framework of the smooth Tamm problem was studied numerically in Ref. 7. After the termination of the charge motion the resulting configuration of the shock waves presented itself an indivisible complex having the sickle moon form and consisting of two shock waves intersecting the motion axis at the right angle. The following paradoxical result was obtained there: the arising configuration of shock waves does not tend to that of the original Tamm problem when the length along which a charge moves nonuniformly tends to zero. Therefore, a qualitative analysis of the arising situation is needed. In the spectral representation, the smooth Tamm problem was studied in Ref. 8 on the observational sphere of an infinite radius. It was shown that the radiation intensity suddenly drops for the angle greater than the Cherenkov angle θ_c corresponding to the velocity β_0. For $\theta<\theta_c$, the radiation intensity falls more slowly. It was suggested there that such behavior of the radiation intensity in the $\theta<\theta_c$ angular region is due to the shock waves arising when the charge velocity coincides with c_n.

We intend to study the radiation intensities in the $z=$const plane. The typical spectral radiation intensities shown in Fig. 5 have a plateau with a sudden drop at the right of this plateau and with moderate amplitude oscillations at its left. Below, in the framework of the exactly solvable model we show that to the right of this plateau only the nonsingular BS shock waves (associated with the beginning and the end of motion) contribute to the radiation intensity while 2 singular shock waves (arising at the accelerated and decelerated parts of the charge trajectory) contribute to the radiation intensity to the left of this plateau. The intensity oscillations in this region are due to the interference of these shock waves.

B. Analytical consideration

In the smooth Tamm problem a charge is at rest at the spatial point $z=-z_0$ up to an instant $t'=-t_0$. In the space–time interval $-t_0<t'<-t_1$, $-z_0<z<-z_1$ (we refer to this interval as to region 1) it moves with constant acceleration a,

$$\xi(t') = -z_0 + \tfrac{1}{2}a(t'+t_0)^2, \quad v(t') = a(t'+t_0).$$

In the space–time interval $-t_1<t'<t_1$, $-z_1<z<z_1$ (region 2) it moves with the constant velocity v_0,

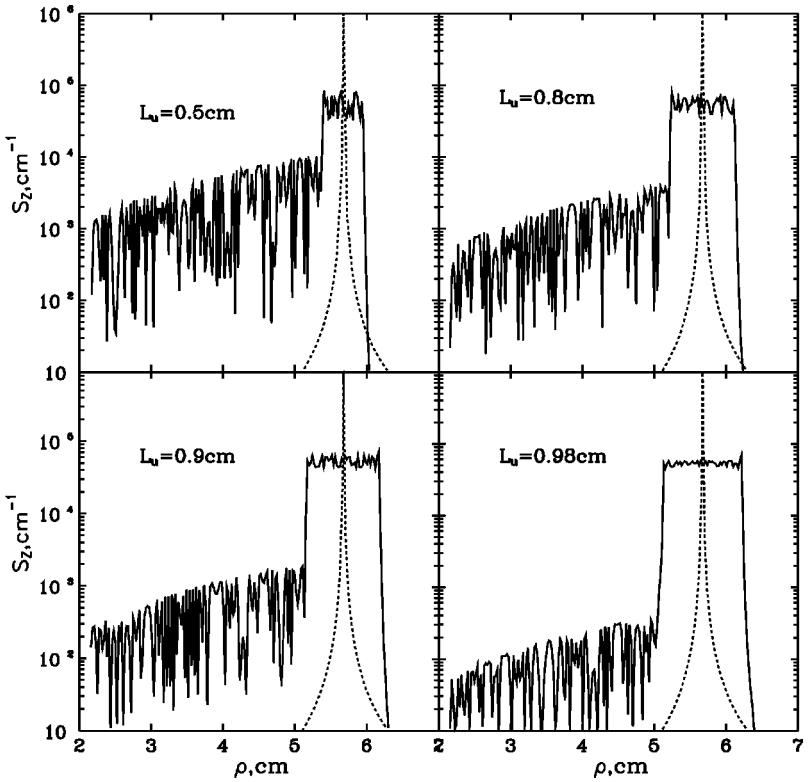

FIG. 5. Spectral radiation intensities for the smooth Tamm problem for various lengths L_u of the charge uniform motion. The total motion interval is 1 cm, the observed wavelength $\lambda = 5.893 \times 10^{-5}$ cm, the medium refractive index $n = 1.512$, the uniform charge velocity $\beta_0 = v_0/c = 1$. The plateau in the radiation intensity corresponds to the CSW in Fig. 6(d). The sudden drop of the radiation intensity to the right of this plateau is due to the absence of the singular shock waves above L_1 [see Fig. 6(d)]. The oscillations of the radiation intensities to the left of the plateau are due to the interference of SW_1 and SW_2 shock waves in the region below L_2. The dotted curves are the Tamm approximate radiation intensities corresponding to the charge uniform motion on the interval L_u.

$$\xi(t') = v_0 t', \quad v(t') = v_0.$$

In the space–time interval $t_1 < t' < t_0$, $z_1 < z < z_0$ (region 3) a charge moves with constant deceleration a down reaching the state of rest at $t = t_0$,

$$\xi(t') = z_0 - \tfrac{1}{2} a (t' - t_0)^2, \quad v(t') = a(t_0 - t').$$

The matching conditions of $\xi(t')$ and $v(t')$ at the $z = \pm z_1$ points define a, t_0, and t_1,

$$a = \frac{v_0^2}{2(z_0 - z_1)}, \quad t_0 = \frac{2z_0 - z_1}{v_0}, \quad t_1 = \frac{z_1}{v_0}.$$

1. Space region 1

In the space region 1 equations (4.3) are

$$z = -z_0 + \frac{1}{2} a (t' + t_0)^2 + \frac{c_n^2}{v}(t - t'), \quad \rho = \frac{c_n^2 (t - t')}{v \gamma_n}, \tag{5.1}$$

where $v = a(t' + t_0)$. It follows from this that the charge velocity coincides with the velocity of light in medium $c_n = c/n$ at $t' = -t_c$, $t_c \equiv t_0 - c_n/a$. At this instant

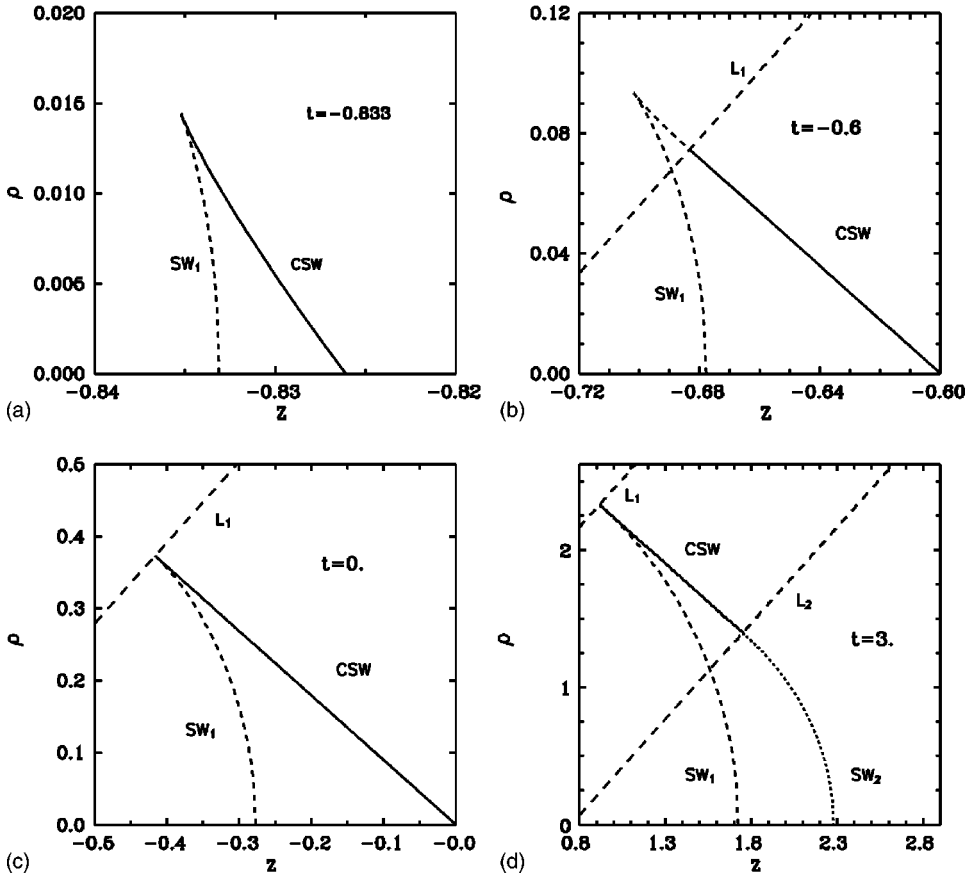

FIG. 6. Shock waves in the smooth Tamm problem. (a), (b), (c) For small and moderate observation times the singularity complex consists of the finite Cherenkov shock wave (CSW) attached to a moving charge and the shock wave SW_1 closing the Cherenkov cone and inclined at the right angle towards the motion axis; (d) for large observation times this complex detaches from a moving charge and propagates with the velocity of light c_n in medium. It consists of the finite CSW and the shock waves SW_1 and SW_2 perpendicular to the motion axis and arising at the accelerated and decelerated parts of the charge trajectory.

$$\rho_c = \rho(t' = -t_c) = 0, \quad z_c^{(1)} = z(t' = -t_c) = c_n t - \left(1 - \frac{1}{\beta_0 n}\right)\left[z_0 - \frac{1}{n\beta_0}(z_0 - z_1)\right]. \tag{5.2}$$

For the observation time t smaller than the time $-t_1$ corresponding to the right boundary of the motion interval 1, $\rho(t')$ has two zeroes (at $t'=t_c$ and $t'=t$). There is a maximum between them [Fig. 6(a)] at

$$t' = t'_m \equiv -t_0 + \left(\frac{c_n}{a}\right)^{2/3}(t + t_0)^{1/3}. \tag{5.3}$$

Obviously, $t_c < t'_m < t$. The corresponding ρ and z are equal to

$$\rho_m = \frac{c_n^2}{a}\left\{\left[\frac{a(t+t_0)}{c_n}\right]^{2/3} - 1\right\}^{3/2}, \quad z_m = -z_0 + \frac{c_n^2}{a}\left\{\frac{3}{2}\left[\frac{a(t+t_0)}{c_n}\right]^{2/3} - 1\right\}. \tag{5.4}$$

This solution coincides with the analytical solution found in Ref. 6 for the semi-infinite motion beginning from the state of rest. The dependence $\rho(z)$ has a moon sicklelike form [Fig. 6(a)]. This complex arises when the charge velocity coincides with the velocity of light c_n in medium. It consists of the curvilinear Cherenkov shock wave CSW attached to a moving charge and the shock

wave closing the Cherenkov cone. As time goes, the dimensions of this complex rise (since a charge moves with the velocity v while SW_1 propagates with the velocity c_n).

For the observation time t greater than the time $-t_1$, ρ has only one zero. It has a maximum if $-t_1<t<-t_0+2(z_0-z_1)v_0/c_n^2$. The corresponding t'_m, ρ_m, and z_m are given by (5.3) and (5.4). In the interval $t'_m<t'<-t_1$, ρ decreases reaching the value

$$\rho_1=\rho(t'=-t_1)=\frac{c_n^2}{v_0\gamma_n}(t+t_1) \tag{5.5}$$

at the boundary point of the motion interval. The corresponding z is equal to

$$\tilde{z}_1=z(t'=-t_1)=\frac{c_n^2}{v_0}(t+t_1)-z_1. \tag{5.6}$$

It is easy to check that z as a function of t' has a minimum at $t'=t'_m$: it decreases from $z_c^{(1)}$ at $t'=-t_c$ down to

$$z_m=-z_0+\frac{c_n^2}{a}\left\{\left[\frac{a(t+t_0)}{c_n}\right]^{2/3}-1\right\} \tag{5.7}$$

at $t'=t'_m$ and then increases up to $\tilde{z}_1$ for $t'=-t_1$ [e.g., Fig. 6(b), dotted line]. For $t>-t_0+2(z_0-z_1)v_0/c_n^2$ there is no maximum of $\rho(t')$ in the space region 1. It rises steadily from 0 for $t'=t_c$ up to ρ_1 given by (5.5) for $t'=-t_1$ [e.g., Fig. 6(c), dotted line]. In particular, $\rho_m=\rho_1$, $z_m=\tilde{z}_1$ for $t=-t_0+2(z_0-z_1)v_0/c_n^2$.

2. Space region 2

In the time interval $-t_1<t'<t_1$ ($t_1=z_1/v_0$) where a charge moves uniformly with the velocity v_0 equations (4.3) look like

$$\rho=\frac{c_n^2}{v_0\gamma_{0n}}(t-t'),\quad z=v_0t'+\frac{c_n^2}{v_0}(t-t'). \tag{5.8}$$

Here $\gamma_{0n}=1/\sqrt{v_0^2/c_n^2-1}$. Excluding t' from these equations one finds

$$\rho=(v_0t-z)\gamma_{0n}, \tag{5.9}$$

where ρ and z change in the intervals

$$\tilde{z}_1<z<v_0t,\quad 0<\rho<\frac{c_n^2}{v_0\gamma_{0n}}(t+t_1)$$

for $-t_1<t<t_1$ and

$$\tilde{z}_1<z<z_2,\quad \rho_2<\rho<\rho_1$$

for $t>t_1$. Here $\tilde{z}_1$ and ρ_1 are the same as above, and

$$z_2=\frac{c_n^2}{v_0}(t-t_1)+z_1,\quad \rho_2=\frac{c_n^2}{v_0\gamma_{0n}}(t-t_1). \tag{5.10}$$

It is seen that for each $t>t_1$ the singular segment (5.9) is enclosed between the straight lines L_1 [$\rho=(z+z_1)/\gamma_{0n}$] and L_2 [$\rho=(z-z_1)/\gamma_{0n}$] originating from the boundary points of the interval 2 and inclined at the angle θ_c ($\cos\theta_c=1/\beta_0 n$) towards the motion axis [Fig. 6(d), solid line]. The singular segment (5.9) is a piece of the Cherenkov shock wave which is enclosed between L_1 and L_2 and perpendicular to both of them. Its normal is inclined at the angle θ_c towards the motion axis. As time goes, it propagates between L_1 and L_2. For $-t_1<t<t_1$ the singular segment (5.9) is enclosed between the moving charge and the straight line L_1 [Fig. 6(c), solid line].

3. Space region 3

In the time interval $t_1 < t' < t_0$ where a charge moves with deceleration a, equations (4.3) look like

$$z = z_0 - \frac{1}{2}a(t' - t_0)^2 + \frac{c_n^2}{v}(t - t'), \quad \rho = \frac{c_n^2(t - t')}{v\gamma_n}, \tag{5.11}$$

where $v = a(t_0 - t')$. The charge velocity changes steadily from v_0 at $t' = t_1$ down to 0 at $t = t_0$. The above singularity surfaces exist only if $c_n < v < v_0$. The charge velocity coincides with the velocity of light in medium $c_n = c/n$ at $t' = t_c$,

$$\rho_c = \rho(t' = t_c) = 0, \quad z_c^{(2)} = z(t' = t_c) = c_n t + \left(1 - \frac{1}{\beta_0 n}\right)\left[z_0 - \frac{1}{\beta_0 n}(z_0 - z_1)\right]. \tag{5.12}$$

The radius $\rho(t')$ vanishes at the position of a moving charge $(t' = t)$ for $t < t_c$ and at $t' = t_c$ for $t > t_c$. It is maximal at the start of the third motion interval $(t' = t_1)$ where

$$\rho(t' = t_1) = \rho_2, \quad z(t' = t_1) = z_2$$

[ρ_2 and z_2 are the same as in (5.10)].

C. Discussion of the results obtained in this section

A complete singular contour composed of its singular pieces defined in the regions 1, 2, and 3 is always closed for the fixed observation time t. In fact, for $-t_c < t < -t_1$ the singular contour lies completely in the region 1. It begins at the point $z = z_c^{(1)}$, $\rho = 0$ and ends at the point $\rho = 0$, $z = -z_0 + a(t + t_0)^2/2$ coinciding with the current charge position [Fig. 6(a)]. For $-t_1 < t < t_1$ the singular contour lies in the regions 1 and 2 [Figs. 6(b) and 6(c)]. Its branch lying in the region 1 begins at the point $z = z_c^{(1)}$, $\rho = 0$ and ends at the point $z = \tilde{z}_1$, $\rho = \rho_1$. Its branch lying in the region 2 begins at the point $z = \tilde{z}_1$, $\rho = \rho_1$ and ends at the point $z = v_0 t$, $\rho = 0$ coinciding with the current charge position. For $t > t_1$ the singular contour lies in the regions 1, 2, and 3 [Fig. 6(d)]. Its branch in region 1 is the same as above. Its branch lying in the region 2 begins at the point $z = \tilde{z}_1$, $\rho = \rho_1$ and ends at the point $z = z_2$, $\rho = \rho_2$. Its branch lying in the region 3 begins at the point $z = z_2$, $\rho = \rho_2$ and ends at the point $z = z_c^{(2)}$, $\rho = 0$.

D. Transition to instantaneous velocity jumps

It is instructive to consider the limit $z_1 \to z_0$ corresponding to the instantaneous velocity jumps at the start and the end of the charge motion. Intuitively it is expected that the original Tamm problem should appear in this limit. Turning to (5.1) we observe that the second term entering into z equals zero in this limit. In fact, it equals

$$\frac{1}{2}a(t' + t_0)^2 = \frac{z_0 - z_1}{\beta^2 n^2}$$

at $t' = -t_c$ and

$$\frac{1}{2}a(t' + t_0)^2 = \frac{z_0 - z_1}{\beta^2 n^2}$$

at $t' = -t_1$. Therefore, in the limit $z_1 \to z_0$ it disappears at the boundaries of the charge motion interval and, therefore, inside this interval since the above term is a monotone function of t'. Then, (5.1) reduces to

$$z = -z_0 + \frac{2(z_0 - z_1)}{\beta_0^2 n^2}\frac{t - t_0}{t' + t_0},$$

$$\rho = \frac{2(z_0 - z_1)}{\beta_0^2 n^2} \frac{t - t_0}{t' + t_0} \left\{ \left[\frac{n\beta_0^2 c(t' + t_0)}{2(z_0 - z_1)} \right]^2 - 1 \right\}^{1/2}. \tag{5.13}$$

On the other hand, we cannot drop the terms with $(z_0 - z_1)$ in (5.13) since the denominator $(t' + t_0)$ is of the same order of smallness. It is seen that $z = z_c^{(1)}$, $\rho = \rho_c^{(1)} = 0$ at $t' = -t_c$ and $z = \tilde{z}_1$, $\rho = \rho_1$ at $t' = -t_1$. Here

$$z_c^{(1)} = c_n t - z_0 \left(1 - \frac{1}{\beta_{0n}} \right), \quad \tilde{z}_1 = \frac{c_n^2}{v_0} t - z_0 \left(1 - \frac{1}{\beta_{0n}^2} \right), \quad \rho_1 = \frac{c_n^2}{v_0 \gamma_{0n}} (t + t_0).$$

It follows from (5.13) that

$$\rho^2 + (z + z_0)^2 = c_n^2 (t + t_0)^2 \tag{5.14}$$

coincides with the equation of the BS shock wave arising at the beginning of the charge motion (BS_1, for short). This singular contour [SW_1 in Fig. 3(b)] begins at the point $z = z_c^{(1)}$, $\rho = \rho_c^{(1)} = 0$ and ends at the point $z = \tilde{z}_1$, $\rho = \rho_1$. It represents the shock wave arising when the charge velocity coincides with the velocity of light in medium at the accelerated part of the charge trajectory.

The fact that SW_1 and BS_1 are described by the same equation (5.14) is physically understandable since both these waves, due to the instantaneous velocity jump, are created at the same instant $t = -t_0$, at the same space point $z = -z_0$, and propagate with the same velocity c_n. It should be noted that the BS_1 shock wave is distributed over the whole sphere (5.14) while the singular shock wave SW_1 fills only its part.

The second part of the singular contour is the Cherenkov shock wave [CSW in Fig. 3(b)] extending from the point $z = \tilde{z}_1$, $\rho = \rho_1$ to the point $z = z_2$, $\rho = \rho_2$. Here

$$z_2 = \frac{c_n^2}{v_0} t + z_0 \left(1 - \frac{1}{\beta_{0n}^2} \right), \quad \rho_2 = \frac{c_n^2}{v_0 \gamma_{0n}} (t - t_0).$$

The third part of the singularity contour [SW_2 in Fig. 3(b)] begins at the point $z = z_2$, $\rho = \rho_2$ and ends at $z = z_c^{(2)}$, $\rho = \rho_c^{(2)} = 0$. Here

$$z_c^{(2)} = c_n t + z_0 \left(1 - \frac{1}{\beta_{0n}} \right).$$

This part of the singularity contour represents the shock wave arising at the decelerated part of the charge trajectory. It is described by the equation

$$\rho^2 + (z - z_0)^2 = c_n^2 (t - t_0)^2 \tag{5.15}$$

coinciding with the equation of the BS_2 shock wave emitted at the end $(t = t_0, z = z_0)$ of a charge motion. Again, the singularity fills only part of the sphere (5.15).

VI. DISCUSSION

Turning to Fig. 5 we observe the existence of the radiation intensity plateau, its sudden drop to the right of the plateau and its moderate decreasing to the left of the plateau. The sudden drop of the radiation intensity to the right of the plateau takes place in the space region where only the nonsingular BS shock waves associated with the beginning and the end of a charge motion exist. In Fig. 6(d), this space region lies above L_1. The plateau corresponds to the space region lying between L_2 and L_1 [Fig. 6(d)] where the singular wave CSW (Cherenkov shock wave) and SW_1 (singular shock wave associated with the transition of the light velocity barrier at the accelerated part of the charge trajectory) exist. The moderate decrease in the radiation intensity to the left of the plateau is due to the existence of SW_1 and SW_2 shock waves (the latter arises at the decelerated part of the charge trajectory). The oscillations of the radiation intensity in this region are due

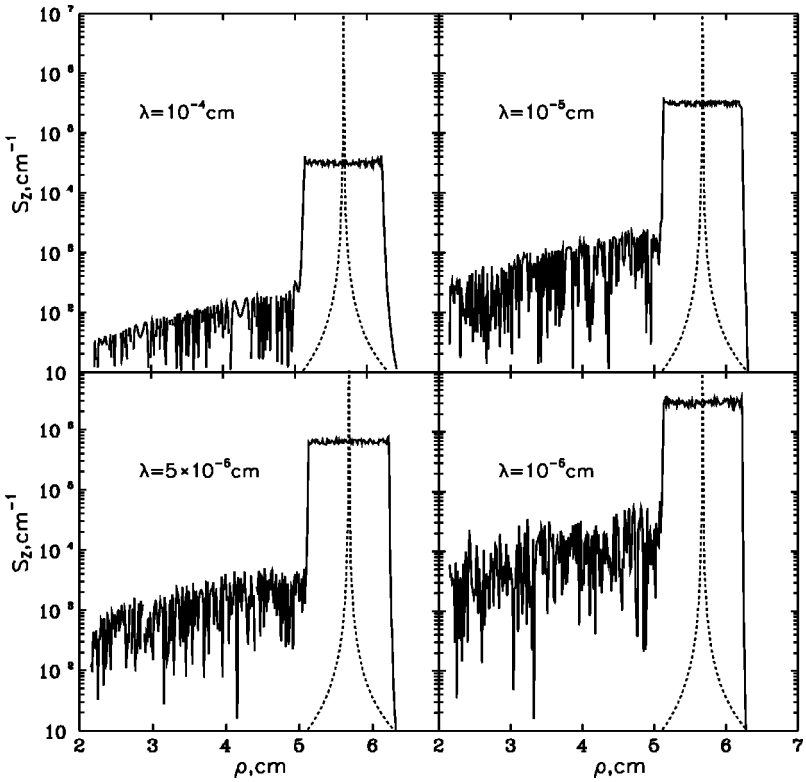

FIG. 7. Spectral radiation intensities for the smooth Tamm problem for the uniform motion interval $L_u=0.98$ cm and various wavelengths λ. Other parameters are the same as in Fig. 5. The radiation intensities rise with the diminishing of λ to the left of the plateau and are very small to the right of the plateau.

to the interference of SW_1 and SW_2. The smallness of oscillations inside the plateau indicates that the contribution of the CSW to the radiation intensity is much larger than that of SW_1.

Now we discuss why the configuration of the shock waves in the limiting case of the smooth Tamm problem [Fig. 3(b)] does not coincide with that of the original Tamm problem [Fig. 3(a)]. It was shown in Ref. 9 that in the spectral representation the radiation intensity (for the fixed observation wavelength) of the smooth Tamm problem transforms into the radiation intensity of the original Tamm problem when the length of the trajectory along which a charge moves nonuniformly tends to zero. Figure 5 supports this claim. However, Figs. 3(a) and 3(b) describe the position of the EMF singularities at the fixed moment of the observational time [or, in other words, Figs. 3(a) and 3(b) correspond to the time representation]. The time and spectral representations of the EMF are related by the Fourier transformation. For an arbitrary small but finite length l of the charge nonuniform motion in the smooth Tamm problem, the contribution of the nonuniform motion to the radiation intensity becomes essential and comparable with the contribution of the uniform motion for high frequencies. This is clearly shown in the last of Refs. 5 and in Ref. 8 and in Fig. 7. Thus, the appearance of additional shock waves in Fig. 3(b) is due to the contribution of high frequencies.

Turning to Fig. 3(b) describing the position of the shock waves in the limiting case of the smooth Tamm problem, we see that three shock waves (BS_1, SW_1, and CSW) are intersected on the straight line L_1. Therefore, the radiation intensity should be large there. Above L_1 (this corresponds to the region lying to the right of the plateau in Fig. 5) only the nonsingular shock waves BS_1 and BS_2 contribute to the radiation intensity. Therefore, the radiation intensity should be very small there. The experimental curve shown in Fig. 2 partly supports these claims.

However, the experimental intensity decreases smoothly in the space region where the theory predicts the existence of plateau. The picture similar to Fig. 2 might be possible if the focusing

devices (their use is wide-spread in the Cherenkov-type experiments) projecting the γ rays emitted at the Cherenkov angle into the narrow Cherenkov ring (and transforming the plateau of the radiation intensity into this ring) were used. However, no focusing lens was used in the experiments discussed in which the Cherenkov light left the radiator along the direction perpendicular to the radiator surface.

There are two possible reasons for the deviation of the theoretical data from the experimental ones. The first of them is the medium dispersion. A charge moving uniformly in medium, in a finite spatial interval, emits all frequencies [contrary to the unbounded charge motion when only the frequencies satisfying the Tamm–Frank radiation condition $\beta n(\omega)>1$ (see, e.g., Ref. 10) are emitted]. In the experiment treated, where no frequency filters were used, the dependence on the frequency enters through the refractive index n of the sample (where a charge moves) and through the spectral sensitivity of the photographic film placed in the observational plane perpendicular to the motion axis. Let the intervals where a charge is accelerated and decelerated be arbitrarily small but finite. For large frequencies the radiation intensity in the space region to the left of the plateau shown in Fig. 7 begins to rise. The resulting radiation intensities are obtained from those presented in Fig. 7 by convoluting them with the spectral sensitivity of the photofilm and integrating over all ω. If the integrand differs from zero for large frequencies, then the arising radiation intensity will resemble the experimental curve of Fig. 2. However, to perform concrete calculations the knowledge of the frequency dependence of the refractive index and the spectral sensitivity of the photofilm is needed. The second reason is due to the finite diameter (0.5 cm) of the proton beam used in experiments described in Ref. 4. The averaging of the radiation intensities over the proton beam diameter leads to their smoothing (and, in particular, to the disappearance of the pronounced peaks at the ends of the Cherenkov plateau).

The transition from the time representation to the spectral one involves the time integration. Since the space regions to which the above shock waves are confined do not depend on time (e.g., CSW is always between L_1 and L_2, etc.), the shock waves are in the same space regions in both representations.

A. The physical meaning of the smooth Tamm problem

Before discussing how the smooth Tamm problem is related to the experimental situation, we recall the usual physical interpretation of the original Tamm problem (see, e.g., Ref. 11). Let the uniformly moving charge move consecutively in vacuum, in dielectric sample and again in vacuum. Since the charge uniformly moving in medium does not radiate if $\beta n<1$ and radiates if $\beta n>1$, the charge passing through the sample is interpreted as a charge instantaneous acceleration at one side of the sample, the instantaneous deceleration at its other side and uniform motion inside the sample. Turning to the physical justification of the smooth Tamm problem, we observe that according to Born,[12] "The assumption on the jump-like transition from one substance to another is a far-reaching idealization. One substance is separated from another by some transition layer in which the dielectric constant changes continuously from ϵ_1 to ϵ_2." Let a charge move uniformly consecutively in vacuum, in a dielectric sample and again in vacuum. A charge begins to radiate with increasing intensity as it moves through the above layer where ϵ changes from ϵ_1 to ϵ_2. Then, in the spirit of the standard interpretation[11] of the original Tamm problem we suggest that the charge uniform motion through this layer is equivalent to its smooth acceleration inside the sample (in both cases βn varies from $\beta n<1$ to $\beta n>1$). That is, the charge passage through the sharp and diffused boundaries is effectively described by its instantaneous and smooth accelerations, respectively.

B. Reflections on the experimental setup

The experiments described in Ref. 4 (performed by Zrelov more than 40 years ago) were not especially designated for the discovering of the shock waves associated with the overcoming of the light velocity barrier (their existence was predicted much later). The following experimental conditions should be fulfilled for the reliable identification of the above shock waves.

(1) The frequency filter should be used. This permits one to escape complications and uncertainties associated with the integration over the frequency spectrum.

(2) The diameter of the charged particles beam should be as small as possible. The radiation intensity peaks associated with the above shock waves will be more pronounced for the thin beam (since the averaging over the beam diameter leads to their smoothing).

(3) No focusing devices (they are frequently used in the Cherenkov-type experiments) projecting the extended Cherenkov radiation into the thin Cherenkov ring should be used.

When these conditions are fulfilled, the observed spectral radiation intensity should resemble those shown in Fig. 7. The peaks of the radiation intensity at the boundaries of the Cherenkov plateau (similar to those shown at the right part of Fig. 1) will certainly indicate the existence of shock waves arising at the light velocity barrier.

VII. CONCLUSION

We briefly summarize the main results obtained.

(1) The position and the time evolution of the electromagnetic singular shock waves in the smooth Tamm problem are found. They consist of the Cherenkov shock wave and the shock waves arising at the accelerated and decelerated parts of the charge trajectory. Theory predicts the existence of the plateau in the spectral radiation intensity (associated with the finite Cherenkov shock wave), its sudden drop to the right of this plateau (associated with the absence of the singular shock waves in this spatial region), and small oscillations to its left (associated with the interference of the shock waves arising at the accelerated and decelerated parts of the charge trajectory).

(2) In the limiting case of the smooth Tamm problem (when the lengths along which a charge moves nonuniformly tend to zero), the resulting configuration of the electromagnetic singular shock waves does not coincide with that of the original Tamm problem (corresponding to the instantaneous velocity jumps at the beginning and the end of the charge motion). This is due to the contribution of high frequencies.

(3) It is studied how the electromagnetic shock waves occurring in the original and smooth Tamm problems reproduce the experimental situation. The recommendations on the performance of experiments aiming to discover shock waves associated with the overcoming of the light velocity barrier are given.

Recently we were aware of the interesting paper[13] in which the Cherenkov waves of the finite width were observed. We associate their finite width with the plateau of the radiation intensities shown in Figs. 1, 5, and 7.

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An inequality for the Gibbs mean number of clusters

Camillo Cammarota[a)]
Dipartimento di Matematica, Universitá di Roma "La Sapienza," Piazzale A. Moro 2, 00185 Roma, Italy

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The number of percolation clusters for configurations of the Ising model at zero external field and ferromagnetic first neighbors interaction on a general finite graph is considered. The mean number of clusters with respect to the Gibbs measure at any inverse temperature β is proved to be smaller or equal than the one at $\beta=0$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1845972]

I. INTRODUCTION

Let $G=(V,E)$ be a finite connected graph, of vertexes set V and edges set E. The Gibbs measure on G is the probability measure μ_β on $\Sigma=\{-1,1\}^V$ of weight

$$e^{\beta\Sigma_{\{i,j\}\in E}\,\sigma(i)\sigma(j)}, \quad \sigma\in\Sigma.$$

We denote by $\mathbb{E}^G_{\mu_\beta}$ the mean with respect to this measure. The measure μ_β describes an Ising model with spin variables on vertexes, ferromagnetic interaction on edges, zero external field, and inverse temperature β. Given any configuration $\sigma\in\Sigma$, the + (−) clusters of σ are the maximal connected components of $\sigma^{-1}(+1)$ $(\sigma^{-1}(-1))$. We denote by $C^{+(-)}(\sigma)$ the set of + (−) clusters of σ; the number of + (−) clusters $N^{+(-)}(\sigma)$ is the cardinality of $C^{+(-)}(\sigma)$, also denoted $|C^{+(-)}(\sigma)|$. The number of clusters of σ, denoted $N(\sigma)$, is defined as $N(\sigma)=N^+(\sigma)+N^-(\sigma)$ and obviously one has by symmetry

$$\mathbb{E}^G_{\mu_\beta}(N^+)=\mathbb{E}^G_{\mu_\beta}(N^-).$$

It is useful to consider the family μ_β, $\beta\in[0,\infty]$. One easily recognizes that μ_0 is a Bernoulli measure of parameter $\frac{1}{2}$ and that $\mu_\infty=\frac{1}{2}\delta_+ +\frac{1}{2}\delta_-$, where $\delta_+(\delta_-)$ is the point mass concentrated on the constant +(−) configuration. Consequently one has $\mathbb{E}^G_{\mu_\infty}(N)=1$, while the value of $\mathbb{E}^G_{\mu_0}(N)$ depends on the graph.

The random variable number of clusters plays a central role in percolation theory, and in the case of Bernoulli percolation it has been extensively studied (for a general reference see Ref. 7). We are interested in monotonicity properties with respect to β of the mean number of clusters $\mathbb{E}^G_{\mu_\beta}(N)$, as a particular case of the general problem of monotonicity in β for variables used in percolation theory. As an example, it is an open problem to extend the coexistence of + and − infinite clusters proved in the cubic lattice for the Ising model at β close to 0 (Ref. 5) to a larger range of temperatures.

The Gibbs measure is FKG for fixed temperature (for instance see Ref. 8), but there is not a satisfactory notion of stochastic ordering with respect to temperature. To circumvent this problem one method is to represent the measure on spins by means of a measure on edges configurations. A widespread approach is the random cluster model given by the Fortuin–Kasteleyn representation. For a review we refer to Ref. 8. Since random cluster measures are stochastically ordered in temperature, it is enough to prove that a particular observable in edge representation is monotonic in the partial ordering of these configurations. Using this method some observables related to percolation can be proved to have monotonicity properties.[3,10]

[a)]Electronic mail: cammar@mat.uniroma1.it

However other approaches have been used, and in particular we refer to the group representation of the Ising model, for which a basic reference is Ref. 9. Combining this representation and the notion of stochastic order has been fruitful. In particular some monotonicity properties of local observables can be re-obtained and new ones are proved.[4,6] The main idea is that the Gibbs measure on spins configurations is represented by a measure on edges configurations conditioned to a group, and that conditioned measures are stochastically ordered.

Despite some evident similarities with the random cluster model, one advantage of this approach is that the measure at $\beta=0$ is a delta mass concentrated on the empty configuration on edges. This feature can be exploited to treat a simpler type of problem, i.e., the inequality between the means at $\beta>0$ and at $\beta=0$. In Ref. 2 the mean number of clusters was proved to be smaller at $\beta>0$ than at $\beta=0$, if the graph has degree not greater than 3. In the present paper we prove an extension of this inequality for any degree.

Proposition 1.1: For any graph G the mean number of clusters with respect to the Gibbs measure at inverse temperature $\beta>0$ is less or equal to the one at $\beta=0$,

$$\mathbb{E}^G_{\mu_\beta}(N) \leqslant \mathbb{E}^G_{\mu_0}(N).$$

The main contribution of the present paper essentially consists in reducing the problem for a general graph G to the one for a graph G' with degree not greater than 3. This is achieved using a vertex resolution procedure, similar to the one used in Ref. 11, and conditioning the measure μ_β to a suitable configurations subset Δ. Hence the main ingredients of our proof can be summarized by the following equations:

$$\mathbb{E}^G_{\mu_\beta}(N) = \mathbb{E}^{G'}_{\mu_\beta}(N|\Delta) \leqslant \mathbb{E}^{G'}_{\mu_0}(N|\Delta) = E^G_{\mu_0}(N). \tag{1}$$

The inequality in the middle is an extension of the one proved in Ref. 2 and the external equalities are the result of the resolution procedure. In the present paper we also provide an exposition of the basic elements of the group representation, in order to make the paper self-consistent.

II. VERTEX RESOLUTION

In this section we prove the following lemma.

Lemma 2.1: There is a graph $G'=(V',E')$ with degree not greater than 3 and a subset Δ of $\Sigma'=\{-1,1\}^{V'}$ such that for the number of clusters N the following equation holds:

$$\mathbb{E}^G_{\mu_\beta}(N) = \mathbb{E}^{G'}_{\mu_\beta}(N|\Delta).$$

On the right-hand side there is the conditional expectation with respect to Δ, and the Gibbs measure on G' is defined as the one on G.

Proof: Given a vertex $i \in V$ we denote ∂i the set of the vertexes adjacent to i (first neighbors): the degree of i, denoted $\deg(i)$, is the cardinality of ∂i. For each i we define a set B_i, the resolution of the vertex i, as follows. If $\deg(i)\leqslant 3$, we set $B_i=\{i\}$: if $\deg(i)>3$, the set B_i is defined as a replica of ∂i, and we denote j' the element of B_i which corresponds to j. The new vertexes set is

$$V' = \cup_{i\in V} B_i.$$

In order to define E', we first replace the edges $\{i,j\}\in E$, $j\in\partial i$, by the edges $\{j,j'\}$, $j\in\partial i$. This defines a set of edges on V', called "conduction" edges and denoted E'_C, which are in one to one correspondence with E. We then put in each of the B_i's having cardinality greater than 3 edges such that make it connected; if $B_i=\{k_1,k_2,\ldots,k_n\}$, for instance we choose the edges $\{k_1,k_2\},\ldots,\{k_n,k_1\}$, forming a loop on B_i. We call these "identification" edges and denote them E'_C. The set E' can now be defined as a union of conduction edges E'_C and identification edges E'_I. The vertexes with degree not greater than 3 keep unchanged their degree; the other ones have exactly one conduction edge and two identification edges; hence the degree of G' is at most 3. This formal definition can be made more transparent with the help of Fig. 1.

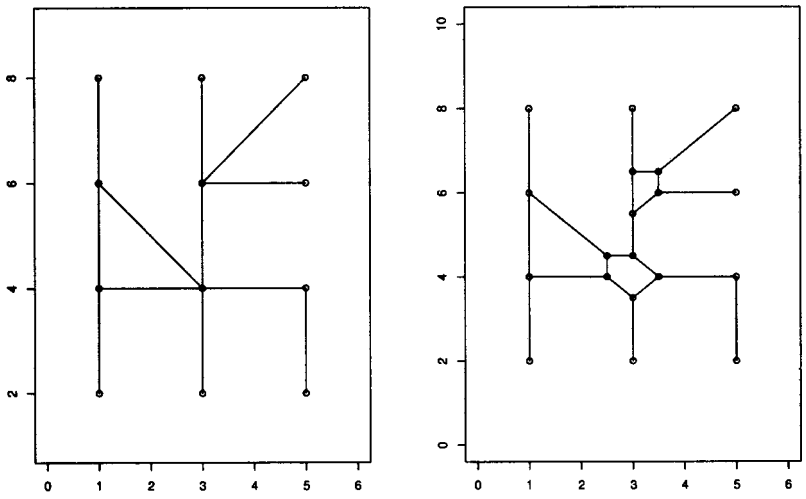

FIG. 1. Resolution procedure applied to the graph on the left, having one vertex of degree 4, of coordinates (3, 6), and one of degree 5, of coordinates (3, 4); on the right the graph obtained after resolution of these vertexes.

For the graph G' the Gibbs measure on $\Sigma'=\{-1,1\}^{V'}$ is formally defined as the one on G, and we use the same notation. We define the identification subset $\Delta\subset\Sigma'$ as the intersection over $i\in V$ of the identification event which forces all spins in B_i to be equal: $\sigma'(k_1)=\cdots=\sigma'(k_n)$. There is a trivial one to one map between configurations spins in Σ and Δ, such that if $\sigma\in\Sigma$ and $\sigma'\in\Delta$ one has $\sigma(i)=\sigma'(k)$, $k\in B_i$. An important consequence of the above definitions is that the number of clusters satisfies the equation

$$N(\sigma)=N(\sigma'). \tag{2}$$

Furthermore the interactions that define the Gibbs weights differ for a constant depending only on the graph,

$$\sum_{\{i,j\}\in E'}\sigma'(i)\sigma'(j)=\sum_{\{i,j\}\in E'_C}\sigma'(i)\sigma'(j)+\sum_{\{i,j\}\in E'_I}\sigma'(i)\sigma'(j)=\sum_{\{i,j\}\in E}\sigma(i)\sigma(j)+\sum_{i\in V,\deg(i)>3}|B_i|,$$

where we have used that conduction edges reproduce exactly E and that each identification edge gives a constant contribution of value 1. This suffices to conclude that conditioned to Δ the mean number of clusters on G' has the same value as the one on G. ■

Remark 1: Identification edges on B_i can be chosen in several ways, subject to the condition that they make B_i connected and that $\deg(j)\leqslant 3$; for instance one of the edges of the loop above defined can be dropped.

Remark 2: Equation (2) may not be true for other percolation variables. Let us consider the cardinality of the (say +) cluster containing a fixed vertex: if $W_k^+(\sigma')$ denotes the + cluster on G' containing the vertex $k\in V'$, where $k\in B_i$ and $\sigma'\in\Delta$, and if $W_k^+(\sigma')$ denotes the corresponding cluster on G, they are related by the nontrivial relationship

$$|W_k^+(\sigma')|=\sum_{j\in W_i^+(\sigma)}|B_j|.$$

III. GROUP REPRESENTATION OF CONDITIONED GIBBS MEASURES

We first discuss the representation of unconditioned Gibbs measures following Ref. 6. Given $\sigma\in\Sigma$ we associate to it the edge configuration $\omega\in\Omega=\{0,1\}^E$, defined as $\omega(i,j)=0$ if $\sigma(i)=\sigma(j)$ and $\omega(i,j)=1$ if $\sigma(i)\neq\sigma(j)$. This defines a map ψ from spins to edges configurations; by symmetry one has $\psi(\sigma)=\psi(-\sigma)$. The range of this map, denoted Γ, can be characterized as the set

of edges configurations such that any loop contains an even number of 1's (this was noticed, for instance, in Ref. 10, but with the opposite coding). A next step is to recognize that this set has a group structure, as a subgroup of Ω.[1] Actually in Ω there is a product defined as

$$\omega_1\omega_2(e) = \omega_1(e) + \omega_2(e) \mod 2, \quad e \in E$$

and the identity is the null element $0(e)=0$, $e \in E$. We call Γ the "parity" group.

The Gibbs weight can be written as

$$e^{\beta|\omega^{-1}(0)|-\beta|\omega^{-1}(1)|}, \quad \omega \in \Gamma.$$

This is the same as the one of a Bernoulli product measure ν_p of parameters p for the 1's and $1-p$ for the 0's, where $p=e^{-\beta}/(e^{\beta}+e^{-\beta})$, conditioned to Γ. Since we are interested in variables invariant with respect to total spin flip, their means with respect to the measure μ_β can be written in terms of means with respect to the Bernoulli measure ν_p conditioned to the subgroup Γ. If X denotes such a variable, both as a function of spins configurations and of edges configurations, we have

$$\mathbb{E}_{\mu_\beta}(X) = \mathbb{E}_{\nu_p}(X|\Gamma). \tag{3}$$

We now consider the general problem of representing the Bernoulli measure ν_p conditioned to a subgroup Θ. We need some definitions. The cylinder of base $A \subset E$, given $\alpha \in \{0,1\}^A$, is

$$K_\alpha^A = \{\omega \in \Omega | \omega(e) = \alpha(e), e \in A\}.$$

We include the case $A=\emptyset$ setting $K_\alpha^\emptyset = \Omega$. In particular one has that K_0^A is a subgroup and K_α^A is a coset for any α. If X is a function on Ω and Θ is a subgroup, we define a function on the subsets of E,

$$X_\Theta(A) = |\Theta \cap K_0^A|^{-1} \sum_{\omega \in \Theta \cap K_0^A} X(\omega). \tag{4}$$

We also introduce a probability measure λ_p^Θ on the subsets of E,

$$\lambda_p^\Theta(A) = \nu_p(\Theta)^{-1}(1-2p)^{|A|}p^{|E\setminus A|}|\Theta \cap K_0^A|. \tag{5}$$

With these notation we have the following.

Proposition 3.1 (Ref. 6): The mean of X with respect to the Bernoulli measure ν_p conditioned to a subgroup Θ can be represented by

$$\mathbb{E}_{\nu_p}(X|\Theta) = \sum_{A \subset E} X_\Theta(A)\lambda_p^\Theta(A). \tag{6}$$

Proof: Denoting for brevity $\omega=\omega^{-1}(1)$ and $\omega^c=\omega^{-1}(0)$ and considering ω as a subset of E, one has

$$\nu_p(\omega) = p^{|\omega|}(1-2p+p)^{|\omega^c|} = \sum_{A \subset \omega^c} (1-2p)^{|A|}p^{|E\setminus A|}.$$

Hence

$$\sum_{\omega \in \Theta} \nu_p(\omega)X(\omega) = \sum_{A \subset E} (1-2p)^{|A|}p^{|E\setminus A|} \sum_{\omega \in \Theta \cap K_0^A} X(\omega)$$

and this concludes the proof. ■

We can now discuss the representation of conditioned Gibbs measures; in particular we are looking for a suitable representation of $\mathbb{E}_{\mu_\beta}^{G'}(N|\Delta)$. We first notice that the image of Δ on edges configurations is a subgroup of Ω'. In particular it is the cylinder $K_0^{E_I'}$ obtained setting 0's on

identification edges of E'; we use the same notation Δ and call it "identification" group. We shall use the following property. Since the representation of the Gibbs measure requires conditioning to the parity group Γ, the representation of the Gibbs measure conditioned to identification group Δ can be achieved conditioning to the intersection of these two groups. We can write

$$\mathbb{E}^{G'}_{\mu_\beta}(N|\Delta) = \mathbb{E}^{G'}_{\nu_p}(N|\Gamma \cap \Delta). \tag{7}$$

Since $\Theta = \Gamma \cap \Delta$ is a group, we can apply Eq. (6) and get

$$\mathbb{E}^{G'}_{\mu_\beta}(N|\Delta) = \sum_{A \subset E} N_\Theta(A) \lambda^\Theta_p(A). \tag{8}$$

We now remark that for $\beta = 0$, i.e., $p = 1/2$, the corresponding measure $\lambda^\Theta_{1/2}$ is a delta mass concentrated on the empty set. Hence,

$$\mathbb{E}^{G'}_{\mu_0}(N|\Delta) = N_\Theta(\emptyset). \tag{9}$$

Hence in order to have

$$\mathbb{E}^{G'}_{\mu_\beta}(N|\Delta) \leqslant E^{G'}_{\mu_0}(N|\Delta) \tag{10}$$

it is sufficient the condition

$$N_\Theta(A) \leqslant N_\Theta(\emptyset), \quad A \subset E'. \tag{11}$$

The next section is devoted to prove this inequality.

IV. A PRUNING TREE ARGUMENT

We shall prove that the function N_Θ over the subsets of E' has the following weak monotonicity property.

Proposition 4.1: For any $A \subset E'$, $A \neq \emptyset$, there is $e \in A$ such that

$$N_\Theta(A) \leqslant N_\Theta(A \setminus e). \tag{12}$$

One easily recognizes that this property is sufficient to give Eq. (11). The case that Θ is the parity group was considered in Ref. 2. Here we recall that proof, adapting it to the present context.

Proof: Equation (12) is equivalent to

$$|\Theta \cap K_0^{A\setminus e}| \sum_{\omega \in \Theta \cap K_0^A} N(\omega) \leqslant |\Theta \cap K_0^A| \sum_{\omega \in \Theta \cap K_0^{A\setminus e}} N(\omega). \tag{13}$$

We use

$$|\Theta \cap K_0^{A\setminus e}| = |\Theta \cap K_{0\,0}^{A\setminus ee}| + |\Theta \cap K_{0\,1}^{A\setminus ee}|$$

and

$$\sum_{\omega \in \Theta \cap K_0^{A\setminus e}} N(\omega) = \sum_{\omega \in \Theta \cap K_{0\,0}^{A\setminus ee}} N(\omega) + \sum_{\omega \in \Theta \cap K_{0\,1}^{A\setminus ee}} N(\omega),$$

and so Eq. (13) is equivalent to

$$|\Theta \cap K_{0\,1}^{A\setminus ee}| \sum_{\omega \in \Theta \cap K_{0\,0}^{A\setminus ee}} N(\omega) \leqslant |\Theta \cap K_{0\,0}^{A\setminus ee}| \sum_{\omega \in \Theta \cap K_{0\,1}^{A\setminus ee}} N(\omega), \tag{14}$$

where we have used $\Theta \cap K_{0\,0}^{A\setminus ee} = \Theta \cap K_0^A$.

If the set $\Theta \cap K_{0\,1}^{A\setminus ee}$ is empty, we define zero the sum extended to it and we have by definition

$$N_\Theta(A) = N_\Theta(A \setminus e).$$

Since $\Theta = \Delta \cap \Gamma$, the set $\Theta \cap K_{0\,1}^{A\setminus ee}$ is empty if the value 1 on the edge e violates the identification or the parity condition. The first case happens if e is an identification edge; the second one if e belongs to a loop of A, since any loop must contain an even numbers of 1's.

If the set $\Theta \cap K_{0\,1}^{A\setminus ee}$ is nonempty, it is a coset of the group $\Theta \cap K_{0\,0}^{A\setminus ee}$ and so it has the same cardinality. Hence Eq. (12) is equivalent to

$$\sum_{\omega \in \Theta \cap K_{0\,0}^{A\setminus ee}} N(\omega) \leqslant \sum_{\omega \in \Theta \cap K_{0\,1}^{A\setminus ee}} N(\omega). \tag{15}$$

From the previous argument we can now suppose that A does not contain loops, i.e., it is union of disjoint trees and we shall prove that pruning any end line e preserves Eq. (12), since Eq. (15) holds. It is convenient to rewrite this equation in spins language, getting

$$\sum_{\sigma \in \Delta \cap K_{=\,=}^{A\setminus ee}} N(\sigma) \leqslant \sum_{\sigma \in \Delta \cap K_{=\,\neq}^{A\setminus ee}} N(\sigma), \tag{16}$$

where the set $K_{=\,\neq}^{A\setminus ee}$ is the spin version of $K_{0\,1}^{A\setminus ee}$. If $e=\{i,j\}$ where j is an endpoint of the tree $T \cup \{j\}$ of A, in order to get Eq. (15) it is sufficient that

$$N(\sigma_{++}^{Tj}) + N(\sigma_{--}^{Tj}) \leqslant N(\sigma_{+-}^{Tj}) + N(\sigma_{-+}^{Tj}), \quad \sigma \in \{-1,1\}^{V' \setminus T \cup \{j\}}, \tag{17}$$

where for instance σ_{+-}^{Tj} denotes the completion of σ with +'s on T and $-$ on j.

We denote for instance by $C_T^+(\sigma)$ and $C_j^+(\sigma)$, respectively, the set of + clusters of σ adjacent to T and j. We have

$$N(\sigma_{++}^{Tj}) = N(\sigma) - \left|C_T^+(\sigma) \cup C_j^+(\sigma)\right| + 1, \tag{18}$$

$$N(\sigma_{+-}^{Tj}) = N(\sigma) - \left|C_T^+(\sigma)\right| + 1 - \left|C_j^+(\sigma)\right| + 1, \tag{19}$$

$$N(\sigma_{--}^{Tj}) = N(\sigma) - \left|C_T^-(\sigma) \cup C_j^-(\sigma)\right| + 1, \tag{20}$$

$$N(\sigma_{-+}^{Tj}) = N(\sigma) - \left|C_T^-(\sigma)\right| + 1 - \left|C_j^+(\sigma)\right| + 1. \tag{21}$$

The first equation, for instance, uses the fact that if one turns on +'s over T and j, the + clusters adjacent to T or to j become a unique cluster. Using in Eq. (17) the above equations we get

$$\left|C_T^+(\sigma) \cap C_j^+(\sigma)\right| + \left|C_T^-(\sigma) \cap C_j^-(\sigma)\right| \leqslant 2. \tag{22}$$

The left-hand side is bounded by the number of vertexes that are simultaneously adjacent to T and j. Since T and j are adjacent and $\deg(j) \leqslant 3$, this number is not greater than 2. This proves Eq. (22) and completes the proof of the proposition. ■

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On the monotonicity of scalar curvature in classical and quantum information geometry

Paolo Gibilisco[a)]
Dipartimento di Studi Economico-Finanziari e Metodi Quantitativi, Facoltà di Economia, Università di Roma "Tor Vergata," Via Columbia 2, Rome 00133, Italy and Centro "Vito Volterra," Università di Roma "Tor Vergata," Via Columbia 2, Rome 00133, Italy

Tommaso Isola[b)]
Dipartimento di Matematica, Università di Roma "Tor Vergata," Via della Ricerca Scientifica, 00133 Rome, Italy

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We study the monotonicity under mixing of the scalar curvature for the α-geometries on the simplex of probability vectors. From the results obtained and from numerical data, we are led to some conjectures about quantum α-geometries and Wigner–Yanase–Dyson information. Finally, we show that this last conjecture implies the truth of the Petz conjecture about the monotonicity of the scalar curvature of the Bogoliubov–Kubo–Mori monotone metric. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1834693]

I. INTRODUCTION

The Bogoliubov–Kubo–Mori (BKM) metric is a distinguished element among the monotone metrics which are the quantum analog of Fisher information on the quantum state space.[35,36] In a definite sense BKM metric is the geometry on the state space that is related to von Neumann entropy (say, Umegaki relative entropy). Other well-known elements of this family are the right logarithmic derivative (RLD) metric, the symmetric logarithmic derivative (SLD or Bures) metric, and the Wigner–Yanase–Dyson (WYD) metrics. In Ref. 34 Petz made a conjecture on the scalar curvature of the BKM metric. Many arguments and numerical calculations suggest that the conjecture is true; nevertheless, a complete proof is still missing (see Refs. 3, 4, 12, 24, and 32).

One can state this conjecture in the following way: the BKM scalar curvature is a quantitative measure of symmetry (like entropy), namely it is increasing under mixing. Let us emphasize that it is also possible to relate the conjecture to quantities with direct physical meaning. An equivalent formulation, still due to Petz,[34] is that "…the scalar curvature is an increasing function of the temperature…." Moreover, the asymptotic relation between volume and curvature in Riemannian geometry and Jeffrey's approach to priors in statistics induced Petz to interpret the scalar curvature as the average statistical uncertainty (that should increase under coarse graining; see Ref. 36).

The original motivations given by Petz for the conjecture rely on the truth of the 2×2 case and on some numerical results for the general case. Petz and Sudar observed in Ref. 38 that "…monotonicity of Kubo metric is not surprising because this result is a kind of reformulation of Lieb convexity theorem.[30] However the monotonicity of the scalar curvature seems to be an inequality of new type (provided the conjecture is really true)…." A recent clear reference for Lieb's result and related inequalities can be found in the paper by Ruskai.[40]

The goals of the present paper are the following.

(1) We want to look at "higher mathematics from an elementary point of view." This means that we want to furnish an elementary motivation for the Petz conjecture. We do this by studying

[a)]Electronic-mail: gibilisco@voterra.mat.uniroma2.it
[b)]Electronic-mail: isola@mat.uniroma2.it

the monotonicity of the curvature for α-geometries in the plane. The results obtained in this case are very intuitive if one looks at the unit sphere of the L^p spaces. We conjecture that a similar behavior occurs for α-geometries in higher dimensions and in the noncommutative case, too.

(2) On the basis of the results of point (1) we make a conjecture about the monotonicity of scalar curvature for the WYD metrics. Further, we show that, using a continuity argument, this WYD conjecture would imply the Petz conjecture as a limit case (Theorem 8.1).

(3) We review what is known about monotonicity of scalar curvature for quantum Fisher information. In particular, we emphasize a result on the Bures metric, attributed to Dittmann, according to which the scalar curvature, in this case, is neither Schur-increasing nor Schur-decreasing (see Sec. II for precise definitions). This implies that an example of a monotone metric for which the scalar curvature (or its opposite) is strictly increasing under mixing does not exist yet. Note that Andai (using an integral decomposition of Ref. 15) proved that also in the 2×2 case there exist monotone metrics whose scalar curvature is not monotone.[3]

Finally, let us note that, related to this area, there exist other interesting papers. Some authors have suggested that, when statistical mechanics is geometrized, then the scalar curvature should have important physical meaning (for example, it should be proportional to the inverse of the free energy; see Refs. 8, 9, 25–27, and 39).

II. MAJORIZATION AND SCHUR-INCREASING FUNCTIONS

For the content of this section we refer to Refs. 1, 5–7, and 31.

A. Commutative case

We shall denote by $\mathcal{P}_n$ the manifold of positive vectors of $\mathbb{R}^n$, and by $\mathcal{P}_n^1 \subset \mathcal{P}_n$ the submanifold of density vectors, namely

Definition 2.1:

$$\mathcal{P}_n^1 := \left\{ \rho \in \mathbb{R}^n \middle| \sum_i \rho_i = 1,\ \rho_i > 0 \right\}.$$

We set $e := (1, \ldots, 1)$. The trace of a vector is $\mathrm{Tr}(v) = \Sigma_{i=1}^n v_i$. For an $n \times n$ real matrix, consider the following properties:

(I) $t_{ij} \geqslant 0 \quad i,j = 1, \ldots, n,$
(II) $\Sigma_{i=1}^n t_{ij} = 1 \quad j = 1, \ldots, n,$
(III) $\Sigma_{j=1}^n t_{ij} = 1 \quad i = 1, \ldots, n.$

Definition 2.2:

(a) *T is said to be stochastic if (I),(II) hold*;
(b) *T is said to be doubly stochastic if (I),(II),(III) hold.*

When T is seen as an operator $T: \mathbb{R}^n \to \mathbb{R}^n$ (by $(Tv)_j = \Sigma_{i=1}^n t_{ji} v_i$), then the properties (I),(II),(III) can be written as

(I)′ (positivity preserving) $Tv \geqslant 0$ if $v \geqslant 0$;
(II)′ (trace-preserving) $\mathrm{Tr}(Tv) = \mathrm{Tr}(v) \quad \forall v \in \mathbb{R}^n$;
(III)′ (unital) $Te = e$.

Let $x \in \mathbb{R}^n$ be a vector. We define $x^{\downarrow}$ as a vector with the same components in a decreasing order so that

$$x_1^{\downarrow} \geqslant x_2^{\downarrow} \geqslant \cdots \geqslant x_n^{\downarrow}.$$

Definition 2.3: x is more mixed (more chaotic,…) than y (denoted by $x \succ y$) if and only if

$$x_1^{\downarrow} \leqslant y_1^{\downarrow},$$

$$x_1^{\downarrow} + x_2^{\downarrow} \leqslant y_1^{\downarrow} + y_2^{\downarrow},$$

$$\cdots,$$

$$x_1^{\downarrow} + \cdots + x_{n-1}^{\downarrow} \leqslant y_1^{\downarrow} + \cdots + y_{n-1}^{\downarrow},$$

$$x_1^{\downarrow} + \cdots + x_n^{\downarrow} = y_1^{\downarrow} + \cdots + y_n^{\downarrow}.$$

For example, if $(\rho_1, \ldots, \rho_n)$ is a density vector then

$$\left(\frac{1}{n}, \frac{1}{n}, \ldots, \frac{1}{n}\right) \succ (\rho_1, \ldots, \rho_n) \succ (1,0, \ldots, 0,0).$$

The relation $\succ$ is a preordering but not a partial ordering. If $x \succ y$ and $y \succ x$ then $x = Ty$ for some permutation matrix T.

Theorem 2.1:

$$x \succ y \Leftrightarrow x = Ty \text{ where } T \text{ is doubly stochastic}.$$

Definition 2.4 (see Ref. 31 pp. 14 and 54): A real-valued function f defined on a set $\mathcal{A} \subset \mathbb{R}^n$ is said to be Schur-increasing on $\mathcal{A}$ if

$$x \succ y \text{ on } \mathcal{A} \Rightarrow \quad f(x) \geqslant f(y).$$

If, in addition, $f(x) > f(y)$ whenever $x \succ y$ but x is not a permutation of y, then f is said to be strictly Schur-increasing. Similarly f is said to be Schur-decreasing on $\mathcal{A}$ if

$$x \succ y \text{ on } \mathcal{A} \Rightarrow f(x) \leqslant f(y),$$

and f is strictly Schur-decreasing if strict inequality $f(x) < f(y)$ holds when x is not a permutation of y.

Of course, f is Schur-increasing if and only if $-f$ is Schur-decreasing.

Remark 2.1 (see Ref. 31, p. 54): $\mathcal{A} \subset \mathbb{R}^n$ is symmetric if $x \in \mathcal{A} \Rightarrow \Pi x \in \mathcal{A}$ for all permutations Π. A function f is symmetric on $\mathcal{A}$ if $f(x) = f(\Pi x)$ for all permutations Π. Let $\mathcal{D} := \{x | x_1 \geqslant \cdots \geqslant x_n\}$. If f is symmetric on a symmetric set $\mathcal{A}$ and Schur-increasing on $\mathcal{D} \cap \mathcal{A}$, then f is Schur-increasing on $\mathcal{A}$.

Remark 2.2: Let us consider the following identification $I: (0, \pi/2) \to \mathcal{P}_2^1$ defined by $I(\theta) := (\cos^2\theta, \sin^2\theta)$. Evidently, if $\theta_1, \theta_2 \leqslant \pi/4$, then

$$\theta_1 \leqslant \theta_2 \Leftrightarrow I(\theta_1) \prec I(\theta_2).$$

Any function on $\mathcal{P}_2^1$ can be seen as a function on $(0, \pi/2)$. By abuse of language we shall use the same symbols to denote the two functions. Since $\mathcal{P}_2^1$ is symmetric we have, because of Remark 2.1

Proposition 2.2: A symmetric function f on $\mathcal{P}_2^1$ is Schur-increasing if and only if f is increasing as a function on $(0, \pi/4)$.

B. Noncommutative case

Let M_n be the space of complex $n \times n$ matrices. We shall denote by H_n the real subspace of Hermitian matrices, by $\mathcal{D}_n$ the manifold of strictly positive elements of M_n, and by $\mathcal{D}_n^1 \subset \mathcal{D}_n$ the submanifold of density matrices, namely

Definition 2.5:

$$\mathcal{D}_n^1 := \{\rho \in M^n | \mathrm{Tr}\ \rho = 1,\ \rho > 0\}.$$

If $A \in M_n$, let $\lambda(A)$ be the n-vector of its eigenvalues, arranged in any order with multiplicities counted. If A is Hermitian then $\lambda(A)$ is a real n-vector. Let A, B be Hermitian.

Definition 2.6:

$$A \succ B \Leftrightarrow \lambda(A) > \lambda(B).$$

Definition 2.7: A linear map Φ on M_n is doubly stochastic if it is positive-preserving, trace-preserving, and unital.

Theorem 2.3:

$$A \succ B \Leftrightarrow A = \Phi(B), \textit{where } \Phi \textit{ is doubly stochastic}.$$

Definition 2.8: A real-valued function f defined on a set $\mathcal{A} \subset H_n$ is said to be Schur-increasing on $\mathcal{A}$ if

$$A \succ B \Rightarrow f(A) \geqslant f(B).$$

Similarly, f is said to be Schur-decreasing on $\mathcal{A}$ if

$$A \succ B \Rightarrow f(A) \leqslant f(B).$$

Of course, f is Schur-increasing if and only if $-f$ is Schur-decreasing.

III. PULL-BACK OF DUALITY PAIRINGS

To make the paper self-contained, we recall some constructions from Ref. 18.

Let V, W be vector spaces over $\mathbb{R}$ (or $\mathbb{C}$). One can say that there is a duality pairing if there exists a separating bilinear form

$$\langle \cdot, \cdot \rangle : V \times W \to \mathbb{R}.$$

Let $\mathcal{M}, \mathcal{N}, \widetilde{\mathcal{N}}$ be differentiable manifolds.

Definition 3.1: Suppose we have a pair of immersions (φ, χ), where $\varphi : \mathcal{M} \to \mathcal{N}$ and $\chi : \mathcal{M} \to \widetilde{\mathcal{N}}$, such that a duality pairing exists between $T_{\varphi(\rho)}\mathcal{N}$ and $T_{\chi(\rho)}\widetilde{\mathcal{N}}$ for any $\rho \in \mathcal{M}$. Then, we may pull-back this pairing on $\mathcal{M}$ by defining

$$\langle u, v \rangle_\rho^{\varphi,\chi} := \langle D_\rho \varphi(u), D_\rho \chi(u) \rangle, \quad u, v \in T_\rho \mathcal{M}.$$

The most elementary example is given by the case where $\mathcal{N} = \widetilde{\mathcal{N}}$ is a Riemannian manifold, $\varphi = \chi$, and the duality pairing is just given by the Riemannian scalar product on $T_{\varphi(\rho)}\mathcal{N}$ (this is the pull-back metric induced by the map φ).

A nontrivial example is the following. Let X be a uniformly convex Banach space such that the dual $\widetilde{X}$ is uniformly convex. We denote by $\langle \cdot, \cdot \rangle$ the standard duality pairing between X and $\widetilde{X}$. Let $J : X \to \widetilde{X}$ be the duality mapping, that is J is the differential of the map $v \to \frac{1}{2}\|v\|^2$. $J(v)$ is the unique element of the dual such that $\langle v, J(v) \rangle = \|v\|^2 = \|J(v)\|^2$.

Definition 3.2: Let $\mathcal{M}$ be a manifold. If we have a map $\varphi : \mathcal{M} \to X$ we can consider a dualized pull-back that is a bilinear form defined on the tangent space of $\mathcal{M}$ by

$$\langle A, B \rangle_\rho^\varphi := \langle A, B \rangle_\rho^{\varphi, J \circ \varphi} = \langle D_\rho \varphi(A), D_\rho (J \circ \varphi)(B) \rangle.$$

Example 3.1: For X a Hilbert space, J is the identity, and this is again the definition of pull-back metric induced by the map φ.

In what follows, if $p \in \mathbb{R} \setminus \{0\}$ then $\tilde{p}$ is defined by $(1/p) + (1/\tilde{p}) = 1$. If $p = 1$ then $\tilde{p} = +\infty$.

Example 3.2: Let $(X, \mathcal{F}, \mu)$ be a measure space. If f is a measurable function and $p \in (1, +\infty)$ then $\|f\|_p := (\int |f|^p d\mu)^{1/p}$. Set

$$L^p = L^p(X,\mathcal{F},\mu) = \{f \text{ is measurable and } \|f\|_p < \infty\}.$$

Define N^p as L^p with the norm

$$\|f\|_{N^p} := \frac{\|f\|_p}{p}.$$

Obviously $\tilde{N^p}$ (the dual of N^p) can be identified with $N^{\tilde{p}}$.

Now, suppose that $\rho > 0$ is measurable and $\int \rho = 1$, namely ρ is a strictly positive density. Then, $v = p\rho^{1/p}$ is an element of the unit sphere of N^p and it is easy to see that $J(v) = \tilde{p}\rho^{1/p}$. The family of maps $\rho \to p\rho^{1/p}$ is known as Amari embeddings.

Let $X = \{1, \ldots, n\}$ and let μ be the counting measure. In this case N^p is just $\mathbb{R}^n$ with the norm $\|\cdot\|_p / p$.

Proposition 3.1: Consider the Amari embedding $\varphi: \rho \in \mathcal{P}_n^1 \to p\rho^{1/p} \in N^p$ *for an arbitrary* $p \in (1, +\infty)$. *Then, the bilinear form*

$$\langle A,B\rangle_\rho^\varphi := \langle A,B\rangle_\rho^{\varphi, J\circ\varphi} = \langle D_\rho\varphi(A), D_\rho(J\circ\varphi)(B)\rangle, \quad A,B \in T_\rho\mathcal{P}_n^1,$$

is just the Fisher information.

Proof:

$$\langle D_\rho\varphi(A), D_\rho(J\circ\varphi)(B)\rangle = \int (\rho^{(1/p)-1}A)(\rho^{(1/p)-1}B) = \int \frac{AB}{\rho}.$$

□

The above result can be stated in much greater generality using the machinery of Refs. 19 and 14.

IV. SCALAR CURVATURE OF α-GEOMETRIES

The α-geometries are one of the fundamental objects of information geometry (see Refs. 2 and 20). The study of the monotonicity of their curvatures does not appear in the literature as far as we know. In this section we start such an investigation.

A. The plane case

Definition 4.1: The α*-geometry on* $\mathcal{P}_2^1$ *is the pull-back geometry induced by the map* $A_p(\rho): \mathcal{P}_2^1 \to \mathbb{R}^2$ *defined by*

$$A_p(\rho) := \begin{cases} p\rho^{1/p}, & p \in \mathbb{R}\setminus\{0\}, \\ \log(\rho), & p = \infty, \end{cases}$$

where $p = 2/(1-\alpha)$.

Definition 4.2: We denote by $c_p(\rho)$ *the curvature of the* α*-geometry* [*with* $p = 2/(1-\alpha)$] *at the point* $\rho \in \mathcal{P}_2^1$.

Remark 4.1: For the curvature $c_p(\cdot)$ there are two easy cases:

—if $p = 1$ then $c_p(\cdot) = \text{const} = 0$;

—if $p = 2$ then $c_p(\cdot) = \text{const} = \frac{1}{2}$.

Taking a look at the unit sphere of $\mathbb{R}^2$ with respect to the L^p-norm, one can easily understand the following general result.

Theorem 4.1: *For the function* $c_p(\cdot): \mathcal{P}_2^1 \to R$ *one has the following properties*:

—*if* $p \in (1,2)$ *then* $c_p(\cdot)$ *is a strictly Schur-decreasing function*;

—*if* $p \in (2, +\infty]$ *then* $c_p(\cdot)$ *is a strictly Schur-increasing function.*

Proof: Let us first consider $p \in (1,\infty)$. Then, the α-geometry, $\alpha = (p-2)/p$, on $\mathcal{P}_2^1$ is the geometry of the set

$$\mathcal{B}:=\left\{(x,y)\in\mathbb{R}^2:\left(\frac{x}{p}\right)^p+\left(\frac{y}{p}\right)^p=1,\quad x>0,\quad y>0\right\}.$$

Let us introduce the parametrization

$$x=p(\cos\ \vartheta)^{2/p},\quad y=p(\sin\ \vartheta)^{2/p},\quad 0<\vartheta<\frac{\pi}{2}.$$

Then

$$x'=2(\cos\ \vartheta)^{(2/p)-1}(-\sin\ \vartheta),\quad y'=2(\sin\ \vartheta)^{(2/p)-1}\cos\ \vartheta,$$

$$x''=2(\cos\ \vartheta)^{(2/p)-2}\left(\frac{2}{p}\sin^2\ \vartheta-1\right),\quad y''=2(\sin\ \vartheta)^{(2/p)-2}\left(\frac{2}{p}\cos^2\ \vartheta-1\right).$$

Let us parametrize density vectors as $(\cos^2\ \theta,\sin^2\ \vartheta)$. In this way the curvature of α-geometry at the point ρ, namely $c_p(\rho)$, is

$$\begin{aligned}c_p(\vartheta):&=\frac{|x'y''-x''y'|}{[(x')^2+(y')^2]^{3/2}}=\frac{p-1}{p}\frac{(\sin\ \vartheta\cos\ \vartheta)^{(2/p)+2}}{[(\sin\ \vartheta(\cos\ \vartheta)^{1/p})^4+((\sin\ \vartheta)^{1/p}\cos\ \vartheta)^4]^{3/2}}\\&=\frac{p-1}{p}\left(\frac{1}{2}\right)^{2[1-(2/p)]}\cdot\frac{(\sin 2\vartheta)^{2[1-(2/p)]}}{[(\cos\ \vartheta)^{4/\tilde{p}}+(\sin\ \vartheta)^{4/\tilde{p}}]^{3/2}}=A_p\cdot\frac{g_p(\vartheta)}{f_p(\vartheta)^{\frac{3}{2}}},\end{aligned}$$

where we set

$$A_p:=\frac{p-1}{p}\left(\frac{1}{2}\right)^{2[1-(2/p)]},$$

$$g_p(\vartheta):=(\sin 2\vartheta)^{2-(4/p)},$$

$$f_p(\vartheta):=(\cos\ \vartheta)^{4/\tilde{p}}+(\sin\ \vartheta)^{4/\tilde{p}}.$$

We want to compute the monotonicity properties of c_p with respect to the preordering $>$. We have

$$g_p'(\vartheta):=4(\sin 2\vartheta)^{1-(4/p)}\cdot(\cos\ \vartheta+\sin\ \vartheta)\left(1-\frac{2}{p}\right)(\cos\ \vartheta-\sin\ \vartheta);$$

since $0<\vartheta<\pi/2$, then

$$4(\sin 2\vartheta)^{1-(4/p)}\cdot(\cos\ \vartheta+\sin\ \vartheta)>0,$$

and therefore

$$g_p'(\vartheta)>0\Leftrightarrow\left(1-\frac{2}{p}\right)(\cos\ \vartheta-\sin\ \vartheta)>0.$$

Moreover

$$f_p'(\vartheta)=\frac{4}{\tilde{p}}\sin\ \vartheta\cos\ \vartheta((\sin\ \vartheta)^{(2/\tilde{p})-1}+(\cos\ \vartheta)^{(2/\tilde{p})-1})((\sin\ \vartheta)^{(2/\tilde{p})-1}-(\cos\ \vartheta)^{(2/\tilde{p})-1});$$

again, since $0<\vartheta<\pi/2$, then

$$4\sin\ \vartheta\cos\ \vartheta((\sin\ \vartheta)^{(2/\tilde{p})-1}+(\cos\ \vartheta)^{(2/\tilde{p})-1})>0,$$

and therefore

$$f_p'(\vartheta) > 0 \Leftrightarrow \frac{1}{\tilde{p}}((\sin\ \vartheta)^{(2/\tilde{p})-1} - (\cos\ \vartheta)^{(2/\tilde{p})-1}) > 0.$$

$c_p(\cdot)$ is evidently symmetric on $\mathcal{P}_2^1$ and therefore (because of Proposition 2.2) the fact that the curvature is strictly Schur-increasing (decreasing) is equivalent to the fact that $c_p(\vartheta)$ is strictly increasing (decreasing) for $0<\vartheta<\pi/4$.

We have the following cases:

Case: $1<p<2$.

This implies $1-(2/p)<0, (2/\tilde{p})-1<0$, and therefore

$$g_p'(\vartheta) > 0 \Leftrightarrow \cos\ \vartheta < \sin\ \vartheta \Leftrightarrow \frac{\pi}{4} < \vartheta < \frac{\pi}{2},$$

$$f_p'(\vartheta) > 0 \Leftrightarrow (\sin\ \vartheta)^{(2/\tilde{p})-1} > (\cos\ \vartheta)^{(2/\tilde{p})-1} \Leftrightarrow \sin\ \vartheta < \cos\ \vartheta \Leftrightarrow 0 < \vartheta < \frac{\pi}{4}.$$

Therefore, for $0<\vartheta<\pi/4$, g is decreasing, f is increasing, and $1/f^{3/2}$ is decreasing. This implies that

$$c_p = A_p \frac{g_p}{f_p^{3/2}}$$

is strictly decreasing for $0<\vartheta<\pi/4$.

Case: $2<p<\infty$.

This implies $1-(2/p)>0, (2/\tilde{p})-1>0$, and therefore

$$g_p'(\vartheta) > 0 \Leftrightarrow \cos\ \vartheta > \sin\ \vartheta \Leftrightarrow 0 < \vartheta < \frac{\pi}{4},$$

$$f_p'(\vartheta) > 0 \Leftrightarrow (\sin\ \vartheta)^{(2/\tilde{p})-1} > (\cos\ \vartheta)^{(2/\tilde{p})-1} \Leftrightarrow \sin\ \vartheta > \cos\ \vartheta \Leftrightarrow \frac{\pi}{4} < \vartheta < \frac{\pi}{2}.$$

Therefore, for $0<\vartheta<\pi/4$, g is increasing, f is decreasing, and $1/f^{3/2}$ is increasing. This implies that

$$c_p = A_p \frac{g_p}{f_p^{3/2}}$$

is strictly increasing for $0<\vartheta<\pi/4$.

Case: $p=\infty$.

Use now the following parametrization:

$$x = 2\ \log(\cos\ \theta), \quad y = 2\ \log(\sin\ \theta),$$

for the curve $e^x+e^y=1$. Then

$$x' = -2\frac{\sin\ \theta}{\cos\ \theta}, \quad y' = 2\frac{\cos\ \theta}{\sin\ \theta},$$

$$x'' = \frac{-2}{\cos^2\ \theta}, \quad y'' = \frac{-2}{\sin^2\ \theta},$$

$$c_\infty(\vartheta) := \frac{|x'y'' - x''y'|}{[(x')^2 + (y')^2]^{3/2}} = \frac{(\sin\ \theta \cos\ \theta)^2}{[(\cos\ \theta)^4 + (\sin\ \theta)^4]^{3/2}}$$
$$= \lim_{p\to+\infty} \frac{p-1}{p}\left(\frac{1}{2}\right)^{2[1-(2/p)]} \cdot \frac{(\sin 2\vartheta)^{2[1-(2/p)]}}{[(\cos\ \vartheta)^{4/\tilde{p}} + (\sin\ \vartheta)^{4/\tilde{p}}]^{3/2}}.$$

Note that

$$c_\infty(\vartheta) = \lim_{p\to+\infty} c_p(\theta).$$

If we set

$$g_\infty(\vartheta) := (\sin\ \theta \cos\ \theta)^2, \quad f_\infty(\vartheta) := (\cos\ \theta)^4 + (\sin\ \theta)^4,$$

then

$$g'_\infty(\vartheta) = 2 \sin\ \vartheta \cos\ \vartheta(\cos\ \vartheta + \sin\ \vartheta)(\cos\ \vartheta - \sin\ \vartheta),$$

$$f'_\infty(\vartheta) = 4 \sin\ \vartheta \cos\ \vartheta(\cos\ \vartheta + \sin\ \vartheta)(\sin\ \vartheta - \cos\ \vartheta).$$

This implies

$$g'_\infty(\vartheta) > 0 \Leftrightarrow \cos\ \vartheta > \sin\ \vartheta,$$

$$f'_\infty(\vartheta) > 0 \Leftrightarrow \sin\ \vartheta > \cos\ \vartheta.$$

We have the same situation of the case $2<p<\infty$ and therefore the same conclusion.

This ends the proof. □

Note that we have also

Proposition 4.2: For the function $c_p(\cdot):\mathcal{P}_2^1 \to \mathbb{R}$ *one has the following properties: if* $p \in (-\infty, 0)$ *then* $c_p(\cdot)$ *is strictly Schur-increasing.*

Proof: Since

$$1 - \frac{2}{p} > 0, \quad \frac{2}{\tilde{p}} - 1 > 1 > 0, \quad 0 < \tilde{p} < 1,$$

we have the same situation of the case $2<p<\infty$ in the preceding Theorem 4.1 and therefore the same conclusion. □

If $p \in (0,1)$ then $c_p(\cdot)$ can have an arbitrary behavior (Schur-increasing, Schur-decreasing, neither of the two).

B. The general case

Definition 4.3: The α*-geometry on* $\mathcal{P}_n^1$ *is the pull-back geometry induced by the map* $A_p(\rho):\mathcal{P}_n^1 \to \mathbb{R}^n$ *defined by*

$$A_p(\rho) := \begin{cases} p\rho^{1/p}, & p \in \mathbb{R}\setminus\{0\}, \\ \log(\rho), & p = \infty, \end{cases}$$

where $p = 2/(1-\alpha)$.

Definition 4.4: We denote by $\mathrm{Scal}_p(\rho)$ *the scalar curvature of the* α*-geometry* [*with* $p = (2/(1-\alpha))$] *at the point* $\rho \in \mathcal{P}_n^1$.

Of course the cases $p=1$ (flat geometry) and $p=2$ (geometry of a $(n-1)$-dimensional sphere with radius 2) are easy to study. One has

—if $p=1$ then $\mathrm{Scal}_p(\cdot) = \mathrm{const} = 0$;

—if $p=2$ then $\mathrm{Scal}_p(\cdot) = \mathrm{const} = \frac{1}{4}(n-1)(n-2)$.

Again taking a look at the unit sphere of $\mathbb{R}^n$ equipped with L^p-norm, one can easily understand the following conjecture.

Conjecture 4.1: Suppose $n>2$. *For the function* $\mathrm{Scal}_p(\cdot):\mathcal{P}_n^1\to R$ *one has the following properties:*

—*if* $p\in(1,2)$ *then* $\mathrm{Scal}_p(\cdot)$ *is a strictly Schur-decreasing function*;

—*if* $p\in(2,+\infty]$ *then* $\mathrm{Scal}_p(\cdot)$ *is a strictly Schur-increasing function*.

C. Non-commutative case

Definition 4.5: The α*-geometry on* $\mathcal{D}_n^1$ *is the geometry induced by the pull-back of the map* $A_p(\rho):\mathcal{D}_n^1\to M_n$ *defined by*

$$A_p(\rho):=\begin{cases}p\rho^{1/p}, & p\in\mathbb{R}\setminus\{0\},\\ \log(\rho), & p=\infty,\end{cases}$$

where $p=2/(1-\alpha)$.

Since the commutativity or noncommutativity of the context will always be clear, we perform a little abuse of language in the following definition.

Definition 4.6: We denote by $\mathrm{Scal}_p(\rho)$ *the scalar curvature of the* α*-geometry* [*with* $p=(2/(1-\alpha))$] *at the point* $\rho\in\mathcal{D}_n^1$.

Again, the case $p=1$ (flat geometry) is obvious. The case $p=2$ is known (see Refs. 16 and 17 or Theorem 7.2 below), and we have

—if $p=1$ then $\mathrm{Scal}_p(\cdot)=\mathrm{const}=0$;

—if $p=2$ then $\mathrm{Scal}_p(\cdot)=\mathrm{const}=\frac{1}{4}(n^2-1)(n^2-2)$.

Motivated by the commutative plane case we formulate the following conjecture.

Conjecture 4.2: Suppose $n\geqslant 2$. *For the function* $\mathrm{Scal}_p(\cdot):\mathcal{D}_n^1\to\mathbb{R}$ *one has the following properties:*

—*if* $p\in(1,2)$ *then* $\mathrm{Scal}_p(\cdot)$ *is a strictly Schur-decreasing function*;

—*if* $p\in(2,+\infty]$ *then* $\mathrm{Scal}_p(\cdot)$ *is a strictly Schur-increasing function*.

V. MONOTONE METRICS AND THEIR SCALAR CURVATURES

A commutative Markov morphism $T:\mathbb{R}^n\to\mathbb{R}^m$ is a stochastic map. A noncommutative Markov morphism is a linear map $T:M_n\to M_m$ that is completely positive and trace-preserving (note that in the commutative case complete positivity is equivalent to positivity; see, for example, Ref. 41).

In the commutative case a monotone metric is a family of Riemannian metrics $g=\{g^n\}$ on $\{\mathcal{P}_n^1\}$, $n\in\mathbb{N}$ such that

$$g^m_{T(\rho)}(TX,TX)\leqslant g^n_\rho(X,X)$$

holds for every Markov morphism $T:\mathbb{R}^n\to\mathbb{R}^m$ and all $\rho\in\mathcal{P}_n^1$ and $X\in T_\rho\mathcal{P}_n$.

In perfect analogy, a monotone metric in the noncommutative case is a family of Riemannian metrics $g=\{g^n\}$ on $\{\mathcal{D}_n^1\}$, $n\in\mathbb{N}$ such that

$$g^m_{T(\rho)}(TX,TX)\leqslant g^n_\rho(X,X)$$

holds for every Markov morphism $T:M_n\to M_m$ and all $\rho\in\mathcal{D}_n^1$ and $X\in T_\rho\mathcal{D}_n^1$.

Let us recall that a function $f:(0,\infty)\to\mathbb{R}$ is called an operator monotone if for any $n\in\mathbb{N}$, any A, $B\in M_n$ such that $0\leqslant A\leqslant B$, the inequalities $0\leqslant f(A)\leqslant f(B)$ hold. An operator monotone function is said to be symmetric if $f(x)=xf(x^{-1})$ and normalized if $f(1)=1$. In what follows, by operator monotone we mean normalized symmetric operator monotone. With each operator monotone function f one associates also the so-called Chentsov–Morotzova function

$$c_f(x,y) := \frac{1}{yf\left(\frac{x}{y}\right)} \quad \text{for } x,y>0.$$

Define $L_\rho(A) := \rho A$, and $R_\rho(A) := A\rho$. Since L_ρ, R_ρ commute we may define $c(L_\rho, R_\rho)$. Now, we can state the fundamental theorems about monotone metrics (uniqueness and classification are up to scalars).

Theorem 5.1 (Ref. 10): *There exists a unique monotone metric on $\mathcal{P}_n^1$ given by the Fisher information.*

Theorem 5.2 (Ref. 35): *There exists a bijective correspondence between monotone metrics on $\mathcal{D}_n^1$ and operator monotone functions given by the formula*

$$\langle A,B\rangle_{\rho,f} := \mathrm{Tr}(A\cdot c_f(L_\rho,R_\rho)(B)).$$

To state the general formula for the scalar curvature of a monotone metric we need some auxiliary functions. In what follows $c', (\log c)'$ denote derivatives with respect to the first variable, and $c=c_f$.

$$h_1(x,y,z) := \frac{c(x,y)-zc(x,z)c(y,z)}{(x-z)(y-z)c(x,z)c(y,z)},$$

$$h_2(x,y,z) := \frac{(c(x,z)-c(y,z))^2}{(x-y)^2c(x,y)c(x,z)c(y,z)},$$

$$h_3(x,y,z) := z\frac{(\ln c)'(z,x)-(\ln c)'(z,y)}{x-y},$$

$$h_4(x,y,z) := z(\ln c)'(z,x)(\ln c)'(z,y),$$

$$h := h_1 - \tfrac{1}{2}h_2 + 2h_3 - h_4. \tag{5.1}$$

The functions h_i have no essential singularities if arguments coincide.

Note that $\langle A,B\rangle_\rho^f := \mathrm{Tr}(A\cdot c_f(L_\rho,R_\rho)(B))$ defines a Riemannian metric also over $\mathcal{D}_n$ ($\mathcal{D}_n^1$ is a submanifold of codimension 1). Let $\mathrm{Scal}_f(\rho)$ be the scalar curvature of $(\mathcal{D}_n,\langle\cdot,\cdot\rangle_\rho^f)$ at ρ and $\mathrm{Scal}_f^1(\rho)$ be the scalar curvature of $(\mathcal{D}_n^1,\langle\cdot,\cdot\rangle_\rho^f)$.

Theorem 5.3 (Ref. 12): *Let $\sigma(\rho)$ be the spectrum of ρ. Then*

$$\mathrm{Scal}_f(\rho) = \sum_{x,y,z\in\sigma(\rho)} h(x,y,z) - \sum_{x\in\sigma(\rho)} h(x,x,x),$$

$$\mathrm{Scal}_f^1(\rho) = \mathrm{Scal}_f(\rho) + \tfrac{1}{4}(n^2-1)(n^2-2).$$

These results have the following form in the simplest case (2×2 matrices). From Theorem 5.3 it follows that (see Ref. 3)

Corollary 5.4: If $\rho\in D_2$ has eigenvalues λ_1,λ_2, one has

$$\mathrm{Scal}(\rho) = h(\lambda_1,\lambda_1,\lambda_2) + h(\lambda_1,\lambda_2,\lambda_1) + h(\lambda_2,\lambda_1,\lambda_1) + h(\lambda_2,\lambda_2,\lambda_1) + h(\lambda_2,\lambda_1,\lambda_2) + h(\lambda_1,\lambda_2,\lambda_2) + \tfrac{3}{2}.$$

Theorem 5.5 (Ref. 3): *If $\rho\in D_2$ has eigenvalues λ_1,λ_2, and $a=2\lambda_1-1$, then*

$$r_f(a) := \mathrm{Scal}_f(\rho) = \frac{14(a-1)\left[f'\left(\frac{1-a}{1+a}\right)\right]^2}{(1+a)^3\left[f\left(\frac{1-a}{1+a}\right)\right]^2} + \frac{2(a^2+7a-6)f'\left(\frac{1-a}{1+a}\right)}{(1+a)^2 a f\left(\frac{1-a}{1+a}\right)} + \frac{8(1-a)f''\left(\frac{1-a}{1+a}\right)}{(1+a)^3 f\left(\frac{1-a}{1+a}\right)} + \frac{2(1+a)f\left(\frac{1-a}{1+a}\right)}{a^2} + \frac{3a^3+5a^2+8a-4}{2(1+a)a^2}.$$

VI. THE WYD METRICS

We are going to study a particular class of monotone metrics.

Definition 6.1:

$$f_p(x) := \frac{1}{p\tilde{p}} \cdot \frac{(x-1)^2}{(x^{1/p}-1)(x^{1/\tilde{p}}-1)}, \quad p \in \mathbb{R}\setminus\{0,1\},$$

$$f_1(x) = f_\infty(x) := \frac{x-1}{\log(x)}, \quad p = 1,\infty.$$

Obviously $f_p = f_{\tilde{p}}$ and

$$f_1 = \lim_{p\to 1} f_p = \lim_{p\to\infty} f_p = f_\infty.$$

Theorem 6.1 (Refs. 22 and 23): *The function f_p is operator monotone if and only if $p \in A := (-\infty,-1]\cup\left[\frac{1}{2},+\infty\right]$.*

Note that $p \in A$ if and only if $\alpha \in [-3,3]$.

Definition 6.2: The WYD(p) metric of parameter p is the monotone metric associated with f_p (where $p \in A$).

We have that f_{-1} is the function of the RLD-metric, $f_1 = f_\infty$ is the function of the BKM-metric, and f_2 is the function of the Wigner–Yanase metric.

In what follows $p \in (1,+\infty)$ and we use again the symbol N_p to denote M_n with the norm

$$\|A\|_{N^p} = p^{-1}(\mathrm{Tr}(|A|^p))^{1/p}.$$

All the commutative construction of Example 3.2 goes through. The following Proposition is the noncommutative analogous of Proposition 3.1 (see also Refs. 16, 21, 23, 28, and 37).

Proposition 6.2 (Ref. 18): Let $\varphi: \rho \in \mathcal{D}_n^1 \to p\rho^{1/p} \in N_p$ be the Amari embedding. The dualized pull-back

$$\langle A,B\rangle_\rho^\varphi := \langle A,B\rangle_\rho^{\varphi, J\circ\varphi} = \langle D_\rho\varphi(A), D_\rho(J\circ\varphi)(B)\rangle$$

coincides with the Wigner–Yanase–Dyson information.

VII. KNOWN RESULTS ON MONOTONICITY

In this short section we review what is known about monotonicity of scalar curvature for monotone metrics. This is useful to emphasize that, up to now, no examples exist of a monotone metrics with Schur-increasing (or Schur-decreasing) scalar curvature.

The Bures or SLD metric is the monotone metric associated with the function $f=(1+x)/2$.

Theorem 7.1 (Refs. 11 and 13): *The scalar curvature of SLD metric is neither Schur-increasing nor Schur-decreasing.*

Proof: By Ref. 11 the SLD-metric has a global minimum at the most mixed state for any n. On

the other hand (this is due to Ref. 13), if $\sigma=\mathrm{diag}(\frac{2}{9},\frac{1}{9},\frac{2}{3})$ and $\rho=\mathrm{diag}(\frac{1}{6},\frac{1}{6},\frac{2}{3})$ then $\rho\succ\sigma$. Using Theorem 5.3 one can calculate $\mathrm{Scal}(\sigma)=3078/25>3447/28=\mathrm{Scal}(\rho)$ and so the conclusion follows. □

Theorem 7.2 (Ref. 17): *The scalar curvature of WY metric is a constant equal to* $\frac{1}{4}(n^2-1)\times(n^2-2)$.

VIII. A CONJECTURE ON THE WYD SCALAR CURVATURE AND ITS RELATION TO PETZ CONJECTURE

In this section we want to suggest that a whole family of monotone metrics with Schur-increasing scalar curvature may exist.

Conjecture 8.1: There exist $\varepsilon>0$ *such that for* p *in the interval* $I:=(1,1+\varepsilon)$ *the scalar curvature of the* WYD(p) *metrics is a Schur-increasing function.*

Conjecture 8.2 (Petz conjecture): The scalar curvature of BKM metric is a Schur-increasing function. This can be rephrased as

$$\rho\succ\sigma\Rightarrow \mathrm{Scal}_{f_1}(\rho)\geqslant \mathrm{Scal}_{f_1}(\sigma).$$

The motivations for Conjecture 8.1 are the following. The WYD(p) metrics come from the dualized pull-back of Proposition 6.2. This means that the WYD(p) metrics depend, indeed, on the pair $(p,\tilde{p})$. Note that when p is in the Schur-decreasing region $(1,2)$ we have that $\tilde{p}$ is in the Schur-increasing region $(2,+\infty)$ (Theorem 4.1, Conjectures 4.1, 4.2). When p approaches 1 then $\tilde{p}$ goes to infinity. Near the boundary values $\{1,+\infty\}$ the increasing–decreasing "symmetry" should be broken: in this case WYD(p) geometry comes from a geometry converging to a flat limit ($p\to1$) and a geometry converging to a (conjectured) Schur-increasing scalar curvature ($\tilde{p}\to\infty$).

Theorem 8.1: *If Conjecture 8.1 is true then Conjecture 8.2 (Petz conjecture) is true.*

Proof: For an arbitrary manifold M let us denote by $\mathcal{M}(M)$ the manifold of Riemannian metrics of M. If $\rho\in M$ is fixed and $g\in\mathcal{M}(M)$ then the function $F_\rho(\cdot):\mathcal{M}(M)\to\mathbb{R}$ defined by $F_\rho(g):=\mathrm{Scal}_g(\rho)$ is a smooth function (see Refs. 29 and 33). Identifying f_p with the metric

$$\langle A,B\rangle_{\rho,f_p}:=\mathrm{Tr}(Ac_{f_p}(L_\rho,R_\rho)(B)),$$

we may consider the function $p\to f_p$ as a continuous curve in $\mathcal{M}(\mathcal{D}_n^1)$. This implies that, by composition, the function $p\to\mathrm{Scal}_{f_p}(\rho)$ is a real, continuous function for each $\rho\in\mathcal{D}_n^1$. Suppose now that Conjecture 8.1 is true.

We have for arbitrary $\rho,\sigma\in\mathcal{D}_n^1$, such that $\rho\succ\sigma$

$$\mathrm{Scal}_{f_1}(\rho)=\lim_{p\to1}\mathrm{Scal}_{f_p}(\rho)\geqslant\lim_{p\to1}\mathrm{Scal}_{f_p}(\sigma)=\mathrm{Scal}_{f_1}(\sigma).$$

But, this is precisely the Petz conjecture. □

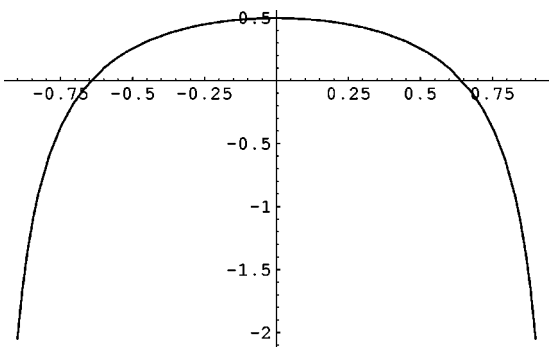

FIG. 1. Case $p=1+10^{-1}$.

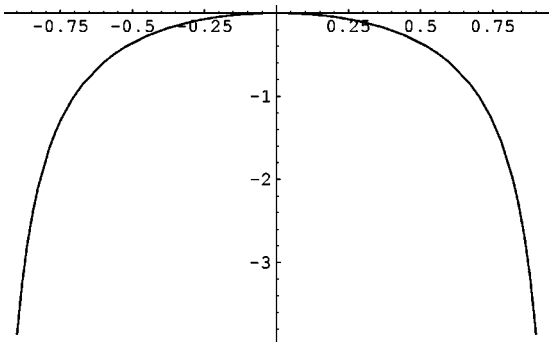

FIG. 2. Case $p=1+10^{-6}$.

A. Numerical results

Conjecture 8.1 would have many consequences. An example is the following theorem.

Theorem 8.2: *Conjecture 8.1 implies that there exists* $\varepsilon>0$ *such that for* $p\in(1,1+\varepsilon)$ *the functions* $r_p:=r_{f_p}$ *of Theorem 5.5 are concave and have their maximum at zero.*

Proof: It follows immediately by Theorem 5.5. □

Using MATHEMATICA, one has the following graphs for the function r_p:

Case $p=1+10^{-1}$; see Fig. 1;

Case $p=1+10^{-6}$; see Fig. 2.

Let us emphasize what we said in the Introduction: a recent result of Andai[3] shows the nontriviality of the above behavior. Indeed, also in the 2×2 case there exist many monotone metrics with nonincreasing scalar curvature.

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Large-time asymptotics for nonlinear diffusions: the initial-boundary value problem

F. Salvarani and G. Toscani
Dipartimento di Matematica, Università degli Studi di Pavia, Via Ferrata, 1 - 27100 Pavia, Italy

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In this paper we investigate the large-time behavior of solutions to the first initial-boundary value problem for the nonlinear diffusion $u_t=(u^m)_{xx}$, $m>0$. In particular, we prove exponential decay of $u(x,t)$ towards its own steady state in L^1-norm for long times and we give an explicit upper bound for the rate of decay. The result is based on a new application of entropy estimates, and on detailed lower bounds for the entropy production in this situation. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1828587]

I. INTRODUCTION

In recent years, entropy dissipation methods (also called *entropy–entropy production* methods) have been successfully applied to reckon decay rates towards equilibrium of weak solutions to Cauchy problems for nonlinear second- and fourth-order parabolic equations and their systems.[1,3,8–10,13,18]

However only rarely, at least to our knowledge, such strategies have been applied to the study of initial-boundary value problems with nonhomogeneous or nonperiodic boundary conditions.[17]

The main reason for this fact relies in the lack of mass conservation, which is one of the main ingredients to handle the problem and to obtain L^1 estimates from the entropy decay by means of Csiszár–Kullback inequalities.[2,12]

An entropy dissipation method to handle almost general Dirichlet boundary conditions will be developed in this paper. Our results show that entropy methods can be fruitfully applied also to initial-boundary value problems with nonhomogeneous Dirichlet boundary conditions.

In more details, we will be concerned with the large-time behavior of the solution to the initial-boundary value problem,

$$u_t(x,t) = [u^m(x,t)]_{xx}, \quad (x,t) \in \Omega \times (0,+\infty), \tag{1}$$

$$u(-L,t) = \varphi_-, \quad u(L,t) = \varphi_+, \tag{2}$$

$$u(x,0) = u_0(x) \tag{3}$$

in $\Omega=(-L,L)$, $L>0$, with $m>0$. The initial data $u_0(x)$ and the boundary conditions φ_+ and φ_- are non-negative real constants satisfying the hypotheses stated in the following definition.

Definition 1.1: The initial and boundary conditions of problem (1)–(3) are said to be admissible if and only if

(1) φ_+ *and* φ_- *are non-negative and* $(\varphi_+ + \varphi_-)>0$*;*
(2) $u_0(x) \in C([-L,L])$ *is a non-negative function which satisfies the compatibility conditions* $u_0(-L)=\varphi_-$ *and* $u_0(L)=\varphi_+$.

While the large-time behavior of solutions to the Cauchy problem for the nonlinear equation (1) was intensively studied for many years (cf. the excellent survey paper of Vázquez[19] and the references therein), the behavior of solutions to the initial-boundary value problem with nonho-

mogenous Dirichlet boundary conditions was less studied (see Refs. 4 and 7; results on the logarithmic nonlinearity can however be found in Ref. 6). Other related results in bounded domains deserve to be referred in. A complete study of the asymptotic behavior of solutions to the initial-Dirichlet problem with homogeneous boundary condition has been recently presented by Vázquez.[20] However, the techniques used there are different from ours. The question of the possible application of the entropy method to the study of the problem treated in Ref. 20 is to our knowledge open in higher dimensions. In dimension one, the analysis of the asymptotic behavior with homogeneous boundary conditions (namely when $\varphi_+ = \varphi_- = 0$) can be performed, by means of the entropy dissipation method, in a rather standard way. We focus therefore our attention only to the case when at least one of the boundary conditions does not vanish.

As we will discuss later on, our method works in the whole range $m > 0$, covering both the fast diffusion equation ($m < 1$) and the porous media equation ($m > 1$).

In order to study the large-time behavior, we shall analyze the time-decay of a suitable relative entropy, where the word "relative" means *relative to the steady state* of Eqs. (1)–(3).

The method introduced in this work, useful to handle second-order diffusions in one dimension, cannot be easily generalized due to a main fact. The entropy associated to the steady state is explicit as the steady state is; in the general case (higher dimensions or higher order diffusions), the steady states are not explicit nor are the entropy functionals. Therefore, the application of the entropy–entropy production method based on the knowledge of the derivative in time of the functional becomes rather difficult.

The results on the large-time behavior will be reached by steps.

The existence and uniqueness theorem for Eqs. (1)–(3) will be stated in Sec. II.

Section III deals with the study of the entropy functional for the same initial-boundary value problem. The sublinear case (i.e., $0 < m \leqslant 1$) and the superlinear case ($m > 1$) lead to different relative entropies, and are treated in a slightly different way. It is interesting to remark that, in the limit $m \to 1$, the entropy functionals of both the superlinear case and the sublinear cases coincide, but the rate of convergence obtained in the linear case as limit of the nonlinear case is worse than the rate obtained from a direct inspection.

The case of strictly positive initial-boundary conditions is considered in Sec. IV, where the rate of decay of the solution towards the steady state is discussed, both in the sublinear case and in the superlinear one.

Finally, the general case of non-negative initial-boundary conditions, obtained by removing the limitation on the data, is studied in Sec. V.

II. MAIN PROPERTIES OF THE SOLUTION

We will start the study of our problem by discussing the well posedness of equations (1)–(3) and the main properties of the solution. Following Ref. 14, the precise characterization of a weak solution to problem (1)–(3) is obtained by the following definition.

Definition 2.1: A function $u(x,t)$ defined on $\overline{\Omega} \times [0,T]$ is a weak solution of problem (1)–(3) if and only if

(1) *$u(x,t)$ is real, non-negative and continuous on $\overline{\Omega} \times [0,T]$;*
(2) *$u(-L,t) = \varphi_-$ and $u(L,t) = \varphi_+$ for all $t \in [0,T]$;*
(3) *$u^m(x,t)$ has a square-integrable generalized derivative with respect to x in $\Omega \times [0,T]$;*
(4) *$u(x,t)$ satisfies the identity*

$$\int_0^T \int_\Omega [(u^m)_x \phi_x - u\phi_t] \mathrm{d}x\, \mathrm{d}t = \int_\Omega \phi(x,0) u_0(x) \mathrm{d}x, \tag{4}$$

for all $\phi \in C(\overline{\Omega} \times [0,T]) \cap H^1(\Omega \times (0,T))$ which vanish for $|x| = L$ and for $t = T$.

The main result of this section is due to Gilding.[14–16] We remark that, as far as the well-posedness of (1)–(3) is concerned, more recent contributions are present in the literature. We refer

in particular to the paper of Bénilan and Touré,[5] where well-posedness is investigated in the framework of the nonlinear semigroup theory. Gilding proved (in a more general form) the following theorem.

Theorem 2.1: *Let us consider the initial-boundary value problem (1)–(3) with admissible (in the sense of Definition 1.1) non-negative initial data* $u(x,0)=u_0(x)\in C(\overline{\Omega})$ *and boundary conditions* $u(-L,t)=\varphi_-$ *and* $u(L,t)=\varphi_+$.

Then problem (1)–(3) has exactly one and only one non-negative weak solution $u(x,t)$.

Moreover, $u(x,t)$ *is a classical solution in a neighborhood of any point* $(x_0,t_0)\in\overline{\Omega}\times[0,T]$ *where* $u(x_0,t_0)>0$.

Finally, if we denote with $u_1(x,t)$ *and* $u_2(x,t)$ *two solutions of Eq. (1) with initial and boundary conditions* $u_{0,1}(x)$, $\varphi_-^{(1)}$, $\varphi_+^{(1)}$ *and* $u_{0,2}(x)$, $\varphi_-^{(2)}$, $\varphi_+^{(2)}$, *respectively,*

$$u_{0,1}(x)\leqslant u_{0,2}(x) \text{ for all } x\in\overline{\Omega}$$

and

$$\varphi_-^{(1)}\leqslant\varphi_-^{(2)},\quad \varphi_+^{(1)}\leqslant\varphi_+^{(2)},$$

imply $u_1(x,t)\leqslant u_2(x,t)$ *for all* $(x,t)\in\overline{\Omega}\times[0,T]$.

The stationary state for problem (1)–(3) can be easily found. We have the following lemma.

Lemma 2.1: Problem (1)–(2) admits one and only one stationary solution. This solution is given by

$$\overline{u^m}(x)=ax+b, \tag{5}$$

where

$$a=\frac{1}{2L}[\varphi_+^m-\varphi_-^m],\quad b=\frac{1}{2}[\varphi_+^m+\varphi_-^m].$$

Proof: The stationary solution of Eqs. (1)–(3) satisfies

$$\overline{u^m}(x)_{xx}=0 \quad \text{in } \Omega, \tag{6}$$

$$\overline{u}(-L)=\varphi_-,\quad \overline{u}(L)=\varphi_+. \tag{7}$$

Integration of (6), together with the use of boundary conditions (7) gives (5). □

Obviously, when $\varphi_+=\varphi_-=0$, we have that $\overline{u}(x)=0$ for all $x\in\overline{\Omega}$. Since this case can be easily solved directly, from now on we will suppose that at least one of the boundary conditions φ_+ or φ_- does not vanish.

III. THE ENTROPY FUNCTIONAL

In order to prove the exponential decay of the solution of problem (1)–(3), we will consider an auxiliary problem and use an entropy monotonicity approach.

We suppose from now on and until the end of Sec. IV that both the initial and boundary conditions are not allowed to take the value zero. If it were the case, we would consider a modified problem, obtained by lifting up the data in a suitable way, as we will see in Sec. V.

Let us define $f=u/\overline{u}$; by the hypotheses on φ_+ and φ_-, $\overline{u}(x)\neq 0$ for all $x\in\Omega$, so that f is always well defined.

It is immediate to show that f satisfies the initial-boundary value problem,

$$\overline{u}f_t=2a(f^m)_x+(ax+b)(f^m)_{xx}, \tag{8}$$

$$f(-L,t)=1,\quad f(L,t)=1, \tag{9}$$

$$f(x,0) = u_0(x)/\overline{u}(x) \tag{10}$$

in Ω.

It will be clear later on that it is convenient to consider separately the two cases $0<m\leqslant 1$ and $m>1$, respectively. Both cases, however, can be treated by studying the time decay of a suitable entropy, defined by the convex functional,

$$H(f) = \int_\Omega \Phi(f)\overline{u}\,\mathrm{d}x, \tag{11}$$

where the convex function Φ, which is defined in the next sections, depends on the case we are considering.

A. The sublinear case

In the sublinear case (i.e., $0<m\leqslant 1$) we consider the convex function Φ given by

$$\Phi(f) = \left[\frac{1}{m(2-m)(3-m)}f^{3-m} - \frac{1}{m(2-m)}f + \frac{1}{m(3-m)}\right]. \tag{12}$$

Note that the linear part of Φ is chosen so that $\Phi(1)=\Phi'(1)=0$.

We prove the following lemma.

Lemma 3.1: Let $u_0(x)$, φ_-, φ_+ be admissible initial-boundary conditions, and moreover be such that φ_-, $\varphi_+>0$ and $u_0(x)$ is strictly positive for all $x\in\Omega$. Then, if $0<m\leqslant 1$, the functional $H(f)$, with $\Phi(f)$ given by (12), is an entropy for problem (8)–(10), that is

$$\frac{\mathrm{d}H(f)}{\mathrm{d}t} = -I(f),$$

where the (non-negative) entropy production $I(f)$ is

$$I(f) = \int_\Omega \overline{u}^m (f_x)^2\,\mathrm{d}x. \tag{13}$$

Proof: Let us multiply both sides of Eq. (8) by $\Phi'(f)$. Integrating over Ω with respect to x, we obtain

$$\int_\Omega \overline{u}\Phi'(f)\frac{\partial f}{\partial t}\mathrm{d}x = \int_\Omega \Phi'(f)(ax+b)(f^m)_{xx}\,\mathrm{d}x.$$

Let us integrate by parts the right-hand side. Thanks to the boundary conditions (9) and to the property $\Phi'(1)=0$ we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \overline{u}\Phi(f)\mathrm{d}x = -\int_\Omega [\overline{u}^m\Phi'(f)]_x (f^m)_x\,\mathrm{d}x = -m\int_\Omega \overline{u}^m\Phi''(f)f^{m-1}(f_x)^2\,\mathrm{d}x.$$

Since $m\Phi''(f)f^{m-1}=1$, the lemma is fully proven. □

B. The superlinear case

In the superlinear case (which corresponds to the choice $m>1$), we introduce the function Φ given by

$$\Phi(f) = \left[\frac{m+f^{m+1}}{m+1} - f\right]. \tag{14}$$

As in the previous case, $\Phi(1)=\Phi'(1)=0$.

We prove the following lemma.

Lemma 3.2: Let $u_0(x)$, φ_-, φ_+ be admissible initial-boundary conditions, and moreover be such that φ_-, $\varphi_+ > 0$ and $u_0(x)$ is strictly positive for all $x \in \Omega$.

Then, if $m > 1$, the functional

$$H(f) = \int_\Omega \Phi(f)\overline{u}\,\mathrm{d}x, \tag{15}$$

where $\Phi(f)$ is given in (14), is an entropy for problem (8)–(10), that is

$$\frac{\mathrm{d}H(f)}{\mathrm{d}t} = -I(f),$$

and the (non-negative) entropy production is

$$I(f) = \int_\Omega \overline{u}^m (f^m)_x^2\,\mathrm{d}x. \tag{16}$$

Proof: Let us multiply both sides of Eq. (8) by $\Phi'(f) = (f^m - 1)$ and integrate over Ω with respect to x,

$$\int_\Omega \overline{u}\Phi'(f)\frac{\partial f}{\partial t}\mathrm{d}x = \int_\Omega \Phi'(f)[2a(f^m)_x + (ax+b)(f^m)_{xx}]\mathrm{d}x.$$

Integrating by parts on the right-hand side, taking into account the boundary conditions (9) and the property $\Phi'(1) = 0$ we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \overline{u}\Phi(f)\mathrm{d}x &= 2a\int_\Omega (f^m - 1)(f^m)_x\,\mathrm{d}x + \int_\Omega \overline{u}^m (f^m - 1)(f^m)_{xx}\,\mathrm{d}x \\ &= -\int_\Omega (f^m)_x[\overline{u}^m (f^m - 1)]_x \mathrm{d}x = -\int_\Omega \overline{u}^m (f^m)_x^2\,\mathrm{d}x,\end{aligned} \tag{17}$$

which is the thesis of the lemma. □

IV. CONVERGENCE FOR STRICTLY POSITIVE INITIAL DATA

In order to investigate the entropy decay rate, we look now for lower bounds to the entropy production functional

$$I(f) = \int_\Omega \overline{u}^m (f^n)_x^2\,\mathrm{d}x,$$

with $m > 0$ and $n \geqslant 1$. In order to achieve this goal, we prove the following Lemma.

Lemma 4.1: Let f belong to $H^1(\Omega)$, and let $\overline{u}(x)$ be the stationary solution of problem (6)–(7). Then, for any $m > 0$ and $n \geqslant 1$,

$$\int_\Omega \overline{u}^m [(f^n)_x]^2\,\mathrm{d}x \geqslant \frac{1}{16\,L^2} J(\varphi_+, \varphi_-)\left(\int_\Omega |u - \overline{u}|\mathrm{d}x\right)^2,$$

where

$$J(\varphi_+,\varphi_-)=\begin{cases}\dfrac{1}{mL}\left[\dfrac{\varphi_+^m-\varphi_-^m}{\varphi_+^2-\varphi_-^2}\right] & \text{if} \quad \varphi_+\neq\varphi_-,\\ \dfrac{1}{2L}\varphi^{m-2} & \text{if} \quad \varphi_+=\varphi_-=\varphi.\end{cases}$$

Proof: Let us first suppose that $\overline{u}^m$ is nondecreasing. The opposite case can be treated in the same way.

Given any function $g\in H^1(\Omega)$, such that $g(L)=1$,

$$\begin{aligned}\|\overline{u}(g-1)\|_{L^1}&\leqslant\int_{-L}^{L}\overline{u}(x)\int_x^L|g'(y)|\mathrm{d}y\,\mathrm{d}x\leqslant\int_{-L}^{L}\overline{u}(x)^{(2-m)/2}\int_x^L\overline{u}(y)^{m/2}|g'(y)|\mathrm{d}y\,\mathrm{d}x\\&\leqslant\int_{-L}^{L}\overline{u}(x)^{(2-m)/2}\left(\int_x^L\overline{u}(y)^m|g'(y)|^2\,\mathrm{d}y\right)^{1/2}(L-x)^{1/2}\,\mathrm{d}x\\&\leqslant\|\overline{u}^{m/2}g'\|_{L^2}\left(\int_{-L}^{L}\overline{u}(x)^{2-m}\,\mathrm{d}x\right)^{1/2}\left(\int_{-L}^{L}(L-x)\mathrm{d}x\right)^{1/2}.\end{aligned}\tag{18}$$

For any $m>0$, the function $\overline{u}^{2-m}=(ax+b)^{2/m-1}$ is integrable on Ω. If we denote

$$J(\varphi_+,\varphi_-)=\left(\int_\Omega(ax+b)^{2/m-1}\,\mathrm{d}x\right)^{-1},$$

we have in fact that

$$J(\varphi_+,\varphi_-)=\begin{cases}\dfrac{1}{mL}\left[\dfrac{\varphi_+^m-\varphi_-^m}{\varphi_+^2-\varphi_-^2}\right] & \text{if} \quad \varphi_+\neq\varphi_-,\\ \dfrac{1}{2L}\varphi^{m-2} & \text{if} \quad \varphi_+=\varphi_-=\varphi.\end{cases}$$

Hence, (18) implies

$$\int_\Omega\overline{u}(x)^m|g'(x)|^2\,\mathrm{d}x\geqslant\frac{J(\varphi_+,\varphi_-)}{2L^2}\|\overline{u}(g-1)\|_{L^1}^2.\tag{19}$$

Next, if $n\geqslant1$, we have $|r^n-1|\geqslant|r-1|$ for $r\geqslant0$. Consequently,

$$\frac{J(\varphi_+,\varphi_-)}{2L^2}\|\overline{u}(f-1)\|_{L^1}^2\leqslant\frac{J(\varphi_+,\varphi_-)}{2L^2}\|\overline{u}(f^n-1)\|_{L^1}^2\leqslant\int_\Omega\overline{u}(x)^m[(f^n(x))_x]^2\,\mathrm{d}x.\tag{20}$$

□

Remark 4.1: We remark that $J(\varphi_+,\varphi_-)$ is monotone decreasing with respect to m. This is consistent with the fact that we expect a faster convergence towards equilibrium in the fast diffusion case.

Remark 4.2: The proof of Lemma 4.1, which is nothing but the proof of a weighted Poincaré inequality, takes essential advantage from the simple form of the steady state $\overline{u}$. Of course, other proofs can be found in the literature, and the constant could be improved. Recent results on weighted Poincaré inequalities are due to Chua and Wheeden.[11]

In order to obtain a proof of the exponential convergence of the solution $u(x,t)$ to problem (1)–(3) towards its stationary state $\overline{u}(x)$ when $u_0(x)>0$, it remains to show that the relative entropy satisfies an inequality of the Csiszár–Kullback type.[12] This result is contained in the following lemma.

Lemma 4.2: Let $f(x,t)$ be the solution of problem (8)–(10), $\overline{u}(x)$ the solution of problem (6)–(7). Let

$$\xi(m) = \min_{0\leqslant\alpha\leqslant 1} \frac{1-\alpha}{\Phi(\alpha)} + \frac{2}{\Phi''(\alpha)}, \tag{21}$$

where Φ is given by (12) if $m<1$, or by (14) if $m\geqslant 1$. Then the following Csiszár–Kullback-type inequality holds:

$$\int_\Omega \Phi(f)\overline{u}\,\mathrm{d}x \geqslant \frac{\xi(m)}{\int_\Omega \overline{u}\,\mathrm{d}x}\left(\int_\Omega |u-\overline{u}|\mathrm{d}x\right)^2. \tag{22}$$

Proof: First, we note that the function

$$\Psi(r) = \frac{\Phi(r)}{1-r}, \quad 0\leqslant r\leqslant 1,$$

is nonincreasing. Since

$$\Psi'(r) = \frac{\Phi'(r)}{1-r} + \frac{\Phi(r)}{(1-r)^2} = \frac{1}{(1-r)^2}[\Phi'(r)(1-r)+\Phi(r)],$$

it is enough to show that the function $z(r)=\Phi'(r)(1-r)+\Phi(r)$ is nonpositive in the set $0\leqslant r\leqslant 1$. This follows easily considering that $\Phi(1)=0$, while the convexity of Φ implies

$$z'(r) = \Phi''(r)(1-r) \geqslant 0.$$

Fix $\alpha\in(0,1)$. Since Ψ is nonincreasing, and

$$\int_{\{f<\alpha\}} \overline{u}|f-1|\mathrm{d}x \leqslant \left(\int_{\{f<\alpha\}} \overline{u}|f-1|\mathrm{d}x\right)^{1/2}\left(\int_\Omega \overline{u}\,\mathrm{d}x\right)^{1/2},$$

we obtain

$$\int_{\{f<\alpha\}} \overline{u}\Phi(f)\mathrm{d}x \geqslant \Psi(\alpha)\int_{\{f<\alpha\}} \overline{u}|f-1|\mathrm{d}x \geqslant \frac{\Psi(\alpha)}{\|\overline{u}\|_{L^1}}\left(\int_{\{f<\alpha\}} \overline{u}|f-1|\mathrm{d}x\right)^2. \tag{23}$$

On the other hand, since both $\Phi(1)=0$ and $\Phi'(1)=0$, by the monotonicity of Φ'' we have

$$\int_{\{f\geqslant\alpha\}} \overline{u}\Phi(f)\mathrm{d}x = \int_{\{f\geqslant\alpha\}} \overline{u}\frac{(f-1)^2}{2}\Phi''(1+\vartheta(f)(f-1))\mathrm{d}x \geqslant \frac{\Phi''(\alpha)}{2}\int_{\{f\geqslant\alpha\}} \overline{u}(f-1)^2\,\mathrm{d}x$$

$$\geqslant \frac{\Phi''(\alpha)}{2\|\overline{u}\|_{L^1}}\left(\int_{\{f\geqslant\alpha\}} \overline{u}|f-1|\mathrm{d}x\right)^2. \tag{24}$$

Grouping together inequalities (23) and (24) we finally obtain

$$\|u-\overline{u}\|_{L^1}^2 \leqslant 2\left(\int_{\{f<\alpha\}} \overline{u}|f-1|\mathrm{d}x\right)^2 + 2\left(\int_{\{f\geqslant\alpha\}} \overline{u}|f-1|\mathrm{d}x\right)^2 \leqslant 2\|\overline{u}\|_{L^1}\left(\frac{1-\alpha}{\Phi(\alpha)} + \frac{2}{\Phi''(\alpha)}\right)\int_\Omega \overline{u}\Phi(f)\mathrm{d}x. \tag{25}$$

Optimizing with respect to α we conclude the proof. □

The previous results are at the basis of the following theorem.

Theorem 4.3: *Let $u(x,t)$ be the solution of problem (1)–(3), where $u_0(x)$, φ_- and φ_+ are strictly positive, and $H(u_0/\overline{u})$ is bounded. Then $u(x,t)$ decays exponentially fast towards the stationary solution $\overline{u}(x)$ in L^1-norm, and the following bound holds*:

$$\left(\int_\Omega |u-\overline{u}|\mathrm{d}x\right)^2 \leqslant \frac{\int_\Omega \overline{u}\,\mathrm{d}x}{\xi(m)} H(u_0/\overline{u})\exp\left[-\frac{\int_\Omega \overline{u}\,\mathrm{d}x}{16L^2\xi(m)}\left(\int_\Omega \overline{u}^{2/m-1}\,\mathrm{d}x\right)^{-1} t\right]. \tag{26}$$

Proof: In consequence of Lemmas 3.1, 3.2, 4.1, and 4.2 we deduce that

$$\left(\int_\Omega |u-\overline{u}|\mathrm{d}x\right)^2 \leqslant \frac{\int_\Omega \overline{u}\,\mathrm{d}x}{\xi(m)}\left[H(u_0/\overline{u}) - \frac{1}{16L^2}\left(\int_\Omega \overline{u}^{2/m-1}\,\mathrm{d}x\right)^{-1}\int_0^t\left(\int_\Omega |u-\overline{u}|\mathrm{d}x\right)^2 \mathrm{d}t'\right]. \tag{27}$$

Gronwall's lemma then implies (26). □

V. NON-NEGATIVE INITIAL-BOUNDARY CONDITIONS

In this section we briefly sketch the procedure to adopt when the initial and boundary conditions are non-negative only, provided that the stationary solution $\overline{u}(x)$ is not identically zero on $\overline{\Omega}$. This corresponds to suppose that $(\varphi_+ + \varphi_-) > 0$.

We consider two cases. In the first one, the boundary conditions are strictly positive, but the initial data can vanish somewhere on Ω. In the second one we admit the possibility of a vanishing boundary condition in $x=-L$ or in $x=L$.

We note that, while in the former case the result is a simple corollary of Theorem 4.3, in the latter the regularity of the initial data plays an important role.

A. Non-negative initial data

Let $u(x,t)$ be the solution of Eqs. (1)–(3), with admissible non-negative initial datum $u(x,0)$, and boundary conditions $u(-L,t)=\varphi_-$ and $u(L,t)=\varphi_+$ for all $t>0$, such that $u_0(-L)=\varphi_-$ and $u_0(L)=\varphi_+$, where φ_+ and φ_- are strictly positive.

To prove the exponential decay also in this case, we lift up the initial data of a small quantity, depending on a parameter $\varepsilon>0$ and vanishing as $\varepsilon\to 0$, and then pass to the limit.

We denote by $u_\varepsilon(x,t)$ the solution of the lifted problem, where the initial data are

$$u_\varepsilon(x,0) = u_{0,\varepsilon}(x) = u_0(x) + \varepsilon\cos\left(\frac{\pi}{2L}x\right).$$

The corresponding stationary solutions remains unchanged. Thanks to Theorem 4.3,

$$\|u_\varepsilon(x,t)-\overline{u}(x)\|_1^2 \leqslant \frac{\int_\Omega \overline{u}\,\mathrm{d}x}{\xi(m)} H(u_{0,\varepsilon}/\overline{u})\exp\left[-\frac{\int_\Omega \overline{u}\,\mathrm{d}x}{16L^2\xi(m)}\left(\int_\Omega \overline{u}^{2/m-1}\,\mathrm{d}x\right)^{-1} t\right].$$

In the sublinear case,

$$H(u_{0,\varepsilon}/\overline{u}) = \int_\Omega\left[\frac{1}{m(2-m)(3-m)} f_\varepsilon^{3-m} - \frac{1}{m(2-m)} f_\varepsilon + \frac{1}{m(3-m)}\right]\overline{u}\,\mathrm{d}x,$$

with $f_\varepsilon = u_{0,\varepsilon}(x)/\overline{u}$.

Since f_ε decreases as $\varepsilon\to 0^+$, and the integrand is continuous and well defined on $\overline{\Omega}$, we can apply the monotone convergence theorem to obtain

$$\lim_{\varepsilon\to 0^+}\int_\Omega f_\varepsilon^{3-m}\overline{u}\,dx=\int_\Omega\left[\frac{u_0(x)}{\overline{u}}\right]^{3-m}\overline{u}\,dx.$$

The same argument shows that also

$$\lim_{\varepsilon\to 0^+}\int_\Omega f_\varepsilon\overline{u}\,dx=\int_\Omega u_0\,dx.$$

Hence,

$$\lim_{\varepsilon\to 0}H(u_{0,\varepsilon}/\overline{u})=H(u_0/\overline{u}).$$

The superlinear case can be equally treated. We proved the following theorem.

Theorem 5.1: *Let $u(x,t)$ be the solution of problem (1)–(3), where the initial data are admissible, φ_- and φ_+ are strictly positive, and $H(u_0/\overline{u})$ is bounded. Then $u(x,t)$ decays exponentially fast towards the stationary solution $\overline{u}(x)$ in L^1-norm, and bound (26) holds.*

B. Non-negative initial-boundary conditions

More involved is the case when we allow that a boundary condition can be zero, which is the most general situation taken into account in the paper.

In what follows, we will suppose that the vanishing boundary condition is in $x=-L$ (i.e., $\varphi_-=0$); the other case is specular.

Denote by $u(x,t)$ the solution of Eqs. (1)–(3), with admissible initial data $u(x,0)=u_0(x)\geqslant 0$ and boundary conditions $u(-L,t)=0$ and $u(L,t)=\varphi_+$ for all $t>0$, such that $u_0(-L)=0$ and $u_0(L)=\varphi_+$, where $\varphi_+>0$.

Given a positive constant $\varepsilon<\varphi_+$, we introduce a lifted problem where $\varphi_-=\varepsilon$. The corresponding stationary solutions are given by

$$\overline{u}^m(x)=ax+b \text{ and } \overline{u}_\varepsilon^m(x)=a_\varepsilon x+b_\varepsilon,$$

respectively, where

$$a_\varepsilon=\frac{1}{2L}[\varphi_+^m-\varepsilon^m],\quad b_\varepsilon=\frac{1}{2}[\varphi_+^m+\varepsilon^m].$$

Moreover, we lift the initial value $u_0(x)$ in the following way:

$$u_{0,\varepsilon}(x)=\overline{u_\varepsilon}(x)\quad \text{if}\quad -L\leqslant x<-L+\varepsilon,$$

$$u_{0,\varepsilon}(x)=u_\varepsilon^*(x)\quad \text{if}\quad -L+\varepsilon\leqslant x<-L+\varepsilon+\varepsilon^{m+1}.$$

In the above formula $0\leqslant u_\varepsilon^*(x)\leqslant C$ is any function in $C(\overline{\Omega})$ which connects continuously $\overline{u_\varepsilon}(-L+\varepsilon)$ with $u_0(-L+\varepsilon+\varepsilon^{m+1})$. Finally

$$u_{0,\varepsilon}(x)=u_0(x)\quad \text{if}\quad -L+\varepsilon+\varepsilon^{m+1}\leqslant x\leqslant L.$$

Let $u_\varepsilon(x,t)$ be the solution of the lifted problem, with initial data $u_\varepsilon(x,0)=u_{0,\varepsilon}(x)$ and boundary conditions $u_\varepsilon(-L,t)=\varepsilon$ and $u_\varepsilon(L,t)=\varphi_+$, where $\varepsilon>0$. Since $u_\varepsilon(x,t)$ satisfies the conditions of Theorem 5.1, we have immediately that

$$\|u_\varepsilon(x,t)-\overline{u_\varepsilon}(x)\|_1^2 \leqslant \frac{\int_\Omega \overline{u_\varepsilon}\,\mathrm{d}x}{\xi(m)} H(u_{0,\varepsilon}/\overline{u_\varepsilon}) \exp\left[-\frac{\int_\Omega \overline{u_\varepsilon}\,\mathrm{d}x}{16\,L^2\xi(m)}\left(\int_\Omega \overline{u_\varepsilon}^{2/m-1}\,\mathrm{d}x\right)^{-1} t\right].$$

Since all integrals containing $\overline{u_\varepsilon}$ converge to the right limit as $\varepsilon\to 0$, the only problem comes out from the limit of the lifted entropy, which in the superlinear case reads

$$H(u_{0,\varepsilon}/\overline{u_\varepsilon}) = \frac{1}{m+1}\int_\Omega \left(\frac{u_{0,\varepsilon}}{\overline{u_\varepsilon}}\right)^{m+1}\overline{u_\varepsilon}\,\mathrm{d}x - \int_\Omega u_{0,\varepsilon}\,\mathrm{d}x + \frac{m}{m+1}\int_\Omega \overline{u_\varepsilon}\,\mathrm{d}x.$$

The linear part converges to the right limit as $\varepsilon\to 0$. For the nonlinear term, by construction we have the bounds

$$\int_{-L}^{-L+\varepsilon}\left(\frac{u_{0,\varepsilon}}{\overline{u_\varepsilon}}\right)^{m+1}\overline{u_\varepsilon}\,\mathrm{d}x = \int_{-L}^{-L+\varepsilon}\overline{u_\varepsilon}\,\mathrm{d}x \leqslant \varphi_+\varepsilon,$$

and

$$\int_{-L+\varepsilon}^{-L+\varepsilon+\varepsilon^{m+1}}\left(\frac{u_{0,\varepsilon}}{\overline{u_\varepsilon}}\right)^{m+1}\overline{u_\varepsilon}\,\mathrm{d}x \leqslant C^{m+1}\int_{-L+\varepsilon}^{-L+\varepsilon+\varepsilon^{m+1}}\frac{1}{\overline{u_\varepsilon}^m}\mathrm{d}x \leqslant C^{m+1}\varepsilon,$$

where the last inequality follows considering that $\overline{u_\varepsilon}(x)^m \geqslant \varepsilon^m$. Finally, since $\overline{u_\varepsilon}\geqslant\overline{u}$,

$$\int_{-L+\varepsilon+\varepsilon^{m+1}}^{L}\left(\frac{u_{0,\varepsilon}}{\overline{u_\varepsilon}}\right)^{m+1}\overline{u_\varepsilon}\,\mathrm{d}x = \int_{-L+\varepsilon+\varepsilon^{m+1}}^{L}\left(\frac{u_0}{\overline{u}}\right)^{m+1}\overline{u}\left(\frac{\overline{u}}{\overline{u_\varepsilon}}\right)^{m}\mathrm{d}x \leqslant \int_{-L+\varepsilon+\varepsilon^{m+1}}^{L}\left(\frac{u_0}{\overline{u}}\right)^{m+1}\overline{u}\,\mathrm{d}x$$

$$\leqslant \int_{-L}^{L}\left(\frac{u_0}{\overline{u_\varepsilon}}\right)^{m+1}\overline{u}\,\mathrm{d}x.$$

Grouping these inequalities together we obtain the bound

$$H(u_{0,\varepsilon}/\overline{u_\varepsilon}) \leqslant H(u_0/\overline{u}) + o(\varepsilon). \tag{28}$$

On the other hand, Fatou's lemma implies

$$H(u_0/\overline{u}) \leqslant \lim_{\varepsilon\to 0} H(u_{0,\varepsilon}/\overline{u_\varepsilon}).$$

Hence we proved that, for the superlinear case

$$H(u_0/\overline{u}) = \lim_{\varepsilon\to 0} H(u_{0,\varepsilon}/\overline{u_\varepsilon}). \tag{29}$$

Since the sublinear case can be equally treated, the following theorem holds.

Theorem 5.2: *Let $u(x,t)$ be the solution of problem (1)–(3), where the initial data u_0 is admissible, $\varphi_- + \varphi_+ > 0$ and $H(u_0/\overline{u})$ is bounded. Then $u(x,t)$ decays exponentially fast towards the stationary solution $\overline{u}(x)$ in L^1-norm, and bound (26) holds.*

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Approximate conditional symmetries and approximate solutions of the perturbed Fitzhugh–Nagumo equation

M. Shih, E. Momoniat,[a] and F. M. Mahomed
Centre for Differential Equations, Continuum Mechanics and Applications, School of Computational and Applied Mathematics, University of the Witwatersrand, Private Bag 3, Wits 2050, Johannesburg, South Africa

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We consider a perturbation of the Fitzhugh–Nagumo equation. The perturbation is proportional to the electric potential across the cell membrane. The purpose of this investigation is to determine the effects of a change in electric potential across the cell membrane. Exact solutions of the perturbed equation are easily obtained from the well-known solutions of the unperturbed Fitzhugh–Nagumo equation. The method of approximate conditional symmetries is used to obtain first-order approximate solutions of the perturbed Fitzhugh-Nagumo equation. The approximate solutions are compared with the exact solutions of the perturbed equation. The exact solutions of the perturbed equation do not indicate a change in the wave front connecting one constant state to another. There is only a proportional increase or decrease in the constant nonzero state. The approximate solutions do show a change in the shape of the wave front connecting two constant states as well as a proportional increase or decrease in the constant nonzero state. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1839276]

I. INTRODUCTION

The Hodgkin–Huxley (HH)[8] model describes the ionic current flows for axonal membranes. The equation is based on data obtained by experimenting on the giant axon of a squid. The HH equation is intractable for analytic investigation. The Fitzhugh–Nagumo (FN) model reduces the complexity of the HH model while maintaining many excitation–propagation phenomena. This FN model is a two variable reaction–diffusion system for nerve-impulse propagation. One variable corresponds to the electric voltage across the cell membrane, also called the fast variable; the other variable corresponds to ion concentration, called the slow variable. The slow variable changes slowly and its coefficient is small. The small variable is set to zero and only the behavior of the fast variables are considered. The resulting model is then described by the nonlinear diffusion equation,

$$u_t = u_{xx} + u(u-a)(1-u), \quad 0 < a < 1, \tag{1}$$

where $u(t,x)$ is the electric potential across the cell membrane. The interested reader is referred to the papers of Fitzhugh[7] and Nagumo[13] for more information on the derivation of (1). The FN equation has also been used in mathematical models in the area of population genetics.[1]

Exact solutions of the unperturbed FN equation (1) are given by

$$u(t,x) = \frac{a\kappa_1 e^{(1/2)(\sqrt{2}ax+a^2t)} + \kappa_2 e^{(1/2)(\sqrt{2}x+t)}}{\kappa_1 e^{(1/2)(\sqrt{2}ax+a^2t)} + \kappa_2 e^{(1/2)(\sqrt{2}x+t)} + \kappa_3 e^{at}}, \tag{2}$$

[a]Electronic mail: ebrahim@cam.wits.ac.za

$$u(t,x) = \frac{1}{1 + \overline{C_1} e^{[(2a-1)t/2] + (x/\sqrt{2})}}, \tag{3}$$

$$u(t,x) = \frac{a}{1 + a\overline{C_3} e^{[(2a-a^2)t/2] + (ax/\sqrt{2})}}, \tag{4}$$

$$u(t,x) = \frac{e^{[(1+a)t/2] + (ax/\sqrt{2}) + \overline{C_5}} - a e^{(x/\sqrt{2}) + a([(1+a)t/2] + \overline{C_5})}}{e^{[(1+a)t/2] + (ax/\sqrt{2}) + \overline{C_5}} - e^{(x/\sqrt{2}) + a([(1+a)t/2] + \overline{C_5})}}, \tag{5}$$

where κ_i, $i=1,2,3$; $\overline{C_1}$, $\overline{C_3}$, and $\overline{C_5}$ are constants. These exact solutions have been determined by Kawahara and Tanaka.[10] These results are also obtained in a more systematic way by Nucci and Clarkson[14] using the nonclassical symmetry method introduced by Bluman and Cole.[3] Further discussions on the use of the nonclassical symmetry method on determining exact solutions of (1) are presented by Clarkson and Mansfield.[5] The nonclassical symmetry approach (also known as the conditional symmetry approach) has been used with much success in obtaining new solutions for differential equations, see, e.g., Refs. 6, 11, and 15–17. These solutions have not been found using Lie's classical approach (see, e.g., Bluman and Kumei[4] and Ibragimov[9]). The solutions (2)–(4) show a wave front connecting two constant states (for the model under consideration in this paper states and electric potentials may be used interchangeably). These states are (0, 1), (1, 0), and (a, 0), respectively. The solution (5) has a singularity at

$$x = x^* = \frac{2\overline{C_5} + t(a+1)}{\sqrt{2}}. \tag{6}$$

In this paper we consider a perturbation of the FN equation where the perturbation is proportional to the electric potential across the cell membrane. The resulting equation is given by

$$u_t = u_{xx} + u(u-a)(1-u) + \epsilon u, \quad 0 < a < 1, \quad \epsilon \ll 1. \tag{7}$$

The approximate equation (7) is solved using the approximate conditional symmetry method of Mahomed and Qu.[12]

II. EXACT SOLUTIONS

We note that the perturbed FN equation (7) can be written in the form

$$u_t = u_{xx} + u(u-a+k)(1-u+k), \quad 0 < a < 1, \quad \epsilon \ll 1, \tag{8}$$

where

$$k = \tfrac{1}{2}((a-1) \pm \sqrt{(a-1)^2 + 4\epsilon}). \tag{9}$$

The expression of the cubic nonlinearity in (8) is not unique. However, the form used is beneficial in this analysis as it indicates the effect of the perturbation on the constant solutions $u=a$ and $u=1$ of the unperturbed FN equation (7). From (8) we note that the stable solution at $u=0$ remains unchanged while two new constant solutions are found, viz.,

$$u = a - k, \quad u = 1 + k. \tag{10}$$

Analytical solutions admitted by (8) are easily found from the solutions (2)–(5) by making the transformations

TABLE I. Symmetries of unperturbed Fitzhugh–Nagumo equation.

	$\tau_0(t,x,u)$	$\xi_0(t,x,u)$	$\eta_0(t,x,u)$	
Case 1	1	$3/\sqrt{2}(u-a+1/3)$	$-\frac{3}{2}(u^3-(a+1)u^2+au)$	(1a)
Case 2	0	1	$1/\sqrt{2}u(u-1)$	(2a)
	0	1	$1/\sqrt{2}u(u-a)$	(2b)
	0	1	$1/\sqrt{2}(u-1)(u-a)$	(2c)

$$a \to a-k, \quad 1 \to 1+k. \tag{11}$$

These transformations do not affect the shape of the wave front connecting two constant states. We will show in the next section that this is not the case when one considers approximate conditional symmetries. The solutions obtained indicate a change in the shape of the wave front. The singularity (6) admitted by (5) is transformed in a similar way. To first order in ϵ we find that the two new constant states are given by

$$u \approx a + \frac{\epsilon}{a-1}, \quad u \approx 1 + \frac{\epsilon}{1-a}. \tag{12}$$

III. APPROXIMATE CONDITIONAL SYMMETRIES

The unperturbed FN equation (1), as is well known, admits the classical Lie point symmetries,

$$Z_1 = \partial_t, \quad Z_2 = \partial_x \tag{13}$$

while it is easy to show that the perturbed FN equation (7) admits the approximate Lie point symmetries (in the sense of Baikov *et al.*[2])

$$W_1 = \partial_t, \quad W_2 = \epsilon\partial_t, \quad W_3 = \partial_x, \quad W_4 = \epsilon\partial_x. \tag{14}$$

The approximate Lie point symmetries (14) of the perturbed FN equation are not true approximate symmetries as they are just a constant multiple of the classical Lie point symmetries of the exact equation. Both the classical and approximate Lie point symmetries lead to the standard traveling wave solutions. Nontrivial symmetries are obtained via the conditional and approximate conditional symmetry approaches.

The conditional symmetries admitted by (1) have been determined by Nucci and Clarkson[14] (see also Clarkson and Mansfield[5]) and are presented in Table I. The generator of these conditional symmetries is written as

$$Y = \tau_0\frac{\partial}{\partial t} + \xi_0\frac{\partial}{\partial x} + \eta_0\frac{\partial}{\partial u}, \tag{15}$$

where the coefficients τ_0, ξ_0, and η_0 are presented in Table I. Solutions admitted by (1) of the form $u=\Phi(t,x)$ are determined from these conditional symmetries by solving the first-order quasilinear partial differential equation,

$$Y(u-\Phi(t,x))\big|_{u=\Phi(t,x)} = 0. \tag{16}$$

These solutions are given by Eqs. (2)–(5).

Using the approach presented by Mahomed and Qu[12] we find the approximate conditional symmetries admitted by (7). The main features of this approach as utilized here can be summarized as follows. An operator $X=X_0+\epsilon X_1$ with

TABLE II. Approximate conditional symmetries of perturbed Fitzhugh–Nagumo equation.

	$\tau(t,x,u;\epsilon)$	$\xi(t,x,u;\epsilon)$	$\eta(t,x,u;\epsilon)$	
Case 1	1	$3/\sqrt{2}(u-a+1/3)$	$-\frac{3}{2}(u^3-(a+1)u^2+au)+\epsilon(\frac{3}{2}u)$	(1b)
Case 2				
(2a)	0	1	$1/\sqrt{2}u(u-1)+\epsilon 1/\sqrt{2}(a-1)u$	(2d)
(2b)	0	1	$1/\sqrt{2}u(u-a)-\epsilon 1/\sqrt{2}(a-1)u$	(2e)
(2c)	0	1	$1/\sqrt{2}(u-1)(u-a)-\epsilon 1/\sqrt{2}$	(2f)

$$X_b = \xi_b^i(x,u)/\partial x^i + \eta_b^\alpha(x,u)/\partial u^\alpha, \quad b = 0,1,$$

is a first-order approximate symmetry generator of an rth-order partial differential equation system $[F]$ perturbed up to order one in the small parameter ϵ, viz.,

$$F^\beta = F_0^\beta(x,u,u_{(1)},\ldots,u_{(r)}) + \epsilon F_1^\beta(x,u,u_{(1)},\ldots,u_{(r)}) = O(\epsilon^2),$$

in which $x=(x^1,x^2,\ldots,x^n)$, $u=(u^1,u^2,\ldots,u^m)$, $u_{(1)},u_{(2)},\ldots,u_{(r)}$ are the collections of partial derivatives up to order r, if

$$X^{[r]}(F^\beta)|_{[W]\cap[F]} = O(\epsilon^2),$$

where

$$X^{[r]} = X_0^{[r]} + \epsilon X_1^{[r]},$$

$$X_b^{[r]} = X_b + \sum_{s=1}^{r} D_{i_1}\cdots D_{i_s}(W_b^\alpha) + \xi_b^j u^\alpha_{ji_1\cdots i_s}\frac{\partial}{\partial u^\alpha_{i_1\cdots i_s}}, \quad b = 0,1,$$

$$W_b^\alpha = \eta_b^\alpha - \xi_b^j u_j^\alpha, \quad \alpha = 1,\ldots,m,$$

and $[W]$ is the surface given by the invariant surface conditions $W_0^\alpha+\epsilon W_1^\alpha=O(\epsilon^2)$ together with

$$D_{i_1}\cdots D_{i_s}[W_0^\alpha + \epsilon W_1^\alpha] = O(\epsilon^2), \quad s = 1,\ldots,r-1.$$

The first order in ϵ approximate conditional symmetries of (7), using the above approach, are presented in Table II.

The generators of the approximate conditional symmetries are written as follows:

$$X = \tau\frac{\partial}{\partial t} + \xi\frac{\partial}{\partial x} + \eta\frac{\partial}{\partial u}, \tag{17}$$

where the coefficients τ, ξ, and η are presented in Table II. We note from Table II that the perturbation affects only the η terms. To determine approximate solutions,

$$u(t,x) = u_0(t,x) + \epsilon u_1(t,x), \quad \epsilon \ll 1, \tag{18}$$

corresponding to the approximate conditional symmetries indicated in Table II we solve the first-order quasilinear partial differential equation[12]

$$X(u - u_0(t,x) - \epsilon u_1(t,x))|_{u=u_0(t,x)+\epsilon u_1(t,x)} = 0. \tag{19}$$

The resulting first-order quasilinear partial differential equation is separated to first order in the small parameter in ϵ. For each of the cases indicated in Table II we choose the appropriate u_0 from (2)–(5).

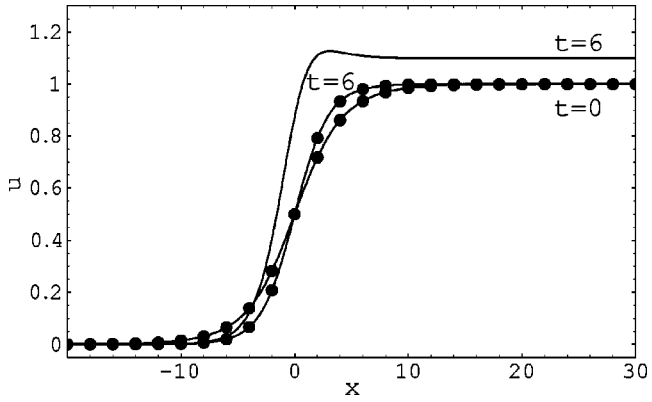

FIG. 1. Plot of the numerical solution $u=u_0+\epsilon u_1$ for case (1b) obtained from the numerical solution of the characteristic equations (22)–(25) and the exact solution (2) (-·-·-·-) of the unperturbed equation on the same system of axes. We have chosen $\epsilon=0.05$, $a=0.5$, and $\kappa_1=\kappa_2=\kappa_3=1$.

For case (1b), we obtain the system of partial differential equations,

$$u_{0_t}+\frac{3}{\sqrt{2}}\left(u_0-\frac{(a+1)}{3}\right)u_{0_x}=-\frac{3}{2}(u_0^3-(a+1)u_0^2+au_0), \tag{20}$$

$$u_{1_t}+\frac{3}{\sqrt{2}}\left(u_0-\frac{(a+1)}{3}\right)u_{1_x}=-\frac{3}{2}(3u_0^2u_1-2(a+1)u_0u_1+au_1-u_0)-\frac{3}{\sqrt{2}}u_1u_{0_x}, \tag{21}$$

where the exact solution of (20) is given by (2). We substitute (2) for u_0 into (21). Unfortunately, we cannot determine an analytical solution to (21). Instead we solve the system (20) and (21) numerically. The characteristic equations for the system (20) and (21) are given by

$$\frac{dt}{ds}=1, \tag{22}$$

$$\frac{dx}{ds}=\frac{3}{\sqrt{2}}\left(u_0-\frac{a+1}{3}\right), \tag{23}$$

$$\frac{du_0}{ds}=-\frac{3}{2}(u_0^3-(a+1)u_0^2+au_0), \tag{24}$$

$$\frac{du_1}{ds}=-\frac{3}{2}(3u_0^2u_1-2(a+1)u_0u_1+au_1-u_0)-\frac{3}{\sqrt{2}}u_1u_{0_x}. \tag{25}$$

We solve the system (22)–(25) numerically subject to

$$t(0,q)=0,\quad x(0,q)=q,\quad u_0(0,q)=F(q),\quad u_1(0,q)=0. \tag{26}$$

$F(q)$ is the initial profile and is obtained from (2) by setting $t=0$. We find that

$$F(q)=\frac{a\kappa_1e^{(1/2)(\sqrt{2}aq)}+\kappa_2e^{(1/2)(\sqrt{2}q)}}{\kappa_1e^{(1/2)(\sqrt{2}aq)}+\kappa_2e^{(1/2)(\sqrt{2}q)}+\kappa_3}. \tag{27}$$

The numerical solution for the perturbed equation and the exact solution for the unperturbed equation are plotted in Fig. 1.

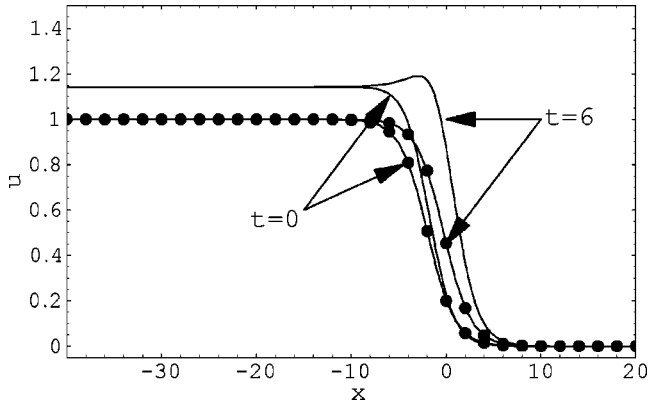

FIG. 2. Plot of the approximate solution $u=u_0+\epsilon u_1$ where u_0 is given by (3) and u_1 is given by (30). The unperturbed solution (3) (-·-·-·-) is plotted on the same system of axes. We have chosen $\epsilon=0.1$, $a=0.3$, $\overline{C}_1=4$, and $\overline{C}_2=5$.

From Fig. 1 we observe that the perturbation has no effect on the zero constant state. The shape of the wave front connecting the zero constant state to the nonzero constant state has changed. The wave front is now steeper and has a pronounced hump. In terms of our model, the hump is indicative of the membrane trying to correct for the perturbation to bring the potential back down to the constant state one. However, the cell is only able to correct this perturbation to a average slightly higher than one.

The system of equations we are required to solve for case (2d) is given by

$$\epsilon^0: u_{0x} - \frac{1}{\sqrt{2}}u_0^2 + \frac{1}{\sqrt{2}}u_0 = 0, \tag{28}$$

$$\epsilon^1: u_{1x} - \sqrt{2}u_0u_1 + \frac{1}{\sqrt{2}}u_1 - \frac{1}{\sqrt{2}(a-1)}u_0 = 0. \tag{29}$$

Substituting in the solution (3) for u_0 we can solve (29) to find that

$$u_1(t,x) = \frac{e^{-t/2}(-2e^{t/2} + e^{at+(x/\sqrt{2})}(2(a-2)\overline{C}_1t + \sqrt{2}\overline{C}_1x + 2(a-1)\overline{C}_2))}{2(a-1)(1+\overline{C}_1e^{(a-(1/2))t+(x/\sqrt{2})})^2}. \tag{30}$$

The approximate solution (18) is plotted in Fig. 2 where u_0 is given by (3) and u_1 is given by (30).

From the solution u_0 given by (3) and u_1 given by (30) we find that

$$\lim_{x\to-\infty} u_0(t,x) = 1, \quad \lim_{x\to\infty} u_0(t,x) = 0 \tag{31}$$

while

$$\lim_{x\to-\infty} (u_0(t,x) + \epsilon u_1(t,x)) = 1 + \frac{\epsilon}{1-a},$$

$$\lim_{x\to\infty} (u_0(t,x) + \epsilon u_1(t,x)) = 0. \tag{32}$$

The system of equations we are required to solve for case (2e) is given by

$$\epsilon^0: u_{0x} - \frac{1}{\sqrt{2}}u_0^2 + \frac{1}{\sqrt{2}}au_0 = 0, \tag{33}$$

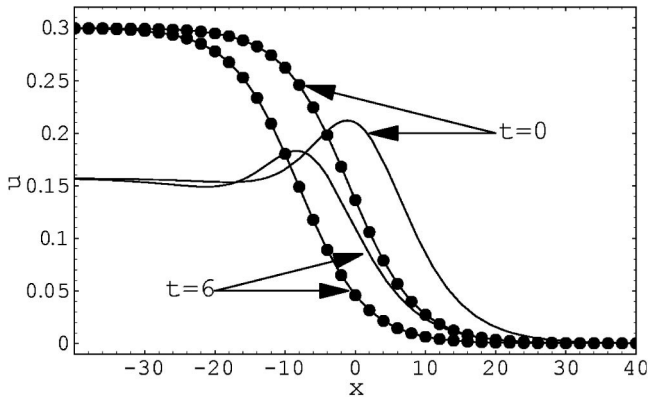

FIG. 3. Plot of the approximate solution $u=u_0+\epsilon u_1$ where u_0 is given by (4) and u_1 is given by (35). The unperturbed solution (4) (-·-·-·-) is plotted on the same system of axes. We have chosen $\epsilon=0.1$, $a=0.3$, $\overline{C_3}=4$, and $\overline{C_4}=5$.

$$\epsilon^1: u_{1x} - \sqrt{2}u_0u_1 + \frac{1}{\sqrt{2}}au_1 + \frac{1}{\sqrt{2}(a-1)}u_0 = 0. \tag{34}$$

Substituting in the solution (4) for u_0 we can solve (34) to find that

$$u_1(t,x) = \frac{1}{2(a-1)(1+a\overline{C_3}e^{[(2a-a^2)t/2]+(ax/\sqrt{2})})^2}(2 - \sqrt{2}a^2e^{[(2a-a^2)t/2]+(ax/\sqrt{2})}x\overline{C_3} + 2e^{[-((-2+a)at)/2]+(ax/\sqrt{2})}$$
$$\times(-a^2t\overline{C_3} + 2a^3t\overline{C_3} - \overline{C_4} + a\overline{C_4})). \tag{35}$$

The approximate solution (18) is plotted in Fig. 3 where u_0 is given by (4) and u_1 is given by (35).

From the solution u_0 given by (4) and u_1 given by (35) we find that

$$\lim_{x\to-\infty} u_0(t,x) = a, \quad \lim_{x\to\infty} u_0(t,x) = 0 \tag{36}$$

while

$$\lim_{x\to-\infty}(u_0(t,x) + \epsilon u_1(t,x)) = a + \frac{\epsilon}{a-1},$$
$$\lim_{x\to\infty}(u_0(t,x) + \epsilon u_1(t,x)) = 0. \tag{37}$$

From Figs. 2 and 3 we observe that the gradient of the wave front has increased. Also, as is indicated in (32) and (37) there is a slight change in the nonzero constant state. In the case of Fig. 2 the potential tends to a nonzero constant state of one as $x\to-\infty$ for the exact solution (3) and $1+\epsilon/(1-a)$ for the perturbed case. While from Fig. 3 we observe that the potential tends to a constant nonzero state of a as $x\to-\infty$ for the exact solution (4) and $a+\epsilon/(a-1)$ for the perturbed case. The zero states are unaffected. We observe the formation of a hump in the wave front. The hump is indicative of the cell membrane trying to correct for the perturbation to bring the potential down to one from $1+\epsilon/(1-a)$ in Fig. 2 and up to a from $a+\epsilon/(a-1)$ in Fig. 3. We note that in Fig. 2 the hump in the perturbed solution grows much larger in size than the unperturbed solution. Also, in Fig. 3, for the parameters given, the perturbed solution becomes negative for larger values of t.

The system of equations we are required to solve for case (2f) is given by

$$\epsilon^0: u_{0x} - \frac{1}{\sqrt{2}}u_0^2 + \frac{1}{\sqrt{2}}(a+1)u_0 - \frac{1}{\sqrt{2}}a = 0, \tag{38}$$

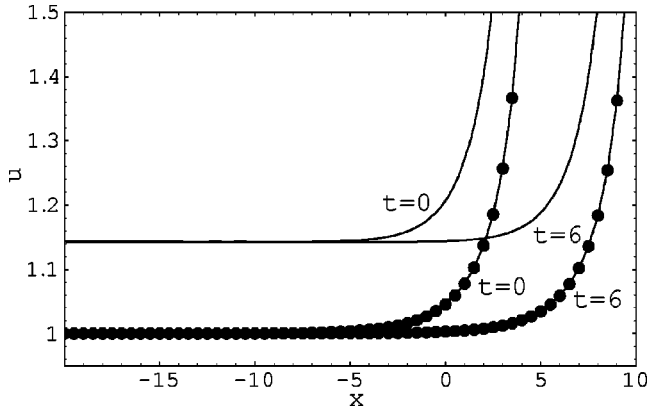

FIG. 4. Plot of the approximate solution $u=u_0+\epsilon u_1$ where u_0 is given by (5) and u_1 is given by (40) on the interval $x \in [-20, x^*]$. The unperturbed solution (5) (-·-·-·-) is plotted on the same system of axes. We have chosen $\overline{C_5}=4$, $\overline{C_6}=5$, $a=0.3$, and $\epsilon=0.1$.

$$\epsilon^1: u_{1x} - \sqrt{2}u_0 u_1 + \frac{1}{\sqrt{2}}(a+1)u_1 + \frac{1}{\sqrt{2}} = 0. \tag{39}$$

Substituting in the solution (5) for u_0 we can solve (39) to find that

$$\begin{aligned} u_1(t,x) = {} & \frac{1}{(a-1)(e^{[(1+a)t/2]+(ax/\sqrt{2})+\overline{C_5}} - e^{(x/\sqrt{2})+a([(1+a)t/2]+\overline{C_5})})^2}[e^{(1+a)^2 t/2}(-e^{[(t-a^2 t+2\sqrt{2}ax+4\overline{C_5})/2]} \\ & + e^{[(a^2-1)t/2]+\sqrt{2}x+2a\overline{C_5}} - (a^2-1)e^{[(1+a)x/\sqrt{2}]+(1+a)\overline{C_5}}t + \sqrt{2}(-1+a)e^{(1+a)(\sqrt{2}x+2\overline{C_5})/2}x \\ & + (a-1)e^{[(1+a)x/\sqrt{2}]}\overline{C_6})]. \end{aligned} \tag{40}$$

We note that (40) also has a singularity at $x=x^*$ where x^* is given by (6). The approximate solution (18) is plotted in Figs. 4 and 5 where u_0 is given by (5) and u_1 is given by (40) on either side of the singularity $x=x^*$.

From the solution u_0 given by (5) and u_1 given by (40) we find that

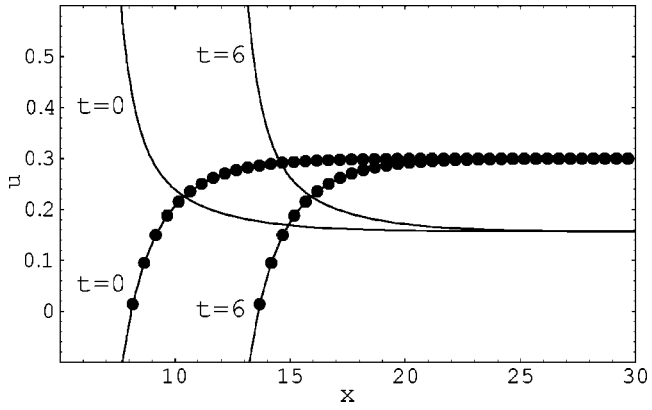

FIG. 5. Plot of the approximate solution $u=u_0+\epsilon u_1$ where u_0 is given by (5) and u_1 is given by (40) on the interval $x \in [x^*, 30]$. The unperturbed solution (5) (-·-·-·-) is plotted on the same system of axes. We have chosen $\overline{C_5}=4$, $\overline{C_6}=5$, $a=0.3$, and $\epsilon=0.1$.

$$\lim_{x\to-\infty} u_0(t,x) = 1, \quad \lim_{x\to\infty} u_0(t,x) = a, \tag{41}$$

while

$$\lim_{x\to-\infty} (u_0(t,x) + \epsilon u_1(t,x)) = 1 + \frac{\epsilon}{1-a},$$
$$\lim_{x\to\infty} (u_0(t,x) + \epsilon u_1(t,x)) = a + \frac{\epsilon}{a-1}. \tag{42}$$

The singular behavior of the solutions for case (2f) destroys the wave front connecting two constant states. However, we note from Figs. 4 and 5 that both the exact and perturbed solutions tend to constant behavior as $x \to \pm\infty$. This solution is not physical in terms of our model of electric potential across a cell membrane.

IV. DISCUSSION

In this paper we have determined approximate solutions for a perturbed Fitzhugh–Nagumo equation where the perturbation is proportional to the electric potential across the cell membrane. This choice of perturbation allows us to write the perturbed equation in an exact form given by (8). The transformations (11) allow us to convert the known solutions of the Fitzhugh–Nagumo equation into exact solutions of the perturbed equation. The physically meaningful solutions represent wave fronts connecting the constant states $(0,1+k)$, $(1+k,0)$, and $(a+k,0)$.

Approximate solutions determined from the approximate conditional symmetries admitted by the perturbed equation (7) were then investigated. The approximate solutions are stable (by the definition of Mahomed and Qu[12]) with one of the solutions having singular behavior. The physically meaningful approximate solutions represent wave fronts joining the constant states $(0,1+\epsilon/(1-a))$, $(1+\epsilon/(1-a),0)$, and $(a+\epsilon/(a-1),0)$. These constant states are just a first-order approximation to the constant states indicated above.

For our investigation into the behavior of the cell membrane it is appropriate to consider only short-time behavior as signals move across the cell membrane in a very short period of time. Over a short time period the difference in the constant states for each of the physically meaningful solutions is given by $|k-\epsilon/(1-a)|$ and $|k-\epsilon/(a-1)|$. We also note a difference in the shape of the wave front connecting the constant states. The approximate solution shows the formation of a hump while the exact solution of the approximate equation shows a smooth transition from one constant state to another.

The difference in the constant state could be used to explain some of the experimental error found when measuring nerve conductivity (see, e.g., Refs. 7 and 13). Also, the formation of the hump is indicative of the cell membrane trying to get down to a constant state given by (12).

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Maurer–Cartan equations for Lie symmetry pseudogroups of differential equations

Jeongoo Cheh[a] and Peter J. Olver[b]
School of Mathematics, University of Minnesota, Minneapolis, Minnesota 55455

Juha Pohjanpelto[c]
Department of Mathematics, Oregon State University, Corvallis, Oregon 97331

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A new method of constructing structure equations of Lie symmetry pseudogroups of differential equations, dispensing with explicit solutions of the (infinitesimal) determining systems of the pseudogroups, is presented, and illustrated by the examples of the Kadomtsev–Petviashvili and Korteweg–de Vries equations. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1836015]

I. INTRODUCTION

The theory of continuous groups of transformations created by Sophus Lie in the late nineteenth century has evolved to become one of the most important tools for geometric and algebraic study of general nonlinear partial differential equations. Lie himself made no essential distinction between finite-dimensional Lie group actions and infinite-dimensional pseudogroup actions. However, since his time, the two subjects have developed in very different directions. The theoretical foundations of finite-dimensional Lie groups and Lie algebras were well-established in the early twentieth century. In contrast, despite its evident importance in both mathematics and applications, the basic theory for infinite-dimensional Lie pseudogroups remains in relatively primitive shape. Unlike Lie groups, to this day, there is no generally accepted abstract object that represents an infinite-dimensional pseudogroup, and so, like Lie and Cartan,[3] we can only study them in the context of their action on a manifold. This makes the subject considerably more difficult than the finite-dimensional case, and a significant effort has been made in establishing a proper rigorous foundation for pseudogroups.[8,11–13,24,27]

Lie pseudogroups appear in gauge theories, Hamiltonian mechanics, symplectic and Poisson geometry, conformal geometry of surfaces, conformal field theory, and geometry of real hypersurfaces, as symmetry groups of both linear and nonlinear partial differential equations arising in fluid mechanics, solitons, relativity, etc., and as foliation-preserving groups of transformations. In general, a Lie pseudogroup $\mathcal{G}$ is defined in terms of a system $\mathcal{R}$ of (typically nonlinear) differential equations, called its *determining system*, whose solutions are the local diffeomorphisms constituting the pseudogroup. One immediate issue is to determine their local structure, which is usually expressed in the form of Maurer–Cartan structure equations, as in the case of finite-dimensional Lie groups. Both Lie's attempt to use his infinitesimal method based on the infinitesimal determining system obtained by linearizing the determining system, and Cartan's method using intricate recursive prolongation of exterior differential systems are either limited in scope or impractical from the standpoint of applications. Along this line of research in the last decade, Reid *et al.*,[14–16,25,26] developed methods for determining Cartan structure equations of Lie pseudogroups, which depended only on algebraic and differential manipulation, without any integration, of infinitesimal determining systems, hence increasing the feasibility of their computer algebra implementation. Their algorithms were successfully applied to certain types of Lie symmetry pseudo-

[a]Electronic mail: cheh@math.umn.edu
[b]Electronic mail: olver@math.umn.edu; URL:http://www.math.umn.edu/~olver/
[c]Electronic mail: juha@math.oregonstate.edu; URL:http://www.oregonstate.edu/~pohjanpp/

groups of differential equations. A major drawback, however, is that their methods were based on *ad hoc* series expansions and became significantly more complicated, requiring more case-by-case analyses, if they worked at all, when it came to intransitive pseudogroup actions.

More recently, Olver and Pohjanpelto developed a theory[22] where the invariant contact forms on the diffeomorphism jet bundle were interpreted as the Maurer–Cartan forms of the Lie pseudogroup. (For finite-dimensional symmetry groups, Morozov[20] has introduced a related approach based on the method of moving coframes.[7]) As a result, a very efficient method for constructing the structure equations of the Maurer–Cartan forms was discovered. This method bypasses the troublesome process of integrating either the determining system $\mathcal{R}$ or its linearization, or the complicated Cartan prolongation process. Moreover, the algorithm directly applies to completely general Lie pseudogroup actions, whether finite or infinite dimensional, transitive or intransitive, and can be easily implemented in computer algebra systems.

The goal of this paper is to show how to use the method to directly construct structure equations for Lie (point) symmetry pseudogroups of differential equations. Our algorithm works for any general Lie symmetry pseudogroup, and it will also give us better understanding of known local symmetry structures, as well as revealing those of a wide range of differential equations that still wait to be investigated. We also wrote some Mathematica routines to facilitate the computations needed for the implementation of our method on specific differential equations. To illustrate our algorithm, we will use the Kadomtsev–Petviashvili (KP) equation

$$(u_t + \tfrac{3}{2}uu_x + \tfrac{1}{4}u_{xxx})_x + \tfrac{3}{4}\epsilon u_{yy} = 0, \quad \epsilon = \pm 1, \tag{1}$$

and the Korteweg–de Vries (KdV) equation

$$u_t + u_{xxx} + uu_x = 0, \tag{2}$$

both of which are integrable soliton equations, possessing, respectively, infinite- and finite-dimensional Lie symmetry pseudogroups.[1,4–6,17–19]

Let us recall how the classical Lie symmetry method[21] works in the context of the KP equation. Let $M=\mathbb{R}^4$ with coordinates t,x,y,u given by the independent and dependent variables in the differential equation, and let $J^\infty(M,3)$ stand for the jet bundle of equivalence classes of three-dimensional submanifolds $u=f(t,x,y)$ of M under the equivalence relation of infinite-order contact. The infinitesimal symmetry algebra $\mathfrak{g}$ of the KP equation consists of the local vector fields

$$\mathbf{v} = \tau\partial_t + \xi\partial_x + \eta\partial_y + \phi\partial_u \tag{3}$$

on M such that their prolongations $\mathbf{v}^{(\infty)}$ are tangent to the variety in $J^\infty(M,3)$ defined by Eq. (1). This characterizing condition yields the system of partial differential equations

$$\begin{gathered}
\eta_u = 0, \quad \eta_x = 0, \quad \xi_u = 0, \quad \eta_t + \tfrac{3}{2}\epsilon\xi_y = 0, \quad 3\xi_x - \tau_t = 0, \\
\tfrac{3}{2}\phi - \xi_t + u\tau_t = 0, \quad \tfrac{3}{2}\eta_y - \tau_t = 0, \quad \tau_u = 0, \quad \tau_x = 0, \quad \tau_y = 0, \\
\tau_t + \tfrac{3}{2}\phi_u = 0, \quad \tfrac{2}{3}\tau_{tt} - 3\phi_x = 0, \quad \phi_{tx} + \tfrac{3}{2}u\phi_{xx} + \tfrac{1}{4}\phi_{xxxx} + \tfrac{3}{4}\epsilon\phi_{yy} = 0,
\end{gathered} \tag{4}$$

for the coefficient functions of the infinitesimal symmetries $\mathbf{v}$. These equations are the minimal *infinitesimal* (or *linearized*) *determining system* of the Lie symmetry pseudogroup $\mathcal{G}$ of the KP equation. Once the system (4) is completed to involution, all the higher order equations are obtained by differentiation with respect to t,x,y,u. The key point of this paper is to determine the local structure of $\mathcal{G}$ directly from its infinitesimal determining system (4). This setup has an obvious counterpart for the KdV equation (2), too, which, for brevity, we will not elaborate on until the end of the paper.

Our subsequent discussions in the paper are organized in such a way that the results of each section are applied to the case of the KP equation within that section, and, starting from the current section, consistent notation without further comment will be used for the examples. It is worth

emphasizing that both finite-dimensional and infinite-dimensional symmetry pseudogroups are handled, on an equal footing, by precisely the same algorithms to be presented here.

II. MAURER–CARTAN FORMS FOR THE PSEUDOGROUP OF LOCAL DIFFEOMORPHISMS

Let M be a smooth manifold of dimension m, and $\mathcal{D}=\mathcal{D}(M)$ the pseudogroup of local diffeomorphisms on M. For each $0\leqslant n\leqslant\infty$, let $\mathcal{D}^{(n)}=\mathcal{D}^{(n)}(M)$ be the bundle of n-jets of maps in $\mathcal{D}$. The bundle $\mathcal{D}^{(n)}$ is double-fibered over M with fibrations being the source projection

$$\boldsymbol{\sigma}^{(n)}:\mathcal{D}^{(n)}\to M,\quad \boldsymbol{\sigma}^{(n)}(j^n_z\phi)=z,$$

and the target projection

$$\boldsymbol{\tau}^{(n)}:\mathcal{D}^{(n)}\to M,\quad \boldsymbol{\tau}^{(n)}(j^n_z\phi)=\phi(z),$$

where $z\in M$ and $\phi\in\mathcal{D}$. Composition of local diffeomorphisms turns $\mathcal{D}^{(n)}$ into a Lie groupoid with multiplication law

$$(j^n_z\phi)\cdot(j^n_w\psi):=j^n_w(\phi\circ\psi)\quad\text{provided}\quad \boldsymbol{\sigma}^{(n)}(j^n_z\phi)=z=\psi(w)=\boldsymbol{\tau}^{(n)}(j^n_w\psi).$$

Local coordinates of the base space M and the total space $\mathcal{D}^{(n)}$ are denoted by $z=(z^i)$ and $(z,Z^{(n)})=(z^i,Z^a_J)$, respectively, where $Z=(Z^a)$ and Z^a_J, with J a symmetric multi-index, represents the derivative $\partial^J Z^a/\partial z^J$. The natural identification, obtained by viewing maps in terms of their graphs, of $\mathcal{D}^{(\infty)}$ with an open subbundle of the jet bundle $J^\infty(M\times M)$ of infinite jets of local sections of the trivial bundle

$$M\times M\to M,\quad (z,Z)\mapsto z,$$

induces a variational bicomplex structure[2,9,10] on the cotangent bundle $T^*\mathcal{D}^{(\infty)}$, where the horizontal subbundle is spanned by the horizontal forms $\mathrm{d}z^1,\dots,\mathrm{d}z^m$, and the vertical subbundle is spanned by the basic contact forms

$$\Upsilon^a_J:=\mathrm{d}Z^a_J-\sum_{i=1}^m Z^a_{J,i}\,\mathrm{d}z^i,\quad a=1,\dots,m,\quad \#J\geqslant 0.$$

Accordingly, the exterior differential $\mathrm{d}=\mathrm{d}_M+\mathrm{d}_G$ on $\mathcal{D}^{(\infty)}$ splits into the horizontal differential[28] d_M and the contact (or vertical) differential d_G, so that

$$\mathrm{d}F=\mathrm{d}_MF+\mathrm{d}_GF=\sum_{i=1}^m(\mathbb{D}_{z^i}F)\mathrm{d}z^i+\sum_{a=1}^m\sum_{\#J\geqslant 0}(\partial_{Z^a_J}F)\Upsilon^a_J,$$

for any smooth function $F:\mathcal{D}^{(\infty)}\to\mathbb{R}$. Here, $\mathbb{D}_{z^i}$ is the total differential operator with respect to the base coordinate function z^i, and $\partial_{Z^a_J}$ is the partial differential operator with respect to the fiber coordinate function Z^a_J.

Let

$$R_\psi(j^n_z\phi):=(j^n_z\phi)\cdot(j^n_z\psi)^{-1}=j^n_{\psi(z)}(\phi\circ\psi^{-1})$$

denote the right action of the diffeomorphism pseudogroup on its jets. A differential form μ on $D^{(n)}$ is said to be *right-invariant* if $R^*_\psi\mu=\mu$, whenever defined, for all $\psi\in\mathcal{D}$. In particular, the target coordinate functions Z^a are right invariant. Since the right action preserves the splitting of $T^*\mathcal{D}^{(\infty)}$, the horizontal and contact differentials of invariant forms are invariant. Thus,

$$\sigma^a:=\mathrm{d}_MZ^a=\sum_{i=1}^m Z^a_i\,\mathrm{d}z^i,\quad \mu^a:=\mathrm{d}_GZ^a=\Upsilon^a,\quad a=1,\dots,m,$$

are, respectively, *invariant horizontal forms* and *invariant contact forms*. The *invariant differential operators*, denoted $\mathbb{D}_{Z^a}$, are dual to the invariant horizontal forms σ^a, so

$$\mathrm{d}_M F = \sum_{a=1}^{m} (\mathbb{D}_{Z^a} F)\sigma^a \quad \text{for all } F \in C^\infty(\mathcal{D}^{(\infty)}).$$

Lie derivatives of invariant differential forms with respect to the invariant differential operators are invariant. Thus, the *higher order invariant contact forms*,

$$\mu^a_J := \mathbb{D}^J_Z \mu^a := \mathbb{D}_{Zj_1}\mathbb{D}_{Zj_2}\cdots\mathbb{D}_{Zj_k}\mu^a,$$

are obtained by repeated Lie differentiation. As argued in earlier papers,[22,23] these invariant contact forms play the role of the *Maurer–Cartan forms* for $\mathcal{D}$.

Let us present the explicit formulas in the case relevant to the KP equation. Since the KdV case is completely similar, except with one fewer independent variable, it will not be explicitly presented.

KP equation 1: The KP equation has independent variables t,x,y and dependent variable u, which we regard as coordinates on the total space $M=\mathbb{R}^4$. We denote the corresponding local coordinates of the diffeomorphism groupoid $\mathcal{D}^{(\infty)}$ by

$$(t,x,y,u,T,X,Y,U,T_t,T_x,T_y,T_u,X_t,X_x,X_y,X_u,\ldots).$$

The horizontal forms on $\mathcal{D}^{(\infty)}$ are $\mathrm{d}t,\mathrm{d}x,\mathrm{d}y,\mathrm{d}u$, and the contact forms are

$$\Upsilon^t := \mathrm{d}_G T = \mathrm{d}T - T_t\,\mathrm{d}t - T_x\,\mathrm{d}x - T_y\,\mathrm{d}y - T_u\,\mathrm{d}u,$$

$$\Upsilon^x := \mathrm{d}_G X = \mathrm{d}X - X_t\,\mathrm{d}t - X_x\,\mathrm{d}x - X_y\,\mathrm{d}y - X_u\,\mathrm{d}u,$$

$$\Upsilon^y := \mathrm{d}_G Y = \mathrm{d}Y - Y_t\,\mathrm{d}t - Y_x\,\mathrm{d}x - Y_y\,\mathrm{d}y - Y_u\,\mathrm{d}u,$$

$$\Upsilon^u := \mathrm{d}_G U = \mathrm{d}U - U_t\,\mathrm{d}t - U_x\,\mathrm{d}x - U_y\,\mathrm{d}y - U_u\,\mathrm{d}u,$$

$$\Upsilon^t_t := \mathbb{D}_t\Upsilon^t = \mathrm{d}_G T_t = \mathrm{d}T_t - T_{tt}\,\mathrm{d}t - T_{tx}\,\mathrm{d}x - T_{ty}\,\mathrm{d}y - T_{tu}\,\mathrm{d}u,$$

$$\ldots \text{ and, in general,} \quad \Upsilon^a_{h,k,l,n} := \mathbb{D}^h_t\mathbb{D}^k_x\mathbb{D}^l_y\mathbb{D}^n_u\Upsilon^a,$$

where we use a to signify either t, x, y or u, and $h,k,l,n\geqslant 0$, with $\mathbb{D}_t,\mathbb{D}_x,\mathbb{D}_y,\mathbb{D}_u$ denoting the total differential operators. The invariant horizontal forms are

$$\sigma^t := \mathrm{d}_M T = T_t\,\mathrm{d}t + T_x\,\mathrm{d}x + T_y\,\mathrm{d}y + T_u\,\mathrm{d}u,$$

$$\sigma^x := \mathrm{d}_M X = X_t\,\mathrm{d}t + X_x\,\mathrm{d}x + X_y\,\mathrm{d}y + X_u\,\mathrm{d}u,$$

$$\sigma^y := \mathrm{d}_M Y = Y_t\,\mathrm{d}t + Y_x\,\mathrm{d}x + Y_y\,\mathrm{d}y + Y_u\,\mathrm{d}u,$$

$$\sigma^u := \mathrm{d}_M U = U_t\,\mathrm{d}t + U_x\,\mathrm{d}x + U_y\,\mathrm{d}y + U_u\,\mathrm{d}u,$$

and the invariant contact forms are

$$\mu^t := \mathrm{d}_G T = \Upsilon^t, \quad \mu^x := \mathrm{d}_G X = \Upsilon^x, \quad \mu^y := \mathrm{d}_G Y = \Upsilon^y, \quad \mu^u := \mathrm{d}_G U = \Upsilon^u,$$

$$\mu^t_T := \mathbb{D}_T\mu^t, \quad \mu^t_X := \mathbb{D}_X\mu^t, \quad \dots \quad \text{and, in general, } \mu^a_{h,k,l,n} := \mathbb{D}_T^h\mathbb{D}_X^k\mathbb{D}_Y^l\mathbb{D}_U^n\mu^a,$$

where $a=t$, x, y or u, and

$$\begin{bmatrix} \mathbb{D}_T \\ \mathbb{D}_X \\ \mathbb{D}_Y \\ \mathbb{D}_U \end{bmatrix} = \begin{bmatrix} T_t & X_t & Y_t & U_t \\ T_x & X_x & Y_x & U_x \\ T_y & X_y & Y_y & U_y \\ T_u & X_u & Y_u & U_u \end{bmatrix}^{-1} \begin{bmatrix} \mathbb{D}_t \\ \mathbb{D}_x \\ \mathbb{D}_y \\ \mathbb{D}_u \end{bmatrix} \tag{5}$$

are the invariant differential operators.

III. STRUCTURE EQUATIONS OF THE DIFFEOMORPHISM PSEUDOGROUP

The invariant coframe for the diffeomorphism pseudogroup are the invariant horizontal and contact forms σ^a, μ^a_J. The structure equations amount to writing their differentials $\mathrm{d}\sigma^a$, $\mathrm{d}\mu^a_J$ as linear combinations of wedge products of the invariant differential forms. A concise way to write down the structure equations, as first described in an earlier paper,[22] rests on a formal power series expansion.[29] To this end, we define the vector-valued formal power series

$$\mu[\![H]\!] := (\mu^a[\![H]\!]) = \left(\sum_{\#J\geq 0} \frac{1}{J!}\mu^a_J H^J \right) \tag{6}$$

whose coefficients are the invariant contact forms on $\mathcal{D}^{(\infty)}$. In particular, if we set $H=(H^a)=0$ in (6), then $\mu[\![0]\!]=\mu:=(\mu^a)$. The key result, proved in an earlier paper,[22] is that the structure equations of the invariant coframe can be read off from certain matrix identities.

Lemma III.1: Let

$$\nabla\mu[\![H]\!] := \left(\frac{\partial \mu^a[\![H]\!]}{\partial H^b} \right)$$

denote the Jacobian matrix of the vector $\mu[\![H]\!]$ of power series in the variables $H=(H^a)$. Then

$$\mathrm{d}\mu[\![H]\!] = \nabla\mu[\![H]\!] \wedge (\mu[\![H]\!] - \mathrm{d}Z). \tag{7}$$

The structure equations of the invariant horizontal forms are given by

$$\mathrm{d}\sigma = -\,\mathrm{d}\mu, \tag{8}$$

where $\sigma := (\sigma^a)$.

The coefficients of the powers H^J in Eq. (7), along with (8), form the complete system of structure equations for the diffeomorphism pseudogroup $\mathcal{D}$.

KP equation 2: We use the capital letters $H,K,L,N \in \mathbb{R}$ to denote variables for power series. The structure equations for the invariant contact forms on $\mathcal{D}^{(\infty)}$ are given by the identity

$$\mathrm{d}\mu[\![H,K,L,N]\!] = \nabla\mu[\![H,K,L,N]\!] \wedge (\mu[\![H,K,L,N]\!] - \mathrm{d}Z), \tag{9}$$

where

$$\mathrm{d}\mu[\![H,K,L,N]\!] = \sum_{h,k,l,n\geq 0} \frac{H^h K^k L^l N^n}{h!\,k!\,l!\,n!} \begin{bmatrix} \mathrm{d}\mu^t_{h,k,l,n} \\ \mathrm{d}\mu^x_{h,k,l,n} \\ \mathrm{d}\mu^y_{h,k,l,n} \\ \mathrm{d}\mu^u_{h,k,l,n} \end{bmatrix},$$

$$\nabla\mu[\![H,K,L,N]\!] = \sum_{h,k,l,n\geqslant 0} \frac{H^h K^k L^l N^n}{h!\,k!\,l!\,n!} \begin{bmatrix} \mu^t_{h+1,k,l,n} & \mu^t_{h,k+1,l,n} & \mu^t_{h,k,l+1,n} & \mu^t_{h,k,l,n+1} \\ \mu^x_{h+1,k,l,n} & \mu^x_{h,k+1,l,n} & \mu^x_{h,k,l+1,n} & \mu^x_{h,k,l,n+1} \\ \mu^y_{h+1,k,l,n} & \mu^y_{h,k+1,l,n} & \mu^y_{h,k,l+1,n} & \mu^y_{h,k,l,n+1} \\ \mu^u_{h+1,k,l,n} & \mu^u_{h,k+1,l,n} & \mu^u_{h,k,l+1,n} & \mu^u_{h,k,l,n+1} \end{bmatrix},$$

$$\mu[\![H,K,L,N]\!] - \mathrm{d}Z = -\begin{bmatrix} \sigma^t \\ \sigma^x \\ \sigma^y \\ \sigma^u \end{bmatrix} + \sum_{\substack{h,k,l,n\geqslant 0 \\ h+k+l+n\geqslant 1}} \frac{H^h K^k L^l N^n}{h!\,k!\,l!\,n!} \begin{bmatrix} \mu^t_{h,k,l,n} \\ \mu^x_{h,k,l,n} \\ \mu^y_{h,k,l,n} \\ \mu^u_{h,k,l,n} \end{bmatrix}.$$

Once the structure equations for the invariant contact forms are established, those for the invariant horizontal forms are immediately obtained by

$$\begin{bmatrix} \mathrm{d}\sigma^t \\ \mathrm{d}\sigma^x \\ \mathrm{d}\sigma^y \\ \mathrm{d}\sigma^u \end{bmatrix} = -\begin{bmatrix} \mathrm{d}\mu^t \\ \mathrm{d}\mu^x \\ \mathrm{d}\mu^y \\ \mathrm{d}\mu^u \end{bmatrix}.$$

IV. MAURER–CARTAN EQUATIONS FOR LIE SYMMETRY PSEUDOGROUPS

Let $\mathcal{X}=\mathcal{X}(M)$ denote the space of locally defined vector fields

$$\mathbf{v} = \sum_{a=1}^{m} \zeta^a \partial_{z^a}$$

on M, i.e., the space of local sections of its tangent bundle TM. Given a sub-pseudogroup $\mathcal{G}\subset\mathcal{D}$, let $\mathfrak{g}\subset\mathcal{X}$ denote its local Lie algebra of infinitesimal generators, and $\mathfrak{g}^{(n)}$ their jets. With each sufficiently large n, the subbundle $\mathfrak{g}^{(n)}\subset J^nTM$ is characterized by the linearized (or infinitesimal) determining equations

$$L^{(n)}(z^i,\zeta^a_J) = 0 \tag{10}$$

for the pseudogroup $\mathcal{G}$. Here $\zeta^a_J=\partial^J_z\zeta^a$ are the jet coordinates of a vector field $\mathbf{v}$. If $\mathcal{G}$ is the symmetry group of a system of differential equations, then (10) are (the involutive completion of) the usual determining equations obtained through Lie's infinitesimal symmetry method.

A complete, though certainly not minimal, system of invariant differential one-forms for $\mathcal{G}$ is obtained by restricting the invariant coframe $\{\sigma^a,\mu^a_J\}$ to the Lie subgroupoid $\mathcal{G}^{(\infty)}\subset\mathcal{D}^{(\infty)}$ given by the jets of pseudogroup diffeomorphisms. For simplicity, we will not explicitly employ the pull-back notation on these restricted forms. The resulting dependencies among the restricted forms are elucidated by the following theorem.[22]

Theorem IV.1: *The invariant forms μ^a_J on $\mathcal{G}^{(n)}$ satisfy the linear system*

$$L^{(n)}(Z^i,\mu^a_J) = 0 \tag{11}$$

obtained by replacing z^i by Z^i and ζ^a_J by μ^a_J in the linearized determining equations (10).

In accordance with an earlier paper,[22] we refer to (11) as the *lifted determining equations* for the pseudogroup.

Theorem IV.2: *The structure equations of the invariant coframe for a Lie pseudogroup $\mathcal{G}$ are obtained by restricting the diffeomorphism structure equations (7) and (8) to the space of solutions of the lifted determining equations (11).*

Since the target coordinates $Z=(Z^a)$ are right invariant, the individual fibers of the target fibration $\boldsymbol{\tau}^{(n)}:\mathcal{G}^{(n)}\to M$ are invariant under the right-action of $\mathcal{G}$ and, for that matter, $\mathcal{G}^{(n)}$. The

Cartan structure equations of a Lie pseudogroup,[3] are obtained by restricting the invariant coframe to a single fiber $\mathcal{G}^{(n)}|_Z=(\boldsymbol{\tau}^{(n)})^{-1}(Z)$, where $Z\in M$ is fixed. Since $0=\mathrm{d}Z^a=\sigma^a+\mu^a$ when restricted to a fiber $\mathcal{G}^{(n)}|_Z$, we can replace σ^a by $-\mu^a$, and hence only the independent invariant contact forms μ^a_J will appear in the resulting structure equations. For example, if the pseudogroup is defined by the (local) action of a finite-dimensional Lie transformation group G on M, then, under some mild regularity assumptions, $\mathcal{G}^{(n)}\to M$ has the structure of a principal G-bundle for n sufficiently large. Each fiber can be identified with a copy of the Lie group, and the restrictions of the independent invariant contact forms to $\mathcal{G}^{(n)}|_Z\simeq G$ are a system of classical (right-invariant) Maurer–Cartan forms for the group G.

These results form the foundation for a general, intrinsic algorithm for directly determining the structure of the symmetry group of a system of differential equations, as well as the structure of its algebra of differential invariants, as fixed by a choice of a moving frame.[7,9] The key point is that the required computations rely exclusively on linear differential algebra, and so can be readily implemented in any standard symbolic computation package. In this paper, we have concentrated on the first part of the method, the determination of the structure of the symmetry (pseudo)group. The second part, on the structure of the differential invariant algebra and the invariant variational bicomplex[9,10] will be explained in more detail in a subsequent publication.

KP equation 3: Let $\mathcal{G}$ denote the infinite-dimensional symmetry pseudogroup of the KP equation (1). We begin by writing out the lifted determining equations

$$\mu^y_U=0,\quad \mu^y_X=0,\quad \mu^x_U=0,\quad \mu^y_T+\tfrac{3}{2}\epsilon\mu^x_Y=0,\quad 3\mu^x_X-\mu^t_T=0,$$

$$\tfrac{3}{2}\mu^u-\mu^x_T+U\mu^t_T=0,\quad \tfrac{3}{2}\mu^y_Y-\mu^t_T=0,\quad \mu^t_U=0,\quad \mu^t_X=0,\quad \mu^t_Y=0, \tag{12}$$

$$\mu^t_T+\tfrac{3}{2}\mu^u_U=0,\quad \tfrac{2}{3}\mu^t_{TT}-3\mu^u_X=0,\quad \mu^u_{TX}+\tfrac{3}{2}U\mu^u_{XX}+\tfrac{1}{4}\mu^u_{XXXX}+\tfrac{3}{4}\epsilon\mu^u_{YY}=0,$$

and so on, which are obtained from the KP symmetry determining equations (4) by replacing t,x,y,u by T,X,Y,U and τ,ξ,η,ϕ by the invariant contact forms μ^t,μ^x,μ^y,μ^u, respectively. These and their higher order counterparts obtained by Lie differentiation with respect to the invariant differential operators (5) form a complete system of linear dependencies among the invariant contact forms when restricted to the symmetry groupoid $\mathcal{G}^{(\infty)}$.

We solve the lifted system of equations (12) [or, equivalently, the original system (4) of infinitesimal determining equations prior to the lifting] through cross-differentiations and Gaussian elimination to determine the following basis of linearly independent Maurer–Cartan forms,

$$\omega^1:=\mu^t,\quad \omega^2:=\mu^x,\quad \omega^3:=\mu^y,\quad \omega^4:=\mu^u,\quad \omega^5:=\mu^t_T=\mu^t_{1,0,0,0},$$

$$\omega^6:=\mu^y_T=\mu^y_{1,0,0,0},\quad \alpha^i:=\mu^u_{i,0,0,0},\quad \beta^i:=\mu^u_{i-1,1,0,0},\quad \gamma^i:=\mu^u_{i-1,0,1,0}, \tag{13}$$

for $i=1,2,3,\ldots$. For example,

$$\mu^x_T=\tfrac{3}{2}\omega^4+U\omega^5,\quad \mu^t_X=0,\quad \mu^x_X=\tfrac{1}{3}\omega^5,$$

$$\mu^y_X=0,\quad \mu^t_Y=0,\quad \mu^x_Y=-\tfrac{2}{3}\epsilon\omega^6,\quad \mu^y_Y=\tfrac{2}{3}\omega^5,$$

$$\mu^t_U=0,\quad \mu^x_U=0,\quad \mu^y_U=0,\quad \mu^u_U=-\tfrac{2}{3}\omega^5, \tag{14}$$

$$\mu^t_{TT}=\tfrac{9}{2}\beta^1,\quad \mu^x_{TT}=\tfrac{3}{2}\alpha^1+\tfrac{9}{2}U\beta^1,\quad \mu^y_{TT}=-\tfrac{9}{4}\epsilon\gamma^1,$$

$$\mu^t_{TX}=0,\quad \mu^x_{TX}=\tfrac{3}{2}\beta^1,\quad \mu^y_{TX}=0,\quad \mu^t_{TY}=0,\quad \ldots.$$

The independent invariant contact forms (13) together with the restricted invariant horizontal forms $\{\sigma^t, \sigma^x, \sigma^y, \sigma^u\}$ form an invariant coframe on the Lie groupoid $\mathcal{G}^{(\infty)}$. The structure equations of this coframe are obtained by imposing the dependence relation (14) on the structure equations (9) for the full diffeomorphism groupoid $\mathcal{D}^{(\infty)}$. The resulting structure equations are

$$\mathrm{d}\sigma^t = \omega^5 \wedge \sigma^t,$$

$$\mathrm{d}\sigma^x = \tfrac{3}{2}\omega^4 \wedge \sigma^t + U\omega^5 \wedge \sigma^t + \tfrac{1}{3}\omega^5 \wedge \sigma^x - \tfrac{2}{3}\epsilon\omega^6 \wedge \sigma^y,$$

$$\mathrm{d}\sigma^y = \tfrac{2}{3}\omega^5 \wedge \sigma^y + \omega^6 \wedge \sigma^t,$$

$$\mathrm{d}\sigma^u = -\tfrac{2}{3}\omega^5 \wedge \sigma^u + \alpha^1 \wedge \sigma^t + \beta^1 \wedge \sigma^x + \gamma^1 \wedge \sigma^y,$$

$$\mathrm{d}\omega^1 = -\omega^5 \wedge \sigma^t,$$

$$\mathrm{d}\omega^2 = -\tfrac{3}{2}\omega^4 \wedge \sigma^t - U\omega^5 \wedge \sigma^t - \tfrac{1}{3}\omega^5 \wedge \sigma^x + \tfrac{2}{3}\epsilon\omega^6 \wedge \sigma^y,$$

$$\mathrm{d}\omega^3 = -\tfrac{2}{3}\omega^5 \wedge \sigma^y - \omega^6 \wedge \sigma^t,$$

$$\mathrm{d}\omega^4 = \tfrac{2}{3}\omega^5 \wedge \sigma^u - \alpha^1 \wedge \sigma^t - \beta^1 \wedge \sigma^x - \gamma^1 \wedge \sigma^y,$$

$$\mathrm{d}\omega^5 = -\tfrac{9}{2}\beta^1 \wedge \sigma^t,$$

$$\mathrm{d}\omega^6 = -\tfrac{1}{3}\omega^5 \wedge \omega^6 - 3\beta^1 \wedge \sigma^y + \tfrac{9}{4}\epsilon\gamma^1 \wedge \sigma^t,$$

$$\mathrm{d}\alpha^1 = -\tfrac{3}{2}\omega^4 \wedge \beta^1 - \tfrac{5}{3}\omega^5 \wedge \alpha^1 - U\omega^5 \wedge \beta^1 - \omega^6 \wedge \gamma^1 + 3\beta^1 \wedge \sigma^u - \alpha^2 \wedge \sigma^t - \beta^2 \wedge \sigma^x - \gamma^2 \wedge \sigma^y,$$

$$\mathrm{d}\beta^1 = -\omega^5 \wedge \beta^1 - \beta^2 \wedge \sigma^t,$$

$$\mathrm{d}\gamma^1 = -\tfrac{4}{3}\omega^5 \wedge \gamma^1 + \tfrac{2}{3}\epsilon\omega^6 \wedge \beta^1 + \tfrac{4}{3}\epsilon\beta^2 \wedge \sigma^y - \gamma^2 \wedge \sigma^t,$$

$$\mathrm{d}\alpha^2 = -3\omega^4 \wedge \beta^2 - \tfrac{8}{3}\omega^5 \wedge \alpha^2 - 2U\omega^5 \wedge \beta^2 - 2\omega^6 \wedge \gamma^2 + 9\alpha^1 \wedge \beta^1 + 3\beta^2 \wedge \sigma^u - \alpha^3 \wedge \sigma^t - \beta^3 \wedge \sigma^x - \gamma^3 \wedge \sigma^y,$$

$$\mathrm{d}\beta^2 = -2\omega^5 \wedge \beta^2 - \beta^3 \wedge \sigma^t,$$

$$\mathrm{d}\gamma^2 = -\tfrac{7}{3}\omega^5 \wedge \gamma^2 + 2\epsilon\omega^6 \wedge \beta^2 - \tfrac{9}{2}\beta^1 \wedge \gamma^1 - \gamma^3 \wedge \sigma^t + \tfrac{4}{3}\epsilon\beta^3 \wedge \sigma^y, \quad \dots . \tag{15}$$

After restricting the equations (15) to a target fiber $(\boldsymbol{\tau}^{(\infty)})^{-1}(T, X, Y, U)$, i.e., fixing the values of the target coordinates T, X, Y, U, we find the Maurer–Cartan equations for the KP symmetry pseudogroup $\mathcal{G}$ to be

$$\mathrm{d}\omega^1 = -\omega^1 \wedge \omega^5,$$

$$\mathrm{d}\omega^2 = -\tfrac{3}{2}\omega^1 \wedge \omega^4 - U\omega^1 \wedge \omega^5 - \tfrac{1}{3}\omega^2 \wedge \omega^5 + \tfrac{2}{3}\epsilon\omega^3 \wedge \omega^6,$$

$$\mathrm{d}\omega^3 = -\omega^1\wedge\omega^6 - \tfrac{2}{3}\omega^3\wedge\omega^5,$$

$$\mathrm{d}\omega^4 = -\omega^1\wedge\alpha^1 - \omega^2\wedge\beta^1 - \omega^3\wedge\gamma^1 + \tfrac{2}{3}\omega^4\wedge\omega^5,$$

$$\mathrm{d}\omega^5 = -\tfrac{9}{2}\omega^1\wedge\beta^1,$$

$$\mathrm{d}\omega^6 = \tfrac{9}{4}\epsilon\omega^1\wedge\gamma^1 - 3\omega^3\wedge\beta^1 - \tfrac{1}{3}\omega^5\wedge\omega^6,$$

$$\mathrm{d}\alpha^1 = -\omega^1\wedge\alpha^2 - \omega^2\wedge\beta^2 - \omega^3\wedge\gamma^2 + \tfrac{3}{2}\omega^4\wedge\beta^1 - \tfrac{5}{3}\omega^5\wedge\alpha^1 - U\omega^5\wedge\beta^1 - \omega^6\wedge\gamma^1,$$

$$\mathrm{d}\beta^1 = -\omega^1\wedge\beta^2 - \omega^5\wedge\beta^1,$$

$$\mathrm{d}\gamma^1 = -\omega^1\wedge\gamma^2 + \tfrac{4}{3}\epsilon\omega^3\wedge\beta^2 - \tfrac{4}{3}\omega^5\wedge\gamma^1 + \tfrac{2}{3}\epsilon\omega^6\wedge\beta^1,$$

$$\mathrm{d}\alpha^2 = -\omega^1\wedge\alpha^3 - \omega^2\wedge\beta^3 - \omega^3\wedge\gamma^3 - \tfrac{8}{3}\omega^5\wedge\alpha^2 - 2U\omega^5\wedge\beta^2 - 2\omega^6\wedge\gamma^2 + 9\alpha^1\wedge\beta^1,$$

$$\mathrm{d}\beta^2 = -\omega^1\wedge\beta^3 - 2\omega^5\wedge\beta^2,$$

$$\mathrm{d}\gamma^2 = -\omega^1\wedge\gamma^3 + \tfrac{4}{3}\epsilon\omega^3\wedge\beta^3 - \tfrac{7}{3}\omega^5\wedge\gamma^2 + 2\epsilon\omega^6\wedge\beta^2 - \tfrac{9}{2}\beta^1\wedge\gamma^1, \quad \ldots.$$

The structure equations for a slightly different variant of the KP equation obtained by Reid *et al.*,[14–16] involve nine basic Maurer–Cartan forms $\{\boldsymbol{\omega}^i \,|\, i=1,2,\ldots,9\}$. The Maurer–Cartan equations that our algorithm finds for the particular target fiber $U=0$ can be mapped to theirs by the scaling correspondence

$$\omega^3 = \mu^y \mapsto p\boldsymbol{\omega}^1, \quad \omega^2 = \mu^x \mapsto \frac{p^2}{q}\boldsymbol{\omega}^2, \quad \omega^1 = \mu^t \mapsto q\boldsymbol{\omega}^3,$$

$$\omega^4 = \mu^u \mapsto -\frac{p^2}{q^2}\boldsymbol{\omega}^4, \quad \gamma^1 = \mu^u_Y \mapsto -\frac{p}{q^2}\boldsymbol{\omega}^5, \quad \beta^1 = \mu^u_X \mapsto -\frac{1}{q}\boldsymbol{\omega}^6,$$

$$\alpha^1 = \mu^u_T \mapsto -\frac{p^2}{q^3}\boldsymbol{\omega}^7, \quad \omega^5 = \mu^t_T \mapsto -\frac{3}{2}\boldsymbol{\omega}^8, \quad \omega^6 = \mu^y_T \mapsto -\frac{2p}{q}\boldsymbol{\omega}^9,$$

$$\beta^2 = \mu^u_{TX} \mapsto \frac{1}{q^2}\boldsymbol{\pi}^1, \quad \gamma^2 = \mu^u_{TY} \mapsto -\frac{p}{q^3}\boldsymbol{\pi}^2, \quad \alpha^2 = \mu^u_{TT} \mapsto -\frac{p^2}{q^4}\boldsymbol{\pi}^3,$$

where p,q are any nonzero constants. Moreover, the other invariant forms $\{\boldsymbol{\pi}^1,\boldsymbol{\pi}^2,\boldsymbol{\pi}^3\}$ appearing in their list of structure equations will correspond to rescalings of our next three second-order Maurer–Cartan forms $\alpha^2,\beta^2,\gamma^2$.

KdV equation: Now let $\mathcal{G}$ denote the symmetry group of the KdV equation (2). Applying Lie's algorithm, the infinitesimal symmetries $\mathbf{v}=\tau\partial_t+\xi\partial_x+\phi\partial_u$ must satisfy the (minimal) determining equations

$$\xi_u = 0, \quad 3\xi_x - \tau_t = 0, \quad \phi - \xi_t + \tfrac{2}{3}u\tau_t = 0, \quad \tau_u = 0,$$

$$\tau_x = 0, \quad \phi_{uu} = 0, \quad \phi_{xu} = 0, \quad \phi_t + u\phi_x + \phi_{xxx} = 0.$$

When this system is completed to involution, all the higher order equations are obtained by differentiation. The corresponding lifted determining equations are

$$\mu^x_U = 0, \quad 3\mu^x_X - \mu^t_T = 0, \quad \mu^u - \mu^x_T + \tfrac{2}{3}U\mu^t_T = 0, \quad \mu^t_U = 0,$$

$$\mu^t_X = 0, \quad \mu^u_{UU} = 0, \quad \mu^u_{XU} = 0, \quad \mu^u_T + U\mu^u_X + \mu^u_{XXX} = 0,$$

and so on, where the higher-order equations are obtained by repeated Lie differentiation with respect to $\mathbb{D}_T, \mathbb{D}_X, \mathbb{D}_U$. Restricting to the symmetry groupoid $\mathcal{G}^{(\infty)}$, there are precisely four independent invariant contact forms,

$$\omega^1 := \mu^t, \quad \omega^2 := \mu^x, \quad \omega^3 := \mu^u, \quad \omega^4 := \mu^t_T,$$

which reflects the fact that the symmetry group of the KdV equation is a four-dimensional Lie group. The structure equations of the coframe are

$$\mathrm{d}\sigma^t = \omega^4 \wedge \sigma^t,$$

$$\mathrm{d}\sigma^x = \omega^3 \wedge \sigma^t + \tfrac{2}{3}U\omega^4 \wedge \sigma^t + \tfrac{1}{3}\omega^4 \wedge \sigma^x,$$

$$\mathrm{d}\sigma^u = -\tfrac{2}{3}\omega^4 \wedge \sigma^u,$$

$$\mathrm{d}\omega^1 = -\omega^4 \wedge \sigma^t,$$

$$\mathrm{d}\omega^2 = -\omega^3 \wedge \sigma^t - \tfrac{2}{3}U\omega^4 \wedge \sigma^t - \tfrac{1}{3}\omega^4 \wedge \sigma^x,$$

$$\mathrm{d}\omega^3 = \tfrac{2}{3}\omega^4 \wedge \sigma^u,$$

$$\mathrm{d}\omega^4 = 0,$$

where $\sigma^t, \sigma^x, \sigma^u$ are the invariant horizontal forms. The Maurer–Cartan equations for the Lie symmetry group $\mathcal{G}$ are obtained by restricting to a target fiber where T, X, U are fixed, whence

$$\mathrm{d}\omega^1 = -\omega^1 \wedge \omega^4,$$

$$\mathrm{d}\omega^2 = -\omega^1 \wedge \omega^3 - \tfrac{2}{3}U\omega^1 \wedge \omega^4 - \tfrac{1}{3}\omega^2 \wedge \omega^4,$$

$$\mathrm{d}\omega^3 = \tfrac{2}{3}\omega^3 \wedge \omega^4,$$

$$\mathrm{d}\omega^4 = 0.$$

V. DISCUSSION

An efficient method for finding the local structure of Lie symmetry pseudogroups of differential equations was explained, and was demonstrated for the particular cases of the KP and KdV equations. The algorithm can be straightforwardly applied to any system of differential equations, irrespective of whether its symmetry group is finite dimensional or infinite dimensional. To apply our method to other more complicated differential equations, we should optimize our computational procedure and develop more efficient symbolic algebra routines.

The next stage of applications of our method is to develop the moving frame algorithms for pseudogroup actions on submanifolds,[23] which will construct complete systems of differential invariants and invariant differential forms, classify their syzygies and recurrence relations, analyze invariant variational principles,[9,10] and solve equivalence and symmetry problems arising in geometry and physics.

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Local and nonlocal symmetries for nonlinear telegraph equation

G. W. Bluman,[a] Temuerchaolu,[b] and R. Sahadevan[c]
Department of Mathematics, University of British Columbia, Vancouver, BC, Canada V6T 1Z2

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In this paper, local and nonlocal symmetry classifications are considered for four equivalent nonlinear telegraph equations. A complete potential symmetry classification of a scalar nonlinear telegraph equation is given through the point symmetry classification of a related potential system. Six new classes of equations are shown to admit potential symmetries. The relationships between local (including contact) and nonlocal (potential) symmetries of these equations are explored. A physical example is considered for possible applications of the obtained potential symmetries. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1841481]

I. INTRODUCTION

In Refs. 1–4, an algorithmic procedure has been developed to find nonlocal symmetries (potential symmetries) of partial differential equations (PDEs) to extend the classes of symmetries admitted by PDEs. Various researchers have found examples of PDEs that admit potential symmetries or extended the procedure to find potential systems.[5]

In recent years, there have been several investigations (Refs. 6–8) to find symmetries for nonlinear telegraph equations of the form

$$u_{tt} = [F(u)u_x]_x + [G(u)]_x. \tag{1}$$

PDE (1) is equivalent to the potential system

$$v_x = u_t,$$

$$v_t = F(u)u_x + G(u). \tag{2}$$

In particular, if $(u,v)=(U(x,t),V(x,t))$ solves (2), then $u=U(x,t)$ solves (1). Conversely, for any $u=U(x,t)$ solving (1), there exists a pair of functions $(u,v)=(U(x,t),V(x,t))$ solving (2) with $V(x,t)$ unique to within a constant.

Similarly, the potential system (2) is equivalent to the potential system

$$w_t = v,$$

$$w_x = u, \tag{3}$$

[a]Electronic mail: bluman@math.ubc.ca
[b]Permanent address: Inner Mongolia Polytechnic University, Hohhot, 010062, Peoples Republic of China. Electronic mail: tmchaolu@impu.edu.cn
[c]Permanent address: Ramanujan Institute for Advanced Study in Mathematics, University of Madras, Chepauk, Chennai 600 005, Tamil Nadu, India. Electronic mail: sahadevan@unom.ac.in and riasm@md3.vsnl.net.in

$$v_t = F(u)u_x + G(u),$$

and hence to the potential equation

$$w_{tt} = F(w_x)w_{xx} + G(w_x). \tag{4}$$

In particular, if $u=U(x,t)$ solves (1), then from the integrability conditions associated with (3) there exists a triplet $(u,v,w)=(U(x,t),V(x,t),W(x,t))$ solving system (3) with $w=W(x,t)$ solving (4). Conversely, if $w=W(x,t)$ solves (4), then $(u,v)=(W_x(x,t),W_t(x,t))$ solves (2) and $u=W_x(x,t)$ solves (1).

Consequently, a symmetry of any one of the PDE systems (1)–(4) defines a symmetry of the remaining three equivalent systems. Moreover, due to the relationship connecting these four equivalent systems, it is possible for a local symmetry of any one of these systems to yield a nonlocal symmetry of another one.[9]

Equations related to (1) include the nonlinear heat conduction equation when $F(u)=0$, and the nonlinear inhomogeneous vibrating string equation when $G(u)=0$.

The group properties of the nonlinear heat equation for both the scalar form (1) and the potential system (2) are presented in Ref. 2. The point symmetry classification of the nonlinear wave equation (1) with $G(u)=0$ and $F(u)$ replaced by $F(x,u)$ is discussed in Ref. 6. The complete point symmetry classifications of equation (1) and the equivalent potential equation (4) are given in Refs. 7 and 8, respectively. Some exact solutions of system (2) are given in Ref. 10 for special forms of $F(u)$ and $G(u)$.

Among the equivalent systems (1)–(4), it appears that the potential system (2) arises most directly in physical situations. One physical example directly related to system (2) is represented by the equations of telegraphy of a two-conductor transmission line with v as the current in the conductors, u as the voltage between the conductors, $G(u)$ as the leakage current per unit length, $F(u)$ as the differential capacitance, t as a spatial variable and x as time.[11] Another physical example related to system (2) is the equation of motion of a hyperelastic homogeneous rod whose cross-sectional area varies exponentially along the rod. Here u is the displacement gradient related to the difference between a spatial Eulerian coordinate and a Lagrangian coordinate x, v is the velocity of a particle displaced by this difference, $G(u)$ is essentially the stress tensor, $F(u)=\lambda G'(u)$ for some constant λ, and t is time (see Refs. 12 and 13).

In this paper we give the complete point symmetry classification of the potential system (2) and compare our results with the complete point symmetry classification of the scalar equation (1) included in Ref. 7 and the complete point symmetry classification of the potential equation (4) given in Ref. 8. In particular, we will show the following.

(I) The point symmetry classifications of the scalar equations (1) and (4) are identical, i.e., for any $F(u)$ and $G(u)$, a point symmetry admitted by (1) induces a point symmetry admitted by (4) and vice versa.

(II) For wide classes of $F(u)$ and $G(u)$, there exist point symmetries of the potential system (2) which are nonlocal symmetries of the scalar equation (1).

(III) Each point symmetry of the potential system (2) which is a nonlocal symmetry of (1) yields a contact symmetry of the potential equation (4) that is *not* a point symmetry of (4).

(IV) For all but one particular class of $F(u)$ and $G(u)$, a point symmetry of the scalar equation (1) is a point symmetry of (2).

In Sec. II, we give the set of determining equations for point symmetries of the potential system (2) and the complete potential symmetry classification of the scalar equation (1) related to (2). In Secs. III and IV, we present the complete point symmetry classifications of the scalar equations (1) and (4) given in Refs. 7 and 8, respectively. In Sec. V, we compare the point symmetry classifications of the systems (1), (2), and (4) by proving theorems that yield statements (I)–(IV). The second physical example is considered in Sec. VI. Further comments are given in Sec. VII.

II. POTENTIAL SYMMETRY CLASSIFICATION OF THE SCALAR EQUATION (1)

Consider the potential system (2).

The point symmetry

$$x^* = x + \varepsilon\xi(x,t,u,v) + O(\varepsilon^2),$$

$$t^* = t + \varepsilon\tau(x,t,u,v) + O(\varepsilon^2),$$

$$u^* = u + \varepsilon\eta(x,t,u,v) + O(\varepsilon^2),$$

$$v^* = v + \varepsilon\phi(x,t,u,v) + O(\varepsilon^2), \tag{5}$$

is admitted by system (2) if and only if it satisfies the determining equations,

$$X^{(1)}(v_x - u_t) = 0,$$

$$X^{(1)}(v_t - F(u)u_x - G(u)) = 0, \tag{6}$$

for *any* (u,v) that solves system (2);

$$X = \xi(x,t,u,v)\frac{\partial}{\partial x} + \tau(x,t,u,v)\frac{\partial}{\partial t} + \eta(x,t,u,v)\frac{\partial}{\partial u} + \phi(x,t,u,v)\frac{\partial}{\partial v}$$

is the infinitesimal generator of the point symmetry (5);

$$X^{(1)} = X + \eta^{(1)}\frac{\partial}{\partial u_x} + \eta^{(2)}\frac{\partial}{\partial u_t} + \phi^{(1)}\frac{\partial}{\partial v_x} + \phi^{(2)}\frac{\partial}{\partial v_t},$$

with

$$\eta^{(1)} = \frac{D\eta}{Dx} - \frac{D\xi}{Dx}u_x - \frac{D\tau}{Dx}u_t, \quad \eta^{(2)} = \frac{D\eta}{Dt} - \frac{D\xi}{Dt}u_x - \frac{D\tau}{Dt}u_t,$$

$$\phi^{(1)} = \frac{D\phi}{Dx} - \frac{D\xi}{Dx}v_x - \frac{D\tau}{Dx}v_t, \quad \phi^{(2)} = \frac{D\phi}{Dt} - \frac{D\xi}{Dt}v_x - \frac{D\tau}{Dt}v_t,$$

is the first extension (prolongation) of X;

$$\frac{D}{Dx} = \frac{\partial}{\partial x} + u_x\frac{\partial}{\partial u} + v_x\frac{\partial}{\partial v} + u_{xx}\frac{\partial}{\partial u_x} + u_{xt}\frac{\partial}{\partial u_t} + v_{xx}\frac{\partial}{\partial v_x} + v_{xt}\frac{\partial}{\partial v_t},$$

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u_t\frac{\partial}{\partial u} + v_t\frac{\partial}{\partial v} + u_{xt}\frac{\partial}{\partial u_x} + u_{tt}\frac{\partial}{\partial u_t} + v_{xt}\frac{\partial}{\partial v_x} + v_{tt}\frac{\partial}{\partial v_t}$$

are total derivative operators. Note that $\eta^{(i)}, \phi^{(i)}$ are functions of x,t,u,v,u_x,u_t,v_x,v_t, $i=1,2$.

The global one-parameter (ε) Lie group of point symmetries associated with (5) is obtained by solving the initial value problem for the first order system of ordinary differential equations (ODEs)

$$\frac{dx^*}{d\varepsilon} = \xi(x^*,t^*,u^*,v^*),$$

$$\frac{dt^*}{d\varepsilon} = \tau(x^*, t^*, u^*, v^*),$$

$$\frac{du^*}{d\varepsilon} = \eta(x^*, t^*, u^*, v^*),$$

$$\frac{dv^*}{d\varepsilon} = \phi(x^*, t^*, u^*, v^*), \tag{7}$$

with $x^* = x$, $t^* = t$, $u^* = u$, $v^* = v$ at $\varepsilon = 0$.

A point symmetry (5) yields a *nonlocal symmetry* of the scalar equation (1) if and only if $\xi_v^2 + \tau_v^2 + \eta_v^2 \neq 0$, i.e., if and only if the infinitesimals ξ, τ, and η have an essential dependence on the potential variable v. Such a nonlocal symmetry is called a *potential symmetry* of scalar equation (1) related to the potential system (2) (for details, see Ref. 3).

The determining equations (6) simplify to

$$\xi_v - \tau_u = 0,$$

$$\eta_u - \phi_v + \xi_x - \tau_t = 0,$$

$$G(u)\eta_v + \eta_t - \phi_x + G(u)\tau_x = 0,$$

$$\xi_u - F(u)\tau_v = 0,$$

$$\phi_u - G(u)\tau_u - F(u)\eta_v = 0,$$

$$G(u)\xi_v + \xi_t - F(u)\tau_x = 0,$$

$$[\phi_v - \tau_t - 2G(u)\tau_v - \eta_u + \xi_x]F(u) - F'(u)\eta = 0,$$

$$[\phi_v - \tau_t - G(u)\tau_v]G(u) - F(u)\eta_x - G'(u)\eta + \phi_t = 0. \tag{8}$$

We now consider the classification problem of finding all $F(u)$, $G(u)$ such that the potential system (2) yields a potential symmetry of (1).

If

$$F(u) = \frac{c}{(au+b)^2}, \quad G(u) = \frac{d}{au+b} + f \tag{9}$$

for arbitrary constants a, b, c, d, f, or if

$$F(u) \text{ is arbitrary}, \quad G(u) = \text{const},$$

then through the potential system (2), the scalar equation admits an infinite number of potential symmetries and the potential system (2) is linearizable by a point transformation (see Refs. 3 and 4).

Various symbolic manipulation algorithms exist to solve the set of determining equations (8) (for example, see Refs. 14 and 15). Using the symmetry manipulation algorithm presented in Ref. 15, one can prove the following results.

Theorem 1: *The scalar equation (1) admits a potential symmetry related to potential system (2) if and only if the functions $F(u)$ and $G(u)$, with $G'(u) \neq 0$, satisfy the system of ODEs,*

$$(c_4u + c_5)F'(u) - 2(c_1 - c_3 - c_2G(u))F(u) = 0, \tag{10}$$

$$(c_4u + c_5)G'(u) + c_2G^2(u) - (c_1 - 2c_3 + c_4)G(u) - c_6 = 0, \tag{11}$$

for any fixed constants $c_1, c_2, \ldots, c_6$ *with* $c_2 \neq 0$.

In the linearizable case (9),

$$c_1 = 0, \quad c_6 = \frac{c_3(c_4 - c_3)}{c_2}.$$

Theorem 2: *For any* $F(u)$, $G(u)$ *satisfying the system of ODEs (10) and (11) with* $c_2 \neq 0$, *the potential system (2) admits the point symmetry (5) with*

$$\xi = c_1x + c_2 \int F(u)\mathrm{d}u,$$

$$\tau = c_3t + c_2v,$$

$$\eta = c_4u + c_5,$$

$$\phi = c_6t + (c_1 - c_3 + c_4)v, \tag{12}$$

and hence the scalar equation (1) admits the corresponding potential symmetry.

Now we find the functions $F(u)$ and $G(u)$ satisfying (10), (11) and the corresponding potential symmetries (12).

Note that the point transformation

$$\overline{x} = ax + b, \quad \overline{t} = ct + d, \quad \overline{u} = \alpha u + \beta, \quad \overline{v} = \gamma v + \rho t$$

for any constants a, b, c, d, α, β, γ, and ρ such that $ac\alpha\gamma \neq 0$ and $a\alpha = c\gamma$ is an equivalence transformation for system (2). Under this transformation, system (2) becomes the equivalent system

$$\overline{v}_{\overline{x}} = \overline{u}_{\overline{t}}, \quad \overline{v}_{\overline{t}} = \overline{F}(\overline{u})\overline{u}_{\overline{x}} + \overline{G}(\overline{u}),$$

where

$$\overline{F}(\overline{u}) = \frac{a\gamma}{c\alpha}F\left(\frac{\overline{u} - \beta}{\alpha}\right)$$

and

$$\overline{G}(\overline{u}) = \frac{\gamma}{c}G\left(\frac{\overline{u} - \beta}{\alpha}\right) + \frac{\rho}{c}.$$

We use such equivalence transformations to simplify the analysis. For example, if $G(u) = a_0(b_0u + c_0)^{d_0} + f_0$, without loss of generality we can assume that $G(u) = u^{d_0}$.

Modulo translations and scalings in u and G, we obtain six distinct classes of ODEs for $F(u)$ and $G(u)$ where scalar equation (1) admits potential symmetries. These six classes of ODEs and their solutions [modulo equivalence classes of $F(u)$ and $G(u)$] are presented in Table I. In Table II for each class we display the corresponding infinitesimals (ξ, τ, η, ϕ) and global group (x^*, t^*, u^*, v^*) obtained from solving the corresponding ODEs (7).

All symmetries presented in Tables I and II are new for each of the equivalent systems (1)–(4). Note that classes 1 and 6 are linearizable[4] if $\beta = 0$ and $\alpha = 1/2$.

TABLE I. Classes of $F(u)$ and $G(u)$ yielding potential symmetries of (1).

Class	ODEs satisfied by $F(u)$ and $G(u)$	$G(u)$	$F(u)$	Relationship between $F(u)$ and $G(u)$
1	$uG'-\alpha(1-G^2)=0$ $uF'-(\beta-1-2\alpha G)F=0$	$(u^{2\alpha}-1)/(u^{2\alpha}+1)$ $(u^{2\alpha}+1)/(u^{2\alpha}-1)$	$4u^{2\alpha+\beta-1}/(u^{2\alpha}+1)^2$ $-4u^{2\alpha+\beta-1}/(u^{2\alpha}-1)^2$	$F(u)=(u^\beta/\alpha)G'(u)$
2	$uG'-\alpha(1+G^2)=0$ $uF'+(1-\beta-2\alpha G)F=0$	$\tan(\alpha \ln u)$	$u^{\beta-1}\sec^2(\alpha \ln u)$	,,
3	$uG'+G^2=0$ $uF'-(\beta-1-2G)F=0$	$(\ln u)^{-1}$	$-u^{\beta-1}(\ln u)^{-2}$	,,
4	$G'-G^2-1=0$ $F'-2(\beta+G)F=0$	$\tan u$	$e^{2\beta u}\sec^2 u$	$F(u)=e^{2\beta u}G'(u)$
5	$G'+G^2-1=0$ $F'-2(\beta-G)F=0$	$\tanh u$ $\coth u$	$e^{2\beta u}\operatorname{sech}^2 u$ $-e^{2\beta u}\operatorname{csch}^2 u$	,,
6	$G'+G^2=0$ $F'-2(\beta-G)F=0$	u^{-1}	$-u^{-2}e^{2\beta u}$	,,

III. POINT SYMMETRY CLASSIFICATION OF THE SCALAR EQUATION (1)

In Ref. 7, Kingston and Sophocleous considered the classification problem of finding all $F(u)$, $G(u)$ such that the scalar equation (1) admits a point symmetry. The point symmetry

$$x^* = x + \varepsilon\xi(x,t,u) + O(\varepsilon^2),$$

TABLE II. Potential symmetries of (1) for each class $[\Gamma(\beta,F,\varepsilon)=\int^{ue^{2\varepsilon}} s^{-(1+\beta)}(\int^s F(x)\mathrm{d}x)\mathrm{d}s,\ \Omega(\beta,F,\varepsilon)=\int^{u+\varepsilon} e^{-2\beta s}(\int^s F(x)\mathrm{d}x)\mathrm{d}s]$.

	Class	Infinitesimals ξ,τ,η,ϕ	Global group
1	$F(u)=4u^{2\alpha+\beta-1}/(u^{2\alpha}+1)^2$ $G(u)=(u^{2\alpha}-1)/(u^{2\alpha}+1)$ or $F(u)=-4u^{2\alpha+\beta-1}/(u^{2\alpha}-1)^2$ $G(u)=(u^{2\alpha}+1)/(u^{2\alpha}-1)$	$\xi=2(\beta x+\alpha\int F(u)\mathrm{d}u)$ $\tau=(\beta+1)t+2\alpha v$ $\eta=2u$ $\phi=2\alpha t+(\beta+1)v$	$x^*=e^{2\beta\varepsilon}[x+\alpha u^\beta(\Gamma(\beta,F,\varepsilon)-\Gamma(\beta,F,0))]$ $t^*=(1/2)e^{(\beta+1)\varepsilon}[(t+v)e^{2\alpha\varepsilon}+(t-v)e^{-2\alpha\varepsilon}]$ $u^*=ue^{2\varepsilon}$ $v^*=(1/2)e^{(\beta+1)\varepsilon}[(t+v)e^{2\alpha\varepsilon}-(t-v)e^{-2\alpha\varepsilon}]$
2	$F(u)=u^{\beta-1}\sec^2(\alpha \ln u)$ $G(u)=\tan(\alpha \ln u)$	$\xi=2(\beta x-\alpha\int F(u)\mathrm{d}u)$ $\tau=(\beta+1)t-2\alpha v$ $\eta=2u$ $\phi=2\alpha t+(\beta+1)v$	$x^*=e^{2\beta\varepsilon}[x-\alpha u^\beta(\Gamma(\beta,F,\varepsilon)-\Gamma(\beta,F,0))]$ $t^*=e^{(\beta+1)\varepsilon}[t\cos 2\alpha\varepsilon-v\sin 2\alpha\varepsilon]$ $u^*=ue^{2\varepsilon}$ $v^*=e^{(\beta+1)\varepsilon}[v\cos 2\alpha\varepsilon+t\sin 2\alpha\varepsilon]$
3	$F(u)=-u^{\beta-1}(\ln u)^{-2}$ $G(u)=(\ln u)^{-1}$	$\xi=2(\beta x+\int F(u)\mathrm{d}u)$ $\tau=(\beta+1)t+2v$ $\eta=2u$ $\phi=(\beta+1)v$	$x^*=e^{2\beta\varepsilon}[x+u^\beta(\Gamma(\beta,F,\varepsilon)-\Gamma(\beta,F,0))]$ $t^*=e^{(\beta+1)\varepsilon}(2v\varepsilon+t)$ $u^*=ue^{2\varepsilon}$ $v^*=ve^{(\beta+1)\varepsilon}$
4	$F(u)=e^{2\beta u}\sec^2 u$ $G(u)=\tan u$	$\xi=2\beta x-\int F(u)\mathrm{d}u$ $\tau=\beta t-v$ $\eta=1$ $\phi=t+\beta v$	$x^*=e^{2\beta\varepsilon}[x-e^{2\beta u}(\Omega(\beta,F,\varepsilon)-\Omega(\beta,F,0))]$ $t^*=e^{\beta\varepsilon}(t\cos\varepsilon-v\sin\varepsilon)$ $u^*=u+\varepsilon$ $v^*=e^{\beta\varepsilon}(v\cos\varepsilon+t\sin\varepsilon)$
5	$F(u)=e^{2\beta u}\operatorname{sech}^2 u$ $G(u)=\tanh u$ or $F(u)=-e^{2\beta u}\operatorname{csch}^2 u$ $G(u)=\coth u$	$\xi=2\beta x+\int F(u)\mathrm{d}u$ $\tau=\beta t+v$ $\eta=1$ $\phi=t+\beta v$	$x^*=e^{2\beta\varepsilon}[x+e^{2\beta u}(\Omega(\beta,F,\varepsilon)-\Omega(\beta,F,0))]$ $t^*=(1/2)e^{\beta\varepsilon}((t+v)e^{\varepsilon}+(t-v)e^{-\varepsilon})$ $u^*=u+\varepsilon$ $v^*=(1/2)e^{\beta\varepsilon}((t+v)e^{\varepsilon}-(t-v)e^{-\varepsilon})$
6	$F(u)=-u^{-2}e^{2\beta u}$ $G(u)=u^{-1}$	$\xi=2\beta x+\int F(u)\mathrm{d}u$ $\tau=\beta t+v$ $\eta=1$ $\phi=\beta v$	$x^*=e^{2\beta\varepsilon}[x+e^{2\beta u}(\Omega(\beta,F,\varepsilon)-\Omega(\beta,F,0))]$ $t^*=e^{\beta\varepsilon}(t+v\varepsilon)$ $u^*=u+\varepsilon$ $v^*=ve^{\beta\varepsilon}$

TABLE III. Classes of $F(u)$ and $G(u)$ yielding point symmetries of (1).

Class	$G(u)$	$F(u)$	Infinitesimals ξ, τ, η
A	e^u	$e^{(\alpha+1)u}$	$\xi=2\alpha x, \tau=(\alpha-1)t, \eta=2$
B	$u^{\alpha+\beta+1}$	u^α	$\xi=2\beta x, \tau=(\alpha+2\beta)t, \eta=-2u$
C	u^{-1}	u^{-2}	Those in class B and $\xi=e^x, \tau=0, \eta=-ue^x$
D	$\ln u$	u^α	$\xi=2(\alpha+1)x, \tau=(\alpha+2)t, \eta=2u$
E	u	$e^{\alpha u}$	$\xi=2\alpha x, \tau=\alpha t, \eta=2$
F	u^{-3}	u^{-4}	Those in class B and $\xi=0, \tau=t^2, \eta=ut$

$$t^* = t + \varepsilon\tau(x,t,u) + O(\varepsilon^2),$$

$$u^* = u + \varepsilon\eta(x,t,u) + O(\varepsilon^2), \tag{13}$$

is admitted by the scalar equation (1) if and only if it satisfies the determining equation

$$X^{(2)}(u_{tt} - (F(u)u_x)_x - G(u)_x) = 0 \tag{14}$$

for any u solving the scalar equation (1);

$$X = \xi(x,t,u)\frac{\partial}{\partial x} + \tau(x,t,u)\frac{\partial}{\partial t} + \eta(x,t,u)\frac{\partial}{\partial u},$$

is the infinitesimal generator of the point symmetry (13); $X^{(2)}$ is the second extension of X.

From (14), the determining equations for $\xi(x,t,u)$, $\tau(x,t,u)$, and $\eta(x,t,u)$ are given by

$$\xi_u = \tau_x = \tau_u = \eta_{uu} = 0,$$

$$\xi_t - F(u)\tau_x = 0,$$

$$2F(u)(\xi_x - \tau_t) - F'(u)\eta = 0,$$

$$\eta_{tt} - F(u)\eta_{xx} - G'(u)\eta_x = 0,$$

$$2\eta_{tu} - \tau_{tt} + F(u)\tau_{xx} + G'(u)\tau_x = 0,$$

$$2F(u)\eta_{xu} + \xi_{tt} - F(u)\xi_{xx} + 2F'(u)\eta_x - G'(u)(\xi_x - 2\tau_t) + G''(u)\eta = 0.$$

For arbitrary $F(u)$ and $G(u)$, clearly each of the equivalent systems (1)–(4) admits translations in $x(\xi=1, \tau=0)$ and $t(\xi=0, \tau=1)$. For specific $F(u)$ and $G(u)$ with $G'(u)\neq 0$, the results are summarized in Table III.

Note that the classes presented in Ref. 7 where $F(u)=1$, $G(u)=e^{\lambda u}$ as well as $F(u)=1$, $G(u)=u^{\lambda+1}$ can be obtained, respectively, by appropriately scaling u in class A and setting $\alpha=0$ in class B.

IV. POINT SYMMETRY CLASSIFICATION OF THE SCALAR EQUATION (4)

In Ref. 8, the authors considered the classification problem of finding all $F(u)$, $G(u)$ such that the scalar equation (4) admits a point symmetry. The point symmetry

$$x^* = x + \varepsilon\xi(x,t,w) + O(\varepsilon^2),$$

TABLE IV. Classes of $F(u)$ and $G(u)$ yielding point symmetries of (4).

Class	$G(u)=G(w_x)$	$F(u)=F(w_x)$	Infinitesimals ξ, τ, η
A	e^u	$e^{(\alpha+1)u}$	$\xi=2\alpha x, \tau=(\alpha-1)t, \Omega=2(\alpha w+x)$
B	$u^{\alpha+\beta+1}$	u^α	$\xi=2\beta x, \tau=(\alpha+2\beta)t, \Omega=2(\beta-1)w$
C	u^{-1}	u^{-2}	Those in class B and $\xi=e^x, \tau=0, \Omega=0$
D	$\ln u$	u^α	$\xi=2(\alpha+1)x, \tau=(\alpha+2)t, \Omega=2(\alpha+2)w+t^2$
E	u	$e^{\alpha u}$	$\xi=2\alpha x, \tau=\alpha t, \Omega=2\alpha w+t^2+2x$
F	u^{-3}	u^{-4}	Those in class B and $\xi=0, \tau=t^2, \Omega=tw$

$$t^* = t + \varepsilon\tau(x,t,w) + O(\varepsilon^2),$$

$$w^* = w + \varepsilon\Omega(x,t,w) + O(\varepsilon^2), \tag{15}$$

is admitted by the scalar equation (4) if and only if it satisfies the determining equation

$$X^{(2)}(w_{tt} - F(w_x)w_{xx} - G(w_x)) = 0$$

for any w solving the scalar equation (4);

$$X = \xi(x,t,w)\frac{\partial}{\partial x} + \tau(x,t,w)\frac{\partial}{\partial t} + \Omega(x,t,w)\frac{\partial}{\partial w},$$

is the infinitesimal generator of the point symmetry (15); $X^{(2)}$ is the second extension of X.

Modulo equivalence transformations, the results presented in Ref. 8 are summarized in Table IV.

V. DISCUSSION OF THE SYMMETRY CLASSIFICATIONS

In this section we prove the statements (I)–(IV) presented in the Introduction through proofs of the following four theorems.

Theorem 3: *The point symmetry classifications of the scalar equations (1) and (4) are identical, i.e., for any $F(u)$ and $G(u)$ a point symmetry admitted by (1) induces a point symmetry admitted by (4) and vice versa.*

Proof: The infinitesimals of a point symmetry of the scalar equation (1) are of the form

$$\xi = \xi(x), \quad \tau = \tau(t), \quad \eta = (f(t) - \xi'(x))u + b$$

for some functions $\xi(x)$, $\tau(t)$, $f(t)$ and constant b. A corresponding point symmetry of the potential scalar equation (4) (with $u=w_x$) must have $\xi=\xi(x)$, $\tau=\tau(t)$, $\Omega=\Omega(x,t,w)$ with $\Omega(x,t,w)$ satisfying

$$\Omega^{x(1)} = \eta$$

in terms of its first extended infinitesimal $\Omega^{x(1)}$, i.e.,

$$\Omega^{x(1)} = \frac{D\Omega}{Dx} - \frac{D\xi}{Dx}w_x - \frac{D\tau}{Dx}w_t = \Omega_x + \Omega_w w_x - \xi'(x)w_x = (f(t) - \xi'(x))w_x + b. \tag{16}$$

Hence from Eq. (16), we must have

$$\Omega_x = b, \quad \Omega_w = f(t).$$

Then it is necessary that

$$\Omega = bx + f(t)w + g(t), \tag{17}$$

for some $g(t)$ in order that a point symmetry of the scalar equation (1) yields a point symmetry of the scalar equation (4). From Tables III and IV, it is easy to check that condition (17) is satisfied for each point symmetry of the scalar equation (4).

Conversely, the infinitesimals of a point symmetry of (4) are of the form

$$\xi = \xi(x), \quad \tau = \tau(t), \quad \Omega = f(t)w + \beta(x,t)$$

for some functions $\xi(x)$, $\tau(t)$, $f(t)$, and $\beta(x,t)$. A corresponding point symmetry of the scalar equation (1) with $u = w_x$ must have

$$\xi = \xi(x), \quad \tau = \tau(t), \quad \eta = \eta(x,t,u).$$

In terms of the first extended infinitesimal $\Omega^{x(1)}$, the infinitesimal $\eta(x,t,u)$ must satisfy

$$\eta = \Omega^{x(1)} = \frac{D\Omega}{Dx} - \frac{D\xi}{Dx}w_x - \frac{D\tau}{Dx}w_t = \Omega_x + \Omega_w w_x - \xi'(x)w_x = \beta_x + (f(t) - \xi'(x))w_x. \tag{18}$$

From Tables III and IV, it is easy to check that condition (18) is satisfied for each point symmetry of (1). ■

Theorem 4: *For each of the six classes of $F(u)$ and $G(u)$ listed in Table I, there exist point symmetries of the potential system (2) which are nonlocal symmetries of the scalar equation (1).*

Proof: Since each point symmetry in Table II has $\tau_v \neq 0$, it follows that for all classes of $F(u)$ and $G(u)$ listed in Table I (also repeated in Table II) there exist point symmetries of the potential system (2) which are nonlocal (potential) symmetries of the scalar equation (1). ■

Note that only the class $F(u) = u^{-2}$, $G(u) = u^{-1}$ is common for Tables I and III. This class is linearizable since it admits potential symmetries leading to the linearization of (2) by a point transformation.[4]

Theorem 5: *Each point symmetry of the potential system (2) which is a nonlocal symmetry of the scalar equation (1) yields a contact symmetry of the potential equation (4) that is* not *a point symmetry of (4).*

Proof: A *contact symmetry* of a PDE with dependent variable w and independent variables x and t is defined by

$$x^* = x + \varepsilon\xi(x,t,w,w_x,w_t) + O(\varepsilon^2),$$

$$t^* = t + \varepsilon\tau(x,t,w,w_x,w_t) + O(\varepsilon^2),$$

$$w^* = w + \varepsilon\Omega(x,t,w,w_x,w_t) + O(\varepsilon^2), \tag{19}$$

if and only if

$$\frac{\partial\Omega}{\partial w_x} = \frac{\partial\xi}{\partial w_x}w_x + \frac{\partial\tau}{\partial w_x}w_t, \quad \frac{\partial\Omega}{\partial w_t} = \frac{\partial\xi}{\partial w_t}w_x + \frac{\partial\tau}{\partial w_t}w_t. \tag{20}$$

Let characteristic function $W = \Omega - \xi w_x - \tau w_t$. A contact symmetry (19) is a point symmetry if and only if

$$\frac{\partial^2 W}{\partial(w_x)^2} = \frac{\partial^2 W}{\partial(w_t)^2} = \frac{\partial^2 W}{\partial w_x \partial w_t} = 0. \tag{21}$$

For details, see Chap. 5 of Ref. 3.

A point symmetry of potential system (2) which is a nonlocal symmetry of the scalar equation (1) (see Table II) is of the form

$$\xi = ax + b\int^{u} F(s)\mathrm{d}s, \quad \tau = ct + dv,$$

$$\eta = fu + g, \quad \phi = ht + kv, \tag{22}$$

for some constants a, b, c, d, f, g, h, and k with $d \neq 0$, $a+f=c+k$.

Solving (20), after using the substitution (22), we find that

$$\Omega(x,t,w,w_x,w_t) = b\int^{w_x} sF(s)\mathrm{d}s + \frac{d}{2}w_t^2 + A(x,t,w) \tag{23}$$

yields a contact symmetry for an arbitrary function $A(x,t,w)$.

Now we find $A(x,t,w)$ so that (23) yields a contact symmetry of the potential equation (4). Since $u=w_x$, $v=w_t$, it follows that we must have

$$\eta = \Omega^{x(1)} = \frac{D\Omega}{Dx} - \frac{D\xi}{Dx}w_x - \frac{D\tau}{Dx}w_t,$$

$$\phi = \Omega^{t(1)} = \frac{D\Omega}{Dt} - \frac{D\xi}{Dt}w_x - \frac{D\tau}{Dt}w_t, \tag{24}$$

in terms of first extended infinitesimals $\Omega^{x(1)}$ and $\Omega^{t(1)}$. After solving the equations (24), we find that $A(x,t,w)=gx+(a+f)w+\frac{1}{2}ht^2$ and hence

$$\xi = ax + b\int^{w_x} F(s)\mathrm{d}s, \quad \tau = ct + dw_t,$$

$$\Omega = b\int^{w_x} sF(s)\mathrm{d}s + \frac{d}{2}w_t^2 + gx + (a+f)w + \frac{1}{2}ht^2, \tag{25}$$

defines a contact symmetry of the scalar potential equation (4). Using condition (21), it is clear that (25) is *not* a point symmetry of (4) since $d \neq 0$. ■

Theorem 6: *A point symmetry of the scalar equation (1) yields a point symmetry of the potential equation (2) if and only if the infinitesimals for $F(u)$ and $G(u)$ belong to classes A–E in Table III.*

Proof: A point symmetry $(\xi(x,t,u), \tau(x,t,u), \eta(x,t,u))$ of the scalar equation (1) yields a point symmetry of (2) if and only if the set of determining equations (8) has a solution for $\phi(x,t,u,v)$. A solution of (8) exists if and only if the six integrability conditions involving the second order mixed partial derivatives of $\phi(x,t,u,v)$ are satisfied. Consequently, it is easy to show that a point symmetry of (1) yields a point symmetry of (2) if and only if it satisfies the additional conditions

$$\tau_{tt} = 0, \quad \eta_{xu} + \xi_{xx} = 0, \quad \eta_{tt} = 0, \quad F'(u)\eta_x - 2F(u)\xi_{xx} = 0. \tag{26}$$

The infinitesimals for classes A–E in Table III satisfy (26) but those for class F do not since here $\tau_{tt} \neq 0$. ■

As a consequence of Theorem 6, we see that the point symmetry $X=t^2(\partial/\partial t)+ut(\partial/\partial u)$ for $G(u)=u^{-3}$, $F(u)=u^{-4}$ yields a *nonlocal symmetry* of the potential system (2).

TABLE V. Physical examples $[F(u)=G'(u)]$ yielding potential symmetries of (1).

	Class	Infinitesimals ξ,τ,η,ϕ	Global group
1.1	$G(u)=(u^{2\alpha}-1)/(u^{2\alpha}+1)$	$\xi=2\alpha((u^{2\alpha}-1)/(u^{2\alpha}+1))$	$x^*=x+\ln((u^{2\alpha}e^{4\alpha\varepsilon}+1)/(u^{2\alpha}+1))-2\alpha\varepsilon$
		$\tau=t+2\alpha v$	$t^*=\frac{1}{2}e^{\varepsilon}[(t+v)e^{2\alpha\varepsilon}+(t-v)e^{-2\alpha\varepsilon}]$
		$\eta=2u$	$u^*=ue^{2\varepsilon}$
		$\phi=2\alpha t+v$	$v^*=\frac{1}{2}e^{\varepsilon}[(t+v)e^{2\alpha\varepsilon}-(t-v)e^{-2\alpha\varepsilon}]$
1.2	$G(u)=(u^{2\alpha}+1)/(u^{2\alpha}-1)$	$\xi=2\alpha((u^{2\alpha}+1)/(u^{2\alpha}-1))$	$x^*=x+\ln\lvert(u^{2\alpha}e^{4\alpha\varepsilon}-1)/(u^{2\alpha}-1)\rvert-2\alpha\varepsilon$
		$\tau=t+2\alpha v$	$t^*=\frac{1}{2}e^{\varepsilon}[(t+v)e^{2\alpha\varepsilon}+(t-v)e^{-2\alpha\varepsilon}]$
		$\eta=2u$	$u^*=ue^{2\varepsilon}$
		$\phi=2\alpha t+v$	$v^*=\frac{1}{2}e^{\varepsilon}[(t+v)e^{2\alpha\varepsilon}-(t-v)e^{-2\alpha\varepsilon}]$
2	$G(u)=\tan(\alpha\ln u)$	$\xi=-2\alpha\tan(\alpha\ln u)$	$x^*=x+\ln\lvert\cos(\alpha(\ln u+2\varepsilon))/\cos(\alpha\ln u)\rvert$
		$\tau=t-2\alpha v$	$t^*=e^{\varepsilon}[t\cos 2\alpha\varepsilon-v\sin 2\alpha\varepsilon]$
		$\eta=2u$	$u^*=ue^{2\varepsilon}$
		$\phi=2\alpha t+v$	$v^*=e^{\varepsilon}[v\cos 2\alpha\varepsilon+t\sin 2\alpha\varepsilon]$
3	$G(u)=(\ln u)^{-1}$	$\xi=2(\ln u)^{-1}$	$x^*=x+\ln\lvert1+2\varepsilon/\ln u\rvert$
		$\tau=t+2v$	$t^*=e^{\varepsilon}(2v\varepsilon+t)$
		$\eta=2u$	$u^*=ue^{2\varepsilon}$
		$\phi=v$	$v^*=ve^{\varepsilon}$
4	$G(u)=\tan u$	$\xi=-\tan u$	$x^*=x+\ln\lvert\cos(u+\varepsilon)/\cos u\rvert$
		$\tau=-v$	$t^*=t\cos\varepsilon-v\sin\varepsilon$
		$\eta=1$	$u^*=u+\varepsilon$
		$\phi=t$	$v^*=v\cos\varepsilon+t\sin\varepsilon$
5.1	$G(u)=\tanh u$	$\xi=\tanh u$	$x^*=x+\ln((e^{2(u+\varepsilon)}+1)/(e^{2u}+1))-\varepsilon$
		$\tau=v$	$t^*=\frac{1}{2}((t+v)e^{\varepsilon}+(t-v)e^{-\varepsilon})$
		$\eta=1$	$u^*=u+\varepsilon$
		$\phi=t$	$v^*=\frac{1}{2}((t+v)e^{\varepsilon}-(t-v)e^{-\varepsilon})$
5.2	$G(u)=\coth u$	$\xi=\coth u$	$x^*=x+\ln\lvert(e^{2(u+\varepsilon)}-1)/(e^{2u}-1)\rvert-\varepsilon$
		$\tau=v$	$t^*=\frac{1}{2}((t+v)e^{\varepsilon}+(t-v)e^{-\varepsilon})$
		$\eta=1$	$u^*=u+\varepsilon$
		$\phi=t$	$v^*=\frac{1}{2}((t+v)e^{\varepsilon}-(t-v)e^{-\varepsilon})$
6	$G(u)=u^{-1}$	$\xi=u^{-1}$	$x^*=x+\ln\lvert1+\varepsilon/u\rvert$
		$\tau=v$	$t^*=t+v\varepsilon$
		$\eta=1$	$u^*=u+\varepsilon$
		$\phi=0$	$v^*=v$

VI. A PHYSICAL EXAMPLE

We now specialize to the situation for the second physical example mentioned in the Introduction. Here $F(u)=\lambda G'(u)$. Consequently, in Tables I and II, we have $\beta=0$ and $\int F(u)\mathrm{d}u=G(u)$. In Table V, we give the corresponding global group for each of the six classes yielding potential symmetries of the scalar equation (1).

After translations and scalings of u and G, class 5 includes bounded monotonic stress tensor functions $G(u)=\alpha\tanh(\beta u+\gamma)$ for arbitrary constants α, β, γ, and δ.

VII. FURTHER DISCUSSION

In this paper we found new symmetries for equivalent telegraph equations (1)–(4). These symmetries can be used to find families of solutions from any given solution and to construct invariant solutions from the invariants of the symmetries or through the direct method discussed in Ref. 3.

In future papers, we will find conservation laws for (1)–(4) through techniques introduced in Refs. 16–18. Systems (1)–(4) are not self-adjoint. Hence a symmetry of (1)–(4) does not yield a conservation law through Noether's theorem.

For the physical case $F(u)=G'(u)$, the second equation in the potential system (2) becomes

$$(e^x v)_t = (e^x G(u))_x.$$

This leads to another equivalent potential system

$$v_x = u_t, \quad w_x = e^x v, \quad w_t = e^x G(u).$$

The problem of finding equivalent potential systems for a given PDE is considered in Refs. 4 and 5.

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Finite propagation speed for the Camassa–Holm equation

Adrian Constantin
Department of Mathematics, Lund University, Box 118, SE-221 00 Lund, Sweden

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We prove that any classical solution of the Camassa–Holm equation will have compact support if its initial data has this property. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1845603]

I. INTRODUCTION

The Camassa–Holm equation

$$m_t + 2mu_x + m_x u = 0, \quad x \in \mathbb{R}, \quad t > 0, \tag{1}$$

with $m = u - u_{xx}$, was first derived by Fokas and Fuchssteiner[18] as a bi-Hamiltonian system, and then as a model for shallow water waves by Camassa and Holm;[2] see also Refs. 6 and 22 for alternative derivations within the shallow water regime. Equation (1) was also obtained as a model for wave propagation in hyperelastic rods,[16] and shown to describe geodesic flow on the diffeomorphism group of the circle;[24] see also Refs. 11 and 12. The Camassa–Holm equation satisfies the least action principle[11,12] and is an integrable infinite-dimensional Hamiltonian system (for various aspects of the direct/inverse scattering approach and of the direct/inverse spectral problem we refer to Refs. 7, 13, 17–19, 21, and 23). It has both classical solutions that exist for all times as well as smooth solutions which develop singularities in finite time.[3,5,8–10] Note that we can write (1) as

$$u_t - u_{txx} + 3uu_x = 2u_x u_{xx} + uu_{xxx}, \quad t \geqslant 0, \quad x \in \mathbb{R}. \tag{2}$$

The solitary wave solutions of (2) are the peaked waves

$$u_c(x,t) = ce^{|x-ct|}, \quad t \geqslant 0, \quad x \in \mathbb{R},$$

traveling at constant speed $c > 0$, cf. Ref. 2. These peaked waves, called *peakons*, are not classical solutions of (2). They satisfy the conservation law form of the Camassa–Holm equation

$$u_t + uu_x + \partial_x(1 - \partial_x^2)^{-1}(u^2 + \tfrac{1}{2}u_x^2) = 0 \tag{3}$$

(see Refs. 9 and 14). The peakons are solitons, retaining their form and speed through the nonlinear interaction with other peakons (see Refs. 1 and 2). Moreover, the peakons are orbitally stable,[15] i.e., their shape is stable even under perturbations of a more general nature than those occuring through the interaction with other peakons.

This paper is concerned with establishing the finite propagation speed property for the Camassa–Holm equation (1). Due to the nonlocal nature of the conservation law form (3) of the equation, it is not *a priori* clear that a localized initial data $m(x,0)$ (that is, of compact support) will not spread out instantly to the whole spatial domain. Below we will give a simple proof of this property.

[a]Electronic mail: adrian.constantin@math.lu.se

II. MAIN RESULTS

Let us first prove the following.

Theorem: *Assume that $m_0:\mathbb{R}\to\mathbb{R}$ is a smooth function with compact support. If $T>0$ is the maximal existence time of the smooth solution $m(x,t)$ to (1) with initial data $m_0(x)$, then for any $t\in[0,T)$ the smooth function $x\mapsto m(x,t)$ has compact support.*

Before proceeding with the proof, a few comments are in order. First of all, the restriction to smooth functions is just for convenience since the same approach will work (the local well-posedness of solutions and other technicalities needed to pursue our approach within this setting are available from the considerations made in Refs. 5 and 9) for initial data in the Sobolev space $H^1(\mathbb{R})$ of square integrable functions with square integrable distributional derivative. It is also well known that the solution of the Camassa–Holm equation inherits at any later time the spatial smoothness of the initial data, measured on a Sobolev space scale with integer index (see Refs. 4 and 9). Finally, we would like to point out that smooth initial data with compact support develop into solutions that might exist for all times or could exhibit singularities in finite time cf. Refs. 3, 5, and 8.

Proof of the theorem: We associate to the solution m with initial data $m(x,0)=m_0(x)$ the family $\{\varphi(\cdot,t)\}_{t\in[0,T)}$ of smooth diffeomorphisms of the line defined by

$$\varphi_t(x,t)=u(\varphi(x,t),t),\quad t\in[0,T), \tag{4}$$

with

$$\varphi(x,0)=x,\quad x\in\mathbb{R}. \tag{5}$$

Using (1), (4), and (5), is easy to check the following identity:

$$m(\varphi(x,t),t)\cdot\varphi_x^2(x,t)=m(x,0),\quad x\in\mathbb{R},\quad t\in[0,T). \tag{6}$$

On the other hand, from (4) and (5) we infer

$$\varphi_x(x,t)=\exp\left(\int_0^t u_x(\varphi(x,s),s)\mathrm{d}s\right),\quad x\in\mathbb{R},\quad t\in[0,T). \tag{7}$$

If m_0 is supported in the compact interval $[a,b]$, since $\varphi_x(x,t)>0$ on $\mathbb{R}\times[0,T)$ in view of (7), we deduce from (6) that $m(x,t)$ has its support in the interval $[\varphi(a,t),\varphi(b,t)]$. This completes the proof. ■

We established that the solutions to the Camassa–Holm equation (1) have finite propagation speed. Since (1) is equivalent to (2), the natural question arises whether this property is captured by the time evolution of the function u. We will now show that this is not the case.

Proposition: *Assume that $u_0:\mathbb{R}\to\mathbb{R}$ is a smooth function with compact support. Let $T>0$ be the maximal existence time of the smooth solution $u(x,t)$ to (2) with initial data $u_0(x)$. If at every $t\in[0,T)$ the smooth function $x\mapsto u(x,t)$ has compact support, then u is identically zero.*

Proof: For $(x,t)\in\mathbb{R}\times[0,T)$, let $m(x,t)=(1-\partial_x^2)u(x,t)$. Clearly $m(x,0)$ has compact support since u_0 does. From our theorem we deduce that for every $t\in[0,T)$ the smooth function $x\mapsto m(x,t)$ is also of compact support. Recall that by the Paley–Wiener theorem,[20,25] an entire analytic function $g(\xi)$ of the complex variable $\xi=\eta+i\zeta$ (with $\eta,\zeta\in\mathbb{R}$) is the Fourier transform $\mathcal{F}_f$ of a smooth function $f:\mathbb{R}\to\mathbb{R}$ with compact support in the ball $\{x\in\mathbb{R}:|x|\leqslant R\}$, where $\mathcal{F}_f(\xi)=\int_{\mathbb{R}}e^{-i\xi x}f(x)\mathrm{d}x$ for $\xi\in\mathbb{C}$, if and only if for every integer $n\geqslant 0$ there is a constant $c_n>0$ so that $|g(\xi)|\leqslant c_n e^{R|\zeta|}/(1+|\xi|)^n$ for all $\xi\in\mathbb{C}$. Notice that

$$\mathcal{F}_m(\xi)=(1+\xi^2)\mathcal{F}_u(\xi),\quad \xi\in\mathbb{C},\quad t\in[0,T). \tag{8}$$

By assumption $u(\cdot,t)$ has compact support at every $t\in[0,T)$. Hence the Paley–Wiener theorem ensures that $\mathcal{F}_u$ and $\mathcal{F}_m$ are entire functions. Then (8) forces $\mathcal{F}_m(\pm i)=0$ at any fixed $t\in[0,T)$, or

$$\int_{\mathbb{R}} e^x m(x,t)\mathrm{d}x = \int_{\mathbb{R}} e^{-x} m(x,t)\mathrm{d}x = 0, \quad t \in [0,T). \tag{9}$$

However, we infer from (1) that for all $t \in (0,T)$,

$$\begin{aligned}
\frac{d}{\mathrm{d}t}\int_{\mathbb{R}} e^x m(x,t)\mathrm{d}x = \int_{\mathbb{R}} e^x m_t \,\mathrm{d}x &= -2\int_{\mathbb{R}} e^x m u_x \,\mathrm{d}x - \int_{\mathbb{R}} e^x m_x u \,\mathrm{d}x \\
&= -\int_{\mathbb{R}} e^x m u_x \,\mathrm{d}x + \int_{\mathbb{R}} e^x m u \,\mathrm{d}x \\
&= -\int_{\mathbb{R}} e^x u u_x \,\mathrm{d}x + \int_{\mathbb{R}} e^x u_x u_{xx} \,\mathrm{d}x + \int_{\mathbb{R}} e^x u^2 \,\mathrm{d}x - \int_{\mathbb{R}} e^x u u_{xx} \,\mathrm{d}x \\
&= -\int_{\mathbb{R}} e^x u u_x \,\mathrm{d}x - \frac{1}{2}\int_{\mathbb{R}} e^x u_x^2 \,\mathrm{d}x + \int_{\mathbb{R}} e^x u^2 \,\mathrm{d}x + \int_{\mathbb{R}} e^x u_x^2 \,\mathrm{d}x \\
&\quad + \int_{\mathbb{R}} e^x u u_x \,\mathrm{d}x
\end{aligned}$$

since all boundary terms obtained after integration by parts vanish as $u(\cdot,t)$ has compact support for every $t \in [0,T)$. Hence

$$\frac{d}{\mathrm{d}t}\int_{\mathbb{R}} e^x m(x,t)\mathrm{d}x = \int_{\mathbb{R}} e^x \left(u^2 + \frac{1}{2}u_x^2\right)\mathrm{d}x, \quad t \in (0,T). \tag{10}$$

But (9) and (10) can hold simultaneously if and only if $u \equiv 0$. The proof is complete. ■

Remark: *If $u_0 \not\equiv 0$ is smooth, the corresponding solution $u(\cdot,t)$ of the Camassa–Holm equation (2) loses instantly the property of having compact support. To prove this statement, we just go through the previous argumentation restricting our attention to an arbitrarily small time interval $[0,\varepsilon)$.*

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Recursive calculation of effective potential and variational resummation

Sebastian F. Brandt and Hagen Kleinert
Freie Universität Berlin, Institut für Theoretische Physik, Arnimallee 14, 14195 Berlin, Germany

Axel Pelster
Universität Duisburg-Essen, Campus Essen, Fachbereich Physik, Universitätsstraße 5, 45117 Essen, Germany

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We set up a method for a recursive calculation of the effective potential which is applied to a cubic potential with imaginary coupling. The result is resummed using variational perturbation theory, yielding an exponentially fast convergence. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1824212]

I. INTRODUCTION

Perturbation theory is the most commonly used technique for an approximate description of nonexactly solvable systems. However, most perturbation series are divergent and yield acceptable results only after resummation. In recent years, based on a variational approach due to Feynman and Kleinert,[1] a systematic and uniformly convergent *variational perturbation theory* (VPT) has been developed.[2–5] It permits the conversion of divergent weak-coupling into convergent strong-coupling expansions and has been applied successfully in quantum mechanics, quantum statistics, condensed matter physics, and the theory of critical phenomena.

The convergence of VPT has been proved to be exponentially fast,[3,4] and this has been verified for the ground-state energy of different quantum mechanical model systems. If the underlying potential is mirror symmetric, one introduces a trial oscillator whose frequency Ω is regarded as a variational parameter and whose influence is minimized according to the *principle of minimal sensitivity*.[6] In this way, the ground-state energy of the quartic anharmonic oscillator was analyzed up to very high orders in Refs. 7 and 8.

If the potential is not mirror symmetric, the center of fluctuations no longer lies at the origin but at some nonzero place X. In VPT, this situation is accounted for by regarding the nonvanishing center of fluctuations X as a second variational parameter. An extreme example is a complete antisymmetric potential, such as $V(x)=Ax^3$, which for real A does not correspond to a stable system. Interestingly, if the parameter A is chosen to be imaginary, so that there does not exist a classical system at all, the quantum-mechanical system turns out to be well defined, and the spectrum of the Hamilton operator

$$H=-\frac{1}{2}\frac{\partial^2}{\partial x^2}+ix^3 \tag{1}$$

is real and positive. This remarkable property of the non-Hermitian Hamilton operator, found in Refs. 9–13, can be attributed to the fact that it possesses a different symmetry: it is invariant under the combined application of the parity and the time-reversal operation.

In this paper, we apply VPT to the $\mathcal{PT}$-symmetric Hamilton operator (1). In a first naive approach, we ignore the necessary shift X of the center of fluctuations and resum the weak-coupling series of the ground-state energy for the anharmonic oscillator

$$V(x) = \frac{\omega^2}{2}x^2 + igx^3 \tag{2}$$

in the strong-coupling limit. In this limit, the potential (2) reduces to the purely cubic potential of (1). It turns out that the VPT results approach the corresponding numerical value for the ground-state energy of (1) with increasing order, but the rate of convergence is not satisfactory. Afterwards, we allow for a nonvanishing center of fluctuations X by using the effective potential, whose calculation is accomplished by an efficient recursion scheme. This refined approach improves the convergence of the results drastically.

In Sec. II, we derive the weak-coupling series for the ground-state energy of (2) by evaluating connected vacuum diagrams. In Sec. III, we show how this perturbation series can be obtained more efficiently by means of the Bender–Wu recursion method.[14] In Sec. IV, we resum the weak-coupling series for the ground-state energy of (2) by applying VPT and examine the resulting convergence. In Sec. V, we determine the effective potential with the *background method*[15,16] from one-particle irreducible vacuum diagrams. In Sec. VI, we set up new recursion relations for a more efficient calculation of the effective potential. In Sec. VII, we finally treat the resulting expansion with VPT and examine the improved convergence.

II. PERTURBATION THEORY

The perturbation series for the ground-state energy of the anharmonic oscillator (2) can be calculated from connected vacuum diagrams. Up to the fourth order in the coupling constant g, the ground-state energy is given by the Feynman diagrams

$$E = \frac{\hbar\omega}{2} - \lim_{\beta\to\infty}\frac{1}{\beta}\Bigg\{\frac{1}{8}\,\bigcirc\!\!-\!\!\bigcirc + \frac{1}{12}\,\ominus + \frac{1}{24}\,\otimes + \frac{1}{16}\,\oslash + \frac{1}{8}\,\bigcirc\!\!-\!\!\bigcirc\!\!\!\!\bigcirc + \frac{1}{16}\,\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc + \frac{1}{48}\,\curlyvee + \mathcal{O}(g^6)\Bigg\}, \tag{3}$$

with the propagator

$$i \bullet\!\!\!-\!\!\!-\!\!\!\bullet\, j \to G_\omega(\tau_i,\tau_j) = \frac{\hbar}{2\omega}e^{-\omega|\tau_i-\tau_j|} \tag{4}$$

and the vertices

$$\overset{i}{\curlyvee} \to -\frac{6ig}{\hbar}\int_0^{\hbar\beta} \tau_i. \tag{5}$$

Evaluating the Feynman diagrams (3) leads to the following analytical expression for the ground-state energy:

$$E = \hbar\omega\left[\frac{1}{2} + \frac{11g^2\hbar}{8\omega^5} - \frac{465g^4\hbar^2}{32\omega^{10}} + \mathcal{O}(g^6)\right]. \tag{6}$$

Since evaluating Feynman diagrams of higher orders is cumbersome, only low perturbation orders are feasible by this procedure. If we want to study higher orders, we better use the Bender–Wu recursion relations.[14]

TABLE I. Expansion coefficients for the ground-state energy of the anharmonic oscillator (2) up to the 10th order.

k	1	2	3	4	5
ϵ_k	0	$\frac{11}{8}$	0	$-\frac{465}{32}$	0
k	6	7	8	9	10
ϵ_k	$\frac{39\,709}{128}$	0	$-\frac{19\,250\,805}{2048}$	0	$\frac{2\,944\,491\,879}{8192}$

III. BENDER–WU RECURSION RELATIONS

The Schrödinger eigenvalue equation for the anharmonic oscillator (2),

$$-\frac{\hbar^2}{2}\psi''(x)+\left(\frac{\omega^2}{2}x^2+igx^3\right)\psi(x)=E\psi(x), \tag{7}$$

is solved as follows: We write the wave function $\psi(x)$ as

$$\psi(x)=\left(\frac{\omega}{\pi\hbar}\right)^{1/4}\exp\left[-\frac{\hat{x}^2}{2}+\phi(\hat{x})\right], \tag{8}$$

with the abbreviation $\hat{x}=x\sqrt{\omega/\hbar}$, and expand the exponent in powers of the dimensionless coupling constant $\hat{g}=g\sqrt{\hbar/\omega^5}$ by using

$$\phi(\hat{x})=\sum_{k=1}^{\infty}\hat{g}^k\phi_k(\hat{x}). \tag{9}$$

The $\phi_k(\hat{x})$ are expanded in powers of the rescaled coordinate $\hat{x}$,

$$\phi_k(\hat{x})=\sum_{m=1}^{k+2}c_m^{(k)}\hat{x}^m. \tag{10}$$

For the ground-state energy we make the ansatz

$$E=\hbar\omega\left(\frac{1}{2}+\sum_{k=1}^{\infty}\hat{g}^k\epsilon_k\right). \tag{11}$$

Inserting (8)–(11) into (7), we obtain to first order

$$c_1^{(1)}=-i,\quad c_2^{(1)}=0,\quad c_3^{(1)}=-\frac{i}{3},\quad \epsilon_1=0. \tag{12}$$

For $k\geqslant 2$, we find the following recursion relation for the expansion coefficients in (10):

$$c_m^{(k)}=\frac{(m+2)(m+1)}{2m}c_{m+2}^{(k)}+\frac{1}{2m}\sum_{l=1}^{k-1}\sum_{n=1}^{m+1}n(m+2-n)c_n^{(l)}c_{m+2-n}^{(k-l)}, \tag{13}$$

with $c_m^{(k)}\equiv 0$ for $m>k+2$. The expansion coefficients of the ground-state energy follow from

$$\epsilon_k=-c_2^{(k)}-\frac{1}{2}\sum_{l=1}^{k-1}c_1^{(l)}c_1^{(k-l)}. \tag{14}$$

Table I shows the coefficients ϵ_k up to the 10th order. We observe that all odd orders vanish for

symmetry reasons and that the first two even orders agree, indeed, with the earlier result (6).

IV. RESUMMATION OF GROUND-STATE ENERGY

In this section, we consider the strong-coupling limit of the perturbation series (11). Rescaling the coordinate according to $x \to x g^{-1/5}$, the Schrödinger equation (7) becomes

$$-\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2}\psi(x) + \left(\frac{1}{2}g^{-4/5}\omega^2 x^2 + ix^3\right)\psi(x) = g^{-2/5}E\psi(x). \tag{15}$$

Expanding the wave function and the energy in powers of the coupling constant yields

$$\psi(x) = \psi_0(\hat{x}) + \hat{g}^{-4/5}\psi_1(\hat{x}) + \hat{g}^{-8/5}\psi_2(\hat{x}) + \cdots \tag{16}$$

and

$$E = \hbar\omega\hat{g}^{2/5}(b_0 + \hat{g}^{-4/5}b_1 + \hat{g}^{-8/5}b_2 + \cdots). \tag{17}$$

By considering (15) in the limit $g \to \infty$, we find that the leading strong-coupling coefficient b_0 equals the ground-state energy associated with the Hamilton operator (1). A precise numerical value for this ground-state energy was given by Bender,[9,18]

$$b_0 = 0.762\,851\,773\ \ldots\ . \tag{18}$$

The weak-coupling series (11) is of the form

$$E^{(N)}(\alpha,\omega) = \hbar\omega\left[\frac{1}{2} + \sum_{k=1}^{N}\left(\frac{\hbar\alpha}{\omega^5}\right)^k \epsilon_{2k}\right], \tag{19}$$

with the abbreviation $\alpha = g^2$. Table I suggests that (19) represents a divergent Borel series which is resummable by applying VPT.[2–5] To this end, an artificial parameter is introduced in the perturbation series, which is most easily obtained by Kleinert's square-root trick,

$$\omega \to \Omega\sqrt{1+\alpha r}, \tag{20}$$

with

$$r = \frac{\omega^2 - \Omega^2}{\alpha\Omega^2}. \tag{21}$$

Thus, one replaces the frequency ω in the weak-coupling series (19) according to (20) and re-expands the resulting expression in powers of α up to the order α^N. Afterwards, the auxiliary parameter r is replaced according to (21). The ground-state energy thus becomes dependent on the variational parameter Ω, $E^{(N)}(\alpha,\omega) \to E^{(N)}(\alpha,\omega,\Omega)$. The influence of Ω is then optimized according to the principle of minimal sensitivity,[6] i.e., one approximates the ground-state energy to Nth order by

$$E^{(N)} = E^{(N)}(\alpha,\omega,\Omega^{(N)}), \tag{22}$$

where $\Omega^{(N)}$ denotes that value of the variational parameter for which $E^{(N)}(\alpha,\omega,\Omega)$ has an extremum or a turning point.

Consider, as an example, the weak-coupling series (19) to first order,

$$E^{(1)}(\alpha,\omega) = \frac{\hbar\omega}{2} + \alpha\frac{11\hbar^2}{8\omega^4}. \tag{23}$$

Inserting (20), re-expanding in α to first order, and taking into account (21), we obtain

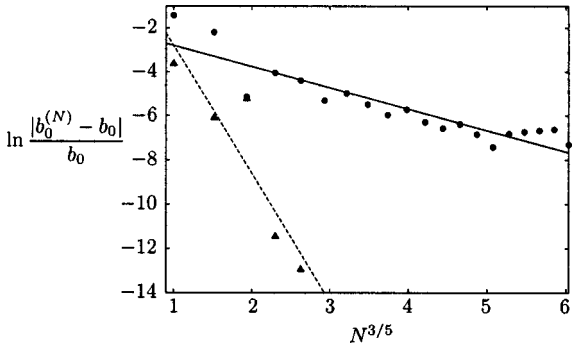

FIG. 1. Convergence of the results for the strong-coupling coefficient b_0 obtained from resummation of the weak-coupling series of the ground-state energy (circles). The resummation involving a variational path average X converges much faster (triangles). The lines represent fits of the respective data to straight lines.

$$E^{(1)}(\alpha,\omega,\Omega) = \frac{\hbar\Omega}{4} + \frac{\hbar\omega^2}{4\Omega} + \alpha\frac{11\hbar^2}{8\Omega^4}. \tag{24}$$

Extremizing this and going to large coupling constants, we obtain the strong-coupling behavior of the variational parameter,

$$\Omega^{(1)} = \omega\hat{\alpha}^{1/5}(\Omega_0^{(1)} + \Omega_1^{(1)}\hat{\alpha}^{-2/5} + \Omega_2^{(1)}\hat{\alpha}^{-4/5} + \cdots), \tag{25}$$

with the abbreviation $\hat{\alpha}=\hat{g}^2$ and the coefficients

$$\Omega_0^{(1)} = \sqrt[5]{22},\ \ \Omega_1^{(1)} = \frac{1}{5\sqrt[5]{22}},\ \ \Omega_2^{(1)} = \frac{1}{25\sqrt[5]{10\,648}},\ \ \ldots\ . \tag{26}$$

Inserting the result (25) and (26) into (24), we obtain the strong-coupling series (17) with the first-order coefficients

$$b_0^{(1)} = \frac{5\sqrt[5]{22}}{16},\quad b_1^{(1)} = \frac{4}{\sqrt[5]{22}},\quad b_2^{(1)} = \frac{-1}{100\sqrt[5]{22}},\quad \ldots\ . \tag{27}$$

The numerical value of the leading strong-coupling coefficient is $b_0^{(1)} \approx 0.5799$. Thus, to first order, the relative deviation of the result from the precise value (18) is

$$\frac{|b_0^{(1)} - b_0|}{b_0} \approx 24\%. \tag{28}$$

Despite this relatively poor agreement, it turns out that the VPT results for $b_0^{(N)}$ in higher orders converge towards the exact value (18). In Refs. 3 and 4 it is proved that VPT in general yields approximations whose relative deviation from the exact value vanishes exponentially. In our case we have

$$\frac{|b_0^{(N)} - b_0|}{b_0} \propto \exp(-CN^{3/5}), \tag{29}$$

where the exponent $3/5$ is determined by the structure of the strong-coupling series (17).

In Fig. 1 the exponential convergence of our variational results is shown up to the 20th order. Fitting the logarithm of the relative deviation to a straight line yields

$$\ln \frac{|b_0^{(N)} - b_0|}{b_0} = -0.96(11)N^{3/5} - 1.83(44). \tag{30}$$

In the following, we show how this exponential convergence is improved drastically by allowing for a shift of the center of fluctuations.

V. DIAGRAMMATIC APPROACH TO EFFECTIVE POTENTIAL

In the presence of a constant external current j, the quantum statistical partition function reads

$$Z(j) := \oint \mathcal{D}x \exp\left\{-\frac{1}{\hbar}\mathcal{A}[x](j)\right\}, \tag{31}$$

where $\mathcal{A}[x](j)$ is the Euclidean action,

$$\mathcal{A}[x](j) = \int_0^{\hbar\beta} \mathrm{d}\tau \left[\frac{1}{2}\dot{x}^2(\tau) + V(x(\tau)) - jx(\tau)\right]. \tag{32}$$

The free energy thus becomes a function of the external current,

$$F(j) = -\frac{1}{\beta}\ln Z(j). \tag{33}$$

The path average,

$$X = \frac{1}{Z(j)}\oint \mathcal{D}x \left[\int_0^{\hbar\beta} \frac{\mathrm{d}\tau}{\hbar\beta} x(\tau)\right] \exp\left\{-\frac{1}{\hbar}\mathcal{A}[x](j)\right\}, \tag{34}$$

then follows from the first derivative of the free energy with respect to the external current:

$$X = -\frac{\partial F(j)}{\partial j}. \tag{35}$$

Assuming that the last identity can be inverted to yield the current j as a function of the average X, one defines the effective potential $V_{\mathrm{eff}}(X)$ as the Legendre transform of the free energy with respect to the external current:

$$V_{\mathrm{eff}}(X) = F(j(X)) + j(X)X. \tag{36}$$

Furthermore, the first derivative of the effective potential gives back the external current j:

$$\frac{\partial V_{\mathrm{eff}}(X)}{\partial X} = j(X). \tag{37}$$

Thus, the free energy $F \equiv F(j=0)$ can be obtained by extremizing the effective potential,

$$F = V_{\mathrm{eff}}(X_e), \tag{38}$$

with

$$\left.\frac{\partial V_{\mathrm{eff}}(X)}{\partial X}\right|_{X=X_e} = 0. \tag{39}$$

In the zero-temperature limit, extremizing the effective potential then yields the ground-state energy.

The effective potential is usually not calculated by performing explicitly the Legendre transformation (36) but by a diagrammatic technique derived via the so-called background method.[15,16] There, the effective potential is expanded in powers of the Planck constant $\hbar$, and the expansion terms are one-particle irreducible vacuum diagrams. The result is

$$V_{\text{eff}}(X) = V(X) + \frac{\hbar}{2}\text{Tr}\ln G^{-1} + V^{(\text{int})}(X), \tag{40}$$

where the trace-log term is given by the ground-state energy of a harmonic oscillator of X-dependent frequency $\tilde{\omega} = \sqrt{V''(X)}$,

$$\frac{\hbar}{2}\text{Tr}\ln G^{-1} = \frac{\hbar\tilde{\omega}}{2}. \tag{41}$$

The interaction term $V^{(\text{int})}(X)$ contains the sum of all one-particle irreducible vacuum diagrams. For the anharmonic oscillator (2), the relevant subset of the diagrams in (3) is

$$V^{(\text{int})}(X) = -\lim_{\beta\to\infty}\frac{1}{\beta}\left\{\frac{1}{12}\ \ominus\ + \frac{1}{24}\ \otimes\ + \frac{1}{16}\ \text{oo}\right\} + \mathcal{O}(\hbar^4). \tag{42}$$

These one-particle irreducible vacuum diagrams are derived most easily by an efficient graphical recursion method.[17] The frequency of the propagators is now given by

$$\tilde{\omega} = \sqrt{\omega^2 + 6igX}. \tag{43}$$

By evaluating the diagrams (42) we obtain

$$V_{\text{eff}}(X) = \frac{\omega^2}{2}X^2 + igX^3 + \frac{\hbar}{2}\sqrt{\omega^2 + 6igX} + \frac{\hbar^2 g^2}{4(\omega^2 + 6igX)^2} - \frac{51\hbar^3 g^4}{32(\omega^2 + 6igX)^{9/2}} + \mathcal{O}(\hbar^4). \tag{44}$$

The ground-state energy of the anharmonic oscillator (2) is found by extremizing the effective potential (44). To this end, we expand the extremal background according to

$$X_e = i(X_0 + \hbar X_1 + \hbar^2 X_2 + \hbar^3 X_3) + \mathcal{O}(\hbar^4). \tag{45}$$

Inserting (45) into the vanishing first derivative of (44) and re-expanding in $\hbar$, we obtain a system of equations which are solved by

$$X_0 = 0, \quad X_1 = -\frac{3g}{2\omega^3}, \quad X_2 = \frac{33g^3}{2\omega^8}. \tag{46}$$

Inserting (45) and (46) into (44) and re-expanding in $\hbar$ yields again the ground-state energy (6).

In order to go to higher orders, we shall now develop a recursion relation for the effective potential.

VI. RECURSIVE APPROACH TO EFFECTIVE POTENTIAL

In the presence of a constant external current j, the Schrödinger eigenvalue equation for the anharmonic oscillator (2) reads

$$-\frac{\hbar^2}{2}\psi''(x) + \left(\frac{\omega^2}{2}x^2 + igx^3 - jx\right)\psi(x) = E\psi(x). \tag{47}$$

Taking into account the Legendre identities (36) and (37), Eq. (47) becomes

$$-\frac{\hbar^2}{2}\psi''(x)+\left(\frac{\omega^2}{2}x^2+igx^3-V'_{\rm eff}(X)x\right)\psi(x)=[V_{\rm eff}(X)-V'_{\rm eff}(X)X]\psi(x). \tag{48}$$

If the coupling constant g vanishes, Eq. (48) is solved by

$$\psi(x)=\mathcal{N}\exp\left(\hat{X}\hat{x}-\frac{\hat{x}^2}{2}\right), \tag{49}$$

$$V_{\rm eff}(X)=\hbar\omega\left(\frac{1}{2}+\frac{\hat{X}}{2}\right), \tag{50}$$

where the path average has been rescaled by the oscillator length, $\hat{X}=X\sqrt{\omega/\hbar}$. For a nonvanishing coupling constant g, we solve the differential equation (48) by the expansions

$$\psi(x)=\mathcal{N}\exp\left[\hat{X}\hat{x}-\frac{\hat{x}^2}{2}+\phi(\hat{x})\right], \tag{51}$$

$$V_{\rm eff}(X)=\hbar\omega\left[\frac{1}{2}+\frac{\hat{X}^2}{2}+\sum_{k=1}^{\infty}\hat{g}^kV_k(\hat{X})\right]. \tag{52}$$

For the correction to the wave function, $\phi(\hat{x})$, we make again the ansatz (9) and (10). Thus, we obtain from (48) for $k=1$,

$$c_1^{(1)}=\frac{i}{2}+2i\hat{X}^2,\ \ c_2^{(1)}=-\frac{i\hat{X}}{2},\ \ c_3^{(1)}=-\frac{i}{3},\ \ V_1(\hat{X})=\frac{3i\hat{X}}{2}+i\hat{X}^3. \tag{53}$$

For $k\geqslant 2$ one finds for $m\geqslant 2$ the following recursion relation for the expansion coefficients of the wave function:

$$c_m^{(k)}=\frac{(m+2)(m+1)}{2m}c_{m+2}^{(k)}+\frac{\hat{X}(m+1)}{m}c_{m+1}^{(k)}+\frac{1}{2m}\sum_{l=1}^{k-1}\sum_{n=1}^{m+1}n(m+2-n)c_n^{(l)}c_{m+2-n}^{(k-l)}, \tag{54}$$

with $c_m^{(k)}\equiv 0$ for $m>k+2$. For $m=1$, we have

$$c_1^{(k)}=3c_3^{(k)}+2\hat{X}c_2^{(k)}+V'_k(\hat{X})+\sum_{l=1}^{k-1}(c_2^{(k-l)}c_1^{(l)}+c_1^{(k-l)}c_2^{(l)}). \tag{55}$$

The expansion coefficients of the effective potential follow from

$$V_k(\hat{X})=-c_2^{(k)}-3\hat{X}c_3^{(k)}-2\hat{X}^2c_2^{(k)}-\hat{X}\sum_{l=1}^{k-1}(c_2^{(k-l)}c_1^{(l)}+c_1^{(k-l)}c_2^{(l)})-\frac{1}{2}\sum_{l=1}^{k-1}c_1^{(l)}c_1^{(k-l)}. \tag{56}$$

Using these results, the effective potential can be determined recursively, yielding an expansion in the coupling constant g,

$$V_{\rm eff}(X)=\frac{\hbar\omega}{2}+\frac{\omega^2}{2}X^2+ig\left(\frac{3\hbar X}{2\omega}+X^3\right)+g^2\frac{\hbar(\hbar+9\omega X^2)}{4\omega^4}$$
$$-ig^3\frac{3\hbar X(4\hbar+9\omega X^2)}{4\omega^6}-g^4\frac{3\hbar(17\hbar^2+288\hbar X^2+270X^4\omega^2)}{32\omega^9}+\mathcal{O}(g^5). \tag{57}$$

This result is in agreement with the expansion of (44) in powers of g and can be carried to higher orders without effort. The expansion coefficients for the $\hbar$-expansion

TABLE II. Expansion coefficients for the effective potential of (2) up to five loops.

l	0	1	2
$V^{(l)}(X)$	$\omega^2X^2/2+igX^3$	$\tilde{\omega}/2$	$g^2/4\tilde{\omega}^4$
l	3	4	5
$V^{(l)}(X)$	$-51g^4/32\tilde{\omega}^9$	$3331g^6/128\tilde{\omega}^{14}$	$-1\,371\,477g^8/2048\tilde{\omega}^{19}$

$$V_{\text{eff}}(X) = \sum_{l=0}^{N} \hbar^l V^{(l)}(X) + \mathcal{O}(\hbar^{N+1}) \tag{58}$$

can then be obtained easily.[19] Iterating the recursion relations (54)–(56) up to the order g^8, we obtain the effective potential up to five loops as shown in Table II.

VII. RESUMMATION OF EFFECTIVE POTENTIAL

We now apply VPT to the loop expansion of the effective potential (58). Since the Planck constant $\hbar$ is now the expansion parameter rather than the coupling constant g, Kleinert's square-root trick will be modified accordingly,

$$\omega \to \Omega\sqrt{1+\hbar r}, \tag{59}$$

with

$$r = \frac{\omega^2 - \Omega^2}{\hbar\Omega^2}. \tag{60}$$

As an example, we consider again the first order

$$V_{\text{eff}}^{(1)}(X) = \frac{\omega^2}{2}X^2 + igX^3 + \frac{\hbar}{2}\sqrt{\omega^2 + 6igX}. \tag{61}$$

After substituting ω according to (59), re-expanding in $\hbar$, and taking into account (60), we obtain

$$V_{\text{eff}}^{(1)}(X,\Omega) = \frac{\omega^2}{2}X^2 + igX^3 + \frac{\hbar}{2}\sqrt{\Omega^2 + 6igX}. \tag{62}$$

In order to calculate an approximation for the ground-state energy, we now optimize in Ω and extremize in X, yielding

$$\frac{\partial}{\partial\Omega}V_{\text{eff}}^{(1)}(X,\Omega)\bigg|_{X=X^{(1)},\Omega=\Omega^{(1)}} = 0, \tag{63}$$

$$\frac{\partial}{\partial X}V_{\text{eff}}^{(1)}(X,\Omega)\bigg|_{X=X^{(1)},\Omega=\Omega^{(1)}} = 0. \tag{64}$$

Equation (63) is solved by

$$\Omega^{(1)} = 0. \tag{65}$$

Afterwards, we obtain from (64),

TABLE III. Variational results for the ground-state energy of (1) compared to the numerical result (18) of Refs. 9 and 18.

1-loop VPT	0.742 751 023
2-loop VPT	0.764 570 478
3-loop VPT	0.758 783 545
4-loop VPT	0.762 843 684
5-loop VPT	0.762 849 959
Numerical	0.762 851 773

$$X^{(1)} + \frac{\omega^2}{3ig} + \frac{\hbar}{2\sqrt{6ig}(X^{(1)})^{3/2}} = 0. \tag{66}$$

This equation allows us to determine the strong-coupling behavior of X,

$$X^{(1)} = -i\hat{g}^{-1/5}\sqrt{\frac{\hbar}{\omega}}(X_0^{(1)} + X_1^{(1)}\hat{g}^{-4/5} + X_2^{(1)}\hat{g}^{-8/5} + \cdots), \tag{67}$$

where the coefficients read

$$X_0^{(1)} = \frac{1}{\sqrt[5]{24}}, \quad X_1^{(1)} = -\frac{2}{15}, \quad X_2^{(1)} = \frac{\sqrt[5]{24}}{75}, \ \ldots \ . \tag{68}$$

Inserting the results (65), (67), and (68) into (62) yields the strong-coupling behavior of the ground-state energy (17), with the new coefficients

$$b_0^{(1)} = \frac{5}{2\sqrt[5]{432}}, \quad b_1^{(1)} = -\frac{1}{4\sqrt[5]{18}}, \quad b_2^{(1)} = \frac{1}{15\sqrt[5]{24}}, \ \ldots \ . \tag{69}$$

The new numerical value of the leading strong-coupling coefficient is $b_0^{(1)} \approx 0.7428$, which is in much better agreement with (18) than the previous value of (27),

$$\frac{|b_0^{(1)} - b_0|}{b_0} \approx 3\%. \tag{70}$$

Thus, the variational path average has led to a significant improvement of the first-order result. Table III summarizes our results for $b_0^{(N)}$ up to the fifth order.

Figure 1 shows the much faster exponential convergence up to the fifth order. A least square fit of the data yields

$$\ln \frac{|b_0^{(N)} - b_0|}{b_0} = -5.8(1.6)N^{3/5} + 3.0(3.0) \tag{71}$$

which is to be compared with (30).

VIII. CONCLUSION AND OUTLOOK

We have developed a recursive technique to determine the effective potential, which is far more efficient than diagrammatic methods. In combination with VPT, this leads to a fast converging determination of the ground-state energy of quantum-mechanical systems with nonmirror symmetric potentials. It will be interesting to analyze in a similar way systems with a coordinate dependent mass term, where only a lowest order effective potential has been calculated so far.[20] Interesting future applications will address the effective potential of ϕ^4 theories in $4-\epsilon$ dimensions to obtain equations of state near to a critical point. A first attempt in this direction is Ref. 21.

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$\mathcal{PT}$ symmetric models with nonlinear pseudosupersymmetry

A. Sinha[a)]
Department of Applied Mathematics, Calcutta University, 92, APC Road, Kolkata-700 009, India

P. Roy[b)]
Physics and Applied Mathematics Unit, Indian Statistical Institute, Kolkata-700 108, India

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By applying the higher order Darboux algorithm to an exactly solvable non-Hermitian $\mathcal{PT}$ symmetric potential, we obtain a hierarchy of new exactly solvable non-Hermitian $\mathcal{PT}$ symmetric potentials with real spectra. It is shown that the symmetry underlying the potentials so generated and the original one is *nonlinear pseudosupersymmetry.* We also show that this formalism can be used to generate a larger class of new solvable potentials when applied to non-Hermitian systems.
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I. INTRODUCTION

There are not many exactly solvable potentials in quantum mechanics. As a result there have always been efforts to enlarge the class of exactly solvable potentials. Some of the different methods which have been used time and again to generate a hierarchy of isospectral potentials are the factorization method of Infeld and Hull,[1] the Darboux algorithm,[2] the method of supersymmetric quantum mechanics (SUSY QM),[3] or the integral transformations of Abraham–Moses–Pursey,[4] etc. Among these methods the Darboux algorithm and the SUSY QM are closely related and these methods have found numerous applications in different areas of theoretical and mathematical physics.[3]

At the same time, the scheme is still narrow as conventional SUSY fails to explain certain phenomena, e.g., the disappearance of the leading Borel singularity of the perturbation correction for the ground state energy of a SUSY theory.[5] In order to explain such behavior and also to widen the scope of SUSY QM, an idea was put forward to extend SUSY to higher orders.[6] We recall that in the conventional intertwining technique, two one-dimensional Schrödinger Hamiltonians H and $\tilde{H}$ are intertwined by means of differential operators L as

$$\tilde{H}L = LH, \quad HL^{\dagger} = L^{\dagger}\tilde{H}. \tag{1}$$

If L is of the first order in derivatives, the standard SUSY QM, with supercharges built of first order Darboux transformation operators, and the factorization method are recovered. On the other hand, if higher order differential operators are involved in the construction of L, it is variously referred to as *polynomial SUSY*,[6] or *nonlinear SUSY*,[7] or *higher order SUSY* (*n-SUSY*),[8,9] or $\mathcal{N}$*-fold SUSY*,[5,10] the study of which has attracted the attention of a lot of researchers in recent times.[5–10] Contrary to standard SUSY, anticommutator of the supercharges no longer coincides with the Hamiltonian in general. Instead, it becomes a polynomial of the Hamiltonian in degree N, and is sometimes referred to as the *Mother Hamiltonian*.[5,10]

[a)]Electronic mail: anjana23@rediffmail.com
[b)]Electronic mail: pinaki@isical.ac.in

Furthermore, the equivalence between an Nth order Darboux transformation and a chain of N first order Darboux transformation is well established.[9] Every chain of N first order Darboux transformation creates a chain of exactly solvable Hamiltonians $h_0 \to h_1 \to \cdots \to h_N$. Hence the intertwining operator $L^{(N)}$ between the initial Hamiltonian h_0 and the final Hamiltonian h_N can always be presented as a product of N first order Darboux transformation operators between every two juxtaposed Hamiltonians $h_0, h_1, \ldots, h_N$,

$$L^{(N)} = L_N L_{N-1} \cdots L_2 L_1, \quad h_p L_p = L_p h_{p-1}, \quad p = 1,2,\ldots,N. \tag{2}$$

In conventional higher order SUSY, h_0 and h_N are essentially self-adjoint Hermitian operators in a Hilbert space, with square integrable eigenfunctions. If all the intermediate potentials $V_1(x)$, $V_2(x), \ldots, V_{N-1}(x)$ are real valued functions in their common domain of definition (a,b), the chain is called *reducible*, and the Nth order Darboux transformation is called *reducible* as well. Additionally, if all the intermediate potentials are free of singularities in (a,b), the chain and the corresponding transformation are called *completely reducible*. When at least one intermediate potential is a complex valued function, the chain and the corresponding transformation are called *irreducible*.

At the same time, non-Hermitian Hamiltonians have made an important place for themselves in the recent development of quantum mechanics, because of their intrinsic interest[11] and possible applications.[12] It is well known by now that a non-Hermitian $\mathcal{PT}$ symmetric Hamiltonian admits real eigenvalues if the eigenfunctions, too, respect the $\mathcal{PT}$ invariance (the so-called unbroken $\mathcal{PT}$ symmetry), whereas the eigenvalues occur as complex conjugate pairs if $\mathcal{PT}$ symmetry is spontaneously broken (in this case the eigenfunctions are no longer $\mathcal{PT}$ invariant). For such non-Hermitian $\mathcal{PT}$ symmetric Hamiltonians,

$$\mathcal{PT}H = H\mathcal{PT}, \tag{3}$$

where $\mathcal{P}$ stands for the *space inversion* operator and $\mathcal{T}$ denotes *time reversal*,

$$\begin{aligned} &\mathcal{P}: \quad x \to -x, \quad p \to -p, \\ &\mathcal{T}: \quad x \to x, \quad p \to -p, \quad i \to -i \end{aligned} \tag{4}$$

The reality of the spectrum may be attributed to the so-called η-pseudo Hermiticity of the non-Hermitian Hamiltonian[13]

$$H^{\dagger} = \eta H \eta^{-1}, \tag{5}$$

where η is a linear, invertible, Hermitian operator. Several non-Hermitian Hamiltonians, whether possessing $\mathcal{PT}$ invariance or not, have been identified as η pseudo-Hermitian under $\eta = e^{-\theta p}$, where θ is real, and $p = -i(d/dx)$, or $\eta = e^{-\phi(x)}$, where $\phi(x)$ is some gaugelike transformation. We note that for $\mathcal{PT}$ symmetric Hamiltonians, η may simply be taken as the parity operator $\mathcal{P}$, whereas for conventional Hermitian Hamiltonians, $\eta = 1$.

Moreover, the square integrability of the wave functions is no longer a prerequisite for non-Hermitian Hamiltonians. Instead, the orthonormalization of the wave function for Hermitian quantum mechanics

$$\int \Psi_m^* \Psi_n \, dx = \delta_{m,n} \tag{6}$$

is replaced by[14]

$$\int [\mathcal{CPT}\Psi_m]\Psi_n \, dx = \delta_{m,n,} \tag{7}$$

where $\mathcal{C}$ plays the role of a linear charge operator, obeying the relationship

$$[\mathcal{C},H]=0, \quad [\mathcal{C},\mathcal{PT}]=0 \tag{8}$$

and has the property $\mathcal{C}^2=1$. In the position representation $\mathcal{C}$ is given as

$$\mathcal{C}(x,y)=\sum_n \psi_n(x)\psi_n(y) \tag{9}$$

and the completeness relation gets modified to

$$\sum_n [\mathcal{CPT}\psi_n(x)]\psi_n(y)=\delta(x-y). \tag{10}$$

While nonlinear SUSY for $N=2$ has been investigated widely for Hermitian Hamiltonians,[5–10] such studies have not been carried out as yet for non-Hermitian Hamiltonians. Motivated by the importance of such systems in the recent development of quantum mechanics, our aim in the present work is to generalize the concept of nonlinear SUSY to include non-Hermitian quantum systems. In analogy with the first order systems, where the partner Hamiltonians $H_\pm$ of non-Hermitian systems were found to be related through *pseudosupersymmetry*,[13,15] it will be shown that the underlying symmetry between the isospectral partners h_0 and h_N is a generalization of $\mathcal{N}$ SUSY and may be called *nonlinear pseudosupersymmetry*. The nature of the intermediate Hamiltonians as well as the corresponding wave functions will also be investigated.

The organization of the paper is as follows. For the sake of completeness, in Sec. II we briefly outline conventional nonlinear SUSY for Hermitian quantum mechanics. In Sec. III we describe a similar framework for non-Hermitian Hamiltonians and show that the underlying symmetry for the potentials produced by higher order Darboux algorithm is nonlinear pseudosupersymmetry. Some explicit examples are given in Secs. IV and V, while Sec. VI is devoted to a conclusion.

II. NONLINEAR SUSY FOR HERMITIAN HAMILTONIANS

In the conventional first order supersymmetric quantum mechanics, if a given solvable Hamiltonian

$$H=-\frac{d^2}{dx^2}+V(x) \tag{11}$$

possesses a discrete spectrum of bound states E_n, $n=0,1,2,\ldots$, together with the square-integrable eigenfunctions $\psi_n(x)$, then a pair of first-order operators L_0 and $L_0^\dagger$ can be constructed from the ground state ψ_0, given by

$$L_0=\frac{d}{dx}+W_0(x), \quad L_0^\dagger=-\frac{d}{dx}+W_0(x), \tag{12}$$

where

$$W_0(x)=-[\ln \psi_0(x)]' \tag{13}$$

such that L_0 and $L_0^\dagger$ play the role of intertwining operators for the initial and final Hamiltonians H and $\tilde{H}$, respectively,

$$\tilde{H}L_0=L_0H, \quad HL_0^\dagger=L_0^\dagger\tilde{H} \tag{14}$$

with

$$H=L_0^\dagger L_0, \quad \tilde{H}=L_0L_0^\dagger. \tag{15}$$

Simple straightforward algebra shows that the partner potentials $V(x)$ and $\tilde{V}(x)$ can be expressed as

$$V(x) = W_0^2(x) - W_0'(x), \tag{16}$$

$$\tilde{V}(x) = W_0^2(x) + W_0'(x) = V(x) + 2W_0'(x). \tag{17}$$

The eigenfunctions $\psi(x)$ and $\tilde{\psi}(x)$ of H and $\tilde{H}$ are interrelated through L_0 and $L_0^\dagger$:

$$L_0\psi_0(x) = 0, \quad L_0(x)\psi_i(x) = \frac{W_{0,i}(x)}{\psi_0(x)}\alpha\,\tilde{\psi}_i(x), \quad L_0^\dagger\tilde{\psi}_i(x)\alpha\,\psi_i(x), \quad i = 1,2,\ldots, \tag{18}$$

where $W_{0,i}(x) = \{\psi_0(x)\psi_i'(x) - \psi_0'(x)\psi_i(x)\}$ is the Wronskian of $\psi_0(x)$ and $\psi_i(x)$. The concise algebraic form of spectral equivalence is given by the superalgebra for the partners H and $\tilde{H}$, and the supercharges Q and $Q^\dagger$,

$$Q = \begin{pmatrix} 0 & L_0 \\ 0 & 0 \end{pmatrix}, \quad Q^\dagger = \begin{pmatrix} 0 & 0 \\ L_0^\dagger & 0 \end{pmatrix}, \tag{19}$$

$$\mathcal{H} = \{Q, Q^\dagger\} = \begin{pmatrix} H & 0 \\ 0 & \tilde{H} \end{pmatrix} = \begin{pmatrix} L_0^\dagger L_0 & 0 \\ 0 & L_0 L_0^\dagger \end{pmatrix} \tag{20}$$

satisfying the relations

$$\{Q,Q\} = \{Q^\dagger, Q^\dagger\} = 0, \quad [Q,\mathcal{H}] = [Q^\dagger,\mathcal{H}] = 0. \tag{21}$$

Thus H and $\tilde{H}$ are isospectral except for the lowest eigenvalue E_0 which is missing in $\tilde{H}$, as $\tilde{\psi}_0$ is not normalizable.

To generalize standard SUSY to higher order, the supercharges are built of higher order intertwining operators.[9] The two Hamiltonians h_0 and h_N are intertwined through an Nth order differential operator $L^{(N)}$, as

$$L^{(N)}h_0 = h_N L^{(N)}, \quad h_0 L^{(N)\dagger} = L^{(N)\dagger} h_N, \tag{22}$$

where h_0 and h_N are self-adjoint operators. The proper eigenfunctions ψ_i of the original Hamiltonian h_0 are known exactly, $h_0\psi_i = E_i\psi_i$. Any such operator $L^{(N)}$ can always be presented in the form known as Crum–Krein formula[16]

$$L^{(N)} = W^{-1}(u_1,u_2,\ldots,u_N)\begin{vmatrix} u_1 & u_2 & \cdots & 1 \\ u'_1 & u'_2 & \cdots & \dfrac{d}{dx} \\ \vdots & \vdots & \ddots & \vdots \\ u_1^{(N)} & u_2^{(N)} & \cdots & \dfrac{d^N}{dx^N} \end{vmatrix}, \tag{23}$$

where $W(u_1,u_2,\ldots,u_N)$ stands for the usual symbol for the Wronskian of the functions $u_1, u_2, \ldots, u_N$. The functions u_i $(i = 1,2,\ldots,N)$ called the transformation functions are eigenfunctions of h_0, $h_0 u_i = \alpha_i u_i$, and they need not necessarily satisfy any physical boundary condition. The final potential has the form

$$V_N(x) = V(x) - 2\frac{d^2}{dx^2}\ln W(u_1, u_2, \ldots, u_N) \tag{24}$$

and will be free of singularities whenever the Wronskian is nodeless, which in turn requires that only consecutive eigenfunctions of h_0 must be considered.[9] The eigenfunctions $\psi(x)$ and $\tilde{\psi}(x)$ of h_0 and h_N are connected by the intertwiners $L^{(N)}$ and $L^{(N)\dagger}$ as

$$\tilde{\psi}_i(x) = L^{(N)}\psi_i(x) = \frac{W_{j,j+1,\ldots,j+N,i}(x)}{W_{j,j+1,\ldots,j+N}(x)}, \tag{25}$$

where $W_{j,j+1,\ldots,j+N,i}(x)$ and $W_{j,j+1,\ldots,j+N}(x)$ are the Wronskians of the eigenfunctions of h_0 associated with the corresponding subindices. Thus if $\psi_i(x)$ is an eigenfunction of h_0 with energy E_i, then $\tilde{\psi}_i(x)$ is an eigenfunction of h_N with the same energy E_i. Evidently

$$L^{(N)}\psi_i = 0, \quad i = 1, 2, \ldots, N. \tag{26}$$

However, for energies E_i $(i=1,2,\ldots,N)$, the corresponding eigenfunctions of h_N,

$$\tilde{\psi}(x)\alpha\frac{\psi(x)}{W_{j,j+1,\ldots,j+N}(x)},$$

have growing asymptotics at both infinities. Consequently, these are not physically acceptable solutions of h_N, and the corresponding eigenvalues E_i $(i=1,2,\ldots,N)$ are excluded from the spectrum of h_N. Thus

$$h_N\tilde{\psi}_E = E\tilde{\psi}_E \tag{27}$$

with the exception of the levels $E=E_i$, $i=1,2,\ldots,N$, which will be absent in the spectrum of the new Hamiltonian h_N, as the corresponding eigenfunctions are not square integrable.

It has already been shown[17] that the operator $L^{(N)}$ can always be presented as a product of N first order Darboux transformation operators between every two Hamiltonians $h_0, h_1, \ldots, h_N$,

$$L^{(N)} = L_N L_{N-1}\cdots L_1, \quad h_p L_p = L_p h_{p-1}, \quad p = 1, 2, \ldots, N. \tag{28}$$

We note that the final Hamiltonian h_N is Hermitian, although some of the intermediate Hamiltonians h_i could be unphysical, e.g., their associated potentials might contain extra singularities that were not present in the initial one. The supercharges Q_N and $Q_N^\dagger$ are constructed as

$$Q_N = \begin{pmatrix} 0 & L^{(N)} \\ 0 & 0 \end{pmatrix}, \quad Q_N^\dagger = \begin{pmatrix} 0 & 0 \\ L^{(N)\dagger} & 0 \end{pmatrix}. \tag{29}$$

Evidently, Q_N and $Q_N^\dagger$ are nilpotent

$$\{Q_N, Q_N\} = \{Q_N^\dagger, Q_N^\dagger\} = 0. \tag{30}$$

The super-Hamiltonian

$$H_N = \begin{pmatrix} h_0 & 0 \\ 0 & h_N \end{pmatrix} \tag{31}$$

satisfies the relations

$$[Q_N, H_N] = [Q_N^\dagger, H_N] = 0. \tag{32}$$

The anticommutator can be generally expressed by a Nth order polynomial $\mathcal{P}_\mathcal{N}$ of the Hamiltonian H_N,

$$\mathcal{H}_N = \{Q_N^\dagger, Q_N\} = \begin{pmatrix} L^{(N)\dagger}L^{(N)} & 0 \\ 0 & L^{(N)}L^{(N)\dagger} \end{pmatrix} = \prod_{k=1}^{N} (H_N - \alpha_k \mathcal{I}), \tag{33}$$

where $\mathcal{I}$ is the 2×2 unit matrix, and

$$L^{(N)\dagger}L^{(N)} = \prod_{k=1}^{N} (h_0 - \alpha_k), \tag{34}$$

$$L^{(N)}L^{(N)\dagger} = \prod_{k=1}^{N} (h_N - \alpha_k). \tag{35}$$

Since the right-hand side of (33) is a polynomial in H_N, it is called nonlinear SUSY or N-fold SUSY. The operator $\mathcal{H}_\mathcal{N}$ is termed as the *Mother Hamiltonian* and satisfies the commutation relations[9]

$$[Q_N, \mathcal{H}_N] = [Q_N^\uparrow, \mathcal{H}_N] = 0. \tag{36}$$

For $N=1$, N-fold SUSY reduces to standard SUSY.

The most widely studied higher order SUSY is for $N=2$,[8,9] where the formalism reduces to

$$L^{(2)} = L_2 L_1, \tag{37}$$

where

$$L_1 = -\partial_x + (\ln u_1)', \quad L_2 = -\partial_x + (\ln v)', \quad v = L_1 u_2, \tag{38}$$

and the isospectral potential turns out to be

$$\tilde{V}_2(x) = V(x) - 2\frac{d^2}{dx^2} \ln W_{j,j+1}(x). \tag{39}$$

III. NONLINEAR PSEUDO-SUSY FOR NON-HERMITIAN HAMILTONIANS

In this section we extend the concept of nonlinear or N-fold supersymmetry to non-Hermitian quantum mechanics. Though the Darboux algorithm and (nonlinear) supersymmetric quantum mechanics are equivalent for Hermitian Hamiltonians, the situation is different for non-Hermitian Hamiltonians. However, intertwining operators $A^{(N)}$ and $B^{(N)}$ can still be constructed with the help of Darboux transformation. Analogous to the case of Hermitian quantum mechanics, it will be shown that once a non-Hermitian Schrödinger potential $V(x)$ is exactly solvable, one can construct an isospectral partner $\tilde{V}_N(x)$ from (24),

$$\tilde{V}_N(x) = V(x) - 2\frac{d^2}{dx^2} \ln W(u_1, u_2, \ldots, u_N), \tag{40}$$

where W stands for the usual symbol for the Wronskian of the functions $u_1, u_2, \ldots, u_N$, which are eigenfunctions of h_0, $h_0 u_i = \alpha_i u_i$. As before the functions $u_i(x)$ may be just formal eigenfunctions. Our aim will be to study the spectrum of the new Hamiltonian in detail, to investigate the nature of the potential and the eigenfunctions, and to determine the symmetry which connects the original Hamiltonian h_0 and the transformed one h_N. For this purpose, we look for two intertwining operators $A^{(N)}$ and $B^{(N)}$ such that

$$A^{(N)}h_0 = h_N A^{(N)}, \quad h_0 B^{(N)} = B^{(N)} h_N, \tag{41}$$

where h_0 and h_N are no longer self-adjoint operators ($h_{0,(N)} \neq h_{0,(N)}^{\dagger}$); on the contrary, to ensure the reality of the spectrum, they are η pseudo-Hermitian,

$$\eta h_{0,(N)} \eta^{-1} = h_{0,(N)}^{\dagger}, \tag{42}$$

where η is a linear, invertible, Hermitian operator. However, the choice of η is not unique. For $\mathcal{PT}$ invariant potentials, a simple representation of η may be given by the parity operator,

$$\eta = \mathcal{P}, \quad \mathcal{P}f(x) = f(-x). \tag{43}$$

It follows that for real potentials, (43) leads to $\eta=1$ so that $B^{(N)}=A^{(N)\dagger}$, thus reproducing the standard result of supersymmetry.

It follows from Eqs. (41) and (42) that the operators $A^{(N)}$ and $B^{(N)}$ are pseudo-adjoint:

$$B^{(N)} = A^{(N)\#} = \eta^{-1} A^{(N)\dagger} \eta. \tag{44}$$

Considering first order Darboux transformation between every two juxtaposed Hamiltonians $h_{0,}h_{1,},\ldots,h_N$, each pair intertwined by first order operators L_k $(k=1,2,\ldots,N)$

$$h_k L_k = L_k h_{k-1,} \quad k = 1,2,3,\ldots,N, \tag{45}$$

$$L_k^{\#} h_k = h_{k-1} L_k^{\#}, \quad k = 1,2,3,\ldots,N, \tag{46}$$

where

$$L_k^{\#} = \eta^{-1} L_k \eta \tag{47}$$

then, analogous to the Hermitian case, the final Hamiltonian h_N is found to be related to the initial (or starting) Hamiltonian h_0 through

$$h_N = L_N L_{N-1} \cdots L_2 L_1 \; h_0 \; L_1^{\#} L_2^{\#} \cdots L_N^{\#} \tag{48}$$

so that the operator $A^{(N)}$ can be represented as a product of the N first order Darboux transformations

$$A^{(N)} = L_N L_{N-1} \cdots L_2 L_1 \tag{49}$$

with its pseudo-adjoint

$$B^{(N)} = A^{(N)\#} = \eta^{-1} L_1 L_2 \cdots L_N \eta = L_1^{\#} \cdots L_{N-1}^{\#} L_N^{\#}. \tag{50}$$

It is worth mentioning here that in contrast to Hermitian quantum mechanics, all the intermediate Hamiltonians h_k are physically acceptable as their associated potentials contain no extra singularities which are not present in the initial potential $V(x)$. This is essentially because the associated eigenfunctions do not have nodes on the real line, and they are normalizable in the sense of Eq. (7).

Thus the initial and the transformed Hamiltonians h_0 and h_N are related by *nonlinear pseudosupersymmetry*. The super-Hamiltonian of this system consists of the pseudosupersymmetric pair of Hamiltonians h_0 and h_N as

$$H_N = \begin{pmatrix} h_0 & 0 \\ 0 & h_N \end{pmatrix}. \tag{51}$$

The supercharges generating this form of pseudosupersymmetry are constructed in the following way:

$$Q_N = \begin{pmatrix} 0 & A^{(N)} \\ 0 & 0 \end{pmatrix}, \quad Q_N^{\#} = \eta^{-1} Q_N^{\dagger} \eta = \begin{pmatrix} 0 & 0 \\ B^{(N)} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ A^{(N)\#} & 0 \end{pmatrix} \tag{52}$$

so that the supercharge Q_N and its pseudoadjoint $Q_N^{\dagger}$ of standard Hermitian quantum mechanics are replaced by Q_N and its pseudoadjoint $Q_N^{\#}$ for non-Hermitian Hamiltonians. Obviously, Q_N and $Q_N^{\#}$ are nilpotent

$$\{Q_N, Q_N\} = \{Q_N^{\#}, Q_N^{\#}\} = 0 \tag{53}$$

and satisfy the following closed algebra:

$$[Q_N, H_N] = [Q_N^{\#}, H_N] = 0, \tag{54}$$

$$\mathcal{H}_N \equiv \{Q_N^{\#}, Q_N\} = \begin{pmatrix} A^{(N)\#} A^{(N)} & 0 \\ 0 & A^{(N)} A^{(N)\#} \end{pmatrix} = \prod_{k=1}^{N} (H_N - \alpha_k \mathcal{I}), \tag{55}$$

i.e.,

$$A^{(N)\#} A^{(N)} = \prod_{k=1}^{N} (h_0 - \alpha_k), \tag{56}$$

$$A^{(N)} A^{(N)\#} = \prod_{k=1}^{N} (h_N - \alpha_k), \tag{57}$$

and $\mathcal{I}$ is the 2×2 unit matrix. Evidently, if $\psi_i(x)$ is an eigenfunction of h_0 with energy eigenvalue E_i, then $\tilde{\psi}_i(x) = A^{(N)} \psi_i(x)$ is an eigenfunction of h_N with the same energy E_i. However, for $i = 1, 2, \ldots, N$,

$$\tilde{\psi}(x) \alpha \frac{\psi(x)}{W(\psi_1, \psi_2, \ldots, \psi_N)}. \tag{58}$$

Clearly, the eigenfunctions $\tilde{\psi}_i(x)$ $(i = 1, 2, \ldots N)$ of h_N corresponding to the eigenvalues E_i $(i = 1, 2, \ldots, N)$ grow asymptotically, and so cannot be included in the set of solutions of h_N. Consequently, E_i $(i = 1, 2, \ldots, N)$ are excluded from the spectrum of h_N.

Next we note two interesting results which are in contrast to the Hermitian case.

(1) For $\tilde{V}_N(x)$ to be free of singularities, the Wronskian $W(\psi_1, \psi_2, \ldots, \psi_N) = W_{\psi_1, \psi_2, \ldots, \psi_N}(x)$ must be nodeless. In the case of Hermitian potentials, this is guaranteed only when ψ_i, $i = 1, 2, \ldots, N$ represent N consecutive eigenfunctions. However, in the case of generic non-Hermitian potentials, the eigenfunctions $\psi_n(x)$ $(n = 0, 1, 2, \ldots)$ have no nodes on the real line. Consequently, the Wronskian is free of real singularities for any value of $i, j, k, \ldots$, and thus can be used to generate a wider class of isospectral Hamiltonians.

(2) The intermediate Hamiltonians are also physically acceptable, as the corresponding potentials are free of singularities, for the same reason as given above. For example, the first intertwining gives

$$V_1(x) = V(x) - 2 \frac{d^2}{dx^2} \ln \psi_i(x) \tag{59}$$

which is well defined. However, this may not always be true for Hermitian potentials due to the presence of additional singularities in $V_1(x)$, which are not present in $V(x)$.

For the sake of simplicity, in the present work we shall restrict ourselves to second order nonlinear pseudosupersymmetry. Thus if an intertwining operator $A=L_2L_1$ is constructed from the two first order Darboux transformation operators L_1 and L_2, given by

$$L_1 = -\partial_x + (\ln u_i)', \quad L_2 = -\partial_x + (\ln v)', \quad v = L_1 u_j, \tag{60}$$

where u_i and u_j are any two eigenfunctions of the non-Hermitian Hamiltonian h_0, then the transformed isospectral Hamiltonian,

$$h_2 = -\frac{d^2}{dx^2} + \tilde{V}_{i,j}(x) \tag{61}$$

has eigenfunctions

$$\tilde{\psi}_n(x) = \frac{W(\psi_i, \psi_j, \psi_n)}{W(\psi_i, \psi_j)} = -E_n\psi_n + E_i\psi_i\frac{W(\psi_n, \psi_j)}{W(\psi_i, \psi_j)} + E_j\psi_j\frac{W(\psi_i, \psi_n)}{W(\psi_i, \psi_j)}, \tag{62}$$

where

$$\tilde{V}_{i,j}(x) = V(x) - 2\frac{d^2}{dx^2}\ln W(u_i, u_j). \tag{63}$$

The mother Hamiltonian $\mathcal{H}_2$ is constructed from the anticommutator by

$$\mathcal{H}_2 = \{Q_2^{\#}, Q_2\} = \begin{pmatrix} A^{\#}A & 0 \\ 0 & AA^{\#} \end{pmatrix} = \begin{pmatrix} (h_0 - \alpha_1\mathcal{I})(h_0 - \alpha_2\mathcal{I}) & 0 \\ 0 & (h_2 - \alpha_1\mathcal{I})(h_2 - \alpha_2\mathcal{I}) \end{pmatrix}, \tag{64}$$

where $\mathcal{I}$ is 2×2 unit matrix and H_2 is given by (51).

In the following sections we shall investigate this formalism further with the help of explicit examples.

IV. $\mathcal{PT}$ SYMMETRIC OSCILLATOR

In this section we shall apply our formalism to the well-known example of the $\mathcal{PT}$ symmetric oscillator[18]

$$V(x) = (x - i\epsilon)^2 + \frac{\alpha^2 - \frac{1}{4}}{(x - i\epsilon)^2} \tag{65}$$

with eigenfunctions

$$\psi_n(x) = e^{-(1/2)(x - i\epsilon)^2}(x - i\epsilon)^{-q\alpha+1/2}L_n^{-q\alpha}((x - i\epsilon)^2) \tag{66}$$

and eigenvalues

$$E_n = 4n - 2q\alpha + 2, \quad n = 0, 1, 2, \ldots, \tag{67}$$

where $q=\pm 1$ is called the quasiparity.

In this study we shall restrict ourselves to $N=2$ only. If one performs Darboux transformations with two eigenfunctions $\psi_i(x)$ and $\psi_j(x)$ of the potential $V(x)$, corresponding to energies E_i and E_j (i and j need not be consecutive), then the intertwining operators take the form

$$L_1 = -\frac{d}{dx} + \frac{\psi_i'}{\psi_i}, \quad L_1^{\#} = \frac{d}{dx} + \frac{\psi_i'}{\psi_i}, \tag{68}$$

$$L_2 = -\frac{d}{dx} + \frac{W'_{i,j}}{W_{i,j}} - \frac{\psi'_i}{\psi_i}, \quad L_2^{\#} = \frac{d}{dx} + \frac{W'_{i,j}}{W_{i,j}} - \frac{\psi'_i}{\psi_i}, \tag{69}$$

where $W_{i,j}$ is the usual Wronskian given by

$$W_{i,j} = W(\psi_i, \psi_j) = \psi_i(x)\psi'_j(x) - \psi'_i(x)\psi_j(x) \tag{70}$$

and η has been taken as in (43). Replacing the intertwining operators $A^{(2)}$ (and $B^{(2)}$) by A (and B) for simplicity, we obtain

$$A = L_2 L_1 = \frac{d^2}{dx^2} + \beta_{i,j}\frac{d}{dx} - \beta_{i,j}\frac{\psi'_i}{\psi_i} - \frac{\psi''_i}{\psi_i}, \tag{71}$$

$$B = A^{\#} = \eta^{-1}A^{\dagger}\eta = \frac{d^2}{dx^2} - \beta_{i,j}\frac{d}{dx} - \beta_{i,j}\frac{\psi'_i}{\psi_i} - \frac{\psi''_i}{\psi_i} - \beta'_{i,j}, \tag{72}$$

where

$$\beta_{i,j} = -\frac{W'_{i,j}}{W_{i,j}} \tag{73}$$

and η is simply the parity operator $\mathcal{P}$ for $\mathcal{PT}$ symmetric potentials. The new exactly solvable non-Hermitian potential, which is isospectral to the $\mathcal{PT}$ symmetric oscillator in (65), is obtained from

$$\tilde{V}_{i,j}(x) = V(x) - 2\frac{d^2}{dx^2}\ln W_{i,j} \tag{74}$$

with solutions

$$\tilde{\psi}_k(x) = A\psi_k(x). \tag{75}$$

Thus for each set (i,j), one obtains two sets of $\tilde{V}_{i,j}(x)$ because of the presence of quasiparity q. Obviously, $\tilde{\psi}_k(x) = 0$ for $k = i, j$. Thus the new potential so constructed in (74) above, has all the eigenenergies of the original $\mathcal{PT}$ symmetric oscillator except for the levels i, j, which are missing from the spectrum of (74).

For the simplicity of calculations we shall now construct and examine some potentials using low values of i and j in further detail.

A. New potential for $i=1$, $j=2$

Applying the above formalism with the two eigenstates $\psi_1(x)$ and $\psi_2(x)$ of the potential in (65), the Wronskian is found to be

$$W(\psi_1, \psi_2) = c_{12}e^{-(x-i\epsilon)^2}(x - i\epsilon)^{2-2q\alpha}g, \tag{76}$$

where c_{12} is some real constant and

$$g = (1 - q\alpha)(2 - q\alpha) - 2(1 - q\alpha)(x - i\epsilon)^2 + (x - i\epsilon)^4. \tag{77}$$

The intertwining operators A and $A^{\#}$ are obtained from $A = L_2L_1$, $A^{\#} = L_1^{\#}L_2^{\#}$, where

$$L_1 = -\frac{d}{dx} + \frac{\psi'_1}{\psi_1} = -\frac{d}{dx} - (x - i\epsilon) + \frac{-q\alpha + \frac{1}{2}}{(x - i\epsilon)} - \frac{2(x - i\epsilon)}{1 - q\alpha - (x - i\epsilon)^2}, \tag{78}$$

$$L_2 = -\frac{d}{dx} + \frac{d}{dx}\ln(L_1\psi_2) = -\frac{d}{dx} - (x - i\epsilon) + \frac{-q\alpha + \frac{3}{2}}{(x - i\epsilon)} + \frac{2(x - i\epsilon)}{1 - q\alpha - (x - i\epsilon)^2} + \frac{g'}{g}, \tag{79}$$

so that

$$A = \frac{d^2}{dx^2} - \left\{ -2(x - i\epsilon) + \frac{2(1 - q\alpha)}{(x - i\epsilon)} + \frac{g'}{g} \right\} \frac{d}{dx} + (x - i\epsilon)^2 + \frac{(-q\alpha + \frac{1}{2})(-q\alpha + \frac{5}{2})}{(x - i\epsilon)^2} + 2q\alpha - 1$$
$$+ \left\{ -(x - i\epsilon) + \frac{-q\alpha + \frac{1}{2}}{(x - i\epsilon)} - \frac{2(x - i\epsilon)}{1 - q\alpha - (x - 1\epsilon)^2} \right\} \frac{g'}{g}, \tag{80}$$

$$A^{\#} = \frac{d^2}{dx^2} + \left\{ -2(x - i\epsilon) + \frac{2(1 - q\alpha)}{(x - i\epsilon)} + \frac{g'}{g} \right\} \frac{d}{dx} + (x - i\epsilon)^2 + \frac{(-q\alpha + \frac{3}{2})(-q\alpha - \frac{1}{2})}{(x - i\epsilon)^2} + 2q\alpha - 3$$
$$+ \left\{ -(x - i\epsilon) + \frac{-q\alpha + \frac{1}{2}}{(x - 1\epsilon)} - \frac{2(x - i\epsilon)}{1 - q\alpha - (x - i\epsilon)^2} \right\} \frac{g'}{g} + \frac{g''}{g} - \left(\frac{g'}{g}\right)^2. \tag{81}$$

Applying Eq. (74), the new potential isospectral to the one in (65) except for the states corresponding to $\psi_1(x)$ and $\psi_2(x)$, comes out as

$$\tilde{V}_{1,2}(x) = (x - i\epsilon)^2 + \frac{(-q\alpha + \frac{3}{2})(-q\alpha + \frac{5}{2})}{(x - i\epsilon)^2} - 2\frac{g''}{g} + 2\left(\frac{g'}{g}\right)^2 + 4 \tag{82}$$

which has solutions

$$\tilde{\psi}_n(x) = -E_{n+2}\psi_{n+2} + E_1\psi_1 \frac{W(\psi_{n+2}, \psi_2)}{W(\psi_1, \psi_2)} + E_2\psi_2 \frac{W(\psi_1, \psi_{n+2})}{W(\psi_1, \psi_2)} \tag{83}$$

with energy eigenvalues

$$\tilde{E}_n = E_{n+2} = 4n + 10 - 2q\alpha, \quad n = 1, 2, 3, \ldots . \tag{84}$$

The ground state is given by

$$\tilde{\psi}_0(x) = e^{-(1/2)(x - i\epsilon)^2}(x - i\epsilon)^{-q\alpha + 1/2}\left\{ B_1 + \frac{B_2(x - i\epsilon)^2}{g} \right\} \tag{85}$$

with eigenvalue

$$\tilde{E}_0 = E_0 = 2 - 2q\alpha, \tag{86}$$

where B_1 and B_2 are some x, ϵ independent constants. Thus the energies E_1 and E_2 of $V(x)$ are absent in the spectrum of $\tilde{V}_{1,2}(x)$. It can be verified that the eigenfunctions $\tilde{\psi}$ are also $\mathcal{PT}$ invariant, and can be normalized using (7). Furthermore, the supercharges Q_2 and $Q_2^{\#}$, generated from the operators A and $A^{\#}$, satisfy the following algebra :

$$\mathcal{H}_2 = \{Q_2, Q_2^{\#}\} = H_2^2 - 4(4 - q\alpha)H_2 + (6 - 2q\alpha)(10 - 2q\alpha), \tag{87}$$

where H_2 is given by (51). The intermediate potential given by

$$V_1(x) = V(x) - 2\frac{d^2}{dx^2}\ln \psi_1(x) = (x - i\epsilon)^2 + \frac{(-q\alpha + \frac{1}{2})(-q\alpha + \frac{3}{2})}{(x - i\epsilon)^2} + \frac{12}{1 - q\alpha - (x - i\epsilon)^2} - \frac{8(1 - q\alpha)}{\{1 - q\alpha - (x - i\epsilon)^2\}^2} + 4 \tag{88}$$

does not have any singularity on the real line, and hence is physically acceptable as well. By arguments similar to those given above, its ground state eigenfunction is given by

$$\phi_0 = \frac{1}{1 - q\alpha - (x - i\epsilon)^2} e^{-(1/2)(x - i\epsilon)^2} (x - i\epsilon)^{-q\alpha + (3/2)} \tag{89}$$

with energy

$$e_0 = E_0 = 2 - 2q\alpha \tag{90}$$

and the excited states

$$\phi_n = \frac{W(\psi_{n+1}, \psi_1)}{\psi_1} \tag{91}$$

with corresponding energies

$$e_n = E_{n+1} = 4n + 6 - 2q\alpha, \quad n = 1,2,3,\ldots . \tag{92}$$

It is easy to observe that applying (4), both the intermediate and the final potentials (as well as their eigenfunctions) satisfy (3), and hence are $\mathcal{PT}$ invariant, having real spectra.

B. New potentials for *i*=0, *j*=2

In a similar manner, the expressions for the different quantities are obtained as follows:

$$W(\psi_0, \psi_2) = c_{02} e^{-(x - i\epsilon)^2} (x - i\epsilon)^{-2q\alpha + 2} \left\{ \frac{(x - i\epsilon)^2}{2 - q\alpha} - 1 \right\} \tag{93}$$

with c_{02} some real constant

$$L_1 = -\frac{d}{dx} - (x - i\epsilon) + \frac{(-q\alpha + \frac{1}{2})}{(x - i\epsilon)}, \tag{94}$$

$$L_2 = -\frac{d}{dx^2} - (x - i\epsilon) + \frac{(-q\alpha + \frac{3}{2})}{(x - i\epsilon)} + \frac{2(x - i\epsilon)}{\left[(x - i\epsilon)^2 - (2 - q\alpha)\right]}, \tag{95}$$

$$A = \frac{d^2}{dx^2} + 2\left\{ (x - i\epsilon) + \frac{(q\alpha - 1)}{(x - i\epsilon)} - \frac{(x - i\epsilon)}{(x - i\epsilon)^2 - (2 - q\alpha)} \right\} \frac{d}{dx} + (x - i\epsilon)^2 + \frac{(-q\alpha + \frac{1}{2})(-q\alpha + \frac{5}{2})}{(x - i\epsilon)^2} - \frac{3}{(x - i\epsilon)^2 - (2 - q\alpha)} + 2q\alpha - 3, \tag{96}$$

$$A^{\#} = -\frac{d}{dx^2} - 2\left\{ (x - i\epsilon) + \frac{(q\alpha - 1)}{(x - i\epsilon)} + \frac{(x - i\epsilon)}{(x - i\epsilon)^2 - (2 - q\alpha)} \right\} \frac{d}{dx} + (x - i\epsilon)^2 + \frac{(-q\alpha - \frac{1}{2})(-q\alpha + \frac{3}{2})}{(x - i\epsilon)^2} - \frac{5}{\{(x - i\epsilon)^2 - (2 - q\alpha)\}} - \frac{4(-q\alpha + 2)}{\{(x - i\epsilon)^2 - (2 - q\alpha)\}^2} + 2q\alpha - 5. \tag{97}$$

The new potential

$$\tilde{V}_{0,2}(x) = (x - i\epsilon)^2 + \frac{\sigma(\sigma-1)}{(x-i\epsilon)^2} + \frac{4}{(x-i\epsilon)^2 - (2-q\alpha)} + \frac{8(2-q\alpha)}{\{(x-i\epsilon)^2 - (2-q\alpha)\}^2} + 4, \tag{98}$$

where

$$\sigma = -q\alpha + \tfrac{5}{2} \tag{99}$$

is totally different from the initial potential of the $\mathcal{PT}$ symmetric oscillator, yet shares the same spectrum except for the states $n=0$, 2 of the original potential, which are missing in the partner.

The ground state wave function of the Hamiltonian in (98) is given by

$$\tilde{\psi}_0(x) = \left\{ A_1(x-i\epsilon)^2 + A_2 + \frac{A_3}{(x-i\epsilon)^2 - (2-q\alpha)} \right\} e^{-(1/2)(x-i\epsilon)^2} (x-i\epsilon)^{-q\alpha+(1/2)} \tag{100}$$

with ground state energy

$$\tilde{E}_0 = E_1 = 6 - 2q\alpha, \tag{101}$$

where A_1, A_2, A_3 are x-independent constants, while the excited states are obtained from (62)

$$\tilde{\psi}_n = A\psi_{n+2} = -E_{n+2}\psi_{n+2} + E_0\psi_0 \frac{W(\psi_{n+2}, \psi_2)}{W(\psi_0, \psi_2)} + E_2\psi_2 \frac{W(\psi_0, \psi_{n+2})}{W(\psi_0, \psi_2)} \tag{102}$$

with energies

$$\tilde{E}_n = E_{n+2} = 4n + 10 - 2q\alpha, \quad n = 1,2,\ldots . \tag{103}$$

It can also be verified that eigenfunctions $\tilde{\psi}_n(x)$ have correct asymptotic behavior and are also $\mathcal{PT}$ invariant. Consequently, they also satisfy Eq. (7). The intermediate potential is given by

$$V_1(x) = (x-i\epsilon)^2 + \frac{(-q\alpha + \frac{1}{2})(-q\alpha + \frac{3}{2})}{(x-i\epsilon)^2} + 2 \tag{104}$$

which is also physically acceptable. By arguments similar to those given above, its ground state eigenfunction is given by

$$\phi_0 = e^{-(1/2)(x-i\epsilon)^2} (x-i\epsilon)^{-q\alpha+(3/2)} \tag{105}$$

with energy

$$e_0 = 6 - 2q\alpha \tag{106}$$

and excited states

$$\phi_n = \frac{W(\psi_{n+1}, \psi_0)}{\psi_0} \tag{107}$$

with energies

$$e_n = E_{n+1} = 4n + 6 - 2q\alpha, \quad n = 1,2,3,\ldots . \tag{108}$$

Once again, both the intermediate and the final potentials (as well as their eigenfunctions) are $\mathcal{PT}$ invariant, having real spectra.

The supercharges Q_2 and $Q_2^\dagger$ generated from the intertwining operators A and $A^\#$ can be shown to satisfy the following algebra:

$$\mathcal{H}_2 = \{Q_2, Q_2^\#\} = H_2^2 - 4(3-q\alpha)H_2 + (2-q\alpha)(10-2q\alpha) \tag{109}$$

where H_2 is given by (51).

We note that the potentials obtained in this section are unique in the sense that they do not have any counterpart in standard quantum mechanics (i.e., in the Hermitian case).

V. $\mathcal{PT}$ SYMMETRIC SCARF II POTENTIAL

We note that the generalized oscillator problem considered in the last section was made non-Hermitian by an imaginary displacement of the coordinate variable x. However, there are other methods of constructing non-Hermitian models. To see how the formalism described in Sec. III works with such models, in this section we shall study an example, viz., the $\mathcal{PT}$ symmetric non-Hermitian Scarf II potential, which has been $\mathcal{PT}$ symmetrized in a different way. This exactly solvable potential, given by

$$V(x) = -\lambda \operatorname{sech}^2 x - i\mu \operatorname{sech} x \tanh x, \quad \lambda > 0,\ \mu \neq 0 \tag{110}$$

has a discrete spectrum that admits both real as well as complex conjugate energies, depending on the relative strengths of its parameters λ and μ. For $|\mu| \leqslant \lambda + \frac{1}{4}$, the system possesses a real and discrete bound state spectrum, whereas for $|\mu| > \lambda + \frac{1}{4}$, the system exhibits spontaneous $\mathcal{PT}$ symmetry breaking, with complex conjugate pairs of energies. The normalized wave functions for this potential are well known, being given by[15,19]

$$\psi_n(x) = \frac{\Gamma(n - 2p + \frac{1}{2})}{n!\Gamma(\frac{1}{2} - 2p)} z^{-p} (z^*)^{-q} P_n^{-2p-1/2,-2q-1/2}(i \sinh x), \tag{111}$$

where $P_n^{\alpha,\beta}$ are the Jacobi polynomials,[20]

$$P_n^{\alpha,\beta}(i \sinh x) = \frac{\Gamma(n + \alpha + 1)}{\Gamma(n + 1)\Gamma(\alpha + 1)} F(-n, n + \alpha + \beta + 1; \alpha + 1; z) \tag{112}$$

and

$$z = \frac{1 - i \sinh x}{2}, \tag{113}$$

$$p = -\frac{1}{4} \pm \frac{1}{2}\sqrt{\frac{1}{4} + \lambda + \mu} = -\frac{1}{4} \pm \frac{t}{2}, \tag{114}$$

$$q = -\frac{1}{4} \pm \frac{1}{2}\sqrt{\frac{1}{4} + \lambda - \mu} = -\frac{1}{4} \pm \frac{s}{2}. \tag{115}$$

However, for normalization of the wave functions, only the positive sign is allowed in p. The energy spectrum

$$E_n = -(n - p - q)^2, \quad n = 0, 1, 2, \ldots < \left(\frac{s + t - 1}{2}\right) \tag{116}$$

is real and bound for $|\mu| \leqslant \lambda + \frac{1}{4}$, i.e., for real p and q, with two towers characterized by the two values of q.

If the formalism developed above is applied to this example for $N=2$, with states $\psi_0(x)$ and $\psi_2(x)$, then the Wronskian is calculated to be

$$W(\psi_0, \psi_2) = (1 - i \sinh x)^{-2p}(1 + i \sinh x)^{-2q} \cosh x\{-i(p - q) + (p + q - \tfrac{3}{2})\sinh x\} \tag{117}$$

and the intertwining operators A and $A^{\#}$ are given by

$$A = L_2 L_1, \quad A^{\#} = L_1^{\#} L_2^{\#}, \tag{118}$$

where L_1 and L_2 take the form

$$L_1 = -\frac{d}{dx} + \frac{\psi_0'}{\psi_0} = \frac{d}{dx} + i(p-q)\operatorname{sech} x - (p+q)\tanh x, \tag{119}$$

$$\begin{aligned} L_2 = &-\frac{d}{dx} + \frac{W_{0,2}'}{W_{0,2}} - \frac{\psi_0'}{\psi_0} = \frac{d}{dx} + i(p-q)\operatorname{sech} x - (p+q)\tanh x \\ &+ \frac{(-p-q+\frac{3}{2}) + i(p-q)\sinh x + (-2p-2q+3)\sinh^2 x}{i(p-q)\cosh x + (-p-q+\frac{3}{2})\sinh x \cosh x}. \end{aligned} \tag{120}$$

Now using (40) the new potential is found to be

$$\tilde{V}_{0,2}(x) = -\tilde{\lambda}\operatorname{sech}^2 x - i\tilde{\mu}\operatorname{sech} x \tanh x - 2\left(\frac{\sigma^2 \operatorname{sech}^2 x - i\rho\sigma \operatorname{sech} x \tanh x}{(\rho \operatorname{sech} x - i\sigma \tanh x)^2}\right), \tag{121}$$

where

$$\tilde{\lambda} = \lambda - 4p - 4q + 2, \tag{122}$$

$$\tilde{\mu} = \mu - 4p + 4q, \tag{123}$$

$$\lambda = 2(p^2 + q^2) + (p+q), \tag{124}$$

$$\mu = 2(p^2 - q^2) + (p-q), \tag{125}$$

$$\rho = p - q, \tag{126}$$

$$\sigma = -p - q + \tfrac{3}{2}. \tag{127}$$

Once again, the final potential $\tilde{V}_{0,2}(x)$ is also $\mathcal{PT}$ invariant. The eigenfunctions are obtained from (62), with the ground state as

$$\tilde{\psi}_0 = (E_0 - E_1)\psi_1 + (E_2 - E_0)\psi_2 \frac{P_1'}{P_2'} \tag{128}$$

and excited states

$$\tilde{\psi}_n = (E_0 - E_{n+2})\psi_{n+2} + (E_2 - E_0)\psi_2 \frac{P_{n+2}'}{P_2'} \tag{129}$$

where P_n denotes the Jacobi polynomial $P_n^{-2p-1/2-2q-1/2}(i \sinh x)$ and P_n' denotes its derivative with respect to x. It can be shown that for $|\mu| \leqslant \lambda + \frac{1}{4}$, the wave functions $\tilde{\psi}$ are also $\mathcal{PT}$ invariant, and can be normalized following (7). The new potential $\tilde{V}_{0,2}(x)$ has real bound state spectrum given by

$$\tilde{E}_0 = -(1-p-q)^2, \tag{130}$$

$$\tilde{E}_n = -(n+2-p-q)^2, \quad n = 1,2,\ldots, < \left(\frac{s+t-5}{2}\right), \tag{131}$$

and the algebra satisfied by the supercharges turns out to be

$$\mathcal{H}_2 = \{Q_2, Q_2^{\#}\} = H_2^2 + (2 - 2p - 2q)H_2 + (p + q)(p + q - 2), \tag{132}$$

where H_2 is given by (51).

The intermediate potential takes the form

$$V_1(x) = -\tilde{v}_1 \operatorname{sech}^2 x - i\tilde{v}_2 \operatorname{sech} x \tanh x, \tag{133}$$

where

$$\tilde{v}_1 = \lambda - 2(p + q), \tag{134}$$

$$\tilde{v}_2 = \mu - 2(p - q) \tag{135}$$

with eigenfunctions

$$\phi_n = \frac{W(\psi_{n+1}, \psi_0)}{\psi_0} \tag{136}$$

and the corresponding energies

$$e_n = E_{n+1} = -(n + 1 - p - q)^2, \quad n = 0, 1, \ldots, < \left(\frac{s + t - 3}{2}\right). \tag{137}$$

Thus $V_1(x)$ and the corresponding wave functions (136) are also physically acceptable as well as $\mathcal{PT}$ invariant.

VI. CONCLUSIONS

In this paper we have suggested an application of higher order Darboux algorithm to non-Hermitian $\mathcal{PT}$ symmetric potentials. For the sake of definiteness the method has been applied to two specific potentials, namely, the generalized oscillator and the Scarf II potentials and a number of new potentials having nearly the same spectrum as the original ones have been obtained. It may be noted that in each of these cases, starting from a $\mathcal{PT}$ symmetric potential we have obtained new potentials which are again $\mathcal{PT}$ symmetric. In other words the higher order Darboux algorithm does not induce spontaneous $\mathcal{PT}$ symmetry breaking. Among the different cases considered here the one involving nonconsecutive levels deserves special mention. The potentials thus obtained have no Hermitian analogues. Also the intermediate potentials in all the cases are perfectly well behaved since the Darboux algorithm does not introduce any new singularity or break $\mathcal{PT}$ symmetry. Furthermore it has been shown that the symmetry underlying the original and the new potentials is a fusion of *nonlinear SUSY* and $\mathcal{PT}$ symmetry which we call *nonlinear pseudosupersymmetry*. Finally we note that analogous to the study of breaking N-fold supersymmetry,[21] it would be of interest to examine breaking of this new symmetry.

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Universality of low-energy scattering in 2+1 dimensions: The nonsymmetric case

N. N. Khuri
Department of Physics, The Rockefeller University, New York, New York 10021

André Martin
Department of Physics, The Rockefeller University, New York, New York 10021 and Department of Physics, CERN, Theory Division, Geneva, Switzerland

Pierre C. Sabatier
Laboratoire de Physique Mathématique, Université de Montpellier II, Sciences et Techniques du Languedoc, F-34095, Montpellier, France

Tai Tsun Wu
Gordon McKay Laboratory, Harvard University, Cambridge, Massachusetts 02138 and Department of Physics, CERN, Theory Division, Geneva, Switzerland

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For a very large class of potentials, $V(\vec{x}), \vec{x} \in R^2$, we prove the universality of the low-energy scattering amplitude, $f(\vec{k}', \vec{k})$. The result is $f = \sqrt{\pi/2}(1/\log k) + o(1)/[\log(1/k)]$. The only exceptions occur if V happens to have a zero-energy bound state. Our new result includes as a special subclass the case of rotationally symmetric potentials, $V(|\vec{x}|)$. © *2005 American Institute of Physics.*
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I. INTRODUCTION

In a recent paper we proved an interesting universality property for the low-energy scattering limit in two space dimensions.[1] This was done both for massive quantum field theory in 2+1 dimensions, and for nonrelativistic quantum mechanics in two space dimensions for a centrally symmetric force.

The result briefly stated that the S-wave phase shift, $\delta_0(k)$, k being the c.m. momentum, vanishes as $\delta_0 \to c/\log(k/m)$ as $k \to 0$, or in exceptional cases, $\delta_0 = O(k^2)$. The constant, c, is universal, $c = \pi/2$ independent of the dynamics. For potential scattering this kind of universality was first noted in Ref. 2, albeit with an incomplete proof which missed among other things the exceptional class of potentials. For the field theoretic case the result can be found in an earlier paper.[3] But it is buried in a much more general context and its physical significance was not discussed.

Physics in two space dimensions was initially mostly of theoretical and mathematical interest. However, especially in the 5 years since Ref. 1 appeared, we have had several physical, experimentally accessible systems which have two space dimensions. These systems appear in condensed matter physics, and a recent review is given in Ref. 4. We also note more recent theoretical papers by Lieb and Yngvasson[5] and also by Ren.[6] It is important to note that in the condensed matter systems the forces are often not rotationally symmetric and in some cases they are also nonlocal.

In the present paper we return to the nonrelativistic case but treat potentials which have no rotational symmetry, $V \equiv V(\vec{x})$, $\vec{x} \in R^2$. In this case there are no phase shifts, but we obtain the corresponding low-energy result for the full amplitude which agrees with that obtained in the rotationally symmetric case. This is obtained under very general and "reasonable" conditions on

$V(\vec{x})$ which have the following three properties: (a) they are linear in V; (b) they are invariant under a shift of origin; and (c) they include the previously studied case of Ref. 1.

Section II is devoted to preliminaries and definitions, including the Green's function in R^2 and the scattering integral equation.

In Sec. III we study the Fredholm integral equation with the two-dimensional (2D) zero-energy Green's function, $G_0=(1/2\pi)\log|\vec{x}-\vec{y}|$. The main task in this section is to define the general class of potentials, $V(\vec{x})$, to be considered.

In Sec. IV, we consider the Lippmann–Schwinger equation for $k>0$. We prove that, given our class of potentials, then for any real fixed k with $k>0$, this equation has a unique solution, $\psi(\vec{k},\vec{x})$, with $\psi\in C$, where C is the Banach space of continuous functions on R^2 with a sup norm. We also obtain a k-dependent upper bound for $\|\psi\|$, which will prove useful in the succeeding sections.

Section V is devoted to proving that the zero-energy kernel defines a compact operator on C. We also show that even in the case where there exist nontrivial solutions of the homogeneous integral equation with a zero-energy kernel, one still has solutions of the inhomogeneous equation. However these are not unique. This helps in solving the "exceptional case" where ϕ_j, $j=1\ldots,N$, are solutions of the homogeneous equation but with $\int \mathrm{d}^2x\ \phi_j(\vec{x})V(\vec{x})=0$.

We end up with two cases to consider. Case A is where the solution(s) of the inhomogeneous equation, $\tilde{\phi}$, are such that $\int \mathrm{d}^2x\tilde{\phi}(\vec{x})V(\vec{x})\neq 0$. Case B is where the solutions of the inhomogeneous equations satisfy $\int \mathrm{d}^2x\tilde{\phi}(\vec{x})V(\vec{x})=0$.

In Sec. VI we prove the universality of the low-energy scattering amplitude for case A. The result for the full scattering amplitude $f(\vec{k}',\vec{k})$ is $f=-\sqrt{\pi/2}[\log(1/k)]^{-1}+o(1)/(\log k)$. This agrees with our result for the symmetric case given in Ref. 1.

In Sec. VII, we treat the "exceptional case," i.e., mainly case B, and obtain the result $f=o(1)/[\log(1/k)]$. Finally in Sec. VIII we discuss two additional exceptional cases, $\mathrm{A_{II}}$ and $\mathrm{B_I}$.

We briefly discuss the case of nonlocal potentials in Sec. IX. This is limited to giving the class of nonlocal potentials, $W(\vec{x},\vec{y})$, that can be studied by our methods.

Finally, in the last section we give a series of comments and conclusions related to issues raised by this work.

II. NONRELATIVISTIC SCATTERING IN 2D

The free Green's function in two dimensions is given by

$$G(\vec{x},\vec{y}) \equiv \frac{1}{4i}H_0^{(1)}(k|\vec{x}-\vec{y}|), \tag{2.1}$$

where

$$(\nabla^2 + k^2)G(\vec{x},\vec{y}) = \delta^2(\vec{x}-\vec{y}), \tag{2.2}$$

with $\vec{x},\vec{y}\in R^2$, and $H_0^{(1)}$ is the standard Hankel function.

The scattering integral equation is

$$\psi(\vec{k},\vec{x}) = e^{i\vec{k}\cdot\vec{x}} + \frac{1}{4i}\int \mathrm{d}^2y\ H_0^{(1)}(k|\vec{x}-\vec{y}|)V(\vec{y})\psi(\vec{k},\vec{y}). \tag{2.3}$$

The class of noncentral potentials, V, will be specified in the next section.

The asymptotic behavior of ψ for large $|\vec{x}|$ is given by

$$\psi(\vec{k},\vec{x}) \underset{|\vec{x}|\to\infty}{\to} e^{i\vec{k}\cdot\vec{x}} + \frac{i}{\sqrt{k}}f(\vec{k}',\vec{k})\frac{e^{i(kr-\pi/4)}}{\sqrt{r}}, \quad r=|\vec{x}|, \quad \vec{k}'=k\frac{\vec{x}}{|\vec{x}|}. \tag{2.4}$$

Here we have used the large $|z|$ behavior of $H_0^{(1)}(z)$. This leads to

$$G \underset{|\vec{x}-\vec{y}|\to\infty}{\to} \frac{1}{i}\sqrt{\frac{1}{8\pi k|\vec{x}-\vec{y}|}}e^{i(k|\vec{x}-\vec{y}|-\pi/4)}. \tag{2.5}$$

Equation (2.4) defines the scattering amplitude, $f(\vec{k}',\vec{k})$. One should note that in Eq. (2.4) we have chosen a center, i.e., the point $\vec{x}=0$. Unlike the rotationally symmetric case, the definition of f is only unique up to a phase. Shifting the center by $\vec{a}$, $\vec{x}\to\vec{x}+\vec{a}$, the new amplitude differs by a factor $\exp[i(\vec{k}'-\vec{k})\cdot\vec{a}]$. One should note that the forward scattering amplitude is invariant under this shift, as one would expect from the optical theorem. In this paper, we are only interested in the $k\to 0$ limit, which is clearly independent of the choice of a center.

From Eqs. (2.2) and (2.4) we have the standard expression for f,

$$f(\vec{k}',\vec{k}) = -\frac{1}{\sqrt{8\pi}}\int \mathrm{d}^2x\; e^{-i\vec{k}'\cdot\vec{x}}V(\vec{x})\psi(\vec{k},\vec{x}), \tag{2.6}$$

where $|\vec{k}'|=|\vec{k}|$.

The problem we face in this paper originates from the logarithmic singularity of $H_0^{(1)}(z)$ at $z=0$.

We define $R(z)$ by the following:

$$H_0^{(1)}(z) \equiv C_0 + \frac{2i}{\pi}\log z + R(z), \tag{2.7}$$

where

$$C_0 \equiv 1 + \frac{2i}{\pi}[\gamma - \log 2], \tag{2.8}$$

and γ is Euler's constant. For small $|z|$ we have

$$R(z) = O(|z|^2|\log|z||). \tag{2.9}$$

Substituting Eq. (2.7) in (2.3), we obtain

$$\psi(\vec{k},\vec{x}) = e^{i\vec{k}\cdot\vec{x}} + \int \mathrm{d}^2y\left[\frac{\log k|\vec{x}-\vec{y}|}{2\pi} + \frac{C_0}{4i} + \frac{R(k|\vec{x}-\vec{y}|)}{4i}\right]V(\vec{y})\psi(\vec{k},\vec{y}). \tag{2.10}$$

From Eq. (2.7) we also have

$$R(k|\vec{x}|) = H_0^{(1)}(k|\vec{x}|) - \frac{\log k|\vec{x}|}{2\pi} - \frac{C_0}{4i}. \tag{2.11}$$

Using this result, we obtain

$$\psi(\vec{k},\vec{x}) = e^{i\vec{k}\cdot\vec{x}} + F(\vec{k})\left[\frac{H_0^{(1)}(k|\vec{x}|)}{4i} - \frac{\log|\vec{x}|}{2\pi}\right] + \frac{1}{2\pi}\int \mathrm{d}^2y(\log|\vec{x}-\vec{y}|)V(\vec{y})\psi(\vec{k},\vec{y})$$
$$-\frac{1}{4i}\int [R(k|\vec{x}|) - R(k|\vec{x}-\vec{y}|)]V(\vec{y})\psi(\vec{k},\vec{y}), \tag{2.12}$$

where F is defined as

$$F(\vec{k}) \equiv \int \mathrm{d}^2y\; V(\vec{y})\psi(\vec{k},\vec{y}). \tag{2.13}$$

We stress that in going from Eq. (2.3)–(2.12) we have made no approximations. We will show in Appendix B that the last term in (2.12) is, for small k, proportional to $[o(1)/|\log k|] \times (\sup_{\vec{y}}|\psi(\vec{k},\vec{y})|)$, and is thus small compared to the preceding term.

It is clear then from Eq. (2.12) that our first task is to study the zero-energy kernel, $K(\vec{x},\vec{y}) = [(1/2\pi)\log|\vec{x}-\vec{y}|]V(\vec{y})$, which is the main term in (2.12). This analysis will also give us the definition of the broadest class of V's that we will investigate.

III. THE ZERO-ENERGY KERNEL AND THE CLASS OF POTENTIALS

In this section we consider the integral equation with the zero-energy Green's function, $G_0 = (1/2\pi)\log|\vec{x}-\vec{y}|$. We use it to define our class of potentials $V(\vec{x})$, essentially as those that lead to a kernel, K, which is bounded on a Banach space of continuous functions on R^2.

We start with

$$\phi(\vec{x}) = 1 + \frac{1}{2\pi}\int d^2y[\log|\vec{x}-\vec{y}|]V(\vec{y})\phi(\vec{y}). \tag{3.1}$$

It is more convenient to deal with functions that have a finite sup norm. We define

$$u(\vec{x}) = \frac{\phi(\vec{x})}{\log(2+|\vec{x}|)}, \tag{3.2}$$

$$u_0(\vec{x}) = \frac{1}{\log(2+|\vec{x}|)}. \tag{3.3}$$

The resulting integral equation is

$$u(\vec{x}) = u_0(\vec{x}) + \int d^2y\ K(\vec{x},\vec{y})u(\vec{y}), \tag{3.4}$$

with

$$K(\vec{x},\vec{y}) = \frac{1}{2\pi}(\log|\vec{x}-\vec{y}|)V(\vec{y})\frac{\log(2+|\vec{y}|)}{\log(2+|\vec{x}|)}. \tag{3.5}$$

The objective is to study Eq. (3.4) for $u \in C$, the Banach space of all bounded continuous functions on R^2. The norm on C is

$$\|u\| = \sup_{\vec{x}\in R^2}|u(\vec{x})|. \tag{3.6}$$

C is complete and convergence in the norm is uniform convergence.

Our task in this section is to define suitable conditions on $V(\vec{x})$ that are needed to guarantee that $K(\vec{x},\vec{y})$ is a bounded operator on C, i.e., we seek some sufficient conditions on $V(\vec{x})$ such that

$$\int d^2y|\log|\vec{x}-\vec{y}|V(\vec{y})|\frac{\log(2+|\vec{y}|)}{\log(2+|\vec{x}|)} < M, \tag{3.7}$$

for all $\vec{x} \in R^2$.

By suitable conditions we mean the following:

(i) the conditions are linear in $|V(\vec{x})|$;
(ii) the conditions are invariant under a shift of origin;
(iii) the conditions are invariant under a scale change;
(iv) the previous symmetrical case of Ref. 1 is included.

Here (iii) implies that k can be replaced by any positive multiple of k. In particular, the k of Sec. II can be replaced by any positive number, an especially convenient choice being 1. To show this explicitly, note that, for $k>0$, there is the following inequality:

$$\frac{2+k|\vec{x}|}{2+|\vec{x}|} \leqslant \max(1,k). \tag{3.8}$$

This inequality implies immediately

$$\log(2+k|\vec{x}|) - \log(2+|\vec{x}|) \leqslant \max(0,\log k)$$

and

$$\log(2+k|\vec{x}|) - \log(2+|\vec{x}|) \leqslant \max\left(\log k, \log\frac{1}{k}\right). \tag{3.9}$$

We prove that the following two conditions are sufficient to guarantee the validity of Eq. (3.7) and hence the boundedness of K,

$$\text{(A)} \quad \int \mathrm{d}^2y |V(\vec{y})| (\log(2+|\vec{y}|))^2 < M \tag{3.10}$$

and

$$\text{(B)} \quad \int_0^1 y \, \mathrm{d}y |\log y| |V(\vec{y})|_R < M, \tag{3.11}$$

where $|V(\vec{y})|_R$ is the rearrangement of $|V(\vec{y})|$.

We remind the reader that the circular decreasing rearrangement of a non-negative function, $f(\vec{x})$, is a decreasing function, $f_R(|\vec{x}|)$, such that

$$\mu[f_R(|\vec{x}|) \geqslant A] = \mu[f(\vec{x}) \geqslant A], \quad \forall A, \tag{3.12}$$

where μ is the Lebesgue measure.

For the proof, we introduce for positive r,

$$\log^+ r = \max(\log r, 0),$$

$$\log^- r = \max(-\log r, 0). \tag{3.13}$$

Hence we have

$$\log r = \log^+ r - \log^- r,$$

$$|\log r| = \log^+ r + \log^- r. \tag{3.14}$$

This splits Eq. (3.7) into two inequalities,

$$\int \mathrm{d}^2y \, \log^+|\vec{x}-\vec{y}| |V(\vec{y})| \frac{\log(2+|\vec{y}|)}{\log(2+|\vec{x}|)} < M \tag{3.15}$$

and

$$\int \mathrm{d}^2y \, \log^-|\vec{x}-\vec{y}| |V(\vec{y})| \frac{\log(2+|\vec{y}|)}{\log(2+|\vec{x}|)} < M. \tag{3.16}$$

We consider Eq. (3.15) first. Fixing $\vec{y}$, we have

$$\max_{\vec{x}} \frac{\log^+|\vec{x}-\vec{y}|}{\log(2+|\vec{x}|)} = \max_{\vec{x}} \frac{\log|\vec{x}-\vec{y}|}{\log(2+|\vec{x}|)} = \max_{\vec{x}} \frac{\log(x+y)}{\log(2+x)}. \tag{3.17}$$

But, for fixed y, the last expression above is monotonic in x. Therefore we obtain

$$\max_{\vec{x}} \frac{\log^+|\vec{x}-\vec{y}|}{\log(2+|\vec{x}|)} \leqslant \frac{\log(2+y)}{\log 2}. \tag{3.18}$$

Hence the inequality (3.15) is satisfied provided that the condition (A), given in Eq. (3.10), is true. One should note that condition (A) is invariant under a change of origin.

Next, we go to the inequality (3.16). Because of the factor $\log^-|\vec{x}-\vec{y}|$, we know that the integrand in (3.15) is zero if $|\vec{x}-\vec{y}|>1$. Hence our domain of integration is such that

$$x-1<y<x+1. \tag{3.19}$$

This gives

$$\log(2+y)<\log(3+x). \tag{3.20}$$

But since $[\log(3+x)/\log(2+x)] \leqslant \log 3/\log 2$, the validity of Eq. (3.16) reduces to

$$\int d^2y \, \log^-|\vec{x}-\vec{y}| \cdot |V(\vec{y})| < \frac{\log 3}{\log 2} M. \tag{3.21}$$

For any $f(\vec{r})$ we denote by $f_R(r)$ the rearrangement of $|f(\vec{r})|$. One has the inequality

$$\int d^2y |f(\vec{y})| \cdot |g(\vec{y})| \leqslant \int d^2y \, f_R(y) g_R(y), \tag{3.22}$$

and using this result

$$\int d^2y \, \log^-|\vec{x}-\vec{y}| \cdot |V(\vec{y})| \leqslant \int d^2y (\log^-|\vec{x}-\vec{y}|)_R \cdot |V(\vec{y})|_R \leqslant \int d^2y (\log^- y)_R \cdot |V(\vec{y})|_R$$

$$\leqslant \int d^2y (\log^- y) |V(\vec{y})|_R. \tag{3.23}$$

But $\log^- y = 0$ for $y>1$, and thus

$$\int_0^1 y \, dy |\log y| |V(\vec{y})|_R \leqslant \frac{\log 3}{\log 2} M. \tag{3.24}$$

This establishes Eq. (3.16), and completes our proof that for potentials, $V(\vec{x})$, satisfying conditions (A) and (B), K is a bounded operator on C.

In Sec. V we prove that K is compact on C, and also prove other important properties of the zero-energy integral equation.

IV. SOLUTIONS OF THE LIPPMANN–SCHWINGER EQUATION FOR $k>0$

We shall now proceed to prove that for our class of potentials the integral equation (2.3), for any fixed real k with $k>0$, has a unique solution, $\psi(\vec{k},\vec{x})$, with $\psi \in C$. The norm of ψ, $\|\psi\|$, will depend on k, but it is bounded for any fixed $k>0$.

The integral equation (2.3) can be written as

$$\psi(\vec{k},\vec{x}) = e^{i\vec{k}\cdot\vec{x}} + \int \mathrm{d}^2 y \tilde{K}(k;\vec{x},\vec{y})\psi(\vec{k},\vec{y}), \tag{4.1}$$

where

$$\tilde{K}(k;\vec{x},\vec{y}) \equiv \frac{1}{4i} H_0^{(1)}(k|\vec{x}-\vec{y}|)V(\vec{y}). \tag{4.2}$$

We first prove the boundedness of $\tilde{K}$.

Lemma 4.1: For any real k, $k>0$, $\tilde{K}$ is a bounded operator on C, with

$$\|\tilde{K}(k)\| < M(k) < \infty, \tag{4.3}$$

where $M(k)=M_1[1+\log(1/k)]$.

Proof: We use the bound on $H_0^{(1)}(\lambda)$,

$$|H_0^{(1)}(\lambda)| \leqslant |H_0^{(1)}(\lambda_0)| + \log^+\left(\frac{\lambda_0}{\lambda}\right). \tag{4.4}$$

This is proved in Appendix A. Hence we have

$$|H_0^{(1)}(k|\vec{x}-\vec{y}|)| < |H_0^{(1)}(k_0|\vec{x}-\vec{y}|)| + \log\frac{k_0}{k}. \tag{4.5}$$

For our case we can set $k_0=1$.

Next, we need the following bounds on $H_0^{(1)}(|\vec{x}-\vec{y}|)$:

$$|H_0^{(1)}(|\vec{x}-\vec{y}|)| < \begin{cases} C_1 + C_2|\log|\vec{x}-\vec{y}|| & \text{for } |\vec{x}-\vec{y}|<1, \\ C_3 & \text{for } |\vec{x}-\vec{y}| \geqslant 1. \end{cases} \tag{4.6}$$

Hence, for any $\chi \in C$, we get

$$\frac{1}{4}\int |H_0^{(1)}(|\vec{x}-\vec{y}|)||V(\vec{y})\chi(\vec{y})|\mathrm{d}^2 y \leqslant \|\chi\|\Bigg[C_1\int_{|\vec{x}-\vec{y}|<1} \mathrm{d}^2 y|V(\vec{y})| + C_2\int_{|\vec{x}-\vec{y}|<1} \mathrm{d}^2 y|\log|\vec{x}-\vec{y}|||V(\vec{y})| + C_3\int_{|\vec{x}-\vec{y}|>1} \mathrm{d}^2 y|V(\vec{y})|\Bigg]. \tag{4.7}$$

But in the preceding section we proved that the middle integral above is bounded.

Hence we have

$$\|\tilde{K}\| = \sup_{\chi\in C}\frac{\|\tilde{K}\chi\|}{\|\chi\|} \leqslant M_1\left(1+\log\frac{1}{k}\right). \tag{4.8}$$

The theorems in textbooks for compact bounded operators on C are usually given for finite domains $|\vec{x}|<\infty$. We use the following lemma which is a generalization of the ones in the textbooks.

Lemma 4.2: Let B be the Banach space of bounded continuous functions on R^m ($m\geqslant 1$) and B_0 the subset of B formed by functions which tend to 0 at infinity. B_0 is a closed subspace of B.

Let Q denote an operator on B satisfying the following three conditions.

(1) For any $g\in B$,

$$(Qg)(x) = \int q(x,y)g(y)\mathrm{d}^m y, \tag{4.9}$$

where q is an L^1 function on $R^m\times R^m$.

(2) $\int|q(x,y)|\mathrm{d}^m y$ exists and is bounded from above by $h(x)$, where h is a continuous positive function which tends to 0 at infinity.

(3) There exists a function η on $[0,a]$ (for some $a>0$) such that $\eta(r)\to 0$ when $r\to 0$, and such that, for every $g\in B$ and every $(x,x')\in R^m\times R^m$ satisfying $|x-x'|\leqslant a$,

$$|Qg(x)-Qg(x')|<\|g\|\,\eta(|x-x'|). \tag{4.10}$$

Then Q is compact from B to B, and in fact from B to B_0.

A proof of this lemma will be given in Appendix B.[7]

Next, we will use Lemma 4.2 to prove the compactness of the operator $\tilde{K}(k)$.

Lemma 4.3: For any fixed real k, $k>0$, the operator $\tilde{K}(k)$ defined by the kernel in Eq. (4.2) is compact on C.

Proof: From Lemma 4.1 the operators, $\tilde{K}(k)$, defined by the kernel

$$\tilde{K}(k;\vec{x},\vec{y})\equiv\frac{1}{4i}H_0^{(1)}(k|\vec{x}-\vec{y}|)V(\vec{y}), \tag{4.11}$$

are, for fixed nonzero k, also bounded operators on C. In addition for any $\vec{x}\in R^2$ we have

$$\int \mathrm{d}^2y|\tilde{K}(k;\vec{x},\vec{y})|\leqslant M<\infty, \tag{4.12}$$

which follows from the boundedness on C. But for large $|\vec{x}|$, $|\vec{x}|\gg 1/k$, we have

$$\int \mathrm{d}^2y|\tilde{K}(k;\vec{x},\vec{y})|=O\left(\frac{1}{\sqrt{|\vec{x}|}}\right). \tag{4.13}$$

This is due to the asymptotic behavior of $H_0^{(1)}(z)$. Hence, we can always find a constant, $M(k)$, such that

$$\int \mathrm{d}^2y|\tilde{K}(k;\vec{x},\vec{y})|\leqslant\frac{M(k)}{\sqrt{1+|\vec{x}|}}, \tag{4.14}$$

for all $\vec{x}\in R^2$.

Thus $\tilde{K}(k)$ satisfies the first condition, i.e., (4.10), of Lemma 4.2 with

$$\tilde{h}(|\vec{x}|)=\frac{M(k)}{\sqrt{1+|\vec{x}|}}. \tag{4.15}$$

To establish the uniform continuity of $f(\vec{x})$, with $f\equiv(\tilde{K}g)(\vec{x})$, we note that, as given in Eq. (2.7),

$$H_0^{(1)}(k|\vec{x}-\vec{y}|)=C_0+\frac{2i}{\pi}\log\, k|\vec{x}-\vec{y}|+R(k|\vec{x}-\vec{y}|), \tag{4.16}$$

and uniform continuity for the kernel $\log|\vec{x}-\vec{y}|V(\vec{y})$ will be established in the next section. The same result for the operator (RV) will be given in Appendix C. Hence, the conditions of Lemma 4.2 are satisfied and therefore $\tilde{K}(k)$ is compact on C for any fixed nonzero k. This completes the proof of Lemma 4.3.

Using the Fredholm alternative we can now assert that a unique solution, $\psi(\vec{k},\vec{x})$, of Eq. (4.1) exists for any fixed $k>0$, unless the homogeneous equation,

$$\psi_0(\vec{k},\vec{x})=(\tilde{K}(k)\psi_0(\vec{k}))(\vec{x}), \tag{4.17}$$

has a nontrivial solution, ψ_0. But one can easily prove that this leads to a contradiction.

Lemma 4.4: For any real fixed k, $k>0$, there is no nontrivial solution, $\psi_0(\vec{k},\vec{x})$, of the equation

$$\psi_0(\vec{k},\vec{x}) = \int \mathrm{d}^2 y \widetilde{K}(k;\vec{x},\vec{y})\psi_0(\vec{k},\vec{y}). \tag{4.18}$$

Proof: Since $\widetilde{K}=(1/4i)H_0^{(1)}(k|\vec{x}-\vec{y}|)V(\vec{y})$, we get for large $k|\vec{x}|$, $|\vec{x}| \gg 1/k$,

$$\psi_0(\vec{k},\vec{x}) = ie^{i(kx-\pi/4)}\left[\frac{\widetilde{f}_0}{\sqrt{kx}} + O\left(\frac{1}{(kx)^{3/2}}\right)\right], \tag{4.19}$$

where

$$\widetilde{f}_0 = -\frac{1}{\sqrt{8\pi}}\int \mathrm{d}^2 y\ e^{-i\vec{k}\cdot\vec{y}}V(\vec{y})\psi_0(\vec{k},\vec{y}), \tag{4.20}$$

with $\vec{k}'/|\vec{k}| = \vec{x}/|\vec{x}|$, and $|\vec{k}'| = |\vec{k}| = k$.

Next, $\psi_0(\vec{k},\vec{x})$ satisfies the Schrödinger equation

$$-\nabla^2\psi_0 + V\psi_0 = k^2\psi_0. \tag{4.21}$$

This leads to

$$\psi_0^*\nabla^2\psi_0 - \psi_0\nabla^2\psi_0^* = 0, \tag{4.22}$$

since V is real. Integrating Eq. (4.22) over a large disk A, we get

$$\int_{\partial A}(\psi_0^*\vec{\nabla}\psi_0 - \psi_0\vec{\nabla}\psi_0^*)\cdot \mathrm{d}\vec{e} = 0, \quad \vec{e} = \vec{x}/|\vec{x}|. \tag{4.23}$$

We note that

$$\vec{\nabla}\left(\frac{e^{i(kx-\pi/4)}}{\sqrt{kx}}\right) = \frac{ike^{i(kx-\pi/4)}}{\sqrt{kx}}\cdot\frac{\vec{x}}{|\vec{x}|} + \frac{\vec{x}}{|\vec{x}|\sqrt{kx}}O(1/x), \tag{4.24}$$

where the $O(1/x)$ factor has no k dependence.

Using the asymptotic expression (4.24) for ψ_0, and substituting in Eq. (4.23), we finally obtain as $|\vec{x}|\to\infty$,

$$2\pi\int \mathrm{d}\theta|\widetilde{f}_0(k,\theta)|^2 = 0. \tag{4.25}$$

This leads to a contradiction and completes the proof of Lemma 4.4.

In conclusion, for our class of potentials, and any $k>0$, a unique solution, $\psi(\vec{k},\vec{x})$, of Eq. (4.1) exists and is in C, i.e.,

$$\|\psi\| = \sup_{\vec{x}}|\psi(\vec{k},\vec{x})| \leqslant M_1(k) < \infty. \tag{4.26}$$

The norm $\|\psi\|$ of course depends on k, and in principle could grow as $k\to 0$.

V. COMPACTNESS OF THE ZERO-ENERGY OPERATOR

We consider the integral equation (3.4),

$$u = u_0 + Ku, \tag{5.1}$$

with $u\in C$, $u_0(x)=1/\log(2+|\vec{x}|)$, and

$$K(\vec{x},\vec{y}) = \frac{1}{2\pi}(\log|\vec{x}-\vec{y}|)\frac{\log(2+|\vec{y}|)}{\log(2+|\vec{x}|)}V(\vec{y}). \tag{5.2}$$

It is easy to check that Lemma 4.2 does not apply to $K(\vec{x},\vec{y})$ because of the large $|\vec{x}|$ behavior of $K(\vec{x},\vec{y})$. This difficulty can be bypassed by writing

$$K \equiv K^{(1)} + B, \tag{5.3}$$

where

$$K^{(1)}(\vec{x},\vec{y}) = \frac{1}{2\pi}\{\log|\vec{x}-\vec{y}| - \log(2+|\vec{x}|)\}\frac{\log(2+|\vec{y}|)}{\log(2+|\vec{x}|)}V(\vec{y}), \tag{5.4}$$

and B is a separable kernel

$$B(\vec{x},\vec{y}) = \frac{1}{2\pi}\log(2+|\vec{y}|)V(\vec{y}). \tag{5.5}$$

Lemma 5.1: $K^{(1)}$ defines a compact operator on C.

Proof: The first condition of Lemma 4.2 applies to $K^{(1)}$. Indeed we have

$$\int |K^{(1)}(\vec{x},\vec{y})|\mathrm{d}^2y \leqslant \tilde{h}(\vec{x}). \tag{5.6}$$

Here $\tilde{h}(|\vec{x}|)=o(1)$ for large x, and $\tilde{h}\to 0$ as $|\vec{x}|\to\infty$. This can be easily shown using the methods of Sec. III.

Next, we must establish uniform continuity as given in inequality (4.10) in Lemma 4.2.

We have, for any $u(\vec{x}) \in C$, the image $w(\vec{x})$ given by

$$w(\vec{x}) = \frac{1}{\log(2+|\vec{x}|)}\int \mathrm{d}^2y[\log|\vec{x}-\vec{y}| - \log(2+|\vec{x}|)]\log(2+|\vec{y}|)V(\vec{y})u(\vec{y}). \tag{5.7}$$

For any $\vec{x}_0$, $\delta>0$, we take the disks,

$$|\vec{x}-\vec{x}_0| \leqslant 2\delta \text{ and } |\vec{x}'-\vec{x}_0| \geqslant 2\delta. \tag{5.8}$$

We want to find a uniform bound on $|w(\vec{x})-w(\vec{x}')|$ which depends only on δ and not on $\vec{x}'$ or $\vec{x}$. Clearly, the second term in the square brackets in (5.7) presents no difficulty and we only need to bound $|\tilde{w}(\vec{x})-\tilde{w}(\vec{x}')|$, where

$$\tilde{w}(\vec{x}) = \frac{1}{2\pi}\frac{1}{\log(2+|\vec{x}|)}\int \mathrm{d}^2y(\log|\vec{x}-\vec{y}|)V(\vec{y})\log(2+|\vec{y}|)u(\vec{y}). \tag{5.9}$$

We can now write

$$\begin{aligned}\tilde{w}(\vec{x}) - \tilde{w}(\vec{x}') = {} & \frac{1}{2\pi}\left[\frac{1}{\log(2+|\vec{x}|)} - \frac{1}{\log(2+|\vec{x}'|)}\right]\int \mathrm{d}^2y(\log|\vec{x}-\vec{y}|)V(\vec{y})\log(2+|\vec{y}|)u(\vec{y}) \\ & + \frac{1}{2\pi}\frac{1}{\log(2+|\vec{x}'|)}\int \mathrm{d}^2y\left(\log\left|\frac{\vec{x}-\vec{y}}{\vec{x}'-\vec{y}}\right|\right)V(\vec{y})\log(2+|\vec{y}|)u(\vec{y}).\end{aligned} \tag{5.10}$$

We treat the two terms in (5.10) separately,

$$\tilde{w}(\vec{x}) - \tilde{w}(\vec{x}') \equiv I_1 + I_2. \tag{5.11}$$

It follows immediately that

$$|I_1| \leqslant \frac{|\vec{x}'|-|\vec{x}|}{(2+|\vec{z}|)[\log(2+|\vec{x}|)]^2}\left|\int \mathrm{d}^2y\ \log|\vec{x}-\vec{y}|V(\vec{y})\log(2+|\vec{y}|)u(\vec{y})\right|, \tag{5.12}$$

where we have assumed $|\vec{x}'|>|\vec{x}|$, and

$$|\vec{x}| < |\vec{z}| < |\vec{x}'|. \tag{5.13}$$

The integral in (5.12) is bounded for $u \in C$, since it is almost identical to the integrals studied in Eqs. (3.7) and (3.10). Thus we have

$$|I_1| \leqslant \frac{|\vec{x}-\vec{x}'|}{2\,\log(2+|\vec{x}|)} \frac{C}{2+|\vec{x}|}. \tag{5.14}$$

For I_2 we introduce two potentials, $V_{x_0,\delta}(\vec{x})$ and $W_{x_0,\delta}(\vec{x})$, such that

$$V_{x_0,\delta} = \begin{cases} V & \text{for } |\vec{x}-\vec{x}_0| \leqslant 2\delta, \\ 0 & \text{for } |\vec{x}-\vec{x}_0| > 2\delta \end{cases} \tag{5.15}$$

and

$$W_{x_0,\delta} = \begin{cases} 0 & \text{for } |\vec{x}-\vec{x}_0| < 2\delta, \\ V & \text{for } |\vec{x}-\vec{x}_0| > 2\delta. \end{cases} \tag{5.16}$$

In terms of these potentials, let

$$I_2 = I_2^{(1)} + I_2^{(2)}, \tag{5.17}$$

where

$$I_2^{(1)} = \frac{1}{2\pi} \frac{1}{\log(2+|\vec{x}'|)} \int \mathrm{d}^2 y \left(\log \left| \frac{\vec{x}-\vec{y}}{\vec{x}'-\vec{y}} \right| \right) W_{x_0,\delta}(\vec{y}) \log(2+|\vec{y}|) u(y) \tag{5.18}$$

and

$$I_2^{(2)} = \frac{1}{2\pi} \frac{1}{\log(2+|\vec{x}'|)} \int d^2 y \left(\log \left| \frac{\vec{x}-\vec{y}}{\vec{x}'-\vec{y}} \right| \right) V_{x_0,\delta}(\vec{y}) \log(2+|\vec{y}|) u(\vec{y}). \tag{5.19}$$

First, we have

$$\begin{aligned} |I_2^{(1)}| &\leqslant \frac{\|u\|}{\log(2+|\vec{x}'|)} \int \mathrm{d}^2 y \left| \log \frac{|\vec{x}-\vec{y}|}{|\vec{x}'-\vec{y}|} \right| |W_{x_0,\delta}(\vec{y})| \log(2+|\vec{y}|) \\ &\leqslant \frac{\|u\|}{\log(2+|\vec{x}'|)} \int d^2 y \left| \left[\log \frac{|\vec{x}'-\vec{y}|+|\vec{x}-\vec{x}'|}{|\vec{x}'-\vec{y}|} + \log \frac{|\vec{x}'-\vec{y}|+|\vec{x}-\vec{x}'|}{|\vec{x}-\vec{y}|} \right] \right| |W_{x_0,\delta}(\vec{y})| \log(2+|\vec{y}|). \end{aligned} \tag{5.20}$$

But in this integral $W_{\vec{x}0,\delta}(\vec{y})$ vanishes for $|\vec{y}-\vec{x}_0| \leqslant 2\delta$. Hence it follows from Eq. (5.9) that our region of integration over $\vec{y}$ is such that

$$|\vec{x}'-\vec{y}| > 2\delta - \delta > \delta,$$

$$|\vec{x}-\vec{y}| > 2\delta > \delta. \tag{5.21}$$

Hence

$$|I_2^{(1)}| \leqslant \frac{C_2}{\log(2+|\vec{x}'|)} \cdot \frac{|\vec{x}-\vec{x}'|}{\delta} \int \mathrm{d}^2 y |V_N(\vec{y})| \log(2+|\vec{y}|) \leqslant \frac{C_2 |\vec{x}-\vec{x}'|}{\delta} \|u\|. \tag{5.22}$$

Next, we estimate $I_2^{(2)}$,

$$|I_2^{(2)}| \leqslant \frac{\|u\|}{\log(2+|\vec{x}'|)} \int \mathrm{d}^2 y \left| \log \frac{|\vec{x}-\vec{y}|}{|\vec{x}'-\vec{y}|} \right| |V_{x0,\delta}(\vec{y})| \log(2+|\vec{y}|). \tag{5.23}$$

If we take $\delta < \frac{1}{3}$, then $|\vec{x}-\vec{y}|$ and $|\vec{x'}-\vec{y}|$ in this integral are both less than 1, and hence

$$|I_2^{(2)}| \leqslant C \int \mathrm{d}^2 y [|\log|\vec{x}-\vec{y}|| + |\log|\vec{x}'-\vec{y}||] |V_{x0,\delta}(\vec{y})| \|u\|. \tag{5.24}$$

We can replace $\log|\vec{x}-\vec{y}|$ and $\log|\vec{x'}-\vec{y}|$ by $\log^-|\vec{x}-\vec{y}|$ and $\log^-|\vec{x'}-\vec{y}|$. Following the same arguments as in Sec. III, we get

$$|I_2^{(2)}| \leqslant C_3 \|u\| \int_0^1 y \, \mathrm{d}y |\log y| |V_{x0,\delta}(\vec{y})|_R. \tag{5.25}$$

Now, $V_{x0,\delta}(\vec{y})$ vanishes outside a disk of radius 2δ. Thus, $|V_{x0,\delta}(\vec{y})|_R = 0$ for $y > 2\delta$. Note also that $|V_{x0,\delta}(\vec{y})| \leqslant |V(\vec{x})|$ which implies that

$$0 \leqslant |V_{x0,\delta}(\vec{y})|_R \leqslant |V(\vec{y})|_R. \tag{5.26}$$

We finally get

$$|I_2^{(2)}| \leqslant \int_0^{2\delta} y \, \mathrm{d}y |\log y| |V(\vec{y})|_R \|u\|. \tag{5.27}$$

The consequence of the above integral allows us to choose δ such that for any small ϵ,

$$\int_0^{2\delta} y \, \mathrm{d}y |\log y| |V(\vec{y})|_R < \epsilon. \tag{5.28}$$

Adding up I_1, $|I_2^{(1)}|$, and $|I_2^{(2)}|$, we obtain

$$|\tilde{w}(\vec{x}) - \tilde{w}(\vec{x}')| \leqslant \left\{ \frac{|\vec{x}| - |\vec{x}'|}{\log(2+|\vec{x}|)(2+|\vec{x}|)} C_1 + \frac{C_2 |\vec{x}-\vec{x}'|}{\log(2+|\vec{x}'|)\delta} + \frac{C_3 \epsilon}{\log(2+|\vec{x}'|)} \right\} \|u\|. \tag{5.29}$$

We can choose now $|\vec{x}-\vec{x}'| < \min(\epsilon/\delta, \delta < 1)$, and hence

$$|\tilde{w}(\vec{x}) - \tilde{w}(\vec{x}')| < \frac{C_4 \epsilon \|u\|}{\log(2+|\vec{x}'|)}. \tag{5.30}$$

This proves the uniform continuity of $\tilde{w}(\vec{x})$ and hence of $w(\vec{x})$. Thus by Lemma 4.2, $K^{(1)}$ is compact. The separable kernel B is compact for our class of V. Hence, since $K = K^{(1)} + B$, the operator, K, is compact on C.

The Fredholm alternative thus holds for K, i.e., either a unique solution of the inhomogeneous equation, (5.1), exists with $u \in C$, and $u_0 = 1/\log(2+|\vec{x}|)$, or there must be at least one solution of the homogeneous equation

$$u_1 = K u_1. \tag{5.31}$$

[From the compactness it follows that, when we have u_j, $j = 1, \ldots, N$ satisfying Eq. (5.31), N is finite.]

Returning to the notation of Eq. (3.1) with $u = \phi/\log(2+|\vec{x}|)$, we have two cases to consider.

(I) A unique solution for Eq. (3.1) exists,

$$\phi = 1 + K_\ell \phi, \tag{5.32}$$

with

$$K_\ell = \frac{1}{2\pi}(\log|\vec{x}-\vec{y}|)V(\vec{y}) \tag{5.33}$$

and

$$|\phi(\vec{x})| \leqslant C\,\log|\vec{x}|, \quad \text{as } |\vec{x}| \to \infty, \quad C \neq 0. \tag{5.34}$$

Otherwise we have the following.

(II) There exist nontrivial, linearly independent, $\phi_j(\vec{x})$, $j=1,\ldots,N$, such that

$$\phi_j = K_\ell \phi_j. \tag{5.35}$$

Case (II) can be divided into two subcases:

$$\int V(\vec{x})\phi_j(\vec{x})\mathrm{d}^2x = V_j \neq 0. \tag{5.36}$$

In this case it is easy to see that if we define

$$\phi_a(x) \equiv -\frac{\phi_j(\vec{x})}{V_j\,\log\,k_1}, \tag{5.37}$$

then

$$\phi_a(\vec{x}) = 1 + \frac{1}{2\pi}\int \mathrm{d}^2y[\log\,k_1|\vec{x}-\vec{y}|]V(\vec{y})\phi_a(\vec{y}), \tag{5.38}$$

which, except for the change of scale, $1 \to k_1$, is essentially the same as Eq. (5.32).

For the second subcase a finite set of ϕ_j's exist, each satisfying the homogeneous equation (5.36) and, in addition,

$$\int \mathrm{d}^2x\; V(\vec{x})\phi_j(\vec{x}) = 0, \quad j = 1,\ldots,N. \tag{5.39}$$

In Appendix D we give a proof of the following theorem.

Theorem 5.1: If the homogeneous equation,

$$\phi(\vec{x}) = \frac{1}{2\pi}\int \mathrm{d}^2y(\log|\vec{x}-\vec{y}|)V(\vec{y})\phi(\vec{y}), \tag{5.40}$$

has nontrivial solutions, ϕ_j, which satisfy

$$\int V(\vec{x})\phi_j(\vec{x})\mathrm{d}^2x = 0, \quad j = 1,\ldots,N, \tag{5.41}$$

then the inhomogeneous integral equation has nonunique solutions, ϕ_a,

$$\phi_a(\vec{x}) = 1 + \frac{1}{2\pi}\int \mathrm{d}^2y(\log|\vec{x}-\vec{y}|)V(\vec{y})\phi_a(\vec{y}), \tag{5.42}$$

where Eq. (5.41) is a necessary and sufficient condition for Eq. (5.42) to hold. Note that this theorem holds whether or not $\int \mathrm{d}^2x\; V(\vec{x})\phi_a(\vec{x})$ is zero.

With this last theorem it becomes clear that we have four cases to consider: $\mathrm{A_I}$, $\mathrm{A_{II}}$, $\mathrm{B_I}$, $\mathrm{B_{II}}$. These are defined as follows.

Case A_I: $\phi = 1 + K_\ell\phi$ has a unique solution, and $\int \mathrm{d}^2x\; V(\vec{x})\phi(\vec{x}) \neq 0$.

Case $\mathrm{A_{II}}$: There exist N linearly independent solutions, $\phi_j(\vec{x})$, $j=1,\ldots,N$, for the homogeneous equation, $\phi_j = K_\ell\phi_j$. But all the ϕ_j satisfy $\int V(\vec{x})\phi_j(\vec{x})\mathrm{d}^2x \neq 0$.

Case B_I: $\phi=1+K_\ell\phi$ has a unique solution but $\int d^2x V(\vec{x})\phi(\vec{x})=0$.

Case B_{II}: The homogeneous equation, $\phi=K_\ell\phi$, has N linearly independent solutions, ϕ_j, $j=1,\ldots,N$, but $\int d^2x\, V(\vec{x})\phi_j(\vec{x})=0$.

One should note that the trivial case $V\equiv 0$ belongs to case B_I, since $\phi=1$ is a unique solution of $\phi=1+K_\ell\phi$ when $V\equiv 0$. One should also note that in both cases A_I and A_{II} we have the bound

$$|\phi(\vec{x})| \leqslant \text{const } \log(2+|\vec{x}|), \tag{5.43}$$

while in cases B_I and B_{II} we have stronger results. In Appendix E we prove that for these two cases $|\phi(\vec{x})|$ is bounded for all $\vec{x}\in R_2$, and more precisely $|\phi|\to 0$ as $|\vec{x}|\to\infty$ in the case B_{II}.

We have referred to these cases as "zero-energy bound states." They are the limits, for a potential $V=g\tilde{V}$, of the trajectories of negative-energy bound states $E_n(g)$, when g decreases to a critical value g_n, where $E_n(g_n)=0$. For $E<0$, the wave functions decrease exponentially, and they cannot approach a solution growing like $\log|\vec{x}|$ for $g=g_n$.

For any $\kappa>0$, $k=i\kappa$, there is a discrete set of couplings, $g_n(\kappa)$, such that a physical bound state exists at $E=-\kappa^2$. Here $(1/g_n(\kappa))$ is an eigenvalue of the homogeneous Lippmann-Schwinger equation (2.3). The discrete nature of $g_n(\kappa)$ follows from the compactness of the operator in (2.3), as does the fact that at each E the degeneracy is finite. But in addition to these general properties, two of the authors (A.M. and T.T.W.) have shown[8] that there exists an explicit bound on the number of zero-energy bound states.

VI. UNIVERSALITY FOR CASE A_I: $\int d^2x\, V(\vec{x})\phi(\vec{x})\neq 0$

Without introducing any approximations we can rewrite our original integral equation for $k>0$, i.e., Eq. (2.3), in the form of Eq. (2.12),

$$\psi(\vec{k},\vec{x}) = e^{i\vec{k}\cdot\vec{x}} + F(\vec{k})\left[\frac{H_0^{(1)}(k|\vec{x}|)}{4i} - \frac{\log|\vec{x}|}{2\pi}\right] + K_\ell\psi + \Delta_R\psi, \tag{6.1}$$

where F is given in Eq. (2.13),

$$K_\ell(\vec{x},\vec{y}) = \frac{1}{2\pi}(\log|\vec{x}-\vec{y}|)V(\vec{y}) \tag{6.2}$$

and

$$\Delta_R(k;\vec{x},\vec{y}) = -\frac{1}{4i}\{R(k|\vec{x}|) - R(k|\vec{x}-\vec{y}|)\}V(\vec{y}). \tag{6.3}$$

A unique solution for Eq. (6.1), ψ, exists and $\psi\in C$, with $k>\epsilon>0$. This was proved in Sec. IV, for our class of potentials.

We now introduce a new Banach space, $\mathcal{B}$, with a norm given by

$$\|\phi\|_\ell \equiv \sup_{\vec{x}\in R^2}\left|\frac{\phi(\vec{x})}{\log(2+x)}\right|, \tag{6.4}$$

where ϕ is a continuous function on R^2.

Our first task is to estimate the norm of the operator, Δ_R for small k, where Δ_R is now considered as an operator on $\mathcal{B}$.

In Appendix C, the following is proved.

Theorem 6.1: As a bounded operator on the Banach space $\mathcal{B}$, we have for Δ_R,

$$\|\Delta_R\|_\ell = \epsilon(k), \quad \epsilon(k)=o(1), \quad 0<k\ll 1. \tag{6.5}$$

One should note at this stage the cancellations that occur in Eq. (6.1) for both $x\to\infty$ and $x\to 0$. First, the $(1/2\pi)\log|\vec{x}|$ term in the square brackets is, for $x\to\infty$, exactly cancelled by the contribution of $K_\ell\psi$. Second, for $x\to 0$, the $\log|\vec{x}|$ in the square brackets is cancelled by a $\log|\vec{x}|$ coming from $H_0^{(1)}(k|\vec{x}|)/4i$ for small $|\vec{x}|$.

Our second task is to get a bound on $\|\psi(\vec{k},\vec{x})\|_\ell$.

Lemma 6.1: For any $k>0$, we have the bound

$$\|\psi(\vec{k},\vec{x})\|_\ell \leqslant C_1 + C_2|F(\vec{k})|\left(\log\frac{1}{k}\right). \tag{6.6}$$

Proof: Equation (6.1) may be rearranged as

$$(1-K_\ell-\Delta_R)\psi = e^{i\vec{k}\cdot\vec{x}} + F(\vec{k})B(\vec{k},\vec{x}), \tag{6.7}$$

with

$$B \equiv \frac{H_0^{(1)}(k|\vec{x}|)}{4i} - \frac{\log|\vec{x}|}{2\pi}. \tag{6.8}$$

Define $I_\ell \equiv (1-K_\ell)^{-1}$. Then,

$$I_\ell(I_\ell^{-1}-\Delta_R)\psi = I_\ell\{e^{i\vec{k}\cdot\vec{x}} + F(\vec{k})B\}, \tag{6.9}$$

or

$$(1-I_\ell\Delta_R)\psi = I_\ell\{e^{i\vec{k}\cdot\vec{x}} + F(\vec{k})B\}. \tag{6.10}$$

We finally obtain

$$\psi = (1-I_\ell\Delta_R)^{-1}I_\ell\{e^{i\vec{k}\cdot\vec{x}} + F(\vec{k})B\} = (I_\ell + I_\ell\Delta_R I_\ell)\{e^{i\vec{k}\cdot\vec{x}} + F(\vec{k})B\} + O(\|\Delta_R\|_\ell^2). \tag{6.11}$$

But, $\|I_\ell\|_\ell \leqslant M$ and

$$\|B\|_\ell \leqslant C_2\left(\log\frac{1}{k}\right) + C_0, \tag{6.12}$$

so that

$$\|\psi\|_\ell \leqslant C_1 + C_2\left(\log\frac{1}{k}\right)|F(\vec{k})|, \tag{6.13}$$

which completes the proof.

Next, we obtain the universal behavior of $F(\vec{k})$ for small k. We take, $\phi(x)$, the solution of the zero-energy integral equation,

$$\phi = 1 + K_\ell\phi, \tag{6.14}$$

which in the case A_I is such that

$$V_0 \equiv \int d^2x\, V(\vec{x})\phi(\vec{x}) \neq 0, \tag{6.15}$$

and thus $\phi(x) = O(\log x)$ for large $|\vec{x}|$. We multiply both sides of Eq. (6.1) by $\phi(\vec{x})V(\vec{x})$ and integrate over d^2x obtaining

$$\int \phi(\vec{x})V(\vec{x})\psi(\vec{k},\vec{x})\mathrm{d}^2x = V_0 + \int \mathrm{d}^2x(e^{i\vec{k}\cdot\vec{x}}-1)V(\vec{x})\phi(\vec{x}) + F(\vec{k})\int \mathrm{d}^2x\ \phi(\vec{x})V(\vec{x})B(\vec{k},\vec{x})$$
$$+\frac{1}{2\pi}\int \mathrm{d}^2x \int \mathrm{d}^2y\ \phi(\vec{x})V(\vec{x})\log|\vec{x}-\vec{y}|V(\vec{y})\psi(\vec{k},\vec{y})$$
$$+\int \mathrm{d}^2x \int \mathrm{d}^2y\ \phi(\vec{x})V(\vec{x})\Delta_R(k;\vec{x},\vec{y})\psi(\vec{k},\vec{y}), \tag{6.16}$$

where $B(\vec{k},\vec{x})$ is given by Eq. (6.8).

Using the integral equation for $\phi(\vec{x})$, we obtain

$$F(\vec{k})[1-X_2] = V_0 + X_1 + X_3, \tag{6.17}$$

where

$$X_1(\vec{k}) \equiv \int \mathrm{d}^2x(e^{i\vec{k}\cdot\vec{x}}-1)V(\vec{x})\phi(\vec{x}),$$

$$X_2(\vec{k}) \equiv \int \mathrm{d}^2x\ B(\vec{k},\vec{x})V(\vec{x})\phi(\vec{x}),$$

$$X_3(\vec{k}) \equiv \int \mathrm{d}^2x \int \mathrm{d}^2y\ \phi(\vec{x})V(\vec{x})\Delta_R(k;\vec{x},\vec{y})\psi(\vec{k},\vec{y}). \tag{6.18}$$

Lemma 6.2: The following estimates hold for small k,

$$X_1(\vec{k}) = o(1)\Big/\left(\log\frac{1}{k}\right), \tag{6.19}$$

$$X_2(\vec{k}) = \frac{1}{2\pi}V_0\log k + \frac{C_0}{4i}V_0 + o(1), \tag{6.20}$$

and

$$|X_3(\vec{k})| = o(1)\left[|F(\vec{k})|\left(\log\frac{1}{k}\right) + C_4\right]. \tag{6.21}$$

Proof: We define $x_0(k)$ as

$$x_0(k) = \frac{1}{k\left(\log\frac{1}{k}\right)^p}, \quad p > 2. \tag{6.22}$$

From Eq. (6.18) it follows that

$$|X_1(\vec{k})| < C_1\left\|\frac{\phi(x)}{\log(2+x)}\right\|\left[\int_{x<x_0(k)} \mathrm{d}^2x|V(\vec{x})|\log(2+x)\left(\frac{1}{\left(\log\frac{1}{k}\right)^p}\right)\right] + 2\int_{x>x_0(k)} \mathrm{d}^2x|V(\vec{x})||\phi(\vec{x})|. \tag{6.23}$$

Thus,

$$|X_1(\vec{k})| \leqslant O\left(\frac{1}{\left(\log\frac{1}{k}\right)^p}\right) + 2\int_{|\vec{x}|>x_0(k)} \mathrm{d}^2x|V(\vec{x})||\phi(\vec{x})|. \tag{6.24}$$

But, $|\phi(\vec{x})| < C\log(2+|\vec{x}|)$, and we get

$$\begin{aligned}\int_{x>x_0(k)} \mathrm{d}^2x|V(\vec{x})||\phi(\vec{x})| &\leqslant C\int_{x>x_0} \mathrm{d}^2x|V(\vec{x})|\log(2+x)\\ &\leqslant \frac{C}{\log(2+x_0(k))}\int_{x>x_0} \mathrm{d}^2x|V(\vec{x})|[\log(2+x)]^2 \leqslant \frac{o(1)}{\log\frac{1}{k}}.\end{aligned} \tag{6.25}$$

Hence Eq. (6.19) holds.

The estimate of X_2 follows again by splitting the region of integration into two parts. For $|\vec{x}| < x_0(k)$,

$$\begin{aligned}B(\vec{k},\vec{x}) &= \frac{H_0^{(1)}(k|\vec{x}|)}{4i} - \frac{\log x}{2\pi}\\ &= -\frac{1}{2\pi}\left(\log\frac{1}{k}\right) + \frac{C_0}{4i} + o(1);\end{aligned} \tag{6.26}$$

and that gives the main part of the estimate (6.20). The integration over the domain $|\vec{x}| > x_0(k)$ is obviously $o(1)$.

Finally, Lemma 6.1 gives us a bound $\|\psi\|_\ell$ given in Eq. (6.6). This leads to

$$|\psi(\vec{y})| < \left[C_1 + C_2|F(\vec{k})|\left(\log\frac{1}{k}\right)\right]\log(2+y). \tag{6.27}$$

From Appendix C, we have

$$|\Delta_R(\vec{x},\vec{y},\vec{k})| < C\log(1+ky)|V(\vec{y})|. \tag{6.28}$$

Substituting these last two equations in the formula (6.18) for $X_3(\vec{k})$, we get

$$|X_3(\vec{k})| \leqslant \tilde{C}_1\left[|F|\left(\log\frac{1}{k}\right) + \tilde{C}_2\right]\int \mathrm{d}^2x \int \mathrm{d}^2y\, \log(2+x)|V(x)||V(y)|\log(1+ky)\log(2+y). \tag{6.29}$$

By splitting the y integration into two regions, $|\vec{y}| < x_0(k)$ and $|\vec{y}| \geqslant x_0(k)$, with $x_0(k)$ given in Eq. (6.22), one can easily show that

$$\int \mathrm{d}^2y|V(\vec{y})|\log(1+ky)\cdot\log(2+y) = o(1). \tag{6.30}$$

The result given in Eq. (6.21) now follows immediately and Lemma 6.2 is proved.

We now insert our estimates of the X_j, $j=1,2,3$, in Eq. (6.15) and obtain

$$F(\vec{k})\left[1 - \frac{1}{2\pi}V_0\log k - \frac{C_0}{4i}V_0 + o(1)\right] = V_0 + \frac{o(1)}{\log\frac{1}{k}} + o(1)\left[|F(k)|\left(\log\frac{1}{k}\right) + C_4\right]. \tag{6.31}$$

We write

$$|F| = Fe^{i(\arg F)}, \tag{6.32}$$

and obtain

$$F = \frac{V_0 + o(1)}{\left[\left(\frac{1}{2\pi}V_0 + o(1)\right)\left(\log\frac{1}{k}\right) + \left(-\frac{C_0 V_0}{4i} + 1\right) + o(1)\right]}. \tag{6.33}$$

Hence, we finally have for small k,

$$F(\vec{k}) = -\frac{2\pi}{\log k} + \frac{o(1)}{\log\frac{1}{k}}. \tag{6.34}$$

The first important consequence of this result on F is to give a bound on $\|\psi\|_\ell$ which is independent of k and finite. Indeed from Lemma 6.1 and the bound result (6.34), we obtain

$$\|\psi\|_\ell \leqslant M \leqslant \infty. \tag{6.35}$$

The definition of the scattering amplitude, $f(\vec{k}',\vec{k})$, is given in Eq. (2.6), and using the definition of F in Eq. (2.12), we have

$$f(\vec{k}',\vec{k}) = -\frac{1}{\sqrt{8\pi}}F(\vec{k}') - \frac{1}{\sqrt{8\pi}}\int \mathrm{d}^2x(e^{i\vec{k}'\cdot\vec{x}} - 1)V(\vec{x})\psi(\vec{k},\vec{x}). \tag{6.36}$$

But

$$\begin{aligned}\left|\frac{1}{\sqrt{8\pi}}\int \mathrm{d}^2x(e^{i\vec{k}'\cdot\vec{x}} - 1)V(\vec{x})\psi(\vec{k}',\vec{x})\right| &\leqslant C_1\|\psi\|_\ell \int_{|\vec{x}|\leqslant x_0(k)} \mathrm{d}^2x|e^{i\vec{k}'\cdot\vec{x}} - 1||V(\vec{x})|\log(2+x) \\ &\quad + 2M\int_{x\geqslant x_0(k)} \mathrm{d}^2x|V(\vec{x})|\log(2+x) \\ &\leqslant O\left(\frac{1}{\left(\log\frac{1}{k}\right)^p}\right) + \frac{o(1)}{\log\frac{1}{k}}, \quad p > 2. \end{aligned} \tag{6.37}$$

This leads to

$$f = -\frac{1}{\sqrt{8\pi}}F + \frac{o(1)}{\log k}, \tag{6.38}$$

and hence from (6.28) our final universal result,

$$f = -\sqrt{\frac{\pi}{2}}\left(\frac{1}{\log\frac{1}{k}}\right) + \frac{o(1)}{\log k}, \tag{6.39}$$

which agrees with our result for the symmetric case (see Sec. IX).

In closing we prove that in this case

$$\lim_{k\to 0}\psi(\vec{k},\vec{x}) \equiv 0. \tag{6.40}$$

To prove this we return to the rewritten integral equation (6.1),

$$\psi(\vec{k},\vec{x}) = e^{i\vec{k}\cdot\vec{x}} + F(\vec{k})\left[\frac{H_0^{(1)}(k|\vec{x}|)}{4i} - \frac{\log|\vec{x}|}{2\pi}\right] + K_\ell\psi + \Delta_R\psi. \tag{6.41}$$

The last term vanishes as $k\to 0$. For small $k|\vec{x}|$,

$$H_0^{(1)} = \frac{2i}{\pi}\log\, k|\vec{x}| + C_0 + O(|kx|^2\, \log\, k|\vec{x}|). \tag{6.42}$$

Hence

$$\lim_{k\to 0} F(\vec{k})\left[\frac{H_0^{(1)}(k|\vec{x}|)}{4i} - \frac{\log|\vec{x}|}{2\pi}\right] = \lim_{k\to 0} F(\vec{k})\left(\frac{\log\, k}{2\pi}\right), \tag{6.43}$$

and given the universality for F, i.e., Eq. (6.28), we get

$$\lim_{k\to 0} F(\vec{k})\left[\frac{H_0^{(1)}(k|\vec{x}|)}{4i} - \frac{\log|\vec{x}|}{2\pi}\right] = -1. \tag{6.44}$$

Thus in the limit we get

$$\psi(0,\vec{x}) = \frac{1}{2\pi}\int \mathrm{d}^2y\, \log|\vec{x}-\vec{y}|V(\vec{y})\psi(0,\vec{y}). \tag{6.45}$$

But we are in the case where no homogeneous solutions exist and (6.45) leads to a contradiction unless

$$\psi(0,\vec{x}) \equiv 0. \tag{6.46}$$

VII. UNIVERSALITY FOR CASE B_{II}: $\int d^2x\, V(\vec{x})\phi(\vec{x}) = 0$

In this section we consider the case B_{II}. This B_{II} case is quite exceptional. As stressed before, if we introduce a coupling parameter replacing V by λV, we have this case for a discrete infinite set of coupling values, λ_q, $q=1,2,\ldots$. The multiplicity of homogeneous solutions for each λ_q is finite. This follows from the compactness of the zero-energy kernel.

In case B_{II} the homogeneous zero-energy equation has N solutions ($N\geqslant 1$), ϕ_j,

$$\phi_j(\vec{x}) = \frac{1}{2\pi}\int \mathrm{d}^2y\, \log|\vec{x}-\vec{y}|V(\vec{y})\phi_j(\vec{y}), \quad j=1,\ldots,N, \tag{7.1}$$

all with

$$\int \mathrm{d}^2x\, V(\vec{x})\phi_j(\vec{x}) = 0. \tag{7.2}$$

From Theorem 5.1, proved in Appendix D, we know that nonunique solutions, $\phi_a(\vec{x})$, of the inhomogeneous equation exist, i.e.,

$$\phi_a(\vec{x}) = 1 + \frac{1}{2\pi}\int \mathrm{d}^2y(\log|\vec{x}-\vec{y}|)V(\vec{y})\phi_a(\vec{y}). \tag{7.3}$$

Here there are two possibilities,

$$\int \mathrm{d}^2x\, V(\vec{x})\phi_a = 0 \tag{7.4}$$

or

$$\int d^2x\, V(\vec{x})\phi_a \neq 0. \tag{7.5}$$

We consider the case (7.4) first.

For small k, $0<k\ll 1$, the solutions $\psi(\vec{k},\vec{x})$ exist and we can write Eq. (6.1) formally as

$$\psi = [e^{i\vec{k}\cdot\vec{x}} + F(\vec{k})B(\vec{k},\vec{x})] + [K_\ell + \Delta_R]\psi. \tag{7.6}$$

Here B is given in (6.28). K_ℓ and Δ_R are operators on the Banach space $\mathcal{B}$, defined in Sec. VI.

We now follow a procedure analogous to that used in Ref. 1, and first introduced by Pais and Wu. The idea is to split Eq. (7.6) into two equations with the same kernel but different inhomogeneous terms. We define $\psi_\alpha(\vec{k},\vec{x})$ and $\psi_\beta(\vec{k},\vec{x})$ as follows:

$$\psi(\vec{k},\vec{x}) \equiv \psi_\alpha(\vec{k},\vec{x}) - \frac{F(\vec{k})}{2\pi}\left(\log\frac{1}{k}\right)\psi_\beta(\vec{k},\vec{x}), \tag{7.7}$$

where now we have two integral equations defining ψ_α and ψ_β,

$$\psi = e^{i\vec{k}\cdot\vec{x}} + (K_\ell + \Delta_R)\psi_\alpha \tag{7.8}$$

and

$$\psi_\beta = -\frac{2\pi B(\vec{k},\vec{x})}{\log\frac{1}{k}} + (K_\ell + \Delta_R)\psi_\beta. \tag{7.9}$$

These last two equations are equivalent to Eq. (7.6).

Note first that both inhomogeneous terms are in $\mathcal{B}$,

$$\|e^{i\vec{k}\cdot\vec{x}}\|_\ell = \frac{1}{\log 2}, \tag{7.10}$$

and from (6.26),

$$\left\| \frac{2\pi B(\vec{k},\vec{x})}{\log\frac{1}{k}} \right\|_\ell \leqslant 1. \tag{7.11}$$

The operators K_ℓ and Δ_R act on $\mathcal{B}$, and we have shown in Sec. VI and Appendix C that $\|\Delta_R\|_\ell = \epsilon(k) = o(1)$ as $k\to 0$. Thus for small k, we have

$$\|K_\ell + \Delta_R\|_\ell = \|K_\ell\|_\ell + o(1) \tag{7.12}$$

and also

$$\lim_{k\to 0}\|K_\ell + \Delta_R\|_\ell = \|K_\ell\|_\ell. \tag{7.13}$$

We can now see the power and significance of the theorem proved in Appendix D. As an operator on $\mathcal{B}$, $(K_\ell+\Delta_R)\to K_\ell$ as $k\to 0$. Thus if $\psi_\alpha(k,x)$, which for $k>0$ is an element of $\mathcal{B}$, remains in $\mathcal{B}$ as $k\to 0$, we will have

$$\psi_\alpha(0,\vec{x}) = 1 + K_\ell\psi_\alpha(0,\vec{x}). \tag{7.14}$$

But without the results of Appendix D, this will be puzzling. However, with those results it follows that, if $\psi_\alpha(0,\vec{x})$ exists,

$$\psi_\alpha(0,\vec{x}) = \phi_a(\vec{x}) + \sum_{j=1}^{N} c_j \phi_j(\vec{x}), \tag{7.15}$$

where $\phi_a = 1 + K_\ell \phi_a$ and $\phi_j = K_\ell \phi_j$. At this stage the c_j's are arbitrary, but we will sketch later how they can be fixed by a perturbative argument.

For any $k > 0$, we know that $\psi(\vec{k},\vec{x})$ exists and is bounded for all $\vec{x}$. It is easy to show that the same holds for both $\psi_\alpha(\vec{k},\vec{x})$ and $\psi_\beta(\vec{k},\vec{x})$. Next, we assert that in any interval $0 < k \leqslant \sigma \ll 1$, and with a fixed $\vec{x}$, the ψ, ψ_α, and ψ_β are continuous functions of k. We now assume that $\psi(0,\vec{x})$ exists. This leads to both $\psi_\alpha(0,\vec{x})$ and $\psi_\beta(0,\vec{x})$ being finite.

With this physical assumption, we now get

$$|\psi_\alpha(\vec{k},\vec{x})| \leqslant C_\alpha(\vec{x}) = \sup_{0 \leqslant k \leqslant \sigma} |\psi_\alpha(\vec{k},\vec{x})| \tag{7.16}$$

and

$$|\psi_\beta(\vec{k},\vec{x})| \leqslant C_\beta(\vec{x}) = \sup_{0 \leqslant k \leqslant \sigma} |\psi_\beta(\vec{k},\vec{x})|. \tag{7.17}$$

Both C_α and C_β are finite for any $\vec{x}$, since there can be no k_0, $0 \leqslant k_0 \leqslant \sigma$, such that the sup above is infinite. That will lead to a contradiction with the statements of the previous paragraph, especially continuity.

It now follows that for any $\vec{x}$,

$$\lim_{k \to 0} |\nabla_R \psi_\alpha| = 0,$$

$$\lim_{k \to 0} |\nabla_R \psi_\beta| = 0. \tag{7.18}$$

Hence we obtain

$$\psi_\alpha(0,\vec{x}) = \tilde{\phi}_\alpha(\vec{x}) = \phi_a + \sum_{j=1}^{N} c_j^{(\alpha)} \phi_j,$$

$$\psi_\beta(0,\vec{x}) = \tilde{\phi}_\beta(\vec{x}) = \phi_a + \sum_{j=1}^{N} c_j^{(\beta)} \phi_j. \tag{7.19}$$

From Appendix E we have the result that both $\tilde{\phi}_\alpha$ and $\tilde{\phi}_\beta$ are bounded by constants for all $\vec{x}$ including $\vec{x} \to \infty$. This fact plus continuity leads to the result that both $C_\alpha(\vec{x})$ and $C_\beta(\vec{x})$ in Eqs. (7.16) and (7.17) are bounded for all $\vec{x}$. Thus for a closed interval $0 \leqslant k \leqslant \sigma \ll 1$, we have

$$|\psi_\alpha(\vec{k},\vec{x})| \leqslant \tilde{C}_\alpha = \sup_{\vec{x} \in R^2} C_\alpha(\vec{x}),$$

$$|\psi_\beta(\vec{k},\vec{x})| \leqslant \tilde{C}_\beta = \sup_{\vec{x} \in R^2} C_\beta(\vec{x}). \tag{7.20}$$

From Eq. (7.7) we have

$$F(\vec{k}) = \int d^2x \; V \psi_\alpha(\vec{k},\vec{x}) - \frac{1}{2\pi}\left(\log\frac{1}{k}\right) F(\vec{k}) \int d^2x \; V(\vec{x}) \psi_\beta(\vec{k},\vec{x}). \tag{7.21}$$

Denoting the integrals above by F_α and F_β, respectively, we get

$$F(\vec{k}) = \frac{F_\alpha(\vec{k})}{1 + \frac{1}{2\pi}\left(\log\frac{1}{k}\right)F_\beta(\vec{k})}. \tag{7.22}$$

We now multiply both sides of Eq. (7.8), i.e., the α-equation, by $\tilde{\phi}_\alpha V$, and integrate. After using the fact that $\tilde{\phi}_\alpha = 1 + K_\ell \tilde{\phi}_\alpha$, and that $\int V(\vec{x})\tilde{\phi}_\alpha(\vec{x})\mathrm{d}^2x = 0$, we obtain as before

$$F_\alpha(\vec{k}) = \int (e^{i\vec{k}\cdot\vec{x}} - 1)V(\vec{x})\tilde{\phi}(\vec{x})\mathrm{d}^2x + Y_\alpha(\vec{k}), \tag{7.23}$$

with

$$Y_\alpha(\vec{k}) = \int \mathrm{d}^2x \int \mathrm{d}^2y\ \tilde{\phi}(\vec{x})\Delta_R(\vec{x},\vec{y},\vec{k})\psi_\alpha(\vec{k},\vec{y}). \tag{7.24}$$

Given the fact that $|\tilde{\phi}_\alpha|$ is bounded (Appendix E), we get

$$\left|\int \mathrm{d}^2x(e^{i\vec{k}\cdot\vec{x}} - 1)V(\vec{x})\tilde{\phi}(\vec{x})\right| = \frac{o(1)}{\left(\log\frac{1}{k}\right)^2}. \tag{7.25}$$

Using the bound given in Appendix C,

$$|\Delta_R(\vec{x},\vec{y},\vec{k})| \leqslant C|V(\vec{y})|\log(1 + ky), \tag{7.26}$$

and the fact that $|\psi_\alpha(\vec{k},\vec{x})|$ is bounded for small k, we get

$$Y_\alpha(\vec{k}) \leqslant C\int \mathrm{d}^2x \int \mathrm{d}^2y|V(\vec{x})\|V(\vec{y})\log(1 + ky)$$

$$\leqslant .9C' \int \mathrm{d}^2y|V(\vec{y})|\log(1 + ky) = \frac{o(1)}{\log\frac{1}{k}}. \tag{7.27}$$

We obtain the last equality by subdividing the d^2y integration into $y < x_0(k)$ and $y > x_0(k)$, as done previously. We finally obtain, as $k \to 0$,

$$F_\alpha(\vec{k}) = \frac{o(1)}{\log\frac{1}{k}}. \tag{7.28}$$

Next, we apply the same trick to Eq. (7.9). We obtain

$$F_\beta = -\frac{2\pi}{\log\frac{1}{k}} \int \mathrm{d}^2x\ \tilde{\phi}_\beta(\vec{x})V(\vec{x})B(\vec{k},\vec{x}) + Y_\beta(\vec{k}), \tag{7.29}$$

where Y_β is given by Eq. (7.24) with $\psi_\alpha \to \psi_\beta$.

The estimate of the first integral in Eq. (7.29) is given by

$$\frac{2\pi}{\log\frac{1}{k}}\int \mathrm{d}^2x\ \tilde{\phi}_\beta(\vec{x})V(\vec{x})B(\vec{k},\vec{x})=\frac{2\pi}{\log\frac{1}{k}}\int \mathrm{d}^2x\ \tilde{\phi}_\beta(\vec{x})V(\vec{x})\left[B(\vec{k},\vec{x})+\frac{1}{2\pi}\log\frac{1}{k}-\frac{C_0}{4i}\right]. \quad (7.30)$$

But from Eq. (6.28) we get

$$\left[B(\vec{k},\vec{x})+\frac{1}{2\pi}\left(\log\frac{1}{k}\right)-\frac{C_0}{4i}\right]=o(1), \quad |\vec{x}|<x_0(k), \quad (7.31)$$

where $x_0(k)$ is given in Eq. (6.24). On the other hand, for $|\vec{x}|>x_0(k)$ we have from (6.28),

$$\left|B(\vec{k},\vec{x})+\frac{1}{2\pi}\left(\log\frac{1}{k}\right)\right|<C\ \log(2+x). \quad (7.32)$$

Splitting the integration domain in (7.30), we finally obtain

$$\frac{2\pi}{\log\frac{1}{k}}\int \mathrm{d}^2x\ \tilde{\phi}_\beta(\vec{x})V(\vec{x})B(\vec{k},\vec{x})=\frac{o(1)}{\log\frac{1}{k}}. \quad (7.33)$$

Hence we get

$$F_\beta=\frac{o(1)}{\log\frac{1}{k}}+Y_\beta(\vec{k}). \quad (7.34)$$

But again, as in Eq. (7.27), we have

$$Y_\beta=\frac{o(1)}{\log\frac{1}{k}}, \quad (7.35)$$

and hence finally

$$F_\beta=\frac{o(1)}{\log\frac{1}{k}} \quad \text{as } k\to 0. \quad (7.36)$$

Substituting our results for F_α and F_β in Eq. (7.22), we get

$$F=\frac{o(1)}{\log\frac{1}{k}} \quad \text{as } k\to 0, \quad (7.37)$$

and a similar result holds for f.

We are left with the case of Eq. (7.5), when

$$V_a\equiv\int \mathrm{d}^2x\ \phi_a(\vec{x})V(\vec{x})\neq 0. \quad (7.38)$$

It is easy to see that in this case we obtain the result of Sec. VI.

Using the same method as above, we get as $k\to 0$,

$$F_\alpha=V_a+o(1),$$

$$F_\beta = V_a + o(1), \tag{7.39}$$

and finally

$$F(\vec{k}) = \frac{V_a + o(1)}{1 + \frac{V_a}{2\pi}\log\frac{1}{k}}$$

$$= \frac{2\pi}{\log\frac{1}{k}} + \frac{o(1)}{\log\frac{1}{k}}. \tag{7.40}$$

This is the same leading term as in the standard case of Sec. VI.

In closing this section we sketch how the coefficients $c_j^{(\alpha)}$ and $c_j^{(\beta)}$ can be determined. We write Eq. (7.8) as

$$\psi_\alpha = f_\alpha + K_\ell \psi_\alpha, \tag{7.41}$$

where

$$f_\alpha \equiv e^{i\vec{k}\cdot\vec{x}} + \Delta_R \psi_\alpha. \tag{7.42}$$

From Appendix D we see that a necessary and sufficient condition for (7.42) to have a solution is

$$\int \phi_j(\vec{x}) V(\vec{x}) f_\alpha(\vec{x}) \mathrm{d}^2x = 0, \quad j = 1, \ldots, N. \tag{7.43}$$

Setting $\psi_\alpha = \tilde{\phi}_\alpha + o(1) = \phi_\alpha + \Sigma_{k=1}^N c_k^{(\alpha)} \phi_k + o(1)$ in Eq. (7.43), and using Eq. (7.44), we obtain

$$\sum_{k=1}^N A_{jk} c_k^{(\alpha)} = \omega_j + \int \mathrm{d}^2x \ \phi_j(\vec{x}) V(\vec{x}) (e^{i\vec{k}\cdot\vec{x}} - 1), \tag{7.44}$$

with

$$A_{jk} \equiv -\int \phi_j(\vec{x}) V(\vec{x}) [\Delta_R \phi_k](\vec{x}) \mathrm{d}^2x,$$

$$\omega_j = \int \phi_j(\vec{x}) V(\vec{x}) [\Delta_R \phi_a](\vec{x}) \mathrm{d}^2x. \tag{7.45}$$

The integral in (7.44) is $o(1)/[\log(1/k)]^2$, while both A_{jk} and ω_j are $O(\|\Delta_R\|_\ell) = o(1)$. Thus to first order in $\|\Delta_R\|_\ell$, the degeneracy can be removed if the matrix A_{jk} has an inverse, and $A^{-1}\vec{\omega}$ will then give $c_k^{(\alpha)}$ for $k = 1, \ldots, N$.

VIII. THE CASES A_{II} AND B_I

We recall that under case A_{II}, we have N solutions, ϕ_j, $j = 1, \ldots, N$, of the homogeneous equation $\phi_j = K_{\ell\phi j}$, with $\int \mathrm{d}^2x \ V(\vec{x}) \phi_j(\vec{x}) \neq 0$. This case depends critically on whether $N = 1$ or $N \geqslant 2$.

For $N = 1$, we can carry out a rescaling of ϕ_j, and define $\hat{\phi}_1$ as

$$\hat{\phi}_1 = -\frac{2\pi\phi_1}{V_1 \log k_1}, \quad V_1 \equiv \int \mathrm{d}^2x \ V(\vec{x}) \phi_1(\vec{x}). \tag{8.1}$$

Then $\hat{\phi}_1(\vec{x})$ is a solution of the inhomogeneous equation

$$\hat{\phi}_1(\vec{x}) = 1 + \frac{1}{2\pi}\int d^2y(\log\, k_1|\vec{x}-\vec{y}|)V(\vec{y})\hat{\phi}(\vec{y}). \tag{8.2}$$

Hence, for $N=1$, case A_{II} will lead to the same result for $f(\vec{k}',\vec{k})$ that was obtained in Sec. VI for the case A_I.

However, for $N\geqslant 2$, we can always take linear combinations of the ϕ_j's, such that

$$\int d^2x\; V(\vec{x})\left(\sum_{j=1}^{N} b_j\phi_j\right) = 0. \tag{8.3}$$

This reduces case A_{II} for $N\geqslant 2$ to the case B_{II} treated in Sec. VII.

In the case B_I one has a unique solution of the inhomogeneous equation, $\phi=1+K_\ell\phi$, but with $\int d^2x\; V(\vec{x})\phi(\vec{x})=0$. In Appendix E we show that in this case $|\phi(\vec{x})|$ is bounded for all $\vec{x}$. The result for F can now be obtained by setting $V_0=0$ in Eq. (6.35), and noting that since $|\phi|$ is bounded,

$$X_1(\vec{k}) = \int d^2x(e^{i\vec{k}\cdot\vec{x}}-1)V(\vec{x})\phi(\vec{x}) = \frac{o(1)}{\left(\log\frac{1}{k}\right)^2}, \tag{8.4}$$

with an additional power of $[\log(1/k)]$ than in Eq. (6.21).

In addition in this case we have

$$X_3(\vec{k}) = o(1)\Big/\left(\log\frac{1}{k}\right). \tag{8.5}$$

The final result for F is then

$$F(\vec{k}) = \frac{o(1)\Big/\left(\log\frac{1}{k}\right)^2}{1+o(1)} = \frac{o(1)}{\left(\log\frac{1}{k}\right)^2}. \tag{8.6}$$

IX. NONLOCAL POTENTIALS

This is the case where the interaction term in the Schrödinger equation is of the form $\int d^2y\; W(\vec{x},\vec{y})\psi(\vec{y})$, replacing the standard local term, $V(\vec{x})\psi(\vec{x})$.

Due to the length of this paper we shall only deal now with the definition of the class of nonlocal potentials, $W(\vec{x},\vec{y})$. More detailed results will be given elsewhere.

The zero-energy integral equation in this case is

$$\phi(\vec{x}) = 1 + \frac{1}{2\pi}\int d^2y\int d^2z(\log|\vec{x}-\vec{y}|)W(\vec{y},\vec{z})\phi(\vec{z}), \tag{9.1}$$

where the norm is given by

$$|\phi| = \sup_{\vec{x}\in R^2}\frac{|\phi(\vec{x})|}{\log(2+|\vec{x}|)}. \tag{9.2}$$

As in the local case we write

$$u \equiv \frac{|\phi(\vec{x})|}{\log(2+|\vec{x}|)}, \tag{9.3}$$

and obtain

$$u(\vec{x}) = u_0(\vec{x}) + \frac{1}{2\pi \log(2+|\vec{x}|)} \int d^2y \int d^2z \, \log|\vec{x}-\vec{y}| W(\vec{y},\vec{z}) \log(2+|\vec{z}|) u(\vec{z}). \tag{9.4}$$

We need conditions on W to guarantee the boundedness of the double integral,

$$I = \frac{1}{\log(2+|\vec{x}|)} \int d^2y \int d^2z (\log|\vec{x}-\vec{y}|) W(\vec{y},\vec{z}) \log(2+|\vec{z}|) u(\vec{z}). \tag{9.5}$$

Using again $\log A = \log^+ A - \log^- A$, we write for $A = |\vec{x}-\vec{y}|$,

$$I = I^+ - I^-. \tag{9.6}$$

We now have

$$|I^+| \leqslant \frac{\|u\|}{\log(2+|\vec{x}|)} \int d^2y \int d^2z \, \log^+|\vec{x}-\vec{y}| |W(\vec{y},\vec{z})| \log(2+|\vec{z}|). \tag{9.7}$$

But

$$\log^+|\vec{x}-\vec{y}| \leqslant \log(2+|\vec{x}|) + \log(2+|\vec{y}|). \tag{9.8}$$

Hence

$$|I^+| \leqslant \|u\| \int d^2y \int d^2z |W(\vec{y},\vec{z})| \log(2+|\vec{z}|) + \frac{\|u\|}{\log(2+|\vec{x}|)} d^2y \int d^2z \, \log(2+|\vec{y}|) \log(2+|\vec{z}|) |W(\vec{y},\vec{z})|. \tag{9.9}$$

This leads to our first condition on W, namely,

$$\text{(A)} \quad \int d^2y \int d^2z \, \log(2+|\vec{y}|) \log(2+|\vec{z}|) |W(\vec{y},\vec{z})| < \infty. \tag{9.10}$$

For I^- we have

$$|I^-| \leqslant \frac{\|u\|}{\log(2+|\vec{x}|)} \int d^2y \int d^2z |\log^-|\vec{x}-\vec{y}|| W(\vec{y},\vec{z})| \log(2+|\vec{z}|). \tag{9.11}$$

Next, one uses the inequality

$$\log(2+|\vec{z}|) \leqslant \log(2+|\vec{y}|) + \log(1+|\vec{y}-\vec{z}|), \tag{9.12}$$

and notes that when $|\vec{x}-\vec{y}| > 1$, $\log^-|\vec{x}-\vec{y}| = 0$. This allows us to write $\log(2+|\vec{y}|) \leqslant C \log(2+|\vec{x}|)$ in Eq. (9.12) when substituted in (9.11). We obtain

$$|I^-| \leqslant \frac{\|u\|}{\log(2+|\vec{x}|)} \int d^2y \int d^2z |\log^-|\vec{x}-\vec{y}|| W(\vec{y},\vec{z})| \log(|1+\vec{y}-\vec{z}|) + C\|u\| \int d^2y \int d^2z |\log^-||\vec{x}-\vec{y}|| W(\vec{y},\vec{z})|. \tag{9.13}$$

We define two decreasing rearrangements,

$$R_W^{(1)}(y) \equiv [\int d^2z |W(\vec{y},\vec{z})| \log(1+|\vec{y}-\vec{z}|)]_R \tag{9.14}$$

and

$$R_W^{(2)}(y) \equiv \left[\int \mathrm{d}^2 z |W(\vec{y},\vec{z})| \right]_R . \tag{9.15}$$

This leads us to two conditions on $R^{(1)}$ and $R^{(2)}$, namely,

$$\mathrm{B}^{(1)}, \quad \int_0^1 y \, \mathrm{d}y |\log y| R_W^{(1)}(y) < \infty \tag{9.16}$$

and

$$\mathrm{B}^{(2)}, \quad \int_0^1 y \, \mathrm{d}y |\log y| R_W^{(2)}(y) < \infty . \tag{9.17}$$

X. MISCELLANEOUS REMARKS

Remark 1: In Ref.1, the next to leading term for the low-energy behavior of the phase shift, $\delta_0(k)$, was given as $O(k^2)$, i.e., $\delta_0 = (\pi/2)(\log k)^{-1} + O(k^2)$. This is true for massive relativistic field theories. It is also certainly true in nonrelativistic potential scattering for rotationally symmetric potentials that are $O(e^{-\mu r})$ for large r with some $\mu > 0$. For potentials that saturate the condition $\int_1^\infty r \, \mathrm{d}r |V(r)| (\log r)^2 < \infty$, the $O(k^2)$ above should be replaced by $o(1)/[\log(1/k)]$. This will remove the inconsistency between Ref. 1 and the present paper.

A similar remark holds for the results in the exceptional case where $\delta_0 = O(k^2)$ is only necessarily true for massive or exponentially decreasing potentials. Otherwise one has $\delta_0 = o(1)/(\log k)$, as in the present case for the full f.

Remark 2: This paper could be significantly shortened and simplified if we were willing to strengthen the condition (A) on $V(\vec{x})$ given by $\int \mathrm{d}^2 x |V(\vec{x})| [\log(2 + |\vec{x}|)]^2 < \infty$. Even changing the power of the log from 2 to $2+\epsilon$ will simplify the proof somewhat. We are however convinced that this condition is the critical one, and in a certain sense we have the optimal result. The difference between the V's for which the $(\log)^2$ integral is convergent and those for which it diverges is apparent in our paper on the number of bound states.[9]

Remark 3: Finally, and indirectly related to the above remark, we must answer the question why we chose to work on a Banach space of wave functions, ϕ, instead of working on a Hilbert space where the elements of the space are $\sqrt{\tilde{V}}\phi$, and $\tilde{V} = V$ where $V(\vec{x}) > 0$, and $\tilde{V} = -V$ otherwise. In fact it can be shown that the nonlinear condition introduced and studied in detail by one of the authors (P.C.S.),

$$\int \mathrm{d}^2 x \int \mathrm{d}^2 y |V(\vec{x})| (\log|\vec{x} - \vec{y}|)^2 |V(\vec{y})| < \infty \tag{10.1}$$

(which gives an L_2 kernel for the zero-energy integral equation), follows from our linear conditions (A) and (B) given in Sec. III, i.e., $\int \mathrm{d}^2 x |V(\vec{x})| [\log(2 + |\vec{x}|)]^2 < \infty$, and $\int \mathrm{d}^2 x |V(\vec{x})|_R \log^- |\vec{x}| < \infty$. Thus conditions (A) and (B) together give a smaller class of potentials.[8]

The reason we use the Banach space approach is also apparent if one reads Sec. VII dealing with the exceptional case, and especially Appendix D.

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APPENDIX A

In this appendix we prove the bound

$$|H_0^{(1)}(x)| < |H_0^{(1)}(x_0)| + \log^+\left(\frac{x_0}{x}\right). \tag{A1}$$

First we prove

$$|H_0^{(1)}(x)| < \sqrt{\frac{2}{\pi}}\left(\frac{1}{\sqrt{x}}\right). \tag{A2}$$

From Nicholson's formula (Ref.10, p.31),

$$|H_0^{(1)}(x)|^2 = \frac{8}{\pi^2}\int_0^\infty K_0(2x\ \sinh\ t)\mathrm{d}t, \tag{A3}$$

we have

$$|H_0^{(1)}(x)|^2 < \frac{8}{\pi^2}\int_0^\infty K_0(2x\ \sinh\ t)\cosh\ t\ \mathrm{d}t = \frac{8}{\pi^2}\left(\frac{1}{2x}\right)\int_0^\infty K_0(u)\mathrm{d}u. \tag{A4}$$

But, from Ref.10, p.33, $\int_0^\infty K_0(u)\mathrm{d}u = \pi/2$, and this proves the inequality (A2).

Now using the notation of Abramovitz and Stegun,[11]

$$|H_0^{(1)}(x)| \equiv M_0(x), \tag{A5}$$

M_0 satisfies a nonlinear differential equation,

$$x^2M_0'' + xM_0' + x^2M_0 - \frac{4}{\pi^2M_0^3} = 0. \tag{A6}$$

From (A2) it follows that

$$x^2M_0 - \frac{4}{\pi^2M_0^3} < 0. \tag{A7}$$

Hence,

$$x^2M_0'' + xM_0' > 0, \tag{A8}$$

or

$$\frac{d}{\mathrm{d}x}(xM_0') > 0. \tag{A9}$$

This leads to

$$xM_0'(x) \geqslant \lim_{y\to 0}(yM_0'(y)) = -1, \tag{A10}$$

since $M_0(x) \sim -\log\ x$ as $x \to 0$.

For $0 < x < x_0$,

$$M_0(x_0) - M_0(x) = -\int_{x_0}^x M_0'(y)\mathrm{d}y = -\int_{x_0}^x (yM_0'(y))\frac{\mathrm{d}y}{y} > -\int_{x_0}^x \frac{\mathrm{d}y}{y} = -\log\frac{x_0}{x}. \tag{A11}$$

Thus for $x < x_0$,

$$|H_0^{(1)}(x)| < |H_0^{(1)}(x_0)| + \log\frac{x_0}{x}. \tag{A12}$$

But $|H_0^{(1)}(x)|$ is decreasing. This follows from Nicholson's formula since K_0 is also decreasing. Thus we finally obtain the result (A1).

APPENDIX B

A proof of Lemma 4.2 follows.

We use Ascoli's theorem:[7] Any bounded equicontinuous set of functions on a compact metric space is relatively compact in the sup norm topology.

Since B is a metric space, it suffices to prove that any sequence $\{g_n\}_{n=1,2,\ldots}$ in B satisfying $\|g_n\| \leqslant M$, $\forall n$, contains a subsequence $\{g_{n_k}\}_{k=1,2,\ldots}$ such that $\{Qg_{n_k}\}_{k=1,2,\ldots}$ converges in norm, i.e., such that, for every integer $\ell \leqslant 1$ there exists a constant $L_\ell \geqslant 0$ such that

$$k,k' \geqslant L_\ell \Rightarrow \|Qg_{n_k} - Qg_{n_{k'}}\| < 2^\ell. \tag{B1}$$

Let $\{g_n\}_{n=1,2,\ldots}$ be a sequence in B satisfying $\|g_n\| \leqslant M$ for every n. Then $|Qg_n(x)| \leqslant Mh(x)$ for all n and all $x \in R^m$.

Let $R_1 > 0$ be such that $|x| \geqslant R_1 \Rightarrow Mh(x) < 1/8$. Since the ball $B_1 = \{x \in R^m : |x| \leqslant R_1\}$ is compact, and the sequence of the restrictions of the Qg_n to B_1 are equicontinuous, there exists a subsequence $\{g_n^{(1)}\}$ of $\{g_n\}$ and a constant $L_1 > 0$ such that

$$n,n' \geqslant L_1 \Rightarrow |Qg_n^{(1)}(x) - Qg_{n'}^{(1)}(x)| < 1/4, \quad \forall\, x \in B_1, \tag{B2}$$

and hence

$$n,n' \geqslant L_1 \Rightarrow |Qg_n^{(1)}(x) - Qg_{n'}^{(1)}(x)| < 1/2, \quad \forall\, x. \tag{B3}$$

Suppose we have defined, for every integer $p \in [1, \ell-1]$, a subsequence $\{g_n^{(p)}\}$ of $\{g_n\}$ and a constant $L_p > 0$ such that,

if $b > 1$, $\{g_n^{(p)}\}$ is a subsequence of $\{g_n^{(p-1)}\}$, and for all p,

$$n,n' \geqslant L_p \Rightarrow |Qg_n^{(p)}(x) - Qg_{n'}^{(p)}(x)| < 2^{-p}, \quad \forall\, x. \tag{B4}$$

We can then define $\{g_n^\ell\}$ in the same way as in the first step: let R_ℓ be such that $|x| \geqslant R_\ell \Rightarrow Mh(x) < 1/2^{2+\ell}$, and $B_\ell = \{x \in R^m : |x| \leqslant R_\ell\}$. Let $\{g_n^{(\ell)}\}$ be a subsequence of $\{g_n^{\ell-1}\}$ which converges uniformly on B_ℓ, and L_ℓ be a constant such that

$$n,n' \geqslant L_\ell \Rightarrow |Qg_n^{(\ell)}(x) - Qg_{n'}^{(\ell)}(x)| < 1/2^{2+\ell}, \quad \forall\, x \in B_\ell, \tag{B5}$$

and hence

$$n,n' \geqslant L_\ell \Rightarrow |Qg_n^{(\ell)}(x) - Qg_{n'}^{(\ell)}(x)| < 1/2^\ell, \quad \forall\, x. \tag{B6}$$

The sequence $\{Qg_n^{(n)}\}$ is uniformly convergent on the whole space.

APPENDIX C

In this appendix we give a proof of Theorem 6.1 regarding the norm of the operator Δ_R, where

$$\Delta_R(k;\vec{x},\vec{y}) \equiv -\frac{1}{4i}\{R(k|\vec{x}|) - R(k|\vec{x}-\vec{y}|)\}V(\vec{y}), \tag{C1}$$

and $R(z)$ is defined by

$$R(z) = H_0^{(1)}(z) - C_0 - \frac{2i}{\pi}\log z, \tag{C2}$$

with C_0 given in Eq. (2.8). We want to prove that, as an operator on the Banach space $\mathcal{B}$, $\|\Delta_R\|_\ell$ has a bound for small k, $0<k\ll 1$,

$$\|\Delta_R\|_\ell = o(1). \tag{C3}$$

At the end of this appendix, in Lemma C.1, we will prove the following inequality:

$$|R(k|\vec{x}|) - R(k|\vec{x}-\vec{y}|)| < C_1 \log(1+k|\vec{y}|). \tag{C4}$$

From Eq. (C1), we have

$$\|\Delta_R\|_\ell \leqslant \sup_x \int \mathrm{d}^2y |R(k|\vec{x}|) - R(k|\vec{x}-\vec{y}|)||V(\vec{y})|\log(2+y). \tag{C5}$$

Using (C4) we obtain

$$\|\Delta_R\|_\ell \leqslant C_1 \int \mathrm{d}^2y \log(1+k|\vec{y}|)|V(\vec{y})|\log(2+y). \tag{C6}$$

We set

$$y_0(k) = \frac{1}{k(\log k)^2}, \tag{C7}$$

and write

$$\|\Delta_R\|_\ell \leqslant C_1\left\{\int_{|\vec{y}|<y_0} \mathrm{d}^2y \log(1+k|\vec{y}|)|V(\vec{y})|\log(2+y) + \int_{|\vec{y}|>y_0} \mathrm{d}^2y \log(1+k|\vec{y}|)|V(\vec{y})|\log(2+y)\right\}. \tag{C8}$$

This leads to

$$\|\Delta_R\|_\ell \leqslant C_1\left\{\frac{1}{(\log k)^2}\int_{|\vec{y}|<y_0} \log(2+y)|V(\vec{y})|\mathrm{d}^2y + C_2\int_{|\vec{y}|>y_0} [\log(2+|\vec{y}|)]^2|V(y)|\mathrm{d}^2y\right\}. \tag{C9}$$

Since the last integral is convergent over all of R^2, and $y_0(k)\to\infty$ as $k\to 0$, we finally obtain

$$\|\Delta_R\|_\ell \leqslant o(1), \tag{C10}$$

which proves Theorem 6.1.

This result is, in a certain sense, optimal since if we take the special case $\vec{x}=0$, we get for any $\psi\in C$,

$$(\Delta_R\psi)(0) = -\frac{1}{4i}\int \mathrm{d}^2y\, R(k|\vec{y}|)V(\vec{y})\psi(\vec{y}). \tag{C11}$$

By taking a special $V(\vec{y})$,

$$|V(\vec{y})| = \begin{cases} 0, & y\leqslant 1, \\ \dfrac{1}{y^2|\log y|^{3+\epsilon}}, & y>1, \end{cases} \tag{C12}$$

we can easily show that

$$|(\Delta_R\psi)(0)| = O\left(\frac{1}{\left(\log\frac{1}{k}\right)^{1+\epsilon}}\right)\|\psi\|, \tag{C13}$$

for any $\epsilon>0$.

We now prove Eq. (C4).

Lemma C.1:

$$|R(k|\vec{x}|) - R(k|\vec{x}-\vec{y}|)| < C\,\log(1+k|\vec{y}|). \tag{C14}$$

Proof: The bound given in Eq. (A2) for $|H_0^{(1)}(z)|$ and the definition of $R(z)$ given in (B2) lead us immediately to the following bound on $|R(z)|$:

$$|R(z)| \leqslant \sqrt{\frac{2}{\pi z}} + |C_0| + \frac{2}{\pi}|\log z|. \tag{C15}$$

For small $|z|$ the behavior of the Hankel function gives us

$$|R(z)| \leqslant C|z|^2[|\log z| + 1]. \tag{C16}$$

Combining (C15) and (C16), we get for real $z>0$,

$$|R(z)| < C\,\log(1+|z|), \quad \forall\, z>0. \tag{C17}$$

Next, we want to prove that, for $u>0$ and $v>0$,

$$|R(u) - R(v)| < C\,\log[1+|u-v|]. \tag{C18}$$

We shall do this in two steps. First we will prove that

$$|R(u) - R(v)| < \text{const}\,|u-v|; \tag{C19}$$

then we prove that

$$|R(u) - R(v)| < C_1 + C_2\,\log(1+|u-v|). \tag{C20}$$

On taking the best of (C19) and (C20), and using the fact that

$$\log(1+x) > \frac{x\,\log(1+x_0)}{x_0} \quad \text{for} \quad 0<x<x_0,$$

(C18) follows.

To prove (C19) we proceed as follows. Assuming, without loss of generality, that $v>u>0$, we have,

$$|R(v) - R(u)| = \left|H_0^{(1)}(u) - H_0^{(1)}(v) + \frac{i}{2\pi}\log\frac{v}{u}\right| \leqslant \int_u^v \left|H_1^{(1)}(x) + \frac{i}{2\pi x}\right| \mathrm{d}x, \tag{C21}$$

where we used the property

$$\frac{\mathrm{d}H_0^{(1)}(x)}{\mathrm{d}x} = -H_1^{(1)}(x).$$

The expansion of $H_1^{(1)}(x)$ near $x=0$ is

$$H_1^{(1)}(x) = J_1(x) + i\left[\frac{2}{\pi}J_1(x)\log\frac{\gamma x}{2} - \frac{x}{2\pi}\sum_{\ell=0}^{\infty} c_\ell x^{2\ell} - \frac{1}{2\pi x}\right], \tag{C22}$$

where $\Sigma c_\ell x^{2\ell}$ is an entire function with $c_0=1$. We thus get

$$\left|H_1^{(1)}(x) + \frac{i}{2\pi x}\right| < Ax + Bx|\log x|, \quad x<1. \tag{C23}$$

On the other hand, we have also the bound

$$|H_1^{(1)}(x)| < C\left[\frac{1}{x} + \frac{1}{\sqrt{x}}\right], \tag{C24}$$

which follows from Nicholson's formula for $\nu=1$. Combining (C23) and (C24), we get

$$\left|H_1^{(1)}(x) + \frac{i}{2\pi x}\right| \leqslant \text{const}, \quad \forall\, x>0. \tag{C25}$$

Thus, by integration of (C21),

$$|R(|u|) - R(|v|)| < \text{const}\,|u-v|. \tag{C26}$$

Finally, we need to prove (C20). Here, we distinguish three cases with $v>u>0$.

(i) $v>2$, $u>1$. From Eq. (C21) and from the bound (A2), we obtain

$$|R(u) - R(v)| \leqslant \text{const} + \frac{1}{2\pi}\log\left(\frac{v}{u}\right) \leqslant \text{const} + \frac{1}{2\pi}\log(1+v-u). \tag{C27}$$

(ii) $v>2, u<1$,

$$|R(u) - R(v)| \leqslant C_1 + C_2\,\log(1+v), \tag{C28}$$

which follows from (C17). Hence we have

$$|R(u) - R(v)| \leqslant C_1 + C_2\,\log(1+v-u)\frac{\log 3}{\log 2}. \tag{C29}$$

(iii) $v<2$. Here we get from (C26)

$$|R(|u|) - R(|v|)| \leqslant C_1 + C_2\,\log(1+v-u)\frac{2}{\log 2}. \tag{C30}$$

Finally, we stress that (C19) is exactly sufficient to establish the uniform continuity of the full kernel of the Lippmann–Schwinger equation given in Eq. (6.1). The uniform continuity for $\log|\vec{x}-\vec{y}|V(\vec{y})$ has already been established in the main text. It remains to prove that $\Delta_R(k;\vec{x},\vec{y})$ operating on any $\chi \in C$ leads to a $(\Delta_R\chi)(\vec{x})$ which is uniformly continuous in $\vec{x}$. From (C19) we have

$$|[R(k|\vec{x}|) - R(k|\vec{x}-\vec{y}|)] - [R(k|\vec{x}'|) - R(k|\vec{x}'-\vec{x}|)]| \leqslant \text{const}\, k|\vec{x}-\vec{x}'|, \tag{C31}$$

which is what we need.

APPENDIX D

In this appendix we give a proof of Theorem 5.1 stated in Sec. V. This theorem starts with the case where the zero-energy homogeneous integral equation,

$$\phi(\vec{x}) = \frac{1}{2\pi}\int \mathrm{d}^2y\ \log|\vec{x}-\vec{y}|V(\vec{y})\phi(\vec{y}), \tag{D1}$$

has N nontrivial solutions, $\phi_j(\vec{x})$, $j=1,\ldots,N$, which all satisfy the condition

$$\int \mathrm{d}^2x\ V(\vec{x})\phi_j(\vec{x}) = 0. \tag{D2}$$

It then follows that the inhomogeneous integral equation,

$$\phi(\vec{x}) = 1 + \frac{1}{2\pi}\int \mathrm{d}^2y\ \log|\vec{x}-\vec{y}|V(\vec{y})\phi(\vec{y}), \tag{D3}$$

has a solution, ϕ_a. This solution is of course not unique.

To establish (D3), we first show that (D1) and (D2) imply that

$$\int \mathrm{d}^2x\ V(\vec{x})[\phi_j(\vec{x})]^2 \neq 0. \tag{D4}$$

This result will be proved at the end of this appendix.

The number, N, of linearly independent solutions of (D1) is finite. This follows from Fredholm theory and the compactness of the operator K. We use the notation

$$\phi_0(\vec{x}) = \sum_{j=1}^{N} c_j\phi_j(\vec{x}). \tag{D5}$$

Next, we generalize Eq. (D3) slightly, replacing 1 by $f(x)$,

$$\phi(\vec{x}) = f(\vec{x}) + \frac{1}{2\pi}\int \mathrm{d}^2y\ \log|\vec{x}-\vec{y}|V(\vec{y})\phi(\vec{y}). \tag{D6}$$

We multiply by $\phi_0(\vec{x})V(\vec{x})$ and integrate over $\vec{x}$,

$$\int \phi_0(\vec{x})V(\vec{x})\phi(\vec{x})\mathrm{d}^2x - \int \phi_0(\vec{x})V(\vec{x})f(x)\mathrm{d}^2x = \frac{1}{2\pi}\int \mathrm{d}^2x \int \mathrm{d}^2y\ \phi_0(\vec{x})V(\vec{x})\log|\vec{x}-\vec{y}|V(\vec{y})\phi(\vec{y})$$
$$= \frac{1}{2\pi}\int \mathrm{d}^2y\ \phi(\vec{y})V(\vec{y})\phi_0(\vec{y}). \tag{D7}$$

Therefore if (D1) has a solution, it follows that

$$\int \mathrm{d}^2x\ f(\vec{x})V(\vec{x})\phi_0(\vec{x}) = 0. \tag{D8}$$

In other words, (D2) is a necessary condition.

We proceed to show that (D2) is also sufficient. Of course, (D2) is satisfied for all $\phi_0(\vec{x})$, and for this purpose, we have to be more careful.

Equation (D6) is defined on a Banach space, B. Thus

$$f \in B \quad \text{and } \phi \in B. \tag{D9}$$

We define

$$(K\phi)(\vec{x}) = \frac{1}{2\pi}\int \mathrm{d}^2y\ \log|\vec{x}-\vec{y}|V(\vec{y})\phi(\vec{y}). \tag{D10}$$

The Banach space B is chosen such that K is a compact operator from B to B. Thus we write (D1) and (D6) as

$$\phi = K\phi, \tag{D11}$$

$$\phi = f + K\phi. \tag{D12}$$

Starting with B, we want to define a second Banach space as follows. The elements of B_1 are the equivalence classes, $\{f+\Sigma_{j=1}^{N} c_j\phi_j\}$ in B, where the c_j run over all real numbers. We denote this equivalence class by F, and $F \in B_1$. We verify that B_1 is indeed a Banach space under the norm

$$\|F\|_1 = \min_{c_j}\left\| f + \sum_{j=1}^{N} c_j\phi_j \right\|. \tag{D13}$$

Because the ϕ_j satisfy (D1), K is also an operator from B_1 to B_1. The point is that

$$K\left(f + \sum c_j\phi_j\right) = Kf + \sum_{j=1}^{N} c_jK\phi_j = Kf + \sum_{j=1}^{N} c_j\phi_j, \tag{D14}$$

which satisfies the definition of being an equivalence class. In the second Banach space B_1, (D3) takes the form

$$\Phi = F + K\Phi. \tag{D15}$$

We verify that K is a compact operator from B_1 to B_1. Thus (D15) is a Fredholm equation in B_1.

Next, we apply the Fredholm alternative to (D15). The Banach space B_1 is constructed such that the homogeneous equation,

$$\Phi = K\Phi, \tag{D16}$$

has no nontrivial solutions in B_1. To show this we assume the contrary, i.e., that there is a nontrivial Φ. Translated back to the original Banach space, B, (D16) is

$$\phi = \phi_0 + K\phi, \tag{D17}$$

where ϕ_0 satisfies (D1) and (D2). By (D8), the existence of a solution implies that

$$\int \phi_0(\vec{x})V(\vec{x})\phi_0(\vec{x})\mathrm{d}^2x = 0, \tag{D18}$$

i.e.,

$$\int \mathrm{d}^2x\ V(\vec{x})[\phi_0(\vec{x})]^2 = 0. \tag{D19}$$

But this contradicts (D4). Therefore (D16) cannot have a nontrivial solution.

From the Fredholm alternative, we know that (D15) always has a solution in the Banach space B_1. Translated back to the original space B, this means that

$$\phi = f + \sum_{j=1}^{N} c_j\phi_j + K\phi \tag{D20}$$

has a solution in B for a suitably chosen set of coefficients c_j.

It therefore remains to show that

$$c_j = 0, \quad j = 1, \ldots, N. \tag{D21}$$

To prove this, we again assume the opposite, i.e., not all c_j are zero, or $\phi_0 = \Sigma_{j=1}^{N} c_j \phi_j$ is nontrivial. Then we have both

$$\int [f(\vec{x}) + \phi_0(\vec{x})] V(\vec{x}) \phi_0(\vec{x}) \mathrm{d}^2x = 0 \tag{D22}$$

and

$$\int f(\vec{x}) V(\vec{x}) \phi_0(\vec{x}) \mathrm{d}^2x = 0. \tag{D23}$$

The latter is just (D8). Subtracting (D23) from (D22), we obtain

$$\int V(\vec{x}) [\phi_0(\vec{x})]^2 \, \mathrm{d}^2x = 0. \tag{D24}$$

But this again contradicts (D4).

The conclusion is therefore reached that the necessary and sufficient condition for (D6) to have a solution is (D8), or

$$\int f(\vec{x}) V(\vec{x}) \phi_j(\vec{x}) \mathrm{d}^2x = 0, \quad j = 1, \ldots, N. \tag{D25}$$

It only remains to specialize (D6) to the case $f=1$. Thus the necessary and sufficient condition for (D3) to have a solution is $\int \mathrm{d}^2x \; V(\vec{x}) \phi_j(\vec{x}) = 0$, $j = 1, \ldots, N$.

We are now only left with the task of proving (D4), i.e., that $\int V(\vec{x}) [\phi_0(\vec{x})]^2 \, \mathrm{d}^2x \neq 0$. A zero-energy bound state is characterized by the solution, $\phi_0(\vec{x})$, of the equation

$$\phi_0(\vec{x}) = \frac{1}{2\pi} \int \mathrm{d}^2y \, \log k_0 |\vec{x} - \vec{y}| V(\vec{y}) \phi_0(\vec{y}), \tag{D26}$$

with the condition

$$\int \mathrm{d}^2x \; V(\vec{x}) \phi_0(\vec{x}) = 0. \tag{D27}$$

From (D26) we see that (D27) is independent of the scale k_0. We set $k_0 = 1$. Then, using the Schrödinger equation

$$-\nabla^2 \phi_0 + V(\vec{x}) \phi_0 = 0, \tag{D28}$$

we get, after multiplication by ϕ_0 and integration,

$$-\int_{|\vec{x}| \leqslant R} \mathrm{d}^2x \; \phi_0 \nabla^2 \phi_0 + \int_{|\vec{x}| \leqslant R} \mathrm{d}^2x V(|\vec{x}|) \phi_0(\vec{x})^2 = 0. \tag{D29}$$

Integrating by parts, we get

$$F(R) = \int_{|\vec{x}| < R} |\nabla \phi_0|^2 \mathrm{d}^2x + \int_{|\vec{x}| < R} V(\vec{x}) \phi_0^2(\vec{x}) \mathrm{d}^2x = \int_{|\vec{x}| = R} \mathrm{d}s (\vec{\nabla} \phi_0) \phi_0. \tag{D30}$$

Using polar coordinates, we have

$$\frac{F(R)}{R} = \int \mathrm{d}\theta \ \phi_0(R_1) \ \left. \frac{\partial \phi_0(r,\theta)}{\partial r} \right|_{r=R}. \tag{D31}$$

Taking $R_1 \leqslant R \leqslant R_2$, we obtain

$$\int_{R_1}^{R_2} \frac{F(R)}{R} \mathrm{d}\, R = \frac{1}{2} \int \mathrm{d}\theta [\phi_0^2(R_2,\theta) - \phi_0^2(R_1,\theta)]. \tag{D32}$$

In Appendix E we prove that if (D26) and (D27) hold, then $\int \mathrm{d}\theta \ \phi_0^2(R,\theta) \to 0$ as $R \to \infty$. If this result is true, we then have

$$\int_{R_1}^{R_2} \frac{F(R)}{R} \mathrm{d}\, R \leqslant \text{const}, \quad \forall\, R_2 > R_1 \gg R_0. \tag{D33}$$

Hence using the mean-value theorem, there exists a $\overline{R}$, $R_1 < \overline{R} < R_2$, such that

$$F(\overline{R}) \leqslant \frac{C}{\log(R_2/R_1)}. \tag{D34}$$

Therefore there is a sequence, $\overline{R}_1, \overline{R}_2, \ldots, \overline{R}_j$, such that $F(\overline{R}_j) \to 0$ as $j \to \infty$.

But $\int \mathrm{d}^2x |V| [\phi_0(\vec{x})]^2$ is convergent since $|\phi_0| < \text{const} \log(2+|\vec{x}|)$ for large $|\vec{x}|$. Potentials with $\int \mathrm{d}^2x |V| [\log(2+|\vec{x}|)]^2 < \infty$ belong to our class. Hence we conclude that $\int_{|\vec{x}|<R} V\phi_0^2 \ \mathrm{d}^2x$ has a limit as $R \to \infty$.

On the other hand, the first term on the right-hand side of (D29), i.e., $\int_{|\vec{x}|<R} |\vec{\nabla}\phi_0|^2 \mathrm{d}^2x$, is a monotonically increasing function of R, so it either has a limit as $R \to \infty$ or it tends to $+\infty$. The latter case is in contradiction with the fact that $F(\overline{R}_j) \to 0$ as $j \to \infty$. Therefore, $\int_{|\vec{x}| \leqslant R} \mathrm{d}^2x |\vec{\nabla}\phi|^2$ has a limit as $R \to \infty$, and $F(R)$ has a limit which is identically zero. But, $\int \mathrm{d}^2x |\vec{\nabla}\phi_0|^2 > 0$ strictly, and therefore

$$\int V[\phi_0]^2 \mathrm{d}^2x < 0. \tag{D35}$$

APPENDIX E

In this appendix we prove the following: Given $\phi(\vec{x}) \in \mathcal{B}$ which satisfies the integral equation

$$\phi(\vec{x}) = c_0 + \frac{1}{2\pi} \int \mathrm{d}^2y (\log|\vec{x}-\vec{y}|) V(\vec{y}) \phi(\vec{y}), \tag{E1}$$

with c_0 finite or zero, then if

$$\int \mathrm{d}^2x \ V(\vec{x}) \phi(\vec{x}) = 0, \tag{E2}$$

$|\phi(\vec{x})|$ is uniformly bounded for all $\vec{x} \in R_2$.

We stress first that, as in Appendix D, the $\phi(\vec{x})$ considered here are all in the Banach space $\mathcal{B}$, and hence $\|\phi\|_\ell \leqslant \text{const}$. This means that we have *ab initio* the bound

$$|\phi(\vec{x})| \leqslant C \ \log(2+|\vec{x}|). \tag{E3}$$

Thus to complete the task of this appendix we only have to study the large $|\vec{x}|$ behavior of $|\phi|$.

Using again the notation $\log A = \log^+ A - \log^- A$, we set

$$\frac{1}{2\pi}\int d^2y(\log|\vec{x}-\vec{y}|)V(\vec{y}) \equiv I^+(\vec{x}) - I^-(\vec{x}). \tag{E4}$$

First we prove that

$$I^+(\vec{x}) \to 0, \quad \text{as} \quad |x| \to \infty. \tag{E5}$$

Given (E2) we can write I^+ as

$$I^+(\vec{x}) = \frac{1}{2\pi}\int \mathrm{d}^2y[\log^+|\vec{x}-\vec{y}| - \log(2+|\vec{x}|)]V(\vec{y})\phi(\vec{y}). \tag{E6}$$

We define $y_0(x)$ as

$$y_0 \equiv \frac{x}{\log(2+x)}. \tag{E7}$$

Next, we split the integration in (E6),

$$\begin{aligned}|I^+| \leqslant \frac{1}{2\pi}\int_{y<y_0(x)} \mathrm{d}^2y|\log|\vec{x}-\vec{y}| - \log(2+x)||V(\vec{y})\phi(\vec{y})| \\ + \frac{1}{2\pi}\int_{y>y_0(x)} \mathrm{d}^2y[2\,\log(2+x) + \log(2+y)]|V(\vec{y})\phi(\vec{y})|.\end{aligned} \tag{E8}$$

In the first integral, for x large enough,

$$|\log|\vec{x}-\vec{y}| - \log(2+x)| < \frac{2}{\log(2+x)}. \tag{E9}$$

But as $x \to \infty$,

$$\int_{y<y_0(x)} \mathrm{d}^2y|\log|\vec{x}-\vec{y}| - \log(2+x)||V(\vec{y})||\phi(\vec{y})| \leqslant \frac{C}{\log(2+x)}\int_{y<y_0(x)} \mathrm{d}^2y\|V(y)\|\log(2+y). \tag{E10}$$

Hence the first integral vanishes as $x \to \infty$. The second integral, I_2^+, satisfies

$$|I_2^+(\vec{x})| \leqslant C\int_{y>y_0(x)} \mathrm{d}^2y|V(y)|[\log(2+y)]^2 = o(1), \tag{E11}$$

as $x \to \infty$. Thus Eq. (E5) is proved.

At this stage we have

$$|\phi(\vec{x})| \leqslant C + \frac{1}{2\pi}\int d^2y(\log^-|\vec{x}-\vec{y}|)|V(\vec{y})||\phi(\vec{y})|. \tag{E12}$$

Next, we define $M(r)$ and $B(r)$ as follows:

$$M(r) = \sup_{|\vec{x}|\leqslant r}|\phi(\vec{x})|, \tag{E13}$$

$$B(r) = r \sup_{\rho \leqslant r} \frac{M(\rho)}{\rho} \geqslant M(r). \tag{E14}$$

$B(r)$ exists because $M(r) \leqslant C \log(2+r)$. If $|\phi(\vec{x})|$ grows to infinity as $|\vec{x}| \to \infty$, there must exist a sequence $\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_n$, $|\vec{x}_n| \to \infty$ as $n \to \infty$, where $M(|\vec{x}_n|) = |\phi(\vec{x}_n)|$, and there must be a subsequence $\vec{x}_1', \vec{x}_2', \ldots, \vec{x}_N'$, where

$$B(|\vec{x}_N'|) = M(|\vec{x}_N'|) = |\phi(\vec{x}_N')|. \tag{E15}$$

We take such an $\vec{x}_N'$, and obtain

$$B(|\vec{x}_N'|) \leqslant C + \frac{1}{2\pi} \int \mathrm{d}^2 y (\log^- |\vec{x}_N' - \vec{y}|) |V(\vec{y})| B(|\vec{x}_N'|) \left(\frac{|\vec{x}_N'| + 1}{|\vec{x}_N'|} \right), \tag{E16}$$

where we recall that in the integral

$$|\vec{x}_N'| - 1 \leqslant |\vec{y}| \leqslant |\vec{x}_N'| + 1. \tag{E17}$$

Now we obtain

$$\int \mathrm{d}^2 y \, \log^- |\vec{x}_N' - \vec{y}| V(\vec{y})$$

$$\leqslant \int_{|\vec{z}|<\Delta} (\log^- |\vec{z}|) |V(\vec{z})|_R \, d^2 z + |\log \Delta| \int_{|\vec{y}|>|\vec{x}_N'|-1} |V(\vec{y})| \mathrm{d}^2 y. \tag{E18}$$

The first integral can be made arbitrarily small by taking Δ small enough. Once Δ is fixed we can make the second integral as small as we please by taking $|\vec{x}_N'|$ large enough. Hence we finally have

$$B(|\vec{x}_N'|) \leqslant C + \epsilon B(|\vec{x}_N'|), \tag{E19}$$

with $\epsilon < 1/2$ for $|\vec{x}_N'|$ large enough.

Therefore B is bounded, and it follows that $|\phi|$ is bounded. From this it is easy to see that

$$\int \mathrm{d}^2 y (\log^- |\vec{x} - \vec{y}|) |V(\vec{y})| |\phi(\vec{y})| \to 0, \tag{E20}$$

as $|\vec{x}| \to \infty$, because from (E18),

$$\int \mathrm{d}^2 y (\log^- |\vec{x} - \vec{y}|) |V(\vec{y})| \to 0 \quad \text{as } |\vec{x}| \to \infty. \tag{E21}$$

As a consequence, if in Eq. (E1), $C_0 = 0$, then $|\phi| \to 0$ as $|\vec{x}| \to \infty$.

In the case where $\int \mathrm{d}^2 x \, V(\vec{x}) \phi(\vec{x}) \neq 0$, we have

$$\left| \int d^y \, \log^- |\vec{x} - \vec{y}| V(\vec{y}) \phi(\vec{y}) \right| \leqslant C \, \log(2+x) \int \mathrm{d}^2 y \, \log^- |\vec{x} - \vec{y}| \| V(\vec{y}) \|. \tag{E22}$$

Combining this with (E2) and using Eq. (E21), we get

$$|\phi| \cong \frac{1}{2\pi} \log(2+x) \left| \int \mathrm{d}^2 y \, V(\vec{y}) \phi(\vec{y}) + o(1) \right| \quad \text{for } |\vec{x}| \to \infty. \tag{E23}$$

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Sz.-Nagy–Foias theory and Lax–Phillips type semigroups in the description of quantum mechanical resonances

Y. Strauss[a)]
Einstein Institute of Mathematics, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

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A quantum mechanical version of the Lax–Phillips scattering theory was recently developed. This theory is a natural framework for the description of quantum unstable systems. However, since the spectrum of the generator of evolution in this theory is unbounded from below, the existing framework does not apply to a large class of quantum mechanical scattering problems. It is shown in this work that the fundamental mathematical structure underlying the Lax–Phillips theory, i.e., the Sz.-Nagy–Foias theory of contraction operators on Hilbert space, can be used for the construction of a formalism in which models associated with a semibounded spectrum may be accomodated. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The Lax–Phillips scattering theory[22] was originally devised for the analysis of the scattering of electromagnetic or acoustic waves off compact obstacles; it is most sutible for handling hyperbolic wave equations in which the generator of evolution, or wave group, naturally has a continuous specrum on the whole real line. More recently Sjöstrand and Zworski[33] extended the scope of the Lax–Phillips theory to include more general cases of semibounded, compactly supported, perturbations of the Laplacian in the wave equation. The extended version of the theory plays a role in the ongoing effort in recent years to obtain various upper and lower bounds on the number of resonances.[33,27] The Lax–Phillips theory also plays an important role in geometric analysis where certain problems can be naturally formulated as scattering problems (see Ref. 40 and references therein).

The description of resonances in the framework of the Lax–Phillips theory possess certain properties which may be considered as defining properties of an appropriate description of these objects. Resonances are identified according to their evolution in time under the action of a dynamical semigroup, i.e., the Lax–Phillips semigroup. Specifically, resonances are identified as eigenvalues of the generator of the Lax–Phillips semigroup. In fact, Sjöstrand and Zworski prove in Ref. 33 that in the case of the Lax–Phillips theory, the eigenvalues of the generator of the Lax–Phillips semigroup coincide with the generally accepted identification of resonances with poles of (a generalized form of) the resolvent.

Many recent studies indicate that resonances should formally be treated in the same way as eigenvalues (see Refs. 24 and 40 and references therein). Taking the analogy a step forward it is natural to ask whether it is possible to show that resonances are indeed eigenvalues of an operator closely related to the generator of evolution. This is known to be the case in the procedure of complex scaling[2,4,14,20,31,30,32,15] and the method of rigged Hilbert space.[5,3,19,26,6] For a recent abstract treatment of the problem of resonances along these lines see Ref. 1. The structure of the Lax–Phillips theory is again very appealing in this respect since the Lax–Phillips semigroup is just the projection of the evolution into a subspace of the Hilbert space for the scattering problem.

[a)]Electronic mail: ystrauss@math.huji.ac.il

If we require that the description of resonances would have the properties mentioned above, i.e.,

(I) the time evolution of resonances is given in terms of a continuous, one parameter, contractive semigroup,

$$\mathbf{Z}(t_1)\mathbf{Z}(t_2) = \mathbf{Z}(t_1 + t_2), \quad t_1, t_2 \geqslant 0; \tag{1.1}$$

(II) a resonance is assigned, for each time t, a pure state in a Hilbert space;

then for most scattering problems in quantum mechanics the situation is not as favorable as in the Lax–Phillips theory. In fact, the standard treatment of the time evolution of resonances through the notion of the survival amplitude does not generically yield a semigroup law of evolution even in the pole approximation in which the propagator is approximated by taking only the contributions coming from the scattering poles. This fact becomes evident in the case of multiple scattering poles where the residues of the resolvent at different points in the complex plane are not orthogonal to each other and generate interference effects which destroy the semigroup property.[17] In particular, it is interesting to relate the statements made here to some recent efforts to obtain resonance expansions of propagators[24] and to recent work on time dependent theory of resonances.[23,34,8]

There has been some recent work on a quantum mechanical adaptation of the Lax–Phillips theory. Some progress has been made in Refs. 11, 18, and 10, and in Ref. 37 a general formalism was developed which was subsequently applied to certain simple Lee–Friedrichs type models in relativistic quantum field theory.[35,36] More recently, the general formalism developed in Ref. 37 has been used for the analysis of the Stark effect [Ben Ari and Horwitz, Stark effect in the Lax–Phillips scattering theory (in preparation)]. However, the formalism developed in Ref. 37 essentially retains the original structure of the Lax–Phillips theory and hence it is not suitable for the analysis of a large class of quantum mechanical problems, since the generator of evolution is required to have an unbounded spectrum from below as well as from above. A natural question then arises whether this situation can be amended. One of the goals of this paper is to show that, in a sense, the answer to this question is in the affirmative. More specifically, it is shown that the fundamental mathematical theory underlying the Lax–Phillips structure, i.e., the Sz.-Nagy–Foias theory of contraction operators on Hilbert space,[38] can be used in the description of resonances for problems for which the generator of evolution has a semibounded spectrum.

The purpose of this paper is twofold. First, it is shown in Sec. II below that a formalism analogous to that of the Lax–Phillips scattering theory may be constructed for the description of resonances in scattering problems for which the generator of evolution has a semibounded spectrum. Thus, two "representations" of the problem are defined, analogous to the Lax–Phillips translation representations, in which the evolution of the scattering system is transformed into the analogue of translation, i.e., into a translation semigroup of Toeplitz operators on Hardy space. It is also possible to define an S-matrix, analogous to the Lax–Phillips S-matrix, mapping the incoming "representation" onto the outgoing "representation." Beyond mere analogy, in the formalism developed in Sec. II scattering resonances are defined exactly as in the Lax–Phillips theory, i.e., as eigenvalues of the generator of a Lax–Phillips type semigroup.

The second goal of this paper is to suggest that the tool box of methods available for the analysis of resonance phenomena should include the Sz.-Nagy–Foias theory of contraction operators on Hilbert space and, more generally, the part of operator theory dealing with model operators and decompositions.[21] The Sz.-Nagy–Foias theory of contractions is an important part of the subject of model operators. Let $\mathcal{B}(\mathcal{H})$ be the space of bounded linear operators on a Hilbert space $\mathcal{H}$. An operator is a *model operator* for a class of operators in $\mathcal{B}(\mathcal{H})$ if every operator in that class is similar to a multiple of a part of it (a part of an operator is defined to be the restriction of the operator to an invariant subspace). In the case of contractions on Hilbert space the model operator is the backward shift (see Refs. 28 and 21). If a resonance is characterized by conditions (I) and (II) above it is then quite natural that its description will eventually be given in terms of the model for contractions, i.e., essentially by the restriction of the backward shift to an invariant subspace.

Taking this point of view, the role of the Sz.-Nagy–Foias theory in the structures developed in Sec. II is not surprising and in fact unavoidable.

The rest of this paper is organized as follows: The Lax–Phillips scattering theory is briefly reviewed in Sec. I A. Section I B provides a self-contained, but rather restricted in scope, exposition of the parts of the Sz.-Nagy–Foias theory which are relevant to the rest of the paper. The Sz.-Nagy–Foias theory is thoroughly discussed in Ref. 38. Section I B also describes the way that the Lax–Phillips semigroup can be naturally understood in the context of the Sz.-Nagy–Foias theory. Section II contains the main results in this paper. After a preliminary discussion in Sec. II A, concerning Hilbert space nesting, a formalism enabling the use of the Sz.-Nagy–Foias theory for the description of resonances is developed in Sec. II B. Section III contains some comments on the framework introduced in Sec. II and concluding remarks are found in Sec. IV.

A. The Lax–Phillips scattering theory

This section provides a brief review of the Lax–Phillips scattering theory and establishes some of the notation which is used throughout the rest of this paper.

Consider a Hilbert space $\mathcal{H}$ and an evolution group of unitary operators $\{\mathbf{U}(t)\}_{t\in\mathbb{R}}$ on $\mathcal{H}$. Suppose that there exists two distinguished subspaces $\mathcal{D}_-$ and $\mathcal{D}_+$ which have the properties that $\mathcal{D}_-$ is orthogonal to $\mathcal{D}_+$ and

$$\begin{aligned} &\mathbf{U}(t)\mathcal{D}_- \subset \mathcal{D}_-, \quad t \leqslant 0, \\ &\mathbf{U}(t)\mathcal{D}_+ \subset \mathcal{D}_+, \quad t \geqslant 0, \\ &\cap_t \mathbf{U}(t)\mathcal{D}_\pm = \{0\}, \\ &\overline{\cup_t \mathbf{U}(t)\mathcal{D}_\pm} = \mathcal{H}. \end{aligned} \tag{1.2.}$$

We call $\mathcal{D}_-$ the *incoming subspace* and $\mathcal{D}_+$ the *outgoing subspace*. $\mathcal{D}_-$ corresponds to incoming waves which do not interact with the target prior to $t=0$ and $\mathcal{D}_+$ corresponds to outgoing waves which do not interact with the target after $t=0$. These properties are reflected in the stability properties of $\mathcal{D}_-$ and $\mathcal{D}_+$ in Eq. (1.2).

Let $L^2_{\mathcal{N}}(\mathbb{R})$ be the space of L^2 functions defined on $\mathbb{R}$ and taking their values in a Hilbert space $\mathcal{N}$. Sinai[7] proved the following theorem.

Theorem 1.1 (Sinai): *If $\mathcal{D}_+$ is an outgoing subspace with respect to a group of unitary operators $\mathbf{U}(t)$, then the Hilbert space $\mathcal{H}$ can be represented isometrically as the Hilbert space of functions $L^2_{\mathcal{N}}(\mathbb{R})$ for some auxiliary Hilbert space $\mathcal{N}$ so that $\mathbf{U}(t)$ goes into translation to the right by t units, and $\mathcal{D}_+$ is mapped onto $L^2_{\mathcal{N}}(\mathbb{R}^+)$. This representation is unique up to an isomorphism of $\mathcal{N}$.*

A representation of this kind is called *outgoing translation representation*. An analogous representation theorem holds for an incoming subspace $\mathcal{D}_-$, i.e., there is a representation in which $\mathcal{H}$ is mapped onto the Hilbert space $L^2_{\mathcal{N}}(\mathbb{R})$, $\mathcal{D}_-$ is mapped onto $L^2_{\mathcal{N}}(\mathbb{R}^-)$ and $\mathbf{U}(t)$ acts as translation to the right by t units. This representation is called the *incoming translation representation*.

For most purposes it is more convenient not to work with the translation representations but with two different representations, called spectral representations. By Fourier transformation of the incoming translation representation and the outgoing translation representation we obtain the *incoming spectral representation* and *outgoing spectral representation*, respectively. According to the Paley–Wiener theorem[25] in the incoming spectral representation, the subspace $\mathcal{D}_-$ is represented by the Hilbert space of functions $H^+_{\mathcal{N}}(\mathbb{R})$ consisting of boundary values on $\mathbb{R}$ of functions in the Hardy space $H^2_{\mathcal{N}}(\Pi)$. Denoting the upper half of the complex plane by Π, the space $H^2_{\mathcal{N}}(\Pi)$ is characterized as the space of analytic vector valued functions on Π, taking their values in the auxiliary Hilbert space $\mathcal{N}$, and such that for any function $f \in H^2_{\mathcal{N}}(\Pi)$ we have

$$\sup_{y>0}\int_{-\infty}^{+\infty}\|f(x+iy)\|_{\mathcal{N}}^2\,dx<C$$

for some constant $C>0$. In the outgoing spectral representation the subspace $\mathcal{D}_+$ is represented, according to the Paley–Wiener theorem, by the function space $H_{\mathcal{N}}^-(\mathbb{R})$ consisting of boundary values of functions in $H_{\mathcal{N}}^2(\overline{\Pi})$, a Hardy space of vector valued functions (taking values in $\mathcal{N}$) on the lower half-plane $\overline{\Pi}$. In the case of scalar valued functions used in the sequel in Sec. II below the same notation will be used but the subscript $\mathcal{N}$ for the auxiliary Hilbert space is omitted.

Let $\mathbf{W}_+$ and $\mathbf{W}_-$ denote the operators that map elements of $\mathcal{H}$ to their outgoing, respectively, incoming, translation representers. We call the operator

$$\mathbf{S}^{L.P}\equiv\mathbf{W}_+\mathbf{W}_-^{-1} \tag{1.3}$$

the *abstract scattering operator* associated with the group $\mathbf{U}(t)$ and the pair of spaces $\mathcal{D}_-$ and $\mathcal{D}_+$. It was proved by Lax and Phillips (LP) that $\mathbf{S}^{\mathrm{LP}}$ is equivalent to the standard definition of the scattering operator. The abstract scattering operator has the following properties:

(a) $\mathbf{S}^{\mathrm{LP}}$ is unitary,
(b) $\mathbf{S}^{\mathrm{LP}}$ commutes with translations,
(c) $\mathbf{S}^{\mathrm{LP}}$ maps $L_{\mathcal{N}}^2(\mathbb{R}^-)$ into itself.

Property (b) is due to the fact that $\mathbf{S}^{\mathrm{LP}}$ is a map between two translation representations. One can understand property (c) by noting that in the incoming translation representation the subspace $\mathcal{D}_-$ is identified with the space of functions $L_{\mathcal{N}}^2(\mathbb{R}^-)$ and in the outgoing translation representation $\mathcal{D}_+$ is represented as $L_{\mathcal{N}}^2(\mathbb{R}^+)$. The orthogonality of $\mathcal{D}_-$ and $\mathcal{D}_+$ then implies that in the outgoing translation representation $\mathcal{D}_-$ is represented by a subspace of $L_{\mathcal{N}}^2(\mathbb{R}^-)$ and property (c) above follows.

Going over to the spectral representations the scattering operator transforms into $\mathcal{S}^{\mathrm{LP}}\equiv\mathbf{F}\mathbf{S}^{\mathrm{LP}}\mathbf{F}^{-1}$, where $\mathbf{F}$ is the Fourier transform operator. Properties (a)–(c) above then imply corresponding properties for $\mathcal{S}^{\mathrm{LP}}$,

(a′) $\mathcal{S}^{\mathrm{LP}}$ is unitary,
(b′) $\mathcal{S}^{\mathrm{LP}}$ commutes with multiplication by scalar functions,
(c′) $\mathcal{S}^{\mathrm{LP}}$ maps $H_{\mathcal{N}}^+(\mathbb{R})$ into itself.

According to a special case of a theorem of Foures and Segal,[12] an operator satisfying properties (a′)–(c′) can be realized as a multiplicative, operator valued function $\mathcal{S}$, such that $\mathcal{S}(\sigma)$ maps $\mathcal{N}$ into $\mathcal{N}$ for each $\sigma\in\mathbb{R}$. This operator valued function satisfies

(a″) $\mathcal{S}(\sigma)$ is the boundary value of an operator valued function $\mathcal{S}(z)$ analytic for $\mathrm{Im}\,z>0$,
(b″) $\|\mathcal{S}(z)\|_{\mathcal{N}}\leqslant 1$ for $\mathrm{Im}\,z>0$,
(c″) $\mathcal{S}(\sigma)$, $\sigma\in\mathbb{R}$ is, pointwise, a unitary operator on the auxiliary Hilbert space $\mathcal{N}$.

Consider the family $\{\mathbf{Z}(t)\}_{t\geqslant 0}$ of operators on $\mathcal{H}$ defined by

$$\mathbf{Z}(t)\equiv\mathbf{P}_+\mathbf{U}(t)\mathbf{P}_-\quad(t\geqslant 0). \tag{1.4}$$

Here $\mathbf{P}_+$ is the orthogonal projection of $\mathcal{H}$ onto the orthogonal complement of $\mathcal{D}_+$ and $\mathbf{P}_-$ is the orthogonal projection of $\mathcal{H}$ onto the orthogonal complement of $\mathcal{D}_-$. Lax and Phillips prove the following theorem.

Theorem 1.2: *The operators* $\{\mathbf{Z}(t)\}_{t\geqslant 0}$ *annihilate* $\mathcal{D}_+$ and $\mathcal{D}_-$, *map the orthogonal complement* $\mathcal{K}=\mathcal{H}\ominus(\mathcal{D}_-\oplus\mathcal{D}_+)$ *into itself, and form a strongly continuous semigroup* [*i.e.* $\mathbf{Z}(t_1)\mathbf{Z}(t_2)=\mathbf{Z}(t_1+t_2)$] *of contraction operators on* $\mathcal{K}$. *Furthermore,* $\mathbf{Z}(t)$ *tends strongly to zero as* $t\to\infty$: $s-\lim_{t\to\infty}\mathbf{Z}(t)x=0$ *for every* x *in* $\mathcal{K}$.

The family of operators $\{\mathbf{Z}(t)\}_{t\geqslant 0}$ is called the Lax–Phillips semigroup. The operator valued

function $\mathcal{S}$, with properties (a″)–(c″) above, is called the Lax–Phillips *S*-matrix. Properties (a″)–(c″) characterize the Lax–Phillips *S*-matrix as an analytic function on the upper half-plane. The analytic continuation of $\mathcal{S}$ to the lower half-plane is given by

$$\mathcal{S}(z) \equiv [\mathcal{S}^*(\overline{z})]^{-1}, \quad \operatorname{Im} z < 0. \tag{1.5}$$

One of the main results of the Lax–Phillips scattering theory is the following theorem.

Theorem 1.3: *Let* $\mathbf{B}$ *denote the generator of the semigroup* $\mathbf{Z}(t)$. *If* $\operatorname{Im}\mu<0$, *then* μ *belongs to the point spectrum of* $\mathbf{B}$ *if and only if* $\mathcal{S}^*(\overline{\mu})$ *has a nontrivial null space*.

This theorem establishes a very important relation between the eigenvalues of the generator $\mathbf{B}$ of the Lax–Phillips semigroup and zeros of the Lax–Phillips *S*-matrix $\mathcal{S}$ in the upper half-plane or poles of the analytic continuation of $\mathcal{S}$ to the lower half-plane.

B. Lax–Phillips theory and Sz.-Nagy–Foias theory of contractions

In this section the structure of the Lax–Phillips theory is put into the context of the more general theory of Sz.-Nagy and Foias concerning contraction operators on Hilbert space.[38]

Consider the Lax–Phillips semigroup $\{\mathbf{Z}(t)\}_{t\geqslant 0}$. According to Theorem 1.2 this semigroup acts nontrivially on the subspace $\mathcal{K}=\mathcal{H}\ominus(\mathcal{D}_-\oplus\mathcal{D}_+)$. For a vector $f\in\mathcal{K}$ and for $t_1,t_2\geqslant 0$ we have

$$\mathbf{Z}(t_1)\mathbf{Z}(t_2)f=\mathbf{P}_+\mathbf{U}(t_1)\mathbf{P}_-\mathbf{Z}(t_2)f=\mathbf{P}_+\mathbf{U}(t_1)\mathbf{Z}(t_2)f=\mathbf{P}_+\mathbf{U}(t_1)\mathbf{P}_+\mathbf{U}(t_2)f. \tag{1.6}$$

The stability properties of the subspace $\mathcal{D}_+$ [Eq. (1.2)] imply the following identity

$$\mathbf{P}_+\mathbf{U}(t)(\mathbf{I}-\mathbf{P}_+)=0, \quad t\geqslant 0. \tag{1.7}$$

Inserting this identity into the right-hand side (rhs) of the previous equation we find, for $f\in\mathcal{K}\oplus\mathcal{D}_-$ and $t_1,t_2\geqslant 0$,

$$\mathbf{P}_+\mathbf{U}(t_1)\mathbf{P}_+\mathbf{U}(t_2)f=\mathbf{P}_+\mathbf{U}(t_1)[(\mathbf{I}-\mathbf{P}_+)+\mathbf{P}_+]\mathbf{U}(t_2)f=\mathbf{P}_+\mathbf{U}(t_1)\mathbf{U}(t_2)f=\mathbf{P}_+\mathbf{U}(t_1+t_2)f. \tag{1.8}$$

We note that, since for $f\in\mathcal{K}$ we have $\mathbf{P}_+\mathbf{U}(t_1+t_2)f=\mathbf{P}_+\mathbf{U}(t_1+t_2)\mathbf{P}_-f=\mathbf{Z}(t_1+t_2)f$, Eq. (1.8) implies the semigroup law. Given a Lax–Phillips structure with an evolution group $\mathbf{U}(t)$ on the Hilbert space $\mathcal{H}$, consider the family of operators $\{\mathbf{T}(t)\}_{t\geqslant 0}$ such that $\mathbf{T}(t)$: $\mathcal{H}\mapsto\mathcal{H}$, $t\geqslant 0$ and

$$\mathbf{T}(t)\equiv\mathbf{P}_+\mathbf{U}(t), \quad t\geqslant 0. \tag{1.9}$$

Each element of this family of operators annihilates the subspace $\mathcal{D}_+$, as can be seen, for example, from Eq. (1.7). By Eq. (1.8) we find that for any vector $f\in\mathcal{D}_-\oplus\mathcal{K}$ we have

$$\mathbf{T}(t_1)\mathbf{T}(t_2)f=\mathbf{T}(t_1+t_2)f, \quad t_1,t_2\geqslant 0 \tag{1.10}$$

and so the family $\{\mathbf{T}(t)\}_{t\geqslant 0}$ forms a one parameter continuous semigroup. We observe from Eq. (1.6) that, for $f\in\mathcal{K}$, we have

$$\mathbf{Z}(t_1)\mathbf{Z}(t_2)f=\mathbf{T}(t_1)\mathbf{T}(t_2)f, \quad t_1,t_2\geqslant 0, \quad f\in\mathcal{K}. \tag{1.11}$$

Consider now the Lax–Phillips outgoing translation representation. Denote the outgoing translation representer of an operator $\mathbf{T}(t)$ from the family defined in Eq. (1.9) by $\widetilde{\mathbf{T}}(t)$. Given any vector valued function $f\in L^2_{\mathcal{N}}(\mathbb{R})$ in the outgoing translation representation we have

$$(\widetilde{\mathbf{T}}(t)f)(s)=\begin{cases} f(s-t), & s\leqslant 0,\\ 0, & s>0,\end{cases} \qquad t\geqslant 0. \tag{1.12}$$

Denote the generator of the semigroup $\{\mathbf{T}(t)\}_{t\geqslant 0}$ by $\mathbf{A}$. It is easy to show that the spectrum of $\mathbf{A}$ is $\sigma(\mathbf{A})=\{\mu\,|\,\operatorname{Im}\mu<0\}$. Denoting the outgoing translation representer of $\mathbf{A}$ by $\widetilde{\mathbf{A}}$, the eigenfunctions of $\widetilde{\mathbf{A}}$ are given by

$$f_{\mu,n}(s)=\begin{cases} e^{i\mu s}n, & s\leqslant 0,\\ 0, & s>0,\end{cases}\qquad \forall\ \mu\ \ \mathrm{Im}\,\mu<0,\quad \forall\ n\in\mathcal{N}, \tag{1.13}$$

where $f_{\mu,n}$ is an eigenfunction of $\tilde{\mathbf{A}}$ with eigenvalue μ.

As mentioned above one usually works in the spectral representations rather than in the translation representations. Hence, we would like to find the representation of the semigroup $\{\mathbf{T}(t)\}_{t\geqslant 0}$ and the eigenfunctions $f_{\mu,n}$ in the outgoing spectral representation. For this we need the definition of a Toeplitz operator on the Hardy space $H^+_{\mathcal{N}}(\mathbb{R})$ (see, for example, Ref. 28 and references therein):

Definition [*Toeplitz operator on* $H^+_{\mathcal{N}}(\mathbb{R})$]: *Let* $W\in L^\infty_{\mathcal{B}(\mathcal{N})}(\mathbb{R})$ [$\mathcal{B}(\mathcal{N})$ *is the space of bounded linear operators on* $\mathcal{N}$]. *Let* P_+ *denote the projection of* $L^2_{\mathcal{N}}(\mathbb{R})$ *on* $H^+_{\mathcal{N}}(\mathbb{R})$. *The operator* $T_W: H^+_{\mathcal{N}}(\mathbb{R})\to H^+_{\mathcal{N}}(\mathbb{R})$ *defined by*

$$T_W f=P_+Wf,\quad f\in H^+_{\mathcal{N}}(\mathbb{R})$$

is called a Toeplitz operator [*on* $H^+_{\mathcal{N}}(\mathbb{R})$] *with symbol W. Here Wf is the operator of pointwise application of W to f i.e.,* $(Wf)(\sigma)=W(\sigma)f(\sigma)$, $\sigma\in\mathbb{R}$.

Define $\{u(t)\}_{t\in\mathbb{R}}$, a family of multiplicative operators on $L^2_{\mathcal{N}}(\mathbb{R})$, by

$$[u(t)f](\sigma)=e^{-i\sigma t}f(\sigma),\quad f\in L^2_{\mathcal{N}}(\mathbb{R}),\quad \sigma\in\mathbb{R}. \tag{1.14}$$

Denote by $\hat{\mathbf{T}}(t)$ the outgoing spectral representer of the semigroup element $\mathbf{T}(t)$. Taking the Fourier transform of Eq. (1.12) and using the definition of a Toeplitz operator we find that $\hat{\mathbf{T}}(t)$ is given by

$$\hat{\mathbf{T}}(t)f=P_+u(t)f=T_{u(t)}f,\quad f\in H^+_N(\mathbb{R}),\quad t\geqslant 0 \tag{1.15}$$

and $\hat{\mathbf{T}}(t)f=0$ for $f\in H^-_{\mathcal{N}}(\mathbb{R})$. The semigroup $\{\mathbf{T}(t)\}_{t\geqslant 0}$ is, therefore, represented in the outgoing spectral representation, by the semigroup of Toeplitz operators on $H^+_{\mathcal{N}}(\mathbb{R})$ with symbols $u(t)$ [and a trivial action on $H^-_{\mathcal{N}}(\mathbb{R})$].

Define the map $\hat{\mathbf{W}}_+:\mathcal{H}\mapsto L^2_{\mathcal{N}}(\mathbb{R})$ by $\hat{\mathbf{W}}_+\equiv\mathbf{F}\mathbf{W}_+$ (recall that $\mathbf{W}_+$ is the map of $\mathcal{H}$ onto the outgoing translation representation and $\mathbf{F}$ is the Fourier transform operator). Then $\hat{\mathbf{W}}_+$ maps $\mathcal{H}$ onto the Lax–Phillips outgoing spectral representation and we can summarize the discussion above by the observation that for any $f\in\mathcal{K}$ we have

$$\hat{\mathbf{W}}_+\mathbf{Z}(t)f=\hat{\mathbf{W}}_+\mathbf{T}(t)f=\hat{\mathbf{T}}(t)f_{\mathrm{out}}=T_{u(t)}f_{\mathrm{out}},\quad t\geqslant 0,\quad f\in\mathcal{K}, \tag{1.16}$$

where $f_{\mathrm{out}}=\hat{\mathbf{W}}_+f$ is the outgoing spectral representer of $f\in\mathcal{K}$. Put differently, letting $\hat{\mathbf{Z}}(t)=\hat{\mathbf{W}}_+\mathbf{Z}(t)\hat{\mathbf{W}}_+^{-1}$ be the outgoing spectral representer of $\mathbf{Z}(t)$ and letting $\hat{\mathcal{K}}=\hat{\mathbf{W}}_+\mathcal{K}$ be the subspace of $L^2_{\mathcal{N}}(\mathbb{R})$ representing $\mathcal{K}$ in the outgoing spectral representation, we have

$$\hat{\mathbf{Z}}(t)=T_{u(t)}|\hat{\mathcal{K}}. \tag{1.17}$$

Taking the Fourier transform of Eq. (1.13) we find that in the outgoing spectral representation the eigenfunctions of the generator $\hat{\mathbf{A}}$ of the semigroup $\{\hat{\mathbf{T}}(t)\}_{t\geqslant 0}=\{T_{u(t)}\}_{t\geqslant 0}$ are given by

$$\hat{f}_{\mu,n}(\sigma)=i\frac{n}{\sigma-\mu}\quad \forall\ \mu\quad \mathrm{Im}\,\mu<0,\quad \forall\ n\in\mathcal{N}. \tag{1.18}$$

Equations (1.17) and (1.18) raise the question of the characterization, out of all of the eigenvectors of the generator of the semigroup $\{T_{u(t)}\}_{t\geqslant 0}$ given in Eq. (1.18), of those which are contained in $\hat{\mathcal{K}}$. These will be the eigenvectors of the Lax–Phillips semigroup. The rest of this section deals with this question.

We start with the observation that following the discussion of the properties of the Lax–Phillips S-matrix in the preceding section we know that the subspace $\hat{\mathcal{K}}$, representing $\mathcal{K} \in \mathcal{H}$ in the outgoing spectral representation, is given by

$$\hat{\mathcal{K}} = H^+_{\mathcal{N}}(\mathbb{R}) \ominus \mathcal{S}H^+_{\mathcal{N}}(\mathbb{R}), \tag{1.19}$$

where $\mathcal{S}$ is an operator valued function with the properties (a″)–(c″) listed in the preceding section. Such a function is identified as belonging to the class of operators on $H^+_{\mathcal{N}}(\Pi)$ known as *inner functions*. Thus we conclude that the representation of an element $\mathbf{Z}(t)$ of the Lax–Phillips semigroup in the outgoing spectral representation is always of the form

$$\hat{\mathbf{Z}}(t) = T_{u(t)}|(H^+_{\mathcal{N}}(\mathbb{R}) \ominus \mathcal{S}H^+_{\mathcal{N}}(\mathbb{R})), \quad t \geqslant 0, \tag{1.20}$$

where $\mathcal{S}$ is some inner function. By a slight abuse of terminology a semigroup of the type of Eq. (1.20) will be called in the rest of this paper a Lax–Phillips semigroup. From Eq. (1.20) we can infer the general form of an element of the adjoint semigroup $\mathbf{Z}^*(t)$. Using the notation of Eq. (1.19) we get

$$\hat{\mathbf{Z}}^*(t) = P_{\hat{\mathcal{K}}}T^*_{u(t)}|\hat{\mathcal{K}} = P_{\hat{\mathcal{K}}}T_{\overline{u}(t)}|\hat{\mathcal{K}}, \quad t \geqslant 0. \tag{1.21}$$

In order to understand the structure described here and the origin of Theorem 1.3, we turn to the Sz.-Nagy–Foias theory of contraction operators on Hilbert space.[38] We start with the observation that the family $\{T_{u(t)}\}_{t\geqslant 0}$ is a continuous semigroup of contraction operators and the adjoint family $\{T^*_{u(t)}\}_{t\geqslant 0}=\{T_{\overline{u}(t)}\}_{t\geqslant 0}$ is also a semigroup of contractions. Moreover, $\{T^*_{u(t)}\}_{t\geqslant 0}$ is an isometric semigroup. It is a basic result of the Sz.-Nagy–Foias theory that the study of continuous semigroups of contractions can be reduced to the study of a single contraction operator. If $\{T(t)\}_{t\geqslant 0}$ is a one parameter continuous semigroup of contractions with generator A defined by

$$Ah = \lim_{t\to 0^+} \frac{1}{t}(T(t) - I)h \tag{1.22}$$

then the study of $\{T(t)\}_{t\geqslant 0}$ reduces to the study of its *cogenerator* T defined by

$$T = \frac{A + I}{A - I}. \tag{1.23}$$

It is easy to show that the cogenerator T is a contraction. The elements of a semigroup $\{T(t)\}_{t\geqslant 0}$ are given in terms of the cogenerator T by

$$T(t) = \exp\left(t\frac{T + I}{T - I}\right). \tag{1.24}$$

Denoting the cogenerator of the semigroup $\{T_{\overline{u}(t)}\}_{t\geqslant 0}$ by $S_T: H^+_{\mathcal{N}}(\mathbb{R}) \to H^+_{\mathcal{N}}(\mathbb{R})$, one finds that

$$(S_T f)(\sigma) = \frac{\sigma - i}{\sigma + i} f(\sigma), \quad \sigma \in \mathbb{R}, \quad f \in H^+_{\mathcal{N}}(\mathbb{R}). \tag{1.25}$$

The cogenerator of $\{T_{\overline{u}(t)}\}_{t\geqslant 0}$ is then identified as the canonical shift operator on $H^+_{\mathcal{N}}(\mathbb{R})$ (see, for example, Ref. 28). By Eq. (1.24) we then have

$$T^*_{u(t)} = T_{\overline{u}(t)} = \exp\left(t\frac{S_T + I}{S_T - I}\right). \tag{1.26}$$

Using Eq. (1.21) we find that

$$\hat{\mathbf{Z}}^*(t) = P_{\hat{\mathcal{K}}} \exp\left(t\frac{S_T + I}{S_T - I}\right)\Big| \hat{\mathcal{K}}. \tag{1.27}$$

Two other important ingredients of the Sz.-Nagy–Foias theory are the notions of *unitary and isometric dilation* of a contraction operator and the *functional calculus for completely nonunitary (cnu) contractions*. A dilation of an operator is defined as follows.

Definition (*dilation*): *Assume that for an operator B on a Hilbert space* $\mathcal{H}$ *and an operator A on a Hilbert space* $\mathcal{H}'$ *the following relations hold:*

(i) $\mathcal{H}$ *is a subspace of* $\mathcal{H}'$,
(ii) $Bx = P_{\mathcal{H}}Ax$ *for all* $x \in \mathcal{H}$, *where* $P_{\mathcal{H}}$ *denotes the orthogonal projection from* $\mathcal{H}'$ *into* $\mathcal{H}$.

We call A a dilation of B if (i) and (ii) hold and if

$$B^n x = P_{\mathcal{H}} A^n x, \quad x \in \mathcal{H}, \quad n = 1,2,3, \ldots . \tag{1.28}$$

Sz.-Nagy and Foias prove (Ref. 38, Chap. I) that for every contraction T on a Hilbert space $\mathcal{H}$ there exists an isometric (and a unitary) dilation V on some Hilbert space $\mathcal{R}$, which is moreover minimal in the sense that

$$\mathcal{R} = \vee_0^\infty V^n \mathcal{H}. \tag{1.29}$$

The minimal isometric dilation is determined up to an isomorphism. The space $\mathcal{H}$ is invariant for V^* and we have

$$TP_{\mathcal{H}} = P_{\mathcal{H}} V, \quad T^* = V^*|\mathcal{H}, \tag{1.30}$$

where $P_{\mathcal{H}}$ denotes the orthogonal projection from $\mathcal{R}$ onto $\mathcal{H}$.

Sz.-Nagy and Foias show (Ref. 38, Chap. III) that the function space $H^\infty(D)$ (D is the open unit disk), regarded as an algebra with an involution under the usual addition and multiplication of functions, can be used to define a *functional calculus for completely nonunitary (cnu) contractions*. By this we mean that, for a cnu contraction T on a Hilbert space $\mathcal{H}$ there exists an algebra homomorphism of $H^\infty(D)$ into $B(\mathcal{H})$ (the space of bounded operators on $\mathcal{H}$). The map providing this homomorphism is defined, for a function $a \in H^\infty(D)$ having the series expansion $a(z) = \Sigma_{n=0}^\infty c_n z^n$, by

$$a(z) = \sum_{n=0}^{\infty} c_n z^n \to a(T) = \lim_{r \to 1^-} a(rT) = \lim_{r \to 1^-} \left(\sum_{n=0}^{\infty} c_n r^n T^n \right).$$

Under this mapping we find, for a function $a \in H^\infty(D)$ and an isometric dilation V of a cnu contraction T, the following relation:

$$a(T)h = P_{\mathcal{H}} a(V)h, \quad h \in \mathcal{H}, \quad a \in H^\infty(D). \tag{1.31}$$

Define

$$T_{\hat{\mathbf{Z}}^*} \equiv P_{\hat{\mathcal{K}}} S_T | \hat{\mathcal{K}}, \tag{1.32}$$

where $\hat{\mathcal{K}} \in H^+(\mathbb{R})$ is defined in Eq. (1.19). The operator $P_{\hat{\mathcal{K}}} S_T | \hat{\mathcal{K}}$ is called a *compression of the shift* into the subspace $\hat{\mathcal{K}}$. It can be shown that, for any inner function $\mathcal{S}$, the shift S_T is an isometric dilation of the compression of S_T into $\hat{\mathcal{K}}$, i.e., it is an isometric dilation of $T_{\hat{\mathbf{Z}}^*}$. Since the function

$$e_t(z) \equiv \exp\left(t\frac{z+1}{z-1}\right) \tag{1.33}$$

is inner, Eq. (1.31) implies that

$$\exp\left(t\frac{T_{\hat{\mathbf{Z}}^*}+I}{T_{\hat{\mathbf{Z}}^*}-I}\right)=P_{\hat{\mathcal{K}}}\exp\left(t\frac{S_T+I}{S_T-I}\right)\Big|\hat{\mathcal{K}}=P_{\hat{\mathcal{K}}}T_{\overline{u}(t)}|\hat{\mathcal{K}}=\hat{\mathbf{Z}}^*(t). \tag{1.34}$$

The operator $T_{\hat{\mathbf{Z}}^*}$ is therefore the cogenerator of the semigroup $\{\hat{\mathbf{Z}}^*(t)\}_{t\geqslant 0}$. Indeed, given the family of functions $\phi_t\in H^\infty(D)$ defined by

$$\phi_t(z)=\frac{z-1+t}{z-1-t},\quad t>0,$$

Sz.-Nagy and Foias prove (Ref. 38, Chap. III, Theorem 8.1) that the cogenerator T of a contractive semigroup $\{T(t)\}_{t\geqslant 0}$ is obtained by

$$T=\lim_{t\to 0^+}\phi_t(T(t))$$

and applying this relation to $\{\hat{\mathbf{Z}}^*(t)\}_{t\geqslant 0}$ we get

$$\lim_{t\to 0^+}\phi_t(\hat{\mathbf{Z}}^*(t))=\lim_{t\to 0^+}\phi_t\circ e_t(T_{\hat{\mathbf{Z}}^*(t)})=\lim_{t\to 0^+}P_{\hat{\mathcal{K}}}\phi_t\circ e_t(S_T)|\hat{\mathcal{K}}=\lim_{t\to 0^+}P_{\hat{\mathcal{K}}}\phi_t(\overline{u}(t))|\hat{\mathcal{K}}=P_{\hat{\mathcal{K}}}S_T|\hat{\mathcal{K}}=T_{\hat{\mathbf{Z}}^*}.$$

We conclude that *the compression of the shift to the subspace $\hat{\mathcal{K}}$ is the cogenerator of the semigroup* $\{\hat{\mathbf{Z}}^*(t)\}_{t\geqslant 0}$ and hence

$$T_{\hat{\mathbf{Z}}^*}=P_{\hat{\mathcal{K}}}S_T|\hat{\mathcal{K}}=\frac{\hat{\mathbf{B}}^*+I}{\hat{\mathbf{B}}^*-I}, \tag{1.35}$$

where $\hat{\mathbf{B}}^*$ is the generator of the semigroup $\{\hat{\mathbf{Z}}^*(t)\}_{t\geqslant 0}$. We note also that, using Eq. (1.30), we obtain

$$T_{\hat{\mathbf{Z}}}=\frac{\hat{\mathbf{B}}+I}{\hat{\mathbf{B}}-I}=S_T^*|\hat{\mathcal{K}}, \tag{1.36}$$

where $\hat{\mathbf{B}}$ is the generator and $T_{\hat{\mathbf{Z}}}$ is the cogenerator of the Lax–Phillips semigroup $\{\mathbf{Z}(t)\}_{t\geqslant 0}$.

For a contraction T on a Hilbert space $\mathcal{H}$ we define the *defect operators* D_T and D_{T^*} by

$$D_T\equiv(I-T^*T)^{1/2},\quad D_{T^*}\equiv(I-TT^*)^{1/2}.$$

The *defect spaces* $\mathcal{D}_T$ and $\mathcal{D}_{T^*}$ are defined by

$$\mathcal{D}_T=\overline{D_T\mathcal{H}},\quad \mathcal{D}_{T^*}=\overline{D_{T^*}\mathcal{H}}.$$

For every complex number λ for which the operator $I-\lambda T^*$ is boundedly invertible, define

$$\Theta_T(\lambda)\equiv\left[-T+\lambda D_{T^*}(I-\lambda T^*)^{-1}D_T\right]|\mathcal{D}_T \tag{1.37}$$

the values of the operator valued function $\Theta_T(\lambda)$ are bounded operators from $\mathcal{D}_T$ into $\mathcal{D}_{T^*}$. When considered on the unit disk D, $\Theta_T(\lambda)$ is a purely contractive, analytic, operator valued function, i.e., it is a contraction from $\mathcal{D}_T$ into $\mathcal{D}_{T^*}$ for every λ in the unit disk. The function $\Theta_T(\lambda)$ is called the *characteristic function of the contraction T* (see Ref. 38, Chap. VI). The main theorem of the Lax–Phillips scattering theory, relating eigenvalues of the generator of the Lax–Phillips semigroup and singularities of the Lax–Phillips *S*-matrix, is then a direct result of the following theorem, proved by Sz.-Nagy and Foias (Ref. 38, Chap. VI, Theorem 4.1).

Theorem 1.4: *Let T be a cnu contraction on $\mathcal{H}$. Denote by α_T the set of points $\mu\in D$ for which the operator $\Theta_T(\mu)$ is not boundedly invertible, together with the points $\mu\in C$ not lying on any of the open arcs of C on which $\Theta_T(\lambda)$ is a unitary operator valued analytic function of λ. Furthermore, denote by α_T^0 the set of points $\mu\in D$ for which $\Theta_T(\lambda)$ is not invertible at all. Then*

$$\sigma(T) = \alpha_T$$

and

$$\sigma_p(T) = \alpha_T^0.$$

Given the cogenerator $T_{\hat{\mathbf{Z}}^*}$ we can define its characteristic function $\Theta_{T_{\hat{\mathbf{Z}}^*}}(\lambda)$ and obtain the spectrum of $T_{\hat{\mathbf{Z}}^*}$ in the closed unit disk through Theorem 1.4. In this particular case the function $\Theta_{T_{\hat{\mathbf{Z}}^*}}$ is an inner function on the unit disk. We can now pass from the unit disk to the upper half-plane by setting

$$\mathcal{S}(z) = \Theta_{T_{\hat{\mathbf{Z}}^*}}\left(\frac{z-i}{z+i}\right), \quad \mathrm{Im}\, z > 0. \tag{1.38}$$

The operator valued function $\mathcal{S}$ on the left-hand side (lhs) of Eq. (1.38) is exactly the inner function appearing in Eq. (1.19) or Eq. (1.20), defining the subspace $\hat{\mathcal{K}} \subset H^+_{\mathcal{N}}(\mathbb{R})$ and identical to the Lax–Phillips *S*-matrix. Theorem 1.4 above then immediately implies Theorem 1.3.

Recapitulating the discussion in this section, we have seen that $\hat{\mathbf{Z}}(t)$, the outgoing spectral representer of an element of the Lax–Phillips semigroup $\mathbf{Z}(t)$, is of the form of a restriction of a Toeplitz operator $T_{u(t)}$ to a subspace $\hat{\mathcal{K}} \subset H^+_{\mathcal{N}}(\mathbb{R})$ given by $\hat{\mathcal{K}} = H^+_{\mathcal{N}}(\mathbb{R}) \ominus \mathcal{S}H^+_{\mathcal{N}}(\mathbb{R})$, for some inner function $\mathcal{S}$. The Lax–Phillips *S*-matrix $\mathcal{S}$ is essentially the characteristic function for the generator $\hat{\mathbf{B}}^*$ of the semigroup $\hat{\mathbf{Z}}^*(t)$. The cogenerator $T_{\hat{\mathbf{Z}}^*}$ of $\hat{\mathbf{Z}}^*(t)$ is identified as a compression of the shift and its characteristic function is an inner function. The correspondence between the points in Π where $\mathcal{S}$ has a nontrivial null space (or poles of the analytic continuation of $\mathcal{S}$ to $\overline{\Pi}$) and eigenvalues of the generator of $\hat{\mathbf{Z}}(t)$ [or $\mathbf{Z}(t)$] then arises from a theorem in operator theory (namely Theorem 1.4 above) relating the points of singularity of the characteristic function for a contraction T to the spectrum of T.

II. DESCRIPTION OF RESONANCES

A. Preliminary discussion

In this section the structures described in Sec. I B are utilized for the description of quantum mechanical resonances. The structures developed below bear general resemblance to the structure of the Lax–Phillips scattering theory. For a given scattering problem an "incoming representation" and an "outgoing representation" are defined, as well as the "*S*-matrix" transforming between the two. The evolution goes in these "representations" into the analogue of translation, i.e., the semigroup of Toeplitz operators $\{T_{u(t)}\}_{t\geq 0}$. Moreover, beyond general resemblance, the framework developed below makes explicit use of the fundamental structures of the Lax–Phillips theory originating from the Sz.-Nagy–Foias theory of contractions. Time evolution of resonances is actually described by a Lax–Phillips type semigroup of the form of Eq. (1.20) and the relation between eigenvalues corresponding to resonances and zeros of the *S*-matrix results from the Sz.-Nagy–Foias theory in the same way as described above in Sec. I B.

The starting point for the developments in this section is a method, proposed by Grossmann,[13] for the description of quantum mechanical resonances through the use of Hilbert space nesting.

Let $\mathcal{H}_0$ and $\mathcal{H}_1$ be (infinitely dimensional, separable) Hilbert spaces. A nesting map of $\mathcal{H}_1$ into $\mathcal{H}_0$ is a linear mapping θ such that

(1) the domain of θ is $\mathcal{H}_1$ and θ is continuous on $\mathcal{H}_1$,
(2) the range of θ is dense in $\mathcal{H}_0$,
(3) θ is one to one.

The adjoint of θ is defined in the usual way by the relation

$$(f,\theta g)_{\mathcal{H}_0} = (\theta^* f, g)_{\mathcal{H}_1} \tag{2.1}$$

θ^* is a nesting map of $\mathcal{H}_0$ into $\mathcal{H}_1$. We note that the properties of the map θ puts it in the class of *quasiaffine transforms* between $\mathcal{H}_1$ and $\mathcal{H}_0$ (see, for example, Refs. 38 and 21). A nested Hilbert space is defined as follows.

Definition (nested Hilbert space): A nested Hilbert space $(\mathcal{H}_1,\mathcal{H}_0,\theta)$ *is defined to be a structure consisting of the two Hilbert spaces* $\mathcal{H}_0$ *and* $\mathcal{H}_1$*, a nesting map* θ *of* $\mathcal{H}_1$ *into* $\mathcal{H}_0$ *and the adjoint nesting map* θ^*.

Given a nested Hilbert space $(\mathcal{H}_1,\mathcal{H}_0,\theta)$ and an operator $\mathbf{A}$ on $\mathcal{H}_0$, Grossmann considereds two types of operators, $\tilde{\mathbf{A}}$ and $\hat{\mathbf{A}}$ defined on $\mathcal{H}_1$. Respectively, these operators are defined to be

$$\tilde{\mathbf{A}} = \theta^* \mathbf{A} \theta \tag{2.2}$$

and

$$\hat{\mathbf{A}} = \theta^{-1} \mathbf{A} \theta. \tag{2.3}$$

We observe that the operator $\hat{\mathbf{A}}$ in Eq. (2.3) is well defined for any operator $\mathbf{A}$ which leaves the range of θ invariant. Let $f \in \mathcal{H}_1$ be in the domain of $\tilde{\mathbf{A}}$. For every $g \in \mathcal{H}_1$ we then have

$$(g,\tilde{\mathbf{A}} f)_{\mathcal{H}_1} = (g,\theta^* \mathbf{A} \theta f)_{\mathcal{H}_1} = (\theta g, \mathbf{A} \theta f)_{\mathcal{H}_0}.$$

We see that matrix elements of $\mathbf{A}$ on the dense set $\theta\mathcal{H}_1 \subset \mathcal{H}_0$ can be calculated as matrix elements of $\tilde{\mathbf{A}}$ on $\mathcal{H}_1$. Put differently, the operator $\tilde{\mathbf{A}}$ on $\mathcal{H}_1$ may be defined through the knowledge of a subset of the matrix elements of $\mathbf{A}$ on $\mathcal{H}_0$. Moreover, if $\mathbf{A}$ is bounded and self-adjoint then $\tilde{\mathbf{A}}$ is also bounded and self-adjoint. Grossmann considers the resolvent $\mathbf{G}(z)=(z-\mathbf{H})^{-1}$ of a scattering Hamiltonian $\mathbf{H}$ and defines through the nesting $(\mathcal{H}_1,\mathcal{H}_0,\theta)$ the operator $\tilde{\mathbf{G}}(z)$ according to Eq. (2.2). Since the matrix elements of $\tilde{\mathbf{G}}(z)$ between elements of $\mathcal{H}_1$ are a subset of the set of matrix elements of $\mathbf{G}(z)$ on $\mathcal{H}_0$, it may happen that $\tilde{\mathbf{G}}(z)$ has a larger domain of analyticity than $\mathbf{G}(z)$. In particular, the domain of analyticity of $\tilde{\mathbf{G}}(z)$ may cross the natural boundary of analyticity of $\mathbf{G}(z)$ along the positive real axis so that it may be possible to reach a second Riemann sheet resonance pole of the resolvent.

The matrix elements of $\hat{\mathbf{A}}$ are, on the other hand, generically different from those of $\mathbf{A}$ due to the different scalar product and, in general, $\hat{\mathbf{A}}$ is neither bounded nor symmetric. It is possible to show that the eigenvalues of $(\hat{\mathbf{A}})^*$ include the "improper" eigenvalues of $\mathbf{A}^*$.

Let $\mathbf{A}$ be a densely defined operator on $\mathcal{H}_0$ such that the operator $(\hat{\mathbf{A}^*})^*$ is also densely defined. A complex number z_0 is defined to be a generalized eigenvalue of $\mathbf{A}$ if there is an element $f \in \mathcal{H}_1$ such that

$$(\hat{\mathbf{A}^*})^* f = z_0 f. \tag{2.4}$$

In particular, it is easy to show that eigenvalues of $\mathbf{A}$ are also eigenvalues of $(\hat{\mathbf{A}^*})^*$.

If in the Hilbert space nesting $(\mathcal{H}_1,\mathcal{H}_0,\theta)$ the map $\theta:\mathcal{H}_1 \mapsto \mathcal{H}_0$ is a contraction then we have a *contractive nesting* of $\mathcal{H}_1$ into $\mathcal{H}_0$. This property of θ *a priori* adds more structure to the resulting framework. A short discussion of this point is found in Sec. III below.

B. Main results

In a similar way to the Lax–Phillips scattering theory, this work centers around three main results: the existence of appropriate incoming and outgoing nesting structures, the existence of a continuous semigroup of contraction operators and the identification of the resonances of the theory, the eigenvalues of the generator of the semigroup, with zeros of the "*S*-matrix" mapping between the incoming and outgoing nesting structures.

Starting with the nesting structures, we have the following theorem.

Theorem 2.1. (outgoing contractive nesting): *Let* $\mathbf{H}_0$ *and* $\mathbf{H}$ *be self-adjoint operators on a Hilbert space* $\mathcal{H}$. *Let* $\{\mathbf{U}(t)\}_{t\in\mathbb{R}}$ *be the unitary evolution group on* $\mathcal{H}$ *generated by* $\mathbf{H}$ *[i.e.,* $\mathbf{U}(t)=\exp(-i\mathbf{H}t)$*]. Denote by* $\mathcal{H}_{ac}^0$ *and* $\mathcal{H}_{ac}$, *respectively, the absolutely continuous subspaces of* $\mathbf{H}_0$ *and* $\mathbf{H}$. *Assume that the absolutely continuous spectrum of* $\mathbf{H}_0$ *and* $\mathbf{H}$ *has multiplicity one and that it satisfies* $\sigma_{ac}(\mathbf{H}_0)=\sigma_{ac}(\mathbf{H})=\mathbb{R}^+$. *Assume furthermore that the Møller wave operator* $\mathbf{\Omega}^-\equiv\mathbf{\Omega}^-(\mathbf{H}_0,\mathbf{H}):\mathcal{H}_{ac}^0\mapsto\mathcal{H}_{ac}$ *exists and is complete. Then there exists a map* $\hat{\mathbf{\Omega}}_+:\mathcal{H}_{ac}\mapsto H^+(\mathbb{R})$ *such that*

(a) $(\mathcal{H}_{ac},H^+(\mathbb{R}),\hat{\mathbf{\Omega}}_+)$ *is a contractive Hilbert space nesting of* $\mathcal{H}_{ac}$ *into* $H^+(\mathbb{R})$.

(b) *For every* $t\geqslant 0$ *define the Grossmann type operator* $\hat{\mathbf{U}}^*(t):H^+(\mathbb{R})\mapsto H^+(\mathbb{R})$ *according to Eq. (2.3), i.e.,* $\hat{\mathbf{U}}^*(t)=(\hat{\mathbf{\Omega}}_+^*)^{-1}\mathbf{U}^*(t)\hat{\mathbf{\Omega}}_+^*$. *These operators are well defined and, for every* $t\geqslant 0$ *and every* $f\in\mathcal{H}_{ac}$ *we have*

$$\hat{\mathbf{\Omega}}_+\mathbf{U}(t)f=(\widehat{\mathbf{U}^*(t)})^*\hat{\mathbf{\Omega}}_+f=T_{u(t)}f_{\text{out}},\quad t\geqslant 0, \tag{2.5}$$

where $f_{\text{out}}=\hat{\mathbf{\Omega}}_+f$ *and* $T_{u(t)}$ *is the Toeplitz operator with symbol* $u(t)$ *given by Eq. (1.14).*

The nesting $(\mathcal{H}_{ac},H^+(\mathbb{R}),\hat{\mathbf{\Omega}}_+)$ is referred to below as the *outgoing contractive nesting of* $\mathcal{H}_{ac}$. *Remarks:*

(1) It follows from Eq. (2.4) and the discussion above that eigenvalues of $(\widehat{\mathbf{U}^*(t)})^*:H^+(\mathbb{R})\mapsto H^+(\mathbb{R})$, are generalized eigenvalues of $\mathbf{U}(t)$ (for $t\geqslant 0$).

(2) Obviously, the lhs of Eq. (2.5) can be defined for every $t\in(-\infty,\infty)$. Equation (2.5), however, is valid for $t\geqslant 0$.

Proof of Theorem 2.1: At the center of the proof of Theorem 2.1 lie two theorems, proved by Van Winter, that enable us to define a contractive nesting of $L^2(\mathbb{R}^+)$ into $H^+(\mathbb{R})$. Taken together, the following theorems are referred to below as the Van Winter theorem.[39]

Theorem 2.2 (Van Winter): *The class of functions* f *which are analytic, regular in the upper half-plane, and have the property that*

$$\int_0^\infty \mathrm{d}r|f(re^{i\phi})|^2 \tag{2.6}$$

is uniformly bounded in ϕ *for* $0<\phi<\pi$, *is identical to the Hardy class* $H^2(\Pi)$. *For each such* f *there exists a boundary value function* $f(r)$ $(r>0)$ *on* $\mathbb{R}^+$. *The boundary values* $f(r)$ *of functions* $f(re^{i\phi})$ *in* $H^2(\Pi)$ *are dense in* $L^2(\mathbb{R}^+)$.

Theorem 2.3 (Van Winter): *A complex valued function* f *defined on the upper half-plane* Π *is in* $H^2(\Pi)$ *if and only if it is given by an inverse Mellin transform as*

$$f(re^{i\phi})=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\mathrm{d}s\,E(s)(re^{i\phi})^{-is-1/2} \tag{2.7}$$

for some function $E(s)$ *satisfying*

$$\int_{-\infty}^{+\infty}\mathrm{d}s(1+e^{2\pi s})|E(s)|^2<\infty$$

in this case the Mellin transform of f *is given by*

$$E(s,\phi)=\frac{1}{\sqrt{2\pi}}\int_0^\infty \mathrm{d}r\,f(re^{i\phi})r^{is-1/2}=e^{\phi s-i(\phi/2)}E(s). \tag{2.8}$$

It can be shown[39] that in Eq. (1.8) it is possible to take ϕ to zero, i.e., that if $f(r)$ is the boundary value on $\mathbb{R}^+$ of a function $f(re^{i\phi})$ in $H^2(\Pi)$ then

$$E(s) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \mathrm{d}r\, f(r) r^{is-1/2}. \tag{2.9}$$

By combining Theorem 2.2 and Theorem 2.3 we find that any function in $H^2(\Pi)$ can be reconstructed from its boundary value on the positive real axis. Define $\theta: H^+(\mathbb{R}) \mapsto L^2(\mathbb{R}^+)$ by taking, for each function $f \in H^2(\Pi)$, the restriction to $\mathbb{R}^+$ of the boundary value of f on the real axis. Then θ is one to one and θ^{-1} can be defined. It is also important to note that the Van Winter theorem can be applied to boundary values of Hardy class functions on the negative real axis, a fact which is used below.

Using the Van Winter theorem we easily obtain the following result.

Proposition 2.1: The map $\theta: H^+(\mathbb{R}) \to L^2(\mathbb{R}^+)$ is a contractive nesting map, $(H^+(\mathbb{R}), L^2(\mathbb{R}^+), \theta)$ is a contractive nesting of $H^+(\mathbb{R})$ into $L^2(\mathbb{R}^+)$ and $(L^2(\mathbb{R}^+), H^+(\mathbb{R}), \theta^*)$ is a contractive nesting of $L^2(\mathbb{R}^+)$ into $H^+(\mathbb{R})$.

Proof: From the Van Winter theorem we know that the map θ is injective and that $\theta H^+(\mathbb{R}) \subset L^2(\mathbb{R}^+)$ is dense in $L^2(\mathbb{R}^+)$. Denote by $H^-(\mathbb{R})$ the space of boundary values on $\mathbb{R}$ of functions belonging to $H^2(\overline{\Pi})$ (recall that $\overline{\Pi}$ is the lower half of the complex plane). We have

$$L^2(\mathbb{R}) = H^-(\mathbb{R}) \oplus H^+(\mathbb{R}). \tag{2.10}$$

$H^+(\mathbb{R})$ is then a subspace of $L^2(\mathbb{R})$ and it inherits its scalar product from that of $L^2(\mathbb{R})$. By the definition of θ we have for $f \in H^+(\mathbb{R})$,

$$\|\theta f\|^2_{L^2(\mathbb{R}^+)} = (\theta f, \theta f)_{L^2(\mathbb{R}^+)} < (f,f)_{L^2(\mathbb{R})} = (f,f)_{H^+(\mathbb{R})} = \|f\|^2_{H^+(\mathbb{R})}. \tag{2.11}$$

$\theta: H^+(\mathbb{R}) \mapsto L^2(\mathbb{R}^+)$ is therefore a contraction and $(H^+(\mathbb{R}), L^2(\mathbb{R}^+), \theta)$ is a contractive nesting of $H^+(\mathbb{R})$ into $L^2(\mathbb{R}^+)$. Defining the adjoint map $\theta^*: L^2(\mathbb{R}^+) \mapsto H^+(\mathbb{R})$ through the relation

$$(\theta x, y)_{L^2(\mathbb{R}^+)} = (x, \theta^* y)_{H^+(\mathbb{R})}, \quad x \in H^+(\mathbb{R}), \quad y \in L^2(\mathbb{R}^+) \tag{2.12}$$

we conclude that $(L^2(\mathbb{R}^+), H^+(\mathbb{R}), \theta^*)$ is a contractive nesting of $L^2(\mathbb{R}^+)$ into $H^+(\mathbb{R})$.

■

Consider the spectral (or energy) representation for $\mathbf{H}_0$. The assumption $\sigma_{ac}(\mathbf{H}_0) = \mathbb{R}^+$ (and that the multiplicity is one) leads to the existence of a unitary map $U: \mathcal{H}^0_{ac} \mapsto L^2(\mathbb{R}^+)$ defining a representation of $\mathcal{H}^0_{ac}$ in terms of the space $L^2(\mathbb{R}^+)$. We can now use the unitarity of the Møller wave operator $\mathbf{\Omega}^-: \mathcal{H}^0_{ac} \mapsto \mathcal{H}_{ac}$ and define a unitary map $\mathbf{W}^+: \mathcal{H}_{ac} \mapsto L^2(\mathbb{R}^+)$ by

$$\mathbf{W}^+ \equiv U(\mathbf{\Omega}^-)^*. \tag{2.13}$$

$\mathbf{W}^+$ is a transformation to a spectral representation for $\mathbf{H}|\mathcal{H}_{ac}$. Applying the contractive nesting $(L^2(\mathbb{R}^+), H^+(\mathbb{R}), \theta^*)$ then allows us to define a map

$$\hat{\mathbf{\Omega}}_+: \mathcal{H}_{ac} \mapsto H^+(\mathbb{R})$$

by

$$\hat{\mathbf{\Omega}}_+ \equiv \theta^* \mathbf{W}^+ = \theta^* U (\mathbf{\Omega}^-)^*. \tag{2.14}$$

Since $\mathbf{W}^+$ is unitary and θ^* is a contractive nesting map we find that $(\mathcal{H}_{ac}, H^+(\mathbb{R}), \hat{\mathbf{\Omega}}_+)$ is a contractive nesting of $\mathcal{H}_{ac}$ into $H^+(\mathbb{R})$ and (a) is proved.

Next, we turn to the proof of (b). Assume that the range of $\hat{\mathbf{\Omega}}^*_+$ is invariant for an operator $\mathbf{A}: \mathcal{H}_{ac} \mapsto \mathcal{H}_{ac}$. Then, it is possible to use the nesting $(H^+(\mathbb{R}), \mathcal{H}_{ac}, \hat{\mathbf{\Omega}}^*_+)$ to define the Grossmann type operator $\hat{\mathbf{A}}: H^+(\mathbb{R}) \mapsto H^+(\mathbb{R})$ according to Eq. (2.3), i.e.,

$$\hat{\mathbf{A}} = (\hat{\mathbf{\Omega}}_+^*)^{-1}\mathbf{A}\hat{\mathbf{\Omega}}_+^*. \tag{2.15}$$

The generalized eigenvalues of $\mathbf{A}$ are then eigenvalues of the operator $(\hat{\mathbf{A}^*})^*: H^+(\mathbb{R}) \mapsto H^+(\mathbb{R})$ given by

$$(\hat{\mathbf{A}^*})^* = \hat{\mathbf{\Omega}}_+\mathbf{A}^{**}((\hat{\mathbf{\Omega}}_+^*)^{-1})^*. \tag{2.16}$$

The first equality in Eq. (2.5) results from the following proposition

Proposition 2.2: For any bounded operator $\mathbf{A}: \mathcal{H}_{ac} \mapsto \mathcal{H}_{ac}$ *satisfying* $\mathbf{A}^{**} = \mathbf{A}$ *and such that* $\hat{\mathbf{\Omega}}_+^* H^+(\mathbb{R}) \subset \mathcal{H}_{ac}$ *is invariant for* $\mathbf{A}$*, and for any* $h \in \mathcal{H}_{ac}$ *we have*

$$(\hat{\mathbf{A}^*})^* \hat{\mathbf{\Omega}}_+ h = \hat{\mathbf{\Omega}}_+ \mathbf{A} h.$$

Proof: Since $\hat{\mathbf{\Omega}}_+^*$ is a nesting map of $H^+(\mathbb{R})$ into $\mathcal{H}_{ac}$ the map $(\hat{\mathbf{\Omega}}_+^*)^{-1}$ is defined on the dense set $\hat{\mathbf{\Omega}}_+^* H^+(\mathbb{R}) \subset \mathcal{H}_{ac}$ and we can define the map $((\hat{\mathbf{\Omega}}_+^*)^{-1})^*$ through the relation

$$(g,f)_{H^+(\mathbb{R})} = ((\hat{\mathbf{\Omega}}_+^*)^{-1}\hat{\mathbf{\Omega}}_+^* g, f)_{H^+(\mathbb{R})} = (\hat{\mathbf{\Omega}}_+^* g, ((\hat{\mathbf{\Omega}}_+^*)^{-1})^* f)_{\mathcal{H}_{ac}}$$

which holds for any $f \in D(((\hat{\mathbf{\Omega}}_+^*)^{-1})^*)$ and any $g \in H^+(\mathbb{R})$. It is then true that

$$((\hat{\mathbf{\Omega}}_+^*)^{-1})^* = (\hat{\mathbf{\Omega}}_+^{**})^{-1} = \hat{\mathbf{\Omega}}_+^{-1}. \tag{2.17}$$

From Eq. (2.16) and Eq. (2.17) we conclude that, for any $f \in \hat{\mathbf{\Omega}}_+ \mathcal{H}_{ac}$ we have

$$(\hat{\mathbf{A}^*})^* f = \hat{\mathbf{\Omega}}_+ \mathbf{A}^{**} \hat{\mathbf{\Omega}}_+^{-1} f, \quad f \in \hat{\mathbf{\Omega}}_+ \mathcal{H}_{ac}. \tag{2.18}$$

By the injective property of $\hat{\mathbf{\Omega}}_+$, for any $f \in \hat{\mathbf{\Omega}}_+ \mathcal{H}_{ac}$ there is a unique $h \in \mathcal{H}_{ac}$ such that $f = \hat{\mathbf{\Omega}}_+ h$. Hence, by Eq. (2.18) we have

$$(\hat{\mathbf{A}^*})^* \hat{\mathbf{\Omega}}_+ h = \hat{\mathbf{\Omega}}_+ \mathbf{A}^{**} h, \quad h \in \mathcal{H}_{ac}. \tag{2.19}$$

In particular, if $\mathbf{A}$ satisfies $\mathbf{A}^{**} = \mathbf{A}$ we find that

$$(\hat{\mathbf{A}^*})^* \hat{\mathbf{\Omega}}_+ h = \hat{\mathbf{\Omega}}_+ \mathbf{A} h, \quad h \in \mathcal{H}_{ac}. \tag{2.20}$$

■

It is easy to see that, for $t \geqslant 0$, $\mathbf{U}(t)\hat{\mathbf{\Omega}}_+^* H^+(\mathbb{R}) \subset \hat{\mathbf{\Omega}}_+^* H^+(\mathbb{R})$. Indeed we have

$$\mathbf{U}(t)\hat{\mathbf{\Omega}}_+^* H^+(\mathbb{R}) = \mathbf{U}(t)(\mathbf{W}^+)^* \theta H^+(\mathbb{R}) = (\mathbf{W}^+)^* \overline{u}(t) \theta H^+(\mathbb{R}) \subset (\mathbf{W}^+)^* \theta H^+(\mathbb{R}) = \hat{\mathbf{\Omega}}_+^* H^+(\mathbb{R})$$

hence, we can apply Proposition 2.2 to $\mathbf{U}(t)$ $(t \geqslant 0)$ and obtain the first equality in Eq. (2.5).

In order to prove the second equality in Eq. (2.5) we need to obtain a more explicit expression for the map $\hat{\mathbf{\Omega}}_+$. We have

Proposition 2.3: Define the inclusion map $\mathbf{I}: L^2(\mathbb{R}^+) \mapsto L^2(\mathbb{R})$ *by*

$$(\mathbf{I}\phi)(\sigma) = \begin{cases} \phi(\sigma), & \sigma \geqslant 0, \\ 0, & \sigma < 0, \end{cases} \quad \phi \in L^2(\mathbb{R}^+). \tag{2.21}$$

Let $\mathbf{P}_+$ *be the orthogonal projection of* $L^2(\mathbb{R})$ *onto* $H^+(\mathbb{R})$ *and let* $\mathbf{W}^+$ *be the unitary map defined in Eq. (2.13). Then the map* $\hat{\mathbf{\Omega}}_+: \mathcal{H}_{ac} \mapsto H^+(\mathbb{R})$ *is given by*

$$\hat{\mathbf{\Omega}}_+ = \mathbf{P}_+ \mathbf{I} \mathbf{W}^+. \tag{2.22}$$

Proof: We first need an explicit expression for the map θ^*. Regarding $L^2(\mathbb{R}^+)$ as a closed

subspace of $L^2(\mathbb{R})$, the inclusion map $\mathbf{I}: L^2(\mathbb{R}^+) \mapsto L^2(\mathbb{R})$ is given by Eq. (2.21). The lhs of Eq. (2.12) can be written then as

$$(\theta x, y)_{L^2(\mathbb{R}^+)} = (\mathbf{I}\theta x, \mathbf{I}y)_{L^2(\mathbb{R})}. \tag{2.23}$$

Making use of the decomposition of $L^2(\mathbb{R})$, Eq. (2.10), we observe that any $y \in L^2(\mathbb{R}^+)$ correspond to the following decompositon into an orthogonal sum:

$$\mathbf{I}y = y_+ + y_-, \quad y_+ \in H^+(\mathbb{R}), \quad y_- \in H^-(\mathbb{R}). \tag{2.24}$$

Equation (2.21) then implies that

$$y_+(\sigma) = -y_-(\sigma), \quad \sigma < 0. \tag{2.25}$$

Inserting the decomposition, Eq. (2.24), into the rhs of Eq. (2.23) we obtain

$$(\theta x, y)_{L^2(\mathbb{R}^+)} = (\mathbf{I}\theta x, y_+ + y_-)_{L^2(\mathbb{R})} = \int_{-\infty}^{+\infty} \mathrm{d}\sigma \overline{(\mathbf{I}\theta x)(\sigma)}(y_+(\sigma) + y_-(\sigma)). \tag{2.26}$$

We can now use Eq. (2.26) to obtain the following identity:

$$\int_{-\infty}^{+\infty} \mathrm{d}\sigma \overline{(\mathbf{I}\theta x)(\sigma)}(y_+(\sigma) + y_-(\sigma)) = \int_{-\infty}^{+\infty} \mathrm{d}\sigma\, \overline{x(\sigma)}(y_+(\sigma) + y_-(\sigma)) = \int_{-\infty}^{+\infty} \mathrm{d}\sigma\, \overline{x(\sigma)} y_+(\sigma) = (x, y_+)_{H^+(\mathbb{R})}, \tag{2.27}$$

where the second equality follows from the orthogonality of $H^+(\mathbb{R})$ and $H^-(\mathbb{R})$. Equations (2.26) and (2.27) imply that

$$(\theta x, y)_{L^2(\mathbb{R}^+)} = (x, y_+)_{H^+(\mathbb{R})}. \tag{2.28}$$

Comparing Eq. (2.12) and Eq. (2.28) we find the desired expression for the map $\theta^*: L^2(\mathbb{R}^+) \mapsto H^+(\mathbb{R})$,

$$\theta^* y = y_+ = \mathbf{P}_+ \mathbf{I} y, \quad y \in L^2(\mathbb{R}^+), \quad y_+ \in H^+(\mathbb{R}). \tag{2.29}$$

Equation (2.14) can now be written in the form

$$\hat{\mathbf{\Omega}}_+ = \mathbf{P}_+ \mathbf{I} \mathbf{W}^+. \tag{2.30}$$

■

Observe that, for any $h \in \mathcal{H}_{ac}$ we have

$$\mathbf{I}\mathbf{W}^+ \mathbf{U}(t) h = \mathbf{I} U \hat{\mathbf{\Omega}}^{-*} \mathbf{U}(t) h = \mathbf{I} U \mathbf{U}_0(t) \hat{\mathbf{\Omega}}^{-*} h = u(t) \mathbf{I} \mathbf{W}^+ h, \tag{2.31}$$

where $u(t)$ is the multiplicative operator defined in Eq. (1.14). Using again the decomposition in Eq. (2.10) we have

$$\mathbf{I}\mathbf{W}^+ h = \mathbf{P}_+ \mathbf{I}\mathbf{W}^+ h + \mathbf{P}_- \mathbf{I}\mathbf{W}^+ h = h_+ + h_-, \tag{2.32}$$

where $h_+ = \mathbf{P}_+ \mathbf{I}\mathbf{W}^+ h = \hat{\mathbf{\Omega}}^+ h$ and $h_- = \mathbf{P}_- \mathbf{I}\mathbf{W}^+ h$. Here $\mathbf{P}_+$ is the projection on $H^+(\mathbb{R})$ defined above and $\mathbf{P}_-: L^2(\mathbb{R}) \mapsto H^-(\mathbb{R})$ is the orthogonal projection of $L^2(\mathbb{R})$ on $H^-(\mathbb{R})$. From Eqs. (2.30)–(2.32) we obtain, for any $h \in \mathcal{H}_{ac}$,

$$\hat{\mathbf{\Omega}}_+ \mathbf{U}(t) h = \mathbf{P}_+ u(t) \mathbf{I}\mathbf{W}^+ h = \mathbf{P}_+ u(t)(h_+ + h_-). \tag{2.33}$$

We conclude the proof of Theorem 2.1 by observing that $H^-(\mathbb{R})$ is stable under the action of $u(t)$ for $t \geqslant 0$. Hence we have $u(t) h_- \in H^-(\mathbb{R})$ and so

$$\hat{\mathbf{\Omega}}_+\mathbf{U}(t)h = \mathbf{P}_+u(t)h_+ = T_{u(t)}\hat{\mathbf{\Omega}}_+h. \tag{2.34}$$

This completes the proof of Theorem 2.1.

■

Theorem 2.1 provides the analogue of the Fourier transform of the representation in Theorem 1.1 in Sec. I, that is, it is the analogue of the outgoing spectral representation of the Lax–Phillips scattering theory. One may think of it as the "outgoing contractive nesting" associated with $\mathcal{H}_{ac}$ and $\mathbf{U}(t)$.

As in the case of the Lax–Phillips theory, there is another nesting structure which may be thought of as the "incoming contractive nesting" associated with $\mathcal{H}_{ac}$ and $\mathbf{U}(t)$. In a similar fashion to Eq. (2.14) we define a contractive nesting map $\hat{\mathbf{\Omega}}_-:\mathcal{H}_{ac}\mapsto H^+(\mathbb{R})$ by

$$\hat{\mathbf{\Omega}}_- \equiv \theta^*\mathbf{W}^- = \theta^*U(\mathbf{\Omega}^+)^*. \tag{2.35}$$

For $\hat{\mathbf{\Omega}}_-$ we have the following theorem.

Theorem 2.4 (incoming contractive nesting): *Let* $\mathbf{H}_0$ *and* $\mathbf{H}$ *be self-adjoint operators on a Hilbert space* $\mathcal{H}$ *and let* $\{\mathbf{U}(t)\}_{t\in\mathbb{R}}$ *be the unitary evolution group on* $\mathcal{H}$ *generated by* $\mathbf{H}$. *Denote by* $\mathcal{H}_{ac}^0$ *and* $\mathcal{H}_{ac}$, *respectively, the absolutely continuous subspaces of* $\mathbf{H}_0$ *and* $\mathbf{H}$. *Assume that the absolutely continuous spectrum of* $\mathbf{H}_0$ *and* $\mathbf{H}$ *has multiplicity one and that it satisfies* $\sigma_{ac}(\mathbf{H}_0) = \sigma_{ac}(\mathbf{H}) = \mathbb{R}^+$. *Assume furthermore that the Møller wave operator* $\mathbf{\Omega}^+ \equiv \mathbf{\Omega}^+(\mathbf{H}_0,\mathbf{H}):\mathcal{H}_{ac}^0\mapsto\mathcal{H}_{ac}$ *exists and is complete. Then there exists a map* $\hat{\mathbf{\Omega}}_-:\mathcal{H}_{ac}\mapsto H^+(\mathbb{R})$ *such that*

(a) $(\mathcal{H}_{ac}, H^+(\mathbb{R}), \hat{\mathbf{\Omega}}_-)$ *is a contractive Hilbert space nesting of* $\mathcal{H}_{ac}$ *into* $H^+(\mathbb{R})$.

(b) *For every* $t\geqslant 0$ *define the Grossmann type operator* $\hat{\mathbf{U}}^*(t):H^+(\mathbb{R})\mapsto H^+(\mathbb{R})$ *according to Eq. (2.3), i.e.,* $\hat{\mathbf{U}}^*(t) = (\hat{\mathbf{\Omega}}_-^*)^{-1}\mathbf{U}^*(t)\hat{\mathbf{\Omega}}_-^*$. *These operators are well defined and, for every* $t\geqslant 0$ *and every* $f\in\mathcal{H}_{ac}$ *we have*

$$\hat{\mathbf{\Omega}}_-\mathbf{U}(t)f = (\widehat{\mathbf{U}^*(t)})^*\hat{\mathbf{\Omega}}_-f = T_{u(t)}f_{\text{in}}, \quad t\geqslant 0, \tag{2.36}$$

where $f_{\text{in}} = \hat{\mathbf{\Omega}}_-f$ *and* $T_{u(t)}$ *is the Toeplitz operator with symbol* $u(t)$ *given by Eq. (1.14).*

Once the existence of the incoming contractive nesting and the outgoing contractive nesting are established we can turn to the definition of the analogue of the Lax–Phillips S-matrix. Let $f_{\text{in}} = \hat{\mathbf{\Omega}}_-f \in H^+(\mathbb{R})$ be the "incoming nested representer" of an element $f\in\mathcal{H}_{ac}$. Let $f_{\text{out}} = \hat{\mathbf{\Omega}}_+f \in H^+(\mathbb{R})$ be the "outgoing nested representer" of the same element f. We have

$$f_{\text{out}} = \hat{\mathbf{\Omega}}_+\hat{\mathbf{\Omega}}_-^{-1}f_{\text{in}} = \theta^*U(\mathbf{\Omega}^-)^*\mathbf{\Omega}^+U^*(\theta^*)^{-1}f_{\text{in}} = \theta^*U\mathbf{S}U^*(\theta^*)^{-1}f_{\text{in}} = \theta^*\widetilde{\mathbf{S}}(\theta^*)^{-1}f_{\text{in}}, \tag{2.37}$$

where $\mathbf{S} = (\mathbf{\Omega}^-)^*\mathbf{\Omega}^+$ is the scattering operator and $\widetilde{\mathbf{S}}:L^2(\mathbb{R}^+)\mapsto L^2(\mathbb{R}^+)$ is defined by $\widetilde{\mathbf{S}} \equiv U\mathbf{S}U^*$. The operator $\widetilde{\mathbf{S}}$ is the representer of $\mathbf{S}$ in the spectral (energy) representation for $\mathbf{H}_0$ and is a multiplicative operator in this representation, i.e.,

$$(\widetilde{\mathbf{S}}f)(E) = \widetilde{\mathbf{S}}(E)f(E), \quad f\in L^2(\mathbb{R}^+).$$

Equation (2.37) provides the definition of the *nested scattering matrix* as follows:

Definition (nested scattering matrix): Let $\mathbf{S} = (\mathbf{\Omega}^-)^*\mathbf{\Omega}^+$ *be the scattering operator associated with* $\mathbf{H}_0$ *and* $\mathbf{H}$. *Let* $\widetilde{\mathbf{S}}:L^2(\mathbb{R}^+)\mapsto L^2(\mathbb{R}^+)$ *be given by*

$$\widetilde{\mathbf{S}} \equiv U\mathbf{S}U^*. \tag{2.38}$$

The nested scattering matrix $\mathbf{S}_{\text{nest}}:H^+(\mathbb{R})\mapsto H^+(\mathbb{R})$ *is defined to be*

$$\mathbf{S}_{\text{nest}} \equiv \theta^*\widetilde{\mathbf{S}}(\theta^*)^{-1}. \tag{2.39}$$

Of course, for every $f \in \mathcal{H}_{ac}$ we have $f_{\text{out}} = \mathbf{S}_{\text{nest}} f_{\text{in}}$ where $f_{\text{out}} = \hat{\mathbf{\Omega}}_+ f$ and $f_{\text{in}} = \hat{\mathbf{\Omega}}_- f$. We have the following theorem.

Theorem 2.5: *Consider* $L^2(\mathbb{R}^+)$ *and* $L^2(\mathbb{R}^-)$ *as closed subspaces of* $L^2(\mathbb{R})$. *Denote* $\mathbf{P}_{\mathbb{R}^+}: L^2(\mathbb{R}) \mapsto L^2(\mathbb{R})$ *the orthogonal projection of* $L^2(\mathbb{R})$ *on* $L^2(\mathbb{R}^+)$ *and, similarly,* $\mathbf{P}_{\mathbb{R}^-}: L^2(\mathbb{R}) \mapsto L^2(\mathbb{R})$ *the orthogonal projection of* $L^2(\mathbb{R})$ *on* $L^2(\mathbb{R}^-)$. *Let* $\tilde{\mathbf{S}}$ *be defined as in Eq. (2.38). Then, for every* $f_{\text{in}} \in \hat{\mathbf{\Omega}}_- \mathcal{H}_{ac} \subset H^+(\mathbb{R})$ *we have*

$$[\mathbf{S}_{\text{nest}} f_{\text{in}}](\sigma) = \frac{1}{2\pi} \int_0^\infty \mathrm{d}E \frac{i}{\sigma - E + i0^+} \tilde{\mathbf{S}}(E) [\mathbf{P}_{\mathbb{R}^+} f_{\text{in}}](E) + \frac{1}{4\pi^2} \int_0^\infty \mathrm{d}E \frac{i}{\sigma - E + i0^+} \tilde{\mathbf{S}}(E) \times \left\{ \int_{-\infty}^\infty \mathrm{d}s \int_{-\infty}^0 \mathrm{d}\sigma' [\mathbf{P}_{\mathbb{R}^-} f_{\text{in}}](\sigma') \sigma'^{-is-1/2} E^{is-1/2} \right\}. \tag{2.40}$$

Proof: We need to obtain a realization of the maps θ^* and $(\theta^*)^{-1}$ on the functional level. For θ^* we have the following.

Lemma 2.1: The map $\theta^*: L^2(\mathbb{R}^+) \mapsto H^+(\mathbb{R})$ *is given, for any* $f \in L^2(\mathbb{R}^+)$, *by*

$$(\theta^* f)(\sigma) = \frac{1}{2\pi} \int_0^\infty \mathrm{d}E \frac{i}{\sigma - E + i0^+} f(E).$$

Proof: The starting point is Eq. (2.29). The inclusion map $\mathbf{I}: L^2(\mathbb{R}^+) \mapsto L^2(\mathbb{R})$ is realized in a simple way: given a function $f \in L^2_{\mathcal{N}}(\mathbb{R}^+)$, and for any $s \in \mathbb{R}$, we have

$$(\mathbf{I}f)(s) = \int_0^\infty \mathrm{d}E \; \delta(s - E) f(E), \tag{2.41}$$

where $\delta(\cdot)$ is the Dirac delta distribution.

Now for the realization of the projection $\mathbf{P}_+: L^2(\mathbb{R}) \mapsto H^+(\mathbb{R})$. For this we Fourier transform $L^2(\mathbb{R})$ and note that, denoting the Fourier transform operator by $\mathbf{F}$, we have $H^+(i\mathbb{R}) = L^2(\mathbb{R}^+)$ and $\mathbf{F}H^-(\mathbb{R}) = L^2(\mathbb{R}^-)$. For any $f \in L^2(\mathbb{R})$ we therefore obtain

$$\mathbf{P}_+ f = \mathbf{F}^{-1} \mathbf{P}_{\mathbb{R}^+} \mathbf{F} f$$

and hence, for $f \in L^2(\mathbb{R})$

$$(\mathbf{P}_+ f)(\sigma) = \frac{1}{2\pi} \int_{-\infty}^\infty \mathrm{d}t \, e^{i\sigma t} \left(\theta(t) \int_{-\infty}^\infty \mathrm{d}s \, e^{-its} f(s) \right) = \frac{1}{2\pi} \int_{-\infty}^\infty \mathrm{d}s \int_0^\infty \mathrm{d}t \, e^{i(\sigma - s + i0^+)t} f(s) = \frac{1}{2\pi} \int_{-\infty}^\infty \mathrm{d}s \frac{i}{\sigma - s + i0^+} f(s). \tag{2.42}$$

Combining Eq. (2.41) and Eq. (2.42) we get, for $f \in L^2(\mathbb{R}^+)$,

$$(\theta^* f)(\sigma) = (\mathbf{P}_+ \mathbf{I} f)(\sigma) = \frac{1}{2\pi} \int_{-\infty}^\infty \mathrm{d}s \frac{i}{\sigma - s + i0^+} \left[\int_0^\infty \mathrm{d}E \; \delta(s - E) f(E) \right] = \frac{1}{2\pi} \int_0^\infty \mathrm{d}E \frac{i}{\sigma - E + i0^+} f(E). \tag{2.43}$$

■

Next, we need to find an explicit expression for the inverse map $(\theta^*)^{-1}$. We have the following lemma.

Lemma 2.2: The map $(\theta^*)^{-1}: \theta^* L^2(\mathbb{R}^+) \mapsto L^2(\mathbb{R}^+)$ *is given, for any* $f \in \theta^* L^2(\mathbb{R}^+)$ *by*

$$[(\theta^*)^{-1} f](E) = [\mathbf{P}_{\mathbb{R}^+} f](E) + \frac{1}{2\pi} \int_{-\infty}^\infty \mathrm{d}s \int_{-\infty}^0 \mathrm{d}\sigma [\mathbf{P}_{\mathbb{R}^-} f](\sigma) \sigma^{-is-1/2} E^{is-1/2},$$

where $E \geqslant 0$, $\mathbf{P}_{\mathbb{R}^+}$ *and* $\mathbf{P}_{\mathbb{R}^-}$ *are the orthogonal projections of* $L^2(\mathbb{R})$ *on* $L^2(\mathbb{R}^+)$ *and* $L^2(\mathbb{R}^-)$, *respectively* [$L^2(\mathbb{R}^+)$ *and* $L^2(\mathbb{R}^-)$ *are considered as subspaces of* $L^2(\mathbb{R})$].

Proof: The procedure for constructing $(\theta^*)^{-1}$ is as follows: Given $y_+ \in H^+(\mathbb{R})$ in the range of θ^*, there is some vector $y \in L^2(\mathbb{R}^+)$ such that $\mathbf{I}y = y_+ + y_-$ [y_- is in $H^-(\mathbb{R})$] and Eq. (2.25) is valid. $y_-(\sigma)$ for $\sigma < 0$ are then the restriction to $\mathbb{R}^-$ of the values of some function $y_- \in H^-(\mathbb{R})$. Van Winter's theorem then implies that $y_- \in H^2(\overline{\Pi})$, and hence also $y_- \in H^-(\mathbb{R})$, can be uniquely reconstructed from its boundary value on the negative real axis. We conclude that, for each y_+ in the range of θ^* we can assign a unique $y_- \in H^-(\mathbb{R})$ such that Eq. (2.25) holds. Therefore, $y = y_+ + y_-$ can be identified with a unique element in $L^2(\mathbb{R}^+)$ corresponding to a given $y_+ \in \theta^* L^2(\mathbb{R}^+)$. This construction defines an inverse $(\theta^*)^{-1}$ such that

$$(\theta^*)^{-1} y_+ = y, \quad y_+ \in \theta^* L^2(\mathbb{R}^+), \quad y \in L^2(\mathbb{R}^+).$$

Observe that the main step in the procedure described above is the construction, through the Van Winter theorem, of a function $f \in H^2(\overline{\Pi})$ from data on the boundary value function of f on the negative real axis $\mathbb{R}^-$.

Given the boundary value function $\theta h \in L^2(\mathbb{R}^+)$ for a function $h \in H^2(\Pi)$, Van Winter's theorem implies that one can reconstruct the function $h \in H^2(\Pi)$ by using an inverse Mellin transform. We first find the Mellin transform

$$E(s) = \frac{1}{\sqrt{2\pi}} \int_0^\infty h(x) x^{is-1/2} \, dx \tag{2.44}$$

and then we reconstruct the analytic function via the inverse Mellin transform as follows:

$$h(re^{i\phi}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty E(s)(re^{i\phi})^{-is-1/2} \, ds, \quad z = re^{i\phi}, \quad r > 0, \quad 0 \leqslant \phi \leqslant \pi. \tag{2.45}$$

For a function $h \in H^2(\Pi)$, define a new function by $\tilde{h}(z) = \overline{h(\overline{z})}$, $\operatorname{Im} z < 0$. Then $\tilde{h} \in H^2(\overline{\Pi})$. In fact, each function $\tilde{h} \in H^2(\overline{\Pi})$ can be obtained from some function $h \in H^2(\Pi)$ by this procedure. From Eqs. (2.44) and (2.45) we obtain

$$\overline{E}(s) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \overline{h}(x) x^{-is-1/2} \, dx \tag{2.46}$$

and

$$\overline{h(\overline{re^{i\phi}})} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty \overline{E}(s)(re^{i\phi})^{is-1/2} \, ds, \quad z = re^{i\phi}, \quad r \geqslant 0, \quad -\pi \leqslant \phi \leqslant 0. \tag{2.47}$$

Denoting $\tilde{E}(s) = \overline{E}(s)$ and taking notice of the fact that $\tilde{h}(x) = \overline{h}(x)$ for real x, we can write Eq. (2.46) and Eq. (2.47) in the form

$$\tilde{E}(s) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \tilde{h}(x) x^{-is-1/2} \, dx \tag{2.48}$$

and

$$\tilde{h}(re^{i\phi}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty \tilde{E}(s)(re^{i\phi})^{is-1/2} \, ds, \quad z = re^{i\phi}, \quad r \geqslant 0, \quad -\pi \leqslant \phi \leqslant 0. \tag{2.49}$$

Using Eq. (2.48) and Eq. (2.49) we can reconstruct a function $\tilde{h} \in H^2(\overline{\Pi})$ from its boundary value function on $\mathbb{R}^+$. This is not quite our goal since we would like to reconstruct the function from its boundary value on the negative real axis $\mathbb{R}^-$. This problem, however, is solved by taking advantage

of the analyticity properties of $\tilde{h}$. Closing a contour integration in the lower half-plane we obtain (s is a real number)

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{0}\tilde{h}(x)x^{-is-1/2}\,dx+\frac{1}{\sqrt{2\pi}}\int_{0}^{\infty}\tilde{h}(x)x^{-is-1/2}\,dx=0$$

and hence

$$\tilde{E}(s)=-\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{0}\tilde{h}(x)x^{-is-1/2}\,dx. \tag{2.50}$$

Using Eq. (2.50) at the rhs of Eq. (2.49) and taking $\phi\to 0$ we obtain

$$\tilde{h}(x)=-\frac{1}{2\pi}\int_{-\infty}^{\infty}ds\int_{-\infty}^{0}dx'\,\tilde{h}(x')x'^{-is-1/2}x^{is-1/2},\quad x>0. \tag{2.51}$$

Given the boundary value on $\mathbb{R}^-$ of a function $\tilde{h}\in H^2(\overline{\Pi})$, Eq. (2.51) enables us to obtain its boundary value on $\mathbb{R}^+$. We can now construct the inverse map $(\theta^*)^{-1}$ according to the procedure described above. Given a function $h_+\in\theta^*L^2(\mathbb{R}^+)$ we have for, $E\geqslant 0$,

$$[(\theta^*)^{-1}h_+](E)=[\mathbf{P}_{\mathbb{R}^+}h_+](E)+\frac{1}{2\pi}\int_{-\infty}^{\infty}ds\int_{-\infty}^{0}d\sigma[\mathbf{P}_{\mathbb{R}^-}h_+](\sigma)\sigma^{-is-1/2}E^{is-1/2}. \tag{2.52}$$

This completes the proof of Lemma 2.2. ■

Equation (2.39), Lemma 2.1 and Lemma 2.2 imply Eq. (2.40) and Theorem 2.5 is proved. ■

Theorem 2.1, Theorem 2.4, and Theorem 2.5 provide the basic nesting structure for the description of quantum mechanical resonances. The fact that for each $t\geqslant 0$ the evolution $\mathbf{U}(t)$ transforms, both in the incoming contractive nesting and in the outgoing contractive nesting, into elements of $\{T_{u(t)}\}_{t\geqslant 0}$, the semigroup of Toeplitz operators on $H^+(\mathbb{R})$, suggests that the Sz.-Nagy–Foias theory, providing the basic mechanism of the Lax–Phillips scattering theory, may be used in the description of resonances. In particular, the Lax–Phillips semigroup in Eq. (1.20) may be used in the description of the time evolution of quantum mechanical resonances and the relation between resonances and second sheet poles of the S-matrix in the lower half-plane (or first sheet zeros of the S-matrix in the upper half-plane) may be shown in some cases to be a result of the Sz.-Nagy–Foias theory of contractions.

The following proposition indicates on the way the Sz.-Nagy–Foias theory may be used.

Proposition 2.4 (H^∞ case): Assume that in Eq. (2.38) $\tilde{\mathbf{S}}$: $L^2(\mathbb{R}^+)\mapsto L^2(\mathbb{R}^+)$ *is the boundary value on* $\mathbb{R}^+$ *of some function* $\mathcal{S}\in H^\infty(\Pi)$. *Suppose, furthermore, that* $\mathcal{S}$ *has a single, simple, zero at the point* $z=\overline{\mu}$, $\mathrm{Im}\,\mu<0$ *in* Π. *Let* $f_{\mathrm{in}}=\hat{\mathbf{\Omega}}_-f$ *and* $f_{\mathrm{out}}=\hat{\mathbf{\Omega}}_+f$ *for some* $f\in\mathcal{H}_{ac}$. *We have*

$$f_{\mathrm{out}}(\sigma)=[\mathbf{S}_{\mathrm{nest}}f_{\mathrm{in}}](\sigma)=\frac{\sigma-\overline{\mu}}{\sigma-\mu}[\mathbf{S}'_{\mathrm{nest}}f_{\mathrm{in}}](\sigma)-i2\,\mathrm{Im}\,\mu[\mathbf{P}_-\mathcal{S}'f_{\mathrm{in}}^-](\mu)\frac{1}{\sigma-\mu}, \tag{2.53}$$

where $f_{\mathrm{in}}^-\in H^-(\mathbb{R})$ *is such that* $\mathbf{P}_{\mathbb{R}^-}(f_{\mathrm{in}}+f_{\mathrm{in}}^-)=0$, $\mathbf{S}'_{\mathrm{nest}}=\theta^*\tilde{\mathcal{S}}'(\theta^*)^{-1}$, $\tilde{\mathcal{S}}'$ *is the boundary value on* $\mathbb{R}^+$ *of a function* $\mathcal{S}'\in H^\infty(\Pi)$ *and* $\mathcal{S}'$ *has no zeros in* Π.

Proof: We need first to consider the structure theory of H^p functions on the upper half-plane.[16,9] We have the following definition and subsequent theorem.

Definition (Blaschke product): A Blaschke product on the upper half-plane is an analytic function $b(z)$ *on* Π *of the form*

$$b(z)=\left(\frac{z-i}{z+i}\right)^m\prod_n\frac{|z_n^2+1|}{z_n^2+1}\cdot\frac{z-z_n}{z-\overline{z}_n}, \tag{2.54}$$

here m is a non-negative integer and z_n, $\mathrm{Im}\, z>0$, *are zeros of* $b(\cdot)$ *in* Π, *finite or infinite in number*.

Theorem 2.6: *If* $f\in H^p(\Pi)$ $(0<p\leqslant\infty)$ *and* $f\not\equiv 0$, *then* $f(\cdot)=b(\cdot)g(\cdot)$, *where* $g(\cdot)$ *is a non-vanishing* $H^p(\Pi)$ *function. The boundary value function of* $f(\cdot)$ *on* $\mathbb{R}$ *satisfies* $|g(x)|=|f(x)|$ *a.e.* $(x\in\mathbb{R})$. *The function* $b(\cdot)$ *is a Blaschke product of the form given in Eq. (2.54) and* z_n *are the zeros* $(z_n\neq i)$ *of* f *in* Π.

By the definition of a Blaschke product and Theorem 2.6, if the function $\mathcal{S}\in H^\infty(\Pi)$ has only a single zero in Π then it must be of the form

$$\mathcal{S}(z)=\frac{z-\overline{\mu}}{z-\mu}\mathcal{S}'(z),\quad \mathrm{Im}\, z>0,\quad \mathrm{Im}\,\mu<0, \tag{2.55}$$

where $\mathcal{S}'\in H^\infty(\Pi)$ has no zeros in Π. By assumption $\tilde{\mathbf{S}}$ is the boundary function of $\mathcal{S}$ on $\mathbb{R}^+$ and so

$$\tilde{\mathbf{S}}(E)=\frac{E-\overline{\mu}}{E-\mu}\mathcal{S}'(E),\quad E\geqslant 0. \tag{2.56}$$

Inserting this form of $\tilde{\mathbf{S}}$ into Eq. (2.40) we get

$$\begin{aligned}[\mathbf{S}_{\mathrm{nest}}f_{\mathrm{in}}](\sigma)=&\frac{1}{2\pi}\int_0^\infty \mathrm{d}E\frac{i}{\sigma-E+i0^+}\frac{E-\overline{\mu}}{E-\mu}\mathcal{S}'(E)[\mathbf{P}_{\mathbb{R}^+}f_{\mathrm{in}}](E)+\frac{1}{4\pi^2}\\&\times\int_0^\infty \mathrm{d}E\frac{i}{\sigma-E+i0^+}\frac{E-\overline{\mu}}{E-\mu}\mathcal{S}'(E)\int_{-\infty}^\infty \mathrm{d}s\int_{-\infty}^0 \mathrm{d}\sigma'[\mathbf{P}_{\mathbb{R}^-}f_{\mathrm{in}}](\sigma')\sigma'^{-is-1/2}E^{is-1/2}\end{aligned}$$

in the first integral we can change the integration interval to the negative real axis by using a contour integration in the upper half-plane [we recall that $H^\infty(\Pi)$ can be regarded as an algebra on $H^2(\Pi)$]. We get

$$\begin{aligned}\frac{1}{2\pi}\int_0^\infty \mathrm{d}E\frac{i}{\sigma-E+i0^+}\frac{E-\overline{\mu}}{E-\mu}\mathcal{S}'(E)[\mathbf{P}_{\mathbb{R}^+}f_{\mathrm{in}}](E)=&\frac{\sigma-\overline{\mu}}{\sigma-\mu}\mathcal{S}'(\sigma)f_{\mathrm{in}}(\sigma)\\&-\frac{1}{2\pi}\int_{-\infty}^0 \mathrm{d}E\frac{i}{\sigma-E+i0^+}\frac{E-\overline{\mu}}{E-\mu}\mathcal{S}'(E)[\mathbf{P}_{\mathbb{R}^-}f_{\mathrm{in}}](E).\end{aligned} \tag{2.57}$$

Since $f_{\mathrm{in}}\in\hat{\mathbf{\Omega}}^-\mathcal{H}_{ac}$ it is in the range of θ^* hence (see the proof of Theorem 2.5) there is some function $f_{\mathrm{in}}^-\in H^2(\overline{\Pi})$ such that $\mathbf{P}_{\mathbb{R}^-}(f_{\mathrm{in}}+f_{\mathrm{in}}^-)=0$. Using Eq. (2.51) we obtain

$$[\mathbf{P}_{\mathbb{R}^+}f_{\mathrm{in}}^-](E)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}s\int_{-\infty}^0 \mathrm{d}\sigma'[\mathbf{P}_{\mathbb{R}^-}f_{\mathrm{in}}](\sigma')\sigma'^{-is-1/2}E^{is-1/2},\quad E\geqslant 0. \tag{2.58}$$

Thus we get

$$[\mathbf{S}_{\mathrm{nest}}f_{\mathrm{in}}](\sigma)=\frac{\sigma-\overline{\mu}}{\sigma-\mu}\mathcal{S}'(\sigma)f_{\mathrm{in}}(\sigma)+\frac{1}{2\pi}\int_{-\infty}^\infty \mathrm{d}E\frac{i}{\sigma-E+i0^+}\frac{E-\overline{\mu}}{E-\mu}\mathcal{S}'(E)f_{\mathrm{in}}^-(E). \tag{2.59}$$

For the second term on the rhs of Eq. (2.59) we have the following decomposition:

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dE \frac{i}{\sigma - E + i0^+}\frac{E-\overline{\mu}}{E-\mu}\mathcal{S}'(E)f_{\text{in}}^-(E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dE \frac{i}{\sigma - E + i0^+}\frac{E-\overline{\mu}}{E-\mu}[(\mathbf{P}_+ + \mathbf{P}_-)\mathcal{S}'f_{\text{in}}^-](E)$$
$$= \frac{\sigma-\overline{\mu}}{\sigma-\mu}[\mathbf{P}_+\mathcal{S}'f_{\text{in}}^-](\sigma) - i2\ \text{Im}\ \mu[\mathbf{P}_-\mathcal{S}'f_{\text{in}}^-](\mu)\frac{1}{\sigma-\mu}. \tag{2.60}$$

The second equality on the rhs of Eq. (2.60) is obtained by making use of the properties of the projections $\mathbf{P}_+$ and $\mathbf{P}_-$ in order to close contour integrals in the upper, respectively, lower half-plane. Taking notice of the fact that $\mathcal{S}'$ is in $H^\infty(\Pi)$ and hence $\mathcal{S}'f_{\text{in}} \in H^+(\mathbb{R})$ we finally obtain

$$[\mathbf{S}_{\text{nest}}f_{\text{in}}](\sigma) = \frac{\sigma-\overline{\mu}}{\sigma-\mu}[\mathbf{P}_+\mathcal{S}'(f_{\text{in}} + f_{\text{in}}^-)](\sigma) - i2\ \text{Im}\ \mu[\mathbf{P}_-\mathcal{S}'f_{\text{in}}^-](\mu)\frac{1}{\sigma-\mu}. \tag{2.61}$$

Moreover, from the procedure for the construction of $(\theta^*)^{-1}$ it follows that $f_{\text{in}} + f_{\text{in}}^- = \mathbf{I}(\theta^*)^{-1}f_{\text{in}}$, so that $\mathbf{P}_+\mathcal{S}'(f_{\text{in}} + f_{\text{in}}^-) = \mathbf{P}_+\mathcal{S}'\mathbf{I}(\theta^*)^{-1}f_{\text{in}} = \mathbf{P}_+\mathbf{I}\tilde{\mathcal{S}}'(\theta^*)^{-1}f_{\text{in}} = \theta^*\tilde{\mathcal{S}}'(\theta^*)^{-1}f_{\text{in}}$ and the proof of Proposition 2.4 is complete.

■

The Blaschke factor B_μ defined by [see Eq. (2.54)]

$$B_\mu(z) = \frac{z-\overline{\mu}}{z-\mu} \tag{2.62}$$

is an inner function, hence we can define the subspace $\hat{\mathcal{K}}_\mu \subset H^+(\mathbb{R})$ by

$$\hat{\mathcal{K}}_\mu \equiv H^+(\mathbb{R}) \ominus B_\mu H^+(\mathbb{R}) \tag{2.63}$$

and the Lax–Phillips semigroup $\{\hat{\mathbf{Z}}(t)\}_{t\in\mathbb{R}^+}$ according to Eq. (1.20), i.e.,

$$\hat{\mathbf{Z}}(t) = T_{u(t)}|\hat{\mathcal{K}}_\mu. \tag{2.64}$$

The dimension of the subspace $\hat{\mathcal{K}}_\mu$ is one and, up to a multiplicative constant, the eigenvector $x_\mu \in \hat{\mathcal{K}}_\mu$ of $\hat{\mathbf{Z}}(t)$ is given by

$$x_\mu(\sigma) = \frac{1}{\sigma-\mu}. \tag{2.65}$$

Equation (2.53) can be written then in the form

$$f_{\text{out}} = B_\mu\mathbf{S}'_{\text{nest}}f_{\text{in}} - i2\ \text{Im}\ \mu[\mathbf{P}_-\mathcal{S}'f_{\text{in}}^-](\mu)x_\mu \tag{2.66}$$

and, using Eq. (2.5) we have, for $t \geqslant 0$,

$$\hat{\mathbf{\Omega}}_+\mathbf{U}(t)f = T_{u(t)}f_{\text{out}} = T_{u(t)}B_\mu\mathbf{S}'_{\text{nest}}f_{\text{in}} - i(2\ \text{Im}\ \mu[\mathbf{P}_-\mathcal{S}'f_{\text{in}}^-](\mu))\hat{\mathbf{Z}}(t)x_\mu$$
$$= T_{u(t)}B_\mu\mathbf{S}'_{\text{nest}}f_{\text{in}} - i(2\ \text{Im}\ \mu[\mathbf{P}_-\mathcal{S}'f_{\text{in}}^-](\mu))e^{-i\mu t}x_\mu. \tag{2.67}$$

Equation (2.67) can be interpreted as implying that in the outgoing nesting "representation" the zero of the *S*-matrix in the upper half-plane corresponds, through the mechanism of the Sz.-Nagy–Foias theory described in Sec. I, to a resonance for which the characteristic, exponentially decaying, evolution in time is given in terms of the action of a Lax–Phillips type semigroup. The resonance state is identified with the eigenvector x_μ of this semigroup. Equation (2.67) clearly exhibits the decomposition, in the nesting space $H^+(\mathbb{R})$, of the state $f_{\text{out}} = \hat{\mathbf{\Omega}}_+ f$ corresponding to an element $f \in \mathcal{H}_{ac}$, into a resonance part and a contribution coming from the subspace in $H^+(\mathbb{R})$ orthogonal to the resonance.

Define

$$\Lambda_{\hat{\mathbf{\Omega}}_+} = \hat{\mathbf{\Omega}}_+^* \hat{\mathbf{\Omega}}_+ \mathcal{H}_{ac} \subset \mathcal{H}_{ac}.$$

The set $\Lambda_{\hat{\mathbf{\Omega}}_+}$ is a linear space in $\mathcal{H}_{ac}$ which is dense in $\mathcal{H}_{ac}$. For an element g in $\Lambda_{\hat{\mathbf{\Omega}}_+}$ there is a unique element $h \in \mathcal{H}_{ac}$ such that $g = \hat{\mathbf{\Omega}}_+^* \hat{\mathbf{\Omega}}_+ h$. Then, for $t \geqslant 0$ and $f, g \in \Lambda_{\hat{\mathbf{\Omega}}_+}$ we have

$$\begin{aligned}(g, \mathbf{U}(t) f)_{\mathcal{H}_{ac}} &= (\hat{\mathbf{\Omega}}_+^* \hat{\mathbf{\Omega}}_+ h, \mathbf{U}(t) f)_{\mathcal{H}_{ac}} = (\hat{\mathbf{\Omega}}_+ h, \hat{\mathbf{\Omega}}_+ \mathbf{U}(t) f)_{H^+(\mathbb{R})} = (h_{\text{out}}, T_{u(t)} f_{\text{out}})_{H^+(\mathbb{R})} \\ &= (h_{\text{out}}, u(t) B_\mu \mathbf{S}'_{\text{nest}} f_{\text{in}})_{H^+(\mathbb{R})} - i2 \text{ Im } \mu [\mathbf{P}_- \mathcal{S}' f_{\text{in}}^-](\mu) (h_{\text{out}}, \hat{\mathbf{Z}}(t) x_\mu)_{H^+(\mathbb{R})} \\ &= (h_{\text{out}}, u(t) B_\mu \mathbf{S}'_{\text{nest}} f_{\text{in}})_{H^+(\mathbb{R})} - i2 \text{ Im } \mu [\mathbf{P}_- \mathcal{S}' f_{\text{in}}^-](\mu) e^{-i\mu t} (h_{\text{out}}, x_\mu)_{H^+(\mathbb{R})}, \end{aligned} \tag{2.68}$$

where $g = \hat{\mathbf{\Omega}}_+^* \hat{\mathbf{\Omega}}_+ h$, $h_{\text{out}} = \hat{\mathbf{\Omega}}_+ h$, and $u(t)$ is the unitary group defined in Eq. (1.14). Thus, on a dense set in $\mathcal{H}_{ac}$, matrix elements of the evolution can be calculated in the outgoing contractive nesting. The example of an H^∞ S-matrix gives a clear demonstration for the possible use of the Sz.-Nagy–Foias theory of contractions in the framework of quantum mechanical scattering problems.

III. COMMENTS—THE CONTRACTIVE CONTAINMENT OF HILBERT SPACES

Consider the following definition of a *bounded and contractive containment* of Hilbert space.[29]

Definition (bounded and contractive containment): If $\mathcal{H}_0$ is a Hilbert space, one says that another Hilbert space $\mathcal{H}_1$ is contained boundedly in $\mathcal{H}_0$ if it is a vector subspace of $\mathcal{H}_0$ and if the inclusion map of it into $\mathcal{H}_0$ is bounded. If the inclusion map is a contraction, one says that $\mathcal{H}_1$ is contained contractively in $\mathcal{H}_0$.

If $\mathbf{A}$ is a bounded operator from the Hilbert space $\mathcal{H}_1$ into the Hilbert space $\mathcal{H}_0$, then we define $\mathcal{M}(\mathbf{A}) \subset \mathcal{H}_0$ to be the range of $\mathbf{A}$ with the Hilbert space structure that makes $\mathbf{A}$ a coisometry from $\mathcal{H}_1$ onto $\mathcal{M}(\mathbf{A})$. Thus if x and y are vectors in $\mathcal{H}_1$ and if they are orthogonal to the kernel of $\mathbf{A}$ then

$$(\mathbf{A}x, \mathbf{A}y)_{\mathcal{M}(\mathbf{A})} = (x, y)_{\mathcal{H}_1}. \tag{3.1}$$

The space $\mathcal{M}(\mathbf{A})$ is contained boundedly in $\mathcal{H}_0$, and if $\mathbf{A}$ is a contraction from $\mathcal{H}_1$ into $\mathcal{H}_0$ then $\mathcal{M}(\mathbf{A})$ is contained contractively in $\mathcal{H}_0$. Every Hilbert space contained boundedly in $\mathcal{H}_0$ is such an operator range, since it is the range of the inclusion map of it into $\mathcal{H}_0$.

Another important notion is that of a *complementary space*.[29] If $\mathbf{A}$: $\mathcal{H}_1 \mapsto \mathcal{H}_0$ is a Hilbert space contraction, then $\mathcal{H}(\mathbf{A}) \equiv \mathcal{M}((1 - \mathbf{A}\mathbf{A}^*)^{1/2}) \subset \mathcal{H}_0$ is called the complementary space of $\mathcal{M}(\mathbf{A})$. If $\mathcal{M}(\mathbf{A})$ is an ordinary subspace, that is, if $\mathbf{A}$ is a partial isometry, then $\mathbf{A}\mathbf{A}^*$ and $1 - \mathbf{A}\mathbf{A}^*$ are complementary orthogonal projections, and $\mathcal{H}(\mathbf{A})$ is the ordinary orthogonal complement of $\mathcal{M}(\mathbf{A})$. If $\mathbf{A}$ is not a partial isometry then the intersection $\mathcal{M}(\mathbf{A}) \cap \mathcal{H}(\mathbf{A})$, called the *overlapping space*,[29] is nontrivial. In this case we have

$$\mathcal{M}(\mathbf{A}) \cap \mathcal{H}(\mathbf{A}) = \mathbf{A}\mathcal{H}(\mathbf{A}^*). \tag{3.2}$$

In addition we have

$$\mathcal{H}_0 = \mathcal{H}(\mathbf{A}) + \mathcal{M}(\mathbf{A}), \tag{3.3}$$

where is Eq. (3.3) vectors in $\mathcal{M}(\mathbf{A})$ and $\mathcal{H}(\mathbf{A})$ are considered as elements of $\mathcal{H}_0$.

Applying the definition above and the subsequent discussion to the nesting structure $(\mathcal{H}_{ac}, H^+(\mathbb{R}), \hat{\mathbf{\Omega}}_+)$ it is clear that $\mathcal{M}(\hat{\mathbf{\Omega}}_+) \subset H^+(\mathbb{R})$ is contractively contained in $H^+(\mathbb{R})$ [of course, the same statement is valid for $\mathcal{M}(\hat{\mathbf{\Omega}}_-) \subset H^+(\mathbb{R})$]. Moreover, since $\hat{\mathbf{\Omega}}_+$: $\mathcal{H}_{ac} \mapsto H^+(\mathbb{R})$ is injective, the scalar product in $\mathcal{M}(\hat{\mathbf{\Omega}}_+)$ defined in Eq. (3.1) can be written in the form

$$(x,y)_{\mathcal{M}(\hat{\mathbf{\Omega}}_+)} \equiv (\hat{\mathbf{\Omega}}_+^{-1}x, \hat{\mathbf{\Omega}}_+^{-1}y)_{\mathcal{H}_{ac}}. \tag{3.4}$$

Regarding $\hat{\mathbf{\Omega}}_+$ as a map from $\mathcal{H}_{ac}$ onto $\mathcal{M}(\hat{\mathbf{\Omega}}_+)$, equipped with the scalar product defined in Eq. (3.4), we find that it is unitary and $\mathcal{M}(\hat{\mathbf{\Omega}}_+)$ is a representation of $\mathcal{H}_{ac}$ [in terms of functions belonging to $H^+(\mathbb{R})$]. Since $\hat{\mathbf{\Omega}}_+$ is a contraction we can construct the complementary space $\mathcal{H}(\hat{\mathbf{\Omega}}_+) \subset H^+(\mathbb{R})$ by

$$\mathcal{H}(\hat{\mathbf{\Omega}}_+) = \mathcal{M}((1 - \hat{\mathbf{\Omega}}_+\hat{\mathbf{\Omega}}_+^*)^{1/2})$$

and Eq. (3.2) and Eq. (3.3) imply that

$$\mathcal{M}(\hat{\mathbf{\Omega}}_+) \cap \mathcal{H}(\hat{\mathbf{\Omega}}_+) = \hat{\mathbf{\Omega}}_+\mathcal{H}(\hat{\mathbf{\Omega}}_+^*) \neq \{0\} \tag{3.5}$$

and

$$H^+(\mathbb{R}) = \mathcal{H}(\hat{\mathbf{\Omega}}_+) + \mathcal{M}(\hat{\mathbf{\Omega}}_+). \tag{3.6}$$

We know that $\hat{\mathbf{\Omega}}_+\mathcal{H}_{ac}$ is dense in $H^+(\mathbb{R})$, hence for any $f \in H^+(\mathbb{R})$ there exists some sequence of elements $\{f_n\}_{n\in N}$, $f_n \in \mathcal{H}_{ac}$ such that

$$\lim_{n\to\infty} \|f - \hat{\mathbf{\Omega}}_+ f_n\|_{H^+(\mathbb{R})} = 0. \tag{3.7}$$

Observe that by the one to one correspondence between $\mathcal{H}_{ac}$ and $\mathcal{M}(\hat{\mathbf{\Omega}}_+)$, the continuity of $\hat{\mathbf{\Omega}}_+$ and its contractive property, if a sequence $\{f_n\}_{n\in N}$ of elements $f_n \in \mathcal{H}_{ac}$ converges to an element $f \in \mathcal{H}_{ac}$ we have

$$\lim_{n\to\infty} \|\hat{\mathbf{\Omega}}_+ f - \hat{\mathbf{\Omega}}_+ f_n\|_{H^+(\mathbb{R})} \leqslant \lim_{n\to\infty} \|f - f_n\|_{\mathcal{M}(\hat{\mathbf{\Omega}}_+)} = \lim_{n\to\infty} \|f - f_n\|_{\mathcal{H}_{ac}} = 0. \tag{3.8}$$

Hence all converging sequences in $\mathcal{H}_{ac}$ correspond, under the mapping $\hat{\mathbf{\Omega}}_+$, to sequences in $H^+(\mathbb{R})$ converging to elements in $\mathcal{M}(\hat{\mathbf{\Omega}}_+)$ *in the topology of the space* $H^+(\mathbb{R})$. Conversly, any element in $\mathcal{M}(\hat{\mathbf{\Omega}}_+)$, regarded as a subset of $H^+(\mathbb{R})$, corresponds (under the mapping by $\hat{\mathbf{\Omega}}_+$) to some sequence converging in $\mathcal{H}_{ac}$. Thus elements in $\mathcal{M}(\hat{\mathbf{\Omega}}_+)$ are associated with the existence of converging sequences in $\mathcal{H}_{ac}$. We conclude that elements in $H^+(\mathbb{R})$ that do not correspond (under the mapping by $\hat{\mathbf{\Omega}}_+$) to any converging sequence in $\mathcal{H}_{ac}$ are all in $\mathcal{H}(\hat{\mathbf{\Omega}}_+)\backslash\mathcal{M}(\hat{\mathbf{\Omega}}_+)$. In particular, resonances, which are not elements of $\mathcal{H}_{ac}$ and do not correspond to any converging sequence in $\mathcal{H}_{ac}$, always belong to the complementary space $\mathcal{H}(\hat{\mathbf{\Omega}}_+)$. In the discussion above of an S-matrix associated with an $H^\infty(\Pi)$ function this observation implies that the subspace $\hat{\mathcal{K}}_\mu$ containing the resonance has the property that $\hat{\mathcal{K}}_\mu \subset \mathcal{H}(\hat{\mathbf{\Omega}}_+)\backslash\hat{\mathbf{\Omega}}_+\mathcal{H}_{ac}$.

IV. CONCLUSIONS

This paper introduces an application of the Sz.-Nagy–Foias theory of contraction operators on Hilbert space for the description of resonances in quantum mechanical scattering problems for which the generator of evolution is bounded from below. This approach is based on the construction, in Sec. II above, of a framework analogous to that of the Lax–Phillips scattering theory. Thus, in this framework there exists an outgoing nesting structure, an incoming nesting structure and a nested S-matrix, which are analogous to the Lax–Phillips translation representations and the Lax–Phillips S-matrix, respectively. In the outgoing and incoming nesting structures the evolution is transformed, for times $t \geqslant 0$ into a continuous semigroup of Toeplitz operators. It was shown that, in the case that the original S-matrix is a bounded analytic function in the upper half-plane, its zeros in the upper half-plane (or poles of its analytic continuation to the lower half-plane) correspond to the existence of a subspace of the nesting space such that the (nested) evolution restricted

to this subspace defines a Lax–Phillips type semigroup providing the typical exponential decay behavior of the resonance. The relation between the zeros of the *S*-matrix and the eigenvalues of the generator of the semigroup are seen to be a result of the Sz.-Nagy–Foias theory of contractions. One may note, furthermore, that the two conditions for an appropriate description of a resonance, set in Sec. I, are formally satisfied. However, the interpretation of the resonance state [the eigenvector x_μ of the generator of the Lax–Phillips type semigroup $\{\hat{\mathbf{Z}}(t)\}_{t\geqslant 0}$ appearing in Eq. (2.68)] merits some additional investigation. The problem of interpretation amounts to the understanding of the contribution of the resonance to observable quantities. Since the resonance state is identified with a well defined closed subspace of the Hardy space, which is a Hilbert space, an appropriate interpretation can be achieved, in principle, by the transfer of the action of operators corresponding to quantum mechanical observables from the original Hilbert space to the Hardy space via the nesting maps. Associating matrix elements of observables to matrix elements of the transformed operators (in a manner similar to the treatment of the evolution in the present paper) should enable for the isolation of the contribution of the resonance. The question of interpretation of the resonance state as well as the natural question regarding the relation of the formalism developed in this paper to standard methods for the description of resonances, such as complex scaling, are best addressed through the analysis of simple concrete models using the framework introduced here and its comparison to the results of analysis by other methods. Such an analysis will be considered elsewhere.

The results presented in this work are limited in two obvious ways. The first is the fact that the nesting structures are constructed for scalar valued functions and the second stems from the fact that the appearance of the Lax–Phillips semigroup was shown under the assumption that the *S*-matrix is the boundary value function on $\mathbb{R}^+$ of an H^∞ function in the upper half-plane. An extension of the nesting framework to the case of an absolutely continuous spectrum of $\mathbf{H}_0$ and $\mathbf{H}$ with finite multiplicity seem to follow in a straightforward way from the framework developed here. More general cases may present additional difficulties.

Concerning the second difficulty raised above, it should be emphasized that the general framework developed in Sec. II, up to and including Theorem 2.5, exist regardless of any particular assumptions on the properties of the original *S*-matrix. More elaborate tools from operator theory may be invoked if more general assumptions, other than the simplifying assumption of an H^∞ *S*-matrix, are made. Possible extensions of the framework presented in this paper, along these lines, will be investigated elsewhere.

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Euclidean quantum mechanics in the momentum representation

Nicolas Privault[a)]
Département de Mathématiques, Université de La Rochelle, Avenue Michel Crépeau, 17042 La Rochelle, France

Jean-Claude Zambrini[b)]
Grupo de Física Matemática, Universidade de Lisboa, Avenida Prof. Gama Pinto 2, 1649-003 Lisboa, Portugal

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A time reversible probabilistic representation of solutions of the (Euclidean) Schrödinger equation in momentum representation is constructed using Lévy processes and bridges. Each diffusion in the position representation is associated with a jump diffusion in the momentum space. Our method can be looked upon as a rigorous version of Feynman's path integral approach. Several examples are studied. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1850178]

I. INTRODUCTION AND NOTATION

Feynman's path integral approach to quantum mechanics can be regarded as an informal reinterpretation of this theory in intrinsically stochastic terms. More than 50 years after its creation,[9] this approach has proved to be deep enough to provide basic insights into an amazing list of physical models, far beyond what could be anticipated originally. However, it is only "informal" because the (complex) probability measures on the various path spaces underlying Feynman's approach do not exist. Of course, a number of mathematical counterparts of such informal probability measures have been known, and used with profit, for a very long time (cf. Refs. 1,18, and references therein for historical perspectives on the issue and, in particular, on the role of the Trotter formula as a kind of alternative). The basic one, for configuration representation, is as old as quantum theory itself: it is Wiener measure, induced by Brownian motion. Its original (sample) path space, also named after Wiener, is of the form

$$\Omega_0 = \{\omega \in C(\mathbb{R}_+;\mathbb{R}^d) : \omega(0) = 0\},$$

and its relation with quantum theory appears in the famous Feynman–Kac formula[19]

$$(e^{-(t/\hbar)H}\chi^*)(q) = \int_{\Omega_0} \chi^*(\omega(t)+q)e^{-(1/\hbar)\int_0^t V(\omega(r)+q)\mathrm{d}r}\,\mathrm{d}P_W(\omega), \tag{1.1}$$

where $H=-(\hbar^2/2)\Delta+V$ is a lower bounded Hamiltonian observable on $L^2(\mathbb{R}^d)$, $V(q)$ a scalar potential, χ^* belongs to the dense domain $\mathcal{D}(H)$ of H in $L^2(\mathbb{R})$, $\hbar$ is the Planck constant, and P_W is the Wiener measure.

It is often more appropriate to consider path spaces on a compact time interval $[0,t]$ instead of $\mathbb{R}_+$, for instance

$$\Omega^{q,t} = \{\omega \in C([0,t];\mathbb{R}^d) : \omega(t) = q\}.$$

Then the Feynman–Kac formula becomes

a)Electronic mail: nprivaul@univ-lr.fr
b)Electronic mail: zambrini@cii.fc.ul.pt

$$(e^{-(t/\hbar)H}\chi^*)(q) = \int_{\Omega^{q,t}} \chi^*(\omega(0)) e^{-(1/\hbar)\int_0^t V(\omega(r))\mathrm{d}r}\, \mathrm{d}P_W(\omega). \tag{1.2}$$

The right-hand side of (1.2) is a legitimate path integral representation of the solution of the Cauchy problem in $L^2(\mathbb{R}^d)$,

$$\begin{aligned} -\hbar \frac{\partial \eta_t^*}{\partial t} &= H\eta_t^*, \\ \eta_0^*(q) &= \chi^*(q), \end{aligned} \tag{1.3}$$

regarded as counterpart of Feynman's one for Schrödinger equation,[10] resulting informally from the "Wick rotation" $t \to -it$ in (1.3). The representation (1.2) is the Euclidean (or imaginary time) viewpoint of Feynman's formula for the wave function ψ, too often considered as the only rigorous one. In relation with the physicists standard manipulations of paths integrals,[27] however, the representation (1.2) is not always appropriate. Indeed, in Feynman's framework, the configuration representation is only one of those where the path integral approach should apply successfully. What are the associated probabilistic counterparts of path integrals in momentum or energy representation, for example? We will really be able to claim that the mathematical content of Feynman's approach is under control when a general probabilistic construction valid in any representation, and providing at once the existence of all underlying probability measures, will be available (at least for a restricted class of potentials). This is, of course, still far from being the case.

Such a general construction would, presumably, also be a great advance to Stochastic Analysis itself[23] since it would provide as well new relations (Euclidean counterparts of quantum unitary transformations) between stochastic processes, or measures, usually regarded as unrelated in probability theory.

A probabilistic counterpart of Feynman's formula in configuration representation, distinct from (1.2), has been introduced in the mid-eighties (cf. Refs. 35,6, and references therein). It is founded on the elementary observation that the Feynman–Kac formula is just a conditional expectation, a concept never defined in quantum mechanics where only absolute expectations appear, and in a very specific manner. Precisely, for the quantum system with the same Hamiltonian as before,

$$\int_A \psi_t(q)\overline{\psi_t}(q)\mathrm{d}q, \tag{1.4}$$

is interpreted as the (unconditional or absolute) probability measure, for this system, to be in the Borelian A at time t, where $\overline{\psi}$ denotes the complex conjugate of the wave function ψ. Of course, the product form of the density in (1.4) is in fact independent of the representation.

Since various probabilistic interpretations of the solutions of (1.3) as conditional expectations are available, (1.4) suggests to look, among those, for a special class of diffusion processes whose absolute probability density is the product of positive solutions η_t^* of (1.3) and of positive solutions η_t of the equation,

$$\begin{aligned} \hbar \frac{\partial \eta_t}{\partial t} &= H\eta_t, \\ \eta_v(q) &= \chi(q), \end{aligned} \tag{1.5}$$

adjoint to (1.3) with respect to the time parameter on a compact time interval, say $t \in I=[r,v]$. Such diffusions are indeed well defined and it can be shown that their qualitative properties are much closer to what is needed to understand Feynman's approach than those of (1.2), cf. Refs. 6,7. In particular, they are time inhomogeneous but still time reversible. The above mentioned product

form of their probability at the time t becomes a mathematical expression of their reversibility (and their Markovian character, actually) since (1.5) can be interpreted as the time reversal of (1.3). In fact, the qualitative properties of these processes are so close to the quantum ones that they allow to understand, for example, fresh aspects of quantum symmetries in Hilbert space, generally ignored.[21,6]

The purpose of this paper is to show that the structure of this probabilistic construction (EQM, or Euclidean quantum mechanics) is preserved in momentum representation, suggesting that this structure is, somehow, independent of the representation. If this is indeed the case, a global mathematical picture of Feynman's path integral approach should be accessible, with a number of exciting consequences, both at the conceptual level of quantum physics and in the infinite dimensional analysis context of (Euclidean) quantum field theory. In this infinite dimensional context, the need for such a unification has been known for a long time in physics and in mathematics (cf. for instance, Refs. 27,13).

As observed by Feynman and Hibbs,[10] Sec. 5.1, it is expected that in momentum representation, the underlying stochastic processes belong to a special class of jump processes. In other words, and in contrast with the configuration representation, the elements ω of the momentum path space cannot be made continuous, in general, but at best continuous on the right.

The organization of our paper is as follows. Section II is devoted to a review of Lévy processes and the use of the Lévy–Khintchine representation to represent potentials. In Sec. III we present a summary of the relations between Lévy processes and pseudodifferential or Hamiltonian operators, and we show how to construct the two adjoint equations corresponding, in momentum representation, to (1.3) and (1.5). What plays the role of the Hamiltonian operator H in (1.3) and (1.5), is now a pseudodifferential operator, denoted by $\hat{H}$, whose explicit form depends, of course, on the scalar potential V in (1.1).

Section IV describes the construction of the new class of reversible diffusions with jumps $\hat{z}_t, t \in I$ (our "momentum process") whose absolute probability density at any time $t \in I$ is a product $\hat{\eta}_t^* \hat{\eta}_t$ of positive solutions of the two adjoint equations above. One way to describe them is to give the two stochastic integro-differential equations solved by $\hat{z}_t, t \in I$, whose coefficients depend exclusively on the two positive solutions $\hat{\eta}_t^*$ and $\hat{\eta}_t$ on I (Euclidean counterparts of the momentum wave function and its complex conjugate). The dual aspect of this construction is fundamental. In particular, two families of σ-algebras (or "filtrations") are necessary, here, for the description of $\hat{z}_t$ in $I=[r,v]$. Let us recall that traditional constructions of stochastic processes require only one such filtration, the nondecreasing family $(\mathcal{P}_t)$, generated by $\hat{z}_t, t \in I$, and describing its past (more precisely the set of all events whose occurrence can result from the observation of $\hat{z}_s, r \leqslant s \leqslant t$). The information about $\mathcal{P}_t$ is contained in the solutions $\hat{\eta}_t^*$ of the Cauchy problem for $\hat{H}$, given a positive initial condition $\hat{\eta}_r^*$. But we will need as well a nonincreasing filtration $\mathcal{F}_t$, describing the future of $\hat{z}_t$ on I. This will correspond to the information included in the solution $\hat{\eta}_t$ of the adjoint PDE, for a positive final condition $\hat{\eta}_v$. Another aspect of this duality can be expressed by saying that the resulting Markovian process $\hat{z}_t, t \in I=[r,v]$, is built from the data of two positive probability densities at the boundary ∂I of our time interval, say π_r and π_v, instead of the traditional initial probability density and a transition function. Our data of π_v is not contradictory, however, because $\hat{z}_t$ is the Markovian representative of a wider class of processes built from $\{\pi_r, \pi_v\}$, called Bernstein (or "local Markov," or "reciprocal," cf. Refs. 6,7) and satisfying the property

$$E[f(\hat{z}_t)|\mathcal{P}_s \vee \mathcal{F}_u] = E[f(\hat{z}_t)|\hat{z}_s, \hat{z}_u], \quad s < t < u, \tag{1.6}$$

for all f bounded measurable, where $E[\cdot|\mathcal{A}]$ denotes the conditional expectation given a σ-algebra $\mathcal{A}$. In other words, the knowledge of all the past $\mathcal{P}_s$ and the future $\mathcal{F}_u$ of the process is irrelevant to compute the conditional expectations; only the boundary values $\hat{z}_s, \hat{z}_u$ matter. Property (1.6) is more general than the Markov property but this one is sufficient for quantum physics, as shown by the product form of the integrand of (1.4).

Sections V and VI describe the dynamics of the momentum process $\hat{z}_t, t \in I$. Here, again, we follow Feynman's approach. His (unpublished) Princeton Ph.D. thesis was entitled "The least

action principle in quantum mechanics" and this principle can be regarded as a stationary phase method in infinite dimension.[1] In our probabilistic context some methods of controlled Markov processes can be adapted to our purpose. They provide a (stochastic) action functional, and in particular a Lagrangian, whose critical points are precisely the diffusion process with jumps constructed in Sec. IV. The method exploits the maximum principle for a class of PDEs which can be interpreted as quantum deformations of the classical Hamilton–Jacobi equation in momentum representation. The equations of motion of Sec. VI are the ones solved by the critical points of the action functional and provide the probabilistic version of the quantum Heisenberg equations in momentum representation. In this sense, the structure of the present construction is, indeed, the same as the one of the reinterpretation of Feynman's approach in configuration representation of Refs. 6 and 35. In particular, the study of the symmetries of this framework (not done here) should have interesting surprises in store as in the configuration representation.[6,33] A number of explicit examples illustrate our construction.

II. LÉVY–KHINTCHINE REPRESENTATION AND POTENTIALS

Let $V:\mathbb{R}^d\to\mathbb{C}$ with $V(0)\geqslant 0$ and such that e^{-tV} is continuous positive definite. In this case the function V admits the Lévy–Khintchine representation

$$V(q)=a+i\langle c,q\rangle+\frac{1}{2}\|q\|^2-\int_{\mathbb{R}^d\setminus\{0\}}(e^{-i\langle q,k\rangle}+i\langle q,k\rangle 1_{\{|k|\leqslant 1\}}-1)\,\nu(\mathrm{d}k), \tag{2.1}$$

where $k\in\mathbb{R}^d$ is called the wave vector, $a,c\in\mathbb{R}^d$, $\langle\cdot,\cdot\rangle$ denotes the scalar product in $\mathbb{R}^d$ with norm $\|\cdot\|$, and ν is a Lévy measure on $\mathbb{R}^d\setminus\{0\}$, i.e., ν satisfies $\int_{\mathbb{R}^d}(\|k\|^2\wedge 1)\,\nu(\mathrm{d}k)<\infty$. Note however that the above hypothesis on V is not satisfied by potentials of the form $V(q)=q^\alpha$ for $\alpha>2$, thus excluding quartic potentials in particular. See, e.g., Refs. 3,29 for background on Lévy processes. A stochastic process ξ_t, $t\geqslant 0$, defined on a probability space $(\Omega,\mathcal{P},P)$ is called a Lévy process if it has right continuous paths starting from the origin and its increments are independent and stationary:

(a) $P(\xi_0=0)=1$,
(b) for all $0\leqslant s\leqslant t$, $\xi_t-\xi_s$ is independent of $\mathcal{P}_s\subset\mathcal{P}$, the past filtration generated by all ξ_r, $r\leqslant s$,
(c) for all $0\leqslant s\leqslant t$, $\xi_t-\xi_s$ is equal in distribution to ξ_{t-s}.

The Lévy process ξ_t of characteristic exponent $V(q)$ is defined by

$$E[e^{-(i/\hbar)\langle\xi_t,q\rangle}]=e^{-(t/\hbar)V(q)},\quad q\in\mathbb{R}^d, \tag{2.2}$$

so that, from now on, the Lévy process ξ_t will have the units of the momentum $p=\hbar k$ and V, of course, the ones of a (potential) energy. Lévy processes form a large class of Markov processes, including the two most commonly used in mathematical physics: Brownian motion and the Poisson process.

The $\mathbb{R}^d$-valued process $\xi_t, t\in\mathbb{R}_+$, admits the following canonical ("Lévy–Itô") decomposition:

$$\xi_t=ct+W_t^\hbar+\int_0^t\int_{\{|k|>1\}}k\mu(\mathrm{d}k,\mathrm{d}s)+\int_0^t\int_{\{0<|k|\leqslant 1\}}k(\mu(\mathrm{d}k,\mathrm{d}s)-\nu(\mathrm{d}k)\mathrm{d}s), \tag{2.3}$$

where $W_t^\hbar=\hbar^{1/2}W_t$ is a Brownian motion with covariance $\hbar$, $\mu(\mathrm{d}k,\mathrm{d}s))$ is a Poisson random measure (or "canonical jump measure") counting the jumps $\Delta\xi_s=\xi_s-\xi_{s^-}$ (where $\xi_{s^-}=\lim_{r\nearrow s}\xi_r$), namely,

$$\mu(\mathrm{d}k,\mathrm{d}s)=\sum_{\Delta\xi_s\neq 0}\delta_{(\Delta\xi_s,s)}(\mathrm{d}k,\mathrm{d}s).$$

Notice that the jump process in (2.3) is independent of $W_t^\hbar$. The first Stieltjes integral in the decomposition (2.3) describes the sum of all large jumps (of size bigger than one) up to time t. It

is called a "compound Poisson process" and is of bounded variation, but may have no finite moments. The Poisson random measure $\mu(\mathrm{d}k,\mathrm{d}s)$ is determined by its compensator

$$\nu(\mathrm{d}k)\mathrm{d}s := E[\mu(\mathrm{d}k,\mathrm{d}s)]. \tag{2.4}$$

As a function of t, the jump process

$$M_t = \int_0^t \int_{\{0<|k|\leqslant 1\}} k(\mu(\mathrm{d}k,\mathrm{d}s) - \nu(\mathrm{d}k)\mathrm{d}s) \tag{2.5}$$

in (2.3) (the "compensated sum of small jumps") is a $\mathcal{P}_t$-martingale, i.e., it satisfies $E[|M_t|]<\infty$, $t\geqslant 0$, and

$$E[M_t|\mathcal{P}_s] = M_s, \quad a.s., \ 0\leqslant s\leqslant t. \tag{2.6}$$

If one takes the absolute expectation, the martingale property (2.6) implies that $t\mapsto E[M_t]$ is constant. A physically interesting example of martingale follows from the definition (2.2) of the characteristic exponent of ξ_t, indeed

$$\exp\left(-\frac{1}{\hbar}(iq\xi_t + tV(q))\right), \quad t>0, \tag{2.7}$$

is a $\mathcal{P}_t$-martingale. It has been shown in Euclidean quantum mechanics that most martingales play, in point of fact, the role of constants of the motion (cf. Refs. 6,21 and references therein).

Remarks:

(1) If $\hbar=0$ the only possible term of unbounded variation paths in (2.3) is the process (2.5) of small jumps. A criterion for bounded variation paths is

$$\int_{\mathbb{R}^d} (|k|\wedge 1)\nu(\mathrm{d}k) < \infty, \tag{2.8}$$

and, in this case, M_t can be decomposed as

$$M_t = \int_0^t \int_{\{0<|k|\leqslant 1\}} k\mu(\mathrm{d}k,\mathrm{d}s) - t\int_{\{|k|\leqslant 1\}} k\nu(\mathrm{d}k), \quad t>0.$$

Condition (2.8) may be verified even when $\nu(\mathbb{R}^d)=\infty$, i.e., when there are infinitely many jumps in any compact time interval. It follows also clearly from (2.1)–(2.3) that the paths $t\mapsto\xi_t$ are continuous if and only $\nu=0$.

(2) A formal expression of the Lévy–Itô decomposition (2.3), used later on when ν is symmetric, is

$$\xi_t = ct + W_t^{\hbar} + \int_0^t \int_{\mathbb{R}^d\setminus\{0\}} k\mu(\mathrm{d}k,\mathrm{d}s), \tag{2.9}$$

but it should be stressed that although the integrals in (2.3) of large and small jumps are convergent, the last term in (2.9) does not make sense in general.

(3) From (2.1) and (2.3) it is clear that, in such a framework, the Brownian motion W_t (in the purely diffusive case) has the characteristic exponent $V(q)=\frac{1}{2}\|q\|^2$. We could say as well that $W_t^{\hbar}$ corresponds to $V(q)=(\hbar/2)\|q\|^2$ but the first version is more natural for our purpose.

(4) Compound Poisson process.

Let Z_n, $n\in\mathbb{N}$, denote a sequence of independent identically distributed $\mathbb{R}^d$-valued random variables with common probability law μ_Z on $\mathbb{R}^d\setminus\{0\}$, and let N_t be a Poisson process with intensity $\gamma>0$, independent of all the Z_n, $n\in\mathbb{N}$. This means that $N_0=0$ and

$$P(N_t = n) = \frac{(\gamma t)^n}{n!} e^{-\gamma t}, \quad n \in \mathbb{N}.$$

Notice that the compensated Poisson process is $\tilde{N}_t = N_t - \gamma t$, so that $E[\tilde{N}_t] = 0$ and $E[\tilde{N}_t^2] = \gamma t$. The compound Poisson process is defined as

$$\xi_t = Z_1 + \cdots + X_{N_t}, \quad t \in \mathbb{R}_+.$$

It is a Lévy process with Lévy measure $\nu = \gamma \mu_Z$. The Lévy–Khintchine representation reduces here to

$$V(q) = \gamma \int_{\mathbb{R}^d \setminus \{0\}} (e^{-iqk} - 1) \mu_Z(\mathrm{d}k).$$

The paths of ξ_t are piecewise constant, and discontinuities occur only at random ("waiting") times

$$T_n = \inf\{t \geqslant 0 : \xi_t = n\}, \quad n \geqslant 1,$$

with $T_0 = 0$, and the jump sizes are random within the range of the Z_n. For example, reducing $\mu_Z(\mathrm{d}k)$, in the above Lévy–Khintchine formula, to $\delta_1(\mathrm{d}k)$, we recover the above elementary Poisson process $\xi_t = N_t$, with jumps of size +1 at each T_n. Those T_n are gamma distributed (see, e.g., Ref. 20), i.e., their probability density has the form

$$\gamma e^{-\gamma s} \frac{(\gamma s)^{n-1}}{(n-1)!} 1_{[0,\infty)}(s).$$

(5) One of the main difficulties in handling Lévy processes is that they can easily be of unbounded variation, i.e.,

$$\sum_{0 \leqslant s \leqslant t} |\Delta \xi_s| = \infty, \quad a.s. \tag{2.10}$$

However it is always true that

$$\sum_{0 \leqslant s \leqslant t} |\Delta \xi_s|^2 < \infty,$$

a.s., and this second property allows to control the problems due to (2.10), see, e.g., Ref. 2.

III. HAMILTONIANS AND PSEUDODIFFERENTIAL OPERATORS

We refer to the survey[15] and to the references therein for the notions summarized in this section on the links between Lévy processes and pseudodifferential operators. In order to proceed with the definition of pseudodifferential operators and the momentum representation, we need to introduce the Fourier transform

$$\mathcal{F}u(p) = \frac{1}{(2\pi\hbar)^{d/2}} \int_{\mathbb{R}^d} e^{-(i/\hbar)\langle p,q \rangle} u(q) \mathrm{d}q, \quad u \in \mathcal{S}(\mathbb{R}^d),$$

and its inverse

$$\mathcal{F}^{-1}v(q) = \frac{1}{(2\pi\hbar)^{d/2}} \int_{\mathbb{R}^d} e^{(i/\hbar)\langle p,q \rangle} v(p) \mathrm{d}p, \quad v \in \mathcal{S}(\mathbb{R}^d).$$

Given any (measurable) classical observable $f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ such that $q \mapsto f(p,q)$ is continuous with polynomial growth, the pseudodifferential operator with symbol $f(p,q)$ is defined as

$$f(p,i\hbar\nabla)u(p) = \frac{1}{(2\pi\hbar)^{d/2}}\int_{\mathbb{R}^d} e^{-(i/\hbar)\langle p,q\rangle} f(p,q)\mathcal{F}^{-1}u(q)\mathrm{d}q$$
$$= \mathcal{F}(f(p,\cdot)\mathcal{F}^{-1}u(\cdot))(p), \quad p \in \mathbb{R}^d, \quad u \in \mathcal{S}(\mathbb{R}^d).$$

In particular, the pseudodifferential operator $V(i\hbar\nabla)$, for V as in (2.1), satisfies

$$V(i\hbar\nabla)u(p) = au(p) - \hbar\langle c, \nabla u\rangle - \frac{\hbar^2}{2}\Delta u - \int_{\mathbb{R}^d}(u(p+\hbar k) - u(p) - \langle \hbar k, \nabla u(p)\rangle 1_{\{|k|\leqslant 1\}})\nu(\mathrm{d}k).$$

Let $(P_t)_{t\in\mathbb{R}_+}$ denote the Markov semigroup associated with the Lévy process $(\xi_t)_{t\in\mathbb{R}_+}$. This means that

$$\begin{aligned} P_t u(p) &= E[u(p+\xi_t)] \\ &= E[(\mathcal{F}\mathcal{F}^{-1}u)(p+\xi_t)] \\ &= \frac{1}{(2\pi\hbar)^{d/2}}\int_{\mathbb{R}^d} E\left[\exp\left(-\frac{i}{\hbar}\langle \xi_t, q\rangle - \frac{i}{\hbar}\langle p,q\rangle\right)\right]\mathcal{F}^{-1}u(q)\mathrm{d}q \\ &= \frac{1}{(2\pi\hbar)^{d/2}}\int_{\mathbb{R}^d} \exp\left(-\frac{t}{\hbar}V(q) - \frac{i}{\hbar}\langle p,q\rangle\right)\mathcal{F}^{-1}u(q)\mathrm{d}q \\ &= \exp\left(-\frac{t}{\hbar}V(i\hbar\nabla)\right)u(p), \quad u \in \mathcal{S}(\mathbb{R}^d), \quad t \in \mathbb{R}_+, \end{aligned}$$

hence the infinitesimal generator of the Markovian semigroup of $(\xi_t)_{t\in\mathbb{R}_+}$ is $-(1/\hbar)V(i\hbar\nabla)$.

We are only interested in real-valued scalar potentials $V(q)$, i.e., the following conditions are assumed to be satisfied from now on:

(H1) the constant c in (2.1) is equal to 0, and

(H2) ν is symmetric with respect to $k \mapsto -k$.

According to (2.1)–(2.3), (H1) says that our basic Lévy process has no constant drift and from (H2) its measure ν is invariant under time reversal, as it should be for any Hamiltonian observable in the class considered now. We shall also assume that the parameter a is zero, i.e., $V(0)=0$, without loss of generality from the physical point of view, since the energy is defined up to an additive constant. Hence, we shall restrict ourselves to V compatible with the Lévy–Khintchine representation

$$V(q) = \frac{1}{2}\|q\|^2 - \int_{\mathbb{R}^d\setminus\{0\}}(e^{-i\langle q,k\rangle} - 1)\nu(\mathrm{d}k), \tag{3.1}$$

and therefore for all $u \in \mathcal{S}(\mathbb{R})$,

$$V(i\hbar\nabla)u(p) = -\frac{\hbar^2}{2}\Delta u(p) - \int_{\mathbb{R}^d}(u(p+k) - u(p))\nu(\mathrm{d}k).$$

Notice that the conditions (H1) and (H2) imply that we could write as well

$$V(q) = \frac{1}{2}\|q\|^2 - \int_0^\infty (\cos(qk) - 1)\nu(\mathrm{d}k).$$

Then we would have

$$V(i\hbar\nabla)u(p) = -\frac{\hbar^2}{2}\Delta u(p) - \frac{1}{2}\int_0^\infty (u(p+\hbar k) - 2u(p) + u(p-\hbar k))\,\nu(\mathrm{d}k). \tag{3.2}$$

Consider any Hamiltonian H of the form

$$H = -\frac{\hbar^2}{2}\Delta_q + V(q) \tag{3.3}$$

and the associated Schrödinger equation in the position representation

$$i\hbar\frac{\partial\Phi}{\partial t}(q,t) = H\Phi(q,t) = -\frac{1}{2}\hbar^2\Delta_q\Phi(q,t) + V(q)\Phi(q,t).$$

The Euclidean version of this equation results from the substitution $t\mapsto it$,

$$\hbar\frac{\partial\eta_t}{\partial t}(q) = H\eta_t(q) = -\frac{1}{2}\hbar^2\Delta_q\eta_t(q) + V(q)\,\eta_t(q), \quad t\in[r,v]. \tag{3.4}$$

The equation adjoint to (3.4) is given by the substitution $t\mapsto -it$,

$$-\hbar\frac{\partial\eta_t^*}{\partial t}(q) = H\eta_t^*(q) = -\frac{1}{2}\hbar^2\Delta_q\eta_t^*(q) + V(q)\,\eta_t^*(q), \quad t\in[r,v]. \tag{3.5}$$

Let us define the Hamiltonian $\hat{H}=\mathcal{F}H\mathcal{F}^{-1}$ in momentum representation, i.e.,

$$\begin{aligned}\hat{H}\hat{\eta}_t(p) &= \mathcal{F}(H\mathcal{F}^{-1}\hat{\eta}_t)(p) = \frac{1}{2}\|p\|^2\hat{\eta}_t(p) + \mathcal{F}(V\mathcal{F}^{-1}\hat{\eta}_t)(p)\\ &= \frac{1}{2}\|p\|^2\hat{\eta}_t(p) + V(i\hbar\nabla)\hat{\eta}_t(p)\\ &= \frac{1}{2}\|p\|^2\hat{\eta}_t(p) - \frac{\hbar^2}{2}\Delta\hat{\eta}_t(p) - \int_{\mathbb{R}^d}(\hat{\eta}_t(p+\hbar k) - \hat{\eta}_t(p))\,\nu(\mathrm{d}k).\end{aligned} \tag{3.6}$$

Using this, the momentum representation of the Euclidean system described by (3.4) becomes

$$\hbar\frac{\partial\hat{\eta}_t}{\partial t}(p) = \hat{H}\hat{\eta}_t(p) = \frac{1}{2}\|p\|^2\hat{\eta}_t(p) + V(i\hbar\nabla)\hat{\eta}_t(p), \tag{3.7}$$

and $\eta, \hat{\eta}$ are linked by the relation $\hat{\eta}_t=\mathcal{F}\eta_t$. Similarly for equation (3.5),

$$-\hbar\frac{\partial\hat{\eta}_t^*}{\partial t}(p) = \hat{H}\hat{\eta}_t^*(p) = \frac{1}{2}\|p\|^2\hat{\eta}_t^*(p) + V(i\hbar\nabla)\hat{\eta}_t^*(p). \tag{3.8}$$

We call (somewhat improperly) integral kernel the kernel $h(t,p,u,\mathrm{d}l)$, $0<t<u$, $p,l\in\mathbb{R}^d$, associated with

$$e^{-(1/\hbar)(u-t)\hat{H}}f(p) = \int_{\mathbb{R}^d} f(l)h(t,p,u,\mathrm{d}l).$$

The following proposition shows how to compute the kernel $h(t,p,u,\mathrm{d}l)$ starting from the law μ_t of the Lévy process ξ_t at time t.

Proposition 3.1: For any $0<t<v$ and $p,l\in\mathbb{R}$ we have

$$h(t,p,u,\mathrm{d}l) = \alpha(u-t,p,l)\mu_{u-t}(-p+\mathrm{d}l), \tag{3.9}$$

where

$$\alpha(u-t,p,l) = E[e^{-(1/2\hbar)\int_0^{u-t}\|p+\xi_\tau\|^2\,\mathrm{d}\tau}\big|\xi_{u-t} = l-p],$$

and $\mu_{u-t}(-p+\mathrm{d}l)$ *denotes the image measure of* μ_{u-t} *under* $l\mapsto l+p$.

Proof: Since $-(1/\hbar)V(i\hbar\nabla)$ is the generator of $(\xi_t)_{t\in[0,u]}$, we have from the Feynman–Kac formula for Markov processes (see, e.g., Sec. III.19 of Ref. 28),

$$e^{-(1/\hbar)(u-t)\hat{H}}f(p) = E[f(\xi_u)e^{-(1/2\hbar)\int_t^u\|\xi_\tau\|^2\,\mathrm{d}\tau}\big|\xi_t = p] = E[f(p+\xi_{u-t})e^{-(1/2\hbar)\int_0^{u-t}\|p+\xi_\tau\|^2\,\mathrm{d}\tau}], \quad t<u,$$

where we used the stationarity of the increments of ξ_t. So, by definition of the integral kernel $h(t,p,u,\mathrm{d}l)$ and the Feynman–Kac formula,

$$\begin{aligned}\int_{\mathbb{R}^d} h(t,p,u,\mathrm{d}l)f(l) &= e^{-(1/\hbar)(u-t)\hat{H}}f(p)\\ &= E[f(\xi_{u-t}+p)e^{-(1/2\hbar)\int_0^{u-t}\|p+\xi_\tau\|^2\,\mathrm{d}\tau}]\\ &= \int_{\mathbb{R}^d} E[f(\xi_{u-t}+p)e^{-(1/2\hbar)\int_0^{u-t}\|p+\xi_\tau\|^2\,\mathrm{d}\tau}\big|\xi_{u-t}=l]\mu_{u-t}(\mathrm{d}l)\\ &= \int_{\mathbb{R}^d} f(p+l)E[e^{-(1/2\hbar)\int_0^{u-t}\|p+\xi_\tau\|^2\,\mathrm{d}\tau}\big|\xi_{u-t}=l]\mu_{u-t}(\mathrm{d}l)\\ &= \int_{\mathbb{R}^d} f(l)E[e^{-(1/2\hbar)\int_0^{u-t}\|p+\xi_\tau\|^2\,\mathrm{d}\tau}\big|\xi_{u-t}=l-p]\mu_{u-t}(-p+\mathrm{d}l).\end{aligned}$$

Consequently we obtain (3.9). ■

We are going to consider five one-dimensional examples in a detailed way, as illustrations of our approach.

Examples:

(1) $V(q)=(1-\cos(\alpha q))$, $\alpha>0$. This case corresponds to

$$\nu(\mathrm{d}k) = \tfrac{1}{2}(\delta_\alpha(\mathrm{d}k) + \delta_{-\alpha}(\mathrm{d}k))$$

in (2.1). By (3.6),

$$\hat{H}u(p) = \tfrac{1}{2}\|p\|^2u(p) - \tfrac{1}{2}\Delta_\alpha u(p),$$

where Δ_α denotes the discretized Laplace operator

$$\Delta_\alpha u(p) = \frac{u(p+\alpha)-2u(p)+u(p-\alpha)}{\alpha^2}.$$

The random jump measure is of the form

$$\mu(\mathrm{d}k,\mathrm{d}s) = \sum_{n=1}^{\infty}\delta_{(\alpha,T_n^1)}(\mathrm{d}k,\mathrm{d}s) + \delta_{(-\alpha,T_n^2)}(\mathrm{d}k,\mathrm{d}s),$$

where $(T_k^1)_{k\geqslant 1}$ and $(T_k^2)_{k\geqslant 1}$ are two independent sequences of Poissonian waiting times, with the same intensity $1/(2\alpha^2)$. The Lévy–Itô decomposition reduces here to the compensated sum of jumps. After introduction of ν and μ as above we find

$$\xi_t = \int_0^t \int_{\mathbb{R}} k(\mu(\mathrm{d}k,\mathrm{d}s) - \nu(\mathrm{d}k)\mathrm{d}s) = \alpha(N_t^1 - N_t^2),$$

where $(N_t^1)_{t\in\mathbb{R}_+}$ and $(N_t^2)_{t\in\mathbb{R}_+}$ are independent standard Poisson processes with intensity $1/(2\alpha^2)$ since (2.5) reduces to a sum, for $k=\pm\alpha$, of all jumps at the waiting times T_n^i, $i=1$, 2, up to the time t. As an illustration, let us check the property (2.4) of the compensator, in this special case. For any integrable f, we have, since T_n^1 and T_n^2 have the same distribution (cf. Remark 2):

$$\begin{aligned}
E\left[\int_0^t \int_{\mathbb{R}} f(k)\mu(\mathrm{d}k,\mathrm{d}s)\right] &= E\left[\sum_{k=1}^{\infty} \int_0^t \int_{\mathbb{R}} f(k)\,\delta_{(\alpha,T_k^1)}(\mathrm{d}k,\mathrm{d}s) + \int_0^t \int_{\mathbb{R}} f(k)\,\delta_{(-\alpha,T_k^2)}(\mathrm{d}k,\mathrm{d}s)\right] \\
&= E\left[\sum_{k=1}^{\infty} f(\alpha)1_{\{T_k^1\leqslant t\}} + f(-\alpha)1_{\{T_k^1\leqslant t\}}\right] \\
&= (f(\alpha)+f(-\alpha))\sum_{k=1}^{\infty} P(T_k^1 \leqslant t) \\
&= \frac{1}{2\alpha^2}(f(\alpha)+f(-\alpha))\sum_{k=1}^{\infty} \int_0^t e^{-s/(2\alpha^2)}\frac{(s/(2\alpha^2))^{k-1}}{(k-1)!}\mathrm{d}s \\
&= \frac{t}{2\alpha^2}(f(\alpha)+f(-\alpha)) = \int_0^t \int_{\mathbb{R}} f(k)\,\nu(\mathrm{d}k)\mathrm{d}s,
\end{aligned}$$

hence $E[\mu(\mathrm{d}k,\mathrm{d}s)] = \nu(\mathrm{d}k)\mathrm{d}s$, as claimed. Here we can compute

$$\begin{aligned}
e^{-(1/\hbar)t\hat{H}}f(p) &= E[f(p+\alpha(N_t^1 - N_t^2))e^{-(1/2\hbar)\int_0^t \|p+\alpha(N_\tau^1 - N_\tau^2)\|^2\,\mathrm{d}\tau}] \\
&= e^{-t}\sum_{k,l\geqslant 0}\left(\frac{1}{2}\right)^{k+l} f(p+\alpha(k-l)) \\
&\quad \times \int_0^t\int_0^{t_k}\cdots\int_0^{t_2}\int_0^t\int_0^{s_l}\cdots\int_0^{s_2} e^{-(1/2\hbar)\int_0^t \|p+\alpha(\sum_{i=1}^{k} i1_{[t_i,t]}(\tau)} \\
&\quad - \sum_{i=j}^{l} i1_{[s_j,t]}(\tau))\|^2\,\mathrm{d}\tau \mathrm{d}s_1\cdots\mathrm{d}s_l\,\mathrm{d}t_1\cdots\mathrm{d}t_k.
\end{aligned}$$

It is generally hard to solve difference equations like (3.7) for $\hat{H}$ given before. As an illustration, let us observe that the solution of its time independent version, namely the stationary equation associated with (3.7),

$$\frac{p^2}{2}u(p) - \frac{1}{2}(u(p+1)+u(p-1)-2u(p)) = Eu(p),$$

is given, for $u(0)=u_0$ and $u(1)=u_1$, by

$$\begin{aligned}
u(p) = &-\frac{(-2)^{p+1}(au_1 - u_1\sqrt{a^2-4} + a^2u_0 - au_0\sqrt{a^2-4} - 2u_0)}{(a-\sqrt{a^2-4})^{p+2}\sqrt{a^2-4}} \\
&+ \frac{(-2)^{p+1}(au_1 + u_1\sqrt{a^2-4} + a^2u_0 + au_0\sqrt{a^2-4} - 2u_0)}{(a+\sqrt{a^2-4})^{p+2}\sqrt{a^2-4}} \\
&+ \frac{(a+\sqrt{a^2-4})^{p+1} + (a-\sqrt{a^2-4})^{p+1}}{(-2)^{p+1}(a+2)^2} + \frac{a-(a+2)(p^2+8p+12)}{(a+2)^2},
\end{aligned}$$

with $a=E+2$ (computation done using the command rsolve in Maple).

(2) Harmonic oscillator: $V(q)=\frac{1}{2}\|q\|^2$. This is the case $\nu(\mathrm{d}k)=0$ in (2.1), and

$$\hat{H}u(p)=\frac{1}{2}\|p\|^2u(p)-\frac{\hbar^2}{2}\Delta u(p).$$

Clearly, the Lévy–Itô decomposition reduces to $\xi_t=W_t^{\hbar}$, i.e., the underlying Lévy process is a Brownian motion (with variance $\hbar$). Notice that this case can be regarded as the limit $\alpha\searrow 0$ of Example 1.

(3) $V(q)=c\|q\|^{\alpha}$, $c>0$, $\alpha\in(0,2]$. Then

$$\nu(\mathrm{d}k)=\begin{cases}0, & \text{when } \alpha=2 \text{(this is the case in Example 2)},\\ \dfrac{c_\alpha}{|k|^{1+\alpha}}\mathrm{d}k, & \text{when } \alpha\neq 2,\end{cases}$$

where $c_\alpha>0$ depends on the value of α. The associated Lévy process is called a "stable process of order α" (and α its "index of stability"). Recall that by (2.2), the existence of moments of order up to $n\geqslant 1$ for ξ_t implies the nth differentiability of $V(q)$ at $q=0$, the converse being true for moments of even order, see, e.g., Ref. 32, Theorem 1, p. 278. In particular, α-stable distributions on $\mathbb{R}$ have finite mean if and only if $\alpha>1$.

Those processes are important because of their rotational invariance (in dimension $d>1$) and also because they are self-similar. Recall that a stochastic process Z_t is self-similar with Hurst index $H>0$ if, $\forall a\geqslant 0$, Z_{at} and a^HZ_t, $t\geqslant 0$, have same finite-dimensional distributions (we refer to Ref. 8 for more about self-similar processes). In particular the stable process $(\xi_t)_{t\geqslant 0}$ of order α is self-similar with Hurst index $1/\alpha$, i.e., we have $\xi_{at}=a^{1/\alpha}\xi_t$, $a\geqslant 0$. For such processes the Hamiltonian (3.6) becomes

$$\hat{H}u(p)=\tfrac{1}{2}\|p\|^2u(p)-c\hbar^{\alpha}\Delta^{\alpha/2}u(p),$$

involving the fractional power of the Laplacian, a highly nonlocal operator, often linked with relativistic Hamiltonians, cf. Ref. 14. When $\alpha=2$, i.e., in the case of the Brownian motion $W_t^{\hbar}$ appearing in (2.3), this scaling property can be traced back to one of the "isovectors" of the symmetry group of the classical heat equation (1.5) for the free Hamiltonian $H_0=-(\hbar^2/2)\Delta$, cf. Ref. 21.

(4) $V(q)=(1/a^2)\log\cosh aq$, $a>0$. The Lévy measure is of the form

$$\nu(\mathrm{d}k)=\frac{1}{2a^2}\frac{\mathrm{d}k}{k\sinh(k\pi/(2a))},$$

see, e.g., Refs. 5,12,30 [note that in Eq. (2) of Ref. 12 as well as in Eq. (4) of Ref. 5, cosh should be replaced by sinh]. Notice that in the limit $a\searrow 0$ this measure reduces to 0, and the potential V becomes the harmonic one of Example 2. The associated process ξ_t is called Meixner process,[24] and its Lévy–Itô decomposition has no diffusive part. Its expectation and variance are, respectively, given by $E[\xi_t]=0$, $E[\xi_t^2]=t$, $t>0$. The corresponding Hamiltonian is

$$\hat{H}u(p)=\frac{1}{2}\|p\|^2u(p)-\frac{1}{2a^2}\int_{\mathbb{R}^d\setminus\{0\}}(u(p+\hbar k)-u(p))\frac{\mathrm{d}k}{k\sinh(k\pi/(2a))}.$$

(5) $V(q)=(1/a^2)\log(1+a^2q^2)$, $a>0$. The Lévy measure

$$\nu(\mathrm{d}k)=\frac{1}{a^2|k|}e^{-|k|/a}\,\mathrm{d}k$$

is one of the (symmetric) variance gamma process (cf., for instance, Ref. 22), whose expectation and variance are, respectively, $E[\xi_t]=0$, $E[\xi_t^2]=2t$, $t>0$. Notice that when the param-

eter a is large the exponential decay of $\nu(\mathrm{d}k)$ is lower around zero and so the probability of large jumps increases. According to Remark 2, the paths of the variance gamma process are of bounded variation. This process has no continuous martingale component but is a pure jump process with infinite number of jumps in any compact time interval. Of course the associated Hamiltonian operator is given by

$$\hat{H}u(p) = \frac{1}{2}\|p\|^2 u(p) - \frac{1}{a^2}\int_{\mathbb{R}\setminus\{0\}} (u(p+\hbar k) - u(p))\frac{e^{-|k|/a}}{|k|}\mathrm{d}k.$$

As in Example 4, this case reduces to the harmonic one when $a \searrow 0$.

Before explaining how the existence of the relevant class of Bernstein processes can be proved, let us introduce some notation and assumptions. In the sequel we make the absolute continuity hypothesis, with an obvious abuse of notation,

$$h(t,p,u,\mathrm{d}l) = h(t,p,u,l)\lambda(\mathrm{d}l), \quad \lambda(\mathrm{d}p) - a\,.\,e\,., \tag{3.10}$$

$0<t<u$, $p,l \in \mathbb{R}^d$, where λ denotes a given reference measure. In particular, for $r \leqslant t \leqslant v$, we have

$$\hat{\eta}_t^*(p) = e^{-(1/\hbar)(t-r)\hat{H}}\hat{\eta}_r^*(p) = \int_{\mathbb{R}^d} \hat{\eta}_r^*(i)h(r,i,t,p)\lambda(\mathrm{d}i)$$

and

$$\hat{\eta}_t(p) = e^{-(1/\hbar)(v-t)\hat{H}}\hat{\eta}_v(p) = \int_{\mathbb{R}^d} \hat{\eta}_v(m)h(t,p,v,m)\lambda(\mathrm{d}m).$$

This condition is satisfied, for example, if

(i) the law of $\xi_t, t>0$, has a density with respect to Lebesgue measure, e.g., in the case of stable processes (see Example 3) and for Lévy processes with Brownian component, or

(ii) $\mu_{t-s}(-j+\mathrm{d}p)$ has a density with respect to $\lambda(\mathrm{d}p), \lambda(\mathrm{d}j)$, a.e. In particular this will follow from Proposition 3.1 if λ is absolutely continuous under the translation $p \mapsto j+p$, $\lambda(\mathrm{d}j)$, a.e., and μ_{t-s} is absolutely continuous with respect to λ,

$$\mu_{t-s}(\mathrm{d}p) = \mu_{t-s}(p)\lambda(\mathrm{d}p).$$

This is the case in particular for the symmetric Poisson process of Example 1 with $\lambda(\mathrm{d}p) = \Sigma_{n=-\infty}^{\infty}\delta_{\alpha\times n}(\mathrm{d}p)$.

Note that we have $h(s,j,t,p) = h(t,p,s,j)$, since $\hat{H}$ that is symmetric with respect to λ.

IV. MOMENTUM REPRESENTATION AND BERNSTEIN–LÉVY PROCESSES

This section summarizes the existence results for Bernstein processes established in Ref. 25. Let $\hat{\eta}_r^*, \hat{\eta}_v : \mathbb{R}^d \to \mathbb{R}_+$ be two λ-a.e. strictly positive initial and final conditions of (1.3) and (1.5), respectively, such that for some $t \in I = [r,v]$, and therefore for any such t,

$$\int_{\mathbb{R}^d} \hat{\eta}_t^*(p)\,\hat{\eta}_t(p)\lambda(\mathrm{d}p) = 1. \tag{4.1}$$

As explained in the introduction, this relation will be interpreted as a Euclidean version of Born's probabilistic interpretation of the wave function in momentum representation. More precisely, and since no specific relation between $\hat{\eta}_t^*$ and $\hat{\eta}_t$ is needed for the last identity to make sense, (4.1) will be regarded as the Euclidean counterpart of the time invariance of any transition amplitudes in Feynman's approach. So the following result shows in particular that, quite in contrast with the

quantum case, this Euclidean (Born) probabilistic interpretation of the wave function in momentum representation is mathematically justifiable.

Theorem 4.1: (Ref. 25) *There exists a* $\mathbb{R}^d$*-valued process* $(\hat{z}_t)_{t\in[r,v]}$ *whose probability density at time* t *with respect to* λ *is precisely given by the product*

$$\rho_t(p) = \hat{\eta}_t^*(p)\,\hat{\eta}_t(p).$$

This process $(\hat{z}_t)_{t\in[r,v]}$ *is both forward and backward Markovian, with forward transition probability kernel, for* $r<s<t<u<v$ *and* $j,p,l\in\mathbb{R}^d$*, given by*

$$\hat{\mathrm{p}}(t,p,u,l) = \frac{\hat{\eta}_u(l)}{\hat{\eta}_t(p)}h(t,p,u,l), \tag{4.2}$$

and backward transition probability kernel

$$\hat{\mathrm{p}}^*(s,j,t,p) = \frac{\hat{\eta}_s^*(j)}{\hat{\eta}_t^*(p)}h(s,j,t,p). \tag{4.3}$$

In particular, the initial and final laws of $(\hat{z}_t)_{t\in[r,v]}$ are of the form

$$\pi_r(\mathrm{d}i) = \hat{\eta}_r(i)\,\hat{\eta}_r^*(i)\lambda(\mathrm{d}i) \quad \text{and } \pi_v(\mathrm{d}m) = \hat{\eta}_v(m)\,\hat{\eta}_v^*(m)\lambda(\mathrm{d}m).$$

In fact, if $h(s,j,t,p)$ is continuous in (j,p) and strictly positive for all $0<s<t$, Theorem 1 of Ref. 4 (see also Theorem 3.2 of Ref. 17, and Theorem 3.4 of Ref. 35) state that given any two strictly positive probability densities $\pi_r(i)$ and $\pi_v(m)$, it is indeed possible to find two strictly positive functions $\hat{\eta}_r^*$, $\hat{\eta}_v:\mathbb{R}^d\to\mathbb{R}_+$ such that

$$\pi_r(i) = \hat{\eta}_r^*(i)\,\hat{\eta}_r(i), \quad \pi_v(m) = \hat{\eta}_v(m)\,\hat{\eta}_v^*(m).$$

A posteriori, $\hat{\eta}_r^*$ and $\hat{\eta}_v$ can, therefore, be interpreted as (positive) initial and final boundary conditions of the two underlying adjoint equations (1.3) and (1.5). The resulting process $(\hat{z}_t)_{t\in[r,v]}$ is a (Markovian) Bernstein process (cf. Ref. 7, for example). As observed in (1.6) this means in particular that

$$P(\hat{z}_t\in\mathrm{d}p|\mathcal{P}_s\vee\mathcal{F}_u) = P(\hat{z}_t\in\mathrm{d}p|\hat{z}_s,\hat{z}_u),$$

and that the joint law $P(\hat{z}_r\in A,\hat{z}_v\in B)$, for A,B two Borelians of $\mathbb{R}^d$, has the special form

$$P(\hat{z}_r\in A,\hat{z}_v\in B) = \int_{A\times B}\hat{\eta}_r^*(i)h(r,i,v,m)\,\hat{\eta}_v(m)\lambda(\mathrm{d}i)\lambda(\mathrm{d}m).$$

Conversely, we also have a uniqueness result, i.e., if $(\hat{z}_t)_{t\in[r,v]}$ is a Markovian Bernstein process with Bernstein kernel $h(s,j,t,\mathrm{d}p,u,l)=P(\hat{z}_t\in\mathrm{d}p\,|\,\hat{z}_s=j,\hat{z}_u=l)$ (cf. Refs. 7,25) such that

$$h(s,j,t,\mathrm{d}p,u,l)h(s,j,u,l) = h(s,j,t,p)h(t,p,u,l)\lambda(\mathrm{d}p),$$

$s\leqslant t\leqslant u$ and $j,p,\ l\in\mathbb{R}^d$, then there exist positive density functions $\hat{\eta}_r^*(i)$ and $\hat{\eta}_v(m)$ such that

$$P(\hat{z}_r\in A,\hat{z}_v\in B) = \int_{A\times B}\hat{\eta}_r^*(i)h(r,i,v,m)\,\hat{\eta}_v(m)\lambda(\mathrm{d}i)\lambda(\mathrm{d}m),$$

see Theorem 7.1 in Ref. 25. The processes $(\hat{z}_t)_{t\in[r,v]}$ resulting from the construction of Theorem 4.1 can be regarded as generalizations of the usual concept of Markovian bridges (cf., for example, Ref. 6 in the more familiar case of diffusion processes), which corresponds to Dirac boundary conditions at the boundary of the time interval $[r,v]$. In contrast, here, we allow for any (λ-a.e. strictly positive) probability densities π_r and π_v. We shall give a description of Markovian bridges of Theorem 4.1 in terms of forward and backward stochastic integro-differential equations driven

by the Lévy process $(\xi_t)_{t\in[r,v]}$ of Sec. II. Let us recall that, for stochastic equations, the analog of classical solutions of integro-differential equations is called a strong solution (in this case the solution is a process). It requires, indeed, strong regularity conditions on the coefficients of the equation, for example Lipschitz conditions for stochastic differential equations. When more general coefficients are needed, there is a concept of weak solution, where one looks for a unique process with the proper set of finite-dimensional distributions (cf. Ref. 16 for instance). Then the solution is a probability measure. Let z_{t^-}, respectively, z_{t^+}, denote the left, respectively, the right, limit of z_t at $t\in[r,v]$.

The proof of the next Proposition 4.2 relies on Lemma 4.3 below, (cf. Ref. 25) which gives the forward and backward generators of the process $(\hat{z}_t)_{t\in I}$ constructed in Theorem 4.1. Indeed, the knowledge of the generators of $(\hat{z}_t)_{t\in I}$ provides the forward and backward representations (4.4) and (4.5) of $(\hat{z}_t)_{t\in I}$ as weak solutions of stochastic integro-differential equations, using Theorem 13.58, Theorem 14.80 of Ref. 16, pp. 438 and 481, and references therein. In order for these representations to hold, we need to assume that the conditions given on p. 434 of Ref. 16 are fulfilled:

(H3) The functions

$$(t,p)\mapsto \int_{\mathbb{R}^d}(1\wedge\|k\|^2)\frac{\hat{\eta}_t(p+\hbar k)}{\hat{\eta}_t(p)}\nu(\mathrm{d}k),$$

$$(t,p)\mapsto \int_{\{0<|k|\leqslant 1\}}k\frac{\hat{\eta}_t(p+\hbar k)-\hat{\eta}_t(p)}{\hat{\eta}_t(p)}\nu(\mathrm{d}k),$$

$$(t,p)\mapsto \nabla\ \log\ \hat{\eta}_t(p),$$

(H4) as well as

$$(t,p)\mapsto \int_{\mathbb{R}^d}(1\wedge\|k\|^2)\frac{\hat{\eta}^*_t(p-\hbar k)}{\hat{\eta}^*_t(p)}\nu(\mathrm{d}k),$$

$$(t,p)\mapsto \int_{\{0<|k|\leqslant 1\}}k\frac{\hat{\eta}^*_t(p-\hbar k)-\hat{\eta}^*_t(p)}{\hat{\eta}^*_t(p)}\nu(\mathrm{d}k),$$

$$(t,p)\mapsto \nabla\ \log\ \hat{\eta}^*_t(p),$$

are bounded on compacts of $\mathbb{R}_+\times\mathbb{R}^d$.

Proposition 4.2: *The process $(\hat{z}_t)_{t\in[r,v]}$ is solution, in the weak sense and with respect to the forward filtration $(\mathcal{P}_t)_{t\in[r,v]}$, of*

$$\mathrm{d}\hat{z}_t=\mathrm{d}W^{\hbar}_t+\int_{\mathbb{R}^d}k\mu(\mathrm{d}k,\mathrm{d}t)+\hbar\ \nabla\ \log\ \hat{\eta}_t(\hat{z}_{t^-})\mathrm{d}t, \tag{4.4}$$

under a probability P for which $W^{\hbar}_t$ is a (forward) Brownian motion with variance $\hbar$, and $\mu(\mathrm{d}k,\mathrm{d}s)$ is the canonical point measure with compensator $[\hat{\eta}_t(\hat{z}_{t^-}+\hbar k)/\hat{\eta}_t(\hat{z}_{t^-})]\nu(\mathrm{d}k)\mathrm{d}t$.

In terms of backward differentials, $(\hat{z}_t)_{t\in[r,v]}$ solves weakly, with respect to the decreasing filtration $(\mathcal{F}_t)_{t\in[r,v]}$:

$$\mathrm{d}_*\hat{z}_t = \mathrm{d}_*W_t^{\hbar *} + \int_{\mathbb{R}^d} k\mu_*(\mathrm{d}k,\mathrm{d}t) - \hbar\,\nabla\,\log\,\hat{\eta}_t^*(\hat{z}_{t^+})\mathrm{d}t, \tag{4.5}$$

where $W_t^{\hbar *}$ denotes a backward Brownian motion with variance $\hbar$, and $\mu_*(\mathrm{d}k,\mathrm{d}t)$ is the backward Poisson random measure with compensator $[\hat{\eta}_t^*(\hat{z}_{t^+}-\hbar k)/\hat{\eta}_t^*(\hat{z}_{t^+})]\nu(\mathrm{d}k)\mathrm{d}t$. In (4.4) and (4.5), $(\hat{z}_t)_{t\in[r,v]}$ represents the process (associated with our system in the momentum representation) whose probability density is of the form $\rho_t(p)$, as in Theorem 4.1. Let us define for $f\in\mathcal{S}(\mathbb{R}^d)$ and $g:\mathbb{R}^d\mapsto(0,\infty)$ the integro differential operator $\mathcal{L}_g$ by

$$\mathcal{L}_g f(p) = \frac{\hbar}{2}\Delta f(p) + \frac{1}{\hbar}\int_{\mathbb{R}^d}(f(p+\hbar k)-f(p))\frac{g(p+\hbar k)}{g(p)}\nu(\mathrm{d}k) + \hbar\langle\nabla\,\log g(p),\,\nabla f(p)\rangle. \tag{4.6}$$

The forward and backward generators $\mathcal{L}_{\hat{\eta}_t}$ and $-\mathcal{L}_{\hat{\eta}_t^*}$ of $(\hat{z}_t)_{t\in I}$ are given from the next lemma.

Lemma 4.3: *The kernels* $\hat{\mathrm{p}}(t,p,u,l)$ *and* $\hat{\mathrm{p}}^*(s,j,t,p)$ *defined in* (4.2) and (4.3) *satisfy the partial integro-differential (Kolmogorov forward or Fokker–Planck) equations*

$$\frac{\partial\hat{\mathrm{p}}}{\partial u}(t,p,u,l) = (\mathcal{L}_{\hat{\eta}_u})_l^\dagger\hat{p}(t,p,u,l), \tag{4.7}$$

where † *denotes the adjoint,* $\mathcal{L}_{\hat{\eta}_s}$ *is the forward generator given by*

$$\mathcal{L}_{\hat{\eta}_s} f = \frac{\hbar}{2}\Delta f(p) + \frac{1}{\hbar}\int_{\mathbb{R}^d}(f(p+\hbar k)-f(p))\frac{\hat{\eta}_t(p+\hbar k)}{\hat{\eta}_t(p)}\nu(\mathrm{d}k) + \hbar\langle\nabla\,\log\,\hat{\eta}_t(p),\,\nabla f(p)\rangle, \tag{4.8}$$

and

$$\frac{\partial\hat{\mathrm{p}}^*}{\partial s}(s,j,t,p) = -(\mathcal{L}_{\hat{\eta}_s^*})_j^\dagger\hat{\mathrm{p}}(s,j,t,p),$$

where $-\mathcal{L}_{\hat{\eta}_s^*}$ *is the backward generator given by*

$$-\mathcal{L}_{\hat{\eta}_s^*} f = -\frac{\hbar}{2}\Delta f(p) - \frac{1}{\hbar}\int_{\mathbb{R}^d}(f(p+\hbar k)-f(p))\frac{\hat{\eta}_t^*(p+\hbar k)}{\hat{\eta}_t^*(p)}\nu(\mathrm{d}k) - \hbar\langle\nabla\,\log\,\hat{\eta}_t^*(p),\,\nabla f(p)\rangle. \tag{4.9}$$

Let the forward and backward derivative operators D_t and D_t^* be defined informally, on two appropriate domains of real-valued functions f, in terms of the Hamiltonian H and two positive solutions $\hat{\eta}_t$, $\hat{\eta}_t^*$ of (3.7) and (3.8) by

$$D_t f = \frac{1}{\hat{\eta}_t}\left(\frac{\partial}{\partial t} - \frac{1}{\hbar}\hat{H}\right)(\hat{\eta}_t f)$$

and

$$D_t^* f = \frac{1}{\hat{\eta}_t^*}\left(\frac{\partial}{\partial t} + \frac{1}{\hbar}\hat{H}\right)(\hat{\eta}_t^* f).$$

Lemma 4.3 is proved using the following decompositions of D_t and D_t^*, which are straightforward to verify

$$D_t = \frac{\partial}{\partial t} + \mathcal{L}_{\hat{\eta}_t} \quad \text{and } D_t^* = \frac{\partial}{\partial t} - \mathcal{L}_{\hat{\eta}_t^*}. \tag{4.10}$$

Let us observe that for constant f, in particular, these two derivative operators are zero by definition. But many nontrivial functions $f:\mathbb{R}^d\times I\to\mathbb{R}$ in these domains have the same property. For

instance let $(\tilde{\eta}_t)_{t\in[r,v]}$ denote a positive solution of (3.7) on I, distinct from $(\hat{\eta}_t)_{t\in[r,v]}$. Then clearly we have $D_t f=0$ as well when $f=\tilde{\eta}_t/\hat{\eta}_t$.

V. VARIATIONAL CHARACTERIZATION AND LAGRANGIAN

As indicated in the introduction, a natural way to interpret the version of Euclidean quantum mechanics advocated here is as a mathematical counterpart of Feynman's path integral approach. In Feynman's perspective, the variational derivations of the quantum laws of motion (as well as some kinematical characterizations of the paths) is fundamental (cf. Refs. 1,10). We prove in this section and the next one that as far as the dynamics of the momentum representation is concerned, such a variational approach is well defined and provides a characterization of the stochastic process constructed before. More precisely, we will use the approach to stochastic control for jump processes of Refs. 31,11, to obtain a variational characterization of the Markovian Bernstein processes (or reversible diffusions with jumps) considered above. We consider the stochastic control problem $\inf_{\hat{S}} J(t,p;\hat{S})$ with action functional

$$J(t,p;\hat{S}) = E_{(t,p)}\left[\int_t^v \mathcal{L}(\hat{z}(s),\hat{S}_s)\mathrm{d}s - \hbar \log \hat{\eta}_v(\hat{z}(v))\right], \tag{5.1}$$

where $E_{(t,p)}$ denotes the conditional expectation given $\{\hat{z}_t=p\}$, the infimum is taken on the set of control variables made of all measurable scalar functions $\hat{S}_\cdot:\mathbb{R}^d\times\mathbb{R}_+\to\mathbb{R}$, and the integrand $\mathcal{L}(p,\hat{S}_s)$ is defined as

$$\begin{aligned}
\mathcal{L}(p,\hat{S}_s) &= \mathcal{L}_{\exp(\hat{S}_s/\hbar)}\hat{S}_s(p) + e^{-\hat{S}_s(p)/\hbar}\hat{H}e^{\hat{S}_s(p)/\hbar} \\
&= \frac{1}{2}\|p\|^2 + \frac{1}{2}\|\nabla \hat{S}_s(p)\|^2 + \int_{\mathbb{R}^d}\left(1+\left(\frac{\hat{S}_s(p+\hbar k)-\hat{S}_s(p)}{\hbar}-1\right)e^{(\hat{S}_s(p+\hbar k)-\hat{S}_s(p))/\hbar}\right)\nu(\mathrm{d}k) \\
&= \frac{1}{2}\|p\|^2 + \frac{1}{2}\|\nabla \hat{S}_s(p)\|^2 + \int_{\mathbb{R}^d}\frac{\hat{S}_s(p+\hbar k)-\hat{S}_s(p)}{\hbar}e^{(\hat{S}_s(p+\hbar k)-\hat{S}_s(p))/\hbar}\nu(\mathrm{d}k) \\
&\quad - \int_{\mathbb{R}^d}(e^{(\hat{S}_s(p+\hbar k)-\hat{S}_s(p))/\hbar}-1)\nu(\mathrm{d}k).
\end{aligned}$$

In particular, when $\hat{S}_s=\hbar \log \hat{\eta}_s$,

$$\begin{aligned}
\mathcal{L}(p,\hbar \log \hat{\eta}_t) &= \hbar\mathcal{L}_{\hat{\eta}_t}\log \hat{\eta}_t(p) + \frac{1}{\hat{\eta}_t(p)}\hat{H}\hat{\eta}_t(p) = \hbar\mathcal{L}_{\hat{\eta}_t}\log \hat{\eta}_t(p) + \frac{\hbar}{\hat{\eta}_t(p)}\frac{\partial}{\partial t}\hat{\eta}_t(p) = \hbar\mathcal{L}_{\hat{\eta}_t}\log \hat{\eta}_t(p) \\
&\quad + \hbar\frac{\partial}{\partial t}\log \hat{\eta}_t(p) = \hbar D_t \log \hat{\eta}_t(p).
\end{aligned}$$

In other terms we have

$$\begin{aligned}
\mathcal{L}(p,\hbar \log \hat{\eta}_t) &= \frac{1}{2}\|p\|^2 + \frac{\hbar^2}{2}\|\nabla \log \hat{\eta}_t(p)\|^2 + \int_{\mathbb{R}^d}(\log \hat{\eta}_t(p+\hbar k) - \log \hat{\eta}_t(p))\frac{\hat{\eta}_t(p+\hbar k)}{\hat{\eta}_t(p)}\nu(\mathrm{d}k) \\
&\quad - \int_{\mathbb{R}^d}\frac{\hat{\eta}_t(p+\hbar k)-\hat{\eta}_t(p)}{\hat{\eta}_t(p)}\nu(\mathrm{d}k).
\end{aligned}$$

Now let us observe that

$$D_t p = \mathcal{L}_{\hat{\eta}_t} p = \hbar \nabla \log \hat{\eta}_t(p) + \int_{\mathbb{R}^d} k \frac{\hat{\eta}_t(p+\hbar k)}{\hat{\eta}_t(p)} \nu(\mathrm{d}k).$$

From now on, we will denote by $L(p, D_t p)$ and call Lagrangian, the integrand $\mathcal{L}(p, \hbar \log \hat{\eta}_t)$ of the action functional, when re-expressed in terms of the variables $p, D_t p$. We have, using (3.2) and the expression of $D_t p$,

$$\begin{aligned} L(p, D_t p) = {} & \frac{1}{2}\|p\|^2 + \hbar \left\langle \frac{\nabla \hat{\eta}_t}{\hat{\eta}_t}, D_t p \right\rangle + \frac{V(i\hbar \nabla)\hat{\eta}_t}{\hat{\eta}_t} + \frac{\hbar^2}{2}\frac{\Delta \hat{\eta}_t}{\hat{\eta}_t} - \frac{\hbar^2}{2}\left\| \frac{\nabla \hat{\eta}_t}{\hat{\eta}_t} \right\|^2 \\ & + \int_{\mathbb{R}^d} (\log \hat{\eta}_t(p+\hbar k) - \log \hat{\eta}_t(p)) \frac{\hat{\eta}_t(p+\hbar k)}{\hat{\eta}_t(p)} \nu(\mathrm{d}k) \\ & - \hbar \int_{\mathbb{R}^d} \langle k, \nabla \log \hat{\eta}_t(p) \rangle \frac{\hat{\eta}_t(p+\hbar k)}{\hat{\eta}_t(p)} \nu(\mathrm{d}k). \end{aligned}$$

By Taylor's formula applied inside the integral term we obtain the Lagrangian

$$\begin{aligned} L(p, D_t p) = {} & \frac{1}{2}\|p\|^2 + \hbar \left\langle \frac{\nabla \hat{\eta}_t}{\hat{\eta}_t}, D_t p \right\rangle + \frac{V(i\hbar \nabla)\hat{\eta}_t}{\hat{\eta}_t} \\ & + \frac{\hbar^2}{2}\Delta \log \hat{\eta}_t(p) \int_{\mathbb{R}^d} (1 + \|k\|^2 + o(\hbar^3)) \frac{\hat{\eta}_t(p+\hbar k)}{\hat{\eta}_t(p)} \nu(\mathrm{d}k). \end{aligned} \tag{5.2}$$

Let us observe that the action functional for $\hat{S}_s = \hbar \log \hat{\eta}_s$ can be expressed in various equivalent ways,

$$\begin{aligned} J(t,p;\hat{S}) &= E_{(t,p)}\left[\int_t^v D_s \hat{S}_s(\hat{z}_s)\mathrm{d}s - \hbar \log \hat{\eta}_v(\hat{z}(v)) \right] \\ &= E_{(t,p)}\left[\int_t^v \mathcal{L}(\hat{\eta}_t(\hat{z}_s), \hat{S}_s)\mathrm{d}s \right] - E_{(t,p)}[\hbar \log \hat{\eta}_v(\hat{z}_v)] \\ &= E_{(t,p)}[\hat{S}_v(\hat{z}_v) - \hat{S}_t(p) - \hbar \log \hat{\eta}_v(\hat{z}(v))] = E_{(t,p)}\left[\int_t^v \mathrm{d}\hat{S}_s(\hat{z}_s) - \hbar \log \hat{\eta}_v(\hat{z}(v)) \right] \\ &= E_{(t,p)}\left[\int_t^v \nabla \hat{S}_s(\hat{z}_s) \circ \mathrm{d}\hat{z}_s + \int_t^v \int_{\mathbb{R}^d} (\hat{S}_s(\hat{z}_{s^-} + \hbar k) - \hat{S}_s(\hat{z}_{s^-}))\mu(\mathrm{d}k, \mathrm{d}s) \right. \\ &\quad \left. + \int_t^v \frac{\partial}{\partial s}\hat{S}_s(\hat{z}_s)\mathrm{d}s - \hbar \log \hat{\eta}_v(\hat{z}(v)) \right] \\ &= E_{(t,p)}\left[\int_t^v \nabla \hat{S}_s(\hat{z}_s) \circ \mathrm{d}\hat{z}_s + \int_t^v \int_{\mathbb{R}^d} \hat{S}_s(\hat{z}_{s^-} + \hbar k)\nu(\mathrm{d}k)\mathrm{d}s \right. \\ &\quad \left. + \int_t^v \frac{\partial}{\partial s}\hat{S}_s(\hat{z}_s)\mathrm{d}s - \hbar \log \hat{\eta}_v(\hat{z}(v)) \right], \end{aligned}$$

where we have used the extension of Itô's calculus to our diffusions with jumps. The symbol $\circ$ denotes the Fisk–Stratonovich differential (cf., e.g., Ref. 26). Let us show that the diffusion processes with jumps constructed before can also be regarded as minima of a stochastic action functional associated with the starting $\hat{H}$. The infima are taken on all measurable functions $\hat{S}_t : \mathbb{R}^d \to \mathbb{R}$:

Proposition 5.1. *The dynamic programming equation with final boundary condition*

$$\frac{\partial A_t}{\partial t}(p) + \min_{\hat{S}_t}(\mathcal{L}_{\exp(\hat{S}/\hbar)}A_t(p) + L(p,\hat{S}_t)) = 0, \quad A_v = -\hbar \log \hat{\eta}_v, \tag{5.3}$$

associated with the action functional (5.1) *is equivalent to the Hamilton–Jacobi–Bellman equation*

$$\frac{\partial A_t}{\partial t}(p) = -\frac{1}{2}\|p\|^2 - \frac{\hbar}{2}\Delta A_t(p) + \frac{1}{2}\|\nabla A_t(p)\|^2 + \int_{\mathbb{R}^d}(e^{-\hbar^{-1}(A_t(p+\hbar k)-A_t(p))} - 1)\mathrm{d}\nu(k), \quad A_v = -\hbar \log \hat{\eta}_v, \tag{5.4}$$

with solution $A_t = -\hbar \log \hat{\eta}_t$, $r \leqslant t \leqslant v$. *Moreover, in* (5.3), *the minimum in* $\hat{S}_t$ *is attained on* $\hat{S}_t = \hbar \log \hat{\eta}_t$.

Proof: Given $\hat{S}_t$ and A_t two suitable functions, let us define

$$F(p,k) = \frac{A_t(p+\hbar k) - A_t(p)}{\hbar} e^{(\hat{S}_t(p+\hbar k)-\hat{S}_t(p))/\hbar} + \frac{\hat{S}_t(p+\hbar k) - \hat{S}_t(p)}{\hbar} e^{(\hat{S}_t(p+\hbar k)-\hat{S}_t(p))/\hbar}$$
$$- e^{(\hat{S}_t(p+\hbar k)-\hat{S}_t(p))/\hbar} + e^{-(A_t(p+\hbar k)-A_t(p))/\hbar}.$$

We have

$$\begin{aligned}\mathcal{L}(p,\hat{S}_t) + \mathcal{L}_{\exp(\hat{S}_t/\hbar)}A_t(p) - e^{A_t(p)/\hbar}\hat{H}e^{-A_t(p)/\hbar} &= \mathcal{L}_{\exp(\hat{S}_t/\hbar)}(A_t(p) + \hat{S}_t(p)) \\ &\quad + e^{-\hat{S}_t(p)/\hbar}\hat{H}e^{\hat{S}_t(p)/\hbar} - e^{A_t(p)/\hbar}\hat{H}e^{-A_t(p)/\hbar} \\ &= \hbar\int_{\mathbb{R}^d} F(p,k)\,\nu(\mathrm{d}k) + \frac{1}{2}\|\nabla A_t(p) + \nabla \hat{S}_t(p)\|^2 \\ &\geqslant \hbar\int_{\mathbb{R}^d} F(p,k)\,\nu(\mathrm{d}k).\end{aligned}$$

Now, for all $a > 0$,

$$\min_{x\in\mathbb{R}}(xa + a\log a - a + e^{-x}) = 0,$$

hence taking $x = (A_t(p+\hbar k) - A_t(p))/\hbar$ and $a = e^{(\hat{S}_t(p+\hbar k)-\hat{S}_t(p))/\hbar}$, we have $F(p,k) \geqslant 0$, and

$$\mathcal{L}(p,\hat{S}_t) + \mathcal{L}_{\exp(\hat{S}_t/\hbar)}A_t(p) - e^{A_t(p)/\hbar}\hat{H}e^{-A_t(p)/\hbar} \geqslant 0,$$

the minimum (zero) being attained for $\hat{S}_t = -A_t$, i.e.,

$$\min_{\hat{S}_t}(L(p,\hat{S}_t) + \mathcal{L}_{\exp(\hat{S}_t/\hbar)}A_t) = e^{A_t(p)/\hbar}\hat{H}e^{-A_t(p)/\hbar}.$$

The dynamic programming equation (5.3) can be formulated as

$$\frac{\partial A_t}{\partial t} + e^{A_t/\hbar}\hat{H}e^{-A_t/\hbar} = 0,$$

and its solution is $A_t = -\hbar \log \hat{\eta}_t$. Finally, from the relation

$$\frac{1}{\hbar}\Delta A_t = -e^{A_t/\hbar}\Delta e^{-A_t/\hbar} + \frac{1}{\hbar^2}\|\nabla A_t\|^2,$$

we have

$$e^{A_t(p)/\hbar}\hat{H}e^{-A_t(p)/\hbar} = e^{A_t(p)/\hbar}\left(\frac{1}{2}\|p\|^2 e^{-A_t(p)/\hbar} - \frac{\hbar}{2}\Delta e^{-A_t(p)/\hbar} - \int_{\mathbb{R}^d}(e^{-(A_t(p+\hbar k)-A_t(p))/\hbar})\,\nu(\mathrm{d}k)\right)$$

$$= \frac{1}{2}\|p\|^2 + \frac{\hbar}{2}\Delta A_t - \frac{1}{2}\|\nabla A_t\|^2 - \int_{\mathbb{R}^d}(e^{-\hbar^{-1}(A_t(p+\hbar k)-A_t(p))} - 1)\,\nu(\mathrm{d}k),$$

which yields (5.4). ■

In the backward case we consider the action functional time reversed of (5.1),

$$J^*(t,p;\hat{S}^*) = E_{(t,p)}\left[\int_r^t \mathcal{L}(\hat{z}(s),\hat{S}^*)\mathrm{d}s - \hbar\log\hat{\eta}_r^*(\hat{z}(r))\right]. \tag{5.5}$$

Similarly when $\hat{S}_s = \hbar\log\hat{\eta}_s^*$ we verify that

$$\mathcal{L}(p,\hbar\log\hat{\eta}_s^*) = -\hbar D_s^*\log\hat{\eta}_s^*(p),$$

where we have used (4.10) and the backward generator (4.9). Then

$$\begin{aligned}
J^*(t,p;\hat{S}^*) &= -E_{(t,p)}\left[\int_r^t D_s^*\hat{S}_s^*(\hat{z}_s^*)\mathrm{d}s + \hbar\log\hat{\eta}_r^*(\hat{z}(r))\right]\\
&= E_{(t,p)}[\hat{S}_r^*(\hat{z}_r) - \hat{S}_t^*(\hat{z}_t) - \hbar\log\hat{\eta}_r^*(\hat{z}(r))]\\
&= -E_{(t,p)}\left[\int_r^t \mathrm{d}\hat{S}_s^*(\hat{z}_s^*) + \hbar\log\hat{\eta}_r^*(\hat{z}(r))\right]\\
&= -E_{(t,p)}\left[\int_r^t \nabla\hat{S}_s^*(\hat{z}_s) \mp d_*\hat{z}_s^* + \int_r^t\int_{\mathbb{R}^d}(\hat{S}_s^*(\hat{z}_{s^+}+\hbar k) - \hat{S}_s^*(\hat{z}_{s^+}))\mu_*(\mathrm{d}k,\mathrm{d}s)\right.\\
&\quad \left. + \int_r^t \frac{\partial}{\partial s}\hat{S}_s^*(\hat{z}_s^*)\mathrm{d}s + \hbar\log\hat{\eta}_r^*(\hat{z}(r))\right]\\
&= -E_{(t,p)}\left[\int_r^t \nabla\hat{S}_s^*(\hat{z}_s)\mathrm{od}_*\hat{z}_s^* + \int_r^t\int_{\mathbb{R}^d}\hat{S}_s^*(\hat{z}_{s^+}+\hbar k)\,\nu(\mathrm{d}k)\mathrm{d}s + \int_r^t \frac{\partial}{\partial s}\hat{S}_s^*(\hat{z}_s^*)\mathrm{d}s\right.\\
&\quad \left. + \hbar\log\hat{\eta}_r^*(\hat{z}(r))\right].
\end{aligned}$$

With respect to the underlying filtration $\mathcal{F}_t$, the Lagrangian now takes the form

$$L(p,D_t^*p) = \frac{1}{2}\|p\|^2 - \hbar\left\langle\frac{\nabla\hat{\eta}_t^*}{\hat{\eta}_t^*}, D_t^*p\right\rangle + \frac{V(i\hbar\nabla)\hat{\eta}_t^*}{\hat{\eta}_t^*} - \frac{\hbar^2}{2}\Delta\log\hat{\eta}_t^*(p)\int_{\mathbb{R}^d}(1+\|k\|^2 + o(\hbar^3))\frac{\hat{\eta}_t^*(p+\hbar k)}{\hat{\eta}_t^*(p)}\nu(\mathrm{d}k), \tag{5.6}$$

and the following backward version of Proposition 5.1 holds true.

Proposition 5.2: *The backward dynamic programming equation with initial boundary condition*

$$\frac{\partial A_t^*}{\partial t}(p) + \min_{\hat{S}_t^*}(\mathcal{L}_{\exp(\hat{S}^*/\hbar)}A_t^*(p) + L(p,\hat{S}_t^*)) = 0, \quad A_r^* = -\hbar\log\hat{\eta}_r^*, \tag{5.7}$$

associated with (5.5), *is equivalent to the backward Hamilton–Jacobi–Bellman equation*

$$\frac{\partial A_t^*}{\partial t}(p) = \frac{1}{2}\|p\|^2 + \frac{\hbar}{2}\Delta A_t^*(p) - \frac{1}{2}\|\nabla A_t^*(p)\|^2 - \int_{\mathbb{R}^d}(e^{-\hbar^{-1}(A_t^*(p+\hbar k)-A_t^*(p))} - 1)\mathrm{d}\nu(k), \quad A_r^* = -\hbar \log \hat{\eta}_r^*, \tag{5.8}$$

with solution $A_t^* = -\hbar \log \hat{\eta}_t^*$, $r \leqslant t \leqslant v$. *Moreover, in* (5.7), *the minimum in* $\hat{S}_t^*$ *is attained at* $\hat{S}_t^*(p) = \hbar \log \hat{\eta}_t^*(p)$.

Proof: Of course, Propositions 5.1 and 5.2 will not be formally used. The key point is that $\hat{z}_t$, $t \in I$, can be regarded as critical point of a stochastic variational principle. Proposition 5.1 is sufficient since $\hat{z}_t$, $t \in I$, is time reversible in the above mentioned sense. But it is illustrative to show that its critical property takes two slightly different forms with respect to the filtrations $\mathcal{P}_t$ and $\mathcal{F}_t$. So we summarize the $\mathcal{F}_t$ proof only for completeness. We first show that

$$\min_{\hat{S}_t^*}(\mathcal{L}^*_{\exp(\hat{S}_t^*/\hbar)}A_t^*(p) + L(p,\hat{S}_t^*)) = -e^{A_t^*/\hbar}\hat{H}e^{-A_t^*/\hbar}, \tag{5.9}$$

and the minimum is attained for $\hat{S}_t^* = A_t^*$. Let

$$F^*(p,k) = e^{(\hat{S}_t^*(p-\hbar k)-\hat{S}_t^*(p))/\hbar}\frac{A_t^*(p+\hbar k) - A_t^*(p)}{\hbar} + e^{(\hat{S}_t^*(p-\hbar k)-\hat{S}_t^*(p))/\hbar}\frac{f_t^*(p+\hbar k) - f_t^*(p)}{\hbar}$$
$$- e^{(\hat{S}_t^*(p-\hbar k)-\hat{S}_t^*(p))/\hbar} + e^{-(A_t^*(p-\hbar k)-A_t^*(p))/\hbar}.$$

We have

$$L(p,\hat{S}^*) + \mathcal{L}^*_{\exp(\hat{S}_t^*/\hbar)}A_t^*(p) - e^{A_t^*(p)/\hbar}\hat{H}e^{-A_t^*(p)/\hbar} = \hbar\int_{\mathbb{R}^d}F^*(p,k)\nu(\mathrm{d}k) + \frac{1}{2}\|\nabla A_t^*(p) + \nabla \hat{S}_t^*(p)\|^2$$
$$\geqslant \hbar\int_{\mathbb{R}^d}F^*(p,k)\nu(\mathrm{d}k),$$

Proceeding as in the forward case we obtain (5.9) and the dynamic programming equation (5.3) becomes

$$\frac{\partial A_t^*}{\partial t} - e^{A_t^*/\hbar}\hat{H}e^{-A_t^*/\hbar} = 0,$$

with solution $A_t^* = -\hbar \log \hat{\eta}_t^*$. Finally we have

$$e^{A_t^*(p)/\hbar}\hat{H}e^{-A_t^*(p)/\hbar} = \frac{1}{2}\|p\|^2 - e^{A_t^*(p)/\hbar}\left(\frac{\hbar^2}{2}\Delta e^{-A_t^*(p)/\hbar} + \int_{\mathbb{R}^d}(e^{-A_t^*(p+\hbar k)/\hbar} - e^{-A_t^*(p)/\hbar})\nu(\mathrm{d}k)\right)$$
$$= \frac{1}{2}\|p\|^2 + \frac{\hbar}{2}\Delta A_t^*(p) - \frac{1}{2}\|\nabla A_t^*(p)\|^2 - \int_{\mathbb{R}^d}(e^{-\hbar^{-1}(A_t^*(p+\hbar k)-A_t^*(p))} - 1)\nu(\mathrm{d}k),$$

which yields (5.8). ■

The action (5.1), with Lagrangian (5.2) may seen relatively artificial. As a matter of fact, and as Sec. VI will show, they are natural $\hbar$-deformations of their classical (Euclidean) counterparts in momentum representation.

VI. EQUATIONS OF MOTION

We now derive a.s. equations of motion associated with $(\hat{z}_t)_{t\in 1}$. Those equations justify, in a way, our whole strategy, including the variational approach of Sec. V. Here, $(\hat{z}_t)_{t\in[r,v]}$ represents the process associated to our system in momentum representation, and the expectations of the almost sure equations of motion can be interpreted as the probabilistic counterpart of the Ehrenfest

theorem in quantum dynamics of Ref. 6. The forward and backward derivatives defined before as the generators $D_t=(\partial/\partial t)+\mathcal{L}_{\hat{\eta}_t}$ and $D_t^*=(\partial/\partial t)-\mathcal{L}_{\hat{\eta}_t^*}$ have natural probabilistic interpretations as the following limits of conditional expectations, for f regular enough

$$D_t f_t(\hat{z}_t)=\lim_{\Delta t\downarrow 0} E\left[\left.\frac{ft+\Delta t^{(\hat{z}_{t+\Delta t})}-f_t(\hat{z}_t)}{\Delta t}\right|\mathcal{P}_t\right]=E\left[\left.\frac{d}{\mathrm{d}t^+}f_t(\hat{z}_t)\right|\mathcal{P}_t\right], \tag{6.1}$$

and

$$D_t^* f_t(\hat{z}_t)=\lim_{\Delta t\downarrow 0} E\left[\left.\frac{f_t(\hat{z}_t)-f_{t-\Delta t}(\hat{z}_{t-\Delta t})}{\Delta t}\right|\mathcal{F}_t\right]=E\left[\left.\frac{d}{\mathrm{d}t^-}f_t(\hat{z}_t)\right|\mathcal{F}_t\right], \tag{6.2}$$

where $(d/\mathrm{d}t^+)f,(d/\mathrm{d}t^-)f$ denote the right-hand side and left-hand side derivatives corresponding to the formal limits of (6.1) and (6.2) when Planck's constant $\hbar$ is equal to 0. Of course, the expectation E denotes, here, the one with respect to the process $\hat{z}_t$ solving Eqs. (4.4) and (4.5). The definitions (6.1) and (6.2) provide a probabilistic interpretation of M_t, M_t^* such that $D_tM_t=0$ and $D_t^*M_t^*=0$. Indeed, when this happens we have clearly for all $\Delta t>0$,

$$E[M_{t+\Delta t}(\hat{z}_{t+\Delta t})|\mathcal{P}_t]=M_t(\hat{z}_t) \quad \text{and } M_t^*(\hat{z}_t)=E[M_{t-\Delta t}^*(\hat{z}_{t-\Delta t})|\mathcal{F}_t].$$

As indicated after (2.6), the first condition means that $M_t(\hat{z}_t)$ is a $\mathcal{P}_t$-martingale and the second that $M_t^*(\hat{z}_t^*)$ is a $\mathcal{F}_t$-martingale. For instance, $f_t(\hat{z}_t)=\hat{\eta}_t(\hat{z}_t)/\hat{\eta}_t(\hat{z}_t)$, as defined above, is a $\mathcal{P}_t$-martingale.

The relation with quantum dynamics is clearer when expressed in terms of (absolute, in contrast with conditional) expectations. For this purpose it is sufficient to observe the following.

Corollary 6.1: *Under (absolute) expectations and when f_t, D_tf, D_t^*f are integrable we have*

$$\frac{d}{\mathrm{d}t}E[f_t(\hat{z}_t)]=E[D_tf_t(\hat{z}_t)]=E[D_t^*f_t(\hat{z}_t)], \quad f\in\mathcal{S}(\mathbb{R}^{d+1}).$$

Proof: This follows from the Itô formula, written as

$$\mathrm{d}f_t(\hat{z}_t)=D_tf_t(\hat{z}_t)\mathrm{d}t+\langle\nabla f_t(\hat{z}_t),\mathrm{d}W_t^{\hbar}\rangle+\int_{\mathbb{R}^d}(f_t(\hat{z}_{t^-}+\hbar k)-f_t(\hat{z}_{t^-}))\left(\mu(\mathrm{d}k,\mathrm{d}t)-\frac{\hat{\eta}_t(\hat{z}_{t^-}+\hbar k)}{\hat{\eta}_t(\hat{z}_{t^-})}\nu(\mathrm{d}k)\mathrm{d}t\right)$$

and

$$\mathrm{d}_*f(\hat{z}_t)=D_t^*f_t(\hat{z}_t)\mathrm{d}t+\langle\nabla f(\hat{z}_t),\mathrm{d}_*W_t^{\hbar *}\rangle+\int_{\mathbb{R}^d}(f(\hat{z}_{t^+})-f(\hat{z}_{t^+}-\hbar k))\left(\mu_*(\mathrm{d}k,\mathrm{d}t)-\frac{\hat{\eta}_t^*(\hat{z}_{t^+}-\hbar k)}{\hat{\eta}_t^*(\hat{z}_{t^+})}\nu(\mathrm{d}k)\mathrm{d}t\right).$$

■

In the next proposition we make the assumption:

$$\int_{\mathbb{R}^d}\|k\|\nu(\mathrm{d}k)<\infty, \tag{6.3}$$

and let $D_tp_{|p=\hat{z}_t}$ be denoted by $D_t\hat{z}_t$.

Proposition 6.2: *The process $(\hat{z}_t)_{t\in[r,v]}$, critical point of the action functional introduced before Proposition 5.1, solves the almost sure equations of motion,*

$$D_t\left(\hbar\frac{\nabla\hat{\eta}_t}{\hat{\eta}_t}\right)(\hat{z}_t)=\hat{z}_t, \tag{6.4}$$

where ∇ denotes ∇_p except if otherwise specified, and

$$D_t\hat{z}_t=\frac{1}{\hat{\eta}_t(\hat{z}_t)}(-i\nabla_qV)(i\hbar\nabla_p)\hat{\eta}_t(\hat{z}_t). \tag{6.5}$$

Proof: By (3.1),

$$-i\nabla_q V(q) = -iq + \frac{1}{\hbar}\int_{\mathbb{R}^d} k e^{-(i/\hbar)\langle q,k\rangle}\nu(\mathrm{d}k).$$

Therefore

$$(-i\nabla_q V)(i\hbar\,\nabla)\,\hat{\eta}_t(p) = \hbar\,\nabla\,\hat{\eta}_t(p) + \int_{\mathbb{R}^d} k\,\hat{\eta}_t(p+\hbar k)\,\nu(\mathrm{d}k).$$

On the other hand, we have

$$D_t p = \mathcal{L}_{\hat{\eta}_t} p = \hbar\,\nabla\,\log\,\hat{\eta}_t(p) + \int_{\mathbb{R}^d} \hbar k \frac{\hat{\eta}_t(p+\hbar k)}{\hat{\eta}_t(\hbar k)}\nu(\mathrm{d}k)$$

which proves the first relation (6.5). Concerning (6.4) we have

$$D_t\left(\hbar\frac{\nabla\hat{\eta}_t}{\hat{\eta}_t}\right)(p) = \frac{1}{\hat{\eta}_t}\left(\frac{\partial}{\partial t} - \frac{1}{\hbar}\hat{H}\right)(\hbar\,\nabla\,\hat{\eta}_t) = p + \frac{1}{\hat{\eta}_t}\,\nabla\left(\hbar\frac{\partial}{\partial t} - \hat{H}\right)\hat{\eta}_t = p.$$

This relation can also be obtained by differentiation with respect to p of the heat equation for $\hat{\eta}$,

$$\frac{\partial\,\nabla\,\hat{\eta}_t}{\partial t}(p) = \nabla\,\frac{\partial\hat{\eta}_t}{\partial t}(p) = \frac{1}{\hbar}\,\nabla\,\hat{H}\hat{\eta}_t(p) = \frac{1}{\hbar}\hat{H}\,\nabla\,\hat{\eta}_t(p) + p.$$

■

In the backward case, similar calculations yield

$$D_t^*\hat{z}_t = \frac{1}{\hat{\eta}_t^*(\hat{z}_t)}(i\nabla_q\overline{V})(i\hbar\nabla_p)\,\hat{\eta}_t^*(\hat{z}_t), \quad D_t^*\left(\hbar\frac{\nabla\hat{\eta}_t^*}{\hat{\eta}_t^*}\right)(\hat{z}_t) = -\hat{z}_t.$$

Since $D_t \mapsto -D_t^*$ and $p \mapsto -p$ under time reversal, it is clear that these equations are time reversed of (6.5). The (forward) analog of the Newton equation in momentum representation becomes

$$D_t D_t\left(\frac{\nabla\hat{\eta}_t}{\hat{\eta}_t}\right)(\hat{z}_t) = \frac{1}{\hat{\eta}_t(\hat{z}_t)}(-i\nabla_q V)(i\hbar\,\nabla)\,\hat{\eta}_t(\hat{z}_t).$$

If $V(q)=q^2/2$ we obtain $D_t\hat{z}_t=\hbar\nabla\,\log\,\hat{\eta}_t$ and $D_tD_t\hat{z}_t=\hat{z}_t$. This is the purely diffusive case, already known.[6]

Let us come back on the interpretation of what we found and, in particular, on its associated classical limit. In position representation the classical action functional S should be regarded as the integral of the ("reduced") Poincaré–Cartan differential form,

$$\tilde{\omega}_q = p(q,t)\mathrm{d}t - h(q,p(q,t))\mathrm{d}t,$$

where $p=p(q,t)$ denotes the momentum expressed as a function of the position and time and $h=h(q,p(q,t))$ the Hamiltonian observable. This means that the underlying flow is the one associated with the first equation of Hamilton, for our elementary class of $h(q,p)=(\|p\|^2/2)+V(q)$, reduced to the q-variable:

$$\frac{\mathrm{d}q}{\mathrm{d}t} = p(q,t). \tag{6.6}$$

The second Hamilton equation follows from the integrability condition of $\tilde{\omega}_q$. For Lipschitz p, let $s\mapsto q(s)$ be the solution of (6.6) such that $q(t)=q$. Let us denote by $\int^{q,t}\tilde{\omega}_q$ the associated line

integral. When it is locally univocal, this integral defines the action functional, say $S(q,t)$. Then S solves the Hamilton–Jacobi equation,

$$\frac{\partial S}{\partial t} + h(q, \nabla_q S) = 0,$$

whose ∇_q coincides with the above second Hamilton equation. For the momentum representation, the construction is symmetric. Instead of $\tilde{\omega}_q$ we have to consider the reduced form

$$\tilde{\omega}_p = q(p,t)\mathrm{d}p + h(q(p,t),p)\mathrm{d}t$$

whose underlying flow is the one associated with the second equation of Hamilton reduced to its p-variable:

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\nabla V(q(p,t)).$$

When

$$\hat{S}(p,t) = \int^{p,t} \tilde{\omega}_p$$

makes sense, so does the Hamilton–Jacobi equation,

$$\frac{\partial \hat{S}}{\partial t} + h(-\nabla_p \hat{S}, p) = 0 \tag{6.7}$$

whose gradient ∇_p coincides with the integrability condition of $\tilde{\omega}_p$.

Let us specialize this to our class of elementary Hamiltonians which are classical limits of (3.3). Then the action function becomes

$$\hat{S}(p,t) = \int \left(q(p(s),s)\frac{\mathrm{d}p}{\mathrm{d}s} + h(q(p(s),s),p) \right)\mathrm{d}s = \int \left(\frac{1}{2}p^2 - \nabla_p \hat{S}.\dot{p}(s) + V(-\nabla_p \hat{S}) \right)\mathrm{d}s$$
$$= \int L(p(s),\dot{p}(s))\mathrm{d}s, \tag{6.8}$$

whose integrand defines the Lagrangian L of our system. So, for the elementary class of Hamiltonians H considered here, the equations of motion reduce to

$$\frac{d}{\mathrm{d}t}(-\nabla_p \hat{S}) = p,$$
$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\nabla V(-\nabla_p \hat{S}). \tag{6.9}$$

Now let us compare this with the Lagrangian and a.s. equation of motion obtained for our class of time-reversible processes $\hat{z}_t$ with jumps. First notice that, in the above classical summary, the parameter is the usual ("real") time. In order to obtain the Euclidean counterpart we have to introduce the "Wick rotation" $t \mapsto -it$ seen in Sec. I. It is easy to check that (6.9) can be transformed into

$$\frac{d}{dt}(i\nabla_p \hat{\mathcal{S}}) = ip,$$
$$i\frac{dp}{dt} = -\nabla_q V(i\nabla_p \hat{\mathcal{S}}), \tag{6.10}$$

where $\hat{\mathcal{S}}=\hat{\mathcal{S}}(p,t)$ solves the Euclidean counterpart of the Hamilton–Jacobi equation (6.7). Comparing with (6.5), those equations can be regarded as the quantum deformation of (6.10) when the smooth trajectories $t\mapsto ip(t)$ are replaced by the very irregular ones of our diffusion process with jumps $\hat{z}_t$. Since the classical (strong) time derivative does not make sense anymore, it is natural to replace it by its probabilistic counterpart D_t (6.1) or, regarded as an operator, by (4.10). The role of the classical action function $\hat{S}(p,t)$ is manifestly played, in (6.5), by $A_t(p)=-\hbar \log \hat{\eta}_t(p)$ solving the Hamilton–Jacobi–Bellman equation (5.4). In particular, it is clear from our first equation (6.5) that the position observable is now proportional to $\hbar\nabla \log \hat{\eta}_t(p)=-\nabla A_t(p)$. So the Hamilton–Jacobi–Bellman equation (5.4) is a quantum deformation of the Euclidean version of the classical equation (6.7). The integrand of the action functional, i.e., our Lagrangian $L(p,D_t p)$ defined in (5.2) of Sec. V, is also a (Euclidean) deformation of the classical integrand of (6.8). The main deformation term, of order $o(\hbar^2)$, involves an integral with respect to the Lévy measure $\nu(\mathrm{d}k)$. This "small" term is, however, necessary to validate the variational characterization of the process $\hat{z}_t$ given in Sec. V. Notice that, because of the relation between the action function and the positive solution $\hat{\eta}_t$ of (3.7) (cf. Proposition 5.1) $A_t(p)=-\hbar \log \hat{\eta}_t(p)$, and also the fact that the underlying Lévy measure $\nu(\mathrm{d}k)$ does not depend on the Planck constant $\hbar$, the limit $\hbar\to 0$ of the probabilistic construction is not trivial. In particular, the first term under the integral of the Hamilton–Jacobi–Bellman equation (5.4), which coincides with the factor $\hat{\eta}_t(p+\hbar k)/\hat{\eta}_t(p)$ in the integral term of the forward generator $\mathcal{L}_{\hat{\eta}_t}$ of $\hat{z}_t$, reduces to

$$\int e^{-\hbar\langle(\nabla\hat{\eta}_t/\hat{\eta}_t)(p),k\rangle}\nu(\mathrm{d}k) \to \int e^{\langle\nabla\hat{S}(p),k\rangle}\nu(\mathrm{d}k) \equiv \int e^{-\langle q,k\rangle}\nu(\mathrm{d}k),$$

namely the Laplace transform of ν (or Fourier transform in imaginary time). Indeed, both quantically and classically, the position q is proportional to the gradient of the action. Using this and the representation (3.1) of the classical potential V, one can reinterpret our first order classical equation of motion (6.10) for p as the solution of a deterministic variational principle, limit of the one given in Sec. V, whose "control" $u(k)$ becomes optimal precisely when $u^*(k)=e^{-\langle q,k\rangle}$. Of course, then, the associated classical Lagrangian reduces to the Euclidean version of the one in (6.8) or, equivalently, to the classical limit of $L(p,D_t p)$ as given in Sec. V, for the semiclassical state $\hat{\eta}_t(p)=\exp-(1/\hbar)\hat{\mathcal{S}}_t(p)$. However, since this deterministic variational principle does not seem to have an obvious physical interpretation it will not be given here (cf. Ref. 31).

A number of the properties of these processes remains to be investigated. Many of those known to hold for pure diffusions should survive for the much richer class of diffusions with jumps considered here. In particular, a systematic study of their symmetries, in term of a Noether theorem, on the model of Refs. 33,34, is possible and should provide further information on the general structure of the construction. A more geometrical approach to these symmetries[21] can probably be extended as well to this class. Moreover, the almost sure equations of motion could be more elegantly deduced from an appropriate generalization of the stochastic calculus of variations used in Ref. 7.

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Control of finite-dimensional quantum systems: Application to a spin-$\frac{1}{2}$ particle coupled with a finite quantum harmonic oscillator

C. Rangan
Department of Physics, University of Windsor, Ontario, Canada N9B 3P4

A. M. Bloch
Department of Mathematics, The University of Michigan, Ann Arbor, Michigan 48109-1109

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In this paper, we consider the problem of the controllability of a finite-dimensional quantum system in both the Schrödinger and interaction pictures. Introducing a Quantum Transfer Graph, we elucidate the role of Lie algebra rank conditions and the complex nature of the control matrices. We analyze the example of a sequentially coupled N-level system: a spin-$\frac{1}{2}$ particle coupled to a finite quantum harmonic oscillator. This models an important physical paradigm of quantum computers—the trapped ion. We describe the control of the finite model obtained, under the right conditions, from the original infinite-dimensional system. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1852701]

I. INTRODUCTION

The control and controllability of finite-dimensional quantum systems are of topical interest to the chemical dynamics, coherent control and quantum computing communities.[1–9] Indeed, several methods of proving controllability of quantum systems[3,4,10–13] have been developed from corresponding techniques used in the control of finite-dimensional classical systems. In these treatments, specifically in the graphical methods, the role of the drift (or field-free) Hamiltonian is not obvious. In quantum mechanics, it is fairly standard to use an interaction picture, where the drift term does not appear explicitly in the Schrödinger equation. In these cases, the presence of only one matrix, namely the control matrix in the interaction picture, makes it not amenable to use of the rigorous Lie algebraic method[11] to determine controllability.

In this paper, we present fresh insights into the controllability and control of quantum systems both in the Schrödinger and interaction pictures. We propose a new graphical method—the Quantum Transfer Graph—that will explicitly demonstrate both the roles of the drift and control matrices, and also the importance of considering the control matrix as one with complex entries. Then we analyze a very interesting example of a sequentially coupled N-level system: a spin-$\frac{1}{2}$ particle coupled with a quantum harmonic oscillator. This models an important physical paradigm of quantum computers—the trapped ion. The analysis in this paper expands on our earlier work on the trapped-ion problem (Ref. 17) and illustrates the key role played by the Quantum Transfer Graph in understanding the complex matrices that describe the interactions between the field and the ion. To our knowledge this is the only example of a quantum control problem where the interaction matrices are complex. Our general analysis of a sequentially connected system can also be extended to understanding the control of N-level chain systems used in adiabatic schemes such as STIRAP,[14] as well as the control of transitions between sequentially connected Zeeman states.

II. SCHRÖDINGER PICTURE

The Schrödinger equation for a particle in a static and dynamic potential (in atomic units, wherein $e=m=\hbar=1$) is written as

$$\imath|\dot{\Psi}\rangle = (H_0 + H_I)|\Psi\rangle. \tag{1}$$

Here, H_0 is the Hamiltonian of the particle in the static potential, with a finite number (N) of eigenvalues E_n corresponding to the eigenvectors ϕ_n. The interaction with the time-dependent potential is given by the control Hamiltonian H_I, which includes the time dependence. In general, we consider problems where the time dependence is separable and linear, for example, $H_I = \sum_i u_i(t) * \mu_i$. Here the operator μ_i represents the transition couplings between the various eigenstates of H_0 due to the time-dependent field $u_i(t)$. Unitarity demands that H_0 and H_I be Hermitian. The eigenvalues of H_0 are therefore real. In the control literature, the Schrödinger equation is written equivalently as

$$\dot{X} = \left(A + \sum_i u_i(t) B_i\right) X. \tag{2}$$

In vector representation, X is the state vector, A is the drift matrix, B_i are the control matrices and $u_i(t)$ are controls, generally chosen to be piecewise smooth. In the eigenbasis of H_0, A is $-\imath$ times a real matrix with only diagonal terms. Each matrix B_i is skew-Hermitian. It can, in general, be written as a sum of a $\imath$ times a real symmetric matrix and a skew-symmetric matrix, $B_i = \imath * B_i^S + B_i^K$. More generally, $A, B_i \in \mathfrak{su}(N)$. In most quantum applications considered up to this point[2,4,15] the matrix elements of the B_i are of the form $\imath$ times a symmetric matrix. Consider a special case, where the eigenstates of H_0 are sequentially coupled by control fields $u_i(t)$. It is well known[3,9,11] that a sufficient condition for controllability is that the dimension of the span of the Lie algebra generated by A and the B_i be equal to the dimension of $\mathfrak{su}(n)$. Rather than take the specific values for the matrix elements of the control matrices, B_i, it will be instructive to consider its general structure—a skew-Hermitian, tridiagonal matrix with zero diagonal elements. In the case where B is of the form $\imath$ times a symmetric matrix, this matrix can be decomposed into $N-1$ matrices—simple roots of the Lie algebra $\mathfrak{su}(n)$, as shown below. These matrices represent the nearest-neighbor couplings. We want to elucidate how these nearest-neighbor couplings generate the Lie algebra. Note that we do not have control over each individual coupling. Nevertheless, one can see how decomposing the control matrix into the simple roots is a powerful way to examine the controllability properties of the system.

Using standard notation for a basis of $\mathfrak{su}(N)$, let $e_{i,j}$ denote the matrix with unit ij entry and zeros elsewhere. Define $x_{i,j} = e_{i,j} - e_{j,i}$ and $y_{i,j} = \imath(e_{i,j} + e_{j,i})$. B is decomposed into the $\imath$-times-symmetric roots

$$S_1 = y_{1,2} = \imath \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & \cdots \\ 1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{3}$$

$$S_2 = y_{2,3}, \tag{4}$$

$$S_3 = y_{3,4}, \tag{5}$$

$$\cdots. \tag{6}$$

The Lie bracket of these roots with each other give the $N-2$ skew-symmetric matrices that represent next-nearest-neighbor coupling as shown below. These matrices form a closed Lie algebra with the matrices from which they were formed, for example, S_1, S_2 and their commutator

$K_N=[S_1,S_2]$ form a Lie subalgebra, similarly for S_2, S_3 and their commutator K_{N+1}, and so on. This generation of alternate symmetric and skew-symmetric elements of the algebra has been observed earlier,[3,13]

$$[S_1,S_2]=x_{1,3}\equiv K_N, \tag{7}$$

$$K_{N+1}=x_{2,4}, \tag{8}$$

$$\cdots. \tag{9}$$

Similarly,

$$[x_{1,3},x_{2,4}]=y_{1,4}\equiv S_{2N-1}. \tag{10}$$

Carrying on in a similar fashion through the matrix that represents the coupling between the first and Nth state (here N is assumed even),

$$S_{N(N-1)/2}=y_{1,N}. \tag{11}$$

It can be shown that the number of linearly independent commutators formed by this set of matrices is $N(N-1)/2$. Thus, the roots of the control Hamiltonian can be used to produce $N(N-1)/2$ independent elements of the algebra.

An interesting observation can be made if the control matrices B_i representing the nearest-neighbor couplings are all skew-symmetric. The Lie algebra generated by these matrices consists of the skew-symmetric matrices, i.e., the symmetric matrices S_n are not generated. These matrices also number $N(N-1)/2$. This is the set of generators for the rotation group $O(N)$, each pairwise coupling representing an independent rotation in N-dimensions.[16]

Thus, if the eigenstates are sequentially connected by the transition matrix elements (usually real), then the Lie algebra generated by the roots of the control terms alone span a space of $N(N-1)/2$. If the drift matrix is strongly regular,[12] it can be decomposed into N linearly independent traceless diagonal matrices $h_i=e_{i,i}-e_{i+1,i+1}$. The Lie brackets formed by the drift matrix and the $N(N-1)/2$ matrices computed above yield another $N(N-1)/2$ matrices of the opposite symmetry. For example, $[A,S_1]$ gives K_1, etc. Thus the total number of linearly independent matrices are $2*N(N-1)/2+N=N^2$, which is sufficient to show controllability.

III. QUANTUM TRANSFER GRAPHS

Graphical methods used to analyze controllability of quantum systems[4,17] are drawn from similar techniques used in the controllability analysis of classical systems.[12] These methods are very elegant. However, they do not bring out two features intrinsic to the controllability of quantum systems—the special role of the drift matrix, and the intrinsically skew-Hermitian nature of the control matrices. To address these issues, we propose that transfer graphs representing the control of quantum systems should be drawn with each eigenstate represented by a double node, representing the real and imaginary parts of the complex wave function. The transition matrix elements are represented by edges of the graph. However, a real matrix element will couple the real part of one state with the real part of the other; and the imaginary part of one state with the imaginary part of the other. A purely imaginary matrix element will couple the real part of one state with the imaginary part of the other. This graph will truly be transitively connected only if the transition matrix elements are complex numbers with both real and imaginary parts. Otherwise the presence of a strongly regular drift matrix (which in time produces a rotation from real to imaginary space) can generate the "missing" elements of the Lie algebra, i.e., complete the transitivity of the Quantum Transfer Graph. These features of Quantum Transfer Graphs are shown in Fig. 1. Other modifications introduced in a recent paper[17] such as ordering the state in energy and the thickness of the edges representing the strength of the couplings are retained.

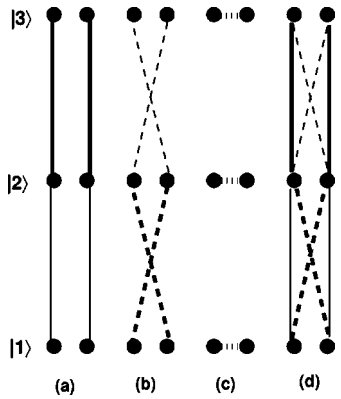

FIG. 1. Features of a Quantum Transfer Graph. Three nondegenerate eigenstates of the field-free Hamiltonian are represented by double nodes, representing the real (left) and imaginary (right) parts of the complex wave function. States that are transitively connected in the classical sense are not necessarily connected when the doublet structure is employed. A control matrix with $\imath$ times symmetric structure connects nodes as shown in (a). A control matrix with real, skew-symmetric structure connects nodes as shown in (b). The drift Hamiltonian causes rotations between the real and imaginary nodes of each eigenstate as in (c). The control matrix with a general complex, skew-Hermitian structure transitively connects the real *and* imaginary parts of the eigenstates as in (d).

IV. CONTROL IN THE INTERACTION PICTURE

In quantum physics, one often uses the interaction picture by making a unitary transformation that is very similar to transforming into the rotating frame in classical physics. Remembering that A is diagonal and $=\imath H_0$, this is carried out as follows:

$$Y = \exp(-At)X, \tag{12}$$

$$\dot{Y} = -A\exp(-At)X + \exp(-At)\dot{X} \tag{13}$$

$$= -A\exp(-At)X + \exp(-At)(A + \sum_i u_i(t)B_i)X \tag{14}$$

$$= \sum_i u_i(t)\exp(-At)B_iX \tag{15}$$

$$= \sum_i u_i(t)\exp(-At)B_i\exp(At)Y \tag{16}$$

$$= \sum_i u_i(t)\left[B_i + \frac{-t}{1!}[A,B_i] + \frac{(-t)^2}{2!}[A,[A,B_i]] + \cdots\right]Y \tag{17}$$

$$= \sum_i u_i(t)\tilde{B}_iY. \tag{18}$$

The transformed state vector Y evolves on an adjoint orbit of $U(n)$ with a span of $N(N-1)$. The last expansion (Baker–Campbell–Hausdorff expansion) contains the Lie algebra formed by the drift and control matrices. In the case that the system is controllable, these matrices span a space of dimension $N(N-1)$. Therefore, the presence of a strongly regular drift matrix, and a transitively

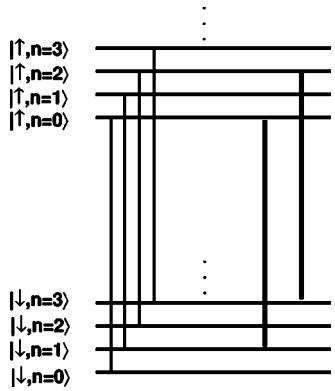

FIG. 2. Trapped-ion quantum states coupled by control fields with frequencies ω_c and ω_r. They cause transitions denoted by solid (carrier) and dashed (red sideband) lines, respectively. By changing the strength of the trap, it is possible to reduce one of the transition strengths to zero, thus truncating the infinitely large Hilbert space.

connected set of eigenstates is sufficient to show controllability. In exactly the same manner, if a set of eigenstates is transitively connected in the interaction picture, and the drift matrix is strongly regular, then these are sufficient conditions to establish controllability as well.

We note that if we have a control matrix that has both symmetric and skew-symmetric parts as in Fig. 1(d), we know that we can generate the $N(N-1)$ elements of the algebra. The Quantum Transfer Graph is transitively connected even without the consideration of the drift matrix. In such a case the demand for the strongly regular drift matrix can be relaxed, and controllability can be shown even with drift matrices that are not strongly regular.[12]

V. SPIN-$\frac{1}{2}$ PARTICLE COUPLED TO FINITE HARMONIC OSCILLATOR

We now apply controllability analysis to a quantum system that is one of the scalable paradigms of a future quantum computer. The system is also interesting from the viewpoint of control, because the control matrices contain both symmetric and skew-symmetric elements. Our analysis can be extended to other systems with sequentially connected eigenstates such as those in N-level STIRAP, and the control of Zeeman states.

In a recent paper,[17] we showed that under certain circumstances, the model of a spin-$\frac{1}{2}$ particle coupled to finite harmonic oscillator is a good representation of a trapped ion with two essential internal states. The spin-$\frac{1}{2}$ model represents a two-level atom with an energy splitting $\hbar\omega_0$, where the frequency $\omega_0/2\pi$ is in the several GHz range. The atomic levels are coupled to the motion of the ion in a harmonic trap.[18] These quantized vibrational energy levels are separated by a frequency $\omega_m/2\pi$ in the MHz range. The Hamiltonian of this system without a control field applied to it (in atomic units) is

$$H_0 = \omega_0 \frac{\sigma_z}{2} + \omega_m \hat{n}. \tag{19}$$

The Pauli operator σ describes the equivalent spin-$\frac{1}{2}$ system, and the operator $\hat{n}$ is the number operator of the quantized simple harmonic oscillator. The eigenstates of the field-free system are characterized by two quantum numbers S_z, and n. When a bichromatic field is applied that causes transitions between states $|\downarrow,n\rangle$ and $|\uparrow,n\rangle$ (carrier transitions), and between states $|\downarrow,n\rangle$ and $|\uparrow,n-1\rangle$ (red sideband transitions), the system is sequentially connected. An important parameter of this system is the Lamb–Dicke parameter η_m that describes the extent of the ion's motion compared to the wavelength of the applied electromagnetic field. It is possible to adjust the strength of the trap (thereby adjusting η_m) such that one of the transition couplings goes to zero, and the state space is truncated to N-levels as shown in Fig. 2.

In the case when the extent of the ion's motion is comparable to the wavelength of the applied field, a matrix element of the control Hamiltonian in the field-free eigenbasis in the interaction picture can be written as[17]

$$\langle S'n'|H_I'|Sn\rangle = \Omega(t)2\ \mathrm{Re}[\langle S'|\sigma_+|S\rangle \otimes \langle n'|\exp(\imath(\eta_m(a_m + a_m^\dagger)))|n\rangle]. \tag{20}$$

The harmonic oscillator part of this matrix element[18] is written as

$$\langle n'|\exp(\imath(\eta_m(a_m + a_m^\dagger)))|n\rangle = \exp(-\eta_m/2)\sqrt{\frac{n_<!}{n_>!}}(\imath\eta_m)^{|n'-n|}L_n^{|n'-n|}(\eta_m^2). \tag{21}$$

The symbol $n_>$ refers to the larger of n and n', and $n_<$ refers to the smaller of n and n'. $L_n^\alpha(x)$ is the associated Laguerre polynomial. When the applied field connects states $|\downarrow,n\rangle$ and $|\uparrow,n\rangle$ (carrier transitions), $n'=n$, and when the applied field connects states $|\downarrow,n\rangle$ and $|\uparrow,n-1\rangle$ (red sideband transitions), $n'=n-1$. The matrix elements are zero for all other values of n'. The strength of the ion trap can be adjusted (thereby adjusting η_m) so that the coupling strength of one of the (red or carrier) transitions becomes zero, the system is transformed into a finite closed subsystem, and a remaining infinite subsystem. For example, if the argument of the Laguerre polynomial η_m^2 is adjusted to 0.527 667 so that $L_6^1(\eta_m^2)=0$, the $|\downarrow,6\rangle$ to $|\uparrow,7\rangle$ transition is turned off.

The truncated finite system is now an N-level sequentially dipole coupled system. The electric field corresponding to the frequencies that cause the carrier and red transitions are dubbed E_c and E_r, respectively. The eigenstates can be ordered as $|\uparrow,0\rangle$, $|\downarrow,0\rangle$, $|\uparrow,1\rangle$, $|\downarrow,1\rangle,\ldots$. The drift Hamiltonian H_0 of this system can be written in matrix form as

$$\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \omega_0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & 0 & \omega_m & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & 0 & 0 & \omega_0+\omega_m & 0 & 0 & \cdots & 0 & 0 \\
0 & 0 & 0 & 0 & 2\omega_m & 0 & \cdots & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \omega_0+2\omega_m & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & & \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & \left(\frac{N}{2}-1\right)\omega_m & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & \omega_0+\left(\frac{N}{2}-1\right)\omega_m
\end{pmatrix}. \tag{22}$$

In the interaction picture, the Schrödinger equation is written as

$$\dot{Y} = (u(t)B_c + v(t)B_r)Y. \tag{23}$$

In general, we can assume that fields $E_c(t)$ and $E_r(t)$ do not have a phase difference between them. Then,

$$u(t) = c_1E_c(t) = 0.25\mu_0\exp(-\eta^2/2)E_c(t), \tag{24}$$

$$v(t) = c_2E_r(t) = 0.25\eta\mu_0\exp(-\eta^2/2)E_r(t), \tag{25}$$

$$B_c = \imath \begin{pmatrix} 0 & L_0(\eta^2) & 0 & 0 & 0 & 0 & \cdots \\ L_0(\eta^2) & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & L_1(\eta^2) & 0 & 0 & \cdots \\ 0 & 0 & L_1(\eta^2) & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & L_2(\eta^2) & \cdots \\ 0 & 0 & 0 & 0 & L_2(\eta^2) & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{26}$$

$$B_r = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & L_0^{(1)}(\eta^2) & 0 & 0 & 0 & \cdots \\ 0 & -L_0^{(1)}(\eta^2) & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & L_1^{(1)}(\eta^2) & 0 & \cdots \\ 0 & 0 & 0 & -L_1^{(1)}(\eta^2) & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & -L_2^{(1)}(\eta^2) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{27}$$

The associated Laguerre polynomials $L_n^{\alpha}(x)$ can be written as

$$L_n^{\alpha}(x) = \sum_{k=0}^{n} (-1)^k \binom{n+\alpha}{n-k} \frac{x^k}{k!}. \tag{28}$$

The argument of the polynomials is the square of the Lamb–Dicke parameter η which gives a measure of how much the ion moves in the harmonic potential as compared to the wavelength of the light applied. We note that the control matrices for this system are different from the usual control matrices in quantum physics problems. The control matrix $\tilde{B}_c$ has the usual $\imath$ times symmetric structure. The control matrix $\tilde{B}_r$ has a real, skew-symmetric structure. If we take the Lie algebra formed by these two matrices, we get $N(N-1)/2$ independent matrices. As the drift matrix is strongly regular this system is completely controllable. We can further analyze this behavior in a four-dimensional model problem.

A. Example: A model four-dimensional system

Using a simple four-dimensional example,[2,19] we show how the Lie algebra produces successive elements, and spans the space. Consider a general matrix A for a four-dimensional Hilbert space with sequentially coupled eigenstates. In particular, we have

$$A = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & c & 0 \\ 0 & 0 & 0 & d \end{pmatrix}, \tag{29}$$

$$B_c = \imath \begin{pmatrix} 0 & \alpha & 0 & 0 \\ \alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma \\ 0 & 0 & \gamma & 0 \end{pmatrix}, \tag{30}$$

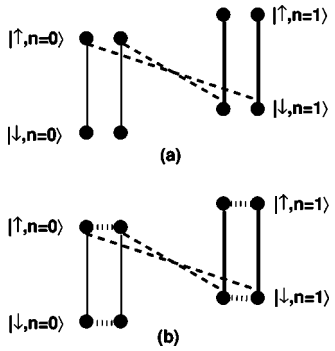

FIG. 3. Quantum Transfer Graph of a model four-level system. Control fields with frequencies ω_c and ω_r cause transitions denoted by solid (carrier) and dashed (red sideband) lines, respectively. The dotted lines in (b) demonstrate the effect of the drift Hamiltonian in rotating between the real and imaginary parts of each eigenfunction.

$$B_r = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \beta & 0 \\ 0 & -\beta & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{31}$$

Taking the Lie brackets of B_c and B_r, we produce four more linearly independent matrices $C=[B_c,B_r]/\beta$, $D=([B_c,C]-B_r*(\alpha^2+\gamma^2)/b)/(2\alpha\gamma)$, $E=[B_c,D]$, and $F=[E,B_r]/(-\beta)$. Thus the control matrices themselves produce $N(N-1)/2=6$ elements of the Lie algebra. Taking the Lie brackets of these six matrices with the drift matrix A, we get six more independent matrices with the opposite symmetry as the first six. Further Lie brackets of the two sets of six matrices produce the remaining four diagonal traceless matrices into which the strongly regular drift matrix can be decomposed.

B. Graphical analysis

We create a Quantum Transfer Graph to represent and analyze this system. We represent the various eigenstates $|\hat{S},n_m\rangle$ by double-vertices of a graph as shown in Fig. 3. When a resonant electromagnetic field is applied, the coupling between two eigenstates caused by the interaction form the edges. The eigenstates are ordered in energy, and the edges on the graph will represent the matrix elements of the interaction between the eigenstates (not a population flow between them), their thickness qualitatively indicating the strength of the coupling. The carrier field (with frequency ω_c) acting on an ion connects states $|\downarrow n\rangle$ and $|\uparrow n\rangle$. As the coupling matrix consists of real elements, this field connects the real parts to the real parts and the imaginary parts to the imaginary parts. The red sideband field (with frequency ω_r) connects states $|\downarrow n\rangle$ and $|\uparrow n-1\rangle$. Since the coupling matrix consists of imaginary elements, this field connects the real parts to the imaginary parts and vice versa. When both fields are applied simultaneously, we see that the Quantum Transfer Graph splits into two very interesting subgraphs. In the sense of the usual transfer graph,[4,20] all eigenstates are transitively connected. However, we can directly see the role of the drift Hamiltonian in moving this system from one subgraph to the other, and truly making the eigenstates transitively connected.

VI. SPECIFIC CONTROL SCHEME

We now discuss a specific control scheme for the *infinite* system, and show how the Quantum Transfer Graph helps us to describe the roles of the control and drift matrices in this scheme. In 1996, Law and Eberly[21] showed that by using the carrier and red fields *alternately* it is possible to produce arbitrary superpositions of a finite number of harmonic oscillator states. References 22 and 23 show that the same scheme can be used to generate arbitrary finite superposition states in

a spin-$\frac{1}{2}$/harmonic oscillator system. This scheme works by designing a sequence of alternately applied carrier and red sideband fields interspersed with a waiting time (action of the drift) in order to transfer the population from an arbitrary superposition to the ground state of the system $|\downarrow, n=0\rangle$. As seen by the Quantum Transfer Graph in Fig. 3(b), there are many combinations of the drift and control matrices that can be applied in order to get to the ground state (both in the finite and the infinite systems). The optimal combination will be one that time-optimizes the process subject to the constraint on the fields' intensities. This time-optimized Law–Eberly scheme is an interesting avenue for future work. Aspects of the controllability of the infinite-dimensional problem are discussed in related work by the authors.[24]

VII. CONCLUSION

A Quantum Transfer Graph is an effective tool in elucidating the controllability of finite quantum systems both in the Schrödinger and interaction pictures. We have shown the equivalence of sufficient conditions for controllability in both pictures, and explicitly presented the role of the drift matrix. We analyze the example of a sequentially connected N-level system as implemented by suitably designed quantum states of a trapped ion. Showing the mechanism of control, we explain how the specific Law–Eberly control scheme can be efficiently implemented.

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Asymptotic of complex hyperbolic geometry and L^2-spectral analysis of Landau-like Hamiltonians

Allal Ghanmi[a] and Ahmed Intissar[b]
Department of Mathematics, Faculty of Sciences, Agdal Mohammed V University, Rabat, Morocco

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In this paper we show that the flat Hermitian complex geometry of $\mathbb{C}^n$, $n \geqslant 1$, is approximated by the complex hyperbolic geometry of the Bergman complex balls $\mathbb{B}^n_\rho \subset \mathbb{C}^n$ of radius $\rho > 0$. Furthermore, it will be shown that some elements of the L^2-spectral analysis, such as the spectrum, the L^2-eigenprojector and the resolvent kernels, associated to the so-called Landau-like Hamiltonian $H_{B,\rho}$ on $\mathbb{B}^n_\rho$ give rise to their analogous of the Landau-like Hamiltonian $H_{B,\infty}$ on $\mathbb{C}^n$ by letting ρ tend to infinity. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1853505]

I. INTRODUCTION

Let $\mathcal{P}=\{w=x+iy; y>0\}$ be the upper-half plane endowed with the Poincaré metric

$$ds^2(\rho) = \frac{\rho^2}{4}\left(\frac{dx^2+dy^2}{y^2}\right),$$

where ρ is a non-negative real number. The metric $ds^2(\rho)$ is scaled such that the constant scalar curvature of the real hyperbolic plane $\mathcal{P}$ is equal to $-4/\rho^2$.

In Ref. 6, A. Comtet considered one parameter family of magnetic Schrödinger operators (or Maass Laplacians) $H_{B,\rho}$ given on $\mathcal{P}$ by

$$H_{B,\rho} = -4\left\{\frac{y^2}{\rho^2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right) - 2iBy\frac{\partial}{\partial x} - B^2\rho^2\right\}, \quad B>0, \tag{1}$$

and discussed some of their asymptotic spectral properties when ρ goes to $+\infty$. In particular, the finite point spectrum in $L^2(\mathcal{P};(\rho^2/4)(dx\,dy/y^2))$ of $H_{B,\rho}$ goes to the Landau levels

$$4B(2l+1), \quad l=0,1,2,\ldots,$$

that correspond to the pure point spectrum in $L^2(\mathbb{R}^2;dxdy)$ of the magnetic Schrödinger operator $H_{B,\infty}$, associated to the vector potential $A=(2By,-2Bx,0)$, given in x,y coordinates by

$$H_{B,\infty} = -\left\{\left(\frac{\partial^2}{\partial x^2}+2iBy\right)^2 + \left(\frac{\partial^2}{\partial y^2}-2iBx\right)^2\right\}$$

or in the complex coordinate $z=x+iy$ as

$$H_{B,\infty} = -4\left\{\frac{\partial^2}{\partial z\,\partial\bar{z}} + B\left(z\frac{\partial}{\partial z}-\bar{z}\frac{\partial}{\partial\bar{z}}\right) - B^2|z|^2\right\}.$$

The operators $H_{B,\rho}$ and $H_{B,\infty}$ (called also Landau Hamiltonians) describe the Hamiltonians of a charged nonrelativistic particle moving under the action of an external uniform magnetic field

[a]Electronic mail: aghanmi@math.net
[b]Electronic mail: intissar@fsr.ac.ma

acting on $\mathcal{P}$ and $\mathbb{R}^2$, respectively. The magnetic Schrödinger operator $H_{B,\rho}$ on $\mathcal{P}$ given by (1) can be intertwined, via Cayley transform, with the Laplacian $H_{B,\rho}$ of the hyperbolic complex disc $\mathbb{B}^1_\rho=\{z\in\mathbb{C};|z|<\rho\}$, which is given in the complex coordinate z of $\mathbb{B}^1_\rho$ by

$$H_{B,\rho}=-4\left(1-\left|\frac{z}{\rho}\right|^2\right)\left\{\left(1-\left|\frac{z}{\rho}\right|^2\right)\frac{\partial^2}{\partial z\,\partial\bar{z}}+B\left(z\frac{\partial}{\partial z}-\bar{z}\frac{\partial}{\partial\bar{z}}\right)\right\}+4B^2|z|^2.$$

Therefore, to have a natural generalization of the above Laplacians $H_{B,\rho}$ and $H_{B,\infty}$ to higher complex dimensions, one may replace the plane $\mathbb{C}$ by the Hermitian complex space $\mathbb{C}^n$, $n\geqslant 1$, and the real hyperbolic disc $\mathbb{B}^1_\rho$ by the Bergman complex ball $\mathbb{B}^n_\rho$ of radius $\rho>0$. Here, the Bergman ball $\mathbb{B}^n_\rho$ will be viewed as the bounded realization of the rank one Hermitian symmetric space of noncompact type [i.e., the complex hyperbolic space $\mathbb{H}^n(\mathbb{C})$] whose holomorphic sectional curvature S_ρ is known to be a negative constant that we will be scaling here to be equal to $-4/\rho^2$. Namely, we can set the following.

Definition 1: Let B be a fixed real number and $\rho>0$. Then

(i) *The Landau-like Hamiltonian $H_{B,\rho}$ on the Bergman ball $\mathbb{B}^n_\rho$ is defined to be equal to*

$$H_{B,\rho}=-4\left(1-\left|\frac{z}{\rho}\right|^2\right)\left\{\sum_{i,j=1}^{n}(\delta_{ij}-\frac{z_i\bar{z}_j}{\rho^2})\frac{\partial^2}{\partial z_i\,\partial\bar{z}_j}+B\sum_{j=1}^{n}\left(z_j\frac{\partial}{\partial z_j}-\bar{z}_j\frac{\partial}{\partial\bar{z}_j}\right)\right\}+4B^2|z|^2.$$

(ii) *The Landau-like Hamiltonian $H_{B,\infty}$ on the Hermitian space $\mathbb{C}^n$ is defined to be equal to*

$$H_{B,\infty}=-4\left\{\sum_{j=1}^{n}\frac{\partial^2}{\partial z_j\,\partial\bar{z}_j}+B\sum_{j=1}^{n}\left(z_j\frac{\partial}{\partial z_j}-\bar{z}_j\frac{\partial}{\partial\bar{z}_j}\right)-B^2|z|^2\right\}.$$

Here we shall note that such Hamiltonians had been considered and studied by many authors in different contexts of both mathematics and physics. Thus, for the unit complex disc case ($n=1$ and $\rho=1$), one can refer to the interest papers (Refs. 14, 17, 8, 18, and 9). And for the unit complex ball ($n\geqslant 2$, $\rho=1$), the reader can refer to the works in Refs. 11, 13, 19, 1, 5, and 3. Also let us note that the operators $H_{B,\infty}$ on $\mathbb{C}^n=\mathbb{R}^{2n}$, which go back to Landau (for $n=1$), play an important role in many different contexts such as Feynman path integral. (in Feynman–Kac formula), oscillatory stochastic integral and theory of lattices electrons in uniform magnetic field. See Bellissard[4] and the rich list of references therein. However, apart Comtet work's[6] for $n=1$ (see also Ref. 7), both Landau-like Hamiltonians $H_{B,\rho}$ and $H_{B,\infty}$ had been studied separately in all previous cited works.

In the present paper, we discuss, when $\rho\to+\infty$, the asymptotic of the Kähler–Bergman geometry on the hyperbolic Bergman balls $\mathbb{B}^n_\rho$ of radius ρ centered at the origin of $\mathbb{C}^n$, $n\geqslant 1$. Further, we follow in spirit Comtet approach to give an analytic treatment which connect many aspect as spectral theory of the Landau-like Hamiltonians $H_{B,\rho}$ on $\mathbb{B}^n_\rho$ (L^2-point spectrum, the L^2-eigenprojectors and the resolvent kernels) to that of the Landau-like Hamiltonians $H_{B,\infty}$ on $\mathbb{C}^n$ ($n\geqslant 1$) by letting ρ go to infinity. Namely, the objective of our work is aimed to show in a rigorous mathematical sense the following statements.

(1) The curved complex hyperbolic geometry of the complex Bergman balls $\mathbb{B}^n_\rho$ of radius $\rho>0$ approximates in a natural intuitive way the flat Hermitian geometry of $\mathbb{C}^n$. This means that all geometrical elements on $\mathbb{B}^n_\rho$ such as the metric ds^2_ρ, the distance d_ρ, the volume form $d\mu_\rho$, the group of motions $G_\rho,\ldots$, converge to their analogous on $\mathbb{C}^n$ when $\rho\to+\infty$; see Table I.

(2) Let

$$\sigma_d(H_{B,\rho})=\left\{4B(2l+n)-4\frac{l(l+n)}{\rho^2};l\in\mathbb{Z}^+,0\leqslant l<B\rho^2-\frac{n}{2}\right\}$$

be the finite set of the point spectrum of the Landau-like Hamiltonian $H_{B,\rho}$ in the Hilbert space $L^2(\mathbb{B}^n_\rho;d\mu_\rho)$. Then obviously we have

TABLE I. Asymptotic of metric and action objects on $\mathbb{B}_\rho^n$.

Metric and action objects on $\mathbb{B}_\rho^n$, $\rho>0$	Their asymptotic on $\mathbb{C}^n=\lim_{\rho\to+\infty}\mathbb{B}_\rho^n$
Hermitian metric ds_ρ^2, $ds_\rho^2=(1-\lvert z/\rho\rvert^2)^{-2}\times\Sigma_{i,j=1}^n((1-\lvert z/\rho\rvert^2)\delta_{i,j}+\bar z_i z_j/\rho^2)dz_j\otimes d\bar z_j$	Euclidean metric ds_∞^2, $ds_\infty^2:=\Sigma_{j=1}^n dz_j\otimes d\bar z_j$
Holomorphic sectional curvature $S_\rho=-4/\rho^2$	Flat curvature $S_\infty=0$
Bergman distance $d_\rho(z,w)$, $\cosh^2(d_\rho(z,w)/\rho)=\lvert\rho^2-\langle z,w\rangle\rvert^2/(\rho^2-\lvert z\rvert^2)(\rho^2-\lvert w\rvert^2)$	Euclidean distance $d_\infty(z,w)d_\infty(z,w):=\lvert z-w\rvert$
Volume form $d\mu_\rho(z)$, $d\mu_\rho(z)=(1-\lvert z/\rho\rvert^2)^{-n-1}\,dm(z)$	Lebesgue form $d\mu_\infty(z)$, $d\mu_\infty(z)=dm(z)$
Kähler 2-form $\Omega_\rho(z)$, $\Omega_\rho(z)=(1-\lvert z/\rho\rvert^2)^{-2}\times\Sigma_{i,j=1}^n((1-\lvert z/\rho\rvert^2)\delta_{i,j}+\bar z_i z_j/\rho^2)dz_i\wedge d\bar z_j$	Kähler 2-form $\Omega_\infty(z)$, $\Omega_\infty(z)=\Sigma_{j=1}^n dz_j\wedge d\bar z_j$
Vector potential $\theta_\rho(z)$, $\theta_\rho(z)=-i(1-\lvert z/\rho\rvert^2)^{-1}\times\Sigma_{j=1}^n(\bar z_j\,dz_j-z_j\,d\bar z_j)$	Vector potential $\theta_\infty(z)$, $\theta_\infty(z)=-i\Sigma_{j=1}^n(\bar z_j\,dz_j-z_j\,d\bar z_j)$
Group of motions G_ρ on $(\mathbb{B}_\rho^n,ds_\rho^2)$, $G_\rho=\{g_\rho=\left(\begin{smallmatrix}A_\rho & B_\rho\\ C_\rho & D_\rho\end{smallmatrix}\right)\in M_{n+1}(\mathbb{C});g_\rho J^{-1}(\rho)g_\rho^*=J^{-1}(\rho),\det(g_\rho)=1\}$	Group of motions G_∞ on $(\mathbb{C}^n,ds_\infty^2)$, $G_\infty=\{g_\infty=\left(\begin{smallmatrix}A & B\\ 0 & (\det A)^{-1}\end{smallmatrix}\right);A\in U(n),B\in\mathbb{C}^n\}$
Homographic action of G_ρ on $\mathbb{B}_\rho^n$, $g_\rho.z=(A_\rho z+B_\rho)\times(C_\rho z+D_\rho)^{-1}$	Affine action of G_∞ on $\mathbb{C}^n$, $g_\infty.z=(\det A)(Az+B)$
Automorphic factor $j_\rho^B(g_\rho,z)$, $B\in\mathbb{R}$, $j_\rho^B(g_\rho,z)=\left(\rho^2-\overline{\langle z,g_\rho^{-1}.0\rangle}/\rho^2-\langle z,g_\rho^{-1}.0\rangle\right)^{B\rho^2}$	Automorphic factor $j_\infty^B(g_\infty,z)$, $\underline{B\in\mathbb{R}}$, $j_\infty^B(g_\infty,z)=e^{B(\langle z,g_\infty^{-1}.0\rangle-\langle z,g_\infty^{-1}.0\rangle)}$

$$\lim_{\rho\mapsto+\infty}\sigma_d(H_{B,\rho})=\{\lambda_l:=4B(2l+n);\quad l=0,1,2,\ldots\},$$

which gives the so-called Landau energy levels for the Landau-like Hamiltonian $H_{B,\infty}$ on $\mathbb{C}^n$. Further, if $K_{l,\rho}^B(z,w)$ denotes the L^2-eigenprojector kernel of the L^2-eigenspace

$$A_l^{2,B}(\mathbb{B}_\rho^n)=\left\{F\in L^2(\mathbb{B}_\rho^n;d\mu_\rho)/H_{B,\rho}F=\left(4B(2l+n)-4\frac{l(l+n)}{\rho^2}\right)F\right\}$$

then $K_{l,\rho}^B(z,w)$ converges, when ρ tends to $+\infty$, to $K_{l,\infty}^B(z,w)$ the L^2-eigenprojector kernel of the L^2-eigenspace

$$A_l^{2,B}(\mathbb{C}^n)=\{F\in L^2(\mathbb{C}^n;dm)/H_{B,\infty}F=4B(2l+n)F\};$$

see Theorem 1.

(3) Appropriately modified, the resolvent kernel of the Landau-like Hamiltonian $H_{B,\rho}$ converges, when $\rho\to+\infty$, to the resolvent kernel of the Landau Hamiltonian $H_{B,\infty}$ (Theorem 2).

Thus the paper is organized as follows: in Sec. II, we show that the Bergman–Kähler geometry on the Bergman balls $\mathbb{B}_\rho^n$ gives rise to the flat geometry of $\mathbb{C}^n$ by letting $\rho\to+\infty$; see Propositions 1 and 2, and Table I. In Sec. III, we give the geometrical realization of the Landau Hamiltonians on both $\mathbb{B}_\rho^n$ and $\mathbb{C}^n$ and we establish some of their invariance properties under the action of the groups of motions; see Proposition 4. In Sec. IV, we recall and we precise some L^2-spectral properties of $H_{B,\rho}$ and $H_{B,\infty}$. Finally, in Sec. V, we give the asymptotic proofs for L^2-spectral analysis of the Landau-like Hamiltonian $H_{B,\rho}$, when $\rho\to+\infty$, such as the L^2-eigenprojector kernels in Theorem 1 and resolvent kernels in Theorem 2.

We conclude this introduction by pointing out that our convergence theorems cannot be obtained just by a simple application of the general theorems in perturbation theory of the operator $H_{B,\rho}$ as in Rauch and Taylor work's.[16] Here the setting is quite different.

II. HERMITIAN STRUCTURE OF $\mathbb{C}^n$ AND BERGMAN–KÄHLER GEOMETRY OF THE BALLS $\mathbb{B}_\rho^n$.

Let $(\mathbb{C}^n,\langle .,.\rangle)$ be the usual n-dimensional Hermitian complex space endowed with its flat Kähler metric ds_∞^2,

$$ds_\infty^2 = \sum_{j=1}^{n} dz_j \otimes d\bar{z}_j. \tag{2}$$

The Euclidean distance $d_\infty(z,w)$ and the volume measure $d\mu_\infty(z)$ associated to ds_∞^2 are given, respectively, by

$$d_\infty(z,w) = |z-w|,$$

$$d\mu_\infty(z) = dm(z) \quad \text{(Usual Lebesgue measure on } \mathbb{C}^n).$$

For ρ fixed in $]0,+\infty[$, let $\mathbb{B}_\rho^n$ be the centered ball in $\mathbb{C}^n$ of radius ρ. That is

$$\mathbb{B}_\rho^n = \{z=(z_1,z_2,\ldots,z_n) \in \mathbb{C}^n;\ |z|^2 = |z_1|^2 + |z_2|^2 + \cdots + |z_n|^2 < \rho^2\}.$$

We equip $\mathbb{B}_\rho^n$ with the scaled Bergman–Kähler metric ds_ρ^2,

$$ds_\rho^2 = \frac{\rho^2}{(\rho^2-|z|^2)^2} \sum_{i,j=1}^{n} \left((\rho^2-|z|^2)\delta_{i,j} + \bar{z}_i z_j\right) dz_i \otimes d\bar{z}_j. \tag{3}$$

The hyperbolic distance $d_\rho(z,w)$ and the volume measure $d\mu_\rho(z)$ associated to ds_ρ^2 on $\mathbb{B}_\rho^n$ are given, respectively, by

$$\cosh^2\left(\frac{d_\rho(z,w)}{\rho}\right) = \frac{|\rho^2 - \langle z,w\rangle|^2}{(\rho^2-|z|^2)(\rho^2-|w|^2)} \tag{4}$$

and

$$d\mu_\rho(z) = \frac{\rho^{2(n+1)}\, dm(z)}{(\rho^2-|z|^2)^{n+1}}.$$

Both $(\mathbb{C}^n, ds_\infty^2)$ and $(\mathbb{B}_\rho^n, ds_\rho^2)$ are complete Kähler manifolds. Further, the holomorphic sectional curvature of $(\mathbb{B}_\rho^n, ds_\rho^2)$ is a negative constant and is equal here to $S_\rho = -4/\rho^2$. Note that $\lim_{\rho\mapsto+\infty} S_\rho = 0$, which corresponds to the flat curvature of $(\mathbb{C}^n, ds_\infty^2)$.

Associated to $(\mathbb{C}^n, ds_\infty^2)$ and $(\mathbb{B}_\rho^n, ds_\rho^2)$ are their groups of motions G_∞ and "G_ρ". The group G_∞ can be represented by the solvable semidirect group $U(n) \ltimes \mathbb{C}^n$, where $U(n)$ denotes the unitary group of $\mathbb{C}^n$ with respect to $\langle .,.\rangle$. The elements $g_\infty \in G_\infty$ can be written as matrices in the form

$$g_\infty = \begin{pmatrix} A & B \\ 0 & (\det A)^{-1} \end{pmatrix}, \quad A \in U(n), \quad B \in \mathbb{C}^n.$$

Also, for fixed $\rho > 0$, the group "G_ρ" of $(\mathbb{B}_\rho^n, ds_\rho^2)$ is essentially isomorphic, as a Lie group, to the complex Lorentz group $SU(n,1)$. But, since we will be varying ρ in $]0,+\infty[$, we need to make the groups "G_ρ" varying smoothly in ρ. To do this let W^∞ be the group of smooth infinite paths in the vector space $M_{n+1}(\mathbb{C})$ of $(n+1)\times(n+1)$ complex matrices of $\mathbb{C}^{n+1}$. That is $W^\infty = \mathcal{C}^\infty(]0,+\infty[, M_{n+1}(\mathbb{C}))$. Instead of W^∞, we consider the following subgroup Σ^∞ of all paths $g \in W^\infty$ "preserving" the nondegenerate Hermitian form J_ρ on $\mathbb{C}^{n+1}$, corresponding to the $(n+1)\times(n+1)$-matrix $J(\rho)$ given by

$$J(\rho) := \begin{pmatrix} I_n & 0 \\ 0 & -\rho^2 \end{pmatrix},$$

such that $\lim_{\rho\to+\infty} g(\rho)$ exists and $\det(g(\rho))=1$ for every fixed $\rho>0$. That is

$$\Sigma^{\infty} = \left\{ g \in W^{\infty}; g^*(\rho)J(\rho)g(\rho) = J(\rho), \lim_{\rho\to+\infty} g(\rho) \text{exists and } \det(g(\rho)) = 1 \right\}.$$

Now, for every fixed $\rho>0$, let G_ρ denote the set of evaluations at ρ of all paths $g\in\Sigma^{\infty}$. That is $G_\rho := \{g(\rho);\quad g\in\Sigma^{\infty}\}$. Then G_ρ is a Lie group of dimension n^2+2n and it can be described as follows:

$$G_\rho = \{g(\rho) \in M_{n+1}(\mathbb{C});\quad g^*(\rho)J(\rho)g(\rho) = J(\rho),\quad \det(g(\rho)) = 1\},$$

or equivalently

$$G_\rho = \{g(\rho) \in M_{n+1}(\mathbb{C});\quad g(\rho)J^{-1}(\rho)g^*(\rho) = J^{-1}(\rho),\quad \det(g(\rho)) = 1\}. \tag{5}$$

Below, we will discuss the asymptotic of the groups G_ρ, when $\rho\to+\infty$. Namely, we have the following proposition.

Proposition 1: (i) Let g be a smooth path in Σ^{∞}. *Then we have* $\lim_{\rho\to+\infty} g(\rho)\in G_\infty = \mathrm{U}(n)\ltimes\mathbb{C}^n$.

(ii) For $g_\infty\in G_\infty$ *there exists at least one path* $g:\rho\mapsto g(\rho)$ *in* Σ^{∞} *such that* $g_\infty=\lim_{\rho\to+\infty} g(\rho)$.

Proof: For (i), we use (5) to see that for every fixed $\rho>0$ the element $g(\rho)=\left(\begin{smallmatrix} A(\rho) & B(\rho) \\ C(\rho) & D(\rho) \end{smallmatrix}\right)\in G_\rho$, satisfies the identity

$$g(\rho)\begin{pmatrix} I_n & 0 \\ 0 & -1/\rho^2 \end{pmatrix} g^*(\rho) = \begin{pmatrix} I_n & 0 \\ 0 & -1/\rho^2 \end{pmatrix}.$$

Therefore, if we set $g_\infty := \lim_{\rho\to+\infty} g(\rho)$, which exists by definition, we see that g_∞ satisfies the identity

$$g_\infty\begin{pmatrix} I_n & 0 \\ 0 & 0 \end{pmatrix} g_\infty^* = \begin{pmatrix} I_n & 0 \\ 0 & 0 \end{pmatrix}. \tag{6}$$

Therefore, writing g_∞ in the form $g_\infty=\left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)$, where A, B, C, and D are, respectively, the limit when $\rho\to+\infty$ of $A(\rho)$, $B(\rho)$, $C(\rho)$, and $D(\rho)$, we conclude from the identity (6) that A is a unitary matrix and that $C=0$. Finally, since $\det(g_\infty)=\lim_{\rho\to+\infty}\det(g(\rho))=1$, it follows that $D=(\det A)^{-1}$.

Now, for (ii), let us fix $g_\infty=\left(\begin{smallmatrix} A & B \\ 0 & D \end{smallmatrix}\right)\in G_\infty$ and set $B=\left(\begin{smallmatrix} v \\ t+is \end{smallmatrix}\right)$ with $v\in\mathbb{C}^{n-1}$, $n\geqslant 2$, and s, $t\in\mathbb{R}$. Also, for every fixed $\rho>0$, let us consider the matrix

$$g(\rho) = \begin{pmatrix} A & 0 \\ 0 & D \end{pmatrix} \cdot a_t(\rho) \cdot n_{v,s}(\rho), \tag{7}$$

where $a_t(\rho)$ and $n_{v,s}(\rho)$ are given, respectively, by

$$a_t(\rho) = \begin{pmatrix} I_{n-1} & 0 & 0 \\ 0 & \cosh\left(\dfrac{t}{\rho}\right) & \rho\sinh\left(\dfrac{t}{\rho}\right) \\ 0 & \dfrac{1}{\rho}\sinh\left(\dfrac{t}{\rho}\right) & \cosh\left(\dfrac{t}{\rho}\right) \end{pmatrix}$$

and

$$n_{(v,s)}(\rho)=\begin{pmatrix} I_{n-1} & -\dfrac{v}{\rho} & v \\ \dfrac{v^*}{\rho} & 1-\dfrac{|v|^2}{2\rho^2}-\dfrac{is}{\rho} & \dfrac{|v|^2}{2\rho}+is \\ \dfrac{v^*}{\rho^2} & -\dfrac{|v|^2}{2\rho^3}-\dfrac{is}{\rho} & 1+\dfrac{|v|^2}{2\rho^2}+\dfrac{is}{\rho} \end{pmatrix}.$$

Then it is clear from the above explicit formulas, that $a_t(\rho)$ and $n_{v,s}(\rho)$ are smooth paths in $\rho\in]0,+\infty[$. Further, for every fixed $\rho>0$, we can show by direct computation that the matrices $a_t(\rho)$ and $n_{v,s}(\rho)$ are in G_ρ. Hence, the element $g(\rho)$ belongs to G_ρ for all fixed ρ and so the mapping $\rho\mapsto g(\rho)$ is in Σ^∞. Furthermore, using again the explicit expressions involved in the construction of $g(\rho)$ in (7), it becomes easy to check that $\lim_{\rho\to+\infty} g(\rho)=g_\infty$. Thus, the proof of the proposition is completed.

Remark 1: (i) Note that the complex space $\mathbb{C}^n$ as well as the balls $\mathbb{B}_\rho^n$ can be realized as homogeneous spaces. Indeed, for $\mathbb{B}_\rho^n$, we have $\mathbb{B}_\rho^n=G_\rho/K_\rho$, where K_ρ, given by

$$K_\rho=\left\{k(\rho)=\begin{pmatrix} A(\rho) & 0 \\ 0 & (\det A(\rho))^{-1}\end{pmatrix};A(\rho)\in U(n)\ \text{and}\ \lim_{\rho\to+\infty} A(\rho)\ \text{exists}\right\},$$

is the isotropic group at the origin $0\in\mathbb{B}_\rho^n$ of the transitive action of the group G_ρ on $\mathbb{B}_\rho^n$ that is given by

$$g(\rho)\,.\,z=\big(A(\rho)z+B(\rho)\big)\big(C(\rho)z+D(\rho)\big)^{-1}, \tag{8}$$

where we have set $g(\rho)=\left(\begin{smallmatrix} A(\rho) & B(\rho)\\ C(\rho) & D(\rho)\end{smallmatrix}\right)\in G_\rho$, with $A(\rho)\in M_{n,n}(\mathbb{C})$, $B(\rho)\in M_{1,n}(\mathbb{C})$, $C(\rho)\in M_{n,1}(\mathbb{C})$ and $D(\rho)\in\mathbb{C}$ depending smoothly in ρ. In (8) the point $z\in\mathbb{B}_\rho^n$ is viewed as a $(1\times n)$-matrix so that $C(\rho)z+D(\rho)$ is nothing than a complex number.

Similarly we have $\mathbb{C}^n=(\mathrm{U}(n)\ltimes\mathbb{C}^n)/\mathrm{U}(n)$, where the group $G_\infty=\mathrm{U}(n)\ltimes\mathbb{C}^n$ acts on $\mathbb{C}^n$ by

$$g_\infty\,.\,z=\det(A)\big(Az+B\big)\quad\text{for } g_\infty=\begin{pmatrix} A & B\\ 0 & (\det A)^{-1}\end{pmatrix}\in G_\infty. \tag{9}$$

(ii) The actions of the groups G_ρ on $\mathbb{B}_\rho^n$ and G_∞ on $\mathbb{C}^n$, as defined above by (8) and (9), can be extended to smooth complex-valued functions by considering the following transformations:

$$[T_\rho^B(g_\rho)f](z):=j_\rho^B(g_\rho;z)f(g\,.\,z)\quad \textit{for } g_\rho\in G_\rho,\quad f\in C^\infty(\mathbb{B}_\rho^n),\quad z\in\mathbb{B}_\rho^n,$$

$$[T_\infty^B(g_\infty)f](z):=j_\infty^B(g_\infty;z)f(g\,.\,z),\quad \textit{for } g_\infty\in G_\infty,\quad f\in C^\infty(\mathbb{C}^n),\quad z\in\mathbb{C}^n,$$

where the automorphic factors $j_\rho^B(g_\rho;z)$ and $j_\infty^B(g_\infty;z)$ are given, respectively, by

$$j_\rho^B(g_\rho;z):=\left(\frac{\rho^2-\overline{\langle z,g_\rho^{-1}\,.\,0\rangle}}{\rho^2-\langle z,g_\rho^{-1}\,.\,0\rangle}\right)^{B\rho^2}\quad \textit{for } g_\rho\in G_\rho,\quad z\in\mathbb{B}_\rho^n, \tag{10}$$

$$j_\infty^B(g_\infty;z):=e^{B(\langle z,g_\infty^{-1}.0\rangle-\overline{\langle z,g_\infty^{-1}\,.\,0\rangle})}\quad \textit{for } g_\infty\in G_\infty,\quad z\in\mathbb{C}^n. \tag{11}$$

Now, for the limit of the metric objects associated to ds_ρ^2 and the action objects associated to the groups G_ρ on the hyperbolic Bergman ball $\mathbb{B}_\rho^n$, when $\rho\to+\infty$, we have the following.

Proposition 2:

(i) *The Bergman metric ds_ρ^2 converges to the Euclidean metric ds_∞^2 of $\mathbb{C}^n$.*
(ii) *The hyperbolic Bergman distance d_ρ converges to the Euclidean distance d_∞.*
(iii) *Let $g\in\Sigma^\infty$ and $g_\infty=\lim_{\rho\to+\infty} g(\rho)$. Then $\lim_{\rho\to+\infty} j_\rho^B(g(\rho),\cdot)=j_\infty^B(g_\infty,\cdot)$.*

Proof: (i) follows easily from the explicit expressions of the metrics ds_ρ^2 and ds_∞^2 as given in (3) and (2). Just note that the limit $\lim_{\rho\to+\infty} ds_\rho^2 = ds_\infty^2$ means here that for every fixed $z\in\mathbb{C}^n$ and ρ large enough the form $ds_\rho^2(u,v)$ is well defined for every u, v in the tangent space $T_z\mathbb{B}_\rho^n = T_z\mathbb{C}^n = \mathbb{C}^n$, and that we have $\lim_{\rho\to+\infty} ds_\rho^2(u,v) = ds_\infty^2(u,v)$.

To prove (ii) fix $(z,w)\in\mathbb{C}^n\times\mathbb{C}^n$. Then for ρ large enough the Bergman distance $d_\rho(z,w)$ is well defined through the identity (4), i.e.,

$$\cosh^2\left(\frac{d_\rho(z,w)}{\rho}\right) = \frac{|\rho^2 - \langle z,w\rangle|^2}{(\rho^2-|z|^2)(\rho^2-|w|^2)}.$$

Furthermore, using the explicit expression of the inverse function of $\cosh^2(x)$, $x\in[0,+\infty[$, we can rewrite it as follows:

$$d_\rho(z,w) = \frac{\rho}{2}\,\mathrm{Log}\left(1 + 2\sqrt{y-1}\left[\sqrt{y} + \sqrt{y-1}\right]\right), \quad \text{for } y\in[1,+\infty[,$$

where we have set

$$y = y_\rho(z,w) = \frac{|\rho^2 - \langle z,w\rangle|^2}{(\rho^2-|z|^2)(\rho^2-|w|^2)}.$$

Now, after direct computation, we can write $y-1$ in the following form:

$$y - 1 = \frac{\rho^2|z-w|^2}{(\rho^2-|z|^2)(\rho^2-|w|^2)} + \frac{|\langle z,w\rangle|^2 - |z|^2|w|^2}{(\rho^2-|z|^2)(\rho^2-|w|^2)}.$$

Thus, for $z\neq w$ and $\rho\to+\infty$, we have

$$y = 1 + O\left(\frac{1}{\rho^2}\right) \quad \text{and } y-1 = \frac{|z-w|^2}{\rho^2} + O\left(\frac{1}{\rho^2}\right).$$

Hence,

$$\sqrt{y} = 1 + O\left(\frac{1}{\rho}\right) \quad \text{and } \sqrt{y-1} = \frac{|z-w|}{\rho} + O\left(\frac{1}{\rho}\right).$$

Therefore, using the asymptotic of the logarithmic function $\mathrm{Log}(1+x) = x(1+O(x))$ for $x\to 0$, we deduce easily that the limit of $d_\rho(z,w)$ when $\rho\to+\infty$ exists and this limit is equal to $|z-w| =: d_\infty(z,w)$.

For the proof of (iii), it is clear that, for fixed $z\in\mathbb{C}^n$ and ρ large enough, the automorphic factor $j_\rho^B(g_\rho,z)$, $g_\rho = g(\rho)\in G_\rho$, as given in (10), is well defined. Thus, we can write it in the form

$$j_\rho^B(g_\rho,z) = \exp\left\{B\rho^2\left(\mathrm{Log}\left(1 - \frac{\langle z, g_\rho^{-1}.0\rangle}{\rho^2}\right) - \mathrm{Log}\left(1 - \frac{\overline{\langle z, g_\rho^{-1}.0\rangle}}{\rho^2}\right)\right)\right\},$$

where Log is the principal determination of the complex logarithm. But, since $\lim_{\rho\to+\infty} g_\rho\cdot w = g_\infty\cdot w$ for every $w\in K$, where $g_\infty := \lim_{\rho\to+\infty} g_\rho$, we get

$$\lim_{\rho\to+\infty} j_\rho^B(g_\rho,z) = e^{B\left(\langle z, g_\infty^{-1}.0\rangle - \overline{\langle z, g_\infty^{-1}.0\rangle}\right)}.$$

Hence in view of (11), we see that $\lim_{\rho\to+\infty} j_\rho^B(g_\rho,z) = j_\infty^B(g_\infty,z)$. With this we have finished the proof of the proposition.

There are many other geometrical elements of the Bergman–Kähler geometry on $\mathbb{B}_\rho^n$ that converge to their analogous on $\mathbb{C}^n = \lim_{\to}\mathbb{B}_\rho^n$. Table I summarizes the relevant items on $\mathbb{B}_\rho^n$ and $\mathbb{C}^n$ that we will consider in this paper.

Remark 2: The above list of geometrical elements is not exhaustive. Indeed, one can consider

other items such as the three points function $J_\rho^B(z_1,z_2,z_3)$, $z_1,z_2,z_3\in\mathbb{B}_\rho^n$, *defined by*

$$J_\rho^B(z_1,z_2,z_3)=\left(\frac{\rho^2-\langle z_1,z_2\rangle}{\rho^2-\langle z_2,z_1\rangle}\right)^{B\rho^2}\left(\frac{\rho^2-\langle z_2,z_3\rangle}{\rho^2-\langle z_3,z_2\rangle}\right)^{B\rho^2}\left(\frac{\rho^2-\langle z_3,z_1\rangle}{\rho^2-\langle z_1,z_3\rangle}\right)^{B\rho^2}=e^{2iB\mathcal{V}_\rho(z_1,z_2,z_3)},$$

where the three phase point $\mathcal{V}_\rho$ *is given by*

$$\mathcal{V}_\rho(z_1,z_2,z_3)=\rho^2\left[\arg\left(1-\frac{\langle z_1,z_2\rangle}{\rho^2}\right)+\arg\left(1-\frac{\langle z_1,z_2\rangle}{\rho^2}\right)+\arg\left(1-\frac{\langle z_3,z_1\rangle}{\rho^2}\right)\right].$$

Here, $\arg(Z)$ *denotes the principal argument of the complex number* Z. *Then it is easy to check that*

$$\lim_{\rho\mapsto+\infty}\mathcal{V}_\rho(z_1,z_2,z_3)=\mathcal{V}_\infty(z_1,z_2,z_3)=\frac{i}{2}\left[(\langle z_1,z_2\rangle-\overline{\langle z_1,z_2\rangle})+(\langle z_2,z_3\rangle-\overline{\langle z_2,z_3\rangle})+(\langle z_3,z_1\rangle-\overline{\langle z_3,z_1\rangle})\right] \tag{12}$$

for every fixed three points z_1, z_2, z_3 *in* $\mathbb{C}^n$. *In particular, for the case* $n=1$, *the obtained result (12) is geometrically consistent since the three phase points* $\mathcal{V}_\rho(z_1,z_2,z_3)$ *is the area of the geodesic triangle of summits* z_1, z_2, z_3 *in the disc* $\mathbb{B}_\rho^1$ *and that* $\mathcal{V}_\infty(z_1,z_2,z_3)$ *represents the area of the Euclidean triangle of summits* z_1, z_2, z_3 *in* $\mathbb{R}^2=\mathbb{C}$.

III. GEOMETRICAL REALIZATION OF LANDAU-LIKE HAMILTONIANS AND INVARIANCE PROPERTIES

Let $H_{B,\rho}$ be the Landau-like Hamiltonians on the balls $\mathbb{B}_\rho^n$, $\rho\in]0,+\infty]$, as given in Definition 1. Then in this section, we give a geometrical realization of them as Schrödinger operators in the presence of uniform magnetic field on $\mathbb{B}_\rho^n$ and we establish some of their invariance properties.

A. Geometrical realization of the Landau-like Hamiltonians $H_{B,\rho}$

For $\rho\in]0,+\infty]$, let θ_ρ be the real differential 1-form defined by

$$\theta_\rho(z)=i\left(1-\left|\frac{z}{\rho}\right|^2\right)^{-1}\sum_{j=1}^n(\bar{z}_j\,dz_j-z_j\,d\bar{z}_j),\quad z\in\mathbb{B}_\rho^n\quad(i=\sqrt{-1}) \tag{13}$$

and let $\Lambda_c^p(\mathbb{B}_\rho^n)$ denote the space of smooth differential p-forms on $\mathbb{B}_\rho^n$ with compact support. For fixed $B\in\mathbb{R}$, let ∇_ρ^B be the first order differential operator acting on $\Lambda_c^p(\mathbb{B}_\rho^n)$ by

$$\nabla_\rho^B:=d+\sqrt{-1}B\,\mathrm{ext}\,\theta_\rho.$$

Here d is the exterior derivative of differential p-forms and $\mathrm{ext}\,\theta_\rho$ is the operator of exterior left multiplication by θ_ρ. Precisely, $\mathrm{ext}\,\theta_\rho\omega=\theta_\rho\wedge\omega$ for all $\omega\in\Lambda^p(\mathbb{B}_\rho^n)$. Also, let $(\nabla_\rho^B)^*$ denote the formal adjoint of ∇_ρ^B with respect to the Hermitian scalar product

$$(\alpha,\beta)_p=\int_{\mathbb{B}_\rho^n}\alpha\wedge\star\beta,\quad\alpha,\beta\in\Lambda_c^p(\mathbb{B}_\rho^n), \tag{14}$$

where $\star$ denotes the Hodge star operator associated to the appropriate metric on $\mathbb{B}_\rho^n$, $\rho\in]0,+\infty]$. Thus, using the above notations, we fix the following definition.

Definition 2: Let $B\in\mathbb{R}$. *For* $\rho\in]0,+\infty]$ *set*

$$H_{B,\rho}:=(\nabla_\rho^B)^*\nabla_\rho^B \tag{15}$$

acting on the space of smooth functions $\mathcal{C}^\infty(\mathbb{B}_\rho^n)=\Lambda^0(\mathbb{B}_\rho^n)$. *The operators* $H_{B,\rho}$ *will be called Landau-like Hamiltonians of* $\mathbb{B}_\rho^n$ *associated to the vector potential* θ_ρ.

Remark 3: The definition (15) *of the Landau-like Hamiltonians acting on scalar functions can be extended to the case of differential p-forms,* $1\leqslant p\leqslant 2n$, *of* $\mathbb{B}_\rho^n$, $\rho\in]0,+\infty]$, *by considering*

$$H^p_{B,\rho} = (\nabla^B_\rho)^* \nabla^B_\rho + \nabla^B_\rho (\nabla^B_\rho)^*. \tag{16}$$

The following proposition, giving the explicit expressions of the Landau-like Hamiltonians $H_{B,\rho}$, asserts that the Laplacians $H_{B,\rho}$ in Definition 2 is in fact a geometrical realization of those in Definition 1. Namely, we have

Proposition 3: Let B fixed in $\mathbb{R}$. *Then*

(i) The explicit expression of the Landau-like Hamiltonian $H_{B,\rho}$, *(15), in the complex coordinates* $z=(z_1,\ldots,z_n)\in\mathbb{B}^n_\rho$, $\rho\in]0,+\infty[$, *is given by*

$$H_{B,\rho} = -4\left(1-\left|\frac{z}{\rho}\right|^2\right)\left\{\sum_{i,j=1}^n\left(\delta_{ij}-\frac{z_i\bar{z}_j}{\rho^2}\right)\frac{\partial^2}{\partial z_i\,\partial\bar{z}_j}+B\sum_{j=1}^n\left(z_j\frac{\partial}{\partial z_j}-\bar{z}_j\frac{\partial}{\partial\bar{z}_j}\right)\right\}+4B^2|z|^2.$$

(ii) The explicit expression of the Landau-like Hamiltonian $H_{B,\infty}$, (15), *in the complex coordinates* $z=(z_1,\cdots,z_n)\in\mathbb{B}^n_\infty=\mathbb{C}^n$ *is given by*

$$H_{B,\infty} = -4\left\{\sum_{j=1}^n\frac{\partial^2}{\partial z_j\,\partial\bar{z}_j}+B\sum_{j=1}^n\left(z_j\frac{\partial}{\partial z_j}-\bar{z}_j\frac{\partial}{\partial\bar{z}_j}\right)\right\}+4B^2|z|^2.$$

Proof: The proof relies essentially on the construction of the Hodge star operator. For $n=1$ this is easy to handle since in this case the metric ds^2_ρ is conformal to the Euclidean metric $|\mathrm{dz}|^2$ of the disc $\mathbb{B}^1_\rho$ for which we have

$$\star 1=\frac{i}{2}\left(1-\left|\frac{z}{\rho}\right|^2\right)^{-2}\mathrm{dz}\wedge\mathrm{d}\bar{z},\quad \star\mathrm{dz}=i\mathrm{d}\bar{z},\quad \star\mathrm{d}\bar{z}=-i\,\mathrm{dz},\quad \text{and } \star(\mathrm{dz}\wedge\mathrm{d}\bar{z})=2i\left(1-\left|\frac{z}{\rho}\right|^2\right)^2.$$

For $n\geqslant 2$ the Kählerian metric

$$\mathrm{ds}^2_\rho(z)=-\sum_{i,j=1}^n\frac{\partial^2}{\partial z_i\,\partial\bar{z}_j}\mathrm{Log}(\rho^2-|z|^2)\mathrm{dz}_i\otimes\mathrm{d}\bar{z}_j$$

on $\mathbb{B}^n_\rho$ is no more conformal to the Euclidean metric $|\mathrm{dz}|^2=|\mathrm{dz}_1|^2+\cdots+|\mathrm{dz}_n|^2$. Indeed, for $z\in\mathbb{B}^n_\rho$, $z\neq 0$, the eigenvalues of the Hermitian metric ds^2_ρ are explicitly given by

$$\lambda_1(\rho)=\frac{\rho^4}{(\rho^2-|z|^2)^2}\quad\text{and }\lambda_2(\rho)=\frac{\rho^2}{\rho^2-|z|^2}.$$

The first eigenvalue $\lambda_1(\rho)$ is of complex multiplicity one with the vector column z as eigenvector while the eigenvalue $\lambda_2(\rho)$ occurs with $n-1$ multiplicity with eigenspace the hyperplane $z^\perp=\{u\in\mathbb{C}^n;\langle u,z\rangle=0\}$. Thus, using the Gram–Schmidt procedure, we can construct a unitary coframe at the point z of differential 1-forms φ_j, $j=1,2,\ldots,n$, with

$$\varphi_1(z)=\frac{\rho^2\bar{z}_j\,\mathrm{dz}_j}{|z|(\rho^2-|z|^2)}$$

and in which the metric can be written as

$$\mathrm{ds}^2_\rho=\varphi_1(z)\otimes\overline{\varphi}_1(z)+\varphi_2(z)\otimes\overline{\varphi}_2(z)+\cdots+\varphi_n(z)\otimes\overline{\varphi}_n(z),$$

and the vector potential θ_ρ has the form $\theta_\rho(z)=i|z|(\varphi_1(z)-\overline{\varphi_1}(z))$.

Using such coframe, the Hodge star operator, $\star$, can be defined as

$$\varphi_j(z)\wedge\star\varphi_k(z)=\overline{\varphi_j}(z)\wedge\star\overline{\varphi_k}(z)=2\delta_{jk}\,\mathrm{d}\mu_\rho(z),$$

$$\varphi_j(z) \wedge \star\overline{\varphi_k}(z) = \overline{\varphi_j}(z) \wedge \star\varphi_k(z) = 0.$$

Now, using the definition of the Landau-like Hamiltonian $H_{B,\rho}=(\nabla_\rho^B)^*\nabla_\rho^B$, we can write it in the form

$$H_{B,\rho} = \mathrm{d}^*\mathrm{d} + iB(\mathrm{d}^* \text{ ext } \theta_\rho - (\text{ext } \theta_\rho)^*\mathrm{d}) + B^2(\text{ext } \theta_\rho)^*(\text{ext } \theta_\rho). \tag{17}$$

Thus, to obtain explicit differential expression in z of $H_{B,\rho}$ it will be enough to find those of the operators $\mathrm{d}^*\mathrm{d}$, $\mathrm{d}^*(\text{ext } \theta_\rho)$, $(\text{ext } \theta_\rho)^*\mathrm{d}$, and $(\text{ext } \theta_\rho)^*(\text{ext } \theta_\rho)$ acting on functions. For this, recall that the adjoints operators d^* of d and $(\text{ext } \theta_\rho)^*$ of ext θ_ρ with respect to (14) are known to be given, respectively, by

$$\mathrm{d}^* = -\star\mathrm{d}\star \quad \text{and } (\text{ext } \theta_\rho)^* = \star \text{ ext } \theta_\rho\star.$$

Also note that the operator $\mathrm{d}^*\mathrm{d}$ is nothing than the Laplace–Beltrami operator of $(\mathbb{B}_\rho^n, \mathrm{d}s_\rho^2)$, $\rho\in]0,+\infty]$, whose explicit expression in the complex coordinates $z=(z_1,z_2,\ldots,z_n)$ is given by

$$\mathrm{d}^*\mathrm{d} = -4\left(1-\left|\frac{z}{\rho}\right|^2\right)\sum_{i,j=1}^{n}\left(\delta_{ij}-\frac{z_i\bar{z}_j}{\rho^2}\right)\frac{\partial^2}{\partial z_i\,\partial\bar{z}_j}. \tag{18}$$

For the other involved operators occurring in (17), we have the following lemma whose proof can be done by straightforward computation keeping in mind that $\theta_\rho=-i\rho^2(\partial-\bar{\partial})\mathrm{Log}(1-|z/\rho|^2)$; see also Ref. 3.

Lemma 1: *Let f be any smooth function on $\mathbb{B}_\rho^n$ and $z\in\mathbb{B}_\rho^n$. Then we have*

$$(1)\quad \mathrm{d}^*\theta_\rho = 0,$$

$$(2)\quad (\text{ext } \theta_\rho)^*\,\mathrm{d}f(z) = -2i\left(1-\left|\frac{z}{\rho}\right|^2\right)(E-\overline{E})f(z), \tag{19}$$

$$(3)\quad \mathrm{d}^*(\text{ext } \theta_\rho)f(z) = 2i\left(1-\left|\frac{z}{\rho}\right|^2\right)(E-\overline{E})f(z), \tag{20}$$

$$(4)\quad (\text{ext } \theta_\rho)^*(\text{ext } \theta_\rho)f(z) = 4|z|^2 f(z). \tag{21}$$

Hence, by combining (18)–(21), we obtain the desired expression of $H_{B,\rho}$ as stated in (i) of the above proposition.

The explicit expression given in (ii) of $H_{B,\infty}$ on the complex space $\mathbb{C}^n$ can easily be handled since the metric $\mathrm{d}s_\infty^2$ is the Euclidean metric itself.

B. Invariance properties

In below, we establish some invariance properties of the Landau-like Hamiltonians $H_{B,\rho}^p$ acting on p-forms of $\mathbb{B}_\rho^n$, $p=0,1,\ldots,2n$, $\rho\in]0,+\infty]$. To do this remind that the vector potential θ_ρ and the automorphic factor j_ρ^B, are given, respectively, by

$$\theta_\rho(z) = -i\rho^2(\partial-\bar{\partial})\mathrm{Log}(\rho^2-|z|^2), \quad z\in\mathbb{B}_\rho^n, \tag{22}$$

$$j_\rho^B(g;z) := \left(\frac{\rho^2-\overline{\langle z,g^{-1}.0\rangle}}{\rho^2-\langle z,g^{-1}.0\rangle}\right)^{B\rho^2} \quad \text{for } g=g_\rho\in G_\rho, \quad z\in\mathbb{B}_\rho^n, \tag{23}$$

for which we have the following.

Lemma 2: Let $\rho>0$, $g=g_\rho\in G_\rho$, and denote by $g^*\theta_\rho$ the pull-back of the differential 1*-form θ_ρ by the map $z\mapsto g.z$. Then for every $z\in\mathbb{B}_\rho^n$, we have*

$$\text{(i)}\quad (g^*\theta_\rho)(z) = \theta_\rho(z) - i\rho^2 \mathrm{d}\left[\mathrm{Log}\left(\frac{\rho^2 - \overline{\langle z, g^{-1}\cdot 0\rangle}}{\rho^2 - \langle z, g^{-1}\cdot 0\rangle}\right)\right],$$

$$\text{(ii)}\quad \mathrm{d}\left(j_\rho^B(g,z)\right) = B\rho^2 j_\rho^B(g,z)\mathrm{d}\left[\mathrm{Log}\left(\frac{\rho^2 - \overline{\langle z, g^{-1}\cdot 0\rangle}}{\rho^2 - \langle z, g^{-1}\cdot 0\rangle}\right)\right].$$

Proof: Let $g\in G_\rho$ and $z\in\mathbb{B}_\rho^n$. Then using definition of G_ρ, we get the identity

$$\rho^2 - |g\cdot z|^2 = \rho^2\frac{(\rho^2 - |g^{-1}\cdot 0|^2)(\rho^2 - |z|^2)}{|\rho^2 - \langle z, g^{-1}\cdot 0\rangle|^2}.$$

Then using (22) and the fact that the pull-back operation $g^*:\omega\mapsto g^*\omega$ commutes with the operators ∂ and $\bar\partial$ (i.e., $\partial g^* = g^*\partial$ and $\bar\partial g^* = g^*\bar\partial$), it follows that

$$g^*\theta_\rho(z) = \theta_\rho(z) - i\rho^2(\partial - \bar\partial)\mathrm{Log}(|\rho^2 - \langle z, g^{-1}\cdot 0\rangle|^2).$$

But, since $z\mapsto\rho^2 - \langle z, g^{-1}\cdot 0\rangle$ is holomorphic and $\mathrm{d} = \partial + \bar\partial$ it follows

$$(\partial - \bar\partial)\mathrm{Log}(|\rho^2 - \langle z, g^{-1}\cdot 0\rangle|^2) = \mathrm{d}\left[\mathrm{Log}\left(\frac{\rho^2 - \overline{\langle z, g^{-1}\cdot 0\rangle}}{\rho^2 - \langle z, g^{-1}\cdot 0\rangle}\right)\right].$$

Hence, (i) holds. Similarly, a direct computation yields (ii).

Now, let $L^2(\mathbb{B}_\rho^n;\Lambda^p)$ be the Hilbert space obtained as completion of $\Lambda_c^p(\mathbb{B}_\rho^n)$ with respect to (14). For $g = g_\rho\in G_\rho$, let $T_\rho^B(g)$ be the transformation defined by

$$T_\rho^B(g)\omega = j_\rho^B(g,\cdot)g^*(\omega),\quad \omega\in\Lambda_c^p(\mathbb{B}_\rho^n),\quad \rho\in 0,+\infty, \tag{24}$$

where $j_\rho^B(g,\cdot)$ is the automorphic factor as given in (23) and $g^*\omega$ is the pull-back of the differential p-form ω by the biholomorphic mapping $z\mapsto g_\rho\cdot z$. Then T_ρ^B is a projective representation of the group G_ρ on $L^2(\mathbb{B}_\rho^n;\Lambda^p)$. That is

(i) T_ρ^B acts unitary on $L^2(\mathbb{B}_\rho^n;\Lambda^p)$ for every $g\in G_\rho$;

(ii) for all $g_1, g_2\in G_\rho$, we have $T_\rho^B(g_1g_2) = e^{2iB\phi(g_1,g_2)}T_\rho^B(g_2)T_\rho^B(g_1)$, where ϕ is a phase factor given here by

$$\phi(g_1,g_2) = \rho^2\arg\left(1 - \frac{\langle g_1^{-1}\cdot 0, g_2\cdot 0\rangle}{\rho^2}\right).$$

(iii) For each function $f\in L^2(\mathbb{B}_\rho^n;\Lambda^p)$, the map $g\in G_\rho\mapsto T_\rho^B(g)f\in L^2(\mathbb{B}_\rho^n;\Lambda^p)$ is continuous.

Thus the following invariance properties hold.

Proposition 4: Let $B\in\mathbb{R}$ fixed and $g = g_\rho\in G_\rho$ for $\rho\in]0,+\infty]$. Then for $p = 0,1,\ldots,2n$, we have

(i) *The first order differential operators $\nabla_\rho^B = d + \sqrt{-1}\,\mathrm{ext}\,\theta_\rho$ are invariant with respect to the transformations $T_\rho^B(g)$. That is*

$$T_\rho^B(g)\nabla_\rho^B = \nabla_\rho^B T_\rho^B(g).$$

(ii) *The Landau-like Hamiltonians $H_{B,\rho}^p = (\nabla_\rho^B)^*\nabla_\rho^B + \nabla_\rho^B(\nabla_\rho^B)^*$ are also T_ρ^B-invariant. More exactly we have*

$$T_\rho^B(g)H_{B,\rho}^p = H_{B,\rho}^p T_\rho^B(g).$$

Proof: By a direct computation of $\nabla_\rho^B[T_\rho^B(g)\omega]$ in (i) for $g\in G_\rho$, $\omega\in\Lambda_c^p(\mathbb{B}_\rho^n)$ and $z\in\mathbb{B}_\rho^n$, where $T_\rho^B(g)\omega$ is as given in (24), we get

$$\nabla_\rho^B[T_\rho^B(g)\omega]=\nabla_\rho^B[j_\rho^B(g,z)g^*\omega]=\mathrm{d}(j_\rho^B(g,z)g^*\omega)+iBj_\rho^B(g,z)\theta_\rho\wedge g^*\omega$$

$$=j_\rho^B(g,z)\mathrm{d}(g^*\omega)+(\mathrm{d}j_\rho^B(g,z))\wedge g^*\omega+iBj_\rho^B(g,z)\theta_\rho\wedge g^*\omega.$$

Now, using the above lemma and the well known facts that $g^*\mathrm{d}=\mathrm{d}g^*$ and $g^*(\theta\wedge\omega)=g^*\theta\wedge g^*\omega$, we get

$$\nabla_\rho^B[T_\rho^B(g)\omega]=j_\rho^B(g,z)g^*(\mathrm{d}\omega)+B\rho^2j_\rho^B(g,z)\mathrm{d}\left[\mathrm{Log}\left(\frac{\rho^2-\overline{\langle z,g^{-1}.0\rangle}}{\rho^2-\langle z,g^{-1}.0\rangle}\right)\right]\wedge g^*\omega+iBj_\rho^B(g,z)$$
$$\times\left\{g^*\theta_\rho+i\rho^2\mathrm{d}\left[\mathrm{Log}\left(\frac{\rho^2-\overline{\langle z,g^{-1}.0\rangle}}{\rho^2-\langle z,g^{-1}.0\rangle}\right)\right]\right\}\wedge g^*\omega=j_\rho^B(g,z)g^*(\mathrm{d}\omega+iB\theta_\rho\wedge\omega).$$

Hence, we obtain the desired result (i) as cited in the proposition.

Now, for the proof of (ii), we use (i) and the fact that $T_\rho^B(g)$ is unitary, to show that $T_\rho^B(g)$ commutes also with the formal adjoint $(\nabla_\rho^B)^*$. Hence, the invariance property of the Hamiltonian $H_{B,\rho}^p$ with respect to $T_\rho^B(g)$, $g\in G_\rho$, holds and so the proof of the proposition is completed.

IV. BACKGROUND ON L^2-CONCRETE SPECTRAL THEORY OF THE LANDAU-LIKE HAMILTONIANS $H_{B,\rho}$.

In this section, we we recall some well established L^2-spectral properties of $H_{B,\rho}$ for $\rho\in]0,+\infty]$.

A. L^2-spectrum and L^2-eigenfunctions of $H_{B,\rho}$ on $L^2(\mathbb{B}_\rho^n;\mathrm{d}\mu_\rho)$

We start with the following.

Proposition 5: (Spectrum of the Landau-like Hamiltonians). Let $n\geqslant 1$, $B>0$ *and let* $H_{B,\rho}$ *be the Landau-like Hamiltonians on* $\mathbb{B}_\rho^n$ *for* $\rho\in]0,+\infty]$. *Then we have the following.*

(i) For fixed $\rho\in]0,+\infty[$, *the Landau-like Hamiltonian* $H_{B,\rho}$ *is densely defined on the Hilbert space* $L^2(\mathbb{B}_\rho^n;\mathrm{d}\mu_\rho)$ *and admits a unique self-adjoint realization denoted* $H_{B,\rho}$, *whose spectrum on* $L^2(\mathbb{B}_\rho^n;\mathrm{d}\mu_\rho)$ *is given by*

$$\sigma(H_{B,\rho})=\sigma_d(H_{B,\rho})\cup\left[\frac{n^2}{\rho^2}+4B^2\rho^2,+\infty\right],$$

where the finite discrete part $\sigma_d(H_{B,\rho})$ *of the spectrum is given by*

$$\sigma_d(H_{B,\rho})=\left\{\lambda_l(\rho):=4B(2l+n)-4\frac{l(l+n)}{\rho^2};l\in\mathbb{Z}^+,\ 0\leqslant l<B\rho^2-\frac{n}{2}\right\}.$$

Here, each L^2-*eigenvalue* $\lambda_l(\rho)$ *occurs with infinite multiplicity.*

(ii) For $\rho=+\infty$, *the Landau-like Hamiltonian* $H_{B,\infty}$ *is also densely defined on the Hilbert space* $L^2(\mathbb{C}^n;\mathrm{d}m)$ *and admits unique self-adjoint realization. The spectrum* $\sigma(H_{B,\infty})$ *of* $H_{B,\infty}$ *in* $L^2(\mathbb{C}^n;\mathrm{d}m)$ *is reduced only to a pure point spectrum with infinite degenerated multiplicities. More exactly we have*

$$\sigma(H_{B,\infty})=\sigma_d(H_{B,\infty})=\{\lambda_l(\infty):=4B(2l+n);\ l=0,1,2,\ldots\}.$$

Proof: For the proof of assertion (i), the reader can refer, for example, to Refs. 8, 18, and 9 for $n=1$ and to Refs. 19 and 5 for $n\geqslant 2$. The assertion (ii) is well known, in both mathematics and physics literature, as Landau energy levels for Schrödinger operators with uniform magnetic field on $\mathbb{R}^{2n}=\mathbb{C}^n$.

Below, we give concrete characterization of the L^2-eigenfunctions of the Landau-like Hamiltonians $H_{B,\rho}$ acting on $L^2(\mathbb{B}^n_\rho;\mathrm{d}\mu_\rho)$, $\rho\in]0,+\infty]$. Mainly, we have the following.

Proposition 6: Let $B>0$ and $\rho\in]0,+\infty]$.

(i) Let $\rho\in]0,+\infty[$ *such that* $B\rho^2>n/2$ *and* $l\in\mathbb{Z}^+$ *satisfying* $0\leqslant l<B\rho^2-n/2$. *Then any* F *solution of* $H_{B,\rho}F=(4B(2l+n)-4[l(l+n)/\rho^2])F$, *in* $L^2(\mathbb{B}^n_\rho;\mathrm{d}\mu_\rho)$, *can be expanded in* $L^2(\mathbb{B}^n_\rho;\mathrm{d}\mu_\rho)$ *as follows:*

$$F(z)=\left(1-\left|\frac{z}{\rho}\right|^2\right)^{B\rho^2-l}\sum_{p=0}^{+\infty}\sum_{q=0}^{l}{}_2F_1\left(q-l,2B\rho^2+p-l;n+p+q;\left|\frac{z}{\rho}\right|^2\right)h^{pq}_{B,\rho,l}(z,\bar{z}),$$

where $h^{pq}_{B,\rho,l}(z,\bar{z})$ *denotes the harmonic polynomials on* $\mathbb{C}^n$ *that are homogeneous of degree* p *in* z *and degree* q *in* $\bar{z}$ *(see Ref. 10). Furthermore, its norm is given by* $\|F\|^2_{L^2(\mathbb{B}^n_\rho;\,\mathrm{d}\mu_\rho)}=\sum_{p=0}^{+\infty}\sum_{q=0}^{l}\gamma^{n,pq}_{B,\rho}(l)\|h^{pq}_{B,\rho,l}\|^2_{L^2(S^{2n-1})}$ *with*

$$\gamma^{n,pq}_{B,\rho}(l)=\frac{(l-q)!\Gamma^2(n+p+q)}{2\Gamma(n+p+l)}\frac{\rho^{2(n+p+q)}\Gamma(2B\rho^2-n-q-l+1)}{(2B\rho^2-n-2l)\Gamma(2B\rho^2+p-l)}. \tag{25}$$

(ii) For $\rho=+\infty$ *and* $l=0,1,2,\ldots$. *Then any function* F *solution of* $H_{B,\infty}F=4B(2\lambda+n)F$ *in* $L^2(\mathbb{C}^n;\mathrm{d}m)$ *can be expanded as follows:*

$$F(z)=e^{-B|z|^2}\sum_{p=0}^{+\infty}\sum_{q=0}^{l}{}_1F_1(q-l,n+p+q;2B|z|^2)h^{pq}_{B,l}(z,\bar{z}),$$

where its norm is given by

$$\|F\|^2_{L^2(\mathbb{C}^n;\mathrm{d}m)}=\sum_{p=0}^{+\infty}\sum_{q=0}^{l}\gamma^{n,pq}_{B}(l)\|h^{pq}_{B,l}\|^2_{L^2(S^{2n-1})}$$

with

$$\gamma^{n,pq}_{B}(l)=\left(\frac{1}{2B}\right)^{n+p+q}\frac{(l-q)!\Gamma^2(n+p+q)}{2\Gamma(n+p+l)}.$$

Proof: (Sketch of the proof.) For $n=1$, the result in (i) is contained in the works of Elstrodt[8] and Patterson.[18] For $n\geqslant 2$, one can check (i) by the use of the weighted Plancherel formula established in Ref. 19 on the unit Bergman ball.

For the computation of the norm, we use the polar coordinates $z=\rho r\omega$, $0\leqslant r<1$, $\omega\in S^{2n-1}$, and Parseval equality to have

$$\|F\|^2=\|F\|^2_{L^2(\mathbb{B}^n_\rho,d\mu_\rho)}=\sum_{p=0}^{+\infty}\sum_{q=0}^{l}\gamma^{n,pq}_{B,\rho}(l)\|h^{pq}_{B,\rho,l}\|^2_{L^2(S^{2n-1})}.$$

The quantities $\gamma^{n,pq}_{B,\rho}(l)$ are defined by

$$\gamma^{n,pq}_{B,\rho}(l):=\frac{\rho^{2n}}{2}\int_0^1 x^{n+p+q-1}(1-x)^{2(B\rho^2-l)-n-1}\left|{}_2F_1(q-l,2B\rho^2+p-l;n+p+q;x)\right|^2\mathrm{d}x,$$

where we have set $x=r^2$. Then the above integral involving the product of two hypergeometric functions can be computed by applying the following well known identity:

$$ {}_2F_1(-m,b;c;x) = \frac{1}{(c)_m} x^{1-c}(1-x)^{c-b+m}\left(\frac{d}{dx}\right)^m (x^{c+m-1}(1-x)^{b-c}), $$

where m is in $\mathbb{Z}^+$ and $(c)_m = c(c+1)\cdots(c+m-1)$ is the Pochhammer symbol, and using integration by parts and the fact

$$ \left(\frac{d}{dx}\right)^m \left((1-x)^{a+m-1} {}_2F_1(a,b;c;x)\right) = \frac{(-1)^m (a)_m (c-b)_m}{(\gamma)_m} (1-x)^{a-1} {}_2F_1(a+m,b;c+m;x). $$

Thus, we get the norm of F as given by (25).

The result (ii), for $\rho = +\infty$, is well known for Schrödinger operators with constant magnetic field on $\mathbb{R}^{2n} = \mathbb{C}^n$. For the norm the proof is similar to the one given for Theorem 2.1 in Ref. 2.

Remark 4: Note that the bottom eigenvalue $\lambda_0(\rho) = 4Bn$, corresponding to $l = 0$, is independent of ρ. The associated L^2-eigenspace is isomorphic to the usual weighted Bergman–Hilbert space of holomorphic functions on $\mathbb{B}_\rho^n$ that are square integrable with respect to the density $(1 - |z/\rho|^2)^{2B\rho^2 - n - 1}\, dm$,

$$ \left\{ G_\rho(z) \text{ holomorphic}; \int_{\mathbb{B}_\rho^n} |G_\rho(z)|^2 \left(1 - \left|\frac{z}{\rho}\right|^2\right)^{2B\rho^2 - n - 1} dm(z) < +\infty \right\}. $$

Also, the L^2-eigenspace associated to the ground state $4Bn$ of the Landau-like Hamiltonian $H_{B,\infty}$ on $\mathbb{C}^n$ is isometric to the Bargmann–Fock space

$$ \left\{ G: \mathbb{C}^n \to \mathbb{C}, \quad G \text{ entire and } \quad \int_{\mathbb{C}^n} |G(z)|^2 e^{-2B|z|^2}\, dm(z) < +\infty \right\}. $$

B. Explicit formulas for the L^2-eigenprojector kernels for the discrete spectrum of $H_{B,\rho}$

Now, let $B > 0$ and $l \in \mathbb{Z}^+$ be fixed. For $\rho > 0$ such that $\rho^2 > (2l+n)/(2B)$, let $A_l^{2,B}(\mathbb{B}_\rho^n)$ be the following Hilbert space corresponding to the L^2-eigenvalue:

$$ \lambda_l(\rho) = 4B(2l+n) - 4\frac{l(l+n)}{\rho^2} $$

of the Landau-like Hamiltonian $H_{B,\rho}$. That is

$$ A_l^{2,B}(\mathbb{B}_\rho^n) = \left\{ F \in L^2(\mathbb{B}_\rho^n; d\mu_\rho) / H_{B,\rho} F = \left(4B(2l+n) - 4\frac{l(l+n)}{\rho^2}\right) F \right\}. $$

Also, let $A_l^{2,B}(\mathbb{C}^n)$ be the following Hilbert space associated to the L^2-eigenvalue $\lambda_l(\rho) = 4B(2l+n)$ (Landau energy level) of the Landau-like Hamiltonian $H_{B,\infty}$ on $\mathbb{C}^n$,

$$ A_l^{2,B}(\mathbb{C}^n) = \{ F \in L^2(\mathbb{C}^n; dm) / H_{B,\infty} F = 4B(2l+n) F \}. $$

Then one can show that the above Hilbert spaces $A_l^{2,B}(\mathbb{B}_\rho^n)$ and $A_l^{2,B}(\mathbb{C}^n)$ admit L^2-eigenprojector kernels which we denote here, respectively, by $K_{l,\rho}^B(z,w)$ with $z, w \in \mathbb{B}_\rho^n$ and $K_{l,\infty}^B(z,w)$ with $z, w \in \mathbb{C}^n$. Therefore, the following proposition gives the explicit closed expressions of such L^2-eigenprojector kernels. Namely, we have the following.

Proposition 7: Let $B > 0$ fixed. Then we have the following.

(i) For fixed $l \in \mathbb{Z}^+$ such that $0 \leqslant l < B\rho^2 - n/2$, the L^2-eigenprojector kernel $K_{l,\rho}^B(z,w)$ of the L^2-eigenspace $A_l^{2,B}(\mathbb{B}_\rho^n)$ is given in term of the Bergman distance $d_\rho(z,w)$ by the following closed explicit formula:

$$K^B_{l,\rho}(z,w) = A_{n;B;l}(\rho)\left(\frac{\rho^2 - \overline{\langle z,w\rangle}}{\rho^2 - \langle z,w\rangle}\right)^{B\rho^2}\left(\cosh\left(\frac{d_\rho(z,w)}{\rho}\right)\right)^{-2(B\rho^2-l)} \times {}_2F_1\left(-l, 2B\rho^2 - l; n; \tanh^2\left(\frac{d_\rho(z,w)}{\rho}\right)\right), \tag{26}$$

where the constant $A_{n;B;l}(\rho)$ is given explicitly in terms of gamma functions by

$$A_{n;B;l}(\rho) = \frac{1}{\pi^n}\frac{\Gamma(n+l)}{\Gamma(n)l!} \times \frac{(2B\rho^2 - n - 2l)\Gamma(2B\rho^2 - l)}{\rho^{2n}\Gamma(2B\rho^2 - n - l + 1)}. \tag{27}$$

(ii) For $\rho = +\infty$ and $l = 0, 1, 2, \ldots$, the L^2-eigenprojector kernel $K^B_{l,\infty}(z,w)$ of $A^{2,B}_l(\mathbb{C}^n)$ is given by the following explicit closed formula:

$$K^B_{l,\infty}(z,w) = \left(\frac{2B}{\pi}\right)^n \frac{\Gamma(n+l)}{\Gamma(n)l!} e^{B(\langle z,w\rangle - \overline{\langle z,w\rangle})} e^{-B|z-w|^2} {}_1F_1(-l, n; 2B|z-w|^2).$$

Proof: Using the invariance property of the Landau-like Hamiltonians $H_{B,\rho}$ under the action T^B_ρ of the group of motions G_ρ (see Proposition 4), we cheek that the L^2-eigenprojector kernel $K^B_{l,\rho}(z,w)$, $\rho \in]\sqrt{n/2B}, +\infty[$, is G_ρ-invariant which means that we have

$$K^B_{l,\rho}(z,w) = j^B_\rho(g;z)\overline{j^B_\rho(g;w)} K^B_{l,\rho}(g \,.\, z, g \,.\, w)$$

for every $g = g_\rho \in G_\rho$, where $j^B_\rho(g;z)$ is the automorphic factor of g at point z. Hence, we get

$$K^B_{l,\rho}(z,w) = j^B_\rho(g_w;z)\overline{j^B_\rho(g_w;w)} K^B_{l,\rho}(g_w \,.\, z, 0),$$

where g_w is in G_ρ such that $g_w \cdot w = 0$. Now let us note that

$$j^B_\rho(g_w;z)\overline{j^B_\rho(g_w;w)} = j^B_\rho(g_w;z) = \left(\frac{\rho^2 - \overline{\langle z,w\rangle}}{\rho^2 - \langle z,w\rangle}\right)^{B\rho^2}$$

and that the function $z \mapsto K^B_{l,\rho}(z,0)$ is a radial L^2-eigenfunction of $H_{B,\rho}$. Therefore, we get

$$K^B_{l,\rho}(z,0) = \{\gamma^{n,00}_{B,\rho}(l)\}^{-1}\left(1 - \left|\frac{z}{\rho}\right|^2\right)^{B\rho^2 - l} {}_2F_1\left(-l, 2B\rho^2 - l; n; \left|\frac{z}{\rho}\right|^2\right).$$

Here, the factor $\{\gamma^{n,00}_{B,\rho}(l)\}^{-1} =: A_{n;B;l}(\rho)$ is due to the normalization and is given through the formula (25) in which we take $p = q = 0$. Hence, we obtain

$$K^B_{l,\rho}(g_w \,.\, z, 0) = A_{n;B;l}(\rho)\left(1 - \left|\frac{g_w \,.\, z}{\rho}\right|^2\right)^{B\rho^2 - l} {}_2F_1\left(-l, 2\nu\rho^2 - l; n; \left|\frac{g_w \,.\, z}{\rho}\right|^2\right).$$

Next using the fact that

$$1 - \left|\frac{g_w \,.\, z}{\rho}\right|^2 = \frac{(\rho^2 - |z|^2)(\rho^2 - |w|^2)}{|\rho^2 - \langle z,w\rangle|^2},$$

we get the desired result (i) of the above proposition.

The result in (ii) can be obtained in a similar way and the reader can refer, for example, to Ref. 2.

C. Resolvent kernels of $H_{B,\rho}$ on $L^2(\mathbb{B}^n_\rho; d\mu_\rho)$

Fix $\mu \in \mathbb{C}$ and $\rho \in]0, +\infty]$. Then by resolvent kernel $R_{B,\rho}(\mu;z,w)$, z, $w \in \mathbb{B}^n_\rho$, we mean the kernel of the integral operator $R_{B,\rho}(\mu)$ that solves

$$[H_{B,\rho} - h_{B,\rho}(\mu)]R_{B,\rho}(\mu) = I,$$

where I is the identity operator and $h_{B,\rho}(\mu)$ is the complex number given by

$$\begin{aligned} h_{B,\rho}(\mu) &= \frac{\mu^2 + n^2}{\rho^2} + 4B^2\rho^2 \qquad \text{for } \rho \in \ ]0; +\infty[; \\ h_{B,\infty}(\mu) &= \mu =: \mu_\infty \qquad\qquad \text{for } \rho = +\infty. \end{aligned} \tag{28}$$

That is for every $\varphi \in \mathcal{C}_c^\infty(\mathbb{B}_\rho^n)$, we have

$$[R_{B,\rho}(\mu)\varphi](z) = \int_{\mathrm{B}_\rho^n} R_{B,\rho}(\mu; z, w)\varphi(w)\mathrm{d}\mu_\rho(w).$$

More particularly, we seek for $R_{B,\rho}(\mu; z, w)$ such that

(1) $R_{B,\rho}(\mu; z, w)$ is T_ρ^B bi-invariant. That is, for every $g_\rho \in G_\rho$, $\rho \in]0, +\infty]$, we have

$$R_{B,\rho}(\mu; g_\rho \,.\, z, g_\rho \,.\, w) = j_\rho^{-B}(g_\rho, z)\overline{j_\rho^{-B}(g_\rho, w)}R_{B,\rho}(\mu; z, w). \tag{29}$$

(2) $R_{B,\rho}(\mu; z, w)$ is solution of the differential equation

$$[H_{B,\rho} - h_{B,\rho}(\mu)]R_{B,\rho}(\mu; z, w) = \delta_w(z), \tag{30}$$

where $\delta_w(z)$ is the "Dirac density" concentrated at the point w with respect to the volume measure $\mathrm{d}\mu_\rho$ of $\mathbb{B}_\rho^n$. The solution of the above equations (29) and (30) is given by the following proposition.

Proposition 8: Let $B > 0$ *be fixed and* μ, $\mu_\infty \in \mathbb{C}$. *Then we have the following,*

(i) For $\rho \in]0, +\infty[$ *and* $\mu \neq -i(2l + n \pm 2B\rho^2)$ *for* $l = 0, 1, 2, \ldots$, *a resolvent kernel* $R_{B,\rho}(\mu; z, w)$, $z, w \in \mathbb{B}_\rho^n$, *of the Landau-like Hamiltonian* $H_{B,\rho}$ *associated to* $h_{B,\rho}(\mu) := (\mu^2 + n^2)/\rho^2 + 4B^2\rho^2$ *is given explicitly by*

$$\begin{aligned} R_{B,\rho}(\mu; z, w) = C_{B,\rho}^n(\mu)&\left(\frac{\rho^2 - \overline{\langle z, w\rangle}}{\rho^2 - \langle z, w\rangle}\right)^{B\rho^2}\left(\frac{(\rho^2 - |z|^2)(\rho^2 - |w|^2)}{|\rho^2 - \langle z, w\rangle|^2}\right)^{n - i\mu/2} \\ &\times {}_2F_1\left(\frac{n - i\mu}{2} + B\rho^2, \frac{n - i\mu}{2} - B\rho^2; 1 - i\mu; \frac{(\rho^2 - |z|^2)(\rho^2 - |w|^2)}{|\rho^2 - \langle z, w\rangle|^2}\right), \end{aligned}$$

where the constant $C_{B,\rho}^n(\mu)$ *is given by*

$$C_{B,\rho}^n(\mu) = \left(\frac{1}{2\pi^n}\right)\frac{\Gamma\left(\frac{n - i\mu}{2} + B\rho^2\right)\Gamma\left(\frac{n - i\mu}{2} - B\rho^2\right)}{\rho^{2(n-1)}\Gamma(1 - i\mu)}.$$

(ii) *For* $\rho = +\infty$ *and* $\mu_\infty \neq 4B(2l + n)$ *for* $l = 0, 1, 2, \ldots$, *a resolvent kernel* $R_{B,\infty}(\mu_\infty; z, w)$, $z, w \in \mathbb{C}^n$, *of the Landau-like Hamiltonian* $H_{B,\infty}$ *associated to* $h_{B,\infty}(\mu_\infty) := \mu_\infty$ *is given explicitly by*

$$R_{B,\infty}(\mu_\infty; z, w) = \left(\frac{2B}{\pi}\right)^n \frac{\Gamma\left(\frac{n}{2} - \frac{\mu_\infty}{8B}\right)}{4B} \times e^{B(\langle z, w\rangle - \overline{\langle z, w\rangle})}e^{-B|z - w|^2}G\left(\frac{n}{2} - \frac{\mu_\infty}{8B}; n; 2B|z - w|^2\right),$$

where $G(\alpha; \gamma; x)$ *is the degenerate hypergeometric function of the second kind.*[15]

Proof: Proof of (i). Let $\rho \in]0, +\infty[$ be fixed. Since the resolvent kernel $R_{B,\rho}$, we are looking for, is T_ρ^B bi-invariant, it follows that it has the following form:

$$R_{B,\rho}(\mu;z,w)=\left(\frac{\rho^2-\overline{\langle z,w\rangle}}{\rho^2-\langle z,w\rangle}\right)^{B\rho^2}\phi\left(\mu;\frac{d_\rho(z,w)}{\rho}\right),$$

where ϕ is a function of the distance $d_\rho(z,w)$ on $(\mathbb{B}_\rho^n,\mathrm{ds}_\rho^2)$. Using the geodesic polar coordinates $z=\rho\tanh(r/\rho)\omega$, where $r=d_\rho(z,0)$ and $\omega\in S^{2n-1}$, we see that the radial part $\mathrm{rad}(H_{B,\rho})$ of the Landau-like Hamiltonian $H_{B,\rho}$ is given by

$$\mathrm{rad}(H_{B,\rho})=-\left\{\frac{d^2}{\mathrm{d}r^2}+\left([2n-1]\coth\left(\frac{r}{\rho}\right)+\tanh\left(\frac{r}{\rho}\right)\right)\left(\frac{1}{\rho}\right)\frac{d}{\mathrm{d}r}+\frac{4B^2\rho^2}{\cosh^2\left(\frac{r}{\rho}\right)}-4B^2\rho^2\right\}.$$

Hence, the function $\phi(\mu;r/\rho)$ is the irregular solution at the point $r/\rho=0$ of the following ordinary differential equation:

$$\frac{d^2}{\mathrm{d}r^2}+\left([2n-1]\coth\left(\frac{r}{\rho}\right)+\tanh\left(\frac{r}{\rho}\right)\right)\left(\frac{1}{\rho}\right)\frac{d}{\mathrm{d}r}+\frac{4B^2\rho^2}{\cosh^2\left(\frac{r}{\rho}\right)}-4B^2\rho^2+h_{B,\rho}(\mu)=-\delta(r)$$

with $r\geqslant 0$.

Therefore, by making the change $s=r/\rho$ and substituting $h_{B,\rho}(\mu)$ by its value given in (28), we see that the above differential equation reduces to the following ordinary differential equation of Jacobi's type:

$$\frac{d^2}{\mathrm{d}s^2}+\big([2n-1]\coth(s)+\tanh(s)\big)\frac{d}{\mathrm{d}s}+\frac{(2B\rho^2)^2}{\cosh^2(s)}+\mu^2+n^2=0,\quad s>0,$$

whose singular solution is given through the expression

$$[\cosh(s)]^{-(n-i\mu)}{}_2F_1\left(\frac{n-i\mu+2B\rho^2}{2},\frac{n-i\mu-2B\rho^2}{2};1-i\mu;\cosh^{-2}(s)\right). \tag{31}$$

In view of the above explicit singular solution (31), the solution of (29) and (30) is then given by

$$R_{B,\rho}(\mu;z,w)=C_{B,\rho}^n(\mu)\left(\frac{\rho^2-\overline{\langle z,w\rangle}}{\rho^2-\langle z,w\rangle}\right)^{B\rho^2}\left(\cosh\left(\frac{d_\rho(z,w)}{\rho}\right)\right)^{-(n-i\mu)}$$
$$\times{}_2F_1\left(\frac{n-i\mu}{2}+B\rho^2,\frac{n-i\mu}{2}-B\rho^2;1-i\mu;\cosh^{-2}\left(\frac{d_\rho(z,w)}{\rho}\right)\right),$$

where $C_{B,\rho}^n(\mu)$ is a normalization constant that ensures the identity (30). It is given explicitly by

$$C_{B,\rho}^n(\mu)=\left(\frac{1}{2\pi^n\rho^{2(n-1)}}\right)\frac{\Gamma\left(\frac{n-i\mu}{2}-B\rho^2\right)\Gamma\left(\frac{n-i\mu}{2}+B\rho^2\right)}{\Gamma(1-i\mu)}.$$

The proof of (ii) is similar to the first one. Just let mention that the radial part of the Landau-like Hamiltonian $H_{B,\infty}$ is given by

$$-\left\{\frac{d^2}{\mathrm{d}r^2}+\frac{2n-1}{r}\frac{d}{\mathrm{d}r}-4B^2r^2\right\},$$

where $r=|z|$. And using the appropriate change of function

$$R_{B,\infty}(\mu_\infty;r)=e^{-x/2}y(x)$$

with $x=2Br^2$, we see that the ordinary differential equation resulting here is of the following form:

$$xy''(x) + (n - x)y'(x) + \lambda y(x) = \delta(x), \quad x \geqslant 0,$$

whose irregular solution at $x=0$ is the degenerate hypergeometric function of the second kind $G(-\lambda; n; x)$.

V. ASYMPTOTIC OF L^2-SPECTRAL PROPERTIES OF THE LANDAU-LIKE HAMILTONIANS $H_{B,\rho}$

According to (i) of Proposition 6, it is clear that the point spectrum $\sigma_d(H_{B,\rho})$ in $L^2(\mathbb{B}_\rho^n; d\mu_\rho)$ of the Landau-like Hamiltonian $H_{B,\rho}$ on $\mathbb{B}_\rho^n$ converges, when $\rho \to +\infty$, to the "Landau levels" that constitute the point spectrum of the Landau-like Hamiltonian $H_{B,\infty}$ on $\mathbb{C}^n$, which recover, for $n=1$, the Comtet's result[6] as mentioned in the introduction. Whereas the continuous part of the spectrum of $H_{B,\rho}$ becomes empty. In this section, we will be interested in the asymptotic of the L^2-eigenprojector kernels of L^2-eigenspaces of the Landau-like Hamiltonian $H_{B,\rho}$ as well as of their resolvent kernels by letting ρ tend to infinity. Mainly, we show that they give rise to their analogous of $H_{B,\infty}$ on the n-complex space $\mathbb{C}^n$.

A. Asymptotic of the L^2-eigenprojector kernels when ρ tends to $+\infty$

The first main result gives asymptotic of the L^2-eigenprojector kernel $K_{l,\rho}^B(z,w)$ of the Landau-like Hamiltonian $H_{B,\rho}$ on the balls $\mathbb{B}_\rho^n$ when $\rho \to +\infty$. Precisely, we have the following.

Theorem 1: *Let $B>0$, $l \in \mathbb{Z}^+$ fixed, and $K_{l,\rho}^B(z,w)$ and $K_{l,\infty}^B(z,w)$ are, respectively, the L^2-eigenprojector kernels of the L^2-eigenspaces of $H_{B,\rho}$ and $H_{B,\infty}$ corresponding to their point spectrum. Then for every fixed $(z,w) \in \mathbb{C}^n \times \mathbb{C}^n$, we have*

$$\lim_{\rho \to +\infty} K_{l,\rho}^B(z,w) = K_{l,\infty}^B(z,w).$$

Proof: Let $l \in \mathbb{Z}^+$ and $(z,w) \in \mathbb{C}^n \times \mathbb{C}^n$ fixed. Then it is clear, from the established explicit formulas (26) (Proposition 7), that the L^2-eigenprojector kernel $K_{l,\rho}^B(z,w)$ is well defined for every $\rho > \mathrm{Max}(|z|, |w|, \sqrt{(2l+n)/2B})$. Thus according to the explicit expression of the constant $A_{n;B;l}(\rho)$ as given by (27) and using the Binet formula

$$\frac{\Gamma(x+a)}{\Gamma(x+b)} = x^{a-b}\left(1 + O\left(\frac{1}{x}\right)\right)$$

with $x = 2B\rho^2$, $a = -l$, $b = -n-l+1$, we derive easily that we have

$$\lim_{\rho \to +\infty} A_{n;B;l}(\rho) = \left(\frac{2B}{\pi}\right)^n \frac{\Gamma(n+l)}{\Gamma(n)l!}. \tag{32}$$

Also, let us note that we have

$$\lim_{\rho \to +\infty} \left(\frac{\rho^2 - \overline{\langle z,w\rangle}}{\rho^2 - \langle z,w\rangle}\right)^{-B\rho^2} = e^{B(\langle z,w\rangle - \overline{\langle z,w\rangle})} \tag{33}$$

and

$$\lim_{\rho \to +\infty} \left(\cosh\left(\frac{d_\rho(z,w)}{\rho}\right)\right)^{2(B\rho^2 - l)} = \lim_{\rho \to +\infty} \left(\frac{(\rho^2 - |z|^2)(\rho^2 - |w|^2)}{|\rho^2 - \langle z,w\rangle|^2}\right)^{B\rho^2 - l} = e^{-B|z-w|^2}. \tag{34}$$

Next, since

$$\tanh^2\left(\frac{d_\rho(z,w)}{\rho}\right) = 1 - \frac{(\rho^2 - |z|^2)(\rho^2 - |w|^2)}{|\rho^2 - \langle z,w\rangle|^2} \sim \frac{|z-w|^2}{\rho^2}$$

for $\rho \to +\infty$, we conclude by the use of the following standard fact:

$$\lim_{m\mapsto+\infty} {}_2F_1\left(a,m+b;c;\frac{z}{m}\right) = {}_1F_1(a;c;z), \tag{35}$$

that we have

$$\lim_{\rho\mapsto+\infty} {}_2F_1\left(-l,2B\rho^2-l;n;1-\frac{(\rho^2-|z|^2)(\rho^2-|w|^2)}{|\rho^2-\langle z,w\rangle|^2}\right) = {}_1F_1(-l,n;2B|z-w|^2). \tag{36}$$

Thus, from (32)–(34) and (36), we see that

$$\lim_{\rho\mapsto+\infty} K_l^B(\rho;z,w) = \left(\frac{2B}{\pi}\right)^n \frac{\Gamma(n+l)}{\Gamma(n)l!} e^{B(\langle z,w\rangle-\overline{\langle z,w\rangle})} e^{-B|z-w|^2} {}_1F_1(-l,n;2B|z-w|^2).$$

The right-hand side in the above equality is nothing more than the L^2-eigenprojector kernel $K_{l,\infty}^B(z,w)$ of $A_l^{2,B}(\mathbb{C}^n)$ given in (ii) of Proposition 7. This finishes the proof of Theorem 1.

Next, in the following section, we will look for the asymptotic of the resolvent kernels associated to the Landau-like Hamiltonians $H_{B,\rho}$, when $\rho\to+\infty$.

B. Asymptotic of resolvent kernels of $H_{B,\rho}$ when $\rho\to+\infty$

For λ in a suitable region of $\mathbb{C}$, we will be constructing modified T_ρ^B bi-invariant resolvent kernel $R_{B,\rho}(\lambda;z,w)$ solution of the differential equation

$$[H_{B,\rho}-h_{B,\rho}(\lambda)]R_{B,\rho}(\lambda;z,w) = \delta_w(z) \quad \text{with } h_{B,\rho}(\lambda) = 4B(2\lambda+n) - 4\frac{\lambda(\lambda+n)}{\rho^2}.$$

Thus, the solution we seek can be deduced from Proposition 8 by setting $\mu=-i(2\lambda+n-2B\rho^2)$. Namely, we have the following.

Proposition 9: LET $B>0$ and $\lambda\in\mathbb{C}$. Then We have the following. (i) *For fixed $\rho\in]0,+\infty[$ and $\lambda\in\mathbb{C}\setminus(\mathbb{Z}^+\cup 2B\rho^2+\mathbb{Z}^+)$, a resolvent kernel $R_{B,\rho}(\lambda;z,w)$, $z,w\in\mathbb{B}_\rho^n$ with $z\neq w$, of the Landau-like Hamiltonian $H_{B,\rho}$ associated to $h_{B,\rho}(\lambda):=4B(2\lambda+n)-4\lambda(\lambda+n)/\rho^2$ is given explicitly by*

$$R_{B,\rho}(\lambda;z,w) = C_{B,\rho}^n(\lambda)\left(\frac{\rho^2-\overline{\langle z,w\rangle}}{\rho^2-\langle z,w\rangle}\right)^{B\rho^2}\left(\frac{(\rho^2-|z|^2)(\rho^2-|w|^2)}{|\rho^2-\langle z,w\rangle|^2}\right)^{B\rho^2-\lambda}$$
$$\times {}_2F_1\left(-\lambda,2B\rho^2-\lambda;2B\rho^2-2\lambda-n+1;\frac{(\rho^2-|z|^2)(\rho^2-|w|^2)}{|\rho^2-\langle z,w\rangle|^2}\right),$$

where the constant $C_{B,\rho}^n(\lambda)$ is given by

$$C_{B,\rho}^n(\lambda) = \left(\frac{\Gamma(-\lambda)}{2\pi^n}\right)\frac{\Gamma(2B\rho^2-\lambda)}{\rho^{2(n-1)}\Gamma(2B\rho^2-\lambda-n+1)}.$$

(ii) For $\rho=+\infty$ and $\lambda\in\mathbb{C}\setminus\mathbb{Z}^+$, a resolvent kernel $R_{B,\infty}(\lambda;z,w)$, $z,w\in\mathbb{C}^n$ with $z\neq w$, of the Landau-like Hamiltonian $H_{B,\infty}$ associated to $h_{B,\infty}(\lambda):=4B(2\lambda+n)$, is given explicitly by

$$R_{B,\infty}(\lambda;z,w) = \frac{(2B)^{n-1}}{2\pi^n}\Gamma(-\lambda)e^{B(\langle z,w\rangle-\overline{\langle z,w\rangle})}e^{-B|z-w|^2}G(-\lambda;n;2B|z-w|^2).$$

Therefore, we have the following.

Theorem 2: *Let $B>0$ and $\lambda\in\mathbb{C}\setminus\mathbb{R}^+$ be fixed, and $R_{B,\rho}(\lambda;.,.)$ and $R_{B,\infty}(\lambda;.,.)$ be the resolvent kernels of the Landau-like Hamiltonians $H_{B,\rho}$ and $H_{B,\infty}$, respectively. Then for every fixed $(z,w)\in\mathbb{C}^n\times\mathbb{C}^n$ such that $z\neq w$, we have*

$$\lim_{\rho\mapsto+\infty} R_{B,\rho}(\lambda;z,w) = R_{B,\infty}(\lambda;z,w).$$

Proof: Let λ be fixed in $\mathbb{C}\backslash\mathbb{R}^+$. Then without loss of generality, we can assume that $w=0$. Hence, for fixed $z\neq 0$ *in* $\mathbb{C}^n$, the resolvent kernel $R_{B,\rho}(\lambda;z,0)=:R^n_{B,\rho}(\lambda;z)$ simplifies to be given by

$$R^n_{B,\rho}(\lambda;z)=\frac{\Gamma(-\lambda)\Gamma(2B\rho^2-\lambda)}{2\pi^n\rho^{2(n-1)}\Gamma(2B\rho^2-2\lambda-n+1)}\left(1-\left|\frac{z}{\rho}\right|^2\right)^{B\rho^2-\lambda}$$
$$\times{}_2F_1\left(-\lambda,2B\rho^2-\lambda;2B\rho^2-2\lambda-n+1;1-\left|\frac{z}{\rho}\right|^2\right).$$

Further, we may write $R^n_{B,\rho}(\lambda;z)$ as follows:

$$R^n_{B,\rho}(\lambda;z)=\frac{(2B)^{n-1}}{2\pi^n}\Gamma(-\lambda)\left(1-\left|\frac{z}{\rho}\right|^2\right)^{B\rho^2-\lambda}\lim_{\gamma\mapsto n}\phi^{\gamma}_{B,\rho}(\lambda;z),$$

where we have set for γ close to n (and $\gamma\neq n$),

$$\phi^{\gamma}_{B,\rho}(\lambda;z)=\frac{\Gamma(2B\rho^2-\lambda)(2B\rho^2)^{1-\gamma}}{\Gamma(2B\rho^2-2\lambda-\gamma+1)}\times{}_2F_1\left(-\lambda,2B\rho^2-\lambda;2B\rho^2-2\lambda-\gamma+1;1-\left|\frac{z}{\rho}\right|^2\right).$$

Now, by appealing to the hypergeometric identity

$${}_2F_1(a,b;c;x)=\frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}{}_2F_1(a,b;a+b-c+1;1-x)+\frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}$$
$$\times(1-x)^{c-a-b}{}_2F_1(c-a,c-b;c-a-b+1;1-x),$$

and applying it to the hypergeometric function involved in $\phi^{\gamma}_{B,\rho}(\lambda;z)$ with $a=-\lambda$, $b=2B\rho^2-\lambda$, $c=2B\rho^2-2\lambda-\gamma+1$, and $x=1-|z/\rho|^2$, we see after the use of the duplication formula

$$\Gamma(z)\Gamma(1-z)=\frac{\pi}{\sin\pi z}$$

and easy simplification that the above function $\phi^{\gamma}_{B,\rho}(\lambda;z)$ can be rewritten as a sum in the following form:

$$\phi^{\gamma}_{B,\rho}(\lambda;z)=\frac{\pi}{\sin\pi\gamma}\{\phi^{\gamma,1}_{B,\rho}(\lambda;z)-\phi^{\gamma,2}_{B,\rho}(\lambda;z)\},$$

where

$$\phi^{\gamma,1}_{B,\rho}(\lambda;z)=\frac{\Gamma(2B\rho^2-\lambda)(2B\rho^2)^{1-\gamma}}{\Gamma(2B\rho^2-\lambda-\gamma+1)}\cdot\frac{{}_2F_1\left(-\lambda,2B\rho^2-\lambda;\gamma;\left|\frac{z}{\rho}\right|^2\right)}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\tag{37}$$

and

$$\phi^{\gamma,2}_{B,\rho}(\lambda;z)=\frac{(2B|z|^2)^{1-\gamma}{}_2F_1\left(2B\rho^2-\lambda-\gamma+1,-\lambda-\gamma+1;2-\gamma;\left|\frac{z}{\rho}\right|^2\right)}{\Gamma(-\lambda)\Gamma(2-\gamma)}.\tag{38}$$

Therefore, since $\phi^{\gamma}_{B,\rho}(\lambda;z)$ and $\phi^{\gamma,j}_{B,\rho}(\lambda;z)$, $j=1,2$, are analytic functions in γ, we see that the singularity in γ produced by $1/(\sin\pi\gamma)$ can be eliminated by applying the Hopital rule and doing so, we end by writing the resolvent kernel $R^n_{B,\rho}(\lambda;z)$ as follows:

$$R^n_{B,\rho}(\lambda;z)=S^{n,1}_{B,\rho}(\lambda;z)-S^{n,2}_{B,\rho}(\lambda;z),$$

where

$$S_{B,\rho}^{n,j}(\lambda;z)=\frac{(-1)^n(2B)^{n-1}}{2\pi^n}\Gamma(-\lambda)\left(1-\left|\frac{z}{\rho}\right|^2\right)^{B\rho^2-\lambda}\frac{d}{d\gamma}[\phi_{B,\rho}^{\gamma,j}(\lambda;z)]_{|_{\gamma=n}},\quad j=1,2.$$

Hence, to obtain the limit of $R_{B,\rho}^n(\lambda;z)$ when $\rho\to+\infty$, we use the following lemma (whose proof will be given later in the Appendix).

Lemma 3: Using the above notations, we have the following.

$$(i)\quad \lim_{\rho\to+\infty}\frac{d}{d\gamma}[\phi_{B,\rho}^{\gamma,1}(\lambda;z)]_{|_{\gamma=n}}=\frac{d}{d\gamma}\left[\frac{{}_1F_1(-\lambda;\gamma;2B|z|^2)}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\right]_{|_{\gamma=n}},$$

$$(ii)\quad \lim_{\rho\to+\infty}\frac{d}{d\gamma}[\phi_{B,\rho}^{\gamma,2}(\lambda;z)]_{|_{\gamma=n}}=\frac{1}{\Gamma(-\lambda)}\frac{d}{d\gamma}\left[(2B|z|^2)^{1-\gamma}\frac{{}_1F_1(-\lambda-\gamma+1;2-\gamma;2B|z|^2)}{\Gamma(2-\gamma)}\right]_{|_{\gamma=n}},$$

where ${}_1F_1(a;c;x)$ *is the confluent hypergeometric function.*

Therefore, using the above lemma and the well established fact

$$\lim_{\rho\to+\infty}\left(1-\left|\frac{z}{\rho}\right|^2\right)^{B\rho^2-\lambda}=e^{-B|z|^2}$$

we conclude that

$$\lim_{\rho\to+\infty}R_{B,\rho}^n(\lambda;z)=(-1)^n\frac{(2B)^{n-1}}{2\pi^n}\Gamma(-\lambda)e^{-B|z|^2}\times\frac{\partial}{\partial\gamma}\left[\frac{{}_1F_1(-\lambda;\gamma;2B|z|^2)}{\Gamma(\gamma)\Gamma(-\lambda-\gamma+1)}-\frac{1}{\Gamma(-\lambda)}(2B|z|^2)^{1-\gamma}\frac{{}_1F_1(-\lambda-\gamma+1;2-\gamma;2B|z|^2)}{\Gamma(2-\gamma)}\right]_{|_{\gamma=n}}.$$

But, since

$$G(\alpha;n;z)=(-1)^n\left\{\frac{\partial}{\partial\gamma}\left[\frac{{}_1F_1(\alpha;\gamma;z)}{\Gamma(\gamma)\Gamma(\alpha-\gamma+1)}\right]_{|_{\gamma=n}}-\frac{1}{\Gamma(\alpha)}\frac{\partial}{\partial\gamma}\left[z^{1-\gamma}\frac{{}_1F_1(\alpha-\gamma+1;2-\gamma;z)}{\Gamma(2-\gamma)}\right]_{|\gamma=n}\right\}.$$

we can rewrite the above limit as

$$\lim_{\rho\to+\infty}R_{B,\rho}^n(\lambda;z)=\frac{(2B)^{n-1}}{2\pi^n}\Gamma(-\lambda)e^{-B|z|^2}G(-\lambda;n;2B|z|^2),\tag{39}$$

where the right-hand side of (39) is nothing more than the resolvent kernel $R_{B,\infty}(\lambda;z,0)$ of $H_{B,\infty}$ associated to the spectral parameter $h_{B,\infty}(\lambda)=4B(2\lambda+n)$. Hence, the proof of the theorem is ended.

Remark 5: The previous theorem is the generalization to $n\geqslant 2$ *of Comtet result's on the asymptotic of the resolvent kernel when* ρ *tends to* $+\infty$. *But, here, we have produced a rigorous proof of this result for* $n\geqslant 1$.

VI. CONCLUDING REMARKS AND COMMENTS

In the preceding sections, we have investigated the asymptotic of the geometrical structure of the hyperbolic balls $\mathbb{B}_\rho^n$ when the radius $\rho\to\infty$ as well as the asymptotic of some aspect of stationary spectral properties (spectrum, L^2-eigenprojector kernels, resolvent kernels) of the so-called Landau-like Hamiltonians acting on functions. And we have shown that they give rise to their analogous of the flat case $\mathbb{C}^n$.

Added to the asymptotic of the stationary spectral analysis of the Landau-like Hamiltonians, they are other aspects of spectral theory related to the Landau-like Hamiltonians such as evolution spectral theory, essentially the heat and wave kernels for which it is likely to investigate their

asymptotic when $\rho \to +\infty$ and to compare the obtained asymptotic formulas (if they exist) to their analogous of the Landau-like Hamiltonians on the flat case $\mathbb{C}^n$. We hope to come back to these matters in the future.

Moreover, in view of the explicit formulas obtained for the Landau Hamiltonians acting on differential 1-forms of the disc, see Ref. 12, which lead to the so-called Pauli Hamiltonians, it seems to be also of interest to discuss and study the concrete spectral analysis of Landau-like Hamiltonians, as defined in (16), acting on differential p-forms, $1 \leqslant p \leqslant n$, as well as their asymptotic. Such Pauli Hamiltonians describes the motion of a nonrelativistic particle with spin $\frac{1}{2}$ under the action of an external uniform magnetic field. Their action on differential 1-forms $\omega = f\,\mathrm{d}z + g\,\mathrm{d}\bar{z}$, identified to the matrix column $\binom{f}{g}$, are given explicitly by

$$H^1_{B,\rho} = \begin{pmatrix} H_{B,\rho} & 0 \\ 0 & \overline{H_{-B,\rho}} \end{pmatrix} - 4B\sigma_3,$$

where

$$H_{B,\rho} = -4\left(1 - \left|\frac{z}{\rho}\right|^2\right)\left\{\left(1 - \left|\frac{z}{\rho}\right|^2\right)\frac{\partial^2}{\partial z\,\partial \bar{z}} + Bz\frac{\partial}{\partial z} - \left(B + \frac{2}{\rho^2}\right)\bar{z}\frac{\partial}{\partial \bar{z}}\right\} + 4B\left(B + \frac{2}{\rho^2}\right)|z|^2.$$

Above $\overline{H_{-B,\rho}}$ is the "complex conjugate" of $H_{-B,\rho}$ and $\sigma_3 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ is the third Pauli spin matrix.

All previous considerations can be generalized to the case of the complex projective space $\mathbb{P}^n_\rho(\mathbb{C})$; the compact counterpart of $\mathbb{B}^n_\rho$; whose holomorphic sectional curvature is equal to $+4/\rho^2$. The space $\mathbb{P}^n_\rho(\mathbb{C})$ is endowed with the scaled Fubini-study metric $\widetilde{\mathrm{ds}^2_\rho}$ given in the complex coordinates $z_1, z_2, \ldots, z_n$ of the chart $\mathbb{C}^n$ by

$$\widetilde{\mathrm{ds}^2_\rho} = \left(1 + \left|\frac{z}{\rho}\right|^2\right)^{-2} \sum_{i,j=1}^{n} \left(\left(1 + \left|\frac{z}{\rho}\right|^2\right)\delta_{i,j} - \frac{\bar{z}_i z_j}{\rho^2}\right)\mathrm{d}z_i \otimes \mathrm{d}\bar{z}_j,$$

whose associated invariant Landau-like Hamiltonian is given by

$$\widetilde{H}_{B,\rho} = -4\left(1 + \left|\frac{z}{\rho}\right|^2\right)\left\{\sum_{i,j=1}^{n}\left(\delta_{ij} + \frac{z_i\bar{z}_j}{\rho^2}\right)\frac{\partial^2}{\partial z_i\,\partial \bar{z}_j} + B\sum_{j=1}^{n}\left(z_j\frac{\partial}{\partial z_j} - \bar{z}_j\frac{\partial}{\partial \bar{z}_j}\right)\right\} + 4B^2|z|^2.$$

Thus, the discussion for $\mathbb{P}^n_\rho(\mathbb{C})$ can be carried over in a similar way. The major difference is that the spectrum of $\widetilde{H}_{B,\rho}$ reduces only to the discrete part where their eigenvalues occur with finite multiplicities. We intend to return to this subject in future work.

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APPENDIX (PROOF OF LEMMA 3)

Here, we give the proof of Lemma 3 in the preceding section. For this, we start by the following lemma for series functions.

Lemma 4: Let $u_k(m)$ be a sequence of functions in $m, m > m_0$, satisfying the following assumptions:

(i) $|u_k(m)| < \alpha_k$ *for some* α_k *independent of* $m, m > m_0$, *such that* $\Sigma_{k=0}^{+\infty}\alpha_k < +\infty$.
(ii) *For every fixed* k, *we have* $\lim_{m\to+\infty} u_k(m) = v_k$, *where* $\Sigma_{k=0}^{+\infty}|v_k| < +\infty$. *Then*

$$\lim_{m\mapsto+\infty}\sum_{k=0}^{+\infty}u_k(m)=\sum_{k=0}^{+\infty}\lim_{m\mapsto+\infty}u_k(m).$$

Proof of (i) of Lemma 3: According to (37) and by the use of Leibnitz formula we have

$$\frac{d}{d\gamma}[\phi_{B,\rho}^{\gamma,1}(\lambda;z)]_{|\gamma=n}=I_\rho^1+I_\rho^2,$$

where

$$I_\rho^1=\frac{d}{d\gamma}\left[\frac{\Gamma(2B\rho^2-\lambda)(2B\rho^2)^{1-\gamma}}{\Gamma(2B\rho^2-\lambda-\gamma+1)}\right]_{|\gamma=n}\cdot\frac{{}_2F_1\left(-\lambda,2B\rho^2-\lambda;n;\left|\frac{z}{\rho}\right|^2\right)}{\Gamma(-\lambda-n+1)\Gamma(n)}$$

and

First, we will show that $\lim_{\rho\mapsto+\infty}I_\rho^1=0$. Indeed, the term I_ρ^1 can be written as a product of three factors. Namely, we have

$$I_\rho^1=\frac{\Gamma(2B\rho^2-\lambda)(2B\rho^2)^{1-n}}{\Gamma(2B\rho^2-\lambda-n+1)}\times\{\psi(2B\rho^2-\lambda-n+1)-\mathrm{Log}(2B\rho^2)\}\times\frac{{}_2F_1\left(-\lambda,2B\rho^2-\lambda;n;\left|\frac{z}{\rho}\right|^2\right)}{\Gamma(-\lambda-n+1)\Gamma(n)},$$

where $\psi(z)=\Gamma'(z)/\Gamma(z)$ is the logarithmic derivative of the function $\Gamma(z)$. Then using the Binet formula $\Gamma(x+a)/\Gamma(x+b)=x^{a-b}(1+O(1/x))$ and the fact that

$$\psi(x+b)-\mathrm{Log}(x)=O\left(\frac{1}{x}\right)$$

with $a=-\lambda$, $b=-\lambda-\gamma+1$, $x=2B\rho^2$, we see that we have

$$\lim_{\rho\mapsto+\infty}\frac{\Gamma(2B\rho^2-\lambda)(2B\rho^2)^{1-n}}{\Gamma(2B\rho^2-\lambda-n+1)}=1 \tag{A1}$$

and

$$\lim_{\rho\mapsto+\infty}\{\psi(2B\rho^2-\lambda-n+1)-\mathrm{Log}(2B\rho^2)\}=0.$$

Further, since $\lim_{x\mapsto+\infty}{}_2F_1(a,x+b;c;\xi/x)={}_1F_1(a;c;\xi)$ (Lemma 35), we see that for $a=b=-\lambda$, $x=2B\rho^2$, $c=n$, and $\xi=2B|z|^2$, we have

$$\lim_{\rho\mapsto+\infty}{}_2F_1\left(-\lambda,2B\rho^2-\lambda;n;\left|\frac{z}{\rho}\right|^2\right)={}_1F_1(-\lambda;n;2B|z|^2),$$

which is finite. Hence, we conclude easily that $\lim_{\rho\mapsto+\infty}I_\rho^1=0$.

Therefore, to get (i) of the Lemma 4, we must show that

$$\lim_{\rho\mapsto+\infty}I_\rho^2=\frac{d}{d\gamma}\left[\frac{{}_1F_1(-\lambda;\gamma;2B|z|^2)}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\right]_{|\gamma=n}.$$

To do this let us note that in view of (A1), it follows

$$\lim_{\rho\mapsto+\infty} I_\rho^2 = \lim_{\rho\mapsto+\infty} \frac{d}{d\gamma}\left[\frac{{}_2F_1\left(-\lambda;2B\rho^2-\lambda;\gamma;\left|\frac{z}{\rho}\right|^2\right)}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\right]_{|_{\gamma=n}},$$

if the last limit exists. Hence, using the expansion in series of the above involved Gauss hypergeometric function ${}_2F_1$ given by

$${}_2F_1\left(-\lambda,2B\rho^2-\lambda;\gamma;\left|\frac{z}{\rho}\right|^2\right) = \sum_{k=0}^{+\infty} \frac{(-\lambda)_k(2B\rho^2-\lambda)_k}{(\gamma)_k}\cdot\frac{\left(\left|\frac{z}{\rho}\right|^2\right)^k}{k!},$$

where $(\alpha)_k$ is the Pochhammer symbol, we then get

$$\frac{d}{d\gamma}\left[\frac{{}_2F_1\left(-\lambda;2B\rho^2-\lambda;\gamma;\left|\frac{z}{\rho}\right|^2\right)}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\right]_{|_{\gamma=n}} = \sum_{k=0}^{+\infty} U_k(\rho),$$

where we have set for every fixed $k\in\mathbb{Z}^+$ and ρ varying in $]0,+\infty[$,

$$U_k(\rho) := (-\lambda)_k \frac{(2B\rho^2-\lambda)_k}{(\rho^2)^k}\frac{d}{d\gamma}\left[\frac{1}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\cdot\frac{1}{(\gamma)_k}\right]_{|_{\gamma=n}}\cdot\frac{(|z|^2)^k}{k!}.$$

At once, one can check easily that for every fixed k, we have

$$\lim_{\rho\mapsto+\infty} U_k(\rho) = (-\lambda)_k \frac{d}{d\gamma}\left[\frac{1}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\cdot\frac{1}{(\gamma)_k}\right]_{|_{\gamma=n}}\cdot\frac{(2B|z|^2)^k}{k!} =: v_k.$$

Thus, proceeding formally, we get

$$\begin{aligned}\lim_{\rho\mapsto+\infty} I_\rho^2 &= \lim_{\rho\mapsto+\infty}\frac{d}{d\gamma}\left[\frac{{}_2F_1\left(-\lambda;2B\rho^2-\lambda;\gamma;\left|\frac{z}{\rho}\right|^2\right)}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\right]_{|_{\gamma=n}}\\ &= \lim_{\rho\mapsto+\infty}\sum_{k=0}^{+\infty} U_k(\rho) = \sum_{k=0}^{+\infty} v_k = \frac{d}{d\gamma}\left[\frac{1}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\sum_{k=0}^{+\infty}\frac{(-\lambda)_k}{(\gamma)_k}\cdot\frac{(2B|z|^2)^k}{k!}\right]_{|_{\gamma=n}}\\ &= \frac{d}{d\gamma}\left[\frac{{}_1F_1(-\lambda;\gamma;2B|z|^2)}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\right]_{|_{\gamma=n}}.\end{aligned}$$

But, to conclude rigorously that

$$\lim_{\rho\mapsto+\infty} I_\rho^2 = \frac{d}{d\gamma}\left[\frac{{}_1F_1(-\lambda;\gamma;2B|z|^2)}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\right]_{|_{\gamma=n}},$$

we apply Lemma 4. For this, we should see that the series $\Sigma_{k=0}^{+\infty}U_k(\rho)$ is absolutely convergent. Indeed, for every fixed k, we have

$$|U_k(\rho)| \leqslant (|\lambda|)_k \frac{(2B\rho^2+|\lambda|)_k}{(\rho^2)^k}\left|\frac{d}{d\gamma}\left[\frac{1}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\cdot\frac{1}{(\gamma)_k}\right]_{|_{\gamma=n}}\right|\cdot\frac{(|z|^2)^k}{k!}.$$

And for fixed α such that $0<\alpha<1$ and arbitrary fixed real number R, $R>0$, set $\rho_0=R/\alpha$. Then since

$$\frac{(2B\rho^2+|\lambda|)_k}{(\rho^2)^k}=\prod_{j=1}^{k}\left(2B+\frac{|\lambda|+j-1}{\rho^2}\right),$$

it follows that for every $\rho>\rho_0=R/\alpha$ (i.e, $1/\rho^2<\alpha^2/R^2$) and fixed k, we have the following estimate:

$$\frac{(2B\rho^2+|\lambda|)_k}{(\rho^2)^k}\leqslant(2B\rho_0^2+|\lambda|)_k\left(\frac{\alpha^2}{R^2}\right)^k. \tag{A2}$$

Also, the factor

$$\left|\frac{d}{\mathrm{d}\gamma}\left[\frac{1}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\cdot\frac{1}{(\gamma)_k}\right]_{|_{\gamma=n}}\right|$$

can be easily estimated. Indeed, we have

$$\left|\frac{d}{\mathrm{d}\gamma}\left[\frac{1}{\Gamma(-\lambda-\gamma+1)\Gamma(\gamma)}\cdot\frac{1}{(\gamma)_k}\right]_{|_{\gamma=n}}\right|\leqslant C(n)(1+k)\frac{1}{(n)_k}. \tag{A3}$$

Setting together the estimates (A2) and (A3), we see that we have

$$|U_k(\rho)|\leqslant C(n)\frac{(|\lambda|)_k(2B\rho_0^2+|\lambda|)_k}{(n)_k}\cdot(1+k)\cdot\frac{(\alpha^2)^k}{k!}=:\alpha_k, \tag{A4}$$

for every $\rho>\rho_0$ and $z\in\mathbb{C}^n$ such that $|z|<R$. Finally, since $0<\alpha<1$, we may use the ratio test to see that the series $\Sigma_{k=0}^{+\infty}\alpha_k$, where α_k is as given in (A4), is convergent.

For the proof of (ii), one can proceed similarly as above [using the expansion in series of the Gauss hypergeometric function ${}_2F_1$ involved in (38) and Leibnitz formula] to split $\lim_{\rho\to+\infty}(d/\mathrm{d}\gamma)[\phi_{B,\rho}^{\gamma,2}(\lambda;z)]_{|_{\gamma=n}}$ as follows:

$$\lim_{\rho\to+\infty}\frac{d}{\mathrm{d}\gamma}[\phi_{B,\rho}^{\gamma,2}(\lambda;z)]_{|_{\gamma=n}}=J_\rho^1+J_\rho^2,$$

where J_ρ^1 and J_ρ^2 are given, respectively, by

$$J_\rho^1=\frac{(2B|z|^2)^{1-n}}{\Gamma(-\lambda)}\sum_{k=0}^{+\infty}\frac{\frac{d}{\mathrm{d}\gamma}[(2B\rho^2-\lambda-\gamma+1)_k]_{|_{\gamma=n}}}{(\rho^2)^k}\cdot\frac{(-\lambda-n+1)_k}{\Gamma(2-n)(2-n)_k}\cdot\frac{(|z|^2)^k}{k!}$$

and

$$J_\rho^2=\sum_{k=0}^{+\infty}\frac{(2B\rho^2-\lambda-n+1)_k}{(\rho^2)^k}\times\frac{d}{\mathrm{d}\gamma}\left[\frac{(2B|z|^2)^{1-\gamma}(-\lambda-\gamma+1)_k}{\Gamma(-\lambda)\Gamma(2-\gamma)}\cdot\frac{1}{(2-\gamma)_k}\right]_{|_{\gamma=n}}\cdot\frac{(|z|^2)^k}{k!}.$$

For every fixed $\lambda\in\mathbb{C}\backslash\mathbb{R}^+$ and $z\in\mathbb{C}\backslash\{0\}$, we have $\lim_{\rho\to+\infty}J_\rho^1=0$. To show this, we use again the Lemma 4 this time for

$$U_k(\rho)=\frac{\frac{d}{\mathrm{d}\gamma}[(2B\rho^2-\lambda-\gamma+1)_k]_{|_{\gamma=n}}}{(\rho^2)^k}\cdot\frac{(-\lambda-n+1)_k}{\Gamma(2-n)(2-n)_k}\cdot\frac{(|z|^2)^k}{k!},$$

$$v_k=\lim_{\rho\to+\infty}U_k(\rho)=0,$$

$$\alpha_k = \frac{1}{\rho^2} C_1(n) \cdot \frac{(|\lambda| + n + 1)_k (2B\rho_0^2 + |\lambda| + n + 1)_k}{(2+n)_k} \cdot k \cdot \frac{(\alpha^2)^k}{k!}.$$

Also, we can show in a similar way (as for I_ρ^2) that

$$\lim_{\rho \mapsto +\infty} J_\rho^2 = \frac{1}{\Gamma(-\lambda)} \frac{d}{d\gamma} \left[(2B|z|^2)^{1-\gamma} \frac{{}_1F_1(-\lambda - \gamma + 1; 2 - \gamma; 2B|z|^2)}{\Gamma(2-\gamma)} \right]_{|\gamma=n}.$$

Here, we apply again the Lemma 4 for

$$U_k(\rho) = \frac{(2B\rho^2 - \lambda - \gamma + 1)_k}{(2B\rho^2)^k} \times \frac{d}{d\gamma} \left[\frac{(2B|z|^2)^{1-\gamma} (-\lambda - \gamma + 1)_k}{\Gamma(-\lambda)\Gamma(2-\gamma)} \cdot \frac{1}{(2-\gamma)_k} \right]_{|\gamma=n} \cdot \frac{(2B|z|^2)^k}{k!},$$

$$v_k = \lim_{\rho \mapsto +\infty} U_k(\rho) = \frac{d}{d\gamma} \left[\frac{(2B|z|^2)^{1-\gamma} (-\lambda - \gamma + 1)_k}{\Gamma(-\lambda)\Gamma(2-\gamma)} \cdot \frac{1}{(2-\gamma)_k} \right]_{|\gamma=n} \cdot \frac{(2B|z|^2)^k}{k!},$$

$$\alpha_k = C_2(n) \cdot \frac{(|\lambda| + n + 1)_k (2B\rho_0^2 + |\lambda| + n + 1)_k}{(2+n)_k} \cdot (1+k) \cdot \frac{(\alpha^2)^k}{k!}.$$

Thus, the proof of Lemma 3 is completed.

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Pure point spectrum for the time evolution of a periodically rank-*N* kicked Hamiltonian

James McCaw[a] and B. H. J. McKellar[b]
School of Physics, Research Centre for High Energy Physics, The University of Melbourne, Victoria, 3010, Australia

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We find the conditions under which the spectrum of the unitary time evolution operator for a periodically rank-*N* kicked system remains pure point. This stability result allows one to analyze the onset of, or lack of chaos in this class of quantum mechanical systems, extending the results for rank-1 systems produced by Combescure and others. This work includes a number of unitary theorems equivalent to those well known and used in the self-adjoint theory. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1841482]

I. INTRODUCTION

We will derive conditions on the time-periodic perturbations to the base Hamiltonian for the spectrum of the Floquet operator to remain pure point. We consider Hamiltonians of the form

$$H(t) = H_0 + A^* W A \sum_{n=0}^{\infty} \delta(t - nT) \tag{1}$$

where A is bounded, W is self adjoint and H_0 has pure point (discrete) spectrum. The time evolution of such Hamiltonians is of great interest in quantum chaos, and of central importance is the spectral properties of the Floquet operator, defined as

$$V = e^{iA^* WA/\hbar} e^{-iH_0 T/\hbar} \tag{2}$$

which comes directly from considering the time evolution of the kicked system

$$U(t) = \left[\exp\left(-\frac{i}{\hbar} \int_0^t \mathrm{d}t' \; H(t') \right) \right]_+$$

with $H(t')$ given by (1). The spectrum of the Floquet operator is known as the "quasienergy spectrum."

This work is an extension of a result of Combescure.[1] Our results are based on the self-adjoint work by Howland.[2] If we choose A to be a rank-1 perturbation,

$$A = |\psi\rangle\langle\psi|,$$

$$W = \lambda I,$$

we reproduce the work of Combescure.[1] The vector $|\psi\rangle$ is a linear combination of orthonormal basis states, $|\phi_n\rangle$ of the unperturbed Hamiltonian H_0,

[a]Electronic mail: j.mccaw@physics.unimelb.edu.au
[b]Electronic mail: b.mckellar@physics.unimelb.edu.au

$$|\psi\rangle = \sum_{n=0}^{\infty} a_n |\phi_n\rangle. \tag{3}$$

Combescure showed that if $\psi \in l_1(H_0)$, that is if

$$\sum_{n=0}^{\infty} |a_n| < \infty \tag{4}$$

then the quasienergy spectrum remains pure point for almost every perturbation strength λ. We will generalize this result to all finite rank perturbations,

$$A = \sum_{k=1}^{N} A_k = \sum_{k=1}^{N} |\psi_k\rangle\langle\psi_k|,$$

$$W = \sum_{k=1}^{N} \lambda_k |\psi_k\rangle\langle\psi_k|, \tag{5}$$

where $\lambda_k \in \mathbb{R}$ and each vector $|\psi_k\rangle$ is a linear combination of the H_0 basis states, $|\phi_n\rangle$,

$$|\psi_k\rangle = \sum_{n=0}^{\infty} (a_k)_n |\phi_n\rangle. \tag{6}$$

The states $|\psi_k\rangle$ are orthogonal,

$$\langle\psi_k|\psi_l\rangle = \delta_{kl}.$$

The basic result is that if each $|\psi_k\rangle$ is in $l_1(H_0)$, the spectrum of V will remain pure point for almost every perturbation strength.

The perturbation for which we prove that the quasienergy spectrum remains pure point is in fact more general than the finite rank perturbation presented above. The finite rank result is however the motivation for undertaking this work.

Howland[2] showed that the Hamiltonian (1) has a pure point spectrum if the ψ_k's are in $l_1(H_0)$. Here, we follow a similar argument, showing that the continuous part of the spectrum of V is empty, allowing us to conclude that the spectrum of V must be pure point.

Associated with what we have termed the Floquet operator, is the "Floquet Hamiltonian"

$$K = -id/\mathrm{d}t + H(t).$$

It turns out that K provides a different way to access similar information to what we are seeking. Developed in papers by Howland[3–5] and linked to our Floquet operator in Ref. 6 (p. 808), K was introduced, in some part, because directly working with V proved too difficult. The large body of knowledge on self-adjoint operators provides a mature basis for proving theorems about K. As discussed in Ref. 6, the spectrum of K is easily related algebraically to that of V, so results on the spectrum for K and V are equivalent.

Working directly with V, however, as we do here, is valuable in that it gives a transparent, direct insight into the dynamics of the perturbed system $H(t)$. After the completion of this work, which is a unitary equivalent to that of Howland,[2] we discovered that Howland had used his work[2] on the spectrum of self-adjoint operators to obtain similar results to what we do here.[5]

The relationship between our work and Howland's works (Refs. 2 and 5) is similar to the relationship between the self-adjoint rank-1 work of Simon and Wolff[7] and the unitary rank-1 work of Combescure.[1]

The techniques developed in this paper provide new, general theorems applicable to unitary operators and show that it is possible to develop the theory of the spectrum of time evolution operators directly, without need for the techniques of Ref. 3 briefly mentioned here.

A. Motivation

The classical study of chaos is now a well established and flourishing field of research in mathematics and mathematical physics. Chaotic behavior seems to pervade a vast spectrum of dynamical systems, and an appreciation of it is essential for a detailed understanding of such systems. The classic example of the earth's weather patterns always comes to mind when chaos is mentioned.

The microscopic world, however, is not governed by the laws of classical dynamics. In the realm of small quantum numbers the dynamics of a system is governed by the Schrödinger equation. In such systems, the simple and elegant definitions of chaos such as positive Lyapunov exponent, which hold for classical systems, are not applicable. In fact, there is no universally accepted definition of quantum chaos. Some model systems show what many would consider "chaotic behavior," yet there are general arguments made by some[8] to the effect that "quantum chaos" does not exist. Our study of one aspect of "quantum chaos" is motivated by much of this work. Taking note of these uncertainties and conflicting views, two questions arise that are of central importance.

(a) What properties of a quantum mechanical system determine whether or not the corresponding classical system that derives from it will display chaotic behavior?
(b) Are there in fact quantum systems that display chaotic behavior at the quantum level?

The former question is intimately linked to the "correspondence principle" and theories of quantum measurement. Needless to say, this area of fundamental physics is infamous for its interpretational difficulties and seemingly inconsistent behavior.

The latter question too, is the source of much debate in the literature. As in any immature study, quantum chaos is struggling to be self-consistently defined. A wide range of possible definitions and interpretations of what quantum chaos actually is have been put forward, many in direct contradiction with one another. At some stage in the future presumably, we will find a satisfactory criteria for what constitutes quantum chaos. Until then, many attempts to look at particular aspects of the dynamics of quantum systems will be (and have been) made. Some papers, courtesy of their definition of quantum chaos, come to the conclusion that there is no such thing as quantum chaos. That is, they conclude that no quantum system can display chaotic behavior. Other papers, simply as a consequence of a different starting point, come to the conclusion that there are quantum systems that display chaos.

There are general arguments that allow one to categorize the behavior of a quantum system based upon the spectral composition of the quasienergy spectrum. Hence, Combescure's work on the spectrum is relevant to the study of chaos. Our work, by extending the result of Combescure, may allow for the further categorization of classes of Hamiltonian systems as chaotic or otherwise. This is further discussed in the next section.

B. Spectral analysis of operators and a link to chaos

The intuitive definition for the energy spectrum of a quantum system is best seen through example, say the hydrogen atom. The bound states of hydrogen are a countable number of isolated, discrete energies. Each energy corresponds to an eigenvalue of the system and the set of these points makes up the point energy spectrum. The positive energy scattering states form the continuous energy spectrum. Thus, the energy spectrum for the hydrogen system consists of two disjoint parts: the negative energy discrete (or "point") spectrum, and the positive energy continuous spectrum.

For hydrogen, $\sigma_p(H)=\{\alpha_n;\alpha_n\approx -13.6/n^2 \text{ for } n\in\mathbb{N}\}$, and $\sigma_{\text{cont}}(H)=(0,\infty)$.

As another simple example, the harmonic oscillator quantum system has only discrete energy levels, and thus is said to be "pure point." That is, the eigenvectors of the harmonic oscillator form a basis of the Hilbert space.

While these simple examples have shown clearly that we can split the energy spectrum into point and continuous parts, this is not the whole story. The mathematical treatment of operators and measures shows that the spectrum in fact consists of three parts, the point, absolutely continuous and singularly continuous spectrum. For an appreciation of the work that follows, a mathematically rigorous understanding of the spectra is necessary. The introductory chapters in Ref. 9 are essential reading.

One must note that the concept of spectrum is associated with a particular operator. Typically, we talk of the energy spectrum, associated with the Hamiltonian. However, all operators (e.g., Hamiltonian, Floquet, etc.) have a spectrum. A failure to realize this has lead to a number of confused papers (see, for example, Ref. 10) which use results on the spectrum of the Hamiltonian in a discussion of the spectrum of the Floquet operator. With these words of warning, we return to a discussion of the Floquet (or quasienergy) spectrum of a quantum system.

The link between spectral properties and dynamics is an active field of research and is not yet fully understood. The introduction to the paper of Last[11] provides an informative overview of the field and gives details on some of the most relevant theorems and results, including the RAGE theorem (Ref. 12, p. 341, Theorem XI.115). See also Ref. 13 (Ref. 28). Last's paper deals with systems where the Hamiltonian spectrum is of interest. In time-periodic Hamiltonian systems, the spectrum of the Floquet operator takes over that role. Yajima and Kitada[14] show that RAGE like results apply to time-periodic systems, as we have here, and thus an analysis of the Floquet operator spectrum is of interest.

Refering to either the Hamiltonian spectrum or the Floquet spectrum where appropriate, and the appropriate RAGE like theorem, we now comment on the "typical" manifestation of the spectrum. A typical quantum mechanical system does not possess a singularly continuous spectral component and thus, singular continuity is not usually mentioned in texts on quantum mechanics. This however, is not to say that it cannot exist, or that it does not manifest itself in the dynamical behavior of appropriate systems. With an understanding that Milek and Seba meant to refer to the RAGE like theorem in Ref. 14 rather than the RAGE theorem itself, the argument presented in Sec. II of their paper[10] shows that if a system possesses a singularly continuous quasienergy spectrum then its energy growth over time may be characteristic of a classically chaotic system. Thus, establishing the existence or otherwise of singular continuous spectra for the Floquet operator can be seen as of central importance to the question of whether or not a quantum mechanical system is chaotic. It must be noted that the arguments presented by Milek and Seba are acknowledged to be anything but rigorous—a point clearly established by Antoniou and Suchanecki[29,30]

It is with the application of the RAGE like theorem in mind,[14] that we undertook the following work on the analysis of the quasienergy spectrum of the class of Hamiltonians as defined by (1). The aforementioned work by Milek and Seba,[10] utilizing the rank-1 work of Combescure, has shown the manifestation of singularly continuous spectra in numerical simulations of rank-1 kicked rotor quantum systems. The work here has the potential to extend upon this, and provide a rigorous mathematical basis to numerical calculations on the time evolution of higher rank kicked quantum systems.

C. Outline and summary of results

In Sec. II we will present the main theorems of the paper, concerned with establishing when systems of the form given by (1) maintain a pure point quasienergy spectrum. Parallelling Howland's paper[2] on self-adjoint perturbations of pure point Hamiltonians, the key ideas are those of U-finiteness and the absolute continuity of the multiplication operator $\mathbb{V}$. To establish the second of these concepts for our unitary case (remember that we are concerned with the spectral properties of the unitary time evolution operator and not with the spectral properties of the self-adjoint

Hamiltonian itself), we require a modified version of the Putnam–Kato theorem.[15] This, and associated theorems are the topic of Sec. III. Sec. IV uses the results of Secs. II and III to give the final results, which are then discussed in Sec. V.

D. Notation

We inherit our notation directly from the work of Howland.[2] $\mathcal{H}$ and $\mathcal{K}$ will denote Hilbert spaces throughout this paper. They will always be separable. The inner product of two vectors x and y is $\langle x,y\rangle$, and the norm of a vector x is $\|x\|=\langle x,x\rangle^{1/2}$. For an operator $A:\mathcal{H}\to\mathcal{K}$ we define the following:

(i) the domain $D(A)$; the vectors $x\in\mathcal{H}$ for which Ax is defined,
(ii) the range $R(A)=\{y\in\mathcal{K}:y=Ax \text{ for some } x\in\mathcal{H}\}$,
(iii) the kernel $\ker A=\{x\in\mathcal{H}:Ax=0\}$, and
(iv) the operator norm $\|A\|=\sup_{x\in D(A):\|x\|=1}\{\|Ax\|\}$.

For any set $S\in\mathbb{C}$, $\overline{S}$ is the closure of S. If A_n is a sequence of operators, s-lim A_n (also $A_n\to{}^sA$) denotes the strong limit, $\|(A_n-A)g\|\to 0$ for all $g\in\mathcal{H}$. w-lim A_n (also $A_n\to{}^wA$) denotes the weak limit, $|\langle A_ng,f\rangle-\langle Ag,f\rangle|\to 0$ for all $g,f\in\mathcal{H}$. By the Schwartz inequality, the weak limit exists if the condition above is satisfied for $f=g$. We will also have need for the norm limit of an operator, $\|A_n-A\|\to 0$.

For a unitary operator $V=\int e^{-i\theta}E(\mathrm{d}\theta)$ on $\mathcal{H}$, we define for any Borel set S, $E[S]=\int_S E(\mathrm{d}\theta)$. The $E(\mathrm{d}\theta)$ are orthogonal projection operators, i.e., $E^2=E$ and thus

$$\int |f(\theta)|^2E(\mathrm{d}\theta)=\left|\int f(\theta)E(\mathrm{d}\theta)\right|^2.$$

We decompose our operator into its pure point (V^p), singular continuous (V^{sc}) and absolutely continuous (V^{ac}) components. $V^s=V^p+V^{sc}$ is the singular part of the operator V. Similarly, we define the corresponding spectral measures E^p, E^{sc}, E^{ac}, and E^s. For a vector $x\in\mathcal{H}$, m_x is the measure

$$m_x(S)=\langle E(S)x,x\rangle.$$

Again, we define m_x^p, m_x^{sc}, m_x^{ac}, and m_x^s. See Ref. 9, pp. 19–23, for an excellent description of these. By their definition, m_x^p, m_x^{sc}, and m_x^{ac} are mutually singular, so we may write the Hilbert space as a direct sum (i.e., each of the spaces below is invariant)

$$\mathcal{H}=\mathcal{H}_{pp}\oplus\mathcal{H}_{ac}\oplus\mathcal{H}_{sc}.$$

The spectrum of V is $\sigma(V)$, defined by

$$\sigma(V)=\{\alpha\in\mathbb{C}:\alpha I-V \text{ is not invertible}\}.$$

If $Tx=\alpha x$ for some $x\in\mathcal{H}$ and $\alpha\in\mathbb{C}$, then x is an eigenvector, with corresponding eigenvalue α. The closure of the set of α's forms the point spectrum of V,

$$\sigma_p(V)=\overline{\{\alpha:\alpha \text{ an eigenvalue of } V\}}=\sigma(V\restriction\mathcal{H}_p).$$

We say that V is *pure point* if and only if the eigenvectors of V form a basis of $\mathcal{H}$. The absolutely (singularly) continuous spectrum, $\sigma_{ac(sc)}(V)$ is similarly defined by

$$\sigma_{ac(sc)}(V)=\sigma(V\restriction\mathcal{H}_{ac(sc)}).$$

For a complete discussion and analysis of these topics, the most convenient reference is (Ref. 9, pp. 19–23, 188, 230–231) or Ref. 16.

A set $\mathcal{S} \in \mathcal{H}$ is said to reduce an operator A if both $\mathcal{S}$ and its orthocomplement $\mathcal{H} \ominus \mathcal{S}$ are invariant subspaces for A.

A vector ϕ is cyclic for an operator A if and only if finite linear combinations of elements of $\{A^n\phi\}_{n=0}^{\infty}$ are dense in $\mathcal{H}$. This motivates the definition that a set $\mathcal{S}$ is cyclic for $\mathcal{H}$ if and only if the smallest closed reducing subspace of $\mathcal{H}$ containing $\mathcal{S}$ is $\mathcal{H}$.

We will also use some basic set notation. $A \cap B$ and $A \cup B$ are, as usual, the intersection and union of sets A and B, respectively. A^c is the complement of A. $A \sim B$ is $A \cap B^c$. Note that $(A \sim B) \sim C$ is not equal to $A \sim (B \sim C)$, the former being a subset of the latter.

The function $\chi_S(x)$ is the characteristic function for a set S.

II. SPECTRAL PROPERTIES OF THE FLOQUET OPERATOR

Let U be unitary on $\mathcal{H}$ and let $\mathcal{K}$ be an auxiliary Hilbert space. Define the closed operator $A: \mathcal{H} \to \mathcal{K}$, with dense domain $D(A)$. For our purposes, A bounded on $\mathcal{H}$ is adequate. We work with a modification (multiplication by $e^{i\theta}$) of the resolvent of U,

$$F(\theta; U) = (1 - Ue^{i\theta})^{-1}, \tag{7}$$

and define for $\theta \in [0, 2\pi)$, and $\epsilon > 0$ the function $G_\epsilon: \mathcal{K} \to \mathcal{K}$,

$$G_\epsilon(\theta; U, A) = AF^*(\theta_+; U)F(\theta_+; U)A^*, \tag{8}$$

where $\theta_\pm = \theta \pm i\epsilon$. Let J be a subset of $[0, 2\pi)$.

Definition II.1 (*U-finite*): *The operator A is U-finite if and only if the operator* $G_\epsilon(\theta; U, A)$ *has a bounded extension to* $\mathcal{K}$, *and*

$$G(\theta; U, A) = s\text{-}\lim_{\epsilon \downarrow 0} G_\epsilon(\theta; U, A) \tag{9}$$

exists for almost every $\theta \in J$.

We define the function

$$\delta_\epsilon(t) = \frac{1}{2\pi}\left(\sum_{n=0}^{\infty} e^{in(t+i\epsilon)} + \sum_{n=-\infty}^{0} e^{in(t-i\epsilon)} - 1\right) = \frac{1}{2\pi}\frac{1 - e^{-2\epsilon}}{1 - 2e^{-\epsilon}\cos(t) + e^{-2\epsilon}}. \tag{10}$$

The limit as $\epsilon \to 0$ of $\delta_\epsilon(t)$ is a series representation of the δ-function. The proof is based on showing that

$$\lim_{\epsilon \downarrow 0} \int_{-\pi}^{\pi} g(t)\delta_\epsilon(t)\mathrm{d}t = 0,$$

where $g(t) = f(t) - f(0)$ and $f(t)$ is bounded in $(-\pi, \pi)$. One splits the integral into three parts, $\int_{-\pi}^{-\xi} + \int_{-\xi}^{\xi} + \int_{\xi}^{\pi}$. One must assume that $f(t)$ is continuous at $t = 0$ [otherwise $\int f(t)\delta(t)\mathrm{d}t$ is not well defined] so that

$$\forall\, \eta, \exists\, \xi > 0 \text{s.t.} \forall\, t, |t| < \xi \quad \text{we have } |f(t) - f(0)| < \eta.$$

The assumption that $f(t)$ is bounded on $(-\pi, \pi)$ is also required.

The first and third integrals are zero because $\delta_\epsilon(t) \to 0$ for $t \neq 0$ from (10) and the assumption that $g(t)$ is bounded. The second integral from $-\xi$ to ξ is zero by the continuity of $f(t)$ at $t = 0$, the positivity of $\delta_\epsilon(t)$ and Ref. 17, p. 435, (3.792.1).

Given (10) and the spectral decomposition of U, we may write

$$\delta_\epsilon(1 - Ue^{i\theta}) = \int \delta_\epsilon(1 - e^{i(\theta - \theta')})E(\mathrm{d}\theta') = \int \delta_\epsilon(\theta - \theta')E(\mathrm{d}\theta') = \frac{1}{2\pi}(1 - e^{-2\epsilon})F^*(\theta_+; U)F(\theta_+; U). \tag{11}$$

The existence of a nontrivial U-finite operator will have important consequences for the spectrum of the Floquet operator V. We introduce the set

$$N(U,A,J) = \{\theta \in J : s\text{-}\lim_{\epsilon \downarrow 0} G_\epsilon(\theta;U,A) \text{ does not exist}\}$$

of measure zero, which enters the theorem. We will often refer to this set simply as N during proofs.

Theorem II.2: *If A is U-finite on J and $R(A^*)$ is cyclic for U, then*

(a) *U has no absolutely continuous spectrum in J, and*
(b) *the singular spectrum of U in J is supported by $N(U,A,J)$.*

Proof: (a) Following Howland, we note that the absolutely continuous spectral measure, $m_y^{ac}(J)$, is the $\epsilon \to 0$ limit of $\langle \delta_\epsilon(1-Ue^{i\theta})y,y\rangle$ for $\theta \in J$. If $y \in \mathcal{H}$ is in $R(A^*)$, allowing us to write $y=A^*x$ for some $x \in \mathcal{K}$, then

$$\lim_{\epsilon \downarrow 0}\langle \delta_\epsilon(1-Ue^{i\theta})y,y\rangle = \lim_{\epsilon \downarrow 0}\langle \delta_\epsilon(1-Ue^{i\theta})A^*x,A^*x\rangle = \lim_{\epsilon \downarrow 0}\frac{\epsilon(1-\epsilon)}{\pi}\langle G_\epsilon(\theta;U,A)x,x\rangle = 0$$

for almost every $\theta \in J$. The set $\mathcal{Y}$ of vectors y for which $m_y^{ac}(J)=0$ is a closed reducing subspace of $\mathcal{H}$, and by construction contains the cyclic set $R(A^*)$ as a subset. Because $\mathcal{Y}$ is invariant, finite linear combinations of action with U^n leaves us in $\mathcal{Y}$. Due to the cyclicity, these same linear combinations allow us to reach any $y \in \mathcal{H}$. Thus, the set $\mathcal{Y}$ of vectors y with $m_y^{ac}(J)=0$ must be the whole Hilbert space $\mathcal{H}$. So there is no absolutely continuous spectrum of U in J.

(b) A theorem of de la Vallée Pousin [Ref. 18, p. 127, (9.6)] states that the singular part of the spectrum of a function is supported on the set where the derivative is infinite. In our case, this corresponds to finding where $m_y(\mathrm{d}\theta) \to \infty$. We calculate

$$\lim_{\epsilon \downarrow 0}\langle \delta_\epsilon(1-Ue^{i\theta})y,y\rangle = \int \delta(\theta-\theta')\langle E(\mathrm{d}\theta')y,y\rangle = \int \delta(\theta-\theta')m_y(\mathrm{d}\theta') = m_y(\mathrm{d}\theta).$$

Thus, $m_y^s = m_y^{sc} + m_y^{pp}$ is supported on the set where

$$\lim_{\epsilon \downarrow 0}\langle \delta_\epsilon(1-Ue^{i\theta})y,y\rangle = \infty. \tag{12}$$

From the proof to part (a), if $y=A^*x$ then the limit (12) is zero for $\theta \in J$, $\theta \notin N$, so m_y^s in J must be supported by N. The set of vectors y with $m_y^s(J \cap N^c) \equiv m_y^s(J \sim N) = 0$ is closed, invariant and contains $R(A^*)$, so must be $\mathcal{H}$ by the argument above. Thus, the singular spectrum of U is supported on the set N. ■

We now define a new operator, $Q(z):\mathcal{K} \to \mathcal{K}$,

$$Q(z) = A(1-Uz)^{-1}A^*.$$

Note that

$$Q(e^{i\theta_\pm}) = AF(\theta_\pm;U)A^*. \tag{13}$$

$Q(z)$ is clearly well defined for $|z| \neq 1$. Proposition II.3 shows that the definition can be extended to $|z|=1$.

Proposition II.3: Let A be bounded. If $\theta \in J$, but $\theta \notin N(U,A,J)$, then

(a) *the operator $Q(e^{i\theta}) = A(1-Ue^{i\theta})^{-1}A^*$ is bounded on K, and*
(b) *one has s-$\lim_{\epsilon \downarrow 0} Q(e^{\pm i(\theta \pm i\epsilon)}) = Q(e^{\pm i\theta})$.*

Proof: (a) Without loss of generality, take $\theta=0$ $(z=1)$. By Theorem II.2, $e^{-i0} \notin \sigma_p(U)$, so

$(1-Ue^{i0})^{-1}$ exists as a densely defined operator. As A is a bounded operator, it suffices to show that $(1-Ue^{i0})^{-1}A^*$ is bounded. We have

$$\begin{aligned}\|(1-Ue^{i0_+})^{-1}A^*x\|^2 &= \langle F(0_+;U)A^*x, F(0_+;U)A^*x\rangle \\ &= \langle AF^*(0_+;U)F(0_+;U)A^*x, x\rangle \\ &= \langle G_\epsilon(0;U,A)x,x\rangle \leqslant C|x|^2 \text{ (as } \theta \notin N) \end{aligned} \tag{14}$$

for some real constant C. If $y=A^*x$, noting $U=\int e^{-i\theta}E(\mathrm{d}\theta)$, we also have

$$\|(1-Ue^{i0_+})^{-1}A^*x\|^2 = \int \left(\frac{1}{1-e^{-i\theta}e^{-\epsilon}}\right)\left(\frac{1}{1-e^{i\theta}e^{-\epsilon}}\right)\langle E(\mathrm{d}\theta)y,y\rangle.$$

In light of (14), we may safely take ϵ to zero, to obtain

$$\int \left(\frac{1}{1-e^{-i\theta}}\right)\left(\frac{1}{1-e^{i\theta}}\right)\langle E(\mathrm{d}\theta)y,y\rangle \leqslant C\|x\|^2 < \infty. \tag{15}$$

From (15), we have

$$\int \left(\frac{1}{1-e^{-i\theta}}\right)\left(\frac{1}{1-e^{i\theta}}\right)\langle E(\mathrm{d}\theta)y,y\rangle = \langle [1-U]^{-1}y, [1-U]^{-1}y\rangle \leqslant C\|x\|^2 < \infty, \tag{16}$$

so $y \in D[(1-U)^{-1}]$. Thus, $Q(1)=A(1-U)^{-1}A^*$ is defined on all $\mathcal{K}$ and bounded.

(b) For $y \in D((1-U)^{-1})$, we show that the difference between $Q(e^{\pm i(0\pm i\epsilon)})$ and $Q(e^{\pm i0})$ tends to zero as $\epsilon \to 0$. Again, due to the boundedness of A, we need only show that

$$\|((1-Ue^{i0_+})^{-1}-(1-U)^{-1})A^*x\|$$

tends to zero. Consider

$$\begin{aligned}|(1-Ue^{-\epsilon})^{-1}y-(1-U)^{-1}y|^2 &= \int \left|\frac{1}{1-e^{-i\theta}e^{-\epsilon}}-\frac{1}{1-e^{-i\theta}}\right|^2\langle E(\mathrm{d}\theta)y,y\rangle \\ &= \int \left(\frac{(1-e^{-\epsilon})^2}{1-2e^{-\epsilon}\cos\theta+e^{-2\epsilon}}\right)\frac{\langle E(\mathrm{d}\theta)y,y\rangle}{(1-e^{-i\theta})(1-e^{i\theta})}. \end{aligned} \tag{17}$$

The first factor is bounded and tends to zero for $\theta \neq 0$. The second factor is the measure from (15). Clearly, away from the origin, the integral tends to zero. About the origin, we must take some care to show that there is no contribution to the integral.

Using (10), we have

$$\frac{(1-e^{-\epsilon})^2}{1-2e^{-\epsilon}\cos\theta+e^{-2\epsilon}} = \frac{(1-e^{-\epsilon})^2}{1-e^{-2\epsilon}}2\pi\delta_\epsilon(\theta).$$

On substitution into (17), we obtain

$$\frac{(1-e^{-\epsilon})^2}{1-e^{-2\epsilon}}2\pi\int_{-\alpha}^{\alpha}\delta_\epsilon(\theta)\frac{m_y(\mathrm{d}\theta)}{2(1-\cos\theta)} = \frac{(1-e^{-\epsilon})^2}{1-e^{-2\epsilon}}2\pi\int_{-\alpha}^{\alpha}\frac{\mathrm{d}\Theta_\epsilon}{\mathrm{d}\theta}\frac{g_y(\theta)}{2(1-\cos\theta)}\mathrm{d}\theta.$$

The function $\Theta_\epsilon(\theta)=\int\delta_\epsilon(\theta')\mathrm{d}\theta'$ is the step function in the $\epsilon\to 0$ limit. For nonzero ϵ it is positive, monotonic, increasing and bounded by unity. As $\theta \notin N$ we have also written $m_y(\mathrm{d}\theta)=g_y(\theta)\mathrm{d}\theta$ for some well behaved positive function $g_y(\theta)$. By integration by parts (see Ref. 19, p. 32 for existence conditions, which are satisfied) we obtain

$$\frac{(1-e^{-\epsilon})^2}{1-e^{-2\epsilon}}2\pi\left\{\left[\Theta_\epsilon(\theta)\frac{g_y(\theta)}{2(1-\cos\ \theta)}\right]_{-\alpha}^{\alpha}-\int_{-\alpha}^{\alpha}\Theta_\epsilon(\theta)\frac{d}{d\theta}\frac{g_y(\theta)}{2(1-\cos\ \theta)}d\theta\right\}.$$

The first term within the curly braces is clearly some finite value. The second term is less than

$$\int_{-\alpha}^{\alpha}\frac{d}{d\theta}\frac{g_y(\theta)}{2(1-\cos\ \theta)}d\theta=\left[\frac{g_y(\theta)}{2(1-\cos\ \theta)}\right]_{\alpha}^{-\alpha}$$

from the properties of the Θ_ϵ function mentioned above. As with the first term, it is clearly some finite value. Noting that

$$\lim_{\epsilon\downarrow 0}\frac{(1-e^{-\epsilon})^2}{1-e^{-2\epsilon}}=0$$

we see that part (b) follows. ■

Theorem II.4: *Let A be bounded and U-finite on J, with $R(A^*)$ cyclic for U. Let W be bounded and self-adjoint on $\mathcal{K}$, and define the Floquet operator*

$$V=e^{iA^*WA/\hbar}U.$$

We assume that for $|z|\neq 1$, $Q(z)$ is compact, and that $Q(e^{\pm i(\theta\pm i\epsilon)})$ converges to $Q(e^{\pm i\theta})$ in operator norm as $\epsilon\rightarrow 0$ for a.e. θ in J. Define the set

$$M(U,A,J)=\{\theta\in J: Q(e^{\pm i(\theta\pm i0)})\ \textit{does not exist in norm}\}.$$

Then

(a) *V has no absolutely continuous spectrum in J, and*
(b) *the singular continuous part of the spectrum of V in J is supported by the set $N(U,A,J)\cup M(U,A,J)$.*

Proof: (a) For convenience, we write the Floquet operator as

$$V=(1+A^*Z\ A)U,$$

where Z is defined appropriately by requiring $\exp(iA^*WA/\hbar)=1+A^*ZA$. [For the rank-$N$ perturbation case where $W=\Sigma_{k=1}^{N}\lambda_k|\psi_k\rangle\langle\psi_k|$ and $A=\Sigma_{k=1}^{N}|\psi_k\rangle\langle\psi_k|$, we have $Z=\Sigma_{k=1}^{N}(\exp(i\lambda_k/\hbar)-1)|\psi_k\rangle\langle\psi_k|$.]

Noting (7) and (13) allows us to define

$$Q_1=AF(\theta;V)A^*=A(1-Ve^{i\theta})^{-1}A^*.$$

Consider some vector $y'\in\mathcal{H}$. $Ay'=x\in\mathcal{K}$ is defined for such y'. $A^*x=y''$ is some vector in $\mathcal{H}$. The cyclicity of $R(A^*)$ means that action with linear combinations of powers of U on y'' allows us to obtain any $y\in\mathcal{H}$, our original y' being one of them. Thus, we have a construction of A^{-1}, namely, operation with A^* followed by the linear combination of powers of U. As y' was arbitrary, A^{-1} exists for all $y\in\mathcal{H}$. This allows us to introduce $I=A^{-1}A$ in what follows. [The particular choice of A as a projection in (5) does not have an inverse, but we will see in Sec. IV that we can define a subspace of $\mathcal{H}$ on which $R(A^*)$ is cyclic, and apply this theorem.]

We now proceed by use of the resolvent equation,

$$\begin{aligned}Q_1-Q&=A\left\{\frac{1}{1-Ve^{i\theta}}-\frac{1}{1-Ue^{i\theta}}\right\}A^*\\&=A\left\{\frac{1}{1-Ve^{i\theta}}(A^*Z\ AUe^{i\theta})\frac{1}{1-Ue^{i\theta}}\right\}A^*=Q_1(e^{i\theta})Z\ AUA^{-1}e^{i\theta}Q(e^{i\theta}).\end{aligned}\tag{18}$$

Thus, briefly using $L=Z\ AUA^{-1}e^{i\theta}$ for clarity, we have

$$LQ_1 - LQ = LQ_1LQ \Rightarrow (1 + LQ_1)(1 - LQ) = 1$$
$$\Rightarrow 1 + e^{i\theta}Z\,AUA^{-1}Q_1(e^{i\theta}) = [1 - e^{i\theta}Z\,AUA^{-1}Q(e^{i\theta})]^{-1}. \tag{19}$$

Denote by N and M the sets $N(U,A,J)$ and $M(U,A,J)$. If $\theta \in (J \sim N) \sim M$, i.e., $\theta \in J \cap N^c \cap M^c$, and $1 - e^{i\theta}Z\,AUA^{-1}Q(e^{i\theta})$ is not invertible, then the compactness of $-LQ(e^{i\theta})$ [which follows from the compactness of $Q(e^{i(\theta+i\epsilon)})$, the norm convergence of $Q(e^{i(\theta+i\epsilon)})$ and Theorem VI.12 in Ref. 9] allows us to use the Fredholm alternative (Ref. 9, p. 201, Theorem VI.14) to assert that

$$\exists x \in \mathcal{K}, \text{s.t. } [1 - e^{i\theta}Z\,AUA^{-1}Q(e^{i\theta})]x = 0.$$

That is, there is some vector $x \in \mathcal{K}$ which satisfies the equation

$$x - e^{i\theta}Z\,AUA^{-1}A(1 - Ue^{i\theta})^{-1}A^*x = 0. \tag{20}$$

As $\theta \in J \sim N$, by Proposition II.3 $y = A^*x \in D[(1 - Ue^{i\theta})^{-1}]$ so define ϕ as

$$\phi = (1 - Ue^{i\theta})^{-1}A^*x. \tag{21}$$

ϕ is a well-defined vector on $\mathcal{H}$ and we have

$$x = e^{i\theta}Z\,AU\phi.$$

By (21), $x \neq 0$ implies $\phi \neq 0$, so we have

$$(1 - Ue^{i\theta})\phi = A^*x = e^{i\theta}A^*Z\,AU\phi$$

or

$$V\phi = e^{-i\theta}\phi. \tag{22}$$

We conclude that $e^{-i\theta} \in \sigma_p(V)$.

The multiplicity of the eigenvalue is given by the dimension of the kernel of $1 - e^{i\theta}Z\,AUA^{-1}Q$, which is finite by the compactness of Q and Theorem 4.25 of Ref. 20.

Therefore, if $\theta \in J \sim (N \cup M \cup \sigma_p(V))$, which is a set of full Lebesgue measure (that the set M has measure zero is a consequence of Lemma II.5), then the vector

$$x(\epsilon) = [1 + e^{i(\theta+i\epsilon)}Z\,AUA^{-1}Q_1(e^{i(\theta+i\epsilon)})]x \equiv [1 + L_+Q_1(e^{i\theta_+})]x \tag{23}$$

must be bounded in norm as $\epsilon \to 0$ because we have just seen that if it is unbounded, we have an eigenvalue of the operator V. For $y = A^*x \in R(A^*)$, the absolutely continuous spectrum, m_y^{ac} of V is the limit of

$$\langle \delta_\epsilon(1 - Ve^{i\theta})y, y\rangle = \langle A\delta_\epsilon(1 - Ve^{i\theta})A^*x, x\rangle.$$

Our aim is to show that this is zero for all $y \in \mathcal{H}$. We define

$$F_1(\theta) = (1 - Ve^{i\theta})^{-1}, \tag{24}$$

$$F(\theta) = (1 - Ue^{i\theta})^{-1}, \tag{25}$$

and in a similar fashion to (18) and (19), obtain

$$F_1(\theta) = F(\theta)[1 + (V - U)e^{i\theta}F_1(\theta)] \tag{26}$$

and

$$(1 + (V - U)e^{i\theta}F_1(\theta)) = (1 - (V - U)e^{i\theta}F(\theta))^{-1}.$$

Writing $X = V - U$, on substituting (26) into our expression for the δ-function (11) we obtain

$$2\pi\delta_\epsilon(1-Ve^{i\theta}) = (1-e^{-2\epsilon})F_1^*(\theta_+)F_1(\theta_+) = [1+e^{i\theta_+}XF_1(\theta_+)]^* 2\pi\delta_\epsilon(1-Ue^{i\theta})[1+e^{i\theta_+}XF_1(\theta_+)].$$

Substitution of (13) and noting that

$$X = V-U = (1+A^*Z\,A)U - U = A^*Z\,AU$$

gives us

$$\begin{aligned} A\delta_\epsilon(1-Ve^{i\theta})A^* &= A[1+Xe^{i\theta_+}F_1(\theta_+)]^*\delta_\epsilon(1-Ue^{i\theta})[1+Xe^{i\theta_+}F_1(\theta_+)]A^* \\ &= [1+L_+Q_1(\theta_+)]^* A\delta_\epsilon(1-Ue^{i\theta})A^*[1+L_+Q_1(\theta_+)]. \end{aligned}$$

The absolutely continuous spectrum, m_y^{ac} of V is the limit of

$$\begin{aligned} \langle A\delta_\epsilon(1-Ve^{i\theta})A^*x,x\rangle &= \langle [1+L_+Q_1(\theta_+)]^* A\delta_\epsilon(1-Ue^{i\theta})A^*[1+L_+Q_1(\theta_+)]x,x\rangle \\ &= \langle A\delta_\epsilon(1-Ue^{i\theta})A^*x(\epsilon),x(\epsilon)\rangle = \frac{\epsilon(1-\epsilon)}{\pi}\langle G_\epsilon(\theta;U,A)x(\epsilon),x(\epsilon)\rangle \end{aligned} \tag{27}$$

which tends to zero as $\epsilon\to 0$ if both $G_\epsilon(\theta;U,A)$ and $x(\epsilon)$ are bounded. $G_\epsilon(\theta;U,A)$ is bounded as we have $\theta\in J\sim N$ and $x(\epsilon)$ is bounded by (23).

Part (a) follows since $R(A^*)$ cyclic for U implies that $R(A^*)$ is cyclic for V.

(b) Let $N_1=N(V,A,J)$. We have just shown that $\theta\in J\sim(N\cup M\cup\sigma_p(V))$ implies that

$$\frac{\epsilon}{\pi}\langle G_\epsilon(\theta;V,A)x(\epsilon),x(\epsilon)\rangle \to 0 \tag{28}$$

and therefore

$$\langle \delta_\epsilon(1-Ve^{i\theta})y,y\rangle \to 0. \tag{29}$$

If we can infer the strong limit from this weak limit then we have established that $\theta\notin N_1$. We use the result that if $x_n\to^w x$ and $\|x_n\|\to\|x\|$, then $x_n\to^s x$ (Ref. 21, p. 244). Writing G_ϵ and G for $G_\epsilon(\theta;V,A)$ and $G(\theta;V,A)$, and F_ϵ and F for $F(\theta_+;V)$ and $F(\theta;V)$, consider

$$|\|G_\epsilon x\|^2 - \|Gx\|^2| = |\langle (G_\epsilon^2-G^2)x,x\rangle| = |\langle A\{(F_\epsilon^*F_\epsilon - F^*F)A^*AF_\epsilon^*F_\epsilon + F^*FA^*A(F_\epsilon^*F_\epsilon - F^*F)\}A^*x,x\rangle|.$$

If A, F_ϵ, and F are bounded operators, then if $F_\epsilon^*F_\epsilon - F^*F$ tends to zero as $\epsilon\to 0$ we can conclude that the strong limit exists. A short calculation shows that

$$F_\epsilon^*F_\epsilon - F^*F = [(1-e^{-2\epsilon}) - (1-e^{-\epsilon})(Ue^{i\theta}+U^*e^{-i\theta})]F_\epsilon^*F_\epsilon F^*F$$

which trivially tends to zero as $\epsilon\to 0$ given the boundedness of F_ϵ and F. Finally, A is bounded by assumption and (23) shows that $Q_1(\theta_+)$ is a bounded operator as $\epsilon\to 0$ and thus both F_ϵ and F are bounded.

Moving on from (29), we have now established that $N_1\subset N\cup M\cup\sigma_p(V)$ so N_1 must have measure zero, again remembering that we need Lemma II.5 below to prove that M has measure zero. By Theorem II.2, N_1 supports the singular spectrum of V. That is,

$$m^s(N_1^c) = 0,$$

where the set N_1^c is the complement of N_1. As the measure is positive and $m^s=m^{sc}+m^p$, we know that

$$m^{sc}(N_1^c) = 0.$$

Trivially, $(N\cup M)\sim\sigma_p(V)$ contains $N_1\sim\sigma_p(V)$. Thus

$$m^{sc}([N_1\cap\sigma_p(V)^c]^c) = m^{sc}(N_1^c\cup\sigma_p(V)) = m^{sc}(N_1^c) + m^{sc}(\sigma_p(V)) = 0+0 = 0$$

as the (continuous) measure of single points is zero.

The set $N \cup M \cap \sigma_p(V)^c$ must support m^{sc} as $N_1 \cap \sigma_p(V)^c$ is a subset. Therefore

$$m^{sc}([N \cup M \cap \sigma_p(V)^c]^c) = 0.$$

This equals

$$m^{sc}([N \cup M]^c \cup \sigma_p(V)) = m^{sc}([N \cup M]^c) + m^{sc}(\sigma_p(V)) = m^{sc}([N \cup M]^c)$$

so we conclude that the set $N \cup M$ supports the singular continuous part of the spectrum. ■

Theorem II.4 has shown us that V has an empty absolutely continuous component, and that the singular continuous component is supported by the set $N \cup M$, which is independent of λ. We know that N has measure zero, and Lemma II.5 below shows us that M also has measure zero. This will allow us to apply Theorem II.6 to show that the singular continuous spectrum of V is also empty. Thus, with both the *ac* and *sc* spectra empty, we can conclude that V must have pure point spectrum.

Lemma II.5: Let $Q(z)$ be a trace class valued analytic function inside the complex unit circle, with $|z| < 1$. Then for almost every θ,

$$\lim_{\epsilon \downarrow 0} Q(e^{i(\theta + i\epsilon)}) \equiv Q(e^{i(\theta + i0)})$$

exists in the Hilbert–Schmidt norm.

Proof: We parallel the proof of de Branges theorem (see Ref. 22 and pp. 149–150 in Ref. 23). Consider

$$\begin{aligned} Q(e^{i(\theta+i\epsilon)}) + Q^*(e^{i(\theta+i\epsilon)}) &= \int A^* \left\{ \frac{1}{1 - e^{-i(\theta' - \theta)} e^{-\epsilon}} + \frac{1}{1 - e^{i(\theta' - \theta)} e^{-\epsilon}} \right\} AE(\mathrm{d}\theta') \\ &= \int A^* \left\{ \frac{2(1 - e^{-\epsilon} \cos(\theta' - \theta))}{1 + e^{-2\epsilon} - 2e^{-\epsilon} \cos(\theta' - \theta)} \right\} AE(\mathrm{d}\theta'). \end{aligned}$$

The factor within the curly braces is greater than zero for all θ', θ and thus we have

$$Q(e^{i(\theta+i\epsilon)}) + Q^*(e^{i(\theta+i\epsilon)}) \geqslant 0 \quad \forall\, \epsilon \geqslant 0.$$

Therefore, following de Branges,

$$|\det(1 + Q(e^{i(\theta+i\epsilon)}))|^2 \geqslant \det(1 + Q^*(e^{i(\theta+i\epsilon)}) Q(e^{i(\theta+i\epsilon)})) = \prod (1 + |\alpha_n|^2) \geqslant \begin{cases} \sum |\alpha_n|^2 = \|Q(e^{i(\theta+i\epsilon)})\|_{\mathrm{HS}}^2, \\ 1. \end{cases}$$

$\{\alpha_n\}$ are the eigenvalues of Q. From the two bounds on $|\det(1 + Q(e^{i(\theta+i\epsilon)}))|$ above, we obtain

$$\left\| \frac{Q(e^{i(\theta+i\epsilon)})}{\det(1 + Q(e^{i(\theta+i\epsilon)}))} \right\|_{\mathrm{HS}} \leqslant 1 \quad \text{and} \quad \left| \frac{1}{\det(1 + Q(e^{i(\theta+i\epsilon)}))} \right| \leqslant 1.$$

The definition of an analytic operator Ref. 9, p. 189) implies the analyticity of the eigenvalues, and thus the operations of taking the determinant and the Hilbert–Schmidt norm are analytic. Hence, both functions above are analytic and bounded within the complex unit circle ($\epsilon > 0$). Application of Fatou's theorem (Ref. 24, p. 454) establishes the existence in the limit as $\epsilon \to 0$ and hence both functions exist on the boundary almost everywhere. Taking the quotient we establish the existence of $Q(e^{i(\theta+i0)})$ in the Hilbert–Schmidt norm. ■

Let (Ω, μ) be a separable measure space, and

$$V(\lambda) = \int e^{-i\theta} E_\lambda(\mathrm{d}\theta)$$

a measurable family of unitary operators on $\mathcal{H}$. We denote by

$$\mathbb{V} = \int e^{-i\theta}\mathbb{E}(\mathrm{d}\theta)$$

the multiplication operator

$$(\mathbb{V}u)(\lambda) = V(\lambda)u(\lambda)$$

on $L^2(\Omega,\mu;\mathcal{H})$, where $u(\lambda) \in L^2(\Omega,\mu;\mathcal{H})$.

A vector $u(\lambda)$ is an element of $L^2(\Omega,\mu;\mathcal{H})$ if, for $u(\lambda) \in \mathcal{H}$,

$$\int_{-\infty}^{\infty} \|u(\lambda)\|^2 \mathrm{d}\mu < \infty.$$

It is important to note the difference between $V(\lambda)$ acting on $\mathcal{H}$ and $\mathbb{V}$ acting on $L^2(\Omega,\mu;\mathcal{H})$. To obtain our goal of showing that for almost every λ, $V(\lambda)$ has a pure point spectrum, we must show that $\mathbb{V}$ is absolutely continuous as a function of λ on the space $L^2(\Omega,\mu;\mathcal{H})$.

Theorem II.6 is taken directly from Ref. 2. The proof given is, apart from some small notational changes, identical to that in Ref. 2. Due to a number of typographical errors however, we have reproduced the proof here for reference and clarity.

Theorem II.6: *Let $\mathbb{V}$ be absolutely continuous on $L^2(\Omega,\mu;\mathcal{H})$, and assume that there is a fixed set S of Lebesgue measure zero which supports the singular continuous spectrum of $V(\lambda)$ in the interval J for μ-a.e. λ. Then $V(\lambda)$ has no singular continuous spectrum in J for μ-a.e. λ.*

Proof: For fixed $x \in \mathcal{H}$, and any measurable subset Γ of Ω, let $u(\lambda) = \chi_\Gamma(\lambda)x$ be a vector in $L^2(\Omega,\mu;\mathcal{H})$. Then

$$\int_\Gamma |E_\lambda^{sc}[J]x|^2 \mu(\mathrm{d}\lambda) \leqslant \int_\Gamma |E_\lambda[S]x|^2 \mu(\mathrm{d}\lambda)$$

$$= \int |E_\lambda[S]u(\lambda)|^2 \mu(\mathrm{d}\lambda) = \int |\mathbb{E}[S]u(\lambda)|^2 \mu(\mathrm{d}\lambda) = \|\mathbb{E}[S]u(\lambda)\|^2 = 0.$$

$\int_\Gamma |E_\lambda^{sc}[J]x|^2 \mu(\mathrm{d}\lambda) = 0$ implies that $|E_\lambda^{sc}[J]x|^2 = 0$ for μ-a.e. λ. Thus

$$E_\lambda^{sc}[J]x = 0$$

for every $x \in \mathcal{H}$. ■

The application of Theorem II.6 relies on finding a fixed set S of measure zero which supports the singularly continuous spectrum. $S = N \cup M$ is sufficient.

We have now established all the basic requirements for V to be pure point, given U pure point. They are now combined to produce the main theorem of the paper. There is still quite a lot of manipulation to satisfy the condition $\mathbb{V}$ *ac* on $L^2(\mathbb{R};\mathcal{H})$ of Theorem II.6, and this will be the focus for the remainder of Sec. II and III.

Theorem II.7. *Let U and A satisfy the hypotheses of Theorem II.4 and define for $\lambda \in \mathbb{R}$,*

$$V(\lambda) = e^{i\lambda A^* A/\hbar} U.$$

Then $V(\lambda)$ is pure point in J for a.e. λ.

Proof: By Theorem II.4, with $W = \lambda I$, $V(\lambda)$ has no absolutely continuous spectrum in J, and its singularly continuous spectrum is supported on the fixed set $S = N \cup M$. Application of Lemma II.5 shows that S is of measure zero. Theorem II.6 applies and shows that the singular continuous spectrum is empty, if we can show that $\mathbb{V}$ is absolutely continuous on $L^2(\mathbb{R};\mathcal{H})$. We show this in the following sections.

As we have shown that both the absolutely continuous and singular continuous parts of the spectrum are empty, we conclude that $V(\lambda)$ is pure point for almost every $\lambda \in \mathbb{R}$. ■

To show that $\mathbb{V}$ is *ac*, we apply a modified version of the Putnam–Kato theorem which is proved in Sec. III. The unitary Putnam–Kato theorem is the following.

Theorem III.3: *Let V be unitary, and D a self-adjoint bounded operator. If* $C=V[V^*,D]\geqslant 0$, *then V is absolutely continuous on* $R(C^{1/2})$. *Hence, if* $R(C^{1/2})$ *is cyclic for V, then V is absolutely continuous on* $\mathcal{H}$.

We apply this theorem on the space $L^2(\mathbb{R};\mathcal{H})$. A naive application to obtain the desired result is as follows. We slightly change notation and explicitly include the λ dependence of W in our definition of V. If we choose $\mathbb{D}=-i(d/d\lambda)$, with $V=e^{i\lambda A^*WA}U$, we see that

$$-i\frac{dV^*}{d\lambda}=-U^*A^*WAe^{-i\lambda A^*WA}=-V^*A^*WA$$

so that for some $u\in L^2(\mathbb{R};\mathcal{H})$,

$$[\mathbb{V}^*,\mathbb{D}]u=(\mathbb{V}^*\mathbb{D}-\mathbb{D}\mathbb{V}^*)u=-\mathbb{D}\mathbb{V}^*u=i\frac{d}{d\lambda}(V^*u)=\mathbb{V}^*A^*WAu.$$

Therefore,

$$\mathbb{C}=\mathbb{V}[\mathbb{V}^*,\mathbb{D}]=A^*WA.$$

With $W=I$, we obtain $\mathbb{C}=A^*A\geqslant 0$ and thus $R(\mathbb{C}^{1/2})=R(A^*)$ (see the proof to Theorem VI.9 in Ref. 9) is cyclic for V. Hence, $\mathbb{V}$ is *ac* and we satisfy all the requirements of Theorem II.7.

The problem here is that $\mathbb{D}$ is not bounded, and boundedness of $\mathbb{D}$ is essential in the proof of the Putnam–Kato theorem. We use a similar technique as Howland[2] to overcome this issue.

As the norm of A^*A may be scaled however we like, we can rewrite V, for real t as

$$V(t)=e^{ictA^*A}U \tag{30}$$

for some real $c>0$.

Proposition II.8: On $L^2(\mathbb{R};\mathcal{H})$, *consider the unitary multiplication operator* $\mathbb{V}$, *defined by*

$$\mathbb{V}u(t)=V(t)u(t)=e^{ictA^*A}Uu(t)$$

and the bounded self-adjoint operator $\mathbb{D}=-\arctan(p/2)$, *where* $p=-i\mathrm{d}/dt$. *Then* $C=\mathbb{V}[\mathbb{V}^*,D]$ *is positive definite, and* $R(C^{1/2})$ *is cyclic for* $\mathbb{V}$. *Hence, the requirements of Theorem II.7 are fully satisfied.*

Proof: The operator $\mathbb{D}$ on $L^2(\mathbb{R};\mathcal{H})$ is convolution by the Fourier transform of $-\arctan(x/2)$,[2] which is $i\pi t^{-1}e^{-2|t|}$ [Ref. 25, p. 87, (3)]. This is a singular (principal value) integral operator, because $\arctan(p/2)$ does not vanish at infinity. Thus, for $u(t)\in L^2(\mathbb{R};\mathcal{H})$,

$$\mathbb{D}u(t)=i\pi P\int_{-\infty}^{\infty}\frac{e^{-2|t-y|}}{t-y}u(y)\mathrm{d}y$$

and

$$[\mathbb{V}^*,\mathbb{D}]u(t)=i\pi P\int_{-\infty}^{\infty}e^{-2|t-y|}\frac{V^*(t)-V^*(y)}{t-y}u(y)\mathrm{d}y$$

so

$$\mathbb{C}u(t)=\mathbb{V}[\mathbb{V}^*,\mathbb{D}]u(t)=i\pi P\int_{-\infty}^{\infty}e^{-2|t-y|}\frac{1-V(t)V^*(y)}{t-y}u(y)\mathrm{d}y. \tag{31}$$

Inserting our expression (30) for $V(t)$, we obtain

$$\mathbb{C}u(t) = i\pi \int_{-\infty}^{\infty} e^{-2|t-y|} \frac{1 - e^{ic(t-y)A^*A}}{t-y} u(y)\mathrm{d}y$$

$$= i\pi \int_{-\infty}^{\infty} e^{-2|t-y|} \frac{1 - \cos(A^*Ac(t-y)) - i\,\sin(A^*Ac(t-y))}{t-y} u(y)\mathrm{d}y. \tag{32}$$

Note that this is no longer a singular integral. To show that $\mathbb{C}$ is positive, we must show that

$$(u(t), \mathbb{C}u(t)) > 0 \quad \forall\, u(t) \in L^2(\mathbb{R};\mathcal{H}).$$

Note that the inner product on $L^2(\mathbb{R};\mathcal{H})$ is given by

$$(u(t), u'(t)) = \int_{-\infty}^{\infty} u^*(t)u'(t)\mathrm{d}t. \tag{33}$$

We now write our operator A in terms of its spectral components. Please note that λ decomposes A and bears no relation to the strength parameter used at other stages in this paper. When required for clarity, we write $\int_\lambda$ to identify the integral over the variable λ,

$$A = \int \lambda E(\mathrm{d}\lambda).$$

A general vector $u(t)$ may be written

$$u(t) = \int E(\mathrm{d}\lambda)u(t).$$

Then

$$f(A)u(t) = \int f(\lambda)E(\mathrm{d}\lambda)u(t)$$

which implies that we may rewrite (32) as

$$\mathbb{C}u(t) = i\pi \int_{-\infty}^{\infty} \mathrm{d}y \int_{\lambda} e^{-2|t-y|} \frac{1 - e^{ic(t-y)|\lambda|^2}}{t-y} E(\mathrm{d}\lambda)u(y) = \int_{-\infty}^{\infty} \mathrm{d}y \int_{\lambda} \phi_\lambda(t-y)E(\mathrm{d}\lambda)u(y)$$

$$= \int_{\lambda} E(\mathrm{d}\lambda)\mathcal{C}_\lambda(t),$$

where

$$\mathcal{C}_\lambda(t) = \int_{-\infty}^{\infty} \mathrm{d}y \phi_\lambda(t-y)u(y)$$

and we have defined the new function

$$\phi_\lambda(t) = i\pi e^{-2|t|}t^{-1}(1 - e^{ict|\lambda|^2}).$$

By the convolution theorem, note that

$$\tilde{\mathcal{C}}_\lambda(\omega) = \tilde{\phi}_\lambda(\omega)\tilde{u}(\omega),$$

where $\tilde{}$ indicates Fourier transform. Using this decomposition of $u(t)$ and Parseval's theorem, we can now easily write down $(u(t), \mathbb{C}u(t))$. We use $(x,y)_{\mathcal{H}}$ to indicate the inner product on the Hilbert space $\mathcal{H}$, reserving (x,y) for the inner product on $L^2(\mathbb{R};\mathcal{H})$ as in (33).

$$(u(t),\mathbb{C}u(t)) = \int_{-\infty}^{\infty} \mathrm{d}t(u(t),\mathbb{C}u(t))_{\mathcal{H}} = \int_{-\infty}^{\infty} \mathrm{d}t\left(u(t), \int_{\lambda} E(\mathrm{d}\lambda)\mathcal{C}_{\lambda}(t)\right)_{\mathcal{H}}$$
$$= \int_{-\infty}^{\infty} \mathrm{d}t\left(u(t), \int_{\lambda} E(\mathrm{d}\lambda) \int \frac{\mathrm{d}\omega}{2\pi} e^{i\omega t}\tilde{\mathcal{C}}_{\lambda}(\omega)\right)_{\mathcal{H}} = \int_{\lambda} E(\mathrm{d}\lambda) \int \frac{\mathrm{d}\omega}{2\pi} |\tilde{u}_{\lambda}(\omega)|^2 \tilde{\phi}_{\lambda}(\omega).$$

We clearly see that if $\tilde{\phi}_{\lambda}(\omega)$ is positive for all λ, then $\mathbb{C}$ will be positive.

In the following calculation we will find the need to bound $c|\lambda|^2$. The restriction $0 \leqslant c|\lambda|^2 \leqslant 1$ will be employed. We argue that as A^*A is a positive self-adjoint bounded operator we can restrict the integral over λ to (Ref. 26, pp. 262 and 273)

$$A^*A = \int_{-\infty}^{\infty} |\lambda|^2 E(\mathrm{d}\lambda) = \int_{m-0}^{M} |\lambda|^2 E(\mathrm{d}\lambda), \tag{34}$$

where M is the least upper bound and m the greatest lower bound of A^*A. The norm of A^*A is given by $\max(|m|,|M|)$. Thus, if we set

$$c = \frac{1}{\|A^*A\|}$$

then we guarantee each $c|\lambda|^2$ to be less than unity.

Proceeding, the Fourier transform, $\tilde{\phi}_{\lambda}(\omega)$ of

$$\phi_{\lambda}(t) = i\pi e^{-2|t|} t^{-1}[1 - \cos ct|\lambda|^2 - i \sin ct|\lambda|^2] \tag{35}$$

is now calculated. We split (35) into two parts,

$$\phi_{\lambda 1}(t) = i\pi e^{-2|t|} t^{-1}[1 - \cos ct|\lambda|^2], \tag{36}$$

$$\phi_{\lambda 2}(t) = \pi e^{-2|t|} t^{-1} \sin ct|\lambda|^2. \tag{37}$$

The Fourier transform of (36) is

$$\tilde{\phi}_{\lambda 1}(\omega) = i\pi \int_{-\infty}^{\infty} e^{-2|t|} t^{-1}(1 - \cos ct|\lambda|^2) e^{-i\omega t}\, \mathrm{d}t$$
$$= i\pi \left[\int_{0}^{\infty} e^{-2t} t^{-1}(1 - \cos ct|\lambda|^2) e^{-i\omega t}\, \mathrm{d}t + \int_{0}^{\infty} e^{-2t}(-t^{-1})(1 - \cos ct|\lambda|^2) e^{i\omega t}\, \mathrm{d}t \right].$$

Using Ref. 25, p. 157, (59), and setting $S = c|\lambda|^2/(2 + i\omega)$, we obtain

$$\tilde{\phi}_{\lambda 1}(\omega) = \frac{i\pi}{2} \log\left(\frac{1 + S^2}{1 + S^{*2}}\right).$$

The logarithm of a complex number can in general be written as

$$\log(z) = \log(|z|) + i \operatorname{Arg} z$$

so noting that $|(1+S^2)/(1+S^{*2})| = 1$, we see that

$$\tilde{\phi}_{\lambda 1}(\omega) = -\frac{\pi}{2} \operatorname{Arg}\left(\frac{1 + S^2}{1 + S^{*2}}\right) = -\pi \operatorname{Arg}(1 + S^2).$$

With $\kappa = c|\lambda|^2$, the real and imaginary parts of $1 + S^2$ are

TABLE I. Sign of each term in the numerator $n(\omega,\kappa)$ and the denominator $d(\omega,\kappa)$ of (38).

$n(\omega,\kappa)=$	$(4+\omega^2)^2$	$+\kappa\omega(4+\omega^2)^2$	$+\kappa^2(4-\omega^2)$	$-\kappa^3\omega$
$\omega<-2$	$+ve$	$-ve$	$-ve$	$+ve$
$-2<\omega<0$	$+ve$	$-ve$	$+ve$	$+ve$
$0<\omega<2$	$+ve$	$+ve$	$+ve$	$-ve$
$\omega>2$	$+ve$	$+ve$	$-ve$	$-ve$
$d(\omega,\kappa)=$	$(4+\omega^2)^3$	$-2\kappa^2\omega^2(4+\omega^2)$	$-16\kappa^3\omega$	$-\kappa^4(4-\omega^2)$
$\omega<-2$	$+ve$	$-ve$	$+ve$	$+ve$
$-2<\omega<0$	$+ve$	$-ve$	$+ve$	$-ve$
$0<\omega<2$	$+ve$	$-ve$	$-ve$	$-ve$
$\omega>2$	$+ve$	$-ve$	$-ve$	$+ve$

$$\Re(1+S^2)=\frac{(4+\omega^2)^2+\kappa^2(4-\omega^2)}{(4+\omega^2)^2},$$

$$\Im(1+S^2)=\frac{-4\kappa^2\omega}{(4+\omega^2)^2}.$$

With the restriction that $0\leqslant\kappa\leqslant 1$, the real part is positive for all ω and thus $\mathrm{Arg}(z)=\arctan(\Im z/\Re z)$. Thus,

$$\tilde{\phi}_{\lambda 1}(\omega)=-\pi\arctan\left(\frac{\Im(1+S^2)}{\Re(1+S^2)}\right).$$

$\arctan(z)$ is the principal part of $\mathrm{Arctan}(z)$, with range $-\pi/2<\arctan(z)<\pi/2$. The Fourier transform of (37) is similarly calculated using Ref. 25, p. 152, (16), to be

$$\tilde{\phi}_{\lambda 2}(\omega)=\pi[\arctan S+\arctan S^*]=\pi\left[\arctan\left(\frac{c|\lambda|^2}{2+i\omega}\right)+\arctan\left(\frac{c|\lambda|^2}{2-i\omega}\right)\right].$$

Repeated application of the formula $\arctan(z_1)+\arctan(z_2)=\arctan(z_1+z_2/1-z_1z_2)$, valid when $z_1z_2<1$ (true for $0\leqslant\kappa\leqslant 1$), yields (this result is not valid for values of κ larger than around 2, at which point the arctan addition formulas fail—this is a moot point however, as we may trivially restrict κ as already explained)

$$\tilde{\phi}_{\lambda}(\omega)=\tilde{\phi}_{\lambda 1}(\omega)+\tilde{\phi}_{\lambda 2}(\omega)=\pi\arctan\left(\frac{n(\omega,c|\lambda|^2)}{d(\omega,c|\lambda|^2)}\right),\tag{38}$$

where

$$n(\omega,\kappa)=4\kappa[(4+\omega^2)^2+\kappa\omega(4+\omega^2)+\kappa^2(4-\omega^2)-\kappa^3\omega]\tag{39}$$

and

$$d(\omega,\kappa)=(4+\omega^2)^3-2\kappa^2\omega^2(4+\omega^2)-16\kappa^3\omega-\kappa^4(4-\omega^2).\tag{40}$$

One may easily confirm that for $0\leqslant\kappa\leqslant 1$, $n(\omega,\kappa)/d(\omega,\kappa)$ and hence $\tilde{\phi}_{\lambda}(\omega)$ is strictly positive by noting that there are four distinct regions of interest for ω, in which terms in n and d do not change sign. Table I shows these regions and the sign of each term in the region. Note that the global (positive and hence irrelevant) κ factor from (39) is dropped from the numerator for the following discussion.

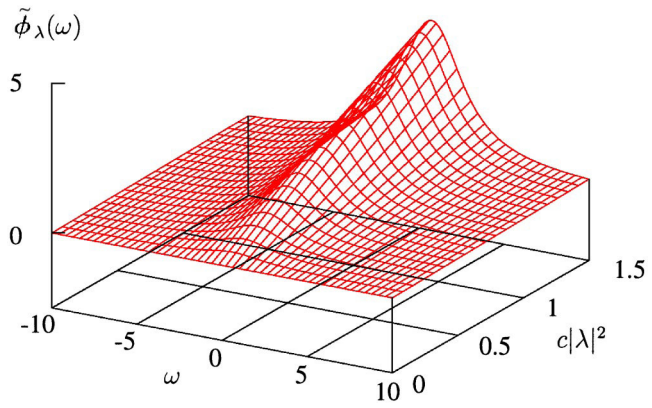

FIG. 1. Plot of $\tilde{\phi}_\lambda(\omega)=\tilde{\phi}_{\lambda 1}(\omega)+\tilde{\phi}_{\lambda 2}(\omega)$, the Fourier transform of $\phi_\lambda(t)=i\pi e^{-2|t|}t^{-1}(1-\cos(ct|\lambda|^2)-i\sin(ct|\lambda|^2))$. $\tilde{\phi}_\lambda(\omega)$ is strictly positive for all ω when $c|\lambda|^2\leqslant 1$.

For each row in the table, we simply need to show that the terms add to produce a strictly positive number. First note that the first column for both the numerator and denominator is independent of κ. To show the positivity of each row, we set all positive κ-dependent terms to zero and then take $\kappa=1$ for the negative terms to maximize their contribution. Expanding out terms, it is then trivially seen in all cases that the first column [$(4+\omega^2)^2$ for the numerator and $(4+\omega^2)^3$ for the denominator] dominates. Thus, no row is negative and we conclude that $\tilde{\phi}_\lambda$ is positive definite.

We have established that the Fourier transform of ϕ_λ is positive definite for $c|\lambda|^2\leqslant 1$. As a visual aid, Fig. 1 shows $\tilde{\phi}_\lambda(\omega)$. The positivity for $c|\lambda|^2\leqslant 1$ is clear.

Thus, $\mathbb{C}$ is strictly positive and $\mathbb{V}$ is absolutely continuous on $R(\mathbb{C}^{1/2})$. As A^*A is a factor of $1-e^{ictA^*A}$ (i.e., A^*A is a factor of $\mathbb{C}$), $R(\mathbb{C}^{1/2})=R(A^*)$. Noting that $R(A^*)$ is cyclic for U and hence cyclic for V, we conclude that $R(\mathbb{C}^{1/2})$ is cyclic for $\mathbb{V}$. Thus, $\mathbb{V}$ is absolutely continuous on $L^2(\mathbb{R};\mathcal{H})$. ■

We have now satisfied all the requirements of Theorem II.7.

III. THE UNITARY PUTNAM–KATO THEOREM

In this section, we will prove a modified version of the Putnam–Kato theorem, as used in the preceding sections. The theorems and proofs follow a similar argument to that of Reed and Simon (Ref. 15, p. 157, Theorem XIII.28) and are motivated by the stroboscopic nature of the kicked Hamiltonian.

Definition III.1. (V-Smooth): Let V be a unitary operator. A is V-smooth if and only if for all $\phi\in\mathcal{H}$, $V(t)\phi\in D(A)$ *for almost every* $t\in\mathbb{R}$ *and for some constant C,*

$$\sum_n \|AV^n\phi\|^2 \leqslant C\|\phi\|^2.$$

Theorem III.2: *If A is V-smooth, then* $\overline{R(A^*)}\subset\mathcal{H}_{ac}(V)$.

Proof: Since $\mathcal{H}_{ac}(V)$ is closed, we need only show $R(A^*)\subset\mathcal{H}_{ac}(V)$. Let $\phi\in D(A^*)$, $\psi=A^*\phi$, and let $d\mu_\psi$ be the spectral measure for V associated with ψ. Define, for the period T in (1),

$$\mathcal{F}_n(T)=\frac{1}{\sqrt{2\pi}}(A^*\phi,[V(T)]^n\psi). \tag{41}$$

We calculate

$$|\mathcal{F}_n| = \frac{1}{\sqrt{2\pi}}|(\phi, AV^n\psi)| \leqslant \frac{1}{\sqrt{2\pi}}\|\phi\|\|AV^n\psi\|.$$

Because A is V-smooth, we see that

$$\sum_n |\mathcal{F}_n|^2 \leqslant \frac{1}{2\pi}\|\phi\|^2 \sum_n \|AV^n\psi\|^2 \leqslant \frac{C}{2\pi}\|\phi\|^2\|\psi\|^2 < \infty.$$

So $\mathcal{F}_n \in L^2(\mathbb{R})$. By the Riesz–Fischer theorem (Ref. 27, pp. 96–97, 4.26 Fourier series), $\mathcal{F}(\theta) = 1/\sqrt{2\pi}\Sigma_n \mathcal{F}_n \bar{e}^{in\theta} \in L^2$.

The spectral resolution of $V[T]$ is

$$V[T] = \int_0^{2\pi} e^{i\theta}\, \mathrm{d}E_T(\theta),$$

so we have

$$(V[T])^n = \int_0^{2\pi} e^{in\theta}\, \mathrm{d}E_T(\theta).$$

Therefore, from (41) we obtain

$$\begin{aligned}\mathcal{F}_n &= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} (A^*\phi, e^{in\theta}\, \mathrm{d}E(\theta)\psi) \\ &= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} e^{in\theta}(\psi, \mathrm{d}E(\theta)\psi) \\ &= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} e^{in\theta}\, \mathrm{d}\mu_\psi(\theta).\end{aligned}$$

Using the inverse of the expression above for $\mathcal{F}(\theta)$ gives

$$\mathcal{F}_n = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} e^{in\theta}\mathcal{F}(\theta)\mathrm{d}\theta.$$

As we have just shown that $\mathcal{F}(\theta) \in L^2$, $\mathrm{d}\mu_\psi(\theta) = \mathcal{F}(\theta)\mathrm{d}\theta$ is absolutely continuous, which implies that $\psi \in R(A^*)$ is in $\mathcal{H}_{ac}(V)$ and so $\overline{R(A^*)} \subset \mathcal{H}_{ac}(V)$. ■

Theorem III.3 (Unitary Putnam–Kato theorem): *Let V be a unitary operator, and A a self-adjoint bounded operator. If $C = V[V^*, A] \geqslant 0$, then V is absolutely continuous on $R(C^{1/2})$. Hence, if $R(C^{1/2})$ is cyclic for V, then V is absolutely continuous.*

Proof: The discrete time evolution of an operator A is given by

$$\mathcal{F}_n = V^{-n}AV^n.$$

We calculate

$$\mathcal{F}_n - \mathcal{F}_{n-1} = V^{-n}V[V^*, A]V^n \equiv G_n,$$

so

$$\sum_{n=a}^{b}(\phi,G_n\phi)=\sum_{n=a}^{b}(\phi,V^{-n}V[V^*,A]V^n\phi)$$

$$=\sum_{n=a}^{b}(V^n\phi,V[V^*,A]V^n\phi)=\sum_{n=a}^{b}(C^{\frac{1}{2}}V^n\phi,C^{\frac{1}{2}}V^n\phi)=\sum_{n=a}^{b}\|C^{\frac{1}{2}}V^n\phi\|^2,$$

where $C=V[V^*,A]$. We also have

$$\sum_{n=a}^{b}(\phi,G_n\phi)=(\phi,V^{-b}AV^b\phi)-(\phi,V^{-(a-1)}AV^{(a-1)}\phi).$$

Taking the modulus and using the Schwartz inequality, we obtain

$$\sum_{n=a}^{b}\|C^{\frac{1}{2}}V^n\phi\|^2\leqslant 2|(\phi,V^{-b}AV^b\phi)|=2|(V^b\phi,AV^b\phi)|\leqslant 2\|A\|\,\|V^b\phi\|^2=2\|A\|\,\|\phi\|^2<\infty$$

and thus we see that $C^{1/2}$ is V-smooth.

That V is absolutely continuous on $R(C^{1/2})$ follows directly from Theorem III.2. ■

IV. FINITE RANK PERTURBATIONS

Here, we utilize the results of Sec. II to show that perturbations of the form (5) lead to the Floquet operator having pure point spectrum for almost every perturbation strength λ.

We use directly the definition of *strongly H-finite* from Howland.

Definition IV.1 (Strongly H-finite): Let H be a self-adjoint operator on $\mathcal{H}$ with pure point spectrum, ϕ_n a complete orthonormal set of eigenvectors, and $H\phi_n=\alpha_n\phi_n$. A bounded operator $A:\mathcal{H}\to\mathcal{K}$ is strongly H-finite if and only if

$$\sum_{n=1}^{\infty}|A\phi_n|<\infty. \tag{42}$$

If H is thought of as a diagonal matrix on l_2, i.e., $H=\Sigma_n\alpha_n|\phi_n\rangle\langle\phi_n|$, and A as an infinite matrix $\{a_{ij}\}$, i.e., $A=\Sigma_{m,n}a_{mn}|\phi_m\rangle\langle\phi_n|$, then (42) says

$$\sum_n\left[\sum_i|a_{in}|^2\right]^{\frac{1}{2}}<\infty. \tag{43}$$

For our purposes, we need to show that if A is strongly H-finite, then it is U-finite. To satisfy the assumption that Q_ϵ is trace class in Lemma II.5 (and hence also compact in Theorem II.4) we also need to show that A is trace class.

Theorem IV.2: *If A is strongly H-finite, then given $U=e^{iTH/\hbar}$, for the period T in* (1) *and $H\phi_n=\alpha_n\phi_n$,*

(a) *A is trace class, and*
(b) *A is U-finite.*

Proof: (a) Simply consider

$$\mathrm{tr}(A)=\sum_l\langle\phi_l|A|\phi_l\rangle=\sum_l a_{ll}\leqslant\sum_l|a_{ll}|. \tag{44}$$

For each term in the sum (44) we trivially have

$$|a_{ll}| \leqslant \sqrt{\sum_i |a_{il}|^2}$$

and thus (44) is finite so A is trace class.

(b) Noting that

$$U|\phi_n\rangle = e^{iTH/\hbar}|\phi_n\rangle$$

we calculate, by insertion of a complete set of states,

$$\sum_n \langle\phi_n|G_\epsilon(\theta;U,A)|\phi_n\rangle = \sum_n \langle\phi_n|A\frac{1}{(1-U^*e^{-i\theta_-})(1-Ue^{i\theta_+})}A^*|\phi_n\rangle = \sum_m \frac{\langle\phi_m|A^*A|\phi_m\rangle}{|1-e^{-\epsilon}e^{iT\alpha_m/\hbar}e^{i\theta}|^2}.$$

The trace norm is then

$$\text{tr } G_\epsilon(\theta) = \sum_n \frac{|A\phi_n|^2}{|1-e^{-\epsilon}e^{iT\alpha_n/\hbar}e^{i\theta}|^2}.$$

If this is bounded for $\epsilon=0$, then it is trivially bounded for all $\epsilon>0$. By (42) and a slightly modified version of Theorem 3.1 in Ref. 2 this is finite almost everywhere for $\epsilon=0$. Thus the trace norm of G_ϵ exists as $\epsilon\to 0$, which implies that the strong limit of G_ϵ exists and we conclude that A is U-finite. ■

THEOREM IV.3: *Let U be a pure point unitary operator, and let $A_1,\ldots,A_N$ be strongly H-finite. Assume that the A_k's commute with each other. Then for almost every $\lambda=(\lambda_1,\ldots,\lambda_N)$ in $\mathbb{R}^N$,*

$$V(\lambda) = e^{i(\Sigma_{k=1}^N \lambda_k A_k^* A_k)/\hbar}U$$

is pure point.

Proof: This is a trivial modification of Theorem 4.3 in Ref. 2. Let

$$\mathrm{K} = \bigoplus_{k=1}^N \overline{R(A_k)}.$$

The elements of $\mathcal{K}$ are represented as column vectors. Our operator $A:\mathcal{H}\to\mathcal{K}$ is defined, for $y\in\mathcal{H}$, by

$$Ay = \begin{bmatrix} A_1 y \\ \vdots \\ A_N y \end{bmatrix} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix}$$

and therefore $A^*:\mathcal{K}\to\mathcal{H}$ is given by

$$A^*x = A_1^*x_1 + \cdots + A_N^*x_N.$$

Accordingly, we introduce $G_\epsilon(\theta):\mathcal{K}\to\mathcal{K}$, the matrix equivalent of Eq. (8),

$$G_\epsilon(\theta;U,A) = A[1-U^*e^{-i\theta_-}]^{-1}[1-Ue^{i\theta_+}]^{-1}A^* = \{A_i[1-U^*e^{-i\theta_-}]^{-1}[1-Ue^{i\theta_+}]^{-1}A_j^*\}_{1\leqslant i,j\leqslant N}.$$

The diagonal terms are finite almost everywhere because each A_k is U-finite by Theorem IV.2. The off-diagonal terms are of the form $X_1^*X_2$, and so the Schwartz inequality,

$$|X_1^*X_2|^2 \leqslant \|X_1\|^2\|X_2\|^2$$

ensures that they are finite almost everywhere too. Hence, A is U-finite as every term in the matrix $G_\epsilon(\theta;U,A)$ is almost everywhere finite as $\epsilon\to 0$.

Our Hamiltonian may now be written as

$$H(\lambda) = H_0 + A^* W(\lambda) A \sum_{n=0}^{\infty} \delta(t - nT) \tag{45}$$

and our Floquet operator as

$$V(\lambda) = e^{iA^* W(\lambda) A/\hbar} U,$$

where $W(\lambda) = \mathrm{diag}\{\lambda_k\}$. In this form, the formalism of Sec. II is essentially fully regained, and we proceed to apply Theorems II.2, II.4, II.6, and II.7.

To establish the absolute continuity of the multiplication operator $\mathbb{V}$ on the space $L^2(\mathbb{R}^N; \mathcal{H})$ we proceed as in Proposition II.8.

We write

$$V(t_1, \ldots, t_N) = e^{ic\Sigma_{k=1}^N t_k A_k^* A_k/\hbar} U,$$

define

$$D = -\sum_{k=1}^{N} \arctan(p_k/2),$$

where $p_k = -id/\mathrm{d}t_k$, and compute

$$C = \mathbb{V}[\mathbb{V}^*, D] = \sum_{k=1}^{N} C_k \geqslant 0.$$

In obtaining C as a direct sum of the C_k, we have had to assume that the A_k's commute with each other. This complication comes when considering the term

$$V(t_1, \ldots, t_N) V^*(t_1, \ldots, t_{k-1}, y_k, t_{k+1}, \ldots, t_N)$$

in the equivalent of (31). To obtain the required form of $e^{ic(t_k - y_k)A_k^* A_k}$ we need the A_k's to commute. [This restriction is not required in Howland's self-adjoint work because the summation over k in the Hamiltonian (45) enters directly, rather than in the exponent of V.]

Moving on, each $C_k \geqslant 0$ is equivalent to C in Proposition II.8 and hence positive. Finally, we must show that $R(C^{1/2})$ is cyclic for $\mathbb{V}$. This is no longer trivial as, for each k, while we have $R(C_k^{1/2}) = R(A_k^*)$, the range of A_k^* is not cyclic for U, hence $\mathbb{V}$. To proceed, first note that

$$R(A^*) = \bigcup_k R(A_k^*).$$

Now, as argued in Howland, we can assume that $R(A^*)$ is cyclic for U. To elaborate, define $\mathcal{M}(U, R(A^*))$ to be the smallest closed reducing subspace of $\mathcal{H}$ containing $R(A^*)$. If $R(A^*)$ is not cyclic for U, then $\mathcal{H} \ominus \mathcal{M}$ is not empty. However, as shown below, if $y \in \mathcal{H} \ominus \mathcal{M}$, then $A^* W A y = 0$, so in $\mathcal{H} \ominus \mathcal{M}$, $V(t) = U$ and is therefore pure point trivially. Thus, we can ignore the space $\mathcal{H} \ominus \mathcal{M}$, and restrict our discussion to $\mathcal{M}$—i.e., we may assume $R(A^*)$ cyclic for U.

The above relied upon showing that $A^* W A y = 0$ for $y \in \mathcal{H} \ominus \mathcal{M}$. We now prove this. If $y \in \mathcal{H} \ominus \mathcal{M}$ and $y' \in \mathcal{M}$, then

$$\langle y, y' \rangle = 0.$$

Given $y' \in \mathcal{M}$, there exists an $x \in \mathcal{K}$ such that $y' = A^* x$, so

$$\langle y, A^* x \rangle = 0.$$

That is

$$\langle Ay, x\rangle = 0.$$

This is true for all $x \in \mathcal{K}$. Suppose $y'' \in \mathcal{H}$. Then $WAy'' \in \mathcal{K}$ and so

$$\langle Ay, WAy''\rangle = 0.$$

That is

$$\langle A^*WAy, y''\rangle = 0.$$

As this is true for any $y'' \in \mathcal{H}$, we conclude that $A^*WAy = 0$ on $\mathcal{H} \ominus \mathcal{M}$.

Thus, $R(A^*)$ [with A acting on $L^2(\mathbb{R}^{\mathbb{N}}; \mathcal{H})$] may be assumed cyclic for U, hence cyclic for $\mathbb{V}$.

We must finally show that $R(C^{1/2}) = R(A^*)$. We have

$$R(A^*) = \bigcup_k R(A_k^*) = \bigcup_k R(C_k^{1/2})$$

and

$$R(C) = \bigcup_k R(C_k).$$

As $R(A^*) = R(A^*A)$, $R(C^{1/2}) = R(C)$ and we have shown that $R(C^{1/2}) = R(A^*)$ as required. ■

Finally, we wish to make the connection with our original aim—to show that Hamiltonians of the form

$$H(t) = H_0 + \sum_{k=1}^{N} \lambda_k |\psi_k\rangle\langle\psi_k| \sum_{n=0}^{\infty} \delta(t - nT) \tag{46}$$

have a pure point quasienergy spectrum.

THEOREM IV.4: *Let H_0 be pure point, and define our time dependent Hamiltonian as in* (46). *If $\psi_1, \ldots, \psi_N \in l_1(H_0)$, then for almost every $\lambda = (\lambda_1, \ldots, \lambda_N)$ in $\mathbb{R}^N$, the Floquet operator*

$$V = e^{i(\Sigma_{k=1}^{N} \lambda_k |\psi_k\rangle\langle\psi_k|)/\hbar} U$$

has pure point spectrum.

Proof: This theorem is just a special case of Theorem IV.3 with the A_k's given by $|\psi_k\rangle\langle\psi_k|$. Clearly, the A_k's commute. As Howland shows, $|\psi\rangle\langle\psi|$ is strongly H-finite if and only if $\psi \in l_1(H_0)$. Thus Theorem IV.3 applies and the result follows. ■

V. DISCUSSION OF RESULTS AND POTENTIAL APPLICATIONS

Of fundamental importance in showing that the quasienergy spectrum remains pure point for almost every perturbation strength λ, was the fact that $\psi_k \in l_1(H_0)$. That is, if we write

$$|\psi_k\rangle = \sum_{n=0}^{\infty} (a_k)_n |\phi_n\rangle$$

where the $|\phi_n\rangle$ are the basis states of H_0, then $\psi_k \in l_1(H_0)$ if and only if

$$\sum_{n=0}^{\infty} |(a_k)_n| < \infty.$$

If this requirement is dropped, and we only retain $\psi_k \in l_2(H_0)$, then Theorem 3.1 in Ref. 2 fails and there is the possibility that $V(\lambda)$ will have a nonempty continuous spectrum. It was this fact that Milek and Seba[10] took advantage of in showing that the rank-1 kicked rotor could contain a singularly continuous spectral component under certain conditions on the ratio of the kicking frequency and the fundamental rotor frequency. They analyzed two regimes of the perturbation.

One where $\psi \in l_1(H_0)$, in which case the numerical results clearly showed pure point recurrent behavior, and the other where $\psi \in l_2(H_0)$, but $\psi \notin l_1(H_0)$. In the second case, the authors further proved that the absolutely continuous part of the spectrum was empty, and thus the system contained a singularly continuous spectral component. The numerical results reflected this, with a diffusive type energy growth being observed.

With the generalization of Combescure's work here, namely our Theorem IV.4, it should now be possible to investigate the full class of rank-N kicked Hamiltonians. A sufficient requirement for recurrent behavior has been shown to be $\psi_k \in l_1(H_0)$ and so we must turn our attention to perturbations where this requirement is no longer satisfied.

The challenge will be of course to find systems for which one can show that the absolutely continuous part of the spectrum is empty. Such systems would be candidates for classification as quantum chaotic systems.

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Exact solution to a supersymmetric Gaudin model

Julia Breiderhoff
Dipartimento di Fisica, Università di Roma TRE, Via Vasca Navale 84, 00146 Roma, Italy

Fabio Musso and Orlando Ragnisco[a)]
Dipartimento di Fisica, Università di Roma TRE, Via Vasca Navale 84, 00146 Roma, Italy and I.N.F.N.-Sezione di Roma TRE, Roma, Italy

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We investigate a special case of the Gaudin model related to the superalgebra $osp(1,2)$. We present an exact solution to that system diagonalizing a complete set of commuting observables, and providing the corresponding eigenvectors and eigenvalues. The approach used in this paper is based on the co-algebra symmetry of the model, already known from the Calogero–Gaudin system. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1853503]

I. INTRODUCTION

The Gaudin model (sometimes called Gaudin magnet),[1,2] introduced by Gaudin in 1976, is a quantum mechanical system involving long-range spin–spin interaction, described by a set of N Hamiltonians $\mathcal{H}_i$ depending on a set of N arbitrary parameters ϵ_i:

$$\mathcal{H}_i = \sum_{j=1, j\neq i}^{N} \frac{\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y + \sigma_i^z\sigma_j^z}{\epsilon_i - \epsilon_j}, \quad j = 1, \ldots, N. \tag{1.1}$$

Out of the operators (1.1) Gaudin constructed the further operator (dependent also on another set of arbitrary parameters η_i)

$$\mathcal{H}_G = \sum_{i<j} \frac{\eta_i - \eta_j}{\epsilon_i - \epsilon_j}(\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y + \sigma_i^z\sigma_j^z) = \sum_{i=1}^{N} \eta_i\mathcal{H}_i \tag{1.2}$$

selecting it as the Hamiltonian of the system: while $\mathcal{H}_i$ describes just the interaction of the ith spin with all the others, $\mathcal{H}_G$ takes care of the mutual interaction among all spins.

Gaudin showed that the Hamiltonians $\mathcal{H}_i$ commute with each other and constructed their common eigenvectors by the coordinate Bethe ansatz. The algebra corresponding to the observables of the model is a loop-algebra, the so-called "rational Gaudin algebra," whose properties underlie the integrability of the system. Later, this model was studied by Sklyanin through the r-matrix approach[3,4] and quite recently its intimate connections with Richardson's work on "pairing force" Hamiltonians[5] and with BCS model of superconductivity has been unveiled.[6,7]

For the special choice $\eta_i = \epsilon_i \forall\, i$, the Gaudin Hamiltonian (1.2) takes the simpler, parameter independent, form:

$$\mathcal{H}_G = \sum_{i,j} (\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y + \sigma_i^z\sigma_j^z). \tag{1.3}$$

In the following we will always work with the "mean-field" Hamiltonian (1.3) and we will continue to refer to it, a bit improperly, as "Gaudin magnet."

[a)]Electronic mail: ragnisco@fis.uniroma3.it

Using co-algebras, Ballesteros and colleagues developed an alternative approach, shortly denoted as BMR in the following, to construct a second family of commuting observables, independent of the Gaudin set $\{\mathcal{H}_i\}$, but sharing with it the element (1.3) (Refs. 8–10). In Ref. 10 Musso and Ragnisco (MR in the following) performed an exact diagonalization of this alternative family of commuting observables, in the simplest finite-dimensional representation, namely the spin-$\frac{1}{2}$ one. We stress that the existence of two independent complete sets of commuting observables implies that the Hamiltonian (1.3) is maximally superintegrable.

The superalgebra extension of the notion of Gaudin algebra, and of the related r-matrix structure, has been worked out in some remarkable papers (see, for instance, Refs. 11 and 12) where the Gaudin magnet related to orthosymplectic Lie superalgebra $osp(1,2)$ has been constructed and solved through a brilliant generalization of the Bethe ansatz.

In the present paper, our purpose is to extend the BMR approach to the supersymmetric Gaudin magnet associated with the $osp(1,2)$ superalgebra and to find a complete family of commuting observables independent of the set found by the previous authors in the context of the Bethe ansatz. These new observables are in fact a sequence of coproducts of the quadratic Casimir of the algebra $osp(1,2)$. By diagonalizing them, we will construct an exact solution of the model, providing an explicit expression for the associated eigenvectors and eigenvalues, thus proving that the Gaudin magnet related to the superalgebra $osp(1,2)$ is still maximally superintegrable.

The paper is organized as follows. In Sec. II we briefly recall the basic notions on superalgebra $osp(1,2)$, as well as the notion of graded tensor-product multiplication, and define a coproduct enjoying the required homomorphicity properties. Then, we show that, as in the $sl(2)$ case, through the coalgebra approach (Refs. 8 and 13) a completely integrable supersymmetric N-body Hamiltonian system can be derived. In Sec. III we construct the common eigenstates of the observables defined in Sec. II and we derive the eigenvalues associated with the partial Casimir operators of the system $\Delta^{(h)}(C)$ $(h=2,\ldots,N)$ (coproducts of the Casimir), paraphrasing the procedure successfully followed in Ref. 10. Namely, starting from the "total pseudovacuum," we first construct an eigenbasis for the kernel of the global fermionic annihilation operator and then on top of it we build up all the remaining eigenstates by acting with fermionic creation operators. In Sec. IV we restrict ourselves to the case of spin $1/2$ and give the explicit construction of the eigenstates for the three-body case. In Sec. V we briefly introduce a more general Hamiltonian, corresponding to the so-called $t-J$ models,[14] which commutes with the complete family of observables defined in Sec. II and therefore is completely integrable as well. The proof that our set of eigenstates is complete is given in the Appendix but only for the case of spin $1/2$.

II. THE GAUDIN MAGNET RELATED TO THE SUPERALGEBRA *osp*(1,2)

The simplest superalgebra that generalizes $sl(2)$ is the orthosymplectic superalgebra $osp(1,2)$ defined by commutation and anticommutation rules (supercommutation rules). As is well known, the basic extra-ingredient characterizing the supersymmetric case is a grading, which allows one to classify the elements of the algebra in two families, the "bosons" with even degree and the "fermions" with odd degree, and leads to the supercommutation rules. The superalgebra $osp(1,2)$ has five generators, three bosonic ones: H, E^+, E^- and two fermionic ones: F^+, F^-. Its defining relations are the following:[15]

$$[H,E^{\pm}]_- = \pm 2E^{\pm}, \quad [E^+,E^-]_- = H, \tag{2.1}$$

$$[H,F^{\pm}]_- = \pm F^{\pm}, \quad [F^+,F^-]_+ = H, \tag{2.2}$$

$$[E^{\pm},F^{\mp}]_- = -F^{\pm}, \quad [F^{\pm},F^{\pm}]_+ = \pm 2E^{\pm}, \tag{2.3}$$

We immediately see that the operators H, E^+, E^- generate the Lie algebra $sl(2)$. Moreover, as the anticommutation rules entail $(F^{\pm})^2=E^{\pm}$, some authors (see, for instance, Ref. 12) define $osp(1,2)$ only in terms of the three generators $\mathcal{H}$, F^+, F^-.

The Casimir of this algebra is

$$C = H^2 + 2(E^+E^- + E^-E^+) - (F^+F^- - F^-F^+). \tag{2.4}$$

As we shall see in the following, the *N*th coproduct of Casimir gives us the Hamiltonian of the "supersymmetric Gaudin magnet:"

$$\begin{aligned} C_N &= \Delta^{(N)}(C) = [\Delta^{(N)}(H)]^2 + 2[\Delta^{(N)}(E^+), \Delta^{(N)}(E^-)]_+ - [\Delta^{(N)}(F^+), \Delta^{(N)}(F^-)]_- \\ &= \sum_{j\neq i}^{N} \mathbf{S}^i\mathbf{S}^j - F_+^iF_-^j + F_-^iF_+^j + 2Nj\left(j+\frac{1}{2}\right)I \equiv \mathcal{H}_{G_s}, \end{aligned} \tag{2.5}$$

where I is the identity operator, the (positive) integer or half-integer j denotes the spin in each site and $\mathbf{S}^l \equiv (H^l, E_+^l + E_-^l, -i(E_+^l - E_-^l))$.

In passing, we note that a further generalization can be obtained by allowing site-dependent representations $(j_1, \ldots, j_N)$: of course in this case the constant $2Nj\left(j+\frac{1}{2}\right)$ is then replaced by $2\Sigma_{k=1}^{N} j_k\left(j_k+\frac{1}{2}\right)$. However, for the sake of simplicity, we will not deal with this more general case in the present paper.

As in the non-supersymmetric case we pose $C_h = \Delta^{(h)}(C)$, $h = 2, \ldots, N$; a complete set of independent commuting observables is provided by

$$\{\Delta^{(N)}(H), C_2, \ldots, C_N\}. \tag{2.6}$$

The operators $\Delta^{(h)}$, $h = 3, \ldots, N$ are defined through the recursive formula:[8]

$$\Delta^{(h)} = (\Delta^{(h-1)} \otimes id)\Delta^{(2)}, \quad h = 3, \ldots, N, \tag{2.7}$$

where $\Delta^{(2)}$ denotes the coproduct associated with the usual Hopf-algebra structure defined on $U(g)$, the universal enveloping algebra of a given Lie (super)algebra g, namely,

$$\Delta^{(2)}(X) = X \otimes 1 + 1 \otimes X \; \forall \, X \in g. \tag{2.8}$$

For the above construction to hold, yielding complete integrability of the composite system (see Ref. 8), (2.8) has to be a coassociative homomorphism of $osp(1,2)$, that is,

$$[\Delta(a), \Delta(b)]_{S\otimes S} = \Delta([a,b]_S), \quad \forall \, a,b \in S, \tag{2.9}$$

$$(\Delta \otimes id)\Delta = (id \otimes \Delta)\Delta, \tag{2.10}$$

where by $[,]$ we have denoted the supercommutator.

We remark that the above-presented formulas involve tensor-products multiplication, which has to be associative if we want the coproduct to be coassociative. This requires the tensor product to be a suitably graded one. The proper definition for binary tensor products is the following:[15]

$$(a \otimes b)(c \otimes d) = ac \otimes bd(-1)^{\deg(b)\deg(c)}. \tag{2.11}$$

Defining the degree of binary tensor-product in the natural way:

$$\deg(a \otimes b) = \deg(a) + \deg(b) \mod 2 \tag{2.12}$$

we obtain the following equations for three element tensor-products:

$$\begin{aligned} ((a \otimes b) \otimes c)((d \otimes e) \otimes f) &= (a \otimes b)(d \otimes e) \otimes cf(-1)^{\deg(c)\deg(d\otimes e)} \\ &= ad \otimes be \otimes cf(-1)^{\deg(b)\deg(d)+\deg(c)\deg(d)+\deg(c)\deg(e)} \end{aligned} \tag{2.13}$$

and

$$(a \otimes (b \otimes c))(d \otimes (e \otimes f)) = ad \otimes (b \otimes c)(e \otimes f)(-1)^{\deg(b\otimes c)\deg(d)}$$
$$= ad \otimes be \otimes cf(-1)^{\deg(b)\deg(d)+\deg(c)\deg(d)+\deg(c)\deg(e)}. \quad (2.14)$$

As (2.13) and (2.14) coincide, the multiplication between three element tensor-products is associative. We can extend this result to the general case of multiplication between N element tensor-products obtaining

$$(a_1 \otimes a_2 \otimes \ldots \otimes a_N)(b_1 \otimes b_2 \otimes \ldots \otimes b_N) = (-1)^{\sum_{i<j=2}^{N}\deg(a_j)\deg(b_i)}$$
$$\times (a_1 b_1 \otimes a_2 b_2 \otimes \ldots \otimes a_N b_N), \quad \forall\, a_j, b_i \in \mathcal{S}. \quad (2.15)$$

Generalizing (2.12), we define the degree of the N element tensor-product as

$$\deg(a_1 \otimes a_2 \otimes \ldots \otimes a_N) = \deg(a_1) + \deg(a_2) + \ldots + \deg(a_N), \quad \mathrm{mod}\, 2. \quad (2.16)$$

From this definition it follows straight away that the coproduct $\Delta^{(N)}(X_i)$ preserves the degree of the generic operator X_i. In fact we have

$$\Delta^{(N)}(X_i) = X_i \otimes \overbrace{1 \otimes \ldots \otimes 1}^{N-1} + 1 \otimes X_i \otimes \overbrace{1 \otimes \ldots \otimes 1}^{N-2} + \ldots + \overbrace{1 \otimes \ldots \otimes 1}^{N-1} \otimes X_i. \quad (2.17)$$

Hence,

$$\deg(\Delta^{(N)}(X_i)) = \deg(X_i) + (N-1)\deg(1). \quad (2.18)$$

But $\deg(1)=0$, so we obtain

$$\deg(\Delta^{(N)}(X_i)) = \deg(X_i). \quad (2.19)$$

We can immediately see that, as in the case $sl(2)$, a completely integrable supersymmetric N-body Hamiltonian system can be constructed through the BMR approach which yields the complete family of commuting observables (2.6).

III. CONSTRUCTION OF THE SIMULTANEOUS EIGENSTATES IN THE CASE *osp*(1,2)

Our aim is to find the common eigenstates of the observables (2.6), which form a basis for the Hilbert space of the problem. As reference state, the so-called "pseudovacuum," we take the tensor-product of the states annihilated by the single-particle operators F_i^-, namely, the tensor-product of the N single-particle lowest weight vectors $|0\rangle_i$, $i=1,\ldots,N$; as in the nonsupersymmetric case, we denote it as $\Psi(0,0)$.

We will show that the common eigenstates of the family of observables (2.6) take the form

$$\Phi(k; m_l, s_{m_l}; \ldots; 0,0) = [\Delta^{(N)}(F^+)]^{k-m_l}\Psi(m_l, s_{m_l}; \ldots; 0,0), \quad (3.1)$$

where $\Psi(m_l, s_{m_l}; \ldots; 0,0)$ is an element of the basis spanning $\mathrm{Ker}(\Delta^{(s_{m_l})}(F^-))$, obtained through the recursive formula

$$\Psi(m_l, s_{m_l}; \ldots; 0,0) = \sum_{i=0}^{m_l - m_{l-1}} a_i \Delta^{(s_{m_l}-1)}(F^+)^{m_l - m_{l-1} - i}(F^+_{s_{m_l}})^i \Psi(m_{l-1}, s_{m_{l-1}}; \ldots; 0,0) \quad (3.2)$$

$$m_l = 1,2,\ldots,N, \quad s_{m_l} = 2,3,\ldots,N, \quad l = 1,2,\ldots,N-1. \quad (3.3)$$

Paraphrasing the procedure followed in Ref. 9 it is possible to prove that the parameters appearing in (3.1) and (3.3) have to satisfy the inequalities:

$$m_{r-1} < m_r, \quad s_{m_{r-1}} < s_{m_r}, \quad 4j \geqslant m_r - m_{r-1} \geqslant 1,$$

$$s_{m_r} - m_r \geqslant 0, \quad k \leqslant 2N - m_r. \tag{3.4}$$

In (3.3) s_{m_l} indicates the number of sites involved; m_l indicates the total excitation of the system, namely, $m_l - N$ is the eigenvalue of $\Delta^{(N)}(H)$. $F^+_{s_{m_l}}$ is a shorthand for

$$\overbrace{id \otimes \ldots \otimes id}^{s_{m_l}-1} \otimes F^+ \otimes \overbrace{id \otimes \ldots \otimes id}^{N-s_{m_l}}$$

and we also define $\Delta^{(1)}(F^\pm) = F^\pm$.

Up to a normalization constant, the coefficients a_i are determined by

$$\Delta^{(s_{m_l})}(F^-)\Psi(m_l, s_{m_l}; \ldots; 0, 0) = 0. \tag{3.5}$$

In fact, a lengthy but straightforward computation shows that they are given by the recursive relation

$$a_{i+1} = a_i(-1)^{m_l - m_{l-1} - i} \frac{\left[\frac{m_l - m_{l-1} - i}{2}\right] + \frac{1}{2}(1 - (-1)^{m_l - m_{l-1} - i})(m_{l-1} - 2j(s_{m_{l-1}}))}{\left[\frac{i+1}{2}\right] - j(1 - (-1)^{i+1})}. \tag{3.6}$$

Another straightforward computation shows that $\Psi(m_l, s_{m_l}; \ldots; 0, 0)$ are eigenvectors for the operators $\Delta^{(s_{m_l})}(H)$:

$$\Delta^{(s_{m_l})}(H)\Psi(m_l, s_{m_l}; \ldots; 0, 0) = (m_l - s_{m_l})\Psi(m_l, s_{m_l}; \ldots; 0, 0). \tag{3.7}$$

Using Eqs. (3.5) and (3.7) it is not difficult to prove that the states (3.1) are indeed eigenstates of the set of observables (2.6) and then calculate the eigenvalues of the partial Casimir operator C_h. First of all we notice that

$$\Delta^{(N)}(H)\Phi(k; m_l, s_{m_l}; \ldots; 0, 0) = (k - N)\Phi(k; m_l, s_{m_l}; \ldots; 0, 0). \tag{3.8}$$

Now we consider the action of the partial Casimir C_h on the generic state (3.1). Using commutation relations (2.1)–(2.3), we rewrite C_h in the equivalent form:

$$\begin{aligned} C_h &= [\Delta^{(h)}(H)]^2 + 2\Delta^{(h)}(E^+)\Delta^{(h)}(E^-) + 2\Delta^{(h)}(E^-)\Delta^{(h)}(E^+) - \Delta^{(h)}(F^+)\Delta^{(h)}(F^-) + \Delta^{(h)}(F^-)\Delta^{(h)}(F^+) \\ &= [\Delta^{(h)}(H)]^2 + 4\Delta^{(h)}(E^+)\Delta^{(h)}(E^-) - \Delta^{(h)}(H) - 2\Delta^{(h)}(F^+)\Delta^{(h)}(F^-). \end{aligned}$$

As the coproduct is a superalgebra homomorphism, all the partial Casimirs C_h commute with the Nth coproduct of any of the generators, in particular

$$[C_h, \Delta^{(N)}(F^+)] = 0.$$

Thus we only have to worry about the action of the partial Casimir $C_h = \Delta^{(h)}(C)$, $(h = 2, \ldots, N)$ on the states (3.2):

$$\begin{aligned} C_h\Psi(m_l, s_{m_l}; \ldots; 0, 0) = &([\Delta^{(h)}(H)]^2 + 4\Delta^{(h)}(E^+)\Delta^{(h)}(E^-) - \Delta^{(h)}(H) - 2\Delta^{(h)}(F^+)\Delta^{(h)}(F^-)) \\ &\times \left(\sum_{i=0}^{m_l - m_{l-1}} a_i \Delta^{(s_{m_l}-1)}(F^+)^{m_l - m_{l-1} - i}(F^+_{s_{m_l}})^i\right)\Psi(m_{l-1}, s_{m_{l-1}}; \ldots; 0, 0). \end{aligned} \tag{3.9}$$

There are two possibilities: (i) $h \geqslant s_{m_l}$ and (ii) $h < s_{m_l}$.

In case (*i*), we know that

$$\Delta^{(h)}(F^-)\Psi(m_l,s_{m_l};\ldots;0,0)=0\rightarrow\Delta^{(h)}(E^-)\Psi(m_l,s_{m_l};\ldots;0,0)=0$$

and using Eq. (3.7) we obtain

$$C_h\Psi(m_l,s_{m_l};\ldots;0,0)=(h-m_l)(h-(m_l-1))\Psi(m_l,s_{m_l};\ldots;0,0). \tag{3.10}$$

On the other hand, in case (*ii*), the Casimir operator C_h commutes both with $F^+_{(s_{m_l})}$ and with $\Delta^{(s_{m_l}-1)}(F^+)$, so that we obtain

$$C_h\Psi(m_l,s_{m_l};\ldots;0,0)=\left(\sum_{i=0}^{m_l-m_{l-1}}a_i\Delta^{(s_{m_l}-1)}(F^+)^{m_l-m_{l-1}-i}(F^+_{s_{m_l}})^i\right)C_h\Psi(m_{l-1},s_{m_{l-1}};\ldots;0,0). \tag{3.11}$$

Again we have two possibilities: if $h\geqslant s_{m_l-1}$, we have

$$C_h\Psi(m_{l-1},s_{m_{l-1}};\ldots;0,0)=(h-(m_{l-1}))(h-(m_{l-1}-1))\Psi(m_{l-1},s_{m_{l-1}};\ldots;0,0), \tag{3.12}$$

otherwise C_h will work directly on $\Psi(m_{l-2},s_{m_{l-2}};\ldots;0,0)$.

We can proceed in this way until we will find a state $\Psi(m_i,s_{m_i};\ldots;0,0)$ for which we have $h\geqslant s_{m_i}$ (it will always exist, as $s_0=0$).

Then, using equations $\Delta^{(h)}(F^-)\Psi(m_i,s_{m_i},\ldots,0,0)=0$ and (3.7) we obtain

$$C_h\Psi(m_i,s_{m_i};\ldots;0,0)=(h-m_i)(h-(m_i-1))\Psi(m_i,s_{m_i};\ldots;0,0). \tag{3.13}$$

Summarizing,

$$C_h\Phi(k;m_l,s_{m_l};\ldots;0,0)=(h-m_i)(h-(m_i-1))\Phi(k;m_l,s_{m_l};\ldots;0,0), \tag{3.14}$$

where the value of $i\in\{0,1,\ldots,l\}$ is selected by the condition:

$$s_{m_i}\leqslant h<s_{m_{i+1}},\quad s_{m_{l+1}}=N+1. \tag{3.15}$$

IV. THE CASE OF SPIN $\frac{1}{2}$

In the special case $j=\frac{1}{2}$, m_l-m_{l-1} can take two values: 1 or 2. So we have two cases.

Case 1: $m_l-m_{l-1}=1\rightarrow i=0,1$,

$$a_{i+1}=a_i(-1)^{1-i}\frac{\left[\frac{1-i}{2}\right]+\frac{1}{2}(1-(-1)^{1-i})(m_{l-1}-s_{m_l}+1)}{\left[\frac{i+1}{2}\right]-\frac{1}{2}(1-(-1)^{i+1})}, \tag{4.1}$$

$$a_1=a_0(m_{l-1}-s_{m_l}+1). \tag{4.2}$$

Case 2: $m_l-m_{l-1}=2\rightarrow i=0,1,2$,

$$a_{i+1}=a_i(-1)^{i}\frac{\left[\frac{2-i}{2}\right]+\frac{1}{2}(1-(-1)^{i})(m_{l-1}-s_{m_l}+1)}{\left[\frac{i+1}{2}\right]-\frac{1}{2}(1-(-1)^{i+1})}, \tag{4.3}$$

$$a_1=-a_0, \tag{4.4}$$

$$a_2 = -a_1(m_{l-1} - s_{m_l} + 1) = a_0(m_{l-1} - s_{m_l} + 1). \tag{4.5}$$

In both cases, we have the condition

$$s_{m_l} > m_{l-1} + 1. \tag{4.6}$$

Indeed, from (3.4) it follows that $s_{m_l} \geqslant m_{l-1}+1$; however, if equality holds a_0 is the only nonvanishing coefficient, and (3.5) cannot be verified.

We rewrite the simultaneous eigenstates of the set of observables (2.6):

$$\Phi(k; m_l, s_{m_l}; \ldots; 0,0) = [\Delta^{(N)}(F^+)]^{k-m}\Psi(m_l, s_{m_l}; \ldots; 0,0), \tag{4.7}$$

$$N \geqslant s_{m_r} \geqslant m_r, \quad s_{m_r} > s_{m_{r-1}}, \quad m_r > m_{r-1},$$

$$s_{m_r} > m_{r-1} + 1, \quad m_l \leqslant k \leqslant 2N - m_l, \quad m_r - m_{r-1} = 1,2, \tag{4.8}$$

$$\Psi(m_l, s_{m_l}; \ldots; 0,0) = \sum_{i=0}^{m_l - m_{l-1}} a_i \Delta^{(s_{m_l}-1)}(F^+)^{m_l - m_{l-1} - i}(F^+_{s_{m_l}})^i \Psi(m_{l-1}, s_{m_{l-1}}; \ldots; 0,0). \tag{4.9}$$

To construct explicit formulas for the eigenstates we recall that, for spin $\frac{1}{2}$, the fundamental representation is three-dimensional: the $osp(1,2)$ generators read

$$H = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad E^+ = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad E^- = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$
$$F^+ = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad F^- = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix}. \tag{4.10}$$

Consequently the vacuum $\Psi(0,0)$ in the spin-$\frac{1}{2}$ representation is

$$\Psi(0,0) = \overbrace{\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \ldots \ldots \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}}^{N} \tag{4.11}$$

Of course, there are three possible single-particle states, namely,

$$\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},$$

where

$$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = F^+ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

denotes the fermionic state and

$$\begin{pmatrix}1\\0\\0\end{pmatrix} = E^{+}\begin{pmatrix}0\\1\\0\end{pmatrix}$$

the bosonic one.

Example: The three-body case: As an example, we give the explicit form of the states (4.9) in the case $N=3$ and for the choice of the normalization parameter $a_0=1$. This is the basis spanning the kernel of $\Delta^{(N)}(F^{-})$:

$$\Psi(0,0) = \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}$$

$$\Psi(1,2;0,0) = \begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix} - \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix},$$

$$\Psi(1,3;0,0) = \begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix} - 2\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix},$$

$$\Psi(2,2;0,0) = \begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix} - \begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix} - \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix},$$

$$\Psi(2,3;0,0) = \begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix} - \begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix} - \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix} - 2\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}1\\0\\0\end{pmatrix},$$

$$\begin{aligned}\Psi(2,3;1,2;0,0) = {} & \begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix} - 2\begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix} - \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix} \\ & - \begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix},\end{aligned}$$

$$\begin{aligned}\Psi(3,3;1,2;0,0) = {} & \begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix} - \begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}1\\0\\0\end{pmatrix} - \begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}1\\0\\0\end{pmatrix} \\ & + \begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix} - \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix} - 2\begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix}.\end{aligned}$$

The remaining 3^3-7 eigenstates are constructed using formula (4.7).

V. A MORE GENERAL HAMILTONIAN

It is easily seen that the basis constructed in Sec. III diagonalizes the more general Hamiltonian $\mathcal{H}$:

$$\mathcal{H} = \lambda\Delta^{(N)}(C_b) + \mu\Delta^{(N)}(C_f), \tag{5.1}$$

which is an arbitrary linear combination of the bosonic and fermionic part of the Gaudin Hamiltonian $\mathcal{H}_{G_s}$, defined in (2.5),

$$\Delta^{(N)}(C) = \Delta^{(N)}(C_b) + \Delta^{(N)}(C_f), \tag{5.2}$$

$$C_b = H^2 + 2(E^+E^- + E^-E^+), \tag{5.3}$$

$$C_f = F^-F^+ - F^+F^-. \tag{5.4}$$

Indeed, $\mathcal{H}$ can be written as

$$\mathcal{H} = \mu\Delta^{(N)}(C) + (\lambda - \mu)\Delta^{(N)}(C_b), \tag{5.5}$$

which obviously commutes with $\Delta^{(h)}(C)$, $(h=2,\ldots,N)$ and $\Delta^{(N)}(H)$. So the complete set of observables

$$\{\Delta^{(N)}(H), C_2, \ldots, C_{N-1}, \mathcal{H}\} \tag{5.6}$$

has the same common eigenstates as the set of observables (2.6). The eigenvalue equation for the more general Hamiltonian $\mathcal{H}$ reads

$$\mathcal{H}\Phi(k;m_l,s_{m-l};\ldots;0,0) = \left(\lambda(N-m_l)(N-(m_l-2)) - \mu(N-m_l) + (\mu-\lambda)(1-(-1)^{k-m_l})\left(N-m_l+\frac{1}{2}\right)\right)\Phi(k;m_l,s_{m_l};\ldots;0,0). \tag{5.7}$$

VI. CONCLUDING REMARKS

A natural generalization of the model presented here will be associated with the q-deformation of the superalgebra $osp(1,2)$ starting from the results first derived by Kulish in the late 1980s, and using the later findings by Lukierski.[16–18] In the coproduct approach integrability of such q-deformed supersymmetric models will follow from the Hopf-algebra structure of $U_q(osp(1,2))$. A further extension is related to the investigation of superalgebras other than $osp(1,2)$, for instance $sl(1,2)$, already introduced within the Bethe ansatz approach.[14,15] Work is progressing in these directions.

APPENDIX

Here we shall prove that our procedure allows one to find all the lowest weight vectors of the representation $(D_{1/2})^N$, i.e., the representation of the N-site chain with spin $\frac{1}{2}$ at each site. These lowest weight vectors are the eigenvectors spanning $\mathrm{Ker}\Delta^{(N)}(F^-)$. In fact the construction of all the common eigenvectors of the set of observables (2.6) consists of two steps. First, we find the "lowest weight vectors" $\Psi(m_l,s_{m_l},\ldots,0,0)$, built up on the "total pseudovacuum" $\Psi(0,0)$. Then we construct all the remaining states by applying $\Delta^{(N)}(F^+)$ repeatedly on $\Psi(m_l,s_{m_l},\ldots,0,0)$. We note that the number of times we can apply $\Delta^{(N)}(F^+)$ on the state $\Psi(m_l,s_{m_l},\ldots,0,0)$ basically depends on the excitation-number m_l and on the magnetization-number k. First of all we notice that it holds:

$$(D_{1/2})^N = (D_{1/2})^{(N-1)} \otimes D_{1/2}. \tag{A1}$$

In general the dimension of $\mathrm{Ker}\Delta^{(N)}(F^-)$ is obtained recurrently from the Clebsch–Gordan series:

$$D_j \otimes D_k = D_{j+k} \oplus \ \ldots \ \oplus D_{|j-k|}, \tag{A2}$$

where $D_{j+k}, \ldots, D_{|j-k|}$ are irreducible representations, each one possessing one lowest weight vector. Thus, the representation $(D_j)^N$ it is associated with a number of lowest weight vectors, which corresponds to the number of irreducible representations appearing in its decomposition.

We have

$$(D_j)^N = \sum_{k=0}^{Nj} c_{j,k}^{(N)} D_k, \quad k = 0, \frac{1}{2}, 1, \ldots, \tag{A3}$$

where $c_{j,k}^{(N)}$ are the appropriate Clebsch-Gordan coefficients.

For $j = \frac{1}{2}$ (A3) obviously becomes

$$(D_{1/2})^N = \sum_{k=0}^{N/2} c_{1/2,k}^{(N)} D_k, \quad k = 0, \frac{1}{2}, 1, \ldots \ . \tag{A4}$$

The dimension of $\mathrm{Ker}\Delta^{(N)}(F^-)$ is given by $\Sigma_{k=0}^{N/2} c_{1/2,k}^{(N)}$. On the other hand (A4) can be written in the form (A1):

$$(D_{1/2})^N = \left(\sum_{k=0}^{(N-1)/2} c_{1/2,k}^{(N-1)} D_k \right) \otimes D_{1/2} = \sum_{k=0}^{(N-1)/2} c_{1/2,k}^{(N-1)} (D_k \otimes D_{1/2}). \tag{A5}$$

Thus, known all the lowest weight vectors of the representation $(D_{1/2})^{N-1}$, by induction we have all the lowest weight vectors of the representation $(D_{1/2})^N$. There are two different cases:

$$D_k \otimes D_{1/2} = D_{1/2}, \quad k = 0. \tag{A6}$$

There is only one lowest weight vector,

$$D_k \otimes D_{1/2} = D_{k-1/2} \oplus D_k \oplus D_{k+1/2}, \quad k \geqslant \tfrac{1}{2}. \tag{A7}$$

We have three lowest weight vectors.

So from the Clebsh–Gordan series we learn that the dimension of $\mathrm{Ker}\Delta^{(N)}(F^-)$ can be obtained recurrently from the dimension of $\mathrm{Ker}\Delta^{(N-1)}(F^-)$, observing that a generic state of the kernel of $\Delta^{(N-1)}(F^-)$ will give rise to one new state of the kernel of $\Delta^{(N)}(F^-)$ for $k=0$ and to three new states otherwise $(k \neq 0)$.

Has our procedure the same starting points and the same properties?

To both questions the answer is affirmative. First, concerning the starting point $(N=2)$, we notice that formula (A1) yields

$$(D_{1/2})^2 = D_0 \oplus D_{1/2} \oplus D_1 \tag{A8}$$

while with our techniques from (4.8), (4.9), and (4.11) we get

$$\Psi(0,0) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},$$

$$\Psi(1,2;0,0) = \sum_{i=0}^{1} a_i (F_1^+)^{(1-i)} (F_2^+)^i \Psi(0,0) = a_0 F_1^+ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + a_1 F_2^+ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},$$

$$\Psi(2,2;0,0,0) = \sum_{i=0}^{2} a_i (F_1^+)^{(2-i)} (F_2^+)^i \Psi(0,0)$$

$$= a_0 (F_1^+)^2 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + a_1 F_1^+ F_2^+ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + a_2 (F_2^+)^2 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \tag{A9}$$

and from the conditions on the coefficients a_i (4.2), (4.4), and (4.5) we get

$$\Psi(1,2;0,0) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

$$\Psi(2,2;0,0) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

So we have three states according to (A8).

Now we turn to consider the general case. Let $\psi^{(N-1)}(m_l, s_{m_l}, \ldots, 0, 0)$ be a state belonging to $\mathrm{Ker}(\Delta^{(N-1)}(F^-))$: we will obtain a state belonging to $\mathrm{Ker}(\Delta^{(N)}(F^-))$ by tensorizing it with a "spin down" state:

$$\psi^{(N)}(m_l, s_{m_l}, \ldots, 0, 0) = \psi^{(N-1)}(m_l, s_{m_l}, \ldots, 0, 0) \otimes \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

As $\psi^{(N-1)}(m_l, s_{m_l}, \ldots, 0, 0)$ spans $\mathrm{Ker}(\Delta^{(N-1)}(F^-))$ we get all states belonging to $\mathrm{Ker}(\Delta^{(N)}(F^-))$ having $s_{m_l} < N$. When generating the complementary subspace of $\mathrm{Ker}(\Delta^{(N)}(F^-))$ through our algorithm, we have to consider two different cases:

(1) $\psi^{(N-1)}(m_l, s_{m_l}, \ldots, 0, 0)$ is annihilated by $\Delta^{(N-1)}(H)$. In this case it holds $m_l - N + 1 = 0 \Rightarrow$ no further element of $\mathrm{Ker}(\Delta^{(N)}(F^-))$ can be constructed, as, from (4.6), it would have $s_{m_{l+1}} > N$.

(2) $\psi^{(N-1)}(m_l, s_{m_l}, \ldots, 0, 0)$ does not belong to $\mathrm{Ker}\Delta^{(N-1)}(H)$. it follows that $m_l \leqslant N-2$, and consequently two more states of $\mathrm{Ker}(\Delta^{(N)}(F^-))$ can be constructed, with $(m_{l+1}, s_{m_{l+1}}) = (m_l + 1, N)$ and $(m_{l+1}, s_{m_{l+1}}) = (m_l + 2, N)$, respectively.

Summarizing, we obtain one element of $\mathrm{Ker}(\Delta^{(N)}(F^-))$ starting from each $(N-1)$-particle state of spin 0, and three elements of $\mathrm{Ker}(\Delta^{(N)}(F^-))$ starting from each $(N-1)$-particle state of spin $k > 0$.

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Two interacting electrons in a uniform magnetic field and a parabolic potential: The general closed-form solution

B. S. Kandemir
Department of Physics, Faculty of Sciences, Ankara University, 06100 Tandoğan, Ankara, Turkey

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We present an analytical analysis of the two-dimensional Schrödinger equation for two interacting electrons subjected to a homogeneous magnetic field and confined by a two-dimensional external parabolic potential. We have found the general closed-form expression for the eigenstates of the problem and its corresponding eigenenergies for particular values of magnetic field and spatial confinement length. The mathematical framework is just based on a rigorous solution of the three-term recursion relation among the coefficients that arises from the series solution of biconfluent Heun (BHE) equation, connected with the radial part of the Schrödinger equation for the internal motion. It is also shown that, by vanishing of Coulomb repulsion strength, the obtained explicit analytical solutions of BHE equation reduces to the well-known polynomials satisfying the associated Laguerre differential equation. Furthermore, in the presence of this interaction, the results are compared with those previously obtained in the literature for first few low-lying states, and are found to be in an exact agreement with them. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1850996]

The study of confined-electron systems is one of the central topics of current theoretical efforts in condensed matter physics, motivated by the recent developments of experimental techniques allowing the creation of ultrasmall nanostructures called quantum dots (QDs).[1–4] Of particular interest are disklike or two-dimensional QDs with two electrons. It is well known that electro-optical properties of such QDs are quite sensitive to the reduction of its dimensionality and to the application of an external magnetic field, and depend strongly on the electron–electron interaction. In recent literature, there exist a large amount of works[5–11] on QDs with two interacting electrons confined in a parabolic potential and/or a magnetic field, wherein a number of approaches, such as exact diagonalization scheme, perturbational and variational methods as well as numerical ones have been successfully applied to this problem. The problem becomes separable by introducing the center-of-mass and internal coordinates. Since the solution of Schrödinger equation for the center-of-mass motion is trivial and simply yields the well-known Fock–Darwin eigenstates,[12,13] the central quantity of interest in the problem therefore arises from the associated radial part of the Schrödinger equation for the relative motion.

From the quantum mechanical point of view, the fact that a system of two interacting Coulomb particles under the influence of a parabolic potential belongs to a class of quasi-exactly-solvable systems is of particular interest in itself. By a quasi-exactly-solvable quantum mechanical problem, it is intended the following: in contrast to the case of standard exactly solvable quantum mechanical problems whose entire spectra can easily be calculated by solving, in general, two-term recursion relations among the coefficients arising from the Frobenius solution to the relevant Schrödinger equation, occurrence of the three-term recursion relations in such problems does not admit an exact solution. Thus, it is only possible to find several eigenvalues and associated eigenstates analytically, under certain circumstances. Introducing accurate group theoretical description of the relevant problem, Turbiner[14] was initially able to show that such a quasi-exact-solvability is purely a consequence of a hidden sl_2 algebraic structure. As discussed in detail by Turbiner, the proof follows immediately from the fact that the eigenvalue equation for the qua-

dratic quasi-exactly-solvable operator constructed from the three generators of sl_2 algebra is directly related to the eigenvalue equation of the relevant problem. Historically, the particular analytical solutions were first found by Verçin[15] in the context of anyon theory, and later by Taut[16] for the two electron case. A different calculation based on the method of factorization was also presented for both Schrödinger and Klein–Gordon equations for a charged particle moving in Coulomb and magnetic fields.[17] There have also been recent other works dealing with this problem.[18–21]

In mathematical physics, the problem is directly linked with the third confluent case of Heun's equation. This equation is, in fact, a generalization of the confluent hypergeometric equation and is called biconfluent Heun equation (BHE).[22] Since it is well-known that, after certain transformations, many Schrödinger equations for a special class of confinement potentials can easily be reduced to BHE, several attempts to solve this equation have been performed in the literature.[23–27] The doubly anharmonic oscillator potential[25] and the potentials of the form $V(r)=\pm Z/r+gr+\lambda r^2$ (Refs. 23, 24, 26, and 27) are the well-known examples of this class of potentials. In particular, the latter (with $\lambda=0$ and with a minus sign) has been studied in the context of nonrelativistic quarkonium model in quantum chromodynamics.[28,29] As can also be easily checked, the problem of interest leads to the same kind of BHE, but with $g=0$ and with a plus sign. To the author's knowledge, so far an exact closed form for the polynomial solutions of this equation has not been achieved.

In this paper, we analyze analytically the two-dimensional (2D) Schrödinger equation for two interacting electrons in a parabolic potential under the influence of a constant, uniform magnetic field perpendicular to the plane of motion. We investigate for the first time its exact general closed form solution by solving the three-term recursion relation among the coefficients arising from the series solutions of the BHE equation. Moreover, we show that, as a particular case, our results reduces to the well-known associated Laguerre polynomials in the absence of the Coulomb interaction between electrons.

The Hamiltonian for a system of two interacting electrons of mass m^* and charge e in two space dimensions subjected to both a uniform magnetic field along the direction perpendicular to the plane and an external parabolic potential is given by

$$H=\sum_{j=1}^{2}\left\{\frac{1}{2m^*}\left[\mathbf{p}(\mathbf{r}_j)+\frac{e}{c}\mathbf{A}(\mathbf{r}_j)\right]^2+U(|\mathbf{r}_j|)\right\}+\frac{e^2}{\epsilon_\infty|\mathbf{r}_1-\mathbf{r}_2|}, \tag{1}$$

where $U(|\mathbf{r}_j|)=(1/2)\,m^*\omega^2\mathbf{r}_j^2$ is the single particle confinement potential, and $\mathbf{A}(\mathbf{r}_j)$ is the vector potential of the magnetic field and will be chosen in the symmetric gauge. It is well known that, by introducing the relative and center-of-mass coordinates, $\mathbf{r}=|\mathbf{r}_1-\mathbf{r}_2|$ and $\mathbf{R}=(\mathbf{r}_1+\mathbf{r}_2)/2$, respectively, Eq. (1) can be decoupled as the sum of two single particle Hamiltonians; one with mass $M=2m^*$ and charge $Q=2e$ and the other with mass $\mu=m^*/2$ and charge $q=e/2$, respectively. The former represents the center-of-mass motion and leads to an eigenvalue equation $H_{2D}(M,\omega)\Psi(\mathbf{R})=E_R\Psi(\mathbf{R})$, wherein H_{2D} is the usual 2D isotropic harmonic oscillator Hamiltonian with frequency ω. Here, ω describes a relation between both strength of magnetic field and the strength of spatial confinement, and is expressed by $\omega_c=QB_0/Mc$ and ω. as $\omega=[\omega_.^2+(\omega_c^2/4)]^{1/2}$. As for the relative motion, we are left with the eigenvalue equation $[H_{2D}(\mu,\omega)+(e^2/\epsilon_\infty|\mathbf{r}|)]\Psi(\mathbf{r})=E_r\Psi(\mathbf{r})$, wherein $H_{2D}(\mu,\omega)$ represent again 2D isotropic harmonic oscillator Hamiltonian with the same frequency ω, but with mass μ. Indeed, for both motion, ω's are the same since $\omega_c=qB_0/\mu c$ is equivalent to eB_0/m^*c as in the case that for the center-of-mass motion. Therefore, by setting $\Psi(\mathbf{r})=e^{im\varphi}R(r)$ due to the cylindrical symmetry of the problem, one can easily obtain the following second-order differential equation for the corresponding radial part of the relative motion

$$\frac{d^2R}{d\rho^2}+\frac{1}{\rho}\frac{dR}{d\rho}-\frac{m^2}{\rho^2}R-\rho^2R-\frac{u}{\rho}R+\tilde{\epsilon}R=0, \tag{2}$$

where $\tilde{\epsilon}=(2E_r-m\hbar\omega_c)/\hbar\omega$, $u=2\mu e^2/\epsilon_\infty\hbar^2\gamma$, $\rho=\gamma r$, $\gamma^2=\mu\omega/\hbar$. The asymptotic behaviors of Eq. (2) at $\rho\to 0$ and $\rho\to\infty$ suggest a solution of the form $R(\rho)=\rho^{\sigma|m|}e^{-\rho^2/2}F(\rho)$ where the function $F(\rho)$ satisfies the differential equation

$$\rho F''+(a-2\rho^2)F'+(d\rho-u)F=0, \tag{3}$$

in which $a=2\sigma|m|+1$ and $d=\tilde{\epsilon}-2(\sigma|m|+1)$. Here, σ takes just $+1$ and -1 values and thus specifies the regular and singular solutions of Eq. (2), respectively, of which only the former one is physically acceptable since the latter diverges at $\rho\to 0$. In fact, Eq. (3) is generally called the biconfluent Heun equation (BHE) in canonical form and its solution is characterized namely by $F(\rho)=N(2\sigma|m|,0,d+2(\sigma|m|+1);\rho)$.[22] The solution of Eq. (3) is obtained through the expansion $F(\rho)=\Sigma_{k=0}^{\infty}A_k\rho^k$ whose coefficients satisfy the following three-term recurrence relation:

$$(k+2)(k+1+a)A_{k+2}=uA_{k+1}-(d-2k)A_k, \tag{4}$$

with $A_0=1$ and $A_1=u/a$. Equation (4) is valid for all values of k greater than and equal to 2. The difficulty in solving Eq. (4) arises from the presence of the Coulomb term u. Without this term, the resulting recurrence relation can easily be solved to construct a series solution of Eq. (3) since all odd coefficients vanish. On the other hand, one can easily express A_{2k} in terms of A_0 by a successive induction, and hence obtains a polynomial of even powers of ρ by just breaking the resulting series off at a certain value of k, say n. However, in the presence of the Coulomb term, studies on Eq. (4) up to now have been restricted to the calculation of the first few terms due to calculational complexities, and could not be able to predict what the general expression for A_k will be. In the present work, by solving A_k's in terms of A_0 and A_1, recursively and taking into account as many terms as we need, and then collecting them together with the same power of ρ, we have achieved to find the general term with ρ^k systematically, and obtained the following infinite series:

$$\begin{aligned}F(\rho)=&\sum_{k=0}^{\infty}\frac{(a-1)!}{k!\,(a+k-1)!}u^k\rho^k-\sum_{k=2}^{\infty}\frac{(a-1)!}{k!\,(a+k-1)!}\sum_{\ell=0}^{k-2}\Theta^{a\ d}(\ell)u^{k-2}\rho^k\\&+\sum_{k=4}^{\infty}\frac{(a-1)!}{k!\,(a+k-1)!}\sum_{\ell=0}^{k-2}\sum_{p>\ell}^{k-3}\Theta^{a\ d}(\ell)\Theta^{a\ d}(p+1)u^{k-4}\rho^k\\&-\sum_{k=6}^{\infty}\frac{(a-1)!}{k!\,(a+k-1)!}\sum_{\ell=0}^{k-2}\sum_{p>\ell}^{k-3}\sum_{r>p}^{k-4}\Theta^{a\ d}(\ell)\Theta^{a\ d}(p+1)\Theta^{a\ d}(r+2)u^{k-6}\rho^k+\cdots,\end{aligned} \tag{5}$$

in which we have defined $\Theta^{a\ d}(\ell)=(\ell+1)(a+\ell)(d-2\ell)$. Equation (5) can easily be rearranged into a more compact form

$$F(\rho)=\sum_{k=0}^{\infty}\frac{(a-1)!}{k!\,(a+k-1)!}\left[u^k-\sum_{s=0(k\geqq 2)}^{[k/2]}(-1)^s u^{k-2s-2}\prod_{t=0}^{s}{\sum_{\ell=0}^{k-t-2}}'\Theta^{a\ d}(\ell+t)\right]\rho^k, \tag{6}$$

where the symbol $[k/2]$ stands for $(k-2)/2$ and $(k-3)/2$ for even and odd k's, respectively. In Eq. (6), the prime above the summation in the square bracket denotes the constraint on summations and implies that only those values of indexes of subsequent summations which satisfy the constraint $\ell>p>r\cdots$ are allowed such that, e.g., for a fixed ℓ, only those values of $\Theta^{a\ d}(p+1)$ in the second sum for which $\ell>p$ will contribute, and so on. Alternatively, it is also possible to write Eq. (5) or equivalently Eq. (6) in the form

$$F(\rho)=\sum_{k=0}^{\infty}\frac{(a-1)!}{k!\,(a+k-1)!}\left[1+\sum_{s=1}^{\infty}(-1)^s\frac{k!\,(a+k-1)!}{(k+2s)!(a+k+2s-1)!}\rho^{2s}\prod_{t=0}^{s-1}\sum_{\ell=0}^{k+2s-t-2}{}'\Theta^{a\ d}(\ell+t)\right]u^k\rho^k. \tag{7}$$

It should be noted that we must have a solution that remains finite as $\rho\to\infty$. Such a solution exists only if the series in Eq. (6) or Eq. (7) are truncated to terminate at a certain value of k to have a finite series. On the other hand, the function $F(\rho)$ becomes a polynomial if and only if the conditions $A_{n+1}=0$ and $d=2n$ are simultaneously fulfilled. Thus, the only solution of Eq. (3) that satisfies these quantization conditions can be finally written as

$$F_{n|m|}(\rho)=\sum_{k=0}^{n}\left[\sum_{s=0(k\geqq 2)}^{[k/2]}\frac{(-1)^s}{k!\,(a)_k}u^{k-2s}\Delta^{a\ n}(k,s)\right]\rho^k. \tag{8}$$

with

$$u^2=\sum_{s=0}^{\|n/2\|}(-1)^s u^{-2s}\prod_{t=0}^{s}\sum_{\ell=0}^{n-t-1}{}'\Theta^{a\ 2n}(\ell+t), \tag{9}$$

where the symbol $\|n/2\|$ stands for $(n-1)/2$ and $(n-2)/2$ for odd and even n's, respectively. In Eq. (8) we have defined a new symbol

$$\Delta^{a\ n}(k,s)=\prod_{t=0}^{s-1}\sum_{\ell=0}^{k-t-2}{}'\Theta^{a\ 2n}(\ell+t),$$

provided that $\Delta^{a\ n}(k,0)=1$, and used the Pochhammer symbol $(a)_k=\Gamma(a+k)/\Gamma(a)$. Therefore, the corresponding energy eigenvalues can be written as $\tilde{\epsilon}_{n\ |m|}=2(n+|m|+1)$. The connection of these eigenvalues with the content of Eq. (9) can be better understood when they are made dimensionless, by expressing them in terms of standard energy and length units, i.e., the effective Bohr radius a_0^* and the Rydberg constant $\mathcal{R}_0^*$. Therefore, one rewrites these eigenvalues and Eq. (9) in the form

$$\bar{E}_r(n,\ |m|)=(n+|m|+1)\bar{\omega}(n,\ |m|)+\frac{m\bar{\omega}_c(n,\ |m|)}{2},$$

$$\bar{\omega}^{-1}(n,\ |m|)=\sum_{s=0}^{\|n/2\|}(-1)^s\bar{\omega}^s(n,\ |m|)\prod_{t=0}^{s}\sum_{\ell=0}^{n-t-1/}\Theta^{a\ 2n}(\ell+t),$$

respectively, where $\bar{E}_r=\bar{E}_r/2\mathcal{R}_0^*$ and $u^2=2\mathcal{R}_0^*/\hbar\omega=1/\bar{\omega}$ are used. Once, a general solution of Eq. (3) has been obtained in the form Eq. (8) together with Eq. (9), one can easily test whether it actually satisfies the differential equation. This can be done by replacing Eq. (8) into Eq. (3), or equivalently by replacing A_k's, which are given by the terms with square brackets in Eq. (8), back into Eq. (4). In the absence of the Coulomb interaction between electrons, i.e., $u=0$, the only nonvanishing term in Eq. (7) is obtained by setting $k=0$, which in fact means that one must retain only the terms with $k=0$, $k=2$, $k=4$, and so on, in Eq. (5). Finally, one finds

$$F(\rho)=1+\sum_{s=1}^{\infty}(-1)^s\frac{(a-1)!}{(2s)!(a+2s-1)!}\prod_{t=0}^{s-1}\sum_{\ell=0}^{2s-t-2\phi}{}'\Theta^{a\ d}(\ell+t)\rho^{2s}. \tag{10}$$

It is also straightforward to verify that the infinite series in Eq. (10) becomes the associated Laguerre polynomials if it terminates at a certain value of s. This is possible if and only if d is an integer, i.e., $d=4n$. This procedure is presented in Appendix A. To check the consistency of our results with those previously obtained in the literature we also give the first few polynomials

together with its associated eigenvalues resulting from Eq. (8) and Eq. (9), respectively, in Appendix B.

In summary, we have explicitly constructed the exact closed-form solution for the problem of two interacting electrons in both uniform magnetic field and external parabolic potential. Besides the polynomial solutions of the problem being obtained from an infinite series for the first time, an alternative representation for the Laguerre polynomials is achieved. The procedure introduced here can easily be extended to its 3D counterpart and can be applied well to the problem of the two- and three-dimensional hydrogen atom in a magnetic field. The results obtained in this paper might also lead to help in understanding the behavior of confined many electron systems under magnetic field, due to the fact that these systems may be considered as interacting pairs. In particular, the present results will be useful in variational and perturbational treatments of the exact spectra of a few particle systems, and thus provide a further insight on discussion of the fractional nature of such systems.

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APPENDIX A

Here, we have presented the key steps of how infinite series given by Eq. (10) become the associated Laguerre polynomials if it is terminated. For this purpose, we start with the expansion of the relevant series given by Eq. (10), i.e.,

$$F(\rho) = 1 - \frac{1}{2!\,(a+1)a}\prod_{t=0}^{0}{\sum_{\ell=0}^{0}}'\Theta^{a\ d}(\ell+t)\rho^2 + \frac{1}{4!\,(a+3)(a+2)(a+1)a}\prod_{t=0}^{1}{\sum_{\ell=0}^{2-t}}'\Theta^{a\ d}(\ell+t)\rho^4$$
$$- \frac{1}{6!\,(a+5)(a+4)(a+3)(a+2)(a+1)a}\prod_{t=0}^{2}{\sum_{\ell=0}^{4-t}}'\Theta^{a\ d}(\ell+t)\rho^6 + \cdots . \tag{A1}$$

By using the definition of $\Theta^{a\ d}(\ell)$ and obeying the constraints on each sum, we obtain the following relations for the products in Eq. (A1):

$$\prod_{t=0}^{0}{\sum_{\ell=0}^{0}}'\Theta^{a\ d}(\ell+t) = \Theta^{a\ d}(0) = 1.a.d,$$

$$\prod_{t=0}^{1}{\sum_{\ell=0}^{2-t}}'\Theta^{a\ d}(\ell+t) = \sum_{\ell=0}^{2}\Theta^{a\ d}(\ell)\sum_{p>\ell}^{1}\Theta^{a\ d}(p+1) = \Theta^{a\ d}(0)\Theta^{a\ d}(1) = 1.3.a.(a+2).d.(d-4),$$

$$\prod_{t=0}^{2}{\sum_{\ell=0}^{4-t/}}'\Theta^{a\ d}(\ell+t) = \sum_{\ell=0}^{4}\Theta^{a\ d}(\ell)\sum_{p>\ell}^{3}\Theta^{a\ d}(p+1)\sum_{r>p}^{2}\Theta^{a\ d}(r+2)$$
$$= \Theta^{a\ d}(0)\Theta^{a\ d}(2)\Theta^{a\ d}(4) = 1.3.5.a.(a+2).(a+4).d\,.\,(d-4).(d-8), \tag{A2}$$

Of course, to get an idea about the behavior of the series one can explore more and more terms with products in Eq. (A1), by following the same procedure as used in Eq. (A2). Therefore, by replacing each term in Eq. (A2) back into Eq. (A1) and collecting the resulting terms into a sum again, one can easily find out what the general term of the series is, and then arrives at a more compact series expansion of Eq. (A1),

$$F(\rho) = 1 + \sum_{s=1}^{\infty} (-1)^s \frac{d.(d-4)\cdots(d-4s+4)}{2s\cdots 4.2.(a+2s-1)\cdots(a+1)} \rho^{2s}. \tag{A3}$$

Now, it remains to show that this infinite series is equal to the associated Laguerre polynomials when it is terminated at a certain value of s. For this, we require $d=4n$ which leads to the energy levels $\tilde{\epsilon}_{n\ |m|}=2(|m|+1)+4n$, i.e., $E_r(n,\ |m|)=(2n+|m|+1)\hbar\omega+(m/2)\hbar\omega_c$. Finally, after necessary algebra, one finds the explicit form of the generalized Laguerre polynomials in the form

$$F_{n|m|}(\rho) = \sum_{s=0}^{n} \frac{(-1)^s}{s!} \binom{n+|m|}{n-s} (\rho^2)^s = L_n^{|m|}(\rho^2) = N(2|m|, 0, 4n + 2(|m|+1); \rho),$$

where $\binom{n}{s} = \Gamma(n+1)/s!\,\Gamma(n+1-s)$ are the binomial coefficients. While, without a spatial confinement, the energy levels connected with the function $F_{n|m|}(\rho)$ are the well-known Landau levels, i.e., $E_r(n,\ |m|)=(2n+|m|+m+1)\hbar\omega_c/2$, in the absence of a magnetic field they reproduce the usual energy levels of 2D isotropic oscillator, i.e., $E_r(n,\ |m|)=(2n+|m|+1)\hbar\omega$. .

APPENDIX B

In this appendix, some special results of Eq. (8) together with Eq. (9) have been presented to show that they reproduce the standard results obtained in the literature. First, we start with $n=1$ ($d=2$) which has $\tilde{\epsilon}_{1\ |m|}=2(|m|+1)+2$; so the solution satisfying Eq. (3) is conveniently extracted from Eq. (8) as

$$F_{1\ |m|}(\rho) = \sum_{k=0}^{1} \frac{(a-1)!}{k!\,(a+k-1)!} u^k \rho^k = 1 + \frac{u}{a}\rho \tag{B1}$$

with the corresponding condition on ω, $u^2=1.a.d$ which is calculated from Eq. (9) with the help of the first equality in Eq. (A1). Second, we consider the case $n=2$ ($d=4$), where $\tilde{\epsilon}_{2\ |m|}=2(|m|+1)+4$. For this case, from Eq. (8) we obtain a solution

$$\begin{aligned} F_{2\ |m|} &= \sum_{k=0}^{2} \frac{(a-1)!}{k!\,(a+k-1)!} \left[u^k - \sum_{s=0(k\geqq 2)}^{0} (-1)^s u^{k-2s-2} \prod_{t=0}^{s} \sum_{\ell=0}^{k+2s-t}{}' \Theta^{a\ d}(\ell+t) \right] \rho^k \\ &= 1 + \frac{u}{a}\rho + \frac{1}{2!\,(a+1)a}[u^2 - 1.a.d]\rho^2 \end{aligned} \tag{B2}$$

with $(u^2-1.a.d)-2(a+1)(d-2)=0$, where, again, Eq. (9) has been used here, but together with the help of the second equality in Eq. (A1), besides the first one. We shall finally consider the case $n=3$ ($d=6$), where $\tilde{\epsilon}_{3\ |m|}=2(|m|+1)+6$. In this case, it is straightforward to show that one can easily obtain the following solution:

$$\begin{aligned} F_{3\ |m|} &= \sum_{k=0}^{3} \frac{(a-1)!}{k!(a+k-1)!} \left[u^k - \sum_{s=0(k\geqq 2)}^{[k/2]} (-1)^s u^{k-2s-2} \prod_{t=0}^{s} \sum_{\ell=0}^{k+2s-t}{}' \Theta^{a\ d}(\ell+t) \right] \rho^k \\ &= 1 + \frac{u}{a}\rho + \frac{1}{2!(a+1)a}[u^2 - 1.a.d]\rho^2 + \frac{u}{3!(a+2)(a+1)a}[(u^2 - 1.a.d) - 2(a+1)(d-2)]\rho^3 \end{aligned} \tag{B3}$$

with $u^4=u^2[1.a.d+2(a+1)(d-2)+3(a+2)(d-4)]-1.a.d.3.(a+2)(d-4)$. In the last step of Eq. (B3) we have used again Eq. (A1). All the exact analytical results presented here are in complete agreement with the results obtained in Refs. 15 and 16.

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Yang–Mills action from minimally coupled bosons on $\mathbb{R}^4$ and on the four-dimensional Moyal plane

Juha Loikkanen and Cornelius Paufler
Mathematical Physics/AlbaNova, Royal Institute of Technology, SE-10691 Stockholm, Sweden

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We consider bosons on (Euclidean) $\mathbb{R}^4$ that are minimally coupled to an external Yang–Mills field. We compute the logarithmically divergent part of the cutoff regularized quantum effective action of this system. We confirm the known result that this term is proportional to the Yang–Mills action. We use pseudodifferential operator methods throughout to prepare the ground for a generalization of our calculation to the noncommutative four-dimensional Moyal plane $\mathbb{R}^4_\theta$. We also include a detailed comparison of our cutoff regularization to heat kernel techniques. In the case of the noncommutative space, we complement the usual technique of asymptotic expansion in the momentum variable with operator theoretic arguments in order to keep separated quantum from noncommutativity effects. We show that the result from the commutative space $\mathbb{R}^4$ still holds if one replaces all pointwise products by the noncommutative Moyal product. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1839277]

I. INTRODUCTION

In this paper we study the determinant of certain differential operators. Such determinants naturally arise in quantum field theory at the one loop level. As the determinant of an operator on an infinite dimensional Hilbert space is not an *a priori* well-defined object, one must choose some regularization scheme. The latter means generally the choice of a recipe for how to replace the formal expressions by something that is both amenable to a rigorous definition and close in its properties. In our case of the regularization of determinants, a common starting point is the well-known identity

$$\log\det A = \mathrm{Tr}\log A, \tag{1}$$

which holds for (finite dimensional) matrices A. The task is now to give meaning to the trace on the right-hand side, since the operators of interest do not have a finite trace in general. In this paper, we restrict the trace to run over a subspace of our Hilbert space only. Loosely speaking, this subspace is spanned by wave functions that have a momentum expectation value smaller than a certain cutoff Λ. The precise definition will follow below. It is known that the cutoff regularized logarithm of the determinant, now viewed as a function of Λ, contains a term that scales like $\log\Lambda$ for large Λ. This term is closely related to the Wodzicki residue for the operator under consideration, a quantity that is of interest in the study of infinite dimensional geometry, see Ref. 15 for a recent review.

Motivated by the observation[14] that for fermions minimally coupled to an external Yang–Mills field, the logarithmically divergent part of the cutoff regularized logarithm of the determinant of the (massive) Dirac operator is proportional to the corresponding Yang–Mills action, we consider the case of bosons in an external Yang–Mills field on $\mathbb{R}^4$. With our work, we confirmed that the above result also applies to the bosonic case. The former result was proposed to be interpreted in two ways. On the one hand, the spectral action principle[2] states that the spectrum of the Dirac

operator should provide exhaustive information about the complete bare action including the Yang–Mills expression. On the other hand, it is known that the logarithmically divergent part plays a critical role in the selection of the finite part of an effective action because of its behavior under rescaling of the regularization parameter Λ. From the latter viewpoint, it is desirable that the logarithmically divergent term in the regularized effective action produce expressions that occur in the complete bare action already.

To understand the connection between these two interpretations, it is interesting to consider the case of (scalar) bosons coupled to an external Yang–Mills field.

It is generally accepted that space–time might lose its smooth properties at very small scales. One possible mathematical framework for this is noncommutative geometry.[3] We are interested in a particular example, the four-dimensional (4D) Moyal plane,[10] also known as noncommutative flat space $\mathbb{R}^4_\theta$. Roughly speaking, the 4D Moyal plane differs from its Euclidean counterpart $\mathbb{R}^4$ in that there is an uncertainty relation for the simultaneous measurement of coordinates coming from the nonvanishing commutator

$$[x^\mu, x^\nu] = i\Theta^{\mu\nu}.$$

Here x^μ, $\mu = 1, \ldots, 4$ are coordinates of $\mathbb{R}^4$ and Θ is some (antisymmetric) matrix. In this paper we take Θ to be proportional to the constant symplectic matrix, see Eq. (16). We refer to Ref. 5 for a treatment of Lorentz covariant generalization of this equation.

Although the results of our analysis for the case of bosons on the commutative space $\mathbb{R}^4$ are not new and can be found already in deWitt's book,[4] our consistent use of pseudodifferential operator methods technically makes possible the generalization to the noncommutative Moyal plane. We refer to Refs. 18 and 11 for a generalization of heat kernel regularization calculations to the noncommutative torus and the Moyal plane, respectively.

The remainder of this paper is structured as follows. Section II sets up the notation used in our work and states the results in the form of two propositions. Section III provides the necessary tools from the theory of pseudodifferential operators. The proofs of the statements from Sec. II can be found in Secs. IV and V, with detailed calculations postponed to the appendix. Also, Sec. IV contains additional arguments that make contact with the case of fermions on $\mathbb{R}^4$ and to an alternative regularization scheme, the heat kernel regularization. Section VI concludes with what we consider to be the lessons from our calculations.

II. NOTATION AND STATEMENT OF THE RESULTS

We consider the Klein–Gordon operator with minimally coupled external field on the four-dimensional flat Euclidean space $\mathbb{R}^4$, given by

$$\begin{aligned}\Box_A = D_A^\mu D_{A,\mu} = (\partial^\mu + ieA^\mu)(\partial_\mu + ieA_\mu) &= \partial^\mu\partial_\mu + ie\partial^\mu A_\mu + 2ieA^\mu\partial_\mu - e^2A^\mu A_\mu \\ &= \Box_0 + ie\partial^\mu A_\mu + 2ieA^\mu\partial_\mu - e^2A^\mu A_\mu. \qquad (2)\end{aligned}$$

Here, $\mu = 1, \ldots, 4$ are the (Euclidean) indices of $\mathbb{R}^4$, $\partial_\mu = \partial/\partial x^\mu$, and A_μ are gl_N-valued Yang–Mills fields on $\mathbb{R}^4$. The bosonic wave functions are elements of the Hilbert space

$$\mathcal{H} = L^2(\mathbb{R}^4) \otimes \mathbb{C}^N_{\text{color}},$$

where the last factor carries a gl_N representation from the external Yang–Mills fields. As an unbounded operator in $\mathcal{H}$, $\Box_0$ can be defined on smooth functions in $\mathcal{H}$ by its formal expression and then extended to a self-adjoint operator. We assume the Yang–Mills fields A_μ to be regular, i.e., to be smooth and to fall off (together with all their derivatives) at infinity like $|x|^{-2-\epsilon}$, $\epsilon > 0$. The latter assumption ensures that all our spatial integrals below will converge. Also, for regular A_μ, the self-adjoint extension of $\Box_A$ can be computed from that of $\Box_0$. In what follows, we will not distinguish between the formal expression for $\Box_A$ and its self-adjoint extension.

We consider the cutoff regularized logarithm of the determinant of the massive Klein–Gordon operator

$$S_\Lambda(A) := \mathrm{Tr}_\Lambda\left(\log\left(\frac{-\Box_A + m^2}{\Lambda_0^2}\right) - \log\left(\frac{-\Box_0 + m^2}{\Lambda_0^2}\right)\right), \tag{3}$$

where the cutoff regularized Hilbert space trace Tr_Λ sums over states with momentum bounded by Λ. More precisely, if D is an operator on $\mathcal{H}$ and Tr denotes the operator trace on $\mathcal{H}$, then the cutoff trace is defined by

$$\mathrm{Tr}_\Lambda D := \mathrm{Tr}\{\theta(\Lambda^2 + \Box_0)D\}, \tag{4}$$

where θ is the Heaviside step function. As is well-known, the expression (3) occurs in quantum field theory as the one-loop effective action. Using the formal identity $\log\det = \mathrm{Tr}\log$, it can be viewed as the generalization of the determinant to operators on an infinite-dimensional Hilbert space.

The parameter Λ_0 has been introduced to balance physical dimensions. It also provides a useful tool for cross checking since in the result of our calculations, it should cancel. Moreover, in the definition of the regularized determinant, we have subtracted a term containing the free Klein–Gordon operator as a reference. Whereas this term is needed for turning the expression under the trace into a pseudodifferential operator, it also comes in—at least in the corresponding expression for fermions—when interpreting the determinant as a subsummation of the one loop diagrams in the Feynman path integral.[16]

The regularized determinant (3) has an asymptotic expansion in Λ for large values of Λ as

$$S_\Lambda(A) = c_2(A,m)\Lambda^2 + c_1(A,m)\Lambda^1 + c_{\log}(A,m)\log\Lambda + c_0(A,m) + \cdots, \tag{5}$$

where the dots indicate terms that vanish at least like $1/\Lambda$ in the limit $\Lambda \to \infty$.

We are interested in the coefficient $c_{\log}(A,m) \equiv c_{\log}(A)$.

Proposition II.1: For the regularized determinant $S_\Lambda(A)$ defined as above, the coefficient $c_{\log}(A,m)$ is proportional to the Yang–Mills action of A_μ,

$$c_{\log}(A) = \frac{1}{96\pi^2}\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}_N(F^{\mu\nu}F_{\mu\nu}), \tag{6}$$

where tr_N is the matrix trace in gl_N and the curvature $F_{\mu\nu}$ of A_μ is given by

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + ie[A_\mu, A_\nu]. \tag{7}$$

The proof is contained in Sec. IV A. Note that the numerical factor in front of $F^{\mu\nu}F_{\mu\nu}$ differs from the one obtained in Ref. 4 Eqs. (24.16), etc., by $\frac{1}{2}$. By the considerations below, this can be understood as coming from the usage of a nongauge invariant regularization for $S_\Lambda(A)$. However, the latter allows a straightforward generalization to the noncommutative Moyal plane.

It is well-known that

$$(\not{D}_A)^2 = \mathbb{1}_4\Box_A - ie\sigma\cdot F, \tag{8}$$

where $\not{D}_A = \gamma^\mu(\partial_\mu + ieA_\mu)$, $\sigma\cdot F = \frac{1}{4}\sigma^{\mu\nu}F_{\mu\nu} = \frac{1}{2}\gamma^\mu\gamma^\nu F_{\mu\nu}$, and γ^μ are the four-dimensional gamma matrices, i.e., 4×4 matrices that satisfy

$$\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\eta^{\mu\nu}\mathbb{1}_4, \tag{9}$$

$\eta^{\mu\nu}$ being the Euclidean flat metric. Using this identity, we are able to rederive the result of Ref. 14 concerning the determinant of the Dirac operator. This is demonstrated in Sec. IV B. Our

computation has the advantage of avoiding extensive calculations involving the gamma matrices γ^μ.

It is at first sight surprising that the nongauge invariant definition of the determinant yields a gauge invariant logarithmically divergent part. It is therefore natural to consider the manifestly gauge invariant expression

$$\widetilde{S}_\Lambda(A) := \mathrm{Tr}_\Lambda^{\Box_A} \log\left(\frac{-\Box_A + m^2}{\Lambda_0^2}\right) - \mathrm{Tr}_\Lambda \log\left(\frac{-\Box_0 + m^2}{\Lambda_0^2}\right), \tag{10}$$

where in the first trace, the cutoff is taken with respect to the operator $\Box_A$ rather than $\Box_0$. As before, $\widetilde{S}_\Lambda(A)$ has an asymptotic expansion,

$$\widetilde{S}_\Lambda(A) = \widetilde{c}_2(A,m)\Lambda^2 + \widetilde{c}_1(A,m)\Lambda^1 + \widetilde{c}_{\log}(A,m)\log\Lambda + \widetilde{c}_0(A,m) + \cdots, \tag{11}$$

the dots subsuming terms scaling at least like $1/\Lambda$. A calculation in Sec. IV C reveals that the coefficient$\widetilde{c}_{\log}(A,m) \equiv \widetilde{c}_{\log}(A)$ in (11) equals half of the corresponding expression in $S_\Lambda(A)$,

$$\widetilde{c}_{\log}(A) = \tfrac{1}{2} c_{\log}(A). \tag{12}$$

This result agrees with the one obtained in Ref. 4.

A widely used alternative regularization of the determinant of a differential operator makes use of the ζ-function and the asymptotic expansion of the trace of the heat kernel operator. We want to compare our coefficient with earlier results that have been obtained with these methods[6] [see also the review articles Ref. 1, and references therein]. In this approach, one considers asymptotic expansions for the trace of the heat operator,

$$K(f,D) := \mathrm{Tr}_{L^2}(f e^{-tD}) = t^{-2} a_0(f,D) + t^{-3/2} a_1(f,D) + \cdots + a_4(f,D) + \cdots, \tag{13}$$

for small t, where f is some function on $\mathbb{R}^4$ that serves as a regulator for the spatial integrals. The rightmost dots indicate terms that fall off at least linearly in t. As the heat trace must be integrated on the positive axis together with the function t, the logarithmically divergent contribution to the heat kernel regularized trace is given by the coefficient $a_4(f,D)$. For the comparison of this coefficient to our result, let $c_{(\cdot)}(f,A)$, etc., be the coefficients in the expansion of $S_\Lambda(A)$, now spatially regularized in the same way as $K(f,D)$. In Sec. IV D, it is shown that the coefficient $\widetilde{c}_{\log}(f,A)$ in the asymptotic expansion of $\widetilde{S}_\Lambda(A)$ differs from the corresponding expression obtained via heat kernel regularization methods by a term proportional to m^4,

$$-\widetilde{c}_{\log}(f,A) + \frac{1}{32\pi^2} m^4 \int_{\mathbb{R}^4} \mathrm{d}^4x\, f(x) = a_4\left(f, \frac{-\Box_A + m^2}{\Lambda_0^2}\right). \tag{14}$$

The additional mass term can be traced back to the usage of the reference operator $-\Box_0 + m^2$ in (3). The calculations using the heat operator can be generalized to the noncommutative 4D torus[18] and the noncommutative Moyal plane.[11] The only change one encounters is that in all expressions, the commutative product of functions must be replaced by the noncommutative product $\star$.

The main part of our paper is devoted to the study of the case of the 4D Moyal plane as the underlying (noncommutative) "space." In this case, the algebra of functions on $\mathbb{R}^4$ is furnished with the (noncommutative) Moyal–Weyl product $\star := \star_\Theta$. The latter is defined by the integral formula

$$f \star g(x) = \frac{1}{(2\pi)^4} \int_{\mathbb{R}^4} \int_{\mathbb{R}^4} \mathrm{d}^4y\, \mathrm{d}^4\xi\, e^{i\xi(x-y)} f(x - \tfrac{1}{2}\Theta\xi) g(y), \tag{15}$$

where Θ is a 4×4 matrix defined by

$$\Theta = \theta \begin{pmatrix} 0 & \mathbb{1}_2 \\ -\mathbb{1}_2 & 0 \end{pmatrix} \tag{16}$$

for the real parameter θ. In our calculations we do not use asymptotic expansions of this product in powers of θ.

On the Moyal plane, we consider the generalized Klein–Gordon operator

$$\Box_A^\theta = \partial^\mu \partial_\mu + ie(\partial^\mu A_\mu) \star + 2ieA^\mu \star \partial_\mu - e^2(A^\mu \star A_\mu) \star , \tag{17}$$

where $f\star$ is a short-hand notation for the operator that $\star$-multiplies smooth wave functions in $\mathcal{H}$ from the left by the (smooth) function f. We define $S_\Lambda^\theta(A)$ and $c_{(\cdot)}^\theta(A,m)$ in analogy with the formulas (3) and (5) above. Then, our main result is the following.

Proposition II.2: For minimally coupled bosonic fields on the (noncommutative) 4D Moyal plane, the above formula (6) holds with the commutative products replaced by the noncommutative Moyal–Weyl product, i.e., we have

$$c_{\log}^\theta(A) = \frac{1}{96\pi^2} \int_{\mathbb{R}^4} \mathrm{d}^4x \, \mathrm{tr}_N F^{\theta,\mu\nu} \star F_{\mu\nu}^\theta, \tag{18}$$

where

$$F_{\mu\nu}^\theta = \partial_\mu A_\nu - \partial_\nu A_\mu + e[A_\mu, A_\nu]_\star . \tag{19}$$

III. PSEUDODIFFERENTIAL OPERATOR METHODS

In our work, we deal with a restricted class of *pseudodifferential operators* (ΨDO) which suits our purposes. The statements below may be found in Shubin's book.[17] We consider ΨDOs that act on smooth and compactly supported wave functions u as [$x=(x^\mu)$, $\mu=1,\ldots,4$, and likewise y, p describe points in $\mathbb{R}^4$; $xp=\Sigma_\mu x^\mu p^\mu$ denotes the scalar product, $|x|$ is the length of the vector x]

$$(Au)(x) = \int_{\mathbb{R}^4} \frac{\mathrm{d}^4p}{(2\pi)^4} \int_{\mathbb{R}^4} \mathrm{d}^4y \, \sigma[A](x,p) u(y) e^{ip(x-y)},$$

where the *symbol* $\sigma[A]$ of A is a smooth function that allows an *asymptotic expansion* in p according to

$$\sigma[A](x,p) \sim \sum_{r=0}^{\infty} \sigma_{m-r}[A](x,p).$$

Here, $\sim$ means that for each s, the finite sum $\Sigma_{r=0}^s \sigma_{m-r}[A]$ approximates $\sigma[A]$ up to a function that falls off at most as $|p|^{m-(s+1)}$ for large $|p|$,

$$\left| \partial_x^\alpha \partial_p^\beta \left(\sigma[A](x,p) - \sum_{r=0}^{s} \sigma_{m-r}[A](x,p) \right) \right| \leqslant C_{\alpha\beta} (1+|p|^2)^{[m-(s+1)-|\beta|]/2}$$

for all multi-indices $\alpha=(\alpha_1,\ldots,\alpha_4)$, $\beta=(\beta_1,\ldots,\beta_4)$, where

$$\partial_x^\alpha = \left(\frac{\partial}{\partial x^1}\right)^{\alpha_1} \cdots \left(\frac{\partial}{\partial x^4}\right)^{\alpha_4},$$

$|\alpha| = \alpha_1 + \cdots + \alpha_4$, and $C_{\alpha\beta}$ are constants. The number m above is called the *order* of A. For a given symbol, there are many different asymptotic expansions. One particular choice is the asymptotic

expansion in terms of *homogeneous symbols* $\sigma^h_{m-r}[A]$, i.e., smooth functions that in addition satisfy

$$\sigma^h_{m-r}[A](x,\lambda p) = \lambda^{m-r}\sigma^h_{m-r}[A](x,p) \quad \text{for } |p| = 1,\ \lambda > 1.$$

The first term $\sigma^h_m[A]$ in an asymptotic expansion in homogeneous summands is termed the *principal symbol*.

An asymptotic expansion encodes the information of a given symbol $\sigma[A]$ up to an additive function that falls off in p like a Schwartz test function. This piece of information will be sufficient for our purposes.

While the expansion in homogeneous symbols is appropriate to discuss invariant notions such as the residue of a ΨDO, the expansions obtained from recursion relations in the computation of resolvents of operators are not of this type in general. The two types, however, are related to each other through a finite resummation at every order of the infinite sum.

The action of the ΨDOs considered here can be extended to smooth functions, leading to the useful formula

$$\sigma[A](x,p) = e^{-ixp}Ae^{ixp}.$$

For the product AB of two ΨDOs A and B with respective symbols $\sigma[A]$ and $\sigma[B]$, one has the following asymptotic expansion of the symbol:

$$\sigma[A] * \sigma[B](x,p) = \sigma[AB](x,p) \sim \sum_\alpha \frac{(-i)^{|\alpha|}}{\alpha!}\partial_p^\alpha\sigma[A](x,p)\partial_x^\alpha\sigma[B](x,p), \tag{20}$$

where the sum runs over all 4-indices α and we have used the notation $\alpha! = \alpha_1!\cdots\alpha_4!$. We will use $*$ whenever we mean this product of symbols, in contrast to the noncommutative product $\star$ defined later on.

Interpreting A as an operator in the Hilbert space $L^2(\mathbb{R}^4)\otimes\mathbb{C}^N$, we can compute the trace of A from its symbol according to

$$\mathrm{Tr}(A) = \int_{\mathbb{R}^4}\frac{d^4p}{(2\pi)^4}\int_{\mathbb{R}^4}\mathrm{d}^4x\ \mathrm{tr}_N\,\sigma[A](x,p),$$

where tr_N denotes the matrix trace over the gl_N-part of the symbol.

For operators A that do not have a (finite) trace, one considers the cutoff trace

$$\mathrm{Tr}_\Lambda(A) = \int_{|p|\leqslant\Lambda}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_{\mathbb{R}^4}\mathrm{d}^4x\ \mathrm{tr}_N\,\sigma[A](x,p).$$

Clearly, this coincides with the previous definition of the cutoff regularized trace, Eq. (4).

The above expression has an asymptotic expansion in Λ, as can be seen from the asymptotic expansion of the symbol $\sigma[A]$ in homogeneous symbols. In this case, there appears a term scaling like $\log\Lambda$. On the other hand, the *Wodzicki residue*[19] of the operator A is defined as the angular p-integral and the spatial integral of the coefficient $\sigma^h_{-4}[A]$ in the homogeneous asymptotic expansion,

$$\mathrm{Res}(A) \coloneqq \frac{1}{(2\pi)^4}\int_{|p|=1}\mathrm{d}\Omega_p\int_{\mathbb{R}^4}\mathrm{d}^4x\ \sigma^h_{-4}[A](x,p),$$

whenever the integral exists. It is known that for compact spatial manifolds this quantity determines completely the factor in front of the $\log\Lambda$ term in the asymptotic expansion of $\mathrm{Tr}_\Lambda(A)$. By abuse of notation, and motivated by the above observation, in our calculations we will use the expression $\mathrm{Res}(\cdots)$ to mean the factor in front of the $\log\Lambda$ term in the corresponding cutoff regularized trace.

IV. THE CASE $M=\mathbb{R}^4$

A. The logarithmically divergent part

In this section we compute the logarithmically divergent part of the bosonic effective action on $\mathbb{R}^4$. We define the regularized bosonic action as

$$S_\Lambda(A) := \mathrm{Tr}_\Lambda\left(\log\left(\frac{-\Box_A+m^2}{\Lambda_0^2}\right)-\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\right). \tag{21}$$

We use the following expression for the logarithm:

$$\log(1+a)=\int_0^1 \frac{\mathrm{d}s}{s}(1-(1+sa)^{-1}) \tag{22}$$

and recall the definition for the regularized trace of a pseudodifferential operator

$$\mathrm{Tr}_\Lambda(a) := \int_{|p|\leqslant\Lambda}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,\sigma[a](x,p) \tag{23}$$

to get

$$\begin{aligned}&\mathrm{Tr}_\Lambda\left(\log\left(\frac{-\Box_A+m^2}{\Lambda_0^2}\right)-\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\right)\\&\quad=-\int_{|p|\leqslant\Lambda}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_{\mathbb{R}^4}\mathrm{d}^4x\int_0^1\frac{\mathrm{d}s}{s}\mathrm{tr}_N\left(\sigma\left[\left(I+s\left(\frac{-\Box_A+m^2}{\Lambda_0^2}-I\right)\right)^{-1}\right]\right.\\&\qquad\left.-\sigma\left[\left(I+s\left(\frac{-\Box_0+m^2}{\Lambda_0^2}-I\right)\right)^{-1}\right]\right).\end{aligned} \tag{24}$$

As shown in the first section of the Appendix, the symbol of the resolvent of $\Box_A$ must satisfy the following recursion relation:

$$\sigma[(c_1I+c_2\Box_A)^{-1}](p,x)=\frac{1}{c_1-c_2p^2}-\frac{c_2}{c_1-c_2p^2}(\Box_A+2ip_\mu D_A^\mu)\sigma[(c_1I+c_2\Box_A)^{-1}](p,x).$$

Its formal solution is given by

$$\sigma[(c_1I+c_2\Box_A)^{-1}](x,p)=(c_1I+c_2(-p^2+\Box_A+2ip^\mu D_{A\mu}))^{-1}1,$$

which can be understood as defining an asymptotic expansion, see the Appendix for details. In particular, for our values of c_1 and c_2, we derive

$$\sigma\left[\left(I+s\left[\frac{-\Box_A+m^2}{\Lambda_0^2}-I\right]\right)^{-1}\right]\sim\sum_{n=0}^{\infty}\frac{(s/\Lambda_0^2)^n}{\left(1-s+\frac{sm^2}{\Lambda_0^2}+\frac{s}{\Lambda_0^2}p^2\right)^{n+1}}(\Box_A+2ip_\mu D_A^\mu)^n1.$$

Here and in all what follows, the 1 on the right-hand side (rhs) means that the operators $\Box_A$, $D_{A,\mu}$ should be applied to the N-dimensional constant vector.

Inserting this expansion into the integral and noting that the second symbol just cancels the first term in the expansion we then have

$$\mathrm{Tr}_\Lambda\left(\log\left(\frac{-\Box_A+m^2}{\Lambda_0^2}\right)-\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\right)=-\int_{|p|\leqslant\Lambda}\frac{\mathrm{d}^4p}{(2\pi)^4}\sum_{n=1}^{\infty}\frac{1}{\Lambda_0^{2n}}\int_0^1\mathrm{d}s\frac{s^{n-1}}{\left(1+s\left(\frac{p^2+m^2}{\Lambda_0^2}-1\right)\right)^{n+1}}$$
$$\times\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N(\Box_A+2ip_\mu D_A^\mu)^n1. \tag{25}$$

In the first section of the Appendix we will expand explicitly the terms in (25) and pick out the logarithmically diverging ones. Setting all the relevant terms together then gives

$$\begin{aligned}
&\mathrm{Res}\left(\log\left(\frac{-\Box_A+m^2}{\Lambda_0^2}\right)-\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\right)\\
&=-\frac{1}{8\pi^2}m^2\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\Box_A-\frac{1}{16\pi^2}\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\Box_A^2+\frac{1}{8\pi^2}m^2\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\Box_A+\frac{1}{12\pi^2}\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\Box_A^2\\
&\quad+\frac{1}{24\pi^2}\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,D_A^\mu\Box_AD_{A\mu}-\frac{1}{48\pi^2}\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N(\Box_A^2+D_A^\nu D_A^\mu D_{A\nu}D_{A\mu}+D_A^\mu\Box_AD_{A\mu})\\
&=\frac{1}{48\pi^2}\left(\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,D_A^\mu\Box_AD_{A\mu}-\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,D_A^\nu D_A^\mu D_{A\nu}D_{A\mu}\right).
\end{aligned}\tag{26}$$

A short calculation shows that the terms under the trace are equal to $(e^2/2)F^{\mu\nu}F_{\mu\nu}$, so we finally get the result

$$\mathrm{Res}\left(\log\left(\frac{-\Box_A+m^2}{\Lambda_0^2}\right)-\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\right)=\frac{e^2}{96\pi^2}\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_NF^{\mu\nu}F_{\mu\nu} \tag{27}$$

which proves Proposition II.1.

B. Comparison with fermion calculations

To incorporate fermions, we have to extend the Hilbert space. We take $\mathcal{H}_{\mathrm{fermion}}=L^2(\mathbb{R}^4)\otimes\mathbb{C}^N_{\mathrm{color}}\otimes\mathbb{C}^4_{\mathrm{spin}}$, where the last factor carries a representation of the Dirac gamma matrixes γ^μ, $\mu=1,\ldots,4$.

We begin by computing the square of the Dirac operator $\not{D}$. First some definitions

$$D_{A\mu}=\partial_\mu+ieA_\mu,$$

$$\not{D}_A=\gamma^\mu(\partial_\mu+ieA_\mu).$$

A short calculation yields the well-known formula

$$(\not{D}_A)^2=\mathbb{1}_4\Box_A+\tfrac{1}{2}\gamma^\mu\gamma^\nu[D_{A\mu},D_{A\nu}]=\mathbb{1}_4\Box_A+ie\sigma\cdot F.$$

Here, $\mathbb{1}_4$ denotes the 4×4 unit matrix and

$$\sigma\cdot F:=\tfrac{1}{4}\sigma^{\mu\nu}F_{\mu\nu}=\tfrac{1}{2}\gamma^\mu\gamma^\nu F_{\mu\nu}$$

for the matrices $\sigma^{\mu\nu}:=[\gamma^\mu,\gamma^\nu]$. We use the above identity to obtain

$$(-i\not{D}_A+im)(-i\not{D}_A-im)=-(\not{D}_A)^2+m^2=-\mathbb{1}_4\Box_A-ie\sigma\cdot F+m^2.$$

Taking the logarithm on both sides, for the left-hand side we arrive at

$$\log\left(\frac{-i\not{D}_A+im}{\Lambda_0}\right)\left(\frac{-i\not{D}_A-im}{\Lambda_0}\right)=\log\left(\frac{-i\not{D}_A+im}{\Lambda_0}\right)+\log\left(\frac{-i\not{D}_A-im}{\Lambda_0}\right),$$

while the right-hand side gives

$$\begin{aligned}\log(-\mathbb{1}_4\Box_A-ie\sigma\cdot F+m^2)&=\log\left(\frac{\mathbb{1}_4(-\Box_A+m^2)}{\Lambda_0^2}\right)\left(\mathbb{1}_4-\frac{ie}{-\Box_A+m^2}\sigma\cdot F\right)\\&=\log\left(\frac{\mathbb{1}_4(-\Box_A+m^2)}{\Lambda_0^2}\right)\\&\quad+\log\left(\mathbb{1}_4-\frac{ie}{-\Box_A+m^2}\sigma\cdot F\right)+\text{commutator terms}.\end{aligned}$$

The extra commutator terms can be computed from the Baker–Campbell–Hausdorff formula.

It is known that on compact manifolds the Wodzicki residue vanishes on commutators.[19] We therefore expect that from the above expression, the commutator terms will not contribute to the logarithmically divergent part of the regularized trace. In the second section of the Appendix it is shown explicitly that this is indeed the case. Rather than using integration-by-parts arguments, this is readily seen from the fact that the $\mathbb{C}_{\text{spin}}$-trace over $\sigma\cdot F$ gives zero. Also, the pertinent contributions from the first two terms of the right-hand side are calculated in the Appendix.

Furthermore, from Langmann's results[14] we know that $\mathrm{Tr}_\Lambda \log[(-i\not{D}_A+im)/\Lambda_0]$ is independent of the sign of m, so we have

$$\begin{aligned}2\,\mathrm{Tr}_\Lambda\log\left(\frac{-i\not{D}_A+im}{\Lambda_0}\right)&=4\,\mathrm{Tr}_\Lambda\log\left(\frac{-\Box_A+m^2}{\Lambda_0^2}\right)+\frac{e^2}{16\pi^2}\log\Lambda\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}(\sigma\cdot F)^2\\&\quad+\text{terms finite in }\Lambda,\end{aligned}$$

where the trace tr runs over both the $\mathbb{C}^N_{\text{color}}$ and the $\mathbb{C}^4_{\text{spin}}$ parts. Performing the trace over the γ-matrices yields

$$\mathrm{tr}(\sigma\cdot F)^2=-2\mathrm{tr}_N F^{\mu\nu}F_{\mu\nu}.$$

The result is then

$$\begin{aligned}\mathrm{Tr}_\Lambda\log\left(\frac{-i\not{D}_A+im}{\Lambda_0}\right)&=2\,\mathrm{Tr}_\Lambda\log\left(\frac{-\Box_A+m^2}{\Lambda_0^2}\right)-\frac{e^2}{16\pi^2}\log\Lambda\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N F^{\mu\nu}F_{\mu\nu}+\cdots\\&=\left(\frac{e^2}{48\pi^2}\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N F^{\mu\nu}F_{\mu\nu}-\frac{e^2}{16\pi^2}\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N F^{\mu\nu}F_{\mu\nu}\right)\log\Lambda+\cdots\\&=-\frac{e^2}{24\pi^2}\log\Lambda\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N F^{\mu\nu}F_{\mu\nu}+\text{terms finite in }\Lambda,\end{aligned}$$

in agreement with Ref. 14.

C. Dependence on the regularization scheme

So far we have been looking at the cutoff regularized determinant

$$S_\Lambda(A) = \mathrm{Tr}_\Lambda\left(\log\left(\frac{-\Box_A + m^2}{\Lambda_0^2}\right) - \log\left(\frac{-\Box_0 + m^2}{\Lambda_0^2}\right)\right). \tag{28}$$

As the cutoff in this regularization is taken with respect to the reference operator $\Box_0$, the above expression is not manifestly gauge invariant. It is thus surprising that the coefficient $c_{\log}(A)$ turns out to be gauge invariant.

One could use the spectral projection with respect to $\Box_A$ instead, but again the resulting expression would fail to be manifestly gauge invariant now because of the reference term $\log[(-\Box_0+m^2)/\Lambda_0^2]$. The latter had to be included to make the calculations tractable by the methods of classical ΨDOs.

Of course, there are gauge invariant regularization schemes such as heat kernel regularization (see the review articles in Ref. 1 for recent developments in this field) readily available. However, cutoff regularized traces seem to be closer to physical intuition.

An acceptable, manifestly gauge invariant expression would be

$$\widetilde{S}_\Lambda(A) := \mathrm{Tr}_\Lambda^{\Box_A} \log\left(\frac{-\Box_A + m^2}{\Lambda_0^2}\right) - \mathrm{Tr}_\Lambda \log\left(\frac{-\Box_0 + m^2}{\Lambda_0^2}\right), \tag{29}$$

where

$$\mathrm{Tr}_\Lambda^{\Box_A} \log\left(\frac{-\Box_A + m^2}{\Lambda_0^2}\right) := \mathrm{Tr}\left\{P_\Lambda(\Box_A)\log\left(\frac{-\Box_A + m^2}{\Lambda_0^2}\right)\right\}$$

is defined using the spectral projections $P_\Lambda(\Box_A) := \theta(\Lambda^2-\Box_A)$ of $\Box_A$, where θ denotes the Heaviside step function that is zero for negative arguments and equal to 1 otherwise. It turns out that $\widetilde{S}_\Lambda(A)$ has an asymptotic expansion as

$$\widetilde{S}_\Lambda(A) = \tilde{c}_2(A)\Lambda^2 + \tilde{c}_1(A)\Lambda + \tilde{c}_{\log}(A)\log\Lambda + \cdots . \tag{30}$$

The dots indicate terms that are finite in the large Λ limit.

In this section we want to compare the coefficient $\tilde{c}_{\log}(A)$ of the logarithmically divergent part in the above expression to the coefficient $c_{\log}(A)$ computed earlier.

A short calculation reveals how to proceed,

$$\begin{aligned}
&\mathrm{Tr}_\Lambda^{\Box_A} \log\frac{-\Box_A + m^2}{\Lambda_0^2} - \mathrm{Tr}_\Lambda^{\Box_0} \log\frac{-\Box_0 + m^2}{\Lambda_0^2} \\
&\quad= \mathrm{Tr}_\Lambda^{\Box_0}\left(\log\frac{-\Box_A + m^2}{\Lambda_0^2} - \log\frac{-\Box_0 + m^2}{\Lambda_0^2}\right) + (\mathrm{Tr}_\Lambda^{\Box_A} - \mathrm{Tr}_\Lambda^{\Box_0})\left(\log\frac{-\Box_A + m^2}{\Lambda_0^2} - \log\frac{-\Box_0 + m^2}{\Lambda_0^2}\right) \\
&\qquad+ (\mathrm{Tr}_\Lambda^{\Box_A} - \mathrm{Tr}_\Lambda^{\Box_0})\log\frac{-\Box_0 + m^2}{\Lambda_0^2}.
\end{aligned} \tag{31}$$

Obviously, the coefficient $\tilde{c}_{\log}(A)$ receives contributions from three different terms, only the first of which is given by $c_{\log}(A)$. From the calculation of the pertinent part in the third term, it will be apparent that the second one in fact does not contribute to $\tilde{c}_{\log}(A)$. For the computation of the third term in (31), however, we must introduce an additional regulator that deals with the noncompactness of $\mathbb{R}^4$. Let f be a smooth, compactly supported function on $\mathbb{R}^4$, interpreted as a multiplication operator on $\mathcal{H}$. Then

$$\mathrm{Tr}\left\{ f\theta(\Lambda^2+\Box_A)\log\frac{-\Box_0+m^2}{\Lambda_0^2}\right\}=\int_{\mathbb{R}^4}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_{\mathbb{R}^4}f(x)\sigma[\theta(\Lambda^2+\Box_A)]\sigma\left[\log\frac{-\Box_0+m^2}{\Lambda_0^2}\right]+\cdots . \tag{32}$$

The dots indicate contributions from the star product of symbols that are uniformly bounded in Λ. Use has been made of the fact that f and $\sigma[\log(-\Box_0+m^2)/\Lambda_0^2]$ are independent of p and x, respectively.

As a next step, we need to derive an asymptotic expansion for the symbol of the theta function. We start with the following sum expression for a smooth approximation of the Heaviside θ function (Ref. 9, p. 248, etc.):

$$\theta_\epsilon(x)=\frac{1}{\epsilon}\sum_{r=-\infty}^{\infty}\frac{e^{i\omega_r 0^+}}{x+i\omega_r}=\frac{e^{-x0^+}}{e^{-x\epsilon}+1},\quad \omega_r=(2r+1)\pi/\epsilon, \tag{33}$$

for $\epsilon>0$. The step function is regained in the limit $\epsilon\to\infty$. Using this equation, we derive an asymptotic expansion for the symbol of $\theta(\Lambda^2+\Box_A)$ as (for details we refer to the third section of the Appendix)

$$\sigma[\theta_\epsilon(\Lambda^2+\Box_A)]=\frac{1}{2\pi i}\int \mathrm{d}z\, e^{iz\epsilon}\sigma\left[\frac{1}{z-i(\Lambda^2+\Box_A)}\right]\sim\sum_{n=0}^{\infty}\frac{1}{n!}\delta_\epsilon^{(n-1)}(\Lambda^2-p^2)(\Box_A+2ip^\mu D_{A\mu})1.$$

As before, for mnemonic purposes, this asymptotic series can be summarized as

$$\sigma[\theta(\Lambda^2+\Box_A)](x,p)=\theta(\Lambda^2-p^2+\Box_A+2ip^\mu D_{A\mu})1, \tag{34}$$

where the x dependence originates from the external fields A.

Combining our results, we find

$$\begin{aligned}&\mathrm{Tr}\left\{ f\theta(\Lambda^2+\Box_A)\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\right\}-\mathrm{Tr}\left\{ f\theta(\Lambda^2+\Box_0)\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\right\}\\&\quad=\sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{R}^4}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_{\mathbb{R}^4}\mathrm{d}^4x\, f(x)\delta_\epsilon^{(n-1)}(\Lambda^2-p^2)\log\left(\frac{p^2+m^2}{\Lambda_0^2}\right)\mathrm{tr}_N\{(\Box_A+2ip^\mu D_{A\mu})^n1\}.\end{aligned}$$

Obviously, we can now drop the regulator f.

For large Λ, the δ_ϵ-functions cancel the radial p-integration. Therefore, the only contributions to the logarithmically divergent part in the above expression can originate from terms where the derivatives of the δ_ϵ-functions exclusively hit the trace under the integral of the measure d^4p but not the factor $\log[(-\Box_0+m^2)/\Lambda_0^2]$. This is only possible as long as $2(n-1)\leqslant 3+n$ (the derivatives of δ_ϵ count twice because of the p^2 in the argument, and the 3 on the rhs comes from the measure d^4p) and hence $n\leqslant 5$. Moreover, since the angular p-integration over an odd number of factors p^μ gives always zero, the $n=5$ term cannot contribute either.

As shown in the Appendix, we can now expand the powers $(\Box_A+2ip^\mu D_{A\mu})^n1$ for $n\leqslant 4$, perform the angular p-integrations, substitute $p^2\to u$ and use partial integration to get rid of the derivatives of the δ_ϵ-functions. We arrive at

$$
\begin{aligned}
&\mathrm{Tr}_{\Lambda}^{\Box_A}\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)-\mathrm{Tr}_{\Lambda}^{\Box_0}\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\\
&\quad=\frac{1}{16\pi^2}\int_1^\infty du\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\delta_\epsilon(\Lambda^2-u)u(1-1)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\Box_A 1+\frac{1}{16\pi^2}\int_1^\infty du\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\\
&\qquad\times\delta_\epsilon(\Lambda^2-u)\left(\frac{1}{2}-\frac{2}{3}+\frac{1}{6}\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\mathrm{tr}_N\Box_A^2 1+\frac{1}{16\pi^2}\int_1^\infty du\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\delta_\epsilon(\Lambda^2-u)(-\tfrac{1}{3}+\tfrac{1}{6})\\
&\qquad\times\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N D_A^\mu\Box_A D_{A\mu}1+\frac{1}{16\pi^2}\int_1^\infty du\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\frac{1}{6}\delta_\epsilon(\Lambda^2-u)\\
&\qquad\times\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N D_A^\mu D_A^\nu D_{A\mu}D_{A\nu}1+\cdots\\
&\quad=-\frac{1}{96\pi^2}\log\left(\frac{\Lambda^2+m^2}{\Lambda_0^2}\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N D_A^\mu\Box_A D_{A\mu}1\\
&\qquad+\frac{1}{96\pi^2}\log\left(\frac{\Lambda^2+m^2}{\Lambda_0^2}\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N D_A^\mu D_A^\nu D_{A\mu}D_{A\nu}1+\cdots\\
&\quad=-\frac{1}{2}\frac{1}{96\pi^2}\log\left(\frac{\Lambda^2+m^2}{\Lambda_0^2}\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N F^{\mu\nu}F_{\mu\nu}+\cdots,
\end{aligned}
$$

where the dots indicate finite or polynomially divergent contributions.

Finally, we will turn back to the second term in (31). The difference as compared to the previous calculation is that now the symbol of the operator under the traces has an asymptotic expansion that is a power series in $1/p$. Therefore, in contrast to the above, no logarithmically divergent term will occur in a large Λ expansion.

Combining these results with our previous expression for $c_{\log}(A)$, we find

$$
\tilde{c}_{\log}(A)=\frac{1}{2}\frac{1}{96\pi^2}\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N F^{\mu\nu}F_{\mu\nu}=\frac{1}{2}c_{\log}(A). \tag{35}
$$

D. Comparison with heat kernel regularization

In this section we want to compare our results with previous ones in the literature[18,11] obtained by heat kernel techniques. For a given differential operator D, we consider the trace of the heat operator for D,

$$
K(t,f,D)=\mathrm{Tr}(fe^{-tD}),
$$

where the auxiliary smooth function $f(x)$ is introduced to make spatial integrals converge on $\mathbb{R}^n$. We write the effective action for D as

$$
S=-\int_0^\infty\frac{\mathrm{d}t}{t}K(t,f,D).
$$

Here the formula $\log\det(D)=\mathrm{Tr}\log(D)$ has been used again together with the following formal expression for the logarithm:

$$\log \lambda = -\int_0^\infty \frac{dt}{t} e^{-t\lambda},$$

which holds up to an (infinite) integration constant.

There is an asymptotic expansion for the heat trace as $t \to 0$ given by

$$\mathrm{Tr}(f e^{-tD}) \sim \sum_{k \geqslant 0} t^{(k-n)/2} a_k(f,D).$$

Next we define the ζ-function for D as follows:

$$\zeta(s,f,D) = \mathrm{Tr}(f D^{-s}).$$

Writing the ζ-function in terms of the heat trace as

$$\zeta(s,f,D) = \frac{1}{\Gamma(s)} \int_0^\infty dt\, t^{s-1} K(t,f,D),$$

we see that $\Gamma(s)\zeta(s,f,D)$ has simple poles at the points $s=(n-k)/2$ and the complex residue at $s=(n-k)/2$ is given by

$$\mathrm{Res}_{s=(n-k)/2}(\Gamma(s)\zeta(s,f,D)) = a_k(f,D). \tag{36}$$

From the asymptotic expansion of the heat trace and the integral formula for the effective action S we see that the logarithmically divergent part is given when $k=n$ so we are interested in computing the coefficient $a_n(f,(-\Box_A+m^2)/\Lambda_0^2)$. In our case $n=4$.

The first task is to compute the ζ-function for the operator $(-\Box_A+m^2)/\Lambda_0^2$. From the definition of the ζ-function we have

$$\zeta\left(s,f,\frac{-\Box_A+m^2}{\Lambda_0^2}\right) = \int_{\mathbb{R}^4} \frac{d^4p}{(2\pi)^4} \int_{\mathbb{R}^4} d^4x\, \mathrm{tr}_N\, \sigma[f] * \sigma\left[\left(\frac{-\Box_A+m^2}{\Lambda_0^2}\right)^{-s}\right](x,p).$$

We next use the expansion

$$(a+x)^{-s} = \sum_{r=0}^\infty (-1)^r \frac{\Gamma(s+r)}{r!\Gamma(s)} a^{-(r+s)} x^r$$

to write the symbol of $(-\Box_A+m^2)/\Lambda_0^2$ as

$$\sigma\left[\left(\frac{-\Box_A+m^2}{\Lambda_0^2}\right)^{-s}\right] = \left(\frac{p^2+m^2-\Box_A-2ip^\mu D_{A\mu}}{\Lambda_0^2}\right)^{-s}$$
$$\sim \sum_{r=0}^\infty (-1)^r \frac{\Gamma(s+r)}{r!\Gamma(s)} \Lambda_0^{2s} \frac{1}{p^{2(s+r)}} (m^2-\Box_A-2ip^\mu D_{A\mu})^r 1.$$

Splitting the integration in the ζ-function into two parts we then have

$$\zeta\left(s,f,\frac{-\Box_A+m^2}{\Lambda_0^2}\right) = \int_{|p|\leqslant 1} \frac{d^4p}{(2\pi)^4} \int_{\mathbb{R}^4} d^4x\, f(x) \mathrm{tr}_N\, \sigma\left[\left(\frac{-\Box_A+m^2}{\Lambda_0^2}\right)^{-s}\right](x,p)$$
$$+ \sum_{r=0}^\infty \frac{(-1)^r\,\Gamma(s+r)}{r!\Gamma(s)} \Lambda_0^{2s} \int_1^\infty |p|^3 d|p| \frac{1}{p^{2(r+s)}} \int_{S^3} \frac{d\Omega_p}{(2\pi)^4} \int_{\mathbb{R}^4} d^4x\, f(x)$$
$$\times \mathrm{tr}_N (m^2-\Box_A-2ip^\mu D_{A\mu})^r 1. \tag{37}$$

Using the fact that under the angular integration odd powers of p give zero we can write

$$\int_{S^3}\frac{d\Omega_\xi}{(2\pi)^4}\int_{\mathbb{R}^4} d^4x\, f(x)\mathrm{tr}_N(m^2-\Box_A-2ip^\mu D_{A\mu})^r 1=\sum_{k=0}^{[r/2]}(-2i)^{2k}p^{2k}\,\mathrm{d}(f,r,2k)$$

for some functions $\mathrm{d}(f,r,2k)$ of f, $\Box_A$ and $D_{A\mu}$ determined from the expansion of $(m^2-\Box_A-2ip^\mu D_{A\mu})^r$. In particular, we have

$$\mathrm{d}(f,0,0)=\frac{1}{8\pi^2}\int_{\mathbb{R}^4} d^4x\, f(x).$$

We then find

$$\zeta\left(s,f,\frac{-\Box_A+m^2}{\Lambda_0^2}\right)=\chi(s)+\sum_{r=0}^{\infty}\frac{(-1)^r\Lambda_0^{2s}\Gamma(s+r)}{r!\Gamma(s)}\int_1^\infty |p|^3\,\mathrm{d}|p|\frac{1}{p^{2(r+s)}}\sum_{t=0}^{[r/2]}(-2i)^{2t}p^{2t}\,\mathrm{d}(f,r,2t),$$

where $\chi(s)$ denotes the first integral in the rhs of (37), a holomorphic function in s. We can evaluate explicitly the p-integral in the above expression to obtain the following formula for the ζ-function:

$$\zeta\left(s,f,\frac{-\Box_A+m^2}{\Lambda_0^2}\right)=\chi(s)+\frac{\Lambda_0^{2s}}{\Gamma(s)}\sum_{r=0}^{\infty}\sum_{t=0}^{[r/2]}\frac{1}{2}\frac{(-1)^{r+t}4^t\Gamma(s+r)}{r!}\frac{1}{s-(2-r+t)}\mathrm{d}(f,r,2t). \tag{38}$$

There are two parts of the ζ-function contributing to the residue at $s=0$; the gamma function $\Gamma(s+r)$ and the poles of $1/[s-(2-r+t)]$. The first one gives a contribution for $r=0$ and the latter one when $r=2+t$. From the summation we see that $t\leqslant r/2$ so it follows that only the terms with $t\leqslant 2$ contribute to the residue:

$$\begin{aligned}a_4\left(f,\frac{-\Box_A+m^2}{\Lambda_0^2}\right)&=\mathrm{Res}_{s=0}\,\Gamma(s)\zeta\left(s,f,\frac{-\Box_A+m^2}{\Lambda_0^2}\right)\\&=\chi(0)-\frac{1}{4}\mathrm{d}(f,0,0)+\sum_{t=0}^{2}\frac{4^t\Gamma(2+t)}{(2+t)!}\frac{1}{2}\mathrm{d}(f,t+2,2t),\end{aligned}$$

where $\chi(0)$ is given by

$$\chi(0)=\frac{1}{(2\pi)^4}\int_{|p|\leqslant 1}d^4p\int_{\mathbb{R}^4}d^4x\,f(x)=\int_0^1|p|^3\,\mathrm{d}|p|\mathrm{d}(f,0,0)=\frac{1}{4}\mathrm{d}(f,0,0).$$

We have thus obtained the following expression for $a_4(f,(-\Box_A+m^2)/\Lambda_0^2)$:

$$a_4\left(f,\frac{-\Box_A+m^2}{\Lambda_0^2}\right)=\sum_{t=0}^{2}\frac{1}{2}\frac{4^t\Gamma(2+t)}{(2+t)!}\mathrm{d}(f,t+2,2t).$$

We now compute directly the logarithmically divergent part of $S_\Lambda(A)$. For this we need the following formula:

$$\sigma\left[\log\left(\frac{-\Box_A+m^2}{\Lambda_0^2}\right)-\log\left(\frac{-\Box+m^2}{\Lambda_0^2}\right)\right]=\sum_{r=1}^{\infty}\frac{(-1)^{r+1}}{r}\frac{1}{p^{2r}}[(m^2-\Box_A-2ip^\mu D_{A\mu})^r-m^{2r}].$$

Note that for this asymptotic expansion, we have divided the recursion formula (A8) differently.

We split the p-integration in the trace into two parts to get

$$\mathrm{Tr}_\Lambda \log\left(f\left(\frac{-\Box_A+m^2}{\Lambda_0^2}-\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\right)$$
$$= \text{finite terms in } \Lambda + \sum_{r=1}^{\infty}\sum_{t=0}^{[r/2]}\frac{(-1)^{r+1}}{r}\int_1^\Lambda |p|^3\,\mathrm{d}|p|\frac{1}{p^{2(r-t)}}(-1)^t 4^t\,\mathrm{d}(f,r,2t)$$
$$-\sum_{r=1}^{\infty}\frac{(-1)^{r+1}}{r}m^{2r}\int_1^\Lambda |p|^3\,\mathrm{d}|p|\frac{1}{p^{2r}}\mathrm{d}(f,0,0).$$

The logarithmically divergent part is then given by

$$c_{\log}(A) = -\sum_{t=0}^{2}4^t\frac{1}{t+2}\mathrm{d}(f,t+2,2t)+\frac{1}{2}m^4\,\mathrm{d}(f,0,0)$$

so we finally have the result

$$-\frac{1}{2}c_{\log}(A)+\frac{1}{4}m^4\,\mathrm{d}(f,0,0)=a_4(f,(-\Box_A+m^2)/\Lambda_0^2).$$

Remarks: (1) The coefficients $\mathrm{d}(f,r,2k)$ defined below Eq. (37) are given by spatial integrals over the $gl(N)$-trace of certain polyomials in the external fields and their derivatives. They can be easily computed by expanding the power on the left-hand side of the defining formula, using the well-known expressions for the angular p-integration of polynomials in p^μ.

(2) Note that the argument relating a_{-4} and $c_{\log}$ did not use the specific form of the coefficients $\mathrm{d}(f,r,2k)$. Therefore, it can be extended to a larger class of operators.

(3) Combining Eqs. (36) and (38), we have a formula for the calculation of the coefficients a_k at hand. In particular, evaluating the function $\chi(s)$ for negative integer s amounts to the computation of the symbol of $(-\Box_A+m^2)^l$ for positive integer powers of l. The latter can be obtained from the formula

$$\sigma[(-\Box_A+m^2)^{l+1}]=(p^2+m^2-\Box_A-2ip_\mu D_A^\mu)\sigma[(-\Box_A+m^2)^l]$$

and the symbol of $-\Box_A+m^2$.

V. GENERALIZATION TO THE MOYAL PLANE

A. The Moyal plane $\mathbb{R}^4_\theta$: generalities

In this section, we want to replace the manifold $\mathbb{R}^4$ by the four-dimensional Moyal plane $\mathbb{R}^4_\theta$, an example of a noncommutative manifold.

For the definition of the latter, one must specify (among other things; see Ref. 3 for the general theory, Ref. 10 for the treatment of the Moyal plane in this context) a (noncommutative) associative algebra $\mathcal{A}$, the elements of which generalize the notion of (smooth) functions on an ordinary manifold. In the case of the 4D Moyal plane, the algebra $\mathcal{A}$ is taken to include the rapidly decaying Schwartz test functions on $\mathbb{R}^4$, while the product of two such elements f, g is given by the integral formula

$$(f\star g)(x)=\frac{1}{(2\pi)^4}\int_{\mathbb{R}^4}\int_{\mathbb{R}^4}\mathrm{d}^4y\,\mathrm{d}^4\xi\,e^{i\xi(x-y)}f(x-\tfrac{1}{2}\Theta\xi)g(y), \tag{39}$$

where Θ is a 4×4 matrix defined by

$$\Theta=\theta\begin{pmatrix}0 & \mathbb{1}_2\\ -\mathbb{1}_2 & 0\end{pmatrix} \tag{40}$$

for the real parameter θ.

The elements of $\mathcal{A}$ act on the Hilbert space $L^2(\mathbb{R}^4)$ by left $\star$-multiplication (see Ref. 8 for an extension of the above formula to distributions). For an element $f \in \mathcal{A}$, we will write the corresponding operator on $L^2(\mathbb{R}^4)$ as $f\star$. From the integral formula (39) of $\star$, we can see that $f\star$ is a ΨDO with the symbol

$$\sigma[f\star\,](x,p) = f(x - \tfrac{1}{2}\Theta p). \tag{41}$$

Note that the asymptotic behavior of f is transferred to the p dependence of the symbol of $f\star$. In particular, for rapidly decaying f, $f\star$ is infinitely smoothing.[10]

A natural class of functions suitable for the Moyal product is the set $\mathcal{P}$ of infinitely differentiable functions f on $\mathbb{R}^4$ such that, for a real number s and for every multi-index α,

$$|(\partial_x^\alpha f)(x)| \leqslant C_\alpha (1 + x^2)^{(s-|\alpha|)/2}, \tag{42}$$

s is called the *order* of f. For $f, g \in \mathcal{P}$ and of order s_1, s_2, respectively, $f\star g$ is again in $\mathcal{P}$ and of order $s_1 + s_2$ (Ref. 12, Sect. 7).

B. Calculation of the logarithmically divergent part

With the commutative product of functions on $\mathbb{R}^4$ replaced by the Moyal product $\star$, Eq. (39), we are led to study the following variant of the Klein–Gordon operator

$$\Box_A^\theta \psi = \partial^\mu \partial_\mu \psi + ie(\partial^\mu A_\mu) \star \psi + 2ieA^\mu \star \partial_\mu \psi - e^2 A^\mu \star A_\mu \star \psi$$

for any rapidly decaying smooth function ψ in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^4) \otimes \mathbb{C}^N_{\text{color}}$. Here, the matrix valued Yang–Mills fields A_μ are taken to be in the set $\mathcal{P}$ above with order strictly smaller than -4, i.e., to satisfy (42) with $s < -4$.

We will also need the operator $D_{A\mu}^\theta$, defined by

$$D_{A\mu}^\theta \psi = \partial_\mu \psi + ieA_\mu \star \psi, \quad \psi \in \mathcal{S}(\mathbb{R}^4).$$

In analogy with the first section, we consider the cutoff regularized determinant of $(-\Box_A^\theta + m^2)/\Lambda_0^2$,

$$S_\Lambda^\theta(A) := \mathrm{Tr}_\Lambda \left\{ \log \frac{-\Box_A^\theta + m^2}{\Lambda_0^2} - \log \frac{-\Box_0 + m^2}{\Lambda_0^2} \right\}.$$

As before, the trace will be computed from the symbol of $\log[(-\Box_A^\theta + m^2)/\Lambda_0^2]$. For the latter, we will need an expression for the symbol of the resolvent of $\Box_A^\theta$. Again, this will be obtained via a recursion relation.

As explained in the Appendix, we find for $c_1, c_2 \in \mathbb{C}$, $c_1 \cdot c_2 < 0$ or $c_2 = 0$,

$$\sigma[(c_1 + c_2\Box_A^\theta)^{-1}](x,p) = \frac{1}{c_1 - c_2 p^2} - \frac{c_2}{c_1 - c_2 p^2}(\Box^\theta_{A(\cdot - (1/2)\Theta p)} + 2ip^\mu D^\theta_{A(\cdot-(1/2)\Theta p)})\sigma[(c_1 + c_2\Box_A^\theta)^{-1}] \times (x,p),$$

where $A\big(\cdot - \frac{1}{2}\Theta p\big)$ is a short-hand notation for the external fields A_μ shifted by $-\frac{1}{2}\Theta p$ in their argument, $A\big(\cdot - \frac{1}{2}\Theta p\big)(x) = A\big(x - \frac{1}{2}\Theta p\big)$. In the derivation of the recursion relation, we have used the identity[13]

$$e^{ip(x-y)} f(x) = [f(\cdot + \tfrac{1}{2}\theta) \star e^{ip(\cdot - y)}](x)$$

and associativity of the Moyal product.

From the recursion relation, one readily obtains the formal expression

$$\sigma[(c_1+c_2\Box_A^\theta)^{-1}](x,p)\sim\sum_{n=0}^{\infty}\frac{(-1)^n}{(c_1-c_2p^2)^{n+1}}(\Box^\theta_{A(\cdot-(1/2)\Theta p)}+2ip^\mu D^\theta_{A(\cdot-(1/2)\Theta p)})^n 1.$$

A thorough investigation reveals, however, that an interpretation of this equation as an asymptotic expansion in p would be misleading: The p dependence through the arguments of the external fields $A_\mu\left(x-\frac{1}{2}\Theta p\right)$ is superficial in that it goes away under the spatial integral. Therefore, one must develop different tools to tackle the situation. As shown in the Appendix, the operator R_N defined by the sum of the first N terms in the above series, for N sufficiently large, differs from the operator $(c_1+c_2\Box_A^\theta)^{-1}$ by a trace-class operator only. Hence, for the singular behavior of the cutoff regularized trace, it suffices to consider this operator R_N.

Inserting the expression for the symbol of R_N into the integral formula for the logarithm, Eq. (22), we find

$$S^\theta_\Lambda(A)=-\sum_{n=1}^{N}\int_{|p|\leqslant\Lambda}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_0^1\frac{\mathrm{d}s}{s}\frac{s^{n-1}}{\left(1+s\left(\frac{p^2+m^2}{\Lambda_0^2}-1\right)\right)^{n+1}}\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N(\Box^\theta_{A(\cdot-(1/2)\Theta p)}$$
$$+2ip^\mu D^\theta_{A(\cdot-(1/2)\Theta p),\mu})^n 1+\text{terms finite in }\Lambda.$$

Now, for every term in the sum, we can shift the x-integration by $-\frac{1}{2}\Theta p$. After this substitution the contribution to the Λ-behavior is apparent: It is only the first four terms that can contribute to $c^\theta_{\log}(A)$. Moreover, the resulting expression differs from the corresponding $S_\Lambda(A)$, Eq. (25), solely in the appearance of the product $\star$ in place of the commutative product. As the replacement of the latter by the Moyal product does not affect the asymptotic behavior in the variable p, we conclude

$$c^\theta_{\log}(A)=\frac{e^2}{96\pi^2}\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N F^{\theta,\mu\nu}\star F^\theta_{\mu\nu},\tag{43}$$

where $F^\theta_{\mu\nu}$ is defined by

$$F^\theta_{\mu\nu}=-ie[D^\theta_{A\mu},D^\theta_{A\nu}].$$

This proves the claim of Proposition II.2.

VI. CONCLUSION

In the first part of our paper, we considered the regularized determinant of the Klein–Gordon operator $\Box_A$ with minimal coupling on $\mathbb{R}^4$. For the regularization, we restricted the Hilbert space trace to run over states of momentum below some cutoff Λ.

Although similar results have been obtained before, we choose to present here an approach that consistently uses the pseudodifferential operator methods to prepare the ground for calculations on a particular noncommutative manifold.

A useful formula for the calculations with symbols of pseudodifferential operators (ΨDO) is given by

$$\sigma[f(\Box_A)](x,p)=f(-p^2+\Box_A+2ip^\mu D_{A\mu})1\tag{44}$$

for any function f of the Klein–Gordon operator $\Box_A$. This formula originates from a recursion relation for the symbol $\sigma[f(\Box_A)]$. It is to be understood as defining an asymptotic expansion of the symbol for large p.

Using this asymptotic expansion we could indeed confirm that the cutoff regularized trace does have an asymptotic expansion in the cutoff Λ as in Eq. (5). Although our approach did not use a manifestly gauge invariant regularization, the term scaling like $\log\Lambda$ in the regularized trace of the logarithm of the massive Klein–Gordon operator was found to be gauge invariant. However, the numerical coefficient in front of this expression differs from that obtained via manifestly gauge

invariant methods[4,11] by a factor of −2, see Eqs. (12) and (14). This difference can be verified through a comparison of our approach to heat kernel regularization. It turns out that this argument does not rely on the particular structure of the operator $\Box_A$, cf. the use of the functions $\mathrm{d}(f,r,2t)$ in Sec. IV D, so we expect it to hold even for more general operators as well. It would be interesting to understand this feature in more detail. Also, we propose a gauge invariant version of the cutoff regularization, Eq. (10), which reproduces the result of Refs. 4 and 11.

Recently, zeta functions have been found to show a pole structure on noncommutative torus[7] that differs from the commutative case. It would be interesting to see a similar effect for the Moyal plane by means of the development in Sec. IV D.

In the second and main part of our work, we considered the generalized Klein–Gordon operator for minimally coupled bosons on the four-dimensional Moyal plane, a particular example for a noncommutative geometry. The difference to the previous case is that now the external Yang–Mills fields act on wave functions by the noncommutative Moyal multiplication. This leads in a natural way to the generalized Klein–Gordon operator $\Box_A^\theta$. As it turns out, the machinery of ΨDOs is still applicable, with (44) generalizing to

$$\sigma[f(\Box_A^\theta)](x,p) = f(-p^2 + \Box^\theta_{A(\cdot-(1/2)\Theta p)} + 2ip^\mu D^\theta_{A(\cdot-(1/2)\Theta p)\mu})1. \tag{45}$$

Here, $A\left(\cdot-\frac{1}{2}\Theta p\right)$ denotes the external fields A shifted by the amount $\frac{1}{2}\Theta p$.

From this formula, one might think that the new p-dependence in the external fields leads to an improvement in the decay properties of the symbol for large p. This point of view is however misleading when one wants to draw conclusions for the asymptotic expansion of the regularized trace: By a change of variables, the p-dependence in the external fields disappears under the spatial integral of the trace. This fact comes solely from the noncompactness of $\mathbb{R}^4$. It may be viewed as another manifestation of the UV/IR mixing. A similar effect can be seen for instance in the example of an infinitely smoothing operator on $\mathbb{R}$ that has a nonvanishing trace, see the end of the fourth section of the Appendix. Therefore, on noncompact manifolds (commutative or noncommutative), arguments linking the asymptotic expansion of the regularized trace of an operator to the expansion of its symbol must be taken with caution. For our case, we propose to use the asymptotic expansion in p of the shifted symbol

$$\sigma[f(\Box_A^\theta)](x+\tfrac{1}{2}\Theta p,p)$$

instead. This proposal is justified rigorously by operator theoretic arguments which show that the difference between the original operator and a certain truncation of the asymptotic expansion of the above shifted symbol is trace-class. Hence, it does not contribute to the divergent part of the regularized trace and we can safely exchange the full symbol by its truncation. This argument can even be extended to the commutative case, thereby proving that the coefficient of the $\log\Lambda$ part of the regularized trace is indeed given by the (noncompact) Wodzicki residue. The latter observation now can be used to explain why the expression for $c_{\log}$ is a gauge invariant quantity: Since a gauge transformation conjugates the Klein–Gordon operator by some unitary operator, the fact that $c_{\log}$ is gauge invariant is equivalent to the vanishing of the Wodzicki residue on commutators.

To conclude, we have seen that the methods of ΨDOs are a powerful tool for the investigation of the case studied here, yet they need to be modified in the described way for the case of the noncommutative Moyal plane. It would be interesting to see what modifications are necessary to study the coupling of gravity to the bosons through a varying metric in $\Box_A$. This is presently under investigation.

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APPENDIX: DETAILS OF THE COMPUTATIONS

Computation of $c_{\log}(A)$

We are using the following convention for the Klein–Gordon operator:

$$\begin{aligned}\Box_A = D_A^\mu D_{A\mu} = (\partial^\mu + ieA^\mu)(\partial_\mu + ieA_\mu) &= \partial^\mu\partial_\mu + ie\partial^\mu A_\mu + 2ieA_\mu\partial^\mu - e^2A^\mu A_\mu \\ &= \Box_0 + ie\partial^\mu A_\mu + 2ieA_\mu - e^2A^\mu A_\mu. \end{aligned} \tag{A1}$$

Recall the definition of the symbol $\sigma[a]$ of a pseudodifferential operator a:

$$(af)(x) = \int_{\mathbb{R}^4} \frac{\mathrm{d}^4p}{(2\pi)^4} \int_{\mathbb{R}^4} \mathrm{d}^4y\, e^{ip\cdot(x-y)}\sigma[a](p,x)f(y). \tag{A2}$$

In the computation we need the symbol of the resolvent of the Klein–Gordon operator, i.e., of the operator $(c_1I+c_2\Box_A)^{-1}$. To determine an asymptotic expansion for this symbol we start with the following expression:

$$\begin{aligned}(c_1I + c_2\Box_A)af(x) &= c_1I + c_2(\partial^\mu\partial_\mu + ie\partial^\mu A_\mu + 2ieA_\mu\partial^\mu - e^2A^\mu A_\mu) \\ &\quad\times \int_{\mathbb{R}^4} \frac{\mathrm{d}^4p}{(2\pi)^4} \int_{\mathbb{R}^4} \mathrm{d}^4y\, e^{ip\cdot(x-y)}\sigma[a](p,x)f(y) \\ &= \int_{\mathbb{R}^4} \frac{\mathrm{d}^4p}{(2\pi)^4} \int_{\mathbb{R}^4} \mathrm{d}^4y\, e^{ip\cdot(x-y)}(c_1I + c_2(-p^2 - 2eA_\mu p^\mu + \partial^\mu\partial_\mu \\ &\quad + ie\partial^\mu A_\mu + 2ieA_\mu\partial^\mu + 2ip_\mu\partial^\mu - e^2A^\mu A_\mu))\sigma[a](p,x)f(y). \end{aligned} \tag{A3}$$

Next replacing a by $(c_1I+c_2\Box_A)^{-1}a$ we get

$$\begin{aligned}(c_1I + c_2\Box_A)(c_1I + c_2\Box_A)^{-1}af(x) = af(x) &= \int_{\mathbb{R}^4} \frac{\mathrm{d}^4p}{(2\pi)^4} \int_{\mathbb{R}^4} \mathrm{d}^4y\, e^{ip\cdot(x-y)}(c_1I + c_2(-p^2 - 2eA_\mu p^\mu \\ &\quad + \partial^\mu\partial_\mu + ie\partial^\mu A_\mu + 2ieA_\mu\partial^\mu + 2ip_\mu\partial^\mu - e^2A^\mu A_\mu)) \\ &\quad\times\sigma[(c_1I + c_2\Box_A)^{-1}a](p,x)f(y) \\ &= \int_{\mathbb{R}^4} \frac{\mathrm{d}^4p}{(2\pi)^4} \int_{\mathbb{R}^4} \mathrm{d}^4y\, e^{ip\cdot(x-y)}\sigma[a](p,x)f(y). \end{aligned} \tag{A4}$$

So we have

$$\begin{aligned}&(c_1I + c_2(-p^2 - 2eA_\mu p^\mu + \partial^\mu\partial_\mu + ie\partial^\mu A_\mu + 2ieA_\mu\partial^\mu - e^2A^\mu A_\mu + 2ip_\mu\partial^\mu))\sigma[(c_1I + c_2\Box_A)^{-1}a](p,x) \\ &\quad = \sigma[a](p,x) \end{aligned} \tag{A5}$$

which can be written as

$$(c_1 I - c_2 p^2)\sigma[(c_1 I + c_2 \Box_A)^{-1} a](p,x) + c_2(\Box_A + 2ip_\mu D_A^\mu)\sigma[(c_1 I + c_2 \Box_A)^{-1} a](p,x) = \sigma[a](p,x), \tag{A6}$$

giving us the recursive relation

$$\sigma[(c_1 I + c_2 \Box_A)^{-1} a](p,x) = \frac{1}{c_1 - c_2 p^2}\sigma[a](p,x) - \frac{c_2}{c_1 - c_2 p^2}(\Box_A + 2ip_\mu D_A^\mu)\sigma[(c_1 I + c_2 \Box_A)^{-1} a](p,x). \tag{A7}$$

We can now get the desired asymptotic expansion by setting $a=1, \sigma[a]=1$,

$$\sigma[(c_1 I + c_2 \Box_A)^{-1}](p,x) \sim \sum_{n=0}^{\infty} \frac{(-1)^n c_2^n}{(c_1 - c_2 p^2)^{n+1}}(\Box_A + 2ip_\mu D_A^\mu)^n 1. \tag{A8}$$

Next we evaluate explicitly the terms contributing to the logarithmically diverging part in the expansion (25) of the effective action. When taking the angular integrals the following formulas are used:

$$\langle p^\mu p^\nu \rangle = \tfrac{1}{4} p^2 \eta^{\mu\nu},$$

$$\langle p^{\mu_1} p^{\mu_2} p^{\mu_3} p^{\mu_4} \rangle = \tfrac{1}{24} p^4 (\eta^{\mu_1\mu_2}\eta^{\mu_3\mu_4} + \eta^{\mu_1\mu_3}\eta^{\mu_2\mu_4} + \eta^{\mu_1\mu_4}\eta^{\mu_2\mu_3}),$$

where the brackets denote integration over the unit sphere in $\mathbb{R}^4$, that is

$$\langle f(p) \rangle := \frac{1}{2\pi^2}\int_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\delta(|p|-1) f(p). \tag{A9}$$

Also the angular integral over an odd number of components p^μ is zero. The s-integrals in the expansion can be evaluated exactly using the formula

$$\int_0^1 \mathrm{d}s \frac{s^{n-1}}{(1+sa)^{n+1}} = \frac{1}{n(1+a)^n} \tag{A10}$$

which holds for $\mathfrak{Re}\, a > 0$. The effective action can now be written as

$$\begin{aligned} &\mathrm{Tr}_\Lambda\left(\log\left(\frac{-\Box_A + m^2}{\Lambda_0^2}\right) - \log\left(\frac{-\Box_0 + m^2}{\Lambda_0^2}\right)\right) \\ &\quad = -\frac{1}{(2\pi)^4}\sum_{n=1}^{\infty}\int_1^\Lambda \mathrm{d}|p||p|^3 \frac{1}{n(p^2+m^2)^n}\int_{\mathbb{R}^4}\mathrm{d}^4 x \int_{S^3}\mathrm{d}\Omega_p \mathrm{tr}_N(\Box_A + 2ip_\mu D_A^\mu)^n 1 + \text{const}, \end{aligned} \tag{A11}$$

where the constant (in Λ) term arises from the integration of the symbol over the region $|p| \leqslant 1$ for which the asymptotic expansion is not valid.

When expanding the integrand in terms of p, the leading term is of the order p^{3-2n} times a term of order at most p^n coming from the angular integration—so the highest order term is of order p^{3-n}. For the terms contributing to logarithmic divergences of the effective action the leading order must be larger than or equal to -1, so the relevant terms in the expansion above are terms of order up to four. To find the parts contributing to the logarithmic divergence we derivate the terms in (A11) with respect to Λ and then pick the terms proportional to $1/\Lambda$. We denote by I_n the nth term in the expansion. Writing the expansions of the first four terms explicitly we then have

$$\frac{\partial I_1}{\partial \Lambda} = -\frac{1}{8\pi^2}\frac{\Lambda^3}{\Lambda_0^2}\frac{\Lambda_0^2}{\Lambda^2+m^2}\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}_N \Box_A 1 = \frac{1}{8\pi^2}\left(\Lambda - m^2\frac{1}{\Lambda} + O\left(\frac{1}{\Lambda^3}\right)\right)\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}_N \Box_A 1,$$

$$\begin{aligned}\frac{\partial I_2}{\partial \Lambda} &= -\frac{1}{8\pi^2}\frac{\Lambda^3}{2(\Lambda^2+m^2)^2}\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}_N \Box_A^2 1 - \frac{1}{8\pi^2}\frac{\Lambda^5}{(\Lambda^2+m^2)^2}\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}_N \Box_A 1 \\ &= -\frac{1}{8\pi^2}\frac{1}{2\Lambda}\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}_N \Box_A^2 1 + \cdots + \frac{1}{8\pi^2}m^2\frac{1}{\Lambda}\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}_N \Box_A 1 + \cdots,\end{aligned}$$

$$\begin{aligned}\frac{\partial I_3}{\partial \Lambda} &= -\frac{1}{8\pi^2}\frac{\Lambda^3}{3(\Lambda^2+m^2)^3}\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{Tr}_N \Box_A^3 + \frac{1}{4\pi^2}\frac{\Lambda^5}{3(\Lambda^2+m^2)^3}\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}_N \Box_A^2 \\ &\quad + \frac{1}{8\pi^2}\frac{\Lambda^5}{3(\Lambda^2+m^2)^3}\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}_N (D_A^\mu \Box_A D_{A\mu}) \\ &= -\frac{1}{8\pi^2}O\left(\frac{1}{\Lambda^3}\right) + \cdots + \frac{1}{4\pi^2}\frac{1}{3\Lambda}\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}_N \Box_A^2 + \cdots + \frac{1}{8\pi^2}\frac{1}{3\Lambda}\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}_N (D_A^\mu \Box_A D_{A\mu}),\end{aligned}$$

$$\begin{aligned}\frac{\partial I_4}{\partial \Lambda} &= -\frac{1}{8\pi^2}\frac{\Lambda^3}{4(\Lambda^2+m^2)^4}\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}_N\Big(\Box_A^4 - \Lambda^2(3\Box_A^3 + \Box_A D_A^\mu \Box_A D_{A\mu} + D_{A\mu}\Box_A^2 D_{A\mu}) + \frac{2}{3}\Lambda^4(\Box_A^2 \\ &\quad + D_A^\nu D_A^\mu D_{A\nu} D_{A\mu} + D_A^\mu \Box_A D_{A\mu})\Big) \\ &= -\frac{1}{8\pi^2}\frac{2}{3}\frac{1}{4\Lambda}\int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}_N(\Box_A^2 + D_A^\nu D_A^\mu D_{A\nu} D_{A\mu} + D_A^\mu \Box_A D_{A\mu}) + \cdots.\end{aligned}$$

Comparison with fermion calculations

We now compute the traces of the relevant terms in the identity

$$\begin{aligned}\log(-\mathbb{1}_4(\Box_A + m^2) - ie\sigma\cdot F) &= \log\left(\frac{\mathbb{1}_4(-\Box_A + m^2)}{\Lambda_0^2}\right) + \log\left(\mathbb{1}_4 - \frac{ie}{-\Box_A + m^2}\sigma\cdot F\right) \\ &\quad + \frac{1}{2}\left[\log\left(\mathbb{1}_4\frac{-\Box_A + m^2}{\Lambda_0^2}\right), \log\left(\mathbb{1}_4 - \frac{ie}{-\Box_A + m^2}\sigma\cdot F\right)\right] \\ &\quad + \frac{1}{12}\left(\left[\log\left(\mathbb{1}_4\frac{-\Box_A + m^2}{\Lambda_0^2}\right), \left[\log\left(\mathbb{1}_4\frac{-\Box_A + m^2}{\Lambda_0^2}\right),\right.\right.\right. \\ &\quad \left.\left.\left.\log\left(\mathbb{1}_4 - \frac{ie}{-\Box_A + m^2}\sigma\cdot F\right)\right]\right] + \left[\log\left(\mathbb{1}_4 - \frac{ie}{-\Box_A + m^2}\sigma\cdot F\right),\right. \\ &\quad \left.\left.\left[\log\left(\mathbb{1}_4 - \frac{ie}{-\Box_A + m^2}\sigma\cdot F\right), \log\left(\mathbb{1}_4\frac{-\Box_A + m^2}{\Lambda_0^2}\right)\right]\right]\right) + O\left(\frac{1}{\Lambda^5}\right).\end{aligned}$$

The commutator terms come from the Baker–Campbell–Hausdorff formula. Terms that fall off at least as $1/\Lambda^5$ have been suppressed. We find

$$\mathrm{Tr}_\Lambda \log\left(\mathbb{1}_4\left(\frac{-\Box_A+m^2}{\Lambda_0^2}\right)\right) = 4\,\mathrm{Tr}_\Lambda \log\left(\frac{-\Box_A+m^2}{\Lambda_0^2}\right),$$

$$\mathrm{Tr}_\Lambda \log\left(\mathbb{1}_4 - \frac{ie}{m^2-\Box_A}\sigma\cdot F\right) = -\int_{|p|\leqslant\Lambda}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_{\mathbb{R}^4}\mathrm{d}^4x\sum_{n=1}^{\infty}\frac{1}{n}\mathrm{tr}\left(\sigma\left[\frac{ie}{-\Box_A+m^2}\right]*\sigma\cdot F\right)^{*n}.$$

Here, $*$ denotes the product of symbols of two ΨDOs which has the asymptotic expansion (20).

Now using the fact that $\mathrm{tr}\,\sigma\cdot F=0$ and the expansion (A8) for $\sigma[1/(c_1+c_2\Box_A)]$, we get

$$\begin{aligned}
&\mathrm{Tr}_\Lambda \log\left(\mathbb{1}_4 - \frac{ie}{m^2-\Box_A}\sigma\cdot F\right)\\
&\quad= -\frac{1}{2}\int_{|p|\leqslant\Lambda}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}\left(\sigma\left[\frac{ie}{-\Box_A+m^2}\right]*\sigma\cdot F*\sigma\left[\frac{ie}{-\Box_A+m^2}\right]*\sigma\cdot F\right)+O\left(\frac{1}{\Lambda^5}\right)\\
&\quad= \frac{1}{2}\int_{|p|\leqslant\Lambda}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_{\mathbb{R}^4}\mathrm{d}^4x\frac{e^2}{(p^2+m^2)^2}\,\mathrm{tr}\,\sigma\cdot F^2+O\left(\frac{1}{\Lambda^5}\right)\\
&\quad= \frac{e^2}{16\pi^2}\log\Lambda\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}\,\sigma\cdot F^2+O(\Lambda^0).
\end{aligned}$$

This provides the results needed in the main text, since, as will be shown below, there are no contributions to the divergent part of the trace that come from the commutator terms. For this, we expand the logarithm in the first commutator term above which gives us

$$\begin{aligned}
&\frac{1}{2}\,\mathrm{Tr}_\Lambda\left[\log\left(\mathbb{1}_4\frac{-\Box_A+m^2}{\Lambda_0^2}\right),\log\left(\mathbb{1}_4-\frac{ie}{-\Box_A+m^2}\sigma\cdot F\right)\right]\\
&\quad=\frac{1}{2}\,\mathrm{Tr}_\Lambda\left[\log\left(\mathbb{1}_4\frac{-\Box_A+m^2}{\Lambda_0^2}\right),\frac{-ie}{-\Box_A+m^2}\sigma\cdot F\right]+\frac{1}{2}\,\mathrm{Tr}_\Lambda\left[\log\left(\mathbb{1}_4\frac{(-\Box_A+m^2)}{\Lambda_0^2}\right),\right.\\
&\qquad\left.-\frac{1}{2}\left(\frac{ie}{-\Box_A+m^2}\sigma\cdot F\right)^2\right]+O\left(\frac{1}{\Lambda^7}\right).
\end{aligned}$$

The first term on the rhs is zero, so we have

$$\begin{aligned}
&\frac{1}{2}\,\mathrm{Tr}_\Lambda\left[\log\left(\frac{\mathbb{1}_4(-\Box_A+m^2)}{\Lambda_0^2}\right),\log\left(\mathbb{1}_4-\frac{ie}{-\Box_A+m^2}\sigma\cdot F\right)\right]\\
&\quad=\frac{1}{4}e^2\,\mathrm{Tr}_\Lambda\left[\log\left(\frac{\mathbb{1}_4(-\Box_A+m^2)}{\Lambda_0^2}\right),\left(\frac{1}{-\Box_A+m^2}\sigma\cdot F\right)^2\right]+O\left(\frac{1}{\Lambda^7}\right).
\end{aligned}$$

Now

$$\begin{aligned}
\sigma\left[\left[\log\left(\mathbb{1}_4\frac{(-\Box_A+m^2)}{\Lambda_0^2}\right),\left(\frac{1}{-\Box_A+m^2}\sigma\cdot F\right)^2\right]\right] &= \left[\log\frac{p^2+m^2}{\Lambda_0^2},\left(\frac{1}{p^2+m^2}\right)^2\sigma\cdot F^2\right]_*+O\left(\frac{1}{\Lambda^6}\right)\\
&= -i\frac{2p^\mu\Lambda_0^2}{p^2+m^2}\left(\frac{1}{p^2+m^2}\right)^2\partial_\mu(\sigma\cdot F^2)+O\left(\frac{1}{\Lambda^6}\right)\\
&= O\left(\frac{1}{\Lambda^5}\right)
\end{aligned}$$

so there is no contribution to the divergent part of the trace.

Next, we turn to the first triple commutator term in the above identity. Counting the powers of p in the pertinent symbols, the leading term should scale like $1/p^4$. However, this term contains a single $\sigma\cdot F$ which gives zero under the trace tr_N. Therefore, one must take one more term in the expansion of

$$\log\left(\mathbb{1}_4 - \frac{ie}{-\Box_A + m^2}\sigma\cdot F\right).$$

The resulting expression then is of order $1/p^6$ and hence can be dropped. Finally the second triple commutator term can be seen to behave as $1/p^6$. In conclusion, we have shown that for the divergent terms of the cutoff regularized trace, all commutator terms can be neglected in the above identity.

Dependence on the regularization scheme

Computation of the symbol of $\theta(\Lambda+\Box_A)$. We start with the following sum expression for the (regularized) θ-function (Ref. 9, p. 248, etc.):

$$\theta_\epsilon(x) = \frac{1}{\epsilon}\sum_{r=-\infty}^{\infty}\frac{e^{i\omega_r 0^+}}{x+i\omega_r} = \frac{e^{-x0^+}}{e^{-x\epsilon}+1}, \quad \omega_r = (2r+1)\pi/\epsilon, \quad \epsilon>0.$$

(This expression is the discretized version of the well-known integral formula

$$\theta(x) = \int_{\mathbb{R}}\frac{\mathrm{d}z}{2\pi i}\frac{e^{iz0^+}}{z-ix}.$$

The latter is regained for $\epsilon\to\infty$.) Differentiation yields

$$\delta_\epsilon^{(n-1)}(x) = \frac{1}{\epsilon}\sum_{r=-\infty}^{\infty}\frac{e^{i\omega_r 0^+}(-1)^n n!}{(x+i\omega_r)^{n+1}}, \quad n=1,2,3,\ldots,$$

for the $(n-1)$th derivative of the (regularized) Dirac δ-function.

Using the above expression, we have

$$\sigma[\theta_\epsilon(\Lambda^2+\Box_A)] = \frac{1}{\epsilon}\sum_{r=-\infty}^{\infty}\sigma\left[\frac{e^{i\omega_r 0^+}}{(\Lambda^2+\Box_A)+i\omega_r}\right].$$

We derived the asymptotic expansion for the symbol of $(c_1 I + c_2\Box_A)^{-1}$ [see Eq. (A8)] to be given by

$$\sigma[(c_1 I + c_2\Box_A)^{-1}](p,x) \sim \sum_{n=0}^{\infty}\frac{(-1)^n c_2^n}{(c_1 - c_2 p^2)^{n+1}}(\Box_A + 2ip_\mu D_A^\mu)^n 1.$$

Using this we get

$$\sigma[\theta_\epsilon(\Lambda+\Box_A)] \sim \frac{1}{\epsilon}\sum_{r=-\infty}^{\infty}\sum_{n=0}^{\infty}\frac{e^{i\omega_r 0^+}(-1)^n}{((\Lambda^2-p^2)+i\omega_r)^{n+1}}(\Box_A + 2ip^\mu D_{A\mu})^n 1.$$

Using the expressions for $\delta_\epsilon^{(n)}$ in the above expansion we finally have

$$\sigma[\theta_\epsilon(\Lambda+\Box_A)] \sim \sum_{n=0}^{\infty}\frac{1}{n!}\delta_\epsilon^{(n-1)}(\Lambda^2-p^2)(\Box_A + 2ip^\mu D_{A\mu})^n 1.$$

Computation of the traces: We can now proceed with the calculation of the trace. From the

remarks in the main section, we know that we can drop the spatial regulator f since terms proportional to the volume of $\mathbb{R}^4$ cancel exactly. We calculate

$$\begin{aligned}
&\mathrm{Tr}_\Lambda^{\Box_A}\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)-\mathrm{Tr}_\Lambda\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\\
&\quad=\sum_{n=0}^{\infty}\frac{1}{n!}\int_{|p|\geqslant 1}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_{\mathbb{R}^4}\mathrm{d}^4x\;\delta_\epsilon^{(n-1)}(\Lambda^2-p^2)\log\left(\frac{p^2+m^2}{\Lambda_0^2}\right)\mathrm{tr}_N(\Box_A+2ip^\mu D_{A\mu})^n 1+\cdots\\
&\qquad-\mathrm{Tr}_\Lambda\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\\
&\quad=\int_{|p|\geqslant 1}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_{R^4}\mathrm{d}^4x\;\theta_\epsilon(\Lambda^2-p^2)\log\left(\frac{p^2+m^2}{\Lambda_0^2}\right)\mathrm{tr}_N 1+\sum_{n=1}^{\infty}\frac{1}{n!}\int_{|p|\geqslant 1}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_{\mathbb{R}^4}\delta_\varepsilon^{(n-1)}(\Lambda^2-p^2)\\
&\qquad\times\log\left(\frac{p^2+m^2}{\Lambda_0^2}\right)\mathrm{tr}_N(\Box_A+2ip^\mu D_{A\mu})^n 1+\cdots-\mathrm{Tr}_\Lambda\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right),
\end{aligned}$$

where the dots indicate terms that are uniformly bounded in Λ. (In particular, we have split the p-integral in a part over the unit ball and an integral over the rest. The former contributes to the finite part.) Now the first term on the right-hand side matches the last one in the limit $\epsilon\to\infty$. As explained in the main text, we are interested in the terms $n\leqslant 5$ of the sum above. Expanding the pertinent terms and performing the angular p-integrals gives

$$\begin{aligned}
&\mathrm{Tr}_\Lambda^{\Box_A}\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)-\mathrm{Tr}_\Lambda\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\\
&\quad=\frac{1}{8\pi^2}\int_1^\infty \mathrm{d}p\;p^3\delta(\Lambda^2-p^2)\log\left(\frac{p^2+m^2}{\Lambda_0^2}\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\;\mathrm{tr}_N\,\Box_A 1+\frac{1}{2}\frac{1}{8\pi^2}\int_1^\infty \mathrm{d}p\;p^3\delta^{(1)}(\Lambda^2-p^2)\\
&\qquad\times\log\left(\frac{p^2+m^2}{\Lambda_0^2}\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\;\mathrm{tr}_N(\Box_A^2-p^2\Box_A)1+\frac{1}{6}\frac{1}{8\pi^2}\int_1^\infty \mathrm{d}p\;p^3\delta^{(2)}(\Lambda^2-p^2)\\
&\qquad\times\log\left(\frac{p^2+m^2}{\Lambda_0^2}\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\;\mathrm{tr}_N(\Box_A^3-p^2(2\Box_A^2+D_{A\mu}\Box_A D_{A\mu}))1\\
&\qquad+\frac{1}{24}\frac{1}{8\pi^2}\int_1^\infty \mathrm{d}p\;p^3\delta^{(3)}(\Lambda^2-p^2)\log\left(\frac{p^2+m^2}{\Lambda_0^2}\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\;\mathrm{tr}_N\big(\Box_A^4-3p^2\Box_A^3\\
&\qquad-p^2\Box_A D_{A\mu}\Box_A D_A^\mu-p^2 D_{A\mu}\Box_A^2 D_{A\mu}-p^2 D_{A\mu}\Box_A D_A^\mu\Box_A+\tfrac{2}{3}p^4(\Box_A^2\\
&\qquad+D_A^\mu D_A^\nu D_{A\mu}D_{A\nu}+D_A^\mu\Box_A D_{A\mu})\big)1+\cdots\ .
\end{aligned}$$

We have also taken the limit $\epsilon\to\infty$, in which δ_ϵ goes over into the Dirac δ-function.

Gathering terms with equal spatial integral we obtain

$$
\begin{aligned}
&\mathrm{Tr}_{\Lambda}^{\Box_A}\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)-\mathrm{Tr}_{\Lambda}^{\Box_0}\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\\
&\quad=\frac{1}{8\pi^2}\int_1^\infty \mathrm{d}p\,\log\left(\frac{p^2+m^2}{\Lambda_0^2}\right)\left(p^3\delta(\Lambda^2-p^2)-\frac{1}{2}p^5\delta^{(1)}(\Lambda^2-p^2)\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,\Box_A 1\\
&\qquad+\frac{1}{8\pi^2}\int_1^\infty \mathrm{d}p\,\log\left(\frac{p^2+m^2}{\Lambda_0^2}\right)\left(\frac{1}{2}p^3\delta^{(1)}(\Lambda^2-p^2)-\frac{1}{3}p^5\delta^{(2)}(\Lambda^2-p^2)\right.\\
&\qquad\left.+\frac{1}{36}p^7\delta^{(3)}(\Lambda^2-p^2)\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,\Box_A^2 1+\frac{1}{8\pi^2}\int_1^\infty \mathrm{d}p\,\log\left(\frac{p^2+m^2}{\Lambda_0^2}\right)\\
&\qquad\times\left(-\frac{1}{6}p^5\delta^{(2)}(\Lambda^2-p^2)+\frac{1}{36}p^7\delta^{(3)}(\Lambda^2-p^2)\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,D_A^\mu\Box_A D_{A\mu}1\\
&\qquad+\frac{1}{8\pi^2}\int_1^\infty \mathrm{d}p\,\log\left(\frac{p^2+m^2}{\Lambda_0^2}\right)\frac{1}{36}p^7\delta^{(3)}(\Lambda^2-p^2)\\
&\qquad\times\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,D_A^\mu D_A^\nu D_{A\mu}D_{A\nu}1+\frac{1}{8\pi^2}\int_1^\infty dp\,\log\left(\frac{p^2+m^2}{\Lambda_0^2}\right)\left(\frac{1}{6}p^3\delta^{(3)}(\Lambda^2-p^2)\right.\\
&\qquad\left.-\frac{1}{8}p^5\delta^{(4)}(\Lambda^2-p^2)\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,\Box_A^3 1+\cdots\ .
\end{aligned}
$$

Next we make a change of variables $p^2=u$ to get

$$
\begin{aligned}
&\mathrm{Tr}_{\Lambda}^{\Box_A}\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)-\mathrm{Tr}_{\Lambda}^{\Box_0}\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\\
&\quad=\frac{1}{8\pi^2}\int_1^\infty \frac{\mathrm{d}u}{2}\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\left(u\delta(\Lambda^2-u)-\frac{1}{2}u^2\delta^{(1)}(\Lambda^2-u)\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,\Box_A 1\\
&\qquad+\frac{1}{8\pi^2}\int_1^\infty \frac{\mathrm{d}u}{2}\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\left(\frac{1}{2}u\delta^{(1)}(\Lambda^2-u)-\frac{1}{3}u^2\delta^{(2)}(\Lambda^2-u)\right.\\
&\qquad\left.+\frac{1}{36}u^3\delta^{(3)}(\Lambda^2-u)\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,\Box_A^2 1+\frac{1}{8\pi^2}\int_1^\infty \frac{\mathrm{d}u}{2}\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\\
&\qquad\times\left(-\frac{1}{6}u^2\delta^{(2)}(\Lambda^2-u)+\frac{1}{36}u^3\delta^{(3)}(\Lambda^2-u)\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,D_A^\mu\Box_A D_{A\mu}1\\
&\qquad+\frac{1}{8\pi^2}\int_1^\infty \frac{\mathrm{d}u}{2}\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\frac{1}{36}u^3\delta^{(3)}(\Lambda^2-u)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,D_A^\mu D_A^\nu D_{A\mu}D_{A\nu}1\\
&\qquad+\frac{1}{8\pi^2}\int_0^\infty \frac{\mathrm{d}u}{2}\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\left(\frac{1}{6}u\delta^{(2)}(\Lambda^2-u)-\frac{1}{8}u^2\delta^{(3)}(\Lambda^2-u)\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,\Box_A^3 1+\cdots\ .
\end{aligned}
$$

Now by integrating by parts and noting that

$$
\frac{\mathrm{d}^k}{\mathrm{d}u^k}\delta(\Lambda^2-u)=(-1)^k\delta^{(k)}(\Lambda^2-u)
$$

we have

$$
\begin{aligned}
&\mathrm{Tr}_{\Lambda}^{\Box_A}\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)-\mathrm{Tr}_{\Lambda}^{\Box_0}\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)\\
&\quad=\frac{1}{16\pi^2}\int_1^\infty \mathrm{d}u\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\delta(\Lambda^2-u)u(1-1)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,\Box_A 1\\
&\qquad+\frac{1}{16\pi^2}\int_1^\infty \mathrm{d}u\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\delta(\Lambda^2-u)\left(\frac{1}{2}-\frac{2}{3}+\frac{1}{6}\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,\Box_A^2 1\\
&\qquad+\frac{1}{16\pi^2}\int_1^\infty du\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\delta(\Lambda^2-u)\left(-\frac{1}{3}+\frac{1}{6}\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,D_A^\mu\Box_A D_{A\mu}1\\
&\qquad+\frac{1}{16\pi^2}\int_1^\infty \mathrm{d}u\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\frac{1}{6}\delta(\Lambda^2-u)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,D_A^\mu D_A^\nu D_{A\mu}D_{A\nu}1+\cdots\\
&\quad=-\frac{1}{16\pi^2}\frac{1}{6}\int_1^\infty \mathrm{d}u\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\delta(\Lambda^2-u)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{Tr}\,D_A^\mu\Box_A D_{A\mu}1+\frac{1}{16\pi^2}\frac{1}{6}\\
&\qquad\times\int_1^\infty \mathrm{d}u\,\log\left(\frac{u+m^2}{\Lambda_0^2}\right)\delta(\Lambda^2-u)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,D_A^\mu D_A^\nu D_{A\mu}D_{A\nu}1+\cdots\\
&\quad=-\frac{1}{96\pi^2}\log\left(\frac{\Lambda^2+m^2}{\Lambda_0^2}\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,D_A^\mu\Box_A D_{A\mu}1\\
&\qquad+\frac{1}{96\pi^2}\log\left(\frac{\Lambda^2+m^2}{\Lambda_0^2}\right)\int_{\mathbb{R}^4}\mathrm{d}^4x\,\mathrm{tr}_N\,D_A^\mu D_A^\nu D_{A\mu}D_{A\nu}1+\cdots\,.
\end{aligned}
$$

Recalling that

$$
\mathrm{tr}_N(D_A^\mu\Box_A D_{A\mu}-D_A^\nu D_A^\mu D_{A\nu}D_{A\mu})=\frac{e^2}{2}\,\mathrm{tr}_N\,F^{\mu\nu}F_{\mu\nu}
$$

we finally get

$$
\mathrm{Tr}_{\Lambda}^{\Box_A}\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)-\mathrm{Tr}_{\Lambda}^{\Box_0}\log\left(\frac{-\Box_0+m^2}{\Lambda_0^2}\right)=-\frac{1}{2}\frac{1}{96\pi^2}\log\frac{\Lambda}{\Lambda_0}\int_{\mathbb{R}^4}\mathrm{tr}_N\,F^{\mu\nu}F_{\mu\nu}+\cdots\,, \tag{A12}
$$

where again the dots indicate terms that are bounded or polynomial in Λ.

Computation on the Moyal plane

General remarks: The symbol of the operator $c_1+c_2\Box_A^\theta$ is given by

$$
\begin{aligned}
\sigma(x,p)&:=\sigma[c_1+c_2\Box_A^\theta](x,p)\\
&=-p^2-2ep^\mu A_\mu(x-\tfrac{1}{2}\Theta p)+ie(\partial^\mu A_\mu)(x-\tfrac{1}{2}\Theta p)-e^2(A^\mu\star A_\mu)(x-\tfrac{1}{2}\Theta p).
\end{aligned}
$$

From this expression, it is clear that one can bound σ from below by a positive constant and from above by a multiple of p^2 for p^2 greater than a certain constant. Furthermore, the derivatives of σ fall off as long as x is confined to some compact set. Therefore, by Ref. 17, corollary 5.1, there is a ΨDO that inverts $(c_1+c_2\Box_A^\theta)$ up to some infinitely smoothing operator.

Derivation of the recursion relation: As in the first section of this appendix, we start with the following identity for σ:

$$\begin{aligned}\psi(x) &= (c_1 + c_2\Box_A^\theta)(c_1 + c_2\Box_A^\theta)^{-1}\psi(x)\\ &= (c_1 + c_2\Box_A^\theta)\int \frac{\mathrm{d}^4p}{(2\pi)^4}\int \mathrm{d}^4y\, e^{ip(x-y)}\sigma(x,p)\psi(y)\\ &= \int \frac{\mathrm{d}^4p}{(2\pi)^4}\int \mathrm{d}^4y(c_1 + c_2(\partial^\mu\partial_\mu + ie(\partial^\mu A_\mu)\star + 2ieA^\mu\star\partial_\mu - e^2A^\mu\star A_\mu\star))(e^{ip(x-y)}\sigma[(c_1\\ &\quad + c_2\Box_A^\theta)^{-1}](x,p))\psi(y).\end{aligned}$$

To continue we need the following formula:

$$e^{ip(x-y)}\sigma(x,p) = [\sigma(\cdot + \tfrac{1}{2}\Theta p,p)\star e^{ip(\cdot-y)}\chi(\cdot)](x),$$

which can be proved as follows. Using the integral expression for the star product,

$$(f\star g)(x) := (2\pi)^{-4}\int\int e^{i\xi(x-y)}f\left(x - \frac{1}{2}\Theta\xi\right)g(y)\mathrm{d}^4y\,\mathrm{d}^4\xi,$$

we have for a Schwartz test function χ

$$\begin{aligned}\left[\sigma\left(\cdot + \frac{1}{2}\Theta p,p\right)\star e^{ip(\cdot-y)}\chi(\cdot)\right](x) &= \frac{1}{(2\pi)^4}\int\int \mathrm{d}^4\xi\,\mathrm{d}^4z\sigma\left(x - \frac{1}{2}\theta\xi + \frac{1}{2}\Theta p,p\right)e^{ip(z-y)}\chi(z)e^{i\xi(x-z)}\\ &= \frac{1}{(2\pi)^4}\int\int \mathrm{d}^4\xi\,\mathrm{d}^4z\sigma\left(x - \frac{1}{2}\theta\xi + \frac{1}{2}\Theta p,p\right)\chi(z)e^{-iz(\xi-p)}e^{i(\xi x-py)}\\ &= \frac{1}{(2\pi)^2}\int \mathrm{d}^4\xi\,\sigma\left(x - \frac{1}{2}\Theta(\xi-p),p\right)\hat{\chi}(\xi-p)e^{i(\xi x-py)}\\ &= e^{ip(x-y)}\frac{1}{(2\pi)^2}\int \mathrm{d}^4\tilde{\xi}\,\sigma\left(x - \frac{1}{2}\Theta\tilde{\xi},p\right)\hat{\chi}(\tilde{\xi})e^{i\tilde{\xi}x}.\end{aligned}$$

Now in the limit $\chi\to 1$, the Fourier transform $\hat{\chi}$ approximates the delta function. Therefore, in this limit, we obtain the claimed identity. Using this formula in the expression for $\psi(x)$ we get

$$\begin{aligned}\psi(x) &= \int\int \frac{\mathrm{d}^4p\,\mathrm{d}^4y}{(2\pi)^4}(c_1 + c_2(\partial^\mu\partial_\mu + ie(\partial^\mu A_\mu)\star + 2ieA^\mu\star\partial_\mu - e^2A^\mu\star A_\mu\star))(\sigma(x,p)e^{ip(x-y)})\psi(y)\\ &= \int\int \frac{\mathrm{d}^4p\,\mathrm{d}^4y}{(2\pi)^4}(c_1 + c_2(\partial^\mu\partial_\mu + ie(\partial^\mu A_\mu)\star + 2ieA^\mu\star\partial_\mu - e^2A^\mu\star A_\mu\star))\\ &\quad\times\left(\sigma\left(\cdot + \frac{1}{2}\Theta p,p\right)\star e^{ip(\cdot-y)}\right)(x)\psi(y)\\ &= \int\int \frac{\mathrm{d}^4p\,\mathrm{d}^4y}{(2\pi)^4}\Bigg[(c_1 + c_2(\Box_0 + 2ip^\mu\partial_\mu - p^2 + ie(\partial^\mu A_\mu)\star - 2ep^\mu A_\mu\star\\ &\quad + 2ieA^\mu\star\partial_\mu - e^2A^\mu\star A_\mu\star))\sigma\left(\cdot + \frac{1}{2}\Theta p,p\right)\Bigg]\star e^{ip(\cdot-y)}(x)\psi(y)\\ &= \int\int \frac{\mathrm{d}^4p\,\mathrm{d}^4y}{(2\pi)^4}(c_1 + c_2p^2 + c_2(\Box^\theta_{A(\cdot-(1/2)\Theta p)} + 2p^\mu D^\theta_{A(\cdot-(1/2)\Theta p),\mu}))\sigma(\cdot,p)e^{ip(x-y)}\psi(y),\end{aligned}$$

which gives us

$$1 = (c_1 - c_2p^2 + c_2(\Box^\theta_{A(\cdot-(1/2)\Theta p)} + 2ip^\mu D^\theta_{A(\cdot-(1/2)\Theta p),\mu}))\sigma[(c_1 + c_2\Box_A^\theta)^{-1}](x,p)$$

or

$$\sigma[(c_1+c_2\Box_A^\theta)^{-1}](x,p)=\frac{1}{c_1-c_2p^2}-\frac{c_2}{c_1-c_2p^2}(\Box^\theta_{A(\cdot-(1/2)\Theta p)}+2ip^\mu D^\theta_{A(\cdot-(1/2)\Theta p)})\sigma[(c_1+c_2\Box_A^\theta)^{-1}]\times(x,p). \tag{A13}$$

Derivation of the asymptotic expansion: We set $R:=(c_1+c_2\Box_A^\theta)^{-1}$. As $-\Box_A^\theta$ is a positive operator, R is bounded for $c_1\cdot c_2<0$. Indeed, from

$$\int_{\mathbb{R}^4}\mathrm{d}^4x\,\overline{\psi}(x)(A\star\varphi)(x)=\int_{\mathbb{R}^4}\mathrm{d}^4x(\overline{\psi}\star A\star\varphi)(x)=\int_{\mathbb{R}^4}\mathrm{d}^4x(\overline{\psi}\star A)(x)\varphi(x),$$

which holds for $\psi,A,\varphi\in L^2(\mathbb{R}^4)$ (Ref. 10, lemma 2.10) and $\overline{\overline{A}\star\psi}=\overline{\psi}\star A$ we conclude

$$\langle\psi,A\star\varphi\rangle=\langle\overline{A}\star\psi,\varphi\rangle$$

and hence $(D^\theta_{A\mu})^\dagger=-D^\theta_{A\mu}$. Therefore,

$$\langle\varphi,-\Box_A^\theta\varphi\rangle=\sum_{\mu=1}^4\langle D^\theta_{A\mu}\varphi,D^\theta_{A\mu}\varphi\rangle\geqslant 0.$$

In our case, we have $c_1=1-s+s(m^2/\Lambda_0^2)$ and $c_2=-s/\Lambda_0^2$ for $0\leqslant s\leqslant 1$ which meets the above requirement of $c_1\cdot c_2<0$ for $0<s\leqslant 1$. For $s=0$, we have $c_2=0$, $c_1\neq 0$, and R is a multiple of the identity.

Next, let R_N be the ΨDO defined by the symbol

$$\sigma[R_N](x,p)=\sum_{n=0}^N\frac{(-c_2)^n}{(c_1-c_2p^2)^{n+1}}(\Box^\theta_{A(\cdot-(1/2)\Theta p)}+2ip^\mu D^\theta_{A(\cdot-(1/2)\Theta p),\mu})^n1.$$

We will show that the difference $R-R_N$ is a trace-class operator.

For this, we first apply $c_1+c_2\Box_A^\theta$ from the left to obtain

$$(c_1+c_2\Box_A^\theta)(R-R_N)=1-(c_1+c_2\Box_A^\theta)R_N.$$

Here, 1 denotes the identity operator. We will compute the symbol of the ΨDO on the right-hand side of this equation. On the level of symbols, multiplication of R_N by $c_1+c_2\Box_A^\theta$ from the left amounts to the application of $c_1+c_2(-p^2+\Box^\theta_{A(\cdot-(1/2)\Theta p)}+2ip^\mu D^\theta_{A(\cdot-(1/2)\Theta p),\mu})$ to $\sigma[R_N]$, cf. the derivation of the recursion relation above. Hence, we find

$$\begin{aligned}\sigma[1-(c_1+c_2\Box_A^\theta)R_N](x,p)&=1-(c_1+c_2(-p^2+\Box^\theta_{A(\cdot-(1/2)\Theta p)}+2ip^\mu D^\theta_{A(\cdot-(1/2)\Theta p),\mu}))\sigma[R_N](x,p)\\&=1-(c_1-c_2p^2)\sigma[R_N]-c_2(\Box^\theta_{A(\cdot-(1/2)\Theta p)}+2ip^\mu D^\theta_{A(\cdot-(1/2)\Theta p),\mu})\sigma[R_N]\\&=-\sum_{n=1}^N\frac{(-c_2)^n}{(c_1-c_2p^2)^n}(\Box^\theta_{A(\cdot-(1/2)\Theta p)}+2ip^\mu D^\theta_{A(\cdot-(1/2)\Theta p),\mu})^n1\\&\quad+\sum_{n=0}^N\frac{(-c_2)^{n+1}}{(c_1-c_2p^2)^{n+1}}(\Box^\theta_{A(\cdot-(1/2)\Theta p)}+2ip^\mu D^\theta_{A(\cdot-(1/2)\Theta p),\mu})^{n+1}1\\&=\frac{(-c_2)^{N+1}}{(c_1-c_2p^2)^{N+1}}(\Box^\theta_{A(\cdot-(1/2)\Theta p)}+2ip^\mu D^\theta_{A(\cdot-(1/2)\Theta p),\mu})^{N+1}1.\end{aligned}$$

Let r_N be defined by the last expression,

$$\sigma[r_N](x,p) := \frac{(-c_2)^{N+1}}{(c_1 - c_2 p^2)^{N+1}} (\Box^{\theta}_{A(\cdot - (1/2)\Theta p)} + 2ip^{\mu} D^{\theta}_{A(\cdot - (1/2)\Theta p),\mu})^{N+1} 1.$$

We will show that r_N is a trace-class operator for sufficiently large N. Expanding the power of operators in the symbol $\sigma[r_N]$ yields terms of the form

$$\text{const} \times \frac{1}{(c_1 - c_2 p^2)^{N+1}} \times f_1 \star \cdots \star f_k \left(x - \frac{1}{2}\Theta p \right),$$

$k = 1, \ldots, 2(N+1)$, the f_i denoting the external fields A_μ or derivatives thereof. [We have used the fact that $(f(\cdot - \frac{1}{2}\Theta p) \star g(\cdot - \frac{1}{2}\Theta p))(x) = (f \star g)(x - \frac{1}{2}\Theta p)$.]

As A_μ is in $\mathcal{P}$ and of order $-2-\epsilon$, Moyal multiplication by it increases the decay property of the x-dependent part by 2. On the other hand, differentiation increases it only by 1. Therefore, the leading term of the above type will be the one where N derivatives of $D^{\theta}_{A(\cdot - (1/2)\Theta p),\mu}$ hit a single A_μ. The resulting term can be bounded from above by

$$\text{const} \times \frac{1}{(1+p^2)^{N+1}} \times (p^2)^{N/2} \times \frac{1}{(1 + (x - \frac{1}{2}\Theta p)^2)^{(4+\epsilon+N)/2}}$$

which is integrable in $x-p$ space for sufficiently large N.

Application from the left of the bounded operator R to r_N does not change the property of being trace-class. On the other hand, we find

$$R r_N = R(c_1 + c_2 \Box^{\theta}_A)(R - R_N) = R - R_N.$$

To summarize, if we are interested in the singular behavior of the cutoff regularized trace of R, we may use the symbol $\sigma[R_N]$ for N sufficiently large in the integral formula of the trace. This amounts to the iteration of the recursion relation (A13) N times.

Remarks: It is easy to see that a blind application of the machinery of ΨDO leads astray. As already mentioned in the main text, the symbol of the operator $f\star$ is given by

$$\sigma[f\star](x,p) = f(x - \tfrac{1}{2}\Theta p).$$

Hence, $f\star$ is an infinitely smoothing operator if f is a Schwartz test function. In other words, the noncommutative Klein–Gordon operator $\Box^{\theta}_A$ differs from the free operator $\Box_0$ by an infinitely smoothing operator,

$$\begin{aligned}\sigma[\Box^{\theta}_A](x,p) &= -p^2 - 2ep^{\mu} A_{\mu}(x - \tfrac{1}{2}\Theta p) + ie(\partial^{\mu} A_{\mu})(x - \tfrac{1}{2}\Theta p) - e^2 (A^{\mu} \star A_{\mu})(x - \tfrac{1}{2}\Theta p) \\ &= \sigma[\Box_0](x,p) + \text{smoothing}.\end{aligned}$$

One might therefore expect that the dependence on the fields A of the resolvent R is in the part that is not seen by an asymptotic expansion in p and hence does not contribute to the divergent behavior of the trace. For ΨDOs on *noncompact* manifolds M this line of reasoning must be taken with caution, since there might be additional divergent terms from the x-integration in the trace integral. This is nicely illustrated by the above computation and the following example. Consider the function

$$f(x,p) = e^{-x^2 e^{-p^2} - (1/4)p^2},$$

where x and p are one-dimensional variables. Clearly

$$|\partial_p^{\alpha} \partial_x^{\beta} f(x,p)| \leqslant C_{K,\alpha,\beta} e^{-(1/4)p^2}, \quad x \in K \subset \mathbb{R} \text{ compact}, \ p \in \mathbb{R},$$

hence f defines an infinitely smoothing operator. On the other hand,

$$\int_{\mathbb{R}} \mathrm{d}x\, f(x,p) = \sqrt{\pi} e^{(1/4)p^2},$$

and the operator f does have a diverging trace. Note that in this example, it is the noncompactness that yields the surprise. We conclude that even in the commutative case, the correspondence between the logarithmically divergent part of the trace and the residue needs some additional justification.

In the above calculation, however, the $p-x$ mixing in the arguments of the fields A_μ—which originates from the noncommutativity of the Moyal plane—makes it impossible to distinguish between the asymptotic p-expansion and an (infinitely smoothing) remainder. There, additional arguments are imperative. Observe, however, that our lines of reasoning above can be taken over to the commutative case, thereby solving the raised objection.

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Variational two-fermion wave equations in quantum electrodynamics: Muoniumlike systems

Andrei G. Terekidi[a] and Jurij W. Darewych[b]
Department of Physics and Astronomy, York University, Toronto, Ontario, Canada M3J 1P3

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We consider a reformulation of quantum electrodynamics in which covariant Green functions are used to solve for the electromagnetic field in terms of the fermion fields. The resulting modified Hamiltonian contains the photon propagator directly. A simple Fock-state variational trial function is used to derive relativistic two-fermion equations variationally from the expectation value of the Hamiltonian of the field theory. The interaction kernel of the equation is shown to be, in essence, the invariant $\mathcal{M}$ matrix in lowest order. Solutions of the two-body equations are presented for muoniumlike systems for small coupling strengths. The results compare well with the observed muonium spectrum, as well as that for hydrogen and muonic hydrogen. Anomalous magnetic moment effects are discussed. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1845602]

I. INTRODUCTION

It has been pointed out in previous publications that various models in quantum field theory (QFT), including quantum electrodynamics (QED), can be reformulated, using mediating-field Green functions, into a form that is particularly convenient for variational calculation.[1,2] This approach was applied to the study of relativistic two-body eigenstates in the scalar Yukawa (Wick–Cutkosky) theory.[3–5] We shall implement such an approach to two-fermion states in QED in this paper.

The Lagrangian of two-fermion fields interacting electromagnetically is ($\hbar=c=1$)

$$\mathcal{L}=\bar{\psi}(x)(i\gamma^{\mu}\partial_{\mu}-m_1-q_1\gamma^{\mu}A_{\mu}(x))\psi(x)+\bar{\phi}(x)(i\gamma^{\mu}\partial_{\mu}-m_2-q_2\gamma^{\mu}A_{\mu}(x))\phi(x)-\tfrac{1}{4}(\partial_{\alpha}A_{\beta}(x)-\partial_{\beta}A_{\alpha}(x))(\partial^{\alpha}A^{\beta}(x)-\partial^{\beta}A^{\alpha}(x)). \tag{1}$$

The corresponding Euler–Lagrange equations of motion are the coupled Dirac–Maxwell equations,

$$(i\gamma^{\mu}\partial_{\mu}-m_1)\psi(x)=q_1\gamma^{\mu}A_{\mu}(x)\psi(x), \tag{2}$$

$$(i\gamma^{\mu}\partial_{\mu}-m_2)\phi(x)=q_2\gamma^{\mu}A_{\mu}(x)\phi(x), \tag{3}$$

and

$$\partial_{\mu}\partial^{\mu}A^{\nu}(x)-\partial^{\nu}\partial_{\mu}A^{\mu}(x)=j^{\nu}(x), \tag{4}$$

where

[a]Electronic mail: terekidi@yorku.ca
[b]Electronic mail: darewych@yorku.ca

$$j^{\nu}(x) = q_1 \overline{\psi}(x) \gamma^{\nu} \psi(x) + q_2 \overline{\phi}(x) \gamma^{\nu} \phi(x). \tag{5}$$

Equations (2)–(4) can be decoupled in part by using the well-known formal solution[6,7] of the Maxwell equation (4), namely

$$A_{\mu}(x) = A^0_{\mu}(x) + \int \mathrm{d}^4x'\, D_{\mu\nu}(x-x') j^{\nu}(x'), \tag{6}$$

where $D_{\mu\nu}(x-x')$ is a Green function (or photon propagator in QFT terminology), defined by

$$\partial_{\alpha}\partial^{\alpha} D_{\mu\nu}(x-x') - \partial_{\mu}\partial^{\alpha} D_{\alpha\nu}(x-x') = g_{\mu\nu}\delta^4(x-x'), \tag{7}$$

and $A^0_{\mu}(x)$ is a solution of the homogeneous (or "free field") equation (4) with $j^{\mu}(x)=0$.

We recall that equation (7) does not define the covariant Green function $D_{\mu\nu}(x-x')$ uniquely. For one thing, one can always add a solution of the homogeneous equation [Eq. (7) with $g_{\mu\nu} \rightarrow 0$]. This allows for a certain freedom in the choice of $D_{\mu\nu}$, as is discussed in standard texts (e.g., Refs. 6 and 7). In practice, the solution of Eq. (7), like that of Eq. (4), requires a choice of gauge. However, we do not need to specify one at this stage.

Substitution of the formal solution (6) into Eqs. (2) and (3) yields the "partly reduced" equations,

$$(i\gamma^{\mu}\partial_{\mu} - m_1)\psi(x) = q_1 \gamma^{\mu}\left(A^0_{\mu}(x) + \int \mathrm{d}^4x'\, D_{\mu\nu}(x-x') j^{\nu}(x') \right)\psi(x), \tag{8}$$

$$(i\gamma^{\mu}\partial_{\mu} - m_2)\phi(x) = q_2 \gamma^{\mu}\left(A^0_{\mu}(x) + \int \mathrm{d}^4x'\, D_{\mu\nu}(x-x') j^{\nu}(x') \right)\phi(x). \tag{9}$$

These are coupled nonlinear Dirac equations. To our knowledge no exact (analytic or numeric) solution of Eqs. (8) and (9) for classical fields have been reported in the literature, though approximate (perturbative) solutions have been discussed by various authors, particularly Barut and co-workers (see Refs. 8 and 9 and citations therein). However, our interest here is in the quantized field theory.

The partially reduced equations (8) and (9) are derivable from the stationary action principle,

$$\delta S[\psi, \phi] = \delta \int \mathrm{d}^4x\, \mathcal{L}_R = 0 \tag{10}$$

with the Lagrangian density

$$\begin{aligned} \mathcal{L}_R = {} & \overline{\psi}(x)(i\gamma^{\mu}\partial_{\mu} - m_1 - q_1\gamma^{\mu}A^0_{\mu}(x))\psi(x) + \overline{\phi}(x)(i\gamma^{\mu}\partial_{\mu} - m_2 - q_2\gamma^{\mu}A^0_{\mu}(x))\phi(x) \\ & - \frac{1}{2}\int \mathrm{d}^4x'\, j^{\mu}(x') D_{\mu\nu}(x-x') j^{\nu}(x) \end{aligned} \tag{11}$$

provided that the Green function is symmetric in the sense that

$$D_{\mu\nu}(x-x') = D_{\mu\nu}(x'-x) \quad \text{and } D_{\mu\nu}(x-x') = D_{\nu\mu}(x-x'). \tag{12}$$

The interaction part of (11) has a somewhat modified structure from that of the usual formulation of QED. Thus, there are two interaction terms. The last term of (11) is a "current–current" interaction which contains the photon propagator sandwiched between the fermionic currents. We shall use this modified formulation together with a variational approach to obtain relativistic few-fermion equations, and to study their bound state solutions.

II. HAMILTONIAN

We shall consider the quantized theory in the equal-time formalism. To this end we write down the Hamiltonian density corresponding to the Lagrangian (11), namely

$$\mathcal{H}_R = \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_{\rm II}, \tag{13}$$

where

$$\mathcal{H}_0 = \psi^\dagger(x)(-i\vec{\alpha}\cdot\nabla + m_1\beta)\psi(x) + \phi^\dagger(x)(-i\vec{\alpha}\cdot\nabla + m_2\beta)\phi(x), \tag{14}$$

$$\mathcal{H}_1 = \frac{1}{2}\int \mathrm{d}^4x'\; j^\mu(x')D_{\mu\nu}(x-x')j^\nu(x), \tag{15}$$

$$\mathcal{H}_{\rm II} = q_1\overline{\psi}(x)\gamma^\mu A^0_\mu(x)\psi(x) + q_2\overline{\phi}(x)\gamma^\mu A^0_\mu(x)\phi(x), \tag{16}$$

and where we have suppressed the kinetic-energy term of the free photon field. We construct a quantized theory by imposing equal-time anticommutation rules for the fermion fields, namely

$$\{\psi_\alpha(\mathbf{x},t),\psi^\dagger_\beta(\mathbf{y},t)\} = \{\phi_\alpha(\mathbf{x},t),\phi^\dagger_\beta(\mathbf{y},t)\} = \delta_{\alpha\beta}\delta^3(\mathbf{x}-\mathbf{y}), \tag{17}$$

and all others vanish. In addition, there are the usual commutation rules for the A^0_μ field, and commutation of the A^0_μ field operators with the ψ and ϕ field operators.

To specify our notation, we quote the Fourier decomposition of the field operators, namely

$$\psi(x) = \sum_s \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^{3/2}}\left(\frac{m_1}{\omega_p}\right)^{1/2}[b_{\mathbf{p}s}u(\mathbf{p},s)e^{-ip\cdot x} + \mathrm{d}^\dagger_{\mathbf{p}s}v(\mathbf{p},s)e^{ip\cdot x}], \tag{18}$$

with $p=p^\mu=(\omega_p,\mathbf{p})$, $\omega_p=\sqrt{m_1^2+\mathbf{p}^2}$ and

$$\phi(x) = \sum_s \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^{3/2}}\left(\frac{m_2}{\Omega_p}\right)^{1/2}[B_{\mathbf{p}s}U(\mathbf{p},s)e^{-ip\cdot x} + D^\dagger_{\mathbf{p}s}V(\mathbf{p},s)e^{ip\cdot x}], \tag{19}$$

with $p=p^\mu=(\Omega_p,\mathbf{p})$, $\Omega_p=\sqrt{m_2^2+\mathbf{p}^2}$. Note that the mass-$m_1$ free-particle Dirac spinors $u(\mathbf{p},s)$, $v(\mathbf{p},s)$ where $(\gamma^\mu\hat{p}_\mu - m_1)u(\mathbf{p},s)=0$, $(\gamma^\mu\hat{p}_\mu + m_1)v(\mathbf{p},s)=0$, are normalized such that

$$\begin{aligned} u^\dagger(\mathbf{p},s)u(\mathbf{p},\sigma) = v^\dagger(\mathbf{p},s)v(\mathbf{p},\sigma) &= \frac{\omega_p}{m_1}\delta_{s\sigma}, \\ u^\dagger(\mathbf{p},s)v(\mathbf{p},\sigma) = v^\dagger(\mathbf{p},s)u(\mathbf{p},\sigma) &= 0. \end{aligned} \tag{20}$$

Analogous properties apply to the mass-m_2 spinors U, V. The creation and destruction operators $b^\dagger$, b of the (free) particles of mass m_1, and $d^\dagger$, d for the corresponding antiparticles, satisfy the usual anticommutation relations. The nonvanishing ones are

$$\{b_{\mathbf{p}s},b^\dagger_{\mathbf{q}\sigma}\} = \{d_{\mathbf{p}s},d^\dagger_{\mathbf{q}\sigma}\} = \delta_{s\sigma}\delta^3(\mathbf{p}-\mathbf{q}). \tag{21}$$

Again, the analogous properties apply to the mass-m_2 operators $B^\dagger$, B, $D^\dagger$, D. As a concrete example, we can think of the mass-m_1 particles as electrons, and the mass-m_2 particles as muons, though any pairs of charged fermions could be considered.

III. VARIATIONAL PRINCIPLE, TWO-FERMION TRIAL STATES AND EQUATIONS

The Hamiltonian formalism of QFT is based on the covariant eigenvalue equation

$$\hat{P}^\mu|\psi\rangle = Q^\mu|\psi\rangle, \tag{22}$$

where $\hat{P}^\mu=(\hat{H},\hat{\mathbf{P}})$ is the energy momentum operator, $Q^\mu=(E,\mathbf{P})$ is the four-vector of energy and momentum, with $E^2-\mathbf{P}^2=M^2$, where M is the invariant mass of the system. There are very few problems in QFT for which exact solution of the $\mu=0$ equation (22) can be written down. In practice, it is necessary to use approximation methods to solve it, such as the widely used covariant perturbation theory or lattice methods. Here we concentrate on the variational approach, which is based on the variational principle

$$\delta\langle\psi|\hat{H}-E|\psi\rangle_{t=0} = 0, \tag{23}$$

which we shall consider in the rest frame, i.e., $\mathbf{P}=0$. Variational solutions are only as good as the trial states that are used. Thus, it is important that the trial states possess as many features of the exact solution as possible. For a system like μ^+e^-, the simplest Fock-space trial state that can be written down in the rest frame is

$$|\psi_{\text{trial}}\rangle = \sum_{s_1s_2}\int \mathrm{d}^3\mathbf{p}\, F_{s_1s_2}(\mathbf{p}) b^\dagger_{\mathbf{p}s_1} D^\dagger_{-\mathbf{p}s_2}|0\rangle, \tag{24}$$

where $F_{s_1s_2}$ are four adjustable functions. We use this trial state to evaluate the matrix elements needed to implement the variational principle (23), that is

$$\langle\psi_{\text{trial}}|:\hat{H}_0-E:|\psi_{\text{trial}}\rangle = \sum_{s_1s_2}\int \mathrm{d}^3\mathbf{p}\, F^*_{s_1s_2}(\mathbf{p})F_{s_1s_2}(\mathbf{p})(\omega_p+\Omega_p-E) \tag{25}$$

and

$$\begin{aligned}\langle\psi_{\text{trial}}|:\hat{H}_{\text{I}}:|\psi_{\text{trial}}\rangle = &-\frac{q_1q_2m_1m_2}{(2\pi)^3}\sum_{\sigma_1\sigma_2s_1s_2}\int \frac{\mathrm{d}^3\mathbf{p}\,\mathrm{d}^3\mathbf{q}}{\sqrt{\omega_p\omega_q\Omega_p\Omega_q}}F^*_{s_1s_2}(\mathbf{p})F_{\sigma_1\sigma_2}(\mathbf{q})\overline{u}(\mathbf{p},s_1)\gamma^\mu u(\mathbf{q},\sigma_1)\\ &\times D_{\mu\nu}(p-q)\overline{V}(-\mathbf{q},\sigma_2)\gamma^\nu V(-\mathbf{p},s_2),\end{aligned} \tag{26}$$

where the Fourier transform of the Green function was used,

$$D_{\mu\nu}(x-x') = \int \frac{\mathrm{d}^4k}{(2\pi)^4}D_{\mu\nu}(k)e^{-ik(x-x')}. \tag{27}$$

The Green function $D_{\mu\nu}(p-q)$ consists of two parts

$$D_{\mu\nu}(p-q) = \tfrac{1}{2}(D^{(1)}_{\mu\nu}(p-q)+D^{(2)}_{\mu\nu}(q-p)), \tag{28}$$

where $D^{(1)}_{\mu\nu}(p-q)$ and $D^{(2)}_{\mu\nu}(q-p)$ are the Green functions of particles with masses m_1 and m_2, respectively.

For a particle–antiparticle system like positronium an additional virtual-annihilation interaction term,

$$\overline{u}(\mathbf{p},s_1)\gamma^\mu v(-\mathbf{p},s_2)D_{\mu\nu}(\omega_p)\overline{v}(-\mathbf{q},\sigma_2)\gamma^\nu u(\mathbf{q},\sigma_1) \tag{29}$$

appears in (26).[10] Note that we have normal-order the entire Hamiltonian, since this circumvents the need for mass renormalization which would otherwise arise. Not that there is a difficulty with handling mass renormalization in the present formalism (as shown in various earlier papers; see, for example, Ref. 11 and citations therein). It is simply that we are not interested in mass renormalization here, since it has no effect on the two-body bound state energies that we obtain in this

paper. Furthermore, the approximate trial state (24), which we use in this work, is incapable of sampling loop effects. Thus, the normal ordering of the entire Hamiltonian does not "sweep under the carpet" loop renormalization effects, since none arise at the present level of approximation. Note, also, that $\langle\psi_{\text{trial}}|:\hat{H}_{\text{II}}:|\psi_{\text{trial}}\rangle=0$, that is the variational trial state (24) is insensitive to that part of the interaction Hamiltonian which is linear in $A^0_\mu(x)$. This means that, with the simple anzatz (24) only stable bound states and elastic scattering can be described, but not processes that involve radiation.

The variational principle (23) leads to the following equation;

$$\sum_{s_1s_2}\int \mathrm{d}^3\mathbf{p}(\omega_p+\Omega_p-E)F_{s_1s_2}(\mathbf{p})\,\delta F^*_{s_1s_2}(\mathbf{p})-\frac{m_1m_2}{(2\pi)^3}\sum_{\sigma_1\sigma_2s_1s_2}\int\frac{\mathrm{d}^3\mathbf{p}\,\mathrm{d}^3\mathbf{q}}{\sqrt{\omega_p\omega_q\Omega_p\Omega_q}}F_{\sigma_1\sigma_2}(\mathbf{q})$$
$$\times(-i)\mathcal{M}^{ope}_{s_1s_2\sigma_1\sigma_2}(\mathbf{p},\mathbf{q})\,\delta F^*_{s_1s_2}(\mathbf{p})=0, \tag{30}$$

where $\mathcal{M}^{ope}_{s_1s_2\sigma_1\sigma_2}(\mathbf{p},\mathbf{q})$ is the usual invariant matrix element corresponding to the one-photon exchange Feynman diagram:

$$\mathcal{M}^{ope}_{s_1s_2\sigma_1\sigma_2}(\mathbf{p},\mathbf{q})=-\overline{u(}\mathbf{p},s_1)(-iq_1\gamma^\mu)u(\mathbf{q},\sigma_1)iD_{\mu\nu}(p-q)\overline{V(}-\mathbf{q},\sigma_2)(-iq_2\gamma^\nu)V(-\mathbf{p},s_2). \tag{31}$$

As mentioned above, for a fermion–antifermion system like positronium we obtain[10] the additional virtual-annihilation term ($q_1=q_2\equiv e$)

$$\mathcal{M}^{ann}_{s_1s_2\sigma_1\sigma_2}(\mathbf{p},\mathbf{q})=\overline{u(}\mathbf{p},s_1)(-ie\gamma^\mu)v(-\mathbf{p},s_2)iD_{\mu\nu}(\omega_p)\overline{v(}-\mathbf{q},\sigma_2)(-ie\gamma^\nu)u(\mathbf{q},\sigma_1). \tag{32}$$

Note that the $\mathcal{M}$-matrix arises naturally in this formalism, that is $\mathcal{M}$ is not put in by hand, nor does its derivation require additional Fock-space terms in the variational trial state (24), as is the case in traditional formulations (e.g., Refs. 12 and 13).

In the nonrelativistic limit, the functions $F_{s_1s_2}$ can be written as

$$F_{s_1s_2}(\mathbf{p})=F(\mathbf{p})\Lambda_{s_1s_2}, \tag{33}$$

where the nonzero elements of Λ_{ij} for total spin singlet ($S=0$) states are $\Lambda_{12}=-\Lambda_{21}=1/\sqrt{2}$, while for the spin triplet ($S=1$) states the nonzero elements are $\Lambda_{11}=1$ for $m_s=+1$, $\Lambda_{12}=\Lambda_{21}=1/\sqrt{2}$ for $m_s=0$, and $\Lambda_{22}=1$ for $m_s=-1$. We use the notation that the subscripts 1 and 2 of Λ correspond to $m_s=1/2$ and $m_s=-1/2$ (or $\uparrow$ and $\downarrow$), respectively. Substituting (33) into (30), multiplying the result by $\Lambda_{s_1s_2}$ and summing over s_1 and s_2, gives the equation

$$(\omega(\mathbf{p})+\Omega(\mathbf{p})-E)F(\mathbf{p})=\frac{1}{(2\pi)^3}\int\mathrm{d}^3\mathbf{q}\,\mathcal{K}(\mathbf{p},\mathbf{q})F(\mathbf{q}), \tag{34}$$

where

$$\mathcal{K}(\mathbf{p},\mathbf{q})=-i\sum_{s_1s_2\sigma_1\sigma_2}\Lambda_{s_1s_2}\mathcal{M}_{s_1s_2\sigma_1\sigma_2}(\mathbf{p},\mathbf{q})\Lambda_{\sigma_1\sigma_2}. \tag{35}$$

To lowest order in $(|\mathbf{p}|,|\mathbf{q}|)/(m_1,m_2)$ (i.e., in the nonrelativistic limit), the kernel (35) reduces to $\mathcal{K}=q_1q_2/|\mathbf{p}-\mathbf{q}|^2$, and so (34) reduces to the (momentum-space) Schrödinger equation

$$\left(\frac{\mathbf{p}^2}{2m_r}-\varepsilon\right)F(\mathbf{p})=\frac{q_1q_2}{(2\pi)^3}\int\mathrm{d}^3\mathbf{q}\frac{1}{|\mathbf{p}-\mathbf{q}|^2}F(\mathbf{q}), \tag{36}$$

where $\varepsilon=E-M$ and $m_r=m_1m_2/M$, $M=m_1+m_2$. This verifies that the relativistic two-fermion equation (30) has the required nonrelativistic limit.

IV. PARTIAL-WAVE DECOMPOSITION AND CLASSIFICATION OF STATES

In the relativistic case we shall not complete the variational procedure in (30) at this stage to get final equations for the four functions $F_{s_1s_2}$, because they are not independent in general. We require that the trial state must be an eigenstate of the relativistic total angular momentum operator, its projection, and parity. Namely

$$\begin{bmatrix} \hat{\mathbf{J}}^2 \\ \hat{J}_3 \\ \hat{\mathcal{P}} \end{bmatrix} |\psi_{\text{trial}}\rangle = \begin{bmatrix} J(J+1) \\ m_J \\ P \end{bmatrix} |\psi_{\text{trial}}\rangle. \tag{37}$$

For a system like positronium charge conjugation invariance is an additional requirement, that is

$$\hat{\mathcal{C}}|e^+e^-\rangle = C|e^+e^-\rangle, \tag{38}$$

however this does not apply for $m_1 \neq m_2$. Explicit forms for the operators $\hat{\mathbf{J}}^2$, $\hat{J}_3$ are given in Appendix A. The functions $F_{s_1s_2}(\mathbf{p})$ can be written in the general form

$$F_{s_1s_2}(\mathbf{p}) = \sum_{\ell_{s_1s_2}} \sum_{m_{s_1s_2}} f^{\ell_{s_1s_2} m_{s_1s_2}}_{s_1s_2}(p) Y^{m_{s_1s_2}}_{\ell_{s_1s_2}}(\hat{\mathbf{p}}), \tag{39}$$

where $Y^{m_{s_1s_2}}_{\ell_{s_1s_2}}(\hat{\mathbf{p}})$ are the usual spherical harmonics. Here and henceforth we will use the notation $p=|\mathbf{p}|$, etc. (four-vectors will be written as p^μ). The orbital indices $\ell_{s_1s_2}$ and $m_{s_1s_2}$ depend on the spin indices s_1 and s_2 and are specified by Eq. (37). The radial coefficients of expansion (39) $f^{\ell_{s_1s_2} m_{s_1s_2}}_{s_1s_2}(p)$ also depend on the spin variables. Substitution of (39) into (24) and then into (37) leads to two categories of relations among the adjustable functions.

A. Mixed-spin states

In this case $\ell_{s_1s_2} \equiv \ell = J$ and the general solution of the system (37) is

$$F_{s_1s_2}(\mathbf{p}) = C_1 F^{(sg)}_{s_1s_2}(\mathbf{p}) + C_2 F^{(tr)}_{s_1s_2}(\mathbf{p}), \tag{40}$$

where C_1 and C_2 are arbitrary constants. $F^{(sg)}_{s_1s_2}(\mathbf{p})$ and $F^{(tr)}_{s_1s_2}(\mathbf{p})$ are functions, which correspond to pure singlet states with the total spin $S=0$ and triplet states with $S=1$, respectively. The singlet functions have the form

$$F^{(sg)}_{s_1s_2}(\mathbf{p}) = f^{(sg)\ell}_{s_1s_2}(p) Y^{m_{s_1s_2}}_{\ell}(\hat{\mathbf{p}}), \tag{41}$$

where $m_{11}=m_{22}=0$ and $m_{12}=m_{21}=m_J$. The relations between $f^{(sg)J}_{12}(p)$ and $f^{(sg)J}_{21}(p)$ involve the Clebsch–Gordan (CG) coefficients $C^{(sg)m_{s_1s_2}}$, that is

$$f^{(sg)J}_{s_1s_2}(p) = C^{(sg)m_{s_1s_2}} f^J(p), \tag{42}$$

as is shown in Appendix A. We see that the spin and radial variables separate in the sense that the factors $f^{(sg)J}_{s_1s_2}(p)$ have a common radial function $f^J(p)$, that is for the singlet functions we obtain

$$F^{(sg)}_{s_1s_2}(\mathbf{p}) = C^{(sg)m_{s_1s_2}} f^J(p) Y^{m_{s_1s_2}}_J(\hat{\mathbf{p}}). \tag{43}$$

The CG coefficients $C^{(sg)m_{s_1s_2}}$ have a simple form, $C^{(sg)m_{11}}=C^{(sg)m_{22}}=0$, $C^{(sg)m_{12}}=-C^{(sg)m_{21}}=1$ (see Appendix A). Thus the nonzero components of $F^{(sg)}_{s_1s_2}(\mathbf{p})$ are $F^{(sg)}_{\uparrow\downarrow}(\mathbf{p}) \equiv F^{(sg)}_{12}(\mathbf{p})$, $F^{(sg)}_{\downarrow\uparrow}(\mathbf{p}) \equiv F^{(sg)}_{21}(\mathbf{p})$.

The triplet functions have the form

$$F^{(tr)}_{s_1s_2}(\mathbf{p}) = f^{(tr)J}_{s_1s_2}(p) Y_J^{m_{s_1s_2}}(\hat{\mathbf{p}}), \tag{44}$$

where

$$m_{11} = m_J - 1, \quad m_{12} = m_{21} = m_J, \quad m_{22} = m_J + 1. \tag{45}$$

The expressions for $f^{(tr)J}_{s_1s_2}(p)$ involve the CG coefficients $C^{(tr)Jm_s}_{Jm_J}$ for $S=1$ listed in Appendix A, that is

$$f^{(tr)J}_{s_1s_2}(p) = C^{(tr)Jm_s}_{Jm_J} f^{\ell}(p), \tag{46}$$

where the index m_s is defined as

$$m_s = +1, \quad \text{when } m_{s_1s_2} = m_{11},$$

$$m_s = 0, \quad \text{when } m_{s_1s_2} = m_{12} = m_{21}, \tag{47}$$

$$m_s = -1, \quad \text{when } m_{s_1s_2} = m_{22}.$$

Thereupon, the triplet function is

$$F^{(tr)}_{s_1s_2}(\mathbf{p}) = C^{(tr)Jm_s}_{Jm_J} f^J(p) Y_J^{m_{s_1s_2}}(\hat{\mathbf{p}}). \tag{48}$$

We need to note that (43) is true for $J \geqslant 0$, while (48) is true for $J \geqslant 1$. Thus the coefficient C_2 in (40) is zero when $J=0$. In other words, for $J=0$, only the pure singlet state arises. For a system like positronium the requirement (38) decouples the singlet and triplet states for all J. Indeed, the charge conjugation eigenstates are

$$|sg\rangle = \sum_{s_1s_2} C^{(sg)m_{s_1s_2}} \int \mathrm{d}^3\mathbf{p}\, f^J(p) Y_J^{m_J}(\hat{\mathbf{p}}) b^{\dagger}_{\mathbf{p}s_1} d^{\dagger}_{-\mathbf{p}s_2} |0\rangle \tag{49}$$

with $C=(-1)^J$ for the pure singlet states, and

$$|tr\rangle = \sum_{s_1s_2} C^{(tr)Jm_{s_1s_2}}_{Jm_J} \int \mathrm{d}^3\mathbf{p}\, f^J(p) Y_J^{m_J}(\hat{\mathbf{p}}) b^{\dagger}_{\mathbf{p}s_1} d^{\dagger}_{-\mathbf{p}s_2} |0\rangle \tag{50}$$

with $C=(-1)^{J+1}$ for the pure triplet states, as is discussed in Appendix A.

The states (49) and (50) diagonalize the Hamiltonian (13). Thus, for positroniumlike systems, the states can be characterized by the spin quantum number S, and the mixed states (40) separate into singlet states (parastates $S=0$) and triplet states (orthostates $S=1$). For distinct particles ($m_1 \neq m_2$) C is not conserved and there is no separation into pure singlet and triplet states in general. Thus for arbitrary mass ratios we need to diagonalize the expectation value of the Hamiltonian (13) (Appendix E). This can be achieved by the following linear transformation

$$\begin{bmatrix} |sg_q\rangle \\ |tr_q\rangle \end{bmatrix} = \hat{U} \begin{bmatrix} |sg\rangle \\ |tr\rangle \end{bmatrix}, \tag{51}$$

where $\hat{U}$ is the unimodular matrix

$$\hat{U} = \begin{bmatrix} a & -b \\ b & a \end{bmatrix} \tag{52}$$

with components

TABLE I. The quasistate coefficients $C^{(s)Jm_{s_1s_2}}_{Jm_J}$ for $s=s_s, s_t$.

	$m_{11}=m_J-1$	$m_{12}=m_J$	$m_{21}=m_J$	$m_{22}=m_J+1$
s_s	$b\left(\frac{(J+m_J)(J-m_J+1)}{J(J+1)}\right)^{1/2}$	$-b\frac{m_J}{(J(J+1))^{1/2}}+a$	$-b\frac{m_J}{(J(J+1))^{1/2}}-a$	$-b\left(\frac{(J-m_J)(J+m_J+1)}{J(J+1)}\right)^{1/2}$
s_t	$-a\left(\frac{(J+m_J)(J-m_J+1)}{J(J+1)}\right)^{1/2}$	$a\frac{m_J}{(J(J+1))^{1/2}}+b$	$a\frac{m_J}{(J(J+1))^{1/2}}-b$	$a\left(\frac{(J-m_J)(J+m_J+1)}{J(J+1)}\right)^{1/2}$

$$a=\sqrt{\frac{1+\xi}{2}},\quad b=\sqrt{\frac{1-\xi}{2}}, \tag{53}$$

where

$$\xi=(4((m_1-m_2)/(m_1+m_2))^2J(J+1)+1)^{-1/2}. \tag{54}$$

The new states, which diagonalize the expectation value of $\hat{H}$, shall be called quasisinglet $|sg_q\rangle$ and quasitriplet $|tr_q\rangle$ states

$$\begin{aligned}|sg_q\rangle&=\sum_{s_1s_2}C^{(s_s)Jm_{s_1s_2}}_{Jm_J}\int \mathrm{d}^3\mathbf{p}\, f^J(p)Y^{m_J}_J(\hat{\mathbf{p}})b^\dagger_{\mathbf{p}s_1}D^\dagger_{-\mathbf{p}s_2}|0\rangle,\\ |tr_q\rangle&=\sum_{s_1s_2}C^{(s_t)Jm_{s_1s_2}}_{Jm_J}\int \mathrm{d}^3\mathbf{p}\, f^J(p)Y^{m_J}_J(\hat{\mathbf{p}})b^\dagger_{\mathbf{p}s_1}D^\dagger_{-\mathbf{p}s_2}|0\rangle,\end{aligned} \tag{55}$$

where the coefficients $C^{(s_s)Jm_{s_1s_2}}_{Jm_J}$ and $C^{(s_t)Jm_{s_1s_2}}_{Jm_J}$ are listed in Table I, and satisfy the following condition:

$$\sum_{\nu_1\nu_2m_J}(C^{(s_s)Jm_\nu}_{Jm_J})^2=\sum_{\nu_1\nu_2m_J}(C^{(s_t)Jm_\nu}_{Jm_J})^2=2(2J+1). \tag{56}$$

Note that these coefficients differ from CG coefficients, because of the coupled system we are dealing with. Remember that these coupled quasistates arise only for $J>0$. For $J=0$ purely $S=0$ states occur. Quasisinglet and quasitriplet states are both characterized by the same quantum numbers J, m_J and $P=(-1)^{J+1}$. Because of the unimodularity of matrix (52) we can identify quasisinglet and quasitriplet states by quasispin (like isospin) $t=1/2$ with $t_3=\mp 1/2$, which is a new quantum number (or label). However, for our purpose it is more convenient to use the value $s=t_3+1/2$, which gives $s=s_s=0$ or $s=s_t=1$ for quasisinglet and quasitriplet states, respectively. In this case the labels s_s and s_t reflect better the meaning of the indicated quasistates. It is easy to see from (55) and Table I that for positronium the quasistates become true singlet ($b=0$) and triplet ($a=0$) states with different charge conjugation quantum numbers. It is useful to note for subsequent calculations that the coefficients C_1 and C_2 in (40) are $C_1=a$, $C_2=-b$ for quasisinglet states $s=s_s=0$, and $C_1=b$, $C_2=a$ for quasitriplet states $s=s_t=1$.

B. The triplet ℓ-mixing states

These states occur for $\ell_{s_1s_2}\equiv\ell=J\mp 1$ (see Appendix A). The adjustable functions have the form

$$F_{s_1s_2}(\mathbf{p}) = C^{(tr)(J-1)m_s}_{Jm_J} f^{J-1}(p) Y^{m_{s_1s_2}}_{J-1}(\hat{\mathbf{p}}) + C^{(tr)(J+1)m_s}_{Jm_J} f^{J+1}(p) Y^{m_{s_1s_2}}_{J+1}(\hat{\mathbf{p}}), \tag{57}$$

where $m_{s_1s_2}$ are defined in (47), while the coefficients $C^{(tr)(J\mp1)m_s}_{Jm_J}$, which are precisely the CG coefficients, can be found in Appendix A. Expression (57) involves two radial functions $f^{J-1}(p)$ and $f^{J+1}(p)$ which correspond to $\ell = J-1$ and $\ell = J+1$. This reflects the fact that the orbital angular momentum is not conserved and ℓ is not a good quantum number. The system in these states is characterized by J, m_J, and $P=(-1)^J$. In spectroscopic notation, these states are a mixture of $^3(J-1)_J$, and $^3(J+1)_J$ states. The exception is the state with $J=0$, for which the orbital angular momentum is a good quantum number. Indeed, for $J=0$ the function $f^{J-1}(p)$ does not exist (see Appendix A), thus the function $F_{s_1s_2}(\mathbf{p})$ is defined only by the second term in (57). Note that ℓ-mixing states appear for principal quantum number $n \geqslant 3$ only.

V. THE RELATIVISTIC RADIAL EQUATIONS FOR TWO-FERMION SYSTEMS

It is not possible to write a universal two-fermion wave equation, because the adjustable functions have different form for different states. Thus it was important to classify all states of the system before deriving final radial equations. Now we return to the variational equation (30) and replace the functions $F_{s_1s_2}(\mathbf{p})$ by the expression (40) for the quasistates and by (57) for the triplet states. After completing the variational procedure we obtain the following results.

For the states with $\ell = J$, $P=(-1)^{J+1}$ the radial equations are

$$(\omega_p + \Omega_p - E) f^J(p) = \frac{m_1 m_2}{(2\pi)^3} \int \frac{q^2\, dq}{\sqrt{\omega_p \omega_q \Omega_p \Omega_q}} \mathcal{K}(p,q) f^J(q), \tag{58}$$

where the kernel $\mathcal{K}(p,q)$ is defined by invariant $\mathcal{M}$-matrices as follows from (30). For the pure singlet states with $J=0$ the kernel $\mathcal{K}(p,q)$ is

$$\mathcal{K}(p,q) = -\frac{i}{4\pi} \int d\hat{\mathbf{p}}\, d\hat{\mathbf{q}} (\mathcal{M}_{1212}(\mathbf{p},\mathbf{q}) - \mathcal{M}_{1221}(\mathbf{p},\mathbf{q}) - \mathcal{M}_{2112}(\mathbf{p},\mathbf{q}) + \mathcal{M}_{2121}(\mathbf{p},\mathbf{q})). \tag{59}$$

For quasisinglet and quasitriplet states ($J \geqslant 1$) we have

$$\mathcal{K}(p,q) = -i \sum_{s_1s_2\sigma_1\sigma_2 m_J} \int d\hat{\mathbf{p}}\, d\hat{\mathbf{q}}\, C^{(s)s_1s_2\sigma_1\sigma_2}_{Jm_J} \mathcal{M}_{s_1s_2\sigma_1\sigma_2}(\mathbf{p},\mathbf{q}) Y^{m_J *}_J(\hat{\mathbf{p}}) Y^{m_J}_J(\hat{\mathbf{q}}), \tag{60}$$

where the coefficients $C^{(s)s_1s_2\sigma_1\sigma_2}_{Jm_J}$ are expressed through the coefficients $C^{(s)Jm_{s_1s_2}}_{Jm_J}$,

$$C^{(s)s_1s_2\sigma_1\sigma_2}_{Jm_J} \equiv C^{(s)Jm_{s_1s_2}}_{Jm_J} C^{(s)Jm_{\sigma_1\sigma_2}}_{Jm_J} \Big/ \sum_{\nu_1\nu_2 m_J} (C^{(s)Jm_{\nu_1\nu_2}}_{Jm_J})^2, \tag{61}$$

where $s=s_s$, s_t. In (60) we have summed over m_J, because of the $2J+1$ energy degeneracy.

For the triplet states with $\ell = J \mp 1$, we have two independent radial functions $f^{J-1}(p)$ and $f^{J+1}(p)$. Thus the variational equation (30) leads to a system of coupled equations for $f^{J-1}(p)$ and $f^{J+1}(p)$. It is convenient to write them in matrix form,

$$(\omega_p + \Omega_p - E) \mathbb{F}(p) = \frac{m_1 m_2}{(2\pi)^3} \int \frac{q^2\, dq}{\sqrt{\omega_p \omega_q \Omega_p \Omega_q}} \mathbb{K}(p,q) \mathbb{F}(q), \tag{62}$$

where

$$\mathbb{F}(p) = \begin{bmatrix} f^{J-1}(p) \\ f^{J+1}(p) \end{bmatrix} \tag{63}$$

and

$$\mathbb{K}(p,q) = \begin{bmatrix} \mathcal{K}_{11}(p,q) & \mathcal{K}_{12}(p,q) \\ \mathcal{K}_{21}(p,q) & \mathcal{K}_{22}(p,q) \end{bmatrix}. \tag{64}$$

The kernels $\mathcal{K}_{ij}$ are similar in form to (60), that is

$$\mathcal{K}_{ij}(p,q) = -i \sum_{s_1 s_2 \sigma_1 \sigma_2 m_J} C^{s_1 s_2 \sigma_1 \sigma_2}_{J m_J i j} \int \mathrm{d}\hat{\mathbf{p}}\, \mathrm{d}\hat{\mathbf{q}}\, \mathcal{M}_{s_1 s_2 \sigma_1 \sigma_2}(\mathbf{p},\mathbf{q}) Y^{m_{s_1 s_2}\,*}_{\ell_i}(\hat{\mathbf{p}}) Y^{m_{\sigma_1 \sigma_2}}_{\ell_j}(\hat{\mathbf{q}}). \tag{65}$$

However the coefficients $C^{s_1 s_2 \sigma_1 \sigma_2}_{J m_J i j}$ are defined by the expression

$$C^{s_1 s_2 \sigma_1 \sigma_2}_{J m_J i j} = C^{(tr)\ell_i m_{s_1 s_2}}_{J m_J} C^{(tr)\ell_j m_{\sigma_1 \sigma_2}}_{J m_J} \Big/ \sum_{s_1 s_2 m_J} (C^{(tr)\ell_i m_s}_{J m_J})^2, \tag{66}$$

where $\ell_1 = J-1$, $\ell_2 = J+1$. The system (62) reduces to a single equation for $f^{J+1}(p)$ when $J=0$, since $f^{J-1}(p)=0$ in that case.

To our knowledge, it is not possible to obtain analytic solutions of the relativistic radial momentum-space equations (58) and (62). Thus one must resort to numerical or other approximation methods. Numerical solutions of such equations are discussed, for example, in Ref. 11, while variational approximations have been employed in Ref. 5. However, in this paper we shall resort to perturbative approximations, in order to verify that our equations agree with known results for positronium to $O(\alpha^4)$. We expect that this must be so, given that the interaction kernels (i.e., momentum-space potentials) of our equations involve the "tree-level" Feynman diagrams only.

Beyond $O(\alpha^4)$ our equations are evidently incomplete. One could, of course, augment them by the addition of invariant matrix elements corresponding to one-loop Feynman diagrams to the existing $\mathcal{M}$-matrices in the kernels of our equations. Indeed such an approach has been used in a similar though not variational treatment of positronium and muonium by Zhang and Koniuk.[14,15] These authors show that the inclusion of single-loop diagrams yields positronium energy eigenstates which are accurate to $O(\alpha^5, \alpha^5 \ln \alpha)$. However such *ad-hoc* augmentation of the kernels would be contrary to the spirit of the present variational treatment, and we shall not pursue it in this work.

VI. THE KERNELS IN SEMIRELATIVISTIC EXPANSION AND THE NONRELATIVISTIC LIMIT

For perturbative solutions of our radial equations, it is necessary to work out expansions of the relevant expressions to first order beyond the nonrelativistic limit. This shall be summarized in the present section. We shall do the calculation in the Coulomb gauge, in which the photon propagator has the form[16]

$$D_{00}(\mathbf{k}) = \frac{1}{\mathbf{k}^2}, \quad D_{0l}(\mathbf{k}) = 0, \quad D_{kl}(k^\mu) = \frac{1}{k^\mu k_\mu}\left(\delta_{kl} - \frac{k_k k_l}{\mathbf{k}^2}\right), \tag{67}$$

where $k^\mu = (\omega_p - \omega_q, \mathbf{p}-\mathbf{q})$.

To expand the amplitudes $\mathcal{M}$ of (31) and (32) up to the lowest nontrivial order of $(p/m)^2$, we take the free-particle spinors to be

$$u(\mathbf{p},i) = \begin{bmatrix} \left(1 + \dfrac{\mathbf{p}^2}{8m^2}\right) \\ \dfrac{(\vec{\sigma}\cdot\mathbf{p})}{2m} \end{bmatrix} \varphi_i, \quad v(\mathbf{p},i) = \begin{bmatrix} \dfrac{(\vec{\sigma}\cdot\mathbf{p})}{2m} \\ \left(1 + \dfrac{\mathbf{p}^2}{8m^2}\right) \end{bmatrix} \chi_i, \tag{68}$$

as discussed in Appendix C. Analogously, the photon propagator takes on the form

$$D_{00}(\mathbf{p}-\mathbf{q}) = \frac{1}{(\mathbf{p}-\mathbf{q})^2}, \quad D_{kl}(\mathbf{p}-\mathbf{q}) \simeq -\frac{1}{(\mathbf{p}-\mathbf{q})^2}\left(\delta_{kl} - \frac{(p-q)_k(p-q)_l}{(\mathbf{p}-\mathbf{q})^2}\right). \tag{69}$$

In this case the total photon propagator (28) coincides with (69). Corresponding calculations give for the orbital part of the $\mathcal{M}$-matrix,

$$\mathcal{M}^{ope(orb)}_{s_1s_2\sigma_1\sigma_2}(\mathbf{q},\mathbf{p}) = \frac{iq_1q_2}{(\mathbf{p}-\mathbf{q})^2}\delta_{s_1\sigma_1}\delta_{s_2\sigma_2} + \frac{iq_1q_2}{m_1m_2}\left(\frac{1}{2}\left(\frac{m_1}{m_2}+\frac{m_2}{m_1}\right)\left(\frac{1}{4}+\frac{\mathbf{q}\cdot\mathbf{p}}{(\mathbf{p}-\mathbf{q})^2}\right) + \frac{(\mathbf{p}\times\mathbf{q})^2}{(\mathbf{p}-\mathbf{q})^4}\right)\delta_{s_1\sigma_1}\delta_{s_2\sigma_2}. \tag{70}$$

The linear spin terms, which are responsible for spin–orbit interaction, become

$$\mathcal{M}^{ope(s-o)}_{s_1s_2\sigma_1\sigma_2}(\mathbf{q},\mathbf{p}) = -\frac{q_1q_2}{4m_1m_2}\varphi^\dagger_{s_1}\chi^\dagger_{\sigma_2}\left(\left(\frac{m_2}{m_1}+2\right)\vec{\sigma}_1 - \left(\frac{m_1}{m_2}+2\right)\vec{\sigma}_2\right)\cdot\frac{\mathbf{p}\times\mathbf{q}}{(\mathbf{p}-\mathbf{q})^2}\varphi_{\sigma_1}\chi_{s_2}. \tag{71}$$

Here $\vec{\sigma}_1$ and $\vec{\sigma}_2$ are spin matrices of the first and second particles, respectively, which are defined by the following operations: $\vec{\sigma}_1\varphi_{\sigma_1}\chi_{s_2}=(\vec{\sigma}_1\varphi_{\sigma_1})\chi_{s_2}$, $\vec{\sigma}_2\varphi_{\sigma_1}\chi_{s_2}=\varphi_{\sigma_1}(\vec{\sigma}_2\chi_{s_2})$. The quadratic spin terms or spin–spin interaction terms are

$$\mathcal{M}^{ope(s-s)}_{s_1s_2\sigma_1\sigma_2}(\mathbf{q},\mathbf{p}) = \frac{iq_1q_2}{4m_1m_2}\varphi^\dagger_{s_1}\chi^\dagger_{\sigma_2}\left\{-\frac{(\vec{\sigma}_2\cdot(\mathbf{p}-\mathbf{q}))(\vec{\sigma}_1\cdot(\mathbf{p}-\mathbf{q}))}{(\mathbf{p}-\mathbf{q})^2} + (\vec{\sigma}_1\cdot\vec{\sigma}_2)\right\}\varphi_{\sigma_1}\chi_{s_2}. \tag{72}$$

The annihilation contribution, which arises for a particle–antiparticle system,[10] is given by the term

$$\mathcal{M}^{ann}_{s_1s_2\sigma_1\sigma_2}(\mathbf{p},\mathbf{q}) = -\frac{ie^2}{4m^2}\varphi^\dagger_{s_1}\chi^\dagger_{\sigma_2}\{\vec{\sigma}_1\cdot\vec{\sigma}_2\}\varphi_{\sigma_1}\chi_{s_2}, \tag{73}$$

where we have excluded a divergent term, which appears in the Coulomb gauge. In this case $m_1=m_2\equiv m$ and $q_1=q_2\equiv e$ in formulas (70)–(72).

The kernels are calculated from (59), (60), and (65) with (70)–(72). They consist of three parts, namely

$$\mathcal{K}(p,q) = \mathcal{K}^{(orb)}(p,q) + \mathcal{K}^{(s-o)}(p,q) + \mathcal{K}^{(s-s)}(p,q). \tag{74}$$

A. The singlet state ($\ell=J=0$, $P=-1$)

Details of the calculations can be found in Appendix D. We use the notation, $z=(p^2+q^2)/2pq$, and $Q_\lambda(z)$ are the Legendre functions of the second kind.[17] The contributions of the various terms to the kernel are as follows:

Orbital term,

$$\mathcal{K}^{(sgl)(orb)}(p,q) = \frac{2\pi q_1q_2}{pq}Q_0(z) + \frac{\pi q_1q_2}{2m_1m_2}\left(\left(\frac{m_1}{m_2}+\frac{m_2}{m_1}+1\right)\left(\frac{p}{q}+\frac{q}{p}\right)Q_0(z) + 2Q_1(z) - \left(\frac{m_1}{m_2}+\frac{m_2}{m_1}+2\right)\right). \tag{75}$$

Spin–orbit interaction,

$$\mathcal{K}^{(sgl)(s-o)}(p,q) = 0. \tag{76}$$

Spin–spin interaction

$$\mathcal{K}^{(sgl)(s-s)}(p,q) = \frac{2\pi q_1q_2}{m_1m_2}. \tag{77}$$

B. The quasistates [$\ell = J (J \geqslant 1)$, $P = (-1)^{J+1}$, $s = 0,1$]

The contributions of the various terms to the kernel are as follows.
Orbital term,

$$\mathcal{K}^{(orb)}(p,q) = \frac{\pi q_1 q_2}{pq} Q_J(z) + \frac{\pi q_1 q_2}{2m_1 m_2}\left(\left(\frac{m_1}{m_2} + \frac{m_2}{m_1} - (J-1)\right)\left(\frac{p}{q} + \frac{q}{p}\right)Q_J(z) + 2(J+1)Q_{J+1}(z)\right), \tag{78}$$

Spin–orbit interaction,

$$\mathcal{K}^{(s-o)}(p,q) = \frac{\pi q_1 q_2}{2m_1 m_2}\left(-C_2^2\left(\frac{m_1}{m_2} + \frac{m_2}{m_1} + 4\right) + 2C_1 C_2 \sqrt{J(J+1)}\left|\frac{m_2}{m_2} - \frac{m_1}{m_1}\right|\right) \times \frac{1}{2J+1}(Q_{J+1}(z) - Q_{J-1}(z)). \tag{79}$$

Spin–spin interaction,

$$\mathcal{K}^{(s-s)}(p,q) = C_2^2 \frac{\pi q_1 q_2}{2m_1 m_2}\left(\frac{p}{q} + \frac{q}{p}\right)Q_J(z) - C_2^2 \frac{\pi q_1 q_2}{m_1 m_2}\frac{1}{2J+1}\{JQ_{J+1}(z) + (J+1)Q_{J-1}(z)\}, \tag{80}$$

where C_1 and C_2 are defined in Sec. IV.

C. The triplet states [$\ell = J-1 (J \geqslant 1)$, $\ell = J+1 (J \geqslant 0)$, $P = (-1)^J$]

From (65), it follows that the kernels $\mathcal{K}_{12}$ and $\mathcal{K}_{21}$ are responsible for mixing of states with $\ell = J-1$ and $\ell = J+1$. These kernels have the form

$$\mathcal{K}_{12}(p,q) = \mathcal{K}_{21}(p,q) = \frac{\pi q_1 q_2}{5m_1 m_2}\frac{\sqrt{J(J+1)}}{(2J+1)}\left(\frac{p}{q}Q_{J+1}(z) + \frac{q}{p}Q_{J-1}(z) - 2Q_J(z)\right), \tag{81}$$

where only spin–spin interactions contribute. For kernels $\mathcal{K}_{11}$ and $\mathcal{K}_{11}$ we have the following from (65):
Orbital terms,

$$\mathcal{K}_{11}^{(o)}(p,q) = \frac{2\pi q_1 q_2}{pq}Q_{J-1}(z) + \frac{\pi q_1 q_2}{2m_1 m_2}\left(\frac{m_1}{m_2} + \frac{m_2}{m_1} + 2 - J\right)\left(\frac{p}{q} + \frac{q}{p}\right)Q_{J-1}(z) + \frac{\pi q_1 q_2}{m_1 m_2}JQ_J(z) - \frac{\pi q_1 q_2}{2m_1 m_2}\left(\frac{m_1}{m_2} + \frac{m_2}{m_1} + 2\right)\delta_{J,1}, \tag{82}$$

$$\mathcal{K}_{22}^{(o)}(p,q) = \frac{2\pi q_1 q_2}{pq}Q_{J+1}(z_1) + \frac{\pi q_1 q_2}{2m_1 m_2}\left(\frac{m_1}{m_2} + \frac{m_2}{m_1} - J\right)\left(\frac{p}{q} + \frac{q}{p}\right)Q_{J+1}(z_1) + \frac{\pi q_1 q_2}{m_1 m_2}(J+2)Q_{J+2}(z). \tag{83}$$

Spin–orbit interaction,

$$\mathcal{K}_{11}^{(s-o)}(p,q) = \frac{\pi q_1 q_2}{2m_1 m_2}\frac{J-1}{2J-1}\left(\frac{m_2}{m_1} + \frac{m_1}{m_2} + 4\right)(Q_J(z) - Q_{J-2}(z)), \tag{84}$$

$$\mathcal{K}_{22}^{(s-o)}(p,q) = -\frac{\pi q_1 q_2}{2m_1 m_2}\left(\frac{m_2}{m_1} + \frac{m_1}{m_2} + 4\right)\frac{J+2}{2J+3}(Q_{J+2}(z) - Q_J(z)). \tag{85}$$

Spin–spin interaction,

$$\mathcal{K}_{11}^{(s-s)}(p,q)=\frac{\pi q_1 q_2}{2m_1 m_2}\frac{1}{2J+1}\left(\left(\frac{p}{q}+\frac{q}{p}\right)Q_{J-1}(z)-2Q_J(z)\right), \tag{86}$$

$$\mathcal{K}_{22}^{(s-s)}(p,q)=\frac{\pi q_1 q_2}{2m_1 m_2}\frac{1}{2J+3}\left(\left(\frac{p}{q}+\frac{q}{p}\right)Q_{J+1}(z)-2Q_{J+2}(z)\right). \tag{87}$$

Annihilation term (particle–antiparticle system only, with $m_1=m_2=m$, $q_1=q_2=e$),

$$\mathcal{K}^{ann}(p,q)=-\frac{2\pi e^2}{m^2}\delta_{J,1}. \tag{88}$$

We note that in the nonrelativistic limit the only terms that survive are the first terms of the orbital part of the kernels. They have the common form $2\pi q_1 q_2 Q_\ell(z)/pq$, where

$$Q_\ell(z)=\frac{pq}{2\pi}\int\frac{d\hat{\mathbf{q}}\,d\hat{\mathbf{p}}}{(\mathbf{p}-\mathbf{q})^2}Y_\ell^{m_\ell *}(\hat{\mathbf{p}})Y_\ell^{m_\ell}(\hat{\mathbf{q}}). \tag{89}$$

Thus, Eqs. (58) and (62) reduce to the form

$$(\omega_p+\Omega_p-E)f^\ell(p)=\frac{m_1 m_2 q_1 q_2}{\pi\sqrt{\omega_p\Omega_p}p}\int_0^\infty dq\frac{q}{\sqrt{\omega_q\Omega_q}}Q_\ell(z)f^\ell(q). \tag{90}$$

If we expand the relativistic free-particle energy,

$$\omega_p\simeq m_1\left(1+\frac{1}{2}\left(\frac{\mathbf{p}}{m_1}\right)^2\right),\quad \Omega_p\simeq m_2\left(1+\frac{1}{2}\left(\frac{\mathbf{p}}{m_2}\right)^2\right), \tag{91}$$

we obtain the two-particle Schrödinger radial equation in momentum space[18]

$$\left(\frac{\mathbf{p}^2}{2m_r}-\varepsilon\right)f^\ell(p)=\frac{\alpha}{\pi p}\int_0^\infty dq\,qQ_\ell(z)f^\ell(q), \tag{92}$$

where $\alpha=q_1q_2/4\pi$. The solutions of these equations are well known. They are given in Appendix D [formula (D12)].

VII. ENERGY EIGENVALUES AND RELATIVISTIC CORRECTIONS TO $O(\alpha^4)$ FOR ARBITRARY MASS RATIO

The energy eigenvalues $E_{n,J}$ for the states, when $\ell=J$, can be calculated from the equation

$$E\int_0^\infty dp\,p^2 f^J(p)f^J(p)=\int_0^\infty dp\,p^2(\omega_p+\Omega_p)f^J(p)f^J(p) - \frac{m_1m_2}{(2\pi)^3}\int_0^\infty\frac{p^2\,dp}{\sqrt{\omega_p\Omega_p}}\int_0^\infty\frac{q^2\,dq}{\sqrt{\omega_q\Omega_q}}\mathcal{K}(p,q)f^J(p)f^J(q). \tag{93}$$

For the $\ell=J\mp1$ triplet states we have the equation

$$E\int_0^\infty dp\,p^2 f^{\ell_i}(p)f^{\ell_i}(p)=\int_0^\infty dp\,p^2(\omega_p+\Omega_p)f^{\ell_i}(p)f^{\ell_i}(p) - \frac{m_1m_2}{(2\pi)^3}\int_0^\infty\frac{p^2\,dp}{\sqrt{\omega_p\Omega_p}}\int_0^\infty\frac{q^2\,dq}{\sqrt{\omega_q\Omega_q}}\mathcal{K}_{ij}(p,q)f^{\ell_i}(p)f^{\ell_j}(q). \tag{94}$$

To obtain results for E to $O(\alpha^4)$ we use the forms of the kernels expanded to $O(p^2/m^2)$ [expressions (75)–(88)] and replace $f^\ell(p)$ by their nonrelativistic (Schrödinger) form (D12) (see Appendix

D). The most important integrals, which we used for calculating (93) and (94), are given in Appendix D. It has been shown in Ref. 10 that the contribution of the kernels $\mathcal{K}_{12}$ and $\mathcal{K}_{21}$ in (94), which are responsible for coupling of the equations (62), is zero. Thus in the framework of the present approximation, the energy corrections for the triplet states with $\ell=J-1$ and $\ell=J+1$ can be calculated independently. We present the results in the form $\Delta\varepsilon=E+(\alpha^2 m_r/2n^2)-M$, $M=m_1+m_2$, $m_r=m_1m_2/(m_1+m_2)$.

A. Singlet states ($\ell=J=0$, $P=-1$) (which include the ground state)

The kinetic energy corrections,

$$\Delta\varepsilon_n^{(sg)(k)}=-\frac{\alpha^4 m_r}{n^3}\left(1-\frac{3}{8n}\right)\left(1-\frac{3m_r}{M}\right). \tag{95}$$

Orbital energy corrections,

$$\Delta\varepsilon_n^{(sg)(o)}=-\frac{\alpha^4 m_r}{n^3}\left(-\frac{1}{2}+\frac{3m_r}{M}-\frac{m_r}{M}\frac{1}{n}\right). \tag{96}$$

Spin–orbit energy corrections,

$$\Delta\varepsilon_n^{(sg)(s\text{-}o)}=0. \tag{97}$$

Spin–spin energy corrections,

$$\Delta\varepsilon_n^{(sg)(s-s)}=-\frac{\alpha^4 m_r}{n^3}\frac{2m_r}{M}. \tag{98}$$

The total energy corrections,

$$\Delta\varepsilon_n^{(sg)}=-\frac{\alpha^4 m_r}{n^3}\left(\frac{1}{2}+\frac{2m_r}{M}-\frac{1}{8n}\left(3-\frac{m_r}{M}\right)\right). \tag{99}$$

B. Quasisinglet, quasitriplet states [$\ell=J(J\geqslant 1)$, $P=(-1)^{J+1}$]

The kinetic energy and orbital energy corrections are common for quasisinglet and quasitriplet states,

$$\Delta\varepsilon_{n,J}^{(k)}=-\frac{\alpha^4 m_r}{2n^3}\left(1-\frac{3m_r}{M}\right)\left(\frac{2}{2J+1}-\frac{3}{4n}\right). \tag{100}$$

Orbital energy corrections,

$$\Delta\varepsilon_{n,J}^{(orb)}=-\frac{\alpha^4 m_r}{n^3}\frac{m_r}{M}\left(\frac{3}{2J+1}-\frac{1}{n}\right). \tag{101}$$

Spin–orbit energy corrections,

$$\Delta\varepsilon_{n,J}^{(s-o)}=\frac{\alpha^4 m_r}{2n^3}\frac{1}{M^2}\frac{-C_2^2((m_1+m_2)^2+2m_1m_2)+2C_1C_2\sqrt{J(J+1)}|m_2^2-m_1^2|}{(2J+1)(J+1)J}. \tag{102}$$

Spin–spin energy corrections,

$$\Delta\varepsilon_{n,J}^{(s-s)}=\frac{\alpha^4 m_r}{n^3}\frac{m_r}{M}\frac{C_2^2}{(2J+1)(J+1)J}. \tag{103}$$

The coefficients C_1 and C_2 are defined here in the same way as in formulas (79) and (80).

Thus, the total energy corrections are

$$\Delta\varepsilon_{n,J,s} = -\frac{\alpha^4 m_r}{n^3}\left(\frac{1}{2J+1}\left(1+\frac{1\mp\xi^{-1}}{4J(J+1)}\right)-\frac{1}{8n}\left(3-\frac{m_r}{M}\right)\right), \tag{104}$$

where upper and lower signs correspond to quasisinglet $s=s_s=0$ and quasitriplet $s=s_t=1$ states, respectively.

C. Triplet states $[\ell=J-1(J\geqslant 1),\ P=(-1)^J]$

Kinetic energy corrections,

$$\Delta\varepsilon_{n,J}^{(tr)(k)} = -\frac{\alpha^4 m_r}{n^3}\left(\frac{1}{2J-1}-\frac{3}{8n}\right)\left(1-\frac{3m_r}{M}\right). \tag{105}$$

Orbital energy corrections,

$$\Delta\varepsilon_{n,J}^{(tr)(o)} = -\frac{\alpha^4 m_r}{n^3}\left(-\frac{\delta_{J,1}}{2}+\left(\frac{3}{2J-1}-\frac{\delta_{J,1}}{2}-\frac{1}{n}\right)\frac{m_r}{M}\right). \tag{106}$$

Spin–orbit energy corrections,

$$\Delta\varepsilon_{n,J}^{(tr)(s-o)} = \frac{\alpha^4 m_r}{n^3}\frac{1-\delta_{J,1}}{2J(2J-1)}\left(1+\frac{2m_r}{M}\right). \tag{107}$$

Spin–spin energy corrections,

$$\Delta\varepsilon_{n,J}^{(tr)(s-s)} = -\frac{\alpha^4 m_r}{n^3}\left(\frac{1-\delta_{J,1}}{J(2J+1)(2J-1)}-\frac{2}{3}\delta_{J,1}\right)\frac{m_r}{M}. \tag{108}$$

The total energy corrections,

$$\Delta\varepsilon_{n,J}^{tr} = -\frac{\alpha^4 m_r}{n^3}\left(\frac{1}{2J-1}\left(1-\frac{1}{2J}-\frac{2m_r}{M}\frac{1}{2J+1}\right)-\frac{1}{8n}\left(3-\frac{m_r}{M}\right)\right). \tag{109}$$

The annihilation term for positroniumlike systems is

$$\Delta\varepsilon_{n}^{(anh)} = \frac{\alpha^4 m}{4n^3}\delta_{J,1}. \tag{110}$$

D. Triplet states $[\ell=J+1(J\geqslant 0),\ P=(-1)^J]$

The kinetic energy corrections,

$$\Delta\varepsilon_{n,J}^{(tr)(k)} = -\frac{\alpha^4 m_r}{n^3}\left(\frac{1}{2J+3}-\frac{3}{8n}\right)\left(1-\frac{3m_r}{M}\right). \tag{111}$$

Orbital energy corrections,

$$\Delta\varepsilon_{n,J}^{(tr)(o)} = -\frac{\alpha^4 m_r}{n^3}\left(\frac{3}{2J+3}-\frac{1}{n}\right)\frac{m_r}{M}. \tag{112}$$

Spin–orbit energy corrections,

$$\Delta\varepsilon_{n,J}^{(tr)(s-o)} = -\frac{\alpha^4 m_r}{n^3}\frac{1}{2(J+1)(2J+3)}\left(1+\frac{2m_r}{M}\right). \tag{113}$$

Spin–spin energy corrections,

$$\Delta\varepsilon_{n,J}^{(tr)(s-s)} = -\frac{\alpha^4 m_r}{n^3}\frac{1}{(J+1)(2J+3)(2J+1)}\frac{m_r}{M}. \tag{114}$$

The total energy corrections,

$$\Delta\varepsilon_{n,J}^{tr} = -\frac{\alpha^4 m_r}{n^3}\left(\frac{1}{2J+3}\left(1+\frac{1}{2(J+1)}+\frac{2m_r}{M}\frac{1}{2J+1}\right)-\frac{1}{8n}\left(3-\frac{m_r}{M}\right)\right). \tag{115}$$

For two equal masses our calculations agree with positronium results.[19] In the limit when one of the masses becomes infinite, say $m_2\to\infty$, the above results reduce to those obtained for a one-electron Dirac equation in a static Coulomb potential [to $O(\alpha^4)$], namely

$$\Delta\varepsilon_{n,j} = -\frac{\alpha^4 m_1}{n^3}\left(\frac{1}{2j+1}-\frac{3}{8n}\right). \tag{116}$$

Indeed, when $m_2\to\infty$ not only the total angular momentum, but also $\mathbf{J}_1^2=(\mathbf{L}_1+\mathbf{S}_1)^2$ and $\mathbf{S}_2^2$ are independently conserved. Thus, in this case, we can replace the quantum number J by $j-1/2$ in (100)–(104) (when $s=0$) and (111)–(115), and by $j+1/2$ in expressions (100)–(104) (when $s=1$) and (105)–(109). In other words,

$$\begin{aligned} &J\to j-1/2 \quad \text{for } |sg_q\rangle \text{ and } |tr_{\ell=J+1}\rangle,\\ &J\to j+1/2 \quad \text{for } |tr_q\rangle \text{ and } |tr_{\ell=J-1}\rangle. \end{aligned} \tag{117}$$

The quantum number $j=|\ell\pm 1/2|$ belongs here to the particle with mass m_1.

The results (99), (104), (109), and (115) agree with the calculations of Connell, based on a quasipotential reduction of the Bethe–Salpeter equation,[20] with those of Hersbach, who used a relativistic Lippman–Schwinger formulation,[21] and with those of Duviryak and Darewych based on a two-fermion Breit equation.[22] Grandy[8] obtained the same results from a perturbative solution of the coupled, nonlinear Dirac equations (8) and (9).

VIII. FINE AND HYPERFINE STRUCTURE: RECOIL EFFECTS

In this section we shall analyze the formulas obtained in the preceding section and we shall apply them to the energy spectra of some exotic atoms. To compare our calculations with experimental data we shall use the standard spectroscopical notation. First of all, it follows from (95)–(97) and (105)–(107) that the difference between the energy levels of $2S$ and $1S$ states (see Fig. 1) is given by formula

$$E(2S)-E(1S) = \frac{3\alpha^2 m_r}{8}+\frac{\alpha^4 m_r}{128}\left(11+15\frac{m_r}{M}\right). \tag{118}$$

Note that the formula (118) ignores hyperfine splitting(HFS), that is we exclude the spin–spin interaction. The fine structure [FS] of the $2P$-state follows similarly from (105)–(107) and (111)–(113), provided that we exclude the spin–spin interaction (108) and (114),

$$\Delta E_{\rm fs}(2P) \equiv E(2P_{3/2})-E(2P_{1/2}) = \frac{\alpha^4 m_r}{32}\left(1+\frac{2m_r}{M}\right). \tag{119}$$

The HFS of $1S_{1/2}$ and $2S_{1/2}$ is obtained from (99) and (109),

$$\Delta E_{\rm hfs}(1S_{1/2}) = \alpha^4 m_r\frac{8m_r}{3M}, \tag{120}$$

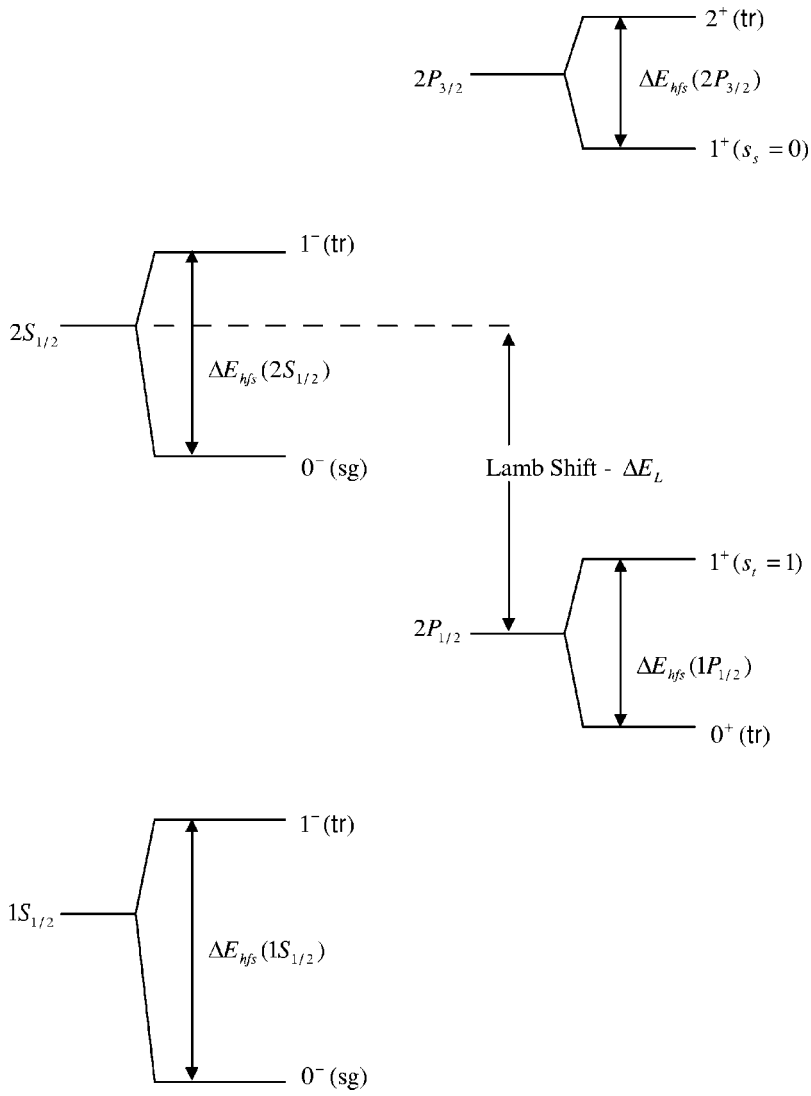

FIG. 1. Energy level diagram of a two-fermion system for $n=1$, 2 shells.

$$\Delta E_{\rm hfs}(2S_{1/2}) = \alpha^4 m_r \frac{m_r}{3M}. \tag{121}$$

Actually this hyperfine splitting, expressions (120) and (121), arises from the difference of spin–spin terms (98) and (108). The formulas (120) and (121) give the usual Fermi splitting.[18]

The HFS of states with $\ell>0$ is more complicated. For each $\ell>0$ we have two sorts of states with different J and s: states with $J=\ell+1$ and $J=\ell$, $s=s_s$ and states with $J=\ell-1$ and $J=\ell$, $s=s_t$. From (104), (109), and (115) we obtain the general HFS formulas for all quantum numbers n, ℓ and for any mass ratio,

$$\Delta E_{\rm hfs}(n,\ell,s_s) \equiv \Delta\varepsilon^{tr}_{n,J=\ell+1} - \Delta\varepsilon_{n,J=\ell,s_s} = \frac{\alpha^4 m_r}{n^3}\frac{1}{2\ell+1}\left(\frac{2\ell+1-\xi^{-1}}{4\ell(\ell+1)} + \frac{2m_r}{M}\frac{1}{2\ell+3}\right), \tag{122}$$

TABLE II. Hyperfine structure in muonium for $n=2$.

μ^+e^-	Experiment (Ref. 24)	Theory (126) and (127)	Theory with a_μ correction
$\Delta E_{\rm hfs}(2P_{1/2})$	186 MHz	185.80 MHz	186.01 MHz
$\Delta E_{\rm hfs}(2P_{3/2})$	74 MHz	74.43 MHz	74.52 MHz

$$\Delta E_{\rm hfs}(n,\ell,s_t) \equiv \Delta\varepsilon_{n,J=\ell,s_t} - \Delta\varepsilon^{tr}_{n,J=\ell-1} = \frac{\alpha^4 m_r}{n^3}\frac{1}{2\ell+1}\left(\frac{2\ell+1-\xi^{-1}}{4\ell(\ell+1)} + \frac{2m_r}{M}\frac{1}{2\ell-1}\right). \quad (123)$$

The quantity ξ is defined by (54), but with the quantum number J replaced by ℓ.

For the particular case when $m_2 \gg m_1$ we obtain from (122) and (123),

$$\Delta E_{\rm hfs}(n,l,s_s) = \frac{\alpha^4 m_1}{n^3}\frac{8(\ell+1)}{(2\ell+1)^2(2\ell+3)}\frac{m_1}{m_2}, \quad (124)$$

$$\Delta E_{\rm hfs}(n,\ell,s_t) = \frac{\alpha^4 m_1}{n^3}\frac{8\ell}{(2\ell+1)^2(2\ell-1)}\frac{m_1}{m_2}, \quad (125)$$

to leading order in m_1/m_2.

The approximate results (124) and (125) are the HFS formulas usually quoted in the literature (e.g., Ref. 18, p. 110, and Ref. 24, p. 836). As mentioned in Sec. VII, in the one-body limit ($m_2 \to \infty$), states with labels s_s and s_t can be characterized by the quantum numbers $j=\ell+1/2$ and $j=\ell-1/2$, respectively. In this one-body picture, the labels s_s and s_t should be replaced by j in the formulas (124) and (125). Note here that, because of the mixed nature of the states $n\ell_{\ell-1/2}(\ell=J, s_t=1)$ and $n\ell_{\ell+1/2}(\ell=J, s_s=0)$, the spin–orbit interaction contributes to the spliting as well. The splitting is largest when $m_1=m_2$ (positronium) and disappears for all states in the one-body limit.

It is easy to get the HFS of $2P_{1/2}$, $2P_{3/2}$ states from (122) and (123):

$$\Delta E_{\rm hfs}(2P_{1/2}) = \alpha^4 m_r\left(\frac{1}{64} - \frac{\xi^{-1}}{192} + \frac{1}{12}\frac{m_r}{M}\right), \quad (126)$$

$$\Delta E_{\rm hfs}(2P_{3/2}) = \alpha^4 m_r\left(\frac{1}{64} - \frac{\xi^{-1}}{192} + \frac{1}{60}\frac{m_r}{M}\right), \quad (127)$$

where $\xi^{-1}=\sqrt{8[(m_1-m_2)/M]^2+1}$. Note that, if we use the pure triplet state instead of the mixed states, we get the following expressions for hyperfine splitting: $E_{\rm hfs}(2P_{1/2})=\alpha^4 m_r\left[\frac{1}{96}+(m_r/12M)\right]$, $E_{\rm hfs}(2P_{3/2})=\alpha^4 m_r\left[\frac{1}{96}+(m_r/60M)\right]$. These give the correct results only for $m_1=m_2$.

The energy level diagram for $n=1$, 2 shells is presented in Fig. 1. Our calculations for FS (119) and HFS (120) and (121) reproduce the well-known result (see, for example, the recent and comprehensive reviews of Refs. 23 and 27). Thus we concentrate here on the discussion of HFS of exited states described by (122) and (123). As already mentioned, formulas (122) and (123) are a consequence of the general formulas (104), (109), and (115), which have been obtained also in Refs. 8 and 20–22. However, to the best of our knowledge, the derivation and analysis of (122) and (123) have never been presented. The results of our calculations of HFS and comparison with experimental data for muonium and hydrogen are summarized in Tables II and III. Because of the absence of experimental data for muonic hydrogen we compare our results with the calculations of Pachucki[28] in Table IV.

Although hydrogen and muonic hydrogen are not strictly leptonic atoms, we can take into account the proton anomalous magnetic moment in the hyperfine splitting in the same phenomenological manner as was done by Barker and Glover.[29] Thus, to get the corrected result for HFS in hydrogen and muonic hydrogen, we multiply the expression for $\Delta E_{\rm hfs}$ by the factor $(1+k_p)$,

TABLE III. Hyperfine structure in hydrogen for $n=2$.

H	Experiment (Refs. 25,26)	Theory (126) and (127)	Theory with k_p correction
$\Delta E_{\mathrm{hfs}}(2P_{1/2})$	59.1721 MHz (Ref. 25)	21.1698 MHz	59.1241 MHz
$\Delta E_{\mathrm{hfs}}(2P_{3/2})$	23.6541 MHz (Ref. 25)	8.4696 MHz	23.6543 MHz

where $k_p=1.792\,847$ is the anomalous magnetic moment of the proton. The last columns in Tables III and IV give the HFS corrected by the factor $(1+k_p)$. The anomalous magnetic moment of the muon is very small, nevertheless for the sake of completeness, we provide the same corrections for muonium, where we use the factor $(1+a_\mu)(a_\mu=0.001\,166)$ to get the result of the last column in Table II from those of the third column. We note that doing so improves the agreement between the calculated and the experimental HFS results in most cases, and dramatically so for hydrogen and muonic hydrogen.

From Tables II and III we see that the calculated $O(\alpha^4)$ results agree with observation remarkably well. Note that if we use the approximate m_1/m_2 expansion formulas (124) and (125), for example, for HFS of $2P_{1/2}$ and $2P_{3/2}$ states we would get, for muonium (with a_μ corrections), the result $\Delta E_{\mathrm{hfs}}(2P_{1/2})=188.50$ MHz, $\Delta E_{\mathrm{hfs}}(2P_{3/2})=75.40$ MHz. These approximate results do not agree as well with observation as the values calculated without the m_1/m_2 expansion, and hence they differ from what we give in the last column of Table II. Note that this difference can be of the same order as the contribution of higher order in α for HFS. Using (124) and (125) for muonic hydrogen gives (with k_p corrections) $\Delta E_{\mathrm{hfs}}(2P_{1/2})=10.47$ meV, $\Delta E_{\mathrm{hfs}}(2P_{3/2})=4.19$ meV. The m_1/m_2 expansion approximation is not significant for hydrogen for which the mass ratio is very small, but it is appreciable for muonium and particularly for muonic hydrogen. Since our results are true for arbitrary mass ratios we can speak here about recoil *effects* rather than about recoil *corrections* to α^4.

IX. CONCLUDING REMARKS

We have used the variational method within the Hamiltonian formalism of QED to derive relativistic momentum-space wave equations for two-fermion systems like muonium. The trial states are chosen to be eigenstates of the total angular momentum operators $\hat{\mathbf{J}}^2, \hat{J}_3$ and parity, as well as charge conjugation for particle–antiparticle systems. A general relativistic reduction of the wave equations to radial form is given for arbitrary masses of the two fermions. For given J there is a single radial equation for total spin zero singlet states, but for spin triplet states there are, in general coupled equations. We have shown how classification of the states follows naturally from the system of eigenvalue equations (37), given our trial state.

It is not possible, as far as we know, to obtain analytic solutions of our relativistic radial equations nor the resulting eigenvalues of the two fermion system that they describe. However, it is possible to obtain $O(\alpha^4)$ corrections to the energy eigenvalues analytically for all states using perturbation theory.

We have compared our calculated results with experiment for hyperfine splitting of low-lying levels in muonium and hydrogen. We find good agreement for muonium, as well as for hydrogen provided that we take into account the anomalous magnetic moment of the proton.

TABLE IV. Hyperfine structure in muonic hydrogen for $n=2$.

μ^-H	Theory (Ref. 27)	Theory (126) and (127)	Theory with k_p correction
$\Delta E_{\mathrm{hfs}}(2P_{1/2})$	7.96 meV	2.79 meV	7.79 meV
$\Delta E_{\mathrm{hfs}}(2P_{3/2})$	3.39 meV	1.16 meV	3.23 meV

The method presented here can be generalized to include effects of higher order in alpha by using dressed propagators in place of the bare propagators. This shall be the subject of a forthcoming work.

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APPENDIX A: TOTAL ANGULAR MOMENTUM OPERATOR IN RELATIVISTIC FORM

The total angular momentum operator is defined by the expression

$$\hat{\mathbf{J}} = \int \mathrm{d}^3\mathbf{x}\ \psi^\dagger(x)(\hat{\mathbf{L}} + \hat{\mathbf{S}})\psi(x) + \int \mathrm{d}^3\mathbf{x}\ \phi^\dagger(x)(\hat{\mathbf{L}} + \hat{\mathbf{S}})\phi(x), \tag{A1}$$

where $\hat{\mathbf{L}}$ is the orbital angular momentum and $\hat{\mathbf{S}}$ is the spin operator, $\hat{\mathbf{L}} = \hat{\mathbf{x}} \times \hat{\mathbf{p}}$ and $\hat{\mathbf{S}} = \frac{1}{2}\hat{\vec{\sigma}}$. We use the standard representation for the Pauli matrices,

$$\hat{\vec{\sigma}} = \begin{bmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{bmatrix}, \tag{A2}$$

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{A3}$$

Using the field operators $\psi(x)$ and $\phi(x)$ in the form (18) and (19), after tedious calculations we obtain the expression for operator $\hat{\mathbf{J}}$. It consists of three parts, two total angular momentum operators of each particle–antiparticle system[10] and the following part, relevant to our considerations:

$$\hat{J}_1 = \int \mathrm{d}^3\mathbf{q} \begin{pmatrix} \hat{L}_{q1}(b^\dagger_{\mathbf{q}\uparrow} b_{\mathbf{q}\uparrow} + b^\dagger_{\mathbf{q}\downarrow} b_{\mathbf{q}\downarrow} + D^\dagger_{\mathbf{q}\uparrow} D_{\mathbf{q}\uparrow} + D^\dagger_{\mathbf{q}\downarrow} D_{\mathbf{q}\downarrow}) \\ + \frac{1}{2}(b^\dagger_{\mathbf{q}\uparrow} b_{\mathbf{q}\downarrow} + b^\dagger_{\mathbf{q}\downarrow} b_{\mathbf{q}\uparrow} + D^\dagger_{\mathbf{q}\downarrow} D_{\mathbf{q}\uparrow} + D^\dagger_{\mathbf{q}\uparrow} D_{\mathbf{q}\downarrow}) \end{pmatrix},$$

$$\hat{J}_2 = \int \mathrm{d}^3\mathbf{q} \begin{pmatrix} \hat{L}_{q2}(b^\dagger_{\mathbf{q}\uparrow} b_{\mathbf{q}\uparrow} + b^\dagger_{\mathbf{q}\downarrow} b_{\mathbf{q}\downarrow} + D^\dagger_{\mathbf{q}\uparrow} D_{\mathbf{q}\uparrow} + D^\dagger_{\mathbf{q}\downarrow} D_{\mathbf{q}\downarrow}) \\ + \frac{i}{2}(- b^\dagger_{\mathbf{q}\uparrow} b_{\mathbf{q}\downarrow} + b^\dagger_{\mathbf{q}\downarrow} b_{\mathbf{q}\uparrow} - D^\dagger_{\mathbf{q}\uparrow} D_{\mathbf{q}\downarrow} + D^\dagger_{\mathbf{q}\downarrow} D_{\mathbf{q}\uparrow}) \end{pmatrix}, \tag{A4}$$

$$\hat{J}_3 = \int \mathrm{d}^3\mathbf{q} \begin{pmatrix} \hat{L}_{q3}(b^\dagger_{\mathbf{q}\uparrow} b_{\mathbf{q}\uparrow} + b^\dagger_{\mathbf{q}\downarrow} b_{\mathbf{q}\downarrow} + D^\dagger_{\mathbf{q}\uparrow} D_{\mathbf{q}\uparrow} + D^\dagger_{\mathbf{q}\downarrow} D_{\mathbf{q}\downarrow}) \\ + \frac{1}{2}(b^\dagger_{\mathbf{q}\uparrow} b_{\mathbf{q}\uparrow} - b^\dagger_{\mathbf{q}\downarrow} b_{\mathbf{q}\downarrow} + D^\dagger_{\mathbf{q}\uparrow} D_{\mathbf{q}\uparrow} - D^\dagger_{\mathbf{q}\downarrow} D_{\mathbf{q}\downarrow}) \end{pmatrix}.$$

Here $\hat{\mathbf{L}}_q$ is the orbital angular momentum operator in momentum representation,

$$(\hat{\mathbf{L}}_q)_i \equiv \hat{L}_{qi} = -i(\mathbf{q} \times \nabla_q)_i. \tag{A5}$$

Note that these expressions are valid for any t, since the time-dependent phase factors of the form $e^{i\omega_q t}$ cancel out. For the operator $\hat{\mathbf{J}}^2 = \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2$ we have

$$\hat{\mathbf{J}}^2 = \int \mathrm{d}^3\mathbf{q}\begin{pmatrix} \left(\hat{\mathbf{L}}_q^2 + \frac{3}{4}\right)(b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\uparrow} + b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\downarrow} + D^\dagger_{\mathbf{q}\uparrow}D_{\mathbf{q}\uparrow} + D^\dagger_{\mathbf{q}\downarrow}D_{\mathbf{q}\downarrow}) \\ + \hat{L}_{q-}b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\downarrow} + \hat{L}_{q+}b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\uparrow} + \hat{L}_{q-}D^\dagger_{\mathbf{q}\uparrow}D_{\mathbf{q}\downarrow} + \hat{L}_{q+}D^\dagger_{\mathbf{q}\downarrow}D_{\mathbf{q}\uparrow} \\ + \hat{L}_{q3}(b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\uparrow} - b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\downarrow} + D^\dagger_{\mathbf{q}\uparrow}D_{\mathbf{q}\uparrow} - D^\dagger_{\mathbf{q}\downarrow}D_{\mathbf{q}\downarrow}) \end{pmatrix}$$

$$+ \frac{1}{2}\int d^3\mathbf{q}'d^3\mathbf{q}\begin{pmatrix} 2\hat{\mathbf{L}}_{q'}\cdot\hat{\mathbf{L}}_q\begin{pmatrix} b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}D^\dagger_{\mathbf{q}\uparrow}D_{\mathbf{q}\uparrow} + b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}D^\dagger_{\mathbf{q}\downarrow}D_{\mathbf{q}\downarrow} \\ + b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}D^\dagger_{\mathbf{q}\uparrow}D_{\mathbf{q}\uparrow} + b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}D^\dagger_{\mathbf{q}\downarrow}D_{\mathbf{q}\downarrow} \end{pmatrix} \\ + \frac{1}{2}(b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}D^\dagger_{\mathbf{q}\uparrow}D_{\mathbf{q}\uparrow} - b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}D^\dagger_{\mathbf{q}\downarrow}D_{\mathbf{q}\downarrow}) \\ - \frac{1}{2}(b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}D^\dagger_{\mathbf{q}\uparrow}D_{\mathbf{q}\uparrow} - b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}D^\dagger_{\mathbf{q}\downarrow}D_{\mathbf{q}\downarrow}) \\ + b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\downarrow}D^\dagger_{\mathbf{q}\downarrow}D_{\mathbf{q}\uparrow} + b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\uparrow}D^\dagger_{\mathbf{q}\uparrow}D_{\mathbf{q}\downarrow} \\ + \hat{L}_{q'+}\begin{pmatrix} b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}D^\dagger_{\mathbf{q}\downarrow}D_{\mathbf{q}\uparrow} + b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}D^\dagger_{\mathbf{q}\downarrow}D_{\mathbf{q}\uparrow} \\ + b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\uparrow}D^\dagger_{\mathbf{q}'\uparrow}D_{\mathbf{q}'\uparrow} + b^\dagger_{\mathbf{q}\downarrow}b_{\mathbf{q}\uparrow}D^\dagger_{\mathbf{q}'\downarrow}D_{\mathbf{q}'\downarrow} \end{pmatrix} \\ + \hat{L}_{q'-}\begin{pmatrix} b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}D^\dagger_{\mathbf{q}\uparrow}D_{\mathbf{q}\downarrow} + b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}D^\dagger_{\mathbf{q}\uparrow}D_{\mathbf{q}\downarrow} \\ + b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\downarrow}D^\dagger_{\mathbf{q}'\uparrow}D_{\mathbf{q}'\uparrow} + b^\dagger_{\mathbf{q}\uparrow}b_{\mathbf{q}\downarrow}D^\dagger_{\mathbf{q}'\downarrow}D_{\mathbf{q}'\downarrow} \end{pmatrix} \\ + (\hat{L}_{q'3} + \hat{L}_{q3})(b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}D^\dagger_{\mathbf{q}\uparrow}D_{\mathbf{q}\uparrow} - b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}D^\dagger_{\mathbf{q}\downarrow}D_{\mathbf{q}\downarrow}) \\ - (\hat{L}_{q'3} - \hat{L}_{q3})(b^\dagger_{\mathbf{q}'\uparrow}b_{\mathbf{q}'\uparrow}D^\dagger_{\mathbf{q}\downarrow}D_{\mathbf{q}\downarrow} - b^\dagger_{\mathbf{q}'\downarrow}b_{\mathbf{q}'\downarrow}D^\dagger_{\mathbf{q}\uparrow}D_{\mathbf{q}\uparrow}) \end{pmatrix}, \tag{A6}$$

where

$$\hat{L}_{q+} = \hat{L}_{q1} + i\hat{L}_{q2}, \quad \hat{L}_{q-} = \hat{L}_{q1} - i\hat{L}_{q2}. \tag{A7}$$

The formulas (A4) and (A6) apply to the particle–antiparticle system[10] as well if the operators $D^\dagger$ and D are formally replaced by $d^\dagger$ and d, respectively.

The requirements (37) with trial state in the form of (24) lead to the system of equations $[F_{s_1s_2}(\mathbf{p}) \equiv F_{s_1s_2}]$:

$$\begin{gathered} (\hat{L}_3 + 1)F_{11} = m_J F_{11}, \\ \hat{L}_3 F_{12} = m_J F_{12}, \\ \hat{L}_3 F_{21} = m_J F_{21}, \\ (\hat{L}_3 - 1)F_{22} = m_J F_{22}, \end{gathered} \tag{A8}$$

$$\begin{gathered} (J(J+1) - \hat{\mathbf{L}}^2 - 2 - 2\hat{L}_3)F_{11} = \hat{L}_-(F_{12} + F_{21}), \\ (J(J+1) - \hat{\mathbf{L}}^2 - 1)F_{12} = F_{21} + \hat{L}_+F_{11} + \hat{L}_-F_{22}, \\ (J(J+1) - \hat{\mathbf{L}}^2 - 1)F_{21} = F_{12} + \hat{L}_+F_{11} + \hat{L}_-F_{22}, \end{gathered} \tag{A9}$$

$$(J(J+1)-\hat{\mathbf{L}}^2-2+2\hat{L}_3)F_{22}=\hat{L}_+(F_{12}+F_{21}).$$

After substitution of the functions $F_{s_1s_2}$, Eq. (39), into the system (A8) and (A9) we get

$$m_{12}=m_{21}=m_J,\quad m_{11}=m_J-1,\quad m_{22}=m_J+1, \tag{A10}$$

$$\ell_{11}=\ell_{22}=\ell_{12}=\ell_{21}\equiv\ell, \tag{A11}$$

and

$$(J(J+1)-\ell(\ell+1)-2m_J)f^\ell_{11}(p)=\sqrt{(\ell-m_J+1)(\ell+m_J)}f^\ell_{12}(p)+\sqrt{(\ell-m_J+1)(\ell+m_J)}f^\ell_{21}(p), \tag{A12}$$

$$(J(J+1)-\ell(\ell+1)-1)f^\ell_{12}(p)=f^\ell_{21}(p)+\sqrt{(\ell+m_J)(\ell-m_J+1)}f^\ell_{11}(p)+\sqrt{(\ell-m_J)(\ell+m_J+1)}f^\ell_{22}(p), \tag{A13}$$

$$(J(J+1)-\ell(\ell+1)-1)f^\ell_{21}(p)=f^\ell_{12}(p)+\sqrt{(\ell+m_J)(\ell-m_J+1)}f^\ell_{11}(p)+\sqrt{(\ell-m_J)(\ell+m_J+1)}f^\ell_{22}(p), \tag{A14}$$

$$(J(J+1)-\ell(\ell+1)+2m_J)f^\ell_{22}(p)=\sqrt{(\ell+m_J+1)(\ell-m_J)}f^\ell_{12}(p)+\sqrt{(\ell+m_J+1)(\ell-m_J)}f^\ell_{21}(p). \tag{A15}$$

The solution of this system leads to two categories of relations among the functions $f^\ell_{s_1s_2}(p)$. The first category, which we call the trivial one, is obtained when $f^\ell_{11}(p)=f^\ell_{22}(p)=0$. In this case, as is easy to see from (A12) and (A15), we get $f^\ell_{12}(p)=-f^\ell_{21}(p)$. This solution corresponds to the singlet states of the system with $\ell=J(J\geqslant 0)$ [as follows from (A13) or (A14)]. This simple relation allows us to write the general formula for the components $f^\ell_{s_1s_2}(p)$ in the following form:

$$f^\ell_{s_1s_2}(p)=C^{(sg)m_{s_1s_2}}f^J(p), \tag{A16}$$

where the radial function $f^J(p)$ is common for all components, and the coefficients $C^{(sg)m_{s_1s_2}}$ have the following properties:

$$C^{(sg)m_{11}}=C^{(sg)m_{22}}=0,\quad C^{(sg)m_{21}}=-C^{(sg)m_{12}}=1. \tag{A17}$$

The formulas (A16) and (A17) with the notation $f^\ell_{s_1s_2}(p)\equiv f^{(sg)J}_{s_1s_2}(p)$ make Eq. (42) evident.

The second category corresponds to the triplet states, when $f^\ell_{11}(p), f^\ell_{22}(p)\neq 0$. First of all, it is not difficult to see from (A13) and (A14) that $f^\ell_{12}(p)=f^\ell_{21}(p)\equiv f^\ell(p)$, and after some simple calculations we get for $\ell=J-1(J\geqslant 1)$,

$$(J-m_J)f^{J-1}_{11}(p)=\sqrt{(J-m_J)(J+m_J-1)}f^{J-1}(p), \tag{A18}$$

$$(J+m_J)f^{J-1}_{22}(p)=\sqrt{(J+m_J)(J-m_J-1)}f^{J-1}(p), \tag{A19}$$

for $\ell=J(J\geqslant 1)$,

$$m_Jf^J_{11}(p)=-\sqrt{(J+m_J)(J-m_J+1)}f^J(p), \tag{A20}$$

$$m_Jf^J_{22}(p)=\sqrt{(J-m_J)(J+m_J+1)}f^J(p), \tag{A21}$$

for $\ell=J+1(J\geqslant 0)$,

TABLE V. The CG coefficients for triplet states (total spin $S=1$).

	$m_s=+1$	$m_s=0$	$m_s=-1$
$\ell=J-1$	$\left(\frac{(J+m_J-1)(J+m_J)}{J(2J-1)}\right)^{1/2}$	$\left(\frac{(J-m_J)(J+m_J)}{J(2J-1)}\right)^{1/2}$	$\left(\frac{(J-m_J-1)(J-m_J)}{J(2J-1)}\right)^{1/2}$
$\ell=J$	$-\left(\frac{(J+m_J)(J-m_J+1)}{J(J+1)}\right)^{1/2}$	$\frac{m_J}{(J(J+1))^{1/2}}$	$\left(\frac{(J-m_J)(J+m_J+1)}{J(J+1)}\right)^{1/2}$
$\ell=J+1$	$\left(\frac{(J-m_J+1)(J-m_J+2)}{(J+1)(2J+3)}\right)^{1/2}$	$-\left(\frac{(J-m_J+1)(J+m_J+1)}{(J+1)(2J+3)}\right)^{1/2}$	$\left(\frac{(J+m_J+2)(J+m_J+1)}{(J+1)(2J+3)}\right)^{1/2}$

$$(J+1+m_J)f_{11}^{J+1}(p) = -\sqrt{(J-m_J+2)(J+m_J+1)}\,f^{J+1}(p), \tag{A22}$$

$$(J+1-m_J)f_{22}^{J+1}(p) = -\sqrt{(J-m_J+1)(J+m_J+2)}\,f^{J+1}(p). \tag{A23}$$

It is convenient to introduce the table of coefficients $C_{Jm_J}^{(tr)\ell m_s}$, which represent the relations in (A18)–(A23). (See Table V.)

Thus, we can write the relations between the components $f_{s_1s_2}^{\ell}(p)$ in the compact form

$$f_{s_1s_2}^{\ell}(p) = C_{Jm_J}^{(tr)\ell m_s} f^{\ell}(p). \tag{A24}$$

The coefficients $C_{Jm_J}^{(tr)\ell m_s}$ coincide with the usual Clebsch–Gordan coefficients for total spin $S=1$ except for a factor $\sqrt{2}$ in the denominator. The expression (39) can now be written in an explicit form

$$F_{s_1s_2}(\mathbf{p}) = C_{Jm_J}^{(tr)(J-1)m_s} f^{J-1}(p) Y_{J-1}^{m_{s_1s_2}}(\hat{\mathbf{p}}) + C_{Jm_J}^{(tr)(J)m_s} f^{J}(p) Y_{J}^{m_{s_1s_2}}(\hat{\mathbf{p}}) + C_{Jm_J}^{(tr)(J+1)m_s} f^{J+1}(p) Y_{J+1}^{m_{s_1s_2}}(\hat{\mathbf{p}}). \tag{A25}$$

However, as is shown in Appendix B, the first and third terms have parity $P=(-1)^J$, while the second term has parity $P=(-1)^{J+1}$. Thus, we get the result (57) by suppressing the second term in (A25). The second term in (A25) is associated with the singlet solution (43) for the mixed-spin states, which have the same parity.

APPENDIX B: PARITY AND CHARGE CONJUGATION

We consider the application of the parity operator to the trial state (24),

$$\hat{\mathcal{P}}|\psi_{\text{trial}}\rangle = \sum_{s_1s_2}\int \mathrm{d}^3\mathbf{p}\, F_{s_1s_2}(\mathbf{p})\hat{\mathcal{P}}b_{\mathbf{p}s_1}^{\dagger}D_{-\mathbf{p}s_2}^{\dagger}|0\rangle = \sum_{s_1s_2}\int \mathrm{d}^3\mathbf{p}\, F_{s_1s_2}(\mathbf{p})\hat{\mathcal{P}}b_{\mathbf{p}s_1}^{\dagger}\hat{\mathcal{P}}^{-1}\hat{\mathcal{P}}D_{-\mathbf{p}s_2}^{\dagger}\hat{\mathcal{P}}^{-1}\hat{\mathcal{P}}|0\rangle. \tag{B1}$$

Making use of the properties

$$\hat{\mathcal{P}}b_{\mathbf{p}s_1}^{\dagger}\hat{\mathcal{P}}^{-1} = \eta^P b_{-\mathbf{p}s_1}^{\dagger}, \quad \hat{\mathcal{P}}D_{-\mathbf{p}s_2}^{\dagger}\hat{\mathcal{P}}^{-1} = -\eta^P D_{\mathbf{p}s_2}^{\dagger}, \quad \hat{\mathcal{P}}|0\rangle = |0\rangle, \tag{B2}$$

where η^P is the intrinsic parity ($(\eta^P)^2=1$), it follows that

$$\begin{aligned}\hat{\mathcal{P}}|\psi_{\text{trial}}\rangle &= \sum_{s_1s_2}\int \mathrm{d}^3\mathbf{p}\, F_{s_1s_2}(\mathbf{p})\hat{\mathcal{P}}b_{\mathbf{p}s_1}^{\dagger}D_{-\mathbf{p}s_2}^{\dagger}|0\rangle \\ &= -\sum_{s_1s_2}\int \mathrm{d}^3\mathbf{p}\, F_{s_1s_2}(-\mathbf{p})b_{\mathbf{p}s_1}^{\dagger}D_{-\mathbf{p}s_2}^{\dagger}|0\rangle = P\sum_{s_1s_2}\int \mathrm{d}^3\mathbf{p}\, F_{s_1s_2}(\mathbf{p})b_{\mathbf{p}s_1}^{\dagger}D_{-\mathbf{p}s_2}^{\dagger}|0\rangle,\end{aligned} \tag{B3}$$

where the parity eigenvalue P depends on the symmetry of $F_{s_1s_2}(p)$ in different states. For the singlet states ($\ell=J$) we get from (43) $F_{s_1s_2}(-p)=(-1)^J F_{s_1s_2}(p)$, so $P=(-1)^{J+1}$. For the triplet states

with $\ell=J$ we get from (48) $F_{s_1s_2}(-p)=(-1)^J F_{s_1s_2}(p)$, so $P=(-1)^{J+1}$. For the triplet states with $\ell=J\pm1$ we get from (57) $F_{s_1s_2}(-p)=(-1)^{J+1}F_{s_1s_2}(p)$, so $P=(-1)^J$.

Charge conjugation is associated with the interchange of the particle and antiparticle. Applying the charge conjugation operator to the trial state of the form (24) we get

$$\hat{C}|\psi_{\text{trial}}\rangle=\sum_{s_1s_2}\int \mathrm{d}^3\mathbf{p}\, F_{s_1s_2}(\mathbf{p})\hat{C}b^\dagger_{\mathbf{p}s_1}d^\dagger_{-\mathbf{p}s_2}|0\rangle=\sum_{s_1s_2}\int \mathrm{d}^3\mathbf{p}\, F_{s_1s_2}(\mathbf{p})\hat{C}b^\dagger_{\mathbf{p}s_1}\hat{C}^{-1}\hat{C}d^\dagger_{-\mathbf{p}s_2}\hat{C}^{-1}\hat{C}|0\rangle. \tag{B4}$$

Using the relations

$$\hat{C}b^\dagger_{\mathbf{p}s_1}\hat{C}^{-1}=\eta^C d^\dagger_{\mathbf{p}s_1},\quad \hat{C}d^\dagger_{-\mathbf{p}s_2}\hat{C}^{-1}=\eta^C b^\dagger_{-\mathbf{p}s_2},\quad \hat{C}|0\rangle=|0\rangle, \tag{B5}$$

where $(\eta^C)^2=1$, we obtain

$$\hat{C}|\psi_{\text{trial}}\rangle=-\sum_{s_1s_2}\int \mathrm{d}^3\mathbf{p}\, F_{s_2s_1}(-\mathbf{p})b^\dagger_{\mathbf{p}s_1}d^\dagger_{-\mathbf{p}s_2}|0\rangle=C\sum_{s_1s_2}\int \mathrm{d}^3\mathbf{p}\, F_{s_1s_2}(\mathbf{p})b^\dagger_{\mathbf{p}s_1}d^\dagger_{-\mathbf{p}s_2}|0\rangle, \tag{B6}$$

where the charge conjugation quantum number C depends on the symmetry of $F_{s_1s_2}(p)$ in different states.

For the singlet states ($\ell=J$) we get from (43) $F_{s_2s_1}(-p)=(-1)^{J+1}F_{s_1s_2}(p)$, so $C=(-1)^J$.

For the triplet states with $\ell=J$ we get from (48) $F_{s_2s_1}(-p)=(-1)^J F_{s_1s_2}(p)$, so $C=(-1)^{J+1}$.

For the triplet states with $\ell=J\pm1$ we get from (57) $F_{s_2s_1}(-p)=(-1)^{J+1}F_{s_1s_2}(p)$, so $C=(-1)^J$.

APPENDIX C: EXPANSION OF THE SPINORS AND $\mathcal{M}$-MATRIX ELEMENTS

We recall the form of the particle spinors,

$$u(\mathbf{p},i)=N_{\mathbf{p}}\begin{bmatrix}1\\ \dfrac{(\vec{\sigma}\cdot\mathbf{p})}{\omega_p+m_1}\end{bmatrix}\varphi_i, \tag{C1}$$

where

$$\varphi_1=\begin{bmatrix}1\\0\end{bmatrix},\quad \varphi_2=\begin{bmatrix}0\\1\end{bmatrix},\quad N_{\mathbf{p}}=\sqrt{\frac{\omega_p+m_1}{2m_1}}. \tag{C2}$$

The antiparticle or "positron" representation for the $v_i(p)$ spinors has the form

$$v(\mathbf{p},i)=N_{\mathbf{p}}\begin{bmatrix}\dfrac{(\vec{\sigma}\cdot\mathbf{p})}{\omega_p+m_1}\\ 1\end{bmatrix}\chi_i, \tag{C3}$$

where

$$\chi_1=\begin{bmatrix}0\\1\end{bmatrix},\quad \chi_2=-\begin{bmatrix}1\\0\end{bmatrix}. \tag{C4}$$

The normalization is

$$\overline{u}(\mathbf{p},i)u(\mathbf{p},j)=\delta_{ij},\quad \overline{v}(\mathbf{p},i)v(\mathbf{p},j)=-\delta_{ij}. \tag{C5}$$

Expanding in powers of p/m_1 and keeping the lowest order nontrivial terms,

$$\frac{(\vec{\sigma}\cdot\mathbf{p})}{\omega_p + m_1} \simeq \frac{(\vec{\sigma}\cdot\mathbf{p})}{2m_1}, \tag{C6}$$

$$N_{\mathbf{p}} = \sqrt{\frac{\omega_p + m_1}{2m_1}} \simeq 1 + \frac{\mathbf{p}^2}{8m_1^2}, \tag{C7}$$

we obtain the result

$$u(\mathbf{p},i) \simeq \left(1 + \frac{\mathbf{p}^2}{8m_1^2}\right)\begin{bmatrix} 1 \\ \dfrac{(\vec{\sigma}\cdot\mathbf{p})}{2m_1} \end{bmatrix}\varphi_i = \begin{bmatrix} \left(1 + \dfrac{\mathbf{p}^2}{8m_1^2}\right) \\ \dfrac{(\vec{\sigma}\cdot\mathbf{p})}{2m_1} \end{bmatrix}\varphi_i, \tag{C8}$$

$$v(\mathbf{p},i) \simeq \left(1 + \frac{\mathbf{p}^2}{8m_1^2}\right)\begin{bmatrix} \dfrac{(\vec{\sigma}\cdot\mathbf{p})}{2m_1} \\ 1 \end{bmatrix}\chi_i = \begin{bmatrix} \dfrac{(\vec{\sigma}\cdot\mathbf{p})}{2m_1} \\ \left(1 + \dfrac{\mathbf{p}^2}{8m_1^2}\right) \end{bmatrix}\chi_i. \tag{C9}$$

The M-matrix elements (70)–(73) have the following nonzero components.

Orbital,

$$\begin{aligned}\mathcal{M}^{(orb)}_{1111}(\mathbf{q},\mathbf{p}) = \mathcal{M}^{(orb)}_{1212}(\mathbf{q},\mathbf{p}) = \mathcal{M}^{(orb)}_{2121}(\mathbf{q},\mathbf{p}) \\ = \mathcal{M}^{(orb)}_{2222}(\mathbf{q},\mathbf{p}) = \frac{iq_1q_2}{(\mathbf{p}-\mathbf{q})^2} + \frac{iq_1q_2}{m_1m_2}\left(\frac{1}{2}\left(\frac{m_1}{m_2} + \frac{m_2}{m_1}\right)\right. \\ \left.\times\left(\frac{1}{4} + \frac{\mathbf{q}\cdot\mathbf{p}}{(\mathbf{p}-\mathbf{q})^2}\right) + \frac{(\mathbf{p}\times\mathbf{q})^2}{(\mathbf{p}-\mathbf{q})^4}\right),\end{aligned} \tag{C10}$$

Spin–orbit,

$$\mathcal{M}^{(s-o)}_{1111}(\mathbf{q},\mathbf{p}) = \frac{iq_1q_2}{8m_1m_2}\left(\frac{m_2}{m_1} + \frac{m_1}{m_2} + 4\right)\frac{p_-q_+ - p_+q_-}{(\mathbf{p}-\mathbf{q})^2}, \tag{C11}$$

$$\mathcal{M}^{(s-o)}_{2222}(\mathbf{q},\mathbf{p}) = \frac{iq_1q_2}{8m_1m_2}\left(\frac{m_2}{m_1} + \frac{m_1}{m_2} + 4\right)\frac{p_+q_- - p_-q_+}{(\mathbf{p}-\mathbf{q})^2}, \tag{C12}$$

$$\mathcal{M}^{(s-o)}_{1112}(\mathbf{q},\mathbf{p}) = \mathcal{M}^{(s-o)}_{2122}(\mathbf{q},\mathbf{p}) = \frac{iq_1q_2}{4m_1m_2}\left(\frac{m_1}{m_2} + 2\right)\frac{p_3q_- - p_-q_3}{(\mathbf{p}-\mathbf{q})^2}, \tag{C13}$$

$$\mathcal{M}^{(s-o)}_{1211}(\mathbf{q},\mathbf{p}) = \mathcal{M}^{(s-o)}_{2221}(\mathbf{q},\mathbf{p}) = \frac{iq_1q_2}{4m_1m_2}\left(\frac{m_1}{m_2} + 2\right)\frac{p_+q_3 - p_3q_+}{(\mathbf{p}-\mathbf{q})^2}, \tag{C14}$$

$$\mathcal{M}^{(s-o)}_{1121}(\mathbf{q},\mathbf{p}) = \mathcal{M}^{(s-o)}_{1222}(\mathbf{q},\mathbf{p}) = \frac{iq_1q_2}{4m_1m_2}\left(\frac{m_2}{m_1} + 2\right)\frac{p_3q_- - p_-q_3}{(\mathbf{p}-\mathbf{q})^2}, \tag{C15}$$

$$\mathcal{M}^{(s-o)}_{2111}(\mathbf{q},\mathbf{p}) = \mathcal{M}^{(s-o)}_{2212}(\mathbf{q},\mathbf{p}) = \frac{iq_1q_2}{4m_1m_2}\left(\frac{m_2}{m_1} + 2\right)\frac{p_+q_3 - p_3q_+}{(\mathbf{p}-\mathbf{q})^2}, \tag{C16}$$

$$\mathcal{M}^{(s-o)}_{1212}(\mathbf{q},\mathbf{p}) = -\mathcal{M}^{(s-o)}_{2121}(\mathbf{q},\mathbf{p}) = \frac{iq_1q_2}{8m_1m_2}\left(\frac{m_2}{m_1}-\frac{m_1}{m_2}\right)\frac{p_-q_+ - p_+q_-}{(\mathbf{p}-\mathbf{q})^2}, \tag{C17}$$

Spin–spin,

$$\mathcal{M}^{(s-s)}_{1111}(\mathbf{q},\mathbf{p}) = \mathcal{M}^{(s-s)}_{2222}(\mathbf{q},\mathbf{p}) = -\mathcal{M}^{(s-s)}_{1212}(\mathbf{q},\mathbf{p}) = (\mathcal{M}^{(s-s)}_{2121}(\mathbf{q},\mathbf{p}))^* = \frac{iq_1q_2}{4m_1m_2}\left(\frac{(q_3-p_3)^2}{(\mathbf{q}-\mathbf{p})^2}-1\right), \tag{C18}$$

$$\mathcal{M}^{(s-s)}_{1112}(\mathbf{q},\mathbf{p}) = (\mathcal{M}^{(s-s)}_{2221}(\mathbf{q},\mathbf{p}))^* = -(\mathcal{M}^{(s-s)}_{1211}(\mathbf{q},\mathbf{p}))^* = -\mathcal{M}^{(s-s)}_{2122}(\mathbf{q},\mathbf{p})$$

$$\mathcal{M}^{(s-s)}_{1121}(\mathbf{q},\mathbf{p}) = (\mathcal{M}^{(s-s)}_{2212}(\mathbf{q},\mathbf{p}))^* = -\mathcal{M}^{(s-s)}_{1222}(\mathbf{q},\mathbf{p}) = -(\mathcal{M}^{(s-s)}_{2111}(\mathbf{q},\mathbf{p}))^*$$
$$= \frac{iq_1q_2}{4m_1m_2}\left(\frac{q_-q_3 - p_-q_3 - p_3q_- + p_-p_3}{(\mathbf{q}-\mathbf{p})^2}\right), \tag{C19}$$

$$\mathcal{M}^{(s-s)}_{1122}(\mathbf{q},\mathbf{p}) = -(\mathcal{M}^{(s-s)}_{2211}(\mathbf{q},\mathbf{p}))^* = \frac{iq_1q_2}{4m_1m_2}\frac{q_-^2 - 2q_-p_- + p_-^2}{(\mathbf{q}-\mathbf{p})^2}, \tag{C20}$$

$$\mathcal{M}^{(s-s)}_{1221}(\mathbf{q},\mathbf{p}) = \mathcal{M}^{(s-s)}_{2112}(\mathbf{q},\mathbf{p}) = \frac{iq_1q_2}{4m_1m_2}\left(\frac{q_+q_- - p_+q_- - p_-q_+ + p_+p_-}{(\mathbf{q}-\mathbf{p})^2}-2\right). \tag{C21}$$

Here $p=(p_1,p_2,p_3)$ and

$$p_+ = p_1 + ip_2 = -\sqrt{\frac{8\pi}{3}}pY^1_1(\theta,\varphi), \quad p_- = p_1 - ip_2 = \sqrt{\frac{8\pi}{3}}pY^{-1}_1(\theta,\varphi), \tag{C22}$$

$$p_3 = \sqrt{\frac{4\pi}{3}}pY^0_1(\theta,\varphi). \tag{C23}$$

For a particle–antiparticle system the annihilation components are

$$\mathcal{M}^{anh}_{1111} = \mathcal{M}^{anh}_{2222} = \frac{ie^2}{2m^2}, \tag{C24}$$

$$\mathcal{M}^{anh}_{1212} = \mathcal{M}^{anh}_{1221} = \mathcal{M}^{anh}_{2112} = \mathcal{M}^{anh}_{2121} = \frac{ie^2}{4m^2}. \tag{C25}$$

APPENDIX D: SOME USEFUL EXPRESSIONS, IDENTITIES, AND INTEGRALS

The following expressions and identities are useful for evaluating the M-matrix:

$$\frac{1}{(\mathbf{q}-\mathbf{p})^2} = \frac{2\pi}{|\mathbf{p}|\,|\mathbf{q}|}\sum_\lambda Q_\lambda(z)\sum_{m_\lambda=-\lambda}^{+\lambda} Y^{m_\lambda}_\lambda(\hat{\mathbf{p}})Y^{m_\lambda *}_\lambda(\hat{\mathbf{q}}), \tag{D1}$$

where $z=(p^2+q^2)/2pq$, and $Q_\lambda(z)$ is the Legendre function of the second kind of order λ.[17] Then

$$\frac{((\mathbf{p}-\mathbf{q})\cdot\mathbf{p})^2}{(\mathbf{p}-\mathbf{q})^4} = \frac{\mathbf{p}^2}{(\mathbf{p}-\mathbf{q})^2} - \frac{(\mathbf{p}\times\mathbf{q})^2}{(\mathbf{p}-\mathbf{q})^4}. \tag{D2}$$

The angular integration in (59), (60), and (65) involves the following integrals:

$$\int \mathrm{d}\hat{\mathbf{p}}\,\mathrm{d}\hat{\mathbf{q}}\,F(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})Y_{J'}^{m_J'}(\hat{\mathbf{q}})Y_{J'}^{m_J*}(\hat{\mathbf{p}}) = 2\pi\delta_{J'J}\delta_{m_J'm_J}\int d(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})F(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})P_J(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}}), \tag{D3}$$

$$\int d(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})\frac{\hat{\mathbf{p}}\cdot\hat{\mathbf{q}}}{(\mathbf{p}-\mathbf{q})^2}P_J(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}}) = \frac{1}{|\mathbf{p}|\,|\mathbf{q}|}\left(\frac{J+1}{2J+1}Q_{J+1}(z)+\frac{J}{2J+1}Q_{J-1}(z)\right), \tag{D4}$$

$$\int d(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})\frac{(\mathbf{p}\times\mathbf{q})^2}{(\mathbf{p}-\mathbf{q})^4}P_J(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}}) = \frac{(J+1)(J+2)}{2(2J+1)}Q_{J+1}(z)-\frac{J(J-1)}{2(2J+1)}Q_{J-1}(z). \tag{D5}$$

Here $F(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})$ is an arbitrary function of $\hat{\mathbf{p}}\cdot\hat{\mathbf{q}}$, $P_J(x)$ is the Legendre polynomial of order J.

The integrals in the form

$$\int \mathrm{d}\hat{\mathbf{p}}\;Y_J^{m_J*}(\hat{\mathbf{p}})Y_{J'}^{m_J'}(\hat{\mathbf{p}})Y_{J''}^{m_J''}(\hat{\mathbf{p}}) \tag{D6}$$

can be calculated using the Wigner–Eckart theorem.[17]

The calculation of the relativistic energy corrections involves the integrals

$$\int_0^\infty\int_0^\infty \mathrm{d}p\,\mathrm{d}q\,p^2q^2f^J(p)f^J(q) = 2\pi\left(\frac{\alpha m_r}{n}\right)^3\delta_{J,0}, \tag{D7}$$

$$\int_0^\infty\int_0^\infty \mathrm{d}p\,\mathrm{d}q\,pqf^J(p)f^J(q)Q_J(z_1) = \frac{\pi\alpha m_r}{n^2}, \tag{D8}$$

$$\int_0^\infty\int_0^\infty \mathrm{d}p\,\mathrm{d}q\,p^2q^2f^J(p)f^J(q)Q_J(z_1) = \int_0^\infty\int_0^\infty \mathrm{d}p\,\mathrm{d}q\,p^3qf^J(p)f^J(q)Q_J(z_1) = \pi\left(\frac{\alpha m_r}{n}\right)^3\left(\frac{4}{2J+1}-\frac{1}{n}\right), \tag{D9}$$

$$\int_0^\infty\int_0^\infty \mathrm{d}p\,\mathrm{d}q\,p^2q^2f^J(p)f^J(q)Q_{J-1}(z_1) = \pi\left(\frac{\alpha m_r}{n}\right)^3\left(\frac{2}{J}-\frac{1}{n}\right), \tag{D10}$$

$$\int_0^\infty\int_0^\infty \mathrm{d}p\,\mathrm{d}q\,p^2q^2f^J(p)f^J(q)Q_{J+1}(z_1) = \pi\left(\frac{\alpha m_r}{n}\right)^3\left(\frac{2}{J+1}-\frac{1}{n}\right). \tag{D11}$$

Here f^J is the nonrelativistic hydrogenlike radial wave function in momentum space,[18]

$$f^J(p)\equiv f_n^J(p) = \left(\frac{2}{\pi}\frac{(n-J-1)!}{(n+J)!}\right)^{1/2}\frac{n^{J+2}x^J2^{2(J+1)}J!}{(n^2x^2+1)^{J+2}}\mathcal{G}_{n-J-1}^{J+1}\left(\frac{n^2x^2-1}{n^2x^2+1}\right), \tag{D12}$$

where $x=p/(\alpha m_r)$ is a scaled momentum, and $\mathcal{G}_{n-J-1}^{J+1}$ are the Gegenbauer functions.

APPENDIX E: DIAGONALIZATION OF THE EXPECTATION VALUE OF THE HAMILTONIAN

The matrix representation of the perturbing Hamiltonian $\Delta\hat{H}=\hat{H}-\hat{H}_{NR}-M$, in the basis of the states $|sg\rangle, |tr\rangle$ (49) and (50), is ($J\neq 0$),

$$\langle\psi|\Delta\hat{H}|\psi\rangle_{t=0} = [a_{ij}] \quad (i,j=1,2), \tag{E1}$$

where the matrix elements a_{ij} are

$$a_{11} = \langle sg|\Delta\hat{H}|sg\rangle = -\frac{\alpha^4 m_r}{n^3}\left(\frac{1}{2J+1} - \left(3 - \frac{m_r}{M}\right)\frac{1}{8n}\right), \tag{E2}$$

$$a_{22} = \langle tr|\Delta\hat{H}|tr\rangle = -\frac{\alpha^4 m_r}{n^3}\left(\frac{1}{2J+1} - \frac{1}{2J(J+1)(2J+1)} - \left(3 - \frac{m_r}{M}\right)\frac{1}{8n}\right), \tag{E3}$$

$$a_{12} = a_{21} = \langle sg|\Delta\hat{H}|tr\rangle = \langle tr|\Delta\hat{H}|sg\rangle = \frac{\alpha^4 m_r}{n^3}\frac{|m_1 - m_2|}{2M}\frac{1}{2J+1}\frac{1}{\sqrt{J(J+1)}}. \tag{E4}$$

Note that, in the case of positronium, the elements a_{11} and a_{22} give the energy corrections for pure singlet and triplet states, respectively. Diagonalization of this matrix leads to (104) with eigenvectors (55).

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Charge superselection sectors for QCD on the lattice

J. Kijowski
Center for Theoretical Physics, Polish Academy of Sciences, al. Lotników 32/46, 02-668 Warsaw, Poland

G. Rudolph
Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, 04109 Leipzig, Germany

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We study quantum chromodynamics (QCD) on a finite lattice Λ in the Hamiltonian approach. First, we present the field algebra $\mathfrak{A}_\Lambda$ as comprising a gluonic part, with basic building block being the crossed product C^*-algebra $C(G)\otimes_\alpha G$, and a fermionic (CAR-algebra) part generated by the quark fields. By classical arguments, $\mathfrak{A}_\Lambda$ has a unique (up to unitary equivalence) irreducible representation. Next, the algebra $\mathfrak{O}^i_\Lambda$ of internal observables is defined as the algebra of gauge invariant fields, satisfying the Gauss law. In order to take into account correlations of field degrees of freedom inside Λ with the "rest of the world," we must extend $\mathfrak{O}^i_\Lambda$ by tensorizing with the algebra of external gauge invariant operators. This way we construct the full observable algebra $\mathfrak{O}_\Lambda$. It is proved that its irreducible representations are labelled by $\mathbb{Z}_3$-valued boundary flux distributions. Then, it is shown that there exist unitary operators (charge carrying fields), which intertwine between irreducible sectors leading to a classification of irreducible representations in terms of the $\mathbb{Z}_3$-valued global boundary flux. By the global Gauss law, these three inequivalent charge superselection sectors can be labeled in terms of the global color charge (triality) carried by quark fields. Finally, $\mathfrak{O}_\Lambda$ is discussed in terms of generators and relations. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1851604]

I. INTRODUCTION

In a series of papers (cf. Refs. 1–6), we have started to analyze the nonperturbative structure of gauge theories, with the final aim being the formulation and investigation of gauge models purely in terms of observables. To start with one should clarify basic structures like that of the field algebra, the observable algebra and the superselection structure of the Hilbert space of physical states. It is well-known that the standard Doplicher–Haag–Roberts theory[7,8] for models, which do not contain massless particles, does not apply here. Nonetheless, there are interesting partial results within the framework of general quantum field theory both for quantum electrodynamics (QED) and for non-Abelian models, see Refs. 9–12.

To approach the problem in a rigorous way, we set the system on a finite (regular cubic) lattice and formulate the model within the Hamiltonian approach. For basic notions concerning lattice gauge theories (including fermions) we refer to Ref. 13 and references therein. Within the finite lattice context, we have analyzed the structure of the observable algebra both for spinorial and scalar QED and we have shown that the physical Hilbert space decomposes into a direct sum of superselection sectors labelled by the total electric charge, see Refs. 1–3. Finally, of course, one wants to construct the continuum limit. In full generality, this is an extremely complicated problem of constructive field theory. However, the results obtained until now suggest that there is some hope, to control the thermodynamic limit, see Ref. 1 for a heuristic discussion. We also mention that for simple toy models, these problems can be solved, see Ref. 14.

In Ref. 4 we have started to investigate quantum chromodynamics (QCD) within the above framework. In particular, we have analyzed the global Gauss law and the notion of global color

charge (triality). Comparing with QED, the notion of global charge in QCD is much more complicated, according to the fact that the local Gauss law is neither built from gauge invariant operators nor is it linear. We have shown that one can extract from the local Gauss equation of QCD a gauge invariant, additive law for operators with eigenvalues in $\mathbb{Z}_3$ [the center of SU(3)]. This implies—as in QED—a gauge invariant conservation law: The global $\mathbb{Z}_3$-valued color charge is equal to the global $\mathbb{Z}_3$-valued gauge invariant color electric flux through the boundary.

We stress that within lattice gauge theories, the above notion of color charge is already implicitly contained in a paper by Kogut and Susskind, see Ref. 15. In particular, Mack[16] used it to propose a certain (heuristic) scheme of color screening and quark confinement, based upon a dynamical Higgs mechanism with Higgs fields built from gluons. For similar ideas we also refer to papers by 't Hooft, see Ref. 17 and references therein. This concept was also used in a paper by Borgs and Seiler,[18] where the confinement problem for Yang–Mills theories with static quark sources at nonzero temperature was discussed.

In the present paper, we continue to investigate lattice QCD as initiated in Ref. 4, with the main topic being the analysis of the observable algebra. Our main result is the proof that all its irreducible representations are labelled by the global charge (triality). For this purpose, we use a special functional analytical framework developed by Woronowicz. To illustrate it, consider the Heisenberg algebra, generated by the canonical commutation relation $[p,q]=-i$, $p^*=p$, $q^*=q$. It is not properly defined unless we impose an appropriately defined "strong commutation rule." In this case, one usually uses the Weyl method which consists in "exponentiating" the commutation relations: $U(t)V(s)=\exp(its)V(s)U(t)$, where $U(t):=\exp(itp)$ and $V(s):=\exp(isq)$. In this context, uniqueness of irreducible representations can be proved and as the observable algebra one can take the algebra $\mathfrak{B}(H)$ of all *bounded* operators acting on the unique (Hilbert) representation space $L^2(\mathbb{R}^1)$.

Unfortunately, this technique does not work in the case of more complicated algebraic relations between the generators of the algebra in question. Already in the case of scalar quantum electrodynamics, the "exponentiation" of complicated algebraic relations defining the observable algebra was impossible (see Ref. 3). The situation is similar to the theory of quantum groups, where a "naive" definition in terms of (in general unbounded) generators and their relations leads to contradictions, as long as one does not find some way to give a precise meaning to the relations in question. One of the most powerful techniques, making it possible to deal even with the most difficult examples of such algebras, was introduced by Woronowicz (see Ref. 19). It enables one to consider algebras defined uniquely in terms of (even *unbounded*) generators and algebraic relations between them. In most cases, the generators themselves *do not belong* to the algebra, but are only *affiliated* with it. Applying this approach to the Heisenberg algebra, yields the algebra of compact operators $\mathfrak{K}(L^2(\mathbb{R}^1))$, whereas p and q are only affiliated with this algebra. The algebra of all bounded operators $\mathfrak{B}(L^2(\mathbb{R}^1))$ is then obtained as the *multiplier algebra* $M(\mathfrak{K}(L^2(\mathbb{R}^1)))$. It may be called *extended* observable algebra.

The fact that bounded operators are not "observables" in the strict sense, but only in the extended sense, whereas unbounded operators like p and q may be called observables in an even more generalized sense, as operators *affiliated* with the observable algebra, can be considered to be a drawback of this approach. But this is the price, which we pay for the rigorous mathematical tractability of the observable algebra. We have earlier used this approach in scalar QED and the present paper is consistently written in this language.

We begin our construction with the algebra $\mathfrak{A}_\Lambda$ of field operators, see Sec. II. Here, the Weyl method would provide an alternative (and, probably, simpler) construction of the algebra. But having in mind the observable algebra, where the Weyl method fails, we use the Woronowicz approach from the very beginning. In this context, we show uniqueness of irreducible representations of $\mathfrak{A}_\Lambda$. Next, we discuss local gauge transformations, the Gauss law and boundary data. In Sec. III, the algebra of internal observables $\mathfrak{O}^i_\Lambda$ is defined as the algebra of gauge invariant fields, satisfying the Gauss law. We show that its irreducible representations are labelled by distributions of color electric fluxes running through the boundary to infinity. It is remarkable that for the very classification of irreducible representations the abstract characterization of $\mathfrak{O}^i_\Lambda$ as the subalgebra,

invariant under the group of local gauge transformations, factorized with respect to the ideal generated by the Gauss law, is sufficient. This is due to the fact that here we work within the compact formulation, which implies that we "stay within" the representation space of the field algebra. This remark does not apply to QED in the noncompact formulation (cf. Refs. 1–3, where the corresponding construction is much more complicated).

In Chap. IV, we extend both the algebra of internal observables $\mathfrak{O}_\Lambda^i$, by adding certain "external observables," and the Hilbert space $\mathcal{H}_\Lambda$, by tensorizing with the Hilbert space of tensors at "external points." By external points we mean endpoints of lattice links connecting the finite lattice Λ with the rest of the world. These external observables enable us to take into account the correlations between the field degrees of freedom contained in Λ and the rest of the world. The algebra obtained this way is called full observable algebra and is denoted by $\mathfrak{O}_\Lambda$. Within this context, we show that different Hilbert space sectors, corresponding to different boundary flux distributions, carry equivalent representations of $\mathfrak{O}_\Lambda$ if and only if their global $\mathbb{Z}_3$-valued flux is the same, with intertwiners given by charge carrying fields (cf. Ref. 20). This reduces the irreducible representations of $\mathfrak{O}_\Lambda$ to three inequivalent sectors, labeled by the $\mathbb{Z}_3$-valued global color electric flux. By the global Gauss law, this flux coincides with the global color charge (triality) carried by the quark fields.

Our proposal to take into account also the external observables is motivated by our strategy to construct the thermodynamical limit of the theory *via* an inductive (respectively, projective) limit procedure for observable algebras (respectively, state spaces). This strategy was discussed in Ref. 1. Physically, it reduces considerably the number of superselection sectors of the theory, which are no longer numbered by the electric flux distribution at the boundary, but only by the global charge. In Sec. IV we thoroughly discuss our motivation for this proposal, which we consider one of the most important ideas of this paper.

Finally, in Sec. V, $\mathfrak{O}_\Lambda$ is discussed in terms of generators and relations. We start with presenting a set of genuine invariants generating $\mathfrak{O}_\Lambda$, which is, however, highly redundant. In the remainder of this section, we use some gauge fixing methods to reduce this set. In this context, a couple of delicate questions arises—all in some sense related to the Gribov problem and to the fact that the underlying classical configuration space has a complicated stratified structure with respect to the gauge group action. A more complete treatment of $\mathfrak{O}_\Lambda$ as an algebra presented by generators and relations will be given in two separate papers, see Refs. 21 and 22.

II. THE FIELD ALGEBRA

A. Basic definitions

We consider QCD in the Hamiltonian framework on a finite regular cubic lattice $\Lambda \subset \mathbb{Z}^3$, with $\mathbb{Z}^3$ being the infinite regular lattice in three dimensions. We denote the lattice boundary by $\partial\Lambda$ and the set of oriented, i-dimensional elements of Λ, respecitively, $\partial\Lambda$, by Λ^i, respectively, $\partial\Lambda^i$, where $i=0,1,2,3$. Such elements are (in increasing order of i) called sites, links, plaquettes, and cubes. Moreover, we denote the set of external links connecting boundary sites of Λ with "the rest of the world" by Λ_∞^1 and the set of endpoints of external links by Λ_∞^0. For the purposes of this paper, we may assume that for each boundary site there is exactly one external link. Then, external links are labeled by boundary sites and we can denote them by (x,∞) with $x \in \partial\Lambda^0$. The set of nonoriented i-dimensional elements will be denoted by $|\Lambda|^i$. If, for instance, $(x,y) \in \Lambda^1$ is an oriented link, then by $|(x,y)| \in |\Lambda|^1$ we mean the corresponding nonoriented link. The same notation applies to $\partial\Lambda^1$ and Λ_∞^1.

The basic fields of lattice QCD are quarks living at lattice sites and gluons living on links, including external links. The field algebra is thus, by definition, the C^*-tensor product of fermionic and bosonic algebras:

$$\mathfrak{A}_\Lambda := \mathfrak{F}_\Lambda \otimes \mathfrak{B}_\Lambda, \tag{2.1}$$

with

$$\mathfrak{F}_\Lambda := \bigotimes_{x\in\Lambda^0} \mathfrak{F}_x \tag{2.2}$$

and

$$\mathfrak{B}_\Lambda := \mathfrak{B}^i_\Lambda \otimes \mathfrak{B}^b_\Lambda = \bigotimes_{|(x,y)|\in|\Lambda|^1} \mathfrak{B}_{|(x,y)|} \bigotimes_{x\in\partial\Lambda^0} \mathfrak{B}_{|(x,\infty)|}. \tag{2.3}$$

Here, $\mathfrak{B}^i_\Lambda$ and $\mathfrak{B}^b_\Lambda$ are the internal and boundary bosonic algebras, respectively. We impose *locality* of the lattice quantum fields by *postulating* that the algebras corresponding to different elements of Λ (anti)commute with each other.

Remark: The bosonic boundary data represent nontrivial color electric flux through the boundary, which—as will be seen later—allows for nontrivial color charge. As will be shown, nontrivial boundary flux is necessary for taking into account correlations of field degrees of freedom inside Λ with the "rest of the world." Even if, for some reasons, the global charge of the Universe vanishes, there is no reason to assume that an arbitrary finite part Λ is also neutral.

The fermionic field algebra $\mathfrak{F}_x$ associated with a lattice site x is the algebra of canonical anticommutation relations (CAR) of quarks at x. The quark field generators are denoted by

$$\Lambda^0 \ni x \to \psi^{aA}(x) \in \mathfrak{F}_x, \tag{2.4}$$

where a stands for bispinorial and (possibly) flavor degrees of freedom and $A=1,2,3$ is the color index corresponding to the fundamental representation of the gauge group $G=\mathrm{SU}(3)$. [In what follows, writing G we have in mind SU(3), but essentially our discussion can be extended to arbitrary compact groups and their representations.] The conjugate quark field is denoted by $\psi^*_{aA}(x)$, where we raise and lower indices by the help of the canonical Hermitian metric tensor g_{AB} in $\mathbb{C}^3$ and the canonical skew-symmetric structure ϵ_{ab} in the spinor space. The only nontrivial canonical anticommutation relations for generators of $\mathfrak{F}_x$ read

$$[\psi^*_{aA}(x), \psi^{bB}(x)]_+ = \delta^B{}_A \delta^b{}_a. \tag{2.5}$$

The bosonic field algebra $\mathfrak{B}_{|(x,y)|}$ associated with the nonoriented link $|(x,y)|$ (where y also stands for ∞), is given in terms of its isomorphic copies $\mathfrak{B}_{(x,y)}$ and $\mathfrak{B}_{(y,x)}$, corresponding to the two orientations of the link (x,y). The algebra $\mathfrak{B}_{(x,y)}$ is generated (in the sense of Woronowicz, as explained below) by matrix elements of the gluonic gauge potential on the link (x,y),

$$\Lambda^1 \ni (x,y) \to U^A{}_B(x,y) \in \mathfrak{C}_{(x,y)}, \tag{2.6}$$

with $\mathfrak{C}_{(x,y)} \cong C(G)$ being the commutative C^*-algebra of continuous functions on G and $A, B=1,2,3$ denoting color indices, and by color electric fields, spanning the Lie algebra $\mathfrak{g}_{(x,y)} \cong \mathrm{su}(3)$. Choosing an orthonormal basis $\{t_i\}$, $i=1,\ldots,8$, of su(3) we denote by $\{E_i(x,y)\}$ the corresponding basis of $\mathfrak{g}_{(x,y)}$,

$$\Lambda^1 \ni (x,y) \to E_i(x,y) := t_i \in \mathfrak{g}_{(x,y)}. \tag{2.7}$$

These elements, satisfying the su(3) commutation relations, generate, in the sense of Woronowicz,[19] the C^*-algebra $\mathfrak{P}_{(x,y)} \cong C^*(G)$ (for the definition see Remark 1 below).

Observe that G acts on $C(G)$ naturally by the left regular representation,

$$\alpha_g(u)(g') := u(g^{-1}g'), \quad u \in C(G). \tag{2.8}$$

Differentiating this relation, we get an action of $e \in \mathrm{su}(3)$ on $u \in C^\infty(G)$ by the corresponding right invariant vector field e^R. Thus, we have a natural commutator between generators of $\mathfrak{P}_{(x,y)}$ and smooth elements of $\mathfrak{C}_{(x,y)}$,

$$i[e,u] := e^R(u). \tag{2.9}$$

Thus, we have a C^*-dynamical system $(\mathfrak{C}_{(x,y)}, G, \alpha)$, with automorphism α given by the left action (2.8). The field algebra $\mathfrak{B}_{(x,y)}$ is, by definition, the corresponding crossed product C^*-algebra,

$$\mathfrak{B}_{(x,y)} := \mathfrak{C}_{(x,y)} \otimes_\alpha G, \tag{2.10}$$

see Refs. 23 and 24 for these notions.

For the convenience of the reader we add a number of comments on the mathematical framework used here.

Remarks:

(1) We give the definition of $C^*(G)$ (cf. Refs. 23 and 25). Take the group algebra of G, which is the space $L^1(G)$ of integrable functions on the group, with convolution providing the product structure. Complete it with respect to the following norm:

$$\|f\| := \sup_\pi \|\pi(f)\|, \tag{2.11}$$

where $f \in L^1(G)$. The supremum is taken over all representations (π, H) of the group and $\pi(f)$ denotes the operator obtained by smearing the corresponding representation in $L^2(G,H)$ over the group with the function f, see Refs. 26 and 25. We stress that $C^*(G)$ is a C^*-algebra without unit. Moreover, its su(3)-generators t_i do not belong to $C^*(G)$, but are only affiliated in the C^*-sense, see Ref. 19.

(2) We define the crossed product algebra $C(G) \otimes_\alpha G$. First take $L^1(G, C(G))$, defined as the *-algebra of $C(G)$-valued L^1-functions on G, with multiplication given by the twisted convolution

$$(z \times w)(g') := \int_G z(g) \alpha_g(w(g^{-1}g'))\mathrm{d}g,$$

involution induced from the *-structure of $C(G)$,

$$z^*(g) = \alpha_g(z(g^{-1})^*),$$

and equipped with the standard L^1-norm. Next, consider all its nondegenerate Hilbert space representations. Finally, $C(G) \otimes_\alpha G \supset L^1(G, C(G))$ is defined as the completion of $L^1(G, C(G))$ in the sup-norm taken over all these representations. This way we obtain a C^*-algebra without unit. This algebra can be viewed as a skew tensor product of $C(G)$ with $C^*(G)$ in the following sense: For each $u \in C(G)$ and $f \in L^1(G)$ denote by $u \otimes f$ the element of $L^1(G, C(G))$ given by $(u \otimes f)(g) := uf(g)$. Then, the linear span of such elements is dense in $L^1(G, C(G))$. It is easily seen that

$$f \to 1 \otimes f \tag{2.12}$$

is an isomorphism onto its image, which enables us to identify $C^*(G)$ with the corresponding subalgebra

$$C^*(G) \subset C(G) \otimes_\alpha G. \tag{2.13}$$

As already noted, the group algebra $C^*(G)$ is a C^*-algebra generated by unbounded elements in the sense of Woronowicz, see Ref. 19. Consequently, $C(G) \otimes_\alpha G$ is of this type, too. It is generated by elements (e, u) fulfilling canonical commutation relations (2.9). We stress that both the (unbounded) su(3)-generators e and the (bounded) generators u do not belong to the algebra, but are only affiliated in the C^*-sense. Moreover, note that—contrary to (2.12)—the mapping $u \to u \otimes 1$ *does not* preserve the algebraic structure of $C(G)$ and, whence, cannot be used to imbed $C(G)$ into $C(G) \otimes_\alpha G$. Hence, $C(G) \nsubseteq C(G) \otimes_\alpha G$, but belongs to its multiplier algebra $M(C(G) \otimes_\alpha G)$. An embedding similar to (2.13) does not hold for a noncompact group G, because here we have to take instead of $C(G)$ the algebra $C_\infty(G)$ of functions

vanishing at infinity, which is an algebra without unit. Thus, the mapping (2.12) does not exist.

(3) Formula (2.9) is a natural generalization of the Heisenberg commutation relation $[p,q]=-i$, describing the Abelian case $G=\mathbb{R}^1$. It corresponds to "canonical quantization" over the phase space

$$T^*(G) \cong \mathfrak{g}^* \times G,$$

with $\mathfrak{g}=\mathrm{su}(3)$ being the Lie algebra of G and $\mathfrak{g}^*$ being the dual space. Quantization applies to functions on $\mathfrak{g}^* \times G$, hence, in particular, to elements of $\mathfrak{g}$. Thus, from the purely algebraic point of view, one would then define $\mathfrak{P}_{(x,y)}$ as the enveloping algebra $\mathfrak{U}(\mathfrak{g})$ of $\mathfrak{g}$, see Ref. 4, yielding for the bosonic field algebra $\mathfrak{B}_{(x,y)}$ the following crossed product structure of Hopf algebras:

$$C^\infty(G) \otimes_\alpha \mathfrak{U}(\mathfrak{g}).$$

This is an example of a Heisenberg double of Hopf algebras, see of Refs. 27 and 28. This choice has, however, substantial drawbacks related to the fact that the operators assigned to the Lie algebra elements e are necessarily unbounded. This is why we choose the functional-analytic framework above, where all fields are compact, hence *bounded* operators in a Hilbert space. We call the algebra (2.10) the algebra of *generalized canonical commutation relations* (CCR) over the group G.

(4) Within the above framework, one can prove a generalization of the classical uniquess theorem by von Neumann,[29] stating that any irreducible representation of the above CCR-algebra is equivalent to the *generalized Schrödinger representation*, acting on the Hilbert space $L^2(G)$ (with respect to the Haar measure). This will be shown in Sec. II B.

The transformation law of elements of $\mathfrak{B}_{(x,y)}$ under the change of the link orientation is derived from the fact that the (classical) G-valued parallel transporter $g(x,y)$ on (x,y) transforms to $g^{-1}(x,y)$ under the change of orientation. This transformation lifts naturally to an isomorphism

$$\mathcal{I}_{(x,y)}: \mathfrak{B}_{(x,y)} \to \mathfrak{B}_{(y,x)} \tag{2.14}$$

of field algebras, defined by

$$\mathcal{I}_{(x,y)}(f) := \check{f}, \quad \mathcal{I}_{(x,y)}(e) := \check{e}, \tag{2.15}$$

where $\check{f}(g) := f(g^{-1})$ and $\check{e}$ is the left invariant vector field on G, generated by $-e$. The bosonic field algebra $\mathfrak{B}_{|(x,y)|}$ is obtained from $\mathfrak{B}_{(x,y)}$ and $\mathfrak{B}_{(y,x)}$ by identifying them via $\mathcal{I}_{(x,y)}$.

Now, we give a full list of relations satisfied by generators of $\mathfrak{B}_{|(x,y)|}$. Being entries of the fundamental representation of SU(3), the generators of $\mathfrak{C}_{(x,y)}$ must fulfill the following conditions:

$$(U^A{}_B(x,y))^* U_A{}^C(x,y) = \delta^C{}_B \mathbf{1}, \tag{2.16}$$

$$\epsilon_{ABC} U^A{}_D(x,y) U^B{}_E(x,y) U^C{}_F(x,y) = \epsilon_{DEF} \mathbf{1}. \tag{2.17}$$

In what follows, we will use the traceless matrix

$$E^A{}_B(x,y) := \sum_i E_i(x,y) t_i{}^A{}_B, \tag{2.18}$$

built from generators of $\mathfrak{P}_{(x,y)}$. Its entries obviously fulfill

$$(E^A{}_B(x,y))^* = E_B{}^A(x,y). \tag{2.19}$$

The transformation law (2.15) of these objects under the change of the link orientation is given by the following relations:

$$U^A{}_B(y,x) = \check{U}^A{}_B(x,y) = (U_B{}^A(x,y))^*, \tag{2.20}$$

$$E^A{}_B(y,x) = \check{E}^A{}_B(x,y) = -U^A{}_D(y,x)U^C{}_B(x,y)E^D{}_C(x,y). \tag{2.21}$$

The su(3)-commutation relations read

$$[E^A{}_B(x,y),E^C{}_D(u,z)] = \delta_{xu}\delta_{yz}(\delta^C{}_B E^A{}_D(x,y) - \delta^A{}_D E^C{}_B(x,y)), \tag{2.22}$$

[formula (2.15) implies that all the components $E^A{}_B(x,y)$ commute with all the components $E^C{}_D(y,x)$, because the left invariant and the right invariant fields on the group commute]. The canonical commutation relations (2.9) take the following form:

$$\begin{aligned} i[E^A{}_B(x,y),U^C{}_D(u,z)] = &+ \delta_{xu}\delta_{yz}\left(\delta^C{}_B U^A{}_D(x,y) - \tfrac{1}{3}\delta^A{}_B U^C{}_D(x,y)\right) \\ &- \delta_{xz}\delta_{yu}\left(\delta^A{}_D U^C{}_B(y,x) - \tfrac{1}{3}\delta^A{}_B U^C{}_D(y,x)\right). \end{aligned} \tag{2.23}$$

To summarize, the field algebra $\mathfrak{A}_\Lambda$, given by (2.1)–(2.3), is a C^*-algebra, generated by elements

$$\{\psi^{aA}(x),\psi^*{}_{aA}(x),U^A{}_B(x,y),E^A{}_B(x,y)\}, \tag{2.24}$$

fulfilling relations (2.16), (2.17), and (2.19)–(2.21), together with canonical (anti)commutation relations (2.5), (2.22), and (2.23).

Remark: According to formula (2.21), the transformation of the color electric field E from (x,y) to (y,x) consists of two steps.

(1) The parallel transport from point x to y by means of the two parallel transporters U, each of them acting appropriately on the two indices of E.
(2) The change of the sign due to the change of the orientation.

In what follows, we always treat $E(x,y)$ as being attached to the site x.

B. Uniqueness of irreducible representations

Here, we prove uniqueness of the generalized canonical commutation relations as announced in Sec. II A.

We use the one-to-one correspondence between nondegenerate representations of crossed products and covariant representations of C^*-dynamical systems, see Ref. 23. Thus, let us consider the following covariant representation of $(C(G),G,\alpha)$ on $L^2(G)$ (with respect to the Haar measure):

(1) Take the representation π of the commutative C^*-algebra $C(G)$ given by multiplication with elements of $C(G)$. This, obviously, a representation by bounded operators on $L^2(G)$.
(2) Consider the left regular (unitary) representation $\hat{\pi}$ of G on $L^2(G)$,

$$(\hat{\pi}(g)\xi)(g') := \xi(g^{-1}g'), \quad \xi \in L^2(G). \tag{2.25}$$

We calculate

$$\begin{aligned} (\hat{\pi}(g)\circ\pi(u)\circ\hat{\pi}(g^{-1}))(\xi)(g') &= ((\pi(u)\circ\hat{\pi}(g^{-1}))(\xi))(g^{-1}g') = u(g^{-1}g')\cdot(\hat{\pi}(g^{-1})(\xi))(g^{-1}g') \\ &= u(g^{-1}g')\cdot\xi(g') = \pi(\alpha_g(u))(\xi)(g'). \end{aligned}$$

This yields

$$\hat{\pi}(g)\circ\pi(u)\circ\hat{\pi}(g^{-1}) = \pi(\alpha_g(u)), \tag{2.26}$$

showing that the pair $(\pi,\hat{\pi})$ defines a *covariant* representation of $(C(G),G,\alpha)$ on $L^2(G)$, indeed.

We call this representation *generalized Schrödinger representation.* Observe that differentiat-

ing relation (2.26) yields the generalized canonical commutation relations (2.9).

Now, consider an arbitrary *covariant* representation $(\rho,\hat{\rho})$ of the the C^*-dynamical system $(C(G),G,\alpha)$, with ρ being a nondegenerate representation of $C(G)$ on a Hilbert space H and $\hat{\rho}$ being a strongly continuous unitary representation of G on H. By the Gelfand–Najmark theorem for commutative C^*-algebras, we have a spectral measure $\mathrm{d}E$ on G, such that

$$\rho(u) = \int u(g)\mathrm{d}E(g), \tag{2.27}$$

for $u\in C(G)$, and by covariance, the pair $(\rho,\hat{\rho})$ also fulfills (2.26). Thus, we get

$$\hat{\rho}(g)\circ\mathrm{d}E(g')\circ\hat{\rho}(g^{-1}) = \mathrm{d}E(gg'). \tag{2.28}$$

We conclude that the spectral measure $\mathrm{d}E$ defines a transitive system of imprimitivity for the representation $\hat{\rho}$ of G based on the group manifold G. Then, the imprimitivity theorem, see Refs. 30 and 31, yields the following.

Theorem 2.1: *Any irreducible representation of* $(C(G),G,\alpha)$ *is equivalent to the generalized Schrödinger representation.*

Remarks:

(1) Disregarding the C^*-context, Theorem 2.1 is a classical result of Mackey, see Ref. 31 and references therein.
(2) Within the C^*-context, there is a formulation of the commutation relations (2.26) for an arbitrary locally compact group in terms of the pentagon equation, which generalizes to quantum groups.[32]

The following statement is a consequence of Theorem 7.7.12 in Ref. 23, but for the reader's convenience we add the proof here.

Lemma 2.2: For any compact Lie group, the generalized Schrödinger representation defines the following isomorphism of C^**-algebras:*

$$C(G)\otimes_{\alpha}G \cong \mathfrak{K}(L^2(G)), \tag{2.29}$$

where $\mathfrak{K}(L^2(G))$ *denotes the algebra of compact operators on* $L^2(G)$.

Proof: Any nondegenerate, irreducible representation of $L^1(G,C(G))$ is equivalent to the following representation in $L^2(G)$:

$$(\pi\times\hat{\pi})(z) = \int \pi(z(g))\hat{\pi}(g)\mathrm{d}g, \tag{2.30}$$

with $z\in L^1(G,C(G))$. This follows from the one-to-one correspondence between nondegenerate representations of $L^1(G,C(G))$ and covariant representations of the C^*-dynamical system $(C(G),G,\alpha)$ (cf. Ref. 23, Proposition 7.6.4) and from the uniqueness theorem above.

Thus, for every $\xi\in L^2(G)$ we have

$$(((\pi\times\hat{\pi})(z))\xi)(h) = \left(\int \pi(z(g))\hat{\pi}(g)\xi\,\mathrm{d}g\right)(h) = \int z(g,h)\xi(g^{-1}h)\mathrm{d}g, \tag{2.31}$$

where we have denoted $(z(g))(h)\equiv z(g,h)$. Note that continuous functions

$$C(G,C(G)) \cong C(G\times G) \subset L^1(G,C(G))$$

form a dense subset. Thus, for algebraically special functions of type $z(g,h)=\overline{x}(g^{-1}h)\cdot y(h)$, with x, $y\in C(G)\subset L^2(G)$, we obtain one-dimensional operators of the following type:

$$(((\pi \times \hat{\pi})(z))\xi)(h) = y(h) \int \bar{x}(g)\xi(g)\mathrm{d}g, \tag{2.32}$$

or, equivalently, in physics notation

$$(\pi \times \hat{\pi})(z) = |y\rangle\langle x|. \tag{2.33}$$

Of course, linear combinations of such elements form a dense subset in $L^1(G, C(G))$ and, thus, also in $C(G) \otimes_\alpha G$. On the other hand, linear combinations of one-dimensional operators exhaust finite dimensional operators and their C^*-closure in the operator norm gives precisely the algebra of all compact operators $\mathfrak{K}(L^2(G))$. ■

Remark:

(1) Consider the isomorphism (2.29). Using the generators (e, u) of $C(G) \otimes_\alpha G$ we built typical elements of $\mathfrak{K}(L^2(G))$ as follows: For any basis $\{t_i\}$, take operators $(1+t_i^2)^{-1}$, which are compact, and multiply them from both sides by any function of matrix elements $U^A{}_B$ (compare with Ref. 19, example 3 of Sec. III).

(2) We stress that Lemma 2.2 holds for noncompact Lie groups, too. In that case, we have to take $x \in C_0(G)$ (function with compact support) and $y \in C_\infty(G)$ (function vanishing at infinity) in the above proof. In particular, for the case of canonical commutation relations $[p, q] = -i$, we take $G = \mathbb{R}^1$ and the above approach yields the algebra $\mathfrak{K}(L^2(\mathbb{R}^1))$. A typical element belonging to this algebra is $(1+q^2)^{-1}(1+p^2)^{-1}(1+q^2)^{-1}$ (compare with Ref. 19, example 4 of Sec. III).

Now, we take the tensor product of generalized Schrödinger representations over all links,

$$\bigotimes_{(x,y)\in\Lambda^1} L^2(\mathcal{C}_{(x,y)}) \bigotimes_{x\in\partial\Lambda^0} L^2(\mathcal{C}_{(x,\infty)}) \cong L^2(\mathcal{C}), \tag{2.34}$$

with

$$\mathcal{C} := \prod_{(x,y)\in\Lambda^1} \mathcal{C}_{(x,y)} \prod_{x\in\partial\Lambda^0} \mathcal{C}_{(x,\infty)}$$

and each of the spaces $\mathcal{C}_{(x,y)}$ being diffeomorphic to the group space of G.

This is, by Theorem 2.1, the unique representation space of the gluonic field algebra $\mathfrak{B}_\Lambda$. Moreover, using the classical uniqueness theorem for CAR-representations by Jordan and Wigner,[33] any representation of fermionic fields is equivalent to the fermionic Fock representation. Consequently, using Lemma 2.2, we get the following.

Corollary 2.3: The field algebra $\mathfrak{A}_\Lambda$ can be identified with the algebra $\mathfrak{K}(H_\Lambda)$ of compact operators on the Hilbert space

$$H_\Lambda = \mathcal{F}(\mathbb{C}^{12N}) \otimes L^2(\mathcal{C}), \tag{2.35}$$

with $\mathcal{F}(\mathbb{C}^{12N})$ denoting the fermionic Fock space generated by $12N$ anticommuting pairs of quark fields.

The subspace $\mathcal{F}(\mathbb{C}^{12N})$ is spanned by vectors

$$\psi^*_{a_1 A_1}(x_1) \cdots \psi^*_{a_n A_n}(x_n)|0\rangle, \tag{2.36}$$

obtained from the fermionic Fock vacuum by the action of quark creation operators. Consequently, any element of H_Λ is a linear combination of these *fermionic* vectors with coefficients being L^2-functions depending on gluonic potentials U.

From the physicists point of view, it might seem to be more natural to choose the whole algebra $\mathfrak{B}(H_\Lambda)$ of all bounded operators as the field algebra. In mathematical terms this means taking the *multiplier algebra*

$$\mathfrak{B}(H_\Lambda) = M(\mathfrak{K}(H_\Lambda))$$

of our field algebra $\mathfrak{K}(H_\Lambda)$. We call $\mathfrak{B}(H_\Lambda)$ *extended field algebra* of our model. Moreover, we denote the set of affiliated elements of the algebra $\mathfrak{K}(H_\Lambda)$ by $(\mathfrak{K}(H_\Lambda))^\eta$. Hence, our approach leads to the triple,

$$\mathfrak{K}(H_\Lambda) \subset \mathfrak{B}(H_\Lambda) \subset (\mathfrak{K}(H_\Lambda))^\eta,$$

which contains physical fields in a (1) restricted, (2) extended, and (3) even more extended sense, but which may all be reconstructed from the first element of the triple. On the level of the observable algebra we will proceed the same way.

The main reason for choosing the above approach, based on $\mathfrak{K}(H_\Lambda)$ and not on $\mathfrak{B}(H_\Lambda)$, is that in this context unbounded generators are structurally related to the field (respectively, observable) algebra, which is defined in terms of algebraic relations between these generators.

C. Gauge transformations and local Gauss law

The group G_Λ of local gauge transformations related to the lattice Λ consists of mappings

$$\Lambda^0 \ni x \to g(x) \in G,$$

which represent internal gauge transformations, and of gauge transformations at external points,

$$\Lambda^0_\infty \ni z \to g(z) \in G.$$

Thus,

$$G_\Lambda := G^i_\Lambda \times G^\infty_\Lambda = \prod_{x\in\Lambda^0} G_x \prod_{z\in\Lambda^0_\infty} G_z, \tag{2.37}$$

with $G_y \cong \mathrm{SU}(3)$, for every y. We denote the corresponding Lie algebra by

$$\mathfrak{g}_\Lambda := \mathfrak{g}^i_\Lambda \oplus \mathfrak{g}^\infty_\Lambda = \bigoplus_{x\in\Lambda^0} \mathfrak{g}_x \oplus \bigoplus_{z\in\Lambda^0_\infty} \mathfrak{g}_z, \tag{2.38}$$

with $\mathfrak{g}_y \cong \mathrm{su}(3)$, for every y.

The group G_Λ acts on the classical configuration space $\mathcal{C}$ as follows:

$$\mathcal{C}_{(x,y)} \ni g(x,y) \to g(x)g(x,y)g(y)^{-1} \in \mathcal{C}_{(x,y)}, \tag{2.39}$$

with $g(x) \in G_x$ and $g(y) \in G_y$. This action lifts naturally to functions on $\mathcal{C}$. Moreover, we have an action of G_x on itself by inner automorphisms. This yields an action of G_Λ by automorphisms on each C^*-dynamical system $(\mathfrak{C}_{(x,y)}, G, \alpha)$ and, therefore, on the gluonic field algebra $\mathfrak{B}_\Lambda$. For generators of $\mathfrak{B}_{(x,y)} \subset \mathfrak{B}_\Lambda$, this action is given by

$$U^A{}_B(x,y) \to g^A{}_C(x) U^C{}_D(x,y) (g^{-1})^D{}_B(y), \tag{2.40}$$

$$E^A{}_B(x,y) \to g^A{}_C(x) E^C{}_D(x,y) (g^{-1})^D{}_B(x), \tag{2.41}$$

with y standing also for ∞. Fermionic generators transform under the fundamental representation:

$$\psi^{aA}(x) \to g^A{}_B(x) \psi^{aB}(x). \tag{2.42}$$

To summarize, the group of local gauge transformation G_Λ acts on the field algebra $\mathfrak{A}_\Lambda$ in a natural way by automorphisms.

It is easy to check that, for $x \in \Lambda^0$, the above automorphisms are generated by the following derivations of the field algebra:

$$\mathcal{G}^A{}_B(x) := \rho^A{}_B(x) - \sum_{y \leftrightarrow x} E^A{}_B(x,y), \tag{2.43}$$

where $y \leftrightarrow x$ means that the sum is taken over all nearest neighbors y of x (with y also standing for ∞), and where

$$\rho^A{}_B(x) = \sum_a \left(\psi^{*aA}(x)\psi^a{}_B(x) - \frac{1}{3}\delta^A{}_B \psi^{*aC}(x)\psi^a{}_C(x) \right) \tag{2.44}$$

is the local matter charge density, fulfilling $\rho^A{}_A(x) = 0$. Observe that both (2.43) and (2.44) satisfy the su(3)-commutation relations separately and that the set $\{\mathcal{G}^A{}_B(x)\}$ of generators spans the Lie algebra $\mathfrak{g}^i_\Lambda$.

The local Gauss law at $x \in \Lambda^0$ reads

$$\sum_{y \leftrightarrow x} E^A{}_B(x,y) = \rho^A{}_B(x), \tag{2.45}$$

meaning that the gauge generator $\mathcal{G}^A{}_B(x)$ defined by formula (2.43) vanishes. Observe that for every $x \in \partial\Lambda^0$, the corresponding boundary flux $E^A{}_B(x,\infty)$ enters the Gauss law. All the Gauss laws at boundary points can thus be easily "solved" by expressing the boundary fluxes in terms of internal fields.

For $z \in \Lambda^0_\infty$, the generator (2.43) of gauge transformations reduces to the boundary flux $E^A{}_B(z,x)$. Nonvanishing of this flux means gauge dependence of the quantum state under the action of $G_z \subset G^\infty_\Lambda$. Neglecting these boundary fluxes means neglecting the possibility that a nontrivial color charge occurs.[4] As will be discussed in Sec. IV A, such a "truncated theory" is not useful as a discrete approximation of the continuum theory. [The continuum limit should be constructed[1] in terms of an inductive (respectively, projective) limit of observable algebras (respectively, quantum states). In this context, "external fluxes" represent the necessary link between any two intersecting lattices belonging to a whole sequence of lattices.]

Remark:

(1) We stress that the Gauss law (2.45) is the lattice counterpart of the "covariant divergence law"

$$D_k E^k \equiv \partial_k E^k + [A_k, E^k] = \rho$$

in the continuum theory. There, the volume integration yields on the left-hand side a standard boundary flux term (by applying Stokes theorem) and an additional volume integral contribution corresponding to the $[A_k, E^k]$-term. In our lattice formulation, the volume integration corresponds to summation over all local Gauss laws. This yields a sum over boundary terms living on external links (x,∞) *and* a volume contribution equal to $E(x,y)+E(y,x)$ on each lattice link. This term mimics the term $[A_k, E^k]$ of the continuum theory, [e.g., it vanishes only if the parallel transporter $U(x,y)$ is trivial, which corresponds to the case $A_k = 0$ in the continuum theory].

(2) We add the "naive" Hamiltonian. Starting from the classical Hamiltonian

$$H = \int \left\{ \frac{1}{4} Tr(E^k(x)E_k(x) + B^k(x)B_k(x)) - \Re(\bar{\psi}(x) i \gamma^k D_k \psi(x)) + \bar{\psi}(x) m \psi(x) \right\} d^3x$$

of continuum QCD, we obtain the following self-adjoint operator acting on the Hilbert space H_Λ of our lattice model:

$$H = \frac{a}{2} \sum_{|(x,y)|\in|\Lambda|^1} E^A{}_B(x,y) E^B{}_A(x,y) + \frac{1}{2g^2 a}\left(\sum_{\sigma\in|\Lambda|^2} U^A{}_A(\partial\sigma) + \text{h.c.} \right)$$
$$+ \frac{a^2}{2} \sum_{|(x,x+\hat{k})|\in|\Lambda|^1} \overline{\psi}_A(x) i\gamma^k U^A{}_B(x,x+\hat{k}) \psi^B(x+\hat{k}) + \text{h.c.} + a^3 \sum_{x\in|\Lambda|^0} \overline{\psi}_A(x) m \psi^A(x), \tag{2.46}$$

where a is the lattice spacing and $\hat{k}$ is the vector of length a in the direction of the kth axis. Here, by $U^A{}_B(\partial\sigma)$ we denote the Wilson loop corresponding to the plaquette σ. By writing "naive" Hamiltonian we mean that we disregard terms, by which H must be supplemented in order to avoid the so-called doubling problem. The dynamical content of this model is based upon this Hamiltonian, which however will not be investigated in the present paper.

III. THE ALGEBRA OF INTERNAL OBSERVABLES

A. Basic definitions

Physical observables, internal relative to Λ, are, by definition, gauge invariant fields respecting the Gauss law. Hence, we must take the subalgebra

$$\mathfrak{A}^{G_\Lambda} \subset \mathfrak{A}_\Lambda$$

of G_Λ-invariant elements of the field algebra $\mathfrak{A}_\Lambda$. This means, in particular, that observables must commute with all gauge generators $\mathcal{G}^A{}_B(x)$.

Moreover, we must impose all relations inherited from the local Gauss laws at all internal lattice sites (*not* including external sites) as defining relations of the observable algebra. This means that the generators $\mathcal{G}^A{}_B(x)$ of G^i_Λ must vanish in all possible gauge-invariant algebraic combinations. Hence, imposing (2.45) at the algebraic (representation-independent) level means that we require vanishing of the ideal $\mathfrak{I}^i_\Lambda \cap \mathfrak{A}^{G_\Lambda}$, with $\mathfrak{I}^i_\Lambda$ being the ideal generated by $\mathfrak{g}^i_\Lambda$. Thus, the algebra $\mathfrak{O}^i_\Lambda$ of internal observables is obtained from $\mathfrak{A}^{G_\Lambda}$ by factorizing with respect to this ideal.

Definition 3.1: The algebra of internal observables relative to Λ *is defined as*

$$\mathfrak{O}^i_\Lambda = \mathfrak{A}^{G_\Lambda}/\{\mathfrak{I}^i_\Lambda \cap \mathfrak{A}^{G_\Lambda}\}, \tag{3.1}$$

where $\mathfrak{A}^{G_\Lambda} \subset \mathfrak{A}_\Lambda$ *is the subalgebra of* G_Λ*-invariant elements of* $\mathfrak{A}_\Lambda$ *and* $\mathfrak{I}^i_\Lambda \subset \mathfrak{A}_\Lambda$ *is the ideal generated by* $\mathfrak{g}^i_\Lambda$*. By the extended algebra of internal observables we mean the multiplier algebra* $M(\mathfrak{O}^i_\Lambda)$.

Remark: The above ideal $\mathfrak{I}^i_\Lambda$ is generated by unbounded elements in the sense of Woronowicz. It is obtained by multiplying its generators $\mathcal{G}^A{}_B(x)$ from both sides by elements of $\mathfrak{A}_\Lambda$ belonging to their common dense domain, e.g., the so-called *smooth* elements (corresponding to C^∞-functions on G).

B. Classification of irreducible representations

By Corollary 2.3, we can identify $\mathfrak{A}_\Lambda$ with the algebra of compact operators acting on the Hilbert space H_Λ, given by (2.35). Under this identification, we have a unitary representation of the gauge group G_Λ on H_Λ and the subalgebra $\mathfrak{A}^{G_\Lambda}$ can be viewed as the commutant $(G_\Lambda)'$ of this representation in $\mathfrak{K}(H_\Lambda)$.

Consider the closed subspace $\mathcal{H}_\Lambda \subset H_\Lambda$ consisting of vectors, which are invariant with respect to internal gauge transformations,

$$\mathcal{H}_\Lambda := \{h \in H_\Lambda | G^i_\Lambda h = h\}. \tag{3.2}$$

Theorem 3.2: *The algebra of internal observables (respectively, extended internal observables) is canonically isomorphic with the algebra of those compact (respectively, bounded) operators on the Hilbert space* $\mathcal{H}_\Lambda$*, which commute with the action of the group* G^∞_Λ*. This means*

$$\mathfrak{O}^i_\Lambda \cong \mathfrak{K}(\mathcal{H}_\Lambda) \cap (G^\infty_\Lambda)'. \tag{3.3}$$

Proof: Consider the direct sum decomposition

$$H_\Lambda = \mathcal{H}_\Lambda \oplus \mathcal{H}^\perp_\Lambda, \tag{3.4}$$

with $\mathcal{H}^\perp_\Lambda$ denoting the orthogonal complement of $\mathcal{H}_\Lambda$. Since the actions of G^i_Λ and G^∞_Λ commute, $\mathcal{H}_\Lambda$ is invariant under the action of G^∞_Λ and, thus, under the full gauge group G_Λ. Consequently, by unitarity of G_Λ, $\mathcal{H}^\perp_\Lambda$ is invariant, too. This implies the following block-diagonal structure of elements of G_Λ with respect to the decomposition (3.4):

$$\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix},$$

with A and B denoting unitary operators on $\mathcal{H}_\Lambda$ and $\mathcal{H}^\perp_\Lambda$, respectively. It can be easily shown that

$$(G_\Lambda)' = \left\{ \begin{pmatrix} C & 0 \\ 0 & D \end{pmatrix} \in \mathfrak{K}(H_\Lambda) : [A,C] = 0 = [B,D], \text{ for all } \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \in G_\Lambda \right\}. \tag{3.5}$$

Indeed, an arbitrary element $\left(\begin{smallmatrix} C & E \\ F & D \end{smallmatrix}\right)$ belongs to $(G_\Lambda)'$ iff

$$AC = CA, \quad AE = EB, \quad BF = FA, \quad BD = DB,$$

for any $\left(\begin{smallmatrix} A & 0 \\ 0 & B \end{smallmatrix}\right) \in G_\Lambda$. For $\left(\begin{smallmatrix} h \\ 0 \end{smallmatrix}\right) \in \mathcal{H}_\Lambda$ we have $\left(\begin{smallmatrix} 0 \\ Fh \end{smallmatrix}\right) \in \mathcal{H}^\perp_\Lambda$. On the other hand, any element of G^i_Λ has the form $\left(\begin{smallmatrix} \mathbf{1} & 0 \\ 0 & B \end{smallmatrix}\right)$. Thus,

$$\begin{pmatrix} \mathbf{1} & 0 \\ 0 & B \end{pmatrix} \begin{pmatrix} 0 \\ Fh \end{pmatrix} = \begin{pmatrix} 0 \\ BFh \end{pmatrix} = \begin{pmatrix} 0 \\ Fh \end{pmatrix},$$

for all elements of G^i_Λ, yielding $\left(\begin{smallmatrix} 0 \\ Fh \end{smallmatrix}\right) \in \mathcal{H}_\Lambda$. Thus, $Fh = 0$, for all $h \in \mathcal{H}_\Lambda$, implying $F = 0$. In an analogous way one shows $E = 0$. This gives formula (3.5).

We decompose $\left(\begin{smallmatrix} C & 0 \\ 0 & D \end{smallmatrix}\right) = \left(\begin{smallmatrix} C & 0 \\ 0 & 0 \end{smallmatrix}\right) + \left(\begin{smallmatrix} 0 & 0 \\ 0 & D \end{smallmatrix}\right)$. Since the restriction of a compact operator to a closed subspace is compact, we have $\left(\begin{smallmatrix} C & 0 \\ 0 & 0 \end{smallmatrix}\right) \in \mathfrak{K}(\mathcal{H}_\Lambda)$. Moreover, $\left(\begin{smallmatrix} 0 & 0 \\ 0 & D \end{smallmatrix}\right) \in \mathfrak{I}^i_\Lambda$. This yields the direct sum decomposition

$$(G_\Lambda)' = (\mathfrak{K}(\mathcal{H}_\Lambda) \cap (G_\Lambda)') \oplus (\mathfrak{I}^i_\Lambda \cap (G_\Lambda)'). \tag{3.6}$$

Consequently, the algebra of internal observables $\mathfrak{O}^i_\Lambda = (G_\Lambda)' / \{\mathfrak{I}^i_\Lambda \cap (G_\Lambda)'\}$ is represented by the direct sum complement

$$\mathfrak{K}(\mathcal{H}_\Lambda) \cap (G_\Lambda)' = \mathfrak{K}(\mathcal{H}_\Lambda) \cap (G^i_\Lambda)' \cap (G^\infty_\Lambda)'$$

in $(G_\Lambda)'$. Finally, by (3.5) we have that arbitrary elements of $(G^i_\Lambda)'$ have the form $\left(\begin{smallmatrix} C & 0 \\ 0 & D \end{smallmatrix}\right)$, with $C \in \mathfrak{K}(\mathcal{H}_\Lambda)$ and $[D,B] = 0$, for any unitary B acting on $\mathcal{H}^\perp_\Lambda$. Thus, $\mathfrak{K}(\mathcal{H}_\Lambda) \subset (G^i_\Lambda)'$, yielding the isomorphism (3.3). Taking the multiplier algebra of $\mathfrak{K}(\mathcal{H}_\Lambda) \cap (G^\infty_\Lambda)'$ yields $\mathfrak{B}(\mathcal{H}_\Lambda) \cap (G^\infty_\Lambda)'$. ■

To find a presentation of this algebra in terms of generators and relations is a nontrivial task, which will be dealt with in Sec. V. Here, we only stress that obvious observables like Wilson loops are represented in $\mathcal{H}_\Lambda$ as multiplication operators and, therefore, belong to the extended algebra $M(\mathfrak{O}^i_\Lambda)$. It is impossible, to build compact operators from Wilson loops only. For that purpose, one must consider combinations of them with gauge invariant combinations of color electric fields, compare with the Remark after the proof of Lemma 2.2.

Now observe that the restriction of the unitary action of G^∞_Λ to the subspace $\mathcal{H}_\Lambda$ is not irreducible. Thus, $\mathcal{H}_\Lambda$ splits into the direct sum of irreducible subspaces. Each irreducible representation of G_z, $z \in \Lambda^0_\infty$, is labeled by its highest weight (m,n) and is equivalent to the corresponding tensor representation in the space $\mathbb{S}^m_n(\mathbb{C}^3)$ of m-contravariant, n-covariant, traceless and totally symmetric tensors over $\mathbb{C}^3$, endowed with the natural scalar product induced by the scalar product on $\mathbb{C}^3$. Therefore, irreducible representations of G^∞_Λ are labeled by sequences of highest weights

$$(\mathbf{m},\mathbf{n}) = (m_{z_1},\ldots,m_{z_M};n_{z_1},\ldots,n_{z_M}), \tag{3.7}$$

where $(z_1,\ldots,z_M)$ label the lattice external sites. These representations are equivalent to tensor products of representations in spaces $\mathbb{S}^{m_{z_i}}_{n_{z_i}}(\mathbb{C}^3)$. Let us denote by $\mathcal{H}^{(\mathbf{m},\mathbf{n})}_\Lambda$ the sum of all the irreducible subspaces with respect to the action of G^∞_Λ, which carry the same type $(\mathbf{m},\mathbf{n})$. Then we have

$$\mathcal{H}_\Lambda = \oplus\, \mathcal{H}^{(\mathbf{m},\mathbf{n})}_\Lambda. \tag{3.8}$$

Obviously, every subspace of type $(\mathbf{m},\mathbf{n})$ is invariant under the action of the observable algebra,

$$\mathfrak{O}^i_\Lambda \mathcal{H}^{(\mathbf{m},\mathbf{n})}_\Lambda \subset \mathcal{H}^{(\mathbf{m},\mathbf{n})}_\Lambda.$$

This yields the following.

Corollary 3.3: The irreducible representations of $\mathfrak{O}^i_\Lambda$ are labelled by highest weight representations $(\mathbf{m},\mathbf{n})$ of G^∞_Λ. For any $(\mathbf{m},\mathbf{n})$, the corresponding irreducible representation of $\mathfrak{O}^i_\Lambda$ coincides with the algebra of those compact operators on $\mathcal{H}^{(\mathbf{m},\mathbf{n})}_\Lambda$, which commute with the action of the group G^∞_Λ.

We call the pair $(\mathbf{m},\mathbf{n})$ the boundary flux distribution carried by the gluonic field. In the next section, it will become obvious that all distributions $(\mathbf{m},\mathbf{n})$ occur.

C. Explicit description of irreducible representations

Now we give an explicit description of the above irreducible representations, using the explicit form (2.35) of H_Λ. Any element of H_Λ is a linear combination of fermionic vectors (2.36) with coefficients being L^2-functions depending on gluonic potentials U. The invariant subspace $\mathcal{H}_\Lambda \subset H_\Lambda$ is spanned by vectors from H_Λ, which are scalars with respect to G^i_Λ. This means that for every $x \in \Lambda^0$, all the color indices $(A_1,\ldots,A_n)$ of the fermionic state (2.36) must be saturated with the upper indices of either $U^A{}_B(x,y)$ or the canonical tensor $\boldsymbol{\epsilon}^{ABC}$. After such contractions, we are—in general—left with free indices at external points $z_i \in \Lambda^0_\infty$. Finally, such a vector can be multiplied by gauge invariant functions of gluonic potentials U. The general form of such functions is as follows:

$$f([U]) = f(\mathrm{Tr}(U_{\gamma_1}),\ldots,\mathrm{Tr}(U_{\gamma_n})),$$

where f is a function of n scalar variables, each $\gamma=(x_1,x_2,\ldots,x_m)$ is an arbitrary closed lattice path and U_γ is the corresponding *parallel transporter* along γ,

$$U^A_{\gamma B} = U^A{}_{C_2}(x_1,x_2)U^{C_2}{}_{C_3}(x_2,x_3)\cdots U^{C_{m-1}}{}_B(x_{m-1},x_m). \tag{3.9}$$

Let us denote the result of these operations by

$$\boldsymbol{\Psi} = \left(\Psi^{\ldots,A_1,\ldots,A_{m_{z_i}},\ldots}_{\ldots,B_1,\ldots,B_{n_{z_i}},\ldots}\right). \tag{3.10}$$

This is a collection of G^i_Λ-invariant vectors belonging to H_Λ, labeled by tensor indices assigned to external points $z_i \in \Lambda^0_\infty$, i,e., an H_Λ-valued tensor over

$$\mathbb{C}^{3M} = \bigoplus_{z_i \in \Lambda^0_\infty} \mathbb{C}^3_{z_i}.$$

Linear combinations of those elements span the invariant subspace $\mathcal{H}_\Lambda$, with coefficients built from products of tensors

$$t(z_i) = \left(t^{B_1,\ldots,B_{n_{z_i}}}_{A_1,\ldots,A_{m_{z_i}}}(z_i)\right) \in \mathbb{T}^{n_{z_i}}_{m_{z_i}}(\mathbb{C}^3). \tag{3.11}$$

The resulting vector belonging to $\mathcal{H}_\Lambda$ is a scalar obtained by contraction of (3.10) with these tensors,

$$\Psi = \Psi(t(z_1),\ldots,t(z_M)) = t^{B_1,\ldots,B_{n_{z_i}}}_{A_1,\ldots,A_{m_{z_i}}}(z_i)\cdots\Psi^{\ldots,A_1,\ldots,A_{m_{z_i}},\ldots}_{\ldots,B_1,\ldots,B_{n_{z_i}},\ldots}. \tag{3.12}$$

Each of the irreducible components $\mathcal{H}_\Lambda^{(\mathbf{m},\mathbf{n})}$ is composed of combinations (3.12), for which all the tensors $t(z_i)$ are irreducible (symmetric, traceless), i.e., where $t(z_i)\in \mathbb{S}^{n_{z_i}}_{m_{z_i}}(\mathbb{C}^3)\subset \mathbb{T}^{n_{z_i}}_{m_{z_i}}(\mathbb{C}^3)$. If t's are not irreducible, (3.12) is a sum of irreducible components belonging to different weights $(\mathbf{m},\mathbf{n})$, according to the decomposition of tensors $t(z_i)$ into the sum of products of irreducible (symmetric, traceless) tensors with canonical tensors $\delta^A_{\ B}$, ϵ^{ABC} and ϵ_{ABC}.

IV. THE FULL ALGEBRA OF OBSERVABLES

A. Motivation and basic definitions

One of the main perspectives of this work is the construction of the thermodynamical limit of finite lattice QCD. In Ref. 1 we have, in the context of finite lattice QED, outlined a strategy based upon an inductive (respectively, projective) limit procedure for observable algebras (respectively, state spaces). In what follows, we will argue that in order to implement this strategy, we must extend both the algebra of observables $\mathfrak{O}^i_\Lambda$ (by adding certain "external observables") and the Hilbert space $\mathcal{H}_\Lambda$ (by tensorizing with the Hilbert space of tensors at external points). Then, each collection $(\Psi^{\ldots,A_1,\ldots,A_{m_{z_i}},\ldots}_{\ldots,B_1,\ldots,B_{n_{z_i}},\ldots})$ of G^i_Λ-invariant H_Λ-vectors labelled by free indices at external points [see (3.10)] will constitute a physical state.

Thus, let us consider two lattices Λ_1 and Λ_2 which are disjoint $(\Lambda_1\cap\Lambda_2=\emptyset)$ and have a common wall such that their sum $\tilde{\Lambda}=\Lambda_1\cup\Lambda_2$ is also a cubic lattice. If $x\in\Lambda_1$ and $y\in\Lambda_2$ are adjacent points in $\tilde{\Lambda}$, then we identify their external points. This joint external point z may be visualized e.g., as the middle point of the connecting link (x,y). The parallel transporter on (x,y) is defined by

$$U^A_{\ B}(x,y) := U^A_{\ C}(x,z)U^C_{\ B}(z,y). \tag{4.1}$$

Observables internal relative to Λ_1 (respectively, Λ_2) are built, among others, from parallel transporters U_γ along lattice paths γ, which are completely contained in Λ_1 (respectively, Λ_2). On the other hand, there exist observables internal relative to $\tilde{\Lambda}$, built from parallel transporters along paths crossing the set of joint external points. Such observables describe correlations between phenomena occurring in the two disjoint regions Λ_1 and Λ_2. As examples, consider the $\tilde{\Lambda}$-internal observables

$$J^{ab}_\gamma(x,y) := \psi^{*a}_{\ A}(x)U^A_{\gamma B}\psi^{bB}(y),$$

with γ being a path from $x\in\Lambda_1$ to $y\in\Lambda_2$, or observables

$$U_\gamma := U^A_{\gamma A},$$

with γ being a closed path lying partially in Λ_1 and partially in Λ_2. These are operators belonging to the multiplier algebra $M(\mathfrak{O}^i_{\tilde{\Lambda}})$ and, whence, are *observables* in the extended sense. According to the above-mentioned inductive limit procedure, the observable algebra related to $\tilde{\Lambda}$ should be constructed from observables related to Λ_1 and Λ_2. But, in order to construct observables related to $\tilde{\Lambda}$ of the above type (describing correlations), we must admit fields "having free external tensor indices," like $\psi^{*a}_{\ A}(x)U^A_{\gamma_1 C}(x,z)$ and $U^C_{\gamma_2 B}(z,y)\psi^{bB}(y)$, with z being a joint external point. Quantities of this type are usually called "charge carrying fields," they were first introduced by Mandelstam (see Ref. 20).

Observe that charge carrying fields do not act neither on $\mathcal{H}_{\Lambda_1}$ nor on $\mathcal{H}_{\Lambda_2}$. They carry the fundamental (respectively, its contragredient) representation of SU(3) associated with the corre-

sponding external point. Thus, we must extend the Hilbert space $\mathcal{H}_\Lambda$ by tensorizing it with the Hilbert space $\mathbb{T}_\infty$ generated by the fundamental and its contragredient representations of SU(3) associated with all external points,

$$\mathbb{T}_\infty := \bigotimes_{z\in\Lambda^0_\infty} \mathbb{T}(z), \quad \mathbb{T}(z) := \bigoplus_{(m,n)} \mathbb{T}^m_n(z). \tag{4.2}$$

Here, $\mathbb{T}^m_n(z)$ denotes the space of all—not necessarily irreducible—m-contravariant, n-covariant tensors over $\mathbb{C}^3_z$. This way, we are led to consider the Hilbert space $\mathbb{T}_\infty \otimes \mathcal{H}_\Lambda$. The action of the gauge group G^∞_Λ extends in a natural way from $\mathcal{H}_\Lambda$ to this tensor product,

$$T(g)(t\otimes\Psi) := t\otimes(g\cdot\Psi), \quad t\otimes\Psi\in\mathbb{T}_\infty\otimes\mathcal{H}_\Lambda, \quad g\in G^\infty_\Lambda. \tag{4.3}$$

On the other hand, the natural action of G^∞_Λ on $\mathbb{T}_\infty$ can be also extended to this product,

$$R(g)(t\otimes\Psi) := (g\cdot t)\otimes\Psi. \tag{4.4}$$

It is clear that elements of $\mathbb{T}_\infty\otimes\mathcal{H}_\Lambda$ may be represented as "wave functions with free boundary indices," i.e., objects of type (3.10). Indeed, such tensors can be naturally viewed as antilinear mappings

$$\mathbb{T}_\infty \ni s \mapsto (t\otimes\Psi)(s) := (s|t)\Psi \in \mathcal{H}_\Lambda, \tag{4.5}$$

where $(\cdot|\cdot)$ denotes the scalar product in $\mathbb{T}_\infty$. Obviously, wave functions (3.10) are mappings of this type, too.

The above extension of the Hilbert space is necessary if we want to construct the thermodynamical limit of the theory by the above-mentioned projective limit procedure. According to this procedure, physical states related to Λ_1 are obtained from physical states related to $\tilde{\Lambda}$ by applying a projection operator $P_{\Lambda_1,\tilde{\Lambda}}$, which consists in averaging over the degrees of freedom located in Λ_2. More precisely, consider a wave function $\tilde{\psi}\in\mathcal{H}_{\tilde{\Lambda}}$, given by (3.12), take the corresponding projector $|\tilde{\psi}\rangle\langle\tilde{\psi}|$, split all parallel transporters on links joining Λ_1 and Λ_2 according to (4.1), and integrate over all degrees of freedom related to Λ_2 (including those located on external links of Λ_2). The result is a mixed state related to Λ_1, which can be represented as a mixture of pure states, each of them being a $\mathcal{H}_{\Lambda_1}$-valued tensor $\mathbf{\Psi}$ with respect to joint infinities of Λ_1 and Λ_2. In other words, the averaging procedure produces, in general, free indices on the common boundary between Λ_1 and Λ_2. To be consistent, we must admit such free indices from the very beginning.

From the above discussion we see that tensors $t(z)$ occurring in elements $t\otimes\Psi\in\mathbb{T}_\infty\otimes\mathcal{H}_\Lambda$ are not *a priori* given c-number quantities, but quantum averages over external (i.e., contained in Λ_2) degrees of freedom.

There is, however, an additional requirement, which we impose on physical states of the system: the averaging procedure described above should be compatible with gauge transformations. Assume that we average a state $\tilde{\psi}\in\mathcal{H}_{\tilde{\Lambda}}$ over Λ_2, with the parallel transporters on links joining Λ_1 and Λ_2 split according to (4.1). Any gauge transformation g at a common external point z between Λ_1 and Λ_2, acting on $\tilde{\psi}$ can be either implemented by the action of $G^\infty_{\Lambda_1}$ or $G^\infty_{\Lambda_2}$. After averaging over Λ_2, the action of the gauge group $G^\infty_{\Lambda_1}$ is of course still represented by $T(g)$, whereas the action of $G^\infty_{\Lambda_2}$ reduces to $R(g)$ representing gauge transformations in "the rest of the world." But, compatibility of averaging with gauging means that the result of this gauge transformation should not depend upon its implementation. Hence, we postulate

$$T(g)\mathbf{\Psi} = R(g)\mathbf{\Psi}. \tag{4.6}$$

As a result of our discussion, we define the physical Hilbert space as

$$\mathbf{H}_\Lambda := \{\mathbf{\Psi} \in \mathbb{T}_\infty \otimes \mathcal{H}_\Lambda | T(g)\mathbf{\Psi} = R(g)\mathbf{\Psi}, \text{ for any } g \in G_\Lambda^\infty\}, \tag{4.7}$$

with gauge transformation being, according to the above discussion, represented by T. The property (4.6) is obviously not shared by elements, which have partially contracted external indices or indices which do not come from the bosonic wave functions $U(x,\infty)$. To illustrate this, we consider the following examples:

$$\Psi^{\ldots,A_1,\ldots,A_m,\ldots}_{\ldots,B_1,\ldots,B_n,\ldots} r^{B_n}_{A_m}(z) \text{ or } \Psi^{\ldots,A_1,\ldots,A_m,\ldots}_{\ldots,B_1,\ldots,B_n,\ldots} r^{A_{m+1}}_{B_{n+1}}(z), \quad \text{with } r(z) \in \mathbb{T}^1_1(z). \tag{4.8}$$

Thus, (4.6) is fulfilled precisely by elements of type (3.10) having all indices free. Admitting objects of type (4.8) would mean admitting additional degrees of freedom r, which would live at joint external points z and would be relevant for the description of physical states on the lattice $\tilde{\Lambda} = \Lambda_1 \cup \Lambda_2$. In that case, these joint external points could not be removed from $\tilde{\Lambda}$.

Using (4.2), we have

$$\mathbf{H}_\Lambda = \bigoplus_{(\mathbf{m},\mathbf{n})} \mathbf{H}_\Lambda^{(\mathbf{m},\mathbf{n})}. \tag{4.9}$$

Here, $\mathbf{H}_\Lambda^{(\mathbf{m},\mathbf{n})}$ denotes the intersection of $\mathbf{H}_\Lambda$ with $\mathbb{T}_\infty^{(\mathbf{m},\mathbf{n})} \otimes \mathcal{H}_\Lambda$, where

$$\mathbb{T}_\infty^{(\mathbf{m},\mathbf{n})} := \bigotimes_{z \in \Lambda_\infty^0} \mathbb{T}^{m_z}_{n_z}(z) \tag{4.10}$$

is the subspace of tensorial type (m_z, n_z) at each $z \in \Lambda_\infty^0$. Note that, contrary to (3.8), (4.9) is *not* a decomposition into irreducible components.

Next, observe that the scalar products on $\mathbf{H}_\Lambda$ and on $\mathbb{T}_\infty$ induce a natural scalar product on $\mathbf{H}_\Lambda$. Using the representation (3.10), it is given by

$$(\mathbf{\Psi}|\mathbf{\Phi})_{\mathbf{H}_\Lambda} = \left(\Psi^{\ldots,A_1,\ldots,A_{m_{z_i}},\ldots}_{\ldots,B_1,\ldots,B_{n_{z_i}},\ldots} \middle| \Phi^{\ldots,C_1,\ldots,C_{m_{z_i}},\ldots}_{\ldots,D_1,\ldots,D_{n_{z_i}},\ldots} \right)_{H_\Lambda} \times \cdots g_{A_1 C_1} \cdots g_{A_{m_{z_i}} C_{m_{z_i}}} \cdots g^{B_1 D_1} \cdots g^{B_{m_{z_i}} B_{m_{z_i}}} \cdots . \tag{4.11}$$

Tensors with different valences (i.e., having a different number of indices) are, by definition, orthogonal.

We define the full algebra of observables related to Λ as the C^*-algebra of gauge invariant compact operators acting on $\mathbf{H}_\Lambda$,

$$\mathfrak{O}_\Lambda := \mathfrak{K}(\mathbf{H}_\Lambda) \cap (G_\Lambda^\infty)'. \tag{4.12}$$

As before, we define the *extended* full observable algebra as $M(\mathfrak{O}_\Lambda) = \mathfrak{B}(\mathbf{H}_\Lambda) \cap (G_\Lambda^\infty)'$. Consider the algebra $\mathfrak{O}_\Lambda^\infty$ of those compact operators acting on $\mathbb{T}_\infty$, which are invariant with respect to the action of G_Λ^∞. By classical invariant theory, this algebra is generated (in the sense of Woronowicz) by operations of tensorizing or contracting with SU(3)-invariant tensors $\delta^A{}_B$, ϵ^{ABC}, and ϵ_{ABC}, and by projection operators $P^{(\mathbf{m},\mathbf{n})}$ onto $\mathbb{T}_\infty^{(\mathbf{m},\mathbf{n})} \subset \mathbb{T}_\infty$.

Proposition 4.1: The full observable algebra can be characterized as follows:

$$\mathfrak{O}_\Lambda \cong \mathfrak{O}_\Lambda^i \otimes \mathfrak{O}_\Lambda^\infty. \tag{4.13}$$

Proof: Any compact gauge invariant operator A acting on $\mathbf{H}_\Lambda$ can be extended to a gauge invariant operator on the whole tensor product $\mathbb{T}_\infty \otimes \mathcal{H}_\Lambda$, using contractions and tensor products with boundary tensors r in $\mathbb{T}_\infty$, see formula (4.8). More precisely, we set

$$A(C(r \otimes \mathbf{\Psi})) := C(r \otimes A(\mathbf{\Psi})), \tag{4.14}$$

for any tensor $r \in \mathbb{T}_\infty$ and any contraction operator C (the result of the contraction on the right-hand-side vanishes *by definition* if a corresponding index is missing in $A\mathbf{\Psi}$). This way we have proved that

$$\mathfrak{K}(\mathbf{H}_\Lambda) \cap (G_\Lambda^\infty)' \cong \mathfrak{K}(\mathbb{T}_\infty \otimes \mathcal{H}_\Lambda) \cap (G_\Lambda^\infty)'. \tag{4.15}$$

But we have

$$\mathfrak{K}(\mathbb{T}_\infty \otimes \mathcal{H}_\Lambda) \cong \mathfrak{K}(\mathbb{T}_\infty) \otimes \mathfrak{K}(\mathcal{H}_\Lambda), \tag{4.16}$$

and, consequently,

$$\mathfrak{K}(\mathbf{H}_\Lambda) \cap (G_\Lambda^\infty)' \cong \mathfrak{K}(\mathbb{T}_\infty) \otimes (\mathfrak{K}(\mathcal{H}_\Lambda) \cap (G_\Lambda^\infty)') \cong \mathfrak{K}(\mathbb{T}_\infty) \otimes \mathfrak{O}_\Lambda^i. \tag{4.17}$$

Taking again the intersection with $(G_\Lambda^\infty)'$ and implementing it by the representation R yields the thesis. ■

Elements of $\mathfrak{O}_\Lambda^\infty$ representing the rest of the world are called *external observables*.

Adopting the point of view that t occurring in $t \otimes \Psi$ represents the "quantum averages over the external field degrees of freedom," one can argue that the only trace of the action of external observables, which may be seen from Λ, are external gauge invariant operators on $\mathbb{T}_\infty$. Hence, formula (4.13) could be taken as an axiomatic definition of the full observable algebra. The results of the following section show that this approach is equivalent to the one used in the present section.

B. Classification of irreducible representations

Obviously, $\mathbb{T}_\infty$ is not irreducible with respect to the action of $\mathfrak{O}_\Lambda^\infty$. If $t(z) \in \mathbb{T}_n^m(z)$, then its image under this action is a sum of components belonging to $\mathbb{T}_l^k(z)$ with (k,l) fulfilling

$$(m-n) \bmod 3 = (k-l) \bmod 3.$$

We see that the $\mathbb{Z}_3$-valued flux

$$\Phi(z) := (m_z - n_z) \bmod 3 \tag{4.18}$$

through each external link (x,z), $z \in \Lambda_\infty^0$, is conserved under the action of $\mathfrak{O}_\Lambda^\infty$. Let us denote the sequence of $\mathbb{Z}_3$-valued fluxes assigned to all boundary points by

$$\mathbf{\Phi} := (\Phi(z_1), \Phi(z_2), \ldots).$$

In what follows, we call $\mathbf{\Phi}$ boundary flux distribution. Consequently, we define the subspace $\mathbf{H}_\Lambda^{\mathbf{\Phi}} \subset \mathbf{H}_\Lambda$ as the space spanned by those tensors (3.10) which fulfill condition $\Phi(z_i) = (m_{z_i} - n_{z_i}) \bmod 3$. In other words, we set

$$\mathbf{H}_\Lambda^{\mathbf{\Phi}} := \bigoplus_{m(z_i) - n(z_i) \bmod 3 = \Phi(z_i)} \mathbf{H}_\Lambda^{(\mathbf{m},\mathbf{n})}, \tag{4.19}$$

with $\mathbf{H}_\Lambda^{(\mathbf{m},\mathbf{n})}$ given by decomposition (4.9). Obviously, these subspaces are invariant under the action of the full observable algebra $\mathfrak{O}_\Lambda$ and $\mathfrak{O}_\Lambda$ acts irreducibly on each of them. Moreover, the physical Hilbert space $\mathbf{H}_\Lambda$ splits into the direct sum of them,

$$\mathbf{H}_\Lambda = \bigoplus_{\mathbf{\Phi}} \mathbf{H}_\Lambda^{\mathbf{\Phi}}. \tag{4.20}$$

We obviously have the following.

Lemma 4.2: The spaces $\mathbf{H}_\Lambda^{\mathbf{\Phi}}$ *provide all the irreducible representations of the algebra of observables* $\mathfrak{O}_\Lambda$.

We denote the irreducible component of $\mathfrak{O}_\Lambda$ acting on $\mathbf{H}_\Lambda^{\mathbf{\Phi}}$, by $\mathfrak{O}_\Lambda^{\mathbf{\Phi}}$.

Now, we define the global flux associated with a given boundary flux distributions $\mathbf{\Phi}$ setting

$$\mathbf{\Phi}_{\partial\Lambda} := \left(\sum_{z\in\Lambda^0_\infty} \mathbf{\Phi}(z) \right) \mathrm{mod}\, 3. \tag{4.21}$$

Let us denote the total number of gluonic and antigluonic flux lines running through the boundary by

$$m := \sum_{z_i\in\Lambda^0_\infty} m(z_i), \tag{4.22}$$

$$n := \sum_{z_i\in\Lambda^0_\infty} n(z_i). \tag{4.23}$$

Then, we get

$$\Phi_{\partial\Lambda} = (m-n) \mathrm{mod}\, 3. \tag{4.24}$$

Lemma 4.3: The irreducible representations of $\mathfrak{O}_\Lambda$ *in* $\mathbf{H}^{\mathbf{\Phi}}_\Lambda$ *and in* $\mathbf{H}^{\mathbf{\Phi}'}_\Lambda$ *are unitarily equivalent, if and only if* $\mathbf{\Phi}$ *and* $\mathbf{\Phi}'$ *carry the same global flux,*

$$\Phi_{\partial\Lambda} = \Phi'_{\partial\Lambda}.$$

Proof: Suppose that we are given a pair $(\mathbf{\Phi},\mathbf{\Phi}')$ such that $\Phi_{\partial\Lambda}=\Phi'_{\partial\Lambda}$. Then, $\mathbf{H}^{\mathbf{\Phi}}_\Lambda$ is given by (4.19) and, similarly,

$$\mathbf{H}^{\mathbf{\Phi}'}_\Lambda = \bigoplus_{m'(z_i)-n'(z_i)\mathrm{mod}\,3=\Phi'(z_i)} \mathbf{H}^{(\mathbf{m}',\mathrm{n}')}_\Lambda.$$

For $\Phi_{\partial\Lambda}=\Phi'_{\partial\Lambda}$, formula (4.24) implies that we can choose a pair of labels $(\mathbf{m}_0,\mathbf{n}_0)$ and $(\mathbf{m}'_0,\mathbf{n}'_0)$ such that $m_0=m'_0$, $n_0=n'_0$, Acting with tensorial operators $\xi\in\mathfrak{O}^\infty_\Lambda$ (tensorising and contracting with canonical tensors $\delta^A{}_B$, ϵ^{ABC} and ϵ_{ABC}) on $\mathbf{H}^{(\mathbf{m}_0,\mathbf{n}_0)}_\Lambda$ (respectively, $\mathbf{H}^{(\mathbf{m}'_0,\mathbf{n}'_0)}_\Lambda$), we may pass to any other subspace $\mathbf{H}^{(\mathbf{m},\mathbf{n})}_\Lambda$ of $\mathbf{H}^{\Phi}_\Lambda$ (respectively, any other subspace $\mathbf{H}^{(\mathbf{m}',\mathbf{n}')}_\Lambda$ of $\mathbf{H}^{\mathbf{\Phi}'}_\Lambda$). This way we construct a bijection between the two sets $(\mathbf{m},\mathbf{n})$ and $(\mathbf{m}',\mathbf{n}')$ corresponding to $\mathbf{\Phi}$ and $\mathbf{\Phi}'$, preserving the total number of gluonic and antigluonic lines, $m=m'$ and $n=n'$.

We shall construct an intertwining operator between representations on $\mathbf{H}^{\Phi}_\Lambda$ and $\mathbf{H}^{\Phi'}_\Lambda$. For this purpose, we first define a sequence of isometric isomorphisms of Hilbert spaces,

$$\mathbf{U}_{(\mathbf{m}',\mathbf{n}')(\mathbf{m},\mathbf{n})} : \mathbf{H}^{(\mathbf{m},\mathbf{n})}_\Lambda \to \mathbf{H}^{(\mathbf{m}',\mathbf{n}')}_\Lambda$$

corresponding to the above bijection, as follows. We choose two finite families $\{\beta_a\}$ and $\{\gamma_b\}$ of lattice paths in Λ, fulfilling the following conditions:

(i) their starting points x_a and y_b, together with their end points z_a and w_b belong to the boundary $\partial\Lambda$,
(ii) for every $x\in\Lambda^0_\infty$ there are exactly $\Delta n(x) := n(x)-n'(x)$ paths β starting from x if $\Delta n(x) > 0$ and zero otherwise,
(iii) for every $x\in\Lambda^0_\infty$ there are exactly $\Delta m(x) := m(x)-m'(x)$ paths γ ending at x if $\Delta m(x)>0$ and zero otherwise,
(iv) for every $x\in\Lambda^0_\infty$ there are exactly $-\Delta n(x)$ paths β ending at x if $\Delta n(x)<0$ and zero otherwise,
(v) for every $x\in\Lambda^0_\infty$ there are exactly $-\Delta m(x)$ paths γ starting from x if $\Delta m(x)<0$ and zero otherwise.

Now, the action of the operator $\mathbf{U}_{(\mathbf{m}',\mathbf{n}')(\mathbf{m},\mathbf{n})}$ on a vector $\mathbf{\Psi}\in\mathbf{H}^{(\mathbf{m},\mathbf{n})}_\Lambda$ is defined as follows. We multiply the tensor (3.10) by all parallel transporters $U^{B_a}_{\beta_a A_a}$ and $U^{B_b}_{\gamma_b A_b}$, see formula (3.9). Then, we contract all the subsequent upper indices B_a with the corresponding subsequent lower indices B_i of

$\mathbf{\Psi}$ at the starting points of the curves β and all the subsequent lower indices A_b with the corresponding upper indices A_i of $\mathbf{\Psi}$ at the end points of the curves γ. It is easy to see that the inverse (adjoint) operator consists in multiplying $\mathbf{\Psi}$ by the same transporters, but in contracting indices A_a with the corresponding subsequent upper indices A_i of $\mathbf{\Psi}$ at the starting points of the curves β and all the subsequent indices B_b with the corresponding lower indices B_i of $\mathbf{\Psi}$ at the end points of the curves γ. This implies that

$$\mathbf{U}^{*}_{(\mathbf{m}',\mathbf{n}')(\mathbf{m},\mathbf{n})}\mathbf{U}_{(\mathbf{m}',\mathbf{n}')(\mathbf{m},\mathbf{n})} = \mathrm{id} = \mathbf{U}_{(\mathbf{m}',\mathbf{n}')(\mathbf{m},\mathbf{n})}\mathbf{U}^{*}_{(\mathbf{m}',\mathbf{n}')(\mathbf{m},\mathbf{n})}.$$

Organizing the operators $\mathbf{U}_{(\mathbf{m}',\mathbf{n}')(\mathbf{m},\mathbf{n})}$ into a block matrix, we get an isometric isomorphism denoted by

$$\mathbf{U}_{\mathbf{\Phi}'\mathbf{\Phi}}:\mathbf{H}^{\mathbf{\Phi}}_{\Lambda} \to \mathbf{H}^{\mathbf{\Phi}'}_{\Lambda}. \tag{4.25}$$

Next, observe that the action

$$\mathbf{U}^{*}_{\mathbf{\Phi}'\mathbf{\Phi}}\mathfrak{O}^{\mathbf{\Phi}'}_{\Lambda}\mathbf{U}_{\mathbf{\Phi}'\mathbf{\Phi}}:\mathbf{H}^{\mathbf{\Phi}}_{\Lambda} \to \mathbf{H}^{\mathbf{\Phi}}_{\Lambda},$$

defines an irreducible representation of $\mathfrak{O}_\Lambda$ on $\mathbf{H}^{\mathbf{\Phi}}_{\Lambda}$. By Lemma 4.2, this representation must be unitarily equivalent to $\mathfrak{O}^{\mathbf{\Phi}}_{\Lambda}$, i.e., there exists a unitary (intertwining) operator

$$\mathbf{S}:\mathbf{H}^{\mathbf{\Phi}}_{\Lambda} \to \mathbf{H}^{\mathbf{\Phi}}_{\Lambda}, \tag{4.26}$$

such that

$$\mathbf{S}^{*}\mathbf{U}^{*}_{\mathbf{\Phi}'\mathbf{\Phi}}\mathfrak{O}^{\mathbf{\Phi}'}_{\Lambda}\mathbf{U}_{\mathbf{\Phi}'\mathbf{\Phi}}\mathbf{S} = \mathfrak{O}^{\mathbf{\Phi}}_{\Lambda}.$$

It remains to show that equivalent representations yield equal global fluxes: If $\mathbf{H}^{\mathbf{\Phi}}_{\Lambda}$ and $\mathbf{H}^{\mathbf{\Phi}'}_{\Lambda}$ carry equivalent representations, then there exists an intertwiner $\mathbf{V}_{\mathbf{\Phi}'\mathbf{\Phi}}$, such that

$$\Phi'_{\partial\Lambda} = \mathbf{V}_{\mathbf{\Phi}'\mathbf{\Phi}}\Phi_{\partial\Lambda}\mathbf{V}^{-1}_{\mathbf{\Phi}'\mathbf{\Phi}}.$$

But, according to formula (4.24), $\Phi_{\partial\Lambda}$ is a scalar on every irreducible representation space of $\mathfrak{O}_\Lambda$. Thus, it commutes with $\mathbf{V}_{\mathbf{\Phi}'\mathbf{\Phi}}$ yielding $\Phi'_{\partial\Lambda}=\Phi_{\partial\Lambda}$. ■

Theorem 4.4: *There are three inequivalent representations of* $\mathfrak{O}_\Lambda$ *labeled by values of the global flux* $\Phi_{\partial\Lambda}$. *Consequently, the space* $\mathbf{H}_\Lambda$ *splits into the sum of three eigenspaces of* $\Phi_{\partial\Lambda}$

$$\mathbf{H}_\Lambda = \bigoplus_{\lambda=-1,0,1} \mathbf{H}^{\lambda}_{\Lambda}.$$

Each of the spaces $\mathbf{H}^{\lambda}_{\Lambda}$ *is a sum of superselection sectors* $\mathbf{H}^{\mathbf{\Phi}}_{\Lambda}$ *corresponding to all possible distributions* $\mathbf{\Phi}$ *of the global flux* λ. *They carry equivalent representations of* $\mathfrak{O}_\Lambda$.

Anticipating the final result, we call the spaces $\mathbf{H}^{\lambda}_{\Lambda}$ "charge superselection sectors," in contrast to the "boundary-flux-distribution superselection sectors" $\mathbf{H}^{\Phi}_{\Lambda}$. (For an analogous discussion in continuum QED see Ref. 34.)

C. Global color charge and superselection structure

Here we show that, according to the global Gauss law, irreducible representations of $\mathfrak{O}_\Lambda$ are, alternatively, labeled by global color charge (triality), which is carried by the quark fields. We briefly recall the notion of triality and derive the global Gauss law, for details see Ref. 4.

Consider any integrable representation F of the Lie algebra su(3) on a Hilbert space H, i.e., a collection of operators $F^{A}{}_{B}$ in H, fulfilling $F^{A}{}_{A}=0$, $(F^{A}{}_{B})^{*}=F_{B}{}^{A}$, and

$$[F^A{}_B, F^C{}_D] = \delta^C{}_B F^A{}_D - \delta^A{}_D F^C{}_B. \tag{4.27}$$

By (2.22), (2.44), and (2.5), the operators $E^A{}_B(x,y)$ and $\rho^A{}_B(x)$, occurring on both sides of the local Gauss law, are of this type. Integrability means that for each F there exists a unitary representation $G \ni g \to \overline{F}(g) \in B(H)$ of the group G such that F is its derivative. If F_1 and F_2 are two commuting (integrable) representations of su(3), then so is $F_1 + F_2$. Such a collection of operators is an *operator domain* in the sense of Woronowicz, see Ref. 35.

We define an operator function on this domain, i.e., a mapping $F \to \varphi(F)$, which satisfies $\varphi(UFU^{-1}) = U\varphi(F)U^{-1}$ for an arbitrary isometry U, as follows: For any integrable representation F of su(3), consider the corresponding representation $\overline{F}$ of G. Its restriction to the center $\mathcal{Z}$ of G acts as a multiple of the identity on each irreducible subspace H_α of $\overline{F}$,

$$\overline{F}(z)|_{H_\alpha} = \chi^\alpha_F(z) \cdot \mathbf{1}_{H_\alpha}, \quad z \in Z.$$

Obviously, χ^α_F is a character on $\mathcal{Z}$ and, therefore, $(\chi^\alpha_F(z))^3 = 1$. We identify the group of characters on $\mathcal{Z} = \{\zeta \cdot \mathbf{1}_3 | \zeta^3 = 1, \zeta \in \mathbb{C}\}$ with the additive group $\mathbb{Z}_3 \cong \{-1, 0, 1\}$ by assigning to any character χ^α_F a number $k(\alpha) \in \{-1, 0, 1\}$ fulfilling

$$\chi^\alpha_F(\zeta \cdot \mathbf{1}_3) = \zeta^{k(\alpha)}.$$

Hence, there exists a $\mathbb{Z}_3$-valued operator function $F \to \varphi(F)$, defined by

$$\zeta^{\varphi_\alpha(F)} = \chi^\alpha_F(\zeta \cdot \mathbf{1}_3), \tag{4.28}$$

$$\varphi(F) = \sum_\alpha \varphi_\alpha(F) \mathbf{1}_{H_\alpha}. \tag{4.29}$$

Since χ^α_F are characters, we have

$$\varphi(F_1 + F_2) = \varphi(F_1) + \varphi(F_2), \tag{4.30}$$

for F_1 and F_2 commuting. Now, using the equivalence of each irreducible representation α of G with highest weight $(m(\alpha), n(\alpha))$ with the tensor representation in the space $\mathbb{T}^{m(\alpha)}{}_{n(\alpha)}(\mathbb{C}^3)$ of $m(\alpha)$-contravariant, $n(\alpha)$-covariant, completely symmetric and traceless tensors over $\mathbb{C}^3$, we get

$$\chi^\alpha_F(z) = \zeta^{\varphi_\alpha(F)} = \zeta^{m(\alpha) - n(\alpha)}, \tag{4.31}$$

for $z = \zeta \cdot \mathbf{1}_3 \in \mathcal{Z}$. Thus, we have

$$\varphi_\alpha(F) = (m(\alpha) - n(\alpha)) \bmod 3 \tag{4.32}$$

for every irreducible highest weight representation $(m(\alpha), n(\alpha))$. In Ref. 4 we have given an explicit construction of $\varphi(F)$ in terms of Casimir operators of F.

Applying φ to the local Gauss law (2.45) and using additivity (4.30) we obtain a gauge invariant equation for operators with eigenvalues in $\mathbb{Z}_3$,

$$\sum_{y \leftrightarrow x} \varphi(E(x,y)) = \varphi(\rho(x)), \tag{4.33}$$

valid at every lattice site x. The quantity on the right-hand side is the (gauge invariant) local color charge density carried by the quark field.

Using the transformation law (2.15) for $E(x,y)$ under the change of the link orientation and additivity (4.30) of φ, we have for every lattice bond (x,y):

$$\varphi(E(x,y)) + \varphi(E(y,x)) = \varphi(E(x,y)) + \varphi(\check{E}(x,y)) = \varphi(E(x,y) + \check{E}(x,y)), \tag{4.34}$$

because representations E and $\check{E}$ commute. But the following identity holds:

$$\varphi(E(x,y) + \check{E}(x,y)) = 0, \tag{4.35}$$

because both representations have the same irreducible subspaces H_α, with the values of $m(\alpha)$ and $n(\alpha)$ exchanged. [The identity follows also directly from formula (2.21). It implies that the second order Casimirs for E and $\check{E}$ coincide, $K_2(E)=K_2(\check{E})$, whereas $K_3(E)=-K_3(\check{E})$, cf. Ref. 4.]

Now, we take the sum of equations (4.33) over all lattice sites $x\in\Lambda^0$. Due to the above identity, all terms on the left-hand side cancel, except for contributions $\varphi(E(x,\infty))\equiv\varphi(E(x,z))$, $z\in\Lambda^0_\infty$, coming from the boundary. The irreducible subspace $\mathbf{H}^\Phi_\Lambda\subset\mathbf{H}_\Lambda$ characterized by the flux distribution $\mathbf{\Phi}$, see (4.19), is an eigenspace of the gauge invariant operator $\varphi(E(x,z))$, with eigenvalue $(m_z-n_z)\mathrm{mod}\,3=\Phi(z)$, according to formula (4.32). Thus, using (4.21) we obtain

$$\sum_{x\in\partial\Lambda^0} \varphi(E(x,\infty)) = \Phi_{\partial\Lambda}, \tag{4.36}$$

with $\Phi_{\partial\Lambda}$ being the global $\mathbb{Z}_3$-valued boundary flux corresponding to the flux distribution $\mathbf{\Phi}$. On the right-hand side we get the (gauge invariant) global color charge (*triality*), carried by the matter field

$$\mathfrak{t}_\Lambda := \sum_{x\in\Lambda^0} \varphi(\rho(x)). \tag{4.37}$$

Thus, the *global Gauss law* takes the following form:

$$\Phi_{\partial\Lambda} = \mathfrak{t}_\Lambda. \tag{4.38}$$

Both quantities appearing here take eigenvalues in the center $\mathcal{Z}\cong\mathbb{Z}_3$ of G.

Comparing with Theorem 4.4, the global Gauss law yields another, equivalent characterization of irreducible representations of the observable algebra.

Corollary 4.5: The inequivalent representations of $\mathfrak{O}_\Lambda$ are labeled by eigenvalues of global color charge $\mathfrak{t}_\Lambda$.

Remark: We illustrate the main result of this paper. Observe that we can assign to single quark fields [being in the defining representation of SU(3)] triality $+1$ and, consequently to antiquarks -1 (or the other way around). A single lattice gluon field has, of course, triality 0. Now, imagine a state with m quarks and n antiquarks, located in an arbitrary way inside Λ. By additivity of triality, $\mathfrak{t}_\Lambda$ has eigenvalue $m-n\,\mathrm{mod}\,3$ on this state. As discussed already, gauge invariance of states with respect to internal gauge transformations implies that all quark indices inside Λ must be contracted. Basically, this can be done by connecting quark–antiquark pairs *inside* Λ with flux lines built from gluonic parallel transporters and by contracting with canonical tensors $\delta^A{}_B$, ϵ^{ABC}, and ϵ_{ABC}. On the other hand, some of the flux lines starting at a antiquark (or ending at a quark) inside can run through the boundary to end at a quark (or start from an antiquark) *outside* of Λ. By the global Gauss law, the total number of gluonic flux lines minus the number of antigluonic flux lines, calculated modulo 3, is equal to the eigenvalue of triality. But the external quark and antiquark fields are not taken into account by a theory on Λ. After averaging over external fields we are left with the action of external gauge invariant operators $\delta^A{}_B$, ϵ^{ABC} and ϵ_{ABC}. The flux lines running through the boundary may by contracted at points $z\in\Lambda^0_\infty$ with these tensors, eventually leaving either none ($\mathfrak{t}_\Lambda=0$), or one gluonic ($\mathfrak{t}_\Lambda=+1$) or one antigluonic ($\mathfrak{t}_\Lambda=-1$) noncontracted line. These three values of triality correspond to the only possible inequivalent representations of the observable algebra. Thus, in particular, we have rigorously confirmed the heuristic picture, which earlier was taken as a starting point for discussing the quark confinement problem, see e.g., Ref. 16.

V. GENERATORS AND RELATIONS

In this section we wish to find a presentation of the observable algebra in terms of generators and relations, inherited from canonical commutation relations of fields and from the Gauss law. In

order to formulate and to study field dynamics, we rather need a presentation in terms of a set of independent generators. Thus, we wish to solve the Gauss law relations explicitly, to end up with a reduced set of generators and their (anti)commutation relations. We show how to implement this idea by a special gauge fixing procedure based upon the choice of a lattice tree. This procedure leaves us, however, with some discrete gauge freedom. Moreover, we restrict ourselves to the generic stratum of the gauge group action, disregarding all nongeneric strata. But even there, our method works only on a dense subset. These two obstructions to global gauge fixing reflect the Gribov problem, which is well known in the continuum theory, see also Ref. 36 for a discussion of this problem in the Ashtekar theory. Thus, following the gauge fixing idea leads to some delicate problems.

How to overcome these problems will be discussed in separate papers, see Refs. 21 and 22. Instead of trying to fix the gauge, one rather must find a generating set of genuine invariants. Below we show that it is quite easy, to write down a highly redundant set of invariants, but it is very hard to reduce it. If we want to work with genuine invariants we are automatically forced to consider higher order monomials, built from basic bosonic and fermionic fields. These invariants inherit, of course, some (anti)commutation relations, but the algebra generated by them does not close on the linear level. This way interesting new algebras occur. We refer to Ref. 37 for some first remarks on their structure. It turns out that algebras of similar types have been discussed in different areas of mathematical physics throughout the last decade, see the list of references in Ref. 37.

Since the generators of $\mathfrak{O}_\Lambda^\infty$ have been already listed before, it remains to discuss $\mathfrak{O}_\Lambda^i$ in terms of generators and relations.

A. Generators of $\mathfrak{O}_\Lambda^i$

Below, we define a set of generators of $\mathfrak{O}_\Lambda^i$ in terms of gauge-invariant combinations of the fields (U,E,ψ,ψ^*). In the next sections, we will systematically reduce the number of generators to a minimal set.

Theorem 5.1: *The observable algebra $\mathfrak{O}_\Lambda^i$ is generated by the following gauge invariant elements (together with their conjugates):*

$$U_\gamma := U^A_{\gamma A}, \tag{5.1}$$

$$E_\gamma(x,y) := U^A_{\gamma B} E^B{}_A(x,y), \tag{5.2}$$

$$J^{ab}_\gamma(x,y) := \psi^{*a}{}_A(x) U^A_{\gamma B} \psi^{bB}(y), \tag{5.3}$$

$$W^{abc}_{\alpha\beta\gamma}(x,y,z) := \tfrac{1}{6}\epsilon_{ABC} U^A_{\alpha D} U^B_{\beta E} U^C_{\gamma F} \psi^{aD}(x)\psi^{bE}(y)\psi^{cF}(z), \tag{5.4}$$

with γ denoting an arbitrary closed lattice path in formula (5.1), a closed lattice path starting and ending at x in (5.2) and a path from x to y in (5.3). In formula (5.4), α, β and γ are paths starting at some reference point t and ending at x, y, and z, respectively. In formula (5.2), both x and y stand also for ∞.

For the proof see Appendix B.

Note that the observables J^{ab}_γ and $W^{abc}_{\alpha\beta\gamma}$ represent hadronic matter of mesonic and baryonic type. They will play a basic role in future investigations towards a construction of an effective theory of interacting hadrons. Looking at the lattice Hamiltonian, given by (2.46), we see that the kinetic energy E^2 of the gluonic field is given by second Casimirs and its potential energy B^2 is given by Wilson loops U_γ. By the above theorem, the Casimirs can be expressed in terms of the above invariants. It is easy to see that the matter field part is given in terms of J's (which, however, are related with W's *via* nonlinear constraints). At present, it is not quite clear, which parametrization of the Hamiltonian in terms of observables will be the most efficient one for future applications.

B. The reduction idea

The above generating set turns out to be highly redundant. There is a number of nontrivial relations between generators, inherited from the canonical (anti) commutation relations and from the local Gauss laws. Below, we will show how to solve the local Gauss laws explicitly. This will be done by using a technique, based upon the choice of a *lattice tree*. This way we shall prove that $\mathfrak{O}^i_\Lambda$ can be decomposed (in a tree-dependent way) into the tensor product of a gluonic and a matter field part. This presentation of $\mathfrak{O}^i_\Lambda$ can be constructed in two steps:

(1) First we fix a lattice point x_0 and impose gauge invariance with respect to the pointed gauge group at x_0,

$$G^0_\Lambda = G^{i,0}_\Lambda \times G^\infty_\Lambda \tag{5.5}$$

with

$$G^{i,0}_\Lambda = \prod_{x_0 \neq x \in \Lambda^0} G_x. \tag{5.6}$$

Moreover, we implement the Gauss laws at all points $\Lambda^0 \ni x \neq x_0$, i.e., we factorize with respect to the ideal $\mathfrak{I}^0_\Lambda \cap (G^0_\Lambda)'$, with $\mathfrak{I}^0_\Lambda$ being generated by the Lie algebra $\mathfrak{g}^{i,0}_\Lambda \subset \mathfrak{g}^i_\Lambda$ of $G^{i,0}_\Lambda$. This gives the pointed algebra of internal observables,

$$\mathfrak{O}^{i,0}_\Lambda := (G^0_\Lambda)'/\{\mathfrak{I}^0_\Lambda \cap (G^0_\Lambda)'\}. \tag{5.7}$$

(2) Next, we impose on $\mathfrak{O}^{i,0}_\Lambda$ gauge invariance with respect to the residual gauge group G_{x_0}, and factorize with respect to the ideal $\mathfrak{I}_{x_0} \subset \mathfrak{O}^{i,0}_\Lambda$ generated by the local Gauss law at x_0.

Whereas the first step can be performed without any obstructions, in the second step, all the problems mentioned at the beginning of this chapter show up.

Theorem 5.2: *The internal observable algebra can be viewed as follows:*

$$\mathfrak{O}^i_\Lambda \cong (G_{x_0})'/\{\mathfrak{I}_{x_0} \cap (G_{x_0})'\}, \tag{5.8}$$

where $(G_{x_0})'$ and $\mathfrak{I}_{x_0}$ *are considered as subalgebras of* $\mathfrak{O}^{i,0}_\Lambda$.

Proof: Since G_{x_0} commutes with G^0_Λ, we have $(G_\Lambda)' = (G^0_\Lambda)' \cap (G_{x_0})'$. Moreover, the invariant subspaces H^0 and H_{x_0} of $G^{i,0}_\Lambda$ and G_{x_0} are both closed subspaces of H_Λ, whereas $\mathfrak{I}^0_\Lambda$ and $\mathfrak{I}_{x_0}$ are composed of operators vanishing on H^0 and H_{x_0}, respectively. Observe that

$$H^0 \cap H_{x_0} = \mathcal{H}_\Lambda$$

and that the ideal

$$\mathfrak{I}_\Lambda = \mathfrak{I}^0_\Lambda \oplus \mathfrak{I}_{x_0}$$

is composed of those operators which vanish on this intersection. Using completely analogous arguments as in the proof of Theorem 3.2, we obtain

$$\mathfrak{O}^{i,0}_\Lambda = \mathfrak{K}(H^0) \cap (G^\infty_\Lambda)'. \tag{5.9}$$

In the second step we must factorize the commutant $(G_{x_0})'$ of G_{x_0} in $\mathfrak{O}^{i,0}_\Lambda$ with respect to $\mathfrak{I}_{x_0} \cap (G_{x_0})'$. But by (5.9) we have

$$(G_{x_0})' = (G_{x_0})'(\mathfrak{K}(H^0)) \cap (G^\infty_\Lambda)',$$

where $(G_{x_0})'(\mathfrak{K}(H^0))$ is the commutant taken in $\mathfrak{K}(H^0)$. Again, using similar arguments as in the proof of Theorem 3.2, we get

$$(G_{x_0})'/\{\mathfrak{I}_{x_0} \cap (G_{x_0})'\} \cong \mathfrak{K}(\mathcal{H}_\Lambda) \cap (G_\Lambda^\infty)',$$

which is isomorphic to $\mathfrak{O}_\Lambda^i$, by formula (3.3). ■

C. Reduction with respect to pointed gauge transformations

As already mentioned, a convenient way to solve relations between generators is to choose a *tree*, i.e., to assign a unique path connecting any pair of lattice sites. More precisely, a tree is a pair $(x_0, \mathcal{T})$, where x_0 is a distinguished lattice site (called *root*) and $\mathcal{T}$ is a set of lattice links such that for any lattice site x there is exactly one path from x to x_0, with links belonging to $\mathcal{T}$. We denote this path by $\beta(x)$. Consequently, for any pair (x,y) of lattice sites, there is a unique *along tree* path from x to y, equal to $\beta^{-1}(y)\circ\beta(x)$, where $\alpha\circ\beta$ denotes the composition of the two paths (a path obtained by first running through β and next through α) and β^{-1} denotes the path taken with the opposite orientation. This does apply also to external sites, because *external links* are treated as belonging to the tree *a priori*.

To find an explicit set of generators of the pointed observable algebra $\mathfrak{O}_\Lambda^{i,0}$, given by (5.9), we "parallel transport" all generators of the field algebra to the lattice root using the above *along tree* paths. The transported generators feel only gauge transformations at x_0 and, therefore, are invariant with respect to $G_\Lambda^{i,0}$. Hence, $(G_\Lambda^0)'$ is generated by

(1)

$$\{U_{\gamma B}^A, E_{\mathcal{T}B}^A(x,y), \psi_{\mathcal{T}}^{aA}(x), \psi_{\mathcal{T}}^{*aA}(x)\}, \tag{5.10}$$

where γ is an arbitrary closed curve starting and ending at x_0 and

$$E_{\mathcal{T}B}^A(x,y) := U_{\beta(x)C}^A U_{\beta(x)^{-1}B}^D E^C{}_D(x,y), \tag{5.11}$$

$$\psi_{\mathcal{T}}^{aA}(x) := U_{\beta(x)B}^A \psi^{aB}(x), \tag{5.12}$$

with $\beta(x)$ denoting the unique tree path from x to x_0.

(2) Boundary fluxes,

$$E_{\mathcal{T}B}^A(x,\infty) := U_{\beta(x)C}^A U_{\beta(x)^{-1}B}^D E^C{}_D(x,\infty). \tag{5.13}$$

The generating set (5.10) is still enormously redundant. To reduce this redundancy, in a first step, we restrict the admissible paths to the form

$$\gamma(x,y) := \beta(x)\circ(x,y)\circ\beta^{-1}(y). \tag{5.14}$$

We denote

$$U_{\mathcal{T}B}^A(x,y) := U_{\gamma(x,y)B}^A.$$

It is obvious that any $U_{\gamma B}^A$ may be reconstructed from those quantities. Thus,

$$\{U_{\mathcal{T}B}^A(x,y), E_{\mathcal{T}B}^A(x,y), \psi_{\mathcal{T}}^{aA}(x), \psi_{\mathcal{T}}^{*aA}(x)\} \tag{5.15}$$

can be taken, together with boundary fluxes, as a set of generators of $(G_\Lambda^0)'$. The bosonic and fermionic generators fulfill the same commutation relations as generators $U^A{}_B(x,y)$ and $E^A{}_B(x,y)$ (see Sec. II). The local Gauss law can be easily rewritten,

$$\rho_{\mathcal{T}B}^A(x) = \sum_{y\leftrightarrow x} E_{\mathcal{T}B}^A(x,y), \tag{5.16}$$

where $\rho_{\mathcal{T}}$ is given by (2.44) with $\psi^{aA}(x)$ replaced by $\psi_{\mathcal{T}}^{aA}(x)$. However, a nontrivial commutator between $E_{\mathcal{T}B}^A(x,y)$ and the latter occurs.

Next, observe that for any on-tree-link $(x,y)\in\mathcal{T}$ we have

$$U^A_{TB}(x,y) = \delta^A{}_B.$$

Thus, the relevant information is carried by those $U_{\mathcal{T}}$'s, which correspond to off-tree-links $(x,y) \notin \mathcal{T}$. On the other hand, exactly those among the fields $E_{\mathcal{T}}$, which correspond to off-tree-links, may be chosen as independent generators. Indeed, the on-tree $E_{\mathcal{T}}$'s can be calculated by solving the local Gauss law at all the points $x \neq x_0$. Observe that the off-tree $E_{\mathcal{T}}$'s have trivial commutators with $\psi_{\mathcal{T}}$'s. Thus, factorization of $(G^0_\Lambda)'$ with respect to the local Gauss laws at all points $x \neq x_0$ consists in taking only independent internal generators, i.e., those among (5.15), which correspond to off-tree links.

Let us denote the number of lattice sites by N and by L the number of links. Since the number of on-tree links is equal to $N-1$, the number of off-tree links is equal to

$$K = L - N + 1.$$

Enumerate these links setting $(x_i,y_i) =: \ell_i$, where $i=1,\ldots,K$. We have thus the following set of independent generators of $\mathfrak{O}^{i,0}_\Lambda$:

$$\{U^A_{TB}(\ell_i), E^A_{TB}(\ell_i), \psi^{aA}_{\mathcal{T}}(x), \psi^{*aA}_{\mathcal{T}}(x)\}, \tag{5.17}$$

together with the boundary fluxes (5.13). The latter commute with all generators (5.17) and, after the final reduction with respect to G_{x_0}, they will generate the center of the algebra.

Generators (5.17) fulfill canonical (anti)commutation relations, given by formulas (2.22), (2.23), and (2.5). They are all subject to gauge transformations at the tree root x_0. Observe that, since bosonic and fermionic generators commute, we have

$$\mathfrak{O}^{i,0}_\Lambda = \tilde{\mathfrak{O}}^{\mathrm{glu}}_{\mathcal{T}} \otimes \tilde{\mathfrak{O}}^{\mathrm{mat}}_{\mathcal{T}} \otimes \mathfrak{O}^b_\Lambda, \tag{5.18}$$

where $\tilde{\mathfrak{O}}^{\mathrm{glu}}_{\mathcal{T}}$ is the gluonic part generated by $\{U^A_{TB}(\ell_i), E^A_{TB}(\ell_i)\}$ and $\tilde{\mathfrak{O}}^{\mathrm{mat}}_{\mathcal{T}}$ is the matter field part, generated by $\{\psi^{aA}_{\mathcal{T}}(x), \psi^{*aA}_{\mathcal{T}}(x)\}$. According to the above discussion, the gluonic algebra $\tilde{\mathfrak{O}}^{\mathrm{glu}}_{\mathcal{T}}$ is isomorphic to the generalized CCR-algebra over the group G, spanned by K pairs of generators, and $\tilde{\mathfrak{O}}^{\mathrm{mat}}_{\mathcal{T}}$ is isomorphic to the CAR-algebra, generated by $12N$ pairs of anticommuting elements. The subalgebra $\mathfrak{O}^b_\Lambda$ denotes the component generated by boundary fluxes (5.13).

D. Removing the residual gauge freedom

In the first part of this paper we have mentioned that G can be, basically, an arbitrary compact Lie group. Here, we definitely consider $G=\mathrm{SU}(3)$ only. In what follows, we denote the K-fold Cartesian product of G by $\mathbf{G}^K = G \times \cdots \times G$ and elements of $\mathbf{G}^K$ by $\mathbf{g} = (g_1,\ldots,g_K)$.

Let us denote the off-tree variables by

$$E_i = E_{\mathcal{T}}(\ell_i), \quad U_i = U_{\mathcal{T}}(\ell_i), \quad i = 1,\ldots,K.$$

The residual gauge group $G_{x_0} \cong G$ acts on this set of variables by

$$(E_i, U_i) \to (gE_ig^{-1}, gU_ig^{-1}), \tag{5.19}$$

with $g = g(x_0) \in G_{x_0}$. In what follows, we want to fix this residual gauge freedom. Thus, we must consider the action of G on $\mathbf{G}^K$ by inner automorphisms

$$G \times \mathbf{G}^K \ni (h,(g_1,\ldots,g_K)) \mapsto (hg_1h^{-1},\ldots,hg_Kh^{-1}) \in \mathbf{G}^K.$$

We wish to parametrize, by choosing a gauge, the space of equivalence classes of elements of $\mathbf{G}^K$ with respect to this group action, which by abuse of language, will be called $\mathrm{Ad}\,G$. Factorizing with respect to this action, we obtain the orbit space $\mathbf{G}^K/\mathrm{Ad}\,G$. This is a complicated stratified set, which will be more deeply discussed in Ref. 21. Here, we restrict ourselves to the generic orbit type, respectively, the generic stratum $\mathbf{G}^K_{\mathrm{gen}}$, which is an open and dense submanifold in $\mathbf{G}^K$. An element $\mathbf{g} = (g_1,\ldots,g_K) \in \mathbf{G}^K$ belongs to the generic stratum, iff its stabilizer is the center $\mathbb{Z}_3$ of G.

It is quite obvious that **g** belongs to the generic stratum, iff there does not exist any common eigenvector of the matrices $(g_1,\ldots,g_K)$. Moreover, one can show[21] that **g** belongs to the generic stratum, iff there exists a pair (g_i,g_j) or a triple (g_i,g_j,g_k) of elements not possessing any common eigenvector. Using arguments developed in Ref. 36 one can prove that the bundle

$$\pi:\mathbf{G}^K_{\mathrm{gen}} \to \mathbf{G}^K_{\mathrm{gen}}/\mathrm{Ad}\, G$$

is nontrivial, for $K \geqslant 2$. It can be considered as a principal fiber bundle with structure group $G/\mathbb{Z}_3$. Moreover, one can find a system of local trivializations (respectively, local sections) of this bundle, defined over a covering of $\mathbf{G}^K_{\mathrm{gen}}/\mathrm{Ad}\, G$ with open subsets, which are all dense with respect to the natural measure (the one induced by the Haar measure).

Thus, let

$$\mathbf{G}^K_{\mathrm{gen}}/\mathrm{Ad}\, G \supset \mathcal{U} \ni [\mathbf{g}] \to \mathbf{s}([\mathbf{g}]) \equiv (s_1,\ldots,s_K)([\mathbf{g}]) \in \mathbf{G}^K$$

be one of these local sections, with $\mathcal{U}$ being dense in $\mathbf{G}^K_{\mathrm{gen}}/\mathrm{Ad}\, G$. Since Ad G acts (pointwise) on this section, we can fix the gauge by bringing **s** to a special form. Since pairs of group elements being in a nongeneric position form a set of measure zero in $\mathbf{G}^2$, we can—without loss of generality—assume that s_{K-1} and s_K are in generic position on $\mathcal{U}$. That means they have no common eigenvector. Thus, on this neighborhood, we can fix the gauge in two steps: First, we diagonalize s_{K-1} and next we use the stabilizer of this diagonal element to bring s_K to a special form. Since s_{K-1} and s_K have no common eigenvector, this fixes the (remaining) stabilizer gauge completely (up to $\mathbb{Z}_3$). Let us denote the function (which obviously depends only on s_{K-1} and s_K) implementing this gauge transformation by

$$\pi^{-1}(\mathcal{U}) \ni (s_1,\ldots,s_K) \mapsto f(s_1,\ldots,s_K) = f(s_{K-1},s_K) \in G$$

and the local section after gauge fixing by

$$\mathbf{G}^K_{\mathrm{gen}}/\mathrm{Ad}\, G \supset \mathcal{U} \ni [\mathbf{g}] \to \mathbf{f}([\mathbf{g}]) \equiv (f_1,\ldots,f_K)([\mathbf{g}]) \in \mathbf{G}^K, \tag{5.20}$$

with

$$f_i = f(s_{K-1},s_K)\cdot s_i \cdot f(s_{K-1},s_K)^{-1}, \quad i=1,\ldots,K.$$

The section **f** can be made explicit by using a system of local trivializations of G as an SU(2)-principal bundle over S^5. We refer to Ref. 21 for details and to Appendix A for one example of a local section of this bundle.

Suppose that we had started with another section $\tilde{\mathbf{s}}$, related to **s** by a gauge transformation given by $g \in G$. Then, the function $\tilde{f}(s_{K-1},s_K) = f(s_{K-1},s_K)\cdot g^{-1}$ yields the same section **f**. Thus, f is equivariant with respect to gauge transformations,

$$f(g\cdot s_{K-1}\cdot g^{-1}, g\cdot s_K \cdot g^{-1}) = f(s_{K-1},s_K)\cdot g^{-1}, \tag{5.21}$$

and in this sense, we can consider the f_i as being "gauge invariant." It is challenging to parametrize classes $[\mathbf{g}]$ of gauge equivalent configurations more intrinsically, namely in terms of genuine invariants. In Ref. 21 we will prove the following.

Theorem 5.3: *Any function on* $\mathbf{G}^2$ *invariant with respect to the action by inner automorphisms*

$$G \times \mathbf{G}^2 \ni (h,(g_1,g_2)) \mapsto (hg_1h^{-1}, hg_2h^{-1}) \in \mathbf{G}^2$$

can be expressed as a function in the following invariants and their complex conjugates:

$$T_1(g_1,g_2) := tr(g_1),$$

$$T_2(g_1,g_2) := tr(g_2),$$

$$T_3(g_1,g_2) := tr(g_1 g_2),$$

$$T_4(g_1,g_2) := tr(g_1 g_2{}^2),$$

$$T_5(g_1,g_2) := tr(g_1{}^2 g_2{}^2 g_1 g_2) - tr(g_1{}^2 g_2 g_1 g_2{}^2).$$

Moreover, there is one algebraic relation between those invariants such that for given values of T_i, $i=1,\ldots,4$, *there are at most two possible values of* T_5.

By this theorem, it follows that the entries of f_i, $i=K-1$, K, and, therefore, the group elements f_i themselves can be expressed in terms of the above set of invariants,

$$f_i = f_i(T_1(g_{K-1},g_K),\ldots,T_5(g_{K-1},g_K)), \quad i = K-1,K.$$

Since the section **f** parametrizes the gauge orbit space, it is clear that the remaining group elements f_i, $i=1,\ldots,K-2$, can be expressed as a function of traces (5.1), too.

To summarize, applying this special gauge-fixing to a gauge configuration $(U_1,\ldots,U_K)$, with generic (U_{K-1},U_K) corresponding to the pair (x_{K-1},y_{K-1}), (x_K,y_K) of off-tree links, we obtain a local parametrization of its gauge equivalence class by $(\mathfrak{u}_1,\ldots,\mathfrak{u}_K)$ defined by

$$\mathfrak{u}_i := f(U_{K-1},U_K)\cdot U_i \cdot (f(U_{K-1},U_K))^{-1}. \tag{5.22}$$

We denote the indices of these matrices by $r,s,\ldots,\mathfrak{u}_i=\{\mathfrak{u}_i{}^r{}_s\}$, and, consequently, the matrix elements of f by $f=\{f^r{}_A\}$. Then we have

$$\mathfrak{u}_{is}^r = f^r{}_A \cdot U_i^A{}_B \cdot (f^{-1})^B{}_s \tag{5.23}$$

and the gauge transformation (5.21) reads

$$f^r{}_B \to f^r{}_A \cdot (g^{-1})^A{}_B, \tag{5.24}$$

(the color indices $A,B,C,\ldots$ feel gauge transformations, whereas indices $r,s,\ldots$ — assuming the same values 1,2,3—label "gauge-invariant quantities").

By inspecting formula (A1), we see that there are two independent degrees of freedom in the matrix $\mathfrak{u}_{K-1}$ and six independent degrees of freedom in the matrix $\mathfrak{u}_K$. They may be combined into eight degrees of freedom of a single element of G in the following way:

$$\mathfrak{u}_0 := \mathfrak{u}_{K-1}\cdot \mathfrak{u}_K \cdot (\mathfrak{u}_{K-1})^{-1}. \tag{5.25}$$

The above procedure is defined up to a discrete symmetry only. This symmetry arises from the action of the permutation group $S_3 \subset \mathrm{Ad}\,\mathrm{SU}(3)$ on entries of the diagonal matrix $\mathfrak{u}_{K-1} \in T^2 \subset \mathrm{SU}(3)$. To fix this S_3-gauge freedom means choosing for each element of T^2/S_3 a unique representative on the torus T^2. Changing this representative by an even permutation does not change the image of the mapping $(\mathfrak{u}_{K-1},\mathfrak{u}_K)\mapsto \mathfrak{u}_0$ given by (5.25), which *does not cover* the entire group SU(3) but only " half of it." Using also odd permutations we cover a dense subset of SU(3), but then the discrete symmetry $\mathfrak{u}_0 \to \overline{\mathfrak{u}}_0$ must be taken into account.

It can be shown that the decomposition of $\mathfrak{u}_0$ into the above product of elements of special form is unique (up to the discrete symmetry) and both $\mathfrak{u}_{K-1}$ and $\mathfrak{u}_K$ may be reconstructed from $\mathfrak{u}_0$. By the above discussion, we can consider the observable $\mathfrak{u}_0$ as SU(3)-valued, provided we keep the discrete symmetry $\mathfrak{u}_0 \to \overline{\mathfrak{u}}_0$. To summarize, we have shown that, locally, the full information carried by the fields U_i is encoded in $K-1$ elements $\mathfrak{u}_i$, $i=0,\ldots,K-2$, of G, modulo the discrete symmetry just described.

Analogously, we construct K gauge invariant generators

$$\mathfrak{e}_{is}^r = f^r{}_A \cdot E_i^A{}_B \cdot (f^{-1})^B{}_s, \tag{5.26}$$

which have to fulfill the residual Gauss law at x_0. To describe the unconstrained information carried by the fields $\mathfrak{e}_i$, we divide the information contained in $\mathfrak{e}_{K-1}$ and $\mathfrak{e}_K$ (16 gauge invariant

generators) into eight independent generators encoded in the momentum $\mathfrak{e}_0$ canonically conjugate to $\mathfrak{u}_0$ and eight other combinations of $\mathfrak{e}_{K-1}$ and $\mathfrak{e}_K$, which can be reconstructed from the global Gauss law at x_0. More precisely, at each point of the section (5.20), we decompose the pair $(\mathfrak{e}_{K-1},\mathfrak{e}_K)$ into a pair $(\mathfrak{e}^{\|}_{K-1},\mathfrak{e}^{\|}_K)$ of vectors tangent to this section and a pair $(\mathfrak{e}^{\perp}_{K-1},\mathfrak{e}^{\perp}_K)$ of vectors orthogonal to it. Here, orthogonality is of course meant in the sense of the natural scalar product induced by the Killing metric. The tangent components sum up to the momentum $\mathfrak{e}_0$ canonically conjugate to $\mathfrak{u}_0$. More precisely, $\mathfrak{e}_0$ is the image of $(\mathfrak{e}^{\|}_{K-1},\mathfrak{e}^{\|}_K)$ under the tangent mapping of $(\mathfrak{u}_{K-1},\mathfrak{u}_K)\mapsto\mathfrak{u}_0$ given by (5.25). By a simple calculation, we get

$$\mathfrak{e}_0 = (\mathrm{Ad}\,\mathfrak{u}_0^{-1} - 1)\circ\mathrm{Ad}\,\mathfrak{u}_{K-1}(\mathfrak{e}^{\|}_{K-1}) + \mathrm{Ad}\,\mathfrak{u}_{K-1}(\mathfrak{e}^{\|}_K), \tag{5.27}$$

This formula is invertible and enables us to calculate uniquely both $\mathfrak{e}^{\|}_{K-1}$ and $\mathfrak{e}^{\|}_K$ once we know $\mathfrak{e}_0$. On the other hand, the sum $\mathfrak{e}_{K-1}+\mathfrak{e}_K$ is given from the Gauss law. This enables us to calculate $(\mathfrak{u}_{K-1},\mathfrak{u}_K,\mathfrak{e}_{K-1},\mathfrak{e}_K)$ once we know $(\mathfrak{u}_0,\mathfrak{e}_0)$. We end up with $2(K-1)$ independent generators $(\mathfrak{e}_i,\mathfrak{u}_i)$, $i=0,\ldots,K-2$, of the gluonic part of the observable algebra.

It is easy to show that these bosonic generators satisfy the generalized canonical commutation relations over G :

$$[\mathfrak{e}^r_{is},\mathfrak{e}^p_{jq}] = \delta_{ij}(\delta^p{}_s\mathfrak{e}^r_{iq} - \delta^r{}_q\mathfrak{e}^p{}_{is}), \tag{5.28}$$

$$[\mathfrak{e}^r_{is},\mathfrak{u}^p_{jq}] = \delta_{ij}\left(\delta^p{}_s\mathfrak{u}^r_{iq} - \tfrac{1}{3}\delta^r{}_s\mathfrak{u}^p_{iq}\right), \tag{5.29}$$

$$[\mathfrak{u}^r_{is},\mathfrak{u}^p_{jq}] = 0. \tag{5.30}$$

For the fermionic observables, we denote

$$\mathfrak{a}^{ar}(x) := f^r{}_A\psi^{aA}_T(x) = f^r{}_A U^A_{\beta(x)B}\psi^{aB}(x). \tag{5.31}$$

Introducing the joint index $k=(a,r,x)$, $k=1,\ldots,12N$, we get,

$$\mathfrak{a}_k := \mathfrak{a}^{ar}(x). \tag{5.32}$$

Formally, these quantities fulfill the canonical anticommutation relations

$$[\mathfrak{a}^{*k},\mathfrak{a}_l]_+ = \delta^k_l, \tag{5.33}$$

but again, an additional discrete symmetry must be taken into account. This symmetry arises, because the section **f**, given by (5.20), is defined only up to the stabilizer $\mathbb{Z}_3$ of the generic stratum. Observe that this ambiguity does not affect the bosonic quantities $\mathfrak{u}$ and $\mathfrak{e}$, because they are "quadratic" in f.

Let us denote the bosonic (respectively, fermionic) observable algebra part, obtained from $\tilde{\mathfrak{O}}^{\mathrm{glu}}_T$ (respectively, $\tilde{\mathfrak{O}}^{\mathrm{mat}}_T$) after fixing the residual gauge, by $\mathfrak{O}^{\mathrm{glu}}_T$ (respectively $\mathfrak{O}^{\mathrm{mat}}_T$). Then we have

$$\mathfrak{O}_\Lambda = \mathfrak{O}^{\mathrm{glu}}_T \otimes \mathfrak{O}^{\mathrm{mat}}_T \otimes \mathfrak{O}^b_\Lambda \otimes \mathfrak{O}^\infty_\Lambda. \tag{5.34}$$

The above discussion shows that locally (on a dense subset of the generic stratum) and up to discrete symmetries, $\mathfrak{O}^{\mathrm{glu}}_T$ (respectively, $\mathfrak{O}^{\mathrm{mat}}_T$) coincides with the algebra of generalized canonical commutation (respectively, anticommutation) relations for the reduced data $(\mathfrak{u}_i,\mathfrak{e}_i)$, with $i=0$, …, $K-2$ [respectively $(\mathfrak{a}_k,\mathfrak{a}^{*k})$, with $k=1,\ldots,12N$].

As already mentioned at the beginning of this section, a systematic study of $\mathfrak{O}_\Lambda$ as an algebra defined in terms of generators and relations on the level of genuine invariants will be presented in Refs. 21 and 22. In particular, we will show that the fermionic part is generated by the following sesquilinear and trilinear combinations of $\mathfrak{a}_k$ and $\mathfrak{a}^{*k}$:

$$\mathfrak{j}^k{}_l = \mathfrak{a}^{*k}\mathfrak{a}_l, \tag{5.35}$$

$$\mathfrak{w}_{pqr} = \mathfrak{a}_p \mathfrak{a}_q \mathfrak{a}_r, \tag{5.36}$$

$$\mathfrak{w}^{*ijk} = \mathfrak{a}^{*k} \mathfrak{a}^{*j} \mathfrak{a}^{*i}. \tag{5.37}$$

Similarly, to parametrize the bosonic part in terms of genuine invariants, one must take—according to classical invariant theory—all trace invariants, built from $\mathfrak{e}$ and $\mathfrak{u}$. This set is, however, highly redundant and it is a complicated task to find, for a fixed number K, the full set of relations.

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APPENDIX A: A LOCAL PARAMETRIZATION OF $(\mathrm{SU}(3)\times\mathrm{SU}(3))_{\mathrm{gen}}/\mathrm{Ad}\,\mathrm{SU}(3)$

Consider the action of the group of inner automorphisms, here denoted by Ad SU(3), on $\mathrm{SU}(3)\times\mathrm{SU}(3)$. In Sec. V D we have used an explicit local parametrization of the generic stratum of this action in terms of a bundle section. Such a section can be obtained as follows. Let $(g_1, g_2) \in \mathrm{SU}(3)\times\mathrm{SU}(3)$ be a pair of group elements lying in the generic stratum. First, we diagonolize g_1. Since g_1 is generic, the stabilizer of the Ad-action is isomorphic to $\mathrm{U}(1)\times\mathrm{U}(1)$. Next, treating SU(3) as an SU(2)-principal bundle over S^5, one can bring g_2 to a special form using the $\mathrm{U}(1)\times\mathrm{U}(1)$-action. This yields a family of local sections defined on dense subsets over the generic stratum, corresponding to a family of local trivializations of the SU(2)-principal bundle $\mathrm{SU}(3)\to S^5$. For details we refer to Ref. 21.

As a local section of the above type one can choose

$$f_1 = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}, \quad f_2 = \begin{bmatrix} a & -\delta^{-1} b^\dagger \\ b & \delta\left(1 - \dfrac{bb^\dagger}{1+|a|}\right) \end{bmatrix} \times \begin{bmatrix} 1 & 0 & 0 \\ 0 & c & d \\ 0 & -\bar{d} & \bar{c} \end{bmatrix}. \tag{A1}$$

Here, λ_i are eigenvalues of g_1, fulfilling

$$|\lambda_1| = |\lambda_2| = |\lambda_3| = 1, \quad \lambda_1\lambda_2\lambda_3 = 1.$$

The entries

$$a, \delta \in \mathbb{C}, b = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}, \quad b_1, b_2 \in \mathbb{R}_+,$$

of the first factor in f_2 fulfill

$$|a|^2 + b_1^2 + b_2^2 = 1, \quad |\delta| = 1, a = |a|\delta^{-2}$$

and the lower diagonal block of the second factor is an SU(2)-matrix in the standard parametrization, with

$$|c|^2 + |d|^2 = 1.$$

APPENDIX B: PROOF OF THEOREM 5.1

Using basic results from invariant theory, see Ref. 38, we get that the only gauge invariant combinations built exclusively from generators $U^A{}_B$ are traces of their products and, whence, quantities of type (5.1).

Any other invariant is built by contracting the color indices of the fields $E^A{}_B(x,y)$, $U^A{}_B(x,y)$, $\psi^{aA}(x)$, and $\psi^*{}_{aA}(x)$. Consider such an invariant I and replace in its definition the above fields by their gauge invariant counterparts $\mathfrak{e}$, $\mathfrak{u}$, $\mathfrak{a}$, and $\mathfrak{a}^*$. In particular, the missing on-tree quantities $\mathfrak{e}$ and $\mathfrak{u}$, are defined as combinations of the off-tree ones, using the Gauss law (for $\mathfrak{e}$) and the Bianchi identities (for $\mathfrak{u}$). Formally, the new invariant obtained this way coincides with I, because the factors f and f^{-1} coming from the definition of the quantities $\mathfrak{e}$, $\mathfrak{u}$, $\mathfrak{a}$, and $\mathfrak{a}^*$ disappear under contraction. Moreover, all the fermionic quantities $\mathfrak{a}$ and $\mathfrak{a}^*$ appearing in the invariant may be grouped to give quantities $\mathfrak{j}$, $\mathfrak{w}$, and $\mathfrak{w}^*$.

As already mentioned in Sec. V D, the invariant quantities $\mathfrak{u}$ can be expressed as (nonlinear) functions of traces of U [invariants (5.1)]. We show that also $\mathfrak{e}$, $\mathfrak{j}$, $\mathfrak{w}$, and $\mathfrak{w}^*$ can be expressed in terms of invariants (5.1)–(5.4), listed in Theorem 5.1. Invariants $\mathfrak{e}^r_{is}$ can be dealt with as follows: We contract them with eight different $\mathfrak{u}$'s and use formulas (5.23) and (5.26) to obtain the following system of linear equations for the eight independent components of $\mathfrak{e}^r_{is}$:

$$\mathfrak{e}^r_{is}\mathfrak{u}^{(1)s}{}_r = E_{\gamma_1}, \ldots, \mathfrak{e}^r_{is}\mathfrak{u}^{(8)s}{}_r = E_{\gamma_8},$$

with the right-hand sides all being invariants of type (5.2). Analogously, we can write down systems of linear equations of this type for the quantities $\mathfrak{j}$, $\mathfrak{w}$, and $\mathfrak{w}^*$. Solving these systems of linear equations, we obtain $\mathfrak{e}$, $\mathfrak{u}$, $\mathfrak{j}$, $\mathfrak{w}$, and $\mathfrak{w}^*$ as functions, linear with respect to invariants (5.2)–(5.4) and nonlinear with respect to invariants (5.1) listed in Theorem 5.1.

Hence, we have formally expressed I as a combination $\tilde{I}$ of invariants listed in Theorem 5.1. In particular all Casimir operators, built from the electric fields E may be expressed in terms of these generators.

The above formulas, expressing any gauge invariant field I as a combination $\tilde{I}$ of the invariants listed in Theorem 5.1, were derived by the help of the gauge fixing section (5.20), which is not globally defined. Hence, equality $I=\tilde{I}$ holds on a dense subset of the configuration space only. But I is a differential operator (with smooth coefficients) on the whole configuration space (the rank of such an operator is equal to its algebraic order with respect to variables E). The invariant $\tilde{I}$ is a differential operator of the same rank, but *a priori* its coefficients are well defined on a dense set of the configuration space only. But, if two such operators coincide on a dense set, they coincide everywhere.

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Square-integrable wave packets from the Volkov solutions

Stephan Zakowicz[a)]
Institut für Theoretische Physik, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

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Rigorous mathematical proofs of some properties of the Volkov solutions are presented, which describe the motion of a relativistic charged Dirac particle in a classical, plane electromagnetic wave. The Volkov solutions are first rewritten in a convenient form, which clearly reveals some of the symmetries of the underlying Dirac equation. Assuming continuity and boundedness of the electromagnetic vector potential, it is shown how one may construct square-integrable wave packets from momentum distributions in the space $\mathcal{C}_0^\infty(\mathbb{R}^3)^4$. If, in addition, the vector potential is $\mathcal{C}^1$ and the derivative is bounded, these wave packets decay in space faster than any polynomial and fulfill the Dirac equation. The mapping which takes momentum distributions into wave packets is shown to be isometric with respect to the $L^2(\mathbb{R}^3)^4$ norm and may therefore be continuously extended to a mapping from $L^2(\mathbb{R}^3)^4$. For a momentum function in $L^1(\mathbb{R}^3)^4 \cap L^2(\mathbb{R}^3)^4$, an integral representation of this extension is presented. © *2005 American Institute of Physics.*
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I. INTRODUCTION

There exist only few exact solutions of the Dirac equation, the relativistic equation which describes the motion of a charged particle with spin $1/2$ in an external electromagnetic field. One important class was discovered by Volkov in 1935,[1] who treated the field of a classical, plane electromagnetic wave. Ever since then, the Volkov solutions have experienced a wide range of applications in the physics of interactions of electrons and positrons with a laser beam, of which we enumerate a few.

In 1952, Sengupta[2] calculated the scattering of electromagnetic waves by a free electron; to the author's knowledge, he was the first to have employed the Volkov solutions explicitly. Ten years later, Reiss[3] computed the probability for electron–positron pair production in two nonparallel classical photon fields, of which one is treated as a perturbation but the other one may be of arbitrary strength. In a more mathematical paper,[4] the same author proved that for this field configuration, the perturbation expansion converges for small parameters. Brown and Kibble[5] as well as Gol'dman[6] studied the Compton scattering of a free electron in a high-intensity laser and used the Volkov solutions to calculate the cross section for this process. Nikishov and Ritus[7] and Narozhnyĭ *et al.*[8] analyzed the $\pi \to \mu + \nu$ decay in the presence of an electromagnetic wave. The scattering of electrons by a scalar potential in the presence of an intense laser field was considered by Bergou and Varró[9]. Moreover, the production of electron–positron pairs in a laser was considered by Nikishov and Ritus[10] and by Narozhnyĭ *et al.*[8] In atomic physics, the Volkov solutions are used in the calculation of ionization rates in strong laser fields within the so-called strong-field approximation (see, for example, Refs. 11 and 12). Szymanowski and co-workers examined laser-assisted scattering of electrons in a Coulomb potential[13] and in a Yukawa potential.[14] The cross section for pair production may be enhanced in the presence of a bare atomic nucleus—a situation which was investigated by Yakovlev[15] and Müller *et al.*[16,17]

[a)]Electronic mail: zakowicz@physik.uni-giessen.de

The Volkov solutions for given "asymptotic momenta," which will be written out explicitly in the subsequent section, are not square integrable. Therefore, a direct interpretation of a physical particle that is localized in space is not easily possible. In the case of the free Dirac equation, where the same problem occurs, square-integrable solutions—so-called *wave packets*—may be constructed from complex-valued functions in momentum space by multiplying these with the free plane-wave solutions and integrating over momentum space.[18,19] The construction of such wave packets from the Volkov solutions was suggested for the Klein–Gordon equation by Neville and Rohrlich[20] and for the Dirac equation by San Román and co-workers.[21–24]

Mathematically spoken, the integration over momentum space for the free Dirac equation represents nothing but the usual Fourier transformation with a minor modification, which accounts for the spinor structure of the Dirac equation.[19] This procedure automatically guarantees the "normalization" and "completeness" of the free plane-wave solutions, i.e., corresponding functions in momentum space and in spatial space have identical L^2 norms, and any L^2 function in spatial space may be represented as such a wave packet. In the literature, only peripheral attention has been paid to a study of the "normalization" and "completeness" properties for the Volkov solutions. There exist several treatments that offer physically motivated arguments for the normalization. Bergou and Varró[9] as well as Filipowicz,[25] for example, make use of delta functions and interchange the orders of divergent integrals in order to obtain the desired result. The standard textbook by Berestetskiĭ *et al.*[26] assumes electromagentic vector potentials that decrease far away from the origin, such that—according to the authors' reasoning—the normalization integral is practically not influenced by this potential.

However, there seem to be no rigorous mathematical proofs for the claims of "normalization" and "completeness." Nevertheless, many authors use these properties in their calculations more or less explicitly. For example, San Román and collaborators[21–24] determine the time evolution of a free electron wave packet in a laser beam by first calculating the momentum distribution of the initial wave packet at time $t=0$ and then computing the resulting wave packets for positive times. The validity of this procedure relies on both "normalization" and "completeness." Furthermore, calculations of cross sections or production rates with the help of the nonsquare-integrable Volkov solutions and "delta functions"—as performed, for example, in Refs. 5–17—implicitly assume "normalization" and "completeness." To be more precise, an incorrect "normalization" would lead to wrong factors in the differential cross sections. On the other hand, the derivation of the total cross section requires an integration and summation of the differential cross section over *all* final states, i.e., these final states need to satisfy "completeness."

It is the purpose of this paper to fill part of the gap indicated above and to provide a proof for the "normalization" of the Volkov solutions. In Sec. II, we present the explicit form of the Volkov solutions. Some symmetries of the Dirac equation that will be useful in the further development are discussed in Sec. III. Section IV is devoted to the construction of *regular wave packets* from $\mathcal{C}_0^\infty$ functions in momentum space in the case where the electromagnetic vector potential is continuous and bounded. Assuming also continuous differentiability of the vector potential and boundedness of its derivative, these regular wave packets are shown to decay rapidly in spatial space and to fulfill the Dirac equation. In Sec. V, which is the central part of the paper, we state the main theorem asserting that the norms of a momentum distribution and of its corresponding wave packet are identical. The statement of the theorem is related to the physical concepts of "normalization to a delta function" and "orthogonality." The construction of wave packets from *any* L^2 functions in momentum space is exhibited in Sec. VI, which is achieved by a continuous extension from the space $\mathcal{C}_0^\infty$. Finally, in the Appendix, we give the proof of the main theorem from Sec. V.

II. THE VOLKOV SOLUTIONS

We treat a relativistic spin-1/2 particle with charge e and mass m that moves in the four-potential $A^\mu \equiv (A^0, \mathbf{A})$ of an electromagnetic field. The motion of the particle is described by the Dirac equation, which reads

$$(i\partial\!\!\!/ - eA\!\!\!/ - m)\psi = 0, \tag{1}$$

where we have used the Feynman slash notation

$$a\!\!\!/ := \gamma^\mu a_\mu$$

with the 4×4 Dirac matrices γ^μ.[18,19] These matrices fulfill

$$\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}\mathbf{1}.$$

Here as in the entire paper, we use natural units ($\hbar = c = 1$) and the signature $(+---)$ of the metric tensor $g_{\mu\nu}$. Scalar products shall be noted as

$$(ab) \equiv a^\mu b_\mu.$$

In the Lorentz gauge,

$$(\partial A) \equiv \partial_\mu A^\mu(x) = 0,$$

a plane electromagnetic wave propagating in the direction of the unit vector $\mathbf{n} \in \mathbb{R}^3$ may be represented by the four-potential

$$A^\mu(x) = \tilde{A}^\mu(\xi), \quad \xi = (nx), \tag{2}$$

with the four-vector

$$n^\mu = (1, \mathbf{n})$$

and the additional conditions

$$A^0 = \mathbf{A}\cdot\mathbf{n} \equiv 0.$$

The analytical Volkov solutions of the Dirac equation (1) with this potential are[9]

$$\psi_{\mathbf{p},r}(\mathbf{r},t) = \mathbf{M}^{(\epsilon_r)}(\mathbf{p}, t - \mathbf{n}\cdot\mathbf{r})u_r(\mathbf{p})e^{iS^{(\epsilon_r)}(\mathbf{p},\mathbf{r},t)}, \tag{3}$$

where

$$\epsilon_r = \begin{cases} 1, & r = 1,2, \\ -1, & r = 3,4, \end{cases}$$

$$\mathbf{M}^{(\pm)}(\mathbf{p},\xi) = 1 \pm \frac{e\tilde{A}\!\!\!/(\xi)}{2(E(\mathbf{p}) - \mathbf{n}\cdot\mathbf{p})} \in \mathbb{C}^{4\times 4}, \tag{4}$$

$$S^{(\pm)}(\mathbf{p},\mathbf{r},t) = \pm\left(\mathbf{p}\cdot\mathbf{r} - E(\mathbf{p})t - \int_0^{t-\mathbf{n}\cdot\mathbf{r}} J_{\mathbf{p}}^{(\pm)}(\xi)\mathrm{d}\xi\right), \tag{5}$$

$$J_{\mathbf{p}}^{(\pm)}(\xi) = \frac{1}{E(\mathbf{p}) - \mathbf{n}\cdot\mathbf{p}}\left(\mp e\mathbf{p}\cdot\tilde{\mathbf{A}}(\xi) - \frac{e^2}{2}\tilde{A}(\xi)^2\right) = \frac{1}{E(\mathbf{p}) - \mathbf{n}\cdot\mathbf{p}}\left(\mp e\mathbf{p}\cdot\tilde{\mathbf{A}}(\xi) + \frac{e^2}{2}|\tilde{\mathbf{A}}(\xi)|^2\right), \tag{6}$$

and

$$E(\mathbf{p}) = \sqrt{m^2 + |\mathbf{p}|^2} \tag{7}$$

is the energy of the particle. The spinors $u_r(\mathbf{p})$ are the free Dirac spinors, which can be written as columns of a certain matrix[19]

$$\mathbf{u}(\mathbf{p}) \equiv (u_1(\mathbf{p})u_2(\mathbf{p})u_3(\mathbf{p})u_4(\mathbf{p})) = \sqrt{\frac{E(\mathbf{p})+m}{2E(\mathbf{p})}}\left(\mathbf{1} + \frac{\boldsymbol{\alpha}\cdot\mathbf{p}}{E(\mathbf{p})+m}\right). \tag{8}$$

Here,

$$\boldsymbol{\alpha} = \gamma^0\boldsymbol{\gamma}$$

is the three-vector of the Dirac α matrices. The functions $u_r(\mathbf{p})$ are $\mathcal{C}^\infty$ in the argument $\mathbf{p}$ and satisfy

$$\not{p}u_r(\mathbf{p}) = \epsilon_r m u_r(\mathbf{p}). \tag{9}$$

In addition, they obey the orthogonality relations

$$u_r(\epsilon_r\mathbf{p})^\dagger u_s(\epsilon_s\mathbf{p}) \equiv \langle u_r(\epsilon_r\mathbf{p}), u_s(\epsilon_s\mathbf{p})\rangle_{\mathbb{C}^4} = \delta_{r,s}.$$

We remark that equation (3) is actually not the original form that was published by Volkov,[1] who considered only the superposition of at most countably many unifrequent electromagentic waves. In his formulas, infinite series over the amplitudes and phases of the external potential occur. Brown and Kibble[5] and Nikishov and Ritus[10] seem to be the first to have written down the solutions in a form that involves a more or less arbitrary form of the electromagnetic potential which involves an integral in the phase factor. A recent derivation of the Volkov solutions can be found in Ref. 21, where also the cases $r=3,4$ are treated. In addition, we mention that the authors cited above use $-\infty$ instead of 0 as the lower integration limit in the phase (5). Taking 0 (or any other finite number) does not require the vector potential to decay for large values $|\xi|$ of the argument ξ in order for the integral to converge.

For the sake of simplicity, we set $\mathbf{n}=\mathbf{e}_z$, so that

$$t - \mathbf{n}\cdot\mathbf{r} = t - z$$

and

$$E(\mathbf{p}) - \mathbf{n}\cdot\mathbf{p} = E(\mathbf{p}) - p_z.$$

The spatial part of the vector potential is then of the form

$$\mathbf{A}(\mathbf{r},t) = \tilde{A}_x(t-z)\mathbf{e}_x + \tilde{A}_y(t-z)\mathbf{e}_y \equiv \tilde{\mathbf{A}}(t-z) \in \mathbb{R}^2. \tag{10}$$

Here as in the following, we make the identification

$$\mathbb{R}^2 \cong \mathbb{R}^2 \times \{0\} \subset \mathbb{R}^3$$

in order to suppress an overduly complex notation. We also set

$$\mathbf{p}_\perp := (p_x, p_y) \in \mathbb{R}^2 \tag{11}$$

and

$$\mathbf{r}_\perp := (x,y) \in \mathbb{R}^2, \tag{12}$$

so that

$$\mathbf{p}\cdot\mathbf{A}(\mathbf{r},t) = \mathbf{p}_\perp\cdot\tilde{\mathbf{A}}(t-z).$$

In addition, we will assume throughout that the functions $\tilde{A}_x, \tilde{A}_y : \mathbb{R}\to\mathbb{R}$ are $\mathcal{C}_b$, i.e., continuous and bounded, and set

$$\|\mathbf{A}\| := \sup_{\xi\in\mathbb{R}} \sqrt{\tilde{A}_x(\xi)^2 + \tilde{A}_y(\xi)^2} < \infty. \tag{13}$$

III. SYMMETRIES OF THE VOLKOV SOLUTIONS

The construction of the Volkov solutions (3) relies heavily on certain symmetries of the Dirac equation (1): The three differential operators ∂_x, ∂_y, and $\partial_t+\partial_z$ commute formally with $(i\not{\partial}-e\not{A}-m)$, which has already been noticed by Nikishov and Ritus.[10] These translational symmetries allow the separation of variables in the equation, which is inherited by the relations

$$-i\partial_x\psi_{\mathbf{p},r} = \epsilon_r p_x \psi_{\mathbf{p},r}, \tag{14a}$$

$$-i\partial_y\psi_{\mathbf{p},r} = \epsilon_r p_y \psi_{\mathbf{p},r}, \tag{14b}$$

$$-i(\partial_t+\partial_z)\psi_{\mathbf{p},r} = \epsilon_r (p_z - E(\mathbf{p}))\psi_{\mathbf{p},r}. \tag{14c}$$

[For more symmetries of the Dirac equation (1) and a detailed group theoretical analysis, see the work of Janner and Janssen.[27]] Using the Hamiltonian form of (1), i.e.,

$$i\partial_t\psi(\mathbf{r},t) = H(t)\psi(\mathbf{r},t) \tag{15}$$

with the formally self-adjoint Hamiltonian operator

$$H(t) = \boldsymbol{\alpha}(-i\boldsymbol{\nabla} - e\mathbf{A}) + \beta m, \tag{16}$$

we easily derive from (14c) that for every t,

$$(H(t)+i\partial_z)\psi_{\mathbf{p},r} = \epsilon_r(E(\mathbf{p})-p_z)\psi_{\mathbf{p},r} \equiv \epsilon_r\kappa(\mathbf{p})\psi_{\mathbf{p},r}, \tag{17}$$

where we have introduced

$$\kappa(\mathbf{p}) := E(\mathbf{p}) - p_z = \sqrt{m^2+|\mathbf{p}|^2} - p_z > 0. \tag{18}$$

The Volkov solutions are thus simultaneous eigenfunctions of the three operators $-i\partial_x$, $-i\partial_y$, and $H(t)+i\partial_z$ with corresponding eigenvalues $\epsilon_r p_x$, $\epsilon_r p_y$, and $\epsilon_r\kappa(\mathbf{p})$, which do not depend on the chosen time t. It will be useful to define

$$\hat{\boldsymbol{\tau}}:\mathbb{R}^3 \to \mathbb{R}^2\times\mathbb{R}^+, \quad \mathbf{p}\mapsto\hat{\boldsymbol{\tau}}(\mathbf{p}) := (\mathbf{p}_\perp, \kappa(\mathbf{p})). \tag{19}$$

Note that the inverse is given by

$$\boldsymbol{\tau} := \hat{\boldsymbol{\tau}}^{-1}:\mathbb{R}^2\times\mathbb{R}^+ \to \mathbb{R}^3, \quad \boldsymbol{\tau}(\mathbf{p}_\perp,\lambda) := \left(\mathbf{p}_\perp, \frac{m^2+|\mathbf{p}_\perp|^2-\lambda^2}{2\lambda}\right). \tag{20}$$

The matrix part (4) and the phase (5) of the Volkov solutions may be rewritten in a simple form in terms of the eigenvalues

$$\mathbf{M}^{(\epsilon_r)}(\mathbf{p},\xi) = \mathbf{1} + \frac{e\not{\tilde{A}}(\xi)}{2\epsilon_r\kappa(\mathbf{p})} \in \mathbb{C}^{4\times4} \tag{21}$$

and

$$
\begin{aligned}
S^{(\epsilon_r)}(\mathbf{p},\mathbf{r},t) &= \epsilon_r \mathbf{p}_\perp \cdot \mathbf{r}_\perp - \epsilon_r \kappa(\mathbf{p}) t - \epsilon_r p_z (t-z) - \epsilon_r \int_0^{t-z} J_{\mathbf{p}}^{(\epsilon_r)}(\xi)\mathrm{d}\xi \\
&= \epsilon_r \mathbf{p}_\perp \cdot \mathbf{r}_\perp - \epsilon_r \kappa(\mathbf{p}) t - \epsilon_r \left[\left(p_z - \frac{|\mathbf{p}_\perp|^2}{2(E(\mathbf{p}) - p_z)} \right)(t-z) \right. \\
&\quad \left. + \frac{1}{2(E(\mathbf{p}) - p_z)} \int_0^{t-z} |\epsilon_r \mathbf{p}_\perp - e\tilde{\mathbf{A}}(\xi)|^2 \, \mathrm{d}\xi \right] \\
&= \epsilon_r \mathbf{p}_\perp \cdot \mathbf{r}_\perp - \epsilon_r \kappa(\mathbf{p}) t - \frac{1}{2}\left(\frac{m^2}{\epsilon_r \kappa(\mathbf{p})} - \epsilon_r \kappa(\mathbf{p}) \right)(t-z) - \frac{1}{2\epsilon_r \kappa(\mathbf{p})} \\
&\quad \times \int_0^{t-z} |\epsilon_r \mathbf{p}_\perp - e\tilde{\mathbf{A}}(\xi)|^2 \, \mathrm{d}\xi. \qquad (22)
\end{aligned}
$$

A similar form of the phase $S^{(\epsilon_r)}$ has already been found by Gol'dman.[6] Defining

$$
\pi_\perp(\xi,\mathbf{p}_\perp) := \begin{cases} \left(\frac{1}{\xi} \int_0^\xi |\mathbf{p}_\perp - e\tilde{\mathbf{A}}(\xi')|^2 \, \mathrm{d}\xi' \right)^{1/2}, & \xi \neq 0, \\ |\mathbf{p}_\perp - e\tilde{\mathbf{A}}(0)|, & \xi = 0, \end{cases} \qquad (23)
$$

$$
\boldsymbol{\nu}_\xi : \mathbb{R}^2 \times (\mathbb{R} \setminus \{0\}) \to \mathbb{R}^3, \boldsymbol{\nu}_\xi(\mathbf{p}_\perp,\lambda) := \left(\mathbf{p}_\perp, \frac{1}{2}\left[\frac{m^2 + \pi_\perp(\xi,\mathbf{p}_\perp)^2}{\lambda} - \lambda \right] \right), \qquad (24)
$$

$$
\mathbf{q}_\xi^{(\pm)}(\mathbf{p}) := \boldsymbol{\nu}_\xi(\pm\hat{\boldsymbol{\pi}}(\mathbf{p})) = \pm \left(\mathbf{p}_\perp, \frac{1}{2}\left[\frac{m^2 + \pi_\perp(\xi, \pm\mathbf{p}_\perp)^2}{\kappa(\mathbf{p})} - \kappa(\mathbf{p}) \right] \right), \qquad (25)
$$

and

$$
\mathbf{s}_t(\mathbf{r}) := (x,y,z-t), \qquad (26)
$$

we may write this as

$$
S^{(\epsilon_r)}(\mathbf{p},\mathbf{r},t) = \mathbf{q}_{t-z}^{(\epsilon_r)}(\mathbf{p}) \cdot \mathbf{s}_t(\mathbf{r}) - \epsilon_r \kappa(\mathbf{p}) t. \qquad (27)
$$

Note that

$$
0 \leqslant \pi_\perp(\xi,\mathbf{p}_\perp) \leqslant |\mathbf{p}_\perp| + |e|\|\mathbf{A}\|. \qquad (28)
$$

Moreover, for $\tilde{\mathbf{A}} \equiv 0$, $\pi_\perp(\xi,\mathbf{p}_\perp) = |\mathbf{p}_\perp|$, so that $\pi_\perp(\xi,\mathbf{p}_\perp)$ may be thought of as a modified "perpendicular momentum."

IV. REGULAR WAVE PACKETS

In this section, we shall construct square-integrable wave packets from the Volkov solutions. These wave packets will be of the form

$$
\psi(\mathbf{r},t) = \frac{1}{(2\pi)^{3/2}} \sum_{r=1}^{4} \int_{\mathbb{R}^3} \phi_r(\mathbf{p}) \psi_{\mathbf{p},r}(\mathbf{r},t) \mathrm{d}^3 p. \qquad (29)
$$

This integral representation was used, for example, by San Román *et al.*[21–24] in their calculations of the time evolution of wave packets. It will be our task to make sense of (29), i.e., we will ensure the existence of this integral for as many functions ϕ_r as possible and to show that the resulting wave packet ψ fulfills the Dirac equation (1).

In this section, we will start with momentum distributions ϕ_r that are in $\mathcal{C}_0^\infty$ and show that the wave packets defined by these decay faster than any power of $|\mathbf{r}|$ for $|\mathbf{r}|\to\infty$. In order to control the $\mathbf{p}$ dependence of the phase (27), we need to determine the inverses of the mappings $\mathbf{q}_\xi^{(\pm)}$ from (25),

$$\tilde{\mathbf{q}}_\xi^{(\pm)}(\tilde{\mathbf{p}}) := (\mathbf{q}_\xi^{(\pm)})^{-1}(\tilde{\mathbf{p}}) = \boldsymbol{\pi}(\pm\boldsymbol{\nu}_\xi^{-1}(\tilde{\mathbf{p}})) = \boldsymbol{\pi}(\pm(\mathbf{p}_\perp, \sqrt{m^2+\pi_\perp(\xi,\pm\tilde{\mathbf{p}}_\perp)^2+\tilde{p}_z^2}\mp\tilde{p}_z)), \tag{30}$$

which are $\mathcal{C}^\infty$. We claim the following.

Lemma 1: For every compact set $K\subset\mathbb{R}^3$ and every $n_x,n_y,n_z\in\mathbb{N}_0$, there is a constant $c_{n_x,n_y,n_z}(K)$ satisfying

$$\left\|\left(\frac{\partial}{\partial\tilde{p}_x}\right)^{n_x}\left(\frac{\partial}{\partial\tilde{p}_y}\right)^{n_y}\left(\frac{\partial}{\partial\tilde{p}_z}\right)^{n_z}\tilde{\mathbf{q}}_\xi^{(\pm)}(\tilde{\mathbf{p}})\right\| \leqslant c_{n_x,n_y,n_z}(K), \quad \tilde{\mathbf{p}}\in K, \quad \xi\in\mathbb{R}.$$

Proof: By the chain rule, one sees that the derivatives of $\tilde{\mathbf{q}}_\xi^{(\pm)}$ depend continuously on $\tilde{\mathbf{p}}$ as well as on $\pi_\perp(\xi,\tilde{\mathbf{p}}_\perp)^2$, $\partial_{\tilde{p}_x}[\pi_\perp(\xi,\tilde{\mathbf{p}}_\perp)]^2$, and $\partial_{\tilde{p}_y}[\pi_\perp(\xi,\tilde{\mathbf{p}}_\perp)]^2$. [Note that higher-order derivatives of $[\pi_\perp(\xi,\tilde{\mathbf{p}}_\perp)]^2$ vanish, see the definition (23).] The last three expressions are bounded for $\xi\in\mathbb{R}$ and $\tilde{\mathbf{p}}_\perp$ in a fixed compact set, which is due to the boundedness of $\tilde{\mathbf{A}}$ and (28). The derivatives of $\tilde{\mathbf{q}}_\xi^{(\pm)}$ are therefore bounded on the compact set K. ∎

We may now state the first main theorem, which allows the construction of L^2 wave packets.

Theorem 2: *Let $\phi\equiv(\phi_1,\ldots,\phi_4)\in\mathcal{C}_0^\infty(\mathbb{R}^3)^4$.*

(a) *The wave packet ψ defined by*

$$\psi(\mathbf{r},t) = \frac{1}{(2\pi)^{3/2}}\sum_{r=1}^4\int_{\mathbb{R}^3}\phi_r(\mathbf{p})\psi_{\mathbf{p},r}(\mathbf{r},t)\mathrm{d}^3p \tag{31}$$

is continuous in $\mathbf{r}$ and t.

(b) *For any $n\in\mathbb{N}_0$, there is a constant c_n such that*

$$\|\psi(\mathbf{r},t)\|_{\mathbb{C}^4} \leqslant c_n\frac{1+|t|^n}{1+|\mathbf{s}_t(\mathbf{r})|^n} = c_n\frac{1+|t|^n}{1+[x^2+y^2+(z-t)^2]^{n/2}}. \tag{32}$$

In particular $\psi(\cdot,t)\in L^p(\mathbb{R}^3)^4$ for all $t\in\mathbb{R}$ and $p\in[1,\infty]$.

Proof: (a) It suffices to show the result for the summands r independently. Let $\mathbf{r}_n\to\mathbf{r}$ and $t_n\to t$. Then $\psi_{\mathbf{p},r}(\mathbf{r}_n,t_n)\to\psi_{\mathbf{p},r}(\mathbf{r},t)$ by continuity of the Volkov solutions (3), so the integrand in (31) converges pointwise. Furthermore, since $\psi_{\mathbf{p},r}(\mathbf{r},t)$ is bounded in $\mathbf{p}\in\operatorname{supp}\phi_r$ as well as in $\mathbf{r}$ and t, continuity of ψ is established by dominated convergence, see, e.g., Theorem I.11 in Ref. 28.

(b) We will show that for any $n_x,n_y,n_z\in\mathbb{N}_0$, there is a constant c_{n_x,n_y,n_z} such that

$$|x|^{n_x}|y|^{n_y}|z-t|^{n_z}\|\psi(\mathbf{r},t)\|_{\mathbb{C}^4} \leqslant c_{n_x,n_y,n_z}(1+|t|^{n_x+n_y+n_z}). \tag{33}$$

The estimate in (32) follows from this by using

$$[x^2+y^2+(z-t)^2]^{n/2} = (\sqrt{x^2+y^2+(z-t)^2})^n \leqslant (\sqrt{(|x|+|y|+|z-t|)^2})^n = (|x|+|y|+|z-t|)^n,$$

where the right-hand side is a polynomial of degree n in $|x|$, $|y|$, and $|z-t|$.

In order to prove the estimate (33), we shall apply the stationary-phase method (see, for example, Theorem XI.14 in Ref. 29). We only need to look at the case $\mathbf{r}\equiv(x,y,z)\in\mathbb{R}^3$ with $x,y,z-t\neq0$; for x, y, or $z-t$ equal to zero, (33) follows by continuity. Setting $\epsilon := \epsilon_r$ for abbreviation, we find

$$\begin{aligned}\int_{\mathbb{R}^3}\phi_r(\mathbf{p})\psi_{\mathbf{p},r}(\mathbf{r},t)\mathrm{d}^3p &= \int_{\mathbb{R}^3}\phi_r(\mathbf{p})\mathbf{M}^{(\epsilon)}(\mathbf{p},t-z)u_r(\mathbf{p})\exp[i(\mathbf{q}^{(\epsilon)}_{t-z}(\mathbf{p})\cdot\mathbf{s}_t(\mathbf{r})-\epsilon\kappa(\mathbf{p})t)]\mathrm{d}^3p\\ &= \int_{\mathbb{R}^3}\phi_r(\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}))\mathbf{M}^{(\epsilon)}(\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}),t-z)u_r(\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}))\\ &\quad\times\exp[i(\tilde{\mathbf{p}}\cdot\mathbf{s}_t(\mathbf{r})-\epsilon\kappa(\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}))t)]|\det(D\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}))|\mathrm{d}^3\tilde{p}\\ &= \frac{(-i)^{n_x+n_y+n_z}}{x^{n_x}y^{n_y}(z-t)^{n_z}}\int_{\mathbb{R}^3}\phi_r(\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}))\mathbf{M}^{(\epsilon)}(\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}),t-z)u_r(\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}))\\ &\quad\times\exp(-i\epsilon\kappa(\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}))t)|\det(D\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}))|\\ &\quad\times\left[\left(\frac{\partial}{\partial\tilde{p}_x}\right)^{n_x}\left(\frac{\partial}{\partial\tilde{p}_y}\right)^{n_y}\left(\frac{\partial}{\partial\tilde{p}_z}\right)^{n_z}\exp(i\tilde{\mathbf{p}}\cdot\mathbf{s}_t(\mathbf{r}))\right]\mathrm{d}^3\tilde{p},\end{aligned}$$

where (27) has been used and the transformation formula for integrals has been applied. Since $\phi_r\in\mathcal{C}_0^\infty$ and all other $\tilde{\mathbf{p}}$ dependences are $\mathcal{C}^\infty$, we may perform integrations by parts and obtain

$$\begin{aligned}\int_{\mathbb{R}^3}\phi_r(\mathbf{p})\psi_{\mathbf{p},r}(\mathbf{r},t)\mathrm{d}^3p &= \frac{i^{n_x+n_y+n_z}}{x^{n_x}y^{n_y}(z-t)^{n_z}}\int_{\mathbb{R}^3}\exp(i\tilde{\mathbf{p}}\cdot\mathbf{s}_t(\mathbf{r}))\left(\frac{\partial}{\partial\tilde{p}_x}\right)^{n_x}\left(\frac{\partial}{\partial\tilde{p}_y}\right)^{n_y}\left(\frac{\partial}{\partial\tilde{p}_z}\right)^{n_z}\\ &\quad\times[\phi_r(\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}))\mathbf{M}^{(\epsilon)}(\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}),t-z)u_r(\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}))\\ &\quad\times\exp(-i\epsilon\kappa(\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}))t)|\det(D\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}))|]\mathrm{d}^3\tilde{p}.\end{aligned}\tag{34}$$

Observe that by the chain rule,

$$\left|\left(\frac{\partial}{\partial\tilde{p}_x}\right)^{m_x}\left(\frac{\partial}{\partial\tilde{p}_y}\right)^{m_y}\left(\frac{\partial}{\partial\tilde{p}_z}\right)^{m_z}\exp(-i\epsilon\kappa(\tilde{\mathbf{q}}^{(\epsilon)}_{t-z}(\tilde{\mathbf{p}}))t)\right|\leqslant d_{m_x,m_y,m_z}(1+|t|^{m_x+m_y+m_z}),\quad\tilde{\mathbf{p}}\in\operatorname{supp}\phi_r,$$

for some constants d_{m_x,m_y,m_z}. Again by the chain rule and by Lemma 1, the derivatives in (34) are uniformly bounded in $\mathbf{r}$, and we may conclude that the integral is bounded in $\mathbf{r}$ and that the t dependence is governed by the above inequality. Thus,

$$|x|^{n_x}|y|^{n_y}|z-t|^{n_z}\left\|\int_{\mathbb{R}^3}\phi_r(\mathbf{p})\psi_{\mathbf{p},r}(\mathbf{r},t)\mathrm{d}^3p\right\|_{\mathbb{C}^4}\leqslant\tilde{c}_{r,n_x,n_y,n_z}(1+|t|^{n_x+n_y+n_z})$$

for some constants $\tilde{c}_{r,n_x,n_y,n_z}$, from which (33) follows after summation over r.

■

Theorem 2 allows us to define regular wave packets.

Definition 1: For $t\in\mathbb{R}$, define

$$\mathcal{F}_t{:}\mathcal{C}_0^\infty(\mathbb{R}^3)^4\to L^2(\mathbb{R}^3)^4\cap\mathcal{C}_\infty(\mathbb{R}^3)^4,\quad\phi\mapsto\mathcal{F}_t(\phi),$$

where

$$(\mathcal{F}_t(\phi))(\mathbf{r}):=\frac{1}{(2\pi)^{3/2}}\sum_{r=1}^4\int_{\mathbb{R}^3}\phi_r(\mathbf{p})\psi_{\mathbf{p},r}(\mathbf{r},t)\mathrm{d}^3p\tag{35}$$

and $\mathcal{C}_\infty(\mathbb{R}^3)^4\subset\mathcal{C}_b(\mathbb{R}^3)^4$ is the space of continuous functions $\mathbb{R}^3\to\mathbb{C}^4$ that vanish at infinity. The elements of the range $\mathcal{F}_t(\mathcal{C}_0^\infty(\mathbb{R}^3)^4)$ will be called regular (Volkov) wave packets.

The following theorem assures that under weak assumptions, the wave packets defined above actually fulfill the Dirac equation in the Hamiltonian form (15). We only need the additional requirement that $\tilde{\mathbf{A}} \in \mathcal{C}_b^1$, i.e., $\tilde{\mathbf{A}}$ is continuously differentiable and both $\tilde{\mathbf{A}}$ and its derivative $\tilde{\mathbf{A}}'$ are bounded.

Theorem 3: *Let* $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^3)^4$, *and set*

$$\psi(\mathbf{r},t) := \mathcal{F}_t(\phi)(\mathbf{r}).$$

Assume that $\tilde{\mathbf{A}} \in \mathcal{C}_b^1$. *Then the following assertions hold:*

(a) $\psi \in \mathcal{C}^1(\mathbb{R}^4)^4$ *and*

$$i\partial_t \psi(\mathbf{r},t) = H(t)\psi(\mathbf{r},t) \equiv [\alpha(-i\boldsymbol{\nabla} - e\tilde{\mathbf{A}}(t-z)) + \beta m]\psi(\mathbf{r},t). \tag{36}$$

(b) *There are constants* c_n, $n \in \mathbb{N}_0$, *satisfying*

$$\|(H(t)\psi(\cdot,t))(\mathbf{r})\| \leqslant c_n \frac{1+|t|^n}{1+[x^2+y^2+(z-t)^2]^{n/2}}.$$

Therefore, $H(t)\psi(\cdot,t) \in L^2(\mathbb{R}^3)^4$ *for all* t.

(c) *The mapping* $\mathbb{R} \to L^2(\mathbb{R}^3)^4$, $t \mapsto \psi(\cdot,t)$, *is* $\mathcal{C}^1$, *and*

$$i\frac{d}{dt}\psi(\cdot,t) = H(t)\psi(\cdot,t), \tag{37}$$

where the derivative is taken in the space $L^2(\mathbb{R}^3)^4$.

Proof: (a) Since the Volkov solutions $\psi_{\mathbf{p},r}$ are $\mathcal{C}^1$ and satisfy the Dirac equation (15), we only have to show that the differentiations in (36) may be interchanged with the integration in (35). This is possible since the derivatives of $\psi_{\mathbf{p},r}(\mathbf{r},t)$ with respect to t, x, y, and z are continuous functions of $\mathbf{p}$, $\mathbf{r}$, and t and since the support of ϕ is compact.

(b) Upon interchange of differentiation and integration and using the boundedness of the derivative $\tilde{\mathbf{A}}'$, this statement follows as in the proof of Theorem 2.

(c) We need to show that for every t_0,

$$i\lim_{\tau\to 0}\frac{\psi(\cdot,t_0+\tau)-\psi(\cdot,t_0)}{\tau} = H(t_0)\psi(\cdot,t_0), \tag{38}$$

where the limit is to be understood in the L^2 norm. In view of part (a), pointwise convergence for every $\mathbf{r} \in \mathbb{R}^3$ is given. It remains to show that the left-hand side of (38) is bounded by a common L^2 function for $|\tau| < 1$; the statement follows then by dominated convergence. For $\tau > 0$,

$$\left\|\frac{\psi(\mathbf{r},t_0+\tau)-\psi(\mathbf{r},t_0)}{\tau}\right\| \leqslant \sup_{\sigma\in(0,\tau)}\left\|\partial_t\psi(\mathbf{r},t)\big|_{t=t_0+\sigma}\right\| = \sup_{\sigma\in(0,\tau)}\|(H(t_0+\sigma)\psi(\cdot,t_0+\sigma))(\mathbf{r})\|$$
$$\leqslant C\sup_{\sigma\in(0,\tau)}\frac{1+|t_0+\sigma|^2}{1+x^2+y^2+(z-(t_0+\sigma))^2}$$

for a certain constant C, which is clear by part (b). For $\tau < 0$, we obtain a similar result, in which $\sup_{\sigma\in(0,\tau)}$ is replaced by $\sup_{\sigma\in(\tau,0)}$. With little effort, we see that for $|\tau| \leqslant 1$,

$$\left\|\frac{\psi(\mathbf{r},t_0+\tau)-\psi(\mathbf{r},t_0)}{\tau}\right\| \leqslant C\frac{1+(|t_0|+1)^2}{1+x^2+y^2+\max\{|z-t_0|-1,0\}^2},$$

where the right-hand side is an L^2 function of x, y, and z. This confirms (38) and concludes the proof. ■

For the usual Fourier transformation, the Riemann–Lebesgue lemma holds, which states that the Fourier transformation defined on $\mathcal{C}_0^\infty$ extends uniquely to a bounded map from L^1 into $\mathcal{C}_\infty$, the continuous functions vanishing at infinity, see Theorem IX.7 in Ref. 30. In the case of the Volkov solutions, a similar result is true.

Theorem 4:

(a) *There is a constant C with*

$$\|\mathcal{F}_t(\phi)\|_\infty \leqslant C\|\phi\|_{L^1(\mathbb{R}^3)^4}$$

for all $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^3)^4 \subset L^1(\mathbb{R}^3)^4$ *and all* $t \in \mathbb{R}$.

(b) *The unique bounded extension* $\mathcal{F}_t^{(1)}$ *to* $L^1(\mathbb{R}^3)^4$ *fulfills*

$$\mathcal{F}_t^{(1)}: L^1(\mathbb{R}^3)^4 \to \mathcal{C}_\infty(\mathbb{R}^3)^4,$$

i.e., $\mathcal{F}_t^{(1)}(\phi)$ *vanishes at infinity for all* $\phi \in L^1(\mathbb{R}^3)^4$.

(c) *For* $\phi \in L^1(\mathbb{R}^3)^4$,

$$(\mathcal{F}_t^{(1)}(\phi))(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \sum_{r=1}^{4} \int_{\mathbb{R}^3} \phi_r(\mathbf{p})\psi_{\mathbf{p},r}(\mathbf{r},t)\mathrm{d}^3p, \tag{39}$$

i.e., the same formula as in (35) *holds for all* $\phi \in L^1(\mathbb{R}^3)^4$.

Proof: (a) In order to adapt the proof for the usual Fourier transformation in Ref. 30, we have to check first that the Volkov solutions are bounded in $\mathbf{p}$. Since this is not directly clear from the defining equation (3), we shall first rewrite the Volkov solutions. To this end, observe that

$$\not{n}\tilde{\not{A}}(\xi) = -\tilde{\not{A}}(\xi)\not{n}.$$

Employing (9), we can write

$$\psi_{\mathbf{p},r}(\mathbf{r},t) = \tilde{\mathbf{M}}^{(\epsilon_r)}(\mathbf{p},t-z)u_r(\mathbf{p})e^{iS^{(\epsilon_r)}(\mathbf{p},\mathbf{r},t)} \tag{40}$$

with

$$\tilde{\mathbf{M}}^{(\pm)}(\mathbf{p},\xi) := 1 \mp e\tilde{\not{A}}(\xi)\frac{E(\mathbf{p})\not{n} \pm m - \not{p}}{2E(\mathbf{p})(E(\mathbf{p})-p_z)} = \mathbf{1} \mp e\tilde{\not{A}}(\xi)\left(\frac{\pm m + p_x\gamma^1 + p_y\gamma^2}{2E(\mathbf{p})(E(\mathbf{p})-p_z)} - \frac{1}{2E(\mathbf{p})}\gamma^3\right).$$

Using the equality

$$\frac{1}{E(\mathbf{p})(E(\mathbf{p})-p_z)} + \frac{1}{E(\mathbf{p})(E(\mathbf{p})+p_z)} = \frac{2E(\mathbf{p})}{E(\mathbf{p})(m^2+|\mathbf{p}_\perp|^2)} = \frac{2}{m^2+|\mathbf{p}_\perp|^2},$$

we find the estimate

$$\frac{m^2+|\mathbf{p}_\perp|^2}{E(\mathbf{p})(E(\mathbf{p})-p_z)} \leqslant 2$$

and conclude that $\tilde{\mathbf{M}}^{(\pm)}(\mathbf{p},\xi)$ are bounded with respect to $\mathbf{p}$ and ξ. Consequently, $\psi_{\mathbf{p},r}(\mathbf{r},t)$ is bounded in $\mathbf{p}$, $\mathbf{r}$, and t,

$$\|\psi_{\mathbf{p},r}(\mathbf{r},t)\| \leqslant c_r \tag{41}$$

for some constants $c_r \geqslant 0$. For $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^3)^4$, this results in the estimate

$$\|(\mathcal{F}_t(\phi))(\mathbf{r})\| \leqslant \frac{1}{(2\pi)^{3/2}}\sum_{r=1}^{4}\int_{\mathbb{R}^3}|\phi_r(\mathbf{p})|\|\psi_{\mathbf{p},r}(\mathbf{r},t)\|\mathrm{d}^3p \leqslant \frac{1}{(2\pi)^{3/2}}\sum_{r=1}^{4} c_r\|\phi_r\|_{L^1}.$$

(b) This follows as for the Riemann–Lebesgue lemma: For a given $\phi\in L^1(\mathbb{R}^3)^4$, choose a sequence $(\phi_n)_{n\in\mathbb{N}}$ in $\mathcal{C}_0^\infty(\mathbb{R}^3)^4$ with $\phi_n\to\phi$, $n\to\infty$, in the $L^1(\mathbb{R}^3)^4$ norm. By Theorem 2, $\mathcal{F}_t^{(1)}(\phi_n)=\mathcal{F}_t(\phi_n)\in\mathcal{C}_\infty(\mathbb{R}^3)^4$ for all $n\in\mathbb{N}$. On the other hand, part (a) of the present theorem ensures that $\mathcal{F}_t^{(1)}(\phi_n)\to\mathcal{F}_t^{(1)}(\phi)$, $n\to\infty$, uniformly on $\mathbb{R}^3$. Therefore, we also have $\mathcal{F}_t(\phi)\in\mathcal{C}_\infty(\mathbb{R}^3)^4$.

(c) In view of (41), the integral on the right-hand side of (39) exists for $\phi\in L^1(\mathbb{R}^3)^4$. Taking again a sequence as in the proof of part (b), the statement follows by dominated convergence. ■

V. NORMALIZATION

The following theorem may be considered as the central point of this paper.

Theorem 5: *Let $\tilde{\mathbf{A}}\in\mathcal{C}_b^1$. Then for every $t\in\mathbb{R}$, $\mathcal{F}_t$ is an isometry with respect to the L^2 norm, i.e., for every $\phi\in L^2(\mathbb{R}^3)^4$,*

$$\|\mathcal{F}_t(\phi)\|_{L^2(\mathbb{R}^3)^4}=\|\phi\|_{L^2(\mathbb{R}^3)^4}. \tag{42}$$

As a simple conclusion, we note the following.

Corollary 6: Under the assumptions of Theorem 5,

$$\langle\mathcal{F}_t(\phi),\mathcal{F}_t(\chi)\rangle_{L^2(\mathbb{R}^3)^4}=\langle\phi,\chi\rangle_{L^2(\mathbb{R}^3)^4} \tag{43}$$

for every $\phi,\chi\in L^2(\mathbb{R}^3)^4$.

The lengthy proof of Theorem 5 will be deferred to the Appendix. Here we shall only verify Corollary 6 and then point out the connection with the "normalization to a delta function" and "orthogonality" of the Volkov solutions.

Proof of Corollary 6: This corollary is just the application of a general theorem valid for any isometry between two complex Hilbert spaces: We use the polarization identity

$$\langle x,y\rangle=\tfrac{1}{4}(\|x+y\|^2+\|x-y\|^2+i\|x-iy\|^2-i\|x+iy\|^2),$$

which follows from taking appropriate linear combinations from

$$\|x+y\|^2=\langle x+y,x+y\rangle=\|x\|^2+\|y\|^2+2\,\mathrm{Re}\langle x,y\rangle$$

and similar expressions for $\|x-y\|^2$, $\|x+iy\|^2$, and $\|x-iy\|^2$. For an isometry T (satisfying $\|Tz\|=\|z\|$ for all z), this leads to

$$\begin{aligned}\langle Tx,Ty\rangle&=\tfrac{1}{4}(\|T(x+y)\|^2+\|T(x-y)\|^2+i\|T(x-iy)\|^2-i\|T(x+iy)\|^2)\\&=\tfrac{1}{4}(\|x+y\|^2+\|x-y\|^2+i\|x-iy\|^2-i\|x+iy\|^2)=\langle x,y\rangle.\end{aligned}$$

■

In the physical literature, e.g., Refs. 10, 16, 26, and 31, the "normalization" and "orthogonality" property is laxly written as follows:

$$\int_{\mathbb{R}^3}\psi^\dagger_{\mathbf{p},r}(\mathbf{r},t)\psi_{\mathbf{p}',r'}(\mathbf{r},t)\mathrm{d}^3r=(2\pi)^3\delta_{r,r'}\delta^{(3)}(\mathbf{p}-\mathbf{p}'), \tag{44}$$

where $\delta^{(3)}$ is the three-dimensional delta function. The property (44) is used for the verification of (43),

$$\langle \mathcal{F}_t(\phi), \mathcal{F}_t(\chi)\rangle = \frac{1}{(2\pi)^3}\sum_{r,r'=1}^{4}\int_{\mathbb{R}^3}\left(\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\overline{\phi_r(\mathbf{p})}\chi_{r'}(\mathbf{p}')\langle\psi_{\mathbf{p},r}(\mathbf{r},t),\psi_{\mathbf{p}'r'}(\mathbf{r},t)\rangle_{\mathbb{C}^4}\,\mathrm{d}^3p\,\mathrm{d}^3p'\right)\mathrm{d}^3r$$

$$= \frac{1}{(2\pi)^3}\sum_{r,r'=1}^{4}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\overline{\phi_r(\mathbf{p})}\chi_{r'}(\mathbf{p}')\left(\int_{\mathbb{R}^3}\langle\psi_{\mathbf{p},r}(\mathbf{r},t),\psi_{\mathbf{p}'r'}(\mathbf{r},t)\rangle_{\mathbb{C}^4}\,\mathrm{d}^3r\right)\mathrm{d}^3p\,\mathrm{d}^3p'$$

$$= \sum_{r=1}^{4}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\overline{\phi_r(\mathbf{p})}\chi_r(\mathbf{p}')\,\delta^{(3)}(\mathbf{p}-\mathbf{p}')\mathrm{d}^3p\,\mathrm{d}^3p'$$

$$= \sum_{r=1}^{4}\int_{\mathbb{R}^3}\overline{\phi_r(\mathbf{p})}\chi_r(\mathbf{p})\mathrm{d}^3p = \langle\phi,\chi\rangle_{L^2(\mathbb{R}^3)^4}.$$

This calculation certainly involves an unjustified interchange of integration orders and is therefore rather questionable from a mathematical point of view.

We mention that a different "normalization" has been employed by Neville and Rohrlich[20] and Bergou and Varró.[9] These authors use a scalar product that is calculated on those hyperplanes in Minkowski space–time where the vector potential **A** is constant, i.e., their considerations involve integrals of the form

$$\int_{\{(\mathbf{r},t)\in\mathbb{R}^4:t-z=u\}}\cdots\mathrm{d}^3r\,\mathrm{d}t$$

for fixed $u\in\mathbb{R}$. However, the L^2 norms determined from this integration cannot be regarded as a normalization for the probability to find a particle. For a probability interpretation, one would have to integrate over space for a fixed time, at least for a certain specified inertial frame. That is, one would need a spacelike hyperplane, whereas the above integration is over a lightlike hyperplane. Even though the lightlike hyperplane and the related coordinates seem more adopted to the symmetry of the problem, an integration over a spacelike hyperplane as in (43) or (44) appears much more "physical."

VI. EXTENSION TO L^2

Theorem 5 allows us to pronounce the following definition.

Definition 2: In the case $\tilde{\mathbf{A}}\in\mathcal{C}_b^1$, *let*

$$\mathcal{F}_t^{(2)}:L^2(\mathbb{R}^3)^4\to L^2(\mathbb{R}^3)^4$$

be the unique isometric extension of $\mathcal{F}_t$ *from Definition 1 to* $L^2(\mathbb{R}^3)^4$.

It will be profitable to have an integral representation of $\mathcal{F}_t^{(2)}$ for a larger subspace of L^2 than just $\mathcal{C}_0^\infty$. This is indeed possible for amplitude functions in $L^1\cap L^2$:

Theorem 7: *For* $\phi\in L^1(\mathbb{R}^3)^4\cap L^2(\mathbb{R}^3)^4$, *we have*

$$\mathcal{F}_t^{(2)}(\phi)=\mathcal{F}_t^{(1)}(\phi)\in\mathcal{C}_\infty(\mathbb{R}^3)^4, \tag{45}$$

or more explicitly,

$$(\mathcal{F}_t^{(2)}(\phi))(\mathbf{r})=\frac{1}{(2\pi)^{3/2}}\sum_{r=1}^{4}\int_{\mathbb{R}^3}\phi_r(\mathbf{p})\psi_{\mathbf{p},r}(\mathbf{r},t)\mathrm{d}^3p. \tag{46}$$

Proof: We adapt here a proof from the usual Fourier transformation, which can be found in the book of Weidmann.[32] Let $(\phi_n)_n$ be a sequence in $\mathcal{C}_0^\infty(\mathbb{R}^3)^4$ with $\phi_n\to\phi$, $n\to\infty$, in $L^1(\mathbb{R}^3)^4$ and in $L^2(\mathbb{R}^3)^4$ simultaneously. Fix $t\in\mathbb{R}$ and set $\psi_n:=\mathcal{F}_t(\phi_n)$. Theorem 2 yields $\psi_n\in L^1(\mathbb{R}^3)^4\cap\mathcal{C}_\infty(\mathbb{R}^3)^4$. We have

$$\mathcal{F}_t^{(1)}(\phi) = \lim_{n\to\infty} \psi_n \in \mathcal{C}_b(\mathbb{R}^3)^4$$

and

$$\mathcal{F}_t^{(2)}(\phi) = \lim_{n\to\infty} \psi_n \in L^2(\mathbb{R}^3)^4,$$

where the limits are understood in $\mathcal{C}_b(\mathbb{R}^3)^4$ and $L^2(\mathbb{R}^3)^4$, respectively. Choose a subsequence $(\psi_{n_k})_k$ such that

$$\psi_{n_k}(\mathbf{r}) \to \mathcal{F}_t^{(2)}(\phi)(\mathbf{r}), \quad k\to\infty, \quad \text{a.e.}$$

But since

$$\psi_{n_k}(\mathbf{r}) \to \mathcal{F}_t^{(1)}(\phi)(\mathbf{r}), \quad k\to\infty,$$

for all $\mathbf{r}$, we conclude that

$$\mathcal{F}_t^{(1)}(\phi)(\mathbf{r}) = \mathcal{F}_t^{(2)}(\phi)(\mathbf{r}), \quad \text{a.e.} \tag{47}$$

■

Corollary 8: Let $\phi \in L^2(\mathbb{R}^3)^4$ *and* $K_n := \{x \in \mathbb{R}^3 : \|x\|_2 \leqslant n\}$. *Then*

$$(\mathcal{F}_t^{(2)}\phi)(\mathbf{r}) = \lim_{n\to\infty} \frac{1}{(2\pi)^{3/2}} \sum_{r=1}^{4} \int_{K_n} \phi_r(\mathbf{p}) \psi_{\mathbf{p},r}(\mathbf{r},t) \mathrm{d}^3p. \tag{48}$$

Proof: Again adapting a proof from Weidmann,[32] let χ_n be the characteristic function of the set K_n and fix $t \in \mathbb{R}$. Then $\chi_n\phi \in L^1(\mathbb{R}^3)^4 \cap L^2(\mathbb{R}^3)^4$, and we have $\chi_n\phi \to \phi$ in $L^2(\mathbb{R}^3)^4$. According to Theorem 7,

$$(\mathcal{F}_t^{(2)}(\chi_n\phi))(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \sum_{r=1}^{4} \int_{K_n} \phi_r(\mathbf{p}) \psi_{\mathbf{p},r}(\mathbf{r},t) \mathrm{d}^3p.$$

The claim follows from the fact that $\mathcal{F}_t^{(2)}(\chi_n\phi) \to \mathcal{F}_t^{(2)}(\phi)$ in $L^2(\mathbb{R}^3)^4$.

■

VII. SUMMARY AND OUTLOOK

In this paper, we have put some assertions concerning the relativistic Volkov solutions on solid mathematical ground. As a general assumption, we took the electromagnetic vector potential to be continuous and bounded. In Theorem 2, we have justified the construction of regular wave packets from Volkov solutions as used, for example, in Ref. 21 and have proved their rapid decay in spatial space. Theorem 3 shows that these wave packets satisfy the Dirac equation, as long as the vector potential is also $\mathcal{C}^1$ and has a bounded derivative. The "normalization" property is verified in the central Theorem 5 and allows the definition of wave packets for any L^2 function in momentum space. Finally, Theorem 7 provides a useful integral representation for the momentum-space functions contained in $L^1 \cap L^2$.

As mentioned in the introduction, it is still desirable to find a rigorous proof of the "completeness" of the Volkov solutions, i.e., for the hypothesis that for any initial wave packet $\psi_0 \in L^2(\mathbb{R}^3)^4$ at time $t=0$, there is a momentum distribution $\phi \in L^2(\mathbb{R}^3)^4$ from which ψ_0 and also the time-dependent solution $\psi(\mathbf{r},t)$ with $\psi(\cdot,0)=\psi_0$ follows. In other words, the mapping $\mathcal{F}_t^{(2)}$ from (2) should be surjective and therefore unitary for a "reasonable" vector potential $\tilde{\mathbf{A}}$. A comparison with the field-free case $\tilde{\mathbf{A}} \equiv 0$ suggests that the inverse

$$\mathcal{G}_t := (\mathcal{F}_t^{(2)})^{-1}$$

might be obtainable by the formula

$$\phi(\mathbf{p}) := (\mathcal{G}_t(\psi))(\mathbf{p}) = \left(\frac{1}{(2\pi)^{3/2}} \sum_{r=1}^{4} \int_{\mathbb{R}^3} \langle \psi_{\mathbf{p},r}(\mathbf{r},t), \psi(\mathbf{r}) \rangle \mathrm{d}^3 p \right)_{r=1,\ldots,4}, \tag{49}$$

at least when $\psi \in \mathcal{C}_0^\infty$. The "physical" version of the above inversion formula (49) is

$$\sum_{r=1}^{4} \int_{\mathbb{R}^3} \psi_{\mathbf{p},r}^\dagger(\mathbf{r},t) \psi_{\mathbf{p},r}(\mathbf{r}',t) \mathrm{d}^3 p = (2\pi)^3 \delta^{(3)}(\mathbf{r}-\mathbf{r}').$$

The validity of the inversion formula (49) would allow one to write the unitary propagator for the Dirac equation (15) as

$$U(t,t') = \mathcal{F}_t^{(2)} \circ \mathcal{G}_{t'}. \tag{50}$$

This conjecture is used by San Román and co-workers in Refs. 21–24 for the calculation of the time evolution of a Volkov wave packet. Having established (49), one might also try to understand on a more analytical level the squeezing and distortion of wave packets observed in Refs. 21 and 22.

In order to prove (49), one should (i) verify the existence of the integral on the right-hand side for $\psi \in \mathcal{C}_0^\infty$, (ii) show that $\phi \in L^1 \cap L^2$, and (iii) demonstrate with the help of Theorem 7 that

$$\psi = F_t^{(2)}(\mathcal{G}_t(\psi)).$$

There are strong indications to the author that the assertions (i) and (ii) are correct for a bounded vector potential $\tilde{\mathbf{A}} \in \mathcal{C}^2$ with bounded first and second derivates. More details and results shall be supplied in a future publication.

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APPENDIX: PROOF OF THEOREM 5

In this appendix, we provide the proof for the main Theorem 5.

Proof: Fix $t \in \mathbb{R}$ and $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^3)^4$. We have to show that

$$\|\mathcal{F}_t(\phi)\|_{L^2(\mathbb{R}^3)^4}^2 \equiv \frac{1}{(2\pi)^3} \sum_{r,r'=1}^{4} \int_{\mathbb{R}^3} I_{r,r'}(\mathbf{r}) \mathrm{d}^3 r = \|\phi\|_{L^2(\mathbb{R}^3)^4}^2 \tag{A1}$$

with

$$I_{r,r'}(\mathbf{r}) := \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \overline{\phi_r(\mathbf{p})} \phi_{r'}(\mathbf{p}') \langle \psi_{\mathbf{p},r}(\mathbf{r},t), \psi_{\mathbf{p}'r'}(\mathbf{r},t) \rangle_{\mathbb{C}^4} \, \mathrm{d}^3 p \, \mathrm{d}^3 p', \tag{A2}$$

where the bar denotes complex conjugation. Note that all integrals appearing above exist since $\mathcal{F}_t(\phi) \in L^2(\mathbb{R}^3)^4$ by virtue of Theorem 2.

Inserting the Volkov solutions (3), we find

$$
\begin{aligned}
I_{r,r'}(\mathbf{r}) &= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \overline{\phi_r(\mathbf{p})}\phi_{r'}(\mathbf{p}')\exp[i(S^{(\epsilon_{r'})}(\mathbf{p}',\mathbf{r},t) - S^{(\epsilon_r)}(\mathbf{p},\mathbf{r},t))] \\
&\quad \times \langle \mathbf{M}^{(\epsilon_r)}(\mathbf{p},t-z)u_r(\mathbf{p}), \mathbf{M}^{(\epsilon_{r'})}(\mathbf{p}',t-z)u_{r'}(\mathbf{p}')\rangle \mathrm{d}^3p\, \mathrm{d}^3p' \\
&= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \overline{\phi_r(\mathbf{p})}\phi_{r'}(\mathbf{p}')\exp[i(\epsilon_r\kappa(\mathbf{p}) - \epsilon_{r'}\kappa(\mathbf{p}'))t] \\
&\quad \times \langle \mathbf{M}^{(\epsilon_r)}(\mathbf{p},t-z)u_r(\mathbf{p}), \mathbf{M}^{(\epsilon_{r'})}(\mathbf{p}',t-z)u_{r'}(\mathbf{p}')\rangle \\
&\quad \times \exp[i(\mathbf{q}_{t-z}^{(\epsilon_{r'})}(\mathbf{p}') - \mathbf{q}_{t-z}^{(\epsilon_r)}(\mathbf{p}))\cdot \mathbf{s}_t(\mathbf{r})]\mathrm{d}^3p\, \mathrm{d}^3p'.
\end{aligned}
$$

Note that the only x and y dependence is contained in the term $\mathbf{s}_t(\mathbf{r})$. This fact is intimately connected with the validity of the eigenvalue equations (14a) and (14b). We thus perform the integration over these two variables $\mathbf{r}_\perp \equiv (x,y)$ first and obtain

$$
\int_{\mathbb{R}^2} I_{r,r'}(\mathbf{r})\mathrm{d}^2r_\perp = \int_{\mathbb{R}^2}\left(\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \langle \tilde{\phi}_r(\mathbf{p}_\perp,z), \tilde{\phi}_{r'}(\mathbf{p}'_\perp,z)\rangle_{\mathbb{C}^4} e^{i(\epsilon_{r'}\mathbf{p}'_\perp - \epsilon_r\mathbf{p}_\perp)\cdot\mathbf{r}_\perp}\, \mathrm{d}^2p_\perp\, \mathrm{d}^2p'_\perp\right)\mathrm{d}^2r_\perp,
$$

where

$$
\begin{aligned}
\tilde{\phi}_r(\mathbf{p}_\perp,z) &:= \int_{\mathbb{R}} \phi_r(\mathbf{p})\psi_{\mathbf{p},r}(\mathbf{r},t)e^{-i\epsilon_r\mathbf{p}_\perp\cdot\mathbf{r}_\perp}\,\mathrm{d}p_z = \int_{\mathbb{R}} \phi_r(\mathbf{p})\mathbf{M}^{(\epsilon_r)}(\mathbf{p},t-z)u_r(\mathbf{p})e^{-i\epsilon_r\kappa(\mathbf{p})t} \\
&\quad \times \exp\left[i\frac{\epsilon_r}{2}\left(\frac{m^2+\pi_\perp(t-z,\epsilon_r\mathbf{p}_\perp)^2}{\kappa(\mathbf{p})} - \kappa(\mathbf{p})\right)(z-t)\right]\mathrm{d}p_z. \qquad \text{(A3)}
\end{aligned}
$$

Since $\phi_r \in \mathcal{C}_0^\infty(\mathbb{R}^3)$, we see that for every z,

$$
\tilde{\phi}_r(\cdot,z) \in \mathcal{C}_0^\infty(\mathbb{R}^2)^4 \subset L^2(\mathbb{R}^2)^4.
$$

Using Parseval's identity, we find

$$
\int_{\mathbb{R}^2} I_{r,r'}(\mathbf{r})\mathrm{d}^2r_\perp = (2\pi)^2\int_{\mathbb{R}^2} \langle \tilde{\phi}_r(\epsilon_r\mathbf{p}_\perp,z), \tilde{\phi}_{r'}(\epsilon_{r'}\mathbf{p}_\perp,z)\rangle_{\mathbb{C}^4}\,\mathrm{d}^2p_\perp. \qquad \text{(A4)}
$$

Moreover, with the method applied in the proof of Theorem 2, we can even show that

$$
\tilde{\phi}_r \in L^2(\mathbb{R}^3)^4.
$$

We may therefore interchange the order of integrations by Fubini's theorem

$$
\begin{aligned}
\|\mathcal{F}_t(\phi)\|^2_{L^2(\mathbb{R}^3)^4} &= \frac{1}{2\pi}\sum_{r,r'=1}^4 \int_{\mathbb{R}}\left(\int_{\mathbb{R}^2} \langle \tilde{\phi}_r(\epsilon_r\mathbf{p}_\perp,z), \tilde{\phi}_{r'}(\epsilon_{r'}\mathbf{p}_\perp,z)\rangle_{\mathbb{C}^4}\,\mathrm{d}^2p_\perp\right)\mathrm{d}z \\
&= \frac{1}{2\pi}\sum_{r,r'=1}^4 \int_{\mathbb{R}^2}\left(\int_{\mathbb{R}} \langle \tilde{\phi}_r(\epsilon_r\mathbf{p}_\perp,z), \tilde{\phi}_{r'}(\epsilon_{r'}\mathbf{p}_\perp,z)\rangle_{\mathbb{C}^4}\,\mathrm{d}z\right)\mathrm{d}^2p_\perp.
\end{aligned}
$$

The identity (A1)—i.e., the statement of the theorem—is true if for every $\mathbf{p}_\perp$,

$$
\begin{aligned}
\frac{1}{2\pi}\int_{\mathbb{R}} \langle \tilde{\phi}_r(\epsilon_r\mathbf{p}_\perp,z), \tilde{\phi}_{r'}(\epsilon_{r'}\mathbf{p}_\perp,z)\rangle_{\mathbb{C}^4}\,\mathrm{d}z &\equiv \frac{1}{2\pi}\langle \tilde{\phi}_r(\epsilon_r\mathbf{p}_\perp,\cdot), \tilde{\phi}_{r'}(\epsilon_{r'}\mathbf{p}_\perp,\cdot)\rangle_{L^2} \\
&= \delta_{r,r'}\int_{\mathbb{R}} |\phi_r(\epsilon_r\mathbf{p}_\perp,p_z)|^2\,\mathrm{d}p_z. \qquad \text{(A5)}
\end{aligned}
$$

For the rest of the proof, we shall fix $\mathbf{p}_\perp$ and verify (A5). In preparation for exploiting the symmetry (17) of the Volkov solutions, we set

$$\tilde{\boldsymbol{\pi}}^{(\pm)}(\lambda) := \boldsymbol{\pi}(\pm\mathbf{p}_\perp,\lambda) = \left(\pm\mathbf{p}_\perp, \frac{m^2+|\mathbf{p}_\perp|^2-\lambda^2}{2\lambda}\right) \tag{A6}$$

and find

$$\tilde{E}(\lambda) := E(\tilde{\boldsymbol{\pi}}^{(\pm)}(\lambda)) = \left(m^2+|\mathbf{p}_\perp|^2+\frac{(m^2+|\mathbf{p}_\perp|^2-\lambda^2)^2}{4\lambda^2}\right)^{1/2} = \frac{m^2+|\mathbf{p}_\perp|^2+\lambda^2}{2\lambda} \tag{A7}$$

for $\lambda>0$. In view of the equalities

$$\tilde{\boldsymbol{\pi}}^{(\pm)}(\kappa(\mathbf{p})) = (\pm\mathbf{p}_\perp, p_z) \tag{A8}$$

and

$$\kappa(\tilde{\boldsymbol{\pi}}^{(\pm)}(\lambda)) = \lambda, \quad \lambda>0, \tag{A9}$$

we may write

$$\tilde{\phi}_r(\epsilon_r\mathbf{p}_\perp,z) = \int_{\mathbb{R}} \phi_r(\tilde{\boldsymbol{\pi}}^{(\epsilon_r)}(\kappa(\mathbf{p})))\tilde{\psi}_{\kappa(\mathbf{p}),r}(z)\mathrm{d}p_z. \tag{A10}$$

Here,

$$\tilde{\psi}_{\lambda,r}(z) := \psi_{\tilde{\boldsymbol{\pi}}^{(\epsilon_r)}(\lambda),r}(\mathbf{r},t)e^{-i\mathbf{p}_\perp\cdot\mathbf{r}_\perp} = \left(\mathbf{1}+\frac{e\tilde{\not{A}}(t-z)}{2\epsilon_r\lambda}\right)\tilde{u}_r(\lambda)e^{-i\epsilon_r\lambda t}\exp[i\epsilon_r(z-t)\tilde{\nu}_{t-z}(\lambda)], \tag{A11}$$

where

$$\tilde{\nu}_\xi(\lambda) := \frac{1}{2}\left(\frac{m^2+\pi_\perp(\xi,\mathbf{p}_\perp)^2}{\lambda}-\lambda\right) \tag{A12}$$

is the third component of $\boldsymbol{\nu}_\xi$ defined in (24). Furthermore,

$$\tilde{u}_r(\lambda) := u_r(\tilde{\boldsymbol{\pi}}^{(\epsilon_r)}(\lambda)), \tag{A13}$$

or, more explicitly,

$$\tilde{u}_r(\lambda) = \sqrt{\frac{\tilde{E}(\lambda)+m}{2\tilde{E}(\lambda)}}\left(\mathbf{1}+\frac{\boldsymbol{\alpha}\cdot\tilde{\boldsymbol{\pi}}^{(\epsilon_r)}(\lambda)}{\tilde{E}(\lambda)+m}\right)_r, \tag{A14}$$

where the index r on the right-hand side denotes the rth column of the enclosed matrix.

The functions $\tilde{\psi}_{\lambda,r}$ fulfill an eigenvalue equation closely related to (17),

$$\Xi\tilde{\psi}_{\lambda,r}(z) = \epsilon_r\lambda\tilde{\psi}_{\lambda,r}(z), \tag{A15}$$

where

$$\Xi := \alpha_x p_x+\alpha_y p_y - i\alpha_z\partial_z - e\boldsymbol{\alpha}\tilde{\mathbf{A}}(t-z)+\beta m + i\partial_z = i(\mathbf{1}-\alpha_z)\partial_z+\alpha_x p_x+\alpha_y p_y - e\boldsymbol{\alpha}\tilde{\mathbf{A}}(t-z)+\beta m \tag{A16}$$

is a formally self-adjoint ordinary differential operator. The validity of (A15) is shown easily. From (A11) we infer that

$$\psi_{\tilde{\boldsymbol{\tau}}^{(\epsilon_r)}(\lambda),r}(\mathbf{r},t) = e^{i\mathbf{p}_\perp\cdot\mathbf{r}_\perp}\tilde{\psi}_{\lambda,r}(z),$$

so that by (17),

$$(H(t)+i\partial_z)(e^{i\mathbf{p}_\perp\cdot\mathbf{r}_\perp}\tilde{\psi}_{\lambda,r}(z)) = \epsilon_r\kappa(\tilde{\boldsymbol{\tau}}^{(\epsilon_r)}(\lambda))\psi_{\tilde{\boldsymbol{\tau}}^{(\epsilon_r)}(\lambda),r}(\mathbf{r},t) = \epsilon_r\lambda e^{i\mathbf{p}_\perp\cdot\mathbf{r}_\perp}\tilde{\psi}_{\lambda,r}(z).$$

Since

$$(-i\alpha_x\partial_x - i\alpha_y\partial_y)(e^{i\mathbf{p}_\perp\cdot\mathbf{r}_\perp}\tilde{\psi}_{\lambda,r}(z)) = (\alpha_x p_x + \alpha_y p_y)(e^{i\mathbf{p}_\perp\cdot\mathbf{r}_\perp}\tilde{\psi}_{\lambda,r}(z)),$$

equation (A15) follows immediately.

Performing the substitution

$$\sigma: p_z \mapsto \kappa(\mathbf{p}) \equiv \lambda,$$

we are led to

$$\tilde{\phi}_r(\epsilon_r\mathbf{p}_\perp,z) = \frac{1}{2}\int_0^\infty \phi_r(\tilde{\boldsymbol{\tau}}^{(\epsilon_r)}(\lambda))\tilde{\psi}_{\lambda,r}(z)\left(\frac{m^2+|\mathbf{p}_\perp|^2}{\lambda^2}+1\right)\mathrm{d}\lambda, \tag{A17}$$

where we have used

$$\frac{d}{\mathrm{d}\lambda}\sigma^{-1}(\lambda) = \frac{d}{\mathrm{d}\lambda}\frac{m^2+|\mathbf{p}_\perp|^2-\lambda^2}{2\lambda} = -\frac{1}{2}\left(\frac{m^2+|\mathbf{p}_\perp|^2}{\lambda^2}+1\right).$$

An attempt to prove (A5) with $\tilde{\phi}_r$ from (A17) directly by interchanging the orders of integration fails because the assumptions of Fubini's theorem are not fulfilled. In order to apply the theorem, the term $\tilde{\psi}_{\lambda,r}(z)$ would have to decay for large values of $|z|$. As we shall see, we can avoid this problem by constructing an analytic continuation of (A11) to values $\lambda\in\mathbb{C}$ with $\mathrm{Re}\,\lambda>0$, and then in a limiting procedure, the desired result will follow. For this purpose we need to examine the Dirac spinor $\tilde{u}_r$ because its definition (A14) might produce a singularity and a branch cut at certain values of λ. However, for $\lambda\in\mathbb{C}\backslash\{0\}$,

$$\mathrm{Re}\,\tilde{E}(\lambda) = \left(\frac{m^2+|\mathbf{p}_\perp|^2}{2|\lambda|^2}+\frac{1}{2}\right)\mathrm{Re}\,\lambda.$$

So whenever $\mathrm{Re}\,\lambda>0$, we also have $\mathrm{Re}\,\tilde{E}(\lambda)>0$ and

$$\mathrm{Re}\,\frac{\tilde{E}(\lambda)+m}{2\tilde{E}(\lambda)} > 0.$$

Consequently, we may extend the definition (A14) also to complex arguments λ with $\mathrm{Re}\,\lambda>0$ if we choose the branch cut of the square root to lie on the negative real axis. Observing that both sides of (A15) are analytic with respect to λ and identical for real λ, we deduce the validity of this equation for *all* complex λ with $\mathrm{Re}\,\lambda>0$.

Next inspect the function $\tilde{\nu}_\xi$ for complex arguments $\mu=\lambda+i\delta$ with $\lambda>0$ and $\delta\in\mathbb{R}$,

$$\tilde{\nu}_\xi(\lambda+i\delta) = \frac{\lambda}{2}\left(\frac{m^2+\pi_\perp(\xi,\mathbf{p}_\perp)^2}{\lambda^2+\delta^2}-1\right) - \frac{i\delta}{2}\left(\frac{m^2+\pi_\perp(\xi,\mathbf{p}_\perp)^2}{\lambda^2+\delta^2}+1\right),$$

so that we obtain for the exponential in (A11),

$$|\exp[i\epsilon_r(z-t)\tilde{\nu}_{t-z}(\lambda+i\delta)]| = \exp[-\epsilon_r(z-t)\mathrm{Im}\,\tilde{\nu}_{t-z}(\lambda+i\delta)]$$
$$= \exp\left[\epsilon_r(z-t)\frac{\delta}{2}\left(\frac{m^2+\pi_\perp(t-z,\mathbf{p}_\perp)^2}{\lambda^2+\delta^2}+1\right)\right].$$

In addition,

$$\frac{\partial}{\partial\lambda}\tilde{\nu}_\xi(\lambda+i\delta) = \tilde{\nu}'_\xi(\lambda+i\delta) = -\frac{1}{2}\left(\frac{m^2+\pi_\perp(\xi,\mathbf{p}_\perp)^2}{(\lambda+i\delta)^2}+1\right),$$

for which we find

$$|\tilde{\nu}'_\xi(\lambda+i\delta)| = \frac{|m^2+\pi_\perp(\xi,\mathbf{p}_\perp)^2+(\lambda+i\delta)^2|}{2|\lambda+i\delta|^2} = \frac{\sqrt{[m^2+\pi_\perp(\xi,\mathbf{p}_\perp)^2+\lambda^2-\delta^2]^2+4\lambda^2\delta^2}}{2(\lambda^2+\delta^2)} \neq 0, \quad \lambda>0.$$

So for $\lambda>0$,

$$(z-t)\tilde{\psi}_{\lambda+i\delta,r}(z) = \left(\mathbf{1}+\frac{e\not{\tilde{A}}(t-z)}{2\epsilon_r(\lambda+i\delta)}\right)\tilde{u}_r(\lambda+i\delta)e^{-i\epsilon_r(\lambda+i\delta)t}$$
$$\times\frac{-i\epsilon_r}{\tilde{\nu}'_{t-z}(\lambda+i\delta)}\frac{\partial}{\partial\lambda}\exp[i\epsilon_r(z-t)\tilde{\nu}_{t-z}(\lambda+i\delta)]. \tag{A18}$$

Now define

$$\hat{\phi}_{r,\delta}(z) := \frac{1}{2}\int_0^\infty \phi_r(\tilde{\tau}^{(\epsilon_r)}(\lambda))\tilde{\psi}_{\lambda-i\delta\cdot\mathrm{sgn}[\epsilon_r(z-t)],r}(z)\left(\frac{m^2+|\mathbf{p}_\perp|^2}{\lambda^2}+1\right)\mathrm{d}\lambda \tag{A19}$$

for $\delta\geqslant 0$. This integral exists because the integrand is continuous and $\phi_r\circ\tilde{\tau}^{(\epsilon_r)}$ is compactly supported in $(0,\infty)$. Comparing with (A17), we recognize that for $\delta=0$,

$$\hat{\phi}_{r,0} = \tilde{\phi}_r(\epsilon_r\mathbf{p},\cdot).$$

The sign of the imaginary part in (A19) was chosen such that for $\delta>0$, we observe exponential decay with z,

$$\|\tilde{\psi}_{\lambda-i\delta\cdot\mathrm{sgn}[\epsilon_r(z-t)],r}(z)\| \leqslant \left(\mathbf{1}+\frac{|e|}{2|\lambda-i\delta\cdot\mathrm{sgn}[\epsilon_r(z-t)]|}\|\not{\tilde{A}}(t-z)\|\right)$$
$$\times\|\tilde{u}_r(\lambda-i\delta\cdot\mathrm{sgn}[\epsilon_r(z-t)]\|e^{-\epsilon_r\delta\cdot\mathrm{sgn}[\epsilon_r(z-t)]t}$$
$$\times\exp\left[-\epsilon_r|z-t|\frac{\delta}{2}\left(\frac{m^2+\pi_\perp(t-z,\mathbf{p}_\perp)^2}{\lambda^2+\delta^2}+1\right)\right], \tag{A20}$$

where (A18) was used. From this we obtain that

$$(z\mapsto\tilde{\psi}_{\lambda-i\delta\cdot\mathrm{sgn}[\epsilon_r(z-t)],r}(z))\in L^2(\mathbb{R})^4, \quad \delta>0.$$

This enables us to inspect the decay properties of $\hat{\phi}_{r,\delta}$ for $|z-t|\to\infty$. We first see that

$$\|\hat{\phi}_{r,\delta}(z)\|\leqslant C_0(\phi), \quad \delta\in[0,1],$$

for a constant $C_0(\phi)$. This is clear since the integrand in (A19) is continuous with respect to δ as well as λ and again since $\phi_r\circ\tilde{\tau}^{(\epsilon_r)}$ has compact support. Furthermore, application of (A18) gives

$$(z-t)\hat{\phi}_{r,\delta}(z) = \frac{1}{2}\int_0^\infty \phi_r(\tilde{\boldsymbol{\tau}}^{(\epsilon_r)}(\lambda))\left(\frac{m^2+|\mathbf{p}_\perp|^2}{\lambda^2}+1\right)\left(\mathbf{1}+\frac{e\tilde{\not{A}}(t-z)}{2\epsilon_r(\lambda-i\delta\cdot\mathrm{sgn}[\epsilon_r(z-t)])}\right)$$
$$\times \tilde{u}_r(\lambda-i\delta\cdot\mathrm{sgn}[\epsilon_r(z-t)])\exp[-i\epsilon_r\lambda t]\exp\{-\epsilon_r\delta\cdot\mathrm{sgn}[\epsilon_r(z-t)]t\}$$
$$\frac{\times -i\epsilon_r}{\tilde{\nu}'_{t-z}(\lambda+i\delta)}\frac{\partial}{\partial\lambda}\exp[i\epsilon_r(z-t)\tilde{\nu}_{t-z}(\lambda-i\delta\cdot\mathrm{sgn}[\epsilon_r(z-t)])]\mathrm{d}\lambda.$$

Performing an integration by parts, we notice that also

$$|z-t|\|\hat{\phi}_{r,\delta}(z)\| \leqslant C_1(\phi), \quad \delta\in[0,1].$$

Concludingly,

$$\|\hat{\phi}_{r,\delta}(z)\| \leqslant \frac{C_0(\phi)+C_1(\phi)}{1+|z-t|} \equiv \frac{C(\phi)}{1+|z-t|}, \quad \delta\in[0,1], \tag{A21}$$

so that the functions $\hat{\phi}_{r,\delta}$, $\delta\in[0,1]$, are uniformly bounded in L^2. In addition, we easily see by dominated convergence that

$$\forall z\in\mathbb{R}: \hat{\phi}_{r,\delta}(z)\to\hat{\phi}_{r,0}(z)=\tilde{\phi}_r(\epsilon_r\mathbf{p}_\perp,z), \quad \delta\to 0^+.$$

Therefore,

$$\hat{\phi}_{r,\delta}\to\tilde{\phi}_r(\epsilon_r\mathbf{p}_\perp,\cdot), \quad \delta\to 0^+, \quad \text{in } L^2. \tag{A22}$$

The above considerations lead us to

$$\langle\tilde{\phi}_r(\epsilon_r\mathbf{p}_\perp,\cdot),\tilde{\phi}_{r'}(\epsilon_{r'}\mathbf{p}_\perp,\cdot)\rangle_{L^2} = \lim_{\delta\to 0^+}\langle\hat{\phi}_{r,\delta},\hat{\phi}_{r',\delta}\rangle_{L^2}, \tag{A23}$$

which necessitates the evaluation of the right-hand side for $\delta>0$. Due to the decay property (A20) that is fulfilled for positive δ, we may now invoke Fubini's theorem,

$$\langle\hat{\phi}_{r,\delta},\hat{\phi}_{r',\delta}\rangle_{L^2} = \frac{1}{4}\int_{\mathbb{R}}\int_{\mathbb{R}}\overline{\phi_r(\tilde{\boldsymbol{\tau}}^{(\epsilon_r)}(\lambda))}\phi_{r'}(\tilde{\boldsymbol{\tau}}^{(\epsilon_{r'})}(\lambda'))\times\left(\frac{m^2+|\mathbf{p}_\perp|^2}{\lambda^2}+1\right)\left(\frac{m^2+|\mathbf{p}_\perp|^2}{\lambda'^2}+1\right)$$
$$\times J_{r,r',\delta}(\lambda,\lambda')\mathrm{d}\lambda\mathrm{d}\lambda', \tag{A24}$$

where

$$J_{r,r',\delta}(\lambda,\lambda') := \int_{\mathbb{R}}\langle\tilde{\psi}_{\lambda-i\delta\cdot\mathrm{sgn}[\epsilon_r(z-t)],r}(z),\tilde{\psi}_{\lambda'-i\delta\cdot\mathrm{sgn}[\epsilon_{r'}(z-t)],r'}(z)\rangle\mathrm{d}z$$
$$= \int_{-\infty}^t\langle\tilde{\psi}_{\lambda+i\epsilon_r\delta,r}(z),\tilde{\psi}_{\lambda'+i\epsilon_{r'}\delta,r'}(z)\rangle\mathrm{d}z + \int_t^\infty\langle\tilde{\psi}_{\lambda-i\epsilon_r\delta,r}(z),\tilde{\psi}_{\lambda'-i\epsilon_{r'}\delta,r'}(z)\rangle\mathrm{d}z$$
$$\equiv J^{(-)}_{r,r',\delta}(\lambda,\lambda')+J^{(+)}_{r,r',\delta}(\lambda,\lambda'). \tag{A25}$$

These integrals can be evaluated by employing the eigenvalue equation (A15) as follows:

$$\int_{-\infty}^t\langle\tilde{\psi}_{\lambda+i\epsilon_r\delta,r}(z),\Xi\tilde{\psi}_{\lambda'+i\epsilon_{r'}\delta,r'}(z)\rangle\mathrm{d}z = \epsilon_{r'}(\lambda'+i\epsilon_{r'}\delta)J^{(-)}_{r,r',\delta}(\lambda,\lambda') = (\epsilon_{r'}\lambda'+i\delta)J^{(-)}_{r,r',\delta}(\lambda,\lambda')$$

and

$$\int_{-\infty}^{t} \langle \Xi \tilde{\psi}_{\lambda+i\epsilon_r\delta,r}(z), \tilde{\psi}_{\lambda'+i\epsilon_{r'}\delta,r'}(z)\rangle = \overline{\epsilon_r(\lambda+i\epsilon_r\delta)} J^{(-)}_{r,r',\delta}(\lambda,\lambda') = (\epsilon_r\lambda - i\delta) J^{(-)}_{r,r',\delta}(\lambda,\lambda').$$

Remembering the formal self-adjointness of Ξ and performing an integration by parts, we see that

$$\begin{aligned}
&\int_{-\infty}^{t} \langle \tilde{\psi}_{\lambda+i\epsilon_r\delta,r}(z), \Xi \tilde{\psi}_{\lambda'+i\epsilon_{r'}\delta,r'}(z)\rangle \mathrm{d}z - \int_{-\infty}^{t} \langle \Xi \tilde{\psi}_{\lambda+i\epsilon_r\delta,r}(z), \tilde{\psi}_{\lambda'+i\epsilon_{r'}\delta,r'}(z)\rangle \mathrm{d}z \\
&\quad = \int_{-\infty}^{t} \langle \tilde{\psi}_{\lambda+i\epsilon_r\delta,r}(z), i(\mathbf{1}-\alpha_z)\partial_z \tilde{\psi}_{\lambda'+i\epsilon_{r'}\delta,r'}(z)\rangle \mathrm{d}z - \int_{-\infty}^{t} \langle i(\mathbf{1}-\alpha_z)\partial_z \tilde{\psi}_{\lambda+i\epsilon_r\delta,r}(z), \tilde{\psi}_{\lambda'+i\epsilon_{r'}\delta,r'}(z)\rangle \mathrm{d}z \\
&\quad = i\langle \tilde{\psi}_{\lambda+i\epsilon_r\delta,r}(t), (\mathbf{1}-\alpha_z)\tilde{\psi}_{\lambda'+i\epsilon_{r'}\delta,r'}(t)\rangle.
\end{aligned}$$

From the last three equations we derive that

$$J^{(-)}_{r,r',\delta}(\lambda,\lambda') = \frac{i}{\epsilon_{r'}\lambda' - \epsilon_r\lambda + 2i\delta} \langle \tilde{\psi}_{\lambda+i\epsilon_r\delta,r}(t), (\mathbf{1}-\alpha_z)\tilde{\psi}_{\lambda'+i\epsilon_{r'}\delta,r'}(t)\rangle.$$

In a similar way, one may show that

$$J^{(+)}_{r,r',\delta}(\lambda,\lambda') = -\frac{i}{\epsilon_{r'}\lambda' - \epsilon_r\lambda - 2i\delta} \langle \tilde{\psi}_{\lambda+i\epsilon_r\delta,r}(t), (\mathbf{1}-\alpha_z)\tilde{\psi}_{\lambda'+i\epsilon_{r'}\delta,r'}(t)\rangle,$$

so that

$$\begin{aligned}
J_{r,r',\delta}(\lambda,\lambda') &= \left(\frac{i}{\epsilon_{r'}\lambda' - \epsilon_r\lambda + 2i\delta} - \frac{i}{\epsilon_{r'}\lambda' - \epsilon_r\lambda - 2i\delta} \right) \langle \tilde{\psi}_{\lambda+i\epsilon_r\delta,r}(t), (\mathbf{1}-\alpha_z)\tilde{\psi}_{\lambda'+i\epsilon_{r'}\delta,r'}(t)\rangle \\
&= \frac{4\delta}{(\epsilon_r\lambda - \epsilon_{r'}\lambda')^2 + 4\delta^2} \langle \tilde{\psi}_{\lambda+i\epsilon_r\delta,r}(t), (\mathbf{1}-\alpha_z)\tilde{\psi}_{\lambda'+i\epsilon_{r'}\delta,r'}(t)\rangle. \qquad \text{(A26)}
\end{aligned}$$

This leads to

$$\begin{aligned}
\langle \hat{\phi}_{r,\delta}, \hat{\phi}_{r',\delta}\rangle_{L^2} = \frac{\pi}{2}\int_0^\infty \int_0^\infty \eta_\delta(\epsilon_r\lambda - \epsilon_{r'}\lambda') \overline{\phi_r(\tilde{\boldsymbol{\tau}}^{(\epsilon_r)}(\lambda))} \phi_{r'}(\tilde{\boldsymbol{\tau}}^{(\epsilon_{r'})}(\lambda')) \left(\frac{m^2+|\mathbf{p}_\perp|^2}{\lambda^2} + 1 \right) \\
\times \left(\frac{m^2+|\mathbf{p}_\perp|^2}{\lambda'^2} + 1 \right) \times \langle \tilde{\psi}_{\lambda+i\epsilon_r\delta,r}(t), (\mathbf{1}-\alpha_z)\tilde{\psi}_{\lambda'+i\epsilon_{r'}\delta,r'}(t)\rangle \mathrm{d}\lambda\, \mathrm{d}\lambda' \qquad \text{(A27)}
\end{aligned}$$

with

$$\eta_\delta(x) := \frac{2}{\pi}\frac{\delta}{x^2+4\delta^2}. \qquad \text{(A28)}$$

The integral in (A27) is of the form

$$\langle \hat{\phi}_{r,\delta}, \hat{\phi}_{r',\delta}\rangle_{L^2} = \frac{\pi}{2}\int_0^\infty \int_0^\infty \eta_\delta(\epsilon_r\lambda - \epsilon_{r'}\lambda') f(\delta,\lambda,\lambda')\mathrm{d}\lambda\, \mathrm{d}\lambda'$$

with a function f depending continuously on δ, λ, and λ'. The restriction $f|_{[0,1]\times[0,\infty)\times[0,\infty)}$ has compact support in $[0,1]\times(0,\infty)\times(0,\infty)$. The trivial extension to $[0,1]\times\mathbb{R}^2$, i.e.,

$$\tilde{f}(\delta,\lambda,\lambda') := \begin{cases} f(\delta,\lambda,\lambda'), & \lambda,\lambda' > 0, \\ 0, & \text{otherwise}, \end{cases} \qquad \text{(A29)}$$

is therefore continuous, and we may write

$$\langle \hat{\phi}_{r,\delta}, \hat{\phi}_{r',\delta} \rangle_{L^2} = \frac{\pi}{2} \int_{\mathbb{R}} \int_{\mathbb{R}} \eta_\delta(\epsilon_r \lambda - \epsilon_{r'} \lambda') \tilde{f}(\delta, \lambda, \lambda') \mathrm{d}\lambda \, \mathrm{d}\lambda'$$

$$= \frac{\pi}{2} \int_{\mathbb{R}} \int_{\mathbb{R}} \eta_\delta(\lambda - \lambda') \tilde{f}(\delta, \epsilon_r \lambda, \epsilon_{r'} \lambda') \mathrm{d}\lambda \, \mathrm{d}\lambda'. \tag{A30}$$

We are required to determine the limit of (A27) for $\delta \to 0^+$, see (A23). This can be accomplished with the help of Lemma 9 below. The result is

$$\lim_{\delta \to 0^+} \langle \hat{\phi}_{r,\delta}, \hat{\phi}_{r',\delta} \rangle_{L^2} = \frac{\pi}{2} \int_{\mathbb{R}} \tilde{f}(0, \epsilon_r \lambda, \epsilon_{r'} \lambda) \mathrm{d}\lambda. \tag{A31}$$

Owing to (A23) and (A29), we have

$$\langle \tilde{\phi}_r(\epsilon_r \mathbf{p}_\perp, \cdot), \tilde{\phi}_{r'}(\epsilon_{r'} \mathbf{p}_\perp, \cdot) \rangle_{L^2} = \lim_{\delta \to 0^+} \langle \hat{\phi}_{r,\delta}, \hat{\phi}_{r',\delta} \rangle_{L^2} = 0 \tag{A32}$$

for $\epsilon_r \neq \epsilon_{r'}$, which validates (A5) in this case.

Now assume $\epsilon_r = \epsilon_{r'} =: \epsilon$. Then again by (A23) and Lemma 9,

$$\langle \tilde{\phi}_r(\epsilon_r \mathbf{p}_\perp, \cdot), \tilde{\phi}_{r'}(\epsilon_{r'} \mathbf{p}_\perp, \cdot) \rangle_{L^2} = \frac{\pi}{2} \int_0^\infty \overline{\phi_r(\tilde{\boldsymbol{\tau}}^{(\epsilon)}(\lambda))} \phi_{r'}(\tilde{\boldsymbol{\tau}}^{(\epsilon)}(\lambda)) \left(\frac{m^2 + |\mathbf{p}_\perp|^2}{\lambda^2} + 1 \right)^2$$

$$\times \langle \tilde{\psi}_{\lambda,r}(t), (\mathbf{1} - \alpha_z) \tilde{\psi}_{\lambda,r'}(t) \rangle \mathrm{d}\lambda$$

$$= \pi \int_{\mathbb{R}} \overline{\phi_r(\tilde{\boldsymbol{\tau}}^{(\epsilon)}(\kappa(\mathbf{p})))} \phi_{r'}(\tilde{\boldsymbol{\tau}}^{(\epsilon)}(\kappa(\mathbf{p}))) \left(\frac{m^2 + |\mathbf{p}_\perp|^2}{\kappa(\mathbf{p})^2} + 1 \right)$$

$$\times \langle \tilde{\psi}_{\kappa(\mathbf{p}),r}(t), (\mathbf{1} - \alpha_z) \tilde{\psi}_{\kappa(\mathbf{p}),r'}(t) \rangle \mathrm{d}p_z, \tag{A33}$$

where we have substituted back from λ to p_z. By virtue of the identities

$$\mathbf{1} - \alpha_z = \gamma^0(\gamma^0 - \gamma^3) = \gamma^0 \not{n},$$

which is a Hermitian matrix, and

$$\not{n}^2 = n^2 = 0,$$

we find

$$\langle \tilde{\psi}_{\lambda,r}(t), (\mathbf{1} - \alpha_z) \tilde{\psi}_{\lambda,r'}(t) \rangle = \left\langle \left(\mathbf{1} + \frac{e \not{n} \tilde{\not{A}}(t)}{2\epsilon\lambda} \right) \tilde{u}_r(\lambda), \gamma^0 \not{n} \left(\mathbf{1} + \frac{e \not{n} \tilde{\not{A}}(t)}{2\epsilon\lambda} \right) \tilde{u}_{r'}(\lambda) \right\rangle$$

$$= \left\langle \left(\mathbf{1} + \frac{e \not{n} \tilde{\not{A}}(t)}{2\epsilon\lambda} \right) \tilde{u}_r(\lambda), \gamma^0 \not{n} \tilde{u}_{r'}(\lambda) \right\rangle$$

$$= \left\langle \gamma^0 \not{n} \left(\mathbf{1} + \frac{e \not{n} \tilde{\not{A}}(t)}{2\epsilon\lambda} \right) \tilde{u}_r(\lambda), \tilde{u}_{r'}(\lambda) \right\rangle$$

$$= \langle \gamma^0 \not{n} \tilde{u}_r(\lambda), \tilde{u}_{r'}(\lambda) \rangle = \langle \tilde{u}_r(\lambda), \gamma^0 \not{n} \tilde{u}_{r'}(\lambda) \rangle = \langle u_r(\tilde{\boldsymbol{\tau}}^{(\epsilon)}(\lambda)), \gamma^0 \not{n} u_{r'}(\tilde{\boldsymbol{\tau}}^{(\epsilon)}(\lambda)) \rangle. \tag{A34}$$

In order to evaluate this scalar product, fix λ and set $\mathbf{p} := \tilde{\boldsymbol{\tau}}^{(\epsilon)}(\lambda)$. We will make use of the 4×4 matrices[18]

$$\Lambda_{\pm}(\mathbf{p}) := \frac{\pm \not{p} + m}{2m} \equiv \frac{\pm(\gamma^0 E(\mathbf{p}) - \gamma^1 p_x - \gamma^2 p_y - \gamma^3 p_z) + m}{2m}, \tag{A35}$$

which obey

$$\Lambda_{\epsilon_r}(\mathbf{p}) u_r(\mathbf{p}) = u_r(\mathbf{p}), \tag{A36}$$

and the fact that for any four-vector a,

$$\not{a}^\dagger = \gamma^0 \not{a} \gamma^0.$$

This gives

$$\begin{aligned}\langle \tilde{\psi}_{\lambda,r}(t), (\mathbf{1} - \alpha_z)\tilde{\psi}_{\lambda,r'}(t)\rangle &= \langle \Lambda_\epsilon(\mathbf{p}) u_r(\mathbf{p}), \gamma^0 \not{n} \Lambda_\epsilon(\mathbf{p}) u_{r'}(\mathbf{p})\rangle \\ &= \langle u_r(\mathbf{p}), \gamma^0 \Lambda_\epsilon(\mathbf{p}) \not{n} \Lambda_\epsilon(\mathbf{p}) u_{r'}(\mathbf{p})\rangle = \langle u_r(\mathbf{p}), \gamma^0 M u_{r'}(\mathbf{p})\rangle \end{aligned} \tag{A37}$$

with the 4×4 matrix

$$M := \Lambda_\epsilon(\mathbf{p}) \not{n} \Lambda_\epsilon(\mathbf{p}) = \frac{\epsilon \not{p} + m}{2m} \not{n} \frac{\epsilon \not{p} + m}{2m} = \frac{1}{4m^2}[\not{p} \not{n} \not{p} + \epsilon m(\not{p} \not{n} + \not{n} \not{p}) + m^2 \not{n}]. \tag{A38}$$

Using

$$\not{a} \not{b} + \not{b} \not{a} = 2(ab)\mathbf{1},$$

which is valid for any four-vectors a and b of real numbers, and

$$\not{p}^2 = p^2 = m^2,$$

we continue

$$M = \frac{1}{4m^2}[2(np)\not{p} - m^2 \not{n} + 2\epsilon m(np) + m^2 \not{n}] = \frac{\epsilon(np)}{m} \Lambda_\epsilon(\mathbf{p}) = \frac{\epsilon \kappa(\mathbf{p})}{m} \Lambda_\epsilon(\mathbf{p}).$$

Hence,

$$\langle \tilde{\psi}_{\lambda,r}(t), (\mathbf{1} - \alpha_z)\tilde{\psi}_{\lambda,r'}(t)\rangle = \frac{\epsilon \kappa(\mathbf{p})}{m} \langle u_r(\mathbf{p}), \gamma^0 \Lambda_\epsilon(\mathbf{p}) u_{r'}(\mathbf{p})\rangle = \frac{\epsilon \kappa(\mathbf{p})}{m} \langle u_r(\mathbf{p}), \gamma^0 u_{r'}(\mathbf{p})\rangle = \delta_{r,r'} \frac{\kappa(\mathbf{p})}{E(\mathbf{p})}, \tag{A39}$$

where

$$\langle u_r(\mathbf{p}), \gamma^0 u_{r'}(\mathbf{p})\rangle \equiv u_r(\mathbf{p})^\dagger \gamma^0 u_{r'}(\mathbf{p}) = \epsilon_r \delta_{r,r'} \frac{m}{E(\mathbf{p})}$$

was exploited.[18] Therefore, we obtain from (A33),

$$\begin{aligned}\langle \tilde{\phi}_r(\epsilon_r \mathbf{p}_\perp, \cdot), \tilde{\phi}_{r'}(\epsilon_{r'} \mathbf{p}_\perp, \cdot)\rangle_{L^2} &= \delta_{r,r'} \pi \int_{\mathbb{R}} \overline{\phi_r(\tilde{\boldsymbol{\tau}}^{(\epsilon)}(\kappa(\mathbf{p})))} \phi_{r'}(\tilde{\boldsymbol{\tau}}^{(\epsilon)}(\kappa(\mathbf{p}))) \left(\frac{m^2 + |\mathbf{p}_\perp|^2}{\kappa(\mathbf{p})^2} + 1 \right) \frac{\kappa(\mathbf{p})}{E(\mathbf{p})} \mathrm{d}p_z \\ &= 2\pi \delta_{r,r'} \int_{\mathbb{R}} \overline{\phi_r(\tilde{\boldsymbol{\tau}}^{(\epsilon)}(\kappa(\mathbf{p})))} \phi_{r'}(\tilde{\boldsymbol{\tau}}^{(\epsilon)}(\kappa(\mathbf{p}))) \mathrm{d}p_z \\ &= 2\pi \delta_{r,r'} \int_{\mathbb{R}} |\phi_r(\epsilon_r \mathbf{p}_\perp, p_z)|^2 \, \mathrm{d}p_z, \end{aligned} \tag{A40}$$

which confirms (A5) also in the case $\epsilon_r = \epsilon_{r'}$. This completes the proof. ■

We are left with showing the following.

Lemma 9: Let $f \in \mathcal{C}_0([0,1]\times\mathbb{R}^2,\mathbb{C})$. *Then*

$$I_\delta := \int_{\mathbb{R}^2} \eta_\delta(x-x')f(\delta,x,x')\mathrm{d}x\,\mathrm{d}x' \to \int_{\mathbb{R}} f(0,x,x)\mathrm{d}x, \quad \delta\to 0^+, \tag{A41}$$

with η_δ *from* (A28).

Proof: We first collect some properties of the functions η_δ,

$$\forall\,\delta>0, \quad x\in\mathbb{R}: \eta_\delta(x)>0, \tag{A42}$$

$$\forall\,\delta>0: \int_{\mathbb{R}} \eta_\delta(x)\mathrm{d}x = 1,$$

and

$$\forall\,\gamma>0: \int_{\mathbb{R}\setminus[-\gamma,\gamma]} \eta_\delta(x)\mathrm{d}x \to 0, \quad \delta\to 0^+. \tag{A43}$$

Set

$$g(\delta,x) := \int_{\mathbb{R}} \eta_\delta(x-x')f(\delta,x,x')\mathrm{d}x' \tag{A44}$$

for $\delta>0$, so that

$$I_\delta = \int_{\mathbb{R}} g(\delta,x)\mathrm{d}x. \tag{A45}$$

The compactness of supp f implies the existence of a compact interval $[a,b]$ such that

$$g(\delta,x)=0 \text{ for } \delta>0, \quad x\notin[a,b].$$

Therefore,

$$I_\delta = \int_a^b g(\delta,x)\mathrm{d}x.$$

Note that

$$|g(\delta,x)| \leqslant \int_{\mathbb{R}} \eta_\delta(x-x')|f(\delta,x,x')|\mathrm{d}x' \leqslant \|f\|_\infty < \infty.$$

We claim that

$$\forall x\in[a,b]: \lim_{\delta\to 0^+} g(\delta,x) = f(0,x,x). \tag{A46}$$

The statement in the lemma follows then by dominated convergence.

In order to prove (A46), fix $x\in[a,b]$. For any $\gamma,\delta>0$, we estimate

$$|g(\delta,x)-f(0,x,x)| = \left| \int_{\mathbb{R}} \eta_\delta(x-x')[f(\delta,x,x')-f(0,x,x)]\mathrm{d}x' \right|$$
$$= \left| \int_{\mathbb{R}} \eta_\delta(y)[f(\delta,x,x-y)-f(0,x,x)]\mathrm{d}y \right|$$
$$\leqslant 2\|f\|_\infty \int_{\mathbb{R}\setminus[-\gamma,\gamma]} \eta_\delta(y)\mathrm{d}y + \sup_{r\in[-\gamma,\gamma]} |f(\delta,x,x+r)-f(0,x,x)|, \qquad \text{(A47)}$$

where (A42) was employed twice. Choose any $\epsilon>0$. Since f is continuous, we find $\gamma,\alpha>0$ such that

$$\sup_{r\in[-\gamma,\gamma]} |f(\delta,x,x+r)-f(0,x,x)| < \frac{\epsilon}{2} \quad \text{for } \delta\in(0,\alpha).$$

In view of (A43), we find $\beta\in(0,\alpha)$ with

$$2\|f\|_\infty \int_{\mathbb{R}\setminus[-\gamma,\gamma]} \eta_\delta(y)\mathrm{d}y < \frac{\epsilon}{2} \quad \text{for } \delta\in(0,\beta).$$

Therefore,

$$|g(\delta,x)-f(0,x,x)| < \epsilon \quad \text{for } \delta\in(0,\beta), \qquad \text{(A48)}$$

and the lemma is proved. ■

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Upper limit on the critical strength of central potentials in relativistic quantum mechanics

Fabian Brau[a)]
Groupe de Physique Nucléaire Théorique, Académie Universitaire Wallonie-Bruxelles, Université de Mons-Hainaut, B-7000 Mons, Belgium

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In the context of relativistic quantum mechanics, where the Schrödinger equation is replaced by the spinless Salpeter equation, we show how to construct a large class of upper limits on the critical value, $g_c^{(\ell)}$, of the coupling constant, g, of the central potential, $V(r)=-gv(r)$. This critical value is the value of g for which a first ℓ-wave bound state appears. © *2005 American Institute of Physics.*
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I. INTRODUCTION

A covariant description of bound states of two particles is achieved with the Bethe–Salpeter equation.[1] This equation reduces to the spinless Salpeter equation[2] when the following approximations are performed:

(i) elimination of any dependences on timelike variables (which leads to the Salpeter equation[3]),
(ii) any references to the spin degrees of freedom of particles are neglected as well as negative energy solutions.

The spinless Salpeter equation takes the form ($\hbar=c=1$)

$$[\sqrt{\mathbf{p}^2+m^2}+V(\mathbf{r})]\Psi(\mathbf{r})=M\Psi(\mathbf{r}), \tag{1}$$

where m is the mass of the particle and M is the mass of the eigenstate ($M=m+E$, E is the binding energy). We restrict our attention to interactions which are introduced in the free equation through the substitution $M\rightarrow M-V(\mathbf{r})$, where $V(\mathbf{r})$ is the time component of a relativistic four-vector. The interaction could also, in principle, be introduced through the substitution $\mathbf{p}\rightarrow\mathbf{p}-\mathbf{A}(\mathbf{r})$, where $\mathbf{A}(\mathbf{r})$ is the spatial component of a relativistic four-vector. However we do not consider this kind of potential since the derivation of the spinless Salpeter equation from the Bethe–Salpeter equation leads to $\mathbf{A}(\mathbf{r})=0$. Equation (1) is generally used when kinetic relativistic effects cannot be neglected and when the particles under consideration are bosons or when the spin of the particles is neglected or is only taken into account via spin-dependent interactions. Despite its apparent complexity, this equation is often preferred to the Klein–Gordon equation. Equation (1) appears, for example, in mesons and baryons spectroscopy in the context of potential models (see, for example, Refs. 4–8). [For a review of several aspects of the "semirelativistic" description of bound states with the spinless Salpeter equation see W. Lucha and F. F. Schöberl, Int. J. Mod. Phys. A **14**, 2309 (1999), and references therein.]

Due to the pseudodifferential nature of the kinetic energy operator, few exact results are known about this equation. Most of these results have been obtained for a Coulomb potential (for example, upper and lower bounds on energy levels).[9–13] Recently, upper and lower limits on energy levels have also been obtained for some other particular interactions.[14–17]

[a)]Electronic mail: fabian.brau@umh.ac.be

Conversely to the Schrödinger equation, for which a fairly large number of results giving both upper and lower limits on the number of bound states can be found in the literature (see, for example, Refs. 18–27), only two results are known for the spinless Salpeter equation.[28,29] The first result, obtained in Ref. 28, is an upper bound on the total number of bound states yielding a lower limit on the critical value, $g_c^{(0)}$, of the coupling constant (strength), g, for which a first S-wave ($\ell=0$) bound state appears (ℓ being obviously the angular momentum) in the potential $V(r)=-gv(r)$. The second results, obtained in Ref. 29, is an upper limit on the number of ℓ-wave bound states which yields a lower limit on the critical value, $g_c^{(\ell)}$ for which a first ℓ-wave bound state appears.

In this paper, we obtain accurate upper limits on the critical strength $g_c^{(\ell)}$ applicable to attractive (purely negative) central potentials which are less singular than $-r^{-1}$ at the origin. This limitation has a deep reason. Indeed, it is known that for the spinless Salpeter equation, a potential which behaves like $-r^{-1}$ at the origin is characterized by a maximal value of the coupling constant above which the spectrum is no longer bounded from below. This particularity has been studied in detail for the Coulomb potential (see, for example, Ref. 9). The $-r^{-1}$ singularity is a critical singularity for the spinless Salpeter equation just as the $-r^{-2}$ singularity is a critical singularity for the Schrödinger equation. So in this paper we discard this class of potentials which should be treated separately. Moreover we suppose that the central potential $V(r)$ is piecewise continuous for $r\in]0,\infty[$. The upper limits on $g_c^{(\ell)}$ we obtain in Sec. II are compared with the exact critical value obtained numerically for some test potentials. These comparisons indicate that the new upper limits are very restrictive. Some conclusions are presented in Sec. III.

II. UPPER LIMIT ON THE CRITICAL STRENGTH

The idea used to derive the upper limit on $g_c^{(\ell)}$ is to transform the standard eigenvalue problem obtained with the time independent spinless Salpeter equation (1), and where the eigenvalues are the eigenenergies, into an eigenvalue problem where the eigenvalues are the critical coupling constants. These critical values of the strength of the potential correspond to the occurrence of an eigenstate with a vanishing binding energy. We thus consider the zero binding energy spinless Salpeter equation that we need to write as an integral equation. This has been done in Ref. 29 but since we need some modifications in the development, we recall the main line here.

We must calculate the Green function of the kinetic energy operator. Similar calculations have also already been performed previously.[30,31] In contrast to results found in Ref. 31, we need here to calculate the Green functionof the following operator:

$$T(\mathbf{p}^2)=\sqrt{\mathbf{p}^2+m^2}-m. \tag{2}$$

This is done by performing the integral

$$G(m,\Delta)=\frac{1}{(2\pi)^3}\int \mathrm{d}\mathbf{p}\frac{\exp(-i\mathbf{p}\cdot\boldsymbol{\Delta})}{\sqrt{p^2+m^2}-m}, \tag{3}$$

where $\boldsymbol{\Delta}=\mathbf{r}-\mathbf{r}'$ and $\Delta=|\boldsymbol{\Delta}|$. We find that

$$G(m,\Delta)=\frac{m}{4\pi\Delta}\left[1+\frac{2}{\pi}F(m\Delta)\right]\equiv\frac{m}{4\pi\Delta}H(m\Delta), \tag{4a}$$

with

$$F(y)=\int_y^\infty\frac{\mathrm{d}z}{z}K_1(z)+\frac{\pi}{2}=K_1(y)+\frac{\pi}{2}-\int_y^\infty \mathrm{d}z\,K_0(z), \tag{4b}$$

and where $K_\nu(y)$ is a modified Bessel function (see, for example, Ref. 32, p. 374). The zero binding energy spinless Salpeter equation takes thus the form of the following integral equation:

$$\Psi(\mathbf{r}) = -\int \mathrm{d}\mathbf{r}'\, G(m,\Delta)V(\mathbf{r}')\Psi(\mathbf{r}'), \tag{5}$$

with $G(m,\Delta)$ given by (4). We now restrict our attention to central potentials $V(\mathbf{r})=V(r)$, with $r=|\mathbf{r}|$.

Integration over angular variables reduces the integral equation (5) to the following one-dimensional integral equation

$$u_\ell(r) = -\int_0^\infty \mathrm{d}r'\, G_\ell(m,r,r')V(r')u_\ell(r'), \tag{6a}$$

with

$$G_\ell(m,r,r') = \frac{mrr'}{2}\int_0^\pi \mathrm{d}\theta'\, \sin\theta' \frac{H(m\Delta)}{\Delta} P_\ell(\cos\theta'), \tag{6b}$$

where $u_\ell(r)$ is the radial wave function, $\Psi(\mathbf{r})=(u_\ell(r)/r)Y_{\ell m}(\hat{\mathbf{r}})$ and where $H(x)$ is defined by (4a).

An important technical difficulty, to obtain a symmetrical kernel, appears if the potential possesses some change of sign [see relation (7) below]. This is overcome when one searches for necessary conditions, or upper bound on the number of bound states, by replacing the potential by its negative part $V(r)\to V^-(r)=-\max(0,-V(r))$. Indeed, the potential $V^-(r)$ is more attractive than $V(r)$ and thus a necessary condition for existence of bound states in $V^-(r)$ is certainly a valid necessary condition for $V(r)$. This procedure can no longer be used to obtain sufficient conditions. For this reason we consider potentials that are nowhere positive, $V(r)=-gv(r)$, with $v(r)\geqslant 0$.

The integral equation (6) can be written with a symmetrical kernel provided we introduce a new wave function

$$\phi_\ell(r) = |V(r)|^{1/2}u_\ell(r). \tag{7}$$

This change of function leads to the following integral equation:

$$\phi_\ell(r) = g\int_0^\infty \mathrm{d}r' K_\ell(m,r,r')\phi_\ell(r'), \tag{8a}$$

with

$$K_\ell(m,r,r') = v(r)^{1/2}G_\ell(m,r,r')v(r')^{1/2}. \tag{8b}$$

The relation (8) is thus an eigenvalue problem and, for each value of ℓ, the smallest characteristic number is just the critical value $g_c^{(\ell)}$. The other characteristic numbers correspond to the critical values of the strength of the potential for which a second, a third,…, ℓ-wave bound state appears. The kernel (8b) acting on the Hilbert space $L^2(\mathbb{R})$ is an Hilbert–Schmidt operator for potentials which decrease faster than r^{-1} at infinity. Thus this kernel satisfies the inequality

$$\int_0^\infty \int_0^\infty \mathrm{d}x\, \mathrm{d}y\, K_\ell(x,y)K_\ell(x,y) < \infty. \tag{9}$$

Consequently the eigenvalue problem (8) always possesses at least one characteristic number (Ref. 33, pp. 102–106) (in general, this problem has an infinity of characteristic numbers).

Now we use the theorem (see, for example, Ref. 33, pp. 118–119) which states that, for a symmetric Hilbert–Schmidt kernel, we have the variational principle

$$\max_{\varphi}\left|\int_0^\infty \mathrm{d}x\,\mathrm{d}y\,K_\ell(x,y)\varphi(x)\varphi(y)\right| = \frac{1}{|g_1|}, \tag{10}$$

for $\varphi(r)$ satisfying

$$\int_0^\infty \mathrm{d}r\,\varphi(r)^2 = 1. \tag{11}$$

The maximal value is reached for $\varphi(x)=\varphi_1(x)$, where $\varphi_1(x)$ is the eigenfunction associated to the smallest eigenvalue g_1. Consequently, for an arbitrary normalized function, $f(x)$, we obtain the following upper limit on g_1:

$$|g_1| \leqslant \left|\int_0^\infty \mathrm{d}x\,\mathrm{d}y\,K_\ell(x,y)f(x)f(y)\right|^{-1}. \tag{12}$$

For the clarity of the discussion we now consider in two separate sections the ultrarelativistic regime ($m=0$) and the relativistic regime ($m>0$).

A. Ultrarelativistic regime $m=0$

In this section, we derive an (among others) upper limit on the critical value, $g_c^{(\ell)}$, of the coupling constant, g, of the potential, $V(r)=-gv(r)$, for which a first ℓ-wave bound state appears in the ultrarelativistic regime ($m=0$). In this limit, the kernel takes a simple form since $mK_1(my)=1/y$ when m goes to zero. This implies that

$$\lim_{m\to 0} mH(m\Delta) = \frac{2}{\pi\Delta}. \tag{13}$$

The function $G_\ell(0,r,r')$ takes then the form

$$G_\ell(0,r,r') = \frac{rr'}{\pi}\int_0^\pi \mathrm{d}\theta' \frac{\sin\theta'}{\Delta^2}P_\ell(\cos\theta'). \tag{14}$$

A simple change of variable leads to (Ref. 32, p. 335)

$$G_\ell(0,r,r') = \frac{1}{2\pi}\int_{-1}^{1}\mathrm{d}y\frac{P_\ell(y)}{(r^2+r'^2)/(2rr')-y} = \frac{1}{\pi}Q_\ell\left(\frac{r^2+r'^2}{2rr'}\right), \tag{15}$$

where the function $Q_\ell(x)$ is a Legendre function of the second kind. The function $G_\ell(0,r,r')$ can thus be evaluated explicitly for each value of the angular momentum ℓ. We have, for example,

$$G_0(0,r,r') = \frac{1}{\pi}\ln\left|\frac{r+r'}{r-r'}\right| \tag{16}$$

and

$$G_1(0,r,r') = \frac{1}{\pi}\left[\frac{r^2+r'^2}{2rr'}\ln\left|\frac{r+r'}{r-r'}\right| - 1\right]. \tag{17}$$

Since the function $G_\ell(0,r,r')$ is given by the relation (15), it follows that the kernel $K_\ell(0,r,r')$, see (8b), is known for each value of ℓ. Now, we just need to choose a suitable normalized function $f(r)$ to apply the variational principle reported above.

For simplicity we restrict the rest of the following discussion to $\ell=0$ but extensions to nonvanishing values of the angular momentum is obvious, one just needs to compute the corresponding expression of the function $G_\ell(0,r,r')$.

TABLE I. Comparison, for some typical potentials, between the exact critical values, $g_c^{(0)}$, the upper limits $g_{\mathrm{up},1}^{m=0}$ (19), $g_{\mathrm{up},2}^{m=0}$ (21) and the lower limits obtained in Refs. 28 and 29.

$v(x)$	Reference 29	Reference 28	$g_c^{(0)}$	$g_{\mathrm{up},1}^{m=0}$	$g_{\mathrm{up},2}^{m=0}$
$\exp(-x)$	4.443	4.370	5.574	5.584	7.411
$[\cosh(x)]^{-2}$	4.126	3.886	5.008	5.018	6.769
$\exp(-x^2)$	4.513	4.169	5.426	5.442	7.399
$x\exp(-x)$	3.696	3.349	4.360	4.364	5.964

The function $f(r)$ should be as close as possible to the zero binding energy wave function but also should be general and simple enough to obtain a neat formula. We simply choose

$$f(r) = A[r^{p-1}v(r)^p]^{1/2}, \quad p > 0, \tag{18}$$

where A is the normalization factor. The relations (8b), (12), (16), and (18) lead to the following upper limit on $g_c^{(0)}$:

$$g_c^{(0)} \leqslant \frac{\alpha\pi\int_0^\infty \mathrm{d}x\, F_1(2p-1;x)}{2\int_0^\infty \mathrm{d}x\, F_1(p;x)\int_0^x \mathrm{d}y\, F_1(p;y)\ln\left(\frac{x+y}{x-y}\right)} \equiv g_{\mathrm{up},1}^{m=0}, \tag{19}$$

where $F_1(q;x)=x^{(q-1)/2}v(x)^{(q+1)/2}$ and where we have introduced the parameter α which takes the value 1, respectively, 2 for one, respectively, two (identical) particle problems. The most stringent upper limit is obviously obtained by minimizing the right-hand side of (19) with respect to all positive values of p.

A simpler, but less stringent, version of this upper limit can be obtained with the help of the following minorization:

$$\ln\left(\frac{x+y}{x-y}\right) \geqslant \frac{2y}{x}, \tag{20}$$

$$g_c^{(0)} \leqslant \frac{\alpha\pi\int_0^\infty \mathrm{d}x\, F_1(2p-1;x)}{4\int_0^\infty \mathrm{d}x\, x^{-1}F_1(p;x)\int_0^x \mathrm{d}y\, yF_1(p;y)} \equiv g_{\mathrm{up},2}^{m=0}. \tag{21}$$

The accuracy of these upper limits can be tested with some typical potentials. The comparison between the exact results (obtained by solving numerically the spinless Salpeter equation) and the upper limits (19) and (21) is reported in Table I. We have also added two lower limits on $g_c^{(0)}$ obtained with the upper limits on the number of bound states derived in Refs. 28 and 29. Note that for these tests, we choose a two identical particles problem, $\alpha=2$.

The results reported in Table I indicate clearly that the accuracy of the upper limit (19) is quite remarkable. The upper limit (21) is obviously less stringent but could prove to be useful to obtain explicit formulas. The typical value of p which optimize these upper limits varies between 2 and 3. We do not consider other choices for $f(r)$ [see (18)] here since the relation (19) is already very accurate.

As an additional indication that the upper limits obtained with the method proposed in this work are quite accurate, we report in Table II a comparison between the exact value of the critical strength $g_c^{(1)}$ ($\ell=1$) and the corresponding upper limit obtained with the relations (12), (17), and (18) and noted $g_{\mathrm{up}}^{m=0,\ell=1}$ in this table.

TABLE II. Comparison, for some typical potentials, between the exact critical values, $g_c^{(1)}$ and the upper limit $g_{\text{up}}^{m=0,l=1}$ obtained with the relations (12), (17), and (18).

$v(x)$	$g_c^{(1)}$	$g_{\text{up}}^{m=0,l=1}$
$\exp(-x)$	10.975	10.992
$[\cosh(x)]^{-2}$	8.1174	8.1268
$\exp(-x^2)$	10.200	10.231
$x\exp(-x)$	9.5442	9.5636

B. Relativistic regime $m>0$

To obtain an upper limit on $g_c^{(\ell)}$ for a nonvanishing mass m, we need to calculate the expression of the function $G_\ell(m,r,r')$. To this end we note that

$$K_1(y) \leqslant F(y) \leqslant K_1(y) + \frac{\pi}{2}. \tag{22}$$

From the relation (12), it is obvious that a minorization of the kernel $K_\ell(m,r,r')$ is enough to obtain the upper limit. However, the minorization (22) of the function $F(y)$ is too crude to obtain good results. Instead we use

$$F(y) \geqslant K_1(y) + \frac{\pi}{2} - \frac{\pi}{2}\exp(-y). \tag{23}$$

This minorization (23) is proved in the Appendix. From the definition of $G_\ell(m,r,r')$ (6b) and the inequality (23) we obtain

$$G_\ell(m,r,r') \geqslant \frac{1}{\pi}\mathcal{G}_\ell(m,r,r') + \mathcal{S}_\ell(m,r,r') - \frac{1}{2}\mathcal{T}_\ell(m,r,r'), \tag{24}$$

where

$$\mathcal{G}_\ell(m,r,r') = m\int_{|r-r'|}^{r+r'} \mathrm{d}y\, K_1(my) P_\ell\left(\frac{r^2+r'^2-y^2}{2rr'}\right), \tag{25}$$

$$\mathcal{S}_\ell(m,r,r') = m\int_{|r-r'|}^{r+r'} \mathrm{d}y\, P_\ell\left(\frac{r^2+r'^2-y^2}{2rr'}\right) = \frac{2m}{2\ell+1} r_<^{\ell+1} r_>^{-\ell}, \tag{26}$$

with $r_< = \min[r,r']$ and $r_> = \max[r,r']$ and Ref. 34,

$$\begin{aligned}\mathcal{T}_\ell(m,r,r') &= mrr'\int_{-1}^{1} \mathrm{d}y \frac{\exp(-m\sqrt{r^2+r'^2-2rr'y})}{\sqrt{r^2+r'^2-2rr'y}} P_\ell(y) \\ &= \sqrt{\frac{2}{\pi}} m^2 rr' \int_{-1}^{1} \mathrm{d}y \frac{K_{1/2}(-m\sqrt{r^2+r'^2-2rr'y})}{[m^2(r^2+r'^2-2rr'y)]^{1/4}} P_\ell(y) \\ &= 2m\sqrt{rr'} K_{\ell+1/2}(mr_>) I_{\ell+1/2}(mr_<),\end{aligned} \tag{27}$$

where $I_\nu(x)$ is a modified Bessel function (see, for example, Ref. 32, p. 374). The kernel $\mathcal{S}_\ell(m,r,r')$ is actually the Green function of the nonrelativistic kinetic energy operator and takes a simple form while the kernel $\mathcal{G}_\ell(m,r,r')$ can be calculated analytically for each value of ℓ.[30,31] We find, for example,

TABLE III. Comparison, for some typical potentials, between the exact critical values, $g_c^{(0)}$ and the upper limit $g_{\rm up}^{m>0}$ (31).

$v(x)$	$\exp(-x)$		$[\cosh(x)]^{-2}$		$\exp(-x^2)$	
β	$g_c^{(0)}$	$g_{\rm up}^{m>0}$	$g_c^{(0)}$	$g_{\rm up}^{m>0}$	$g_c^{(0)}$	$g_{\rm up}^{m>0}$
0.1	4.694	5.390	4.461	4.994	4.927	5.363
0.5	2.387	2.547	2.766	3.006	3.309	3.589
1	1.361	1.407	1.742	1.843	2.198	2.352
2	0.7133	0.7206	0.9598	0.9862	1.257	1.307
3	0.4804	0.4817	0.6549	0.6642	0.8669	0.8880
4	0.3607	0.3615	0.4956	0.4994	0.6589	0.6694
5	0.2890	0.2893	0.3981	0.3999	0.5305	0.5364

$$\mathcal{G}_0(m,r,r') = K_0(m|r-r'|) - K_0(m(r+r')), \tag{28}$$

$$\mathcal{G}_1(m,r,r') = K_0(m|r-r'|) + K_0(m(r+r')) + \frac{1}{mrr'}[(r+r')K_1(m(r+r')) - |r-r'|K_1(m|r-r'|)]. \tag{29}$$

Now, we just need to choose a suitable normalized function $f(r)$ to apply the variational principle reported above [see (12)]. We take the following expression for $f(r)$:

$$f(r) = A[r^{2p-1}v(r)^p]^{1/2}, \quad p > 0. \tag{30}$$

For simplicity we again restrict the rest of the following discussion to $\ell = 0$ but extensions to nonvanishing values of the angular momentum is obvious, one just needs to compute the corresponding expression of the function $G_\ell(m,r,r')$.

The relations (8b), (12), (18), and (28) lead to the following upper limit on $g_c^{(0)}$:

$$g_c^{(0)} \leqslant \frac{\alpha \int_0^\infty \mathrm{d}x \sqrt{x} F_2(2p-1;x)}{2\int_0^\infty \mathrm{d}x\, F_2(p;x) \int_0^x \mathrm{d}y\, F_2(p,y) T(x,y)} \equiv g_{\rm up}^{m>0}, \tag{31a}$$

with

$$T(x,y) = \frac{1}{\pi}[K_0(\beta(x-y)) - K_0(\beta(x+y))] + 2\beta y + \frac{1}{2}[\exp(-\beta(x+y)) - \exp(-\beta(x-y))], \tag{31b}$$

where $F_2(q,x) = x^{q-1/2}v(x)^{(q+1)/2}$ and where $\beta = mR$, R being the scale of length which appears in the potential $[v(r) = v(Rx)]$. Again, we have introduced in (31a) the parameter α which takes the value 1, respectively, 2 for one, respectively, two (identical) particle problems.

The accuracy of this upper limit can be tested with some typical potentials. The comparison between the exact results and the upper limit (31) is reported in Table III. Note that for these tests, we also choose a two identical particles problem, $\alpha = 2$.

The results reported in Table III indicate clearly that the accuracy of the upper limit (31) is quite good. But for a small value of β the upper limit is however less restrictive. Thus for a small value of β it is preferable to use an intermediate form for $f(r)$. We then propose in general to use

$$f(r) = A[r^{ap-1}v(r)^p]^{1/2}, \quad p > 0, \tag{32}$$

with $1 \leqslant a \leqslant 2$. This last expression for $f(r)$ improves significantly the restriction on the possible values of $g_c^{(0)}$. Indeed, for $\beta = 0.1$, $a = 1.18$ and for the exponential potential, the upper limit is then equal to 4.812 instead of 5.390. But this additional flexibility is only significant for a small value of β, indeed for $\beta = 0.5$ the best upper limit is found to be equal to 2.521 (for the exponential potential and $a = 1.69$) instead of 2.547.

However, even with the choice (32) for $f(r)$, the upper limit (31) still yields less restrictive results for small β than those obtained for larger values of β or those obtained with the upper limit (19). This is easy to understand, since this is in the sector of small β, that the error introduced by the inequality (23) is the most important. Indeed, in the limit of β going to zero, the upper limit (31) coincides with the upper limit (19) and for β going to infinity, only the nonrelativistic kernel $\mathcal{S}_\ell(m, r, r')$ contributes.

III. CONCLUSIONS

In this paper we have shown how to construct upper limits on the critical value, $g_c^{(\ell)}$, of the coupling constant, g, of a central potential, $V(r) = -gv(r)$. The method used to derive the upper limits is quite general and other (possibly more complicated) families of upper limits yielding (possibly) stronger restrictions on $g_c^{(\ell)}$ could also be obtained. Indeed, the method is based on a variational principle for which a trial zero energy wave function is needed. There is no limitation on the accuracy of such a trial function, which imply that there is, in principle, no limitation on the accuracy of the upper limit on $g_c^{(\ell)}$ derived with this procedure. However, this remark is only true for the ultrarelativistic regime, $m = 0$, where the kernel of the integral equation has been calculated exactly. For $m > 0$, a minorization of the kernel has been used yielding some errors in the restrictions on the possible values of the critical value $g_c^{(\ell)}$ which cannot be compensated by a better choice of the trial zero energy wave function. In this paper we have proposed in Sec. II a compromise between accuracy and simplicity of the final formula. The accuracy of the upper limits on $g_c^{(\ell)}$ was then tested with some typical potentials.

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APPENDIX: MAJORIZATION OF THE PRIMITIVE OF $K_0(x)$

We choose the following integral representation for the modified Bessel function $K_0(x)$ (Ref. 32, p. 376):

$$K_0(x) = \int_0^\infty \mathrm{d}t \exp(-\, x \cosh t). \tag{A1}$$

We have

$$\int_y^\infty \mathrm{d}x\, K_0(x) = \int_0^\infty \mathrm{d}t \frac{\exp(-\, y \cosh t)}{\cosh t} \leqslant \exp(-\, y) \int_0^\infty \mathrm{d}t \frac{1}{\cosh t} = \frac{\pi}{2} \exp(-\, y). \tag{A2}$$

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Matrix theory of unoriented membranes and Jordan algebras

Peter Varga[a)]
Institute of Mathematics and Informatics, University of Debrecen, H-4010 Debrecen, Hungary

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We express the equations of motion of unoriented membranes with the help of Jordan algebras. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1857032]

I. INTRODUCTION

The proposal of the matrix theory as a fundamental theory of physics[1] and its connection with the supermembrane theory[2] gave a strong impetus to the study of noncommutative space-time models. The starting point of these investigations is often the correspondence between the Poisson algebra of functions on the surface of the membrane and the associative algebra of the regularized matrix coordinates. Nevertheless, there are models where even the assumption of the associativity of the space-time coordinates is dropped. We demonstrate that the nonassociative Jordan algebras can be used to describe the motion of the bosonic membrane. In contrast to the case of Poisson algebras, our construction does not require orientable surfaces, so it can describe nonorientable surfaces, too. Let us note that Jordan algebras were used for example in string theory[3] and matrix string theory.[4]

In Sec. II we briefly review the matrix theory—membrane correspondence—while Sec. III contains the Jordan algebraic reformulation of this theory.

II. A SHORT REVIEW OF THE ORIENTED MEMBRANE

The classical equation of motion of a membrane is derived from the action

$$S = -T \int d^3\sigma \sqrt{-\det \partial_\alpha X^\mu \partial_\beta X_\mu}, \tag{2.1}$$

where the $X^\mu(\sigma_0,\sigma_1,\sigma_2)$ coordinates describe the embedding of the membrane's world volume into the ambient Minkowski space. The Hamiltonian equations of motion in the light-front coordinates are generated by the Hamiltonian

$$H = \frac{\nu T}{4} \int d^2\sigma \left(\dot{X}^i \dot{X}^i + \frac{2}{\nu^2} \{X^i, X^j\}\{X^i, X^j\} \right) \tag{2.2}$$

and the supplementary constraint

$$\{\dot{X}^i, X^i\} = 0. \tag{2.3}$$

The equation of motion is

a)Electronic mail: varga@math.klte.hu

$$\ddot{X}^i = \frac{4}{\nu^2}\{\{X^i, X^j\}, X^j\}. \tag{2.4}$$

(For references, explanation of notation, and further review of this topic we refer to Ref. 5.)

In the regularization procedure of Hoppe,[6] the X^i coordinate functions are replaced by finite size matrices, Poisson brackets by matrix commutators, and the integration over the membrane's surface by suitably normalized traces. The regularized Hamiltonian and the equations of motion are

$$H = \frac{1}{2\pi l_p^3}\,\mathrm{Tr}\left(\frac{1}{2}\dot{\mathbb{X}}^i\dot{\mathbb{X}}^i - \frac{1}{4}[\mathbb{X}^i,\mathbb{X}^j][\mathbb{X}^i,\mathbb{X}^j]\right),$$
$$\ddot{\mathbb{X}}^i + [[\dot{\mathbb{X}}^i,\dot{\mathbb{X}}^j],\dot{\mathbb{X}}^j] = 0, \quad [\dot{\mathbb{X}}^i,\mathbb{X}^i] = 0, \tag{2.5}$$

where the $\mathbb{X}^i$ coordinates are now Hermitian matrices.

This reformulation requires orientable surfaces. Nevertheless, this procedure can be extended to nonorientable surfaces, too.[7] Indeed a nonorientable surface has an orientable double cover (the orientation bundle). Inside the Poisson algebra of the functions of the double cover, one can identify the sub-Lie-algebra of those functions, which generate the area-preserving transformations of the nonorientable surface.[8,9] On $\mathbb{RP}^2$ one obtains the $USp(N)$ Lie algebra.

III. THE UNORIENTED MEMBRANE

The surface of the membrane has no intrinsic orientation. Indeed, the Hamiltonian (2.2) is invariant against the flip of the sign of the symplectic form ω of the Poisson bracket. This fact suggests that it might be possible to rewrite the expressions (2.2) and (2.3) with no reference to the sign of ω. Since the correspondence between (2.2) and (2.3) uses the replacement of the commutative algebra of the X^i functions by the noncommutative $\mathbb{X}^i$ matrices via deformation quantization, it is quite reasonable to search for a deformed algebraic structure that does not depend on the sign of ω. Let us recall that on $\mathbb{R}^2$ with $\omega = dx \wedge dy$ the deformed Moyal products look like

$$f *_h g = fg + \frac{ih}{2}(f_x g_y - f_y g_x) + \frac{h^2}{8}\left[f_{xy}g_{xy} - \frac{1}{2}(f_{xx}g_{yy} + f_{yy}g_{xx})\right] + \cdots . \tag{3.1}$$

The second-order term is symmetric with respect to the exchange of the x and y variables, so it makes no reference to the orientation of the surface. Exactly this term is the first nontrivial term in the Jordan product of f and g

$$f \circ_h g = \frac{1}{2}(f *_h g - g *_h f) = fg + \frac{h^2}{8}\left[f_{xy}g_{xy} - \frac{1}{2}(f_{xx}g_{yy} + f_{yy}g_{xx})\right] + \cdots , \tag{3.2}$$

so we try to rewrite (2.3) and (2.4) with the help of anticommutators (Jordan products) instead of commutators.

The Hamiltonian can be rewritten using the following calculation:

$$\mathrm{Tr}([\mathbb{X},\mathbb{Y}][\mathbb{X},\mathbb{Y}]) = 2\ \mathrm{Tr}(\mathbb{X}\mathbb{Y})^2 - 2\ \mathrm{Tr}(\mathbb{X}^2\mathbb{Y}^2),$$
$$\mathrm{Tr}(\mathbb{X}\circ\mathbb{X})\circ(\mathbb{Y}\circ\mathbb{Y}) = \mathrm{Tr}(\mathbb{X}^2\mathbb{Y}^2), \tag{3.3}$$
$$\mathrm{Tr}\{\mathbb{X}\circ[\mathbb{Y}\circ(\mathbb{X}\circ\mathbb{Y})]\} = \frac{1}{2}\ \mathrm{Tr}(\mathbb{X}\mathbb{Y})^2 + \frac{1}{2}\ \mathrm{Tr}(\mathbb{X}^2\mathbb{Y}^2)$$

[here $\circ$ is the usual Jordan product of matrices $\mathbb{X}\circ\mathbb{Y} = (\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X})/2$].

Consequently,

$$H = \frac{1}{2\pi l_p^3}\,\mathrm{Tr}\left(\frac{1}{2}\dot{\mathbb{X}}^i \circ \dot{\mathbb{X}}^i - \mathbb{X}^i \circ (\mathbb{X}^j \circ (\mathbb{X}^i \circ \mathbb{X}^j)) + (\mathbb{X}^i \circ \mathbb{X}^i) \circ (\mathbb{X}^j \circ \mathbb{X}^j)\right). \tag{3.4}$$

The accelerations $\ddot{\mathbb{X}}^i$ of the matrix coordinates are given by double commutators (2.4), so it can be expressed by with the help of the associator of the Jordan algebra

$$(\mathbb{X},\mathbb{Y},\mathbb{Z}) = (\mathbb{X}\circ\mathbb{Y})\circ\mathbb{Z} - \mathbb{X}\circ(\mathbb{Y}\circ\mathbb{Z}) = \frac{1}{4}[\mathbb{Y},[\mathbb{X},\mathbb{Z}]], \tag{3.5}$$

whose identity gives the following equation of motion:

$$\ddot{\mathbb{X}}^i = 4(\mathbb{X}^i,\mathbb{X}^j,\mathbb{X}^j) = [\mathbb{X}^j,[\mathbb{X}^i,\mathbb{X}^j]]. \tag{3.6}$$

The substitution of double commutators by associators occurs in almost all papers on the Jordan algebraic reformulation of quantum mechanics. Our next task is to express the constraints $[\dot{\mathbb{X}}^i,\mathbb{X}^i]=0$ with the Jordan product of matrices. This is obviously impossible directly. The best we can do is to require that

$$4(\dot{\mathbb{X}}^i,\mathbb{U},\mathbb{X}^i) = [\mathbb{U},[\dot{\mathbb{X}}^i,\mathbb{X}^i]] = 0 \tag{3.7}$$

for any matrix $\mathbb{U}$. Since only the multiples of the identity matrix commute with all the other matrices, this equation implies that $[\dot{\mathbb{X}}^i,\mathbb{X}^i]=c\cdot\mathbb{1}$, but it is well known that this is impossible for finite size matrices (by taking the trace of both sides).

So we managed to rewrite the Eqs. (2.3) and (2.4) in a Jordan algebraic language. Since these equations are only finite dimensional approximations of the continuous equation (2.2), we expect that a similar procedure can be repeated for (2.2), at least up to the leading orders of a deformation parameter. For this purpose, we would like to express $\int d\sigma^2\{f,g\}^2$ with the help of the Jordan multiplication $\circ_h$. This is possible in the sense that the following identity holds on $\mathbb{R}^2$:

$$\{f,g\}^2 = (f_x g_y - f_y g_x)^2 = -\frac{4}{h^2}[f\circ_h(g\circ_h(f\circ_h g)) - (f\circ_h f)\circ_h(g\circ_h g)] + O(h^2) + \alpha_x + \beta_y, \tag{3.8}$$

where the explicit forms of α and β are

$$\begin{aligned}\alpha &= f_x(fg_y^2 - 2f_y g g_y) + g_x(2f_y^2 g - f f_y g_y),\\ \beta &= f_y(fg_x^2 - 2f_x g g_x) + g_x(2f_x^2 g - f f_x g_x).\end{aligned} \tag{3.9}$$

The verification of these formulas consists of a fairly direct but quite long calculation, which can be easily performed by a symbolic algebra package. It is amusing to compare this to the simplicity of the matrix version (3.3) and (3.4) of these identities. Since the integral of the $\alpha_x+\beta_y$ term is zero if f and g have compact support (or the integration is done over a compact closed surface), (2.2) can be expressed with the help of the deformed Jordan multiplication up to terms of order $O(h^2)$.

Next we would like to see what sort of Jordan algebra can be associated to a nonorientable surface. We treat here only the simplest case of the real projective plane $\mathbb{RP}^2$, but we believe that the same conclusion would be true for the other nonorientable surfaces, too. (It was demonstrated in Ref. 10 that the Goldstone–Hoppe regularization procedure is applicable for higher genus orientable surfaces, too.)

Let us recall that the Goldstone–Hoppe construction on the unit sphere S^2 uses the correspondence

$$x_i \leftrightarrow \frac{2}{N} J_i, \quad \{x_i, x_j\} = \epsilon_{ijk} x_k, \quad -i[J_i, J_j] = \epsilon_{ijk} J_k, \tag{3.10}$$

where the $x_{1,2,3}$ are the three-dimensional coordinates of S^2 satisfying $x_1^2+x_2^2+x_3^2=1$, while $J_{1,2,3}$ are the Hermitian generators of the N-dimensional irreducible representation of $SU(2)$. As an algebra, these matrices generate $Mat_N(\mathbb{C})$, while as a (unital) Jordan algebra they generate the self-adjoint part of $Mat_N(\mathbb{C})$, which is denoted by $H_N(\mathbb{C})$. This is probably well known for Jordan algebrists, but with the help of the standard representation of $SU(2)$

$$N = 2j + 1, \quad J_3|m\rangle = m|m\rangle,$$

$$\begin{aligned} J_+|m\rangle &= \sqrt{j(j+1) - m(m+1)}|m\rangle, \\ J_-|m\rangle &= \sqrt{j(j+1) - m(m-1)}|m\rangle, \end{aligned} \tag{3.11}$$

$$J_1 = \frac{J_+ + J_-}{2}, \quad j_2 = \frac{J_+ - J_-}{2i},$$

this can be demonstrated quite explicitly. Let us denote by e_{ij} the matrix with zero entries except at $(e_{ij})_{ij}=1$. Then e_{ii} can be written as a suitable polynomial of J_3, since J_3 is diagonal with different diagonal entries. Furthermore,

$$\begin{aligned} (e_{ii} \circ J_1) \circ e_{i+1,i+1} &= \frac{1}{4}(J_1)_{i,i+1}(e_{i+1,i} + e_{i,i+1}), \\ (e_{ii} \circ J_2) \circ e_{i+1,i+1} &= \frac{1}{4}(J_1)_{i,i+1}(-ie_{i+1,i} + ie_{i,i+1}). \end{aligned} \tag{3.12}$$

The successive Jordan products of these types of matrices generate the whole of $H_N(\mathbb{C})$. (For example,

$$(e_{i+1,i} + e_{i,i+1}) \circ (-ie_{i+1,i+2} + ie_{i+2,i+1}) = \frac{1}{2}(-ie_{i,i+2} + ie_{i+2,i}), \tag{3.13}$$

etc.)

Now let us turn our attention to the case of $\mathbb{RP}^2$. This projective plane is the quotient of S^2 by the antipodal map $(x_1,x_2,x_3) \to (-x_1,-x_2,-x_3)$, so we would like to keep those elements of the Jordan algebra generated by $J_{1,2,3}$ that are invariant with respect to the substitution $J_{1,2,3} \to -J_{1,2,3}$. This part can be generated by the matrices $\{J_i \circ J_k;\ i,k=1,2,3\}$. We restrict ourself to the very simple case when N is odd, so J_i represents $SO(3)$. In this case J_i can be chosen to be purely imaginary and antisymmetric, so $J_i \circ J_k$ is a symmetric real matrix. The Jordan algebra generated by these matrices is formally real, i.e., $\Sigma_i a_i^2=0$ implies $a_i=0$. Such unital and finite dimensional Jordan algebras are direct sums of simple ones (p. 72).[11] If this direct sum were nontrivial, or the generated algebra were realized as a diagonal embedding of, for example, $H_{N/2}(\mathbb{R})$ into $H_N(\mathbb{R})$, that would implicate the existence of a nontrivial decomposition of the vector space $\mathbb{C}^N$ into the direct sum of vector spaces, with invariant factors with respect to the action of $SO(3)$ [since the linear span of the generating set $\{J_i \circ J_k,\ i,k=1,2,3\}$ is also invariant against $SO(3)$], but this would contradict to the irreducibility of the representation. So we conclude that the Matrix theoretic description of a membrane with topology of the real projective space requires the use of the Jordan algebra of real symmetric matrices. This result is in sharp contrast compared to the construction of Ref. 7, where the Lie algebra of $USp(N)$ was used, since the closest Jordan algebraic relative of $USp(N)$ is $H_N(\mathbb{H})$, i.e., the set of self-adjoint quaternionic matrices.

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Consistent and mimetic discretizations in general relativity

Cayetano Di Bartolo
Departamento de Física, Universidad Simón Bolívar, Aptdo. 89000, Caracas 1080-A, Venezuela

Rodolfo Gambini
Instituto de Física, Facultad de Ciencias, Iguá 4225, esq. Mataojo, Montevideo, Uruguay

Jorge Pullin
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803-4001

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A discretization of a continuum theory with constraints or conserved quantities is called *mimetic* if it mirrors the conserved laws or constraints of the continuum theory at the discrete level. Such discretizations have been found useful in continuum mechanics and in electromagnetism. We have recently introduced a new technique for discretizing constrained theories. The technique yields discretizations that are consistent, in the sense that the constraints and evolution equations can be solved simultaneously, but it cannot be considered mimetic since it achieves consistency by determining the Lagrange multipliers. In this paper we would like to show that when applied to general relativity linearized around a Minkowski background the technique yields a discretization that is mimetic in the traditional sense of the word. We show this using the traditional metric variables and also the Ashtekar new variables, but in the latter case we restrict ourselves to the Euclidean case. We also argue that there appear to exist conceptual difficulties to the construction of a mimetic formulation of the full Einstein equations, and suggest that the new discretization scheme can provide an alternative that is nevertheless close in spirit to the traditional mimetic formulations. [DOI: 10.1063/1.1841483]

I. INTRODUCTION

Continuum theories, either mechanical systems or field theories, usually have conservation laws and sometimes constraints. When one discretizes the equations of these theories, for instance in order to solve them numerically on a computer, or for "quantization on the lattice" purposes, the resulting discrete equations will usually fail to preserve the conserved quantities of the continuum theory upon evolution. Similar comments apply to constraints. Although one may have discrete equations resulting from discretizing the constraints of the continuum theory, if one chooses initial data that solve these equations exactly, they will fail to be solved upon discrete evolution.

Mimetic discretizations are discretizations of continuum theories that preserve conserved quantities or constraints in the discrete theory that mimic those of the continuum theory. There is quite a body of literature[1] on mimetic discretizations in the context of continuum mechanics and electromagnetism. The literature on Hamiltonian lattice QCD implicitly considers a mimetic discretization of Yang–Mills theory, although this fact is not usually emphasized.

Some authors have considered the question of whether mimetic discretizations of general relativity can be constructed.[2,3] It is well known that if one discretizes the Einstein equations, the Hamiltonian and momentum constraint, which should hold for all time if satisfied initially (ignoring for the moment the issue of spatial boundaries), fail to do so in the discrete theory. Although there has been success in generating mimetic formulations of linearized relativity, it appears unlikely that something similar will be available for the full theory (or even for the linearized

theory on nontrivial backgrounds or slicings). This is due to the fact that discretized derivatives fail to satisfy Leibnitz's rule and therefore the nonlinear terms when discretized do not have properties that mirror those of the continuum.[3]

We have recently introduced a new approach to the discretization of theories, particularly of theories with constraints[4,5] called "consistent discretization." The technique guarantees that the resulting discrete equations are compatible, i.e., they admit a common set of solutions (something that is not generically true if one discretizes the equations of a constrained theory). The technique has been tried out in the context of cosmological solutions of the Einstein equations,[6] of BF theory and of Maxwell and Yang–Mills theories on the lattice.[4] Current investigations are testing it for the Gowdy models.

In this paper we would like to show that the technique we proposed, when applied to the Einstein theory linearized around a Minkowski background yields a discrete formulation that is mimetic. That is, the discretized constraints are exactly preserved under evolution without determining the Lagrange multipliers. We first consider linearized general relativity in terms of the traditional metric variables. We then consider it in terms of Ashtekar's variables, which have the advantage of being closer to the discretizations used in Yang–Mills theories (although in this case we restrict ourselves to Euclidean general relativity).

In the consistent discretization scheme, equations are discretized with variables evaluated at two (or more) different levels in time. This includes the constraints of general relativity, which in the discrete theory therefore can only be viewed as "pseudo" constraints (we will reserve the word constraint for expressions that involve all variables evaluated at the same instant of time, as in traditional canonical terminology). These equations, with variables discretized at mixed instants of time are the equations that are solved by the consistent discretization scheme. Of course, if one is in a regime in which the time-step is small, then satisfying the pseudoconstraints implies that the usual discrete constraints (with all the variables at the same time-step) are approximately satisfied as well. Therefore the resulting scheme cannot be strictly called mimetic, although it approximately is. We will show that if one uses a discretization for general relativity that is mimetic in the linearized case, one further improves the accuracy with which the consistent scheme for the full nonlinear theory satisfies the constraints. This encourages further studies of these discretization schemes in the context of numerical applications.

In the next section we will present a brief summary of the consistent discretizations scheme. In the following two sections we apply it to linearized gravity, first with the traditional variables and then with the Ashtekar variables. We end with a discussion and proposals for further research.

II. CONSISTENT DISCRETIZATION OF CONSTRAINED THEORIES

We illustrate the technique with a mechanical system for simplicity, but there is no problem working it out for field theories, since upon discretization the latter become mechanical systems. We assume we start from an action in the continuum, written in first-order form,

$$S = \int L(q,p)\mathrm{d}t \tag{1}$$

with

$$L(q,p) = p\dot{q} - H(q,p) - \lambda\phi(q,p), \tag{2}$$

where λ is a Lagrange multiplier and the theory has a single (it is immediate to incorporate several) constraint $\phi(q,p)=0$. The discretization of the action yields $S=\Sigma_0^N L(n,n+1)$, where

$$L(n,n+1) = p_n(q_{n+1} - q_n) - \epsilon H(q_n,p_n) - \lambda_n\phi(q_n,p_n), \tag{3}$$

where $\epsilon=t_{n+1}-t_n$ and we have absorbed an ϵ in the definition of the Lagrange multipliers.

We will now view the Lagrangian as the generator of a type 1 canonical transformation between the instant n and the instant $n+1$. In ordinary classical mechanics parlance, given a

canonical transformation between a canonical pair q,p and a new canonical pair Q,P, the generating function of a type 1 canonical transformation is a function of q,Q, $F(q,Q)$ and the canonically conjugate momenta are defined by $P=\partial F/\partial Q$, $p=\partial F/\partial q$. In our case we will view q_n, p_n, λ_n and q_{n+1}, p_{n+1}, λ_{n+1} as "configuration variables" and will assign to each of them a canonically conjugate momentum through the canonical transformation,

$$P^q_{n+1}=\frac{\partial L(n,n+1)}{\partial q_{n+1}}, \tag{4}$$

$$P^p_{n+1}=\frac{\partial L(n,n+1)}{\partial p_{n+1}}, \tag{5}$$

$$P^\lambda_{n+1}=\frac{\partial L(n,n+1)}{\partial \lambda_{(n+1)}}, \tag{6}$$

$$P^q_n=-\frac{\partial L(n,n+1)}{\partial q_n}, \tag{7}$$

$$P^p_n=-\frac{\partial L(n,n+1)}{\partial p_n}, \tag{8}$$

$$P^\lambda_n=-\frac{\partial L(n,n+1)}{\partial \lambda_{(n)}}. \tag{9}$$

If one explicitly computes the partial derivatives with the Lagrangian given, one can eliminate the p, P^p, and P^λ to yield a more familiar-looking set of equations,

$$P^q_{n+1}-P^q_n=-\epsilon\frac{\partial H(q_n,P^q_{n+1})}{\partial q_n}-\lambda_{nB}\frac{\partial \phi^B(q_n,P^q_{n+1})}{\partial q_n},$$

$$q_{n+1}-q_n=\epsilon\frac{\partial H(q_n,P^q_{n+1})}{\partial P^q_{n+1}}+\lambda_{nB}\frac{\partial \phi^B(q_n,P^q_{n+1})}{\partial P^q_{n+1}}, \tag{10}$$

$$\phi^B(q_n,P^q_{n+1})=0.$$

These indeed look like a discrete version of equations for a system with constraints. However, there are important differences. First of all, notice that as an evolution system the equations are implicit. Second, if one solves the first two equations one obtains P^q and q as functions of the initial data and the Lagrange multipliers. The last equation however, will generically not hold. One will have to choose specific values for the Lagrange multipliers at each time-step (and if one is dealing with a field theory at each point in space) for all the equations to be solved.

Notice that there can be particular cases in which the system does not determine the Lagrange multipliers. For instance, consider a totally constrained system like general relativity. There the Hamiltonian vanishes. Suppose now that the constraint in (10) is only a function of q_n. Then the evolution equation for q_{n+1} implies that $q_{n+1}=q_n$ and the constraint is automatically preserved. Therefore the resulting formulation is mimetic in the traditional sense of the word, a constraint that is just the discrete version of the continuum constraint is preserved under evolution by the discrete evolution equations. A similar situation develops if the constraint is only a function of P^q.

If the Hamiltonian is nonvanishing, and the constraint depends only on P^q_{n+1} then the latter is not automatically preserved upon evolution, but it cannot be satisfied by choosing the Lagrange

multipliers either since they drop out from the relevant evolution equations. On the other hand, if the constraint is only a function of q_n, its preservation could be enforced by choosing the Lagrange multipliers (the asymmetry between P^q and q in this treatment comes from the fact that we chose to write the equations as "propagating forward" in time, if one had chosen to propagate backwards, the roles of q and P^q in this discussion would be reversed).

Summarizing, the consistent discretization technique consists of discretizing the action and working out the resulting equations of motion for the discrete theory from it through the canonical transformation that implements time evolution. The resulting evolution equations (and constraints) are made of a consistent set of nonlinear algebraic equations by considering the Lagrange multipliers as dynamical variables one must solve for. In particular situations, the Lagrange multipliers are not determined by the equations. In such cases the resulting set of equations and constraints must be consistent since it has been derived from a variational principle and the resulting discrete theory is mimetic in the traditional sense of the word, the constraints are automatically preserved upon evolution. In the other case, when the Lagrange multipliers are determined the resulting discrete theory is based on a consistent set of algebraic equations, but as one can see in Eq. (10), one is enforcing the constraints with some variables evaluated at instant n and some at instant $n+1$. For small step sizes, this implies that the constraints with all the variables evaluated at the same instant of time are approximately preserved. The resulting theory therefore cannot be called mimetic in the traditional sense of the word, although it can do a good job of preserving (approximately) the discrete constraints.

In the next two sections we apply this technique to linearized general relativity. We will see that the resulting theories do not determine the Lagrange multipliers, preserve the constraints automatically, and therefore are mimetic in the traditional sense of the word. We will not discuss the case of full general relativity here, but in several examples we have considered elsewhere for the nonlinear theory (cosmologies,[6] Gowdy space–times) the Lagrange multipliers are determined. Therefore it is unlikely that this method will yield a mimetic formulation for full GR. However, as we argued above, it will yield a formulation that approximates general relativity well in certain regimes and in such regimes the discrete constraints are enforced approximately very well. We believe it is likely that this is "as close as one will get" to a mimetic formulation of full general relativity.

III. LINEARIZED GENERAL RELATIVITY IN TERMS OF METRIC VARIABLES

In this section we will apply the technique we described in the preceding section to linearized general relativity written in terms of the traditional variables. We assume the background is the Minkowski metric.

A. Continuum formulation

We start with the Arnowitt, Deser, and Misner (ADM)[7] form of the action of general relativity,

$$S = \int \mathrm{d}^4x[\pi^{ab}\dot{q}_{ab} - NC - N_aC^a], \tag{11}$$

where

$$C = \frac{1}{\sqrt{q}}\left[\pi^{ab}\pi_{ab} - \frac{1}{2}(\pi^b_b)^2\right] - \sqrt{q}^{(3)}R, \tag{12}$$

$$C^a = -2\pi^{ab}_{;b}, \tag{13}$$

and the variables (q_{ab}, N, N_a) are related to the four dimensional metric ${}^{(4)}g_{\mu\nu}$ through,

$$q_{ab} = {}^{(4)}g_{ab}, \tag{14}$$

$$N = (-{}^{(4)}g_{00})^{-1/2}, \tag{15}$$

$$N_a = {}^{(4)}g_{0a}. \tag{16}$$

The indices a,b,c run from 1 to 3. $\sqrt{q}$ is the determinant of the spatial metric q_{ab} and ${}^{(3)}R$ is its Ricci curvature scalar. The momenta π^{ab} are related to the extrinsic curvature of the spacelike surfaces $x^0=t=$constant through $\pi^{ab}=-\sqrt{q}[K^{ab}-q^{ab}K^c_c]$ and indices are raised and lowered with the spatial metric. The semicolon denotes covariant differentiation with respect to the Christoffel connection of the spatial metric. Variation with respect to π^{ab},q_{ab},N,N_a yields the Einstein equations. In particular variation of N,N_a gives rise to four constraints $C=0,C^a=0$ usually referred to as (super-) Hamiltonian and momentum (or diffeomorphism) constraints.

We have chosen the ADM action since it is one of the most traditionally used in general relativity. Modern numerical implementations favor the use of formulations in which the evolution equations are manifestly symmetric-hyperbolic. This is not the case for the ADM equations. In principle there is no obstruction in applying our technique to any action, but it just is the case that there has been little investigation about formulating the symmetric-hyperbolic formulations as deriving from an action principle. This will require further study and therefore we decided to concentrate on this paper on the ADM action for simplicity.

We now consider that the space–time metric is given by a static background metric plus small perturbations ${}^{(4)}g_{\mu\nu}={}^{(4)}g^{(0)}_{\mu\nu}+h_{\mu\nu}$. For simplicity we make the further choice that the foliation is such that the zeroth order shift $N_a=0$ and the zeroth order extrinsic curvature is therefore zero $\pi^{ab}=0$. The constraint equations to leading order in the perturbations are given by[8]

$$C^a = -2p^{ab}{}_{;b}, \tag{17}$$

$$C = -\sqrt{q}[h_{ab}{}^{;ab} - h_{;a}{}^{;a} - h_{ab}{}^{(3)}R^{ab}]. \tag{18}$$

In these expressions p^{ab} is the linear portion of the canonical momentum π^{ab} and ${}^{(3)}R^{ab}$ is the Ricci tensor of the background metric. The action for the linearized theory is

$$S = \int \mathrm{d}^4x[p^{ab}\dot{h}_{ab} - N^{(0)}H - N^{(1)}_a C^a - N^{(1)}C], \tag{19}$$

where we have kept track of the order in the perturbation expansion of the lapse and the shift (recall that we assume zero shift in the background). The constraints C, C^a are given by the expressions above, where only terms up to order linear have been kept. The quantity

$$H = \frac{1}{\sqrt{q}}\left[p^{ab}p_{ab} - \frac{1}{2}p^2\right] + \frac{1}{2}\sqrt{q}\left[\frac{1}{2}h_{ab;c}h^{ab;c} - h_{ab;c}h^{ac;b} - \frac{1}{2}h_{;a}h^{;a} + 2h_{;a}h^{ab}{}_{;b} + hh^{ab}{}_{;ab} - hh_{ab}{}^{(3)}R^{ab}\right] \tag{20}$$

is a true Hamiltonian density (not a constraint) that is responsible for the evolution of the canonical variables, and is multiplied in the action times the lapse of the background space–time.

At this point we can make an important observation. The momentum constraint (17) is only a function of the momenta p^{ab} (the covariant derivative is with respect to the background metric) and the Hamiltonian constraint (18) is only a function of the configuration variables q^{ab}. Therefore, as we discussed in Sec. II, our discretization technique will not determine the value of the Lagrange multipliers. The resulting theory therefore can only either be mimetic or inconsistent. We will proceed to show that the resulting discrete theory is indeed consistent.

B. Discretization

We start by discretizing the linearized action, $S=\Sigma_{n=1}^{N}L(n,n+1)$, where

$$L(n,n+1)=\sum_{\vec{m}}\left(\sum_{a,b=1}^{3}\{p_{ab}(n,\vec{m})(h_{ab}(n+1,m)-h_{ab}(n,m))-N(n,\vec{m})[h_{ab}(n,\vec{m}+\vec{e}_a+\vec{e}_b)\right.$$
$$-h_{ab}(n,\vec{m}-\vec{e}_a+\vec{e}_b)-h_{ab}(n,\vec{m}+\vec{e}_a-\vec{e}_b)+h_{ab}(n,\vec{m}-\vec{e}_a-\vec{e}_b)-h_{aa}(n,\vec{m}+2\vec{e}_b)$$
$$+2h_{aa}(n,\vec{m})-h_{aa}(n,\vec{m}-2\vec{e}_b)]-N_a(n,\vec{m})[2p_{ab}(n,\vec{m}+\vec{e}_b)-2p_{ab}(n,\vec{m}-\vec{e}_b)]\}$$
$$\left.-H(n,\vec{m})\right) \tag{21}$$

and

$$H(n,\vec{m})=\sum_{a,b=1}^{3}\left[p_{ab}(n,\vec{m})^2-\frac{1}{2}p_{aa}(n,\vec{m})p_{bb}(n,\vec{m})\right]+\frac{1}{2}\sum_{a,b,c=1}^{3}\left[\frac{1}{2}(h_{ab}(n,\vec{m}+\vec{e}_c)-h_{ab}(n,\vec{m}-\vec{e}_c))^2\right.$$
$$-(h_{ab}(n,\vec{m}+\vec{e}_c)-h_{ab}(n,\vec{m}-\vec{e}_c))(h_{ac}(n,\vec{m}+\vec{e}_b)-h_{ac}(n,\vec{m}-\vec{e}_b))-\frac{1}{2}(h_{aa}(n,\vec{m}+\vec{e}_c)$$
$$-h_{aa}(n,\vec{m}-\vec{e}_c))(h_{bb}(n,\vec{m}+\vec{e}_c)-h_{bb}(n,\vec{m}-\vec{e}_c))+2(h_{cc}(n,\vec{m}+\vec{e}_a)-h_{cc}(n,\vec{m}-\vec{e}_a))$$
$$\times(h_{ab}(n,\vec{m}+\vec{e}_b)-h_{ab}(n,\vec{m}-\vec{e}_b))+h_{cc}(n,\vec{m})[h_{ab}(n,\vec{m}+\vec{e}_a+\vec{e}_b)-h_{ab}(n,\vec{m}+\vec{e}_a-\vec{e}_b)$$
$$\left.+h_{ab}(n,\vec{m}-\vec{e}_a-\vec{e}_b)-h_{ab}(n,\vec{m}-\vec{e}_a+\vec{e}_b)]\right], \tag{22}$$

where we have assumed that the background metric is Minkowski and we have chosen the zeroth order lapse equal to unity and we have dropped the (1) superscript from the first order and shift. We have also chosen a centered prescription for spatial derivatives, with the following conventions, i.e., $\phi(i)_{,x}=\phi(i+1)-\phi(i-1)$ and $\phi(i)_{,xx}=\phi(i+2)+\phi(i-2)-2\phi(i)$ and similarly for higher derivatives. This choice of prescription is needed for two reasons, (i) it ensures that "summation by parts" (ignoring boundaries) is satisfied, which is important when taking variations of the action, (ii) it makes the successive application of two first derivatives the second derivative, etc. This is important when proving mimetism.

The Lagrangian is the generator of the canonical transformation that materializes evolution from instant n to instant $n+1$. Specifically, we will introduce the canonically conjugate momenta as we discussed in the preceding section,

$$P^h_{ab}(n+1,\vec{m})=p_{ab}(n,\vec{m}), \tag{23}$$

$$P^p_{ab}(n+1,\vec{m})=0, \tag{24}$$

$$P^N(n+1,m)=0, \tag{25}$$

$$P^N_a(n+1,m)=0, \tag{26}$$

$$P^h_{ab}(n,\vec{m})=p_{ab}(n,\vec{m})+N(n,\vec{m}-\vec{e}_a-\vec{e}_b)-N(n,\vec{m}-\vec{e}_a+\vec{e}_b)-N(n,\vec{m}+\vec{e}_a-\vec{e}_b)+N(n,\vec{m}+\vec{e}_a+\vec{e}_b)$$
$$-\delta_{ab}\sum_{c=1}^{3}(N(n,\vec{m}-2\vec{e}_c)-2N(n,\vec{m})+N(n,\vec{m}+2\vec{e}_c))+\frac{1}{2}\sum_{c=1}^{3}[(h_{ab}(n,\vec{m})-h_{ab}(n,\vec{m}-2\vec{e}_c))$$
$$-(h_{ab}(n,\vec{m}+2\vec{e}_c)-h_{ab}(n,\vec{m}))]-\frac{1}{2}\sum_{c=1}^{3}[(h_{ac}(n,\vec{m}+\vec{e}_b-\vec{e}_c)-h_{ac}(n,\vec{m}-\vec{e}_b-\vec{e}_c))$$

$$- (h_{ac}(n,\vec{m}+\vec{e}_b+\vec{e}_c) - h_{ac}(n,\vec{m}-\vec{e}_b+\vec{e}_c))] - \frac{1}{2}\sum_{c=1}^{3}[(h_{bc}(n,\vec{m}+\vec{e}_a-\vec{e}_c)$$

$$- h_{bc}(n,\vec{m}-\vec{e}_a-\vec{e}_c)) - (h_{bc}(n,\vec{m}+\vec{e}_a+\vec{e}_c) - h_{bc}(n,\vec{m}-\vec{e}_a+\vec{e}_c))] - \frac{1}{2}\delta_{ab}\sum_{c,d=1}^{3}[(h_{dd}(n,\vec{m})$$

$$- h_{dd}(n,\vec{m}-2\vec{e}_c)) - (h_{dd}(n,\vec{m}+2\vec{e}_c) - h_{dd}(n,\vec{m}))] + \frac{\delta_{ab}}{2}\sum_{c,d=1}^{3}[h_{cd}(n,\vec{m}+\vec{e}_d-\vec{e}_c)$$

$$- h_{cd}(n,\vec{m}-\vec{e}_d-\vec{e}_c) - h_{cd}(n,\vec{m}+\vec{e}_c+\vec{e}_d) + h_{cd}(n,\vec{m}+\vec{e}_c-\vec{e}_d)]$$

$$+ \frac{1}{2}\sum_{c=1}^{3}[(h_{cc}(n,\vec{m}+\vec{e}_a-\vec{e}_b) - h_{cc}(n,\vec{m}-\vec{e}_a-\vec{e}_b)) - (h_{cc}(n,\vec{m}+\vec{e}_a+\vec{e}_b)$$

$$- h_{cc}(n,\vec{m}-\vec{e}_a+\vec{e}_b))], \tag{27}$$

$$P^{p}_{ab}(n,\vec{m}) = - (h_{ab}(n+1,\vec{m}) - h_{ab}(n,\vec{m})) + 2p_{ab}(n,\vec{m}) - \sum_{c=1}^{3} p_{cc}(n,\vec{m})\,\delta_{ab} + N_a(n,\vec{m}-\vec{e}_b)$$

$$- N_a(n,\vec{m}+\vec{e}_b) + N_b(n,\vec{m}-\vec{e}_a) - N_b(n,\vec{m}+\vec{e}_a), \tag{28}$$

$$P^{N_a}(n,m) = \sum_{b=1}^{3}[2p_{ab}(n,\vec{m}+\vec{e}_b) - 2p_{ab}(n,\vec{m}-\vec{e}_b)], \tag{29}$$

$$P^{N}(n,m) = \sum_{a,b=1}^{3}[h_{ab}(n,\vec{m}+\vec{e}_a+\vec{e}_b) - h_{ab}(n,\vec{m}-\vec{e}_a+\vec{e}_b) - h_{ab}(n,\vec{m}+\vec{e}_a-\vec{e}_b) + h_{ab}(n,\vec{m}-\vec{e}_a-\vec{e}_b)$$

$$- h_{aa}(n,\vec{m}+2\vec{e}_b) + 2h_{aa}(n,\vec{m}) - h_{aa}(n,\vec{m}-2\vec{e}_b)]. \tag{30}$$

The system has four primary constraints (24)–(27). Preserving these constraints in time implies, via (28)–(30) that the linearized Hamiltonian and momentum constraints are satisfied,

$$C_a = 2\sum_{b=1}^{3}[P^{h}_{ab}(n,\vec{m}+\vec{e}_b) - P^{h}_{ab}(n,\vec{m}-\vec{e}_b)] = 0, \tag{31}$$

$$C = \sum_{a,b=1}^{3}[h_{ab}(n,\vec{m}+\vec{e}_a+\vec{e}_b) - h_{ab}(n,\vec{m}-\vec{e}_a+\vec{e}_b) - h_{ab}(n,\vec{m}+\vec{e}_a-\vec{e}_b) + h_{ab}(n,\vec{m}-\vec{e}_a-\vec{e}_b)$$

$$- h_{aa}(n,\vec{m}+2\vec{e}_b) + 2h_{aa}(n,\vec{m}) - h_{aa}(n,\vec{m}-2\vec{e}_b)] = 0. \tag{32}$$

Constraints (24) and (27) can be imposed strongly, the second constraint determines the variable p_{ab}. This eliminates the variable p_{ab} and its canonically conjugate momenta from the theory.

We now combine (23) and (27) to get the evolution equation for P^h,

$$P^{h}_{ab}(n+1,\vec{m}) = P^{h}_{ab}(n,\vec{m}) - N(n,\vec{m}-\vec{e}_a-\vec{e}_b) + N(n,\vec{m}-\vec{e}_a+\vec{e}_b) + N(n,\vec{m}+\vec{e}_a-\vec{e}_b)$$

$$- N(n,\vec{m}+\vec{e}_a+\vec{e}_b) + \delta_{ab}\sum_{c=1}^{3}(N(n,\vec{m}-2\vec{e}_c) - 2N(n,\vec{m}) + N(n,\vec{m}+2\vec{e}_c))$$

$$- \frac{1}{2}\sum_{c=1}^{3}[(h_{ab}(n,\vec{m}) - h_{ab}(n,\vec{m}-2\vec{e}_c)) - (h_{ab}(n,\vec{m}+2\vec{e}_c) - h_{ab}(n,\vec{m}))]$$

$$+\frac{1}{2}\sum_{c=1}^{3}[(h_{ac}(n,\vec{m}+\vec{e}_b-\vec{e}_c)-h_{ac}(n,\vec{m}-\vec{e}_b-\vec{e}_c))-(h_{ac}(n,\vec{m}+\vec{e}_b+\vec{e}_c)$$

$$-h_{ac}(n,\vec{m}-\vec{e}_b+\vec{e}_c))]+\frac{1}{2}\sum_{c=1}^{3}[(h_{bc}(n,\vec{m}+\vec{e}_a-\vec{e}_c)-h_{bc}(n,\vec{m}-\vec{e}_a-\vec{e}_c))$$

$$-(h_{bc}(n,\vec{m}+\vec{e}_a+\vec{e}_c)-h_{bc}(n,\vec{m}-\vec{e}_a+\vec{e}_c))]+\frac{1}{2}\delta_{ab}\sum_{c,d=1}^{3}[(h_{dd}(n,\vec{m})$$

$$-h_{dd}(n,\vec{m}-2\vec{e}_c))-(h_{dd}(n,\vec{m}+2\vec{e}_c)-h_{dd}(n,\vec{m}))]$$

$$-\frac{\delta_{ab}}{2}\sum_{c,d=1}^{3}[(h_{cd}(n,\vec{m}+\vec{e}_d-\vec{e}_c)-h_{cd}(n,\vec{m}-\vec{e}_d-\vec{e}_c))-(h_{cd}(n,\vec{m}+\vec{e}_c+\vec{e}_d)$$

$$-h_{cd}(n,\vec{m}+\vec{e}_c-\vec{e}_d))]-\frac{1}{2}\sum_{c=1}^{3}[(h_{cc}(n,\vec{m}+\vec{e}_a-\vec{e}_b)-h_{cc}(n,\vec{m}-\vec{e}_a-\vec{e}_b))$$

$$-(h_{cc}(n,\vec{m}+\vec{e}_a+\vec{e}_b)-h_{cc}(n,\vec{m}-\vec{e}_a+\vec{e}_b))], \tag{33}$$

and from (28) we get the evolution equation for h,

$$h_{ab}(n+1,\vec{m})=h_{ab}(n,\vec{m})+2P^h_{ab}(n,\vec{m})-\delta_{ab}\sum_{f=1}^{3}P^h_{ff}(n,\vec{m})+N_a(n,\vec{m}-\vec{e}_b)-N_a(n,\vec{m}+\vec{e}_b)$$

$$+N_b(n,\vec{m}-\vec{e}_a)-N_b(n,\vec{m}+\vec{e}_a)-2N(n,\vec{m}-\vec{e}_a-\vec{e}_b)+2N(n,\vec{m}-\vec{e}_a+\vec{e}_b)$$

$$+2N(n,\vec{m}+\vec{e}_a-\vec{e}_b)-2N(n,\vec{m}+\vec{e}_a+\vec{e}_b)-\sum_{c=1}^{3}[2h_{ab}(n,\vec{m})-h_{ab}(n,\vec{m}-2\vec{e}_c)$$

$$-h_{ab}(n,\vec{m}+2\vec{e}_c)]+\sum_{c=1}^{3}[h_{ac}(n,\vec{m}+\vec{e}_b-\vec{e}_c)-h_{ac}(n,\vec{m}-\vec{e}_b-\vec{e}_c)-h_{ac}(n,\vec{m}+\vec{e}_b+\vec{e}_c)$$

$$+h_{ac}(n,\vec{m}-\vec{e}_b+\vec{e}_c)]+\sum_{c=1}^{3}[h_{bc}(n,\vec{m}+\vec{e}_a-\vec{e}_c)-h_{bc}(n,\vec{m}-\vec{e}_a-\vec{e}_c)$$

$$-h_{bc}(n,\vec{m}+\vec{e}_a+\vec{e}_c)+h_{bc}(n,\vec{m}-\vec{e}_a+\vec{e}_c)]+\frac{1}{2}\delta_{ab}\sum_{c,d=1}^{3}[2h_{dd}(n,\vec{m})-h_{dd}(n,\vec{m}-2\vec{e}_c)$$

$$-h_{dd}(n,\vec{m}+2\vec{e}_c)]-\frac{1}{2}\delta_{ab}\sum_{c,d=1}^{3}[h_{cd}(n,\vec{m}+\vec{e}_d-\vec{e}_c)-h_{cd}(n,\vec{m}-\vec{e}_d-\vec{e}_c)$$

$$-h_{cd}(n,\vec{m}+\vec{e}_c+\vec{e}_d)+h_{cd}(n,\vec{m}+\vec{e}_c-\vec{e}_d)]-\sum_{c=1}^{3}[h_{cc}(n,\vec{m}+\vec{e}_a-\vec{e}_b)$$

$$-h_{cc}(n,\vec{m}-\vec{e}_a-\vec{e}_b)-h_{cc}(n,\vec{m}+\vec{e}_a+\vec{e}_b)+h_{cc}(n,\vec{m}-\vec{e}_a+\vec{e}_b)]. \tag{34}$$

A first point to be noted is that the evolution equations have resulted in an explicit evolution scheme. This is usually not the case, it is a particularity of the linearized theory that the evolution is explicit. It should be noted that the evolution equations obtained are just a straightforward discretization of the evolution equations one would obtain in the continuum by working out the variations of the continuum action.

We have checked, using a computer algebra code, that the evolution equations (34) and (33) exactly preserve the constraints (31) and (32), or more precisely that

$$C_a(n+1,m) = C_a(n,m), \tag{35}$$

$$C(n+1,m) = C(n,m) + \sum_{a=1}^{3} [C_a(n,m+\vec{e}_a) - C_a(n,m-\vec{e}_a)]. \tag{36}$$

This result was expected since we used differentiation operators that ensure that mixed discrete spatial derivatives commute, and that one can integrate by parts (more precisely "sum by parts"), and that is all that is needed in a linear theory on a Minkowski background to show that the constraints are preserved upon evolution. It is interesting to compare this result with that of Meier.[3] He finds a mimetic discretization of linearized general relativity around Minkowski space–time, but using staggered grids. This is a natural approach, for instance, in electromagnetism and Yang–Mills theory (and it is the one we will take in the next section where we deal with gravity with the Ashtekar variables).

It would be interesting to generalize these results to the case of linearization around a static background. In that case it is not obvious that the formulation would result automatically mimetic. In fact, the failure of the Leibnitz rule at a discrete level implies that it will be difficult to find a mimetic formulation since the equations now will have nonconstant coefficients and one will need Leibnitz' rule to show conservation. Our formalism will yield a consistent formulation, but it is possible that it will require determining the Lagrange multipliers.

C. Stability

We have discretized the time derivatives without centering them (that is, we have used a stencil that is first order accurate only). The reason for this is that the canonical theory is much cleaner with only two levels in time involved in the derivatives. It is possible to use derivatives that are second order accurate in time and use our construction by rewriting the theory in terms of new variables in such a way that the resulting theory has derivatives that are first order accurate, but we will not do this here.

The spatial derivatives, on the other hand, were centered (this was required in order to have summation by parts). The resulting scheme is therefore "forward in time centered in space," a recipe that is not stable, for instance, for the advection or the wave equation. We therefore would like to check if our scheme is stable. To simplify things, we will consider (34) and (33) and make the following assumptions: the metric and extrinsic curvatures are diagonal and only depend on the coordinates t,x, the lapse is unity and the shift is zero. The resulting equations therefore are

$$P^h_{11}(n+1,\vec{m}) = P^h_{11}(n,\vec{m}) - \frac{1}{2}\sum_{c=2}^{3} [2h_{cc}(n,\vec{m}) - h_{cc}(n,\vec{m}-2\vec{e}_1) - h_{cc}(n,\vec{m}+2\vec{e}_1)], \tag{37}$$

$$P^h_{22}(n+1,\vec{m}) = P^h_{22}(n,\vec{m}) + \tfrac{1}{2}[2h_{33}(n,\vec{m}) - h_{33}(n,\vec{m}-2\vec{e}_1) - h_{33}(n,\vec{m}+2\vec{e}_1)], \tag{38}$$

$$P^h_{33}(n+1,\vec{m}) = P^h_{33}(n,\vec{m}) + \tfrac{1}{2}[2h_{22}(n,\vec{m}) - h_{22}(n,\vec{m}-2\vec{e}_1) - h_{22}(n,\vec{m}+2\vec{e}_1)], \tag{39}$$

$$\begin{aligned} h_{11}(n+1,\vec{m}) = h_{11}(n,\vec{m}) + 2P^h_{11}(n,\vec{m}) - \sum_{f=1}^{3} P^h_{ff}(n,\vec{m}) - \frac{1}{2}\sum_{d=2}^{3} [2h_{dd}(n,\vec{m}) - h_{dd}(n,\vec{m}-2\vec{e}_1) \\ - h_{dd}(n,\vec{m}+2\vec{e}_1)], \end{aligned} \tag{40}$$

$$h_{22}(n+1,\vec{m}) = h_{22}(n,\vec{m}) + 2P^h_{22}(n,\vec{m}) - \sum_{f=1}^{3} P^h_{ff}(n,\vec{m}) - \frac{1}{2}[2h_{22}(n,\vec{m}) - h_{22}(n,\vec{m}-2\vec{e}_1)$$

$$- h_{22}(n,\vec{m}+2\vec{e}_1)] + \frac{1}{2}[2h_{33}(n,\vec{m}) - h_{33}(n,\vec{m}-2\vec{e}_1) - h_{33}(n,\vec{m}+2\vec{e}_2)], \quad (41)$$

$$h_{33}(n+1,\vec{m}) = h_{33}(n,\vec{m}) + 2P^h_{33}(n,\vec{m}) - \sum_{f=1}^{3} P^h_{ff}(n,\vec{m}) - \frac{1}{2}[2h_{33}(n,\vec{m}) - h_{33}(n,\vec{m}-2\vec{e}_1)$$

$$- h_{33}(n,\vec{m}+2\vec{e}_1)] + \frac{1}{2}[2h_{22}(n,\vec{m}) - h_{22}(n,\vec{m}-2\vec{e}_1) - h_{22}(n,\vec{m}+2\vec{e}_2)]. \quad (42)$$

As a test case, we concentrate on a subfamily of solutions of the equations, in which $h_{11}=P_{11}=0$ and $h_{22}=-h_{33}$ and $P_{22}=-P_{33}$. In that case, the equations reduce to

$$P^h_{22}(n+1,\vec{m}) = P^h_{22}(n,\vec{m}) - \tfrac{1}{2}[2h_{22}(n,\vec{m}) - h_{22}(n,\vec{m}-2\vec{e}_1) - h_{22}(n,\vec{m}+2\vec{e}_1)], \quad (43)$$

$$h_{22}(n+1,\vec{m}) = h_{22}(n,\vec{m}) + 2P^h_{22}(n,\vec{m}) - [2h_{22}(n,\vec{m}) - h_{22}(n,\vec{m}-2\vec{e}_1) - h_{22}(n,\vec{m}+2\vec{e}_1)]. \quad (44)$$

We have performed a Von Neumann analysis of this system and confirmed that the scheme is stable provided the Courant factor is less than 1. So at least for this particular subcase the scheme is stable. A more complete analysis is needed to guarantee stability in general.

IV. LINEARIZED GENERAL RELATIVITY IN TERMS OF ASHTEKAR VARIABLES

A. Continuum formulation

We will now apply the technique we outlined in the preceding section to general relativity linearized around Minkowski space using the Ashtekar formulation. The formulation of linearized gravity with the new variables was first discussed by Ashtekar and Lee.[9] The discussion presented in that paper required the use of complex variables if one was to describe general relativity with metrics with a Lorentzian signature (alternatively, one could consider real variables, but then the theory described the Euclidean signature sector). Developments that have taken place in the field since the publication of that paper that allow one to consider the Lorentzian sector using real variables,[10,11] but we will see that the discretized theory is more problematic in this case and we will not discuss it in detail in this paper.

The Ashtekar canonical variables consist of a set of triads with density weight 1, E^{ai} and a (complex) SO(3) connection A_{ai}. In this notation $a,b,\ldots$ are spatial vector indices and $i,j,\ldots$ range from 1 to 3. Following Ashtekar and Lee we omit using tildes to denote density weights since in this context they do not play an important role. To linearize the theory around Minkowski, we choose a fixed background ($E^{ai}=E^{ai}_0, A_{ai}=0$) in the phase space and consider fluctuations around it. In Cartesian coordinates, $E^{ai}_0=\delta^{ai}$. The triad is therefore given by

$$E^{ai} = \delta^{ai} + e^{ai}, \quad (45)$$

and therefore the background metric has components $q^{ab}=\delta^{ab}$ and its determinant is unity and therefore density weights are all trivial. We will denote by A_{ai} the fluctuations of the connection. The Poisson bracket of the canonical variables is $\{e^{ai}(x),A_{bj}(y)\}=i\delta^a_b\delta^i_j\delta(x-y)$.

The Ashtekar formulation has, in addition to the usual diffeomorphism and Hamiltonian constraints of the metric canonical formulation of general relativity, a set of additional constraints that make the formulation invariant under triad rotations. The additional constraints take the form of a Gauss law, which linearized will read

$$\mathcal{G}_L^i = \partial_a e^{ai} + \epsilon^{ija} A_{aj} = 0, \tag{46}$$

where from now on the subscript L means we have kept the minimum required number of terms in the perturbative expansion. In spite of the second term, one can check that if one computes the Poisson bracket of two Gauss laws, they commute, that is, they form an Abelian algebra. The internal symmetry group of the linearized theory is therefore U(1) (Ref. 3).

Ignoring boundary terms, the (super-) Hamiltonian for general relativity can be written as

$$H = \int \mathrm{d}^3x \left[N E_i^a E_j^b \left(F_{ab}^k \epsilon_{ijk} - \frac{(\beta^2 - \sigma)}{\beta^2} (\Gamma_a^i - \sigma\beta A_a^i)(\Gamma_b^j - \sigma\beta A_b^j) \right) + N^a E_i^a F_{ab}^i \right], \tag{47}$$

and in the full theory it vanishes identically. The parameter β is called the Immirzi parameter and the parameter σ is equal to +1 for the Euclidean case and −1 for the Lorentzian signature. Classically, different values of the Immirzi parameter correspond to different representations of the same theory. The quantities Γ_a^i are the spin connections compatible with the triads, defined by

$$\partial_{[a} \overline{E^i}_{b]} + \epsilon_{jk}^i \Gamma_{[a}^j \overline{E^k}_{b]} = 0, \tag{48}$$

where the $\overline{E}$'s are the triads (without density weight), related to the Ashtekar variables by $E_i^a = \det(\overline{E}) \overline{E}_i^a$, or equivalently, $E_i^a = \overline{E_b^j} \overline{E_c^k} \epsilon^{abc} \epsilon_{ijk}$. Indices are lowered and raised with the flat Euclidean metric. One can obtain an explicit expression for the spin connection in terms of the triads,

$$\Gamma_c^i = \epsilon_c^{ab} (\partial_a e_b^i - \partial_a \mathrm{Tr}(e) \delta_b^i). \tag{49}$$

To study it in the linearized theory, we need to choose a lapse and a shift. The natural choice is to use as zeroth order lapse and shift the ones that would preserve the spatial background metric explicitly time independent. This corresponds to a lapse $N=1$ and a shift $N^a=0$. So we will write $N_L = 1 + \nu$ and $N_L^a = \nu^a$, and these will become Lagrange multipliers in the linearized theory. The super-Hamiltonian then separates into two pieces, one that acts as a Hamiltonian and another piece that is given by the Lagrange multipliers times constraints of the linearized theory. These constraints are

$$C_a^L = -i f_{ab}^b = 0, \tag{50}$$

$$C^L = -i \epsilon_c^{ab} f_{ab}^c = 0, \tag{51}$$

where $f_{ab}^i = 2\partial_{[a} A^i{}_{b]}$ is the linearized field strength, and the first one is the linearized momentum constraint and the latter the linearized Hamiltonian constraint. The nonvanishing Hamiltonian for the linearized theory is given by

$$H_L = \int \mathrm{d}^3x \left(2\epsilon_k^{ib} f_{ab}^k e_i^a + (A_a^a A_b^b - A_a^b A_b^a) - \frac{\beta^2 - \sigma}{\beta^2} [(\Gamma_a^a - \sigma\beta A_a^a)(\Gamma_a^b - \sigma\beta A_a^b)) \right.$$
$$\left. - (\Gamma_a^b - \sigma\beta A_a^b)(\Gamma_b^a - \sigma\beta A_b^a) \right]. \tag{52}$$

B. Discretizing the full theory on the lattice

In this section we review some results of Refs. 4 and 5 where we discretized general relativity on the lattice. In the next section we will particularize these results to the case of linearized general relativity. We start by considering an action for general relativity written in terms of Ashtekar's variables (see for instance Ref. 12 and the book by Ashtekar,[13] p. 47),

$$L = \int E^{ai} F^{i}_{a0} - H, \tag{53}$$

where N and N^a are the lapse and shift and H the super-Hamiltonian (47). We will particularize to the Euclidean case $\sigma=1$ and choose the Immirzi parameter $\beta=1$ which correspond to the original form of Ashtekar's variables, for simplicity (see Sec. VI for more details). From now on we will not assume Einstein's summation convention and present the summations explicitly, since many expressions would otherwise be confusing. The Lagrangian can be discretized as follows:

$$L(n,n+1) = -\frac{1}{4}\sum_{v} \mathrm{Tr}\Bigg[\sum_{a} E^{a}_{n,v}(h^{a0}_{n,v} - h^{0a}_{n,v}) - \sum_{a,b} K^{ab}_{n,v}(h^{ab}_{n,v} - h^{ba}_{n,v}) + \sum_{a} \alpha_{a,n,v}(h^{a}_{n,v}(h^{a}_{n,v})^{\dagger} - 1) + \beta_{n,v}(h^{0}_{n,v}(h^{0}_{n,v})^{\dagger} - 1)\Bigg], \tag{54}$$

where h^{a}_{n+1} represents an holonomy along the a direction at instant $n+1$, h^{0}_{n} represents the "vertical" (timelike) holonomy. The holonomy associated with a plaquette in the $\alpha\beta$ $(\alpha\neq\beta)$ plane $(\alpha,\beta=0,\ldots,3)$ is

$$h^{\alpha\beta}_{n,v} \equiv h^{\alpha}_{n,v} h^{\beta}_{n,v+e_\alpha} (h^{\alpha}_{n,v+e_\beta})^{\dagger} (h^{\beta}_{n,v})^{\dagger}, \tag{55}$$

and

$$K^{ab}_{n,v} \equiv \tfrac{1}{2}[(E^{a}_{n,v}E^{b}_{n,v} - E^{b}_{n,v}E^{a}_{n,v})N_{n,v} + N^{a}_{n,v}E^{b}_{n,v} - N^{b}_{n,v}E^{a}_{n,v}]. \tag{56}$$

We will assume that the holonomies are matrices of the form $h=\Sigma_I h^I T^I$ where $T^0=I$ and $T^a=-i\sigma^a$ where σ^a are the Pauli matrices. The indices n,v represent a label for "time" n and a spatial label for the vertices of the lattice v. The elementary unit vectors along the spatial directions are labeled as e_a, so for instance $n+e_1$ labels the nearest neighbor to n along the e_1 direction. The unit vector in the timelike direction is e_0 and we chose $h^{\alpha}_{n,v+e_0} \equiv h^{\alpha}_{n+1,v}$. The quantities $E^{a}_{n,v}$ are elements of the algebra of su(2) and α and β are Lagrange multipliers, the last two terms of the Lagrangian enforcing the condition that the holonomies are elements of SU(2). We use the usual conventions of lattice gauge theories in which one has oriented links and the natural variables are the holonomies in a given orientation and based at a given vertex. If we need to traverse back, as in the case of closed loops one then considers the adjoint of the holonomy based at the vertex one is ending at.

The discretization of the field tensor is based on

$$F^{i}_{ab} \to -\tfrac{1}{4}\mathrm{Tr}[(h^{ab}_{n,v} - h^{ba}_{n,v})T^{i}]. \tag{57}$$

Instead of working out the equations of motion for this action, we will, in the next section, particularize it to the linearized case and work out the relevant equations of motion, which is equivalent to working the equations first and then linearizing if appropriate perturbative orders are kept.

C. The linearized theory on the lattice

We now proceed to linearize the action. We start with the holonomies. The explicit form of the linearized holonomy is

$$h^{\alpha}_{v} = 1 + \sum_{i} \phi^{\alpha i}_{v} T^{i}, \tag{58}$$

where we have dropped the subscript n we used in the last section to indicate the time level in order to make the notation more compact (but we will make it explicit when things are evaluated at $n+1$). In this equation $\phi^{\alpha i}_{v} T^{i}$ is an element of the algebra that can be viewed as a "phase" (it corresponds to the logarithm of the path-ordered exponential of the connection along the direction

α). The holonomy of a plaquette in the plane $\alpha\beta$ is (neglecting higher order terms)

$$h_v^{\alpha\beta} = h_v^{\alpha} h_{v+e_\alpha}^{\beta} (h_{v+e_\beta}^{\alpha})^{\dagger} (h_v^{\beta})^{\dagger} = \left(1 - \sum_i \Phi_{2v}^{\alpha\beta ii}\right) 1 + \sum_i (\Phi_{1v}^{\alpha\beta i} + \Phi_{2v}^{\alpha\beta i}) T^i. \tag{59}$$

The first order contribution is

$$\Phi_{1v}^{\alpha\beta k} \equiv + \phi_v^{\alpha k} - \phi_v^{\beta k} - \phi_{v+\hat{e}_\beta}^{\alpha k} + \phi_{v+\hat{e}_\alpha}^{\beta k}, \tag{60}$$

and the second order contribution is

$$\Phi_{2v}^{\alpha\beta ij} \equiv - \phi_v^{\alpha i} \phi_v^{\beta j} + \phi_v^{\alpha i} \phi_{v+\hat{e}_\alpha}^{\beta j} + \phi_{v+\hat{e}_\beta}^{\alpha i} \phi_v^{\beta j} - \phi_{v+\hat{e}_\beta}^{\alpha j} \phi_{v+\hat{e}_\alpha}^{\beta i} - \phi_v^{\alpha i} \phi_{v+\hat{e}_\beta}^{\alpha j} - \phi_v^{\beta j} \phi_{v+\hat{e}_\alpha}^{\beta i}, \tag{61}$$

$$\Phi_{2v}^{\alpha\beta k} \equiv \sum_{ij} \epsilon^{ijk} \Phi_{2v}^{\alpha\beta ij}. \tag{62}$$

We now linearize the expression for K defined in the preceding section, by noting that to first order,

$$e_v^a = \sum_i (\delta^{ai} + e_v^{ai}) T^i \tag{63}$$

and ignoring higher order terms we get that

$$K_v^{ab} = \sum_i (\epsilon^{abi} + K_{1,v}^{abi}) T^i \tag{64}$$

with

$$K_1^{abk} \equiv \epsilon^{abk} \nu_v + \frac{1}{2} (\nu_v^a \delta^{bk} - \nu_v^b \delta^{ak}) + \sum_i (e_v^{ai} \epsilon^{ibk} - e_v^{bi} \epsilon^{iak}). \tag{65}$$

We now consider the first term in the discretized Lagrangian (54). Substituting the expression for the holonomy around a plaquette (59) we get the following identity, valid up to second order:

$$-\frac{1}{4} \mathrm{Tr} \left[\sum_a E_{n,v}^a (h_{n,v}^{a0} - h_{n,v}^{0a}) \right] = \sum_a \Phi_{1v}^{a0a} + \sum_a \Phi_{2v}^{a0a} + \sum_{ak} e_v^{ak} \Phi_{1v}^{a0k} \tag{66}$$

and we note that when one considers the sum over all vertices, the first term on the right-hand side yields a total derivative with respect to time that can be ignored in the Lagrangian.

For the second term in (54) we use (59) and (64), getting the following identity, valid up to second order:

$$\frac{1}{4} \mathrm{Tr} \left[\sum_{ab} K_{n,v}^{ab} (h_{n,v}^{ab} - h_{n,v}^{ba}) \right] = - \sum_{abk} (\epsilon^{abk} \Phi_{1v}^{abk} + \epsilon^{abk} \Phi_{2v}^{abk} + K_{1v}^{abk} \Phi_{1v}^{abk}). \tag{67}$$

When one considers the sum over all vertices the first term on the right-hand side of this expression vanishes. The resulting Lagrangian therefore can be written as

$$\begin{aligned} L = - \sum_v \Bigg\{ & \sum_{ai} e_v^{ai} (\phi_{n+1,v}^{ai} - \phi_{n,v}^{ai}) + \sum_{ijk} \epsilon_{ijk} (\phi_v^{ij} \phi_{n+1,v}^{ik} + \Phi_{2v}^{ijk} + \nu_v \Phi_{1v}^{ijk}) + \sum_{aijk} 2 e_v^{ai} \epsilon^{ijk} \Phi_{1v}^{ajk} + \sum_{ab} \nu_v^a \Phi_{1v}^{abb} \\ & + \sum_{ij} (\phi_v^{0i} - \phi_{v+\hat{e}_j}^{0i}) e_v^{ji} + \sum_{ijk} \epsilon_{ijk} \phi_v^{0i} (\phi_{n+1,v}^{kj} + \phi_{v+\hat{e}_j}^{0k} + \phi_v^{jk}) - \sum_{ijk} \phi_{v+\hat{e}_j}^{0i} \epsilon_{ijk} (\phi_v^{jk} + \phi_{n+1,v}^{jk}) \Bigg\}. \end{aligned} \tag{68}$$

Now that we have an explicit expression for the Lagrangian we can proceed to identify the various terms. The theory has the following Lagrange multipliers: ϕ_v^{0i} the "vertical component of the phase" (which plays a role analogous to the time component of the vector potential in Maxwell

theory) and the linearized lapse and shift. These quantities multiply times the constraints of the linearized theory. Explicitly, the momentum and Hamiltonian constraint read

$$C_v^a = \sum_b \Phi_{1v}^{abb}, \tag{69}$$

$$C_v = \sum_{ijk} \epsilon_{ijk} \Phi_{1v}^{ijk}. \tag{70}$$

In order to get Gauss' law, we first take the variation of the Lagrangian with respect to the Lagrange multiplier ϕ_v^{0i} to get

$$G_v^i \equiv \sum_a (\xi_{n+1,v}^{ai} + \xi_{n+1,v}^{\bar{a}i}) = 0, \tag{71}$$

where

$$\xi_{n+1,v}^{ai} \equiv + \delta^{ai} + e_{n,v}^{ai} + \sum_k \epsilon_{aik}(- \phi_{n,v}^{ak} - \phi_{n,v+\hat{e}_a}^{0k} - \phi_{n,v}^{0k} + \phi_{n+1,v}^{ak}), \tag{72}$$

$$\xi_{n+1,v}^{\bar{a}i} \equiv - \delta^{ai} - e_{n,v-\hat{e}_a}^{ai} + \sum_k \epsilon_{aik}(\phi_{n,v-\hat{e}_a}^{ak} + \phi_{n,v}^{0k} + \phi_{n,v-\hat{e}_a}^{0k} + \phi_{n+1,v-\hat{e}_a}^{ak}). \tag{73}$$

At the moment this does not appear to be a true constraint since it involves variables at instant n and at instant $n+1$. To see that it actually is a constraint, we will call $\xi_{n+1,v}^{ai}$ the component in the direction $\hat{e}_a$ of a quantity that we will think of as an "electric field" (in the sense that it is the quantity that satisfies the usual form of Gauss law) and we will call $\xi_{n+1,v}^{\bar{a}i}$ the component in the direction $-\hat{e}_a$, both at point $(n+1,v)$. To make this more transparent, we need to see how they transform under gauge transformations. To leading order the field $e_{n,v}^a$ is $e_{0,n,v}^a = \Sigma_i \delta^{ai} T^i$. We then define

$$\check{e}_{n,v}^a = e_{n,v}^a + \frac{1}{4}[h_{n,v}^{0a} e_{0,n,v}^a (h_{n,v}^{0a})^\dagger - h_{n,v}^{a0} e_{0,n,v}^a (h_{n,v}^{a0})^\dagger] = e_{n,v}^a + \sum_{jk} \epsilon_{ajk} \Phi_{1v}^{0ak} T^j, \tag{74}$$

with the second equality valid up to second order. By inspection one sees that the field $\check{e}_{n,v}^a$ is an element of the algebra that transforms like an electric field at (n,v) under gauge transformation. One can also show the following identities, valid to first order:

$$\xi_{n+1,v}^a \equiv \sum_i \xi_{n+1,v}^{ai} T^i = (h_{n,v}^0)^\dagger \check{e}_{n,v}^a h_{n,v}^0, \tag{75}$$

$$\xi_{n+1,v}^{\bar{a}} \equiv \sum_i \xi_{n+1,v}^{\bar{a}i} T^i = - (h_{n+1,v-\hat{e}_a}^a)^\dagger \xi_{n+1,v-\hat{e}_a}^a h_{n+1,v-\hat{e}_a}^a \tag{76}$$

from which one immediately sees that the quantities we identified as components of the electric field have the appropriate transformation properties under gauge transformations.

Therefore we can identify (71) as the usual intuitive expression of Gauss' law stating that field lines cannot emanate from a point in vacuum.

We now turn our attention to the equations of motion. Given the Lagrangian (68) we work out the equations of motion from the canonical transformation. We start by computing the canonical conjugate momentum to e,

$$P_{n+1,v}^{(e)ak} \equiv \frac{\partial L(n,n+1)}{\partial e_{n+1,v}^{ak}} = 0, \tag{77}$$

$$P_v^{(e)ak} \equiv -\frac{\partial L(n,n+1)}{\partial e_v^{ak}} = -\Phi_{1v}^{a0k} + 2\sum_{ij} \epsilon^{kij}\Phi_{1v}^{aij} = 0. \tag{78}$$

Therefore the dynamics of $P^{(e)}$ is trivial. However, the last equation can be viewed as an evolution equation for ϕ through (60),

$$\phi_{n+1,v}^{ak} = \phi_v^{ak} - \phi_v^{0k} + \phi_{v+\hat{e}_a}^{0k} - 2\sum_{ij} \epsilon^{kij}\Phi_{1v}^{aij}. \tag{79}$$

Notice that by adding over indices a belonging to a given plaquette equation (79), one effectively gets an evolution equation for all the horizontal ϕ's in the plaquette. This is due to the fact that the vertical contributions in (60) will cancel out in pairs when adding through the plaquette. Explicitly,

$$\Phi_{1,n+1,v}^{abk} = \Phi_{1v}^{abk} - 2\sum_{ij} \epsilon^{kij}(\Phi_{1v}^{aij} + \Phi_{1v+\hat{e}_a}^{bij} - \Phi_{1v+\hat{e}_b}^{aij} - \Phi_{1v}^{bij}) \equiv \Phi_{1v}^{abk} - 2\sum_{ij} \epsilon^{kij} \sum_{d\in P_{ab}} \Phi_{1v_d}^{dij}, \tag{80}$$

where in the last term v_d is the vertex in which the link d originates and P_{ab} is the plaquette spanned by a and b.

We now consider the momentum canonically conjugate to ϕ. We start by computing the canonical conjugate momentum at instant $n+1$,

$$P_{n+1,v}^{(\phi)ak} \equiv \frac{\partial L(n,n+1)}{\partial \phi_{n+1,v}^{ak}} = -e_v^{ak} + \sum_i \epsilon^{aki}(\phi_v^{ai} + \phi_v^{0i} + \phi_{v+\hat{e}_a}^{0i}). \tag{81}$$

The momentum can be written in terms of the electric field in an expression that parallels the usual relation between the electric field and the canonical momentum in the lattice ξ^{ak} as

$$P_{n+1,v}^{(\phi)ak} = \delta_{ak} - \xi_{n+1,v}^{ak} + \sum_i \epsilon_{aki}\phi_{n+1,v}^{ai} \tag{82}$$

and in terms of it, Gauss' law (71) can be written as

$$G_{n+1,v}^{k} = -\sum_a \left(P_{n+1,v}^{(\phi)ak} - P_{n+1,v-\hat{e}_a}^{(\phi)ak} - \sum_i \epsilon^{aki}(\phi_{n+1,v}^{ai} + \phi_{n+1,v-\hat{e}_a}^{ai}) \right). \tag{83}$$

This final expression for Gauss' law is a genuine constraint, in the sense that all variables are expressed at the same instant of time.

We now compute the momentum conjugate to ϕ at instant n,

$$\begin{aligned} P_v^{(\phi)ab} = -\frac{\partial L(n,n+1)}{\partial \phi_v^{ab}} &= -e_v^{ab} + \nu_v^a - \nu_{v-\hat{e}_b}^a + \delta_{ab}\sum_i (-\nu_v^i + \nu_{v-\hat{e}_i}^i) + 2(-\phi_{v-\hat{e}_b}^{aa} + \phi_{v+\hat{e}_b}^{aa} + \phi_v^{ba} - \phi_{v+\hat{e}_a}^{ba} \\ &\quad - \phi_{v-\hat{e}_b}^{ba} - \phi_{v+\hat{e}_a-\hat{e}_b}^{ba}) + 2\delta_{ab}\sum_i (\phi_{v-\hat{e}_i}^{ai} - \phi_{v+\hat{e}_i}^{ai} - \phi_v^{ii} + \phi_{v+\hat{e}_a}^{ii} + \phi_{v-\hat{e}_i}^{ii} + \phi_{v+\hat{e}_a-\hat{e}_i}^{ii}) \\ &\quad + \sum_i \epsilon_{abi}(-2\nu_v + 2\nu_{v-\hat{e}_i} + \phi_v^{0i} - \phi_{v+\hat{e}_a}^{0i} - 2e_v^{aa} + 2e_{v-\hat{e}_i}^{aa} - 2e_v^{bi} + 2e_{v-\hat{e}_b}^{bi} - 2e_v^{ii} + 2e_{v-\hat{e}_i}^{ii} + \phi_{n+1,v}^{ai}) \\ &\quad + 2\delta_{ab}\sum_{i,j} \epsilon_{aij}(e_v^{ai} - e_{v-\hat{e}_j}^{ai}). \end{aligned} \tag{84}$$

One still needs to replace the expressions for the e's and for the ϕ's evaluated at instant $n+1$. The resulting substitutions lead to lengthy expressions that are not particularly illuminating, and will not be needed in what follows, so we will not display them here. We point out however, that the resulting scheme is not an explicit one for the $P^{(\phi)}$'s. Since these variables do not arise in the constraints, we do not need this evolution equation to show mimetism.

One now needs to show that the evolution is mimetic, that is, it preserves the discrete constraints (69), (70), and (83). Using the evolution equation (80) one gets that

$$C^a_{n+1,v} = C^a_v + C_v - C_{v+\hat{e}_a}, \tag{85}$$

$$C_{n+1,v} = C_v + 4\sum_a (C^a_{v+\hat{e}_a} - C^a_v). \tag{86}$$

To study the time evolution of Gauss' law one needs Eqs. (79), (81), and (84) and one gets that

$$G^k_{n+1,v} = G^k_{n,v}. \tag{87}$$

As in the preceding section, we have checked these identities using computer algebra.

V. DISCUSSION AND CONCLUSIONS

The consistent discretization scheme is such that it yields a set of discrete equations for the evolution equations and the constraints of general relativity that is compatible, that is, all can be solved simultaneously. It does so at the price of determining the Lagrange multipliers (the lapse and the shift). In the linearized case we have shown that one can discretize the theory in such a way that the Lagrange multipliers are not determined and nevertheless the theory is consistent.

When one discretizes a theory there is always an ambiguity in how to proceed. Among the ambiguities we have the dependence on how one chooses to represent the derivatives. What we have found is that in the linearized case one can choose certain derivative operators for which the Lagrange multipliers are not determined. It should be noted that the consistent discretization scheme would work even if one did not choose the derivatives this way, but the Lagrange multipliers will be determined in order to have a consistent set of equations. This is true both in the case of the traditional variables and also in the Ashtekar variables. In the latter case there is an additional element that is the presence of an extra constraint: the Gauss law. We have also chosen a specific way of discretizing the theory in such a way that Gauss' law is implemented exactly in the discrete theory (this is standard in Yang–Mills theory on the lattice, and implies that the discrete formulation is gauge invariant, and also that these discretizations are mimetic, though this is rarely emphasized in the Yang–Mills literature). In the case of the traditional variables, one can also associate mimetism with gauge invariance. The action we chose to work with is invariant under linearized coordinate transformations of the form $h'_{\mu\nu}=h_{\mu\nu}+\xi_{(\mu,\nu)}$. The discrete action, if one chooses a derivative operator such that the second derivatives coincide with the derivative of a first derivative and satisfies summation by parts, is invariant under a discrete version of the above symmetry. This symmetry is generated canonically by the discrete constraints. This explains in a geometrically nice way why mimetism was possible in the linearized case.

In the case of Lorentzian general relativity written in terms of Ashtekar's variables, the presence of the terms $(\Gamma^i_a - \sigma\beta A^i_a)$ in the Hamiltonian make it more difficult to discretize the action in such a way that the Gauss law is preserved exactly. This is because the Γ^i_a's have to be written in terms of the triads and the resulting expressions are not easy to discretize on the lattice preserving the internal symmetry (unlike the A^i_a's which are readily discretized by considering a parallel transport operator along the elementary links). It may be possible using dual lattices to discretize such terms in an invariant way, but this will require further study. There is no problem applying our discretization technique to this case directly, but what will happen is that the internal symmetry will be broken, the Lagrange multipliers associated with the Gauss law will be determined and the resulting discretization will not be mimetic in the traditional sense of the word. It is clear that further work is needed before this kind of discretizations will be useful numerically.

In the full nonlinear case either with the traditional or the new variables, the constraints involve both coordinates and momenta and therefore the application of our technique will determine the Lagrange multipliers and will therefore not furnish a mimetic discretization in the traditional sense. The resulting discrete theory is consistent, but it does so at the expense of determining the Lagrange multipliers. Based on what we learned from the linearized case, we can conclude that the only remaining possibility for a formulation that is mimetic in the traditional sense would be to implement the symmetries implied by the constraints exactly in the lattice.

Since the symmetries implied by the diffeomorphism constraint are broken by the introduction of the lattice it appears unlikely that such a formulation would ever be found.

The conclusion we can draw from this is that for the case of full nonlinear general relativity, the closest one can come to a formulation that preserves the constraints under evolution is the proposal of consistent discretizations we have introduced. Such proposal is not mimetic in the traditional sense in that it imposes the constraints by determining the Lagrange multipliers. This proposal has many new aspects that are currently in investigation. It has been successfully applied in cosmological examples and is now being studied in detail for the Gowdy space–times. If it works for this example, it is likely that it could be applied successfully in general, but this obviously requires further study.

Something to be noticed is that it is not clear that the formulations we presented are going to be useful numerically. In particular, the fact that they are not based on manifestly hyperbolic equations. We have presented a first step towards showing stability of the scheme in a particular situation, but a fuller analysis should be carried out to determine if the scheme is stable in general. Numerical relativity codes also use more sophisticated time stepping techniques than the one we use. It is clear, however, that our method can accommodate more elaborate discretizations of the time derivatives and the calculations in this paper could be repeated in that case. Another interesting point would be to attempt to apply the techniques in this paper to the several manifestly hyperbolic formulations of the Einstein equations that have been proposed in the last few years. Unfortunately, few of them have been worked out in the context of an action principle, but this difficulty could presumably be remedied. This would also allow one to study within our framework manifolds with boundaries.

Another element of interest is the impact of the choice of the derivative operators on the construction of consistent discrete theories. The consistent technique will work no matter what derivative operators are chosen. But here we have learned that one can choose them in such a way that the linearized theory is automatically mimetic. We would like to argue that the level of accuracy with which the consistent discretization enforces the constraints is improved when one chooses a formulation that is mimetic at the linear level, at least for weak fields. The argument is simple. In the consistent discretization scheme the constraints that are enforced exactly have the form $\phi(q_n, p_{n+1})=0$. The constraints one would like to see enforced are of the form $\phi(q_n, p_n)=0$. Starting from the former, and using the equations of motion one has that $\phi(q_n, p_n+O(p^2))=0$ where the terms that correct p_n are of order p^2 (or q^2 or mixed but quadratic). This is true if the theory is mimetic in the linearized level. Otherwise one would have $\phi(q_n, p_n+O(p))=0$. Therefore choosing a discretization that is mimetic at the linearized level, at least for weak fields, implies that the constraints are tracked more accurately in the full nonlinear theory when one discretizes consistently.

Summarizing, we have shown that the consistent discretization scheme we have introduced recently, when applied to general relativity discretized around Minkowski space–time yields a formulation that is mimetic. That is, a formulation in which the discrete constraints are exactly preserved upon discrete evolution. We have also argued that for the full nonlinear case, the use of consistent discretizations appears as a possibility to yield a formulation that is close to the intention of mimetic formulations, although only approximately.

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General relativity via complete integrals of the Hamilton–Jacobi equation

Enrique Montiel-Piña
Facultad de Ciencias Físico Matemáticas de la Universidad Autónoma de Puebla, Apartado Postal 1152, Puebla, Pue., México

Ezra Ted Newman
Department of Physics and Astronomy, University of Pittsburgh, Pennsylvania 15260

Gilberto Silva-Ortigoza
Facultad de Ciencias Físico Matemáticas de la Universidad Autónoma de Puebla, Apartado Postal 1152, Puebla, Pue., México

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The aim of this work is to present a formulation to general relativity, which is analogous to the null surface formulation, but now instead of starting with a complete integral of the eikonal equation we start with a complete integral of the Hamilton–Jacobi equation. In the first part of this work we show that on the space of solutions of a certain class of systems of six second-order partial differential equations, $u_{ss}=\Lambda(s,s^*,\gamma,u,u_s,u_{s^*},u_\gamma), u_{s^*s^*}=\Lambda^*(s,s^*,\gamma,u,u_s,u_{s^*},u_\gamma)$, $u_{\gamma\gamma}=\Upsilon(s,s^*,\gamma,u,u_s,u_{s^*},u_\gamma), u_{ss^*}=\Phi(s,s^*,\gamma,u,u_s,u_{s^*},u_\gamma)$, $u_{s\gamma}=\Psi(s,s^*,\gamma,u,u_s,u_{s^*},u_\gamma), u_{s^*\gamma}=\Psi^*(s,s^*,\gamma,u,u_s,u_{s^*},u_\gamma)$, a four-dimensional (definite or indefinite) metric, g_{ab}, can be constructed on the four-dimensional solution space with local coordinates x^a. Furthermore the solutions, $u=Z(x^a,s,s^*,\gamma)$, satisfy the four-dimensional Hamilton–Jacobi equation, $g^{ab}u_{,a}u_{,b}=1$. We remark that this structure is invariant under a subset of contact transformations. In the next section, as an example, we apply these results to the Schwarzschild metric. Finally we use the four-dimensional metric obtained in the first part and we impose the Einstein equations. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1850366]

I. INTRODUCTION

Many years ago, Wünschmann, Cartan, and Chern,[1–6] while studying the structure and transformation properties of third-order ODE's, discovered that all three-dimensional conformal Lorentzian geometries were encoded in equivalence classes (under contact transformations) of third-order ODE's, that were characterized by the vanishing of a certain function, $W[F]$, defined from the differential equation itself, that is referred to as the Wünschmann invariant. In other words, from the solutions to equations of the form

$$\frac{d^3z}{dt^3}=F\left(z,\frac{dz}{dt},\frac{d^2z}{dt^2},t\right),$$

with $W[F]=0$, all three-dimensional conformal Lorentzian metrics could be constructed.

In a more recent series of papers Frittelli, Kozameh, Newman, Kamran, and Nurowski,[7–14] were able to generalize this result. They showed that all four-dimensional conformal Lorentzian geometries were encoded in equivalence classes (under contact transformations) of pairs of second-order partial differential equations (PDE's) that were characterized by the vanishing of an analogous (generalized) Wünschmann invariant, referred to as the *metricity conditions.*

In this work, referred to as the null surface formulation of general relativity, the metric of the space–time is a derived concept. The fundamental objects are two functions, $Z(x^a,\zeta,\zeta^*)$ and $\Omega(x^a,\zeta,\zeta^*)$, of the space–time points x^a and parametrized by points on the sphere; that is, by

functions defined on $\mathcal{M}\times\mathcal{S}^2$ (the sphere bundle over the space–time). The first of the functions, $Z(x^a,\zeta,\zeta^*)$, which encodes all the conformal information of the space–time, describes a sphere's worth of surfaces through each space–time point. It is from these surfaces that a conformal metric can be constructed. The second function, $\Omega(x^a,\zeta,\zeta^*)$, which plays the role of a conformal factor, converts it into any metric in the conformal class. The level surfaces of $Z(x^a,\zeta,\zeta^*)$ in $\mathcal{M}$, for each fixed value of ζ, are null hypersurfaces with respect to this metric. As ζ takes different values on $\mathcal{S}^2$ at a fixed point x^a in $\mathcal{M}$, the normals to the null hypersurfaces sweep out the null-cone at x^a.

To establish this new approach to general relativity, these authors began with a four-dimensional Lorentzian manifold, already containing a metric g_{ab} and a complete integral to the eikonal equation

$$g^{ab}(x^a)\nabla_a Z\cdot\nabla_b Z=0. \tag{1}$$

A complete integral, expressed as

$$u=Z(x^a,\zeta,\zeta^*), \tag{2}$$

contains the space–time coordinates, x^a, and the needed (for a complete integral) two parameters (ζ,ζ^*). By constructing the four functions,

$$\theta^i\equiv(u,\omega,\omega^*,R)\equiv(Z,\partial_\zeta Z,\partial_{\zeta^*}Z,\partial_{\zeta^*\zeta}Z) \tag{3}$$

from Eq. (2) and its derivatives, and by eliminating x^a, via the algebraic inversion

$$x^a=X^a(\zeta,\zeta^*,\theta^i), \tag{4}$$

they found that $u=Z(x^a,\zeta,\zeta^*)$ satisfies in addition to Eq. (2) the pair of second-order partial differential equations in ζ, ζ^*, of the form

$$\partial_{\zeta\zeta}Z=\Lambda(Z,\partial_\zeta Z,\partial_{\zeta^*}Z,\partial_{\zeta\zeta^*}Z,\zeta,\zeta^*),$$

$$\partial_{\zeta^*\zeta^*}Z=\Lambda^*(Z,\partial_\zeta Z,\partial_{\zeta^*}Z,\partial_{\zeta\zeta^*}Z,\zeta,\zeta^*). \tag{5}$$

The x^a, in the solution of Eq. (5), appear now as constants of integration. The roles of x^a and (ζ,ζ^*) are thereby interchanged. Note that the metric has disappeared from the equations.

The question then was, could this procedure be reversed? Could one start with a pair of equations of the form, (5), and then find the eikonal equation, (1), with a metric $g^{ab}(x^a)$.

It was shown that when the functions (Λ,Λ^*) satisfy an integrability condition, a weak inequality and a certain set of differential conditions (the metricity or generalized Wünschmann conditions), the procedure can be reversed. The solutions to the pair do determine a conformal four-dimensional Lorentzian metric and, in fact, all conformal Lorentzian metrics can be obtained from equivalence classes of equations of the form Eq. (5). When certain specific conditions,[15] in addition to the Wünschmann condition, are imposed on the (Λ,Λ^*), the metrics, determined by the solutions, are in the vacuum conformal Einstein class.

The aim of the present work is to present an approach to general relativity, which is similar to the null surface formulation, but now instead of using a complete integral to the eikonal equation, we use a complete integral to the Hamilton–Jacobi (HJ) equation.

In Sec. II we begin with a four-dimensional manifold, $\mathcal{M}$, with no further structure and then investigate arbitrary three-parameter families of surfaces on $\mathcal{M}$ given by

$$u=\text{constant}=Z(x^a,\alpha,\beta,\gamma). \tag{6}$$

(The x^a are local coordinates on $\mathcal{M}$ and α, β, and γ parametrize the families and can take values on $\mathcal{S}^3$, $\mathcal{S}^1\times\mathcal{R}^2$, $\mathcal{S}^2\times\mathcal{R}$ or on $\mathcal{R}^3$. However, in this work we combine the real α and β parameters into a pair of conjugate parameters s and s^*; γ will be real.) More specifically, we then ask when do such families of surfaces define a four-dimensional metric, $g_{ab}(x^a)$, such that

$$g^{ab}\nabla_a Z(x^a,s,s^*,\gamma)\nabla_b Z(x^a,s,s^*,\gamma)=1. \tag{7}$$

We have here either taken the mass in the HJ equation to be *one* or set it into the g^{ab} as a factor.

By taking (s,s^*,γ) derivatives of Eq. (6) and eliminating the x^a, we will show that the $u=Z(x^a,s,s^*,\gamma)$ must also satisfy a system of six second-order PDE's,

$$\begin{aligned}
\partial_{ss}Z&=\Lambda(u,w,w^*,R,s,s^*,\gamma),\\
\partial_{s^*s^*}Z&=\Lambda^*(u,w,w^*,R,s,s^*,\gamma),\\
\partial_{\gamma\gamma}Z&=\Upsilon(u,w,w^*,R,s,s^*,\gamma),\\
\partial_{ss^*}Z&=\Phi(u,w,w^*,R,s,s^*,\gamma),\\
\partial_{s\gamma}Z&=\Psi(u,w,w^*,R,s,s^*,\gamma),\\
\partial_{s^*\gamma}Z&=\Psi^*(u,w,w^*,R,s,s^*,\gamma),
\end{aligned} \tag{8}$$

with

$$w\equiv\partial_s Z,\quad w^*\equiv\partial_{s^*}Z,\quad \text{and } R\equiv\partial_\gamma Z,$$

and where Λ, Λ^*, Υ, Φ, Ψ, and Ψ^* are restricted to satisfy certain metricity or "Wünschmann-like" conditions.

Here ∂_s, ∂_{s^*}, and ∂_γ, denote the partial derivatives with respect to the parameters s, s^*, and γ, respectively. Observe that in the solutions of Eqs. (8) $u=Z(x^a,s,s^*,\gamma)$, the x^a are four constants of integration for Eqs. (8) while the s, s^*, and γ are three integration constants for Eq. (7). Observe that $u=Z(x^a,s,s^*,\gamma)$ is a complete integral to the Hamilton–Jacobi equation (7).

In this section we also remark that the four-dimensional metric $g_{ab}(x^a)$ associated with the system of partial differential equations, (8), is invariant under a subset of contact transformations of the differential equations.

In Sec. III, as an example, we apply the results derived in Sec. II to the Schwarzschild metric.

In Sec. IV, we present our formulation of general relativity. For this purpose we substitute the four-dimensional metric already obtained in Sec. II into the Einstein equations. From our results we conclude that the Einstein equations can be reformulated as equations for families of three-dimensional surfaces given by the level surfaces of $u=Z(x^a,s,s^*,\gamma)$.

This new point of view can be given in either of two versions. In the first version, the variables are the six functions, $(\Lambda,\Lambda^*,\Upsilon,\Phi,\Psi,\Psi^*)$ of the seven variables, (u,w,w^*,R,s,s^*,γ) i.e., the right-hand side of Eqs. (8). These functions must satisfy three sets of equations; the integrability conditions, the Wünschmann-like conditions and a further condition obtained from the Einstein equations. The metric, on a four-manifold, can be written down directly in terms of these six functions and their derivatives. *No use need be made of the set*, Eqs. (8). In the second version one uses the same set of $(\Lambda,\Lambda^*,\Upsilon,\Phi,\Psi,\Psi^*)$ in the right-hand side of Eqs. (8) and solves for the $Z(x^a,s,s^*,\gamma)$. The metric is then written in terms of the $Z(x^a,s,s^*,\gamma)$ and its derivatives. The advantage of the first version is that one does not need to solve Eqs. (8), but one has to extract (algebraically) the four-manifold from the (u,w,w^*,R) while in the second version the four-manifold is explicitly given by the four constants of integration, x^a.

There is no claim being made that this approach to the Einstein equations has any obvious advantage over the usual metric approach. It however does give certain mathematical insights into the differential geometry associated with general relativity.

II. 4D METRICS AND THE METRICITY OR WÜNSCHMANN-LIKE CONDITIONS

In this section we prove that in the space of solutions of a certain class of systems of six second-order PDE's, a four-dimensional definite or indefinite metric, g_{ab}, can be constructed such that the solutions satisfy the four-dimensional HJ equation. We start with a four-dimensional manifold $\mathcal{M}$ [with local coordinates $x^a=(x^0,x^1,x^2,x^3)$] and assume we are given a three-parameter set of functions $u=Z(x^a,\alpha,\beta,\gamma)$. In general the parameters α, β, and γ can take values on $\mathcal{S}^3$, $\mathcal{S}^1\times\mathcal{R}^2$, $\mathcal{S}^2\times\mathcal{R}$ or on $\mathcal{R}^3$. As we said, we combine the real α and β parameters into a pair of conjugate parameters s and s^*, and γ is real. We also assume that for fixed values of the parameters s, s^*, and γ the level surfaces

$$u = \text{constant} = Z(x^a,s,s^*,\gamma), \tag{9}$$

locally foliate the manifold $\mathcal{M}$ and that $u=Z(x^a,s,s^*,\gamma)$ satisfies the HJ equation

$$g^{ab}(x^a)\nabla_a Z(x^a,s,s^*,\gamma)\nabla_b Z(x^a,s,s^*,\gamma)=1, \tag{10}$$

for some unknown metric $g_{ab}(x^a)$.

The basic idea now is to solve Eq. (10) for the components of the metric in terms of $\nabla_a Z(x^a,s,s^*,\gamma)$. To do so, we will consider a number of parameter derivatives of the condition (10), and then by manipulation of these derivatives, obtain both the four-dimensional metric and the six partial differential equations defining the surfaces plus the conditions these PDE's must satisfy. They will be referred to as the metricity or Wünschmann-like conditions.

Remark 1: The notation is as follows: there will be two types of differentiation, one is with respect to the local coordinates, x^a, of the manifold $\mathcal{M}$, denoted by ∇_a or "comma a," the other is with respect to the parameters s, s^* and γ, denoted by ∂_s, ∂_{s^*}, and ∂_γ.

From the assumed existence of $u=Z(x^a,s,s^*,\gamma)$, we define four parameterized scalars θ^i in the following way:

$$\begin{aligned}
\theta^0 &= u \equiv Z(x^a,s,s^*,\gamma),\\
\theta^+ &= w \equiv \partial_s Z(x^a,s,s^*,\gamma),\\
\theta^- &= w^* \equiv \partial_{s^*} Z(x^a,s,s^*,\gamma),\\
\theta^1 &= R \equiv \partial_\gamma Z(x^a,s,s^*,\gamma).
\end{aligned} \tag{11}$$

Remark 2: For each value of s, s^* and γ, Eqs. (11) can be thought of as a coordinate transformation between the x^a's and (u,w,w^*,R).

We also define the following six important scalars:

$$\tilde{\Lambda} = \partial_{ss} Z(x^a,s,s^*,\gamma),$$

$$\tilde{\Lambda}^* = \partial_{s^*s^*} Z(x^a,s,s^*,\gamma),$$

$$\tilde{\Upsilon} = \partial_{\gamma\gamma} Z(x^a,s,s^*,\gamma),$$

$$\tilde{\Phi} = \partial_{ss^*} Z(x^a,s,s^*,\gamma),$$

$$\tilde{\Psi} = \partial_{s\gamma} Z(x^a,s,s^*,\gamma),$$

$$\tilde{\Psi}^* = \partial_{s^*\gamma} Z(x^a, s, s^*, \gamma). \tag{12}$$

In what follows we will assume that Eqs. (11) can be inverted, i.e., solved for the x^a's;

$$x^a = X^a(u, w, w^*, R, s, s^*, \gamma).$$

Equations (12) can then be rewritten as

$$\begin{aligned}
\partial_{ss} Z &= \Lambda(u, w, w^*, R, s, s^*, \gamma), \\
\partial_{s^*s^*} Z &= \Lambda^*(u, w, w^*, R, s, s^*, \gamma), \\
\partial_{\gamma\gamma} Z &= \Upsilon(u, w, w^*, R, s, s^*, \gamma), \\
\partial_{ss^*} Z &= \Phi(u, w, w^*, R, s, s^*, \gamma), \\
\partial_{s\gamma} Z &= \Psi(u, w, w^*, R, s, s^*, \gamma), \\
\partial_{s^*\gamma} Z &= \Psi^*(u, w, w^*, R, s, s^*, \gamma).
\end{aligned} \tag{13}$$

This means that the three-parameter family of level surfaces, Eq. (9), can be obtained as solutions to the system of six second-order PDE's (13). Note that $(\Lambda, \Lambda^*, \Upsilon, \Phi, \Psi, \Psi^*)$ satisfy the integrability conditions

$$\begin{aligned}
&D_{s^*}\Lambda = D_s\Phi, \quad D_\gamma\Lambda = D_s\Psi, \quad D_\gamma\Phi = D_{s^*}\Psi, \\
&D_s\Lambda^* = D_{s^*}\Phi, \quad D_\gamma\Lambda^* = D_{s^*}\Psi^*, \quad D_\gamma\Phi = D_s\Psi^*, \\
&D_\gamma\Psi = D_s\Upsilon, \quad D_\gamma\Psi^* = D_{s^*}\Upsilon, \quad D_{s^*}\Psi = D_s\Psi^*,
\end{aligned} \tag{14}$$

where we have the following.

Definition 1: *The total* s, s^*, *and* γ *derivatives of a function* $F = F(u, w, w^*, R, s, s^*, \gamma)$ *are defined by*

$$\begin{aligned}
D_s F &\equiv F_s + F_u w + F_w \Lambda + F_{w^*}\Phi + F_R \Psi, \\
D_{s^*} F &\equiv F_{s^*} + F_u w^* + F_w \Phi + F_{w^*}\Lambda^* + F_R \Psi^*, \\
D_\gamma F &\equiv F_\gamma + F_u R + F_w \Psi + F_{w^*}\Psi^* + F_R \Upsilon,
\end{aligned} \tag{15}$$

respectively.

The solution space of Eqs. (13) is four dimensional. This can be seen in the following way. The system of PDE's (13) is equivalent to the vanishing of the four one-forms, ω^i,

$$\begin{aligned}
\omega^0 &= \mathrm{d}u - w\,\mathrm{d}s - w^*\,\mathrm{d}s^* - R\,\mathrm{d}\gamma, \\
\omega^+ &= \mathrm{d}w - \Lambda\,\mathrm{d}s - \Phi\,\mathrm{d}s^* - \Psi\,\mathrm{d}\gamma, \\
\omega^- &= \mathrm{d}w^* - \Phi\,\mathrm{d}s - \Lambda^*\,\mathrm{d}s^* - \Psi^*\,\mathrm{d}\gamma,
\end{aligned}$$

$$\omega^1 = \mathrm{d}R - \Psi\,\mathrm{d}s - \Psi^*\,\mathrm{d}s^* - \Upsilon\,\mathrm{d}\gamma. \tag{16}$$

A simple calculation, using the integrability conditions on $(\Lambda, \Lambda^*, \Upsilon, \Phi, \Psi, \Psi^*)$, leads to $\mathrm{d}\omega^i = 0$ (modulo ω^i) from which, via the Frobenius theorem, the solution space of Eqs. (13) is four dimensional.

From the four scalars, θ^i, we have their associated gradient basis $\theta^i{}_{,a}$ given by

$$\theta^i{}_{,a} = \nabla_a \theta^i = \{Z_{,a}, \partial_s Z_{,a}, \partial_{s^*} Z_{,a}, \partial_\gamma Z_{,a}\}, \tag{17}$$

and its dual vector basis θ_i^a, so that

$$\theta_i^a \theta^j{}_{,a} = \delta_i^j, \quad \theta_i^a \theta^i{}_{,b} = \delta_b^a. \tag{18}$$

It is easier to search for the components of the four-dimensional metric in the gradient basis rather than in the original coordinate basis. Furthermore, it is preferable to use the contravariant components rather than the covariant components of the metric; i.e., we want to determine

$$g^{ij}(x^a, s, s^*, \gamma) = g^{ab}(x^a)\,\theta^i{}_{,a}\,\theta^j{}_{,b}. \tag{19}$$

The metric components and the Wünschmann-like conditions are obtained by repeatedly operating with ∂_s, ∂_{s^*}, and ∂_γ on Eq. (10), which, by definition, is

$$g^{00} = g^{ab} Z_{,a} Z_{,b} = 1. \tag{20}$$

Applying ∂_s to Eq. (20) yields $\partial_s g^{00} = 2 g^{ab} \partial_s Z_{,a} Z_{,b} = 0$, i.e.,

$$g^{+0} = 0. \tag{21}$$

In the same way we obtain that $\partial_{s^*} g^{00} = 2 g^{ab} \partial_{s^*} Z_{,a} Z_{,b} = 0$, $\partial_\gamma g^{00} = 2 g^{ab} \partial_\gamma Z_{,a} Z_{,b} = 0$ and thus,

$$\begin{aligned} g^{-0} &= 0, \\ g^{10} &= 0. \end{aligned} \tag{22}$$

A direct computation shows that

$$\partial_{ss}(g^{00}/2) = g^{ab} \partial_{ss} Z_{,a} Z_{,b} + g^{ab} \partial_s Z_{,a} \partial_s Z_{,b} = g^{ab} \Lambda_{,a} Z_{,b} + g^{++} = 0. \tag{23}$$

Since, by the assumed linear independence of $(Z_{,a}, \partial_s Z_{,a}, \partial_{s^*} Z_{,a}, \partial_\gamma Z_{,a})$,

$$\Lambda_{,a} = \Lambda_u Z_{,a} + \Lambda_w \partial_s Z_{,a} + \Lambda_{w^*} \partial_{s^*} Z_{,a} + \Lambda_\gamma \partial_\gamma Z_{,a}, \tag{24}$$

Eq. (23), using Eqs. (20)–(22) and (24), is equivalent to

$$g^{++} = -\Lambda_u. \tag{25}$$

In exactly the same way we find that

$$\partial_{s^* s^*}(g^{00}/2) = \Lambda_u^* + g^{--} = 0,$$

$$\partial_{\gamma\gamma}(g^{00}/2) = \Upsilon_u + g^{11} = 0,$$

$$\partial_{s s^*}(g^{00}/2) = \Phi_u + g^{-+} = 0,$$

$$\partial_{s\gamma}(g^{00}/2) = \Psi_u + g^{1+} = 0,$$

$$\partial_{s^*\gamma}(g^{00}/2) = \Psi_u^* + g^{-1} = 0. \tag{26}$$

Therefore, the final result is

$$(g^{ij}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -\Lambda_u & -\Phi_u & -\Psi_u \\ 0 & -\Phi_u & -\Lambda_u^* & -\Psi_u^* \\ 0 & -\Psi_u & -\Psi_u^* & -\Upsilon_u \end{pmatrix}. \tag{27}$$

Remark 3: We require that $\det(g^{ij})=\Delta$ *be different from zero, with*

$$\Delta \equiv \Upsilon_u\Phi_u^2 - 2\Phi_u\Psi_u\Psi_u^* + \Lambda_u^*\Psi_u^2 + \Lambda_u(\Psi_u^*)^2 - \Lambda_u\Lambda_u^*\Upsilon_u. \tag{28}$$

The metricity or Wünschmann-like conditions are obtained from the third derivatives, i.e., from $\partial_{sss}g^{00}=0$, $\partial_{sss^*}g^{00}=0$, $\partial_{ss^*s^*}g^{00}=0$, $\partial_{s^*s^*s^*}g^{00}=0$, $\partial_{ss\gamma}g^{00}=0$, $\partial_{s\gamma\gamma}g^{00}=0$, $\partial_{\gamma\gamma\gamma}g^{00}=0$, $\partial_{s^*s^*\gamma}g^{00}=0$, $\partial_{s^*\gamma\gamma}g^{00}=0$. By using the integrability conditions, (14), a direct computation shows that they are equivalent to the following nine equations:

$$\begin{aligned}
&\Lambda_{us} + \Lambda_{uu}w + \Lambda_{uw}\Lambda + \Lambda_{uw^*}\Phi + \Lambda_{uR}\Psi = 2[\Lambda_w\Lambda_u + \Lambda_{w^*}\Phi_u + \Lambda_R\Psi_u],\\
&\Lambda_{us^*} + \Lambda_{uu}w^* + \Lambda_{uw}\Phi + \Lambda_{uw^*}\Lambda^* + \Lambda_{uR}\Psi^* = 2[\Phi_w\Lambda_u + \Phi_{w^*}\Phi_u + \Phi_R\Psi_u],\\
&\Lambda_{us}^* + \Lambda_{uu}^*w + \Lambda_{uw^*}^*\Phi + \Lambda_{uw}^*\Lambda + \Lambda_{uR}^*\Psi = 2[\Phi_{w^*}\Lambda_u^* + \Phi_w\Lambda_u + \Phi_R\Psi_u^*],\\
&\Lambda_{us^*}^* + \Lambda_{uu}^*w^* + \Lambda_{uw^*}^*\Lambda^* + \Lambda_{uw}^*\Phi + \Lambda_{uR}^*\Psi^* = 2[\Lambda_{w^*}^*\Lambda_u^* + \Lambda_w^*\Phi_u + \Lambda_R^*\Psi_u^*],\\
&\Lambda_{u\gamma} + \Lambda_{uu}R + \Lambda_{uw}\Psi + \Lambda_{uw^*}\Psi^* + \Lambda_{uR}\Upsilon = 2[\Psi_w\Lambda_u + \Psi_{w^*}\Phi_u + \Psi_R\Psi_u],\\
&\Upsilon_{us} + \Upsilon_{uu}w + \Upsilon_{uw}\Lambda + \Upsilon_{uw^*}\Phi + \Upsilon_{uR}\Psi = 2[\Psi_w\Psi_u + \Psi_{w^*}\Psi_u^* + \Psi_R\Upsilon_u],\\
&\Upsilon_{u\gamma} + \Upsilon_{uu}R + \Upsilon_{uw}\Psi + \Upsilon_{uw^*}\Psi^* + \Upsilon_{uR}\Upsilon = 2[\Upsilon_w\Psi_u + \Upsilon_{w^*}\Psi_u^* + \Upsilon_R\Psi_u],\\
&\Lambda_{u\gamma}^* + \Lambda_{uu}^*R + \Lambda_{uw^*}^*\Psi^* + \Lambda_{uw}^*\Psi + \Lambda_{uR}^*\Upsilon = 2[\Psi_{w^*}^*\Lambda_u^* + \Psi_w^*\Phi_u + \Psi_R^*\Psi_u^*],\\
&\Upsilon_{us^*} + \Upsilon_{uu}w^* + \Upsilon_{uw^*}\Lambda^* + \Upsilon_{uw}\Phi + \Upsilon_{uR}\Psi^* = 2[\Psi_{w^*}^*\Psi_u^* + \Psi_w^*\Psi_u + \Psi_R^*\Upsilon_u].
\end{aligned} \tag{29}$$

Summarizing we have the following.

(a) If we start from a complete integral, $u=Z(x^a,s,s^*,\gamma)$ to the HJ equation, (10), then it satisfies the system of six second-order PDE's (13), with $(\Lambda,\Lambda^*,\Upsilon,\Phi,\Psi,\Psi^*)$ satisfying Eqs. (14) and the Wünschmann-like conditions (29); in other words, in the solution space of Eqs. (13) there is the naturally defined metric,

$$\begin{aligned}
g_{ab} = u_{,a}u_{,b} + \frac{1}{\Delta}[&(\Lambda_u^*\Upsilon_u - (\Psi_u^*)^2)w_{,a}w_{,b} + (\Psi_u\Psi_u^* - \Upsilon_u\Phi_u)(w_{,a}w_{,b}^* + w_{,a}^*w_{,b}) + (\Lambda_u\Upsilon_u - \Psi_u^2)w_{,a}^*w_{,b}^*\\
&+ (\Phi_u\Psi_u^* - \Lambda_u^*\Psi_u)(w_{,a}R_{,b} + R_{,a}w_{,b}) + (\Phi_u\Psi_u - \Lambda_u\Psi_u^*)(w_{,a}^*R_{,b} + R_{,a}w_{,b}^*) + (\Lambda_u\Lambda_u^* - \Phi_u^2)R_{,a}R_{,b}],
\end{aligned} \tag{30}$$

where Δ is defined by Eq. (28).

(b) If we start with a system of six second-order PDE's (13), where $(\Lambda,\Lambda^*,\Upsilon,\Phi,\Psi,\Psi^*)$ satisfy Eqs. (29) and the integrability conditions, (14), then in its solution space there exist a

natural four-dimensional metric given by Eq. (30). Though it might appear as if the metric components depend on the parameters (s, s^*, γ), the Wünschmann-like conditions guarantees that they do not. Furthermore, the solutions $u = Z(x^a, s, s^*, \gamma)$ satisfy the HJ equation

$$g^{ab}\nabla_a Z(x^a, s, s^*, \gamma)\nabla_b Z(x^a, s, s^*, \gamma) = 1$$

with the just determined metric, Eq. (30).

Remark 4: From the results presented above we conclude that solving the four-dimensional HJ equation, in a four-dimensional background space–time, is equivalent to solving a system of six second-order PDE's.

In some of the earlier work on the eikonal equation in three- and four-dimensional Lorentzian spaces, it was proved that the conformal Lorentzian metrics associated with third-order ODE's and pairs of second-order PDE's satisfying the Wünschmann condition and generalized Wünschmann condition, is preserved when the differential equation is transformed by a contact transformation. For our present case, there is an analogous result given by the following.

Theorem 1: *Let Eqs. (13) be a system of six second-order PDE's, with* $(\Lambda, \Lambda^*, \Upsilon, \Phi, \Psi, \Psi^*)$ *satisfying the conditions (14) and (29), and let*

$$\begin{aligned}
\partial_{\overline{ss}}\overline{Z} &= \overline{\Lambda}(\overline{u}, \overline{w}, \overline{w^*}, \overline{R}, \overline{s}, \overline{s^*}, \overline{\gamma}),\\
\partial_{\overline{s^*s^*}}\overline{Z} &= \overline{\Lambda}^*(\overline{u}, \overline{w}, \overline{w^*}, \overline{R}, \overline{s}, \overline{s^*}, \overline{\gamma}),\\
\partial_{\overline{\gamma\gamma}}\overline{Z} &= \overline{\Upsilon}(\overline{u}, \overline{w}, \overline{w^*}, \overline{R}, \overline{s}, \overline{s^*}, \overline{\gamma}),\\
\partial_{\overline{ss^*}}\overline{Z} &= \overline{\Phi}(\overline{u}, \overline{w}, \overline{w^*}, \overline{R}, \overline{s}, \overline{s^*}, \overline{\gamma}),\\
\partial_{\overline{s\gamma}}\overline{Z} &= \overline{\Psi}(\overline{u}, \overline{w}, \overline{w^*}, \overline{R}, \overline{s}, \overline{s^*}, \overline{\gamma}),\\
\partial_{\overline{s^*\gamma}}\overline{Z} &= \overline{\Psi}^*(\overline{u}, \overline{w}, \overline{w^*}, \overline{R}, \overline{s}, \overline{s^*}, \overline{\gamma}),
\end{aligned} \tag{31}$$

be a second system of six second-order PDE's locally equivalent to Eqs. (13) under the subset of contact transformations generated by the generating function

$$H(s, s^*, \gamma, u, \overline{s}, \overline{s^*}, \overline{\gamma}, \overline{u}) = \overline{u} - u - G(s, s^*, \gamma, \overline{s}, \overline{s^*}, \overline{\gamma}). \tag{32}$$

Then under this subset of contact transformations the metric given by Eq. (30) is preserved.

The proof of this theorem is exactly as that presented in Ref. 12 for a system of two second-order PDE's such that on its space of solutions there is a unique four-dimensional conformal Lorentzian metric, g^{ab}, such that $g^{ab}u_{,a}u_{,b} = 0$. Here we only justify the form of the generating function (32). We first review the definition of a general contact transformation.

Theorem 2: *Every contact transformation which is not a prolonged point transformation is determined in terms of a generating function* $H(s, s^*, \gamma, u, \overline{s}, \overline{s^*}, \overline{\gamma}, \overline{u})$ *by solving the following seven implicit equations for* $\overline{s}, \overline{s^*}, \overline{\gamma}, \overline{u}, \overline{w} = \partial_{\overline{s}}\overline{u}, \overline{w^*} = \partial_{\overline{s^*}}\overline{u}, \overline{R} = \partial_{\overline{\gamma}}\overline{u}$:

$$\begin{aligned}
&H(s, s^*, \gamma, u, \overline{s}, \overline{s^*}, \overline{\gamma}, \overline{u}) = 0,\\
&H_s + wH_u = 0,\ H_{\overline{s}} + \overline{w}H_{\overline{u}} = 0,\\
&H_{s^*} + w^*H_u = 0,\ H_{\overline{s^*}} + \overline{w^*}H_{\overline{u}} = 0,
\end{aligned}$$

$$H_\gamma + RH_u = 0,\ H_{\overline{\gamma}} + \overline{R}H_{\overline{u}} = 0. \tag{33}$$

The generating function $H(s, s^*, \gamma, u, \overline{s}, \overline{s^*}, \overline{\gamma}, \overline{u})$ *is an arbitrary smooth function, subject only to the solvability of Eqs. (33) for* $\overline{s}$, $\overline{s^*}$, $\overline{\gamma}$, $\overline{u}$, $\overline{w}$, $\overline{w^*}$ *and* $\overline{R}$.

For a proof of this theorem see, for example, Olver.[16]

Without loss of generality one can take

$$H = \overline{u} - \overline{V}(u, s, s^*, \gamma, \overline{s}, \overline{s^*}, \overline{\gamma}), \tag{34}$$

so that the contact transformation has the form

$$\begin{aligned}
&\overline{u} = \overline{V}(u, s, s^*, \gamma, A(s, s^*, \gamma, u, w, w^*, R), A^*(s, s^*, \gamma, u, w, w^*, R), C(s, s^*, \gamma, u, w, w^*, R)),\\
&\overline{s} = A(s, s^*, \gamma, u, w, w^*, R),\\
&\overline{s^*} = A^*(s, s^*, \gamma, u, w, w^*, R),\\
&\overline{\gamma} = C(s, s^*, \gamma, u, w, w^*, R),\\
&\overline{w} = \overline{V}_{\overline{s}}(u, s, s^*, \gamma, A(s, s^*, \gamma, u, w, w^*, R), A^*(s, s^*, \gamma, u, w, w^*, R), C(s, s^*, \gamma, u, w, w^*, R)),\\
&\overline{w^*} = \overline{V}_{\overline{s^*}}(u, s, s^*, \gamma, A(s, s^*, \gamma, u, w, w^*, R), A^*(s, s^*, \gamma, u, w, w^*, R), C(s, s^*, \gamma, u, w, w^*, R)),\\
&\overline{R} = \overline{V}_{\overline{\gamma}}(u, s, s^*, \gamma, A(s, s^*, \gamma, u, w, w^*, R), A^*(s, s^*, \gamma, u, w, w^*, R), C(s, s^*, \gamma, u, w, w^*, R)),
\end{aligned} \tag{35}$$

where $A(s, s^*, \gamma, u, w, w^*, R)$, $A^*(s, s^*, \gamma, u, w, w^*, R)$, and $C(s, s^*, \gamma, u, w, w^*, R)$ are obtained by solving

$$\begin{aligned}
&\overline{V}_s + w\overline{V}_u = 0,\\
&\overline{V}_{s^*} + w^*\overline{V}_u = 0,\\
&\overline{V}_\gamma + R\overline{V}_u = 0,
\end{aligned} \tag{36}$$

for $\overline{s}$, $\overline{s^*}$, and $\overline{\gamma}$ in terms of s, s^*, γ, u, w, w^*, and R.

As was pointed out earlier, for each value of s, s^*, and γ, the four-parameters, x^a, family of solutions

$$u = Z(x^a, s, s^*, \gamma), \tag{37}$$

of (13) is also a three-parameters, (s, s^*, γ), family of solutions of Eq. (10), i.e., are complete integrals of Eq. (10). We now invoke the envelope construction to take one complete integral of Eq. (10) into another such solution. Consider the function $\overline{u} = \overline{Z}(x^a, \overline{s}, \overline{s^*}, \overline{\gamma})$ defined by

$$\overline{u} = \overline{V}(u, s, s^*, \gamma, \overline{s}, \overline{s}^*, \overline{\gamma}), \tag{38}$$

where u is defined by Eq. (37) and s, s^*, and γ are defined implicitly as functions of x^a, $\overline{s}$, $\overline{s^*}$, and $\overline{\gamma}$ by the envelope conditions[12,17]

$$\overline{V}_u w + \overline{V}_s = 0,$$

$$\overline{V}_u w^* + \overline{V}_{s^*} = 0, \tag{39}$$

$$\overline{V}_u R + \overline{V}_\gamma = 0.$$

Note that although Eqs. (39) have the same form as Eqs. (36), they involve the variables x^a, s, s^*, and γ. Using both Eqs. (38) and (39), we have that

$$\overline{u}_{,a} = \overline{V}_u u_{,a}. \tag{40}$$

By direct substitution of $\overline{u}_{,a}$ into the HJ equation, Eq. (10), we see that it is a new complete integral if and only if $\overline{V}_u^2 = 1$. That is, $\overline{u} = \overline{V}(u, s, s^*, \gamma, \overline{s}, \overline{s^*}, \overline{\gamma})$ has the form $\overline{u} = \pm u + G(s, s^*, \gamma, \overline{s}, \overline{s^*}, \overline{\gamma})$. For simplicity, taking the positive sign, we have that if $u(x^a, s, s^*, \gamma)$ is a complete integral of Eq. (10) then

$$\overline{u} = u + G(s, s^*, \gamma, \overline{s}, \overline{s}^*, \overline{\gamma}), \tag{41}$$

where s, s^*, and γ are defined implicitly as functions of x^a, $\overline{s}$, $\overline{s^*}$, and $\overline{\gamma}$ by the envelope conditions

$$w + G_s = 0,$$

$$w^* + G_{s^*} = 0, \tag{42}$$

$$R + G_\gamma = 0,$$

is a new complete integral of Eq. (10). Equations (41) and (42) define a particular subset of the contact transformations given by contact transformations

$$\overline{u} = u + G(s, s^*, \gamma, \overline{s}, \overline{s^*}, \overline{\gamma}), \tag{43}$$

$$w = -G_s, \tag{44}$$

$$w^* = -G_{s^*}, \tag{45}$$

$$R = -G_\gamma, \tag{46}$$

$$\overline{w} = G_{\overline{s}}, \tag{47}$$

$$\overline{w^*} = G_{\overline{s}^*}, \tag{48}$$

$$\overline{R} = G_{\overline{\gamma}}. \tag{49}$$

The generating function for this set of contact transformations is given by

$$H(s, s^*, \gamma, u, \overline{s}, \overline{s}^*, \overline{\gamma}, \overline{u}) = \overline{u} - u - G(s, s^*, \gamma, \overline{s}, \overline{s}^*, \overline{\gamma}) = 0 \tag{50}$$

thus justifying our choice of the generating function, Eq. (32).

III. EXAMPLE

As an example we apply our results to the motion of a particle in the Schwarzschild space–time. By using the coordinates $x^a = (t, r, \theta, \phi)$, the Hamilton–Jacobi equation for this case can be written as

$$\left(\frac{1}{m^2}\right)\left[\frac{u_{,t}^2}{\left(1-\frac{r_g}{r}\right)}-\left(1-\frac{r_g}{r}\right)u_{,r}^2-\frac{u_{,\theta}^2}{r^2}-\frac{u_{,\phi}^2}{r^2\sin^2\theta}\right]=1, \tag{51}$$

where m is the mass of the particle and $r_g=2M$ with M being the mass of the Schwarzschild solution. By the method of separation of variables one finds that a complete solution to Eq. (51) can be written in the following form:

$$u=Z(x^a,\alpha,\beta,\gamma)=-\gamma t+\beta\phi+\int\sqrt{\alpha^2-\frac{\beta^2}{\sin^2\theta}}\,\mathrm{d}\theta+\int\sqrt{\frac{\gamma^2r^3-(m^2r^2+\alpha^2)(r-r_g)}{r(r-r_g)^2}}\,\mathrm{d}r, \tag{52}$$

where α, β, and γ are three constants of separation. For this problem, γ, is the energy of the particle, β is the value of the angular momentum about the polar axis and α is the magnitude of the total angular momentum. To obtain the system of second-order PDE's associated with this complete integral we take $\alpha=s^*+s$ and $\beta=i(s^*-s)$. Thus the complete integral in terms of the parameters (s,s^*,γ) is given by

$$\begin{aligned}u=Z(x^a,s,s^*,\gamma)=&-\gamma t+\int\sqrt{\frac{\gamma^2r^3-[m^2r^2+(s+s^*)^2](r-r_g)}{r(r-r_g)^2}}\,\mathrm{d}r\\&+\int\sqrt{(s+s^*)^2+(s-s^*)^2\csc^2\theta}\,\mathrm{d}\theta-i(s-s^*)\phi.\end{aligned} \tag{53}$$

A direct computation shows that

$$\begin{aligned}w&=\int\frac{-(s+s^*)\mathrm{d}r}{\sqrt{r}\sqrt{\gamma^2r^3-[m^2r^2+(s+s^*)^2](r-r_g)}}+\int\frac{[(s+s^*)+(s-s^*)\csc^2\theta]\mathrm{d}\theta}{\sqrt{(s+s^*)^2+(s-s^*)^2\csc^2\theta}}-i\phi,\\w^*&=\int\frac{-(s+s^*)\mathrm{d}r}{\sqrt{r}\sqrt{\gamma^2r^3-[m^2r^2+(s+s^*)^2](r-r_g)}}+\int\frac{[(s+s^*)-(s-s^*)\csc^2\theta]\mathrm{d}\theta}{\sqrt{(s+s^*)^2+(s-s^*)^2\csc^2\theta}}+i\phi,\\R&=-t+\int\frac{\sqrt{r}r^2\gamma\,\mathrm{d}r}{(r-r_g)\sqrt{\gamma^2r^3-[m^2r^2+(s+s^*)^2](r-r_g)}}.\end{aligned} \tag{54}$$

By using Eqs. (53) and (54), one sees that the Jacobian of the coordinate transformation, $\theta^i=\theta^i(x^a,s,s^*,\gamma)$, for this case, is given by

$$J=\frac{\partial(u,w,w^*,R)}{\partial(t,r,\theta,\phi)}=\frac{2im^2r^{3/2}(s+s^*)[(s+s^*)^2+(s-s^*)^2\csc^2\theta]^{-1/2}}{[\gamma^2r^3-[m^2r^2+(s+s^*)^2](r-r_g)]^{1/2}}. \tag{55}$$

Using Eqs. (54), our system of six PDE's for a Schwarzschild space–time is obtained as follows.

First we have that

$$\partial_{ss}Z=\mathcal{A}(r,s,s^*,\gamma)+s^{*2}\mathcal{B}(\theta,s,s^*),$$

$$\partial_{s^*s^*}Z=\mathcal{A}(r,s,s^*,\gamma)+s^2\mathcal{B}(\theta,s,s^*),$$

$$\partial_{\gamma\gamma}Z=\mathcal{C}(r,s,s^*,\gamma),$$

$$\partial_{ss^*}Z=\mathcal{A}(r,s,s^*,\gamma)-ss^*\mathcal{B}(\theta,s,s^*),$$

$$\partial_{s\gamma} Z = \mathcal{D}(r,s,s^*,\gamma),$$

$$\partial_{s^*\gamma} Z = \mathcal{D}(r,s,s^*,\gamma), \tag{56}$$

where

$$\mathcal{A}(r,s,s^*,\gamma) = \int \frac{-r^{3/2}[\gamma^2 r - m^2(r-r_g)]\mathrm{d}r}{[\gamma^2 r^3 - [m^2r^2 + (s+s^*)^2](r-r_g)]^{3/2}},$$

$$\mathcal{B}(\theta,s,s^*) = \int \frac{4\csc^2\theta \mathrm{d}\theta}{[(s+s^*)^2 + (s-s^*)^2\csc^2\theta]^{3/2}},$$

$$\mathcal{C}(r,s,s^*,\gamma) = \int \frac{-\sqrt{r}r^2[m^2r^2 + (s+s^*)^2]\mathrm{d}r}{[\gamma^2 r^3 - [m^2r^2 + (s+s^*)^2](r-r_g)]^{3/2}}, \tag{57}$$

$$\mathcal{D}(r,s,s^*,\gamma) = \int \frac{\sqrt{r}r^2(s+s^*)\gamma\,\mathrm{d}r}{[\gamma^2 r^3 - [m^2r^2 + (s+s^*)^2](r-r_g)]^{3/2}}.$$

On the other hand, Eqs. (53) and (54) imply that

$$t = t(u,w,w^*R,s,s^*,\gamma),$$

$$r = r(u,w,w^*R,s,s^*,\gamma),$$

$$\theta = \theta(u,w,w^*R,s,s^*,\gamma), \tag{58}$$

$$\phi = \phi(u,w,w^*R,s,s^*,\gamma).$$

Therefore, the system of six second-order PDE's for a particle moving in the Schwarzschild space–time is given by

$$\partial_{ss} Z = \Lambda = \mathcal{A}(r(u,w,w^*R,s,s^*,\gamma),s,s^*,\gamma) + s^{*2}\mathcal{B}(\theta(u,w,w^*R,s,s^*,\gamma),s,s^*),$$

$$\partial_{s^*s^*} Z = \Lambda^* = \mathcal{A}(r(u,w,w^*R,s,s^*,\gamma),s,s^*,\gamma) + s^2\mathcal{B}(\theta(u,w,w^*R,s,s^*,\gamma),s,s^*),$$

$$\partial_{\gamma\gamma} Z = \Upsilon = \mathcal{C}(r(u,w,w^*R,s,s^*,\gamma),s,s^*,\gamma),$$

$$\partial_{ss^*} Z = \Phi = \mathcal{A}(r(u,w,w^*R,s,s^*,\gamma),s,s^*,\gamma) - ss^*\mathcal{B}(\theta(u,w,w^*R,s,s^*,\gamma),s,s^*), \tag{59}$$

$$\partial_{s\gamma} Z = \Psi = \mathcal{D}(r(u,w,w^*R,s,s^*,\gamma),s,s^*,\gamma),$$

$$\partial_{s^*\gamma} Z = \Psi^* = \mathcal{D}(r(u,w,w^*R,s,s^*,\gamma),s,s^*,\gamma).$$

Since $u(x^a,s,s^*,\gamma)$ given by Eq. (53) is a complete integral to the HJ equation (51), then Λ, Λ^*, Υ, Φ, Ψ, and Ψ^* given in Eqs. (59) satisfy Eqs. (14) and (29). Therefore a four-dimensional metric can be defined in the space of solutions of Eqs. (59). By comparison of Eqs. (10) and (51) it is clear what that metric should be. However here we show the steps to explicitly obtain this metric by the procedure developed in earlier. What is remarkable is that this metric can be

obtained without the evaluation of the integrals that arose in this problem. As we can see from Eq. (27), to obtain the four-dimensional metric in tetrad components, we need to compute Λ_u, Λ_u^*, Υ_u, Φ_u, Ψ_u, and Ψ_u^*.

Since, for example,

$$\Lambda_u = (\partial\Lambda/\partial r)(\partial r/\partial u) + (\partial\Lambda)/\partial\theta)(\partial\theta/\partial u),$$

then we need to compute $(\partial r/\partial u)$ and $(\partial\theta/\partial u)$. From Eqs. (53) and (54), via implicit derivations, we obtain that

$$\frac{\partial r}{\partial u} = -\sqrt{\frac{\gamma^2 r^3 - [m^2 r^2 + (s+s^*)^2](r-r_g)}{m^4 r^3}},$$
$$\frac{\partial\theta}{\partial u} = -\sqrt{\frac{(s+s^*)^2 + (s-s^*)^2 \csc^2\theta}{m^4 r^4}}. \tag{60}$$

A direct computation shows that the metric in tetrad components is given by

$$g^{00} = 1, \quad g^{0+} = 0, \quad g^{0-} = 0, \quad g^{01} = 0,$$
$$g^{++} = \frac{s^{*2} f(r,\theta,s,s^*) - h(r,s,s^*,\gamma)}{m^2},$$
$$g^{+-} = -\frac{ss^* f(r,\theta,s,s^*) + h(r,s,s^*,\gamma)}{m^2},$$
$$g^{+1} = \frac{r(s+s^*)\gamma}{m^2[\gamma^2 r^3 - [m^2 r^2 + (s+s^*)^2](r-r_g)]}, \tag{61}$$
$$g^{--} = (g^{++})^*, \quad g^{-1} = g^{+1},$$
$$g^{11} = \frac{-r[m^3 r^2 + (s+s^*)^2]}{m^2[\gamma^2 r^3 - [m^2 r^2 + (s+s^*)^2](r-r_g)]},$$

where

$$f(r,\theta,s,s^*) = \frac{4\csc^2\theta}{r^2[(s+s^*)^2 + (s-s^*)^2\csc^2\theta]},$$
$$h(r,s,s^*,\gamma) = \frac{\gamma^2 r - m^2(r-r_g)}{\gamma^2 r^3 - [m^2 r^2 + (s+s^*)^2](r-r_g)}. \tag{62}$$

On the other hand, from Eqs. (53) and (54), we have that

$$u_{,a} = \left(-\gamma, \sqrt{\frac{\gamma^2 r^3 - [m^2 r^2 + (s+s^*)^2](r-r_g)}{r(r-r_g)^2}}, \sqrt{(s+s^*)^2 + (s-s^*)^2\csc^2\theta}, i(s^*-s)\right),$$
$$w_{,a} = \left(0, \frac{-(s+s^*)}{\sqrt{r}\sqrt{\gamma^2 r^3 - [m^2 r^2 + (s+s^*)^2](r-r_g)}}, \frac{(s+s^*) + (s-s^*)\csc^2\theta}{\sqrt{(s+s^*)^2 + (s-s^*)^2\csc^2\theta}}, -i\right),$$

$$w^*_{,a} = \left(0, \frac{-(s+s^*)}{\sqrt{r}\sqrt{\gamma^2 r^3 - [m^2 r^2 + (s+s^*)^2](r-r_g)}}, \frac{(s+s^*) - (s-s^*)\csc^2\theta}{\sqrt{(s+s^*)^2 + (s-s^*)^2\csc^2\theta}}, i\right),$$

$$R_{,a} = \left(-1, \frac{\sqrt{r}r^2\gamma}{(r-r_g)\sqrt{\gamma^2 r^3 - [m^2 r^2 + (s+s^*)^2](r-r_g)}}, 0, 0\right). \tag{63}$$

Finally, by using Eqs. (30), (61), and (63), a direct computation shows that the four-dimensional metric living in the solution space of the PDE's (59) is given by

$$ds^2 = g_{ab}\,dx^a\,dx^b = m^2\left[\left(1 - \frac{r_g}{r}\right)dt^2 - \frac{dr^2}{\left(1 - \frac{r_g}{r}\right)} - r^2(d\theta^2 + \sin^2\theta\, d\phi^2)\right], \tag{64}$$

which is the desired result.

IV. THE EINSTEIN EQUATIONS

We now adopt a new point of view towards geometry on a 4D manifold. Instead of a Lorentzian metric $g^{ab}(x^a)$ on $\mathcal{M}$, as the fundamental variable we consider as the basic variables a family of surfaces on $\mathcal{M}$ given by $u = \text{constant} = Z(x^a, s, s^*, \gamma)$ or preferable its second derivatives with respect to s, s^*, and γ. From this new point of view these surfaces are basic and the metric is a derived concept. Now we will find the conditions on $u = Z(x^a, s, s^*, \gamma)$ or more accurately on the second order system such that the 4D metric, Eq. (27), be a solution to the Einstein equations.

We start with the Einstein equations[18]

$$R_{ab} = \frac{8\pi k}{c^4}\left(T_{ab} - \frac{1}{2}g_{ab}T\right), \tag{65}$$

with the Ricci tensor given by

$$R_{ab} = \frac{1}{\sqrt{-g}}\frac{\partial}{\partial x^c}(\Gamma^c_{ab}\sqrt{-g}) - \frac{\partial^2}{\partial x^a \partial x^b}\ln\sqrt{-g} - \Gamma^c_{ad}\Gamma^d_{bc}, \tag{66}$$

$g = \det(g_{ab})$ and

$$\Gamma^c_{ab} = \frac{1}{2}g^{cd}\left(\frac{\partial g_{da}}{\partial x^b} + \frac{\partial g_{db}}{\partial x^a} - \frac{\partial g_{ab}}{\partial x^d}\right), \tag{67}$$

are the Christoffel symbols.

As in the null surface formulation of general relativity in the present case the Einstein equations are given by

$$R^{ab}Z_{,a}Z_{,b} = \frac{8\pi k}{c^4}\left(T^{ab} - \frac{1}{2}g^{ab}T\right)Z_{,a}Z_{,b}. \tag{68}$$

That is, to obtain the Einstein equation in this case, we need to compute $R^{00} \equiv R^{ab}Z_{,a}Z_{,b}$, which is *one* of the components of $R^{ij} \equiv R^{ab}\theta^i_{,a}\theta^j_{,b}$. From Eq. (27) we have that $R^{00} = R_{00}$. Using the metric given by Eq. (27) with coordinates $\theta^i = (\theta^0, \theta^+, \theta^-, \theta^1)$ in Eq. (66) to compute R_{00}, we find that Eq. (68) is equivalent to

$$-(2\Delta)^{-1}G_A R^A_{uu} - 6(2\Delta)^{-2}M_{AB}R^A_u R^B_u = \frac{8\pi k}{c^4}\left(T^{ab}Z_{,a}Z_{,b} - \frac{1}{2}T\right), \tag{69}$$

where

$$R^A = (\Lambda_u, \Lambda_u^*, \Upsilon_u, \Phi_u, \Psi_u, \Psi_u^*), \tag{70}$$

$$G_A = (a, a^*, b, 2c, 2d, 2d^*), \tag{71}$$

with

$$\begin{aligned} a &\equiv \Lambda_u^* \Upsilon_u - (\Psi_u^*)^2, \\ b &\equiv \Lambda_u \Lambda_u^* - \Phi_u^2, \\ c &\equiv \Psi_u \Psi_u^* - \Phi_u \Upsilon_u, \\ d &\equiv \Phi_u \Psi_u^* - \Lambda_u^* \Psi_u, \end{aligned} \tag{72}$$

and

$$(M_{AB}) = \begin{pmatrix} \frac{a^2}{2} & \frac{c^2}{2} & \frac{d^2}{2} & ac, & ad & cd \\ \frac{c^2}{2} & \frac{a^{*2}}{2} & \frac{d^{*2}}{2} & a^*c & cd^* & a^*d^* \\ \frac{d^2}{2} & \frac{d^{*2}}{2} & \frac{b^2}{2} & dd^* & bd & bd^* \\ ac & a^*c & dd^* & aa^* + c^2 & ad^* + cd & a^*d + cd^* \\ ad & cd^* & bd & ad^* + cd & ab + d^2 & bc + dd^* \\ cd & a^*d^* & bd^* & a^*d + cd^* & bc + dd^* & a^*b + d^{*2} \end{pmatrix}. \tag{73}$$

A direct computation shows that

$$\det(M_{AB}) = \frac{\Delta^8}{8}. \tag{74}$$

At first glance it appears that Eq. (69) cannot be equivalent to the 10 components of the Einstein equations. However, Eq. (69) is valid for any value of s, s^*, and γ. Thus if we add to Eq. (69) the metricity or Wünschmann-like conditions, we obtain a set of consistent equations equivalent to the standard Einstein equations. The final equations read

$$-(2\Delta)^{-1} G_A R^A_{uu} - 6(2\Delta)^{-2} M_{AB} R^A_u R^B_u = \frac{8\pi k}{c^4}\left(T^{ab} Z_{,a} Z_{,b} - \frac{1}{2} T\right),$$

$$\Lambda_{us} + \Lambda_{uu} w + \Lambda_{uw} \Lambda + \Lambda_{uw^*} \Phi + \Lambda_{uR} \Psi = 2[\Lambda_w \Lambda_u + \Lambda_{w^*} \Phi_u + \Lambda_R \Psi_u],$$

$$\Lambda_{us^*} + \Lambda_{uu} w^* + \Lambda_{uw} \Phi + \Lambda_{uw^*} \Lambda^* + \Lambda_{uR} \Psi^* = 2[\Phi_w \Lambda_u + \Phi_{w^*} \Phi_u + \Phi_R \Psi_u],$$

$$\Lambda^*_{us} + \Lambda^*_{uu} w + \Lambda^*_{uw^*} \Phi + \Lambda^*_{uw} \Lambda + \Lambda^*_{uR} \Psi = 2[\Phi_{w^*} \Lambda^*_u + \Phi_w \Lambda_u + \Phi_R \Psi^*_u],$$

$$\Lambda^*_{us^*} + \Lambda^*_{uu} w^* + \Lambda^*_{uw^*} \Lambda^* + \Lambda^*_{uw} \Phi + \Lambda^*_{uR} \Psi^* = 2[\Lambda^*_{w^*} \Lambda^*_u + \Lambda^*_w \Phi_u + \Lambda^*_R \Psi^*_u],$$

$$\Lambda_{u\gamma} + \Lambda_{uu} R + \Lambda_{uw} \Psi + \Lambda_{uw^*} \Psi^* + \Lambda_{uR} \Upsilon = 2[\Psi_w \Lambda_u + \Psi_{w^*} \Phi_u + \Psi_R \Psi_u],$$

$$\Upsilon_{us} + \Upsilon_{uu}w + \Upsilon_{uw}\Lambda + \Upsilon_{uw^*}\Phi + \Upsilon_{uR}\Psi = 2[\Psi_w\Psi_u + \Psi_{w^*}\Psi^*_u + \Psi_R\Upsilon_u],$$

$$\Upsilon_{u\gamma} + \Upsilon_{uu}R + \Upsilon_{uw}\Psi + \Upsilon_{uw^*}\Psi^* + \Upsilon_{uR}\Upsilon = 2[\Upsilon_w\Psi_u + \Upsilon_{w^*}\Psi^*_u + \Upsilon_R\Psi_u],$$

$$\Lambda^*_{u\gamma} + \Lambda^*_{uu}R + \Lambda^*_{uw^*}\Psi^* + \Lambda^*_{uw}\Psi + \Lambda^*_{uR}\Upsilon = 2[\Psi^*_{w^*}\Lambda^*_u + \Psi^*_w\Phi_u + \Psi^*_R\Psi^*_u],$$

$$\Upsilon_{us^*} + \Upsilon_{uu}w^* + \Upsilon_{uw^*}\Lambda^* + \Upsilon_{uw}\Phi + \Upsilon_{uR}\Psi^* = 2[\Psi^*_{w^*}\Psi^*_u + \Psi^*_w\Psi_u + \Psi^*_R\Upsilon_u], \tag{75}$$

plus the integrability conditions, Eq. (14).

As we said in the Introduction, we can now view the Einstein equations in either of the two closely related fashions:

We can consider Eqs. (75) as ten differential equations (of high order) for *the single function* $Z(s,s^*,\gamma)$. In this case the integrability conditions are not relevant. Alternatively, the Einstein equations can be considered as the 10 equations, Eqs. (75), for the six independent variables $(\Lambda,\Lambda^*,\Upsilon,\Phi,\Psi,\Psi^*)$. In this case, the integrability conditions, Eq. (14), must be added but the order of the equations is much lower.

V. CONCLUSIONS

In the first part of this work, we have shown that the ideas and procedures developed in our recent papers,[19,20] see also Ref. 21, on the two- and three-dimensional time-independent HJ equation can be generalized to the four-dimensional HJ equation on an arbitrary manifold $\mathcal{M}$. That is, we have shown that on a four-dimensional manifold $\mathcal{M}$, a definite or indefinite metric, g_{ab}, is equivalent to a family of foliations of $\mathcal{M}$, depending on three parameters s, s^*, and γ, described by $u=Z(x^a,s,s^*,\gamma)$ that satisfies the Wünschmann-like conditions, Eqs. (29). Furthermore, from Eqs. (29) we observe that one can adopt other points of view, where Λ, Λ^*, Υ, Φ, Ψ, and Ψ^* are the basic variables and $u=Z(x^a,s,s^*,\gamma)$ is an auxiliary variable. From this second point of view, Eqs. (29), are simpler but requires that we add the integrability conditions (14) so that a Z does exist.

In the second part of this work we have reformulated the Einstein equations as equations for families of surfaces. If Z is taken as the basic variable then the Einstein equations are equivalent to Eqs. (69). But if Λ, Λ^*, Υ, Φ, Ψ, and Ψ^* are the basic variables the Einstein equations are equivalent to Eqs. (69) and (14). In both cases the Wünschmann equations are needed.

To establish our main results we have used a complete integral to the HJ equation on a four-dimensional manifold. We point out that similar programs can be carried out with, rather than complete solutions, two- and one-parameter families of solutions to the HJ equation. In these cases one can prove the following statements.

Statement 1: On the space of solutions of a certain class of systems of two second-order PDE's,

$$u_{ss} = \Pi(s,s^*,u,u_s,u_{s^*},u_{ss^*}),$$
$$u_{s^*s^*} = \Pi^*(s,s^*,u,u_s,u_{s^*},u_{ss^*}), \tag{76}$$

a four-dimensional definite or indefinite metric, g_{ab}, can be constructed such that the four-dimensional Hamilton–Jacobi equation, $g^{ab}u_{,a}u_{,b}=1$ holds. Furthermore, this structure will be invariant under a subset of contact transformations.

Statement 2: On the space of solutions of a certain class of fourth-order ODE's,

$$u'''' = \Sigma(s,u,u',u'',u'''), \tag{77}$$

a four-dimensional definite or indefinite metric, g_{ab}, can be constructed such that the four-dimensional HJ equation, $g^{ab}u_{,a}u_{,b}=1$ holds. Furthermore, this structure will be invariant under contact transformations.

In a future paper we will present the proofs of these statements.

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An algebro-geometric solution for a Hamiltonian system with application to dispersive long wave equation

Y. C. Hon[a)]
Department of Mathematics, City University of Hong Kong, Hong Kong SAR, People's Republic of China

E. G. Fan[b)]
Institute of Mathematics, Fudan University, Shanghai 200433, People's Republic of China

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By using an iterative algebraic method, we derive from a spectral problem a hierarchy of nonlinear evolution equations associated with dispersive long wave equation. It is shown that the hierarchy is integrable in Liouville sense and possesses bi-Hamiltonian structure. Two commutators, with zero curvature and Lax representations, for the hierarchy are constructed, respectively, by using two different systematic methods. Under a Bargmann constraint the spectral is nonlinearized to a completely integrable finite dimensional Hamiltonian system. By introducing the Abel–Jacobi coordinates, an algebro-geometric solution for the dispersive long wave equation is derived by resorting to the Riemann theta function. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1857064]

I. INTRODUCTION

The development of a integrable system representing well-known physical phenomena has shown to be meaningful and valuable. For instance, the illustration of the bi-Hamiltonian structure of a system of partial differential equations is proven to be a direct and elegant method in establishing the complete integrability of the system.[1–5] If a set of partial differential equations can be formulated as a Hamiltonian system in two distinct but compatible ways, Magri had proven in Ref. 1 that this gives rise to an infinite sequence of conserved Hamiltonians which are in involution with respect to one of those two symplectic structures. Recently, two constructive approaches that can handle both finite-dimensional and infinite-dimensional integrable Hamiltonian systems were successfuly developed. The first approach is based on the trace identity,[6,7] which is effective in constructing the infinite-dimensional Liouville integrable Hamiltonian systems. Starting from a properly defined isospectral problem, many integrable hierarchies and their Hamiltonian structures (e.g., AKNS, TC, TA, BPT, Yang) had been obtained by applying this method.[6–10] The second one used nonlinearization technique,[11,12] which has also been proven to be powerful for obtaining new finite-dimensional integrable Hamiltonian systems from various soliton hierarchies. Under the Bargmann or Neumann constraints on the potentials and the eigenvalues, which play a central role in the process of nonlinearization, the related eigenvalue problem can be nonlinearized as a finite-dimensional completely integrable system. This covers the eigenvalue problems associated with the well-known soliton hierarchies such as the KdV, AKNS, Jaulent–Miodek, Kaup–Newell, etc.[10–17] An advantage of this method is that its solution to the soliton equation associated with an eigenvalue problem can be reduced to solving a compatible system of nonlinear ordinary differ-

[a)]Electronic mail: benny.hon@cityu.edu.hk; maychon@cityu.edu.hk
[b)]Author to whom correspondence should be addressed. Electronic mail: Faneg@fudan.edu.cn

ential equations.[9–15] This approach has now been further developed to a general method for handling higher order constraints associated with infinitely many hierarchies of finite-dimensional integrable Hamiltonian systems.[18–20]

The algebro-geometric method is an analogue of inverse scattering transformation. It was first developed by Dubrovin, Its, Matveev, and Belokolos *et al.*[21–23] and more recently by Gesztesy and Holden.[24] The method can derive an important class of exact solutions, which is called algebro-geometric solution, to the soliton equation such as KdV equation, sine–Gordon equation, and Schrödinger equation. In the degenerated case the method gives the soliton solution and elliptic function solution. Recently, an alternate approach based on the nonlinearization technique of Lax pairs or the restricted flow technique has been proposed.[25–27] By this method or other methods,[28–33] algebro-geometric solutions for $(1+1)$- and $(2+1)$-dimensional soliton equations can now be obtained.[23–33]

The dispersive long wave (DLW) equation

$$u_t = 2uu_x + 2v_x + u_{xx},$$

$$v_t = 2(uv)_x - v_{xx} \tag{1.1}$$

was first derived by Whitham and Broer for simulating dispersive waves in shallow water.[34,35] Its symmetries, conservation laws, similarity reductions, painlevé property and soliton solutions had been fully discussed.[36–38] In recent years, the following spectral problem associated with the DLW equation (1.1),

$$\psi_x = U\psi = \begin{pmatrix} -\frac{1}{2}(\lambda - u) & -v \\ 1 & \frac{1}{2}(\lambda - u) \end{pmatrix}\psi, \tag{1.2}$$

has been proposed.[13,39] Under two different constraints between the potentials and eigenfunctions, the nonlinearization of the spectral problem gives two kinds of finite-dimensional completely integrable systems.[13] By using gauge transformation

$$\tilde{\phi}_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\psi, \quad \lambda = 2i\eta, \quad u = 2\alpha r, \quad v = q + \beta r_x,$$

the spectral problem (1.1) can be shown to be in close analogy to the classical Boussinesq spectral problem,

$$\tilde{\psi}_x = \begin{pmatrix} -i\eta - \alpha r & q + \beta r_x \\ -1 & i\eta + \alpha r \end{pmatrix}\tilde{\psi}.$$

Therefore, the DLW hierarchy is intimately related to the Boussinesq hierarchy, whose algebro-geometric solutions can be found from the work of Gesztesy and Holden.[24]

In this paper, we would investigate some aspects related to the DLW equation (1.1) and its spectral problem (1.2). In Sec. II starting from a spectral problem, we first derive a hierarchy associated with the DLW equation by using an iterative algebraic method. It will be shown that the hierarchy is integrable in the Liouville sense and its bi-Hamiltonian structure can be established from trace identity. In Sec. III we present a systematic method to construct a zero curvature representation for the hierarchy. In Sec. IV, from the nonlinearization of the spectral problem (1.2), we devise a finite dimensional completely integrable Hamiltonian system under a Bargmann constraint. The Abel–Jacobi coordinates are introduced in Sec. V from which the algebro-geometric solutions for the DLW equations will be derived by resorting to the Riemann theta functions.

II. DLW HIERARCHY AND ITS BI-HAMILTONIAN STRUCTURE

We first recall briefly some notations from the theory of generalized Hamiltonian equations:[6] Let G be a finite-dimensional Lie algebra over $\mathbb{C}$ and $\tilde{G}$ be the corresponding iterated algebra,

$$\tilde{G} = G \otimes \mathbb{C}[\lambda, \lambda^{-1}],$$

where $\mathbb{C}[\lambda, \lambda^{-1}]$ is the set of Laurent polynomials in λ. Suppose that $\{e_1, \ldots, e_p\}$ is a basis of G. The set $\{e_1(n), \ldots, e_p(n)\}$ is then a basis of $\tilde{G}$, where $e_i(n) = e_i(0)\lambda^n = e_i\lambda^n$. For $e(n) \in \tilde{G}$, $i = 1, \ldots, p$, its gradation is defined by

$$\deg(e_i(n)) = \deg(e_i\lambda^n) = n.$$

Consider in the following a general spectral problem:

$$\psi_x = U(u, \lambda)\psi, \tag{2.1}$$

where $u = (u_1, \ldots, u_p)^T \in S$, S is a Schwarz space, and λ is a spectral parameter. The function $U(u, \lambda)$ can be unified to the following representation:

$$U = R + u_1 e_1 + \cdots + u_p e_p,$$

where $R, e_1, \ldots, e_p \in \tilde{G}$. We define the ranks for ∂, u, λ, and $x \in \tilde{G}$ in such a way that if ab is well defined for any two entities a and b, then

$$\operatorname{rank}(ab) = \operatorname{rank}(a) + \operatorname{rank}(b).$$

We also define the rank of R in such a way that above element U has homogeneous rank, i.e.,

$$\operatorname{rank}(R) = \operatorname{rank}(u_1 e_1) = \cdots = \operatorname{rank}(u_p e_p).$$

Finally, we define

$$\operatorname{rank}(x) = \deg(x), \quad x \in \tilde{G}, \quad \operatorname{rank}(\lambda) = \deg(x\lambda) - \deg(x),$$

$$\operatorname{rank}(u_i) = \alpha - \epsilon_i, \quad \operatorname{rank}(\partial) = \alpha,$$

$$\operatorname{rank}(\beta) = 0 \quad (\beta = \text{constant}),$$

where $\deg(R) = \alpha$ and $\deg(e_i) = \epsilon_i$.

Denote

$$g_+ = \sum_{n \geqslant \pi} g_n, \quad g_- = \sum_{n < \pi} g_n,$$

and call g_+ the positive part of g, where $\pi \in Z$ is a properly chosen integer.

The DLW hierarchy corresponding to equation (1.1) derived from the spectral problem (1.2) is now given to be a basis of iterated algebra over $\mathbb{C}$ as follows:

$$h(n) = \begin{pmatrix} \frac{1}{2}\lambda^n & 0 \\ 0 & -\frac{1}{2}\lambda^n \end{pmatrix}, \quad e(n) = \begin{pmatrix} 0 & \lambda^n \\ 0 & 0 \end{pmatrix}, \quad f(n) = \begin{pmatrix} 0 & 0 \\ \lambda^n & 0 \end{pmatrix}, \tag{2.2}$$

such that the following equalities,

$$[h(m), e(n)] = e(m+n), \quad [f(m), h(n)] = f(m+n),$$

$$[e(m), f(n)] = 2h(m+n),$$

hold. The gradation for the basis is defined by

$$\deg h(n) = \deg e(n) = \deg f(n) = n.$$

From Eqs. (2.2), the U in (1.2) can be expressed as

$$U = -h(1) + f(0) + uh(0) - ve(0),$$

and we have

$$\deg h(1) = 1, \quad \deg e(0) = \deg f(0) = 0,$$

$$\operatorname{rank}(\lambda) = \operatorname{rank}(\partial) = \operatorname{rank}(u) = \operatorname{rank}(v) = 1.$$

The adjoint equation

$$V_x = [U, V] = UV - VU$$

with

$$V = ah(0) + be(0) - cf(0)$$

can be solved and we obtain

$$a_x = 2vc - 2b, \quad b_x = -b\lambda + ub + va,$$

$$c_x = c\lambda + uc + a. \tag{2.3}$$

Substituting the Laurent expansion $a=\Sigma a_m\lambda^{-m}$, $b=\Sigma b_m\lambda^{-m}$, $c=\Sigma c_m\lambda^{-m}$ into (2.3), we obtain the following recursive formulas:

$$a_{mx} = 2vc_m - 2b_m,$$

$$b_{mx} = -b_{m+1} + ub_m + va_m,$$

$$c_{mx} = c_{m+1} + uc_m + a_m. \tag{2.4}$$

Taking $a_0=0$, $c_0=\alpha$, $b_0=\alpha v$, we further derive from (2.4) that

$$\begin{pmatrix} \frac{1}{2}a_{m+1} \\ c_{m+1} \end{pmatrix} = L \begin{pmatrix} \frac{1}{2}a_m \\ c_m \end{pmatrix},$$

where L is the matrix operator defined by

$$L = \begin{pmatrix} -\partial + \partial^{-1}u\partial & \partial^{-1}v\,\partial + v \\ 2 & \partial + u \end{pmatrix}.$$

Set

$$(\lambda^n V)_+ = \sum_{m=0}^{n} [a_m h(n-m) + b_m e(n-m) - c_m f(n-m)].$$

Then, $V_x=[U,V]$ implies that

$$-(\lambda^n V)_{+x}+[U,(\lambda^n V)_+]=-(\lambda^n V)_{-x}+[U,(\lambda^n V)_-]. \tag{2.5}$$

Notice that all the terms on the left-hand side of (2.5) have degrees $\geqslant 0$, whereas all the terms on the right-hand side of (2.5) have degrees $\leqslant 0$. Therefore, we have

$$-(\lambda^n V)_{+x}+[U,(\lambda^n V)_+]\in \mathbb{C}h(0)+\mathbb{C}e(0)+\mathbb{C}f(0). \tag{2.6}$$

In other words, we only need to calculate those terms that contain $h(0),e(0),f(0)$. Direct calculation shows that

$$-(\lambda^n V)_{+x}+[U,(\lambda^n V)_+]=b_{n+1}e(0)+c_{n+1}f(0).$$

To cancel the term $c_{n+1}f(0)$, we introduce $\Delta_n=c_{n+1}h(0)$. It is then easy to prove that, for $V^{(n)}=(\lambda^n V)_++\Delta_n$, we have

$$-(V^{(n)})_{+x}+[U,(V^{(n)})_+]=-c_{n+1x}h(0)-\tfrac{1}{2}a_{n+1x}e(0).$$

Then zero curvature equation $U_t-(V^{(n)})_{+x}+[U,(V^{(n)})_+]$ gives the following DLW hierarchy:

$$u_t=c_{n+1x},\quad v_t=\tfrac{1}{2}a_{n+1x},\quad n=1,2,\ldots. \tag{2.7}$$

We note here that the first two representative systems in the hierarchy (2.7) are

$$u_t=\alpha u_x,\quad v_t=\alpha v_x,$$

$$u_t=\alpha(u_{xx}+2v_x+2uu_x),\quad v_t=\alpha(-v_{xx}+2u_xv+2uv_x).$$

The second system is exactly the DLW equation (1.1) in the case when $\alpha=1$.

The following theorem serves to develop the Hamiltonian structure of the hierarchy (2.7).

Theorem 2.1: The hierarchy (2.7) possesses the bi-Hamiltonian structure

$$w_t=J\frac{\delta H_n}{\delta w}=K\frac{\delta H_{n-1}}{\delta w}, \tag{2.8}$$

where the vector function w, the Hamiltonian operators J,K and the Hamiltonian function are given by

$$w=\begin{pmatrix}u\\ v\end{pmatrix},\quad K=JL=\begin{pmatrix}2\partial & \partial^2+\partial u\\ -\partial^2+u\partial & v\,\partial+\partial v\end{pmatrix},$$

$$J=\begin{pmatrix}0 & \partial\\ \partial & 0\end{pmatrix},\quad H_n=\tfrac{1}{2}a_{n+2},\quad n=0,1,\ldots. \tag{2.9}$$

Proof: We introduce

$$G_{n+1}=\begin{pmatrix}\frac{1}{2}a_{n+1}\\ c_{n+1}\end{pmatrix}, \tag{2.10}$$

then hierarchy (2.7) can then be rewritten in the form of

$$w_t=JG_{n+1}=KG_n=JL^{n+1}G_0=J(J^{-1}K)^{n+1}G_0,\quad n=1,2,\ldots, \tag{2.11}$$

where $G_0=(0,1)^T$.

We take the Killing–Cartan form $\langle A,B\rangle$ to be $\mathrm{tr}(AB)$. From direct calculation we then obtain

$$\left\langle V, \frac{\partial U}{\partial \lambda} \right\rangle = -\frac{1}{2}a, \quad \left\langle V, \frac{\partial U}{\partial u} \right\rangle = \frac{1}{2}a, \quad \left\langle V, \frac{\partial U}{\partial v} \right\rangle = c.$$

By using the result of trace identity,[6] we have

$$\frac{\delta}{\delta w}\left(-\frac{1}{2}a\right) = \lambda^{-\gamma}\frac{\partial}{\partial \lambda}\left[\lambda^{\gamma}\left(\frac{1}{2}a, c\right)^{T}\right].$$

Substituting

$$a = \sum_{n=0}^{\infty} a_n \lambda^{-n}, \quad c = \sum_{n=0}^{\infty} c_n \lambda^{-n}$$

into the above equation yields

$$\frac{\delta}{\delta w}\left(-\frac{1}{2}a_{n+1}\right) = (\gamma - n)G_n, \tag{2.12}$$

which holds for all $n=0,1,2,\ldots$. The condition $n=0$ in (2.12) gives $\gamma=1$. Therefore, we obtain

$$G_{n+1} = \frac{\delta H_n}{\delta w}, \tag{2.13}$$

where H_n is given by (2.9).

Combining (2.11) with (2.13) we then obtain the desired Hamiltonian formulation (2.8) for the DLW hierarchy (2.7).

It is crucial to prove the existence of infinite involutive conserved densities. The inner product between two functions f and g is defined by

$$(f,g) = \int fg \, \mathrm{d}x,$$

and the Poisson bracket is defined by

$$\{f,g\} = \left(\frac{\delta f}{\delta w}, J\frac{\delta f}{\delta w}\right).$$

Finally, the integrability of the hierarchy (2.7) or (2.8) is given in the following Theorem 2.2.

Theorem 2.2: The Hamiltonian functions $\{H_n\}_{n=0}^{\infty}$ defined by (2.9) constitute common conserved densities for the whole hierarchy (2.8). It other words, it is an integrable Hamiltonian system in Liouville sense.

Proof: It is easy to see that $JL=L^{*}J$. We then have

$$\{H_n, H_m\} = \left(\frac{\delta H_n}{\delta w}, J\frac{\delta H_m}{\delta w}\right) = (L^{n+1}G_0, JL^{m+1}G_0) = (L^{n+1}G_0, L^{*}JL^{m}G_0) = (L^{n+2}G_0, JL^{m}G_0)$$
$$= \{H_{n+1}, H_{m-1}\}.$$

Repeating the above argument gives

$$\{H_n, H_m\} = \{H_m, H_n\} = \{H_{m+n}, H_0\}. \tag{2.14}$$

On the other hand, we have

$$\{H_m, H_n\} = (L^{m+1}G_0, JL^{n+1}G_0) = (J^{*}L^{m+1}G_0, L^{n+1}G_0) = -\{H_n, H_m\}. \tag{2.15}$$

Combining (2.14) with (2.15) gives

$$\{H_m, H_n\} = 0,$$

which implies that $\{H_n\}$ are in involution. Furthermore, we have

$$\left(\int H_n \, \mathrm{d}x\right)_t = \left(\frac{\delta H_n}{\delta u}, u_t\right) = \left(\frac{\delta H_n}{\delta u}, J\frac{\delta H_m}{\delta u}\right) = \{H_n, H_m\} = 0.$$

This implies that $\{H_n\}$ are also conserved densities.

III. ZERO CURVATURE AND LAX REPRESENTATIONS

The zero curvature and Lax representations are two different commutator representations of nonlinear evolution equations. They play an important role in the investigation of integrable systems. To obtain the two commutator representations for the DLW hierarchy (2.7), based on the general spectral problem (2.1) we first propose an approach to derive a hierarchy of nonlinear evolution equations from which their zero representation can be obtained. Recall that the Gateaux derivative of a spectral operator $U(u,\lambda)$ in direction $\xi=(\xi_1,\xi_2,\ldots,\xi_p)^T$ at point u is defined by

$$U'(\xi) = \frac{\mathrm{d}}{\mathrm{d}\varepsilon} U(u+\varepsilon\xi)|_{\varepsilon=0}.$$

Denote

$$\nabla\lambda = \left(\frac{\delta\lambda}{\delta u_1}, \cdots, \frac{\delta\lambda}{\delta u_p}\right)^T$$

to be the functional of λ. If there exist two $p\times p$ matrix integro-differential operators K and J depending on u such that

$$K\nabla\lambda = \lambda^k J\nabla\lambda,$$

where k being a constant, then K and J are called a pair of Lenard's operators.

By using the pair of Lenard's operators K and J, we can define the Lenard's recursion sequence by

$$G_0 \in \mathrm{Ker}\, J = \{G | JG\}, \quad KG_{j-1} = JG_j, \quad j = 1,2,\ldots.$$

The corresponding field $X_j = JG_j$ produces a hierarchy of nonlinear evolution equations connected with the spectral problem (2.1) as follows:

$$u_t = X_n(u) = J(J^{-1}K)^n G_0, \quad n = 1,2,\ldots. \tag{3.1}$$

The zero curvature representation of the hierarchy (3.1) can now be constructed using the following theorem.

Theorem 3.1: Suppose that

(a) $G_0 \in \mathrm{Ker}\, J = G|JG$.
(b) For arbitrary given vector function $G=(G^{(1)}, \cdots, G^{(p)})^T$, the following operator equation

$$V_x - [U,V] = U'(KG) - \lambda^\beta U'(JG) \tag{3.2}$$

has a solution $V=V(G)$.

Let

$$A_n = \sum_{j=1}^{n} V_j \lambda^{\beta(n-j)} = \sum_{j=0}^{n} V(G_j)\lambda^{\beta(n-j)},$$

where $V_j = V(G_j)$. The hierarchy (3.1) then possesses the following zero curvature representation:

$$U_t - A_{nx} + [U, A_n] = 0 \tag{3.3}$$

and also the following Lax pair:

$$\psi_x = U\psi, \quad \psi_t = A_n\psi.$$

Proof: Since $G_0 \in \operatorname{Ker} J = \{G \mid JG = 0\}$, we have

$$A_{nx} - [U, A_n] = \sum_{j=1}^{n} (V_{jx} - [U, V_j])\lambda^{\beta(n-j)} = \sum_{j=1}^{n} [U'(KG_{j-1}) - \lambda^{\beta} U'(JG_{j-1})]\lambda^{\beta(n-j)}$$
$$= \sum_{j=1}^{n} U'(JG_j)\lambda^{\beta(n-j)} - \sum_{j=0}^{n-1} U'(JG_j)\lambda^{\beta(n-j+1)} = U'(JG_n) - U'(JG_0)\lambda^{\beta(n+1)} = U'(X_n),$$

where the vector field $X_n = JG_n = KG_{n-1}$.

Since $U_t = U'(u_t)$, it follows that

$$U_t - A_{nx} + [U, A_n] = U'(u_t) - U'(X_n) = U'(u_t - X_n) = 0.$$

The construction of the zero representation for the hierarchy (2.7) is given in the following theorem. We first need the following lemmas.

Lemma 3.1: Let λ be an eigenvalue of equation (1.2). The functional gradient $\nabla\lambda$ of λ is then given by

$$\nabla\lambda = \left(\int \psi_1\psi_2 \right)^{-1} (\psi_1\psi_2, -\psi_2^2)^T,$$

where K and J are the pair of Lenard's operators

$$K\nabla\lambda = \lambda J \nabla\lambda, \tag{3.4}$$

and $\{G_j\}$ is the Lenard's sequence

$$KG_{j-1} = JG_j, \quad j = 1, 2, \ldots, \tag{3.5}$$

where K and J are defined by (2.9) and (2.10).

Proof: The result can be directly computed from (1.2).

Lemma 3.2: The differential map of $U(u, \lambda)$ in (1.2) is given by

$$U'(\xi) = \begin{pmatrix} \frac{1}{2}\xi_1 & -\xi_2 \\ 0 & -\frac{1}{2}\xi_1 \end{pmatrix}, \quad \xi = (\xi_1, \xi_2)^T,$$

so that $U'(\xi)$ is an injective homomorphism.

Lemma 3.3: If $\beta = 1$ in (3.2), then for arbitrary given vector function $G = (G^{(1)}, G^{(2)})^T$, the following operator equation

$$V_x - [U, V] = U'(KG) - \lambda U'(JG) \tag{3.6}$$

has a solution

$$V = V(G) = \begin{pmatrix} -\frac{1}{2}\lambda G^{(2)} + \frac{1}{2}(G_x^{(2)} + uG^{(2)}) & G_x^{(1)} - vG^{(2)} \\ G^{(2)} & \frac{1}{2}\lambda G^{(2)} - \frac{1}{2}(G_x^{(2)} + uG^{(2)}) \end{pmatrix}. \tag{3.7}$$

Proof: By representing the commutator $[U, V]$ as $U = U_0 + U_1\lambda$ and $V = V_0 + V_1\lambda$ such that

$$U_0 = \begin{pmatrix} \frac{1}{2}u & -v \\ 1 & -\frac{1}{2}u \end{pmatrix}, \quad U_1 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix},$$

$$V_0 = \begin{pmatrix} A & B \\ C & -A \end{pmatrix}, \quad V_1 = \begin{pmatrix} D & 0 \\ 0 & -D \end{pmatrix},$$

where A, B, C, D are four undetermined functions, we have

$$\begin{aligned}[U,V] &= [U_0,V_0] + (U_0,V_1] + [U_1,V_0])\lambda + [U_1,V_1]\lambda^2 = [U_0,V_0] + (U_0,V_1] + [U_1,V_0])\lambda \\ &= \begin{pmatrix} -vC - B & 2vA + uB \\ 2A - uC & B + vC \end{pmatrix} + \begin{pmatrix} 0 & 2vD - B \\ 2D + C & 0 \end{pmatrix}\lambda, \end{aligned} \tag{3.8}$$

and

$$KG = \begin{pmatrix} 2G_x^{(1)} + G_{xx}^{(2)} + uG_x^{(2)} + u_xG^{(2)} \\ -G_{xx}^{(1)} + uG_x^{(1)} + 2vG_x^{(2)} + v_xG^{(2)} \end{pmatrix}, \quad JG = \begin{pmatrix} G_x^{(2)} \\ G_x^{(1)} \end{pmatrix}. \tag{3.9}$$

Substituting (3.8) and (3.9) into (3.6) and comparing the corresponding elements in both sides of the matrices, we can determine the values of A, B, C, and D from which the solution V as given in (3.7) can be obtained.

Finally, from Theorem 3.1 we have the following.

Theorem 3.2: Let

$$A_n = \sum_{j=1}^{n} V_j\lambda^{n-j} = \sum_{j=0}^{n} V(G_j)\lambda^{n-j},$$

where $V_j = V(G_j)$ is given by (3.7). The DLW hierarchy (2.7) possesses the following zero curvature representation:

$$U_t - A_{nx} + [U,A_n] = 0, \tag{3.10}$$

and the Lax pair

$$\psi_x = U_\psi, \quad \psi_t = A_n\psi.$$

Similarly we can obtain the Lax representation of the hierarchy (2.7) through the following lemmas and theorem.

Lemma 3.4: The spectral problem (1.2) is equivalent to

$$L\psi = \begin{pmatrix} -2\partial + u & -2v \\ -2 & 2\partial + u \end{pmatrix}\psi = \lambda\psi, \tag{3.11}$$

where the differential map of $L = L(u, v, \lambda)$ is

$$L'(\xi) = \begin{pmatrix} \xi_1 & -2\xi_2 \\ 0 & \xi_1 \end{pmatrix},$$

and $L'(\xi)$ is an injective homomorphism.

Proof: Direct calculation from (1.2).

Lemma 3.5: For arbitrary given vector function $G = (G^{(1)}, G^{(2)})^T$, the following operator equation

$$[V,L] = L'(KG) - L'(JG)L \tag{3.12}$$

has a solution

$$V = V(G) = \begin{pmatrix} \frac{1}{2}(G_x^{(2)} + uG^{(2)}) & G_x^{(1)} - vG^{(2)} \\ G^{(2)} & -\frac{1}{2}(G_x^{(2)} + uG^{(2)}) \end{pmatrix} + \begin{pmatrix} -\frac{1}{2}G^{(2)} & 0 \\ 0 & -\frac{1}{2}G^{(2)} \end{pmatrix}L. \tag{3.13}$$

Proof: Representing the commutator $[V,L]$ of $L = L_0 + L_1\partial_x$ and $V = V_0 + V_1\partial_x$ such that

$$L_0 = \begin{pmatrix} u & -2v \\ -2 & u \end{pmatrix}, \quad U_1 = \begin{pmatrix} -2 & 0 \\ 0 & 2 \end{pmatrix},$$

$$V_0 = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \quad U_1 = \begin{pmatrix} E & 0 \\ 0 & F \end{pmatrix},$$

where A,B,C,D are four undetermined functions, we have

$$\begin{aligned}
[V,L] &= [V_0,L_0] + [V_0,L_1\partial_x] + [V_1\partial_x,L_0]) + [V_1\partial_x,L_1\partial_x] \\
&= [V_0,L_0] + V_1L_{0x} - L_1V_{0x} + ([V_0,L_1] + [V_1,L_0] + V_1L_{1x} - L_1V_{1x})\partial_x \\
&= \begin{pmatrix} -2B + 2vC + u_xE + 2A_x & -2v(A-D) - 2v_xE + 2B_x \\ 2(A-D) - 2C_x & 2B - 2vC + u_xF - 2D_x \end{pmatrix} \\
&\quad + \begin{pmatrix} 2E_x & -2v(E-F) + 4B \\ 2(E-F) - 4C & -2F_x \end{pmatrix}\partial_x. \qquad (3.14)
\end{aligned}$$

We also have

$$\begin{aligned}
L'[KG] - L'(JG)L &= \begin{pmatrix} 2G_x^{(2)} & 4G_x^{(1)} \\ 0 & -2G_x^{(2)} \end{pmatrix}\partial_x \\
&\quad + \begin{pmatrix} 2G_x^{(1)} + G_{xx}^{(2)} + u_xG^{(2)} - 4G_x^{(1)} & 2G_{xx}^{(1)} - 2vG_x^{(2)} - 2v_xG^{(2)} \\ 2G_x^{(2)} & 2G_x^{(1)} + G_{xx}^{(2)} + u_xG^{(2)} \end{pmatrix}. \qquad (3.15)
\end{aligned}$$

Substituting (3.14) and (3.15) into (3.12) and comparing the corresponding elements on both sides of the matrices, we then obtain

$$A = -D = \tfrac{1}{2}G_x^{(2)}, \quad B = G_x^{(1)}, \quad C = 0, \quad E = F = G^{(2)}.$$

Since $\partial_x = L_1^{-1}(L - L_0)$, we have

$$\begin{aligned}
V = V(G) &= \begin{pmatrix} \frac{1}{2}G_x^{(2)} & G_x^{(1)} \\ 0 & -\frac{1}{2}G_x^{(2)} \end{pmatrix} + \begin{pmatrix} {}^{(2)} & 0 \\ 0 & G^{(2)} \end{pmatrix}\partial_x \\
&= \begin{pmatrix} \frac{1}{2}(G_x^{(2)} + uG^{(2)})G_x^{(1)} - vG^{(2)} & \\ G^{(2)} & -\frac{1}{2}(G_x^{(2)} + uG^{(2)}) \end{pmatrix} + \begin{pmatrix} -\frac{1}{2}G^{(2)} & 0 \\ 0 & \frac{1}{2}G^{(2)} \end{pmatrix}L.
\end{aligned}$$

Theorem 3.3: Let

$$B_n = \sum_{j=1}^{n} V_jL^{n-j} = \sum_{j=0}^{n} V(G_j)L^{n-j}, \qquad (3.16)$$

where $V_j = V(G_j)$, $G_j = (G_j^{(1)}, G_j^{(2)})^T$, and the matrix function V satisfies (3.13). The DLW hierarchy (2.7) possesses the following Lax representation:

$$L_t = [B_n, L], \qquad (3.17)$$

and the Lax pair

$$L\psi = \lambda\psi, \quad \psi_t = B_n\psi.$$

Proof: From (3.12) and (3.16), we have

$$[B_n,L]=\sum_{j=1}^{n}[V_j,L])L^{n-j}=\sum_{j=1}^{n}[L'(KG_{j-1})-L'(JG_{j-1})L]L^{n-j}$$
$$=\sum_{j=1}^{n}L'(JG_j)L^{n-j}-\sum_{j=0}^{n-1}L'(JG_j)L^{n-j}=L'(JG_n)-L'(JG_0)=L'(X_n).$$

Since $L_t=L'(u_t)$, it follows that

$$L_t-[B_m,L]=L'(u_t)-L'(X_m)=L'(u_t-X_m)=0.$$

The proof is completed.

IV. A FINITE DIMENSIONAL HAMILTONIAN SYSTEM

To construct the algebro-geometric solution of DLW hierarchy, in this section we investigate the finite dimensional Hamiltonian systems associated with the spectral problem (1.2) through a nonlinearization approach.[12,13] Let λ_j, $j=1,\ldots,N$ be N different eigenvalues of equation (1.2), and (p_j,q_j) be the associated eigenfunctions, i.e., we consider the following N eigenvalues:

$$\begin{pmatrix}p_j\\q_j\end{pmatrix}_x=\begin{pmatrix}-\frac{1}{2}(\lambda_j-u) & -v\\ 1 & \frac{1}{2}(\lambda_j-u)\end{pmatrix}\begin{pmatrix}p_j\\q_j\end{pmatrix}. \tag{4.1}$$

Denote $p=(p_1,p_2,\ldots,p_N)^T$, $q=(q_1,q_2,\ldots,q_N)^T$, and $\wedge=\mathrm{diag}(\lambda_1,\lambda_2,\ldots,\lambda_N)$. From the Bargmann constraint

$$G_1=\begin{pmatrix}v\\u\end{pmatrix}=\sum_{j=1}^{N}\nabla\lambda_j=\begin{pmatrix}\langle p,q\rangle\\-\langle q,q\rangle\end{pmatrix}, \tag{4.2}$$

we then obtain

$$w=\begin{pmatrix}u\\v\end{pmatrix}=\begin{pmatrix}-\langle q,q\rangle\\\langle p,q\rangle\end{pmatrix}\equiv h(p,q). \tag{4.3}$$

From the constraint (4.3), the equation (4.1) can further be nonlinearized into the following finite-dimensional Hamiltonian system:

$$p_x=-\frac{1}{2}\wedge p-\frac{1}{2}\langle q,q\rangle p-\langle p,q\rangle q=-\frac{\partial H}{\partial q},$$

$$q_x=p+\frac{1}{2}\wedge q+\frac{1}{2}\langle q,q\rangle q=\frac{\partial H}{\partial p}, \tag{4.4}$$

whose Hamiltonian function H is given by

$$H=\tfrac{1}{2}\langle p,p\rangle+\tfrac{1}{2}\langle\wedge p,q\rangle+\tfrac{1}{2}\langle q,q\rangle\langle p,q\rangle.$$

In the following, we proceed to show that the Hamilton system (4.4) is completely integrable in the Liouville sense. The Poisson bracket of two functions in symplectic space $(\mathbb{R}^{2N},\mathrm{d}p\wedge\mathrm{d}q)$ is defined as

$$(F,G)=\sum_{j=1}^{N}\left(\frac{\partial F}{\partial q_j}\frac{\partial G}{\partial p_j}-\frac{\partial F}{\partial p_j}\frac{\partial G}{\partial q_j}\right)=\left\langle\frac{\partial F}{\partial q},\frac{\partial G}{\partial p}\right\rangle-\left\langle\frac{\partial F}{\partial p},\frac{\partial G}{\partial q}\right\rangle,$$

which is skew-symmetric, bilinear, and satisfies the Jacobi identity. In particular, F and G are called involution if $(F,G)=0$.

Consider a bilinear function $Q_\lambda(p,q)=\langle(\lambda I-\wedge)^{-1}p,q\rangle$ such that

$$G_\lambda = G_0 + \sum_{j=1}^{N} \frac{\nabla\lambda_j}{\lambda-\lambda_j} = \begin{pmatrix} Q_\lambda(p,q) \\ 1-Q_\lambda(q,q) \end{pmatrix}. \tag{4.5}$$

From (3.4) and (4.5), we have

$$V_\lambda = V(G_\lambda) = \begin{pmatrix} -\frac{1}{2}\lambda - Q_\lambda(p,q) & -\langle p,q\rangle + Q_\lambda(p,p) \\ 1-Q_\lambda(q,q) & \frac{1}{2}\lambda + Q_\lambda(p,q) \end{pmatrix}.$$

Let $F_\lambda=\det V_\lambda$. Then, we have

$$\begin{aligned} F_\lambda &= -\tfrac{1}{4}\lambda^2 - Q_\lambda(\wedge p,q) + Q_\lambda(p,p) + \langle p,p\rangle Q_\lambda(q,q) + \begin{vmatrix} Q_\lambda(p,p) & Q_\lambda(p,q) \\ Q_\lambda(p,q) & Q_\lambda(q,q,) \end{vmatrix} \\ &= -\frac{1}{4}\lambda^2 + \sum_{m=0}^{\infty} F_m \lambda^{-m-1}, \end{aligned} \tag{4.6}$$

where

$$F_0 = 2H,$$

$$F_m = -\langle \wedge^{m+1}p,p\rangle + \langle p,q\rangle\langle \wedge^m q,q\rangle + \sum_{m=0}^{m-1} \begin{vmatrix} \langle \wedge^j p,p\rangle & \langle \wedge^{m-1-j}p,q\rangle \\ \langle \wedge^j p,q\rangle & \langle \wedge^{m-1-j}q,q\rangle \end{vmatrix}.$$

By considering that F_λ is a Hamiltonian in the symplectic space $(\mathbb{R}^{2N}, \mathrm{d}p\wedge\mathrm{d}q)$, the canonical equations of the F_λ-flow can be computed as

$$\frac{\mathrm{d}}{\mathrm{d}\tau_\lambda}\begin{pmatrix} p_k \\ q_k \end{pmatrix} = I\nabla F_\lambda = \begin{pmatrix} -\partial F_\lambda/\partial q_k \\ \partial F_\lambda/\partial p_k \end{pmatrix} = W(\lambda,\lambda_k)\begin{pmatrix} p_k \\ q_k \end{pmatrix},$$

where

$$W(\lambda,\lambda_k) = \frac{2}{\lambda-\lambda_k}V_\lambda + (1-Q_\lambda(p,q))\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Lemma 4.1: The Lax matrix V_μ satisfies the Lax equation (4.7) alone the t_λ-flow:

$$\frac{\mathrm{d}V_\mu}{\mathrm{d}\tau_\lambda} = [W(\lambda,\mu), V_\mu] \tag{4.7}$$

and

$$(F_\mu, F_\lambda) = 0, \quad \forall\, \lambda,\mu \in \mathbb{C}, \tag{4.8}$$

$$(F_j, F_k) = 0, \quad \forall\, j,k = 0,1,\ldots. \tag{4.9}$$

Proof: Notice that

$$Q_\lambda(\wedge\xi,\eta) = \lambda Q_\lambda(\wedge\xi,\eta) - \langle\xi,\eta\rangle,$$

$$\langle(\mu I - \wedge)^{-1}(\lambda I - \wedge)^{-1}\xi,\eta\rangle = \frac{1}{\mu-\lambda}(Q_\lambda(\xi,\eta) - Q_\mu(\xi,\eta)),$$

a direct calculation shows that (4.7) holds. From the Lax equation (4.7) we have

$$(F_\mu, F_\lambda) = \sum_{j=1}^{N} \left(\frac{\partial F_\mu}{\partial q_j}\frac{\partial F_\lambda}{\partial p_j} - \frac{\partial F_\mu}{\partial p_j}\frac{\partial F_\lambda}{\partial q_j} \right) = \sum_{j=1}^{N} \left(\frac{\partial F_\mu}{\partial q_j}\frac{\mathrm{d}q_j}{\mathrm{d}t_\lambda} + \frac{\partial F_\mu}{\partial p_j}\frac{\mathrm{d}p_j}{\mathrm{d}t_\lambda} \right)$$
$$= \frac{\mathrm{d}F_\mu}{\mathrm{d}\tau_\lambda} = \frac{\mathrm{d}}{\mathrm{d}\tau_\lambda}(\det V_\mu) = \frac{\mathrm{d}}{\mathrm{d}\tau_\lambda}\left(-\tfrac{1}{2}\mathrm{tr}V_\mu^2\right) = -\mathrm{tr}\left(V_\mu \frac{\mathrm{d}V_\mu}{\mathrm{d}\tau_\lambda} \right)$$
$$= -\mathrm{tr}\, V_\mu \,\mathrm{tr}[W(\lambda,\mu), V_\mu] = 0.$$

Substituting (4.6) into (4.8) and using the coefficients of λ and μ, we then obtain (4.9).

We conclude the above results in the following theorem.

Theorem 4.1: The finite dimensional Hamiltonian system defined by (4.4) is completely integrable in Liouville sense in the symplectic space $(\mathbb{R}^{2N}, \mathrm{d}p \wedge \mathrm{d}q)$.

Theorem 4.2: Let (p,q) be a solution of the Hamiltonian system (4.4). Then, u and v defined by (4.3) satisfy the following stationary DLW equation

$$X_N + c_1 X_{N-2} + \cdots + c_{N-1} X_0 = 0 \tag{4.10}$$

with suitably chosen constants $c_1, \ldots, c_{N-1}$.

Proof: Operating with $(J^{-1}K)^{k-1}$ upon the expression of (4.2), we get

$$G_k + \beta_1 G_{k-2} + \cdots + \beta_{k-1} G_0 + \beta_k G_{-1} = \sum_{j=1}^{N} \lambda_j^k \nabla \lambda_j, \tag{4.11}$$

where $\beta_1, \ldots, \beta_k$ are arbitrary constants, $G_{-1} = (0,0)^T$, and $J^{-1}KG_{-1} = G_0$.

Consider the polynomial

$$p(\lambda) = \prod_{j=1}^{N} (\lambda - \lambda_j) = \lambda^N + p_1 \lambda^{N-1} + \cdots + p_N.$$

Applying the operator $J\Sigma_{k=1}^{N} p_{N-k}$ on (4.11), we obtain (4.10), where $c_1, \ldots, c_N$ depend on $\beta_1, \ldots, \beta_k$ and $\lambda_1, \ldots, \lambda_N$.

Introduce the generating function $\{g_k\}$,

$$g_\lambda = G_0 + \sum_{k=0}^{\infty} G_k \lambda^{-k}, \tag{4.12}$$

which satisfies

$$(K - \lambda J) g_\lambda = 0,$$

we have

$$V_x(g_\lambda) - [U, V(g_\lambda)] = U'((K - \lambda J) g_\lambda) = 0.$$

This implies that

$$\frac{\partial}{\partial x}(\det V(g_\lambda)) = 0.$$

Hence, we have

$$\det V(g_\lambda) = -\tfrac{1}{4}\lambda^2. \tag{4.13}$$

Define a new set of integrals $\{H_k\}$, respectively, by

$$H_0 = \tfrac{1}{2}F_0, \quad H_1 = -\tfrac{1}{2}F_1, \quad H_2 = -\tfrac{1}{2}F_2,$$

$$H_m = -\tfrac{1}{2}F_m + 2\sum_{j=0}^{m-3} H_j H_{m-j-3}, \quad m \geqslant 3.$$

Equation (4.6) can then be transformed into the following equivalent form:

$$-\frac{4}{\lambda^2}F_\lambda = (1-4H_\lambda)^2, \tag{4.14}$$

where

$$H_\lambda = \sum_{m=1}^{\infty} H_{m-1}\lambda^{-m-1}.$$

The involutivity of $\{H_k\}$ is based on the equality

$$\{H_\mu, H_\lambda\} = \frac{1}{16\sqrt{F_\lambda F_\mu}}\{F_\mu, F_\lambda\} = 0.$$

By using (4.5) and (4.11), we have

$$\begin{aligned} G_\lambda &= G_0 + \sum_{k=0}^{\infty}\lambda^{-k-1}\sum_{j=1}^{N}\lambda_j^k \nabla\lambda_j, \\ &= G_0 + \sum_{k=0}^{\infty} c^{-k-1}(G_k + c_1 G_{k-2} + \cdots + c_{k-1}G_0 + c_k G_{-1}, \\ &= c_\lambda g_\lambda + \sum_{k=0}^{\infty}\lambda^{-k-1}c_k G_{-1}, \end{aligned}$$

where

$$c_\lambda = 1 + \sum_{k=0}^{\infty} c_{k+2}\lambda^{-k-2}. \tag{4.15}$$

Using (4.6) and (4.14) again, we have

$$V_\lambda = V\left(c_\lambda g_\lambda + \sum_{k=0}^{\infty}\lambda^{-k-1}c_k G_{-1}\right) = V(c_\lambda g_\lambda).$$

Therefore, we have

$$F_\lambda = \det V_\lambda = -\tfrac{1}{4}c_\lambda^2 g_\lambda^2. \tag{4.16}$$

From (4.14) and (4.16), we obtain

$$c_\lambda = 1 - 4H_\lambda.$$

Denote the variables of H_λ flow and H_k flow by t_λ and t_k, respectively. Applying the Leibniz rule of the Poisson bracket, we obtain

$$\frac{1}{2\lambda^2}\{\psi, F_\lambda\} = (1-4H_\lambda)\{\psi, H_\lambda\},$$

for any smooth function ψ. Thus,

$$\frac{\mathrm{d}}{\mathrm{d}t_\lambda} = \frac{1}{2\lambda^2(1-4H_\lambda)}\frac{\mathrm{d}}{\mathrm{d}\tau_\lambda} = \frac{1}{2\lambda^2 c_\lambda}\frac{\mathrm{d}}{\mathrm{d}\tau_\lambda}. \tag{4.17}$$

For $w=(u,v)^T=h(p,q)$, we have

$$\frac{\mathrm{d}w}{\mathrm{d}\tau_\lambda} = \begin{pmatrix} -2\left\langle q, \dfrac{\mathrm{d}q}{\mathrm{d}\tau_\lambda}\right\rangle \\ \left\langle p, \dfrac{\mathrm{d}q}{\mathrm{d}\tau_\lambda}\right\rangle + \left\langle \dfrac{\mathrm{d}p}{\mathrm{d}\tau_\lambda}, q\right\rangle \end{pmatrix} = 2JG_\lambda,$$

$$\frac{\mathrm{d}w}{\mathrm{d}t_\lambda} = \frac{1}{2\lambda^2 c_\lambda}\frac{\mathrm{d}w}{\mathrm{d}\tau_\lambda} = \frac{1}{\lambda^2 c_\lambda}JG_\lambda = \frac{1}{\lambda^2}Jg_\lambda$$
$$= \sum_{k=0}^{\infty} JG_K\lambda^{-k-3} = \sum_{k=0}^{\infty} JG_K\lambda^{-k-3}.$$

Finally, we state the above result in the following theorem.

Theorem 4.3: Let $(p(x,t_k),q(x,t_k))$ be a compatible solution of the h_0 and H_k flow. Then, $w(x,t_K)=h(p,q)$ solves the kth DLW equation

$$w_t = X_k(w).$$

V. ALGEBRO-GEOMETRIC SOLUTIONS

Based on results presented in Secs. III and IV, we give the construction of the algebro-geometric solutions for the hierarchy (2.7) in the following lemmas and theorem.

Lemma 5.1: The solutions u and v for the DLW hierarchy (2.7) can be expressed in the form

$$u = \sum_{k=1}^{N}(\lambda_k - \nu_k), \quad \partial_x \ln v = \sum_{k=1}^{N}(\mu_k - \nu_k), \tag{5.1}$$

where μ_k, ν_k are called the elliptic coordinates of the finite-dimensional Hamiltonian system (4.3).

Proof: We express F_λ in the form

$$F_\lambda = -V_\lambda^{11^2} - V_\lambda^{12}V_\lambda^{21} = -\frac{1}{4}\lambda^2 + \sum_{k=1}^{N}\frac{E_k}{\lambda-\lambda_k},$$

where

$$E_k = -\lambda_k p_k q_k + p_k^2 + \langle p,q\rangle q_k^2 + \sum_{j=1,j\neq k}^{N}\frac{(p_j q_k - p_k q_j)^2}{\lambda_j - \lambda_k}.$$

Let

$$F_\lambda = -\frac{b(\lambda)}{4a(\lambda)} = -\frac{R(\lambda)}{4a^2(\lambda)}, \tag{5.2}$$

$$V_\lambda^{12} = -\langle p,q\rangle + Q_\lambda(p,p) = -\langle p,q\rangle \frac{m(\lambda)}{a(\lambda)},$$

$$V_\lambda^{21} = 1 - Q_\lambda(q,q) = \frac{n(\lambda)}{a(\lambda)}, \tag{5.3}$$

where

$$a(\lambda) = \prod_{k=1}^{N} (\lambda - \lambda_k), \quad b(\lambda) = \prod_{k=1}^{N+2} (\lambda - \lambda_{N+k}),$$

$$m(\lambda) = \prod_{k=1}^{N} (\lambda - \mu_k), \quad n(\lambda) = \prod_{k=1}^{N} (\lambda - \nu_k),$$

$$R(\lambda) = a(\lambda)b(\lambda) = \prod_{k=1}^{2N+2} (\lambda - \lambda_k).$$

Comparing the coefficients of λ^{N-1} in (5.2) and (5.3) gives

$$\langle q,q\rangle = -\sum_{k=1}^{N} (\lambda_k - \nu_k), \quad \frac{\langle p,p\rangle}{\langle p,q\rangle} = \sum_{k=1}^{N} (\mu_k - \lambda_k). \tag{5.4}$$

By using (4.2) and (5.4), we then obtain (5.1).

From the Lax equation (4.7), we have

$$\frac{dV_\mu^{12}}{dt_\lambda} = 2(W^{11}V^{12} - W^{12}V^{11}),$$

$$\frac{dV_\mu^{21}}{dt_\lambda} = 2(W^{21}V^{11} - W^{11}V^{21}). \tag{5.5}$$

Taking $\lambda = \mu_k, \nu_k$ in (5.2) and (5.3), we get

$$V_{\mu_k}^{11} = \frac{\sqrt{R(\mu_k)}}{2a(\mu_k)}, \quad V_{\mu_k}^{11} = \frac{\sqrt{R(\nu_k)}}{2a(\nu_k)}.$$

Hence, we have

$$\frac{1}{2\sqrt{R(\mu_k)}} \frac{d\mu_k}{d\tau_\lambda} = \frac{m(\lambda)}{a(\lambda)(\lambda - \mu_k)m'(\mu_k)},$$

$$\frac{1}{2\sqrt{R(\nu_k)}} \frac{d\nu_k}{d\tau_\lambda} = -\frac{n(\lambda)}{a(\lambda)(\lambda - \nu_k)n'(\nu_k)}.$$

By using the polynomials interpolation formula, we have

$$\sum_{k=1}^{N} \frac{\mu_k^{N-j}}{2\sqrt{R(\mu_k)}} \frac{d\mu_k}{d\tau_\lambda} = \frac{\lambda^{N-j}}{a(\lambda)}, \quad \sum_{k=1}^{N} \frac{\mu_k^{N-j}}{2\sqrt{R(\nu_k)}} \frac{d\nu_k}{d\tau_\lambda} = -\frac{\lambda^{N-j}}{a(\lambda)}. \tag{5.6}$$

Define the hyperelliptic curve by

$$\Gamma: \xi^2 - 4R(\lambda) = 0, \tag{5.7}$$

with genus $g=N$ and the usual holomorphic differentials by

$$\tilde{\omega}_j = \frac{\lambda^{N-j}\,\mathrm{d}\lambda}{2\sqrt{R(\lambda)}}, \quad j = 1,2,\ldots,N. \tag{5.8}$$

Denote $P(\mu_k)=(\lambda, \xi=2\sqrt{R(\lambda)}) \in \Gamma$. Let $P_0 \in \Gamma$ be fixed. Define the quasi-Abel–Jacobi coordinates by

$$\tilde{\phi}_j = \sum_{k=1}^{N} \int_{P_0}^{P(\mu_k)} \tilde{\omega}_j, \quad \tilde{\psi}_j = \sum_{k=1}^{N} \int_{P_0}^{P(\nu_k)} \tilde{\omega}_j, \quad j = 1,2,\ldots,N. \tag{5.9}$$

Then, (5.6) can be represented in the form

$$\frac{\mathrm{d}\tilde{\phi}_j}{\mathrm{d}\tau_\lambda} = \frac{\lambda^{N-j}}{a(\lambda)}, \quad \frac{\mathrm{d}\tilde{\psi}_j}{\mathrm{d}\tau_\lambda} = -\frac{\lambda^{N-j}}{a(\lambda)}.$$

Let $a_1, b_1, \ldots, a_N, b_N$ be the canonical basis of cycles on the Γ and

$$C = (A_{jk})^{-1}_{N\times N}, \quad A_{jk} = \int_{a_k} \tilde{\omega}_j.$$

Define the normalized holomorphic differential by

$$\omega_s = \sum_{j=1}^{N} C_{sj}\tilde{\omega}_j, \quad \omega = (\omega_1, \ldots, \omega_N)^T = C\tilde{\omega}.$$

Then, we have

$$\int_{a_k} \omega_s = \delta_{sk}, \quad \int_{b_k} \omega_s = B_{sk},$$

where the matrix $B=(B_{sk})$ is symmetric with positive-definite imaginary part. This is used to define the Riemann theta function of Γ as

$$\theta(\zeta) = \sum_{z\in\mathbb{Z}^N} \exp(\pi i\langle Bz, z\rangle + 2\pi i\langle \zeta, z\rangle), \quad \zeta \in C^N.$$

The Abel map $A(P)$ and the Abel–Jacobi coordinate are defined as

$$A(P) = \int_{P_0}^{P} \omega, \quad A\left(\sum n_k P_k\right) = \sum n_k A(P_k),$$

$$\phi = A\left(\sum_{k=1}^{N} P(\mu_k)\right) = \sum_{k=1}^{N} \int_{P_0}^{P(\mu_k)} \omega = C\tilde{\phi},$$

$$\psi = A\left(\sum_{k=1}^{N} P(\nu_k)\right) = \sum_{k=1}^{N} \int_{P_0}^{P(\nu_k)} \omega = C\tilde{\psi}.$$

Let $S_k=\lambda_1^k+\cdots+\lambda_{2N+2}^k$, and $\tilde{R}(\lambda^{-1})=\Pi_{j=1}^{2N+2}(1=\lambda_j\lambda^{-1})$. The coefficients in

$$\frac{1}{\sqrt{\tilde{R}(\lambda^{-1})}} = \sum_{k=1}^{\infty} \Lambda_k \lambda^{-k}$$

are then given by

$$\Lambda_0 = 1, \quad \Lambda_1 = \frac{1}{2} S_1, \quad \Lambda_k = \frac{1}{2k}\left(S_k + \sum_{i+j=k, i,j \geqslant 1} S_i \Lambda_j \right).$$

From (5.2), we obtain

$$\sqrt{R(\lambda)} = \lambda a(\lambda) c_\lambda,$$

and the lemma is proved.

Lemma 5.2: Let C_k be the kth column vector of the matrix C. Under the Abel–Jacobi coordinate system, we have straightened out the flows to

$$\frac{\mathrm{d}\phi}{\mathrm{d}t_\lambda} = \sum_{k=1}^{\infty} \Omega_{k-1} \lambda^{-k-1}, \quad \frac{\mathrm{d}\psi}{\mathrm{d}t_\lambda} = -\sum_{k=1}^{\infty} \Omega_{k-1} \lambda^{-k-1}, \tag{5.10}$$

$$\frac{\mathrm{d}\phi}{\mathrm{d}t_k} = \Omega_{k-1}, \quad \frac{\mathrm{d}\psi}{\mathrm{d}t_k} = -\Omega_{k-1}, \tag{5.11}$$

where

$$\Omega_0 = \tfrac{1}{2}\Lambda_0 C_1, \quad \Omega_1 = \tfrac{1}{2}(\Lambda_1 C_1 + \Lambda_0 C_2),$$

$$\Omega_k = \tfrac{1}{2}(\Lambda_k C_1 + \cdots + \Lambda_0 C_{k+1}), \quad k \leqslant N-1,$$

$$\Omega_k = \tfrac{1}{2}(\Lambda_k C_1 + \cdots + \Lambda_{k-N+1} C_N), \quad k \geqslant N-1.$$

Proof: Notice that

$$\begin{aligned}
\frac{\mathrm{d}\phi}{\mathrm{d}t_\lambda} = \frac{1}{2\lambda^2 c_\lambda}\frac{\mathrm{d}\phi}{\mathrm{d}\tau_\lambda} &= \frac{1}{2\lambda^2 c_\lambda} C \frac{\mathrm{d}\tilde{\phi}}{\mathrm{d}\tau_\lambda} \\
&= \frac{\lambda^{N-1}}{2\sqrt{R(\lambda)}}(C_1 \lambda^{-1} + \cdots + \cdots C_N \lambda^{-N}) \\
&= \frac{1}{2\lambda^2\sqrt{\tilde{R}(\lambda^{-1})}}(C_1 \lambda^{-1} + \cdots + \cdots_N \lambda^{-N}) \\
&= \frac{1}{2}\sum_{k=0}^{\infty} \Lambda_k \lambda^{-k-2} \sum_{j=1}^{N} C_j \lambda^{-j} = \sum_{k=0}^{\infty} \Omega_k \lambda^{-k-3}.
\end{aligned}$$

Similarly, we can obtain the second formula of (5.10) and compare the coefficients of λ^{-k-1} in (5.10) to obtain (5.11).

From (5.11), we get

$$\phi = \phi_0 + \sum_{k=1}^{\infty} \Omega_{k-1} t_k, \quad \psi = \psi_0 - \sum_{k=1}^{\infty} \Omega_{k-1} t_k.$$

Hence, the evolution picture of the $1+1$ flow is given as

$$\phi = \phi_0 + \Omega_0 x + \Omega_1 t, \quad \psi = \psi_0 - \Omega_0 x - \Omega_1 t. \tag{5.12}$$

Since $\deg R = 2N+2$ on Γ, there are two infinite points ∞_1 and ∞_2 which are not branch points of Γ. From Riemann theorem, there exists two constants $M_1, M_2 \in C^N$ such that $\theta(A(P) - \phi - M_1)$, $\theta(A(P) - \psi - M_2)$ have exactly n zeroes at $\mu_1, \ldots, \mu_N$ and $\nu_1, \ldots, \nu_N$, respectively. That is,

$$\sum_{j=1}^{N} \mu_j = I(\Gamma) - \sum_{j=1}^{2} \mathrm{Res}_{\lambda=\infty_j} \lambda d \ln \theta(A(P) - \phi - M_1), \tag{5.13}$$

$$\sum_{j=1}^{N} \nu_j = I(\Gamma) - \sum_{j=1}^{2} \mathrm{Res}_{\lambda=\infty_j} \lambda d \ln \theta(A(P) - \phi - M_1), \tag{5.14}$$

with the constant

$$I(\Gamma) = \sum_{j=1}^{N} \int_{a_j} \lambda \omega_j.$$

For the same λ, there are two points on the different sheets of the Riemann surface Γ,

$$P_+(\lambda) = (\lambda, \sqrt{R(\lambda)}), \quad P_+(\lambda) = (\lambda, -\sqrt{R(\lambda)}).$$

Under the local coordinate $z = \lambda^{-1}$ at infinity, the hyperelliptic curve $\Gamma: \xi^2 - 4R(\lambda) = 0$ in the neighborhood of infinity is expressed as $\tilde{\xi}^2 - 4\tilde{R}(z) = 0$ with $\tilde{\xi} = z^{N+1}\xi$ and $(z, 2(-1)^{s-1}\sqrt{R(z)})|_{z=0} = (0, 2(-1)^{s-1})$, $s = 1, 2$. Thus, we have

$$\begin{aligned} \omega = C\tilde{\omega} &= (C_1\lambda^{-1} + \cdots + C_N\lambda^{-N}) \frac{\lambda^{N-1} d\lambda}{2\sqrt{R(\lambda)}} \\ &= (C_1\lambda^{-1} + \cdots + C_N\lambda^{-N}) \frac{d\lambda}{2\lambda^2\sqrt{\tilde{R}(\lambda^{-1})}} \\ &= \frac{1}{2}(-1)^{s-1} \sum_{j=0}^{\infty} \Omega_k z^k \, dz \end{aligned}$$

and

$$A(P(z^{-1})) = \int_{P_0}^{P} \omega = -\int_{\infty_s}^{P_0} \omega + \int_{\infty_s}^{P} \omega = -\pi_s + \frac{1}{2}(-)^{s-1} \sum_{k=0}^{\infty} \frac{1}{k+1} \Omega_k z^{k+1}.$$

Since the theta function is an even function, we have

$$\theta(A(P(z^{-1}) - \phi - M_1) = \theta(\phi + M_1 + \eta_s) + \frac{1}{2} z(-1)^{s-1} \frac{\partial}{\partial x} \theta(\phi + M_1 + \eta_s) + o(z^2). \tag{5.15}$$

From (5.13) and (5.15), we obtain

$$\begin{aligned} \sum_{j=1}^{N} \mu_j &= I(\Gamma) - \frac{1}{2}(-1)^{s-1} \frac{\partial}{\partial x} \theta(\phi + M_1 + \eta_s) \\ &= I(\Gamma) + \frac{1}{2} \partial_x \ln \frac{\theta(\phi + M_1 + \eta_2)}{\theta(\phi + M_1 + \eta_1)}. \end{aligned} \tag{5.16}$$

Simiarly, we have

$$\sum_{j=1}^{N} \mu_j = I(\Gamma) + \frac{1}{2}\partial_x \ln \frac{\theta(\psi + M_2 + \pi_1)}{\theta(\psi + M_2 + \pi_2)}. \tag{5.17}$$

Substituting (5.16) and (5.17) into (5.1), we then obtain the following algebro-geometric solution for the DLW equation

$$u = \sum_{k=1}^{N} \lambda_k - I(\Gamma) - \frac{1}{2}\partial_x \ln \frac{\theta(\Omega_0 x + \Omega_1 t + \alpha_1)}{\theta(\Omega_0 x + \Omega_1 t + \alpha_2)},$$

$$v^2 = \frac{\theta(\Omega_0 x + \Omega_1 t + \alpha_2)\theta(\Omega_0 x + \Omega_1 t + \beta_2)}{\theta(\Omega_0 x + \Omega_1 t + \alpha_1)\theta(\Omega_0 x + \Omega_1 t + \beta_1)} v^2(0,t),$$

where

$$\alpha_l = \phi_0 + M_1 + \pi_l, \quad \beta_l = -\psi_0 - M_2 - \pi_l, \quad l = 1,2.$$

VI. CONCLUSION

Spectral problem usually provides many important integrable properties related to nonlinear equations such as Lax pair, *r*-matrix, Hamiltonian structure, Darboux transformation, and algebro-geometric solution. In this paper we investigate a spectral problem associated with the DLW equation and derive a hierarchy of nonlinear evolution equations related to the DLW equation by using an iterated algebraic method. The Hamiltonian structures for the DLW hierarchy are established by using trace identity. These two methods can be extended to other kinds of hierarchies. In constructing the commutator representation, the parameter λ is found to be easier to be computed than the operator L. We thus provide a transformation to change the operator L to λ in order to obtain the Lax representation for the DLW hierarchy. Through nonlinearization technique, a finite dimensional Hamiltonian system is obtained in an explicit form. The Abel–Jacobi coordinates are introduced from which the algebro-geometric solutions for the DLW equation can be derived by resorting to the Riemann theta function. The results given in this paper can be applied to many interesting problems such as higher order constrained flow and *r*-matrix structure.

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Lagrange–Fedosov nonholonomic manifolds

Fernando Etayo,[a] Rafael Santamaría,[b] and Sergiu I. Vacaru[c]
Departamento de Matemáticas, Estadística y Computación, Facultad de Ciencias, Universidad de Cantabria, Avda. de los Castros, s/n, 39071 Santander, Spain

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We outline a unified approach to geometrization of Lagrange mechanics, Finsler geometry and geometric methods of constructing exact solutions with generic off-diagonal terms and nonholonomic variables in gravity theories. Such geometries with induced almost symplectic structure are modeled on nonholonomic manifolds provided with nonintegrable distributions defining nonlinear connections. We introduce the concept of Lagrange–Fedosov spaces and Fedosov nonholonomic manifolds provided with almost symplectic connection adapted to the nonlinear connection structure. We investigate the main properties of generalized Fedosov nonholonomic manifolds and analyze exact solutions defining almost symplectic Einstein spaces. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1855402]

I. INTRODUCTION

The geometry of Fedosov manifolds is a natural generalization of Kähler geometry defining a procedure of canonical deformation quantization.[1–5] By definition, a Fedosov manifold is given by a triple (M,θ,Γ) where M is a $\mathcal{C}^{\infty}$-manifold enabled with symplectic structure θ (a nondegenerated closed exterior two-form) and a symplectic connection structure Γ (i.e., a torsionless linear connection parallelizing the symplectic form). If a Lagrange fundamental function $L:(x,y)\in TM \to \mathbb{R}$ is defined on M (for simplicity, in this work we shall consider only regular Lagrangians; (x,y) denote a set of local coordinates on the tangent bundle TM with $x\in M$), there is a natural almost complex structure adapted to the canonical nonlinear connection (in brief, N-connection) induced by $L(x,y)$.[6–8] Nonlinear connections can also be naturally related to generic off-diagonal metrics and nonholonomic moving frames in (super) gravity and string theories.[9–13] So, if we want to apply the methods of symplectic geometry (and possible generalizations for Poisson manifolds[14]) to various types of Lagrange–Hamilton, and related Finsler–Cartan spaces, we have to consider spaces enabled with N-connection structure.

In this work, we study the geometry of almost symplectic connections (in general, they are not torsion-free but can be symmetrized) which are distinguished by a N-connection structure and preserve an almost symplectic form, for instance, induced by a regular Lagrangian or off-diagonal metric structure. This is related to almost symplectic manifolds (see, for instance, Refs. 15–19) but, in our case, the manifolds are nonholonomic ones.

We shall define and analyze the curvature tensor for such almost symplectic connections and related Einstein equations with nonholonomic variables. For nonholonomic manifolds, i.e., manifolds with nonintegrable distributions (in our case, with a such distribution defined by a N-connection), this is not a trivial task. The problem together with a proposal when the Riemann tensor is interpreted as a modification of the Spencer cohomology and related to solutions of partial differential equations, as well to superspaces, are analyzed in Refs. 20 and 21.

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[a]Electronic mail: etayof@unican.es
[b]Also at: Departamento de Matemáticas, Escuela de Ingenierías Industrial e Informática, Universidad de León, 24071 León; electronic mail: demrss@unileon.es
[c]Also at: Instituto de Matemáticas y Física Fundamental, Consejo Superior de Investigaciones Científicas, Calle Serrano 123, 28006 Madrid, Spain; electronic mail: vacaru@imaff.cfmac.csic.es, sergiu_vacaru@yahoo.com

The geometry of nonholonomic manifolds has a long time historical perspective: For instance, in Ref. 22 it is stated that it is probably impossible to construct an analog of the Riemannian tensor for the general nonholonomic manifold. In two more recent reviews (Refs. 23 and 24), it is emphasized that in the past there were proposed well-defined Riemannian tensors for a number of spaces provided with nonholonomic distributions, like Finsler and Lagrange spaces and various types of their higher order generalizations, i.e., for nonholonomic manifolds possessing corresponding N-connection structures. As some examples of former such investigations, we cite Refs. 25–29.

Essentially, the Fedosov type nonholonomic geometry to be elaborated in this work is based on the notion of N-connection and considers a Whitney-like splitting of the tangent bundle to a manifold into horizontal and vertical subspaces (see the discussion and a bibliography for recent developments and applications in Refs. 30–32). Here we emphasize that the geometrical aspects of the N-connection formalism have been studied since the first papers of Cartan[33] and Kawaguchi[34–36] (who used it in component form for Finsler geometry), then one should mention the so-called Ehresmann connection[37] and the work of Barthel[38] where the global definition of N-connection was given. The monographs (Refs. 6–8) consider the N-connection formalism elaborated and applied to the geometry of generalized Finsler–Lagrange and Cartan–Hamilton spaces, see also the approaches in Refs. 39–42.

The works related to nonholonomic geometry and N-connections have appeared many times in a rather dispersive way when different schools of authors from geometry, mechanics, and physics have worked many times entirely independent of each other. We outline some recent results with explicit applications in modern mathematical physics and particle and string theories: N-connection structures were modeled on Clifford and spinor bundles,[43,44] on superbundles and in some directions of (super) string theory,[45,46] as well as in noncommutative geometry and gravity.[47] The idea to apply the N-connections formalism as a new geometric method of constructing exact solutions in gravity theories was suggested in Refs. 9 and 10 and developed in a number of works, see, for instance, Refs. 11–13).

We begin in Sec. II with an introduction into the N-connection geometry for arbitrary manifolds with tangent bundles admitting splitting into conventional horizontal and vertical subspaces. We illustrate how regular Lagrangians induce natural semispray, N-connection, metric, and almost complex structures on tangent bundles and discuss the relation between Lagrange and Finsler geometry and their generalizations. Then we prove that N-connection structures and corresponding almost complex geometries may be modeled by generic off-diagonal metrics and nonholonomic frames in gravity theories.

Section III is devoted to the theory of linear connections on N-anholonomic manifolds (i.e., on manifolds with nonholonomic structure defined by N-connections). We demonstrate how the linear connections may be adapted to the N-connection splitting of the manifolds and analyze the conditions when such distinguished connections may be naturally related to almost complex structures. This has great *philosophical* interest, because several authors have defined different notions of general connections, looking for associated parallel transport and covariant differential operator satisfying, if possible, the properties of those of a linear connection (e.g., Ehresmann connections on bundles, nonhomogeneous connections of Grifone,[48] quasi- and pseudo-connections (see Ref. 49, etc.), but it always implies losing properties or demanding more assumptions than in the case of a N-connection. [For example, nonhomogeneous connections of Grifone define a covariant derivative $D_X Y$, which in general does not define a vector field on the manifold (see p. 302 of Ref. 48) and which does not satisfy $D_X(fY)=fD_XY+(Xf)Y$ (see p. 305 of Ref. 48). In the case of nonlinear connections used in the book of Yano and Ishihara (Ref. 50, p. 209) it is assumed that horizontal distributions are invariant under dilatations (see also Ref. 51), etc.] In the present paper we shall see that one can define a canonical linear connection adapted to a given N-connection. This shall allow us to avoid extra constructions and additional restrictions.

In Sec. IV, we define the Fedosov N-anholonomic and Lagrange–Fedosov manifolds as certain

generalizations of the Fedosov spaces to nonholonomic configurations. We construct in explict form the curvature tensor of such spaces and define the Einstein equations for N-adapted linear connection and metric structures.

In Sec. V, we analyze the main conditions when vacuum gravitational configurations with N-anholonomic structures can be defined as exact solutions of the Einstein equations. We prove that for a very general five-dimensional ansatz for metric coefficients depending on two, three, and four variables the system of field equations is completely integrable. We illustrate that the method can be reduced to the case of four-dimensional spaces, which gives us the possibility to generate conformal almost complex gravitational metrics.

We shall use both physical and mathematical languages and both coordinate and intrinsic notations, when possible.

II. NONLINEAR CONNECTIONS AND FEDOSOV SPACES

In the following, we recall some results on nonlinear connections and almost symplectic structures, which in certain particular cases, are induced by regular Lagrangians, Finsler fundamental functions, or by generic off-diagonal metrics in gravity theories. From now on, all the manifolds (in general, nonholonomic ones)—in the literature, the equivalent term, anholonomic, is also used—and geometric objects are supposed to be C^∞.

A. Nonlinear connection geometry

Let $\mathbf{V}$ be an $(n+m)$-dimensional manifold. It is supposed that in any point $u\in\mathbf{V}$ there is a local splitting $\mathbf{V}_u=M_u\oplus V_u$, where M is an n-dimensional subspace and V is an m-dimensional subspace. (One has this local decomposition when $\mathbf{V}\to M$ is a surjective submersion. A particular case is that of a fiber bundle, but we can obtain the results in the general case.) We shall split the local coordinates (in general, abstract ones both for holonomic and nonholonomic variables) in the form $u=(x,y)$, or $u^\alpha=(x^i,y^a)$, where $i,j,k,\ldots=1,2,\ldots,n$ and $a,b,c,\ldots=n+1,n+2,\ldots,n+m$. We denote by $\pi^\tau:T\mathbf{V}\to TM$ the differential of a map $\pi:V^{n+m}\to V^n$ defined by fiber preserving morphisms of the tangent bundles $T\mathbf{V}$ and TM. The kernel of π^τ is just the vertical subspace $v\mathbf{V}$ with a related inclusion mapping $i:v\mathbf{V}\to T\mathbf{V}$.

Definition 1: *A nonlinear connection (N-connection)* $\mathbf{N}$ *on a manifold* $\mathbf{V}$ *is defined by the splitting on the left of an exact sequence*

$$0\to v\mathbf{V}\overset{i}{\to}T\mathbf{V}\to T\mathbf{V}/v\mathbf{V}\to 0,$$

i.e., by a morphism of submanifolds $\mathbf{N}:T\mathbf{V}\to v\mathbf{V}$ *such that* $\mathbf{N}\circ\mathbf{i}$ *is the unity in* $v\mathbf{V}$.

In an equivalent form, we can say that a N-connection is defined by a splitting to subspaces with a Whitney sum of conventional horizontal (h) subspace, $(h\mathbf{V})$, and vertical (v) subspace, $(v\mathbf{V})$,

$$T\mathbf{V}=h\mathbf{V}\oplus v\mathbf{V}, \tag{1}$$

where $h\mathbf{V}$ is isomorphic to M. Moreover, one can say that a N-connection is defined by a tensor field of type (1,1) $\mathbf{P}=\mathbf{H}-\mathbf{N}$, where $\mathbf{H}$ (respectively, $\mathbf{N}$) denotes the projection over the horizontal (respectively, vertical) subspace. Observe that $\mathbf{P}\circ\mathbf{P}=\mathbf{I}$, i.e., $\mathbf{P}$ is an almost product structure, horizontal (respectively, vertical) subspace being the eigenspace associated to the eigenvalue $+1$ (respectively, -1).

Locally, a N-connection is defined by its coefficients $N_i^a(u)$,

$$\mathbf{N}=N_i^a(u)\mathrm{d}x^i\otimes\frac{\partial}{\partial y^a}.$$

The well-known class of linear connections consists on a particular subclass with the coefficients being linear on y^a, i.e., $N_i^a(u)=\Gamma_{bj}^a(x)y^b$.

Any N-connection $\mathbf{N}=N_i^a(u)$ may be characterized by an associated frame (vielbein) structure $\mathbf{e}_\nu=(e_i,e_a)$, where

$$e_i=\frac{\partial}{\partial x^i}-N_i^a(u)\frac{\partial}{\partial y^a},\quad e_a=\frac{\partial}{\partial y^a}, \tag{2}$$

and the dual frame (coframe) structure $\vartheta^\mu=(\vartheta^i,\vartheta^a)$, where

$$\vartheta^i=\mathrm{d}x^i,\quad \vartheta^a=\mathrm{d}y^a+N_i^a(u)\mathrm{d}x^i. \tag{3}$$

These vielbeins are called N-adapted frames. In order to preserve a relation with the previous denotations,[8–11,43,44,46] we note that $\mathbf{e}_\nu=(e_i,e_a)$ and $\vartheta^\mu=(\vartheta^i,\vartheta^a)$ are, respectively, the former $\delta_\nu=\delta/\partial u^\nu=(\delta_i,\partial_a)$ and $\delta^\mu=\delta u^\mu=(d^i,\delta^a)$ which emphasize that operators (2) and (3) define, correspondingly, certain "N-elongated" partial derivatives and differentials which are more convenient for calculations on such nonholonomic manifolds.

Any N-connection also defines a N-connection curvature

$$\Omega=\tfrac{1}{2}\Omega_{ij}^a\mathrm{d}^i\wedge\mathrm{d}^j\otimes\partial_a,$$

with N-connection curvature coefficients

$$\Omega_{ij}^a=\delta_{[j}N^a_{i]}=\delta_jN_i^a-\delta_iN_j^a=\frac{\partial N_i^a}{\partial x^j}-\frac{\partial N_j^a}{\partial x^i}+N_i^b\frac{\partial N_j^a}{\partial y^b}-N_j^b\frac{\partial N_i^a}{\partial y^b}. \tag{4}$$

The vielbeins (3) satisfy the nonholonomy (equivalently, anholonomy) relations

$$[\mathbf{e}_\alpha,\mathbf{e}_\beta]=\mathbf{e}_\alpha\mathbf{e}_\beta-\mathbf{e}_\beta\mathbf{e}_\alpha=W_{\alpha\beta}^\gamma\mathbf{e}_\gamma \tag{5}$$

with (antisymmetric) nontrivial anholonomy coefficients $W_{ia}^b=\partial_aN_i^b$ and $W_{ji}^a=\Omega_{ij}^a$.

Definition 2: *A manifold* $\mathbf{V}$ *is called N-anholonomic if on the tangent space* $T\mathbf{V}$ *it is defined as a local (nonintegrable) distribution (1), i.e.,* $T\mathbf{V}$ *is enabled with a N-connection and related nonholonomic vielbein structure (5).*

We note that in this work we use boldfaced symbols for the spaces and geometric objects provided/adapted to a N-connection structure. For instance, a vector field $\mathbf{X}\in T\mathbf{V}$ is expressed as $\mathbf{X}=(X,{}^\vee X)$, or $\mathbf{X}=X^\alpha\mathbf{e}_\alpha=X^ie_i+X^ae_a$, where $X=X^ie_i$ and ${}^\vee X=X^ae_a$ state, respectively, the irreducible (adapted to the N-connection structure) horizontal (h) and vertical (v) components of the vector (which following Ref. 6 and 7 are called distinguished vectors, in brief, d-vector). In a similar fashion, the geometric objects on $\mathbf{V}$ like tensors, spinors, connections, etc., are called, respectively, d-tensors, d-spinors, d-connections if they are adapted to the N-connection splitting.

In secs. II B and II C we show how certain types of N-connection geometries can be naturally derived from Lagrange–Finsler geometry and in gravity theories.

B. N-connections and Lagrangians

We outline the main results on N-connections and almost symplectic structures induced by regular Lagrangians.[6–8] In this case the N-anholonomic manifold $\mathbf{V}$ is to be modeled on the tangent bundle (TM,π,M), where M is an n-dimensional base manifold, π is a surjective projection, and TM is the total space. One denotes by $\widetilde{TM}=TM\backslash\{0\}$ where $\{0\}$ means the null section of map π.

A differentiable Lagrangian $L(x,y)$, i.e., a fundamental Lagrange function, is defined by a map $L:(x,y)\in TM\to L(x,y)\in\mathbb{R}$ of class $\mathcal{C}^\infty$ on $\widetilde{TM}$ and continuous on the null section $0:M\to TM$ of π. A regular Lagrangian is with nondegenerated Hessian,

$${}^{(L)}g_{ij}(x,y)=\frac{1}{2}\frac{\partial^2L(x,y)}{\partial y^i\,\partial y^j} \tag{6}$$

when *rank* $|g_{ij}|=n$ on $\widetilde{TM}$.

Definition 3: *A Lagrange space is a pair* $L^n=[M,L(x,y)]$ *with* ${}^{(L)}g_{ij}(x,y)$ *being of constant signature over* $\widetilde{TM}$.

The notion of Lagrange space was introduced by Kern[52] and elaborated in detail by Miron's school on Finsler and Lagrange geometry, see Refs. 6 and 7, as a natural extension of Finsler geometry[33,53–59] (see also Refs. 45 and 46 on Lagrange–Finsler supergeometry).

By straightforward calculations, there were proved the following results:

1. The Euler–Lagrange equations,

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\left(\frac{\partial L}{\partial y^i}\right)-\frac{\partial L}{\partial x^i}=0,$$

where $y^i=\mathrm{d}x^i/\mathrm{d}\tau$ for $x^i(\tau)$ depending on parameter τ, are equivalent to the "nonlinear" geodesic equations

$$\frac{\mathrm{d}^2x^i}{\mathrm{d}\tau^2}+2G^i\left(x^k,\frac{\mathrm{d}x^j}{\mathrm{d}\tau}\right)=0$$

defining paths of a canonical semispray

$$S=y^i\frac{\partial}{\partial x^i}-2G^i(x,y)\frac{\partial}{\partial y^i},$$

where

$$2G^i(x,y)=\frac{1}{2}{}^{(L)}g^{ij}\left(\frac{\partial^2 L}{\partial y^i\,\partial x^k}y^k-\frac{\partial L}{\partial x^i}\right)$$

with ${}^{(L)}g^{ij}$ being inverse to (6).

2. There exists on $\widetilde{TM}$ a canonical N-connection

$${}^{(L)}N^i_j=\frac{\partial G^i(x,y)}{\partial y^j} \tag{7}$$

defined by the fundamental Lagrange function $L(x,y)$, which prescribes nonholonomic frame structures of types (2) and (3), ${}^{(L)}\boldsymbol{e}_\nu=(e_i,{}^\vee e_k)$ and ${}^{(L)}\vartheta^\mu=(\vartheta^i,{}^\vee\vartheta^k)$. [On the tangent bundle the indices related to the base space run the same values as those related to fibers: we can use the same symbols but have to distinguish like ${}^\vee e_k$ certain irreducible v-components with respect to, (or for) N-adapted bases and cobases.]

3. The canonical N-connection (7) defining ${}^\vee e_i$, induces naturally an almost complex structure $\mathbf{F}:\chi(\widetilde{TM})\to\chi(\widetilde{TM})$, where $\chi(\widetilde{TM})$ denotes the module of vector fields on $\widetilde{TM}$,

$$\mathbf{F}(e_i)={}^\vee e_i,\quad \mathbf{F}\left({}^\vee e_i\right)=-e_i,$$

when

$$\mathbf{F}={}^\vee e_i\otimes\vartheta^i-e_i\otimes{}^\vee\vartheta^i \tag{8}$$

satisfies the condition $\mathbf{F}\rfloor\mathbf{F}=-\mathbf{I}$, i.e., $F^\alpha{}_\beta F^\beta{}_\gamma=-\delta^\alpha_\gamma$, where δ^α_γ is the Kronecker symbol and "$\rfloor$" denotes the interior product.

4. On $\widetilde{TM}$, there is a canonical metric structure

$${}^{(L)}\mathbf{g}={}^{(L)}g_{ij}(x,y)\,\vartheta^i\otimes\vartheta^j+{}^{(L)}g_{ij}(x,y)\,{}^\vee\vartheta^i\otimes{}^\vee\vartheta^j \tag{9}$$

constructed as a Sasaki type lift from M.

One holds (Refs. 6–8) the following

Theorem 1: *The space* $(\widetilde{TM},\mathbf{F},{}^{(L)}\mathbf{g})$ *with almost complex form* $\mathbf{F}$ *(8) defined by* ${}^{(L)}N^i_j$*, see (7), and canonical metric structure* ${}^{(L)}\boldsymbol{g}$ *(9) is an almost Kähler space with almost symplectic structure*

$$ {}^{(L)}\theta = {}^{(L)}\theta_{\alpha\beta}(x,y)\vartheta^\alpha \wedge \vartheta^\beta = {}^{(L)}g_{ij}(x,y)^\vee\vartheta^i \wedge \vartheta^j. \tag{10}$$

Proof: It is evident if we define

$$ {}^{(L)}\theta(\mathbf{X},\mathbf{Y}) \doteqdot {}^{(L)}\mathbf{g}(\mathbf{FX},\mathbf{Y}) $$

and put $\mathbf{X}=\mathbf{e}_\alpha$ and $\mathbf{Y}=\mathbf{e}_\beta$. ■

We conclude that any regular Lagrange mechanics can be geometrized as an almost Kähler space with N-connection distribution. In such a Lagrange–Kähler nonholonomic manifold, the fundamental geometric structures (semispray, N-connection, almost complex structure, and canonical metric on $\widetilde{TM}$) are defined by the fundamental Lagrange function $L(x,y)$.

Remark 1: *For applications in optics of nonhomogeneous media and gravity (see, for instance, Refs. 7, 9, 11, and 12) one considers metric forms of type* $g_{ij}\sim e^{\lambda(x,y)^{(L)}}g_{ij}(x,y)$ *which cannot be derived from a mechanical Lagrangian. In the so-called generalized Lagrange geometry one considers Sasaki-type metrics (9) with certain general coefficients both for the metric and* N*-connection, i.e., when* ${}^{(L)}g_{ij}\to g_{ij}(x,y)$*, and* ${}^{(L)}N^i_j\to N^i_j(x,y)$*. [In this case, we can similarly define an almost Kähler* N*-anholonomic space* $(\widetilde{TM},\mathbf{F},\theta)$ *with the geometric structures induced naturally by the* N*-connection.]*

Remark 2: *Finsler geometry with the fundamental Finsler function* $F(x,y)$*, being homogeneous of type* $F(x,\lambda y)=\lambda F(x,y)$*, for nonzero* $\lambda\in\mathbb{R}$*, may be considered as a particular case of Lagrange geometry when* $L=F^2$*. [In another turn, there is a proof*[59] *that any Lagrange fundamental function L can be modeled as a singular case in a certain class of Finsler geometries of extra dimension.] We shall apply the methods of Finsler geometry and its almost Kähler models in this work. Nevertheless, because the generalized Lagrange spaces are very general ones enabled with N-anholonomic structure inducing a corresponding almost symplectic structure we shall emphasize just such geometric configurations.*

Remark 3: *It is also proved that both generalized Lagrange and Finsler geometries can be modeled on Riemannian–Cartan N-anholonomic manifolds*[13,30–32] *if off-diagonal metrics and N-connections are introduced into consideration.*

Now we shall demonstrate how N-anholonomic configurations can be defined in gravity theories. In this case, it is convenient to work on a general manifold $\mathbf{V}$, $\dim\mathbf{V}=n+m$ with global splitting, instead of the tangent bundle $\widetilde{TM}$.

C. N-connections in gravity

Let us consider a metric structure on $\mathbf{V}$ with the coefficients defined with respect to a local coordinate basis $du^\alpha=(dx^i,dy^a)$,

$$ \mathbf{g} = \underline{g}_{\alpha\beta}(u)du^\alpha\otimes du^\beta $$

with

$$ \underline{g}_{\alpha\beta} = \begin{bmatrix} g_{ij}+N^a_iN^b_jh_{ab} & N^e_jh_{ae} \\ N^e_ih_{be} & h_{ab} \end{bmatrix}. \tag{11}$$

A metric, for instance, parametrized in the form (11) is generic off-diagonal if it cannot be diagonalized by any coordinate transforms. Performing a frame transform with the coefficients

$$ \mathbf{e}^\alpha_\alpha(u) = \begin{bmatrix} e^i_i(u) & N^b_i(u)e^a_b(u) \\ 0 & e^a_a(u) \end{bmatrix}, \tag{12}$$

$$\mathbf{e}_{\underline{\beta}}^{\beta}(u)=\begin{bmatrix} e_{\underline{i}}^{i}(u) & -N_{k}^{b}(u)e_{\underline{i}}^{k}(u) \\ 0 & e_{\underline{a}}^{a}(u) \end{bmatrix}, \tag{13}$$

we write equivalently the metric in the form

$$\mathbf{g}=\mathbf{g}_{\alpha\beta}(u)\vartheta^{\alpha}\otimes\vartheta^{\beta}=g_{ij}(u)\vartheta^{i}\otimes\vartheta^{j}+h_{ab}(u)\overset{\vee}{\vartheta}{}^{a}\otimes\overset{\vee}{\vartheta}{}^{b}, \tag{14}$$

where $g_{ij}\doteq\mathbf{g}(e_i,e_j)$ and $h_{ab}\doteq\mathbf{g}(e_a,e_b)$ and

$$\mathbf{e}_{\alpha}=\mathbf{e}_{\alpha}^{\underline{\alpha}}\partial_{\underline{\alpha}} \text{ and } \vartheta^{\beta}=\mathbf{e}_{\underline{\beta}}^{\beta}du^{\underline{\beta}}.$$

are vielbeins of types (2) and (3) defined for arbitrary $N_i^b(u)$. We can consider a special class of manifolds provided with a global splitting into conventional "horizontal" and "vertical" subspaces (1) induced by the "off-diagonal" terms $N_i^b(u)$ and prescribed type of nonholonomic frame structure.

If the manifold $\mathbf{V}$ is (pseudo) Riemannian, there is a unique linear connection (the Levi-Civita connection) ∇, which is metric, $\nabla\mathbf{g}=\mathbf{0}$, and torsionless, ${}^{\nabla}T=0$. Nevertheless, the connection ∇ is not adapted to the nonintegrable distribution induced by $N_i^b(u)$. In this case, it is more convenient to work with more general classes of linear connections which are N-adapted but contain nontrivial torsion coefficients because of nontrivial nonholonomy coefficients $W_{\alpha\beta}^{\gamma}$ (5). (For instance, in order to construct exact solutions parametrized by generic off-diagonal metrics, or for investigating nonholonomic frame structures in gravity models with nontrivial torsion.)

For a splitting of a (pseudo-) Riemannian–Cartan space of dimension $(n+m)$ [under certain constraints, we can consider (pseudo-) Riemannian configurations], the Lagrange and Finsler type geometries were modeled by N-anholonomic structures as exact solutions of gravitational field equations.[9–13,31,32] In this paper, we shall concentrate on N-anholonomic almost complex structures of vacuum gravity which can be naturally defined as $(n+n)$ configurations, in general, embedded in certain spaces of dimension $(n+m)$, $m\geqslant n$.

III. CONNECTIONS ON ALMOST SYMPLECTIC N-ANHOLONOMIC MANIFOLDS

The geometric constructions can be adapted to the N-connection structure:

Definition 4: A distinguished connection (d-connection) $\mathbf{D}$ *on a manifold* $\mathbf{V}$ *is a linear connection conserving under parallelism the Whitney sum (1) defining a general N-connection. Equivalently,* $\mathbf{DP}=0$, $\mathbf{P}$ *being the almost product structure defined by the N-connection.*

The N-adapted components $\Gamma_{\beta\gamma}^{\alpha}$ of a d-connection $\mathbf{D}_{\alpha}=(\delta_{\alpha}\rfloor\mathbf{D})$ are defined by the equations

$$\mathbf{D}_{\alpha}\delta_{\beta}=\Gamma_{\alpha\beta}^{\gamma}\delta_{\gamma},$$

or

$$\Gamma_{\alpha\beta}^{\gamma}(u)=(\mathbf{D}_{\alpha}\delta_{\beta})\delta^{\gamma}. \tag{15}$$

In its turn, this defines a N-adapted splitting into h- and v-covariant derivatives, $\mathbf{D}=D+\overset{\vee}{D}$, where $D_k=(L_{jk}^i,L_{bk}^a)$ and $\overset{\vee}{D}_c=(C_{jk}^i,C_{bc}^a)$ are introduced as corresponding h- and v-parametrizations of (15),

$$L_{jk}^{i}=(\mathbf{D}_{k}e_{j})\vartheta^{i},\quad L_{bk}^{a}=(\mathbf{D}_{k}e_{b})\vartheta^{a},\quad C_{jc}^{i}=(\mathbf{D}_{c}e_{j})\vartheta^{i},\quad C_{bc}^{a}=(\mathbf{D}_{c}e_{b})\vartheta^{a}.$$

The components $\mathbf{\Gamma}_{\alpha\beta}^{\gamma}=(L_{jk}^i,L_{bk}^a,C_{jc}^i,C_{bc}^a)$ completely define a d-connection $\mathbf{D}$ on a N-anholonomic manifold $\mathbf{V}$.

The simplest way to perform computations with d-connections is to use N-adapted differential forms like $\mathbf{\Gamma}_{\beta}^{\alpha}=\mathbf{\Gamma}_{\beta\gamma}^{\alpha}\vartheta^{\gamma}$ with the coefficients defined with respect to (3) and (2).

We shall say that a d-connection $\mathbf{D}$ preserves an almost symplectic two-form, of Lagrange type ${}^{(L)}\theta$ (10) (or any general one, θ) defined from a generalized Lagrange geometry or N-anholonomic gravity model, if

$$\mathbf{D}\theta = \mathbf{0} \tag{16}$$

or

$$\mathbf{Z}(\theta(\mathbf{X},\mathbf{Y})) = \theta(\mathbf{D}_Z\mathbf{X},\mathbf{Y}) + \theta(\mathbf{X},\mathbf{D}_\mathbf{Z}\mathbf{Y})$$

for any d-vector fields $\mathbf{X}$, $\mathbf{Y}$, $\mathbf{Z}\in T\mathbf{V}$.

Theorem 2: *The torsion* $\mathcal{T}^\alpha \doteqdot \mathbf{D}\vartheta^\alpha = d\vartheta^\alpha + \Gamma^\alpha_\beta \wedge \vartheta^\beta$ *of a d-connection has the irreducible h-, v-components (d-torsions) with N-adapted coefficients*

$$T^i_{jk} = L^i_{[jk]}, \quad T^i_{ja} = -T^i_{aj} = C^i_{ja}, \quad T^a_{ji} = \Omega^a_{ji},$$

$$T^a_{bi} = T^a_{ib} = \frac{\partial N^a_i}{\partial y^b} - L^a_{bi}, \quad T^a_{bc} = C^a_{[bc]}, \tag{17}$$

where $L^i_{[jk]} = L^i_{jk} - L^i_{kj}$ *and so on.* ■

Proof: By a straightforward calculation we can verify the formulas.

Remark 4: *The Levi-Civita linear connection* $\nabla = \{{}^\nabla\mathbf{\Gamma}^\alpha_{\beta\gamma}\}$, *with vanishing both torsion and nonmetricity, is not adapted to the global splitting (1). In fact, if* ∇ *was adapted, then* $\nabla\mathbf{P} = 0$, $\mathbf{P}$ *being the almost product structure defined by the N-connection, and then, as* ∇ *is torsionless, one obtains by means of the Lemma 2.1.6 of Ref. 60 that the Nijenhuis tensor field* $N_\mathbf{P}$ *vanishes, thus proving that both vertical and horizontal distributions are involutive in the sense of Frobenius theorem, which is not our case of anholonomic manifolds. Then, we must look for another connection to study the geometry of these manifolds.*

One holds:

Proposition 3: *There is a preferred, canonical d-connection structure,* $\hat{\mathbf{D}}$, *on N-aholonomic manifold* $\mathbf{V}$ *constructed only from the metric and N-connection coefficients* $[g_{ij}, h_{ab}, N^a_i]$ *and satisfying the conditions* $\hat{\mathbf{D}}\mathbf{g} = 0$ *and* $\hat{T}^i_{jk} = 0$ *and* $\hat{T}^a_{bc} = 0$.

Proof: By straightforward calculations with respect to the N-adapted bases (3) and (2), we can verify that the connection

$$\hat{\mathbf{\Gamma}}^\alpha_{\beta\gamma} = {}^\nabla\mathbf{\Gamma}^\alpha_{\beta\gamma} + \hat{\mathbf{P}}^\alpha_{\beta\gamma} \tag{18}$$

with the deformation d-tensor [$\hat{\mathbf{P}}^\alpha_{\beta\gamma}$ is a tensor field of type (1,2)—as is well known, the sum of a linear connection and a tensor field of type (1,2) is a new linear connection]

$$\hat{\mathbf{P}}^\alpha_{\beta\gamma} = \left(P^i_{jk} = 0, P^a_{bk} = \frac{\partial N^a_k}{\partial y^b}, P^i_{jc} = -\frac{1}{2} g^{ik}\Omega^a_{kj} h_{ca}, P^a_{bc} = 0 \right)$$

satisfies the conditions of this Proposition. It should be noted that, in general, the components $\hat{T}^i_{ja}$, $\hat{T}^a_{ji}$, and $\hat{T}^a_{bi}$ are not zero. This is an anholonomic frame (or, equivalently, off-diagonal metric) effect. ■

With respect to the N-adapted frames, the coefficients $\hat{\mathbf{\Gamma}}^\gamma_{\alpha\beta} = (\hat{L}^i_{jk}, \hat{L}^a_{bk}, \hat{C}^i_{jc}, \hat{C}^a_{bc})$ are computed:

$$\hat{L}^i_{jk} = \frac{1}{2} g^{ir}\left(\frac{\delta g_{jr}}{\partial x^k} + \frac{\delta g_{kr}}{\partial x^j} - \frac{\delta g_{jk}}{\partial x^r} \right),$$

$$\hat{L}^a_{bk} = \frac{\partial N^a_k}{\partial y^b} + \frac{1}{2} h^{ac}\left(\frac{\delta h_{bc}}{\partial x^k} - \frac{\partial N^d_k}{\partial y^b} h_{dc} - \frac{\partial N^d_k}{\partial y^c} h_{db} \right),$$

$$\hat{C}^i_{jc} = \frac{1}{2} g^{ik} \frac{\partial g_{jk}}{\partial y^c},$$

$$\hat{C}^a_{bc} = \frac{1}{2} h^{ad} \left(\frac{\partial h_{bd}}{\partial y^c} + \frac{\partial h_{cd}}{\partial y^b} - \frac{\partial h_{bc}}{\partial y^d} \right). \tag{19}$$

For the canonical d-connection there are satisfied the conditions of vanishing of torsion on the h-subspace and v-subspace, i.e., $\hat{T}^i_{jk} = \hat{T}^a_{bc} = 0$. In more general cases, such components of torsion are not zero, for instance, the metric d-connections of type $\mathbf{\Gamma}^{\gamma}_{\alpha\beta} = (\hat{L}^i_{jk} + l^i_{jk}(u), \hat{L}^a_{bk}, \hat{C}^i_{jc}, \hat{C}^a_{bc} + c^a_{bc}(u))$ are also compatible with metric (14) and has nontrivial T^i_{jk} and $\hat{T}^a_{bc}$.

Let us consider a special case with $\dim \mathbf{V} = n+n$, $h_{ab} \to g_{ij}$ and $N^a_i \to N^j_i$ in (14) when a tangent bundle structure is locally modeled on $\mathbf{V}$. We denote such a space by $\widetilde{\mathbf{V}}_{(n,n)}$. One holds:

Theorem 4: *The canonical d-connection* $\hat{\mathbf{D}}$ *(19) for a local modelling of a* $\widetilde{TM}$ *space on* $\widetilde{\mathbf{V}}_{(n,n)}$ *is defined by* $\hat{\mathbf{\Gamma}}^{\gamma}_{\alpha\beta} = (\hat{L}^i_{jk}, \hat{C}^i_{jk})$ *with*

$$\hat{L}^i_{jk} = \frac{1}{2} g^{ir} \left(\frac{\delta g_{jr}}{\partial x^k} + \frac{\delta g_{kr}}{\partial x^j} - \frac{\delta g_{jk}}{\partial x^r} \right), \quad \hat{C}^i_{jk} = \frac{1}{2} g^{ir} \left(\frac{\partial g_{jr}}{\partial x^k} + \frac{\partial g_{kr}}{\partial x^j} - \frac{\partial g_{jk}}{\partial x^r} \right). \tag{20}$$

This d-connection is almost Hermitian, i.e., it is compatible with the almost Hermitian structure $(\mathbf{g}, \mathbf{F})$, *when*

$$\hat{\mathbf{D}}\theta = 0 \text{ and } \hat{\mathbf{D}}\mathbf{F} = 0 \tag{21}$$

for a two-form [in an intrinsic way, $\theta(X,Y) = \mathbf{g}(\mathbf{F}X, Y)$]

$$\theta = \theta_{\alpha\beta}(x,y)\vartheta^{\alpha} \wedge \vartheta^{\beta} = g_{ij}(x,y)^{\vee}\vartheta^i \wedge \vartheta^j.$$

Proof: It is similar to that for the Theorem 1. ■

On almost symplectic manifolds, usually there are considered symmetric linear connections. In our case, we can always define a symmetric d-connection by taking the symmetric part **[**in coordinate-free notation, $\mathbf{S}_X Y = \frac{1}{2}(\mathbf{D}_X Y + \mathbf{D}_Y X + [X,Y])$**]** of $\mathbf{\Gamma}^{\gamma}_{\alpha\beta}$,

$$\mathbf{S}^{\gamma}_{\alpha\beta} = \tfrac{1}{2}(\mathbf{\Gamma}^{\gamma}_{\alpha\beta} + \mathbf{\Gamma}^{\gamma}_{\beta\alpha}), \tag{22}$$

where $\mathbf{\Gamma}^{\gamma}_{\alpha\beta} = (\hat{L}^i_{jk} + l^i_{jk}(u), \hat{C}^i_{jk} + c^i_{jk}(u))$. On a N-anholonomic manifold $\widetilde{\mathbf{V}}_{(n,n)}$, an almost symplectic form θ is not closed, i.e., $d\theta \neq \mathbf{0}$. But it may be closed under the action of N-adapted derivatives (2) and differentials (3) when

$$\delta\theta = \delta(\theta_{\alpha\beta}(x,y)\vartheta^{\alpha} \wedge \vartheta^{\beta}) = 0,$$

which means that

$$\mathbf{e}_{\gamma}\theta_{\alpha\beta} + \mathbf{e}_{\alpha}\theta_{\gamma\beta} + \mathbf{e}_{\beta}\theta_{\alpha\gamma} = 0. \tag{23}$$

The condition (16) written in N-adapted bases results in

$$\mathbf{e}_{\gamma}\theta_{\alpha\beta} = \mathbf{\Gamma}_{\alpha\gamma\beta} - \mathbf{\Gamma}_{\beta\gamma\alpha}$$

for $\mathbf{\Gamma}_{\alpha\gamma\beta} \doteq \theta_{\alpha\tau}\mathbf{\Gamma}^{\tau}_{\gamma\beta}$.

Definition 5: An almost symplectic two-form θ *is N-symplectic if it satisfies the conditions (23).*

There is a relation between the set of all d-connections $\mathbf{D}$ for which $\mathbf{D}\theta = \mathbf{0}$ for any given θ and $\mathbf{N}$ and the set of all symmetric connections on $\widetilde{\mathbf{V}}_{(n,n)}$. By straightforward calculations we can verify that

$$\mathbf{\Gamma}_{\alpha\gamma\beta} = \tfrac{1}{2}(\mathbf{e}_{\alpha}\theta_{\gamma\beta} - \mathbf{e}_{\gamma}\theta_{\alpha\beta} - \mathbf{e}_{\beta}\theta_{\alpha\gamma}) + (\mathbf{S}_{\alpha\gamma\beta} - \mathbf{S}_{\gamma\beta\alpha} + \mathbf{S}_{\beta\gamma\alpha}) \tag{24}$$

is inverse to (22), which for almost symplectic $\theta_{\alpha\beta}$ satisfying the conditions (23) simplifies to

$$\mathbf{\Gamma}_{\alpha\gamma\beta} = \mathbf{e}_\alpha \theta_{\gamma\beta} + (\mathbf{S}_{\alpha\gamma\beta} - \mathbf{S}_{\gamma\beta\alpha} + \mathbf{S}_{\beta\gamma\alpha}).$$

On holonomic manifolds with trivial N-connection, the formulas (23) and (24) transform into those from Ref. 3 with $\mathbf{e}_\alpha \to \partial/\partial u^\alpha$. We may conclude that N-anholonomic transforms map symplectic forms in almost symplectic ones but preserve the main symmetry properties and compatibility with the linear connection structure if the computations are performed with respect to N-adapted bases.

IV. CURVATURE OF N-SYMPLECTIC d-CONNECTIONS

Let $\mathbf{V}$ (or $\widetilde{\mathbf{V}}_{(n,n)}$) be an N-anholonomic manifold provided with a metric d-connection $\mathbf{\Gamma}^\alpha_\gamma$.

Definition 6: A Fedosov N-anholonomic manifold is defined by an almost symplectic d-connection and almost complex structure induced by the N-connection.

Definition 7: A Lagrange–Fedosov manifold is a Fedosov N-anholonomic manifold with the N-connection and almost complex structure defined by the fundamental Lagrange function, see Theorem 1.

The curvature of a symplectic d-connection $\mathbf{D}$ is defined by the usual formula

$$\mathbf{R}(\mathbf{X},\mathbf{Y})\mathbf{Z} \doteq \mathbf{D}_X\mathbf{D}_Y\mathbf{Z} - \mathbf{D}_Y\mathbf{D}_X\mathbf{Z} - \mathbf{D}_{[X,X]}\mathbf{Z}.$$

Because on N-anholonomic spaces the "simplest" adapted to the N-connection induced almost complex structures is defined by the canonical d-connection, it is convenient to use it as a symplectic d-connection.

By straightforward calculations we prove:

Theorem 5: *The curvature* $\mathcal{R}^\alpha_\beta \doteq \mathbf{D}\mathbf{\Gamma}^\alpha_\beta = d\mathbf{\Gamma}^\alpha_\beta - \mathbf{\Gamma}^\gamma_\beta \wedge \mathbf{\Gamma}^\alpha_\gamma$ *of a d-connection* $\mathbf{\Gamma}^\alpha_\gamma$ *has the irreducible h- v- components (d-curvatures) of* $\mathbf{R}^\alpha_{\beta\gamma\delta}$,

$$R^i_{hjk} = e_k L^i_{hj} - e_j L^i_{hk} + L^m_{hj} L^i_{mk} - L^m_{hk} L^i_{mj} - C^i_{ha}\Omega^a_{kj},$$

$$R^a_{bjk} = e_k L^a_{bj} - e_j L^a_{bk} + L^c_{bj} L^a_{ck} - L^c_{bk} L^a_{cj} - C^a_{bc}\Omega^c_{kj},$$

$$R^i_{jka} = e_a L^i_{jk} - D_k C^i_{ja} + C^i_{jb} T^b_{ka},$$

$$R^c_{bka} = e_a L^c_{bk} - D_k C^c_{ba} + C^c_{bd} T^c_{ka},$$

$$R^i_{jbc} = e_c C^i_{jb} - e_b C^i_{jc} + C^h_{jb} C^i_{hc} - C^h_{jc} C^i_{hb},$$

$$R^a_{bcd} = e_d C^a_{bc} - e_c C^a_{bd} + C^e_{bc} C^a_{ed} - C^e_{bd} C^a_{ec}. \tag{25}$$

Remark 5: *For an N-anholonomic manifold* $\widetilde{\mathbf{V}}_{(n,n)}$ *provided with N-sympletic canonical d-connection* $\hat{\mathbf{\Gamma}}_{\gamma\alpha\beta} = \theta_{\gamma\tau}\hat{\mathbf{\Gamma}}^\tau_{\alpha\beta}$, *see (20), the d-curvatures (25) reduces to three irreducible components*,

$$R^i_{hjk} = e_k L^i_{hj} - e_j L^i_{hk} + L^m_{hj} L^i_{mk} - L^m_{hk} L^i_{mj} - C^i_{ha}\Omega^a_{kj},$$

$$R^i_{jka} = e_a L^i_{jk} - D_k C^i_{ja} + C^i_{jb} T^b_{ka},$$

$$R^a_{bcd} = e_d C^a_{bc} - e_c C^a_{bd} + C^e_{bc} C^a_{ed} - C^e_{bd} C^a_{ec}, \tag{26}$$

where all indices $i,j,k\ldots$ *and* $a,b,\ldots$ *run the same values but label the components with respect to different h- or v-frames.*

The indices of the components of the curvature tensor are lowered as

$$\mathbf{R}_{\tau\beta\gamma\delta} = \theta_{\tau\alpha}\mathbf{R}^{\alpha}_{\beta\gamma\delta}.$$

For Lagrange–Fedosov manifolds, the two-form $\theta_{\tau\alpha}$ has the coefficients defined by the metric structure and Lagrangian, see (10). In this case we can apply the canonical d-connection and the d-metric for definition of the curvature of symplectic d-connections.

Contracting, respectively, the components of (25) and (26) we prove:

Corollary 6: *The Ricci d-tensor* $\mathbf{R}_{\alpha\beta} \doteq \mathbf{R}^{\tau}_{\alpha\beta\tau}$ *has the irreducible h- v-components*

$$R_{ij} \doteq R^{k}_{ijk}, \quad R_{ia} \doteq -R^{k}_{ika}, \quad R_{ai} \doteq R^{b}_{aib}, \quad R_{ab} \doteq R^{c}_{abc}, \tag{27}$$

for a general N-holonomic manifold $\mathbf{V}$, *and*

$$R_{ij} \doteq R^{k}_{ijk}, \quad R_{ia} \doteq -R^{k}_{ika}, \quad R_{ab} \doteq R^{c}_{abc}, \tag{28}$$

for an N-anholonomic manifold $\widetilde{\mathbf{V}}_{(n,n)}$.

Corollary 7: *The scalar curvature of a d-connection is*

$$\overleftarrow{\mathbf{R}} \doteq \mathbf{g}^{\alpha\beta}\mathbf{R}_{\alpha\beta} = g^{ij}R_{ij} + h^{ab}R_{ab,} \quad for \quad \mathbf{V};$$
$$= 2g^{ij}R_{ij} \quad for \quad \widetilde{\mathbf{V}}_{(n,n)}.$$

Corollary 8: *The Einstein d-tensor is computed* $\mathbf{G}_{\alpha\beta} = \mathbf{R}_{\alpha\beta} - \frac{1}{2}\mathbf{g}_{\alpha\beta}\overleftarrow{\mathbf{R}}$.

In modern gravity theories, one considers more general linear connections generated by deformations of type $\mathbf{\Gamma}^{\alpha}_{\beta\gamma} = \hat{\mathbf{\Gamma}}^{\alpha}_{\beta\gamma} + \mathbf{P}^{\alpha}_{\beta\gamma}$. We can split all geometric objects into canonical and postcanonical pieces which results in N-adapted geometric constructions. For instance,

$$\mathcal{R}^{\alpha}_{\beta} = \hat{\mathcal{R}}^{\alpha}_{\beta} + \mathbf{D}\mathcal{P}^{\alpha}_{\beta} + \mathcal{P}^{\alpha}_{\gamma} \wedge \mathcal{P}^{\gamma}_{\beta} \tag{29}$$

for $\mathcal{P}^{\alpha}_{\beta} = \mathbf{P}^{\alpha}_{\beta\gamma}\vartheta^{\gamma}$. This way, for almost complex geometries, the d-tensors (26) and (28) can be redefined just for symmetrized d-connections compatible with the almost complex structure.

V. EINSTEIN FLAT N-ANHOLONOMIC MANIFOLDS

In terms of differential forms, the vacuum Einstein equations are written

$$\eta_{\alpha\beta\gamma} \wedge \hat{\mathcal{R}}^{\beta\gamma} = 0, \tag{30}$$

where, for the volume four-form $\eta \doteq *1$ with the Hodge operator "*," $\eta_{\alpha} \doteq \mathbf{e}_{\alpha} \rfloor \eta$, $\eta_{\alpha\beta} \doteq \mathbf{e}_{\beta} \rfloor \eta_{\alpha}$, $\eta_{\alpha\beta\gamma} \doteq \mathbf{e}_{\gamma} \rfloor \eta_{\alpha\beta}, \ldots$ and $\hat{\mathcal{R}}^{\beta\gamma}$ is the curvature two-form. The deformation of connection (18) defines a deformation of the curvature tensor of type (29) but with respect to the curvature of the Levi-Civita connection, ${}^{\nabla}\mathcal{R}^{\beta\gamma}$. The gravitational field equations (30) transforms into

$$\eta_{\alpha\beta\gamma} \wedge {}^{\nabla}\mathcal{R}^{\beta\gamma} + \eta_{\alpha\beta\gamma} \wedge {}^{\nabla}\mathcal{Z}^{\beta\gamma} = 0, \tag{31}$$

where ${}^{\nabla}\mathcal{Z}^{\beta}_{\gamma} = \nabla\mathcal{P}^{\beta}_{\gamma} + \mathcal{P}^{\beta}_{\alpha} \wedge \mathcal{P}^{\alpha}_{\gamma}$.

A subclass of solutions of the gravitational field equations for the canonical d-connection defines also solutions of the Einstein equations for the Levi-Civita connection if and only if

$$\eta_{\alpha\beta\gamma} \wedge {}^{\nabla}\mathcal{Z}^{\beta\gamma} = 0. \tag{32}$$

This property is very important for constructing exact solutions in Einstein and string gravity, parametrized by generic off-diagonal metrics and anholonomic frames with associated N-connection structure (see reviews of results in Refs. 30–32).

A. The ansatz for metric

In this section we investigate a class of five-dimensional vacuum Einstein solutions with nontrivial associated N-connection and generic off-diagonal metric. We analyze the conditions when such solutions reduce to four dimensions and possess almost complex structure.

Let us consider a five-dimensional ansatz for the metric (14) and frame (3) when $u^{\alpha}=(x^i,y^4=v,y^5)$; $i=1, 2, 3$ and the coefficients

$$g_{ij}=\mathrm{diag}[g_1=\pm\varpi(x^k,v),\varpi(x^k,v)g_2(x^2,x^3),\varpi(x^k,v)g_3(x^2,x^3)],$$

$$h_{ab}=\mathrm{diag}[\varpi(x^k,v)h_4(x^k,v),\varpi(x^k,v)h_5(x^k,v)],$$

$$N_i^4=w_i(x^k,v),N_i^5=n_i(x^k,v) \tag{33}$$

are some functions of necessary smooth class. The partial derivative are briefly denoted $a^{\bullet}=\partial a/\partial x^2$, $a'=\partial a/\partial x^3$, $a^*=\partial a/\partial v$.

Theorem 9: *The vacuum Einstein equations (30) for the canonical d-connection (18) constructed from data (33) are equivalent to the system of equations*

$$g_3^{\bullet\bullet}-\frac{g_2^{\bullet}g_3^{\bullet}}{2g_2}-\frac{(g_3^{\bullet})^2}{2g_3}+g_2''-\frac{g_2'g_3'}{2g_3}-\frac{(g_2')^2}{2g_2}=0, \tag{34}$$

$$h_5^{**}-h_5^*\left(\ln\left|\sqrt{|h_4h_5|}\right|\right)^*=0, \tag{35}$$

$$w_i\beta+\alpha_i=0, \tag{36}$$

$$n_i^{**}+n_i^*=0, \tag{37}$$

where

$$\alpha_i=\partial_i h_5^*-h_5^*\partial_i\ln\left|\sqrt{|h_4h_5|}\right|,\quad \beta=h_5^{**}-h_5^*\left[\ln\left|\sqrt{|h_4h_5|}\right|\right]^*,$$

$$\gamma=3h_5^*/2h_5-h_4^*/h_4, \tag{38}$$

$h_4^*\neq 0$ *and* $h_5^*\neq 0$ *and the functions* h_4 *and* ϖ *must satisfy certain additional conditions*

$$\hat{\delta}_i h_4=0\quad \textit{and}\quad \hat{\delta}_i\varpi=0, \tag{39}$$

for any $\zeta_i(x^k,v)$ *defining* $\hat{\delta}_i=\partial_i-(w_i+\zeta_i)\partial_4+n_i\partial_5$.

Proof: It is a straightforward calculation, see similar ones in Refs. 31, 9, and 11. ■

We note that the conditions (39) are satisfied if

$$\varpi^{q_1/q_2}=h_4 \tag{40}$$

for some nonzero integers q_1 and q_2 and ζ_i defined from

$$\partial_i\varpi-(w_i+\zeta_i)\varpi^*=0. \tag{41}$$

Remark 6: *Under the conditions of the Theorem 9, we can also consider d-metrics with* $h_5^*=0$ *for such functions* $h_4=h^{\#}(x^i,v)$ *when*

$$\lim_{h_5^*\to 0}\left\{h_5^*[\ln\left|\sqrt{|h^{\#}h_5|}\right|]^*\right\}\to 0$$

and

$$\lim_{h_5^*\to 0}\left\{h_5^*\partial_i \ln\left|\sqrt{|h^\# h_5|}\right|\right\}\to 0.$$

In these cases, Eqs. (35) and (36) will be satisfied by any $h^\#(x^i,v)$ *and* $w_i(x^i,v)$ *and we may take* $n_i^*=n_{[1]i}(x^i)h^\#(x^i,v)$ *in order to satisfy (37).*

Theorem 10: *The system of gravitational field equations (30) for the ansatz (33) can be solved in general form if there are given certain values of functions* $g_2(x^2,x^3)$ [*or, inversely,* $g_3(x^2,x^3)$], $h_4(x^i,v)$ [*or, inversely,* $h_5(x^i,v)$].

Proof: We outline the main steps of constructing exact solutions proving this Theorem, see detailed computations presented in the Proof of Theorem 4.3 from Ref. 31.

- The general solution of Eq. (34) can be written in the form

$$\lambda = g_{[0]}\exp[a_2\tilde{x}^2(x^2,x^3)+a_3\tilde{x}^3(x^2,x^3)], \tag{42}$$

were $g_{[0]}$, a_2, and a_3 are some constants and the functions $\tilde{x}^{2,3}(x^2,x^3)$ define any coordinate transforms $x^{2,3}\to\tilde{x}^{2,3}$ for which the two-dimensional line element becomes conformally flat, i.e.,

$$g_2(x^2,x^3)(\mathrm{d}x^2)^2+g_3(x^2,x^3)(\mathrm{d}x^3)^2\to\lambda(x^2,x^3)[(\mathrm{d}\tilde{x}^2)^2+\epsilon(\mathrm{d}\tilde{x}^3)^2], \tag{43}$$

where $\epsilon=\pm 1$ for a corresponding signature. In coordinates $\tilde{x}^{2,3}$, Eq. (34) transforms into

$$\lambda(\lambda^{\bullet\bullet}+\lambda'')-\lambda^{\bullet}-\lambda'=0$$

or

$$\ddot{\psi}+\psi''=0, \tag{44}$$

for $\psi=\ln|\lambda|$. There are three alternative possibilities to generate solutions of (34). For instance, we can prescribe that $g_2=g_3$ and get Eq. (44) for $\psi=\ln|g_2|=\ln|g_3|$. If we suppose that $g_2'=0$, for a given $g_2(x^2)$, we obtain from (34)

$$g_3^{\bullet\bullet}-\frac{g_2^{\bullet}g_3^{\bullet}}{2g_2}-\frac{(g_3^{\bullet})^2}{2g_3}=0,$$

which can be integrated exactly. Similarly, we can generate solutions for a prescribed $g_3(x^3)$ in

$$g_2''-\frac{g_2'g_3'}{2g_3}-\frac{(g_2')^2}{2g_2}=0. \tag{45}$$

We note that a transform (43) is always possible for two-dimensional (2D) metrics and the explicit form of solutions depends on chosen system of 2D coordinates and on the signature $\epsilon=\pm 1$. In the simplest case, Eq. (34) is solved by arbitrary two functions $g_2(x^3)$ and $g_3(x^2)$.

- Equation (35) relates two functions $h_4(x^i,v)$ and $h_5(x^i,v)$ following two possibilities:

a) to compute

$$\sqrt{|h_5|}=h_{5[1]}(x^i)+h_{5[2]}(x^i)\int\sqrt{|h_4(x^i,v)|}\mathrm{d}v,\ h_4^*(x^i,v)\neq 0;$$
$$=h_{5[1]}(x^i)+h_{5[2]}(x^i)v,\ h_4^*(x^i,v)=0, \tag{46}$$

for some functions $h_{5[1,2]}(x^i)$ stated by boundary conditions;

b) or, inversely, to compute h_4 for a given $h_5(x^i,v)$, $h_5^*\neq 0$,

$$\sqrt{|h_4|} = h_{[0]}(x^i)(\sqrt{|h_5(x^i,v)|})^*, \tag{47}$$

with $h_{[0]}(x^i)$ given by boundary conditions.

- The exact solutions of (36) for $\beta \neq 0$ are defined from an algebraic equation, $w_i\beta + \alpha_i = 0$, where the coefficients β and α_i are computed as in formulas (38) by using the solutions for (34) and (35). The general solution is

$$w_k = \partial_k \ln[\sqrt{|h_4 h_5|}/|h_5^*|]/\partial_v \ln[\sqrt{|h_4 h_5|}/|h_5^*|], \tag{48}$$

with $\partial_v = \partial/\partial v$ and $h_5^* \neq 0$. If $h_5^* = 0$, or even $h_5^* \neq 0$ but $\beta = 0$, the coefficients w_k could be arbitrary functions on (x^i, v). For the vacuum Einstein equations this is a degenerated case imposing the compatibility conditions $\beta = \alpha_i = 0$, which are satisfied, for instance, if the h_4 and h_5 are related as in the formula (47) but with $h_{[0]}(x^i) = \text{const}$.
- Having defined h_4 and h_5 and computed γ from (38) we can solve Eq. (37) by integrating on variable "v" the equation $n_i^{**} + \gamma n_i^* = 0$. The exact solution is

$$\begin{aligned} n_k &= n_{k[1]}(x^i) + n_{k[2]}(x^i) \int [h_4/(\sqrt{|h_5|})^3] dv, \quad h_5^* \neq 0 \\ &= n_{k[1]}(x^i) + n_{k[2]}(x^i) \int h_4 \mathrm{d}v, \quad h_5^* = 0 \\ &= n_{k[1]}(x^i) + n_{k[2]}(x^i) \int [1/(\sqrt{|h_5|})^3] \mathrm{d}v, \quad h_4^* = 0, \end{aligned} \tag{49}$$

for some functions $n_{k[1,2]}(x^i)$ stated by boundary conditions.

The exact solution of (41) is given by some functions $\zeta_i = \zeta_i(x^i, v)$ if both $\partial_i \varpi = 0$ and $\varpi^* = 0$, we chose $\zeta_i = 0$ for $\varpi = \text{const}$, and

$$\zeta_i = -w_i + (\varpi^*)^{-1}\partial_i \varpi, \quad \varpi^* \neq 0, = (\varpi^*)^{-1}\partial_i \varpi, \quad \varpi^* \neq 0, \quad \text{for vacuum solutions}. \tag{50}$$

■

Theorem 10 states a general method of constructing five-dimensional exact solutions in various gravity models with generic off-diagonal metrics, nonholonomic frames and, in general, with nontrivial torsion. Such solutions are with associated N-connection structure. This method can also be applied in order to generate, for instance, certain Finsler or Lagrange configurations as v-irreducible components, or for a certain class of conformal factors $\varpi(x^i, v)$ for both h- and v-irreducible components. The five-dimensional ansatz cannot be used to generate directly standard Finsler or Lagrange geometries because the dimension of such spaces cannot be an odd number. Nevertheless, the anholonomic frame method can be applied in order to generate four-dimensional exact solutions containing Finsler–Lagrange configurations. For instance, a four-dimensional configuration can be defined just by an ansatz (14) with the data (33) where the coefficients do not depend on coordinate x^1 and the metric is stated to be four dimensional with the conformal factor $\varpi(x^2, x^3, v)$.

B. An example of induced almost Kähler gravity

Let us consider a four-dimensional ansatz which may mimic under certain constraints a generalized Lagrange geometry and induced almost Kähler structure in Riemann–Cartan space:

$$\begin{aligned} \mathbf{g} = \varpi(x^2,x^3,v)[&g_{22}(x^2,x^3)\mathrm{d}x^2 \otimes \mathrm{d}x^2 + g_{33}(x^2,x^3)\mathrm{d}x^3 \otimes \mathrm{d}x^3 + h_{44}(x^2,x^3,v)\,\delta y^4 \otimes \delta y^4 \\ &+ h_{55}(x^2,x^3,v)\,\delta y^5 \otimes \delta y^5], \end{aligned}$$

where

$$\delta y^4 = \mathrm{d}v + w_2(x^2,x^3,v)\mathrm{d}x^2 + w_3(x^2,x^3,v)\mathrm{d}x^3,$$

$$\delta y^5 = \mathrm{d}y^5 + n_2(x^2,x^3,v)\mathrm{d}x^2 + n_3(x^2,x^3,v)\mathrm{d}x^3.$$

This d-metric will define a class of vacuum solutions of the Einstein equations if the coefficients are subjected to the conditions of Theorem 10, when the dependence on coordinate x^1 is eliminated. We put $g_{22}=g(x^3)$ and $g_{33}=0$ to be a solution of (34) in the form (45), i.e.,

$$2gg'' - (g')^2 = 0$$

and choose $h_5=0$ and

$$h_4 = h^{\#}(x^3,v) = \frac{a^2}{|g(x^3)\times v|}g(x^3)$$

for $a=$const, which satisfies (35), see Remark 6. Taking any functions $w_{2,3}(x^2,x^3,v)$ and $n_{2,3}(x^2,x^3,v)$ satisfying

$$n^{*}_{2,3} = n_{2,3[0]}(x^2,x^3)h^{\#}(x^3,v)$$

we solve, respectively, Eqs. (36) and (37). We may take

$$\varpi = \varpi^{\#}(x^3,v) = [h^{\#}(x^3,v)]^{q_2/q_1}$$

like for (50). All such functions define a vacuum Einstein d-metric

$$\mathbf{g} = \varpi^{\#}(x^3,v)\left[g(x^3)\mathrm{d}x^2\otimes\mathrm{d}x^2 + \frac{a^2}{|g(x^3)\times v^2|}g(x^3)\,\delta y^4\otimes\delta y^4\right],$$

modeling an embedded generalized Lagrange geometry [it is a particular case of d-metrics considered in Ref. 8, see formula (6.3), which in our case is derived from a gravity model]. We construct a conformal almost Kähler geometry if we consider

$$\theta = \varpi^{\#}(x^3,v)g(x^3)\frac{a}{\sqrt{|g(x^3)\times v^2|}}\delta y^4\wedge\mathrm{d}x^2$$

and

$$\mathbf{F} = \frac{\sqrt{|g(x^3)\times v^2|}}{a}\left(\frac{\partial}{\partial v}\otimes\mathrm{d}x^2 + \frac{\partial}{\partial y^5}\otimes\mathrm{d}x^3\right) - \frac{a}{\sqrt{|g(x^3)\times v^2|}}\left(\frac{\delta}{\partial x^2}\otimes\mathrm{d}v + \frac{\delta}{\partial x^3}\otimes\mathrm{d}y^5\right).$$

Finally, we note that if we choose the functions $w_{2,3}(x^2,x^3,v)$ and $n_{2,3}(x^2,x^3,v)$ to parametrize a noncommutative structure, this vacuum gravitational space will possess a noncommutative symmetry like in Refs. 31 and 32. An alternative class of solutions can be generated if we put certain boundary conditions (for instance, for $v=t$ treated as a timelike coordinate, and one of the space coordinates x^2, x^3, y^5 running to infinite) when the N-connection coefficients possess a Lie algebra symmetry. In this case, we generate an explicit example of vacuum gravitational fields (in general, with nontrivial torsion) possessing Lie symmetries.[61] We can select such values of $w_{2,3}$ and $n_{2,3}$ when conditions (32) are satisfied and the solutions coincide with those for the Levi-Civita connection, but this is a very restricted case of N-connection geometry and associated almost complex structures.

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Hamilton–Jacobi equations for nonholonomic dynamics

Michele Pavon[a)]
Dipartimento di Matematica Pura e Applicata, Università di Padova, via Belzoni 7, 35131 Padova, Italy

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We derive generalized Hamilton–Jacobi equations for dynamical systems subject to linear velocity constraints. As long as a solution of the generalized Hamilton–Jacobi equation exists, the action is actually minimized (not just extremized). [DOI: 10.1063/1.1858441]

I. INTRODUCTION

Consider a mechanical system with configuration space $\mathbb{R}^n$. Let L be the Lagrangian, and suppose that the system is subject to $k<n$ nonholonomic constraints of the form

$$\omega_i(x(t))^T\dot{x}(t)=0, \quad i=1,2,\ldots,k, \quad t\in[t_0,t_1], \tag{1.1}$$

where the $\omega_i:\mathbb{R}^n\to\mathbb{R}^n$ are smooth functions and T denotes transpose. Let $\Omega(x)$ be the $k\times n$ matrix whose ith row is $\omega_i(x)^T$. Then, an application of d'Alembert's principle together with the method of Lagrange multipliers, gives that the equations of motion for the system are

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}}-\frac{\partial L}{\partial x}=\Omega^T\lambda, \tag{1.2}$$

where λ is the k-dimensional Lagrange multiplier. Equation (1.2) together with (1.1) constitute a system of $n+k$ equations for the $n+k$ unknowns $x_1,x_2,\ldots,x_n$, $\lambda_1,\lambda_2,\ldots,\lambda_k$. The components of $\Omega^T\lambda$ can be physically interpreted as the components of the (polygenic) force that acts on the mechanical system in order to maintain the given nonholonomic conditions.[10] Notice that d'Alembert's principle is not variational. A variational approach to the dynamics of systems subject to linear velocity constraints was proposed in Ref. 15 (see also Ref. 1, Chap. 1, Sec. 4). A lucid critique of this "Vakonomic dynamics" (variational axiomatic kind dynamics) can be found in Ref. 20. It is shown there that the vakonomic equations may lead to paradoxical behavior. The relation between the vakonomic and holonomic approaches has also been discussed in Refs. 1, 4, 5, 7, 11, and 17.

We show in this paper that the second, hydrodynamic form of Hamilton's principle may be extended to nonholonomic systems. We concentrate on the *optimization aspect* that is largely ignored in the physics literature. As long as a solution of the generalized Hamilton–Jacobi equation exists, the action is *minimized* by a path satisfying the correct equations of motions (1.2). Our derivation relies on general nonlinear Lagrange functionals.[12–14] It would be quite feasible to derive the result, after a suitable transformation, using standard optimal control results such as Ref. 16, Sec. 5.2, Theorem 7, and Ref. 8, Chap. IV. We find, however, that the approach based on Lagrange functionals is more transparent.

The paper is outlined as follows. In Sec. II we recall the hydrodynamic form of the classical Hamilton principle as established in Ref. 19, Sec. II (the latter developed from Ref. 9). In Sec. III, we extend the latter result to systems subject to linear velocity constraints. In Sec. IV the paper concludes with a discussion.

[a)]Electronic mail: pavon@math.unipd.it

II. THE CLASSICAL HAMILTON PRINCIPLE

Consider a dynamical system with configuration space $\mathbb{R}^n$. Let

$$L(x,v) := \frac{1}{2} m v \cdot v - V(x) \tag{2.1}$$

be the Lagrangian function, where $V(\cdot): \mathbb{R}^n \to R$ is of class C^1. The extension of the results of this paper to general Lagrangian functions that are strictly convex with respect to v appears straightforward. We prefer, however, to treat the simple case (2.1) in order to avoid obscuring ideas with technicalities. Let $\mathcal{X}_0$ denote the class of all C^1 paths $x: [t_0, t_1] \to R^n$ such that $x(t_0) = x_0$. Let $\mathcal{V}$ denote the family of continuous functions $v: [t_0, t_1] \to \mathbb{R}^n$. For $(x,v) \in \mathcal{X}_0 \times \mathcal{V}$, we define the functional $J(x,v)$ by

$$J(x,v) = \int_{t_0}^{t_1} L(x(t), v(t)) dt - S_1(x(t)), \tag{2.2}$$

where $S_1: R^n \to \mathbb{R}$ is continuous. Consider the following control problem:

$$\text{minimize } \{J(x,v) | (x,v) \in (\mathcal{X}_0 \times \mathcal{V})\}, \tag{2.3}$$

subject to the constraint

$$\dot{x}(t) = v(t), \quad \forall\, t \in [t_0, t_1]. \tag{2.4}$$

Remark. 1: It is apparent that this control problem is equivalent to minimizing the action functional $I(x) := J(x, \dot{x})$ *over* $\mathcal{X}_0$.

To solve problems (2.3) we rely on the following elementary, albeit fundamental, result in the spirit of Lagrange. Let Y be a nonempty set. Consider the minimization of $J: Y \to \overline{R}$, where $\overline{R}$ denotes the extended reals, over the nonempty subset M of Y.

Lemma 1: (Lagrange Lemma) *Let* $\Lambda: Y \to \overline{\mathbb{R}}$ *and let* $y_0 \in M$ *minimize* $J + \Lambda$ *over* Y. *Assume that* $\Lambda(\cdot)$ *is* finite *and* constant *over* M. *Then* y_0 *minimizes* J *over* M.

Proof: For any $y \in M$, we have $J(y_0) + \Lambda(y_0) \leqslant J(y) + \Lambda(y) = J(y) + \Lambda(y_0)$. Hence $J(y_0) \leqslant J(y)$. Q.E.D.

A functional Λ that is constant and finite on M is called the Lagrange functional. For problem (2.3), let

$$M = \{(x,v) \in \mathcal{X}_0 \times \mathcal{V} | \dot{x}(t) = v(t),\ \forall\, t \in [t_0, t_1]\}.$$

We introduce a suitable class of nonlinear Lagrange functionals for our problem. Let $F: [t_0, t_1] \times \mathbb{R}^n \to R$ be of class C^1. Corresponding to such an F, we define the nonlinear functional Λ^F on $\mathcal{X}_0 \times \mathcal{V}$

$$\Lambda^F(x,v) := F(t_1, x(t_1)) - F(t_0, x(t_0)) + \int_{t_0}^{t_1} \left[-\frac{\partial F}{\partial t}(t, x(t)) - v(t) \cdot \nabla F(t, x(t)) \right] dt.$$

When $(x,u) \in M$, by the chain rule, we have $\Lambda^F(x,u) = 0$. Thus, Λ^F is indeed a Lagrange functional for our problem. The solution procedure is now outlined as follows. Consider the unconstrained minimization

$$\min_{(x,v) \in (\mathcal{X}_0 \times \mathcal{V})} (J + \Lambda^F)(x,v). \tag{2.5}$$

We perform two-stage optimization.

Step 1: For each fixed $x \in \mathcal{X}_0$, we try to compute an optimal control v_x^* through *pointwise minimization* of the integrand of $J + \Lambda^F$. More explicitly, consider for each $x \in \mathcal{X}_0$ and each $t \in [t_0, t_1]$ the finite-dimensional problem

$$\min_{v\in\mathbb{R}^n}\left\{\frac{1}{2}mv\cdot v - V(x(t)) - \frac{\partial F}{\partial t}(t,x(t)) - v\cdot\nabla F(t,x(t))\right\}. \tag{2.6}$$

We get

$$v_x^*(t) = \frac{1}{m}\nabla F(t,x(t)). \tag{2.7}$$

We notice that v_x^* belongs to the class of admissible velocities $\mathcal{V}$.

Step 2: Consider now the minimization of the functional

$$\Gamma^F(x) = (J+\Lambda^F)(x,v_x^*)$$

on the space $\mathcal{X}_0$. We have

$$\Gamma^F(x) = -S_1(x(t_1)) + F(t_1,x(t_1)) - F(t_0,x(t_0)) + \int_{t_0}^{t_1}\left[-\frac{\partial F}{\partial t}(t,x(t)) - \frac{1}{2m}\nabla F(t,x(t))\cdot\nabla F(t,x(t)) - V(x(t))\right]dt.$$

If we can find S such that $\Gamma^S(\cdot)$ is actually constant on $\mathcal{X}_0$, then any pair $(x,v_x^*)\in\mathcal{X}_0\times\mathcal{V}$ solves problem (2.5). Then, by Lemma 1, if the pair (x,v_x^*) satisfies

$$\dot{x}(t) = v_x^*(t) = \frac{1}{m}\nabla S[t,x(t)], \quad \forall\, t\in[t_0,t_1],$$

it also solves the original constrained problem (2.3) and (2.4).

Theorem 1: (Ref. 19) *Let $S(t,x)$ be any C^1 solution on $[t_0,t_1]\times\mathbb{R}^n$ of the terminal value problem*

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\nabla S\cdot\nabla S + V(x) = 0, \tag{2.8}$$

$$S(t_1,x) = S_1(x). \tag{2.9}$$

Let $x^*\in\mathcal{X}_0$ be any solution on $[t_0,t_1]$ of

$$\dot{x}(t) = \frac{1}{m}\nabla S(x(t),t). \tag{2.10}$$

Then $\left(x^*, 1/m\,\nabla S(x^*(t),t)\right)$ solves problem (2.3) and (2.4).

Proof: If S satisfies (2.8) and (2.9), we get $\Gamma^S(x)\equiv -S(x_0,t_0)$ on $\mathcal{X}_0$. Q.E.D.

Notice that when a C^1 solution $S(x,t)$ of (2.8) and (2.9) exists, then there are also solutions x of the differential equation (2.10) satisfying $x(t_0)=x_0$, and therefore optimal pairs. In this case, the action functional is actually *minimized*, not just extremized. The difficulty lies, of course, with the terminal value problem (2.8) and (2.9) that, in general, only has a local in t solution **(**namely, on some interval $(\bar{t},t_1), t_0<\bar{t}$**)**.

Remark 2: Let us now assume that S is of class C^2. Following Ref. 9, let us introduce the *acceleration field* $a(t,x)$ through a substantial time derivative

$$a(t,x) := \left[\frac{\partial}{\partial t} + \frac{1}{m}\nabla S\cdot\nabla\right]\left(\frac{1}{m}\nabla S\right)(t,x) = \frac{1}{m}\nabla\left[\frac{\partial S}{\partial t} + \frac{1}{2m}\nabla S\cdot\nabla S\right](t,x).$$

Then, (2.8) implies the local form of Newton's law

$$a(t,x) = -\frac{1}{m}\nabla V(x). \tag{2.11}$$

III. NONHOLONOMIC DYNAMICAL SYSTEMS

Consider a system subject to linear velocity constraints of the form

$$\Omega(x(t))\dot{x}(t) = 0, \quad t \in (t_0,t_1), \tag{3.1}$$

where $\Omega:\mathbb{R}^n \to \mathbb{R}^{k\times n}$, $k<n$ is a continuous map. We assume that for eack $x\in\mathbb{R}^n$, the rows of Ω are linearly independent. These constraints are called *Pfaffian*. A simple example is provided by a disk rolling on a plane without slipping. More complex nonholonomic systems with Pfaffian constraints occur in many problems of robot motion planning and vehicular dynamics, and have therefore been the subject of intensive study, see Refs. 2, 3, and 18 and references therein. Let

$$\Omega(x(t))v(t) = 0, \quad t \in [t_0,t_1]. \tag{3.2}$$

We now study the control problem (2.3), (2.4), and (3.2), namely the same problem as in the previous section when also constraint (3.2) is present. This problem is equivalent to minimizing the action functional

$$I(x) := J(x,\dot{x}) = \int_{t_0}^{t_1} L(x(t),\dot{x}(t))dt - S_1(x(t_1)), \tag{3.3}$$

under the constraints (3.1). Reformulating the calculus of variations problem as a control problem as before, we let

$$M = \{(x,v) \in \mathcal{X}_0 \times \mathcal{V} | \dot{x}(t) = v(t), \quad \Omega(x(t))v(t) = 0, \quad \forall\, t \in [t_0,t_1]\}.$$

Let $F:[t_0,t_1]\times\mathbb{R}^n \to \mathbb{R}$ be of class C^1 and $g:[t_0,t_1]\times\mathbb{R}^n \to R^k$ be continuous. Corresponding to such a pair, we define the nonlinear functional $\Lambda^{F,g}$ on $\mathcal{X}_0\times\mathcal{V}$ by

$$\Lambda^{F,g}(x,v) := F(t_1,x(t_1)) - F(t_0,x(t_0)) + \int_{t_0}^{t_1}\left[-\frac{\partial F}{\partial t}(t,x(t)) - v(t)\cdot\nabla F(t,x(t)) + g(t,x(t))^T\Omega(x(t))v(t)\right]dt.$$

It is apparent that $\Lambda^{F,g}$ is a Lagrange functional for the problem since it is identically zero when (2.4) and (3.2) are satisfied. Following the same procedure as in the previous section, we consider the *unconstrained* minimization of $(J+\Lambda^{F,g})(x,v)$ over $\mathcal{X}_0\times\mathcal{V}$. For $x\in\mathcal{X}_0$ fixed, the pointwise minimization of the integrand of $J+\Lambda^{F,g}$ at time t gives

$$v_x^*(t) = \frac{1}{m}\left[\nabla F(t,x(t)) - \Omega^T(x(t))g(t,x(t))\right]. \tag{3.4}$$

Notice that $v_x^*\in\mathcal{V}$. We consider next the minimization of the functional

$$\Gamma^{F,g}(x) = (J+\Lambda^{F,g})(x,v_x^*)$$

on the space $\mathcal{X}_0$. We have

$$\Gamma^{F,g}(x) = -S_1(x(t_1)) + F(x(t_1),t_1) - F(x(t_0),t_0) + \int_{t_0}^{t_1} \left[-\frac{\partial F}{\partial t}(t,x(t)) - \frac{1}{2m}\| \nabla F(t,x(t)) - \Omega^T(x(t))g(t,x(t))\|^2 - V(x(t)) \right] dt,$$

where $\|\cdot\|$ denotes the Euclidean norm in R^n. Let $S(t,x)$ of class C^1 and $\mu(t,x)$ continuous solve on $R^n \times [t_0,t_1]$ of the initial value problem

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\| \nabla S - \Omega^T \mu\|^2 + V(x) = 0, \tag{3.5}$$

$$S(x,t_0) = S_0(x). \tag{3.6}$$

Then $\Gamma^{S,\mu}(x) \equiv -S(x_0,t_0)$ on $\mathcal{X}_0$. By Lemma 1, if $x \in \mathcal{X}_0$ satisfies for all $t \in [t_0,t_1]$

$$\dot{x}(t) = \frac{1}{m}\left[\nabla S - (t,x(t)) - \Omega^T(x(t))\mu(t,x(t))\right], \tag{3.7}$$

$$\Omega(x(t))\dot{x}(t) = 0, \tag{3.8}$$

then it solves the problem together with the corresponding feedback velocity (3.4).

Remark 3: As in the unconstrained case, we now show that (3.5) implies the second principle of dynamics. Assume that S is of class C^2 and that Ω, and μ are of class C^1. The acceleration field is again obtained through a substantial derivative of the velocity field

$$\begin{aligned} a(t,x) &:= \left[\frac{\partial}{\partial t} + \frac{1}{m}\left[\nabla S - \Omega^T \mu\right] \cdot \nabla \right] \left(\frac{1}{m}\left[\nabla S - \Omega^T \mu\right] \right)(t,x) \\ &= \frac{1}{m}\left\{ \nabla \left[\frac{\partial S}{\partial t} + \frac{1}{2m}\| \nabla S - \Omega^T \mu\|^2 \right] - \frac{\partial (\Omega^T \mu)}{\partial t} \right\}(t,x). \end{aligned}$$

Then, (3.5) yields

$$a(t,x) = -\frac{1}{m} \nabla V(x) - \frac{1}{m}\Omega^T \frac{\partial \mu}{\partial t}. \tag{3.9}$$

Define

$$\lambda(t,x) := -\frac{\partial \mu}{\partial t}(t,x).$$

For $x \in \mathcal{X}_0$ satisfying (3.7) and of class C^2, let $\lambda(t) := \lambda(t,x(t))$. We then get

$$m\ddot{x}(t) = -\nabla V(x(t)) + \Omega^T(x(t))\lambda(t), \tag{3.10}$$

namely Eq. (1.2). By differentiating (3.8), a simple calculation employing (3.10) shows that the Lagrange multipliers λ may be expressed as an instantaneous function of x and $\dot{x}$, see, e.g., Ref. 20, Sec. 2, and Ref. 18, pp. 269–270.

Next we show how the multiplier μ can be also eliminated in our hydrodynamic context. If x satisfies (3.7) and (3.8), then, plugging (3.7) into (3.8), we get

$$\Omega(x(t))\frac{1}{m}\left[\nabla S(t,x(t)) - \Omega^T(x(t))\mu(t,x(t))\right] = 0.$$

Since Ω has full row rank, the latter is equivalent to

$$\mu(t,x(t)) = (\Omega(x(t))\Omega^T(x(t)))^{-1}\Omega(x(t))\,\nabla S(t,x(t)). \tag{3.11}$$

Plugging this into (3.7), we get

$$\dot{x}(t) = \frac{1}{m}[(I - \pi(x(t)))\,\nabla S(t,x(t))], \tag{3.12}$$

where $\pi(t,x)$ is defined by

$$\pi(x) = \Omega^T(x)(\Omega(x)\Omega^T(x))^{-1}\Omega(x). \tag{3.13}$$

Observe that $\pi(x)^2 = \pi(x)$ and $\pi(x)^T = \pi(x)$. Thus, $\pi(x)$ is an orthogonal projection. In fact, $\pi(x)$ is the orthogonal projection onto range $(\Omega^T(x))$.

Remark 4: Notice that (3.12) implies (3.8). Indeed,

$$\Omega(x(t))\dot{x}(t) = \Omega(x(t))\frac{1}{m}[(I - \pi(x(t)))\,\nabla S(t,x(t))] = 0,$$

since $I - \pi(x)$ projects onto the kernel of $\Omega(x)$.

Remark 5: It is apparent that (3.11)–(3.13) are related to the projection technique introduced in Ref. 6. Indeed, there the constrained dynamics is obtained by suitably projecting the free dynamics.

Now we use the freedom we have in picking S and μ. Since (3.11) must be satisfied by an optimal solution, we impose that the pair (S,μ) satisfies *identically* on all of $[t_0,t_1]\times\mathbb{R}^n$

$$\mu(t,x) = (\Omega(x)\Omega^T(x))^{-1}\Omega(x)\,\nabla S(t,x). \tag{3.14}$$

Hence, we can write $\Gamma^S(x)$ instead of $\Gamma^{S,\mu}(x)$, and Eq. (3.5) becomes

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\|(I - \pi)\,\nabla S\|^2 + (x) = 0. \tag{3.15}$$

We are now ready for our main result.

Theorem 2: *For $x\in R^n$, let $\sigma(x) = I - \pi(x)$ denote the orthogonal projection onto* $\ker\,\Omega(x)$. *Let $S(t,x)$ be any C^1 solution on $[t_0,t_1]\times\mathbb{R}^n$ of*

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\,\nabla S\cdot\sigma\,\nabla S + V(x) = 0, \quad S(t_1,x) = S_1(x). \tag{3.16}$$

Then any $x\in\mathcal{X}_0$ satisfying

$$\dot{x}(t) = \frac{1}{m}\sigma(x(t))\,\nabla S(t,x(t)) \tag{3.17}$$

on $[t_0,t_1]$ solves together with

$$v(t) = \frac{1}{m}\sigma(x(t))\,\nabla S(t,x(t))$$

problems (2.3), (2.4), and (3.2). [*Equivalently, such an $x\in\mathcal{X}_0$ minimizes* (3.3) *subject to* (3.1)]. *If S is of class C^2, and $x\in\mathcal{X}_0$ satisfying* (3.17) *is also of class C^2, then x satisfies* Eq. (3.10)

$$m\ddot{x}(t) = -\,\nabla V(x(t)) + \Omega^T(x(t))\lambda(t),$$

with λ given by

$$\lambda(t) = -\,(\Omega(x(t))\Omega^T(x(t)))^{-1}\Omega(x(t))\,\nabla\frac{\partial S}{\partial t}(t,x(t)). \tag{3.18}$$

Proof: If S solves (3.16), we get $\Gamma^S(x)=-S(x_0,t_0)$ for any $x\in\mathcal{X}_0$. Thus any pair $(x,v)\in\mathcal{X}_0\times\mathcal{V}$ solves the unconstrained minimization problem. Since x satisfies (3.17), constraint (2.4) is fulfilled. Moreover, by Remark 4, (3.2) is also satisfied. By Lemma 1, the pair is optimal for the original constrained minimization. Finally, x satisfies (3.10) with λ as in (3.18) in view of Remark 3 and (3.14). Q.E.D.

IV. DISCUSSION

We conclude this paper with a few simple remarks on how the minimization of the modified action leading to the vakonomic equations relates to the problem studied in the preceding section. Assume that $L:\mathbb{R}\times\mathbb{R}^n\times\mathbb{R}^n\to\mathbb{R}$ is of class C^2. Assume, moreover, that S_1 and Ω are of class C^1. Recall

$$I(x):=\int_{t_0}^{t_1} L(t,x(t),\dot{x}(t))dt - S_1(x(t_1))$$

and the constraint (3.1)

$$\Omega(x(t))\dot{x}(t)=0, \quad t\in[t_0,t_1]. \tag{4.1}$$

For $\mathcal{X}$ taking values in $\mathbb{R}^k$ of class C^1, let

$$\mathcal{L}(t,x,\dot{x}):=L(t,x,\dot{x})+\mathcal{X}^T(t)\Omega(x)\dot{x}.$$

Introduce also the modified action

$$\mathcal{I}(x):=\int_{t_0}^{t_1}\mathcal{L}(t,x(t),\dot{x}(t))dt - S_1(x(t_1)). \tag{4.2}$$

Taking as variations paths $y(t)\in C^1[t_0,t_1]$ such that $y(t)=0$, and setting the first variation of $\mathcal{I}$ equal to zero, we get the equations

$$\frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{x}}-\frac{\partial\mathcal{L}}{\partial x}=0, \tag{4.3}$$

$$\frac{\partial\mathcal{L}}{\partial\dot{x}}(t_1,x(t_1),\dot{x}(t_1))=\frac{\partial S_1}{\partial x}(x(t_1)). \tag{4.4}$$

They read

$$\frac{d}{dt}\frac{\partial L}{\partial\dot{x}}-\frac{\partial L}{\partial x}=-\Omega^T\dot{\mathcal{X}}-\mathcal{X}\cdot\Omega'\dot{x}+\frac{\partial}{\partial x}(\mathcal{X}\cdot\Omega\dot{x}), \tag{4.5}$$

$$\frac{\partial L}{\partial\dot{x}}(t_1,x(t_1),\dot{x}(t_1))+\Omega^T(x(t_1)\mathcal{X}(t_1))=\frac{\partial S_1}{\partial x}(x(t_1)), \tag{4.6}$$

where

$$(\mathcal{X}\cdot\Omega'\dot{x})_i=\sum_{\alpha=1}^{k}\mathcal{X}_a\sum_{j=1}^{n}\frac{\partial\Omega_{\alpha i}}{\partial x_j}\dot{x}_j, \quad \frac{\partial}{\partial x}(\mathcal{X}\cdot\Omega\dot{x})_i=\sum_{\alpha=1}^{k}\mathcal{X}_\alpha\sum_{j=1}^{n}\frac{\partial\Omega_{\alpha j}}{\partial x_i}\dot{x}_j.$$

Equation (4.5) together with (4.1) constitute the equations of the Vakonomic dynamics. Moreover, (4.5) and (4.6) are *necessary* conditions for the *unconstrained* minimization of the modified action (4.2) over $\mathcal{X}_0$. If x does minimize (4.2) over $\mathcal{X}_0$ *and* it satisfies (4.1), then, by Lemma 1, it also minimizes $I(x)$ over $\mathcal{X}_0$ subject to (4.1).

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Exact analytic solutions of nonlinear boundary value problems in fluid mechanics (Blasius equations)

D. E. Panayotounakos[a)] and N. B. Sotiropoulos
Division of Mechanics, Department of Applied Mathematical and Physical Sciences, National Technical University of Athens, Athens, Greece

A. B. Sotiropoulou
A.S.PE.T.E. School of Pedagogical and Technological Education, Athens, Greece

N. D. Panayotounakou
Division of Mechanics, Department of Applied Mathematical and Physical Sciences, National Technical University of Athens, Athens, Greece

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In this work it is shown that, by a series of admissible functional transformations, the generalized Blasius equation in fluids can be exactly reduced to a three-term generalized Emden–Fowler equation. Furthermore, the restricted in axisymmetric flows and simplified forms of this equation can be reduced to (i) two-term generalized Emden–Fowler equations; (ii) generalized Emden–Fowler equations; (iii) Emden–Fowler equations of the normal form; and (iv) Abel equations of the second kind. By means of a recently developed mathematical solution methodology (Panayotounakos, Fifth Greek Congress on Mechanics, Xania, Crete, 22–25 June 2004, Hellas, Greece), we provide exact analytic solutions for the simplified as well as for the restricted forms of the above-mentioned Blasius equations. Thus, it is proved that important, unsolvable in exact form problems in nonlinear fluid dynamics now can be analytically solved. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1819528]

I. INTRODUCTION

There is a wide class of particularly basic second-order nonlinear ordinary differential equations (ODEs) in mathematical physics and nonlinear mechanics that does not admit exact analytic solutions in terms of known (tabulated) functions.[1–3] Among these equations, one of great interest in nonlinear fluid dynamics is that related to uniform flow past a semi-infinite plate. The first to introduce and discuss such a problem was Blasius (Ref. 4). He obtained similarity solutions of the well-known simplified Blasius equation. The generalization of the Blasius problem was introduced in Ref. 5, including nonuniform flow. Later, in Ref. 6 the generalized Blasius equation was investigated numerically, and it was proved that if one of its characteristic parameters is positive or zero, then the related convenient boundary conditions are sufficient to define a unique solution; but, when this parameter becomes negative, the property of uniqueness disappears. The more general problem with arbitrary parameters has been the object of study of many researchers.[7,8]

Several relative problems requiring the solution of the generalized Blasius equation (Falkner–Skan equation) were introduced in Ref. 9, investigating axisymmetric flow due to stretching flat surface; in Ref. 10, performing a series method for the solution of laminar boundary layers or moving surfaces; in Ref. 11, developing self-similar solutions describing thermal capillary flows in viscous layers, and in Ref. 12, using similarity solutions of the boundary equations for a stretching wall. All the above problems have to be solved numerically, or in the form of power series for fixed values of the parameters being introduced.

[a)]Electronic mail: tsakstel@central.ntua.gr

This work deals with the possibility of constructing exact analytic solutions concerning the generalized Blasius equation correlated with a wide class of nonlinear boundary value problems in mathematical physics and nonlinear mechanics. Before we address the issue of these solutions, we prove that, by a series of admissible functional transformations, the above-mentioned equation can be reduced to a three-term generalized Emden–Fowler equation, which in axisymmetric cases (restricted form) becomes two-term. In addition, the simplified Blasius equation can be reduced to a typical generalized Emden–Fowler equation, or to an Emden–Fowler equation of the normal form. Both previous types of Emden–Fowler equations, by means of admissible functional transformations, are further reduced to Abel equations of the second kind of the normal form. Thus, it is proved that the unsolvability of the Blasius problems is due to the fact that both Abel and Emden–Fowler equations do not admit exact analytic solutions in terms of known (tabulated) functions. Only very special cases of these equations can be analytically solved in parametric form, which were tabulated in Ref. 3.

Our goal is that, based on a recently developed mathematical technique leading to the construction of analytic solutions of the Abel equation of the second kind of the normal form,[13] we provide exact analytic solutions of the prescribed two types of Blasius equations: (i) the simplified equation, and (ii) the restricted form of the generalized equation (concerning axisymmetric flows), with convenient boundary conditions.

The solution methodology employed is general and can be applied to a large class of other unsolvable nonlinear ODEs in mathematical physics and nonlinear mechanics such as the Duffing nonlinear oscillator (see Ref. 14), the Van der Pol nonlinear oscillator, the Kidder equation in porous media, the Thomas–Fermi and White–Dwarf (Chandrasekhar) equations in thermodynamics and relativistic mechanics, etc.

II. SOME RESULTS OF THE CLASSES OF EMDEN–FOWLER AND ABEL EQUATIONS

There is a wide class of nonlinear ODEs which can be reduced to equations that traditionally attracted the attention of many researchers: those of the simplest appearance but involving the most difficulties for integration (Abel and Emden–Fowler equations). Both these types of equations are in general unsolvable.[3] Recently, a mathematical methodology was developed in Ref. 13 that leads to the construction of exact analytic solutions of the Abel nonlinear ODEs of the second kind.

Before we address the issue of the construction of exact analytic solutions of the Blasius equations in fluids, we will digress to some well-known classes of nonlinear ODEs, and to admissible functional transformations that reduce a class of ODEs to a different class.

A. The Emden–Fowler equation of the normal form

The Emden-Fowler nonlinear ODE of the normal form is

$$y''_{xx} = Ax^n y^m, \tag{2.1}$$

where A and n, m are arbitrary parameters. Here, the notation $y'_x = dy/dx$, $y''_{xx} = d^2y/dx^2, \ldots$ is used for the total derivatives. We note the following regarding the solution of (2.1):[3]

(i) For $m \neq 1$, Eq. (2.1) possesses the following particular solution:

$$y = \lambda x^{(n+2)/(1-m)}, \quad \text{where } \lambda = [(n+2)(n+m+1)/A(m-1)^2]^{1/(m-1)}. \tag{2.2}$$

(ii) The transformations

$$\mathcal{P}: \quad y = w(t)/t, \quad x = 1/t; \quad t \neq 0, \tag{2.3}$$

transform (2.1) into the following equation of different pair of exponents $\{n, m\}$:

$$w''_{tt} = At^{-n-m-3} w^m. \tag{2.4}$$

Equation (2.1) is, in general, unsolvable. Reference 3 discusses all solvable Emden–Fowler equations, e.g., all possible combinations of parameters A, n, and m for which exact solutions can be constructed in parametric form.

B. The generalized Emden–Fowler equation

The generalized Emden–Fowler ODE is

$$y''_{xx} = Ax^n y^m (y'_x)^\ell. \tag{2.5}$$

For $\ell = 0$ it degenerates to the normal Emden–Fowler form (2.1). To analyze Eq. (2.5) we utilize the triad notation $\{n, m, \ell\}$ to denote the specific exponents of the equation. We note the following:

(i) Considering $x = x(y)$ and introducing the $\mathcal{F}$-transformation

$$\mathcal{F}: \quad y'_x = \frac{dy}{dx} = \frac{1}{dx/dy} = \frac{1}{x'_y}, \tag{2.6}$$

we then derive the following alternative generalized Emden–Fowler equation:

$$x''_{yy} = -Ay^m x^n (x'_y)^{3-\ell}. \tag{2.7}$$

The above transformation can be represented in short-hand notation using the triad symbolism

$$\{n, m, \ell\} \overset{\mathcal{F}}{\leftrightarrow} \{m, n, 3-\ell\}.$$

(ii) If $m \neq 0$, $n \neq -1$, and $\ell \neq 1$, the coordinate transformation

$$\mathcal{J}: \quad w(t) = x^{n+1}, \quad t = (y'_x)^{1-\ell}, \tag{2.8}$$

transforms Eq. (2.5) to the following new Emden–Fowler equation:

$$w''_{tt} = Bt^{1/(1-\ell)} w^{-n/(n+1)} (w'_t)^{(2m+1)/m}, \quad \text{where} \quad B = -\frac{m}{m+1}\left[\frac{A(1-\ell)}{n+1}\right]^{1/m}. \tag{2.9}$$

We denote this transformation symbolically as

$$\{n, m, \ell\} \overset{\mathcal{J}}{\leftrightarrow} \left\{\frac{1}{1-\ell}, -\frac{n}{n+1}, \frac{2m+1}{m}\right\}.$$

Different compositions of transformation $\mathcal{F}$ and $\mathcal{J}$ generate six distinct generalized Emden–Fowler equations corresponding to different triad of exponents $\{n, m, \ell\}$ (Ref. 13, p. 301). When the solution of the transformed equation is obtained in the form $w = w(t)$, the solution of the original equation can be obtained in the parametric form

$$x = w^{1/(1+n)}, \quad y = k(w'_t)^{-1/m}; \quad k = [(n+1)/A(1-\ell)]^{1/m}. \tag{2.10}$$

(iii) In the special case when $\ell = 0$ we showed that transformation (2.3) leads to the normal Emden–Fowler equation (2.4), that is

$$\{n, m, 0\} \overset{\mathcal{P}}{\leftrightarrow} \{-n-m-1, m, 0\}.$$

Then, different compositions of transformations $\mathcal{F}$, $\mathcal{J}$, and $\mathcal{P}$ generate 12 distinct generalized Emden–Fowler equations (Ref. 3, p. 302).

(iv) Finally, with $\ell = 0$ and $n = 1$, different compositions of transformation $\mathcal{F}$, $\mathcal{J}$, and $\mathcal{P}$ generate 24 different generalized Emden–Fowler equations (Ref. 3, p. 303).

C. The Abel equation of the second kind

The Abel nonlinear ODE of the second kind is

$$[g_1(x)y + g_0(x)]y'_x = f_2(x)y^2 + f_1(x)y + f_0(x). \tag{2.11}$$

(i) The transformations

$$w = \left(y + \frac{g_0}{g_1}\right)E, \quad \text{where} \quad E = \exp\left(-\int \frac{f_2}{g_1}dx\right), \tag{2.12}$$

reduce (2.11) into the simplified form

$$w'_x = F_1(x)w + F_0(x), \tag{2.13}$$

in which

$$F_1(x) = \left[\left(\frac{g_0}{g_1}\right)'_x + \frac{f_1}{g_1} - 2\frac{g_0 f_2}{g_1^2}\right]E, \quad F_0 = \left(\frac{f_0}{g_1} - \frac{g_0 f_1}{g_1^2} + \frac{g_0^2 f_2}{g_1^3}\right)E^2. \tag{2.14}$$

(ii) With the aid of the substitution

$$\xi = \int F_1(x)dx, \tag{2.15}$$

the simplified Abel equation (2.13) reduces into the following Abel equation of the second kind of the normal form:

$$ww'_\xi - w = F(\xi), \quad \text{where} \quad F(\xi) = \frac{F_0(x)}{F_1(x)}. \tag{2.16}$$

(iii) If the variable coefficients of the original equation (2.11) satisfy the functional relation

$$g_0(2f_2 + g'_{1_x}) = g_1(f_1 + g'_{0_x}), \quad g_1 \neq 0, \tag{2.17}$$

then its general solution is given by the formula

$$\frac{g_1 y^2 + 2g_0 y}{g_1 J} = 2\int \frac{f_0}{g_1 J}dx + C, \tag{2.18}$$

where C is an integration constant and $J(x)$ the integrating factor

$$J(x) = \exp\left(\int \frac{2f_2}{g_1}dx\right). \tag{2.19}$$

The above result is attributed to Julia in 1933 (Ref. 8, p. 27).

(iv) Consider now the special form of the Abel equation (2.11)

$$yy'_x - y = \alpha x + bx^m, \quad m \text{ any number}. \tag{2.20}$$

In Ref. 3 the following result was provided: if $m \neq 1$, $\alpha > -1/4$, and assuming that

$$\alpha = -\frac{(n+2)(n+m+1)}{(2n+m+3)^2}, \quad \text{where} \quad n_{1,2} = \frac{1}{2}\left(\pm\frac{m-1}{\sqrt{1+4\alpha}} - m - 3\right), \tag{2.21}$$

the coordinate transformations

$$x=\xi^{(n+2)/(m-1)}w(\xi),\quad y=\frac{m-1}{2n+m+3}\xi^{(n+2)/(m-1)}\left(\xi w'_{\xi}+\frac{n+2}{m-1}w\right);\quad n=n_{1,2} \tag{2.22}$$

reduce (2.20) to the Emden–Fowler equation of the normal form

$$w''_{\xi\xi}=A\xi^{n}w^{m},\quad \text{where}\quad A=\left(\frac{2n+m+3}{m-1}\right)^{2}b. \tag{2.23}$$

D. Some basic transformations

(i) Consider the Emden–Fowler nonlinear ODE of the normal form

$$y''_{xx}=Ax^{n}y^{m}, \tag{2.24}$$

with $m\neq 1$ and $m\neq -2n-3$. The transformation

$$\xi=\frac{2n+m+3}{m-1}x^{(n+2)/(m-1)}y,\quad u=x^{(n+2)/(m-1)}\left(xy'_{x}+\frac{n+2}{m-1}y\right), \tag{2.25}$$

leads to the Abel equation of the second kind of the normal form

$$uu'_{\xi}-u=-\frac{(n+2)(n+m+1)}{(2n+m+3)^{2}}\xi+A\left(\frac{m-1}{2n+m+3}\right)^{2}\xi^{m}. \tag{2.26}$$

(ii) Consider the generalized Emden–Fowler equation

$$y''_{xx}=Ax^{n}y^{m}(y'_{x})^{\ell}. \tag{2.27}$$

The substitutions

$$z=\frac{x}{y}y'_{x},\quad \upsilon=Ax^{n-\ell+2}y^{m+\ell-1}, \tag{2.28}$$

reduce (2.27) into the following Abel nonlinear ODE of the second kind:

$$(z^{\ell}\upsilon-z^{2}+z)\upsilon'_{z}=[(m+\ell-1)z+n-\ell+2]\upsilon. \tag{2.29}$$

Furthermore, using the new substitution

$$\xi=\upsilon-z^{2-\ell}+z^{1-\ell}, \tag{2.30}$$

Eq. (2.29) leads to the following equation:

$$\xi\xi'_{z}=[(m+2\ell-3)z+n-2\ell+3]z^{-1}\xi+[(m+\ell-1)z^{2}+(n-m-2\ell+3)z-n+\ell-2]z^{1-2\ell}, \tag{2.31}$$

which is of the Abel form (2.13).

III. THE REDUCTION OF THE EQUATIONS OF BLASIUS

By the generalized equation of Blasius we mean the following nonlinear ODE of the third order:

$$y'''_{xxx} + \alpha y y''_{xx} = \beta(y'^2_x - 1), \tag{3.1}$$

where α and β are arbitrary constants. But, α is in general positive and can be set equal to 1 without loss of generality, as one sees from the transformation $y=\lambda z$, $x=\lambda t$, where $\lambda^2\alpha=1$. The boundary conditions of greatest interest are the following:

For $\alpha \neq 1$

$$y(0) = \alpha_1; \quad y'_x(0) = \beta_1; \quad y'_x(x) \to 0, \quad \text{as} \quad x \to \infty, \tag{3.2}$$

or

$$y(0) = \alpha_2; \quad y''_{xx}(0) = \beta_2; \quad y'_x(x) \to 0, \quad \text{as} \quad x \to \infty, \tag{3.3}$$

and for $\alpha=1$

$$y(0) = y'_x(0) = 0, \quad y'_x(x) \to k \quad \text{as} \quad x \to \infty, \tag{3.4}$$

or

$$y(0) = y''_{xx}(0) = 0, \quad y'_x(x) \to k \quad \text{as} \quad x \to \infty. \tag{3.5}$$

Here, k is a constant. When $\beta \geqslant 0$, the last conditions are sufficient to insure a unique solution of the equation (3.1), but this uniqueness fails when $\beta < 0$.[6]

The equation for the case where $\beta=0$ was originally solved by Blasius, Ref. 4, who introduced it in studying the laminar flow of a fluid. Also, the above simplified Blasius equation ($\beta=0$) was investigated in Ref. 16 for the case $\alpha=1/2$ in studying the flow of an electrically conducting fluid up a hot vertical plate in the presence of strong magnetic field normal to the plate. The generalized Blasius equation (3.1), where $\beta \neq 0$, has been the object of Refs. 5–8. Finally, the restricted form of the Blasius equation

$$y'''_{xxx} + \alpha y y''_{xx} - \beta y'^2_x = 0, \tag{3.6}$$

obeying the boundary conditions (3.2) and (3.3), or (3.4) and (3.5), has been the object of study of Refs. 10–12 and 17.

We emphasize that all the above investigations refer mainly to numerical solutions, as well as to approximate ones by series expansions, similarity variables techniques, etc. Furthermore, all previous investigations refer to concrete values of the parameters α and β.

In what follows we provide a reduction methodology concerning the generalized Blasius equation that leads to equation of the Abel or Emden–Fowler forms. This methodology is realistic and usual for deriving exact analytic solutions of the problem under consideration.

Consider the generalized Blasius equation

$$y'''_{xx} + \alpha y y''_{xx} - \beta y'^2_x + \beta = 0;$$

$$0 \leqslant x < +\infty; \quad \alpha_1 \leqslant y < +\infty; \quad y'_x(0) = \beta_1; \quad y'_x(\infty) = 0; \tag{3.7}$$

where α_1, β_1=constants, $\beta_1 > 0$; α=positive constant, β=positive or negative constant.

The substitution

$$y'_x = z(y) \Rightarrow y''_{xx} = z z'_y, \quad y'''_{xxx} = z^2 z''_{yy} + z z'^2_y, \tag{3.8}$$

reduces (3.7) into the second-order nonlinear ODE

$$z^2 z''_{yy} + z z'^2_y + \alpha y z z'_y - \beta z^2 + \beta = 0;$$

$$\alpha_1 \leqslant y < +\infty; \quad z(\alpha_1) = \beta_1; \quad z(\infty) = 0, (z \in [0, \beta_1]). \tag{3.9}$$

Introduce the transformation

$$z(y)=n(\xi),\quad \xi=\xi(y)\Rightarrow z_y'=n_\xi'\xi_y',\quad z_{yy}''=n_{\xi\xi}''\xi_y'^2+n_\xi'\xi_{yy}'', \tag{3.10}$$

and obtain the equation

$$\xi_y'^2n^2n_{\xi\xi}''+\xi_{yy}''n^2n_\xi'+\xi_y'^2nn_\xi'^2+\alpha y\xi_y'nn_\xi'-\beta n^2+\beta=0. \tag{3.11}$$

We define function $n(\xi)$ such that

$$nn_{\xi\xi}''=-n_\xi'^2\Rightarrow(nn_\xi')_\xi'=0\Rightarrow nn_\xi'=1\Rightarrow n(\xi)=\sqrt{2\xi}=z(y);\quad n\neq 0, \tag{3.12}$$

and thus Eq. (3.11) becomes of the following form, performing only the determinable function $\xi(y)$:

$$\sqrt{2\xi}\xi_{yy}''+\alpha y\xi_y'-2\beta\xi+\beta=0;$$

$$\alpha_1\leqslant y<+\infty;\quad \xi(\alpha_1)=\beta_1^2/2;\quad \xi(\infty)=0,(\xi\in[0,\beta_1^2/2]). \tag{3.13}$$

The new substitution

$$\sqrt{2\xi}=\omega\Rightarrow\xi_y'=\omega\omega_y',\quad \xi_{yy}''=\omega\omega_{yy}''+\omega_y'^2, \tag{3.14}$$

transforms (3.13) to the following second-order nonlinear ODE:

$$\omega^2\omega_{yy}''+\omega\omega_y'^2+\alpha y\omega\omega_y'-\beta\omega^2+\beta=0, \tag{3.15}$$

while the $\mathcal{F}$-transformation (2.6) reduces (3.15) to the equation

$$\omega^2y_{\omega\omega}''-\omega y_\omega'=\alpha\omega yy_\omega'^2-\beta\omega^2y_\omega'^3+\beta y_\omega'^3;$$

$$\alpha_1\leqslant y<+\infty;\quad \text{for } y=\alpha_1,\quad \omega=\beta_1;\quad \text{for}\quad y\to\infty,\quad \omega\to 0,(\omega\in[0,\beta_1]). \tag{3.16}$$

Applying again a [similar to (3.10)] transformation, that is setting

$$y(\omega)=\upsilon(s),\quad s=s(\omega),$$

with concrete form

$$s_\omega'=\omega\Rightarrow s=\omega^2/2;\quad \omega\neq 0, \tag{3.17}$$

we obtain the nonlinear ODE

$$\upsilon_s''=\frac{\alpha}{\sqrt{2}}s^{-1/2}\upsilon\upsilon_s'^2-\beta\sqrt{2}s^{1/2}\upsilon_s'^3+\frac{\beta}{\sqrt{2}}s^{-1/2}\upsilon_s'^3;$$

$$\alpha_1\leqslant\upsilon<+\infty;\quad \text{for } \upsilon=\alpha_1,\quad s=\beta_1^2/2;\quad \text{for } \upsilon\to\infty,s\to 0,(s\in[0,\beta_1^2/2]). \tag{3.18}$$

The $\mathcal{F}$-transformation (2.6) on Eq. (3.18) reduces it to the following three-term generalized Emden–Fowler equation:

$$s_{\upsilon\upsilon}''=A\upsilon s^{-1/2}s_\upsilon'+Bs^{1/2}-\frac{B}{2}s^{-1/2};\quad A=-\frac{\alpha}{\sqrt{2}},\quad B=-\beta\sqrt{2};$$

$$\alpha_1\leqslant\upsilon<+\infty;\quad \text{for}\quad s=\beta_1^2/2,\upsilon=\alpha_1;\quad \text{for}\quad s\to 0,\upsilon\to\infty,(s\in[0,\beta_1^2/2]). \tag{3.19}$$

We distinguish now the following two cases:

Case a: $\beta=0$

This case corresponds to the simplified Blasius equation

$$y'''_{xxx} + \alpha y y''_{xx} = 0;$$

$$0 \leqslant x < +\infty; \quad \alpha_1 \leqslant y < +\infty; \quad y'_x(0) = \beta_1; \quad y'_x(\infty) = 0;$$

$$\alpha = \text{positive constant}; \quad \alpha_1, \beta_1 = \text{constants}, \quad \beta_1 > 0. \tag{3.20}$$

The [equivalent to (3.13)] transformed equation becomes a generalized Emden–Fowler equation, that is

$$\xi''_{yy} = A y \xi^{-1/2} \xi'_y; \quad A = -\alpha/\sqrt{2};$$

$$\alpha_1 \leqslant y < +\infty; \quad \xi(\alpha_1) = \beta_1^2/2; \quad \xi(\infty) = 0, (\xi \in [0, \beta_1^2/2]). \tag{3.21}$$

The $\mathcal{F}$-transformation (2.6) reduces (3.21) to the generalized Emden–Fowler equation with a different pair of exponents

$$y''_{\xi\xi} = -A \xi^{-1/2} y (y'_\xi)^2; \quad A = -\alpha\sqrt{2};$$

$$\alpha_1 \leqslant y < +\infty; \quad \text{for} \quad y = \alpha_1, \xi = \beta_1^2/2; \quad \text{for} \quad y \to \infty, \xi \to 0, (\xi \in [0, \beta_1^2/2]), \tag{3.22}$$

while the $\mathcal{J}$-transformation (2.8) with concrete form

$$w(t) = \xi^{1/2}, \quad t = (y'_\xi)^{-1}, \tag{3.23}$$

transforms (3.22) into the following generalized Emden–Fowler equation:

$$w''_{tt} = B t^{-1} w (w'_t)^3; \quad B = 4\alpha\sqrt{2} = -4A;$$

$$0 \leqslant w \leqslant \beta_1/\sqrt{2}. \tag{3.24}$$

When the solution of Eq. (3.24) is obtained in the form $w = w(t)$, the solution of Eq. (3.22) can be written in the parametric form [see Eqs. (2.10)]

$$\xi = w^2, \quad y = \frac{1}{2A}(w'_t)^{-1}; \quad t = \text{parameter};$$

$$\alpha_1 \leqslant y < +\infty; \quad \text{for} \quad y = \alpha_1, \xi = w^2 = \beta_1^2/2; \quad \text{for} \quad y \to \infty, \xi = w^2 \to 0, (\xi \in [0, \beta_1^2/2]). \tag{3.25}$$

Equation (3.24) is directly reducible to the Emden–Fowler equation of the normal form

$$t''_{ww} = -B w t^{-1}; \quad B = 4\alpha\sqrt{2} = -4A;$$

$$0 \leqslant w \leqslant \beta_1/\sqrt{2}. \tag{3.26}$$

The above generalized Emden–Fowler equation (3.21) and (3.22), or the Emden–Fowler equation of the normal form (3.26), can be reduced to an Abel equation of the second kind of the normal form by means of the admissible functional transformations (2.28) and (2.25), respectively. Consider for example the reduced generalized Emden–Fowler equation (3.21). Then, by the transformation (2.28) with concrete form

$$\overset{\star}{z} = \frac{y}{\xi}\xi'_y, \quad \overset{\star}{v} = Ay^2\xi^{-1/2}, \tag{3.27}$$

(3.21) becomes the Abel equation of the second kind

$$(\overset{\star}{v} - \overset{\star}{z} + 1)\overset{\star}{v}'_z = \frac{4 - \overset{\star}{z}}{2\overset{\star}{z}}\overset{\star}{v};$$
$$\text{for} \quad y_0 = \alpha_1, \xi_0 = \beta_1^2/2, \overset{\star}{v}_0 = \sqrt{2}\alpha_1^2 A/\beta_1; \quad \text{for } y_1 \to \infty, \xi_1 \to 0. \tag{3.28}$$

Furthermore, by the transformation (2.12) with concrete form

$$r = \overset{\star}{v} - \overset{\star}{z} + 1, \tag{3.29}$$

Eq. (3.28) results in

$$rr'_{\overset{\star}{z}} = F_1(\overset{\star}{z})r + F_0(\overset{\star}{z});$$

$$F_1(\overset{\star}{z}) = \frac{4 - 3\overset{\star}{z}}{2\overset{\star}{z}}, \quad F_0(\overset{\star}{z}) = \frac{(\overset{\star}{z} - 1)(4 - \overset{\star}{z})}{2\overset{\star}{z}}. \tag{3.30}$$

Finally, the substitution (2.15) with concrete form

$$s = \int F_1(\overset{\star}{z})d\overset{\star}{z} = \int \frac{4 - 3\overset{\star}{z}}{2\overset{\star}{z}}d\overset{\star}{z} = 2\ \ln|\overset{\star}{z}| - \frac{3}{2}\overset{\star}{z}, \tag{3.31}$$

transforms (3.30) to the Abel equation of the normal form

$$rr'_s - r = \frac{F_0(\overset{\star}{z}(s))}{F_1(\overset{\star}{z}(s))};$$

$$\frac{F_0(\overset{\star}{z}(s))}{F_1(\overset{\star}{z}(s))} = \frac{(\overset{\star}{z} - 1)(4 - \overset{\star}{z})}{4 - 3\overset{\star}{z}}; \quad s = 2\ \ln|\overset{\star}{z}| - \frac{3}{2}\overset{\star}{z}. \tag{3.32}$$

When the Abel equation (3.32) is solved (including one constant of integration), then, by the transformation (3.29) one extracts the solution of the Abel equation (3.28) in the form $\overset{\star}{v} = \overset{\star}{v}(\overset{\star}{z})$, and the solution of the generalized Emden–Fowler equation (3.21) can be obtained parametrically as follows.

Using the first part of (3.27), we have

$$\overset{\star}{z}=y\frac{\xi_y'}{\xi}=\frac{y}{\xi}\frac{\xi_{\overset{\star}{z}}'}{y_{\overset{\star}{z}}'}\Leftrightarrow\frac{y_{\overset{\star}{z}}'}{y}=\frac{1}{\overset{\star}{z}}\frac{\xi_{\overset{\star}{z}}'}{\xi},\tag{3.33}$$

while by the second part we extract

$$y^2=\frac{\overset{\star}{\upsilon}\xi^{1/2}}{A}\Leftrightarrow y=\pm\frac{\overset{\star}{\upsilon}^{1/2}\xi^{1/4}}{A^{1/2}},\quad 2yy_{\overset{\star}{z}}'=\frac{1}{A}\left(\overset{\star}{\upsilon}_{\overset{\star}{z}}'\sqrt{\xi}+\overset{\star}{\upsilon}\frac{\xi_{\overset{\star}{z}}'}{2\sqrt{\xi}}\right).\tag{3.34}$$

Combination of the last two relations results in

$$y_{\overset{\star}{z}}'=\pm\frac{1}{2\sqrt{A}}\left(\frac{\overset{\star}{\upsilon}_{\overset{\star}{z}}'}{\sqrt{\overset{\star}{\upsilon}}}\xi^{1/4}+\sqrt{\overset{\star}{\upsilon}}\frac{\xi_{\overset{\star}{z}}'}{2\xi^{3/4}}\right),\tag{3.35}$$

and thus, by way of (3.28), we obtain

$$\frac{y_{\overset{\star}{z}}'}{y}=\frac{1}{2}\left(\frac{4-\overset{\star}{z}}{2\overset{\star}{z}(\overset{\star}{\upsilon}-\overset{\star}{z}+1)}+\frac{\xi_{\overset{\star}{z}}'}{2\xi}\right).\tag{3.36}$$

Both Eqs. (3.33) and (3.36) perform the following equation for $\xi_{\overset{\star}{z}}'$:

$$\frac{1}{2}\left(\frac{4-\overset{\star}{z}}{2\overset{\star}{z}(\overset{\star}{\upsilon}-\overset{\star}{z}+1)}+\frac{\xi_{\overset{\star}{z}}'}{2\xi}\right)=\frac{1}{\overset{\star}{z}}\frac{\xi_{\overset{\star}{z}}'}{\xi}\Leftrightarrow\frac{\xi_{\overset{\star}{z}}'}{\xi}=\frac{1}{\overset{\star}{\upsilon}-\overset{\star}{z}+1}.$$

Consequently, the variables ξ *and* y in transformation (3.27) are given in parametric form as follows:

$$\xi=\exp\left(C+\int\frac{d\overset{\star}{z}}{\overset{\star}{\upsilon}-\overset{\star}{z}+1}\right);$$

$$y=\pm\frac{\overset{\star}{\upsilon}^{1/2}}{A^{1/2}}\left[\exp\left(C+\int\frac{d\overset{\star}{z}}{\overset{\star}{\upsilon}-\overset{\star}{z}+1}\right)\right]^{1/4};\tag{3.37}$$

$\overset{\star}{\upsilon}=\overset{\star}{\upsilon}(\overset{\star}{z})$=the solution of the Abel equation (3.28) including one constant of integration;

$$\overset{\star}{z}=\text{parameter};C=\text{integration constant}.$$

Equations (3.37) consist the intermediate integral of the simplified Blasius equation (3.20), that is, the solution of the problem under consideration in the phase plane. The solution to the original Blasius equation (3.20) also can be obtained parametrically by means of (i) Eq. (3.12), giving $z(y)=\sqrt{2\xi}$ [y and ξ as in (3.37)] ; (ii) the transformation (3.10), giving $z(y)=n(\xi)=\sqrt{2\xi}$; and (iii) by the substitution (3.8), which permits us to write $dy/z(y)=dy/\sqrt{2\xi}=dx$.

Summarizing, the exact analytic solution of the simplified Blasius equation (3.20) in parametric form is given by the following equations:

$$y = \pm \frac{\overset{\star}{v}^{1/2}}{A^{1/2}} \left[\exp\left(C + \int \frac{d\overset{\star}{z}}{\overset{\star}{v} - \overset{\star}{z} + 1} \right) \right]^{1/4};$$

$$x = \pm \int \frac{\overset{\star}{v}^{1/2}}{\sqrt{2}A^{1/2}} \left[\exp\left(C + \int \frac{d\overset{\star}{z}}{\overset{\star}{v} - \overset{\star}{z} + 1} \right) \right]^{-1/4} \left(\overset{\star}{v}'_{\overset{\star}{z}} + \frac{1}{4(\overset{\star}{v} - \overset{\star}{z} + 1)} \right) d\overset{\star}{z} + \overset{\star}{C};$$

$$C, \overset{\star}{C} = \text{integration constants}; \tag{3.38}$$

$\overset{\star}{v}(\overset{\star}{z})$=the solution of the Abel equation (3.28) including a third constant of integration;

$$\overset{\star}{z} = \text{parameter}.$$

Case b: $\beta \neq 0$

This case corresponds to the generalized Blasius equation (3.1). We shall consider here the restricted form of this equation, that is, Eq. (3.6) governing axisymmetric flows due to stretching flat surfaces. We have already proved that this equation can be reduced to a two-term generalized Emden–Fowler equation, namely

$$s''_{vv} = A v s^{-1/2} s'_v + B s^{1/2}; \quad A = -\frac{\alpha}{\sqrt{2}}, \quad B = -\beta\sqrt{2};$$

$$\alpha_1 \leqslant v < +\infty; \quad \text{for} \quad s = \beta_1^2/2, v = \alpha_1; \quad \text{for} \quad s \to 0, v \to \infty \quad (s \in [0, \beta_1^2/2]). \tag{3.39}$$

Transformation of (2.28) with concrete form

$$\overset{\star}{z} = v\frac{s'_v}{s}, \quad \overset{\star}{t} = A v^2 s^{-1/2}, \tag{3.40}$$

furnishes the results

$$d\overset{\star}{z} = \left(\frac{s'_v}{s} + v\frac{s''_{vv}}{s} - v\frac{s'^2_v}{s^2} \right) dv; \quad d\overset{\star}{t} = A\frac{4vs - v^2 s'_v}{2s^{3/2}} dv.$$

Because of (3.40), these last relations formulate the following equation:

$$\overset{\star}{z}_{\overset{\star}{t}} = 2\frac{\overset{\star}{z} + v^2\frac{s''_{vv}}{s} - \frac{z^2}{v}}{(4 - \overset{\star}{z})\overset{\star}{t}}. \tag{3.41}$$

Solving (3.41) for s''_{vv} and introducing to the resulting new equation the expression (3.39), one obtains

$$s''_{vv} = [(4 - \overset{\star}{z})\overset{\star}{t}\overset{\star}{z}'_t - 2\overset{\star}{z} + 2\overset{\star}{z}^2]\frac{s}{2v^2} = A v s^{-1/2} s'_v + B s^{1/2},$$

which, by means of (3.39), becomes

$$[(4-\overset{\star}{z})\overset{\star}{t}\overset{\star}{z}'_{\overset{\star}{t}}-2\overset{\star}{z}+2\overset{\star}{z}^2]\frac{A}{2\overset{\star}{t}}=A\overset{\star}{z}+B. \tag{3.42}$$

This is an Abel equation of the second kind of the normal form

$$(\overset{\star}{z}-4)\overset{\star}{z}'_{\overset{\star}{t}}=\frac{2}{t}\overset{\star}{z}^2-A\left(1+\frac{1}{\overset{\star}{t}}\right)\overset{\star}{z}-\frac{2B}{A};$$

$$\text{for}\quad \upsilon_0=\alpha_1,\quad s_0=\beta_1^2/2,\quad \overset{\star}{t}_0=\sqrt{2}\alpha_1^2A/\beta_1;\quad \text{for}\quad \upsilon_1\to\infty,s_1\to 0. \tag{3.43}$$

By the transformation

$$r=(\overset{\star}{z}-4)\exp\left(-\int\frac{2}{\overset{\star}{t}}d\overset{\star}{t}\right)=\frac{(\overset{\star}{z}-4)}{\overset{\star}{t}^2}, \tag{3.44}$$

(3.43) is reduced to

$$r\overset{\star}{r}'_{\overset{\star}{t}}=F_1(\overset{\star}{t})r+F_0(\overset{\star}{t});$$

$$F_1(\overset{\star}{t})=-\frac{A(\overset{\star}{t}+1)+16}{\overset{\star}{t}},\quad F_0(\overset{\star}{t})=-\frac{2B\overset{\star}{t}-32A+4A^2(1+\overset{\star}{t})}{A\overset{\star}{t}}. \tag{3.45}$$

Finally, the substitution

$$s=-\int\frac{A(\overset{\star}{t}-1)+16}{\overset{\star}{t}}d\overset{\star}{t}=-A\overset{\star}{t}-(A+16)\ln|\overset{\star}{t}|, \tag{3.46}$$

transforms (3.45) to the following Abel equation of the second kind of the normal form:

$$rr'_s-r=\frac{F_0(\overset{\star}{t}(s))}{F_1(\overset{\star}{t}(s))}=\frac{2B\overset{\star}{t}-32A+4A^2(1+\overset{\star}{t})}{A[A(1+\overset{\star}{t})+16]};\quad s=-A\overset{\star}{t}-(A+16)\ln|\overset{\star}{t}|. \tag{3.47}$$

When the solution of the Abel equation (3.47) is obtained in the form $r=r(s)$ (including one constant of integration), the solution of Eq. (3.43) can be expressed by means of the transformation (3.44) as $\overset{\star}{z}=\overset{\star}{z}(\overset{\star}{t})$ and thus, the solution to the original Emden–Fowler equation (3.39) can be constructed parametrically as follows.

By the first part of (3.40), one obtains

$$\overset{\star}{z}=\upsilon\frac{s'_\upsilon}{s}=\frac{\upsilon}{s}\frac{\overset{\star}{s}'_{\overset{\star}{t}}}{\upsilon'_{\overset{\star}{t}}}\Leftrightarrow\frac{\upsilon'_{\overset{\star}{t}}}{\upsilon}=\frac{1}{\overset{\star}{z}}\frac{\overset{\star}{s}'_{\overset{\star}{t}}}{s}, \tag{3.48}$$

while by the second of these equations we extract

$$\upsilon^2=\frac{\overset{\star}{t}}{A}s^{1/2}\Leftrightarrow 2\upsilon\upsilon'_{\overset{\star}{t}}=\frac{1}{A}\left(s^{1/2}+\frac{\overset{\star}{t}s'_t}{2s^{1/2}}\right). \tag{3.49}$$

Combination of the last two relations results in

$$\overset{\star}{v}{}'_{\overset{\star}{t}} = \pm \frac{1}{2\sqrt{A}}\left(\frac{s^{1/4}}{\overset{\star}{t}{}^{1/2}} + \frac{\overset{\star}{t}{}^{1/2}\overset{\star}{s}{}'_{\overset{\star}{t}}}{2s^{3/4}}\right), \tag{3.50}$$

and thus

$$\frac{\overset{\star}{v}{}'_{\overset{\star}{t}}}{v} = \frac{1}{2}\left(\frac{1}{\overset{\star}{t}} + \frac{s'_t}{2s}\right). \tag{3.51}$$

Introducing expression (3.51) into (3.48), we perform the following equation for $\overset{\star}{s}{}'_{\overset{\star}{z}}$:

$$\frac{1}{2\overset{\star}{t}} + \frac{\overset{\star}{s}{}'_{\overset{\star}{t}}}{4s} = \frac{1}{\overset{\star}{z}}\frac{\overset{\star}{s}{}'_{\overset{\star}{t}}}{s} \Leftrightarrow \frac{\overset{\star}{s}{}'_{\overset{\star}{t}}}{s} = \frac{2\overset{\star}{z}}{\overset{\star}{t}(4-\overset{\star}{z})}. \tag{3.52}$$

Consequently, both s and v in transformation (3.40) are given parametrically as follows:

$$s = \exp\left(C + \int \frac{2\overset{\star}{z}}{\overset{\star}{t}(4-\overset{\star}{z})}d\overset{\star}{t}\right);$$

$$v = \pm \frac{\overset{\star}{t}{}^{1/2}}{A^{1/2}}\left[\exp\left(C + \int \frac{2\overset{\star}{z}}{\overset{\star}{t}(4-\overset{\star}{z})}d\overset{\star}{t}\right)\right]^{1/4}; \tag{3.53}$$

$\overset{\star}{z} = \overset{\star}{z}(\overset{\star}{t})$ = solution of the Abel equation (3.43) including one constant of integration;

$$C = \text{integration constant}; \quad \overset{\star}{t} = \text{parameter}.$$

The solution to the original Blasius equation (3.6) follows the same exactly steps as in case (a).

Summarizing, the simplified Blasius equation (3.20) was reduced: (i) to the generalized Emden–Fowler equations (3.21) and (3.22); (ii) to the Emden–Fowler equation of the normal form (3.26), and (iii) to the Abel equation of the second kind of the normal form (3.32). In addition, the restricted form of the generalized Blasius equation (3.6) was reduced: (i) to the two-term generalized Emden–Fowler equation (3.39), and (ii) to the Abel equation of the second kind of the normal form (3.47). In addition, the solution to the original Blasius equations can be obtained parametrically, as Eqs. (3.38) and (3.53) show. This presupposes the construction of the solution of the Abel equations (3.32) and (3.47), respectively.

In what follows, based on the mathematical construction briefly discussed in Ref. 13, we provide the exact analytic solution of the Abel equation of the second kind of the normal form $yy'_x - y = F(x)$, which consists of the fundamental ODE of the above-mentioned prescribed reduction procedure.

IV. EXACT ANALYTIC SOLUTION OF THE ABEL EQUATION, $yy'_x - y = F(x)$

Before we address the issue of the construction of exact analytic solutions to the Abel ODE of the second kind of the normal form, we will provide a mathematical result given by Julia in 1933 (see Ref. 2, p. 27) concerning the exact solution of an Abel nonlinear ODE of the second kind. According to this result, if the variable coefficients of the equation

$$[g_1(x)y + g_0(x)]y'_x = f_2(x)y^2 + f_1(x)y + f_0(x) \tag{4.1}$$

satisfy the functional relation

$$g_0(2f_2 + g'_{1_x}) = g_1(f_1 + g'_{0_x}), \quad g_1 \neq 0, \tag{4.2}$$

then there exists its general solution, given by the formula

$$\frac{g_1y^2 + 2g_0y}{g_1J} = 2\int \frac{f_0}{g_1J}dx + C, \tag{4.3}$$

where C is an integration constant and J the integrating factor $J(x)=\exp[\int(2f_2/g_1)dx]$.

Consider the Abel equation of the second kind of the normal form

$$yy'_x - y = F(x), \tag{4.4}$$

where $F(x)$ is an arbitrary smooth function of the variable x. We introduce the functional transformation

$$y(x) = f_1(x)n(\xi), \quad \xi = \xi(x), \tag{4.5}$$

which reduces (4.4) to the form

$$f_1^2\xi'_x nn'_\xi + f_1f'_{1_x}n^2 - f_1n = F. \tag{4.6}$$

Here, $f_1(x)$, $\xi(x)$, and $n(\xi)$ are to be determined. Introducing a new function $g(x)$, one rewrites (4.6) as

$$(f_1^2\xi'_x n + g)n'_\xi - 2F = (-f_1^2\xi'_x n + g)n'_\xi - 2f_1f'_{1_x}n^2 + 2f_1n. \tag{4.7}$$

The last equation splits into the following two equations:

$$(f_1^2\xi'_x n + g)n'_\xi - 2F = G(x), \tag{4.8}$$

$$(-f_1^2\xi'_x n + g)n'_\xi - 2f_1f'_{1_x}n^2 + 2f_1n = G(x). \tag{4.9}$$

Here, $g(x)$ and $G(x)$ are also arbitrary smooth functions to be determined. We develop now the following steps.

1st step: We apply Julia's construction on the Abel equation (4.8) and obtain, after integration, the following results:

$$g = f_1^2\xi'_x; \tag{4.10}$$

$$n^2 + 2n - 8\int \frac{G + 2F}{f_1^2}dx + C = 0, \tag{4.11}$$

where C is an integration constant.

2nd step: Similarly, we apply Julia's construction on the Abel equation (4.9) and obtain, after integration, the following results:

$$f_1 = (x + 2\lambda)/2; \quad n^2 - 2n + \frac{8}{(x+2\lambda)^4}\int (x+2\lambda)^2G(x)dx - \frac{\overset{\star}{C}}{(x+2\lambda)^4} = 0, \tag{4.12}$$

where λ is a parameter and $\overset{\star}{C}$ is a new constant of integration.

The problem under consideration demands that from the already introduced three constants of integration λ, C, and $\overset{\star}{C}$ only one exists. If $\lambda=0$, then $f_1(x)=x/2$, and supposing that the original Abel equation (4.4) obeys the condition for $x=0$, $y(0)=y_0\neq 0$, by (4.5) we admit the result $y_0=0\cdot n(\xi_0)=0$. This is unacceptable, and thus one concludes that $\lambda\neq 0$ and $C=\overset{\star}{C}=0$.

Summarizing, the obtained results are the following:

$$f_1(x)=\frac{x+2\lambda}{2},\quad \frac{g(x)}{\xi_x'(x)}=f_1^2, \tag{4.13}$$

$$n^2+2n-8\int\frac{G+2F}{(x+2\lambda)^2}dx=0,\quad n^2-2n+\frac{8}{(x+2\lambda)^4}\int(x+2\lambda)^2G\,dx=0, \tag{4.14}$$

where $g(x)$, $\xi(x)$, and $G(x)$ are to be determined $(x\neq -2\lambda)$.

3rd step: In what follows we are able to construct an exact analytic solution of the problem under consideration, that is of the original Abel equation (4.4). Supposing, without loss of generality, real roots of the last two equations (4.14), solving them for n, and equating the results we deduce the unique relation

$$\sqrt{1+8\int\frac{G}{\omega}dx+16\int\frac{F}{\omega}dx}=2+\sqrt{1-\frac{8}{\omega^2}\int\omega G\,dx}, \tag{4.15}$$

where

$$\omega=(x+2\lambda)^2=(2f_1)^2. \tag{4.16}$$

We rewrite (4.15) in the form

$$\sqrt{\omega^2-M(x)}=\omega\sqrt{1+N(x)}-2\omega, \tag{4.17}$$

with

$$M(x)=8\int\omega G\,dx,\quad N(x)=8\int\frac{G}{\omega}dx+16\int\frac{F}{\omega}dx, \tag{4.18}$$

and, since $M_x'=8\omega G$, $N_x'=8(G/\omega)+16(F/\omega)$, squaring and differentiating (4.17), one extracts the equation

$$6\omega\omega_x'+M_x'+2(1+N)\omega\omega_x'+\omega^2N_x'-8\sqrt{1+N}\omega\omega_x'-2\omega^2\frac{N_x'}{\sqrt{1+N}}=0. \tag{4.19}$$

Finally, introducing M_x' and N_x' by way of (4.18) into the last relation, we perform the following cubic equation for $(1+N)^{1/2}$:

$$(1+N)^{3/2}-4(1+N)+\left[3+\frac{4(G+F)}{x+2\lambda}\right](1+N)^{1/2}-4\frac{G+2F}{x+2\lambda}=0. \tag{4.20}$$

The substitution

$$(1+N)^{1/2}=\overline{N}+\tfrac{4}{3}, \tag{4.21}$$

transforms (4.20) to the Cardan form

$$\overline{N}^3+p\overline{N}+q=0, \tag{4.22}$$

where

$$p=-\frac{\boldsymbol{a}^2}{3}+b,\quad q=2\left(\frac{\boldsymbol{a}}{3}\right)^3-\frac{\boldsymbol{a}b}{3}+c,\quad \boldsymbol{a}=-4,\quad b=3+\frac{4(G+F)}{x+2\lambda},\quad c=-\frac{4(G+2F)}{x+2\lambda}. \tag{4.23}$$

It is well known that the solution of the cubic equation (4.22) can be expressed in analytic form, depending on the sign of the discriminant

$$Q=\left(\frac{p}{3}\right)^3+\left(\frac{q}{2}\right)^2. \tag{4.24}$$

When $Q<0$, (4.22) possesses three real roots, whereas when $Q>0$ there exists a single real root and a complex conjugate pair of roots. The case $Q=0$ furnishes three real roots, two of which are equal. Based on these observations and noting that only real roots are of interest, we list the specific forms of the roots of (4.22) as follows:

Case 1: $Q<0$ $(p<0)$,

$$N(x)=\left(\overline{N}(x)+\frac{4}{3}\right)^2-1;$$

$$\overline{N}_1(x)=2\sqrt{-\frac{p}{3}}\cos\frac{a}{3},\quad \overline{N}_2(x)=2\sqrt{-\frac{p}{3}}\cos\frac{a-\pi}{3},\quad \overline{N}_3(x)=-2\sqrt{-\frac{p}{3}}\cos\frac{a+\pi}{3};$$

$$\cos a=-\frac{q}{2\sqrt{-\left(\frac{p}{3}\right)^3}};\quad 0<a<\pi,\quad p,q \text{ as in (4.23)}, \tag{4.25}$$

Case 2: $Q>0$,

$$N(x)=\left(\overline{N}(x)+\frac{4}{3}\right)^2-1;\quad \overline{N}(x)=\sqrt[3]{-\frac{q}{2}+\sqrt{Q}}+\sqrt[3]{-\frac{q}{2}-\sqrt{Q}},\quad p,q \text{ as in (4.23)}. \tag{4.26}$$

Case 3: $Q=0$,

$$N(x)=\left(\overline{N}(x)+\frac{4}{3}\right)^2-1;\quad \overline{N}_1(x)=2\sqrt[3]{-\frac{q}{2}},\quad \overline{N}_2(x)=\overline{N}_3(x)=-\sqrt[3]{-\frac{q}{2}},\quad p,q \text{ as in (4.23)}. \tag{4.27}$$

By now the problem can be solved according to the following procedure.

a) Combination of the second of Eqs. (4.18) together with the substitution (4.21) results in

$$N(x)=8\int\frac{G+2F}{\omega}=\left[N(x)+\frac{4}{3}\right]^2-1. \tag{4.28}$$

Furthermore, Eq. (4.17), together with the second part of (4.14), yields the expressions

$$\sqrt{1-\frac{M}{\omega^2}}=\sqrt{1+N}-2,\quad (n-1)^2=1-\frac{M}{\omega^2}, \tag{4.29}$$

by means of which we extract the equation

$$\sqrt{1+8\int\frac{G+2F}{\omega}dx}=2+(n-1). \tag{4.30}$$

Thus, combining (4.28) and (4.30), one obtains the following solution for $n(x)$:

$$n(x)=\overline{N}(x)+\tfrac{1}{3}=[N(x)+1]^{1/2}-1, \tag{4.31}$$

where $\overline{N}(x)$ as in Eqs. (4.25)–(4.27). Since $N(x)$ has been evaluated already in (4.28), the subsidiary function $M(x)$ provided in (4.18) also can be evaluated.

Summarizing, we perform the following solutions:

$$n(x)=\overline{N}+\tfrac{1}{3}=\sqrt{1+N}-1,$$

$$N(x)=8\int\frac{G+2F}{(x+2\lambda)^2}dx=\left(\overline{N}+\frac{4}{3}\right)^2-1,$$

$$\frac{M(x)}{(x+2\lambda)^4}=\frac{8}{(x+2\lambda)^4}\int(x+2\lambda)^2Gdx=-\left(\overline{N}+\frac{1}{3}\right)\left(\overline{N}-\frac{5}{3}\right),$$

$$\overline{N}(x)\quad\text{as in Eqs. (4.25) to (4.27).} \tag{4.32}$$

Note that both $N(x)$ and $M(x)$ denote integrals, and they are expressed in terms of the unknown subsidiary function $G(x)$, which is to be determined.

b) It is easy now to show that the already constructed solution $n(x)$ in Eq. (4.31) verifies all the transformed Abel equations (4.6), (4.8), and (4.9) if and only if the derivative $\overline{N}'_x$ of the function $\overline{N}(x)$ is given by the differentiation of the second of (4.32). In other words, the set

$$n=\overline{N}+\frac{1}{3},\quad \overline{N}'_x=\frac{4(G+2F)}{(x+2\lambda)^2\left(\overline{N}+\frac{4}{3}\right)} \tag{4.33}$$

verifies all the aforementioned Abel equations.

Indeed, introducing (4.33) together with the expression for $f_1(x)$ given in (4.12) into the above Abel equations, simultaneously setting $\xi'_x=1$ ($\xi=x$), we extract the cubic equations (4.20). For example, Eq. (4.9) provides

$$(\sqrt{1+N}-2)\frac{2(G+2F)}{x+2\lambda}=-(\sqrt{1+N}-1)^2\sqrt{1+N}+2(\sqrt{1+N}-1)\sqrt{1+N}-\frac{2G}{x+2\lambda}\sqrt{1+N},$$

while Eq. (4.6) also provides

$$(\sqrt{1+N}-1)\frac{4(G+2F)}{(x+2\lambda)\sqrt{1+N}}=-(\sqrt{1+N}-1)^2+2(\sqrt{1+N}-1)+\frac{4F}{x+2\lambda},$$

which coincide with the cubic equation (4.20).

This leads to a similar result for the original Abel equation (4.4). Thus, the solution of the original Abel equation can be written

$$y(x)=\tfrac{1}{2}(x+2\lambda)[\overline{N}(x)+\tfrac{1}{3}], \tag{4.34}$$

where $\overline{N}(x)$ is given in Eqs. (4.25)–(4.27) in terms of the unknown subsidiary function $G(x)$.

c) In determining $G(x)$ we refer to the set (4.33) together with the Abel equation (4.8), or (4.9), or equivalently with the following equivalent system of equations resulting from these Abel equations:

$$(f_1 f_x' n^2 - f_1 n - F)(n+1) + n(G+2F) = 0, \tag{4.35}$$

$$n_x' = \frac{f_{1_x}'}{f_1} n^2 - \frac{1}{f_1} n + \frac{F+G}{f_1^2}. \tag{4.36}$$

The functional relation (4.35) together with first part of (4.33) leads to the cubic equation (4.20). On the other hand, the Riccati equation (4.36), by means of the set (4.33), results also in the cubic equation (4.20). This means that $n(x)=\overline{N}+1/3$ is a solution of (4.36) if and only if $\overline{N}_x'=4(G+2F)/(x+2\lambda)^2(\overline{N}+4/3)$.

By the functional transformation

$$n(x) - 1 = \overline{N}(x) - \tfrac{2}{3} = \overline{H}(\overline{\xi}), \quad \overline{\xi} = \ln|x+2\lambda|, \tag{4.37}$$

we reduce the Riccati equation (4.36) to the normal form

$$\overline{H}_{\xi}' = \overline{H}^2 - [1 - 4(G+F)e^{-\overline{\xi}}]. \tag{4.38}$$

Thus, according to the above results, a solution of the Riccati equation (4.38) is given by the following set of equations:

$$\overline{H}(\xi) = \overline{N} - \tfrac{2}{3}, \quad \overline{N}_{\xi}' = \frac{4(G+2F)}{\overline{N} + \frac{4}{3}} e^{-\overline{\xi}}. \tag{4.39}$$

It is well known (see Refs. 2 and 3), that if $\overline{N}-2/3$ is a solution of (4.38), then the general solution is given by the formula

$$\overline{H}_{\mathbb{R}}(\overline{\xi}) = \overline{N}(\overline{\xi}) - \frac{2}{3} + \frac{\phi(\overline{\xi})}{C - \int_0^{\overline{\xi}} \phi(\overline{\xi}) d\overline{\xi}}, \quad \phi(\overline{\xi}) = \exp\left(2\int_0^{\overline{\xi}} \left(\overline{N} - \frac{2}{3}\right) d\overline{\xi}\right);$$

$$\overline{N}_{\overline{\xi}}' = \frac{4(G+2F)e^{-\overline{\xi}}}{\overline{N} + \frac{4}{3}}, \quad C = \text{integration constant}. \tag{4.40}$$

For verification, inserting the quantities

$$\overline{H}_{\mathbb{R}} = \overline{N} - \tfrac{2}{3} + A, \quad A = \frac{\phi}{\left(C - \int_0^{\overline{\xi}} \phi \, d\xi\right)}, \tag{4.41}$$

into Eq. (4.38), we obtain

$$\overline{N}_{\overline{\xi}}' - (\overline{N} - \tfrac{2}{3})^2 + 1 - 4(G+F)e^{-\overline{\xi}} = -A_{\overline{\xi}}' + A^2 + 2(\overline{N} - \tfrac{2}{3})A. \tag{4.42}$$

By means of the expression for $\overline{N}_{\overline{\xi}}'$ given in (4.40), the left-hand side of the last equation results in the cubic form (4.20), which is identically equal to zero. On the other hand, the right-hand side, which is a Bernoulli equation for A, is also identically equal to zero, since the quantity A given in (4.41) is the general solution of this Bernoulli equation.

Furthermore, the same set of equations (4.41), together with the third part of (4.40), must be the solution of the Abel equation (4.6), which in the $(\overline{\xi},\overline{H})$–coordinates can be written as

$$(\overline{H}+1)\overline{H}'_{\overline{\xi}} = -\overline{H}^2 + 1 + 4Fe^{-\overline{\xi}}. \tag{4.43}$$

Introducing (4.41) into (4.43), we obtain

$$(\overline{N}-\tfrac{2}{3}+1)\overline{N}'_{\overline{\xi}} + (\overline{N}-\tfrac{2}{3})^2 - 1 - 4Fe^{-\overline{\xi}} = -(\overline{N}-\tfrac{2}{3}+1)A'_{\overline{\xi}} - A(\overline{N}'_{\overline{\xi}} + A'_{\overline{\xi}}) - A^2 - 2(\overline{N}-\tfrac{2}{3})A. \tag{4.44}$$

The left-hand side of this equation is identically equal to zero, since, by means of the third part of Eqs. (4.40), the cubic form (4.20) results. Thus, the right-hand side becomes

$$(\overline{N}-\tfrac{2}{3}+A+1)A'_{\overline{\xi}} + A\overline{N}'_{\overline{\xi}} + A^2 + 2(\overline{N}-\tfrac{2}{3})A = 0,$$

which, by way of the second part of (4.40), yields the equation

$$(\overline{N}-\tfrac{2}{3}+A+1)A'_{\overline{\xi}} + A^2 + \left[2\left(\overline{N}-\frac{2}{3}\right) + \frac{4(G+2F)e^{-\overline{\xi}}}{\overline{N}+\dfrac{4}{3}}\right]A = 0. \tag{4.45}$$

Introducing $A'_{\overline{\xi}}$ by means of (4.42), taking into account substitution (4.21), and manipulating accordingly, we extract the following cubic equation for $[1+\overline{N}(x)]$:

$$2(1+N)^{3/2} + (3A-4)(1+N) + (A^2-4A)(1+N)^{1/2} + 4(G+2F)e^{-\overline{\xi}} = 0. \tag{4.46}$$

Both cubic equations (4.20) and (4.46) are sufficient for the elimination of N and the evaluation of the subsidiary unknown function G in terms of the second member F of the original Abel equation (4.4), a fact that also ensures the general solution of this Abel equation. But, since Eq. (4.46) is a strongly nonlinear integral equation, this elimination seems to be in general impossible.

However, for the elimination of the function G and thus the construction of an exact analytic solution of the original Abel equation (4.4), one defines a functional relation by the following procedure. We seek a solution for the Riccati equation (4.38) such that

$$\lim_{\overline{\xi}\to+\infty} \overline{H}_{\mathbb{R}}(\overline{\xi}) = \lim_{\overline{\xi}\to+\infty} [\overline{N}(\overline{\xi}) - \tfrac{2}{3}]; \quad \lim_{\overline{\xi}\to-\infty} \overline{H}_{\mathbb{R}}(\overline{\xi}) = \lim_{\overline{\xi}\to-\infty} [\overline{N}(\overline{\xi}) - \tfrac{2}{3}]. \tag{4.47}$$

These assertions by way of (4.40) ensure the equations

$$\lim_{\overline{\xi}\to+\infty} \int_0^{\overline{\xi}} \varphi'_{\overline{\xi}} d\overline{\xi} = 0, \quad \lim_{\overline{\xi}\to-\infty} \int_0^{\overline{\xi}} \varphi'_{\overline{\xi}} d\overline{\xi} = 0,$$

that is, the equation

$$\int_{-\infty}^{+\infty} \varphi'_{\overline{\xi}} d\overline{\xi} = 0. \tag{4.48}$$

It is also well known [see Ref. 15, p. 406 (3.722.8)], that

$$\int_{-\infty}^{+\infty} \frac{\cos(a\overline{\xi})}{\beta - \overline{\xi}} = \pi \sin(a\beta), \quad a > 0.$$

Setting $a=1$ and $\beta=0$, the above integral becomes

$$\int_{-\infty}^{+\infty} -\frac{\cos\overline{\xi}}{\overline{\xi}}d\overline{\xi}=0. \tag{4.49}$$

Combination of (4.48) and (4.49) results in

$$\varphi'_{\overline{\xi}}=-\frac{\cos\overline{\xi}}{\overline{\xi}},$$

and thus [Ref. 15, p. 187 (2.641.2); p. 928 (8.23)], one defines

$$\varphi=\mathrm{ci}(\overline{\xi}),$$

$$\mathrm{ci}(\overline{\xi})=-\int_{\overline{\xi}}^{+\infty}\frac{\cos t}{t}dt=\mathbb{C}+\ln\overline{\xi}+\int_{0}^{\overline{\xi}}\frac{\cos t-1}{t}dt=\text{the cosine integral};$$

$$\mathrm{ci}(\overline{\xi})=\mathbb{C}+\ln\overline{\xi}+\sum_{\nu=1}^{\infty}(-1)^{\nu}\frac{\overline{\xi}^{2\nu}}{(2\nu)(2\nu)!};$$

$$\mathbb{C}=\text{Euler's constant}=0.577\ 215\ 664\ 901\ 532\ 5\ldots. \tag{4.50}$$

By Eqs. (4.50) and the second part of (4.40), one extracts the relation

$$2\int(\overline{N}-\tfrac{2}{3})d\overline{\xi}=\ln|\mathrm{ci}(\overline{\xi})|,$$

and thus defines the solution

$$\overline{N}-\frac{2}{3}=-\frac{1}{2}\frac{\cos\overline{\xi}}{\overline{\xi}\mathrm{ci}(\overline{\xi})}=\mathcal{F}(\overline{\xi}). \tag{4.51}$$

In addition, the general Riccati solution given by the first part of (4.40) becomes

$$\overline{H}_{\mathrm{R}}(\overline{\xi})=-\frac{1}{2}\frac{\cos\overline{\xi}}{\overline{\xi}\mathrm{ci}(\overline{\xi})}-\frac{\mathrm{ci}(\overline{\xi})}{C-\int\mathrm{ci}(\overline{\xi})d\overline{\xi}},$$

which, because [Ref. 15; p. 406 (3.722.7); p. 929 (8.235.2)]

$$\lim_{\overline{\xi}\to 0}\mathrm{ci}(\overline{\xi})=\mathrm{ci}(0)=-\infty,\quad \lim_{\overline{\xi}\to-\infty}\mathrm{ci}(\overline{\xi})=\pm\pi i,$$

$$\int\mathrm{ci}(\overline{\xi})d\overline{\xi}=\left[\mathbb{C}+\ln\overline{\xi}-1+\sum_{\nu=1}^{\infty}(-1)^{\nu}\frac{\overline{\xi}^{2\nu}}{(2\nu+1)(2\nu)(2\nu)!}\right]\overline{\xi},$$

satisfies the assertions (4.47).

By now, in order for the function $\overline{N}-2/3=\mathcal{F}(\overline{\xi})$ being defined in (4.51) to be a solution of the Riccati equation (4.38), and thus of the original Abel equation (4.4), the third part of Eqs. (4.40) must be also valid. Thus, we perform the equation

$$\frac{4(G+2F)e^{-\bar{\xi}}}{\bar{N}+\frac{4}{3}}=\frac{1}{2}\frac{\mathrm{ci}(\bar{\xi})(\bar{\xi}\sin\bar{\xi}+\cos\bar{\xi})+\cos^2\bar{\xi}}{[\bar{\xi}\mathrm{ci}(\bar{\xi})]^2}, \tag{4.52}$$

by means of which, introducing also the expression for $\bar{N}+4/3$, we evaluate the subsidiary function $G(\bar{\xi})$.

The above results complete the solution of the problem under consideration, that is the construction of the exact solution of the original Abel equation (4.4). Indeed, following the inverse course the above solution can be written as follows:

$$y(x)=\tfrac{1}{2}(x+2\lambda)[\bar{N}(x)+\tfrac{1}{3}],$$

$$4(G+2F)e^{-\bar{\xi}}=\frac{1}{4}\frac{[(\bar{\xi}\sin\bar{\xi}+\cos\bar{\xi})\overset{\star}{A}+\cos^2\bar{\xi}](4\bar{\xi}\overset{\star}{A}+\cos\bar{\xi})}{(\bar{\xi}\overset{\star}{A})^3};$$

$$\overset{\star}{A}(\bar{\xi})=\mathrm{ci}(\bar{\xi})=\text{the cosine integral};$$

$$\mathrm{ci}(\bar{\xi})=\mathbb{C}+\ln\,\xi+\int_0^{\bar{\xi}}\frac{\cos\,t-1}{t}dt=\mathbb{C}+\ln\bar{\xi}+\sum_{\nu=1}^{\infty}(-1)^{\nu}\frac{\bar{\xi}^{2\nu}}{(2\nu)(2\nu)!};$$

$$\bar{\xi}=\ln|x+2\lambda|\Rightarrow d\bar{\xi}=\frac{1}{x+2\lambda}dx;$$

$$\bar{N}(x)\text{ as in Eqs. (4.25) to (4.27);}$$

$$\lambda=\text{integration constant}. \tag{4.53}$$

V. EXACT ANALYTIC SOLUTIONS OF THE BLASIUS EQUATION

For simplicity and without loss of generality, we choose to extract the implicit analytic solution of the simplified Blasius equation (3.20) emphasizing that the same exactly mathematical procedure can be followed in the case of the restricted form of the generalized Blasius equation (3.6). According to the solution methodology developed in Sec. IV [formulas (4.53)], as well as in Eqs. (3.31) and (3.29), the solution of the Abel equation (3.28) can be written in exact analytic form as follows:

$$\overset{\star}{v}(\overset{\star}{z})=r(\overset{\star}{z})+\overset{\star}{z}-1=\overset{\star}{z}-1+\tfrac{1}{2}[\bar{N}(\overset{\star}{z})+\tfrac{1}{3}](2\,\ln|\overset{\star}{z}|-\tfrac{3}{2}\overset{\star}{z}+2\lambda);$$

$$4\left[G(\bar{\xi})+2\frac{F_0}{F_1}\right]e^{-\bar{\xi}}=\frac{1}{4}\frac{[(\bar{\xi}\sin\bar{\xi}+\cos\bar{\xi})\overset{\star}{A}+\cos^2\bar{\xi}](4\overset{\star}{A}\bar{\xi}+\cos\bar{\xi})}{(\bar{\xi}\overset{\star}{A})^3};$$

$$\bar{\xi}=\ln\left|2\,\ln\left|\frac{\overset{\star}{z}}{2}\right|-\frac{3}{2}\overset{\star}{z}+2\lambda\right|,\quad \overset{\star}{A}=\mathrm{ci}(\bar{\xi})=\text{the cosine integral};$$

$$\frac{F_0}{F_1}=\frac{(\overset{\star}{z}-1)(4-\overset{\star}{z})}{4-3\overset{\star}{z}},\quad \lambda=\text{integration constant}. \tag{5.1}$$

Here, $\overline{N}(\overset{\star}{z})$ is given in terms of $G(\overset{\star}{z})$ by the formulas (4.23) and (4.25)–(4.27). In order to define the type of the function $\overline{N}(\overset{\star}{z})$ which must be chosen among Eqs. (4.25)–(4.27), as well as to define the function $G(\overset{\star}{z})$ and the constant of integration λ, we must combine the above Abel equation (3.28) with the original Emden–Fowler equation (3.21) through the transformation (3.27) and the boundary data of the problem under consideration. Thus, we have the following conditions:

1st boundary condition: for $y_1\to\infty$, $\xi_1\to 0$.

By the second part of (3.27) we obtain

$$\lim_{\substack{y\to\infty\\ \xi_1\to 0}}\frac{y^2}{\sqrt{\xi}}=\lim_{\substack{y_1\to\infty\\ \xi_1\to 0}}\frac{\overset{\star}{v}_1}{A}=\infty\Rightarrow \overset{\star}{v}_1\to\infty.$$

As $\overset{\star}{v}_1\to\infty$, from substitution of (3.29) it follows that $r_1\to\infty$, and thus the Abel equation (3.30) permits us to write

$$(r'_{\overset{\star}{z}_1}-F_{1,1})r_1=F_{0,1}\Rightarrow \text{for } r_1\to\infty,\quad F_{0,1}\to\infty.$$

But, since $F_{0,1}=(\overset{\star}{z}_1-1)(4-\overset{\star}{z}_1)/2\overset{\star}{z}_1$, we have that for $F_{0,1}\to\infty$, $\overset{\star}{z}_1\to 0$.

2nd boundary condition: for $y_0=\alpha_1$, $\xi_0=\beta_1^2/2$, $\overset{\star}{v}_0=\sqrt{2}\alpha_1^2A/\beta_1$, $\overset{\star}{z}_0=$unknown.

The first boundary condition, that is to say

$$\text{for } y_1\to\infty,\quad \xi_1\to 0 \text{ and } \overset{\star}{z}_1\to 0,$$

insures the type of the function $\overline{N}(\overset{\star}{z}_1)$. In fact, by Eqs. (4.23) we estimate $b=3, c=0, p=-7/3, q=-116/3$, and thus we conclude that the discriminant $Q(\overset{\star}{z}_1)$, Eq. (4.24) , becomes positive $(Q(\overset{\star}{z}_1)=(-7/9)^3+(116/3)^2)$. This means that the form of $\overline{N}(\overset{\star}{z}_1)$ is expressed by Eq. (4.26).

Based on the above observations, one distinguishes the following two cases concerning the solution of the intermediate Emden–Fowler equation (3.21).

Case a:

This case corresponds to a unique solution of Eq. (3.21) inside the main interval $y\in(+\infty,\alpha_1]$, $\xi\in[0,\beta_1^2/2]$, that is to say to a unique solution of the Blasius equation (3.20). Thus, if the solution is unique, then the solution of the Abel equation (3.28) is expressed by Eqs. (5.1), where $\overline{N}(\overset{\star}{z})$ is given by (4.26). In addition, the solution of the Emden–Fowler equation (3.21) is expressed parametrically by Eqs. (3.37), in which $\overset{\star}{v}(\overset{\star}{z})$ is the already constructed solution given in (5.1). For the evaluation of the two constants of integration λ and C, we apply the second of the prescribed boundary conditions, that is to say the boundary condition

$$\text{for } y_0=\alpha_1,\quad \xi_0=\beta_1^2/2 \text{ and } \overset{\star}{v}_0=\sqrt{2}\alpha_1^2A/\beta_1.$$

Applying these conditions on Eqs. (5.1) and (3.37), we perform the following:

$$\frac{\sqrt{2}\alpha_1^2A}{\beta_1}=\overset{\star}{z}_0-1+\frac{1}{2}\left[\overline{N}(\overset{\star}{z}_0)+\frac{1}{3}\right]\left(2\ln|\overset{\star}{z}_0|-\frac{3}{2}\overset{\star}{z}_0+2\lambda\right),$$

$$4\left[G(\bar{\xi}_0)+2\frac{F_0}{F_1}\bigg|_{\overset{\star}{z}_0}e^{-\bar{\xi}_0}=\frac{1}{4}\frac{[(\bar{\xi}_0\sin\bar{\xi}_0+\cos\bar{\xi}_0)\overset{\star}{A}_0+\cos^2\bar{\xi}_0](4\overset{\star}{A}_0\bar{\xi}_0+\cos\bar{\xi}_0)}{(\bar{\xi}_0\overset{\star}{A}_0)^3},\right.$$

$$\frac{\beta_1^2}{2}=\exp[C+R(\overset{\star}{z}_0)],$$

$$\alpha_1=\pm\frac{\overset{\star}{\nu}{}^{1/2}(\overset{\star}{z}_0)}{A^{1/2}}\{\exp[C+R(\overset{\star}{z}_0)]\}^{1/4} \tag{5.2}$$

where

$$R(\overset{\star}{z}_0)=\int\frac{d\overset{\star}{z}}{\overset{\star}{\nu}(\overset{\star}{z})-\overset{\star}{z}+1}\Bigg|_{\overset{\star}{z}_0},\quad \bar{\xi}_0=\ln\left|2\ln\left|\frac{\overset{\star}{z}_0}{2}\right|-\frac{3}{2}\overset{\star}{z}_0+2\lambda\right|,\quad \overset{\star}{A}_0=\mathrm{ci}(\bar{\xi}_0),$$

$$\frac{F_0}{F_1}\bigg|_{\overset{\star}{z}_0}=\frac{(\overset{\star}{z}_0-1)(4-\overset{\star}{z}_0)}{4-3\overset{\star}{z}_0}. \tag{5.3}$$

In the above equations $\overset{\star}{\nu}(\overset{\star}{z})$ is given by the first of Eqs. (5.1), and $\bar{N}(\overset{\star}{z}_0)$ by Eq. (4.26).

Equations (5.2) consist of a strongly nonlinear (transcendental) system of four equations including five unknown parameters, that is, the parameters $\overset{\star}{z}_0; G(\overset{\star}{z}_0); \lambda; C$, and $R(\overset{\star}{z}_0)$. Thus, one more relation must be added for the estimation of the above five parameters. This relation is the cubic equation (4.22) at $\overset{\star}{z}=\overset{\star}{z}_0$.

The above-mentioned calculations permit us to construct the solution of the reduced Emden–Fowler equation (3.21), that is, the solution of the problem under consideration in the phase plane. The solution to the original Blasius equation (3.20) can be obtained by way of Eqs. (3.38) in combination with the third boundary condition $(y_x'(0)=\beta_1)$, indispensable for the evaluation of the third constant of integration $\overset{\star}{C}$ being introduced in (3.38).

Case b:

The solution of the intermediate Emden–Fowler equation (3.21) is not unique inside the main interval $y\in(+\infty,\alpha_1]; \xi\in[0,\beta_1^2/2]$, but it can be divided into several branches of solutions valid separately inside consecutive subintervals $y^{(n-1)}\in(y_n=+\infty,y_{n-1}), y^{(n-2)}\in[y_{n-1},y_{n-2}),\ldots,\quad y^{(0)}\in[y_1,y_0=\alpha_1];\quad \xi^{(n-1)}\in[\xi_n=0,\xi_{n-1}),\quad \xi^{(n-2)}\in[\xi_{n-1},\xi_{n-2}),\ldots,\quad \xi^{(0)}\in[\xi_1,\xi_0=\beta_1^2/2]$. Here, the superscript in parentheses denotes quantity inside the corresponding subinterval.

For simplicity, and without loss of generality, we assume two branches of solutions valid inside two consecutive subintervals $(y_2=+\infty,y_1),\quad [y_1,y_0=\alpha_1]$; and $[\xi_2=0,\xi_1),\quad [\xi_1,\xi_0=\beta_1^2/2]$. In each pair $\{+\infty,\xi_2\},\{y_1,\xi_1\}$, and $\{\alpha_1,\beta_1^2/2\}$ correspond three concrete values $\overset{\star}{z}_2$, $\overset{\star}{z}_1$, and $\overset{\star}{z}_0$ of the parameter $\overset{\star}{z}$, respectively. We note also that in each of the above subintervals two constants of integration $\lambda^{(1)}$ and $\lambda^{(0)}$, as well as two subsidiary determinable functions $G^{(1)}(\overset{\star}{z})$ and $G^{(0)}(\overset{\star}{z})$ exist, being introduced separately by the corresponding solutions of two Abel equations of the type (3.28). The same conclusion results for the parametric solutions (3.37) of two Emden–Fowler equations of the type (3.21) valid separately in the above subintervals and introducing two constants of integration $C^{(1)}$ and $C^{(0)}$, as well as two integrands $(1/(\overset{\star}{\nu}{}^{(1)}(\overset{\star}{z})-\overset{\star}{z}+1))$ and $(1/(\overset{\star}{\nu}{}^{(0)}(\overset{\star}{z})$

$-(\overset{\star}{z})+1))$. Thus, the whole problem is focused on the determination of the before-mentioned concrete values $\xi_1, y_1, \overset{\star}{z}_1$, as well as on the kind of solutions valid inside of each of the above discrete subintervals.

The first boundary condition, that is to say

$$\text{for } y_2 \to \infty, \quad \xi_2 \to 0, \quad \overset{\star}{z}_2 \to 0 \quad (\overset{\star}{v}{}^{(2)} \to \infty),$$

insures only that the discriminant $Q^{(1)}(\overset{\star}{z}{}^{(1)})$ is positive. This means that the solution $\overline{N}^{(1)}(\overset{\star}{z}{}^{(1)})$ valid inside the first subinterval $(y_2=\infty, y_1);[\xi_2=0, \xi_1)$ is given by Eq. (4.26). In other words, in the first subinterval we admit the following solution of the Abel equation (3.28):

$$\overset{\star}{v}{}^{(1)}(\overset{\star}{z}{}^{(1)}) = \overset{\star}{z}{}^{(1)} - 1 + \frac{1}{2}\left[\overline{N}^{(1)}\left(\overset{\star}{z}{}^{(1)} + \frac{1}{3}\right)\right]\left(2\ \ln|\overset{\star}{z}{}^{(1)}| - \frac{3}{2}\overset{\star}{z}{}^{(1)} + 2\lambda^{(1)}\right),$$

$$4\left[G(\overline{\xi}^{(1)}) + 2\frac{F_0}{F_1}\right]e^{-\overline{\xi}^{(1)}} = \frac{1}{4}\frac{[(\overline{\xi}^{(1)}\sin\ \overline{\xi}^{(1)} + \cos\ \overline{\xi}^{(1)})\overset{\star}{A}{}^{(1)} + \cos^2\ \overline{\xi}^{(1)}](4\overset{\star}{A}{}^{(1)}\overline{\xi}^{(1)} + \cos\ \overline{\xi}^{(1)})}{(\overline{\xi}^{(1)}\overset{\star}{A}{}^{(1)})^3},$$

$$\overline{\xi}^{(1)} = \ln\left|2\ \ln\ \left|\frac{\overset{\star}{z}{}^{(1)}}{2}\right| - \frac{3}{2}\overset{\star}{z}{}^{(1)} + 2\lambda^{(1)}\right|, \quad \overset{\star}{A}{}^{(1)} = \mathrm{ci}(\overline{\xi}^{(1)}),$$

$$\left.\frac{F_0}{F_1}\right|_{\overset{\star}{z}{}^{(1)}} = \frac{(\overset{\star}{z}{}^{(1)} - 1)(4 - \overset{\star}{z}{}^{(1)})}{4 - 3\overset{\star}{z}{}^{(1)}}, \tag{5.4}$$

where $\overline{N}^{(1)}(\overset{\star}{z}{}^{(1)})$ as in Eq. (4.26) and $\overset{\star}{z}{}^{(1)} \in (+\infty, \overset{\star}{z}_1)$.

Similarly, the solution of the corresponding Emden–Fowler equation (3.21) in the above subinterval is given parametrically as follows:

$$\xi^{(1)} = \exp(C^{(1)} + R^{(1)}(\overset{\star}{z}{}^{(1)}));$$

$$y^{(1)} = \pm\frac{\overset{\star}{v}{}^{(1)^{1/2}}(\overset{\star}{z}{}^{(1)})}{A^{1/2}}[\exp(C^{(1)} + R^{(1)}(\overset{\star}{z}{}^{(1)}))]^{1/4};$$

$$\overset{\star}{v}{}^{(1)}(\overset{\star}{z}{}^{(1)}) \text{ as in Eqs.(5.3);}$$

$$R^{(1)}(\overset{\star}{z}{}^{(1)}) = \int \frac{d\overset{\star}{z}{}^{(1)}}{\overset{\star}{v}{}^{(1)}(\overset{\star}{z}{}^{(1)}) - \overset{\star}{z}{}^{(1)} + 1}. \tag{5.5}$$

At the concrete unknown value $\overset{\star}{z}{}^{(1)} = \overset{\star}{z}_1$, where the solution changes, the continuity and the smoothness demand the validity of the following equations:

$$\overline{N}^{(1)}(\overset{\star}{z}_1) = \overline{N}^{(0)}(\overset{\star}{z}_1), \quad \overset{\star}{v}{}^{(1)}(\overset{\star}{z}_1) = \overset{\star}{v}{}^{(0)}(\overset{\star}{z}_1), \quad \overset{\star}{v}{}_{\star}^{\prime(1)}(\overset{\star}{z}_1) = \overset{\star}{v}{}_{\star}^{\prime(0)}(\overset{\star}{z}_1). \tag{5.6}$$

We emphasize that $\overline{N}^{(0)}(\overset{\star}{z}{}^{(0)})$, $\overset{\star}{v}{}^{(0)}(\overset{\star}{z}{}^{(0)})$, and $\overset{\star}{v}{}_z^{\prime(0)}(\overset{\star}{z}{}^{(0)})$ denote the corresponding quantities valid inside the second subinterval $[y_1, y_0=\alpha_1];[\xi_1, \xi_0=\beta_1^2/2]$ and including one new constant of inte-

gration $\lambda^{(0)}$, as well as a determinable function $G^{(0)}(\overset{\star}{z}{}^{(0)})$ (in terms of the unknown expression $\overline{N}^{(0)}(\overset{\star}{z}{}^{(0)})$). The expression for $\overline{N}^{(0)}(\overset{\star}{z}{}^{(0)})$ must be selected between formulas (4.25)–(4.27), while the solution for $\overset{\star}{v}{}^{(0)}(\overset{\star}{z}{}^{(0)}), G^{(0)}(\overset{\star}{z}{}^{(0)})$ is given by Eqs. (5.1) where, instead of $\lambda^{(1)}$ and $\overline{N}^{(1)}(\overset{\star}{z}{}^{(1)})$, the new expressions $\lambda^{(0)}$ and $\overline{N}^{(0)}(\overset{\star}{z}{}^{(0)})$ must be introduced.

Similarly, the continuity and the smoothness of the solution at $\overset{\star}{z}{}^{(0)}=\overset{\star}{z}_1$ demand the validity of the following two equations:

$$\xi_1^{(1)} = \xi_1^{(0)}, \quad y_1^{(1)} = y_1^{(0)}, \tag{5.7}$$

in which $\xi_1^{(1)}$ and $y_1^{(1)}$ as in Eqs. (5.5), and

$$\xi_1^{(0)} = \exp(C^{(0)} + R_1^{(0)}(\overset{\star}{z}_1));$$

$$y_1^{(0)} = \pm \frac{\overset{\star}{v}{}_1^{(0)1/2}(\overset{\star}{z}_1)}{A^{1/2}}[\exp(C^{(0)} + R_1^{(0)}(\overset{\star}{z}_1))]^{1/4};$$

$\overset{\star}{v}{}_1^{(0)}(\overset{\star}{z}_1)$ as in Eqs.(5.4) for $\overset{\star}{z}{}^{(0)} = \overset{\star}{z}_1$with $\lambda^{(0)}$ and $\overline{N}^{(0)}(\overset{\star}{z}{}^{(0)})$;

$$R_1^{(0)}(\overset{\star}{z}_1) = \left[\int \frac{d\overset{\star}{z}{}^{(0)}}{\overset{\star}{v}{}^{(0)}(\overset{\star}{z}{}^{(0)}) - \overset{\star}{z}{}^{(0)} + 1}\right]\Bigg|_{\overset{\star}{z}{}^{(0)}=\overset{\star}{z}_1}. \tag{5.8}$$

The five equations (5.6) and (5.7) introduce nine unknowns $\lambda^{(1)}, \overline{N}^{(1)}(\overset{\star}{z}_1), \lambda^{(0)}$, $\overline{N}^{(0)}(\overset{\star}{z}_1)$, $R_1^{(1)}, R_1^{(0)}, \overset{\star}{z}_1, C^{(1)}$, and $C^{(0)}$. Four additional equations of the types (5.1) and (3.37) hold true at $\overset{\star}{z}{}^{(0)}=\overset{\star}{z}_0$, that is to say at the point $y^{(0)}=y_0=\alpha_1$ and $\xi^{(0)}=\xi_0=\beta_1^2/2$, namely

$$\frac{\sqrt{2}\alpha_1^2 A}{\beta_1} = \overset{\star}{z}_0 - 1 + \frac{1}{2}\left[\overline{N}^{(0)}(\overset{\star}{z}_0) + \frac{1}{3}\right]\left(2\ \ln|\overset{\star}{z}_0| = \frac{3}{2}\overset{\star}{z}_0 + 2\lambda^{(0)}\right);$$

$$4\left[G(\overline{\xi}_0) + 2\ \frac{F_0}{F_1}\Bigg|_{\overset{\star}{z}_0}\right]e^{-\overline{\xi}_0} = \frac{1}{4}\frac{[(\overline{\xi}_0\ \sin\ \overline{\xi}_0 + \cos\ \overline{\xi}_0)\overset{\star}{A}_0 + \cos^2\ \overline{\xi}_0](4\overset{\star}{A}_0\overline{\xi}_0 - \cos\ \overline{\xi}_0)}{(\overline{\xi}_0\overset{\star}{A}_0)^3},$$

$$\frac{\beta_1^2}{2} = \left(\exp\left[C^{(0)} + \int \frac{d\overset{\star}{z}{}^{(0)}}{\overset{\star}{v}{}^{(0)}(\overset{\star}{z})^{(0)} - \overset{\star}{z}{}^{(0)} + 1}\right]\right)\Bigg|_{\overset{\star}{z}{}^{(0)}=\overset{\star}{z}_0};$$

$$a_1 = \pm \frac{\overset{\star}{v}{}^{(0)1/2}(\overset{\star}{z}_0)}{A^{1/2}} \left(\exp\left[C^{(0)} + \int \frac{d\overset{\star}{z}{}^{(0)}}{\overset{\star}{v}{}^{(0)}(\overset{\star}{z}{}^{(0)}) - \overset{\star}{z}{}^{(0)} + 1}\right]^{1/4}\right)\Bigg|_{\overset{\star}{z}{}^{(0)}=\overset{\star}{z}_0}. \tag{5.9}$$

These equations introduce the new fixed parameter $\overset{\star}{z}_0$, as well as the new integrand value

$$R_0^{(0)} \equiv \left[\int \frac{dz^{\overset{\star}{(0)}}}{\upsilon^{\overset{\star}{(0)}}(\overset{\star}{z}^{(0)}) - z^{\overset{\star}{(0)}} + 1} \right]\Bigg|_{\overset{\star}{z}^{(0)}=\overset{\star}{z}_1}.$$

Thus, a nonlinear (transcendental) system of nine equations (5.6), (5.7), and (5.9) with 11 unknowns $\lambda^{(1)}, \lambda^{(0)}, \overline{N}^{(1)}(\overset{\star}{z}_1), \overline{N}^{(0)}(\overset{\star}{z}_1), R_1^{(1)}(\overset{\star}{z}_1), \quad R_1^{(0)}(\overset{\star}{z}_1), R_0^{(0)}(\overset{\star}{z}_0), C^{(1)}, C^{(0)}, \overset{\star}{z}_1$, and $\overset{\star}{z}_0$ results, which must be enriched by two additional cubic equations of the type (4.22) valid at $\overset{\star}{z}=\overset{\star}{z}_1$ and $\overset{\star}{z}=\overset{\star}{z}_0$. The solution of the above system furnishes all the unknown parameters of the problem under consideration.

The prescribed analysis can be extended to cases of several branches of different solutions valid inside several consecutive subintervals demanding successive solutions of strongly nonlinear (transcendental) systems of the type (5.6), (5.7), and (5.9).

VI. CONCLUSIONS

Through a series of admissible functional transformations, we reduced the generalized Blasius equation in fluids to a three-term generalized Emden–Fowler equation. In addition, the restricted and the simplified forms of this equation were reduced to (i) a two-term generalized Emden–Fowler's equation; (ii) Emden–Fowler's equations of the normal form; and (iii) Abel's equations of the second kind.

By a mathematical solution methodology concerning the construction of exact analytic solutions of the Abel equation of the second kind of the normal form, we succeeded in constructing exact analytic solutions for the simplified as well as for the restricted form of the generalized Blasius equation in axisymmetric flows. Thus, important unsolvable in exact form problems in nonlinear mechanics, such as manufacturing of polymer and metal sheets, cooling of an infinite metallic plate, boundary layer along a liquid film in condensation process, thermal capillary flow in viscous layer, etc., now can be analytically solved.

The mathematical methodology introduced is general and can be applied to a wide class of unsolvable nonlinear ODEs in mathematical physics and nonlinear mechanics.

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Uniform estimates on the velocity in Rayleigh–Bénard convection

Manuel Núñez[a)]
Departamento de Análisis Matemático, Universidad de Valladolid, 47005 Valladolid, Spain

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The kinetic energy of a fluid located between two plates at different temperatures is easily bounded by classical inequalities. However, experiments and numerical simulations indicate that when the convection is turbulent, the volume of the domains in which the speed is large, is rather small. This could imply that the maximum of the speed, in contrast with its quadratic mean, does not admit an *a priori* upper bound. It is proved that, provided the pressure remains bounded, a uniform estimate for the speed maximum does indeed exist, and that it depends on the maxima of certain ratios between temperature, pressure, and velocity. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1855400]

I. INTRODUCTION

The study of thermal convection of a fluid powered by the difference of temperature between two plates, known as Rayleigh–Bénard convection, has been an extensively studied subject for a long time. Computer modeling and physical experiments have produced an enormous wealth of information: for recent reviews, see Refs. 1 and 2. Perhaps unavoidably, there has not been a comparable volume of rigorous studies, if we except the study of the stability of different patterns (Ref. 3, pp. 23–95). It is well known that when the difference of temperature between the top and bottom plates exceeds a certain amount, usually measured in terms of the Rayleigh constant R, convection sets in. Near the onset, convection cells occur; with increasing R, and depending also on the ratio between viscosity and thermal diffusivity (the Prandtl number) more complex patterns appear and bifurcations to chaotic states may occur. The same may be said of the temperature: for a colorful illustration, starting with regular rolls, see e.g., Ref. 4.

The standard mathematical model of Reyleigh–Bénard convection is given by the Boussinesq approximation to the equations of motion, which we repeat here for convenience. We will consider a d-dimensional domain U of the form $\Omega\times[0,h]$, and as usual we will assume that the temperature is constant at the lower and upper lids, $T=T_0$ at $\Omega\times\{0\}$ and $T=T_h<T_0$ at $\Omega\times\{h\}$. The rest of the boundary conditions will be discussed later. Let us denote by $\mathbf{v}$ the fluid velocity, T the temperature, ν the kinematic viscosity, κ the thermal diffusivity, and π the kinetic pressure. Then the nondimensionalized Boussinesq approximation (see, e.g., Ref. 5) to the equations of motion is

$$\frac{\partial \mathbf{v}}{\partial t}=\nu\Delta\mathbf{v}-\mathbf{v}\cdot\nabla\mathbf{v}-\nabla\pi+(T-T_h)\mathbf{e}_d, \tag{1}$$

$$\frac{\partial T}{\partial t}=\kappa\Delta T-\mathbf{v}\cdot\nabla T, \tag{2}$$

[a)]Electronic mail: mnjmhd@am.uva.es

$$\nabla \cdot \mathbf{v} = 0. \tag{3}$$

$\mathbf{e}_d$ denotes the vertical unit vector. Traditionally the difference θ of the actual temperature with the linear one between the lids (associated to pure heat conduction) is used,

$$\theta = T - T_0 + \beta x_d, \qquad \beta = \frac{T_0 - T_h}{h}. \tag{4}$$

π is also changed to $\pi + \beta x_d^2/2 - (T_0 - T_h)x_d$ (which we denote again by π). The final system is

$$\frac{\partial \mathbf{v}}{\partial t} = \nu \Delta \mathbf{v} - \mathbf{v} \cdot \nabla \mathbf{v} - \nabla \pi + \theta \mathbf{e}_d, \tag{5}$$

$$\frac{\partial \theta}{\partial t} = \kappa \Delta \theta - \mathbf{v} \cdot \nabla \theta + \beta v_d, \tag{6}$$

$$\nabla \cdot \mathbf{v} = 0. \tag{7}$$

Boundary conditions are usually the following ones: the upper and lower plates are taken either rigid, where we assume a no-slip condition and $\mathbf{v}$ vanishes there, or stress free, in which case $v_d = 0$ and the vertical derivatives of the remaining components of the velocity are also zero, $\partial_d v_i = 0$. The lateral walls are assumed rigid and conducting, so that $\mathbf{v}$ and θ vanish there.

Let us state some classical results, since T satisfies (2), which is a scalar parabolic equation without terms in T, it also satisfies the maximum and minimum principles (see, e.g., Ref. 6). That means that T lies always between T_0 and T_h, which makes excellent physical sense. Therefore θ is uniformly bounded. By multiplying (5) by $\mathbf{v}$, integrating in U and making use of the boundary conditions, one gets

$$\frac{1}{2}\frac{d}{dt}\int_U v^2 \, dV + \nu \int_U |\nabla \mathbf{v}|^2 \, dV = \int_U \theta v_d \, dV \leqslant \|\theta\|_\infty \, \mathrm{Vol}(U)^2 \|v_d\|_2, \tag{8}$$

where $\mathrm{Vol}(U)$ denotes the volume (area in dimension two) of U. Since with our boundary conditions a Poincaré inequality holds, there exists a positive constant c such that

$$c \int_U |v^2| dV \leqslant \int_U |\nabla \mathbf{v}|^2 \, dV.$$

Thus, by standard inequalities,

$$\frac{1}{2}\frac{d}{dt}\|\mathbf{v}\|_2^2 + \frac{\nu c}{2}\|\mathbf{v}\|_2^2 \leqslant \frac{1}{2\nu^2 c^2}\|\theta\|_\infty^2 \, \mathrm{Vol}(U), \tag{9}$$

which implies that $\|\mathbf{v}\|_2$ is bounded for all time.

As in many other turbulent situations, modeling of the chaotic phase of convection shows a tendency of the flow to concentrate the velocity in regions of small volume.[7] Thus the boundedness of the kinetic energy does not provide an *a priori* bound upon the maximum of the speed. It is true that physically it seems obvious that this maximum cannot grow without limit, but nevertheless it is interesting to obtain rigorous estimates in terms of the main magnitudes of the

problem. Our only hypothesis will be the boundedness of the pressure π [or, to be specific, of $\pi/(1+v)$].

II. ANALYSIS OF THE MOMENTS OF THE VELOCITY

Let us start with the momentum equation

$$\frac{\partial \mathbf{v}}{\partial t} = \nu \Delta \mathbf{v} - \mathbf{v} \cdot \nabla \mathbf{v} - \nabla \pi + \theta \mathbf{e}_d, \tag{10}$$

and for $p=1,2\ldots$, let

$$F_p = \int_U v^p \, \mathrm{d}V, \tag{11}$$

where $v=|\mathbf{v}|$ represents the modulus of $\mathbf{v}$. F_p is a function of time. Since $v^2=\mathbf{v}\cdot\mathbf{v}$,

$$\frac{\partial v^{2p}}{\partial t} = 2pv^{2p-2}\mathbf{v} \cdot \frac{\partial \mathbf{v}}{\partial t}.$$

Therefore

$$\frac{1}{2p}\dot{F}_{2p} = \int_U v^{2p-2}\mathbf{v} \cdot \frac{\partial \mathbf{v}}{\partial t} \mathrm{d}V,$$

and taking into account the momentum equation,

$$\frac{1}{2p}\dot{F}_{2p} = -\int_U v^{2p-2}(\mathbf{v} \cdot \nabla \mathbf{v}) \cdot \mathbf{v} \, \mathrm{d}V + \nu \int_U v^{2p-2}\mathbf{v} \cdot \Delta \mathbf{v} \, \mathrm{d}V + \int_U (\theta v^{2p-2} v_d - v^{2p-2}\mathbf{v} \cdot \nabla \pi) \mathrm{d}V. \tag{12}$$

In the first place,

$$\int_U v^{2p-2}(\mathbf{v} \cdot \nabla \mathbf{v}) \cdot \mathbf{v} \, \mathrm{d}V = \int_U \frac{1}{2p}\mathbf{v} \cdot \nabla v^{2p} \, \mathrm{d}V = 0. \tag{13}$$

As for the dissipative term,

$$\begin{aligned}\int_U v^{2p-2}\mathbf{v} \cdot \Delta \mathbf{v} \, \mathrm{d}V &= \int_U \sum_j (\nabla \cdot (v_j v^{2p-2} \nabla v_j) - \nabla v_j \cdot \nabla (v^{2p-2} v_j)) \mathrm{d}V \\ &= \frac{1}{2}\int_{\partial U} v^{2p-2}\frac{\partial v^2}{\partial n} \mathrm{d}\sigma - \int_U \left(v^{2p-2} |\nabla \mathbf{v}|^2 + \frac{p-1}{2} v^{2p-4} |\nabla v^2|^2 \right) \mathrm{d}V. \end{aligned} \tag{14}$$

It is understood that the last term (multiplied by $p-1$) vanishes when $p=1$; there are never negative powers of v. As for the boundary integral, it also vanishes, since $\partial v^2/\partial n$ vanishes in all the boundary, including possible stress-free surfaces.

The last term we must consider is

$$\int_U (\theta v^{2p-2} v_d - v^{2p-2}\mathbf{v}\cdot\nabla\pi)\mathrm{d}V. \tag{15}$$

Since

$$-\int_U v^{2p-2}\mathbf{v}\cdot\nabla\pi\,\mathrm{d}V = -\int_{\partial U} v^{2p-2}\pi\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}\sigma + \int_U (p-1)\pi v^{2p-4}\mathbf{v}\cdot\nabla v^2\,\mathrm{d}V, \tag{16}$$

and again the boundary integral vanishes, the term in (16) is

$$\int_U (v^{2p-2}\theta v_d + (p-1)\pi v^{2p-4}\mathbf{v}\cdot\nabla v^2)\mathrm{d}V, \tag{17}$$

with the same meaning as before when $p=1$. We may bound (17) in several ways. We first choose

$$\begin{aligned}\left|\int_U v^{2p-2}\theta v_d + (p-1)\pi v^{2p-4}\mathbf{v}\cdot\nabla v^2\,\mathrm{d}V\right| &= \left|\int_U \frac{\theta}{1+v}(v_d v^{2p-2} + v_d v^{2p-1}) + (p-1)\frac{\pi}{1+v}(v^{2p-4}\right.\\ &\quad \left. + v^{2p-3})\mathbf{v}\cdot\nabla v^2\,\mathrm{d}V\right|\\ &\leqslant \left\|\frac{\theta}{1+v}\right\|_\infty \int_U (v^{2p-2}+v^{2p-1})|v_d|\mathrm{d}V + (p-1)\left\|\frac{\pi}{1+v}\right\|_\infty\\ &\quad \times\int_U (v^{2p-4}+v^{2p-3})|\mathbf{v}\cdot\nabla v^2|\mathrm{d}V\\ &\leqslant \left\|\frac{\theta}{1+v}\right\|_\infty \int_U (v^{2p-1}+v^{2p})\mathrm{d}V + (p-1)\left\|\frac{\pi}{1+v}\right\|_\infty\\ &\quad \times\int_U (v^{2p-3}+v^{2p-2})|\nabla v^2|\mathrm{d}V. \end{aligned}\tag{18}$$

From now on we will denote

$$\alpha = \left\|\frac{\theta}{1+v}\right\|_\infty,$$

$$\beta = \left\|\frac{\pi}{1+v}\right\|_\infty.$$

Notice that they are functions of t. Thus

$$\begin{aligned}\frac{1}{2p}\dot{F}_{2p} &\leqslant -\nu\int_U v^{2p-2}|\nabla\mathbf{v}|^2\,\mathrm{d}V - \frac{\nu(p-1)}{2}\int_U v^{2p-4}|\nabla v^2|^2\,\mathrm{d}V + \alpha\int_U (v^{2p-1}+v^{2p})\mathrm{d}V\\ &\quad + (p-1)\beta\int_U (v^{2p-3}+v^{2p-2})|\nabla v^2|\mathrm{d}V.\end{aligned}\tag{19}$$

For our first estimate we will not make use of the first dissipative term. We have

$$\alpha\int_U (v^{2p-2}+v^{2p-1})\mathrm{d}V \leqslant \alpha(F_{2p-1}+F_{2p}). \tag{20}$$

As for the second term, by using Cauchy–Schwarz and Young's inequalities,

$$(p-1)\beta\int_U (v^{p-1}+v^p)v^{p-2}|\nabla v^2|\mathrm{d}V \leqslant (p-1)\beta\left(\int_U (v^{p-1}+v^p)^2\,\mathrm{d}V\right)^{1/2}\left(\int_U v^{2p-4}|\nabla v^2|^2\,\mathrm{d}V\right)^{1/2}$$
$$\leqslant (p-1)\beta^2\frac{1}{\nu}\int_U (v^{p-1}+v^p)^2\,\mathrm{d}V + \frac{(p-1)\nu}{4}\int_U v^{2p-4}|\nabla v^2|^2\,\mathrm{d}V$$
$$\leqslant (p-1)\beta^2\frac{2}{\nu}(F_{2p-2}+F_{2p}) + \frac{(p-1)\nu}{4}\int_U v^{2p-4}|\nabla v^2|^2\,\mathrm{d}V. \tag{21}$$

We have proved the recursive inequality

$$\frac{1}{2p}\dot{F}_{2p} \leqslant -\frac{\nu(p-1)}{4}\int_U v^{2p-4}|\nabla v^2|^2\,\mathrm{d}V + \alpha F_{2p-1} + \alpha F_{2p} + \frac{2(p-1)\beta^2}{\nu}F_{2p-2} + \frac{2(p-1)\beta^2}{\nu}F_{2p}. \tag{22}$$

We use now the fact that U has finite volume to bound all the F_k in terms of F_{2p},

$$F_{2p-2} \leqslant \mathrm{Vol}(U)^{1/p}F_{2p}^{1-1/p},$$
$$F_{2p-1} \leqslant \mathrm{Vol}(U)^{1/2p}F_{2p}^{1-1/2p}. \tag{23}$$

Let us begin studying a series of alternatives. It may happen

(A) $F_{2p}<1$. Otherwise,
(B) $F_{2p-2}\leqslant \mathrm{Vol}(U)^{1/p}F_{2p}$, $F_{2p-1}\leqslant \mathrm{Vol}(U)^{1/2p}F_{2p}$.

We will consider the consequences of alternative (B). We have

$$\frac{1}{2p}\dot{F}_{2p} + \frac{\nu(p-1)}{4}\int_U v^{2p-4}|\nabla v^2|^2\,\mathrm{d}V \leqslant \left(\alpha(1+m(U)^{1/2p}) + \frac{2(p-1)\beta^2}{\nu}(1+\mathrm{Vol}(U)^{1/p})\right)F_{2p}, \tag{24}$$

and if we call $k=1+\max\{\mathrm{Vol}(U),1\}$,

$$\frac{1}{2p}\dot{F}_{2p} + \frac{\nu(p-1)}{4}\int_U v^{2p-4}|\nabla v^2|^2\,\mathrm{d}V \leqslant k\left(\alpha + \frac{2(p-1)\beta^2}{\nu}\right)F_{2p}. \tag{25}$$

Let us now remember a particular case of the Gagliardo–Nirenberg inequality (Ref. 8, pp. 69 and 70). For any function $f\in H^1(U)$, there exists a constant C depending only on U such that

$$\|f\|_2^{d+2} \leqslant C(\|\nabla f\|_2 + \|f\|_1)^d\|f\|_1^2. \tag{26}$$

Since $(x+y)^d\leqslant 2^{d-1}(x^d+y^d)$, by taking $\lambda=\max\{2^{d-1}C,1\}$,

$$\|f\|_2^{d+2} \leqslant \lambda(\|\nabla f\|_2^d + \|f\|_1^d)\|f\|_1^2, \tag{27}$$

with $\lambda\geqslant 1$. Notice that for $f=v^p$,

$$\|f\|_2 = F_{2p}^{1/2}, \quad \|f\|_1 = F_p, \quad \nabla f = \frac{p}{2}v^{2p-2}\nabla v^2, \quad \|\nabla f\|_2^2 = \frac{p^2}{4}\int_U v^{2p-4}|\nabla v^2|^2\,\mathrm{d}V. \tag{28}$$

In the inequality (27), there exist two alternatives. Either

$$\text{(b1)} \quad \|f\|_2 < \lambda^{1/(d+2)}\|f\|_1, \tag{29}$$

or

$$\text{(b2)} \quad \|\nabla f\|_2^2 \geqslant \left(\frac{\|f\|_2^{d+2} - \lambda\|f\|_1^{d+2}}{\lambda\|f\|_1^2}\right)^{2/d}. \tag{30}$$

With our election of f, the first alternative means

$$F_{2p} < \lambda^{2/(d+2)}F_p^2. \tag{31}$$

Alternative (b2), when taken into (25), yields

$$\frac{1}{2p}\dot{F}_{2p} \leqslant -\frac{\nu(p-1)}{p^2}\left(\frac{F_{2p}^{(d+2)/2} - \lambda F_p^{d+2}}{\lambda F_p^2}\right)^{2/d} + k\left(\alpha + \frac{2(p-1)\beta^2}{\nu}\right)F_{2p}. \tag{32}$$

Take now, for $p \geqslant 2$,

$$\gamma_p = \lambda\left(1 + k^{d/2}\left(\frac{p^2}{\nu(p-1)}\right)^{d/2}\left(\alpha + \frac{2(p-1)\beta^2}{\nu}\right)^{d/2}\right). \tag{33}$$

Notice that $\gamma_p \geqslant \lambda \geqslant \lambda^{2/(d+2)} \geqslant 1$. A short calculation will convince us that if $F_{2p} > \gamma_p F_p^2$ and (b2) occurs, then $\dot{F}_{2p} \leqslant 0$. Since alternative (b1) is included in

$$\text{(B1)} \quad F_{2p} \leqslant \gamma_p F_p^2,$$

the remaining possibility is

$$\text{(B2)} \quad F_{2p} \leqslant 0.$$

Recall that all this assumes (B). Therefore the alternatives are (A) $F_{2p} \leqslant 1$, (B1) or (B2).

III. UNIFORM ESTIMATES IN TIME

Let us consider a time interval $[0,\tau]$, and let

$$\begin{aligned} \Phi_p(\tau) &= \max\{1, \max\{F_p(t): t \in [0,\tau]\}\} \\ \Gamma_p(\tau) &= \max\{\gamma_p(t): t \in [0,\tau]\}. \end{aligned} \tag{34}$$

For every $t \in [0,\tau]$ where (A) or (B1) occurs, certainly

$$F_{2p}(t) \leqslant \Gamma_p(\tau)\Phi_p(\tau)^2. \tag{35}$$

Now, if (35) occurs for every $t \in [0,\tau]$, obviously

$$\Phi_{2p}(\tau) \leqslant \Gamma_p(\tau)\Phi_p(\tau)^2. \tag{36}$$

The other possibility is that for a certain $t_1 \in [0,\tau]$,

$$F_{2p}(t_1) > \Gamma_p(\tau)\Phi_p(\tau)^2, \tag{37}$$

which implies that (B2) holds, i.e., $\dot{F}_{2p}(t_1) \leqslant 0$. Let $(t_0, t_1]$ be a maximal left interval where (37) occurs. We know that F_{2p} is decreasing there. If $t_0 > 0$, $F_{2p}(t_0) = \Gamma_p(\tau)\Phi_p(\tau)^2$, which, since $F_{2p}(t_1) \leqslant F_{2p}(t_0)$, contradicts our hypothesis. The only possibility is that (35) occurs nowhere, i.e., $t_0 = 0$. In that case, F_{2p} is decreasing in $[0,t_1]$ and therefore $F_{2p}(t_1) \leqslant F_{2p}(0)$. Thus, in every case

$$\Phi_{2p}(\tau) \leqslant \max\{\Gamma_p(\tau)\Phi_p(\tau)^2, F_{2p}(0)\}. \tag{38}$$

Since $\|\mathbf{v}(t)\|_p = F_p(t)^{1/p}$, if we denote

$$\phi_p(\tau) = \max\{1, \max\{\|\mathbf{v}(t)\|_p : t \in [0,\tau]\}\}, \tag{39}$$

the $2p$th root of (38) yields

$$\phi_{2p}(\tau) \leqslant \max\{\Gamma_p(\tau)^{1/2p}\phi_p(\tau), \|\mathbf{v}(0)\|_{2p}\}. \tag{40}$$

Hence

$$\begin{gathered}
\phi_4(\tau) \leqslant \max\{\Gamma_2(\tau)^{1/4}\phi_2(\tau),\ \|\mathbf{v}(0)\|_4\},\\
\phi_8(\tau) \leqslant \max\{\Gamma_4(\tau)^{1/8}\Gamma_2(\tau)^{1/4}\phi_2(\tau), \Gamma_4(\tau)^{1/8}\|\mathbf{v}(0)\|_4,\ \|\mathbf{v}(0)\|_8\}\cdots,\\
\phi_{2^n}(\tau) \leqslant \{\Gamma_{2^{n-1}}(\tau)^{1/2^n}\Gamma_{2^{n-2}}(\tau)^{1/2^{n-1}}\cdots\Gamma_2(\tau)^{1/4}\phi_2(\tau),\\
\Gamma_{2^{n-1}}(\tau)^{1/2^n}\Gamma_{2^{n-2}}(\tau)^{1/2^{n-1}}\cdots\Gamma_4(\tau)^{1/8}\|\mathbf{v}(0)\|_4\ldots,\ \|\mathbf{v}(0)\|_{2^n}.
\end{gathered} \tag{41}$$

Let us study the infinite product

$$\Gamma_2(\tau)^{1/4}\Gamma_4(\tau)^{1/8}\cdots\Gamma_{2^{n-1}}(\tau)^{1/2^n}\cdots. \tag{42}$$

Recall that

$$\alpha(t) = \left\|\frac{\theta(t)}{1+v(t)}\right\|_\infty, \quad \beta(t) = \left\|\frac{\pi(t)}{1+v(t)}\right\|_\infty. \tag{43}$$

Let us denote by $\overline{\alpha}(\tau)$, $\overline{\beta}(\tau)$ their respective maxima in $[0,\tau]$. By the expression in (33),

$$\begin{aligned}
\Gamma_{2^n}(\tau) &\leqslant \lambda\left(1 + k^{d/2}\left(\frac{2^{2n}}{\nu(2^n-1)}\right)^{d/2}\left(\overline{\alpha}(\tau) + \frac{2(2^n-1)}{\nu}\overline{\beta}(\tau)^2\right)^{d/2}\right)\\
&\leqslant \lambda\left(1 + \left(2^{2n+2}k\left(\frac{\overline{\alpha}(\tau)}{\nu} + \frac{\overline{\beta}(\tau)^2}{\nu^2}\right)\right)^{d/2}\right) \leqslant \lambda\left(1 + \left(2^{2n+2}k\left(\frac{\overline{\alpha}(\tau)}{\nu} + \frac{\overline{\beta}(\tau)^2}{\nu^2} + 1\right)\right)^{d/2}\right).
\end{aligned} \tag{44}$$

The addition of 1 to the parentheses is intended to ensure that

$$x = \left(2^{2n+2}k\left(\frac{\overline{\alpha}(\tau)}{\nu} + \frac{\overline{\beta}(\tau)^2}{\nu^2} + 1\right)\right)^{d/2} \geqslant 1.$$

Since for those x, $\log(1+x) \leqslant 1 + \log x$ holds,

$$\log\Gamma_{2^n}(\tau) \leqslant \log\lambda + 1 + \frac{d}{2}\left(\log k + (2n+2)\log 2 + \log\left(\frac{\overline{\alpha}(\tau)}{\nu} + \frac{\overline{\beta}(\tau)^2}{\nu^2} + 1\right)\right).$$

Hence the sum of the logarithms of Γ_{2^n} satisfies

$$\sum_{n=1}^{\infty}\frac{1}{2^{n+1}}\log\Gamma_{2^n}(\tau) \leqslant \frac{1}{2}\left(1 + \log\lambda + \frac{d}{2}\log k\right) + \frac{d}{2}\log 2\sum_{n=1}^{\infty}\frac{2n+2}{2^{n+1}} + \frac{d}{4}\log\left(\frac{\overline{\alpha}(\tau)}{\nu} + \frac{\overline{\beta}(\tau)^2}{\nu^2} + 1\right). \tag{45}$$

Thus, since the sum of the series $\Sigma(2n+2)/2^{n+1}$ is 3,

$$\prod_{n=1}^{\infty}\Gamma_{2^n}(\tau)^{1/2^{n+1}} \leqslant 2^{3d/2}(\lambda e)^{1/2}k^{d/4}\left(\frac{\overline{\alpha}(\tau)}{\nu} + \frac{\overline{\beta}(\tau)^2}{\nu^2} + 1\right)^{d/4}, \tag{46}$$

and the same may be said of any finite product

$$\prod_{n=1}^{m} \Gamma_{2^n}(\tau)^{1/2^{n+1}}. \tag{47}$$

Since, on the other hand,

$$\|\mathbf{v}(0)\|_p \leqslant \|\mathbf{v}(0)\|_\infty \operatorname{Vol}(U)^{1/p} \leqslant k\|\mathbf{v}(0)\|_\infty, \tag{48}$$

we find

$$\phi_{2^n}(\tau) \leqslant 2^{3d/2}(\lambda e)^{1/2}k^{d/4}\left(\frac{\overline{\alpha}(\tau)}{\nu} + \frac{\overline{\beta}(\tau)^2}{\nu^2} + 1\right)^{d/4} \max\{\phi_2(\tau), k\|\mathbf{v}(0)\|_\infty\}. \tag{49}$$

It is well known that $\|\mathbf{v}\|_p \to \|\mathbf{v}\|_\infty$ as $p \to \infty$, so that $\phi_{2^n}(\tau) \to \max\{1, \|\mathbf{v}(t)\|_\infty : t \in [0,\tau]\}$. Also, $\phi_2(\tau)$ represents the maximum of the kinetic energy in $[0,\tau]$, which we denote by $E(\tau)$. Calling M the universal constant written in (49), we obtain our main estimate

$$\begin{aligned}\max\{\|\mathbf{v}(t)\|_\infty : t \in [0,\tau]\} \leqslant M\left(\frac{1}{\nu}\max_{[0,\tau]}\left\|\frac{\theta(t)}{1+v(t)}\right\|_\infty + \frac{1}{\nu^2}\max_{[0,\tau]}\left\|\frac{\pi(t)}{1+v(t)}\right\|_\infty^2 + 1\right)^{d/4} \\ \times \max\{E(\tau), k\|\mathbf{v}(0)\|_\infty\}.\end{aligned} \tag{50}$$

IV. COMMENTS AND EXTENSIONS OF THE ESTIMATES

In principle it could look as if the estimates in terms of θ and π divided by $1+v$ are unnecessary, since if v is bounded so are θ and π. While there is no conceptual gain in taking these magnitudes divided by $1+v$, the estimate (50) is in fact finer than one involving only $\|\theta\|_\infty$ and $\|\pi\|_\infty$. It can be far better if the regions where θ and/or π are larger coincide with regions of high velocity. In particular, high temperature deviation propels the fluid faster, so it is likely that $\theta/(1+v)$ is considerably smaller than θ.

When the flow is chaotic, the temperature may become irregular. Therefore it is possible that some primitive of θ (e.g., a function Θ such that for some coordinate j, $\partial_j\Theta = \theta$) may have a better behavior than the temperature deviation: portions where θ is positive may compensate with others where it is negative to obtain a smooth result. We will see that $\|\mathbf{v}\|_\infty$ may also be bounded in terms of $\Theta/(1+v)$. The method follows the steps of the previous one: the term

$$\int_U \theta v^{2p-2} v_d \, \mathrm{d}V \tag{51}$$

may be written as

$$\int_U (\partial_j\Theta) v^{2p-2} v_d \, \mathrm{d}V = -\int_U \Theta \partial_j (v^{2p-2} v_d) \mathrm{d}V = -\int_U \Theta (v^{2p-2}\partial_j v_d + 2(p-1)v^{2p-4} v_d \mathbf{v}\cdot\partial_j\mathbf{v}) \mathrm{d}V. \tag{52}$$

This may be bounded by

$$(2p-1)\int_U \left|\frac{\Theta}{1+v}\right| (v^{2p-2} + v^{2p-1}) |\nabla \mathbf{v}| \mathrm{d}V \leqslant (2p-1)\left\|\frac{\Theta}{1+v}\right\|_\infty \int_U (v^{2p-2} + v^{2p-1}) |\nabla \mathbf{v}| \mathrm{d}V. \tag{53}$$

Using now the Cauchy–Schwarz inequality, the term is bounded by

$$(2p-1)^2\left\|\frac{\Theta}{1+v}\right\|_\infty \frac{1}{2\nu}\int_U (v^{2p-2}+v^{2p})\mathrm{d}V+\nu\int_U v^{2p-2}|\nabla \mathbf{v}|^2\,\mathrm{d}V. \tag{54}$$

The last term may now be cancelled with the first of the dissipative terms (which we did not use in our previous proof) and we are left with

$$(2p-1)^2\left\|\frac{\Theta}{1+v}\right\|_\infty^2 \frac{1}{2\nu}(F_{2p-2}+F_{2p}). \tag{55}$$

The rest of the proof is analogous to the previous one. We are left with a bound of the form

$$\max\{\|\mathbf{v}(t)\|_\infty : t\in[0,\tau]\} \leqslant M\left(\frac{1}{\nu^2}\max_{[0,\tau]}\left\|\frac{\Theta(t)}{1+v(t)}\right\|_\infty^2+\frac{1}{\nu^2}\max_{[0,\tau]}\left\|\frac{\pi(t)}{1+v(t)}\right\|_\infty^2+1\right)^{d/4} \times \max\{E(\tau),k\|\mathbf{v}(0)\|_\infty\}. \tag{56}$$

Notice, however, that now a factor of the form $1/\nu^2$ appears before the maximum norm of $\Theta/(1+v)$, and this is squared, while before we had only $1/\nu$ and the power of $\theta/(1+v)$ was one. This may be important when the viscosity is low.

V. CONCLUSIONS

While the kinetic energy of the flow in Rayleigh–Bénard convection may be easily bounded by classical inequalities, the maximum of the velocity is harder to handle. As soon as the flow becomes chaotic small islands or filaments of high velocity are observed, which makes compatible the boundedness of the square mean of the velocity (the kinetic energy) with the existence of large velocity peaks. It is proved here that, provided the pressure remains uniformly bounded, so does the velocity, and its maximum may be estimated by the maxima of the temperature deviation and pressure divided by one plus the velocity modulus. Other estimates may be made in terms of certain means of the temperature, which may be considerably smaller than the temperature itself if its distribution is irregular. The bounds depend on certain powers, depending on the dimension, of the previously mentioned magnitudes and the flow viscosity.

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Study on boundary–boundary correlation functions of the two-dimensional Ising model using topological interaction method

Masuo Suzuki[a] and Hidenori Suzuki[b]
Department of Applied Physics, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku-ku, Tokyo 162-8601, Japan

Shu-Chiuan Chang[c]
Department of Applied Physics, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku-ku, Tokyo 162-8601, Japan and Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

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The topological interaction method is applied to the evaluation of boundary–boundary correlation functions, which yield the square of the spontaneous magnetization m_b at the boundary in the thermodynamic limit. One of the remarkable results is that the boundary–boundary correlation function C_M is found to be nonmonotonic with respect to the system size M for $T<T_c$, because of boundary effects. On the other hand, it is monotonic above T_c, $C_M \simeq (A_+(T)/\sqrt{M})\exp(-M/\xi)$ with the correlation length ξ and with $A_+(T)\sim\sqrt{T-T_c}$ near the critical point T_c. At the critical point, $C_M \sim 1/M$, and below T_c, $C_M \simeq m_b^2+(-A_-(T)\sqrt{M}+B(T)+C(T)/\sqrt{M})\exp(-M/\xi)$, where $A_-(T)\sim m_b^3$, $B(T)\sim m_b^2$, $C(T)\sim m_b \sim \sqrt{T-T_c}$. Fisher's finite-size scaling is confirmed in this respect. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1845954]

I. INTRODUCTION

A second-order phase transition[1–8] is characterized by spontaneous symmetry breaking (SSB) accompanied by the appearance of long-range order (LRO),[5,6,9]

$$\mathrm{LRO} = \lim_{R\to\infty}\langle Q(0)Q(R)\rangle \tag{1.1}$$

for the relevant local order-parameter Q_j or $Q(R)$ of the system. The global order parameter Q is defined by the sum or integral

$$Q = \sum_j Q_j = \int Q(R)\mathrm{d}^d R \tag{1.2}$$

in d dimensions. A standard method to study SSB is to evaluate the generalized partition function of the form

$$Z(T,\Lambda) = \mathrm{Tr}\exp[-\beta(\mathcal{H}_0 - \Lambda Q)], \tag{1.3}$$

where Λ is a parameter conjugate to the order parameter Q. Then, the thermal average of Q is given by

[a]Electronic mail: msuzuki@rs.kagu.tus.ac.jp
[b]Electronic mail: j1202706@ed.kagu.tus.ac.jp
[c]Electronic mail: scchang@mail.ncku.edu.tw

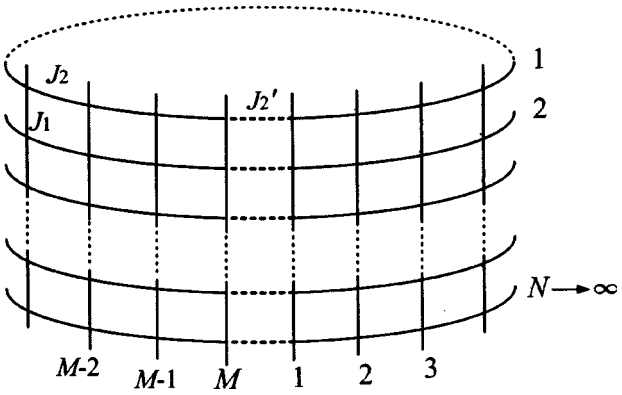

FIG. 1. Topological interaction J_2' to connect the two opposite boundary spins.

$$\langle Q\rangle_\Lambda = \frac{\partial}{\partial(\beta\Lambda)}\log Z(T,\Lambda). \tag{1.4}$$

The spontaneous order parameter is obtained by taking the following limits:

$$\langle Q\rangle_+ = \lim_{\Lambda\to+0}\lim_{N\to\infty}\langle Q\rangle_\Lambda \tag{1.5}$$

for the system size N. The order of the above two limits is crucial, as is well known. It has been proved[5,6,9] that

$$\mathrm{LRO} = \langle Q\rangle_+^2. \tag{1.6}$$

It is extremely difficult to calculate $Z(T,\Lambda)$ for a nonvanishing Λ. Yang[2] used a trick to make a magnetic field H go to zero proportionally to $N^{-1/2}=L^{-1}$ (i.e., $H\sim N^{-1/2}=L^{-1}$), in order to evaluate the spontaneous magnetization m_s of the two-dimensional Ising model. It might be impossible to obtain m_s if we set $H\sim N^{-1}$ (which means that the Zeeman energy is of the order of unity even below the critical point T_c), as was discussed by Suzuki and Suzuki.[10]

In the present paper, we study SSB in the two-dimensional Ising model by using the topological interaction method (TIM) proposed by Suzuki.[11,12] The scheme of TIM in the present model (Fig. 1) is described by the following Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 - J_2'\sum_{k=1}^{N} S_{1,k}S_{M,k}, \tag{1.7}$$

where

$$\mathcal{H}_0 = -J_1\sum_{j=1}^{M}\sum_{k=1}^{N} S_{j,k}S_{j,k+1} - J_2\sum_{j=1}^{M-1}\sum_{k=1}^{N} S_{j,k}S_{j+1,k} \tag{1.8}$$

with $S_{j,k}=\pm 1$. Clearly, J_2' changes the topology of the system, according to the conditions $J_2'\neq 0$ or $J_2'=0$. Physically, if $J_2'\neq 0$, then $\{\langle S_{1,i}S_{M,i}\rangle\}$ denote short-range correlations. However, if $J_2'=0$, then they denote the long-range correlation for $M\to\infty$, under the limit $N\to\infty$ first before setting $J_2'=0$. This condition is vital for evaluating the long-range order below T_c. This corresponds to the situation that the thermodynamic limit ($N\to\infty$) should be taken before a magnetic field H is made to vanish ($H\to+0$) in order to calculate the spontaneous magnetization in a uniform system.

Even when M is finite, this topological interaction method yields the boundary–boundary correlation function $C_M(0)=\langle S_1S_M\rangle_{J_2'=0}$ as follows:

$$C_M(0) = \lim_{J_2' \to +0} \lim_{N \to \infty} \frac{1}{\beta N} \frac{\partial \ln Z_{2D}(J_2')}{\partial J_2'}, \tag{1.9}$$

where $Z_{2D}(J_2')$ is the partition function of the system and β is the inverse temperature (i.e., $\beta = 1/k_B T$). The nearest-neighbor correlation function, denoted as $C_M(J_2)$, can be treated at the same time as

$$C_M(J_2) = \lim_{J_2' \to J_2} \lim_{N \to \infty} \frac{1}{\beta N} \frac{\partial \ln Z_{2D}(J_2')}{\partial J_2'}. \tag{1.10}$$

In the present paper, we derive boundary–boundary correlation functions in the two-dimensional Ising model and we study their asymptotic behavior for large system size.

II. PARTITION FUNCTION, CORRELATION FUNCTIONS AND BOUNDARY SPONTANEOUS MAGNETIZATION

Consider the rectangular Ising model with the spin–spin interaction $J_1(>0)$ in the vertical direction and $J_2(>0)$ in the horizontal direction. Impose the topological spin–spin interaction J_2' between column 1 and column M, as is shown in Fig. 1. The Hamiltonian of the system is the same as that given in Eqs. (1.7) and (1.8), namely

$$\mathcal{H} = -J_1 \sum_{j=1}^{M} \sum_{k=1}^{N} S_{j,k} S_{j,k+1} - J_2 \sum_{j=1}^{M-1} \sum_{k=1}^{N} S_{j,k} S_{j+1,k} - J_2' \sum_{k=1}^{N} S_{1,k} S_{M,k} \tag{2.1}$$

with periodic boundary condition in the vertical direction. The partition function of this system is expressed as

$$Z_{2D} = 2^{MN-1} (\cosh K_1)^{NM} (\cosh K_2)^{N(M-1)} (\cosh K_2')^N (-\mathrm{Pf}\, A_1 + \mathrm{Pf}\, A_2 + \mathrm{Pf}\, A_3 + \mathrm{Pf}\, A_4), \tag{2.2}$$

using the standard Pfaffian (Pf) method.[4,13–15] Here, the above four Pfaffians are evaluated in Appendix A to give the following expressions:

$$\{\mathrm{Pf}\, A_i\}^2 = \det A_i = \prod_{n=1}^{N} \{z_2(1-z_1^2)\}^M \{(f + f'\zeta^2)\alpha(\theta_n)^M + (f' + f\zeta^2)\alpha(\theta_n)^{-M} + 2(-1)^i \zeta\} \tag{2.3}$$

for $i=1$, 2, 3, and 4 with the notations $K_{1,2} = \beta J_{1,2}$, $K_2' = \beta J_2'$, $z_{1,2} = \tanh K_{1,2}$, $z_2' = \tanh K_2'$ and $\zeta = z_2'/z_2$. The arguments $\{\theta_n\}$ denote $2n\pi/N$ for $i=1$, 2 and $(2n-1)\pi/N$ for $i=3$, 4. The functions $f = f(\alpha)$ and $f' = f(1/\alpha)$ are given by

$$f = f(\alpha) = \frac{(\alpha - z_2/x_1)(\alpha - z_2 x_1)}{(1-z_2^2)(\alpha^2 - 1)} \tag{2.4}$$

and

$$f' = f(1/\alpha) = 1 - f(\alpha) = \frac{(1 - \alpha z_2/x_1)(1 - \alpha z_2 x_1)}{(1-z_2^2)(1-\alpha^2)}, \tag{2.5}$$

respectively, where $x_1 = (1-z_1)/(1+z_1) = e^{-2K_1}$ and $\alpha = \alpha(\theta)$ is the larger solution of the following equation:

$$(1+z_1^2)(1+z_2^2) - 2z_1(1-z_2^2)\cos\theta - z_2(1-z_1^2)(\alpha + \alpha^{-1}) = 0. \tag{2.6}$$

More explicitly, we have

$$\alpha = \alpha(\theta) = \frac{1}{2(1-z_1^2)z_2}[(1+z_1^2)(1+z_2^2) - 2z_1(1-z_2^2)\cos\theta + \sqrt{\{(1+z_1^2)(1+z_2^2) - 2z_1(1-z_2^2)\cos\theta\}^2 - 4(1-z_1^2)^2 z_2^2}]. \tag{2.7}$$

The correct branch of the solution differs above and below T_c. This remark is important in evaluating explicitly the root of Eq. (2.7). Namely, the function $\alpha=\alpha(\theta)$ is such a branch of the root as connects with $\alpha(0)=(1-z_1)/\{z_2(1+z_1)\}$ for $T>T_c$ and $\alpha(0)=z_2(1+z_1)/(1-z_1)$ for $T<T_c$.

Then, the correlation function $\langle S_{1,i}S_{M,i}\rangle$ for $N\to\infty$ can be evaluated as

$$C_M(J_2') \equiv \langle S_{1,i}S_{M,i}\rangle = \lim_{N\to\infty}\frac{1}{N}\frac{\partial \log Z(K_1,K_2,K_2')}{\partial K_2'} = z_2\zeta + \frac{1-z_2^2\zeta^2}{2\pi z_2}\int_0^{2\pi}\frac{(f'\alpha^M + f\alpha^{-M})\zeta + 1}{(f+f'\zeta^2)\alpha^M + (f'+f\zeta^2)\alpha^{-M} + 2\zeta}\mathrm{d}\theta, \tag{2.8}$$

where ζ denotes the topological parameter defined by $\zeta=\tanh(\beta J_2')\coth(\beta J_2)$. The above integral formula of $C_M(J_2')$ is very basic in our investigation on the boundary–boundary correlation. Note that $\alpha(\theta)\geqslant\alpha(0)>1$ except the critical point [where $\alpha(0)=1$]. Then, the limit $M\to\infty$ is easily taken in the above integral (2.8) to give the result

$$C_\infty(J_2') = z_2\zeta + \frac{1-z_2^2\zeta^2}{2\pi z_2}\int_0^{2\pi}\frac{\zeta f(1/\alpha(\theta))}{f(\alpha(\theta)) + \zeta^2 f(1/\alpha(\theta))}\mathrm{d}\theta. \tag{2.9}$$

This shows how the nearest-neighbor correlation function changes according to the change of one-line interaction ($\{J_2\}\to\{J_2'\}\neq 0$).

It is shown here from the idea of topological interaction method that the limit $J_2'\to+0$ of the function $C_\infty(J_2')$ yields the square of the boundary spontaneous magnetization m_b obtained first by McCoy and Wu[13] as follows. It should be noted first that if we set $\zeta=0$ in the integral of Eq. (2.9) then the integral (2.9) will vanish. This comes from the wrong limit for studying SSB; we must integrate Eq. (2.9) first ($N\to\infty$) before setting $J_2'=0$ (namely $\zeta=0$). No SSB occurs for finite N. This is a quite general remark in studying SSB. This situation makes our calculations very difficult or subtle in our paper, as will be seen later.

Now, we take the correct limit $J_2'\to+0$ after the integration with respect to θ in Eq. (2.9) using the delta function $\delta(x)$ as

$$\lim_{J_2'\to+0} C_\infty(J_2') = \frac{1}{2\pi z_2}\lim_{\zeta\to+0}\int_{-\pi}^{\pi}\frac{\zeta}{f(\alpha(\theta))/f(1/\alpha(\theta)) + \zeta^2}\mathrm{d}\theta = \frac{1}{2z_2}\int_{-\pi}^{\pi}\delta(\sqrt{f(\alpha(\theta))/f(1/\alpha(\theta))})\mathrm{d}\theta = \begin{cases} 0 & (T>T_c), \\ \dfrac{z_2^2(1+z_1)^2-(1-z_1)^2}{4z_1z_2^2} & (T\leqslant T_c), \end{cases} \tag{2.10}$$

because it is easily shown from Eqs. (2.4), (2.5), and (2.7) that

$$f(\alpha(\theta)) = 1 + \mathrm{O}(\theta^2) \quad \text{and } f(1/\alpha(\theta)) = \mathrm{O}(\theta^2) \quad \text{for } T>T_c \tag{2.11}$$

and

$$f(\alpha(\theta)) = \hat{f}\theta^2 + \mathrm{O}(\theta^4) \quad \text{and } f(1/\alpha(\theta)) = 1 - \hat{f}\theta^2 + \mathrm{O}(\theta^4) \quad \text{for } T<T_c \tag{2.12}$$

near $\theta=0$, where

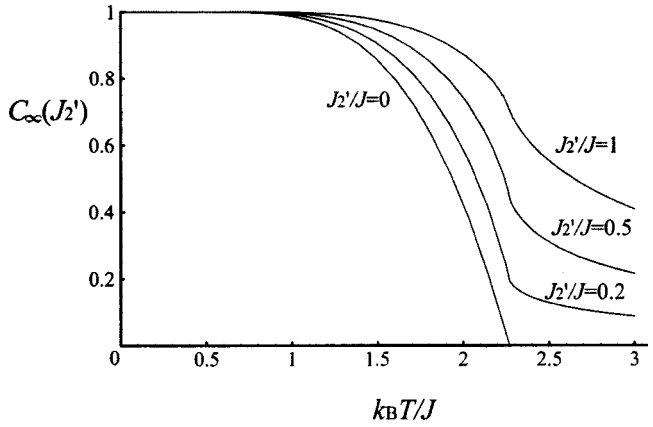

FIG. 2. Temperature dependence of the correlation functions $C_\infty(J_2')$ for various values of the ratio J_2'/J with $J_1=J_2=J$. They are all singular at T_c (where $k_BT_c/J=2.269\ldots$).

$$\hat{f}=\frac{4z_1^2z_2^2}{\{z_2^2(1+z_1)^2-(1-z_1)^2\}^2}. \tag{2.13}$$

It should be remarkable that the first integrand of Eq. (2.10) is essentially singular at $\theta=0$ and $\zeta=0$ only below the critical point T_c. Equivalently, the argument of the delta function in Eq. (2.10), $z_2\{f(\alpha(\theta))/f(1/\alpha(\theta))\}^{1/2}$, has a zero point in the integral range $(-\pi\leqslant\theta\leqslant\pi)$ only below T_c. Thus, we arrive at the following result:

$$\lim_{J_2'\to+0} C_\infty(J_2')=m_b^2, \quad m_b=\left\{\frac{\cosh 2K_2-\coth 2K_1}{\cosh 2K_2-1}\right\}^{1/2}, \tag{2.14}$$

below T_c. This is an alternative derivation of McCoy–Wu's formula on m_b.

It will be instructive to study $C_\infty(J_2')$ for various values of the ratio J_2'/J_2. In particular, $C_\infty(J_2)$ is confirmed to be equal to the uniform nearest-neighbor correlation function[16,17]

$$C_\infty(J_2)=\frac{1}{4\pi z_2}\int_{-\pi}^{\pi}\left\{1+z_2^2+\frac{(1-z_2^2)\{2z_1(1+z_2^2)\cos\theta-(1+z_1^2)(1-z_2^2\}}{\sqrt{\{(1+z_1^2)(1+z_2^2)-2z_1(1-z_2^2)\cos\theta\}^2-4z_2^2(1-z_1^2)^2}}\right\}\mathrm{d}\theta, \tag{2.15}$$

as it should be. All the functions $C_\infty(J_2')$ are singular at T_c for any values of J_2', as shown in Fig. 2.

III. BOUNDARY–BOUNDARY CORRELATION FUNCTION

The main purpose of the present paper is to evaluate the boundary–boundary correlation function both for finite M and infinite $M(\to\infty)$, using the above topological interaction method. In principle, this should be performed by taking the limit $J_2'\to+0$ (and consequently $\zeta=z_2'/z_2\to+0$) in the above basic integral formula (2.8). In fact, we obtain an integral representation of the form

$$C_M\equiv C_M(0)=\frac{1}{2\pi z_2}\int_{-\pi}^{\pi}\frac{1}{f_M(\theta)}\mathrm{d}\theta, \tag{3.1}$$

where

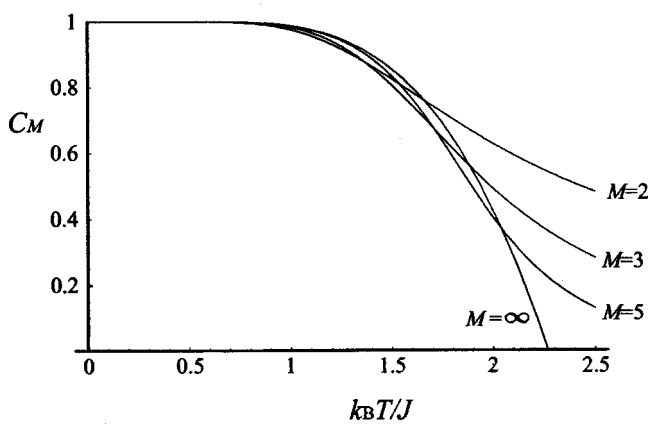

FIG. 3. Temperature dependence of C_M for various values of M with $J_1=J_2=J$. It is seen numerically that C_M is less than C_∞ at low temperatures.

$$f_M(\theta) = f(\alpha(\theta))\alpha(\theta)^M + f\left(\frac{1}{\alpha(\theta)}\right)\alpha(\theta)^{-M}. \tag{3.2}$$

It is easily found from Eqs. (2.4), (2.5), and (2.7) that $f_M(\theta)$ is an Mth order polynomial of $\cos\theta$.

For example, we have, for $M=2$,

$$f_2(\theta) = \frac{1}{z_2^2(1-z_1^2)^2}[(1+z_1^2-2z_1\cos\theta)^2 + 4z_1^2z_2^2\sin^2\theta]. \tag{3.3}$$

Then, we obtain the correlation function

$$C_2 = \frac{z_2(1+z_1^2)}{\sqrt{(1-z_1^2)^2+4z_1^2z_2^2}} = 1 - 8e^{-4K_1-2K_2} + \cdots = C_\infty - 4e^{-4K_1-2K_2} + \cdots . \tag{3.4}$$

The second expression of Eq. (3.4) is a low temperature series expansion. The third expression shows the quite remarkable fact that C_2 is less than C_∞ at low temperatures. This surprising result is found to be universal for any values of M as shown in Fig. 3, which has been calculated numerically from (3.1).

It will be interesting and useful in the theory of critical phenomena to study analytically the asymptotic behavior of the boundary–boundary correlation function C_M. First note that the integrand of Eq. (3.1) for large M is singular at $\theta=0$ below T_c. Thus, it seems to be rather complicated to evaluate Eq. (3.1) for large M below T_c. We must integrate first Eq. (3.1) before taking the limit $M\to\infty$, or at least, to perform the two procedures simultaneously. In fact, we obtain, below T_c,

$$C_\infty = C_\infty(0) = \frac{1}{2\pi z_2}\lim_{M\to\infty}\int_{-\pi}^{\pi}\frac{\alpha(0)^{-M}}{c^2\theta^2+\alpha(0)^{-2M}}\mathrm{d}\theta = \frac{1}{2\pi z_2 c}\lim_{M\to\infty}\int_{-\pi c\alpha(0)^M}^{\pi c\alpha(0)^M}\frac{\mathrm{d}x}{x^2+1}$$
$$= \frac{1}{2\pi z_2 c}\int_{-\infty}^{\infty}\frac{\mathrm{d}x}{x^2+1} = \frac{1}{2cz_2} \tag{3.5}$$

with

$$c = \sqrt{\hat{f}} = \left\{\lim_{\theta\to 0} f(\alpha(\theta))/\theta^2\right\}^{1/2} = \frac{1}{2z_2m_b^2}. \tag{3.6}$$

This relation is derived from Eqs. (2.12) and (2.13). Thus, we arrive again at the relation

$$\lim_{M\to\infty} C_M = m_b^2. \tag{3.7}$$

Clearly we have $C_\infty = 0$ for $T > T_c$. This can be also derived using the delta function as

$$\lim_{M\to\infty} C_M(0) = \frac{1}{2\pi z_2} \lim_{M\to\infty} \int_{-\pi}^{\pi} \frac{\alpha(0)^{-M}}{f + f'\alpha(0)^{-2M}} \mathrm{d}\theta$$
$$= \frac{1}{2z_2} \int_{-\pi}^{\pi} \frac{\delta(\sqrt{f/f'})}{f'} \mathrm{d}\theta = \begin{cases} 0 & (T > T_c), \\ \dfrac{z_2^2(1+z_1)^2 - (1-z_1)^2}{4z_1 z_2^2} & (T \leqslant T_c). \end{cases} \tag{3.8}$$

The above two derivations (2.14) and (3.7) of m_b^2 yield

$$\lim_{J_2'\to+0} \lim_{M\to\infty} C_M(J_2') = \lim_{M\to\infty} \lim_{J_2'\to+0} C_M(J_2') = m_b^2. \tag{3.9}$$

This exchangeability of the two limits comes from the fact that J_2' changes only the topology (not symmetry) of the system.

Next we study the asymptotic behavior of $C_M \equiv C_M(0)$.

A. Asymptotic form of C_M above T_c

Noting the property (2.11), we find, from Eq. (3.1),

$$C_M \simeq \frac{1}{2\pi z_2} \int_{-\pi}^{\pi} e^{-M \log \alpha(\theta)} \, \mathrm{d}\theta \simeq \frac{e^{-M \log \alpha(0)}}{2\pi z_2} \int_{-\infty}^{\infty} e^{-kM\theta^2} \, \mathrm{d}\theta = A_+(T) e^{-M/\xi_b} / \sqrt{M}. \tag{3.10}$$

Here, we have used the relation

$$\log \alpha(\theta) \simeq \log \alpha(0) + k\theta^2, \quad k \equiv \frac{z_1(1-z_2^2)}{(1-z_1)^2 - z_2^2(1+z_1)^2}. \tag{3.11}$$

The coefficient $A_+(T)$ is given by

$$A_+(T) = \frac{1}{2z_2} \left[\frac{(1-z_1)^2 - z_2^2(1+z_1)^2}{\pi z_1 (1-z_1^2)} \right]^{1/2} \sim \sqrt{T - T_c}. \tag{3.12}$$

The correlation length ξ_b is exactly expressed by

$$\xi_b = \frac{1}{\log \alpha(0)} = \frac{1}{\log\left(\dfrac{1-z_1}{z_2(1+z_1)} \right)}, \tag{3.13}$$

which diverges as follows:

$$\xi_b \sim \frac{1}{T - T_c} \to \infty \quad \text{as } T \to T_c, \quad \nu_b = 1. \tag{3.14}$$

It is interesting to note that the above correlation length ξ_b is exactly the same as the ordinary correlation length ξ defined by the correlation function $C(R)$ in the K_2 direction for an infinite system[18]

$$\xi^{-1} = \log \coth K_2 - 2K_1. \tag{3.15}$$

That is, from Eq. (3.13), we obtain

$$\xi_b = \xi, \quad \nu_b = \nu = 1. \tag{3.16}$$

It should be also noted that the above asymptotic form including the prefactor $(1/\sqrt{M})$ agrees with that of the ordinary correlation function[19,20]

$$C(R,T) \simeq \frac{B_+ e^{-R/\xi}}{\sqrt{R}}, \quad T > T_c, \quad R \to \infty. \tag{3.17}$$

However, the situation is different at and below T_c, as will be seen later.

B. Asymptotic form of C_M at T_c [or for $M(T-T_c)/T_c \ll 1$]

It will be interesting to evaluate the asymptotic form of C_M at T_c or for $M(T-T_c)/T_c \ll 1$. We find easily that

$$\alpha(\theta) = 1 + a\theta + \cdots = e^{a\theta} + \mathrm{O}(\theta^2), \quad a \equiv \frac{2z_{1,c}}{1-z_{1,c}^2}, \tag{3.18}$$

and

$$f(\alpha(\theta)) = \tfrac{1}{2} + \mathrm{O}(\theta) \quad \text{and } f(1/\alpha(\theta)) = \tfrac{1}{2} + \mathrm{O}(\theta), \tag{3.19}$$

using Eqs. (2.4), (2.5), and (2.7), as is shown in Appendix B. Here, $z_{1,c}$ denotes the value of z_1 at T_c. Then, we obtain

$$\begin{aligned} C_M &= \frac{1}{2\pi z_{2,c}} \int_{-\pi}^{\pi} \frac{\alpha(\theta)^{-M}}{f(\alpha(\theta)) + f(1/\alpha(\theta))\alpha(\theta)^{-2M}} \mathrm{d}\theta \simeq \frac{2}{\pi z_{2,c}} \int_0^{\infty} \frac{e^{-aM\theta}}{1+e^{-2aM\theta}} \mathrm{d}\theta \\ &= \frac{2}{\pi a M z_{2,c}} \int_0^1 \frac{\mathrm{d}t}{1+t^2} = \frac{(1+z_{1,c})^2}{4z_{1,c}} \cdot \frac{1}{M} \equiv \frac{A(T_c)}{M}, \end{aligned} \tag{3.20}$$

where $z_{2,c}=(1-z_{1,c})/(1+z_{1,c})$. [In particular, we have $A(T_c)=(\sqrt{2}+1)/2$ for $J_1=J_2$.] This asymptotic form $(C_M \sim 1/M)$ is different from the ordinary asymptotic form[1,18] $C(R,T_c) \sim R^{-1/4}$ $(\eta=1/4)$. A similar form was obtained by McCoy and Wu[13] in a different situation.

C. Asymptotic form of C_M below T_c

It is more complicated to study the asymptotic behavior of the boundary–boundary correlation function C_M below T_c, because of the existence of long-range order. We can derive, from Eq. (3.1), the following asymptotic form:

$$C_M \sim m_b^2 + \left\{ -A_-(T)\sqrt{M} + B(T) + \frac{C(T)}{\sqrt{M}} \right\} e^{-M/\xi}, \tag{3.21}$$

and

$$\xi = \frac{1}{\log \alpha(0)} = \frac{1}{\log\left(\dfrac{z_2(1+z_1)}{1-z_1} \right)} \tag{3.22}$$

for $M(T_c-T)/T_c \gg 1$, using the renormalized evaluation method of singular integrals,[21] as will be shown in Appendix C. Here, the coefficients $A_-(T)$ and $B(T)$ are given by

$$A_-(T) = 2\sqrt{\frac{1-z_2^2}{\pi}} \left[\frac{z_2^2(1+z_1)^2 - (1-z_1)^2}{4z_1 z_2^2} \right]^{3/2} = 2m_b^3 \sqrt{\frac{1-z_2^2}{\pi}} \tag{3.23}$$

and

$$B(T) = \frac{1}{2\pi z_2}\int_{-\pi}^{\pi} \frac{2(1-\cos\theta)\hat{f} - f(\alpha(\theta))}{f(\alpha(\theta))2(1-\cos\theta)\hat{f}}\mathrm{d}\theta = \mathrm{O}(1) \quad \text{in } M, \tag{3.24}$$

respectively. The function $\hat{f}$ (of T) is defined in $f(\alpha(\theta)) = \hat{f}\theta^2 + \mathrm{O}(\theta^4)$, namely by (2.13). It is easily shown that

$$A_{-}(T) \sim m_b^3, \quad B(T) \sim m_b^2, \quad \text{and } C(T) \sim m_b. \tag{3.25}$$

This yields the following finite-size scaling law:

$$C_M - \langle S_1\rangle\langle S_M\rangle \simeq P_{\mathrm{sc}}^{(\pm)}(m_b\sqrt{M})\frac{1}{M}e^{-M/\xi}, \tag{3.26}$$

where

$$P_{\mathrm{sc}}^{(\pm)}(x) = a_{\pm}x^3 + b_{\pm}x^2 + c_{\pm}x + d. \tag{3.27}$$

It is easily understood that $m_b\sqrt{M}$ is the scaling variable in Eq. (3.26), because $m_b \sim (T_c - T)^{1/2} \sim \xi^{-1/2} \sim M^{-1/2}$ to give the invariance property of $m_b\sqrt{M} \sim \sqrt{M/\xi}$. The above scaling form (3.26) is a typical example of Fisher's finite-size scaling law.[22,23]

D. Nonmonotonicity of C_M below T_c

One of the remarkable features on C_M is that it is nonmonotonic with respect to the system-size M below T_c, as is seen from Eq. (3.21). It is easily found that $A_{-}(T) > 0$ (see Appendix C). This yields the nonmonotonicity of C_M. This behavior seems to be surprising, at first. Thus, we have confirmed this result in three ways. The first one is analytic, as in Eq. (3.21) with $A_{-}(T) > 0$.

The second one is to make use of the low-temperature expansion of C_M, as was already exemplified for C_2 in Eq. (3.4). It is possible in principle to calculate the low-temperature expansion of C_M. However, it is so complicated that we are here satisfied, for the second confirmation of the nonmonotonicity of C_M, to find the following expansion up to the first order of x_2 ($=e^{-2K_2}$ with $x_1 = e^{-2K_1}$):

$$C_M = \frac{1}{2\pi z_2}\int_{-\pi}^{\pi} \frac{1}{f(\alpha(\theta))\alpha^M + f(1/\alpha(\theta))\alpha^{-M}}\mathrm{d}\theta = 1 - \frac{4\{x_1^2 + (M-1)(1-x_1^2)x_1^M - x_1^{2M}\}}{(1-x_1^2)(1+x_1^M)^2}x_2 + \mathrm{O}(x_2^2) \tag{3.28}$$

for an arbitrary value of M. On the other hand, the square of the boundary magnetization $C_\infty = m_b^2$ is generally expanded as

$$C_\infty = m_b^2 = \frac{\{1 + x_1 - (1-x_1)x_2\}\{1 - x_1 - (1+x_1)x_2\}}{(1-x_1^2)(1-x_2)^2} = 1 - \frac{4x_1^2}{1-x_1^2}\sum_{n=1}^{\infty} n x_2^n. \tag{3.29}$$

Therefore, we find

$$C_M - C_\infty = -\frac{4x_1^M\{M(1-x_1^2) - (1+x_1^2)(1+x_1^M)\}}{(1-x_1^2)(1+x_1^M)^2}x_2 + \mathrm{O}(x_2^2) \tag{3.30}$$

to confirm the inequalities $C_1 > C_M$ and $C_M < C_\infty$ at sufficiently low temperatures for $M \geqslant 2$.

The third method to confirm this behavior is to integrate Eq. (3.1) numerically. Two examples of typical monotonic behavior and nonmonotonic behavior are shown in Fig. 4. In more detail, assuming $J_1 = J_2 = J$ for simplicity, we find the inequality $C_M < C_\infty$ except for $M = 1$ below $k_BT/J = 1.6616\ldots$ as is shown in the above low-temperature expansion. For $1.6616\ldots < k_BT/J < 1.8883\ldots$, we find $C_M < C_{\ldots}$ except for $M = 1$, 2. From Fig. 4(b), it is found that C_M with M

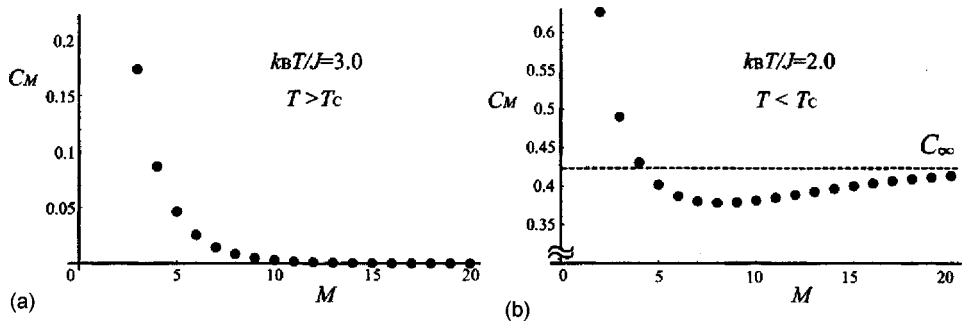

FIG. 4. Size dependence of C_M for $J_1=J_2=J$ (where $k_BT_c/J=2.269\ldots$); (a) above T_c ($k_BT/J=3.0$) and (b) below T_c ($k_BT/J=2.0$). The correlation function C_M is nonmonotonic with respect to M only below T_c.

$=1, 2, 3, 4$ are larger than C_∞ at $k_BT/J=2.0$. In addition, the minimum value of C_M is found at finite $M_{\min}\geqslant 2$. For example, C_2 takes the minimum value for $k_BT/J<1.3696\ldots$ and C_8 is minimum at $k_BT/J=2.0$ [Fig. 4(b)]. For $T\geqslant T_c$, we have $M_{\min}=\infty$.

Above T_c, the function C_M is monotonic with respect to the system size M. The reason why C_M becomes nonmonotonic only below T_c is because the finite-size effect on C_M becomes dominant only below T_c, namely because the difference between C_M and C_∞ comes from the remaining correlations longer than M. These correlations become larger at low temperatures [where the long-range order (LRO) appears]. Except at very low temperatures, the function C_M for small M denotes the short-range correlation effect coming mainly from a finite strip and consequently it decreases as M increases.

IV. SUMMARY AND DISCUSSION

We have applied a new scheme of topological interaction method to the evaluation of the boundary–boundary correlation function C_M for the system-size M. An exact integral formula of C_M has been derived to give the asymptotic scaling form,

$$C_M - m_b^2 = C_M - \langle S_0\rangle\langle S_M\rangle \simeq \tilde{P}_{\mathrm{sc}}^{(\pm)}(\sqrt{M/\xi})\frac{1}{M}e^{-M/\xi}. \tag{4.1}$$

This confirms Fisher's finite-size scaling law. More explicitly, we have

$$C_M \simeq A_+(T)e^{-M/\xi}/\sqrt{M} \quad \text{above } T_c,$$

$$C_M \simeq \frac{A(T_c)}{M},$$

$$C_M \simeq m_b^2 + \left\{-A_-(T)\sqrt{M} + B(T) + \frac{C(T)}{\sqrt{M}}\right\}e^{-M/\xi} \quad \text{below } T_c, \tag{4.2}$$

where ξ is given by Eq. (3.13) for $T>T_c$ and by Eq. (3.22) for $T<T_c$. The nonmonotonicity of C_M with respect to M has been found to appear only below T_c, owing to the competing effect of the strong short-range correlation, long-range correlation dominant at low temperatures and finite-size effect.

It will be interesting to remark that present formula $C_M\simeq(A_+(T)/\sqrt{M})\exp(-M/\xi)$ above T_c is consistent with Morita's sum rule,[24]

$$\lim_{N\to\infty}\frac{1}{N}\sum_{i,j=1}^{N}\langle S_{1,i}S_{M,j}\rangle=(e^{2K_1}\tanh K_2)^M\coth K_2=e^{-M/\xi}\coth K_2 \tag{4.3}$$

which is valid above T_c. For more details, see Appendix D.

The present topological interaction method will be applicable to many other systems to evaluate not only the boundary magnetization but also other physical quantities such as the boundary energy and boundary many-body interactions, $\langle Q_{1,i_1,i_2,\ldots,i_n}\rangle$ by introducing the topological interaction $-J_Q\Sigma Q_{1,i_1,\ldots,i_n}Q_{M,i_1,\ldots,i_n}$. The TIM will be also useful in studying quantum spin systems.[25]

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APPENDIX A: EVALUATION OF PFAFFIANS $\{\mathrm{Pf}\,A_i\}$

By the standard Pfaffian method,[4,13,14] the partition function can be calculated to be

$$\begin{aligned}Z(J_2')&=(\cosh\beta J_1)^{NM}(\cosh\beta J_2)^{N(M-1)}(\cosh\beta J_2')^N\sum_{\{S\}}\left[\left\{\prod_{j=1}^{M}\prod_{k=1}^{N}(1+z_1S_{j,k}S_{j,k+1})\right\}\right.\\&\left.\times\left\{\prod_{j=1}^{M-1}\prod_{k=1}^{N}(1+z_2S_{j,k}S_{j+1,k})\right\}\left\{\prod_{j=1}^{N}(1+z_2'S_{1,k}S_{M,k})\right\}\right]\\&=2^{NM-1}(\cosh K_1)^{NM}(\cosh K_2)^{N(M-1)}(\cosh K_2')^N(-\mathrm{Pf}\,A_1+\mathrm{Pf}\,A_2+\mathrm{Pf}\,A_3+\mathrm{Pf}\,A_4),\end{aligned} \tag{A1}$$

where we use the notations $z_{1,2}=\tanh\beta J_{1,2}=\tanh K_{1,2}$ and $z_2'=\tanh\beta J_2'=\tanh K_2'$. The antisymmetrical matrices A_1 and A_3 are given by

$$A_i(j,k;j,k)=\begin{bmatrix}0&1&-1&-1\\-1&0&1&-1\\1&-1&0&1\\1&1&-1&0\end{bmatrix}\quad\text{for } i=1,3,\quad 1\leqslant j\leqslant M,\quad 1\leqslant k\leqslant N,$$

$$A_1(j,k;j,k+1)=-A_1^T(j,k+1;j,k)=\begin{bmatrix}0&z_1&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{bmatrix}\quad\text{for } 1\leqslant j\leqslant M,\quad 1\leqslant k\leqslant N,$$

$$A_3(j,k;j,k+1)=-A_3^T(j,k+1;j,k)=\begin{bmatrix}0&z_1&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{bmatrix}\quad\text{for } 1\leqslant j\leqslant M,\quad 1\leqslant k\leqslant N-1,$$

$$A_3(j,N;j,1)=-A_3^T(j,1;j,N)=\begin{bmatrix}0&-z_1&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{bmatrix}\quad\text{for } 1\leqslant j\leqslant M,$$

$$A_i(j,k;j+1,k) = -A_i^T(j+1,k;j,k) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z_2 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \text{for } i=1,3, \quad 1 \leqslant j \leqslant M-1, \quad 1 \leqslant k \leqslant N,$$

$$A_i(M,k;1,k) = -A_i^T(1,k;M,k) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z_2' \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \text{for } i=1,3, \quad 1 \leqslant k \leqslant N. \tag{A2}$$

The matrix A_2 (A_4) is exactly the same as A_1 (A_3) except that the sign of z_2' should be reversed. The determinant of the matrix A_1 is the square of the Pfaffian of A_1, and can be calculated by the same procedure as given in Ref. 13 to be

$$\det A_1 = \prod_{\theta} [|1+z_1 e^{i\theta}|^{2M} \det D_1(\theta)], \tag{A3}$$

where $\theta = 2n\pi/N$ with $n = 1,2,\ldots,N$, and $D_1(\theta)$ is a $2M \times 2M$ matrix with the form

$$D_1(\theta) = \begin{bmatrix} -a & b & & & & & & & & & -z_2' \\ -b & a & z_2 & & & & & & & & \\ & -z_2 & -a & b & & & & & & & \\ & & -b & a & z_2 & & & & & & \\ & & & -z_2 & -a & b & & & & & \\ & & & & -b & a & \ddots & & & & \\ & & & & & \ddots & \ddots & \ddots & & & \\ & & & & & & \ddots & -a & b & & \\ & & & & & & & -b & a & z_2 & \\ & & & & & & & & -z_2 & -a & b \\ z_2' & & & & & & & & & -b & a \end{bmatrix}. \tag{A4}$$

Here all the unwritten elements in the upper-right and lower-left triangles in Eq. (A4) are zero and we use the definitions

$$a = 2iz_1 \sin\theta |1+z_1 e^{i\theta}|^{-2}, \quad b = (1-z_1^2)|1+z_1 e^{i\theta}|^{-2}. \tag{A5}$$

The determinant of the matrix $D_1(\theta)$ can be calculated to be

$$\det D_1(\theta) = (f+\zeta^2 f')\lambda^M + (f'+\zeta^2 f)\lambda'^M - 2\zeta(bz_2)^M, \tag{A6}$$

where

$$f = \frac{1}{2}\left(1 + \frac{z_2^2 + a^2 - b^2}{\lambda' - \lambda}\right), \quad f' = \frac{1}{2}\left(1 - \frac{z_2^2 + a^2 - b^2}{\lambda' - \lambda}\right),$$

$$\lambda = |1+z_1 e^{i\theta}|^{-2} z_2 (1-z_1^2)\alpha, \quad \lambda' = |1+z_1 e^{i\theta}|^{-2} z_2 (1-z_1^2)\alpha^{-1},$$

$$\zeta = z_2'/z_2 = \tanh(\beta J_2')\coth(\beta J_2) \tag{A7}$$

and α is given by Eq. (2.7). As the matrix A_2 is similar to A_1 with the sign of z_2' reversed, we have

$$\{\mathrm{Pf}\, A_i\}^2 = \det A_i = \prod_{n=1}^{N} \{z_2(1-z_1^2)\}^M \{(f+f'\zeta^2)\alpha(\theta_n)^M + (f'+f\zeta^2)\alpha(\theta_n)^{-M} + 2(-1)^i\zeta\} \quad \text{(A8)}$$

with $\theta_n = 2n\pi/N$. The expression of the determinants for A_3 and A_4 are the same except that $\theta_n = (2n-1)\pi/N$. If $z_2' = z_2$, it is easily shown that the partition function Z reduces to the regular rectangular Ising lattice with toroidal boundary conditions.

It will be instructive to separate the free energy $-k_BT \log Z_{2D}$ into the following two parts:

$$-k_BT \log Z_{2D} = NMf_0 + Nf_1, \quad \text{(A9)}$$

where f_0 is the bulk free energy defined in

$$-\beta f_0 = \log[2\cosh K_1 \cosh K_2] + \frac{1}{4\pi}\int_{-\pi}^{\pi} \log[z_2(1-z_1^2)\alpha(\theta)]\mathrm{d}\theta, \quad \text{(A10)}$$

and the remaining part f_1 contains the boundary and topological terms,

$$-\beta f_1 = \log[\cosh K_2'] - \log[\cosh K_2] + \frac{1}{4\pi}\int_{-\pi}^{\pi} \log[\{(f+f'\zeta^2) + (f'+f\zeta^2)\alpha(\theta)^{-2M} + 2\zeta\alpha(\theta)^{-M}\}]\mathrm{d}\theta. \quad \text{(A11)}$$

Note that only $\mathrm{Pf}\, A_2$ and $\mathrm{Pf}\, A_4$ contribute to the free energy and consequently that the factor $(-1)^i$ in (A8) is equal to unity. The correlation function $C_M(J_2')$ is thus given by

$$C_M(J_2') = -\frac{\partial}{\partial J_2'} f_1 = \frac{\partial}{\partial K_2'}(-\beta f_1) = \frac{1-z_2^2\zeta^2}{z_2}\frac{\partial}{\partial \zeta}(-\beta f_1). \quad \text{(A12)}$$

This gives Eq. (2.8).

APPENDIX B: PROPERTIES OF $\alpha(\theta)$, $f(\alpha(\theta))$, AND $f(1/\alpha(\theta))$ NEAR $\theta=0$

It is easy to show, from Eqs. (2.4), (2.5), and (2.7), for $T=T_c$,

$$\alpha(\theta) = \frac{(1+z_{1,c}^2)^2 - 4z_{1,c}^2\cos\theta + 4z_{1,c}\sin(\theta/2)\sqrt{1+z_{1,c}^4 - 2z_{1,c}^2\cos\theta}}{(1-z_{1,c}^2)^2} = 1 + \frac{2z_{1,c}}{1-z_{1,c}^2}\theta + \mathrm{O}(\theta^2), \quad \text{(B1)}$$

$$f(\alpha(\theta)) = \frac{1}{2}\left(1 + \frac{(1+z_{1,c}^2)\sin(\theta/2)}{\sqrt{1+z_{1,c}^4 - 2z_{1,c}^2\cos\theta}}\right) = \frac{1}{2} + \mathrm{O}(\theta) \quad \text{(B2)}$$

and

$$f(1/\alpha(\theta)) = \frac{1}{2}\left(1 - \frac{(1+z_{1,c}^2)\sin(\theta/2)}{\sqrt{1+z_{1,c}^4 - 2z_{1,c}^2\cos\theta}}\right) = \frac{1}{2} + \mathrm{O}(\theta), \quad \text{(B3)}$$

where we have substituted $z_{2,c} = (1-z_{1,c})/(1+z_{1,c})$. The above linear dependence of $\alpha(\theta)$ near $\theta = 0$ at T_c is a big contrast to the following θ^2-dependence of $\alpha(\theta)$ for $T \neq T_c$:

$$\alpha(\theta) = \begin{cases} \dfrac{1-z_1}{z_2(1+z_1)} + \dfrac{z_1(1-z_1)(1-z_2^2)}{z_2(1+z_1)\{(1-z_1)^2 - z_2^2(1+z_1)^2\}}\theta^2 + \mathrm{O}(\theta^4) \quad (T > T_c), \\ \dfrac{z_2(1+z_1)}{1-z_1} + \dfrac{z_1z_2(1+z_1)(1-z_2^2)}{(1-z_1)\{z_2^2(1+z_1)^2 - (1-z_1)^2\}}\theta^2 + \mathrm{O}(\theta^4) \quad (T < T_c). \end{cases} \quad \text{(B4)}$$

Equivalently we have

$$\log \alpha(\theta) = \begin{cases} \log\dfrac{1-z_1}{z_2(1+z_1)} + \dfrac{z_1(1-z_2^2)}{(1-z_1)^2 - z_2^2(1+z_1)^2}\theta^2 + \mathrm{O}(\theta^4) & (T > T_c) \\ \log\dfrac{z_2(1+z_1)}{1-z_1} + \dfrac{z_1(1-z_2^2)}{z_2^2(1+z_1)^2 - (1-z_1)^2}\theta^2 + \mathrm{O}(\theta^4) & (T < T_c). \end{cases} \tag{B5}$$

APPENDIX C: DERIVATION OF C_M BELOW T_c

In order to investigate the asymptotic behavior of the correlation function C_M expressed by the integral (3.1), we must study f_M near $\theta=0$, namely $f(\alpha(\theta))$ and $f(1/\alpha(\theta))$. Then we easily find

$$f(\alpha(\theta)) = \hat{f}\theta^2 + \mathrm{O}(\theta^4) \quad \text{and } f(1/\alpha(\theta)) = 1 - \hat{f}\theta^2 + \mathrm{O}(\theta^4), \tag{C1}$$

for $T<T_c$. Thus, the integral of C_M, (3.1) is essentially singular at $\theta=0$ and for $M\to\infty$. It will be useful to set

$$\varepsilon = \alpha(0)^{-M} = e^{-M/\xi}, \tag{C2}$$

which goes to zero as $M\to\infty$. Now we try to evaluate C_M given in the form

$$C_M = \frac{1}{2\pi z_2}\int_{-\pi}^{\pi} \frac{\varepsilon\tilde{\alpha}(\theta)^{-M}}{f(\alpha(\theta)) + \varepsilon^2 f(1/\alpha(\theta))\tilde{\alpha}(\theta)^{-2M}}\mathrm{d}\theta \tag{C3}$$

for large M (and consequently $\varepsilon\to 0$), where

$$\tilde{\alpha}(\theta) = \alpha(\theta)/\alpha(0). \tag{C4}$$

As was mentioned above, the integral (C3) is extremely subtle to calculate because $f(\alpha(\theta)) \simeq \hat{f}\theta^2$ and $f(1/\alpha(\theta)) \simeq 1$ near $\theta=0$ and because $\varepsilon\to 0$ and $\tilde{\alpha}(\theta)^{-M}\to 0$ $(\theta\neq 0)$ for $M\to\infty$. The main term gives m_b^2 and the remaining term becomes of the order of ε. In order to evaluate this remaining term, we make use of the renormalized evaluation method[21] of singular integrals as follows:

$$\begin{aligned} C_M &= \frac{1}{2\pi z_2}\int_{-\pi}^{\pi} \frac{\varepsilon}{f(\alpha(\theta)) + \varepsilon^2 f(1/\alpha(\theta))\tilde{\alpha}(\theta)^{-2M}}\mathrm{d}\theta - \frac{\varepsilon}{2\pi z_2}\int_{-\pi}^{\pi} \frac{1-\tilde{\alpha}(\theta)^{-M}}{f(\alpha(\theta)) + \varepsilon^2 f(1/\alpha(\theta))\tilde{\alpha}(\theta)^{-2M}}\mathrm{d}\theta \\ &\equiv C_M^{(B)} - C_M^{(A)}. \end{aligned} \tag{C5}$$

Noting that the term $C_M^{(B)}$ contains m_b^2 and using the "magic representation" of m_b^2 of the form

$$m_b^2 = \frac{1}{2\pi z_2}\int_{-\pi}^{\pi} \frac{\varepsilon}{2(1-\cos\theta)\hat{f} + \varepsilon^2}\mathrm{d}\theta + \mathrm{O}(\varepsilon^2), \tag{C6}$$

we obtain the following relation:

$$\begin{aligned} C_M^{(B)} - m_b^2 &= \frac{\varepsilon}{2\pi z_2}\int_{-\pi}^{\pi}\left\{\frac{1}{f(\alpha(\theta)) + \varepsilon^2 f(1/\alpha(\theta))\tilde{\alpha}(\theta)^{-2M}} - \frac{1}{2(1-\cos\theta)\hat{f} + \varepsilon^2}\right\}\mathrm{d}\theta + \mathrm{O}(\varepsilon^2) \\ &= \frac{\varepsilon}{2\pi z_2}\int_{-\pi}^{\pi}\left\{\frac{1}{f(\alpha(\theta)) + \varepsilon^2} - \frac{1}{2(1-\cos\theta)\hat{f} + \varepsilon^2}\right\}\mathrm{d}\theta + \mathrm{O}(\varepsilon^2) \\ &= -\varepsilon\left[\frac{1}{2\pi z_2}\int_{-\pi}^{\pi}\frac{f(\alpha(\theta)) - 2(1-\cos\theta)\hat{f}}{2f(\alpha(\theta))(1-\cos\theta)\hat{f}}\mathrm{d}\theta\right] + \mathrm{O}(\varepsilon^2) \equiv B(T)\varepsilon + \mathrm{O}(\varepsilon^2). \end{aligned} \tag{C7}$$

The function $B(T)$ defined in (C7) is easily confirmed to be finite because the integrand of it is finite in the limit $\theta\to 0$. It is also shown that $B(T)\sim m_b^2$. It should be remarked that the replacement

of the term $\varepsilon^2 f(1/\alpha(\theta))\tilde{\alpha}(\theta)^{-2M}$ by ε^2 in the above calculation gives corrections of the order of ε^2.

The term $C_M^{(A)}$ is calculated as follows:

$$C_M^{(A)} = \frac{\varepsilon}{2\pi z_2}\int_{-\pi}^{\pi} \frac{1-\tilde{\alpha}(\theta)^{-M}}{f(\alpha(\theta)) + \varepsilon^2 f(1/\alpha(\theta))\tilde{\alpha}(\theta)^{-2M}} \mathrm{d}\theta$$
$$= \frac{\varepsilon}{2\pi z_2}\int_{-\pi}^{\pi} \frac{1-\tilde{\alpha}(\theta)^{-M}}{f(\alpha(\theta))} \mathrm{d}\theta + \mathrm{O}(\varepsilon^2) = \frac{\varepsilon}{2\pi z_2}\int_{-\pi}^{\pi} \frac{1-e^{-Mb\theta^2}}{\hat{f}\theta^2} \mathrm{d}\theta + \mathrm{O}(\varepsilon^2), \tag{C8}$$

where

$$\tilde{\alpha}(\theta) \simeq e^{b\theta^2}, \quad b = \frac{z_1(1-z_2^2)}{z_2^2(1+z_1)^2 - (1-z_1)^2} = \frac{1-z_2^2}{4z_2^2 m_b^2} \sim m_b^{-2}. \tag{C9}$$

Thus, for large M (and consequently, $\varepsilon \to 0$), we obtain

$$\frac{C_M^{(A)}}{\varepsilon} = \frac{1}{2\pi z_2}\int_{-\pi}^{\pi} \frac{1-e^{-Mb\theta^2}}{\hat{f}\theta^2} \mathrm{d}\theta = \frac{\sqrt{Mb}}{2\pi z_2 \hat{f}}\int_{-\sqrt{Mb}\pi}^{\sqrt{Mb}\pi} \frac{1-e^{-t^2}}{t^2} \mathrm{d}t$$
$$\simeq \frac{\sqrt{(1-z_2^2)M}}{\pi} m_b^3 \int_{-\infty}^{\infty} \frac{1-e^{-t^2}}{t^2} \mathrm{d}t = 2m_b^3 \sqrt{\frac{(1-z_2^2)M}{\pi}} = A_-(T)\sqrt{M}, \tag{C10}$$

where we have used Eqs. (3.6) and (C9), and the following formula;

$$\int_{-\infty}^{\infty} \frac{1-e^{-t^2}}{t^2} \mathrm{d}t = 2\sqrt{\pi}. \tag{C11}$$

Thus, we arrive at the following asymptotic formula:

$$C_M^{(A)} \simeq A_-(T)\sqrt{M} e^{-M/\xi}, \quad A_-(T) = 2\sqrt{\frac{1-z_2^2}{\pi}} m_b^3. \tag{C12}$$

Note that $A_-(T) \geqslant 0$ and $A_-(T) \sim m_b^3$.

Therefore, we arrive finally at

$$C_M \sim m_b^2 + \left\{ -A_-(T)\sqrt{M} + B(T) + \frac{C(T)}{\sqrt{M}} \right\} e^{-M/\xi}. \tag{C13}$$

Here, the coefficient $C(T)$ is shown to be of the order of m_b. The details of this derivation are omitted here.

APPENDIX D: CONSISTENCY OF EQ. (3.10) ON C_M WITH MORITA'S SUM RULE

Morita's sum rule is confirmed by extending our result on C_M given in Eq. (3.10) to correlations in oblique directions, $\{\langle S_{1,i} S_{M,j}\rangle\}$ in the form

$$C(|i-j|, M) \equiv \langle S_{1,i} S_{M,j}\rangle \simeq \frac{A' e^{-R/\xi}}{\sqrt{R}}, \quad R = \sqrt{x^2 + M^2}, \quad x = a_0|i-j|, \tag{D1}$$

where a_0 is an anisotropy parameter depending on z_1 and z_2, the coefficient A' may depend on the angle of the direction of the correlation, and it is proportional to $\sqrt{\kappa} = \sqrt{1/\xi}$. Then, Morita's sum rule will be asymptotically given by

$$J(M) \equiv \int_{-\infty}^{\infty} \frac{e^{-\kappa\sqrt{x^2+M^2}}}{\sqrt{\kappa}(x^2+M^2)^{1/4}} d(kx), \quad \kappa = \frac{1}{\xi}. \tag{D2}$$

In order to study the asymptotic form of this integral, we consider the following ratio:

$$I(M) \equiv J(M)/e^{-\kappa M} = \sqrt{\kappa}\int_{-\infty}^{\infty} \frac{e^{-\kappa(\sqrt{x^2+M^2}-M)}}{(x^2+M^2)^{1/4}} \mathrm{d}x \equiv \sqrt{\kappa}\int_{-\infty}^{\infty} f(x,M)\mathrm{d}x. \tag{D3}$$

The integrand $f(x,M)$ is rewritten as

$$f(x,M) = (x^2+M^2)^{-1/4} \exp\left[- \frac{\kappa x^2}{\sqrt{x^2+M^2}+M} \right]. \tag{D4}$$

Then, we separate the integral (D3) into the two parts $I(M) = \sqrt{\kappa}(I_1(M) + I_2(M))$, where

$$I_1(M) = 2\int_0^M f(x,M)\mathrm{d}x \quad \text{and } I_2(M) = 2\int_M^{\infty} f(x,M)\mathrm{d}x. \tag{D5}$$

It is easily shown that

$$\lim_{M\to\infty} I_2(M) \leqslant \lim_{M\to\infty} 2\int_M^{\infty} \frac{e^{-\kappa x}}{\sqrt{x}}\mathrm{d}x = 0 \tag{D6}$$

for $\kappa > 0$. As the function $f(x,M)$ satisfies the inequalities

$$\frac{e^{-\kappa x^2/2M}}{2^{1/4}\sqrt{M}} \leqslant f(x,M) \leqslant \frac{e^{-\kappa x^2/\{(\sqrt{2}+1)M\}}}{\sqrt{M}} \tag{D7}$$

for $0 \leqslant x \leqslant M$, we obtain the inequalities

$$2^{1/4}\sqrt{\pi} \leqslant I(\infty) \leqslant (\sqrt{2}+1)^{1/2}\sqrt{\pi} \tag{D8}$$

for $T \geqslant T_c$. Thus, we finally arrive at

$$J(M) \simeq A'_+(T)e^{-M/\xi}, \quad A'_+(T_c) \neq 0. \tag{D9}$$

This is nothing but Morita's sum rule.

It will be instructive to present here a rough but direct estimate of the integral (D2) as follows:

$$J(M) \simeq \sqrt{\frac{\kappa}{M}}\int_{-\infty}^{\infty} \exp\left[- \kappa M\left(1 + \frac{x^2}{2M^2}\right)\right]\mathrm{d}x = \sqrt{2\pi}e^{-\kappa M}. \tag{D10}$$

The prefactor $\sqrt{2\pi}$ in Eq. (D10) satisfies the inequality (D8). This rough estimation has been already made in Ref. 26 in applications of Morita's sum rule to the coherent anomaly method.[27]

The above extended form (D1) will be derived rigorously[28] using again the topological interaction method by applying the interaction $J''\Sigma_{k=1}^{N} S_{1,i+k}S_{M,j+k}$ for fixed i and j to the two-dimensional Ising model with width M and length N.

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On the largest singular values of random matrices with independent Cauchy entries

Alexander Soshnikov[a)]
Department of Mathematics, University of California at Davis, One Shields Avenue, Davis, California 95616

Yan V. Fyodorov[b)]
Department of Mathematical Sciences, Brunel University, Uxbridge UB83PH, United Kingdom

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We apply the method of determinants to study the distribution of the largest singular values of large $m \times n$ real rectangular random matrices with independent Cauchy entries. We show that for a special one-parametric class of statistics the properties of the largest singular values (rescaled by a factor $1/m^2n^2$) agree in the limit with the statistical properties of the Poisson random point process with the intensity $(1/\pi)x^{-3/2}$ and, therefore, are different from the Tracy–Widom law. Among other corollaries of our method we show an interesting connection between the mathematical expectations of the determinants of the complex rectangular $m \times n$ standard Wishart ensemble and the real rectangular $2m \times 2n$ standard Wishart ensemble. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1855932]

I. INTRODUCTION AND FORMULATION OF RESULTS

The main goal of this paper is to study the spectral properties of a large random matrix with independent identically distributed (i.i.d.) Cauchy entries. In other words we consider a rectangular $m \times n$ matrix $A=(a_{ij}), 1 \leqslant i \leqslant m, 1 \leqslant j \leqslant n$, where $\{a_{ij}\}$ are independent identically distributed Cauchy random variables with the probability density $f(x)=1/\pi(1+x^2)$. Our goal is to study the singular values of A as the dimensions of a matrix go to infinity, $m \to \infty$, $n \to \infty$. This is clearly equivalent to studying the eigenvalues of a positive-definite $n \times n$ matrix $M=A^tA$. Matrices of such type are quite often called sample covariance matrices in random matrix literature. Positive-definite matrices are of particular importance in statistics (we refer to Refs. 33, 50, and 20 for the classical works on statistical applications of the spectral properties of Wishart matrices, and Refs. 21, 14, 16, and 30 for a few recent developments and applications to various fields). They also are of long-standing interest in nuclear physics, starting with the classical works of Refs. 49 and 9. More recently they were used to model the "dissipative" part of the effective Hamiltonian in quantum chaotic scattering (see Ref. 19 and references therein) and appeared to be very intimately connected with the "chiral" ensembles studied in quantum chromodynamics (see Ref. 45). As other important applications of random positive-definite matrices we mention that they are used in a branch of condensed matter theory known as mesoscopics to model famous universal conductance fluctuations and other transport properties of small metallic samples and quantum dots (see Ref. 4) and also emerged in theory of information communication in random environment.[44]

It is well known that if the entries of A are i.i.d. random variables with zero mean and finite variance σ^2, the empirical distribution function of the eigenvalues of $(1/n)A^tA$ converges in the limit $m \to \infty$, $n \to \infty$, $m/n \to \gamma \in (0, +\infty)$ to the Marchenko–Pastur law (see, e.g., Refs. 29 and 2) defined by its density

[a)]Electronic mail: soshniko@math.ucdavis.edu.
[b)]Electronic mail: yan.fyodorov@brunel.ac.uk.

$$p_\gamma(x) = (2\pi x\gamma\sigma^2)^{-1}\sqrt{(b-x)(x-a)}, \quad a \leqslant x \leqslant b, \tag{1}$$

where $a=\sigma^2(1-\gamma^{-1/2})^2$ and $b=\sigma^2(1+\gamma^{-1/2})^2$ (we assume here $\gamma \geqslant 1$). Since the spectrum of A^tA differs from the spectrum of AA^t only by the multiplicity of the eigenvalue $\lambda=0$ (for $m \geqslant n$ the matrix AA^t has $m-n$ additional zero eigenvalues) for the rest of the paper we can assume $m \geqslant n$. Under the assumption that the fourth moment of a_{ij} is finite, Yin, Bai, and Krishnaiah (Ref. 51, see also Refs. 34 and 3) showed that the largest eigenvalue of $(1/n)A^tA$ converges to b almost surely. Recently Johnstone proved that in the standard Wishart case [i.e., $\{a_{ij}\}$ are i.i.d. $N(0,1)$ random variables] the properly rescaled largest eigenvalue converges in distribution to the $\beta=1$ Tracy–Widom distribution,[42] (see also Ref. 41). Soshnikov[38] generalized the result of Johnstone to the non-Gaussian case provided $n-m=O(n^{1/3})$ and the moments of the matrix entries do not grow very fast. There are quite a few standard methods that have been successfully used for Wigner and sample covariance matrices in the case when second and higher moments of matrix entries exist, most notably the method of moments,[47,48,35–38] the method of resolvents,[29,28,2] the method of orthogonal polynomials,[13,25] the method used by Johansson[23] (and recently extended by Ben Arous and Péché to the case of sample covariance matrices) which is based on the Kazakov–Brézin–Hikami trick,[27,7,8] etc. Unfortunately, the above-mentioned approaches are not suitable for the Cauchy case. In particular, one can expect the spectral properties of A^tA in the Cauchy case to be rather different from the case of a finite variance. In our view this makes the studies of the Cauchy case especially interesting. Denote the eigenvalues of A^tA by $\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant \cdots \geqslant \lambda_n$. It is expected that the majority of the eigenvalues are proportional to mn. We would like to specifically single out Ref. 11 where Cizeau and Bouchard studied the spectral properties of the Wigner random matrices with the heavy tails (see also Refs. 10 and 22 for physical papers on the so-called Lévy–Smirnov unitary ensembles). Among other things, Cizeau and Bouchard argued (on a physical level of rigor) that the empirical distribution function of the eigenvalues of a properly normalized Wigner matrix (with the heavy tails of the marginal distribution of matrix entries) converges to a limiting distribution that can be obtained as a solution of a quite complicated system of two integral equations [we refer to the formulas (15), (12a), (12b) in Ref. 11]. It is not difficult to guess the right order of the normalization: after the normalization, the norm of any given matrix row has to be of order of a constant (in particular in the Cauchy case one has to normalize the matrix entries by n^{-1} and in the case of a finite variance the normalization is $1/\sqrt{n}$). The support of the limiting distribution is the whole real line. One can expect (arguing at the same level of physical rigor) to derive a similar system of integral equations for the limiting distribution function of the eigenvalues of $(1/mn)A^tA$ in the case of the i.i.d. Cauchy entries of A. The support of the limiting distribution should be the positive half of the real line. Our results formulated below indicate that the asymptotics of the spectral density at infinity should be $1/\pi x^{3/2}$. This suggests that the largest eigenvalues of A^tA grow faster than mn; in fact, we will show below that the largest eigenvalues are of the order of m^2n^2. Let us rescale the eigenvalues by that factor:

$$\tilde{\lambda}_i = \frac{\lambda_i}{n^2m^2}, \quad i = 1, \ldots, n. \tag{2}$$

The goal of this paper is to study the local distribution of the largest eigenvalues by the method of determinants. Our main results are Theorems 1.1 and 1.2 formulated below.

Theorem 1.1: *Let A be a random rectangular $m \times n$ matrix $(m \geqslant n)$ with i.i.d. Cauchy entries and z a complex number with a positive real part. Then as $n \to \infty$ we have*

$$\lim_{n\to\infty} E\left(\det\left(1+\frac{z}{m^2n^2}A^tA\right)\right)^{-1/2} = E\prod_{i=1}^{n}(1+z\tilde{\lambda}_i)^{-1/2} = \exp\left(-\frac{2}{\pi}\sqrt{z}\right) \tag{3}$$

$$= \mathbf{E}\prod_{i=1}^{\infty}(1+zx_i)^{-1/2}, \tag{4}$$

where we consider the branch of $\sqrt{z}$ *on* $D=\{z:\Re z>0\}$ *such that* $\sqrt{1}=1$, *E denotes the mathematical expectation with respect to the random matrix ensemble defined above,* **E** *denotes the mathematical expectation with respect to the inhomogeneous Poisson random point process on the positive half-axis with the intensity* $1/\pi x^{3/2}$, *and the convergence is uniform inside D* (*i.e., it is uniform on the compact subsets of D*). *For a real positive* $z=t^2$, $t\in\mathbb{R}$, *one can estimate the rate of convergence, namely,*

$$\lim_{n\to\infty} E\left(\det\left(1+\frac{t^2}{m^2n^2}A^tA\right)\right)^{-1/2}=\lim_{n\to\infty} E\prod_{i=1}^{n}(1+t^2\tilde{\lambda}_i)^{-1/2}=\exp\left(-\frac{2}{\pi}|t|(1+o(n^{-1/2+\epsilon}))\right), \quad (5)$$

where ϵ *is an arbitrary small positive number and the convergence is uniform on the compact subsets of* $[0,+\infty)$.

We will discuss the properties of Poisson random point processes in the Appendix. A very useful introduction to the elementary theory and methods of random point processes is Ref. 12. It is not a coincidence that the intensity of the Poisson random process in the above theorem is equal to the leading term of the asymptotics of the density of the square of a standard Cauchy random variable.

We claim that the result can be generalized to the case of a sparse random matrix with Cauchy entries. Let, as before, $\{a_{jk}\}$, $1\leqslant j\leqslant m$, $1\leqslant k\leqslant n$, be i.i.d. Cauchy random variables, and $Q=(q_{jk})$ be a $m\times n$ nonrandom rectangular $0-1$ matrix such that the number of nonzero entries in each column is fixed and equals to b_n. For technical reasons we assume that b_n grows to infinity as some power of n, i.e., $b_n\geqslant n^{\alpha}$, for some $0<\alpha\leqslant 1$, and $\ln m$ is much smaller than any power of n. We define a $m\times n$ rectangular matrix A with the entries $\Gamma_{jk}=q_{jk}a_{jk}$, $1\leqslant j\leqslant m$, $1\leqslant k\leqslant n$. As before we denote by $\lambda_1\geqslant\lambda_2\cdots\geqslant\lambda_n$ the eigenvalues of $\Gamma^t\Gamma$. The appropriate rescaling for the largest eigenvalues in this case is going to be $\tilde{\lambda}_i=\lambda_i/m^2b_n^2$, $i=1,\ldots,n$. We claim that the result of Theorem 1.1 can be extended to the case of a sparse random matrix Γ.

Theorem 1.2: *Let* Γ *be a sparse random rectangular* $m\times n$ *matrix* ($m\geqslant n$) *defined as above and z a complex number with a positive real part. Then as* $n\to\infty$ *we have*

$$\lim_{n\to\infty} E\left(\det\left(1+\frac{z}{m^2b_n^2}\Gamma^t\Gamma\right)\right)^{-1/2}=\lim_{n\to\infty} E\prod_{i=1}^{n}(1+z\tilde{\lambda}_i)^{-1/2}=\exp\left(-\frac{2}{\pi}\sqrt{z}\right) \quad (6)$$

$$=\mathbf{E}\prod_{i=1}^{\infty}(1+zx_i)^{-1/2}, \quad (7)$$

where, as in Theorem 1.1, we consider the branch of $\sqrt{z}$ *on* $D=\{z:\Re z>0\}$ *such that* $\sqrt{1}=1$, *E denotes the mathematical expectation with respect to the random matrix ensemble defined in the paragraph above the theorem,* **E** *denotes the mathematical expectation with respect to the inhomogeneous Poisson random point process on the positive half-axis with the intensity* $1/\pi x^{3/2}$, *and the convergence is uniform inside D* (*i.e., it is unform on the compact subsets of D*). *For a real positive* $z=t^2$, $t\in R$, *one can get an estimate on the rate of convergence, namely,*

$$E\left(\det\left(1+\frac{t^2}{m^2b_n^2}\Gamma^t\Gamma\right)\right)^{-1/2}=E\prod_{i=1}^{n}(1+t^2\tilde{\lambda}_i)^{-1/2}=\exp\left(-\frac{2}{\pi}t(1+o(b_n^{-1/2+\epsilon}))\right), \quad (8)$$

where ϵ *is an arbitrary small positive number and the convergence is uniform on the compact subsets of* $[0,+\infty)$.

The result of Theorem 1.2 can be generalized even further. Let the setting be as in Theorem 1.2 but relax the condition that the number of nonzero entries in each column is exactly b_n to the condition $\Sigma_{k=1}^{n}q_{jk}=b_n(1+o(1))$, $j=1,\ldots,m$ (for example, the relaxed condition is satisfied by a typical realization of a random matrix Q with independent Bernoulli $0-1$ entries with $\Pr(q_{jk}=1)=b_n/n$]. Then we still have

$$E\left(\det\left(1+\frac{z}{m^2b_n^2}\Gamma^t\Gamma\right)\right)^{-1/2}=\exp\left(-\frac{2}{\pi}\sqrt{z}\right)(1+o(1)).$$

The proof is almost identical to the proof of Theorem 1.2 and will be left to the reader.

The case when the number of nonzero terms of Q is fixed in each row can be treated in a similar manner.

An important consequence of Theorems 1.1 and 1.2 is that the statistical properties of the largest eigenvalues $\tilde{\lambda}_1,\tilde{\lambda}_2,\ldots$ are drastically different from the statistical properties of the (rescaled) largest eigenvalues in the GOE[42] and real Wishart cases[25] that are described by the ($\beta=1$) Tracy–Widom law.

Theorems 1.1 and 1.2 follow from Proposition 1 formulated below.

Proposition 1: *Let $A=(a_{jk})$ be a random rectangular $m\times n$ matrix with independent (not necessarily identically distributed) entries with the characteristic functions of the matrix entries $g_{jk}(s)=E\exp(isa_{jk})$. Let $t_i>0$, $i=1,\ldots,r$, be some positive parameters. Then the following formula holds.*

$$E\left(\prod_{i=1}^{r}\det(1+t_i^2A^tA)\right)^{-1/2}=(2\pi)^{-r(n+m)/2}\int_{R^{r(n+m)}}\prod_{i=1}^{r}d^ns^{(i)}d^mp^{(i)}\times\exp\left(-\sum_{i=1}^{r}(|s^{(i)}|^2/2+|p^{(i)}|^2/2)\right)\prod_{1\leqslant j\leqslant m,1\leqslant k\leqslant n}g_{jk}\left(\sum_{i=1}^{r}t_ip_j^{(i)}s_k^{(i)}\right). \tag{9}$$

Theorems 1.1 and 1.2 imply several important corollaries that are given in the next section.

The proofs of Theorems 1.1 and 1.2 and Proposition 1 are given in the next section. Section III is devoted to application of the method of determinants to random matrices with i.i.d. complex entries. We prove in Sec. III the analogue of Proposition 1 (Proposition 2) in the complex case and as a corollary establish an interesting connection between the determinants in the $2m\times 2n$ rectangular real Wishart case and the $m\times n$ rectangular complex Wishart case (see Lemma 1).

II. PROOFS OF THEOREMS 1.1 AND 1.2

We start with the proof of Proposition 1. Consider $(\det(1+t^2A^tA))^{-1/2}$, $t>0$. Let $s=(s_1,\ldots,s_n)^t$, $p=(p_1,\ldots,p_m)^t$ be real n- and m-dimensional column vectors. Let $B=B(t)=\left(\begin{smallmatrix} Id & tiA \\ tiA^t & Id\end{smallmatrix}\right)$ and $d^nsd^mp=\Pi_{i=1}^n ds_i\Pi_{j=1}^m p_i$.

Then

$$(\det(1+t^2A^tA))^{-1/2}=\left(\det\begin{pmatrix}1 & tiA\\ tiA^t & 1\end{pmatrix}\right)^{-1/2}=(\det(B))^{-1/2},$$

and, since the Hermitian part of the matrix B is positive definite, $(\det(B))^{-1/2}$ can be written as the Gaussian integral over $\mathbb{R}^{m+n}$ [according to our notations introduced above (s,p) is an $(m+n)$-dimensional vector; in the next formula $(s,p)B(s,p)^t$ stands for the value of the quadratic form associated with the matrix B on the vector (s,p)]:

$$\begin{aligned}(\det(1+t^2A^tA))^{-1/2}&=(\det(B))^{-1/2}\\&=\left(\frac{1}{\pi}\right)^{(n+m)/2}\int d^nsd^mp\exp(-(s,p)B(s,p)^t)\\&=\left(\frac{1}{\pi}\right)^{(n+m)/2}\int d^nsd^mp\exp(-(|s|^2+|p|^2))\left(\exp\left(-2i\sum_{1\leqslant j\leqslant m,1\leqslant k\leqslant n}ta_{jk}p_js_k\right)\right).\end{aligned} \tag{10}$$

The formula (10) and the independence of matrix entries imply

$$E\left(\prod_{i=1}^{r}\det(1+t_i^2A^tA)\right)^{-1/2}=\pi^{-r(n+m)/2}\int_{R^{r(n+m)}}\prod_{i=1}^{r}d^ns^{(i)}d^mp^{(i)}\exp\left(-\sum_{i=1}^{r}(|s^{(i)}|^2+|p^{(i)}|^2)\right)$$
$$\times E\prod_{1\leqslant j\leqslant m,1\leqslant k\leqslant n}\exp\left(2ia_{jk}\sum_{i=1}^{r}t_ip_j^{(i)}s_k^{(i)}\right)$$
$$=(2\pi)^{-r(n+m)/2}\int_{R^{r(n+m)}}\prod_{i=1}^{r}d^ns^{(i)}d^mp^{(i)}\exp\left(-\sum_{i=1}^{r}(|s^{(i)}|^2/2+|p^{(i)}|^2/2)\right)$$
$$\times\prod_{1\leqslant j\leqslant m,1\leqslant k\leqslant n}g_{jk}\left(\sum_{i=1}^{r}t_ip_j^{(i)}s_k^{(i)}\right). \tag{11}$$

The Proposition is proven.

To prove Theorem 1.1 we observe that the functions on the lhs of (3) are analytic and uniformly bounded in $D=\{z:\Re z>0\}$. Therefore, by the Vitali's theorem it is enough to prove the convergence for real positive z. Let us denote $z=t^2$, where t is a positive real number, and apply the result of the proposition in the case $r=1$. Since the matrix entries of A are i.i.d. Cauchy we have $g_{jk}(s)=g(s)=\exp(-|s|)$ and

$$E(\det(1+t^2A^tA))^{-1/2}=(2\pi)^{-(n+m)/2}\int_{R^{n+m}}d^nsd^mp\exp(-(|s|^2+|p|^2)/2)\prod_{1\leqslant j\leqslant n,1\leqslant k\leqslant m}\exp(-t|s_kp_j|)$$
$$=2^m\int_{R^n}d^ns(2\pi)^{-n/2}\exp\left(-\frac{1}{2}|s|^2\right)\int_{R_+^m}(2\pi)^{-m/2}$$
$$\times\exp\left(-\frac{1}{2}\sum_{j=1}^{m}(p_j^2+2p_jt\sum_{k=1}^{n}|s_k|)\right)$$
$$=\int_{R^n}d^ns(2\pi)^{-n/2}\exp\left(-\frac{1}{2}|s|^2\right)\Psi^m\left(t\sum_{k=1}^{n}|s_k|\right), \tag{12}$$

where $\Psi(y)=2e^{y^2/2}\int_y^{+\infty}(1/\sqrt{2\pi})e^{-t^2/2}dt$. In particular, $\Psi(0)=1$ and $\Psi'(0)=-(2/\pi)^{1/2}$. It is easy to see that the function $\Psi(y)$ is monotonically decreasing on $[0,+\infty)$, in particular $1=\Psi(0)=\max_{[0,+\infty)}\Psi(y)$. Indeed, $\Psi'(y)=2ye^{y^2/2}\int_y^{+\infty}(1/\sqrt{2\pi})e^{-t^2/2}dt-2(1/\sqrt{2\pi})$. The assertion then follows from the inequality $y^{-1}e^{-y^2/2}>\int_y^{+\infty}e^{-t^2/2}dt$ for $y>0$.

Replacing t by t/nm we arrive at

$$E\left(\det\left(1+\frac{t^2}{n^2m^2}A^tA\right)\right)^{-1/2}=\int_{R^n}d^ns(2\pi)^{-n/2}\exp\left(-\frac{1}{2}|s|^2\right)\Psi\left(\frac{t}{nm}\sum_{k=1}^{n}|s_k|\right)^m. \tag{13}$$

The rhs of the last formula suggests to use the law of large numbers and large deviations estimates for the sum of the absolute values of n standard Gaussian random variables. Since $\int(1/2\pi)|s|e^{-s^2/2}ds=(2/\pi)^{1/2}$, we see that $(1/n)\Sigma_{j=1}^{n}|s_j|=(2/\pi)^{1/2}+o(n^{-1/2+\epsilon})$ with probability $1-O(\exp(-n^{1.99\epsilon}))$. Recalling that $\Psi(0)=1$ and $\Psi'(0)=-(2/\pi)^{1/2}$ we get

$$E\left(\det\left(1+\frac{t^2}{n^2m^2}A^tA\right)\right)^{-1/2}=\int_{R^n}d^ns(2\pi)^{-n/2}\exp\left(-\frac{1}{2}|s|^2\right)\left(1-\frac{2t(1+o(n^{-1/2+\epsilon}))}{\pi m}\right)^m$$
$$=\left(1-\frac{2t(1+o(n^{-1/2+\epsilon}))}{\pi m}\right)^m=\exp\left(-\frac{2t(1+o(n^{-1/2+\epsilon}))}{\pi}\right),\quad(14)$$

for any $\epsilon>0$ Theorem 1.1 is then followed by the Vitali theorem.

The proof of Theorem 1.2 is very similar. Again we can restrict our attention to the case when z is a real positive number, $z=t^2$. We have

$$E(\det(1+t^2\Gamma^t\Gamma))^{-1/2}=\int_{R^n}d^ns(2\pi)^{-n/2}\exp\left(-\frac{1}{2}|s|^2\right)\prod_{j=1}^m\Psi\left(t\sum_{k=1}^n q_{jk}|s_k|\right).\quad(15)$$

Let $k_1^{(j)},k_2^{(j)},\ldots,k_{b_n}^{(j)}$ be the indices k for which $q_{jk}=1$. Then $\Sigma_{k=1}^n q_{jk}|s_k|=\Sigma_{l=1}^{b_n}|s_{k_l^{(j)}}|$ and we can claim that $(1/b_n\Sigma_{l=1}^{b_n}|s_{k_l^{(j)}}|=(2/\pi)^{1/2}+o(b_n^{-1/2+\epsilon})$ with probability $1-O(\exp(-b_n^{1.99\epsilon}))$ for each $1\leqslant j\leqslant m$. Since we assumed that $\ln(m)$ is much smaller than any power of n we get similarly to (14) that

$$E\left(\det\left(1+\frac{t^2}{m^2b_n^2}\Gamma^t\Gamma\right)\right)^{-1/2}=\int_{R^n}d^ns(2\pi)^{-n/2}\exp\left(-\frac{1}{2}|s|^2\right)\left(1-\frac{2t(1+o(b_n^{-1/2+\epsilon}))}{\pi m}\right)^m$$
$$=\left(1-\frac{2t(1+o(b_n^{-1/2+\epsilon}))}{\pi m}\right)^m=\exp\left(-\frac{2t(1+o(b_n^{-1/2+\epsilon}))}{\pi}\right).\quad(16)$$

Theorem 1.2 is proven.

Below we restrict our attention to the corollaries of Theorem 1.1 (full matrix case). The corollaries of Theorem 1.2 are basically identical to those of Theorem 1.1 (with an obvious change of n to b_n where it is needed).

Remark 0: We are not aware that the results of Theorems 1.1 and 1.2 are enough to imply that ths statistics of the largest eigenvalues are Poisson in the limit of $n\to\infty$. Indeed, to prove the Poisson statistics in the limit one has to show that

$$\lim_{n\to\infty}E\prod_{i=1}^n(1+f(\tilde{\lambda}_i))=\mathbf{E}\prod_{i=1}^{+\infty}(1+f(x_i))\quad(17)$$

for a sufficiently large class of the test functions f. The results of Theorems 1.1 and 1.2 claim that (17) is valid for $f(x)=(1+zx)^{-1/2}-1$ for all z such that $\Re z>0$. Below we formulate several corollaries of our main result that are weaker than the claim about the Poisson statistics, but still give us some information about the behavior of the largest eigenvalues. The proof of the Poisson statistics for the largest eigenvalues in Wigner random matrices with heavy tails will appear in Ref. 39.

Remark 1: It follows immediately from the result of Theorem 1.1 that "only a finite number" of the eigenvalues λ_i are of the order of n^2m^2. Indeed, let $N_{n,m}$ be an integer growing to infinity arbitrarily slowly as $n\to\infty$ and let $\delta>0$ be an arbitrarily small positive number. Then $\Pr(\#(\lambda_i\geqslant\delta n^2m^2)\geqslant N_{n,m})\to 0$ as $n\to\infty$. Indeed, suppose this is not the case. Then $\Pr(\#(\lambda_i\geqslant\delta n^2m^2)\geqslant N_{n,m})\geqslant\kappa>0$ and $E(\det(1+(t^2/n^2m^2)A^tA))^{-1/2}\leqslant\kappa(1+t^2\kappa)^{-N_{n,m}}+(1-\kappa)1$. One obtains a contradiction since for $t=N_{n,m}^{-1}$ the rhs of the last inequality does not go to zero (see also the next remark). One can also rewrite the statement of this remark in the following way: for any positive δ, κ, there exist $n_0(\delta,\kappa)$ and $C(\delta,\kappa)$ such that $\Pr(\#(\lambda_i\geqslant\delta n^2m^2)\geqslant C)<\kappa$ for all $n_0\leqslant n\leqslant m$.

Remark 2: It is clear from the proof of Theorem 1.1 that the asymptotic result

$$E\left(\det\left(1+\frac{t^2}{n^2m^2}A^tA\right)\right)^{-1/2}=\exp\left(-\frac{2t(1+o(n^{-1/2+\epsilon}))}{\pi}\right)$$

holds uniformly in t on compact subsets of $[0,+\infty)$. In particular the result is valid for a sequence $t_n\to 0$.

Below we formulate and prove some additional consequences of Theorem 1.1. Our first observation is that one can repeatedly differentiate (3) with respect to parameter z.

Corollary 1: Let $\Re z>0$. *Then*

$$\lim_{n\to\infty}E\prod_{i=1}^{n}(1+z\tilde{\lambda}_i)^{-1/2}\left(\sum_{j=1}^{n}\frac{\tilde{\lambda}_i}{1+z\tilde{\lambda}_i}\right)=\frac{2}{\pi}z^{-1/2}\exp\left(-\frac{2}{\pi}\sqrt{z}\right) \tag{18}$$

$$=\mathbf{E}\prod_{i=1}^{\infty}(1+zx_i)^{-1/2}\left(\sum_{j=1}^{\infty}\frac{x_i}{1+zx_i}\right), \tag{19}$$

where, as above, **E** *stands for the mathematical expectation with respect to the inhomogeneous Poisson random point process on* $(0,+\infty)$ *with the intensity* $\rho(x)=1/\pi x^{3/2}$.

Remark 3: If we let $z\to 0$ in (18), one gets $E(\Sigma_{j=1}^{n}\tilde{\lambda}_i)=+\infty$, which trivially follows from the fact that matrix entries of A are Cauchy random variables. Essentially the result of the corollary can tell us how fast the mathematical expectation $E(\Sigma_j\tilde{\lambda}_j)$ grows if we restrict the summation only to $\tilde{\lambda}_i\leqslant L$ where L is large.

Proof of Corollary 1: The result immediately follows from the uniform convergence of the analytic functions in (3) and (4).

By differentiating (3) twice one can obtain in a similar fashion that

$$\lim_{n\to\infty}E\prod_{i=1}^{n}(1+z\tilde{\lambda}_i)^{-1/2}\left(\left(\sum_{j=1}^{n}\frac{\tilde{\lambda}_i}{1+z\tilde{\lambda}_i}\right)^2+\sum_{i=1}^{n}\frac{(\tilde{\lambda}_i)^2}{(1+z\tilde{\lambda}_i)^2}\right)=\left(\frac{4}{\pi^2}z^{-1}+\frac{2}{\pi}z^{-3/2}\right)\exp\left(-\frac{2}{\pi}\sqrt{z}\right). \tag{20}$$

Corollary 2: There is a constant C *which depends on* γ *such that for* $\Pr(\lambda_1/n^2m^2>x)<Cx^{-1/2}$ *uniformly for large* $n\leqslant m$ *and* x.

Indeed, it follows from Theorem 1.1 and Remark 1 that $E(1+t^2\tilde{\lambda}_1)^{-1/2}\geqslant\exp(-2t(1+o(n^{-1/2+\epsilon}))/\pi)$ uniformly in t on compact subsets of $[0,\infty)$. Therefore $(1-\Pr(\tilde{\lambda}_1>x))+1/\sqrt{1+t^2x}\times\Pr(\tilde{\lambda}_1>x)\geqslant\exp(-(2/\pi)t(1+o(n^{-1/2+\epsilon})))$, which implies $1-\exp(-(2/\pi)t(1+o(n^{-1/2+\epsilon})))\geqslant(1-1/\sqrt{1+t^2x})\Pr(\tilde{\lambda}_1>x)$. Choosing $t^2x=1$ we obtain that $(2/\pi)\gamma x^{-1/2}(1+\delta)\geqslant(1-2^{-1/2})\Pr(\tilde{\lambda}_1>x)$ for all sufficiently large n, m, and x.

Remark 4: It is not difficult to show that in probability $\lambda_1=O(n^2m^2)$. To see this we observe that the operator norm $\|A\|$ can be bounded from below by $\max_{1\leqslant j\leqslant m,1\leqslant k\leqslant n}|a_{jk}|$. The maximum of $n\times m$ i.i.d. Cauchy random variables is of the order $O(nm)$ [with the limiting distribution of $1/nm\times\max_{1\leqslant j\leqslant m,1\leqslant k\leqslant n}|a_{jk}|$ easily computable, namely $\Pr((1/nm)\max_{1\leqslant j\leqslant m,1\leqslant k\leqslant n}|a_{jk}|\leqslant x)\to\exp(-2/\pi x)$]. We expect that the limiting distribution λ_1/n^2m^2 also exists and is given by the distribution of the rightmost particle in the Poisson process with the intensity $\rho(x)=(1/\pi)x^{-3/2}$, in other words, $\lim_{n\to\infty}\Pr(\tilde{\lambda}_1<x)=\exp(-(2/\pi)x^{-1/2})$.

It is a useful exercise to see what Proposition 1 gives in the Wishart case. Below we treat the case of one determinant:

$$
\begin{aligned}
E(\det(1+t^2A^tA))^{-1/2} &= (2\pi)^{-(n+m)/2}\int_{R^{n+m}} d^n s d^m p\, \exp(-(|s|^2+|p|^2)/2) \\
&\quad \times \prod_{1\leqslant j\leqslant n,1\leqslant k\leqslant m} \exp\left(-\frac{1}{2}(ts_kp_j)^2\right) \\
&= \int_{R^n} d^n s (2\pi)^{-n/2} \exp\left(-\frac{1}{2}|s|^2\right)\int_{R^m} d^m p (2\pi)^{-m/2} \\
&\quad \times \prod_{k=1}^{m} \exp\left(-\frac{1}{2}p_k^2\left(1+t^2\sum_{j=1}^{n} s_j^2\right)\right) \\
&= \int_{R^n} d^n s (2\pi)^{-n/2} \exp\left(-\frac{1}{2}|s|^2\right)\left(1+t^2\sum_{j=1}^{n} s_j^2\right)^{-m/2} \\
&= c_n\int_0^{+\infty} \exp\left(-\frac{1}{2}r^2\right) r^{n-1}(1+t^2r^2)^{-m/2}\, dr \\
&= c_n 2^{n/2-1}\int_0^{+\infty} e^{-r} r^{n/2-1}(1+2t^2r)^{-m/2}\, dr, \qquad (21)
\end{aligned}
$$

where c_n is the normalization constant, $c_n^{-1}=\int_0^{+\infty}\exp\left(-\frac{1}{2}r^2\right)r^{n-1}\,dr=2^{n/2-1}\Gamma(n/2)$. To study the global distribution of the eigenvalues in the Wishart ensemble one has to consider rescaling $t^2 \to t^2/n$ (since typical eigenvalues of A^tA are of the order of n). It follows that

$$
\begin{aligned}
E\left(\det\left(1+\frac{t^2}{n}A^tA\right)\right)^{-1/2} &= [\Gamma(n/2)]^{-1}\int_0^{+\infty} e^{-r} r^{n/2-1}\left(1+2t^2\frac{r}{n}\right)^{-m/2} dr \\
&= [\Gamma(2/n)]^{-1}(2/n)^{n/2}\int_0^{+\infty} e^{-n/2r} r^{n/2}(1+t^2r)^{-m/2} r^{-1}\, dr \\
&= [\Gamma(2/n)]^{-1}(2/n)^{n/2}\int_0^{+\infty} e^{-n/2\mathcal{L}(z)} z^{-1}\, dz, \qquad (22)
\end{aligned}
$$

where $\mathcal{L}(z)=z+(m/n)\ln(1+t^2z)-\ln z$. The asymptotics of the last integral can be obtained by the steepest descent method. The formulas are especially simple in the square case $m=n$. One then can find a positive solution of the equation

$$
\frac{d\mathcal{L}}{dz} = 1+\frac{t^2}{1+t^2z}-\frac{1}{z} = \frac{t^2z^2+z-1}{z(1+t^2z)} = 0 \qquad (23)
$$

to be $z(t)=(-1+\sqrt{4t^2+1})/2t^2$. Taking into account that $d^2\mathcal{L}/dz^2=\sqrt{4t^2+1}$ at $z=z(t)$ we obtain that in the square Wishart case

$$
\begin{aligned}
E\left(\det\left(1+\frac{t^2}{n}A^tA\right)\right)^{-1/2} &= \frac{2^n n^{n/2}}{\Gamma(n/2)}\exp\left(-n\frac{-1+\sqrt{4t^2+1}}{4t^2}\right)(1 \\
&\quad +\sqrt{4t^2+1})^{-n}\sqrt{\frac{2\pi\sqrt{4t^2+1}}{n}}\frac{2t^2}{-1+\sqrt{4t^2+1}}(1+o(1)). \qquad (24)
\end{aligned}
$$

The fact that the asymptotics in (24) is exponential in n is standard. Indeed, it is a straightforward exercise to verify that

$$\lim_{n\to\infty}\frac{1}{n}\ln\left(E\left(\det\left(1+\frac{t^2}{n}A^tA\right)\right)^{-1/2}\right)=-\frac{1}{2}\int_0^4(\ln(1+t^2x)p_1(x))\,dx, \tag{25}$$

where $p_1(x)$ is the probability density of the Marchenko–Pastur law defined in (1), which reflects the law of large numbers for the linear statistics $\Sigma_{i=1}^n \ln(1+t^2\lambda_i n^{-1})$ where $\{\lambda_i\}_{i=1}^n$ are the eigenvalues of the real Wishart matrix. The variance of the linear statistics is bounded and has a limit as $n\to\infty$ (for a rather general class of polynomial ensembles of random matrices it was first discovered by Johansson in (Ref. 24), thus contributing a constant term to the rhs of (24), so that

$$\begin{aligned}E\left(\det\left(1+\frac{t^2}{n}A^tA\right)\right)^{-1/2}&=E\left(\exp\left(-\frac{1}{2}\sum_{i=1}^n\ln(1+t^2\lambda_i n^{-1})\right)\right)\\&=\exp\left(-\frac{1}{2}E\left(\sum_{i=1}^n(\ln(1+t^2\lambda_i n^{-1}))\right)+\frac{1}{8}d(t)+o(1)\right),\end{aligned} \tag{26}$$

where $d(t):=\lim_{n\to\infty}\mathrm{Var}(\Sigma_{i=1}^n(\ln(1+t^2\lambda_i n^{-1})))$ and can be explicitely calculated (see Ref. 24, Theorem 2.4).

Remark 5: Another class of random matrices we are particularly interested in is the Rademacher random matrices (i.e., square random matrices with ±1 i.i.d. entries), which we are going to denote by $\mathcal{R}$. It appears that the questions of the invertibility of a Rademacher random matrix and the estimate of the norm of the inverse are of great importance in geometric functional analysis (for example, in connection with a deterministic construction of Euclidean sections of convex bodies). Similar to the previous analysis one can obtain

$$E\frac{1}{\sqrt{\det(1+t^2\mathcal{R}^t\mathcal{R})}}=\frac{1}{(2\pi)^n}\int_{R^{2n}}\prod_{i=1}^n du_i dv_i\exp\left(-\frac{1}{2}\sum_{i=1}^n(u_i^2+v_i^2)\right)\prod_{j,k=1}^n\cos(tu_jv_k). \tag{27}$$

The fact that a Rademacher matrix R is invertible with probability going to 1 as $n\to\infty$ was proved by J.Komlós (see, e.g., Ref. 6, Chap. 14). More recently, Kahn, Komlós and Szemeredi[26] proved that the probability that R is invertible is exponentially close to 1. To the best of our knowledge there is no known estimate on the norm of the inverse matrix (which, in our language, corresponds to the estimate of the smallest eigenvalue of R^tR).

III. COMPLEX MATRICES WITH i.i.d. ENTRIES

In this section we consider the ensemble of $n\times n$ complex random matrices $M=A^*A$, $A=(A_{jk})_{1\leqslant j\leqslant m,1\leqslant k\leqslant n}$, with the joint distribution of the matrix entries of A given by the formula

$$\Pr(A)dA\overline{dA}=\prod_{1\leqslant j\leqslant m,\ 1\leqslant k\leqslant n}\left\{d\Re a_{jk}d\Im a_{jk}\frac{1}{\pi}f(|a_{jk}|^2)\right\}. \tag{28}$$

In other words $\{a_{jk},1\leqslant j\leqslant m,1\leqslant k\leqslant n\}$ are independent indentically distributed random variables with a distribution depending only on the radial component, and $f(x)$ is the density of the distribution of $|a_{jk}|^2$. The ensemble (28) is a generalization of the standard Wishart (Laguerre) ensemble which corresponds to the choice $f(x)=e^{-x}$.

In the standard Wishart (Laguerre) case it is known that the smallest eigenvalues are proportional to $1/n^2$, and the (rescaled) k-point correlation functions are given in the limit $n\to\infty$ by the determinants

$$\rho_k(x_1,\ldots,x_k)=\det(K(x_i,x_j))_{i,j=1,\ldots,k},\quad k=1,2,3,\ldots, \tag{29}$$

with the Bessel kernel (with $\alpha=0$). Then

$$K^{(\alpha)}(x,y) = \frac{J_\alpha(2\sqrt{x})\sqrt{y}J'_\alpha(2\sqrt{y}) - J_\alpha(2\sqrt{y})\sqrt{x}J'_\alpha(2\sqrt{x})}{x-y}, \tag{30}$$

where J_ν is the J-Bessel function, appears as the limit of the rescaled correlation kernel at the hard edge in the Laguerre and Jacobi ensembles (see, e.g., Refs. 15 and 43).

Ban Arous and Péché,[5] following the approach suggested by Johansson[23] for Wigner matrices, have recently shown universality of the limiting distribution of the smallest eigenvalues (as well as in the bulk of the spectrum) for a special class of sample covariance matrices. Their technique requires that entries of A have a Gaussian component.

One of the possible ways to attack this problem for an ensemble (28) (assuming that all moments exist, i.e., and do not grow very fast) is to study the mathematical expectation of the ratio of determinants

$$Z(\eta_1, \eta_2, \ldots, \eta_k, \mu_1, \ldots, \mu_l) = E\frac{\prod_{i=1}^{k} \det(1 + \eta_i^2 A^* A)}{\prod_{j=1}^{l} \det(1 + t_j^2 A^* A)}$$

for appropriately scaled (large) real numbers $\eta_1, \ldots, \eta_k, t_1, \ldots, t_l$. For the standard complex Wishart (Laguerre) case these expectation values were calculated exactly for any k, l, n (see Refs. 17 and 40 and references therein), and also used to address objects interesting in mesoscopic physics,[18] and quantum chromodynamics.[1]

In particular, one can easily see that $(\partial/\partial\eta)Z(\eta,t)|_{\eta=t} = E\Sigma_{i=1}^{n} 2\eta\lambda_i/(t^2+\lambda_i)$, where $0 \leqslant \lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n$ are the eigenvalues of A^*A. Such an object can be used to extract the mean eigenvalue density. In a similar fashion, by taking partial derivatives of $Z(\eta_1, \ldots, \eta_k, t_1, \ldots, t_l)$ of higher orders, one can study the correlations of the eigenvalues of A^*A. To show the universality of the distribution of the smallest eigenvalues one needs to show that local statistical quantities at the edge of the spectrum (near the origin) do not depend (in the limit $n \to \infty$) on the second and higher moments of f.

The next proposition is analogous to Proposition 1 in the real case.

Proposition 2: Let A be a random rectangular $m \times n$ matrix with the probability distribution given by (28). Let $t_l > 0$, $l = 1, \ldots, r$, be some positive parameters. Then the following formula holds:

$$E\left(\prod_{l=1}^{r} \det(1 + t_l^2 A^t A)\right)^{-1} = \pi^{-r(n+m)/} \int_{R^{2r(n+m)}} \prod_{l=1}^{r} d^n\Re s^{(l)} d^n\Im s^{(l)} d^m\Re p^{(l)} d^m\Im p^{(l)} \times \exp\left(-\sum_{l=1}^{r} (|s^{(l)}|^2 + |p^{(l)}|^2)\right) \prod_{1\leqslant j\leqslant n, 1\leqslant k\leqslant m} G\left(\left|\sum_{l=1}^{r} t_l s_k^{(l)} p_j^{(l)}\right|^2\right), \tag{31}$$

where $s^{(l)} = (s_1^{(l)}, \ldots, s_n^{(l)})$ are n-dimensional complex vectors, $p^{(l)} = (p_1^{(l)}, \ldots, p_m^{(l)})$ are m-dimensional complex vectors, $l = 1, \ldots, r$,

$$G(y) = \frac{1}{2\pi}\int_0^{2\pi} d\theta \int_0^{+\infty} f(x)\, dx \exp(2i(xy)^{1/2}\cos(\theta)) = \int_0^{+\infty} dx f(x)\phi(xy), \tag{32}$$

and

$$\phi(x) = \sum_{l=0}^{+\infty} \frac{(-1)^l}{(l!)^2} x^l = J_0(2x^{1/2}). \tag{33}$$

In the special case of single determinant $(r=1)$ the formula (31) can be simplified:

$$E(\det(1+t^2A^*A))^{-1}=\int_{(0,+\infty)^{m+n}}\prod_{i=1}^{n}e^{-u_i}\,du_i\prod_{j=1}^{m}e^{-v_i}\,dv_i\prod_{k,l}G(t^2u_kv_l). \tag{34}$$

Remark 6: As in Sec. II we can consider the case when the the matrix entries $\{|a_{jk}|\}$ are independent but not identically distributed with the densities $f_{jk}(|x|)$, $1\leqslant j\leqslant m$, $1\leqslant n\leqslant n$. The result of Proposition 2 still holds true provided we replace G in (31) and (32) by $G_{jk}(y)=(1/2\pi)\int_0^{2\pi}d\theta\int_0^{+\infty}f_{jk}(x)dx\exp(2i(xy)^{1/2}\cos(\theta))=\int_0^{+\infty}dxf_{jk}(x)\phi(xy)$.

Remark 7: In (33) $J_0(z)=(1/2\pi)\int_0^{2\pi}\exp(iz\cos\theta)d\theta$ is the standard Bessel function.[46]

Remark 8: In the special Wishart (Laguerre) case [which corresponds to $f(x)=e^{-x}$] one has $G(y)=e^{-y}$. If all moments of $f(x)$ exist and do not grow very fast, one can write $G(y)=\sum_{l=0}^{+\infty}[(-1)^l\alpha_l/(l!)^2]y^l$, where $\{\alpha_n\}_{n\geqslant 1}$ are the moments of $f(x)$.

Proof of Proposition 2: Let $\underline{s}=(s_1,\ldots,s_n)^t$, $\underline{p}=(p_1,\ldots,p_m)^t$ be complex n-and m-dimensional column vectors and $s^*=(\overline{s_1},\ldots,\overline{s_n})$, $p^*=(\overline{p_1},\ldots,\overline{p_m})$. In what follows $d^{2n}s$ and $d^{2m}p$ will stand for $d^n\Re s\,d^n\Im s$ and $d^m\Re p\,d^m\Im p$ correspondingly. Then

$$\begin{aligned}(\det(1+t^2A^*A))^{-1}&=\left(\det\begin{pmatrix}1 & tiA\\ tiA^* & 1\end{pmatrix}\right)^{-1}\\&=\left(\frac{1}{\pi}\right)^{n+m}\int d^{2n}s\,d^{2m}p\exp(-(s^*,p^*)B(t)(s,p)^t)\\&=\left(\frac{1}{\pi}\right)^{n+m}\int d^{2n}s\,d^{2m}p\exp(-(|s|^2+|p|^2))\\&\quad\times\exp\left(-i\sum_{1\leqslant j\leqslant n,1\leqslant k\leqslant m}(ta_{jk}p_k\overline{s_j}+t\overline{a_{jk}p_k}s_j)\right),\end{aligned}$$

where as before $B(t)=\left(\begin{smallmatrix}Id & itA\\ itA^* & Id\end{smallmatrix}\right)$ and $d^{2n}sd^{2m}p=\Pi_{i=1}^n d\Re s_i d\Im s_i\Pi_{j=1}^m\Re p_i d\Im p_i$.

We can then write down

$$\begin{aligned}E\left(\prod_{l=1}^{r}\det(1+t_i^2A^tA)\right)^{-1}&=\pi^{-r(n+m)}\int_{R^{2r(n+m)}}\prod_{l=1}^{r}d^{2n}s^{(l)}\,d^{2m}p^{(l)}\exp\left(-\sum_{l=1}^{r}(|s^{(l)}|^2+|p^{(l)}|^2)\right)\\&\quad\times\prod_{1\leqslant j\leqslant n,1\leqslant k\leqslant m}E\left(\exp\left(-i\left(a_{kj}\sum_{l=1}^{r}t_ls_j^{(l)}\overline{p_k^{(l)}}+\overline{a_{kj}}\sum_{l=1}^{r}t_l\overline{s_j^{(l)}}p_k^{(l)}\right)\right)\right).\end{aligned} \tag{35}$$

Let $u=\sum_{l=1}^{r}t_ls_j^{(l)}\overline{p_k^{(l)}}$. Then we can write

$$\begin{aligned}E(\exp(-i(a_{jk}u+\overline{a_{jk}u}))&=\frac{1}{\pi}\int d\Re z\,d\Im z f(|z|^2)\exp(-i(zu+\overline{zu}))\\&=\frac{1}{\pi}\int_0^{2\pi}d\theta\int_0^{+\infty}drrf(r^2)\exp(-ir(e^{i\theta}u+e^{-i\theta}\overline{u}))\\&=\frac{1}{2\pi}\int_0^{2\pi}d\theta\int_0^{+\infty}dxf(x)\exp(-i\sqrt{x}(e^{i\theta}u+e^{-i\theta}\overline{u}))\\&=\int_0^{+\infty}dxf(x)\phi(x|u|^2),\end{aligned} \tag{36}$$

where $\phi(x)$ has been defined in (33). Combining (35) and (36) we arrive at

$$E\prod_{l=1}^{r}(\det(1+t_l^2A^*A))^{-1}=\left(\frac{1}{\pi}\right)^{r(m+n)}\prod_{l=1}^{r}\int d^{2n}s^{(l)}\,d^{2m}p^{(l)}\exp\left(-\sum_{j=1}^{n}|s_j^{(l)}|^2-\sum_{k=1}^{m}|p_k^{(l)}|^2\right)$$
$$\times\prod_{1\leqslant j\leqslant n,1\leqslant k\leqslant m}G\left(\left|\sum_{l=1}^{r}t_l s_j^{(l)}p_k^{(l)}\right|^2\right). \tag{37}$$

In the special case $r=1$ the formula can be simplified further:

$$E(\det(1+t^2A^*A))^{-1}=\left(\frac{1}{\pi}\right)^{m+n}\int_{R^{2(n+m)}}d^{2n}s\,d^{2m}p\exp\left(-\sum_{j=1}^{n}|s_j|^2-\sum_{k=1}^{m}|p_k|^2\right)$$
$$\times\prod_{1\leqslant j\leqslant n,1\leqslant k\leqslant m}\int_0^\infty dx f(x)\left\{\sum_{l=0}^{\infty}\frac{1}{(l!)^2}(-x)^l t^{2l}|p_k|^{2l}|s_j|^{2l}\right\}$$
$$=2^{m+n}\int_{(0,+\infty)^{m+n}}\prod_{i=1}^{n}r_i\,dr_i\prod_{j=1}^{m}\rho_j\,d\rho_j\exp\left(-\sum_{i=1}^{n}r_i^2-\sum_{j=1}^{m}\rho_j^2\right)\prod_{k=1}^{n}\prod_{l=1}^{m}G(t^2r_k^2\rho_l^2)$$
$$=\int_{(0,+\infty)^{m+n}}\prod_{i=1}^{n}e^{-u_i}du_i\prod_{j=1}^{m}e^{-v_i}dv_i\prod_{k,l}G(t^2u_kv_l). \tag{38}$$

In the Wishart case one can simplify things even further. The calculations are very similar to the real Wishart case considered in Remark 4 (Sec. II). Since typical eigenvalues of A^*A are of the order of n, the scaling of t^2 by a factor $1/n$ allows us to study the limiting distribution of the eigenvalues. It follows from (38) that we are left with the task of evaluating the integral $E(\det(1+(t^2/n)A^*A))^{-1}\int_{(0,+\infty)^{2n}}\Pi_{i=1}^{n}e^{-u_i}\,du_i\Pi_{j=1}^{m}e^{-v_j}\,dv_j\exp(-(t^2/n)\Sigma_{k=1}^{n}u_k\Sigma_{l=1}^{m}v_l)$, which can be reduced to

$$\int_{(0,+\infty)^{m+n}}\prod_{i=1}^{n}e^{-u_i}\,du_i\prod_{j=1}^{m}e^{-v_j}\,dv_j\exp\left(-\frac{t^2}{n}\sum_{k=1}^{n}u_k\sum_{l=1}^{m}v_l\right)$$
$$=\int_{(0,+\infty)^{n}}\prod_{i=1}^{n}e^{-u_i}\,du_i\left(1+\frac{t^2}{n}\sum_{l=1}^{n}u_l\right)^{-m}$$
$$=\int_0^{+\infty}\frac{z^{n-1}}{(n-1)!}e^{-z}\left(1+\frac{t^2}{n}z\right)^{-m}dz$$
$$=\frac{n^n}{\Gamma(n)}\int_0^{+\infty}z^{n-1}e^{-nz}(1+t^2z)^{-m}\,dz=\frac{n^n}{\Gamma(n)}\int_0^{+\infty}e^{-n\mathcal{L}(z)}z^{-1}\,dz, \tag{39}$$

where $\mathcal{L}(z)=z+(m/n)\ln(1+t^2z)-\ln z$. It is remarkable that the formulas in the complex case are identical to those in the real case [(21) and (22)] modulo trivial change of parameters. We thus proved the following result.

Lemma 1: Let m and n be positive integers and $z\in\mathbb{C}\backslash(-\infty,0)$. *Then*

$$E_{2m,2n,\ real}\left(\det\left(1+\frac{z}{2}A^tA\right)\right)^{-1/2}=E_{m,n,\ complex}(\det(1+zA^*A))^{-1}, \tag{40}$$

where on the lhs we have the mathematical expectation with respect to the ensemble of rectangular $2m\times 2n$ *real matrices A with i.i.d. standard Gaussian entries (standard real Wishart ensemble), and on the rhs we have the mathematical expectation with respect to the ensemble of rectangular* $m\times n$ *complex matrices A with i.i.d. standard Gaussian entries (standard complex Wishart ensemble).*

As before, it was enough to prove the result for positive real $z=t^2$. We remind the reader that in the standard real Wishart case all entries $\{a_{j,k}\}$ are i.i.d. N(0,1) random variables, and in the standard complex Wishart case all entries $\{\Re a_{j,k}, \Im a_{j,k}\}$ are i.i.d. $N(0,1/2)$ random variables (so in both cases $E|a_{j,k}|^2=1$).

Remark 9: If all moments of $f(x)$ exist, then under some technical conditions the asymptotics of $E(\det(1+t^2A^*A))^{-1}$ in the global regime depend on the first and second moments of $f(x)dx$, (i.e., on the second and fourth moments of the matrix entries A_{kl}). This phenomena is known in random matrix theory: for example, in the case of Wigner random matrices, the limiting distribution of a global linear statistics $Tr\, h(A)-E(Tr\, h(A))$ (where h is a test function, say a polynomial, and A is a random Wigner matrix normalized so that a typical eigenvalue is of the order of a constant) depends on the second and fourth moments of the matrix entries (see e.g., Refs. 28 and 35). It is conjectured (and, in a few interesting special cases, verified) that in the local regime the dependence on the fourth moment goes away.

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APPENDIX

A Poisson random point process on the positive half-axis with the locally integrable intensity function $\rho(x)$ is defined in such a way that the counting functions (e.g., numbers of particles) in the disjoint intervals $I_1, \dots, I_k$ are independent Poison random variables with the parameters $\int_{I_j}\rho(x)dx$, $j=1,\dots,k$. Equivalently, one can define the Poisson random point by requiring that the k-point correlations functions are given by the products of one-point correlation functions (intensities), i.e., $\rho_k(x_1,\dots,x_k)=\Pi_{j=1}^k\rho(x_j)$.

Let $f:(0,+\infty)\to\mathbb{C}$ be a test function with a nice behavior at the origin and infinity. Then

$$\begin{aligned}\mathbf{E}\prod_{i=1}^{\infty}(1+f(x_i)) &= 1+\sum_{k=1}^{\infty}\mathbf{E}\sum_{1\le i_1<i_2<\cdots<i_k}\prod_{j=1}^{k}f(x_{i_j})\\ &= \sum_{k=0}^{\infty}\frac{1}{k!}\int_{(0,+\infty)^k}\prod_{j=1}^{k}f(x_j)\rho_k(x_1,\dots,x_k)\,dx_1\cdots dx_k\\ &= \sum_{k=0}^{\infty}\frac{1}{k!}\left(\int_{(0,+\infty)}f(x)\rho(x)\,dx\right)^k=\exp\left(\int_{(0,+\infty)}f(x)\rho(x)\,dx\right).\end{aligned}\tag{A1}$$

If the test function $f(x)$ equals $(1+zx)^{-1/2}-1$, and $\rho(x)=1/\pi x^{3/2}$, we have

$$\int_{(0,+\infty)}f(x)\rho(x)\,dx=\int_{(0,+\infty)}((1+zx)^{-1/2}-1)\frac{1}{\pi x^{3/2}}\,dx=-\frac{2}{\pi}\sqrt{z},$$

which is exactly the exponent in (4). For random Schrödinger operators the Poisson statistics of the eigenvalues in the localization regime was first proved by Molchanov in Ref. 32 (see also Ref. 31).

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Limit theorems for statistics of combinatorial partitions with applications to mean field Bose gas

Giuseppe Benfatto[a)]
Dipartimento di Matematica, Università di Roma tor Vergata, 00133 Rome, Italy

Marzio Cassandro[b)]
Dipartimento di Fisica, Università di Roma la Sapienza, INFM, Sezione di Roma, 00185 Rome, Italy

I. Merola[c)] and E. Presutti[d)]
Dipartimento di Matematica, Università di Roma tor Vergata, 00133 Rome, Italy

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In this paper we study the statistics of combinatorial partitions of the integers, which arise when studying the occupation numbers of loops in the mean field Bose gas. We review the results of Lewis and collaborators and get some more precise estimates on the behavior at the critical point (fluctuations of the condensate component, finite volume corrections to the pressure). We then prove limit shape theorems for the loops occupation numbers. In particular we prove that in a certain range of the parameters, a finite fraction of the total mass is, in the limit, supported by infinitely long loops. We also show that this mass is equal to the mass of the condensed state where all particles have zero momentum. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1855933]

I. INTRODUCTION

Statistics of combinatorial partitions arises in many areas of science as number theory, combinatorics, probability and statistical mechanics, as illustrated by Vershik in his 1996 paper on the subject.[14]

The problem is about decomposing a positive integer $N \in \mathbb{N}_+$ into a sum of positive integers, $N=j_1+\cdots+j_k$, $k \in \mathbb{N}_+$. Let $(j_1,\dots,j_k)$ the sequence of terms in the sum and consider two such sequences equivalent if they differ by a permutation. A partition of N is then the equivalence class of a sequence whose terms sum up to N. Following Vershik we describe partitions by sequences $\underline{n}=\{n_j, j \in \mathbb{N}_+\}$, where n_j is the number of elements equal to j in a sequence representative of the partition, thus $\Sigma_j j n_j = N$. Statistics enters once we assign a statistical weight to the partitions, the choice of the weights is determined by the particular applications we have in mind and the goal is to derive limit theorems and characterize the typical partitions when N is large.

As in Ref. 14 we will consider multiplicative weights, namely we will suppose that the statistical weight of $\underline{n}$ is

$$w(\underline{n}) = \prod_{j=1}^{\infty} w(j,n_j), \quad \underline{n} = \{n_j, j \in \mathbb{N}_+\} \tag{1.1}$$

where $w(j,\cdot): \mathbb{N}_+ \to \mathbb{R}_+$.

[a)]Electronic mail: benfatto@mat.uniroma2.it
[b)]Electronic mail: marzio.cassandro@roma1.infn.it
[c)]Electronic mail: merola@mat.uniroma2.it
[d)]Electronic mail: presutti@mat.uniroma2.it

In the language of statistical mechanics, the assumption restricts the analysis to noninteracting systems and we will relax it, to study mean field interactions as well. To make clear the connection with physics, it is convenient to generalize the above context by considering j as an element of some countable space J. For instance, a quantum gas of particles in a finite box with Bose–Einstein statistics, can be represented in terms of occupation numbers $\{n_j, j \in J\}$, with J the momentum eigenvalues of a single particle (which are countably many because particles are in a finite box). In the free case, the equilibrium distribution of such occupation numbers is determined by multiplicative weights of the form (1.1), as it will be discussed in the next section.

Bose condensation is then the phenomenon for which a positive fraction of the total number of particles occupies the state with zero momentum, the fraction converging to a deterministic value in the thermodynamic limit. The other particles are distributed over the remaining momenta and their random distribution, suitably normalized, also converges to a deterministic curve, in the thermodynamic limit. The fraction with zero momentum, thought of as a Dirac delta of positive mass added to the remaining distribution, is referred to as the mass of the condensed gas, while the remaining mass is that of the gas in its "normal state." All that happens for suitable values of temperature and density, the theory is very well known and can be found in textbooks and review papers (see, for instance, Refs. 6 and 15). The extension to the mean field case is due to Lewis and collaborators (see, for instance, Ref. 10).

Our model is the same free Bose gas discussed so far, but regarded in terms of "loops" which arise when enforcing the symmetry of the wave functions under particles permutations (Bose statistics). To make this paper self contained, in Appendix A, we derive the representation of the canonical partition function for a Bose gas in the loops language. Thus in our scheme $j \in \mathbb{N}_+$ is the "loop length," representing a cycle with j particles which describe the permutations among particles when imposing the symmetry of the wave function, see Ginibre[5] for a detailed analysis of the model also when interparticles interactions are present.

Feynman conjectured,[4] that Bose condensation is related to the appearance of long loops, namely a fraction of the total number of particles is concentrated on loops whose length diverges when Bose condensation occurs, and this fraction should be exactly the same as the condensed mass of the gas.

Results of this kind for the free gas, and also in the case when obstacles are present as well, have been proved by Kac and Luttinger,[7,8] and Suto.[13]

The purpose of this paper is to show that many properties of the free gas are easily and naturally expressed in terms of the loop representation, which in some instances could provide an alternative picture of the system with some advantages over the more usual momentum-occupation representation. We will indeed prove very detailed estimates on the statistics of the loops, both in the free and in the mean field case.

In particular our large deviation estimates can be used to extend our analysis in the case the Kac potential with $\gamma^{-1}/L \sim 1$. An extension to a more general class has been obtained in Ref. 9.

In Sec. II we present the model. In Sec. III we study the thermodynamics of the mean field Bose gas, showing that the phase diagram can be recovered by solving a variational problem in terms of a free energy functional. We also compute the finite volume corrections to the pressure. In Sec. IV we analyze the statistics of the "long loops" whose length goes to infinity faster than L^2, L being the size of the volume. In Sec. V we state large deviation theorems for the "short loops." In Sec. VI, we prove that the mass density supported by the long loops is equal to the density of the condensed state, where all particles have zero momentum.

Proofs are given in the appendixes.

II. THE FREE AND MEAN FIELD BOSE GAS

We will consider the weights $w(j,n)$ in (1.1) as dependent on the parameters $L>0$, $\beta>0$, $\lambda \in \mathbb{R}$ and given by the expression

$$w(j,n) = \frac{1}{n!}\left(\frac{L^d a(\beta j, L)}{j} e^{\beta \lambda j}\right)^n, \tag{2.1}$$

$$a(\beta j,L)=\sum_{k\in\mathbb{Z}^d}\frac{e^{-(kL)^2/(2\beta j)}}{(2\pi\beta j)^{d/2}}. \tag{2.2}$$

The quantity $L^d a(\beta j,L)$ is the partition function at temperature βj of a free quantum particle of unitary mass in a periodic cubic box of side L, namely

$$L^d a(\beta j,L)=\sum_{k\in\mathbb{Z}^d} e^{-1/2\beta j(2\pi k/L)^2}. \tag{2.3}$$

The elementary equality (2.3) is proved in Lemma A.2.

By the help of the weights (2.1), we construct three probability measures on $\mathbb{N}_+^{\mathbb{N}}$, the canonical, the grand canonical and the mean field measures. The canonical measure with $N\in\mathbb{N}_+$ particles is the probability

$$\mu_{N,L}(\mathfrak{n})=Z_{N,L}^{-1}\mathbf{1}_{\Sigma jn_j=N}w(\mathfrak{n}), \tag{2.4}$$

the partition function $Z_{N,L}$ being the normalization factor and $w(\mathfrak{n})$ is given by (1.1) with $w(j,n_j)$ as in (2.1) with $\lambda=0$. We are not making explicit the dependence on β, as it will be kept fixed throughout the sequel. As we will see in Appendix A, $Z_{N,L}$ is equal to the partition function of a Bose gas in a cubic box of length L with periodic boundary conditions and inverse temperature β.

The grand canonical probability is

$$P_{\lambda,L}(\mathfrak{n})=\Xi_{\lambda,L}^{-1}w(\mathfrak{n}), \tag{2.5}$$

where

$$\Xi_{\lambda,L}=\exp\left\{L^d\sum_j e^{\beta\lambda j}\frac{a(\beta j,L)}{j}\right\} \tag{2.6}$$

and the definition is well posed if $\lambda<0$. Indeed, the right-hand side (rhs) of (2.6) diverges for $\lambda\geqslant 0$ because $a(\beta j,L)\geqslant 1/L^d$, as follows from (2.3).

Finally, the mean field grand canonical probability is

$$P_{\lambda,L}^{mf}(\mathfrak{n})=\Xi_{\lambda,L}^{mf\,-1}e^{-\beta(\Sigma_j n_j)^2/(2L^d)}w(\mathfrak{n}) \tag{2.7}$$

(having set equal to 1 the interaction strength). Due to the presence of the interaction, which ensures convergence at infinity, the value of the chemical potential λ is now unrestricted.

To establish the connection of these measures with the Gibbs measures of the Bose gas in the momentum representation, we realize the above processes in the following way. Let $\alpha(\beta j,p,L)>0$, $j\in\mathbb{N}_+$, $p\in\Pi$, Π a countable set, be such that

$$L^d a(\beta j,L)=\sum_{p\in\Pi}\alpha(\beta j,p,L). \tag{2.8}$$

We then define new weights,

$$w(j,p,n)=\frac{1}{n!}\left(\frac{\alpha(\beta j,p,L)}{j}e^{\beta\lambda j}\right)^n, \tag{2.9}$$

and call $\mu_{N,L}^*(\mathfrak{n})$, $P_{\lambda,L}^*(\mathfrak{n})$, $P_{\lambda,L}^{mf,*}(\mathfrak{n})$, $\mathfrak{n}=\{n_{j,p},j\in\mathbb{N}_+,p\in\Pi\}$, the measures given as in (2.4)–(2.7) with the new weights $w(j,p,n)$ of (2.9) and replacing $\Sigma_j jn_j\to\Sigma_{j,p}jn_{j,p}$. Calling

$$n_j=\sum_{p\in\Pi}n_{j,p},\quad n_p=\sum_{j>0}jn_{j,p}, \tag{2.10}$$

a simple combinatorial computation, which is omitted, shows that the laws of the variables n_j under $\mu_{N,L}^*$, $P_{\lambda,L}^*$, and $P_{\lambda,L}^{mf,*}$ are the same as those under $\mu_{N,L}$, $P_{\lambda,L}$, and $P_{\lambda,L}^{mf}$.

We will see that some proofs become simpler using the representation (2.10) after a suitable choice of $\alpha(\beta j,p,L)$. To recover the momentum representation, we set $\Pi=\mathbb{Z}^d$ and

$$\alpha(\beta j,p,L)=e^{-(\beta j/2)(2\pi p/L)^2} \tag{2.11}$$

that satisfies (2.8) [cf. (2.3)]. Moreover, the law under $\mu^*_{N,L}$, $P^*_{\lambda,L}$, and $P^{mf,*}_{\lambda,L}$ of the variables n_p defined in (2.10) is the usual free Bose canonical and grand-canonical and mean field laws of the momentum occupation numbers. Examining for simplicity only the free Bose grand canonical measure, the probability to have $\nu\in\mathbb{N}$ particles of unitary mass with momentum p is

$$\frac{e^{-\beta\nu[-\lambda+1/2(2\pi p/L)^2]}}{\sum_{n\geqslant 0}e^{-\beta n[-\lambda+1/2(2\pi p/L)^2]}}. \tag{2.12}$$

This is equal to $P^*_{\lambda,L}(\{n_p=\nu\})$, because,

$$e^{-\beta\nu[-\lambda+1/2(2\pi p/L)^2]}=\sum_{\{n_{j,p},j>0\}:\Sigma_j jn_{j,p}=\nu}\prod_{j>0}\frac{1}{n_{j,p}!}\left(\frac{e^{-\beta j[-\lambda+1/2(2\pi p/L)^2]}}{j}\right)^{n_{j,p}} \tag{2.13}$$

which follows from the combinatorial identity

$$1=\sum_{\{n_j,j>0\}:\Sigma_j jn_j=\nu}\prod_{j>0}\frac{1}{n_j!}\left(\frac{1}{j}\right)^{n_j}. \tag{2.14}$$

It turns out that this identity could be proved by checking that

$$1=\frac{1}{\nu!}\left.\frac{\mathrm{d}^\nu f(x)}{\mathrm{d}x^\nu}\right|_{x=0},\quad f(x)=\sum_{\{n_j,j>0\}}\prod_{j>0}\frac{1}{n_j!}\left(\frac{x^j}{j}\right)^{n_j}. \tag{2.15}$$

III. THERMODYNAMICS OF THE MEAN FIELD BOSE GAS

By replacing the factorials in $w(\underline{n})$ with the leading terms of the Stirling formula, we obtain the following heuristics for the distribution of the loops occupation numbers at large L:

$$w(\underline{n})e^{-\beta(\Sigma_j jn_j)^2/(2L^d)}\approx e^{-\beta L^d F_\lambda(\underline{\rho})},\quad \underline{\rho}=\{jn_j/L^d, j>0\}, \tag{3.1}$$

where $F_\lambda(\underline{\rho}):[0,+\infty)^{\mathbb{N}_+}\to\mathbb{R}\sqcup\{+\infty\}$, is defined by the expression

$$F_\lambda(\underline{\rho})=\frac{1}{2}\left(\sum_j\rho_j\right)^2-\lambda\sum_j\rho_j-\frac{S(\underline{\rho})}{\beta}, \tag{3.2}$$

$$S(\underline{\rho})=-\sum_{j=1}^{\infty}\frac{\rho_j}{j}\left(\log\frac{\rho_j}{\rho^*_j}-1\right),\quad \rho^*_j=\frac{1}{(2\pi\beta)^{d/2}j^{d/2}}. \tag{3.3}$$

Besides the above heuristic derivation, the functional $F_\lambda(\underline{\rho})$ has an important role in the sequel. Indeed, as suggested by (3.1) and proved in this paper, in the thermodynamic limit $L\to\infty$, the distribution concentrates on the minimizers of F_λ, thus reducing the computation of the "macroscopic observables" to variational problems for the "limit functional" F_λ. In particular this applies to the thermodynamic potentials. Indeed, interpreting $F_\lambda(\underline{\rho})$ as the Gibbs thermodynamic potential and applying the corresponding version of the second principle of thermodynamics, we have the following expression for the equilibrium thermodynamical pressure:

$$\pi(\lambda) := -\inf_{\varrho} F_\lambda(\varrho). \tag{3.4}$$

The validity of such an interpretation is confirmed by equality with the mean field grand canonical pressure,

$$\pi(\lambda) = \lim_{L\to\infty} \frac{1}{\beta L^d} \ln \Xi^{mf}_{\lambda,L}. \tag{3.5}$$

According to thermodynamics, the free energy functional which corresponds to the Gibbs potential $F_\lambda(\varrho)$ is $F_\lambda(\varrho)+\lambda\{\Sigma\rho_j\}$; we can then use the latter to define the equilibrium thermodynamical free energy,

$$a(u) := \inf_{\varrho:\Sigma_j\rho_j=u} \{F_\lambda(\varrho) + \lambda u\}. \tag{3.6}$$

The validity of (3.6) follows from equality with the mean field canonical free energy, which can be written, if $Z^{mf}_{N_L,L}$ denotes the mean field canonical partition function,

$$a(u) = -\lim_{\substack{L\to\infty \\ N_L/L^d\to u}} \frac{1}{\beta L^d} \ln Z^{mf}_{N_L,L} \tag{3.7}$$

and thermodynamic consistency follows from checking that $a(u)$ is the Legendre transform of $\pi(\lambda)$.

Equations (3.4)–(3.7) show that the thermodynamics of the mean field Bose gas is the same thermodynamics of the free energy functional F_λ, which can be quite explicitly computed. All that, including the proofs of (3.4)–(3.7), are reported in Appendix G.

The thermodynamics of the Bose gas (in the free and in the mean field cases) is very well known and does not need to be discussed again here, but its features in terms of loops are not so familiar and, on the other hand, quite interesting and transparent. Recall first that in the free gas there is, in any dimension $d\geqslant 3$, a Bose condensation characterized by the existence of a critical density u^*, so that the free energy

$$a^0(u) := a(u) - \frac{u^2}{2} \tag{3.8}$$

[i.e., the mean field free energy $a(u)$ minus the mean field energy when the particles density is u] is constant past u^*,

$$a^0(u) = a^0(u^*). \tag{3.9}$$

Such a property is indeed verified by $a^0(u)$ as defined by (3.8) with $a(u)$ as in (3.6), which means, recalling (2.4) and (3.7), that, if $u\geqslant u^*$ and $[\cdot]$ denotes the integer part,

$$\lim_{L\to\infty} \lim_{\substack{N_L=[L^d u] \\ N^*_L=[L^d u^*]}} \frac{1}{\beta L^d} \ln\left\{\frac{Z_{N_L,L}}{Z_{N^*_L,L}}\right\} = 0. \tag{3.10}$$

Equation (3.10) shows that the ratio $Z_{N_L,L}/Z_{N^*_L,L}\to 1$ (in a very weak sense, indeed). The closeness to equality before the limit is an indication of validity of the Bose condensation phenomenon in finite volumes. We have a result (proved in Appendix B) which shows that the infinite volume description is very accurate,

Theorem 3.1: *Let* $d\geqslant 3$ *and*

$$u^* = \sum_{j>0} \rho^*_j. \tag{3.11}$$

Then, given any density $u > u^*$ and any two sequences, N_L and N_L^*, such that $N_L = [L^d u]$ and $N_L^* = [L^d u^*]$, there is a constant c_0, only dependent on d, such that

$$\lim_{L\to\infty} \frac{Z_{N_L,L}}{Z_{N_L^*,L}} = c_0. \tag{3.12}$$

Moreover, there exists another dimension dependent constant c_1, such that, if $\lambda > u^*$,

$$\lim_{L\to\infty} \frac{\Xi^{mf}_{\lambda,L} e^{-\beta\lambda^2 L^d/2}}{\Xi^{mf}_{u^*,L} e^{-\beta(u^*)^2 L^d/2}} = c_1. \tag{3.13}$$

Let us now describe the condensation phenomenon in terms of loops, starting from the analysis of the functional $F_\lambda(\underline{\rho})$. In any dimension $d \geqslant 3$, there is a critical chemical potential

$$\lambda^* = \sum_{j>0} \rho_j^* = u^* \tag{3.14}$$

and, for $\lambda > \lambda^*$, the inf in (3.4) is not a minimum, but (cf. Appendix G) it is obtained by any minimizing sequence $\underline{\rho}^{(n)} = \{\rho_j^{(n)}, j > 0\}$, such that, for any fixed j,

$$\lim_{n\to\infty} \rho_j^{(n)} = \rho_j^* \tag{3.15}$$

while

$$\rho(\lambda) := \lim_{n\to\infty} \sum_{j>0} \rho_j^{(n)} = \sum_{j>0} \rho_j^* + (\lambda - \lambda^*) = \lambda. \tag{3.16}$$

Equation (3.15) and (3.16) show that a fraction $\lambda - \lambda^*$ of the total mass $\rho(\lambda)$ concentrates on "infinite loops." The phenomenon is absent for $\lambda \leqslant \lambda^*$, where instead the rhs of (3.4) has a unique minimizer $\underline{\rho}(\lambda) = \{\rho_j(\lambda), j > 0\}$, where

$$\rho_j(\lambda) = \rho_j^* e^{\beta j \lambda_0(\lambda)} \tag{3.17}$$

and $\lambda_0(\lambda)$ is strictly positive for $\lambda < \lambda^*$, and =0 otherwise. Thus the total mass of the fluid is

$$\rho(\lambda) = \begin{cases} \sum_{j>0} \rho_j(\lambda) & \text{if } \lambda \leqslant \lambda^*, \\ \sum_{j>0} \rho_j^* + (\lambda - \lambda^*) & \text{if } \lambda \geqslant \lambda^*, \end{cases} \tag{3.18}$$

and no mass concentrates on infinite loops for $\lambda \leqslant \lambda^*$. Note that, by (3.14), $\rho(\lambda^*) = \lambda^*$.

The validity of the above interpretation follows from the following theorem, which is a corollary of the large deviation estimates proved in Appendix E.

Theorem 3.2: *For any* λ, (3.19)–(3.21) *below hold,*

$$\lim_{L\to\infty} P^{mf}_{\lambda,L}\left(\left| \frac{j n_j}{L^d} - \rho_j(\lambda) \right| > \delta \right) = 0, \quad \forall\, \delta > 0, \tag{3.19}$$

$$\lim_{L\to\infty} P^{mf}_{\lambda,L}\left(\left| \sum_{j \leqslant J(L)} \left\{ \frac{j n_j}{L^d} - \rho_j(\lambda) \right\} \right| > \delta \right) = 0, \quad \forall\, \delta > 0, \tag{3.20}$$

independently of the choice of $J(L)$, provided $J(L)$ is an increasing function of L and $J(L) \leqslant L^2$,

$$\lim_{L\to\infty} P^{mf}_{\lambda,L}\left(\left| \sum_{j \geqslant 1} \left\{ \frac{j n_j}{L^d} - \rho(\lambda) \right\} \right| > \delta \right) = 0, \quad \forall\, \delta > 0. \tag{3.21}$$

While the statements relative to global quantities, like pressure, free energy, and total number of particles are known in the literature, the results on the way the mass distributes among the different loops are new for the mean field interaction; Suto[13] has analogous results in the context of the canonical free measure.

But all this is not really in the focus of our study, which is rather aimed at relaxing the assumption of mean field, for instance considering Kac potentials, with the hope that the loops language may provide some simplification. In this perspective it is important to derive sharp estimates on the deviations of the densities in (3.19)–(3.21) which have been used in Ref. 9 to prove the occurrence of Bose condensation with Kac potentials in suitable scaling limits and to get nontrivial estimates for the low momenta distribution in the condensed region for a class of long but finite range potential. Results and proofs can be found in Sec. V and Appendix B.

The rate functions of the large deviations of the above macroscopic quantities are faithfully described by the functional $F_\lambda(\varrho)$, whose suitably constrained minima give the correct large deviations rate functions. Thus, like in the case of the thermodynamical potentials, the analysis of the functional $F_\lambda(\varrho)$ gives the right answer.

The functional $F_\lambda(\varrho)$ is instead inadequate for studying how the mass of the condensed fluid (in the Bose condensation regime $\lambda > \lambda^*$) distributes among the long loops. The issue is discussed in the next section.

IV. DISTRIBUTION OF LONG LOOPS

To study the Bose condensation phenomenon, we restrict to $d \geqslant 3$ and to $\lambda > \lambda^*$. Then, see (3.18)–(3.21) and (3.14), the total mass (after the thermodynamic limit) is $\rho(\lambda) = u^* + (\lambda - \lambda^*)$, u^* is the mass of the "normal fluid" and $(\lambda - \lambda^*)$ of the condensed one. By (3.20),

$$\lim_{L\to\infty} P^{mf}_{\lambda,L}\left(\left| \sum_{j \leqslant L^2} \frac{jn_j}{L^d} - u^* \right| > \delta \right) = 0, \quad \forall\, \delta > 0 \tag{4.1}$$

which shows that in finite volumes the mass of the normal fluid is essentially carried by loops with length $\leqslant L^2$, while the mass of the condensed concentrates on loops of length $> L^2$,

$$\lim_{L\to\infty} P^{mf}_{\lambda,L}\left(\left| \sum_{j > L^2} \frac{jn_j}{L^d} - (\lambda - \lambda^*) \right| > \delta \right) = 0, \quad \forall\, \delta > 0. \tag{4.2}$$

Actually most of the mass is on loops whose length is a fraction of the whole volume,

$$\lim_{L\to\infty} E^{mf}_{\lambda,L}\left(\frac{1}{L^d} \sum_{j > L^2}^{\delta L^d} jn_j \right) = \delta. \tag{4.3}$$

Furthermore the number $\tilde{X}_L$ of loops larger than L^2 goes like $\ln L$ and becomes deterministic in the limit $L \to \infty$ (i.e., $\tilde{X}_L / \ln L \to a > 0$), while the cardinality of the subset of loops larger than δL^d, $\delta > 0$, is finite and has a nontrivial (i.e., nondeterministic) limit distribution.

We summarize this result in the following theorem proved in Appendix F, where we use the following notation:

$$y_{\delta,L} \equiv \frac{1}{L^d} \sum_{j \geqslant \delta L^d} jn_j, \quad X_{\delta,L} \equiv \sum_{j \geqslant \delta L^d} n_j, \quad X_L \equiv \frac{1}{\log L} \sum_{j \geqslant L^2} n_j,$$

$$j_{\max} := \max\{j : n_j > 0\}. \tag{4.4}$$

Theorem 4.1: *Suppose that* $\lambda > \lambda^*$ *and* $0 < \delta < \lambda - \lambda^*$, *then*

$$\lim_{L\to\infty} E^{mf}_{\lambda,L}(y_{\delta,L}) = \lambda - \lambda^* - \delta, \tag{4.5}$$

$$\lim_{L\to\infty}\{E^{mf}_{\lambda,L}(y^2_{\delta,L}) - E^{mf}_{\lambda,L}(y_{\delta,L})^2\} = \tfrac{1}{2}\delta^2, \tag{4.6}$$

$$\lim_{L\to\infty} E^{mf}_{\lambda,L}(X_{\delta,L}) = \log\frac{\lambda-\lambda^*}{\delta}, \quad \lim_{L\to\infty} E^{mf}_{\lambda,L}(X_L) = d-2, \tag{4.7}$$

$$\lim_{L\to\infty}\{\sqrt{\log L}[E^{mf}_{\lambda,L}(X^2_L) - E^{mf}_{\lambda,L}(X_L)^2]\} = d-2, \tag{4.8}$$

$$\lim_{L\to\infty}\{E^{mf}_{\lambda,L}(X^2_{\delta,L}) - E^{mf}_{\lambda,L}(X_{\delta,L})^2\} = D_\delta = \log\frac{\lambda-\lambda^*}{\lambda-\lambda^*-\delta}\left(1-\log\frac{\lambda-\lambda^*}{\delta}\right) + \int_\delta^{\lambda-\lambda^*-\delta}\frac{dx}{x}\left(1-\log\frac{\lambda-\lambda^*}{\lambda-\lambda^*-x}\right), \tag{4.9}$$

$$\frac{D_\delta}{\log[(\lambda-\lambda^*)/\delta]} \underset{\delta\to 0}{\longrightarrow} 1. \tag{4.10}$$

Furthermore, for any $\xi\in(1/2,1]$,

$$\lim_{L\to\infty} P^{mf}_{\lambda,L}\left(\frac{j_{\max}}{L^d} > \xi(\lambda-\lambda^*)\right) = -\ln\xi. \tag{4.11}$$

Suto[13] has already a proof of (4.3) in the free canonical case, but he has not analyzed in detail the statistics of long loops.

V. SMALL AND LARGE DEVIATIONS

A. Small deviations

Theorem 5.1 (small fluctuations for N): *Let*

$$\sigma^2 := \lim_{L\to\infty}\frac{1}{L^d}E^{mf}_{\lambda,L}\left(\left[\sum_{j>0} j(n_j - \langle n_j\rangle)\right]^2\right), \quad \langle n_j\rangle := E^{mf}_{\lambda,L}(n_j). \tag{5.1}$$

Then, if $\lambda_0(\lambda)$ *is defined as in Appendix G,*

$$\sigma^2 = \left[\beta + \frac{\mathbf{1}_{\{\lambda<\lambda^*\}}}{\sum_j \rho^*_j j e^{\lambda_0(\lambda)\beta j}}\right]^{-1} \tag{5.2}$$

for any λ, *if* $d=3,4$, *and for* $\lambda\neq\lambda^*$, *if* $d\geqslant 5$. *Moreover, under the same conditions on* λ, *the function*

$$\mathfrak{I}(v) := \inf_{\varrho:\Sigma\rho_j=\rho(\lambda)+v} F_\lambda(\varrho) - \inf_\varrho F_\lambda(\varrho) \tag{5.3}$$

with $\rho(\lambda)$ *given by (3.18), is twice differentiable in* $v=0$ *and*

$$\sigma^2 = \left(\beta\left[\frac{d^2\mathfrak{I}(v)}{dv^2}\right]_{v=0}\right)^{-1}. \tag{5.4}$$

Proof: The value of σ^2 is calculated in Appendix C, Theorem C.2, in the case $\lambda\geqslant\lambda^*$; the case $\lambda<\lambda^*$ could be treated in a similar (simpler) way. The relation with the free energy functional, Eq. (5.4), follows from (I6) of Appendix I. ■

Remark: If $d=3$ and $\lambda\neq\lambda^*$, Eq. (5.2) was already obtained by Ref. 2, but the case $\lambda=\lambda^*$

seems new. To check that the expression given in Ref. 2 coincides with (5.2) for $\lambda \neq \lambda^*$, it is sufficient to note that, since $\rho(\lambda)=\lambda-\lambda_0(\lambda)$ and, in $d=3$, $\rho_j^*=1/(2\pi\beta j)^{3/2}$,

$$\sum_j \rho_j^* \beta j e^{\lambda_0(\lambda)\beta j} = \frac{\beta}{(2\pi\beta)^{3/2}} \sum_j \frac{1}{j^{1/2}} e^{(\lambda-\rho(\lambda))\beta j} \equiv \frac{\beta}{(2\pi\beta)^{3/2}} \mathfrak{g}_{1/2}(\lambda-\rho(\lambda)), \tag{5.5}$$

where $\mathfrak{g}_{1/2}(\mu)$ is defined in formulas 17–18 of Ref. 2.

We will also study deviations of other macroscopic quantities. In particular we will consider the following sets:

$$V_1 := \mathbb{Z}^+, \quad V_2 := \{\ell\}, \quad V_3 := \{J(L)\}, \quad V_4 := \{1,2,\ldots,J(L)\} \tag{5.6}$$

with $J(L)$ as in Theorem 3.2, namely $J(L) \in \mathbb{N}^+$ is an increasing function of L, such that $\lim_{L\to\infty} J(L)=\infty$ and $\lim_{L\to\infty} J(L)/L^2<\infty$.

For $k=1,\ldots,4$, we then define

$$\mathcal{A}_{L,\delta}^{(k)}(v) \equiv \mathcal{A}_{L,\delta}^{(k)} := \left\{ \varrho : \frac{1}{L^d} N^{(k)} \in \left(\sum_{j\in V_k} \rho_j(\lambda) + v - \delta, \sum_{j\in V_k} \rho_j(\lambda) + v + \delta \right) \right\}, \tag{5.7}$$

$$A_L^{(k)}(v) \equiv A_L^{(k)} := \left\{ \varrho : \sum_{j\in V_k} \rho_j = \sum_{j\in V_k} \rho_j(\lambda) + v \right\}, \tag{5.8}$$

with

$$N^{(k)} = \sum_{j\in V_k} j n_j \tag{5.9}$$

and $\rho_j(\lambda)$ as in (3.17).

The small deviations for $N^{(k)}$, $k\neq 1$, $N^{(k)}$ as in (5.9), are discussed in Appendix D for $\lambda>\lambda^*$. The relation of the corresponding covariances with the free energy functional goes along the same lines of Appendix I and we omit it.

B. Large deviations

In this section we will express the rate functions of large deviations for the quantities (5.7) and (5.8) in terms of variational problems for the limit functional with corresponding constraints.

Theorem 5.2: *For any* λ, *if* $k=1$, *and for any* $\lambda\neq\lambda^*$, *if* $k>1$,

$$\lim_{\delta\to 0} \lim_{L\to\infty} \left[\frac{\frac{1}{\beta L^d} \ln P_{\lambda,L}^{mf}(\mathcal{A}_{L,\delta}^{(k)})}{-\inf_{\varrho\in A_L^{(k)}} F_\lambda(\varrho) + \inf_{\varrho} F_\lambda(\varrho)} \right] = 1. \tag{5.10}$$

Proof: The proof of this theorem in the case $k=4$ and $\lambda>\lambda^*$ (the most interesting case) follows from Theorem E.3 in Appendix E and Appendix H. The other cases can be treated along the same lines. ■

Remark: The case $\lambda=\lambda^*$ is more involved, if $k>1$, so we did not study it in detail, but we think that Theorem 5.2 is still valid.

Corollary 5.3 (large deviations for $N^{(1)}\equiv N$):

$$\lim_{\delta\to 0} \lim_{L\to\infty} \frac{\ln P(\mathcal{A}_{L,\delta}^{(1)})}{\beta L^d} = -\overline{t}(\rho(\lambda)+v) + \frac{v^2}{2} + \rho(\lambda)v + \pi^0_{\lambda_0(\lambda+\overline{t})} - \pi^0_{\lambda_0(\lambda)}, \tag{5.11}$$

where $\lambda_0(\lambda)$ *is defined in* (G5), $\pi^0_{\lambda_0}$ *is the pressure of the free system with chemical potential* λ_0 [cf. Eq. (G2)] *and* $\overline{t}$ *is the solution of the equation* $\overline{t}=\lambda_0(\lambda+\overline{t})-\lambda_0(\lambda)+v$.

Remark: If $\lambda > \lambda^*$ and $\lambda + v > \lambda^*$, then $\rho(\lambda) = \lambda$, $\lambda_0 = 0$ and the expression on the rhs of (5.11) becomes $-v^2/2$.

Corollary 5.4 (large fluctuations for $N^{(2)}$ and $N^{(3)}$): *If* $\lambda \geq \lambda^*$, $-\rho_\ell^* < v < \lambda - \lambda^*$ *and we define* $\theta := v/\rho_\ell^*$, *then*

$$\lim_{\delta\to 0}\lim_{L\to\infty}\frac{1}{\beta L^d}\ln P(\mathcal{A}^{(2)}_{L,\delta}) = -\frac{1}{\beta}\frac{v}{\ell}[(\theta^{-1}+1)\ln(1+\theta)-1] \tag{5.12}$$

while, if $\lambda \geq \lambda^*$ *and* $v > \lambda - \lambda^*$,

$$\lim_{\delta\to 0}\lim_{L\to\infty}\frac{1}{\beta L^d}\ln P(\mathcal{A}^{(2)}_{L,\delta}) = -\frac{1}{\beta}\frac{v}{\ell}[(\theta^{-1}+1)\ln(1+\theta)-1] + \frac{\lambda_0^2}{2} - \lambda_0 + \pi^0_{\lambda_0} - \pi^0_0, \tag{5.13}$$

where $\lambda_0 = \lambda_0(\lambda - \rho_\ell^* - v)$.

If $\lambda > \lambda^*$ *and* $v > 0$,

$$\lim_{\delta\to 0}\lim_{L\to\infty}\frac{J(L)}{\beta L^d \ln J(L)}\ln P(\mathcal{A}^{(3)}_{L,\delta}) = -\frac{vd}{2}. \tag{5.14}$$

For $\lambda > \lambda^*$ *and* $v < 0$ *we get*

$$\lim_{\delta\to 0}\lim_{L\to\infty}\frac{1}{\beta L^d}\ln P(\mathcal{A}^{(3)}_{L,\delta}) = -\frac{c(v)d}{2}, \tag{5.15}$$

where $c(v) > 0$ *and vanishes as* $v \to 0$ (cf. *Corollary 5.5*).

Proof: By Theorem 5.2 and Appendix H,

$$\lim_{\delta\to 0}\lim_{L\to\infty}\frac{1}{\beta L^d}\ln P(\mathcal{A}^{(2)}_{L,\delta}) = -\overline{t}(\rho_\ell(\lambda)+v) + \pi_{\lambda,\overline{t}} - \pi_\lambda, \tag{5.16}$$

where $\overline{t}$ is the solution of the equation $\rho_\ell(\lambda)e^{\overline{t}\beta\ell} = \rho_\ell(\lambda) + v$. The solution does exist when $v > -\rho_\ell(\lambda)$ and is given by

$$\overline{t} = \frac{1}{\beta\ell}\ln\left(\frac{\rho_\ell(\lambda)+v}{\rho_\ell(\lambda)}\right). \tag{5.17}$$

When $\lambda > \lambda_*$ and $-\rho_\ell^* < v < \lambda - \lambda^*$, we see that $\tilde{\pi}_{\lambda,\overline{t}} - \pi_\lambda = (\lambda^2/2) + (1/\beta)\Sigma_j[(\rho_j^* + v\mathbf{1}_{j=\ell})/j] - (\lambda^2/2) - (1/\beta)\Sigma_j(\rho_j^*/j) = v/\beta\ell$, so that, defining $\theta := v/\rho_\ell^*$,

$$\lim_{\delta\to 0}\lim_{L\to\infty}\frac{1}{\beta L^d}\ln P(\mathcal{A}^{(2)}_{L,\delta}) = -\frac{1}{\beta}\frac{v}{\ell}[(\theta^{-1}+1)\ln(1+\theta)-1] \tag{5.18}$$

while, if $v > \lambda - \lambda^*$, we get an extra term coming from the difference $\tilde{\pi}_{\lambda,\overline{t}} - \pi_\lambda$.

Equation (5.14) is a direct consequence of (5.12), obtained in the limit $\theta \to \infty$. ■

Notice that, when $\lambda > \lambda^*$, in the limit $L \to \infty$, the fluctuation of ρ_ℓ has the law of a free Poisson distribution with parameter ρ_ℓ^*.

Corollary 5.5 (large deviations for $N^{(4)}$): *For* $\lambda > \lambda^*$; $v > 0$,

$$\lim_{\delta\to 0}\lim_{L\to\infty}\frac{J(L)}{\beta L^d \ln J(L)}\ln P(\mathcal{A}^{(4)}_{L,\delta}) = -v\left(\frac{d}{2}-1\right). \tag{5.19}$$

For $v < 0$ *and all* $\lambda \geq \lambda^*$, *we have instead,*

$$\limsup_{L\to\infty}\frac{1}{L^d}\log P^{mf}_{\lambda,L}\left(\sum_{j=1}^{j(L)} jn_j \leq [u^* - |v|]L^d\right) \leq -c(v), \tag{5.20}$$

where $c(v) > 0$ *and vanishes as* $v \to 0$ *as*

$$c(v) \sim \begin{cases} v^2, & d \geqslant 5, \\ \dfrac{v^2}{|\log|v||}, & d = 4, \\ |v|^3, & d = 3. \end{cases} \tag{5.21}$$

Proof: See Theorem E.3 and Appendix H. ■

VI. LONG LOOPS AND BOSE CONDENSATION

In this section we show that, in the mean field model, the excess density concentration $\rho - \rho^*$ on large loops implies the phenomenon of condensation (i.e., a finite fraction of the number of particles occupies the state of zero momentum).

The reduced density matrices (RDM) are the quantum analogue of correlation functions[1,12] and the Fourier transform of the one point RDM, in the case of periodic boundary conditions with translational invariant potentials, gives (Penrose[11]) the average number of particles of momentum $2\pi p/L$, $p \in \mathbb{Z}^d$,

$$\hat{\rho}_\Lambda(p) = \int_\Lambda \rho_\Lambda(0,z) e^{i(2\pi p/L)z} \mathrm{d}z. \tag{6.1}$$

Using the language of loops, in the mean field case, where the interaction does not depend on the position of the particles, the one point RDM reads[5]

$$\rho_\Lambda^{mf}(x,y) = \sum_{j_0} \Xi_{\lambda,L}^{-1} \sum_{\mathfrak{n}} w(\mathfrak{n}) e^{-\beta[(\Sigma_j j(n_j + \delta_{j,j_0}))^2/2L^d]} e^{\lambda\beta j_0} \sum_{k \in \mathbb{Z}^d} \frac{e^{-[(kL + (x-y))^2/2\beta j_0]}}{(2\pi\beta j_0)^{d/2}}. \tag{6.2}$$

Theorem 6.1: *For* $d \geqslant 3$ *and any* β, *when* λ *is larger than* λ^*,

$$\lim_{L\to\infty} \frac{\hat{\rho}_\Lambda^{mf}(0)}{L^d} = \lambda - \lambda^*. \tag{6.3}$$

Proof: From (6.1) and (6.2) we get that

$$\begin{aligned} \hat{\rho}_\Lambda^{mf}(0) &= \int_\Lambda \rho_\Lambda^{mf}(0,z)\mathrm{d}z = \sum_{j_0} \Xi_{\lambda,L}^{-1} \sum_{\mathfrak{n}} w(\mathfrak{n}) e^{-\beta[(\Sigma_j j(n_j + \delta_{j,j_0}))^2/2L^d]} e^{\lambda\beta \sum_j j(n_j + \delta_{j,j_0})} \\ &= E_{\lambda,L}^{mf}\left(\sum_j \frac{j n_j}{L^d a(\beta j, L)} \right). \end{aligned} \tag{6.4}$$

The theorem is proved using (4.5) and [cf. (D62)]

$$0 < a(\beta j, L) - \rho_j \leqslant C\rho_j e^{-L^2/(2\beta j)}.$$

■

APPENDIX A

In this appendix we recall the relation between the usual definition of the canonical partition function for a free Bose gas and its representation in the loops language given in (2.4).

The canonical partition function for a system of N identical bosons is

$$Z_N = \mathrm{Tr}\, e^{-\beta H_N},$$

where H_N is the Hamiltonian operator and the trace involves only symmetrized states.

Theorem A.1: *Let $H_N=-\Sigma_{i=1}^N\Delta_i$ be the Hamiltonian of N free Bosons in a cubic box of size L with periodic boundary conditions, then*

$$Z_{N,L}=\sum_{\boldsymbol{\nu}:|\boldsymbol{\nu}|=N} e^{-\beta\Sigma_p(2\pi p/L)^2\nu_p}=\sum_{\mathbf{n}:\Sigma jn_j=N}\prod_j\frac{1}{n_j!}\left(\frac{\sum_p e^{-\beta j(2\pi p/L)^2}}{j}\right)^{n_j}. \tag{A1}$$

Proof: The Bosons states in the momentum representation can be written as $|\boldsymbol{\nu}\rangle=|\nu_p, p\in\mathbb{Z}^d\rangle$, ν_p being the number of Bosons with momentum equal to $k=2\pi pL^{-1}$. The energy in such a state is equal to $\Sigma_p\epsilon_p\nu_p$, $\epsilon_p=(2\pi pL^{-1})^2$, hence the first equality in (A1).

To prove the second one, let $\lambda<0$ and define,

$$\mathcal{Z}(\lambda):=\sum_N e^{\beta\lambda N}\sum_{\boldsymbol{\nu}:|\boldsymbol{\nu}|=N} e^{-\beta\Sigma_p\epsilon_p\nu_p} \tag{A2}$$

that can be rewritten as

$$\mathcal{Z}(\lambda)=\exp\left\{-\sum_p \ln(1-e^{-\beta(\epsilon_p-\lambda)})\right\}=\exp\left\{\sum_j\left(\sum_p\frac{e^{-\beta(\epsilon_p-\lambda)j}}{j}\right)\right\}=\sum_M\frac{1}{M!}\left[\sum_j\left(\sum_p\frac{e^{-\beta(\epsilon_p-\lambda)j}}{j}\right)\right]^M$$

$$=\sum_{\mathbf{n}}\prod_j\left[\sum_p\frac{e^{-\beta(\epsilon_p-\lambda)j}}{j}\right]^{n_j}\frac{1}{n_j!}=\sum_N e^{\beta\lambda N}\sum_{\mathbf{n}:\Sigma_j jn_j=N}\prod_j\left[\frac{\sum_p e^{-\beta j\epsilon_p}}{j}\right]^{n_j}\frac{1}{n_j!}. \tag{A3}$$

Since $\mathcal{Z}(\lambda)$ is analytic in λ for $\mathrm{Re}\,\lambda<0$, (A1) follows. ■

An alternative proof working in the configuration representation can be obtained as follows:

$$Z_{N,L}=\frac{1}{N!}\sum_\pi\int \mathrm{d}r_1\cdots\mathrm{d}r_N\langle r_{\pi_1}\cdots r_{\pi_N}|e^{-\beta H_N}|r_1\cdots r_N\rangle,$$

where Σ_π is the sum over all permutations of $(1,2,\ldots,N)$. Since any permutation breaks up into cycles (loops), we have

$$Z_N=\frac{1}{N!}\sum_{n_1,n_2,\ldots}c(n_1,n_2,\ldots)\prod_j Z^{n_j},$$

where

(a) $c(n_1,n_2,\ldots)=N!\Pi_j(1/j^{n_j})(1/n_j!)$ is the number of ways of having n_1 loops of length 1, n_2 of length 2, etc.,
(b) the sum is over all combinations of permutations s.t. $\Sigma jn_j=N$,
(c) $Z(j)=\Sigma_p e^{-\beta j\epsilon_p}$, where $-\epsilon_p$ are the eigenvalues of the Laplace operator Δ.

In the case of a free Bose gas in a cubic box of size L with periodic boundary conditions

$$Z_{N,L}=\sum_{\mathbf{n}:\Sigma jn_j=N}\prod_j\frac{1}{n_j!}\left(\frac{\sum_p e^{-\beta j(2\pi p/L)^2}}{j}\right)^{n_j}$$

thus deriving again the last equality in (A1).

Finally, to justify Eq. (2.3), we prove the following lemma.

Lemma A.2: For any L and $\alpha>0$

$$L^d\sum_{k\in\mathbb{Z}^d}\frac{e^{-(kL)^2/(2\alpha)}}{(2\pi\alpha)^{d/2}}=\sum_{k\in\mathbb{Z}^d}e^{-1/2\alpha(2\pi k/L)^2}. \tag{A4}$$

Proof: Equation (A4) follows from the identities:

$$e^{-(kL)^2/(2\alpha)} = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-x^2/2 + iLkx/\sqrt{\alpha}}\, dx \tag{A5}$$

and

$$\frac{1}{(2\pi)^d} \sum_{k \in \mathbb{Z}^d} e^{ivk} = \sum_{k \in \mathbb{Z}^d} \delta(v - 2\pi k). \tag{A6}$$

■

APPENDIX B

The canonical partition function (A1) of the free Bose gas can be written as

$$Z_{N,L} = \sum_{\{n_k\}} \mathbf{1}_{\Sigma n_k = N} e^{-\beta \Sigma_k n_k E_k} = \sum_{M=0}^{N} \tilde{Z}_{M,L}, \tag{B1}$$

$$\tilde{Z}_{M,L} = \sum_{\{n_k, k \neq 0\}} \mathbf{1}_{\Sigma_{k \neq 0} n_k = M} e^{-\beta \Sigma_{k \neq 0} n_k E_k}, \tag{B2}$$

where the momentum k takes values in the set $\{2\pi u/L, u \in \mathbb{Z}^d\}$, $n_k \in \mathbb{Z}$, and $E_k = k^2/2$.

In this appendix we study the tail properties of the probability distribution on $\mathbb{N}$ with density,

$$P_L(M) = \frac{\tilde{Z}_{M,L}}{Q_L}, \quad Q_L = \sum_{M=0}^{\infty} \tilde{Z}_{M,L} \tag{B3}$$

and mean value

$$\langle M \rangle_L = \sum_{k \neq 0} \frac{1}{e^{\beta E_k} - 1} \equiv L^d \lambda_L^*. \tag{B4}$$

We remark that this probability distribution is the canonical distribution of the total number of particles with $k \neq 0$ for a free Bose gas. These results will be used in the sequel to prove small and large deviation both in the free and mean field case.

We want to study the asymptotic properties of the probability measure P_L as $L \to \infty$. To begin with, note that, if $d \geqslant 3$, $\lim_{L \to \infty} \lambda_L^*$ does exist and

$$\lambda^* = \lim_{L \to \infty} \lambda_L^* = \int_{\mathbb{R}^d} \frac{dk}{(2\pi)^d} \frac{1}{e^{\beta E_k} - 1}. \tag{B5}$$

Let us define

$$c_L = L^{d-2}(\lambda^* - \lambda_L^*). \tag{B6}$$

Lemma B.1: For any $d \geqslant 3$, c_L has a limit as $L \to \infty$ and

$$c^* \equiv \lim_{L \to \infty} c_L = \int_0^\infty dt \left[1 - \sum_{u \neq 0} \frac{e^{-u^2/(2\beta t)}}{(2\pi\beta t)^{d/2}} \right]. \tag{B7}$$

Proof: (3.2) and (B4) imply that

$$L^d \lambda_L^* = \sum_{k \neq 0} \sum_{j=1}^{\infty} e^{-\beta j E_k} = \sum_{j=1}^{\infty} [L^d a(\beta j, L) - 1] \tag{B8}$$

while (B5) implies that

$$L^d\lambda^* = L^d\sum_{j=1}^{\infty}\frac{1}{(2\pi\beta j)^{d/2}} \tag{B9}$$

hence, by using the definition of $a(t,L)$ in (3.2), we get

$$c_L = \frac{1}{L^2}\sum_{j=1}^{\infty}\left[1-\sum_{n\neq 0}\frac{e^{-n^2/(2\beta t_j)}}{(2\pi\beta t_j)^{d/2}}\right], \quad t_j=\frac{j}{L^2}. \tag{B10}$$

The lemma follows from this expression, easily implying the convergence of the sum over $j\leqslant L^2$, and the identity, following from (3.2) (with $L=1$):

$$1-\sum_{n\neq 0}\frac{e^{-n^2/(2t)}}{(2\pi t)^{d/2}} = \frac{1}{(2\pi t)^{d/2}} - \sum_{n\neq 0} e^{-2\pi^2 t n^2} \tag{B11}$$

which implies immediately the convergence of the sum over $j\geqslant L^2$. ■

Let us now define

$$y_L = \frac{M-L^d\lambda_L^*}{h_L}, \quad h_L = \begin{cases} L^2, & d=3,\\ L^2\sqrt{\log L} & d=4,\\ L^{d/2}, & d\geqslant 5. \end{cases} \tag{B12}$$

An important role in this appendix has the following theorem.

Theorem B.2: *If M is a random variable with probability (B3), the distribution function of the random variable y_L converges, as $L\to\infty$, to the distribution function of a random variable y on $\mathbb{R}$ with mean 0 and smooth density $\rho(y)$ strictly positive, whose Laplace transform $F(\sigma)=\int dy\,\rho(y)\exp(-\sigma y)$, $\sigma\in\mathbb{C}$, is given, if $d=3$ and $\Re\sigma>-2\pi^2\beta$, by*

$$F(\sigma)=\exp\left(\sum_{n\neq 0} G\left(\frac{\sigma}{2\pi^2\beta n^2}\right)\right), \quad G(u)=u-\log(1+u) \tag{B13}$$

while, if $d\geqslant 4$ and $\Re\sigma\in\mathbb{R}$,

$$F(\sigma)=e^{1/2c_0\sigma^2}, \quad c_0=\begin{cases}\dfrac{1}{2\pi^2\beta^2}, & d=4\\[2ex] \dfrac{1}{(2\pi\beta)^{d/2}}\displaystyle\sum_{j=1}^{\infty} j^{1-d/2}, & d\geqslant 5.\end{cases} \tag{B14}$$

Moreover, there exists a constant C, independent of L and M, such that

$$(1+y_L^2)h_L P_L(M)\leqslant C \tag{B15}$$

and, given any $y\in\mathbb{R}$, if we choose $M=M_L^*$ so that $y_L^*=(M_L^*-L^d\lambda_L^*)/h_L\to_{L\to\infty} y$, then

$$h_L P_L(M_L^*)\xrightarrow[L\to\infty]{}\rho(y). \tag{B16}$$

Proof: To begin with, we shall prove that the Laplace transform of y_L, $F_L(\sigma)=\Sigma_{M=0}^{\infty}P_L(M)\exp[-\sigma(M-L^d\lambda_L^*)/h_L]$, is well defined and convergent as $L\to\infty$, if $\Re\sigma\in(\sigma_0,\infty)$, where $\sigma_0=-2\pi^2\beta$, if $d=3$, and $\sigma_0=-\infty$, if $d\geqslant 4$; this implies in particular that the characteristic function $f_L(t)=F_L(-it)$, $t\in\mathbb{R}$, is convergent for any t. By analyzing the decaying properties in t of $f_L(t)$, we shall also prove the bound (B15), implying that the distribution function of y_L is convergent and that its limit is the distribution function of a probability measure on $\mathbb{R}$; in fact, by a simple application of dominated convergence theorem,

$$\sum_{0\leqslant M\leqslant h_L y+L^d\lambda_L^*} P_L(M) = \frac{1}{h_L} \sum_{0\leqslant M\leqslant h_L y+L^d\lambda_L^*} h_L P_L(M) \xrightarrow[L\to\infty]{} \int_{-\infty}^{y} \rho(z)\mathrm{d}z. \tag{B17}$$

Note that this result follows from the convergence of $f_L(t)$ to $f(t)$, without using the bound (B15), since $P_L(M)$ is a probability measure.[3] We are stressing here the role of (B15) only because we shall generalize in the following the previous argument to some cases where $P_L(M)$ is not a probability measure, even if $\Sigma_{M=0}^{\infty} P_L(M)=1$.

Finally, by analyzing the properties of the limiting measure Laplace transform, we shall prove that this measure has a smooth and strictly positive density.

By a straightforward calculation, one can see that

$$\begin{aligned}\log F_L(\sigma) &= \frac{L^d\lambda_L^*}{h_L}\sigma - \sum_{k\neq 0} \log \frac{1-e^{-\beta E_k-\sigma/h_L}}{1-e^{-\beta E_k}} = \sum_{k\neq 0}\left[\frac{\sigma}{h_L}\frac{1}{e^{\beta E_k}-1} - \log\left(1+\frac{1-e^{-\sigma/h_L}}{e^{\beta E_k}-1}\right)\right] \\ &= \sum_{k\neq 0}\frac{1}{e^{\beta E_k}-1}\left[\frac{\sigma}{h_L} - (1-e^{-\sigma/h_L})\right] + \sum_{n\neq 0} G\left(\frac{1-e^{-\sigma/h_L}}{e^{2\pi^2\beta n^2/L^2}-1}\right),\end{aligned} \tag{B18}$$

where $G(u)=u-\log(1+u)$.

Let us consider first the case $d=3$. Then $h_L=L^2$, so that $F_L(\sigma)$ is well defined for $\Re\sigma>\sigma_0 \equiv -2\pi^2\beta$; hence we shall fix σ so that this condition is satisfied. Then the first term in the third line of (B18) goes to 0 as $L\to\infty$, since it is bounded by CL^{-1}, where C (here and in the following) denotes a suitable positive constant, depending on σ but independent of L. Note that

$$u_{n,L} \equiv \frac{1-e^{-\sigma/h_L}}{e^{2\pi^2\beta n^2/L^2}-1} \xrightarrow[L\to\infty]{} u_n^* \equiv \frac{\sigma}{2\pi^2\beta n^2} \tag{B19}$$

and that $|u_{n,L}|$, $|u_n^*|\leqslant Cn^{-2}$, and $|u_{n,L}-u_n^*|\leqslant C/L^2$. On the other hand, $\Re u_{n,L}$ and $\Re u_n^*$ are larger of some constant $u_0>-1$, for any n; since $G'(u)=u/(1+u)$, it immediately follows that

$$|G(u_{n,L})-G(u_n^*)| \leqslant C|u_{n,L}-u_n^*|n^{-2} \leqslant Cn^{-7/2}|u_{n,L}-u_n^*|^{1/4} \leqslant C|n|^{-7/2}L^{-1/2}. \tag{B20}$$

It follows that $\log F_L(\sigma)$ and $F_L(\sigma)$ are convergent for $L\to\infty$ and that, if $F(\sigma)=\lim_{L\to\infty} F_L(\sigma)$,

$$\Pi(\sigma) \equiv \log F(\sigma) = \sum_{n\neq 0} G\left(\frac{\sigma}{2\pi^2\beta n^2}\right). \tag{B21}$$

It is not hard to show that $\Pi(\sigma)$ is differentiable and that

$$\Pi'(\sigma) = \sum_{n\neq 0} \frac{\sigma}{2\pi^2\beta n^2(\sigma+2\pi^2\beta n^2)} \tag{B22}$$

implying that, if $x\in\mathbb{R}$,

$$\lim_{x\to+\infty} \Pi'(x) = +\infty, \quad \lim_{x\to\sigma_0^+} \Pi'(x) = -\infty. \tag{B23}$$

Let us now call $P(\mathrm{d}y)$ the probability measure such that

$$F(\sigma) = e^{\Pi(\sigma)} = \int P(\mathrm{d}y) e^{-\sigma y}. \tag{B24}$$

The property (B23) easily implies that the support of $P(\mathrm{d}x)$ is the full real line. Moreover, the characteristic function $f(t)$ of $P(\mathrm{d}x)$ is given by the equation

$$f(t) = e^{\Pi(-it)} = \prod_{n\neq 0} \frac{e^{-ita n^{-2}}}{1 - ita n^{-2}}, \quad a = (2\pi^2\beta)^{-1}. \tag{B25}$$

By using the bound $\log(1+x) \geq 2x/3$, valid for $0 \leq x \leq 1/2$, we get, if $|t| \geq 1$,

$$|f(t)| \leq \prod_{n\neq 0} (1 + t^2 a^2 |n|^{-4})^{-1/2} \leq \prod_{|n|\leq(\sqrt{2}a|t|)^{1/2}} (3/2)^{-1/2} \prod_{|n|>(\sqrt{2}a|t|)^{1/2}} e^{-t^2 a^2 |n|^{-4}/3} \leq e^{-C|t|^{3/2}}. \tag{B26}$$

This bound and the support properties of $P(\mathrm{d}y)$ imply that $P(\mathrm{d}y) = \rho(y)\mathrm{d}y$, with $\rho(y)$ a strictly positive smooth function on $\mathbb{R}$.

In order to complete the proof of the theorem in the case $d=3$, we still have to prove the strong convergence property (B16), together with the uniform bound (B15) on $h_L P_L(M)$. Note that the definition of characteristic function implies that

$$h_L P_L(M) = \frac{1}{2\pi} \int_{-\pi h_L}^{+\pi h_L} \mathrm{d}t\, e^{-ity_L} f_L(t). \tag{B27}$$

By using (B18), we see that

$$f_L(t) = F_L(-it) = \prod_{n\neq 0} \frac{e^{v_{n,L}}}{1 + u_{n,L}}, \tag{B28}$$

where $u_{n,L}$ is given by (B19) with $\sigma = -it$ and

$$v_{n,L} = \frac{-it}{L^2(e^{2\pi^2\beta n^2/L^2} - 1)}. \tag{B29}$$

It follows that $|f_L(t)| \leq \Pi_{n\neq 0} |1+u_{n,L}|^{-1}$. Moreover, by using (B19), we see that, if $|t| \leq \pi L^2/2$ and $|n|^2 \leq |t|$, $|1+u_{n,L}| \geq 1+\delta$, with a suitable $\delta > 0$. Hence, if $|t| \leq \pi L^2/2$, $|f_L(t)| \leq \Pi_{0<|n|\leq|t|^{1/2}} (1+\delta)^{-1}$ $\leq \exp(-C|t|^{-3/2})$. If $\pi L^2/2 \leq |t| \leq \pi L^2$, the same result is obtained, by observing that in this case, if $|n| \leq L$, $|1+u_{n,L}| \geq 1 + 1/(e^{2\pi^2\beta} - 1)$, so that $|f_L(t)| \leq \exp(-CL^3) \leq \exp(-C|t|^{-3/2})$. Hence, we can show that, uniformly in L,

$$|f_L(t)| \leq \exp(-C|t|^{3/2}), \quad |t| \leq \pi h_L \tag{B30}$$

which implies, together with (B27), that $h_L P_L(M) \leq C$, with C independent of L and M. Moreover, by the dominated Lebesgue convergence theorem, we get, for any $y \in \mathbb{R}$,

$$y_L \xrightarrow[L\to\infty]{} y \Rightarrow h_L P_L(M) \xrightarrow[L\to\infty]{} \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ity} f(t) = \rho(y). \tag{B31}$$

In order to complete the proof of (B15), we use the identity

$$(-iy_L)^2 h_L P_L(M) = \frac{1}{2\pi} \int_{-\pi h_L}^{+\pi h_L} e^{-ity_L} f_L''(t). \tag{B32}$$

Since $f_L''(t) = f_L(t)[\Pi_L'(-it)^2 + \Pi_L''(-it)]$, where $\Pi_L(-it) = \log F_L(-it)$, and, as one can check easily by proceeding as in the analysis given before of $\log F_L(\sigma)$, uniformly in L,

$$|\Pi_L'(-it)| \leq C|t|, \quad |\Pi_L(-it)| \leq C \tag{B33}$$

the bound (B15) immediately follows from the bound (B30).

Let us now suppose that $d=4$. Then $h_L = L^2\sqrt{\log L}$, so that, given any $x<0$, $F_L(\sigma)$ is well defined for $\Re\sigma > x$, if $L > \exp(-x/(2\pi^2\beta))$. Moreover, as in the case $d=3$, the first term in the third line of (B18) goes to 0 as $L \to \infty$, since it is bounded by $C(\log L)^{-1/2}$.

If we define $u_{\mathfrak{a},L}$ as in (B19), $|u_{\mathfrak{a},L}| \leqslant C(\mathfrak{a}^2\sqrt{\log L})^{-1}$, with C only depending on σ if L is large enough. Hence, if $\tilde{G}(u) = u - \log(1+u) - u^2/2$,

$$\left| \sum_{\mathfrak{a}\neq 0} \tilde{G}(u_{\mathfrak{a},L}) \right| \leqslant \frac{C}{(\log L)^{3/2}} \sum_{\mathfrak{a}\neq 0} \frac{1}{|\mathfrak{a}|^6} \xrightarrow[L\to\infty]{} 0. \tag{B34}$$

Note also that $L^{-4}\Sigma_{|\mathfrak{a}|\geqslant L}[\exp(a\mathfrak{a}^2/L^2)-1]^{-2}$ is bounded for $L\to\infty$, for any $a>0$, and that

$$\frac{1}{\log L} \sum_{0<|\mathfrak{a}|\leqslant L} \left[\frac{1}{(a\mathfrak{a}^2)^2} - \frac{1}{L^4(e^{a\mathfrak{a}^2/L^2}-1)^2} \right] \leqslant \frac{C}{L^2 \log L} \sum_{0<|\mathfrak{a}|\leqslant L} \frac{1}{|\mathfrak{a}|^4} \xrightarrow[L\to\infty]{} 0 \tag{B35}$$

so that $(\log L)^{-1}L^{-4}\Sigma_{\mathfrak{a}\neq 0}[\exp(a\mathfrak{a}^2/L^2)-1]^{-2}$ is convergent for $L\to\infty$ and

$$c_0 = \lim_{L\to\infty} \frac{1}{\log L} \sum_{\mathfrak{a}\neq 0} \frac{1}{L^4(e^{a\mathfrak{a}^2/L^2}-1)^2} = \lim_{L\to\infty} \frac{1}{\log L} \sum_{0<|\mathfrak{a}|\leqslant L} \frac{1}{a^2|\mathfrak{a}|^4} = \frac{1}{a^2} \lim_{L\to\infty} \frac{1}{\log L} \int_{1\leqslant|\mathfrak{x}|\leqslant L} \frac{\mathrm{d}^4\mathfrak{x}}{|\mathfrak{x}|^4} = \frac{2\pi^2}{a^2}. \tag{B36}$$

By using (B18) and (B36) with $a = 2\pi^2\beta$, it is now easy to prove that $\log F_L(\sigma)$ is convergent for $L\to\infty$ and that

$$\Pi(\sigma) = \lim_{L\to\infty} \log F_L(\sigma) = \frac{1}{2}\sigma^2 \lim_{L\to\infty} \frac{1}{L^4 \log L} \sum_{\mathfrak{a}\neq 0} \frac{1}{(e^{2\pi^2\beta\mathfrak{a}^2/L^2}-1)^2} = \frac{1}{2}\frac{2}{(2\pi\beta)^2}\sigma^2. \tag{B37}$$

It follows immediately, if we define $P(\mathrm{d}y)$ as in the case $d=3$, that $P(\mathrm{d}y)$ is a Gaussian probability measure with density $\rho(y) = (2\pi c_0)^{-1/2}\exp[-y^2/(2c_0)]$, with $c_0 = 2/(2\pi\beta)^2$. The proof of (B15) and (B16) in the case $d=3$ can be easily extended to this case; we omit the details.

Let us finally consider the case $d\geqslant 5$. Then $h_L = L^{d/2}$ and we can proceed as in the previous case, the only relevant difference being that now $\Pi(\sigma)$ gets a contribution also from the first term in the third line of (B18). We find that $\Pi(\sigma) = \frac{1}{2}c_0\sigma^2$, with

$$\begin{aligned} c_0 &= \lim_{L\to\infty} \frac{1}{L^d} \sum_{\mathfrak{a}\neq 0} \left[\frac{1}{e^{2\pi^2\beta\mathfrak{a}^2/L^2}-1} + \frac{1}{(e^{2\pi^2\beta\mathfrak{a}^2/L^2}-1)^2} \right] = \int \frac{\mathrm{d}^d\mathfrak{k}}{(2\pi)^d} \frac{e^{-\beta E_{\mathfrak{k}}}}{(1-e^{-\beta E_{\mathfrak{k}}})^2} \\ &= \sum_{j_1,j_2\geqslant 0} \int \frac{\mathrm{d}^d\mathfrak{k}}{(2\pi)^d} e^{-\beta E_{\mathfrak{k}}(j_1+j_2+1)} = \sum_{j\geqslant 1} \frac{j}{(2\pi\beta j)^{d/2}}. \end{aligned} \tag{B38}$$

The proof of (B15) and (B16) in the case $d=3$ can be easily extended also to this case, so completing the proof of the theorem. ■

APPENDIX C: PROOF OF THEOREM 3.1

Note that the mean field grand canonical partition function can be written as

$$\Xi^{mf}_{\lambda,L} = e^{1/2\beta\lambda^2 L^d} \sum_{N=0}^{\infty} e^{-(\beta/2)L^d[(N/L^d)-\lambda]^2} Z_{N,L} \tag{C1}$$

and that

$$P_L(M\leqslant N) = P_L\left(y_L \leqslant \frac{L^d}{h_L}(\lambda-\lambda^*) + \frac{L^{d/2}}{h_L}x_N + \frac{L^2}{h_L}c_L \right),$$

$$x_N = L^{d/2}\left(\frac{N}{L^d} - \lambda\right). \tag{C2}$$

Let us now define

$$\Gamma_{\lambda,L} \equiv \frac{\Xi^{mf}_{\lambda,L}}{e^{1/2\beta\lambda^2 L^d} Q_L L^{d/2}} = \frac{1}{L^{d/2}} \sum_{N=0}^{\infty} e^{-\beta/2L^d[(N/L^d)-\lambda]^2} P_L(M \leqslant N). \tag{C3}$$

Theorem 3.1 follows from the following Lemma.

Lemma C.1: If $\lambda \geqslant \lambda^*$, *the quantity* $\Gamma_{\lambda,L}$ *has a limit as* $L \to \infty$. *If* $\lambda > \lambda^*$, *we have, for any* $d \geqslant 3$,

$$\lim_{L\to\infty} \Gamma_{\lambda,L} = \sqrt{\frac{2\pi}{\beta}} \tag{C4}$$

while, if $\lambda = \lambda_*$, *we have*

$$0 < \lim_{L\to\infty} \Gamma_{\lambda,L} = \begin{cases} \sqrt{\dfrac{2\pi}{\beta}} \displaystyle\int_{-\infty}^{c^*} dy\, \rho(y), & d = 3, \\ \sqrt{\dfrac{\pi}{2\beta}}, & d = 4, \\ \displaystyle\int_{-\infty}^{+\infty} dx\, e^{-\beta x^2/2} \int_{-\infty}^{x} dy\, \rho(y), & d \geqslant 5, \end{cases} \tag{C5}$$

where $\rho(y)$ *is the density probability defined in Theorem B.2.*

Moreover, if $N_L = [uL^d]$ ($[\cdot]$ *denotes the integer part*), $u > \lambda^*$, *and* $N_L^* = [\lambda^* L^d]$, *then*

$$\lim_{L\to\infty} \frac{Z_{N_L,L}}{Z_{N_L^*,L}} = \begin{cases} 1/P(y \leqslant c_*), & d = 3, \\ 2, & d \geqslant 4. \end{cases} \tag{C6}$$

Proof: By Theorem B.2, $P_L(y_L \leqslant \overline{y}) \to_{L\to\infty} \int_0^{\overline{y}} dy\, \rho(y)$, for any fixed $\overline{y}$, $\rho(y)$ being a strictly positive function depending on the dimension d. Hence, by using (C2) and Lemma B.1, we can easily show that, if $\lambda > \lambda^*$ and $x_N \to_{L\to\infty} x$

$$P_L(M \leqslant N) \xrightarrow[L\to\infty]{} 1, \quad \forall\, x \tag{C7}$$

while, if $\lambda = \lambda^*$ and $x_N \to_{L\to\infty} x$,

$$P_L(M \leqslant N) \xrightarrow[L\to\infty]{} \begin{cases} P(y \leqslant c_*), & d = 3, \\ P(y \leqslant 0) = 1/2, & d = 4, \\ P(y \leqslant x), & d \geqslant 5. \end{cases} \tag{C8}$$

Then (C4) and (C5) follow from (C3) and a simple application of the dominated Lebesgue convergence theorem. The proof of (C6) is a simple consequence of (C2), (C8) and the equation, valid if $N_L = [uL^d]$, $u > \lambda^*$, and $N_L^* = [\lambda^* L^d]$,

$$\lim_{L\to\infty} \frac{Z_{N_L,L}}{Z_{N_L^*,L}} = \lim_{L\to\infty} \frac{P_L(M \leqslant N_L)}{P_L(M \leqslant N_L^*)} = \lim_{L\to\infty} \frac{P_L\left(y_L \leqslant \dfrac{L^d}{h_L}(u - \lambda^*)\right)}{P_L(y_L \leqslant c_L L^2/h_L)}. \tag{C9}$$

■

By similar arguments, one can prove the following theorem (see also Ref. 2 for the case $\lambda > \lambda^*$).

Theorem C.2: *If* $\lambda > \lambda^*$, *the distribution of the random variable* x_N *converges, as* $L \to \infty$, *to a Gaussian distribution with density* $\exp(-\beta x^2/2)$; *the same result is true if* $\lambda = \lambda^*$ *and* $d = 3, 4$. *However, if* $d > 4$, *the limiting distribution is still well defined, but it is not Gaussian anymore; it is proportional to* $e^{-\beta x^2/2} \int_{-\infty}^{x} dy\, \rho(y)$, $\rho(y)$ *being the density probability defined in Theorem B.2.*

APPENDIX D: DISTRIBUTION OF "SHORT LOOPS"

In this appendix we will restrict to $d \geqslant 3$ and $\lambda \geqslant \lambda^*$ and study the distribution of the variables,

$$y_{A,L} = \frac{\sum_{j \in A} j n_j - L^d \rho_{A,L}}{h_{A,L}}, \quad \rho_{A,L} = \sum_{j \in A} \rho_{j,L}, \tag{D1}$$

where A is a finite subset of $\mathbb{N}^+$, $L^D \rho_{j,L}$ is the mean value of $j n_j$ with respect to the mean field measure and $h_{A,L}$ is a suitable scaling factor. The main results are stated in Theorems D.4 and D.5 below, the main ingredient in the proofs is the reduction to the analysis of the probability distribution $P_L(M)$ defined in Appendix B.

We start by deriving the following expression for $\rho_{j,L}$:

$$\rho_{j,L} = a(\beta j, L) \alpha_{j,L}, \tag{D2}$$

where

$$\alpha_{j,L} = \frac{1}{\Gamma_{\lambda,L}} \frac{1}{L^{d/2}} \sum_{N \geqslant 0} e^{-\beta x_N^2/2} P_L(M \leqslant N - j) \tag{D3}$$

with x_N as in (C2).

Proof of (D2): Let $w^0(j, n_j)$ be as in (2.1) with $\lambda = 0$, then

$$\rho_{j^*,L} = \frac{e^{(\beta\lambda^2/2)L^d}}{\Xi^{mf}_{\lambda,L}} \sum_N e^{-\beta(x_N^2/2)} \sum_{\underline{n}: \Sigma_j j n_j = N} \prod_j w^0(j, n_j) \frac{j^* n_{j^*}}{L^d} = \frac{e^{(\beta\lambda^2/2)L^d}}{\Xi^{mf}_{\lambda,L}} a(\beta j^*, L) \sum_N e^{-\beta(x_N^2/2)} Z_{N-j^*,L}. \tag{D4}$$

By (B1) and (B3) we get

$$\rho_{j^*,L} = \frac{e^{(\beta\lambda^2/2)L^d}}{\Xi^{mf}_{\lambda,L}} a(\beta j^*, L) Q_L \sum_N e^{-\beta(x_N^2/2)} P_L(M < N - j^*) \tag{D5}$$

hence (D2) follows by (C3). ■

Lemma D.1: For any $\lambda \geqslant \lambda^*$, *there is a constant* C, *independent of* L *and* j, *such that, if* h_L *is defined as in* (B12),

$$0 < 1 - \alpha_{j,L} \leqslant C \frac{j}{h_L}. \tag{D6}$$

Moreover, if $\lambda = \lambda^*$,

$$\lim_{L\to\infty}\frac{h_L}{j}(1-\alpha_{j,L})=\begin{cases}\dfrac{\rho(c^*)}{\displaystyle\int_{-\infty}^{c^*}\mathrm{d}y\,\rho(y)}, & d=3,\\ 2\rho(0), & d=4,\\ \dfrac{\displaystyle\int_{-\infty}^{+\infty}\mathrm{d}x\,e^{-\beta x^2/2}\rho(x)}{\displaystyle\int_{-\infty}^{+\infty}\mathrm{d}x\,e^{-\beta x^2/2}\int_{-\infty}^{x}\mathrm{d}y\,\rho(y)}, & d\geqslant 5,\end{cases}\tag{D7}$$

where $\rho(y)$ is defined as in Lemma C.1.

Proof: Note that

$$1-\alpha_{j,L}=\frac{1}{\Gamma_{\lambda,L}}\frac{1}{L^{d/2}}\sum_{N\geqslant 0}e^{-\beta x_N^2/2}P_L(N-j<M\leqslant N).\tag{D8}$$

By using the claim in Lemma C.1 that $h_L P_L(M)$ is bounded uniformly in L and M, we get

$$P_L(N-j<M\leqslant N)=\frac{1}{h_L}\sum_{M=N-j+1}^{N}h_L P_L(M)\leqslant C\frac{j}{h_L}\tag{D9}$$

which immediately implies (D6), by using Lemma C.1. On the other hand, if $\lambda=\lambda^*$ and $M=N-r$, $r\geqslant 1$, the corresponding y_L variable is equal, see (C2), to $(L^{d/2}x_N+L^2c_L-r)/h_L$, so that, by using (B16),

$$h_L P_L(M=N-r)\xrightarrow[L\to\infty]{}\begin{cases}\rho(c^*), & d=3,\\ \rho(0), & d=4,\\ \rho(x), & d\geqslant 5.\end{cases}\tag{D10}$$

Equations (D7) then follows from Lemma C.1 and dominated convergence theorem. ■

If $\lambda>\lambda^*$, $h_L P_L(M=N-r)$ goes to 0 as $L\to\infty$, so we expect the bound (D6) can be improved. This is especially true if j is taken as a diverging function of L; in particular, if $j>(\lambda-\lambda^*)L^d$, it is easy to see that $\alpha_{j,L}\to 0$ as $L\to\infty$. In order to get good bounds in all these cases, we shall use the following large deviation bound for the probability measure $P_L(M)$.

Lemma D.2: Let $0<u_1<u_2$; then there exist $\bar{L}(u_1)$, such that the probabilities,

$$S_L^+(u_1,u_2)\equiv P_L(L^d\lambda_L^*+L^d u_1\leqslant M\leqslant L^d\lambda_L^*+L^d u_2),\tag{D11}$$

$$S_L^-(u_1,u_2)\equiv P_L(L^d\lambda_L^*-L^d u_2\leqslant M\leqslant L^d\lambda_L^*-L^d u_1),\tag{D12}$$

satisfy, for $L\geqslant\bar{L}(u_1)$, the following bounds:

$$e^{-a_1u_2L^{d-2}(1+\delta_L)}\leqslant S_L^+(u_1,u_2)\leqslant e^{-a_1u_1L^{d-2}(1-\delta_L)},\quad\forall\,u_1>0,\tag{D13}$$

$$e^{-f(u_2)(L^d/h_L)^2(1+\delta_L)}\leqslant S_L^-(u_1,u_2)\leqslant e^{-f(u_1)(L^d/h_L)^2(1-\delta_L)},\quad u_2<\lambda^*,\tag{D14}$$

where δ_L is a function which goes to 0 as $L\to\infty$, a_1 is a positive constant, depending on d, and $f(u)$ is a positive function of order u^2 for $u\to 0$ (equal indeed to a_2u^2 for $d=2,3$).

Proof: By (C2), we can write

$$S_L^+(u_1,u_2)=\int_{u_1L^d/h_L}^{u_2L^d/h_L} P_L(\mathrm{d}y)=e^{\Pi_L(t)}\int_{u_1L^d/h_L}^{u_2L^d/h_L} e^{ty}P_{t,L}(\mathrm{d}y), \tag{D15}$$

where $\Pi_L(t)=\log F_L(t)$, $F_L(t)$ is the Laplace transform of $P_L(\mathrm{d}y)$ given by (B18), t is any real number such that $F_L(t)$ is well defined and $P_{t,L}(\mathrm{d}y)$ is the probability measure

$$P_{t,L}(\mathrm{d}y)=\frac{e^{-ty}P_L(\mathrm{d}y)}{F_L(t)}. \tag{D16}$$

By looking at (B18), we see that $F_L(t)$ is defined for $t>t_L^*$, where t_L^* is the value of t such that the argument $u_{n,L}$ of the function $G(u)=u-\log(1+u)$ is equal to -1 if $|\mathbf{n}|=1$, that is $t_L^*=-ah_L/L^2$. We choose t so that

$$-\Pi_L'(t)=\int \mathrm{d}y\, yP_{t,L}(\mathrm{d}y)=v\frac{L^d}{h_L},\quad v=\frac{u_1+u_2}{2}. \tag{D17}$$

By using (B18), this condition can be written

$$\frac{1}{h_L}\sum_{\mathbf{n}\neq 0}\frac{(e^{-t/h_L}-1)e^{a\mathbf{n}^2/L^2}}{(e^{a\mathbf{n}^2/L^2}-e^{-t/h_L})(e^{a\mathbf{n}^2/L^2}-1)}=v\frac{L^d}{h_L},\quad a=2\pi^2\beta. \tag{D18}$$

By proceeding as in the proof of Theorem B.2, it is easy to see that the sum in the lhs is bounded by $C|t|$, if we extract from it the terms with $|\mathbf{n}|=1$; hence we get

$$c_L-d\frac{t}{h_L^2}\frac{1}{a/L^2+t/h_L}\frac{L^2}{a}(1+\delta_{1,L})=v\frac{L^d}{h_L} \tag{D19}$$

with $\delta_{1,L}\to 0$ and $c_L\to c$ as $L\to\infty$. It follows that

$$t\frac{L^d}{h_L}=-aL^{d-2}(1+\delta_{2,L}) \tag{D20}$$

with $\delta_{2,L}\to 0$ as $L\to\infty$. It is easy to see that, for such a value of t, $\Pi_L(t)$ diverges as $C\log L$ for $d=3,4$ and as L^{d-4} for $d\geqslant 5$, so that we can write

$$S_L^+(u_1,u_2)=e^{-av L^{d-2}(1+\delta_L)}\int_{u_1L^d/h_L}^{u_2L^d/h_L} e^{t(y-vL^d/h_L)}P_{t,L}(\mathrm{d}y) \tag{D21}$$

with $\delta_L\to 0$ as $L\to\infty$. The upper bound in (D13) easily follows from this equation. In order to prove the lower bound we have also to show that

$$\int_{u_1L^d/h_L}^{u_2L^d/h_L} P_{t,L}(\mathrm{d}y)\geqslant 1-\delta_L \tag{D22}$$

with $\delta_L\to 0$. This result can be deduced as the other ones from the properties of the Laplace transform of the measure $P_{t,L}(\mathrm{d}y)$; we omit the details.

Let us now consider the upper bound of (D14). We proceed as before, by writing

$$S_L^-(u_1,u_2)=e^{\Pi_L(t)-t\Pi_L'(t)}\int_{-u_2L^d/h_L}^{-u_1L^d/h_L} e^{t(y+u_1L^d/h_L)}P_{t,L}(\mathrm{d}y)\leqslant e^{\Pi_L(t)-t\Pi_L'(t)}, \tag{D23}$$

where t is chosen so that $\Pi_L'(t)=u_1L^d/h_L$. It is easy to see that $\Pi_L'(t)$ is a monotone function and that $\lim_{t\to\infty}\Pi_L'(t)=\lambda_L^*L^d/h_L$, so that t is well defined for L large enough, if $u_1<\lambda^*$. It turns out that $\lim_{L\to\infty}t(h_L/L^d)=f_0(u)>0$, with $f_0(u)$ of order u for $u\to 0$ (and equal to c_du for $d=3,4$, for some $c_d>0$). Moreover

$$\Pi_L(t) - t\Pi'_L(t) = -\int_0^t ds \int_0^s du\, \Pi''_L(u), \quad C/2 < \Pi''_L(u) \leq C \tag{D24}$$

and one can prove that $\lim_{L\to\infty} \Pi''_l(u) = C_d > 0$, uniformly for $0 \leq u \leq t$; this allows us to get the upper bound in (D14). The lower bound is obtained in a similar way, by choosing t so that $\Pi'_L(t) = u_2 L^d/h_L$ and by proving that $\int_{-u_2 L^d/h_L}^{-u_1 L^d/h_L} P_{t,L}(dy) \to 1/2$ for $L \to \infty$. ■

We can now prove the following bounds on the factors $\alpha_{j,L}$.

Lemma D.3: Given $d \geq 3$, $\lambda > \lambda^*$ and a sequence j_L such that

$$\lim_{L\to\infty} j_L/L^d = \gamma < (\lambda - \lambda^*) \tag{D25}$$

there exists $\bar{L}$ such that, if $L \geq \bar{L}$ and $j \leq j_L$,

$$1 - \alpha_{j,L} \leq Ce^{-a_3(\lambda-\lambda^*-\gamma)L^{d-2}}, \tag{D26}$$

where C and a_3 are constants independent of L and of j.

Moreover, if $\lambda \geq \lambda^*$ and $\gamma > \lambda - \lambda^*$, there exist C, a_4 and $\bar{L}$ such that, if $L \geq \bar{L}$ and $j \geq j_L$,

$$\alpha_{j,L} \leq Ce^{-a_4[\gamma - [\lambda-\lambda^*)]\, L^{d-1}}. \tag{D27}$$

Proof. Note that

$$P_L(N - j < M \leq N) \leq P_L\left(y_L \geq \frac{(\lambda - \lambda^*)L^d + c_L L^2 + x_N L^{d/2} - j}{h_L}\right). \tag{D28}$$

Hence, if $j \leq j_L$, with $j_L/L^d \to \gamma$ as $L \to \infty$, and $|x_N| \leq L^{(d-1)/2}$, so that $|x_N| L^{d/2}/h_L \leq L^{-1/2} L^d/h_L$,

$$P_L(N - j < M \leq N) \leq P_L\left(y_L \geq \frac{(\lambda - \lambda^* - \gamma - \delta_L)L^d}{h_L}\right) \tag{D29}$$

with $\delta_L \to 0$ as $L \to \infty$. On the other hand,

$$\frac{1}{L^{d/2}} \sum_{N=0}^{\infty} e^{-(\beta/2)x_N^2} \mathbf{1}_{|x_N| \geq L^{(d-1)/2}} \leq Ce^{-(\beta/4)L^{d-1}}. \tag{D30}$$

The bound (D26) then easily follows from (D8) and Lemma D.2 since the upper bound in (D13) is independent of the u_2 value (equal to $+\infty$ in this case).

The bound (D27) is proved in a similar way, by using the upper bound in (D14) and the remark that $L^{d-1} \leq (L^d/h_L)^2$. ■

We have now all the technical ingredients to study the Laplace transform $F_{A,L}(\sigma)$ of the probability distribution of the random variables $y_{A,L}$ defined in (D1). We have

$$F_{A,L}(\sigma) = \frac{e^{\sigma(L^d \rho_{A,L}/h_{A,L})}}{\Gamma_{\lambda,L}} \frac{1}{L^{d/2}} \sum_{N \geq 0} e^{-\beta x_N^2/2} \frac{1}{Q_L} \sum_{\{n_j \geq 0, j \geq 1\}} \mathbf{1}_{\Sigma j n_j = N} \cdot \prod_{j \notin A} w(j, n_j) \prod_{j \in A} w(j, n_j) e^{-\sigma(j n_j/h_{A,L})}. \tag{D31}$$

By using (2.14) and the identity

$$w(j,n)e^{-\sigma(j n_j/h_{A,L})} = \sum_{\{n', n'' \geq 0\}} \mathbf{1}_{n'+n''=n} \frac{1}{n'!} \left[\frac{L^d a(\beta j, L) e^{-\sigma(j/h_{A,L})} - 1}{j}\right]^{n'} \frac{1}{n''!} \left(\frac{1}{j}\right)^{n''} \tag{D32}$$

we see that

$$F_{A,L}(\sigma) = G_{A,L}(\sigma)\frac{1}{\Gamma_{\lambda,L}}\frac{1}{L^{d/2}}\sum_{N\geqslant 0} e^{-\beta x_N^2/2} P_{A,L,\sigma}(M \leqslant N), \tag{D33}$$

where

$$P_{A,L,\sigma}(M) = Q_{A,L,\sigma}^{-1} \sum_{\{n_j\geqslant 0, j\geqslant 1\}} \mathbf{1}_{\Sigma j n_j = M} \prod_{j\notin A} \tilde{w}(j,n_j) \prod_{j\in A} \tilde{w}(j,n_j,\sigma), \tag{D34}$$

$$Q_{A,L,\sigma} = \sum_{\{n_j\geqslant 0, j\geqslant 1\}} \prod_{j\notin A} \tilde{w}(j,n_j) \prod_{j\in A} \tilde{w}(j,n_j,\sigma), \tag{D35}$$

$$\tilde{w}(j,n,\sigma) = \frac{1}{n!}\left[\frac{L^d a(\beta j,L) e^{-\sigma(j/h_{A,L})} - 1}{j}\right]^n, \tag{D36}$$

$$G_{A,L}(\sigma) = e^{\sigma(L^d \rho_{A,L}/h_{A,L})}\frac{Q_{A,L,\sigma}}{Q_L}. \tag{D37}$$

Note that $P_{A,L,\sigma}(M)$ in general is not a probability distribution for any value of σ (this is clear only for σ real and negative). Moreover, in all the choices of the set A we shall consider, $P_{A,L,\sigma}(M)$ is absolutely summable over M and its sum is equal to 1 (which is formally true by definition). Hence, we can consider it as a finite complex measure on $\mathbb{R}$ (with support on a lattice set) and we shall study its convergence, as $L\to\infty$, to a measure with smooth density.

A few simple calculations show that

$$\log Q_{A,L,\sigma} = \sum_{j\in A} \frac{L^d a(\beta j,L) e^{-\sigma(j/h_{A,L})} - 1}{j} + \sum_{j\notin A} \frac{L^d a(\beta j,L) - 1}{j}, \tag{D38}$$

so that

$$\begin{aligned}\log G_{A,L}(\sigma) &= \sigma\frac{L^d \rho_{A,L}}{h_{A,L}} + \sum_{j\in A} \frac{L^d a(\beta j,L)}{j}(e^{-\sigma(j/h_{A,L})} - 1) \\ &= \sigma r_{A,L}^* + \sum_{j\in A} \frac{L^d a(\beta j,L)}{j}\left(e^{-\sigma(j/h_{A,L})} - 1 + \sigma\frac{j}{h_{A,L}}\right),\end{aligned} \tag{D39}$$

where

$$r_{A,L}^* = \frac{L^d}{h_{A,L}}\sum_{j\in A} a(\beta j,L)(\alpha_{j,L} - 1). \tag{D40}$$

It will also useful to consider the random variable

$$y_{A,L,\sigma} = \frac{M - M_{A,L,\sigma}^*}{h_L}, \tag{D41}$$

where M is a random variable with measure $P_{A,L,\sigma}(M)$ and h_L is defined as in (B12).

The mean value of M is given by

$$M_{A,L,\sigma}^* \equiv \sum_{M=0}^{\infty} M P_{A,L,\sigma}(M) = \sum_{j\in A} (L^d a(\beta j,L) e^{-\sigma(j/h_{A,L})} - 1) + \sum_{j\notin A} (L^d a(\beta j,L) - 1). \tag{D42}$$

By using (B8) and (B4), we see that

$$M^*_{A,L,\sigma} = L^d \lambda^*_L + L^d \sum_{j \in A} a(\beta j, L)(e^{-\sigma(j/h_{A,L})} - 1), \tag{D43}$$

so that

$$P_{A,L,\sigma}(M \leqslant N) = P_{A,L,\sigma}\left(y_{A,L,\sigma} \leqslant \frac{L^d(\lambda - \lambda^*) + L^{d/2} x_N + L^2 c_L}{h_L} + y^*_{A,L,\sigma} \right), \tag{D44}$$

$$y^*_{A,L,\sigma} = \frac{L^d}{h_L} \sum_{j \in A} a(\beta j, L)(1 - e^{-\sigma(j/h_{A,L})}). \tag{D45}$$

As in the proof of Theorem B.2, the limiting distribution of $y_{A,L,\sigma}$ will be obtained by studying the Laplace transform $H_{A,L,\sigma}(w)$ of its measure. We have

$$\log H_{A,L,\sigma}(w) = \sum_{j=1}^{\infty} \frac{L^d a(\beta j, L) - 1}{j} \left(e^{-w(j/h_L)} - 1 + w \frac{j}{h_L} \right) + \log R_{A,L,\sigma}(w), \tag{D46}$$

$$\log R_{A,L,\sigma}(w) = \sum_{j \in A} \frac{L^d a(\beta j, L)}{j} (e^{-\sigma(j/h_{A,L})} - 1) \left(e^{-w(j/h_L)} - 1 + w \frac{j}{h_L} \right). \tag{D47}$$

If we define $f_{A,L,\sigma}(t) = H_{A,L,\sigma}(-it)$, we have also

$$h_L P_{A,L,\sigma}(M) = \frac{1}{2\pi} \int_{-\pi h_L}^{+\pi h_L} e^{-it y_{A,L,\sigma}} f_{A,L,\sigma}(t). \tag{D48}$$

Moreover, if $\sigma = 0$, the function $H_{A,L,\sigma}(w)$ has to coincide [as one could check by using the identity (A4) and some easy algebra] with the function $F_L(w)$ defined in (B18). It follows that

$$\log H_{A,L,\sigma}(w) = \log F_L(w) + \log R_{A,L,\sigma}(w),$$

$$f_{A,L,\sigma}(t) = f_L(t) R_{A,L,\sigma}(-it). \tag{D49}$$

We shall consider some special cases for the set A. First of all, we consider the simplest one, that is the case where A contains only one element; we prove the following theorem.

Theorem D.4: *If $A = \{j\}$ and $h_{A,L} = L^{d/2}$, then, if $d \geqslant 3$ and $\lambda \geqslant \lambda^*$,*

$$\rho_{\{j\},L} \xrightarrow[L \to \infty]{} \rho_j \equiv (2\pi\beta j)^{-d/2}. \tag{D50}$$

Moreover, if $d \geqslant 3$ and $\lambda > \lambda^*$ or $d = 3, 4$ and $\lambda = \lambda^*$, the probability distribution of $y_{A,L}$ converges, as $L \to \infty$, to a Gaussian distribution with variance $j\rho_j$. Finally, if $d \geqslant 5$ and $\lambda = \lambda^*$, the limiting distribution is still well defined, but its Laplace transform is given by

$$\lim_{L \to \infty} \log F_{\{j\},L}(\sigma) = -\sigma r^* j \rho_j + \frac{1}{2} \sigma^2 j \rho_j + \log \left\{ \frac{\displaystyle\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-\beta x^2/2} \int_{-\infty}^{x + \sigma j \rho_j} \mathrm{d}y\, \rho(y)}{\displaystyle\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-\beta x^2/2} \int_{-\infty}^{x} \mathrm{d}y\, \rho(y)} \right\}, \tag{D51}$$

where

$$r^* = \frac{\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-\beta x^2/2} \rho(x)}{\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-\beta x^2/2} \int_{-\infty}^{x} \mathrm{d}y\, \rho(y)}. \tag{D52}$$

Proof: By using the definition of $a(\beta j, L)$ in (2.2), we see that, for any j,

$$a(\beta j, L) \xrightarrow[L\to\infty]{} (2\pi\beta j)^{-d/2} = \rho_j. \tag{D53}$$

Moreover, by Lemma (D1) and (D2), $\forall \lambda \geqslant \lambda^*$,

$$\lim_{L\to\infty} \alpha_{j,L} = 1 \Rightarrow \lim_{L\to\infty} \rho_{j,L} = \rho_j. \tag{D54}$$

Let us now observe that, by (D47), for any fixed σ and w,

$$|\log R_{\{j\},L,\sigma}(w)| \leqslant C \frac{L^d}{L^{d/2} h_L^2} j^{2-d/2} \xrightarrow[L\to\infty]{} 0. \tag{D55}$$

Moreover, if we set $w = -it$, $t \in \mathbb{R}$, for any fixed σ, we have

$$|\log R_{\{j\},L,\sigma}(-it)| \leqslant C|t| \frac{L^d}{L^{d/2} h_L} j^{1-d/2} \leqslant C|t|. \tag{D56}$$

Hence we see, by using (D49) and the bound (B30), that $|f_{A,L,\sigma}(t)| \leqslant \exp(-C|t|^{3/2})$. It is easy to prove that this bound is valid also for $f''_{A,L,\sigma}(t)$, which implies that the measure $P_{\{j\},L,\sigma}(M)$ satisfies the analogous of (B15) and (B16) (we omit the details); and that $P_{\{j\},L,\sigma}(y \leqslant \overline{y})$ converges to $P(y \leqslant \overline{y})$ for any $\overline{y}$, if $P(\mathrm{d}y)$ is the limiting probability measure of Theorem B.2. On the other hand, we have, see (D45),

$$y^*_{\{j\},L,\sigma} \xrightarrow[L\to\infty]{} \begin{cases} 0, & d = 3,4, \\ \sigma j \rho_j, & d \geqslant 5. \end{cases} \tag{D57}$$

Note also that, by Lemmas D.1 and D.3, see (D40),

$$r^*_{\{j\},L} \xrightarrow[L\to\infty]{} \begin{cases} 0, & d = 3,4, \quad \lambda \geqslant \lambda^*, \\ 0, & d \geqslant 5, \quad \lambda > \lambda^*, \\ -r^* j \rho_j & d \geqslant 5, \quad \lambda = \lambda^*. \end{cases} \tag{D58}$$

If $d=3$ or $d=4$, it follows, by using (D33) and (D39), that, for any $\lambda \geqslant \lambda^*$,

$$\lim_{L\to\infty} \log F_{\{j\},L}(\sigma) = \lim_{L\to\infty} \log G_{\{j\},L}(\sigma) = \tfrac{1}{2}\sigma^2 j \rho_j. \tag{D59}$$

The same result is true, if $d \geqslant 5$ and $\lambda > \lambda^*$. However, if $d \geqslant 5$ and $\lambda = \lambda^*$, we get (D51).

The fact that the Laplace transform converges for any σ implies that also the characteristic function is convergent. As it is well known,[3] this is sufficient to prove the convergence of the probability distribution of $y_{A,L}$. ■

We now consider a more interesting choice of the set A.

Theorem D.5: *Let $A = \{1 \leqslant j \leqslant j_L\}$, with j_L a monotone diverging function of L such that $j_L \leqslant L^2$. Then, if $d \geqslant 3$ and $\lambda \geqslant \lambda^*$,*

$$\rho_{A,L} \xrightarrow[L\to\infty]{} \sum_{j=1}^{\infty} \rho_j = \lambda^*. \tag{D60}$$

Moreover, if $j_L/L^2 \to_{L\to\infty} 0$ *and* $\lambda > \lambda^*$, *the probability distribution of* $y_{A,L}$ *converges, as* $L \to \infty$, *to a Gaussian distribution, provided we take*

$$h_{A,L} = \begin{cases} L^2 (j_L/L^2)^{1/4}, & d = 3, \\ L^2 \sqrt{\log j_L}, & d = 4, \\ L^{d/2}, & d \geqslant 5. \end{cases} \tag{D61}$$

The same result is true, if $\lambda = \lambda^*$, *provided* $d = 3$ *or* $d = 4$ *and* $\lim_{L\to\infty} \sqrt{\log j_L / \log L} = 0$; *in the other cases the limiting distribution is still well defined but it is not Gaussian.*

Proof: By using (2.2), it is easy to prove that, if $j \leqslant L^2$, there is a constant C, independent of j and L, such that

$$a(\beta j, L) \leqslant C\rho_j, \quad 0 < a(\beta j, L) - \rho_j \leqslant C\rho_j e^{-L^2/(2\beta j)}. \tag{D62}$$

Hence, since $0 \leqslant \alpha_{j,L} \leqslant 1$,

$$0 \leqslant \sum_{j \leqslant j_L} (\rho_{j,L} - \rho_j \alpha_{j,L}) \leqslant C \sum_{j \leqslant L^2} j^{-d/2} e^{-L^2/(2\beta j)} \leqslant C L^{2-d} \xrightarrow[L\to\infty]{} 0. \tag{D63}$$

On the other hand, by (D6),

$$0 \leqslant \sum_{j \leqslant j_L} \rho_j (1 - \alpha_{j,L}) \leqslant \frac{C}{h_L} \sum_{j \leqslant L^2} j^{-d/2+1} \xrightarrow[L\to\infty]{} 0. \tag{D64}$$

Equation (D60) is an easy consequence of the last two bounds.

In order to study the limiting distribution of $y_{A,L}$, we proceed as in the proof of Theorem D.4. First of all we observe that, by (D47), if $h_{A,L}$ is chosen as in (D61), for any fixed σ and w,

$$|\log R_{A,L,\sigma}(w)| \leqslant C \frac{L^d}{h_{A,L} h_L^2} \sum_{j=1}^{j_L} j^{2-d/2} \xrightarrow[L\to\infty]{} 0. \tag{D65}$$

Moreover, if we set $w = -it$, $t \in \mathbb{R}$, for any fixed σ, we have

$$|\log R_{\{j\},L,\sigma}(-it)| \leqslant C|t| \frac{L^d}{h_{A,L} h_L} \sum_{j=1}^{j_L} j^{1-d/2} \leqslant C|t|. \tag{D66}$$

Once again, by proceeding as in the proof of Theorem D.4, one can prove that the measure $P_{A,L,\sigma}(M)$ satisfies the analogous of (B15) and (B16); we omit the details. This implies the convergence of $P_{A,L,\sigma}(y \leqslant \overline{y})$ to $P(y \leqslant \overline{y})$ for any $\overline{y}$, if $P(\mathrm{d}y)$ is the limiting probability measure of Theorem B.2. On the other hand, we have, see (D45),

$$y^*_{A,L,\sigma} \xrightarrow[L\to\infty]{} \begin{cases} 0, & d = 3, \\ \sigma (2\pi^2 \beta)^{-2} \lim_{L\to\infty} \sqrt{\log j_L / \log L}, & d = 4, \\ \sigma \sum_{j=1}^{\infty} j \rho_j, & d \geqslant 5. \end{cases} \tag{D67}$$

Let us now suppose that $\lambda > \lambda^*$. Then, by using (D26), we can easily show that, for any $d \geqslant 3$, $r^*_{A,L}$, [see (D40)] goes to 0 as $L \to \infty$. It is also very easy to show that the factor which multiplies $G_{A,L}(\sigma)$ on the rhs of (D33) goes to 1 as $L \to \infty$. Hence, by using (D39), we get

$$\lim_{L\to\infty} \log F_{A,L}(\sigma) = \lim_{L\to\infty} \log G_{A,L}(\sigma) = \lim_{L\to\infty} \sum_{j=1}^{j_L} \frac{L^d a(\beta j, L)}{j} \left(e^{-\sigma(j/h_{A,L})} - 1 + \sigma \frac{j}{h_{A,L}} \right). \tag{D68}$$

If we insert the value of $h_{A,L}$ given in (D61) on the rhs of this equation, we can see that only the terms of order σ^2 survive in the limit $L\to\infty$. Moreover, the fact that the Laplace transform converges for any σ implies that also the characteristic function is convergent. Therefore the limiting distribution of $y_{A,L}$ is well defined and is Gaussian; we can also easily calculate its variance.

If $\lambda = \lambda^*$, we get a different result for $d \geqslant 4$, because we can see, by using Lemma D.1, that

$$r^*_{A,L} \xrightarrow[L\to\infty]{} \begin{cases} 0, & d = 3, \\ -2\rho_0 (2\pi^2\beta)^{-2} \lim_{L\to\infty} \sqrt{\log j_L / \log L}, & d = 4, \\ -r^* \sum_{j=1}^{\infty} j\rho_j, & d \geqslant 5. \end{cases} \tag{D69}$$

Moreover, the factor which multiplies $G_{A,L}(\sigma)$ on the rhs of (D33) is still convergent, but it goes to 1 as $L\to\infty$ only for $d=3$ and for $d=4$, if $\lim_{L\to\infty} \sqrt{\log j_L / \log L} = 0$. It follows that the limiting distribution of $y_{A,L}$ is still well defined and its Laplace transform can be explicitly calculated; however, it is Gaussian only for $d=3$ and for $d=4$, if $\lim_{L\to\infty} \sqrt{\log j_L / \log L} = 0$. ■

APPENDIX E: LARGE DEVIATIONS FOR "SHORT LOOPS"

In this appendix we consider $d \geqslant 3$ and $\lambda > \lambda^*$; our main result is stated in Theorem E.3.

Given any finite subset A of $\mathbb{N}^+$, we define

$$S_{A,L}(v,\delta) \equiv P^{mf}_{\lambda,L} \left[L^d(\rho_{A,L} + v - \delta) \leqslant \sum_{j\in A} j n_j \leqslant L^d(\rho_{A,L} + v + \delta) \right] \tag{E1}$$

with $\rho_{A,L}$ defined as in (D1). We want to show that, if $A=\{j\}$ or $A=\{j \leqslant j_L\}$, with j_L a monotone diverging function of L, such that $j_L \leqslant L^2$, we can evaluate the behavior for $L\to\infty$ on the rhs of (E1) by substituting the measure $P^{mf}_{\lambda,L}$ with the measure, independent of λ (recall that $\lambda > \lambda^*$ in this section)

$$P_{A,L}(n_j, j \in A) = Z^{-1}_{A,L} \prod_{j\in A} w(j, n_j). \tag{E2}$$

We shall consider in detail only the case $A=\{j \leqslant j_L\}$; the other case can be treated in a similar (simpler) way.

Let us define $\Pi_{A,L}(t) = \log F_{A,L}(t h_{A,L})$ and

$$\tilde{\Pi}_{A,L}(t) = \log G_{A,L}(t h_{A,L}) - t h_{A,L} r^*_{A,L} = \sum_{j\in A} \frac{L^d a(\beta j, L)}{j} (e^{-tj} - 1 + tj), \tag{E3}$$

where $F_{A,L}(\sigma)$ and $G_{A,L}(\sigma)$ are defined as in (D33) and $r^*_{A,L}$ is defined as in (D40). Choose $t \equiv t_L(v)$ so that

$$-\tilde{\Pi}'_{A,L}(t) = v L^d. \tag{E4}$$

Lemma E.1: Let $A=\{1 \leqslant j \leqslant j_L\}$, with j_L a monotone diverging function of L such that $j_L \leqslant L^2$. Then the equation (E4) *has a solution for any $v > -\lambda^*$. Moreover, if $0 > v > -\lambda^*$, $t_L(v)$ has a finite positive limit $t(v)$ for $L\to\infty$, such that, for $v\to 0$ and suitable constants c_d,*

$$t(v) \sim \begin{cases} c_3 v^2, & d = 3, \\ c_4 v / \log(1/v), & d = 4, \\ c_d v, & d \geqslant 5, \end{cases} \tag{E5}$$

while, if $v>0$, $t_L(v)<0$ *and*

$$\lim_{L\to\infty}\frac{j_L|t_L(v)|}{\log(vj_L^{d/2-1})}=1. \tag{E6}$$

Proof: By using (D39), we see that Eq. (E4) can be written as

$$H_L(t)\equiv\sum_{j=1}^{j_L}a(\beta j,L)(e^{-tj}-1)=v. \tag{E7}$$

Note that the sign of t is the opposite of the sign of v. Let us consider first the case $v<0$. In this case $t>0$ and $H_L(t)\to-\Sigma_{j\leqslant j_L}a(\beta j,L)$, as $t\to+\infty$; since $\lim_{L\to\infty}\Sigma_{j\leqslant j_L}a(\beta j,L)=\lambda^*$, Eq. (E7) has a unique solution $t_L(v)$ only if $v>-\lambda^*$. It is an easy exercise to show that $t_L(v)$ converges, as $L\to\infty$, to a limit $t(v)$, verifying (E5).

If $v>0$, there is a unique negative solution $t_L(v)$ of (E7) for any v, since $H_L(t)\to+\infty$ as $t\to-\infty$, and it is easy to see that $\lim_{L\to\infty}t_L(v)=0$. A more careful analysis shows that Eq. (E6) is verified. ■

Lemma E.2: Let $A=\{1\leqslant j\leqslant j_L\}$, *with* j_L *a monotone diverging function of* L *such that* $j_L\leqslant L^2$. *Then, if* t *is defined as in (E4), there exists* $\eta>0$ *such that, for* L *large enough,*

$$F_{A,L}(th_{A,L})=G_{A,L}(th_{A,L})[1+\delta_L(t)],\quad |\delta_L(t)|\leqslant e^{-L^\eta}, \tag{E8}$$

$$\Pi'_{A,L}(t)=\tilde{\Pi}'_{A,L}(t)+\delta_L(t),\quad |\delta_L(t)|\leqslant e^{-L^\eta}. \tag{E9}$$

Proof: By using (D33), we see that (E8) is satisfied, if we define

$$\delta_L(t)=\delta_{L,1}+\delta_{L,2}(t), \tag{E10}$$

$$\delta_{L,1}=\frac{1}{\Gamma_{\lambda,L}}\frac{1}{L^{d/2}}\sum_{N\geqslant 0}e^{-\beta x_N^2/2}-1, \tag{E11}$$

$$\delta_{L,2}(t)=-\frac{1}{\Gamma_{\lambda,L}}\frac{1}{L^{d/2}}\sum_{N\geqslant 0}e^{-\beta x_N^2/2}P_{A,L,t}(M>N), \tag{E12}$$

where $P_{A,L,t}(M)$ is the measure defined in (D34), with $\sigma=th_{A,L}$, t being the solution of (E7). By using (C3), we see that

$$\delta_{L,1}=\frac{1}{\Gamma_{\lambda,L}}\frac{1}{L^{d/2}}\sum_{N\geqslant 0}e^{-\beta x_N^2/2}P_L(M>N), \tag{E13}$$

where $P_L(M)$ is the probability measure defined in (B3). By using (C4) and the large deviation estimates of Lemma D.2, it is easy to prove that $|\delta_{L,1}|\leqslant\exp(-L^\eta)$, with $0<\eta<d-2$.

In order to prove a similar bound for $\delta_{L,2}(t)$, we need a large deviation estimate for the measure $P_{A,L,t}(M)$. Let us consider first the case $v>0$, that is $t<0$, when $P_{A,L,t}(M)$ is a probability measure. In this case, if $\lambda-\lambda^*-v>0$ and $|x_N|\leqslant L^{d/4}$, by using (D43) and (E7), we see that, for L large enough

$$\begin{aligned}P_{A,L,t}(M>N)&=P_{A,L,t}(M-M^*_{A,L,t}>L^d(\lambda-\lambda^*-v)+L^{d/2}x_N+L^2c_L+h_{A,L}r^*_{A,L})\\&\leqslant P_{A,L,t}(M-M^*_{A,L,t}>L^d\epsilon)\end{aligned} \tag{E14}$$

if $0<\epsilon<\lambda-\lambda^*-v$, so that, for L large enough,

$$|\delta_{L,2}(t)|\leqslant 2e^{-\beta L^{d/2}/2}+2P_{A,L,t}(M-M^*_{A,L,t}>L^d\epsilon). \tag{E15}$$

Let us consider the Laplace transform $H_{L,t}(w)$ of the random variable $y=M-M^*_{A,L,t}$; it is related to the analogous function $H_{A,L,\sigma}(w)$ defined in (D46) by the relation

$$H_{L,t}(w) = H_{A,L,th_{A,L}}(wh_L). \tag{E16}$$

By proceeding as in the proof of Lemma D.2, we can write

$$P_{A,L,t}(M - M^*_{A,L,t} > L^d\epsilon) = e^{\Pi_{L,t}(w)} \int_{\epsilon L^d}^{+\infty} e^{wy} P_{L,t,w}(\mathrm{d}y), \tag{E17}$$

where $\Pi_{L,t}(w)=\log H_{L,t}(w)$ and $P_{L,t,w}(\mathrm{d}y)=e^{-wy}P_{L,t}(\mathrm{d}y)/H_{L,t}(w)$. We now fix w so that $-\Pi'_{L,t}(w) = \epsilon L^d$; it is to see that this condition can be written as

$$\epsilon L^d = L^d \sum_{j=1}^{j_L} a(\beta j, L)(e^{-tj} - 1)(1 - e^{-wj}) + \sum_{j=1}^{\infty} (L^d a(\beta j, L) - 1)(1 - e^{-wj}). \tag{E18}$$

Since $t<0$, the solution of this equation must be negative and one can show that $\Pi_{L,t}(w)+w\epsilon L^d = \Pi_{L,t}(w)-w\Pi'_{L,t}(w)$ is negative and of order L^{d-2}. It follows that

$$P_{A,L,t}(M - M^*_{A,L,t} > L^d\epsilon) \leqslant e^{\Pi_{L,t}(w)-w\Pi'_{L,t}(w)} \leqslant e^{-cL^{d-2}} \tag{E19}$$

for some $c>0$.

The case $v<0$, that is $t>0$, is a bit more involved, since in this case $P_{A,L,t}(M)$ is not necessarily a probability measure. However, it is easy to prove, by using (D34), that

$$\sum_{M=0}^{\infty} |P_{A,L,t}(M)| \leqslant e^{2\,\log j_L} \tag{E20}$$

so that, instead of the bound (E15), we have

$$|\delta_{L,2}(t)| \leqslant 2e^{-\beta L^{d/2}/2+2\,\log j_l} + 2|P_{A,L,t}(M - M^*_{A,L,t} > L^d\epsilon)|. \tag{E21}$$

Moreover, since it is still true that $\Pi_{L,t}(w)-w\Pi'_{L,t}(w)$ is negative and of order L^{d-2}, instead of bound (E19), we get

$$|P_{A,L,t}(M - M^*_{A,L,t} > L^d\epsilon)| \leqslant e^{-cL^{d-2}} \sum_{M=0}^{\infty} |P_{L,t,w}(M)| \tag{E22}$$

which is a negligible difference, since $|w|L^2 \leqslant c$, so that, as one can easily check,

$$\sum_{M=0}^{\infty} |P_{L,t,w}(M)| \leqslant e^{2e^{cj_L/L^2}\,\log j_L}. \tag{E23}$$

We still must prove (E9). By setting $\sigma=th_{A,L}$ in (D33) and by doing the derivative with respect to t, we get

$$\frac{d}{\mathrm{d}t}F_{A,L}(th_{A,L}) = L^d\rho_{A,L}F_{A,L}(th_{A,L}) - G_{A,L}(th_{A,L})\sum_{j=1}^{j_L} L^d a(\beta j, L)e^{-tj}[1 + \delta_{L,2,k}(t) + \delta_{L,1}], \tag{E24}$$

where $\delta_{L,1}$ is defined as in (E11) and

$$\delta_{L,2,k}(t) = -\frac{1}{\Gamma_{\lambda,L}}\frac{1}{L^{d/2}}\sum_{N\geqslant 0} e^{-\beta x_N^2/2} P_{A,L,t}(M > N-k). \tag{E25}$$

Since $k \leqslant j_L \leqslant L^2$, we can find as before that $|\delta_{L,2,k}(t)| \leqslant e^{-L^\eta}$. On the other hand, $\Sigma_{j\leqslant j_L} L^d a(\beta j, L) e^{-tj}$ is always of order L^d. It follows that

$$\Pi'_{A,L}(t) = \frac{\frac{d}{dt}F_{A,L}(th_{A,L})}{F_{A,L}(th_{A,L})} = L^d\rho_{A,L} - \sum_{j=1}^{j_L} L^d a(\beta j, L) e^{-tj} + O(e^{-L^\eta}) = \tilde{\Pi}'_{A,L}(t) + O(e^{-L^\eta}). \tag{E26}$$

■

Theorem E.3: *If* $\mathcal{A}^{(4)}_{L,\delta}(v)$ *is defined as in* (5.7) *and* $0 < v < \lambda - \lambda^*$, *then*

$$v - \delta \leqslant -\lim_{L\to\infty}\frac{1}{L^d}\frac{j_L}{\log(v j_L^{d/2-1})}\log P^{mf}_{\lambda,L}(\mathcal{A}^{(4)}_{L,\delta}) \leqslant u + \delta \tag{E27}$$

while, if $-\lambda^* < v < 0$, *there are positive functions* $t_d(v)$ *and* $a_d(v)$, *depending on* d, *such that*

$$a_d(v) - t_d(v)\delta \leqslant -\lim_{L\to\infty}\frac{1}{L^d}\log P^{mf}_{\lambda,L}(\mathcal{A}^{(4)}_{L,\delta}) \leqslant a_d(v) + t_d(v)\delta. \tag{E28}$$

Moreover, the two bounds above do not change if we substitute $P^{mf}_{\lambda,L}(\mathcal{A}^{(4)}_{L,\delta})$ *with* $\tilde{\Pi}_{A,L}(t_L(v)) - t\tilde{\Pi}'_{A,L}(t_L(v))$, $t_L(v)$ *being the solution of (E4).*

Proof: By (E1) $P^{mf}_{\lambda,L}(\mathcal{A}^{(4)}_{L,\delta}) = S_{A,L}(v,\delta)$. By proceeding as in the proof of Lemma D.2, we can write

$$S_{A,L}(v,\delta) = e^{\Pi_{A,L}(t) - t\Pi'_{A,L}(t)} \int_{(v-\delta)L^d}^{(v+\delta)L^d} e^{t(y - vL^d)} P_{A,L,t}(\mathrm{d}y), \tag{E29}$$

where t is chosen so that $vL^d = -\Pi'_{A,L}(t)$. By using Lemma E.2, we see that $\Pi_{A,L}(t)$ and its derivative can be substituted with $\tilde{\Pi}_{A,L}(t)$ and $\tilde{\Pi}'_{A,L}(t)$, and that t can be taken as the solution of (E4), without changing the asymptotic behavior of $S_{A,L}(v,\delta)$.

Let us consider first the case $0 < v < \lambda - \lambda^*$. It is easy to check that, in this case, $\tilde{\Pi}_{A,L}(t)$ is negligible, for $L \to \infty$, with respect to $|t| v L^d$, so that we get immediately, by using also (E6), the lower bound in (E27). In order to prove the upper bound, we need also a lower bound on $\int_{(v-\delta)L^d}^{(v+\delta)L^d} P_{A,L,t}(\mathrm{d}y)$, which can be obtained by studying the Laplace transform of $P_{A,L,t}(\mathrm{d}y)$; this analysis shows that $\int_{(v-\delta)L^d}^{(v+\delta)L^d} P_{A,L,t}(\mathrm{d}y) \to 1$ as $L \to \infty$.

If $-\lambda^* < v < 0$, as shown in Lemma E.1, the solution of (E4) converges, as $L \to \infty$, to the function $t(v)$ defined in (E5). Moreover, it is easy to check that, up to negligible corrections, for any fixed t,

$$\lim_{L\to\infty} L^{-d}[\Pi_{A,L}(t) - t\Pi'_{A,L}(t)] = -a_d(v), \tag{E30}$$

where $a_d(v)$ is a positive function equal to

$$a_d(v) = \sum_{j=1}^{\infty} \frac{1}{(2\pi\beta j)^{d/2}}\left(\frac{1-e^{-tj}}{j} - te^{-tj}\right). \tag{E31}$$

Since it is still true that $\int_{(v-\delta)L^d}^{(v+\delta)L^d} P_{A,L,t}(\mathrm{d}y) \to 1$ as $L \to \infty$, we get the bound (E28). ■

APPENDIX F: PROOF OF THEOREM 4.1

By (D2),

$$E^{mf}_{\lambda,L}(y_{\delta,L}) = \frac{1}{L^d} \sum_{j \geqslant \delta L^d} L^d a(\beta j, L) \alpha_{j,L},$$

$$E^{mf}_{\lambda,L}(X_{\delta,L}) = \sum_{j \geqslant \delta L^d} \frac{L^d a(\beta j, L)}{j} \alpha_{j,L}, \tag{F1}$$

$$E^{mf}_{\lambda,L}(X_L) = \sum_{j \geqslant L^2} \frac{L^d a(\beta j, L)}{j} \alpha_{j,L}.$$

On the other hand, by (2.3),

$$|L^d a(\beta j, L) - 1| \leqslant C \exp(-Cj/L^2), \quad \forall\, j \geqslant L^2 \tag{F2}$$

which allows us to prove very easily the limits in (4.5) and (4.7), by using Lemma D3.

The arguments given at the beginning of Appendix D can be used to prove also that

$$E^{mf}_{\lambda,L}(n_{j_1} n_{j_2}) = \frac{L^d a(\beta j_1, L)}{j_1} \frac{L^d a(\beta j_2, L)}{j_2} \alpha_{j_1+j_2,L} \quad \text{if } j_1 \neq j_2, \tag{F3}$$

$$E^{mf}_{\lambda,L}(n_j^2) = E^{mf}_{\lambda,L}(n_j(n_j-1)) + E^{mf}_{\lambda,L}(n_j) = \left(\frac{L^d a(\beta j, L)}{j} \right)^2 \alpha_{2j,L} + \frac{L^d a(\beta j, L)}{j} \alpha_{j,L}. \tag{F4}$$

It follows that

$$E^{mf}_{\lambda,L}(y^2_{\delta,L}) - E^{mf}_{\lambda,L}(y_{\delta,L})^2 = \sum_{j_1, j_2 \geqslant \delta L^d} a(\beta j_1, L) a(\beta j_2, L) (\alpha_{j_1+j_2,L} - \alpha_{j_1,L} \alpha_{j_2,L}) + \sum_{j \geqslant \delta L^d} j a(\beta j, L) \alpha_{j,L}. \tag{F5}$$

The limit (4.6) follows through some simple calculations from this identity, the bound (F2) and Lemma D.3. In a similar way, one can prove also (4.8)–(4.10).

We still must prove (4.11). The previous arguments imply that, if $\xi \in (1/2, 1]$ and $j > \xi(\lambda - \lambda^*)L^d$, then

$$\lim_{L\to\infty} P^{mf}_{\lambda,L}(n_j = 1) = \lim_{L\to\infty} E^{mf}_{\lambda,L}(n_j) \tag{F6}$$

and

$$\lim_{L\to\infty} P^{mf}_{\lambda,L}(X_{\xi(\lambda-\lambda^*)} \geqslant 1) = \lim_{L\to\infty} \sum_{j > \xi(\lambda-\lambda^*)L^d} P^{mf}_{\lambda,L}(n_j = 1) = -\log \xi. \tag{F7}$$

APPENDIX G: THE LIMIT FUNCTIONAL

Theorem G.1: *There is a nondecreasing, negative, continuous function* $\lambda_0(\lambda)$ *on* $\mathbb{R}$, *strictly negative in* $d \leqslant 2$, *such that*

$$\pi(\lambda) := -\inf_{\varrho} F_\lambda(\varrho) = \frac{[\lambda - \lambda_0(\lambda)]^2}{2} + \pi^0_{\lambda_0(\lambda)}, \tag{G1}$$

$$\pi^0_{\lambda_0(\lambda)} = \beta^{-1} \sum_j \frac{\rho_j^*}{j} e^{\lambda_0(\lambda)\beta j}. \tag{G2}$$

Moreover, $\rho(\lambda) := \lambda - \lambda_0(\lambda)$*, is a positive, strictly increasing, continuous function of* λ *with range the whole* $(0,\infty)$ *and*

$$\inf_{\varrho} F_\lambda(\varrho) = \inf_{\varrho:\Sigma_j \rho_j = \rho(\lambda)} F_\lambda(\varrho). \tag{G3}$$

Remark 1: In Ref. 10 it is proved that the grand canonical mean field, thermodynamical pressure coincides with $\pi(\lambda)$, namely

$$\pi(\lambda) = \lim_{L\to\infty} \frac{1}{L^d} \Xi^{mf}_{\lambda,L} \tag{G4}$$

thus proving our claim in the text that the computation of the pressure using the limit functional gives the correct result.

Remark 2: The proof of Theorem G.1 identifies the function $\lambda_0(\lambda)$ as follows. There exists a dimension dependent constant λ^*, equal to $+\infty$ in $d \leqslant 2$ and $<\infty$ in $d \geqslant 3$ such that for $\lambda \leqslant \lambda^*$ (by which we will mean, here and in the sequel, *any* λ *in* $d \leqslant 2$ *and* $\lambda \leqslant \lambda^*$ *in* $d \geqslant 3$) there is a unique solution λ_0 of

$$\lambda - \lambda_0 = \sum_j \rho_j^* e^{\lambda_0 \beta j}. \tag{G5}$$

This solution, which depends on λ, coincides with the function $\lambda_0(\lambda)$ of Theorem G.1 for $\lambda \leqslant \lambda^*$, while the latter is identically 0 for $\lambda > \lambda^*$.

We will also prove that the inf in (G1) is a minimum when $\lambda \leqslant \lambda^*$, and, in such a case, the minimizer is unique and given by

$$\rho_j = \rho_j^* e^{\lambda_0 \beta j} \tag{G6}$$

in agreement with (G3), because $\Sigma_j \rho_j^* e^{\lambda_0 \beta j} = \rho(\lambda)$ by (G5).

The rhs of (G6) is the equilibrium density of j loops in the free, grand canonical ensemble with chemical potential λ_0, so that λ_0 has the meaning of an effective chemical potential.

If $d \geqslant 3$ and $\lambda > \lambda^*$, the inf in (G1) is not attained and there is a finite fraction of the density which "concentrates on infinitely long loops."

By (G3), $\rho(\lambda)$ can be interpreted as the equilibrium density when the chemical potential is λ; since the range of $\rho(\lambda)$ is the whole $(0,\infty)$, there is no "forbidden interval" for the equilibrium density, namely there is no first order phase transition in our system. This is due to the assumption that the interaction energy $u^2/2$, $u = \Sigma_j \rho_j$, is convex.

Proof of Theorem G.1: Call $m(\alpha) = \Sigma_j \rho_j^* e^{\beta \alpha j}$, $\alpha < 0$ in $d \leqslant 2$ and $\alpha \leqslant 0$ in $d \geqslant 3$. The graph of $m(\alpha)$ is as in Fig. 1, having set $\lambda^* = m(0)$ in $d \geqslant 3$. Existence and uniqueness of the solution λ_0 of (G5) for $\lambda \leqslant \lambda^*$ follow from monotonicity of $m(\cdot)$. Graphically λ_0 is the α-coordinate of the intersection point in Fig. 1.

Let us next prove (G1) and (G2) when $\lambda \leqslant \lambda^*$. With λ_0 as in (G5) we write

$$F_\lambda(\varrho) = \left[\frac{\rho^2}{2} - (\lambda - \lambda_0)\rho \right] + [-\lambda_0 \rho - \beta^{-1} S(\varrho)], \quad \rho = \sum_j \rho_j. \tag{G7}$$

Then

$$F_\lambda(\varrho) \geqslant \inf_{\varrho} \left\{ \frac{\rho^2}{2} - (\lambda - \lambda_0)\rho \right\} + \inf_{\varrho} \{-\lambda_0 \rho - \beta^{-1} S(\varrho)\}. \tag{G8}$$

We have

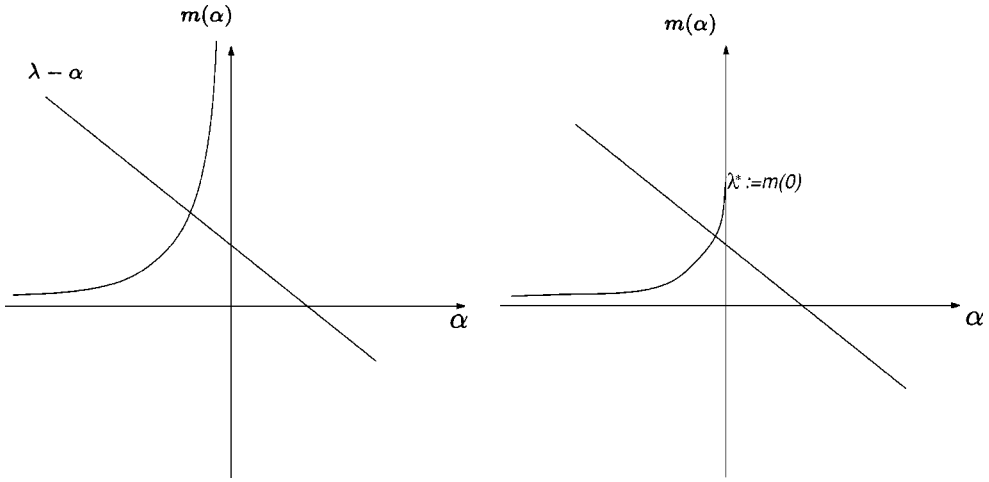

FIG. 1. The two graphs, on the left and right, refer, respectively, to $d \leqslant 2$ and $d \geqslant 3$.

$$\inf_{\varrho}\{-\lambda_0\rho - \beta^{-1}S(\varrho)\} = -\pi^0_{\lambda_0} \tag{G9}$$

with a unique minimizer given by (G6). On the other hand,

$$\inf_{\varrho}\left\{\frac{\rho^2}{2} - (\lambda - \lambda_0)\rho\right\} = -\frac{(\lambda - \lambda_0)^2}{2} \tag{G10}$$

with minimizer any ϱ such that $\Sigma_j \rho_j = \lambda - \lambda_0$. By (G5), the previous minimizer ϱ, given by (G6), satisfies such a condition, hence (G1) and (G3).

Suppose next that $d \geqslant 3$ and $\lambda > \lambda^*$. Then

$$F_\lambda(\varrho) \geqslant \inf_{\varrho}\left\{\frac{\rho^2}{2} - \lambda\rho\right\} + \inf_{\varrho}\{-\beta^{-1}S(\varrho)\} \geqslant -\frac{\lambda^2}{2} - \pi^0_0, \tag{G11}$$

where the minimizers of the first inf are those ϱ such that $\Sigma_j \rho_j = \lambda$, while the minimizer of the second inf is unique and given by $\{\rho^*_j\}$. We thus need to show that there is a sequence $\varrho^{(n)}$ such that $\Sigma_j \rho^{(n)}_j = \lambda$ and

$$\lim_{n\to\infty} S(\varrho^{(n)}) = S(\varrho^*). \tag{G12}$$

Let $a := \lambda - \rho^*$ be the excess mass, λ being the mass ρ which minimizes $\rho^2/2 - \lambda\rho$ and $\rho^* = \Sigma_j \rho^*_j$. Set

$$\varrho^{(n)}_j = \begin{cases} \rho^*_j & \text{if } j \neq n, \\ \rho^*_j + a & \text{if } j = n. \end{cases} \tag{G13}$$

Then

$$S(\varrho^{(n)}) = S(\varrho^*) + \left(\frac{\rho^*_n}{n} + \left(\frac{\rho^*_n}{n} + \frac{a}{n}\right)\left(\log\left(\frac{\rho^*_n + a}{\rho^*_n}\right) - 1\right)\right) \tag{G14}$$

with the last parentheses vanishing as $n \to \infty$.

Equations (G1)–(G3) are therefore proved. We will next show that $\rho(\lambda)$ is continuous, strictly increasing, and with range $(0, \infty)$. Let $\lambda < \lambda^*$ and λ_0' the derivative of λ_0 with respect to λ. Then

$$\frac{d\rho(\lambda)}{d\lambda} = 1 - \lambda_0' \tag{G15}$$

and, by differentiating (G5),

$$\lambda_0'\left(\beta\sum_j j\rho_j^* e^{\lambda_0\beta j} + 1\right) = 1. \tag{G16}$$

Hence $\lambda_0(\cdot)$ is a nondecreasing function, as claimed in Theorem G.1; moreover, since $\lambda_0' < 1$, $d\rho(\lambda)/d\lambda > 0$, for $\lambda < \lambda^*$. For $\lambda > \lambda^*$, $\rho(\lambda) = \lambda$ and since $\lim_{\lambda \nearrow \lambda^*} \rho(\lambda) = \lambda^*$, because $\lambda^* = m(0)$ and

$$\lim_{\alpha \nearrow 0} \sum_j \rho_j^* e^{\alpha\beta j} = \sum_j \rho_j^* = m(0), \quad d \geqslant 3 \tag{G17}$$

we conclude that $\rho(\lambda)$ is continuous and strictly increasing.

Obviously, $\lim_{\lambda\to\infty} \rho(\lambda) = \lim_{\lambda\to\infty} \lambda = \infty$. It remains to prove that $\lim_{\lambda\to-\infty} \rho(\lambda) = 0$. By monotonicity, the limit exists. Since $\rho(\cdot) > 0$, $\lambda - \lambda_0(\lambda) > 0$, so that $\lim_{\lambda\to-\infty} \lambda_0(\lambda) = -\infty$. Then

$$\lim_{\lambda\to-\infty} \sum_j \rho_j^* e^{\lambda_0(\lambda)\beta j} = \lim_{\alpha\to-\infty} \sum_j \rho_j^* e^{\alpha\beta j} = 0. \tag{G18}$$

Theorem G.1 is proved. ■

Remark: The construction of the minimizing sequence $\underline{\rho}^{(n)}$ in the case $\lambda > \lambda^*$ shows that the excess mass $\lambda - \lambda^*$ concentrates in the limit on infinitely long loops.

Let

$$a(u) := \inf_{\Sigma_j \rho_j = u} (F_\lambda(\underline{\rho}) + \lambda u) \tag{G19}$$

observing that the rhs does not depend on λ. Obviously

$$a(u) \geqslant \sup_\lambda \{\lambda u + \inf_{\underline{\rho}} F_\lambda(\underline{\rho})\}. \tag{G20}$$

We will prove that equality actually holds, namely

$$a(u) = \sup_\lambda \{\lambda u + \inf_{\underline{\rho}} F_\lambda(\underline{\rho})\} \tag{G21}$$

which then shows that

$$a(u) = \sup_\lambda \{\lambda u - \pi(\lambda)\}, \tag{G22}$$

namely that $a(u)$ is the Legendre transform of $\pi(\lambda)$. In Ref. 10 an equivalence of ensembles theorem is proved, namely that

$$-\lim_{\substack{L\to\infty \\ N_L = [L^d u]}} \frac{1}{L^d} \ln Z^{mf}_{N_L, L} = \sup_\lambda \{\lambda u - \pi(\lambda)\} \tag{G23}$$

which, together with (G22) shows that

$$\inf_{\Sigma_j \rho_j = u} (F_\lambda(\underline{\rho}) + \lambda u) = -\lim_{\substack{L\to\infty \\ N_L = [L^d u]}} \frac{1}{L^d} \ln Z^{mf}_{N_L, L} \tag{G24}$$

as claimed in the text.

Proof of (G21): By (G3) the inf of $F_\lambda(\underline{\rho})$ is achieved on the set $\{\underline{\rho} : \Sigma_j \rho_j = \lambda - \lambda_0\}$. Call α the value of λ such that

$$\rho(\alpha) = \alpha - \lambda_0(\alpha) = u \tag{G25}$$

(existence and uniqueness follow from Theorem G.1). Then

$$\sup_{\lambda}\{\lambda u + \inf_{\varrho} F_\lambda(\varrho)\} \geqslant \{\alpha u + \inf_{\varrho} F_\alpha(\varrho)\} = \{\alpha u + \inf_{\varrho:\Sigma_j \rho_j = \rho(\alpha) = u} F_\alpha(\varrho)\} = a(u) \tag{G26}$$

which, together with (G20), proves (G21). ■

By general thermodynamic relations, and making explicit now the dependence on β, the entropy $\sigma(\beta,u)$ and the internal energy, $e(\beta,u)$, are

$$\sigma(\beta,u) = \beta^2 \frac{\partial a(\beta,u)}{\partial \beta}, \quad a(\beta,u) = e(\beta,u) - \frac{\sigma(\beta,u)}{\beta}. \tag{G27}$$

In our model $e(\beta,u) = (u^2/2) + k(\beta,u)$, with $k(\beta,u)$ the kinetic part of the internal energy. By direct inspection, $\sigma(\beta,u)$ and $k(\beta,u)$ as functions of the particles density u, become constant for $u \geqslant u^*$. This is the Bose condensation phenomenon, which is interpreted by saying that the fluid added when increasing the density past u^* does not carry entropy nor momentum.

APPENDIX H

Let $\boldsymbol{\lambda} := \{\lambda_j, j > 0\}$ be the sequence defined by

$$\lambda_j := \begin{cases} \lambda + \lambda', & j \in V_k, \\ \lambda & \text{otherwise}, \end{cases} \tag{H1}$$

and

$$F_{\boldsymbol{\lambda}}(\varrho) := \frac{1}{2}\left(\sum_{j>0} \rho_j\right)^2 - \left(\sum_{j>0} \lambda_j \rho_j\right) - \frac{1}{\beta} S(\varrho), \tag{H2}$$

$$\pi_{\boldsymbol{\lambda}} := -\inf_{\varrho} F_{\boldsymbol{\lambda}}(\varrho), \quad \rho^{(k)}(\lambda) := \sum_{j \in V_K} \rho_j(\lambda). \tag{H3}$$

Then

$$\begin{aligned} \inf_{\varrho:\Sigma_{j\in V_k}\rho_j = \rho^{(k)}(\lambda)+\upsilon} F_\lambda(\varrho) &= \inf_{\varrho:\Sigma_{j\in V_k}\rho_j = \rho^{(k)}(\lambda)+\upsilon} \left[F_\lambda(\varrho) - \lambda'\left(\sum_{j\in V_k}\rho_j - (\rho^{(k)}(\lambda)+\upsilon)\right)\right] \\ &= \inf_{\varrho:\Sigma_{j\in V_k}\rho_j = \rho^{(k)}(\lambda)+\upsilon} F_{\boldsymbol{\lambda}}(\varrho) + \lambda'(\rho^{(k)}(\lambda)+\upsilon) \geqslant -\pi_{\boldsymbol{\lambda}} + \lambda'(\rho^{(k)}(\lambda)+\upsilon). \end{aligned} \tag{H4}$$

The equality in line (H4) holds if λ' is chosen in such a way that the minimizer sequence $\varrho_n(\lambda,\lambda')$ satisfies the constraint $\Sigma_{j\in V_k}\rho_j = \rho^{(k)}(\lambda)+\upsilon$.

The case $V_k = N^+$ follows directly from the arguments used in Appendix G, by changing the chemical potential from $\lambda \to \lambda + \lambda'$, where λ' is

$$\lambda' = \rho(\lambda) + \upsilon - \lambda + \tilde{\lambda}_0 \tag{H5}$$

with $\tilde{\lambda}_0 \equiv \tilde{\lambda}_0(\lambda,\upsilon) = 0$ when $\rho(\lambda)+\upsilon \geqslant \lambda^*$, while otherwise is the unique solution of the equation

$$\sum_j e^{\rho_j^* \tilde{\lambda}_0 \beta j} = \rho(\lambda) + \upsilon. \tag{H6}$$

The minimizer sequence $\{\rho_j^{(n)}\}_{j\in\mathbb{N}^+}$ is then given by

$$\rho_j^{(n)} = \rho_j^* e^{\beta j \tilde{\lambda}_0} + \mathbf{1}_{\{j=n\}}[\lambda + \lambda' - \lambda^*]_+, \tag{H7}$$

where we have indicated by $[\cdot]_+$ the positive part. In particular, if $\lambda > \lambda^*$, $v > -(\lambda - \lambda^*)$, then $\lambda' = v$.

For $k=2,3,4$, we set $\tilde{\lambda}_0(\lambda, v)$ as the solution of the equation

$$\sum_{j \notin V_k} \rho_j^* e^{\tilde{\lambda}_0 \beta j} = \lambda - \tilde{\lambda}_0 - \rho^{(k)}(\lambda) - v \tag{H8}$$

when this solution exists, otherwise we take $\tilde{\lambda}_0 = 0$. Then λ' is given by the unique solution of the equation

$$\sum_{j \in V_k} \rho_j^* e^{(\tilde{\lambda}_0 + \lambda')\beta j} = \rho^{(k)}(\lambda) + v \tag{H9}$$

whose existence and uniqueness follows (for any given value of $\tilde{\lambda}_0$) by monotonicity arguments, since V_k is bounded for $k > 1$.

Then the minimizer sequence $\{\rho_j^{(n)}\}_{j \in \mathbb{N}^+}$, $n > \max V_k$, is given by

$$\rho_j^{(n)} = \rho_j^* e^{\beta j(\tilde{\lambda}_0 + \lambda')} \mathbf{1}_{j \in V_k} + (\rho_j^* e^{\beta j \tilde{\lambda}_0} + \mathbf{1}_{\{j=n\}}[\lambda - \lambda_{\notin}^* - \rho^{(k)}(\lambda) - v]_+) \mathbf{1}_{j \notin V_k}, \tag{H10}$$

where $\lambda_{\notin}^* := \Sigma_{j \notin V_k} \rho_j^*$. Notice that, when the positive part is null, $\{\rho_j^{(n)}\}$ does not depend on n and it is actually a minimum.

In the case $k \neq 1$, $\lambda > \lambda^*$ ($\Rightarrow \rho^k(\lambda) = \lambda_{\in}^*$) and $v < \lambda - \lambda^*$,

$$\pi_\lambda = \frac{\lambda^2}{2} + \frac{1}{\beta} \sum_{j \in V_K} \frac{\rho_j^*}{j} e^{\lambda' \beta j} + \frac{1}{\beta} \sum_{j \notin V_K} \frac{\rho_j^*}{j}, \tag{H11}$$

where λ' is the unique solution of $\Sigma_{j \in V_k} \rho_j^* (e^{\lambda' \beta j} - 1) = v$.

Collecting Eqs. (G1) and (H4), we get

$$\inf_{\varrho : \Sigma_{j \in V_k} \rho_j = \rho^{(k)}(\lambda) + v} F_\lambda(\varrho) - \inf_{\varrho} F_\lambda(\varrho) = -\pi_\lambda + \lambda'(\rho^{(k)}(\lambda) + v) + \pi(\lambda). \tag{H12}$$

To prove Theorem 5.2, one must show (see proof of Theorem E.3 for notation) that

$$\lim_{L \to \infty} \frac{\log S_{A,L}(v, \delta)}{[\Pi_{A,L}(t) - t\Pi'_{A,L}(t)]} = \lim_{L \to \infty} \left[\frac{\frac{1}{\beta L^d} \ln P^{mf}_{\lambda,L}(\mathcal{A}^{(k)}_{L,\delta})}{-\inf_{\varrho \in A_L^{(k)}} F_\lambda(\varrho) + \inf_{\varrho} F_\lambda(\varrho)} \right]. \tag{H13}$$

For example, if $\lambda > \lambda^*$, $v < \lambda - \lambda^*$ and $k \neq 1$, one has

$$\inf_{\varrho : \Sigma_{j \in V_k} \rho_j = \rho^{(k)}(\lambda) + v} F_\lambda(\varrho) - \inf_{\varrho} F_\lambda(\varrho) = -\frac{1}{\beta} \sum_{j \in V_k} \frac{\rho_j^*}{j} (e^{\lambda' \beta j} - 1) + \lambda'(\rho^{(k)}(\lambda) + v). \tag{H14}$$

Hence, by using (E3), (E4), (E8), and (E9), it is easy to check that the two limits are equal in the case $k=4$. The other cases can be treated in a similar way.

APPENDIX I

If $k=1$, by the analysis in Appendix H, substituting the value of λ' as a function of λ and $\tilde{\lambda}_0$ in (H4), we get

$$\inf_{\varrho:\Sigma_j \rho_j = \rho(\lambda)+v} F_\lambda(\varrho) = \frac{1}{2}(\rho+v)^2 - (\lambda - \tilde{\lambda}_0)(\rho(\lambda)+v) - \frac{1}{\beta}\sum_j \frac{\rho_j^*}{j} e^{\beta j \tilde{\lambda}_0}. \tag{I1}$$

If $\lambda \neq \lambda^*$, this expression is twice differentiable and we get

$$\left.\frac{d^2\mathfrak{I}(v)}{dv^2}\right|_{v=0} = 1 + \mathbf{1}_{\{\lambda<\lambda^*\}}\left[2\frac{d\tilde{\lambda}_0}{dv} + \frac{d^2\tilde{\lambda}_0}{dv^2}(\rho(\lambda)+v) - \frac{d^2\tilde{\lambda}_0}{dv^2}\sum_j \rho_j^* e^{\tilde{\lambda}_0 \beta j} - \left(\frac{d\tilde{\lambda}_0}{dv}\right)^2 \sum_j \rho_j^* \beta j e^{\tilde{\lambda}_0 \beta j}\right]_{v=0}. \tag{I2}$$

On the other hand, if $\lambda < \lambda^*$ and v is small enough, $\tilde{\lambda}_0$ satisfies the equation $\rho(\lambda)+v = \Sigma_j \rho_j^* e^{\tilde{\lambda}_0 \beta j}$, so that

$$\frac{d\tilde{\lambda}_0}{dv}\sum_j \rho_j^* \beta j e^{\tilde{\lambda}_0 \beta j} = 1 \tag{I3}$$

and we get

$$\left.\frac{d^2\mathfrak{I}(v)}{dv^2}\right|_{v=0} = 1 + \mathbf{1}_{\{\lambda<\lambda^*\}}\left[2\frac{d\tilde{\lambda}_0}{dv} + \left(\frac{d\tilde{\lambda}_0}{dv}\right)^2 \sum_j \rho_j^* \beta j e^{\tilde{\lambda}_0 \beta j}\right]_{v=0} = 1 + \mathbf{1}_{\{\lambda<\lambda^*\}} \frac{1}{\sum_j \rho_j^* \beta j e^{\lambda_0 \beta j}}, \tag{I4}$$

where we used also the fact that, if $v=0$, $\tilde{\lambda}_0 = \lambda_0$, λ_0 being defined as in (G5).

If $\lambda = \lambda^*$, the right and left limit of the derivative of $\tilde{\lambda}_0$ in $v=0$ do exist and are given by

$$\lim_{v\to 0^+} \frac{d\tilde{\lambda}_0(\lambda^*, v)}{dv} = 0,$$

$$\lim_{v\to 0^-} \frac{d\tilde{\lambda}_0(\lambda^*, v)}{dv} = \lim_{v\to 0^-}\left[\frac{1}{\sum_j \rho_j^* \beta j e^{\tilde{\lambda}_0(\lambda^*, v)\beta j}}\right] = \frac{1}{\sum_j \rho_j^* \beta j}, \tag{I5}$$

so that, if $d \leqslant 4$, the second derivative of $\mathfrak{I}(v)$ in $v=0$ does exist and is given by

$$\left.\frac{d^2\mathfrak{I}(v)}{dv^2}\right|_{v=0} = \left[1 + \frac{\mathbf{1}_{\{\lambda<\lambda^*\}}}{\beta \sum_j \rho_j^* j e^{\lambda_0(\lambda)\beta j}}\right]^{-1}. \tag{I6}$$

It follows that, if $d=3,4$, $d^2\mathfrak{I}(v)/dv^2$ is given by Eq. (I6) for any λ, while, if $d>4$, the same result is true, but only for $\lambda \neq \lambda^*$.

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A classification of generalized quantum statistics associated with classical Lie algebras

N. I. Stoilova[a] and J. Van der Jeugt[b]
Department of Applied Mathematics and Computer Science, University of Ghent, Krijgslaan 281-S9, B-9000 Gent, Belgium

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Generalized quantum statistics such as para-Fermi statistics is characterized by certain triple relations which, in the case of para-Fermi statistics, are related to the orthogonal Lie algebra $B_n=\mathrm{so}(2n+1)$. In this paper, we give a quite general mathematical definition of "a generalized quantum statistics associated to a classical Lie algebra G." This definition is closely related to a certain $\mathbb{Z}$-grading of G. The generalized quantum statistics is then determined by a set of root vectors (the creation and annihilation operators of the statistics) and the set of algebraic relations for these operators. Then we give a complete classification of all generalized quantum statistics associated to the classical Lie algebras A_n, B_n, C_n, and D_n. In the classification, several new classes of generalized quantum statistics are described. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1827324]

I. INTRODUCTION

In classical quantum statistics one works exclusively with Bose and Fermi statistics (bosons and fermions). A historically important extension or generalization of these quantum statistics has been known for 50 years, namely the para-Bose and para-Fermi statistics as developed by Green.[1] Instead of the classical bilinear commutators or anticommutators as for bosons and fermions, parastatistics is described by means of certain trilinear or triple relations. For example, for n pairs of para-Fermi creation and annihilation operators f_i^{ξ} ($\xi=\pm$ and $i=1,\ldots,n$), the defining relations are

$$[[f_j^{\xi},f_k^{\eta}],f_l^{\epsilon}]=\tfrac{1}{2}(\epsilon-\eta)^2\delta_{kl}f_j^{\xi}-\tfrac{1}{2}(\epsilon-\xi)^2\delta_{jl}f_k^{\eta},$$

$$\xi,\eta,\epsilon=\pm\,\text{or}\,\pm 1,\quad j,k,l=1,\ldots,n. \tag{1.1}$$

About 10 years after the introduction of para-Fermi relations by Green, it was proved that these relations are associated with the orthogonal Lie algebra $\mathrm{so}(2n+1)=B_n$.[2] More precisely, the Lie algebra generated by the $2n$ elements f_i^{ξ}, with $\xi=\pm$ and $i=1,\ldots,n$, subject to the relations (1.1), is $\mathrm{so}(2n+1)$ (as a Lie algebra defined by means of generators and relations). In fact, this can be considered as an alternative definition instead of the common definition by means of Chevalley generators and their known relations expressed by means of the Cartan matrix elements (inclusive the Serre relations). Moreover, there is a certain representation of $\mathrm{so}(2n+1)$, the so-called Fermi representation $\mathcal{F}$, that yields the classical Fermi relations. In other words, the representatives $\mathcal{F}(f_i^{\xi})$ satisfy the bilinear relations of classical Fermi statistics. Thus the usual Fermi statistics corresponds to a particular realization of para-Fermi statistics. For general para-Fermi statistics, a class of finite dimensional $\mathrm{so}(2n+1)$ representations (of Fock type) needs to be investigated.

[a]Permanent address: Institute for Nuclear Research and Nuclear Energy, Boul. Tsarigradsko Chaussee 72, 1784 Sofia, Bulgaria. Electronic mail: neli.stoilova@ugent.be
[b]Electronic mail: joris.vanderjeugt@ugent.be

Twenty years after the connection between para-Fermi statistics and the Lie algebra so$(2n+1)$, a new connection, between para-Bose statistics and the orthosymplectic Lie superalgebra osp$(1|2n)=B(0,n)$ (Ref. 3) was discovered.[4] The situation here is similar, the Lie superalgebra generated by $2n$ odd elements b_i^ξ, with $\xi=\pm$ and $i=1,\ldots,n$, subject to the triple relations of para-Bose statistics, is osp$(1|2n)$ (as a Lie superalgebra defined by means of generators and relations). Also there is a particular representation of osp$(1|2n)$, the so-called Bose representation $\mathcal{B}$, that yields the classical Bose relations, i.e., where the representatives $\mathcal{B}(b_i^\xi)$ satisfy the relations of classical Bose statistics. For more general para-Bose statistics, a class of infinite dimensional osp$(1|2n)$ representations needs to be investigated, and one of these representations corresponds with ordinary Bose statistics.

From these historical examples it is clear that parastatistics, as introduced by Green[1] and further developed by many other research teams (see Ref. 5 and the references therein), can be associated with representations of the Lie (super)algebras of class B [namely B_n and $B(0,n)$]. The question that arises is whether alternative interesting types of generalized quantum statistics can be found in the framework of other classes of simple Lie algebras or superalgebras. In this paper we shall classify all the classes of generalized quantum statistics for the classical Lie algebras A_n, B_n, C_n, and D_n, by means of their algebraic relations. In a forthcoming paper we hope to perform a similar classification for the classical Lie superalgebras.

We should mention that certain generalizations related to other Lie algebras have already been considered,[6–10] although a complete classification was never made. For example, for the Lie algebra sl$(n+1)=A_n$,[7] a set of creation and annihilation operators has been described, and it was shown that n pairs of operators a_i^ξ, with $\xi=\pm$ and $i=1,\ldots,n$, subject to the defining relations

$$[[a_i^+,a_j^-],a_k^+]=\delta_{jk}a_i^+ + \delta_{ij}a_k^+,$$

$$[[a_i^+,a_j^-],a_k^-]=-\delta_{ik}a_j^- - \delta_{ij}a_k^-, \tag{1.2}$$

$$[a_i^+,a_j^+]=[a_i^-,a_j^-]=0$$

$(i,j,k=1,\ldots,n)$, generate the special linear Lie algebra sl$(n+1)$ (as a Lie algebra defined by means of generators and relations). Just as in the case of para-Fermi relations, (1.2) has two interpretations. On the one hand, (1.2) describes the algebraic relations of a new kind of generalized statistics, in this case A-statistics or statistics related to the Lie algebra A_n. On the other hand, (1.2) yields a set of defining relations for the Lie algebra A_n in terms of generators and relations. Observe that certain microscopic and macroscopic properties of A-statistics have already been studied.[11,12]

The description (1.2) was given for the first time by Jacobson[13] in the context of "Lie triple systems." Therefore, this type of generators is often referred to as the "Jacobson generators" of sl$(n+1)$. In this context, we shall mainly use the terminology "creation and annihilation operators (CAOs) for sl$(n+1)$."

In the following section we shall give a mathematical definition of "generalized quantum statistics associated with a Lie algebra G" and the corresponding creation and annihilation operators. It will be clear that this notion is closely related to gradings of G, and to regular subalgebras of G. Following the definition, we go on to describe the actual classification method. In the remaining sections of this paper, the classification results are presented. The paper ends with some closing remarks and further outlook.

II. DEFINITION AND CLASSIFICATION METHOD

Let G be a (classical) Lie algebra. A generalized quantum statistics associated with G is determined by a set of N creation operators x_i^+ and N annihilation operators x_i^-. Inspired by the para-Fermi case and the example of A-statistics, these $2N$ operators should satisfy certain condi-

tions. First of all, these $2N$ operators should generate the Lie algebra G, subject to certain triple relations like (1.1) and (1.2). Let G_{+1} and G_{-1} be the subspaces of G spanned by these elements:

$$G_{+1} = \text{span}\{x_i^+;\ i = 1, \ldots, N\}, \quad G_{-1} = \text{span}\{x_i^-;\ i = 1, \ldots, N\}. \tag{2.1}$$

Then $[G_{+1}, G_{+1}]$ can be zero [in which case the creation operators mutually commute, as in (1.2)] or nonzero [as in (1.1)]. A similar statement holds for the annihilation operators and $[G_{-1}, G_{-1}]$. The fact that the defining relations should be triple relations, implies that it is natural to make the following requirements:

$$[[x_i^+, x_j^+], x_k^+] = 0,$$

$$[[x_i^+, x_j^+], x_k^-] = \text{a linear combination of } x_l^+,$$

$$[[x_i^+, x_j^-], x_k^+] = \text{a linear combination of } x_l^+,$$

$$[[x_i^+, x_j^-], x_k^-] = \text{a linear combination of } x_l^-,$$

$$[[x_i^-, x_j^-], x_k^+] = \text{a linear combination of } x_l^-,$$

$$[[x_i^-, x_j^-], x_k^-] = 0.$$

So let $G_{\pm 2} = [G_{\pm 1}, G_{\pm 1}]$ and $G_0 = [G_{+1}, G_{-1}]$, then we may require $G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}$ (direct sum as vector spaces) to be a $\mathbb{Z}$-grading of a subalgebra of G. Furthermore, since we want G to be generated by the $2N$ elements subject to the triple relations, one must have $G = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}$.

There are two additional assumptions, again inspired by the known examples (1.1) and (1.2). One is related to the fact that creation and annihilation operators are usually considered to be each other's conjugate. So, let ω be the standard antilinear anti-involutive mapping of the Lie algebra G [characterized by $\omega(x) = x^\dagger$ in the standard defining representation of G, where $x^\dagger$ denotes the transpose complex conjugate of the matrix x in this representation] then we should have $\omega(x_i^+) = x_i^-$. And finally, we shall assume that the generating elements $x_i^\pm$ are certain root vectors of the Lie algebra G.

Definition 1: Let G be a classical Lie algebra, with antilinear anti-involutive mapping ω. A set of 2N root vectors $x_i^\pm$ $(i = 1, \ldots, N)$ *is called a set of creation and annihilation operators for G if,*

(i) $\omega(x_i^\pm) = x_i^\mp$,

(ii) $G = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}$ *is a* $\mathbb{Z}$*-grading of G, with* $G_{\pm 1} = span\{x_i^\pm,\ i = 1 \ldots, N\}$ *and* $G_{j+k} = [G_j, G_k]$.

The algebraic relations $\mathcal{R}$ *satisfied by the operators* $x_i^\pm$ *are the relations of a generalized quantum statistics (GQS) associated with G.*

Observe that this is a mathematical generalization of quantum statistics, inspired by the examples mentioned. Whether all such GQS actually lead to physically acceptable quantum statistics remains to be seen; in this sense one should interpret our GQS as "candidates for generalizations of quantum statistics." So with this terminology, a GQS is characterized by a set $\{x_i^\pm\}$ of CAOs and the set of algebraic relations $\mathcal{R}$ they satisfy. A consequence of this definition is that G is generated by G_{-1} and G_{+1}, i.e., by the set of CAOs. Furthermore, since $G_{j+k} = [G_j, G_k]$, it follows that

$$G = \text{span}\{x_i^\xi, [x_i^\xi, x_j^\eta];\ i, j = 1, \ldots, N, \xi, \eta = \pm\}. \tag{2.2}$$

This implies that it is necessary and sufficient to give all relations of the following type:

(R1) The set of all linear relations between the elements $[x_i^\xi, x_j^\eta]$ $(\xi, \eta = \pm,\ i, j = 1, \ldots, N)$.

(R2) The set of all triple relations of the form $[[x_i^{\xi},x_j^{\eta}],x_k^{\zeta}]$=linear combination of x_l^{θ}.

So in general $\mathcal{R}$ consists of a set of quadratic relations (linear combinations of elements of the type $[x_i^{\xi},x_j^{\eta}]$) and a set of triple relations. This also implies that, as a Lie algebra defined by generators and relations, G is uniquely characterized by the set of generators $x_i^{\pm}$ subject to the relations $\mathcal{R}$.

Another consequence of this definition is that G_0 itself is a subalgebra of G spanned by root vectors of G, i.e., G_0 is a regular subalgebra of G. Even more, G_0 is a regular subalgebra containing the Cartan subalgebra H of G. And by the adjoint action, the remaining G_i's are G_0-modules. Thus the following technique can be used in order to obtain a complete classification of all GQS associated with G:

(1) Determine all regular subalgebras G_0 of G. If not yet contained in G_0, replace G_0 by G_0+H.
(2) For each regular subalgebra G_0, determine the decomposition of G into simple G_0-modules g_k $(k=1,2,\ldots)$.
(3) Investigate whether there exists a $\mathbb{Z}$-grading of G of the form

$$G=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}, \tag{2.3}$$

where each G_i is either directly a module g_k or else a sum of such modules $g_1\oplus g_2\oplus\cdots$, such that $\omega(G_{+i})=G_{-i}$.

The first stage in this technique is a known one, to find regular subalgebras one can use the method of extended Dynkin diagrams.[14] The second stage is straightforward by means of Lie algebra representation techniques. The third stage requires most of the work, one must try out all possible combinations of the G_0-modules g_k, and see whether it is possible to obtain a grading of the type (2.3). In this process, if one of the simple G_0-modules g_k is such that $\omega(g_k)=g_k$, then it follows that this module should be part of G_0. In other words, such a case reduces essentially to another case with a larger regular subalgebra.

In general, when the rank of the semisimple regular subalgebra is equal or close to the rank of G, the corresponding $\mathbb{Z}$-grading of G is "short" in the sense that $G_i=0$ for $|i|>1$ or $|i|>2$. When the rank of the regular subalgebra becomes smaller, the corresponding $\mathbb{Z}$-grading of G is "long," and $G_i\neq 0$ for $|i|>2$. Thus the analysis shows that it is usually sufficient to consider maximal regular subalgebras (same rank), or almost maximal regular subalgebras (rank of G minus 1 or 2).

Note that in Ref. 10 a definition of CAOs was already given. Our Definition 1 is inspired by the definition in Ref. 10, however it is different in the sense that the grading conditions $G_{j+k}=[G_j,G_k]$ are new. It is thanks to these new conditions that we are able to give a complete classification of CAOs and the corresponding GQS.

In the following sections we shall give a summary of the classification process for the classical Lie algebras A_n, B_n, C_n, and D_n. Note that, in order to identify a GQS associated with G, it is sufficient to give only the set of CAOs, or alternatively, to give the subspace G_{-1} [then the x_i^- are the root vectors of G_{-1}, and $x_i^+=\omega(x_i^-)$]. The set $\mathcal{R}$ then consist of all quadratic relations (i.e., the linear relations between the elements $[x_i^{\xi},x_j^{\eta}]$) and all triple relations, and all of these relations follow from the known commutation relations in G. Because, in principle, $\mathcal{R}$ can be determined from the set $\{x_i^{\pm};i=1,\ldots,N\}$, we will not always give it explicitly. In fact, when N is large, the corresponding relations can become rather numerous and long. Such examples of GQS would be too complicated for applications in physics. For this reason, we shall give $\mathcal{R}$ explicitly only when N is not too large, more precisely when N is either equal to the rank of G or at most double the rank of G.

Finally, observe that two different sets of CAOs $\{x_i^{\pm};\ i=1,\ldots,N\}$ and $\{y_i^{\pm};\ i=1,\ldots,N\}$ (same N) are said to be isomorphic if, for a certain permutation τ of $\{1,2,\ldots,N\}$, the relations between the elements $x_{\tau(i)}^{\pm}$ and $y_i^{\pm}$ are the same. In that case, the regular subalgebra G_0 spanned by $\{[x_i^+,x_j^-]\}$ is isomorphic (as a Lie algebra) to the regular subalgebra spanned by $\{[y_i^+,y_j^-]\}$.

TABLE I. Classical Lie algebras, their (extended) Dynkin diagrams with a labeling of the nodes and the corresponding simple roots.

Lie algebra	Dynkin diagram	Extended Dynkin diagram
A_n $(n>0)$	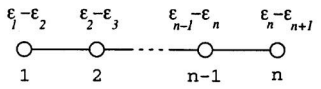	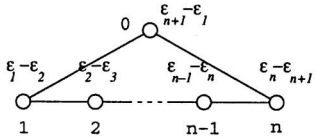
B_n $(n>1)$	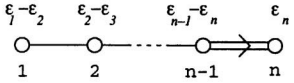	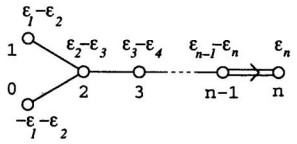
C_n $(n>2)$	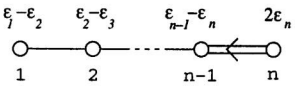	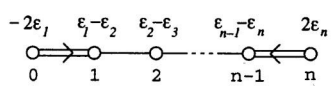
D_n $(n>3)$	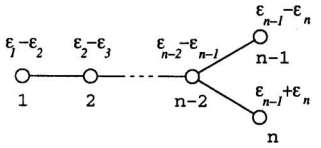	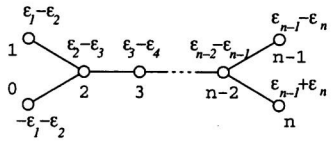

III. THE LIE ALGEBRA $A_n = \mathrm{sl}(n+1)$

Let G be the special linear Lie algebra $\mathrm{sl}(n+1)$, consisting of traceless $(n+1)\times(n+1)$ matrices. The Cartan subalgebra H of G is the subspace of diagonal matrices. The root vectors of G are known to be the elements e_{jk} $(j\neq k=1,\ldots,n+1)$, where e_{jk} is a matrix with zeros everywhere except a 1 on the intersection of row j and column k. The corresponding root is $\epsilon_j-\epsilon_k$, in the usual basis. The anti-involution is such that $\omega(e_{jk})=e_{kj}$. The simple roots and the Dynkin diagram of A_n are given in Table I, and so is the extended Dynkin diagram.

In order to find regular subalgebras of $G=A_n$, one should delete nodes from the Dynkin diagram of G or from its extended Dynkin diagram. We shall start with the ordinary Dynkin diagram of A_n, and subsequently consider the extended diagram.

Step 1: Delete node i from the Dynkin diagram. The corresponding diagram is the Dynkin diagram of $\mathrm{sl}(i)\oplus\mathrm{sl}(n-i+1)$, so $G_0=H+\mathrm{sl}(i)\oplus\mathrm{sl}(n-i+1)$. In this case, there are only two G_0 modules and we can set

$$G_{-1}=\mathrm{span}\{e_{kl};\ k=1,\ldots,i,\ l=i+1,\ldots,n+1\},\quad G_{+1}=\omega(G_{-1}). \tag{3.1}$$

Therefore $\mathrm{sl}(n+1)$ has the following grading:

$$\mathrm{sl}(n+1)=G_{-1}\oplus G_0\oplus G_{+1}, \tag{3.2}$$

and the number of creation and annihilation operators is $N=i(n-i+1)$. Note that the cases i and $n+1-i$ are isomorphic.

The most interesting cases are those with $i=1$ and $i=2$, for which we shall explicitly give the relations $\mathcal{R}$ between the CAOs.

For $i=1$, $N=n$, the rank of A_n. Setting

$$a_j^- = e_{1,j+1}, \quad a_j^+ = e_{j+1,1}, \quad j = 1, \ldots, n \tag{3.3}$$

(for A_n, the possible sets $\{x_i^\pm\}$ will be denoted $\{a_i^\pm\}$, for B_n, they will be denoted $\{b_i^\pm\}$, etc.) the corresponding relations $\mathcal{R}$ read $(j,k,l=1,\ldots,n)$,

$$[a_j^+, a_k^+] = [a_j^-, a_k^-] = 0,$$

$$[[a_j^+, a_k^-], a_l^+] = \delta_{jk} a_l^+ + \delta_{kl} a_j^+, \tag{3.4}$$

$$[[a_j^+, a_k^-], a_l^-] = -\delta_{jk} a_l^- - \delta_{jl} a_k^-.$$

These are the relations of A-statistics[6,7,10–12] as considered in the Introduction.

For $i=2$, $N=2(n-1)$, let

$$a_{-j}^- = e_{1,j+2}, \quad a_{+j}^- = e_{2,j+2}, \quad j = 1, \ldots, n-1,$$

$$a_{-j}^+ = e_{j+2,1}, \quad a_{+j}^+ = e_{j+2,2}, \quad j = 1, \ldots, n-1. \tag{3.5}$$

Now the corresponding relations are $(\xi, \eta, \epsilon = \pm;\ j,k,l=1,\ldots,n-1)$

$$[a_{\xi j}^+, a_{\eta k}^+] = [a_{\xi j}^-, a_{\eta k}^-] = 0,$$

$$[a_{\xi j}^+, a_{-\xi k}^-] = 0, \quad j \neq k,$$

$$[a_{-j}^+, a_{-k}^-] = [a_{+j}^+, a_{+k}^-], \quad j \neq k,$$

$$[a_{+j}^+, a_{-j}^-] = [a_{+k}^+, a_{-k}^-], \tag{3.6}$$

$$[a_{-j}^+, a_{+j}^-] = [a_{-k}^+, a_{+k}^-],$$

$$[[a_{\xi j}^+, a_{\eta k}^-], a_{\epsilon l}^+] = \delta_{\eta\epsilon}\delta_{jk} a_{\xi l}^+ + \delta_{\xi\eta}\delta_{kl} a_{\epsilon j}^+,$$

$$[[a_{\xi j}^+, a_{\eta k}^-], a_{\epsilon l}^-] = -\delta_{\xi\epsilon}\delta_{jk} a_{\eta l}^- - \delta_{\xi\eta}\delta_{jl} a_{\epsilon k}^-.$$

These relations are already more complicated than (3.4). But they are still defining relations for the Lie algebra A_n.

Step 2: Delete node i and j from the Dynkin diagram. By the symmetry of the Dynkin diagram, it is sufficient to consider $1 \leqslant i \leqslant \lfloor n/2 \rfloor$ and $i < j < n+1-i$. We have $G_0 = H + \mathrm{sl}(i) \oplus \mathrm{sl}(j-i) \oplus \mathrm{sl}(n+1-j)$. In this case, there are six simple G_0-modules. All the possible combinations of these modules give rise to gradings of the form

$$\mathrm{sl}(n+1) = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}.$$

There are essentially three different ways in which these G_0-modules can be combined. To characterize these three cases, it is sufficient to give only G_{-1},

$$G_{-1} = \mathrm{span}\{e_{kl}, e_{lp};\ k = 1, \ldots, i,\ l = i+1, \ldots, j,\ p = j+1, \ldots, n+1\},$$

$$\text{with } N = (j-i)(n+1-j+i); \tag{3.7}$$

$$G_{-1} = \mathrm{span}\{e_{kl}, e_{pk};\ k = 1, \ldots, i,\ l = i+1, \ldots, j,\ p = j+1, \ldots, n+1\}, \quad \text{with } N = i(n+1-i); \tag{3.8}$$

$$G_{-1} = \mathrm{span}\{e_{kl}, e_{lp};\ k = 1, \ldots, i,\ p = i+1, \ldots, j,\ l = j+1, \ldots, n+1\}, \quad \text{with } N = j(n+1-j). \tag{3.9}$$

It turns out that the sets of CAOs corresponding to (3.8) and (3.9) are isomorphic to (3.7), so it is sufficient to consider only (3.7). Each case of (3.7) with $1 \leqslant i \leqslant \lfloor n/2 \rfloor$ and $i < j < n+1-i$ gives rise to a distinct GQS. For reasons explained earlier, we shall give the corresponding set of relations explicitly only for small N. In this case, it is interesting to give $\mathcal{R}$ for $j-i=1$, because then the number of creation or annihilation operators is $N=n$. One can label the CAOs as follows:

$$\begin{aligned} a_k^- &= e_{k,i+1}, \quad a_k^+ = e_{i+1,k}, \quad k = 1, \ldots, i, \\ a_k^- &= e_{i+1,k+1}, \quad a_k^+ = e_{k+1,i+1}, \quad k = i+1, \ldots, n. \end{aligned} \tag{3.10}$$

Using

$$\langle k \rangle = \begin{cases} 0 & \text{if } k = 1, \ldots, i, \\ 1 & \text{if } k = i+1, \ldots, n \end{cases} \tag{3.11}$$

the quadratic and triple relations read

$$[a_k^+, a_l^+] = [a_k^-, a_l^-] = 0, \quad k,l = 1, \ldots, i \text{ or } k,l = i+1, \ldots, n,$$

$$[a_k^-, a_l^+] = [a_k^+, a_l^-] = 0, \quad k = 1, \ldots, i, \quad l = i+1, \ldots, n,$$

$$\begin{aligned} [[a_k^+, a_l^-], a_m^+] &= (-1)^{\langle l \rangle + \langle m \rangle} \delta_{kl} a_m^+ + (-1)^{\langle l \rangle + \langle m \rangle} \delta_{lm} a_k^+, \quad k,l = 1, \ldots, i \text{ or } k,l = i+1, \ldots, n, \\ [[a_k^+, a_l^-], a_m^-] &= -(-1)^{\langle l \rangle + \langle m \rangle} \delta_{kl} a_m^- - (-1)^{\langle l \rangle + \langle m \rangle} \delta_{km} a_l^-, \quad k,l = 1, \ldots, i \text{ or } k,l = i+1, \ldots, n, \end{aligned} \tag{3.12}$$

$$[[a_k^\xi, a_l^\xi], a_m^{-\xi}] = -\delta_{km} a_l^\xi + \delta_{lm} a_k^\xi, \ k = 1, \ldots, i, \ l = i+1, \ldots, n,$$

$$[[a_k^\xi, a_l^\xi], a_m^\xi] = 0 \quad (\xi = \pm;\ k,l,m = 1, \ldots, n).$$

The existence of the set of CAOs (3.10) is pointed out in Ref. 6 as a possible example. The relations (3.12) with $n=2m$ and $i=m$ are the commutation relations of the so-called causal A-statistics investigated in Ref. 9.

Step 3: If we delete three or more nodes from the Dynkin diagram, the resulting $\mathbb{Z}$-gradings of $\mathrm{sl}(n+1)$ are no longer of the form $\mathrm{sl}(n+1) = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}$, but there would be non-zero G_i with $|i| > 2$, so these cases are not relevant for our classification.

Step 4: Next, we move on to the extended Dynkin diagram of G. If we delete node i from the extended Dynkin diagram, then remaining diagram is again of type A_n, so $G_0 = G$, and there are no CAOs.

Step 5: If we delete node i and j from the extended Dynkin diagram ($0 \leqslant i < j \leqslant n+1$), then $\mathrm{sl}(n+1) = G_{-1} \oplus G_0 \oplus G_{+1}$ with $G_0 = H + \mathrm{sl}(j-i) \oplus \mathrm{sl}(n-j+i+1)$, and

$$G_{-1} = \mathrm{span}\{e_{kl};\ k = i+1 \ldots, j,\ l \neq i+1, \ldots, j\}.$$

The number of annihilation operators is $N = (j-i)(n+1-j+i)$. It is not difficult to see that all these cases are isomorphic to those of step 1. This can also be deduced from the symmetry of the Dynkin diagram.

Step 6: If we delete nodes i, j, and k from the extended Dynkin diagram ($i < j < k$), then the corresponding $\mathbb{Z}$-gradings are of the form

$$\mathrm{sl}(n+1) = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}.$$

All the corresponding CAOs, however, are isomorphic to those of step 2 (which can again be seen from the remaining Dynkin diagram).

Step 7: If we delete four or more nodes from the extended Dynkin diagram, the corresponding $\mathbb{Z}$-grading of $\mathrm{sl}(n+1)$ has no longer the required properties (i.e., there are nonzero subspaces G_i with $|i|>2$).

IV. THE LIE ALGEBRA $B_n = \mathrm{so}(2n+1)$

$G=\mathrm{so}(2n+1)$ is the subalgebra of $\mathrm{sl}(2n+1)$ consisting of matrices of the form

$$\begin{pmatrix} a & b & c \\ d & -a^t & e \\ -e^t & -c^t & 0 \end{pmatrix}, \tag{4.1}$$

where a is any $(n\times n)$-matrix, b and d are antisymmetric $(n\times n)$-matrices, and c and e are $(n\times 1)$-matrices. The Cartan subalgebra H of G is again the subspace of diagonal matrices. The root vectors and corresponding roots of G are given by

$$e_{jk} - e_{k+n,j+n} \leftrightarrow \epsilon_j - \epsilon_k, \quad j \neq k = 1, \ldots, n,$$

$$e_{j,k+n} - e_{k,j+n} \leftrightarrow \epsilon_j + \epsilon_k, \quad j < k = 1, \ldots, n,$$

$$e_{j+n,k} - e_{k+n,j} \leftrightarrow -\epsilon_j - \epsilon_k, \quad j < k = 1, \ldots, n,$$

$$e_{j,2n+1} - e_{2n+1,j+n} \leftrightarrow \epsilon_j, \quad j = 1, \ldots, n,$$

$$e_{n+j,2n+1} - e_{2n+1,j} \leftrightarrow -\epsilon_j, \quad j = 1, \ldots, n.$$

The anti-involution is such that $\omega(e_{jk})=e_{kj}$. The simple roots, the Dynkin diagram and the extended Dynkin diagram of B_n are given in Table I. Just as for A_n, we now start the process of deleting nodes from the Dynkin diagram or from the extended Dynkin diagram.

Step 1: Delete node 1 from the Dynkin diagram. The remaining diagram is that of B_{n-1}, so $G_0=H+\mathrm{so}(2n-1)\equiv H+B_{n-1}$. There are two G_0-modules:

$$G_{-1} = \mathrm{span}\{e_{1,2n+1} - e_{2n+1,n+1},\ e_{1,k+n} - e_{k,n+1},\ e_{1k} - e_{k+n,n+1};\ k = 2, \ldots, n\}, \tag{4.2}$$

and $G_{+1}=\omega(G_{-1})$. Thus $\mathrm{so}(2n+1)$ has the following grading:

$$\mathrm{so}(2n+1) = G_{-1} \oplus G_0 \oplus G_{+1}$$

and the number of (mutually commuting) creation and annihilation operators is $N=2n-1$. Let us denote the CAOs by

$$b_{00}^- = e_{1,2n+1} - e_{2n+1,n+1}, \quad b_{00}^+ = e_{2n+1,1} - e_{n+1,2n+1},$$

$$b_{-k}^- = e_{1,n+k+1} - e_{k+1,n+1}, \quad b_{-k}^+ = e_{n+k+1,1} - e_{n+1,k+1}, \quad k = 1, \ldots, n-1, \tag{4.3}$$

$$b_{+k}^- = e_{1,k+1} - e_{n+k+1,n+1}, \quad b_{+k}^+ = e_{k+1,1} - e_{n+1,n+k+1}, \quad k = 1, \ldots, n-1.$$

The corresponding relations $\mathcal{R}$ are given by $(\xi, \eta, \epsilon=0, \pm;\ i,j,k=1,\ldots,n-1)$

$$[b_{\xi i}^+, b_{\eta j}^+] = [b_{\xi i}^-, b_{\eta j}^-] = 0,$$

$$[b^+_{-i}, b^-_{-j}] = [b^-_{+i}, b^+_{+j}], \quad i \neq j,$$

$$[b^+_{00}, b^-_{-j}] = [b^-_{00}, b^+_{+j}],$$

$$[b^+_{00}, b^-_{+j}] = [b^-_{00}, b^+_{-j}], \tag{4.4}$$

$$[[b^+_{\xi i}, b^-_{\eta j}], b^+_{\epsilon k}] = \delta_{ij}\delta_{\xi\eta}b^+_{\epsilon k} + \delta_{jk}\delta_{\eta\epsilon}b^+_{\xi i} - \delta_{ik}\delta_{\xi,-\epsilon}b^+_{-\eta j},$$

$$[[b^+_{\xi i}, b^-_{\eta j}], b^-_{\epsilon k}] = -\delta_{ij}\delta_{\xi\eta}b^-_{\epsilon k} - \delta_{ik}\delta_{\xi\epsilon}b^-_{\eta j} + \delta_{jk}\delta_{\eta,-\epsilon}b^-_{-\xi i}.$$

Step 2: Delete node i $(i=2,\ldots,n)$ from the Dynkin diagram; then the corresponding subalgebra is $G_0=H+\mathrm{sl}(i)\oplus\mathrm{so}(2(n-i)+1)$. Now there are four G_0-modules, with the following grading for G:

$$\mathrm{so}(2n+1) = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}$$

with

$$G_{-1} = \mathrm{span}\{e_{j,2n+1} - e_{2n+1,n+j},\ e_{j,k+n} - e_{k,n+j},\ e_{jk} - e_{k+n,n+j};\quad j=1,\ldots,i,\ k=i+1,\ldots,n\},$$

$$G_{-2} = \mathrm{span}\{e_{j,k+n} - e_{k,j+n};\ 1 \leqslant j < k \leqslant i\}. \tag{4.5}$$

The number of the annihilation operators is $N=2i(n-i)+i$. The most interesting case is that with $i=n$: this is the para-Fermi case presented in the Introduction. Indeed, let

$$f^-_j = \sqrt{2}(e_{j,2n+1} - e_{2n+1,n+j}), \quad f^+_j = \sqrt{2}(e_{2n+1,j} - e_{n+j,2n+1}), \quad j=1,\ldots,n. \tag{4.6}$$

Then there are no quadratic relations, and $\mathcal{R}$ consists of triple relations only

$$[[f^\xi_j, f^\eta_k], f^\epsilon_l] = \tfrac{1}{2}(\epsilon-\eta)^2\delta_{kl}f^\xi_j - \tfrac{1}{2}(\epsilon-\xi)^2\delta_{jl}f^\eta_k,$$

$$\xi,\eta,\epsilon = \pm \text{ or } \pm 1, \quad j,k,l = 1,\ldots,n. \tag{4.7}$$

Step 3: Delete two or more nodes from the Dynkin diagram. Then the corresponding $\mathbb{Z}$-grading of $\mathrm{so}(2n+1)$ no longer has the required properties (i.e., there are nonzero G_i with $|i|>2$).

Step 4: Now we turn to the extended Dynkin diagram. Deleting node i from this diagram, leaves the Dynkin diagram of $\mathrm{so}(2n+1)$ for $i=0,1$, of $\mathrm{so}(2n)$ for $i=n$, of $\mathrm{sl}(2)\oplus\mathrm{sl}(2)\oplus\mathrm{so}(2n-3)$ for $i=2$, of $\mathrm{sl}(4)\oplus\mathrm{so}(2n-5)$ for $i=3$, and of $\mathrm{so}(2i)\oplus\mathrm{so}(2n-2i+1)$ for $i\geqslant 4$. In all these cases there is only one G_0-module, so there are no contributions to our classification.

Step 5: Delete the adjacent nodes $(i-1)$ and i $(i=3,\ldots,n)$ from the extended Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=\mathrm{sl}(2)\oplus\mathrm{sl}(2)\oplus\mathrm{so}(2(n-i)+1)$ for $i=3$, of $\tilde{G}_0=\mathrm{sl}(4)\oplus\mathrm{so}(2(n-i)+1)$ for $i=4$, and of $\tilde{G}_0=\mathrm{so}(2(i-1))\oplus\mathrm{so}(2(n-i)+1)$ for $i>4$. In each case, there are five $\tilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one must set $G_0=H+\tilde{G}_0+g_1$, and in each case one finds $G_0\equiv H+B_{n-1}$.

Now, there are only two G_0-modules and

$$\mathrm{so}(2n+1) = G_{-1} \oplus G_0 \oplus G_{+1}$$

with

$$G_{-1} = \mathrm{span}\{e_{i,2n+1} - e_{2n+1,n+i}, e_{ik} - e_{k+n,n+i}, e_{i,k+n} - e_{k,n+i};\ k \neq i = 1,\ldots,n\}. \tag{4.8}$$

The number of the anihilation operators is $N=2n-1$, and all these cases are isomorphic to those of step 1.

Step 6: Delete two nonadjacent nodes from the extended Dynkin diagram, say i and j, $i<j$, $i,j\neq 0,1$. The remaining diagram is that of $\tilde{G}_0=\mathrm{so}(2i)\oplus\mathrm{sl}(j-i)\oplus\mathrm{so}(2(n-j)+1)$ [if $i=2$ we have $\mathrm{sl}(2)\oplus\mathrm{sl}(2)$ instead of $\mathrm{so}(2i)$]. There are seven $\tilde{G}_0$-modules g_k, one of which (say g_1) with $\omega(g_1)=g_1$. Thus one must take $G_0=H+\tilde{G}_0+g_1$, and this is in fact $G_0\equiv H+\mathrm{so}(2(n-j+i)+1)\oplus\mathrm{sl}(j-i)$.

The corresponding grading is

$$\mathrm{so}(2n+1)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$$

with

$$G_{-1}=\mathrm{span}\{e_{k,2n+1}-e_{2n+1,n+k},e_{kl}-e_{l+n,n+k},e_{k,n+l}-e_{l,n+k};\ k=i+1,\ldots,j,l=1,\ldots,i,j+1,\ldots,n\},$$

$$G_{-2}=\mathrm{span}\{e_{k,n+l}-e_{l,n+k};\ i+1\leqslant k<l\leqslant j\}. \tag{4.9}$$

The number of the annihilation operators is $N=2(j-i)(n-j+i)+j-i$, and all these cases turn out to be isomorphic to those of step 2.

Step 7: If we delete three or more nodes from the extended Dynkin diagram, the corresponding $\mathbb{Z}$-grading of $\mathrm{so}(2n+1)$ has no longer the required properties (i.e., there are nonzero subspaces G_i with $|i|>2$).

V. THE LIE ALGEBRA $C_n=\mathrm{sp}(2n)$

$G=\mathrm{sp}(2n)$ is the subalgebra of $\mathrm{sl}(2n)$ consisting of matrices of the form

$$\begin{pmatrix} a & b \\ c & -a^t \end{pmatrix}, \tag{5.1}$$

where a is any $(n\times n)$-matrix, and b and c are symmetric $(n\times n)$-matrices. The Cartan subalgebra H consist of the diagonal matrices, and the root vectors and corresponding roots of G are

$$e_{jk}-e_{k+n,j+n}\leftrightarrow\epsilon_j-\epsilon_k,\quad j\neq k=1,\ldots,n,$$

$$e_{j,k+n}+e_{k,j+n}\leftrightarrow\epsilon_j+\epsilon_k,\quad j\leqslant k=1,\ldots,n,$$

$$e_{j+n,k}+e_{k+n,j}\leftrightarrow-\epsilon_j-\epsilon_k,\quad j\leqslant k=1,\ldots,n.$$

The simple roots, Dynkin diagram and extended Dynkin diagram are given in Table I. Again, the anti-involution is such that $\omega(e_{jk})=e_{kj}$. Next, we describe the process of deleting nodes and its consequences for the classification of GQS.

Step 1: Delete node i ($i=1,\ldots,n-1$) from the Dynkin diagram. The remaining diagram is that of $\mathrm{sl}(i)\oplus\mathrm{sp}(2(n-i))$, so $G_0=H+\mathrm{sl}(i)\oplus\mathrm{sp}(2(n-i))$. There are four G_0-modules, leading to the following grading:

$$\mathrm{sp}(2n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$$

with

$$\begin{aligned} G_{-1}&=\mathrm{span}\{e_{k,n+l}+e_{l,n+k},e_{kl}-e_{n+l,n+k};k=1,\ldots,i,l=i+1,\ldots,n\},\\ G_{-2}&=\mathrm{span}\{e_{k,n+l}+e_{l,n+k};1\leqslant k\leqslant l\leqslant i\}. \end{aligned} \tag{5.2}$$

The number of the annihilation operators is $N=2i(n-i)$. The most interesting cases are $i=1$ and $i=n-1$, which we shall describe in more detail.

For $i=1$, let us denote the CAOs by

$$c^{-}_{-j} = e_{1,n+j+1} + e_{j+1,n+1}, \quad c^{-}_{+j} = e_{1,j+1} - e_{n+j+1,n+1}, \quad j = 1, \ldots, n-1,$$
$$c^{+}_{-j} = e_{n+j+1,1} + e_{n+1,j+1}, \quad c^{+}_{+j} = e_{j+1,1} - e_{n+1,n+j+1}, \quad j = 1, \ldots, n-1. \tag{5.3}$$

Then the corresponding relations $\mathcal{R}$ read, with $\xi, \eta, \epsilon, \gamma = \pm$ or ± 1, and $j, k, l = 1, \ldots, n-1$,

$$[c^{\eta}_{\xi j}, c^{\eta}_{\xi k}] = 0,$$

$$[c^{+}_{-j}, c^{-}_{-k}] = [c^{-}_{+j}, c^{+}_{+k}], \quad j \neq k,$$

$$[c^{-}_{-j}, c^{-}_{+k}] = [c^{+}_{-j}, c^{+}_{+k}] = 0, \quad j \neq k,$$

$$[[c^{+}_{\xi j}, c^{-}_{\eta k}], c^{+}_{\epsilon l}] = \delta_{\xi\eta}\delta_{jk}c^{+}_{\epsilon l} + \delta_{\eta\epsilon}\delta_{kl}c^{+}_{\xi j} + (-1)^{\eta\epsilon}\delta_{\xi,-\epsilon}\delta_{jl}c^{+}_{-\eta k}, \tag{5.4}$$

$$[[c^{+}_{\xi j}, c^{-}_{\eta k}], c^{-}_{\epsilon l}] = -\delta_{\xi\eta}\delta_{jk}c^{-}_{\epsilon l} - \delta_{\xi\epsilon}\delta_{jl}c^{-}_{\eta k} + (-1)^{\xi\eta}\delta_{\eta,-\epsilon}\delta_{kl}c^{-}_{-\xi j},$$

$$[[c^{\xi}_{-j}, c^{\xi}_{+k}], c^{-\xi}_{\eta l}] = 2\eta\delta_{jk}c^{\xi}_{-\eta l},$$

$$[[c^{\gamma}_{\xi j}, c^{\gamma}_{\eta k}], c^{\gamma}_{\epsilon l}] = 0.$$

For $i = n-1$, let us also denote the CAOs by $c^{\pm}_{j}$,

$$c^{-}_{-j} = e_{j,2n} + e_{n,n+j}, \quad c^{-}_{+j} = e_{jn} - e_{2n,n+j}, \quad j = 1, \ldots, n-1,$$
$$c^{+}_{-j} = e_{2n,j} + e_{n+j,n}, \quad c^{+}_{+j} = e_{nj} - e_{n+j,2n}, \quad j = 1, \ldots, n-1. \tag{5.5}$$

Now, the corresponding relations read, with $\xi, \eta, \epsilon, \gamma = \pm$ or ± 1, $j, k, l = 1, \ldots, n-1$,

$$[c^{\eta}_{\xi j}, c^{\eta}_{\xi k}] = 0,$$

$$[c^{+}_{+j}, c^{-}_{-k}] = [c^{-}_{+j}, c^{+}_{-k}] = 0, \quad j \neq k,$$

$$[[c^{\epsilon}_{\xi j}, c^{-\epsilon}_{\xi k}], c^{\epsilon}_{\eta l}] = \xi\eta\delta_{jk}c^{\epsilon}_{\eta l} + \delta_{kl}c^{\epsilon}_{\eta j},$$

$$[[c^{\epsilon}_{+j}, c^{-\epsilon}_{-k}], c^{\xi}_{\eta l}] = (\epsilon\xi - \eta)\delta_{jk}c^{\xi}_{-\eta l}, \tag{5.6}$$

$$[[c^{\epsilon}_{+j}, c^{\epsilon}_{-k}], c^{-\epsilon}_{\xi l}] = -\xi\delta_{jl}c^{\epsilon}_{-\xi k} - \xi\delta_{kl}c^{\epsilon}_{-\xi j},$$

$$[[c^{\gamma}_{\xi j}, c^{\gamma}_{\eta k}], c^{\gamma}_{\epsilon l}] = 0.$$

This set of CAOs, together with their relations (5.6), was constructed earlier in Ref. 6. Also the CAOs (5.3) were already mentioned in Ref. 6 as a possible example, without giving the actual relations (5.4).

Step 2: When node n is deleted from the Dynkin diagram of C_n, the corresponding diagram is that of sl(n), and $G_0 = H + \mathrm{sl}(n)$. In this case, there are two G_0-modules, and sp($2n$) has the grading $\mathrm{sp}(2n) = G_{-1} \oplus G_0 \oplus G_{+1}$ with

$$G_{-1} = \{e_{j,n+k} + e_{k,n+j};\ 1 \leqslant j \leqslant k \leqslant n\}. \tag{5.7}$$

There are $N = n(n+1)/2$ commuting annihilation operators, and the relations $\mathcal{R}$ will not be given explicitly.

Step 3: Upon deleting two or more nodes from the Dynkin diagram of C_n, the corresponding

$\mathbb{Z}$-gradings have no longer the required property (there are nonzero G_i with $|i|>2$).

Step 4: Now we turn to the extended Dynkin diagram. Deleting one node from this diagram leads to a situation with only one G_0-module, irrelevant for our classification.

Step 5: Delete the adjacent nodes $(i-1)$ and i $(i=2,\ldots,n)$ from the extended Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=\mathrm{sp}(2(i-1))\oplus\mathrm{sp}(2(n-i))$. There are seven $\tilde{G}_0$-modules g_k, one of which satisfies $\omega(g_1)=g_1$. Setting $G_0=H+\tilde{G}_0+g_1$, it turns out that $G_0\equiv H+C_{n-1}$. In that case, there are only four G_0-modules and G has the grading $\mathrm{sp}(2n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$ with

$$G_{-1}=\mathrm{span}\{e_{i,n+j}+e_{j,n+i},e_{ij}-e_{n+j,n+i};\ j\neq i=1,\ldots,n\}. \tag{5.8}$$

The number of the annihilation operators is $N=2(n-1)$, and all these cases are isomorphic to the $i=1$ case of step 1.

Step 6: Delete two nonadjacent nodes $i<j$ (excluding the case $i=1$ and $j=n$) from the extended Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=\mathrm{sp}(2i)\oplus\mathrm{sl}(j-i)\oplus\mathrm{sp}(2(n-j))$. There are again seven $\tilde{G}_0$-modules g_k, among which one with $\omega(g_1)=g_1$. Then $G_0=H+\tilde{G}_0+g_1$ $\equiv H+\mathrm{sl}(j-i)\oplus\mathrm{sp}(2(n-j+i))$. There are only four G_0-modules and the grading is $\mathrm{sp}(2n)=G_{-2}$ $\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$ with

$$G_{-1}=\mathrm{span}\{e_{k,n+l}+e_{l,n+k},e_{kl}-e_{n+l,n+k};\ k=i+1,\ldots,j,l\neq i+1,\ldots,j\}. \tag{5.9}$$

The number of annihilation operators is $N=2(j-i)(n-j+i)$, and all these cases are isomorphic to those of step 1 with $i\neq 1$.

Step 7: Delete node 1 and n from the extended Dynkin diagram. The remaining diagram is that of $\mathrm{sl}(2)\oplus\mathrm{sl}(n-1)$. With $G_0=\mathrm{sl}(2)\oplus\mathrm{sl}(n-1)$, there are four G_0-modules and the corresponding grading is $\mathrm{sp}(2n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$ with

$$G_{-1}=\mathrm{span}\{e_{1,n+k}+e_{k,n+1},e_{k1}-e_{n+1,n+k};\ k=2,\ldots,n\}. \tag{5.10}$$

This case is isomorphic to the $i=n-1$ case of step 1.

Step 8: If we delete three or more nodes from the extended Dynkin diagram, the corresponding $\mathbb{Z}$-grading of $\mathrm{sp}(2n)$ no longer has the required properties (i.e., there are nonzero subspaces G_i with $|i|>2$).

VI. THE LIE ALGEBRA $D_n=\mathrm{so}(2n)$

$G=\mathrm{so}(2n)$ is the subalgebra of $\mathrm{sl}(2n)$ consisting of matrices of the form

$$\begin{pmatrix} a & b \\ c & -a^t \end{pmatrix}, \tag{6.1}$$

where a is any $(n\times n)$-matrix, and b and c are antisymmetric $(n\times n)$-matrices. The Cartan subalgebra H consist of the diagonal matrices, and the root vectors and corresponding roots of G are

$$e_{jk}-e_{k+n,j+n}\leftrightarrow\epsilon_j-\epsilon_k,\quad j\neq k=1,\ldots,n,$$

$$e_{j,k+n}-e_{k,j+n}\leftrightarrow\epsilon_j+\epsilon_k,\quad j<k=1,\ldots,n,$$

$$e_{j+n,k}-e_{k+n,j}\leftrightarrow-\epsilon_j-\epsilon_k,\quad j<k=1,\ldots,n.$$

The simple roots, Dynkin diagram and extended Dynkin diagram are given in Table I. Again, the anti-involution is such that $\omega(e_{jk})=e_{kj}$. Next, we describe the process of deleting nodes and its consequences for the classification of GQS.

Step 1: When node 1 is deleted from the Dynkin diagram of D_n, the remaining diagram is that of D_{n-1}, so $G_0=H+D_{n-1}=H+\mathrm{so}(2(n-1))$. There are two G_0-modules,

$$G_{-1} = \mathrm{span}\{e_{1i} - e_{n+i,n+1}, e_{1,n+i} - e_{i,n+1}; i = 2, \ldots, n\}, \tag{6.2}$$

and $G_{+1} = \omega(G_{-1})$. G has the corresponding grading $\mathrm{so}(2n) = G_{-1} \oplus G_0 \oplus G_{+1}$, and there are $N = 2(n-1)$ commuting annihilation operators. Denoting the CAOs by

$$d^-_{-i} = e_{1,n+i+1} - e_{i+1,n+1}, \quad d^-_{+i} = e_{1,i+1} - e_{n+i+1,n+1}, \quad i = 1, \ldots, n-1,$$

$$d^+_{-i} = e_{n+i+1,1} - e_{n+1,i+1}, \quad d^+_{+i} = e_{i+1,1} - e_{n+1,n+i+1}, \quad i = 1, \ldots, n-1, \tag{6.3}$$

then, for $\xi, \eta, \epsilon = \pm$ and $i, j, k = 1, \ldots, n-1$, the relations $\mathcal{R}$ are given by

$$\begin{gathered}
[d^\epsilon_{\xi i}, d^\epsilon_{\eta j}] = 0, \\
[d^+_{-i}, d^-_{+i}] = [d^+_{+i}, d^-_{-i}] = 0, \\
[[d^+_{\xi i}, d^-_{\eta j}], d^-_{\epsilon k}] = -\delta_{\xi\eta}\delta_{ij} d^-_{\epsilon k} - \delta_{\xi\epsilon}\delta_{ik} d^-_{\eta j} + \delta_{\eta,-\epsilon}\delta_{jk} d^-_{-\xi,i}, \\
[[d^+_{\xi i}, d^-_{\eta j}], d^+_{\epsilon k}] = \delta_{\xi\eta}\delta_{ij} d^+_{\epsilon k} + \delta_{\eta\epsilon}\delta_{jk} d^+_{\xi i} - \delta_{\xi,-\epsilon}\delta_{ik} d^+_{-\eta,j}.
\end{gathered} \tag{6.4}$$

Although the relations (6.4) are new, the existence of the set of CAOs (6.3) was pointed out in Ref. 6.

Step 2: When node i ($i = 2, \ldots, n-2$) is deleted from the Dynkin diagram of D_n, the remaining diagram is that of $\mathrm{sl}(i) \oplus \mathrm{so}(2(n-i))$ [or $\mathrm{sl}(n-2) \oplus \mathrm{sl}(2) \oplus \mathrm{sl}(2)$ in the case $i = n-2$]. With $G_0 = \mathrm{sl}(i) \oplus \mathrm{so}(2(n-i))$, there are four G_0-modules, and $\mathrm{so}(2n)$ has the following grading $\mathrm{so}(2n) = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}$ with

$$G_{-1} = \mathrm{span}\{e_{kl} - e_{n+l,n+k}, e_{k,n+l} - e_{l,n+k};\ k = 1, \ldots, i, l = i+1, \ldots, n\}. \tag{6.5}$$

The number of annihilation operators is $N = 2i(n-i)$.

Step 3: Delete node $n-1$ or n from the Dynkin diagram; the remaining diagram is that of $\mathrm{sl}(n)$, and $G_0 = H + \mathrm{sl}(n)$. There are only two G_0-modules and G has the grading $\mathrm{so}(2n) = G_{-1} \oplus G_0 \oplus G_{+1}$, with

$$G_{-1} = \mathrm{span}\{e_{j,n+k} - e_{k,n+j};\ 1 \leqslant j < k \leqslant n-1\} \cup \mathrm{span}\{e_{jn} - e_{2n,n+j};\ j = 1, \ldots, n-1\}, \text{ for } i = n-1,$$

$$G_{-1} = \mathrm{span}\{e_{j,k+n} - e_{k,j+n};\ 1 \leqslant j < k \leqslant n\}, \text{ for } i = n. \tag{6.6}$$

There are $N = n(n-1)/2$ commuting annihilation operators, and these two cases are isomorphic. The relations are not given explicitly.

Step 4: Upon deleting two nodes i and j ($i < j = 1, \ldots, n-2$) or more from the Dynkin diagram of D_n, the corresponding $\mathbb{Z}$-gradings have no longer the required property (there are nonzero G_i with $|i| > 2$).

Step 5: Delete nodes $n-1$ and n from the Dynkin diagram. The remaining diagram is that of $\mathrm{sl}(n-1)$. For $G_0 = H + \mathrm{sl}(n-1)$, there are six G_0-modules. There are three different ways in which these G_0-modules can be combined, each of them yielding a $\mathbb{Z}$-grading of the form $\mathrm{so}(2n) = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}$, namely,

$$G_{-1} = \mathrm{span}\{e_{jn} - e_{2n,n+j},\ e_{j,2n} - e_{n,n+j};\ j = 1, \ldots, n-1\}, \tag{6.7}$$

$$G_{-1} = \mathrm{span}\{e_{jn} - e_{2n,n+j},\ j = 1, \ldots, n-1; \quad e_{n+j,k} - e_{n+k,j},\ 1 \leqslant j < k \leqslant n-1\}, \tag{6.8}$$

$$G_{-1} = \text{span}\{e_{j+n,n} - e_{2n,j},\ j = 1, \ldots, n-1; \quad e_{j,k+n} - e_{k,j+n},\ 1 \leqslant j < k \leqslant n-1\}. \tag{6.9}$$

For (6.7), we have $N=2(n-1)$; for (6.8) and (6.9), we have $N=n(n-1)/2$. It turns out that (6.8) and (6.9) are isomorphic to each other. Here, we shall give the relations only for (6.7). Denote the CAOs of (6.7) by

$$d^-_{-i} = e_{i,2n} - e_{n,n+i},\ d^-_{+i} = e_{in} - e_{2n,n+i}, \quad i = 1, \ldots, n-1,$$

$$d^+_{-i} = e_{2n,i} - e_{n+i,n}, d^+_{+i} = e_{ni} - e_{n+i,2n}, \quad i = 1, \ldots, n-1. \tag{6.10}$$

Then, with $\xi, \eta, \epsilon, \gamma = \pm$ or ± 1 and $i, j, k = 1, \ldots, n-1$, the relations are explicitly given by

$$\begin{gathered}
[d^\eta_{\xi i}, d^\eta_{\xi j}] = 0, \\
[d^+_{-i}, d^-_{+j}] = [d^+_{+i}, d^-_{-j}] = 0, \\
[d^-_{+i}, d^-_{-i}] = [d^+_{+i}, d^+_{-i}] = 0, \\
[[d^\gamma_{\xi i}, d^\gamma_{\eta j}], d^\gamma_{\epsilon k}] = 0, \\
[[d^\xi_{+i}, d^\xi_{-j}], d^{-\xi}_{\epsilon k}] = -\delta_{ik} d^\xi_{-\epsilon j} + \delta_{jk} d^\xi_{-\epsilon i}, \\
[[d^\eta_{\xi i}, d^{-\eta}_{\xi j}], d^\eta_{\epsilon k}] = \xi\epsilon\delta_{ij} d^\eta_{\epsilon k} + \delta_{jk} d^\eta_{\epsilon i}.
\end{gathered} \tag{6.11}$$

The set of CAOs (6.10) with relations (6.11) is the example that was considered earlier in Refs. 6 and 8.

Step 6: Now we move to the extended Dynkin diagram. Deleting node i leaves the Dynkin diagram of so$(2n)$ for $i=0,1,n-1,n$, of sl$(2)\oplus$sl$(2)\oplus$so$(2(n-2))$ for $i=2$, of sl$(3)\oplus$so$(2(n-3))$ for $i=3$, and of $=$so$(2i)\oplus$so$(2(n-i))$ for $i\geqslant 4$. In all these cases there is only one G_0-module, so there are no contributions to our classification.

Note that deleting nodes i and j $[1<i<j<\lfloor(n+1)/2\rfloor]$ from the extended Dynkin diagram is equivalent to delete nodes $(n-j)$ and $(n-i)$.

Step 7: Delete the adjacent nodes $(j-1)$ and j. For $j=1$ we are back to step 1, and for $j=2$ to step 2 with $i=2$. For $j\geqslant 3$ the remaining diagram is that of $\tilde{G}_0=$so$(2(j-1))\oplus$so$(2(n-j))$ [for $j=3$ this is sl$(2)\oplus$sl$(2)\oplus$so$(2(n-j))$ and for $j=4$ this is sl$(4)\oplus$so$(2(n-j))$]. There are five $\tilde{G}_0$-modules g_k, one with $\omega(g_5)=g_5$, so one must set $G_0=H+\tilde{G}_0+g_5\equiv H+so(2(n-1))$. Now, there are only two G_0-modules, G has the grading so$(2n)=G_{-1}\oplus G_0\oplus G_{+1}$, and all these cases are isomorphic to those of step 1.

Step 8: Delete the nonadjacent nodes i and j $(i<j-1)$ from the extended Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=$so$(2i)\oplus$sl$(j-i)\oplus$so$(2(n-j))$ [for $i=2$ this is sl$(2)\oplus$sl$(2)\oplus$sl$(j-i)\oplus$so$(2(n-j))$; for $i=3$ this is sl$(3)\oplus$sl$(j-i)\oplus$so$(2(n-j))$]. There are nine $\tilde{G}_0$-modules g_k, one with $\omega(g_9)=g_9$. Setting $G_0=H+\tilde{G}_0+g_9\equiv H+sl(j-i)\oplus$so$(2(n-j+i))$, there are only four G_0-modules. All these cases are isomorphic to those of step 2.

Step 9: If we delete three or more nodes from the extended Dynkin diagram, the corresponding $\mathbb{Z}$-grading of so$(2n)$ no longer has the required properties (i.e., there are nonzero subspaces G_i with $|i|>2$).

VII. SUMMARY AND CONCLUSIONS

We have obtained a complete classification of all GQS associated with the classical Lie algebras. The familiar cases (para-Fermi statistics and A-statistics) appear as simple examples in our classification. It is worth observing that some other examples in this classification are also

TABLE II. Summary of the classification: all nonisomorphic GQS associated with a classical Lie algebra are given. For each GQS, we list the Dynkin diagram of G_0 (described in terms of the Dynkin diagram D of G), the subspace G_{-1} (as a reference to the main text), the number of annihilation operators (N), and the relations $\mathcal{R}$ (when given in the text).

Lie algebra	Dynkin diagram of G_0	G_{-1}	N	$\mathcal{R}$
A_n	$D-\{i\}$ $(i\leqslant\lfloor(n+1)/2\rfloor)$	(3.1)	$i(n+1-i)$	$i=1$ (3.4) $i=2$ (3.6)
	$D-\{i,j\}$ $(i\leqslant\lfloor n/2\rfloor$ $i<j<n+1-i)$	(3.7)	$(j-i)(n+1-j+i)$	$j-i=1$ (3.12)
B_n	$D-\{1\}$	(4.2)	$2n-1$	(4.4)
	$D-\{i\}$ $(2\leqslant i\leqslant n)$	(4.5)	$2i(n-i)+i$	$i=n$ (4.7)
C_n	$D-\{i\}$ $(1\leqslant i\leqslant n-1)$	(5.2)	$2i(n-i)$	$i=1$ (5.4) $i=n-1$ (5.6)
	$D-\{n\}$	(5.7)	$n/(n+1)2$	
D_n	$D-\{1\}$	(6.2)	$2(n-1)$	(6.4)
	$D-\{i\}$ $(2\leqslant i\leqslant n-2)$	(6.5)	$2i(n-i)$	
	$D-\{n\}$	(6.6)	$n/(n-1)2$	
	$D-\{n-1,n\}$	(6.7) (6.8)	$2(n-1)$ $n/(n-1)2$	(6.11)

rather simple. The GQS given in (3.6) and (3.12), e.g., seem to be closely related to *A*-statistics, except that there are two kinds of particles corresponding to the CAOs [see (3.5) and (3.11)]. The GQS of type *D* given in (6.4) has also particularly simple defining relations. For convenience, a comprehensive summary of the classification of all GQS is given in Table II.

As we have already mentioned in the main text, several cases in our classification appear as examples in Refs. 7–12 and in Palev's thesis.[6] In these papers or in the thesis, however, no classification is given, only a number of examples inspired by the para-Fermi case are considered. Furthermore, for some of these examples Fock-type representations are constructed.

In this paper, we have dealt only with a mathematical definition of generalized quantum statistics. In order to talk about a quantum statistics in the physical sense, one should take into account additional requirements for the CAOs, related to certain quantization postulates.[7] First of all, there should be a state space (possibly a Fock space) in which the CAOs act. Here, the Lie algebraic framework could be useful, since such a state space can coincide with a Lie algebra representation space (and automatically all elements in the Lie algebra G and in its universal enveloping algebra have a well-defined action in any representation). Physical observables, and in particular the Hamiltonian, should be Hermitian operators and expressible via the CAOs. The Hermiticity conditions for physical observables usually lead to conjugacy relations for the CAOs; these are often such that, for example, $(x_i^-)^\dagger = x_i^+$ (for the representatives of the CAOs in a representation). In other words, such Hermiticity conditions are often related to the anti-involution ω. The representation spaces in which the inner product is such that the Hermitian conjugate of the representative of $x \in G$ is equal to the representative of $\omega(x)$ are often called the unitary representations (with respect to the given anti-involution ω). Whether the class of finite dimensional representations of G plays a role, or whether it is a class of infinite dimensional representations, depends on the choice of ω. With the standard choice considered in this paper, the unitary representations are finite dimensional. For another choice of ω [still with $\omega(G_{-1}) = G_{+1}$, but no longer all plus signs in $\omega(x_i^-) = \pm x_i^+$], our classification of GQS remains valid, but the unitary representations will be infinite dimensional.

It is only after an investigation of such further properties, that one can talk about a quantum statistics. If one can furthermore classify the state spaces for a particular GQS, then one can study its macroscopic and microscopic properties. Such a program is feasible, and could give rise to interesting quantum statistical properties. For example, for A-statistics, the microscopic properties (i.e., the properties of the CAOs and their action on the Fock spaces) have been described in Refs. 7–11, whereas the macroscopic properties (i.e., the statistical properties of ensembles of particles satisfying this GQS) have been studied in Ref. 12. We hope that some other cases of this classification will yield similar interesting GQS.

From the mathematical point of view, a set of CAOs together with a complete set of relations $\mathcal{R}$ unambiguously describes the Lie algebra. So each case of our classification also gives the description of a classical Lie algebra in terms of a number of generators subject to certain relations. This can also be reformulated in terms of the notion of Lie triple systems.[13] According to the definition, a Lie triple system L of an associative algebra A is a subspace of A that is closed under the ternary composition $[[a,b],c]$, where $[a,b]=ab-ba$. It is easy to see that in our case the subspace $G_{-1}\oplus G_{+1}$ (i.e., the subspace spanned by all CAOs) is a Lie triple system for the universal enveloping algebra $\mathrm{U}(G)$.

This paper was devoted to classical Lie algebras only. The exceptional Lie algebras are not considered here. Although it would be possible to perform a mathematical classification of the GQS associated with G_2, F_4, E_6, E_7, and E_8, it is obvious that in such a case the number of CAOs is a fixed integer. For physical applications, it is of importance that the number of CAOs is not a fixed number but an integer parameter N. In fact, in quantum field theoretical applications, one is mainly interested in the case $N\to\infty$.

As mentioned in the Introduction, para-Bose statistics is connected with a Lie superalgebra, the orthosymplectic superalgebra $\mathrm{osp}(1|2n)$. In a future paper, we hope to classify all GQS associated with the classical Lie superalgebras.

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Solitonlike excitations in a one-dimensional electrical transmission line

François B. Pelap[a] and Mansour M. Faye
Département de Physique, Faculté des Sciences et Techniques, Université Cheikh Anta Diop de Dakar, BP 5005 Dakar–Fann, Senegal

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Dynamics of modulated waves is studied in a one-dimensional discrete nonlinear electrical transmission line. Contribution of a linear dispersive capacitance is appreciated and it is shown via a reductive perturbation method that evolution of such waves in this system is governed by a higher order nonlinear Schrödinger equation. Passing through the Stokes wave analysis, a generalized criterion for the Benjamin–Feir instability in the network is presented and exact solutions of the obtained wave equation are determined by the means of the Pathria and Morris approach. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1843272]

I. INTRODUCTION

It is well known that exactly integrable nonlinear differential equations have soliton solutions that travel stationary and collide elastically. Many wave spread phenomena can be explained by integrable equations in some ideal conditions and there is a great variety of applications of the concept of solitons in condensed matter physics.[1] It is possible to divide these applications into the following two parts: In one part continuum media are treated, e.g., in hydrodynamics,[2] and solitons arise as solutions of partial differential equations (PDE's). In the other part, intrinsically discrete models are considered, e.g., chains of magnetic ions or hydrogen-bonded chains in proteins.[1,3] Here differential-difference equations must be solved instead of the PDE's of the first part. However, apart from very few exceptions like Toda lattice,[4] the differential-difference equations cannot be solved exactly. Therefore, several soliton perturbation theories have been developed to study the effect of small perturbations on integrable equations. In these theories, the reductive perturbation method[5,6] is well known. Within this method, we have the semidiscrete approximation that consists of considering the continuum approximation to describe the envelope of the signal and treats the carrier wave with its discrete character.

The main purpose of this paper is to study the dynamics of modulated wave trains in a discrete nonlinear electrical transmission line using the semidiscrete approximation. This paper is organized as follows. In Sec. II, we present a nonlinear electrical network representing a bandpass filter with a linear dispersive capacitance C_s. In Sec. III, we use the reductive perturbation method to derive the higher order nonlinear Schrödinger equation (HONLSE) describing the propagation of modulated waves in the line. The impact of C_s on the dispersion relation is discussed. In Sec. IV, the resulting HONLSE is utilized to determine the condition for instability of slowly modulated waves. A calculation to predict the modulational instability (MI) is presented. In Sec. V, the Pathria and Morris method is exploited to check whether the HONLSE possesses solitary wave solutions which show that solitons can propagate in the network. Finally, Sec. VI is devoted to concluding remarks.

[a]Author to whom correspondence should be addressed. Permanent address: Department of Physics, Physics Laboratory, University of Dschang, P.O. Box 69, Dschang, Cameroon.

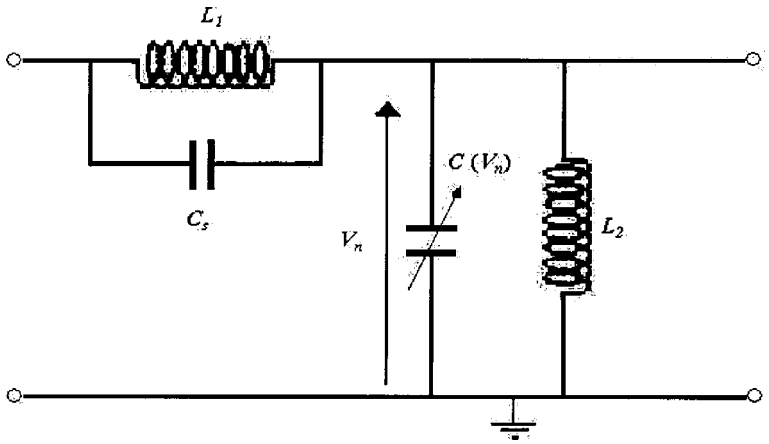

FIG. 1. Schematic representation of one unit cell of a discrete nonlinear electrical transmission line. The network is composed of N identical cells.

II. MODEL DESCRIPTION

The model under consideration is a lossless discrete nonlinear transmission line made of N identical unit cells as illustrated in Fig. 1. Each unit cell contains a linear inductance L_1 in parallel with a linear capacitance C_s in the series branch and, a linear inductance L_2 in parallel with a nonlinear capacitance $C(V)$ in the shunt branches. This nonlinear capacitance consists of a reversed-biased diode with differential capacitance function of the voltage V_n across the nth capacitor[7] and biased by a constant voltage V_0: $C(V_0+V_n)=\mathrm{d}Q_n/\mathrm{d}V_n$ in which Q_n is the corresponding nonlinear charge. For low voltages chosen around V_0 the quantity $Q_n(V_n)$ can be approximated by[8]

$$Q_n(V_n) = C_0(V_n - \alpha V_n^2 + \beta V_n^3), \tag{2.1}$$

where $C_0=C(V_0)$, α and β are positive constants, C_0 designates the characteristic capacitance, and α and β denote the nonlinear parameter. From the Kirchhoff's laws applied to the circuit of Fig. 1, we derive the following system of nonlinear equations for the voltage $V_n(t)$:

$$\frac{\mathrm{d}^2V_n}{\mathrm{d}t^2} + u_0^2(2V_n - V_{n-1} - V_{n+1}) + \lambda\frac{\mathrm{d}^2}{\mathrm{d}t^2}(2V_n - V_{n-1} - V_{n+1}) + \omega_0^2V_n = \alpha\frac{\mathrm{d}^2V_n^2}{\mathrm{d}t^2} - \beta\frac{\mathrm{d}^2V_n^3}{\mathrm{d}t^2},$$

$$n = 1,2, \ldots ,N \tag{2.2}$$

where N is the number of cells considered. In Eq. (2.2), we have set

$$u_0^2 = \frac{1}{L_1C_0}, \quad \omega_0^2 = \frac{1}{L_2C_0}, \quad \text{and } \lambda = \frac{C_s}{C_0}. \tag{2.3}$$

During computations, the following values of the network's parameters are used[8,9]

$$L_1 = 200 \pm 5\mu H, \quad L_2 = 470 \pm 10\mu H, \quad V_0 = 2V, \quad C_0 = 370 \pm 10pF,$$

$$\alpha = 0.21V^{-1}, \quad \beta = 0.0197V^{-2}, \quad \text{and } C_s = 1850 \pm 10pF. \tag{2.4}$$

III. OSCILLATORY SOLUTIONS

Now, our attention is focused on the propagation of modulated waves in the system. For this aim, the semidiscrete approximation[5,6] is employed to obtain short wavelength envelope solitons.

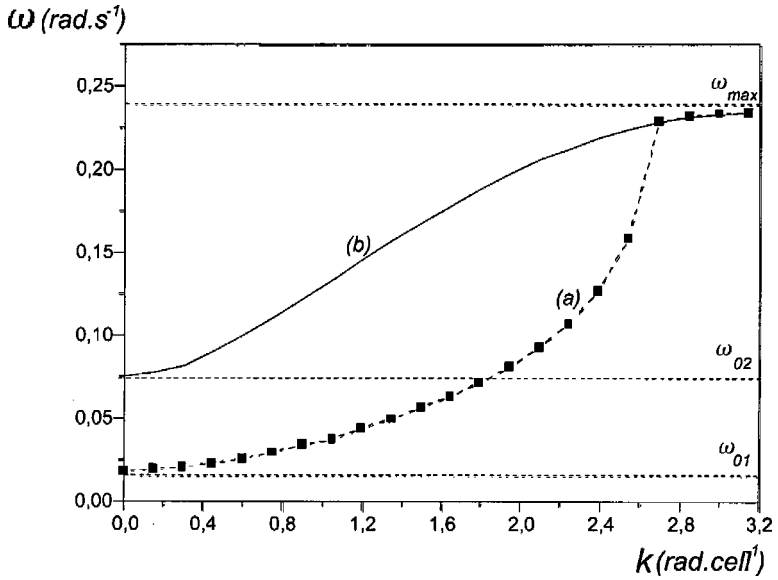

FIG. 2. Linear dispersion curve defined by relation (3.2) for the constants given by expression (2.2). (a) Case where $\lambda \neq 0$; (b) case where $\lambda = 0$. While comparing these two plots, we note that the gap zone is larger in the absence of the linear capacitance C_s (i.e., for $\lambda = 0$).

This approach allows us to treat properly the carrier with its discrete character and to describe the envelope in the continuum approximation. Therefore, slow variables (ξ, τ) are introduced as follows: $\xi = \varepsilon(n - V_g t)$, $\tau = \varepsilon^2 t$ where ε is a small parameter and V_g denotes the group velocity of the packet wave.

Leaning on the idea developed by Taniuti and Yajima,[10] the solution $V_n(t)$ of Eq. (2.2) can be taken in the following form:[11]

$$\begin{aligned} V_n(t) = {} & \varepsilon^{1/2} V_{11}(n,t) e^{i\theta} + \varepsilon [V_{20}(n,t) + V_{22}(n,t) e^{2i\theta}] + \varepsilon^{3/2} [V_{30}(n,t) + V_{33}(n,t) e^{3i\theta}] \\ & + \varepsilon^2 [V_{40}(n,t) + V_{42}(n,t) e^{2i\theta} + V_{44}(n,t) e^{4i\theta}] + \varepsilon^{5/2} [V_{50}(n,t) + V_{53}(n,t) e^{3i\theta} + V_{55}(n,t) e^{5i\theta}] \\ & + \text{c.c.} + O(\varepsilon^{7/2}), \end{aligned} \tag{3.1}$$

in which θ is the phase given by $\theta = kn - \omega t$; c.c. stands for the complex conjugation and ε is the smallness parameter that measures the size of the amplitude of the perturbation. During the computations, there are nonzero voltages $V_{lm}(n \pm 1, t)$ which are expanded in the continuum limit around $V_{lm}(x,t)$ with $n = x$. So the fast changes of the phase θ in Eq. (3.1) are correctly taken into account by considering differences in the phase for the discrete variable n. We have also scaled time and space derivatives as $\partial/\partial t \sim 0(\varepsilon)$ and $\partial/\partial x \sim 0(\varepsilon)$, respectively, and neglected consistently high order in ε terms. Then we keep up to the second order derivative terms of $V_n(t)$ to balance dispersion and nonlinearity. Introduction of $V_n(t)$ and its derivatives into Eq. (2.2) yields a series of equations distinguished by the power of ε.

From the equations of $(\varepsilon^{1/2}, e^{i\theta})$, that is the terms of $0(\varepsilon^{1/2})$ for the first harmonic, we derive the following linear dispersion law:

$$(1 + 4\lambda \cos^2(k/2))\omega^2 = \omega_0^2 + 4u_0^2 \sin^2(k/2) \tag{3.2}$$

in which the wave number k is taken in the Brillouin zone. The linear dispersion curve that deals with expression (3.2) is shown in Fig. 2(a) and represents a bandpass filter. As displayed in this figure, the corresponding linear spectrum has a gap $f_{01} = \omega_{01}/2\pi$ which is the lower cutoff frequency introduced by the parallel inductance L_2 and it is limited by the cutoff frequency

$$f_{\max} = \frac{\omega_{\max}}{2\pi} = \frac{1}{2\pi}(\omega_0^2 + 4u_0^2)^{1/2} \tag{3.3}$$

due to the lattice effects. On the other hand, Fig. 2(b) presents the plot of relation (3.2) in the case where $\lambda = 0$ that corresponds to $C_s = 0$. While comparing the graphs of Figs. 2(a) and 2(b), we note that the upper cutoff frequency $f_{\max}$ has not changed in the presence of the linear dispersion capacitance C_s in the system. But the existence of C_s reduces the value of the lower cutoff frequency since $f_{01} < f_{02}$ with $f_{02} = \omega_{02}/2\pi$. The direct physical consequence of such result is that the gap zone in the system is highly reduced. Because the width of the interval $[f_{01}, f_{\max}]$ is bigger than that of $[f_{02}, f_{\max}]$, introduction of C_s in the circuit has increased the propagation domain of the signal.

From the terms proportional to $\varepsilon^{3/2}e^{i\theta}$, we obtain the expression

$$i\left[V_g\frac{\partial V_{11}}{\partial \xi} + \frac{\partial V_{11}}{\partial \tau}\right] = -Q(k)|V_{11}|^2 V_{11} \tag{3.4}$$

in which

$$Q(k) = \frac{\omega}{2}[2\alpha(N_{20} + N_{22}) - 3\beta] = \frac{\omega}{2}\left\{4\alpha^2\left(\frac{2\omega^2}{D} + \frac{V_g^2}{V_g^2 - u_0^2}\right) - 3\beta\right\}$$

with

$$D = 4\omega^2(1 + 4\lambda\cos^2 k) - 4u_0^2\sin^2 k - \omega_0^2.$$

Here we follow the Kakutani and Michihiro idea[12] and assume that $\Delta k = k - k_c$ is of $O(\varepsilon)$ and write $Q = \varepsilon Q_1$ where Q_1 is of $O(1)$ and is given approximately by

$$Q_1(k) = \frac{\Delta k}{\varepsilon}\left(\frac{\mathrm{d}Q(k)}{\mathrm{d}k}\right)_{k=k_c} = \frac{V_g}{\omega}Q(k) - \left(\frac{\omega u_0^2}{V_g^2}\right)N_{20}^2\left[\frac{6\lambda\omega}{\chi}\sin k - \frac{V_g}{\omega} + \frac{\cos k}{\sin k}\right] + 2\alpha N_{22}V_g$$

$$- \frac{N_{22}^2}{\omega}[2\omega V_g(1 + 4\lambda\cos^2 k) - (u_0^2 + 4\lambda\omega^2)\sin 2k]. \tag{3.5}$$

In relation (3.5), the group velocity is expressed as

$$V_g = \frac{\partial \omega}{\partial k} = \frac{2}{\chi}(u_0^2 + \lambda\omega^2)\sin k, \quad \chi = \omega(1 + 4\lambda\cos^2(k/2)) \tag{3.6}$$

and real k_c designates the critical value of the wave number k of the signal. Therefore at $O(\varepsilon^{3/2})$, Eq. (3.4) becomes

$$V_g\frac{\partial V_{11}}{\partial \xi} + \frac{\partial V_{11}}{\partial \tau} = 0. \tag{3.7}$$

This result means that in the reference frame moving with the group velocity V_g, the complex amplitude V_{11} of the signal remains constant to the concerned scale.[13] Hence, the right-hand side (rhs) of Eq. (3.4) is shifted to the corresponding nonsecular condition at $O(\varepsilon^{5/2})$.

From the equations of $(\varepsilon^{5/2}, e^{i\theta})$, we establish that the resulting equation that describes dynamics of a packet wave in the discrete nonlinear transmission line (of Fig. 1) is the higher order nonlinear Schrödinger equation (HONLSE),

$$i\frac{\partial V_{11}}{\partial \tau} + P\frac{\partial^2 V_{11}}{\partial \xi^2} = Q_1|V_{11}|^2 V_{11} + Q_2|V_{11}|^4 V_{11} + iQ_3 V_{11}^2\frac{\partial V_{11}^*}{\partial \xi} + iQ_4|V_{11}|^2\frac{\partial V_{11}}{\partial \xi} \tag{3.8}$$

in which the different coefficients are defined by

$$P = \frac{1}{2\omega}[(u_0^2 + \lambda\omega_0^2)\cos k - 4\lambda V_g^2 \sin^2(k/2) - 4\omega V_g \sin k], \tag{3.9}$$

$$Q_2 = \omega\left[\alpha(N_{40} + N_{42} + N_{22}N_{33}) - \frac{3\beta}{2}(2N_{22}^2 + N_{33} + N_{20}^2 + 2N_{20}N_{22})\right], \tag{3.10}$$

$$Q_3 = 2V_g[\beta - \alpha(N_{20} + N_{22})], \tag{3.11}$$

$$Q_4 = \alpha\omega\tilde{N}_{42} + 2Q_3, \tag{3.12}$$

and Q_1 is given by relation (3.5). The diverse parameters and voltages that appear in the coefficients of Eq. (3.8) are determined in the Appendix.

The HONLSE (3.8) is known to govern modulations of weakly nonlinear ions in acoustic plasma waves,[5] ferromagnetic chain[14] and evolutions of Stokes waves.[12,15] This relation is also used as an envelope equation for describing a weakly subcritical bifurcation to counter propagating waves[16] and also accounts for the slow modulations of an oscillatory mode closed to a subcritical bifurcation[17,18] when $Q_3 = Q_4 = 0$. In Eq. (3.8), the first two terms of the rhs are the nonlinear terms while the others represent the nonlinear dispersion.

Using the line parameters (2.2) the spatial dispersion coefficient (3.9) is plotted as a function of k (Fig. 3). We could remark from these graphs that the coefficient P has both positive and negative values whether λ is null or not. When comparing Figs. 3(a)–3(c) we note that the presence of C_s (i.e., for $\lambda \neq 0$) increases the interval of the values of P. In other words, introduction of C_s adds the dispersion in the system. This result will be useful to predict the stability of modulated waves in the network.

IV. MODULATIONAL INSTABILITY

In this section, we research under which conditions a uniform wave train moving along the discrete nonlinear electrical transmission line of Fig. 1 will become unstable to a small perturbation. For this purpose, we use the HONLSE (3.8) derived from the exact equations (2.2) describing the wave propagation in the network. First, we look for solutions of Eq. (3.8) in the form

$$V_{11}(\xi, \tau) = E_0 \exp[i(k_n\xi - \omega_n\tau)], \tag{4.1}$$

where E_0 is a complex constant amplitude. Substitution of (4.1) into Eq. (3.8) yields the nonlinear dispersion law[5]

$$\omega_n = \omega_n(k_n, |E_0|^2) = Pk_n^2 + Q_1|E_0|^2 + Q_2|E_0|^4 + k_n(Q_3 - Q_4)|E_0|^2 \tag{4.2}$$

in which k_n and ω_n are, respectively, the wave number and the angular frequency of the carrier wave. From relation (4.2), the plane wave (4.1) is nonlinear and the principle of superposition is invalid. To investigate the MI[18] of the carrier wave, a small perturbation of (4.1) is taken as follows:[5,19–21]

$$V_{11}(\xi, \tau) = [1 + A(\xi, \tau)]E_0 \exp[i(k_n\xi - \omega_n\tau)], \tag{4.3}$$

where $A(\xi, \tau)$ is a complex quantity. Substituting this solution into (3.8) and linearizing the result with respect to $A(\xi, \tau)$ gives the differential equation

$$\begin{aligned} iA_\tau + P(A_{\xi\xi} + 2ik_nA_\xi) = {} & Q_1(A + A^*)|E_0|^2 + 2Q_2(A + A^*)|E_0|^4 + i(Q_3A_\xi^* + Q_4A_\xi)|E_0|^2 \\ & + k_n(Q_3 - Q_4)(A + A^*)|E_0|^2 \end{aligned} \tag{4.4}$$

in which the asterisk denotes the complex conjugation. Following the idea developed by Parkes,[5] solutions of Eq. (4.4) could be found in the form

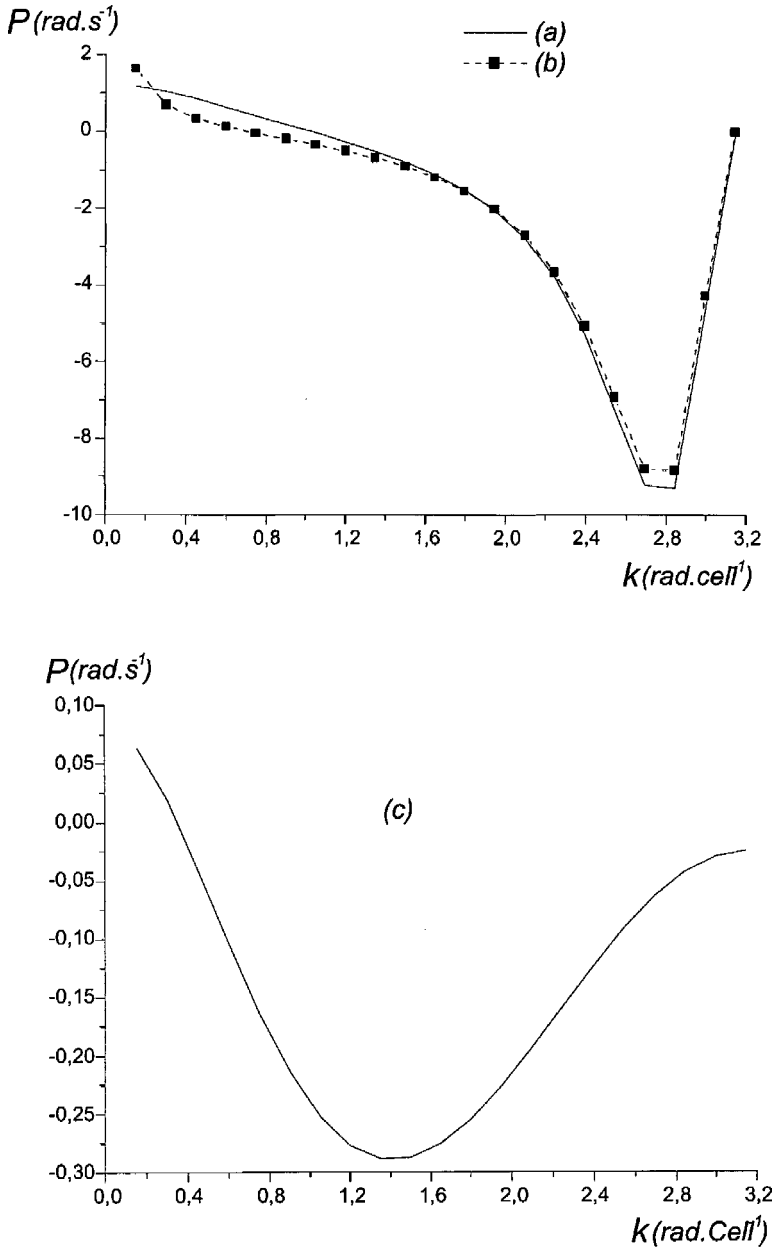

FIG. 3. Dispersive coefficient in terms of the wave number k taken in the Brillouin zone for the line parameters (2.2). (a) Case where $\lambda \neq 0$ and $\omega_0 \neq 0$; (b) case where $\lambda \neq 0$ and $\omega_0 = 0$; (c) case where $\lambda = 0$ and $\omega_0 \neq 0$. These plots show that P admits both positive and negative values and inform that the range values of the dispersion coefficient P increases with the introduction of C_s in the system.

$$A(\xi,\tau) = A_1 \exp[i(l\xi + \Omega\tau)] + A_2^* \exp[-i(l\xi + \Omega * \tau)], \tag{4.5}$$

where l and Ω indicate, respectively, the wave number and the angular frequency of the perturbation. Parameters A_1 and A_2 are complex constants. Introduction of relation (4.5) into Eq. (4.4) yields a dispersion law for the perturbation wave

$$\Omega^2 + 2b\Omega + (b^2 - P^2 l^4 - l^2 Q_3^2 |E_0|^4 - 2cPl^2) = 0, \tag{4.6}$$

which is a second order equation for Ω with real coefficients; the quantities b and c are defined by

$$b = 2k_n lP - lQ_4|E_0|^2 \quad \text{and} \quad c = Q_1|E_0|^2 + 2Q_2|E_0|^4 + k_n(Q_3 - Q_4)|E_0|^2.$$

The MI phenomenon is observed when the angular frequency Ω of the perturbation has a nonzero imaginary part leading to an exponential growth of the amplitude versus time. This situation occurs when the discriminant (Δ) of Eq. (4.6) possesses a negative value ($\Delta<0$) leading up to

$$PQ_1 - r < -\left(\frac{l^2P^2 + Q_3^2|E_0|^4}{2|E_0|^2}\right) < 0 \tag{4.7}$$

and necessarily

$$PQ_1 - r < 0 \tag{4.8}$$

with

$$r = -k_n(Q_3 - Q_4)|E_0|^2 - PQ_2|E_0|^2. \tag{4.9}$$

Relation (4.8) together with (4.9) represents the MI criterion associated to the HONLSE in the electrical transmission line of Fig. 1. We deduce from Eq. (4.7) that the wave number of the perturbation l should be taken in a finite interval namely,

$$0 < l < \frac{|E_0|}{|P|}[2(r - PQ_1) - Q_3^2|E_0|^2]^{1/2}. \tag{4.10}$$

The MI condition (4.8) is function of the nonlinear and dispersive parameters β and λ since it depends on the coefficients of Eq. (3.8) which are related to β and λ. The result (4.8) is more general than the one obtained by Ketchakeu *et al.*[11] during the study of ϕ^4 models. It also generalizes the family criterion for the standard nonlinear Schrödinger (NLS) equations.[18,22] However this criterion is similar to that established by Kakutani and Michihiro[12] when they examine the motion of water waves near the marginal state of instability.

V. EXACT SOLITARY SOLUTIONS

The main purpose of this section is to check whether the discrete nonlinear transmission line under study can support solitary waves. Hence we follow the Pathria and Morris[23] method and set $\tau = Pt$. Therefore, the amplitude wave equation (3.8) takes the form:

$$iV_{11,\tau} + V_{11,\xi\xi} + q_c|V_{11}|^2V_{11} + q_q|V_{11}|^4V_{11} + iq_mV_{11}^2V_{11,\xi}^* + iq_u|V_{11}|^2V_{11,\xi} = 0 \tag{5.1}$$

with $q_c = -Q_1/P$, $q_q = -Q_2/P$, $q_m = -Q_3/P$, and $q_u = -Q_4/P$. At this level, we introduce the following notations:

$$Q_c = q_c, \quad Q_q = q_q + \tfrac{1}{16}(q_u + q_m)(3q_m - 5q_u),$$

$$Q_m = q_m - \tfrac{1}{2}(q_u + q_m) = -\tfrac{1}{2}(q_u - q_m) \quad \text{and} \quad Q_u = q_u - q_m. \tag{5.2}$$

The solutions of Eq. (5.1) strongly depend on the sign of the coefficient[23] Q_q. Two cases can be distinguished. When $Q_q<0$, the solution of Eq. (5.1) is given by

$$V_{11}(\xi,t) = \left(\frac{r_1r_2}{r_1 + (r_1 - r_2)\sinh^2(\chi_0)}\right)^{1/2} \exp[i\phi(\xi,t)] \tag{5.3}$$

in which

$$\phi(\xi,t) = -\left(\frac{q_u+q_m}{4}\right)\sqrt{-3/Q_q}\tanh^{-1}\left(\sqrt{\frac{r_2}{r_1}}\tanh(\chi_0)\right) + \frac{\eta}{2}(\xi-\mu t) + \vartheta_0,$$

with $\chi_0=(-r_1r_2Q_q/3)^{1/2}(\xi-\eta t)+\vartheta_1$. In expressions (5.3), the quantities μ and η denote the speeds of the carrier and envelope waves of V_{11}, respectively; ϑ_0 and ϑ_1 are arbitrary constants. The values of r_1 and r_2 determine the form of this solution. Solitary waves arise in the system if r_1 and r_2 are real, with[23] $r_1>r_2>0$.

On the other hand, if $Q_q>0$, r_1 and r_2 are real with $r_1>0>r_2$, a solitary wave also exists and the corresponding solution for Eq. (5.1) is[23]

$$V_{11}(\xi,t) = \left(\frac{r_1r_2}{r_2+(r_2-r_1)\sinh^2(\chi_0)}\right)^{1/2}\exp[i\phi(\xi,t)] \tag{5.4}$$

with

$$\phi(\xi,t) = -\left(\frac{q_u+q_m}{4}\right)\sqrt{3/Q_q}\tan^{-1}\left(\sqrt{-\frac{r_1}{r_2}}\tanh(\chi_0)\right) + \frac{\eta}{2}(\xi-\mu t) + \vartheta_0,$$

and

$$\chi_0 = (-r_1r_2Q_q/3)^{1/2}(\xi-\eta t) + \vartheta_1.$$

Furthermore, if r_1 and r_2 are real with $r_1>r_2>0$, then the solution is oscillatory and has the following form:[23]

$$V_{11}(\xi,t) = \left(\frac{r_1r_2}{r_1+(r_2-r_1)\cos^2(\chi_1)}\right)^{1/2}\exp[i\phi(\xi,t)], \tag{5.5}$$

where

$$\phi(\xi,t) = -\left(\frac{q_u+q_m}{4}\right)\sqrt{3/Q_q}\tan^{-1}\left(\sqrt{\frac{r_2}{r_1}}\tanh(\chi_1)\right) + \frac{\eta}{2}(\xi-\mu t) + \vartheta_0,$$

and $\chi_1=(r_1r_2Q_q/3)^{1/2}(\xi-\eta t)+\vartheta_1$. From these investigations, we note that the HONLSE possesses solitary wave solutions for both positive and negative values of Q_q.

VI. CONCLUSION

In this paper, we have considered a discrete nonlinear electrical transmission line and examined dynamics of modulated waves. Exploiting the reductive perturbation method, it has been shown in the semidiscrete limit that propagations of modulated wave trains are governed by a modified form of the NLS equation that involves higher orders nonlinearities, i.e., the HONLSE. Through our investigations, it has been obtained that the capacitance C_s adds the linear dispersive effects in the circuit with the consequence that the gap zone is greatly reduced and the range of frequencies for the propagation of the signal has substantially increased given way to more applications of the model.

Based on the obtained amplitude wave equation, we have utilized the Stokes wave analysis to construct a criterion for the MI of a plane wave introduced in the electrical line. It has appeared that the obtained criterion generalizes the family criterion for NLS equations and depends both on the amplitude and wave number of the propagating signal.

Besides this study of the asymptotic behavior of a signal in the network, the Pathria and Morris method has been exploited to show that this discrete nonlinear transmission line can support solitary waves. This last result is of higher importance since it is known that solitons are good waves for the transport of information in some physical systems.

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APPENDIX

The equations of $(\varepsilon^3, e^{0i\theta})$ lead to the potential

$$V_{20} = N_{20}|V_{11}|^2 \quad \text{with } N_{20} = \frac{2\alpha V_g^2}{V_g^2 - u_0^2}. \tag{A1}$$

From the equations of $(\varepsilon, e^{2i\theta})$, we get

$$V_{22} = N_{22}(V_{11})^2, \quad \text{where } N_{22} = \frac{4\alpha\omega^2}{D}. \tag{A2}$$

Terms proportional to $\varepsilon^{5/2}e^{2i\theta}$ and $\varepsilon^3 e^{i\theta}$ yield, respectively, the voltages

$$V_{30} = 0 \quad \text{and} \quad V_{50} = 0. \tag{A3}$$

From the equations of $(\varepsilon^{3/2}, e^{3i\theta})$, we obtain the potential

$$V_{33} = N_{33}(V_{11})^3 \quad \text{in which } N_{33} = \frac{1}{D_1}(18\alpha\omega^2 N_{22} - 9\beta\omega^2) \tag{A4}$$

with

$$D_1 = 9\omega^2(1 + 4\lambda\cos^2(3k/2)) - 4u_0^2\sin^2(3k/2) - \omega_0^2.$$

The equations of $(\varepsilon^3, e^{0i\theta})$ liberate

$$V_{40} = N_{40}|V_{11}|^4 \quad \text{with } N_{40} = \frac{1}{2}N_{20}(N_{20}^2 + 2N_{22}^2) - \frac{\beta}{\alpha}N_{20}(2N_{20} + 3N_{22}). \tag{A5}$$

From the terms proportional to $\varepsilon^2 e^{2i\theta}$, we determine the voltage

$$V_{42} = N_{42}|V_{11}|^2 V_{11}^2 + i\tilde{N}_{42}(V_{11}^2)_\xi \tag{A6}$$

in which the diverse coefficients are defined by

$$N_{42} = \frac{4\omega^2}{D}[2\alpha(N_{33} + N_{20}N_{22}) - 3\beta(N_{20} + 2N_{22})]$$

and

$$\tilde{N}_{42} = \frac{2}{D}[2\omega V_g N_{22}(1 + 4\lambda\cos^2 k) - (u_0^2 + 4\lambda\omega^2)N_{22}\sin k - 2\alpha\omega V_g].$$

Note: There exist other nonzero coefficients that do not contribute in the establishment of the amplitude wave equation (3.8) which characterizes the motion of a signal in the line. Nevertheless, their expressions are found and listed below.

From the equations of $(\varepsilon^2, e^{4i\theta})$, we deduce

$$V_{44} = N_{44}(V_{11})^4 \quad \text{wherein } N_{44} = \frac{1}{D_2}[16\alpha\omega^2(N_{22}^2 + 2N_{33}) - 48\beta\omega^2 N_{22}] \tag{A7}$$

with $D_2 = 16\omega^2(1 + 4\lambda\cos^2(2k)) - 4u_0^2\sin^2(2k) - \omega_0^2$.

The equations of $(\varepsilon^{5/2}, e^{2i\theta})$ help to determine the voltage

$$V_{53} = N_{53}|V_{11}|^2 V_{11}^3 + iN'_{53}(V_{11}^2)_\xi V_{11} + iN''_{53}(V_{11}^3)_\xi \tag{A8}$$

in which the different parameters are given by

$$N_{53} = \frac{18\omega^2}{D_1}[\alpha(N_{42} + N_{44} + N_{20}N_{33}) - \beta(2N_{33} + 2N_{20}N_{22} + 2N_{22}^2)],$$

$$N'_{53} = \frac{6\alpha\omega}{D_1}(3\omega\tilde{N}_{42} - 2V_g N_{22}),$$

and

$$N''_{53} = \frac{1}{D_1}[6\omega V_g N_{33}(1 + 4\lambda \cos^2(3k/2)) - 2(u_0^2 + 9\lambda\omega^2)N_{33}\sin 3k + 6\beta\omega V_g].$$

From the equations of $(\varepsilon^{5/2}, e^{5i\theta})$, we get

$$V_{55} = N_{44}(V_{11})^5 \quad \text{in which } N_{44} = \frac{25\omega^2}{D_3}[2\alpha(N_{44} + N_{22}N_{33}) - 3\beta(N_{22}^2 + N_{33})], \tag{A9}$$

where

$$D_3 = 25\omega^2(1 + 4\lambda \cos^2(5k/2)) - 4u_0^2 \sin^2(5k/2) - \omega_0^2.$$

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Brownian pants and Deligne cohomology

Rémi Léandre[a)]
Institut Elie Cartan, Faculté des Sciences, Université Henry Poincaré, 54000 Vandoeuvre-les-Nancy, France and Centre Emile Borel, Institut Henri Poincaré, Rue Marie Curie, 75231 Paris Cedex 05, France

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We define stochastic pants, and the stochastic parallel transport over them for the Felder–Gawedzki–Kupiainen line bundle over the loop space. It is related to the construction of stochastic integrals, where we cannot use martingale theory in order to define them. We get a stochastic fusion of the two line bundles when the two loops meet. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1847707]

I. INTRODUCTION

In conformal field theory or in string theory (see Refs. 1–3), people look at random applications ψ from a Riemann surface Σ into a Riemannian manifold M endowed with the probability measure:

$$d\mu(\psi) = Z^{-1} \exp[-I(\psi)]dD(\psi), \tag{1.1}$$

where $dD(\psi)$ is the formal Lebesgue measure over the set of maps ψ and $I(\psi)$ the energy of the map ψ. Z is the partition function of the theory such that μ is a probability measure. Z is formally infinite, but physicists regularize Z and the correlators. If Σ has boundaries, let us say exit boundaries which are circle S_i^1 and input boundaries which are circles S_i^2, the amplitude related to the measure (1.1) should realize a map from $\otimes_{\text{output}} H$ into $\otimes_{\text{input}} H$ where H is an Hilbert space associated to the loop space (see Ref. 4).

In the case where the manifold is the linear space R^n, (1.1) is a Gaussian measure, which corresponds to the free field measure. Since in two dimension, the Green kernel associated to the Laplacian has a singularity on the diagonal, the random field lives on random distributions (see Ref. 5). It is difficult to state what is a distribution with values in a curved manifold, because the notion of distribution is linear.

If $\Sigma = [0,1] \times [0,1]$, there is another process indexed by Σ with values in R, which is the Brownian sheet and which is continuous. $(\partial^2 / \partial_s \partial_t)\psi = \eta_{s,t}$ is the white noise over $[0,1] \times [0,1]$. It is a formal Gaussian random field with average 0 and covariance $\langle \eta_{s,t}, \eta_{s',t'} \rangle = \delta_{s,t}(s',t')$ where $\delta_{s,t}$ is the Dirac delta function in (s,t). On Σ, there is a natural order, and it is possible after the work of Cairoli[6] to study the stochastic differential equation in Itô meaning,

$$\delta_{s,t} x_{s,t} = A(x_{s,t}) \delta_{s,t} \psi, \tag{1.2}$$

by using martingale theory, where A is a vector field over R. This gives an example of a non-Gaussian random field parametrized by the square. In the Gaussian case, this gives the Brownian motion over the path space. Doss and Dozzi[7] have studied the formal action which is associated to (1.2), that is they have studied the large deviation theory. Léandre and Russo[8] studied the behavior of the density of the solution $x_{s,t}$ of (1.2) when $(s,t) \to (0,0)$ by using the Malliavin calculus over the Brownian sheet.[9] Norris[10] has succeeded to give a geometrical meaning to (1.2) and has constrained $x_{s,t}$ to live over a curved manifold.

[a)]Present address: Institut de Mathématiques, Faculté des Sciences, Université de Bourgogne, 21000 Dijon, France.

But it is difficult to generalize (1.2) to the case where the world sheet is not the square $[0,1]\times[0,1]$, because (1.2) uses the multiparameter martingale theory, which requests the presence of an order relation on the world sheet.

Airault–Malliavin in a series of papers (some of them are published, for instance, in Refs. 11–14) have constructed the Brownian motion over a loop group. For that, they use the Brownian motion in a Sobolev space with values in the Lie algebra of the group G. This gives a random field from the cylinder $[0,1]\times S^1$ into G. Various works were done later (see Ref. 15 for instance). Fang and Zhang[16] and Léandre[17] have studied the formal action which gives the Brownian motion over a loop group, that is they have performed the large deviation theory.

Infinite dimensional diffusion processes over infinite dimensional manifolds have a long story initiated by Kuo[18] in 1972. The Russian school has studied infinite dimensional processes over infinite dimensional manifolds (see Refs. 19 and 20). Brzezniak–Elworthy[21] have done a general theory of infinite dimensional diffusion processes over infinite dimensional manifolds over $M-2$ Banach spaces. The interest of $M-2$ Banach spaces is that there is a Doob inequality for martingales over them. They apply their theory to the case of the free loop space of a manifold. This produces random cylinders with values in a compact Riemannian manifold, or the Brownian motion with values in the loop space of a Riemannian manifold. The loops are only Hoelder.

Brzezniak–Léandre[22] have extended the construction of Ref. 21 to the case where we consider Brownian pants. The world sheet has two output boundaries and one input boundary. This gives one application from $E_c\otimes E_c$ into E_c, where E_c is the Banach space of continuous functions over the loop space. This means that the Brownian pants are Feller. This gives an approach to one of Segal's axiom of conformal field theory,[4] the Hilbert space of the loop space being replaced by the Banach space of continuous functionals over it.

Our query is to replace this Banach space by a suitable Hilbert space of sections over a suitable line bundle over the loop space.

Line bundle over C^1 loops are highly studied in the literature: they are the purpose of Kac–Moody groups[23,24] or to the works of Brylinsky[25] by starting from the transgression of a 3-form over the manifold M. In these works, the authors suppose that the free loop space is simply connected and constructed the line bundle by using its curvature. Felder–Gawedzki–Kupiainen have a more general approach by using Deligne cohomology of a line bundle over the loop space.[26] If they consider a Riemann surface with boundaries, they show that the Riemann surface realizes a map from the tensor product of the line bundles over the exit boundaries to the tensor product of the line bundles over the input boundaries.

Brzezniak–Léandre[27] have studied the diffusion over C^1-loops and the parallel transport of the Felder–Gawedzki–Kupiainen line bundle over random paths. This realizes an isometry from the Hilbert space of sections of the exit boundary to the Hilbert space of sections of the input boundary, because the parallel transport is an isometry.

We are motivated by two generalizations of this work.

(i) We work over the Hoelder loop space, that is we consider bundles with fibers almost surely defined.
(ii) We consider random pants instead of cylinders.

In the case of random cylinders, they are two possibilities to study line bundles over the loop space and the parallel transport over a path over the loop space.

Léandre[28] considers a C^1 path over the Brownian bridge and a stochastic line bundle over the Brownian bridge (with fibers almost surely defined). He shows that the parallel transport over C^1 paths of an element of the stochastic line bundle is related to multiparameter integrals: it is a classical integral in the time of propagation of the loop and a stochastic integral in the internal time of the loop[25] requested in understanding the stochastic line bundles over the loop space, and therefore in understanding the stochastic Z-valued forms over the loop space. A new stochastic differential Calculus was established in Refs. 28–31 inspired by the considerations of Iglésias,[32] Souriau,[33] and Chen[34] about diffeology. One of the main theorem of Refs. 29 and 31 is that the

stochastic cohomology of Chen–Souriau is equal of the de Rham cohomology of the Hoelder loop space. Therefore a stochastic line bundle (with fiber almost surely defined) over the Brownian bridge is isomorphic to a true line bundle over the Hoelder loop space.

Brzezniak–Léandre[27] consider a diffusion process over the set of C^1 loops in a manifold. The parallel transport of an element of a true line bundle over the C^1 loop space is related to two parameters integrals, the integral in the propagation time of the loop being stochastic and the integral in the internal time of the loop being an ordinary integral.

In this paper, we are concerned by the case where the parallel transport is related to a two-dimensional stochastic integral.

Let us consider the pant Σ. This gives a propagation time of the loop t and if $t \leqslant 1$, an internal time of the loop $s \to x_t(s)$. If $t > 1$, there are two loops, $s \to (x_t^1(s), x_t^2(s))$. The loop $s \to x_t(s)$ is only continuous as well as the two loops $s \to x_t^1(s)$ and $s \to x_t^2(s)$. Although, we can define line integrals over these loop spaces associated to a one form. We can apply the apparatus of Léandre[35] in order to define Felder–Gawedzki–Kupiainen line bundle ξ_t over the random paths $x_t(.)$ for $t \leqslant 1$, with fibers almost surely defined. For $t > 1$, we can define the tensor product of the bundles $\xi_t^1 \otimes \xi_t^2$ over the product of the two loops $x_t^1(.)$ and $x_t^2(.)$ with fibers almost surely defined with respect to the join law of $(x_t^1(.), x_t^2(.))$. Let us remark that $(x_t^1(.), x_t^2(.))$ are not independent.

In $t=1$, where the two loops $(x_1^1(.), x_1^2(.))$ meet in only one loop $x_1(.)$, there is a natural application map π, $(x_1^1(.), x_1^2(.)) \to x_1(.))$ which is the concatenation map. The beautiful properties of Felder–Gawedzki–Kupiainen line bundle imply that $\pi^*(\xi_1) = \xi_1^1 \otimes \xi_1^2$.

The parallel transport in time t is related to the existence of two-dimensional stochastic integrals. We cannot apply martingale theory to define them (we refer to Ref. 36 and references therein and Ref. 37 for analoguous considerations for one-dimensional stochastic integrals for the fractional Brownian motion where we cannot apply the martingale theory and to Ref. 38 for analoguous considerations on the sphere). We can define a stochastic parallel transport from $\xi_2^1 \otimes \xi_2^2$ into $\xi_1^1 \otimes \xi_1^2 = \xi_1$ which is almost surely an isometry and the stochastic parallel transport from ξ_1 over the fiber over the constant loop $s \to x$, because we start from the constant loop. The composite realized a map from a random section of $\xi_2^1 \otimes \xi_2^2$ over C, called $\tau_{0,2}$. We get the following theorem.

Theorem: $\tau_{0,2}$ realizes an isometry from $L^2(\xi_2^1 \otimes \xi_2^2)$ into L^2.

But since $x_2^1(.)$ and $x_2^2(.)$ are not independent, the Hilbert space of sections of $\xi_2^1 \otimes \xi_2^2$ over the product of random loops $(x_2^1(.), x_2^2(.))$ is not the tensor product of Hilbert spaces of sections of the line bundle ξ_2^1 over $x_2^1(.)$ and of L^2 sections of the Hilbert space of sections over $x_2^2(.)$ over ξ_2^2. In some sense, we have replaced the Banach space of continuous functions over the loop space by the Hilbert space of L^2 sections of the Gawedzki–Felder–Kupiainen line bundle over the loop space, but our program failed in part because $x_2^1(.)$ and $x_2^2(.)$ are not independent.

For analysis over loop space, we refer to the two surveys of Léandre.[39,40]

Let us remark that this kind of mechanism of splitting a loop in two loops is very classical in physics. We refer to the survey of Mandelstam[41] about that. Moreover, we are in this work in presence of a $1+1$ dimensional theory, we consider a diffusion process on loop space. The reader interested by a $1+2$ dimensional theory, that is a diffusion process on pants, can see Refs. 42 and 43.

II. CONSTRUCTION OF THE BROWNIAN PANTS

We recall briefly the construction of the Brownian pants of Brzezniak–Léandre.[22]

We consider a compact Riemannian manifold M of dimension d imbedded in R^n isometrically. If $x \in M$, $\Pi(x)$ is the orthogonal projection from R^n into $T_x(M)$. It can be extended to a map from R^n into the linear applications over R^n, which is smooth and have bounded derivatives of all orders. We introduce the Hilbert space $H = H^{1,2}(S^1; R^n)$ of the set of loops in R_n such that

$$\int_0^1 |\gamma(s)|^2 \, ds + \int_0^1 |d/ds\, \gamma(s)|^2 ds = \|\gamma\|^2 < \infty. \tag{2.1}$$

Let $B_t(.)$ be the Brownian motion with values in H.

We can construct it as follows. Let Ψ_s be the linear map from H into R^n defined as follows: $\Psi_s(\gamma(.)) = \gamma(s)$. Since H is an Hilbert space and since Ψ_s is continuous, we get

$$\Psi_s(\gamma(.)) = \int_0^1 \langle \gamma(u), e_s(u)\rangle du + \int_0^1 \langle d/du\ \gamma(u), d/du\ e_s(u)\rangle du, \tag{2.2}$$

$t \to B_t(s)$ is a Brownian motion with covariance $\|e_s(.)\|^2$ (we did as we were working on R in order to simplify the notation, but it is easy to reduce our study to the case of R by looking at the coordinates of Ψ_s). Moreover, if $s \neq s'$, Ψ_s is independent of $\Psi_{s'}$ as a linear map. This shows us that $e_s(.)$ and $e_{s'}(.)$ are independents and that the couple $t \to (B_t(s), B_t(s'))$ realized a nondegenerated Brownian motion over $R^n \times R^n$, although $t \to B_t(s)$ and $t \to B_t(s')$ are not independent. We have $\langle B_t(s), B_t(s')\rangle = t\langle e_s, e_s'\rangle$. Moreover the covariance matrix of $B_t(s)$ and $B_t(s')$ is not degenerated. In others words, we can write

$$B_t(s') = \alpha_1(s,s')B_t(s) + \alpha_2(s,s')B_t(s,s'), \tag{2.3}$$

where $B_t(s,s')$ is independent of $B_t(s)$ and where the two constants in the decomposition (2.3) are not equal to 0.

We can construct the Brownian motion with values in H in a more global setup. Let γ_j be an orthonormal basis of H. Let $B_t(j)$ be some independent R-valued Browian motion. We set

$$B_t(s) = \sum B_t(j)\gamma_j(s). \tag{2.4}$$

This series does not converge in H, but in a bigger space. Namely, we get, if d is the Riemannian distance on the circle $\langle B_t(s) - B_t(s'), B_t(s) - B_t(s')\rangle \leqslant Cd(s,s')$. We deduce, since $(t,s) \to B_t(s)$ is a Gaussian process, that $(t,s) \to B_t(s)$ has almost surely a version which is Hoelder, by Kolmogorov lemma. We can show that

$$\langle B_t(s), B_t(s')\rangle = t\langle e_s, e_{s'}\rangle. \tag{2.5}$$

The family of Stratonovitch equations

$$d_t x_t(s) = \Pi(x_t(s)) d_t B_t(s); \quad x_0(s) = x \tag{2.6}$$

has a meaning. It constitutes a family of Brownian motions over the manifold over M parametrized by the circle (in this work, s will denote the internal time of the loop and t the propagation time of the loop). We recall[17] that $(s,t) \to x_t(s)$ has almost surely a version which is $1/2 - \epsilon$ Hoelder for all ϵ.

Let $s_1 < s_2$ be two times. We constrain the elliptic diffusion $t \to (x_t(s_1), x_t(s_2))$ to be equal at y at time 1.

Let us recall that if we consider an elliptic diffusion $\tilde{y}_t(\tilde{x})$ over a compact manifold $\tilde{M}$, it has a heat kernel $q_t(\tilde{x}, \tilde{y})$ satisfying the estimate

$$\text{grad} \log q_t(\tilde{x}, \tilde{y}) \leqslant C \frac{\tilde{d}(\tilde{x}, \tilde{y})}{t} \tag{2.7}$$

for $\tilde{y}$ close to $\tilde{x}$ for the associated Riemannian metric and the natural Riemannian distance $\tilde{d}$ associated to the elliptic diffusion (see Refs. 44 and 45). Let us recall that if the stochastic differential equation of the elliptic diffusion is given by

$$\mathrm{d}\tilde{y}_t(\tilde{x}) = \sum \tilde{X}_i(\tilde{y}_t(\tilde{x})\mathrm{d}\tilde{w}_t^i + \tilde{X}_0(\tilde{y}_t(\tilde{x})\mathrm{d}t \tag{2.8}$$

over the compact manifold, the bridge between $\tilde{x}$ and $\tilde{y}$ satisfies to the following stochastic differential equation (in Stratonovitch sense):

$$\mathrm{d}\tilde{y}_t(\tilde{x},\tilde{y}) = \sum \tilde{X}_i(\tilde{y}_t(\tilde{x},\tilde{y})(\mathrm{d}\tilde{w}_t^i + \langle \tilde{X}_i(\tilde{y}_t(\tilde{x},\tilde{y}),\ \mathrm{grad}\log q_{1-t}(\tilde{y}_t(\tilde{x},\tilde{y}),\tilde{y})\rangle) + \tilde{X}_0(\tilde{y}_t(\tilde{x},\tilde{y})\mathrm{d}t \tag{2.9}$$

(see Refs. 44 and 45). This means that we transform $\mathrm{d}\tilde{w}_t^i$ into $\mathrm{d}\tilde{w}_t^i + \alpha_t^i\,\mathrm{d}t$ by using the equation (2.9). By the estimate (2.7), we have

$$E\left[\int_0^1 |\alpha_t^i|\mathrm{d}t\right] < \infty. \tag{2.10}$$

We write

$$B_t(s_2) = \alpha(s_1,s_2)B_t(s_1) + \beta(s_1,s_2)B_t(s_1,s_2),$$

$$B_t(s) = \alpha(s_1,s_2,s)B_t(s_1) + \beta(s_1,s_2,s)B_t(s_1,s_2) + \gamma(s_1,s_2,s)B_t(s_1,s_2,s), \tag{2.11}$$

where the Brownian motion $B_t(s_1,s_2,s)$ is independent of the Brownian motions $B_t(s_1)$ and $B_t(s_1,s_2)$. Conditionating by $x_1(s_1)=x_1(s_2)=y$ is nothing else to do the following transformation in (2.11):

$$\begin{aligned}\mathrm{d}\tilde{B}_t(s) = {}& \alpha(s_1,s_2,s)(\mathrm{d}B_t(s_1) + \alpha_t^1(s_1,s_2)\mathrm{d}t) + \beta(s_1,s_2,s)(\mathrm{d}B_t(s_1,s_2) + \alpha_t^2(s_1,s_2)\mathrm{d}t)\\ &+ \gamma(s_1,s_2,s)\mathrm{d}B_t(s_1,s_2,s).\end{aligned} \tag{2.12}$$

We set $\mathrm{d}\tilde{B}_t(s_1)=\mathrm{d}B_t(s_1)+\alpha_t^1(s_1,s_2)\mathrm{d}t$ and $\mathrm{d}\tilde{B}_t(s_2)=\mathrm{d}B_t(s_1,s_2)+\alpha_t^2(s_1,s_2)\mathrm{d}t$. Moreover,

$$\begin{aligned}\mathrm{d}\tilde{B}_t(s') = {}& \alpha(s_1,s_2,s,s')\mathrm{d}\tilde{B}_t(s_1) + \beta(s_1,s_2,s,s')\mathrm{d}\tilde{B}_t(s_2) + \gamma(s_1,s_2,s,s')\mathrm{d}B_t(s_1,s_2,s)\\ &+ \delta(s_1,s_2,s,s')\mathrm{d}B_t(s_1,s_2,s,s'),\end{aligned} \tag{2.13}$$

where $\mathrm{d}B_t(s_1,s_2,s,s')$ is independent of the others processes in (2.13).

Moreover, we have

$$\begin{aligned}|\delta(s_1,s_2,s,s')| &\leqslant C\sqrt{d(s,s')},\\ |\gamma(s_1,s_2,s,s') - \gamma(s_1,s_2,s)| &\leqslant C\sqrt{d(s,s')},\\ |\beta(s_1,s_2,s,s') - \beta(s_1,s_2,s)| &\leqslant C\sqrt{d(s,s')},\\ |\alpha(s_1,s_2,s,s') - \alpha(s_1,s_2,s,s')| &\leqslant C\sqrt{d(s,s')},\end{aligned} \tag{2.14}$$

where $d(s,s')$ is the Riemannian distance over the circle. Let us justify this fact. We have namely

$$\langle B_t(s) - B_t(s'), B_t(s) - B_t(s')\rangle \leqslant Cd(s,s'). \tag{2.15}$$

But this variance is equal to the sum of the square of the left-side hand of (2.14).

Lemma II.1: If $\int_0^1|\alpha_t^i|\mathrm{d}t<K$ (Hypothesis K), we have

$$E[|x_t(s) - x_t(s')|^p]\ |x_1(s_1) = x_1(s_2) = y\ ] \leqslant Cd(s,s')^{p/2}. \tag{2.16}$$

Proof: $x_t(s)-x_t(s')$ satisfies the equality in the Stratonovitch sense,

$$\mathrm{d}x_t(s) - \mathrm{d}x_t(s') = (\Pi(x_t(s)) - \Pi(x_t(s')))\mathrm{d}\tilde{B}_t(s) + \Pi(x_t(s'))(\mathrm{d}\tilde{B}_t(s) - \mathrm{d}\tilde{B}_t(s')). \tag{2.17}$$

By the estimates (2.14) and (Hypothesis K), the result arises by using Burkholder–Davies–Gundy inequality and Gronwall lemma. ■

By using the Kolmogorov lemma (see Ref. 46), we deduce that there exists an Hoelder version of the random field $(t,s)\to x_t(s)$ where we have conditionated by $x_1(s_1)=x_1(s_2)=y$. The loop $s\to x_1(s)$ is splitted in two loops $s\to x_i^1(s)$ and $s\to x_1^2(s)$ starting from y and satisfying the estimates if (Hypothesis K) is satisfied,

$$E[|x_1^1(s) - x_1^1(s')|^p] \leqslant Cd(s,s')^{p/2} \tag{2.18}$$

and

$$E[|x_1^2(s) - x_1^2(s')|^p] \leqslant Cd(s,s')^{p/2}. \tag{2.19}$$

Following the idea of Brzezniak–Léandre,[22] we introduce two others Brownian motion with values in the Hilbert space H $B_t^1(.)$ and $B_t^2(.)$ independent of each other and independent of the first Brownian motion $B_t(.)$. We consider the equations after time 1,

$$d_t x_{t+1}^1(s) = \Pi(x_{t+1}^1(s))\mathrm{d}B_t^1(s), \quad x_1^1(s) = x_1^1(s) \tag{2.20}$$

and

$$d_t x_{t+1}^2(s) = \Pi(x_{t+1}^2(s))\mathrm{d}B_t^2(s), \quad x_1^2(s) = x_1^2(s) \tag{2.21}$$

We have

$$x_{t+1}^1(s) - x_{t+1}^1(s') = x_1^1(s) - x_1^1(s') + \int_0^t (\Pi(x_{1+u}^1(s)) - \Pi(x_{u+1}^1(s'))\ \mathrm{d}B_u^1(s)$$

$$+ \int_0^t \Pi(x_{u+1}^1(s'))(\mathrm{d}B_u^1(s) - \mathrm{d}B_u^1(s')) \tag{2.22}$$

Lemma II.2: If (Hypothesis K) is satisfied, we have

$$E[|x_t^1(s) - x_t^1(s')|^p] \leqslant Cd(s,s')^{p/2} \tag{2.23}$$

and we have

$$E[|x_t^2(s) - x_2^2(s')|^p] \leqslant Cd(s,s')^{p/2}. \tag{2.24}$$

Proof: The result comes from (2.18), (2.19), and (2.15) and from Gronwall lemma (see Refs. 17, 43, and 47 for analoguous statements). ■

Definition II.3: The random pant is constituted for $t\leqslant 1$ by the random field $(t,s)\to x_t(s)$ with the constrain $x_1(s_1)=x_1(s_2)=y$ and for $t>1$ by the couple of diffusion processes $t\to(x_t^1(.),x_t^2(.))$

There are one input boundary at $t=0$ and two output boundaries to the pant $(x_2^1(.),x_2^2(.))$.

III. LINE INTEGRALS

The material of this part and of the following part follows closely the construction of stochastic integrals of Refs. 43, 47, and 48. So we do not give all the details, referring to these references.

We consider a 1 form ω over M conveniently extended in a 1-form over R^n with bounded derivatives of all orders. We consider $t\leqslant 1$. We consider a segment l of S^1. We would like to give a meaning to the stochastic integral $\int_l\langle\omega(x_t(s)),d_s x_t(s)\rangle$. In a second case, we consider $t>1$, and we would like to give a meaning to the two stochastics integrals $\int_l\langle\omega(x_t^1(s)),d_s x_t^1(s)\rangle$ and $\int_l\langle\omega(x_t^2(s)),d_s x_t^2(s)\rangle$. t is the time of the dynamic and s is the internal time of the loop.

We will do the exact treatment for $t=1$, the others case being similar.

Let us come back to the Brownian motion over the Sobolev space given by (2.1). Let us introduce $0 \leqslant s < t \leqslant 1$ and $\Delta s \geqslant 0$ and $\Delta t \geqslant 0$ such that $s + \Delta s \leqslant t \leqslant t + \Delta t \leqslant 1$. Let us compute the covariance of $B_\cdot(s+\Delta s) - B_\cdot(s)$ and of $B_\cdot(t+\Delta t) - B_\cdot(t)$.

For that, let us define $e(s)$ such that for all paths $\gamma(.)$ in the Sobolev space,

$$\gamma(0) = \int_0^1 \langle e(s), \gamma(s) \rangle \mathrm{d}s + \int_0^1 \langle e'(s), \gamma'(s) \rangle \mathrm{d}s, \tag{3.1}$$

$$e(s) = \lambda \exp[-s] + \mu \exp[s] \tag{3.2}$$

for some λ and some μ for $0 \leqslant s \leqslant 1$. Therefore, $e(.)$ is smooth with bounded derivatives over the closed interval $[0,1]$ with $e(0) = e(1)$ and not $e'(0) = e'(1)$. Moreover, using the natural rotational invariance of the norms given by (2.1), we get

$$\gamma(t) = \int_{S^1} \langle e(s-t), \gamma(s) \rangle \mathrm{d}s + \int_{S^1} \langle e'(s-t), \gamma'(s) \rangle \mathrm{d}s. \tag{3.3}$$

This shows us that for the Hilbert structure (2.1),

$$\langle e(.-t-\Delta t) - e(.-t), e(.-s-\Delta s) - e(.-\Delta s) \rangle = e(t+\Delta t - s - \Delta s) - e(t-s-\Delta s) - e(t+\Delta t - s) + e(t-s) = e''(t-s)\Delta t \Delta s + O(\Delta t + \Delta s)^3. \tag{3.4}$$

We can diagonalize $B_\cdot(s_1)$, $B_\cdot(s_2)$, $B_\cdot(s+\Delta s)$, $B_\cdot(t)$, $B_\cdot(t+\Delta t)$. We can find two couples of independent Brownian motion $((w_\cdot(1), w_\cdot(2))$ and $(w_\cdot(3), w_\cdot(4))$ such that

$$B_\cdot(s) = \alpha_1(s_1,s_2,s) B_t(s_1) + \beta(s_1,s_2,s) B_\cdot(s_2) + \gamma(s_1,s_2,s) w_\cdot(1),$$

$$B_\cdot(s+\Delta s) = \alpha_1(s_1,s_2,s,\Delta s) B_\cdot(s_1) + \beta(s_1,s_2,s,\Delta s) B_\cdot(s_2) + \gamma(s_1,2,s,\Delta s) w_\cdot(1) + \delta(s_1,s_2,s,\Delta s) w_\cdot(2), \tag{3.5}$$

$$B_\cdot(s') = \alpha_1(s_1,s_2,s') B_\cdot(s_1) + \beta(s_1,s_2,s') B_t(s_2) + \gamma(s_1,s_2,s') w_\cdot(3),$$

$$B_\cdot(s'+\Delta s') = \alpha_1(s_1,s_2,s',\Delta s') \tilde{B}_\cdot(s_1) + \beta(s_1,s_2,s',\Delta s') B_\cdot(s_2) + \gamma(s_1,s_2,s',\Delta s') w_\cdot(3) + \delta(s_1,s_2,s',\Delta s') w_\cdot(4),$$

$0 \leqslant s + \Delta s \leqslant s' \leqslant s' + \Delta s' \leqslant 1$. $(w_\cdot(1), w_\cdot(2))$ are independent of $(B_\cdot(s_1), B_\cdot(s_2))$. $(w_\cdot(3), w_\cdot(4))$ is independent of $(B_\cdot(s_1), B_\cdot(s_2))$. Moreover, $\alpha_1(s_1,s_2,s) - \alpha_1(s_1,s_2,s,\Delta s) = C(s_1,s_2,s)\Delta s + O(\Delta s)^{3/2}$. $\beta(s_1,s_2,s) - \beta(s_1,s_2,s,\Delta s) = C(s_1,s_2,s)\Delta s + O(\Delta s)^{3/2}$. $\gamma(s_1,s_2,s) - \gamma(s_1,s_2,s,\Delta s) = C(s_1,s_2,s)\Delta s + O(\Delta s)^{3/2}$. We have too the estimate $\delta(s_1,s_2,s,\Delta s) = C(s_1,s_2,s)\sqrt{\Delta s} + O(\Delta s)$. We deduce that $\langle w_\cdot(4), w_\cdot(1) \rangle = O(\sqrt{\Delta t})$, $\langle w_\cdot(4), w_\cdot(2) \rangle = O(\sqrt{\Delta t}\sqrt{\Delta s})$, $\langle w_\cdot(2), w_\cdot(3) \rangle = O(\sqrt{\Delta s})$.

Lemma III.1: Let H_1 be the Hilbert space spanned by $e(s_1)$ and $e(s_2)$ and P be the othogonal projection of H_1 on it. $t \to P(e(t))$ is of finite energy.

Proof: H_1 has an orthonormal basis constituted of linear combinations of $e(s_1)$ and $e(s_2)$. But $t \to \langle e(s_1), e(t) \rangle = e(s_1 - t)$ is of finite energy. The same holds for $t \to \langle e(s_2), e(t) \rangle$. Therefore the result. ■

In the sequel, we will suppose always that (Hypothesis K) is satisfied, we will remove this hypothesis only in the last part.

Since the solution of a stochastic differential equation in Stratonovitch sense is unique in law, we can replace in order to study $x_t(s)$, $x_t(s+\Delta s)$, $x_t(s')$, $x_t(s'+\Delta s')$ the leading Brownian motion by the diagonalization (3.5). If we conditionate by $x_1(s_1) = x_1(s_2) = y$, we replace $B_t(s_1)$ by $\tilde{B}_t(s_1)$, the same operation holding for $B_t(s_2)$.

If we look at the linear equation:

$$d\phi_t(s) = \frac{\partial}{\partial x}\Pi(x_t(s))\phi_t(s)d\tilde{B}_t(s) \tag{3.6}$$

it has a solution bounded in all the L^p independently of s, after doing the conditionating. Moreover $\phi_t^{-1}(s)$ is bounded in all the L^p. We deduce from (3.5) that in law

$$g_t^1(s) = \frac{\partial}{\partial\sqrt{\Delta s}}x_t(s+\Delta s)_{\Delta s=0} \tag{3.7}$$

is solution of the linear equation

$$dg_t^1(s) = \frac{\partial}{\partial x}\Pi(x_t(s))g_t^1(s)d\tilde{B}_t(s) + \Pi(x_t(s))\frac{\partial}{\partial\sqrt{\Delta s}}\delta(s_1,s_2,s,\Delta s)_{\Delta s=0}\,dw_t(2), \tag{3.8}$$

which can be solved by the method of variation of constant[46]

$$g_t^1(s) = \phi_t(s)\int_0^t \phi_u^{-1}(s)\Pi(x_t(u))\frac{\partial}{\partial\sqrt{\Delta s}}\delta(s_1,s_2,s,\Delta s)dw_u(2). \tag{3.9}$$

We deduce that in law

$$x_1(s+\Delta s) = x_1(s) + \sqrt{\Delta s}g_1^1(s) + \Delta s g_1^2(s) + O(\Delta s)^{3/2}. \tag{3.10}$$

In $g_1^2(s)$, there is a double integral in $dw_u(2)$ and a single integral in $dw_u(1)$. Lemma III.1 allows us namely to handle the finite energy terms in $d\tilde{B}_t(s_1)$ and $d\tilde{B}_t(s_2)$, there are of finite energy in s, and appear linearly in $g_1^2(s)$. $g_1^1(s)$ is a linear expression in $dw_u(2)$.

Lemma. III.2: We have the estimate

$$E[f(x_1(s))f(x_1(s'))g_1^1(s)g_1^1(s')] = C(s,s')\sqrt{\Delta s\Delta s'} + O(\sqrt{\Delta s} + \sqrt{\Delta s'})^{3/2}. \tag{3.11}$$

Proof: The proof is very similar to Lemma III.3 of Ref. 48. But before to apply Itô formula and Clark–Ocone formula,[49] we conditionate in $B_\cdot(s_1)$ and $B_\cdot(s_2)$. [The drift in $\tilde{B}_\cdot(s_1)$ and $\tilde{B}_\cdot(s_2)$ is namely $B_\cdot(s_1)$ and $B_\cdot(s_2)$ measurables]. ■

We consider N a big integer, and 2^N and the dyadic subdivision of $[0,1]$ associated to 2^N. We call its elements s_i with $s_i < s_{i+1}$ such that $s_{i+1} - s_i = 2^{-N}$. If $s \in [s_i, s_{i+1}]$, we set

$$x_t^N(s) = x_t(s_i) + \frac{(s-s_i)}{(s_{i+1}-s_i)}(x_t(s_{i+1}) - x_t(s_i)). \tag{3.12}$$

We consider

$$A^N = \int_l \langle\omega(x_1^N(s)), d_s x_1^N(s)\rangle. \tag{3.13}$$

We get the following.

Proposition III.3: When $N\to\infty$, the sequence of random variables A^N tends in L^2 to a random variable called $\int_l\langle\omega(x_1(s)), d_s x^1(s)\rangle$.

Proof: We write

$$A^N = \sum A_i^N = \sum \int_{s_i}^{s_{i+1}} \langle\omega(x_1^N(s)), d_s x_1^N(s)\rangle. \tag{3.14}$$

Let us decompose A_i^N. We write

$$A_i^N = B_i^N + C_i^N \tag{3.15}$$

with

$$B_i^N = \omega(x_1(s_i))\Delta_s x_1^N(s_i) \tag{3.16}$$

and

$$C_i^N = \int_{s_i}^{s_{i+1}} \langle \omega(x_1^N(s)) - \omega(x_1(s_i)), d_s x_t^N(s) \rangle. \tag{3.17}$$

B_i^N will converge to the Itô part of the integral in the Proposition III.3 and C_i^N to the Stratonovitch counterterm in this integral.

First step: Study of ΣB_i^N.

By (3.10), we have

$$B_i^N = \sqrt{\Delta s_i}\omega(x_1(s_i))g_1^1(s_i) + \Delta s_i \omega(x_1(s_i))g_1^2(s_i). \tag{3.18}$$

Let us show that the quantity $\Sigma \Delta s_i \omega(x_1(s_i))g_1^2(s_i)$ converges in L^2. In $g_t^2(s_i)$, there are two terms: the terms with derivatives of order two of $\delta(s_1, s_2, s, \Delta s)$ and the term where derivative of $\alpha(s_1, s_2, s, \Delta s)$, $\beta(s_1, s_2, s, \Delta s)$ and $\gamma(s_1, s_2, \Delta s)$ appear which lead to linear contributions.

The contribution of the finite variational part in $\tilde{B}_1(s_1)$ and in $\tilde{B}_1(s_2)$ is of finite energy in s by Lemma III.1 and does not cause any difficulty. We can see the contribution of the other linear tems in $g_1^2(s_1)$. As a matter of fact, these terms can be handled by the following considerations: if we do not conditionate by $x_1(s_1) = x_1(s_2) = y$, we can write

$$B_\cdot(s) = w_\cdot(1),$$

$$B_\cdot(s + \Delta s) = \alpha(s, \Delta s) w_\cdot(1) + \beta(s, \Delta s) w_\cdot(2), \tag{3.19}$$

where $\alpha(t, \Delta t) = 1 + C(t)(\Delta t) + O(\Delta t)^{3/2}$, we get

$$\alpha_1(s_1, s_2, s, \Delta s) = \alpha_1(s_1, s_2, s) C\alpha(s, \Delta s),$$

$$\beta(s_1, s_2, s, \Delta s) = \beta(s_1, s_2, s)\alpha(s, \Delta s), \tag{3.20}$$

$$\gamma(s_1, s_2, s, \Delta s) = \gamma(s_1, s_2, s)\alpha(s, \Delta s),$$

such that the linear term in g_1^2 are in fact stochastic integrals in $\mathrm{d}B_t(s)$ mutiplied by Δs. This term does not cause any difficulty.

Let us compute the behavior of the quadratic term in $g_1^2(s_i)$. $\Delta s_i g_1^2(s_i)$ modulo a term in $(\Delta s_i)^{3/2}$ behaves as a double Stratonovitch integral $\alpha_\cdot(s_i)$ in $B_\cdot(s_i + \Delta s_i) - B_\cdot(s_i)$.

We refer to Ref. 47, pp. 5539, 5540, and 5541 for details. In order to do the conditionating, we conditionate in addition by $B_\cdot(s_1)$ and by $B_\cdot(s_2)$ with respect of this reference. Moreover, we replace (3.47) in Ref. 47 by the the use of the Itô–Stratonovitch formula of Ref. 50. Let X_t and Y_t be two semimartingales with values in R^n. We would like to solve the stochastic differential equation in the Stratonovitch sense,

$$\mathrm{d}x_t = \Pi(x_t)(\mathrm{d}X_t + \mathrm{d}Y_t). \tag{3.21}$$

We solve first the equation

$$\mathrm{d}y_t = \Pi(y_t)\mathrm{d}Y_t. \tag{3.22}$$

Equation (3.22) has a stochastic flow ϕ and we have $x_t = \phi(z_t)$ where z_t is the solution of the stochastic differential equation

$$\mathrm{d}z_t = \phi_t^* \Pi(z_t)\mathrm{d}X_t \tag{3.23}$$

Let N' a bigger subdivision associate to $2^{N'}$. We suppose in the sequel that $[s_j, s_{j+1}] \subseteq [s_i, s_{i+1}]$. We write

$$\sum \omega(x_t(s_i))\alpha_1(s_i) - \sum \omega(x_t(s_j))\alpha_t(s_j) = \sum \Big(\omega(x_t(s_i)) - \omega(x_t(s_j))\alpha_t(s_j) + \sum \omega(x_t(s_i))\Big) \times \Big(\sum_{[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}]} (\alpha_t(s_i) - \alpha_t(s_j))\Big) \tag{3.24}$$

The first term tends clearly to 0. In the double integral which compose $\alpha_t(s_i)$, we write

$$\mathrm{d}B_\cdot(s_i + \Delta s_i) - \mathrm{d}B_\cdot(s_i) = \sum \mathrm{d}B_\cdot(s_j + \Delta s_j) - \mathrm{d}B_\cdot(s_j) \tag{3.25}$$

and we distribute in the double stochastic integral. The integrand before $B_\cdot(s_i+\Delta s_i)$ is $\widetilde{B}_\cdot(s_i)$ measurable, and continuous in u. Therefore, we can replace the integrand before $B_\cdot(s_i+\Delta s_i) - B_\cdot(s_i)$ by the integrand before $B_\cdot(s_j+\Delta s_j) - B_\cdot(s_j)$. When we distribute over $[s_j, s_{j+1}] \subseteq [s_i, s_{i+1}]$, the term where we take twice the same $[s_j, s_{j+1}]$ cancel with $\alpha_t(s_j)$. Therefore, we must take the sum

$$E_t = \sum_i \sum_{[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}];[s_{j'},s_{j'+1}]\subseteq[s_i,s_{i+1}];j\neq j'} \omega(x_t(s_i)) \int_{0<u<v<t} r_u(s_j) d_u(B(s_j + \Delta s_j) - B(s_j)) r_v(s_{j'}) \mathrm{d}v(B(s_{j'} + \Delta s_{j'}) - B_\cdot(s_{j'})) \tag{3.26}$$

where $r_\cdot(s_j)$ is $B_\cdot(s_j)$ measurable and adapted. Let us show that the previous expression converges to 0.

First, we convert the Stratonovitch integral in Itô integral. Since $\langle B_\cdot(s_j+\Delta s_j) - B_\cdot(s_j), B_\cdot(s_{j'} + \Delta s_{j'}) - B_\cdot(s_{j'})\rangle = c(s_i, s_j)\Delta s_i \Delta s_j + O(\Delta s_i + \Delta s_j)^{3/2}$, this leads to a term in 2^{-N2}. This shows that the finite variational term E_t tends to 0. Let us study the martingale part of E_t and let us study the quadratic variation. This leads to a sum of quadruplets of intervalles $[s_j, s_{j+1}]$.

Let us remark, if we do not conditionate by $x_1(s_1) = x_1(s_2) = y$,

$$\langle B_\cdot(s), B_\cdot(s' + \Delta s') - B_\cdot(s')\rangle = O(\Delta s'), \tag{3.27}$$

if s is not included in the time interval $]s', s' + \Delta s'[$.

Let us suppose that all the elements of the quadruplet $[s_j, s_{j+1}]$ are different. We diagonalize $B_\cdot(s_1)$, $B_\cdot(s_2)$, $B_\cdot(s_{i'})$ and $B_\cdot(s_j)$, $B_\cdot(s_j+\Delta s_j)$ as it was done before. We start from $B_\cdot(s_1)$, $B_\cdot(s_2)$, $B_\cdot(s_i)$, $B_\cdot(s_j)$, and $B_\cdot(s_j+\Delta s_j)$ as before. By using (3.27) and (3.4) and an analoguous of (3.5), we find that the contribution where we have a quadruplet without coincidence is in $2^{-N'4}$. They are $2^{2N}2^{4(N'-N)}$ such contributions. Therefore the total contribution behaves as 2^{-2N}.

If we suppose, they are three different terms, that can come from two cases, the two last terms in the double integral are equal. Therefore we must estimate (where $k \neq j \neq j'$)

$$\int_0^t r_u(s_j)(d_u B(s_j + \Delta s_j) - d_u B(s_j)) \int_0^t r_u(s_{j'})(d_u B_u(s_{j'} + \Delta s_{j'}) - d_u B(s_j)) r_t^2(s_k)\Delta s_k. \tag{3.28}$$

By conditionating as before, this leads to a contribution in $2^{-3N'}$.

Or the two last terms are different. This leads to a contribution where $k \neq k' \neq j$

$$\int_0^t r_u(s_j)(d_u B(s_j + \Delta s_j) - d_u B(s_j))^2 r_t(s_k) r_t(s_{k'})\Delta s_k \Delta s_{k'}. \tag{3.29}$$

By diagonalizing as before, this leads to a contribution in $2^{-3N'}$. This possibility occurs $2^N 2^{3(N'-N)}$. This gives a total contribution which vanishes.

The terms where there are only two $[s_j, s_{j+1}]$ leads to a behavior in $2^{-2N'}$ because it is of the shape

$$\int_0^t r_u(s_j)(dB_u(s_j+\Delta s_j)-d_uB(s_j))^2 r_t(s_k)^2 \Delta s_k. \tag{3.30}$$

The last possibility occurs $2^N 2^{2(N'-N)}$.

This gives a total contribution which vanishes.

We write $\Sigma\sqrt{s_{i+1}-s_i}\omega(x_t(s_i))g_1^1(s_i)=\Sigma B^N(s_i)$. Let us study its convergence. We write

$$C_i = B^N(s_i) - \sum_{[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}]} B_{s_j}^{N'} \tag{3.31}$$

and we would like to show that ΣC_i converges in L^2 to 0.

Let us study the contribution of $E[C_iC_{i'}]$ when $i\neq i'$. We must estimate the quantity

$$E[\omega(x_1(s))g_1^1(s)\omega(x_1(s'))g_1^1(s')] \tag{3.32}$$

if $0\leqslant s\leqslant s+\Delta s\leqslant t\leqslant t+\Delta t\leqslant 1$. We have seen (Lemma III.2) that it behaves as $C(s,t)\sqrt{\Delta s\Delta t}+O(\sqrt{\Delta s}+\sqrt{\Delta t})^{3/2}$. Therefore,

$$\sum_{i\neq i'} E[C_iC_{i'}] \to 2\int_{l\times l} C_2(s,t)\mathrm{d}s\,\mathrm{d}t - 2\int_{l\times l} C(s,t)\mathrm{d}s\,\mathrm{d}t \tag{3.33}$$

which is 0.

Let us estimate $E[C_i^2]$.

We have seen that

$$B^N(s_i) = \omega(x_1(s_i))\Delta x_1(s_i) + O(s_{i+1}-s_i) \tag{3.34}$$

and the remaining term converges as before by the consideration given before. Therefore, it is enough to study the contribution of

$$C_i' = \omega(x_1(s_i))\Delta x_1(s_i) - \sum_{[s_j,s_{j+1}]} \omega(x_1(s_j))\Delta x_1(s_j) = \sum_{[s_j,s_{j+1}]} (\omega(x_1(s_i))-\omega(x_1(s_j))\Delta x_1(s_j). \tag{3.35}$$

We have to study the contribution of $E[|C_i''|^2]$ where

$$C_i'' = \sqrt{s_{j+1}-s_j}\sum_{[s_j,s_{j+1}]} (\omega(x_1(s_i))-\omega(x_1(s_j))g_1^1(s_j). \tag{3.36}$$

In $C_i''^2$, there are two contributions: the contribution where we have twice the same $[s_j,s_{j+1}]$ which leads the expression $\Sigma(s_{j+1}-s_j)O(2^{-N})=(s_{i+1}-s_i)O(2^{-N})$. This leads to a contribution where we sum over all $j\neq j'$.

So we must estimate

$$E[(\omega(x_1(s_i)))-\omega(x_1(s_j))g_1^1(s_j)(\omega(x_1(s_i)))-\omega(x_1(s_{j'}))g_1^1(s_{j'})] = \alpha_{j,j'}. \tag{3.37}$$

This leads to some improvement. Instead of diagonalizing only $B_\cdot(s_1)$, $B_\cdot(s_2)$, $B_\cdot(s_j)$, and $B_\cdot(s_j+\Delta s_j)$ as it was done before in order to get $g_1^1(s_j)$, we will diagonalize $B_\cdot(s_1)$, $B_\cdot(s_2)$, $B_\cdot(s_i)$, $B_\cdot(s_j+\Delta s_j)$, and $B_\cdot(s_j)$ in order to get $g_1^1(s_j)$. We find an expression of $\alpha_{j,j'}$ in

$$o(1/N)\sqrt{\Delta s_j}\sqrt{\Delta s_{j'}}. \tag{3.38}$$

Therefore

$$\sum \alpha_{j,j'} \sqrt{\Delta s_j} \sqrt{\Delta s_{j'}} = 2^{-2N} o(1/N) \tag{3.39}$$

is obtained exactly as in Ref. 47, p. 5542 (3.41), where we conditionate in $B_.(s_1)$ and $B_.(s_2)$ in addition, the drift namely in $\tilde{B}_t(s_1)$ and $\tilde{B}_t(s_2)$ are $B_.(s_1)$ and $B_.(s_2)$ measurables. Therefore, $\Sigma_i E[|C_i''|^2] \to 0$. It remains to see that the error term in (3.34) converges. This arises exactly from the previous considerations, because in the double integrals which appear in $g_1^2(s_j)$, we consider as leading term the double integrals in $d_u B(s_j + \Delta s_j) - d_u B(s_j)$ which are treated as before.

Second step: Let us study the convergence of ΣC_i^N in (3.17). We write

$$C_i^N = \langle \omega'(x_1(s_i)) g_1^1(s_i) g_1^1(s_i) \rangle (s_{i+1} - s_i) + O(\Delta s_i)^{3/2}. \tag{3.40}$$

We use Itô–Stratonovitch formula in order to write $g_1^1(s_i) g_1^1(s_i)$ as a double Stratonovitch integral, and we proceed as before in order to show that

$$\sum (s_{i+1} - s_i) \omega'(x_1(s_i)) g_1^1(s_i) g_1^1(s_i) \tag{3.41}$$

converges in L^2. ■

We consider a more intrinsic approximation of the stochastic integral in the Stratonovitch sense $\int_l \langle \omega(x_1(s)), d_s x_1(s) \rangle$. If $x_1(s_{i+1})$ is close of $x_1(s_i)$, we use the function

$$F_N[s, x_1(s_i), x_1(s_{i+1})] = \exp_{x_1(s_i)} \left[\frac{s - s_i}{s_{i+1} - s_i} (x_1(s_{i+1}) - x_1(s_i)) \right], \tag{3.42}$$

where exp is the Riemannian exponential and $(x_1(s_{i+1}) - x_1(s_i))$ is the unique vector in the tangent space at $x_1(s_i)$ such that $\exp_{x_1(s_i)}[x_1(s_{i+1}) - x_1(s_i)] = x_1(s_{i+1})$. We extend this map conveniently. We get another approximation $\tilde{x}_1^N(s)$.

Theorem III.4: $\int_l \langle \omega(\tilde{x}_1^N(s)), d_s \tilde{x}_1^N(s) \rangle$ converges in L^2 to $\int_l \langle \omega(x_1(s)), d_s x_1(s) \rangle$.

Proof: We have

$$\tilde{x}_1^N(s) = x_1(s_i) + \frac{s - s_i}{s_{i+1} - s_i} (x_1(s_{i+1}) - x_1(s_i)) + O\left(\left(\frac{s - s_i}{s_{i+1} - s_i} \right)^2 (x_1(s_{i+1}) - x_1(s_i))^2 \right). \tag{3.43}$$

Moreover,

$$\int_{s_i}^{s_{i+1}} \frac{(s - s_i)^2}{(s_{i+1} - s_i)^2} O(x_1(s_{i+1}) - x_1(s_i))^2 = O(s_{i+1} - s_i)^2 \tag{3.44}$$

whose sum converges to p. Therefore the result. ■

Remark: We ignore if the stochastic integral of Theorem III.2 is equal to the stochastic integral of Proposition III.1, although the Itô parts in both are equal. In the sequel we will use the stochastic integral of Theorem III.2, because it is more intrinsic.

We can repeat the argument in order to define $\int_l \langle \omega(x_{1+t}^1(s)), d_s x_{1+t}^1(s) \rangle$ and to define the line integral $\int_l \langle \omega(x_{1+t}^2(s)), d_s x_{1+t}^2(s) \rangle$ as limit in L^2 of the deterministic integral for the intrinsic polygonal approximations $\tilde{x}_{1+t}^{1,N}(s)$ or $\tilde{x}_{1+t}^{2,N}(s)$ of $s \to x_{1+t}^1(s)$ or $s \to x_{1+t}^2(s)$.

Theorem III.5: $\int_l \langle \omega(\tilde{x}_{1+t}^{1,N}(s)) d_s \tilde{x}_{1+t}^{1,N}(s) \rangle$ and $\int_l \langle \omega(\tilde{x}_{1+t}^{2,N}(s)), d_s \tilde{x}_{1+t}^{2,N}(s) \rangle$ converges in L^2 to the line integral $\int_l \langle \omega(x_{1+t}^1(s)), d_s x_{1+t}^1(s) \rangle$ and to the line integral $\int_l \langle \omega(x_{1+t}^2(s)), d_s x_{1+t}^2(s) \rangle$.

Remark: If we consider the case where $\omega = df$, Theorem III.5 leads to an Itô–Stratonovitch formula.

IV. INTEGRAL OF A TWO FORM

Let us consider a 2-form ω over M, extended in a 2-form over R^n with bounded derivatives of all orders. Consider a deterministic interval of the circle, and let $\tau \leqslant \tau'$ be two stopping times smaller than 1. We would like to define the integral $\int_\tau^{\tau'} \int_l \omega(d_t x_t(s), d_s x_t(s))$. In order to simplify the exposition, we will take $\tau = 0$ and $\tau' = 1$. Moreover, if we consider two stopping time 1

$\leqslant \tau, \tau' \leqslant 2$, we would like to define the stochastic integrals $\int_\tau^{\tau'} \int_l \omega(d_t x_t^1(s), d_s x_t^1(s))$ and $\int_\tau^{\tau'} \int_l \omega(d_t x_t^2(s), d_s x_t^2(s))$. t is the time of the dynamic, where we can apply martingale theory in order to define the stochastic integral and s is the internal time of the loop where we cannot apply martingale theory in order to define the stochastic integral but the considerations of the previous part.

We still suppose (Hypothesis K) is satisfied.

Since the second case is very similar to the first one, we will consider only the first case. After extending ω over the whole linear space R^n, we consider

$$A^N = \int_0^1 \int_{S^1} \omega(x_t^N(s))(d_t x_t^N(s), d_s x_t^N(s)), \tag{4.1}$$

where we consider the approximation $x_t^N(s)$ of $x_t(s)$ (we take the full circle S^1 instead of the interval l in order to simplify the exposition).

Proposition IV. 1: When $N \to \infty$, A^N tends in L^2 to the double stochastic Stratonovitch integral $\int_0^1 \int_{S^1} \langle \omega(x_t(s)), d_t x_t(s), d_s x_t(s) \rangle$.

Proof: Let us write

$$A^N = \sum_i \int_{[0,1]\times[s_i, s_{i+1}]} \langle \omega(x_t^N(s)), d_t x_t^N(s), d_s x_t^N(s) \rangle = \sum A_i^N. \tag{4.2}$$

Let us decompose A_i^N. We write

$$A_i^N = B_i^N + C_i^N \tag{4.3}$$

with

$$B_i^N = \int_{[0,1]\times[s_i, s_{i+1}]} \langle \omega(x_t^N(s_i)), d_t x_t^N(s_i), d_s x_t^N(s_i) \rangle = \int_{[0,1]} \langle \omega(x_t(s_i)), d_t x_t(s_i), \Delta x_t^N(s_i) \rangle \tag{4.4}$$

and

$$C_i^N = \int_{[0,1]\times[s_i, s_{i+1}]} \langle \omega(x_t^N(s)), d_t x_t^N(s), d_s x_s^N(s) \rangle - B_i^N. \tag{4.5}$$

First step: Study of B_i^N.

In the stochastic integrals which appear in B_i^N, we do the separation in a martingale part and a finite variational part. There are three problems.

The finite variational part in $\widetilde{B}_\cdot(s_1)$ and $\widetilde{B}_\cdot(s_2)$ which can be treat by Lemma III.1.

The second problem arises from a contraction betwee $d_t x_t(s_i)$ and $\Delta x_t(s_i)$, which leads to a term in Δs_i which converge.

The last one comes from the contraction between $\omega(x_t^N(s))$ and $d_t x_t^N(s)$ which leads to a double integral, which is a classical integral in t and which is in s of the type of the stochastic integral treated in Proposition III.2.

In the sequel, δ means that we take the martingale part of the processes considered and the associated Itô integral. So we must to consider only the martingale

$$(B_i^N)' = \int_{[0,1]\times[s_i, s_{i+1}]} \langle \omega(x_t(s_i),\ \delta_t x_t(s_i), \Delta x_t(s_i) \rangle. \tag{4.6}$$

We write as in (3.10) and we get

$$(B_i^N)' = \int_{[0,1]} \langle \omega(x_t(s_i)), \delta_t x_t(s_i), \sqrt{\Delta s_i} g_t^1(s_i) \rangle + \int_{[0,1]} \Delta s_i \langle \omega(x_t(s_i)), \delta x_t(s_i), g_t^2(s_i) \rangle + O(\Delta s_i^{3/2}). \tag{4.7}$$

Let us show that the sum of the second term converges in L^2. Following the notations of the previous part, we must estimate

$$\begin{aligned} &\sum_i \sum_{[s_j,s_{j+1}] \subseteq [s_i,s_{i+1}]} \Delta s_j \left(\int_0^1 \langle \omega(x_t(s_i)), \delta x_t(s_i), g_t^2(s_i) \rangle - \int_0^1 \langle \omega(x_t(s_j)), \delta_t x_t(s_j), g_t^2(s_j) \rangle \right) \\ &= \sum_i \sum_{[s_j,s_{j+1}] \subseteq [s_i,s_{i+1}]} \Delta s_j \left(\int_0^1 \langle \omega(x_t(s_i)), \delta x_t(s_i), g_t^2(s_i) \rangle - \int_0^1 \langle \omega(x_t(s_j)), \delta x_t(s_j), g_t^2(s_i) \rangle \right) \\ &\quad + \sum_i \sum_{[s_j,s_{j+1}] \subseteq [s_i,s_{i+1}]} \Delta s_j \left(\int_0^1 \langle \omega(x_t(s_j)), \delta x_t(s_j), g_t^2(s_i) - g_t^2(s_j) \rangle \right). \end{aligned} \tag{4.8}$$

The first term in (4.8) tends clearly to 0 in L^2. Namely, we can consider in $g_t^2(s_j)$ the linear term, where we consider the finite variation part of $\tilde{B}_\cdot(s_1)$ and of $\tilde{B}_\cdot(s_2)$ which can be treated by Lemma III.1. We can consider the term in $dw_u(1)$ which leads to a term in $dB_u(s_j)$ [see (3.19) and (3.20)]. Let us consider the term in $g_t^2(s)$ which leads to double stochastic integrals. We look at the right bracket of the martingale which is associated and we conclude by the same considerations as in the proof of Proposition III.1, first step [see (3.26)].

Let us study the behavior of the first term in (4.7). We write

$$C_i = \int_{[0,1]} \langle \omega(x_t(s_i)), \delta_t x_t(s_i), \sqrt{\Delta s_i} g_t^1(s_i) \rangle - \sum_{[s_j,s_{j+1}] \subseteq [s_i,s_{i+1}]} \int_0^1 \langle \omega(x_t(s_j)), \delta_t x_t(s_j), \sqrt{\Delta s_j} g_t^1(s_j) \rangle. \tag{4.9}$$

We would like to show that ΣC_i tends in 0 in L^2 when $N \to \infty$. This leads to two types of different contributions.

The contribution of $\Sigma_{i \neq i'} E[C_i C_{i'}]$. We can do as in the previous part in order to estimate the quantity

$$E\left[\int_0^1 \langle \omega(x_u(s)), \delta_u x_u(s), g_u^1(s) \rangle \int_0^1 \langle \omega(x_u(t)), \delta_u x_u(t), g_u^1(t) \rangle \right] = \alpha(s,t). \tag{4.10}$$

As in the previous part, $\alpha(s,t)$ has the asymptotic expansion $\alpha(s,t) = C_2(s,t)\sqrt{\Delta s}\sqrt{\Delta t} + O((\sqrt{\Delta s} + \sqrt{\Delta t})^3)$. In order to see that, we apply Itô formula in order to compute $\alpha(s,t)$ and we use Lemma III.2. This shows us that when $N, N' \to \infty$,

$$\sum_{i \neq i'} E[C_i C_{i'}] \to 2 \int_{S^1 \times S^1} C_2(s,t) ds\, dt - 2 \int_{S^1 \times S^1} C_2(s,t) ds\, dt. \tag{4.11}$$

The contribution of $\Sigma E[C_i^2]$. We can write if $[s_j, s_{j+1}] \subseteq [s_i, s_{i+1}]$,

$$\sqrt{\Delta s_i} \int_0^1 \langle \omega(x_t(s_i)), \delta_t x_t(s_i), g_t^1(s_i) \rangle = \int_0^1 \langle \omega(x_t(s_i)), \delta_t x_t(s_i), \Delta x_t(s_i) \rangle + O(\Delta s_i). \tag{4.12}$$

The remaining term converges in L^2 by the previous considerations. Let us write $\Delta x_t(s_i) = \Sigma \Delta x_t(s_j)$. We must estimate the L^2 norm of

$$D_i = \sum_{[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}]} \left(\int_0^1 \langle \omega(x_t(s_i)), \delta_t x_t(s_i), \Delta x_t(s_j)\rangle - \int_0^1 \langle \omega(x_t(s_j)), \delta_t x_t(s_j), \Delta x_t(s_j)\rangle \right) \tag{4.13}$$

or

$$D_i' = \sum_{[s_j,s_{j+1}]\subseteq[s_i,s_{i+1}]} \left(\int_0^1 \langle \omega(x_t(s_i)), \delta_t x_t(s_i), g_t^1(s_j)\rangle - \int_0^1 \langle \omega(x_t(s_j)), \delta_t x_t(s_j), g_t^1(s_j)\rangle \right). \tag{4.14}$$

We compute $E[(D_i')^2]$ by using Itô formula. This leads to expressions similar to (3.37) to estimate. They can be estimated by the techniques of (3.36)–(3.39),

$$E[(C_i)^2] = (s_{i+1} - s_i) O(2^{-N}), \tag{4.15}$$

after using (3.11) for different times t and t' instead of 1 and a diagonalization of $B_\cdot(s_1), B_\cdot(s_2), B_\cdot(s_j), B_\cdot(s_j+\Delta s_j), B_\cdot(s_{j'}), B_\cdot(s_{j'}+\Delta s_{j'})$.

Second step: study of C_i^N.

We write

$$C_i^N = D_i^N + E_i^N \tag{4.16}$$

with

$$D_i^N = \int_{[0,1]\times[s_i,s_{i+1}]} \langle \omega(x_t^N(s)) - \omega(x_t^N(s_i)), d_t x_t^N(s_i), d_s x_t^N(s)\rangle \tag{4.17}$$

and

$$E_i^N = \int_{[0,1]\times[s_i,s_{i+1}]} \langle \omega(x_t(s_i)), d_t x_t^N(s) - d_t x_t(s_i), d_s x_t^N(s)\rangle. \tag{4.18}$$

We write

$$\omega(x_t^N(s)) - \omega(x_t(s_i)) = \frac{s - s_i}{\sqrt{s_{i+1} - s_i}} g_t^1(s_i) B(x_t(s_i)) + O(s - s_i). \tag{4.19}$$

We write

$$d_t x_t^N(s) = d_t x_t(s_i) + \frac{s - s_i}{\sqrt{s_{i+1} - s_i}} d_t g_t^1(s_i) + O(s - s_i) \tag{4.20}$$

and we write too

$$d_s x_t^N(s) = \frac{\mathrm{d}s}{\sqrt{s_{i+1} - s_i}} g_t^1(s_i) + \mathrm{d}s\, g_t^2(s_i) + \mathrm{d}s\, O(s - s_i). \tag{4.21}$$

The more singular term in D_i^N is

$$\int_{[0,1]\times[s_i,s_{i+1}]} \frac{s - s_i}{s_{i+1} - s_i} \langle g_t^1(s_i) B(x_t(s_i)), d_t x_t(s_i), g_t^1(s_i)\rangle = (s_{i+1} - s_i) \int_0^1 \langle B(x_t(s_i)), d_t x_t(s_i), (g_t^1(s_i))^2\rangle, \tag{4.22}$$

$(g_t^1(s_i))^2$ is a quadratic polynomial in $(g_t^1(s_i))$ and is a product of stochastic integrals. It is by the Itô formula an iterated integral of length 2 which has exactly the same behavior of $g_t^2(s_i)$, and we can apply the same procedures in order to estimate its contribution. Therefore this term converges in L^2.

The more singular term in E_i^N is

$$\int_{[0,1]\times[s_i,s_{i+1}]} \left\langle \omega(x_t(s_i)), \frac{s-s_i}{\sqrt{s_{i+1}-s_i}} d_t g_t^1(s_i), \frac{ds}{\sqrt{s_{i+1}-s_i}} g_t^1(s_i) \right\rangle$$

$$= (s_{i+1}-s_i) \int_0^1 \langle \omega(g_t(s_i)), d_t g_t^1(s_i), g_t^1(s_i) \rangle$$

$$= (s_{i+1}-s_i)(g_1(s_i))^2 \omega(x_1(s_i)) - \int_0^1 (g_t^1(s_i))^2 \omega'(x_t(s_i)) d_t x_t(s_i), \tag{4.23}$$

where $(g_t^1(s_i))^2$ is an homogeneous polynomial of order 2 in its components. We can treat this term as the contribution of $g_t^2(s_i)$. ■

We consider a more intrinsic approximation of $x_t(s)$ between $x_t(s_{i+1})$ and $x_t(s_i)$. As in the previous part, we choose

$$F_N[s, x_t(s_i), x_t(s_{i+1})] = \exp_{x_t(s_i)}\left[\frac{s-s_i}{s_{i+1}-s_i} (x_t(s_{i+1}) - x_t(s_i)) \right] = \tilde{x}_t^N(s) \tag{4.24}$$

and we can show the following theorem.

Theorem IV.2: When $N \to \infty$, the random ordinary two parameter integral $\int_0^1 \int_{S^1} \langle \omega(\tilde{x}_t^N(s)), d_t \tilde{x}_t^N(s), d_s \tilde{x}_t^N(s) \rangle$ tends in L^2 to the stochastic Stratonovitch integral $\int_0^1 \int_{S^1} \langle \omega(x_t(s)), d_t x_t(s), d_s x_t(s) \rangle$.

Remark: We ignore if the double stochastic integral of Theorem IV.2 is equal to the stochastic integral of Proposition IV.1. In the sequel, we will use the version of theorem IV.2, because it is an intrinsic version.

Remark: We have an analoguous theorem when the 2-form ω depends smoothly of a finite dimensional parameter.

V. DELIGNE COHOMOLOGY

In this part, we do not suppose that Hypothesis K is satisfied, but the stochastic integrals we consider are almost surely defined by (2.10).

Let us consider the product of loop spaces $L(M) \times L(M)$. We endow it with the probability law of $(x_2^1(.), x_2^2(.))$ We will construct a line bundle over $L(M) \times L(M)$, by using the arguments of Felder–Gawedzki–Kupiainen.[26] We will not suppose that the loop space is simply connected, because our construction is motivated by Deligne cohomology.[25]

Let O_α be a cover of M by convex contractibles open subsets of M, such that $O_{\alpha_1,\alpha_2} = O_{\alpha_1} \cap O_{\alpha_2}$, $O_{\alpha_1,\alpha_2,\alpha_3} = O_{\alpha_1} \cap O_{\alpha_2} \cap O_{\alpha_3}$ and $O_{\alpha_1,\alpha_2,\alpha_3,\alpha_4} = O_{\alpha_1} \cap O_{\alpha_2} \cap O_{\alpha_3} \cap O_{\alpha_4}$.

Let $g_{\alpha_1,\alpha_2,\alpha_3}$ be a family of smooth functions S^1-valued which are multiplicatively antisymmetric in $\alpha_1, \alpha_2, \alpha_3$ and such that

$$g_{\alpha_1,\alpha_2,\alpha_3} g_{\alpha_0,\alpha_2,\alpha_3}^{-1} g_{\alpha_0,\alpha_1,\alpha_3} g_{\alpha_0,\alpha_1,\alpha_3}^{-1} = 1 \tag{5.1}$$

over $O_{\alpha_0,\alpha_1,\alpha_2,\alpha_3}$.

Also, let $\eta_{\alpha_1,\alpha_2} = -\eta_{\alpha_2,\alpha_1}$ be a smooth real 1-form over O_{α_1,α_2} such that

$$\eta_{\alpha_1,\alpha_2} - \eta_{\alpha_0,\alpha_2} + \eta_{\alpha_0,\alpha_1} = 1/i g_{\alpha_0,\alpha_1,\alpha_2}^{-1} dg_{\alpha_0,\alpha_1,\alpha_2} \tag{5.2}$$

on $O_{\alpha_0,\alpha_1,\alpha_2}$. Finally, we suppose that ω_α is a real 2-form defined on O_α such that

$$\omega_{\alpha_1} - \omega_{\alpha_0} = \mathrm{d}\eta_{\alpha_0,\alpha_1} \tag{5.3}$$

on O_{α_0,α_1}. These data define an element of the second Deligne hypercohomology group of the manifold (see Ref. 25, pp. 250–251). If we look at the 3-form $\mathrm{d}\omega_\alpha = \omega$, they patch together by (5.3) in order to give a closed 3-form ω on M.

Consider a system (l,v) which constitutes a triangulation of the circle S^1 such that b is an edge and $v \in \partial b$ is one of its vertex. To each edge, we associate an element α_b and to each vertex v we associate a number α_v such that the following hold: we consider the set of loops γ such that for each edge $b\,\gamma(b) \subseteq O_{\alpha_b}$ and such for all vertices $\gamma(v) \in O_{\alpha_v}$. This defines an open subset

$$U_{A,\alpha} = \{\gamma : S^1 \to M | \gamma(b) \subseteq O_{\alpha_b}, \gamma(v) \in O_{\alpha_v} \quad \text{for each } (b,v) \in A\}. \tag{5.4}$$

If we consider the product of the loop space, we consider the product $U_{A,\alpha} \times U_{A',\alpha'}$ which constitutes a cover by open subsets of the product of the loop space.

We would like to define a system of transition maps of $(U_{A_1\alpha_1} \times U_{A_1',\alpha_1'}) \cap (U_{A_2,\alpha_2}) \times U_{A_2',\alpha_2'}$. Let us define the refined triangulation of both triangulation A_1 and A_2 by $(b,\overline{v})$, $\overline{v} \in \partial b$, the triangulation A_1 by (b_i,v_i), $v_i \in \partial b_i$ and the second triangulation by (b_2,v_2), $v_2 \in \partial b_2$. Let us set $\alpha_{\overline{b}}^1 = \alpha_{b_1}^1$ and $\alpha_{\overline{b}}^2 = \alpha_{b_2}^2$. If $\overline{v}$ is a vertex of the new triangulation, we set $\alpha_{\overline{v}}^1 = \alpha_{v_1}^1$ if $\overline{v} = v_1$ and $\alpha_{\overline{v}}^1 = \alpha_{b_1}^1$ if $\overline{v}$ is in the interior point of the interval b_1. We define $\alpha_{\overline{v}}^2$ analoguously. The system of transition functionals of the stochastic line bundle over $L(M) \times L(M)$ is defined by

$$\rho = \rho_{A_1,\alpha_1,A_2,\alpha_2}(x_2^1)\rho_{A_1',\alpha_1',A_2',\alpha_2'}(x_2^2), \tag{5.5}$$

where

$$\rho_{A_1,\alpha_1,A_2,\alpha_2}(x_2^1) = \exp\left[i \sum_b \int_{\overline{b}} \eta_{\alpha_{\overline{b}^1}\alpha_{\overline{b}^2}}(d_s x_2^1(s)) \right] \prod_{\overline{v},b,\overline{v} \in \partial b} \frac{g_{\alpha_{\overline{v}}^1 \alpha_{\overline{v}}^2 \alpha_{\overline{b}}^2}}{g_{\alpha_{\overline{v}}^1 \alpha_{\overline{b}}^1 \alpha_{\overline{b}}^2}}(x_2^1(v)) \tag{5.6}$$

and the analoguous formula holds for $\rho_{A_1',\alpha_1',A_2',\alpha_2'}(x_2^2)$. The transition functions are almost surely defined. So we cannot define $\xi = \xi_1 \otimes \xi_2$, but we will follow the lines of Ref. 29 in order to define the Hilbert space of L^2 sections of it.

Definition V.2: A L^2 section of the line bundle $\xi_1 \otimes \xi_2$ over $L(M) \times L(M)$ is a system of functionals over $U_{A,\alpha} \times U_{A',\alpha'}$ $f_{A,\alpha,A,\alpha'}$ submitted to the relations: almost surely, over $(U_{A_1,\alpha_1} \times U_{A_1' \times \alpha_1'}) \cap (U_{A_2,\alpha_2} \times U_{A_2',\alpha_2'})$, we get $f_{A_1,\alpha_1,A_1',\alpha_1'} = \rho f_{A_2,\alpha_2,A_2',\alpha_2'}$. We can define since ρ defined by (5.6) is of modulus 1 the norm of a section $|f|$. We suppose $E[|f|^2] < \infty$ in order to define the space of L^2 sections of $\xi_1 \otimes \xi_2$.

In order this definition has some consistency, we recall that almost surely over $(U_{A_1,\alpha_1} \times U_{A_1',\alpha_1'}) \cap (U_{A_2,\alpha_2} \times U_{A_2',\alpha_2'})$, we get

$$\begin{aligned} &\rho_{A_1,\alpha_1,A_2,\alpha_2}(x_2^1)\rho_{A_2,\alpha_2,A_1,\alpha_1}(x_2^1) = 1, \\ &\rho_{A_1',\alpha_1',A_2',\alpha_2'}(x_2^2)\rho_{A_2',\alpha_2',A_1',\alpha_1'}(x_2^2) = 1, \end{aligned} \tag{5.7}$$

and that on $U_{A_1,\alpha_1} \cap U_{A_2,\alpha_2} \cap U_{A_3,\alpha_3}$, we get almost surely

$$\rho_{A_1,\alpha_1,A_2,\alpha_2}(x_2^1)\rho_{A_2,\alpha_2,A_3,\alpha_3}(x_2^1)\rho_{A_3,\alpha_3,A_1,\alpha_1}(x_2^1) = 1. \tag{5.8}$$

This identity works still for the product of transition functions defined by $\rho_{A_1,\alpha_1,A_2,\alpha_2}(x_2^1)$ $\rho_{A_1',\alpha_1',A_2',\alpha_2'}(x_2^1)$.

In the previous definition, we have supposed that the section is almost surely defined over the product of random loops (x_2^1,x_2^2) and is (x_2^1,x_2^2) measurable. We can suppose that $f_{A,\alpha,A',\alpha'}$ depends from all the random pants, or if we choose $1 \leqslant t \leqslant 2$, $1 \leqslant t \leqslant 2$, it depends from all the paths between t and 2. $f_{A,\alpha,A',\alpha'}$ becomes an element of $L^2(\text{pant}) \otimes L^2(U_{A,\alpha}(x_2^1) \otimes U_{A',\alpha'}(x_2^1))$ and satisfies still to the consistency relations of Definition V.2. We can define the L^2 norm of the section f. This increases the degree of freedom and is done in order to define what is the parallel transport over the random path from (x_2^1,x_2^2) into the path (x_1^1,x_1^2). We will get a section of the bundle over $L_y(M) \times L_y(M)$, $\xi_1 \otimes \xi_2$ for the measure defined by (x_1^1,x_1^2), but with an extra degree of freedom,

that is the path between (x_2^1,x_2^2) to (x_1^1,x_1^2). In order to define the stochastic parallel transport from a random section over $\xi_1\otimes\xi_2$ over (x_2^1,x_2^2) to (x_1^1,x_2^1) along the path $t\to(x_t^1,x_t^2)$, we will use the double integral of the previous part.

Let us divise the time interval[1,2] into the stochastic intervals $[\tau_i,\tau_{i+1}[$ where (x_t^1,x_t^2) over $[\tau_i,\tau_{i+1}[$ the process (x_t^1,x_t^2) lives over some open subset $U_{A,\alpha}\times U_{A',\alpha'}$. We have described the time interval into a finite number of random intervals. Moreover, the times τ_i are stopping times.

Let us suppose that the parallel transport from $(x_{\tau_i}^1,x_{\tau_i}^2)$ to (x_1^1,x_1^2) is well defined. Let us call it $\tau_{1,\tau_i}=\tau_{1,\tau_i}^1\otimes\tau_{1,\tau_i}^2$ (the product formula will be explained by the next considerations). If $t\in[\tau_i,\tau_{i+1}[$, we have

$$\tau_{1,t}=\tau_{1,\tau_i}\left\{\exp\left[\sqrt{-1}\int_{\tau_i}^{t\wedge\tau_{i+1}}\sum_b\omega_{\alpha_b}(d_sx_t^1(s),d_tx_t^1(s))+\sqrt{-1}\sum_{v,b,v\in\partial b}\int_{\tau_i}^{t\wedge\tau_{i+1}}\eta_{\alpha_v,\alpha_b}(d_tx_t^1(v))\right]\right\}$$
$$\otimes\left\{\exp\left[\sqrt{-1}\int_{\tau_i}^{t\wedge\tau_{i+1}}\sum_{b'}\omega_{\alpha_{b'}}(d_sx_t^2(s),d_tx_t^2(s))+\sqrt{-1}\int_{\tau_i}^{t\wedge\tau_{i+1}}\sum_{v',b',v'\in\partial b'}\eta_{\alpha_v,\alpha_b}(d_tx_t^2(v))\right]\right\}. \tag{5.9}$$

Let us remark that by induction the parallel transport is of modulus one (5.9). The rules given in the previous parts of approximation of Stratonovitch integrals allow to state this definition.

Theorem V.3: If f is a section of $L(M)\times L(M)$ for the measure of (x_2^1,x_2^2) and measurable for (x_2^1,x_2^2), $\tau_{1,2}f$ is a section of $\xi_1\otimes\xi_2$ for the measure of (x_1^1,x_2^1) (but in an extended sense, because there are many paths joining (x_2^1,x_2^2) to (x_1^1,x_1^2). Moreover,

$$E[|\tau_{1,2}f|^2]=E[|f|^2]. \tag{5.10}$$

(We refer to Refs. 26 and 27 for analoguous results.)

Let us work in time 1. We consider the product of loop space $L_y(M)\times L_y(M)$ for the measure (x_1^1,x_1^2) and the loop $L(M)$ induced by concatenation of the two loops for the measure induced by x_1. This induces a map π,

$$L_y(M)\times L_y(M)\to L(M) \tag{5.11}$$

which preserves the measure. Over $L_y(M)\times L_y(M)$, we have the stochastic line bundle $\xi_1\otimes\xi_2$ and over $L(M)$ we have the stochastic line bundle ξ defined by the previous considerations for the random loop x_1.

For x_1, we define a triangulation by choosing vertices s_1 and s_2. We have $\gamma(s_1)=\gamma(s_2)=y\in O_{\alpha_y}$. We choose another triangulation (b^1,v^1) where we have chosen s_1 and s_2 among the vertices. For the first triangulation, we suppose $\gamma(b)\subseteq O_{\alpha_b}$ and $\gamma(v)\in O_{\alpha_v}$ where $O_{\alpha_{s_1}}=O_{\alpha_{s_2}}=\overline{O}$ is fixed, and for the second triangulation, we choose $\gamma(b')\subseteq O_{\alpha_{b'}}$ and $\gamma(v')\in O_{\alpha_{v'}}$ where $O_{\alpha_{s_1}}=O_{\alpha_{s_2}}=\overline{O}$ for the same open subset $\overline{O}$ than the first triangulation.

We deduce from the previous triangulation two triangulations of $L_y(M)$ and from the second triangulation two triangulations of $L_y(M)$. The transition map for the big loop space $L(M)$ is given by (5.6) where we replace $d_sx_2^1(s)$ by $d_sx_1(s)$ and $x_2^1(v)$ by $x_1(v)$ for the refined triangulation of the two big triangulations of the big circle. But it is almost surely equal to the product of the two transition functions where we consider the couple of loops $(x_1^1(s),x_2^1(s))$. This shows us that $\xi_1\otimes\xi_2=\pi^*\xi$. This means that a L^2 section of ξ over the random loops x_1 for $L(M)$ corresponds naturally to a L^2 section of $\xi_1\otimes\xi_2$ over $L_x(M)\times L_x(M)$ for the law (x_1^1,x_1^2) and the L^2 norms are conserved. We assimilate $\tau_{1,2}f$ to a section over x_1. Afterwards, we use the stochastic parallel transport from x_1 to x_0 $\tau_{0,1}$. We set $\tilde{f}=\tau_{0,1}\tau_{1,2}f$. Since x_0 is the constant loop $s\to x$, $\tilde{f}$ is a random variable.

Theorem V.4: $E[|\tilde{f}|^2]=E[|f|^2]$.

This comes from the fact that $\tau_{0,1}$ is a random isometry from the stochastic fiber of the bundle over the random loop x_1 to the fiber over the constant loop.

Remark: In order to define the connection form $\omega_{A,\alpha}$ over $U_{A,\alpha}$ of the stochastic bundle, we can consider the formal expression

$$\omega_{A,\alpha}=\sum_b \int_b \omega_{\alpha_b}(\mathrm{d}\gamma_s,X_s)+\sum_{v,b,v\in\partial b}\langle \eta_{\alpha_v,\alpha_b}(\gamma_v),X_v\rangle \tag{5.12}$$

(see Refs. 25–27) which can be treated by using the apparatus of the stochastic Chen–Souriau calculus. The curvature of this stochastic line bundle is the transgression of the 3-form ω, which can be treated by using the stochastic Chen–Souriau calculus, because we have line integrals in $\mathrm{d}_s x_t(s)$ (see Ref. 25), and because we can consider in the part II integral of a one-form which depends on a finite dimensional parameter.

Remark: For analoguous considerations with the measure of physicists, we refer to the work of Tsukuda.[51]

Remark: It is much more simpler to get pants by this procedure than by Dirichlet forms (see Refs. 52–55). The reader interested by various aspects and applications of infinite dimensional processes to physics can see the survey of Albeverio.[55]

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Method of variation of constants for difference equations and its application to the calculation of atomic integrals

J. Zamastil, M. Šimánek, J. Čížek, and L. Skála
Department of Chemical Physics and Optics, Charles University, Faculty of Mathematics and Physics, Ke Karlovu 3, 121 16 Prague 2, Czech Republic and Department of Applied Mathematics, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

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In this paper we extend the method for numerically stable calculation of the atomic integrals suggested in our previous paper for the *S*-states of two-electron atoms to the states with arbitrary total angular momenta. The extension consists in finding numerically stable forms of the solution of difference equations appearing in the calculation of the radial part of the atomic integrals. These equations become for some value of the independent variable homogenous and their solution in that region is described by one of the two linearly independent solutions. Modification of the method of the variation of constants for this special type of linear second order inhomogenous difference equations is suggested and applied. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1849811]

I. INTRODUCTION

This work grew out from the search for a numerically stable method of the solution of linear inhomogenous second order difference equations appearing in the calculation of the radial part of the atomic integrals.[1] Generally, once we know one of the two linearly independent solutions of the homogenous equation, the second solution can be obtained by the method of the reduction of order.[2] The solution of the inhomogenous equation is then obtained by the method of the variation of constants.[2] However, it turns out that for the difference equations appearing in the calculation of the atomic integrals this general well-known procedure is of little use in its standard form. The reason is that these difference equations become for certain values of the independent variable homogenous and their solution in that region is described by one of the two linearly independent solutions. This behavior results from the general formula by several cancellations of large numbers. If these cancellations are left on the computer working, for example, in double precision arithmetics, totally wrong results are obtained.

Therefore, a general method for obtaining a numerically stable solution of this type of difference equation is given in this paper. The method is applied to the special case of difference equations appearing in the calculation of the radial part of the atomic integrals. Thus, the method suggested in our previous paper for the *S*-states of the two-electron atoms is extended here to the states with arbitrary total angular momenta. Since in general there are at most two-electron interactions, these results can be extended to all atoms and more generally to all one-center integrals.

The paper is organized as follows. In Sec. II we briefly summarize the calculation of the atomic integrals via the multipole expansion of Coulomb potential. Here, we proceed along the lines of our previous paper.[1] After integrating out angular degrees of freedom, we use analog of the Wigner–Eckart theorem for the radial functions. This reduces the integration over four radial functions to the integration over two radial functions. Then we write down a generalization of the difference equations for the reduced radial integrals derived in Ref. 1 for the *S*-states to the states of arbitrary total angular momenta of the electrons. The main difference is the fact that for the states of the nonzero total angular momentum the difference equations are inhomogenous. In Sec. III we discuss solutions of these equations. We present results of numerical experiments that show

that the difference equations are in a region where they are homogenous described by just one of the two linearly independent solutions. In Sec. IV we first briefly summarize general methods of the reduction of order and the variation of constants. We modify the method of the variation of constants for the cases when the second of the two linearly independent solutions of homogenous equations is obtained by the method of the reduction of order. The form proposed by us is more suitable for computational purposes. We then turn our attention to the special type of equations appearing in the calculation of the atomic integrals and derive numerically stable forms of their solution. In Sec. V we apply the general method of Sec. IV to the difference equations for the reduced radial integrals and test it for the case of very large quantum numbers. In Sec. VI, a summary of the achieved results and perspectives of their further applications are given. In the Appendix computationally suitable forms of the hypergeometric functions needed in Secs. II and III are given.

II. CALCULATION OF THE ATOMIC INTEGRALS

In this section we derive the difference equations for the reduced radial part of the atomic integrals. The derivation of these equations was given in great detail in Ref. 1 for the *S*-states of two-electron atoms. What is difficult in the extension of the method described in Ref. 1 for the *S*-states to the general state is the *solution* of these difference equations, not their derivation. Therefore, we shall proceed very briefly.

We search for the exact two-electron wave function by the expansion into the symmetry adapted products of the one-electron wave functions

$$|i\rangle = 2^{-(1+\delta_{l_{i1},l_{i2}}\delta_{n_{i1},n_{i2}})/2}[R_{n_{i1},l_{i1}}(r_1)R_{n_{i2},l_{i2}}(r_2)|(l_{i1},l_{i2})L\rangle \pm R_{n_{i2},l_{i2}}(r_1)R_{n_{i1},l_{i1}}(r_2)|(l_{i2},l_{i1})L\rangle]. \tag{1}$$

Here, the states $|(l_1,l_2)L\rangle$ are the eigenfunctions of the square and the third component of the sum of the angular momenta of two electrons

$$|(l_1,l_2)L\rangle = \sum_{m_1=-l_1}^{l_1} (l_1,m_1,l_2,M-m_1|L,M)|l_1,m_1\rangle^{(1)}|l_2,M-m_1\rangle^{(2)}, \tag{2}$$

where $(\,|\,)$ denotes Clebsch–Gordan coefficients. Their explicit form is given, for example, in Refs. 3–5. The radial functions $R_{n,l}$ are eigenfuctions of one of the generators of the so(2,1) algebra[1] and will be described in greater detail later.

A. Multipole expansion

The matrix elements of the Coulomb interaction, i.e., repulsion integrals, are calculated by means of the multipole expansion of the operator r_{12}^{-1},

$$r_{12}^{-1} = \frac{1}{r_>}\sum_{l=0}^{\infty}\left(\frac{r_<}{r_>}\right)^l P_l(\vec{n}_1 \,.\, \vec{n}_2), \tag{3}$$

where $r_< = \min(r_1,r_2)$ and $r_> = \max(r_1,r_2)$, $P_l(x)$ denotes the Legendre polynomials. With the usual definition of the inner product (to avoid confusion we note that the inner product used in Ref. 1 differs from the usual one by the factor r^{-1}) and multipole expansion (3) the matrix elements of the operator r_{12}^{-1} between the states (1) can be written as

$$\langle i|r_{12}^{-1}|j\rangle = 2^{-(\delta_{n_{i1},n_{i2}}\delta_{l_{i1},l_{i2}}+\delta_{n_{j1},n_{j2}}\delta_{l_{j1},l_{j2}})/2}\left[\sum_{l=\max(|l_{i1}-l_{j1}|,|l_{i2}-l_{j2}|)}^{\min(l_{i1}+l_{j1},l_{i2}+l_{j2})} \theta_{l_{i1},l_{i2},l_{j1},l_{j2},l} X^{l_{i1},l_{i2},l_{j1},l_{j2},l}_{n_{i1},n_{i2},n_{j1},n_{j2}}\right.$$
$$\left. \pm \sum_{l=\max(|l_{i1}-l_{j2}|,|l_{j1}-l_{i2}|)}^{\min(l_{i1}+l_{j2},l_{j1}+l_{i2})} \theta_{l_{i1},l_{i2},l_{j2},l_{j1},l} X^{l_{i1},l_{i2},l_{j2},l_{j1},l}_{n_{i1},n_{i2},n_{j2},n_{j1}}\right], \tag{4}$$

where l in the summation increases by 2.

The angular part $\theta_{l_{i1},l_{i2},l_{j1},l_{j2},l}$ corresponds to the matrix elements of the Legendre polynomials $P_l(\vec{n}_1.\vec{n}_2)$ between the coupled states (2),

$$\begin{aligned}\theta_{l_{i1},l_{i2},l_{j1},l_{j2},l} &= \langle (l_{i1},l_{i2})L|P_l(\vec{n}_1\,.\,\vec{n}_2)|(l_{j1},l_{j2})L\rangle \\ &= (-1)^{L+l+l_{i1}-l_{j1}+l_{i2}-l_{j2}}\frac{\sqrt{(2l_{i1}+1)(2l_{i2}+1)(2l_{j1}+1)(2l_{j2}+1)}}{2l+1} \\ &\quad\times W(l_{i1},l_{j1},l_{i2},l_{j2},l,L)(l_{i1},0,l_{j1},0|l,0)(l_{i2},0,l_{j2},0|l,0),\end{aligned} \tag{5}$$

where $W(a,b,c,d;e,f)$ are the so-called Racah coefficients and their explicit form is given, for example, in Refs. 4 and 5. The Clebch–Gordan coefficients $(a,0,b,0|c,0)$ are zero unless a, b, and c satisfy the triangle inequality $|a-b|\leqslant c\leqslant a+b$ and $a+b+c$ is even. This reduces the infinite sum in Eq. (3) to the finite number of terms in Eq. (4).

The radial part of the integration reads

$$\begin{aligned}X^{l_{i1},l_{i2},l_{j1},l_{j2},l}_{n_{i1},n_{i2},n_{j1},n_{j2}} &= \int_0^\infty \mathrm{d}r_1\int_0^\infty \mathrm{d}r_2\, r_1^2 r_2^2 R_{n_{i1},l_{i1}}(r_1)R_{n_{i2},l_{i2}}(r_2)\frac{r_<^l}{r_>^{l+1}}R_{n_{j1},l_{j1}}(r_1)R_{n_{j2},l_{j2}}(r_2) \\ &= \int_0^\infty \mathrm{d}r_1\, R_{n_{i1},l_{i1}}(r_1)R_{n_{j1},l_{j1}}(r_1)r_1^{l+2}\int_{r_1}^\infty \mathrm{d}r_2\, R_{n_{i2},l_{i2}}(r_2)R_{n_{j2},l_{j2}}(r_2)r_2^{-l+1} \\ &\quad+\int_0^\infty \mathrm{d}r_1\, R_{n_{i1},l_{i1}}(r_1)R_{n_{j1},l_{j1}}(r_1)r_1^{-l+1}\int_0^{r_1} \mathrm{d}r_2\, R_{n_{i2},l_{i2}}(r_2)R_{n_{j2},l_{j2}}(r_2)r_2^{l+2}.\end{aligned} \tag{6}$$

B. Reduction of the radial integrals

Using the analog of the Wigner–Eckart theorem for so(2,1) algebra[1] we can write the integrals over four radial functions as a linear combination of the integrals over two radial functions

$$\begin{aligned}X^{l_{i1},l_{i2},l_{j1},l_{j2},l}_{n_{i1},n_{i2},n_{j1},n_{j2}} &= 2^{-2}A^{l_{i1},l_{j1}}_{n_{i1},n_{j1}}A^{l_{i2},l_{j2}}_{n_{i2},n_{j2}}\sum_{n_1=-1}^{n_{i1}+n_{j1}-l_{i1}-l_{j1}-2} c^{l_{i1},l_{j1}}_{n_{i1},n_{j1},n_1}\sum_{n_2=-1}^{n_{i2}+n_{j2}-l_{i2}-l_{j2}-2} c^{l_{i2},l_{j2}}_{n_{i2},n_{j2},n_2} \\ &\quad\times \tilde{Q}^{l_{i1}+l_{j1},l_{i2}+l_{j2},l}_{n_{i1}+n_{j1}-1-n_1,n_{i2}+n_{j2}-1-n_2},\end{aligned} \tag{7}$$

where the multiplicative factor $A^{l_i,l_j}_{n_i,n_j}$ equals

$$A^{l_i,l_j}_{n_i,n_j} = \frac{2^{1-n_i-n_j}(n_i+n_j-l_i-l_j-2)!(n_i+l_i+n_j+l_j)!}{(n_i-l_i-1)!(n_j-l_j-1)!}\sqrt{\frac{(n_i-l_i-1)!}{(n_i+l_i)!}}\sqrt{\frac{(n_j-l_j-1)!}{(n_j+l_j)!}}. \tag{8}$$

The coefficients $c^{l_i,l_j}_{n_i,n_j,n}$ of the linear combination read

$$c^{l_i,l_j}_{n_i,n_j,n} = C^{l_i,l_j}_{n_i,n_j,n} - \frac{(n_i+n_j-l_i-l_j-2-n)}{(n_i+n_j+l_i+l_j-n-1)}C^{l_i,l_j}_{n_i,n_j,n+1}, \tag{9}$$

where the coefficients $C^{l_i,l_j}_{n_i,n_j,n}$ are given as

$$C^{l_i,l_j}_{n_i,n_j,n} = \frac{F(-n_i+l_i+1,-n;-n_i-n_j+l_i+l_j+2;2)F(-n_i-l_i,-n;-n_i-n_j-l_i-l_j;2)}{(n_i+l_i+n_j+l_j-n-1)!n!} \tag{10}$$

for $n\geqslant 0$ and equal zero otherwise. Here, $F(\alpha,\beta;\gamma;z)$ denotes the hypergeometric function (see, e.g., Refs. 6–8). We note that Eq. (43) in Ref. 1 is incorrect.

$\tilde{Q}^{L_1,L_2,l}_{N_1,N_2}$ denotes the integrals over two radial functions

$$\tilde{Q}^{L_1,L_2,l}_{N_1,N_2} = \tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2} + \tilde{Q}^{-,L_1,L_2,l}_{N_1,N_2}. \tag{11}$$

Here,

$$\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2} = \int_0^\infty \mathrm{d}r_1\, \tilde{R}_{N_1,L_1}(2r_1) r_1^{l+1} \int_{r_1}^\infty \mathrm{d}r_2\, \tilde{R}_{N_2,L_2}(2r_2) r_2^{-l} \tag{12}$$

and

$$\tilde{Q}^{-,L_1,L_2,l}_{N_1,N_2} = \int_0^\infty \mathrm{d}r_1\, \tilde{R}_{N_1,L_1}(2r_1) r_1^{-l} \int_0^{r_1} \mathrm{d}r_2\, \tilde{R}_{N_2,L_2}(2r_2) r_2^{l+1}, \tag{13}$$

where $\tilde{R}_{N,L}(r)$ differs from $R_{N,L}(r)$ by the normalization factor

$$\tilde{R}_{N,L}(r) = 2\sqrt{\frac{(N+L)!}{(N-L-1)!}} R_{N,L}(r). \tag{14}$$

We note that due to the selection rules for the Clebsch–Gordan coefficients mentioned earlier the difference $|L_1 - L_2|$ is always even. Moreover, the sum $L_1 + L_2 + l$ must be even as well.

C. Difference equations for the reduced integrals

Proceeding in complete analogy with the considerations made in Ref. 1 we obtain the following difference equations for the integrals $\tilde{Q}^{\pm,L_1,L_2,l}_{N_1,N_2}$,

$$(N_2 - L_2)\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2+1} - (N_2 + L_2)\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2-1} - 2l\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2} = -p^{L_1,L_2}_{N_1,N_2} \tag{15}$$

and

$$(N_1 - L_1)\tilde{Q}^{+,L_1,L_2,l}_{N_1+1,N_2} - (N_1 + L_1)\tilde{Q}^{+,L_1,L_2,l}_{N_1-1,N_2} + 2(l+1)\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2} = p^{L_1,L_2}_{N_1,N_2}. \tag{16}$$

The values of $\tilde{Q}^{-,L_1,L_2,l}_{N_1,N_2}$ are obtained from the relation[1]

$$\tilde{Q}^{-,L_1,L_2,l}_{N_1,N_2} = \tilde{Q}^{+,L_2,L_1,l}_{N_2,N_1}. \tag{17}$$

Here, the right-hand side of equations $p^{L_1,L_2}_{N_1,N_2}$ equals

$$p^{L_1,L_2}_{N_1,N_2} = \int_0^\infty \mathrm{d}r\, r^2 \tilde{R}_{N_1,L_1}(2r)\tilde{R}_{N_2,L_2}(2r). \tag{18}$$

Using the explicit form of the radial functions,[9]

$$\tilde{R}_{n,l}(r) = 2^2 e^{-r}(2r)^l L^{2l+1}_{n-l-1}(2r), \tag{19}$$

and the expression for the generalized Laguerre polynomials (see, e.g., Refs. 6–8)

$$L^\alpha_K(r) = \frac{1}{K!} e^r r^{-\alpha} \frac{d^K}{\mathrm{d}r^K}(e^{-r} r^{K+\alpha}), \tag{20}$$

we obtain for $L_1 > L_2 + 1$ integrating by parts (see, e.g., Ref. 5),

$$p_{N_1,N_2}^{L_1,L_2} = \frac{(L_1+L_2+2)!}{2} \sum_{q=\max(0,N_2-L_1-2)}^{\min(N_1-L_1-1,N_2-L_2-1)} (-1)^{N_2-L_2-1-q} \times \binom{N_1-L_2-q-3}{L_1-L_2-2} \binom{L_1+L_2+2+q}{L_1+L_2+2} \binom{L_1-L_2+1}{N_2-L_2-1-q} \tag{21}$$

for $N_2 \leqslant N_1+1$ and

$$p_{N_1,N_2}^{L_1,L_2} = 0 \tag{22}$$

otherwise. The values of $p_{N_1,N_2}^{L_1,L_2}$ for $L_2 > L_1+1$ are obtained from the obvious symmetry $p_{N_1,N_2}^{L_1,L_2} = p_{N_2,N_1}^{L_2,L_1}$, see Eq. (18).

Using difference equations (15) and (16) the integrals are reduced to the integrals over nodeless functions that can be calculated analytically,[1]

$$\tilde{Q}_{L_1+1,L_2+1}^{+,L_1,L_2,l} = 2^{-1}(L_1+L_2+1)!F(1,-L_2+l;-L_1-L_2-1;2). \tag{23}$$

The difference equations (15) and (16) were programmed in MAPLE in form of the recursive algorithm and solved both in rational and 16 digit arithmetics. From these numerical experiments we found that for large quantum numbers N_1, N_2, L_1, and L_2 numerical instabilities appear. Moreover, after some time the recursive algorithm took so much computer memory that further computation was not feasible.

Therefore, we search for the explicit solution of Eqs. (15) and (16). This is done in the following section.

III. SOLUTION OF DIFFERENCE EQUATIONS

In this section we discuss the explicit solution of Eqs. (15) and (16). We argue that the method of variation of constants cannot be used in its standard form and discuss the result of our numerical experiments. These experiments show that Eqs. (15) and (16) are in the region where they are homogenous described by just one of the two linearly independent solutions.

A. The extension of the method given in Ref. 1

In our previous paper[1] we solved Eqs. (15) and (16) for the *S*-states. It follows from the properties of the Clebsch–Gordan coefficients that we must consider the only case $L_1=L_2=L$. In such a case the situation is simplified by virtue of the fact that the right-hand side $p_{N_1,N_2}^{L,L}$ vanishes whenever $|N_1-N_2|>1$.[1] That means that Eqs. (15) and (16) are for most of the values N_1 and N_2 homogenous. Therefore, it was sufficient to find two linearly independent solutions (fundamental system) of homogenous equations (15) and (16) for $l<L$. The two linearly independent solutions of homogenous equation (15) are

$$a_{N_2} = (-1)^{N_2-L_2-1}F(N_2-L_2,-L_2+l;-2L_2;2) \tag{24}$$

and

$$b_{N_2} = F(N_2-L_2,-L_2-l;-2L_2;2). \tag{25}$$

The two linearly independent solutions of the homogenous equation (16) are

$$a_{N_1} = F(N_1-L_1-1,-L_1+l+1;-2L_1;2) \tag{26}$$

and

$$b_{N_1} = (-1)^{N_1-L_1-1} F(N_1 - L_1, -L_1 - l - 1; -2L_1, 2). \tag{27}$$

For $l=L$, behavior of Eqs. (15) and (16) was so simple that it was possible to guess the result directly from the numerical analysis.

The task of solving Eqs. (15) and (16) is therefore twofold.

First, to determine two linearly independent solutions of homogenous equations (15) and (16) in the cases when $l=\min(L_1,L_2)$. In these cases solutions are not hypergeometric functions. In the Appendix we give a method for finding the solution of Eqs. (15) and (16) in terms of the power series in N_1 or N_2. For $l<\min(L_1,L_2)$ we obtain in this way an alternative expression for the hypergeometric functions. For $l=\min(L_1,L_2)$ this method yields at least one of the two linearly independent solutions. The second solution is found by the method of the reduction of order described in Sec. IV A below.

Second, the fundamental system is used for the solution of inhomogenous equations by the method of the variation of constants. One possibility is to apply this method to Eq. (16) and fix constants on the values $\tilde{Q}^{+,L_1,L_2,l}_{L_1+1,N_2}$ and $\tilde{Q}^{+,L_1,L_2,l}_{L_1+2,N_2}$. Then we apply the method first to Eq. (15) for $N_1=L_1+1$ and fix constants on the values of $\tilde{Q}^{+,L_1,L_2,l}_{L_1+1,L_2+1}$ and $\tilde{Q}^{+,L_1,L_2,l}_{L_1+1,L_2+2}$. Second, we apply the method to Eq. (16) for $N_1=L_1+2$ and fix constants on the values of $\tilde{Q}^{+,L_1,L_2,l}_{L_1+2,L_2+1}$ and $\tilde{Q}^{+,L_1,L_2,l}_{L_1+2,L_2+2}$. Such solution, however, is neither fast nor numerically stable. The reason is that solution of Eqs. (15) and (16) is simplified by virtue of the fact that these equations become homogenous for $L_1<L_2$ and $N_1>N_2+1$ or $L_1>L_2$ and $N_2>N_1+1$, see Eq. (22). Further simplifications were found from numerical experiments given below. All these simplifications must be carefully examined and taken into account to get numerically stable formulas.

B. Numerical experiments

We found that Eq. (15) can be for $L_1>L_2$ and $N_2>N_1+1$ described by just one of the two linearly independent solutions,

$$Q^{+,L_1,L_2,l}_{N_1,N_2} = K(N_1,L_1,L_2,l) a_{N_2}, \tag{28}$$

where a_{N_2} is given by Eq. (24). This equation holds for $l<L_2$. For $l=L_2$ the dependence of $Q^{+,L_1,L_2,L_2}_{N_1,N_2}$ on N_2 can be described as

$$Q^{+,L_1,L_2,L_2}_{N_1,N_2} = K(N_1,L_1,L_2)(-1)^{N_2-L_2-1}. \tag{29}$$

Equation (16) behaves in the same way for $L_2>L_1$ and $N_1>N_2+1$,

$$Q^{+,L_1,L_2,l}_{N_1,N_2} = K(N_2,L_1,L_2,l) a_{N_1}, \tag{30}$$

where a_{N_1} is given by Eq. (26). This equation holds for $l<L_1$. For $l=L_1$ and $N_1>N_2$ we found

$$Q^{+,L_1,L_2,L_1}_{N_1,N_2} = 0. \tag{31}$$

These results show that Eq. (15) is for $L_1>L_2$ and $N_2>N_1+1$ described by just *one* of the two linearly independent solutions. Equation (16) behaves in this way for $L_1<L_2$ and $N_1>N_2+1$. A consequence of this is that although Eqs. (15) and (16) are three term recursion relations we need in the case of Eq. (15) for $L_1>L_2$ and in the case of Eq. (16) for $L_1<L_2$ just *one* initial condition instead of two. In the case of Eq. (16) for $L_1<L_2$ and $l=L_1$ we do not need initial conditions at all. From numerical experiments given in Sec. V below, we were able to determine these initial conditions, that means to determine behavior of $\tilde{Q}^{+,L_1,L_2,l}_{N_1,L_2+1}$ for $L_1>L_2$ and $\tilde{Q}^{+,L_1,L_2,l}_{L_1+1,N_2}$ for $L_1<L_2$ and $l<L_1$.

This simplifies the situation tremendously because it means that *instead of solving both Eqs. (16) and (15) simultaneously, we must solve only Eq. (16) for $L_1<L_2$ and Eq. (15) for $L_1>L_2$.*

As it is clear from the above discussion we need modification of the method of the variation of constants for the case when one of the solutions is obtained by the method of the reduction of order [the case $l=\min(L_1,L_2)$] and for special types of equations when for some value of independent variable equations become homogenous and their solution in that region is described by one of the two linearly independent solutions [Eq. (16) for $L_1<L_2$ and Eq. (15) for $L_1>L_2$]. A general theory of the variation of constants for these cases is given in the following section.

IV. GENERAL THEORY

In this section a general modification of the method of variation of constants is described. We consider general linear second order inhomogenous difference equations for the discrete function f_n,

$$f_{n+1} + q_n f_n + r_n f_{n-1} = s_n. \tag{32}$$

We assume that $f_n=0$ for $n<L+1$ where L is integer and that $s_n=0$ for all $n>M+1$. Equation (15) is obtained from this general equation by setting $n=N_2$, $L=L_2$, $M=N_1$, and $f_{N_2}=\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2}$. Equation (16) is obtained from this general equation by setting $n=N_1$, $L=L_1$, $M=N_2$, and $f_{N_1}=\tilde{Q}^{+,L_1,L_2,l}_{N_1,N_2}$. With these assignments we have for both cases

$$r_n = -\frac{n+L}{n-L}. \tag{33}$$

We first show the method of the reduction of order. This is not new, but for the sake of further considerations we describe it in greater detail. Then we summarize the method of the variation of constants and modify it for the cases when one of the solutions was obtained by the reduction of order and for special types of equations appearing in the calculation of atomic integrals.

A. Reduction of order

Let a_n be a solution of the homogenous equation

$$a_{n+1} + q_n a_n + r_n a_{n-1} = 0. \tag{34}$$

The second linearly independent solution can be found by the method of the reduction of order. We search for it in the form

$$b_n = (x_n - x_L)a_n. \tag{35}$$

Inserting it into homogenous equation (32) (with $s_n=0$) and using Eq. (34) we obtain after some manipulation

$$d_{n+1} = r_n \frac{a_{n-1}}{a_{n+1}} d_n, \tag{36}$$

where

$$d_n = x_n - x_{n-1}. \tag{37}$$

Considering the last equation successively for descending n we get

$$x_j - x_n = \sum_{i=n+1}^{j} d_i. \tag{38}$$

Considering Eq. (36) successively for descending n we get

$$d_n = \prod_{k=n-m}^{n-1} r_k \frac{a_{n-m}a_{n-m-1}}{a_n a_{n-1}} d_{n-m}. \tag{39}$$

Since $a_n=0$ for $n<L+1$ we set $n-m-1=L+1$ in the last equation. Then we obtain for d_n,

$$d_n = \frac{\prod_{k=L+2}^{n-1} r_k}{a_n a_{n-1}} a_{L+2}a_{L+1}d_{L+2}. \tag{40}$$

Inserting this equation into Eq. (38) we get finally

$$x_j - x_n = a_{L+2}a_{L+1}d_{L+2} \sum_{i=n+1}^{j} \frac{\prod_{k=L+2}^{i-1} r_k}{a_i a_{i-1}}. \tag{41}$$

B. Variation of constants

Having two linearly independent solutions a_n and b_n of the homogenous equation a general solution of the inhomogenous equation (32) is obtained by the method of variation of constants[2]

$$f_n = c_1 a_n + c_2 b_n + \sum_{j=L+2}^{n-1} T_j (b_j a_n - a_j b_n). \tag{42}$$

Here, T_j denotes the ratio

$$T_j = \frac{s_j}{W_j}, \tag{43}$$

where W_j is the Wronskian of the solutions

$$W_j = a_{j+1}b_j - a_j b_{j+1}. \tag{44}$$

The constants c_1 and c_2 in Eq. (42) are fixed by the initial values f_{L+1} and f_{L+2}.

For further considerations we derive an alternative form of the Wronskian W_j, see also Ref. 2. Inserting b_j from Eq. (35) we rewrite Eq. (44) into the form

$$W_j = -a_{j+1}a_j(x_{j+1} - x_j). \tag{45}$$

Inserting the difference $x_{j+1}-x_j$ from Eq. (41) into the last equation we obtain

$$W_j = -a_{L+2}a_{L+1}d_{L+2} \prod_{k=L+2}^{j} r_k. \tag{46}$$

Since

$$W_{L+1} = -a_{L+2}a_{L+1}d_{L+2} \tag{47}$$

we can write

$$W_j = W_{L+1} \prod_{k=L+2}^{j} r_k. \tag{48}$$

By means of Eq. (47) we can rewrite also Eq. (41) into the form

$$x_j - x_n = -W_{L+1} \sum_{i=n+1}^{j} \frac{\prod_{k=L+2}^{i-1} r_k}{a_i a_{i-1}}. \tag{49}$$

We note that, quite generally, formula (42) can be set into an alternative form. Inserting b_n from Eq. (35) we get

$$f_n = a_n[c_1 + c_2(x_n - x_L) + \sum_{j=L+2}^{n-1} T_j a_j (x_j - x_n)], \tag{50}$$

where the difference $x_j - x_n$ is given by Eq. (49). This form of the solution is likely to be less numerically unstable than the form (42), especially in the cases where one of the solutions was obtained by the method of the reduction of order. The reason is that in Eq. (42) we subtract the numbers $b_j a_n$ and $a_j b_n$. Inserting b_j from Eq. (35) we see that we subtract in fact $a_j a_n (x_j - x_L)$ and $a_j a_n (x_n - x_L)$. These two numbers can be very large especially for large n and j. Therefore their subtraction can cause a loss of significant digits. The advantage of Eq. (50) is that we directly calculate the *result* of the subtraction.

C. Special type of equations

Until now, our considerations were quite general. Now we turn to the special type of Eq. (32) for which $s_n = 0$ for all $n > M+1$ where M is integer and the solution of Eq. (32) in this region is fully described by just *one* of the two linearly independent solutions of the homogenous equation

$$f_n = K a_n, \tag{51}$$

where K is independent on n. Comparing Eqs. (50) and (51) we get

$$K = c_1 + (x_n - x_L)c_2 + \sum_{j=L+2}^{M+1} T_j a_j (x_j - x_n) \tag{52}$$

for arbitrary $n > M+1$. Since this equation holds for $n > M+1$ independently on the value of n we get

$$c_1 - x_L c_2 + \sum_{j=L+2}^{M+1} T_j a_j x_j = K \tag{53}$$

and

$$c_2 - \sum_{j=L+2}^{M+1} T_j a_j = 0. \tag{54}$$

The last two equations are a source of numerical instabilities if constants c_1 and c_2 are determined from the initial values f_{L+1} and f_{L+2}. To avoid these instabilities *we use Eqs. (53) and (54) as equations determining constants* c_1 *and* c_2. If we do so and insert the result into Eq. (50) we obtain

$$f_n = a_n \left[K - \sum_{j=n}^{M+1} T_j a_j (x_j - x_n) \right]. \tag{55}$$

Considering this equation for $n = L+1$ we determine the constant K,

$$K = \frac{f_{L+1}}{a_{L+1}} + \sum_{j=L+1}^{M+1} T_j a_j (x_j - x_{L+1}). \tag{56}$$

Inserting this back into Eq. (55) we obtain finally

$$f_n = a_n \left[\frac{f_{L+1}}{a_{L+1}} + \sum_{j=L+2}^{n-1} T_j a_j (x_j - x_{L+1}) + \sum_{j=n}^{M+1} T_j a_j (x_n - x_{L+1}) \right]. \tag{57}$$

Alternatively, we can use Eq. (35) and rewrite Eq. (57) in terms of a_n and b_n,

$$f_n = \frac{a_n}{a_{L+1}} \left[f_{L+1} - \sum_{j=L+2}^{M+1} T_j a_j b_{L+1} \right] + a_n \sum_{j=L+2}^{n-1} T_j b_j + b_n \sum_{j=n}^{M+1} T_j a_j. \tag{58}$$

The last two equations are likely to be more convenient for computational purposes than Eq. (42) since there are no cancellations of large numbers in these equations. The possible exception is the subtraction in the square brackets in Eq. (58), but for the special case of interest (see Sec. V) we avoid this difficulty.

V. APPLICATION OF THE METHOD

General theory outlined in the preceding section will be applied to the difference equations (15) and (16). To do so, we need to calculate T_j from Eq. (43).

A. Calculation of T_j

First we calculate Wronskian (44) from Eq. (48). Inserting r_k from Eq. (33) into this equation we get that Wronskian behaves for both Eqs. (15) and (16) as

$$W_j = (-1)^{j-L-1} \frac{(j+L)!}{(j-L)!} \frac{W_{L+1}}{(2L+1)!}, \tag{59}$$

where we set either $L=L_2$ or $L=L_1$. We note that W_{L+1} is the only quantity in this equation that depends on the concrete form of a_j and b_j.

Second, we take the right-hand side s_j of Eq. (32) equal to

$$s_j = -\frac{p_{N_1,j}^{L_1,L_2}}{j - L_2} \tag{60}$$

in case of Eq. (15) and

$$s_j = \frac{p_{N_2,j}^{L_2,L_1}}{j - L_1} \tag{61}$$

in case of Eq. (16).

Equations (59), (60), and (61) can be used to simplify formula (43). By inserting Eq. (59) with $L=L_2$ and Eq. (60) into Eq. (43) we get in the case of Eq. (15),

$$T_j = -\frac{P_{N_1,j}^{L_1,L_2}}{W_{L_2+1}}. \tag{62}$$

Analogously, by inserting Eq. (59) with $L=L_1$ and Eq. (61) into Eq. (43) we get in the case of Eq. (16),

$$T_j = \frac{P_{N_2,j}^{L_2,L_1}}{W_{L_1+1}}. \tag{63}$$

Here, $P_{N_1,N_2}^{L_1,L_2}$ denotes

$$P_{N_1,N_2}^{L_1,L_2} = \frac{p_{N_1,N_2}^{L_1,L_2} W_{L_2+1}}{(N_2 - L_2) W_{N_2}}. \tag{64}$$

This quantity was introduced because of the symmetry

$$P_{N_1,N_2}^{L_1,L_2} = P_{N_2,N_1}^{L_2,L_1} \tag{65}$$

[see the notes after Eqs. (22) and (59)]. By combining Eqs. (21) and (59) we can write for $L_1 > L_2+1$,

$$P_{N_1,N_2}^{L_1,L_2} = \frac{(L_1 - L_2 + 1)!(2L_2 + 1)!}{2} \sum_{q=\max(0,N_2-L_1-2)}^{\min(N_1-L_1-1,N_2-L_2-1)} (-1)^q \times \binom{N_1 - L_2 - q - 3}{L_1 - L_2 - 2} \binom{N_2 - L_2 - 1}{q} \binom{L_1 + L_2 + 2 + q}{N_2 + L_2}. \tag{66}$$

The case $L_2 > L_1+1$ is calculated by means of Eq. (65).

B. Numerical experiments and final formulas

1. Case $l < \min(L_1, L_2)$

By numerical experiments we found that the initial values f_{L+1} for Eq. (15) with $L_1 > L_2$ and $l < L_2$ and for Eq. (16) with $L_1 < L_2$ and $l < L_1$ are given as

$$f_{L+1} = (a_{L+1} + b_{L+1}) \sum_{j=L+1}^{M+1} T_j a_j. \tag{67}$$

In the case of Eq. (15) this equation holds with $L = L_2$, $M = N_1$, $f_{L+1} = \tilde{Q}_{N_1,L_2+1}^{+,L_1,L_2,l}$ and with a_j, b_j, and T_j given by Eqs. (24), (25), and (62). In the case of Eq. (16) this equation holds with $L = L_1$, $M = N_2$, $f_{L+1} = \tilde{Q}_{L_1+1,N_2}^{+,L_1,L_2,l}$ and with a_j, b_j, and T_j given by Eqs. (26), (27), and (63).

Then Eq. (58) can be brought to the form

$$f_n = a_n \sum_{j=L+1}^{n-1} T_j (a_j + b_j) + (a_n + b_n) \sum_{j=n}^{M+1} T_j a_j. \tag{68}$$

2. Case $l = L_2$

It follows from Eq. (29) that in this case one of the two linearly independent solutions is

$$a_{N_2} = (-1)^{N_2 - L_2 - 1}. \tag{69}$$

The second one is determined by the reduction of order. We use Eq. (57) for $f_{N_2} = \tilde{Q}_{N_1,N_2}^{+,L_1,L_2,L_2}$ with $n = N_2$, $L = L_2$, $M = N_1$, and T_j given by Eq. (62). The value of f_{L+1} was found from numerical analysis to be

$$\tilde{Q}_{N_1,L_2+1}^{+,L_1,L_2,L_2} = \frac{(L_1 + L_2 + 1)!(N_1 - L_2 - 2)!}{2(L_1 - L_2 - 1)!(N_1 - L_1 - 1)!}. \tag{70}$$

3. Case $l=L_1$

It follows from Eq. (31) that the constant K in Eq. (51) is equal to zero, so we can use Eq. (55) for $f_{N_1}=\tilde{Q}^{+,L_1}_{N_1,N_2,L_2,L_1}$ with $n=N_1$, $L=L_1$, $M=N_2$, and T_j calculated from Eq. (63).

One of the two linearly independent solutions of homogenous equation (16) is given by Eq. (A6) of the Appendix with $J=2L_1+1$,

$$a_{N_1}=(-1)^{N_1-L_1-1}\sum_{j=0}^{2L_1+1} h_j(N_1-L_1)^j, \tag{71}$$

where h_j are given by Eq. (A11) and where $h_{2L_1+1}=1$.

Using Eqs. (33) and (49) we can write Eq. (55) for the case considered as

$$f_n=-a_n\frac{W_{L+1}}{(2L+1)!}\sum_{j=n+1}^{M+1} T_j a_j \sum_{k=n+1}^{j}\frac{(-1)^{k-L-1}(k+L-1)!}{a_k a_{k-1}(k-L-1)!}. \tag{72}$$

This expression is still not entirely satisfactory. We found that there is residual instability for n close to $L+1$. To eliminate it we rewrite the double summation in the last equation

$$f_n=-a_n\frac{W_{L+1}}{(2L+1)!}\sum_{k=n+1}^{M+1}\frac{(-1)^{k-L-1}(k+L-1)!}{a_k a_{k-1}(k-L-1)!}\sum_{j=k}^{M+1} T_j a_j. \tag{73}$$

The source of instability for n close to $L+1$ is an interesting identity,

$$\sum_{j=L+1}^{M+1} T_j a_j=0. \tag{74}$$

Therefore, we use this identity in Eq. (73) and rewrite this equation to the form

$$f_n=a_n\frac{W_{L+1}}{(2L+1)!}\sum_{k=n+1}^{M+1}\frac{(-1)^{k-L-1}(k+L-1)!}{a_k a_{k-1}(k-L-1)!}\sum_{j=L+1}^{k-1} T_j a_j. \tag{75}$$

This equation is stable for all n from $L+1$ to M. For $n>M$, it yields zero as it should.

C. Numerical tests

We tested derived formulas numerically for very large quantum numbers. First we set $L_1=16$ and $L_2=14$, second we considered $L_1=20$ and $L_2=10$. We took $N_1=50$ and varied N_2 from L_2+1 to 70 and l from 2 to L_2. Then we reversed the role of L_1 and L_2 and also N_1 and N_2. These tests are rather severe; in normal calculation one encounters much more favorable situations. The formulas were run in double precision arithmetics and compared with the exact solutions of Eqs. (15) and (16) programmed in MAPLE in the form of the recursive algorithm run in rational arithmetics. For $l<\min(L_1,L_2)$, the hypergeometric functions (24)–(27) were calculated from the MAPLE subroutine. The numerical stable way of their calculations is given in the Appendix. For $|L_1-L_2|=2$ the relative error of the derived formulas was typically of order 10^{-15}. For the case $|L_1-L_2|=10$ the relative error was typically two orders higher. This shows that numerical stability of formulas slightly deteriorates with increasing difference $|L_1-L_2|$. However, one can expect that with increasing difference of the angular momenta of the electrons the contributions of the terms with large numbers of nodes to the energy is relatively small. Therefore, the achieved numerical stability is sufficient for all practical purposes.

VI. CONCLUSIONS

In this paper we extended the method of numerically stable calculation of the atomic integrals suggested in our previous paper[1] for the S-states of two-electron atoms to the states of arbitrary

total angular momenta. Thus, in these two papers the complete solution of the numerically stable calculation of the atomic integrals is given. In the first paper[1] we succeeded in transformation of the problem of the numerical stable calculation of the atomic integrals to the problem of the numerical stable solution of the difference equations. In this paper we completed our program by solving the latter problem in required generality. To achieve this aim we suggested a computationally stable method for the solution of inhomogenous difference equations that for certain values of the discrete independent variable become homogenous and in that region are described by just one of the two linearly independent solutions. The method was applied to the difference equations appearing in the radial part of the atomic integrals and tested for very large quantum numbers. These tests show high numerical stability of the suggested method. The stability slightly decreases with increasing difference of the angular momenta of the electrons.

The method suggested in these two papers can be used for the calculation of the radial part of the Coulomb interaction between electrons whose orbitals are expanded from the same center. This covers all atoms and the simplest molecules. The results obtained in these papers can be directly used for the configuration interaction calculation of the excited states of two electron atoms. This will be reported elsewhere.

Because of the potential importance of the achieved results it would be desirable to put them on a rigorous basis. The paper is based on the observation that Eqs. (15) and (16) can be in the region where they become homogenous described by just *one* of the two linearly independent solutions. Although we are certain about this observation, one should see *why* equations behave in this way. The same applies to our guesses (67), (70), and (74), and for Eq. (A17) in the Appendix.

Therefore, we believe that the results achieved in this paper are of some interest from the point of view of atomic physics as well as pure mathematics.

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APPENDIX

In this appendix we suggest a solution of the homogenous equations (15) and (16). Since this solution is given in terms of the hypergeometric function $F(a,b,c,2)$ we find a particularly useful form of these functions that can be used also in Eq. (10).

Let us rewrite homogenous equations (15) and (16) into a general form,

$$(n-L)g_{n+1}-(n+L)g_{n-1}-2(J-L)g_n=0. \tag{A1}$$

This equation is obtained from the original homogenous equation (16),

$$(n-L)f_{n+1}-(n+L)f_{n-1}+2(l+1)f_n=0, \tag{A2}$$

by setting either $f_n=g_n$ and $J=L-l-1$ or $f_n=(-1)^n g_n$ and $J=L+l+1$. Equation (A1) is obtained also from homogenous equation (15),

$$(n-L)f_{n+1}-(n+L)f_{n-1}-2lf_n=0, \tag{A3}$$

by setting either $f_n=g_n$ and $J=L+l$ or $f_n=(-1)^n g_n$ and $J=L-l$. Due to the selection rules for Clebsch–Gordan coefficients mentioned after Eq. (5), the difference $L-l$ is always even. Therefore, the parameter J is odd in the case of Eq. (16) and even in the case of Eq. (15).

For $J<L-1$ the solution of Eq. (A1) is given by the hypergeometric function

$$g_n=F(n-L,-J;-2L;2). \tag{A4}$$

Let us remind the form of the hypergeometric function $F(a,b,c,z)$ here,

$$F(a,b,c,z) = 1 + \frac{ab}{c}z + \frac{a(a+1)b(b+1)}{c(c+1)}\frac{z^2}{2!} + \cdots . \tag{A5}$$

It turns out that this form of the hypergeometric functions is useful only for a close to zero, i.e., only for n close to L. For larger n, a more suitable form is needed.

Since we want to get expression also for the hypergeometric functions appearing in Eq. (10), we allow L to be half-integral and n to be half-integral and smaller than $L+1$.

We search for the solution of Eq. (A1) in the form of the series

$$g_n = \sum_{j=0}^{J} h_j (n-L)^j . \tag{A6}$$

Later on, it will be clear why we choose the upper bound of summation J. The advantage of this expansion is that the coefficients h_j do not change the sign. Therefore, for n larger than L this way of calculating the hypergeometric functions is numerically stable and can be used for the hypergeometric functions appearing in Eqs. (24)–(27).

Since J must be a non-negative integer, for $L=l$ we obtain only one solution in the form (A6). If $l<L$, we obtain in this way two linearly independent solutions.

The remaining hypergeometric functions to be calculated are those appearing in Eq. (10). For these functions argument a in the definition (A5) is always negative. As it is clear from Eq. (A4) it corresponds to the situation when $n<L$. The use of Eq. (A6) is not advantageous in this case, because for negative value of $n-L$ we get in (A6) the sum of terms with changing signs. When n is close to L, the best way is to calculate the hypergeometric functions from the definition (A5). For n more distant from L we calculate the hypergeometric functions from the series

$$g_n = \sum_{j=0}^{J} c_j n^j . \tag{A7}$$

It appears that for even J the coefficients c_j with odd j equal zero and for odd J the coefficients c_j with even j equal zero. From this fact it immediately follows that

$$F(-n-L,-J;-2L;2) = (-1)^J F(n-L,-J;-2L,2). \tag{A8}$$

Using this equation we can always raise the value of the parameter a over $-L$.

In the following we first show how to calculate the coefficients h_j in the expansion (A6), then we calculate the coefficients c_j in the expansion (A7).

Expansion around $n=L$

We make substitution $N=n-L$ in Eq. (A1). Then Eq. (A1) reads

$$Ng_{N+1} - (N+2L)g_{N-1} - 2(J-L)g_N = 0. \tag{A9}$$

Inserting the expansion (A6) and using the binomial formula we obtain after some manipulation

$$\sum_{j=0}^{J}\left[\sum_{k=0}^{j}\binom{j}{k}N^{k+1}(1-(-1)^{j-k}) - 2L\sum_{k=0}^{j}N^k(-1)^{j-k} - 2(J-L)N^j\right]h_j = 0. \tag{A10}$$

Comparing now terms with the same powers of N we get for the highest power N^J identically zero. It means that the coefficient h_J is free for the normalization of the solution. This is the reason why we chose in Eq. (A6) the upper bound of the summation equal to J. Going then successively to the lower powers of N we obtain recurrence relations for the coefficients h_j,

$$\frac{h_{J-j}}{h_J} = \frac{1}{j(J-j)!}\sum_{p=0}^{j-1}\frac{(J-p)!}{(1+j-p)!}\left[\frac{1-(-1)^{j-p-1}}{2}(J-j) - L(1+j-p)(-1)^{j-p}\right]\frac{h_{J-p}}{h_J}. \quad \text{(A11)}$$

Normalization of the series (A6) to the hypergeometric function is done by comparing Eqs. (A4) and (A6) for some value of n. The best choice is $n=L$ since then we have

$$1 = h_J\frac{h_0}{h_J}, \quad \text{(A12)}$$

where we used the identity $F(0,-J;-2L;2)=1$. The ratio h_0/h_J is calculated from Eq. (A11).

Expansion around $n=0$

We proceed along the same lines as in the derivation of recurrence relations for the coefficients h_j. We insert the expansion (A7) into Eq. (A1), use binomial formula and compare the terms with the same powers of n. After some manipulation we obtain

$$\frac{c_{J-2p}}{c_J} = \frac{1}{2p(J-2p)!}\sum_{j=0}^{p-1}\frac{c_{J-2j}}{c_J}\frac{(J-2j)!}{(2p-2j+1)!}[J-2p-L(2p-2j+1)] \quad \text{(A13)}$$

for p running from 1 to $J/2$ for J even and to $(J-1)/2$ for J odd. The coefficients c_{J-2p-1} equal zero.

The coefficient c_J is determined by comparing series (A7) and the hypergeometric function (A4) for some n. Setting $n=L$ we obtain

$$1 = c_J\sum_{j=0}^{J}\frac{c_j}{c_J}L^j, \quad \text{(A14)}$$

where we used the identity $F(0,-J;-2L;2)=1$. For practical purposes, however, this form is not very convenient, since there is a cancellation of large numbers in the sum on the right-hand side. For this reason the use of series (A7) is not suitable for calculation of the hypergeometric functions with n comparable or greater than L. Instead we determine the constant c_J as follows.

For even values of $J=2P$ the constant c_{2P} is found by comparing Eqs. (A4) and (A7) for $n=0$,

$$F(-L,-2P;-2L;2) = c_{2P}\frac{c_0}{c_{2P}}, \quad \text{(A15)}$$

where the ratio c_0/c_{2P} is calculated from Eq. (A13). The values of $F(-L,-2P;-2L,2)$ were found from the numerical experiments to be

$$F(-L,-2P,-2L,2) = \prod_{p=0}^{P-1}\frac{2p+1}{2L-2p-1}. \quad \text{(A16)}$$

For odd values of $J=2P+1$, comparison of Eqs. (A4) and (A7) yields for $n=0$ nothing, since both sides are identically equal to zero. However, the constant c_{2P+1} can be calculated from remarkable identity

$$c_{2P+1} = \frac{c_{2P}}{L-P} \quad \text{(A17)}$$

found by numerical experiments.

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SO(10) group theory for the unified model building

Takeshi Fukuyama[a)]
Department of Physics, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan

Amon Ilakovac[b)]
Department of Physics, University of Zagreb, P.O. Box 331, Bijenička cesta 32, HR-10002 Zagreb, Croatia

Tatsuru Kikuchi[c)]
Department of Physics, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan

Stjepan Meljanac[d)]
Institut Rudjer Bošković, Bijenička cesta 54, P.O. Box 180, HR-10002 Zagreb, Croatia

Nobuchika Okada[e)]
Theory Group, KEK, Oho 1-1, Tsukuba, Ibaraki 305-0801, Japan

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The complete tables of Clebsch–Gordan (CG) coefficients for a wide class of SO(10) SUSY grand unified theories (GUTs) are given. Explicit expressions of states of all corresponding multiplets under standard model gauge group $G_{321}=\mathrm{SU}(3)_C\times\mathrm{SU}(2)_L\times\mathrm{U}(1)_Y$, necessary for evaluation of the CG coefficients are presented. The SUSY SO(10) GUT model considered here includes most of the Higgs irreducible representations usually used in the literature, **10**, **45**, **54**, **120**, **126**, **126**, and **210**. Mass matrices of all G_{321} multiplets are found for the most general superpotential. These results are indispensable for the precision calculations of the gauge couplings unification and proton decay, etc. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1847709]

I. INTRODUCTION

A particularly attractive idea for the physics beyond the standard model (SM) is the possible appearance of grand unified theories (GUTs).[1] The idea of GUTs bears several profound features. Perhaps the most obvious one is that GUTs have the potential to unify the diverse set of particle representations and parameters found in the SM into a single, comprehensive, and hopefully predictive framework. For example, through the GUT symmetry one might hope to explain the quantum numbers of the fermion spectrum, or even the origins of fermion mass. Moreover, by unifying all U(1) generators within a non-Abelian theory, GUTs would also provide an explanation for the quantization of electric charge. By combining GUTs with supersymmetry (SUSY), we hope to unify the attractive features of GUTs simultaneously with those of SUSY into a single theory, SUSY GUTs.[2] The apparent gauge couplings unification of the minimal supersymmetric standard model (MSSM) is strong circumstantial evidence in favor of the emergence of a SUSY GUT near $M_G\simeq 2\times 10^{16}$ GeV.[3]

While there are *a priori* many choices for such possible groups, the list can be narrowed down by requiring groups of rank $\geqslant 4$ that have complex representations. The smallest groups satisfying these requirements are SU(5), SU(6), SO(10), and E_6. Amongst these choices, SO(10) is particu-

[a)]Electronic mail: fukuyama@se.ritsumei.ac.jp
[b)]Electronic mail: ailakov@rosalind.phy.hr
[c)]Electronic mail: rp009979@se.ritsumei.ac.jp
[d)]Electronic mail: meljanac@irb.hr
[e)]Electronic mail: nobuchika.okada@kek.jp

larly attractive,[4] because SO(10) is the smallest simple Lie group for which a single anomaly-free irreducible representation (irrep) (namely the spinor **16** representation) can accommodate the entire SM fermion content of each generation.

Once we fix SO(10) as the gauge group, we have also many choices of the Higgs fields though they are limited by the gauge symmetry. The Higgs fields play an essential role in the spontaneous symmetry breaking of the SO(10) gauge group and as a source of the observed fermion masses. The SO(10) gauge group must be broken down to the standard model gauge group $G_{321}=\mathrm{SU}(3)_C\times\mathrm{SU}(2)_L\times\mathrm{U}(1)_Y$ gauge group, and each SO(10) irrep must be decomposed into G_{321} multiplets. In this paper, we make an explicit construction of the states of these G_{321} multiplets. Using these states, we calculate the CG coefficients appearing in the mass matrices for the states belonging to G_{321} irreps and corresponding mass matrices in a wide class of the SO(10) models. The purpose of the present paper is to give detailed structures of the SO(10) GUTs based on a general model as far as has been possible, and to serve a wide range of unified model builders.

The paper is organized as follows. In Sec. II, we give a class of SUSY SO(10) GUTs and give an explicit form of the most general superpotential. In such a superpotential, we postulate a renormalizability in order to keep the predictability.[5–7] However, the result developed here is also applicable to the nonrenormalizable models.[8–14] The symmetry breakings are considered in Sec. III. Section IV is devoted to present explicit forms of the states in the G_{321} multiplets for all SO(10) irreps. This is the central part of the present paper. Using these tables, we give in Sec. V the mass matrices with the CG coefficients for a class of SUSY SO(10) GUTs, together with suitable tests and consistency checks for them. In Sec. VI, we consider the quark and lepton mass matrices in general SUSY SO(10) models. Section VII is devoted to conclusion. We list the decompositions of each SO(10) irreps under G_{321} subgroup in Appendix A. In Appendix B, we present the complete list of the CG coefficients for the G_{321} multiplets for all SO(10) irreps.

II. A CLASS OF SUSY SO(10) GUTs

In this section, we consider a class of renormalizable SUSY SO(10) models. They include three families of matter fields Ψ_i $(i=1,2,3)$ transforming as 16 dimensional fundamental spinor representation, **16**, gauge fields contained in the adjoint representation, and set of SO(10) multiplets of Higgs fields, enabling most general Yukawa couplings. The most general Yukawa couplings follow from decomposition of $\mathbf{16}\times\mathbf{16}=\mathbf{10}+\mathbf{120}+\mathbf{126}$, i.e., they include the Higgs fields in $H=\mathbf{10}$, $D=\mathbf{120}$, $\bar{\Delta}=\overline{\mathbf{126}}$ irreps, respectively. Furthermore, to consider as general case of the symmetry breaking of SO(10) to the standard model gauge group G_{321} as possible, we add several Higgs fields containing G_{321} singlets. They are $A=\mathbf{45}$, $\Delta=\mathbf{126}$, $\Phi=\mathbf{210}$, and $E=\mathbf{54}$ irreps. Of course, that is not the most general case. However, this set of Higgs fields is quite rich and gives rise to several realistic SUSY SO(10) models. Our aim is to give a systematic method for treatment of models with complicated Higgs sectors. This is a generalization of the method proposed in Refs. 15–17. We shall assume that the SUSY is preserved so that we consider the breaking of SUSY SO(10) to the MSSM.

Then the Yukawa couplings are

$$W_Y = Y_{10}^{ij}\Psi_i H\Psi_j + Y_{120}^{ij}\Psi_i D\Psi_j + Y_{126}^{ij}\Psi_i\bar{\Delta}\Psi_j, \tag{1}$$

where $i,j=1,2,3$ denote the generation indices. Note that H is a fundamental SO(10) irrep, and A, D, Φ, and $\Delta+\bar{\Delta}$ are antisymmetric tensors of rank 2, 3, 4, and 5, respectively. E is a symmetric traceless tensor of rank 2.

The most general Higgs superpotential is given by

$$W = \frac{1}{2}m_1\Phi^2 + m_2\overline{\Delta}\Delta + \frac{1}{2}m_3H^2 + \frac{1}{2}m_4A^2 + \frac{1}{2}m_5E^2 + \frac{1}{2}m_6D^2 + \lambda_1\Phi^3 + \lambda_2\Phi\overline{\Delta}\Delta + (\lambda_3\Delta + \lambda_4\overline{\Delta})H\Phi$$
$$+ \lambda_5A^2\Phi - i\lambda_6A\overline{\Delta}\Delta + \frac{\lambda_7}{120}\varepsilon A\Phi^2 + E(\lambda_8E^2 + \lambda_9A^2 + \lambda_{10}\Phi^2 + \lambda_{11}\Delta^2 + \lambda_{12}\overline{\Delta^2} + \lambda_{13}H^2)$$
$$+ D^2(\lambda_{14}E + \lambda_{15}\Phi) + D\{\lambda_{16}HA + \lambda_{17}H\Phi + (\lambda_{18}\Delta + \lambda_{19}\overline{\Delta})A + (\lambda_{20}\Delta + \lambda_{21}\overline{\Delta})\Phi\}, \tag{2}$$

where SO(10) invariants are defined in the fundamental SO(10) basis $1',2',\ldots,9',0'$ and in the Y diagonal basis $1,2,\ldots,9,0$ (which we will define in the next section) as follows:

$$\Phi^2 \equiv \Phi_{a'b'c'd'}\Phi_{a'b'c'd'} = \Phi_{abcd}\Phi_{\bar{a}\bar{b}\bar{c}\bar{d}},$$

$$\overline{\Delta}\Delta \equiv \overline{\Delta}_{a'b'c'd'e'}\Delta_{a'b'c'd'e'} = \overline{\Delta}_{abcde}\Delta_{\bar{a}\bar{b}\bar{c}\bar{d}\bar{e}},$$

$$H^2 \equiv H_{a'}H_{a'} = H_aH_{\bar{a}},$$

$$A^2 \equiv A_{a'b'}A_{a'b'} = A_{ab}A_{\bar{a}\bar{b}},$$

$$E^2 \equiv E_{a'b'}E_{a'b'} = E_{ab}E_{\bar{a}\bar{b}},$$

$$D^2 \equiv D_{a'b'c'}D_{a'b'c'} = D_{abc}D_{\bar{a}\bar{b}\bar{c}},$$

$$\Phi^3 \equiv \Phi_{a'b'c'd'}\Phi_{a'b'e'f'}\Phi_{c'd'e'f'} = \Phi_{\bar{a}\bar{b}\bar{c}\bar{d}}\Phi_{abef}\Phi_{cd\bar{e}\bar{f}},$$

$$\Phi\overline{\Delta}\Delta \equiv \Phi_{a'b'c'd'}\overline{\Delta}_{a'b'e'f'g'}\Delta_{c'd'e'f'g'} = \Phi_{\bar{a}\bar{b}\bar{c}\bar{d}}\overline{\Delta}_{abefg}\Delta_{cd\bar{e}\bar{f}\bar{g}},$$

$$\Delta H\Phi \equiv \Delta_{a'b'c'd'e'}H_{a'}\Phi_{b'c'd'e'} = \Delta_{\bar{a}\bar{b}\bar{c}\bar{d}\bar{e}}H_a\Phi_{bcde},$$

$$\overline{\Delta}H\Phi \equiv \overline{\Delta}_{a'b'c'd'e'}H_{a'}\Phi_{b'c'd'e'} = \overline{\Delta}_{\bar{a}\bar{b}\bar{c}\bar{d}\bar{e}}H_a\Phi_{bcde},$$

$$A^2\Phi \equiv A_{a'b'}A_{c'd'}\Phi_{a'b'c'd'} = A_{\bar{a}\bar{b}}A_{cd}\Phi_{ab\bar{c}\bar{d}},$$

$$-iA\overline{\Delta}\Delta \equiv -iA_{a'b'}\overline{\Delta}_{a'c'd'e'f'}\Delta_{b'c'd'e'f'} = -iA_{\bar{a}\bar{b}}\overline{\Delta}_{acdef}\Delta_{b\bar{c}\bar{d}\bar{e}\bar{f}},$$

$$\tfrac{1}{120}\varepsilon A\Phi^2 \equiv \tfrac{1}{120}\varepsilon_{a'_1a'_2a'_3a'_4a'_5a'_6a'_7a'_8a'_9a'_0}A_{a'_1a'_2}\Phi_{a'_3a'_4a'_5a'_6}\Phi_{a'_7a'_8a'_9a'_0}$$
$$= \tfrac{1}{120}\varepsilon_{\bar{a}_1\bar{a}_2\bar{a}_3\bar{a}_4\bar{a}_5\bar{a}_6\bar{a}_7\bar{a}_8\bar{a}_9\bar{a}_0}A_{a_1a_2}\Phi_{a_3a_4a_5a_6}\Phi_{a_7a_8a_9a_0}, \tag{3}$$

$$E^3 \equiv E_{a'b'}E_{a'c'}E_{b'c'} = E_{\bar{a}\bar{b}}E_{ac}E_{b\bar{c}},$$

$$EA^2 \equiv E_{a'b'}A_{a'c'}A_{b'c'} = E_{\bar{a}\bar{b}}A_{ac}A_{b\bar{c}},$$

$$E\Phi^2 \equiv E_{a'b'}\Phi_{a'c'd'e'}\Phi_{b'c'd'e'} = E_{\bar{a}\bar{b}}\Phi_{acde}\Phi_{b\bar{c}\bar{d}\bar{e}},$$

$$E\Delta^2 \equiv E_{a'b'}\Delta_{a'c'd'e'f'}\Delta_{b'c'd'e'f'} = E_{\bar{a}\bar{b}}\Delta_{acdef}\Delta_{b\bar{c}\bar{d}\bar{e}\bar{f}},$$

$$E\overline{\Delta}^2 \equiv E_{a'b'}\overline{\Delta}_{a'c'd'e'f'}\overline{\Delta}_{b'c'd'e'f'} = E_{\overline{ab}}\overline{\Delta}_{acdef}\overline{\Delta}_{bc\overline{de}\overline{f}},$$

$$EH^2 \equiv E_{a'b'}H_{a'}H_{b'} = E_{\overline{ab}}H_aH_b,$$

$$ED^2 \equiv E_{a'b'}D_{a'c'd'}D_{b'c'd'} = E_{\overline{ab}}D_{acd}D_{bc\overline{d}},$$

$$D^2\Phi \equiv D_{a'b'c'}D_{a'd'e'}\Phi_{b'c'd'e'} = D_{\overline{abc}}D_{ade}\Phi_{bc\overline{de}},$$

$$DHA \equiv D_{a'b'c'}H_{a'}A_{b'c'} = D_{\overline{abc}}H_aA_{bc},$$

$$DH\Phi \equiv D_{a'b'c'}H_{d'}\Phi_{a'b'c'd'} = D_{\overline{abc}}H_d\Phi_{abc\overline{d}},$$

$$D\Delta A \equiv D_{a'b'c'}\Delta_{a'b'c'd'e'}A_{d'e'} = D_{\overline{abc}}\Delta_{abcde}A_{\overline{de}},$$

$$D\overline{\Delta}A \equiv D_{a'b'c'}\overline{\Delta}_{a'b'c'd'e'}A_{d'e'} = D_{\overline{abc}}\overline{\Delta}_{abcde}A_{\overline{de}},$$

$$D\Delta\Phi \equiv D_{a'b'c'}\Delta_{a'b'd'e'f'}\Phi_{c'd'e'f'} = D_{\overline{abc}}\Delta_{abdef}\Phi_{c\overline{def}},$$

$$D\overline{\Delta}\Phi \equiv D_{a'b'c'}\overline{\Delta}_{a'b'd'e'f'}\Phi_{c'd'e'f'} = D_{\overline{abc}}\overline{\Delta}_{abdef}\Phi_{c\overline{def}}.$$

Here $a',b',c',\ldots$ $(a,b,c,\ldots)$ run over all the SO(10) vector (Y diagonal) indices and ε is a totally antisymmetric SO(10) invariant tensor with

$$\varepsilon_{1'2'3'4'5'6'7'8'9'0'} = i\varepsilon_{1234567890} = 1. \tag{4}$$

III. SYMMETRY BREAKING

Here we first introduce Y diagonal basis (see also Ref. 18): $1=1'+2'i$, $2=1'-2'i$, $3=3'+4'i$, $4=3'-4'i$, $5=5'+6'i$, $6=5'-6'i$, $7=7'+8'i$, $8=7'-8'i$, $9=9'+0'i$, $0=9'-0'i$, up to the normalization factor $1/\sqrt{2}$. It is more convenient since (1,3,5,7,9) transforms as **5**-plet and (2,4,6,8,0) transforms as $\overline{\mathbf{5}}$-plet under $\mathrm{SU}(5)\times\mathrm{U}(1)_X$ [for that reason Y diagonal basis could also be called SU(5) basis]. Consequently, (1,3) and (2,4) are $\mathrm{SU}(2)_L$ doublets with definite hypercharges $Y=\frac{1}{2}$ and $Y=-\frac{1}{2}$, respectively. Similarly, (5,7,9) and (6,8,0) transform under $\mathrm{SU}(3)_C$ as **3** and $\overline{\mathbf{3}}$ with definite hypercharges $Y=-\frac{1}{3}$ and $Y=\frac{1}{3}$, respectively. Note that under the complex conjugation (c.c.), $\overline{1}=2$, $\overline{3}=4$, $\overline{5}=6$, $\overline{7}=8$, $\overline{9}=0$, and vice versa. The SO(10) invariants are built in such a way that an index a is contracted (summed) with the corresponding c.c. index $\overline{a}$, for example, $T_{\ldots a\cdot\ldots}T_{\ldots\overline{a}\cdot\ldots}$.

The basis in $A=\mathbf{45}$, $D=\mathbf{120}$, $\Phi=\mathbf{210}$, and $\Delta+\overline{\Delta}=\mathbf{126}+\overline{\mathbf{126}}$ dimensional spaces are defined by totally antisymmetric (unit) tensors $(a'b')$, $(a'b'c')$, $(a'b'c'd')$, and $(a'b'c'd'e')$, respectively, and similarly in a, b, c, d, e indices in Y diagonal basis. The states of the Δ and $\overline{\Delta}$ have additional properties,

$$\begin{aligned} i\varepsilon_{\overline{a}_1\overline{a}_2\overline{a}_3\overline{a}_4\overline{a}_5\overline{a}_6\overline{a}_7\overline{a}_8\overline{a}_9\overline{a}_{10}}\overline{\Delta}_{a_6a_7a_8a_9a_{10}} &= \overline{\Delta}_{\overline{a}_1\overline{a}_2\overline{a}_3\overline{a}_4\overline{a}_5}, \\ i\varepsilon_{\overline{a}_1\overline{a}_2\overline{a}_3\overline{a}_4\overline{a}_5\overline{a}_6\overline{a}_7\overline{a}_8\overline{a}_9\overline{a}_{10}}\Delta_{a_6a_7a_8a_9a_{10}} &= -\Delta_{\overline{a}_1\overline{a}_2\overline{a}_3\overline{a}_4\overline{a}_5}, \end{aligned} \tag{5}$$

that allow one to project out the Δ and $\overline{\Delta}$ states, respectively, from the 256 antisymmetric states $(abcde)$. The explicit expressions for antisymmetric tensors are, for example,

$$(ab) = ab - ba,$$

$$(abc) = abc + cab + bca - bac - acb - cba, \tag{6}$$

etc. Important relations are

$$(12) = -i(1'2'),$$

$$(34) = -i(3'4'),$$

$$(56) = -i(5'6'), \tag{7}$$

$$(78) = -i(7'8'),$$

$$(90) = -i(9'0').$$

Symmetric $E=\mathbf{54}$ dimensional space is spanned by traceless symmetric states $\{a'b'\} \equiv a'b' + b'a'(a', b' = 1', 2', \ldots, 9', 0')$ and $\Sigma_{a'} c_{a'} \{a'a'\}$ with $\Sigma_{a'} c_{a'} \equiv 0$. Also, important relations are

$$\{12\} = 1'1' + 2'2',$$

$$\{34\} = 3'3' + 4'4',$$

$$\{56\} = 5'5' + 6'6', \tag{8}$$

$$\{78\} = 7'7' + 8'8',$$

$$\{90\} = 9'9' + 0'0'.$$

Now, the Higgs fields A, E, Δ, $\overline{\Delta}$, and Φ contain eight directions of singlets under the G_{321} subgroup (see Appendix A). The corresponding vacuum expectation values (VEVs) are defined by

$$\langle A \rangle = \sum_{i=1}^{2} A_i \hat{A}_i, \tag{9}$$

$$\langle E \rangle = E\hat{E}, \tag{10}$$

$$\langle \Delta \rangle = v_R \hat{v_R}, \tag{11}$$

$$\langle \overline{\Delta} \rangle = \overline{v_R}\,\widehat{\overline{v_R}}, \tag{12}$$

$$\langle \Phi \rangle = \sum_{i=1}^{3} \Phi_i \hat{\Phi}_i, \tag{13}$$

where unit directions $\hat{A}_i$ $(i=1,2)$, $\hat{E}$, $\hat{v_R}$, $\widehat{\overline{v_R}}$ and $\hat{\Phi}_i$ $(i=1,2,3)$ in the Y diagonal basis are

$$\hat{A}_1 = \hat{A}^{(1,1,0)}_{(1,1,3)} = \frac{i}{2}(12 + 34), \tag{14}$$

$$\hat{A}_2 = \hat{A}^{(1,1,0)}_{(15,1,1)} = \frac{i}{\sqrt{6}}(56 + 78 + 90), \tag{15}$$

$$\hat{E} = \hat{E}^{(1,1,0)}_{(1,1,1)} = \frac{1}{\sqrt{60}}\{3 \times [12 + 34] - 2 \times [56 + 78 + 90]\}, \tag{16}$$

$$\widehat{v_R} = \hat{\Delta}^{(1,1,0)}_{(10,1,3)} = \frac{1}{\sqrt{120}}(24\,680), \tag{17}$$

$$\widehat{\overline{v_R}} = \hat{\overline{\Delta}}^{(1,1,0)}_{(10,1,3)} = \frac{1}{\sqrt{120}}(13\,579), \tag{18}$$

$$\hat{\Phi}_1 = \hat{\Phi}^{(1,1,0)}_{(1,1,1)} = -\frac{1}{\sqrt{24}}(1234), \tag{19}$$

$$\hat{\Phi}_2 = \hat{\Phi}^{(1,1,0)}_{(15,1,1)} = -\frac{1}{\sqrt{72}}(5678 + 5690 + 7890), \tag{20}$$

$$\hat{\Phi}_3 = \hat{\Phi}^{(1,1,0)}_{(15,1,3)} = -\frac{1}{12}([12 + 34][56 + 78 + 90]). \tag{21}$$

Here and hereafter, the upper and the lower indices indicate the $SU(3)_C \times SU(2)_L \times U(1)_Y$, $SU(4) \times SU(2)_L \times SU(2)_R$ quantum numbers, respectively in the case of double indices. A word about notation: the square brackets are used for grouping of indices. This grouping of indices is used to emphasize the $SU(2)_L$ and $SU(3)_C$ structures within the state vectors. The square brackets satisfy usual distributive law with respect to summation of indices and tensor product of indices, e.g.,

$$\begin{aligned}([12 + 34][56 + 78 + 90]) &= (1256 + 1278 + 1290 + 3456 + 3478 + 3490)\\ &= (1256) + (1278) + (1290) + (3456) + (3478) + (3490),\end{aligned}$$

$$\begin{aligned}([1,3][5[78 + 90], 7[56 + 90], 9[56 + 78]]) &= (1578 + 1590, 1756 + 1790, 1956 + 1978, 3578\\ &\quad + 3590, 3756 + 3790, 3956 + 3978)\\ &= (1578, 1756, 1956, 3578, 3756, 3956)\\ &\quad + (1590, 1790, 1978, 3590, 3790, 3978).\end{aligned} \tag{22}$$

Further, the numerical factors which could be misinterpreted as additional SO(10) indices are written in italics.

The unit directions appearing in VEVs satisfy the following orthonormality relations:

$$\hat{A}_i \cdot \hat{A}_j = \delta_{ij} \quad (i,j = 1,2),$$

$$\hat{E}^2 = 1,$$

$$\widehat{v_R} \cdot \widehat{v_R} = \widehat{\overline{v_R}} \cdot \widehat{\overline{v_R}} = 0, \tag{23}$$

$$\widehat{v_R}\cdot\widehat{\overline{v_R}}=1,$$

$$\widehat{\Phi_i}\cdot\widehat{\Phi_j}=\delta_{ij}\quad(i,j=1,2,3).$$

Due to the D-flatness condition the absolute values of the VEVs, v_R and $\overline{v_R}$ are equal,

$$|v_R|=|\overline{v_R}|. \tag{24}$$

The superpotential of Eq. (2) calculated at the VEVs in Eqs. (14)–(21) is

$$\langle W\rangle=\frac{1}{2}m_1\langle\Phi\rangle^2+m_2\langle\overline{\Delta}\rangle\langle\Delta\rangle+\frac{1}{2}m_4\langle A\rangle^2+\frac{1}{2}m_5\langle E\rangle^2+\lambda_1\langle\Phi\rangle^3+\lambda_2\langle\Phi\rangle\langle\overline{\Delta}\rangle\langle\Delta\rangle+\lambda_5\langle A\rangle^2\langle\Phi\rangle$$
$$-i\lambda_6\langle A\rangle\langle\overline{\Delta}\rangle\langle\Delta\rangle+\frac{\lambda_7}{120}\varepsilon\langle A\rangle\langle\Phi\rangle^2+\langle E\rangle[\lambda_8\langle E\rangle^2+\lambda_9\langle A\rangle^2+\lambda_{10}\langle\Phi\rangle^2]. \tag{25}$$

Inserting the VEVs from Eqs. (14)–(21), one obtains

$$\langle W\rangle=\frac{1}{2}m_1[\Phi_1^2+\Phi_2^2+\Phi_3^2]+m_2v_R\overline{v_R}+\frac{1}{2}m_4(A_1^2+A_2^2)+\frac{1}{2}m_5E^2$$
$$+\lambda_1\left[\Phi_2^3\frac{1}{9\sqrt{2}}+3\Phi_1\Phi_3^2\frac{1}{6\sqrt{6}}+3\Phi_2\Phi_3^2\frac{1}{9\sqrt{2}}\right]+\lambda_2\left[\Phi_1\frac{1}{10\sqrt{6}}+\Phi_2\frac{1}{10\sqrt{2}}+\Phi_3\frac{1}{10}\right]v_R\overline{v_R}$$
$$+\lambda_5\left[A_1^2\Phi_1\frac{1}{\sqrt{6}}+A_2^2\Phi_2\frac{\sqrt{2}}{3}+A_1A_2\Phi_3\frac{2}{\sqrt{6}}\right]+\lambda_6\left[A_1\left(-\frac{1}{5}\right)+A_2\left(-\frac{3}{5\sqrt{6}}\right)\right]v_R\overline{v_R}$$
$$+\lambda_7\left[2A_2\Phi_1\Phi_2\frac{\sqrt{2}}{5}+A_2\Phi_3^2\frac{2\sqrt{2}}{5\sqrt{3}}+2A_1\Phi_2\Phi_3\frac{\sqrt{2}}{5}\right]+\lambda_8E^3\frac{1}{2\sqrt{15}}+\lambda_9E\left[A_1^2\frac{\sqrt{3}}{2\sqrt{5}}+A_2^2\left(-\frac{1}{\sqrt{15}}\right)\right]$$
$$+\lambda_{10}E\left[\Phi_1^2\frac{\sqrt{3}}{2\sqrt{5}}+\Phi_2^2\left(-\frac{1}{\sqrt{15}}\right)+\Phi_3^2\frac{1}{4\sqrt{15}}\right]. \tag{26}$$

The VEVs are determined by the following equation:

$$\left\{\frac{\partial}{\partial\Phi_1},\frac{\partial}{\partial\Phi_2},\frac{\partial}{\partial\Phi_3},\frac{\partial}{\partial v_R},\frac{\partial}{\partial\overline{v_R}},\frac{\partial}{\partial A_1},\frac{\partial}{\partial A_2},\frac{\partial}{\partial E}\right\}\langle W\rangle=0. \tag{27}$$

From Eq. (27), we obtain seven equations for Φ_1, Φ_2, Φ_3, A_1, A_1, E, and $v_R\overline{v_R}$. They are the following:

$$0=m_1\Phi_1+\frac{\lambda_1\Phi_3^2}{2\sqrt{6}}+\frac{\lambda_2v_R\overline{v_R}}{10\sqrt{6}}+\frac{\lambda_5A_1^2}{\sqrt{6}}+\frac{2\sqrt{2}\lambda_7A_2\Phi_2}{5}+\frac{\sqrt{3}\lambda_{10}\Phi_1E}{\sqrt{5}},$$

$$0=m_1\Phi_2+\frac{\lambda_1\Phi_2^2}{3\sqrt{2}}+\frac{\lambda_1\Phi_3^2}{3\sqrt{2}}+\frac{\lambda_2v_R\overline{v_R}}{10\sqrt{2}}+\frac{\sqrt{2}}{3}\lambda_5A_2^2+\frac{2\sqrt{2}\lambda_7\Phi_1A_2}{5}+\frac{2\sqrt{2}\lambda_7A_1\Phi_3}{5}-\frac{2\lambda_{10}\Phi_2E}{\sqrt{15}},$$

$$0=m_1\Phi_3+\frac{\lambda_1\Phi_1\Phi_3}{\sqrt{6}}+\frac{\sqrt{2}\lambda_1\Phi_2\Phi_3}{3}+\frac{\lambda_2v_R\overline{v_R}}{10}+\frac{\sqrt{2}\lambda_5A_1A_2}{\sqrt{3}}+\frac{2\sqrt{2}\lambda_7A_1\Phi_2}{5}+\frac{4\sqrt{2}\lambda_7A_2\Phi_3}{5\sqrt{3}}+\frac{\lambda_{10}\Phi_3E}{2\sqrt{15}},$$

$$0=v_R\overline{v_R}\left[m_2+\frac{\lambda_2\Phi_1}{10\sqrt{6}}+\frac{\lambda_2\Phi_2}{10\sqrt{2}}+\frac{\lambda_2\Phi_3}{10}-\frac{\lambda_6A_1}{5}-\frac{\sqrt{3}\lambda_6A_2}{5\sqrt{2}}\right], \tag{28}$$

$$0 = m_4 A_1 + \frac{\sqrt{2}\lambda_5 A_1 \Phi_1}{\sqrt{3}} + \frac{\sqrt{2}\lambda_5 A_2 \Phi_3}{\sqrt{3}} - \frac{\lambda_6 v_R \overline{v_R}}{5} + \frac{2\sqrt{2}\lambda_7 \Phi_2 \Phi_3}{5} + \frac{\sqrt{3}\lambda_9 A_1 E}{\sqrt{5}},$$

$$0 = m_4 A_2 + \frac{\sqrt{2}\lambda_5 A_1 \Phi_3}{\sqrt{3}} + \frac{2\sqrt{2}\lambda_5 A_2 \Phi_2}{3} - \frac{\sqrt{3}\lambda_6 v_R \overline{v_R}}{5\sqrt{2}} + \frac{2\sqrt{2}\lambda_7 \Phi_3^2}{5\sqrt{3}} + \frac{2\sqrt{2}\lambda_7 \Phi_1 \Phi_2}{5} - \frac{2\lambda_9 A_2 E}{\sqrt{15}},$$

$$0 = m_5 E + \frac{\sqrt{3}\lambda_8 E^2}{2\sqrt{5}} + \frac{\sqrt{3}\lambda_9 A_1^2}{2\sqrt{5}} - \frac{\lambda_9 A_2^2}{\sqrt{15}} + \frac{\sqrt{3}\lambda_{10} \Phi_1^2}{2\sqrt{5}} - \frac{\lambda_{10} \Phi_2^2}{\sqrt{15}} + \frac{\lambda_{10} \Phi_3^2}{4\sqrt{15}}.$$

If we assume $v_R \overline{v_R} \neq 0$, we obtain five quadratic equations and one linear equation for Φ_i, A_i, and E. For that case there are 32 solutions. Two of them correspond to SU(5) symmetry and remaining 30 solutions to G_{321} standard gauge group symmetry solutions. If we set $v_R = 0$, we find six quadratic equations for Φ_1, Φ_2, Φ_3, A_1, A_2, and E with 64 solutions with symmetry groups having rank 5. They are isomorphic to $G_{3211} \equiv \mathrm{SU}(3)_C \times \mathrm{SU}(2)_L \times \mathrm{U}(1)_R \times \mathrm{U}(1)_{B-L}$. However, there are solutions with higher symmetries. They are G_{3221}, G_{421}, G_{422}, and G_{51} (for the reader's convenience, we list the decompositions of each representation in Appendix A). For general coupling constants $\lambda_1, \ldots, \lambda_{21}$, $m_1, \ldots, m_8$, the solutions with higher symmetries are specified by the following relations. Solutions with higher symmetries are characterized by the following:

(1) $\mathrm{SU}(5) \times \mathrm{U}(1)_X$ and $(\mathrm{SU}(5) \times \mathrm{U}(1))^{\mathrm{flipped}}$ symmetry solutions,

$$E = v_R = 0,$$
$$\Phi_1 = \frac{\varepsilon}{\sqrt{6}} \Phi_3, \quad \Phi_2 = \frac{\varepsilon}{\sqrt{2}} \Phi_3, \quad A_1 = \frac{2\varepsilon}{\sqrt{6}} A_2, \tag{29}$$

where $\varepsilon = 1$ and $\varepsilon = -1$ correspond to the $\mathrm{SU}(5) \times \mathrm{U}(1)_X$ symmetric vacua and $(\mathrm{SU}(5) \times \mathrm{U}(1))^{\mathrm{flipped}}$ symmetric vacua, respectively.

(2) SU(5) symmetry solutions,

$$E = 0,$$
$$\Phi_1 = \frac{1}{\sqrt{6}} \Phi_3, \quad \Phi_2 = \frac{1}{\sqrt{2}} \Phi_3, \quad A_1 = \frac{2}{\sqrt{6}} A_2, \quad v_R \neq 0. \tag{30}$$

(3) $G_{422} \equiv \mathrm{SU}(4) \times \mathrm{SU}(2)_L \times \mathrm{SU}(2)_R$ symmetry solutions,

$$\Phi_2 = \Phi_3 = A_1 = A_2 = v_R = 0,$$
$$\Phi_1 \neq 0, \quad E \neq 0. \tag{31}$$

(4) $G_{3221} \equiv \mathrm{SU}(3)_C \times \mathrm{SU}(2)_L \times \mathrm{SU}(2)_R \times \mathrm{U}(1)_{B-L}$ symmetry solutions,

$$\Phi_3 = A_1 = v_R = 0,$$
$$\Phi_1 \neq 0, \quad \Phi_2 \neq 0, \quad A_2 \neq 0, \quad E \neq 0. \tag{32}$$

(5) $G_{421} \equiv \mathrm{SU}(4) \times \mathrm{SU}(2)_L \times \mathrm{U}(1)$ symmetry solutions,

$$\Phi_2 = \Phi_3 = A_2 = v_R = 0,$$
$$\Phi_1 \neq 0, \quad A_1 \neq 0, \quad E \neq 0. \tag{33}$$

(6) $G_{3211} \equiv \mathrm{SU}(3)_C \times \mathrm{SU}(2)_L \times \mathrm{U}(1)_R \times \mathrm{U}(1)_{B-L}$ symmetry solutions,

$$v_R = 0,$$
$$\Phi_i \neq 0 \quad (i=1,2,3), \quad A_i \neq (i=1,2), \quad E \neq 0. \tag{34}$$

The higher symmetry solutions given in Eqs. (29)–(34) lead to the crucial consistency checks for all results in this paper.

IV. THE STATES AND CLEBSCH–GORDAN COEFFICIENTS

A. The states in the G_{321} multiplets

In order to obtain and study the mass matrices, it is convenient to decompose the Higgs representations under the G_{321} gauge group. The explicit decompositions of **10**, **45**, **54**, **120**, **126**, $\overline{\mathbf{126}}$, and **210** representations in Y diagonal basis are presented according to the G_{321} multiplets with the same quantum numbers which generally mix among themselves. The eight singlets $(\mathbf{1},\mathbf{1},0)$ are already given in Eqs. (14)–(21). There are $45-12=33$ would-be NG modes. They are in the following multiplets: $(\mathbf{1},\mathbf{1},0)$, $[(\mathbf{3},\mathbf{2},-\frac{5}{6})+\text{c.c.}]$, $[(\mathbf{1},\mathbf{1},1)+\text{c.c.}]$, $[(\mathbf{3},\mathbf{1},\frac{2}{3})+\text{c.c.}]$, and $[(\mathbf{3},\mathbf{2},\frac{1}{6})+\text{c.c.}]$. The corresponding orthonormal states are listed in Table 1 (Ref. 19) in Y-diagonal basis. The physically important modes, so-called, Higgs doublets $[(\mathbf{1},\mathbf{2},\frac{1}{2})+\text{c.c.}]$ and color triplets $[(\mathbf{3},\mathbf{1},-\frac{1}{3})+\text{c.c.}]$ states are listed in Tables 2 (Ref. 19) and 3 (Ref. 19), respectively. The remaining G_{321} multiplets are listed in Tables 4 (Ref. 19) and 5 (Ref. 19). There are altogether 691 states accommodated in G_{321} multiplets [see Table 6 (Ref. 19)]. There are 26 mass matrices, five containing NG modes, one containing doublets, one containing color triplets, 19 containing the other modes. There are five multiplets (33 states) with zero mass and 69 G_{321} multiplets with masses different from zero (containing $691-33=658$ states). Hence the mass spectrum contains 70 different mass eigenvalues. For the SU (5) solutions, there are only 21 different masses and G_{321} multiplets are grouped into multiplets transforming under the SU (5) group. For the G_{422} solutions, there are 27 different mass eigenvalues and G_{321} multiplets are grouped into multiplets transforming under the G_{422} group (see Appendix A). The higher symmetries serve as a strong consistency check of our mass matrices and CG coefficients.

We point out that the main basic blocks in all 691 states are $\mathrm{SU}(2)_L$ irreps **1**, **2**, and **3**, and SU (3) irreps **1**, **3**, $\overline{\mathbf{3}}$, **6**, $\overline{\mathbf{6}}$, and **8**:

$$\mathrm{SU}(2)_L,$$

$$\mathbf{1} \quad [12+34],\ (13),(24),\ (1234),$$

$$\mathbf{2} \quad [1,3],\ [-3,1],\ [2,4],[-4,2],$$

$$\mathbf{3} \quad \left[14,32,\frac{12-34}{\sqrt{2}}\right],\ \left\{\frac{11}{2},-\frac{33}{2},-\frac{13}{\sqrt{2}}\right\},\ \left\{\frac{22}{2},-\frac{44}{2},-\frac{24}{\sqrt{2}}\right\} \tag{35}$$

$$\mathrm{SU}(3)_C,$$

$$\mathbf{1} \quad [56+78+90],\ (579),\ (680),\ (5678+5690+7890),$$

$$\mathbf{3} \quad [5,7,9],\ (80,06,68),\ (5680,7806,9068),$$

$$\overline{\mathbf{3}} \quad [6,8,0],\ (79,95,57),\ (5697,7859,9075),$$

$$\mathbf{6} \quad \left(580,670,689,\frac{6[90-78]}{\sqrt{2}},\frac{8[56-90]}{\sqrt{2}},\frac{0[78-56]}{\sqrt{2}}\right),$$
$$\left\{\frac{55}{2},\frac{77}{2},\frac{99}{2},\frac{79}{\sqrt{2}},\frac{95}{\sqrt{2}},\frac{57}{\sqrt{2}}\right\}, \tag{36}$$

$$\overline{\mathbf{6}} \quad \left(679,589,570,\frac{5[09-78]}{\sqrt{2}},\frac{7[65-09]}{\sqrt{2}},\frac{9[87-65]}{\sqrt{2}}\right),$$
$$\left\{\frac{66}{2},\frac{88}{2},\frac{00}{2},\frac{\{80\}}{\sqrt{2}},\frac{\{06\}}{\sqrt{2}},\frac{\{68\}}{\sqrt{2}}\right\},$$

$$\mathbf{8} \quad \left[58,50,70,76,96,98,\frac{56-78}{\sqrt{2}},\frac{56+78-2\times 90}{\sqrt{6}}\right],$$
$$\left(5890,5078,7056,7690,9678,9856,\frac{5690-7890}{\sqrt{2}},\frac{2\times 5678-5690-7890}{\sqrt{6}}\right).$$

All states can be constructed combining and antisymmetrizing or symmetrizing the basic blocks. The basic blocks (35) and (36) which appear only in antisymmetric tensors are embraced by parentheses, the basic blocks which appear only in the symmetric tensors are embraced by curly brackets ($\{aa\}/2=aa$), while the basic blocks that appear both in symmetric and antisymmetric tensors are embraced by square brackets.

B. $\mathcal{H}$ operators and Clebsch–Gordan coefficients

Let us denote by R the sum of all representations **10**, **45**, **54**, **120**, **126**, $\overline{\mathbf{126}}$, and **210**,

$$R=\sum_I R^I, \quad \dim R=691. \tag{37}$$

There are 21 cubic invariants [see Eq. (3)],

$$\mathcal{I}(R^I,R^J,R^{\bar{K}})\equiv \mathcal{I}^{IJ\bar{K}}, \quad \overline{R^K}\equiv R^{\bar{K}}, \tag{38}$$

where $R^I\times R^J=\Sigma_K R^K$.

Let us denote $\mathcal{H}$-operators (see Refs. 15 and 16),

$$\mathcal{H}_K(R^I,R^J)=\mathcal{H}_K(R^J,R^I)\sim R^K \tag{39}$$

transforming as R^K and

$$\mathcal{H}_K(R^I,R^J)=\frac{1}{N}\frac{\partial \mathcal{I}^{IJ\bar{K}}}{\partial R^{\bar{K}}}. \tag{40}$$

The normalization factor N is chosen so that

$$\mathcal{H}_K(R^I,R^J)R^{\bar{K}}=\mathcal{I}^{IJ\bar{K}}. \tag{41}$$

For example, in the Y-diagonal basis

$$[\mathcal{H}_\Phi(\Phi_1,\Phi_2)]_{abcd} = \tfrac{1}{6}[(\Phi_1)_{abef}(\Phi_2)_{cd\overline{ef}} - (\Phi_1)_{acef}(\Phi_2)_{bd\overline{ef}} + (\Phi_1)_{adef}(\Phi_2)_{bc\overline{ef}} + (\Phi_1)_{cdef}(\Phi_2)_{ab\overline{ef}} - (\Phi_1)_{bdef}(\Phi_2)_{ac\overline{ef}} + (\Phi_1)_{bcef}(\Phi_2)_{ad\overline{ef}}]. \tag{42}$$

For invariants of the type $\mathcal{I}^{III}$, there is only one $\mathcal{H}$ operator, $\mathcal{H}_I$, for invariants of the type $\mathcal{I}^{II\overline{K}}$ there are two $\mathcal{H}$ operators, $\mathcal{H}_{\overline{I}}$ and $\mathcal{H}_K$, and for invariants of the type $\mathcal{I}^{IJ\overline{K}}$ there are three $\mathcal{H}$ operators, $\mathcal{H}_{\overline{I}}$, $\mathcal{H}_{\overline{J}}$, and $\mathcal{H}_K$. The $\mathcal{H}$ operators are symmetric in R^I and R^J, $\mathcal{H}(R^I,R^J)=\mathcal{H}(R^J,R^I)$. More generally,

$$\mathcal{I}^{IJ\overline{K}} = \mathcal{I}^{JI\overline{K}} = \mathcal{I}^{I\overline{K}J} = \mathcal{I}^{J\overline{K}I} = \mathcal{I}^{\overline{K}IJ} = \mathcal{I}^{\overline{K}JI}. \tag{43}$$

We are especially interested in CG coefficients when at least one of the states transforms as a singlet under the G_{321} group. That requires the decomposition of each SO(10) irrep R^I into G_{321} irreps,

$$R^I = \sum_i R_i^I, \tag{44}$$

where indices "i" just enumerate the G_{321} irreps with fixed Y contained in a specific R^I irrep. There are eight singlets, denoted here shortly by S_i^I, defined in Eqs. (14)–(21). For this choice of G_{321}-singlet states, the action of $\mathcal{H}$ operators are reduced to the invariant subspaces of states with fixed G_{321} quantum numbers, which are listed in Tables 1–5 (Ref. 19),

$$\mathcal{H}_K(\hat{S}_i^I,R_j^J) = \sum_k C_{ijk}^{IJK} R_k^K, \tag{45}$$

where R_j^J and R_k^K transform as identical G_{321} irreps (have the same G_{321} quantum numbers). For example, for the evaluation of the first column in the $(\mathbf{1},\mathbf{3},1)$ mass matrix [see Eq. (74)], the following $\mathcal{H}$ operators must be evaluated:

$$\mathcal{H}_E(\hat{E},\hat{E}_{(1,3,3)}^{(1,3,1)}) = \frac{\sqrt{3}}{2\sqrt{5}}\hat{E}_{(1,3,3)}^{(1,3,1)},$$
$$\mathcal{H}_{\overline{\Delta}}(\widehat{v_R},\hat{E}_{(1,3,3)}^{(1,3,1)}) = \frac{1}{5}\hat{\overline{\Delta}}_{(10,3,1)}^{(1,3,1)}. \tag{46}$$

Note that

$$C_{ijk}^{IJK} = \mathcal{I}(\hat{S}_i^I,\hat{R}_j^J,\hat{R}_k^{\overline{K}}) \equiv \hat{S}_i^I\hat{R}_j^J\hat{R}_k^{\overline{K}} \tag{47}$$

[the second part of Eq. (47) defines shortand notation] where

$$\hat{R}_i^{\overline{I}} \equiv \overline{\hat{R}_i^I} \tag{48}$$

is the complex conjugated irrep of $\hat{R}_i^I$. The CG coefficients are listed in 25 tables in Appendix B. Note that the CG coefficients depend only on the indices $i,j,\ldots$, that represent G_{321} multiplets and not on the specific states within the G_{321} multiplets. That can be used as a consistency check of the states belonging to the specific G_{321} multiplets.

We choose all SO(10) invariants in Eq. (3) to be real, except for invariants containing the Δ or the $\overline{\Delta}$ field separately (for example, $\Delta H\Phi$ or $E\overline{\Delta}^2$). In this last case, the sum of the two invariants, one containing Δ field and the other having $\overline{\Delta}$ field in place of Δ, are real. Generally, CG coefficients are complex (in our case they are either real or pure imaginary). Starting with cubic invariants in Eq. (3), our choice of phases of states in Tables 1–5 (Ref. 19) is such that it leads to the minimal number of imaginary terms in the mass matrices.

Symmetry relations imply

$$C_{ijk}^{IJK} = C_{jik}^{JIK}. \tag{49}$$

CG coefficients also satisfy Hermiticity relations,

$$\overline{C_{ijk}^{IJK}} = C_{\bar{i}kj}^{\bar{I}KJ}. \tag{50}$$

Here the $\bar{i}$ represents the label assigned to the irrep complex conjugated to the irrep designated by i.

Furthermore, following relations are valid:

$$\sum_j C_{ijj}^{IJ\bar{J}} \dim R_j^J = 0, \quad \sum_j \dim R_j^J = \dim R^J, \tag{51}$$

$$\sum_i \sum_j C_{ijk}^{IJK} C_{\bar{i}\bar{j}\bar{l}}^{\bar{I}\bar{J}\bar{K}} \dim R_i^I \dim R_j^J = C(I,J,K)\delta_{kl}^{-},$$

$$\sum_i \dim R_i^I = \dim R^I, \quad \sum_j \dim R_j^J = \dim R^J, \tag{52}$$

where $C(I,J,K)$ are constants depending on irreps R^I, R^J, and R^K.

V. MASS MATRICES

A. Mass matrices

For the sum of all representations R [see Eq. (37)], we define fluctuations of the Higgs field around the VEVs as

$$R = \langle R \rangle + \sum_{I,i} r_i^I. \tag{53}$$

Then the matrix element of the mass matrix corresponding to G_{321} multiplets i,j (R_i^I and R_j^J transform identically under G_{321}) is

$$\mathcal{M}_{ij}^{IJ} = \left(\frac{\partial^2 W}{\partial r_i^I \partial \overline{r_j^J}} \right)_{R=\langle R \rangle}, \tag{54}$$

$$\mathcal{M}_{ij}^{IJ} = m_I \delta_{IJ} \delta_{ij} + \sum_{K,k} \lambda^{IJK} S_i^I C_{ijk}^{IJK}, \tag{55}$$

where $\lambda^{III}=6\lambda_p$, $\lambda^{IIK}=2\lambda_p$, and $\lambda^{IJK}=\lambda_p$ for invariants containing three identical representations, two identical representations (different from the third one), and three different representations, respectively. Specifically, $\{\lambda^{IJK}\}=\{6\lambda_1, 6\lambda_8, 2\lambda_5, 2\lambda_7, 2\lambda_9, 2\lambda_{10}, 2\lambda_{11}, 2\lambda_{12}, 2\lambda_{13}, 2\lambda_{14}, 2\lambda_{15}, \lambda_2, \lambda_3, \lambda_4, \lambda_6, \lambda_{16}, \lambda_{17}, \lambda_{18}, \lambda_{19}, \lambda_{20}, \lambda_{21}\}$.

According to Eq. (51) the trace of the total mass matrix over all $\dim R$ states in R is

$$\mathrm{Tr}\, \mathcal{M} = \sum_I m_I \dim R^I. \tag{56}$$

The mass matrices are generally non-Hermitian. So the squares of physical masses are equal to the eigenvalues of matrices $\mathcal{M}^\dagger \mathcal{M}$ and $\mathcal{M}\mathcal{M}^\dagger$. (One can obtain Hermitian matrices $\mathcal{M}^\dagger \mathcal{M}$, i.e., $\mathcal{M}\mathcal{M}^\dagger$ with the same spectra.) For a real superpotential, that is for $\lambda_3=\lambda_4$, $\lambda_{11}=\lambda_{12}$, $\lambda_{18}=\lambda_{19}$, and $\lambda_{20}=\lambda_{21}$ and all coupling constants and VEVs real, the matrices are Hermitian due to the Hermiticity relation (50).

Now we are ready to present the explicit forms of the mass matrices calculated from the superpotential of Eq. (2). Every matrix is designated with the corresponding G_{321} multiplet and appears dim R_i^I times in the total mass matrix $\mathcal{M}$. A mass matrix associated with a G_{321} multiplet and the mass matrix associated with the corresponding complex conjugated G_{321} multiplet are equal up to transposition, and therefore for multiplets with $Y \neq 0$ we list only one of the two mass matrices. Of course, when enumerating the total degrees of freedom, one must include all mass eigenvalues (691 in total). The basis designating the columns ($\mathbf{c}$:) of the mass matrices listed below is given in the same way as shown in Tables 1, 2, 3, 4, and 5 (Ref. 19), while the rows are designated by the corresponding complex conjugated G_{321} multiplets ($\mathbf{r}$:),

$(\mathbf{1},\mathbf{1},0)$

$\mathbf{c}$: $\hat{A}^{(1,1,0)}_{(1,1,3)}, \hat{A}^{(1,1,0)}_{(15,1,1)}, \hat{E}^{(1,1,0)}_{(1,1,1)}, \hat{\Delta}^{(1,1,0)}_{(\overline{10},1,3)}, \hat{\bar{\Delta}}^{(1,1,0)}_{(10,1,3)}, \hat{\Phi}^{(1,1,0)}_{(1,1,1)}, \hat{\Phi}^{(1,1,0)}_{(15,1,1)}, \hat{\Phi}^{(1,1,0)}_{(15,1,3)}$

$\mathbf{r}$: $\hat{A}^{(1,1,0)}_{(1,1,3)}, \hat{A}^{(1,1,0)}_{(15,1,1)}, \hat{E}^{(1,1,0)}_{(1,1,1)}, \hat{\bar{\Delta}}^{(1,1,0)}_{(10,1,3)}, \hat{\Delta}^{(1,1,0)}_{(\overline{10},1,3)}, \hat{\Phi}^{(1,1,0)}_{(1,1,1)}, \hat{\Phi}^{(1,1,0)}_{(15,1,1)}, \hat{\Phi}^{(1,1,0)}_{(15,1,3)}$

$$\begin{pmatrix}
m_{11}^{(1,1,0)} & \sqrt{\frac{2}{3}}\lambda_5\Phi_3 & \sqrt{\frac{3}{5}}\lambda_9 A_1 & -\frac{\lambda_6 \overline{v_R}}{5} & -\frac{\lambda_6 v_R}{5} & \sqrt{\frac{2}{3}}\lambda_5 A_1 & \frac{2\sqrt{2}\lambda_7\Phi_3}{5} & m_{81}^{(1,1,0)} \\
\sqrt{\frac{2}{3}}\lambda_5\Phi_3 & m_{22}^{(1,1,0)} & -\frac{2\lambda_9 A_2}{\sqrt{15}} & -\frac{1}{5}\sqrt{\frac{3}{2}}\lambda_6 \overline{v_R} & -\frac{1}{5}\sqrt{\frac{3}{2}}\lambda_6 v_R & \frac{2\sqrt{2}\lambda_7\Phi_2}{5} & m_{72}^{(1,1,0)} & m_{82}^{(1,1,0)} \\
\sqrt{\frac{3}{5}}\lambda_9 A_1 & -\frac{2\lambda_9 A_2}{\sqrt{15}} & m_{33}^{(1,1,0)} & 0 & 0 & \sqrt{\frac{3}{5}}\lambda_{10}\Phi_1 & -\frac{2\lambda_{10}\Phi_2}{\sqrt{15}} & \frac{\lambda_{10}\Phi_3}{2\sqrt{15}} \\
-\frac{\lambda_6 v_R}{5} & -\frac{1}{5}\sqrt{\frac{3}{2}}\lambda_6 v_R & 0 & m_{44}^{(1,1,0)} & 0 & \frac{\lambda_2 v_R}{10\sqrt{6}} & \frac{\lambda_2 v_R}{10\sqrt{2}} & \frac{\lambda_2 v_R}{10} \\
-\frac{\lambda_6 \overline{v_R}}{5} & -\frac{1}{5}\sqrt{\frac{3}{2}}\lambda_6 \overline{v_R} & 0 & 0 & m_{44}^{(1,1,0)} & \frac{\lambda_2 \overline{v_R}}{10\sqrt{6}} & \frac{\lambda_2 \overline{v_R}}{10\sqrt{2}} & \frac{\lambda_2 \overline{v_R}}{10} \\
\sqrt{\frac{2}{3}}\lambda_5 A_1 & \frac{2\sqrt{2}\lambda_7\Phi_2}{5} & \sqrt{\frac{3}{5}}\lambda_{10}\Phi_1 & \frac{\lambda_2 \overline{v_R}}{10\sqrt{6}} & \frac{\lambda_2 v_R}{10\sqrt{6}} & m_{66}^{(1,1,0)} & \frac{2\sqrt{2}\lambda_7 A_2}{5} & \frac{\lambda_1\Phi_3}{\sqrt{6}} \\
\frac{2\sqrt{2}\lambda_7\Phi_3}{5} & m_{72}^{(1,1,0)} & -\frac{2\lambda_{10}\Phi_2}{\sqrt{15}} & \frac{\lambda_2 \overline{v_R}}{10\sqrt{2}} & \frac{\lambda_2 v_R}{10\sqrt{2}} & \frac{2\sqrt{2}\lambda_7 A_2}{5} & m_{77}^{(1,1,0)} & m_{87}^{(1,1,0)} \\
m_{81}^{(1,1,0)} & m_{82}^{(1,1,0)} & \frac{\lambda_{10}\Phi_3}{2\sqrt{15}} & \frac{\lambda_2 \overline{v_R}}{10} & \frac{\lambda_2 v_R}{10} & \frac{\lambda_1\Phi_3}{\sqrt{6}} & m_{87}^{(1,1,0)} & m_{88}^{(1,1,0)}
\end{pmatrix}, \tag{57}$$

where

$$m_{11}^{(1,1,0)} \equiv m_4 + \sqrt{\tfrac{2}{3}}\lambda_5\Phi_1 + \sqrt{\tfrac{3}{5}}\lambda_9 E,$$

$$m_{22}^{(1,1,0)} \equiv m_4 + \frac{2\sqrt{2}\lambda_5\Phi_2}{3} - \frac{2\lambda_9 E}{\sqrt{15}},$$

$$m_{33}^{(1,1,0)} \equiv m_5 + \sqrt{\tfrac{3}{5}}\lambda_8 E,$$

$$m_{44}^{(1,1,0)} \equiv m_2 + \frac{\lambda_2\Phi_1}{10\sqrt{6}} + \frac{\lambda_2\Phi_2}{10\sqrt{2}} + \frac{\lambda_2\Phi_3}{10} - \frac{\lambda_6 A_1}{5} - \frac{\sqrt{3}\lambda_6 A_2}{5\sqrt{2}}$$

$$m_{66}^{(1,1,0)} \equiv m_1 + \sqrt{\tfrac{3}{5}}\lambda_{10} E,$$

$$m_{72}^{(1,1,0)} \equiv \frac{2\sqrt{2}\lambda_5 A_2}{3} + \frac{2\sqrt{2}\lambda_7 \Phi_1}{5}, \tag{58}$$

$$m_{77}^{(1,1,0)} \equiv m_1 + \frac{\sqrt{2}\lambda_1 \Phi_2}{3} - \frac{2\lambda_{10} E}{\sqrt{15}},$$

$$m_{81}^{(1,1,0)} \equiv \sqrt{\frac{2}{3}}\lambda_5 A_2 + \frac{2\sqrt{2}\lambda_7 \Phi_2}{5},$$

$$m_{82}^{(1,1,0)} \equiv \sqrt{\frac{2}{3}}\lambda_5 A_1 + \frac{4}{5}\sqrt{\frac{2}{3}}\lambda_7 \Phi_3,$$

$$m_{87}^{(1,1,0)} \equiv \frac{\sqrt{2}\lambda_1 \Phi_3}{3} + \frac{2\sqrt{2}\lambda_7 A_1}{5},$$

$$m_{88}^{(1,1,0)} \equiv m_1 + \frac{\lambda_1 \Phi_1}{\sqrt{6}} + \frac{\sqrt{2}\lambda_1 \Phi_2}{3} + \frac{4}{5}\sqrt{\frac{2}{3}}\lambda_7 A_2 + \frac{\lambda_{10} E}{2\sqrt{15}}.$$

$[(\mathbf{1},\mathbf{1},1)+\text{c.c.}]$

c: $\hat{A}^{(1,1,1)}_{(1,1,3)}, \hat{D}^{(1,1,1)}_{(10,1,1)}, \hat{\Delta}^{(1,1,1)}_{(10,1,3)}$

r: $\hat{A}^{(1,1,-1)}_{(1,1,3)}, \hat{D}^{(1,1,-1)}_{(10,1,1)}, \hat{\Delta}^{(1,1,-1)}_{(10,1,3)}$

$$\begin{pmatrix} m_4 + \frac{\sqrt{2}\lambda_5\Phi_1}{\sqrt{3}} + \frac{\sqrt{3}\lambda_9 E}{\sqrt{5}} & -\frac{i\lambda_{19}\overline{v_R}}{\sqrt{10}} & -\frac{\lambda_6\overline{v_R}}{5} & -\sqrt{\frac{2}{3}}\lambda_5 A_2 - \frac{2\sqrt{2}\lambda_7\Phi_2}{5} \\ \frac{i\lambda_{18}v_R}{\sqrt{10}} & m_6 - \frac{2\lambda_{14}E}{\sqrt{15}} + \frac{\sqrt{2}\lambda_{15}\Phi_2}{3} & -\frac{i\lambda_{18}A_1}{\sqrt{10}} - \frac{\lambda_{20}\Phi_3}{2\sqrt{10}} & -\frac{\lambda_{20}v_R}{\sqrt{10}} \\ -\frac{\lambda_6 v_R}{5} & \frac{i\lambda_{19}A_1}{\sqrt{10}} - \frac{\lambda_{21}\Phi_3}{2\sqrt{10}} & m_{33}^{(1,1,1)} & -\frac{\lambda_2 v_R}{10} \\ -\sqrt{\frac{2}{3}}\lambda_5 A_2 - \frac{2\sqrt{2}\lambda_7\Phi_2}{5} & -\frac{\lambda_{21}\overline{v_R}}{\sqrt{10}} & -\frac{\lambda_2\overline{v_R}}{10} & m_{44}^{(1,1,1)} \end{pmatrix}, \tag{59}$$

where

$$m_{33}^{(1,1,1)} \equiv m_2 + \frac{\lambda_2 \Phi_1}{10\sqrt{6}} + \frac{\lambda_2 \Phi_2}{10\sqrt{2}} - \frac{1}{5}\sqrt{\frac{3}{2}}\lambda_6 A_2,$$

$$m_{44}^{(1,1,1)} \equiv m_1 + \frac{\lambda_1 \Phi_1}{\sqrt{6}} + \frac{\sqrt{2}\lambda_1 \Phi_2}{3} + \frac{4}{5}\sqrt{\frac{2}{3}}\lambda_7 A_2 + \frac{\lambda_{10} E}{2\sqrt{15}}. \tag{60}$$

$[(\mathbf{3},\mathbf{1},\tfrac{2}{3})+\text{c.c.}]$

c: $\hat{A}^{(3,1,2/3)}_{(15,1,1)}, \hat{D}^{(3,1,2/3)}_{(6,1,3)}, \hat{\Delta}^{(3,1,2/3)}_{(10,1,3)}, \hat{\Phi}^{(3,1,2/3)}_{(15,1,1)}, \hat{\Phi}^{(3,1,2/3)}_{(15,1,3)}$

r: $\hat{A}^{(3,1,-2/3)}_{(15,1,1)}, \hat{D}^{(3,1,-2/3)}_{(6,1,3)}, \hat{\Delta}^{(3,1,-2/3)}_{(10,1,3)}, \hat{\Phi}^{(3,1,-2/3)}_{(15,1,1)}, \hat{\Phi}^{(3,1,-2/3)}_{(15,1,3)}$

$$\begin{pmatrix} m_{11}^{(3,1,2/3)} & -\frac{i\lambda_{18}v_R}{\sqrt{10}} & -\frac{\lambda_6 v_R}{5} & -\frac{\sqrt{2}}{3}\lambda_5 A_2 - \frac{2\sqrt{2}\lambda_7\Phi_1}{5} & -\sqrt{\frac{2}{3}}\lambda_5 A_1 - \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7\Phi_3 \\ \frac{i\lambda_{19}\overline{v_R}}{\sqrt{10}} & m_{22}^{(3,1,2/3)} & m_{23}^{(3,1,2/3)} & \frac{\lambda_{21}\overline{v_R}}{2\sqrt{30}} & \frac{\lambda_{21}\overline{v_R}}{2\sqrt{15}} \\ -\frac{\lambda_6\overline{v_R}}{5} & m_{32}^{(3,1,2/3)} & m_{33}^{(3,1,2/3)} & -\frac{\lambda_2\overline{v_R}}{10\sqrt{3}} & -\frac{\lambda_2\overline{v_R}}{5\sqrt{6}} \\ -\frac{\sqrt{2}}{3}\lambda_5 A_2 - \frac{2\sqrt{2}\lambda_7\Phi_1}{5} & \frac{\lambda_{20}v_R}{2\sqrt{30}} & -\frac{\lambda_2 v_R}{10\sqrt{3}} & m_{44}^{(3,1,2/3)} & m_{45}^{(3,1,2/3)} \\ -\sqrt{\frac{2}{3}}\lambda_5 A_1 - \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7\Phi_3 & \frac{\lambda_{20}v_R}{2\sqrt{15}} & -\frac{\lambda_2 v_R}{5\sqrt{6}} & m_{45}^{(3,1,2/3)} & m_{55}^{(3,1,2/3)} \end{pmatrix}, \tag{61}$$

where

$$\begin{aligned} m_{11}^{(3,1,2/3)} &\equiv m_4 + \frac{\sqrt{2}\lambda_5\Phi_2}{3} - \frac{2\lambda_9 E}{\sqrt{15}}, \\ m_{22}^{(3,1,2/3)} &\equiv m_6 + \frac{4\lambda_{14}E}{3\sqrt{15}} + \frac{1}{3}\sqrt{\frac{2}{3}}\lambda_{15}\Phi_1 + \frac{2\lambda_{15}\Phi_3}{9}, \\ m_{23}^{(3,1,2/3)} &\equiv -\frac{i\lambda_{19}A_2}{\sqrt{15}} + \frac{\lambda_{21}\Phi_2}{6\sqrt{5}} + \frac{\lambda_{21}\Phi_3}{3\sqrt{10}}, \\ m_{32}^{(3,1,2/3)} &\equiv \frac{i\lambda_{18}A_2}{\sqrt{15}} + \frac{\lambda_{20}\Phi_2}{6\sqrt{5}} + \frac{\lambda_{20}\Phi_3}{3\sqrt{10}}, \\ m_{33}^{(3,1,2/3)} &\equiv m_2 + \frac{\lambda_2\Phi_1}{10\sqrt{6}} + \frac{\lambda_2\Phi_2}{30\sqrt{2}} + \frac{\lambda_2\Phi_3}{30} - \frac{\lambda_6 A_1}{5} - \frac{\lambda_6 A_2}{5\sqrt{6}}, \\ m_{44}^{(3,1,2/3)} &\equiv m_1 + \frac{\lambda_1\Phi_2}{3\sqrt{2}} - \frac{2\lambda_{10}E}{\sqrt{15}}, \\ m_{45}^{(3,1,2/3)} &\equiv \frac{\lambda_1\Phi_3}{3\sqrt{2}} + \frac{2\sqrt{2}\lambda_7 A_1}{5}, \\ m_{55}^{(3,1,2/3)} &\equiv m_1 + \frac{\lambda_1\Phi_1}{\sqrt{6}} + \frac{\lambda_1\Phi_2}{3\sqrt{2}} + \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7 A_2 + \frac{\lambda_{10}E}{2\sqrt{15}}. \end{aligned} \tag{62}$$

$\left[(\mathbf{3},\mathbf{2},-\frac{5}{6})+\text{c.c.}\right]$

$\mathbf{c}$: $\hat{A}_{(6,2,2)}^{(3,2,-5/6)}, \hat{E}_{(6,2,2)}^{(3,2,-5/6)}, \hat{\Phi}_{(6,2,2)}^{(3,2,-5/6)} \hat{\Phi}_{(10,2,2)}^{(3,2,-5/6)}$

$\mathbf{r}$: $\hat{A}_{(6,2,2)}^{(3,2,5/6)}, \hat{E}_{(6,2,2)}^{(3,2,5/6)}, \hat{\Phi}_{(6,2,2)}^{(3,2,5/6)} \hat{\Phi}_{(10,2,2)}^{(3,2,5/6)}$

$$\begin{pmatrix} m_4 - \frac{\lambda_5\Phi_3}{3} + \frac{\lambda_9 E}{2\sqrt{15}} & -\frac{\lambda_9 A_1}{2} - \frac{\lambda_9 A_2}{\sqrt{6}} & -\frac{\lambda_5 A_1}{\sqrt{3}} + \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7\Phi_2 & -\frac{2\lambda_5 A_2}{3} + \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7\Phi_3 \\ -\frac{\lambda_9 A_1}{2} - \frac{\lambda_9 A_2}{\sqrt{6}} & m_5 + \frac{1}{2}\sqrt{\frac{3}{5}}\lambda_8 E & \frac{\lambda_{10}\Phi_1}{2\sqrt{2}} + \frac{\lambda_{10}\Phi_3}{4\sqrt{3}} & \frac{\lambda_{10}\Phi_2}{2\sqrt{3}} + \frac{\lambda_{10}\Phi_3}{2\sqrt{6}} \\ -\frac{\lambda_5 A_1}{\sqrt{3}} + \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7\Phi_2 & \frac{\lambda_{10}\Phi_1}{2\sqrt{2}} + \frac{\lambda_{10}\Phi_3}{4\sqrt{3}} & m_1 - \frac{\lambda_1\Phi_3}{6} + \frac{7\lambda_{10}E}{4\sqrt{15}} & \frac{\lambda_1\Phi_3}{3\sqrt{2}} - \frac{4\lambda_7 A_2}{5\sqrt{3}} \\ -\frac{2\lambda_5 A_2}{3} + \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7\Phi_3 & \frac{\lambda_{10}\Phi_2}{2\sqrt{3}} + \frac{\lambda_{10}\Phi_3}{2\sqrt{6}} & \frac{\lambda_1\Phi_3}{3\sqrt{2}} - \frac{4\lambda_7 A_2}{5\sqrt{3}} & m_{44}^{(3,2,-5/6)} \end{pmatrix}, \tag{63}$$

where

$$m_{44}^{(3,2,-5/6)} \equiv m_1 + \frac{\lambda_1\Phi_2}{3\sqrt{2}} - \frac{\lambda_1\Phi_3}{6} - \frac{2\lambda_7 A_1}{5} - \frac{1}{4}\sqrt{\frac{3}{5}}\lambda_{10}E. \tag{64}$$

$\left[\left(\mathbf{3},\mathbf{2},\frac{1}{6}\right)+\text{c.c.}\right]$

c: $\hat{A}_{(6,2,2)}^{(3,2,1/6)}, \hat{E}_{(6,2,2)}^{(3,2,1/6)}, \hat{D}_{(15,2,2)}^{(3,2,1/6)}, \hat{\Delta}_{(15,2,2)}^{(3,2,1/6)}, \hat{\bar{\Delta}}_{(15,2,2)}^{(3,2,1/6)}, \hat{\Phi}_{(6,2,2)}^{(3,2,1/6)}, \hat{\Phi}_{(10,2,2)}^{(3,2,1/6)}$

r: $\hat{A}_{(6,2,2)}^{(3,2,-1/6)}, \hat{E}_{(6,2,2)}^{(3,2,-1/6)}, \hat{D}_{(15,2,2)}^{(3,2,-1/6)}, \hat{\bar{\Delta}}_{(15,2,2)}^{(3,2,-1/6)}, \hat{\Delta}_{(15,2,2)}^{(3,2,-1/6)}, \hat{\Phi}_{(6,2,2)}^{(3,2,-1/6)}, \hat{\Phi}_{(10,2,2)}^{(3,2,-1/6)}$

$$\begin{pmatrix} m_{11}^{(3,2,1/6)} & \frac{\lambda_9 A_1}{2} - \frac{\lambda_9 A_2}{\sqrt{6}} & -\frac{i\lambda_{19}\bar{v}_R}{\sqrt{10}} & -\frac{\lambda_6\bar{v}_R}{5} & 0 & m_{61}^{(3,2,1/6)} & m_{71}^{(3,2,1/6)} \\ \frac{\lambda_9 A_1}{2} - \frac{\lambda_9 A_2}{\sqrt{6}} & m_5 + \frac{1}{2}\sqrt{\frac{3}{5}}\lambda_8 E & 0 & 0 & -\frac{2\lambda_{12}v_R}{5} & \frac{\lambda_{10}\Phi_3}{4\sqrt{3}} - \frac{\lambda_{10}\Phi_1}{2\sqrt{2}} & \frac{\lambda_{10}\Phi_2}{2\sqrt{3}} - \frac{\lambda_{10}\Phi_3}{2\sqrt{6}} \\ \frac{i\lambda_{18}v_R}{\sqrt{10}} & 0 & m_{33}^{(3,2,1/6)} & m_{34}^{(3,2,1/6)} & m_{35}^{(3,2,1/6)} & -\frac{\lambda_{20}v_R}{2\sqrt{30}} & -\frac{\lambda_{20}v_R}{2\sqrt{15}} \\ -\frac{\lambda_6 v_R}{5} & 0 & m_{43}^{(3,2,1/6)} & m_{44}^{(3,2,1/6)} & \frac{\lambda_{12}E}{\sqrt{15}} & -\frac{\lambda_2 v_R}{10\sqrt{3}} & -\frac{\lambda_2 v_R}{5\sqrt{6}} \\ 0 & -\frac{2\lambda_{11}v_R}{5} & m_{53}^{(3,2,1/6)} & \frac{\lambda_{11}E}{\sqrt{15}} & m_{55}^{(3,2,1/6)} & 0 & 0 \\ m_{61}^{(3,2,1/6)} & \frac{\lambda_{10}\Phi_3}{4\sqrt{3}} - \frac{\lambda_{10}\Phi_1}{2\sqrt{2}} & -\frac{\lambda_{21}\bar{v}_R}{2\sqrt{30}} & -\frac{\lambda_2\bar{v}_R}{10\sqrt{3}} & 0 & m_{66}^{(3,2,1/6)} & \frac{\lambda_1\Phi_3}{3\sqrt{2}} + \frac{4\lambda_7 A_2}{5\sqrt{3}} \\ m_{71}^{(3,2,1/6)} & \frac{\lambda_{10}\Phi_2}{2\sqrt{3}} - \frac{\lambda_{10}\Phi_3}{2\sqrt{6}} & -\frac{\lambda_{21}\bar{v}_R}{2\sqrt{15}} & -\frac{\lambda_2\bar{v}_R}{5\sqrt{6}} & 0 & \frac{\lambda_1\Phi_3}{3\sqrt{2}} + \frac{4\lambda_7 A_2}{5\sqrt{3}} & m_{77}^{(3,2,1/6)} \end{pmatrix}, \tag{65}$$

where

$$m_{11}^{(3,2,1/6)} \equiv m_4 + \frac{\lambda_5\Phi_3}{3} + \frac{\lambda_9 E}{2\sqrt{15}},$$

$$m_{33}^{(3,2,1/6)} \equiv m_6 - \frac{\lambda_{14}E}{3\sqrt{15}} + \frac{\sqrt{2}\lambda_{15}\Phi_2}{9} + \frac{2\lambda_{15}\Phi_3}{9},$$

$$m_{34}^{(3,2,1/6)} \equiv -\frac{i\lambda_{18}A_1}{2\sqrt{10}} - \frac{i\lambda_{18}A_2}{2\sqrt{15}} - \frac{\lambda_{20}\Phi_1}{4\sqrt{15}} - \frac{\lambda_{20}\Phi_2}{6\sqrt{5}} - \frac{\lambda_{20}\Phi_3}{4\sqrt{10}},$$

$$
\begin{aligned}
m_{35}^{(3,2,1/6)} &\equiv -\frac{i\lambda_{19}A_1}{2\sqrt{10}} + \frac{i\lambda_{19}A_2}{2\sqrt{15}} - \frac{\lambda_{21}\Phi_1}{4\sqrt{15}} + \frac{\lambda_{21}\Phi_2}{6\sqrt{5}} - \frac{\lambda_{21}\Phi_3}{12\sqrt{10}},\\
m_{43}^{(3,2,1/6)} &\equiv \frac{i\lambda_{19}A_1}{2\sqrt{10}} + \frac{i\lambda_{19}A_2}{2\sqrt{15}} - \frac{\lambda_{21}\Phi_1}{4\sqrt{15}} - \frac{\lambda_{21}\Phi_2}{6\sqrt{5}} - \frac{\lambda_{21}\Phi_3}{4\sqrt{10}},\\
m_{44}^{(3,2,1/6)} &\equiv m_2 + \frac{\lambda_2\Phi_2}{30\sqrt{2}} + \frac{\lambda_2\Phi_3}{20} - \frac{\lambda_6 A_1}{10} - \frac{1}{5}\sqrt{\frac{2}{3}}\lambda_6 A_2,\\
m_{53}^{(3,2,1/6)} &\equiv \frac{i\lambda_{18}A_1}{2\sqrt{10}} - \frac{i\lambda_{18}A_2}{2\sqrt{15}} - \frac{\lambda_{20}\Phi_1}{4\sqrt{15}} + \frac{\lambda_{20}\Phi_2}{6\sqrt{5}} - \frac{\lambda_{20}\Phi_3}{12\sqrt{10}},\\
m_{55}^{(3,2,1/6)} &\equiv m_2 + \frac{\lambda_2\Phi_2}{30\sqrt{2}} + \frac{\lambda_2\Phi_3}{60} + \frac{\lambda_6 A_1}{10} + \frac{1}{5}\sqrt{\frac{2}{3}}\lambda_6 A_2,\\
m_{61}^{(3,2,1/6)} &\equiv -\frac{\lambda_5 A_1}{\sqrt{3}} - \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7\Phi_2,\\
m_{66}^{(3,2,1/6)} &\equiv m_1 + \frac{\lambda_1\Phi_3}{6} + \frac{7\lambda_{10}E}{4\sqrt{15}},\\
m_{71}^{(3,2,1/6)} &\equiv -\frac{2\lambda_5 A_2}{3} - \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7\Phi_3,\\
m_{77}^{(3,2,1/6)} &\equiv m_1 + \frac{\lambda_1\Phi_2}{3\sqrt{2}} + \frac{\lambda_1\Phi_3}{6} + \frac{2\lambda_7 A_1}{5} - \frac{1}{4}\sqrt{\frac{3}{5}}\lambda_{10}E.
\end{aligned}
\tag{66}
$$

$\left[\left(\mathbf{1},\mathbf{2},\frac{1}{2}\right)+\text{c.c.}\right]$

$\mathbf{c}$: $\hat{H}^{(1,2,1/2)}_{(1,2,2)}, \hat{D}^{(1,2,1/2)}_{(1,2,2)}, \hat{D}^{(1,2,1/2)}_{(15,2,2)}, \hat{\Delta}^{(1,2,1/2)}_{(15,2,2)}, \hat{\overline{\Delta}}^{(1,2,1/2)}_{(15,2,2)}, \hat{\Phi}^{(1,2,1/2)}_{(6,2,2)}$

$\mathbf{r}$: $\hat{H}^{(1,2,-1/2)}_{(1,2,2)}, \hat{D}^{(1,2,-1/2)}_{(1,2,2)}, \hat{D}^{(1,2,-1/2)}_{(15,2,2)}, \hat{\overline{\Delta}}^{(1,2,-1/2)}_{(15,2,2)}, \hat{\Delta}^{\left(1,2,-\frac{1}{2}\right)}_{(15,2,2)}, \hat{\Phi}^{(1,2,-1/2)}_{(6,2,2)}$

$$
\begin{pmatrix}
m_3+\sqrt{\frac{3}{5}}\lambda_{13}E & -\frac{i\lambda_{16}A_1}{\sqrt{6}}-\frac{\lambda_{17}\Phi_1}{2} & -\frac{i\lambda_{16}A_2}{\sqrt{3}}-\frac{\lambda_{17}\Phi_3}{2\sqrt{2}} & \frac{\lambda_3\Phi_2}{\sqrt{10}}-\frac{\lambda_3\Phi_3}{2\sqrt{5}} & -\frac{\lambda_4\Phi_2}{\sqrt{10}}-\frac{\lambda_4\Phi_3}{2\sqrt{5}} & -\frac{\lambda_4\overline{v_R}}{\sqrt{5}}\\
\frac{i\lambda_{16}A_1}{\sqrt{6}}-\frac{\lambda_{17}\Phi_1}{2} & m_6+\sqrt{\frac{3}{5}}\lambda_{14}E & \frac{\lambda_{15}\Phi_3}{3\sqrt{3}} & -\frac{i\lambda_{18}A_2}{2\sqrt{5}}+\frac{\lambda_{20}\Phi_3}{4\sqrt{30}} & -\frac{i\lambda_{19}A_2}{2\sqrt{5}}+\frac{\lambda_{21}\Phi_3}{4\sqrt{30}} & -\frac{\lambda_{21}\overline{v_R}}{2\sqrt{30}}\\
\frac{i\lambda_{16}A_2}{\sqrt{3}}-\frac{\lambda_{17}\Phi_3}{2\sqrt{2}} & \frac{\lambda_{15}\Phi_3}{3\sqrt{3}} & m_{33}^{(1,2,1/2)} & m_{34}^{(1,2,1/2)} & m_{35}^{(1,2,1/2)} & -\frac{\lambda_{21}\overline{v_R}}{2\sqrt{10}}\\
\frac{\lambda_4\Phi_2}{\sqrt{10}}-\frac{\lambda_4\Phi_3}{2\sqrt{5}} & \frac{i\lambda_{19}A_2}{2\sqrt{5}}+\frac{\lambda_{21}\Phi_3}{4\sqrt{30}} & m_{43}^{(1,2,1/2)} & m_{44}^{(1,2,1/2)} & \frac{\lambda_{12}E}{\sqrt{15}} & 0\\
-\frac{\lambda_3\Phi_2}{\sqrt{10}}-\frac{\lambda_3\Phi_3}{2\sqrt{5}} & \frac{i\lambda_{18}A_2}{2\sqrt{5}}+\frac{\lambda_{20}\Phi_3}{4\sqrt{30}} & m_{53}^{(1,2,1/2)} & \frac{\lambda_{11}E}{\sqrt{15}} & m_{55}^{(1,2,1/2)} & \frac{\lambda_2\overline{v_R}}{10}\\
-\frac{\lambda_3 v_R}{\sqrt{5}} & -\frac{\lambda_{20}v_R}{2\sqrt{30}} & -\frac{\lambda_{20}v_R}{2\sqrt{10}} & 0 & \frac{\lambda_2 v_R}{10} & m_{66}^{(1,2,1/2)}
\end{pmatrix},
\tag{67}
$$

where

$$
\begin{aligned}
m_{33}^{(1,2,1/2)} &\equiv m_6 - \frac{\lambda_{14}E}{3\sqrt{15}} + \frac{2\sqrt{2}\lambda_{15}\Phi_2}{9},\\
m_{34}^{(1,2,1/2)} &\equiv -\frac{i\lambda_{18}A_1}{2\sqrt{10}} + \frac{i\lambda_{18}A_2}{\sqrt{15}} + \frac{\lambda_{20}\Phi_1}{4\sqrt{15}} - \frac{\lambda_{20}\Phi_3}{6\sqrt{10}},\\
m_{35}^{(1,2,1/2)} &\equiv -\frac{i\lambda_{19}A_1}{2\sqrt{10}} - \frac{i\lambda_{19}A_2}{\sqrt{15}} + \frac{\lambda_{21}\Phi_1}{4\sqrt{15}} + \frac{\lambda_{21}\Phi_3}{6\sqrt{10}},\\
m_{43}^{(1,2,1/2)} &\equiv \frac{i\lambda_{19}A_1}{2\sqrt{10}} - \frac{i\lambda_{19}A_2}{\sqrt{15}} + \frac{\lambda_{21}\Phi_1}{4\sqrt{15}} - \frac{\lambda_{21}\Phi_3}{6\sqrt{10}},\\
m_{44}^{(1,2,1/2)} &\equiv m_2 + \frac{\lambda_2\Phi_2}{15\sqrt{2}} - \frac{\lambda_2\Phi_3}{30} + \frac{\lambda_6 A_1}{10},\\
m_{53}^{(1,2,1/2)} &\equiv \frac{i\lambda_{18}A_1}{2\sqrt{10}} + \frac{i\lambda_{18}A_2}{\sqrt{15}} + \frac{\lambda_{20}\Phi_1}{4\sqrt{15}} + \frac{\lambda_{20}\Phi_3}{6\sqrt{10}},\\
m_{55}^{(1,2,1/2)} &\equiv m_2 + \frac{\lambda_2\Phi_2}{15\sqrt{2}} + \frac{\lambda_2\Phi_3}{30} - \frac{\lambda_6 A_1}{10},\\
m_{66}^{(1,2,1/2)} &\equiv m_1 + \frac{\lambda_1\Phi_2}{\sqrt{2}} + \frac{\lambda_1\Phi_3}{2} + \frac{2\lambda_7 A_1}{5} - \frac{1}{4}\sqrt{\frac{3}{5}}\lambda_{10}E.
\end{aligned}
\tag{68}
$$

$\left[\left(\mathbf{3},\mathbf{1},-\frac{1}{3}\right)+\text{c.c.}\right]$

c: $\hat{H}_{(6,1,1)}^{(3,1,-1/3)}$, $\hat{D}_{(6,1,3)}^{(3,1,-1/3)}$, $\hat{D}_{(10,1,1)}^{(3,1,-1/3)}$, $\hat{\Delta}_{(6,1,1)}^{(3,1,-1/3)}$, $\hat{\bar{\Delta}}_{(6,1,1)}^{(3,1,-1/3)}$, $\hat{\bar{\Delta}}_{(10,1,3)}^{(3,1,-1/3)}$, $\hat{\Phi}_{(15,1,3)}^{(3,1,-1/3)}$

r: $\hat{H}_{(6,1,1)}^{(\bar{3},1,1/3)}$, $\hat{D}_{(6,1,3)}^{(\bar{3},1,1/3)}$, $\hat{D}_{(\bar{10},1,1)}^{(\bar{3},1,1/3)}$, $\hat{\bar{\Delta}}_{(6,1,1)}^{(\bar{3},1,1/3)}$, $\hat{\Delta}_{(6,1,1)}^{(\bar{3},1,1/3)}$, $\hat{\Delta}_{(\bar{10},1,3)}^{(\bar{3},1,1/3)}$, $\hat{\Phi}_{(15,1,3)}^{(\bar{3},1,1/3)}$

$$
\begin{pmatrix}
m_3 - \frac{2\lambda_{13}E}{\sqrt{15}} & m_{12}^{(3,1,-1/3)} & m_{13}^{(3,1,-1/3)} & m_{14}^{(3,1,-1/3)} & m_{15}^{(3,1,-1/3)} & -\sqrt{\frac{2}{15}}\lambda_4\Phi_3 & \frac{\lambda_4\overline{v_R}}{\sqrt{5}}\\
m_{21}^{(3,1,-1/3)} & m_{22}^{(3,1,-1/3)} & \frac{2\lambda_{15}\Phi_3}{9} & m_{24}^{(3,1,-1/3)} & m_{25}^{(3,1,-1/3)} & m_{26}^{(3,1,-1/3)} & \frac{\lambda_4\overline{v_R}}{2\sqrt{15}}\\
m_{31}^{(3,1,-1/3)} & \frac{2\lambda_{15}\Phi_3}{9} & m_{33}^{(3,1,-1/3)} & m_{34}^{(3,1,-1/3)} & m_{35}^{(3,1,-1/3)} & m_{36}^{(3,1,-1/3)} & \frac{\lambda_{21}\overline{v_R}}{2\sqrt{15}}\\
m_{41}^{(3,1,-1/3)} & m_{42}^{(3,1,-1/3)} & m_{43}^{(3,1,-1/3)} & m_2 + \frac{\lambda_6 A_2}{5\sqrt{6}} & \frac{2\lambda_{12}E}{\sqrt{15}} & 0 & 0\\
m_{51}^{(3,1,-1/3)} & m_{52}^{(3,1,-1/3)} & m_{53}^{(3,1,-1/3)} & \frac{2\lambda_{11}E}{\sqrt{15}} & m_2 - \frac{\lambda_6 A_2}{5\sqrt{6}} & \frac{\lambda_2\Phi_3}{15\sqrt{2}} & -\frac{\lambda_2\overline{v_R}}{10\sqrt{3}}\\
-\sqrt{\frac{2}{15}}\lambda_3\Phi_3 & m_{62}^{(3,1,-1/3)} & m_{63}^{(3,1,-1/3)} & 0 & \frac{\lambda_2\Phi_3}{15\sqrt{2}} & m_{66}^{(3,1,-1/3)} & -\frac{\lambda_2\overline{v_R}}{5\sqrt{6}}\\
\frac{\lambda_3 v_R}{\sqrt{5}} & \frac{\lambda_{20}v_R}{2\sqrt{15}} & \frac{\lambda_{20}v_R}{2\sqrt{15}} & 0 & -\frac{\lambda_2 v_R}{10\sqrt{3}} & -\frac{\lambda_2 v_R}{5\sqrt{6}} & m_{77}^{(3,1,-1/3)}
\end{pmatrix},
\tag{69}
$$

where

$$m_{12}^{(3,1,-1/3)} \equiv -\frac{i\lambda_{16}A_1}{\sqrt{3}} - \frac{\lambda_{17}\Phi_3}{2\sqrt{3}},$$

$$m_{13}^{(3,1,-1/3)} \equiv -\frac{i\sqrt{2}\lambda_{16}A_2}{3} - \frac{\lambda_{17}\Phi_2}{\sqrt{6}},$$

$$m_{14}^{(3,1,-1/3)} \equiv \frac{\lambda_3\Phi_2}{\sqrt{30}} - \frac{\lambda_3\Phi_1}{\sqrt{10}},$$

$$m_{15}^{(3,1,-1/3)} \equiv -\frac{\lambda_4\Phi_1}{\sqrt{10}} - \frac{\lambda_4\Phi_2}{\sqrt{30}},$$

$$m_{21}^{(3,1,-1/3)} \equiv \frac{i\lambda_{16}A_1}{\sqrt{3}} - \frac{\lambda_{17}\Phi_3}{2\sqrt{3}},$$

$$m_{22}^{(3,1,-1/3)} \equiv m_6 + \frac{4\lambda_{14}E}{3\sqrt{15}} + \frac{1}{3}\sqrt{\frac{2}{3}}\lambda_{15}\Phi_1,$$

$$m_{24}^{(3,1,-1/3)} \equiv -\frac{i\lambda_{18}A_1}{2\sqrt{5}} + \frac{\lambda_{20}\Phi_3}{12\sqrt{5}},$$

$$m_{25}^{(3,1,-1/3)} \equiv -\frac{i\lambda_{19}A_1}{2\sqrt{5}} + \frac{\lambda_{21}\Phi_3}{12\sqrt{5}},$$

$$m_{26}^{(3,1,-1/3)} \equiv -\frac{i\lambda_{19}A_2}{\sqrt{15}} + \frac{\lambda_{21}\Phi_2}{6\sqrt{5}},$$

$$m_{31}^{(3,1,-1/3)} \equiv \frac{i\sqrt{2}\lambda_{16}A_2}{3} - \frac{\lambda_{17}\Phi_2}{\sqrt{6}},$$

$$m_{33}^{(3,1,-1/3)} \equiv m_6 - \frac{2\lambda_{14}E}{\sqrt{15}} + \frac{\sqrt{2}\lambda_{15}\Phi_2}{9}$$

$$m_{34}^{(3,1,-1/3)} \equiv \frac{i\lambda_{18}A_2}{\sqrt{30}} - \frac{\lambda_{20}\Phi_2}{6\sqrt{10}},$$

$$m_{35}^{(3,1,-1/3)} \equiv -\frac{i\lambda_{19}A_2}{\sqrt{30}} + \frac{\lambda_{21}\Phi_2}{6\sqrt{10}},$$

$$m_{36}^{(3,1,-1/3)} \equiv -\frac{i\lambda_{19}A_1}{\sqrt{10}} + \frac{\lambda_{21}\Phi_3}{6\sqrt{10}},$$

$$m_{41}^{(3,1,-1/3)} \equiv \frac{\lambda_4\Phi_2}{\sqrt{30}} - \frac{\lambda_4\Phi_1}{\sqrt{10}},$$

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$$m_{42}^{(3,1,-1/3)} \equiv \frac{i\lambda_{19}A_1}{2\sqrt{5}} + \frac{\lambda_{21}\Phi_3}{12\sqrt{5}},$$

$$m_{43}^{(3,1,-1/3)} \equiv -\frac{i\lambda_{19}A_2}{\sqrt{30}} - \frac{\lambda_{21}\Phi_2}{6\sqrt{10}},$$

$$m_{51}^{(3,1,-1/3)} \equiv -\frac{\lambda_3\Phi_1}{\sqrt{10}} - \frac{\lambda_3\Phi_2}{\sqrt{30}},$$

$$m_{52}^{(3,1,-1/3)} \equiv \frac{i\lambda_{18}A_1}{2\sqrt{5}} + \frac{\lambda_{20}\Phi_3}{12\sqrt{5}},$$

$$m_{53}^{(3,1,-1/3)} \equiv \frac{i\lambda_{18}A_2}{\sqrt{30}} + \frac{\lambda_{20}\Phi_2}{6\sqrt{10}},$$

$$m_{62}^{(3,1,-1/3)} \equiv \frac{i\lambda_{18}A_2}{\sqrt{15}} + \frac{\lambda_{20}\Phi_2}{6\sqrt{5}},$$

$$m_{63}^{(3,1,-1/3)} \equiv \frac{i\lambda_{18}A_1}{\sqrt{10}} + \frac{\lambda_{20}\Phi_3}{6\sqrt{10}},$$

$$m_{66}^{(3,1,-1/3)} \equiv m_2 + \frac{\lambda_2\Phi_1}{10\sqrt{6}} + \frac{\lambda_2\Phi_2}{30\sqrt{2}} - \frac{\lambda_6 A_2}{5\sqrt{6}},$$

$$m_{77}^{(3,1,-1/3)} \equiv m_1 + \frac{\lambda_1\Phi_1}{\sqrt{6}} + \frac{\lambda_1\Phi_2}{3\sqrt{2}} + \frac{2\lambda_1\Phi_3}{3} + \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7 A_2 + \frac{\lambda_{10}E}{2\sqrt{15}}.$$

$[(\mathbf{1},\mathbf{1},2)+\text{c.c.}]$
c: $\hat{\Delta}^{(1,1,2)}_{(10,1,3)}$
r: $\hat{\bar{\Delta}}^{(1,1,-2)}_{(10,1,3)}$

$$m_2 + \frac{\lambda_2\Phi_1}{10\sqrt{6}} + \frac{\lambda_2\Phi_2}{10\sqrt{2}} - \frac{\lambda_2\Phi_3}{10} + \frac{\lambda_6 A_1}{5} - \frac{1}{5}\sqrt{\frac{3}{2}}\lambda_6 A_2. \tag{71}$$

$\left[(\mathbf{1},\mathbf{2},\frac{3}{2})+\text{c.c.}\right]$
c: $\hat{\Phi}^{(1,2,3/2)}_{(10,2,2)}$
r: $\hat{\bar{\Phi}}^{(1,2,-3/2)}_{(10,2,2)}$

$$m_1 + \frac{\lambda_1\Phi_2}{\sqrt{2}} - \frac{\lambda_1\Phi_3}{2} - \frac{2}{5}\lambda_7 A_1 - \frac{1}{4}\sqrt{\frac{3}{5}}\lambda_{10}E. \tag{72}$$

$(\mathbf{1},\mathbf{3},0)$
c: $\hat{A}^{(1,3,0)}_{(1,3,1)}$, $\hat{E}^{(1,3,0)}_{(1,3,3)}$, $\hat{\Phi}^{(1,3,0)}_{(15,3,1)}$
r: $\hat{A}^{(1,3,0)}_{(1,3,1)}$, $\hat{E}^{(1,3,0)}_{(1,3,3)}$, $\hat{\Phi}^{(1,3,0)}_{(15,3,1)}$

$$\begin{pmatrix} m_4 - \sqrt{\frac{2}{3}}\lambda_5\Phi_1 + \sqrt{\frac{3}{5}}\lambda_9 E & \lambda_9 A_1 & -\sqrt{\frac{2}{3}}\lambda_5 A_2 + \frac{2}{5}\sqrt{2}\lambda_7\Phi_2 \\ \lambda_9 A_1 & m_5 + 3\sqrt{\frac{3}{5}}\lambda_8 E & -\frac{\lambda_{10}\Phi_3}{2} \\ -\sqrt{\frac{2}{3}}\lambda_5 A_2 + \frac{2}{5}\sqrt{2}\lambda_7\Phi_2 & -\frac{\lambda_{10}\Phi_3}{2} & m_1 - \frac{\lambda_1\Phi_1}{\sqrt{6}} + \frac{\sqrt{2}\lambda_1\Phi_2}{3} - \frac{4}{5}\sqrt{\frac{2}{3}}\lambda_7 A_2 + \frac{\lambda_{10}E}{2\sqrt{15}} \end{pmatrix}. \tag{73}$$

$[(\mathbf{1},\mathbf{3},1)+\text{c.c.}]$
c: $\hat{E}^{(1,3,1)}_{(1,3,3)}$, $\hat{\bar{\Delta}}^{(1,3,1)}_{(\bar{10},3,1)}$
r: $\hat{E}^{(1,3,-1)}_{(1,3,3)}$, $\hat{\Delta}^{(1,3,-1)}_{(10,3,1)}$

$$\begin{pmatrix} m_5 + 3\sqrt{\frac{3}{5}}\lambda_8 E & \frac{2\lambda_{12}\overline{v_R}}{5} \\ \frac{2\lambda_{11}v_R}{5} & m_2 - \frac{\lambda_2\Phi_1}{10\sqrt{6}} + \frac{\lambda_2\Phi_2}{10\sqrt{2}} + \frac{1}{5}\sqrt{\frac{3}{2}}\lambda_6 A_2 \end{pmatrix}. \tag{74}$$

$[(\mathbf{3},\mathbf{1},-\frac{4}{3})+\text{c.c.}]$
c: $\hat{D}^{(3,1,-4/3)}_{(6,1,3)}$, $\hat{\bar{\Delta}}^{(3,1,-4/3)}_{(\bar{10},1,3)}$
r: $\hat{\bar{D}}^{(3,1,4/3)}_{(\bar{6},1,3)}$, $\hat{\Delta}^{(3,1,4/3)}_{(10,1,3)}$

$$\begin{pmatrix} m_6 + \frac{4\lambda_{14}E}{3\sqrt{15}} + \frac{1}{3}\sqrt{\frac{2}{3}}\lambda_{15}\Phi_1 - \frac{2\lambda_{15}\Phi_3}{9} & -\frac{i\lambda_{19}A_2}{\sqrt{15}} + \frac{\lambda_{21}\Phi_2}{6\sqrt{5}} - \frac{\lambda_{21}\Phi_3}{3\sqrt{10}} \\ \frac{i\lambda_{18}A_2}{\sqrt{15}} + \frac{\lambda_{20}\Phi_2}{6\sqrt{5}} - \frac{\lambda_{20}\Phi_3}{3\sqrt{10}} & m_2 + \frac{\lambda_2\Phi_1}{10\sqrt{6}} + \frac{\lambda_2\Phi_2}{30\sqrt{2}} - \frac{\lambda_2\Phi_3}{30} + \frac{\lambda_6 A_1}{5} - \frac{\lambda_6 A_2}{5\sqrt{6}} \end{pmatrix}. \tag{75}$$

$[(\mathbf{3},\mathbf{1},\frac{5}{3})+\text{c.c.}]$
c: $\hat{\Phi}^{(3,1,5/3)}_{(\bar{15},1,3)}$
r: $\hat{\Phi}^{(3,1,-5/3)}_{(15,1,3)}$

$$m_1 + \frac{\lambda_1\Phi_1}{\sqrt{6}} + \frac{\lambda_1\Phi_2}{3\sqrt{2}} - \frac{2\lambda_1\Phi_3}{3} + \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7 A_2 + \frac{\lambda_{10}E}{2\sqrt{15}}. \tag{76}$$

$[(\mathbf{3},\mathbf{2},\frac{7}{6})+\text{c.c.}]$
c: $\hat{D}^{(3,2,7/6)}_{(\bar{15},2,2)}$, $\hat{\Delta}^{(3,2,7/6)}_{(15,2,2)}$, $\hat{\bar{\Delta}}^{(3,2,7/6)}_{(\bar{15},2,2)}$
r: $\hat{\bar{D}}^{(3,2,-7/6)}_{(15,2,2)}$, $\hat{\bar{\Delta}}^{(3,2,-7/6)}_{(15,2,2)}$, $\hat{\Delta}^{(3,2,7/6)}_{(15,2,2)}$

$$\begin{pmatrix} m_{11}^{(3,2,7/6)} & m_{12}^{(3,2,7/6)} & m_{13}^{(3,2,7/6)} \\ m_{21}^{(3,2,7/6)} & m_{22}^{(3,2,7/6)} & \frac{\lambda_{12}E}{\sqrt{15}} \\ m_{31}^{(3,2,7/6)} & \frac{\lambda_{11}E}{\sqrt{15}} & m_{33}^{(3,2,7/6)} \end{pmatrix}, \tag{77}$$

where

$$m_{11}^{(3,2,7/6)} \equiv m_6 - \frac{\lambda_{14}E}{3\sqrt{15}} + \frac{\sqrt{2}\lambda_{15}\Phi_2}{9} - \frac{2\lambda_{15}\Phi_3}{9},$$

$$m_{12}^{(3,2,7/6)} \equiv -\frac{i\lambda_{18}A_1}{2\sqrt{10}} + \frac{i\lambda_{18}A_2}{2\sqrt{15}} + \frac{\lambda_{20}\Phi_1}{4\sqrt{15}} + \frac{\lambda_{20}\Phi_2}{6\sqrt{5}} - \frac{\lambda_{20}\Phi_3}{4\sqrt{10}},$$

$$m_{13}^{(3,2,7/6)} \equiv -\frac{i\lambda_{19}A_1}{2\sqrt{10}} - \frac{i\lambda_{19}A_2}{2\sqrt{15}} + \frac{\lambda_{21}\Phi_1}{4\sqrt{15}} - \frac{\lambda_{21}\Phi_2}{6\sqrt{5}} - \frac{\lambda_{21}\Phi_3}{12\sqrt{10}},$$

$$m_{21}^{(3,2,7/6)} \equiv \frac{i\lambda_{19}A_1}{2\sqrt{10}} - \frac{i\lambda_{19}A_2}{2\sqrt{15}} + \frac{\lambda_{21}\Phi_1}{4\sqrt{15}} + \frac{\lambda_{21}\Phi_2}{6\sqrt{5}} - \frac{\lambda_{21}\Phi_3}{4\sqrt{10}}, \tag{78}$$

$$m_{22}^{(3,2,7/6)} \equiv m_2 + \frac{\lambda_2\Phi_2}{30\sqrt{2}} - \frac{\lambda_2\Phi_3}{20} + \frac{\lambda_6 A_1}{10} - \frac{1}{5}\sqrt{\frac{2}{3}}\lambda_6 A_2,$$

$$m_{31}^{(3,2,7/6)} \equiv \frac{i\lambda_{18}A_1}{2\sqrt{10}} + \frac{i\lambda_{18}A_2}{2\sqrt{15}} + \frac{\lambda_{20}\Phi_1}{4\sqrt{15}} - \frac{\lambda_{20}\Phi_2}{6\sqrt{5}} - \frac{\lambda_{20}\Phi_3}{12\sqrt{10}},$$

$$m_{33}^{(3,2,7/6)} \equiv m_2 + \frac{\lambda_2\Phi_2}{30\sqrt{2}} - \frac{\lambda_2\Phi_3}{60} - \frac{\lambda_6 A_1}{10} + \frac{1}{5}\sqrt{\frac{2}{3}}\lambda_6 A_2.$$

$[(\mathbf{3},\mathbf{3},-\frac{1}{3})+\text{c.c.}]$
c: $\hat{D}^{(3,3,-1/3)}_{(\underline{6},3,1)}$, $\hat{\Delta}^{(3,3,-1/3)}_{(\underline{10},3,1)}$
r: $\hat{D}^{(3,3,1/3)}_{(6,3,1)}$, $\hat{\bar{\Delta}}^{(3,3,1/3)}_{(\overline{10},3,1)}$

$$\begin{pmatrix} m_6 + \frac{4\lambda_{14}E}{3\sqrt{15}} - \frac{1}{3}\sqrt{\frac{2}{3}}\lambda_{15}\Phi_1 & -\frac{i\lambda_{18}A_2}{\sqrt{15}} + \frac{\lambda_{20}\Phi_2}{6\sqrt{5}} \\ \frac{i\lambda_{19}A_2}{\sqrt{15}} + \frac{\lambda_{21}\Phi_2}{6\sqrt{5}} & m_2 - \frac{\lambda_2\Phi_1}{10\sqrt{6}} + \frac{\lambda_2\Phi_2}{30\sqrt{2}} + \frac{\lambda_6 A_2}{5\sqrt{6}} \end{pmatrix}. \tag{79}$$

$[(\mathbf{3},\mathbf{3},\frac{2}{3})+\text{c.c.}]$
c: $\hat{\Phi}^{(3,3,2/3)}_{(\underline{15},3,1)}$
r: $\hat{\Phi}^{(3,3,-2/3)}_{(15,3,1)}$

$$m_1 - \frac{\lambda_1\Phi_1}{\sqrt{6}} + \frac{\lambda_1\Phi_2}{3\sqrt{2}} - \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7 A_2 + \frac{\lambda_{10}E}{2\sqrt{15}}. \tag{80}$$

$[(\mathbf{6},\mathbf{1},-\frac{2}{3})+\text{c.c.}]$
c: $\hat{E}^{(6,1,-2/3)}_{(20',1,1)}$, $\hat{\bar{\Delta}}^{(6,1,-2/3)}_{(10,1,3)}$
r: $\hat{\bar{E}}^{(6,1,2/3)}_{(20',1,1)}$, $\hat{\Delta}^{(6,1,2/3)}_{(\overline{10},1,3)}$

$$\begin{pmatrix} m_5 - 2\sqrt{\frac{3}{5}}\lambda_8 E & \frac{2\lambda_{12}\overline{v_R}}{5} \\ \frac{2\lambda_{11}v_R}{5} & m_2 + \frac{\lambda_2\Phi_1}{10\sqrt{6}} - \frac{\lambda_2\Phi_2}{30\sqrt{2}} + \frac{\lambda_2\Phi_3}{30} + \frac{\lambda_6 A_1}{5} + \frac{\lambda_6 A_2}{5\sqrt{6}} \end{pmatrix}. \tag{81}$$

$[(\mathbf{6},\mathbf{1},\frac{1}{3})+\text{c.c.}]$

c: $\hat{D}^{(6,1,1/3)}_{(10,1,1)}$, $\hat{\bar{\Delta}}^{(6,1,1/3)}_{(10,1,3)}$

r: $\hat{D}^{(6,1,-1/3)}_{(\bar{10},1,1)}$, $\hat{D}^{(6,1,-1/3)}_{(\bar{10},1,3)}$

$$\begin{pmatrix} m_6-\frac{2\lambda_{14}E}{\sqrt{15}}-\frac{\sqrt{2}\lambda_{15}\Phi_2}{9} & -\frac{i\lambda_{19}A_1}{\sqrt{10}}-\frac{\lambda_{21}\Phi_3}{6\sqrt{10}} \\ \frac{i\lambda_{18}A_1}{\sqrt{10}}-\frac{\lambda_{20}\Phi_3}{6\sqrt{10}} & m_2+\frac{\lambda_2\Phi_1}{10\sqrt{6}}-\frac{\lambda_2\Phi_2}{30\sqrt{2}}+\frac{\lambda_6A_2}{5\sqrt{6}} \end{pmatrix}. \tag{82}$$

$[(\mathbf{6},\mathbf{1},\frac{4}{3})+\text{c.c.}]$

c: $\hat{\bar{\Delta}}^{(6,1,4/3)}_{(10,1,3)}$

r: $\hat{\Delta}^{(6,1,-4/3)}_{(\bar{10},1,3)}$

$$m_2+\frac{\lambda_2\Phi_1}{10\sqrt{6}}-\frac{\lambda_2\Phi_2}{30\sqrt{2}}-\frac{\lambda_2\Phi_3}{30}-\frac{\lambda_6A_1}{5}+\frac{\lambda_6A_2}{5\sqrt{6}}. \tag{83}$$

$[(\mathbf{6},\mathbf{2},-\frac{1}{6})+\text{c.c.}]$

c: $\hat{\phi}^{(6,2,-1/6)}_{(10,2,2)}$

r: $\hat{\Phi}^{(6,2,1/6)}_{(\bar{10},2,2)}$

$$m_1-\frac{\lambda_1\Phi_2}{3\sqrt{2}}+\frac{\lambda_1\Phi_3}{6}-\frac{2}{5}\lambda_7A_1-\frac{1}{4}\sqrt{\frac{3}{5}}\lambda_{10}E. \tag{84}$$

$[(\mathbf{6},\mathbf{2},\frac{5}{6})+\text{c.c.}]$

c: $\hat{\Phi}^{(6,2,5/6)}_{(10,2,2)}$

r: $\hat{\Phi}^{(6,2,-5/6)}_{(\bar{10},2,2)}$

$$m_1-\frac{\lambda_1\Phi_2}{3\sqrt{2}}-\frac{\lambda_1\Phi_3}{6}+\frac{2}{5}\lambda_7A_1-\frac{1}{4}\sqrt{\frac{3}{5}}\lambda_{10}E. \tag{85}$$

$[(\mathbf{6},\mathbf{3},1/3)+\text{c.c.}]$

c: $\hat{\Delta}^{(6,3,1/3)}_{(10,3,1)}$

r: $\hat{\bar{\Delta}}^{(6,3,-1/3)}_{(\bar{10},3,1)}$

$$m_2-\frac{\lambda_2\Phi_1}{10\sqrt{6}}-\frac{\lambda_2\Phi_2}{30\sqrt{2}}-\frac{\lambda_6A_2}{5\sqrt{6}}. \tag{86}$$

$(\mathbf{8},\mathbf{1},0)$

c: $\hat{A}^{(8,1,0)}_{(15,1,1)}, \hat{E}^{(8,1,0)}_{(20',1,1)}, \hat{\Phi}^{(8,1,0)}_{(15,1,1)}, \hat{\Phi}^{(8,1,0)}_{(15,1,3)}$

r: $\hat{A}^{(8,1,0)}_{(15,1,1)}, \hat{E}^{(8,1,0)}_{(20',1,1)}, \hat{\Phi}^{(8,1,0)}_{(15,1,1)}, \hat{\Phi}^{(8,1,0)}_{(15,1,3)}$

$$\begin{pmatrix} m_4 - \frac{\sqrt{2}\lambda_5\Phi_2}{3} - \frac{2\lambda_9 E}{\sqrt{15}} & \sqrt{\frac{2}{3}}\lambda_9 A_2 & -\frac{\sqrt{2}\lambda_5 A_2}{3} + \frac{2\sqrt{2}\lambda_7\Phi_1}{5} & -\sqrt{\frac{2}{3}}\lambda_5 A_1 + \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7\Phi_3 \\ \sqrt{\frac{2}{3}}\lambda_9 A_2 & m_5 - 2\sqrt{\frac{3}{5}}\lambda_8 E & -\frac{\lambda_{10}\Phi_2}{\sqrt{6}} & -\frac{\lambda_{10}\Phi_3}{\sqrt{6}} \\ -\frac{\sqrt{2}\lambda_5 A_2}{3} + \frac{2}{5}\sqrt{2}\lambda_7\Phi_1 & -\frac{\lambda_{10}\Phi_2}{\sqrt{6}} & m_1 - \frac{\lambda_1\Phi_2}{3\sqrt{2}} - \frac{2\lambda_{10}E}{\sqrt{15}} & \frac{\lambda_1\Phi_3}{3\sqrt{2}} - \frac{2\sqrt{2}\lambda_7 A_1}{5} \\ -\sqrt{\frac{2}{3}}\lambda_5 A_1 + \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7\Phi_3 & -\frac{\lambda_{10}\Phi_3}{\sqrt{6}} & \frac{\lambda_1\Phi_3}{3\sqrt{2}} - \frac{2\sqrt{2}\lambda_7 A_1}{5} & m_{44}^{(8,1,0)} \end{pmatrix}, \quad (87)$$

where

$$m_{44}^{(8,1,0)} \equiv m_1 + \frac{\lambda_1\Phi_1}{\sqrt{6}} - \frac{\lambda_1\Phi_2}{3\sqrt{2}} - \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7 A_2 + \frac{\lambda_{10}E}{2\sqrt{15}}. \quad (88)$$

$[(\mathbf{8},\mathbf{1},1)+\text{c.c.}]$

c: $\hat{\Phi}^{(8,1,1)}_{(15,1,3)}$

r: $\hat{\Phi}^{(8,1,-1)}_{(15,1,3)}$

$$m_1 + \frac{\lambda_1\Phi_1}{\sqrt{6}} - \frac{\lambda_1\Phi_2}{3\sqrt{2}} - \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7 A_2 + \frac{\lambda_{10}E}{2\sqrt{15}}. \quad (89)$$

$[(\mathbf{8},\mathbf{2},-\frac{1}{2})+\text{c.c.}]$

c: $\hat{D}^{(8,2,1/2)}_{(15,2,2)}, \hat{\Delta}^{(8,2,1/2)}_{(15,2,2)}, \hat{\bar{\Delta}}^{(8,2,1/2)}_{(15,2,2)}$

r: $\hat{D}^{(8,2,-1/2)}_{(15,2,2)}, \hat{\bar{\Delta}}^{(8,2,-1/2)}_{(15,2,2)}, \hat{\Delta}^{(8,2,-1/2)}_{(15,2,2)}$

$$\begin{pmatrix} m_{11}^{(8,2,-1/2)} & m_{12}^{(8,2,-1/2)} & m_{13}^{(8,2,-1/2)} \\ m_{21}^{(8,2,-1/2)} & m_{22}^{(8,2,-1/2)} & \frac{\lambda_{12}E}{\sqrt{15}} \\ m_{31}^{(8,2,-1/2)} & \frac{\lambda_{11}E}{\sqrt{15}} & m_{33}^{(8,2,-1/2)} \end{pmatrix}, \quad (90)$$

where

$$m_{11}^{(8,2,-1/2)} \equiv m_6 - \frac{\lambda_{14}E}{3\sqrt{15}} - \frac{\sqrt{2}\lambda_{15}\Phi_2}{9},$$

$$m_{12}^{(8,2,-1/2)} \equiv -\frac{i\lambda_{18}A_1}{2\sqrt{10}} - \frac{i\lambda_{18}A_2}{2\sqrt{15}} + \frac{\lambda_{20}\Phi_1}{4\sqrt{15}} + \frac{\lambda_{20}\Phi_3}{12\sqrt{10}},$$

$$m_{13}^{(8,2,-1/2)} \equiv -\frac{i\lambda_{19}A_1}{2\sqrt{10}} + \frac{i\lambda_{19}A_2}{2\sqrt{15}} + \frac{\lambda_{21}\Phi_1}{4\sqrt{15}} - \frac{\lambda_{21}\Phi_3}{12\sqrt{10}},$$

$$m_{21}^{(8,2,-1/2)} \equiv \frac{i\lambda_{19}A_1}{2\sqrt{10}} + \frac{i\lambda_{19}A_2}{2\sqrt{15}} + \frac{\lambda_{21}\Phi_1}{4\sqrt{15}} + \frac{\lambda_{21}\Phi_3}{12\sqrt{10}}, \quad (91)$$

$$m_{22}^{(8,2,-1/2)} \equiv m_2 - \frac{\lambda_2\Phi_2}{30\sqrt{2}} + \frac{\lambda_2\Phi_3}{60} + \frac{\lambda_6 A_1}{10},$$

$$m_{31}^{(8,2,-1/2)} \equiv \frac{i\lambda_{18}A_1}{2\sqrt{10}} - \frac{i\lambda_{18}A_2}{2\sqrt{15}} + \frac{\lambda_{20}\Phi_1}{4\sqrt{15}} - \frac{\lambda_{20}\Phi_3}{12\sqrt{10}},$$

$$m_{33}^{(8,2,-1/2)} \equiv m_2 - \frac{\lambda_2\Phi_2}{30\sqrt{2}} - \frac{\lambda_2\Phi_3}{60} - \frac{\lambda_6 A_1}{10}.$$

$(\mathbf{8},\mathbf{3},0)$

$\mathbf{c}$: $\hat{\Phi}_{(15,3,1)}^{(8,3,0)}$

$\mathbf{r}$: $\hat{\Phi}_{(15,3,1)}^{(8,3,0)}$

$$m_1 - \frac{\lambda_1\Phi_1}{\sqrt{6}} - \frac{\lambda_1\Phi_2}{3\sqrt{2}} + \frac{2}{5}\sqrt{\frac{2}{3}}\lambda_7 A_2 + \frac{\lambda_{10}E}{2\sqrt{15}}. \tag{92}$$

B. Tests and consistency checks of the total mass matrix

The following consistency checks of the total mass matrix have been performed (see also Ref. 17):

(1) The CG coefficients appearing in the total mass matrix have been found to satisfy the Hermiticity relation (50).

(2) The trace of the total mass matrix has been evaluated and it has been found that it satisfies Eq. (56).

(3) For the G_{321} symmetric vacuum, the number of the would-be NG modes have been found to be equal to the number of the broken generators, i.e., massive gauge bosons, $45-12=33$. Here, 45 represents the number of gauge bosons in the adjoint irrep of the SO(10) group, and 12 represents the number of the gauge bosons in the standard model (G_{321} group). The check has been performed numerically for several tens of randomly chosen sets of the parameters of the superpotential $\lambda_1,\ldots,\lambda_{21}$ and $m_1,\ldots,m_6$, constrained by VEV Eqs. (28).

(4) For the SU(5) symmetric vacuum, it has been found that the number of the different mass eigenvalues is 21. The number of independent SU(5) irreps contained in the total representation of the model R is 22 (see Appendix A), and the would-be NG bosons are in two multiplets $[(\mathbf{1})+(\mathbf{10}+\overline{\mathbf{10}})]$. Therefore, there are in total 21 mass eigenvalues: 20 different from zero and one equal to zero. All other states must be accommodated in the SU(5) irreps. Further, for the SU(5) symmetric vacuum, all eigenvalues of the doublet Higgs matrix $(\mathbf{1},\mathbf{2},\frac{1}{2})$ are contained in the spectrum of the triplet Higgs matrix $(\mathbf{3},\mathbf{1},-\frac{1}{3})$. The only mass eigenvalue of the triplet Higgs matrix spectrum not contained in the doublet mass spectrum belongs to the SU(5) multiplet **50**, leading to the following relation between determinants of these two matrices:

$$\det(M^{(3,1,-1/3)} - \lambda \times \mathbf{1}) = (m_{50}^{(3,1,-1/3)} - \lambda)\det(M^{(1,2,1/2)} - \lambda \times \mathbf{1}). \tag{93}$$

The above relation gives a very strong test for these two matrices. All above checks have been performed numerically, in the same way as explained in the previous item. Our mass matrices passed all checks. For the SU(5) symmetric vacuum, all VEVs, except E, are different from zero, and they are nontrivially correlated through the VEV Eqs. (28) and SU(5) symmetry conditions (30). Therefore, these tests serve as a strong check of the total mass matrix up to terms which depend on E.

(5) For the G_{422} symmetric vacuum, it has been found that the number of different mass eigenvalues is 27, what is just the number of the independent G_{422} irreps (see Appendix A). The number of NG states, contained in G_{422} irrep $(\mathbf{6},\mathbf{2},\mathbf{2})$ is $45-21=24$. These checks have been performed numerically as explained above. All other states have been found to be accommodated in G_{422} irreps. For the G_{422} symmetric vacuum, VEVs different from zero are Φ_1 and E, and therefore this serves as a check of the E-dependent parts of the total mass matrix.

(6) Similar tests are satisfied for other higher symmetries G_{51}, G_{421}, G_{3221}, and G_{3211}.

We stress that all mass matrices in Ref. 17, derived for minimal SO(10) model ($R=\mathbf{10}+\mathbf{126}+\overline{\mathbf{126}}+\mathbf{210}$), satisfy all of the above consistency checks, and are just a special case of the mass matrices in this paper. Further, all results including CG coefficients and mass matrices were obtained analytically including checks.

In the recent calculations in Refs. 20 and 21, that appeared after Ref. 17, the necessary condition (93) between doublets and triplets is not satisfied. The Hermiticity condition (50) and the total trace relation (56) are also not satisfied in these references. Further, none of the higher symmetry tests is satisfied. That is a consequence of different phase conventions in Ref. 17 and phase conventions in Refs. 20 and 21.

In this paper, all results for the CG coefficients and mass matrices have been also obtained analytically. Checks have been performed numerically and it has been found that the mass matrices satisfy ALL consistency checks.

VI. MASS MATRICES OF QUARKS AND LEPTONS

After the symmetry breaking down to the G_{321} subgroup, the electroweak symmetry breaking $\mathrm{SU}(2)_L\times\mathrm{U}(1)_Y\to\mathrm{U}(1)_{\mathrm{em}}$ can be achieved by the VEVs of doublets included in the fields H, D, Δ, $\overline{\Delta}$, and Φ. These fields are given by [see Table 2 (Ref. 19)] $\tilde{H}_{u/d}=H^{(1,2,\pm1/2)}_{(1,2,2)}$, $D_{u/d}=D^{(1,2,\pm1/2)}_{(1,2,2)}$, $\tilde{D}_{u/d}=D^{(1,2,\pm1/2)}_{(15,2,2)}$, $\overline{\Delta}_{u/d}=\overline{\Delta}^{(1,2,\pm1/2)}_{(15,2,2)}$, $\Delta_{u/d}=\Delta^{(1,2,\pm1/2)}_{(15,2,2)}$, $\Phi_{u/d}=\Phi^{(1,2,\pm1/2)}_{(\overline{10},2,2)}$. The Yukawa couplings of Eq. (1) including these doublets can be written as follows:

$$\begin{aligned}W_Y &= U^c_i(Y^{ij}_{10}\tilde{H}_u + Y^{ij}_{120}D_u + Y^{ij}_{120}\tilde{D}_u + Y^{ij}_{126}\overline{\Delta}_u)Q_j + D^c_i(Y^{ij}_{10}\tilde{H}_d + Y^{ij}_{120}D_d + Y^{ij}_{120}\tilde{D}_d + Y^{ij}_{126}\overline{\Delta}_d)Q_j\\ &\quad + N^c_i(Y^{ij}_{10}\tilde{H}_u + Y^{ij}_{120}D_u - 3Y^{ij}_{120}\tilde{D}_u - 3Y^{ij}_{126}\overline{\Delta}_u)L_j + E^c_i(Y^{ij}_{10}\tilde{H}_d + Y^{ij}_{120}D_d - 3Y^{ij}_{120}\tilde{D}_d - 3Y^{ij}_{126}\overline{\Delta}_d)L_j,\end{aligned} \tag{94}$$

where U^c, D^c, N^c, and E^c are the right-handed $\mathrm{SU}(2)_L$ singlet quark and lepton superfields, Q and L are the left-handed $\mathrm{SU}(2)_L$ doublet quark and lepton superfields, respectively. This is a generalization of the renormalizable minimal SO(10) model,[6,7] including **120**. Note that the successful gauge-couplings unification is realized with only the MSSM particle contents. This means that only one pair of Higgs doublets remains light and others should be heavy ($\geqslant M_G$). Here we accept the simple picture that the low-energy superpotential is described by only one pair of light Higgs doublets (H_u and H_d) in the MSSM. But, in general, these Higgs fields are admixtures of all Higgs doublets having the same quantum numbers in the original model such as

$$\begin{aligned}H_u &= \tilde{\alpha}^1_u\tilde{H}_u + \tilde{\alpha}^2_u D_u + \tilde{\alpha}^3_u\tilde{D}_u + \tilde{\alpha}^4_u\overline{\Delta}_u + \tilde{\alpha}^5_u\Delta_u + \tilde{\alpha}^6_u\Phi_u,\\ H_d &= \tilde{\alpha}^1_d\tilde{H}_d + \tilde{\alpha}^2_d D_d + \tilde{\alpha}^3_d\tilde{D}_d + \tilde{\alpha}^4_d\overline{\Delta}_d + \tilde{\alpha}^5_d\Delta_d + \tilde{\alpha}^6_d\Phi_d,\end{aligned} \tag{95}$$

where $\tilde{\alpha}^i_{u,d}$ ($i=1,2,\ldots,5,6$) denote elements of the unitary matrix which rotate the flavor basis in the original model into the (SUSY) mass eigenstates. As mentioned above, the low-energy superpotential is described only by the light Higgs doublets H_u and H_d,

$$\begin{aligned}W_Y &= U^c_i(\alpha^1_u Y^{ij}_{10} + \alpha^2_u Y^{ij}_{120} + \alpha^3_u Y^{ij}_{120} + \alpha^4_u Y^{ij}_{126})H_u Q_j + D^c_i(\alpha^1_d Y^{ij}_{10} + \alpha^2_d Y^{ij}_{120} + \alpha^3_d Y^{ij}_{120} + \alpha^4_d Y^{ij}_{126})H_d Q_j\\ &\quad + N^c_i(\alpha^1_u Y^{ij}_{10} + \alpha^2_u Y^{ij}_{120} - 3\alpha^3_u Y^{ij}_{120} - 3\alpha^4_u Y^{ij}_{126})H_u L_j + E^c_i(\alpha^1_d Y^{ij}_{10} + \alpha^2_d Y^{ij}_{120} - 3\alpha^3_d Y^{ij}_{120}\\ &\quad - 3\alpha^4_d Y^{ij}_{126})H_d L_j,\end{aligned} \tag{96}$$

where the formulas of the inverse unitary transformation of Eq. (95),

$$\tilde{H}_u = \alpha^1_u H_u, \quad D_u = \alpha^2_u H_u,$$

$$\begin{aligned} \tilde{D}_u &= \alpha_u^3 H_u, \quad \overline{\Delta}_u = \alpha_u^4 H_u, \\ \tilde{H}_d &= \alpha_d^1 H_d, \quad D_d = \alpha_d^2 H_d, \\ \tilde{D}_d &= \alpha_d^3 H_d, \quad \overline{\Delta}_d = \alpha_d^4 H_d, \end{aligned} \tag{97}$$

have been used.

Providing the Higgs VEVs, $H_u = v \sin\beta$ and $H_d = v \cos\beta$ with $v \simeq 174.1(\mathrm{GeV})$, the quark and lepton mass matrices can be read off as

$$\begin{aligned} M_u &= c_{10} M_{10} + c_{120} M_{120} + \tilde{c}_{120} \tilde{M}_{120} + c_{126} M_{126}, \\ M_d &= M_{10} + M_{120} + \tilde{M}_{120} + M_{126}, \\ M_D &= c_{10} M_{10} + c_{120} M_{120} - 3\tilde{c}_{120} \tilde{M}_{120} - 3 c_{126} M_{126}, \\ M_e &= M_{10} + M_{120} - 3\tilde{M}_{120} - 3 M_{126}, \\ M_R &= c_R M_{126}, \end{aligned} \tag{98}$$

where M_u, M_d, M_D, M_e, and M_R denote the up-type quark, down-type quark, neutrino Dirac, charged-lepton, and right-handed neutrino Majorana mass matrices, respectively. Note that the mass matrices at the right-hand side of Eq. (98) are defined as $M_{10} = Y_{10}\alpha_d^1 v \cos\beta$, $M_{120} = Y_{120}\alpha_d^2 v \cos\beta$, $\tilde{M}_{120} = Y_{120}\alpha_d^3 v \cos\beta$, and $M_{126} = Y_{126}\alpha_d^4 v \cos\beta$, respectively, and the coefficients are defined as $c_{10} = (\alpha_u^1/\alpha_d^1)\tan\beta$, $c_{120} = (\alpha_u^2/\alpha_d^2)\tan\beta$, $\tilde{c}_{120} = (\alpha_u^3/\alpha_d^3)\tan\beta$, $c_{126} = (\alpha_u^4/\alpha_d^4)\tan\beta$, and $c_R = v_R/(\alpha_d^4 v \cos\beta)$. These mass matrices are directly connected with low-energy observations and are crucial to model judgement.

VII. CONCLUSION

We have presented a simple method for the calculation of CG coefficients. We have constructed all states for all antisymmetric and symmetric SO(10) tensor irreps. We list all tables for the CG coefficients for the SO(10) irreps **10**, **45**, **54**, **120**, **126**, $\overline{\mathbf{126}}$, and **210**, for all possible cubic invariants. We have constructed all mass matrices for the corresponding Higgs-Higgsino sector is SUSY GUT SO(10) models. We have found a set of consistency checks for the CG coefficients and mass matrices which proved the correctness of all our results. The results obtained here are useful for a wide class of GUT models based on the SO (10) group.

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APPENDIX A: DECOMPOSITION OF REPRESENTATIONS UNDER G_{321}

Here we list the decompositions of **10, 16, 45, 54, 120**, $\overline{\mathbf{126}}$, and **210** representations under the chain of subgroups $G_{422} \supset G_{3122} \supset G_{3121} \supset G_{321}$ in Tables 7, 8, 9, 10, 11, 12, and 13 (Ref. 19), where U(1) groups are related to $\mathrm{SU}(4) \to \mathrm{SU}(3)_C \times \mathrm{U}(1)_{B-L}$, $\mathrm{SU}(2)_L \times \mathrm{SU}(2)_R \to \mathrm{SU}(2)_L$

$\times U(1)_R$. [We use the same notation as Slansky[22] but with the proper U(1) normalizations.] Note also that we may consider another chain of subgroups $SO(10) \rightarrow SU(5) \times U(1)_X$ and $SU(5) \rightarrow G_{321}$. The relations between the generators of $U(1)_{X,Y}$ and $U(1)_{B-L,R}$ are

$$\begin{aligned} \tfrac{1}{10}(-X+4Y) &= B-L, \\ Y &= B-L+T_R^3, \end{aligned} \tag{A1}$$

where T_R^3 denotes the $U(1)_R$ generator.

APPENDIX B: CG COEFFICIENTS

The CG coefficients for HH, AA, EE, DD, $\Delta\Delta$, $\overline{\Delta\Delta}$, $\overline{\Delta}\Delta$, $\Phi\Phi$, EA, $A\Phi$, $E\Delta$, $E\overline{\Delta}$, $E\Phi$, ΔH, $\overline{\Delta}H$, $H\Phi$, $\Phi\Delta$, $\Phi\overline{\Delta}$, $A\Delta$, $A\overline{\Delta}$, DH, DA, $D\Delta$, $D\overline{\Delta}$, and $D\Phi$ combinations are listed in Tables 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, and 39, respectively.[19]

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Quantum integrability of the deformed elliptic Calogero–Moser problem

L. A. Khodarinova[a)]
Magnetic Resonance Centre, School of Physics and Astronomy, University of Nottingham, Nottingham, England NG7 2RD

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The integrability of the deformed quantum elliptic Calogero–Moser problem introduced by Chalykh, Feigin, and Veselov is proven. Explicit recursive formulas for the integrals are found. For integer values of the parameter this implies the algebraic integrability of the systems. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Deformed quantum Calogero–Moser (CM) systems were introduced by Chalykh, Feigin, and Veselov,[1,2] who proved their integrability in rational and trigonometric cases and conjectured that the same is true in the elliptic case. The aim of this paper is to prove this conjecture.

Elliptic deformed CM system corresponds to the following Schrödinger operator:

$$L_m^{(n)} = \sum_{j=1}^{n} \frac{\hat{p}_j^2}{m_j} + 2m(m+1) \sum_{1\leqslant j<k\leqslant n}^{n} m_j m_k \wp(x_j - x_k), \tag{1}$$

where all but one "masses" are equal, $m_1 = m^{-1}$, $m_2 = \cdots = m_n = 1$, m is a real parameter, $\hat{p}_j = i(\partial/\partial x_j)$, $j = 1, \ldots, n$, and $\wp$ is the classical Weierstrass elliptic function. The case when m is integer is a special one: in that case a stronger version of integrability (the so-called algebraic integrability) was conjectured.[2] The first results in this direction were found by Prikhodsky and the author,[3] who proved the conjecture in the simplest nontrivial case $n=3$, $m=2$.

The main result of the present paper is an explicit recursive formula for the quantum integrals of the elliptic deformed CM system. This proves integrability of the system for all n and m and due to a general recent result by Chalykh, Etingof, and Oblomkov[4] this also implies the algebraic integrability for integer values of the parameter m.

As a by-product we have also new formulas for the integrals of the usual quantum elliptic CM problem, which was the subject of many investigations since the 1970s.[5–11] We will be using some technical tricks from these important papers. In trigonometric and rational limits we have the formulas for the quantum integrals of the corresponding deformed CM systems which also seem to be new.

II. PRELIMINARIES AND MAIN FORMULAS

Quantum Hamiltonian of the deformed elliptic CM problem has the following form:

$$H = -(m\partial_1^2 + \partial_2^2 + \cdots + \partial_{n-1}^2 + \partial_n^2) + 2(m+1)\sum_{k=2}^{n} \wp_{1k} + 2m(m+1) \sum_{2\leqslant j<k\leqslant n} \wp_{jk}, \tag{2}$$

where $\partial_i = \partial/\partial x_i$, $\wp_{jk} = \wp(x_j - x_k)$. Here $\wp$ is the classical Weierstrass elliptic function,[12] which can be determined by the differential equation

[a)]Electronic mail: larisakhodarinova@hotmail.com

$$(\mathfrak{p}'(z))^2 = 4(\mathfrak{p}(z) - e_1)(\mathfrak{p}(z) - e_2)(\mathfrak{p}(z) - e_3) = 4\mathfrak{p}^3(z) - g_2\mathfrak{p}(z) - g_3. \tag{3}$$

The Laurent expansion of $\mathfrak{p}$ at the origin is of the following form:[12]

$$\mathfrak{p}(z) = z^{-2} + \sum_{k=1}^{\infty} \gamma_{2k} z^{2k}, \tag{4}$$

where

$$\gamma_2 = \tfrac{1}{20} g_2, \quad \gamma_4 = \tfrac{1}{28} g_3.$$

The coefficients γ_{2k} are related to the so-called *Bernoulli–Hurwitz numbers*[13] BH (k),

$$\gamma_{2k} = \frac{1}{(2k)!} \frac{\mathrm{BH}(2k+2)}{(2k+2)}.$$

There is a recursive formula which allows one to obtain the coefficients γ_{2k+2} from the coefficients of the lower order,

$$\gamma_{2k+2} = \frac{3}{(k-1)(2k+5)} \sum_{j=1}^{k-1} \gamma_{2j}\gamma_{2k-2j}, \quad k = 2,3, \ldots . \tag{5}$$

The relationship (5) is easy to verify. One needs to differentiate (3) to obtain

$$\mathfrak{p}''(z) = 6\mathfrak{p}^2(z) - \tfrac{1}{2} g_2,$$

use the expansion (4) and collect terms at the appropriate degrees of z.

To construct the integrals of the operator (2) we will follow the idea going back to the papers by Sawada and Kotera[6] and Olshanetsky and Perelomov.[7] Namely, the integrals are constructed from the highest one by successive commutators with some function which in our case is $m^{-1}x_1 + x_2 + \cdots + x_n$. This highest integral is of order n and will be denoted below as I. The rest of this section is to explain the main ingredients of the formula for I.

Let us introduce the following differential operators $\mathfrak{D}^k$ in ∂_1 with constant coefficients,

$$\mathfrak{D}^1 = \partial_1, \quad \mathfrak{D}^2 = \frac{(1-m)}{2!}\partial_1^2, \quad \mathfrak{D}^3 = \frac{(1-m)(1-2m)}{3!}\partial_1^3, \quad \mathfrak{D}^4 = \frac{(1-m)(1-2m)(1-3m)}{4!}\partial_1^4,$$

$$\mathfrak{D}^k = p_{0,k}\partial_1^k + \sum_{i=2}^{[k/2]} p_{2i,k}\partial_1^{k-2i}. \tag{6}$$

The constants $p_{0,k}$, $k=2,3,\ldots$, are given by

$$p_{0,k} = \frac{1}{k!} \prod_{l=1}^{k-1} (1 - lm), \quad k = 2,3, \ldots , \tag{7}$$

and constants $p_{2i,k}$, $i=2,3,\ldots$, $k=2i, 2i+1, \ldots$, are determined by the following recursive relations:

$$p_{2i,2i} = 0, \quad i = 2,3, \ldots , \tag{8}$$

$$p_{2i,k} = \frac{(1 - m(k-2i-1))}{k-2i} p_{2i,k-1} - (1+m) \sum_{\substack{j=1 \\ j\neq 2}}^{i-1} (2i-2j)! C_{k-2j+1}^{k-2i} \gamma_{2i-2j} p_{2j-2,k-1},$$

$$i = 2,3, \ldots, \quad k = 2i+1, 2i+2, \ldots, \tag{9}$$

where $C_n^k = n!/(k!(n-k)!)$ is a binomial coefficient. To illustrate the formula (9) let us write explicitly the formulas for the first few values of i,

$$p_{4,k} = \frac{(1-m(k-5))}{k-4} p_{4,k-1} - (1+m)\frac{\prod_{l=1}^{3}(k-l)}{3}\gamma_2 p_{0,k-1}, \quad k = 5,6, \ldots,$$

$$p_{6,k} = \frac{(1-m(k-7))}{k-6} p_{6,k-1} - (1+m)\frac{\prod_{l=1}^{5}(k-l)}{5}\gamma_4 p_{0,k-1}, \quad k = 7,8, \ldots,$$

$$p_{8,k} = \frac{(1-m(k-9))}{k-8} p_{8,k-1} - (1+m)\left(\frac{\prod_{l=1}^{7}(k-l)}{7}\gamma_6 p_{0,k-1} + \frac{\prod_{l=5}^{7}(k-l)}{3}\gamma_2 p_{4,k-1}\right), \quad k = 9,10, \ldots.$$

It is interesting to note that for the special values of parameter $m = 1/l$, where l is a positive integer number, most of the constants (7) and (9) are zero. For example, if $m = \frac{1}{2}$ only $p_{0,2}$ is nonzero, if $m = \frac{1}{3}$ then only $p_{0,2}$ and $p_{0,3}$ are nonzero, if $m = \frac{1}{4}$ then only $p_{0,2}$, $p_{0,3}$, $p_{0,4}$ and $p_{4,5}$, $p_{4,6} = p_{0,2}p_{4,5}$, $p_{4,7} = p_{0,3}p_{4,5}$, $p_{4,8} = p_{0,4}p_{4,5}$ are nonzero and so on.

Let us introduce the following notations:

$$\mathfrak{s}_j = (m+1)\mathfrak{s}(x_1 - x_j), \quad 2 \leqslant j \leqslant n,$$

$$u_{1j} = (m+1)\mathfrak{p}(x_1 - x_j), \quad 2 \leqslant j \leqslant n,$$

$$u_{kl} = m(m+1)\mathfrak{p}(x_k - x_l), \quad 2 \leqslant k < l \leqslant n,$$

where $\mathfrak{s}$ is the standard elliptic $\mathfrak{s}$-function $d\mathfrak{s}(z)/dz = -\mathfrak{p}(z)$.

We will need also to consider all the subsystems of the deformed CM system. Let S be a subset of k indices of the set $\{1,2,\ldots,n\}$ and $\sigma = \{j_1, j_2, \ldots, j_t\}$, $j_1 < j_2 < \cdots < j_t$, be a subset of t indices chosen from S. The set of all different subsets σ of size t of the set S will be denoted by

$$\mathfrak{S}(S;t) = \{\sigma = \{j_1, j_2, \ldots, j_t\} : j_1 < j_2 < \ldots < j_t, j_l \in S\}.$$

If $\sigma \in \mathfrak{S}(S;t)$ define the set $S \setminus \sigma = \{j : j \in S \text{ and } j \notin \sigma\}$. If $S = \{1,2,\ldots,n\}$ we will use short notations $\mathfrak{S}(t) = \mathfrak{S}(\{1,2,\ldots,n\};t)$ and $\hat{\sigma} = \{1,2,\ldots,n\} \setminus \sigma$. If σ contains only one element $\sigma = \{l\}$ the brackets will be omitted: l will denote a set which contains one element $\{l\}$, $S \setminus l = S \setminus \{l\}$ and $\hat{l} = \{1,2,\ldots,n\} \setminus \{l\}$ We will also use notation $\hat{\sigma}_1\hat{\sigma}_2$ to denote the intersection of the subsets $\hat{\sigma}_1$ and $\hat{\sigma}_2$, $\hat{\sigma}_1\hat{\sigma}_2 = \hat{\sigma}_1 \cap \hat{\sigma}_2$.

We will distinguish two cases, $1 \in S$ and $1 \notin S$. In the second case we will use the notation $\mathrm{ad}_{\mathfrak{s}_\sigma}^t(\mathfrak{D}^r)$ for the repeated commutator

$$\mathrm{ad}_{\mathfrak{s}_\sigma}^t(\mathfrak{D}^r) = [\mathfrak{s}_{i_t}, \ldots [\mathfrak{s}_{i_2}, [\mathfrak{s}_{i_1}, \mathfrak{D}^r]]], \quad \sigma = \{i_1, i_2, \ldots, i_t\}. \tag{10}$$

Note that the order in which $\mathfrak{s}_{i_k}$ are used is not important because of the form of the operator $\mathfrak{D}^r$ We will use also the notation e_S^j for the elementary symmetric polynomials of degree j of the symbols ∂_l, $l \in S$, $e_S^0 = 1$, $e_S^1 = \sum_{l \in S}\partial_l$, $e_S^2 = \sum_{l,r \in S}^{l<r} \partial_l\partial_r$, etc.

Now, define

$$\Theta = \mathfrak{D}^n + \sum_{t=1}^{[n/2]} \sum_{\sigma \in \mathfrak{S}(\hat{1};t)} \mathrm{ad}_{\mathfrak{s}_\sigma}^t(\mathfrak{D}^{n-t}) = \sum_{t=0}^{[n/2]} \sum_{\sigma \in \mathfrak{S}(\hat{1};t)} \mathrm{ad}_{\mathfrak{s}_\sigma}^t(\mathfrak{D}^{n-t})$$

and

$$\Theta_S = \mathfrak{D}^k + \sum_{t=1}^{[k/2]} \sum_{\sigma \in \mathfrak{S}(S\setminus 1;t)} \mathrm{ad}^t_{\mathfrak{s}_\sigma}(\mathfrak{D}^{k-t}) = \sum_{t=0}^{[k/2]} \sum_{\sigma \in \mathfrak{S}(S\setminus 1;t)} \mathrm{ad}^t_{\mathfrak{s}_\sigma}(\mathfrak{D}^{k-t}), \tag{11}$$

when the set S consists of k elements and contains 1. Here and below by $[x]$ we mean the integer part of the number x.

Consider now the quantum system with the Hamiltonian,

$$H_S = -\Delta_S + 2 \sum_{\substack{j<k \\ j,k\in S}} u_{jk},$$

where $\Delta_S = m\partial_1^2 + \Sigma_{j\in S\setminus 1}\partial_j^2$ if $1 \in S$ and $\Delta_S = \Sigma_{j\in S}\partial_j^2$ otherwise. If $1 \notin S$ then this is the standard CM system which is well known to have complete set of quantum integrals.[6–10] In particular, it has the integral with the highest term $\partial_S = \Pi_{j\in S}\partial_j$. We will denote this integral I_S.

If the set S consists of k elements and contains 1 then H_S is the Hamiltonian of the deformed CM system (2) with k particles. We claim that this system has the integral (which we also denote as I_S) with the constant highest term of the form

$$E_S = \partial_1 e^{k-1}_{S\setminus 1} + p_{0,2}\partial_1^2 e^{k-2}_{S\setminus 1} + p_{0,3}\partial_1^3 e^{k-3}_{S\setminus 1} + \cdots + p_{0,k}\partial_1^k e^0_{S\setminus 1},$$

where the constants $p_{0,s}$ are given by the formula (7) above. Note that when $m=1$ they all are zero and E_S reduces to $\partial_S = \Pi_{j\in S}\partial_j$, so the integral I_S can be considered as a deformation of the corresponding integral of the usual CM system.

We define I_S inductively. Namely, assuming that we know these integrals for the subsystems consisting of less than n particles define

$$I = \sum_{t=1}^{n-2} (-1)^{t+1} \sum_{\sigma\in\mathfrak{S}(t)} I_{\hat\sigma}\partial_\sigma + (-1)^n (n-1)\partial_1\cdots\partial_n + X. \tag{12}$$

Here

$$X = \Theta + \sum_{t=1}^{[(n-2)/2]} \sum_{\sigma\in\mathfrak{S}(\hat 1;2t)} X_\sigma \Theta_{\hat\sigma} \tag{13}$$

with the coefficients

$$X_S = \sum u_{i_1 j_1} u_{i_2 j_2}\cdots u_{i_p j_p}, \tag{14}$$

where the sum is taken over all partitions of S into two-element subsets $S = \{i_1,j_1\}\cup\{i_2,j_2\}\cup\cdots\cup\{i_p,j_p\}$, in the case when the size of S is even and $X_S=0$ otherwise. These coefficients can also be determined by the recurrent formulas

$$X_{\hat 1} = \sum_{j=2}^{n-1} X_{\{j,n\}} X_{\hat 1\setminus\{j,n\}} \quad \text{if } n = 2p+1 \text{ and } X_{\hat 1} = 0 \text{ if } n = 2p \tag{15}$$

with $X_{\{2,3\}} = u_{23}$.

Theorem 1: *The operator I defined by (12) and (13) commutes with the deformed elliptic CM operator (2).*

Remark: The formula (12) is valid in the nondeformed case also, the operator

$$I_{\hat 1} = \sum_{t=1}^{n-3} (-1)^{t+1} \sum_{\sigma\in\mathfrak{S}(\hat 1,t)} I_{\hat\sigma}\partial_\sigma + (-1)^n (n-2)\partial_2\cdots\partial_n + X_{\hat 1}$$

commutes with the operator

$$H_{\hat{1}} = -(\partial_2^2 + \cdots + \partial_{n-1}^2 + \partial_n^2) + 2m(m+1)\sum_{2\leqslant j<k\leqslant n} \mathfrak{p}_{jk},$$

which is the usual $n-1$ particle elliptic CM operator.

Idea of the proof of Theorem 1: The proof will be done by induction. The main idea behind the formula (12) consists in the observation that one can use the commutativity of $I_{\hat{\sigma}}\partial_\sigma$ with $H_{\hat{\sigma}}$ to simplify the commutator $[I,H]$ to the expression

$$[I,H] = [X,H] + \sum_{j=1}^{n}\left[X_{\hat{j}}\partial_j, 2\sum_{\substack{l=1\\ l\neq j}}^{n} u_{jl}\right] + \sum_{1\leqslant k<l\leqslant n}[X_{\hat{k}\hat{l}}\partial_k\partial_l, 2u_{kl}],$$

where terms X, $X_{\hat{j}}$, and $X_{\hat{k}\hat{l}}$ depend only on ∂_1 and u_{sr}, $1\leqslant s<r\leqslant n$. This is shown in Lemma 1 in Sec. VI. At the next step we notice that if X is given by (13) the commutator $[I,H]$ can be simplified further to the following expression:

$$[I,H] = [\Theta,H] + \sum_{j=2}^{n}\left[\Theta_{\hat{j}}\partial_j, 2\sum_{\substack{l=1\\ l\neq j}}^{n} u_{jl}\right] + \sum_{2\leqslant k<l\leqslant n}[\Theta_{\hat{k}\hat{l}}, 2(u_{1k}+u_{1l})]X_{\{k,l\}},$$

where Θ, $\Theta_{\hat{j}}$, and $\Theta_{\hat{k}\hat{l}}$ depend only on ∂_1 and u_{1s}, $2\leqslant s\leqslant n$. From this we can deduce that

$$\frac{\partial\Theta}{\partial x_k} = [u_{1k}, \Theta_{\hat{k}}]$$

and, therefore, it seems natural to use the operators $\mathrm{ad}_{\mathfrak{s}_\sigma}^t$ to construct Θ. At this stage the only freedom left is in choosing operators $\mathfrak{D}^k$ which must be the operators in ∂_1 with constant coefficients. To ensure that $[I,H]=0$ these operators must satisfy the relation

$$[\mathfrak{D}^n, \mathfrak{p}(x_1-x_i)] + (1+m)[[\mathfrak{s}(x_1-x_i), \mathfrak{D}^{n-1}], \mathfrak{p}(x_1-x_i)] + m[\mathfrak{D}^{n-1}, \mathfrak{p}(x_1-x_i)]\partial_1 - \frac{(1+m)}{2}\mathfrak{p}'(x_1-x_i)\mathfrak{D}^{n-1} - \frac{(1-m)}{2}\mathfrak{D}^{n-1}\mathfrak{p}'(x_1-x_i) = 0,$$

which is equivalent to a large set of identities. It is remarkable that the constants in $\mathfrak{D}^k$ can be chosen in such a way that all these identities are satisfied (Lemma 3 of Sec. VI). The choice of the constants is related to the Bernoulli–Hurwitz numbers and is described above. The complete proof of the theorem is quite technical and is given in a separate section.

III. EXAMPLES: FORMULAS FOR TWO, THREE, AND FOUR PARTICLES

To illuminate our formulas let us consider more explicitly the case of small n.

Two-particle case: In this case we have the operator

$$H = -m\partial_1^2 - \partial_2^2 + 2(m+1)\mathfrak{p}_{12} = -m\partial_1^2 - \partial_2^2 + 2u_{12}$$

which is trivially integrable since the operator $\partial_1+\partial_2$ obviously commutes with it. This system gives the formula for operator $I_{\{1,2\}}$ which starts the recursive construction of the integral I (12). We have

$$I = I_{\{1,2\}} = \frac{1}{2}(H + (\partial_1+\partial_2)^2) = \partial_1\partial_2 + \frac{(1-m)}{2}\partial_1^2 + (m+1)\mathfrak{p}_{12} = \partial_1\partial_2 + \mathfrak{D}^2 + u_{12},$$

$$X = X_{\{1,2\}} = \Theta_{\{1,2\}} = \mathfrak{D}^2 + u_{12} = \mathfrak{D}^2 + [\mathfrak{s}_2, \mathfrak{D}].$$

Three-particle case: The integrals for the problem in this case have been found by the author.[14] The operator of the third order has the form

$$I = \partial_1\partial_2\partial_3 + \frac{(1-m)}{2}(\partial_2+\partial_3)\partial_1^2 + \frac{(1-m)(1-2m)}{3!}\partial_1^3 + (m+1)(m\mathfrak{p}_{23}\partial_1 + \mathfrak{p}_{13}\partial_2 + \mathfrak{p}_{12}\partial_3)$$
$$+ \frac{(1-m)}{2}(m+1)((\mathfrak{p}_{12}+\mathfrak{p}_{13})\partial_1 + \partial_1(\mathfrak{p}_{12}+\mathfrak{p}_{13}))$$
$$= \partial_1\partial_2\partial_3 + p_{0,2}(\partial_2+\partial_3)\partial_1^2 + u_{23}\partial_1 + u_{13}\partial_2 + u_{12}\partial_3 + \mathfrak{D}^3 + [\mathfrak{s}_2,\mathfrak{D}^2] + [\mathfrak{s}_3,\mathfrak{D}^2].$$

Operator I can be rewritten as

$$I = I_{\{2,3\}}\partial_1 + I_{\{1,3\}}\partial_2 + I_{\{1,2\}}\partial_3 - 2\partial_1\partial_2\partial_3 + X,$$

where

$$X = \Theta = \mathfrak{D}^3 + [\mathfrak{s}_2,\mathfrak{D}^2] + [\mathfrak{s}_3,\mathfrak{D}^2] \quad \text{and } I_{\{2,3\}} = \partial_2\partial_3 + u_{23}.$$

Four-particle case: One can check by direct calculation that the operator

$$I = \partial_1\partial_2\partial_3\partial_4 + \frac{(1-m)}{2}(\partial_2\partial_3+\partial_2\partial_4+\partial_3\partial_4)\partial_1^2 + \frac{(1-m)(1-2m)}{3!}(\partial_2+\partial_3+\partial_4)\partial_1^3$$
$$+ \frac{(1-m)(1-2m)(1-3m)}{4!}\partial_1^4 + m(m+1)(\mathfrak{p}_{34}\partial_1\partial_2 + \mathfrak{p}_{24}\partial_1\partial_3 + \mathfrak{p}_{23}\partial_1\partial_4) + (m+1)(\mathfrak{p}_{14}\partial_2\partial_3$$
$$+ \mathfrak{p}_{13}\partial_2\partial_4 + \mathfrak{p}_{12}\partial_3\partial_4) + \frac{(1-m)(m+1)}{2}\partial_1((\mathfrak{p}_{13}+\mathfrak{p}_{14})\partial_2 + (\mathfrak{p}_{12}+\mathfrak{p}_{14})\partial_3 + (\mathfrak{p}_{12}+\mathfrak{p}_{13})\partial_4)$$
$$+ \frac{(1-m)(m+1)}{2}((\mathfrak{p}_{13}+\mathfrak{p}_{14})\partial_2 + (\mathfrak{p}_{12}+\mathfrak{p}_{14})\partial_3 + (\mathfrak{p}_{12}+\mathfrak{p}_{13})\partial_4)\partial_1 + \frac{(1-m)(1-2m)(m+1)}{3!}((\mathfrak{p}_{12}$$
$$+ \mathfrak{p}_{13}+\mathfrak{p}_{14})\partial_1^2 + \partial_1(\mathfrak{p}_{12}+\mathfrak{p}_{13}+\mathfrak{p}_{14})\partial_1 + \partial_1^2(\mathfrak{p}_{12}+\mathfrak{p}_{13}+\mathfrak{p}_{14})) + \frac{(1-m)m(m+1)}{2}(\mathfrak{p}_{34}+\mathfrak{p}_{24}+\mathfrak{p}_{23})\partial_1^2$$
$$+ (m+1)^2((1-m)(\mathfrak{p}_{14}\mathfrak{p}_{24}+\mathfrak{p}_{14}\mathfrak{p}_{34}+\mathfrak{p}_{24}\mathfrak{p}_{34}) + m(\mathfrak{p}_{12}\mathfrak{p}_{34}+\mathfrak{p}_{13}\mathfrak{p}_{24}+\mathfrak{p}_{14}\mathfrak{p}_{23}))$$

commutes with H. The operator I can be rewritten in the following recursive form:

$$I = 3\partial_1\partial_2\partial_3\partial_4 + X + I_{\{2,3,4\}}\partial_1 + I_{\{1,3,4\}}\partial_2 + I_{\{1,2,4\}}\partial_3 + I_{\{1,2,3\}}\partial_4 - I_{\{3,4\}}\partial_1\partial_2 - I_{\{2,4\}}\partial_1\partial_3 - I_{\{2,3\}}\partial_1\partial_4$$
$$- I_{\{1,4\}}\partial_2\partial_3 - I_{\{1,3\}}\partial_2\partial_4 - I_{\{1,2\}}\partial_3\partial_4, \tag{16}$$

where

$$X = \Theta + X_{\{2,3\}}\Theta_{\{1,4\}} + X_{\{2,4\}}\Theta_{\{1,3\}} + X_{\{3,4\}}\Theta_{\{1,2\}}$$
$$= \mathfrak{D}^4 + [\mathfrak{s}_2,\mathfrak{D}^3] + [\mathfrak{s}_3,\mathfrak{D}^3] + [\mathfrak{s}_4,\mathfrak{D}^3] + [\mathfrak{s}_2,[\mathfrak{s}_3,\mathfrak{D}^2]]$$
$$+ [\mathfrak{s}_2,[\mathfrak{s}_4,\mathfrak{D}^2]] + [\mathfrak{s}_3,[\mathfrak{s}_4,\mathfrak{D}^2]] + u_{23}(\mathfrak{D}^2 + [\mathfrak{s}_4,\mathfrak{D}]) + u_{24}(\mathfrak{D}^2 + [\mathfrak{s}_3,\mathfrak{D}]) + u_{34}(\mathfrak{D}^2 + [\mathfrak{s}_2,\mathfrak{D}]).$$

and

$$I_{\{2,3,4\}} = \partial_1\partial_2\partial_3 + u_{23}\partial_1 + u_{13}\partial_2 + u_{12}\partial_3.$$

IV. INTEGRABILITY OF THE DEFORMED ELLIPTIC QUANTUM CM PROBLEM

Let us introduce the function $\theta=m^{-1}x_1+x_2+\cdots+x_n$ and consider the corresponding "ad"-operation: $\mathrm{ad}_\theta(L)=[\theta,L]$. Following to the procedure known for the usual CM system (see, for example, Olshanetsky and Perelomov[8] consider the operators $L_k=\mathrm{ad}_\theta^k(I)$, $k=0,1,\ldots,n-1$.

Theorem 2: *Operators* $L_k=\mathrm{ad}_\theta^k(I)$, $k=0,1,\ldots,n-1$, *where I is given by (12), commute with each other and with operator H*.

Proof: The proof is similar to the nondeformed case.[8,11]

Let us first prove that L_k commute with H and with $\Sigma_{j=1}^n\partial_j$. Proof is by induction in k. For $k=0$ it follows from Theorem 1. Let us assume that this is true for $k=i$, then for $k=i+1$ we have by the Jacobi identity

$$[H,L_{i+1}]=[H,[\theta,L_i]]=[[H,\theta],L_i]+[[L_i,H],\theta]=2\left[\sum_{j=1}^n\partial_j,L_i\right]+[0,\theta]=0$$

and

$$\left[\sum_{j=1}^n\partial_j,L_{i+1}\right]=\left[\sum_{j=1}^n\partial_j,[\theta,L_i]\right]=\left[\left[\sum_{j=1}^n\partial_j,\theta\right],L_i\right]+\left[\left[L_i,\sum_{j=1}^n\partial_j\right],\theta\right]$$
$$=[(m^{-1}+n-1)Id,L_i^m]+[0,\theta]=0.$$

To prove that operators L_k and L_l, $k\neq l$, commute one can use the arguments of Oshima's paper.[11] Consider an involution δ on the space of all differential operators on R^n corresponding to the change $x\to -x$ and the anti-involution $*$ such that the operator L^* is a formal adjoint to L. Our operators L_k have the following properties with respect to these involutions: $L_k^*=L_k^\delta=(-1)^kL_k$. Now, consider the commutator $C=[L_k,L_l]$. By the Jacobi identity $[C,H]=0$, therefore we can use Berezin's lemma[15] which states that in such a case the highest symbol of C is polynomial in x. In this case it is also periodic, hence the highest symbol must be constant. We have

$$C^\delta=[L_k,L_l]^\delta=[L_k^\delta,L_l^\delta]=[L_k^*,L_l^*]=-[L_k,L_l]^*=-C^*. \tag{17}$$

Since the highest symbol of C is constant the highest symbols of C^* and C^δ are the same, which contradicts to (17) unless the highest symbol of C is zero and hence $[L_k,L_l]=0$.

Theorem 3: *Deformed quantum CM problem (1) is integrable for all n and m and algebraically integrable for integer m*.

Proof: The complete family of the commuting quantum integrals for arbitrary m is given by the previous theorems. The algebraic integrability in the case when m is integer follows from the general result due to Chalykh, Etingof, and Oblomkov[4] (see Theorem 3.8).

V. TRIGONOMETRIC AND RATIONAL DEGENERATIONS

Trigonometric degenerations of the Weierstrass $\mathfrak{p}$-function corresponds to the case when one of the half-periods ω_1 or ω_2 is infinite, which happens when two of the roots of the polynomial (3) collide. For example, the case of $e_1=e_2=a$ and $e_3=-2a$ corresponds to $\omega=\infty$, $\tilde{\omega}=i(\pi/\sqrt{12a})$, and $\mathfrak{p}(z)=a+(3a/\sinh^2\sqrt{3a}z)$. Choosing $a=\frac{1}{3}$ we have

$$\mathfrak{p}(z)=\frac{1}{3}+\frac{1}{\sinh^2 z}=z^{-2}-\sum_{k=1}^{\infty}\frac{2^{2k+2}}{(2k+2)}\frac{B_{2k+2}}{(2k)!}z^{2k},\quad \mathfrak{s}(z)=-\frac{1}{3}z+\coth z,$$

$$\gamma_{2k}=-\frac{2^{2k+2}}{(2k+2)}\frac{B_{2k+2}}{(2k)!},$$

where B_{2k+2} are the classical Bernoulli numbers defined by the expansion

$$\frac{z}{e^z-1}=1-\frac{1}{2}z+\sum_{k=1}^{\infty}\frac{B_{2k}}{(2k)!}z^{2k}.$$

In this case the Hamiltonian H takes the form

$$H=-(m\partial_1^2+\partial_2^2+\cdots+\partial_{n-1}^2+\partial_n^2)+\frac{(m+1)(n-1)}{3}\left(1-m+\frac{mn}{2}\right)+\sum_{k=2}^{n}\frac{2(m+1)}{\sinh^2(x_1-x_k)}$$
$$+\sum_{2\leqslant j<k\leqslant n}\frac{2m(m+1)}{\sinh^2(x_j-x_k)}.$$

Therefore, the formulas for the integrals in this case can be obtained using the following recursive formulas for constants $p_{2i,k}$:

$$p_{2i,k}=\frac{(1-m(k-2i-1))}{k-2i}p_{2i,k-1}+(1+m)\sum_{\substack{j=1\\ j\neq 2}}^{i-1}C_{k-2j+1}^{k-2i}\frac{2^{2i-2j+2}}{(2i-2j+2)}B_{2i-2j+2}p_{2j-2,k-1}.$$

The integrability of this problem was shown by Chalykh, Feigin, and Veselov.[2] Sergeev and Veselov[16] found a recurrent formula for the quantum integrals with the highest symbols given by the deformed Newton sums. Our formulas correspond to the deformed elementary symmetric polynomials and seem to be new even in that degenerate case.

The rational degeneration corresponds to both periods being equal to infinity. In this case $\mathfrak{P}(z)=z^{-2}$ and all $\gamma_{2k}=0$. Therefore, in this case only constants $p_{0,k}$ $k=1,2,\ldots$, are nonzero.

VI. PROOF OF THEOREM 1

We prove Theorem 1 by induction in n. For small n we showed this in Sec. III. Now assume that the statement of the theorem is true for all $k<n$ and show that it is true for $k=n$.

Under this assumption, let us first show that commutator $[I,H]$ can be reduced to an expression on the additional terms X, $X_{\hat{j}}$, and $X_{\hat{k}\hat{l}}$.

Lemma 1:

$$[I,H]=[X,H]+\sum_{j=1}^{n}\left[X_{\hat{j}}\partial_j,2\sum_{\substack{l=1\\ l\neq j}}^{n}u_{jl}\right]+\sum_{1\leqslant k<l\leqslant n}[X_{\hat{k}\hat{l}}\partial_k\partial_l,2u_{kl}]. \tag{18}$$

Proof: Using (12) we obtain

$$[I,H]=\sum_{t=1}^{n-2}(-1)^{t+1}\sum_{\sigma\in\mathfrak{S}(t)}[I_{\hat{\sigma}}\partial_\sigma,H]+(-1)^n(n-1)[\partial_1\cdots\partial_n,H]+[X,H],$$

which is equal to

$$(-1)^n(n-1)\left[\partial_1\cdots\partial_n,2\sum_{1\leqslant j<k\leqslant n}u_{jk}\right]+[X,H]+\sum_{j=1}^{n}\left[I_{\hat{j}}\partial_j,H_{\hat{j}}-\Delta_j+2\sum_{\substack{k=1\\ k\neq j}}^{n}u_{jk}\right]$$
$$+\sum_{t=2}^{n-2}(-1)^{t+1}\sum_{\sigma\in\mathfrak{S}(t)}\left[I_{\hat{\sigma}}\partial_\sigma,H_{\hat{\sigma}}-\Delta_\sigma+2\sum_{j\in\sigma}\sum_{\substack{k=1\\ k\neq j}}^{n}u_{jk}-2\sum_{\substack{j<k\\ j,k\in\sigma}}u_{jk}\right].$$

Since $I_{\hat{\sigma}}$ commutes with $H_{\hat{\sigma}}$ (by the induction assumption) and $I_{\hat{\sigma}}$ with $-\Delta_\sigma$ (since it does not depend on x_i, $i\in\sigma$) we have

$$[I,H]=\sum_{j=1}^{n}\left[I_{\hat{j}}\partial_j,2\sum_{\substack{k=1\\k\neq j}}^{n}u_{jk}\right]+\sum_{t=2}^{n-2}(-1)^{t+1}\sum_{\sigma\in\mathfrak{S}(t)}\left[I_{\hat{\sigma}}\partial_\sigma,2\sum_{j\in\sigma}\sum_{\substack{k=1\\k\neq j}}^{n}u_{jk}-2\sum_{\substack{j<k\\j,k\in\sigma}}u_{jk}\right]+(-1)^n(n-1)$$
$$\times\left[\partial_1\cdots\partial_n,2\sum_{1\leqslant j<k\leqslant n}u_{jk}\right]+[X,H].$$

Now we use (12) again and obtain

$$[I,H]=\sum_{j=1}^{n}\sum_{t=1}^{n-3}(-1)^{t+1}\sum_{\sigma\in\mathfrak{S}(\hat{j};t)}\left[I_{\hat{j}\hat{\sigma}}\partial_\sigma\partial_j,2\sum_{\substack{k=1\\k\neq j}}^{n}u_{jk}\right]+(-1)^n(n-1)\left[\partial_1\cdots\partial_n,2\sum_{1\leqslant j<k\leqslant n}u_{jk}\right]$$
$$+\sum_{j=1}^{n}\left[(-1)^{n-1}(n-2)\partial_1\cdots\partial_n+X_{\hat{j}}\partial_j,2\sum_{\substack{k=1\\k\neq j}}^{n}u_{jk}\right]+[X,H]+\sum_{t=2}^{n-2}(-1)^{t+1}$$
$$\times\sum_{\sigma\in\mathfrak{S}(t)}\left[I_{\hat{\sigma}}\partial_\sigma,2\sum_{j\in\sigma}\sum_{\substack{k=1\\k\neq j}}^{n}u_{jk}-2\sum_{\substack{j<k\\j,k\in\sigma}}u_{jk}\right].$$

If we cancel the repeated terms we obtain

$$[I,H]=\sum_{j=1}^{n}\left[(-1)^{n-1}(n-2)\partial_1\cdots\partial_n+X_{\hat{j}}\partial_j,2\sum_{\substack{k=1\\k\neq j}}^{n}u_{jk}\right]+\sum_{t=2}^{n-2}(-1)^t\sum_{\sigma\in\mathfrak{S}(t)}\left[I_{\hat{\sigma}}\partial_\sigma,2\sum_{\substack{j<k\\j,k\in\sigma}}u_{jk}\right]$$
$$+(-1)^n(n-1)\left[\partial_1\cdots\partial_n,2\sum_{1\leqslant j<k\leqslant n}u_{jk}\right]+[X,H].$$

We use (12) again,

$$[I,H]=\sum_{j=1}^{n}\left[(-1)^{n-1}(n-2)\partial_1\cdots\partial_n+X_{\hat{j}}\partial_j,2\sum_{\substack{k=1\\k\neq j}}^{n}u_{jk}\right]+\sum_{t=3}^{n-2}(-1)^t\sum_{\sigma\in\mathfrak{S}(t)}\left[I_{\hat{\sigma}}\partial_\sigma,2\sum_{\substack{j<k\\j,k\in\sigma}}u_{jk}\right]$$
$$+\sum_{1\leqslant j<k\leqslant n}\left[\sum_{t=1}^{n-4}(-1)^{t+1}\sum_{\sigma\in\mathfrak{S}(\hat{j}\hat{k};t)}I_{\hat{\sigma}\hat{j}\hat{k}}\partial_\sigma\partial_j\partial_k,2u_{jk}\right]+\sum_{1\leqslant j<k\leqslant n}[(-1)^{n-2}(n-3)\partial_1\cdots\partial_n$$
$$+X_{\hat{j}\hat{k}}\partial_j\partial_k,2u_{jk}]+(-1)^n(n-1)\left[\partial_1\cdots\partial_n,2\sum_{1\leqslant j<k\leqslant n}u_{jk}\right]+[X,H].$$

Finally, canceling the repeated terms, we get

$$[I,H]=(-1)^n2\left[\partial_1\cdots\partial_n,-(n-2)\sum_{j=1}^{n}\sum_{\substack{k=1\\k\neq j}}^{n}u_{jk}+(n-3)\sum_{1\leqslant j<k\leqslant n}u_{jk}+(n-1)\sum_{1\leqslant j<k\leqslant n}u_{jk}\right]+[X,H]$$
$$+\sum_{j=2}^{n}\left[X_{\hat{j}}\partial_j,2\sum_{\substack{k=1\\k\neq j}}^{n}u_{jk}\right]+\sum_{1\leqslant j<k\leqslant n}[X_{\hat{j}\hat{k}}\partial_j\partial_k,2u_{jk}],$$

which simplifies to

$$[I,H]=[X,H]+\sum_{j=1}^{n}\left[X_{\hat{j}}\partial_j,2\sum_{\substack{k=1\\k\neq j}}^{n}u_{jk}\right]+\sum_{1\leqslant j<k\leqslant n}[X_{\hat{j}\hat{k}}\partial_j\partial_k,2u_{jk}].$$

Lemma 1 is proven.

Lemma 2: In the nondeformed case

$$[I_{\hat{1}},H_{\hat{1}}]=[X_{\hat{1}},H_{\hat{1}}]+\sum_{j=2}^{n}\left[X_{\hat{1}\hat{j}}\partial_j,2\sum_{\substack{l=2\\l\neq j}}^{n}u_{jl}\right]+\sum_{2\leqslant k<l\leqslant n}[X_{\hat{1}\hat{k}\hat{l}}\partial_k\partial_l,2u_{kl}]=0. \tag{19}$$

Proof: To prove that

$$[I_{\hat{1}},H_{\hat{1}}]=[X_{\hat{1}},H_{\hat{1}}]+\sum_{j=2}^{n}\left[X_{\hat{1}\hat{j}}\partial_j,2\sum_{\substack{l=2\\l\neq j}}^{n}u_{jl}\right]+\sum_{2\leqslant k<l\leqslant n}[X_{\hat{1}\hat{k}\hat{l}}\partial_k\partial_l,2u_{kl}]$$

one must repeat the arguments of Lemma 1. We will need the addition theorem for the Weierstrass elliptic function,[12]

$$T_{ijk}\equiv\det\begin{pmatrix}\mathfrak{p}_{ij} & \mathfrak{p}_{jk} & \mathfrak{p}_{ki}\\ \mathfrak{p}'_{ij} & \mathfrak{p}'_{jk} & \mathfrak{p}'_{ki}\\ 1 & 1 & 1\end{pmatrix}\equiv 0.$$

Two cases must be considered to prove the lemma: n is odd and n is even. If n is even (19) is reduced to $2\Sigma_{j=2}^{n}\Sigma_{\substack{l=2\\l\neq j}}^{n}[X_{\hat{1}\hat{j}}\partial_j,u_{jl}]=0$, as $X_{\hat{1}}=0$ and $X_{\hat{1}\hat{k}\hat{l}}=0$, $2\leqslant k<l\leqslant n$. In this case we have

$$\begin{aligned}\sum_{j=2}^{n}\sum_{\substack{l=2\\l\neq j}}^{n}[X_{\hat{1}\hat{j}}\partial_j,u_{jl}]&=\sum_{j=2}^{n}\sum_{\substack{l=2\\l\neq j}}^{n}X_{\hat{1}\hat{j}}[\partial_j,u_{jl}]=m(m+1)\sum_{j=2}^{n}\sum_{\substack{l=2\\l\neq j}}^{n}X_{\hat{1}\hat{j}}\mathfrak{p}'_{jl}\\&=m(m+1)\sum_{2\leqslant j<l\leqslant n}\mathfrak{p}'_{jl}(X_{\hat{1}\hat{j}}-X_{\hat{1}\hat{l}})\\&=m(m+1)\sum_{2\leqslant i<j<k\leqslant n}T_{ijk}X_{\hat{1}\hat{i}\hat{j}\hat{k}}=0.\end{aligned}$$

If n is odd (19) becomes $[X_{\hat{1}},-\Delta_{\hat{1}}]+\Sigma_{2\leqslant k<l\leqslant n}[X_{\hat{1}\hat{k}\hat{l}}\partial_k\partial_l,2u_{kl}]=0$, since in this case $X_{\hat{1}\hat{j}}=0$, $j=2,\ldots,n$. We have

$$\begin{aligned}[X_{\hat{1}},-\Delta_{\hat{1}}]+\sum_{2\leqslant k<l\leqslant n}[X_{\hat{1}\hat{k}\hat{l}}\partial_k\partial_l,2u_{kl}]&=\sum_{k=2}^{n}\frac{\partial^2X_{\hat{1}}}{\partial x_k^2}+2\sum_{k=2}^{n}\frac{\partial X_{\hat{1}}}{\partial x_k}\partial_k+2\sum_{2\leqslant k<l\leqslant n}X_{\hat{1}\hat{k}\hat{l}}(u'_{kl}\partial_l-u'_{kl}\partial_k-u''_{kl})\\&=\sum_{k=2}^{n}\frac{\partial^2X_{\hat{1}}}{\partial x_k^2}-2\sum_{2\leqslant k<l\leqslant n}X_{\hat{1}\hat{k}\hat{l}}u''_{kl}+2\sum_{k=2}^{n}\left(\frac{\partial X_{\hat{1}}}{\partial x_k}-\sum_{\substack{l=2\\l\neq k}}^{n}X_{\hat{1}\hat{k}\hat{l}}u'_{kl}\right)\partial_k=0.\end{aligned}$$

Lemma 2 is proven.

Lemma 3: The operators $\mathfrak{D}^n$ satisfy the relation

$$[\mathfrak{D}^n,\mathfrak{p}(x_1-x_i)]+(1+m)[[\mathfrak{s}(x_1-x_i),\mathfrak{D}^{n-1}],\mathfrak{p}(x_1-x_i)]+m[\mathfrak{D}^{n-1},\mathfrak{p}(x_1-x_i)]\partial-\frac{(1+m)}{2}$$

$$\times\mathfrak{p}'(x_1-x_i)\mathfrak{D}^{n-1}-\frac{(1-m)}{2}\mathfrak{D}^{n-1}\mathfrak{p}'(x_1-x_i)=0 \tag{20}$$

for any $i=2,\ldots,n$, where $\partial=\partial/\partial x_1$.

Proof: Let us denote the left-hand side of the relation (20) by $\mathcal{Y}_n$.

It can be shown by a simple direct calculation that (20) is true if $n=1,2,3,4$. The equations in these cases are

$$n=1:\mathcal{Y}_1=[\partial,\mathfrak{p}]+m[1,\mathfrak{p}]\partial-\frac{(1+m)}{2}\mathfrak{p}'-\frac{(1-m)}{2}\mathfrak{p}'=0,$$

$$n=2:\mathcal{Y}_2=\left[\frac{1-m}{2}\partial^2,\mathfrak{p}\right]+(1+m)[[\mathfrak{s},\partial],\mathfrak{p}]+m[\partial,\mathfrak{p}]\partial-\frac{(1+m)}{2}\mathfrak{p}'\partial-\frac{(1-m)}{2}\partial\mathfrak{p}'=0,$$

$$n=3:\mathcal{Y}_3=\left[\frac{1-2m}{3}\partial^3,\mathfrak{p}\right]+(1+m)[[\mathfrak{s},\partial^2],\mathfrak{p}]+m[\partial^2,\mathfrak{p}]\partial-\frac{(1+m)}{2}\mathfrak{p}'\partial^2-\frac{(1-m)}{2}\partial^2\mathfrak{p}'=0,$$

$$n=4:\mathcal{Y}_4=\left[\frac{1-3m}{4}\partial^4,\mathfrak{p}\right]+(1+m)[[\mathfrak{s},\partial^3],\mathfrak{p}]+m[\partial^3,\mathfrak{p}]\partial-\frac{(1+m)}{2}\mathfrak{p}'\partial^3-\frac{(1-m)}{2}\partial^3\mathfrak{p}'=0.$$

For $n\geqslant 5$ we use (6) to obtain

$$\begin{aligned}\mathcal{Y}_n=&[p_{0,n}\partial^n,\mathfrak{p}]+(1+m)[[\mathfrak{s},p_{0,n-1}\partial^{n-1}],\mathfrak{p}]+m[p_{0,n-1}\partial^{n-1},\mathfrak{p}]\partial-\frac{(1+m)}{2}\mathfrak{p}'p_{0,n-1}\partial^{n-1}\\&-\frac{(1-m)}{2}p_{0,n-1}\partial^{n-1}\mathfrak{p}'+\left[\sum_{i=2}^{[n/2]}p_{2i,n}\partial^{n-2i},\mathfrak{p}\right]+(1+m)\left[\left[\mathfrak{s},\sum_{i=2}^{[(n-1)/2]}p_{2i,n-1}\partial^{n-1-2i}\right],\mathfrak{p}\right]\\&+m\left[\sum_{i=2}^{[(n-1)/2]}p_{2i,n-1}\partial^{n-1-2i},\mathfrak{p}\right]\partial-\frac{(1+m)}{2}\mathfrak{p}'\sum_{i=2}^{[(n-1)/2]}p_{2i,n-1}\partial^{n-1-2i}\\&-\frac{(1-m)}{2}\sum_{i=2}^{[(n-1)/2]}p_{2i,n-1}\partial^{n-1-2i}\mathfrak{p}'.\end{aligned}$$

We can express $p_{0,n}$ through $p_{0,n-1}$ and $p_{2i,n}$ through $p_{2l,n-1}$, $l=0,\ldots,2i$, as described by (9) and obtain

$$\begin{aligned}\mathcal{Y}_n=&\left[\frac{1-m(n-1)}{n}p_{0,n-1}\partial^n,\mathfrak{p}\right]+(1+m)[[\mathfrak{s},p_{0,n-1}\partial^{n-1}],\mathfrak{p}]+m[p_{0,n-1}\partial^{n-1},\mathfrak{p}]\partial\\&-\frac{(1+m)}{2}\mathfrak{p}'p_{0,n-1}\partial^{n-1}-\frac{(1-m)}{2}p_{0,n-1}\partial^{n-1}\mathfrak{p}'+m\left[\sum_{i=2}^{[(n-1)/2]}p_{2i,n-1}\partial^{n-1-2i},\mathfrak{p}\right]\partial-(1+m)\\&\times\left[\sum_{i=2}^{[(n-1)/2]}(2i-2)!C_{n-1}^{n-2i}\gamma_{2i-2}p_{0,n-1}\partial^{n-2i},\mathfrak{p}\right]+\left[\sum_{i=2}^{[(n-1)/2]}\frac{(1-m(n-2i-1))}{n-2i}p_{2i,n-1}\partial^{n-2i},\mathfrak{p}\right]\\&+(1+m)\left[\left[\mathfrak{s},\sum_{i=2}^{[(n-1)/2]}p_{2i,n-1}\partial^{n-1-2i}\right],\mathfrak{p}\right]-\frac{(1+m)}{2}\mathfrak{p}'\sum_{i=2}^{[(n-1)/2]}p_{2i,n-1}\partial^{n-1-2i}\end{aligned}$$

$$-\frac{(1-m)}{2}\sum_{i=2}^{[(n-1)/2]} p_{2i,n-1}\partial^{n-1-2i}\mathfrak{p}'$$
$$-(1+m)\sum_{i=2}^{[(n-1)/2]-2}\left[\sum_{j=i+2}^{[(n-1)/2]}(2j-2i-2)!C_{n-2i-1}^{n-2j}\gamma_{2j-2i-2}p_{2i,n-1}\partial^{n-2j},\mathfrak{p}\right].$$

Denote

$$\mathcal{W}_k=\left[\frac{1-m(k-1)}{k}\partial^k,\mathfrak{p}\right]+(1+m)[[\mathfrak{s},\partial^{k-1}],\mathfrak{p}]+m[\partial^{k-1},\mathfrak{p}]\partial-\frac{(1+m)}{2}\mathfrak{p}'\partial^{k-1}-\frac{(1-m)}{2}\partial^{k-1}\mathfrak{p}'$$
$$-(1+m)\sum_{i=2}^{[(k-1)/2]}[(2i-2)!C_{k-1}^{k-2i}\gamma_{2i-2}\partial^{k-2i},\mathfrak{p}],$$

then

$$\mathcal{Y}_5=p_{0,4}\mathcal{W}_5+p_{4,4}\mathcal{Y}_1,\quad \mathcal{Y}_6=p_{0,5}\mathcal{W}_6+p_{4,5}\mathcal{Y}_2,$$

$$\mathcal{Y}_7=p_{0,6}\mathcal{W}_7+p_{4,6}\mathcal{Y}_3+p_{6,6}\mathcal{Y}_1,\quad \mathcal{Y}_8=p_{0,7}\mathcal{W}_8+p_{4,7}\mathcal{Y}_4+p_{6,7}\mathcal{Y}_2$$

and for $k\geqslant 5$,

$$\mathcal{Y}_{2k-1}=p_{0,2k-2}\mathcal{W}_{2k-1}+\sum_{i=2}^{k-3}p_{2i,2k-2}\mathcal{W}_{2k-1-2i}+p_{2k-4,2k-2}\mathcal{Y}_3+p_{2k-2,2k-2}\mathcal{Y}_1,$$

$$\mathcal{Y}_{2k}=p_{0,2k-1}\mathcal{W}_{2k}+\sum_{i=2}^{k-3}p_{2i,2k-1}\mathcal{W}_{2k-2i}+p_{2k-4,2k-1}\mathcal{Y}_4+p_{2k-2,2k-1}\mathcal{Y}_2.$$

Below we show that $\mathcal{W}_n=0$ for $n\geqslant 5$. First,

$$\frac{10}{1+m}\mathcal{W}_5=2[\partial^4,\mathfrak{p}]\partial-3\partial^4\mathfrak{p}'+10[[\mathfrak{s},\partial^4],\mathfrak{p}]-5\mathfrak{p}'\partial^4-80[\gamma_2\partial^1,\mathfrak{p}]+2\partial[\partial^3,\mathfrak{p}]\partial-3\mathfrak{p}'\partial^4-3\partial^4\mathfrak{p}'$$
$$+10\partial[[\mathfrak{s},\partial^3],\mathfrak{p}]+10[\partial,\mathfrak{p}][\mathfrak{s},\partial^3]+10[\mathfrak{s},\partial][\partial^3,\mathfrak{p}]-80[\gamma_2\partial^1,\mathfrak{p}].$$

We calculate that $\partial[[\mathfrak{s},\partial^3],\mathfrak{p}]=-\frac{1}{4}\partial[\partial^3,\mathfrak{p}]\partial+\frac{1}{2}\partial\mathfrak{p}'\partial^3+\frac{1}{4}\partial^4\mathfrak{p}'$, therefore

$$\frac{10}{1+m}\mathcal{W}_5=-\frac{1}{2}\partial[\partial^3,\mathfrak{p}]\partial-3\mathfrak{p}'\partial^4-\frac{1}{2}\partial^4\mathfrak{p}'+5\partial\mathfrak{p}'\partial^3+10\mathfrak{p}'[\mathfrak{s},\partial^3]+10\mathfrak{p}[\partial^3,\mathfrak{p}]-80\gamma_2\mathfrak{p}'-5\mathfrak{p}'''\partial^2$$
$$-\frac{5}{2}\mathfrak{p}^{(4)}\partial-\frac{1}{2}\mathfrak{p}^{(5)}-80\gamma_2\mathfrak{p}'+10\mathfrak{p}'(3\mathfrak{p}\partial^2+3\mathfrak{p}'\partial+\mathfrak{p}'')+10\mathfrak{p}(3\mathfrak{p}'\partial^2+3\mathfrak{p}''\partial+\mathfrak{p}''')=0.$$

In this calculation the identities which are the derivatives of the differential equation of the Weierstrass elliptic function (3) have been used. At the next step we use the induction assumption that for any $s<k$, $\mathcal{W}_s=0$. Then $\mathcal{W}_k$ can be simplified into

$$\mathcal{W}_k=\frac{1+m}{k}[\partial^{k-1},\mathfrak{p}]\partial-\frac{(1+m)}{2}\frac{k-2}{k}\partial^{k-1}\mathfrak{p}'+(1+m)[[\mathfrak{s},\partial^{k-1}],\mathfrak{p}]-\frac{(1+m)}{2}\mathfrak{p}'\partial^{k-1}$$
$$-(1+m)\sum_{j=2}^{[k-1/2]}[(2j-2)!C_{k-1}^{k-2j}\gamma_{2j-2}\partial^{k-2j},\mathfrak{p}].$$

We consider

$$\frac{1}{1+m}\mathcal{W}_k = \frac{1}{k}[\partial^{k-1},\mathfrak{p}]\partial - \frac{k-2}{2k}\partial^{k-1}\mathfrak{p}' + [[\mathfrak{s},\partial^{k-1}],\mathfrak{p}] - \frac{1}{2}\mathfrak{p}'\partial^{k-1} - \sum_{j=2}^{[k-1/2]}[(2j-2)!C_{k-1}^{k-2j}\gamma_{2j-2}\partial^{k-2j},\mathfrak{p}].$$

If $k=2l$,

$$\frac{1}{1+m}\mathcal{W}_{2l} = \frac{1}{2l}[\partial^{2l-1},\mathfrak{p}]\partial - \frac{l-1}{2l}\partial^{2l-1}\mathfrak{p}' + [[\mathfrak{s},\partial^{2l-1}],\mathfrak{p}] - \frac{1}{2}\mathfrak{p}'\partial^{2l-1} - \sum_{j=2}^{l-1}[(2j-2)!C_{2l-1}^{2l-2j}\gamma_{2j-2}\partial^{2l-2j},\mathfrak{p}]$$

and if $k=2l+1$,

$$\frac{1}{1+m}\mathcal{W}_{2l+1} = \frac{1}{(2l+1)}[\partial^{2l},\mathfrak{p}]\partial - \frac{2l-1}{2(2l+1)}\partial^{2l}\mathfrak{p}' + [[\mathfrak{s},\partial^{2l}],\mathfrak{p}] - \frac{1}{2}\mathfrak{p}'\partial^{2l} - \sum_{j=2}^{l}[(2j-2)!C_{2l}^{2l+1-2j}\gamma_{2j-2}\partial^{2l+1-2j},\mathfrak{p}].$$

We show below that $\mathcal{W}_{2l}=0$. The case of $\mathcal{W}_{2l+1}$ can be dealt with in the same way,

$$\begin{aligned}\frac{1}{1+m}\mathcal{W}_{2l} &= \frac{1}{2l}[\partial^{2l-1},\mathfrak{p}]\partial - \frac{1}{2l}(l-1)\partial^{2l-1}\mathfrak{p}' + [[\mathfrak{s},\partial^{2l-1}],\mathfrak{p}] - \frac{1}{2}\mathfrak{p}'\partial^{2l-1} \\ &\quad - \sum_{j=2}^{l-1}[(2j-2)!C_{2l-1}^{2l-2j}\gamma_{2j-2}\partial^{2l-2j},\mathfrak{p}] \\ &= \frac{1}{2l}[\partial\partial^{2l-2},\mathfrak{p}]\partial - \frac{l-1}{2l}\partial\partial^{2l-2}\mathfrak{p}' + [[\mathfrak{s},\partial\partial^{2l-2}],\mathfrak{p}] - \frac{1}{2}\mathfrak{p}'\partial\partial^{2l-2} \\ &\quad - \sum_{j=2}^{l-1}[(2j-2)!C_{2l-1}^{2l-2j}\gamma_{2j-2}\partial\partial^{2l-2j-1},\mathfrak{p}] \\ &= \frac{1}{2l}\partial[\partial^{2l-2},\mathfrak{p}]\partial - \frac{l-1}{2l}\partial\partial^{2l-2}\mathfrak{p}' - \frac{l-1}{2l}\mathfrak{p}'\partial\partial^{2l-2} \\ &\quad + \partial[[\mathfrak{s},\partial^{2l-2}],\mathfrak{p}] + [\partial,\mathfrak{p}][\mathfrak{s},\partial^{2l-2}] + [\mathfrak{s},\partial][\partial^{2l-2},\mathfrak{p}] - \partial\sum_{j=2}^{l-1}[(2j-2)!C_{2l-1}^{2l-2j}\gamma_{2j-2}\partial^{2l-2j-1},\mathfrak{p}] \\ &\quad - \sum_{j=2}^{l-1}(2j-2)!C_{2l-1}^{2l-2j}\gamma_{2j-2}\mathfrak{p}'\partial^{2l-2j-1}.\end{aligned}$$

From the inductive assumption we have that $\mathcal{W}_{2l-1}=0$, then

$$[[\mathfrak{s},\partial^{2l-2}],\mathfrak{p}] = -\frac{1}{2l-1}[\partial^{2l-2},\mathfrak{p}]\partial + \frac{2l-3}{2(2l-1)}\partial^{2l-2}\mathfrak{p}' + \frac{1}{2}\mathfrak{p}'\partial^{2l-2} + \sum_{j=2}^{l-1}[(2j-2)!C_{2l-2}^{2l-1-2j}\gamma_{2j-2}\partial^{2l-1-2j},\mathfrak{p}]$$

and therefore,

$$
\begin{aligned}
-\frac{1}{1+m}\mathcal{W}_{2l} &= \frac{1}{2l(2l-1)}\partial[\partial^{2l-2},\mathfrak{p}]\partial + \frac{1}{2l(2l-1)}\partial\partial^{2l-2}\mathfrak{p}' - \frac{1}{2}\mathfrak{p}''\partial^{2l-2} - \frac{1}{2l}\mathfrak{p}'\partial\partial^{2l-2} \\
&\quad + \partial\sum_{j=2}^{l-1}\left[\frac{(2l-2)!}{(2l-2j)!}\gamma_{2j-2}\partial^{2l-1-2j},\mathfrak{p}\right] - \mathfrak{p}'[\mathfrak{s},\partial^{2l-2}] - \mathfrak{p}[\partial^{2l-2},\mathfrak{p}] \\
&\quad + \sum_{j=2}^{l-1}(2j-2)!C_{2l-1}^{2l-2j}\gamma_{2j-2}\mathfrak{p}'\partial^{2l-2j-1} \\
&= \frac{1}{2l(2l-1)}\partial[\partial^{2l-1},\mathfrak{p}] - \frac{1}{2}\mathfrak{p}''\partial^{2l-2} - \frac{1}{2l}\mathfrak{p}'\partial^{2l-1} - \mathfrak{p}'[\mathfrak{s},\partial^{2l-2}] \\
&\quad - \mathfrak{p}[\partial^{2l-2},\mathfrak{p}] + \partial\sum_{j=2}^{l-1}\frac{(2l-2)!}{(2l-2j)!}\gamma_{2j-2}[\partial^{2l-1-2j},\mathfrak{p}] + \sum_{j=2}^{l-1}(2j-2)!C_{2l-1}^{2l-2j}\gamma_{2j-2}\mathfrak{p}'\partial^{2l-2j-1}.
\end{aligned}
$$

The commutators can be rewritten as

$$
[\partial^{2l-1},\mathfrak{p}] = \sum_{k=0}^{2l-2} C_{2l-1}^{2l-1-k}\mathfrak{p}^{(2l-1-k)}\partial^k, \quad [\partial^{2l-2},\mathfrak{p}] = \sum_{k=0}^{2l-3} C_{2l-2}^{2l-2-k}\mathfrak{p}^{(2l-2-k)}\partial^k,
$$

$$
[\mathfrak{s},\partial^{2l-2}] = \sum_{k=0}^{2l-3} C_{2l-2}^{2l-2-k}\mathfrak{p}^{(2l-3-k)}\partial^k, \quad [\partial^{2l-1-2j},\mathfrak{p}] = \sum_{k=0}^{2l-2-2j} C_{2l-1-2j}^{2l-1-2j-k}\mathfrak{p}^{(2l-1-2j-k)}\partial^k,
$$

and, hence,

$$
\begin{aligned}
-\frac{1}{1+m}\mathcal{W}_{2l} &= \frac{1}{2l(2l-1)}\sum_{k=1}^{2l-1} C_{2l-1}^{2l-k}\mathfrak{p}^{(2l-k)}\partial^k + \frac{1}{2l(2l-1)}\sum_{k=0}^{2l-2} C_{2l-1}^{2l-1-k}\mathfrak{p}^{(2l-k)}\partial^k - \sum_{k=0}^{2l-3} C_{2l-2}^{2l-2-k}\mathfrak{p}'\mathfrak{p}^{(2l-3-k)}\partial^k \\
&\quad - \sum_{k=0}^{2l-3} C_{2l-2}^{2l-2-k}\mathfrak{p}\mathfrak{p}^{(2l-2-k)}\partial^k + \sum_{j=2}^{l-1}\frac{(2l-2)!}{(2l-2j)!}\gamma_{2j-2}\sum_{k=1}^{2l-1-2j} C_{2l-1-2j}^{2l-2j-k}\mathfrak{p}^{(2l-2j-k)}\partial^k \\
&\quad + \sum_{j=2}^{l-1}\frac{(2l-2)!}{(2l-2j)!}\gamma_{2j-2}\sum_{k=0}^{2l-2-2j} C_{2l-1-2j}^{2l-1-2j-k}\mathfrak{p}^{(2l-2j-k)}\partial^k + \sum_{j=2}^{l-1}(2j-2)!C_{2l-1}^{2l-2j}\gamma_{2j-2}\mathfrak{p}'\partial^{2l-2j-1} \\
&\quad - \frac{1}{2}\mathfrak{p}''\partial^{2l-2} - \frac{1}{2l}\mathfrak{p}'\partial^{2l-1}
\end{aligned}
$$

which can be rewritten as

$$
\begin{aligned}
-\frac{1}{1+m}\mathcal{W}_{2l} &= \frac{1}{2l(2l-1)}\sum_{k=1}^{2l-1} C_{2l-1}^{2l-k}\mathfrak{p}^{(2l-k)}\partial^k + \frac{1}{2l(2l-1)}\sum_{k=0}^{2l-2} C_{2l-1}^{2l-1-k}\mathfrak{p}^{(2l-k)}\partial^k - \frac{1}{2}\mathfrak{p}''\partial^{2l-2} - \frac{1}{2l}\mathfrak{p}'\partial^{2l-1} \\
&\quad - \sum_{k=0}^{2l-3} C_{2l-2}^{2l-2-k}(\mathfrak{p}'\mathfrak{p}^{(2l-3-k)} + \mathfrak{p}\mathfrak{p}^{(2l-2-k)})\partial^k \\
&\quad + \sum_{k=1}^{2l-5}\sum_{j=2}^{l-1-[k/2]}\frac{(2l-2)!}{(2l-2j)!}\gamma_{2j-2}C_{2l-1-2j}^{2l-2j-k}\mathfrak{p}^{(2l-2j-k)}\partial^k \\
&\quad + \sum_{k=0}^{2l-6}\sum_{j=2}^{l-1-[(k+1)/2]}\frac{(2l-2)!}{(2l-2j)!}\gamma_{2j-2}C_{2l-1-2j}^{2l-1-2j-k}\mathfrak{p}^{(2l-2j-k)}\partial^k
\end{aligned}
$$

$$+\sum_{k=1}^{l-2}(2l-2k-2)!C_{2l-1}^{2k}\gamma_{2l-2k-2}\mathfrak{p}'\partial^{2k-1}.$$

It is shown below that the coefficients by all ∂^k, $k=0,1,\ldots,2l-1$, are zero. We have

$$\partial^{2l-1}:\quad \frac{1}{2l(2l-1)}C_{2l-1}^{1}\mathfrak{p}'-\frac{1}{2l}\mathfrak{p}'=0,$$

$$\partial^{2l-2}:\quad \frac{1}{2l(2l-1)}C_{2l-1}^{2}\mathfrak{p}''+\frac{1}{2l(2l-1)}C_{2l-1}^{1}\mathfrak{p}''-\frac{1}{2}\mathfrak{p}''=0,$$

$$\partial^{2l-3}:\quad \frac{1}{2l(2l-1)}C_{2l-1}^{3}\mathfrak{p}^{(3)}+\frac{1}{2l(2l-1)}C_{2l-1}^{2}\mathfrak{p}^{(3)}-2C_{2l-2}^{1}\mathfrak{p}'\mathfrak{p}$$
$$=\left(\frac{12}{2l(2l-1)}C_{2l-1}^{3}+\frac{12}{2l(2l-1)}C_{2l-1}^{2}-2C_{2l-2}^{1}\right)\mathfrak{p}'\mathfrak{p}=0,$$

$$\partial^{2l-4}:\quad \frac{1}{2l(2l-1)}C_{2l-1}^{4}\mathfrak{p}^{(4)}+\frac{1}{2l(2l-1)}C_{2l-1}^{3}\mathfrak{p}^{(4)}-C_{2l-2}^{2}(\mathfrak{p}'\mathfrak{p}'+\mathfrak{p}\mathfrak{p}^{(2)})$$
$$=\left(\frac{12}{2l(2l-1)}C_{2l-1}^{4}+\frac{12}{2l(2l-1)}C_{2l-1}^{3}-C_{2l-2}^{2}\right)(\mathfrak{p}'\mathfrak{p}'+\mathfrak{p}\mathfrak{p}^{(2)})=0.$$

When $k=2l-2q-1$, $q=2,\ldots,l-1$, coefficient by $\partial^{2l-2q-1}$ is

$$K_{2l-2q-1}=\frac{(2l-2)!}{(2l-2q-1)!}\left(\frac{\mathfrak{p}^{(2q+1)}}{(2q+1)!}-\frac{\mathfrak{p}'\mathfrak{p}^{(2q-2)}+\mathfrak{p}\mathfrak{p}^{(2q-1)}}{(2q-1)!}+\sum_{j=2}^{q-1}\frac{\gamma_{2j-2}}{(2q+1-2j)!}\mathfrak{p}^{(2q+1-2j)}\right.$$
$$\left.+\frac{2q}{2q-1}\gamma_{2q-2}\mathfrak{p}'\right).$$

To show that this coefficient is zero let us calculate its Laurent expansion and show that it consists of the terms by the positive degrees of z only. Since it is also a doubly periodic function it can only be zero. The Laurent expansion for the derivatives of the Weierstrass function are given by

$$\mathfrak{p}'=-2z^{-3}+O(z),$$

$$\mathfrak{p}^{(2q+1)}=-(2q+2)!z^{-(2q+3)}+O(z),$$

$$\mathfrak{p}^{(2q+1-2j)}=-(2q+2-2j)!z^{-(2q-2j+3)}+O(z).$$

Therefore, we can find that

$$\mathfrak{p}\mathfrak{p}^{(2q-1)}=-(2q)!z^{-(2q+3)}-(2q)!\sum_{i=1}^{q-1}\gamma_{2i}z^{-(2q+1-2i)}+O(z),$$

$$\mathfrak{p}'\mathfrak{p}^{(2q-2)}=-2(2q-1)!z^{-(2q+3)}-2(2q-2)!\gamma_{2q-2}z^{-3}+(2q-1)!\sum_{i=1}^{q-1}2i\gamma_{2i}z^{-(2q+1-2i)}+O(z),$$

and

$$-\frac{(\wp'\wp^{(2q-2)}+\wp\wp^{(2q-1)})}{(2q-1)!}=(2q+2)z^{-(2q+3)}+\sum_{i=1}^{q-2}(2q-2i)\gamma_{2i}z^{-(2q+1-2i)}+\frac{4q}{2q-1}\gamma_{2q-2}z^{-3}+O(z).$$

Therefore

$$\begin{aligned}K_{2l-2q-1}=&\frac{(2l-2)!}{(2l-2q-1)!}\Bigg(-(2q+2)z^{-(2q+3)}+(2q+2)z^{-(2q+3)}+\sum_{i=1}^{q-2}(2q-2i)\gamma_{2i}z^{-(2q+1-2i)}\\&+\frac{4q}{2q-1}\gamma_{2q-2}z^{-3}-\sum_{i=2}^{q-1}\gamma_{2j-2}(2q+2-2j)z^{-(2q-2j+3)}-\gamma_{2q-2}\frac{4q}{2q-1}z^{-3}+O(z)\Bigg)\\=&\frac{(2l-2)!}{(2l-2q-1)!}(O(z))=0.\end{aligned}$$

When $k=2l-2q$; $q=3,\ldots,l-1$, coefficient by ∂^{2l-2q} is

$$K_{2l-2q}=\frac{(2l-2)!}{(2l-2q)!}\left(\frac{1}{(2q)!}\wp^{(2q)}-\frac{(\wp'\wp^{(2q-3)}+\wp\wp^{(2q-2)})}{(2q-2)!}+\sum_{j=2}^{q-1}\frac{1}{(2q-2j)!}\gamma_{2j-2}\wp^{(2q-2j)}\right).$$

The Laurent expansion for the derivatives of the Weierstrass function are given by

$$\wp^{(2q)}=(2q+1)!z^{-(2q+2)}+(2q)!\gamma_{2q}+O(z^2),$$

$$\wp^{(2q-2j)}=(2q-2j+1)!z^{-(2q-2j+2)}+(2q-2j)!\gamma_{2q-2j}+O(z^2),$$

and we calculate that

$$\begin{aligned}\wp\wp^{(2q-2)}=&(2q-1)!z^{-(2q+2)}+(2q-2)!(2q)\gamma_{2q-2}z^{-2}+(2q-1)!(q+1)\gamma_{2q}\\&+(2q-1)!\left(\sum_{i=1}^{q-2}\gamma_{2i}z^{-(2q-2i)}\right)+O(z^2),\end{aligned}$$

$$\begin{aligned}\wp'\wp^{(2q-3)}=&2(2q-2)!z^{-(2q+2)}-(2q-2)!(2q)\gamma_{2q-2}z^{-2}-(2q-2)!(2q)\left(\frac{2q+2}{3}\right)\gamma_{2q}\\&-(2q-2)!\sum_{i=1}^{q-2}2i\gamma_{2i}z^{-(2q-2i)}+O(z^2),\end{aligned}$$

and

$$\begin{aligned}-\frac{(\wp\wp^{(2q-2)}+\wp'\wp^{(2q-3)})}{(2q-2)!}=&-(2q+1)z^{-(2q+2)}-\sum_{i=1}^{q-2}(2q-1-2i)\gamma_{2i}z^{-(2q-2i)}\\&-\left(\frac{(1+q)(2q-3)}{3}\right)\gamma_{2q}+O(z^2).\end{aligned}$$

Therefore

$$K_{2l-2q} = \frac{(2l-2)!}{(2l-2q)!}\Bigg((2q+1)z^{-(2q+2)} + \gamma_{2q} - (2q+1)z^{-(2q+2)} - \sum_{i=1}^{q-2} (2q-1-2i)\gamma_{2i} z^{-(2q-2i)}$$
$$- \frac{(1+q)(2q-3)}{3}\gamma_{2q} + \sum_{j=2}^{q-1} \gamma_{2j-2}(2q-2j+1)z^{-(2q-2j+2)} + \sum_{j=2}^{q-1} \gamma_{2j-2}\gamma_{2q-2j} + O(z^2)\Bigg)$$
$$= \frac{(2l-2)!}{(2l-2q)!}\Bigg(- \frac{(2q+3)(q-2)}{3}\gamma_{2q} + \sum_{j=2}^{q-1} \gamma_{2j-2}\gamma_{2q-2j} + O(z^2)\Bigg) = 0.$$

Here we have used the identity (5).

The last case to consider is when $k=0$. In this case we need to show that

$$K_0 = \frac{1}{2l(2l-1)}\mathfrak{p}^{(2l)} - (\mathfrak{p}'\mathfrak{p}^{(2l-3)} + \mathfrak{p}\mathfrak{p}^{(2l-2)}) + \sum_{j=2}^{l-1} \frac{(2l-2)!}{(2l-2j)!}\gamma_{2j-2}\mathfrak{p}^{(2l-2j)}$$

is zero. We have

$$K_0 = (2l-2)!\Bigg((2l+1)z^{-(2l+2)} + \gamma_{2l} - (2l+1)z^{-(2l+2)} - \sum_{i=1}^{l-2} (2l-1-2i)\gamma_{2i} z^{-(2l-2i)}$$
$$- \frac{(1+l)(2l-3)}{3}\gamma_{2l} + \sum_{j=2}^{l-1} \gamma_{2j-2}(2l-2j+1)z^{-(2l-2j+2)} + \sum_{j=2}^{l-1} \gamma_{2j-2}\gamma_{2l-2j} + O(z^2)\Bigg)$$
$$= (2l-2)!\Bigg(- \frac{(2l+3)(l-2)}{3}\gamma_{2l} + \sum_{j=2}^{l-1} \gamma_{2j-2}\gamma_{2l-2j} + O(z^2)\Bigg) = 0.$$

The proof of Lemma 3 is now finished.

Lemma 4: The following identity holds:

$$\Bigg[\Theta, \sum_{j=2}^{n} u_{1j}\Bigg] + m\sum_{j=2}^{n} [\Theta_{\hat{j}}, u_{1j}]\partial - \frac{(1+m)}{2}\sum_{j=2}^{n} u'_{1j}\Theta_{\hat{j}} - \frac{(1-m)}{2}\sum_{j=2}^{n} \Theta_{\hat{j}} u'_{1j} + m\sum_{k=2}^{n}\sum_{\substack{l=2 \\ l\neq k}}^{n} [\Theta_{\hat{k}\hat{l}}, u_{1k}]u_{1l} = 0.$$

Here again $\partial = \partial/\partial x_1$.

Proof: From Lemma 3,

$$[\mathfrak{D}^n, u_{1j}] + [[\mathfrak{s}_j, \mathfrak{D}^{n-1}], u_{1j}] + m[\mathfrak{D}^{n-1}, u_{1j}]\partial - \frac{(1+m)}{2}u'_{1j}\mathfrak{D}^{n-1} - \frac{(1-m)}{2}\mathfrak{D}^{n-1}u'_{1j} = 0. \qquad (21)$$

Note also that

$$\sum_{j=2}^{n}\sum_{\sigma\in\mathfrak{S}(1\hat{j};t)} \mathrm{ad}^t_{\mathfrak{s}_\sigma}([\mathfrak{D}^{n-t-1}, u_{1j}]\partial) = \sum_{j=2}^{n}\sum_{\sigma\in\mathfrak{S}(1\hat{j};t)} \mathrm{ad}^t_{\mathfrak{s}_\sigma}([\mathfrak{D}^{n-t-1}, u_{1j}])\partial$$
$$+ \sum_{k=2}^{n}\sum_{\substack{l=2 \\ l\neq k}}^{n}\sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{k}\hat{l};t)} [\mathrm{ad}^t_{\mathfrak{s}_\sigma}(\mathfrak{D}^{n-2-t}), u_{1k}]u_{1l}.$$

We sum (21) and then use (11) to obtain Θ and $\Theta^n_{\hat{k}}$. We have

$$
\begin{aligned}
0 &= \sum_{t=0}^{[n/2]} \sum_{j=2}^{n} \sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{j};t)} \mathrm{ad}_{\mathfrak{s}_\sigma}^t \Big([\mathfrak{D}^{n-t}, u_{1j}] + [[\mathfrak{s}_j, \mathfrak{D}^{n-t-1}], u_{1j}] + m[\mathfrak{D}^{n-t-1}, u_{1j}]\partial - \frac{(1+m)}{2} u'_{1j}\mathfrak{D}^{n-t-1} \\
&\quad - \frac{(1-m)}{2}\mathfrak{D}^{n-t-1}u'_{1j} \Big) \\
&= \sum_{t=0}^{[n/2]} \sum_{j=2}^{n} \sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{j};t)} [\mathrm{ad}_{\mathfrak{s}_\sigma}^t(\mathfrak{D}^{n-t}), u_{1j}] + m \sum_{t=0}^{[(n-2)/2]} \sum_{k=2}^{n} \sum_{\substack{l=2 \\ l\neq k}}^{n} \sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{k}\hat{l};t)} [\mathrm{ad}_{\mathfrak{s}_\sigma}^t(\mathfrak{D}^{n-2-t}), u_{1k}]u_{1l} \\
&\quad + m \sum_{t=0}^{[(n-1)/2]} \sum_{j=2}^{n} \sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{j};t)} \mathrm{ad}_{\mathfrak{s}_\sigma}^t([\mathfrak{D}^{n-t-1}, u_{1j}])\partial + \sum_{t=0}^{[(n-1)/2]} \sum_{j=2}^{n} \sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{j};t)} [\mathrm{ad}_{\mathfrak{s}_{\{j,\sigma\}}}^t(\mathfrak{D}^{n-t-1}), u_{1j}] \\
&\quad - \frac{(1+m)}{2} \sum_{t=0}^{[(n-1)/2]} \sum_{j=2}^{n} \sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{j};t)} u'_{1j}\,\mathrm{ad}_{\mathfrak{s}_\sigma}^t(\mathfrak{D}^{n-t-1}) - \frac{(1-m)}{2} \sum_{t=0}^{[(n-1)/2]} \sum_{j=2}^{n} \sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{j};t)} \mathrm{ad}_{\mathfrak{s}_\sigma}^t(\mathfrak{D}^{n-t-1})u'_{1j} \\
&= \sum_{t=0}^{[n/2]} \sum_{\sigma\in\mathfrak{S}(\hat{1};t)} \left[\mathrm{ad}_{\mathfrak{s}_\sigma}^t(\mathfrak{D}^{n-t}), \sum_{j=2}^{n} u_{1j} \right] + m \sum_{t=0}^{[(n-1)/2]} \sum_{j=2}^{n} \sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{j};t)} \mathrm{ad}_{\mathfrak{s}_\sigma}^t([\mathfrak{D}^{n-t-1}, u_{1j}])\partial \\
&\quad + m \sum_{t=0}^{[(n-2)/2]} \sum_{k=2}^{n} \sum_{\substack{l=2 \\ l\neq k}}^{n} \sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{k}\hat{l};t)} [\mathrm{ad}_{\mathfrak{s}_\sigma}^t(\mathfrak{D}^{n-2-t}), u_{1k}]u_{1l} - \frac{(1+m)}{2} \sum_{t=0}^{[(n-1)/2]} \sum_{j=2}^{n} \sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{j};t)} u'_{1j}\,\mathrm{ad}_{\mathfrak{s}_\sigma^\mu}^t(\mathfrak{D}^{n-t-1}) \\
&\quad - \frac{(1-m)}{2} \sum_{t=0}^{[(n-1)/2]} \sum_{j=2}^{n} \sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{j};t)} \mathrm{ad}_{\mathfrak{s}_\sigma}^t(\mathfrak{D}^{n-t-1})u'_{1j} = \left[\Theta, \sum_{j=2}^{n} u_{1j} \right] + m\sum_{j=2}^{n} [\Theta_{\hat{j}}, u_{1j}]\partial \\
&\quad - \frac{(1+m)}{2}\sum_{j=2}^{n} u'_{1j}\Theta_{\hat{j}} - \frac{(1-m)}{2}\sum_{j=2}^{n} \Theta_{\hat{j}}u'_{1j} + m\sum_{k=2}^{n}\sum_{\substack{l=2 \\ l\neq k}}^{n} [\Theta_{\hat{k}\hat{l}}, u_{1k}]u_{1l}.
\end{aligned}
$$

Lemma 4 is proven.

Lemma 5: The following identity holds:

$$
[\Delta, \Theta] = 2\sum_{k=2}^{n} [u_{1k}, \Theta_{\hat{k}}]\partial_k - 2m\sum_{k=2}^{n} [u_{1k}, \Theta_{\hat{k}}]\partial_1 - (1+m)\sum_{k=2}^{n} [u'_{1k}, \Theta_{\hat{k}}] + m\sum_{k=2}^{n}\sum_{\substack{l=2 \\ l\neq k}}^{n} [u_{1k}, [u_{1l}, \Theta_{\hat{k}\hat{l}}]]. \tag{22}
$$

Proof:

$$
[\Delta, \Theta] = 2m\frac{\partial\Theta}{\partial x_1}\partial_1 + 2\sum_{k=2}^{n}\frac{\partial\Theta}{\partial x_k}\partial_k + m\frac{\partial^2\Theta}{\partial x_1^2} + \sum_{k=2}^{n}\frac{\partial^2\Theta}{\partial x_k^2}.
$$

From (11) it follows that $\partial\Theta/\partial x_k = [u_{1k}, \Theta_{\hat{k}}]$ and $\partial\Theta/\partial x_1 = -\Sigma_{k=2}^n [u_{1k}, \Theta_{\hat{k}}]$, therefore $\partial^2\Theta/\partial x_k^2 = -[u'_{1k}, \Theta_{\hat{k}}]$ and $\partial^2\Theta/\partial x_1^2 = -\Sigma_{k=2}^n [u'_{1k}, \Theta_{\hat{k}}] + \Sigma_{k=2}^n \Sigma_{\substack{l=2 \\ l\neq k}}^n [u_{1k}, [u_{1l}, \Theta_{\hat{k}\hat{l}}]]$, and we arrive at (22).

Lemma 6:

$$
R = [\Theta, H] + \sum_{j=2}^{n} \left[\Theta_{\hat{j}}\partial_j, 2\sum_{\substack{l=1 \\ l\neq j}}^{n} u_{jl} \right] + \sum_{2\leqslant k<l\leqslant n} [\Theta_{\hat{k}\hat{l}}, 2(u_{1k} + u_{1l})]X_{\{k,l\}} = 0.
$$

Proof: We have

$$R=[\Delta,\Theta]+2\sum_{k=2}^{n}[\Theta,u_{1k}]+2\sum_{j=2}^{n}\sum_{\substack{l=1\\ l\neq j}}^{n}[\Theta_{\hat{j}},u_{jl}]\partial_j+2\sum_{j=2}^{n}\sum_{\substack{l=1\\ l\neq j}}^{n}\Theta_{\hat{j}}[\partial_j,u_{jl}]+2\sum_{2\leqslant k<l\leqslant n}[\Theta_{\hat{k}\hat{l}},u_{1k}+u_{1l}]u_{kl}.$$

Using Lemma 5, R is rewritten as

$$R=2\sum_{k=2}^{n}[u_{1k},\Theta_{\hat{k}}]\partial_k-2m\sum_{k=2}^{n}[u_{1k},\Theta_{\hat{k}}]\partial_1-(1+m)\sum_{k=2}^{n}[u'_{1k},\Theta_{\hat{k}}]+m\sum_{k=2}^{n}\sum_{\substack{l=2\\ l\neq k}}^{n}[u_{1k},[u_{1l},\Theta_{\hat{k}\hat{l}}]]$$

$$+2\sum_{k=2}^{n}[\Theta,u_{1k}]+2\sum_{j=2}^{n}[\Theta_{\hat{j}},u_{1j}]\partial_j+2\sum_{j=2}^{n}\sum_{\substack{l=1\\ l\neq j}}^{n}\Theta_{\hat{j}}u'_{jl}+2\sum_{2\leqslant k<l\leqslant n}[\Theta_{\hat{k}\hat{l}},u_{1k}+u_{1l}]u_{kl}$$

and, hence,

$$R=-2m\sum_{k=2}^{n}[u_{1k},\Theta_{\hat{k}}]\partial-(1+m)\sum_{k=2}^{n}[u'_{1k},\Theta_{\hat{k}}]+m\sum_{k=2}^{n}\sum_{\substack{l=2\\ l\neq k}}^{n}[u_{1k},[u_{1l},\Theta_{\hat{k}\hat{l}}]]+2\sum_{k=2}^{n}[\Theta,u_{1k}]-2\sum_{j=2}^{n}\Theta_{\hat{j}}u'_{1j}$$

$$+2\sum_{2\leqslant k<l\leqslant n}(\Theta_{\hat{k}}-\Theta_{\hat{l}})u'_{kl}+2\sum_{2\leqslant k<l\leqslant n}[\Theta_{\hat{k}\hat{l}},u_{1k}+u_{1l}]u_{kl}.$$

Now, let us apply Lemma 4 which simplifies the above expression into the following:

$$R=(1+m)\sum_{k=2}^{n}u'_{1k}\Theta_{\hat{k}}+(1-m)\sum_{k=2}^{n}\Theta_{\hat{k}}u'_{1k}-2m\sum_{k=2}^{n}\sum_{\substack{l=2\\ l\neq k}}^{n}[\Theta_{\hat{k}\hat{l}},u_{1k}]u_{1l}-(1+m)\sum_{k=2}^{n}u'_{1k}\Theta_{\hat{k}}$$

$$+(1+m)\sum_{k=2}^{n}\Theta_{\hat{k}}u'_{1k}+m\sum_{k=2}^{n}\sum_{\substack{l=2\\ l\neq k}}^{n}[u_{1k},[u_{1l},\Theta_{\hat{k}\hat{l}}]]+\sum_{2\leqslant k<l\leqslant n}[\Theta_{\hat{k}\hat{l}},2(u_{1k}+u_{1l})]u_{kl}$$

$$-2\sum_{j=2}^{n}\Theta_{\hat{j}}u'_{1j}+2\sum_{2\leqslant k<l\leqslant n}(\Theta_{\hat{k}}-\Theta_{\hat{l}})u'_{kl}$$

$$=-2m\sum_{k=2}^{n}\sum_{\substack{l=2\\ l\neq k}}^{n}[\Theta_{\hat{k}\hat{l}},u_{1k}]u_{1l}+m\sum_{k=2}^{n}\sum_{\substack{l=2\\ l\neq k}}^{n}[u_{1k},[u_{1l},\Theta_{\hat{k}\hat{l}}]]$$

$$+2\sum_{2\leqslant k<l\leqslant n}[\Theta_{\hat{k}\hat{l}},(u_{1k}+u_{1l})]u_{kl}+2\sum_{2\leqslant k<l\leqslant n}(\Theta_{\hat{k}}-\Theta_{\hat{l}})u'_{kl}.$$

From (11) $\Theta_{\hat{k}}-\Theta_{\hat{l}}=[\varsigma_l-\varsigma_k,\Theta_{\hat{k}\hat{l}}]$ and, therefore, R is simplified to

$$R=m\sum_{k=2}^{n}\sum_{\substack{l=2\\ l\neq k}}^{n}[u_{1k}u_{1l},\Theta_{\hat{k}\hat{l}}]+2\sum_{2\leqslant k<l\leqslant n}[\Theta_{\hat{k}\hat{l}},(u_{1k}+u_{1l})u_{kl}]+2\sum_{2\leqslant k<l\leqslant n}[\varsigma_{1l}-\varsigma_{1k},\Theta_{\hat{k}\hat{l}}]u'_{kl}$$

$$=2\sum_{2\leqslant k<l\leqslant n}[(\varsigma_l-\varsigma_k)u'_{kl}-(u_{1k}+u_{1l})u_{kl}+mu_{1k}u_{1l},\Theta_{\hat{k}\hat{l}}].$$

All derivatives with respect to x_1 of the term

$$(\varsigma_l-\varsigma_k)u'_{kl}-(u_{1k}+u_{1l})u_{kl}+mu_{1k}u_{1l}=m(m+1)^2((\varsigma(x_1-x_l)-\varsigma(x_1-x_k))\wp'_{kl}-(\wp_{1k}+\wp_{1l})\wp_{kl}+\wp_{1k}\wp_{1l})$$

are zero. Indeed, this follows from the fact that the first derivative is the addition theorem for the Weierstrass $\wp$-function,

$$\frac{\partial}{\partial x_1}((\varsigma(x_1-x_l)-\varsigma(x_1-x_k))\wp'_{kl}-(\wp_{1k}+\wp_{1l})\wp_{kl}+\wp_{1k}\wp_{1l})$$
$$=(\wp_{1k}-\wp_{1l})\wp'_{kl}-(\wp'_{1k}+\wp'_{1l})\wp_{kl}+\wp'_{1k}\wp_{1l}+\wp_{1k}\wp'_{1l}=0.$$

Therefore $R=2\Sigma_{2\leqslant k<l\leqslant n}[(\varsigma_{1l}-\varsigma_{1k})u'_{kl}-(u_{1k}+u_{1l})u_{kl}+mu_{1k}u_{1l},\Theta_{\hat{k}\hat{l}}]=0$ and Lemma 6 is proven.

Proof of Theorem 1: We use Lemma 3 to reduce the commutator $[I,H]$ to the expression (18) and we show below that (18) is zero. From (13),

$$X=\Theta+\sum_{t=1}^{[(n-2)/2]}\sum_{\sigma\in\mathfrak{S}(\hat{1};2t)}X_\sigma\Theta_{\hat{\sigma}},$$

therefore we can rewrite (18) as the following:

$$\begin{aligned}
[I,H]&=\left[X_{\hat{1}}\partial_1,2\sum_{l=2}^{n}u_{1l}\right]+\left[\sum_{k=2}^{n}X_{\hat{1}\hat{k}}\partial_1\partial_k,2u_{1k}\right]+\left[\Theta+\sum_{t=1}^{[(n-2)/2]}\sum_{\sigma\in\mathfrak{S}(\hat{1};2t)}X_\sigma\Theta_{\hat{\sigma}},H\right]\\
&+\left[\sum_{j=2}^{n}\left(\Theta_{\hat{j}}+\sum_{t=1}^{[(n-3)/2]}\sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{j};2t)}X_\sigma\Theta_{\hat{j}\hat{\sigma}}\right)\partial_j,2\sum_{\substack{l=1\\l\neq j}}^{n}u_{jl}\right]\\
&+\left[\sum_{2\leqslant i<j\leqslant n}\left(\Theta_{\hat{i}\hat{j}}+\sum_{t=1}^{[(n-4)/2]}\sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{i}\hat{j};2t)}X_\sigma\Theta_{\hat{i}\hat{j}\hat{\sigma}}\right)\partial_i\partial_j,2u_{ij}\right]\\
&=[\Theta,H]+\sum_{t=1}^{[(n-2)/2]}\sum_{\sigma\in\mathfrak{S}(\hat{1};2t)}[X_\sigma,-\Delta_\sigma]\Theta_{\hat{\sigma}}\\
&+\sum_{t=1}^{[(n-2)/2]}\sum_{\sigma\in\mathfrak{S}(\hat{1};2t)}\left[\Theta_{\hat{\sigma}},-\Delta_{\hat{\sigma}}+2\sum_{j=2}^{n}u_{1j}\right]X_\sigma+\sum_{j=2}^{n}\left[\Theta_{\hat{j}}\partial_j,2\sum_{\substack{l=1\\l\neq j}}^{n}u_{jl}\right]\\
&+\sum_{j=2}^{n}\sum_{t=1}^{[(n-3)/2]}\sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{j};2t)}\left[X_\sigma\partial_j,2\sum_{l\in\sigma}u_{jl}\right]\Theta_{\hat{j}\hat{\sigma}}+\sum_{j=2}^{n}\sum_{t=1}^{[(n-3)/2]}\sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{j};2t)}\left[\Theta_{\hat{j}\hat{\sigma}}\partial_j,2\sum_{\substack{l=1\\l\notin j\cup\sigma}}^{n}u_{jl}\right]X_\sigma\\
&+\left[\sum_{2\leqslant i<j\leqslant n}\partial_i\partial_j,2u_{ij}\right]\Theta_{\hat{i}\hat{j}}+\sum_{2\leqslant i<j\leqslant n}\sum_{t=1}^{[(n-4)/2]}\sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{i}\hat{j};2t)}[X_\sigma\partial_i\partial_j,2u_{ij}]\Theta_{\hat{i}\hat{j}\hat{\sigma}}\\
&+\left[X_{\hat{1}}\partial_1,2\sum_{l=2}^{n}u_{1l}\right]+\left[\sum_{k=2}^{n}X_{\hat{1}\hat{k}}\partial_1\partial_k,2u_{1k}\right]
\end{aligned}$$

From the formulas for the system with $n=2$ we have

$$[X_{\{k,l\}},-\Delta_{\{k,l\}}]=-[\partial_k\partial_l,2u_{kl}]\quad\text{and}\quad[\partial_1\partial_k,2u_{1k}]=-[\Theta_{\{1,k\}},H_{\{1,k\}}],$$

and from Lemma 2 we have that for any $\sigma'\in\mathfrak{S}(\hat{1};2t)$, $t\geqslant 2$,

$$[X_{\sigma'},-\Delta_{\sigma'}]=-2\sum_{\substack{k<l\\ k,l\in\sigma'}}[X_{\sigma'\setminus\{k,l\}}\partial_k\partial_l,u_{kl}]$$

and

$$\sum_{t=1}^{[(n-3)/2]}\sum_{j=2}^{n}\sum_{\sigma\in\mathfrak{S}(\sigma'\setminus\{j\};2t)}\left[X_\sigma\partial_j,2\sum_{l\in\sigma}u_{jl}\right]\Theta_{\hat{j}\hat{\sigma}}=0.$$

Hence, $[I,H]$ can be simplified to

$$\begin{aligned}[I,H]=[\Theta,H]&+\sum_{t=1}^{[(n-2)/2]}\sum_{\sigma\in\mathfrak{S}(\hat{1};2t)}[\Theta_{\hat{\sigma}},H_{\hat{\sigma}}]X_\sigma+\sum_{t=1}^{[(n-2)/2]}\sum_{\sigma\in\mathfrak{S}(\hat{1};2t)}\left[\Theta_{\hat{\sigma}},2\sum_{j\in\sigma}u_{1j}\right]X_\sigma\\&+\sum_{j=2}^{n}\left[\Theta_{\hat{j}}\partial_j,2\sum_{\substack{l=1\\ l\neq j}}^{n}u_{jl}\right]+\sum_{j=2}^{n}\sum_{t=1}^{[(n-3)/2]}\sum_{\sigma\in\mathfrak{S}(\hat{1}\hat{j};2t)}\left[\Theta_{\hat{j}\hat{\sigma}}\partial_j,2\sum_{\substack{l=1\\ l\notin j\cup\sigma}}^{n}u_{jl}\right]X_\sigma+\left[X_{\hat{1}}\partial_1,2\sum_{l=2}^{n}u_{1l}\right]\\&-\sum_{k=2}^{n}[\Theta_{\{1,k\}},H_{\{1,k\}}]X_{\hat{1}\hat{k}}.\end{aligned}$$

This expression is equal to zero. To verify this we should use relation (15), apply Lemma 6, which gives us

$$[\Theta,H]=-\sum_{j=2}^{n}\left[\Theta_{\hat{j}}\partial_j,2\sum_{\substack{l=1\\ l\neq j}}^{n}u_{jl}\right]-\sum_{2\leqslant k<l\leqslant n}[\Theta_{\hat{k}\hat{l}},2(u_{1k}+u_{1l})]X_{\{k,l\}}$$

and

$$[\Theta_{\hat{\sigma}},H_{\hat{\sigma}}]=-\sum_{\substack{j=2\\ j\notin\sigma}}^{n}\left[\Theta_{\hat{\sigma}\hat{j}}\partial_j,2\sum_{\substack{l=1\\ l\neq j,\sigma}}^{n}u_{jl}\right]-\sum_{\substack{2\leqslant k<l\leqslant n\\ k,l\notin\sigma}}[\Theta_{\hat{\sigma}\hat{k}\hat{l}},2(u_{1k}+u_{1l})]X_{\{k,l\}},$$

and equality

$$[\Theta_{\{1,k,l\}},H_{\{1,k,l\}}]=-[\partial_1,2(u_{1k}+u_{1l})]X_{\{k,l\}}-[\Theta_{\{1,l\}}\partial_k,2(u_{1k}+u_{kl})]-[\Theta_{\{1,k\}}\partial_l,2(u_{1l}+u_{kl})].$$

The last equality can be obtained by direct calculation or using formulas for the three-particle case. Once all these substitutions are made it can be easily seen that all terms in (18) are canceled. This completes the proof of Theorem 1.

VII. CONCLUDING REMARKS

A more general class of the deformed CM operators related to any Lie superalgebra has been recently introduced by Sergeev and Veselov,[16] who found also recurrent formulas for the quantum integrals in the trigonometric case for the classical series. In the elliptic case the integrability of these systems is an open problem. Within this approach the operator (1) considered in our paper corresponds to the Lie superalgebra $\mathrm{sl}(n-1,1)$. The author hopes that the technique developed in this paper can be applied to more general deformed elliptic CM operators related to the Lie superalgebra $\mathrm{sl}(n,p)$.

In this relation it is worth mentioning that as one can see from our formulas (6) the parameters $m=1/l$, $l=1,2,3,\ldots$ play a special role in the theory of the deformed CM operators. These values

of the parameters have also an interesting geometric interpretation,[16,17] they correspond to the strata in the discriminant variety of the polynomials having a root of multiplicity l.

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Integrable couplings of vector AKNS soliton equations

Wen-Xiu Ma[a)]
Department of Mathematics, University of South Florida, Tampa, Florida 33620-5700

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By enlarging the associated matrix spectral problems, two specific classes of multicomponent integrable couplings of the physically important vector AKNS soliton equations are constructed, which can be linked to each other by a Bäcklund transformation. The resulting two hierarchies of integrable couplings possess the enlarged zero curvature representations and recursion structures, and thus each system in the two hierarchies has infinitely many commuting symmetries. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1845971]

I. INTRODUCTION

It is in the direction of solving the integrability problem of nonlinear differential equations to search for completely integrable differential equations and to accumulate characteristics of integrability. Integrability of ordinary differential equations and $1+1$ dimensional partial differential equations, especially scalar ones, was extensively studied and various criteria such as the Liouville–Arnold theorem, the inverse scattering transform and the Painlevé test were proposed for testing integrability.[1,2] But the higher dimensions of differential equations and the multiplicity of systems of differential equations cause much difficulty in determining their integrability. Both the dimension and the multiplicity bring a diversity of mathematical structures of integrable systems, and indeed, nonlinear differential equations in higher dimensions and systems of nonlinear differential equations often need specific consideration due to complex characteristics of integrability that they may have.

Integrable couplings show one of diverse integrable structures that the multiplicity of integrable systems bring. The problem of integrable couplings was presented and studied extensively by various perturbations in Ref. 3. The interest in studying integrable couplings comes from the study of the symmetry problem and its related Virasoro algebra.

To present the definition of integrable couplings concretely, let us first look at a triangular system of differential equations

$$X(x,u) \equiv X(x,u,D_x u, \dots) = 0, \tag{1a}$$

$$Y(\bar{x},u,v) \equiv Y(\bar{x},u,v,D_{\bar{x}}u, D_{\bar{x}}v, \dots) = 0, \tag{1b}$$

where x, $\bar{x}$, u, v, X, and Y all can be multicomponent vectors, and $D_y w$ means the derivative of w with respect to y. The vector $\bar{x}$ can contain one or more variables in x, or be the same as x, or contain the whole vector x. Such a triangular system is called nontrivial with respect to the system $X(x,u)=0$, if the second subsystem $Y(\bar{x},u,v)=0$ involves the dependent variable u of the first subsystem $X(x,u)=0$. This nontriviality property implies that diagonal systems with $Y(\bar{x},u,v) = Y(\bar{x},v)$, especially $Y(\bar{x},u,v)=X(x,v)$, are trivial, and so they are not interesting and will be excluded from our discussion.

Definition: A non-trivial triangular system of differential equations (1) with respect to a given

a)Electronic mail: mawx@math.usf.edu

system $X(x,u,D_x u,\ldots)=0$ *is called an integrable coupling of the system* $X(x,u,D_x u,\ldots)=0$, *if (1) is integrable*.

Among the primary problems of integrable couplings are how one can construct integrable couplings for a given system and what mathematical structures integrable couplings should possess. The study of integrable couplings will also help classify integrable systems in whatever dimensions, along a direction of transforming them into triangular forms. What is more, all possible methods for constructing integrable couplings will tell us how to extend integrable systems, from small to large and from simple to complicated. The resulting integrable couplings themselves provide us with new models of integrable systems, which are probably difficult to find in other ways.

For evolution equations, the perturbation method to construct integrable couplings was systematically developed and various mathematical properties associated with the resulting integrable couplings were discussed in Ref. 3, motivated by the work on perturbations around solutions of evolution equations by Lakshmanan and Tamizhmani[4] and the perturbation bundle by Fuchssteiner.[5] As by-products, local $2+1$ dimensional integrable bi-Hamiltonian systems were presented among the resulting integrable couplings of the Korteweg–de Vries (KdV) equation,[6] which also provide counter examples for the conjecture on nonexistence of local integrable bi-Hamiltonian systems in higher dimensions, made by Zakharov and Konopelchenko.[7] One of such $2+1$ dimensional integrable bi-Hamiltonian systems is

$$u_t = u_{xxx} + 6uu_x, \tag{2a}$$

$$v_t = v_{xxx} + 3u_{xxy} + 6(uv)_x + 6uu_y, \tag{2b}$$

which was presented in Ref. 8 and whose Painlevé property was studied in Ref. 9. This $2+1$ dimensional system has a local bi-Hamiltonian structure[6]

$$\begin{pmatrix} u \\ v \end{pmatrix}_t = J\begin{pmatrix} \dfrac{\delta \tilde{H}_1}{\delta u} \\ \dfrac{\delta \tilde{H}_1}{\delta v} \end{pmatrix} = M\begin{pmatrix} \dfrac{\delta \tilde{H}_0}{\delta u} \\ \dfrac{\delta \tilde{H}_0}{\delta v} \end{pmatrix}, \tag{3}$$

where $\delta/\delta u$ and $\delta/\delta v$ are variational derivatives with respect to u and v, respectively; the Hamiltonian pair, J and M, is defined by

$$J = \begin{pmatrix} 0 & \partial_x \\ \partial_x & \partial_y \end{pmatrix}, \quad M = \begin{pmatrix} 0 & \partial_x^3 + 2u_x + 4u\partial_x \\ \partial_x^3 + 2u_x + 4u\partial_x & Q \end{pmatrix}, \tag{4}$$

with Q being given by

$$Q = 3\partial_x^2\partial_y + 2v_x + 2u_y + 4v\partial_x + 4u\partial_y; \tag{5}$$

and the Hamiltonian functionals, $\tilde{H}_0$ and $\tilde{H}_1$, are defined by

$$\tilde{H}_0 = \int\int uv\, \mathrm{d}x\, \mathrm{d}y, \quad \tilde{H}_1 = \int\int \left(\frac{1}{2}uv_{xx}uu_{xy} + \frac{1}{2}u_{xx}v + 3u^3v\right)\mathrm{d}x\, \mathrm{d}y. \tag{6}$$

This bi-Hamiltonian structure gives rise to a hereditary recursion operator (see Refs. 10 and 11 for definition) of the system (2),

$$\Phi = \begin{pmatrix} \partial_x^2 + 2u_x\partial_x^{-1} + 4u & 0 \\ 2\partial_x\partial_y - 2u_x\partial_x^{-2}\partial_y + 2(v_x + u_y)\partial_x^{-1} + 4v & \partial_x^2 + 2u_x\partial_x^{-1} + 4u \end{pmatrix}. \tag{7}$$

On the other hand, a basic integrable coupling of an evolution equation $u_t = K(u)$:

$$u_t = K(u), \quad v_t = K'(u)[v] \tag{8}$$

can also be generated by a perturbation around a solution of the equation $u_t=K(u)$. In the above system and elsewhere throughout this paper, $P'(u)[v]$ denotes the Gateaux derivative of $P(u) \equiv P(u, D_x u, \ldots)$ with respect to u in a direction v, i.e.,

$$P'(u)[v] = \left.\frac{\partial}{\partial \varepsilon} P(u+\varepsilon v)\right|_{\varepsilon=0} = \left.\frac{\partial}{\partial \varepsilon} P(u+\varepsilon v, D_x u + \varepsilon D_x v, \ldots)\right|_{\varepsilon=0}.$$

A symmetry $S(u)$ of the equation $u_t=K(u)$ leads to a solution $(u, S(u))$ to the above integrable coupling (8). However, the second component v of a solution (u,v) to the integrable coupling (8) is generally not a symmetry of the equation $u_t=K(u)$. This is because v satisfies the linearized equation $v_t=K'(u)[v]$ only for one solution, not for all solutions of the equation $u_t=K(u)$. Therefore, the integrable coupling (8) is a generalization of the symmetry problem, which also provides a stimulus for us to study the problem of integrable couplings. Moreover, the function $u+\varepsilon v$ presents an approximate solution to the equation $u_t=K(u)$ up to a precision $o(\varepsilon)$, if (u,v) solves the integrable coupling (8). Another basic integrable coupling of an evolution equation $u_t=K(u)$, generated by perturbation, is given by

$$u_t = K(u), \quad v_t = K'(u)[v] + K(u). \tag{9}$$

Interestingly, it has a set of hereditary recursion operators[3]

$$\Phi(\beta_1, \beta_2) = \begin{pmatrix} \beta_1 \Phi(u) & 0 \\ \beta_1 \Phi'(u)[v] + \beta_2 \Phi(u) & \beta_1 \Phi(u) \end{pmatrix} \tag{10}$$

with two arbitrary constants β_1 and β_2, if the original equation $u_t=K(u)$ has a hereditary recursion operator $\Phi(u)$. This also shows that the multiplicity of integrable systems bring the diversity of integrable structures.

A natural and interesting question for us now is whether there are other kinds of integrable couplings and what mathematical structures the resulting integrable couplings can have. In this paper, we aim at presenting two classes of multicomponent integrable couplings for the physically important vector AKNS soliton equations by enlarging the associated spectral problems. All resulting integrable couplings of the vector AKNS soliton equations possess the enlarged zero curvature representations and infinitely many commuting symmetries with recursion structures, but they are different from the integrable couplings obtained through perturbations. Unlike the case of perturbations,[3,6] it is unclear to us whether the resulting integrable couplings have infinitely many commuting conservation laws and Hamiltonian structures. A few concluding remarks will be given in the last section.

II. VECTOR AKNS SOLITON HIERARCHY

A. Soliton hierarchy

Let m be an arbitrary natural number. To display the vector AKNS soliton hierarchy, we start from the following $(m+1)\times(m+1)$ matrix spectral problem:

$$\phi_x = U(u,\lambda)\phi, \quad U(u,\lambda) = \begin{pmatrix} \alpha\lambda & q \\ r & \beta\lambda I_m \end{pmatrix} = U_0\lambda + U_1, \quad \frac{\partial U_0}{\partial \lambda} = \frac{\partial U_1}{\partial \lambda} = 0, \tag{11}$$

where λ is a spectral parameter, α and β are two distinct constants, I_m is the $m\times m$ unit matrix, and

$$q = (q_1, q_2, \ldots, q_m), \quad r = (r_1, r_2, \ldots, r_m)^T, \quad u = (q, r^T)^T. \tag{12}$$

If $m=1$ and $\alpha=-\beta=i$, where i is the square root of -1, the above spectral problem becomes the AKNS spectral problem.[12] Therefore, we say that (11) is the vector AKNS spectral problem. A

special traceless vector AKNS spectral problem, i.e., the case of (11) under $\alpha=-m$ and $\beta=1$, was discussed in Ref. 13.

As usual, to derive an associated soliton hierarchy, we first solve the stationary zero curvature equation

$$V_x = [U,V] \tag{13}$$

of the spectral problem (11). We assume that a solution V can be given by

$$V = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \tag{14}$$

where a is a scalar, b^T and c are m-dimensional columns, and d is an $m\times m$ matrix. Then we have

$$[U,V] = \begin{pmatrix} qc-br & (\alpha-\beta)\lambda b + qd - aq \\ (\beta-\alpha)\lambda c + ra - dr & rb - cq \end{pmatrix}.$$

Therefore, the stationary zero curvature equation (13) becomes

$$a_x = qc - br, \quad b_x = (\alpha-\beta)\lambda b + qd - aq, \tag{15a}$$

$$c_x = (\beta-\alpha)\lambda c + ra - dr, \quad d_x = rb - cq. \tag{15b}$$

Let us seek a formal solution of the type

$$V = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \sum_{k=0}^{\infty} V_k \lambda^{-k}, \quad V_k = \begin{pmatrix} a^{(k)} & b^{(k)} \\ c^{(k)} & d^{(k)} \end{pmatrix}, \quad k \geqslant 0, \tag{16}$$

where $b^{(k)}$, $c^{(k)}$, and $d^{(k)}$ are assumed to be

$$b^{(k)} = (b_1^{(k)}, b_2^{(k)}, \ldots, b_m^{(k)}), \quad c^{(k)} = (c_1^{(k)}, c_2^{(k)}, \ldots, c_m^{(k)})^T, \quad d^{(k)} = (d_{ij}^{(k)})_{m\times m}. \tag{17}$$

Then, the equations (15) equivalently yield the following recursion relation:

$$b^{(0)} = 0, \quad c^{(0)} = 0, \quad a_x^{(0)} = 0, \quad d_x^{(0)} = 0, \tag{18a}$$

$$b^{(k+1)} = \frac{1}{\beta-\alpha}(-b_x^{(k)} + qd^{(k)} - a^{(k)}q), \quad k \geqslant 0, \tag{18b}$$

$$c^{(k+1)} = \frac{1}{\beta-\alpha}(c_x^{(k)} - ra^{(k)} + d^{(k)}r), \quad k \geqslant 0, \tag{18c}$$

$$a_x^{(k+1)} = qc^{(k+1)} - b^{(k+1)}r, \quad d_x^{(k+1)} = rb^{(k+1)} - c^{(k+1)}q, \quad k \geqslant 0. \tag{18d}$$

To uniquely determine $a^{(k)}$, $b^{(k)}$, $c^{(k)}$, and $d^{(k)}$, we fix the following initial data:

$$a^{(0)} = \alpha, \quad d^{(0)} = \beta I_m, \tag{19}$$

which leads to $V_0 = U_0$, and require that

$$V_k|_{u=0} = 0, \quad k \geqslant 1. \tag{20}$$

The requirement (20) implies to identify all constants of integration as zero while using (18) to determine V. One can also release (19) and (20), and choose arbitrary constants of integration. But the results of V_k are just linear combinations of the expressions of V_k under (19) and (20). Now it is direct to generate from (18) under the selections (19) and (20) that

$$b_i^{(1)} = q_i, \quad c_i^{(1)} = r_i, \quad a^{(1)} = 0, \quad d_{ij}^{(1)} = 0,$$

$$b_i^{(2)} = \frac{1}{\alpha-\beta} q_{i,x}, \quad c_i^{(2)} = \frac{1}{\beta-\alpha} r_{i,x}, \quad a^{(2)} = \frac{1}{\beta-\alpha} \sum_{i=1}^{m} q_i r_i, \quad d_{ij}^{(2)} = \frac{1}{\alpha-\beta} r_i q_j,$$

$$b_i^{(3)} = \frac{1}{(\beta-\alpha)^2} \left(q_{i,xx} - 2q_i \sum_{j=1}^{m} q_j r_j \right), \quad c_i^{(3)} = \frac{1}{(\beta-\alpha)^2} \left(r_{i,xx} - 2r_i \sum_{j=1}^{m} q_j r_j \right),$$

$$a^{(3)} = \frac{1}{(\beta-\alpha)^2} \sum_{i=1}^{m} (q_i r_{i,x} - q_{i,x} r_i), \quad d_{ij}^{(3)} = \frac{1}{(\beta-\alpha)^2} (r_i q_{j,x} - r_{i,x} q_j),$$

$$b_i^{(4)} = \frac{1}{(\beta-\alpha)^3} \left[-q_{i,xxx} + 3 \sum_{j=1}^{m} (q_i q_j)_x r_j \right], \quad c_i^{(4)} = \frac{1}{(\beta-\alpha)^3} \left[r_{i,xxx} - 3 \sum_{j=1}^{m} (r_i r_j)_x q_j \right],$$

$$a^{(4)} = \frac{1}{(\beta-\alpha)^3} \left[\sum_{i=1}^{m} (q_i r_{i,xx} - q_{i,x} r_{i,x} + q_{i,xx} r_i) - 3 \sum_{i,j=1}^{m} q_i q_j r_i r_j \right],$$

$$d_{ij}^{(4)} = \frac{1}{(\beta-\alpha)^3} \left(-r_i q_{j,xx} r_{i,x} q_{j,x} - r_{i,xx} q_j + 3 r_i q_j \sum_{k=1}^{m} r_k q_k \right),$$

where $1 \leqslant i, j \leqslant m$. From (18d), we have

$$a^{(k)} = \partial^{-1}(qc^{(k)} - b^{(k)}r), \quad d^{(k)} = \partial^{-1}(rb^{(k)} - c^{(k)}q), \quad k \geqslant 1, \tag{21}$$

where the operator ∂^{-1} is the inverse of the operator ∂,

$$\partial\partial^{-1} = \partial^{-1}\partial = 1, \quad \partial = \partial_x = \frac{\partial}{\partial x}. \tag{22}$$

Then we can obtain the following recursion relation for $b^{(k)}$ and $c^{(k)}$:

$$\begin{pmatrix} c^{(k+1)} \\ b^{(k+1)T} \end{pmatrix} = \Psi \begin{pmatrix} c^{(k)} \\ b^{(k)T} \end{pmatrix}, \quad k \geqslant 1, \tag{23}$$

where the $2m \times 2m$ matrix operator Ψ is given by

$$\Psi = \frac{1}{\beta-\alpha} \begin{pmatrix} \left(\partial - \sum_{k=1}^{m} r_k \partial^{-1} q_k \right) I_m - r\partial^{-1} q & r\partial^{-1} r^T + (r\partial^{-1} r^T)^T \\ -q^T \partial^{-1} q - (q^T \partial^{-1} q)^T & \left(-\partial + \sum_{k=1}^{m} q_k \partial^{-1} r_k \right) I_m + q^T \partial^{-1} r^T \end{pmatrix}. \tag{24}$$

As in the cases of the AKNS spectral problem[12] and the traceless vector AKNS spectral problem,[13] we take the temporal spectral matrices as

$$V^{(n)} = (\lambda^n V)_+ \equiv \sum_{j=0}^{n} V_j \lambda^{n-j} = \sum_{j=0}^{n} \begin{pmatrix} a^{(j)} & b^{(j)} \\ c^{(j)} & d^{(j)} \end{pmatrix} \lambda^{n-j}, \quad n \geqslant 0, \tag{25}$$

and then introduce the temporal spectral problems,

$$\phi_{t_n} = V^{(n)}\phi = V^{(n)}\left(u, u_x, \ldots, \frac{\partial^{n-1}u}{\partial x^{n-1}}; \lambda\right)\phi, \quad n \geqslant 0. \tag{26}$$

The compatibility condition of the spectral spectral problem (11) and the temporal spectral problems (26), i.e., the zero curvature equations

$$U_{t_n} - V_x^{(n)} + [U, V^{(n)}] = 0, \quad n \geqslant 0, \tag{27}$$

lead to a hierarchy of systems of evolution equations

$$u_{t_n} = \begin{pmatrix} q^T \\ r \end{pmatrix}_{t_n} = K_n = \begin{pmatrix} (\alpha-\beta)b^{(n+1)T} \\ (\beta-\alpha)c^{(n+1)} \end{pmatrix} = \Phi^n \begin{pmatrix} (\alpha-\beta)q^T \\ (\beta-\alpha)r \end{pmatrix}, \quad n \geqslant 0, \tag{28}$$

where Φ is the conjugate operator of the operator Ψ, i.e., $\Phi = \Psi^\dagger$. The soliton hierarchy (28) is called the vector AKNS soliton hierarchy with multiplicity m.

The first nonlinear system in (28) reads as

$$(q_i)_{t_2} = \frac{1}{\alpha-\beta}\left[(q_i)_{xx} - 2q_i\sum_{j=1}^{m} q_j r_j\right], \quad 1 \leqslant i \leqslant m, \tag{29a}$$

$$(r_i)_{t_2} = \frac{1}{\beta-\alpha}\left[(r_i)_{xx} - 2r_i\sum_{j=1}^{m} q_j r_j\right], \quad 1 \leqslant i \leqslant m. \tag{29b}$$

In particular, the case of $\alpha-\beta=2i$, where i is the square root of -1, will give us two important reductions of (29).[14] The first is the vector nonlinear Schrödinger equation

$$iq_{t_2} = \tfrac{1}{2}q_{xx} + |q|^2 q,$$

which corresponds to the reduction $r=-q^H=-\overline{q}^T$. The second is the vector defocusing nonlinear Schrödinger equation

$$iq_{t_2} = \tfrac{1}{2}q_{xx} - |q|^2 q,$$

which corresponds to the reduction $r=q^H=\overline{q}^T$.

B. Bi-Hamiltonian structure

To exhibit a bi-Hamiltonian structure of the vector AKNS soliton hierarchy (28), we apply the trace identity proposed by Tu (see Ref. 15 for more applications):

$$\frac{\delta}{\delta u}\int \operatorname{tr}\left(V\frac{\partial U}{\partial \lambda}\right)\mathrm{d}x = \lambda^{-\gamma}\frac{\partial}{\partial\lambda}\left[\lambda^{\gamma}\operatorname{tr}\left(V\frac{\partial U}{\partial u}\right)\right], \tag{30}$$

where γ is a constant to be determined and $\delta/\delta u$ is the variational derivative with respect to u as before. It is direct to compute that

$$\operatorname{tr}\left(V\frac{\partial U}{\partial\lambda}\right) = \alpha a + \beta\operatorname{tr}(d) = \sum_{k\geqslant 0}\left(\alpha a^{(k)} + \beta\sum_{i=1}^{m} d_{ii}^{(k)}\right)\lambda^{-k}, \tag{31}$$

and

$$\operatorname{tr}\left(V\frac{\partial U}{\partial u}\right) = \begin{pmatrix} c \\ b^T \end{pmatrix} = \sum_{k\geqslant 0} G_{k-1}\lambda^{-k}, \quad G_{k-1} = \begin{pmatrix} c^{(k)} \\ b^{(k)T} \end{pmatrix}, \quad k \geqslant 0. \tag{32}$$

Upon inserting these two expressions into the trace identity (30), we obtain

$$\frac{\delta}{\delta u}\int\left(\alpha a^{(k+1)}+\beta\sum_{i=1}^{m}d_{ii}^{(k+1)}\right)\mathrm{d}x=(\gamma-k)G_{k-1},\quad k\geqslant 0.$$

Then considering the case of $k=1$, we know $\gamma=0$, and thus we have

$$\frac{\delta\tilde{H}_n}{\delta u}=G_{n-1},\quad \tilde{H}_n=-\frac{1}{n}\int\left(\alpha a^{(n+1)}+\beta\sum_{i=1}^{m}d_{ii}^{(n+1)}\right)\mathrm{d}x,\quad n\geqslant 1. \tag{33}$$

Now it follows from (33) that the vector AKNS soliton equations (28) have the following bi-Hamiltonian structure

$$u_{t_n}=K_n=JG_n=J\frac{\delta\tilde{H}_{n+1}}{\delta u}=M\frac{\delta\tilde{H}_n}{\delta u}, \tag{34}$$

where the Hamiltonian pair, J and $M=J\Psi$, is defined by

$$J=\begin{pmatrix}0 & (\alpha-\beta)I_m\\ (\beta-\alpha)I_m & 0\end{pmatrix}, \tag{35a}$$

$$M=\begin{pmatrix}q^T\partial^{-1}q+(q^T\partial^{-1}q)^T & \left(\partial-\sum_{k=1}^{M}q_k\partial^{-1}r_k\right)I_m-q^T\partial^{-1}r^T\\ \left(\partial-\sum_{k=1}^{M}r_k\partial^{-1}q_k\right)I_m-r\partial^{-1}q & r\partial^{-1}r^T+(r\partial^{-1}r^T)^T\end{pmatrix}. \tag{35b}$$

Of course, the nth system in (28) has an n-Hamiltonian structure. This bi-Hamiltonian structure leads to infinitely many symmetries $\{K_i\}_{i=0}^{\infty}$ and infinitely many conserved functionals $\{\tilde{H}_i\}_{i=0}^{\infty}$, and the hereditary recursion operator $\Phi=MJ^{-1}$,

$$\Phi=\frac{1}{\beta-\alpha}\begin{pmatrix}\left(-\partial+\sum_{k=1}^{M}q_k\partial^{-1}r_k\right)I_m+q^T\partial^{-1}r^T & q^T\partial^{-1}q+(q^T\partial^{-1}q)^T\\ -r\partial^{-1}r^T-(r\partial^{-1}r^T)^T & \left(\partial-\sum_{k=1}^{M}r_k\partial^{-1}q_k\right)I_m-r\partial^{-1}q\end{pmatrix} \tag{36}$$

for the vector AKNS soliton hierarchy (28). The recursion operator Φ can also be used to generate master symmetries[16] and a τ-algebra[17] of symmetries including time-dependent symmetries for the vector AKNS soliton hierarchy (28) (see Ref. 18 for the discussion in the case of the vector nonlinear Schrödinger equation).

III. INTEGRABLE COUPLINGS

A. Enlarged zero curvature equations

To construct integrable couplings of the vector AKNS soliton equations in the hierarchy (28), we use an idea of enlarging spectral problems[19] to make an enlarged spectral problem of (11) as follows:

$$\bar{\phi}_x=\bar{U}\bar{\phi}=\bar{U}(\bar{u},\lambda)\bar{\phi},\quad \bar{\phi}=(\phi^T,\phi_e^T)^T, \tag{37}$$

with the enlarged spectral square matrix

$$\overline{U} = \overline{U}(\overline{u}) = \begin{pmatrix} U & U_a \\ U_b & 0 \end{pmatrix} = \begin{pmatrix} U(u) & U_a \\ U_b & 0 \end{pmatrix}, \tag{38}$$

where the additional matrices U_a and U_b give additional dependent variables and the new potential $\overline{u}$ consists of both the original dependent variables and additional dependent variables. This enlarged spectral matrix $\overline{U}$ is associated with a larger loop Lie algebra than U. The spectral problem (37) is equivalent to

$$\phi_x = U\phi + U_a\phi_e, \quad (\phi_e)_x = U_b\phi.$$

As usual, solve the stationary zero curvature equation $\overline{V}_x = [\overline{U}, \overline{V}]$ by choosing

$$\overline{V} = \overline{V}(\overline{u}) = \begin{pmatrix} V & V_a \\ V_b & 0 \end{pmatrix} = \begin{pmatrix} V(u) & V_a(\overline{u}) \\ V_b(\overline{u}) & 0 \end{pmatrix}, \tag{39}$$

where V_a and V_b are assumed to have the same sizes as U_a and U_b, respectively. We are then led to a set of differential equations

$$V_x = [U,V] + U_aV_b - V_aU_b, \tag{40a}$$

$$(V_a)_x = UV_a - VU_a, \tag{40b}$$

$$(V_b)_x = U_bV - V_bU, \tag{40c}$$

besides a closed condition for the matrix Lie algebra:

$$U_bV_a - V_bU_a = 0. \tag{41}$$

The system (40) is a linear system of differential equations for V_a and V_b, and thus there always exist solutions, but (41) is a restricted condition for U_a, U_b, V_a, and V_b.

Now we enlarge the associated temporal spectral matrices as follows:

$$\overline{V}^{(n)} = \begin{pmatrix} V^{(n)} & V_a^{(n)} \\ V_b^{(n)} & 0 \end{pmatrix} = \begin{pmatrix} V^{(n)}(u) & V_a^{(n)}(\overline{u}) \\ V_b^{(n)}(\overline{u}) & 0 \end{pmatrix}, \quad n \geqslant 0, \tag{42}$$

where $V_a^{(n)}$ and $V_b^{(n)}$ are assumed to have the same sizes as U_a and U_b, respectively, and usually generated from V_a and V_b. Then, the enlarged zero curvature equations

$$\overline{U}_{t_n} - \overline{V}_x^{(n)} + [\overline{U}, \overline{V}^{(n)}] = 0, \quad n \geqslant 0, \tag{43}$$

equivalently yield the following systems:

$$U_{t_n} - V_x^{(n)} + [U,V^{(n)}] + U_aV_b^{(n)} - V_a^{(n)}U_b = 0, \quad n \geqslant 0, \tag{44a}$$

$$(U_a)_{t_n} - (V_a^{(n)})_x + UV_a^{(n)} - V^{(n)}U_a = 0, \quad n \geqslant 0, \tag{44b}$$

$$(U_b)_{t_n} - (V_b^{(n)})_x + U_bV^{(n)} - V_b^{(n)}U = 0, \quad n \geqslant 0, \tag{44c}$$

together with the closed condition $U_bV_a^{(n)} - V_b^{(n)}U_a = 0$, $n \geqslant 0$. If we assume that

$$U_aV_b^{(n)} - V_a^{(n)}U_b = 0, \quad U_bV_a^{(n)} - V_b^{(n)}U_a = 0, \quad n \geqslant 0, \tag{45}$$

then the hierarchy (44) of systems determined by the enlarged zero curvature equations becomes the following hierarchy of triangular systems:

$$U_{t_n} - V_x^{(n)} + [U, V^{(n)}] = 0, \quad n \geqslant 0, \tag{46}$$

$$(U_a)_{t_n} - (V_a^{(n)})_x + UV_a^{(n)} - V^{(n)}U_a = 0, \quad n \geqslant 0, \tag{47}$$

$$(U_b)_{t_n} - (V_b^{(n)})_x + U_bV^{(n)} - V_b^{(n)}U = 0, \quad n \geqslant 0. \tag{48}$$

The first equation engenders exactly the vector AKNS soliton equations in the hierarchy (28), but the second and third equations present a coupled system involving u, U_a, and U_b. Therefore, they provide a class of candidates of integrable couplings for the vector AKNS soliton equations in (28).

In what follows, we shall assume that

$$\frac{\partial U_a}{\partial \lambda} = 0, \quad \frac{\partial U_b}{\partial \lambda} = 0. \tag{49}$$

Moreover, to satisfy the basic condition in (41), we choose

$$U_b = V_b = 0 \quad \text{or } U_a = V_a = 0,$$

and then the system (40) becomes

$$(V_a)_x = UV_a - VU_a \quad \text{or } (V_b)_x = U_bV - V_bU, \tag{50}$$

together with the original stationary zero curvature equation $V_x = [U, V]$. To satisfy the basic conditions in (45), we shall similarly choose

$$U_b = V_b^{(n)} = 0 \quad \text{or } U_a = V_a^{(n)} = 0,$$

and then (48) or (47) disappears. Those two classes will be discussed in details and two classes of integrable couplings will then be generated for the vector AKNS soliton equations in (28).

B. First class of integrable couplings

1. First enlarged soliton hierarchy

Let us consider the first specific case of the enlarged spectral problem (37),

$$\overline{\phi}_x = \overline{U}\overline{\phi} = \overline{U}(\overline{u}, \lambda)\overline{\phi}, \quad \overline{\phi} = (\phi^T, \phi_a^T)^T, \tag{51}$$

with the enlarged spectral square matrix

$$\overline{U} = \overline{U}(\overline{u}) = \begin{pmatrix} U & U_a \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} U(u) & U_a \\ 0 & 0 \end{pmatrix}, \quad \frac{\partial U_a}{\partial \lambda} = 0. \tag{52}$$

This enlarged spectral problem is equivalent to

$$\phi_x = U\phi + U_a\phi_a, \quad (\phi_a)_x = 0.$$

Choose a solution for $\overline{V} = [\overline{U}, \overline{V}]$ as

$$\overline{V} = \overline{V}(\overline{u}) = \begin{pmatrix} V & V_a \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} V(u) & V_a(\overline{u}) \\ 0 & 0 \end{pmatrix}, \tag{53}$$

and then we are led to the additional equations

$$(V_a)_x = UV_a - VU_a, \tag{54}$$

besides $V_x = [U, V]$. The enlarged temporal spectral matrices read as

$$\overline{V}^{(n)} = \begin{pmatrix} V^{(n)} & V_a^{(n)} \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} V^{(n)}(u) & V_a^{(n)}(\overline{u}) \\ 0 & 0 \end{pmatrix}, \quad n \geqslant 0, \tag{55}$$

and thus the enlarged associated temporal spectral problem

$$\overline{\phi}_{t_n} = \overline{V}^{(n)}\overline{\phi}, \quad \overline{\phi} = (\phi^T, \phi_a^T)^T, \quad n \geqslant 0, \tag{56}$$

are equivalent to

$$\phi_{t_n} = V^{(n)}\phi + V_a^{(n)}\phi_a, \quad (\phi_a)_{t_n} = 0, \quad n \geqslant 0.$$

Therefore, the enlarged zero curvature equations

$$\overline{U}_{t_n} - \overline{V}_x^{(n)} + [\overline{U}, \overline{V}^{(n)}] = 0, \quad n \geqslant 0,$$

equivalently yield the following triangular systems:

$$U_{t_n} - V_x^{(n)} + [U, V^{(n)}] = 0, \quad n \geqslant 0, \tag{57}$$

$$(U_a)_{t_n} - (V_a^{(n)})_x + UV_a^{(n)} - V^{(n)}U_a = 0, \quad n \geqslant 0. \tag{58}$$

To present a realization of the above structure, let us introduce

$$V_a = \sum_{i \geqslant 0} V_{a,i}\lambda^{-i-1}, \quad \frac{\partial V_{a,i}}{\partial \lambda} = 0, \tag{59}$$

and then (54) implies that

$$U_0 V_{a,0} - V_0 U_a = 0, \tag{60}$$

$$(V_{a,i})_x = U_0 V_{a,i+1} + U_1 V_{a,i} - V_{i+1}U_a, \quad i \geqslant 0, \tag{61}$$

where U_0 and U_1 are defined by (11), and V_i, by (16).

We assume that

$$\alpha\beta \neq 0, \quad \text{i.e., } \alpha \neq 0 \quad \text{and } \beta \neq 0, \tag{62}$$

in order to determine V_a. Then, U_0 is invertible, and so the matrix V_a in (59) is uniquely determined by (60) and (61). Define the additional Lax matrices as

$$V_a^{(n)} = (\lambda^n V_a)_+, \quad n \geqslant 0, \tag{63}$$

where the subscript $+$ denotes to take the polynomial part in λ. Then by (54), we have

$$(V_a^{(n)})_x = (\lambda^n U V_a)_+ - (\lambda^n V)_+ U_a = (\lambda^n U V_a)_+ - V^{(n)}U_a,$$

and further, we can compute that

$$\begin{aligned} -(V_a^{(n)})_x + UV_a^{(n)} - V^{(n)}U_a &= -(\lambda^n U V_a)_+ + UV_a^{(n)} = -U_0 V_a^{(n+1)} - U_1 V_a^{(n)} + (\lambda U_0 + U_1)V_a^{(n)} \\ &= -U_0 V_a^{(n+1)} + \lambda U_0 V_a^{(n)} \\ &= -U_0(V_{a,n} + \lambda V_a^{(n)}) + \lambda U_0 V_a^{(n)} = -U_0 V_{a,n}. \end{aligned}$$

It follows that the additional equations determined by (58) become

$$(U_a)_{t_n} = U_0 V_{a,n}, \quad n \geqslant 0, \tag{64}$$

and so the candidates of integrable couplings are given by

$$u_{t_n} = K_n(u), \quad (U_a)_{t_n} = U_0 V_{a,n}, \quad n \geqslant 0, \tag{65}$$

To get the concrete expression of (65), we now specify U_a and $V_{a,i}$ as follows:

$$U_a = \begin{pmatrix} v_1 & \cdots & v_l \\ w_1 & \cdots & w_l \end{pmatrix}, \quad V_{a,i} = \begin{pmatrix} e_1^{(i)} & \cdots & e_l^{(i)} \\ f_1^{(i)} & \cdots & f_l^{(i)} \end{pmatrix}, \quad i \geqslant 0, \tag{66}$$

where l is an arbitrary natural number, v_j and $e_j^{(i)}$ are scalars but w_j and $f_j^{(i)}$ are m-dimensional columns. Then, the recursion relation defined by (60) and (61) yields

$$\begin{pmatrix} e_j^{(0)} \\ f_j^{(0)} \end{pmatrix} = U_0^{-1} V_0 \begin{pmatrix} v_j \\ w_j \end{pmatrix} = \begin{pmatrix} v_j \\ w_j \end{pmatrix}, \quad 1 \leqslant j \leqslant l, \tag{67}$$

$$\begin{pmatrix} e_j^{(i+1)} \\ f_j^{(i+1)} \end{pmatrix} = U_0^{-1} \begin{pmatrix} e_j^{(i)} \\ f_j^{(i)} \end{pmatrix} + U_0^{-1} V_{i+1} \begin{pmatrix} v_j \\ w_j \end{pmatrix} - U_0^{-1} U_1 \begin{pmatrix} e_j^{(i)} \\ f_j^{(i)} \end{pmatrix}, \quad 1 \leqslant j \leqslant l, \quad i \geqslant 0, \tag{68}$$

and the additional equations determined by (64) become

$$\begin{pmatrix} v_1 & \cdots & v_l \\ w_1 & \cdots & w_l \end{pmatrix}_{t_n}, \quad U_0 V_{a,n} = \begin{pmatrix} \alpha e_1^{(n)} & \cdots & \alpha e_l^{(n)} \\ \beta f_1^{(n)} & \cdots & \beta f_l^{(n)} \end{pmatrix}, \quad n \geqslant 0. \tag{69}$$

Therefore, the enlarged hierarchy (65) of the vector AKNS soliton equations reads as

$$\overline{u_{t_n}} \equiv \begin{pmatrix} q^T \\ r \\ v_1 \\ w_1 \\ \vdots \\ v_l \\ w_l \end{pmatrix}_{t_n} = \overline{K_n} \equiv \begin{pmatrix} (\alpha - \beta) b^{(n+1)T} \\ (\beta - \alpha) c^{(n+1)} \\ \alpha e_1^{(n)} \\ \beta f_1^{(n)} \\ \vdots \\ \alpha e_l^{(n)} \\ \beta f_l^{(n)} \end{pmatrix}, \quad n \geqslant 0. \tag{70}$$

2. Recursion structure for the first enlarged hierarchy

Let us now derive a recursion structure for the first enlarged soliton hierarchy (70). From the above recursion relation (68) for $e_j^{(i)}$ and $f_j^{(i)}$, we have

$$\alpha e_j^{(i+1)} = (e_j^{(i)})_x - q f_j^{(i)} + (a^{(i+1)} v_j + b^{(i+1)} w_j), \quad 1 \leqslant j \leqslant l, \; i \geqslant 0, \tag{71a}$$

$$\beta f_j^{(i+1)} = (f_j^{(i)})_x - r e_j^{(i)} + (c^{(i+1)} v_j + d^{(i+1)} w_j), \quad 1 \leqslant j \leqslant l, \; i \geqslant 0. \tag{71b}$$

In particular, this gives rise to

$$e_j^{(1)} = \frac{1}{\alpha}(v_j)_x, \quad f_j^{(1)} = \frac{1}{\beta}(w_j)_x, \quad 1 \leqslant j \leqslant l,$$

$$e_j^{(2)} = \frac{1}{\alpha}\left[\frac{1}{\alpha}(v_j)_{xx} - \frac{1}{\beta} q (w_j)_x + \frac{1}{\beta - \alpha} q r v_j + \frac{1}{\alpha - \beta} q_x w_j\right], \quad 1 \leqslant j \leqslant l,$$

$$f_j^{(2)} = \frac{1}{\beta}\left[\frac{1}{\beta}(w_j)_{xx} - \frac{1}{\alpha} r (v_j)_x + \frac{1}{\beta - \alpha} r_x v_j + \frac{1}{\alpha - \beta} q r w_j\right], \quad 1 \leqslant j \leqslant l.$$

In order to get a recursion structure, we rewrite the equations (69) as

$$\begin{pmatrix} v_j \\ w_j \end{pmatrix}_{t_n} = \begin{pmatrix} \alpha e_j^{(n)} \\ \beta f_j^{(n)} \end{pmatrix} = \overline{\Phi}_j \begin{pmatrix} (\alpha-\beta)b^{(n)T} \\ (\beta-\alpha)c^{(n)} \end{pmatrix} + \overline{\Phi}_0 \begin{pmatrix} \alpha e_j^{(n-1)} \\ \beta f_j^{(n-1)} \end{pmatrix}, \quad 1 \leqslant j \leqslant l,\ n \geqslant 0. \tag{72}$$

Then based on (71) and (21), we find that the $(m+1)\times(m+1)$ matrix $\overline{\Phi}_0$ can be chosen as

$$\overline{\Phi}_0 = \overline{\Phi}_0(q,r) = \begin{pmatrix} \frac{1}{\alpha}\partial & -\frac{1}{\beta}q \\ -\frac{1}{\alpha}r & \frac{1}{\beta}\partial I_m \end{pmatrix}, \tag{73}$$

and further, the $(m+1)\times 2m$ matrix operators $\overline{\Phi}_j$ can be chosen as

$$\overline{\Phi}_j = \overline{\Phi}_j(q,r,v_j,w_j) = \frac{1}{\beta-\alpha}\begin{pmatrix} v_j\partial^{-1}L_{r^T} - L_{w_j^T} & v_j\partial^{-1}L_q \\ -R_{w_j}\partial^{-1}L_T T & v_j I_m - R_{w_j}\partial^{-1}R_q \end{pmatrix}, \quad 1 \leqslant j \leqslant l, \tag{74}$$

where $(R_A)B=BA$, $(L_A)B=AB$, and $TB=B^T$ for two matrices A and B [note that $L_{r^T}A=r^TA$ but $(L_rT)A=rA^T$]. Therefore, the enlarged vector AKNS hierarchy (70) possesses the following recursion structure:

$$\begin{pmatrix} q^T \\ r \\ v_1 \\ w_1 \\ \vdots \\ v_l \\ w_l \end{pmatrix}_{t_n} = \overline{\Phi}\begin{pmatrix} (\alpha-\beta)b^{(n)T} \\ (\beta-\alpha)c^{(n)} \\ \alpha e_1^{(n-1)} \\ \beta f_1^{(n-1)} \\ \vdots \\ \alpha e_l^{(n-1)} \\ \beta f_l^{(n-1)} \end{pmatrix} = \overline{\Phi}^n \begin{pmatrix} (\alpha-\beta)b^{(1)T} \\ (\beta-\alpha)c^{(1)} \\ \alpha e_1^{(0)} \\ \beta f_1^{(0)} \\ \vdots \\ \alpha e_l^{(0)} \\ \beta f_l^{(0)} \end{pmatrix} = \overline{\Phi}^n \begin{pmatrix} (\alpha-\beta)q^T \\ (\beta-\alpha)r \\ \alpha v_1 \\ \beta w_1 \\ \vdots \\ \alpha v_l \\ \beta w_l \end{pmatrix}, \quad n \geqslant 0, \tag{75}$$

if we define the recursion operator $\overline{\Phi}$ as

$$\overline{\Phi} = \begin{pmatrix} \Phi & & & & 0 \\ \overline{\Phi}_1 & \overline{\Phi}_0 & & & \\ \overline{\Phi}_2 & 0 & \overline{\Phi}_0 & & \\ \vdots & \ddots & \ddots & \ddots & \\ \overline{\Phi}_l & 0 & \cdots & 0 & \overline{\Phi}_0 \end{pmatrix}, \tag{76}$$

where $\Phi=\Psi^\dagger$ is the hereditary recursion operator of (28) defined by (36). We point out that there may exist other choices for $\overline{\Phi}_j$ and $\overline{\Phi}_0$ in the recursion structure (72).

The triangular systems in (70) are commutative. This can be shown, for example, by using the uniqueness property of the spectral problem $\phi_x=U\phi$, that is, if a Lax matrix V has zero initial value $V|_{u=0}=0$, i.e., if $U'[K]-V_x+[U,V]=0$ and $V|_{u=0}=0$, then the Lax matrix $V=0$.[17] Keeping the equation (58) in mind, it is easy to verify that if the original spectral problem $\phi_x=U\phi$ possesses the uniqueness property, then so does the enlarged spectral problem (51). In this way, we can prove that the spectral problem (51) has the uniqueness property. On the other hand, the Lax matrices

$$\overline{V}^{k,l}(\overline{u}) \equiv (\overline{V}^{(k)})'(\overline{u})[\overline{K}_l] - (\overline{V}^{(l)})'(\overline{u})[\overline{K}_k] + [\overline{V}^{(k)}(\overline{u}), \overline{V}^{(l)}(\overline{u})], \quad k,l \geqslant 0, \tag{77}$$

have zero initial value $\overline{V}^{k,l}(\overline{u})|_{\overline{u}=0}=0$ (see Refs. 17 and 20 for more discussion). Therefore, the new enlarged soliton hierarchy defined by (70) or (75) is commutative, and so it is a common hierarchy of commuting integrable couplings for all the vector AKNS soliton equations in the

hierarchy (28). The integrability here denotes the existence of infinitely many symmetries.[21] Its first nonlinear system reads as

$$q_{t_2} = \frac{1}{\alpha - \beta}(q_{xx} - 2qrq), \tag{78a}$$

$$r_{t_2} = \frac{1}{\beta - \alpha}(r_{xx} - 2rqr), \tag{78b}$$

$$(v_j)_{t_2} = \frac{1}{\alpha}(v_j)_{xx} - \frac{1}{\beta}q(w_j)_x + \frac{1}{\beta - \alpha}qrv_j + \frac{1}{\alpha - \beta}q_x w_j, \quad 1 \leqslant j \leqslant l, \tag{78c}$$

$$(w_j)_{t_2} = \frac{1}{\beta}(w_j)_{xx} - \frac{1}{\alpha}r(v_j)_x + \frac{1}{\beta - \alpha}r_x v_j + \frac{1}{\alpha - \beta}qrw_j, \quad 1 \leqslant j \leqslant l, \tag{78d}$$

where q^T, r, w_j are m-dimensional columns and v_j are scalar variables.

C. Second class of integrable couplings

1. Second enlarged soliton hierarchy

Let us consider the second specific case of the enlarged spectral problem (37):

$$\tilde{\phi}_x = \tilde{U}\tilde{\phi} = \tilde{U}(\tilde{u}, \lambda)\tilde{\phi}, \quad \tilde{\phi} = (\phi^T, \phi_b^T)^T, \tag{79}$$

with the enlarged spectral square matrix

$$\tilde{U} = \tilde{U}(\tilde{u}) = \begin{pmatrix} U & 0 \\ U_b & 0 \end{pmatrix} = \begin{pmatrix} U(u) & 0 \\ U_b & 0 \end{pmatrix}, \quad \frac{\partial U_b}{\partial \lambda} = 0. \tag{80}$$

It is equivalent to

$$\phi_x = U\phi, \quad (\phi_b)_x = U_b\phi.$$

Choose a solution for $\tilde{V}=[\tilde{U}, \tilde{V}]$ as

$$\tilde{V} = \tilde{V}(\tilde{u}) = \begin{pmatrix} V & 0 \\ V_b & 0 \end{pmatrix} = \begin{pmatrix} V(u) & 0 \\ V_b(\tilde{u}) & 0 \end{pmatrix}, \tag{81}$$

and we are then led to

$$(V_b)_x = U_b V - V_b U, \tag{82}$$

besides $V_x=[U, V]$. The enlarged temporal spectral matrices read as

$$\tilde{V}^{(n)} = \begin{pmatrix} V^{(n)} & 0 \\ V_b^{(n)} & 0 \end{pmatrix} = \begin{pmatrix} V^{(n)}(u) & 0 \\ V_b^{(n)}(\tilde{u}) & 0 \end{pmatrix}, \quad n \geqslant 0, \tag{83}$$

and so the enlarged temporal spectral problems

$$\tilde{\phi}_{t_n} = \tilde{V}^{(n)}\tilde{\phi}, \quad \tilde{\phi} = (\phi^T, \phi_b^T)^T, \quad n \geqslant 0, \tag{84}$$

are equivalent to

$$\phi_{t_n} = V^{(n)}\phi, \quad (\phi_b)_{t_n} = V_b^{(n)}\phi, \quad n \geqslant 0.$$

Now the enlarged zero curvature equations

$$\tilde{U}_{t_n} - \tilde{V}_x^{(n)} + [\tilde{U}, \tilde{V}^{(n)}] = 0, \quad n \geqslant 0,$$

equivalently engender the triangular systems

$$U_{t_n} - V_x^{(n)} + [U, V^{(n)}] = 0, \quad n \geqslant 0, \tag{85}$$

$$(U_b)_{t_n} - (V_b^{(n)})_x + U_b V^{(n)} - V_b^{(n)} U = 0, \quad n \geqslant 0. \tag{86}$$

To present the second enlarged soliton hierarchy, let us similarly introduce

$$V_b = \sum_{i \geqslant 0} V_{b,i} \lambda^{-i-1}, \quad \frac{\partial V_{b,i}}{\partial \lambda} = 0, \tag{87}$$

and then (82) leads to

$$V_{b,0} U_0 - U_b V_0 = 0, \tag{88}$$

$$(V_{b,i})_x = U_b V_{i+1} - V_{b,i+1} U_0 - V_{b,i} U_1, \quad i \geqslant 0, \tag{89}$$

where U_0 and U_1 are defined by (11), and V_i, by (16).

We also assume that the conditions in (62) are satisfied, to determine V_b uniquely. Then, U_0 is invertible, and so the matrix V_b in (87) is uniquely determined by (88) and (89), indeed. Define the additional Lax matrices as

$$V_b^{(n)} = (\lambda^n V_b)_+, \quad n \geqslant 0, \tag{90}$$

where the subscript + denotes to take the polynomial part in λ. Then, using (82), we have

$$(V_b^{(n)})_x = (\lambda^n U_b V)_+ - (\lambda^n V_b U)_+ = U_b V^{(n)} - (\lambda^n V_b U)_+,$$

and we can further compute that

$$\begin{aligned} -(V_b^{(n)})_x + U_b V^{(n)} - V_b^{(n)} U &= (\lambda^n V_b U)_+ - V_b^{(n)} U \\ &= V_b^{(n+1)} U_0 + V_b^{(n)} U_1 - V_b^{(n)} (\lambda U_0 + U_1) \\ &= V_b^{(n+1)} U_0 - \lambda V_b^{(n)} U_0 \\ &= (V_{b,n} + \lambda V_b^{(n)}) U_0 - \lambda V_b^{(n)} U_0 \\ &= V_{b,n} U_0. \end{aligned}$$

It now follows that the additional equations determined by (86) become

$$(U_b)_{t_n} = -V_{b,n} U_0, \quad n \geqslant 0, \tag{91}$$

and thus, the candidates of integrable couplings are determined by

$$u_{t_n} = K_n(u), \quad (U_b)_{t_n} = -V_{b,n} U_0, \quad n \geqslant 0, \tag{92}$$

Let us now proceed to present the concrete expression of (92). Similarly, we specify U_b and $V_{b,i}$ as follows:

$$U_b = \begin{pmatrix} y_1 & z_1 \\ \vdots & \vdots \\ y_l & z_l \end{pmatrix}, \quad V_{b,i} = \begin{pmatrix} g_1^{(i)} & h_1^{(i)} \\ \vdots & \vdots \\ g_l^{(i)} & h_l^{(i)} \end{pmatrix}, \quad i \geqslant 0, \tag{93}$$

where l is an arbitrary natural number, y_j and $g_j^{(i)}$, $1 \leqslant j \leqslant l$, are scalars but z_j and $h_j^{(i)}$, $1 \leqslant j \leqslant l$, are m-dimensional rows. Then, the recursion relation defined by (88) and (89) gives rise to

$$(g_j^{(0)} h_j^{(0)}) = (y_j z_j) V_0 U_0^{-1} = (y_j z_j), \quad 1 \leqslant j \leqslant l, \tag{94}$$

$$(g_j^{(i+1)} h_j^{(i+1)}) = -(g_j^{(i)} h_j^{(i)})_x U_0^{-1} + (y_j z_j) V_{i+1} U_0^{-1} - (g_j^{(i)} h_j^{(i)}) U_1 U_0^{-1}, \quad 1 \leqslant j \leqslant l, \quad i \geqslant 0, \tag{95}$$

and the additional equations determined by (91) become

$$\begin{pmatrix} y_1 & z_1 \\ \vdots & \vdots \\ y_l & z_l \end{pmatrix}_{t_n} = -V_{b,n} U_0 = -\begin{pmatrix} \alpha g_1^{(n)} & \beta h_1^{(n)} \\ \vdots & \vdots \\ \alpha g_l^{(n)} & \beta h_l^{(n)} \end{pmatrix}, \quad n \geqslant 0. \tag{96}$$

Therefore, the enlarged hierarchy (92) of the vector AKNS soliton equations reads as

$$\tilde{u}_{t_n} \equiv \begin{pmatrix} q^T \\ r \\ y_1 \\ z_1^T \\ \vdots \\ y_l \\ z_l^T \end{pmatrix}_{t_n} = \tilde{K}_n \equiv \begin{pmatrix} (\alpha - \beta) b^{(n+1)T} \\ (\beta - \alpha) c^{(n+1)} \\ -\alpha g_1^{(n)} \\ -\beta h_1^{(n)T} \\ \vdots \\ -\alpha g_l^{(n)} \\ -\beta h_l^{(n)T} \end{pmatrix}, \quad n \geqslant 0. \tag{97}$$

2. Recursion structure for the second enlarged hierarchy

Let us now derive a recursion structure for the second enlarged soliton hierarchy (97). From the above recursion relation (95) for $g_j^{(i)}$ and $h_j^{(i)}$, we have

$$\alpha g_j^{(i+1)} = -(g_j^{(i)})_x - h_j^{(i)} r + (y_j a^{(i+1)} + z_j b^{(i+1)}), \quad i \geqslant 0, \tag{98a}$$

$$\beta h_j^{(i+1)} = -(h_j^{(i)})_x - g_j^{(i)} q + (y_j b^{(i+1)} + z_j d^{(i+1)}), \quad i \geqslant 0. \tag{98b}$$

In particular, this generates

$$g_j^{(1)} = -\frac{1}{\alpha}(y_j)_x, \quad h_j^{(1)} = -\frac{1}{\beta}(z_j)_x, \quad 1 \leqslant j \leqslant l,$$

$$g_j^{(2)} = \frac{1}{\alpha}\left[\frac{1}{\alpha}(y_j)_{xx} + \frac{1}{\beta}(z_j)_x r + \frac{1}{\beta - \alpha} y_j q r + \frac{1}{\beta - \alpha} z_j r_x\right], \quad 1 \leqslant j \leqslant l,$$

$$h_j^{(2)} = \frac{1}{\beta}\left[\frac{1}{\beta}(z_j)_{xx} + \frac{1}{\alpha}(y_j)_x q + \frac{1}{\alpha - \beta} y_j q_x + \frac{1}{\alpha - \beta} z_j r q\right], \quad 1 \leqslant j \leqslant l.$$

To obtain a recursion structure, we rewrite the equations (96) as

$$\begin{pmatrix} y_j \\ z_j^T \end{pmatrix}_{t_n} = \begin{pmatrix} -\alpha g_j^{(n)} \\ -\beta h_j^{(n)T} \end{pmatrix} = \tilde{\Phi}_j \begin{pmatrix} (\alpha-\beta) b^{(n)T} \\ (\beta-\alpha) c^{(n)} \end{pmatrix} + \tilde{\Phi}_0 \begin{pmatrix} -\alpha g_j^{(n-1)} \\ -\beta h_j^{(n-1)T} \end{pmatrix}, \quad 1 \leqslant j \leqslant l, \quad n \geqslant 0. \tag{99}$$

Then it follows from (98) and (21) that the $(m+1)\times(m+1)$ matrix $\tilde{\Phi}_0$ can be taken as

$$\tilde{\Phi}_0 = \tilde{\Phi}_0(q,r) = \begin{pmatrix} -\frac{1}{\alpha}\partial & -\frac{1}{\beta} r^T \\ -\frac{1}{\alpha} q^T & -\frac{1}{\beta}\partial I_m \end{pmatrix}, \tag{100}$$

and further, the $(m+1)\times 2m$ matrix operators $\tilde{\Phi}_j$ can be taken as

$$\tilde{\Phi}_j = \tilde{\Phi}_j(q,r,y_j,z_j) = \frac{1}{\beta-\alpha} \begin{pmatrix} -y_j \partial^{-1} L_{r^T} & -y_j \partial^{-1} L_q - L_{z_j} \\ y_j I_m + R_{z_j^T} \partial^{-1} R_{r^T} & R_{z_j^T} \partial^{-1} L_{q^T} T \end{pmatrix}, \quad 1 \leqslant j \leqslant l, \tag{101}$$

where $(R_A)B = BA$, $(L_A)B = AB$, and $TB = B^T$ for two matrices A and B. Therefore, the enlarged vector AKNS hierarchy (97) possesses the following recursion structure:

$$\begin{pmatrix} q^T \\ r \\ y_1 \\ z_1^T \\ \vdots \\ y_l \\ z_l^T \end{pmatrix}_{t_n} = \tilde{\Phi} \begin{pmatrix} (\alpha-\beta) b^{(n)T} \\ (\beta-\alpha) c^{(n)} \\ -\alpha g_1^{(n-1)} \\ -\beta h_1^{(n-1)} \\ \vdots \\ -\alpha g_l^{(n-1)} \\ -\beta h_l^{(n-1)} \end{pmatrix} = \tilde{\Phi}^n \begin{pmatrix} (\alpha-\beta) b^{(1)T} \\ (\beta-\alpha) c^{(1)} \\ -\alpha g_1^{(0)} \\ -\beta h_1^{(0)} \\ \vdots \\ -\alpha g_1^{(0)} \\ -\beta h_1^{(0)} \end{pmatrix} = \tilde{\Phi}^n \begin{pmatrix} (\alpha-\beta) q^T \\ (\beta-\alpha) r \\ -\alpha y_1 \\ -\beta z_1 \\ \vdots \\ -\alpha y_l \\ -\beta z_l^T \end{pmatrix}, \quad n \geqslant 0, \tag{102}$$

once we define the recursion operator $\tilde{\Phi}$ as

$$\tilde{\Phi} = \begin{pmatrix} \Phi & & & & & 0 \\ \tilde{\Phi}_1 & \tilde{\Phi}_0 & & & & \\ \tilde{\Phi}_2 & 0 & \tilde{\Phi}_0 & & & \\ \vdots & \ddots & \ddots & \ddots & & \\ \tilde{\Phi}_l & 0 & \cdots & \cdots & 0 & \tilde{\Phi}_0 \end{pmatrix}, \tag{103}$$

where $\Phi = \Psi^{\dagger}$ is the hereditary recursion operator defined by (36). Note that there may also exist other choices for $\tilde{\Phi}_j$ and $\tilde{\Phi}_0$ in the recursion structure (99).

The triangular systems in (97) are commutative, which can be shown in a similar manner to the proof for the first class. The enlarged spectral problem (79) has the uniqueness property, indeed, which can also be directly verified. Moreover, the Lax matrices

$$\tilde{V}^{k,l}(\tilde{u}) \equiv (\tilde{V}^{(k)})'(\tilde{u})[\tilde{K}_l] - (\tilde{V}^{(l)})'(\tilde{u})[\tilde{K}_k] + [\tilde{V}^{(k)}(\tilde{u}), \tilde{V}^{(l)}(\tilde{u})], \quad k,l \geqslant 0, \tag{104}$$

have zero initial value $\tilde{V}^{k,l}(\tilde{u})|_{\tilde{u}=0} = 0$. Therefore, by the so-called uniqueness property,[17] the new enlarged soliton hierarchy defined by (97) or (102) is commutative, and so it is a common hierarchy of commuting integrable couplings for all the vector AKNS soliton equations in (28). The first nonlinear system in the hierarchy reads as

$$q_{t_2} = \frac{1}{\alpha-\beta}(q_{xx} - 2qrq), \tag{105a}$$

$$r_{t_2} = \frac{1}{\beta - \alpha}(r_{xx} - 2rqr), \tag{105b}$$

$$(y_j)_{t_2} = -\left[\frac{1}{\alpha}(y_j)_{xx} + \frac{1}{\beta}(z_j)_x r + \frac{1}{\beta - \alpha} y_j qr + \frac{1}{\beta - \alpha} y_j r_x\right], \quad 1 \leqslant j \leqslant l, \tag{105c}$$

$$(z_j)_{t_2} = -\left[\frac{1}{\beta}(z_j)_{xx} + \frac{1}{\alpha}(y_j)_x q + \frac{1}{\alpha - \beta} y_j q_x + \frac{1}{\alpha - \beta} z_j rq\right], \quad 1 \leqslant j \leqslant l, \tag{105d}$$

where q, r^T, z_j are m-dimensional rows and y_j are scalar variables.

D. Bäcklund transformation and special solutions

It is known that the adjoint zero curvature equation

$$(-U^T)_t - (-V^T)_x + [-U^T, -V^T] = 0$$

is equivalent to the zero curvature equation

$$U_t - V_x + [U, V] = 0.$$

Therefore, they lead to the same soliton equation. Using this fact, our two classes of enlarged specific spectral problems of the equal sizes can be linked to each other. More specifically, we can take

$$\overline{U} = -(\widetilde{U})^T, \quad \overline{V} = -(\widetilde{V})^T, \quad \overline{V}^{(n)} = -(\widetilde{V}^{(n)})^T, \quad n \geqslant 0,$$

to transform one to another of the equal sizes, and thus the two classes of integrable couplings can be transformed into each other. The resulting Bäcklund transformation from $\overline{U} = -(\widetilde{U})^T$ reads as

$$q \to -r^T, \quad r \to -q^T, \quad v_j \to -y_j, \quad w_j \to -z_j^T, \quad \alpha \to -\alpha, \quad \beta \to -\beta.$$

Under this transformation, the first hierarchy of integrable couplings (70) becomes the second hierarchy (97) of integrable couplings. In particular, the first nonlinear integrable coupling (78) in the first enlarged soliton hierarchy becomes the first nonlinear integrable coupling (105) in the second enlarged soliton hierarchy. Therefore, the above Bäcklund transformation links the two classes of integrable couplings together, and also provides another way to generate the second class of integrable couplings.

On the other hand, we point out that some special classes of exact solutions can be explicitly presented for the resulting integrable coupling (78). First, let us choose

$$q = 0, \quad r_{t_2} = \frac{1}{\beta - \alpha} r_{xx}, \quad (v_j)_{t_2} = \frac{1}{\alpha}(v_j)_{xx}, \quad 1 \leqslant j \leqslant l,$$

and then solving the nonhomogeneous heat equations for w_j,

$$(w_j)_{t_2} = \frac{1}{\beta}(w_j)_{xx} - \frac{1}{\alpha} r (v_j)_x + \frac{1}{\beta - \alpha} r_x v_j, \quad 1 \leqslant j \leqslant l,$$

gives a class of solutions to the integrable coupling (78). Second, let us choose

$$q_{t_2} = \frac{1}{\alpha - \beta} q_{xx}, \quad r = 0, \quad (w_j)_{t_2} = \frac{1}{\beta}(w_j)_{xx}, \quad 1 \leqslant j \leqslant l,$$

and then solving the nonhomogeneous heat equations for v_j,

$$(v_j)_{t_2} = \frac{1}{\alpha}(v_j)_{xx} - \frac{1}{\beta}q(w_j)_x + \frac{1}{\alpha-\beta}q_x w_j, \quad 1 \leqslant j \leqslant l,$$

gives another class of solutions to the integrable coupling (78). In particular, when $m=l=1$, we can have the following two concrete solutions:

$$q = 0, \quad r = \frac{c_1}{\sqrt{t_2-\eta_1}} \exp\left(\frac{(\alpha-\beta)(x-\xi_1)^2}{4(t_2-\eta_1)}\right),$$

$$v_1 = \frac{c_2}{\sqrt{t_2-\eta_1}} \exp\left(-\frac{\alpha(x-\xi_1)^2}{4(t_2-\eta_1)}\right), \quad w_1 = \sum_{i=1}^{k} \frac{d_i}{\sqrt{t_2-\eta_i}} \exp\left(-\frac{\beta(x-\xi_i)^2}{4(t_2-\eta_i)}\right) + d_{k+1},$$

and

$$q = \frac{c_1}{\sqrt{t_2-\eta_1}} \exp\left(\frac{(\beta-\alpha)(x-\xi_1)^2}{4(t_2-\eta_1)}\right), \quad r = 0,$$

$$v_1 = \sum_{i=1}^{k} \frac{d_2}{\sqrt{t_2-\eta_i}} \exp\left(-\frac{\alpha(x-\xi_i)^2}{4(t_2-\eta_i)}\right) + d_{k+1}, \quad w_1 = \frac{c_i}{\sqrt{t_2-\eta_1}} \exp\left(-\frac{\beta(x-\xi_1)^2}{4(t_2-\eta_1)}\right),$$

where k is an arbitrary natural number, and η_i, ξ_i, c_i, and d_i are arbitrary constants. The solution analysis made here also implies that coupled systems of differential equations can possess diverse solutions,[22] like integrable equations in higher dimensions.[23] Actually, even in the case of 1+1 dimensions, a new kind of exact solutions, so-called complexitons, were recently shown to exist for the Korteweg–de Vries equation[24] and the Toda lattice equation.[25]

IV. CONCLUDING REMARKS

Two specific classes of multicomponent integrable couplings have been presented for the physically important vector AKNS soliton hierarchy. The basic idea in our construction is to apply an idea of enlarging the associated spectral problems or the associated loop Lie algebras underlying the spectral problems. The enlarged vector AKNS soliton hierarchies also possess zero curvature representations and recursion structures, which guarantee the existence of infinitely many symmetries of the enlarged soliton hierarchies. Under the reduction of $\alpha=-1$, $\beta=1$, and $m=l=1$, the first class of integrable couplings boil down to the integrable couplings of the scalar AKNS soliton equations presented in Ref. 19.

We point out that there is another successful choice of enlarged spectral matrices

$$\overline{U} = \hat{U}(u,v) \equiv \begin{pmatrix} U(u) & 0 \\ U'(u)[v] & U(u) \end{pmatrix} \quad \text{or} \begin{pmatrix} U(u) & U'(u)[v] \\ 0 & U(u) \end{pmatrix},$$

which correspond to the spectral matrices generated by perturbation.[3] The additional potential v in the above enlarged spectral matrix $\hat{U}(u,v)$ must have the same number of dependent variables as u. But the enlarged spectral matrix $\hat{U}(u,v)$ has a symmetric structure, which ensures that there exist Hamiltonian structures for the enlarged soliton equations.[3] On the other hand, we can relax the conditions in (49), i.e., let the additional matrices U_a and U_b in (38) depend on the spectral parameter λ. For example, we can choose

$$U_a = \sum_{i=1}^{k} U_{a,i}\lambda^{i-1} = \sum_{i=1}^{k} \begin{pmatrix} v_{1,i} & \cdots & v_{l,i} \\ w_{1,i} & \cdots & w_{l,i} \end{pmatrix} \lambda^{i-1}, \quad k,l \geqslant 1,$$

$$U_b = \sum_{i=1}^{k} U_{b,i}\lambda^{i-1} = \sum_{i=1}^{k} \begin{pmatrix} y_{1,i} & z_{1,i} \\ \vdots & \vdots \\ y_{l,i} & z_{l,i} \end{pmatrix} \lambda^{i-1}, \quad k,l \geqslant 1.$$

Then, much more diverse integrable couplings can be expected to obtain.

We would also like to emphasize that the resulting integrable couplings by enlarging spectral problems are different from the ones obtained by the method of perturbations. Actually, the integrable couplings (78) and (105), for example, cannot be obtained through using perturbations at all. On the other hand, it should be very important to investigate the Painlevé property and bilinear forms of the enlarged soliton hierarchies (70) and (97), especially the integrable couplings (78) and (105), from the solution perspective. The systems (78) and (105) reduce to two systems of variable coefficient partial differential equations, if q and r are given.

We finally remark that the integrability property usually requires the existence of infinitely many conservation laws.[26] The perturbation procedure of enlarging spectral problems guarantees Hamiltonian structures and thus infinitely many conservation laws.[3,6] It is an interesting question whether the enlarged vector AKNS soliton hierarchies (70) and (97) possess infinitely many conservation laws of the enlarged type, i.e., involving the additional variables [v_j and w_j in the case of (70), and y_j and z_j in the case of (97)] and their derivatives with respect to x.

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Validity and failure of some entropy inequalities for CAR systems

Hajime Moriya[a)]
Institut des Hautes Études Scientifiques (IHES), Le Bois-Marie, 35, route de Chartres F-91440 Bures-sun-Yvette, France

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Basic properties of von Neumann entropy such as the triangle inequality and what we call MONO–SSA are studied for CAR systems. We show that both inequalities hold for every even state by using symmetric purification which is applicable to such a state. We construct a certain class of noneven states giving examples of the nonvalidity of those inequalities. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Let $\mathcal{H}$ be a Hilbert space and D be a density matrix on $\mathcal{H}$, i.e., a positive trace class operator on $\mathcal{H}$ whose trace is unity. The von Neumann entropy is given by

$$-\mathbf{Tr}(D\log D), \tag{1}$$

where **Tr** denotes the trace which takes the value 1 on each minimal projection. Let ϱ be a normal state of $\mathcal{B}(\mathcal{H})$, the set of all bounded linear operators on $\mathcal{H}$. Then ϱ has its density matrix D_ϱ, and its von Neumann entropy $S(\varrho)$ is given by (1) with $D=D_\varrho$.

It has been known that von Neumann entropy is useful for description and characterization of state correlation for composite systems. Among others, the following inequality called strong subadditivity (SSA) is remarkable:

$$S(\varphi_{I\cup J})-S(\varphi_I)-S(\varphi_J)+S(\varphi_{I\cap J})\leqslant 0, \tag{2}$$

where I, J, $I\cap J$, and $I\cup J$ denote the indexes of subsystems and φ_I denotes the restriction of a state φ to the subsystem indexed by I, and so on. Such entropy inequalities have been studied for quantum systems, see e.g., Refs. 4,5,9,11,13,15, and also their references. However, the composite systems considered there were mostly tensor product of matrix algebras to which we refer as the tensor product systems.

We investigate some well-known entropy inequalities, the triangle inequality and MONO–SSA (which will be specified soon later), for CAR systems. This study is relevant to our previous works on state correlations such as quantum-entanglement[7] and separability[8] for CAR systems. In a certain sense, the conditions of validity and failure of such entropy inequalities which we are going to establish will explain the similarities and differences in the possible forms of state correlations between CAR and tensor product systems.

Let $\mathcal{L}$ be an arbitrary discrete set. The canonical anticommutation relations (CAR) are

$$\{a_i^*,a_j\}=\delta_{i,j}\mathbf{1},$$

a)Electronic mail: moriya@ihes.fr

$$\{a_i^*, a_j^*\} = \{a_i, a_j\} = 0,$$

where $i, j \in \mathcal{L}$, and $\{A,B\}=AB+BA$ (anticommutator). For each subset I of $\mathcal{L}$, $\mathcal{A}(I)$ denotes the subsystem on I given as the $\mathbf{C}^*$-algebra generated by all a_i^* and a_i with $i \in I$. For $I \subset J$, $\mathcal{A}(I)$ is naturally imbedded in $\mathcal{A}(J)$ as its subalgebra.

We have already shown that SSA (2) holds for the CAR systems. For the convenience, we sketch its proof given in Ref. 6 and Theorem 10.1 of Ref. 2 First we check the commuting square property for a CAR system as follows:

$$\begin{array}{ccc} \mathcal{A}(I \cup J) & \xrightarrow{E_1} & \mathcal{A}(I) \\ E_J \downarrow & & \downarrow E_{I\cap J} \\ \mathcal{A}(J) & \xrightarrow[E_{I\cap J}]{} & \mathcal{A}(I \cap J) \end{array},$$

where E denotes the conditional expectation with respect to the tracial state onto the subsystem with a specified index. From this property SSA follows for every state (without any assumption on the state, like its evenness) by a well-known proof method using the monotonicity of relative entropy under the action of conditional expectations.

We move to entropy inequalities for which CAR makes a difference. The following is usually referred to as the triangle inequality:

$$|S(\varphi_I) - S(\varphi_J)| \leqslant S(\varphi_{I\cup J}), \tag{3}$$

where I and J are disjoint. While this is satisfied for the tensor product systems,[1] it is not valid in general for the CAR systems; there is a counter example.[7]

We next introduce our main target,

$$S(\varphi_I) + S(\varphi_J) \leqslant S(\varphi_{K\cup I}) + S(\varphi_{K\cup J}), \tag{4}$$

where I, J, and K are disjoint. We may call (4) "MONO–SSA," because it is equivalent to SSA (2) for the tensor product systems at least, and it obviously implies the monotonicity of the following function:

$$K \mapsto S(\varphi_{K\cup I}) + S(\varphi_{K\cup J}),$$

with respect to the inclusion of the index K. Our question is whether MONO–SSA holds for the CAR systems, if not, under what condition it is satisfied.

The MONO–SSA for the tensor product systems is shown by what is called purification implying the equivalence of MONO–SSA and SSA for those systems (see 3.3 of Ref. 11). We note that the purification is a sort of state extension, and is not automatic for the CAR systems. We shall review the basic concept of state extension.

In the description of a quantum composite system, the total system is given by a $\mathbf{C}^*$-algebra $\mathcal{A}$, and its subsystems are described by $\mathbf{C}^*$-subalgebras $\mathcal{A}_i$ of $\mathcal{A}$ indexed by $i=1,2,\ldots$. Let φ be a state of $\mathcal{A}$. We denote its restrictions to $\mathcal{A}_i$ by φ_i. Surely φ_i is a state of $\mathcal{A}_i$. Conversely, suppose that a set of states φ_i of $\mathcal{A}_i$, $i=1,2,\ldots$, are given. Then a state φ of $\mathcal{A}$ is called an extension of $\{\varphi_i\}$ if its restriction to each $\mathcal{A}_i$ coincides with φ_i.

For tensor product systems, there always exists a state extension for any given prepared states $\{\varphi_i\}$ on disjoint regions, at least their product state extension $\varphi=\varphi_1 \otimes \cdots \otimes \varphi_i \otimes \cdots$, and generically other extensions. On the contrary, it is not always the case for CAR systems. When two (or more than two) prepared states on disjoint regions are not even, there may be no state extension. We have shown that if all of them are noneven pure states, then there exists no state extension.[7,3]

We explain the above-mentioned purification in terms of state extension. We are given a state ϱ_1 of $\mathcal{A}(I)$. We then prepare some state ϱ_2 on some $\mathcal{A}(J)$ with $J \cap I = \varnothing$ such that it has the same nonzero eigenvalues and their multiplicities as ϱ_1 for their density matrices. We want to construct their pure state extension to $\mathcal{A}(I \cup J)$. We use the term "symmetric purification" to refer to this

TABLE I. Truth and the falsity of von Neumann entropy inequalities.

Property	Tensor-product systems	CAR systems
SSA	○	○
Triangle	○	× in general, but ○ for every even state
MONO–SSA	○	× in general, but ○ for every even state

procedure where the "symmetric" may indicate the above specified property of ϱ_2. For the tensor product systems, symmetric purification exists for every ϱ_1. On the contrary for the CAR systems, though we can easily make a pure state extension of ϱ_1, its pair ϱ_2 cannot always be chosen among those states which have the same nonzero eigenvalues and their multiplicities as ϱ_1. In the above and what follows, we shall identify states with their density matrices when there is no fear of confusion.

We will show that MONO–SSA is not satisfied in general in Sec. III. However it is shown to hold for every even state in Sec. II. Table I above shows the truth (○) and the falsity (×) of the entropy inequalities.

We fix our notation. The even–odd grading Θ is determined by

$$\Theta(a_i^*) = -a_i^*, \quad \Theta(a_i) = -a_i. \tag{5}$$

The even and odd parts of $\mathcal{A}(I)$ are given by

$$\mathcal{A}(I)_\pm \equiv \{A \in \mathcal{A}(I) | \Theta(A) = \pm A\}.$$

For an element $A \in \mathcal{A}(I)$ we have the decomposition

$$A = A_+ + A_-, \quad A_\pm \equiv \tfrac{1}{2}(A \pm \Theta(A)) \in \mathcal{A}(I)_\pm.$$

For a finite subset I, define

$$v_I \equiv \prod_{i \in I} v_i, \quad v_i \equiv a_i^* a_i - a_i a_i^*. \tag{6}$$

By a simple computation, v_I is a self-adjoint unitary operator in $\mathcal{A}(I)_+$ implementing Θ, namely

$$\mathrm{Ad}(v_I)(A) = \Theta(A), \quad A \in \mathcal{A}(I). \tag{7}$$

For a finite subset I, every even pure state of $\mathcal{A}(I)$ is given by an eigenvector of v_I as its vector state.

The following is a simple consequence of the CAR given, e.g., in Sec. 4.5 of Ref. 2.

Lemma 1: *Let I be a finite subset and J be a (finite or infinite) subset disjoint with J. Let $\mathcal{A}(I'|I \cup J) \equiv \mathcal{A}(I)' \cap \mathcal{A}(I \cup J)$ and $\mathcal{A}(I'|J) \equiv \mathcal{A}(I)' \cap \mathcal{A}(J)$, the commutant of $\mathcal{A}(I)$ in $\mathcal{A}(I \cup J)$ and that in $\mathcal{A}(J)$, respectively. Then*

$$\mathcal{A}(I'|I \cup J) = \mathcal{A}(J)_+ + v_I \mathcal{A}(J)_-, \tag{8}$$

$$\mathcal{A}(I'|J) = \mathcal{A}(J)_+. \tag{9}$$

In this note we restrict our discussion to finite-dimensional systems so as to exclude from the outset the cases where our statements themselves on von Neumann entropy do not make sense; for infinite-dimensional systems a density matrix does not exist in general for a given state. (However in the proof of Proposition 8 we shall mention possible infinite-dimensional extensions of some results.)

II. SYMMETRIC PURIFICATION FOR EVEN STATES

Symmetric purification is a useful mathematical technique having a lot of applications. For example, we can derive MONO–SSA from SSA for the tensor product systems by using it.

We now discuss symmetric purification for the CAR systems. We shall show its existence for even states.

Lemma 2: *Let I and J be mutually disjoint finite subsets. Let ϱ be an even pure state of $\mathcal{A}(I\cup J)$, and let ϱ_1 and ϱ_2 be its restrictions to $\mathcal{A}(I)$ and $\mathcal{A}(J)$. Then the density matrix of ϱ_1 has the same nonzero eigenvalues and their multiplicities as those of ϱ_2. In particular, $S(\varrho_1)=S(\varrho_2)$.*

Proof: We have $\mathcal{A}(I\cup J)=\mathcal{A}(I)\otimes\mathcal{A}(I'|I\cup J)$ by (8). By some finite-dimensional Hilbert spaces $\mathcal{H}_1$, $\mathcal{H}_2$, and $\mathcal{H}_{1,2}\equiv\mathcal{H}_1\otimes\mathcal{H}_2$, we can write $\mathcal{A}(I\cup J)=\mathcal{B}(\mathcal{H}_{1,2})$, $\mathcal{A}(I)=\mathcal{B}(\mathcal{H}_1)$, and $\mathcal{A}(I'|I\cup J)=\mathcal{B}(\mathcal{H}_2)$.

Since ϱ is a pure state of $\mathcal{A}(I\cup J)$, its density matrix [with respect to the non-normalized trace **Tr** of $\mathcal{B}(\mathcal{H}_{1,2})$] is a one-dimensional projection operator of $\mathcal{B}(\mathcal{H}_{1,2})$, and hence there exists a unit vector $\xi\in\mathcal{H}_{1,2}$ such that $D_\varrho\eta=(\xi,\eta)\xi$ for any $\eta\in\mathcal{H}_{1,2}$. By using the Schmidt decomposition,[12] we have the following decomposed form:

$$\xi=\sum_i \lambda_i\xi_{1i}\otimes\xi_{2i},\quad \lambda_i>0, \tag{10}$$

where $\{\xi_{1i}\}$ and $\{\xi_{2i}\}$ are some orthonormal sets of vectors of $\mathcal{H}_1$ and $\mathcal{H}_2$. For $\nu=1,2$, let $P(\xi_{\nu i})$ denote the projection operator on the one-dimensional subspace of $\mathcal{H}_\nu$ containing $\xi_{\nu i}$. We denote the restricted states of ϱ onto $\mathcal{B}(\mathcal{H}_2)$ by $\tilde{\varrho}_2$. By (10), the density matrices of ϱ_1 and $\tilde{\varrho}_2$ have the following symmetric forms:

$$D_{\varrho_1}=\sum_i \lambda_i^2 P(\xi_{1i}),\quad D_{\tilde{\varrho}_2}=\sum_i \lambda_i^2 P(\xi_{2i}). \tag{11}$$

Since ϱ is an even state, its restriction ϱ_2 is even and hence its density matrix D_{ϱ_2} belongs to $\mathcal{A}(J)_+$.

On the other hand, the even state ϱ is invariant under the action of $\mathrm{Ad}(v_{I\cup J})=\mathrm{Ad}(v_I v_J)$:

$$v_{I\cup J}D_\varrho v_{I\cup J}=v_I v_J D_\varrho v_I v_J=D_\varrho.$$

Acting the conditional expectation onto $\mathcal{B}(\mathcal{H}_2)$ with respect to the tracial state of $\mathrm{B}(\mathcal{H}_{1,2})$ on the above equality, we obtain

$$v_J D_{\tilde{\varrho}_2} v_J=D_{\tilde{\varrho}_2}$$

noting that v_I belongs to $\mathcal{B}(\mathcal{H}_1)=\mathcal{B}(\mathcal{H}_2)'\cap\mathcal{B}(\mathcal{H}_{1,2})$.

We denote $\mathcal{B}(\mathcal{H}_2)_+\equiv\mathcal{B}(\mathcal{H}_2)\cap\mathcal{A}(I\cup J)_+$, the set of all invariant elements under $\mathrm{Ad}(v_I v_J)$ in $\mathcal{B}(\mathcal{H}_2)$. By (8), $\mathcal{B}(\mathcal{H}_2)_+$ is equal to $\mathcal{A}(J)_+$, and also to the set of all invariant elements under $\mathrm{Ad}(v_J)$ in $\mathcal{B}(\mathcal{H}_2)$. Therefore both $D_{\tilde{\varrho}_2}$ and D_{ϱ_2} belong to $\mathcal{B}(\mathcal{H}_2)_+$. Accordingly, $D_{\tilde{\varrho}_2}$ is equal to D_{ϱ_2} as the density of the state ϱ restricted to $\mathcal{B}(\mathcal{H}_2)_+$, and hence

$$D_{\varrho_2}=D_{\tilde{\varrho}_2}=\sum_i \lambda_i^2 P(\xi_{2i}). \tag{12}$$

From (11) and (12), it follows that ϱ_1 and ϱ_2 have the same nonzero eigenvalues and their multiplicities equal to $\{\lambda_i^2\}$. Thus

$$S(\varrho_1)=S(\varrho_2).$$

■

For a subset I of $\mathcal{L}$, $|I|$ denotes the number of sites in I.

Lemma 3. Let I be a finite subset and ϱ_1 be a state of $\mathcal{A}(I)$. Let J be a finite subset such that $J\cap I=\emptyset$ and $|J|\geqslant|I|$. Then there exists a pure state ϱ on $\mathcal{A}(I\cup J)$ satisfying

$$\varrho|_{\mathcal{A}(I)} = \varrho_1. \tag{13}$$

Moreover, if ϱ_1 is even, then the above ϱ can be taken to be even.

Proof: We use the same notation as in the proof of the preceding lemma and write $\mathcal{A}(I\cup J) = \mathcal{B}(\mathcal{H}_{1,2})$, $\mathcal{A}(I)=\mathcal{B}(\mathcal{H}_1)$, and $\mathcal{A}(I'|I\cup J)=\mathcal{B}(\mathcal{H}_2)$. Let $\varrho_1=\Sigma_i\lambda_i^2 P(\xi_{1i})$, where $\lambda_i>0$, $\{\xi_{1i}\}$ is an orthonormal set of $\mathcal{H}_1$, and $P(\xi_{1i})$ is the projection operator on the one-dimensional subspace of $\mathcal{H}_1$ containing ξ_{1i}. Since $|J|\geqslant|I|$ and hence $\dim\mathcal{H}_2\geqslant\dim\mathcal{H}_1$, we can take an orthonormal set of vectors $\{\xi_{2i}\}$ of $\mathcal{H}_2$ having the same cardinality as $\{\xi_{1i}\}$. Define a unit vector $\xi\in\mathcal{H}_{1,2}$ by the same formula as (10) and let ϱ be its vector state, namely the state whose density matrix is the projection operator on the one-dimensional subspace of $\mathcal{H}_{1,2}$ containing ξ. This ϱ is a pure state extension of ϱ_1 to $\mathcal{A}(I\cup J)$ by its definition.

Assume now that ϱ_1 is even, and hence its density matrix is in $\mathcal{A}(I)_+$. For each eigenvalue, the associated spectral projection is also even and commutes with v_I, and its range is invariant under v_I. Therefore we can choose an orthonormal basis of the range of the projection which consists of eigenvectors of v_I. We take $\{\xi_{1i}\}$ to be a set of eigenvectors of v_I.

Since v_J belongs to $\mathcal{B}(\mathcal{H}_2)_+(=\mathcal{A}(J)_+)$, there exists an orthonormal basis of $\mathcal{H}_2$ consisting of eigenvectors of v_J. Due to the assumption $|J|\geqslant|I|$, we can take a set of different eigenvectors $\{\xi_{2i}\}$ of v_J such that for each i its eigenvalue, $+1$ or -1, is equal to that of ξ_{1i} for v_I. Define a unit vector ξ by (10) using these $\{\xi_{1i}\}$ and $\{\xi_{2i}\}$. Since this ξ is an eigenvector of $v_{I\cup J}$ by its definition, its vector state ϱ is even. ■

Combining the above two lemmas we obtain the following.

Proposition 4: Let I be a finite subset and ϱ_1 be an even state of $\mathcal{A}(I)$. Let J be a finite subset such that $J\cap I=\emptyset$ and $|J|\geqslant|I|$. Then there exists an even pure state ϱ on $\mathcal{A}(I\cup J)$ such that its restriction to $\mathcal{A}(I)$ is equal to ϱ_1 and the density matrix of its restricted state $\varrho_2\equiv\varrho|_{\mathcal{A}(J)}$ has the same nonzero eigenvalues and their multiplicities as those of ϱ_1.

We may call the above state extension from ϱ_1 to ϱ the symmetric purification. Thanks to this, we obtain the following two theorems.

Theorem 5: *Let I, J, and K be mutually disjoint finite subsets. For every even state φ, MONO–SSA,*

$$S(\varphi_I)+S(\varphi_J)\leqslant S(\varphi_{K\cup I})+S(\varphi_{K\cup J}) \tag{14}$$

is satisfied.

Proof: The equivalence of MONO–SSA and SSA for even states follows from Proposition 4 in the same way as (3), p. 164 of Ref. 1. Since SSA holds for every state, MONO–SSA is valid for every even state. ■

Similarly, by using Proposition 4 we immediately obtain the triangle inequality for even states in much the same way as (3.1) of Ref. 1. We omit its proof.

Theorem 6: *Let I and J be mutually disjoint finite subsets. For every even state φ, the triangle inequality*

$$|S(\varphi_I)-S(\varphi_J)|\leqslant S(\varphi_{I\cup J}) \tag{15}$$

holds.

III. VIOLATION OF MONO–SSA

In this section we give a certain class of noneven states. We shall give a sketch of our model indicated by Fig. 1 (below). We can take a pure state $\varrho_{I\cup K}$ on $I\cup K$ whose restriction ϱ_K is a pure state, but ϱ_I is nonpure, say the tracial state. Such $\varrho_{I\cup K}$ does not satisfy the triangle inequality, because the entropies on I and on K are different, whereas the entropy on $I\cup K$ is zero. It can be said that the pure state $\varrho_{I\cup K}$ has the asymmetric restrictions in our terminology. This asymmetry is due to the large amount of the oddness of ϱ_K, whose precise meaning will be given soon. [Note however that for the infinite-dimensional case, the GNS representations π_{ϱ_K} and $\pi_{\varrho_K\Theta}$ should be

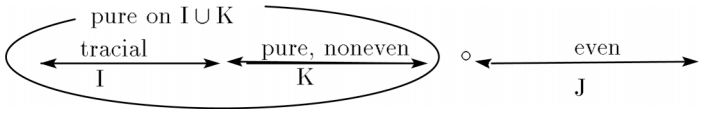

FIG. 1. A state not satisfying MONO–SSA.

unitarily equivalent, see Proposition 8(i).] We take an arbitrary even state ϱ_J on J. The desired state on $\varrho_{I\cup K\cup J}$ on $I\cup K\cup J$ is given by the product state extension of $\varrho_{I\cup K}$ and ϱ_J, which will be denoted by $\varrho_{I\cup K}\circ\varrho_J$.

We recall the definition of the transition probability.[14] For two states φ and ψ of $\mathcal{A}(I)$ (where $|I|$ is finite or infinite), take any representation π of $\mathcal{A}(I)$ on a Hilbert space $\mathcal{H}$ containing vectors Φ and Ψ such that

$$\varphi(A)=(\Phi,\pi(A)\Phi),\quad \psi(A)=(\Psi,\pi(A)\Psi), \tag{16}$$

for all $A\in\mathcal{A}(I)$. The transition probability between φ and ψ is given by

$$P(\varphi,\psi)\equiv\sup|(\Phi,\Psi)|^2, \tag{17}$$

where the supremum is taken over all $\mathcal{H}$, π, Φ, and Ψ as described above. For a state φ of $\mathcal{A}(I)$, we define

$$p_\Theta(\varphi)\equiv P(\varphi,\varphi\Theta)^{1/2}, \tag{18}$$

where $\varphi\Theta$ denotes the state $\varphi\Theta(A)=\varphi(\Theta(A))$, $A\in\mathcal{A}(I)$. Intuitively, $p_\Theta(\varphi)$ quantifies the amount of *oddness* of the state φ. If $p_\Theta(\varphi)=0$ or nearby, then we may say that the difference between φ and $\varphi\Theta$ is large. If φ is even, $p_\Theta(\varphi)$ obviously takes the maximum value 1.

The following is Lemma 3.1 of Ref. 2.

Lemma 7: If ϱ_1 is a pure state of $\mathcal{A}(K)$ and π_{ϱ_1} and $\pi_{\varrho_1\Theta}$ are unitarily equivalent, then there exists a self-adjoint unitary $u_1\in\pi_{\varrho_1}(\mathcal{A}(K)_+)''$ satisfying

$$u_1\pi_{\varrho_1}(A)u_1=\pi_{\varrho_1}(\Theta(A)),\quad A\in\mathcal{A}(K). \tag{19}$$

The next proposition is a basis of our construction. It is a generalization of Ref. 7. The first paragraph is in principle excerpted from Theorem 4 (4) and (5) of Ref. 2. The second paragraph is necessary for the argument of entropy.

Proposition 8. Let K and I be mutually disjoint subsets. Assume that ϱ_1 is a (noneven) pure state of $\mathcal{A}(K)$ satisfying $p_\Theta(\varrho_1)=0$. Assume that ϱ_2 is an even state of $\mathcal{A}(I)$. There exists a joint extension of ϱ_1 and ϱ_2 other than their product state extension if and only if ϱ_1 and ϱ_2 satisfy the following pair of conditions:

(i) *π_{ϱ_1} and $\pi_{\varrho_1\Theta}$ are unitarily equivalent.*

(ii) *There exists a state $\tilde{\varrho}_2$ of $\mathcal{A}(I)$ such that $\tilde{\varrho}_2\neq\tilde{\varrho}_2\Theta$ and*

$$\varrho_2=\tfrac{1}{2}(\tilde{\varrho}_2+\tilde{\varrho}_2\Theta). \tag{20}$$

For each $\tilde{\varrho}_2$ above, there exists the joint extension of ϱ_1 and ϱ_2 to $\mathcal{A}(K\cup I)$ denoted by $\psi_{\tilde{\varrho}_2}$ which satisfies

$$\psi_{\tilde{\varrho}_2}(A_1A_2)=\varrho_1(A_1)\varrho_2(A_{2+})+\overline{\varrho_1}(\pi_{\varrho_1}(A_1)u_1)\tilde{\varrho}_2(A_{2-}), \tag{21}$$

where $\overline{\varrho_1}$ is the GNS-extension of ϱ_1 to $\pi_{\varrho_1}(\mathcal{A}(K))''$.

If K and I are finite subsets, then the entropy of $\tilde{\varrho}_2$ is equal to that of $\psi_{\tilde{\varrho}_2}$.

Proof: We shall show only the sufficiency of the pair of conditions (i) and (ii). For the necessity of (i) see 5.2 in Ref. 2, and for that of (ii) see (d) in the proof of its Theorem 4(4).

Let $(\mathcal{H}_{\varrho_1}, \pi_{\varrho_1}, \Omega_{\varrho_1})$ be a GNS triplet for ϱ_1 and $(\mathcal{H}_{\tilde{\varrho}_2}, \pi_{\tilde{\varrho}_2}, \Omega_{\tilde{\varrho}_2})$ be that for $\tilde{\varrho}_2$. Define

$$\mathcal{H} \equiv \mathcal{H}_{\varrho_1} \otimes \mathcal{H}_{\tilde{\varrho}_2}, \quad \Omega \equiv \Omega_{\varrho_1} \otimes \Omega_{\tilde{\varrho}_2}, \tag{22}$$

$$\pi(A_1A_2) \equiv \pi_{\varrho_1}(A_1) \otimes \pi_{\tilde{\varrho}_2}(A_{2+}) + \pi_{\varrho_1}(A_1)u_1 \otimes \pi_{\tilde{\varrho}_2}(A_{2-}), \tag{23}$$

for $A_1 \in \mathcal{A}(K)$, $A_2 = A_{2+} + A_{2-}$, $A_{2\pm} \in \mathcal{A}(I)_{\pm}$. Let $\mathbf{1}_1$ be the identity operator of $\mathcal{H}_{\varrho_1}$ and $\mathbf{1}_2$ be that of $\mathcal{H}_{\tilde{\varrho}_2}$.

We can check that the operators $\pi(\mathcal{A}(K \cup I))$ satisfy the CAR by using (19), and hence π extends to a representation of $\mathcal{A}(K \cup I)$. We define the state $\psi_{\tilde{\varrho}_2}$ on $\mathcal{A}(K \cup I)$ as

$$\psi_{\tilde{\varrho}_2}(A) \equiv (\Omega, \pi(A)\Omega) \tag{24}$$

for $A \in \mathcal{A}(K \cup I)$. The von Neumann algebra $\pi(\mathcal{A}(K \cup I))''$ is generated by $\pi_{\varrho_1}(\mathcal{A}(K))'' \otimes \mathbf{1}_2$, $\mathbf{1}_1 \otimes \pi_{\tilde{\varrho}_2}(\mathcal{A}(\mathbf{I})_+)''$, and the weak closure of $\mathbf{1}_1 \otimes \pi_{\tilde{\varrho}_2}(\mathcal{A}(I)_-)$, where we have noted $u_1 \in \pi_{\varrho_1}(\mathcal{A}(K)_+)'' = \mathcal{B}(\mathcal{H}_{\varrho_1})$. Therefore

$$\pi(\mathcal{A}(K \cup I))'' = \mathcal{B}(\mathcal{H}_{\varrho_1}) \otimes \pi_{\tilde{\varrho}_2}(\mathcal{A}(I))''. \tag{25}$$

From this it follows that the vector Ω is cyclic for the representation π of $\mathcal{A}(K \cup I)$ in $\mathcal{H}$. Hence $(\mathcal{H}, \pi, \Omega)$ gives a GNS triplet for the state $\psi_{\tilde{\varrho}_2}$ on $\mathcal{A}(K \cup I)$.

We have

$$\psi_{\tilde{\varrho}_2}(A_1A_2) = (\Omega, \pi(A_1A_2)\Omega) = \varrho_1(A_1)\tilde{\varrho}_2(A_{2+}) + \overline{\varrho_1}(\pi_{\varrho_1}(A_1)u_1)\tilde{\varrho}_2(A_{2-}), \tag{26}$$

for $A_1 \in \mathcal{A}(K)$, $A_2 = A_{2+} + A_{2-}$, $A_{2\pm} \in \mathcal{A}(I)_{\pm}$. Taking $A_2 = \mathbf{1}$ in (26), we obtain

$$\psi_{\tilde{\varrho}_2}(A_1) = \varrho_1(A_1). \tag{27}$$

We will then show

$$\psi_{\tilde{\varrho}_2}(A_2) = \varrho_2(A_2). \tag{28}$$

Under the condition of Lemma 7 (which is our case), we have

$$p_\Theta(\varrho_1) = |\overline{\varrho_1}(u_1)|, \tag{29}$$

because the transition probability between the vector states of the algebra $\mathcal{B}(\mathcal{H}_{\varrho_1}) = \pi_{\varrho_1}(\mathcal{A}(K))''$ is equal to the (usual) transition probability of their vectors and hence $p_\Theta(\varrho_1) = |(\Omega_{\varrho_1}, u_1\Omega_{\varrho_1})|$. By the assumption $p_\Theta(\varrho_1) = 0$, (29) implies

$$\overline{\varrho_1}(u_1) = 0. \tag{30}$$

Setting $A_1 = \mathbf{1}$ in (26), we obtain

$$\psi_{\tilde{\varrho}_2}(A_2) = \tilde{\varrho}_2(A_{2+}) + \overline{\varrho_1}(u_1)\tilde{\varrho}_2(A_{2-}) = \tilde{\varrho}_2(A_{2+}). \tag{31}$$

By (20),

$$\varrho_2(A_2) = \varrho_2(A_{2+}) = \tilde{\varrho}_2(A_{2+}). \tag{32}$$

From (31) and (32), (28) follows. We have now shown that $\psi_{\tilde{\varrho}_2}$ is an extension of ϱ_1 and ϱ_2.

We will show the second paragraph. By (25) and the commutant theorem, $\pi(\mathcal{A}(K \cup I))' = \mathbf{1}_1 \otimes \pi_{\tilde{\varrho}_2}(\mathcal{A}(I))'$, where the commutant is taken in each GNS space. Thus we have the following isomorphism:

$$b \mapsto \mathbf{1}_1 \otimes b, \quad b \in \pi_{\tilde{\varrho}_2}(\mathcal{A}(I))' \tag{33}$$

from $\pi_{\tilde{\varrho}_2}(\mathcal{A}(I))'$ onto $\pi(\mathcal{A}(K\cup I))'$. Furthermore by (22) we obtain

$$(\Omega,(\mathbf{1}_1 \otimes b)\Omega) = (\Omega_{\varrho_1} \otimes \Omega_{\tilde{\varrho}_2}, \Omega_{\varrho_1} \otimes b\Omega_{\tilde{\varrho}_2}) = (\Omega_{\tilde{\varrho}_2}, b\Omega_{\tilde{\varrho}_2}). \tag{34}$$

From the assumption that K and I are finite subsets (which we have not used so far), $\pi_{\tilde{\varrho}_2}(\mathcal{A}(I))'$ and $\pi(\mathcal{A}(K\cup I))'$ are both finite-dimensional type I factors.

Now we note the following basic fact about GNS representations for states of finite-dimensional type I factors which can be considered as the counterpart of Lemma 2 for the usual case, namely for a pair of isomorphic systems coupled by tensor product. Let ω be a state of a finite-dimensional type I factor $\mathfrak{U}$ and $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ denote a GNS triplet of ω. The GNS vector Ω_ω of ω induces a state on the commutant $\pi_\omega(\mathfrak{U})'$ whose expectation value for $a \in \pi_\omega(\mathfrak{U})'$ is given by $(\Omega_\omega, a\Omega_\omega)$. We call this state on $\pi_\omega(\mathfrak{U})'$ "ω on the commutant." [In our terminology, the pure state with respect to Ω_ω on $\mathcal{B}(\mathcal{H}_\omega) = \pi_\omega(\mathfrak{U}) \otimes \pi_\omega(\mathfrak{U})'$ gives a symmetric purification of ω. Also ω on the commutant is symmetric to ω.] Then the entropy of ω on $\mathfrak{U}$ [equivalently that on $\pi_\omega(\mathfrak{U})$] is equal to the entropy of ω on the commutant by the same reason described in Lemma 2. We note that this holds for a general $\mathbf{C}^*$-algebra if the GNS representation of a given state generates a type I von Neumann algebra with a discrete center. Similarly the extension of Lemma 2 is possible under the above condition on the state.

From the above fact with (33) and (34), we deduce the equality of the entropies of $\tilde{\varrho}_2$ and of $\psi_{\tilde{\varrho}_2}$. ■

Remark 1: Note that this $\psi_{\tilde{\varrho}_2}$ is a state extension of ϱ_1 and ϱ_2, not that of ϱ_1 and $\tilde{\varrho}_2$. The possibility of the state extension of ϱ_1 and $\tilde{\varrho}_2$ is negated by Theorem 4(3) of Ref. 3.

Remark 2: We can easily make examples of states in this proposition. Take a finite subset K and an odd self-adjoint element A in the algebra $\mathcal{A}(K)$ which we will identify with $\mathcal{B}(\mathcal{H})$ on a finite-dimensional Hilbert space $\mathcal{H}$. Let $\eta \in \mathcal{H}$ be a normalized eigenvector of this A and ω_η denote the associated vector state. Then $\eta \perp v_K\eta$, and $\omega_\eta\Theta$ becomes the vector state with respect to $v_K\eta$. Hence $p_\Theta(\omega_\eta)=0$. This ω_η obviously satisfies (i). For the existence of ϱ_2 satisfying (ii), take, for example, the above ω_η for $\tilde{\varrho}_2$ (with $i \in I$), $\omega_\eta\Theta$ for $\tilde{\varrho}_2\Theta$, and their affine sum (20) for ϱ_2.

Proposition 8 yields the following construction giving counter examples of MONO–SSA and those of the triangle inequality.

Theorem 9: *Let K, I, and J be mutually disjoint subsets. Let $\varrho_K = \varrho_1$ and $\varrho_I = \varrho_2$ where ϱ_1 and ϱ_2 are those states on $\mathcal{A}(K)$ and on $\mathcal{A}(I)$ given in Proposition 8. Let $\varrho_{K\cup I}$ be the state extension of ϱ_K and ϱ_I to $\mathcal{A}(K\cup J)$ given by $\psi_{\tilde{\varrho}_2}$ in the form of (21). Let ϱ_J be an arbitrary even state of $\mathcal{A}(J)$. Then for such $\varrho_{K\cup I}$ and ϱ_J, there exists a (unique) product state extension $\varrho_{K\cup I}\circ\varrho_J$ on $\mathcal{A}(K\cup I\cup J)$. If all K, I, and J are finite subsets, then*

$$S(\varrho_{K\cup I}) + S(\varrho_{K\cup J}) < S(\varrho_I) + S(\varrho_J), \tag{35}$$

and

$$|S(\varrho_I) - S(\varrho_K)| = S(\varrho_I) > S(\varrho_{K\cup I}). \tag{36}$$

Proof: By Ref. 10 or Theorem 1(1) of Ref. 2, there exists a unique product state extension of a pair of states on disjoint regions if (and only if) at least one of them is even, and hence the (unique) existence of $\varrho_{K\cup I}\circ\varrho_J$ follows.

By the second paragraph of Proposition 8, we obtain

$$S(\varrho_{K\cup I}) = S(\psi_{\tilde{\varrho}_2}) = S(\tilde{\varrho}_2). \tag{37}$$

Since $\varrho_2 = \frac{1}{2}(\tilde{\varrho}_2 + \tilde{\varrho}_2\Theta)$ and $\tilde{\varrho}_2 \neq \tilde{\varrho}_2\Theta$, we have

$$S(\varrho_I) = S(\varrho_2) = S(1/2(\tilde{\varrho}_2 + \tilde{\varrho}_2\Theta)) > 1/2S(\tilde{\varrho}_2) + 1/2S(\tilde{\varrho}_2\Theta) \tag{38}$$

by the strict concavity of von Neumann entropy with respect to the affine sum of states (see

Remark 3 below). Due to the unitary invariance of von Neumann entropy,

$$S(\tilde{\varrho}_2) = S(\tilde{\varrho}_2\Theta). \tag{39}$$

By (37), (38), and (39), we have

$$S(\varrho_I) > S(\varrho_{K\cup I}). \tag{40}$$

By the product property of $\varrho_{K\cup J}=\varrho_K\circ\varrho_J$ the density matrix of $\varrho_{K\cup J}$ is a product of the density matrices of ϱ_K and ϱ_J which mutually commute because $\varrho_J\in\mathcal{A}(J)_+$. Hence by a direct computation we have

$$S(\varrho_{K\cup J}) = S(\varrho_K) + S(\varrho_J).$$

Since ϱ_K is assumed to be pure and hence $S(\varrho_K)=0$, we have

$$S(\varrho_{K\cup J}) = S(\varrho_J). \tag{41}$$

From (40) and (41), we obtain (35). From (40) and $S(\varrho_K)=0$, we obtain (36). ■

Remark 3: Let $\mathcal{H}$ be a finite-dimensional Hilbert space. For states φ and ψ on the algebra $\mathcal{B}(\mathcal{H})$ and for $0\leqslant\lambda\leqslant 1$, the following von Neumann entropy inequalities are well known:

$$S(\lambda\varphi + (1-\lambda)\psi) \geqslant \lambda S(\varphi) + (1-\lambda)S(\psi), \tag{42}$$

$$S(\lambda\varphi + (1-\lambda)\psi) \leqslant \lambda S(\varphi) + (1-\lambda)S(\psi) - \lambda\log\lambda - (1-\lambda)\log(1-\lambda). \tag{43}$$

We refer to Proposition 6.2.25 of Ref. 4 for their proofs. We now see the strict concavity of von Neumann entropy which was used in the proof of Theorem 9, namely for $0<\lambda<1$ the equality of (42) holds if and only if $\varphi=\psi$. We employ the proof method given in the above-mentioned reference. Let $\mathcal{K}$ be a two-dimensional Hilbert space and P denote a one-dimensional projection of $\mathcal{B}(\mathcal{K})$. We denote $\mathcal{A}_1\equiv\mathcal{B}(\mathcal{H})$, $\mathcal{A}_2\equiv\mathcal{B}(\mathcal{K})$, and $\mathcal{A}_{1,2}\equiv\mathcal{B}(\mathcal{H}\otimes\mathcal{K})$. Let ω denote a state on $\mathcal{A}_{1,2}$ whose density matrix D_ω is given by

$$\lambda D_\varphi\otimes P + (1-\lambda)D_\psi\otimes(1-P).$$

We denote ω restricted to $\mathcal{A}_1$ (to $\mathcal{A}_2$, respectively) by ω_1 (and ω_2). We see that ω_1 is equal to $\lambda\varphi+(1-\lambda)\psi$, hence

$$S(\omega_1) = S(\lambda\varphi + (1-\lambda)\psi).$$

Also we have

$$S(\omega) - S(\omega_2) = \lambda S(\varphi) + (1-\lambda)S(\psi).$$

Since

$$S(\omega_1) + S(\omega_2) - S(\omega) = \omega(\log D_\omega - \log(D_{\omega_1}\otimes D_{\omega_2})) \equiv S(\omega|\omega_1\otimes\omega_2) \geqslant 0,$$

which is equivalent to the subadditivity of entropy, we obtain (42). This $S(\omega|\omega_1\otimes\omega_2)$ is relative entropy of the two states in its argument and is known to have strict positivity, i.e., $S(\omega|\omega_1\otimes\omega_2)=0$ if and only if $\omega=\omega_1\otimes\omega_2$, which is equivalent to $\varphi=\psi$ for $0<\lambda<1$. Hence our desired strictness of (42) is shown.

Remark 4: We shall give a rough estimation of the amount of violation of the triangle inequality, i.e., $|S(\varphi_I)-S(\varphi_K)|-S(\varphi_{K\cup I})$ of (36) for a general state φ. Let $\hat{\varphi}\equiv 1/2(\varphi+\varphi\Theta)$. Then it obviously satisfies the triangle inequality. By (42) and (43), we have $|S(\hat{\varphi}_{K\cup I})-S(\varphi_{K\cup I})|\leqslant -1/2\log 1/2-1/2\log 1/2=\log 2$, and similarly $|S(\hat{\varphi}_I)-S(\varphi_I)|\leqslant\log 2$ and $|S(\hat{\varphi}_K)-S(\varphi_K)|\leqslant\log 2$. Hence $|S(\varphi_I)-S(\varphi_K)|-S(\varphi_{K\cup I})$ is at most $3\log 2$. However, we do not know its possible maximal value. (The violation of the triangle inequality for our concrete model considered in Ref. 7 ranges from 0 up to $\log 2$.)

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Symmetries of distributional domain wall geometries

Nelson Pantoja and Alberto Sanoja
Centro de Física Fundamental, Universidad de Los Andes, Mérida 5101, Venezuela

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Generalizing the Lie derivative of smooth tensor fields to distribution-valued tensors, we examine the Killing symmetries and the collineations of the curvature tensors of some distributional domain wall geometries. The chosen geometries are rigorously the distributional thin wall limit of self-gravitating scalar field configurations representing thick domain walls and the permanence and/or the rising of symmetries in the limit process is studied. We show that, for all the thin wall space–times considered, the symmetries of the distributional curvature tensors turns out to be the Killing symmetries of the pullback of the metric tensor to the surface where the singular part of these tensors is supported. Remarkably enough, for the nonreflection symmetric domain wall studied, these Killing symmetries are not necessarily symmetries of the ambient space–time on both sides of the wall. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1851603]

I. INTRODUCTION

Consider a family of space–times $(\mathcal{M}, {}^{\gamma}\mathbf{g})$, where ${}^{\gamma}\mathbf{g}$ is C^{∞} metric tensor which depends on a parameter γ. An isometry ψ on $(\mathcal{M}, {}^{\gamma}\mathbf{g})$ is defined to be a diffeomorphism $\psi: \mathcal{M} \to \mathcal{M}$ for which $\psi^{*}{}^{\gamma}\mathbf{g} = {}^{\gamma}\mathbf{g}$. The infinitesimal generator of a one-parameter group ψ_{λ} of local isometries is the C^{∞} vector field $\mathbf{V}$ on $\mathcal{M}$ that satisfies

$$\mathcal{L}_{\mathbf{V}}{}^{\gamma}\mathbf{g} = 0, \tag{1}$$

and $\mathbf{V}$ is called a Killing vector field on $(\mathcal{M}, {}^{\gamma}\mathbf{g})$ relative to this group. To every one-parameter family of Killing symmetries there is an associated conserved quantity along the geodesics of the space–time and these conserved quantities are useful for integrating the geodesic equation.[1]

Although isometries are the most important transformations on $(\mathcal{M}, {}^{\gamma}\mathbf{g})$, geometric symmetries other than Killing symmetries may also be considered. Let ${}^{\gamma}\mathbf{Ric}$ be the Ricci curvature tensor of ${}^{\gamma}\mathbf{g}$. A vector field $\mathbf{V}$ on $\mathcal{M}$ that satisfies

$$\mathcal{L}_{\mathbf{V}}{}^{\gamma}\mathbf{Ric} = 0, \tag{2}$$

is called a Ricci collineation. It is well known that for every vector field $\mathbf{V}$ such that (1) is satisfied, i.e., for every Killing vector field, (2) is also satisfied and the Ricci tensor inherits the symmetries of the metric. However, other vector fields that are not Killing vectors may exist for which (2) is satisfied and these are called proper Ricci collineations. Since **Ric** is obtained by contracting the Riemann curvature tensor, Ricci collineations have a natural geometrical significance and it is believed that they can be useful to understand the interplay between geometry and physics in general relativity (for more details on these and other geometric symmetries, see Refs. 2–5).

Now, consider a space–time $(\mathcal{M}, \mathbf{g})$ of low differentiability, revealing itself through a lack of smoothness of the metric $\mathbf{g}$ and its curvature tensors. Up to what extent can the classical concept of a geometric symmetry (in the smooth case) be carried over to this situation? Let us assume that the metric tensors $\mathbf{g}$ and ${}^{\gamma}\mathbf{g}$ are distribution-valued tensors that satisfy

$$\mathbf{g} \equiv \lim_{\gamma \to 0} {}^{\gamma}\mathbf{g} \tag{3}$$

(in the sense of distributions) and that their corresponding curvature tensors have a well-defined distributional meaning. Further, assume that the following diagram holds;

$$\begin{array}{ccccccc} {}^{\gamma}\mathbf{g} & \longrightarrow & {}^{\gamma}\mathbf{Riem} & \longrightarrow & {}^{\gamma}\mathbf{Ric} & \longrightarrow & {}^{\gamma}\mathbf{G} \\ \downarrow_{\gamma \to 0} & & \downarrow_{\gamma \to 0} & & \downarrow_{\gamma \to 0} & & \downarrow_{\gamma \to 0} \\ \mathbf{g} & \longrightarrow & \mathbf{Riem} & \longrightarrow & \mathbf{Ric} & \longrightarrow & \mathbf{G} \end{array} \tag{4}$$

where ${}^{\gamma}\mathbf{g}$, ${}^{\gamma}\mathbf{Riem}$, ${}^{\gamma}\mathbf{Ric}$, ${}^{\gamma}\mathbf{G}$ and $\mathbf{g}$, **Riem**, **Ric**, **G** are the distribution valued metric, Riemann, Ricci and Einstein tensors of the smooth and the distributional geometries, respectively. Although distributional curvatures are in general ill-defined due to the nonlinearities of general relativity, there is a class of distributional metrics for which the Riemann curvature tensor and its contractions can be interpreted as distributions.[6] Metrics for thin shells[7] are included into this class.[6,8] Furthermore, for such a class an appropriate notion of convergence of metrics has been stated which ensures the convergence of the respective curvatures,[6] in the sense that the diagram (4) holds.

Since the derivative of a distribution is a distribution, for a distributional metric whose curvature tensors make sense as distributions, it makes sense to consider their geometric symmetries. Obviously, this situation should be considered also from the distributional point of view. For example, Eq. (2) contains products of the Ricci tensor and the vector field which generates the symmetry, so that for a distribution-valued Ricci tensor such equation restricts the vector field to be C^{∞}. With this proviso, we can consider geometric symmetries in cases in which the curvature tensors are zero almost everywhere (when obtained within standard differential geometry). Furthermore, for distributional geometries such that the above diagram holds, we can study the permanence and/or the rising of symmetries in the limit process. Thus, from the study of these geometries we expect to get further insight about the nature of distributional curvatures in general relativity.

Killing symmetries of distributional metrics have been considered previously in Ref. 9, where it is shown that the Killing fields of the Schwarzschild metric are also Killing of its ultrarelativistic limit, the last one being a *pp*-wave with a distributional δ profile.[10] In addition, based on the analysis of the adjoint orbits of normal-form-preserving diffeomorphisms, Killing symmetries of impulsive *pp*-waves with distributional profiles have been analyzed[11] and the existence of nonsmooth Killing vectors put forward.[12]

In this paper, adopting a different approach for a rigorous definition of symmetries of distributional geometries, we are concerned with symmetries of domain wall space–times. Such space–times have been the subject of intense investigation, after it was realized in Ref. 13 that our four-dimensional universe might be a thin (codimension one) distributional domain wall embedded in a five-dimensional space–time. Thin wall geometries have distribution-valued curvature tensor fields whose singular parts are proportional to a Dirac distribution supported on the surface where the wall is localized. All the metrics representing the possible backgrounds of an infinitely thin domain wall[14] have been found and classified,[15,16] these being joined at a common boundary, the surface where the wall is localized, following the Darmois–Israel formalism.[7] On the other hand, smooth domain wall geometries can be obtained as solutions to the coupled Einstein-scalar field system with a suitable symmetry breaking potential $V(\phi)$.[14,17–20] The behavior of gravity in some of these models has been also investigated.[21–23] Recently, following the convergence criteria of Ref. 6, the distributional thin wall limit of some classes of domain wall space–times has been rigourously analyzed[24,25] showing that the diagram (4), in which ${}^{\gamma}\mathbf{g}$ and $\mathbf{g}$ are the distribution valued metric tensors of the thick and thin domain wall space–times, respectively, holds. Specifically, we will study the symmetries of the metric and its curvature tensors of these distributional domain wall geometries. Domain walls have drastic gravitational effects in the ambient space and, due to its role in brane-world models, we are interested in their geometric symmetries besides those defining the plane-parallel symmetry since a larger group may exists for various particular models.

In Sec. II, after an overview on the subject of distribution-valued tensors, we give the definition of the Lie derivative of a tensor distribution along a C^∞ vector field. In the next three sections, we examine the Killing symmetries and the collineations of the singular Ricci and Einstein curvature tensors associated to the distributional thin wall limit of some thick domain wall space–times for which the diagram (4) holds.[24] The last section is devoted to summarize and discuss the results.

II. MATHEMATICAL FRAMEWORK

We first recall some fundamental results about distribution-valued tensors on a C^∞ paracompact n-dimensional manifold $\mathcal{M}$.[26–28]

Let $\mathcal{D}_p(\mathcal{M})$ be the space of C^∞ p-tensor fields on $\mathcal{M}$ with compact support endowed with its Schwartz topology, i.e., the space of test p-tensor fields. The space of p-cotensor distributions on $\mathcal{M}$, $\mathcal{D}_p^{*'}(\mathcal{M})$, is defined as the dual of $\mathcal{D}_p(\mathcal{M})$. Now, in order to keep things simple, we endow the C^∞ paracompact manifold $\mathcal{M}$ with a C^∞ metric $\boldsymbol{\eta}$. However, it should be noted that tensor distributions and their derivatives can be described without assuming the presence of a metric[29] and that, by using de Rham currents[30] and replacing test tensors by test n-forms, the introduction of a volume form can also be avoided. Here we shall follow the approach of Ref. 26.

Let $\mathbf{U}$ be a test p-tensor field on $\mathcal{M}$. The identification of a locally integrable p-cotensor field $\mathbf{T}$ with a distribution-valued tensor is defined by

$$\mathbf{T}[\mathbf{U}] \equiv \int_{\mathcal{M}} \mathbf{T}\cdot\mathbf{U}\boldsymbol{\omega}_\eta, \tag{5}$$

where $\mathbf{T}\cdot\mathbf{U}$ denotes the scalar product of $\mathbf{T}$ and $\mathbf{U}$, and $\boldsymbol{\omega}_\eta$ is the volume element of $\boldsymbol{\eta}$. Since (5) is the integral of an n-form with compact support, we have

$$\mathbf{T}[\mathbf{U}] \equiv \int_{\varphi(\mathcal{M})} T_{i_1\cdots i_p} U^{i_1\cdots i_p} |\det\,\eta|^{1/2}\, \mathrm{d}x^1\cdots\,\mathrm{d}x^n \tag{6}$$

in the domain $\varphi(\mathcal{M})$ of the chart $(x^1,\ldots,x^n)$. Obviously, (6) is independent of the choice of coordinate system covering the corresponding domain. Further, although (5) depends on the choice of $\boldsymbol{\eta}$, the space of locally integrable tensor fields does not.[26]

Next, let us define the Lie derivative of a tensor field in the sense of distributions. Let $\mathbf{V}$ be a C^∞ vector field and $\mathbf{T}$ be a C^1 p-cotensor field on $\mathcal{M}$. The Lie derivative of $\mathbf{T}$ is the p-cotensor field $\mathcal{L}_\mathbf{v}\mathbf{T}$ such that, for every test p-tensor field $\mathbf{U}$,

$$\mathcal{L}_\mathbf{v}\mathbf{T}[\mathbf{U}] \equiv \int_{\mathcal{M}} \mathcal{L}_\mathbf{v}\mathbf{T}\cdot\mathbf{U}\boldsymbol{\omega}_\eta = \int_{\mathcal{M}} \mathcal{L}_\mathbf{v}(\mathbf{T}\cdot\mathbf{U}\boldsymbol{\omega}_\eta) - \int_{\mathcal{M}} ((\mathbf{T}\cdot\mathcal{L}_\mathbf{v}\mathbf{U})\boldsymbol{\omega}_\eta + (\mathbf{T}\cdot\mathbf{U})\mathcal{L}_\mathbf{v}\boldsymbol{\omega}_\eta). \tag{7}$$

Now, since $\mathbf{T}\cdot\mathbf{U}\boldsymbol{\omega}_\eta$ is an n-form with compact support, we have

$$\int_{\mathcal{M}} \mathcal{L}_\mathbf{v}(\mathbf{T}\cdot\mathbf{U}\boldsymbol{\omega}_\eta) = \int_{\mathcal{M}} \mathbf{d}\mathbf{i}_\mathbf{v}(\mathbf{T}\cdot\mathbf{U}\boldsymbol{\omega}_\eta) = \int_{\partial\mathcal{M}} \mathbf{i}_\mathbf{v}(\mathbf{T}\cdot\mathbf{U}\boldsymbol{\omega}_\eta) = 0, \tag{8}$$

where $\mathbf{i}_\mathbf{v}$ denotes interior product, in the last step we have used Stokes' theorem and the surface term vanishes because $\mathbf{U}$ has compact support. Therefore

$$\mathcal{L}_\mathbf{v}\mathbf{T}[\mathbf{U}] = -\int_{\mathcal{M}} ((\mathbf{T}\cdot\mathcal{L}_\mathbf{v}\mathbf{U})\boldsymbol{\omega}_\eta + (\mathbf{T}\cdot\mathbf{U})\mathcal{L}_\mathbf{v}\boldsymbol{\omega}_\eta). \tag{9}$$

On the other hand, we have

$$\mathcal{L}_{\mathbf{v}}\boldsymbol{\omega}_{\eta} = (\nabla \cdot \mathbf{V})\boldsymbol{\omega}_{\eta} \tag{10}$$

where ∇ is the torsion free metric compatible Levi–Civita covariant derivative associated with $\boldsymbol{\eta}$ and

$$\nabla \cdot \mathbf{V} \equiv \nabla_j V^j. \tag{11}$$

It follows that

$$\mathcal{L}_{\mathbf{v}}\mathbf{T}[\mathbf{U}] = -\int_{\mathcal{M}} \mathbf{T} \cdot (\mathcal{L}_{\mathbf{v}}\mathbf{U} + \mathbf{U}(\nabla \cdot \mathbf{V}))\boldsymbol{\omega}_{\eta}. \tag{12}$$

Therefore, to have a definition which coincides with the usual one when $\mathbf{T}$ is C^1, we define for $\mathbf{T}$ an arbitrary p-cotensor distribution and $\mathbf{V}$ a C^{∞} vector field on $\mathcal{M}$ the Lie derivative of $\mathbf{T}$ as the p-cotensor distribution given by

$$\mathcal{L}_{\mathbf{v}}\mathbf{T}[\mathbf{U}] \equiv -\mathbf{T}[\mathcal{L}_{\mathbf{v}}\mathbf{U} + (\nabla \cdot \mathbf{V})\mathbf{U}]. \tag{13}$$

Note that (13) makes sense since both $\mathcal{L}_{\mathbf{v}}\mathbf{U}$ and $(\nabla \cdot \mathbf{V})\mathbf{U}$ are test p-tensor fields if $\mathbf{V}$ is a C^{∞} vector field. Further, it should be stressed that the distributional Lie derivative of a tensor distribution, (13), reduce to the classical Lie derivative of an ordinary smooth tensor for a tensor distribution associated to a smooth tensor. This claim follows directly from the derivation of (12).

In the next sections, (13) will be used to define and compute the Lie derivative of a distribution-valued metric tensor $\mathbf{g}$ with $\mathbf{V}$ a C^{∞} vector field that generates a one parameter group of isometries of the space–time $(\mathcal{M}, \mathbf{g})$. We also make use of (13) to define and compute the Ricci and Einstein collineations of the distributional geometry associated to these space–times. Since all the distribution-valued metric tensors that we shall consider are regular metrics in the sense of Ref. 6, let us recall their definition. Suppose that $(\mathcal{M}, \mathbf{g})$ are given such that

(1) $\mathbf{g}$ and $(\mathbf{g}^{-1})$ exist everywhere and are locally bounded,
(2) the first derivative $\nabla\mathbf{g}$ (in the sense of distributions) of $\mathbf{g}$ in some smooth derivative operator ∇ exists and is locally square-integrable, i.e., the outer product of the derivative with itself is locally integrable.

Following Ref. 6, these are the minimal conditions for the Riemann curvature tensor to be definable as a distribution by the usual coordinate formula and we shall say that $\mathbf{g}$ is a regular metric. Since for this class of metrics the outer product of any number of metrics and inverse metrics with the Riemann curvature tensor can be interpreted as distributions, the Ricci and Einstein curvature tensors of a regular metric make sense as distributions. Finally, it should be stressed that for such class an appropriate notion of convergence of metrics exists which ensures the convergence of the respective curvatures,[6] in the sense that the diagram (4) holds (for details, see Ref. 6).

III. A DOMAIN WALL WITH A DE SITTER EXPANSION

Consider the space–time $(\mathbb{R}^4, {}^{\gamma}\mathbf{g})$ where the metric tensor ${}^{\gamma}\mathbf{g}$, in a particular coordinate basis, is given by

$${}^{\gamma}\mathbf{g} = \cosh^{-2\gamma}\frac{\beta x}{\gamma}(-\mathbf{d}t \otimes \mathbf{d}t + \mathbf{d}x \otimes \mathbf{d}x + e^{2\beta t}(\mathbf{d}y \otimes \mathbf{d}y + \mathbf{d}z \otimes \mathbf{d}z)), \tag{14}$$

where β and γ are constants, with $0 < \gamma < 1$. This space–time is generated by a thick domain wall, i.e., a solution to the coupled Einstein-scalar field equations

$${}^{\gamma}\mathbf{G} + {}^{\gamma}\mathbf{g}\Lambda \equiv {}^{\gamma}\mathbf{Ric} - \tfrac{1}{2}{}^{\gamma}\mathbf{g}{}^{\gamma}R + {}^{\gamma}\mathbf{g}\Lambda = 8\pi\left[\mathbf{d}\phi \otimes \mathbf{d}\phi - \mathbf{g}\left(\tfrac{1}{2}\mathbf{d}\phi \cdot \tilde{\mathbf{d}}\phi + V(\phi)\right)\right], \tag{15}$$

where the vector field $\tilde{\mathbf{d}}\phi$ is the metric dual to $\mathbf{d}\phi$ and

$$\Box\phi - \frac{d}{d\phi}V(\phi) = 0, \tag{16}$$

where $-\Box \equiv \boldsymbol{\delta}\mathbf{d} + \mathbf{d}\boldsymbol{\delta}$, with $\mathbf{d}$ and $\boldsymbol{\delta}$ the exterior derivative and the codifferential, respectively. In this case we have

$$\phi = \phi_0 \tan^{-1}(\sinh(\beta x/\gamma)\ , \quad \phi_0 \equiv \sqrt{\gamma(1-\gamma)/4\pi}, \tag{17}$$

$$V(\phi) = \frac{1}{8\pi}\beta^2\left(2 + \frac{1}{\gamma}\right)\cos^{2(1-\gamma)}(\phi/\phi_0), \quad \Lambda = 0. \tag{18}$$

The scalar field takes values $\pm\pi\phi_0/2$ at $x = \pm\infty$ corresponding to two consecutive minima of the potential and interpolates smoothly between these values,[17,18,20] with γ playing the role of the wall's thickness.[24] The five-dimensional analogue of this geometry, considered as a thick brane-world model, has been studied in Ref. 23.

Note that (14) is C^∞ as are also all its curvature tensor fields. In particular, for the Ricci and Einstein tensor fields we obtain

$${}^\gamma\mathbf{Ric} = -\left(2 + \frac{1}{\gamma}\right)\beta^2 \cosh^{-2}\frac{\beta x}{\gamma}\left(-\mathbf{d}t\,\mathbf{d}t + \frac{3}{1+2\gamma}\mathbf{d}x\,\mathbf{d}x + e^{2\beta t}(\mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z)\right) \tag{19}$$

and

$${}^\gamma\mathbf{G} = -\left(1 + \frac{2}{\gamma}\right)\beta^2 \cosh^{-2}\frac{\beta x}{\gamma}\left(-\mathbf{d}t\,\mathbf{d}t + \frac{3\gamma}{2+\gamma}\mathbf{d}x\,\mathbf{d}x + e^{2\beta t}(\mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z)\right), \tag{20}$$

where, following standard practice, we have omitted writing the outer product sign.

Now, from (1) and (14), we obtain six linearly independent Killing vector fields on $(\mathbb{R}^4, {}^\gamma\mathbf{g})$ given by

$$\mathbf{V}_1 = \boldsymbol{\partial}_y, \quad \mathbf{V}_2 = \boldsymbol{\partial}_z, \quad \mathbf{V}_3 = z\boldsymbol{\partial}_y - y\boldsymbol{\partial}_z, \tag{21}$$

$$\mathbf{V}_4 = \boldsymbol{\partial}_t - \beta(y\boldsymbol{\partial}_y + z\boldsymbol{\partial}_z), \tag{22}$$

$$\mathbf{V}_5 = 2\beta y\mathbf{V}_4 + (\beta^2(y^2+z^2) - e^{-2\beta t})\boldsymbol{\partial}_y, \tag{23}$$

$$\mathbf{V}_6 = 2\beta z\mathbf{V}_4 + (\beta^2(y^2+z^2) - e^{-2\beta t})\boldsymbol{\partial}_z. \tag{24}$$

The Killing vectors (21) are generic to the plane parallel symmetry, two spatial translations $\mathbf{V}_1$, $\mathbf{V}_2$ and one spatial rotation $\mathbf{V}_3$. The six vector fields (21)–(24) are also Killing vectors on the (2+1)-dimensional de Sitter space–time $(\mathbb{R}^3, \overline{\mathbf{g}})$ with

$$\overline{\mathbf{g}} = -\mathbf{d}t\,\mathbf{d}t + e^{2\beta t}(\mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z), \tag{25}$$

where $\mathbf{V}_4$ is a quasitime translation and $\mathbf{V}_5$, $\mathbf{V}_6$ are quasi-Lorentz rotations. Note that (21)–(24) are all independent of the thickness γ of the wall. It is straightforward to show that for (21)–(24) we have in the classical (i.e., nondistributional) sense

$$\mathcal{L}_\mathbf{v}\,{}^\gamma\mathbf{Ric} = 0, \quad \mathcal{L}_\mathbf{v}{}^\gamma\mathbf{G} = 0. \tag{26}$$

One can also show that there are no other vector fields for which (26) is satisfied. Hence, the Ricci (19) and Einstein (20) curvature tensors only admit improper collineations.

Next, consider the Lie derivative of (14) in the sense of distributions as given by (13). Let $\boldsymbol{\eta}$ be the ordinary four-dimensional Minkowski metric tensor in Cartesian coordinates

$$\boldsymbol{\eta} = -\,\mathbf{d}t\,\mathbf{d}t + \mathbf{d}x\,\mathbf{d}x + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z, \tag{27}$$

and let ∇ be the Levi–Civita covariant derivative associated with $\boldsymbol{\eta}$. Let $\mathbf{U}$ be a test tensor on $\mathbb{R}^4$. From (13), it is straightforward to verify that for all Killing vectors (21)–(24), we have

$$\mathcal{L}_{\mathbf{v}}{}^{\gamma}\mathbf{g}[\mathbf{U}] = 0, \tag{28}$$

as expected. Indeed, it is to make such things true that the Lie derivative is defined as in (13). For the sake of completeness, let us show explicitly the computation of this derivative for the Killing vector given by (22). We have

$$\mathcal{L}_{\mathbf{v}_4}{}^{\gamma}\mathbf{g}[\mathbf{U}] \equiv -\,{}^{\gamma}\mathbf{g}[\mathcal{L}_{\mathbf{v}_4}\mathbf{U} + (\nabla\cdot\mathbf{V}_4)\mathbf{U}] = -\int_{\mathbb{R}^4} {}^{\gamma}\mathbf{g}\cdot(\mathcal{L}_{\mathbf{v}_4}\mathbf{U} + \mathbf{U}(\nabla\cdot\mathbf{V}_4))\boldsymbol{\omega}_{\eta} = -\int_{\mathbb{R}^4} \cosh^{-2\gamma}\frac{\beta x}{\gamma}((\partial_t - \beta y\partial_y - \beta z\partial_z - 2\beta)(-U^{tt} + U^{xx}) + e^{2\beta t}(\partial_t - \beta y\partial_y - \beta z\partial_z)(U^{yy} + U^{zz}))\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = 0, \tag{29}$$

where in the last step we have integrated by parts and used the fact that $\mathbf{U}$ is of compact support. For all the Killing vector fields (21)–(24), analogous computations show that

$$\mathcal{L}_{\mathbf{v}}{}^{\gamma}\mathbf{Ric}[\mathbf{U}] = 0, \quad \mathcal{L}_{\mathbf{v}}{}^{\gamma}\mathbf{G}[\mathbf{U}] = 0, \tag{30}$$

as expected.

We turn now to consider the $\gamma\to 0$ limit of this geometry. In Ref. 24, it has been proved that (14) provides a sequence of metrics that satisfies the convergence conditions of Ref. 6 such that the limit of the Riemann curvature tensor exists and is the Riemann tensor of the limit metric. The same holds for the other curvature tensors. We have

$$\mathbf{g} \equiv \lim_{\gamma\to 0} {}^{\gamma}\mathbf{g} = (\Theta_x^- e^{2\beta x} + \Theta_x^+ e^{-2\beta x})(-\,\mathbf{d}t\,\mathbf{d}t + \mathbf{d}x\,\mathbf{d}x + e^{2\beta t}(\mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z)), \tag{31}$$

$$\mathbf{Ric} \equiv \lim_{\gamma\to 0} {}^{\gamma}\mathbf{Ric} = 2\beta\delta_0(\mathbf{d}t\,\mathbf{d}t - 3\,\mathbf{d}x\,\mathbf{d}x - e^{2\beta t}(\mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z)), \tag{32}$$

$$\mathbf{G} \equiv \lim_{\gamma\to 0} {}^{\gamma}\mathbf{G} = 4\beta\delta_0(\mathbf{d}t\,\mathbf{d}t - e^{2\beta t}(\mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z)), \tag{33}$$

where Θ_x^- and Θ_x^+ are the Heaviside distributions with support on $x<0$ and $x>0$, respectively, and δ_0 is the Dirac measure with support on the surface $x=0$. Note that $\mathbf{g}$ is piecewise smooth and that the pullback of $\mathbf{g}$ to the surface $x=0$ is the same from both sides. Note also that this pullback is given by (25). Indeed, the above expressions should be understood in the sense of distributions. Thus, $\mathbf{g}\equiv\lim_{\gamma\to 0}{}^{\gamma}\mathbf{g}$ means

$$\mathbf{g}[\mathbf{U}] \equiv \lim_{\gamma\to 0} {}^{\gamma}\mathbf{g}[\mathbf{U}]. \tag{34}$$

In fact, ${}^{\gamma}\mathbf{g}$, $({}^{\gamma}\mathbf{g})^{-1}$ and $\nabla{}^{\gamma}\mathbf{g}$, with ∇ the covariant derivative associated with (27), converge locally (in square integral) to $\mathbf{g}$, $(\mathbf{g})^{-1}$, and $\nabla\mathbf{g}$, respectively.[24] (Remarkably enough, with ${}^{\mathbf{g}}\nabla$ the covariant derivative associated to any regular metric tensor $\mathbf{g}$ we have ${}^{\mathbf{g}}\nabla\mathbf{g}=0$ in the sense of distributions.[6]) Hence, **Ric** and **G** are the distribution-valued Ricci and Einstein curvatures of $\mathbf{g}$.[24] It follows that the diagram (4), in which ${}^{\gamma}\mathbf{g}$ and $\mathbf{g}$ are the distribution valued metric tensors of the thick and thin domain wall space–times, respectively, holds in the sense of distributions.

Now, as follows from the distributional convergence (4) proved in Ref. 24 and the fact that the vectors (21)–(24) are all smooth vector fields independent of the wall's thickness, these are also Killing vectors of $(\mathbb{R}^4,\mathbf{g})$ in the sense that $\mathcal{L}_{\mathbf{v}}\mathbf{g}$ is the zero distribution on $\mathbb{R}^4$. As an example, consider the Killing vector given by (22). For (31) we have

$$\mathcal{L}_{\mathbf{v}_4}\mathbf{g}[\mathbf{U}] \equiv -\mathbf{g}[\mathcal{L}_{\mathbf{v}_4}\mathbf{U} + (\nabla\cdot\mathbf{V}_4)\mathbf{U}] = -\int_{\mathbb{R}^4}\mathbf{g}\cdot(\mathcal{L}_{\mathbf{v}_4}\mathbf{U} + \mathbf{U}(\nabla\cdot\mathbf{V}_4))\boldsymbol{\omega}_\eta = -\int_{x<0} e^{2\beta x}((\partial_t - \beta y\partial_y - \beta z\partial_z - 2\beta)(-U^{tt} + U^{xx}) + e^{2\beta t}(\partial_t - \beta y\partial_y - \beta z\partial_z)(U^{yy} + U^{zz}))\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z - \int_{x>0} e^{-2\beta x}((\partial_t - \beta y\partial_y - \beta z\partial_z - 2\beta)(-U^{tt} + U^{xx}) + e^{2\beta t}(\partial_t - \beta y\partial_y - \beta z\partial_z)(U^{yy} + U^{zz}))\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = 0, \tag{35}$$

where we have integrated by parts and used the fact that **U** is of compact support.

Indeed, (21)–(24) are also improper Ricci collineations. For (32) and (22) we have

$$\mathcal{L}_{\mathbf{v}_4}\mathbf{Ric}[\mathbf{U}] \equiv -\mathbf{Ric}[\mathcal{L}_{\mathbf{v}_4}\mathbf{U} + (\nabla\cdot\mathbf{V}_4)\mathbf{U}] = -\beta\int_{x=0}((\partial_t - \beta y\partial_y - \beta z\partial_z - 2\beta)(2U^{tt} - 3U^{xx}) - 2e^{2\beta t}(\partial_t - \beta y\partial_y - \beta z\partial_z)(U^{yy} + U^{zz}))\mathrm{d}t\,\mathrm{d}y\,\mathrm{d}z = 0, \tag{36}$$

where in the last step we have integrated by parts and used again the fact that **U** is of compact support. Analogous computations show that

$$\mathcal{L}_{\mathbf{v}}\mathbf{Ric}[\mathbf{U}] = 0, \quad \mathcal{L}_{\mathbf{v}}\mathbf{G}[\mathbf{U}] = 0, \tag{37}$$

for all the Killing symmetries of (14), a result that obviously cannot be proved outside the distributional setting. It follows that for this space–time the diagram

$$\begin{array}{ccccc} \mathcal{L}_{\mathbf{v}}{}^{\gamma}\mathbf{g} = 0 & \longrightarrow & \mathcal{L}_{\mathbf{v}}{}^{\gamma}\mathbf{Ric} = 0 & \longrightarrow & \mathcal{L}_{\mathbf{v}}{}^{\gamma}\mathbf{G} = 0 \\ \downarrow_{\gamma\to 0} & & \downarrow_{\gamma\to 0} & & \downarrow_{\gamma\to 0} \\ \mathcal{L}_{\mathbf{v}}\mathbf{g} = 0 & \longrightarrow & \mathcal{L}_{\mathbf{v}}\mathbf{Ric} = 0 & \longrightarrow & \mathcal{L}_{\mathbf{v}}\mathbf{G} = 0 \end{array} \tag{38}$$

holds in the sense of distributions. Besides (21)–(24), there is no other C^∞ vector field for which (37) are satisfied. It should be noted that both diagrams, (4) and (38), hold under γ-dependent smooth diffeomorphisms, whenever in the limit $\gamma\to 0$ these remain bounded in order to avoid different identifications of points in the manifold under these diffeomorphisms.

Finally, it should be stressed that any smooth metric can be chosen as an auxiliary metric in (13). We have made the choice (27) for simplicity. In this sense, any C^∞ metric tensor field $\boldsymbol{\eta}$ whose Killing vectors are given by (21)–(24) is also a convenient choice for explicit calculations since in this case $\nabla\cdot\mathbf{V}=0$. Now, with ${}^{\mathbf{g}}\nabla$ the covariant derivative associated to **g**, we have ${}^{\mathbf{g}}\nabla\cdot\mathbf{V}=0$ for **g** given by (31) and **V** any of its Killing vector fields (21)–(24). However, (31) cannot be chosen as an auxiliary metric, since for **V** an arbitrary C^∞ vector field, $({}^{\mathbf{g}}\nabla\cdot\mathbf{V})$ turns out to be discontinuous at the surface $x=0$ and $({}^{\mathbf{g}}\nabla\cdot\mathbf{V})\mathbf{U}$ is not a test tensor field.

IV. A DOMAIN WALL EMBEDDED IN AN ANTI-DE SITTER SPACE–TIME

Consider the space–time $(\mathbb{R}^4, {}^{\gamma}\mathbf{g})$ where the metric tensor is given by

$${}^{\gamma}\mathbf{g} = \cosh^{-2\gamma}\frac{\beta x}{\gamma}(-\mathbf{d}t\,\mathbf{d}t + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z) + \mathbf{d}x\,\mathbf{d}x, \tag{39}$$

with β and γ constants and $\gamma>0$. This is a thick domain wall space–time, solution to the coupled Einstein-scalar field equations (15) and (16) with $\Lambda=-3\beta^2$ and

$$\phi = \phi_0\tan^{-1}(\sinh(\beta x/\gamma)), \quad \phi_0 \equiv \sqrt{\gamma/4\pi} \tag{40}$$

and

$$V(\phi) = \frac{1}{8\pi}\beta^2\left(3 + \frac{1}{\gamma}\right)\cos^2(\phi/\phi_0). \tag{41}$$

This space–time behaves asymptotically (i.e., far away of the wall) as an anti-de Sitter space–time[24] and its five-dimensional analogue provides a thick domain wall version[22] of the original Randall–Sundrum scenario.[13] Here, γ plays the role of the wall's thickness and the distributional $\gamma \to 0$ limit of this geometry has been analyzed in Ref. 24.

There are six Killing vector fields on $(\mathbb{R}^4, {}^{\gamma}\mathbf{g})$, given by

$$\mathbf{V}_1 = \boldsymbol{\partial}_y, \quad \mathbf{V}_2 = \boldsymbol{\partial}_z, \quad \mathbf{V}_3 = z\boldsymbol{\partial}_y - y\boldsymbol{\partial}_z, \tag{42}$$

$$\mathbf{V}_4 = \boldsymbol{\partial}_t, \quad \mathbf{V}_5 = t\boldsymbol{\partial}_y + y\boldsymbol{\partial}_t, \quad \mathbf{V}_6 = z\boldsymbol{\partial}_t + t\boldsymbol{\partial}_z, \tag{43}$$

where $\mathbf{V}_4$ is a time translation and $\mathbf{V}_5$, $\mathbf{V}_6$ are Lorentz rotations.

The Ricci and Einstein tensor fields of (39) are given by

$${}^{\gamma}\mathbf{Ric} = \Lambda \tanh^2\frac{\beta x}{\gamma}\,{}^{\gamma}\mathbf{g} + \frac{\beta^2}{\gamma}\cosh^{-2}\frac{\beta x}{\gamma}\left(\cosh^{-2\gamma}\frac{\beta x}{\gamma}(-\mathbf{d}t\,\mathbf{d}t + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z) + 3\,\mathbf{d}x\,\mathbf{d}x\right), \tag{44}$$

$${}^{\gamma}\mathbf{G} = -\Lambda \tanh^2\frac{\beta x}{\gamma}\,{}^{\gamma}\mathbf{g} - \frac{2\beta^2}{\gamma}\cosh^{-2(\gamma+1)}\frac{\beta x}{\gamma}(-\mathbf{d}t\,\mathbf{d}t + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z). \tag{45}$$

The distributional thin wall limits of (39), (44), and (45) are given by

$$\mathbf{g} \equiv \lim_{\gamma\to 0}\,{}^{\gamma}\mathbf{g} = (\Theta_x^- e^{2\beta x} + \Theta_x^+ e^{-2\beta x})(-\mathbf{d}t\,\mathbf{d}t + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z) + \mathbf{d}x\,\mathbf{d}x, \tag{46}$$

$$\mathbf{Ric} \equiv \lim_{\gamma\to 0}\,{}^{\gamma}\mathbf{Ric} = \Lambda\mathbf{g} + 2\beta\delta_0(-\mathbf{d}t\,\mathbf{d}t + 3\,\mathbf{d}x\,\mathbf{d}x + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z), \tag{47}$$

$$\mathbf{G} + \mathbf{g}\Lambda \equiv \lim_{\gamma\to 0}\left({}^{\gamma}\mathbf{G} + {}^{\gamma}\mathbf{g}\Lambda\right) = 4\beta\delta_0(\mathbf{d}t\,\mathbf{d}t - \mathbf{d}y\,\mathbf{d}y - \mathbf{d}z\,\mathbf{d}z), \tag{48}$$

where **Ric** and **G** are the distribution-valued Ricci and Einstein curvatures of **g**.[24] The diagram (4), in which ${}^{\gamma}\mathbf{g}$ and **g** are given by (39) and (46), respectively, holds in the sense of distributions.

Note that **g** is piecewise smooth and that the pullback of **g** to the surface $x=0$ is the same from both sides of this surface. Note also that the six vector fields (42) and (43) are also Killing vectors on the $(2+1)$-dimensional Minkowski space–time $(\mathbb{R}^3, \overline{\mathbf{g}})$ with $\overline{\mathbf{g}}$ the Minkowski metric which appears as this pullback.

Next, let $\boldsymbol{\eta}$ be the Minkowski metric tensor (27) and let ∇ be the Levi–Civita covariant derivative associated with $\boldsymbol{\eta}$. Let **U** be a test 2-tensor field on $\mathbb{R}^4$. From (13), it is straightforward to verify that for the vector fields given by (42) and (43), we have

$$\mathcal{L}_{\mathbf{v}}\,{}^{\gamma}\mathbf{g}[\mathbf{U}] = 0, \quad \mathcal{L}_{\mathbf{v}}\mathbf{g}[\mathbf{U}] = 0, \tag{49}$$

as expected. Hence, (42) and (43) are Killing vectors of $(\mathbb{R}^4, \mathbf{g})$ in the sense that $\mathcal{L}_{\mathbf{v}}\mathbf{g}$ along these vectors is the zero distribution on $\mathbb{R}^4$. Analogous computations show that

$$\mathcal{L}_{\mathbf{v}}\,{}^{\gamma}\mathbf{Ric}[\mathbf{U}] = 0, \quad \mathcal{L}_{\mathbf{v}}\,{}^{\gamma}\mathbf{G}[\mathbf{U}] = 0 \tag{50}$$

and

$$\mathcal{L}_{\mathbf{v}}\,\mathbf{Ric}[\mathbf{U}] = 0, \quad \mathcal{L}_{\mathbf{v}}\mathbf{G}[\mathbf{U}] = 0. \tag{51}$$

It follows that for this space–time the diagram (38) holds in the sense of distributions. Besides (42) and (43), there is no other C^∞ vector field for which (50) and (51) are satisfied on $\mathbb{R}^4$.

Next, let $\mathcal{M}^+ \equiv \{(t,x,y,z) \in \mathbb{R}^4, x>0\}$ and let $\mathbf{U}^+$ be a test tensor of compact support $\mathcal{K} \subset \mathcal{M}^+$. From (12) we find that

$$\mathcal{L}_{\mathbf{v}}\mathbf{g}[\mathbf{U}^+] = 0 \tag{52}$$

is satisfied along the C^∞ vector fields on $\mathbb{R}^4$ given by

$$\mathbf{V}_7 = \boldsymbol{\partial}_x + \beta(t\boldsymbol{\partial}_t + y\boldsymbol{\partial}_y + z\boldsymbol{\partial}_z), \tag{53}$$

$$\mathbf{V}_8 = \beta t\mathbf{V}_7 + \left(\tfrac{1}{2}\beta^2(-t^2+y^2+z^2) + \tfrac{1}{8}e^{2\beta x}\right)\boldsymbol{\partial}_t, \tag{54}$$

$$\mathbf{V}_9 = \beta y\mathbf{V}_7 - \left(\tfrac{1}{2}\beta^2(-t^2+y^2+z^2) + \tfrac{1}{8}e^{2\beta x}\right)\boldsymbol{\partial}_y, \tag{55}$$

$$\mathbf{V}_{10} = \beta z\mathbf{V}_7 - \left(\tfrac{1}{2}\beta^2(-t^2+y^2+z^2) + \tfrac{1}{8}e^{2\beta x}\right)\boldsymbol{\partial}_z. \tag{56}$$

It follows that $\mathcal{L}_{\mathbf{v}}\mathbf{g}$ is the zero distribution on $\mathcal{M}^+$, along these vector fields.

Now, let $\mathbf{U}$ be a test tensor on $\mathbb{R}^4$ and let us consider the Lie derivatives (in the sense of distributions) of (39) and (46) along the vector fields (53)–(56). Since ${}^\gamma\mathbf{g}$ and $\nabla{}^\gamma\mathbf{g}$ converge locally to $\mathbf{g}$ and $\nabla\mathbf{g}$ for $\gamma\to 0$,[24] it follows directly that $\mathcal{L}_{\mathbf{v}}{}^\gamma\mathbf{g}$ also converge locally to $\mathcal{L}_{\mathbf{v}}\mathbf{g}$ along the smooth vector fields (53)–(56). Thus, for $\mathbf{V}_7$ we have

$$\mathcal{L}_{\mathbf{V}_7}{}^\gamma\mathbf{g} = 2\beta\cosh^{-2\gamma}\frac{\beta x}{\gamma}\left(1-\tanh\frac{\beta x}{\gamma}\right)(-\mathbf{d}t\,\mathbf{d}t + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z), \tag{57}$$

$$\mathcal{L}_{\mathbf{V}_7}\mathbf{g} = \Theta_x^-\, 4\beta e^{2\beta x}(-\mathbf{d}t\,\mathbf{d}t + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z), \tag{58}$$

that satisfy

$$\lim_{\gamma\to 0}\mathcal{L}_{\mathbf{V}_7}{}^\gamma\mathbf{g}[\mathbf{U}] = \mathcal{L}_{\mathbf{V}_7}\mathbf{g}[\mathbf{U}]. \tag{59}$$

The fact that $\mathcal{L}_{\mathbf{v}_7}\mathbf{g}$ is the zero distribution on $\mathcal{M}^+$ may be interpreted naturally as a Killing symmetry of $\mathbf{g}$ on $\mathcal{M}^+$ generated by $\mathbf{V}_7$. Since this symmetry arises in the limit $\gamma\to 0$ of ${}^\gamma\mathbf{g}$, $\mathbf{V}_7$ is an *asymptotic* Killing vector field on $(\mathbb{R}^4, {}^\gamma\mathbf{g})$. The same considerations holds for the other C^∞ vector fields (54)–(56). Further, since $(\mathbb{R}^4, \mathbf{g})$ is reflection symmetric along the direction perpendicular to the wall, a symmetry inherited from $(\mathbb{R}^4, {}^\gamma\mathbf{g})$, the above considerations can be extended to $\mathcal{M}^- \equiv \{(t,x,y,z) \in \mathbb{R}^4, x<0\}$ under the replacement $x\to -x$. Indeed, these results are by no means unexpected, they simply put in a rigorous setting the emergence of additional symmetries in the $\gamma\to 0$ limit of the space–time $(\mathbb{R}^4, {}^\gamma\mathbf{g})$, where we have an absolute control over what is going on.

For the sake of completeness, let us analyze the action of $\mathcal{L}_{\mathbf{v}}$ on the distribution-valued curvature tensors of the metric (46) along the vector fields (53)–(56). Let us consider again the vector field $\mathbf{V}_7$. We find

$$\mathcal{L}_{\mathbf{V}_7}\mathbf{Ric} = 2\beta(\delta_0' - 2\beta\delta_0)(-\mathbf{d}t\,\mathbf{d}t + 3\,\mathbf{d}x\,\mathbf{d}x + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z) - \Theta_x^-\, 12\beta^3 e^{2\beta x}(-\mathbf{d}t\,\mathbf{d}t + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z) \tag{60}$$

and

$$\mathcal{L}_{\mathbf{V}_7}(8\pi\mathbf{T}) \equiv \mathcal{L}_{\mathbf{V}_7}(\mathbf{G}+\Lambda\mathbf{g}) = 4\beta(\delta_0' + 2\beta\delta_0)(-\,\mathbf{d}t\,\mathbf{d}t + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z). \tag{61}$$

Indeed, $\mathbf{V}_7$ is neither a Ricci collineation nor a matter collineation and the same conclusion extends to the vector fields (54)–(56). In particular, this shows explicitly that the distributional energy momentum tensor of the brane does not inherit all the symmetries of the bulk.

V. AN ASYMMETRIC DOMAIN WALL SPACE–TIME

Let us now to consider the space–time $(\mathbb{R}^4, {}^{\gamma}\mathbf{g})$ where the C^∞ metric tensor ${}^{\gamma}\mathbf{g}$ is given by

$${}^{\gamma}\mathbf{g} = \cosh^{-2\gamma/3}\frac{\beta x}{\gamma}e^{-4\beta x/3}(-\,\mathbf{d}t\,\mathbf{d}t + e^{2\beta x}(\mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z)) + \cosh^{-2\gamma}\frac{\beta x}{\gamma}\mathbf{d}x\,\mathbf{d}x, \tag{62}$$

with β and γ constants and $0<\gamma<1$. This represents a two-parameter family of plane symmetric static domain wall space–times in which the reflection symmetry along the direction perpendicular to the wall has been relaxed, being asymptotically (i.e., far away of the wall) flat for $x>0$ and behaving asymptotically as the Taub space–time for $x<0$.[20] The metric (62) is solution to the coupled Einstein-scalar field equations (15) and (16) with $\Lambda=0$ and

$$\phi = \phi_0 \tan^{-1}(\sinh(\beta x/\gamma), \quad \phi_0 \equiv \tfrac{1}{6}\sqrt{3\gamma(1-\gamma)/\pi} \tag{63}$$

and

$$V(\phi) = \frac{1}{24\pi}\beta^2\frac{1}{\gamma}\cos^{2(1-\gamma)}(\phi/\phi_0), \tag{64}$$

where γ plays the role of the wall's thickness. The distributional $\gamma\to 0$ limit of this geometry has been analyzed in Ref. 25. It should be noted that (62) does not inherit the Z_2 symmetry of $V(\phi)$, a fact that makes very interesting the analysis of the symmetries of this space–time.

The Ricci and Einstein tensor fields of (62) are given by

$${}^{\gamma}\mathbf{Ric} = \frac{\beta^2}{3\gamma}\left(\cosh\frac{\beta x}{\gamma}\right)^{-2(1-2\gamma/3)}(-\,e^{-4\beta x/3}\,\mathbf{d}t\,\mathbf{d}t + e^{2\beta x/3}(\mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z)) + \frac{\beta^2}{3\gamma}(3 - 2\gamma)\cosh^{-2}\frac{\beta x}{\gamma}\mathbf{d}x\,\mathbf{d}x, \tag{65}$$

$${}^{\gamma}\mathbf{G} = \frac{\beta^2}{3\gamma}\left(\cosh\frac{\beta x}{\gamma}\right)^{-2(1-2\gamma/3)}(2-\gamma)(e^{-4\beta x/3}\,\mathbf{d}t\,\mathbf{d}t - e^{2\beta x/3}(\mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z)) - \frac{\beta^2}{3}\cosh^{-2}\frac{\beta x}{\gamma}\mathbf{d}x\,\mathbf{d}x, \tag{66}$$

and the distributional thin wall limits of (62), (65), and (66) are given by[25]

$$\mathbf{g} \equiv \lim_{\gamma\to 0}{}^{\gamma}\mathbf{g} = \Theta_x^-(-\,e^{-2\beta x/3}\,\mathbf{d}t\,\mathbf{d}t + e^{2\beta x}\,\mathbf{d}x\,\mathbf{d}x + e^{4\beta x/3}(\mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z)) + \Theta_x^+(-\,e^{-2\beta x}\,\mathbf{d}t\,\mathbf{d}t + e^{-2\beta x}\,\mathbf{d}x\,\mathbf{d}x + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z), \tag{67}$$

$$\mathbf{Ric} \equiv \lim_{\gamma\to 0}{}^{\gamma}\mathbf{Ric} = \tfrac{1}{3}\beta\delta_0(-\,\mathbf{d}t\,\mathbf{d}t + 3\,\mathbf{d}x\,\mathbf{d}x + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z), \tag{68}$$

$$\mathbf{G} \equiv \lim_{\gamma\to 0}{}^{\gamma}\mathbf{G} = \tfrac{2}{3}\beta\delta_0(\mathbf{d}t\,\mathbf{d}t - \mathbf{d}y\,\mathbf{d}y - \mathbf{d}z\,\mathbf{d}z). \tag{69}$$

Note that $\mathbf{g}$ is piecewise smooth and that the pullback of $\mathbf{g}$ to the surface $x=0$ is the same from both sides and coincides with the ordinary $(2+1)$-dimensional Minkowski metric. Like its smoothed version (62), $\mathbf{g}$ is not reflection symmetric along the coordinate perpendicular to the

wall. The space–time $(\mathbb{R}^4, \mathbf{g})$ for $x>0$ is isometric to the ordinary $(3+1)$-dimensional Minkowski space–time, while for $x<0$ it is the Taub space–time.[20,25]

There are only four independent Killing vector fields on $(\mathbb{R}^4, {}^{\gamma}\mathbf{g})$ and these are given by

$$\mathbf{V}_1 = \boldsymbol{\partial}_y, \quad \mathbf{V}_2 = \boldsymbol{\partial}_z, \quad \mathbf{V}_3 = z\boldsymbol{\partial}_y - y\boldsymbol{\partial}_z, \quad \mathbf{V}_4 = \boldsymbol{\partial}_t. \tag{70}$$

Let ∇ be the derivative operator in the ordinary Minkowski metric tensor (27). Let $\mathbf{U}$ be a test 2-tensor field on $\mathbb{R}^4$. From (13) it is straightforward to show that the four vectors given in (70) generate also isometries of (67) and are improper collineations for the distributional Ricci and Einstein curvature tensors. It follows that for this space–time the diagram (38) holds in the sense of distributions.

Next, consider the C^∞ vector fields given by

$$\mathbf{V}_5 = t\boldsymbol{\partial}_y + y\boldsymbol{\partial}_t, \quad \mathbf{V}_6 = z\boldsymbol{\partial}_t + t\boldsymbol{\partial}_z. \tag{71}$$

We have

$$\mathcal{L}_{\mathbf{V}_5}\mathbf{g}[\mathbf{U}] \equiv -\mathbf{g}[\mathcal{L}_{\mathbf{V}_5}\mathbf{U} + (\nabla\cdot\mathbf{V}_5)\mathbf{U}] = -\int_{\mathbb{R}^4} \mathbf{g}\cdot(\mathcal{L}_{\mathbf{V}_5}\mathbf{U} + \mathbf{U}(\nabla\cdot\mathbf{V}_5))\boldsymbol{\omega}_\eta = -\int_{x<0} (e^{-2\beta x/3} - e^{4\beta x/3})$$
$$\times (U^{ty} + U^{yt})\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z - \int_{x>0} (e^{-2\beta x} - 1)(U^{ty} + U^{yt})\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z, \tag{72}$$

where we have integrated by parts and used the fact that $\mathbf{U}$ is of compact support. It follows

$$\mathcal{L}_{\mathbf{V}_5}\mathbf{g} = 2(\Theta_x^- e^{\beta x/3} + \Theta_x^+ e^{-\beta x})\sinh\beta x(\mathbf{d}t\,\mathbf{d}y + \mathbf{d}y\,\mathbf{d}t). \tag{73}$$

On the other hand, as can be guessed from the explicit form of **Ric**, we have

$$\mathcal{L}_{\mathbf{V}_5}\mathbf{Ric}[\mathbf{U}] \equiv -\mathbf{Ric}[\mathcal{L}_{\mathbf{V}_5}\mathbf{U} + (\nabla\cdot\mathbf{V}_5)\mathbf{U}]$$
$$= -\frac{1}{3}\beta\int_{x=0} (y\partial_t + t\partial_y)(U^{tt} + 3U^{xx} + U^{yy} + U^{zz})\mathrm{d}t\,\mathrm{d}y\,\mathrm{d}z = 0, \tag{74}$$

where in the last step we have integrated by parts and used again the fact that $\mathbf{U}$ is of compact support. Analogous computations show that

$$\mathcal{L}_{\mathbf{V}_6}\mathbf{g} = 2(\Theta_x^- e^{\beta x/3} + \Theta_x^+ e^{-\beta x})\sinh\beta x(\mathbf{d}t\,\mathbf{d}z + \mathbf{d}z\,\mathbf{d}t), \tag{75}$$

$$\mathcal{L}_{\mathbf{V}_6}\mathbf{Ric} = 0. \tag{76}$$

Hence, although V_5 and V_6 are not Killing vectors of $(\mathbb{R}^4, \mathbf{g})$, they are Ricci collineations. Further,

$$\mathcal{L}_{\mathbf{V}_5}\mathbf{G} = 0, \quad \mathcal{L}_{\mathbf{V}_6}\mathbf{G} = 0, \tag{77}$$

and V_5 and V_6 are also Einstein collineations. Indeed, the above expressions should be understood in the sense of distributions. Besides (70) and (71), there is no other C^∞ vector field that generates symmetries of **Ric** and **G**.

It should be noted that $\mathcal{L}_{\mathbf{v}_5}\mathbf{g}$ and $\mathcal{L}_{\mathbf{v}_6}\mathbf{g}$ are piecewise smooth and that the pullbacks of $\mathcal{L}_{\mathbf{v}_5}\mathbf{g}$ and $\mathcal{L}_{\mathbf{v}_6}\mathbf{g}$ to the surface $x=0$ are the same from both sides of the wall and vanish. It follows that the symmetries of the distribution-valued curvature tensors **Ric** and **G** (which are supported on the surface $x=0$) coincide with the Killing symmetries of the pullback of $\mathbf{g}$ to this surface. For the sake of completeness, let us show that the same result is also reached within the standard thin shell formalism.[7,31] For $(\mathbb{R}^4, \mathbf{g})$ with $\mathbf{g}$ given by (67), the pullback $\overline{\mathbf{g}}$ of $\mathbf{g}$ to the surface $x=0$ is the same from both sides and is given by

$$\overline{\mathbf{g}} = (-\mathbf{d}t\,\mathbf{d}t + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z). \tag{78}$$

The extrinsic curvature tensor $\mathbf{K}$ of the surfaces $x=x_0$ as submanifolds of $(\mathbb{R}^4,\mathbf{g})$, is the C^∞ regularly discontinuous tensor across the surface $x=0$ given by

$$\mathbf{K} = -\tfrac{1}{3}\beta\Theta_x^-(e^{-2\beta x_0/3}\,\mathbf{d}t\,\mathbf{d}t + 2e^{-4\beta x_0/3}(\mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z)) - \beta\Theta_x^+ e^{-2\beta x_0}\,\mathbf{d}t\,\mathbf{d}t. \tag{79}$$

Thus, the discontinuity $[[\mathbf{K}]] \equiv \mathbf{K}|_{x_0=0^+} - \mathbf{K}|_{x_0=0^-}$ of $\mathbf{K}$ across the surface $x=0$, which is declared as a purely intrinsic property of this surface, is the ordinary C^∞ tensor field defined on the surface $x=0$ given by

$$[[\mathbf{K}]] = \tfrac{2}{3}\beta(-\mathbf{d}t\,\mathbf{d}t + \mathbf{d}y\,\mathbf{d}y + \mathbf{d}z\,\mathbf{d}z). \tag{80}$$

Therefore, the symmetries of $[[\mathbf{K}]]$ are the symmetries of the pullback $\overline{\mathbf{g}}$ of $\mathbf{g}$ to the surface $x=0$. Now, we have

$$\mathbf{Ric} = \tfrac{1}{2}\delta_0([[\mathbf{K}]] + (\overline{\mathbf{g}}^{-1}\cdot[[\mathbf{K}]])\mathbf{d}x\,\mathbf{d}x), \tag{81}$$

from which it follows that the symmetries of the distributional Ricci tensor of $\mathbf{g}$ turns out to be the Killing symmetries of the induced metric $\overline{\mathbf{g}}$ on the surface $x=0$ where the 2-brane is localized. It should be noted that this is not an example of the well known (trivial) symmetry inheritance. Although, the pullback $\overline{\mathbf{g}}$ of $\mathbf{g}$ to the surface $x=0$ acts a metric on this surface (as follows from the fact that the surface $x=0$ has a well-defined intrinsic geometry) and therefore the Killing vectors of this pullback are naturally collineations of the curvature tensors of this pullback, **Ric** given by (68) or (81) is not the Ricci tensor of $\overline{\mathbf{g}}$. The same conclusions can be extended also to all the thin domain wall geometries considered in the preceding sections.

Remarkably enough, the asymmetric geometry considered here, explicitly shows that the Killing symmetries of the pullback of the metric tensor to the surface where the thin wall is localized may form a larger group than the group of Killing symmetries which are common to the ambient space–time on both sides of the wall.

VI. SUMMARY AND DISCUSSION

In this work, by generalizing the Lie derivative of smooth tensor fields to distribution-valued tensors, we defined and computed the Killing symmetries and the Ricci and Einstein collineations of some distributional domain wall geometries for which the diagram (4), with ${}^\gamma\mathbf{g}$ and $\mathbf{g}$ the distribution valued metric tensors of the thick and thin domain wall space–times, respectively, holds rigourously in the sense of distributions. For all the geometries considered, the distribution-valued curvature tensors of the thin wall limit have singular parts proportional to a Dirac distribution supported on the surface Σ where the thin wall is localized. We found that the Killing symmetries of the distributional geometry of the thin wall space–time $(\mathbb{R}^4,\mathbf{g})$ are the Killing symmetries of the smooth thick domain wall space–time $(\mathbb{R}^4,{}^\gamma\mathbf{g})$ and that, besides these, there are no other isometries. However, as expected, the thin wall geometry may show additional symmetries on the open disjoint sets $\mathcal{M}^+$ and $\mathcal{M}^-$, that admit Σ as a boundary, which are not isometries inherited from the corresponding smooth geometry. These symmetries are the asymptotic (i.e., far away of the wall) Killing symmetries of $(\mathbb{R}^4,{}^\gamma\mathbf{g})$.

For the thin domain walls with reflection symmetry of Secs. III and IV, the Killing vectors of $(\mathbb{R}^4,\mathbf{g})$ are the only symmetries of the corresponding distribution-valued Ricci and Einstein tensors. Therefore the Ricci and Einstein collineations of these thin wall geometries are improper. For the asymmetric thin domain wall of Sec. V, we found that the collineations of the distributional Ricci and Einstein tensors form a larger group than the one formed by the Killing symmetries of the corresponding space–time $(\mathbb{R}^4,\mathbf{g})$. The additional symmetries are then proper Ricci and Einstein collineations. Finally, for all the thin wall space–times $(\mathbb{R}^4,\mathbf{g})$ considered, the symmetries of the distributional curvature tensors turns out to be the Killing symmetries of $(\Sigma,\overline{\mathbf{g}})$, where $\overline{\mathbf{g}}$ is the pullback of $\mathbf{g}$ to Σ.

Although we have restricted ourselves to consider four-dimensional domain wall space–times, these models are straightforwardly generalized to D-dimensional domain wall space–times.[25] On the other hand, the analysis presented here can be carried out, in principle, for all the distribution-valued curvature tensors of a space–time $(\mathcal{M},\mathbf{g})$, whenever the distribution-valued metric tensor $\mathbf{g}$ is a regular metric in the sense of Ref. 6. This generalization and its implications will be discussed in a forthcoming paper.

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SCD patterns have singular diffraction

M. Baake[a)]
Fakultät für Mathematik, Universität Bielefeld, Postfach 100131, 33501 Bielefeld, Germany

D. Frettlöh[b)]
Institut für Mathematik und Informatik, Universität Greifswald, Jahnstr. 15a, 17487 Greifswald, Germany

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Among the many families of nonperiodic tilings known so far, SCD tilings are still a bit mysterious. Here, we determine the diffraction spectra of point sets derived from SCD tilings and show that they have no absolutely continuous part, that they have a uniformly discrete pure point part on the axis $\mathbb{R}\boldsymbol{e}_3$, and that they are otherwise supported on a set of concentric cylinder surfaces around this axis. For SCD tilings with additional properties, more detailed results are given. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1842355]

I. THE TILINGS

After the discovery of families of tiles that permit only aperiodic tilings, the question arose whether there exists a single tile that permits *only* aperiodic tilings by copies of itself (an *aperiodic prototile*). A first example, which gives tilings in Euclidean 3-space, was found by Schmitt in 1988. It was elaborated later by Conway and Danzer (cf. Ref. 7). In particular, they modified Schmitt's prototile to a convex one. We refer to these tilings—which will be described in this section—as SCD tilings.

A *tiling* in $\mathbb{R}^d$ is a collection of tiles $\{T_n\}_{n\geqslant 0}$ which covers $\mathbb{R}^d$ and contains no overlapping tiles, i.e., $\mathrm{int}(T_k)\cap\mathrm{int}(T_n)=\varnothing$ for $k\neq n$. A *tile* is a nonempty compact set $T\subset\mathbb{R}^d$ with the property that $\mathrm{cl}(\mathrm{int}(T))=T$. A tiling $\mathcal{T}$ is called *aperiodic*, if $\mathcal{T}+\boldsymbol{x}=\mathcal{T}$ implies $\boldsymbol{x}=\boldsymbol{0}$.

The SCD tilings are built from a single kind of tile—a single *prototile*—which we refer to as *SCD tile*. Essentially, the main idea is that the only possible tilings are of the following form: The tiles can be put together to form layers, which extend in two dimensions; these layers can be stacked, but only in such a way that two consecutive layers are rotated against each other by a fixed angle, which may be incommensurate to π. Then, the symmetry groups of the resulting tilings may still be nontrivial, even infinite, but they contain no translation. To achieve this, we allow only directly congruent copies of the tiles, but no mirror images (cf. Sec. III).

The SCD tile: Choose $0<\lambda<1$, and positive real numbers b_1, b_2, c. Let $\varphi=\arctan(b_1/b_2)$, set $a=\sqrt{b_1^2+b_2^2}$, and

$$\boldsymbol{a}=(a,0,0),\quad \boldsymbol{b}=(b_1,b_2,0),\quad \boldsymbol{c}=\lambda\boldsymbol{b}+(0,0,c),\quad \boldsymbol{d}=\lambda\boldsymbol{a}-(0,0,c),$$

(cf. Fig. 1). Now, we define the SCD tile as

$$T=\mathrm{conv}(\boldsymbol{0},\boldsymbol{a},\boldsymbol{b},\boldsymbol{a}+\boldsymbol{b},\boldsymbol{c},\boldsymbol{a}+\boldsymbol{c},\boldsymbol{d},\boldsymbol{b}+\boldsymbol{d}), \tag{1}$$

where $\mathrm{conv}(M)$ denotes the convex hull of M. The result is the union of the two triangular prisms $\mathrm{conv}(\boldsymbol{0},\boldsymbol{a},\boldsymbol{b},\boldsymbol{a}+\boldsymbol{b},\boldsymbol{c},\boldsymbol{a}+\boldsymbol{c})$ and $\mathrm{conv}(\boldsymbol{0},\boldsymbol{a},\boldsymbol{b},\boldsymbol{a}+\boldsymbol{b},\boldsymbol{d},\boldsymbol{b}+\boldsymbol{d})$, glued together at the rhomb-shaped

[a)]Electronic mail: mbaake@math.uni-bielefeld.de
[b)]Present address: Fakultät für Mathematik, Universität Bielefeld, 33501 Bielefeld, Germany. Electronic mail: dirk.frettloeh@math.uni-bielefeld.de

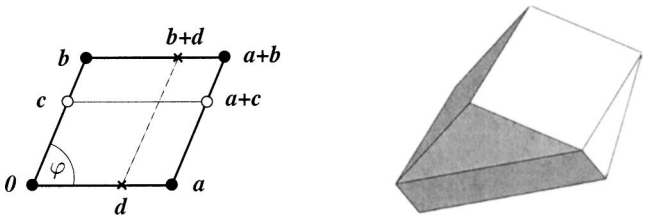

FIG. 1. The construction of an SCD tile (left) and a view of an SCD tile (right).

facet conv($\mathbf{0},\boldsymbol{a},\boldsymbol{b},\boldsymbol{a}+\boldsymbol{b}$). This is the reason that it is sometimes called Conway's biprism. If $\varphi \notin \pi\mathbb{Q}$, we will call the SCD tile *incommensurate* (which is the classical case), otherwise *commensurate*.

We should mention that this is only one possible construction. Several generalizations or variations are possible (cf. Sec. III or Ref. 7). But all these tiles give rise to tilings with basically the same structure.

The SCD tilings: Using translations of the SCD tile, one can put them together (i) by joining triangular facets conv($\mathbf{0},\boldsymbol{b},\boldsymbol{c}$) with conv($\boldsymbol{a},\boldsymbol{a}+\boldsymbol{b},\boldsymbol{a}+\boldsymbol{c}$), and (ii) by joining triangular facets conv($\mathbf{0},\boldsymbol{a},\boldsymbol{d}$) with conv($\boldsymbol{b},\boldsymbol{b}+\boldsymbol{a},\boldsymbol{b}+\boldsymbol{d}$). If we do so inductively until no triangular facet remains uncovered, we end up with a planar layer covering a two-dimensional plane.

This layer is congruent to $L=\{\boldsymbol{x}+T \,|\, \boldsymbol{x}\in\Gamma\}$, where Γ is the two-dimensional point lattice spanned by $\boldsymbol{a}$ and $\boldsymbol{b}$, i.e., $\Gamma=\mathbb{Z}\boldsymbol{a}+\mathbb{Z}\boldsymbol{b}$. The top of L shows ridges and valleys, all parallel to each other, and all parallel to $\boldsymbol{b}$. The bottom of L also shows "down under" (or upside down) valleys and ridges, all of them parallel to $\boldsymbol{a}$. In order to stack the layers, consider a layer $L'=L-\boldsymbol{c}$. Take a second layer $L''=(0,0,c)+RL'$, where R is a rotation through $-\varphi$ around the axis $\mathbb{R}\boldsymbol{e}_3=\langle(0,0,1)\rangle_{\mathbb{R}}$. L'' fits exactly on top of L'. In the same fashion, we proceed stacking layers and obtain

$$\mathcal{T}=\bigcup_{m\in\mathbb{Z}} m(0,0,c)+R^m L', \tag{2}$$

which is a tiling of $\mathbb{R}^3$. There are many other possibilities to build SCD tilings. For example, two consecutive layers can be shifted against each other by an arbitrary translation in the direction of $R^m\boldsymbol{b}$, which is the direction of the matching valleys and ridges of the two layers. Let us mention that Danzer's version restricts these translations to a discrete set $\mathbb{Z}R^m\boldsymbol{b}$ in order to allow crystallographic applications. Therefore, "SC tilings" might be a better notation for the more general tilings we consider here. Nevertheless, we will stick to the well-known notation of SCD tilings throughout this paper, holding in mind that the SCD tilings in Ref. 7 are a proper subset of the SCD tilings here. In this sense, all possible SCD tilings are congruent to

$$\mathcal{T}=\bigcup_{m\in\mathbb{Z}} m(0,0,c)+\boldsymbol{v}_m+R^m L', \tag{3}$$

for some $\boldsymbol{v}_m=(v_1^{(m)},v_2^{(m)},0)$, where $\boldsymbol{v}_{m+1}-\boldsymbol{v}_m$ is a (real) multiple of $R^m\boldsymbol{b}$. For a more thorough discussion of all possible SCD tilings, see Sec. III or Ref. 7.

As with tiles, we will distinguish between *incommensurate* SCD tilings, if they are built from incommensurate SCD tiles, and *commensurate* SCD tilings otherwise. Now, it is easy to see that incommensurate SCD tilings are aperiodic: Since $\varphi\notin\pi\mathbb{Q}$, all layers $m(0,0,c)+\boldsymbol{v}_m+R^mL$ have pairwise different orientations. Consequently, a possible translation $\boldsymbol{x}$ with $\mathcal{T}+\boldsymbol{x}=\mathcal{T}$ must map every layer onto itself. The translation vectors that fix the mth layer $m(0,0,c)+\boldsymbol{v}_m+R^mL$ are those in $R^m\Gamma$. So, the translation vectors which fix the whole tiling are elements of

$$\bigcap_{m\in\mathbb{Z}} R^m\Gamma=\{0\},$$

wherefore all incommensurate SCD tilings are aperiodic.

Note that even in the incommensurate case *finitely* many layers could still possess nontrivial translation symmetries, as two layers might still share a so-called coincidence site lattice Γ' of finite index in Γ. Then, any finite number of layers still may admit one, where the index grows with the number of layers. In the limit of infinitely many layers, only the trivial translation survives, hence the final incommensurate SCD tiling is aperiodic, compare Ref. 7 for details.

II. THE DIFFRACTION SPECTRUM

Since the discovery of quasicrystals, a central point in the study of tilings is the diffraction behavior of tilings or point sets (cf. Ref. 16). With point sets, one can model the structure of quasicrystals quite well, e.g., by representing every atom by a point. But many interesting structures were originally described in terms of tilings. The usual way to examine the diffraction behavior of such structures is to replace every tile by one (or more) reference points, in a way that the tiling and the point set determine each other uniquely by local rules (i.e., they are "mutually locally derivable," cf. Refs. 1 and 3), and then to determine the diffraction behavior of the resulting point set. In this sense, *crystallographic* tilings in $\mathbb{R}^d$—i.e., tilings which permit d linearly independent translations—correspond to crystallographic point sets, which again model ideal crystals. These show a sharp diffraction spectrum consisting of bright spots only, the "Bragg peaks," located on a uniformly discrete point set, compare Refs. 6 and 9.

The Fourier transform of structures like tilings or point sets (this will be made precise below) gives a desription of their diffraction behavior. For example, the diffraction spectrum of quasiperiodic point sets, corresponding to physical quasicrystals (cf. Ref. 9), consists of Bragg peaks only, but their positions need not be discrete. In general, any diffraction spectrum, described in terms of a positive measure μ, consists of three (unique) parts,

$$\mu = \mu_{pp} + \mu_{sc} + \mu_{ac},$$

compare Ref. 2 for examples and further references. The *pure point* part $\mu_{pp} = \Sigma_{\boldsymbol{x} \in \Lambda} I(\boldsymbol{x}) \delta_{\boldsymbol{x}}$ is the sum of weighted Dirac measures (the so-called Bragg peaks) over a countable set Λ, where $\delta_{\boldsymbol{x}}$ is the normalized point measure at $\boldsymbol{x}$ [i.e., $\delta_{\boldsymbol{x}}(M) = 1$, if $\boldsymbol{x} \in M$, and $\delta_{\boldsymbol{x}}(M) = 0$ otherwise] and $I(\boldsymbol{x})$ denotes the intensity. The *singular continuous* part μ_{sc} satisfies $\mu_{sc}(\{\boldsymbol{x}\}) = 0$ for all $\boldsymbol{x}$, but is supported (or concentrated) on a set of Lebesgue measure zero. The *absolutely continuous* part μ_{ac} corresponds to a measure with a locally integrable density function and is supported on a set of positive Lebesgue measure. The diffraction spectrum μ of a structure is called *singular*, if μ_{ac} vanishes. It is called *pure point*, if μ_{ac} and μ_{sc} vanish; i.e., if it consists of Bragg peaks only. For example, the latter case occurs if the considered structure is a *model set* (cf. Ref. 10). In this case, there is a rich theory one may use to examine the diffraction spectrum. In this paper, however, we leave the realm of pure point diffractive structures and have to use different methods.

This section makes use of the calculus of tempered distributions, also known as generalized functions (compare Refs. 4, 13, and 15). In particular, this allows for a unified treatment of functions and measures. The following common notations are used: $\mathcal{S}(\mathbb{R}^d)$ denotes the Schwartz space of rapidly decreasing functions on $\mathbb{R}^d$. The function $\widetilde{f}$ is given by $\widetilde{f}(x) = \overline{f(-x)}$. The Fourier transform of f is denoted by $\hat{f}$. The tempered distributions, $\mathcal{S}'$, are the continuous linear functionals on $\mathcal{S}(\mathbb{R}^d)$. For $T \in \mathcal{S}'$ and $\varphi \in \mathcal{S}(\mathbb{R}^d)$, we will often write $\langle T, \varphi \rangle$ instead of $T(\varphi)$. As described above, one now constructs an *SCD set* Λ_{SCD} from an SCD tiling and determines the diffraction spectrum of Λ_{SCD}, taking up and extending previous work in this direction.[7,12] To do so, choose a point $\boldsymbol{z}$ in the interior of the SCD tile T in (1), choose an SCD tiling $\mathcal{T}$ and set

$$\Lambda := \Lambda_{\mathrm{SCD}} := \{\boldsymbol{v} + R^m \boldsymbol{z} | (\boldsymbol{v} + R^m T) \in \mathcal{T}\},$$

i.e., replace every tile $\boldsymbol{v} + R^m T$ by the corresponding reference point $\boldsymbol{v} + R^m \boldsymbol{z}$. Obviously, Λ consists of layers which are congruent to the lattice Γ. Now, define the measure

$$\omega := \omega_{\mathrm{SCD}} := \sum_{x\in\Lambda} \delta_x .$$

Let $C_r=[-r/2,r/2]^3$ be the closed cube of side length r centered at the origin. The diffraction spectrum of Λ is described by the Fourier transform $\hat{\gamma}$ of the autocorrelation

$$\gamma = \lim_{r\to\infty} r^{-3} \sum_{x,y\in\Lambda\cap C_r} \delta_{x-y},$$

where the limit of these measures is taken in the vague topology. *A priori*, it is not clear whether this limit exists. But since the considered measures are translation bounded, there is at least one convergent subsequence [Ref. 9, Proposition 2.2]. In this case, we restrict to this convergent subsequence. If there is more than one convergent subsequence, we consider each one separately. This way, we can now always assume that γ exists as a tempered measure.

Let $\omega_r=\Sigma_{x\in\Lambda\cap C_r}\delta_x$. Then,

$$\gamma = \lim_{r\to\infty} r^{-3}\omega_r * \tilde{\omega}_r,$$

where $\tilde{\omega}_r := (\omega_r)^{\sim}$. By definition, this means that $\lim_{r\to\infty} r^{-3}\langle \omega_r * \tilde{\omega}_r, \varphi\rangle$ exists for all test functions $\varphi\in\mathcal{S}(\mathbb{R}^3)$. So,

$$\begin{aligned}
\lim_{r\to\infty} r^{-3}\langle \omega_r * \tilde{\omega}_r, \varphi\rangle &= \lim_{r\to\infty} r^{-3} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \varphi(x+y)\,\mathrm{d}\tilde{\omega}_r(y)\,\mathrm{d}\omega_r(x) \\
&= \lim_{r\to\infty} r^{-3} \int_{C_r}\int_{\mathbb{R}^3} \varphi(x+y)\,\mathrm{d}\tilde{\omega}_r(y)\,\mathrm{d}\omega(x) \\
&= \lim_{r\to\infty} r^{-3} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \varphi(x+y)\,\mathrm{d}\tilde{\omega}_r(y)\,\mathrm{d}\omega(x) \\
&= \lim_{r\to\infty} r^{-3}\langle \omega * \tilde{\omega}_r, \varphi\rangle
\end{aligned}$$

and therefore

$$\gamma = \lim_{r\to\infty} r^{-3}\omega * \tilde{\omega}_r. \tag{4}$$

This can also be deduced from Lemma 1.2 in Ref. 14.

In order to determine $\hat{\gamma}$, we compute the Fourier transform of $\lim_{r\to\infty} r^{-3}\omega * \tilde{\omega}_r$. Since the Fourier transform is continuous on the set $\mathcal{S}'$ of tempered distributions, we have

$$\Big(\lim_{r\to\infty} r^{-3}\omega * \tilde{\omega}_r\Big)\hat{} = \lim_{r\to\infty} r^{-3}(\omega * \tilde{\omega}_r)\hat{}.$$

So, we proceed to compute $(\omega * \tilde{\omega}_r)\hat{}$. Since $\tilde{\omega}_r$ has compact support, we have $\hat{\tilde{\omega}}_r\in\mathcal{C}^\infty$ and $\tilde{\omega}_r * \omega = \omega * \tilde{\omega}_r$. The convolution theorem for distributions yields

$$\langle (\omega * \tilde{\omega}_r)\hat{}, \varphi\rangle = \langle \hat{\omega}, \hat{\tilde{\omega}}_r \cdot \varphi\rangle \tag{5}$$

for all $\varphi\in\mathcal{S}(\mathbb{R}^3)$. Let us take a closer look at ω. It can be written as

$$\omega = \sum_{m\in\mathbb{Z}} \delta^{(2)}_{v_m+R^m\Gamma} \otimes \delta^{(1)}_{mc},$$

where $v_m=(v_1^{(m)},v_2^{(m)})$, compare (3). Here and in what follows, $\delta_M := \Sigma_{x\in M}\delta_x$. Note that $\delta^{(2)}_{v_m+R^m\Gamma}$ is a measure on $\mathbb{R}^2$ and $\delta^{(1)}_{mc}$ is one on $\mathbb{R}^1$. Let $\varphi\in\mathcal{S}(\mathbb{R}^3)$ be of the form $\varphi(x_1,x_2,x_3) = f(x_1,x_2)g(x_3)$, i.e., $f\in\mathcal{S}(\mathbb{R}^2)$, $g\in\mathcal{S}(\mathbb{R})$, and $\varphi=f\cdot g$. Since linear combinations of such functions

φ are dense in $\mathcal{S}(\mathbb{R}^3)$, see Ref. 4, the following calculation for tempered distributions holds:

$$\hat{\omega} = \sum_{m\in\mathbb{Z}} \widehat{\delta^{(2)}_{\boldsymbol{v}_m+R^m\Gamma}} \otimes \widehat{\delta^{(1)}_{mc}}.$$

It remains to examine $\widehat{\delta^{(1)}_{mc}}$, which equals $e^{-2\pi imcx_3}$, and

$$\widehat{\delta^{(2)}_{\boldsymbol{v}_m+R^m\Gamma}} = (\delta^{(2)}_{\boldsymbol{v}_m} * \delta^{(2)}_{R^m\Gamma})\hat{} = \widehat{\delta^{(2)}_{\boldsymbol{v}_m}} \cdot \widehat{\delta^{(2)}_{R^m\Gamma}} = e^{-2\pi i(x_1 v_1^{(m)} + x_2 v_2^{(m)})} \mathrm{dens}^{(2)}(\Gamma)\, \delta^{(2)}_{R^m\Gamma^*},$$

where $\mathrm{dens}^{(2)}$ denotes the two-dimensional density of Γ. The last equality uses the Poisson summation formula in distribution form (Ref. 15, p. 254)

$$\widehat{\delta_\Gamma} = \mathrm{dens}(\Gamma)\, \delta_{\Gamma^*}, \tag{6}$$

where $\Gamma^* = \{\boldsymbol{y} \,|\, \boldsymbol{y}\boldsymbol{x} \in \mathbb{Z} \text{ for all } \boldsymbol{x} \in \Gamma\}$ denotes the dual (or reciprocal) lattice. The dual lattice of $R^m\Gamma$ is indeed $R^m\Gamma^*$, since

$$\boldsymbol{y} \in (R^m\Gamma)^* \Leftrightarrow \forall\, \boldsymbol{x}' \in R^m\Gamma : \boldsymbol{y}\boldsymbol{x}' \in \mathbb{Z} \Leftrightarrow \forall\, \boldsymbol{x} \in \Gamma : \boldsymbol{y}R^m\boldsymbol{x} \in \mathbb{Z}$$

$$\Leftrightarrow \forall\, \boldsymbol{x} \in \Gamma : R^{-m}\boldsymbol{y}\boldsymbol{x} \in \mathbb{Z} \;\Leftrightarrow R^{-m}\boldsymbol{y} \in \Gamma^* \Leftrightarrow \boldsymbol{y} \in R^m\Gamma^*.$$

Altogether, we get the following result. Let $\varphi(\boldsymbol{x}) = 0$ for all $\boldsymbol{x} \in M' = (\cup_{m\in\mathbb{Z}} R^m\Gamma^*) \times \mathbb{R}$ [and thus $\varphi(\boldsymbol{x}) = 0$ for all $\boldsymbol{x} \in M := \mathrm{cl}(M')$, since φ is continuous]; in other words, let the interior of the support of φ be contained in the complement of M. Then,

$$\langle \hat{\omega}, \varphi \rangle = \left\langle \sum_{m\in\mathbb{Z}} e^{-2\pi i(x_1 v_1^{(m)} + x_2 v_2^{(m)} + mcx_3)} \mathrm{dens}^{(2)}(\Gamma)\, \delta^{(2)}_{R^m\Gamma^*}, \varphi \right\rangle = 0, \tag{7}$$

where $\hat{\omega}$ is already known to be a tempered distribution. Since the term $\delta^{(2)}_{R^m\Gamma^*}$ refers only to the two coordinates x_1, x_2, we conclude that the support of $\hat{\omega}$ is a subset of M, as is the support of $(\tilde{\omega}_r * \omega)\hat{}$, by (5). So, the support of $\hat{\gamma}$ is a subset of M. So far, we have established the following.

Theorem 2.1: *The diffraction spectrum of any SCD set* Λ_{SCD} *is a singular measure, and it is supported on the set*

$$M = \mathrm{cl}\left(\bigcup_{m\in\mathbb{Z}} R^m\Gamma^* \right) \times \mathbb{R}.$$

■

In the case of incommensurate SCD tilings, M is the union of all concentric cylinder surfaces S with central axis $\mathbb{R}\boldsymbol{e}_3$, where the radius of each S is $\|\boldsymbol{v}\|$ for some $\boldsymbol{v} \in \Gamma^*$. In the case of commensurate SCD tilings, M is a union of lines parallel to $\mathbb{R}\boldsymbol{e}_3$. In this case, as we will see later on in an example, the support of $\hat{\gamma}$ is a true subset of M.

Now, take a closer look at the diffraction spectrum along $\mathbb{R}\boldsymbol{e}_3$. From (7), we conclude

$$\hat{\omega} = \mathrm{dens}^{(2)}(\Gamma) \sum_{m\in\mathbb{Z}} e^{-2\pi i(x_1 v_1^{(m)} + x_2 v_2^{(m)} + mcx_3)}\, \delta^{(2)}_{R^m\Gamma^*}, \tag{8}$$

which might not be a measure in $\mathbb{R}^3$, but has a clear meaning as a tempered distribution. The coefficient of $\delta^{(2)}_0$ can be calculated by means of (6) as follows:

$$\sum_{m\in\mathbb{Z}} e^{-2\pi imcx_3} = \sum_{n\in c\mathbb{Z}} \widehat{\delta^{(1)}_n} = (\delta^{(1)}_{c\mathbb{Z}})\hat{} = \mathrm{dens}^{(1)}(c\mathbb{Z})\, \delta^{(1)}_{(c\mathbb{Z})^*} = c^{-1}\delta^{(1)}_{c^{-1}\mathbb{Z}}, \tag{9}$$

to be read as an equation for tempered distributions in $\mathcal{S}' = \mathcal{S}'(\mathbb{R})$.

On the other hand, since $\widetilde{\omega}_r$ is a finite measure with compact support, its Fourier transform is an analytic function and can be written as

$$\widehat{\widetilde{\omega}_r}(\boldsymbol{x}) = \sum_{\boldsymbol{y}\in\Lambda\cap C_r} e^{2\pi i(x_1y_1+x_2y_2+x_3y_3)}. \tag{10}$$

For $\boldsymbol{x}=(0,0,x_3)$, we thus get

$$\begin{aligned}\lim_{r\to\infty} r^{-3}\widehat{\widetilde{\omega}}_r\hat{\omega} &= \mathrm{dens}^{(2)}(\Gamma)\lim_{r\to\infty} r^{-3}\left(\sum_{\boldsymbol{y}\in\Lambda\cap C_r} e^{2\pi i x_3y_3}\right)\left(\sum_{n\in\mathbb{Z}} e^{-2\pi i n c x_3}\delta^{(2)}_{R^n\Gamma^*}\right)\\ &= \mathrm{dens}^{(2)}(\Gamma)\lim_{r\to\infty} r^{-3}\left(\sum_{m=-\lceil r/2\rceil}^{\lfloor r/2\rfloor} d_r^{(m)} r^2 e^{2\pi i m c y_3}\right)\left(\sum_{n\in\mathbb{Z}} e^{-2\pi i n c x_3}\delta^{(2)}_{R^n\Gamma^*}\right).\end{aligned}$$

Here, $d_r^{(m)}$ is chosen such that $d_r^{(m)}r^2$ counts the number of elements of $\Lambda\cap C_r$ in layer m. So, $d_r^{(m)}$ depends on $\mathrm{dens}^{(2)}(\Gamma)$, and $\lim_{r\to\infty} d_r^{(m)} = \mathrm{dens}^{(2)}(\Gamma)$ for all $m\in\mathbb{Z}$, uniformly in m.

Putting the pieces together, and restricting to the central axis, we obtain

$$\lim_{r\to\infty} r^{-3}\,\widehat{\widetilde{\omega}}_r\hat{\omega}|_{\mathbb{R}\boldsymbol{e}_3} = c^{-1}(\mathrm{dens}^{(2)}(\Gamma))^2\lim_{r\to\infty} r^{-1}\left(\sum_{m=-\lceil r/2\rceil}^{\lfloor r/2\rfloor} e^{-2\pi i m c x_3}\right)\delta^{(1)}_{c^{-1}\mathbb{Z}}.$$

This expression vanishes for $x_3\notin c^{-1}\mathbb{Z}$, while for $x_3\in c^{-1}\mathbb{Z}$ we get

$$c^{-1}(\mathrm{dens}^{(2)}(\Gamma))^2\lim_{r\to\infty} r^{-1}\sum_{m=-\lceil r/2\rceil}^{\lfloor r/2\rfloor} 1 = c^{-1}(\mathrm{dens}^{(2)}(\Gamma))^2 = \mathrm{dens}^{(2)}(\Gamma)\mathrm{dens}^{(3)}(\Lambda_{\mathrm{SCD}}).$$

In analogy to $\mathrm{dens}^{(2)}$, $\mathrm{dens}^{(3)}$ denotes three-dimensional density. It follows:

Theorem 2.2: *The diffraction spectrum $\hat{\gamma}$ of any SCD set Λ_{SCD}, restricted to $\mathbb{R}\boldsymbol{e}_3$, is pure point. In particular,*

$$\hat{\gamma}\big|_{\mathbb{R}\boldsymbol{e}_3} = \mathrm{dens}^{(2)}(\Gamma)\mathrm{dens}^{(3)}(\Lambda_{\mathrm{SCD}})\sum_{\boldsymbol{x}\in c^{-1}\mathbb{Z}\boldsymbol{e}_3}\delta_{\boldsymbol{x}}.$$

■

For special cases, this result already appears in Ref. 12. In the general case, it seems difficult to achieve results about the explicit behavior on the cylinder surfaces. If the SCD tiling has additionial properties, it is possible to show that all existing Bragg peaks are located on $\mathbb{R}\boldsymbol{e}_3$.

Definition 2.3: *A point set Λ in $\mathbb{R}^d$ is called* repetitive, *if for every $r>0$ some $R>0$ exists such that for all $\boldsymbol{x},\boldsymbol{y}\in\mathbb{R}^d$ a congruent copy of $(\boldsymbol{x}+C_r)\cap\Lambda$ occurs in every set $(\boldsymbol{y}+C_R)\cap\Lambda$.*

This definition has a natural extension to the repetitivity of tilings. For our purposes, it suffices to call an SCD tiling repetitive, if the corresponding SCD sets are repetitive. In particular, if $\mathcal{T}$ is repetitive, there are only finitely many ways how two tiles can touch each other. (Otherwise, there would be infinitely many different pairs of tiles, each fitting into a box C_r with $r=2\|\boldsymbol{a}+\boldsymbol{b}\|$. This infinitely many pairs, having all the same positive volume, must be contained in a finite ball of radius R, which is impossible.)

Proposition 2.4: If an SCD tiling $\mathcal{T}$ is repetitive, then $\varphi=\arccos(p/q)$, with $p,q\in\mathbb{Z}$.

Proof: Let $\mathcal{T}$ be repetitive. Then, the tiles of two consecutive layers L_i, L_{i-1} can touch each other in only finitely many ways. Let $L_i=T+\Gamma$, $L_{i-1}=R^{-1}(T+\Gamma)-R^{-1}\boldsymbol{c}$, and $\Gamma=\langle(1,0),(b_1,b_2)\rangle_{\mathbb{Z}}$. By the definition of T and $\mathcal{T}$, it follows that $b_1=\cos(\varphi)$, $b_2=\sin(\varphi)$ and that R^{-1} (recall that R is a rotation through the angle $-\varphi$) is given by

$$\begin{pmatrix} \cos(\varphi) & -\sin(\varphi) \\ \sin(\varphi) & \cos(\varphi) \end{pmatrix}.$$

So, $R^{-1}\Gamma = \langle (b_1,b_2), (b_1^2-b_2^2, 2b_1b_2)\rangle_{\mathbb{Z}}$. Obviously, $\langle (b_1,b_2)\rangle_{\mathbb{Z}} \subseteq \Gamma \cap R^{-1}\Gamma$. Since the tiles of L_i and L_{i-1} touch each other in finitely many ways, there are only finitely many possibilities how a point of Γ is positioned relative to its nearest point in $R^{-1}\Gamma$. Consequently, one has $(\Gamma \cap R^{-1}\Gamma)\backslash\langle (b_1,b_2)\rangle_{\mathbb{Z}} \neq \emptyset$. Therefore, the equation

$$\kappa(1,0) + \lambda(b_1,b_2) = \mu(b_1,b_2) + \nu(b_1^2 - b_2^2, 2b_1b_2) \tag{11}$$

has a solution, where $\kappa \neq 0 \neq \nu$. We must show that this is only possible if b_1 is a rational number p/q. Let b_1 be an irrational number. From $\lambda b_2 = \mu b_2 - \nu 2b_1b_2$ ($\lambda, \mu, \nu \in \mathbb{Z}$), one concludes $\nu = 0$ and $\lambda = \mu$. Therefore,

$$\kappa + \lambda b_1 = \mu b_1 + \nu(b_1^2 - b_2^2)$$

gives $\kappa = 0$, so there is no solution of (11) with $\kappa \neq 0 \neq \nu$. ■

Theorem 2.5: *Let Λ be an incommensurate SCD set. If $R^m\Lambda + m\boldsymbol{c} = \Lambda$ for some $m \geqslant 1$, or if Λ is repetitive and $\varphi = \arccos(p/q)$, where q is odd, then the diffraction spectrum of Λ is singular continuous on $M\backslash\mathbb{R}\boldsymbol{e}_3$.*

Lemma 2.6: Let R be an orthogonal map, μ a measure, and let the measure $R.\mu$ be given by $R.\mu(A) = \mu(R^{-1}A)$. Then

$$R.\widehat{\mu} = \widehat{R.\mu}.$$

Proof: Let $\varphi \in \mathcal{S}(\mathbb{R}^3)$. It is clear that $\langle R.\mu, \varphi\rangle = \langle \mu, \varphi \circ R\rangle$. Since

$$\widehat{\varphi \circ R}(\boldsymbol{x}) = \int \varphi(R\boldsymbol{y}) e^{-2\pi i \boldsymbol{x}\boldsymbol{y}}\, \mathrm{d}\boldsymbol{y} = \int \varphi(\tilde{\boldsymbol{y}}) e^{-2\pi i \boldsymbol{x}(R^{-1}\tilde{\boldsymbol{y}})} \mathrm{d}\tilde{\boldsymbol{y}} = \int \varphi(\tilde{\boldsymbol{y}}) e^{-2\pi i (R\boldsymbol{x})\tilde{\boldsymbol{y}}} \mathrm{d}\tilde{\boldsymbol{y}} = \hat{\varphi}(R\boldsymbol{x}),$$

where $\tilde{\boldsymbol{y}} = R\boldsymbol{y}$, it follows that $\widehat{\varphi \circ R} = \hat{\varphi} \circ R$. Thus

$$\langle \widehat{R.\mu}, \varphi\rangle = \langle R.\mu, \hat{\varphi}\rangle = \langle \mu, \hat{\varphi} \circ R\rangle = \langle \mu, \widehat{\varphi \circ R}\rangle = \langle \hat{\mu}, \varphi \circ R\rangle = \langle R.\hat{\mu}, \varphi\rangle$$

which proves the claim. ■

Proof of Theorem 2.5: Let $R^m\Lambda + m\boldsymbol{c} = \Lambda$. The support of the autocorrelation γ is the closure of the set $\Lambda - \Lambda = \{\boldsymbol{x} - \boldsymbol{y} \,|\, \boldsymbol{x}, \boldsymbol{y} \in \Lambda\}$. Since

$$R^m(\Lambda - \Lambda) = R^m\Lambda + m\boldsymbol{c} - (R^m\Lambda + m\boldsymbol{c}) = \Lambda - \Lambda,$$

we get $\gamma = R^m.\gamma$. Lemma 2.6 implies $\hat{\gamma} = \widehat{R^m.\gamma} = R^m.\hat{\gamma}$, and therefore $\hat{\gamma} = R^{km}.\hat{\gamma}$ for all $k \in \mathbb{Z}$.

Now, let Λ be repetitive and $\varphi = \arccos(p/q)$, where q is odd. Like Λ itself, the set $\Lambda - \Lambda$ consists of equidistant layers. If $\Lambda = \cup_{k\in\mathbb{Z}} R^k\Gamma + \boldsymbol{v}_k + k\boldsymbol{c}_0$ [where $\boldsymbol{c}_0 = (0,0,c)$], then

$$\Lambda - \Lambda = \bigcup_{i\in\mathbb{Z}} \bigcup_{k\in\mathbb{Z}} R^{k+i}\Gamma + \boldsymbol{v}_{k+i} + (k+i)\boldsymbol{c}_0 - (R^k\Gamma + \boldsymbol{v}_k + k\boldsymbol{c}_0).$$

Now, we use a fact from Ref. 7: If $\mathcal{T}$ is a repetitive SCD tiling, and if $\varphi = \arccos(p/q)$ with q odd, then the union of i consecutive layers in $\mathcal{T}$ is congruent to any other such union of i consecutive layers in $\mathcal{T}$. Therefore, all difference sets $R^{k+i}\Gamma + \boldsymbol{v}_{k+i} + (k+i)\boldsymbol{c}_0 - (R^k\Gamma + \boldsymbol{v}_k + k\boldsymbol{c}_0)$ are congruent. This means $\boldsymbol{v}_{k+i} - \boldsymbol{v}_k = R^k(\boldsymbol{v}_i - \boldsymbol{v}_0)$. Since $R\boldsymbol{c}_0 = \boldsymbol{c}_0$, it follows:

$$R(\Lambda-\Lambda)=R\Bigg(\bigcup_{i\in\mathbb{Z}}\bigcup_{k\in\mathbb{Z}}R^k(R^i\Gamma-\Gamma+\boldsymbol{v}_i-\boldsymbol{v}_0)+i\boldsymbol{c}_0\Bigg)$$
$$=R\Bigg(\bigcup_{k\in\mathbb{Z}}R^k\Bigg(\bigcup_{i\in\mathbb{Z}}R^i\Gamma-\Gamma+\boldsymbol{v}_i-\boldsymbol{v}_0+i\boldsymbol{c}_0\Bigg)\Bigg)=\Lambda-\Lambda.$$

Therefore, one has $\hat{\gamma}=R^k.\hat{\gamma}$ for all $k\in\mathbb{Z}$.

In both cases, the following argument applies: If there is a Bragg peak $I(\boldsymbol{x})\delta_{\boldsymbol{x}}$ at $\boldsymbol{x}\in M\backslash\mathbb{R}\boldsymbol{e}_3$ with intensity $I(\boldsymbol{x})>0$, then there are infinitely many Bragg peaks $I(\boldsymbol{x})\delta_{R^{km}\boldsymbol{x}}$, with $k\in\mathbb{Z}$, on a circle of diameter $\|\boldsymbol{x}\|$. But since $\hat{\gamma}$ is a tempered distribution, it is bounded on every compact set $K\subset\mathbb{R}^3$. This is a contradiction. Therefore, no Bragg peaks occur in $M\backslash\mathbb{R}\boldsymbol{e}_3$. The claim now follows from Theorem 2.1. ■

In contrast to this situation, let us ask what happens for a fully periodic SCD tiling. This is only possible if it is a commensurate SCD tiling (which means that R is of finite order), and if the sequence $(v_1^{(m)},v_2^{(m)})$ is periodic (to be precise, periodic mod $R^m\boldsymbol{a}$). Equivalently, there is a $k\geqslant 1$, such that $R^k=\mathrm{id}$ and $v_1^{(m+k)}\equiv v_1^{(m)}, v_2^{(m+k)}\equiv v_2^{(m)} \bmod R^m\boldsymbol{a}$ for all $m\in\mathbb{Z}$. In this case, (8) gives

$$\hat{\omega}=\mathrm{dens}^{(2)}(\Gamma)\sum_{n\in k\mathbb{Z}}\sum_{j=0}^{k-1}e^{-2\pi i(x_1v_1^{(j)}+x_2v_2^{(j)}+(n+j)cx_3)}\delta^{(2)}_{R^{n+j}\Gamma^*}$$
$$=\mathrm{dens}^{(2)}(\Gamma)\sum_{j=0}^{k-1}e^{-2\pi i(x_1v_1^{(j)}+x_2v_2^{(j)}+jcx_3)}\Bigg(\sum_{n\in ck\mathbb{Z}}e^{-2\pi inx_3}\Bigg)\delta^{(2)}_{R^j\Gamma^*}$$
$$=\mathrm{dens}^{(2)}(\Gamma)\sum_{j=0}^{k-1}e^{-2\pi i(x_1v_1^{(j)}+x_2v_2^{(j)}+jcx_3)}(ck)^{-1}(\delta^{(2)}_{R^j\Gamma^*}\otimes\delta^{(1)}_{(ck)^{-1}\mathbb{Z}}).$$

This term vanishes everywhere except on $(\cup_{j=1}^{k}R^j\Gamma^*)\times(ck)^{-1}\mathbb{Z}$. So, the diffraction spectrum of a fully periodic SCD tiling is, as expected, supported on a uniformly discrete point set. It is, in fact, a pure point diffraction spectrum, consisting of isolated Bragg peaks. The support is indeed *uniformly* discrete, since from the periodicity of the tiling the repetitivity follows, wherefore Proposition 2.4 yields $\varphi=\arccos(p/q)$ $(p,q\in\mathbb{Z})$. Since the tiling is commensurate, (p,q) can take the values (0,1) or (1,2) only.

III. FURTHER REMARKS

(1) One special case which occurs is the body-centered-cubic lattice (bcc) as the underlying point set of an SCD tiling. It is the dual of the root lattice D_3, compare Ref. 5,

$$\mathrm{bcc}=D_3^*=\langle(1,0,0),(0,1,0),(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})\rangle_{\mathbb{Z}}.$$

This is achieved by placing the reference point $\boldsymbol{z}$ in the center $\frac{1}{2}(\boldsymbol{a}+\boldsymbol{b})$ of the SCD tile, and choosing (cf. Sec. I),

$$\boldsymbol{a}=(1,0,0),\quad \boldsymbol{b}=(0,1,0),\quad \boldsymbol{c}=(0,\tfrac{1}{2},\tfrac{1}{2}),\quad \boldsymbol{d}=(\tfrac{1}{2},0,-\tfrac{1}{2}),\quad v_1^{(m)}=v_2^{(m)}=\begin{cases}0, & m\text{ even},\\ \frac{1}{2}, & m\text{ odd}.\end{cases}$$

Using (8) and (10), one finds for this case

$$\widehat{\gamma_{\mathrm{bcc}}}=\lim_{r\to\infty}r^{-3}\Bigg(\sum_{\boldsymbol{y}\in\mathrm{bcc}\cap C_r}e^{2\pi i\boldsymbol{x}\boldsymbol{y}}\Bigg)\Bigg(\sum_{m\in\mathbb{Z}}e^{-2\pi i(x_1v_1^{(m)}+x_2v_2^{(m)}+x_3m/2)}\Bigg)\mathrm{dens}^{(2)}(\mathbb{Z}^2)\delta^{(2)}_{\mathbb{Z}^2}.$$

This measure vanishes on $\{\boldsymbol{x}\,|\,(x_1,x_2)\notin\mathbb{Z}^2\}$. For $(x_1,x_2)\in\mathbb{Z}^2$, one finds

$$\lim_{r\to\infty} r^{-3}\left(\sum_{n=-\lfloor r\rfloor}^{\lfloor r\rfloor} r^2 e^{2\pi i x_3 n/2}\right)\left(\sum_{m\in 2\mathbb{Z}+1} e^{-\pi i(x_1+x_2+x_3 m)} + \sum_{m\in 2\mathbb{Z}} e^{-2\pi i x_3 m/2}\right)$$
$$= \lim_{r\to\infty} r^{-1}\left(\sum_{n=-\lfloor r\rfloor}^{\lfloor r\rfloor} e^{2\pi i x_3 n/2}\right)(1+e^{-\pi i(x_1+x_2+x_3)})\sum_{m\in\mathbb{Z}} e^{-2\pi i x_3 m}.$$

From (9), one gets $\Sigma_{m\in\mathbb{Z}} e^{-2\pi i x_3 m} = \delta^{(1)}_{\mathbb{Z}}$. So, this term vanishes for $x_3 \notin \mathbb{Z}$, and for $x_3 \in \mathbb{Z}$ we have to examine the factor $1+e^{-\pi i(x_1+x_2+x_3)}$. It equals 2 (respectively, 0) if $x_1+x_2+x_3$ is even (respectively, odd). In the even case, the first sum does not converge, so the limit is not zero. Altogether, the diffraction spectrum of bcc consists of Bragg peaks on points in

$$D_3 = \{\, \boldsymbol{x} \mid x_1 + x_2 + x_3 \equiv 0 \bmod 2\}.$$

In this way, we retrieve the well-known result that the diffraction image of the bcc is pure point, with Bragg peaks on the points of the dual lattice $(D_3^*)^* = D_3 = 2$ fcc.

In a similar way, one finds further structures that are well known from crystallography or discrete geometry, such as the root lattices $\mathbb{Z}^3$ and D_3 [which is a scaled version of the face-centered-cubic lattice (fcc)], or the hexagonal close packing (compare Ref. 5).

(2) The description of the SCD tile in Sec. I follows the idea of Conway, see Ref. 7. The prototile found by Schmitt is not convex, but showed itself the valleys and ridges, which occur on the layers of our tilings (and his tilings have essentially the same structure as ours). Anyway, both tiles lead to the same SCD sets, and both tiles are examples of aperiodic prototiles. But the latter is only true if we forbid tilings which contain both our SCD tile and its mirror image. For example, let T be as in (1) and T' the mirror image of T under reflection in the plane spanned by $\boldsymbol{a}$ and $\boldsymbol{b}$. The layer $L = T + \Gamma$ contains only translations of T, the layer $L' = T' + \boldsymbol{c} + \Gamma$ contains only translations of T'. The tiling

$$\mathcal{T} = \bigcup_{m\in 2\mathbb{Z}} (0,0,mc) + (L \cup L')$$

is invariant under the translations $t(\boldsymbol{x}) = \boldsymbol{x} + (0,0,2c)$ and $u(\boldsymbol{x}) = \boldsymbol{x} + \boldsymbol{b}$, hence not aperiodic.

In our description, the angle φ can take any value in $]0, \pi/2[$. The SCD tile described by Danzer (Ref. 7) uses $\varphi = \arccos(p/q)$, where p, q are positive integers, $p < q, q \geqslant 3$ (leading to incommensurate SCD tilings). In this case, it is possible to *enforce* SCD tilings which are repetitive. Then, in particular, two tiles can touch each other only in finitely many different ways. (This is clearly not true for all SCD tilings considered in this paper.) Using this, one can modify the shape of the prototile in such a way that the occurrence of mirror images of the prototile is ruled out. This can be done, e.g., by adding protrusions and indentations to the tiles, fitting together like key and keyhole, but only if the tiles are directly congruent. So, in this case, one has indeed a single prototile—no longer convex—permitting only aperiodic tilings, just by its shape.

Anyway, even in the last setting, there may occur other symmetries, namely screw motions. Obviously, the tiling $\mathcal{T}$ in (2) is invariant under the map $s(\boldsymbol{x}) = R\boldsymbol{x} + (0,0,c)$. More generally, if we choose an arbitrary SCD tile as discussed here, then in the set of all tilings built from this tile we will always find tilings invariant under the maps s^k $(k \in \mathbb{Z})$. Thus the symmetry group of such tilings is infinite. In less than three dimensions, aperiodicity is equivalent to finiteness of the symmetry group. The SCD tilings show that this is not true in general. Therefore, it makes sense to rephrase the question "Is there an aperiodic prototile?" as "Is there a prototile that permits only tilings with finite symmetry group?," shortly, "Is there a *strongly aperiodic* prototile?" (cf. Ref. 11). To our knowledge, no answer to this question is known so far.

(3) To some extent, the underlying mechanism of SCD tilings does occur in nature. The structure of smectic C^* liquid crystals resembles the layer structure: planar, two-periodic "sheets" of tilted molecules (called directors) are stacked with a screw order on top of each other.[8] This happens in such a way that the (effective) period in direction $\mathbb{R}\boldsymbol{e}_3$ is on a much greater length scale than the elementary periods within the layers.

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A geometric approach to scalar field theories on the supersphere

A. F. Schunck[a] and Chris Wainwright[b]
Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, United Kingdom

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Following a strictly geometric approach we construct globally supersymmetric scalar field theories on the supersphere, defined as the quotient space $S^{2|2}=\mathrm{UOSp}(1|2)/\mathcal{U}(1)$. We analyze the superspace geometry of the supersphere, in particular deriving the invariant vielbein and spin connection from a generalization of the left-invariant Maurer–Cartan form for Lie groups. Using this information we proceed to construct a superscalar field action on $S^{2|2}$, which can be decomposed in terms of the component fields, yielding a supersymmetric action on the ordinary two-sphere. We are able to derive Lagrange equations and Noether's theorem for the superscalar field itself. © *2005 American Institute of Physics.*
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I. INTRODUCTION

While superspheres have been extensively studied as target spaces for supersymmetric sigma models, see, e.g., Refs. 1 and 2, little attention has been paid to considering the supersphere as the base space for supersymmetric field theories. However, treating the supersphere as such provides us with an interesting model for studying globally supersymmetric field theories in curved space.

In this paper we present a strictly geometric approach to constructing globally supersymmetric scalar field theories on the supersphere, defined here as the coset space $\mathrm{UOSp}(1|2)/\mathcal{U}(1)$,[3,4] the body of which is given by the ordinary two-sphere. We should emphasize here that there is an ambiguity in defining a supersphere, i.e., a supersymmetric generalization of the ordinary two-sphere, the only criterion being that the body of the respective supermanifold coincides with S^2. Another example of a supersymmetric generalization of S^2 would be the quotient space $\mathrm{SU}(2|1)/\mathrm{U}(1|1)$, as considered in, e.g., Ref. 5. If one insists, however, on the additional condition that the resultant coset space is not just a supermanifold but rather a *superspace*, this excludes, for example, the latter possibility and leaves as one obvious choice precisely the coset space $\mathrm{UOSp}(1|2)/\mathcal{U}(1)$.

While it is not important to insist on this additional condition for the purpose of using the supermanifold as the target space for some supersymmetric sigma model, it is crucial to enforce it if one wants to construct a field theory on the supermanifold as the background. This is because the superspace condition ensures first that the tangent space group of the supermanifold under consideration corresponds to the even Grassmann extension of the tangent space group of the body of the respective coset space and second that the fermionic field content of the theory will transform as *spinor* fields under the action of the tangent space group (see Secs. III E and V B).

Note, however, that taking the coset space $\mathrm{UOSp}(1|2)/\mathcal{U}(1)$ as the supersymmetric generalization of the ordinary sphere involves inevitably the usage of a rather unfamiliar extension of complex conjugation to supernumbers, referred to as pseudoconjugation,[6] see Sec. II A, together with the definition of a graded adjoint, see Sec. II B.

[a]Electronic mail: a.f.schunck@damtp.cam.ac.uk
[b]Electronic mail: c.j.wainwright@damtp.cam.ac.uk

We shall emphasize one other important point about our approach to constructing scalar field theories on $S^{2|2}$. While it is possible to construct supersymmetric theories on certain curved backgrounds using component fields from the outset, as in, e.g., Ref. 7 for the case of AdS_2, we instead rigorously pursue a superspace approach; analyzing the superspace geometry of the supersphere we construct in particular the invariant vielbein and spin connection, using a supergeneralization of the left-invariant Maurer–Cartan form for ordinary Lie groups (see Sec. V). Having this information at hand we proceed to construct a *superscalar* field theory on $S^{2|2}$, which only when written in terms of the component fields of the superscalar field under consideration, and after integrating out the odd coordinates, becomes a field theory on the ordinary sphere. Having derived the component field version of the superfield action in Sec. VII, we will be able to briefly discuss supersymmetry breaking in Sec. VIII. Notably, the superspace approach also makes it possible to derive Lagrange equations as well as Noether's theorem for the superscalar field itself, see Sec. IX.

II. THE UNITARY ORTHOSYMPLECTIC GROUP

A. Pseudoconjugation

We expand an arbitrary (complex) supernumber z in terms of the generators of a Grassmann algebra ζ_i, $i=1,\ldots,N$, as

$$z = z_0 + z_i\zeta_i + z_{ij}\zeta_i\zeta_j + z_{ijk}\zeta_i\zeta_j\zeta_k + \cdots . \tag{1}$$

We use a subscript 0 to denote the *body* of the supernumber, the remaining terms are called the *soul*. A supernumber is said to be *even* if the above expansion does not contain terms with an odd number of generators. The set of even supernumbers will be denoted by $\mathbb{C}_c$. A supernumber is said to be *odd* if it contains only terms with an odd number of generators. The odd supernumbers will be denoted by $\mathbb{C}_a$. The set of all supernumbers will be denoted by $\mathbb{C}_N$. We will normally, however, consider the formal limit $N\to\infty$ and denote the supernumbers by $\mathbb{C}_\infty$. Note also that $\mathbb{C}_0\cong\mathbb{C}$ is precisely the set of ordinary complex numbers.

The standard extension of ordinary complex conjugation to supernumbers is given in Ref. 8. It is defined as a map

$$*: \begin{cases} \mathbb{C}_c \to \mathbb{C}_c, \\ \mathbb{C}_a \to \mathbb{C}_a, \end{cases}$$

which agrees with complex conjugation on ordinary numbers and satisfies the following properties:

$$(a+b)^* = a^* + b^*,$$

$$(ab)^* = b^*a^*,$$

$$a^{**} = a,$$

for arbitrary supernumbers a and b. Note that when taking the conjugate of a product the order is reversed. The Grassmann generators can be taken to be real with respect to this conjugation, i.e., $\zeta_i^* = \zeta_i$, and the expansion of z^* is given by

$$z^* = z_0^* + z_i^*\zeta_i - z_{ij}^*\zeta_i\zeta_j - z_{ijk}^*\zeta_i\zeta_j\zeta_k + \cdots .$$

Note that the minus signs are due to the reordering of the Grassmann generators.

It is possible to define another extension of complex conjugation to supernumbers, called *pseudoconjugation*.[6] Pseudoconjugation is defined as a map

$$\diamondsuit: \begin{cases} \mathbb{C}_c \to \mathbb{C}_c, \\ \mathbb{C}_a \to \mathbb{C}_a, \end{cases} \tag{2}$$

which agrees with complex conjugation on ordinary numbers and satisfies the following properties:

$$(a+b)^{\diamond} = a^{\diamond} + b^{\diamond}, \tag{3a}$$

$$(ab)^{\diamond} = a^{\diamond} b^{\diamond}, \tag{3b}$$

$$a^{\diamond\diamond} = (-1)^{\epsilon_a} a, \tag{3c}$$

for arbitrary supernumbers a and b, where $\epsilon_a = 0$ if $a \in \mathbb{C}_c$ and $\epsilon_a = 1$ if $a \in \mathbb{C}_a$. Note that the pseudoconjugate does *not* switch the order when applied to a product. A consequence of this definition is that the generators of the Grassmann algebra can no longer be described as real with respect to pseudoconjugation in the same way as for standard conjugation. To see this note that if we had $\zeta_i^{\diamond} = \zeta_i$ this would imply that $\zeta_i^{\diamond\diamond} = \zeta_i$ which contradicts Eq. (3c). In fact, a definition of how the pseudoconjugate acts on the Grassmann generators which is consistent with Eqs. (2), (3a)–(3c) is not always possible. If however N is even, or indeed infinite, we can proceed as follows. Let W be the N-dimensional vector space of Grassmann generators. Pick a semilinear map[9] $f: W \to W$ such that $f^2 = -1$, for example, the matrix

$$J = \begin{pmatrix} 0 & \mathbb{1}_{N/2} \\ -\mathbb{1}_{N/2} & 0 \end{pmatrix},$$

and then define $\zeta_i^{\diamond} = f(\zeta_i)$. Using this definition of the pseudoconjugate on the Grassmann generators it is possible to write down the expansion for an arbitrary supernumber as

$$z^{\diamond} = z_0^* + z_i^* \zeta_i^{\diamond} + z_{ij}^* \zeta_i^{\diamond} \zeta_j^{\diamond} + z_{ijk}^* \zeta_i^{\diamond} \zeta_j^{\diamond} \zeta_k^{\diamond} + \cdots .$$

B. Graded adjoint

Using ordinary complex conjugation of supernumbers it is possible to define an adjoint operation on *pure supermatrices*. A pure, i.e., *even* or *odd*, $(p|q)$-dimensional supermatrix is written in block form as

$$X = \begin{pmatrix} A & B \\ C & D \end{pmatrix}. \tag{4}$$

The matrix is said to be even if $A \in \mathrm{Mat}_{p\times p}(\mathbb{C}_c)$, $B \in \mathrm{Mat}_{p\times q}(\mathbb{C}_a)$, $C \in \mathrm{Mat}_{q\times p}(\mathbb{C}_a)$, and $D \in \mathrm{Mat}_{q\times q}(\mathbb{C}_c)$. The matrix is called odd if $A \in \mathrm{Mat}_{p\times p}(\mathbb{C}_a)$, $B \in \mathrm{Mat}_{p\times q}(\mathbb{C}_c)$, $C \in \mathrm{Mat}_{q\times p}(\mathbb{C}_c)$, and $D \in \mathrm{Mat}_{q\times q}(\mathbb{C}_a)$. Here $\mathrm{Mat}_{m\times n}(\mathbb{F})$ are $m \times n$ matrices over $\mathbb{F}$.

The standard adjoint operation is defined, as usual, by the conjugate transpose

$$X^{\dagger} = X^{*t}, \tag{5}$$

or in block form

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{\dagger} = \begin{pmatrix} A^{*t} & C^{*t} \\ B^{*t} & D^{*t} \end{pmatrix}.$$

This satisfies the usual properties of an adjoint

$$(XY)^{\dagger} = Y^{\dagger} X^{\dagger},$$

$$X^{\dagger\dagger} = X.$$

It is also possible to use the pseudoconjugate to construct a *graded adjoint*.[6] Note, however, that one cannot construct an adjoint operation which has sensible properties using the pseudoconjugate combined with the ordinary transpose, but rather one must use the *supertranspose*. The supertranspose of a pure $(p|q)$-dimensional supermatrix is defined by

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{st} = \begin{pmatrix} A^t & (-1)^{\epsilon_X} C^t \\ -(-1)^{\epsilon_X} B^t & D^t \end{pmatrix}, \tag{6}$$

where $\epsilon_X = 0$ for even supermatrices, and $\epsilon_X = 1$ for odd supermatrices. Note that with this definition of the supertranspose we have that in general $(X^{st})^{st} \neq X$, see Ref. 6. The graded adjoint is then defined as

$$X^{\ddagger} = X^{\diamond\, st}, \tag{7}$$

and this satisfies a graded version of the properties of the standard adjoint

$$(XY)^{\ddagger} = (-1)^{\epsilon_X \epsilon_Y} Y^{\ddagger} X^{\ddagger},$$

$$X^{\ddagger\ddagger} = (-1)^{\epsilon_X} X.$$

We may also extend the definition of the graded adjoint to *supervectors* in a manner consistent with the definition for supermatrices. We write a pure, i.e., even or odd, $(p|q)$-dimensional supervector as

$$V = \begin{pmatrix} u \\ w \end{pmatrix}.$$

The supervector is said to be even, i.e., $\epsilon_V = 0$, if $u \in \mathrm{Mat}_{p\times 1}(\mathbb{C}_c)$ and $w \in \mathrm{Mat}_{q\times 1}(\mathbb{C}_a)$. It is called odd, i.e., $\epsilon_V = 1$, if $u \in \mathrm{Mat}_{p\times 1}(\mathbb{C}_a)$ and $w \in \mathrm{Mat}_{q\times 1}(\mathbb{C}_c)$. We define the supertranspose of V to be

$$V^{st} = (u^t,\ (-1)^{\epsilon_V} w^t)$$

and the graded adjoint is then defined by

$$V^{\ddagger} = V^{\diamond\, st}.$$

C. Compact form of OSp($n|2m$)

Using the graded adjoint one can define a compact (i.e., unitary) form of the orthosymplectic supergroup $\mathrm{OSp}(n|2m)$ which is not possible with the ordinary adjoint.

The orthosymplectic supergroup is defined by[6]

$$\mathrm{OSp}(n|2m) = \{s \in \mathrm{PL}(n|2m) : s^{st} g s = g\}, \tag{8}$$

where $\mathrm{PL}(n|2m)$ are the invertible even supermatrices of dimension $(n|2m)$ and

$$g = \begin{pmatrix} \mathbb{1}_n & 0 \\ 0 & J_{2m} \end{pmatrix}, \quad J_{2m} = \begin{pmatrix} 0 & \mathbb{1}_m \\ -\mathbb{1}_m & 0 \end{pmatrix}.$$

The algebra is given by

$$\mathrm{osp}(n|2m) = \{X \in \mathrm{pl}(n|2m) : X^{st} g + g X = 0\}, \tag{9}$$

where $\mathrm{pl}(n|2m)$ is the algebra of $\mathrm{PL}(n|2m)$. If we write X in block form, as in Eq. (4), then for X to be in the algebra it must satisfy

$$A^t + A = 0, \tag{10a}$$

$$B + C^t J = 0, \tag{10b}$$

$$D^t J + JD = 0. \tag{10c}$$

From Eqs. (10a) and (10c) we see that the body of the algebra is

$$\mathrm{osp}(n|2m)_0 = o(n) \times \mathrm{sp}(2m).$$

To find a compact form of an algebra we must first complexify it and then impose a consistent anti-Hermitian condition, which yields a unitary group. For the orthosymplectic algebra the standard adjoint of Eq. (5) does not give a consistent anti-Hermitian condition. To see this, note that imposing $X^\dagger = -X$, we find $B^{*t} = -C$ and $C^{*t} = -B$. From Eq. (10b) we have

$$0 = (B + C^t J)^* J = -C^t J + B$$

which together with Eq. (10b) would imply $B = C = 0$. This problem is avoided by using the graded adjoint. Imposing $X^\ddagger = -X$ we have $B^{\diamond t} = C$ and $C^{\diamond t} = -B$. The previous argument now gives

$$0 = (B + C^t J)^{\diamond} J = C^t J + B$$

and hence no inconsistency.

The *unitary* orthosymplectic algebra can now be defined as

$$\mathrm{uosp}(n|2m) = \{X \in \mathrm{osp}(n|2m) \otimes \mathbb{C}_c : X^\ddagger = -X\}, \tag{11}$$

and the group as

$$\mathrm{UOSp}(n|2m) = \{s \in \mathrm{OSp}(n|2m) \otimes \mathbb{C}_c : s^\ddagger = s^{-1}, \mathrm{sdet}(s) = 1\}, \tag{12}$$

where the *superdeterminant* is defined by

$$\mathrm{sdet}\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A - BD^{-1}C)\det(D)^{-1}. \tag{13}$$

Note that in the definition of $\mathrm{UOSp}(n|2m)$ we have imposed the condition $\mathrm{sdet}(s) = 1$, hence strictly speaking we are dealing with the *special* unitary orthosymplectic group, we shall not however refer to it as such.

D. UOSp(1|2)

We will be interested in the particular case of UOSp(1|2). The algebra has three even generators J_i, $i = 0, 1, 2$ and two odd generators Q_α, $\alpha = -, +$, which can be represented as supermatrices

$$J_i = \frac{i}{2}\left(\begin{array}{c|cc} 0 & 0 & 0 \\ \hline 0 & & \\ & & \sigma_i \\ 0 & & \end{array}\right), \quad Q_- = \frac{1}{2}\left(\begin{array}{c|cc} 0 & 0 & 1 \\ \hline 1 & 0 & 0 \\ 0 & 0 & 0 \end{array}\right), \quad Q_+ = \frac{1}{2}\left(\begin{array}{c|cc} 0 & -1 & 0 \\ \hline 0 & 0 & 0 \\ 1 & 0 & 0 \end{array}\right), \tag{14}$$

where $(\sigma_i)^\alpha{}_\beta$ are the standard Pauli matrices. The generators of the algebra satisfy the following commutation and anticommutation relations,

$$[J_i, J_j] = -\epsilon_{ij}{}^k J_k, \tag{15a}$$

$$[J_i, Q_\alpha] = \frac{i}{2}(\sigma_i)_\alpha{}^\beta Q_\beta, \tag{15b}$$

$$[Q_\alpha, Q_\beta] = \frac{i}{2}(\sigma^i)_{\alpha\beta} J_i, \tag{15c}$$

where ϵ_{ijk} is completely antisymmetric with $\epsilon_{012}=1$. The indices $i,j,\ldots$ have been raised and lowered using $\delta^{ij}=\delta_{ij}=\delta^i_j$, whereas $\alpha,\beta,\ldots$ have been raised and lowered using the antisymmetric symbols $\epsilon^{\alpha\beta}$ and $\epsilon_{\alpha\beta}$, with $\epsilon^{-+}=\epsilon_{-+}=1$. The raising and lowering conventions, along with their application to the Pauli matrices, are discussed more in Appendix A. The bracket [,] shall denote the anticommutator whenever both entries are odd, as, e.g., in Eq. (15c). In any other case [,] is to be understood as the commutator.

The Casimir operator C of uosp(1|2) is given by

$$C = J^i J_i - \epsilon^{\alpha\beta} Q_\alpha Q_\beta.$$

A general element of the algebra can be expanded as $X=\theta^i J_i + \eta^\alpha Q_\alpha$, where $\theta^i \in \mathbb{R}_c$ and $\eta^- = \eta^\diamond$, $\eta^+ = \eta$, with $\eta \in \mathbb{C}_a$. We find that X is anti-Hermitian as the generators satisfy the following Hermiticity properties:

$$J_i^\ddagger = -J_i,$$

$$(Q_\alpha)^\ddagger = \epsilon^{\alpha\beta} Q_\beta.$$

Note that if we naively multiplied the generators by a supernumber we would not obtain an anti-Hermitian element X. The correct definition of left and right multiplication is[10]

$$z\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} zA & zB \\ (-1)^{\epsilon_z} zC & (-1)^{\epsilon_z} zD \end{pmatrix},$$

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} z = \begin{pmatrix} Az & (-1)^{\epsilon_z} Bz \\ Cz & (-1)^{\epsilon_z} Dz \end{pmatrix}.$$

The general element of the group UOSp(1|2) can be represented by a supermatrix

$$s(a,b,\eta) = \begin{pmatrix} 1+\frac{1}{4}\eta\eta^\diamond & -\frac{1}{2}\eta & \frac{1}{2}\eta^\diamond \\ -\frac{1}{2}\eta^\diamond & 1-\frac{1}{8}\eta\eta^\diamond & 0 \\ -\frac{1}{2}\eta & 0 & 1-\frac{1}{8}\eta\eta^\diamond \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & a & -b^\diamond \\ 0 & b & a^\diamond \end{pmatrix} \tag{16a}$$

$$= \begin{pmatrix} 1+\frac{1}{4}\eta\eta^\diamond & -\frac{1}{2}(\eta a - \eta^\diamond b) & \frac{1}{2}(\eta b^\diamond + \eta^\diamond a^\diamond) \\ -\frac{1}{2}\eta^\diamond & \left(1-\frac{1}{8}\eta\eta^\diamond\right)a & -\left(1-\frac{1}{8}\eta\eta^\diamond\right)b^\diamond \\ -\frac{1}{2}\eta & \left(1-\frac{1}{8}\eta\eta^\diamond\right)b & \left(1-\frac{1}{8}\eta\eta^\diamond\right)a^\diamond \end{pmatrix}, \tag{16b}$$

where the parameters $a,b \in \mathbb{C}_c$ are constrained by $\mathrm{sdet}(s) = aa^\diamond + bb^\diamond = 1$, and $\eta \in \mathbb{C}_a$ is unconstrained. Note that the first matrix on the right-hand side of Eq. (16a) is just $\exp(\eta^\alpha Q_\alpha)$. The second matrix is of the form $\exp(\theta^i J_i)$, for some $\theta^i \in \mathbb{R}_c$ determining the constrained parameters a and b. From this we see that the body of uosp(1|2) is simply $\mathrm{uosp}(1|2)_0 = \mathrm{su}(2)$ which will be important in the next section.

III. CONSTRUCTING THE SUPERSPHERE

A. General coset spaces

We shall briefly review the general formalism for constructing spaces as coset spaces, covered in, for example, Ref. 11.

Consider a group G with a subgroup H. We define an equivalence relation on G by

$$g_1 \sim g_2 \Leftrightarrow g_2^{-1} g_1 \in H.$$

Each element $g \in G$ lies in an equivalence class

$$gH \equiv \{gh\colon\ h \in H\}.$$

The set of all equivalence classes is the (right-)coset space G/H, written as

$$G/H \equiv \{gH\colon\ g \in G\}.$$

We can define a projection map $\pi\colon\ G \to G/H$ by sending an element $g \in G$ to its equivalence class $gH \in G/H$. Also, for each point in the coset space we may choose a particular element of G which projects down to this point under π, this group element is called a *coset representative*.

The left action of G on itself descends to an action of G on the coset space

$$g'\colon\ G/H \to G/H$$

$$:gH \mapsto g'gH.$$

This is well defined as it is clearly independent of the coset representative chosen.

In Sec. V we will introduce a vielbein and spin connection on G/H which are invariant under this left action, and as such we will think of G as the isometry group of the coset space.

B. The sphere as a coset space

We first review how the ordinary sphere can be constructed as the coset space $S^2 = \mathrm{SU}(2)/\mathrm{U}(1)$. This construction is then straightforward to generalize to the case of the supersphere.

The group SU(2) has the 2×2 matrix representation

$$s(a,b) = \begin{pmatrix} a & -b^* \\ b & a^* \end{pmatrix},$$

where the parameters $a, b \in \mathbb{C}_0$ are just ordinary complex numbers which are constrained by $aa^* + bb^* = 1$. The matrices $s(w,0)$, with $ww^* = 1$, form a U(1) subgroup. We define an equivalence relation on SU(2) by multiplication on the right with an element of this U(1) subgroup,

$$s(a,b) \sim s(a',b') = s(a,b)s(w,0).$$

This equivalence relation defines the coset space SU(2)/U(1). The projection map for this coset space is the standard *Hopf map*, it can be written as

$$\pi\colon\ \mathrm{SU}(2) \to \mathrm{SU}(2)/\mathrm{U}(1)$$

$$:s(a,b) \mapsto s(a,b)\hat{J}_0 s(a,b)^\dagger,$$

where $\hat{J}_0 = (i/2)\sigma_0$ is the element of the algebra su(2) which generates the U(1) subgroup. Note we consider the image of π as a subset of the algebra su(2), which is just $\mathbb{R}^3$ as a vector space. Expanding the image in coordinates we have

$$s(a,b)\hat{J}_0 s(a,b)^\dagger = \sum_{i=0}^{2} x^i \hat{J}_i,$$

where $x^i \in \mathbb{R}$. This equation leads to the constraint

$$(x^0)^2 + (x^1)^2 + (x^2)^2 = 1,$$

hence the coset space SU(2)/U(1) is just an ordinary sphere, $S^2 \subseteq \mathbb{R}^3$.

C. The supersphere as a coset space

The construction of the preceding section naturally generalizes to the case of the supersphere,[3,4] which we will see can be defined as the coset space $S^{2|2}=\mathrm{UOSp}(1|2)/\mathcal{U}(1)$. Here $\mathcal{U}(1)\equiv\{w\in\mathbb{C}_c: ww^{\diamond}=1\}$ is the even Grassmann extension of the group U(1).

We use the matrix representation of UOSp(1|2) defined in Eqs. (16a) and (16b). The equivalence relation on UOSp(1|2) is given by multiplication on the right with an element of a $\mathcal{U}(1)$ subgroup,

$$s(a,b,\eta)\sim s(a',b',\eta')=s(a,b,\eta)s(w,0,0). \tag{17}$$

In terms of the group parameters we have

$$a'=aw,\quad b'=bw,\quad \eta'=\eta.$$

This equivalence relation defines the coset space $\mathrm{UOSp}(1|2)/\mathcal{U}(1)$. Note that the body of this coset space is just SU(2)/U(1), which as we showed in the preceding section is just an S^2. The projection map for this coset is a supersymmetric generalization of the ordinary Hopf map, it can be written as

$$\begin{aligned}\pi:\ &\mathrm{UOSp}(1|2)\to\mathrm{UOSp}(1|2)/\mathcal{U}(1)\\ &:s(a,b,\eta)\mapsto s(a,b,\eta)J_0s(a,b,\eta)^{\ddagger}.\end{aligned} \tag{18}$$

Note that the image of this map is considered as a subset of the algebra uosp(1|2). Expanding the image in coordinates we have

$$s(a,b,\eta)J_0s(a,b,\eta)^{\ddagger}=\sum_{i=0}^{2}x^iJ_i+\sum_{\alpha=\pm}\xi^{\alpha}Q_{\alpha}, \tag{19}$$

where $x^i\in\mathbb{R}_c$ and $\xi^{\pm}\in\mathbb{C}_a$. It is then possible to solve for the coordinates in terms of the group parameters, which yields

$$x^0=(1-\tfrac{1}{4}\eta\eta^{\diamond})(aa^{\diamond}-bb^{\diamond}), \tag{20a}$$

$$x^1=(1-\tfrac{1}{4}\eta\eta^{\diamond})(ab^{\diamond}+a^{\diamond}b), \tag{20b}$$

$$x^2=i(1-\tfrac{1}{4}\eta\eta^{\diamond})(ab^{\diamond}-a^{\diamond}b), \tag{20c}$$

$$\xi^{-}=-\frac{i}{2}(2\eta ab^{\diamond}+\eta^{\diamond}(aa^{\diamond}-bb^{\diamond})), \tag{20d}$$

$$\xi^{+}=-\frac{i}{2}(2\eta^{\diamond}a^{\diamond}b-\eta(aa^{\diamond}-bb^{\diamond})). \tag{20e}$$

These coordinates satisfy the constraint

$$(x^0)^2+(x^1)^2+(x^2)^2-2\xi^{-}\xi^{+}=1, \tag{21}$$

which is the equation for the unit supersphere $S^{2|2}\subseteq\mathbb{R}^{3|2}$. Another way to think about this equation is as a two-sphere in the even coordinates, with a radius dependent on the odd coordinates, given by $1+\xi^{-}\xi^{+}=1-\frac{1}{4}\eta\eta^{\diamond}$. It is also clear from Eq. (21) that the body of the supersphere is just an ordinary sphere, as expected.

The reality of the coordinates x^i and ξ^{α} is defined with respect to the pseudoconjugate; we have $(x^i)^{\diamond}=x^i$ and $(\xi^{-})^{\diamond}=-\xi^{+}$, $((\xi^{+})^{\diamond}=\xi^{-})$. Note that if we expand out the coordinates in terms of

the Grassmann generators as in Eq. (1) then these reality conditions give the same number of constraints, as would be obtained with standard complex conjugation, which reduces the dimensionality down from that of $\mathbb{C}^{3|2}$ to that of $\mathbb{R}^{3|2}$. Obviously for the purposes of counting these constraints we must take the number of Grassmann generators, N, to be finite.

D. Unconstrained coordinates

In this section we will construct unconstrained coordinates on the supersphere. On S^2 we can define, for example, polar and stereographic coordinates and we will generalize these to $S^{2|2}$ in the following.

We first note that the general element of UOSp(1|2) can be written as

$$s = e^{\eta^\alpha Q_\alpha} e^{-\varphi J_0} e^{-\theta J_2} e^{-\psi J_0}.$$

Here $\theta, \varphi, \psi \in \mathbb{R}_c$, and their bodies are chosen to be in the range $0 \leqslant \theta_0 \leqslant \pi$, $-\pi < \varphi_0 \leqslant \pi$ and $-\pi < \psi_0 \leqslant \pi$. Here θ_0, the body of θ, should not be confused with the coordinate θ^0. A convenient choice of coset representative is given by taking $\psi = 0$, i.e.,

$$L_1(\theta, \varphi, \eta, \eta^\diamond) = e^{\eta^\alpha Q_\alpha} e^{-\varphi J_0} e^{-\theta J_2}. \tag{22}$$

Thus we have $(\theta, \varphi, \eta, \eta^\diamond)$ as coordinates on $S^{2|2}$. The constrained coordinates $(x^0, x^1, x^2, \xi^-, \xi^+)$ of Eqs. (20a)–(20e) can be written in terms of these generalized polar coordinates as

$$x^0 = (1 - \tfrac{1}{4}\eta\eta^\diamond)\cos\theta, \tag{23a}$$

$$x^1 = (1 - \tfrac{1}{4}\eta\eta^\diamond)\sin\theta\cos\varphi, \tag{23b}$$

$$x^2 = (1 - \tfrac{1}{4}\eta\eta^\diamond)\sin\theta\sin\varphi, \tag{23c}$$

$$\xi^- = -\frac{i}{2}(\eta e^{-i\varphi}\sin\theta + \eta^\diamond\cos\theta), \tag{23d}$$

$$\xi^+ = -\frac{i}{2}(\eta^\diamond e^{i\varphi}\sin\theta - \eta\cos\theta). \tag{23e}$$

Note that the trigonometric functions for supernumbers are defined in terms of the usual power series; the usual trigonometric identities are satisfied if the angles are even supernumbers. Also note the appearance of the radius factor, $1 - \frac{1}{4}\eta\eta^\diamond$, in Eqs. (23a)–(23c).

To define a generalization of stereographic coordinates we take a different coset representative $L_2(z, z^\diamond, \eta, \eta^\diamond)$, which can be written in the matrix representation of Eq. (16a) as

$$L_2 = \begin{pmatrix} 1 + \frac{1}{4}\eta\eta^\diamond & -\frac{1}{2}\eta & \frac{1}{2}\eta^\diamond \\ -\frac{1}{2}\eta^\diamond & 1 - \frac{1}{8}\eta\eta^\diamond & 0 \\ -\frac{1}{2}\eta & 0 & 1 - \frac{1}{8}\eta\eta^\diamond \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{z^\diamond}{(1+zz^\diamond)^{1/2}} & \frac{-1}{(1+zz^\diamond)^{1/2}} \\ 0 & \frac{1}{(1+zz^\diamond)^{1/2}} & \frac{z}{(1+zz^\diamond)^{1/2}} \end{pmatrix}. \tag{24}$$

The complex coordinate z is related to the previous coordinates by

$$z = \frac{x^1 + ix^2}{1 + \xi^- \xi^+ - x^0} = \frac{e^{i\varphi} \sin\theta}{1 - \cos\theta}, \tag{25}$$

where again the radius factor, $1+\xi^-\xi^+$, appears. We will find later that the coordinate η is not the most convenient for our purposes, with hindsight we thus define a new odd coordinate χ, and its pseudoconjugate $\chi^\diamond$, by

$$\chi = -\frac{i}{2}(\eta^\diamond z + \eta), \quad \chi^\diamond = \frac{i}{2}(\eta^\diamond - \eta z^\diamond). \tag{26}$$

These relations can be inverted, giving

$$\eta = \frac{2i(\chi^\diamond z + \chi)}{(1 + zz^\diamond)}, \quad \eta^\diamond = \frac{2i(\chi z^\diamond - \chi^\diamond)}{(1 + zz^\diamond)}.$$

Rewriting η in terms of χ gives us the coset representative for the point (z,χ), which we write as

$$L_3(z,z^\diamond,\chi,\chi^\diamond) = L_2(z,z^\diamond,\eta(\chi,\chi^\diamond),\eta^\diamond(\chi,\chi^\diamond)). \tag{27}$$

Note that the coordinates (z,χ) cover a single $\mathbb{C}^{1|1}$ chart on $S^{2|2}$. From Eq. (25) we see that as $\theta_0 \to 0$ we have $z \to \infty$, thus these coordinates can be viewed as generalizations of stereographic coordinates projected from the north pole (i.e., $\theta=0$). To cover the entire supersphere we need a second coordinate patch, which we will think of as projection from the south pole. Away from both the north and south pole we define a new (even) complex coordinate by $w=z^{-1}$. A coset representative for the point (w,η) is given by

$$L_2' = \begin{pmatrix} 1 + \frac{1}{4}\eta\eta^\diamond & -\frac{1}{2}\eta & \frac{1}{2}\eta^\diamond \\ -\frac{1}{2}\eta^\diamond & 1 - \frac{1}{8}\eta\eta^\diamond & 0 \\ -\frac{1}{2}\eta & 0 & 1 - \frac{1}{8}\eta\eta^\diamond \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{(1+ww^\diamond)^{1/2}} & \frac{-w}{(1+ww^\diamond)^{1/2}} \\ 0 & \frac{w^\diamond}{(1+ww^\diamond)^{1/2}} & \frac{1}{(1+ww^\diamond)^{1/2}} \end{pmatrix}.$$

This can be obtained from the coset representative L_2 by multiplication on the right with

$$s\left(\frac{z}{(zz^\diamond)^{1/2}},0,0\right) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{z}{(zz^\diamond)^{1/2}} & 0 \\ 0 & 0 & \frac{z^\diamond}{(zz^\diamond)^{1/2}} \end{pmatrix},$$

which, as it should be, is an element of the $\mathcal{U}(1)$ subgroup of UOSp(1|2). We will also need the analogue of the coordinate χ for this patch, which we take to be

$$\zeta = \frac{i}{2}(\eta^\diamond w + \eta). \tag{28}$$

Away from the poles, the two coordinate patches are related by the holomorphic transformations

$$w = \frac{1}{z}, \quad \zeta = -\frac{\chi}{z}. \tag{29}$$

The two patches (z,χ) and (w,ζ) taken together cover the whole supersphere.

E. Other superspheres

At this stage we should mention that the coset space $S^{2|2}=\mathrm{UOSp}(1|2)/\mathcal{U}(1)$ is not the only way in which a supersphere can be defined. There are at least two other possible coset constructions.

(i) $\mathrm{OSp}(3|2)/\mathrm{OSp}(2|2)$—The ordinary two-sphere can be constructed as the coset space O(3)/O(2); since the body of $\mathrm{OSp}(n|2m)$ is just $\mathrm{O}(n)\times\mathrm{Sp}(2m)$ it is natural to consider the coset space $\mathrm{OSp}(3|2)/\mathrm{OSp}(2|2)$ as a supersymmetric generalization of this.[2] The body of this space is clearly just the ordinary two-sphere. Just as $\mathrm{UOSp}(1|2)/\mathcal{U}(1)$ is, as a subset of $\mathbb{R}^{3|2}$, given by Eq. (21), so is $\mathrm{OSp}(3|2)/\mathrm{OSp}(2|2)$. Now, however, the coordinates x^i and ξ^α are just real supernumbers, i.e., when expanded in the Grassmann generators, as in Eq. (1), all the coefficients are real numbers.

(ii) $\mathrm{SU}(2|1)/\mathrm{U}(1|1)$—This construction is a generalization of that of the complex projective plane. The body of this coset space is given by $\mathrm{U}(2)/(\mathrm{U}(1)\times\mathrm{U}(1))=\mathbb{C}P^1$. As the orthosymplectic groups are not used in this construction the use of the pseudoconjugate and graded adjoint is not required. This space, called $\mathbb{C}P^{1|1}$, and its generalizations $\mathbb{C}P^{n|m}$ are considered further in Ref. 5.

However, neither of these two coset spaces can naturally be considered what one calls a *superspace*. A coset space G/H will be a superspace if it satisfies two conditions. First, the subgroup H should be (the even Grassmann extension of) the tangent space group of the body of the coset space. This will correspond to a restriction of the tangent space group of a general supermanifold. Second, we require that under the (co)-adjoint action of H the odd generators of the algebra of G transform as spinors. The coset space $\mathrm{UOSp}(1|2)/\mathcal{U}(1)$ satisfies both of these conditions, U(1) is the tangent space group of the ordinary sphere, and we see from Eq. (15b) that $Q_\pm$ transform as spinors. Most other treatments use the supersphere as a target space for some sigma model[1,2] and thus do not require a superspace structure. Here we shall be treating the supersphere as the base space for our field theories and as such require it to be a superspace. This will be discussed more in Sec. V.

IV. ACTION OF UOSp(1|2) ON $S^{2|2}$

A. Transformation of the coordinates under UOSp(1|2)

Using the general result of Sec. III A we see that the left action of UOSp(1|2) is well defined on the coset space $S^{2|2}$. First we wish to show how such a transformation acts on the unconstrained coordinates (z,χ) which were defined in Sec. III D. The left action of the arbitrary element $s(c,d,\beta)\in\mathrm{UOSp}(1|2)$ transforms the coset representative $L_3(z,z^\diamond,\chi,\chi^\diamond)$ as

$$L_3(z,z^\diamond,\chi,\chi^\diamond)\to L_3(z',z'^\diamond,\chi',\chi'^\diamond)=s(c,d,\beta)L_3(z,z^\diamond,\chi,\chi^\diamond).$$

We can split the transformation as $s(c,d,\beta)=s(1,0,\beta)s(c,d,0)$ and analyze the two parts separately. Using Eqs. (16a) and (27) we find, that under the action of $s(c,d,0)$ the coordinates transform as

$$z'=\frac{c^\diamond z-d}{d^\diamond z+c}, \tag{30a}$$

$$\chi'=\frac{\chi}{d^\diamond z+c}, \tag{30b}$$

whereas under $s(1,0,\beta)$ we have

$$z'=\left(1-\frac{i}{2}\beta^\diamond\chi\right)z-\frac{i}{2}\beta\chi, \tag{31a}$$

$$\chi' = \left(1 + \frac{1}{8}\beta\beta^{\diamond}\right)\chi - \frac{i}{2}(\beta + \beta^{\diamond} z). \tag{31b}$$

Obviously we can take the pseudoconjugate of these equations to find how $z^{\diamond}$ and $\chi^{\diamond}$ transform.

Note that the group element $s(c,d,0)$ is obtained by exponentiating just the J_i generators of the uosp(1|2) algebra. We also see that the form of Eq. (30a) is that of a Möbius transformation corresponding to the rotation of a sphere. We thus refer to the transformations of Eqs. (30a) and (30b) as the rotations of the supersphere. The group element $s(1,0,\beta)$ is obtained by exponentiating only the Q_α algebra generators. We will therefore refer to Eqs. (31a) and (31b) as the supersymmetry transformations.

For completeness we must also consider how the (w,ζ) coordinates of the other patch transform. We find that under rotations given by $s(c,d,0)$ we have

$$w' = \frac{d^{\diamond} + cw}{c^{\diamond} - dw},$$

$$\zeta' = \frac{\zeta}{c^{\diamond} - dw}.$$

Under supersymmetry transformations given by $s(1,0,\beta)$ we have

$$w' = \left(1 - \frac{i}{2}\beta\zeta\right)w - \frac{i}{2}\beta^{\diamond}\zeta,$$

$$\zeta' = \left(1 + \frac{1}{8}\beta\beta^{\diamond}\right)\zeta + \frac{i}{2}(\beta^{\diamond} + \beta w).$$

Again we may take the pseudoconjugate of these equations to find the transformation properties of $w^{\diamond}$ and $\zeta^{\diamond}$.

B. Differential operator representation of uosp(1|2)

We may use the transformation properties of the coordinates under UOSp(1|2) to construct a differential operator representation of the algebra uosp(1|2).

The coordinates $(z,z^{\diamond},\chi,\chi^{\diamond})$ can be represented by a single superspace coordinate X^M, where the index $M=(m,\mu)$ runs over $m=z,z^{\diamond}$, $\mu=\chi,\chi^{\diamond}$. We may then define a superscalar field Φ on the supersphere, which is just a supernumber valued function on $S^{2|2}$. In this coordinate patch it takes the value $\Phi(X)$.

Now consider an infinitesimal active coordinate transformation $X \to X + \delta X$. As discussed more in Appendix F, we may alternatively think of this as a transformation of the field, $\Phi(X)$, given by

$$\Phi(X) \to \Phi'(X) = \Phi(X - \delta X). \tag{32}$$

Expanding to first order we have

$$\delta\Phi(X) = -\delta X^M \partial_M \Phi(X). \tag{33}$$

For the case of an isometry we can write $\delta X^M = \delta u K^M$, where δu is some small parameter, and K^M is a Killing supervector. The quantity $-K^M\partial_M$ will then be the differential operator corresponding to the isometry.

First we shall consider the rotations of Eqs. (30a) and (30b). For a rotation generated by the element J_0 we have $s(c,d,0)=e^{\theta^0 J_0}$, hence

$$c = e^{i\theta^0/2}, \quad d = 0.$$

Expanding Eqs. (30a) and (30b) to first order in θ^0 we find

$$\delta z = -i\theta^0 z, \quad \delta\chi = -\frac{i}{2}\theta^0\chi,$$

$\delta z^\diamond$ and $\delta\chi^\diamond$ are obtained by taking the pseudoconjugate of these equations. Substituting into Eq. (33) gives us the differential operator corresponding to J_0, namely,

$$\tilde{J}_0 = i\left[z\frac{\partial}{\partial z} - z^\diamond\frac{\partial}{\partial z^\diamond} + \frac{1}{2}\chi\frac{\partial}{\partial\chi} - \frac{1}{2}\chi^\diamond\frac{\partial}{\partial\chi^\diamond}\right]. \tag{34a}$$

A similar argument leads to the differential operators for J_1 and J_2,

$$\tilde{J}_1 = \frac{i}{2}\left[(1-z^2)\frac{\partial}{\partial z} - (1-z^{\diamond 2})\frac{\partial}{\partial z^\diamond} - z\chi\frac{\partial}{\partial\chi} + z^\diamond\chi^\diamond\frac{\partial}{\partial\chi^\diamond}\right], \tag{34b}$$

$$\tilde{J}_2 = -\frac{1}{2}\left[(1+z^2)\frac{\partial}{\partial z} + (1+z^{\diamond 2})\frac{\partial}{\partial z^\diamond} + z\chi\frac{\partial}{\partial\chi} + z^\diamond\chi^\diamond\frac{\partial}{\partial\chi^\diamond}\right]. \tag{34c}$$

Now consider the supersymmetry transformations of Eqs. (31a) and (31b). Expanding these to first order in β and $\beta^\diamond$, and substituting into Eq. (33) we find the differential operators corresponding to Q_- and Q_+,

$$\tilde{Q}_- = \frac{i}{2}\left[\chi z\frac{\partial}{\partial z} - \chi^\diamond\frac{\partial}{\partial z^\diamond} + z\frac{\partial}{\partial\chi} - \frac{\partial}{\partial\chi^\diamond}\right], \tag{34d}$$

$$\tilde{Q}_+ = \frac{i}{2}\left[\chi\frac{\partial}{\partial z} + \chi^\diamond z^\diamond\frac{\partial}{\partial z^\diamond} + \frac{\partial}{\partial\chi} + z^\diamond\frac{\partial}{\partial\chi^\diamond}\right]. \tag{34e}$$

It is straightforward to verify that the generators of Eqs. (34a)–(34e) satisfy the uosp$(1|2)$ algebra. As stated earlier they are of the form $-K_p^M\partial_M$, where $p=0,1,2,-,+$ labels the generators. This allows us to read off the Killing supervectors K_p^M of the supersphere.

In order to construct a superfield theory on $S^{2|2}$ we first have to introduce the invariant vielbein and spin connection, which we do next.

V. COSET SPACE GEOMETRY

A. Vielbein and spin connection for reductive coset spaces

Consider some Lie group G, a subgroup H of G and the space of right cosets $G/H = \{gH: g \in G\}$. The Lie algebra $\mathfrak{h}$ of H is spanned by the generators $H_I \in \mathfrak{h}$, $I=1,\ldots,\dim H$. Let the remaining generators of the Lie algebra $\mathfrak{g}$ of G span $\mathfrak{k} \subseteq \mathfrak{g}$. We shall denote these remaining generators by $K_A \in \mathfrak{k}$, $A=1,\ldots,\dim G - \dim H$. As a vector space we then have

$$\mathfrak{g} = \mathfrak{h} \oplus \mathfrak{k}.$$

The structure constants of G are defined by

$$[H_I, H_J] = f_{IJ}{}^K H_K,$$

$$[H_I, K_A] = f_{IA}{}^J H_J + f_{IA}{}^B K_B,$$

$$[K_A,K_B] = f_{AB}{}^J H_J + f_{AB}{}^C K_C.$$

If $\mathfrak{k}$ can be chosen such that the structure constants $f_{IA}{}^J$ vanish, the coset space G/H is said to be *reductive*.

Suppose now that the coset manifold G/H is parametrized by coordinates Y^M, $M=1,\ldots,\dim G-\dim H$, and so the coset representative may be written $L(Y^M)$. For reductive coset spaces we can then define an invariant vielbein E^A and spin connection ω^I by

$$L^{-1}(Y)dL(Y) = E^A K_A + \omega^I H_I, \tag{35}$$

which is a generalization of the left-invariant Maurer–Cartan form for Lie groups. Here $L(Y)$ is assumed to be in a matrix representation.

Note that these are indeed *invariant* one-forms since under a left action of $g \in G$ on the coset space we have

$$L \mapsto gL, \tag{36a}$$

$$L^{-1}dL \mapsto (L^{-1}g^{-1})d(gL) = L^{-1}dL, \tag{36b}$$

where g is constant on the coset space. Hence we can think of this action as an isometry.

In contrast, under a right action of $h^{-1} \in H$ on the coset space we find

$$L \mapsto Lh^{-1}, \tag{37a}$$

$$L^{-1}dL \mapsto hL^{-1}d(Lh^{-1}) = h(L^{-1}dL)h^{-1} + hdh^{-1}, \tag{37b}$$

and hence

$$E^A K_A + \omega^I H_I \mapsto \underbrace{h(E^A K_A)h^{-1}}_{\in \mathfrak{k}} + \underbrace{h(\omega^I H_I)h^{-1} + hdh^{-1}}_{\in \mathfrak{h}}.$$

Here $h=h(Y)$, i.e., h is not necessarily constant on the coset space, but is rather a local transformation. Note that $h(E^A K_A)h^{-1} \in \mathfrak{k}$ is only true for reductive coset spaces. Thus we have

$$E^A K_A \mapsto E'^A K_A = E^A(hK_A h^{-1}), \tag{38a}$$

$$\omega^I H_I \mapsto \omega'^I H_I = \omega^I(hH_I h^{-1}) + hdh^{-1}. \tag{38b}$$

We can rewrite this using the co-adjoint representation[12] of G, i.e., $g \mapsto R_p{}^q(g)$, which is defined as

$$g^{-1}T_p g = R_p{}^q(g)T_q, \tag{39}$$

where T_p, $p=1,\ldots,\dim G$, are the generators of $\mathfrak{g}$. Thus we have

$$hK_A h^{-1} = R_A{}^B(h^{-1})K_B$$

and so we can alternatively write

$$E^A \mapsto E'^A = E^B R_B{}^A(h^{-1}). \tag{40}$$

Rewriting Eq. (38b) in the co-adjoint representation we find

$$\omega'^I(\tilde{H}_I)_A{}^B = \omega^I R_A{}^C(h)(\tilde{H}_I)_C{}^D R_D{}^B(h^{-1}) + R_A{}^C(h)dR_C{}^B(h^{-1}),$$

where $\tilde{H}_I$ denotes the generator H_I in the co-adjoint representation. Defining $\Omega_A{}^B = \omega^I(\tilde{H}_I)_A{}^B$ we can finally write Eq. (38b) as

$$\Omega_A{}^B \mapsto \Omega'^B_A = R_A{}^C(h)\Omega_C{}^D R_D{}^B(h^{-1}) + R_A{}^C(h)dR_C{}^B(h^{-1}).$$

In this sense the right action of h^{-1} on the coset space, defined in Eq. (37a), can be regarded as a local gauge transformation acting on the tangent space.

B. Vielbein and spin connection for $S^{2|2}$

We will now derive the superzweibein and spin connection for $S^{2|2}$ following the construction given in the preceding section.

As mentioned in Sec. III C the supersphere $S^{2|2}$ is, as a coset space, given by $S^{2|2} = \mathrm{UOSp}(1|2)/\mathcal{U}(1)$. As before we will split up the generators of $G=\mathrm{UOSp}(1|2)$ into the generator of the subgroup $H=\mathcal{U}(1)$, which we take to be J_0, and the remaining generators K_A, $A=(a,\alpha)$, which are given by J_a, Q_α, with $a=1,2$, $\alpha=-,+$, see Eqs. (15a)–(15c). In this case we have—apart from $S^{2|2}$ being a reductive coset space—the additional structure that

$$[H,Q] \subseteq Q,$$

$$[H,J] \subseteq J,$$

hence

$$h^{-1}Q_\alpha h = R_\alpha{}^A(h)K_A = R_\alpha{}^\beta(h)Q_\beta,$$

$$h^{-1}J_a h = R_a{}^A(h)K_A = R_a{}^b(h)J_b,$$

Thus $R_A{}^B(h)$ takes block diagonal form

$$R_A{}^B(h) = \begin{pmatrix} R_a{}^b(h) & 0 \\ 0 & R_\alpha{}^\beta(h) \end{pmatrix}. \tag{41}$$

Using the matrix representation of the UOSp(1|2) algebra, see Eq. (14), we find for $R_a{}^b(h)$ and $R_\alpha{}^\beta(h)$, respectively,

$$R_a{}^b(h) = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix}, \tag{42a}$$

$$R_\alpha{}^\beta(h) = \begin{pmatrix} e^{-i\varphi/2} & 0 \\ 0 & e^{i\varphi/2} \end{pmatrix}. \tag{42b}$$

We see that tangent supervectors V^A belong to a (completely) reducible representation of the tangent space group; the components V^a transform in the vector representation, whereas the components V^α transform in the corresponding spinor representation of $\mathcal{U}(1)$. In this sense we are dealing with a superspace rather than just a supermanifold (see Sec. III E).

To construct the superzweibein and spin connection in the particular case of $\mathrm{UOSp}(1|2)/\mathcal{U}(1)$ we must choose an appropriate coset representative. This is given by

$$L_1(\theta,\phi,\eta,\eta^\diamond) = e^{\eta^\alpha Q_\alpha} e^{-\phi J_0} e^{-\theta J_2},$$

as defined in Eq. (22). In matrix form [see Eq. (16a)] we have

$$L_1(\theta,\phi,\eta,\eta^\diamond)=\begin{pmatrix} 1+\frac{1}{4}\eta\eta^\diamond & -\frac{1}{2}\eta & \frac{1}{2}\eta^\diamond \\ -\frac{1}{2}\eta^\diamond & 1-\frac{1}{8}\eta\eta^\diamond & 0 \\ -\frac{1}{2}\eta & 0 & 1-\frac{1}{8}\eta\eta^\diamond \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & a & -b^\diamond \\ 0 & b & a^\diamond \end{pmatrix},$$

where here $a(\theta,\varphi)=e^{-i\varphi/2}\cos(\theta/2)$ and $b(\theta,\varphi)=e^{i\varphi/2}\sin(\theta/2)$. According to the general formalism derived in the preceding section, the superzweibein and spin connection for $S^{2|2}$ as the coset space can be derived from the generalized Maurer–Cartan one-form, Eq. (35),

$$L_1{}^{-1}(\theta,\phi,\eta,\eta^\diamond)dL_1(\theta,\phi,\eta,\eta^\diamond)=E^AK_A+\omega^IH_I,$$

with $H_I=J_0$ and $K_A=(J_a,Q_\alpha)$, $a=1,2$, $\alpha=-,+$. This way we obtain the superzweibein and spin connection in (super)-polar coordinates. Their explicit form is given in Appendix B.

Using instead the coset representative defined in Eq. (27) we find for the superzweibein in complex (stereographic) coordinates

$$(E_M{}^A)=\begin{pmatrix} \frac{-i}{1+zz^\diamond+\chi\chi^\diamond} & \frac{1}{1+zz^\diamond+\chi\chi^\diamond} & \frac{-2i(\chi z^\diamond-\chi^\diamond)}{(1+zz^\diamond)^{3/2}} & 0 \\ \frac{i}{1+zz^\diamond+\chi\chi^\diamond} & \frac{1}{1+zz^\diamond+\chi\chi^\diamond} & 0 & \frac{-2i(\chi^\diamond z+\chi)}{(1+zz^\diamond)^{3/2}} \\ \frac{-i\chi}{1+zz^\diamond} & \frac{\chi}{1+zz^\diamond} & \frac{2i}{(1+zz^\diamond-\chi\chi^\diamond)^{1/2}} & 0 \\ \frac{i\chi^\diamond}{1+zz^\diamond} & \frac{\chi^\diamond}{1+zz^\diamond} & 0 & \frac{2i}{(1+zz^\diamond-\chi\chi^\diamond)^{1/2}} \end{pmatrix},$$

where the index M, as before, runs over z, $z^\diamond$, χ, $\chi^\diamond$. For the inverse superzweibein, which we will make extensive use of later, we have

$$(E_A{}^M)=\begin{pmatrix} \frac{i}{2}(1+zz^\diamond) & -\frac{i}{2}(1+zz^\diamond) & \frac{i}{2}(\chi z^\diamond-\chi^\diamond) & -\frac{i}{2}(\chi^\diamond z+\chi) \\ \frac{1}{2}(1+zz^\diamond) & \frac{1}{2}(1+zz^\diamond) & \frac{1}{2}(\chi z^\diamond-\chi^\diamond) & \frac{1}{2}(\chi^\diamond z+\chi) \\ \frac{i}{2}(1+zz^\diamond)^{1/2}\chi & 0 & -\frac{i}{2}(1+zz^\diamond+\chi\chi^\diamond)^{1/2} & 0 \\ 0 & \frac{i}{2}(1+zz^\diamond)^{1/2}\chi^\diamond & 0 & -\frac{i}{2}(1+zz^\diamond+\chi\chi^\diamond)^{1/2} \end{pmatrix}.$$

Note that the two coset representatives, Eqs. (22) and (27), differ by a gauge transformation only. Thus, the superzweibein in complex coordinates can be derived from the one in polar coordinates by means of a gauge transformation, see Eq. (40).

In order to construct a superfield Lagrangian later on we will make special use of E_- and E_+, which we can read off from $(E_A{}^M)$ above. We have

$$E_-=\frac{i}{2}(1+zz^\diamond+\chi\chi^\diamond)^{1/2}(\chi\partial_z-\partial_\chi), \tag{43a}$$

$$E_+=\frac{i}{2}(1+zz^\diamond+\chi\chi^\diamond)^{1/2}(\chi^\diamond\partial_{z^\diamond}-\partial_{\chi^\diamond}). \tag{43b}$$

The superdeterminant [cf. Eq. (13)] of $(E_M{}^A)$ is given by

$$E \equiv \mathrm{sdet}(E_M{}^A) = \frac{i}{2}\frac{1}{1+zz^\diamond+\chi\chi^\diamond} = \frac{i}{2}\frac{1+zz^\diamond-\chi\chi^\diamond}{(1+zz^\diamond)^2}. \tag{44}$$

Finally, we have for the spin connection in complex coordinates

$$\begin{aligned}\omega^0 &= \frac{i}{1+zz^\diamond+\chi\chi^\diamond}(z^\diamond dz - zdz^\diamond + d\chi\chi^\diamond + d\chi^\diamond\chi)\\ &= -\frac{1}{2}(z^\diamond+z)E^1 + \frac{i}{2}(z^\diamond - z)E^2 + \frac{1}{2}\frac{\chi z^\diamond - \chi^\diamond}{(1+zz^\diamond)^{1/2}}E^- - \frac{1}{2}\frac{\chi^\diamond z+\chi}{(1+zz^\diamond)^{1/2}}E^+,\end{aligned} \tag{45}$$

hence in the co-adjoint representation

$$\Omega_B{}^C = \omega^0 (J_0)_B{}^C,$$

where

$$(J_0)_B{}^C = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \end{pmatrix}.$$

Note that the body of $\Omega_\alpha{}^\beta$ is given by

$$\Omega_\alpha{}^\beta|_0 = \frac{i}{1+z_0 z_0^*}(z_0^* dz_0 - z_0 dz_0^*)(J_0)_\alpha{}^\beta,$$

which matches the result expected for the ordinary sphere. Similar expressions for the super-zweibein, its dual and the spin connection can be obtained for the (w,ζ) coordinate patch (see Sec. III D). They are given in Appendix C.

The results developed in this section can be used to define a covariant derivative on the supersphere. This will be given by

$$\mathcal{D}_A = E_A{}^M(\partial_M + \omega_M^0 J_0) = E_A + \Omega_A, \tag{46}$$

with $\Omega_A = E_A{}^M \omega_M^0 J_0$ and where J_0 is taken to be in the representation appropriate to the field being acted on.

C. Torsion and curvature of $S^{2|2}$

We are now in the position to calculate the torsion components for the supersphere and hence—by Dragon's theorem[13]—the curvature components. This can be done using the fact that the (anti-)commutator of two covariant derivatives is determined in terms of the supertorsion $T_{AB}{}^C$ and the supercurvature R_{AB} as follows:

$$[\mathcal{D}_A, \mathcal{D}_B] = T_{AB}{}^C \mathcal{D}_C + R_{AB}. \tag{47}$$

Here, both the torsion and the curvature are two-forms which have the following symmetry properties:

$$T_{AB}{}^C = -(-1)^{\epsilon_A\epsilon_B} T_{BA}{}^C,$$

$$R_{AB} = -(-1)^{\epsilon_A\epsilon_B} R_{BA},$$

with

$$\epsilon_A = \begin{cases} 0 & \text{if } A = a, \\ 1 & \text{if } A = \alpha. \end{cases}$$

It is convenient to directly express the torsion and curvature components in terms of the superzweibein and spin connection. Defining the so-called *anholonomy* coefficients $\mathcal{C}_{AB}{}^{C}$ by

$$[E_A, E_B] = \mathcal{C}_{AB}{}^{C} E_C,$$

we have

$$T_{AB}{}^{C} = \mathcal{C}_{AB}{}^{C} + \Omega_{AB}{}^{C} - (-1)^{\epsilon_A \epsilon_B} \Omega_{BA}{}^{C},$$

$$R_{ABC}{}^{D} = E_A \Omega_{BC}{}^{D} + \Omega_{AC}{}^{E} \Omega_{BE}{}^{D} - (-1)^{\epsilon_A \epsilon_B} (A \leftrightarrow B) - \mathcal{C}_{AB}{}^{E} \Omega_{EC}{}^{D}.$$

Note that as a result of the Bianchi identities and of the restricted choice of tangent space group the curvature is completely determined in terms of the torsion. This is known as *Dragon's theorem*.

The only nonvanishing torsion components are given by

$$T_{\alpha\beta}{}^{a} = \frac{i}{2} (\sigma^a)_{\alpha\beta}, \tag{48a}$$

$$T_{\alpha a}{}^{\beta} = -\frac{i}{2} (\sigma_a)_{\alpha}{}^{\beta}, \tag{48b}$$

where the invariant tensor $(\sigma^a)^{\alpha}{}_{\beta}$ is given in Appendix A. Note that even for flat superspace one finds nonzero torsion components $T_{\alpha\beta}{}^{a}$. Since the curvature is completely determined in terms of the torsion we must therefore expect some other nonvanishing torsion components in the case of $S^{2|2}$, which is a curved superspace. Thus it is not surprising that we encounter the additional torsion components $T_{\alpha a}{}^{\beta}$.

For the only nonvanishing curvature components we find

$$R_{12B}{}^{C} = -R_{21B}{}^{C} = (J_0)_B{}^{C}, \tag{49a}$$

$$R_{-+B}{}^{C} = R_{+-B}{}^{C} = -\frac{i}{2} (J_0)_B{}^{C}. \tag{49b}$$

Note that the only nonzero components of the body of the curvature tensor, $R_{abc}{}^{d}$, are given by $R_{12a}{}^{b} = -R_{21a}{}^{b} = (J_0)_a{}^{b}$, which matches the result for the ordinary sphere.

In the following we will use the geometric structure developed in this section to formulate scalar field theories on $S^{2|2}$. Before we do so, however, we will discuss superscalar fields on the supersphere and their transformation properties under isometries.

VI. SUPERFIELDS ON THE SUPERSPHERE

A. Component fields

In Sec. IV B we defined a superscalar field, Φ, on the supersphere. Working in the (z, χ) coordinate patch we can perform an expansion in the χ and $\chi^{\diamond}$ variables, giving

$$\Phi = A(z, z^{\diamond}) + \chi \psi_{\chi}(z, z^{\diamond}) + \chi^{\diamond} \psi_{\chi^{\diamond}}(z, z^{\diamond}) + \chi \chi^{\diamond} F(z, z^{\diamond}). \tag{50}$$

The fields A, ψ_{χ}, $\psi_{\chi^{\diamond}}$, and F are called the component fields of Φ, and are functions of z and $z^{\diamond}$ only. F is often referred to as the *auxiliary* field.

Since we know how the superfield Φ transforms under isometries [see Eq. (33)], it is possible to derive how the component fields transform. For example, under the action of J_0 we have $\delta\Phi = \theta^0 \tilde{J}_0 \Phi$, which gives

$$\delta A = i\theta^0 (z\partial_z - z^\diamond \partial_{z^\diamond}) A, \tag{51a}$$

$$\delta \psi_\chi = i\theta^0 (z\partial_z - z^\diamond \partial_{z^\diamond} + \tfrac{1}{2}) \psi_\chi, \tag{51b}$$

$$\delta \psi_{\chi^\diamond} = i\theta^0 (z\partial_z - z^\diamond \partial_{z^\diamond} - \tfrac{1}{2}) \psi_{\chi^\diamond}, \tag{51c}$$

$$\delta F = i\theta^0 (z\partial_z - z^\diamond \partial_{z^\diamond}) F. \tag{51d}$$

Similar expressions for the transformation properties under J_1 and J_2 can also be found. An identical argument gives the transformation of the component fields under the supersymmetry transformation $\delta\Phi = \beta^\alpha \tilde{Q}_\alpha \Phi$. We find

$$\delta A = \frac{i}{2}((\beta^\diamond z + \beta)\psi_\chi + (\beta z^\diamond - \beta^\diamond)\psi_{\chi^\diamond}), \tag{52a}$$

$$\delta \psi_\chi = \frac{i}{2}((\beta z^\diamond - \beta^\diamond)F - (\beta^\diamond z + \beta)\partial_z A), \tag{52b}$$

$$\delta \psi_{\chi^\diamond} = -\frac{i}{2}((\beta^\diamond z + \beta)F + (\beta z^\diamond - \beta^\diamond)\partial_{z^\diamond} A), \tag{52c}$$

$$\delta F = \frac{i}{2}((\beta^\diamond z + \beta)\partial_z \psi_{\chi^\diamond} - (\beta z^\diamond - \beta^\diamond)\partial_{z^\diamond} \psi_\chi). \tag{52d}$$

It is possible to put these equations in a more familiar form by rewriting them using *Killing spinors*, which we do next.

B. Killing spinors

In order to define Killing spinors we must first introduce some more notation concerning the geometry of $S^{2|0}$, the even Grassmann extension of the ordinary two-sphere. The gamma matrices, γ^m, $m = z, z^\diamond$, for $S^{2|0}$, can be taken to be

$$\gamma^z = -i(1 + zz^\diamond)\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

$$\gamma^{z^\diamond} = i(1 + zz^\diamond)\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

These satisfy $\{\gamma^m, \gamma^n\} = 2g^{mn}$ where the metric g_{mn} has the following nonzero components:

$$g_{zz^\diamond} = g_{z^\diamond z} = \frac{2}{(1 + zz^\diamond)^2}.$$

As we can see from Eq. (45), the restriction of the spin connection ω^0 from the supersphere to $S^{2|0}$ is given by

$$\omega \equiv \omega^0|_{\chi,\chi^\diamond=0} = \omega_z dz + \omega_{z^\diamond} dz^\diamond = \frac{i}{(1+zz^\diamond)}(z^\diamond dz - z dz^\diamond)\begin{pmatrix} -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} \end{pmatrix}.$$

This allows us to define the covariant derivative $D_m = \partial_m + \omega_m$.

Killing spinors on $S^{2|0}$ are defined by (see Ref. 14)

$$D_m \boldsymbol{\epsilon} = \frac{i}{2}\kappa\gamma_m\boldsymbol{\epsilon}, \tag{53}$$

where $\kappa = \pm 1$. A solution to this equation with $\kappa = -1$ reads

$$\boldsymbol{\epsilon} = \frac{1}{2(1+zz^\diamond)^{1/2}}\begin{pmatrix} \beta^\diamond - \beta z^\diamond \\ \beta^\diamond z + \beta \end{pmatrix}, \tag{54}$$

where $\beta \in \mathbb{C}_a$ is some arbitrary constant.

In order to rewrite Eqs. (52a)–(52d) using Killing spinors we also need to introduce a new set of component fields, which are obtained from the superfield Φ. In the case of the spinor and auxiliary fields this will require the use of the covariant derivative. We define

$$\widetilde{A} = \Phi|_{\chi,\chi^\diamond=0}, \tag{55a}$$

$$\psi_\alpha = 2(\mathcal{D}_\alpha\Phi)|_{\chi,\chi^\diamond=0}, \tag{55b}$$

$$F_{\alpha\beta} = -((\mathcal{D}_\alpha\mathcal{D}_\beta - \mathcal{D}_\beta\mathcal{D}_\alpha)\Phi)|_{\chi,\chi^\diamond=0}. \tag{55c}$$

We can use $F_{\alpha\beta}$ to alternatively define

$$\widetilde{F} = \epsilon^{\alpha\beta}F_{\alpha\beta}, \tag{55d}$$

where $\epsilon^{-+} = 1$.

The set of fields given by $\widetilde{A}$, ψ_-, ψ_+, and $\widetilde{F}$ turns out to be a conformal rescaling of the original component fields defined in the preceding section. We find

$$\widetilde{A} = A, \tag{56a}$$

$$\psi_- = -i(1+zz^\diamond)^{1/2}\psi_\chi, \tag{56b}$$

$$\psi_+ = -i(1+zz^\diamond)^{1/2}\psi_{\chi^\diamond}, \tag{56c}$$

$$\widetilde{F} = -(1+zz^\diamond)F. \tag{56d}$$

Note that from Eq. (55b) we see immediately that the fields ψ_- and ψ_+, carrying the tangent space index α, indeed transform as spinors under the action of the tangent space group $\mathcal{U}(1)$. The components ψ_- and ψ_+ can be grouped into a two-component spinor, $\boldsymbol{\psi}$, as

$$\boldsymbol{\psi} = \begin{pmatrix} \psi_- \\ \psi_+ \end{pmatrix}.$$

Using these results we can rewrite the transformation of the component fields under the supersymmetry transformations, given in Eqs. (52a)–(52d), in the more compact form

$$\delta\tilde{A} = \boldsymbol{\epsilon}^{\ddagger}\boldsymbol{\psi}, \tag{57a}$$

$$\delta\boldsymbol{\psi} = (-i\partial\!\!\!/\tilde{A} + \tilde{F})\boldsymbol{\epsilon}, \tag{57b}$$

$$\delta\tilde{F} = -i\boldsymbol{\epsilon}^{\ddagger}\not{D}\boldsymbol{\psi}, \tag{57c}$$

where the spinors $\boldsymbol{\epsilon}$ and $\boldsymbol{\psi}$ are considered as $(0|2)$-dimensional even supervectors in order to define their graded adjoints (see Sec. II B). These equations should be compared with standard results, for instance in Ref. 7. Note that here the graded adjoint plays the role of the Dirac conjugate.

VII. SCALAR FIELD ACTIONS ON $S^{2|2}$

A. Kinetic part of superfield action

We are now in the position to write down a Lagrangian in terms of some superscalar field Φ. Remember that we can expand $\Phi(z,\chi)$ in terms of the χ variables as

$$\Phi = A(z,z^{\diamond}) + \chi\psi_{\chi}(z,z^{\diamond}) + \chi^{\diamond}\psi_{\chi^{\diamond}}(z,z^{\diamond}) + \chi\chi^{\diamond}F(z,z^{\diamond}).$$

Here we want to restrict our attention to (pseudo)real superfields only. We therefore impose the reality condition

$$\Phi^{\diamond} = \Phi,$$

which reads in terms of the component fields

$$A^{\diamond} = A,$$

$$(\psi_{\chi^{\diamond}})^{\diamond} = -\psi_{\chi},$$

$$(\psi_{\chi})^{\diamond} = \psi_{\chi^{\diamond}},$$

$$F^{\diamond} = F.$$

Let us consider the following kinetic Lagrangian[15] for the superscalar field Φ,

$$L_{\text{kin}} = \mathcal{D}_{-}\Phi\mathcal{D}_{+}\Phi = E_{-}\Phi E_{+}\Phi. \tag{58}$$

In order to write down an action on the supersphere we will need the invariant volume form $dzdz^{\diamond}d\chi d\chi^{\diamond}E$, with $E=\text{sdet}(E_M{}^A)$ as in Eq. (44). We thus have for the action

$$I_{\text{kin}} = \int dzdz^{\diamond}d\chi d\chi^{\diamond}EE_{-}\Phi E_{+}\Phi. \tag{59}$$

This will be invariant under supersymmetry transformations, as long as the Lagrangian L_{kin} transforms as a scalar, e.g., as Φ. This is the case, provided that under a supersymmetry transformation with parameter β, we have

$$L_{\text{kin}} \to e^{\beta^{\alpha}\tilde{Q}_{\alpha}}L_{\text{kin}}.$$

To check this, note that under a supersymmetry transformation with small β we have

$$\delta L_{\text{kin}} = E_{-}\Phi E_{+}(\beta^{\alpha}\tilde{Q}_{\alpha}\Phi) + E_{-}(\beta^{\alpha}\tilde{Q}_{\alpha}\Phi)E_{+}\Phi.$$

Now using the fact that

$$[E_-,\tilde{Q}_-] = -\frac{i}{4}\chi E_-, \quad [E_+,\tilde{Q}_-] = \frac{i}{4}\chi E_+,$$

$$[E_-,\tilde{Q}_+] = \frac{i}{4}\chi^\diamond E_-, \quad [E_+,\tilde{Q}_+] = -\frac{i}{4}\chi^\diamond E_+,$$

we find that L_{kin} indeed transforms as a scalar under supersymmetry transformations

$$\delta L_{\text{kin}} = \beta^\alpha \tilde{Q}_\alpha L_{\text{kin}}.$$

Similarly the action will be invariant under rotations if the Lagrangian transforms as

$$L_{\text{kin}} \to e^{\theta^i \tilde{J}_i} L_{\text{kin}}.$$

Under rotations, for small θ^i, we have

$$\delta L_{\text{kin}} = E_-\Phi E_+(\theta^i \tilde{J}_i \Phi) + E_-(\theta^i \tilde{J}_i \Phi) E_+ \Phi,$$

which we can rewrite using

$$[E_-,\tilde{J}_0] = \frac{i}{2}E_-, \quad [E_+,\tilde{J}_0] = -\frac{i}{2}E_+,$$

$$[E_-,\tilde{J}_1] = -\frac{i}{4}(z + z^\diamond)E_-, \quad [E_+,\tilde{J}_1] = \frac{i}{4}(z + z^\diamond)E_+,$$

$$[E_-,\tilde{J}_2] = -\frac{1}{4}(z - z^\diamond)E_-, \quad [E_+,\tilde{J}_2] = \frac{1}{4}(z - z^\diamond)E_+.$$

Doing so we find

$$\delta L_{\text{kin}} = \theta^i \tilde{J}_i L_{\text{kin}}.$$

Thus the action is invariant not only under supersymmetry transformations but also under rotations.

Let us rewrite the kinetic part of the superfield action in terms of component fields. To do so first note that we can write the Lagrangian as

$$L_{\text{kin}} = E_-\Phi E_+\Phi = -\tfrac{1}{4}(1 + zz^\diamond + \chi\chi^\diamond)[(\chi\partial_z - \partial_\chi)\Phi][(\chi^\diamond \partial_{z^\diamond} - \partial_{\chi^\diamond})\Phi],$$

and thus we have for the Lagrangian density $\mathcal{L}_{\text{kin}}$,

$$\mathcal{L}_{\text{kin}} = E L_{\text{kin}} = -\frac{i}{8}[(\chi\partial_z - \partial_\chi)\Phi][(\chi^\diamond \partial_{z^\diamond} - \partial_{\chi^\diamond})\Phi]. \tag{60}$$

Expanding $\mathcal{L}_{\text{kin}}$ in terms of the χ variables we need to keep track only of terms proportional to $\chi\chi^\diamond$, as these are the only ones which will survive the Grassmann integration over χ and $\chi^\diamond$ in the action. We have

$$\mathcal{L}_{\text{kin}}|_{\chi\chi^\diamond} = -\frac{i}{8}(\partial_z A \partial_{z^\diamond} A + \psi_\chi \partial_{z^\diamond}\psi_\chi + \psi_{\chi^\diamond}\partial_z \psi_{\chi^\diamond} + F^2).$$

Hence we find for the action in terms of the component fields after integrating out the $\chi,\chi^\diamond$ dependence

$$I_{\mathrm{kin}} = \frac{i}{8}\int dz dz^{\diamond}(\partial_z A \partial_z{}^{\diamond} A + \psi_\chi \partial_z{}^{\diamond}\psi_\chi + \psi_\chi{}^{\diamond}\partial_z \psi_\chi{}^{\diamond} + F^2). \tag{61}$$

Note that had we used the η coordinates instead of the χ coordinates the action would not have taken this simple form. Note further that the kinetic part of the component field action is conformally invariant, see Appendix E.

For the Euler–Lagrange equations we find

$$\partial_z \partial_z{}^{\diamond} A = 0, \tag{62a}$$

$$\partial_z{}^{\diamond}\psi_\chi = 0, \tag{62b}$$

$$\partial_z \psi_\chi{}^{\diamond} = 0, \tag{62c}$$

$$F = 0. \tag{62d}$$

These imply that A is a harmonic function of z and $z^{\diamond}$, ψ_χ is a holomorphic function and $\psi_\chi{}^{\diamond}$ is an antiholomorphic function of z. Thus if we insist on boundedness of the solutions, A as well as ψ_χ and $\psi_\chi{}^{\diamond}$ are constant in this coordinate patch. Remember, however, that only the two coordinate patches (z,χ) and (w,ζ) taken together cover the whole sphere, see Sec. III D. Thus, in order to make a global statement, we also have to consider the field equations following from the action written in the (w,ζ) patch. To do so, first note that we can rewrite the superfield Φ in terms of the w and ζ coordinates as

$$\Phi(z,\chi) = A(z) + \chi\psi_\chi(z) + \chi^{\diamond}\psi_\chi{}^{\diamond}(z) + \chi\chi^{\diamond}F(z) = A(z) - \frac{\zeta}{w}\psi_\chi(z) - \frac{\zeta^{\diamond}}{w^{\diamond}}\psi_\chi{}^{\diamond}(z) + \frac{\zeta\zeta^{\diamond}}{ww^{\diamond}}F(z).$$

Then defining the fields

$$\hat{A}(w) = A(z), \tag{63a}$$

$$\psi_\zeta(w) = -z\psi_\chi(z), \tag{63b}$$

$$\psi_\zeta{}^{\diamond}(w) = -z^{\diamond}\psi_\chi{}^{\diamond}(z), \tag{63c}$$

$$\hat{F}(w) = zz^{\diamond}F(z), \tag{63d}$$

we have

$$\Phi(w,\zeta) \equiv \hat{A}(w) + \zeta\psi_\zeta(w) + \zeta^{\diamond}\psi_\zeta{}^{\diamond}(w) + \zeta\zeta^{\diamond}\hat{F}(w).$$

Using the inverse superzweibein in the (w,ζ) coordinate patch, see Appendix C, we find for the Lagrangian [Eq. (58)]

$$E_-\Phi E_+\Phi = E'_-\Phi E'_+\Phi$$

and hence for the action in terms of the component fields defined in Eqs. (63a)–(63d)

$$I_{\mathrm{kin}} = \frac{i}{8}\int dw dw^{\diamond}(\partial_w \hat{A}\partial_w{}^{\diamond}\hat{A} + \psi_\zeta \partial_w{}^{\diamond}\psi_\zeta + \psi_\zeta{}^{\diamond}\partial_w \psi_\zeta{}^{\diamond} + \hat{F}^2).$$

The Euler–Lagrange equations following from this action are

$$\partial_w \partial_{w^\diamond} \hat{A} = 0, \tag{64a}$$

$$\partial_w \psi_{\zeta^\diamond} = 0, \tag{64b}$$

$$\partial_{w^\diamond} \psi_\zeta = 0, \tag{64c}$$

$$\hat{F} = 0. \tag{64d}$$

Now Eq. (64c), for example, implies that ψ_ζ is a holomorphic function of w. If, however, we insist also on boundedness of the solution we have—since $\psi_\zeta = -z\psi_\chi(z)$ and since Eq. (62b) implies that ψ_χ is constant—that both $\psi_\chi(z)$ and $\psi_\zeta(w)$ must be zero. An analogous argument shows that also $\psi_{\chi^\diamond}(z)$ and $\psi_{\zeta^\diamond}(w)$ must be taken to be zero.

B. Full superfield action

Now let us add a potential term to the kinetic part of the superfield action given in Eq. (59). This will allow us later to study supersymmetry breaking in this theory. Note that adding a potential term breaks the conformal invariance of the action.

The potential part of the superfield action will be taken to be

$$I_{\text{pot}} = \frac{1}{4} \int dz dz^\diamond d\chi d\chi^\diamond E U(\Phi), \tag{65}$$

with $U(\Phi)$ some superpotential. When expanding $U(\Phi)$ in terms of the odd variables one should note that, since

$$E = \frac{i}{2} \frac{1 + zz^\diamond - \chi\chi^\diamond}{(1 + zz^\diamond)^2},$$

the only terms contributing to the action after integrating out the $\chi, \chi^\diamond$ dependence will be the ones proportional to 1 and $\chi\chi^\diamond$. Keeping this in mind we write

$$U(\Phi) = U(A + \chi\psi_\chi + \chi^\diamond \psi_{\chi^\diamond} + \chi\chi^\diamond F) = U(A) + \chi\chi^\diamond (FU'(A) - \psi_\chi \psi_{\chi^\diamond} U''(A)) + \cdots,$$

where the dots stand for the terms proportional to χ and $\chi^\diamond$, respectively. Thus we can rewrite I_{pot} in terms of the component fields as

$$I_{\text{pot}} = \frac{i}{8} \int dz dz^\diamond \left(\frac{U(A)}{(1 + zz^\diamond)^2} - \frac{FU'(A) - \psi_\chi \psi_{\chi^\diamond} U''(A)}{1 + zz^\diamond} \right). \tag{66}$$

The full action $I = I_{\text{kin}} + I_{\text{pot}}$ in terms of the component fields is then given by

$$I = \frac{i}{8} \int dz dz^\diamond \left(\partial_z A \partial_{z^\diamond} A + \psi_\chi \partial_{z^\diamond} \psi_\chi + \psi_{\chi^\diamond} \partial_z \psi_{\chi^\diamond} + F^2 + \frac{U(A)}{(1 + zz^\diamond)^2} - \frac{FU'(A) - \psi_\chi \psi_{\chi^\diamond} U''(A)}{1 + zz^\diamond} \right). \tag{67}$$

The Euler–Lagrange equations corresponding to the full action can be found in Appendix D. Note that we can check the invariance of the action under rotations and supersymmetry transformations explicitly using the transformation laws given in Eqs. (51a)–(51d) and (52a)–(52d).

Seeing as F is just an auxiliary field we may eliminate it from the action. The field equation for F is purely algebraic, we have

$$F = \frac{1}{2}\frac{U'(A)}{1+zz^{\diamond}},$$

and thus eliminating it from the action we find

$$I = \frac{i}{8}\int dzdz^{\diamond}\left(\partial_z A\partial_{z^{\diamond}}A + \psi_\chi\partial_{z^{\diamond}}\psi_\chi + \psi_{\chi^{\diamond}}\partial_z\psi_{\chi^{\diamond}} + \frac{U(A)-\frac{1}{4}(U'(A))^2}{(1+zz^{\diamond})^2} + \frac{U''(A)}{1+zz^{\diamond}}\psi_\chi\psi_{\chi^{\diamond}}\right).$$

For later convenience we define the effective potential V by

$$V(A) = U(A) - \tfrac{1}{4}(U'(A))^2. \tag{68}$$

Note that the factor $(1+zz^{\diamond})^{-2}$ contributes to the invariant volume element of $S^{2|0}$ and as such is not part of the effective potential. Also note that the effective potential will be unbounded from below whenever $U(A)$ is given by a polynomial of degree greater than 2. However, there exist nonpolynomial choices of the potential $U(A)$, for example, a Gaussian, which lead to effective potentials that are bounded from below.

The truncated supersymmetry transformations are

$$\delta A = \frac{i}{2}((\beta^{\diamond}z+\beta)\psi_\chi + (\beta z^{\diamond}-\beta^{\diamond})\psi_{\chi^{\diamond}}),$$

$$\delta\psi_\chi = \frac{i}{2}\left((\beta z^{\diamond}-\beta^{\diamond})\frac{1}{2}\frac{U'(A)}{1+zz^{\diamond}} - (\beta^{\diamond}z+\beta)\partial_z A\right),$$

$$\delta\psi_{\chi^{\diamond}} = -\frac{i}{2}\left((\beta^{\diamond}z+\beta)\frac{1}{2}\frac{U'(A)}{1+zz^{\diamond}} + (\beta z^{\diamond}-\beta^{\diamond})\partial_{z^{\diamond}}A\right).$$

Note that the truncated action will be invariant under these supersymmetry transformations. However, the truncated transformations will not close unless we impose the field equations, i.e., the commutator of two supersymmetry transformations will give a rotation only on-shell.

VIII. SUPERSYMMETRY BREAKING

In this section we will investigate supersymmetry breaking in this model for different choices of the potential $U(\Phi)$. In order to do so let us consider an SO(3) invariant classical vacuum solution given by $A=$constant and $\psi_\chi=\psi_{\chi^{\diamond}}=0$. Under supersymmetry this solution transforms as

$$\delta A = 0,$$

$$\delta\psi_\chi = \frac{i}{4}(\beta z^{\diamond}-\beta^{\diamond})\frac{U'(A)}{1+zz^{\diamond}},$$

$$\delta\psi_{\chi^{\diamond}} = -\frac{i}{4}(\beta^{\diamond}z+\beta)\frac{U'(A)}{1+zz^{\diamond}}.$$

Thus this solution will be supersymmetry preserving if $U'(A)=0$, i.e., if $F=0$. On the other hand, $F\neq 0$ indicates states of broken supersymmetry.

Note that vacuum solutions correspond to critical points of the effective potential V, given in Eq. (68). Since

$$V'(A) = U'(A)(1 - \tfrac{1}{2}U''(A))$$

we have two types of stationary points, namely $U'(A)=0$ and $U''(A)=2$, the former corresponding to states with unbroken supersymmetry, the latter corresponding to states for which supersymmetry is possibly broken.

As a first example consider the potential $U(A)=mA^2$, where $m \in \mathbb{R}_0$ is some constant parameter. Here $\mathbb{R}_0 \cong \mathbb{R}$ denotes the body of $\mathbb{R}_c$. We shall look for critical points of the effective potential, which is

$$V(A) = (m - m^2)A^2. \tag{69}$$

Note that if $m=0$ or 1 the effective potential is identically zero. In the case of $m>1$ or $m<0$ there exists neither a global nor a local minimum. If, however, $0<m<1$ the potential possesses a global minimum at $A=0$. As this implies that $U'(A)=2mA=0$, supersymmetry will be preserved for this solution.

As a second example we will consider the potential

$$U(A) = \tfrac{1}{3}gA^3 + \lambda A,$$

with $g, \lambda \in \mathbb{R}_0$ constant. The extrema of the effective potential

$$V(A) = \lambda A + \tfrac{1}{3}gA^3 - \tfrac{1}{4}(gA^2 + \lambda)^2 \tag{70}$$

are given by

$$U'(A) = gA^2 + \lambda = 0 \Rightarrow A = \pm \sqrt{\frac{-\lambda}{g}},$$

$$U''(A) = 2gA = 2 \Rightarrow A = \frac{1}{g}.$$

In order to decide whether we can have stable supersymmetry preserving vacuum solutions, we need to know for which parameter values $A=\pm\sqrt{-\lambda/g}$ correspond to local minima. Thus we need to investigate $V''(A)$ at these points. We have

$$V''(A) = U''(A)(1 - \tfrac{1}{2}U''(A)) - \tfrac{1}{2}U'(A)U'''(A) = -2\sqrt{-\lambda g}(\sqrt{-\lambda g} \mp 1).$$

One must distinguish between four different cases.

(i) Suppose $\sqrt{-\lambda g}>1$. In this case $V''(A)<0$ for both the roots $A=\pm\sqrt{-\lambda/g}$, hence $U''(A)=2$ must correspond to the local minimum. Thus for this vacuum solution supersymmetry will be broken [see Fig. 1(a)].

(ii) Suppose $0<\sqrt{-\lambda g}<1$. In this case one of the roots $A=\pm\sqrt{-\lambda/g}$ will correspond to a local maximum the other to a local minimum. Thus there exists a supersymmetry preserving vacuum solution [see Fig. 1(b)].

(iii) Suppose $-\lambda g=1$. Then $A=\pm\sqrt{-\lambda/g}=\pm 1/g$ implies that one of the two roots corresponds to $V''(A)=0$, the other to a maximum. Thus there exists no stable supersymmetry preserving vacuum state [see Fig. 1(c)].

(iv) Suppose $\lambda g>0$. There is no solution to $U'(A)=0$, hence supersymmetry will be broken. However, in this case $V(A)$ has a single maximum at $A=1/g$ and thus any vacuum solution will be unstable anyway [see Fig. 1(d)].

Note, however, that the effective potential of Eq. (70) is unbounded from below and as such exhibits only local minima. Therefore there do not exist true vacuum solutions.

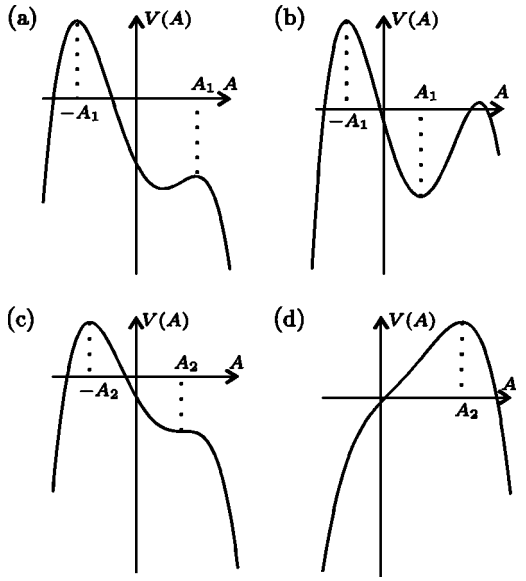

FIG. 1. A sketch of the effective potential $V(A)=\lambda A+\frac{1}{3}gA^3-\frac{1}{4}(gA^2+\lambda)^2$ for the four different cases discussed in the text. Here $A_1=\sqrt{-\lambda/g}$ and $A_2=1/g$.

IX. CONSERVED CURRENTS FROM SUPERFIELD FORMALISM

Using the superfield formalism we will derive in this section a supersymmetric generalization of the energy-momentum tensor.

In order to do so consider some superfield Lagrangian density $\mathcal{L}=\mathcal{L}(\Phi,\partial\Phi)$. Remember that a coordinate transformation $X^M\to X^M+\delta X^M$ is realized on superscalar fields as [see Eq. (33)] $\Phi\to\Phi(X-\delta X)=\Phi(X)+\delta\Phi(X)$ where $\delta\Phi=-\delta X^M\partial_M\Phi$. Note that in the case of an isometry, as we shall assume here, we have $\delta X^M=\delta u K^M$, with K^M a Killing supervector.

Similarly we find that the Lagrangian density transforms under an isometry as

$$\delta\mathcal{L}=-(-1)^M\partial_M(\delta X^M\mathcal{L}). \tag{71}$$

For a derivation of this result see Appendix F. On the other hand, we find that the change in the Lagrangian density obtained by varying the fields is

$$\delta\mathcal{L}=\delta\Phi\frac{\partial\mathcal{L}}{\partial\Phi}+(\partial_M\delta\Phi)\frac{\partial\mathcal{L}}{\partial(\partial_M\Phi)}=\delta\Phi\left(\frac{\partial\mathcal{L}}{\partial\Phi}-\partial_M\left(\frac{\partial\mathcal{L}}{\partial(\partial_M\Phi)}\right)\right)+\partial_M\left(\delta\Phi\frac{\partial\mathcal{L}}{\partial(\partial_M\Phi)}\right). \tag{72}$$

Note that the superzweibein is invariant under an isometry, thus the variation of $\mathcal{L}$ with respect to the superzweibein is zero. From Eq. (72) we see that the Euler–Lagrange equations are

$$\frac{\partial\mathcal{L}}{\partial\Phi}-\partial_M\left(\frac{\partial L}{\partial(\partial_M\Phi)}\right)=0. \tag{73}$$

Thus if we impose the field equations the first term in Eq. (72) vanishes and we can set the remaining term equal to $-(-1)^M\partial_M(\delta X^M\mathcal{L})$. Then using $\delta\Phi=-\delta X^M\partial_M\Phi$ we find

$$\partial_M\left(\delta X^N\left((-1)^M\delta_N{}^M\mathcal{L}-\partial_N\Phi\frac{\partial\mathcal{L}}{\partial(\partial_M\Phi)}\right)\right)=0. \tag{74}$$

We are now in the position to define the superenergy-momentum tensor $\mathcal{T}_N{}^M$,

$$\mathcal{T}_N{}^M = (-1)^M \delta_N{}^M \mathcal{L} - \partial_N \Phi \frac{\partial \mathcal{L}}{\partial(\partial_M \Phi)}. \tag{75}$$

The corresponding super-Noether current $\mathcal{J}^M$ is then defined by

$$\mathcal{J}^M = K^N \mathcal{T}_N{}^M. \tag{76}$$

By means of Eq. (74) $\mathcal{J}^M$ will satisfy the superconservation law

$$\partial_M \mathcal{J}^M = 0. \tag{77}$$

Let us now consider the specific Lagrangian density for $S^{2|2}$ given by [see Eqs. (59) and (65)]

$$\mathcal{L} = E(E_- \Phi E_+ \Phi + \tfrac{1}{4} U(\Phi)). \tag{78}$$

One can check that the field equations given by Eq. (73) indeed coincide—when written in terms of the component fields—with the field equations given in Appendix D, which were directly derived from the action in terms of the component fields.

For the superenergy-momentum tensor we find in this case

$$\mathcal{T}_N{}^M = (-1)^M \delta_N{}^M E(E_- \Phi E_+ \Phi + \tfrac{1}{4} U(\Phi)) - \partial_N \Phi E(E_-{}^M E_+ \Phi + (-1)^M E_- \Phi E_+{}^M).$$

The supercurrents are given by

$$\mathcal{J}_p{}^M = K_p{}^N \mathcal{T}_N{}^M,$$

with $p = 0, 1, 2, -, +$, as before. The Killing supervectors $K_p{}^N$ can be read off from Eqs. (34a)–(34c) and (34e). Note that by taking the $\chi\chi^\diamond$ component of the conservation equation, Eq. (77), we find a conservation equation purely in z

$$(\partial_M \mathcal{J}_p{}^M)|_{\chi\chi^\diamond} = (\partial_z \mathcal{J}_p{}^z + \partial_{z^\diamond} J_p{}^{z^\diamond})|_{\chi\chi^\diamond} = (\partial_m \mathcal{J}_p{}^m)|_{\chi\chi^\diamond} = 0, \tag{79}$$

as both $\partial_\chi \mathcal{J}_p{}^\chi$ and $\partial_{\chi^\diamond} \mathcal{J}_p{}^{\chi^\diamond}$ do not contribute a $\chi\chi^\diamond$ term. It will turn out that it is this $\chi\chi^\diamond$ contribution to the conservation equation that gives rise to the familiar energy-momentum tensor and fermionic currents, which can alternatively be derived directly from the action in terms of the component fields. Considering other components of the conservation equation, say the χ component, we find

$$(\partial_z \mathcal{J}_p{}^z + \partial_{z^\diamond} \mathcal{J}_p{}^{z^\diamond})|_\chi = -(\partial_{\chi^\diamond} \mathcal{J}_p{}^{\chi^\diamond})|_\chi.$$

Note that this also is a conservation equation purely in z. However, the term on the right-hand side of the equation, $-(\partial_{\chi^\diamond} \mathcal{J}_p{}^{\chi^\diamond})|_\chi$, which does not involve any derivatives with respect to z, must be understood as some kind of source term. Yet, the interpretation of these additional conservation equations remains unclear.

Now let us consider the currents $\mathcal{J}_i{}^m$, $i = 0, 1, 2$, in more detail. We have

$$\mathcal{J}_i{}^m = K_i{}^N \mathcal{T}_N{}^m = K_i{}^n \mathcal{T}_n{}^m + K_i{}^\mu \mathcal{T}_\mu{}^m.$$

By direct calculation one finds that the components $\mathcal{T}_\chi{}^m$ are proportional to χ and similarly the components $\mathcal{T}_{\chi^\diamond}{}^m$ are proportional to $\chi^\diamond$. Now, as also $K_i{}^\chi$ is proportional to χ and similarly $K_i{}^{\chi^\diamond}$ is proportional to $\chi^\diamond$ the above equation simplifies to

$$\mathcal{J}_i{}^m = K_i{}^n \mathcal{T}_n{}^m.$$

Note that $K_i{}^n = K_i{}^n|_{\chi\chi^\diamond} \equiv k_i{}^n$ correspond to the usual Killing vectors on the sphere $S^{2|0}$,

$$(k_0^m) = i(z, -z^\diamond),$$

$$(k_1^m) = \frac{i}{2}((1-z^2), -(1-z^{\diamond 2})),$$

$$(k_2^m) = -\tfrac{1}{2}((1+z^2), (1+z^{\diamond 2})).$$

Defining $j_i{}^m$ and $t_m{}^n$ as the $\chi\chi^\diamond$ components of $\mathcal{J}_i^n$ and $\mathcal{T}_m{}^n$, respectively,

$$j_i{}^m \equiv \mathcal{J}_i^m|_{\chi\chi^\diamond}, \quad t_m{}^n \equiv \mathcal{T}_m{}^n|_{\chi\chi^\diamond}$$

we can rewrite the conservation equation, Eq. (79), for the bosonic currents $\mathcal{J}_i^m$ as

$$\partial_m j_i{}^m = \partial_m(k_i{}^n t_n{}^m) = 0.$$

For $t_m{}^n$ we find in terms of the conformally rescaled fields $\tilde{A}, \psi_-, \psi_+$, as given in Eqs. (56a)–(56c),

$$t_{mn} = \frac{i}{8}\sqrt{|g|}\left(\partial_m\tilde{A}\partial_n\tilde{A} + \frac{i}{2}\boldsymbol{\psi}^\ddagger\gamma_m\partial_n\boldsymbol{\psi} - g_{mn}\left[\frac{1}{2}(\partial\tilde{A})^2 - \frac{1}{8}U'(\tilde{A})^2 + \frac{1}{2}U(\tilde{A})\right]\right), \tag{80}$$

where the index has been lowered using the metric g_{mn}. Note that the auxiliary field $\tilde{F}$ has been eliminated.

We shall now consider the $\chi\chi^\diamond$ contribution to the currents $\mathcal{J}_\alpha{}^m$, $\alpha = -, +$. Let us define

$$j_\alpha{}^m \equiv \mathcal{J}_\alpha{}^m|_{\chi\chi^\diamond}$$

and also

$$j^m \equiv \beta^\diamond j_-{}^m + \beta j_+{}^m.$$

From Eq. (79) we see that j^m satisfies the conservation equation

$$\partial_m j^m = 0.$$

Rewriting this fermionic current in terms of the rescaled fields $\tilde{A}, \psi_-, \psi_+$, as we did before in the case of t_{mn}, we find

$$j^m = \frac{i}{8}\sqrt{|g|}\boldsymbol{\epsilon}^\ddagger\left(\not{\partial}\tilde{A} + \frac{i}{2}U'(\tilde{A})\right)\gamma^m\boldsymbol{\psi}, \tag{81}$$

where $\boldsymbol{\epsilon}$ is the Killing spinor defined in Eq. (54).

X. CONCLUSIONS AND OUTLOOK

We have shown how to construct the supersphere $S^{2|2}$ as the coset space $\mathrm{UOSp}(1|2)/\mathcal{U}(1)$, analogous to the construction of flat superspace as the super Poincaré group quotiented by the Lorentz group. The definition of UOSp(1|2), which is the isometry group of the supersphere, required the notions of pseudoconjugation and graded adjoint.

The coset space $\mathrm{UOSp}(1|2)/\mathcal{U}(1)$ has the structure of a superspace, rather than just being a supermanifold as is the case for other coset space definitions of the supersphere. This allowed us to consider the supersphere as a base space for a superscalar field theory. As $S^{2|2}$ is an example of a curved superspace on which we have *rigid* supersymmetry transformations, i.e., the supersymmetry parameter is not position dependent, the theory we constructed exhibits global supersymmetry. Upon integrating out the odd coordinate dependence, this superscalar field theory becomes a supersymmetric theory on the ordinary sphere with a scalar, spinor, and auxiliary field. Choosing a polynomial potential we saw that solutions at local minima may break supersymmetry, provided certain conditions are met. Also recall that, contrary to what is expected, the effective potential for this model is not typically bounded from below. This appears to be due to the Euclidean nature of

the theory. However, as we pointed out, nonpolynomial potentials can be found which will exhibit global minima and thus true vacuum solutions.

Using the superfield formalism we were able to derive Euler–Lagrange equations and Noether's theorem for the superscalar field Φ itself, starting from some general superfield Lagrangian density $\mathcal{L}(\Phi,\partial\Phi)$. When applying Euler–Lagrange equations to the specific Lagrangian density constructed for $S^{2|2}$ we found that the field equations for Φ reduce, when written in terms of the component fields, to the ones derived directly from the action on the ordinary sphere. The superconservation equations derived from Noether's theorem—when applied to the Lagrangian density for the supersphere—give rise to the familiar energy-momentum tensor and fermionic currents expected from the component field action. Notably, though, the super conservation equations also give rise to additional conservation laws, that appear to be independent of the familiar ones and which thus call for some interpretation.

In this work we have concentrated on superscalar field theories on the supersphere. Using the methods we have presented it would be possible to further this study by investigating more general field theories, for example, gauge theories or sigma models with the supersphere as the base space. Another possible extension of this work would be to quantize the scalar field theory, which due to its Euclidean nature would correspond to a statistical field theory.

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APPENDIX A: RAISING AND LOWERING CONVENTIONS FOR SPINOR INDICES

Raising and lowering of spinor indices $\alpha,\beta,\ldots$ is achieved with the use of the antisymmetric epsilon symbols $\epsilon^{\alpha\beta}$ and $\epsilon_{\alpha\beta}$; the convention we will follow is that of Ref. 16. When raising an index we always contract on the second index of $\epsilon^{\alpha\beta}$, e.g.,

$$\psi^{\alpha}=\epsilon^{\alpha\beta}\psi_{\beta}.$$

However, when lowering an index we always contract on the first index of $\epsilon_{\alpha\beta}$, e.g.,

$$\psi_{\beta}=\epsilon_{\gamma\beta}\psi^{\gamma}.$$

Combining the preceding two equations we see that

$$\epsilon^{\alpha\beta}\epsilon_{\gamma\beta}=\delta^{\alpha}{}_{\gamma}.$$

Hence we see that if we choose $\epsilon_{-+}=1$, then we must also have $\epsilon^{-+}=1$. Note that we can think of $\epsilon^{\alpha\beta}$ as $\epsilon_{\alpha\beta}$ with both indices raised.

The (components of the) standard Pauli matrices are taken to be $(\sigma^{i})^{\alpha}{}_{\beta}$. Lowering the first index allows us to construct the quantity

$$(\sigma^{i})_{\alpha\beta}=\epsilon_{\gamma\alpha}(\sigma^{i})^{\gamma}{}_{\beta}=-\epsilon_{\alpha\gamma}(\sigma^{i})^{\gamma}{}_{\beta},$$

which is symmetric in α,β. We can then raise the second index to give

$$(\sigma^{i})_{\alpha}{}^{\beta}=\epsilon_{\gamma\alpha}(\sigma^{i})^{\gamma}{}_{\delta}\epsilon^{\beta\delta}=\epsilon_{\alpha\gamma}(\sigma^{i})^{\gamma}{}_{\delta}\epsilon^{\delta\beta}.$$

Notice that the third terms in the above two equations have been written in a way more suggestive of standard matrix multiplication. In fact, if we define the antisymmetric matrix $\epsilon=(\epsilon_{\alpha\beta})$, we may think of these quantities as the components of the matrices $-\epsilon\sigma^{i}$ and $\epsilon\sigma^{i}\epsilon=(\sigma^{i})^{t}$, respectively.

The quantity $(\sigma^{i})_{\alpha}{}^{\beta}$ [as well as $(\sigma^{a})_{\alpha}{}^{\beta}$] is a $\mathcal{U}(1)$ invariant tensor, i.e.,

$$(\sigma^j)_\alpha{}^\beta = R_\alpha{}^\gamma(h)(\sigma^j)_\gamma{}^\delta R_\delta{}^\beta(h^{-1})R_j{}^i(h^{-1}),$$

where $R_p{}^q(h)$ is as given in Eq. (39).

APPENDIX B: SUPERZWEIBEIN AND SPIN CONNECTION IN POLAR COORDINATES

We obtain for the superzweibein in (super)-polar coordinates

$$(\tilde{E}_M{}^A)$$

$$= \begin{pmatrix} \sin\theta & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ \frac{i}{4}(\eta^\diamond \sin\theta - \eta\cos\theta e^{-i\varphi}) & -\frac{1}{4}\eta e^{-i\varphi} & \left(1+\frac{1}{8}\eta\eta^\diamond\right)\sin\frac{\theta}{2}e^{-i\varphi/2} & \left(1+\frac{1}{8}\eta\eta^\diamond\right)\cos\frac{\theta}{2}e^{-i\varphi/2} \\ \frac{i}{4}(\eta\sin\theta + \eta^\diamond\cos\theta e^{i\varphi}) & -\frac{1}{4}\eta^\diamond e^{i\varphi} & \left(1+\frac{1}{8}\eta\eta^\diamond\right)\cos\frac{\theta}{2}e^{i\varphi/2} & -\left(1+\frac{1}{8}\eta\eta^\diamond\right)\sin\frac{\theta}{2}e^{i\varphi/2} \end{pmatrix},$$

where the index M here runs over $\varphi, \theta, \eta, \eta^\diamond$. The spin connection is in polar coordinates given by

$$\begin{aligned}\omega^0 &= -d\varphi\cos\theta - \frac{i}{4}d\eta^\diamond(\eta\cos\theta - \eta^\diamond e^{i\varphi}\sin\theta) - \frac{i}{4}d\eta(\eta^\diamond\cos\theta + \eta e^{-i\varphi}\sin\theta) \\ &= -\cot\theta\,\tilde{E}^1 + \frac{i}{4}\frac{1}{\sin\theta}\left(\eta e^{-i\varphi/2}\sin\frac{\theta}{2} - \eta^\diamond e^{i\varphi/2}\cos\frac{\theta}{2}\right)\tilde{E}^- + \frac{i}{4}\frac{1}{\sin\theta}\left(\eta e^{-i\varphi/2}\cos\frac{\theta}{2}\right. \\ &\quad \left. + \eta^\diamond e^{i\varphi/2}\sin\frac{\theta}{2}\right)\tilde{E}^+.\end{aligned}$$

APPENDIX C: SUPERZWEIBEIN AND SPIN CONNECTION IN THE (w,ζ) PATCH

We find for the superzweibein in the (w,ζ) coordinate patch

$$(E'_M{}^A) = \begin{pmatrix} \frac{i}{1+ww^\diamond+\zeta\zeta^\diamond} & \frac{-1}{1+ww^\diamond+\zeta\zeta^\diamond} & \frac{2i(\zeta w^\diamond+\zeta^\diamond)}{(1+ww^\diamond)^{3/2}} & 0 \\ \frac{-i}{1+ww^\diamond+\zeta\zeta^\diamond} & \frac{-1}{1+ww^\diamond+\zeta\zeta^\diamond} & 0 & \frac{2i(\zeta^\diamond w-\zeta)}{(1+ww^\diamond)^{3/2}} \\ \frac{-i\zeta}{1+ww^\diamond} & \frac{\zeta}{1+ww^\diamond} & \frac{-2i}{(1+ww^\diamond-\zeta\zeta^\diamond)^{1/2}} & 0 \\ \frac{i\zeta^\diamond}{1+ww^\diamond} & \frac{\zeta^\diamond}{1+ww^\diamond} & 0 & \frac{-2i}{(1+ww^\diamond-\zeta\zeta^\diamond)^{1/2}} \end{pmatrix},$$

where the index M now runs over $w, w^\diamond, \zeta, \zeta^\diamond$. The inverse superzweibein is given by

$$(E'^{M}_{A}) = \begin{pmatrix} -\frac{i}{2}(1+ww^{\diamond}) & \frac{i}{2}(1+ww^{\diamond}) & -\frac{i}{2}(\zeta w^{\diamond}+\zeta^{\diamond}) & \frac{i}{2}(\zeta^{\diamond}w-\zeta) \\ -\frac{1}{2}(1+ww^{\diamond}) & -\frac{1}{2}(1+ww^{\diamond}) & -\frac{1}{2}(\zeta w^{\diamond}+\zeta^{\diamond}) & -\frac{1}{2}(\zeta^{\diamond}w-\zeta) \\ \frac{i}{2}(1+ww^{\diamond})^{1/2}\zeta & 0 & \frac{i}{2}(1+ww^{\diamond}+\zeta\zeta^{\diamond})^{1/2} & 0 \\ 0 & \frac{i}{2}(1+ww^{\diamond})^{1/2}\zeta^{\diamond} & 0 & \frac{i}{2}(1+ww^{\diamond}+\zeta\zeta^{\diamond})^{1/2} \end{pmatrix}.$$

The superdeterminant of (E'^{A}_{M}) is given by

$$E' \equiv \mathrm{sdet}(E'^{A}_{M}) = \frac{i}{2}\frac{1}{1+ww^{\diamond}+\zeta\zeta^{\diamond}}.$$

Finally, we find for the spin connection in the (w,ζ) coordinate patch

$$\begin{aligned}\omega'^{0} &= \frac{i}{1+ww^{\diamond}+\zeta\zeta^{\diamond}}(w^{\diamond}dw - wdw^{\diamond} + d\zeta\zeta^{\diamond} + d\zeta^{\diamond}\zeta) \\ &= \frac{1}{2}(w^{\diamond}+w)E'^{1} - \frac{i}{2}(w^{\diamond}-w)E'^{2} + \frac{1}{2}\frac{\zeta w^{\diamond}+\zeta^{\diamond}}{(1+ww^{\diamond})^{1/2}}E'^{-} - \frac{1}{2}\frac{\zeta^{\diamond}w-\zeta}{(1+ww^{\diamond})^{1/2}}E'^{+}.\end{aligned}$$

APPENDIX D: EULER–LAGRANGE EQUATIONS FOR THE FULL ACTION

The field equations following from the full action given in Eq. (67) are

$$\partial_z\partial_z{}^{\diamond}A = \frac{1}{2}\frac{U'(A)}{(1+zz^{\diamond})^2} - \frac{1}{2}\frac{FU''(A)}{1+zz^{\diamond}} + \frac{1}{2}\frac{\psi_\chi\psi_\chi{}^{\diamond}U'''(A)}{1+zz^{\diamond}},$$

$$\partial_z{}^{\diamond}\psi_\chi = -\frac{1}{2}\frac{\psi_\chi{}^{\diamond}U''(A)}{1+zz^{\diamond}},$$

$$\partial_z\psi_\chi{}^{\diamond} = \frac{1}{2}\frac{\psi_\chi U''(A)}{1+zz^{\diamond}},$$

$$F = \frac{1}{2}\frac{U'(A)}{1+zz^{\diamond}}.$$

APPENDIX E: CONFORMAL INVARIANCE OF THE KINETIC PART OF THE ACTION

The superscalar field action, Eq. (67), can be rewritten using the notation of Sec. VI B. We find it to be

$$I = \frac{i}{16}\int d^2z\sqrt{|g|}\left(g^{mn}\partial_m\tilde{A}\partial_n\tilde{A} + i\boldsymbol{\psi}^{\ddagger}\partial\!\!\!/\boldsymbol{\psi} + \tilde{F}^2 - \frac{1}{2}\boldsymbol{\psi}^{\ddagger}\boldsymbol{\psi}U''(\tilde{A}) + U(\tilde{A}) + \tilde{F}U'(\tilde{A})\right),$$

where g is the determinant of the metric. The kinetic part of the action is obtained by setting $U(\tilde{A})=0$. Note that we could replace the second term, $i\boldsymbol{\psi}^{\ddagger}\partial\!\!\!/\boldsymbol{\psi}$, with $i\boldsymbol{\psi}^{\ddagger}\mathbb{D}\boldsymbol{\psi}$. This is because the term involving the spin connection will vanish due to the anticommuting nature of $\boldsymbol{\psi}$ and the form of the gamma matrices.

Under a conformal transformation, the metric and gamma matrices transform as

$$g_{mn} \to \lambda^2 g_{mn},$$

$$\gamma^m \to \lambda^{-1}\gamma^m,$$

where λ is some positive function on the sphere. It is then possible to define the transformation properties of the component fields in such a way that the kinetic part of the action will remain invariant. We find

$$\tilde{A} \to \tilde{A},$$

$$\boldsymbol{\psi} \to \lambda^{-1/2}\boldsymbol{\psi},$$

$$\tilde{F} \to \lambda^{-1}\tilde{F}.$$

The presence of a nonzero potential will break this conformal invariance.

APPENDIX F: TRANSFORMATION PROPERTIES OF SUPERSCALAR DENSITIES

Using the infinitesimal point transformation $X'^M = X^M + \delta u \Xi^M(X)$ we can define the Lie derivative of any supertensor field $T(X)$ by

$$\mathcal{L}_\Xi T(X) = \lim_{\delta u \to 0} \frac{T(X') - T'(X')}{\delta u}.$$

For instance, a superscalar transforms as $\Phi'(X') = \Phi(X)$, hence the Lie derivative can be calculated by using a Taylor expansion. We find

$$\mathcal{L}_\Xi \Phi(X) = \Xi^M \partial_M \Phi(X).$$

Now, let $\mathfrak{T}(X)$ be a superscalar density of weight +1. It is defined to transform as

$$\mathfrak{T}'(X') = J(X)\mathfrak{T}(X),$$

where $J(X)$ is given by the superdeterminant

$$J(X) = \mathrm{sdet}\left(\frac{\partial X^M}{\partial X'^N}\right) = 1 - \delta u(-1)^M \partial_M \Xi^M + \cdots .$$

Note that in the last line we have expanded the superdeterminant to first order, resulting in the appearance of a supertrace, this explains the factor $(-1)^M$ in the summation over M. Also we can expand

$$\mathfrak{T}(X') = \mathfrak{T}(X) + \delta u \Xi^M \partial_M \mathfrak{T}(X) + \cdots .$$

Combining these gives us the Lie derivative of a superscalar density

$$\mathcal{L}_\Xi \mathfrak{T}(X) = (-1)^M \partial_M (\Xi^M \mathfrak{T}(X)).$$

The same procedure can be used to calculate the Lie derivative of any supertensor field.

Using the Lie derivative we can describe the infinitesimal active coordinate transformation, $X \to X + \delta u \Xi$, alternatively as a transformation of the fields. We need to find the difference between the tensor which has been dragged along $\delta u \Xi$ to the point X, and the tensor which was already at X. For the supertensor field $T(X)$ this difference is given by

$$\delta T(X) = -\delta u \mathcal{L}_\Xi T(X).$$

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Level shift operator and second order perturbation theory

Jan Dereziński[a] and Rafal Früboes[b]
Department of Mathematical Methods in Physics, Warsaw University, Hoża 74, 00-682, Warsaw, Poland

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We give approximate formulas for spectrum and the corresponding spectral projections of perturbed linear operators. The main tool is the so-called *level shift operator*, which expresses the effects of second order perturbation theory on the point spectrum. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1850833]

I. INTRODUCTION

One of the main tools of quantum mechanics is perturbation theory for eigenvalues of family of linear operators of the form $L_\lambda := L_0 + \lambda Q$. This theory is particularly simple if one considers an isolated eigenvalue of L_0 of finite degeneracy and one assumes that L_0 and Q are self-adjoint. In this case, both the eigenvalues and the eigenvectors can be described by functions analytic in the coupling constant $e(\lambda)$. This is described in almost every textbook on quantum mechanics.

In quantum mechanics self-adjoint operators play a prominent role. However, non-self-adjoint operators are also physically relevant. For instance, they are used to describe resonances. In fact, resonances are often defined as complex eigenvalues of analytically deformed Hamiltonians, which are usually non-self-adjoint. The perturbation theory of non-self-adjoint operators is more complicated than that of self-adjoint operators. In the case of non-self-adjoint operators, eigenvalues and eigenvectors are typically described by a multivalued analytic function with a branch point at $\lambda = 0$. This is described, e.g., in Refs. 11 and 16.

The method of analytic functions may be inapplicable if the isolated eigenvalue has infinite degeneracy, because it may then happen that the perturbed operator has continuous spectrum close to the unperturbed eigenvalue. Thus one cannot follow individual eigenvalues.

In practice one is not interested in the full perturbation expansion of eigenvalues or eigenvectors. One usually uses the lowest order approximation. The first order approximation to the eigenvalue is very simple—it is just the appropriate matrix element of the perturbation. More interesting is the second order approximation. Its importance has been noted since the early days of quantum mechanics. Not without a reason the computations based on the second order perturbation theory have been called by Fermi the golden rule of quantum mechanics.

In our paper we describe a method of constructing approximate eigenvalues and approximate eigenprojections that summarizes the usual second order perturbation theory. We do not restrict ourselves to self-adjoint operators. We prove that our construction can be applied without any problem in the case when the eigenvalue has infinite multiplicity. Thus, the formulas that we give are quite robust—they do not need the assumptions typical of the usual approach to perturbation theory through expansion in a power series.

Let us now describe our results a little more closely. Suppose that L_0 is a closed operator having a cluster of isolated eigenvalues Ξ. The spectral projection of L_0 onto Ξ, denoted $\mathbf{1}_\Xi(L_0)$, gives a natural decomposition of the Banach space into a direct sum $\mathcal{H} = \mathcal{H}^v \oplus \mathcal{H}^{\bar{v}}$.

Let Q be a perturbation. Our main object is the perturbed operator

[a]Electronic mail: jan.derezinski@fuw.edu.pl
[b]Electronic mail: rafal.fruboes@fuw.edu.pl

$$L_{\lambda,\beta} := L_0 + \lambda(Q^{v\bar{v}} + Q^{\bar{v}v}) + \beta Q^{\bar{v}\bar{v}}.$$

Note that we assume that inside $\mathcal{H}^v$ the perturbation is zero. This guarantees that there is no first order shift of the spectrum. $Q^{v\bar{v}} + Q^{\bar{v}v}$ is the "off-diagonal" part of the perturbation—it connects $\mathcal{H}^v$ and $\mathcal{H}^{\bar{v}}$. $Q^{\bar{v}\bar{v}}$ is the "external" part of the perturbation—it acts inside $\mathcal{H}^{\bar{v}}$. We use two perturbation parameters, λ for the off-diagonal and β for the diagonal part. We are interested in what happens for small complex λ and β. We will try to estimate carefully the deviations from our predictions in terms of these two coupling constants.

It is easy to see that for small λ and β, the spectrum of $L_{\lambda,\beta}$ does not differ much from the spectrum L_0. Thus, for small λ and β, for any isolated point e of Ξ, there exists a patch of spectrum of $L_{\lambda,\beta}$ located around e, which we will denote by Θ_e. (We say "a patch," not "a cluster," because the spectrum does not have to be discrete.) We will give the formula for a projection p_e that approximates the spectral projection of $L_{\lambda,\beta}$ onto Θ_e. We will show that this projection approximately diagonalizes $L_{\lambda,\beta}$. By this we mean that $L - p_e L_{\lambda,\beta} p_e - (\mathbf{1} - p_e) L_{\lambda,\beta} (\mathbf{1} - p_e)$ is small.

The above results are contained in Theorem 2.1. They are quite easy. What is more interesting is the study of the splitting of the patch Θ_e, which is the subject of Theorem 2.3—the main result of our paper.

We show that if the eigenvalue e is semisimple then the patch of the spectrum around e naturally splits into subpatches separated by a distance of order $O(|\lambda|^2)$. The subpatches will be parametrized by eigenvalues of the so-called *level shift operator* (LSO). The level shift operator is a certain operator that describes the shift of spectrum under the influence of second order perturbation theory. The subpatch of the spectrum of $L_{\lambda,\beta}$ around $e + \lambda^2 m$, where m is an eigenvalue of the LSO, will be denoted by $\Theta_{e,m}$. We will also give a formula for the projection $p_{e,m}$ that approximates the spectral projection of $L_{\lambda,\beta}$ onto $\Theta_{e,m}$. Finally, we will show that $p_{e,m}$ approximately diagonalizes $L_{\lambda,\beta}$.

Clearly, the results that we present are quite general and applicable in many situations. The main motivation for our paper comes, however, from the class of problems first considered by Jaksic and Pillet in Refs. 12, 13, and 15. Using the terminology of Ref. 7 we can say that the results of our paper can be used to describe approximately resonances of Pauli–Fierz Liouvillean. The last section is devoted to a short description of this application.

Let us briefly explain what we mean by resonances of Pauli–Fierz Liouvilleans. We use the name "Pauli–Fierz system" to describe a quantum system consisting of a small system (e.g., an atom) interacting with a bosonic field (e.g., photons or phonons). We are especially interested in the case when the field has a positive density, for instance it is at a positive temperature. The dynamics of this system is generated by a certain self-adjoint operator, which, following Ref. 7, we call the "Pauli–Fierz Liouvillean." Next we apply the so-called Jaksic–Pillet method and we obtain an analytically deformed Pauli–Fierz Liouvillean. Analytically deformed Liouvilleans are non-self-adjoint and have spectrum in the lower half-plane. Moreover, they often have isolated eigenvalues. These eigenvalues are called resonances. They do not depend on the parameter of deformation. They are physically relevant, they are responsible for the decay of certain correlation functions. They can be naturally written as the sum of an explicit operator with discrete eigenvalues and a perturbation. The method of our paper allows us to give approximate predictions about the resonances.

Another class of operators (not discussed in our paper) where our results could be applied are the generators of a Pauli–Fierz dynamics on an operator algebra (called *C*-Liouvilleans in Ref. 14).

Level shift operators appear in the mathematics and physics literature in various disguises whenever the second order perturbation theory is considered. They are often introduced in the case of embedded eigenvalues. For instance, they appeared implicitly in the work of Ref. 6 devoted to the perturbation theory for embedded eigenvalues of Pauli–Fierz operators. The analysis of the point spectrum given in Ref. 6 is very closely related to the analysis given in our paper. Nevertheless, there are some differences. Reference 6 was devoted to the study of *embedded* eigenvalues, and therefore additional tools were required: the limiting absorption principle and Mourre's

positive commutator method. Another difference is the self-adjointness of the operator studied in Ref. 6, whereas in our paper we do not restrict ourselves to self-adjoint operators.

Constructions similar to ours can be found in the papers of Bach–Fröhlich–Sigal.[1,2] The authors study the spectrum of certain operators (similar to the Pauli–Fierz operators considered in Refs. 6 and 7) by an iterative procedure ("renormalization group"). The basic step of this procedure resembles our prescription for locating the spectrum and constructing the approximate spectral projection.

The LSO appears naturally in the so-called weak coupling (van Hove) limit.[4,5,8] In this context it is sometimes called the Davies generator.

II. MAIN RESULTS

A. Notation

If $\Xi \subset \Theta \subset \mathbb{C}$, then we say that Ξ is an isolated subset of Θ if it is closed and open in the relative topology of Θ.

Θ^{cl} denotes the closure of Θ in $\mathbb{C}$.

If L is a linear operator, $\mathrm{sp}\, L$ denotes its spectrum and $\mathrm{Dom}\, L$ its domain. If Ξ is an isolated and bounded subset of $\mathrm{sp}\, L$, then we can define the spectral projection of L onto Ξ by the formula

$$\mathbf{1}_{\Xi}(L) = \frac{1}{2\pi i}\oint_{\gamma} (z-L)^{-1}\, \mathrm{d}z,$$

where γ is a closed path that encircles Ξ counterclockwise.

If e is an isolated point of $\mathrm{sp}\, L$, then we will write $\mathbf{1}_e(L)$ for $\mathbf{1}_{\{e\}}(L)$. For such e set $N_e := (L-e)\mathbf{1}_e(L)$. We say that the degree of nilpotence of e is equal to n iff $N_e^{n-1} \neq 0$ but $N_e^n = 0$. We say that e is semisimple iff $n=1$ (i.e., $N_e = 0$).

If $\Theta \subset \mathbb{C}$ and $\epsilon > 0$, then we set

$$\mathrm{D}(\Theta, \epsilon) := \{z \in \mathbb{C} : \mathrm{dist}(z, \Theta) < \epsilon\}.$$

For $e \in \mathbb{C}$, $\mathrm{D}(e, \epsilon)$ will denote the open disc centered at e with radius ϵ. Moreover, we set $\mathrm{D}(\emptyset, \epsilon) := \emptyset$.

If $A(\lambda, \beta)$ are bounded operators, and $f(\lambda, \beta)$ a positive function, then

$$A(\lambda, \beta) = O(f(\lambda, \beta))$$

means that there exists c such that

$$\|A(\lambda, \beta)\| \leqslant c f(\lambda, \beta).$$

Moreover,

$$A_1(\lambda, \beta) = A_2(\lambda, \beta) + O(f(\lambda, \beta))$$

or

$$A_1(\lambda, \beta) \overset{O(f(\lambda,\beta))}{=} A_2(\lambda, \beta)$$

means that

$$A_1(\lambda, \beta) - A_2(\lambda, \beta) = O(f(\lambda, \beta)).$$

B. Assumptions

Let L_0 be a closed operator on a Banach space $\mathcal{H}$. Suppose that Ξ is an isolated bounded subset of $\mathrm{sp}\, L_0$.

It will be convenient to denote $\mathbf{1}_{\Xi}(L_0)$ by $\mathbf{1}^{vv}$ and set $\mathbf{1}^{\overline{vv}} := \mathbf{1} - \mathbf{1}^{vv}$. We can also introduce the subspaces

$$\mathcal{H}^v := \mathbf{1}^{vv}\mathcal{H}, \quad \mathcal{H}^{\overline{v}} := \mathbf{1}^{\overline{vv}}\mathcal{H},$$

so that $\mathcal{H}$ is decomposed into a direct sum

$$\mathcal{H} = \mathcal{H}^v \oplus \mathcal{H}^{\overline{v}}. \tag{2.1}$$

With respect to the decomposition (2.1) any operator B on $\mathcal{H}$ satisfying

$$\mathrm{Dom}(B) = (\mathrm{Dom}(B) \cap \mathcal{H}^v) \oplus (\mathrm{Dom}(B) \cap \mathcal{H}^{\overline{v}})$$

can be written as

$$B = \begin{bmatrix} B^{vv} & B^{v\overline{v}} \\ B^{\overline{v}v} & B^{\overline{vv}} \end{bmatrix}. \tag{2.2}$$

In particular, we have

$$L_0 = \begin{bmatrix} L_0^{vv} & 0 \\ 0 & L_0^{\overline{vv}} \end{bmatrix}. \tag{2.3}$$

It will be convenient to write E for L_0^{vv}. Note that E is a bounded operator on $\mathcal{H}^v$ and $\mathrm{sp}(E) = \overline{\Xi}$.

Let Q be another operator, that we will treat as a perturbation of L_0. More precisely, we make the following assumptions.

Assumption 2.A: $Q^{vv} = 0$.

Assumption 2.B: Off-diagonal elements of Q, i.e., $Q^{v\overline{v}}$ and $Q^{\overline{v}v}$, are bounded.

We will also use either one of the following two assumptions.

Assumption 2.C: $Q^{\overline{vv}}$ is an operator bounded perturbation of $L_0^{\overline{vv}}$ (Ref. 11).

Assumption 2.D: $\mathcal{H}^{\overline{vv}}$ is a Hilbert space, $L_0^{\overline{vv}}$ is self-adjoint, bounded from below and $Q^{\overline{vv}}$ is a form bounded perturbation of $L_0^{\overline{vv}}$ (Ref. 11).

Let $\lambda, \beta \in \mathbb{C}$. Note that under Assumption 2.C or 2.D the operator $L_0^{\overline{vv}} + \beta Q^{\overline{vv}}$ is well defined for small enough β (Ref. 11). Likewise,

$$L_{\lambda,\beta} := L_0 + \lambda Q^{v\overline{v}} + \lambda Q^{\overline{v}v} + \beta Q^{\overline{vv}} = \begin{bmatrix} E & \lambda Q^{v\overline{v}} \\ \lambda Q^{\overline{v}v} & L_0^{\overline{vv}} + \beta Q^{\overline{vv}} \end{bmatrix}$$

is well defined for small enough β. For simplicity we will write L instead of $L_{\lambda,\beta}$.

Fix an open subset $\Omega \subset \mathbb{C}$ such that $\Omega^{\mathrm{cl}} \cap \mathrm{sp}\, L_0 = \overline{\Xi}$ and $\Xi \subset \Omega$. Note that there exists β_0 such that, for $|\beta| \leqslant \beta_0$, $\mathrm{sp}(L_0^{\overline{vv}} + \beta Q^{\overline{vv}}) \cap \Omega^{\mathrm{cl}} = \varnothing$. We fix β_0 satisfying these conditions.

C. Results

The main results of our paper are stated in the following two theorems. Note that Theorem 2.1 is quite easy and basically describes the well-known stability of spectrum under a perturbation. Theorem 2.3 is more difficult—it describes the splitting of the spectrum according to second order perturbation theory. In that theorem, an important role is played by the level shift operator. Note that we tried to make the two theorems as parallel as possible.

Theorem 2.1: *Suppose that Assumptions 2.A and 2.B hold. We also suppose that either Assumption 2.C or 2.D is satisfied. Then the following is true:*

(1) *There exists a continuous and increasing function*

$$[0, \infty[\ni x \mapsto \delta(x) \in [0, \infty],$$

such that $\lim_{x \to 0} \delta(x) = 0$, *and for* $|\beta| < \beta_0$ *and* $|\lambda| < \lambda_0$, *for some* $\lambda_0 > 0$, *we have*

$$\mathrm{sp}(L) \cap \Omega \subset \mathrm{D}(\mathrm{sp}\, E, \delta(|\lambda|))^{\mathrm{cl}}. \tag{2.4}$$

(2) *In what follows we assume that* $\mathcal{E}$ *is an isolated subset of* sp E. *Clearly,* (1) *implies that there exists* $0<\lambda_{\mathcal{E}}$ *such that, for* $|\lambda|<\lambda_{\mathcal{E}}$,

$$\Theta_{\mathcal{E}} := \mathrm{D}(\mathcal{E}, \delta(|\lambda|))^{\mathrm{cl}} \cap \mathrm{sp}\, L \tag{2.5}$$

is an isolated subset of sp L *and* $\Theta_{\mathcal{E}} \subset \Omega$.

(3) *For* $|\lambda|<\lambda_{\mathcal{E}}$ *we have*

$$\mathbf{1}_{\Theta_{\mathcal{E}}}(L) - \mathbf{1}_{\mathcal{E}}(L_0) = O(|\lambda|). \tag{2.6}$$

(4) *For* $|\lambda|<\lambda_{\mathcal{E}}$ *we have*

$$\dim \mathbf{1}_{\Theta_{\mathcal{E}}}(L) = \dim \mathbf{1}_{\mathcal{E}}(L_0). \tag{2.7}$$

(5) *In what follows we assume that* e *is an isolated point of* sp E. *We will write* Θ_e *for* $\Theta_{\{e\}}$. *If the degree of nilpotence of* e *as an eigenvalue of* E *is equal to* n, *then there exists* C_e *such that*

$$\Theta_e \subset \mathrm{D}(e, C_e|\lambda|^{2/n})^{\mathrm{cl}}.$$

(6) *For*

$$|\lambda| < \|\mathbf{1}_e(L_0) Q^{v\overline{v}} (e\mathbf{1}^{\overline{v}\overline{v}} - L_0^{\overline{v}\overline{v}})^{-2} Q^{\overline{v}v} \mathbf{1}_e(L_0)\|^{-1/2} =: \widehat{\lambda_e}, \tag{2.8}$$

we set

$$\begin{aligned} p_e := {} & (\mathbf{1}_e(L_0) + \lambda (e\mathbf{1}^{\overline{v}\overline{v}} - L_0^{\overline{v}\overline{v}})^{-1} Q^{\overline{v}v} \mathbf{1}_e(L_0))(\mathbf{1}_e(L_0) + \lambda^2 \mathbf{1}_e(L_0) Q^{v\overline{v}} (e\mathbf{1}^{\overline{v}\overline{v}} - L_0^{\overline{v}\overline{v}})^{-2} Q^{\overline{v}v} \mathbf{1}_e(L_0))^{-1} \\ & \times (\mathbf{1}_e(L_0) + \lambda \mathbf{1}_e(L_0) Q^{v\overline{v}} (e\mathbf{1}^{\overline{v}\overline{v}} - L_0^{\overline{v}\overline{v}})^{-1}). \end{aligned} \tag{2.9}$$

Then p_e *is a projection. Moreover,*

(a)

$$\mathbf{1}_{\Theta_e}(L) - p_e = O(|\lambda|); \tag{2.10}$$

(b) *if* e *is a semisimple eigenvalue of* E *then*

$$\mathbf{1}_{\Theta_e}(L) - p_e = O(|\lambda|^2 + |\lambda\beta|); \tag{2.11}$$

(c) *if, in addition,* sp$(E)=\{e\}$, *then*

$$\mathbf{1}_{\Theta_e}(L) - p_e = O(|\lambda|^3 + |\lambda\beta|). \tag{2.12}$$

(7) *For* $|\lambda|<\widehat{\lambda_e}$ *we have*

(a)

$$L - p_e L p_e - (\mathbf{1} - p_e) L (\mathbf{1} - p_e) = O(|\lambda|); \tag{2.13}$$

(b) *if* e *is a semisimple eigenvalue of* E *then*

$$L - p_e L p_e - (\mathbf{1} - p_e) L (\mathbf{1} - p_e) = O(|\lambda|^2 + |\lambda\beta|); \tag{2.14}$$

(c) *if, moreover,* sp$(E)=\{e\}$ *then*

$$L - p_e L p_e - (\mathbf{1} - p_e) L (\mathbf{1} - p_e) = O(|\lambda|^3 + |\lambda\beta|). \tag{2.15}$$

Note that in Eq. (2.9) we use the notation $(e\mathbf{1}^{\overline{v}\overline{v}} - L^{\overline{v}\overline{v}})^{-1}$ for the inverse of the operator $e\mathbf{1}^{\overline{v}\overline{v}} - L^{\overline{v}\overline{v}}$ *restricted to* $\mathcal{H}^{\overline{v}}$. In what follows we will often use similar notation without a comment.

Let us now assume that sp E is a finite set.

Definition 2.2: We define the level shift operator (LSO) as

$$\Gamma := \sum_{e\in \mathrm{sp}(E)} \mathbf{1}_e(E) Q^{\nu\overline{\nu}} (e\mathbf{1}^{\overline{\nu}\overline{\nu}} - L_0^{\overline{\nu}\overline{\nu}})^{-1} Q^{\overline{\nu}\nu} \mathbf{1}_e(E).$$

From now on we will write for shortness $\Gamma^{ee} := \mathbf{1}_e(E)\Gamma\mathbf{1}_e(E)$.

Now we are ready to state our main theorem.

Theorem 2.3: Suppose that Assumptions 2.A and 2.B hold. We also assume either Assumption 2.C or 2.D. Assume also that sp E *is a finite set consisting of semisimple eigenvalues. Then the following is true:*

(1) *There exists a continuous and increasing function*

$$[0,\infty[\ni x \mapsto \delta(x) \in [0,\infty],$$

such that $\lim_{x\to 0}\delta(x)=0$, *and, for* $|\beta|<\beta_0$, $|\lambda|<\lambda_0$, *for some* $\lambda_0>0$, *we have*

$$\mathrm{sp}(L)\cap\Omega \subset \mathrm{D}(\mathrm{sp}(E+\lambda^2\Gamma), |\lambda|^2\delta(|\lambda|^2+|\beta|))^{\mathrm{cl}} = \bigcup_{e\in\mathrm{sp}(E)} \mathrm{D}(e+\lambda^2\,\mathrm{sp}(\Gamma^{ee}), |\lambda|^2\delta(|\lambda|^2+|\beta|))^{\mathrm{cl}}. \tag{2.16}$$

(2) *In what follows we fix* $e\in$ sp E, *and* $\mathcal{M}$ *is an isolated subset of* sp Γ^{ee}. *Clearly, (1) implies that there exists* $0<\lambda_{e,\mathcal{M}}$ *and* $0<\beta_{e,\mathcal{M}}$ *such that for* $|\lambda|<\lambda_{e,\mathcal{M}}$ *and* $|\beta|<\beta_{e,\mathcal{M}}$,

$$\Theta_{e,\mathcal{M}} := \mathrm{D}(e+\lambda^2\mathcal{M}, |\lambda|^2\delta(|\lambda|^2+|\beta|))^{\mathrm{cl}} \cap \mathrm{sp}\, L$$

is an isolated subset of sp L *and* $\Theta_{e,\mathcal{M}}\subset\Omega$.

(3) *For* $|\lambda|<\lambda_{e,\mathcal{M}}$ *and* $|\beta|<\beta_{e,\mathcal{M}}$ *we have*

$$\mathbf{1}_{\Theta_{e,\mathcal{M}}}(L) - \mathbf{1}_{\mathcal{M}}(\Gamma^{ee}) = O(|\lambda|+|\beta|). \tag{2.17}$$

(4) *For* $|\lambda|<\lambda_{e,\mathcal{M}}$ *and* $|\beta|<\beta_{e,\mathcal{M}}$ *we have*

$$\dim \mathbf{1}_{\Theta_{e,\mathcal{M}}}(L) = \dim \mathbf{1}_{\mathcal{M}}(\Gamma^{ee}). \tag{2.18}$$

(5) *Assume now that* m *is an isolated point of* sp Γ^{ee}. *We will write* $\Theta_{e,m}$ *for* $\Theta_{e,\{m\}}$. *Suppose that the degree of nilpotence of* m *as an eigenvalue of* Γ^{ee} *is equal to* n. *Then*

$$\Theta_{e,m} \subset \mathrm{D}(e+\lambda^2 m, C_{e,m}|\lambda|^2(|\lambda|^2+|\beta|)^{1/n})^{\mathrm{cl}},$$

for some $C_{e,m}>0$.

(6) *For*

$$|\lambda| < \|\mathbf{1}_m(\Gamma^{ee})Q^{\nu\overline{\nu}}(e\mathbf{1}^{\overline{\nu}\overline{\nu}} - L_0^{\overline{\nu}\overline{\nu}})^{-2}Q^{\overline{\nu}\nu}\mathbf{1}_m(\Gamma^{ee})\|^{-1/2} =: \widehat{\lambda_{e,m}}, \tag{2.19}$$

we set

$$\begin{aligned} p_{e,m} := {} & (\mathbf{1}_m(\Gamma^{ee}) + \lambda(e\mathbf{1}^{\overline{\nu}\overline{\nu}} - L_0^{\overline{\nu}\overline{\nu}})^{-1}Q^{\overline{\nu}\nu}\mathbf{1}_m(\Gamma^{ee}))(\mathbf{1}_m(\Gamma^{ee}) + \lambda^2\mathbf{1}_m(\Gamma^{ee})Q^{\nu\overline{\nu}}(e\mathbf{1}^{\overline{\nu}\overline{\nu}} - L_0^{\overline{\nu}\overline{\nu}})^{-2} \\ & \times Q^{\overline{\nu}\nu}\mathbf{1}_m(\Gamma^{ee}))^{-1}(\mathbf{1}_m(\Gamma^{ee}) + \lambda\mathbf{1}_m(\Gamma^{ee})Q^{\nu\overline{\nu}}(e\mathbf{1}^{\overline{\nu}\overline{\nu}} - L_0^{\overline{\nu}\overline{\nu}})^{-1}). \end{aligned} \tag{2.20}$$

Then $p_{e,m}$ *is a projection. Moreover*,

(a)

$$\mathbf{1}_{\Theta_{e,m}}(L) - p_{e,m} = O(|\lambda|+|\beta|); \tag{2.21}$$

(b) *if* m *is a semisimple eigenvalue of* Γ^{ee} *then*

$$\mathbf{1}_{\Theta_{e,m}}(L) - p_{e,m} = O(|\lambda|^2+|\beta|). \tag{2.22}$$

(7) *For* $|\lambda| < \widehat{\lambda_{e,m}}$ *we have*

(a)

$$L - p_{e,m}Lp_{e,m} - (\mathbf{1} - p_{e,m})L(\mathbf{1} - p_{e,m}) = O(|\lambda|^2 + |\lambda\beta|);$$

(b) *if* $\mathbf{1}^{vv} = \mathbf{1}_m(\Gamma^{ee})$ *then*

$$L - p_{e,m}Lp_{e,m} - (\mathbf{1} - p_{e,m})L(\mathbf{1} - p_{e,m}) = O(|\lambda|^3 + |\lambda\beta|).$$

Remark 2.4: Note that in both theorems (6) describes how close the projections p_e *and* $p_{e,m}$ *are to the corresponding spectral projections of* L *and (7) describes how well they diagonalize* L.

In Theorem 2.1, we have the same order of smallness in (6) and (7). We will see from the proof, that (7) essentially follows from (6).

On the other hand, in Theorem 2.3, the order of smallness of (7) is much better than that of (6). Thus (7) requires a separate proof.

III. PROOFS

Let us begin with a general fact about the stability of the spectrum of bounded operators (Ref. 11).

Theorem 3.1: *Let* $A \in B(\mathcal{H})$. *Then there exists an increasing and continuous function,*

$$[0,\infty\,[\ni x \mapsto \mu_A(x) \ \in [0,\infty],$$

such that $\lim_{x\to 0} \mu_A(x) = 0$ *and for any* $B \in B(\mathcal{H})$ *we have* $\mathrm{sp}(A+B) \subset \mathrm{D}(\mathrm{sp}(A), \mu_A(\|B\|))^{\mathrm{cl}}$.

If $a \in \mathrm{sp}(A)$ *is an isolated eigenvalue with the degree of nilpotence equal to* n, *then there exists* $\epsilon > 0$ *such that for* $z \in \mathrm{D}(a,\epsilon)\backslash\{a\}$ *we have*

$$\|(z - A)^{-1}\| \leqslant C|z - a|^{-n}, \tag{3.1}$$

for some $C > 0$. *Moreover, for* $|\lambda| < \Lambda_a$ *for some* $\Lambda_a > 0$ *we have*

$$\mathrm{sp}(A + \lambda B) \cap \mathrm{D}(a,\epsilon) \subset \mathrm{D}(a, c|\lambda|^{1/n})^{\mathrm{cl}}, \tag{3.2}$$

where $c = (C\|B\|)^{1/n}$.

Proof: We prove only the last statement. Let $|\lambda| < \epsilon^n(C\|B\|)^{-1}$. If $z \in \mathrm{D}(a,\epsilon)\backslash\mathrm{D}(a,(C\|\lambda B\|)^{1/n})^{\mathrm{cl}}$ then

$$|z - a| > (C\|\lambda B\|)^{1/n},$$

so by the inequality (3.1),

$$1 > C\|\lambda B\|\,|z - a|^{-n} \geqslant \|\lambda B\|\,\|(z - A)^{-1}\| \geqslant \|\lambda B(z - A)^{-1}\|.$$

This shows that $z - A - \lambda B$ is invertible and hence $z \notin \mathrm{sp}(A + \lambda B)$, so we get (3.2). ■

Let us comment on some additional notation that we will use. For $\mathcal{E}$ an isolated subset of $\mathrm{sp}(E)$ we will write

$$\mathbf{1}^{\mathcal{E}\mathcal{E}} := \mathbf{1}_{\mathcal{E}}(E) = \mathbf{1}_{\mathcal{E}}(L_0), \quad \mathbf{1}^{\overline{\mathcal{E}}\overline{\mathcal{E}}} := \mathbf{1} - \mathbf{1}^{\mathcal{E}\mathcal{E}}, \quad \mathbf{1}^{\underline{\mathcal{E}}\underline{\mathcal{E}}} := \mathbf{1}^{vv} - \mathbf{1}^{\mathcal{E}\mathcal{E}},$$

$$\mathcal{H}^{\mathcal{E}} := \mathrm{Ran}\,\mathbf{1}_{\mathcal{E}}(E), \quad \mathcal{H}^{\overline{\mathcal{E}}} := \mathrm{Ran}\,\mathbf{1}^{\overline{\mathcal{E}}\overline{\mathcal{E}}}, \quad \mathcal{H}^{\underline{\mathcal{E}}} := \mathrm{Ran}\,\mathbf{1}^{\underline{\mathcal{E}}\underline{\mathcal{E}}}.$$

Now the Banach space $\mathcal{H}$ can be decomposed in the following way:

$$\mathcal{H} = \mathcal{H}^{\mathcal{E}} \oplus \mathcal{H}^{\overline{\mathcal{E}}} = \mathcal{H}^{\mathcal{E}} \oplus \mathcal{H}^{\underline{\mathcal{E}}} \oplus \mathcal{H}^{\overline{v}},$$

and operator L can be written as

$$L = \begin{bmatrix} E^{\mathcal{E}\mathcal{E}} & \lambda Q^{\mathcal{E}\overline{\mathcal{E}}} \\ \lambda Q^{\overline{\mathcal{E}}\mathcal{E}} & L^{\overline{\mathcal{E}}\overline{\mathcal{E}}} \end{bmatrix} = \begin{bmatrix} E^{\mathcal{E}\mathcal{E}} & 0 & \lambda Q^{\mathcal{E}\overline{v}} \\ 0 & E^{\underline{\mathcal{E}}\underline{\mathcal{E}}} & \lambda Q^{\underline{\mathcal{E}}\overline{v}} \\ \lambda Q^{\overline{v}\mathcal{E}} & \lambda Q^{\overline{v}\underline{\mathcal{E}}} & L_0^{\overline{v}\overline{v}} + \beta Q^{\overline{v}\overline{v}} \end{bmatrix}. \tag{3.3}$$

If e is an isolated point of $\mathrm{sp}(E)$ then we write $\mathbf{1}^{ee}$ for $\mathbf{1}^{\{e\}\{e\}}$, $\mathcal{H}^e$ for $\mathcal{H}^{\{e\}}$, etc. Note that $E^{\overline{\mathcal{E}}\overline{\mathcal{E}}} = E^{\underline{\mathcal{E}}\underline{\mathcal{E}}}$.

We will use the following theorem for several operators and for various decompositions of the space $\mathcal{H}$.

Theorem 3.2: *Let H be a closed operator on a Banach space $\mathcal{H} = \mathcal{H}^{\underline{v}} \oplus \mathcal{H}^{\overline{v}}$. Assume that off-diagonal elements of H,* i.e., *$H^{\underline{v}\overline{v}}$* and *$H^{\overline{v}\underline{v}}$ are bounded. For $z \in \mathbb{C}\backslash \mathrm{sp}(H^{\underline{v}\underline{v}})$ define*

$$G_v(z) := z\mathbf{1}^{\underline{v}\underline{v}} - H^{\underline{v}\underline{v}} - H^{\underline{v}\overline{v}}(z\mathbf{1}^{\overline{v}\overline{v}} - H^{\overline{v}\overline{v}})^{-1}H^{\overline{v}\underline{v}}.$$

Then for $z \notin \mathrm{sp}(H^{\overline{v}\overline{v}})$ we have

(1) $z \in \mathrm{sp}(H)$ *iff* $0 \in \mathrm{sp}(G_v(z))$,
(2) *if* $0 \notin \mathrm{sp}(G_v(z))$ *then*

$$(z - H)^{-1} = (z\mathbf{1}^{\overline{v}\overline{v}} - H^{\overline{v}\overline{v}})^{-1} + (\mathbf{1}^{\underline{v}\underline{v}} + (z\mathbf{1}^{\overline{v}\overline{v}} - H^{\overline{v}\overline{v}})^{-1}H^{\overline{v}\underline{v}})G_v^{-1}(z)(\mathbf{1}^{\underline{v}\underline{v}} + H^{\underline{v}\overline{v}}(z\mathbf{1}^{\overline{v}\overline{v}} - H^{\overline{v}\overline{v}})^{-1}).$$

The last equation is often called the Feshbach formula. We will keep this name. For more information about the above theorem the reader is referred to Refs. 6 and 10.

Lemma 3.3: Suppose that Assumptions 2.A and 2.B hold. We also assume either Assumption 2.C or 2.D. Let $\mathcal{E}$ be an isolated subset of $\mathrm{sp}(E)$ *and fix $r > 0$. Then there exists $0 < \Lambda_{\mathcal{E}}$ such that for $|\lambda| < \Lambda_{\mathcal{E}}$, $|\beta| < \beta_0$ we have $(\Omega\backslash \mathrm{D}(\mathrm{sp}(E^{\overline{\mathcal{E}}\overline{\mathcal{E}}}), r)) \cap \mathrm{sp}(L^{\overline{\mathcal{E}}\overline{\mathcal{E}}}) = \emptyset$ and*

$$\sup_{\substack{z \in \Omega\backslash \mathrm{D}(\mathrm{sp}(E^{\overline{\mathcal{E}}\overline{\mathcal{E}}}), r) \\ |\lambda| < \Lambda_{\mathcal{E}},\ |\beta| < \beta_0}} \|(z\mathbf{1}^{\overline{\mathcal{E}}\overline{\mathcal{E}}} - L^{\overline{\mathcal{E}}\overline{\mathcal{E}}})^{-1}\| < \infty. \tag{3.4}$$

Proof: If $z \in \Omega$ and $|\beta| < \beta_0$ then $z \notin \mathrm{sp}(L^{\overline{v}\overline{v}})$ and hence we can use the Theorem 3.2 for the operator $L^{\overline{\mathcal{E}}\overline{\mathcal{E}}}$ and for decomposition $\mathcal{H}^{\overline{\mathcal{E}}} := \mathcal{H}^{\underline{\mathcal{E}}} \oplus \mathcal{H}^{\overline{v}}$. We obtain that, for some $\Lambda_{\mathcal{E}} > 0$, and $|\lambda| < \Lambda_{\mathcal{E}}$ and for $z \in \Omega\backslash \mathrm{D}(\mathrm{sp}(E^{\underline{\mathcal{E}}\underline{\mathcal{E}}}), r)$,

$$G_{\underline{\mathcal{E}}}(z) = z\mathbf{1}^{\underline{\mathcal{E}}\underline{\mathcal{E}}} - E^{\underline{\mathcal{E}}\underline{\mathcal{E}}} - \lambda^2 Q^{\underline{\mathcal{E}}\overline{v}}(z\mathbf{1}^{\overline{v}\overline{v}} - L^{\overline{v}\overline{v}})^{-1}Q^{\overline{v}\underline{\mathcal{E}}},$$

is invertible and hence $z \notin \mathrm{sp}(L^{\overline{\mathcal{E}}\overline{\mathcal{E}}})$. Moreover, for such z, $G_{\underline{\mathcal{E}}}(z)$ has a uniformly bounded inverse. Therefore, the Feshbach formula implies (3.4). ∎

Proof of the Theorem 2.1: (1) By Theorem 3.2, $z \in \mathrm{sp}(L) \cap \Omega$ iff $z \in \mathrm{sp}(E + \lambda^2 Q^{\underline{v}\overline{v}}(z1^{\overline{v}\overline{v}} - L^{\overline{v}\overline{v}})^{-1}Q^{\overline{v}\underline{v}}) \cap \Omega$. By Theorem 3.1,

$$\mathrm{sp}(E + \lambda^2 Q^{\underline{v}\overline{v}}(z\mathbf{1}^{\overline{v}\overline{v}} - L^{\overline{v}\overline{v}})^{-1}Q^{\overline{v}\underline{v}}) \subset \mathrm{D}(\mathrm{sp}(E), \mu_E(|\lambda|^2 c))^{\mathrm{cl}},$$

where

$$c = \sup_{z \in \Omega, |\beta| < \beta_0} \|Q^{\underline{v}\overline{v}}(z\mathbf{1}^{\overline{v}\overline{v}} - L^{\overline{v}\overline{v}})^{-1}Q^{\overline{v}\underline{v}}\|,$$

(which as we know is finite), and $\mu_E : [0, \infty[\to [0, \infty[$ is a continuous increasing function with $\lim_{x \to 0} \mu_E(x) = 0$. Thus $\mathrm{sp}(L) \cap \Omega \subset \mathrm{D}(\mathrm{sp}(E), \delta(|\lambda|))^{\mathrm{cl}}$, where $\delta(x) = \mu_E(x^2 c)$.

(2) A simple consequence of (1).

(3) For some $0 < \lambda_{\mathcal{E}}$, $|\lambda| < \lambda_{\mathcal{E}}$, and $|\beta| < \beta_0$, there exists a closed path $\gamma \subset \Omega$ that encircles $\Theta_{\mathcal{E}}$ counterclockwise, but no other parts of $\mathrm{sp}(L)$. We have

$$\sup_{\substack{z\in\gamma,\ |\beta|<\beta_0\\ |\lambda|<\lambda_{\mathcal{E}}}} \|(z-L)^{-1}\|<\infty.$$

Besides,

$$(2\pi i)^{-1}\oint_\gamma (z\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}\,\mathrm{d}z=(2\pi i)^{-1}\oint_\gamma (z\mathbf{1}^{\overline{vv}}-L^{\overline{vv}})^{-1}\,\mathrm{d}z=0.$$

Therefore,

$$\begin{aligned}\mathbf{1}_{\Theta_{\mathcal{E}}}(L)-\mathbf{1}_{\mathcal{E}}(L_0)&=(2\pi i)^{-1}\oint_\gamma ((z\mathbf{1}-L)^{-1}-(z\mathbf{1}^{vv}-E)^{-1}-(z\mathbf{1}^{\overline{vv}}-L^{\overline{vv}})^{-1})\mathrm{d}z\\ &=\lambda(2\pi i)^{-1}\oint_\gamma (z\mathbf{1}-L)^{-1}(Q^{v\overline{v}}+Q^{\overline{v}v})((z\mathbf{1}^{vv}-E)^{-1}+(z\mathbf{1}^{\overline{vv}}-L^{\overline{vv}})^{-1})\mathrm{d}z=O(|\lambda|).\end{aligned}$$

(4) Equation (2.6) implies that for $|\lambda|$ sufficiently small we have $\|\mathbf{1}_{\Theta_{\mathcal{E}}}(L)-\mathbf{1}_{\mathcal{E}}(L_0)\|<1$ so by a well-known theorem (Ref. 11) Eq. (2.7) holds for $|\lambda|$ small. But $\lambda\mapsto\dim\mathbf{1}_{\Theta_{\mathcal{E}}}(L)\in\mathbb{N}$ is a continuous function so (2.7) holds for all $|\lambda|<\lambda_{\mathcal{E}}$.

(5) Let $\mathcal{E}$, r, and $\Lambda_{\mathcal{E}}$ be the same as in the Lemma 3.3. For $|\lambda|<\Lambda_{\mathcal{E}}$, $|\beta|<\beta_0$, we can use Theorem 3.2, which implies that for $z\in\Omega\backslash\mathrm{D}(\mathrm{sp}(E^{\overline{\mathcal{E}}\overline{\mathcal{E}}}),r)$ we have $z\in\mathrm{sp}(L)$ iff

$$z\in\mathrm{sp}(E^{\mathcal{E}\mathcal{E}}+\lambda^2Q^{\mathcal{E}\overline{\mathcal{E}}}(z\mathbf{1}^{\overline{\mathcal{E}}\overline{\mathcal{E}}}-L^{\overline{\mathcal{E}}\overline{\mathcal{E}}})^{-1}Q^{\overline{\mathcal{E}}\mathcal{E}}).$$

By Theorem 3.1 we get

$$\mathrm{sp}(E^{\mathcal{E}\mathcal{E}}+\lambda^2Q^{\mathcal{E}\overline{\mathcal{E}}}(z\mathbf{1}^{\overline{\mathcal{E}}\overline{\mathcal{E}}}-L^{\overline{\mathcal{E}}\overline{\mathcal{E}}})^{-1}Q^{\overline{\mathcal{E}}\mathcal{E}})\subset\mathrm{D}(\mathcal{E},\mu_{E^{\mathcal{E}\mathcal{E}}}(|\lambda|^2c))^{\mathrm{cl}},\tag{3.5}$$

where

$$c:=\sup_{\substack{z\in\Omega\backslash\mathrm{D}(\mathrm{sp}(E^{\overline{\mathcal{E}}\overline{\mathcal{E}}}),r)\\ |\beta|<\beta_0,\ |\lambda|<\Lambda_{\mathcal{E}}}}\|Q^{\mathcal{E}\overline{\mathcal{E}}}(z\mathbf{1}^{\overline{\mathcal{E}}\overline{\mathcal{E}}}-L^{\overline{\mathcal{E}}\overline{\mathcal{E}}})^{-1}Q^{\overline{\mathcal{E}}\mathcal{E}}\|$$

is finite by Lemma 3.3.

Now set $\mathcal{E}=\{e\}$ and assume that e has a degree of nilpotence equal to n. Then by Theorem 3.1 we can take $\mu_{E^{ee}}(x):=c_1x^{1/n}$.

(6) For $|\lambda|<\widehat{\lambda_e}$,

$$\mathbf{1}^{ee}+\lambda^2Q^{e\overline{v}}(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-2}Q^{\overline{v}e},$$

is an invertible operator so the expression for p_e makes sense. Direct computations show that $p_e^2=p_e$. Note that

$$(\mathbf{1}^{ee}+\lambda^2Q^{e\overline{v}}(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-2}Q^{\overline{v}e})^{-1}=\mathbf{1}^{ee}-\lambda^2Q^{e\overline{v}}(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-2}Q^{\overline{v}e}+O(\lambda^4)$$

so

$$\begin{aligned}p_e=\mathbf{1}^{ee}&+\lambda(Q^{e\overline{v}}(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}+(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}Q^{\overline{v}e})+\lambda^2((e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}Q^{\overline{v}e}Q^{e\overline{v}}(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}\\ &-Q^{e\overline{v}}(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-2}Q^{\overline{v}e})+O(|\lambda|^3).\end{aligned}\tag{3.6}$$

We have

$$\mathbf{1}_{\Theta_e}(L) = \mathbf{1}_e(L_0) + \lambda(2\pi i)^{-1}\oint_\gamma ((z\mathbf{1}^{vv} - E)^{-1}Q^{v\overline{v}}(z\mathbf{1}^{\overline{vv}} - L_0^{\overline{vv}})^{-1} + (z\mathbf{1}^{\overline{vv}} - L_0^{\overline{vv}})^{-1}Q^{\overline{v}v}(z\mathbf{1}^{vv} - E)^{-1})\mathrm{d}z$$
$$+ \lambda^2(2\pi i)^{-1}\oint_\gamma ((z\mathbf{1}^{vv} - E)^{-1}Q^{v\overline{v}}(z\mathbf{1}^{\overline{vv}} - L_0^{\overline{vv}})^{-1}Q^{\overline{v}v}(z\mathbf{1}^{vv} - E)^{-1}$$
$$+ (z\mathbf{1}^{\overline{vv}} - L_0^{\overline{vv}})^{-1}Q^{\overline{v}v}(z\mathbf{1}^{vv} - E)^{-1}Q^{v\overline{v}}(z\mathbf{1}^{\overline{vv}} - L_0^{\overline{vv}})^{-1})\mathrm{d}z + O(|\lambda|^3 + |\lambda\beta|).$$

e is the only one eigenvalue of E inside γ so $(z\mathbf{1}^{vv}-E)^{-1}$ has only one pole inside γ. All points on and inside γ are not in $\mathrm{sp}(L_0^{\overline{ee}})$ so $(z\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}$ is analytic inside and continuous on γ. If e is semisimple then $(z\mathbf{1}^{vv}-E)^{-1}=(z-e)^{-1}\mathbf{1}^{ee}+$*analytic part* and hence

$$\mathbf{1}_{\Theta_e}(L) = \mathbf{1}_e(L_0) + \lambda(Q^{e\overline{v}}(e\mathbf{1}^{\overline{vv}} - L_0^{\overline{vv}})^{-1} + (e\mathbf{1}^{\overline{vv}} - L_0^{\overline{vv}})^{-1}Q^{\overline{v}e}) + \lambda^2\Bigg((2\pi i)^{-1}\oint_\gamma (z\mathbf{1}^{vv} - E)^{-1}Q^{v\overline{v}}$$
$$\times(z\mathbf{1}^{\overline{vv}} - L_0^{\overline{vv}})^{-1}Q^{\overline{v}v}(z\mathbf{1}^{vv} - E)^{-1}\,\mathrm{d}z + (e\mathbf{1}^{\overline{vv}} - L_0^{\overline{vv}})^{-1}Q^{\overline{v}e}Q^{e\overline{v}}(e\mathbf{1}^{\overline{vv}} - L_0^{\overline{vv}})^{-1}\Bigg) + O(|\lambda|^3$$
$$+ |\lambda\beta|). \tag{3.7}$$

Now part (b) [Eq. (2.11)] is a simple consequence of (3.7) and (3.6). In general, when e is not semisimple, terms of order $O(|\lambda|)$ will not cancel so part (a) [Eq. (2.10)] cannot be improved.

If $\mathrm{sp}(E)=\{e\}$ and e is semisimple then $(z\mathbf{1}^{vv}-E)^{-1}=(z-e)^{-1}\mathbf{1}^{ee}=(z-e)^{-1}\mathbf{1}^{vv}$. Now

$$(2\pi i)^{-1}\oint_\gamma (z\mathbf{1}^{vv} - E)^{-1}Q^{v\overline{v}}(z\mathbf{1}^{\overline{vv}} - L_0^{\overline{vv}})^{-1}Q^{\overline{v}v}(z\mathbf{1}^{vv} - E)^{-1}\,\mathrm{d}z = -\,Q^{e\overline{v}}(e\mathbf{1}^{\overline{vv}} - L_0^{\overline{vv}})^{-2}Q^{\overline{v}e}.$$

Now part (c) [Eq. (2.12)] is a simple consequence of (3.7) and (3.6).

(7) The proof of (6) in the cases (a), (b), and (c) shows actually slightly improved results,

$$(\mathbf{1}_{\Theta_e}(L) - p_e)L = O(|\lambda|), \quad O(|\lambda|^2 + |\lambda\beta|), \quad \text{and } O(|\lambda|^3 + |\lambda\beta|),$$

$$L(\mathbf{1}_{\Theta_e}(L) - p_e) = O(|\lambda|), \quad O(|\lambda|^2 + |\lambda\beta|), \quad \text{and } O(|\lambda|^3 + |\lambda\beta|).$$

To obtain (7) we use

$$L - p_eLp_e - (\mathbf{1} - p_e)L(\mathbf{1} - p_e) = -\,[p_e,[p_e,L]] = -\,[p_e,[p_e - \mathbf{1}_e(L),L]].$$

■

Proof of the Theorem 2.3: (1) Let $e\in\mathrm{sp}(E)$. Let $\mathcal{E}=\{e\}$, $\Lambda_e=\Lambda_{\mathcal{E}}$ and r be the same as in the Lemma 3.3 and in the proof of (5) of the previous theorem. For $|\lambda|<\Lambda_e$, $|\beta|<\beta_0$ and for $z\in\Omega\backslash\mathrm{D}(\mathrm{sp}(E^{\overline{ee}}),r)$ we can use Theorem 3.2 for the operator L and for decomposition $\mathcal{H}:=\mathcal{H}^e\oplus\mathcal{H}^{\overline{e}}$. If $z\in\mathrm{sp}(L)\cap\Omega\backslash\mathrm{D}(\mathrm{sp}(E^{\overline{ee}}),r)$ then

$$0\in\mathrm{sp}(z\mathbf{1}^{ee} - E^{ee} - \lambda^2Q^{e\overline{e}}(z\mathbf{1}^{\overline{ee}} - L^{\overline{ee}})^{-1}Q^{\overline{e}e}). \tag{3.8}$$

Note that $e\in\mathrm{sp}(E)$ is semisimple so $E^{ee}=e\mathbf{1}^{ee}$ and moreover, we have $Q^{\overline{e}e}=Q^{\overline{v}e}$ and $Q^{e\overline{e}}=Q^{e\overline{v}}$. Now (3.8) can be written as

$$\frac{z-e}{\lambda^2}\in\mathrm{sp}(Q^{e\overline{v}}(z\mathbf{1}^{\overline{ee}} - L^{\overline{ee}})^{-1}Q^{\overline{v}e}). \tag{3.9}$$

Note that

$$(z\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1} = (e\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1} + (e-z)(z\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1}(e\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1}$$
$$= (e\mathbf{1}^{\underline{e}\underline{e}} - L_0^{\underline{e}\underline{e}})^{-1} + (e\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1}(\lambda(Q^{\underline{e}\overline{v}} + Q^{\overline{v}\underline{e}}) + \beta Q^{\overline{v}\overline{v}})(e\mathbf{1}^{\underline{e}\underline{e}} - L_0^{\underline{e}\underline{e}})^{-1}$$
$$+ (e-z)(z\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1}(e\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1}, \tag{3.10}$$

and $(e\mathbf{1}^{\underline{e}\underline{e}} - L_0^{\underline{e}\underline{e}})^{-1} = (e\mathbf{1}^{\underline{e}\underline{e}} - E^{\underline{e}\underline{e}})^{-1} + (e\mathbf{1}^{\overline{v}\overline{v}} - L_0^{\overline{v}\overline{v}})^{-1}$. Now we can write

$$Q^{e\overline{v}}(z\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1}Q^{\overline{v}e} = \Gamma^{ee} + \mathbf{I} + \mathbf{II} + \mathbf{III}, \tag{3.11}$$

where

$$\mathbf{I} = \beta Q^{e\overline{v}}(e\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1}Q^{\overline{v}\overline{v}}(e\mathbf{1}^{\underline{e}\underline{e}} - L_0^{\underline{e}\underline{e}})^{-1}Q^{\overline{v}e},$$

$$\mathbf{II} = \lambda Q^{e\overline{v}}(e\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1}(Q^{\overline{v}\underline{e}} + Q^{\underline{e}\overline{v}})(e\mathbf{1}^{\underline{e}\underline{e}} - L_0^{\underline{e}\underline{e}})^{-1}Q^{\overline{v}e}, \tag{3.12}$$

$$\mathbf{III} = (e-z)Q^{e\overline{v}}(z\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1}(e\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1}Q^{\overline{v}e}.$$

Clearly, $\|\mathbf{I}\| \leqslant C_{\mathrm{I}}|\beta|$. If we note that

$$\mathbf{1}^{\overline{v}\overline{v}}(e\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1}\mathbf{1}^{\underline{e}\underline{e}} = \lambda(e\mathbf{1}^{\overline{v}\overline{v}} - L^{\overline{v}\overline{v}})^{-1}Q^{\overline{v}\underline{e}}G_{\underline{e}}^{-1}(e) = O(\lambda)$$

and similarly $\mathbf{1}^{\underline{e}\underline{e}}(e\mathbf{1}^{\underline{e}\underline{e}} - L^{\underline{e}\underline{e}})^{-1}\mathbf{1}^{\overline{v}\overline{v}} = O(\lambda)$ then we get $\|\mathbf{II}\| \leqslant C_{\mathrm{II}}|\lambda|^2$. Moreover, Theorem 2.1 implies that $|z-e| < C\lambda^2$ and hence by the Lemma 3.3 [Eq. (3.4)] we get $\|\mathbf{III}\| \leqslant C_{\mathrm{III}}\lambda^2$. So for $|\lambda| < \Lambda_e$ and $|\beta| < \beta_0$ we have

$$\|\mathbf{I} + \mathbf{II} + \mathbf{III}\| < C_e(|\lambda|^2 + |\beta|)$$

for some $C_e > 0$. Now we can apply the Theorem 3.1 to the expression (3.9) and get for $|\lambda| < \Lambda_e$ and $|\beta| < \beta_0$,

$$\frac{z-e}{\lambda^2} \in \mathrm{D}(\mathrm{sp}(\Gamma^{ee}), \mu_{\Gamma^{ee}}(C_e(|\lambda|^2 + |\beta|)))^{\mathrm{cl}}, \tag{3.13}$$

where functions $\mu_{\Gamma^{ee}}: [0,\infty[\to [0,\infty]$ are continuous, increasing and $\lim_{x\to 0}\mu_{\Gamma^{ee}}(x) = 0$. This implies

$$\mathrm{sp}(L) \cap \Omega \setminus \mathrm{D}(\mathrm{sp}(E^{\underline{e}\underline{e}}), r) \subset \mathrm{D}(e + \lambda^2\,\mathrm{sp}(\Gamma^{ee}), |\lambda|^2\mu_{\Gamma^{ee}}(C_e(|\lambda|^2 + |\beta|)))^{\mathrm{cl}},$$

and hence for $|\lambda| < \lambda_0 := \min_{e\in\mathrm{sp}(E)}\Lambda_e$ and $|\beta| < \beta_0$ we have

$$\mathrm{sp}(L) \cap \Omega \subset \bigcup_{e\in\mathrm{sp}(E)} \mathrm{D}(e + \lambda^2\,\mathrm{sp}(\Gamma^{ee}), |\lambda|^2\delta(|\lambda|^2 + |\beta|))^{\mathrm{cl}},$$

where we denoted $\delta(x) := \max_{e\in\mathrm{sp}(E)}(\mu_{\Gamma^{ee}}(C_e x))$.

(2) A simple consequence of (1).

(3) Let γ be a closed path such that γ encircles $\mathcal{M}$ but no other parts of $\mathrm{sp}(\Gamma^{ee})$. By (1) and (2), for small enough λ and β, the translated and rescaled path $e+\lambda^2\gamma$ encircles only $\Theta_{e,\mathcal{M}}$ but no other parts of $\mathrm{sp}(L)$. Now

$$\mathbf{1}_{\Theta_{e,\mathcal{M}}}(L) = (2\pi i)^{-1}\oint_{e+\lambda^2\gamma} \frac{1}{\eta\mathbf{1} - L}\mathrm{d}\eta.$$

For all $\eta \in e+\lambda^2\gamma$ we can use Feshbach formula for the operator L and for the decomposition $\mathcal{H} = \mathcal{H}^e \oplus \mathcal{H}^{\overline{e}}$. We get

$$\oint_{e+\lambda^2\gamma}(\eta\mathbf{1}-L)^{-1}\,\mathrm{d}\eta=\oint_{e+\lambda^2\gamma}(\mathbf{1}^{ee}+(\eta\mathbf{1}^{\overline{ee}}-L^{\overline{ee}})^{-1}\lambda Q^{\overline{ee}})G_e^{-1}(\eta)(\mathbf{1}^{ee}+\lambda Q^{e\overline{e}}(\eta\mathbf{1}^{\overline{ee}}-L^{\overline{ee}})^{-1})\mathrm{d}\eta,$$

where

$$G_e(\eta)=\eta\mathbf{1}^{ee}-e\mathbf{1}^{ee}-\lambda^2Q^{e\overline{e}}(\eta\mathbf{1}^{\overline{ee}}-L^{\overline{ee}})^{-1}Q^{\overline{e}e}.$$

Note that

$$\begin{aligned}((\eta-e)\mathbf{1}^{ee}-\lambda^2\Gamma^{ee})^{-1}-G_e^{-1}(\eta)=\lambda^2((\eta-e)\mathbf{1}^{ee}-\lambda^2\Gamma^{ee})^{-1}Q^{e\overline{v}}((e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}\\ -\mathbf{1}^{\overline{vv}}(\eta\mathbf{1}^{\overline{ee}}-L^{\overline{ee}})^{-1}\mathbf{1}^{\overline{vv}})Q^{\overline{v}e}G_e^{-1}(\eta),\end{aligned}\tag{3.14}$$

where we used $Q^{\overline{v}e}=Q^{\overline{e}\overline{e}}$ and $Q^{e\overline{v}}=Q^{e\overline{e}}$. Moreover,

$$\begin{aligned}&(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}-\mathbf{1}^{\overline{vv}}(\eta\mathbf{1}^{\overline{ee}}-L^{\overline{ee}})^{-1}\mathbf{1}^{\overline{vv}}\\ &\quad=(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}-(\eta\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}}-\beta Q^{\overline{vv}})^{-1}-\lambda^2(\eta\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}}-\beta Q^{\overline{vv}})^{-1}Q^{\overline{v}\underline{e}}G_{\underline{e}}^{-1}(\eta)\\ &\qquad\times Q^{\underline{e}\overline{v}}(\eta\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}}-\beta Q^{\overline{vv}})^{-1}\\ &\quad=(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}((\eta-e)\mathbf{1}^{\overline{vv}}+\beta Q^{\overline{vv}})(\eta\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}}-\beta Q^{\overline{vv}})^{-1}-\lambda^2(\eta\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}}-\beta Q^{\overline{vv}})^{-1}\\ &\qquad\times Q^{\overline{v}\underline{e}}G_{\underline{e}}^{-1}(\eta)Q^{\underline{e}\overline{v}}(\eta\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}}-\beta Q^{\overline{vv}})^{-1},\end{aligned}\tag{3.15}$$

where

$$G_{\underline{e}}(\eta)=\eta\mathbf{1}^{\underline{ee}}-E^{\underline{ee}}-\lambda^2Q^{\underline{e}\overline{v}}(\eta\mathbf{1}^{\overline{vv}}-L^{\overline{vv}})^{-1}Q^{\overline{v}\underline{e}}.$$

If we change the variable $\eta=e+\lambda^2z$ and use the equations (3.14) and (3.15) we get

$$\begin{aligned}\oint_{e+\lambda^2\gamma}(\eta\mathbf{1}-L)^{-1}\,\mathrm{d}\eta=\oint_{\gamma}(\mathbf{1}^{ee}+((e+\lambda^2z)\mathbf{1}^{\overline{ee}}-L^{\overline{ee}})^{-1}\lambda Q^{\overline{ee}})(z\mathbf{1}^{ee}-\Gamma^{ee})^{-1}\\ \times(\mathbf{1}^{ee}+\lambda Q^{e\overline{e}}((e+\lambda^2z)\mathbf{1}^{\overline{ee}}-L^{\overline{ee}})^{-1})\mathrm{d}z+O(|\lambda|^2+|\beta|).\end{aligned}\tag{3.16}$$

Since

$$(2\pi i)^{-1}\oint_{\gamma}(z\mathbf{1}^{ee}-\Gamma^{ee})^{-1}\,\mathrm{d}z=\mathbf{1}_{\mathcal{M}}(\Gamma^{ee}),$$

we get $\mathbf{1}_{\Theta_{e,\mathcal{M}}}(L)-\mathbf{1}_{\mathcal{M}}(\Gamma^{ee})=O(|\lambda|+|\beta|)$.

(4) Equation (2.17) implies that for $|\lambda|$ and $|\beta|$ sufficiently small we have $\|\mathbf{1}_{\Theta_{e,\mathcal{M}}}(L)-\mathbf{1}_{\mathcal{M}}(\Gamma^{ee})\|<1$ so by a well-known theorem (Ref. 11) equality (2.18) holds. But $\dim\mathbf{1}_{\Theta_{\mathcal{E}}}(L)\in\mathbb{N}$ is a continuous function of λ and β so (2.18) holds for all $|\lambda|<\lambda_{e,\mathcal{M}}$ and $|\beta|<\beta_{e,\mathcal{M}}$.

(5) If the degree of nilpotence of m as an eigenvalue of Γ^{ee} is n then due to the Theorem 3.1, Eq. (3.13) can be written as

$$\frac{z-e}{\lambda^2}\in\mathrm{D}(m,C_{e,m}(|\lambda|^2+|\beta|)^{1/n})^{\mathrm{cl}}\cup\mathrm{D}(\mathrm{sp}(\Gamma^{ee})\setminus\{m\},\mu_{\Gamma^{ee}}(C_e(|\lambda|^2+|\beta|)))^{\mathrm{cl}}.$$

(6) For $|\lambda|<\widehat{\lambda_{e,m}}$,

$$\mathbf{1}_m(\Gamma^{ee})+\lambda^2\mathbf{1}_m(\Gamma^{ee})Q^{v\overline{v}}(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-2}Q^{\overline{vv}}\mathbf{1}_m(\Gamma^{ee})$$

is an invertible operator so the expression for $p_{e,m}$ makes sense. Direct computations show that $p_{e,m}^2=p_{e,m}$.

In the proof of the part (3) we showed that $\mathbf{1}_{\Theta_{e,m}}(L)=\mathbf{1}_m(\Gamma^{ee})+O(|\lambda|+|\beta|)$ so (a) is already done. To show (b), we use the approximation for $\mathbf{1}_{\Theta_{e,m}}(L)$ given by (3.16);

$$\begin{aligned}\mathbf{1}_{\Theta_{e,m}}(L) &\overset{O(|\lambda^2|+|\beta|)}{=} \frac{1}{2\pi i}\oint_\gamma (\lambda((e+\lambda^2 z)\mathbf{1}^{\overline{ee}}-L^{\overline{ee}})^{-1}Q^{\overline{ee}}+\mathbf{1}^{ee})(z\mathbf{1}^{ee}-\Gamma^{ee})^{-1}\\ &\times(\lambda Q^{\overline{ee}}((e+\lambda^2 z)\mathbf{1}^{\overline{ee}}-L^{\overline{ee}})^{-1}+\mathbf{1}^{ee})\mathrm{d}z \overset{O(|\lambda^2|+|\lambda\beta|)}{=} \frac{1}{2\pi i}\oint_\gamma (\lambda(e+\lambda^2 z)\ \mathbf{1}^{\overline{ee}}-L_0^{\overline{ee}})^{-1}\\ &\times Q^{\overline{ee}}+\mathbf{1}^{ee})(z\mathbf{1}^{ee}-\Gamma^{ee})^{-1}(\lambda Q^{e\overline{e}}((e+\lambda^2 z)\mathbf{1}^{\overline{ee}}-L_0^{\overline{ee}})^{-1}+\mathbf{1}^{ee})\mathrm{d}z\\ &=(\lambda((e+\lambda^2 m)\mathbf{1}^{\overline{ee}}-L_0^{\overline{ee}})^{-1}Q^{\overline{ee}}+\mathbf{1}^{ee})\mathbf{1}_m(\Gamma^{ee})(\lambda Q^{e\overline{e}}((e+\lambda^2 m)\mathbf{1}^{\overline{ee}}-L_0^{\overline{ee}})^{-1}+\mathbf{1}^{ee}) \overset{O(|\lambda|^3)}{=} p_{e,m},\end{aligned}$$

where we used

$$((e+\lambda^2 z)\mathbf{1}^{\overline{ee}}-L_0^{\overline{ee}})^{-1}-((e+\lambda^2 z)\mathbf{1}^{\overline{ee}}-L^{\overline{ee}})^{-1}=O(|\lambda|+|\beta|).$$

(7) Let us denote $\mathbf{1}^{mm}:=\mathbf{1}_m(\Gamma^{ee})$, $Q^{m\overline{v}}:=\mathbf{1}^{mm}Q^{v\overline{v}}$ and $Q^{\overline{v}m}:=Q^{\overline{v}\overline{v}}\mathbf{1}^{mm}$, so that

$$\begin{aligned}p_{e,m}=&(\mathbf{1}^{mm}+\lambda(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}Q^{\overline{v}m})(\mathbf{1}^{mm}+\lambda^2 Q^{m\overline{v}}(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-2}Q^{\overline{v}m})^{-1}\\ &\times(\mathbf{1}^{mm}+\lambda Q^{m\overline{v}}(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}).\end{aligned}$$

We compute

$$\begin{aligned}p_{e,m}(L-e)=&(\mathbf{1}^{mm}+\lambda(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}Q^{\overline{v}m})(\mathbf{1}^{mm}+\lambda^2 Q^{m\overline{v}}(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-2}Q^{\overline{v}m})^{-1}\\ &\times(\lambda^2 Q^{m\overline{v}}(e\mathbf{1}^{\overline{vv}}-L^{\overline{vv}})^{-1}Q^{\overline{vv}}+\lambda\beta Q^{m\overline{v}}(e\mathbf{1}^{\overline{vv}}-L^{\overline{vv}})^{-1}Q^{\overline{vv}})=O(|\lambda|^2+|\lambda\beta|),\end{aligned}$$

$$\begin{aligned}p_{e,m}Lp_{e,m}-ep_{e,m}=&(\mathbf{1}^{mm}+\lambda(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1}Q^{\overline{v}m})(\mathbf{1}^{mm}+\lambda^2 Q^{m\overline{v}}(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-2}Q^{\overline{v}m})^{-1}\\ &\times(\lambda^2 Q^{m\overline{v}}(e\mathbf{1}^{\overline{vv}}-L^{\overline{vv}})^{-1}Q^{\overline{v}m}+\lambda^2\beta Q^{m\overline{v}}(e\mathbf{1}^{\overline{vv}}-L^{\overline{vv}})^{-1}Q^{\overline{vv}}(e\mathbf{1}^{\overline{vv}}-L^{\overline{vv}})^{-1}Q^{\overline{v}m})\\ &\times(\mathbf{1}^{mm}+\lambda^2 Q^{m\overline{v}}(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-2}Q^{\overline{v}m})^{-1}(\mathbf{1}^{mm}+\lambda Q^{m\overline{v}}(e\mathbf{1}^{\overline{vv}}-L_0^{\overline{vv}})^{-1})\\ =&O(|\lambda|^2+|\lambda\beta|).\end{aligned}$$

Thus

$$p_{e,m}(L-e)(\mathbf{1}-p_{e,m})=O(|\lambda|^2+|\lambda\beta|).$$

Similarly,

$$(\mathbf{1}-p_{e,m})(L-e)p_{e,m}=O(|\lambda|^2+|\lambda\beta|).$$

Finally, we use

$$L-p_{e,m}Lp_{e,m}-(\mathbf{1}-p_{e,m})L(\mathbf{1}-p_{e,m})=p_{e,m}(L-e)(\mathbf{1}-p_{e,m})+(\mathbf{1}-p_{e,m})(L-e)p_{e,m}.$$

This proves (a).

Assume now that $\mathrm{sp}(E)=\{e\}$. Then

$$Q^{m\overline{v}}(e\mathbf{1}^{\overline{vv}}-L^{\overline{vv}})^{-1}Q^{\overline{vv}}=Q^{m\overline{v}}(e\mathbf{1}^{\overline{vv}}-L^{\overline{vv}})^{-1}Q^{\overline{ve}}=Q^{m\overline{v}}(e\mathbf{1}^{\overline{vv}}-L^{\overline{vv}})^{-1}Q^{\overline{v}m}.$$

[The first identity follows from $\mathrm{sp}(E)=\{e\}$, the second is a consequence of the definition of $\mathbf{1}^{mm}$.] Using this we get

$$p_{e,m}(L-e) = (\mathbf{1}^{mm} + \lambda(e\mathbf{1}^{\overline{\upsilon\upsilon}} - L_0^{\overline{\upsilon\upsilon}})^{-1}Q^{\overline{\upsilon}m})(\mathbf{1}^{mm} + \lambda^2 Q^{m\overline{\upsilon}}(e\mathbf{1}^{\overline{\upsilon\upsilon}} - L_0^{\overline{\upsilon\upsilon}})^{-2}Q^{\overline{\upsilon}m})^{-1}\lambda^2 Q^{m\overline{\upsilon}}(e\mathbf{1}^{\overline{\upsilon\upsilon}} - L^{\overline{\upsilon\upsilon}})^{-1}$$
$$\times Q^{\overline{\upsilon}m}(\mathbf{1}^{mm} + \lambda^2 Q^{m\overline{\upsilon}}(e\mathbf{1}^{\overline{\upsilon\upsilon}} - L_0^{\overline{\upsilon\upsilon}})^{-2}Q^{\overline{\upsilon}m})^{-1}(\mathbf{1}^{mm} + \lambda Q^{m\overline{\upsilon}}(e\mathbf{1}^{\overline{\upsilon\upsilon}} - L_0^{\overline{\upsilon\upsilon}})^{-1}) + O(|\lambda|^3).$$

This proves (b). ■

IV. APPLICATION: ANALYTICALLY DEFORMED PAULI–FIERZ LIOUVILLEANS

In this section we describe a class of operators to which the results of our paper can be applied. These operators arise naturally as models used in quantum physics. They provided for us a part of motivation to write this paper.

In order to introduce these operators we have to introduce a number of concepts taken from operator algebra and mathematical physics. Our presentation is based on Refs. 6, 7, 12, 13, and 9.

A. W^*-dynamical systems and Liouvilleans

Let us start with a brief description of some elements of theory of operator algebras, that we will use.[3,9]

A pair $(\mathfrak{M}, \tau^t)$, where $\mathfrak{M}$ is a W^*-algebra and τ^t is a σ-weakly continuous group of automorphisms of $\mathfrak{M}$, is called a W^*-dynamical system. In many circumstances it is convenient to describe a quantum system by a W^*-dynamical system. One of important results of theory of W^*-algebras says that there exists a distinguished representation, unique up to the unitary equivalence, called the standard representation.[3,9] It is a quadruple $(\pi, \mathcal{W}, J, \mathcal{W}_+)$, where $\mathcal{W}$ is a Hilbert space, $\pi := \mathfrak{M} \to B(\mathcal{W})$ is a *-representation, J an antiunitary involution, called the modular conjugation, and $\mathcal{W}_+$ is a self-dual cone, called the positive cone, in $\mathcal{W}$ satisfying certain axioms. In this representation there exists a unique self-adjoint operator L, called the Liouvillean, that implements the dynamics

$$\pi(\tau^t(A)) := e^{itL}\pi(A)e^{-itL}$$

and leaves invariant the positive cone, $e^{itL}\mathcal{W}_+ = \mathcal{W}_+$.

The properties of the W^*-dynamics τ^t are encoded in a simple way in the Liouvillean. For instance, the dynamics τ^t has no stationary states iff L has no point spectrum; it has a single stationary state iff L has a simple eigenvalue at zero.

One can argue that the resonances of L correspond to metastable states of the system $(\mathfrak{M}, \tau)$.

B. Massless bosons at zero density interacting with a small quantum system

Our main object of interest will be Pauli–Fierz systems at a positive density. They will be introduced in the next section. In order, however, to understand their physical content it is appropriate to describe first Pauli–Fierz systems at a zero density (in other words, at zero temperature), which we will do in this section.

Let $\mathcal{K}$ be a Hilbert space associated with quantum mechanical system and let K be a self-adjoint Hamiltonian for this system.

Let $L^2(\mathbb{R}^d)$ be the one particle bosonic space and let h be the one particle energy operator given by the multiplication by $|\xi|$ where $\xi \in \mathbb{R}^d$. The Hamiltonian $\mathrm{d}\Gamma(h)$ of the Bose gas acts on the symmetric (bosonic) Fock space $\Gamma_s(L^2(\mathbb{R}^d))$.

Let the interaction between systems be given by a measurable operator valued function $\mathbb{R}^d \ni \xi \mapsto v(\xi) \in B(\mathcal{K})$. The following sections are based on Ref. 7 (see also Ref. 6).

The Hilbert space of the system at zero density (zero temperature) is $\mathcal{H} = \mathcal{K} \otimes \Gamma_s(L^2(\mathbb{R}^d))$ and the free Hamiltonian is

$$H_{\mathrm{fr}} := K \otimes \mathbf{1}_{\Gamma_s(L^2(\mathbb{R}^d))} + \mathbf{1}_{\mathcal{K}} \otimes \int |\xi| a^*(\xi) a(\xi) \mathrm{d}\xi,$$

where $a^*(\xi)/a(\xi)$ are the usual creation/annihilation operators of the boson of momentum ξ. The interaction is given by the operator

$$V := \int (v(\xi) \otimes a^*(\xi) + v^*(\xi) \otimes a(\xi)) \mathrm{d}\xi.$$

The full Pauli–Fierz Hamiltonian equals

$$H := H_{\mathrm{fr}} + \lambda V,$$

where $\lambda \in \mathbb{R}$. To guarantee the self-adjointness of H we can assume that $\int (1+|\xi|^{-1}) \|v(\xi)\|^2 \, \mathrm{d}\xi < \infty$.

C. Massless bosons at density ρ interacting with a small quantum system

In this section we explain the notion of a Pauli–Fierz system at density ρ.

Suppose that we are given a measurable function

$$\mathbb{R}^d \ni \xi \mapsto \rho(\xi) \in [0, \infty[.$$

Let us consider the "doubled" Fock space $\Gamma_s(L^2(\mathbb{R}^d) \oplus L^2(\mathbb{R}))$. The creation/annihilation operators corresponding to the left/right $L^2(\mathbb{R}^d)$ will be denoted by $a_{\mathrm{l}}^*(\xi)/a_{\mathrm{l}}(\xi)$ and $a_r^*(\xi)/a_r(\xi)$, respectively. Let us introduce the left and right Araki–Woods creation and annihilation operators

$$a_{\rho,\mathrm{l}}^*(\xi) := \sqrt{1+\rho(\xi)}\, a_{\mathrm{l}}^*(\xi) + \sqrt{\rho(\xi)}\, a_r(\xi),$$

$$a_{\rho,\mathrm{l}}(\xi) := \sqrt{1+\rho(\xi)}\, a_{\mathrm{l}}(\xi) + \sqrt{\rho(\xi)}\, a_r^*(\xi),$$

$$a_{\rho,r}^*(\xi) := \sqrt{\rho(\xi)}\, a_{\mathrm{l}}(\xi) + \sqrt{1+\rho(\xi)}\, a_r^*(\xi),$$

$$a_{\rho,r}(\xi) := \sqrt{\rho(\xi)}\, a_{\mathrm{l}}^*(\xi) + \sqrt{1+\rho(\xi)}\, a_r(\xi).$$

The sub-W^*-algebra of $\mathcal{B}(\mathcal{K} \otimes \overline{\mathcal{K}} \otimes \Gamma_s(L^2(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d)))$ generated by operators of the form

$$A \otimes \mathbf{1}_{\overline{\mathcal{K}}} \otimes \exp\left(i \int f(\xi) a_{\rho,\mathrm{l}}^*(\xi) \mathrm{d}\xi + i \int \overline{f}(\xi) a_{\rho,\mathrm{l}}(\xi) \mathrm{d}\xi \right),$$

where $A \in \mathcal{B}(\mathcal{K})$ and $\int |f(\xi)|^2 \delta(\xi) d\xi < \infty$, will be called the Pauli–Fierz W^*-algebra. It is in a standard representation.

Note that the Pauli–Fierz algebra is isomorphic to the tensor product of the algebra of the small system $\mathcal{B}(\mathcal{K})$ and the algebra of Araki–Woods canonical commutation relations at density ρ.

The free Liouvillean is given by

$$L_{\mathrm{fr}} := K \otimes \mathbf{1} \otimes \mathbf{1} - \mathbf{1} \otimes \overline{K} \otimes \mathbf{1} + \mathbf{1} \otimes \mathbf{1} \otimes \int (|\xi| a_{\mathrm{l}}^*(\xi) a_{\mathrm{l}}(\xi) - |\xi| a_r^*(\xi) a_r(\xi)) \mathrm{d}\xi;$$

the perturbation is

$$Q_\rho := \int v(\xi) \otimes 1 \otimes a_{\rho,\mathrm{l}}^*(\xi) \mathrm{d}\xi + hc - \int (\mathbf{1} \otimes \overline{v}(\xi)) \otimes a_{\rho,r}^*(\xi) \mathrm{d}\xi + hc.$$

Assumption 4.A: If $\int (1+|\xi|^2)(1+\rho(\xi)) \|v(\xi)\|^2 \, \mathrm{d}\xi < \infty$ *holds then*

$$L_\rho := L_{\mathrm{fr}} + \lambda Q_\rho$$

essentially self-adjoint on the intersection of the domains of L_{fr} *and* Q_ρ.

The most important class of densities is that given by the Planck law at the inverse temperature β,

$$\rho_\beta{}^{(\xi)} := (e^{\beta|\xi|} - 1)^{-1}.$$

In particular, $\beta=\infty$ corresponds to the temperature zero (and density zero), and the corresponding Liouvillean is unitarily equivalent to

$$H \otimes \mathbf{1} - \mathbf{1} \otimes \overline{H}. \tag{4.1}$$

Thus in this case all the information is encoded in the Pauli–Fierz Hamiltonian described in the preceding section. One can argue that for a general ρ, L_ρ is a kind of a thermodynamical limit (4.1).

D. Analytically deformed Pauli–Fierz Liouvilleans

Pauli–Fierz Liouvilleans have continuous spectrum that covers the whole real line. They may also have some embedded eigenvalues. In particular, a thermal Pauli–Fierz Liouvillean (i.e., whose density is given by the Planck law) always has a zero eigenvalue corresponding to a KMS state. In general, eigenvalues of a Liouvillean are related to stationary states, therefore their study is very important from the physical point of view.

Another physically relevant question about Pauli–Fierz Liouvilleans is whether they have resonances and if so what is their location. They may manifest themselves as poles of an S-matrix or decay rates of certain correlation functions.

In order to define resonances we use the approach of Jaksic–Pillet. The first step of this approach consists of "gluing" the "left" and "right" one-particle subspaces. This is done as follows. We use the spherical coordinates in $\mathbb{R}^d$ and we introduce the Jaksic–Pillet gluing map defined as

$$L^2(\mathbb{R}^d) \oplus \overline{L^2(\mathbb{R}^d)} \ni (f_+, \overline{f_-}) \mapsto f \in L^2(\mathbb{R}) \otimes L^2(S^{d-1}), \tag{4.2}$$

$$f(p,\omega) := \begin{cases} p^{(d-1)/2} f_+(p\omega), & p > 0, \\ (-p)^{(d-1)/2} \overline{f_-}(-p\omega), & p \leqslant 0. \end{cases}$$

Here, $(p,\omega) \in \mathbb{R} \times S^{d-1}$ and S^{d-1} denotes $(d-1)$ dimensional sphere. The canonical conjugation in $L^2(\mathbb{R}) \otimes L^2(S^{d-1})$ is given by the complex conjugation.

If we assume that

$$v^*(\xi) = v(-\xi), \quad \rho(\xi) = \rho(-\xi)$$

and introduce

$$v_\rho(p,\omega) := \begin{cases} p^{(d-1)/2}(1+\rho(p\omega))^{1/2} v(p\omega), & p > 0, \\ (-p)^{(d-1)/2} \rho(p\omega)^{1/2} v(p\omega), & p \leqslant 0. \end{cases}$$

In the new representation, the free Liouvillean and its perturbation can be written as

$$L_{\mathrm{fr}} := K \otimes \mathbf{1} \otimes \mathbf{1} - \mathbf{1} \otimes \overline{K} \otimes \mathbf{1} + \mathbf{1} \otimes \mathbf{1} \otimes \int p a^*(p,\omega) a(p,\omega) \mathrm{d}p \, \mathrm{d}\omega,$$

$$Q_\rho = \int (v_\rho(p,\omega)\otimes \mathbf{1}\otimes a^*(p,\omega) + v_\rho^*(p,\omega)\otimes \mathbf{1}\otimes a(p,\omega))\mathrm{d}p\,\mathrm{d}\omega$$

$$+ \int (\mathbf{1}\otimes \overline{v_\rho}(p,\omega)\otimes a^*(-p,\omega) + \mathbf{1}\otimes \overline{v_\rho^*}(p,\omega)\otimes a(-p,\omega))\mathrm{d}p\,\mathrm{d}\omega$$

as an operator on $\mathcal{K}\otimes\overline{\mathcal{K}}\otimes\Gamma_s(L^2(\mathbb{R})\otimes L^2(S^{d-1}))$.

Let us make the following assumption.

Assumption 4.B: The function

$$\mathbb{R}\ni p\mapsto v_\rho(p,\cdot)\in\mathcal{B}(\mathcal{K},\mathcal{K}\otimes L^2(S^{d-1}))$$

extends to an analytic function in a strip $|\mathrm{Im}\,p|<\eta_0$ *and*

$$\sup_{|\mathrm{Im}p|<\eta_0}\int \|v_\rho(p,\cdot)\|^2\mathrm{d}(\mathrm{Re}\,p)<\infty.$$

Let $i^{-1}\nabla_p$ be the generator of translations on $L^2(\mathbb{R})$ in the spectral parameter p. Let $S := \mathrm{d}\Gamma(i^{-1}\nabla_p)$ be its second quantization. Note that for any complex η,

$$L_{\mathrm{fr}}(\eta) := e^{i\eta S}L_{\mathrm{fr}}e^{-i\eta S} = L_{\mathrm{fr}} + \eta\mathbf{1}^{\otimes 1}\otimes N,$$

where $N=\mathrm{d}\Gamma(1)$ is the number operator. Moreover, for $|\mathrm{Im}\,\eta|<\eta_0$,

$$Q_\rho(\eta) := e^{i\eta S}Q_\rho e^{-i\eta S}$$

$$= \int v_\rho((p+\eta),\omega)\otimes\mathbf{1}\otimes a^*(p,\omega)\mathrm{d}p\,\mathrm{d}\omega + \int v_\rho^*((p+\overline{\eta}),\omega)\otimes\mathbf{1}\otimes a(p,\omega)\mathrm{d}p\,\mathrm{d}\omega$$

$$+ \int \mathbf{1}\otimes\overline{v_\rho}((p+\overline{\eta}),\omega)\otimes a^*(-p,\omega)\mathrm{d}p\,\mathrm{d}\omega + \int \mathbf{1}\otimes\overline{v_\rho^*}((p+\eta),\omega)\otimes a(-p,\omega)\mathrm{d}p\,\mathrm{d}\omega.$$

Theorem 4.1: *Assume that 4.A, and 4.B hold. Then we have the following.*

(1) *There exists a unique operator-valued function* $\eta\mapsto L_\rho(\eta)$ *defined for* $0\leqslant -\mathrm{Im}\,\eta<\eta_0$ *such that*

- (a) $L_\rho(\eta)=e^{i\eta S}L_\rho e^{-i\eta S}$ *for* $\eta\in\mathbb{R}$.
- (b) *For* $0<\mathrm{Im}\,\eta<\eta_0$, $\eta\mapsto L_\rho(\eta)$ *is an analytic family.*
- (c) *For* $\mathrm{Im}z>0$, $(z-L_\rho(\eta))^{-1}$ *is strongly continuous up to* $\mathrm{Im}\,\eta=0$.

(2) *For and open* $U\subset\mathbb{C}$, $U\cap\mathrm{sp}_{\mathrm{disc}}(L_\rho(\eta))$ *is locally independent of* η, *as long as* $U\cap\mathrm{sp}_{\mathrm{ess}}(L_\rho(\eta))=\emptyset$.

If we assume that $\dim K<\infty$, *then for* $0\leqslant -\mathrm{Im}\,\eta<\eta_0$ *there exists* $\lambda_0>0$ *such that for* $|\lambda|<\lambda_0$ *the following statements hold:*

(3) $\mathrm{sp}L_\rho(\eta)\subset\{z\in\mathbb{C}:\mathrm{Im}z\leqslant 0\}$,

(4) *There exists* $c>0$ *such that*

$$\mathrm{sp}_{\mathrm{ess}}L_\rho(\eta)\subset\{z\in\mathbb{C}:\mathrm{Im}z<-|\mathrm{Im}\,\eta|(1-c|\lambda|)\}.$$

(5) *Real eigenvalues of* $L_\rho(\eta)$ *are semisimple and*

$$\mathrm{sp}_{\mathrm{pp}}L_\rho=\mathrm{sp}\,L_\rho(\eta)\cap\mathbb{R}.$$

So real discrete eigenvalues of $L_\rho(\eta)$ are semisimple, independent of η and coincide with the embedded eigenvalues of L_ρ. The nonreal discrete eigenvalues of $L_\rho(\eta)$, which are called resonances or metastable states, are also independent of η but they do not have to be semisimple.

E. LSO for Pauli–Fierz Liouvilleans

In this section we indicate how one can apply the method described in our paper to an analytically deformed Pauli–Fierz Liouvillean. We will see that many objects, including the LSO, do not depend on the parameter of deformation η, or depend rather mildly.

It is easy to see that $\mathbb{R}\cap \mathrm{sp}\, L_{\mathrm{fr}}(\eta)$ is an isolated subset of $\mathrm{sp}\, L_{\mathrm{fr}}(\eta)$ equal to

$$\mathrm{sp}(K\otimes \mathbf{1}-\mathbf{1}\otimes \overline{K})=\{k_1-k_2: k_1,k_2\in\ \mathrm{sp}\, K\}.$$

The corresponding spectral projection equals the orthogonal projection onto $\mathcal{K}\otimes\overline{\mathcal{K}}\otimes\Omega$, where Ω is the Fock vacuum. Note that it does not depend on η. Denote this projection by $\mathbf{1}^{vv}$. Clearly, $E=\mathbf{1}^{vv}L_{\mathrm{fr}}(\eta)$ does not depend on η either and can be identified with $K\otimes\mathbf{1}-\mathbf{1}\otimes\overline{K}$.

We can apply the method developed in this paper to the operator $L_\rho(\eta)=L_{\mathrm{fr}}(\eta)+\lambda Q_\rho(\eta)$ obtaining the LSO, which again does not depend on η,

$$\Gamma_\rho := \sum_{e\in \mathrm{sp}(E)} \mathbf{1}_e(E)Q_\rho^{v\overline{v}}(\eta)(e\mathbf{1}^{\overline{vv}}-L_{\mathrm{fr}}^{\overline{vv}}(\eta))^{-1}Q_\rho^{\overline{vv}}(\eta)\mathbf{1}_e(E).$$

One can compute Γ_ρ from the undeformed Liouvillean as well,

$$\Gamma_\rho=\lim_{\epsilon\searrow 0}\sum_{e\in \mathrm{sp}(E)} \mathbf{1}_e(E)Q_\rho^{v\overline{v}}((e+i\in)\mathbf{1}^{\overline{vv}}-\ L_{\mathrm{fr}}^{\overline{vv}}))^{-1}Q_\rho^{\overline{vv}}\mathbf{1}_e(E). \tag{4.3}$$

Note that (4.3) coincides with the definition of LSO contained in Ref. 7.

One can also compute the projectors $p_e(\eta)$ and $p_{e,m}(\eta)$. They depend on η, but in a rather controlled way, they are analytic functions of η for satisfying $s\in\mathbb{R}$,

$$p_e(\eta)=e^{isS}p_e(\eta+s)e^{-isS},\quad p_{e,m}(\eta)=e^{isS}p_{e,m}(\eta+s)e^{-isS}.$$

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Hyperbolic octagons and Teichmüller space in genus 2

Aline Aigon-Dupuy, Peter Buser,[a] Michel Cibils, and Alfred F. Künzle[b]
Section de Mathématiques, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Frank Steiner[c]
Abteilung Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, D-89069 Ulm, Germany

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In this paper we study different models of the Teichmüller space of compact hyperbolic surfaces with special emphasis on their construction by geodesic octagons. Such surfaces have become increasingly interesting due to their applications to the physical behavior of chaotic quantum systems. They are, on the one hand, complex enough to show the relevant features, and on the other hand, they possess a simple mathematical structure allowing practical implementations. We give a new description of Teichmüller space and the mapping class group in terms of geometric data of the octagons. This provides modellings based on the vertices and also on the generators of the associated isometry group. In addition, we explicitly connect our approach with other models currently used in the literature (Helling matrices, Fenchel–Nielsen parameters). The result of the paper may be considered as a computational tool kit to work with a specific model and to relate it with the others. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1850177]

I. INTRODUCTION

The purpose of this paper is to provide tools for computation and experimentation on compact Riemann surfaces of genus 2, starting from their description via the pasting of a fundamental octagon. A Riemann surface here is understood as a compact two-dimensional orientable manifold with a Riemannian metric of constant curvature −1. The universal covering of such surfaces is the hyperbolic plane for which we shall use the Poincaré disc model.

Over the years, many authors have studied the particular case of genus 2: this case gives access to quite explicit calculations but is still complex enough for the study of relevant phenomena in a model situation.

In Ref. 10, 12, 19, and 32 , for instance, explicit presentations of the mapping class group are given; in Refs. 7, 15, 20–24, 29, 34, 35, and 39, suitable parameters are introduced for the construction of algebraic and geometric models of Teichmüller space and in order to approach the moduli problem. Computations of explicit examples and numerical experiments are carried out for the Koebe–Poincaré uniformization theorem in Refs. 2, 14, 16, 28, 30, 31, 38, 41, and 42. Bounds and numerical computations for small eigenvalues of the Laplace–Beltrami operator are given in Ref. 25 and 27.

In Refs. 4, 6–9, and 36, the Hadamard–Gutzwiller model is studied from a physical point of view. Eigenvalues and eigenfunctions of a quantum mechanical system which describes the motion of a particle on a surface of constant negative curvature (hyperbolic octagon) are analyzed

[a]Electronic mail: peter.buser@epfl.ch
[b]Electronic mail: alfred.kuenzle@zkb.ch
[c]Electronic mail: frank.steiner@physik.uni-ulm.de

TABLE I. Changes of parameters.

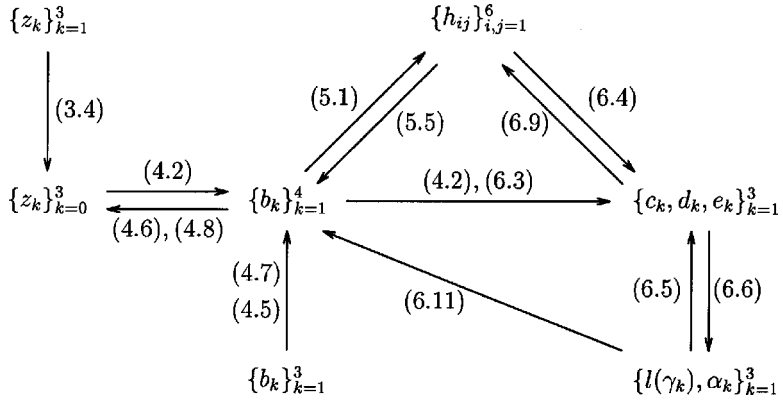

with respect to its strongly chaotic behavior. Numerical experiments are performed in order to investigate the statistical properties of highly excited states[8] and the lengths of periodic orbits are related with an arithmetical structure of chaos.[3,5]

The use of a fundamental polygon as the "input device" for such computations has a number of advantages. First of all, to designate any example, it is sufficient to give the sequence of vertices.[7] Second, a function on the surface (such as an eigenfunction of the Laplacian) is represented simply as a function on a compact plane domain. Finally, by letting the mapping class group operate on these polygons (see Sec. VIII), we obtain geometrically different domains representing the same surface, hence a possibility of checking numerical accuracy experimentally.

The paper is organized as follows. In Sec. II we briefly review the connection between the hyperbolic octagons and the corresponding Riemann surfaces and Fuchsian groups of genus 2. In Sec. III, we show how the octagon is computed if three of its vertices are given. Not all triples lead to a result and so we solve the problem of how to overview the admissible triples in Sec. VII. This yields a new description of the Teichmüller space in genus 2 (Theorem 7.3). In Sec. IV and Theorem 7.2, the same is carried out in terms of Fuchsian groups.

In Secs. V and VI, we relate the parameters used in this paper to other parameters known in the literature. Here we have made an effort to provide simple formulas that are easily programmable. Table I shows the global structure of the formulas for the parameter changes settled in this paper. In this table, z_0, z_1, z_2, z_3 are vertices of the octagon, b_1, b_2, b_3, b_4 are generators of the Fuchsian group related to the octagon, $\{h_{ij}\}$ is Helling's matrix from Ref. 24, c_k, d_k, e_k for $k=1$, 2, 3, are trace parameters (the Fenchel–Nielsen triples) and $l(\gamma_k), \alpha_k$ the corresponding Fenchel–Nielsen length and twist parameters. The arrows point out the different possible ways of expressing one set of parameters in terms of the others. The numbers refer to the corresponding transformation formulas in the text.

Finally, in Sec. VIII, we introduce elementary operations on the octagon and prove that they generate the mapping class group. The proof uses a new technique introduced in the thesis[1] and is different from the usual approach by Dehn twists.

II. OCTAGONS AND TEICHMÜLLER SPACE

In this section we describe the relation between the symmetric hyperbolic octagons and the compact Riemann surfaces of genus 2. The construction is standard, for details see, e.g., Refs. 11 and 40.

We work in the unit disc model

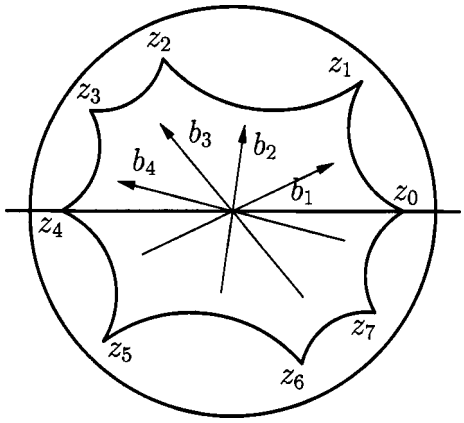

FIG. 1. Symmetric hyperbolic octagon in the unit disk and generators of the Fuchsian group.

$$\mathbb{D} = \{z = x + iy \in \mathbb{C} \,|\, |z| < 1\}$$

of hyperbolic geometry with the Riemannian metric

$$\mathrm{d}s^2 = \frac{4(\mathrm{d}x^2 + \mathrm{d}y^2)}{(1 - x^2 - y^2)^2}$$

of constant curvature -1. The hyperbolic distance of $z, w \in \mathbb{D}$ is denoted by $\mathrm{dist}_{\mathbb{D}}(z, w)$ and the Euclidean distance by $|z - w|$.

The orientation-preserving isometries of $(\mathbb{D}, \mathrm{d}s^2)$ are the Möbius transformations

$$z \mapsto g(z) = \frac{az + b}{\overline{b}z + \overline{a}}, \quad z \in \mathbb{D},$$

where $a, b \in \mathbb{C}$ are complex numbers satisfying $|a|^2 - |b|^2 = 1$, and $\overline{a}, \overline{b}$ are the complex conjugates. The group of all orientation-preserving isometries of $(\mathbb{D}, \mathrm{d}s^2)$ is denoted by $\mathrm{Isom}^+(\mathbb{D})$.

The geodesics in this model are the intersections with $\mathbb{D}$ of the Euclidean circles and the Euclidean straight lines that intersect the boundary $\partial\mathbb{D}$ orthogonally.

A hyperbolic n-gon is a simply connected compact domain $\Omega \subset \mathbb{D}$, whose boundary consists of n geodesic arcs, the *sides* of Ω, whose endpoints are the *vertices*. Denoting the interior angles at these vertices by $\delta_1, \ldots, \delta_n$, we have the *area formula*

$$\mathrm{area}(\Omega) = (n - 2)\pi - (\delta_1 + \cdots + \delta_n). \tag{2.1}$$

Now let $z_1, z_2, z_3 \in \mathbb{D}^+ = \{x + iy \in \mathbb{D} \,|\, y > 0\}$ be points with arguments

$$0 < \arg(z_1) < \arg(z_2) < \arg(z_3) < \pi$$

and let $z_0 \in]0, 1[\subset \mathbb{D}$ be on the positive real axis. Setting

$$z_4 = -z_0, \quad z_5 = -z_1, \quad z_6 = -z_2, \quad z_7 = -z_3$$

we obtain a geodesic octagon $P = P[z_0, z_1, z_2, z_3]$ with vertices $z_0, \ldots, z_7$ and sides $s_k = z_{k-1}z_k$, $k = 1, \ldots, 8$, where we write $z_8 = z_0$. By construction, P is invariant under the rotation $z \mapsto -z$ so that opposite sides have the same lengths. For $k = 1, \ldots, 4$, we therefore have a uniquely defined isometry $b_k \in \mathrm{Isom}^+(\mathbb{D})$ sending side s_{k+4} to s_k in such a way that

$$b_k(z_{k+3}) = z_k, \quad b_k(z_{k+4}) = z_{k-1}.$$

(See Fig. 1.)

For these isometries we have $b_k(P)\cap P=s_k$. Pasting sides s_{k+4} and s_k together, for $k=1, 2, 3, 4$ [by identifying any $z\in s_{k+4}$ with $b_k(z)\in s_k$], we therefore obtain a closed surface S of genus 2, which carries the hyperbolic metric inherited from P. This metric is smooth, except possibly at the point $w_0\in S$ which corresponds to the vertices of P. It follows that the metric is smooth at w_0 if and only if the sum of the interior angles of P equals 2π.

We call P *admissible* if this angle sum equals 2π. By the area formula (2.1), this is the same as requiring that $\text{area}(P)=4\pi$.

A classical result, which can be traced back to Fricke–Klein,[18] says that *any compact Riemann surface of genus 2 can be obtained by the above construction out of some admissible octagon.*

The proof uses the fact that on any such surface S there exists a curve system Σ consisting of simple closed geodesics $\sigma_1,\sigma_2,\sigma_3,\sigma_4$ which intersect each other pairwise at one and the same point w_0. Cutting S open along Σ gives a symmetric octagon.

This brings us as follows to the concept of Teichmüller space (see Ref. 26 for a general account).

If $\phi:S\to S$ is a homeomorphism, then the closed geodesics in the homotopy classes of the image curves $\phi\circ\sigma_k$ also decompose S into an admissible octagon. Hence, different octagons may lead to the same surface. For this reason it has become useful to *mark* a surface by selecting a curve system Σ on it. Two marked surfaces (S,Σ) and (S',Σ') are then called *marking equivalent* if there exists an isometry $h:S\to S'$ sending Σ to Σ'. The *Teichmüller space* $\mathcal{T}_2$ (for genus 2) is the set of all marking equivalence classes.

If, in the above construction, S is marked with the geodesics σ_k that result from the couples of sides s_{k+4}, s_k of the octagon, then it is not difficult to show that there is a one-to-one correspondence between the set $\mathcal{P}_2$ of all admissible octagons and the Teichmüller space $\mathcal{T}_2$. *We may therefore identify $\mathcal{P}_2$ with the Teichmüller space in genus 2.*

The surface obtained from P may also be described in terms of Fuchsian groups. If P is admissible, then by a theorem of Poincaré,[17,33,37] the isometries b_1,b_2,b_3,b_4 generate a Fuchsian group $\Gamma\subset\text{Isom}^+(\mathbb{D})$ with fundamental domain P, and S is the quotient surface $S=\mathbb{D}/\Gamma$. We may *mark* Γ by the selection of the generators $b_1,\ldots,b_4$ and call Γ with these generators and Γ' with generators $b_1',\ldots,b_4'$ marking equivalent if there exist $g\in\text{Isom}^+(\mathbb{D})$ satisfying $b_k'=gb_kg^{-1}$, $k=1,\ldots,4$. It can be shown that this establishes a one-to-one correspondence between the set $\mathcal{P}_2$ of all admissible polygons and the set $\mathcal{F}_2$ of all marking equivalence classes of Fuchsian groups (for genus 2), see, e.g., Refs. 12, 23, and 24.

III. COMPUTATION OF z_0

Definition 3.1: A triple of complex numbers $z_1,z_2,z_3\in\mathbb{D}$ satisfying

$$0<\arg(z_1)<\arg(z_2)<\arg(z_3)<\pi$$

is called admissible *if there exists $z_0\in\,]0,1[$ such that the symmetric octagon $P[z_0,z_1,z_2,z_3]$ is admissible.*

Instead of using the octagon we shall work most of the time with the pentagon $G=G[z_0,z_1,z_2,z_3]$ given by the vertices $z_0,z_1,z_2,z_3,z_4=-z_0$.

The triple z_1,z_2,z_3, and likewise the pentagon G is admissible if and only if $\text{area}(G)=2\pi$. As we shall see in Lemma 3.3, z_0 is uniquely determined by z_1,z_2,z_3.

Lemma 3.2: $G[z_0,z_1,z_2,z_3]$ is an admissible pentagon if and only if

$$\text{Im}\prod_{k=0}^{3}(1-z_k\overline{z_{k+1}})=0. \tag{3.1}$$

Proof: We use the area formula for triangles $D(z_k,z_{k+1})$ with vertices 0, z_k, z_{k+1} given in (A7):

$$\text{area } D(z_k, z_{k+1}) = 2 \arg(1 - z_k \overline{z_{k+1}}) \quad (k = 0,1,2,3). \tag{3.2}$$

The area of this triangle (as for any geodesic triangle in $\mathbb{D}$) is a number between 0 and π. Therefore we have $0 < \arg(1 - z_k \overline{z_{k+1}}) < \pi/2$. The sum of these areas is equal to the area of $G[z_0, z_1, z_2, z_3]$ and, since the latter is less than 3π, we have

$$0 < \sum_{k=0}^{3} \arg(1 - z_k \overline{z_{k+1}}) < \frac{3\pi}{2}.$$

Since all four arguments lie between 0 and $\pi/2$, we have

$$\sum_{k=0}^{3} \arg(1 - z_k \overline{z_{k+1}}) = \arg \prod_{k=0}^{3} (1 - z_k \overline{z_{k+1}})$$

(an equality between real numbers and not an equality modulo 2π). This gives us the formula

$$\text{area } G[z_0, z_1, z_2, z_3] = 2 \arg \prod_{k=0}^{3} (1 - z_k \overline{z_{k+1}}). \tag{3.3}$$

Now the argument of the product equals π if and only if the imaginary part equals zero, and the lemma follows. ■

In the next lemma we show how to compute z_0 out of an admissible triple z_1, z_2, z_3 such that $G[z_0, z_1, z_2, z_3]$ becomes an admissible pentagon. The lemma is formulated in such a way that the formula for z_0 is easily programmable and is valid for all cases.

Lemma 3.3: Let $z_1, z_2, z_3 \in \mathbb{D}$ *be complex numbers satisfying* $0 < \arg(z_1) < \arg(z_2) < \arg(z_3) < \pi$. *Abbreviate*

$$u = (1 - z_1 \overline{z_2})(1 - z_2 \overline{z_3}),$$

$$a = \text{Im}\{-u \overline{z_1} z_3\},$$

$$b = \text{Im}\{u(z_3 - \overline{z_1})\},$$

$$c = \text{Im}\{u\}. \tag{3.4a}$$

The triple z_1, z_2, z_3 *is admissible if and only if* $a + b + c < 0$. *If the triple is admissible, then there exists exactly one* $z_0 \in (0,1)$ *such that* $G[z_0, z_1, z_2, z_3]$ *is admissible. This* z_0 *is given by the formula*

$$z_0 = \frac{2c}{-b + \sqrt{b^2 - 4ac}}. \tag{3.4b}$$

Remark: In the future (but not yet during the proof of the lemma), if an admissible triple is given, then z_0 always means the real number given by this formula. As we shall see, for admissible triples, parameter c is always positive, and therefore if a becomes zero, formula (3.4b) is never singular.

Proof of the lemma: Let us first consider the value of c. By equation (3.3), we have

$$0 < 2 \arg(u) = \text{area } D(z_1, z_2) + \text{area } D(z_2, z_3) < 2\pi.$$

Hence $c = \text{Im}\{u\} > 0$.

Next let us consider the area of $G[z_0, z_1, z_2, z_3]$ where we keep z_1, z_2, z_3 fixed (admissible or not) and vary z_0 from 0 to 1, including the limiting cases $z_0 = 0$ and $z_0 = 1$. For $z_0 = 0$ the pentagon is singular and consists just of two triangles, $G[z_0, z_1, z_2, z_3] = D(z_1, z_2) \cup D(z_2, z_3)$, and its area is

$<2\pi$. As we continuously increase z_0, the area of the pentagon increases strictly to a maximum at $z_0=1$, where area $G[1,z_1,z_2,z_3]=2\arg[(1-\overline{z_1})u(1+z_3)]$. Consequently, the triple z_1,z_2,z_3 is admissible if and only if $\arg[(1-\overline{z_1})u(1+z_3)]>\pi$. Since $\mathrm{Im}((1-\overline{z_1})u(1+z_3))=a+b+c$, this is equivalent to saying that $a+b+c<0$.

Now let us assume that the triple is admissible, and hence $a+b+c<0$. From what we have just seen, there exists exactly one value of z_0 in the interval (0, 1) for which $G[z_0,z_1,z_2,z_3]$ is admissible. By virtue of Lemma 3.2, this value is the unique solution in the interval (0, 1) of the equation $\mathrm{Im}\,\Pi_{k=0}^{3}(1-z_k\overline{z_{k+1}})=0$. This equation is the same as

$$az_0^2+bz_0+c=0 \tag{3.5}$$

(with the above-defined values of a,b,c). In the case $a=0$, we have $b+c=a+b+c<0$. Using that $c>0$, we obtain $b<-c<0$ and the solution of equation (3.5) is $z_0=c/(-b)$. This indeed lies in the interval (0, 1) and is also given by the formula of the lemma.

If $a\neq 0$, (3.5) has the two distinct solutions

$$z_0=\frac{2c}{-b\pm\sqrt{b^2-4ac}},$$

where we already know that exactly one of them lies in the interval (0, 1). In particular, this means that $\sqrt{b^2-4ac}$ is a real number. It remains to be shown that the solution in (0, 1) is the one with the plus sign.

If $a<0$, then $b^2-4ac>b^2$ and therefore $-b-\sqrt{b^2-4ac}<0$. In this case the solution with the minus sign lies in the interval $(-\infty,0)$.

If $a>0$, we first conclude from $a+b+c<0$ that $b<0$. Furthermore, $b^2-4ac<b^2$, so that in this case $-b-\sqrt{b^2-4ac}>0$. Again from $a+b+c<0$, we have $-a>b+c$ and so $b^2-4ac>b^2+4bc+4c^2=(-b-2c)^2$. From this we find $\sqrt{b^2-4ac}>-b-2c$ and thence $-b-\sqrt{b^2-4ac}<2c$.

Altogether $2c/(-b-\sqrt{b^2-4ac})>1$, so that the solution with the minus sign now lies in the interval $(1,\infty)$. This concludes the proof of the lemma. ∎

Remark: The expression $(1/2a)(-b\pm\sqrt{b^2-4ac})$ for the solution of (3.5) is less useful than that given in Lemma 3.3 because a becomes 0 in certain cases.

IV. GENERATORS OF THE FUCHSIAN GROUP

In this section we compute the generators of the Fuchsian group which arise naturally from the octagon and vice versa.

The generators are $b_1,b_2,b_3,b_4\in\mathrm{Isom}^+(\mathbb{D})$, where, for $k=1$, 2, 3, 4, b_k is the (uniquely determined) orientation-preserving isometry mapping side $z_{k+3}z_{k+4}$ onto side z_kz_{k-1} in such a way that $b_k(z_{k+3})=z_k$ and $b_k(z_{k+4})=z_{k-1}$ (with the notation $z_8\doteq z_0$). It is well known that b_1,b_2,b_3,b_4 generate the Fuchsian group Γ of the octagon and that the following relation [which also follows from (4.3) below] holds:

$$b_1b_2^{-1}b_3b_4^{-1}b_1^{-1}b_2b_3^{-1}b_4=\mathrm{id}. \tag{4.1}$$

We express the generators by half turns. Let p_k be the midpoint of side $z_{k-1}z_k$ for $k=1$, 2, 3, 4; set $p_5=0$, $p_6=z_0$ and let m_k be the half turn around p_k ($k=1$, …, 6), i.e., the rotation with angle π and center p_k (so that p_k is the unique fixed point of m_k and $m_k^2=\mathrm{id}$).

In the next lemma, we use the notation

$$B[z]=\frac{az+b}{cz+d}\quad\text{for } B=\begin{bmatrix}a & b\\ c & d\end{bmatrix}\in \mathrm{GL}(2,\mathbb{C}).$$

Lemma 4.1: Let z_1,z_2,z_3 be an admissible triple and assume that z_0 has been computed so that $G[z_0,z_1,z_2,z_3]$ is admissible. Set

$$\omega_k = \frac{z_{k-1}(1-|z_k|^2) + z_k(1-|z_{k-1}|^2)}{1-|z_{k-1}z_k|^2}, \quad k=1,\ldots,4, \tag{4.2a}$$

then $|\omega_k|<1$. *Furthermore, the matrix*

$$B_k = \frac{-1}{\sqrt{1-|\omega_k|^2}}\begin{bmatrix} 1 & \omega_k \\ \overline{\omega_k} & 1 \end{bmatrix}, \quad k=1,\ldots,4 \tag{4.2b}$$

is well defined and satisfies

$$B_k[z] = b_k(z), \quad z \in \mathbb{D}, \quad k=1,\ldots,4,$$

i.e., the B_k *are matrices representing the generators of the Fuchsian group for the octagon* $P[z_0,z_1,z_2,z_3]$.

Proof: From (A1) and (A2) it follows that $|\omega_k|<1$ for $k=1, \ldots, 4$.

Let m_k denote the half turn around the midpoint p_k of side $z_{k-1}z_k$, $k=1, \ldots, 4$, and let m_5 denote the half turn around the point $p_5 \doteq 0$. From (A3), m_k is given by the matrix

$$M_k = \frac{i}{\sqrt{1-|\omega_k|^2}}\begin{bmatrix} 1 & -\omega_k \\ \overline{\omega_k} & -1 \end{bmatrix}, \quad k=1,\ldots,5, \tag{4.2c}$$

where we set $\omega_5 \doteq 0$. From (A4), the midpoints and centers of rotation are

$$p_k = \frac{\omega_k}{1+\sqrt{1-|\omega_k|^2}}, \quad k=1,\ldots,5. \tag{4.2d}$$

Note that $M_kM_5=B_k$, $k=1, \ldots, 4$.

It remains to be shown that

$$b_k = m_km_5. \tag{4.2e}$$

Now $m_5(z)=-z$ for $z \in \mathbb{D}$ and therefore, in particular,

$$m_km_5(z_{k+3}) = m_k(z_{k-1}) = z_k,$$

$$m_km_5(z_{k+4}) = m_k(z_k) = z_{k-1}.$$

Since any isometry from $\mathrm{Isom}^+(\mathbb{D})$ is uniquely determined by the images of two distinct points, this proves that indeed $m_km_5=b_k$ and the proof of Lemma 4.1 is complete. ■

The remainder of this section concerns the converse problem of finding the vertices of the octagon from a given set of generators.

By virtue of the relation (4.1), any one of the generators is determined by the other three. We shall assume that b_1,b_2,b_3 are given and compute b_4 as well as z_0,z_1,z_2,z_3.

For this we first consider some mapping properties of the half turns m_k.

Let α_k be the interior angle of $G=G[z_0,z_1,z_2,z_3]$ at vertex z_k, $k=0, 1, 2, 3, 4$. As may be seen from Fig. 2, the images G, $m_1(G)$, $m_1m_2(G)$, $m_1m_2m_3(G)$, and $m_1m_2m_3m_4(G)$ cover an angular sector of angle $\alpha_0+\alpha_1+\alpha_2+\alpha_3+\alpha_4$ at z_0. Since the angle sum of G is π, it follows that $m_1m_2m_3m_4(G)$ is the same as $\tau(G)$, where τ denotes the isometry with axis through z_4 and z_0 which maps z_4 onto z_0. Denoting by m_6 the half turn around $z_0=p_6$, we can write

$$\tau = m_6m_5.$$

Since $m_1m_2m_3m_4(G)=\tau(G)$, we conclude that $m_1m_2m_3m_4=m_6m_5$, or

$$m_1m_2m_3m_4m_5m_6 = \mathrm{id}. \tag{4.3}$$

Note that (4.3) implies (4.1).

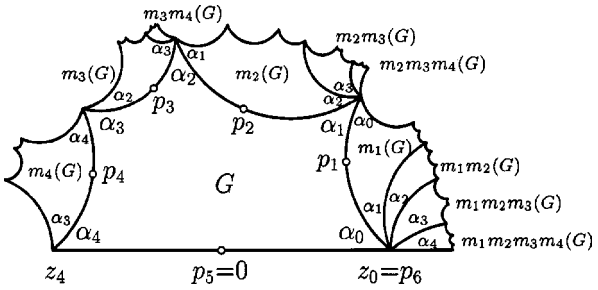

FIG. 2. A succession of half turns.

We also need this relation in terms of the matrices (4.2c). *A priori*, we can only say that $M_1\cdots M_6=\pm\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$. However, the set of all admissible triples z_1,z_2,z_3 is a *connected* open subset of $\mathbb{D}\times\mathbb{D}\times\mathbb{D}$ (Theorem 7.3). Hence, by continuity, the sign is always the same. Taking any example, we see that it is the plus sign. Thus the matrices M_k in (4.2c), representing the half turns m_k satisfy

$$M_1M_2M_3M_4M_5M_6=\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}. \tag{4.4}$$

A convenient way to "input" the generators is to define them by means of the points p_1,p_2,p_3, in much the same way as the octagon is defined by giving z_1,z_2,z_3. For the triple p_1,p_2,p_3, we assume

$$0<\arg(p_1)<\arg(p_2)<\arg(p_3)<\pi$$

and call it *admissible* if there exists an admissible $G[z_0,z_1,z_2,z_3]$ such that p_k is the midpoint of side $z_{k-1}z_k$, $k=1,2,3$ (a more convenient criterion for this admissibility is given in Theorem 7.1).

From (A3) and (A5), the half turn m_k around p_k is given by the matrix

$$M_k=\frac{i}{\sqrt{1-|\omega_k|^2}}\begin{bmatrix}1-\omega_k\\ \overline{\omega_k}-1\end{bmatrix},\quad k=1,2,3, \tag{4.5a}$$

where the invariant ω_k and point p_k are related by

$$\omega_k=\frac{2p_k}{1+|p_k|^2},\quad p_k=\frac{\omega_k}{1+\sqrt{1-|\omega_k|^2}},\quad k=1,2,3. \tag{4.5b}$$

The corresponding generator is given by the matrix

$$B_k\doteq\begin{bmatrix}\beta_k & \delta_k\\ \overline{\delta_k} & \overline{\beta_k}\end{bmatrix}=\frac{-1}{\sqrt{1-|\omega_k|^2}}\begin{bmatrix}1 & \omega_k\\ \overline{\omega_k} & 1\end{bmatrix},\quad k=1,2,3, \tag{4.5c}$$

where

$$\beta_k=\frac{-1}{\sqrt{1-|\omega_k|^2}},\quad \delta_k=\frac{-\omega_k}{\sqrt{1-|\omega_k|^2}},\quad \omega_k=\frac{\delta_k}{\beta_k}. \tag{4.5d}$$

These relations show that it is equivalent to give either B_k, p_k, or ω_k. We call the generators b_1,b_2,b_3, given by B_1,B_2,B_3 *admissible* if the corresponding points p_1,p_2,p_3 form an admissible triple.

In Theorem 7.1 we give a geometric criterion for the admissibility of the triple p_1,p_2,p_3 and we now prove the following

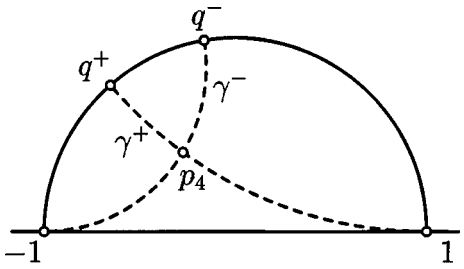

FIG. 3. Construction of p_4 and b_4.

Lemma 4.2: Let b_1, b_2, b_3 be an admissible triple of generators and let

$$A = \begin{bmatrix} \alpha & \beta \\ \overline{\beta} & \overline{\alpha} \end{bmatrix} \doteq B_3 B_2^{-1} B_1$$

be the matrix representing the product $b_3 b_2^{-1} b_1$. Then the octagon has the vertex

$$z_0 = \frac{\omega_6}{1 + \sqrt{1 - \omega_6^2}} \quad \text{with } \omega_6 = \frac{\alpha - \overline{\alpha}}{\beta - \overline{\beta}}, \tag{4.6}$$

The generator b_4 is given by the matrix

$$B_4 = AW \quad \text{where } W \doteq \frac{-1}{\sqrt{1 - \omega_6^2}} \begin{bmatrix} 1 & -\omega_6 \\ -\omega_6 & 1 \end{bmatrix}. \tag{4.7}$$

The remaining vertices are obtained from z_0 via the generators

$$z_4 = -z_0, \quad z_1 = b_1(z_4), \quad z_5 = -z_1, \quad z_2 = b_2(z_5), \quad etc. \tag{4.8}$$

Proof: From (4.3),

$$m_4 = m_3 m_2 m_1 m_6 m_5 = m_3 m_5 m_5 m_2 m_1 m_5 m_5 m_6 m_5 = b_3 b_2^{-1} b_1 m_5 m_6 m_5.$$

The half turn m_4 is represented by the matrix

$$M_4 = \frac{i}{\sqrt{1 - \omega_6^2}} A \begin{bmatrix} 1 & \omega_6 \\ -\omega_6 & -1 \end{bmatrix}.$$

We determine ω_6 such that M_4 is a half turn. This is the case if and only if the trace of the matrix is zero. Evaluating the trace, we find that it is zero if and only if

$$\alpha - \overline{\alpha} + \omega_6(\overline{\beta} - \beta) = 0.$$

The solution to this is $\omega_6 = (\alpha - \overline{\alpha})/(\beta - \overline{\beta})$. The formula for B_4 is now clear and the expression for z_0 (which is the fixed point of m_6 where m_6 is determined by ω_0) is given by (A4). ■

Remark 4.3: There is a simple geometric construction of b_4 out of b_3, b_2, b_1.

We recall that $b_k = m_k m_5$. The construction is described in terms of m_1, m_2, m_3 and yields the center p_4 of the half turn m_4.

Let $q^+ = m_3 m_2 m_1(1)$ and $q^- = m_3 m_2 m_1(-1)$ and draw the geodesics γ^+ from 1 to q^+ and γ^- from -1 to q^- (the points 1, q^+ and $-1, q^-$ are "points at infinity," respectively, of these geodesics). We claim that p_4 is the intersection of γ^- and γ^+. (See Fig. 3.)

To see this, we again use the relation (4.3). The product m_6m_5 is a hyperbolic transformation with axis from -1 to 1, i.e., $m_6m_5(-1)=-1$ and $m_6m_5(1)=1$. Therefore, $m_3m_2m_1(-1)=m_4(-1)$ and $m_3m_2m_1(1)=m_4(1)$. In other words, m_4 exchanges -1 and q^- so that $m_4(\gamma^-)=\gamma^-$ and the fixed point of m_4 lies on γ^-. For the same reason, it also lies on γ^+.

V. THE HELLING MATRIX

It may be desirable to describe the octagon in a way which does not involve its position in the unit disc $\mathbb{D}$. In Ref. 24, Helling introduces the invariants h_{ij} which are defined in the following way. Let again $m_1,\ldots,m_6$ be the half turns around $p_1,\ldots,p_6$, respectively. We use the matrices M_i corresponding to the half turns m_i as in (4.2c), and set

$$h_{ij} = -\tfrac{1}{2}\operatorname{tr} M_iM_j, \quad i,j=1,\ldots,6, \tag{5.1}$$

where tr denotes the trace. We call $H=\{h_{ij}\}$ the *Helling matrix*.

From the sign property (A6) we have $\operatorname{tr} M_iM_j<0$ so that the h_{ij} are positive. The geometric meaning of the h_{ij} is given by

$$h_{ij} = \cosh \operatorname{dist}_{\mathbb{D}}(p_i,\, p_j). \tag{5.2}$$

In order to compute the half turns (and hence the octagon) out of the Helling matrix, we use the following formula which we state in an independent form.

Lemma 5.1: Let M_1,M_2,M_3 be the matrices for the half turns with centers $q_1,q_2,q_3\in\mathbb{D}$, set $a_{ij}=-\frac{1}{2}\operatorname{tr}M_iM_j$ and define

$$a_{123} = \det\begin{bmatrix} 1 & a_{12} & a_{13} \\ a_{21} & 1 & a_{23} \\ a_{31} & a_{23} & 1 \end{bmatrix} = 1 + 2a_{12}a_{23}a_{31} - a_{12}^2 - a_{23}^2 - a_{31}^2. \tag{5.3}$$

It then follows that

$$M_3 = \frac{(a_{12}a_{23}-a_{13})}{a_{12}^2-1}M_1 + \frac{(a_{12}a_{13}-a_{23})}{a_{12}^2-1}M_2 + \frac{1}{2(a_{12}^2-1)}\ \operatorname{or}(q_1,q_2,q_3)\sqrt{a_{123}}(M_1M_2-M_2M_1), \tag{5.4}$$

where or *denotes the orientation of the triple*.

Proof: Since the formula remains invariant if all the half turns are conjugated by the same matrix $\begin{bmatrix} \alpha & \beta \\ \bar\beta & \bar\alpha \end{bmatrix}$ for suitable α,β, we may assume that points q_1,q_2,q_3 are given by

$$q_1=0, \quad q_2=t\in[0,1), \quad q_3=u+iv.$$

The determinant then becomes

$$a_{123} = 16t^2v^2(1-t)^{-2}(1-u^2-v^2)^{-2},$$

and the stated formula reads

$$\frac{t(1+u^2+v^2)-u(1+t^2)}{t(1-u^2-v^2)}\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} + \frac{u(1-t^2)}{t(1-u^2-v^2)}\frac{i}{1-t^2}\begin{bmatrix} 1+t^2 & -2t \\ 2t & -(1+t^2) \end{bmatrix} \pm \frac{2v}{1-u^2-v^2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$
$$= \frac{i}{1-u^2-v^2}\begin{bmatrix} 1+u^2+v^2 & -2(u+iv) \\ 2(u-iv) & -(1+u^2+v^2) \end{bmatrix}.$$

The equality is now easily verified. ∎

To obtain the half turns we first recall that

$$p_5 = 0, \quad M_5 = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}. \tag{5.5a}$$

Furthermore,

$$M_5 M_6 = \frac{-1}{1-p_6^2}\begin{bmatrix} 1+p_6^2 & -2p_6 \\ -2p_6 & 1+p_6^2 \end{bmatrix}, \quad h_{56} = \frac{1+p_6^2}{1-p_6^2},$$

which yields

$$p_6 = \sqrt{\frac{h_{56}-1}{h_{56}+1}}, \quad M_6 = i\begin{bmatrix} h_{56} & -\sqrt{h_{56}^2-1} \\ \sqrt{h_{56}^2-1} & -h_{56} \end{bmatrix}. \tag{5.5b}$$

With Lemma 5.1, and knowing that all triples p_5, p_6, p_k are positively orientated, we obtain

$$M_k = \frac{(h_{56}h_{6k}-h_{5k})}{h_{56}^2-1}M_5 + \frac{(h_{56}h_{5k}-h_{6k})}{h_{56}^2-1}M_6 + \frac{\sqrt{\delta_k}}{\sqrt{h_{56}^2-1}}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{5.5c}$$

for $k=1, 2, 3, 4$, where

$$\delta_k = \det\begin{bmatrix} 1 & h_{56} & h_{5k} \\ h_{56} & 1 & h_{6k} \\ h_{5k} & h_{6k} & 1 \end{bmatrix}. \tag{5.5d}$$

VI. FENCHEL–NIELSEN PARAMETERS

The Fenchel–Nielsen parameters, frequently used in the literature, are another type of parameter arising from certain sets of closed geodesics[14,26,40] and are defined as follows.

Let $p_k' = -p_k$, $k=1,\ldots, 6$, and consider the geodesic arcs c_1 from p_1 to p_2 and c_1' from p_2' to p_1'. On the surface S (obtained by pasting the sides of the octagon), the two arcs together form a smooth closed geodesic γ_1. Similarly, a closed geodesic γ_2 is obtained from the arcs c_2 and c_2', which run, respectively, from p_3 to p_4 and from p_4' to p_3'. The diagonal p_6p_6' yields a closed geodesic γ_3.

The triple $\gamma_1, \gamma_2, \gamma_3$ dissects S into two parts ("pairs of pants") which have the topological type of a sphere from which three pairwise disjoint discs have been removed. The pairs of pants are determined, up to isometry, by the lengths $l(\gamma_1), l(\gamma_2), l(\gamma_3)$. When the pairs of pants are pasted together again to yield S, there arises an additional degree of freedom at each γ_k, the so-called *twist parameter* (see α_k below). This parameter is determined by the lengths of two additional closed geodesics μ_k, η_k. We define them in terms of generators of the fundamental group of S.

For $k=0,\ldots, 4$, we denote the geodesic arc from p_5 to $m_k(p_5)$ by $\tilde{\beta}_k$, and the corresponding curve on S by β_k. Note that $\tilde{\beta}_k$ lies on the axis of the generator b_k of the group Γ which corresponds to the octagon. The geodesics are defined in Table II.

In Table II the expression "$\gamma_1 \sim \beta_2\beta_1^{-1}$" means that γ_1 is the closed geodesic in the free homotopy class of $\beta_2\beta_1^{-1}$, etc., and the symbol $\leftrightarrow$ means that the corresponding $b_2b_1^{-1}$ in Γ is $b_2b_1^{-1} = m_2m_1$, etc. Points $w_1, \ldots, w_6$ on the surface correspond to $p_1, \ldots, p_6$ in the octagon. For $k=1, 2, 3, 4$, the closed geodesic β_k corresponds to the straight line on the octagon joining p_k' to p_k.

For $k=1, 2, 3$, the geodesics μ_k, η_k intersect γ_k—each in two points—and are disjoint from the other γ_i. We call the numbers

$$c_k = \cosh\tfrac{1}{2}l(\gamma_k), \quad d_k = \cosh\tfrac{1}{2}l(\mu_k), \quad e_k = \cosh\tfrac{1}{2}l(\eta_k), \tag{6.1}$$

the *Fenchel–Nielsen triples*. In (6.5) and (6.6) we shall derive the twist parameters from these, but before that we relate them to the half turns and the Helling matrix.

Using the relation for $X \in \mathrm{SL}(2, \mathbb{C})$,

TABLE II. The Fenchel–Nielsen parameter geodesics.

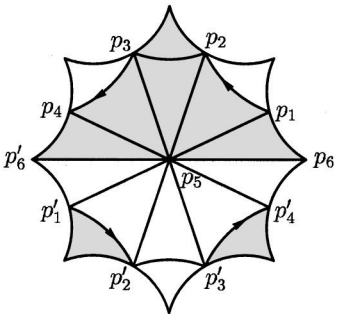

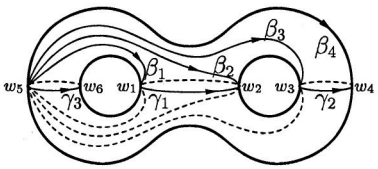

$$\gamma_1 \sim \beta_2\beta_1^{-1} \leftrightarrow m_2m_1$$

$$\mu_1 \sim \beta_1\beta_0^{-1}\beta_1^{-1}\beta_0 \leftrightarrow (m_1m_6m_5)^2$$

$$\eta_1 \sim \beta_2\beta_0^{-1}\beta_2^{-1}\beta_0 \leftrightarrow (m_2m_6m_5)^2$$

$$\gamma_2 \sim \beta_4\beta_3^{-1} \leftrightarrow m_4m_3$$

$$\mu_2 \sim \beta_3\beta_2^{-1}\beta_1\beta_3^{-1}\beta_2\beta_1^{-1} \leftrightarrow (m_3m_2m_1)^2$$

$$\eta_2 \sim \beta_4\beta_2^{-1}\beta_1\beta_4^{-1}\beta_2\beta_1^{-1} \leftrightarrow (m_4m_2m_1)^2$$

$$\gamma_3 \sim \beta_0 \leftrightarrow m_6m_5$$

$$\mu_3 \sim \beta_4^{-1}\beta_3\beta_4\beta_3^{-1} \leftrightarrow (m_5m_4m_3)^2$$

$$\eta_3 \sim \beta_0\beta_4^{-1}\beta_3\beta_0^{-1}\beta_4\beta_3^{-1} \leftrightarrow (m_6m_4m_3)^2$$

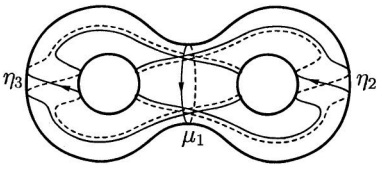

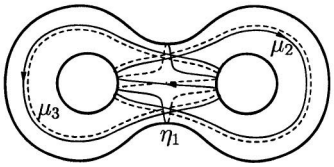

$$\operatorname{tr} X^2 = \operatorname{tr}^2 X - 2, \tag{6.2}$$

for $k=1, 2, 3$ and indices mod 6, the above list gives

$$c_k = -\tfrac{1}{2}\operatorname{tr}(M_{2k-1}M_{2k}),$$

$$d_k = \tfrac{1}{2}\operatorname{tr}^2(M_{2k-1}M_{2k-2}M_{2k-3}) - 1,$$

$$e_k = \tfrac{1}{2}\operatorname{tr}^2(M_{2k}M_{2k-2}M_{2k-3}) - 1. \tag{6.3}$$

Note that c_k is positive by (A6).

In Ref. 24, it is shown that, for $A, B, C \in \mathrm{SL}(2,\mathbb{C})$ with $\operatorname{tr} A = \operatorname{tr} B = \operatorname{tr} C = 0$,

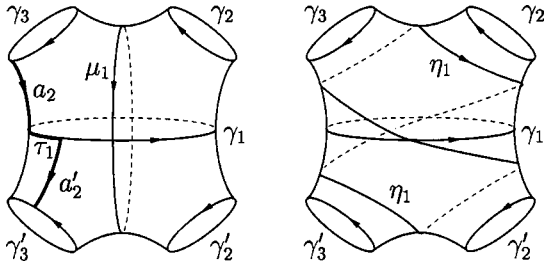

FIG. 4. Defining the twist parameter α_1.

$$\mathrm{tr}^2(ABC) + \mathrm{tr}(AB)\mathrm{tr}(BC)\mathrm{tr}(CA) + \mathrm{tr}^2(AB) + \mathrm{tr}^2(BC) + \mathrm{tr}^2(CA) - 4 = 0.$$

For $k=1, 2, 3$, this yields

$$c_k = h_{2k-1,2k},$$

$$d_k = 2\delta(h_{2k-1,2k-2}, h_{2k-1,2k-3}, h_{2k-2,2k-3}) - 1,$$

$$e_k = 2\delta(h_{2k,2k-2}, h_{2k,2k-3}, h_{2k-2,2k-3}) - 1, \tag{6.4}$$

where δ denotes the polynomial

$$\delta(a,b,c) = \det\begin{bmatrix} 1 & a & b \\ a & 1 & c \\ b & c & 1 \end{bmatrix}.$$

In order to obtain the other parameters from the Fenchel–Nielsen triples, we use twists.

We give the description for γ_1, since the twists along γ_2, γ_3 are defined in the same way and the formulas are obtained by cyclic permutation. (See Fig. 4.)

For convenient viewing we cut S open along γ_2 and γ_3 into a four-holed sphere X. The cuts appear as closed boundary geodesics γ_2, γ_2' and γ_3, γ_3'. The geodesic γ_1 further separates X into two isometric three-holed spheres Y, with boundary geodesics $\gamma_1, \gamma_2, \gamma_3$, and Y' with boundary geodesics $\gamma_1', \gamma_2', \gamma_3'$.

The shortest geodesic arc a_2 on Y from γ_3 to γ_1 and the shortest geodesic arc a_2' on Y' from γ_1 to γ_3' both have the same length given by

$$\cosh^2 l(a_2) = \cosh^2 l(a_2') = \frac{(c_2 + c_1c_3)^2}{(c_1^2 - 1)(c_3^2 - 1)}$$

[see Ref. 13, Theorem 2.4.1(i)]. On γ_1, let τ_1 be the geodesic arc going from the end point of a_2 to the initial point of a_2'. There are infinitely many such arcs (winding around γ_1). We render the selection of τ_1 unique by requiring that the closed curve $a_2\tau_1 a_2'(\gamma_3')^{-1}(a_2')^{-1}\tau_1^{-1}a_2^{-1}\gamma_3$ lies in the free homotopy class of μ_1. The *twist parameter* α_1 is defined as

$$\alpha_1 = \pm\frac{l(\tau_1)}{l(\gamma_1)},$$

where we take the plus sign if τ_1 goes in the same direction as γ_1 and the minus sign if τ_1 goes in the opposite direction.

In Ref. 13 [Proposition 3.3.11 in connection with the above expression for $\cosh^2 l(a_2)$] it is shown that

$$d_1 = \cosh\tfrac{1}{2} l(\mu_1) = F_1(\alpha_1),$$

where F_1 is the function

$$F_1(\alpha) \doteq \frac{1}{c_1^2 - 1}(c_1^2 + c_2^2 + c_3^2 + 2c_1c_2c_3 - 1)(1 + \cosh \alpha l(\gamma_1)) - 1.$$

Replacing τ_1 by the arc τ_1' which winds an additional time around γ_1 gives the curve $a_2\tau_1' a_2'(\gamma_3')^{-1}(a_2')^{-1}(\tau_1')^{-1}a_2^{-1}\gamma_3$ in the free homotopy class of η_1. Accordingly,

$$e_1 = \cosh\tfrac{1}{2} l(\eta_1) = F_1(\alpha_1 + 1).$$

The twist parameters α_2, α_3 are defined in the same way and the relation with the Fenchel–Nielsen triples is as follows.

Lemma 6.1: For $k=1, 2, 3$, *if*

$$p = c_1^2 + c_2^2 + c_3^2 + 2c_1c_2c_3 - 1, \quad \Gamma_k = e_k + 1 - (2c_k^2 - 1)(d_k + 1) + 2p,$$

then

$$c_k = \cosh\tfrac{1}{2} l(\gamma_k),$$

$$d_k = \frac{p}{c_k^2 - 1}(1 + \cosh \alpha_k l(\gamma_k)) - 1,$$

$$e_k = \frac{p}{c_k^2 - 1}(1 + \cosh(\alpha_k + 1) l(\gamma_k)) - 1, \tag{6.5}$$

and

$$\sinh \alpha_k l(\gamma_k) = \frac{\Gamma_k \sqrt{c_k^2 - 1}}{2c_k p}. \tag{6.6}$$

Proof: The first two formulas have already been proved. For the third, we apply the rule

$$\cosh(x + y) = \cosh x \cosh y + \sinh x \sinh y$$

to $x = \alpha_k l(\gamma_k)$ and $y = l(\gamma_k)$. ■

The twists now allow us to solve for the h_{ij} in the system of equations (6.4), using the fact that

$$\cosh\frac{\alpha_k}{2} l(\gamma_k) = \sqrt{\frac{1 + \cosh \alpha_k l(\gamma_k)}{2}} = \frac{1}{\sqrt{2p}}\sqrt{(d_k + 1)(c_k^2 - 1)},$$

$$\sinh\frac{\alpha_k}{2} l(\gamma_k) = \frac{\sinh \alpha_k l(\gamma_k)}{2 \cosh\frac{\alpha_k}{2} l(\gamma_k)} = \frac{\Gamma_k}{2c_k\sqrt{2p}\sqrt{d_k + 1}}. \tag{6.7}$$

The geometric interpretation of the h_{ij} on Y is shown in Fig. 5 for the case where $\alpha_1, \alpha_2, \alpha_3$ have small positive values.

Arcs p_5p_6, p_1p_2, p_3p_4 on the pentagon P correspond, respectively, to one-half of the boundary geodesics $\gamma_1, \gamma_2, \gamma_3$ of Y. Arcs p_6p_1, p_2p_3, p_4p_5 correspond to arcs on Y which decompose Y into two hexagons (which are not isometric and do not generally even have the same area). Since points w_5, w_6 on γ_3, corresponding to p_5, p_6, are opposite, we have

$$h_{56} = c_3. \tag{6.8}$$

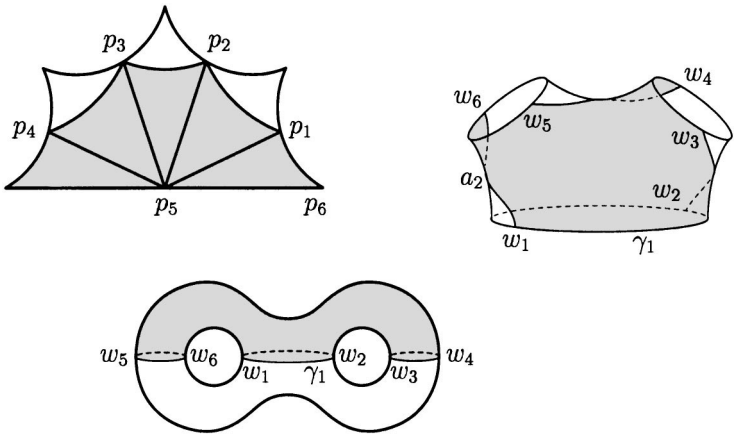

FIG. 5. Geodesic arcs for the Helling matrix.

Arc a_2 and the arc w_1w_6 which corresponds to p_1p_6, form a quadrilateral on Y with right angles at the end points of a_2. Using the trigonometry for such quadrilateral gives

$$h_{61} = G(\alpha_3 l(\gamma_3), \alpha_1 l(\gamma_1)),$$

where G is the function

$$G(x,y) = \cosh a_2 \cosh\frac{x}{2}\cosh\frac{y}{2} + \sinh\frac{x}{2}\sinh\frac{y}{2}.$$

From the arcs connecting p_6 with p_2, etc., we obtain similar quadrilaterals which differ from the first by plus or minus one-half of the boundary geodesics γ_1, γ_2. Thus,

$$h_{62} = G(\alpha_3 l(\gamma_3), (\alpha_1 + 1) l(\gamma_1)),$$

$$h_{51} = G((\alpha_3 - 1) l(\gamma_3), \alpha_1 l(\gamma_1)),$$

$$h_{52} = G((\alpha_3 - 1) l(\gamma_3), (\alpha_1 + 1) l(\gamma_1)).$$

Using the abbreviations, for $k=1, 2, 3$,

$$x_{k,1} = \sqrt{d_k + 1}, \quad y_{k,1} = \frac{\Gamma_k}{2c_k\sqrt{d_k + 1}},$$

$$x_{k,2} = c_k x_{k,1} + y_{k,1}, \quad y_{k,2} = c_k y_{k,1} + (c_k^2 - 1) x_{k,1},$$

$$x_{k,3} = c_k x_{k,1} - y_{k,1}, \quad y_{k,3} = c_k y_{k,1} - (c_k^2 - 1) x_{k,1}, \tag{6.9a}$$

and recalling that

$$\Gamma_k = e_k + 1 - (2c_k^2 - 1)(d_k + 1) + 2p, \quad p = c_1^2 + c_2^2 + c_3^2 + 2c_1c_2c_3 - 1, \tag{6.9b}$$

then, applying cyclic permutations to $\gamma_1, \gamma_2, \gamma_3$ in (6.5)–(6.8), we obtain

$$h_{2k-1,2k} = h_{2k,2k-1} = c_k,$$

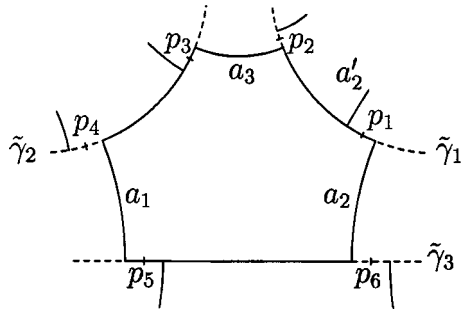

FIG. 6. Twist parameters as seen in the universal covering.

$$h_{2k-2-i,2k-1+j} = h_{2k-1+j,2k-2-i} = \frac{1}{2p}((c_{k+1} + c_k c_{k+2})x_{k,1+j}x_{k-1,1-i} + y_{k,1+j}y_{k-1,1-i}), \tag{6.9c}$$

for $k=1, 2, 3$, $i=0, 1$, $j=0, 1$, where the indices of h are mod 6 and the remaining indices are mod 3.

In order to see how the octagon can follow directly from the twist and length parameters, we use the fact that the shortest connections a_1, a_2, a_3, which, respectively, link γ_2 to γ_3, γ_3 to γ_1, and γ_1 to γ_2, separate the three-holed sphere Y into two right angled geodesic hexagons. Figure 6 shows one of these hexagons drawn in $\mathbb{D}$, the universal covering of $S=\mathbb{D}/\Gamma$.

The selected covering curves of $\gamma_1, \gamma_2, \gamma_3$ are the geodesics $\tilde{\gamma}_1$ through p_1, p_2, $\tilde{\gamma}_2$ through p_3, p_4 and $\tilde{\gamma}_3$ through p_5, p_6. Now a_k appears as the common perpendicular of $\tilde{\gamma}_{k-1}$ and $\tilde{\gamma}_{k+1}$, $k=1, 2, 3$ (indices mod 3). The arc a_2' (see Figs. 4 and 6), which was used to define the twist parameter α_1, now appears as a perpendicular arc of $\tilde{\gamma}_1$ that is opposite to a_2 and shifted along $\tilde{\gamma}_1$ by $|\alpha_1| l(\gamma_1)$. The shift is to the left if α_1 is positive and to the right if α_1 is negative. It is well known that the surface S has a rotational symmetry (the so-called hyperelliptic involution) with fixed points $w_1, \ldots, w_6$, and it therefore follows that p_1 lies at a point on $\tilde{\gamma}_1$ that is equidistant from the end points of a_2 and a_2'. The points $p_2, \ldots, p_6$ have analogous properties. The positions of these points in $\mathbb{D}$ may thus be found by applying the isometries given by the matrices

$$R_t \doteq \begin{bmatrix} 1+\cosh t & \sinh t \\ \sinh t & 1+\cosh t \end{bmatrix}, \quad U_t \doteq \begin{bmatrix} 1+\cosh t & i\sinh t \\ -i\sinh t & 1+\cosh t \end{bmatrix}, \quad t \in \mathbb{R}. \tag{6.10}$$

Geometrically, R_t is a hyperbolic isometry with axis from -1 to 1, shifting 0 to the point $\sinh t/(1+\cosh t)=\tanh(t/2)$, whose hyperbolic distance to 0 is t. Similarly, U_t is a hyperbolic isometry with axis from $-i$ to i, shifting 0 to $i\tanh t/2$ with the same distance. Hence to obtain the points $p_1, \ldots, p_6$ from the lengths $l(\gamma_k)$ and twists α_k, we set

$$\lambda_k = \tfrac{1}{2} l(\gamma_k), \quad c_k = \cosh \lambda_k,$$

$$\vartheta_k = \tfrac{1}{2}\alpha_k l(\gamma_k), \quad a_k = \operatorname{arccosh} \frac{c_k + c_{k-1}c_{k+1}}{\sqrt{(c_{k-1}^2-1)(c_{k+1}^2-1)}}, \tag{6.11a}$$

and apply products of R_t and U_t given by the following list:

$$p_5 = 0, \quad p_6 = R_{\lambda_3}[0],$$

$$p_1 = R_{\lambda_3 - \vartheta_3} U_{a_2} R_{-\vartheta_1}[0],$$

$$p_2 = R_{\lambda_3 - \vartheta_3} U_{a_2} R_{-\lambda_1 - \vartheta_1}[0],$$

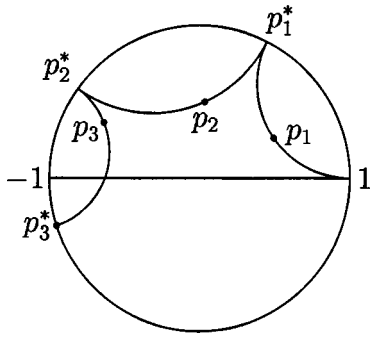

FIG. 7. A non-admissible triple of midpoints.

$$p_3 = R_{-\vartheta_3} U_{a_1} R_{\lambda_2 - \vartheta_2}[0],$$

$$p_4 = R_{-\vartheta_3} U_{a_1} R_{-\vartheta_2}[0]. \tag{6.11b}$$

VII. A PICTURE OF TEICHMÜLLER SPACE

In the first part of this section we give a simple criterion for the admissibility of the triple of generators b_1, b_2, b_3 and thus a geometric picture of Teichmüller space in terms of octagons. In the second part, a similar description is given in terms of the vertices z_1, z_2, z_3. The main results are summarized in Theorems 7.2 and 7.3.

Any b_k is the product of half turns $b_k = m_k m_5$ [cf. (4.2e)], where m_5 is the half turn with center 0. Describing the admissible triples b_1, b_2, b_3 is therefore equivalent to describing the centers of rotation p_1, p_2, p_3 of the corresponding half turns m_1, m_2, m_3.

For any triple of points $p_1, p_2, p_3 \in \mathbb{D}^+$ with

$$0 < \arg(p_1) < \arg(p_2) < \arg(p_3) < \pi,$$

we construct a triple $p_1^*, p_2^*, p_3^* \in \partial\mathbb{D}$ as follows: p_1^* is the second end point at infinity of the geodesic through p_1 whose first end point at infinity is 1; p_2^* is the second end point at infinity of the geodesic through p_1^* and p_2; p_3^* is the end point at infinity of the geodesic through p_2^* and p_3. (See Fig. 7.)

Theorem 7.1: *The triple p_1, p_2, p_3 is admissible if and only if the points p_k^* satisfy*

$$0 < \arg(p_1^*) < \arg(p_2^*) < \arg(p_3^*) < \pi.$$

Proof: We use a continuity argument. Assuming first that p_1, p_2, p_3 is admissible, there is an admissible pentagon $z_0 z_1 z_2 z_3 z_4$ such that p_k is the midpoint of side $z_{k-1} z_k$, $k = 1, 2, 3$, and we label p_4 the midpoint of side $z_3 z_4$.

Shifting z_0 towards 1 by a small amount $t > 0$, i.e., replacing it by the point z_0^t on the geodesic γ from -1 to 1, whose hyperbolic distance from z_0 is t and which lies nearer 1, gives a new pentagon with vertices z_0^t, $z_1^t \doteq m_1(z_0^t)$, $z_2^t \doteq m_2(z_1^t)$, $z_3^t \doteq m_3(z_2^t)$, $z_4^t \doteq m_4(z_3^t)$. Thus, the new pentagon has the same midpoints p_1, p_2, p_3, p_4, but it is no longer centered at 0. (See Fig. 8.)

Now, from (4.3), $z_4^t = m_4 m_3 m_2 m_1(z_0^t) = m_6 m_5(z_0^t)$, where in this case $m_6 m_5$ is the hyperbolic isometry with axis γ. Hence, $z_4^t \in \gamma$ and $\mathrm{dist}_{\mathbb{D}}(z_0^t, z_4^t) = \mathrm{dist}_{\mathbb{D}}(z_0, z_4)$ so that the point z_4 is also shifted towards 1 by t. Since for $k = 1, 2, 3, 4$ the triangles $z_{k-1} z_{k-1}^t p_k$ and $z_k z_k^t p_k$ (being exchanged by m_k) have the same area, *the area of the new pentagon is still* 2π.

Similarly, as t is increased by small amounts, the pentagon retains the area 2π and therefore remains convex. As $t \to \infty$, z_k^t converges to p_k^* for $k = 1, 2, 3$ and z_4^t converges to 1, so the quadrilateral $1 p_1^* p_2^* p_3^*$ is convex. Moreover, p_3^* is the end point at infinity of the geodesic through 1 and p_4 (as observed in a different way at the end of the section precedent). It follows that

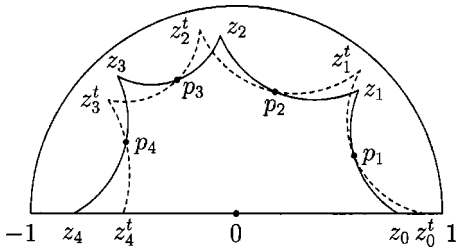

FIG. 8. Deforming the pentagon.

$$0 < \arg(p_1^*) < \arg(p_2^*) < \arg(p_3^*) < \pi.$$

Conversely, if this relation holds, we let $z_0^t \in \gamma$ be a moving point between 0 and 1 and consider the pentagon P^t with vertices z_0^t, $z_1^t = m_1(z_0^t)$, $z_2^t = m_2(z_1^t)$, $z_3^t = m_3(z_2^t)$, $z_4^{tt} = -z_0^t$ [in contrast to $z_4^t = m_4(z_3^t)$ used before]. For $z_0^t = 1$, P^t is an ideal pentagon with area 3π. As z_0^t moves towards 0, P^t remains convex and the area changes continuously. For $z_0^t = 0$, P^t becomes a quadrilateral with area $< 2\pi$. Hence there exists $z_0^t \in (0,1)$ for which the area of the pentagon is exactly 2π, which means that p_1, p_2, p_3 is admissible. ■

Theorem 7.1 provides a convenient way to overview the domain $\mathcal{P} \subset \mathbb{D}^+ \times \mathbb{D}^+ \times \mathbb{D}^+$ of all admissible triples, starting from a random choice of $p_1 \in \mathbb{D}^+$,

For any $p_1 \in \mathbb{D}^+$, the geodesic from -1 to p_1^* separates $\mathbb{D}^+$ into two open convex subsets. If $\mathbb{D}[p_1]$ is the one which does not contain p_1, then, by Theorem 7.1, a triple p_1, p_2, p_3 can only be admissible if $p_2 \in \mathbb{D}[p_1]$. (See Fig. 9.)

Similarly, for $p_2 \in \mathbb{D}[p_1]$ with p_2^* the second end point at infinity of the geodesic through p_1^* and p_2, the geodesic from -1 to p_2^* separates $\mathbb{D}[p_1]$ into two open convex subsets and we let $\mathbb{D}[p_1, p_2]$ be the one which does not contain p_2.

Again by Theorem 7.1, a triple p_1, p_2, p_3 is admissible if and only if $p_3 \in \mathbb{D}[p_1, p_2]$. This yields the following geometric picture of Teichmüller space in genus 2.

Theorem 7.2: *The set $\mathcal{P}$ of all admissible triples p_1, p_2, p_3 is given as*

$$\mathcal{P} = \{(p_1, p_2, p_3) \in \mathbb{D}^+ \times \mathbb{D}^+ \times \mathbb{D}^+ | p_2 \in \mathbb{D}[p_1], p_3 \in \mathbb{D}[p_1, p_2]\}.$$

Clearly, Theorem 7.2 shows that $\mathcal{P}$ is homeomorphic to $\mathbb{D}^+ \times \mathbb{D}^+ \times \mathbb{D}^+$ or, equivalently, to $\mathbb{R}^6$.

Remark: The description may be varied. For instance, if $p_2 \in \mathbb{D}^+$ is chosen freely, then let $\tilde{p}_2$ be the second end point at infinity of the geodesic through -1 and p_2, with $\tilde{\mathbb{D}}[p_2]$ the domain cut away by the geodesic from 1 to $\tilde{p}_2$ which does not contain p_2. A triple $p_1 p_2 p_3$ is then admissible if and only if $p_1 \in \tilde{\mathbb{D}}[p_2]$ and $p_3 \in \tilde{\mathbb{D}}[p_1, p_2]$, etc.

In the second part of this section we outline a similar picture in terms of the set $\mathcal{Z}$ of all admissible triples z_1, z_2, z_3.

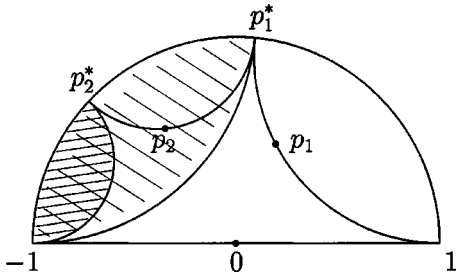

FIG. 9. Domains of admissible midpoints.

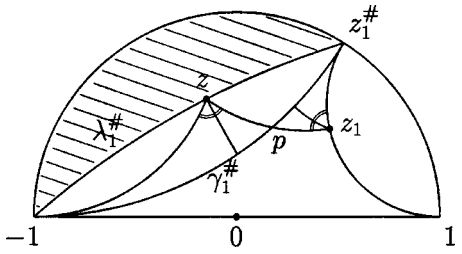

FIG. 10. The connected open component $\mathbb{D}^\#[z_1]$ of $\mathbb{D}^+$ (shaded area).

As before, $z_1 \in \mathbb{D}^+$ is selected arbitrarily and $z_1^\# \in \partial\mathbb{D}$ is the end point of the geodesic through 1 and z_1. If $\gamma_1^\#$ is the geodesic from -1 to $z_1^\#$, then, in the disc model $\mathbb{D}$ of the hyperbolic plane, it is well known that the line $\lambda_1^\#$, consisting of all points $z \in \mathbb{D}^+$ whose distance from $\gamma_1^\#$ is the same as the distance of z_1 to $\gamma_1^\#$ and which lie on the opposite side of $\gamma_1^\#$ to z_1, is a circular arc.

For $z \in \lambda_1^\#$, the geodesic arc from z to z_1 intersects $\gamma_1^\#$ at its midpoint p (there are two right-angled triangles with the same angle at p and the same length of opposite side). Hence, the half turn with center p sends the triangle $pz(-1)$ to $pz_1z_1^\#$. In particular, the angles at z and z_1 are the same. It follows that the quadrilaterals $(-1)(1)z_1z$ and $(-1)(1)z_1z_1^\#$ have the same angle sum π.

Line $\lambda_1^\#$ separates $\mathbb{D}^+$ into two connected open components and we denote the one which does not contain z_1 by $\mathbb{D}^\#[z_1]$ (the shaded area in Fig. 10). For $z_2 \in \mathbb{D}^+$, the quadrilateral $(-1)(1)z_1z_2$ has angle sum $<\pi$ if and only if $z_2 \in \mathbb{D}^\#[z_1]$.

Now taking $z_2 \in \mathbb{D}^\#[z_1]$, but instead of choosing the end point of the geodesic through z_1, z_2 as in the previous step, let $z_2^\# \in \partial\mathbb{D}$ be such that the pentagon $(-1)(1)z_1z_2z_2^\#$ has angle sum π. The remainder of the construction is as before: $\gamma_2^\#$ is the geodesic from -1 to $z_2^\#$; $\lambda_2^\#$ is the line of all points, on the opposite side of $\gamma_2^\#$ from z_2, which are equidistant with z_2 from $\gamma_2^\#$. This line separates $\mathbb{D}^+$ into two connected open components and we denote the one which does not contain z_2 by $\mathbb{D}^\#[z_1, z_2]$.

For a triple z_1, z_2, z_3, the angle sum of the pentagon $(-1)(1)z_1z_2z_3$ is equal to π for $z_3 \in \lambda_2^\#$, it is smaller than π if $z_3 \in \mathbb{D}^\#[z_1, z_2]$ and greater than π otherwise. If the angle sum is smaller than π then there exists $z_0 \in (0,1)$ such that the angle sum of the pentagon $-z_0z_0z_1z_2z_3$ is exactly π.

We summarize the result in the next theorem.

Theorem 7.3: *The set $\mathcal{Z}$ of all admissible triples of vertices z_1, z_2, z_3 is given as*

$$\mathcal{Z} = \{(z_1, z_2, z_3) \in \mathbb{D}^+ \times \mathbb{D}^+ \times \mathbb{D}^+ | z_2 \in \mathbb{D}^\#[z_1], z_3 \in \mathbb{D}^\#[z_1, z_2]\}.$$

VIII. GENERATORS OF THE MODULAR GROUP

A compact Riemann surface of genus 2 may be decomposed into symmetric octagons in infinitely many different ways. We call two octagons *equivalent* if the two surfaces obtained by pasting together the pairs of opposite sides are isometric. From the theory of Teichmüller spaces, it is well known that there exists a group $\mathcal{M}$ operating on the parameter space such that two octagons are equivalent if and only if there exists $\mu \in \mathcal{M}$ sending the first octagon to the second. This group is known as the *modular group*. Generators of $\mathcal{M}$ are described in this section.

The idea is borrowed from the thesis of Aigon[1] who studied group actions on surfaces of signature (0; 2, 2, 2, 2, 2). The generators are similar to those used in Ref. 12.

In the parameter space of the set Z of all admissible triples (z_1, z_2, z_3), each $\mu \in \mathcal{M}$ applied to one such triple yields a new admissible triple,

$$(z_1', z_2', z_3') = \mu[z_1, z_2, z_3],$$

with the property that the corresponding octagon $z_0'z_1' \cdots z_7'$ is equivalent to $z_0z_1 \cdots z_7$. Applying the given generators successively to (z_1, z_2, z_3) and its images yields all equivalent octagons [it re-

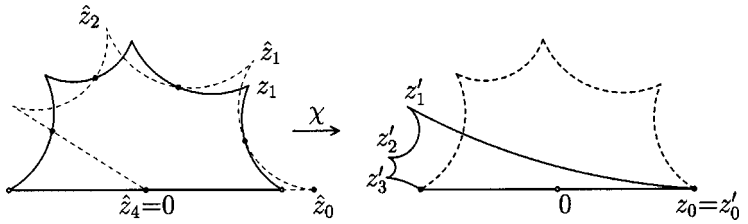

FIG. 11. Shear transformation.

mains however a difficult problem to determine whether or not two given triples (z_1,z_2,z_3) and $(\zeta_1,\zeta_2,\zeta_3)$ lie in the same orbit of $\mathcal{M}$].

Since the octagons are determined by the pentagons, we describe the action of $\mathcal{M}$ in terms of operations on pentagons. When points z_0,p_1,p_2, etc., occur in the formulas, it is always assumed that these are the corresponding points of the octagon determined by the triple z_1,z_2,z_3.

The first operation shears the pentagon and shifts the result into normal position. (See Fig. 11.)

The sheared points are

$$\hat{z}_0 = m_6(0), \quad \hat{z}_k = m_k(\hat{z}_{k-1}), \quad k = 1,2,3,4.$$

By (4.3) we have $\hat{z}_4=0$. The points p_1,p_2,p_3,p_4,p_5 are the midpoints of the sides of the pentagon $\hat{P}$ with vertices $\hat{z}_0,\ldots,\hat{z}_4$ and moreover, P and $\hat{P}$ have the same area (as already observed in the proof of Theorem 7.1). From this it is easily seen that $\hat{P}$ is a fundamental domain for the action of the group Γ^1 generated by $m_1,\ldots,m_5$. If $\hat{P}$ is now shifted using the isometry

$$z \mapsto h(z) = \frac{z - z_0}{1 - z_0 z}, \tag{8.1}$$

then $h(\hat{P})$ is an admissible pentagon equivalent to P. Altogether, this gives the operation $\chi \in \mathcal{M}$ defined as

$$\chi[z_1,z_2,z_3] = (h(\hat{z}_1),h(\hat{z}_2),h(\hat{z}_3)), \tag{8.2}$$

with

$$\hat{z}_0 = m_6(0), \quad \hat{z}_1 = m_1(\hat{z}_0), \quad \hat{z}_2 = m_2(\hat{z}_1), \quad \hat{z}_3 = m_3(\hat{z}_2).$$

The next operation is

$$\tau[z_1,z_2,z_3] = (z_1,z_2,m_3(z_4)). \tag{8.3}$$

The pentagon P' with vertices $z_0,z_1,z_2,m_3(z_4),z_4$ has normal position, area $P'=$area P and the points p_1,p_2,p_3,p_5 are also the midpoints of P'. Hence P' is a fundamental domain for the action of Γ^1 and therefore P and P' are equivalent. (See Fig. 12.)

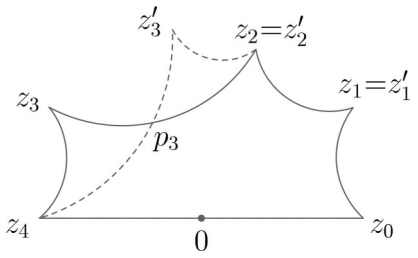

FIG. 12. Transformation of type τ.

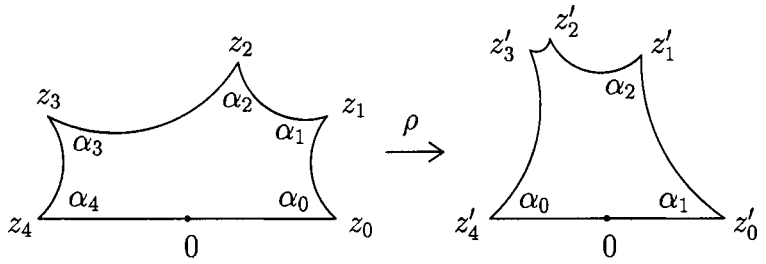

FIG. 13. Rotating the pentagon.

The remaining two operations merely change the position of the pentagon. The first one rotates it

$$\rho[z_1,z_2,z_3] = (r(z_2),r(z_3),r(z_4)), \tag{8.4}$$

with

$$r(z) = \frac{r^1(z)}{r^1(z_1)}|r^1(z_1)|, \quad r^1(z) = \frac{z-p_1}{1-\overline{p_1}z}.$$

The mapping $r^1:\mathbb{D}\to\mathbb{D}$ is the hyperbolic isometry with axis through 0, p_1 which moves p_1 to 0. The multiplication by $|r^1(z_1)|/r^1(z_1)$ is a rotation around 0 bringing $r^1(z_1)$ to the positive part of the real axis. (See Fig. 13.)

The second operation is the symmetry about the imaginary axis

$$\sigma[z_1,z_2,z_3] = (-\overline{z_3},-\overline{z_2},-\overline{z_1}), \tag{8.5}$$

where the bar indicates the complex conjugate.

Theorem 8.1: *The operations χ,ρ,σ,τ generate the modular group $\mathcal{M}$.*

Proof: We have to show that if z_1,z_2,z_3 and z_1',z_2',z_3' are equivalent admissible triples then we can obtain one from the other by a succession of applications of χ,ρ,σ,τ.

Let P,P' be the corresponding pentagons, R,R' the Riemann surfaces obtained by pasting the sides of the corresponding octagons and S,S' the surfaces obtained by pasting the sides of P,P', respectively, in the following way: for $k=1,\ldots,5$, m_k maps side $z_{k-1}z_k$ (i.e., z_4z_0 for $k=5$) onto itself and any point z on this side is pasted to point $m_k(z)$. The resulting surface is topologically a sphere: points $p_1,\ldots,p_5$ turn into points $w_1,\ldots,w_5$ on S and the vertices $z_0,\ldots,z_4$ of P turn into a single point w_6 on S. The surface S carries a hyperbolic metric inherited from P, which is, however, singular at $w_1,\ldots,w_6$. The sides of P become five geodesic arcs at w_6 connecting w_6 with $w_1,\ldots,w_5$. The same holds for S', with singular points $w_1',\ldots,w_6'$.

From the geometry of compact Riemann surfaces of genus 2, it is known that R' is isometric to R if and only if S' is isometric to S with an isometry $g:S'\to S$ sending $w_1',\ldots,w_6'$ to $w_1,\ldots,w_6$. In our case, such an isometry is indeed given, and it carries the arcs from w_6' to $w_1',\ldots,w_5'$ to geodesic arcs on S connecting some w_k to the remaining w_i. These arcs are simple and intersect each other only at w_k. We call them the "*w-curves*."

On P again, these curves are split into a number of geodesic arcs—the *w*-arcs—each of which is either a side of P or else runs through the interior connecting two boundary points of P with each other. Some of the latter have an end point at one of the vertices of P. If the number of these is r and the number of *w*-sides of P is s, then $r+s=5$.

The strategy is to apply χ,ρ,σ,τ successively to P (still calling the successive images P) so that the number of interior *w*-arcs is reduced at each step until eventually they all disappear.

The initial step depends on the above isometry $g:S'\to S$. If $g(w_6')=w_6$ then nothing is carried out in this step. If $g(w_6')=w_k$ with $k\neq 6$, then the position of P is changed using ρ^{5-k}. Corresponding to our notation, this results in a cyclic permutation of the labelling of the points $w_1,\ldots,w_5$ on

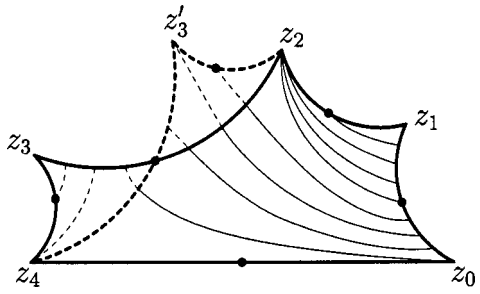

FIG. 14. Reduction of *w*-arcs.

S so that we can now say that g sends w_6' to w_5. We then apply the shear transformation χ. After this initial step we have $g(w_6')=w_6$. The shear χ is not used again in the later steps.

There are now two possible situations. In the first, it is found that, after a suitable change of the position of P via ρ and σ, there exists a *w*-arc from a vertex z_4 to a point on side z_2z_3 which is not z_3 (see Fig. 14 which shows two such arcs). In this case, we apply τ to P so that the vertices are now z_0, z_1, z_2, z_3', z_4. Since *w*-arcs do not intersect each other in the interior of P, no *w*-arc can connect an interior point of side z_3z_4 ("interior" here means different from z_3, z_4) with a boundary point of P which does not lie on side z_2z_3. Any end point of a *w*-arc on p_3z_3 is pasted onto an end point of a *w*-arc on p_3z_2. From this it is easily seen that the number of interior *w*-arcs is reduced at least by one in this step. It is possible that side $z_3'z_4$ is now of *w*-type.

In the remaining case, any *w*-arc in the interior of P and emanating from a vertex of P has its end point on the opposite side. If we change the position of P (via applications of ρ and σ) so that the vertex is z_4 then this arc goes from z_4 to side z_1z_2 and so *any* *w*-arc emanating from a vertex into the interior of P goes from z_4 to side z_1z_2. (See Fig. 15.)

Here we apply $\tau\rho\tau\rho^{-1}$ to P. Under $\rho\tau\rho^{-1}$, P becomes $z_0z_1z_2'z_3z_4$ and under τ it then becomes $z_0z_1z_2'z_3'z_4$. From the same argument as before, the number of *w*-arcs in the interior of P has become smaller and after some steps all interior *w*-arcs have disappeared. This means that the above isometry $g: S' \to S$ maps P' to P, i.e., P and P' are isometric. Hence we may change the position of P using ρ and σ so that finally $P=P'$. ■

Remark: The generators in Theorem 8.1 are for practical use and are not kept to a minimum number. Lu,[32] for the case of genus 2, and later Wajnryb[43] for the general case, showed that the mapping class group of a surface of genus $\geqslant 1$ can be generated by two elements.

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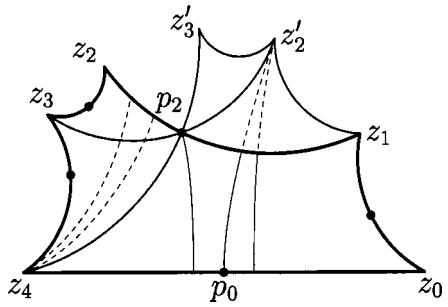

FIG. 15. Reduction of *w*-arcs.

APPENDIX

For convenience we review some facts from hyperbolic geometry in the unit disc model.

For given points $z_1, z_2 \in \mathbb{D}$, let $p = p_{z_1 z_2}$ be the midpoint of the geodesic segment $z_1 z_2$ and $m = m_{z_1 z_2}$ the half turn with center p. Thus,

$$m(p) = p, \quad m(z_1) = z_2, \quad m(z_2) = z_1, \quad m^2 = \mathrm{id}.$$

In order to obtain manageable formulas, we introduce the constant

$$\omega = \omega_{z_1 z_2} \doteq \frac{z_1(1 - |z_2|^2) + z_2(1 - |z_1|^2)}{1 - |z_1 z_2|^2}. \tag{A1}$$

Abbreviating $x = |z_1|$, $y = |z_2|$,

$$x + y = 1 + xy - (1 - x)(1 - y) \text{ and } xy < 1,$$

so that

$$|\omega| < \frac{x(1 - y^2) + y(1 - x^2)}{1 - x^2 y^2} = \frac{(1 - xy)(x + y)}{(1 - xy)(1 + xy)} < 1,$$

i.e.,

$$|\omega_{z_1 z_2}| < 1. \tag{A2}$$

For the half turn we define

$$M = M_{z_1 z_2} \doteq \frac{i}{\sqrt{1 - |\omega_{z_1 z_2}|^2}} \begin{bmatrix} 1 & -\omega_{z_1 z_2} \\ \overline{\omega_{z_1 z_2}} & -1 \end{bmatrix}, \tag{A3}$$

and let $m = m_{z_1 z_2}$ be the isometry $m \in \mathrm{Isom}^+(\mathbb{D})$ defined by this matrix. It follows immediately that $m(z_1) = z_2$, $m(z_2) = z_1$, and $m^2 = \mathrm{id}$. It can also be verified directly that the midpoint of $z_1 z_2$ is

$$p = p_{z_1 z_2} = \frac{\omega_{z_1 z_2}}{1 + \sqrt{1 - |\omega_{z_1 z_2}|^2}}. \tag{A4}$$

Conversely,

$$\omega = \frac{2p}{1 + |p|^2}, \quad M = \frac{i}{1 - |p|^2} \begin{bmatrix} 1 + |p|^2 & -2p \\ 2\overline{p} & -(1 + |p|^2) \end{bmatrix}. \tag{A5}$$

If M and M' are two matrices for half turns as in (A5), then it is easily seen that

$$\mathrm{tr}\, MM' < 0. \tag{A6}$$

In the remaining part we prove the area formula for a geodesic triangle $D(z_1, z_2)$ with vertices $0, z_1, z_2$ used in Sec. III

$$\mathrm{area}\, D(z_1, z_2) = 2 \arg(1 - z_1 \overline{z_2}), \tag{A7}$$

assuming that $0 \leqslant \arg z_1 \leqslant \arg z_2 \leqslant \pi$. [This assumption is unnecessary if we wish to interpret (A7) as a formula for the oriented area.]

The proof is seen from the construction shown in Fig. 16.

If $\mathcal{C} \subset \mathbb{C}$ is the circle through z_1, z_2 which intersects $\partial\mathbb{D}$ orthogonally, then $\mathcal{C} \cap \mathbb{D}$ is the geodesic through z_1, z_2. Since circles orthogonal to $\partial\mathbb{D}$ are invariant under the antiholomorphic involution

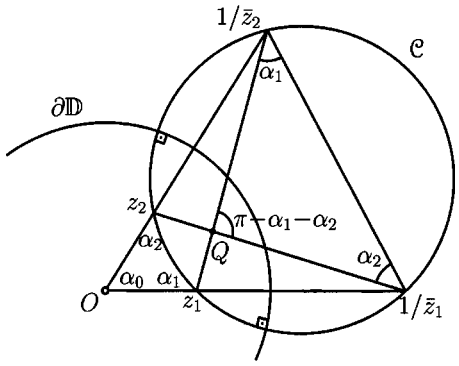

FIG. 16. Angles and area formula.

$z\mapsto 1/\overline{z}$, it follows that $1/\overline{z_1}$ and $1/\overline{z_2}$ lie on $\mathcal{C}$. Denoting the interior angles of $D(z_1,z_2)$ at $0, z_1, z_2$, respectively, by $\alpha_0,\alpha_1,\alpha_2$, then applying the peripheric angle theorem to the Euclidean triangle $(z_2,1/\overline{z_1},1/\overline{z_2})$ inscribed in $\mathcal{C}$ gives the angle at vertex $1/\overline{z_1}$ as

$$\measuredangle(z_2 1/\overline{z_1},1/\overline{z_2})=\alpha_2$$

as marked in the figure. Similarly, triangle $(z_1,1/\overline{z_2},1/\overline{z_1})$ has angle $\measuredangle(z_1,1/\overline{z_2},1/\overline{z_1})=\alpha_1$ at vertex $1/\overline{z_2}$.

The triangle $(1/\overline{z_2},Q,1/\overline{z_1})$ has angle $\pi-\alpha_1-\alpha_2$ at Q, the intersection point of the line segments $(z_1,1/\overline{z_2})$ and $(z_2,1/\overline{z_1})$.

The formula which gives the area of $D(z_1,z_2)$ in terms of z_1 and z_2 is based on the simple fact that if $b_1=r_1e^{i\beta_1}$ and $b_2=r_2e^{i\beta_2}$ are two complex numbers with $0\leqslant\beta_1\leqslant\beta_2\leqslant\pi$, then $\measuredangle(b_2,0,b_1)=\beta_2-\beta_1=\arg(b_2\overline{b_1})$.

Setting

$$b_1=\frac{1}{\overline{z_1}}-z_2 \text{ and } b_2=\frac{1}{\overline{z_2}}-z_1,$$

we have

$$\pi-\alpha_1-\alpha_2=\arg\left(\left(\frac{1}{\overline{z_2}}-z_1\right)\left(\frac{1}{z_1}-\overline{z_2}\right)\right)=\arg\left(\frac{1}{z_1\overline{z_2}}(1-z_1\overline{z_2})^2\right)$$
$$=-\arg(z_1\overline{z_2})+2\arg(1-z_1\overline{z_2})=-(-\alpha_0)+2\arg(1-z_1\overline{z_2}).$$

As area $D(z_1,z_2)=\pi-(\alpha_0+\alpha_1+\alpha_2)$, it follows that

$$\text{area } D(z_1,z_2)=2\arg(1-z_1\overline{z_2}).$$

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SU(*N*) Wigner–Racah algebra for the matrix of second moments of embedded Gaussian unitary ensemble of random matrices

V. K. B. Kota
Physical Research Laboratory, Ahmedabad 380 009, India

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Recently Pluhar and Weidenmüller [Ann. Phys. (N.Y.) **297**, 344 (2002)] showed that the eigenvectors of the matrix of second moments of embedded Gaussian unitary ensemble of random matrices generated by k-body interactions [EGUE(k)] for m fermions in N single particle states are SU(N) Wigner coefficients and derived also an expression for the eigenvalues. Going beyond this work, we will show that the eigenvalues of this matrix are square of a SU(N) Racah coefficient and thus the matrix of second moments of EGUE(k) is solved completely by SU(N) Wigner–Racah algebra. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Interacting finite quantum systems such as nuclei, atoms, quantum dots, nanometer-scale metallic grains, etc., are governed by Hamiltonians of low (compared to the number of particles in the system) particle rank. Therefore, for many purposes, the random matrix models appropriate for these systems are embedded random matrix ensembles of k-body interactions originally introduced, via nuclear shell model calculations, by French and Wong and Bohigas and Flores.[1] For a system of m spinless fermions in N single particle states (we will use fermions throughout this paper and turn briefly to bosons at the end) the embedded Gaussian unitary ensemble of random matrices of k-body interactions [EGUE(k)] is generated by defining the Hamiltonian H, which is given to be k-body, to be GUE in the k-particle spaces and then propagating it to the m particle spaces by using the geometry (direct product structure) of the m-particle spaces. Just as EGUE(k), the EGOE(k) and other embedded ensembles are defined.[2] With m particle space dimension given by $N_m=\binom{N}{m}$, one has the unitary groups SU(N), U(N_k), and U(N_m) with EGUE(k) invariant under U(N_k) and the embedding in m-particle spaces is defined by SU(N); note that a GUE in m particle spaces is invariant under U(N_m) but not the EGUE(k), $k<m$. Very early, using the so-called binary correlation approximation, Mon and French[3] and later French *et al.*[4] derived some analytical properties of embedded ensembles valid in the dilute limit [defined by $(N,m,k)\rightarrow\infty$, $m/N\rightarrow 0$ and $k/m\rightarrow 0$]. However only recently rigorous analytical results, valid for any (N,m,k) are derived for these ensembles by Benet *et al.*[5] and very soon Pluhar and Weidenmüller (hereafter called PW) demonstrated[6] that these results indeed follow from considerations based on the SU(N) embedding algebra. With all the m-particle matrix elements being linear combinations of the k-particle matrix elements [see Eq. (9) ahead], the joint distribution for the matrix elements will be a multivariate Gaussian. Thus all the information about EGUE(k) is in the covariance matrix or the matrix of second moments [Eq. (10) ahead]. PW have shown that the eigenvectors of this matrix are SU(N) Wigner [or Clebsch–Gordon (CG)] coefficients and derived the expression for their eigenvalues using a duality relation for EGUE(k). The purpose of this paper is to show that the eigenvalues can be written as SU(N) Racah coefficients and thus the matrix of second moments is solved completely by SU(N) Wigner–Racah algebra. To this end results for SU(N) Racah coefficients given in Refs. 7–9 are used. We will start with some basic results given in the PW paper.

II. BASIC DEFINITIONS AND RESULTS

Let us begin with m particles in N single particle states (unfortunately in PW ℓ is used in place of N but to keep the notations the same as in our earlier papers,[2,10] we use N). The single particle (sp) creation operator $a_i^\dagger$ for any ith sp state transforms as the irreducible representation $\{1\}$ of U(N) and similarly a product of r creation operators transform, as we have fermions, as the irrep $\{1^r\}$ in Young tableaux notation. Let us add that a U(N) irrep $\{\lambda_1,\lambda_2,\ldots,\lambda_N\}$ defines the corresponding SU(N) irrep as $\{\lambda_1-\lambda_N,\lambda_2-\lambda_N,\ldots,\lambda_{N-1}-\lambda_N\}$ with $N-1$ rows [there are also other equivalent ways of defining SU(N) irreps given a U(N) irrep (Ref. 6)]. This U(N)$\leftrightarrow$SU(N) correspondence is used throughout and therefore we use U(N) and SU(N) interchangeably. In PW, $\{1^r\}$ is denoted by f_r and we will follow this notation from now on. With v_r denoting irreps (and other multiplicity labels) of the groups in a subgroup chain of U(N) that supply the labels needed for a complete specification of any m-particle state (for the purpose of the present paper the subgroup chain need not be specified), the operator $\Pi_{i=1}^r a_i^\dagger$ and a normalized r-particle creation operator $A^\dagger(f_r v_r)$ behave as the SU(N) tensors $T^{f_r v_r}$ and $(1/\sqrt{r!})T^{f_r v_r}$, respectively. Using the composition formula,

$$T^{f_m v_m} = \sum_{v_k,v_s} C^{f_m v_m}_{f_k v_k f_s v_s} T^{f_k v_k} T^{f_s v_s}, \quad s = m-k, \tag{1}$$

where $C^{f_m v_m}_{f_k v_k f_s v_s}$ is a SU(N) CG coefficient, a m-particle state $|f_m v_m\rangle = A^\dagger(f_m v_m)|0\rangle$ can be written as a product of k and $s=m-k$ particle states as

$$|f_m v_m\rangle = \binom{m}{k}^{-1/2} \sum_{v_k v_s} A^\dagger(f_k v_k)|f_s v_s\rangle C^{f_m v_m}_{f_k v_k f_s v_s}. \tag{2}$$

Some properties of the CG coefficients, used later in simplifications, are

$$C^{f_{ab} v_{ab}}_{f_a v_a f_b v_b} = (-1)^{\phi(f_a,f_b,f_{ab})} C^{f_{ab} v_{ab}}_{f_b v_b f_a v_a}, \quad C^{f_{ab} v_{ab}}_{f_a v_a f_b v_b} = C^{\overline{f_{ab}} \overline{v_{ab}}}_{\overline{f_a} v_a \overline{f_b} v_b},$$

$$C^{f_{ab} v_{ab}}_{f_a v_a f_b v_b} = (-1)^{\phi(f_a,f_b,f_{ab})} \sqrt{\frac{d(f_{ab})}{d(f_a)}} C^{f_a v_a}_{f_{ab} v_{ab} \overline{f_b} v_b},$$

$$C^{f_a v_a}_{00 f_a v_a} = 1, \quad C^{00}_{f_a v_a \overline{f_a} v_a} = \frac{1}{\sqrt{d(f_a)}}, \quad (C^{f_{ab} v_{ab}}_{f_a v_a \overline{f_a} v_b})^* = C^{f_{ab} v_{ab}}_{f_a v_b \overline{f_a} v_a},$$

$$\sum_{v_a,v_b} (C^{f_{ab} v_{ab}}_{f_a v_a \overline{f_a} v_b})^* C^{f'_{ab} v'_{ab}}_{f_a v_a \overline{f_a} v_b} = \delta_{f_{ab} f'_{ab}} \delta_{v_{ab} v'_{ab}}. \tag{3}$$

In (3), ϕ is a function that defines the phase for the $1\leftrightarrow 2$ interchange in the CG coefficients, $d(f)$ is the dimension of the irrep f and $\overline{f}$ is the irrep conjugate to f. For $f_r=\{1^r\}$, $\overline{f_r}=\{1^{N-r}\}$ and it also contains a phase factor as given in Eq. (53) of Ref. 7 [this is also seen easily by comparing the second and third equalities in (3) with the corresponding relations for the standard CG coefficients for angular momentum[11]]. Similarly with $f_a=f_k$, $f_b=\overline{f_k}$, one has

$$f_{ab} = g_\nu = \{2^\nu 1^{N-2\nu}\}, \quad \nu = 0,1,\ldots,k.$$

Note that $g_0=\{0\}$ for SU(N) and also $g_\nu=\overline{g_{\nu'}}$. The function ϕ in Eq. (3) is of the form $\phi(\lambda_1,\lambda_2,\lambda_3)=F(\lambda_1)+F(\lambda_2)+F(\lambda_3)$ where F is some function with $F(\lambda)$ an integer and $F(\lambda)=F(\overline{\lambda})$; for SU($N$) irreps that appear in this paper these results are valid as can be seen from Eq. (60) of Ref. 7 except that there can be an overall N dependent factor which will not change any of the final results.

SU(N) irreducible tensors $B_k(g_\nu\omega_\nu)$ constructed out of $A^\dagger(f_k v_k)A(f_k v'_k)$ are defined by

$$B_k(g_\nu\omega_\nu) = \sum_{\upsilon_k,\upsilon_k'} A^\dagger(f_k\upsilon_k)A(f_k\upsilon_k')C^{g_\nu\omega_\nu}_{f_k\upsilon_k\ \overline{f_k}\overline{\upsilon_k'}}. \tag{4}$$

It is useful to note that the tensors B's in (4) multiplied by $k!$ are, to within a phase factor, the same as the tensors defined in Eq. (48) of Ref. 7. Wigner–Eckart theorem decomposes the matrix elements of $B_k(g_\nu\omega_\nu)$ in m-particle spaces into a reduced matrix element $\langle\|\ \|\rangle$ and a CG coefficient,

$$\langle f_m\upsilon_m|B_k(g_\nu\omega_\nu)|f_m\upsilon_m'\rangle = \langle f_m\|B_k(g_\nu)\|f_m\rangle C^{g_\nu\omega_\nu}_{f_m\upsilon_m\ \overline{f_m}\overline{\upsilon_m'}}. \tag{5}$$

Two important properties of $B_k(g_\nu\omega_\nu)$ are

$$\langle\langle B_k(g_\nu\omega_\nu)\rangle\rangle^k = \sqrt{N_k}\delta_{g_\nu,\{0\}},$$

$$\langle\langle B_k(g_\nu\omega_\nu)B_k(g_\mu\omega_\mu)\rangle\rangle^k = \delta_{g_\nu g_\mu}\delta_{\omega_\nu\omega_\mu}. \tag{6}$$

In (6), $\langle\langle\ \rangle\rangle^k$ denotes trace over the k-particle spaces. The first equality in Eq. (6) easily follows from the fact that here $g_\nu=\{0\}$ as traces are scalars with respect to SU(N) and then applying the fifth equality in Eq. (3). Similarly the second equality in Eq. (6) follows from the fact that only $g_\nu=g_\mu$ will give a scalar. Now we will turn to EGOE(k).

Consider a k-body Hamiltonian,

$$H(k) = \sum_{\upsilon_a,\upsilon_b} V_{\upsilon_a\upsilon_b}(k)A^\dagger(f_k\upsilon_a)A(f_k\upsilon_b), \tag{7}$$

where $V_{\upsilon_a\upsilon_b}(k)$ are matrix elements of $H(k)$ in k-particle space and form a GUE, i.e., $V_{\upsilon_a\upsilon_b}(k)$ are independent Gaussian variables with zero center and variance given by

$$\overline{V_{\upsilon_a\upsilon_b}(k)V_{\upsilon_c\upsilon_d}(k)} = \frac{\lambda^2}{N_k}\delta_{\upsilon_a\upsilon_d}\delta_{\upsilon_b\upsilon_c}. \tag{8}$$

In Eq. (8) the overline indicates ensemble average and λ^2 is ensemble averaged variance of $H(k)$ in k-particle space. The m-particle matrix elements of $H(k)$ are, with $s=m-k$,

$$H_{\upsilon_m^1\upsilon_m^2}(k) = \langle f_m\upsilon_m^1|H(k)|f_m\upsilon_m^2\rangle = \binom{m}{k}\sum_{\upsilon_a,\upsilon_b,\upsilon_s}(C^{f_m\upsilon_m^1}_{f_k\upsilon_a f_s\upsilon_s})^* C^{f_m\upsilon_m^2}_{f_k\upsilon_b f_s\upsilon_s}V_{\upsilon_a\upsilon_b}(k). \tag{9}$$

Equation (9) is obtained easily by substituting the definition (7) for $H(k)$, then inserting the complete set of states between $A^\dagger$ and A operators and applying Eq. (2). The EGUE(k) in $m\geqslant k$ spaces is defined by Eqs. (7)–(9). Now it is clear that for any analysis of EGUE(k) all one needs to know is the covariance between any two m-particle matrix elements $H_{\upsilon_m^1\upsilon_m^2}(k)$ and this defines the matrix of second moments,

$$A_{\upsilon_m^1\upsilon_m^4:\upsilon_m^3\upsilon_m^2} = \overline{H_{\upsilon_m^1\upsilon_m^2}(k)H_{\upsilon_m^3\upsilon_m^4}(k)}. \tag{10}$$

As stressed by PW, the most important step in EGUE(k) analysis is to derive a "generalized eigenvalue expansion" of A defined by $A_{ij}=\Sigma_k C_{ik}E_kC_{jk}$ with E_k the eigenvalues and C_{jk} the eigenvectors such that E_k are positive and C's Hermitian. To this end, it is useful to consider the unitary decomposition of $H(k)$ in terms of the SU(N) tensors $B_k(g_\nu\omega_\nu)$,

$$H(k) = \sum_{g_\nu,\omega_\nu} B_k(g_\nu\omega_\nu) W_{g_\nu\omega_\nu}(k). \tag{11}$$

The expansion coefficients $W_{g_\nu\omega_\nu}(k)$ are easily given by

$$W_{g_\nu\omega_\nu}(k) = \langle\langle H(k) B_k(g_\nu\omega_\nu)\rangle\rangle^k \tag{12}$$

and this follows by using the definition (11) and Eq. (6). The most significant property of the W coefficients is that they are independent Gaussian variables with zero center and variance given by [derived using Eqs. (11), (4), (7), and (8) in that order and using the orthonormal properties of the CG coefficients]

$$\overline{W_{g_\nu\omega_\nu}(k) W_{g_\mu\omega_\mu}(k)} = \frac{\lambda^2}{N_k} \delta_{g_\nu g_\mu} \delta_{\omega_\nu\omega_\mu}. \tag{13}$$

III. MATRIX OF SECOND MOMENTS

First we will derive an expression for the covariance $\overline{H^{\upsilon_m^1\upsilon_m^2}(k) H^{\upsilon_m^3\upsilon_m^4}(k)}$ in terms of SU(N) CG coefficients and Racah coefficients and then turn to the eigenvalues and eigenvectors of A, the matrix of second moments. Applying Eqs. (10), (11), and (5) in that order gives

$$\begin{aligned}
\overline{H^{\upsilon_m^1\upsilon_m^2}(k) H^{\upsilon_m^3\upsilon_m^4}(k)} &= \sum_{g_\nu,\omega_\nu,g_\mu,\omega_\mu} \overline{\langle f_m \upsilon_m^1 | B_k(g_\nu\omega_\nu) W_{g_\nu\omega_\nu}(k) | f_m \upsilon_m^2\rangle \langle f_m \upsilon_m^3 | B_k(g_\mu\omega_\mu) W_{g_\mu\omega_\mu}(k) | f_m \upsilon_m^4\rangle} \\
&= \sum_{g_\nu,\omega_\nu,g_\mu,\omega_\mu} \overline{W_{g_\nu\omega_\nu}(k) W_{g_\mu\omega_\mu}(k)} \langle f_m \upsilon_m^1 | B_k(g_\nu\omega_\nu) | f_m \upsilon_m^2\rangle \langle f_m \upsilon_m^3 | B_k(g_\mu\omega_\mu) | f_m \upsilon_m^4\rangle \\
&= \frac{\lambda^2}{N_k} \sum_{g_\nu\omega_\nu} \langle f_m \upsilon_m^1 | B_k(g_\nu\omega_\nu) | f_m \upsilon_m^2\rangle \langle f_m \upsilon_m^3 | B_k(g_\nu\omega_\nu) | f_m \upsilon_m^4\rangle \\
&= \frac{\lambda^2}{N_k} \sum_{g_\nu\omega_\nu} |\langle f_m \| B_k(g_\nu) \| f_m\rangle|^2 C^{g_\nu\omega_\nu}_{f_m \upsilon_m^1 \overline{f_m} \overline{\upsilon_m^2}} C^{g_\nu\omega_\nu}_{f_m \upsilon_m^3 \overline{f_m} \overline{\upsilon_m^4}}.
\end{aligned} \tag{14}$$

Equations (55) and (56) of Ref. 7 together with Eqs. (3) [see also the remark just after Eq. (4)] allows one to write the reduced matrix element in Eq. (14) as a SU(N) Racah or U-coefficient,

$$|\langle f_m \| B_k(g_\nu) \| f_m\rangle|^2 = \frac{(N_m)^2 \binom{m}{k}^2}{d(g_\nu)(N_{m-k})} [\mathrm{U}(f_m f_{N-k} f_m f_k; f_{m-k} g_\nu)]^2. \tag{15}$$

With $\{2^\nu 1^{N-2\nu}\} = \{1^\nu\} \otimes \{1^{N-\nu}\} - \{1^{\nu-1}\} \otimes \{1^{N-\nu+1}\}$ where $\otimes$ denotes Kronecker product, the dimension $d(g_\nu)$ is given by

$$d(g_\nu) = d(\nu) = (N_\nu)^2 - (N_{\nu-1})^2 = \frac{(N!)^2 (N+1)(N-2\nu+1)}{(\nu!)^2 (N-\nu+1!)^2}. \tag{16}$$

Before going further let us define, for a given (m,N), a function $\Lambda^\nu(k)$,

$$\Lambda^\nu(k) = \binom{m-\nu}{k} \binom{N-m+k-\nu}{k}. \tag{17}$$

Now, using Eq. (16) and substituting the expression given by Eq. (61) of Ref. 7 for the U-coefficient in (15), it is seen that

$$|\langle f_m||B_k(g_\nu)||f_m\rangle|^2 = \Lambda^\nu(m-k), \quad \nu = 0,1,2,\ldots,k. \tag{18}$$

Combining (14) with (18) yields an expression for the covariance between H matrix elements in m-particle spaces,

$$\overline{H_{v_m^1 v_m^2}(k) H_{v_m^3 v_m^4}(k)} = \frac{\lambda^2}{N_k} \sum_{\nu=0,1,\ldots,k;\omega_\nu} \frac{(N_m)^2 \binom{m}{k}^2}{d(g_\nu)(N_{m-k})} [\mathrm{U}(f_m f_{N-k} f_m f_k; f_{m-k} g_\nu)]^2 C^{g_\nu \omega_\nu}_{f_m v_m^1 \overline{f_m} \overline{v_m^2}} C^{g_\nu \omega_\nu}_{f_m v_m^3 \overline{f_m} \overline{v_m^4}}$$

$$= \frac{\lambda^2}{N_k} \sum_{\nu=0,1,\ldots,k;\omega_\nu} \{\Lambda^\nu(m-k)\} C^{g_\nu \omega_\nu}_{f_m v_m^1 \overline{f_m} \overline{v_m^2}} C^{g_\nu \omega_\nu}_{f_m v_m^3 \overline{f_m} \overline{v_m^4}}. \tag{19}$$

Equation (19) will be useful in deriving expressions for the moments of H spectrum, i.e., $\overline{\langle H^p \rangle^m}$. However the disadvantage of (19) is that it is not in a proper form to give the eigenvalues and eigenvectors of the matrix A in Eq. (10). In order to obtain them, the CG coefficients in Eq. (14) should be changed to $C^{g_\mu \omega_\mu}_{f_m v_m^1 \overline{f_m} \overline{v_m^4}} C^{g_\mu \omega_\mu}_{f_m v_m^3 \overline{f_m} \overline{v_m^2}}$ and this can be accomplished by a SU(N) Racah transform. Using Eq. (3.2.17) of Ref. 9 one has, for example,

$$\sum_{\omega_\nu} C^{g_\nu \omega_\nu}_{f_m v_m^1 \overline{f_m} \overline{v_m^2}} C^{f_m v_m^4}_{g_\nu \omega_\nu f_m v_m^3} = \sum_{g_\mu \omega_\mu} \mathrm{U}(f_m \overline{f_m} f_m f_m; g_\nu g_\mu) C^{g_\mu \omega_\mu}_{\overline{f_m} v_m^2 f_m v_m^3} C^{f_m v_m^4}_{f_m v_m^1 g_\mu \omega_\mu}. \tag{20}$$

Then Eqs. (20) and (3) will give

$$\sum_{\omega_\nu} C^{g_\nu \omega_\nu}_{f_m v_m^1 \overline{f_m} \overline{v_m^2}} C^{g_\nu \omega_\nu}_{f_m v_m^3 \overline{f_m} \overline{v_m^4}} = \sum_{g_\mu \omega_\mu} \sqrt{\frac{d(g_\nu)}{d(g_\mu)}} \mathrm{U}(f_m \overline{f_m} f_m f_m; g_\nu g_\mu) C^{g_\mu \omega_\mu}_{f_m v_m^1 \overline{f_m} \overline{v_m^4}} C^{g_\mu \omega_\mu}_{f_m v_m^3 \overline{f_m} \overline{v_m^2}}. \tag{21}$$

Finally Eqs. (21) and (15) combined with (14) produce the generalized eigenvalue expansion of the matrix of second moments A,

$$A_{v_m^1 v_m^4 : v_m^3 v_m^2} = \overline{H_{v_m^1 v_m^2}(k) H_{v_m^3 v_m^4}(k)} = \sum_{g_\mu \omega_\mu} C^{g_\mu \omega_\mu}_{f_m v_m^1 \overline{f_m} \overline{v_m^4}} C^{g_\mu \omega_\mu}_{f_m v_m^3 \overline{f_m} \overline{v_m^2}} \left\{ \frac{\lambda^2}{N_k} \frac{(N_m)^2 \binom{m}{k}^2}{(N_{m-k})} \left[\sum_{g_\nu} \sqrt{\frac{1}{d(g_\nu) d(g_\mu)}} \right.\right.$$

$$\left.\left. \times [\mathrm{U}(f_m f_{N-k} f_m f_k; f_{m-k} g_\nu)]^2 \mathrm{U}(f_m \overline{f_m} f_m f_m; g_\nu g_\mu) \right] \right\}. \tag{22}$$

Obviously the quantity in the curly brackets in Eq. (22) gives the eigenvalues of A and the C's are eigenvectors.

IV. EIGENVALUES AS SU(N) RACAH COEFFICIENTS AND THEIR APPLICATIONS

In order to proceed further, it is useful to consider $6j$ symbols of SU(N) and they are defined by [see Eq. (3.2.18) of Ref. 9],

$$\mathrm{U}(\lambda_1 \lambda_2 \lambda \lambda_3; \lambda_{12} \lambda_{23}) = \sqrt{d(\lambda_{12}) d(\lambda_{23})} (-1)^{\phi(\lambda_2, \overline{\lambda_2}, 0) + \phi(\lambda_{12}, \lambda_3, \overline{\lambda}) + \phi(\lambda_1, \lambda_2, \overline{\lambda_{12}})} \begin{Bmatrix} \lambda_1 & \lambda_{23} & \overline{\lambda} \\ \overline{\lambda_3} & \lambda_{12} & \lambda_2 \end{Bmatrix}. \tag{23}$$

In (23) λ's are SU(N) irreps and the four couplings involved in the U-coefficient are assumed to be multiplicity free (for the applications in the present paper this assumption is always valid). Symmetry properties of the $6j$-symbol appearing on the right-hand side of (23) are well known.[8,9] In the present analysis, the Biedenharn–Elliott sum rule extended to SU(N) (Refs. 8 and 9) plays a central role. This sum rule relates a product of three Racah coefficients (weighted appropriately

by dimension factors and phase factors with the irreps in the Racah coefficients appearing in some particular order) with sum over a common irrep label to a product of two Racah coefficients. After converting the Racah coefficients in (22) into 6j symbols of SU(N) using Eq. (23) and then applying the symmetry properties of the 6j symbols, it is seen that the sum in the square brackets in Eq. (22) is exactly in the required form. Applying the Biedenharn–Elliott sum rule, the sum then simplifies to

$$\frac{N_{m-k}}{N_k d(g_\mu)} \mathrm{U}^2(f_m f_{N-m+k} f_m f_{m-k}; f_k g_\mu).$$

Here $\mu = 0, 1, \ldots, m-k$. Now the eigenvalues of the matrix A, in terms of the U(N) Racah coefficients is given by

$$E_\mu = \frac{\lambda^2}{N_k} \frac{(N_m)^2 \binom{m}{k}^2}{d(g_\mu)(N_k)} [\mathrm{U}(f_m f_{N-m+k} f_m f_{m-k}; f_k g_\mu)]^2, \quad \mu = 0, 1, \ldots, m-k \tag{24}$$

with degeneracy $d(g_\mu)$ [see Eq. (16)]. Equation (24) is the central result of this paper. With this, the matrix A is completely specified by the U(N) Wigner and Racah coefficients. Now substituting the formula [Eq. (61) of Ref. 7] for the U-coefficients in Eq. (24) produces the result of PW,

$$A_{\upsilon_m^1 \upsilon_m^4 : \upsilon_m^3 \upsilon_m^2} = \overline{H_{\upsilon_m^1 \upsilon_m^2}(k) H_{\upsilon_m^3 \upsilon_m^4}(k)} = \sum_{g_\mu \omega_\mu} C^{g_\mu \omega_\mu}_{f_m \upsilon_m^1 \overline{f_m} \overline{\upsilon_m^4}} C^{g_\mu \omega_\mu}_{f_m \upsilon_m^3 \overline{f_m} \overline{\upsilon_m^2}} E_\mu, \tag{25}$$

where

$$E_\mu = \frac{\lambda^2}{N_k} \Lambda^\mu(k), \quad \mu = 0, 1, \ldots, m-k. \tag{26}$$

Note that the function $\Lambda^\mu(k)$ is defined by Eq. (17).

Information about EGUE(k) is contained in the ensemble averaged moments $M_p = \overline{\langle H^p \rangle^m}$ and the bivariate moments $\Sigma_{pq} = \overline{\langle H^p \rangle^m \langle H^q \rangle^m}$. In deriving the formulas for the lower order moments, we will show the usefulness of Eq. (19). Obviously, ensemble averaged centroid is zero and the variance is

$$\overline{\langle H^2 \rangle^m} = \frac{1}{N_m} \sum_{\upsilon_m^i, \upsilon_m^j} \overline{H_{\upsilon_m^i \upsilon_m^j} H_{\upsilon_m^j \upsilon_m^i}} = \frac{1}{N_m} \sum_{g_\mu, \omega_\mu} \Lambda^\mu(k) \sum_{\upsilon_m^i, \upsilon_m^j} C^{g_\mu \omega_\mu}_{f_m \upsilon_m^i \overline{f_m} \overline{\upsilon_m^i}} C^{g_\mu \omega_\mu}_{f_m \upsilon_m^j \overline{f_m} \overline{\upsilon_m^j}} = \Lambda^0(k). \tag{27}$$

The second equality follows from (25) and the final result follows by applying (3); note that $\Sigma_{\upsilon_m^i} C^{g_\mu \omega_\mu}_{f_m \upsilon_m^i \overline{f_m} \overline{\upsilon_m^i}} = \sqrt{N_m} \delta_{\mu,0}$. The variance in (27) is in λ^2/N_k units and this factor is dropped as all the quantities we consider from now on are all scaled with respect to $\{\overline{\langle H^2 \rangle^m}\}^{1/2}$. As the third moment is zero, we will turn to the fourth moment,

$$\begin{aligned}
\overline{\langle H^4 \rangle^m} &= \frac{1}{N_m} \sum_{\upsilon_m^i, \upsilon_m^j, \upsilon_m^{k'}, \upsilon_m^l} \overline{H_{\upsilon_m^i \upsilon_m^j} H_{\upsilon_m^j \upsilon_m^{k'}} H_{\upsilon_m^{k'} \upsilon_m^l} H_{\upsilon_m^l \upsilon_m^i}} \\
&= \frac{1}{N_m} \sum_{\upsilon_m^i, \upsilon_m^j, \upsilon_m^{k'}, \upsilon_m^l} \left\{ 2 \left[\sum_{g_\nu, \omega_\nu} \langle f_m \upsilon_m^i | B_k(g_\nu \omega_\nu) | f_m \upsilon_m^j \rangle \langle f_m \upsilon_m^j | B_k(g_\nu \omega_\nu) | f_m \upsilon_m^{k'} \rangle \right] \right. \\
&\quad \times \left[\sum_{g_\mu, \omega_\mu} \langle f_m \upsilon_m^{k'} | B_k(g_\mu \omega_\mu) | f_m \upsilon_m^l \rangle \langle f_m \upsilon_m^l | B_k(g_\mu \omega_\mu) | f_m \upsilon_m^i \rangle \right] + \left[\sum_{g_\nu, \omega_\nu} \langle f_m \upsilon_m^i | B_k(g_\nu \omega_\nu) | f_m \upsilon_m^j \rangle \right. \\
&\quad \left. \left. \times \langle f_m \upsilon_m^{k'} | B_k(g_\nu \omega_\nu) | f_m \upsilon_m^l \rangle \right] \left[\sum_{g_\mu, \omega_\mu} \langle f_m \upsilon_m^j | B_k(g_\mu \omega_\mu) | f_m \upsilon_m^{k'} \rangle \langle f_m \upsilon_m^l | B_k(g_\mu \omega_\mu) | f_m \upsilon_m^i \rangle \right] \right\}
\end{aligned}$$

$$= 2[\Lambda^0(k)]^2 + \frac{1}{N_m} \sum_{v_m^i, v_m^j, v_m^{k'}, v_m^l} \left\{ \sum_{\nu=0,1,\ldots,k;\omega_\nu} \{\Lambda^\nu(m-k)\} C^{g_\nu \omega_\nu}_{f_m v_m^i \overline{f_m} \overline{v_m^j}} C^{g_\nu \omega_\nu}_{f_m v_m^{k'} \overline{f_m} \overline{v_m^l}} \right\}$$

$$\times \left\{ \sum_{\mu=0,1,\ldots,m-k;\omega_\mu} \{\Lambda^\mu(k)\} C^{g_\mu \omega_\mu}_{f_m v_m^j \overline{f_m} \overline{v_m^i}} C^{g_\mu \omega_\mu}_{f_m v_m^l \overline{f_m} \overline{v_m^{k'}}} \right\}$$

$$= 2[\Lambda^0(k)]^2 + \frac{1}{N_m} \sum_{\nu=0}^{\min\{k,m-k\}} \Lambda^\nu(m-k)\Lambda^\nu(k) d(\nu). \tag{28}$$

The second equality in Eq. (28) follows by applying Eqs. (11) and (13). In the third equality, it is easy to recognize the first term. The second term follows by applying Eqs. (19) and (25) to the two pieces in the corresponding term in the second equality. The final result follows by applying the orthonormality of the CG coefficients. Equations (27) and (28) will give the excess (γ_2) parameter of the density of eigenvalues of EGUE(k),

$$\gamma_2 = \frac{\overline{\langle H^4 \rangle^m}}{[\overline{\langle H^2 \rangle^m}]^2} - 3 = \left[\frac{1}{N_m} \sum_{\nu=0}^{\min\{k,m-k\}} \frac{\Lambda^\nu(m-k)\Lambda^\nu(k) d(\nu)}{[\Lambda^0(k)]^2} \right] - 1. \tag{29}$$

Turning now to the lowest bivariate moment Σ_{11}, it is easily seen that

$$\Sigma_{11} = \overline{\langle H \rangle^m \langle H \rangle^m} = \frac{1}{(N_m)^2} \sum_{v_m^i, v_m^j} \overline{H_{v_m^i v_m^i} H_{v_m^j v_m^j}} = \frac{1}{N_m} \Lambda^0(m-k). \tag{30}$$

Applying (19) and recognizing that only $\nu=0$ will contribute to the traces give immediately Eq. (30). However Eq. (25) generates a different formula for Σ_{11} and equating it to (30) gives the identity (derived in PW using the duality transformation),

$$\frac{1}{N_m} \sum_{\nu=0}^{m-k} \Lambda^\nu(k) d(\nu) = \Lambda^0(m-k).$$

The variance of the distribution of centroids of the H spectra over the EGUE(k) ensemble is

$$\hat{\Sigma}_{11} = \frac{\Sigma_{11}}{\overline{\langle H^2 \rangle^m}} = \frac{1}{N_m} \frac{\Lambda^0(m-k)}{\Lambda^0(k)}. \tag{31}$$

Finally Σ_{22} is given by

$$\Sigma_{22} = \overline{\langle H^2 \rangle^m \langle H^2 \rangle^m} = \frac{1}{(N_m)^2} \sum_{v_m^i, v_m^j, v_m^{k'}, v_m^l} \overline{|H_{v_m^i v_m^j}|^2 |H_{v_m^{k'} v_m^l}|^2}$$

$$= \frac{1}{(N_m)^2} \sum_{v_m^i, v_m^j, v_m^{k'}, v_m^l} \overline{|H_{v_m^i v_m^j}|^2}\, \overline{|H_{v_m^{k'} v_m^l}|^2} + \frac{2}{(N_m)^2} \sum_{v_m^i, v_m^j, v_m^{k'}, v_m^l} [\overline{H_{v_m^i v_m^j} H_{v_m^{k'} v_m^l}}]^2$$

$$= [\Lambda^0(k)]^2 + \frac{2}{(N_m)^2} \sum_{\nu=0}^{m-k} [\Lambda^\nu(k)]^2 d(\nu). \tag{32}$$

Here in the second equality used is the property $\overline{x^2 y^2} = (\overline{x^2})(\overline{y^2}) + 2[\overline{xy}]^2$ of Gaussian variables x and y. Similarly the final result follows by applying (25) to the second term in the second equality and simplifying the CG coefficients using Eq. (3). Now, the variance of the distribution of the variances of the H spectra over the EGUE(k) ensemble is

$$\hat{\Sigma}_{22} = \frac{\Sigma_{22}}{[\overline{\langle H^2\rangle^m}]^2} - 1 = \frac{2}{(N_m)^2}\sum_{\nu=0}^{m-k}\left[\frac{\Lambda^\nu(k)}{\Lambda^0(k)}\right]^2 d(\nu). \tag{33}$$

Equations (27), (29), (31), and (33) are also given by Benet *et al.*;[5] this paper neither gives details of the derivations nor uses SU(N) Racah coefficients. Also in this work, $\hat{\Sigma}_{11}$, $\hat{\Sigma}_{22}$, and γ_2+1 are denoted by S, R, and Q, respectively, while we have followed Ref. 3.

V. CONCLUSIONS

Going beyond PW, matrix elements of the matrix of second moments are written explicitly in terms of SU(N) Wigner and Racah coefficients and this result is obtained by recognizing that the reduced matrix elements of $B_k(g_\nu)$ are SU(N) Racah coefficients. With this one has Eq. (19) and this is converted into the generalized eigenvalue expansion form by first applying a SU(N) Racah transform and then applying the Biedenharn–Elliott sum rule extended to SU(N). This gives the eigenvalues of the matrix of second moments explicitly in terms of SU(N) Racah coefficients [Eq. (24)]. The two different forms given by Eqs. (19) and (25) for the covariances of m-particle H matrix elements, give in a simple manner the formulas for the low order moments M_p that define the state density and the bivariate moments Σ_{pq} that give information about fluctuations.

Although EGUE(k) for only fermions is considered in this paper, all the results in fact translate to those of EGUE(k) for bosons by using the well known $N\rightarrow -N$ symmetry,[12,13] i.e., in the fermion results replace N by $-N$ and then take the absolute value of the final result. For example, the m boson space dimension is $d(m)=\left|\binom{-N}{m}\right|=\{(N-m+1)_m\}$. More importantly the eigenvalues of the matrix of the second moments are

$$\Lambda_B^\nu(k) \rightarrow \left|\binom{m-\nu}{k}\binom{-N-m+k-\nu}{k}\right| = \binom{m-\nu}{k}\binom{N+m+\nu-1}{k}. \tag{34}$$

This result was explicitly derived in Ref. 14; see Eq. (14) of this paper. Moreover for bosons, $\{k\}\otimes\{k^{N-1}\}\rightarrow g_\nu=\{2\nu,\nu^{N-2}\}$, $\nu=0,1,\ldots,k$. Also, the $N\rightarrow -N$ symmetry and Eq. (16) give $d(g_\nu)=\{(N+\nu-1)_\nu\}^2-\{(N+\nu-2)_{\nu-1}\}^2$ and this is same as Eq. (15) of Ref. 14. Similarly Eqs. (27), (29), (31), and (33) extend directly to the boson EGUE(k) with $\Lambda^\nu(k)$ replaced by $\Lambda_B^\nu(k)$ defined in Eq. (34). In addition, for fermions to bosons there is also a $m\leftrightarrow N$ symmetry and this connects fermion results (say for M_p and Σ_{pq}) in the dilute limit to boson results in the dense limit.[13]

Recently there is considerable interest in mesoscopic physics to study EGUE(k) for fermions with spin[15] and here the embedding algebra is $\mathrm{U}(2N)\supset\mathrm{U}(N)\otimes\mathrm{SU}(2)$ with SU(2) generating spin. The approach presented in Secs. II–IV is being applied to this system; some useful results for the $\mathrm{U}(2N)\supset\mathrm{U}(N)\otimes\mathrm{SU}(2)$ Wigner–Racah algebra are available in Refs. 16 and 17. Finally, Wigner–Racah algebra analysis of embedded ensembles with more general group symmetries (see Refs. 2, 6, 17, and 18 for examples) should be possible in the future, thus opening up a new direction in random matrix theory.

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Darboux transformations and exact solutions of two dimensional $A_{2n}^{(2)}$ Toda equation

Zi-Xiang Zhou[a)]
Institute of Mathematics, Fudan University, Shanghai 200433, People's Republic of China

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The Darboux transformations for two dimensional $A_{2n}^{(2)}$ Toda equation are constructed. The lowest degree of the Darboux transformation is $2(2n+1)$ if all the spectral parameters are complex, or $2n+1$ if one spectral parameter is real. Exact solutions are written down by computing the Darboux transformations explicitly. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1857033]

I. INTRODUCTION

The two dimensional Toda equation is an important integrable system which has been studied widely (e.g., Refs. 1–15) and has applications to differential geometry.[4–7] A Toda equation corresponding to a Kac–Moody algebra g of affine type can be written as

$$w_{k,xt} = A_k \exp\left(\sum_{i=1}^{n} c_{ki} w_i\right) - A_0 v_k \exp\left(\sum_{i=1}^{n} c_{0i} w_i\right) \quad (k = 1, \ldots, n), \tag{1.1}$$

where $C=(c_{ij})_{0\leqslant i,j\leqslant n}$ is the generalized Cartan matrix of g, $v=(v_0, v_1, \ldots, v_n)^T$ is a nonzero vector such that $Cv=0$, and $A_0, A_1, \ldots, A_n$ are real constants.[8,9] There have been a lot of works on the two dimensional Toda equations which are infinite, or are periodic (with $g=A_n^{(1)}$),[5,10] or having fixed ends,[11,12] or with finite dimensional Lie algebras (Kac–Moody algebras of finite type).[13–15]

As a special case of $g=A_2^{(2)}$, the Tzitzeica equation is a typical equation in affine geometry describing indefinite affine spheres.[4,16] An expression of Darboux transformation of the Tzitzeica equation, whose spectral parameter is real, was discussed in Ref. 17, and the loop group decomposition was presented in Ref. 18.

In this paper, we consider the Toda equation with Kac–Moody algebra $g=A_{2n}^{(2)}$. It is neither periodic nor with fixed ends. It has an $(2n+1)\times(2n+1)$ Lax pair, and the Lax pair has a unitary symmetry, a reality symmetry and a cyclic symmetry of order $2n+1$. To get the Darboux transformations which generate solutions of the same equation, we need to consider all these symmetries in the construction. Therefore, Darboux transformations of high degree are necessary. We shall consider the case where all the spectral parameters are complex, as well as the case where one spectral parameter is real. The main results are presented in Theorem 1 of Sec. IV and Theorem 2 of Sec. V.

In Sec. II, we discuss the Lax pair of the $A_{2n}^{(2)}$ Toda equation. In Sec. III, the formulas of Darboux transformation are listed in terms of the standard construction. In Sec. IV, the Darboux transformation with complex spectral parameters is written down in an explicit way. Correspondingly, the Darboux transformation with a real spectral parameter is written down explicitly in Sec. V. In Sec. VI, the explicit solutions of the Tzitzeica equation are presented.

II. LAX PAIR AND EVOLUTION EQUATIONS

The $A_2^{(2)}$ Toda equation, or the Tzitzeica equation, is

a)Electronic mail: zxzhou@public6.sta.net.cn

$$w_{1,xt} = -A_0 e^{-w_1} + A_1 e^{2w_1}, \tag{2.1}$$

where A_0, A_1 are real constants. It corresponds to the generalized Cartan matrix $C=\left(\begin{smallmatrix} 2 & -1 \\ -4 & 2 \end{smallmatrix}\right)$ of $A_2^{(2)}$ with $C(\frac{1}{2},1)^T=0$.

For $n\geqslant 2$, the $A_{2n}^{(2)}$ Toda equation is

$$w_{1,xt} = -A_0 e^{-w_1} + A_1 e^{2w_1-w_2},$$

$$w_{j,xt} = -A_0 e^{-w_1} + A_j e^{2w_j-w_{j-1}-w_{j+1}} \quad (j=2,\ldots,n-1),$$

$$w_{n,xt} = -A_0 e^{-w_1} + A_n e^{2w_n-2w_{n-1}}, \tag{2.2}$$

where A_0, $A_1,\ldots,A_n$ are real constants. It corresponds to the generalized Cartan matrix

$$C = \begin{pmatrix} 2 & -1 & & & & \\ -2 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -2 & 2 \end{pmatrix} \tag{2.3}$$

of $A_{2n}^{(2)}$ and $C(\frac{1}{2},1,\ldots,1)^T=0$.

For all $n\geqslant 1$, let $w_j=-(u_1+\ldots+u_j)$ $(j=1,\ldots,n)$, then (2.1) becomes

$$u_{1,xt} = A_0 e^{u_1} - A_1 e^{-2u_1}, \tag{2.4}$$

and (2.2) becomes

$$u_{1,xt} = A_0 e^{u_1} - A_1 e^{u_2-u_1},$$

$$u_{j,xt} = A_{j-1} e^{u_j-u_{j-1}} - A_j e^{u_{j+1}-u_j} \quad (2\leqslant j\leqslant n-1),$$

$$u_{n,xt} = A_{n-1} e^{u_n-u_{n-1}} - A_n e^{-2u_n}. \tag{2.5}$$

Hereafter, for any $(2n+1)\times(2n+1)$ matrix A or any $(2n+1)$-vector v, and for any integers i and j, define $A_{ij}=A_{i'j'}$ and $v_i=v_{i'}$ where $i\equiv i' \bmod 2n+1$, $j\equiv j' \bmod 2n+1$, and $1\leqslant i',j'\leqslant 2n+1$. Especially, denote

$$\delta_{ij} = \begin{cases} 1 & \text{if } i-j\equiv 0 \bmod 2n+1, \\ 0 & \text{otherwise.} \end{cases} \tag{2.6}$$

Let $\omega=e^{2\pi i/(2n+1)}$, $\Omega=\mathrm{diag}(1,\omega^{-1},\ldots,\omega^{-2n})$. Let $K=(K_{ij})=(\delta_{i,2n+1-j})_{(2n+1)\times(2n+1)}$ and $J=(J_{ij})=(\delta_{i,j-1})_{(2n+1)\times(2n+1)}$ be two constant matrices and

$$P = (p_i\delta_{ij})_{(2n+1)\times(2n+1)}, \quad Q = (q_i\delta_{i,j+1})_{(2n+1)\times(2n+1)}, \tag{2.7}$$

where

$$p_i = -p_{2n+1-i} = u_{i,x} \quad (1\leqslant i\leqslant n), \quad p_{2n+1}=0,$$

$$q_i = q_{2n-i} = A_i e^{u_{i+1}-u_i} \quad (1\leqslant i\leqslant n-1), \quad q_n = A_n e^{-2u_n}, \quad q_{2n}=q_{2n+1}=A_0 e^{u_1}. \tag{2.8}$$

From (2.7) and (2.8), $\det Q=q_1\ldots q_{2n+1}=A_0^2A_1^2\ldots A_{n-1}^2A_n$ is a constant.

Notice that

$$\Omega^* K = \omega^{-2} K \Omega. \tag{2.9}$$

Here A^* refers to the Hermitian conjugate of a matrix A.

Now consider the Lax pair

$$\Phi_x = U(x,t,\lambda)\Phi \equiv (\lambda J + P(x,t))\Phi, \quad \Phi_t = V(x,t,\lambda)\Phi \equiv \lambda^{-1} Q(x,t)\Phi. \tag{2.10}$$

Its integrability condition

$$U_t - V_x + [U,V] = 0 \tag{2.11}$$

is

$$Q_x = [P,Q], \quad P_t + [J,Q] = 0, \tag{2.12}$$

or equivalently

$$q_{i,x} = (p_{i+1} - p_i) q_i, \quad p_{i,t} = q_{i-1} - q_i. \tag{2.13}$$

These are just the $A_{2n}^{(2)}$ Toda equations (2.4) and (2.5) by considering (2.8).

It is easy to check that J, $P(x,t)$, $Q(x,t)$ satisfy the relations

$$\Omega P \Omega^{-1} = P, \quad \Omega J \Omega^{-1} = \omega J, \quad \Omega Q \Omega^{-1} = \omega^{-1} Q,$$

$$K P K^{-1} = -P^T, \quad K J K^{-1} = J^T, \quad K Q K^{-1} = Q^T. \tag{2.14}$$

Written equivalently in terms of U and V, (2.14) becomes

$$\overline{U(x,t,\lambda)} = U(x,t,\bar{\lambda}), \quad \overline{V(x,t,\lambda)} = V(x,t,\bar{\lambda}),$$

$$\Omega U(x,t,\lambda)\Omega^{-1} = U(x,t,\omega\lambda), \quad \Omega V(x,t,\lambda)\Omega^{-1} = V(x,t,\omega\lambda),$$

$$K U(x,t,\lambda) K^{-1} = -(U(x,t,-\bar{\lambda}))^*, \quad K V(x,t,\lambda) K^{-1} = -(V(x,t,-\bar{\lambda}))^*. \tag{2.15}$$

Conversely, if (P,Q) satisfies (2.12), then $\det Q$ is independent of x, since

$$(\det Q)_x = \det Q \, \mathrm{tr}(Q_x Q^{-1}) = \det Q \, \mathrm{tr}([PQ^{-1}, Q]) = 0. \tag{2.16}$$

Now suppose that $A_0, A_1, \ldots, A_{n-1} \neq 0$ are given constants and (P,Q) is a $(2n+1)\times(2n+1)$ matrix solution of (2.12) satisfying the constraints (2.14) and $\det Q$ is a constant. From (2.14), P and Q must be of form (2.7) with

$$p_i + p_{2n+1-i} = 0, \quad q_i = q_{2n-i} \quad (i = 1,2,\ldots,2n+1). \tag{2.17}$$

In the region where $q_i A_i > 0$ $(i=1,\ldots,n)$, let $q_i = A_i e^{u_{i+1}-u_i}$ $(1 \leqslant i \leqslant n-1)$, $q_{2n} = A_0 e^{u_1}$, then $q_n = A_n e^{-2u_n}$ where $A_n = \det Q / A_0^2 A_1^2 \cdots A_{n-1}^2$. Moreover, from the first equation of (2.12),

$$p_i = -p_{2n+1-i} = u_{i,x} \quad (1 \leqslant i \leqslant n), \quad p_{2n+1} = 0. \tag{2.18}$$

The second equation of (2.12) implies that $(u_1,\ldots,u_n)$ is a solution of the $A_{2n}^{(2)}$ Toda equation (2.4) or (2.5). Therefore, we have the following,

Lemma 1: *Suppose (P,Q) is a $(2n+1)\times(2n+1)$ matrix solution of (2.12) satisfying the constraints (2.14) and $\det Q$ is a constant. Then in the region where $q_i A_i > 0$ $(i=1,\ldots,n)$, $(u_1,\ldots,u_n)$ is a solution of the $A_{2n}^{(2)}$ Toda equation (2.4) or (2.5).*

In order to construct Darboux transformation, we need the following lemma, which is the direct consequence of (2.14).

Lemma 2: *Suppose $\mu \in \mathbf{C}$.*

(i) *If $\Phi(x,t)$ is a solution of (2.10) for $\lambda = \mu$, then $\overline{\Phi}(x,t)$ is a solution of (2.10) for $\lambda = \bar{\mu}$;*

(ii) *If* $\Phi(x,t)$ *is a solution of (2.10) for* $\lambda=\mu$*, then for any integer* k*,* $\Omega^k\Phi(x,t)$ *is a solution of (2.10) for* $\lambda=\omega^k\mu$.

(iii) *If* $\Phi(x,t)$ *is a solution of (2.10) for* $\lambda=\mu$*,* $\Psi(x,t)$ *is a solution of (2.10) for* $\lambda=-\bar{\mu}$*, then* $(\Psi^*K\Phi)_x=0$, $(\Psi^*K\Phi)_t=0$.

III. DARBOUX TRANSFORMATION

The Darboux matrix with unitary reduction can be constructed in the following known procedure.[19,20]

Let $\lambda_1,\ldots,\lambda_M$ be M complex numbers such that λ_j, $-\bar{\lambda}_j$ $(j=1,2,\ldots,M)$ are distinct. Let H_j be a column solution of the Lax pair (2.10) for $\lambda=\lambda_j$ $(j=1,2,\ldots,M)$. Denote

$$\Gamma_{ij}=\frac{H_i^*KH_j}{\bar{\lambda}_i+\lambda_j} \tag{3.1}$$

for $i,j=1,2,\ldots,M$, $\Gamma=(\Gamma_{ij})_{1\leqslant i,j\leqslant M}$,

$$G(x,t,\lambda)=\prod_{l=1}^{M}(\lambda+\bar{\lambda}_l)\left(1-\sum_{i,j=1}^{M}\frac{(\Gamma^{-1})_{ij}H_iH_j^*K}{\lambda+\bar{\lambda}_j}\right). \tag{3.2}$$

Then it can be checked directly that

$$G(x,t,\lambda)^{-1}=\prod_{l=1}^{M}(\lambda+\bar{\lambda}_l)^{-1}\left(1+\sum_{i,j=1}^{M}\frac{(\Gamma^{-1})_{ij}H_iH_j^*K}{\lambda-\lambda_i}\right). \tag{3.3}$$

$G(x,t,\lambda)$ is a polynomial of λ of degree M with matrix coefficients. Write

$$G(x,t,\lambda)=\sum_{j=0}^{M}(-1)^{M-j}G_{M-j}(x,t)\lambda^j,\quad G_0(x,t)=I, \tag{3.4}$$

and define

$$\tilde{U}=GUG^{-1}+G_xG^{-1},\quad \tilde{V}=GVG^{-1}+G_tG^{-1}. \tag{3.5}$$

Lemma 3: $\tilde{U}=\lambda J+\tilde{P}$, $\tilde{V}=(1/\lambda)\tilde{Q}$ *where* $\tilde{P}=P+[J,G_1]$, $\tilde{Q}=G_MQG_M^{-1}$.

Proof: Using (2.14) and the fact that H_j is a solution of the Lax pair (2.10) with $\lambda=\lambda_j$, we have

$$\Gamma_{ij,x}=H_i^*KJH_j,\quad \Gamma_{ij,t}=\frac{1}{\bar{\lambda}_i\lambda_j}H_i^*KQH_j. \tag{3.6}$$

Substituting (3.2), (3.3), and (3.6) into (3.5) and using the symmetries (2.14), we get the conclusion of the lemma by direct calculation.

Lemma 4:

$$G(x,t,-\bar{\lambda})^*KG(x,t,\lambda)=\prod_{l=1}^{M}(\bar{\lambda}_l+\lambda)(\lambda_l-\lambda)K. \tag{3.7}$$

Proof: The equality (3.7) follows from

$$G(x,t,-\bar{\lambda})^*=KG(x,t,\lambda)^{-1}K^{-1}\prod_{l=1}^{M}(\bar{\lambda}_l+\lambda)(\lambda_l-\lambda), \tag{3.8}$$

which is a direct result of (3.2), (3.3) and the fact that Γ is Hermitian. The lemma is proved.

The solution $\tilde{Q}$ has been expressed in terms of G_M. According to (3.2),

$$(-1)^M G_M = \prod_{l=1}^{M} \bar{\lambda}_l \left(1 - \sum_{i,j=1}^{M} \frac{(\Gamma^{-1})_{ij} H_i H_j^* K}{\bar{\lambda}_j} \right) = \prod_{l=1}^{M} \bar{\lambda}_l \left(1 - (2n+1) R^* \Gamma^{-1} S\right), \tag{3.9}$$

where R and S are $M \times (2n+1)$ matrices with

$$R_{ij} = (2n+1)^{-1/2} (\bar{H}_i)_j, \quad S_{ij} = (2n+1)^{-1/2} \bar{\lambda}_i^{-1} \sum_{k=1}^{2n+1} (\bar{H}_i)_{-k}. \tag{3.10}$$

IV. DARBOUX TRANSFORMATION WITH COMPLEX SPECTRAL PARAMETERS

Darboux matrix keeping the reductions (2.14) can be derived by above general construction together with some more constraints on the spectral parameters and the solutions of the Lax pair.

Let μ be a nonzero complex number such that $\arg(\mu) \neq k\pi/(4n+2)$ for any integer k. Let $\lambda_j = \omega^{j-1}\mu$, $\lambda_{2n+1+j} = \omega^{-j+1}\bar{\mu}$ $(j=1,2,\ldots,2n+1)$. Then all λ_j and $-\bar{\lambda}_j$ $(j=1,2,\ldots,2(2n+1))$ are distinct. Let h be a column solution of (2.10) for $\lambda=\mu$, $H_j = \Omega^{j-1} h$, $H_{2n+1+j} = \Omega^{-j+1}\bar{h}$ $(j=1,2,\ldots,2n+1)$. Then H_j is a solution of (2.10) for $\lambda=\lambda_j (j=1,2,\ldots,2(2n+1))$.

We construct Γ, $G(x,t,\lambda)$, $\tilde{U}(x,t,\lambda)$, $\tilde{V}(x,t,\lambda)$ according to Sec. III with $M=2(2n+1)$.

More explicit expressions of Γ_{ij} can be written down from their definition (3.1). For $1 \leqslant i,j \leqslant 2n+1$, let

$$A_{ij} = \Gamma_{ij} = \frac{h^*(\Omega^*)^{i-1} K \Omega^{j-1} h}{\omega^{-i+1}\bar{\mu} + \omega^{j-1}\mu} = \omega^{-i+1} \frac{h^* K \Omega^{i+j-2} h}{\bar{\mu} + \omega^{i+j-2}\mu},$$

$$B_{ij} = \Gamma_{i,2n+1+j} = \frac{h^*(\Omega^*)^{i-1} K \Omega^{-j+1} \bar{h}}{\omega^{-i+1}\bar{\mu} + \omega^{-j+1}\bar{\mu}} = \omega^{-i+1} \frac{h^* K \Omega^{i-j} \bar{h}}{\bar{\mu} + \omega^{i-j}\bar{\mu}},$$

$$C_{ij} = \Gamma_{2n+1+i,j} = \frac{\bar{h}^*(\Omega^*)^{-i+1} K \Omega^{j-1} h}{\omega^{i-1}\mu + \omega^{j-1}\mu} = \omega^{i-1} \frac{\bar{h}^* K \Omega^{j-i} h}{\mu + \omega^{j-i}\mu},$$

$$D_{ij} = \Gamma_{2n+1+i,2n+1+j} = \frac{\bar{h}^*(\Omega^*)^{-i+1} K \Omega^{-j+1} \bar{h}}{\omega^{i-1}\mu + \omega^{-j+1}\bar{\mu}} = \omega^{i-1} \frac{\bar{h}^* K \Omega^{-i-j+2} \bar{h}}{\mu + \omega^{-i-j+2}\bar{\mu}}. \tag{4.1}$$

Then Γ is written as a 2×2 block matrix $\Gamma = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)$ where $A=(A_{ij})$, $B=(B_{ij})$, $C=(C_{ij})$, $D=(D_{ij})$ are $(2n+1)\times(2n+1)$ matrices, and $\Gamma^{-1} = \left(\begin{smallmatrix} \hat{A} & \hat{B} \\ \hat{C} & \hat{D} \end{smallmatrix}\right)$ where

$$\hat{A} = (A - BD^{-1}C)^{-1}, \quad \hat{B} = -A^{-1}B(D - CA^{-1}B)^{-1},$$

$$\hat{C} = -D^{-1}C(A - BD^{-1}C)^{-1}, \quad \hat{D} = (D - CA^{-1}B)^{-1}. \tag{4.2}$$

From (4.1), we know that $D=\bar{A}$, $C=\bar{B}$. Hence, (4.2) leads to $\hat{D}=\bar{\hat{A}}$, $\hat{C}=\bar{\hat{B}}$. Then, from (3.2), we have the following.

Lemma 5: $\overline{G(x,t,\bar{\lambda})} = G(x,t,\lambda)$. *Hence the coefficients of each power of* λ *in* $G(x,t,\lambda)$ *are all real matrices.*

From (4.1), we get

$$A_{i+1,j-1} = \omega^{-1} A_{ij}, \quad B_{i+1,j+1} = \omega^{-1} B_{ij}, \quad C_{i+1,j+1} = \omega C_{ij}, \quad D_{i+1,j-1} = \omega D_{ij}. \tag{4.3}$$

Written equivalently, they are

$$JAJ=\omega^{-1}A,\quad JBJ^{-1}=\omega^{-1}B,\quad J^{-1}CJ=\omega^{-1}C,\quad J^{-1}DJ^{-1}=\omega^{-1}D. \tag{4.4}$$

According to (4.2),

$$J\hat{A}J=\omega^{-1}\hat{A},\quad J\hat{B}J^{-1}=\omega^{-1}\hat{B},\quad J^{-1}\hat{C}J=\omega^{-1}\hat{C},\quad J^{-1}\hat{D}J^{-1}=\omega^{-1}\hat{D}. \tag{4.5}$$

Hence

$$\hat{A}_{i+1,j-1}=\omega^{-1}\hat{A}_{ij},\quad \hat{B}_{i+1,j+1}=\omega^{-1}\hat{B}_{ij},\quad \hat{C}_{i+1,j+1}=\omega\hat{C}_{ij},\quad \hat{D}_{i+1,j-1}=\omega\hat{D}_{ij}. \tag{4.6}$$

Lemma 6: $\Omega G(x,t,\lambda)\Omega^{-1}=G(x,t,\omega\lambda)$.

Proof:

$$\Omega\frac{\Omega^{i-1}h(\Omega^{j-1}h)^*K}{\lambda+\overline{\omega^{j-1}\mu}}\Omega^{-1}=\frac{\omega\Omega^{i}h(\Omega^{j-2}h)^*\Omega^*K\Omega^{-1}}{\omega\lambda+\overline{\omega^{j-2}\mu}}=\frac{\omega^{-1}\Omega^{i}h(\Omega^{j-2}h)^*K}{\omega\lambda+\overline{\omega^{j-2}\mu}}. \tag{4.7}$$

Hence,

$$\Omega\sum_{i,j=1}^{2n+1}\hat{A}_{ij}\frac{\Omega^{i-1}h(\Omega^{j-1}h)^*K}{\lambda+\overline{\omega^{j-1}\mu}}\Omega^{-1}=\sum_{i,j=1}^{2n+1}\hat{A}_{i+1,j-1}\frac{\Omega^{i}h(\Omega^{j-2}h)^*K}{\omega\lambda+\overline{\omega^{j-2}\mu}}=\sum_{i,j=1}^{2n+1}\hat{A}_{ij}\frac{\Omega^{i-1}h(\Omega^{j-1}h)^*K}{\omega\lambda+\overline{\omega^{j-1}\mu}} \tag{4.8}$$

by (4.6). Similar relations hold for the terms in G with B_{ij}, C_{ij}, and D_{ij}. Moreover, $\Pi_{l=1}^{2(2n+1)}(\lambda+\overline{\lambda}_l)=\Pi_{l=1}^{2(2n+1)}(\omega\lambda+\overline{\lambda}_l)$. Hence, by (3.2), the lemma is true.

From Lemma 4, Lemma 5, and Lemma 6, $\tilde{U}$ and $\tilde{V}$ defined by (3.5) are real and satisfy the relations (2.15). Moreover, after the Darboux transformation, they must satisfy the integrability condition (2.11). Hence, by Lemma 1, we have the following.

Proposition 1: $(\tilde{P},\tilde{Q})$ *generated by the Darboux transformation constructed above is a real solution of (2.12) satisfying the relations (2.14). Therefore, it gives a solution of the* $A_{2n}^{(2)}$ *Toda equation (2.4) or (2.5).*

In order to get explicit expressions of the solutions we should derive the explicit expression of $G_{2(2n+1)}$. Equation (3.2) is too complicated to be computed directly even by computer. Therefore, we need to represent the matrix Γ, regarded as a linear transformation, in another basis, so that its inverse can be computed explicitly.

Let $\xi_k=(2n+1)^{-1/2}\Omega^{k-1}(1,1,\ldots,1)^T$, then the ith component of ξ_k is

$$(\xi_k)_i=(2n+1)^{-1/2}\omega^{-(k-1)(i-1)}. \tag{4.9}$$

Using the fact

$$\sum_{j=1}^{2n+1}\omega^{jk}=\begin{cases}0 & \text{if } k\not\equiv 0 \bmod 2n+1,\\ 2n+1 & \text{if } k\equiv 0 \bmod 2n+1,\end{cases} \tag{4.10}$$

we know that $(\xi_1,\ldots,\xi_{2n+1})$ is an orthonormal basis of $\mathbf{C}^{2n+1}$.

From (4.1),

$$A\xi_k=\alpha_k\xi_{3-k},\quad B\xi_k=\overline{\gamma}_{2-k}\xi_{k+1},\quad C\xi_k=\gamma_k\xi_{k-1},\quad D\xi_k=\overline{\alpha}_{2-k}\xi_{1-k}, \tag{4.11}$$

where

$$\alpha_k=\sum_{j=1}^{2n+1}\frac{h^*K\Omega^jh}{\overline{\mu}+\omega^j\mu}\omega^{-(k-1)j},\quad \gamma_k=\sum_{j=1}^{2n+1}\frac{\overline{h}^*K\Omega^jh}{\mu+\omega^j\mu}\omega^{-(k-1)j}. \tag{4.12}$$

Using (2.9), we have $\overline{h^*K\Omega^jh}=(h^*K\Omega^jh)^*=\omega^{-2j}h^*K\Omega^jh$, $\overline{h}^*K\Omega^jh=(\overline{h}^*K\Omega^jh)^T=\omega^{2j}\overline{h}^*K\Omega^{-j}h$. Hence

$$\overline{\alpha}_k = \alpha_{3-k}, \quad \gamma_k = \gamma_{3-k}. \tag{4.13}$$

From (4.2) and (4.11), we obtain

$$\hat{A}\xi_k = \hat{\alpha}_k \xi_{3-k}, \quad \hat{B}\xi_k = \overline{\hat{\gamma}}_{2-k}\xi_{k+1}, \quad \hat{C}\xi_k = \hat{\gamma}_k \xi_{k-1}, \quad \hat{D}\xi_k = \overline{\hat{\alpha}}_{2-k}\xi_{1-k}, \tag{4.14}$$

where

$$\hat{\alpha}_k = \overline{\alpha}_{3-k}(|\alpha_{3-k}|^2 - |\gamma_{3-k}|^2)^{-1}, \quad \hat{\gamma}_k = -\gamma_{3-k}(|\alpha_{3-k}|^2 - |\gamma_{3-k}|^2)^{-1}. \tag{4.15}$$

Let $h=(h_1,\ldots,h_{2n+1})^T$, then the entries of $\overline{H}_i$, $\overline{H}_{2n+1+i}$ $(1\leqslant i\leqslant 2n+1)$ are $(\overline{H}_i)_j=\omega^{(i-1)(j-1)}\overline{h}_j$, $(\overline{H}_{2n+1+i})_j=\omega^{-(i-1)(j-1)}h_j$. Hence, from (3.10), for $1\leqslant i,j\leqslant 2n+1$,

$$R_{ij} = (2n+1)^{-1/2}\omega^{(i-1)(j-1)}\overline{h}_j, \quad R_{2n+1+i,j} = (2n+1)^{-1/2}\omega^{-(i-1)(j-1)}h_j,$$

$$S_{ij} = (2n+1)^{-1/2}\overline{\mu}^{-1}\omega^{-(i-1)j}\overline{h}_{-j}, \quad S_{2n+1+i,j} = (2n+1)^{-1/2}\mu^{-1}\omega^{(i-1)j}h_{-j}. \tag{4.16}$$

Written in matrices, the ith column of R is $(\overline{h}_i\xi_{2-i}, h_i\xi_i)^T$ and the jth column of S is $(\overline{\mu}^{-1}\overline{h}_{-j}\xi_{j+1}, \mu^{-1}h_{-j}\xi_{1-j})^T$.

Let

$$\mathcal{A}_l = \overline{h_l}h_{-l}, \quad \mathcal{C}_l = h_l h_{-l}. \tag{4.17}$$

Lemma 7: *$|\mu|^{-2(2n+1)}G_{2(2n+1)}=1-(2n+1)R^*\Gamma^{-1}S=\mathrm{diag}(g_1,\ldots,g_{2n+1})$ where*

$$g_j = 1 - 2(2n+1)\mathrm{Re}\left(\frac{1}{\mu}\frac{\mathcal{A}_j\alpha_{2-j} - \mathcal{C}_j\overline{\gamma}_{2-j}}{|\alpha_{2-j}|^2 - |\gamma_{2-j}|^2}\right). \tag{4.18}$$

Proof: Using the expressions (3.9) and (4.14), we have $|\mu|^{-2(2n+1)}G_{2(2n+1)}=1-(2n+1)R^*\Gamma^{-1}S$ and

$$(R^*\Gamma^{-1}S)_{ij} = \left(h_i\xi_{2-i}^*, \overline{h}_i\xi_i^*\right)\begin{pmatrix}\hat{A} & \hat{B}\\ \hat{C} & \hat{D}\end{pmatrix}\begin{pmatrix}\overline{\mu}^{-1}\overline{h}_{-j}\xi_{j+1}\\ \mu^{-1}h_{-j}\xi_{1-j}\end{pmatrix} = f_i\delta_{ij}, \tag{4.19}$$

where

$$f_j = \overline{\mu}^{-1}\overline{h}_{-j}(h_j\hat{\alpha}_{j+1} + \overline{h}_j\hat{\gamma}_{j+1}) + \mu^{-1}h_{-j}(\overline{h}_j\overline{\hat{\alpha}}_{j+1} + h_j\overline{\hat{\gamma}}_{j+1}) = \frac{1}{|\alpha_{2-j}|^2 - |\gamma_{2-j}|^2}\left(\overline{\mu}^{-1}\overline{\mathcal{A}}_j\overline{\alpha}_{2-j} - \overline{\mu}^{-1}\overline{\mathcal{C}}_j\gamma_{2-j}\right.$$

$$\left. - \mu^{-1}\mathcal{C}_j\overline{\gamma}_{2-j} + \mu^{-1}\mathcal{A}_j\alpha_{2-j}\right). \tag{4.20}$$

The lemma is proved.

According to Lemma 3, we get the entries $(\tilde{q}_1,\ldots,\tilde{q}_{2n+1})$ of $\tilde{Q}$ in (2.7) as

$$\tilde{q}_j = \frac{g_{j+1}}{g_j}q_j. \tag{4.21}$$

However, the expression of g_j in (4.18) is still not simple enough. To simplify the expressions of the solutions, we need the following two lemmas.

Lemma 8: *Suppose $k-2=(2n+1)s+r$ where s, r are integers, $1\leqslant r\leqslant 2n+1$, then*

$$\alpha_k = \frac{2n+1}{\overline{\mu}^{2n+1} + \mu^{2n+1}}\left(\sum_{l=1}^{r}\mathcal{A}_l(-\mu)^{r-l}\overline{\mu}^{2n+l-r} + \sum_{l=r+1}^{2n+1}\mathcal{A}_l(-\mu)^{2n+1+r-l}\overline{\mu}^{l-r-1}\right),$$

$$\gamma_k = \frac{2n+1}{2\mu^{2n+1}}\left(\sum_{l=1}^{r}\mathcal{C}_l(-\mu)^{r-l}\mu^{2n+l-r} + \sum_{l=r+1}^{2n+1}\mathcal{C}_l(-\mu)^{2n+1+r-l}\mu^{l-r-1}\right). \tag{4.22}$$

Proof: According to (4.12),

$$\alpha_k = \sum_{j=1}^{2n+1}\sum_{l=1}^{2n+1}\frac{\mathcal{A}_l\omega^{-j(k-l-2)}}{\overline{\mu}+\omega^j\mu}. \tag{4.23}$$

Let θ be a constant with $|\theta|<1$. Let

$$\alpha_k^{(\theta)} = \sum_{j=1}^{2n+1}\sum_{l=1}^{2n+1}\frac{\mathcal{A}_l\omega^{-j(k-l-2)}}{\overline{\mu}+\theta\omega^j\mu} = \sum_{j=1}^{2n+1}\sum_{l=1}^{2n+1}\sum_{\rho=0}^{+\infty}\overline{\mu}^{-1}\mathcal{A}_l\omega^{j(\rho+2+l-k)}(-\theta\mu\overline{\mu}^{-1})^{\rho}. \tag{4.24}$$

Using (4.10) we have $\Sigma_{j=1}^{2n+1}\omega^{j(\rho+2+l-k)}=0$ unless $\rho+2+l-k\equiv 0 \bmod 2n+1$. Let $\rho=k-l-2+(2n+1)\sigma$, then, using $k-2=(2n+1)s+r$,

$$\begin{aligned}(2n+1)^{-1}\alpha_k^{(\theta)} &= \sum_{l=1}^{2n+1}\sum_{\sigma\geqslant\frac{1}{2n+1}(l-k+2)}\overline{\mu}^{-1}\mathcal{A}_l(-\theta\mu\overline{\mu}^{-1})^{k-l-2+(2n+1)\sigma}\\ &= \sum_{l=1}^{r}\sum_{\sigma=-s}^{+\infty}\overline{\mu}^{-1}\mathcal{A}_l(-\theta\mu\overline{\mu}^{-1})^{k-l-2+(2n+1)\sigma} + \sum_{l=r+1}^{2n+1}\sum_{\sigma=-s+1}^{+\infty}\overline{\mu}^{-1}\\ &\quad\times\mathcal{A}_l(-\theta\mu\overline{\mu}^{-1})^{k-l-2+(2n+1)\sigma} = \sum_{l=1}^{r}\frac{\mathcal{A}_l(-\theta\mu)^{r-l}\overline{\mu}^{2n+l-r}}{\overline{\mu}^{2n+1}+(\theta\mu)^{2n+1}} + \sum_{l=r+1}^{2n+1}\frac{\mathcal{A}_l(-\theta\mu)^{2n+1+r-l}\overline{\mu}^{l-r-1}}{\overline{\mu}^{2n+1}+(\theta\mu)^{2n+1}}.\end{aligned} \tag{4.25}$$

Here a sum is zero if the lower bound is greater than the upper bound. Since $\arg(\mu)\notin\{k\pi/(4n+2)|k\in\mathbf{Z}\}$, by taking $\theta\to 1$, we get the expression of α_k in (4.22). The expression of γ_k in (4.22) is obtained similarly. The lemma is proved.

Lemma 9: *For any integer k,*

$$|\alpha_{2-k}|^2 - |\alpha_{1-k}|^2 - |\gamma_{2-k}|^2 + |\gamma_{1-k}|^2 = 2(2n+1)\mathrm{Re}\left(\mu^{-1}(\mathcal{A}_k\alpha_{2-k} - \mathcal{C}_k\overline{\gamma}_{2-k})\right). \tag{4.26}$$

Proof: First suppose $-k-1=(2n+1)s+r$, $1\leqslant r\leqslant 2n$, then $(2-k)-2=(2n+1)s+r+1$, $(1-k)-2=(2n+1)s+r$. According to Lemma 8,

$$\alpha_{2-k} = \frac{2n+1}{\overline{\mu}^{2n+1}+\mu^{2n+1}}\left(\sum_{l=1}^{r+1}\mathcal{A}_l(-\mu)^{r+1-l}\overline{\mu}^{2n-1+l-r} + \sum_{l=r+2}^{2n+1}\mathcal{A}_l(-\mu)^{2n+2+r-l}\overline{\mu}^{l-r-2}\right),$$

$$\alpha_{1-k} = \frac{2n+1}{\overline{\mu}^{2n+1}+\mu^{2n+1}}\left(\sum_{l=1}^{r}\mathcal{A}_l(-\mu)^{r-l}\overline{\mu}^{2n+l-r} + \sum_{l=r+1}^{2n+1}\mathcal{A}_l(-\mu)^{2n+1+r-l}\overline{\mu}^{l-r-1}\right). \tag{4.27}$$

Hence

$$\alpha_{1-k} = -\mu^{-1}\overline{\mu}(\alpha_{2-k} - (2n+1)\overline{\mu}^{-1}\mathcal{A}_{r+1}). \tag{4.28}$$

This implies

$$|\alpha_{2-k}|^2 - |\alpha_{1-k}|^2 = 2(2n+1)\mathrm{Re}\left(\mu^{-1}\overline{\mathcal{A}}_{r+1}\alpha_{2-k}\right) - (2n+1)^2|\mu|^{-2}|\mathcal{A}_{r+1}|^2. \tag{4.29}$$

Similarly, we have

$$-|\gamma_{2-k}|^2+|\gamma_{1-k}|^2=-2(2n+1)\mathrm{Re}(\overline{\mu}^{-1}\overline{\mathcal{C}}_{r+1}\gamma_{2-k})+(2n+1)^2|\mu|^{-2}|\mathcal{C}_{r+1}|^2. \tag{4.30}$$

Since $|\mathcal{C}_{r+1}|^2=|\mathcal{A}_{r+1}|^2$,

$$|\alpha_{2-k}|^2-|\alpha_{1-k}|^2-|\gamma_{2-k}|^2+|\gamma_{1-k}|^2=2(2n+1)\mathrm{Re}(\mu^{-1}\overline{\mathcal{A}}_{r+1}\alpha_{2-k})-2(2n+1)\mathrm{Re}(\mu^{-1}\mathcal{C}_{r+1}\overline{\gamma}_{2-k}). \tag{4.31}$$

According to (4.17), $\mathcal{A}_{r+1}=\overline{\mathcal{A}}_k$, $\mathcal{C}_{r+1}=\mathcal{C}_k$. Hence (4.26) holds.

If $-k-1\equiv 0 \bmod 2n+1$, (4.28) still holds. The same result is obtained. This proves the lemma.

From (4.18) and (4.26),

$$g_k=1-\frac{2(2n+1)}{|\alpha_{2-k}|^2-|\gamma_{2-k}|^2}\,\mathrm{Re}\left(\frac{\mathcal{A}_k\alpha_{2-k}-\mathcal{C}_k\overline{\gamma}_{2-k}}{\mu}\right)=\frac{|\alpha_{1-k}|^2-|\gamma_{1-k}|^2}{|\alpha_{2-k}|^2-|\gamma_{2-k}|^2}. \tag{4.32}$$

Using (4.21), we get the transformation of the solution of (2.12),

$$\tilde{q}_k=\frac{\eta_k\eta_{k+2}}{\eta_{k+1}^2}q_k, \tag{4.33}$$

Where $\eta_k=|\alpha_{2-k}|^2-|\gamma_{2-k}|^2$.

Remark 1: *From (4.13), the equality $\eta_{1-k}=\eta_k$ always holds. Hence $\tilde{q}_{-k-1}=\tilde{q}_k$ holds provided that $q_{-k-1}=q_k$ holds. This means that the Darboux transformation does not change the natural relation (2.17).*

η_k's can be written down explicitly. For $k=1,2,\ldots,n+1$, we have $(2-k)-2=-(2n+1)+2n+1-k$. The first equation of (4.27) can be written as

$$\alpha_{2-k}=\frac{2n+1}{\overline{\mu}^{2n+1}+\mu^{2n+1}}\left(\sum_{l=1}^{2n+1-k}\mathcal{A}_l(-\mu)^{2n+1-k-l}\overline{\mu}^{k+l-1}+\sum_{l=2n+2-k}^{2n+1}\mathcal{A}_l(-\mu)^{4n+2-k-l}\overline{\mu}^{k+l-2n-2}\right). \tag{4.34}$$

Similarly,

$$\begin{aligned}\gamma_{2-k}&=\frac{2n+1}{2\mu^{2n+1}}\left(\sum_{l=1}^{2n+1-k}\mathcal{C}_l(-\mu)^{2n+1-k-l}\mu^{k+l-1}+\sum_{l=2n+2-k}^{2n+1}\mathcal{C}_l(-\mu)^{4n+2-k-l}\mu^{k+l-2n-2}\right)\\&=-\frac{2n+1}{2\mu}\left(\sum_{l=1}^{2n+1-k}\mathcal{C}_l(-1)^{k+l}-\sum_{l=2n+2-k}^{2n+1}\mathcal{C}_l(-1)^{k+l}\right).\end{aligned} \tag{4.35}$$

Equation (4.33) leads to the transformation of the solution $(\tilde{u}_1,\ldots,\tilde{u}_n)$ of (2.4) or (2.5) as

$$\tilde{u}_k=u_k+\ln\frac{\eta_{k+1}}{\eta_k}\quad(1\leqslant k\leqslant n) \tag{4.36}$$

If $\eta_1,\ldots,\eta_n$ have the same sign.

In summary, we have the following theorem.

Theorem 1: *Suppose $(u_1,\ldots,u_n)$ is a solution of (2.4) or (2.5). Let $\mu\in\mathbf{C}\backslash\{0\}$ such that $\arg(\mu)\neq k\pi/(4n+2)$ for any inter k. Let $h=(h_1,\ldots,h_{2n+1})^T$ be a column solution of* (2.10) *for $\lambda=\mu$. Let $\lambda_j=\omega^{j-1}\mu$, $\lambda_{2n+1+j}=\omega^{-j+1}\overline{\mu}$, $H_j=\Omega^{j-1}h$, $H_{2n+1+j}=\Omega^{-j+1}\overline{h}(j=1,2,\ldots,2n+1)$. Define $\Gamma_{ij}=H_i^*KH_j/(\overline{\lambda}_i+\lambda_j)$ $(i,j=1,\ldots,2(2n+1))$. Let $G(x,t,\lambda)$ be defined by* (3.2) *with $M=2(2n+1)$. Then G is a Darboux matrix for (2.10) in the sense that for any solution Φ of (2.10), $\tilde{\Phi}=G\Phi$ satisfies*

$$\tilde{\Phi}_x=(\lambda J+\tilde{P})\tilde{\Phi},\quad \tilde{\Phi}_t=\lambda^{-1}\tilde{Q}\tilde{\Phi}, \tag{4.37}$$

where $\tilde{P}=P+[J,G_1]$, $\tilde{Q}=G_{2(2n+1)}QG_{2(2n+1)}^{-1}$.

Let

$$\zeta_k = \frac{1}{|\overline{\mu}^{2n+1} + \mu^{2n+1}|^2} \left| \sum_{l=1}^{2n+1-k} \overline{h}_l h_{-l} (-\mu)^{2n+1-k-l} \overline{\mu}^{k+l-1} + \sum_{l=2n+2-k}^{2n+1} \overline{h}_l h_{-l} (-\mu)^{4n+2-k-l} \overline{\mu}^{k+l-2n-2} \right|^2$$
$$- \frac{1}{4|\mu|^2} \left| \sum_{l=1}^{2n+1-k} h_l h_{-l} (-1)^{k+l} - \sum_{l=2n+2-k}^{2n+1} h_l h_{-l} (-1)^{k+l} \right|^2, \tag{4.38}$$

then in the region where $\zeta_1, \ldots, \zeta_n$ have the same sign, the new solution $(\tilde{u}_1, \ldots, \tilde{u}_n)$ of (2.4) or (2.5) is given by

$$\tilde{u}_k = u_k + \ln \frac{\zeta_{k+1}}{\zeta_k} \quad (k = 1, 2, \ldots, n). \tag{4.39}$$

V. DARBOUX TRANSFORMATION WITH A REAL SPECTRAL PARAMETER

Now suppose a spectral parameter in constructing Darboux matrix is real. Considering the symmetries in Lemma 2, the Darboux matrix can be derived as follows.

Let μ be a nonzero real number, $\lambda_j = \omega^{j-1}\mu (j = 1, 2, \ldots, 2n+1)$, then all λ_j, $-\overline{\lambda}_j$ $(j = 1, \ldots, 2n+1)$ are distinct. Let h be a column solution of (2.10) for $\lambda = \mu$, $H_j = \Omega^{j-1} h$, $(j = 1, 2, \ldots, 2n+1)$. Then H_j is a solution of (2.10) for $\lambda = \lambda_j$ $(j = 1, 2, \ldots, 2n+1)$.

According to Sec. III for $M = 2n+1$, we can also construct Γ and $G(x, t, \lambda)$. From (3.1),

$$\Gamma_{ij} = \frac{h^* (\Omega^*)^{i-1} K \Omega^{j-1} h}{\omega^{-i+1}\mu + \omega^{j-1}\mu} = \omega^{-i+1} \frac{h^* K \Omega^{i+j-2} h}{\mu + \omega^{i+j-2}\mu}. \tag{5.1}$$

Now

$$\Gamma \xi_k = \alpha_k \xi_{3-k}, \quad \alpha_k = \sum_{j=1}^{2n+1} \frac{h^* K \Omega^j h}{\mu + \omega^j \mu} \omega^{-(k-1)j}, \quad \Gamma^{-1} \xi_k = \hat{\alpha}_k \xi_{3-k}, \quad \hat{\alpha}_k = \alpha_{3-k}^{-1}. \tag{5.2}$$

Lemma 10: $\overline{G(x, t, \overline{\lambda})} = G(x, t, \lambda)$.

Proof: Since $\lambda_{2-i} = \overline{\lambda}_i$, $H_{2-i} = \overline{H}_i$, we have

$$\overline{\Gamma}_{2-i,2-j} = \frac{\overline{H}_{2-i}^* K \overline{H}_{2-j}}{\overline{\lambda}_{2-j} + \lambda_{2-i}} = \frac{H_i^* K H_j}{\overline{\lambda}_i + \lambda_j} = \Gamma_{ij}. \tag{5.3}$$

Let L be a constant matrix such that $L_{11} = 1$, $L_{i+1,1-i} = 1$ $(i = 1, 2, \ldots, 2n)$ and $L_{ij} = 0$ for other (i, j). Then Γ satisfies $L\Gamma L = \overline{\Gamma}$. This leads to $L\Gamma^{-1}L = \overline{\Gamma}^{-1}$. Therefore,

$$\sum_{i,j=1}^{2n+1} \overline{\left(\frac{(\Gamma^{-1})_{ij} H_i H_j^* K}{\overline{\lambda} + \overline{\lambda}_j} \right)} = \sum_{i,j=1}^{2n+1} \frac{(\Gamma^{-1})_{2-i,2-j} H_{2-i} H_{2-j}^* K}{\lambda + \overline{\lambda}_{2-j}} = \sum_{i,j=1}^{2n+1} \frac{(\Gamma^{-1})_{ij} H_i H_j^* K}{\lambda + \overline{\lambda}_j}. \tag{5.4}$$

The lemma is proved.

Hence, the coefficients of each power of λ in $G(x, t, \lambda)$ are all real matrices.

Similar to Lemma 6, we have

$$\Omega G(x, t, \lambda) \Omega^{-1} = G(x, t, \omega\lambda). \tag{5.5}$$

From Lemma 4, Lemma 10, and (5.5), $\tilde{U}$ and $\tilde{V}$ defined by (3.5) satisfy the relations (2.15).

Let $h = (h_1, \ldots, h_{2n+1})^T$, then

$$R_{ij} = (2n+1)^{-1/2} \omega^{(i-1)(j-1)} h_j, \quad S_{ij} = (2n+1)^{-1/2} \mu^{-1} \omega^{-(i-1)j} h_{-j}. \tag{5.6}$$

Written in matrices, the ith column of R is $h_i \xi_{2-i}$, and the jth column of S is $\mu^{-1} h_{-j} \xi_{j+1}$.

Therefore, $-\mu^{-2n-1}G_{2n+1}=1-(2n+1)R^*\Gamma^{-1}S=\mathrm{diag}(g_1,\ldots,g_{2n+1})$ where

$$g_j = 1-(2n+1)\mu^{-1}h_jh_{-j}/\alpha_{2-j}. \tag{5.7}$$

Similar to Lemma 8, α_k can be expressed as

$$\begin{aligned}\alpha_k &= \frac{2n+1}{2\mu^{2n+1}}\left(\sum_{l=1}^{r}\mathcal{A}_l(-\mu)^{r-l}\mu^{2n+l-r}+\sum_{l=r+1}^{2n+1}\mathcal{A}_l(-\mu)^{2n+1+r-l}\mu^{l-r-1}\right)\\ &= \frac{2n+1}{2\mu}\left(\sum_{l=1}^{r}(-1)^{r-l}\mathcal{A}_l-\sum_{l=r+1}^{2n+1}(-1)^{r-l}\mathcal{A}_l\right),\end{aligned} \tag{5.8}$$

where $\mathcal{A}_l=h_lh_{-l}$ and $k-2=(2n+1)s+r$ with $s,\ r\in\mathbf{Z}$ and $1\leqslant r\leqslant 2n+1$.

From (5.8), we get $\alpha_{2-k}+\alpha_{1-k}=(2n+1)\mu^{-1}\mathcal{A}_k$ corresponding to Lemma 9. From (5.7), $g_k=1-(2n+1)\mu^{-1}\mathcal{A}_k\alpha_{2-k}^{-1}=-\alpha_{1-k}\alpha_{2-k}^{-1}$. Hence, $\tilde{q}_k=(\eta_k\eta_{k+2}/\eta_{k+1}^2)q_k$ where $\eta_k=\alpha_{2-k}$.

Since $(2-k)-2=-(2n+1)s+2n+1-k$, (5.8) leads to

$$\eta_k=\alpha_{2-k}=-\frac{2n+1}{2\mu}\left(\sum_{l=1}^{2n+1-k}(-1)^{k+l}\mathcal{A}_l-\sum_{l=2n+2-k}^{2n+1}(-1)^{k+l}\mathcal{A}_l\right) \tag{5.9}$$

$(k=1,2,\ldots,n+1)$. Finally,

$$\tilde{u}_k=u_k+\ln\frac{\eta_{k+1}}{\eta_k}. \tag{5.10}$$

If $\eta_1,\ldots,\eta_n$ have the same sign.

The above results are summarized in the following theorem.

Theorem 2: *Suppose $(u_1,\ldots,u_n)$ is a solution of (2.4) or (2.5). Let $\mu\in\mathbf{R}\backslash\{0\}$. Let $h=(h_1,\ldots,h_{2n+1})^T$ be a real column solution of (2.10) for $\lambda=\mu$. Let $\lambda_j=\omega^{j-1}\mu$, $H_j=\Omega^{j-1}h$ $(j=1,2,\ldots,2n+1)$. Define $\Gamma_{ij}=H_i^*KH_j/(\bar{\lambda}_i+\lambda_j)$ $(i,j=1,\ldots,2n+1)$. Let $G(x,t,\lambda)$ be defined by (3.2) with $M=2n+1$. Then G is a Darboux matrix for (2.10) in the sense that for any solution Φ of (2.10), $\tilde{\Phi}=G\Phi$ satisfies*

$$\tilde{\Phi}_x=(\lambda J+\tilde{P})\tilde{\Phi},\quad \tilde{\Phi}_t=\lambda^{-1}\tilde{Q}\tilde{\Phi}, \tag{5.11}$$

Where $\tilde{P}=P+[J,G_1]$, $\tilde{Q}=G_{2n+1}QG_{2n+1}^{-1}$.

Let

$$\zeta_k=\sum_{l=1}^{2n+1-k}(-1)^{k+l}h_lh_{-l}-\sum_{l=2n+2-k}^{2n+1}(-1)^{k+l}h_lh_{-l} \tag{5.12}$$

then in the region where $\zeta_1,\ldots,\zeta_n$ have the same sign, the new solution $(\tilde{u}_1,\ldots,\tilde{u}_n)$ of (2.4) or (2.5) is given by

$$\tilde{u}_k=u_k+\ln\frac{\zeta_{k+1}}{\zeta_k}\quad (k=1,2,\ldots,n). \tag{5.13}$$

VI. APPLICATION TO THE TZITZEICA EQUATION

The Tzitzeica equation

$$u_{xt}=e^u-e^{-2u} \tag{6.1}$$

is a special two dimensional Toda equation with $n=1$.

Suppose u is a solution of (6.1) and $h=(h_1,h_2,h_3)^T$ is a column solution of its Lax pair for $\lambda=\mu$. Using Theorem 1 and Theorem 2, we get the new solution of (6.1). When μ is taken as a complex number,

$$\tilde{u}=u+\ln\frac{4|\mu|^2|\bar{\mu}^2\bar{h}_1h_2+\mu^2h_1\bar{h}_2-|\mu|^2|h_3|^3|^2-(\mu^3+\bar{\mu}^3)^2|2h_1h_2-h_3^2|^2}{(2|\mu|^2\bar{\mu}h_1\bar{h}_2-2|\mu|^2\mu\bar{h}_1h_2+(\mu^3-\bar{\mu}^3)|h_3|^2)^2}. \tag{6.2}$$

When μ is a real number,

$$\tilde{u}=u+\ln\frac{2h_1h_2-h_3^2}{h_3^2}. \tag{6.3}$$

Equation (6.3) is similar to that given by Ref. 17.

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Representations of classical Lie subalgebras of quantum pseudodifferential operators

Carina Boyallian[a] and José I. Liberati[b]
Ciem-FAMAF, Universidad Nacional de Córdoba, Ciudad Universitaria, 5000 Córdoba, Argentina

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We show that there is a family of anti-involutions $\sigma_{\epsilon,k}$ ($\epsilon=\pm 1$ and $k\in\mathbb{Z}$), up to conjugation, of the Lie algebra $\mathcal{S}_q$ of quantum pseudodifferential operators preserving the principal gradation. We classify the irreducible quasifinite highest weight modules over the Lie subalgebras of $\mathcal{S}_q$, fixed by minus $\sigma_{\epsilon,k}$ (k even), and we realize them in terms of irreducible highest weight representations of the Lie algebra of infinite matrices with finitely many nonzero diagonals and its classical Lie subalgebras of B, C, and D types. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1845600]

I. INTRODUCTION

The W-infinity algebras naturally arise in various physical theories, such as conformal field theory, the theory of the quantum Hall effect, etc. The $W_{1+\infty}$ algebra, which is the central extension of the Lie algebra $\mathcal{D}$ of differential operators on the circle, is the most fundamental among these algebras.

When we study the representation theory of a Lie algebra of this kind, we encounter the difficulty that although it admits a $\mathbb{Z}$-gradation, each of the graded subspaces is still infinite dimensional, and therefore the study of highest weight modules which satisfy the quasifiniteness condition, that is, graded subspaces have finite dimension, becomes a nontrivial problem.

The study of representation theory of the Lie algebra $\hat{\mathcal{D}}$ (the universal central extension of the Lie algebra $\mathcal{D}$, also denoted by $\mathcal{W}_{1+\infty}$ in the physicists literature), was initiated in Ref. 5. In that paper, Kac and Radul classified the irreducible quasi-finite highest weight representations of $\hat{\mathcal{D}}$, and it was shown that they can be realized in terms of irreducible highest weight representations of the Lie algebra of infinite matrices. At the end of that article, they did, very briefly, the same for the Lie algebra $\widehat{\mathcal{S}_q}$, the central extension of the Lie algebra of quantum pseudodifferential operators, which contains as a subalgebra the q-analogue of the Lie algebra $\hat{\mathcal{D}}$, the algebra of all regular difference operators on $\mathbb{C}^\times$.

In Ref. 2 we extend the results obtained in Ref. 5, for the central extension of the Lie algebra of $M\times M$ matrix quantum pseudodifferential operators.

In this paper we get analogous results to those obtained in Ref. 6, for $\widehat{\mathcal{S}_q}$. That is, we show that there is a family of anti-involutions $\sigma_{\epsilon,k}$ ($\epsilon=\pm 1$ and $k\in\mathbb{Z}$), up to conjugation, of the Lie algebra $\mathcal{S}_q$, preserving the principal gradation. We classify the irreducible quasifinite highest weight modules over the Lie subalgebras of $\mathcal{S}_q$, fixed by minus $\sigma_{\epsilon,k}$ (k even), and we realize them in terms of irreducible highest weight representations of the Lie algebra of infinite matrices with finitely many nonzero diagonals and its classical Lie subalgebras of B, C, and D types. Here we get a larger family of subalgebras, and this makes the picture much richer than in the classical case.

[a]Electronic mail: boyallia@mate.uncor.edu
[b]Electronic mail: liberati@mate.uncor.edu

The paper is organized as follows. In Sec. II we recall some definitions and notations of $\widehat{g\ell}_\infty$ and its classical subalgebras. In Sec. III we study the structure of $\widehat{\mathcal{S}_q}$, its involutions and we introduce the subalgebras $\widehat{\mathcal{S}_q^{\kappa,\epsilon}}$. In Sec. IV we characterize the quasifiniteness of highest weight modules over $\widehat{\mathcal{S}_q^{\kappa,\epsilon}}$. In Sec. V we establish the relation of this subalgebra with $\widehat{g\ell}(\infty,R_m)$ and finally in Sec. VI we realize and construct the quasifinite highest weight modules over $\widehat{\mathcal{S}_q}$.

II. LIE ALGEBRAS $\widehat{g\ell}_\infty^{[m]}$ AND ITS CLASSICAL SUBALGEBRAS

Denote by $R_m=\mathbb{C}[u]/(u^{m+1})$, the quotient algebra of the polynomial algebra $\mathbb{C}[u]$ by the ideal generated by u^{m+1} ($m\in\mathbb{Z}_+$). Let **1** be the identity element in R_m. Denote by $g\ell_\infty^{[m]}$ the complex Lie algebra of all infinite matrices $(a_{ij})_{i,j\in Z}$ with only finitely many nonzero diagonals with entries in R_m. Denote by E_{ij} the infinite matrix with 1 at (i,j)-place and 0 elsewhere. There is a natural automorphism ν of $g\ell_\infty^{[m]}$ given by

$$\nu(E_{i,j})=E_{i+1,j+1}. \tag{2.1}$$

Let the weight of $E_{i,j}$ be $j-i$. This defines the *principal* $\mathbb{Z}$-gradation $g\ell_\infty^{[m]}=\oplus_{j\in\mathbb{Z}}(g\ell_\infty^{[m]})_j$. Denote by $\widehat{g\ell}_\infty^{[m]}=g\ell_\infty^{[m]}\oplus R_m$ the cental extension of $g\ell_\infty^{[m]}$ given by the following 2-cocycle with values in R_m:

$$C(A,B)=\mathrm{Tr}([J,A]B), \tag{2.2}$$

where $J=\Sigma_{i\leqslant 0}E_{ii}$. The $\mathbb{Z}$-gradation of the Lie algebra $g\ell_\infty^{[m]}$ extends to $\widehat{g\ell}_\infty^{[m]}$ by setting the weight of R_m to be 0. In particular we have the *triangular decomposition*

$$\widehat{g\ell}_\infty^{[m]}=(\widehat{g\ell}_\infty^{[m]})_+\oplus(\widehat{g\ell}_\infty^{[m]})_0\oplus(\widehat{g\ell}_\infty^{[m]})_-, \tag{2.3}$$

where

$$(\widehat{g\ell}_\infty^{[m]})_\pm=\bigoplus_{j\in\mathbb{N}}(\widehat{g\ell}_\infty^{[m]})_{\pm j}\quad\text{and}\quad(\widehat{g\ell}_\infty^{[m]})_0=(g\ell_\infty^{[m]})_0\oplus R_m.$$

Given $\lambda\in(\widehat{g\ell}_\infty^{[m]})_0^*$, we let

$$c_i=\lambda(u^i),$$

$$^a\lambda_j^{(i)}=\lambda(u^iE_{j,j}), \tag{2.4}$$

$$^ah_j^{(i)}={}^a\lambda_j^{(i)}-{}^a\lambda_{1+j}^{(i)}+\delta_{j,0}c_i,$$

where $j\in\mathbb{Z}$ and $i=0,\ldots,m$. Let $L(\widehat{g\ell}_\infty^{[m]},\lambda)$ be the irreducible highest weight $\widehat{g\ell}_\infty^{[m]}$-module with highest weight λ. The $^a\lambda_j^{(i)}$ are called the *labels* and c_i are the *central charges* of $L(\widehat{g\ell}_\infty^{[m]},\lambda)$.

Consider the vector space $R_m[t,t^{-1}]$, and take the R_m-basis $v_i=t^{-i}$, $i\in\mathbb{Z}$. The Lie algebra $g\ell_\infty^{[m]}$ acts on this vector space via the usual formula

$$E_{ij}v_k=\delta_{j,k}v_i. \tag{2.5}$$

Now consider the following $\mathbb{C}$-bilinear form on $R_m[t,t^{-1}]$:

$$B^\pm(u^mv_i,u^nv_j)=u^m(-u^n)(\pm 1)^i\delta_{i,-j}. \tag{2.6}$$

Denote by $\overline{b}_\infty^{-[m]}$ (respectively, $\overline{b}_\infty^{+[m]}$) the Lie subalgebra of $g\ell_\infty^{[m]}$ which preserves the bilinear form $B^-(,)$ [respectively, $B^+(,)$]. We have

$$\overline{b}_\infty^{-[m]} = \{(a_{ij}(u))_{i,j\in\mathbb{Z}} \in g\ell_\infty^{[m]} | a_{ij}(u) = (-1)^{i+j+1} a_{-j,-i}(-u)\},$$

$$\overline{b}_\infty^{+[m]} = \{(a_{ij}(u))_{i,j\in\mathbb{Z}} \in g\ell_\infty^{[m]} | a_{ij}(u) = -a_{-j,-i}(-u)\}.$$

Denote by $b_\infty^{[m]} = \overline{b}_\infty^{-[m]} \oplus R_m$ (respectively, $\widetilde{b}_\infty^{[m]} = \overline{b}_\infty^{+[m]} \oplus R_m$), the central extension of $\overline{b}_\infty^{-[m]}$ (respectively, $\overline{b}_\infty^{+[m]}$) given by the corresponding restriction of the 2-cocycle in (2.2). These subalgebras inherit from $\widehat{g\ell}_\infty^{[m]}$ the principal $\mathbb{Z}$-gradation and the triangular decomposition (see Refs. 6 and 3 for notation),

$$b_\infty^{[m]} = \oplus_{j\in\mathbb{Z}} (b_\infty^{[m]})_j, \quad b_\infty^{[m]} = (b_\infty^{[m]})_+ \oplus (b_\infty^{[m]})_0 \oplus (b_\infty^{[m]})_-$$

and

$$\widetilde{b}_\infty^{[m]} = \oplus_{j\in\mathbb{Z}} (\widetilde{b}_\infty^{[m]})_j, \quad \widetilde{b}_\infty^{[m]} = (\widetilde{b}_\infty^{[m]})_+ \oplus (\widetilde{b}_\infty^{[m]})_0 \oplus (\widetilde{b}_\infty^{[m]})_-.$$

Note that the Lie algebra $\widetilde{b}_\infty^{[m]}$ is isomorphic to $b_\infty^{[m]}$ by mapping $u^k E_{ij} - (-u)^k E_{-j,-i}$ to $u^k E_{ij} + (-1)^{i+j+1}(-u)^k E_{-j,-i}$. When $m=0$, we have the usual Lie subalgebra of $g\ell_\infty$, denoted by b_∞.

Given $\lambda \in (b_\infty^{[m]})_0^*$, denote by $L(b_\infty^{[m]};\lambda)$ the irreducible highest weight module over $b_\infty^{[m]}$ with highest weight λ.

For each $\lambda \in (b_\infty^{[m]})_0^*$, we let

$$\begin{gathered} c_i = \lambda(u^i), \\ {}^b\lambda_0^{(i)} = \lambda(2u^i E_{0,0}) \quad (i \text{ odd}), \\ {}^b\lambda_j^{(i)} = \lambda(u^i E_{j,j} - (-u)^i E_{-j,-j}), \quad i \neq 0, \\ {}^bh_j^{(i)} = {}^b\lambda_j^{(i)} - {}^b\lambda_{1+j}^{(i)}, \\ {}^bh_0^{(i)} = -2\,{}^b\lambda_1^{(i)} + 2c_i \quad (i \text{ even}), \\ {}^bh_0^{(i)} = {}^b\lambda_0^{(i)} - {}^b\lambda_1^{(i)} + c_i \quad (i \text{ odd}), \end{gathered} \tag{2.7}$$

where $j \in \mathbb{N}$ and $i = 0, \ldots, m$. The superscript b stands for type B. The ${}^b\lambda_j^{(i)}$ are called the *labels* and c_i are the *central charges* of $L(b_\infty^{[m]}, \lambda)$.

As before, take the R_m-basis, $v_i = t^{-i}$, $i \in \mathbb{Z}$ of $R_m[t, t^{-1}]$, and consider $R_m[t, t^{-1}]$ equipped with the following $\mathbb{C}$-bilinear form:

$$C(u^m v_i, u^n v_j) = u^m(-u^n)(-1)^i \delta_{i,1-j}. \tag{2.8}$$

Denote by $\overline{c}_\infty^{\pm m]}$ the Lie subalgebra of $g\ell_\infty^{[m]}$ which preserves the bilinear form $C(,)$. We have

$$\overline{c}_\infty^{\pm m]} = \{(a_{ij}(u))_{i,j\in\mathbb{Z}} \in g\ell_\infty^{[m]} | a_{ij}(u) = (-1)^{i+j+1} a_{1-j,1-i}(-u)\}.$$

Denote by $c_\infty^{[m]} = \overline{c}_\infty^{\pm m]} \oplus R_m$ the central extension of $\overline{c}_\infty^{\pm m]}$ given by the restriction of the 2-cocycle (2.2), defined in $g\ell_\infty^{[m]}$. This subalgebra inherits from $\widehat{g\ell}_\infty^{[m]}$ the principal $\mathbb{Z}$-gradation and the triangular decomposition (see Refs. 6 and 3 for notation)

$$c_\infty^{[m]} = \oplus_{j\in\mathbb{Z}} (c_\infty^{[m]})_j, \quad c_\infty^{[m]} = (c_\infty^{[m]})_+ \oplus (c_\infty^{[m]})_0 \oplus (c_\infty^{[m]})_-.$$

In particular when $m=0$, we have the usual Lie subalgebra of $g\ell_\infty$, denoted by c_∞.

Given $\lambda \in (c_\infty^{[m]})_0^*$, denote by $L(c_\infty^{[m]};\lambda)$ the irreducible highest weight module over $c_\infty^{[m]}$ with highest weight λ.

For each $\lambda \in (c_\infty^{[m]})_0^*$, we let

$$c_i = \lambda(u^i),$$

$$\begin{aligned} {}^c\lambda_j^{(i)} &= \lambda(u^i E_{j,j} - (-u)^i E_{1-j,1-j}), \\ {}^c h_j^{(i)} &= {}^c\lambda_j^{(i)} - {}^c\lambda_{1+j}^{(i)}, \end{aligned} \tag{2.9}$$

$${}^c h_0^{(i)} = {}^c\lambda_1^{(i)} + c_i \quad (i \text{ even}),$$

where $j \in \mathbb{N}$ and $i=0,\ldots,m$. Here, the superscript c denotes type C. The ${}^c\lambda_j^{(i)}$ are called the *labels* and c_i are the *central charges* of $L(c_\infty^{[m]},\lambda)$.

Again, take the R_m-basis, $v_i=t^{-i}$, $i \in \mathbb{Z}$ of $R_m[t,t^{-1}]$, but consider $R_m[t,t^{-1}]$ equipped with the following C-bilinear form:

$$D(u^m v_i, u^n v_j) = u^m(-u^n)\delta_{i,1-j}. \tag{2.10}$$

Denote by $\overline{d}_\infty^{[m]}$ the Lie subalgebra of $g\ell_\infty^{[m]}$ which preserves the bilinear form $D(,)$. We have

$$\overline{d}_\infty^{[m]} = \{(a_{ij}(u))_{i,j\in\mathbb{Z}} \in g\ell_\infty^{[m]} | a_{ij}(u) = -a_{1-j,1-i}(-u)\}.$$

Denote by $d_\infty^{[m]} = \overline{d}_\infty^{[m]} \oplus R_m$ the central extension of $\overline{d}_\infty^{[m]}$ given by the restriction of the 2-cocycle (2.2). This subalgebra inherits from $\widehat{g\ell}_\infty^{[m]}$ the principal $\mathbb{Z}$-gradation and the triangular decomposition (see Refs. 6 and 3 for notation)

$$d_\infty^{[m]} = \oplus_{j\in\mathbb{Z}}(d_\infty^{[m]})_j, \quad d_\infty^{[m]} = (d_\infty^{[m]})_+ \oplus (d_\infty^{[m]})_0 \oplus (d_\infty^{[m]})_-.$$

In particular when $m=0$, we have the usual Lie subalgebra of $g\ell_\infty$, denoted by d_∞.

Given $\lambda \in (d_\infty^{[m]})_0^*$, denote by $L(d_\infty^{[m]};\lambda)$ the irreducible highest weight module over $d_\infty^{[m]}$ with highest weight λ.

For each $\lambda \in (d_\infty^{[m]})_0^*$, we let

$$c_i = \lambda(u^i),$$

$$\begin{aligned} {}^d\lambda_j^{(i)} &= \lambda(u^i E_{j,j} - (-u)^i E_{1-j,1-j}), \\ {}^d h_j^{(i)} &= {}^d\lambda_j^{(i)} - {}^d\lambda_{1+j}^{(i)}, \end{aligned} \tag{2.11}$$

$${}^d h_0^{(i)} = -{}^d\lambda_1^{(i)} - {}^d\lambda_2^{(i)} + 2c_i \quad (i \text{ even}),$$

where $j \in \mathbb{N}$ and $i=0,\ldots,m$. Here, the superscript d denotes type D.The ${}^d\lambda_j^{(i)}$ are called the *labels* and c_i are the *central charges* of $L(d_\infty^{[m]},\lambda)$.

III. THE SUBALGEBRA $\mathcal{S}_q$ AND ITS INVOLUTIONS

Denote by T_q, $q \in \mathbb{C}^\times = \mathbb{C}\backslash\{0\}$, the following operator on $\mathbb{C}[z,z^{-1}]$:

$$T_q f(z) = f(qz).$$

Denote by $\mathcal{S}_q^{qs}$ the associative algebra of all pseudodifferential operators, i.e., the operators on $\mathbb{C}[z,z^{-1}]$ of the form

$$E = \sum_{k \in Z} e_k(z) T_q^k, \quad \text{where } e_i(z) \in \mathbb{C}[z, z^{-1}] \quad \text{(sum is finite)}.$$

Any pseudodifferential operator can be written as linear combinations of elements of the form $z^k f(T_q)$, where $f \in \mathbb{C}[w, w^{-1}]$. The product in $\mathcal{S}_q^{as}$ is then given by

$$(z^r f(T_q))(z^s g(T_q)) = z^{r+s} f(q^s T_q) g(T_q).$$

Denote by $\mathcal{S}_q$ the Lie algebra obtained from $\mathcal{S}_q^{as}$ by taking the usual bracket. Let $\mathcal{S}_q' = [\mathcal{S}_q, \mathcal{S}_q]$. It is easy to check that we have

$$\mathcal{S}_q = \mathcal{S}_q' \oplus \mathbb{C} T_q^0 \quad \text{(direct sum of ideals)}.$$

Thus, the representation theory of $\mathcal{S}_q$ reduces to that of $\mathcal{S}_q'$. Taking the trace form in $\mathbb{C}[w, w^{-1}]$, namely $\mathrm{tr}_0(\Sigma_j c_j w^j) = c_0$, we obtain, by a general construction (cf. Sec. 1.3 in Ref. 5), the following 2-cocycle in $\mathcal{S}_q$:

$$\Psi(z^m f(T_q), z^k g(T_q)) = m \, \mathrm{tr}_0(f(q^{-m} w) g(w)) \delta_{m,-k}. \tag{3.1}$$

Let

$$\widehat{\mathcal{S}_q} = \mathcal{S}_q' + \mathbb{C} C$$

denote the central extension of $\mathcal{S}_q'$ corresponding to the cocycle (3.1).

The elements $z^k T_q^m$ $(k, m \in \mathbb{Z})$ form a basis of $\mathcal{S}_q$. Define the *weight* by

$$\mathrm{wt}\, z^k T_q^m = k, \ \mathrm{wt}\, C = 0.$$

This gives us the principal $\mathbb{Z}$-gradation of $\mathcal{S}_q^{as}$, $\mathcal{S}_q$, and $\widehat{\mathcal{S}_q}$,

$$\mathcal{S}_q^{as} = \bigoplus_{j \in \mathbb{Z}} (\mathcal{S}_q^{as})_j, \quad \widehat{\mathcal{S}_q} = \bigoplus_{j \in \mathbb{Z}} (\widehat{\mathcal{S}_q})_j.$$

An *anti-involution* σ of $\mathcal{S}_q^{as}$ is an involutive antiautomorphism of $\mathcal{S}_q^{as}$, i.e., $\sigma^2 = \mathrm{Id}$, $\sigma(ax + by) = a\sigma(x) + b\sigma(y)$ and $\sigma(xy) = \sigma(y)\sigma(x)$, for all $a, b \in \mathbb{C}$ and $x, y \in \mathcal{S}_q^{as}$. From now on we will assume that $|q| \neq 1$.

Proposition 3.1: Any anti-involution σ of $\mathcal{S}_q^{as}$ which preserves the principal $\mathbb{Z}$-gradation is of the following form:

$$\sigma_{A,B,k}(z) = A z T_q^k \quad \textit{and} \quad \sigma_{A,B,k}(T_q) = B T_q^{-1}$$

with $k \in \mathbb{Z}$ and $A, B \in \mathbb{C} - \{0\}$ such that $A^2 B^k = q^k$.

Proof: Since σ preserves $\mathbb{Z}$-gradation we may assume that $\sigma(z) = z f(T_q)$ and $\sigma(T_q) = g(T_q)$, where $f, g, \in \mathbb{C}[w, w^{-1}]$. Now, since T_q is an invertible element in our algebra, so is $g(T_q)$, and therefore of the form $g(T_q) = B T_q^l$ for some $B \in \mathbb{C} - \{0\}$ and $l \in \mathbb{Z}$. Similarly, $f(T_q) = A T_q^k$ with $A \in \mathbb{C} - \{0\}$ and $k \in \mathbb{Z}$. Using that $\sigma^2 = id$ we have

$$1 = f(g(T_q)) f(T_q) \quad \text{and } T_q = g(g(T_q)).$$

Combining the second equation and the expression of $g(T_q)$ we get $T_q = B^{l+1} T_q^{(l^2)}$. We can deduce that either $l = 1$, $B = \pm 1$ or $l = -1$ and $B \in \mathbb{C}$.

Now using the first equation and the expression for $f(T_q)$ we have $1 = A^2 B^k q^{lk} T_q^{(l+1)k}$, and hence $(l+1)k = 0$.

If $l = 1$, then $A = \pm 1$. Since we assumed that q is not a root of unity, it is easy to check that these are not antiautomorphisms. Therefore $l = -1$ and we have finished our proof. ■

It is immediate that $(h \in \mathbb{C}[w, w^{-1}])$,

$$\sigma_{A,B,k}(z^n h(T_q)) = A^n q^{[n(n-1)k]/2} z^n h(B q^{-n} T_q^{-1}) T_q^{nk}. \tag{3.2}$$

Given $s \in \mathbb{C}$, denote by Θ_s the automorphism of $\mathcal{S}_q$ given by sending $a \in \mathcal{S}_q$ to $z^{-s}az^s$. Therefore, using (3.2), we have

$$\theta_s \sigma_{A,B,k} \theta_{-s} = \sigma_{q^{-sk}A,q^{2s}B,k}. \tag{3.3}$$

Denote by $\mathcal{S}_q^{A,B,k}$ the fixed Lie subalgebra of $\mathcal{S}_q$ by $-\sigma_{A,B,k}$, namely

$$\mathcal{S}_q^{A,B,k} = \{a \in \mathcal{S}_q | \sigma_{A,B,k}(a) = -a\}.$$

It inherits a $\mathbb{Z}$-gradation from $\mathcal{S}_q$ since $\sigma_{A,B,k}$ preserves the principal $\mathbb{Z}$-gradation of $\mathcal{S}_q^{as}$: $\mathcal{S}_q^{A,B,k} = \oplus_{j\in\mathbb{Z}}(\mathcal{S}_q^{A,B,k})_j$, where $(\mathcal{S}_q^{A,B,k})_j = \{z^j f(T_q) | f(w) \in \mathbb{C}[w,w^{-1}]$ and $\sigma_{A,B,k}(z^j f(T_q)) = -z^j f(T_q)\}$.

Now, it is straightforward from (3.3) that we have the following.

Lemma 3.2: The Lie algebra $\mathcal{S}_q^{A,B,k}$ for arbitrary choices of A and B is isomorphic to $\mathcal{S}_q^{\epsilon,q,k}$ where ϵ is either 1 *or* -1.

We will write $\sigma_{\epsilon,k}$ and $\mathcal{S}_q^{\epsilon,k}$ instead of $\sigma_{\epsilon,q,k}$ and $\mathcal{S}_q^{\epsilon,q,k}$. From now on k is even.

Let us denote by $\mathbb{C}[w,w^{-1}]^{\epsilon,j}$ (where $\epsilon=1$ or $\epsilon=-1$) the set of Laurent polynomials such that $f(w^{-1}) = -(\epsilon)^j f(w)$.

Now, we can give a complete description of $(\mathcal{S}_q^{\epsilon,k})_j$.

Lemma 3.3: We have

$$(\mathcal{S}_q^{\epsilon,k})_j = \{z^j (q^{(j-1)/2}T_q)^{kj/2} f(q^{(j-1)/2}T_q) | f(w) \in \mathbb{C}[w,w^{-1}]^{\epsilon,j}\}. \tag{3.4}$$

Proof: By (3.2), an element of $(\mathcal{S}_q^{\epsilon,k})_j$ is of the form $(z^j h(T_q) \in \mathcal{S}_q)$,

$$z^j h(T_q) - \sigma_{\epsilon,k}(z^j h(T_q)) = z^j (h(T_q) - (\epsilon)^j (q^{(j-1)/2}T_q)^{jk} h(q^{-j+1}T_q^{-1})) = z^j (q^{(j-1)/2}T_q)^{jk/2} f(q^{(j-1)/2}T_q)$$

with $f(w) = h(q^{(-j+1)/2}w)w^{-jk/2} - (\epsilon)^j h(q^{(-j+1)/2}w^{-1})w^{jk/2}$. It is easy to see that $f(w^{-1}) = -(\epsilon)^j f(w)$, finishing the proof. ■

From this lemma we have that

$$\mathcal{B} = \{z^j (q^{(j-1)/2}T_q)^{jk/2} ((q^{(j-1)/2}T_q)^m - \epsilon^j (q^{(j-1)/2}T_q)^{-m}) | j \in \mathbb{Z}, m \in \mathbb{N}\}$$

form a $\mathbb{C}$-basis of $(\mathcal{S}_q^{\epsilon,k})$ if $\epsilon=1$ and $\mathcal{B} \cup \{z^j (q^{(j-1)/2}T_q)^{jk/2}\}$ is a basis if $\epsilon=-1$.

We denote again by Ψ the restriction of the 2-cocycle in (3.1) to $(\mathcal{S}_q^{\epsilon,k})$, namely

$$\begin{aligned}\Psi(z^m (q^{(m-1)/2}T_q)^{mk/2} f(q^{(m-1)/2}T_q), z^n (q^{(n-1)/2}T_q)^{nk/2} g(q^{(n-1)/2}T_q)) \\ = \delta_{m,-n} m \mathrm{tr}_0(f(q^{(m-1)/2}w) g(q^{(-m-1)/2}w)),\end{aligned} \tag{3.5}$$

where $z^m (q^{(m-1)/2}T_q)^{mk/2} f(q^{(m-1)/2}T_q)$ and $z^n (q^{(n-1)/2}T_q)^{nk/2} g(q^{(n-1)/2}T_q)$ are in $\mathcal{S}_q^{\epsilon,k}$. Denote by $\widehat{\mathcal{S}_q^{\epsilon,k}}$ the central extension of $\mathcal{S}_q^{\epsilon,k}$ by $\mathbb{C}C$ corresponding to the 2-cocycle Ψ. $\widehat{\mathcal{S}_q^{\epsilon,k}}$ is a Lie subalgebra of $\widehat{\mathcal{S}_q}$ by definition.

IV. CHARACTERIZATION OF QUASIFINITENESS OF HWMs OF $\widehat{\mathcal{S}_q^{\epsilon,k}}$

In order to characterize the quasifiniteness of the highest weight modules (HWMs) of $\widehat{\mathcal{S}_q^{\epsilon,k}}$ we will apply general results for quasifinite representations of $\mathbb{Z}$-graded Lie algebras obtained in Ref. 4. We refer to Ref. 4 for proofs and details. Let $\mathfrak{g}$ be a $\mathbb{Z}$-graded Lie algebra over $\mathbb{C}$:

$$\mathfrak{g} = \bigoplus_{j\in\mathbb{Z}} \mathfrak{g}_j, \quad [\mathfrak{g}_i, \mathfrak{g}_j] \subset \mathfrak{g}_{i+j},$$

where $\mathfrak{g}_i$ is not necessarily of finite dimension. Let $\mathfrak{g}_\pm = \oplus_{j>0}\mathfrak{g}_{\pm j}$. A subalgebra $\mathfrak{p}$ of $\mathfrak{g}$ is called *parabolic* if it contains $\mathfrak{g}_0 \oplus \mathfrak{g}_+$ as a proper subalgebra, that is

$$\mathfrak{p} = \bigoplus_{j\in\mathbb{Z}} \mathfrak{p}_j, \quad \text{where } \mathfrak{p}_j = \mathfrak{g}_j \text{ for } j \geqslant 0, \text{ and } \mathfrak{p}_j \neq 0 \text{ for some } j < 0.$$

We assume the following properties of $\mathfrak{g}$:

(P1) $\mathfrak{g}_0$ is commutative,

(P2) if $a \in \mathfrak{g}_{-k}$ $(k>0)$ and $[a,\mathfrak{g}_1]=0$, then $a=0$.

Given $a \in \mathfrak{g}_{-1}$, $a \neq 0$, we define $\mathfrak{p}^a = \oplus_{j\in\mathbb{Z}} \mathfrak{p}^a_j$, where $\mathfrak{p}^a_j = \mathfrak{g}_j$ for all $j \geqslant 0$, and

$$\mathfrak{p}^a_{-1} = \sum [\cdots[[a,\mathfrak{g}_0],\mathfrak{g}_0], \ldots], \quad \mathfrak{p}^a_{-k-1} = [\mathfrak{p}^a_{-1}, \mathfrak{p}^a_{-k}].$$

Lemma 4.1: (a) $\mathfrak{p}^a$ *is the minimal parabolic subalgebra containing* a. (b) $\mathfrak{g}^a_0 := [\mathfrak{p}^a, \mathfrak{p}^a] \cap \mathfrak{g}_0 = [a, \mathfrak{g}_1]$.

In the particular case of the central extension of the Lie algebra of matrix differential operators on the circle (see Ref. 1, Remark 2.2), we observed the existence of some parabolic subalgebras $\mathfrak{p}$ such that $\mathfrak{p}_{-j}=0$ for $j \gg 0$. Having in mind that example, we give the following definition.

Definition 4.2: (a) A parabolic subalgebra $\mathfrak{p}$ is called *nondegenerate* if $\mathfrak{p}_{-j}$ has finite codimension in $\mathfrak{g}_{-j}$, for all $j>0$.

(b) An element $a \in \mathfrak{g}_{-1}$ is called *nondegenerate* if $\mathfrak{p}^a$ is nondegenerate.

Now, we begin our study of quasifinite representations over $\mathfrak{g}$. A $\mathfrak{g}$-module V is called $\mathbb{Z}$*-graded* if $V = \oplus_{j\in\mathbb{Z}} V_j$ and $\mathfrak{g}_i V_j \subset V_{i+j}$. A $\mathbb{Z}$-graded $\mathfrak{g}$-module V is called *quasifinite* if $\dim V_j < \infty$ for all j.

Given $\lambda \in \mathfrak{g}_0^*$, a *highest weight module* is a $\mathbb{Z}$-graded $\mathfrak{g}$-module $V(\mathfrak{g},\lambda)$ generated by a highest weight vector $v_\lambda \in V(\mathfrak{g},\lambda)_0$ which satisfies

$$hv_\lambda = \lambda(h)v_\lambda \quad (h \in \mathfrak{g}_0), \quad \mathfrak{g}_+ v_\lambda = 0.$$

A nonzero vector $v \in V(\mathfrak{g},\lambda)$ is called *singular* if $\mathfrak{g}_+ v = 0$.

The *Verma module* over $\mathfrak{g}$ is defined as usual,

$$M(\mathfrak{g},\lambda) = \mathcal{U}(\mathfrak{g}) \otimes_{\mathcal{U}(\mathfrak{g}_0 \oplus \mathfrak{g}_+)} \mathbb{C}_\lambda,$$

where $\mathbb{C}_\lambda$ is the one-dimensional $(\mathfrak{g}_0 \oplus \mathfrak{g}_+)$-module given by $h \mapsto \lambda(h)$ if $h \in \mathfrak{g}_0$, $\mathfrak{g}_+ \mapsto 0$, and the action of $\mathfrak{g}$ is induced by the left multiplication in $\mathcal{U}(\mathfrak{g})$. Here and further $\mathcal{U}(q)$ stands for the universal enveloping algebra of the Lie algebra $\mathfrak{q}$. Any highest weight module $V(\mathfrak{g},\lambda)$ is a quotient module of $M(\mathfrak{g},\lambda)$. The irreducible module $L(\mathfrak{g},\lambda)$ is the quotient of $M(\mathfrak{g},\lambda)$ by the maximal proper graded submodule. We shall write $M(\lambda)$ and $L(\lambda)$ in place of $M(\mathfrak{g},\lambda)$ and $L(\mathfrak{g},\lambda)$ if no ambiguity may arise.

Consider a parabolic subalgebra $\mathfrak{p} = \oplus_{j\in\mathbb{Z}} \mathfrak{p}_j$ of $\mathfrak{g}$ and let $\lambda \in \mathfrak{g}_0^*$ be such that $\lambda|_{\mathfrak{g}_0 \cap [\mathfrak{p},\mathfrak{p}]} = 0$. Then the $(\mathfrak{g}_0 \oplus \mathfrak{g}_+)$-module $\mathbb{C}_\lambda$ extends to a $\mathfrak{p}$-module by letting $\mathfrak{p}_j$ act as 0 for $j<0$, and we may construct the highest weight module

$$M(\mathfrak{g},\mathfrak{p},\lambda) = \mathcal{U}(\mathfrak{g}) \otimes_{\mathcal{U}(\mathfrak{p})} \mathbb{C}_\lambda$$

called the *generalized Verma module*.

We will also require the following condition on $\mathfrak{g}$.

(P3) If $\mathfrak{p}$ is a nondegenerate parabolic subalgebra of $\mathfrak{g}$, then there exists a nondegenerate element a such that $\mathfrak{p}^a \subseteq \mathfrak{p}$.

Theorem 4.3: *The following conditions on* $\lambda \in \mathfrak{g}_0^*$ *are equivalent*:

(1) $M(\lambda)$ *contains a singular vector* $a \cdot v_\lambda$ *in* $M(\lambda)_{-1}$, *where* a *is nondegenerate*;
(2) *there exist a nondegenerate element* $a \in \mathfrak{g}_{-1}$, *such that* $\lambda([\mathfrak{g}_1, a]) = 0$;
(3) $L(\lambda)$ *is quasifinite*;
(4) *there exist a nondegenerate element* $a \in \mathfrak{g}_{-1}$, *such that* $L(\lambda)$ *is the irreducible quotient of the generalized Verma module* $M(\mathfrak{g},\mathfrak{p}^a,\lambda)$.

Now consider $\mathfrak{g} = \mathcal{S}_q^{\epsilon,k}$. Take a parabolic subalgebra $\mathfrak{p}$ of $\widehat{\mathcal{S}}_q^{\epsilon,k}$, namely, it is a subalgebra of the following form:

$$\mathfrak{p} = \bigoplus_{j\in z} \mathfrak{p}_j, \quad \text{where } \mathfrak{p}_j = (\widehat{\mathcal{S}}_q^{\epsilon,k})_j \text{ for } j \geqslant 0 \text{ and } \mathfrak{p}_j \neq 0 \text{ for some } j < 0.$$

Observe for each $j \in \mathbb{N}$ we have

$$\mathfrak{p}_{-j} = \{z^{-j}(q^{(-j-1)/2}T_q)^{-jk/2} f(q^{(-j-1)/2}T_q) : f \in I_{-j}\},$$

where I_{-j} is a subspace of $\mathbb{C}[w,w^{-1}]^{\epsilon,j}$. Given $f(w) \in \mathbb{C}[w,w^{-1}]^{\epsilon,0}$ and $p(w) \in \mathbb{C}[w,w^{-1}]^{\epsilon,j}$ we have that $[f(q^{-1/2}T_q), z^{-n}(q^{(-n-1)/2}T_q)^{-nk/2} p(q^{(-n-1)/2}T_q)] \in \widehat{\mathcal{S}_q^{\epsilon,k}}$. Computing

$$\begin{aligned}[f(q^{-1/2}T_q), z^{-n}(q^{(-n-1)/2}T_q)^{-nk/2} p(q^{(-n-1)/2}T_q)] &= z^{-n}(q^{(-n-1)/2}T_q)^{-nk/2}(f(q^{-n-1/2}T_q) \\ &\quad - f(q^{-1/2}T_q))p(q^{(-n-1)/2}T_q) \\ &= z^{-n}(q^{(-n-1)/2}T_q)^{-nk/2} g(q^{(-n-1)/2}T_q) p(q^{(-n-1)/2}T_q),\end{aligned} \tag{4.1}$$

where $g(w) = f(q^{-n/2}T_q) - f(q^{n/2}T_q)$. As f ranges over $\mathbb{C}[w,w^{-1}]^{\epsilon,0}$, $g(w)$ ranges over all Laurent polynomials such that $g(w^{-1}) = g(w)$. We denote this set by $\mathbb{C}[w,w^{-1}]^0$. Thus (4.1) implies that if $p(w) \in I_{-n}$, then $p(w)$ multiplied by any Laurent polynomial in $\mathbb{C}[w,w^{-1}]^0$ belongs to I_{-n}. This means that I_{-n} is a $\mathbb{C}[w,w^{-1}]^0$-submodule of $\mathbb{C}[w,w^{-1}]^{\epsilon,n}$, where $\mathbb{C}[w,w^{-1}]^{\epsilon,n}$ is regarded as a module over $\mathbb{C}[w,w^{-1}]^0$ by multiplication.

It is known that every nonzero $\mathbb{C}[w,w^{-1}]^0$-submodule of $\mathbb{C}[w,w^{-1}]^{\epsilon,n}$ is a free rank 1 submodule generated by a monic Laurent polynomial (meaning that the coefficient of the higher degree monomial is 1). Denote by b_n^ϵ such a generator for I_{-n} if $I_{-n} \neq 0$ and $b_n^\epsilon(w) = 0$ if $I_{-n} = 0$. We call $b_n^\epsilon(w)$, $k \in \mathbb{N}$ the *characteristic polynomial* of $\mathfrak{p}$.

Let us check conditions (P1), (P2), and (P3) for $\widehat{\mathcal{S}_q^{\epsilon,k}}$. We can immediately see that condition (P1) is satisfied since

$$(\mathcal{S}_q^{\epsilon,k})_0 = \{h(q^{-1/2}T_q) : h(w^{-1}) = h(w)\}$$

is abelian. Let us check (P2).

Lemma 4.4: If $a \in (\mathcal{S}_q^{\epsilon,k})_{-j}$, $(j>0)$ *such that* $[a, (\mathcal{S}_q^{\epsilon,k})_1] = 0$, *then* $a = 0$.

Proof: Take $a \in (\mathcal{S}_q^{\epsilon,k})_{-j}$, $(j>0)$, then $a = z^{-j}(q^{(-j-1)/2}T_q)^{-jk/2} h(q^{(-j-1)/2}T_q)$ with $h(w^{-1}) = -\epsilon^j h(w)$. Consider an arbitrary element of $(\mathcal{S}_q^{\epsilon,k})_1$, namely, $z(T_q)^{k/2} g(T_q)$ with $g(w^{-1}) = -\epsilon g(w)$. We have that

$$\begin{aligned}0 &= [z^{-j}(q^{(-j-1)/2}T_q)^{-jk/2} h(q^{(-j-1)/2}T_q), z(T_q)^{k/2} g(T_q)] \\ &= z^{-j+1}(q^{-j/2}T_q)^{[(-j+1)k]/2}(h(q^{(-j+1)/2}T_q)g(T_q) - h(q^{(-j-1)/2}T_q)g(q^{-j}T_q)) \\ &= z^{-j+1}(q^{-j/2}T_q)^{[(-j+1)k]/2} f(q^{-j/2}T_q)\end{aligned} \tag{4.2}$$

with $f(T_q) = h(q^{1/2}T_q)g(q^{j/2}T_q) - h(q^{-1/2}T_q)g(q^{-j/2}T_q)$. Suppose that $h(w) = a_n w^n + \textit{lower degree terms}$, with $a_n \neq 0$ and take $g(w) = w^m - \epsilon w^{-m}$ with $n \neq -mj$, then

$$0 = f(w) = a_n(q^{(n+mj)/2} - q^{(-n-mj)/2}) w^{m+n} + \textit{lower degree terms}$$

which is a contradiction, therefore $a = 0$. ∎

To check (P3) we will need the following lemma.

Lemma 4.5: Let $\{b_n^\epsilon : n \in \mathbb{N}\}$ *be the sequence of characteristic polynomials of a parabolic subalgebra* $\mathfrak{p}$ *of the Lie algebra* $\widehat{\mathcal{S}_q^{\epsilon,k}}$. *Then*

(1) $b_n^\epsilon(w) \in \mathbb{C}[w,w^{-1}]^{\epsilon,n}$;
(2) $b_n^\epsilon(w)$ *divides*

$$(q^{(-n-1)/2}w - \epsilon q^{(n+1)/2}w^{-1})((q^{-1}-1)q^{1/2}w - \epsilon^{-n-1}(q-1)q^{-1/2}w^{-1}) b_{n+1}^\epsilon(q^{-1/2}w);$$

(3) $b_{n+m}^\epsilon(w)$ *divides* $(q^{m/2} - q^{-m/2})(w + \epsilon^{-n}w^{-1}) b_n^\epsilon(q^{m/2}w) b_m^\epsilon(q^{n/2}w)$;

(4) $\mathfrak{p}_{-n} \neq 0$ for all $n \in \mathbb{N}$.

In particular all $b_n^\epsilon(w)$ *are nonzero.*

Proof: Part (1) follows from the definition of the characteristic polynomial. Computing

$$[z(T_q)^{k/2}(T_q - \epsilon T_q^{-1}), z^{-n-1}(q^{-n/2-1}T_q)^{[(-n-1)k]/2} b_{n+1}^\epsilon(q^{(-n/2)-1}T_q)]$$
$$= z^{-n}(q^{(-n-1)/2}T_q)^{-nk/2}((q^{-n-1}T_q - \epsilon q^{n+1}T_q^{-1})b_{n+1}^\epsilon(q^{(-n/2)-1}T_q) - (T_q - \epsilon T_q^{-1})b_{n+1}^\epsilon(q^{-n/2}T_q))$$

we see that $b_n^\epsilon(q^{(-n-1)/2}w)$ divides

$$(q^{-n-1}w - \epsilon q^{n+1}w^{-1})b_{n+1}^\epsilon(q^{(-n/2)-1}w) - (w - \epsilon w^{-1})b_{n+1}^\epsilon(q^{-n/2}w). \tag{4.3}$$

From the commutation relation

$$[z(T_q)^{k/2}(T_q - \epsilon T_q^{-1}), z^{-n-1}(q^{(-n/2)-1}T_q)^{[(-n-1)k]/2}(q^{(-n/2)-1}T_q - \epsilon^{-n-1}q^{(n/2)+1}T_q^{-1})b_{n+1}^\epsilon(q^{(-n/2)-1}T_q)]$$
$$= z^{-n}(q^{(-n-1)/2}T_q)^{-nk/2}((q^{-n-1}T_q - \epsilon q^{n+1}T_q^{-1})(q^{(-n/2)-1}T_q - \epsilon^{-n-1}q^{(n/2)+1}T_q^{-1})b_{n+1}^\epsilon(q^{(-n/2)-1}T_q)$$
$$- (T_q - \epsilon T_q^{-1})(q^{-n/2}T_q - \epsilon^{-n-1}q^{n/2}T_q^{-1})b_{n+1}^\epsilon(q^{-n/2}T_q))$$

we see that $b_n^\epsilon(q^{(-n-1)/2}w)$ divides

$$(q^{-n-1}w - \epsilon q^{n+1}w^{-1})((q^{(-n/2)-1}w - \epsilon^{-n-1}q^{(n/2)+1}w^{-1})b_{n+1}^\epsilon(q^{(-n/2)-1}w)$$
$$- (w - \epsilon w^{-1})(q^{-n/2}w - \epsilon^{-n-1}q^{n/2}w^{-1})b_{n+1}^\epsilon(q^{-n/2}w)). \tag{4.4}$$

Now, from (4.3) and (4.4) we see that $b_n^\epsilon(q^{(-n-1)/2}w)$ divides

$$(q^{-n-1}w - \epsilon q^{n+1}w^{-1})((q^{-1}-1)q^{-n/2}w - \epsilon^{-n-1}(q-1)q^{n/2}w^{-1})b_{n+1}^\epsilon(q^{(-n/2)-1}w).$$

This proves (2), and we can deduce that if $b_{n+1}^\epsilon(w) \neq 0$, then $b_n^\epsilon(w) \neq 0$.

Part (3) can be similarly proved by computing the following two commutators:

$$[z^{-n}(q^{(-n-1)/2}T_q)^{(-n)k/2}b_n^\epsilon(q^{(-n-1)/2}T_q), z^{-m}(q^{(-m-1)/2}T_q)^{(-m)k/2}b_m^\epsilon(q^{(-m-1)/2}T_q)]$$

and

$$[z^{-n}(q^{(-n-1)/2}T_q)^{(-n)k/2}(q^{(-n-1)/2}T_q - \epsilon^{-n}q^{(n+1)/2}T_q^{-1})b_n^\epsilon(q^{(-n-1)/2}T_q),$$
$$z^{-m}(q^{(-m-1)/2}T_q)^{(-m)k/2}b_m^\epsilon(q^{(-m-1)/2}T_q)].$$

In particular, if $b_k^\epsilon(w) \neq 0$ and $b_l^\epsilon(w) \neq 0$, then $b_{l+k}^\epsilon(w) \neq 0$. Part (4) follows immediately from (2) and (3). ■

Given $\mathfrak{p}$ a parabolic subalgebra of $\widehat{\mathcal{S}_q^{\epsilon,k}}$, by the lemma above, we have that it is nondegenerate. Take

$$a = z^{-1}(q^{-1}T_q)^{-k/2}b_1^\epsilon(q^{-1}T_q) \in \mathfrak{p}_{-1}, \tag{4.5}$$

where b_1^ϵ is the first characteristic polynomial of $\mathfrak{p}$. Then, $\mathfrak{p}^a$ is, by Lemma 4.1, the minimal parabolic subalgebra containing a. Using again the above lemma, we know that it is nondegenerate, therefore by definition a is nondegenerate, and by construction $\mathfrak{p}^a \subseteq \mathfrak{p}$, proving (P3).

Now, consider $\lambda \in (\widehat{\mathcal{S}_q^{\epsilon,k}})_0^*$. Let $L(\lambda) = L(\widehat{\mathcal{S}_q^{\epsilon,k}}, \lambda)$ denote the unique irreducible quotient of $M(\lambda) = M(\widehat{\mathcal{S}_q^{\epsilon,k}}, \lambda)$. A functional $\lambda \in (\widehat{\mathcal{S}_q^{\epsilon,k}})_0^*$ is described by its labels $\Delta_n = q(n)\lambda((q^{-1/2}T_q)^n - (q^{-1/2}T_q)^{-n})$ with $n \in \mathbb{Z}$, $q(n) = q^{n/2} - q^{-n/2}$, and the central charge $\lambda(C) = c$. We will consider the generating series

$$\Delta(x) = \sum_{n \in \mathbb{Z}} x^n \Delta_n.$$

Recall that a *quasipolynomial* is a linear combination of functions of the form $p(x)q^{\alpha x}$, where

$p(x)$ is a polynomial and $\alpha \in \mathbb{C}$. That is, it satisfies a nontrivial linear differential equation with constant coefficients. We also have the following well-known proposition.

Proposition 4.6: Given a quasipolynomial P, and a polynomial $B(x)=\Pi_i(x-A_i)$, *take* $b(x)=\Pi_i(x-a_i)$ *where* $a_i=e^{A_i}$, *then* $b(x)(\Sigma_{n\in\mathbb{Z}}P(n)x^{-n})=0$ *if and only if* $B(d/dx)P(x)=0$.

If the polynomial B is even we call P an *even quasipolynomial*. We will prove the main theorem of this section.

Theorem 4.7: *An irreducible highest weight* $\widehat{\mathcal{S}_q^{\epsilon,k}}$*-module* $L(\lambda)$ *is quasifinite if and only if one of the following equivalent conditions hold.*

(a) There exists a monic Laurent polynomial $b_1^\epsilon(w)\in\mathbb{C}^{\epsilon,1}[w,w^{-1}]$ *such that*

$$b_1^\epsilon(x)(\Delta(x)-2c)=0. \tag{4.6}$$

(b) There exists an even quasipolynomial $P_\epsilon(x)$ *such that*

$$P_\epsilon(n)=\Delta_n \quad \text{for } n\neq 0 \text{ and } P(0)=2c. \tag{4.7}$$

Proof: We can apply Theorem 4.3. Therefore the quasifiniteness of $L(\lambda)$ is equivalent to show that there exist a nondegenerate element $a\in(\widehat{\mathcal{S}_q^{\epsilon,k}})_{-1}$, such that $\lambda([(\widehat{\mathcal{S}_q^{\epsilon,k}})_1,a])=0$. Take a as in (4.5). Since $b_1^\epsilon(w)\in\mathbb{C}^{\epsilon,1}[w,w^{-1}]$, then we have that $b_1^\epsilon(w)=a_m(w^m-\epsilon w^{-m})+a_{m-1}(w^{m-1}-\epsilon w^{-m+1})+\ldots+a_1(w-\epsilon w^{-1})+a_0(1-\epsilon)$ with $a_m\neq 0$. Recall that a base for $(\widehat{\mathcal{S}_q^{\epsilon,k}})_1$ is

$$\mathcal{B}=\{z(T_q)^{k/2}(T_q^n-\epsilon T_q^{-n}):n\in\mathbb{N}\}$$

if $\epsilon=1$ and $\mathcal{B}\cup\{z(T_q)^{k/2}\}$ if $\epsilon=-1$. Therefore $(\forall n)$,

$$\begin{aligned}
0&=\lambda([z(T_q)^{k/2}(T_q^n-\epsilon T_q^{-n}),a])\\
&=\lambda(b_1^\epsilon(T_q)(T_q^n-\epsilon T_q^{-n})-(q^{-n}T_q^n-\epsilon q^n T_q^{-n})b_1^\epsilon(q^{-1}T_q)-\mathrm{tr}_0(b_1^\epsilon(w)(w^n-\epsilon w^{-n}))C)\\
&=\lambda\left(\sum_{j=0}^m a_j((T_q^j-\epsilon T_q^{-j})(T_q^n-\epsilon T_q^{-n})-(q^{-n}T_q^n-\epsilon q^n T_q^{-n})(q^{-j}T_q^j-\epsilon q^j T_q^{-j}))+\mathrm{tr}_0(b_1^\epsilon(w)(w^n-\epsilon w^{-n}))C\right)\\
&=\sum_{j=0}^m a_j(q\ (n+j)\lambda((q^{-1/2}T_q)^{j+n}-(q^{-1/2}T_q)^{-j-n})-\epsilon q(n-j)\lambda((q^{-1/2}T_q)^{n-j}-(q^{-1/2}T_q)^{-n+j})\\
&\quad-\lambda(\mathrm{tr}_0(b_1^\epsilon(w)(w^n-\epsilon w^{-n}))C)\\
&=\sum_{j=0}^m a_j(\Delta_{j+n}-\epsilon\Delta_{n-j})+2\epsilon a_n c.
\end{aligned} \tag{4.8}$$

We also have for the case $\epsilon=-1$,

$$0=\lambda[a,zT_q^{k/2}]=\lambda(b_1^\epsilon(T_q)-b_1^\epsilon(q^{-1}T_q))=\sum_{j=0}^m a_j\lambda(q(j)((q^{-1/2}T_q)^j-(q^{-1/2}T_q)^{-j}))=\sum_{j=0}^m a_j\Delta_j. \tag{4.9}$$

Multiplying the last equality in (4.8) by $x^n-\epsilon x^{-n}$, adding over $n\in\mathbb{Z}_{\geqslant 0}$, and using the fact that $\Delta_n=\Delta_{-n}$ and (4.9) when $\epsilon=-1$, we get

$$0=\sum_{j=0}^m a_j(x^{-j}-\epsilon x^j)\Delta(x)+2\epsilon b_1^\epsilon(x)c=-\epsilon b_1^\epsilon(x)(\Delta(x)-2c). \tag{4.10}$$

The equivalence of (a) and (b) follows from the fact that Eq. (4.6) holds, if and only if multiplying both sides of this formula by x^m this equation also holds, and now $\widetilde{b}^\epsilon(x)=x^m b_1^\epsilon(x)\in\mathbb{C}[x]$. Observe that $\widetilde{b}^\epsilon(0)=a_m\neq 0$, and since $b_1^\epsilon(x^{-1})=-\epsilon b_1^\epsilon(x)$ it is easy to see that if α is a root of $\widetilde{b}^\epsilon(x)$, then $1/\alpha$

is also a root of $\widetilde{b}^{\epsilon}(x)$. Now we can apply Proposition 4.6 and due to the relationship between the roots of B and b in this proposition it follows that the $B(x)$ corresponding to our $\widetilde{b}^{\epsilon}(x)$ is an even polynomial, finishing our proof. ■

Given a quasifinite irreducible highest weight $\widehat{\mathcal{S}_q^{k,\epsilon}}$-module V by Theorem 4.7, we have that there exists an even quasipolynomial $P(x)$ satisfying (4.7). We will write

$$P(x) = \sum_i p_i(x)\cosh_q(e_i^+ x) + \sum_j q_j(x)\sinh_q(e_j^- x), \tag{4.11}$$

with $p_i(x)$ [respectively, $q_j(x)$] are nonzero even (respectively, odd) polynomials, e_i^+ and e_j^- are distinct complex numbers, $\cosh_q(x)=(q^x+q^{-x})/2$ and $\sin_q(x)=(q^x-q^{-x})/2$. The expression in (4.11) is unique up to a sign of e_i^+ or a simultaneous change of signs of e_j^- and $q_j(x)$. We call e_i^+ (respectively, e_j^-), *even type* (*respectively, odd type*) *exponents* of V with *multiplicities* $p_i(x)$ [respectively, $q_j(x)$]. As in Ref. 6, we denote e^+ the set of even type exponents with multiplicity $p_i(x)$ and by e^- the set of odd type of exponents with multiplicity $q_i(x)$. Therefore the pair $(e^+;e^-)$ uniquely determines V. We will denote this module by $L(\widehat{\mathcal{S}_q^{k,\epsilon}};e^+;e^-)$.

V. EMBEDDING OF $\widehat{\mathcal{S}_q^{\epsilon,k}}$ INTO INFINITE RANK CLASSICAL LIE ALGEBRAS

Let $\mathcal{O}$ be the algebra of all holomorphic functions on $\mathbb{C}^\times$ with the topology of uniform convergence on compact sets, and denote

$$\mathcal{O}^{\epsilon,j} = \{f \in \mathcal{O} | f(w) = -\epsilon^j f(w^{-1})\}.$$

We consider the vector space $\mathcal{S}_q^{\mathcal{O}^{as}}$ spanned by the quantum pseudodifferential operators (of infinite order) of the form $z^k f(T_q)$, where $f \in \mathcal{O}$. The product in $\mathcal{S}_q^{as}$ and its principal gradation extend to $\mathcal{S}_q^{\mathcal{O}^{as}}$. Denote by $\mathcal{S}_q^{\mathcal{O}}$ the corresponding Lie algebra. Then the cocycle Ψ extends by formula (3.1). Let $\widehat{\mathcal{S}}_q^{\mathcal{O}}=\mathcal{S}_q^{\mathcal{O}}+\mathbb{C}C$ be the corresponding central extension. Similarly we define

$$\widehat{\mathcal{S}_q^{k,\epsilon^{\mathcal{O}}}} = \mathcal{S}_q^{k,\epsilon^{\mathcal{O}}} + \mathbb{C}C$$

the central extension of $\mathcal{S}_q^{k,\epsilon^{\mathcal{O}}}$ by the restriction of the cocycle Ψ, where

$$\mathcal{S}_q^{k,\epsilon^{\mathcal{O}}} = \{z^l (q^{(l-1)/2}T_q)^{lk/2} f(q^{(l-1)/2}T_q) | l \in \mathbb{Z}, f \in \mathcal{O}^{\epsilon,l}\}.$$

We shall construct an embedding of $\widehat{\mathcal{S}_q^{\epsilon,k}}$ into the Lie algebra of infinite matrices with only finitely many nonzero diagonal, over the algebra of truncated polynomials and its classical Lie subalgebras of type B, C, and D.

As in Sec. II, consider the associative algebra $R_m=\mathbb{C}[t]/(t^{m+1})$ with $m \in \mathbb{Z}_+$. Recall that $g\ell_\infty^{[m]}$ is the $\mathbb{Z}$-graded complex Lie algebra of all infinite matrices $(a_{i,j})_{i,j\in\mathbb{Z}}$ with finitely many nonzero diagonals with entries in R_m.

Let us fix $s \in \mathbb{C}^\times$, then we have a family of homomorphism $\varphi_s: \mathcal{S}_q \to g\ell_\infty^{[m]}$ which is compatible with the principal gradation, defined by

$$\varphi_{s,t}(z^k f(T_q)) = \sum_{l\in\mathbb{Z}} f(sq^{-l+t})E_{(l-k),l}. \tag{5.1}$$

Observe that it naturally extends to a homomorphism $\varphi_{s,t}: \mathcal{S}_q^{\mathcal{O}} \to g\ell_\infty^{[m]}$. Let

$$I_s^{[m],\epsilon,l} = \{f(q^{(l-1)/2}T_q) | f \in \mathcal{O}^{\epsilon,l} \text{ and } f^{(i)}(sq^j) = 0 \text{ for all } j \in \mathbb{Z}, i = 0,1,\ldots,m\}$$

and

$$J_s^{[m],k,\epsilon} = \bigoplus_{l\in\mathbb{Z}} z^l (q^{(l-1)/2}T_q)^{lk/2} I_s^{[m],\epsilon,l} \in \mathcal{S}_q^{k,\epsilon^{\mathcal{O}}}.$$

Therefore, it follows by the Taylor formula for $\varphi_s^{[m]}: \mathcal{S}_q^{\epsilon,k} \to g\ell_\infty^{[m]}$, that

$$\operatorname{Ker} \varphi_s^{[m]} = J_s^{[m],k,\epsilon}. \tag{5.2}$$

Choose a branch of $\log q$. Let $\tau = \log q/2\pi i$. Then any $s \in \mathbb{C}^\times$ is uniquely written as $s = q^a$, $a \in \mathbb{C}/\tau^{-1}\mathbb{Z}$. Now, let fix $\mathbf{s} = (s_1, \ldots, s_n) \in \mathbb{C}^n$ such that if we write each $s_i = q^{a_i}$, we have

$$a_i - a_j \notin \mathbb{Z} + \tau^{-1}\mathbb{Z} \quad \text{for } i \neq j, \tag{5.3}$$

and fix $\mathbf{m} = (m_1, \ldots, m_n) \in \mathbb{Z}_+^n$.

Let $g\ell_\infty^{[\mathbf{m}]} = \oplus_{i=1}^n g\ell_\infty^{[m_i]}$. Consider the homomorphism

$$\varphi_{\mathbf{s}}^{[\mathbf{m}]} = \bigoplus_{i=1}^n \varphi_{s_i}^{[m_i]}: \mathcal{S}_q^{k,\epsilon^{\mathcal{O}}} \to g\ell_\infty^{[\mathbf{m}]}.$$

Proposition 5.1: Given $\mathbf{s}$ *and* $\mathbf{m}$ *as above, we have the exact sequence of* $\mathbb{Z}$*-graded Lie algebras, provided that* $|q| \neq 1$:

$$0 \to J_{\mathbf{s}}^{[\mathbf{m}],k,\epsilon} \to \mathcal{S}_q^{k,\epsilon^{\mathcal{O}}} \xrightarrow{\varphi_{\mathbf{s}}^{[\mathbf{m}]}} g\ell_\infty^{[\mathbf{m}]} \to 0$$

where $J_{\mathbf{s}}^{[\mathbf{m}],k,\epsilon} = \cap_{i=1}^n J_{s_i}^{[m_i],k,\epsilon}$.

Proof: The first part is clear from (5.2). For the sake of simplicity, we will prove the surjectivity of $\varphi_{\mathbf{s}}^{[\mathbf{m}]}$ in the case $N=1$, $\mathbf{m}=m$ and $\mathbf{s}=s=q^a$. We will use the following well-known fact: for every discrete sequence of points in $\mathbb{C}$ and a non-negative integer m there exists $f(w) \in \mathcal{O}$ having prescribed values of its first m derivatives at these points. By condition (5.3) and $|q| \neq 1$ we have that $\{q^{(n-1)/2-j+a}\}$ and $\{q^{-(n-1)/2+j-a}\}$ are discrete and disjoint sequences of points in $\mathbb{C}$. Therefore we can find $p \in \mathcal{O}$ such that $p^{(i)}(q^{(n-1)/2-j+a}) = p^{(i)}(q^{-(n-1)/2+j-a}) = 0$ for $i = 0, \ldots, m-1$ and $j \in \mathbb{Z}$,

$$p^{(m)}(q^{(n-1)/2-j+a}) = 1, \quad p^{(m)}(q^{-(n-1)/2+j-a}) = -\epsilon^j(-1)^m q^{2m\{[-(n-1)/2]+j-a\}}$$

for a fixed value of j and zero for the remaining points in the sequences. Now let $f(w) = [p(w) - \epsilon^n p(w^{-1})]/2$. Using Taylor formula for φ_s^m and the way we choose p it is a straightforward computation that the image of $z^n(q^{(n-1)/2}T_q)^{nk/2} f(q^{(n-1)/2}T_q)$ is up to a nonzero constant $(t^m/m!)E_{j-n,j}$. Similarly one can show that $[t^{m-1}/(m-1!)]E_{j-n,j}$ is also in the image, and then inductively completing the proof. ∎

Now we want to extend the homomorphism $\varphi_s^{[m]}$ to a homomorphism between the central extensions of the corresponding Lie algebras.

Proposition 5.2: The $\mathbb{C}$*-linear map* $\hat{\varphi}_s^{[m]}: \widehat{\mathcal{S}_q^{k,\epsilon}} \to \widehat{g\ell}_\infty^{[m]}$ *defined by* $(s = q^a)$,

$$\hat{\varphi}_s^{[m]}|_{(\widehat{\mathcal{S}_q^{k,\epsilon}})_j} = \varphi_s^{[m]}|_{(\mathcal{S}_q^{k\epsilon})_j} \quad \text{if } j \neq 0, \tag{5.4}$$

$$\widehat{\varphi_s^{[m]}}(q(n)(q^{-n/2}T_q^n - q^{n/2}T_q^{-n})) = \varphi_s^{[m]}(q(n)(q^{-n/2}T_q^n - q^{n/2}T_q^{-n})) - \sum_{j=1}^m \frac{q^{(a-1/2)n} + (-1)^j q^{(-a+1/2)n}}{q^{n/2} - q^{-n/2}} (n\log q)^j \frac{t^j}{j!} \quad (n \neq 0), \tag{5.5}$$

$$\hat{\varphi}_s^{[m]}(C) = 1 \in R_m, \tag{5.6}$$

is a homomorphism of Lie algebras over $\mathbb{C}$.

Proof: It is straightforward computation restricting the formula of $\widehat{\varphi_s^{[m]}}$ in (6.5) of Ref. 5, to $\widehat{\mathcal{S}_q^{k,\epsilon}}$. ∎

The homomorphism $\varphi_s^{[m]}: \mathcal{S}_q^{k,\epsilon} \to g\ell_\infty^{[m]}$ is defined for any $s \in \mathbb{C}^\times$. However if $s=q^a$ with $a \in \mathbb{Z}/2$, it is no longer surjective. The case $a=1$ is described by the following.

Proposition 5.3: We have the following exact sequences of Lie algebras:

$$0 \to J_q^{[m],k,1} \to \mathcal{S}_q^{k,1} \xrightarrow{\varphi_q^{[m]}} d_\infty^{[m]} \to 0,$$

$$0 \to J_q^{[m],k,-1} \to \mathcal{S}_q^{k,-1} \xrightarrow{\varphi_q^{[m]}} c_\infty^{[m]} \to 0.$$

Proof: By definition of $\varphi_q^{[m]}$, it is easy to see that its image lies in $d_\infty^{[m]}$ or $c_\infty^{[m]}$ depending if $\epsilon=1$ or -1. The proof of the rest is similar to that of Proposition 5.1. ■

Similarly, the case $a=1/2$, is described by the following.

Proposition 5.4: We have the following exact sequences of Lie algebras:

$$0 \to J_{q^{1/2}}^{[m],k,1} \to \mathcal{S}_q^{k,1} \xrightarrow{\varphi_{q^{1/2}}^{[m]}} \overline{b_\infty^{+}}^{[m]} \to 0,$$

$$0 \to J_{q^{1/2}}^{[m],k,-1} \to \mathcal{S}_q^{k,-1} \xrightarrow{\varphi_{q^{1/2}}^{[m]}} \overline{b_\infty^{-}}^{[m]} \to 0.$$

Remark 5.5: For arbitrary $a \in \mathbb{Z}$ the image of $\widehat{\mathcal{S}_q^{k,1}}$ by $\varphi_{q^a}^{[m]}$ is $\nu^{q^a}(d_\infty^{[m]})$ and the image of $\widehat{\mathcal{S}_q^{k,-1}}$ by $\varphi_{q^a}^{[m]}$ is $\nu^{q^a}(c_\infty^{[m]})$, where ν was defined in (2.1). Similarly, for $a \in \mathbb{Z}+1/2$ the image of $\widehat{\mathcal{S}_q^{k,\epsilon}}$ by $\varphi_{q^a}^{[m]}$ is $\nu^{q^a}(b_\infty^{[m]})$. Therefore it is enough to consider $a=1$ and $a=1/2$.

We will say that a vector $\mathbf{s}=(s_1,s_2,\ldots,s_N)=(q^{a_1},\ldots,q^{a_N}) \in \mathbb{C}^N$ satisfies the *condition* if $a_i \in \mathbb{Z}$, then $a_i=1$; if $a_i \in \mathbb{Z}+1/2$ then $a_i=1/2$, and $a_i-a_j \notin \mathbb{Z}+\tau^{-1}\mathbb{Z}$ for $i \neq j$.

Now, given $\mathbf{s}=(s_1,s_2,\ldots,s_N)=(q^{a_1},\ldots,q^{a_N}) \in \mathbb{C}^N$ satisfying the "condition" above and $\mathbf{m}=(m_1,\ldots,m_n) \in \mathbb{Z}^N$, and combining Propositions 5.1–5.4, we obtain a surjective Lie algebra homomorphism

$$\hat{\varphi}_{\mathbf{s}}^{[\mathbf{m}]} = \bigoplus_{i=1}^{n} \varphi_{s_i}^{[m_i]} : \widehat{\mathcal{S}_q^{k,\epsilon}}^{\mathcal{O}} \to \mathfrak{g}^{[\mathbf{m}]} := \bigoplus_{i=1}^{n} \mathfrak{g}^{[m_i]}, \tag{5.7}$$

where

$$\mathfrak{g}^{[m_i]} = \begin{cases} \widehat{g\ell}_\infty^{[m_i]} & \text{if } a_i \notin \mathbb{Z}/2, \\ b_\infty^{[m_i]} & \text{if } a_i = 1/2, \\ d_\infty^{[m_i]} & \text{if } a_i = 1 \text{ and } \epsilon = 1, \\ c_\infty^{[m_i]} & \text{if } a_i = 1 \text{ and } \epsilon = -1. \end{cases} \tag{5.8}$$

VI. REALIZATION OF QUASIFINITE HIGHEST WEIGHT MODULES OF $\widehat{\mathcal{S}_q^{\epsilon,k}}$

Here $\mathfrak{g}^{[m]}$ will be $\widehat{g\ell}_\infty^{[m]}$ or one of its classical subalgebras. The proof of the following result is in Ref. 3.

Proposition 6.1: The $\mathfrak{g}^{[m]}$*-module* $L(\mathfrak{g}^{[m]};\lambda)$ *is quasifinite if and only if all but finitely many of the* ${}^{\dagger}h_j^{(i)}$ *are zero, where* $\dagger$ *represents a, b, c or d depending on whether* $\mathfrak{g}^{[m]}$ *is* $\widehat{g\ell}_\infty^{[m]}$, $b_\infty^{[m]}$, $c_\infty^{[m]}$ *or* $d_\infty^{[m]}$.

Take a quasifinite $\lambda(i) \in (\mathfrak{g}_0^{[m_i]})^*$ for each $i=1,\ldots,N$, and let $L(\mathfrak{g}^{[m_i]};\lambda(i))$ be the corresponding irreducible $\mathfrak{g}^{[m_i]}$-module. The outer tensor product

$$L(\mathfrak{g}^{[\mathbf{m}]};\lambda)=\otimes_{i=1}^{n}L(\mathfrak{g}^{[m_i]};\lambda(i))$$

is an irreducible $\mathfrak{g}^{[\mathbf{m}]}$-module. The module $L(\mathfrak{g}^{[\mathbf{m}]};\lambda)$ can be regarded as $\widehat{\mathcal{S}_q^{\epsilon,k}}$-module via the homomorphism $\widehat{\varphi_{\mathbf{s}}^{[\mathbf{m}]}}$ given by (5.7), which we shall denote by $L_{\mathbf{s}}^{[\mathbf{m}],k,\epsilon}(\lambda)$.

We shall need the following Proposition, whose proof is completely similar to Proposition 4.3 in Ref. 5.

Proposition 6.2: Let V be a quasifinite $\widehat{\mathcal{S}_q^{k,\epsilon}}$-module. Then the action of $\widehat{\mathcal{S}_q^{k,\epsilon}}$ on V naturally extends to the action of $(\widehat{\mathcal{S}_q^{k,\epsilon}}^{\mathcal{O}})_j$ on V for any $j\neq 0$.

Given $\mathbf{m}=(m_1,\ldots,m_n)\in\mathbb{Z}_+^n$, we let $\mathfrak{g}^{[\mathbf{m}]}=\oplus_{i=1}^{n}\mathfrak{g}^{[m_i]}$. Let $\mathbf{s}=(s_1,\ldots,s_n)$ satisfying the "condition." By Proposition 5.1(4), we have that $\hat{\varphi}_{\mathbf{s}}^{[\mathbf{m}]}:\widehat{\mathcal{S}_q^{k,\epsilon}}\to\mathfrak{g}^{[\mathbf{m}]}$ is a surjective homomorphism of Lie algebras over $\mathbb{C}$.

Now we have the following important result.

Theorem 6.3: *Let $\mathbf{s}=(s_1,\ldots,s_n)$ satisfying the "condition." Consider the embedding $\hat{\varphi}_{\mathbf{s}}^{[\mathbf{m}]}:\widehat{\mathcal{S}_q^{k,\epsilon}}\to\mathfrak{g}^{[\mathbf{m}]}$ and let V be a quasifinite $\mathfrak{g}^{[\mathbf{m}]}$-module. Then any $\widehat{\mathcal{S}_q^{k,\epsilon}}$-submodule of V is a $\mathfrak{g}^{[\mathbf{m}]}$-submodule as well. In particular, the $\widehat{\mathcal{S}_q^{k,\epsilon}}$-modules $L_{\mathbf{s}}^{[\mathbf{m}],k,\epsilon}(\lambda)$ are irreducible.*

Proof: The same proof as Theorem 4.5 in Ref. 5. ■

By Proposition 6.1 and Theorem 6.3, we have that the $\widehat{\mathcal{S}_q^{k,\epsilon}}$-modules $L_{\mathbf{s}}^{[\mathbf{m}],k,\epsilon}(\lambda)$ are irreducible quasifinite highest weight modules. Using the formulas (5.4) and (5.6), we can calculate the generating series $\Delta_{\mathbf{m},\mathbf{s},\lambda}^{k,\epsilon}(x)=\Sigma_n\Delta_n x^{-n}$ of the highest weight and the central charge c of the $\widehat{\mathcal{S}_q^{k,\epsilon}}$-module $L_{\mathbf{s}}^{[\mathbf{m}],k,\epsilon}(\lambda)$. We will introduce the following notation:

$$\eta_i(\alpha,\beta):=\frac{q^{\alpha\beta}+(-1)^i q^{-\alpha\beta}}{q^{\alpha/2}-q^{-\alpha/2}}\frac{(\beta\log q)^i}{i!}. \tag{6.1}$$

Proposition 6.4: Take the embedding $\hat{\varphi}_s^{[m]}:\widehat{\mathcal{S}_q^{k,\epsilon}}\to\widehat{g\ell_\infty^{[m]}}$ with $s=q^a$ and $a\notin\mathbb{Z}/2$. The $\widehat{g\ell_\infty^{[m]}}$-module $L(\widehat{g\ell_\infty^{[m]}};\lambda)$ regarded as a $\widehat{\mathcal{S}_q^{k,\epsilon}}$-module is isomorphic to $L(\widehat{\mathcal{S}_q^{k,\epsilon}};e^+,e^-)$ where e^+ and e^- consists of the exponents $a-j-1$, $(j\in\mathbb{Z})$ with multiplicities,

$$\sum_{0\leqslant i\leqslant m,\,i\ even}{}^a\tilde{h}_j^{(i)}\frac{x^i}{i!}\quad and\quad \sum_{0\leqslant i\leqslant m,\,i\ odd}{}^a\tilde{h}_j^{(i)}\frac{x^i}{i!}, \tag{6.2}$$

respectively, with ${}^a\tilde{h}_j^{(i)}=({}^ah_j^{(i)}-\delta_{0,j}c_i)(\log q)^i$.

Proof: By Proposition 6.1 and Theorem 6.3 the $\widehat{\mathcal{S}_q^{k,\epsilon}}$-module $L_s^{[m],k,\epsilon}(\lambda)$ is an irreducible quasifinite highest weight module. By applying λ to (5.5) and using formulas (5.1) and (6.1), we obtain $(n\in\mathbb{Z})$

$$\begin{aligned}(\Delta_{m,s,\lambda}^{k,\epsilon})_n=&-q(n)\lambda\Bigg(\sum_{j\in\mathbb{Z}}\sum_{i=0}^{m}(q^{n(a-j-1/2)}-(-1)^iq^{-n(a-j-1/2)})(n\log q)^i\frac{t^i}{i!}E_{jj}\\&-\sum_{i=0}^{m}\frac{q^{(a-1)n}+(-1)^iq^{(-a+1)n}}{q^{n/2}-q^{-n/2}}\frac{(n\log q)^i}{i!}t^i\Bigg)\\=&-q(n)\lambda\Bigg(\sum_{j\in\mathbb{Z}}\sum_{i=0}^{m}(\eta_i(a-j,n)-\eta_i(a-j-1,n))t^iE_{jj}-\sum_{i=0}^{m}\eta_i(a-1,n)t^i\Bigg).\end{aligned} \tag{6.3}$$

Shifting the index j to $j+1$ in the first sum of the last identity in (6.3) we have

$$(\Delta_{m,s,\lambda}^{k,\epsilon})_n=-q(n)\Bigg(\sum_{j\in\mathbb{Z}}\sum_{i=0}^{m}\eta_i(a-j-1,n)^ah_j^{(i)}-\sum_{i=0}^{m}\eta_i(a-1,n)c_i\Bigg). \tag{6.4}$$

Using the definition of multiplicities and exponents for the quasipolynomial in Theorem 4.7 (b), we finish our proof. ■

Proposition 6.5: Take $s=q^a$, $a=1/2$ *and the embedding* $\hat{\varphi}_s^{[m]}:\widehat{\mathcal{S}_q^{k,\epsilon}}\to b_\infty^{[m]}$. *The* $b_\infty^{[m]}$*-module* $L(b_\infty^{[m]};\lambda)$ *regarded as a* $\widehat{\mathcal{S}_q^{k,\epsilon}}$*-module is isomorphic to* $L(\widehat{\mathcal{S}_q^{k,\epsilon}};e^+,e^-)$ *where* e^+ *and* e^- *consists of the exponents* $-j-1/2$, $(j\in\mathbb{Z}_{\geqslant 0})$ *with multiplicities*

$$\sum_{0\leqslant i\leqslant m,i\ even} {}^b\widetilde{h}_j^{(i)}\frac{x^i}{i!} \quad \text{and} \quad \sum_{0\leqslant i\leqslant m,i\ odd} {}^b\widetilde{h}_j^{(i)}\frac{x^i}{i!}, \tag{6.5}$$

respectively, where ${}^b\widetilde{h}_j^{(i)}={}^bh_j^{(i)}(\log q)^i$ *for* $j>0$ *and* ${}^b\widetilde{h}_0^{(i)}=1/2\,{}^bh_0^{(i)}(\log q)^i$.

Proof: Replacing $a=1/2$ in (6.3) and shifting the index j to $j+1$ in its first summation we get

$$(\Delta_{m,s,\lambda}^{k,\epsilon})_n=-q(n)\lambda\left(\sum_{j\in\mathbb{Z}}\sum_{i=0}^{m}\eta_i(-j-1/2,n)(t^iE_{j+1,j+1}-t^iE_{jj})-\sum_{i=0}^{m}(\eta_i(-1/2,n)t_i\right). \tag{6.6}$$

Now, splitting the summation $\Sigma_{j\in\mathbb{Z}}$ into two, namely $\Sigma_{j\geqslant 0}+\Sigma_{j\leqslant 0}$, changing j by $-j-1$ in the negative index sums, using the fact that $\eta_i(\alpha,\beta)=(-1)^i\eta_i(-\alpha,\beta)$ and formulas (2.7), we have

$$(\Delta_{m,s,\lambda}^{k,\epsilon})_n=-q(n)\sum_{j\geqslant 0}\sum_{i=0}^{m}\eta_i(-j-1/2,n)\,{}^b\widetilde{h}_j^{(i)}/(\log q)^i \tag{6.7}$$

now the proposition follows from the definition of multiplicities and exponents applied to the quasipolynomial given by Theorem 4.7. ■

Proposition 6.6: Consider $s=q^a$, $a=1$.

(*a*) ($\epsilon=1$). *Take the embedding* $\hat{\varphi}_s^{[m]}:\widehat{\mathcal{S}_q^{k,1}}\to d_\infty^{[m]}$. *The* $d_\infty^{[m]}$*-module* $L(d_\infty^{[m]};\lambda)$ *regarded as a* $\widehat{\mathcal{S}_q^{k,1}}$*-module is isomorphic to* $L(\widehat{\mathcal{S}_q^{k,1}};e^+,e^-)$ *where* e^+ *and* e^- *consists of the exponents* $-j$, $(j\in\mathbb{Z}_{\geqslant 0})$ *with multiplicities,*

$$\sum_{0\leqslant i\leqslant m,i\ even} {}^d\widetilde{h}_j^{(i)}\frac{x^i}{i!} \quad \text{and} \quad \sum_{0\leqslant i\leqslant m,i\ odd} {}^d\widetilde{h}_j^{(i)}\frac{x^i}{i!}, \tag{6.8}$$

respectively, with ${}^d\widetilde{h}_j^{(i)}={}^dh_j^{(i)}(\log q)^i$ *if* $j>0$ *and* ${}^0\widetilde{h}_j^{(i)}=1/2({}^dh_0^{(i)}-{}^dh_1^{(i)})(\log q)^i$.

(*b*) ($\epsilon=-1$). *Take the embedding* $\hat{\varphi}_s^{[m]}:\widehat{\mathcal{S}_q^{k,1}}\to c_\infty^{[m]}$. *The* $c_\infty^{[m]}$*-module* $L(c_\infty^{[m]};\lambda)$ *regarded as a* $\widehat{\mathcal{S}_q^{k,1}}$*-module is isomorphic to* $L(\widehat{\mathcal{S}_q^{k,1}};e^+,e^-)$ *where* e^+ *and* e^- *consists of the exponents* $-j$, $(j\in\mathbb{Z}_{\geqslant 0})$ *with multiplicities*

$$\sum_{0\leqslant i\leqslant m,i\ even} {}^c\widetilde{h}_j^{(i)}\frac{x^i}{i!} \quad \text{and} \quad \sum_{0\leqslant i\leqslant m,i\ odd} {}^c\widetilde{h}_j^{(i)}\frac{x^i}{i!}, \tag{6.9}$$

respectively, with ${}^c\widetilde{h}_j^{(i)}={}^ch_j^{(i)}(\log q)^i$.

Proof: We leave the details of the proof to the reader since it is completely similar to the proof of Proposition (6.5). ■

Consider an irreducible quasifinite highest weight $\widehat{\mathcal{S}_q^{k,\epsilon}}$-module V and denote by $P(x)$ its corresponding quasipolynomial. We will write

$$P(x)=\sum_{s=q^a\in\mathbb{C}}\sum_{i=0}^{m_s}a_{s,i}\eta_i(x,a-1)\frac{\sinh_q(x/2)}{2} \tag{6.10}$$

with $a_{s,i}\in\mathbb{C}$, and $a_{s,i}\neq 0$ for only finitely many $s\in\mathbb{C}$. We can fix ambiguities in expressing $P(x)$ in the form (6.10) caused by symmetries of (6.1) [namely $\eta_i(\alpha,\beta)=(-1)^i\eta_i(\alpha,-\beta)$], by the following rule inthe choice of the parameter s: when $s=q^a$, with $a\in\mathbb{Z}$ we require $a\leqslant 0$; when $a\in 1/2+\mathbb{Z}$, we ask $a\leqslant 1/2$; when $a\notin 1/2\mathbb{Z}$ we require that $\mathrm{Im}\,a>0$ if $\mathrm{Im}\,a\neq 0$, or $a>1$ if $a\in\mathbb{R}$, where Im denote the imaginary part of a complex number and [ ] denote the closest integer to the number which is not larger than itself.

Now, we decompose the set $\{s \in \mathbb{C} | a_{s,i} \neq 0 \text{ for some } i\}$ into a disjoint union of equivalence classes S under the relation

$$s = q^a \sim s' = q^{a'} \quad \text{if and only if } a - a' \in \mathbb{Z} + \tau^{-1}\mathbb{Z},$$

Then, we choose a representative s of each equivalence class S such that $s=q$ if a lies in $\mathbb{Z}$ and $s=q^{1/2}$ if a lies in $\mathbb{Z}+1/2$. Let $S=\{s=q^a, s_1=q^{a+k_1}, s_2=q^{a+k_2}, \ldots\}$. Take $k_0=0$ and $m=\max_{s\in S} m_s$. It is easy to see by the rules in picking the parameter s that if $a=1$ or $1/2$, then $k_i \in \mathbb{N}$.

Now, we attach to S a $\mathfrak{g}^{[m]}$-module $L_s^{[m]}(\lambda_S)$ in one of the following ways.

If $a \notin \mathbb{Z}/2$, let ${}^a h_{k_r}^{(i)} = a_{s+k_r,i}(\log q)^i$ with $i=0,\ldots,m_s$ and $r=0,1,2,\ldots$. We associate to S the $\widehat{g\ell}_\infty^{[m]}$-module $L_s^{[m]}(\lambda_S)$ with central charges and labels

$$c_i = \sum_{k_r} {}^a h_{k_r}^{(i)}, \quad {}^a\lambda_j^{(i)} = \sum_{k_r \geqslant j} {}^a\widetilde{h}_{k_r}^{(i)},$$

where ${}^a\widetilde{h}_k^{(i)} = {}^a h_k^{(i)} - c_i \delta_{k,0}$.

If $a=1/2$ let ${}^b h_{k_r}^{(i)} = a_{s+k_r,i}(\log q)^i$ with $i=0,\ldots,m_{q^{1/2}}$ and $r=0,1,2,\ldots$. We associate to S the $b_\infty^{[m]}$-module $L_s^{[m]}(\lambda_S)$ with central charges and labels

$$c_i = \sum_{k_r} {}^b h_{k_r}^{(i)}, \quad (i \text{ even}), \quad c_i = 0, \quad (i \text{ odd}),$$

$${}^b\lambda_j^{(i)} = \sum_{k_r \geqslant j} {}^b h_{k_r}^{(i)}, \quad {}^b\lambda_0^{(i)} = \sum_{k_r \geqslant 0} {}^b h_{k_r}^{(i)} \quad (i \text{ odd}),$$

where $j \in \mathbb{N}$ and $i=0,\ldots,m_{q^{1/2}}$.

If $a=1$ and $\epsilon=-1$, let ${}^c h_{k_r}^{(i)} = a_{s+k_r,i}(\log q)^i$ with $j=0,\ldots,m_q$ and $r=0,1,2,\ldots$. We associate to S the $c_\infty^{[m]}$-module $L_s^{[m]}(\lambda_S)$ with central charges and labels

$$c_i = \sum_{k_r} {}^c h_{k_r}^{(i)} \quad (i \text{ even}), \quad c_i = 0 \quad (i \text{ odd}),$$

$${}^c\lambda_j^{(i)} = \sum_{k_r \geqslant j} {}^c h_{k_r}^{(i)},$$

where $j \in \mathbb{N}$ and $i=0,\ldots,m_q$. If $a=1$ and $\epsilon=1$, let ${}^c h_{k_r}^{(i)} = a_{s+k_r,i}(\log q)^i$ with $j=0,\ldots,m_1$ and $r=0,1,2,\ldots$. We associate to S the $d_\infty^{[m]}$-module $L_s^{[m]}(\lambda_S)$ with central charges and labels

$$c_i = \sum_{k_r} {}^d h_{k_r}^{(i)} \quad (i \text{ even}), \quad c_i = 0 \quad (i \text{ odd}),$$

$${}^d\lambda_j^{(i)} = \sum_{k_r \leqslant i} {}^d h_{k_r}^{(i)},$$

where $j \in \mathbb{N}$ and $i=0,\ldots,m_1$.

Denote by $\{s_1, s_2, \ldots, s_N\}$ a set of representatives of the equivalence classes in the set $\{s \in \mathbb{C} | a_{s,j} \neq 0 \text{ for some } j\}$. Theorem 6.3, the $\widehat{\mathcal{S}_q^{k,\epsilon}}$-module $L_{\mathbf{s}}^{[\mathbf{m}],k,\epsilon}(\lambda)$ is irreducible for $\mathbf{s}=(s_1,\ldots,s_N)$ satisfying the "condition." Then by the above discussion, Theorem 6.3, and Propositions 6.4–6.6 we have proved the following.

Theorem 6.7: *Let V be an irreducible quasifinite highest weight $\widehat{\mathcal{S}_q^{k,\epsilon}}$-module with central charge c and let $P(x)$ be the quasipolynomial given by Theorem 4.7 written in the form (6.10). Then V is isomorphic to the tensor product of the modules $L_s^{[m],k,\epsilon}(\lambda_S)$ with distinct equivalence classes S.*

Remark 6.8: A different choice of representatives $s=q^a$ with $a \notin \mathbb{Z}/2$ in the equivalence class

S has the effect of shifting $\widehat{g\ell}_{\infty}^{[m]}$ via the automorphism ν^i for some i. It is not difficult to see that any irreducible quasifinite highest weight module $L(\widehat{\mathcal{S}_q^{k,\epsilon}}, \zeta)$ can be obtained as above in an essentially unique way up to this shift.

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Erratum: "The use of so(2,1) algebra for the evaluation of atomic integrals: The study of two-electron atoms" [J. Math. Phys. 45, 2674 (2004)]

J. Zamastil, J. Čížek, M. Kalhous, L. Skála, and M. Šimánek
Department of Applied Mathematics, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada and Department of Chemical Physics and Optics, Charles University, Faculty of Mathematics and Physics, Ke Karlovu 3, 121 16 Prague 2, Czech Republic

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Equation (43) should read

$$c^{l_i,l_j}_{n_i,n_j,n} = C^{l_i,l_j}_{n_i,n_j,n} - \frac{n_i + n_j - l_i - l_j - 2 - n}{n_i + n_j + l_i + l_j - n - 1} C^{l_i,l_j}_{n_i,n_j,n+1}.$$

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Inversion time of large spins

Ekatherina A. Karatsuba
Computer Centre of RAS, ul. Vavilova 40, Moscow 119991, Russia

Paolo Moretti[a)]
"Istituto dei Sistemi Complessi" del C.N.R., Sezione di Firenze, Via Panciatichi, 64 - 50127 Florence, Italy

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In order to find an accurate expression for the inversion probability of a large spin, an asymptotic expansion in series of Bessel functions is found, and a formula for the inversion time is obtained. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1860593]

I. INTRODUCTION

Spin dynamics plays a very important role in the study of molecular magnetic clusters. In particular, if Mössbauer spectroscopy is used, the inversion time of the spin is one of the most important parameters in the structure of the experimental spectra.[1] In a pictorial, intuitive description, as the total electronic spin of the surrounding neighbors inverts its direction, the magnetic field on the iron nucleus also changes. Thus, the nuclear energy levels are modified and we are in the presence of the "Mössbauer relaxation spectrum," with a structure that depends on the frequency of the inversion.[2]

In Ref. 3 the coefficient $|b_n(t)|^2$, which gives the probability of finding the system in the nth spin state, has been calculated and it is found to be a somewhat involute trigonometric sum. An approximate expression for $b_n(t)$ by means of the corresponding Bessel functions was obtained only if $n \ll N$, $\alpha t \ll N$ (N is the total number of spin states, α is a parameter), since the trigonometric sum which runs through all the spin states can be replaced by an integral in a careful way only in this case. Using a heuristic argumentation, this form has been assumed to be valid also for $n=N$, which corresponds to the transition from spin-up to spin-down, and the inversion time has been calculated in this way. It is given by the first maximum of $|b_N(t)|^2$. However, due to the important role of the inversion time, which connects the theory with the experimental spectra, a better calculation is in order, thus justifying in a strict way the approach used in Ref. 3.

In this paper a new formula for the probability amplitude $b_N(t)$, for $N \geqslant 2$ and for any t, is obtained. This exact expression in terms of the Bessel functions with large indexes allows the effective computation of $b_N(t)$ with increasing accuracy (see Fig. 1 in Sec. III).

An asymptotically exact expression is obtained for the spin inversion time. An application of this useful formula is shown in the example of the Fe8 cluster.

II. POSITION OF THE PROBLEM

The Hamiltonian of our system, which involves an entire spin S, has the form: $H=H_0+V$, where H_0 is a static Hamiltonian (e.g., a magnetic field) and V is the term responsible for the transitions between spin states.

Starting from the discrete set of the $N(N=2S+1)$ spin eigenstates $|n\rangle$ of H_0 with energies E_n, we can write the wave function as

a)Electronic mail: p.moretti@ifac.cnr.it

$$\psi(t) = \sum_{n=1}^{N} a_n(t)|n\rangle \exp(-iE_n t/\hbar). \tag{1}$$

From the Schrödinger equation, the coefficients $a_n(t)$ result:

$$i\hbar \dot{a}_n(t) = \sum_{l=1}^{N} a_l(t) V_{nl} \exp(i\omega_{nl} t), \quad \omega_{nl} = \frac{E_n - E_l}{\hbar}. \tag{2}$$

Some simplifications are in order. First, we can assume that V connects only neighboring states, and does not have diagonal elements; moreover, $|\omega_{n,n\pm1}| = \omega$, independent of n, and $V^*_{n,n+1} = V_{n,n-1} = k$.

The initial conditions of interest are

$$a_1(0) = 1,$$

$$a_n(0) = 0, \quad n = 2,3,\ldots,N,$$

which correspond to the spin up (or down).

The substitution

$$b_n(t) = a_n(t) \mathrm{e}^{-in\omega t} \tag{3}$$

leads to a set of equations that can be solved by Laplace transform. By considering $n = N$, namely the probability amplitude of the spin inversion, the following result can be obtained:

$$b_N(t) = -2\frac{(-1)^N}{N+1} \sum_{s=1}^{N} \sin\frac{s\pi}{N+1} \sin\frac{Ns\pi}{N+1} \exp\left(2\pi i\beta \cos\frac{s\pi}{N+1}\right), \tag{4}$$

where

$$\beta = \frac{kt}{\pi\hbar} = \alpha\frac{t}{2\pi}, \quad \alpha = \frac{2k}{\hbar}. \tag{5}$$

This equation works for small values of ω; more precisely, if in the full calculation an expansion up to the first order in ω is performed, the coefficient b_N is again given by (4) within a phase factor only.[3]

III. THE ASYMPTOTIC EXPANSION OF b_N

The aim of the present work is to study the function $b_N(t)$ where $N \geqslant 2$.

Theorem: *For $b_N(t)$ holds the formula:*

$$b_N(t) = (-1)^N \frac{2}{\alpha t} \sum_{\nu=1}^{+\infty} i^{(N+1)(2\nu-1)} \{[(N+1)(2\nu-1) - 1] J_{(N+1)(2\nu-1)-1}(\alpha t) + [(N+1)(2\nu-1) + 1] J_{(N+1)(2\nu-1)+1}(\alpha t)\}, \quad N \geqslant 2.$$

To prove the theorem it is necessary to prove three lemmas.

Lemma 1: The following relation is valid for $b_N(t)$:

$$b_N(t) = \frac{(-1)^N}{2(N+1)} [S_1 - S_2 - (S_3 - S_4)],$$

where

$$S_1 = \sum_{j=1}^{N+1} \exp\left[2\pi i\left(\frac{2j-1}{N+1} + \beta\cos\frac{(2j-1)\pi}{N+1}\right)\right],$$

$$S_2 = \sum_{j=1}^{N+1} \exp\left[2\pi i\left(\frac{2j}{N+1} + \beta\cos\frac{2j\pi}{N+1}\right)\right],$$

$$S_3 = \sum_{j=1}^{N+1} \exp\left[2\pi i\beta\cos\frac{(2j-1)\pi}{N+1}\right],$$

$$S_4 = \sum_{j=1}^{N+1} \exp\left(2\pi i\beta\cos\frac{2j\pi}{N+1}\right).$$

Proof: First, one easily verifies that

$$2b_N(t) = -2\frac{(-1)^N}{N+1}\sum_{s=1}^{2(N+1)} \sin\frac{s\pi}{N+1}\sin\frac{Ns\pi}{N+1}\exp\left(2\pi i\beta\cos\frac{s\pi}{N+1}\right),$$

and after straightforward calculations we obtain that

$$b_N(t) = \frac{(-1)^N}{4(N+1)}\sum_{s=1}^{2(N+1)} (-1)^{s+1}\left\{\exp\left[2\pi i\left(\frac{s}{N+1} + \beta\cos\frac{s\pi}{N+1}\right)\right]\right.$$
$$\left. + \exp\left[-2\pi i\left(\frac{s}{N+1} - \beta\cos\frac{s\pi}{N+1}\right)\right] - 2\exp\left[2\pi i\beta\cos\frac{s\pi}{N+1}\right]\right\}. \tag{6}$$

Since the function

$$(-1)^{s+1}\exp\left[2\pi i\left(\frac{s}{N+1} + \beta\cos\frac{s\pi}{N+1}\right)\right]$$

is periodic in s, with the period $2(N+1)$,

$$\sum_{s=1}^{2(N+1)} (-1)^{s+1}\exp\left[2\pi i\left(\frac{s}{N+1} + \beta\cos\frac{s\pi}{N+1}\right)\right] = \sum_{s=1}^{2(N+1)} (-1)^{s+1}\exp\left[-2\pi i\left(\frac{s}{N+1} - \beta\cos\frac{s\pi}{N+1}\right)\right],$$

and therefore

$$b_N(t) = \frac{(-1)^N}{2(N+1)}\sum_{s=1}^{2(N+1)} (-1)^{s+1}\left\{\exp\left[2\pi i\left(\frac{s}{N+1} + \beta\cos\frac{s\pi}{N+1}\right)\right] - \exp\left[2\pi i\beta\cos\frac{s\pi}{N+1}\right]\right\}. \tag{7}$$

We represent (7) in the form of the sum of two sums, one over odd s: $s=2j-1$; $j=1,2,3,\ldots,N+1$; another one over even s: $s=2j$; $j=1,2,3,\ldots,N+1$. From here we have the statement of the lemma.

We consider the function

$$f(x) = e^{2\pi i\beta\cos 2\pi x}, \tag{8}$$

which is a periodic function with the period 1. We expand $f(x)$ as a Fourier series

$$f(x) = \sum_{k=-\infty}^{+\infty} c(k) e^{2\pi i k x}, \tag{9}$$

with the coefficients

$$c(k) = \int_0^1 f(x) e^{-2\pi i k x} \mathrm{d}x = 2 \int_0^{1/2} e^{2\pi i \beta \cos 2\pi x} \cos 2\pi k x \, \mathrm{d}x. \tag{10}$$

Lemma 2: *For* $|k| > 0$, *the following estimate is valid:*

$$|c(k)| \leqslant \frac{(2\pi\beta)^2 + 2\pi|\beta|}{k^2},$$

and, in particular, the Fourier series for the function $f(x)$ *converges absolutely.*

Proof: From (10), $c(k) = c(-k)$. For $k \neq 0$, we find

$$c(k) = \int_0^1 f(x) \frac{\mathrm{d}e^{-2\pi i k x}}{-2\pi i k} = \frac{1}{(2\pi i k)^2} \int_0^1 f''(x) e^{-2\pi i k x} \mathrm{d}x,$$

$$|c(k)| \leqslant \frac{1}{(2\pi k)^2} \int_0^1 |f''(x)| \mathrm{d}x \leqslant \frac{1}{(2\pi k)^2} \max_{0 \leqslant x \leqslant 1} |f''(x)|.$$

Since from (8)

$$f''(x) = -16\pi^4 \beta^2 \sin^2 2\pi x e^{2\pi i \beta \cos 2\pi x} - 8\pi^3 i \beta \cos 2\pi x e^{2\pi i \beta \cos 2\pi x},$$

then

$$|f''(x)| \leqslant (2\pi)^4 \beta^2 + (2\pi)^3 |\beta|.$$

From here we have the statement of the lemma.

Lemma 3: *Assume that* M *and* m *are integers,* $M > 1$, $0 \leqslant m \leqslant M$; *the sums* A *and* B *are defined by the equalities:*

$$A = \sum_{j=1}^{M} \exp\left[2\pi i \left(\frac{m}{M} \left(j - \frac{1}{2} \right) + \beta \cos 2\pi \frac{\left(j - \frac{1}{2} \right)}{M} \right) \right],$$

$$B = \sum_{j=1}^{M} \exp\left[2\pi i \left(\frac{m}{M} j + \beta \cos 2\pi \frac{j}{M} \right) \right].$$

Then the following relations hold:

$$A = M \sum_{r=-\infty}^{+\infty} (-1)^r c(rM - m),$$

$$B = M \sum_{r=-\infty}^{+\infty} c(rM - m),$$

where $c(k)$ *are the Fourier coefficients of the function* $f(x) = e^{2\pi i \beta \cos 2\pi x}$.

Proof: Representing the factor $e^{2\pi i \beta \cos 2\pi x}$ of each summand of the sums A and B in the form of the Fourier series, we find

$$A=\sum_{j=1}^{M}\exp\left[2\pi i\frac{m}{M}\left(j-\frac{1}{2}\right)\right]\sum_{k=-\infty}^{+\infty}c(k)\exp\left(2\pi i\frac{j-\frac{1}{2}}{M}k\right)=\sum_{k=-\infty}^{+\infty}c(k)\sum_{j=1}^{M}\exp\left[2\pi i\frac{m+k}{M}\left(j-\frac{1}{2}\right)\right], \tag{11}$$

$$B=\sum_{j=1}^{M}\exp\left(2\pi i\frac{m}{M}j\right)\sum_{k=-\infty}^{+\infty}c(k)\exp\left(2\pi i\frac{j}{M}k\right)=\sum_{k=-\infty}^{+\infty}c(k)\sum_{j=1}^{M}\exp\left(2\pi i\frac{m+k}{M}j\right). \tag{12}$$

Since

$$\sum_{j=1}^{M}\exp\left[2\pi i\frac{m+k}{M}\left(j-\frac{1}{2}\right)\right]=\begin{cases}(-1)^{r}M & \text{if } m+k=rM, r \text{ is an integer}, -\infty<r<+\infty\\ 0 & \text{if } m+k \text{ is not a multiple of } M,\end{cases}$$

$$\sum_{j=1}^{M}\exp\left(2\pi i\frac{m+k}{M}j\right)=\begin{cases}M & \text{if } m+k=rM, r \text{ is an integer}, -\infty<r<+\infty\\ 0 & \text{if } m+k \text{ is not a multiple of } M,\end{cases}$$

then we have from (11) and (12), respectively,

$$A=M\sum_{r=-\infty}^{+\infty}(-1)^{r}c(rM-m),$$

$$B=M\sum_{r=-\infty}^{+\infty}c(rM-m).$$

The lemma is proved.

Corollary 1: From lemma 1 and lemma 3 we obtain that

$$b_N(t)=(-1)^{N+1}\sum_{\nu=1}^{+\infty}\{c[(N+1)(2\nu-1)-2]+c[(N+1)(2\nu-1)+2]-2c[(N+1)(2\nu-1)]\}. \tag{13}$$

Proof of the theorem: The terms of this series, the functions $c(k)$, are defined by the integrals (10) and can be transformed into a convenient form. By making the change of variable of integration $y=2\pi x$, $\varphi=y-\pi/2$, in (10), we obtain

$$c(k)=\frac{1}{\pi}\int_0^{\pi}e^{i\alpha t\cos y}\cos ky\,\mathrm{d}y=\frac{i^k}{2\pi}\int_0^{2\pi}e^{i(k\varphi-\alpha t\sin\varphi)}\mathrm{d}\varphi,$$

$\alpha=2\pi\beta/t$.

The integral

$$J_k(\alpha t)=\frac{1}{2\pi}\int_0^{2\pi}e^{i(k\varphi-\alpha t\sin\varphi)}\mathrm{d}\varphi \tag{14}$$

is the Bessel function of the kth order; using well-known recurrence formulas,[4] we represent the series (13) in the form

$$b_N(t)=(-1)^{N}\frac{2}{\alpha t}\sum_{\nu=1}^{+\infty}i^{(N+1)(2\nu-1)}\{[(N+1)(2\nu-1)-1]J_{(N+1)(2\nu-1)-1}(\alpha t)+[(N+1)(2\nu-1)+1]J_{(N+1)(2\nu-1)+1}(\alpha t)\},\quad N\geqslant 2. \tag{15}$$

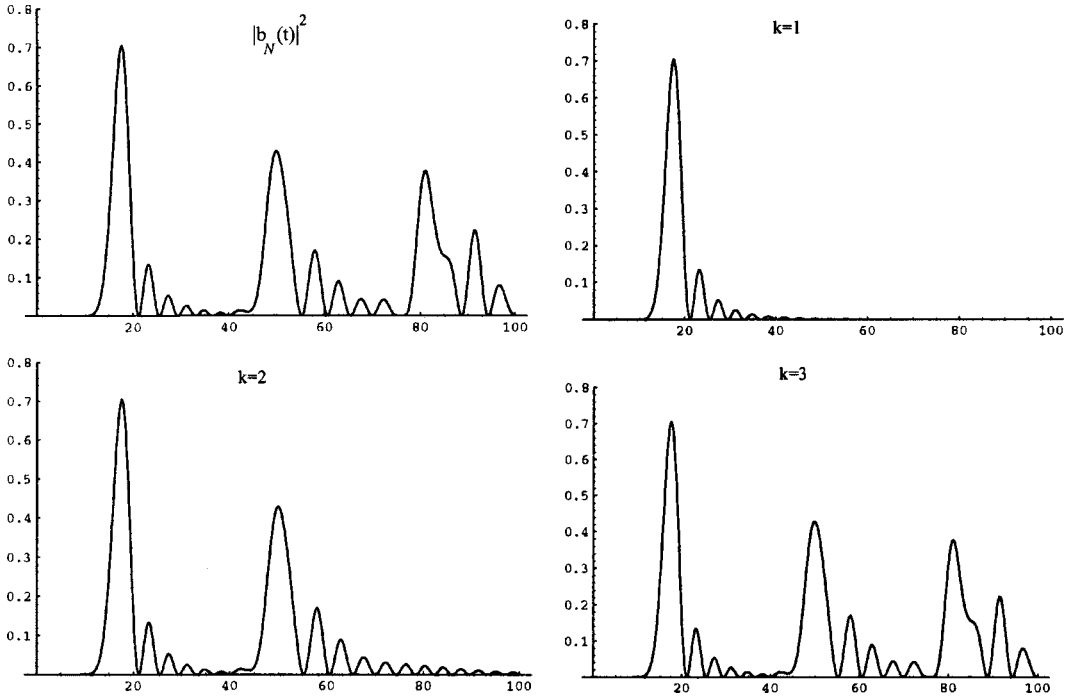

FIG. 1. The value of $|b_N(t)|^2 (N=15, \alpha=1)$ as given by (4), and by approximation (16), with $k=1, 2, 3$.

The theorem is proved.

Remark: Since $J_\nu(\alpha t)$ decreases exponentially as ν increases, and in (15) the summing is over ν, belonging to an arithmetic progression with the difference $2(N+1)$, then the first summands of the sum (15) give already a very good approximation to $b_N(t)$.

Let $k \geqslant 1$, and

$$b_N^{(k)}(t) = (-1)^N \frac{2}{\alpha t} \sum_{\nu=1}^{k} i^{(N+1)(2\nu-1)} \{[(N+1)(2\nu-1)-1] J_{(N+1)(2\nu-1)-1}(\alpha t) + [(N+1)(2\nu-1) + 1] J_{(N+1)(2\nu-1)+1}(\alpha t)\}, \quad N \geqslant 2. \tag{16}$$

We note at once that, also stopping to $k=1$, the result is very satisfactory up to the first maximum, and the expression used in Ref. 3, with a single Bessel function, is improved significantly. This is shown in Fig. 1 for a typical value $N=15$.

IV. CALCULATION OF THE INVERSION TIME

Since function (16) reproduces the behavior of $b_N(\alpha t)$ very well also for $k=1$ in the range of interest, we use this approximate form to find the position of the first maximum of its squared modulus, which gives the inversion time. This maximum corresponds to the first zero of $d/d\tau[b_N^{(1)}(\alpha t)]$, and is given by the equation $(\tau = \alpha t)$

$$0 = \frac{\mathrm{d}}{\mathrm{d}\tau}\left[N\frac{J_N(\tau)}{\tau} + (N+2)\frac{J_{N+2}(\tau)}{\tau} \right] = \frac{\mathrm{d}}{\mathrm{d}\tau}\left[\frac{2N(N+1)}{\tau} J_{N+1}(\tau) + 2J_{N+2}(\tau) \right]$$

and since[4]

$$\frac{\mathrm{d}}{\mathrm{d}\tau} J_{N+2}(\tau) = J_{N+1}(\tau) - \frac{N+2}{\tau} J_{N+2}(\tau),$$

$$J_{N+2}(\tau) = -\frac{\mathrm{d}}{\mathrm{d}\tau}J_{N+1}(\tau) + \frac{N+1}{\tau}J_{N+1}(\tau),$$

we eventually obtain

$$0 = \frac{\mathrm{d}\ J_{N+1}(\tau)}{\mathrm{d}\tau} - \frac{J_{N+1}(\tau)}{\tau}\left[\frac{2N(N+1)+(N+3)(N+1)-\tau^2}{N^2+2N+3}\right] \tag{17}$$

as can easily be verified. By expanding in the neighborhood of the first zero of $\mathrm{d}/\mathrm{d}\tau[J_{N+1}]$, as given by Abramowitz,[5] a straightforward calculation leads to the result

$$\overline{\tau} = N + 1 + 0.8N^{1/3} - 1.16N^{-1/3} + O(N^{-2/3}). \tag{18}$$

V. CONCLUSIONS

The difference between expression (18) and that of Ref. 3, for a typical value of $N \sim 10-20$, is remarkable. With reference to the Fe8 cluster,[6] the value of the experimental parameter (k/D), where D is the anisotropy constant, is found to be about 0.22, less than the value 0.25 given in Ref. 3. It is, therefore, closer to the experimental value 0.16, thus confirming that a precise determination of the inversion time is of fundamental importance in correlating the structure of Mössbauer spectra to the spin Hamiltonian parameters.

We would like to stress that in this system the inversion takes place by means of jumps between the degenerate lowest doublets, and therefore the use of formulas (4) and (18) is well justified. The accurate asymptotic formula (18) would be useless, in the presence of an indeterminate error due to a large value of ω.

An even better calculation can be worked out by observing that, in many cases, the spin states are degenerate in energy only to a first approximation. As indicated in Ref. 3, a full investigation taking into account the energy differences leads to the Laplace transform of Lommel's polynomials, and work is in progress in this direction.

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Quantum kinematics of bosonic vortex loops

Gerald A. Goldin[a)]
Departments of Mathematics and Physics, Rutgers University, SERC Building, Piscataway, New Jersey 08854

Robert Owczarek[b)]
Nuclear Waste and Infrastructure Services Division, Los Alamos National Laboratory, MS J 594, Los Alamos, New Mexico 87544

David H. Sharp[c)]
Applied Physics Division, Theoretical Division, Los Alamos National Laboratory, MS B213, Los Alamos, New Mexico 87545

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In the framework of geometric quantization, filaments of vorticity in a two-dimensional, ideal incompressible superfluid belong to certain coadjoint orbits of the group of area-preserving diffeomorphisms. The Poisson structure for such vortex strings is analyzed in detail. While the Lie algebra associated with area-preserving diffeomorphisms is noncanonical, we can nevertheless find canonical coordinates and their conjugate momenta that describe these systems. We then introduce a Fock-like space of quantum states for the simplest case of bosonic vortex loops, with natural, nonlocal creation and annihilation operators for the quantized vortex filaments. © *2005 American Institute of Physics.*
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I. INTRODUCTION

In this paper we discuss quantized vortex filaments—open or closed strings of vorticity—in the context of a model of an incompressible, inviscid fluid. Vortices are excitations descriptive of the collective motion of the fluid. Such collective coordinates have played an essential role in understanding a variety of quantum many-body systems, of which superfluids are a prominent example.

Quantized vortex configurations in two or three spatial dimensions can be described by means of unitary representations of the group $G=S\,\mathrm{Diff}(\mathbf{R}^n)$, for $n=2$ or 3. Here G is the group (under composition) of area- or volume-preserving diffeomorphisms of the plane or of three-space, respectively, where the diffeomorphisms are compactly supported or become rapidly trivial at infinity. To exploit the full physical content of the representation theory, we would like to have a description that makes use of the ideas associated with canonical creation and annihilation operators in Fock space. Here we take some important steps in this direction, writing canonically conjugate coordinates to describe filaments of vorticity in an idealized thin planar film of fluid, and introducing a Fock-like space of states, with creation and annihilation field operators, to describe bosonic vortex loops.

Knowledge of the symmetry group of a classical system generally permits use of some variant of geometric quantization, where the Hilbert space of quantum states carries an appropriate unitary, irreducible representation of the symmetry group. Thus we construct the quantized vortices so

[a)]Electronic mail: gagoldin@dimacs.rutgers.edu
[b)]On leave from Institute of Fundamental Technological Research, Polish Academy of Sciences, Świetokrzyska 21, 00-049 Warsaw, Poland. Electronic mail: rmo@lanl.gov
[c)]Electronic mail: dhs@lanl.gov

as to respect the classical symmetry of the fluid. The configuration space for the fluid can be identified with the underlying manifold of G, and the symmetry is also described by G, acting on its own group manifold by left multiplication.

Unitary representations are obtained from coadjoint orbits or families of orbits, which serve as reduced phase spaces for the classical system. For $n=2$ we consider the Poisson structure on those coadjoint orbits of G that are associated with filaments of vorticity. Ordinarily the description is noncanonical. However, using a coordinatization intrinsic to the filaments themselves, we are able to write canonically conjugate coordinates for the coadjoint orbits. These turn out to be the position $\Gamma(s)$ of the filament in $\mathbf{R}^2$, parametrized by its own arc length s, and the *cumulative vorticity* function $\tilde{\gamma}(s)$ along the filament.

We next introduce a Fock-like space for bosonic vortex loops. The arguments of the field operators are extended configurations (unparametrized loops), so that the operators are, in a sense, nonlocal. Our formal construction also assumes the existence of a suitable measure on the space of unparametrized loops. We show that the desired measure for systems of loops (i.e., multiloop configurations) should satisfy a multiplicative property with respect to the creation of new loops, in order to yield an appropriate hierarchy of unitary group representations. We give some simple prescriptions for constructing such measures from single-loop measures.

Section II briefly surveys some related research. In Sec. III we review the symplectic structure on coadjoint orbits of diffeomorphism groups, establish notation, and discuss the Poisson structure on coadjoint orbits associated with vortex filaments. Section IV introduces the formal construction of the Fock space, while Sec. V contains conclusions and suggestions for future research directions.

II. BACKGROUND

The diffeomorphism group $G=S\,\mathrm{Diff}(\mathbf{R}^n)$ is taken as the classical symmetry group of an ideal, incompressible fluid by Arnold.[1] Marsden and Weinstein[2] consider coadjoint orbits with point vortices (for $n=2$). We refer to the book by Arnold and Khesin,[3] and references therein.

Goldin, Menikoff, and Sharp examine the quantizability of particular vortex structures from the point of view of geometric quantization on coadjoint orbits.[4,5] They demonstrate that not all the coadjoint orbits of G permit quantization, in the sense of obtaining an irreducible, unitary representation of G. A necessary condition is existence of a polarization which, roughly speaking, encodes the uncertainy principle. It expresses the condition that the coordinates of the orbit (regarded as a reduced, classical phase space) can be partitioned into some maximal set of "configuration space" variables together with another set of "momentum" variables. When a polarization is found, the quantum states can be written as functions of configuration space coordinates only.

For point vortices in two dimensions, and one-dimensional vortex filaments in three dimensions, the requisite polarizations do not exist. However, polarizations do exist for coadjoint orbits containing vortex dipoles, loops (closed strings), and arcs (open strings) in the plane, and for orbits containing vortex ribbons and tubes in three-space.

Owczarek[6,7] obtains similar results in three dimensions using an approach based formally on a field theoretic interpretation of knot theory,[8,9] proposed by Peradzyński.[10] He also discusses the role of topological degrees of freedom for knotted and linked vortices in the thermodynamics of critical superfluid helium,[11] as anticipated in Ref. 5. Brylinski[12] studies the symplectic structure on orbits associated with vortex filaments in three dimensions, noting too that vortex ribbons are better suited for quantization than vortex filaments. He proves that vortex ribbons describe Lagrange manifolds with respect to the standard symplectic structure, remarking that this could be a starting point for geometric quantization. Penna and Spera[13] reconstruct the Poisson structure that generates Hamiltonian dynamics for vortex filaments, within the current algebra framework used here, as a limit of the standard brackets for smooth velocity fields. They also discuss differences between this framework and the canonical quantization of point vortices.

The geometric ideas we use also underlie the so-named α-Euler equation,[14–18] which can be understood as an averaged Euler equation—or, in more functional analytic terms, an H^1-Euler

equation in contrast to the standard L^2-Euler equation. The latter terminology is associated with the variational derivation of the equations. Recall that the elements of the Lie algebra of G are divergenceless velocity fields. Taking the L^2-norm on the space of velocity fields, one obtains the standard Euler equation by variation of this norm with respect to the velocity field. Taking the H^1-norm instead, one obtains the α-Euler equation by the analogous variational procedure. In defining the H^1-norm, one must introduce a constant factor with the dimension of length (which is where α comes into play). One motivation for the modified theory is to achieve greater stability by filtering out short-wavelength modes from the system. The interesting feature of this approach for us is that the diffeomorphism invariance is not destroyed by this change. The geometric framework of Shkoller, Marsden, and Ratiu[19,20] may be as valuable for quantization of vortex solutions to α-Euler equations as the earlier Marsden–Weinstein work[2] is for quantum vortices in the standard Euler fluid.

Questions similar to those addressed in the present paper about the quantum kinematics of vortex filaments are already answered for systems of nonrelativistic, quantum point particles, which are classified by the unitary representations of the group Diff ($\mathbf{R}^n$) of (not necessarily volume-preserving) diffeomorphisms.[21,22] In particular Goldin, Menikoff, and Sharp predict "anyons," particles obeying intermediate statistics modeled on the braid group, using this approach,[22] confirming an earlier idea of Leinaas and Myrheim.[23] More recently Goldin and Sharp propose a general construction of creation and annihilation field operators as intertwining operators in a hierarchy of unitary representations of the diffeomorphism group. For the case of anyons they construct such field operators explicitly, showing how q-commutation rules enter for the operators without having been assumed from the outset.[24] We adopt the same spirit here in our Fock space construction, but for ease of discussion we treat only the bosonic case. We expect to be able to generalize our results to anyonic statistics for systems of planar vortex loops and filaments.

The above-mentioned facts regarding the quantizability of certain vortex structures highlight the possibility of interesting effects on the quantum level associated with the more complicated topology of vortex configuration spaces. Thus there can be "internal statistics" for individual, two-dimensional vortex loops, and effects associated with twistedness, knottedness, and linkedness of vortex ribbons in three dimensions.

Speliotopoulos constructs creation and annihilation operators for vortices in superfluid helium with a heuristic approach that starts from a rule for quantization of vorticity.[25] Treating the vortices as point-like excitations, he postulates an approximate bilinear one-vortex Hamiltonian $H=\epsilon c^* c$, where c^* and c are one-vortex creation and annihilation operators. To avoid singularities in the corresponding wave function, he then modifies the creation and annihilation operators in a way that he interprets as a transition from point vortices to vortex patches. However the vortex patches are homogeneous, and in our framework are also not susceptible to geometric quantization.[4]

Taking coadjoint orbits that allow polarizations, the unitarity of the resulting representations of G further depends on having measures on the configuration space that are quasi-invariant under G. Construction of such measures is difficult, but not essential for our present results on the kinematics of such systems. However, we expect the details to be very important to quantum dynamics. Some ideas regarding properties of measures appropriate to the description of quantum vortices are given in Ref. 26. Related questions about measures are discussed by Ismagilov[27] and Goldin and Moschella;[28,29] a mathematical construction of such measures is proposed by Shavgulidze.[30]

III. POISSON STRUCTURE FOR VORTEX FILAMENTS IN R^2

A. Symplectic structure on coadjoint orbits of diffeomorphism groups

The present notation is a compromise between that used in our previous publications, and the notation of the textbook by Arnold and Khesin.[3] We begin with the general formula for the

Kirillov–Kostant–Souriau (KKS) symplectic structure on coadjoint orbits of a Lie group G. We then take G to be $S\,\mathrm{Diff}(\mathbf{R}^n)$, with $n=2$ or 3 as needed for discussing incompressible hydrodynamics.

Let $\mathcal{G}$ be the Lie algebra of G and $\mathcal{G}^*$ be its dual, with the pairing $\langle\cdot,\cdot\rangle$ mapping $\mathcal{G}^*\times\mathcal{G}\to\mathbf{R}$. Let $[\cdot,\cdot]$ denote the bracket in $\mathcal{G}$. For finite-dimensional groups $\mathcal{G}^*$ is isomorphic as a vector space to $\mathcal{G}$, while if G is an infinite-dimensional group of the sort we consider, then $\mathcal{G}^*$ is in a sense larger than $\mathcal{G}$; they are no longer isomorphic. Denote left translation in G by $L_g(h)=gh$, right translation by $R_g(h)=hg$, and the adjoint action $R_{g^{-1}}\circ L_g$ by $\mathrm{Ad}_g: G\to G$ (where $\circ$ denotes composition); Ad_g (like L_g) is a left action on G.

Given a manifold M and $F: M\to M$, its derivative at the point $x\in M$ is a linear operator $F_*|_x$ from T_xM to $T_{F(x)}M$. The derivative of Ad_g at the identity $e\in G$ is the adjoint representation of G acting in $\mathcal{G}$, denoted also as Ad_g. For $\xi\in\mathcal{G}$, we write

$$\mathrm{ad}_\xi = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \mathrm{Ad}_{g(t)},$$

where $g(t)$ is a curve in G with $g(0)=e$ and

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} g(t) = \xi;$$

then $[\xi,\eta]=\mathrm{ad}_\xi\eta$.

Define the coadjoint representation of $\mathcal{G}$ acting in $\mathcal{G}^*$, for $\xi,\eta\in\mathcal{G}$ and $\mu\in\mathcal{G}^*$, by

$$\langle \mathrm{coad}_\xi\mu,\eta\rangle = \langle \mathrm{ad}^*_\xi\mu,\eta\rangle = \langle \mu,\mathrm{ad}_\xi\eta\rangle = \langle \mu,[\xi,\eta]\rangle. \tag{1}$$

This is the infinitesimal version of the coadjoint representation of G on $\mathcal{G}^*$,

$$\langle \mathrm{Ad}^*_g(\mu),\xi\rangle = \langle \mu,\mathrm{Ad}_g\xi\rangle, \tag{2}$$

which is a right action: $\langle \mathrm{Ad}^*_{g_1g_2}\mu,\xi\rangle = \langle (\mathrm{Ad}^*_{g_2}\circ\mathrm{Ad}^*_{g_1})(\mu),\xi\rangle$. For $\mu\in\mathcal{G}^*$, the coadjoint orbit containing μ is the set $\mathcal{O}_\mu := \{\mathrm{Ad}^*_g(\mu): g\in G\}$. Given an element $\xi\in\mathcal{G}$, the coadjoint representation of G associates to it a vector field $\xi_{\mathcal{G}^*}$ on $\mathcal{O}_\mu$. The KKS symplectic form on $\mathcal{O}_\mu$ is given by

$$\Omega_\mu(\xi_{\mathcal{G}^*}(\mu),\eta_{\mathcal{G}^*}(\mu)) := \langle \mu,[\xi,\eta]\rangle, \tag{3}$$

where $\xi_{\mathcal{G}^*}(\mu)$ is the value of $\xi_{\mathcal{G}^*}$ at μ.

To describe idealized, incompressible hydrodynamics, one considers G to be $S\,\mathrm{Diff}(M)$, where M is a manifold equipped with a volume form. Usually $M=\mathbf{R}^2$ or $\mathbf{R}^3$, with the standard Euclidean metric and volume element, so that $S\,\mathrm{Diff}(M)$ consists of volume-preserving C^∞ diffeomorphisms of M. For M not compact, diffeomorphisms are usually further assumed to be compactly supported, or else to become trivial sufficiently rapidly at infinity. The group law is defined by composition of diffeomorphisms: $\phi_1\phi_2=\phi_1\circ\phi_2$, for $\phi_1,\phi_2\in G$. With this convention we follow Refs. 2 and 3, instead of our previous papers where the opposite order was used. With the present convention, the bracket in $\mathcal{G}$ is the negative of the usual Lie bracket of vector fields (see the following). Now $\mathcal{G}$ can be identified with divergenceless vector fields on M vanishing rapidly at infinity, the space that we call $s\,\mathrm{Vect}(M)$. The left group action in G is $L_{\phi_1}(\phi_2)=\phi_1\phi_2=\phi_1\circ\phi_2$, while $R_{\phi_1}(\phi_2)=\phi_2\circ\phi_1$, so that $(\mathrm{Ad}\,\phi)(\psi)=\phi\psi\phi^{-1}=\phi\circ\psi\circ\phi^{-1}$. Let $\psi^{\mathbf{v}}_t$ be a one-parameter subgroup in G generated by a vector field $\mathbf{v}(x)$ on the manifold M. Then from $(\mathrm{Ad}\,\phi)(\psi^{\mathbf{v}}_t)=\phi\circ\psi^{\mathbf{v}}_t\circ\phi^{-1}$, we have

$$\mathrm{Ad}\;\phi_*|_e\mathbf{v} = (D_\phi\mathbf{v})\circ\phi^{-1}, \tag{4}$$

or in Cartesian coordinates (summing over repeated indices),

$$(\mathrm{Ad}(\phi)v)^j(x) = \left[\left(\frac{\partial\phi(y)^j}{\partial y^k}v^k\right)\circ\phi^{-1}\right](x) = \left.\frac{\partial\phi(y)^j}{\partial y^k}\right|_{y=\phi^{-1}(x)} v^k(\phi^{-1}(x)) = \frac{\partial x^j}{\partial[\phi^{-1}(x)]^k}v^k(\phi^{-1}(x)). \tag{5}$$

Thus the matrix D_ϕ at x is given by

$$[D_\phi]^j_k(x) = \frac{\partial\phi(x)^j}{\partial x^k}, \tag{6}$$

and at $\phi^{-1}(x)$ by

$$[D_\phi]^j_k(\phi^{-1}(x)) = \frac{\partial x^j}{\partial[\phi^{-1}(x)]^k}. \tag{7}$$

This specifies how diffeomorphisms act in the space of velocity fields of the fluid.

The transformation has a counterpart in the adjoint action of diffeomorphisms on stream functions. For divergenceless velocity fields in $\mathbf{R}^3$, the stream function $\chi_\mathbf{v}$ is defined so that $\mathbf{v}=-\mathrm{curl}\,\chi_\mathbf{v}$. In $\mathbf{R}^2$, $\chi_\mathbf{v}$ is a scalar function, and we have $v^i=-\epsilon^{ij}\partial\chi_\mathbf{v}/\partial x_j$, where ϵ_{ij} is the usual antisymmetric symbol with $\epsilon_{12}=1$. The stream function is defined only up to the gradient of a function on $\mathbf{R}^3$, or up to an additive constant on $\mathbf{R}^2$. In the latter case one can obtain $\chi_\mathbf{v}$ from $\mathbf{v}$ by introducing $\mathbf{w}=\nabla^{(2)}\chi_\mathbf{v}=(v_2,-v_1)=\mathbf{v}^\perp$. Then $\chi_\mathbf{v}=\int_\infty^x\mathbf{w}\cdot\mathrm{d}\mathbf{s}$, where the integration is along any path from infinity to x (and is independent of the path); this choice sets $\chi_\mathbf{v}=0$ at infinity. An interesting and convenient relation satisfied by such a stream function is

$$\chi_{[\mathbf{v}_1,\mathbf{v}_2]_L} = \mathbf{v}_2 \times \mathbf{v}_1, \tag{8}$$

where $[\cdot,\cdot]_L$ denotes the standard Lie bracket of vector fields, $[\mathbf{v}_1,\mathbf{v}_2]_L=(\mathbf{v}_1\nabla)\mathbf{v}_2-(\mathbf{v}_2\nabla)\mathbf{v}_1$. We use the subscript L to distinguish this from the bracket in the Lie algebra $\mathcal{G}$ obtained in Eq. (15). The action of diffeomorphisms (in three dimensions), given by

$$\chi_i' = [(\mathrm{Ad}\,\phi)\chi]_i = \left(\frac{\partial y^j}{\partial[\phi(y)]^i}\chi_j\right)\circ\phi^{-1} \tag{9}$$

or

$$\chi_i'(x) = \frac{\partial[\phi^{-1}(x)]^j}{\partial x^i}\chi_j(\phi^{-1}(x)), \tag{10}$$

and (in two dimensions) given by

$$\chi_i'(x) = \chi_i(\phi^{-1}(x)), \tag{11}$$

leads to the correct adjoint representation on the velocity fields.

Now $\mathcal{G}^*$ consists of *generalized* (co-)vector fields; that is, fields $\mathbf{A}(x)$ whose components are generalized functions (distributions). The duality is expressed by the pairing

$$\langle\mathbf{A}(x),\mathbf{v}(x)\rangle := \int_{\mathbf{R}^n}\mathbf{A}(x)\cdot\mathbf{v}(x)\mathrm{d}^n x = \int_{\mathbf{R}^n}A_i(x)v^i(x)\mathrm{d}^n x. \tag{12}$$

For $n=3$, we have

$$\langle\mathbf{A}(x),\mathbf{v}(x)\rangle = -\int_{\mathbf{R}^3}\omega(x)\cdot\chi_\mathbf{v}(x)\mathrm{d}^3x, \tag{13}$$

where $\omega(x)=\mathrm{curl}\,\mathbf{A}(x)$ is a generalized vorticity field.

Now the adjoint action of G on $\mathcal{G}$ should be such that infinitesimally it reduces to the adjoint action of $\mathcal{G}$ on $\mathcal{G}$; this requirement is satisfied by (4) and (5). Consider the one-parameter subgroup $\phi_t^{\mathbf{u}}$ of G, which is the solution of the ordinary differential equation

$$\frac{\mathrm{d}\phi_t^{\mathbf{u}}(x)}{\mathrm{d}t} = \mathbf{u}(\phi_t^{\mathbf{u}}(x)),$$

$$\phi_{t=0}^{\mathbf{u}}(x) = x,$$

describing the flow under the vector field $\mathbf{u}(x) \in s\,\mathrm{Vect}(\mathbf{R}^n)$. Then

$$(\mathrm{Ad}(\phi_t^{\mathbf{u}})\mathbf{v})^j = \frac{\partial[\phi_t^{\mathbf{u}}(x)]^j}{\partial x^k} v^k \circ (\phi_t^{\mathbf{u}})^{-1}, \tag{14}$$

and as a result

$$[\mathbf{u},\mathbf{v}] = \mathrm{ad}(\mathbf{u})\mathbf{v} = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} [\mathrm{Ad}(\phi_t^{\mathbf{u}})\mathbf{v}] = -[\mathbf{u},\mathbf{v}]_L, \tag{15}$$

so we see that the bracket in the Lie algebra $\mathcal{G}$ is the negative of the Lie bracket of the vector fields.

Next we write the symplectic form explicitly. We work in the three-dimensional case, because two-dimensional vector fields can be embedded in three dimensions so that the same formulas are applicable.

For $\mu \in \mathcal{G}^*$ we take the generalized velocity field $\mathbf{A}(x) \in s\,\mathrm{Vect}(\mathbf{R}^n)^*$. For $\xi, \eta \in \mathcal{G}$ we take two divergenceless vector fields $\mathbf{u}_1(x)$, $\mathbf{u}_2(x)$. Then the formula for the KKS form on the coadjoint orbit containing $\mathbf{A}(x)$, taken at $\mathbf{A}(x)$, is

$$\Omega_{\mathbf{A}(x)}(\mathbf{u}_{1\mathcal{G}^*}(\mathbf{A}(x)), u_{2\mathcal{G}^*}(\mathbf{A}(x))) = \langle \mathbf{A}(x), [\mathbf{u}_1(x), \mathbf{u}_2(x)]\rangle = -\int_{\mathbf{R}^3} \mathbf{A}(x) \cdot [\mathbf{u}_1(x), \mathbf{u}_2(x)]_L \mathrm{d}^3x. \tag{16}$$

Using (8) and integration by parts, we obtain

$$\Omega_{\mathbf{A}(x)}(\mathbf{u}_{1\mathcal{G}^*}(\mathbf{A}(x)), u_{2\mathcal{G}^*}(\mathbf{A}(x))) = \int_{\mathbf{R}^3} \omega(x) \cdot [\mathbf{u}_1(x) \times \mathbf{u}_2(x)] \mathrm{d}^3x. \tag{17}$$

B. Vortex filaments

Next we consider the case of coadjoint orbits associated with vortex loops or arcs in $\mathbf{R}^2$. We shall use the term "filament" to refer to either a loop or an arc. For a vortex filament in $\mathbf{R}^2$, the vorticity field can be written as

$$\omega(x) = \kappa \mathbf{e}_z \int_0^{2\pi} \mathrm{d}\alpha\, \delta(x^1 - C^1(\alpha))\delta(x^2 - C^2(\alpha)), \tag{18}$$

where $\mathbf{C}(\alpha)$ is a parametrized filament in $\mathbf{R}^2$; i.e., $\mathbf{C}:[0,2\pi] \to \mathbf{R}^2$; and where κ is proportional to the total vorticity of the filament. The KKS symplectic form is given by

$$
\begin{aligned}
&\Omega_{\mathbf{A}(x)}(\mathbf{u}_{1\mathcal{G}^*}(\mathbf{A}(x)),\mathbf{u}_{2\mathcal{G}^*}(\mathbf{A}(x)))\\
&\quad=\kappa\int_{\mathbf{R}^2}\mathrm{d}x^1\,\mathrm{d}x^2\,\mathbf{e}_z\cdot\int_0^{2\pi}\mathrm{d}\alpha\,\delta(x^1-C^1(\alpha))\delta(x^2-C^2(\alpha))(\mathbf{u}_1(x)\times\mathbf{u}_2(x))\\
&\quad=\kappa\int_0^{2\pi}\mathrm{d}\alpha\,u_1^1(C^1(\alpha),C^2(\alpha))u_2^2(C^1(\alpha),C^2(\alpha))\\
&\qquad-\kappa\int_0^{2\pi}\mathrm{d}\alpha\,u_2^1(C^1(\alpha),C^2(\alpha))u_1^2(C^1(\alpha),C^2(\alpha))\\
&\quad=\kappa\int_0^{2\pi}\mathrm{d}\alpha\,(\delta C^1(\alpha)\wedge\delta C^2(\alpha))(\mathbf{u}_1(\mathbf{C}(\alpha)),\mathbf{u}_2(\mathbf{C}(\alpha))),
\end{aligned}
\tag{19}
$$

where $C^1(\alpha)$, $C^2(\alpha)$ are the first and second components of $\mathbf{C}(\alpha)$ in $\mathbf{R}^2$, and $\delta C^1(\alpha)$, $\delta C^2(\alpha)$ denote the respective infinitesimal variations.

Thus the KKS form on the coadjoint orbit characterized by $\mathbf{C}(\alpha)$ can be written as the two-form

$$
\Omega_{\mathbf{C}(\alpha)}=\kappa\int_0^{2\pi}\mathrm{d}\alpha\,\delta C^1(\alpha)\wedge\delta C^2(\alpha).
\tag{20}
$$

Taking a geometric point of view, it is natural to consider unparametrized filaments instead of parametrized ones. An unparametrized filament is just the *image* of the map $\mathbf{C}(\alpha)$. As remarked in Ref. 4, the unparametrized filaments should serve as the quantum configurations. Given a (sufficiently smooth) unparametrized filament Γ, a naturally available intrinsic parametrization is with respect to its own arc length s (in the case of the loop, calculated from an arbitrary initial point). Then we can use a description of the vortex filament in which the original parametrized filament $\mathbf{C}(\alpha)$ is replaced by the pair (Γ,γ), where γ is the vorticity distribution written as a function of s. The function $\gamma(s)$ is defined from $\mathbf{C}(\alpha)$ by

$$
\gamma(s):=\frac{\mathrm{d}\alpha}{\mathrm{d}s}.
\tag{21}
$$

Thus Γ describes just the shape of the filament; the remaining information is coded in $\gamma(s)$. One expects that the canonical coordinates on the coadjoint orbits can be expressed in terms of these quantities. Therefore, it is desirable to write the principal formulas in terms of them.

To calculate the action of the symplectic form on two vector fields in the intrinsic coordinates, we can introduce internal tangent and normal components of the vector fields. In these coordinates $\mathbf{u}_i(x)=(u_{it}(x),u_{in}(x))$, for $i=1,2$; where x is a point on the filament, $u_{it}(x)$ is the component of $\mathbf{u}_i(x)$ tangent to the curve, and $u_{in}(x)$ the component normal to the curve. Using (19), the action of the symplectic form on the pair of vector fields $\mathbf{u}_1(x)$, $\mathbf{u}_2(x)$ is given by

$$
\Omega_{\mathbf{A}(x)}(\mathbf{u}_{1\mathcal{G}^*}(\mathbf{A}(x)),\mathbf{u}_{2\mathcal{G}^*}(\mathbf{A}(x)))=\int_{\mathbb{R}^2}\mathrm{d}^2x\,\mathbf{e}_z\kappa\int\mathrm{d}s\;\gamma(s)\delta(x-\Gamma(s))(\mathbf{u}_1(x)\times\mathbf{u}_2(x)).
\tag{22}
$$

In intrinsic coordinates, the symplectic form reads

$$
\Omega_{(\gamma(s),\Gamma(s))}=\kappa\int\mathrm{d}s\;\gamma(s)\delta s\wedge\delta\Gamma(s).
\tag{23}
$$

This suggests that we introduce the *cumulative vorticity* function $\tilde{\gamma}(s):=\int_0^s\gamma(s')\mathrm{d}s'$, where the zero in the lower limit of the integral can be taken arbitrarily, so that $\mathrm{d}\tilde{\gamma}(s)=\gamma(s)\mathrm{d}s$. Then

$$\Omega_{(\tilde{\gamma}(s),\Gamma(s))} = \kappa \int \mathrm{d}s\, \delta\tilde{\gamma}(s) \wedge \delta\Gamma(s), \tag{24}$$

which is the canonical form of the symplectic structure.

Next we calculate the Poisson bracket for the coadjoint orbit of a vortex filament, in both systems of coordinates. First, let us consider the parametrization by $\mathbf{C}(\alpha) = (C^1(\alpha), C^2(\alpha))$. For any two functions $F(\mathbf{C})$, $G(\mathbf{C})$ on the coadjoint orbit, one defines the Poisson bracket by

$$\{F,G\}(\mathbf{C}(\alpha)) = \Omega_{\mathbf{C}(\alpha)}(X_F, X_G), \tag{25}$$

where X_F and X_G are the vector fields on the coadjoint orbit associated with F and G. They are given by the formula

$$i_{X_F}(\Omega_{\mathbf{C}(\alpha)}) = -\,\mathrm{d}F(\mathbf{C}(\alpha)), \tag{26}$$

where i_X is the interior product; that is, $i_X(\Omega)$ is here the one-form satisfying $[i_X(\Omega)](Y) = \Omega(X,Y)$ for any vector field Y on the coadjoint orbit.

In general

$$\mathrm{d}F(\mathbf{C}(\alpha)) = \int_0^{2\pi} \mathrm{d}\alpha \left[\frac{\delta F}{\delta C^1(\alpha)} \delta C^1(\alpha) + \frac{\delta F}{\delta C^2(\alpha)} \delta C^2(\alpha) \right], \tag{27}$$

so the vector field associated with $F(\mathbf{C}(\alpha))$ is given by

$$X_F = \int_0^{2\pi} \mathrm{d}\alpha \left[X_F^1(\alpha) \frac{\delta}{\delta C^1(\alpha)} + X_F^2(\alpha) \frac{\delta}{\delta C^2(\alpha)} \right], \tag{28}$$

where $\delta/\delta C^1(\alpha)$ and $\delta/\delta C^2(\alpha)$ are defined to be the basis dual to $\delta C^1(\alpha)$ and $\delta C^2(\alpha)$ as specified by the formulas

$$\begin{aligned}
&\frac{\delta}{\delta C^1(\alpha)} \rfloor \delta C^1(\beta) = \delta(\alpha - \beta), \\
&\frac{\delta}{\delta C^2(\alpha)} \rfloor \delta C^1(\beta) = 0, \\
&\frac{\delta}{\delta C^1(\alpha)} \rfloor \delta C^2(\beta) = 0, \\
&\frac{\delta}{\delta C^2(\alpha)} \rfloor \delta C^2(\beta) = \delta(\alpha - \beta).
\end{aligned} \tag{29}$$

Next we express the components of X_F in terms of derivatives of $F(\mathbf{C})$. Since

$$i_{X_F}(\Omega_{\mathbf{C}(\alpha)}) = \kappa \int_0^{2\pi} \mathrm{d}\alpha [X_F^1 \delta C^2(\alpha) - X_F^2 \delta C^1(\alpha)], \tag{30}$$

we obtain by comparison with (27)

$$X_F^1(\alpha) = -\frac{1}{\kappa} \frac{\delta F}{\delta C^2(\alpha)}, \tag{31}$$

$$X_F^2(\alpha) = \frac{1}{\kappa}\frac{\delta F}{\delta C^1(\alpha)}. \tag{32}$$

As a result,

$$X_F = \int_0^{2\pi} \mathrm{d}\alpha \frac{1}{\kappa}\left[-\frac{\delta F}{\delta C^2(\alpha)}\frac{\delta}{\delta C^1(\alpha)} + \frac{\delta F}{\delta C^1(\alpha)}\frac{\delta}{\delta C^2(\alpha)} \right]. \tag{33}$$

Thus we obtain the Poisson bracket of two functions on our coadjoint orbit,

$$\{F,G\}(\mathbf{C}(\alpha)) = \Omega_{\mathbf{C}(\alpha)}(X_F,X_G) = -\int_0^{2\pi} \mathrm{d}\alpha \frac{1}{\kappa}\left[\frac{\delta F}{\delta C^1(\alpha)}\frac{\delta G}{\delta C^2(\alpha)} - \frac{\delta F}{\delta C^2(\alpha)}\frac{\delta G}{\delta C^1(\alpha)} \right]. \tag{34}$$

Applying a similar procedure, we obtain the formula for the Poisson bracket with respect to the intrinsic coordinates $\tilde{\gamma}(s)$ and $\Gamma(s)$,

$$\{F,G\}(\tilde{\gamma}(s),\Gamma(s)) = \Omega_{(\tilde{\gamma}(s),\Gamma(s))}(X_F,X_G) = \frac{1}{\kappa}\int \mathrm{d}s \left[\frac{\delta F}{\delta \Gamma(s)}\frac{\delta G}{\delta \tilde{\gamma}(s)} - \frac{\delta F}{\delta \tilde{\gamma}(s)}\frac{\delta G}{\delta \Gamma(s)} \right]. \tag{35}$$

Thus the coordinates $\Gamma(s)$ and $\tilde{\gamma}(s)$ serve as canonical coordinates and momenta of the coadjoint orbit. Formula (35) agrees with the result of Ref. 4 concerning the polarization of the orbits. The quantum configuration space is the space of *unparametrized* filaments $\Gamma(s)$. The stability subgroup, or little group, consists of those area-preserving diffeomorphisms which preserve the filament as a set, but which can change arbitrarily the cumulative vorticity distribution $\tilde{\gamma}(s)$, preserving only the total vorticity of the loop.

C. Evaluation of a Poisson bracket

Let us consider the calculation of the Poisson bracket for a concrete, illustrative pair of functions on the coadjoint orbit of vortex filaments, using Eqs. (25) and (26). Suppose first that the vector fields X_F, X_G can be identified with $\mathbf{u}_{\mathcal{G}^*}$ and $\mathbf{v}_{\mathcal{G}^*}$, respectively, for vector fields $\mathbf{u}$ and $\mathbf{v}$ on $\mathbf{R}^2$. We then have Eq. (19), which we write more concisely as

$$\Omega(\mathbf{u}_{\mathcal{G}^*},\mathbf{v}_{\mathcal{G}^*}) = \kappa\int_0^{2\pi} \mathrm{d}\alpha[(u^1\circ\mathbf{C})(v^2\circ\mathbf{C}) - (u^2\circ\mathbf{C})(v^1\circ\mathbf{C})](\alpha). \tag{36}$$

Next introduce a local coordinate system in $\mathbf{R}^2$ defined in a sufficiently narrow, ribbon-like neighborhood of the filament. Such coordinates can be defined locally using integral curves of the vector fields obtained via parallel transport of the tangent and normal vector fields on the filament. We can thus write the coordinates for a point in such a neighborhood as $(s,x^\perp)$, where s is the arclength along the filament, and $x^\perp$ is locally the arclength coordinate along the integral curve of the normal vector field, taking the value 0 on the filament. In this notation, the symplectic form can be formally rewritten

$$\Omega(\mathbf{u}_{\mathcal{G}^*},\mathbf{v}_{\mathcal{G}^*}) = \kappa\int\int \mathrm{d}^2x\,\delta^{(1)}(x^\perp)I_{[0,L_{\mathrm{tot}}]}(s)\gamma(s)[u^1(x)v^2(x) - u^2(x)v^1(x)], \tag{37}$$

where $\mathrm{d}^2x = \mathrm{d}s\,\mathrm{d}x^\perp$, $I_{[0,L_{\mathrm{tot}}]}$ is the indicator function that is 1 on the interval $[0,L_{\mathrm{tot}}]$ and 0 outside it, L_{tot} is the length of the filament, and the integration is taken over a neighborhood of the filament in which the coordinates are defined. Now let us regard F as given, with $X_F = \mathbf{u}_{\mathcal{G}^*}$, and contract both sides of Eq. (34) with an arbitrary vector field $\mathbf{v}_{\mathcal{G}^*}$. The right-hand side becomes

$$\mathrm{d}F(\mathbf{v}_{\mathcal{G}^*})|_{\mathbf{C}} = \mathbf{v}_{\mathcal{G}^*}(F)|_{\mathbf{C}} = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} F(\phi_t^{\mathbf{v}} \circ \mathbf{C}), \tag{38}$$

where $\phi_t^{\mathbf{v}}$ is the flow generated by $\mathbf{v}$, while the left-hand side of (34) becomes just $\Omega(\mathbf{u}_{\mathcal{G}^*}, \mathbf{v}_{\mathcal{G}^*})|_{\mathbf{C}}$ which is (37). Equating (37) and (38), we now consider a particular, highly instructive choice of functions F: let us define $F^j_\beta(\mathbf{C}) = C^j(\beta)$ for $j=1,2$, where β is a fixed value of the parameter α. That is, for each β the F^j_β are coordinate functions on the space of filaments. Then

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} F^j_\beta(\phi_t^{\mathbf{v}} \circ \mathbf{C}) = v^j(\mathbf{C}(\beta)), \tag{39}$$

which may be rewritten as

$$\int\int \mathrm{d}^2x\, v^j(x)\, \delta^{(1)}(x^\perp)\, \delta^{(1)}(s - s(\beta)). \tag{40}$$

Setting (37) equal to (40), and recalling that $\mathbf{v}$ was chosen arbitrarily, the resulting equations are easily solved to obtain formal expressions for $\mathbf{u}$: For $j=1$, we have

$$\begin{aligned} u^1(0,s) &= 0, \\ u^2(0,s) &= -\frac{1}{\kappa\gamma(s)}\,\delta^{(1)}(s - s(\beta)), \end{aligned} \tag{41}$$

while for $j=2$,

$$\begin{aligned} u^1(0,s) &= \frac{1}{\kappa\gamma(s)}\,\delta^{(1)}(s - s(\beta)), \\ u^2(0,s) &= 0. \end{aligned} \tag{42}$$

We make two remarks about these formulas:

1. The vector field $\mathbf{u}$ is singular (a distribution), so that from a rigorous point of view it does not belong to the Lie algebra $\mathcal{G}$. It is, however, straightforward to regularize it. In place of $F^j_\beta(\mathbf{C})$ consider

$$F^{j(a)}_\beta(\mathbf{C}) = \int_0^{2\pi} \mathrm{d}\alpha\; \delta^{(1)}_a(\alpha - \beta) C^j(\beta), \tag{43}$$

   where $\delta^{(1)}_a$ is a family of smooth functions parametrized by a such that the weak limit of $\delta^{(1)}_a(\alpha)$ as $a \to 0$ is $\delta^{(1)}(\alpha)$; we then obtain formulas corresponding to (41) and (42) with $\delta^{(1)}$ replaced by $\delta^{(1)}_a$.
2. The solutions for $\mathbf{u}$ describe it only on the filament, and not in the local neighborhood. Nevertheless, one can extend $\mathbf{u}$ to the neighborhood in a smooth but otherwise arbitrary way.

Finally we calculate the Poisson bracket for the functions

$$F(\mathbf{C}) = C^1(\beta_1), \quad G(\mathbf{C}) = C^2(\beta_2), \tag{44}$$

defined on the coadjoint orbit. Let $\mathbf{u}_1$ and $\mathbf{u}_2$ be vector fields in the plane whose components on the filament $\mathbf{C}$ are given by the formulas (41) and (42), respectively. The Poisson bracket of F and G is then given by

$$
\begin{aligned}
\{F,G\}|_{\mathbf{C}} &= \Omega(X_F,X_G)|_{\mathbf{C}} \\
&= \Omega(\mathbf{u}_{1\mathcal{G}^*},\mathbf{u}_{2G^*})|_{\mathbf{C}} \\
&= \kappa\int_0^{2\pi} \mathrm{d}\alpha[u_1^1(\mathbf{C}(\alpha))u_2^2(\mathbf{C}(\alpha)) - u_1^2(\mathbf{C}(\alpha))u_2^1(\mathbf{C}(\alpha))] \\
&= \kappa\int_0^{L_{\mathrm{tot}}} \mathrm{d}s\ \gamma(s)\frac{1}{\kappa\gamma(s)}\delta^{(1)}(s-s(\beta_1))\frac{1}{\kappa\gamma(s)}\delta^{(1)}(s-s(\beta_2)) \\
&= \frac{1}{\kappa\gamma(s(\beta_1))}\delta(s(\beta_1)-s(\beta_2)).
\end{aligned} \tag{45}
$$

This result confirms the formal expression (34) obtained for the Poisson bracket.

IV. FOCK SPACE FOR BOSONIC VORTEX LOOPS

In this section we construct a Fock space of states for planar vortex loops. We do this for the simplest case of bosonic loops. Despite its relative simplicity, this case is quite rich and illustrates some of the general features. It will serve as a fundamental construction in our continuing study of vortex structures in ideal quantum fluids. Our consideration is formal to the extent that we make no commitment to a specific quasi-invariant measure on the configuration space, which is necessary for the construction of unitary representations; see Ref. 30, however, where a class of such measures is constructed. We expect the particular choice of measure to describe the dynamics of the theory,[31] while here we consider only the kinematics.

In the approach to nonrelativistic quantum systems based on local current algebras and diffeomorphism groups,[21,32,33] the states are vectors in a Hilbert space carrying a unitary representation of the group Diff (M), of (not necessarily volume-preserving) diffeomorphisms of the spatial manifold M that become rapidly trivial at infinity. The states are square-integrable functions defined on the configuration space, with values in a complex inner product space. In quantum mechanics, the configuration space typically consists of N-point subsets of M, while in statistical physics it consists of countably infinite but locally finite subsets.

The representations take the general form

$$
(V(\phi)\Psi)(\Gamma) = \chi_\phi(\Gamma)\Psi(\phi\Gamma)\sqrt{\frac{\mathrm{d}\mu_\phi}{\mathrm{d}\mu}(\Gamma)}, \tag{46}
$$

where ϕ is a diffeomorphism, Γ is an element of the configuration space Δ (on which diffeomorphisms of M act naturally), μ is a measure on Δ quasi-invariant under diffeomorphisms, and $\chi_\phi(\Gamma)$ denotes a unitary cocycle, satisfying (almost everywhere) the relation

$$
\chi_{\phi_1\circ\phi_2}(\Gamma) = \chi_{\phi_2}(\Gamma)\chi_{\phi_1}(\phi_2\Gamma). \tag{47}
$$

In the applications of diffeomorphism groups to the nonrelativistic quantum mechanics of finitely many particles, inequivalent cocycles describe distinct quantum statistics (bosonic, fermionic, anyonic, or plektonic), and can be obtained by inducing from unitary representations of the stability subgroup.[21,22,34] The square root of the Radon–Nikodym derivative in (46) ensures that $V(\phi)$ is unitary with respect to the measure μ; note that this expression also satisfies a cocycle condition.

Our purpose here is to generalize the earlier construction to include configurations that are extended objects—in particular, the quantum vortex filaments in an ideal, incompressible fluid discussed in Sec. III. Thus we consider unitary representations of the subgroup $S\,\mathrm{Diff}(\mathbf{R}^n)$, here with $n=2$.

In general, the configuration space consists of unparametrized loops. It can be decomposed into the disjoint union of submanifolds, each of which consists of configurations having a specified number N of component loops; we call such configurations "multiloops." There is a corresponding

decomposition of the full Hilbert space $\mathcal{H}$ into a direct sum of component subspaces $\mathcal{H}_N$, characterized by the number of loops in a configuration. So far, this is similar to the case of point particles. The new ingredient with extended objects is the further decomposition of the subspace of N-loop configuration space into components invariant under area-preserving diffeomorphisms. These are the topological sectors discussed, for example, in Ref. 26. There is a corresponding decomposition of the Hilbert spaces $\mathcal{H}_N$.

When studying point particles, it is useful to consider creation and annihilation operators. For the diffeomorphism group these intertwine the corresponding N-particle unitary group representations, and the cocycles impose the algebra of canonical commutation, anticommutation, or q-commutation relations on the creation and annihilation fields.[24] We anticipate that this scheme will also work for nonrelativistic extended objects such as vortex filaments.

We now construct representations of creation and annihilation field operators for bosonic vortex loops, where the cocycles are assumed to be trivial. This removes complications due to the different topological sectors in each N-loop subspace—when a loop is created, the operator need not "know" whether it intersects with or overlaps existing loops. For that reason, this case is formally very similar to the case of bosonic point particles. Nevertheless we have the new feature that the arguments of the creation and annihilation operators are extended, unparametrized loops, rather than points in the physical space.

Now the wave functions of this quantum theory are complex-valued functions of multiloops. The N-loop representation of the diffeomorphism group is given by

$$[V(\phi)\Psi]_N(\{\Gamma_1, \ldots, \Gamma_N\}) = \Psi(\{\phi\Gamma_1, \ldots, \phi\Gamma_N\}) \sqrt{\frac{\mathrm{d}\mu_\phi^{(N)}}{\mathrm{d}\mu^{(N)}}(\{\Gamma_1, \ldots, \Gamma_N\})}, \tag{48}$$

with $\{\Gamma_1, \ldots, \Gamma_N\}$ being a multiloop comprised of N unparametrized loops (possibly intersecting, overlapping, knotted, and so forth, according to the number of dimensions of the space). Here $\phi\Gamma_j$ denotes the natural action of the area-preserving diffeomorphism ϕ on the loop Γ_j embedded in $\mathbf{R}^2$.

We define the operators $\psi^*(\Gamma): \mathcal{H}_N \to \mathcal{H}_{N+1}$ and $\psi(\Gamma): \mathcal{H}_{N+1} \to \mathcal{H}_N$ by

$$[\psi(\Gamma)\Psi]_N(\{\Gamma_1, \ldots, \Gamma_N\}) := \Psi_{N+1}(\{\Gamma_1, \ldots, \Gamma_N, \Gamma\}), \tag{49}$$

$$[\psi^*(\Gamma)\Psi]_N(\{\Gamma_1, \ldots, \Gamma_N\}) := \sum_{j=1}^{N} \delta(\Gamma, \Gamma_j)\Psi_{N-1}(\{\Gamma_1, \ldots, \hat{\Gamma}_j, \ldots, \Gamma_N\}), \tag{50}$$

where $\hat{\Gamma}_j$ means that Γ_j is omitted, and where $\delta(\Gamma, \Gamma')$ is formally defined as a distribution over functions $h(\Gamma)$ on the one-loop configuration space by

$$\int \mathrm{d}\mu(\Gamma')\,\delta(\Gamma, \Gamma')h(\Gamma') = h(\Gamma). \tag{51}$$

Straightforward calculation gives the commutation relations for these creation and annihilation operators:

$$[\psi(\Gamma), \psi(\Gamma')] = 0, \quad [\psi^*(\Gamma), \psi^*(\Gamma')] = 0, \quad [\psi(\Gamma), \psi^*(\Gamma')] = \delta(\Gamma, \Gamma'). \tag{52}$$

Necessary conditions for the operators $\psi(\Gamma)$, $\psi^*(\Gamma)$ and the representations $V(\phi)$ to form a hierarchy are the intertwining properties of the form proposed in Ref. 24:

$$\begin{aligned} V_{N+1}(\phi)\psi^*(h) &= \psi^*(V_{N=1}(\phi)h)V_N(\phi), \\ V_N(\phi)\psi(h) &= \psi(V_{N=1}(\phi)h)V_{N+1}(\phi), \end{aligned} \tag{53}$$

where $\psi(h) = \int \mathrm{d}\mu(\Gamma)h(\Gamma)\psi(\Gamma)$ and $\psi^*(h) = \int \mathrm{d}\mu(\Gamma)h(\Gamma)\psi^*(\Gamma)$ are the creation and annihilation operators averaged with respect to $h \in \mathcal{H}_{N=1}$. These intertwining properties restrict the quasi-

invariant measures in an interesting way. Thus, a condition on the $\mu^{(N)}$ sufficient to satisfy (53) is

$$\forall j \in \{1, \ldots, N\}, \quad \frac{\mathrm{d}\mu_\phi^{(N)}}{\mathrm{d}\mu^{(N)}}(\{\Gamma_1, \ldots, \Gamma_j, \ldots, \Gamma_N\}) = \frac{\mathrm{d}\mu_\phi^{(N-1)}}{\mathrm{d}\mu^{(N-1)}}(\{\Gamma_1, \ldots, \hat{\Gamma}_j, \ldots, \Gamma_N\}) \frac{\mathrm{d}\mu_\phi^{(1)}}{\mathrm{d}\mu^{(1)}}(\{\Gamma_j\}). \tag{54}$$

Iteration of this formula leads to the following multiplicative property of the Radon–Nikodym derivatives:

$$\frac{\mathrm{d}\mu_\phi^{(N)}}{\mathrm{d}\mu^{(N)}}(\{\Gamma_1, \ldots, \Gamma_N\}) = \prod_{j=1}^{N} \frac{\mathrm{d}\mu_\phi^{(1)}}{\mathrm{d}\mu^{(1)}}(\{\Gamma_j\}). \tag{55}$$

This is the condition which, when satisfied by the quasi-invariant measure, ensures existence of a hierarchy of representations of the diffeomorphism group. The representations from the hierarchy are indexed by the numbers of loops. The simplest examples of such measures are, of course, products of one-loop measures, so that

$$\mathrm{d}\mu^{(N)}(\{\Gamma_1, \ldots, \Gamma_N\}) = \mathrm{d}\mu^{(1)}(\{\Gamma_1\}) \ldots \mathrm{d}\mu^{(1)}(\{\Gamma_N\}). \tag{56}$$

However, we are mainly interested in more general measures, which can distinguish nonoverlapping and overlapping vortex loops. Such measures should depend on the areas of the overlap regions, which are preserved by the diffeomorphisms in our group. For complicated overlaps there can be many such regions, on whose areas the measures may explicitly depend; some general properties that should be satisfied are discussed in Ref. 26. In particular, suppose that some multiloops $\{\Gamma_1, \ldots, \Gamma_N\}$ consist of N overlapping loops with r distinguished regions of overlap; let the areas be $\beta_1, \ldots, \beta_r$. Then let

$$\mathrm{d}\mu^{(N)}(\{\Gamma_1, \ldots, \Gamma_N\}) = f(\beta_1, \ldots \beta_r)\mathrm{d}\mu^{(1)}(\{\Gamma_1\}) \ldots \mathrm{d}\mu^{(1)}(\{\Gamma_N\}), \tag{57}$$

where f is a general, measurable function of $\beta_1, \ldots, \beta_r$. One can assume that for $\beta_1 = \ldots = \beta_r = 0$, $f(\beta_1, \ldots \beta_r) = 1$. It is easy to prove that for a measure satisfying this condition, (55) is satisfied.

V. SUMMARY AND OUTLOOK

We have written down and analyzed the Poisson structure for coadjoint orbits associated with two-dimensional vortex filaments, and introduced canonical coordinates and momenta—the unparametrized filaments, and the cumulative vorticity functions, respectively. This result confirms the results of Ref. 4, which were obtained by requiring the existence of a polarization for geometric quantization.

We have also constructed a space of quantum states for bosonic vortex loops. This construction is at a formal level, but acquires concrete meaning when an appropriate quasi-invariant measure is chosen.

Similar constructions should be valid for other nonrelativistic extended objects. These may include vortex dipoles in two space dimensions, vortex ribbons and tubes in three space dimensions, or nonrelativistic bosonic strings. We also anticipate further study of the dynamics for extended vortex configurations, where the dynamical role of topological degrees of freedom should become apparent.

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Bounds on integrals of the Wigner function: The hyperbolic case

J. G. Wood and A. J. Bracken
Centre for Mathematical Physics, University of Queensland, Brisbane, Australia 4072

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Wigner functions play a central role in the phase space formulation of quantum mechanics. Although closely related to classical Liouville densities, Wigner functions are not positive definite and may take negative values on subregions of phase space. We investigate the accumulation of these negative values by studying bounds on the integral of an arbitrary Wigner function over noncompact subregions of the phase plane with hyperbolic boundaries. We show using symmetry techniques that this problem reduces to computing the bounds on the spectrum associated with an exactly solvable eigenvalue problem and that the bounds differ from those on classical Liouville distributions. In particular, we show that the total "quasiprobability" on such a region can be greater than 1 or less than zero. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1851971]

I. INTRODUCTION

Since its introduction,[1] the Wigner function has been the subject of extensive study in the fields of quantum physics, quantum chemistry and signal analysis (see Refs. 2–10 and references therein). Since Wigner functions represent quantum states on phase space, they play a key role in the phase space formulation of quantum mechanics. They are also designed to closely resemble the joint densities of position and momentum, known as Liouville densities, that are used in classical mechanics. In quantum physics, such studies have been stimulated in recent times by the development of quantum tomography, which has enabled the reconstruction of Wigner functions corresponding to states of a variety of quantum systems.[11] Such experimental observations have confirmed that Wigner functions can be negative on subregions of phase space. This is one of several properties that can be used to distinguish Wigner functions from classical Liouville densities.

The study of these "quantum properties" has been approached in a number of ways including calculations of pointwise bounds on Wigner functions and bounds on various moments.[12–16] A more recent development has been the study of bounds on integrals of the Wigner function over subregions of the phase space,[17–19] which we denote by Γ. We call such integrals *quasiprobability integrals* (qpis). For a given subregion S of Γ, the problem of determining best possible upper and lower bounds on all possible qpis over S has been shown to be equivalent to the problem of determining the supremum and infimum of the spectrum of the *region operator* associated with S. This operator is just the image under Weyl's quantization map[20] of the characteristic function of S, namely the function that equals 1 on S and 0 elsewhere on Γ. In the special case of a quantum system with one linear degree of freedom, it has been shown that for any subregion of the phase plane enclosed by an ellipse, the eigenvalue problem is exactly solvable and the bounds on qpis can be obtained analytically for ellipses of arbitrary size.[17]

The determination of bounds on qpis is important not only because it provides information about the structure of theoretically possible Wigner functions, which is a question of mathematical interest, but also because an understanding of that structure provides checks on experimentally determined Wigner functions. It is therefore of interest to know if there are other subregions of the phase plane, and more generally of phase space, for which the spectrum of the associated region operators, and hence the best-possible upper and lower bounds on all possible associated qpis, can

be determined exactly. In this paper, we show that an exact formula for the spectrum of the region operator, from which the bounds are easily obtained numerically, can be derived for subregions of the phase plane with hyperbolic symmetry. The solvability of the eigenvalue problems for the corresponding region operators, as in the case of elliptical subregions discussed earlier, relies on the invariance of these regions under one-parameter subgroups of the metaplectic group $Mp(2,\mathbb{R})$ of transformations of the phase plane. This group consists of all real transformations of the form

$$T:(q,p) \to (q',p') = (\alpha q + \beta p + q_0, \gamma q + \delta p + p_0), \tag{1}$$

where $\alpha\delta - \beta\gamma = 1$. In this paper, the subgroup of $Mp(2,\mathbb{R})$ formed by the transformations $T_\sigma:(q,p) \to (\sigma q, p/\sigma), \sigma > 0$ is of particular importance.

Several illustrative examples of eigenvalue problems for hyperbolic regions are considered in what follows, including the interesting limiting case of an infinite wedge. We shall be concerned with quantum systems with one linear degree of freedom, described in terms of a Hilbert space of states $\mathcal{H}$, and with the properties of Wigner functions on the associated (q,p) phase plane Γ. We are not concerned with dynamics, and consider each Wigner function at a fixed time. Dimensionless phase plane coordinates (q,p) are used, and in effect we set $\hbar = 1$. Finally, we note that in the absence of limits of integration, integrals are assumed to run from $-\infty$ to ∞.

II. BOUNDS ON QUASIPROBABILITY INTEGRALS

The Wigner function corresponding to a pure state $\psi \in \mathcal{H}$ has the definition

$$W_\psi(q,p) = \frac{1}{\pi} \int \overline{\psi}(q+\tau)\psi(q-\tau)e^{2ip\tau}\,\mathrm{d}\tau. \tag{2}$$

For a mixed state, the Wigner function is a convex linear combination of such integrals. It is known that Wigner functions are bounded at every point $(q,p) \in \Gamma$ such that $-1/\pi \leqslant W(q,p) \leqslant 1/\pi$ and that they satisfy the normalization conditions

$$\int_\Gamma W\,\mathrm{d}q\,\mathrm{d}p = 1, \quad 0 \leqslant \int_\Gamma W^2\,\mathrm{d}q\,\mathrm{d}p \leqslant \frac{1}{2\pi},$$

where the value $1/2\pi$ is attained if and only if W corresponds to a pure state.

More generally, an operator $\hat{A}$ is unitarily related to a phase space function $A(q,p)$ by the Weyl–Wigner transform[21] and its inverse,

$$A = \mathcal{W}(\hat{A}), \quad \hat{A} = \mathcal{W}^{-1}(A). \tag{3}$$

Here $\mathcal{W}^{-1}$ is Weyl's quantization map and $\mathcal{W}$ is such that the Wigner function corresponding to a quantum density operator $\hat{\rho}$ is given by $W_\rho = \mathcal{W}(\hat{\rho})/(2\pi)$. In this paper we make extensive use of the configuration realization, in which $\hat{A}$ can be expressed as an integral operator

$$(\hat{A}\psi)(x) = \int A_K(x,y)\psi(y)\mathrm{d}y. \tag{4}$$

We refer to the function $A_K(x,y)$ as the configuration kernel of $\hat{A}$. It is related to the phase space function $A(q,p)$ by the formulas[22,23]

$$A(q,p) = \int A_K(q-y/2, q+y/2)e^{ipy}\,\mathrm{d}y, \tag{5}$$

$$A_K(x,y) = \frac{1}{2\pi}\int A((x+y)/2,p)e^{ip(x-y)}\,\mathrm{d}p, \tag{6}$$

which provide an explicit realization of the transformations (3).

An important property of Wigner functions is that quantum averages on phase space take the same form as classical averages, if $A(q,p)$ is the phase space representation of a quantum observable $\hat{A}$, then its quantum average in the state with density operator $\hat{\rho}$ and corresponding Wigner function W_ρ is given by

$$\langle\hat{A}\rangle = \mathrm{Tr}(\hat{A}\hat{\rho}) = \int_\Gamma W_\rho(q,p)A(q,p)\mathrm{d}q\,\mathrm{d}p. \tag{7}$$

The qpi of a Wigner function W over a subregion S of Γ may be written as the functional

$$Q_S[W] = \int_S W(q,p)\mathrm{d}q\,\mathrm{d}p. \tag{8}$$

Note that the integral on the right-hand side can be rewritten in terms of the characteristic function $\chi_S(q,p)$ that equals 1 on S and 0 on its complement,

$$Q_S[W] = \int_\Gamma W(q,p)\chi_S(q,p)\mathrm{d}q\,\mathrm{d}p,$$

and, by comparing with (7), we can write

$$Q_S[W] = \langle\hat{\chi}_s\rangle, \tag{9}$$

where we have introduced the *region operator* $\hat{\chi}_S = \mathcal{W}^{-1}(\chi_S)$,[17] with configuration kernel [as given by (6)]

$$\chi_{S,K}(x,y) = \frac{1}{2\pi}\int \chi_S((x+y)/2,p)e^{ip(x-y)}\,\mathrm{d}p. \tag{10}$$

Since the expectation value of a quantum operator always lies between the extremal values of its spectrum, we deduce from (9) that $Q_S[W]$ must lie between the infimum and the supremum of the spectrum of $\hat{\chi}_S$. Moreover, as the spectral bounds on the expectation value of an operator can be approached arbitrarily closely with normalized states in $\mathcal{H}$, these bounds are best-possible. Hence the best-possible bounds on the qpi functional Q_S are provided by the extremal solutions to the integral equation

$$(\hat{\chi}_S\psi)(x) = \int \chi_{S,K}(x,y)\psi(y)\mathrm{d}y = \lambda\psi(x) \tag{11}$$

that defines the eigenvalue problem for $\hat{\chi}_S$.

For a general region S, the integral equation (11) is not exactly solvable and the bounds on its spectrum must be obtained by using computational methods. However, there is a subclass of regions for which the (generalized) eigenvalues and eigenfunctions can be determined exactly. This subclass is the set of regions that are each invariant under a one-parameter subgroup of the metaplectic (or linear canonical) group of transformations (1) of the phase plane. Any such transformation U has the special property that its inverse Weyl–Wigner transform $\hat{U} = \mathcal{W}^{-1}(U)$ is a unitary (and thus spectrum preserving) operator acting on $\mathcal{H}$. If a subregion S of Γ is invariant under a metaplectic transformation, then it follows that the associated region operator $\hat{\chi}_S$ is invariant under the corresponding unitary operation $\hat{U}$, that is generated by an operator $\hat{r}$ of no

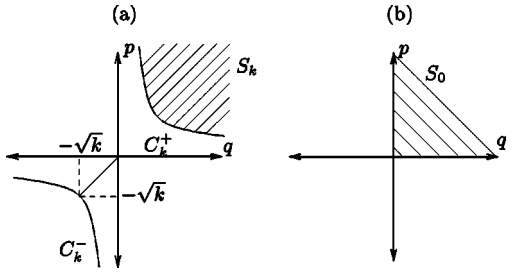

FIG. 1. Graphs of hyperbolic regions and their boundaries, in (a) the hyperbolic region S_k is shown as are the boundary curves C_k^+ and C_k^-, while in (b) the infinite wedge S_0 is depicted.

greater than the second degree in $\hat{q}$ and $\hat{p}$. It follows that $[\hat{\chi}_S, \hat{r}]=0$ and hence that the eigenfunctions of $\hat{\chi}_S$ may be chosen so that they are also eigenfunctions of $\hat{r}$. These are readily obtained by solving the eigenvalue problem for $\hat{r}$.

This approach can be applied to regions that are bounded by ellipses, hyperbolas, parabolas, and straight lines. [If the boundary is composed of several curves, then each curve must be invariant under the same one-parameter subgroup of $Mp(2,\mathbb{R})$.] In the case of elliptical regions, the best-possible bounds have already been described,[17] while the fact that the marginal distributions of the Wigner function are true probability density functions[24] implies that integrals over regions bounded by parallel straight lines must lie in the interval $[0, 1]$. In this paper, we consider the problem of determining the best-possible bounds on qpis over regions with hyperbolic boundaries.

III. BEST-POSSIBLE BOUNDS ON QPIS FOR HYPERBOLIC REGIONS

In order to demonstrate our technique for constructing the bounds on qpis, we begin with a simple example. Let C_k be the hyperbolic curve consisting of all points that satisfy

$$qp = k, \quad k \geqslant 0, \tag{12}$$

as depicted in part (a) of Fig. 1. Note that C_k is itself composed of two curves, namely C_k^+, which lies in the positive (q,p) quadrant of Γ and C_k^-, which lies in the negative (q,p) quadrant of Γ. It is clear that the curves $C_k^\pm$ are separately invariant under the action of the transformation $T_\sigma: (q,p) \to (\sigma q, p/\sigma)$ for all $\sigma > 0$.

Now consider the subregion S_k that contains all points in Γ such that $qp \geqslant k$, $q \geqslant 0$, which is indicated by the shaded region in part (a) of Fig. 1. Since this region can be viewed as the union of all hyperbolic curves C_l^+ with $l \geqslant k$, it is itself invariant under the action of T_σ. In order to apply this symmetry to the problem of determining the bounds on qpis over S_k, we must first construct the corresponding region operator, which we denote by $\hat{\chi}_k$. Note that the characteristic function on S_k, may be written as

$$\chi_k = \begin{cases} 1, & qp \geqslant k, \quad q \geqslant 0 \\ 0, & \text{otherwise} \end{cases} = H(q)H(p - k/q), \tag{13}$$

where H is the Heaviside function. Using (6), the configuration kernel for the region operator can be determined (see the Appendix for details):

$$\chi_{k,K}(x,y) = H\left(\frac{x+y}{2}\right) e^{2ik[(x-y)/(x+y)]} \left[\frac{1}{2}\delta(x-y) - \frac{1}{2\pi i(x-y)}\right], \tag{14}$$

and hence the bounds on qpis are given by the spectral bounds associated with the integral equation

$$\int_{-x}^{\infty} e^{2ik[(x-y)/(x+y)]}\left[\frac{1}{2}\delta(x-y)-\frac{1}{2\pi i(x-y)}\right]\psi(y)\mathrm{d}y=\mu\psi(x). \tag{15}$$

We know, however, that the region operator $\hat{\chi}_k$ is invariant under the set of operator transformations that correspond to the subgroup of $Mp(2,\mathbb{R})$ formed by $T_\sigma, \sigma>0$. Since the effect of T_σ is to squeeze position and stretch momentum (or vice versa) while preserving the canonical commutation relations, the corresponding operator transformation, up to an unimportant phase, is given by the squeezing operator $\hat{U}_\sigma=\exp(i\log\sigma(\hat{q}\hat{p}+\hat{p}\hat{q})/2)$. This implies that $\hat{\chi}_k$ commutes with $\hat{U}_\sigma$ for all $\sigma>0$, and hence

$$[\hat{\chi}_k,\hat{\omega}]=0, \quad \hat{\omega}=(\hat{q}\hat{p}+\hat{p}\hat{q})/2.$$

It follows that the eigenfunctions of $\hat{\chi}_k$ can be chosen such that they are also eigenfunctions of $\hat{\omega}$. We can then obtain a partial solution to the integral equation (15) by solving the equation $\hat{\omega}\psi=\omega\psi$. A number of results connected with this problem can be found in a paper of Chruscinski.[25] On configuration space, this equation appears as the first order differential equation

$$x\frac{\mathrm{d}\psi}{\mathrm{d}x}=\left(i\omega-\frac{1}{2}\right)\psi. \tag{16}$$

The solutions of this equation are complex-valued linear combinations of the functions

$$\psi_\omega^+(x)=\begin{cases}\dfrac{1}{\sqrt{2\pi}}\dfrac{e^{i\omega\log|x|}}{|x|^{1/2}}, & x>0,\\ 0, & x<0,\end{cases} \qquad \psi_\omega^-(x)=\begin{cases}0, & x>0,\\ \dfrac{1}{\sqrt{2\pi}}\dfrac{e^{i\omega\log|x|}}{|x|^{1/2}}, & x<0.\end{cases} \tag{17}$$

Here ω can take any real value. These solutions are generalized functions and are elements of the space of tempered distributions $\mathcal{G}'$,[26] of which $\mathcal{H}$ is a proper subspace. The factor $1/\sqrt{2\pi}$ is inserted to ensure that $(\psi_\omega^\pm,\psi_{\omega'}^\pm)=\delta(\omega-\omega')$. Since they have disjoint support, ψ_ω^+ and $\psi_{\omega'}^-$ are orthogonal for all $\omega,\omega'\in\mathbb{R}$. Note that, since $\log|x|\to-\infty$ as $|x|\to0$, the eigenfunctions become highly oscillatory in the neighborhood of the origin and are undefined at $|x|=0$, due to the $|x|^{1/2}$ term in the denominator.

Since the $\psi_\omega^\pm$ form two independent families of solutions to (16), the eigenfunctions of $\hat{\chi}_k$ are not yet fully determined. In order to construct these solutions, we must solve the reduced eigenvalue problem

$$\hat{\chi}_k\psi_\omega=\mu(\omega,k)\psi_\omega, \quad \psi_\omega=\alpha_\omega\psi_\omega^+ +\beta_\omega\psi_\omega^-, \tag{18}$$

where $\alpha_\omega,\beta_\omega\in\mathbb{C}$. In order to solve (18), we must first determine the action of $\hat{\chi}_k$ on the two-dimensional subspace $\mathcal{G}'_\omega$ of $\mathcal{G}'$ spanned by ψ_ω^+ and ψ_ω^-, $\hat{\chi}_k(\psi_\omega^+,\psi_\omega^-)^T=A(\omega,k)(\psi_\omega^+,\psi_\omega^-)^T$, where $A(\omega,k)$ is given by the matrix

$$A(\omega,k)=\begin{pmatrix}A_{11}(\omega,k) & A_{12}(\omega,k)\\ A_{21}(\omega,k) & A_{22}(\omega,k)\end{pmatrix}. \tag{19}$$

The matrix elements of $A(\omega,k)$ can be computed by using the configuration realization of $\hat{\chi}_k$, details of which are presented in the Appendix. It so happens that the matrix elements of $A(\omega,k)$ depend on the functions $d(\omega,k)$ and $a(\omega,k)$, that are given by

$$d(\omega,k)=\frac{1}{2}\left[\tanh(\pi\omega)+\frac{1}{4\pi}\Im\left\{\oint_{C_0}\frac{e^{i\omega z-2ik\coth(z/2)}}{\cosh(z/2)}\mathrm{d}z\right\}\right], \tag{20}$$

where C_0 is any closed path in the complex plane that contains only the pole at $z=0$, and

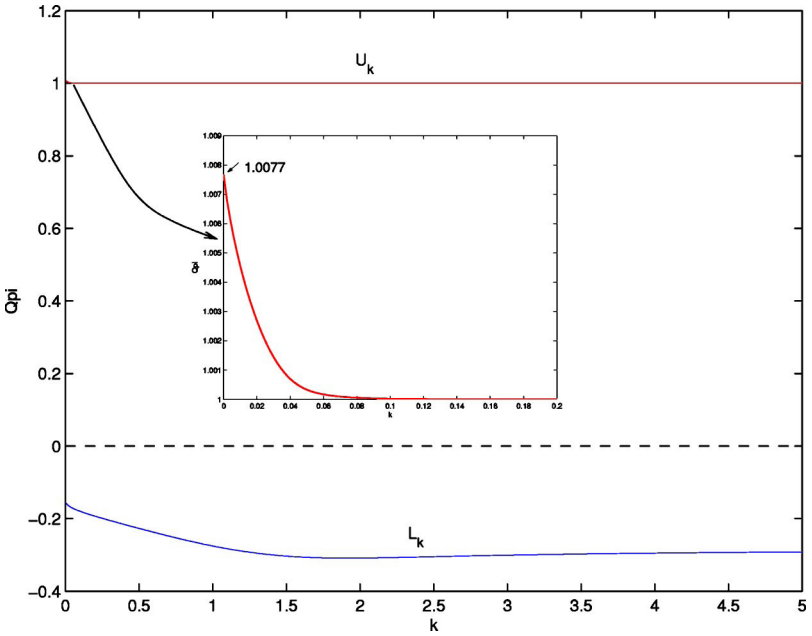

FIG. 2. (Color online) Graph of the best-possible bounds on qpis over S_k for k in the range 0 to 5. The inset graph, with k in the range 0 to 0.2, shows that the upper bound lies above 1, but converges rapidly to 1 as k increases.

$$a(\omega,k)=\frac{e^{-\pi\omega}}{2\pi}\left(\int_0^{\pi}\left(\frac{e^{\omega t-2k\tan(t/2)}}{\sin(t/2)}-\frac{\cos(\omega t-2k\tanh(t/2))}{\sinh(t/2)}\right)\mathrm{d}t-\int_{\pi}^{\infty}\frac{\cos(\omega t-2k\tanh(t/2))}{\sinh(t/2)}\mathrm{d}t\right). \tag{21}$$

The above formula is written in this way, because the individual terms in the first integral are singular at $t=0$, whereas their difference is well defined. In terms of these functions, we may expand $A(\omega,k)$ as

$$A(\omega,k)=\begin{pmatrix}\frac{1}{2}+d(\omega,k) & \frac{1}{2}\left[a(\omega,k)+ie^{-\pi\omega}\left(\frac{1}{2}+d(\omega,k)\right)\right]\\ \frac{1}{2}\left[a(\omega,k)-ie^{-\pi\omega}\left(\frac{1}{2}+d(\omega,k)\right)\right] & 0\end{pmatrix}. \tag{22}$$

Hence the spectrum of the region operator $\hat{\chi}_k$ splits into positive and negative parts, which we label by $\mu_+(\omega,k)$ and $\mu_-(\omega,k)$, respectively,

$$\mu_{\pm}(\omega,k)=\tfrac{1}{2}\left[\tfrac{1}{2}+d(\omega,k)\pm\sqrt{\left(\tfrac{1}{2}+d(\omega,k)\right)^2(1+e^{-2\pi\omega})+a(\omega,k)^2}\right]. \tag{23}$$

Of particular interest are the functions $L_k=\inf_{\omega\in\mathbb{R}}\mu_-(\omega,k)$ and $U_k=\sup_{\omega\in\mathbb{R}}\mu_+(\omega,k)$, since they provide the best-possible bounds on qpis over the hyperbolic regions S_k. Although it does not seem possible to obtain exact expressions for these functions, it is not difficult to compute the bounds after first evaluating a and d numerically.

These bounds are graphed in Fig. 2 for k in the range $[0, 5]$ from which we conclude that the upper bound on qpis over S_k remains close to but greater to 1 for all k and that this difference is greatest when $k=0$ (see inset). The lower bound displays a more marked difference from the classical bound of 0, reaching a minimum value of -0.3089 at approximately $k=1.9$, before rising again. A surprising result is that the lower bound does not approach 0 for large values of k. Nonetheless, this appears to be a characteristic feature of bounds on qpis for many classes of regions.[27]

The infinite wedge: An interesting subclass of hyperbolic regions is provided by taking the limit as $k\to 0$. The region S_0 so obtained is precisely the positive (q,p) quadrant of Γ, as depicted

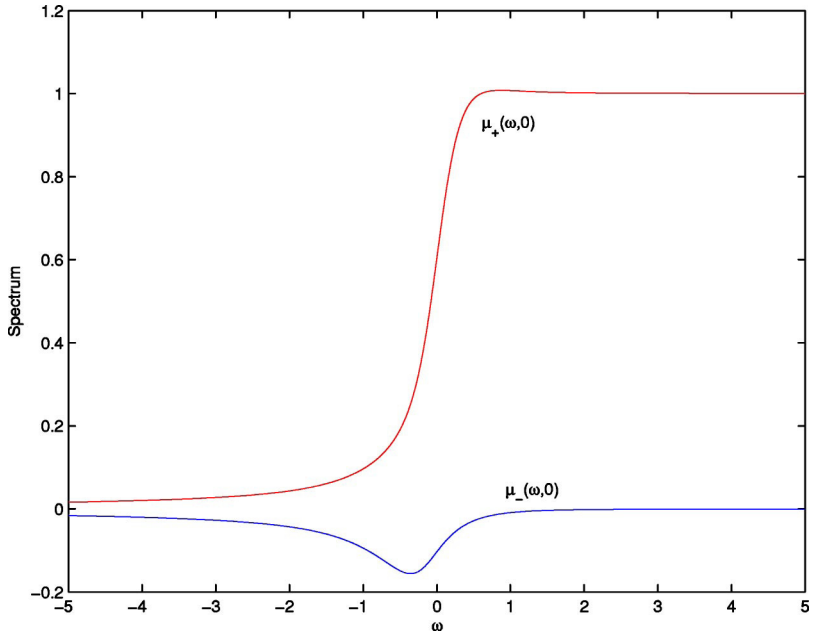

FIG. 3. (Color online) Graph of the spectrum of $\hat{\chi}_0$ which, as labeled, splits into the curves $\mu_+(\omega,0)$ and $\mu_-(\omega,0)$.

in part (b) of Fig. 1. Note that when $k=0$, the functions d and a take a simplified form,

$$d(\omega,0)) = \tfrac{1}{2}\tanh(\pi\omega), \quad a(\omega,0) = -\tfrac{1}{2}\tanh(\pi\omega) + u(\omega), \tag{24}$$

where $u(\omega)$ may be expressed as an infinite sum,[28]

$$u(\omega) = \frac{8\omega}{\pi}\sum_{n=0}^{\infty}\frac{1}{\omega^2 + (4n+1)^2}.$$

If we now apply these simplifications to the spectral formula (23), we obtain the spectrum for $\hat{\chi}_0$:

$$\mu_\pm(\omega,0) = \tfrac{1}{4}(1 + \tanh(\pi\omega) \pm \sqrt{(2u(\omega) - \tanh(\pi\omega))^2 + (1 + \tanh(\pi\omega))^2}), \tag{25}$$

which is graphed in Fig. 3. The infimum and supremum can then be determined numerically, and to an accuracy of $\pm 5\times 10^{-10}$, we have that

$$-0.155\,939\,843 < Q_0[W] < 1.007\,679\,970. \tag{26}$$

An interesting point is that these bounds are also best-possible when applied to regions defined by infinite wedges. This equivalence is due to two factors: first, by an appropriate metaplectic transformation T, the region S_0 can be transformed into any infinite wedge with half-angle $\alpha < \pi/2$. Second, the operator transformation $\hat{U}_T$ that corresponds to T is unitary, and thus the spectrum of $\hat{\chi}_0$ is preserved under its action. This implies that the spectrum of any region operator corresponding to an infinite wedge is given by (25). As a consequence, the integral of a Wigner function over any infinite wedge must lie between the bounds given in (26). Bounds on the spectrum of similar operators have been considered before, in the context of the quantum phase operator[21] and in connection with studies of probability backflow[29] but not to the same level of precision.

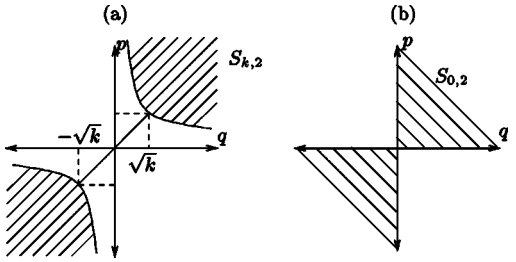

FIG. 4. Regions bounded by two hyperbolic curves, in (a) the hyperbolic region $S_{k,2}$ is shown while in (b) the double wedge $S_{0,2}$ is depicted.

IV. EXAMPLES INVOLVING TWO BOUNDARY CURVES

As a second example, consider the slightly more complicated case of a region with a boundary composed of two curves with T_σ symmetry. There are several possible forms that such a region can take,[27] however, we will concentrate on just the subcase for which the boundary curves lie in positive and negative (q,p) quadrants, as shown in part (a) of Fig. 4.

In order to further simplify matters, we assume that both curves are labeled by the variable k. We label the class of regions that remain by $S_{k,2}$ and note that this region may be written in terms of the region S_k as

$$S_{k,2} = S_k + R_\pi(S_k), \tag{27}$$

where R_π denotes a rotation through an angle π. Note that $R_\pi:(q,p)\to(-q,-p)$ and that the operator that corresponds to this transformation under the Weyl–Wigner transform is just the parity operator $\hat{P}$, which acts on the canonical coordinate and momentum operators according to

$$\hat{P}\hat{q}\hat{P} = -\hat{q}, \quad \hat{P}\hat{p}\hat{P} = -\hat{p}.$$

Due to the linearity of the Weyl quantization map, this implies that the region operator that corresponds to $S_{k,2}$ may be expressed as

$$\hat{\chi}_{k,2} = \hat{\chi}_k + \hat{P}\hat{\chi}_k\hat{P}. \tag{28}$$

This operator also commutes with $\hat{\omega}$, and hence its eigenstates can be chosen such that they are some linear combination of $\psi^\pm_\omega$. In order to find the correct linear combination, we must first determine the matrix representation of $\hat{\chi}_{k,2}$ on the subspace spanned by $\psi^\pm_\omega$. This turns out to quite simple, since the action of $\hat{P}$ on this subspace is given by $\hat{P}\psi^\pm_\omega = \psi^\mp_\omega$. Thus the matrix representation of $\hat{\chi}_{k,2}$ is given by

$$A_2(\omega,k) = A(\omega,k) + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} A(\omega,k) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} + d(\omega,k) & a(\omega,k) \\ a(\omega,k) & \frac{1}{2} + d(\omega,k) \end{pmatrix}. \tag{29}$$

The simple form of this matrix representation leads to the following expression for the spectrum of $\hat{\chi}_{k,2}$:

$$\mu_{2,\pm}(\omega,k) = \tfrac{1}{2} + d(\omega,k) \pm |a(\omega,k)|, \tag{30}$$

In this case, the eigenfunctions are odd and even combinations of $\psi^\pm_\omega$, and are independent of k,

$$\psi^\pm_{2,\omega}(x;k) \equiv \psi^\pm_{2,\omega}(x) = \frac{1}{\sqrt{2}}(\psi^+_\omega(x) \pm \psi^-_\omega(x)), \tag{31}$$

which indicates that the operators $\hat{\chi}_{k,2}$ commute for all $k \geqslant 0$.

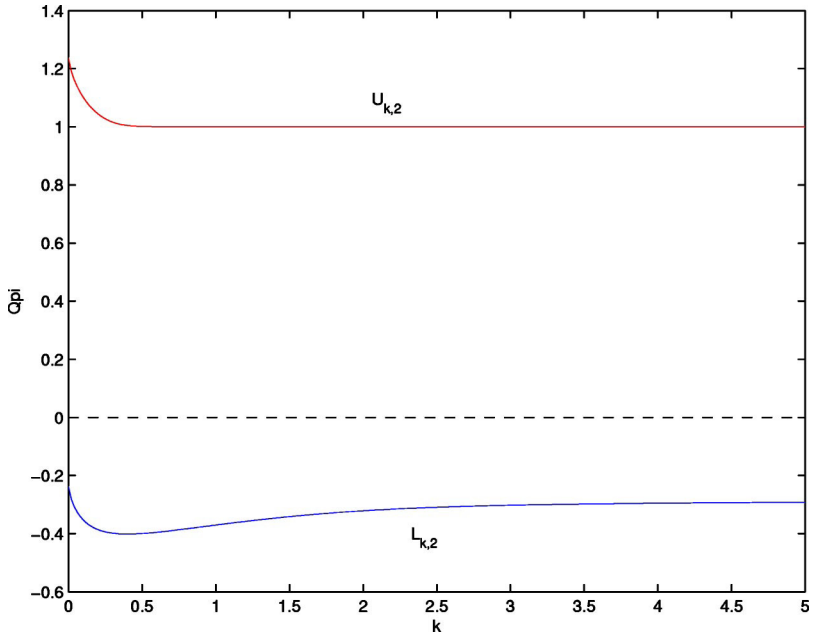

FIG. 5. (Color online) Graph of the best-possible bounds on qpis over $S_{k,2}$ for k in the range 0 to 5.

The properties of the spectrum in this case vary somewhat from the preceding example. In particular, $\mu_{2,-}(\omega,k)$ is not restricted to negative values and, similarly, $\mu_{2,+}(\omega,k)$ is not strictly positive, although clearly the inequality $\mu_{2,+}(\omega,k)\geqslant\mu_{2,-}(\omega,k)$ holds for all $\omega\in\mathbb{R}$, $k\geqslant 0$. Since the bounds on qpis over $S_{k,2}$ are given by the infimum $L_{k,2}$ and supremum $U_{k,2}$ of the spectrum of $\hat{\chi}_{k,2}$, it is these functions that are of primary importance in the context of this paper. Again, closed-form expressions do not appear to exist, so we must resort to computational techniques in evaluating these functions, the results of which are graphed in Fig. 5. In this case, the upper bound is well in excess of 1 for small values of k, but rapidly approaches 1 as k increases. The lower bound, on the other hand, dips initially, reaching a minimum of -0.4014 at $k=0.4$ before rising again, and appears to approach a finite negative value near to -0.3 as $k\rightarrow\infty$.

Double wedges: It is again of interest to consider in more detail the limit as $k\rightarrow 0$ of the region $S_{k,2}$. The resulting region $S_{0,2}$ is the union of the positive and negative (q,p) quadrants [as shown in part (b) of Fig. 4], and one might guess that qpis over such a region should be positive,[24] since it appears to be composed from the union of a set of infinite straight lines, over which the integral of the Wigner function is known to be positive. However, since these lines cross at the origin one cannot immediately apply this result and it will be shown that the true bounds on qpis lie significantly outside the [0,1] interval to which classical probabilities are restricted.

The region operator that corresponds to $\hat{\chi}_{0,2}$ may be expressed in terms of $\hat{\chi}_0$ as $\hat{\chi}_{0,2}=\hat{\chi}_0+\hat{P}\hat{\chi}_0\hat{P}$. The spectrum for this operator can be derived from (30) upon substitution of (24), from which we obtain

$$\mu_{2,\pm}(\omega,0)=\frac{1+\tanh(\pi\omega)}{2}\pm\left|u(\omega)-\frac{\tanh(\pi\omega)}{2}\right|. \tag{32}$$

This spectrum is graphed in Fig. 6, and from this one sees that the function $\mu_2=\frac{1}{2}+u(\omega)$ passes through both the infimum and the supremum of the spectrum of $\hat{\chi}_{0,2}$. Since $u(\omega)$ is an odd function, we need only calculate its global maximum in order to determine the bounds on qpis over $S_{0,2}$. Using computational techniques, this value can be obtained to great accuracy, and we find that the best-possible bounds (accurate to $\pm 5\times 10^{-10}$) on qpis over $S_{0,2}$ are

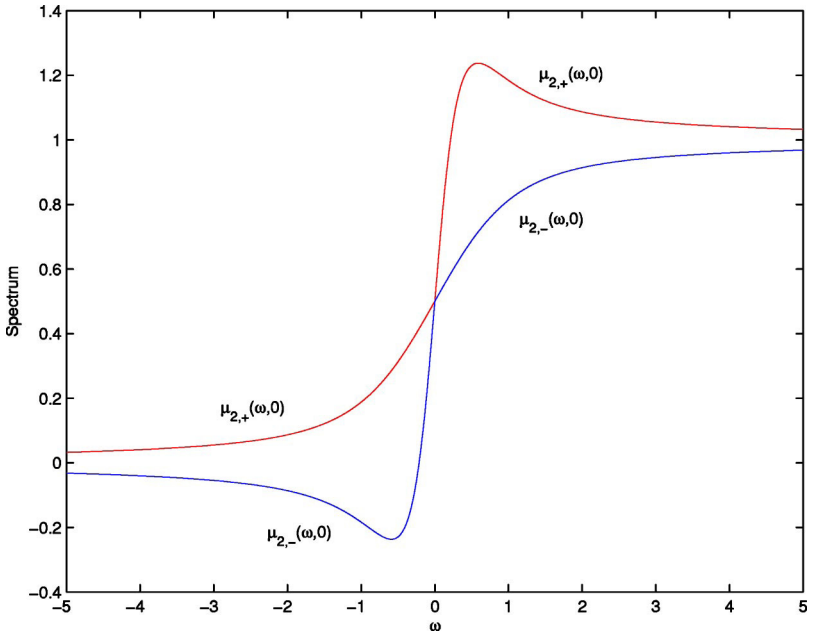

FIG. 6. (Color online) Spectrum of the double wedge operator $\hat{\chi}_{0,2}$.

$$-0.236\,823\,652 < Q_{\alpha,2}[W] < 1.236\,823\,652. \tag{33}$$

Note that the upper and lower bounds sum to 1 since they are symmetric about $1/2$. This symmetry can be explained by noting that if one rotates the region $S_{0,2}$ through an angle $\pi/2$, then one obtains its complement: i.e., $R_{\pi/2}(S_{0,2})=\Gamma/S_{0,2}=S_{0,2}^c$. Note that the integral of a Wigner function over $\Gamma=S\cup S^c$ is normalized to 1. Now, since the operator equivalent of a rotation is a unitary transformation, the region operator that corresponds to the complement of $S_{0,2}$ has precisely the spectrum given in (32). Accordingly, the spectrum of $\hat{\chi}_{0,2}$ must consist of pairs that sum to 1 and, in particular, the upper and lower bounds on this spectrum must be symmetric about $1/2$.

As in the case of the region S_0, the bounds on qpis over $S_{0,2}$ can be applied to a wider class of regions. We shall refer to elements of this wider class as double wedges, since they are formed by taking the union of an infinite wedge with its rotation through an angle π. By applying the appropriate metaplectic transformation, we can transform $S_{0,2}$ into any double wedge. The corresponding operator transformation is unitary and preserves the spectrum of $\hat{\chi}_{0,2}$, so that the spectrum of any region operator corresponding to a double wedge is given by (32). Accordingly, the integral of any Wigner function over an arbitrary double wedge must satisfy the inequality given in (33).

V. CONCLUSION

The problem of constructing best-possible bounds on integrals of the Wigner function is not only of mathematical interest, but should be of practical significance in providing checks on experimentally reconstructed quantum states. Since our approach to the problem relies on specifying the region to be integrated over, it is important to identify the types of region for which the bounds can be easily computed. In this paper, we have considered several examples of regions with a hyperbolic symmetry for which the bounds can be computed numerically from the spectrum of an exactly solvable integral equation. We have demonstrated that the bounds on integrals of the Wigner function for these regions are not equivalent to those on integrals of true probability density functions. In particular, the lower bound is significantly below zero in all cases, although it lacks the scalloped effect arising from eigenvalue crossings as seen in the bounds for elliptical

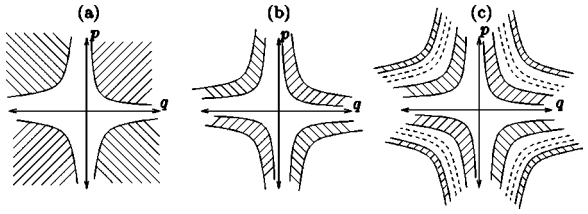

FIG. 7. Examples of generalized hyperbolic regions are shown in (a)–(c).

discs.[17] The upper bound also rises above 1 although for the most part the difference between its value and the classical bound is very small. This contrasts with the case of the disc, for which the upper bound always remains below 1.

The results herein can also be extended to more complicated regions with boundaries given by an arbitrary number of hyperbolic curves sharing the same symmetry,[27] for example, the regions shown in Fig. 7. The problem of determining the spectrum is essentially the same but the matrix representations for operators corresponding to regions with many boundaries are functions of many variables and hence the behavior of the bounds is much more difficult to characterize.

APPENDIX

The configuration kernels that correspond to (13) take the form

$$\chi_{k,K}(x,y) = \frac{H\left(\frac{x+y}{2}\right)}{2\pi}\int_{-\infty}^{\infty} H\left(p - \frac{2k}{x+y}\right)e^{i(x-y)p}\,\mathrm{d}p. \tag{A1}$$

This integral can be computed in a generalized sense,[30] and we find that

$$\chi_{k,K}(x,y) = H\left(\frac{x+y}{2}\right)e^{2ik[(x-y)/(x+y)]}\left[\frac{1}{2}\delta(x-y) - \frac{1}{2\pi i(x-y)}\right]. \tag{A2}$$

This expression for the configuration kernel of $\hat{\chi}_k$ enables us to determine the action of $\hat{\chi}_k$ on the space $\mathcal{G}'_\omega$ [recall that this is given by the matrix $A(\omega,k)$ defined in (19)]. In this representation $\hat{\chi}_k$ acts on ψ_ω as

$$(\hat{\chi}_k\psi_\omega)(x) = \int_{-x}^{\infty} e^{2ik[(x-y)/(x+y)]}\left[\frac{1}{2}\delta(x-y) - \frac{1}{2\pi i(x-y)}\right]\psi_\omega(y)\,\mathrm{d}y. \tag{A3}$$

If we substitute $\psi_\omega = \alpha_\omega\psi^+_\omega + \beta_\omega\psi^-_\omega$, then we find that the action of $\hat{\chi}_k$ when $x<0$ differs from that when $x>0$. Thus, for $x>0$,

$$\begin{aligned}(\hat{\chi}_k\psi_\omega)(x) = {}& \alpha_\omega\int_0^{\infty} e^{2ik[(x-y)/(x+y)]}\left[\frac{1}{2}\delta(x-y) - \frac{1}{2\pi i(x-y)}\right]\frac{e^{i\omega\log y}}{\sqrt{2\pi y}}\mathrm{d}y \\ & + \beta_\omega\int_{-x}^{0} e^{2ik[(x-y)/(x+y)]}\left[\frac{1}{2}\delta(x-y) - \frac{1}{2\pi i(x-y)}\right]\frac{e^{i\omega\log|y|}}{\sqrt{2\pi|y|}}\mathrm{d}y\end{aligned}$$

and for $x<0$,

$$(\hat{\chi}_k\psi_\omega)(x) = \alpha_\omega\int_{|x|}^{\infty} e^{2ik[(x-y)/(x+y)]}\left[\frac{1}{2}\delta(x-y) - \frac{1}{2\pi i(x-y)}\right]\frac{e^{i\omega\log y}}{\sqrt{2\pi y}}\mathrm{d}y.$$

It is immediately clear that $A_{22}(\omega,k)=0$, since the $x>0$ case involves only α_ω.

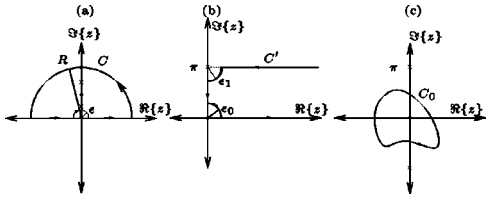

FIG. 8. The contours used in evaluating the functions $b(\omega,k)$, $a(\omega,k)$, and $d(\omega,k)$, in (a) the semicircular contour C, in (b) the contour C' used to relate $b(\omega,k)$ to $d(\omega,k)$, and in (c) an example of a contour C_0 for evaluating $R(\omega,k)$.

The other integrals can be simplified and this process leads to the following expression for the matrix elements of A:

$$A(\omega,k)=\begin{pmatrix} \frac{1}{2}+d(\omega,k) & \frac{1}{2}[a(\omega,k)+ib(\omega,k)] \\ \frac{1}{2}[a(\omega,k)-ib(\omega,k)] & 0 \end{pmatrix}, \tag{A4}$$

where the functions d, a, and b are given by

$$d(\omega,k)=\frac{1}{2\pi}\int_0^\infty \frac{\sin(\omega t-2k\tanh(t/2))}{\sinh(t/2)}\mathrm{d}t, \tag{A5}$$

$$a(\omega,k)=\frac{1}{2\pi}\int_0^\infty \frac{\sin(\omega t-2k\coth(t/2))}{\cosh(t/2)}\mathrm{d}t, \tag{A6}$$

$$b(\omega,k)=\frac{1}{2\pi}\int_0^\infty \frac{\cos(\omega t-2k\coth(t/2))}{\cosh(t/2)}\mathrm{d}t. \tag{A7}$$

Note, however, that although the integrands of a and b are bounded for all t, they become highly oscillatory in the neighborhood of the origin, which poses difficulties for numerical schemes. These problems can be alleviated by using the technique of contour integration.

In the case of $b(\omega,k)$, we consider the following contour integral in the complex plane:

$$I_C=\frac{1}{2\pi}\oint_C \frac{e^{i\omega z-2ik\coth(z/2)}}{\cosh(z/2)}\mathrm{d}z, \tag{A8}$$

where C is the contour shown in part (a) of Fig. 8. Although the contour is divided into four parts, only the integrals along the real axis contribute, since the contributions from the semicircular segments vanish in the respective limits as $\epsilon\to 0$ and $R\to\infty$. Thus one has that

$$\lim_{R\to\infty,\epsilon\to 0} I_C=2\frac{1}{2\pi}\int_0^\infty \frac{e^{i\omega t-2ik\coth(t/2)}}{\cosh(t/2)}\mathrm{d}t, \tag{A9}$$

and as a result, $b(\omega,k)=\Re\{I_C\}/2$.

We can make use of the residue theorem in evaluating I_C,

$$I_C=2\pi i\sum \mathrm{Res}\, f(z), \tag{A10}$$

where $f(z)$ is the integrand in (A8). Note that $f(z)$ has two distinct classes of residues, simple poles at $z=(2n+1)\pi i$ and essential singularities at $z=2m\pi i$, with $m\in\mathbb{Z}$. The contour C encloses only the simple poles with $n\geqslant 0$ and the essential singularities with $m\geqslant 1$, and hence the sum in (A10) is over the residues at these points.

It is easy to evaluate the residues at the simple poles and we find that the total contribution from the simple poles inside C is given by

$$\mathrm{Res}_s = \frac{1}{2\pi i}\sum_{n=0}^{\infty}(-1)^n e^{-(2n+1)\pi\omega} = \frac{\mathrm{sech}(\pi\omega)}{2\pi i}. \tag{A11}$$

The sum of the residues associated with the essential singularities can also be simplified,

$$\mathrm{Res}_e = \frac{1}{2\pi}\sum_{n=1}^{\infty}(-1)^n e^{-2n\pi\omega} R(\omega,k) = \frac{e^{-\pi\omega}\,\mathrm{sech}(\pi\omega)}{2} R(\omega,k), \tag{A12}$$

where $R(\omega,k)$ is the residue of $f(z)$ associated with the essential singularity at the origin.

Ordinarily, one might try to evaluate this residue by constructing the Laurent series for $f(z)$, however in this case the coth term in the exponential makes this extremely difficult. However, one may use the residue theorem in reverse and evaluate $R(\omega,k)$ by considering the integral of $f(z)$ over a closed contour enclosing the origin (and no other poles),

$$R(\omega,k) = \frac{1}{2\pi i}\oint_{C_1} \frac{e^{i\omega z - 2ik\,\coth(z/2)}}{\cosh(z/2)}\mathrm{d}z. \tag{A13}$$

The rapid oscillations due to the coth term do not appear in this calculation, and due to its finite range this integral can be rapidly evaluated to a high degree of accuracy using numerical techniques.

If we now collect the results for the residues together, we discover that

$$b(\omega,k) = \frac{\mathrm{sech}(\pi\omega)}{2}\left[1 + \frac{e^{-\pi\omega}}{2}\Im\{R(\omega,k)\}\right]. \tag{A14}$$

Note that in deriving these results it has been assumed that $\omega \geqslant 0$. A similar procedure (with the semicircular contour defined in the lower half-plane) enables us to extend the validity of (A14) to all $\omega \in \mathbb{R}$.

In order to obtain superior expressions for the functions $a(\omega,k)$ and $d(\omega,k)$, we choose another contour [see part (b) of Fig. 8], this time involving five curves. However, we know from the above calculation that the integral over ϵ_0 vanishes, which leaves four curves to consider. Of these, the integral over the imaginary axis from 0 to π results in a pure imaginary contribution I_π, while the integral over ϵ_1 contributes $-1/2$ in the limit as $\epsilon_1 \to 0$. The integral over the positive real axis is equal to $b(\omega,k)+a(\omega,k)i$ in the limit as $\epsilon_0 \to 0$, while the contribution from the line $(\pi i, \pi i + \infty)$ can be expressed as $-\exp(-\pi\omega)(d(\omega,k)+I_\infty i)$.

By equating the real parts, we find that

$$b(\omega,k) = e^{-\pi\omega}\left(\tfrac{1}{2} + d(\omega,k)\right). \tag{A15}$$

This leads to the expression (20) for $d(\omega,k)$ and the expression (22) for the matrix A. If we equate the imaginary parts, then we discover that

$$a(\omega,k) = e^{-\pi\omega}(I_\pi - I_\infty), \tag{A16}$$

where

$$I_\pi = \frac{1}{2\pi}\int_0^{\pi} \frac{e^{\omega t - 2k\,\tan(t/2)}}{\sin(t/2)}\mathrm{d}t, \tag{A17}$$

$$I_\infty = \frac{1}{2\pi}\int_0^{\infty} \frac{\cos(\omega t - 2k\,\tanh(t/2))}{\sinh(t/2)}\mathrm{d}t. \tag{A18}$$

Neither I_π nor I_∞ are well defined, but their difference is, and provided one expresses $a(\omega,k)$ as in (21), the singularities of these integrals are avoided.

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Alternative descriptions in quaternionic quantum mechanics

A. Blasi,[a] G. Scolarici,[b] and L. Solombrino[c]
Dipartimento di Fisica, Università di Lecce and INFN, Sezione di Lecce, I-73100 Lecce, Italy

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We characterize the quasianti-Hermitian quaternionic operators in quaternionic quantum mechanics by means of their spectra; moreover, we state a necessary and sufficient condition for a set of quasianti-Hermitian quaternionic operators to be anti-Hermitian with respect to a uniquely defined positive scalar product in a infinite dimensional (right) quaternionic Hilbert space. According to such results we obtain two alternative descriptions of a quantum optical physical system, in the realm of quaternionic quantum mechanics, while no alternative can exist in complex quantum mechanics, and we discuss some differences between them. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1873040]

I. INTRODUCTION

Many attempts have been made in the past in order to formulate quantum mechanics in Hilbert spaces over the skew-field **Q** of quaternions. In the early 1960s a systematic approach began to quaternionic quantum mechanics (QQM);[1] at present, a clear and detailed review of this theory, together with the foundations of quaternionic quantum field theory, can be found in Ref. 2.

It is worth noting that an important difference exists between complex and quaternionic quantum mechanics about Hamiltonians operators and observables. In both theories, observables are associated with self-adjoint (or Hermitian) operators, whereas Hamiltonians are Hermitian in complex quantum mechanics (CQM), but they are anti-Hermitian in QQM, and the same happens for the symmetry generators, like the angular momentum operators. Moreover, in CQM any anti-Hermitian operator can be made Hermitian (and vice versa) by multiplying by i. In QQM in contrast, an anti-Hermitian operator cannot be trivially converted to a Hermitian one by multiplying by a c-number; actually in this context in order to obtain such a conversion one needs a "phase" operator.[2]

Thus, if one wishes to enlarge the theoretical framework and to generalize standard quaternionic Hamiltonians and symmetry generators (as happened in CQM where pseudo-Hermiticity has been fruitfully introduced), in QQM one rather needs to deal with *pseudoanti-Hermitian* quaternionic operators.

Definition (Ref. 3): A quaternionic linear operator H is said to be (η-) pseudoanti-Hermitian if a linear invertible Hermitian operator η exists such that

$$\eta H \eta^{-1} = -H^{\dagger}. \tag{1}$$

If Eq. (1) holds with a bounded positive definite η, H is said *quasianti-Hermitian*.

Of course, several η can exist which verify Eq. (1). The properties of pseudoanti-Hermitian Hamiltonians in QQM are analogous to the ones of pseudo-Hermitian in CQM. In particular, a

[a]Electronic mail: blasi@le.infn.it
[b]Electronic mail: scolarici@le.infn.it
[c]Electronic mail: solombrino@le.infn.it

new inner product in the Hilbert space can be associated with any bounded positive definite η which fulfills Eq. (1), and different η's give rise to alternative descriptions.[4]

In this paper, we preliminarly characterize in Sec. II the subclass of quasianti-Hermitian quaternionic operators with discrete spectrum (in finite dimensional vector spaces), showing that they are necessarily diagonalizable operators with imaginary eigenvalues (and vice versa). Next, facing the unity problem, we derive in Sec. III a necessary and sufficient condition for a set of quasianti-Hermitian operators to be anti-Hermitian with respect to a uniquely defined scalar product in quaternionic Hilbert spaces. Finally, we consider in Sec. IV two alternative descriptions of a physical system in quantum optics, which are possible only in the realm of QQM, according with the previous result, and we discuss some differences between them.

II. QUASIANTI-HERMITIAN QUATERNIONIC OPERATORS

In this section, we characterize the subclass of quasianti-Hermitian quaternionic operators by means of their spectra, in strict analogy with similar statements in CQM.[5,6] The following proposition, which holds in finite dimensional Hilbert spaces, provides a necessary and sufficient condition for a quaternionic operator with discrete spectrum to be quasianti-Hermitian.

Proposition 1: Let H be a quaternionic linear operator with discrete spectrum. Then, a definite operator η exists such that H is η-pseudoanti-Hermitian (hence, η-quasianti-Hermitian) if and only if H is diagonalizable with imaginary spectrum.

Proof: Let H be a pseudoanti-Hermitian operator. We preliminarily observe that, being in any case η an invertible operator, all its eigenvalues must be different from zero, so that either η is definite or it is indefinite. Now, let us suppose that a positive (respectively, negative) definite operator η exists which fulfills condition (1); then, an R exists such that $\eta = R^\dagger R$ (Ref. 7) (respectively, $\eta = -R^\dagger R$), and by Eq. (1) we obtain

$$RHR^{-1} = -R^{\dagger -1} H^\dagger R^\dagger = -(RHR^{-1})^\dagger,$$

i.e., RHR^{-1} is anti-Hermitian, hence it is diagonalizable and it has an imaginary spectrum.[2] The same conclusion holds obviously with regard to H, since on a right quaternionic vector space the similarity transformations preserve the properties of the spectrum, in the sense that the real part and the moduli of the imaginary part of the eigenvalues do not change under (quaternionic) similarity transformations.

Conversely, if H is diagonalizable with imaginary spectrum, then by proposition 2 of Ref. 3, a positive definite operator $\eta = SS^\dagger$ exists which fulfills condition (1). ■

We remark that the above Proposition still holds in infinite dimensional Hilbert spaces $\mathcal{H}^Q$ if one assumes that the eigenvalues of H have finite multiplicity and there is a basis on $\mathcal{H}^Q$ in which H is block diagonal with finite dimensional blocks (see also Ref. 6).

As a consequence of Proposition 1, any quasianti-Hermitian operator H with discrete spectrum can be written by means of a set of biorthonormal vectors (if we suitably fix their phases) as[3,2]

$$H = \sum_n \sum_{a=1}^{d_n} |\psi_n, a\rangle i E_n \langle \phi_n, a|, \quad E_n \geqslant 0,$$

where d_n denotes the degeneracy associated to the nth eigenvalue, a is a degeneracy label, and the usual relations for a biorthonormal basis hold,

$$\langle \phi_m, b|\psi_n, a\rangle = \delta_{mn}\delta_{ba},$$

$$\sum_n \sum_{a=1}^{d_n} |\psi_n, a\rangle\langle \phi_n, a| = \sum_n \sum_{a=1}^{d_n} |\phi_n, a\rangle\langle \psi_n, a| = \mathbf{1}.$$

III. ALTERNATIVE DESCRIPTIONS OF QUANTUM SYSTEMS

As we already pointed out in the Introduction, different (alternative) description of the same physical system in a quaternionic Hilbert space $\mathcal{H}^Q$ are possible whenever different η's fulfill condition (1). Indeed, *for any bounded self-adjoint positive definite* η*, the space* H^Q *endowed with the scalar product* $\langle\varphi|\psi\rangle_\eta=\langle\varphi|\eta|\psi\rangle$ *is a Hilbert space* H^Q_η.

We do not report here the explicit proof of this property, which was already stated in CQM;[8] indeed the proof easily follows from the one in the complex case since all the key steps in it still hold in a quaternionic Hilbert space, as for instance the closed graph theorem[9] and the uniticity of the decomposition $\eta=S^2$, with S positive and self-adjoint.[10]

Hence, an undesirable ambiguity can arise, as we will explicitly show in the next section by means of a physical example; in order to remove that and obtain a proper (quaternionic) quantum mechanical interpretation, we will resort to the concept of irreducibility of the physical operators on $\mathcal{H}^Q$.

As a preliminary step, we state the following lemma, which actually is very similar to the quaternionic version of the corollary of the Schur lemma (on the irreducible quaternionic group representations of unitary operators)[10] and can be easily proven in the same way.

Lemma: Let $\{H_i\}$ $(i=1,2,\ldots,N)$ *be an irreducible set of anti-self-adjoint bounded quaternionic linear operators on the (right) quaternionic Hilbert space* $\mathcal{H}^Q$*. Then, the commutant of* $\{H_i\}$*, i.e., the set of all bounded quaternionic linear operators which commute with each* H_i *is composed of the operators* $T=h\mathbf{1}+a\mathbf{I}_a$ (*where* h, $a\in\mathbf{R}$, *and* $\mathbf{I}_a$ *is a unitary, anti-Hermitian operator on* $\mathcal{H}^Q$).

Thus, the following proposition provides a necessary and sufficient condition for a set of η-quasianti-Hermitian quaternionic operators to admit a unique positive definite operator η which satisfy the quasianti-Hermiticity condition.

Proposition 2: Let $\{H_i\}$ *be a set of bounded* η*-quasianti-Hermitian operators on a right quaternionic Hilbert space* $\mathcal{H}^Q$*, where* η *denotes a bounded positive self-adjoint operator. Then,* η *is uniquely determined up to a global normalization factor if and only if the set* $\{H_i\}$ *is irreducible on* $\mathcal{H}^Q$.

Proof: First, we observe that, by assumption, all the quasianti-Hermitian operators in the set $\{H_i\}$ are bounded both on $\mathcal{H}^Q$ and on $\mathcal{H}^Q_\eta$, since $\|H_ix\|_\eta=\|SH_ix\|\leqslant\|SH_iS^{-1}\|\|Sx\|=\|SH_iS^{-1}\|\|x\|_\eta$ (where the decomposition $\eta=S^2$, with S positive, self-adjoint has been used[10]); furthermore, they are anti-self-adjoint on $\mathcal{H}^Q_\eta$ because $\eta H_i=-H_i^\dagger\eta\ \forall i=1,2,\ldots,N$. Assume now that an η' exists with the same properties as η. Then, it follows that $[\eta'^{-1}\eta,H_i]=0\ \forall i=1,2,\ldots,N$. Hence, by the previous lemma, $\eta=\eta'(h\mathbf{1}+a\mathbf{I}_a)$. But imposing the Hermiticity condition on η, one easily obtains $\eta'(h\mathbf{1}+a\mathbf{I}_a)=(h\mathbf{1}-a\mathbf{I}_a)\eta'$, which implies either $a=0$ or $\{\eta',\mathbf{I}_a\}=0$. Denoting by $|\eta'\rangle$ an eigenvector of η': $\eta'|\eta'\rangle=|\eta'\rangle\alpha$ (where $\alpha>0$, since η' is positive) the condition $\{\eta',\mathbf{I}_a\}=0$ would imply $\eta'(\mathbf{I}_a|\eta'\rangle)=-(\mathbf{I}_a|\eta'\rangle)\alpha$, i.e., an eigenvector of η' would exist associated with a negative eigenvalue, contradicting thus the hypothesis on the positive definiteness of η'. Then, $a=0$ and $\eta=\eta'h$.

The converse is easily proven by merely paraphrasing the analogous proof in complex Hilbert spaces.[8] ■

As a consequence of the above proposition, any reducible set $\{H_i\}$ of quasianti-Hermitian operators admits at least two quite different positive operators η and η' which fulfill the quasianti-Hermiticity condition for any operator belonging to this set. This allows us to construct two different Hilbert spaces $\mathcal{H}^Q_\eta$ and $\mathcal{H}^Q_{\eta'}$, endowed with scalar products $\langle\varphi|\eta|\psi\rangle$ and $\langle\varphi|\eta'|\psi\rangle$, respectively, such that any H_i is anti-Hermitian on $\mathcal{H}^Q_\eta$ as well as on $\mathcal{H}^Q_{\eta'}$.

In particular, any reducible set of anti-Hermitian operators $\{H_i\}$ on $\mathcal{H}^Q$ will appear at the same time as a set of anti-Hermitian operators on the Hilbert space $\mathcal{H}^Q_\eta$ where η denotes a bounded, nontrivial, positive operator which commutes with any element of $\{H_i\}$.

This is just the scenario of the example we will study in the next section, which exactly mimics an analogous situation in CQM, where alternative descriptions arise in correspondence with different η's which fulfill the quasi-Hermiticity condition for a set $\{H_i\}$.[4,8]

IV. A PHYSICAL EXAMPLE

Let us consider a two level quantum optical system in the *complex* Hilbert space $\mathcal{H}$ whose dynamics is described by the complex anti-Hermitian time-dependent Hamiltonian,

$$H = 2\Omega_0(t)J_1 + 2\Omega_1(t)J_2 + \omega(t)J_3 \quad (\hbar = 1), \tag{2}$$

where $\Omega_0(t)$, $\Omega_1(t)$, and $\omega(t)$ are real valued functions of the time t, and the anti-Hermitian operators J_l ($l=1,2,3$) obey the usual rules of commutation of the su(2) algebra

$$[J_l, J_m] = -\varepsilon_{lmn}J_n.$$

As we already noted in the Introduction, H times i is of course an observable in CQM, and it coincides with the one introduced in order to describe the interaction of a chirped classical electromagnetic field with a two level atomic system in a complex Hilbert space.[11] This model has been extensively studied also to explain the Berry phase.[12]

By resorting to the irreducible two-dimensional representation of the J operators

$$J_1 = \frac{i}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad J_2 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad J_3 = \frac{i}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3}$$

and setting $\Omega = \Omega_0 + i\Omega_1$, we can write the Hamiltonian (2) as a 2×2 anti-Hermitian complex matrix,

$$H = i\begin{pmatrix} \dfrac{\omega(t)}{2} & \Omega^*(t) \\ \Omega(t) & -\dfrac{\omega(t)}{2} \end{pmatrix}. \tag{4}$$

The set $\mathfrak{h}$ of anti-Hermitian complex operators obtained by changing the entries in Eq. (4), is of course irreducible in the two-dimensional (complex) Hilbert space $\mathcal{H}$, since such is the spinorial representation (3) of the J_l's.

From a different point of view, we can interpret the Hamiltonian (4) as a *anti-Hermitian quaternionic operator* in a (right) quaternionic Hilbert space $\mathcal{H}^Q$, and the dynamics of our quantum system is then described by the Schrödinger equation[2]

$$\frac{d}{dt}|\boldsymbol{\Psi}\rangle = -H|\boldsymbol{\Psi}\rangle, \tag{5}$$

where $|\boldsymbol{\Psi}\rangle$ belongs to $\mathcal{H}^Q$. (We recall that in QQM the eigenvalues of a anti-Hermitian Hamiltonian are imaginary quaternions, whose moduli represent the values of the energy of the system.)

Roughly speaking, $\mathcal{H}^Q$ can be obtained from $\mathcal{H}$ by simply adding to each complex vector $|v\rangle \in \mathcal{H}$ a term $|v'\rangle j$, where $|v'\rangle \in \mathcal{H}$ and $j : j^2 = -1$ is a quaternionic unity different from i; note that $\dim \mathcal{H}^Q = \dim \mathcal{H} = 2$. Actually the various manner in which one can *quaternionify* a complex Hilbert space are all equivalent to this one.[13]

Now, let us denote by $|\boldsymbol{\Psi}\rangle = \begin{pmatrix} \boldsymbol{\Psi}_{\alpha,+} + \boldsymbol{\Psi}_{\beta,+}j \\ \boldsymbol{\Psi}_{\alpha,-} + \boldsymbol{\Psi}_{\beta,-}j \end{pmatrix} \equiv \begin{pmatrix} \boldsymbol{\Psi}_+ \\ \boldsymbol{\Psi}_- \end{pmatrix}$ (where $\boldsymbol{\Psi}_{\alpha,\pm}, \boldsymbol{\Psi}_{\beta,\pm}$ are complex functions of t) the quaternionic state vector representing the system; the components $\boldsymbol{\Psi}_-$ and $\boldsymbol{\Psi}_+$ can be interpreted from a physical point of view as the probability amplitudes for the system of being in the lowest or in the excited state, respectively. From the Schrödinger equation one immediately gets the time evolution of the components $\Psi_\pm$,

$$\boldsymbol{\Psi}'_{\alpha,+} = \frac{i}{2}\omega(t)\boldsymbol{\Psi}_{\alpha,+} + i\Omega^*(t)\boldsymbol{\Psi}_{\alpha,-}, \tag{6a}$$

$$\boldsymbol{\Psi}'_{\alpha,-} = -\frac{i}{2}\omega(t)\boldsymbol{\Psi}_{\alpha,-} + i\Omega(t)\boldsymbol{\Psi}_{\alpha,+}, \tag{6b}$$

$$\boldsymbol{\Psi}'_{\beta,+} = \frac{i}{2}\omega(t)\boldsymbol{\Psi}_{\beta,+} + i\Omega^*(t)\boldsymbol{\Psi}_{\beta,-}, \tag{7a}$$

$$\boldsymbol{\Psi}'_{\beta,-} = -\frac{i}{2}\omega(t)\boldsymbol{\psi}_{\beta,-} + i\Omega(t)\boldsymbol{\Psi}_{\beta,+}. \tag{7b}$$

where the prime denotes a time derivative.

Since the systems in (6) and (7) are identical, and they represent a rotation of the vector $\boldsymbol{\Psi}$ in the complex space, we can write their solutions as a whole using the Cayley–Klein (CK) matrix, *independently on the quaternionic or complex character of* $\boldsymbol{\Psi}_{\pm}$,

$$\begin{pmatrix} \boldsymbol{\Psi}_+ \\ \boldsymbol{\Psi}_- \end{pmatrix} = \begin{pmatrix} F^* & G \\ -G^* & F \end{pmatrix} \begin{pmatrix} \boldsymbol{\Psi}_+(0) \\ \boldsymbol{\Psi}_-(0) \end{pmatrix}, \tag{8}$$

where $F(t)$ and $G(t)$ are complex functions depending on ω and Ω in a rather involved way; furthermore $F(0)=1$, $G(0)=0$, and $|F|^2+|G|^2=1$.[11]

The CK matrix can be regarded as the matrix representation of the time evolution operator U associated with the time-dependent Hamiltonian (4), and it belongs to a two-dimensional (complex) unitary representation of the SU(2) group; by varying H in $\mathfrak{h}$, we correspondingly obtain a set $\mathfrak{U}=\{U\}$.

We remark once again that the form of any element $U \in \mathfrak{U}$ does not depend on the scalar field, **C** or **Q**, adopted. Now, as long as we study the two-level system in $\mathcal{H}$, the set $\mathfrak{U}$ is clearly irreducible, hence, by the corollary of the Schur lemma, no nontrivial η exists which commutes with it. Recalling the discussion at the end of the preceding section, we can conclude that the description of the system in $\mathcal{H}$ is unique.

On the contrary, if we now consider $\mathfrak{U}$ as a quaternionic group representation acting on $\mathcal{H}^Q$, it can be proven that this representation is reducible into the direct sum of two equivalent unidimensional irreducible quaternionic representations on $\mathcal{H}^Q$,[14,15] so that $\mathfrak{U}$ admits a nontrivial commutant. By a direct computation, the most general quaternionic Hermitian matrix η commuting with any $U \in \mathfrak{U}$ (hence with any $H \in \mathfrak{h}$) is

$$\eta = \begin{pmatrix} a & jz \\ -jz & a \end{pmatrix}, \quad z \in \mathbf{C}. \tag{9}$$

Since its matrix elements are independent of ω and Ω, η is a *secular* metric in the sense of Ref. 16.

Moreover, η is positive definite whenever $a > |z|$, as one can prove by solving the eigenvalue problem associated with it.[17]

We can conclude that any element $U \in \mathfrak{U}$ is unitary on $\mathcal{H}^Q$,

$$U^\dagger U = \mathbf{1}, \tag{10}$$

and, moreover, it is η-unitary on $\mathcal{H}^Q_\eta$,[18] i.e.,

$$U^\dagger \eta U = \eta. \tag{11}$$

Alternatively, we can say that the Hamiltonian H given in Eq. (4) is anti-Hermitian on $\mathcal{H}^Q$ as well as on the Hilbert space $\mathcal{H}^Q_\eta$ endowed with the scalar product $\langle\Psi|\eta|\Phi\rangle$, since

$$H = \eta H \eta^{-1} = -H^\dagger, \tag{12}$$

where η is given in Eq. (9).

Then, we may describe the dynamics of our system in $\mathcal{H}^Q$ or in $\mathcal{H}^Q_\eta$. Moreover, if the value $a=1$ is chosen in Eq. (9), one obtains that for each vector $|\psi_c\rangle$ with *complex components* $\langle\psi_c|\psi_c\rangle=\langle\psi_c|\eta|\psi_c\rangle$. The relevant physical quantities with respect to both the alternative descriptions can now be easily computed.

Let us compute first the diagonal matrix elements of the angular momentum operators and of the Hamiltonian when the system is described by the vector $|+\rangle=\binom{1}{0}$ and $|-\rangle=\binom{0}{1}$. (In the sequel by an abuse of language, we will call them *expectation values.*) One easily obtains

$$\langle\pm|J_1|\pm\rangle=0, \quad \langle\pm|\eta J_1|\pm\rangle=\mp\tfrac{1}{2}kz,$$

$$\langle\pm|J_2|\pm\rangle=0, \quad \langle\pm|\eta J_2|\pm\rangle=\mp\tfrac{1}{2}jz,$$

$$\langle\pm|J_3|\pm\rangle=\langle\pm|\eta J_3|\pm\rangle=\pm\frac{i}{2},$$

$$\langle\pm|H|\pm\rangle=\pm\frac{i}{2}\omega, \quad \langle+|\eta H|+\rangle=\frac{i}{2}\omega-kz\Omega, \quad \langle-|\eta H|-\rangle=-\frac{i}{2}\omega-kz\Omega^*.$$

All these values are obviously imaginary quaternions. In particular the moduli of the mean values of H are

$$|\langle\pm|H|\pm\rangle|=\frac{|\omega|}{2}, \quad |\langle\pm|\eta H|\pm\rangle|=\sqrt{\frac{\omega^2}{4}+|z|^2|\Omega|^2}, \tag{13}$$

showing then a sharp difference between the two descriptions, which however vanishes as $|z|\to 0$.

More generally, by using the previous results, one can compute all the expectation values associated with any vector $|\mathbf{\Psi}\rangle=\binom{\mathbf{\Psi}_+}{\mathbf{\Psi}_-}$ ($\mathbf{\Psi}_\pm\in\mathbf{Q}$), being trivially $|\mathbf{\Psi}\rangle=|+\rangle\mathbf{\Psi}_++|-\rangle\mathbf{\Psi}_-$. The only obvious warning concerns the norm of $|\mathbf{\Psi}\rangle$, since (as one can obtain by an easy calculation)

$$\langle\mathbf{\Psi}|\eta|\mathbf{\Psi}\rangle=|\mathbf{\Psi}_+|^2+|\mathbf{\Psi}_-|^2+2\,\mathrm{Re}\{\overline{\mathbf{\Psi}}_+jz\mathbf{\Psi}_-\}\neq\langle\mathbf{\Psi}|\mathbf{\Psi}\rangle. \tag{14}$$

(Here, $\overline{\mathbf{\Psi}}_+$ denotes the quaternionic conjugate of $\mathbf{\Psi}_+$.)

Finally, making resort to the form (8) of the evolution operator U, we can also compute the transition probabilities in both the descriptions. Let us for instance assume that the system is in the excited state $|+\rangle$ at $t=0$; the probability of finding the system in the ground state $|-\rangle$ at the time t is given by

$$\mathcal{P}_{+\to-}(t)=|\langle-|U|+\rangle|^2=|G|^2 \tag{15}$$

according to the first description, and by

$$\mathcal{P}'_{+\to-}(t)=|\langle-|\eta U|+\rangle|^2=|z|^2|F|^2+|G|^2. \tag{16}$$

according to the alternative description.[19]

We emphasize in conclusion that the possibility of an alternative description for this model can only occur in QQM, which then appears as a theory intrinsically different from CQM, and not a mere trascription of it.

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Conditions for multiplicativity of maximal ℓ_p-norms of channels for fixed integer p

Vittorio Giovannetti
NEST-INFM and Scuola Normale Superiore, Piazza dei Cavalieri 7, I-56126, Pisa, Italy

Seth Lloyd
Massachusetts Institute of Technology, Department of Mechanical Engineering and Research Laboratory of Electronics, Cambridge, Massachusetts 02139

Mary Beth Ruskai
Department of Mathematics, Tufts University, Medford, Massachusetts 02155

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We introduce a condition for memoryless quantum channels which, when satisfied guarantees the multiplicativity of the maximal ℓ_p-norm with p a fixed integer. By applying the condition to qubit channels, it can be shown that it is not a necessary condition, although some known results for qubits can be recovered. When applied to the Werner-Holevo channel, which is known to violate multiplicativity when p is large relative to the dimension d, the condition suggests that multiplicativity holds when $d \geqslant 2^{p-1}$. This conjecture is proved explicitly for $p=2,3,4$. Finally, a new class of channels is considered which generalizes the depolarizing channel to maps which are combinations of the identity channel and a noisy one whose image is an arbitrary density matrix. It is shown that these channels are multiplicative for $p=2$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1862094]

I. INTRODUCTION

A noisy quantum channel can be described by[9,26,29] means of a completely positive, trace-preserving (CPT) map $\mathcal{E}$ which transforms the density matrices γ on the Hilbert space $\mathcal{H}$ into the output states $\mathcal{E}(\gamma)$. Such maps can always be represented[8,26,29] in the form

$$\mathcal{E}(\gamma) = \sum_k A_k \gamma A_k^\dagger, \quad \sum_k A_k^\dagger A_k = \mathbb{1}, \tag{1}$$

with $\{A_k\}$ called a set of Kraus operators associated with $\mathcal{E}$. When the channel is memoryless,[6] m successive uses are described by the map $\mathcal{E}^{\otimes m}$. It is natural to ask if entangled inputs can decrease the effects of noise for memoryless channels[5] in some way.

One measure of the effect of noise is the maximal ℓ_p-norm of a channel, which is defined as

$$\nu_p(\mathcal{E}) \equiv \sup_{\gamma \in \mathcal{D}(\mathcal{H})} \|\mathcal{E}(\gamma)\|_p, \quad p \geqslant 1, \tag{2}$$

where $\|A\|_p \equiv (\mathrm{Tr}|A|^p)^{1/p}$ is the p-norm of the operator A and where the supremum is taken over all $\mathcal{D}(\mathcal{H})$, the set of density matrices. The quantity $\mathrm{Tr}[\mathcal{E}(\gamma)^p]$ is a measure of the closeness of the output to a pure state, and $\nu_p(\mathcal{E})=1$ if and only if some output state $\mathcal{E}(\gamma)$ is pure. Because the Rényi entropy[30] can be written as $S_p(\rho)=[-1/(p-1)]\log\|\rho\|_p^p$ one could define a maximal output Rényi entropy[2,13,14] satisfying $(p-1)S_{p,\max}(\mathcal{E})=-p\log\nu_p(\mathcal{E})$.

Amosov, Holevo, and Werner (AHW) conjectured[4] that $\nu_p(\mathcal{E})$ is multiplicative for tensor product channels

$$\nu_p(\mathcal{E}^{\otimes m}) \equiv \sup_{\Gamma \in \mathcal{D}(\mathcal{H}^{\otimes m})} \|\mathcal{E}^{\otimes m}(\Gamma)\|_p = [\nu_p(\mathcal{E})]^m, \tag{3}$$

where $\mathcal{E}^{\otimes m}$ is the CPT map which describes m successive memoryless uses of the channel $\mathcal{E}$, and where the maximization in the second term of Eq. (3) is now performed over the density matrices $\Gamma \in \mathcal{D}(\mathcal{H}^{\otimes m})$. The AHW conjecture requires that a product state Γ saturates the supremum of $\nu_p(\mathcal{E}^{\otimes m})$ for the memoryless channel $\mathcal{E}^{\otimes m}$ so that entangled input states Γ do not increase the output norm. One rationale for the multiplicativity hypothesis[4] is the physical intuition that quantum coherence among successive channel uses should be degraded by the action of a memoryless channel. Since the ℓ_p-norm "measures" the purity of the states emerging from the channel, one might expect separable inputs to perform better than entangled inputs. The multiplicativity of $\nu_p(\mathcal{E}^{\otimes m})$ is equivalent to additivity for the minimum Rényi entropy with the same p.[2,13,14] Moreover, if (3) holds for p arbitrarily close to 1, then it implies[4] the additivity of the minimum output von Neumann entropy,[24] another measure of output purity. This has been shown[33] to be related to a conjectured additivity property of the Holevo information,[15] and to conjectures about additivity and superadditivity of the entanglement of formation.[1,27]

Subsequently, Werner and Holevo[34] showed that the general multiplicativity conjecture is false by producing a channel that violates (3) for $p > 4.79$. Nevertheless, one might still expect multiplicativity to hold for some range of p, most notably $1 \leqslant p \leqslant 2$ and this would suffice for many applications in quantum information theory. However, even the case $p=2$ is still not resolved. It is hence important to understand under which circumstances and for which values of p a given channel satisfies Eq. (3). Many authors have tackled this problem by discussing special situations for which the conjecture can be proved.[2,3,10,13,18–23,25,28,32] In the case of a fixed integer p, we provide an upper bound for $\nu_p(\mathcal{E}^{\otimes m})$, and derive a pair of sufficient conditions, either of which ensures that $\mathcal{E}$ satisfies the multiplicativity conjecture (3).

The material is organized as follows. In Sec. II we introduce some notation and present a linearization technique that allows one to compute the ℓ_p-norm of integer order as the expectation value of an operator defined on an extended Hilbert space. In Sec. III we derive our upper bound and show how it leads to a sufficient condition for the multiplicativity of the ℓ_p-norm. Then we apply our condition to several classes of channels. By considering qubit channels in the case $p=2$, we show in Sec. IV A that our sufficient condition is not necessary. We also obtain new proofs of multiplicativity when the two shortest axes of the image ellipsoid (whether or not shifted) are equal. In Sec. IV B we prove multiplicativity when $p=2$ for a shifted depolarizing channel and further generalizations which do not seem to have been considered in the literature. Finally, in Sec. IV C we consider the Werner–Holevo channel[34] for $p=2,3,4$, and obtain new results about multiplicativity when $p=3,4$. We also conjecture that the channel is multiplicative for *any* p when it acts on a space of dimension $d \geqslant 2^{p-1}$.

We include several appendices. The first reviews useful facts about operators, including Hilbert–Schmidt duality, shift and permutation operators, and double stochastic matrices. Appendix A also contains information about the notation, and the proof of an important identity. Appendix B discusses properties and alternative forms of the linearizing operators we use. Appendix C provides details needed for our analysis of the Werner–Holevo channel.

II. LINEARIZATION OF *p*-NORM FUNCTIONS

A. Basic linearization strategy

In this section we present a method, introduced in Ref. 13, that allows one to compute the ℓ_p-norm from the expectation value of a operator defined in an extended Hilbert space. For any integer p, it is possible to find a linear operator $X(\mathcal{E},p)$ defined in the extended Hilbert space $\mathcal{H}^{\otimes p}$ such that, for any density matrix $\gamma \in \mathcal{H}$, we have

$$\mathrm{Tr}[\mathcal{E}(\gamma)]^p = \mathrm{Tr}[(\underbrace{\gamma \otimes \gamma \otimes \cdots \otimes \gamma}_{p\text{-times}})X(\mathcal{E},p)], \tag{4}$$

where the trace on the left-hand side is computed with respect to an orthonormal basis of $\mathcal{H}$, while

the trace on the right-hand side is computed with respect to an orthonormal basis of $\mathcal{H}^{\otimes p}$. In other words, we can represent the p-purity functionTr$[\mathcal{E}(\gamma)]^p$ as the expectation value of $X(\mathcal{E},p)$ on p copies of γ. The operator $X(\mathcal{E},p)$ is not uniquely defined; in fact, it can be realized by the action of tensor products of the dual map of $\mathcal{E}$ on any permutation operator acting on $\mathcal{H}^{\otimes p}$ whose shortest cycle is length p.

To make this explicit, we need some notation, which is explained in more detail in Appendix A, particularly Appendixes A 1 and A 2. We will use a hat to denote the dual, or adjoint, map $\hat{\mathcal{E}}$ with respect to the Hilbert–Schmidt inner product. Let L_p and R_p denote the left and right cyclic shifts which can be defined by their action on an orthonormal product basis as

$$L_p|\xi_1\xi_2\cdots\xi_{p-1}\xi_p\rangle = |\xi_2\cdots\xi_p\xi_1\rangle, \tag{5a}$$

$$R_p|\xi_1\xi_2\cdots\xi_{p-1}\xi_p\rangle = |\xi_p\xi_1\cdots\xi_{p-1}\rangle, \tag{5b}$$

where $|\xi_1\xi_2\cdots\xi_{p-1}\xi_p\rangle = \otimes_{j=1}^{p}|\xi_j\rangle$ and $\{|\xi_k\rangle\}$ is an orthonormal basis for $\mathcal{H}$. Then the operator

$$\Omega(\mathcal{E},p) = \hat{\mathcal{E}}^{\otimes p}(L_p) \tag{6}$$

satisfies (4). This follows from

$$\begin{aligned}\mathrm{Tr}\ \gamma^{\otimes p}\Omega(\mathcal{E},p) &= \mathrm{Tr}(\gamma\otimes\ \gamma\otimes\ \cdots\ \otimes\ \gamma)\hat{\mathcal{E}}^{\otimes p}(L_p)\\ &= \mathrm{Tr}[\mathcal{E}(\gamma)\otimes\mathcal{E}(\gamma)\otimes\ \cdots\ \otimes\mathcal{E}(\gamma)]L_p = \mathrm{Tr}[\mathcal{E}(\gamma)]^p,\end{aligned} \tag{7}$$

where the last step used (A12). It follows from (A14) that L_p could be replaced by another permutation; however, it is important to make a definite choice for later use.

In previous work,[13,14] a different realization of $X(\mathcal{E},p)$ was used which is valid only for pure states. Let

$$\Theta(\mathcal{E},p) = \Omega(\mathcal{E},p)R_p = \hat{\mathcal{E}}^{\otimes p}(L_p)R_p \tag{8}$$

$$= \sum_{k_1,\ldots,k_p} A_{k_1}^{\dagger}A_{k_2}\otimes A_{k_2}^{\dagger}A_{k_3}\otimes\ \cdots\ \otimes A_{k_p}^{\dagger}A_{k_1}, \tag{9}$$

where $\{A_k\}$ form a set of Kraus operators for $\mathcal{E}$ as in (1). The operator $\Theta(\mathcal{E},p)$ satisfies (4) when $\gamma=|\psi\rangle\langle\psi|$ is a pure state. This relation is proved in Appendix B 1, and implicitly shows that it does not depend on the chosen Kraus representation (1) of $\mathcal{E}$. For $p=2$, (9) and (8) were obtained earlier in Ref. 35.

In general, the operator $\Omega(\mathcal{E},p)$ will not be Hermitian. We have already observed that $X(\mathcal{E},p)$ is not unique and that whenever P_p is a permutation operator whose shortest cycle is length p, the operator $\hat{\mathcal{E}}^{\otimes p}(P_p)$ provides another realization. Since $L_p=R_p^{\dagger}$,

$$[\hat{\mathcal{E}}^{\otimes p}(L_p)]^{\dagger} = \hat{\mathcal{E}}^{\otimes p}(L_p^{\dagger}) = \hat{\mathcal{E}}^{\otimes p}(R_p). \tag{10}$$

This implies that $\Omega(\mathcal{E},2)$ is Hermitian for $p=2$, and that the operator

$$\tfrac{1}{2}[\Omega(\mathcal{E},p) + [\Omega(\mathcal{E},p)]^{\dagger}] = \tfrac{1}{2}[\hat{\mathcal{E}}^{\otimes p}(L_p) + \hat{\mathcal{E}}^{\otimes p}(R_p)] \tag{11}$$

gives a Hermitian realization of $X(\mathcal{E},p)$ for any p. However, we do not expect (11) to have the important multiplicity property (14) for repeated uses of the channel. Further discussion of other realizations $X(\mathcal{E},p)$ is given in Appendixes B 2 and B 3.

Linear operators satisfying (4) provide a useful tool for studying the p-purity functions, which are intrinsically nonlinear objects; it reduces some associated problems to the analysis of the linear operator $X(\mathcal{E},p)$ acting on the extended Hilbert space $\mathcal{H}^{\otimes p}$ obtained by adding $p-1$ "fictitious" copies of the input Hilbert space $\mathcal{H}$. In Refs. 13 and 14, this approach was used to obtain some

additivity properties of Gaussian Bosonic channels. For $p=2$, Eq. (4) was used in Ref. 7 to study the fidelity obtainable in continuous-variable teleportation with finite two-mode squeezing, and in Ref. 35 to analyze the purity of generic quantum channels.

B. Tensor product maps

The results derived in the preceding section can also be applied when the basic CPT map is itself a tensor product. Then Eq. (4) becomes

$$\mathrm{Tr}[\mathcal{E}^{\otimes m}(\Gamma)]^p = \mathrm{Tr}[(\underbrace{\Gamma\otimes\Gamma\otimes\cdots\Gamma}_{p\text{-times}})X(\mathcal{E}^{\otimes m},p)], \tag{12}$$

where Γ is a generic density matrix in the input Hilbert space $\mathcal{H}^{\otimes m}$ and $X(\mathcal{E}^{\otimes m},p)$ is a linear operator on $(\mathcal{H}^{\otimes m})^{\otimes p}=\mathcal{H}^{\otimes mp}$. Following the strategy of Sec. II A, we now choose $X(\mathcal{E}^{\otimes m},p)$ to be the operator,

$$\Omega(\mathcal{E}^{\otimes m},p) \equiv (\widehat{\mathcal{E}^{\otimes m}})^{\otimes p}(\mathbb{L}_p) = (\widehat{\mathcal{E}^{\otimes m}})^{\otimes p}(L_p^{\otimes m}). \tag{13}$$

The operator $\mathbb{L}_p$ is described in more detail in Appendix A 3 where it is proved that $\mathbb{L}_p=L_p^{\otimes m}=(L_{mp})^m$. Using $(\widehat{\mathcal{E}^{\otimes m}})^{\otimes p}=(\hat{\mathcal{E}})^{\otimes mp}$, we find

$$\Omega(\mathcal{E}^{\otimes m},p) = \hat{\mathcal{E}}^{\otimes mp}(L_p^{\otimes m}) = [\hat{\mathcal{E}}^{\otimes p}(L_p)]^{\otimes m} = [\Omega(\mathcal{E},p)]^{\otimes m}. \tag{14}$$

Equation (14) is a key result whose simplicity hides a great deal of subtlety. The essential point is that the linear operator $X(\mathcal{E}^{\otimes m},p)$ which satisfies (1) for the tensor product channel $\mathcal{E}^{\otimes m}$ can be realized by the action of the dual of $\mathcal{E}^{\otimes m}$ on the permutation $L_p^{\otimes m}$.

III. CONDITIONS FOR MULTIPLICATIVITY

A. Upper bound

We now use the singular value decomposition[16,17] to observe that one can write

$$\Omega(\mathcal{E},p) = \sum_j \mu_j |\eta_j\rangle\langle\omega_j|, \tag{15}$$

where $\{|\eta_j\rangle\}$ and $\{|\omega_j\rangle\}$ denote orthonormal bases for $\mathcal{H}^{\otimes p}$ and $\mu_j>0$ are the singular values of $\Omega(\mathcal{E},p)$, i.e., the nonzero eigenvalues of $|\Omega(\mathcal{E},p)| \equiv \sqrt{[\Omega(\mathcal{E},p)]^\dagger\Omega(\mathcal{E},p)}$. Before applying this, it is convenient to introduce the convention of using bold uppercase greek letters to denote tensor product vectors as in $|\mathbf{\Psi}\rangle \equiv |\psi\rangle^{\otimes p} = |\psi\rangle\otimes|\psi\rangle\otimes\cdots\otimes|\psi\rangle \in \mathcal{H}^{\otimes p}$. Then

$$\begin{aligned}
\mathrm{Tr}[\mathcal{E}(|\psi\rangle\langle\psi|)]^p &= \langle\mathbf{\Psi}|\Omega(\mathcal{E},p)|\mathbf{\Psi}\rangle \\
&= \sum_j \mu_j \langle\mathbf{\Psi}|\eta_j\rangle\langle\omega_j|\mathbf{\Psi}\rangle \\
&\leqslant \mu_{\max}\sum_j |\langle\mathbf{\Psi}|\eta_j\rangle\langle\omega_j|\mathbf{\Psi}\rangle| \\
&\leqslant \mu_{\max}\|\mathbf{\Psi}\|^2 = \|\Omega(\mathcal{E},p)\|_\infty,
\end{aligned} \tag{16}$$

where $\mu_{\max}=\sup_j \mu_j=\|\Omega(\mathcal{E},p)\|_\infty$ is the largest singular value of $\Omega(\mathcal{E},p)$. Applying this analysis to multiple uses of the channel, one can similarly conclude that

$$\mathrm{Tr}[\mathcal{E}^{\otimes m}(|\Psi\rangle\langle\Psi|)]^p \leqslant \|\Omega(\mathcal{E}^{\otimes m},p)\|_\infty, \tag{17}$$

where $|\Psi\rangle$ is now an arbitrary vector in $\mathcal{H}^{\otimes m}$. However, it follows from (14) that the singular values of $\Omega(\mathcal{E}^{\otimes m},p)$ are products of those of $\Omega(\mathcal{E},p)$ so that

$$\|\Omega(\mathcal{E}^{\otimes m},p)\|_\infty = (\|\Omega(\mathcal{E},p)\|_\infty)^m = (\mu_{\max})^m. \tag{18}$$

Combining (17) and (18), one finds

$$\mathrm{Tr}[\mathcal{E}^{\otimes m}(|\Psi\rangle\langle\Psi|)]^p \leqslant (\|\Omega(\mathcal{E},p)\|_\infty)^m = (\mu_{\max})^m. \tag{19}$$

Since, the supremum in (2) is attained using a pure state input and (19) holds for all pure inputs $|\Psi\rangle$, we conclude that the upper bound

$$\nu_p(\mathcal{E}^{\otimes m}) \leqslant (\mu_{\max})^{m/p}, \tag{20}$$

holds for all pairs of integers m and p.

B. Multiplicativity condition

The bound (20) leads to a sufficient condition for multiplicativity. We state this formally, and give a condition as a corollary.

Theorem 1: *The channel $\mathcal{E}$ has the multiplicativity property (3) if the largest singular value of $\Omega(\mathcal{E},p)$ satisfies*

$$\|\Omega(\mathcal{E},p)\|_\infty = [\nu_p(\mathcal{E})]^p. \tag{21}$$

Corollary 2: *The channel $\mathcal{E}$ has the multiplicativity property (3) if the largest singular value of $\Omega(\mathcal{E},p)$ is also an eigenvalue of $\Omega(\mathcal{E},p)$ with a product eigenvector of the form $|\phi\rangle^{\otimes p}$.*

To prove Theorem 1, observe that in the notation of the preceding section (21) can be written as $\mu_{\max}=[\nu_p(\mathcal{E})]^p$. Then (20) implies

$$\nu_p(\mathcal{E}^{\otimes m}) \leqslant (\mu_{\max})^{m/p} = [\nu_p(\mathcal{E})]^m. \tag{22}$$

On the other hand, one always has

$$\nu_p(\mathcal{E}^{\otimes m}) \geqslant \|\mathcal{E}^{\otimes m}(\gamma_{\max}^{\otimes m})\|_p = \|\mathcal{E}(\gamma_{\max})\|_p^m = [\nu_p(\mathcal{E})]^m,$$

where $\gamma_{\max}$ denotes the state which achieves the supremum for $\nu_p(\mathcal{E})$. Combining these inequalities gives $\nu_p(\mathcal{E}^{\otimes m})=[\nu_p(\mathcal{E})]^m$. QED

To prove the corollary, observe that its hypothesis holds if and only if there is a state $|\phi\rangle$ in $\mathcal{H}$ such that

$$\mu_{\max} = \langle\mathbf{\Phi}|\Omega(\mathcal{E},p)|\mathbf{\Phi}\rangle = \mathrm{Tr}[\mathcal{E}(|\phi\rangle\langle\phi|)]^p, \tag{23}$$

where the second equality used (7) and our convention that $|\mathbf{\Phi}\rangle=|\phi\rangle^{\otimes p}$. But it is always true that

$$\mathrm{Tr}[\mathcal{E}(|\phi\rangle\langle\phi|)]^p \leqslant \sup_\gamma \mathrm{Tr}[\mathcal{E}(\gamma)]^p \equiv [\nu_p(\mathcal{E})]^p \tag{24}$$

so that $\mu_{\max}\leqslant[\nu_p(\mathcal{E})]^p$. Combining this with (20) when $m=1$, implies that $\mu_{\max}=[\nu_p(\mathcal{E})]^p$ so that the hypothesis of Theorem 1 holds. QED

In Sec. IV A we will see that the condition in Theorem 1 is not necessary. There are unital qubit CPT maps, which are known to be multiplicative, but do not satisfy (21). Verifying the hypothesis of Corollary 2 requires that one find an eigenvector as well as the largest singular value of an operator, but does not require knowledge of $\nu_p(\mathcal{E})$; condition (21) does require the latter, but does not require computation of any eigenvectors. In general, (21) seems easier to check. However, in the examples we analyzed, both conditions hold and the process of verifying one easily yields the other. It would be interesting to know if (21) implies that the singular value of $\Omega(\mathcal{E},p)$ is also an eigenvector with a product eigenvalue as in Corollary 2.

IV. APPLICATIONS

A. Qubit channels

1. Notation

We illustrate our condition by looking at some examples of qubit channels, for which we will use notation similar to that introduced in Refs. 25 and 31. Any 2×2 matrix can be represented in the basis consisting of the 2×2 identity matrix $\mathbb{1}$ and the three Pauli matrices which we often write as a formal vector $\vec{\sigma}\equiv(\sigma_1,\sigma_2,\sigma_3)$. In this basis a density matrix can be written as $\gamma=\frac{1}{2}[\mathbb{1}+\vec{w}\cdot\vec{\sigma}]$ with $\vec{w}$ in $\mathbf{R}^3$ and $|\vec{w}|\leqslant 1$. The density matrix is pure if and only if $|\vec{w}|=1$. Any linear map Φ on a qubit, can be described by two real vectors $\vec{s}$, $\vec{t}\in\mathbf{R}^3$ and by a 3×3 real matrix T, through the expression

$$\Phi(z_0\mathbb{1}+\vec{z}\cdot\vec{\sigma})=(z_0+\vec{s}\cdot\vec{z})\mathbb{1}+(z_0\vec{t}+T\cdot\vec{z})\cdot\vec{\sigma}, \tag{25}$$

which holds for all $z_0\in\mathbb{C}$ and $\vec{z}\in\mathbb{C}^3$. This corresponds to representing Φ in the basis $\{\mathbb{1},\vec{\sigma}\}$ by the 4×4 matrix $\left(\begin{smallmatrix}1 & \vec{s}^{\,t}\\ \vec{t} & T\end{smallmatrix}\right)$ which we have written in block form (with the convention that $\vec{t}$ corresponds to a column vector and $\vec{s}^{\,t}$ a row vector, using the superscript t to denote transpose). It was shown in Ref. 24 that it suffices to consider T diagonal with real elements $\{\lambda_1,\lambda_2,\lambda_3\}$. [In essence, a variant of the SVD (which leads to negative as well as positive λ_k) can be applied to T corresponding to rotations on the input and output bases, respectively.]

In this notation, Φ is trace preserving (TP) if and only if $\vec{s}=0$ and it is unital if and only if $\vec{t}=0$. Additional conditions under which the map is positivity preserving or completely positive (CP) are more complex. A complete set of conditions for the map to be CPT was obtained in Ref. 31. When $t_1=t_2=0$, these CPT conditions reduce to $(\lambda_1\pm\lambda_2)^2\leqslant(1\pm\lambda_3)^2-t_3^2$, as shown in Refs. 11 and 31. Since the dual map of Φ is represented by the adjoint matrix, it satisfies,

$$\hat{\Phi}(z_0\mathbb{1}+\vec{z}\cdot\vec{\sigma})=(z_0+\vec{t}\cdot\vec{z})\mathbb{1}+(z_0\vec{s}+T^t\cdot\vec{z})\cdot\vec{\sigma}. \tag{26}$$

Since $\mathcal{H}$ is now two dimensional, the left shift L_2 is simply the SWAP operator S which satisfies

$$S=\tfrac{1}{2}[\mathbb{1}\otimes\mathbb{1}+\sigma_1\otimes\sigma_1+\sigma_2\otimes\sigma_2+\sigma_3\otimes\sigma_3]. \tag{27}$$

It is then straightforward to use (6) to show that

$$\Omega(\Phi,2)=\hat{\Phi}^{\otimes 2}(S)=\frac{1}{2}\left[(1+|\vec{t}|^2)\mathbb{1}\otimes\mathbb{1}+\sum_{j=1}^{3}\lambda_j^2\sigma_j\otimes\sigma_j+\sum_{j=1}^{3}\lambda_j t_j(\mathbb{1}\otimes\sigma_j+\sigma_j\otimes\mathbb{1})\right]. \tag{28}$$

2. Unital maps

For qubit channels the conjecture (2) has been extensively studied in Refs. 18, 19, 22, and 24. Multiplicativity has been proven for all p for unital qubit channels[18] and for $p=2$ for all qubit channels (Theorem 2 of Ref. 18). Here we will use the case $p=2$ to illustrate the multiplicativity criterion presented in Sec. III B.

It will be useful to choose the subscript "max" in {1, 2, 3} so that $|\lambda_{\max}|=\max_k|\lambda_k|$. For unital qubits maps, the maximum ℓ_2-norm of Φ can be achieved with an input state of the form $\frac{1}{2}[\mathbb{1}\pm\sigma_{\max}]$ for which the output $\frac{1}{2}[\mathbb{1}\pm\lambda_{\max}\sigma_{\max}]$ has eigenvalues $\frac{1}{2}[1\pm\lambda_{\max}]$ and

$$\nu_2(\Phi)=\frac{1}{\sqrt{2}}\sqrt{1+\lambda_{\max}^2}. \tag{29}$$

When Φ is unital, $\vec{t}=0$ and the third term in the expression (28) vanishes. It then follows that in the product basis $\{|00\rangle,|01\rangle,|10\rangle,|11\rangle\}$, the operator $\Omega(\Phi,2)$ is represented by the matrix

$$\frac{1}{2}\begin{pmatrix} 1+\lambda_3^2 & 0 & 0 & \lambda_1^2-\lambda_2^2 \\ 0 & 1-\lambda_3^2 & \lambda_1^2+\lambda_2^2 & 0 \\ 0 & \lambda_1^2+\lambda_2^2 & 1-\lambda_3^2 & 0 \\ \lambda_1^2-\lambda_2^2 & 0 & 0 & 1+\lambda_3^2 \end{pmatrix}. \tag{30}$$

This is easily seen to have two nonzero 2×2 blocks. The "inner" block has eigenvalues $\frac{1}{2}[1-\lambda_3^2\pm(\lambda_1^2+\lambda_2^2)]$ with eigenvectors $2^{-1/2}(0,1,\pm 1,0)^t$ corresponding to the Bell states $2^{-1/2}(|01\rangle\pm|10\rangle)$. The "outer" block has eigenvalues $\frac{1}{2}[1+\lambda_3^2\pm(\lambda_1^2-\lambda_2^2)]$ with eigenvectors $2^{-1/2}(1,0,0,\pm 1)^t$ corresponding to the Bell states $2^{-1/2}(|00\rangle\pm|11\rangle)$. Since $\Omega(\Phi,2)$ is Hermitian, its singular values are simply the absolute values of the eigenvalues above.

When the $|\lambda_k|$ are distinct for $k=1,2,3$, the singular values of $\Omega(\Phi,2)$ are all distinct and correspond to maximally entangled, rather than product, states. Moreover, one of the singular values is always strictly greater than $\nu_2(\Phi)$. For example, when $|\lambda_{\max}|=|\lambda_3|$, one of the "outer" eigenvalues equals $\nu_2(\Phi)^2+\frac{1}{2}(\lambda_1^2-\lambda_2^2)$ which is strictly greater than (29) unless $|\lambda_1|=|\lambda_2|$. Therefore, although Φ is multiplicative, it does not satisfy (21). This establishes that (21) is not a necessary condition for multiplicativity.

Now consider the case $\lambda_3>\lambda_1=\lambda_2\geqslant 0$; such channels are sometimes called "two-Pauli" channels.[5] The image of the Bloch sphere is an ellipsoid shaped like an American football. For these channels, the "outer" block in (30) is diagonal, its (degenerate) eigenvalue $\frac{1}{2}(1+\lambda_3^2)=[\nu_2(\Phi)]^2$ is the largest singular value of $\Omega(\Phi,2)$ and the corresponding eigenvectors $|00\rangle$ and $|11\rangle$ are product states. Thus, Theorem 1 implies that the channel satisfies (3).

3. Nonunital maps

We now consider channels similar to those above, but with the image ellipsoid shifted along the longest axis. It suffices to consider $|\lambda_3|\geqslant\lambda_1=\lambda_2\geqslant 0$ and $t_1=t_2=0$. The same results hold for permutations of 1,2,3 and for $\lambda_1=\lambda_2\leqslant 0$. However, the analysis in the basis we have chosen to represent $\Omega(\Phi,2)$ is simplest when $|\lambda_{\max}|=|\lambda_3|$. The matrix representing $\Omega(\Phi,2)$ is

$$\frac{1}{2}\begin{pmatrix} 1+(t_3+\lambda_3)^2 & 0 & 0 & 0 \\ 0 & 1+t_3^2-\lambda_3^2 & 2\lambda_1^2 & 0 \\ 0 & 2\lambda_1^2 & 1+t_3^2-\lambda_3^2 & 0 \\ 0 & 0 & 0 & 1+(t_3-\lambda_3)^2 \end{pmatrix} \tag{31}$$

which has an "inner" block with eigenvalues $\frac{1}{2}[1+t_3^2-\lambda_3^2\pm 2\lambda_1^2]$ and a diagonal "outer" block with eigenvalues $\frac{1}{2}[1+(t_3\pm\lambda_3)^2]$ and product eigenvectors. One can verify that the largest singular value is $\frac{1}{2}[1+(|t_3|+|\lambda_3|)^2]$. To see that this equals $[\nu_2(\Phi)]^2$, observe that the optimal input state is $\frac{1}{2}[\mathbb{1}+(t_3/|t_3|)\sigma_3]$ for which the output state has eigenvalues $\frac{1}{2}[1\pm(|t_3|+|\lambda_3|)^2]$. Thus, we can again use Theorem 1 to conclude that (3) holds.

The methods introduced here are able to handle qubit channels for which the image of the Bloch sphere is an elongated ellipsoid with a symmetry axis, i.e., in the shape of an American football, both when the channel is unital and when it is shifted in the direction of the longest axis. However, it cannot handle these channels if the shift is orthogonal to the longest axis, i.e., if $t_3=0$ but $t_2\neq 0$ above. When the ellipsoid has a symmetry axis but $|\lambda_1|=|\lambda_2|\geqslant|\lambda_3|$ so that it is shaped like a flying saucer, the methods used here cannot prove multiplicativity. Even for unital channels, for which multiplicativity has been established,[19] neither of the conditions in Theorem 1 holds.

B. Shifted depolarizing channels

1. Shifting and generalizing the depolarizing channel

The unital qubit map with $\lambda_k = \pm|\lambda_{\max}|$ for all k, is a special case of the depolarizing channel which has the form $\mathcal{E}(\gamma) = (1-x)(\mathrm{Tr}\,\gamma)\frac{1}{d}\mathbb{1} + x\gamma$. It is CPT for $-\frac{1}{3} \leqslant x \leqslant 1$. The nonunital qubit map which takes

$$\gamma = \tfrac{1}{2}[\mathbb{1} + \vec{w}\cdot\vec{\sigma}] \mapsto \tfrac{1}{2}[\mathbb{1} + (\vec{t} + \lambda\vec{w})\cdot\vec{\sigma}] = (1 - |\vec{t}| - \lambda)\tfrac{1}{2}\mathbb{1} + |\vec{t}|\tfrac{1}{2}[\mathbb{1} + \hat{t}\cdot\vec{\sigma}] + \lambda\gamma \tag{32}$$

can be regarded as a shifted depolarizing channel because it shifts the output toward the point $\hat{t}$ on the Bloch sphere. By rotating coordinates so that $\vec{t} = (0,0,t_3)$, this is a special case of the qubit maps considered in Sec. IV A 3 above. It is then natural to define a shifted depolarizing channel in dimension d by

$$\mathcal{E}(\gamma) = a(\mathrm{Tr}\,\gamma)\frac{1}{d}\mathbb{1} + b(\mathrm{Tr}\,\gamma)|\psi\rangle\langle\psi| + c\gamma \tag{33}$$

with the state $|\psi\rangle$ fixed and $a+b+c=1$. When a,b,c are positive, this channel is a convex combination of the identity map and two completely noisy channels which maps all states to $\frac{1}{d}\mathbb{1}$ and to $|\psi\rangle\langle\psi|$, respectively.

We now consider the more general class of channels of the form

$$\mathcal{E}(\gamma) = (1-c)(\mathrm{Tr}\,\gamma)\rho + c\gamma, \tag{34}$$

where ρ is a fixed density matrix. For $\rho = (1/d)\mathbb{1}$, this is the usual depolarizing channel; for $\rho = [1/(a+b)][(a/d)\mathbb{1} + b|\psi\rangle\langle\psi|]$ it is the shifted depolarizing channel (33).

When $c \geqslant 0$ additivity was proved for the depolarizing channel in d dimensions using a majorization argument[12] from which multiplicativity immediately follows; for $-[1/(d^2-1)] \leqslant c \leqslant 1$ (which is the range for which the map is CPT) multiplicativity of the depolarizing channel in d dimensions was proved in Ref. 21. Neither shifted depolarizing channels nor the generalization (34) seem to have been explicitly considered in the literature before. One could obtain a proof of multiplicativity for $p=2$ when $c>0$ by verifying that the positive element condition in Ref. 25 is satisfied. (In fact, these maps satisfy the stronger condition considered in Ref. 23.) However, neither of these positive element conditions can be verified when $c<0$. By contrast, the method presented here can establish multiplicativity when $p=2$ for all CPT maps of the form (34), including those with $c<0$.

2. Convex combinations of the identity and completely noisy maps

It will be useful to write the spectral decomposition of ρ as $\rho = \Sigma_j a_j |j\rangle\langle j|$ with the eigenvalues a_j in decreasing order. Then, for $c>0$, the state $\mathcal{E}(|1\rangle\langle 1|)$ majorizes all outputs so that $[\nu_p(\mathcal{E})]^p = [ca_1 + (1-c)]^p + c^p \Sigma_{j>1}^d a_j^p$.

Since, $\hat{\mathcal{E}}(B) = (1-c)[\mathrm{Tr}\,B\rho]\mathbb{1} + cB$, we have

$$\hat{\mathcal{E}}(|j\rangle\langle k|) = (1-c)\langle k|\rho|j\rangle\mathbb{1} + c|j\rangle\langle k| = (1-c)\,\delta_{jk}a_k\mathbb{1} + c|j\rangle\langle k| \tag{35}$$

and

$$\begin{aligned}\Omega(\mathcal{E},2) &= (\hat{\mathcal{E}}\otimes\hat{\mathcal{E}})(S) = \sum_{jk}\hat{\mathcal{E}}(|j\rangle\langle k|)\otimes\hat{\mathcal{E}}(|k\rangle\langle j|)\\ &= \sum_{jk}[(1-c)^2\delta_{jk}a_k^2\mathbb{1}\otimes\mathbb{1} + c(1-c)\,\delta_{jk}a_k(\mathbb{1}\otimes|k\rangle\langle k| + |k\rangle\langle k|\otimes\mathbb{1}) + c^2|j\rangle\langle k|\otimes|k\rangle\langle j|]\\ &= (1-c)^2(\mathrm{Tr}\,\rho^2)\mathbb{1}\otimes\mathbb{1} + c(1-c)[\mathbb{1}\otimes\rho + \rho\otimes\mathbb{1}] + c^2 S.\end{aligned} \tag{36}$$

From this it is easy to see that $\Omega(\mathcal{E},2)$ has d product eigenvectors of the form $|kk\rangle$ with eigenvalues

$$(1-c)^2(\mathrm{Tr}\,\rho^2)+2c(1-c)a_k+c^2=[(1-c)a_k+c]^2+(1-c)^2\sum_{j\neq k}a_j^2, \tag{37}$$

and $\binom{d}{2}$ blocks of the form $[(1-c)^2(\mathrm{Tr}\,\rho^2)+c(1-c)(a_j+a_k)]\mathbb{1}_2+c^2\sigma_x$, with eigenvalues

$$(1-c)^2(\mathrm{Tr}\,\rho^2)+c(1-c)(a_j+a_k)\pm c^2 \tag{38}$$

and entangled eigenvectors $2^{-1/2}(|jk\rangle\pm|kj\rangle)$. When $c>0$ all eigenvalues are non-negative and the largest singular value is $[(1-c)a_1+c]^2+(1-c)^2\Sigma_{j>1}a_j^2=[\nu_2(\mathcal{E})]^2$ associated with the product eigenvector $|11\rangle$. Therefore, one can use Theorem 1, or Corollary 2, to conclude that the channel (34) is multiplicative for $p=2$ when $c>0$.

3. CPT maps with a negative contribution from the identity

To analyze the case $c<0$, write $c=-x$ with $x=|c|>0$, and recall that we assumed that the $\{a_j\}$ are decreasing. It can still happen that all eigenvalues of $\Omega(\mathcal{E},2)$ are non-negative, in which case the largest singular value is $[(1+x)a_d-x]^2+(1+x)^2\Sigma_{j<d}a_j^2$ associated with the product eigenvector $|dd\rangle$. It turns out that the requirement that $\mathcal{E}$ be CPT suffices to ensure that the eigenvalues of $\Omega(\mathcal{E},2)$ are non-negative. Therefore, any CPT map of the form (34) is multiplicative for $p=2$.

To see the relevance of the CPT condition, observe that the CP requirement that $(\mathcal{E}\otimes\mathbb{1})(\Sigma_{jk}|j\rangle\langle k|\otimes|j\rangle\langle k|)$ (which is the Choi matrix) is positive semidefinite holds if and only if

$$B=(1+x)\rho-x\begin{pmatrix}1&\cdots&1\\ \vdots&&\vdots\\ 1&\cdots&1\end{pmatrix}$$

is positive semidefinite. Then B has non-negative diagonal elements, which gives

$$(1+x)a_j-x\geqslant 0\Rightarrow x\leqslant\frac{a_j}{1-a_j}\Rightarrow\frac{x}{1+x}\leqslant a_j. \tag{39}$$

All 2×2 principle minors of B are non-negative, which implies

$$(1+x)^2a_1a_2-x(1+x)(a_1+a_2)\geqslant 0. \tag{40}$$

Now, all eigenvalues of $\Omega(\mathcal{E},2)$ will be positive if $(1-c)^2(\mathrm{Tr}\,\rho^2)+c(1-c)(a_j+a_k)-c^2\geqslant 0$ for all j,k. But the most negative of these is

$$\begin{aligned}(1+x)^2(\mathrm{Tr}\,\rho^2)-x(1+x)(a_1+a_2)-x^2&\geqslant(1+x)^2(a_1^2+a_2^2)-(1+x)^2a_1a_2-x^2\\&=(1+x)^2\left[a_1^2+a_2^2-a_1a_2-\left(\frac{x}{1+x}\right)^2\right]\\&\geqslant(1+x)^2[a_1^2+a_2^2-2a_1a_2]=(1+x)^2(a_1-a_2)^2\geqslant 0,\end{aligned} \tag{41}$$

where the second inequality used (39) with $j=1,2$ to conclude that $[x/(1+x)]^2\leqslant a_1a_2$.

C. The Werner–Holevo channel

In our final example, we apply our condition for $p=3,4$ as well as $p=2$. We study the channels $\mathcal{W}_d$ introduced in Ref. 34 to show that multiplicativity does not hold for sufficiently large p. The channel $\mathcal{W}_d$ is defined on a d dimensional Hilbert space as

$$\mathcal{W}_d(\gamma) \equiv \frac{1}{d-1}[(\mathrm{Tr}\,\gamma)\mathbb{1}_d - \gamma^T] = \frac{1}{(d-1)}\sum_{j<k} W_{jk}^\dagger \gamma W_{jk} \tag{42}$$

with $\mathbb{1}_d$ the identity operator on $\mathcal{H}$, γ^T the matrix transpose with respect to some fixed basis $\{|i\rangle\}$, and W_{jk} the anti-Hermitian operator $|j\rangle\langle k| - |k\rangle\langle j|$. (We will often suppress the subscript d and simply write $\mathcal{W}$ for $\mathcal{W}_d$.) As observed in Ref. 34, any pure input state yields an output state $\mathcal{W}(|\psi\rangle\langle\psi|)$ with eigenvalues$1/(d-1)$ with multiplicity $d-1$. This implies

$$\nu_p(\mathcal{W}_d) = (d-1)^{(1-p)/p}. \tag{43}$$

Werner and Holevo showed that for $d=3$ and $p>4.79$ this map is not ℓ_p multiplicative, by showing that maximally entangled inputs yield output ℓ_p-norm greater than $(d-1)^{(1-p)/p}$. For $d>3$, they also showed that multiplicativity fails for sufficiently large p. Although their results strongly suggest that multiplicativity does hold for smaller p, they do not preclude the possibility that it fails with inputs that are partially entangled. Our results show that this cannot happen when $p=2,3,4$ and $d\geqslant 2^{p-1}$.

The multiplicativity of $\mathcal{W}$ for $p=2$ was established in Ref. 25; the additivity of minimal output entropy and Holevo capacity was proved in Refs. 28 and 10; and, recently, a short elegant proof of multiplicativity for all $1\leqslant p\leqslant 2$ was given in Ref. 2. Here we use Theorem 1 to give another proof of (3) for $p=2$, and then consider multiplicativity of $\Omega(\mathcal{W},p)$ for integer $p>2$.

For $p=2$ it is straightforward to show that (or see Appendix C 1)

$$\Omega(\mathcal{W},2) = (\mathcal{W}\otimes\mathcal{W})(S) = \frac{1}{(d-1)^2}[(d-2)\mathbb{1}\otimes\mathbb{1} + S]. \tag{44}$$

with S the SWAP on $\mathcal{H}\otimes\mathcal{H}$. The eigenvalues of $\Omega(\mathcal{W},2)$ can be computed from those of S which has a diagonal block with d product states $|jj\rangle$ as eigenvectors with eigenvalue 1, and $\binom{d}{2}$ blocks of the form $\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)$ with eigenvalues $+1$ and -1 corresponding to the entangled states $2^{-1/2}(|jk\rangle \pm |kj\rangle)$. This yields eigenvalues $1/(d-1)$ with multiplicity $d(d+1)/2$ and $(d-3)/(d-1)$ with multiplicity $d(d-1)/2$. For $d\geqslant 3$, these are also the singular values of $\Omega(\mathcal{W},2)$; for $d=2$, $1/(d-1)$ is the only singular value. In both cases $\|\Omega(\mathcal{W},2)\|_\infty = 1/(d-1) = \nu_2(\mathcal{W})$. Therefore, (21) is satisfied and the result follows from Theorem 1.

To study $p>2$, we first observe that (C2) implies that $\Omega(\mathcal{W},p)$ is a linear combination of permutation matrices. This has some important consequences.

(a) $\Omega(\mathcal{W},p)$ has a large number of invariant subspaces, giving it a block diagonal structure. Each block describes the restriction of $\Omega(\mathcal{W},p)$ to a subspace spanned by all permutations of a vector $|\xi_{k_1}\xi_{k_2}\cdots\xi_{k_p}\rangle$ with indices $k_1\leqslant k_2\leqslant\cdots\leqslant k_p$.

(b) All row and column sums are equal. Moreover, (C3) implies that every row and column sum of $\Omega(\mathcal{W},p)$ or, equivalently, of each block, is exactly $(d-1)^{1-p}$, which is also the value of $[\nu_p(\mathcal{W})]^p$.

It follows immediately from (b) that $(d-1)^{1-p}$ is an eigenvalue of each block of $\Omega(\mathcal{W},p)$ and hence, an eigenvalue of $\Omega(\mathcal{W},p)$ with very high degeneracy. Therefore, $\Omega(\mathcal{W},p)$ can have a singular value greater that $[\nu_p(\mathcal{W})]^p$ only if some block has a singular value greater than $(d-1)^{1-p}$. The following lemma, which is proved in Appendix C 5, shows that it will suffice to consider this question for one of the largest blocks.

Lemma 3: When $d\geqslant p$, the largest singular value of $\Omega(\mathcal{W},p)$ is a singular value of each of the $p!\times p!$ blocks representing the restriction of $\Omega(\mathcal{W},p)$ to a subspace of $(\mathbb{C}^d)^{\otimes p}$ spanned by all permutations of a vector $|\xi_{k_1}\xi_{k_2}\cdots\xi_{k_p}\rangle$ with distinct k_p.

Based on this and the structure of the largest blocks as described in Appendx C 4, we make the following conjecture.

Conjecture 4: The ℓ_p multiplicativity relation (3) holds for the channel $\mathcal{W}_d$ when the dimension $d\geqslant 2^{p-1}$.

TABLE I. Block structure of $\Omega(\mathcal{W},p)$.

Number of blocks	Size	Type of vectors	Non-neg elements	max sing value $\times(d-1)^p$		
				$d=3$	$d=4$	$d\geqslant 5$
			$p=3$			
d	1×1	$\|kkk\rangle$	yes	2	3	$d-1$
$d(d-1)$	3×3	$\|jjk\rangle$	yes	2	3	$d-1$
$\binom{d}{3}$	6×6	$\|ijk\rangle$	no	4	3	$\max\{d-1,\|7-d\|\}$
			$p=4$			
d	1×1	$\|kkkk\rangle$	yes	2	3	$d-1$
$d(d-1)$	4×4	$\|jjjk\rangle$	yes	2	3	$d-1$
$\binom{d}{2}$	6×6	$\|jjkk\rangle$	yes	2	3	$d-1$
$\frac{1}{2}d(d-1)(d-2)$	12×12	$\|ijkk\rangle$	no	$\sqrt{18}$	$\sqrt{13}$	$\max\{d-1,\sqrt{d^2-12d+45}\}$
$\binom{d}{4}$	24×24	$\|ijk\ell\rangle$	no		11	$\max\{d-1,\|15-d\|\}$

This conjecture is proved for $p=2,3,4$. For larger p we have shown in Appendix C 4 that the largest block of $\Omega(\mathcal{W},p)$ has two eigenvectors which transform as the two one-dimensional representations of $\mathcal{S}_p$. The corresponding eigenvalues are $(d-1)^{1-p}$ and $(d-1)^{-p}(d-2^p+1)$. When $d\geqslant 2^{p-1}$, $|d-2^p+1|\leqslant d-1$. Moreover, no other singular values have the symmetry associated with a one-dimensional representation of $\mathcal{S}_p$. Thus, if we knew that the largest singular value of $\Omega(\mathcal{W},p)$ must be associated with a one-dimensional irreducible representation, we could conclude that the largest singular value of $\Omega(\mathcal{W},p)$ is $d-1$, proving the conjecture.

Now we consider $p=3,4$. The results in Appendix C 1 can be used to write $\Omega(\mathcal{W},p)$ explicitly as

$$\Omega(\mathcal{W},3)=\frac{1}{(d-1)^3}\left[(d-3)\mathbb{1}+\sum_{a<b}S_{ab}-R_3\right], \tag{45}$$

$$\Omega(\mathcal{W},4)=\frac{1}{(d-1)^4}\left[(d-4)\mathbb{1}+\sum_{a<b}S_{ab}-\sum_{a<b<c}R_3(a,b,c)+R_4\right], \tag{46}$$

where the shift $R_3(a,b,c)$ is defined in Appendix A 2. The block structure of $\Omega(\mathcal{W},p)$ for $p=3,4$ is summarized in Table I. In this table, i,j,k,ℓ always denote distinct indices. For readability, $(d-1)^p\mu_{\max}$ is reported in the last three columns, and should be compared to $(d-1)^p[\nu_p(\mathcal{W})]^p=(d-1)$. For $\Omega(\mathcal{W},3)$ and $\Omega(\mathcal{W},4)$, all singular values can be found explicitly with the help of Mathematica, with the largest for each block shown in Table I. The multiplicativity condition (21) holds if the largest singular value is $(d-1)^{1-p}$. For $p=3$, this holds for $d\geqslant 4$; for $p=4$, it holds for $d\geqslant 8$. For $p=3$, an analytic argument, which does not require determining the eigenvalues of $\Omega(\mathcal{W},3)$, is presented in Appendix C 2.

V. CONCLUSION

We have extended the method introduced in Refs. 13 and 14 to study the maximal ℓ_p-norms of a CPT map when p is a fixed integer. This yields a sufficient condition for multiplicativity which requires only that one find the singular values of a particular matrix, rather than performing

a full optimization. Although the matrix will be $d^p \times d^p$, it often has a block structure which makes the problems quite tractable, as shown in several examples. The condition is not necessary, but does allow us to prove new results about multiplicativity in several interesting cases, as well as providing alternative proofs of known results.

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APPENDIX A: SOME OPERATOR PROPERTIES

1. Hilbert–Schmidt duality

For a Hilbert space $\mathcal{H}$ the subspace of operators satisfying $\mathrm{Tr}\, A^\dagger A < \infty$ also forms a Hilbert space (the space of Hilbert–Schmidt operators) with respect to the inner product,

$$\langle A, B\rangle = \mathrm{Tr}\, A^\dagger B. \tag{A1}$$

An operator (sometimes referred to as a "superoperator") $\mathcal{E}$ acting on this space has an adjoint which we will denote $\hat{\mathcal{E}}$ and which satisfies

$$\mathrm{Tr}[\mathcal{E}(A)]^\dagger B = \mathrm{Tr}\, A^\dagger \hat{\mathcal{E}}(B) \quad \forall\, A, B. \tag{A2}$$

Because $[\mathcal{E}(A)]^\dagger = \mathcal{E}(A^\dagger)$, by writing C for $A^\dagger$ one easily sees that (A2) is equivalent to to the condition

$$\mathrm{Tr}[\mathcal{E}(C)]B = \mathrm{Tr}\, C\hat{\mathcal{E}}(B) \quad \forall\, B, C. \tag{A3}$$

The map $\hat{\mathcal{E}}$ is often called the dual of $\mathcal{E}$ because it is defined by the duality property of the Riesz representation theorem applied to the inner product (A1). When $\mathcal{E}$ is a CPT map of the form (1), its dual is the unital CP map with the form

$$\hat{\mathcal{E}}(\gamma) = \sum_k A_k^\dagger B A_k. \tag{A4}$$

One can verify, either directly from (A1) or by using (A4), that the dual of the map $\mathcal{E}^{\otimes m}$ is given by the m-fold tensor product of the dual map of $\mathcal{E}$; i.e., $\widehat{\mathcal{E}^{\otimes m}} = (\hat{\mathcal{E}})^{\otimes m}$.

2. Shift operators

The shift operators defined in (5) are unitary and satisfy $L_p R_p = \mathbb{1}$ so that $L_p^\dagger = L_p^{-1} = R_p$. Moreover, if a vector $|\Psi\rangle$ in $\mathcal{H}^{\otimes p}$ has the expansion

$$|\Psi\rangle = \sum_{j_1 j_2 \cdots j_p} c_{j_1 j_2 \cdots j_p} |\xi_{j_1} \xi_{j_2} \cdots \xi_{j_p}\rangle \tag{A5}$$

then

$$L_p|\Psi\rangle = \sum_{j_1 j_2 \cdots j_p} c_{j_1 j_2 \cdots j_p} |\xi_{j_2} \xi_{j_3} \cdots \xi_p \xi_{j_1}\rangle \tag{A6}$$

$$= \sum_{j_1 j_2 \cdots j_p} c_{j_p j_1 \cdots j_{p-1}} |\xi_{j_1} \xi_{j_2} \cdots \xi_{j_p}\rangle \tag{A7}$$

so that L_p induces a right shift on the expansion coefficients. From this, it follows that L_p and R_p induce left and right shifts on all product states, e.g.,

$$L_p|\phi_1, \phi_2, \ldots, \phi_p\rangle = |\phi_2, \phi_3, \ldots, \phi_p, \phi_1\rangle, \tag{A8a}$$

$$R_p|\phi_1, \phi_2, \ldots, \phi_p\rangle = |\phi_p, \phi_1, \ldots, \phi_{p-1}\rangle, \tag{A8b}$$

where $|\phi_1, \phi_2, \ldots, \phi_p\rangle$ denotes $|\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_p\rangle$. It also follows from (A8) that the shift operators are independent of the choice of orthonormal basis in (5).

To compute operators associated with the WH channel, it will be useful to observe that

$$L_p = \sum_{m_1 \cdots m_p} |m_2 \cdots m_p m_1\rangle\langle m_1 m_2 \cdots m_p|, \tag{A9a}$$

$$R_p = \sum_{m_1 \cdots m_p} |m_p m_1 \cdots m_{p-1}\rangle\langle m_1 m_2 \cdots m_p|, \tag{A9b}$$

where $|m_j\rangle$ denotes any orthonormal basis of $\mathcal{H}$. It will also be useful to introduce some notation for shift operators on a subset of $\mathcal{H}^{\otimes p}$. For example, write $\mathcal{H}^{\otimes 4} = \mathcal{H}_a \otimes \mathcal{H}_b \otimes \mathcal{H}_c \otimes \mathcal{H}_d$. Then $L_3(a,b,d)$ denotes the operator which acts as a left shift on $\mathcal{H}_a \otimes \mathcal{H}_b \otimes \mathcal{H}_d$ and the identity on $\mathcal{H}_c$, i.e.,

$$L_3(a,b,d) = \sum_{m_1 \cdots m_4} |m_2 m_4 m_3 m_1\rangle\langle m_1 m_2 m_3 m_4|. \tag{A10}$$

The SWAP operators $L_2(a,b) = R_2(a,b)$ play such a special role that we denote them as S_{ab}. Using the standard method for writing any permutation as a product of cycles, one can see that any shift can be written as a product of SWAP operators, e.g., $L_3(a,b,d) = S_{ab} S_{ad}$ and $L_4(a,b,c,d) = S_{ab} S_{ac} S_{ad}$.

3. Tensor products of shifts

When the underlying Hilbert is itself a tensor product $\mathcal{H}^{\otimes m}$, we will let $\mathbb{L}_p$ denote the shift operator acting on p copies of $\mathcal{H}^{\otimes m}$, e.g., $\mathbb{L}_3|x,y,z\rangle = |y,z,x\rangle$ with x,y,z denoting vectors in $\mathcal{H}^{\otimes m}$. Then, $\mathbb{L}_p = L_p^{\otimes m} = (L_{mp})^m$. To avoid notation with double subscripts, we prove this in the case $p = 3$. Then

$$\begin{aligned} \mathbb{L}_3|x,y,z\rangle &= \mathbb{L}_3|x_1,x_2, \ldots, x_m, y_1, y_2, \ldots, y_m, z_1, z_2, \ldots, z_m\rangle \\ &= |y_1, y_2, \ldots, y_m, z_1, z_2, \ldots, z_m, x_1, x_2, \ldots, x_m\rangle \\ &= L_3^{\otimes m}|x_1,x_2, \ldots, x_m, y_1, y_2, \ldots, y_m, z_1, z_2, \ldots, z_m\rangle, \end{aligned} \tag{A11}$$

where the last line follows by writing

$$L_3^{\otimes m} = (L_3 \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1})(\mathbb{1} \otimes L_3 \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}) \cdots (\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes L_3)$$

and observing that

$$\begin{aligned} &(L_3 \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1})|x_1,x_2, \ldots, x_m, y_1, y_2, \ldots, y_m, z_1, z_2, \ldots, z_m\rangle \\ &\quad = |y_1, x_2, \ldots, x_m, z_1, y_2, \ldots, y_m, x_1, z_2, \ldots, z_m\rangle. \end{aligned}$$

Note that it is also evident from (A11) that $L_p^{\otimes m} = (L_{mp})^m$.

4. An important trace identity

We now show that for any set of operators $\{B_1, B_2, \ldots, B_p\}$ acting on $\mathcal{H}$,

$$\mathrm{Tr}_{\mathcal{H}}[B_1 B_2 B_3 \cdots B_p] = \mathrm{Tr}_{\mathcal{H}^{\otimes p}}[B_1 \otimes B_2 \otimes \cdots \otimes B_p] L_p, \tag{A12}$$

where we have introduced subscripts to emphasize that the trace on the left-hand side of Eq. (A12) is performed on $\mathcal{H}$, while the trace on the right-hand side is performed on $\mathcal{H}^{\otimes p}$. To verify (A12) observe that

$$\begin{aligned}
\mathrm{Tr}[B_1 B_2 \cdots B_p] &= \sum_{\xi_1} \langle \xi_1 | B_1 B_2 \cdots B_{p-1} B_p | \xi_1 \rangle \\
&= \sum_{\xi_1, \ldots, \xi_p} \langle \xi_1 | B_1 | \xi_2 \rangle \langle \xi_2 | B_2 | \xi_3 \rangle \cdots \langle \xi_{p-1} | B_{p-1} | \xi_p \rangle \langle \xi_p | B_p | \xi_1 \rangle \\
&= \sum_{\xi_1, \ldots, \xi_p} \langle \xi_1, \xi_2, \ldots, \xi_p | B_1 \otimes B_2 \otimes \cdots \otimes B_p | \xi_2, \ldots, \xi_p, \xi_1 \rangle \\
&= \mathrm{Tr}[B_1 \otimes B_2 \otimes \cdots \otimes B_p] L_p,
\end{aligned}$$

where a resolution of the identity operator $\mathbb{1}$ of $\mathcal{H}$ was inserted between the products $B_j B_{j+1}$.

5. General permutations

Shifts are special cases of permutation operators. Let Π_p denote a permutation of $\{1, 2, \ldots, p\}$ and $\mathcal{S}_p$ the set of all such permutations. We will write $\Pi(j) = k_j$ for the permutation that takes $j \mapsto k_j$. For example, $L_p(j) = j + 1$. One can then define a permutation operator on $\mathcal{H}^{\otimes p}$ by

$$\Pi_p |\xi_{j_1} \xi_{j_2} \cdots \xi_{j_p}\rangle = |\xi_{\Pi(j_1)} \xi_{\Pi(j_2)} \cdots \xi_{\Pi(j_p)}\rangle \tag{A13}$$

with $\{|\xi_j\rangle\}$ an orthonormal basis for $\mathcal{H}$ as in (5). A permutation of the indices $\{1, 2, \ldots, p\}$ induces a permutation on the d^p product basis vectors $\mathcal{H}^{\otimes p}$ via (A13). Although we abuse notation by using the same letter for both, there should be no confusion. The permutation operator on $\mathcal{H}^{\otimes p}$ is represented by a $d^p \times d^p$ matrix which has precisely one 1 and $d^p - 1$ 0's in each row and column.

The permutation which takes $k_1 \mapsto k_2 \mapsto \cdots \mapsto k_q \mapsto k_1$ is called a cycle and written $P = (k_1, k_2, \ldots, k_q)$, i.e., $P(k_j) = (k_{j+1})$ with the understanding that $P(k_q) = k_1$ and $\Pi(j) = j$ if j does not appear as one of the k_i in the cycle. Any permutation can be written uniquely as a product of *disjoint* cycles, and the length of the disjoint cycles in $\Pi P \Pi^\dagger$ are the same as those in P. For example $(13) L_5 (13) = (14532)$. If a permutation of $\{1, 2, \ldots, p\}$ has a cycle decomposition with cycles whose length is strictly less than p, then some subset of $\{1, 2, \ldots, p\}$ is invariant. A permutation Π_p whose shortest cycle is of length p has no invariant subsets. Permutations satisfying this condition, which is equivalent to $(\Pi_p)^s(j) \neq j$ for $s < p$ and $(\Pi_p)^p(j) = j$ for all j, are of particular interest.

In fact, when all operators $B_i = B$ are identical, (A12) can be extended to any permutation Π_p of $\{1, 2, \ldots, p\}$ whose shortest cycle is length p. One finds

$$\begin{aligned}
\mathrm{Tr}_{\mathcal{H}} B^p &= \sum_{\xi_1, \ldots, \xi_p} \langle \xi_1 | B | \xi_{\Pi_p(1)} \rangle \langle \xi_{\Pi_p(1)} | B | \xi_{\Pi_p^2(1)} \rangle \cdots \langle \xi_{(\Pi_p)^p(1)} | B | \xi_1 \rangle \\
&= \sum_{\xi_1, \ldots, \xi_p} \langle \xi_1 | B | \xi_{\Pi_p(1)} \rangle \langle \xi_2 | B | \xi_{\Pi_p(2)} \rangle \cdots \langle \xi_p | B | \xi_{\Pi_p(p)} \rangle \\
&= \sum_{\xi_1, \ldots, \xi_p} \langle \xi_1, \xi_2, \ldots, \xi_p | B \otimes B \otimes \cdots \otimes B | \xi_{k_1}, \xi_{k_2}, \ldots, \xi_{k_p} \rangle \\
&= \mathrm{Tr}_{\mathcal{H}^{\otimes p}}[B \otimes B \otimes \cdots \otimes B] \Pi_p = \mathrm{Tr}_{\mathcal{H}^{\otimes p}} B^{\otimes p} \Pi_p.
\end{aligned} \tag{A14}$$

To see where the invariance condition is used, consider the permutation (153) (24). Attempting to apply the process above yields

$$\mathrm{Tr}_{\mathcal{H}} B^5 = \sum_{\xi_1,\xi_3,\xi_5} \langle\xi_1|B|\xi_5\rangle\langle\xi_5|B|\xi_3\rangle\langle\xi_3|B^3|\xi_1\rangle$$
$$= \sum_{\xi_1,\xi_3,\xi_5} \langle\xi_1,\xi_5,\xi_3|B\otimes B\otimes B^3|\xi_5,\xi_3,\xi_1\rangle = \mathrm{Tr}_{\mathcal{H}_a\otimes\mathcal{H}_c\otimes\mathcal{H}_e}[B\otimes B\otimes B^3]L_3$$

or $\mathrm{Tr}_{\mathcal{H}} B^5 = \mathrm{Tr}_{\mathcal{H}^{\otimes 3}}[B\otimes B^3\otimes B]L_3$ or $\mathrm{Tr}_{\mathcal{H}} B^5 = \mathrm{Tr}_{\mathcal{H}^{\otimes 2}}[B\otimes B^4]L_2$.

6. Double stochastic matrices

A double stochastic matrix[16] is a matrix with non-negative elements whose row and column sums are all 1, i.e., B is double stochastic if and only if $b_{jk}\geqslant 0\,\forall\, j,k$ and $\Sigma_j b_{jk}=\Sigma_k b_{jk}=1$. The vector $(1,1,\ldots,1)$ is always an eigenvector with eigenvalue 1. Moreover, all other eigenvalues satisfy $|\lambda_j|\leqslant 1$. A permutation of $\{1,2,\ldots,p\}$ can be represented by a matrix which has precisely one 1 and $p-1$ 0's in each row and column. This is a special type of double stochastic matrix called a "permutation matrix." Moreover, a permutation Π_p of $\{1,2,\ldots,p\}$ has no nontrivial invariant subspaces if and only if its permutation matrix is indecomposable. Note that the corresponding permutation operator on $\mathcal{H}^p$, represented by a $d^p\times d^p$ matrix with precisely one 1 and d^p-1 0's in each row and column, can have invariant subspaces. In fact, it will be block diagonal.

APPENDIX B: PROPERTIES OF LINEARIZING OPERATORS $X(\mathcal{E},p)$

1. Kraus operator form of $\Omega(\mathcal{E},p)$

We first observe that conjugation of a tensor product of operators by a shift operation induces a shift on the tensor product, e.g.,

$$L_p[B_1\otimes B_2\otimes\cdots\otimes B_p]L_p^{-1} = B_2\otimes\cdots\otimes B_p\otimes B_1. \tag{B1}$$

More generally,

$$\Pi_p[B_1\otimes B_2\otimes\cdots\otimes B_p]\Pi_p^{-1} = B_{\Pi(1)}\otimes B_{\Pi(2)}\cdots\otimes B_{\Pi(p)}. \tag{B2}$$

To prove (9), one can use (1) and (B1) to see that

$$[\hat{\mathcal{E}}^{\otimes p}(L_p)]R_p = \left[\sum_{k_1,\ldots,k_p}(A_{k_1}^\dagger\otimes A_{k_2}^\dagger\otimes\cdots\otimes A_{k_p}^\dagger)L_p(A_{k_1}\otimes A_{k_2}\otimes\cdots\otimes A_{k_p})\right]L_p^{-1}$$
$$= \sum_{k_1,\ldots,k_p}(A_{k_1}^\dagger\otimes A_{k_2}^\dagger\otimes\cdots\otimes A_{k_p}^\dagger)(A_{k_2}\otimes A_{k_3}\otimes\cdots\otimes A_{k_p}\otimes A_{k_1})$$
$$= \sum_{k_1,\ldots,k_p} A_{k_1}^\dagger A_{k_2}\otimes A_{k_2}^\dagger A_{k_3}\otimes\cdots\otimes A_{k_p}^\dagger A_{k_1} \tag{B3}$$

which gives the desired result. Moreover, using a similar argument and (B2), one finds

$$R_p[\hat{\mathcal{E}}^{\otimes p}(L_p)] = R_p\left[\sum_{k_1,\ldots,k_p}(A_{k_1}^\dagger\otimes A_{k_2}^\dagger\otimes\cdots\otimes A_{k_p}^\dagger)L_p^{-1}(A_{k_1}\otimes A_{k_2}\otimes\cdots\otimes A_{k_p})\right]$$
$$= \sum_{k_1,\ldots,k_p} A_{k_p}^\dagger A_{k_1}\otimes A_{k_1}^\dagger A_{k_2}\otimes\cdots\otimes A_{k_{p-1}}^\dagger A_{k_p}. \tag{B4}$$

Then by observing that both (B3) and (B4) involve tensor products of operators of the form $A_{k_j}^\dagger A_{k_{j+1}}$, one sees that after a change of variable in the summation indices, e.g., $k_j\to k_{j-1}$ in (B4), the two expressions are identical. Therefore, R_P commutes with $\hat{\mathcal{E}}^{\otimes p}(L_p)$ and $\Theta(\mathcal{E},p)=\Omega(\mathcal{E},p)R_p=R_p\Omega(\mathcal{E},p)$.

2. General permutations

Define $\mathcal{X}(\mathcal{E},p)$ the set of operators $X(\mathcal{E},p)$ of $\mathcal{H}^{\otimes p}$ that satisfy the property (4) for all the input states γ of $\mathcal{H}$. We have already seen that $\hat{\mathcal{E}}^{\otimes p}(L_p)$ is in $\mathcal{X}(\mathcal{E},p)$ which implies that it is nonempty. Moreover, the linearity of Eq. (4) with respect to $X(\mathcal{E},p)$ implies that whenever $X(\mathcal{E},p)$ and $Y(\mathcal{E},p)$ are in $\mathcal{X}(\mathcal{E},p)$, then $aX(\mathcal{E},p)+(1-a)Y(\mathcal{E},p)$ is in $X(\mathcal{E},p)$ is also. This is true for any real number a including $a<0$ and $a>1$, and even for complex a. By choosing $0<a<1$, we can also conclude that $\mathcal{X}(\mathcal{E},p)$ is convex; however, $\mathcal{X}(\mathcal{E},p)$ is not compact. Because $\mathrm{Tr}[\mathcal{E}(\gamma)]^p$ is real,

$$\mathrm{Tr}\ \gamma^{\otimes p}X(\mathcal{E},p) = \overline{\mathrm{Tr}\ \gamma^{\otimes p}X(\mathcal{E},p)} = \mathrm{Tr}[\gamma^{\otimes p}X(\mathcal{E},p)]^\dagger = \mathrm{Tr}[X(\mathcal{E},p)]^\dagger\gamma^{\otimes p} = \mathrm{Tr}\ \gamma^{\otimes p}[X(\mathcal{E},p)]^\dagger \tag{B5}$$

for all density matrices γ. Therefore, whenever $X(\mathcal{E},p)$ is in $\mathcal{X}(\mathcal{E},p)$ so are $[X(\mathcal{E},p)]^\dagger$ and the self-adjoint operator $\frac{1}{2}(X(\mathcal{E},p)+[X(\mathcal{E},p)]^\dagger)$.

In view of the discussion in Appendix A 4 we can also conclude that the operator $\hat{\mathcal{E}}^{\otimes p}(\Pi_p)$ is in $\mathcal{X}$ whenever Π_p is a permutation whose shortest cycle is length p. Moreover, a modification of the argument in the preceding section shows that, for these permutations,

$$\hat{\mathcal{E}}^{\otimes p}(\Pi_p)\Pi_p^\dagger = \Pi_p^\dagger\hat{\mathcal{E}}^{\otimes p}(\Pi_p) = \sum_{k_1,\ldots,k_p} A_{k_1}^\dagger A_{\Pi(k_1)} \otimes A_{k_2}^\dagger A_{\Pi(k_2)} \otimes \cdots \otimes A_{k_p}^\dagger A_{\Pi(k_p)}. \tag{B6}$$

Since $\Pi_p\gamma^{\otimes p}\Pi_p^\dagger=\Pi_p$ for any permutation,

$$\mathrm{Tr}[\gamma^{\otimes p}(\Pi_p X(\mathcal{E},p)\Pi_p^\dagger)] = \mathrm{Tr}[(\Pi_p^\dagger\gamma^{\otimes p}\Pi_p)X(\mathcal{E},p)] = \mathrm{Tr}\ \gamma^{\otimes p}X(\mathcal{E},p) = \mathrm{Tr}[\mathcal{E}(\gamma)^p]. \tag{B7}$$

Note that the map $P_p\mapsto\Pi_pP_p\Pi_p^\dagger$ does not change the cycle structure of P_p, e.g., if P_p is a product of a 3-cycle and a disjoint 2-cycle, then so is $\Pi_pP_p\Pi_p^\dagger$. Thus, $\Pi_pL_p\Pi_p^\dagger$ is a permutation whose shortest cycle is length p irrespective of the cycle structure of Π_p. One can show that $\Pi_p[\hat{\mathcal{E}}^{\otimes p}(L_p)]\Pi_p^\dagger=\hat{\mathcal{E}}^{\otimes p}(\Pi_pL_p\Pi_p^\dagger)$, with a similar result when L_p is replaced by any permutation whose shortest cycle is length p.

3. Linearizing operators for pure inputs

The set $\mathcal{X}(\mathcal{E},p)$ is a subset of $\mathcal{X}_{\mathrm{pure}}(\mathcal{E},p)$, the set of operators, which satisfy the property (4) when $\gamma=|\psi\rangle\langle\psi|$ is pure. We have already observed that $\Theta(\mathcal{E},p)=\Omega(\mathcal{E},p)R_p$ belongs to $\mathcal{X}_{\mathrm{pure}}(\mathcal{E},p)$ but need not belong to $\mathcal{X}(\mathcal{E},p)$. It follows from (B6) that the operators $\hat{\mathcal{E}}^{\otimes p}(\Pi_p)\Pi_p^\dagger$ are also in $\mathcal{X}_{\mathrm{pure}}(\mathcal{E},p)$. In addition, for any $X(\mathcal{E},p)\in\mathcal{X}_{\mathrm{pure}}(\mathcal{E},p)$ the operators $X(\mathcal{E},p)\Pi_p$ and $\Pi_pX(\mathcal{E},p)$ are also in $\mathcal{X}_{\mathrm{pure}}(\mathcal{E},p)$ for all permutations Π_p. This follows from

$$\begin{aligned}\mathrm{Tr}[\gamma\otimes\gamma\otimes\cdots\otimes\gamma]X(\mathcal{E},p)\Pi_p &= \mathrm{Tr}|\psi\rangle\langle\psi|\otimes|\psi\rangle\langle\psi|\otimes\cdots\otimes|\psi\rangle\langle\psi|X(\mathcal{E},p)\Pi_p\\ &= \mathrm{Tr}\,\Pi_p|\psi,\ldots,\psi\rangle\langle\psi,\ldots,\psi|X(\mathcal{E},p)\\ &= \mathrm{Tr}|\psi,\ldots,\psi\rangle\langle\psi,\ldots,\psi|X(\mathcal{E},p)\\ &= \mathrm{Tr}[\gamma\otimes\gamma\otimes\cdots\otimes\gamma]X(\mathcal{E},p) = \mathrm{Tr}\,\mathcal{E}(\gamma)^p,\end{aligned}$$

whenever $\gamma=|\psi\rangle\langle\psi|$ is pure.

APPENDIX C: OPERATORS FOR WERNER–HOLEVO CHANNEL

1. General form of $\Omega(\mathcal{W},p)$

It follows from (42), (A9), and (6) that for the WH channel,

$$\Omega(\mathcal{W},p) = \sum_{\xi_1\cdots\xi_p} \mathcal{W}(|\xi_2\rangle\langle\xi_1|) \otimes \mathcal{W}(|\xi_3\rangle\langle\xi_2|) \otimes \cdots \mathcal{W}(|\xi_p\rangle\langle\xi_{p-1}|)\mathcal{W}(|\xi_1\rangle\langle\xi_p|)$$

$$= \frac{1}{(d-1)^p} \sum_{\xi_1\cdots\xi_p} (\delta_{\xi_2\xi_1}\mathbb{1} - |\overline{\xi_1}\rangle\langle\overline{\xi_2}|) \otimes (\delta_{\xi_3\xi_2}\mathbb{1} - |\overline{\xi_2}\rangle\langle\overline{\xi_3}|) \otimes \cdots \otimes (\delta_{\xi_1\xi_p}\mathbb{1} - |\overline{\xi_p}\rangle\langle\overline{\xi_1}|)$$

$$= \frac{1}{(d-1)^p}\Bigg[d\mathbb{1} - \Bigg(\sum_{\xi_1} |\overline{\xi_1}\rangle\langle\overline{\xi_1}| + \sum_{\xi_2} |\overline{\xi_1}\rangle\langle\overline{\xi_2}| + \cdots + \sum_{\xi_p} |\overline{\xi_1}\rangle\langle\overline{\xi_p}|\Bigg)$$

$$+ \sum_{a<b} \Bigg(\sum_{\xi_a\xi_b} |\overline{\xi_a}\overline{\xi_b}\rangle\langle\overline{\xi_b}\overline{\xi_a}|\Bigg) - \cdots + (-1)^p \sum_{\xi_1\cdots\xi_p} |\overline{\xi_1}\overline{\xi_2}\cdots\overline{\xi_{p-1}}\overline{\xi_p}\rangle\langle\overline{\xi_2}\overline{\xi_3}\cdots\overline{\xi_p}\overline{\xi_1}| \qquad \text{(C1)}$$

$$= \frac{1}{(d-1)^p}\Bigg[(d-p)\mathbb{1} + \sum_{a<b} S_{ab} - \sum_{a<b<c} R_3(a,b,c) + \cdots + (-1)^p R_p \Bigg], \qquad \text{(C2)}$$

where we have used the notation introduced at the end of Appendix A 2. Note that the orthonormal basis $\{|\xi_j\rangle\}$ can be chosen real, but even if it is not, $\{|\overline{\xi_j}\rangle\}$ gives another orthonormal basis for $\mathcal{H}$ for which the representation (A9) is also valid.

It is useful to compare the structure of (C2) to that of a binomial expansion. The term in square brackets is a sum of shift operators R_k of order $k=0,1,2,\ldots,p$. For $k\geqslant 2$ the number of R_k is $\binom{p}{k}$ with coefficient $(-1)^k$. In view of (C1), the $(d-p)\mathbb{1}$ term should be regarded as the sum of a $k=0$ term $d\mathbb{1}$ and a $k=1$ term $-p\mathbb{1}$. The coefficient of the $k=0$ term is anomalous, since it has the value d rather than 1. This implies that the row and column sums of the matrix representing $\Omega(\mathcal{W},p)$ in the orthonormal basis $\{|\overline{\xi_{j1}}\overline{\xi_{j2}}\cdots\overline{\xi_{jp}}\rangle\}$ of $\mathcal{H}^{\otimes p}$ are

$$\frac{1}{(d-1)^p}\left[d + \sum_{k=1}^{p} (-1)^k \binom{p}{k} \right] = \frac{d-1}{(d-1)^p}. \qquad \text{(C3)}$$

One similarly finds that the sum of the absolute values of elements in any row or column sum is bounded above by

$$\frac{1}{(d-1)^p}\left[d + \sum_{k=1}^{p} \binom{p}{k} \right] = \frac{(d-1+2^p)}{(d-1)^p},$$

and will use the fact that

$$\sum_{k=2}^{p} \binom{p}{k} = 2^p - p - 1.$$

2. Singular value analysis for $p=3$

We first remark that one can reduce the analysis of $\Omega(\mathcal{W},3)$ to that of its 6×6 blocks without using Lemma 3. When $p=3$, all blocks with basis vectors $|jjk\rangle$ with $j\neq k$ have only non-negative elements. To see why, note that the only negative contribution comes from R_3, for which $\langle jjk|R_3|jkj\rangle=-1$ is the only nonzero element of the row corresponding to jjk. But $\langle jjk|\Omega|jkj\rangle \geqslant \langle jjk|(S_{ac}-R_3)|jkj\rangle=0$. Therefore, every 3×3 block is represented by a stochastic matrix and, hence, its column sum $(d-1)^{1-p}$ is also its largest singular value. Thus, only the 6×6 blocks of $\Omega(\mathcal{W},3)$ can have negative elements and, hence, a singular value greater than $(d-1)^{1-p}$.

Using an ordered basis whose first three elements are $\{|ijk\rangle, L_3|ijk\rangle, L_3^2|ijk\rangle\}$ and last three $S_{ab}\{|ijk\rangle, S_{bc}|ijk\rangle, S_{ac}|ijk\rangle\}$, one can write each 6×6 block as $(d-1)^{-3}F$ with

TABLE II. Singular value decomposition of $\Omega(\mathcal{W},4)$ on the 12-dimensional subspace generated by the vectors $\{|ijkk\rangle,|jikk\rangle,\ldots,|kjik\rangle\}$ and the 24-dimensional subspace generated by $\{|ijk\ell\rangle,|jjk\ell\rangle,\ldots,|kji\ell\rangle\}$.The singular values $\Omega(\mathcal{W},4)$ are given in the left column, with the corresponding degeneracies in the central and right columns.

Singular value $\times(d-1)^4$	Degeneracy (12×12 blocks)	Degeneracy (24×24 blocks)
$\sqrt{d^2-12d+45}$	2	6
$\lvert d-5\rvert$	1	3
$\lvert d-3\rvert$	3	5
$\sqrt{d^2-4d+5}$	4	6
$\lvert d-1\rvert$	2	3
$\lvert d-15\rvert$	0	1

$$F=(d-3)\mathbb{1}_6+\begin{pmatrix}-L_3 & V\\ V & -L_3\end{pmatrix}\quad\text{and } V=\begin{pmatrix}1&1&1\\1&1&1\\1&1&1\end{pmatrix}. \tag{C4}$$

Then

$$\begin{aligned}F^\dagger F&=(d-3)^2\mathbb{1}+(d-3)[G+G^\dagger]+G^\dagger G\\&=(d^2-5d+7)\mathbb{1}_6+\begin{pmatrix}-d+6 & 2d-8\\ 2d-8 & -d+6\end{pmatrix}\otimes V.\end{aligned} \tag{C5}$$

Since the eigenvalues of V are 3, 0, 0, the nonzero eigenvalues of $F^\dagger F$ are d^2-5d+7 (with fourfold degeneracy) and $(d^2-5d+7)+3[(6-d)\pm(2d-8)]$ or $(d-7)^2$ and $(d-1)^2$. Now $(d^2-5d+7)\leqslant(d-1)^2$ when $d\geqslant2$ and $(d-7)^2\leqslant(d-1)^2$ if and only if $d\geqslant4$. Therefore, when $d\geqslant4$ the largest singular value of this block is $d-1$ which implies that the largest singular value of $\|\Omega(\mathcal{W},3)\|_\infty=(d-1)^{-2}$.

3. Singular value analysis for $p=4$

For $p=4$, one can show that the 4×4 and 6×6 blocks have only non-negative elements. Therefore, their largest singular value is the same as the column sum $(d-1)^{-3}$. $\Omega(\mathcal{W},4)$ also has 12×12 blocks corresponding to permutations of $|ijkk\rangle$, with i,j,k distinct and 24×24 blocks corresponding to permutations of $|ijk\ell\rangle$, with i,j,k,ℓ distinct. By Lemma 3, the largest singular value is associated with the latter. Nevertheless, an analysis of all blocks was performed using Mathematica, yielding the results summarized in Table II. This confirms that the largest singular value of $\Omega(\mathcal{W},4)$ is $(d-1)^{-3}$ when $d\geqslant8$.

4. Structure of largest block

a. Preliminaries

Recall that every permutation P in $\mathcal{S}_p$ can be classified as even or odd, depending on the number of transpositions (or SWAP) operators needed to write it as a product $P=S_{a_1b_1}S_{a_2b_2}\cdots S_{a_mb_m}$. Although this decomposition is not unique, m is either always even or always odd. Let $|P|$ be the minimal number of swaps needed so that

$$(-)^{|P|}=\begin{cases}+1 & \text{if } P \text{ is even}\\ -1 & \text{if } P \text{ is odd}\end{cases}.$$

Note that $S(a,b)$ and $R_4(a,b,c,d)$ are odd and $R_3(a,b,c)$ is even. More generally, a shift of j elements is even when j is odd and odd when j is even. Thus, one can write

$$\Omega(\mathcal{W},p) = \frac{1}{(d-1)^p}[(d-p)\mathbb{1} + \tilde{\Omega}_{\text{odd}} - \tilde{\Omega}_{\text{even}}], \tag{C6}$$

where $\tilde{\Omega}_{\text{odd}}$ is the sum over odd permutations (even shifts) in (C2) and $\tilde{\Omega}_{\text{even}}$ the sum over even permutations (odd shifts) in (C2).

Fix $k_1<k_2<\cdots<k_p$ and let $\mathcal{K}$ denote the subspace spanned by $\{P|\xi_{k_1},\xi_{k_2},\ldots,\xi_{k_p}\rangle : P\in\mathcal{S}_p\}$ where $|\xi_k\rangle$ is an orthonormal basis for $\mathbb{C}^d$ and the action of P is as defined in (A13). The matrix representing a particular permutation operator Π has elements

$$\pi_{st} = \langle \xi_{k_1},\xi_{k_2},\ldots,\xi_{k_p}|P_s^\dagger \Pi P_t|\xi_{k_1},\xi_{k_2},\ldots,\xi_{k_p}\rangle \tag{C7}$$

which depends *only* on the labeling P_s, $s=1,2,\ldots,p!$ of elements of $\mathcal{S}_p$ and not on the choice of indices k_j or vectors ξ_j. It will be convenient to simply use $|k\rangle$ to denote $|\xi_k\rangle$, and to write $|\Pi(k_1,k_2,\ldots,k_p)\rangle$ for $\Pi|\xi_{k_1},\xi_{k_2},\ldots,\xi_{k_p}\rangle$. (The condition $k_j<k_{j+1}$ is only a convenient convention; the essential requirement is that the k_j are distinct.)

b. Irreducible representation structure

The matrix representing the action of a permutation Π on the vectors $\{P|k_1,k_2,\ldots,k_p\rangle : P\in\mathcal{S}_p\}$ is identical to its matrix in the regular representation of $\mathcal{S}_p$. Therefore, one can find a unitary transformation to a basis whose components form disjoint subsets which transform as the irreducible representation of $\mathcal{S}_p$. This basis change simultaneously converts all permutations to a block diagonal form. Thus, $\Omega(\mathcal{W},p)$, is also block diagonal with each block corresponding to an irreducible representation of $\mathcal{S}_p$. The two one-dimensional representations, therefore, yield eigenvectors of $\Omega(\mathcal{W},p)$. In fact

$$\Omega(\mathcal{W},p)|\phi_{\text{sym}}\rangle = \frac{d-1}{(d-1)^p}|\phi_{\text{sym}}\rangle, \tag{C8a}$$

$$\Omega(\mathcal{W},p)|\phi_{\text{anti}}\rangle = \frac{d-2^p+1}{(d-1)^p}|\phi_{\text{anti}}\rangle, \tag{C8b}$$

where

$$|\phi_{\text{sym}}\rangle = \frac{1}{\sqrt{p!}}\sum_{P\in\mathcal{S}_p}|P(k_1,k_2,\ldots,k_p)\rangle = \frac{1}{\sqrt{2}}(|u_{\text{even}}\rangle + |u_{\text{odd}}\rangle), \tag{C9a}$$

$$|\phi_{\text{anti}}\rangle = \frac{1}{\sqrt{p!}}\sum_{P\in\mathcal{S}_p}(-)^{|P|}|P(k_1,k_2,\ldots,k_p)\rangle = \frac{1}{\sqrt{2}}(|u_{\text{even}}\rangle - |u_{\text{odd}}\rangle), \tag{C9b}$$

with

$$|u_{\text{even}}\rangle = \sqrt{\frac{2}{p!}}\sum_{p_{\text{even}}}|P(k_1,k_2,\ldots,k_p)\rangle,$$

and

$$|u_{\text{odd}}\rangle = \sqrt{\frac{2}{p!}}\sum_{p_{\text{odd}}}|P(k_1,k_2,\ldots,k_p)\rangle.$$

If we could conclude that the largest singular value of $(d-1)^p\Omega(\mathcal{W},p)$ is associated with a one-dimensional representation of $\mathcal{S}_p$, then we could conclude that $(d-1)^p\|\Omega(\mathcal{W},p)\|_\infty = \max\{d-1,|d-2^p+1|\}$. Note that this maximum is clearly $d-1$ when $d\geqslant 2^p-1$. For $d<2^p$, the maximum is $d-1$ if and only if $2^p-d-1\leqslant d-1\Leftrightarrow 2d\geqslant 2^p$.

c. Odd/even structure

We now describe the odd/even structure of $\Omega(\mathcal{W},p)$. We can divide the $p!$ basis vectors of $\mathcal{K}$ into two equal subsets, those of the form $P_{\text{even}}|k_1,k_2,\ldots,k_p\rangle$ and those of the form $P_{\text{odd}}|k_1,k_2,\ldots,k_p\rangle$. We will denote their spans as $\mathcal{K}_{\text{even}}$ and $\mathcal{K}_{\text{odd}}$, respectively. Now $\langle k_1,k_2,\ldots,k_p|\Pi|k_1,k_2,\ldots,k_p\rangle=0$ unless Π is the identity permutation. Therefore $\langle P_s(k_1,k_2,\ldots,k_p)|\Pi|P_t(k_1,k_2,\ldots,k_p)\rangle=0$ unless $\Pi=P_sP_t^\dagger=I$. Moreover, since the identity is an even permutation

$$\langle P_{\text{even}}(k_1,k_2,\ldots,k_p)|\Pi_{\text{odd}}|\tilde{P}_{\text{even}}(k_1,k_2,\ldots,k_p)\rangle=\langle P_{\text{odd}}(k_1,k_2,\ldots,k_p)|\Pi_{\text{odd}}|\tilde{P}_{\text{odd}}(k_1,k_2,\ldots,k_p)\rangle=0, \tag{C10}$$

$$\langle P_{\text{even}}(k_1,k_2,\ldots,k_p)|\Pi_{\text{even}}|\tilde{P}_{\text{odd}}(k_1,k_2,\ldots,k_p)\rangle=\langle P_{\text{odd}}(k_1,k_2,\ldots,k_p)|\Pi_{\text{even}}|\tilde{P}_{\text{even}}(k_1,k_2,\ldots,k_p)\rangle=0. \tag{C11}$$

Thus, the largest block of $(d-1)^p\Omega(\mathcal{W},p)$ can be written in the form

$$B=(d-p)\mathbb{1}+\begin{pmatrix}-B_{\text{ee}} & B_{\text{oe}}\\ B_{\text{eo}} & -B_{\text{oo}}\end{pmatrix}$$

with B_{ee} and B_{oo} determined by $\tilde{\Omega}_{\text{even}}$ and B_{eo} and B_{oe} determined by $\tilde{\Omega}_{\text{odd}}$.

It is useful to relate the order of elements within the bases associated with odd and even permutations. Let $P_1,P_2,\ldots,P_M$ with $M=p!/2$ denote the even permutations (with $P_1=\mathbb{1}$) and $P_{t+M}=P_tS$ the odd, where S denotes the swap operator $S(k_1,k_2,k_3,\ldots,k_p)=k_2,k_1,k_3,\ldots,k_p$. (There is nothing special about applying SWAP to the first two elements. Any fixed choice would do.) Then

$$\begin{aligned}b_{s,t+M}&=\langle P_s(k_1,k_2,\ldots,k_p)|\Pi|P_tS(k_1,k_2,\ldots,k_p)\rangle\\&=\langle P_sS(k_2,k_1,\ldots,k_p)|\Pi|P_t(k_2,k_1,\ldots,k_p)\rangle=b_{s+M,t},\end{aligned} \tag{C12}$$

where we used the fact that the matrix representing a permutation is independent of the initial choice of k_i. Thus, $B_{\text{eo}}=B_{\text{oe}}$ and, for the same reason, $B_{\text{ee}}=B_{\text{oo}}$, and we can write

$$B=(d-p)\mathbb{1}+\begin{pmatrix}-W_{\text{e}} & W_{\text{o}}\\ W_{\text{o}} & -W_{\text{e}}\end{pmatrix}=(d-p)\mathbb{1}+B_{\text{off}}, \tag{C13}$$

where W_{e} and W_{o} are determined by $\tilde{\Omega}_{\text{even}}$ and $\tilde{\Omega}_{\text{odd}}$, respectively. By conjugating with $\left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right)$, one finds that B has the same singular values as

$$G=(d-p)\mathbb{1}-\begin{pmatrix}W_{\text{e}} & W_{\text{o}}\\ W_{\text{o}} & W_{\text{e}}\end{pmatrix}=(d-p)\mathbb{1}-G_{\text{off}}. \tag{C14}$$

Note that we have shown that the restriction of $\Omega(\mathcal{W},p)$ to $\mathcal{K}$ is similar to $1/(d-1)^p[(d-p)\mathbb{1}-\tilde{\Omega}_{\text{odd}}-\tilde{\Omega}_{\text{even}}]$ which differs from (C6) by a sign. Although this may seem surprising, it could easily be established directly by observing that any vector $|v\rangle\in\mathcal{K}$ can be written as $|v\rangle=|v_{\text{even}}\rangle+|v_{\text{odd}}\rangle$ with $|v_{\text{even}}\rangle\in\mathcal{K}_{\text{even}}$ and $|v_{\text{odd}}\rangle\in\mathcal{K}_{\text{odd}}$. Using (C3) and related combinatorics, one finds that the row and column sums of B, G, W_{e}, and W_{o} are, respectively, $d-1$, $d-2^p+1$, $2^{p-1}-p$, and $2^{p-1}-1$. It follows that $d-1$ and $d-2^p+1$ are eigenvalues of B and G,

$$B\begin{pmatrix}1\\1\end{pmatrix}=(d-1)\begin{pmatrix}1\\1\end{pmatrix},\quad B\begin{pmatrix}1\\-1\end{pmatrix}=(d-2^p+1)\begin{pmatrix}1\\-1\end{pmatrix}, \tag{C15a}$$

$$G\begin{pmatrix} 1 \\ -1 \end{pmatrix} = (d-1)\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad G\begin{pmatrix} 1 \\ 1 \end{pmatrix} = (d-2^p+1)\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{C15b}$$

where 1 denotes a vector with all 1's. These are easily seen to be equivalent to (C8).

The main reason for changing B to the form (C14) is that G_{off} is a multiple of a double stochastic matrix, its column sum 2^p-p-1 is both its largest eigenvalue and its largest singular value. Therefore, $d-2^p+1$ is the smallest eigenvalue of G; however, even when it is the most negative eigenvalue, we cannot conclude that it is also the largest singular value because G could have a positive, or complex, eigenvalue of greater magnitude.

Remark: Conjugating B with the block Hadamard transform $H=2^{-1/2}\begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & -\mathbb{1} \end{pmatrix}$ corresponds to making the change of basis to (C18). One finds

$$HFH^\dagger = (d-p)\mathbb{1} + \begin{pmatrix} -W_e + W_o & 0 \\ 0 & -W_e - W_o \end{pmatrix}. \tag{C16}$$

5. Proof that $\|\Omega(\mathcal{W},p)\|_\infty$ is attained on the largest blocks

As above, fix $k_1<k_2<\cdots<k_p$ and let B denote the block of $\Omega(\mathcal{W},p)$ corresponding to their span $\mathcal{K}$.

For simplicity, we first compare the singular values of B to those for a block spanned by vectors of the form

$$\{\Pi|j,j,k_3,\ldots,k_p\rangle : \Pi \in \mathcal{S}_p\} \tag{C17}$$

with $j<k_3<\cdots<k_p$. Observe that

$$\left\{ \frac{1}{\sqrt{2}}\Pi(|k_1,k_2,k_3,\ldots,k_p\rangle \pm |k_2,k_1,k_3,\ldots,k_p\rangle) : \Pi \in \mathcal{S}_p,\ \Pi \neq S_{12} \right\} \tag{C18}$$

is another orthonormal basis for $\mathcal{K}$, and let V be the unitary matrix for the basis change from $\{P|k_1,k_2,\ldots,k_p\rangle, P\in\mathcal{S}_p\}$ to (C18). Let $\mathcal{K}_\pm$ denote the subspace spanned by vectors with a $\pm$ sign in (C18), and $\tilde{B}_{++}$ the submatrix for the restriction of $VBV^\dagger$ to the subspace $\mathcal{K}_+$. The effect of any permutation on vectors of the form (C17) and those with a $+$ sign in (C18) is the same. Therefore, $\tilde{B}_{++}$ is identical to the matrix for the restriction of $\Omega(\mathcal{W},p)$ to the span of (C17), and the largest singular value of the latter is the same as

$$\|\tilde{B}_{++}\|_\infty = \sup_{\phi\in\mathcal{K}_+} \frac{\langle\phi,\tilde{B}_{++}^\dagger\tilde{B}_{++}\phi\rangle}{\|\phi\|^2} = \sup_{\phi\in\mathcal{K}_+} \frac{\langle\phi,VB^\dagger BV^\dagger\phi\rangle}{\|\phi\|^2} \leqslant \sup_{\phi\in\mathcal{K}} \frac{\langle\phi,VB^\dagger BV^\dagger\phi\rangle}{\|\phi\|^2} = \|B\|_\infty^2. \tag{C19}$$

In (C16) we showed that $\tilde{B}_{++}=-W_e+W_o$ and that B is block diagonal, which immediately implies that the singular values of $\tilde{B}_{++}$ are a subset of those for B. This is stronger than (C19), but does not necessarily generalize.

Next, consider a block for a subspace spanned by vectors of the form

$$\{\Pi|j,j,\ldots,j,k_{m+1},\ldots,k_p\rangle : \Pi \in \mathcal{S}_p\} \tag{C20}$$

with m occurences of j and $j<k_{m+1}\cdots k_p$. We adopt the convention that $Q\in\mathcal{S}_m$ denotes a permutation of $\{1,2,\ldots,m\}$. Choose $p!/m!$ permutations $P_t\in\mathcal{S}_p$ such that each P_t is in a distinct coset of $\mathcal{S}_p/\mathcal{S}_m$ or, equivalently $P_sP_t^{-1}\notin\mathcal{S}_m\,\forall\, s\neq t$. Then the vectors

$$|\phi_t\rangle = \frac{1}{\sqrt{m!}} \sum_{Q \in \mathcal{S}_m} P_t Q |k_1, \ldots, k_m, k_{m+1}, \ldots, k_p\rangle \tag{C21}$$

transform under permutations exactly as those in (C20). Therefore, the restriction of B to the span of (C21) is represented by the same matrix as the block of $\Omega(\mathcal{W}, p)$ corresponding to (C20). Then, as in (C19), its largest singular value is bounded above by $\|B\|_\infty$.

To deal with the general case, note that the restriction $j < k_{m+1} < k_{m+2} < \cdots < k_p$ does not play an essential role. The same argument works whenever j is distinct from the remaining k_i with $i > m$. Then, for example, the

largest singular value of the block for permutations of $|i,i,i,j,j,k_6, \ldots, k_p\rangle$

$\leqslant$ largest singular value of the block for permutations of $|i,i,i,k_4,k_5, \ldots, k_p\rangle$

$\leqslant$ largest singular value of the block for permutations of $|k_1,k_2, \ldots, k_p\rangle = \|B\|_\infty$.

Proceeding in this way, one can complete the argument by induction. Alternatively, one could consider cosets for repeated indices, such as $\mathcal{S}_p/(\mathcal{S}_3 \times \mathcal{S}_2)$ in this example.

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A rigorous proof of the Landauer–Büttiker formula

Horia D. Cornean[a] and Arne Jensen[a]
Department of Mathematical Sciences, Aalborg University, Fredrik Bajers Vej 7G, 9220 Aalborg, Denmark

Valeriu Moldoveanu
National Institute of Materials Physics, P.O. Box MG-7, Magurele, Romania

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Recently, Avron *et al.* in a series of papers shed new light on the question of quantum transport in mesoscopic samples coupled to particle reservoirs by semi-infinite leads. They rigorously treat the case, when the sample undergoes an adiabatic evolution thus generating a current through the leads, and prove the so-called BPT formula. Using a discrete model, we complement their work by giving a rigorous proof of the Landauer–Büttiker formula, which deals with the current generated by an adiabatic evolution on the leads. As is well known from physics, both of these formulas link the conductance coefficients for such systems to the *S*-matrix of the associated scattering problem. As an application, we discuss resonant transport through a quantum dot. The single charge tunneling processes are mediated by extended edge states, simultaneously localized near several leads. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1862324]

I. INTRODUCTION

Mesoscopic systems have been extensively studied in the last two decades, both from theoretical and experimental points of view. Much effort has been devoted to the understanding of transport phenomena through quantum rings, wires, or dots (see the monographs, Refs. 15 and 18). These nano-devices display several nontrivial effects, for example, Aharonov–Bohm conductance oscillations, quantum Hall effect, and single charge tunneling. Consequently, various theories have been developed in order to explain them. Among such theories, the scattering approach to the transport problem initiated by Landauer,[23,24] and accomplished by Büttiker,[10,11] is perhaps the most frequently utilized one in the physics literature. The basic idea in the Landauer–Büttiker (LB) formalism is that the charge transport through a finite system connected to several (usually semi-infinite) leads is a scattering process. The incident electrons are either transmitted between leads or reflected in the same lead. By a counting argument, the conductance G of a two-lead system is related to its transmittance $\mathcal{T}$ (which still remains to be computed from the S matrix of the problem) by the Landauer formula at zero temperature,

$$G = \frac{e^2}{h}\mathcal{T}. \tag{1}$$

As shown by Büttiker, this formula admits a generalization to a multilead geometry, and also to the case, when a magnetic field is present. In particular, a four-terminal setup is the natural way to put into evidence the quantization of the Hall resistance in strong magnetic fields.

Alternatively, the conductance G can be found from the linear response theory. It is then a natural question, whether the Landauer formula can be derived directly from the Kubo formalism. This problem was addressed in a series of papers in the 1980s (see Refs. 17, 20, 25, and 22). All those papers used the Kubo formula as given for macroscopic samples. Later on, Baranger and

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Stone[6] argued for a Kubo formula adapted to mesoscopic systems with leads. They also presented a formal justification of the equivalence between the linear response theory, and the LB approach.

The main aim of our work is to provide a rigorous derivation of this equivalence, following their ideas. Second, we use the LB formalism to describe the resonant transport through a mesoscopic sample weakly coupled to leads, the so-called quantum dot (see Ref. 21 for a review). These steps are behind the formulas used in Ref. 26 for studying specific properties of such systems.

Now let us describe the strategy followed to achieve the results. First, we establish a Kubo formula for the conductance, and then we perform the thermodynamic and adiabatic limits. Second, we compute the transmission between different leads from scattering theory. A comparison of the two results leads us to the Landauer–Büttiker formula.

We stress that in the present approach we use a tight-binding representation (i.e., a discrete model) for Hamiltonians. This makes some of the delicate technical points easier to handle. For instance, due to the particular form of the current operator (which has finite rank), the trace implied by the Kubo formula is reduced to a simple product of matrix elements of an effective resolvent R_{eff} that comes from the Feshbach formula. Its associated Hamiltonian acts only in the Hilbert space of the finite system, and is non-Hermitian, due to a supplementary term that embodies the effects of the leads. This term is well known in the physics literature as the self-energy of the leads (see Ref. 15). Roughly speaking, it controls the imaginary part of the effective Hamiltonian coming from the Feshbach formula, and is proportional to the square of the hopping integral between the leads and the sample. As a consequence, a weak coupling generates resonances located near the real axis, and a peak in the conductance, as given by the LB formula, each time the energy of the incident electron equals an eigenvalue of the isolated dot. These peaks are the so-called Coulomb oscillations in quantum dots (see Ref. 21 for an introduction to the subject). In fact, our approach shows that the peaks are *not* of Coulomb origin, but a purely resonant effect (as shown numerically in Ref. 26, they are very sensitive to the lead-dot coupling, the interaction adding quantitative differences only).

Other interesting geometric, topological, and adiabatic aspects of transport problems through mesoscopic samples were given by Avron *et al.* in Refs. 1–4. Note that the authors work with adiabatic pumps, i.e., the perturbation occurs on the sample, and not on the leads (the analog of LB formula in that case is the so-called BPT formula[12]).

In Ref. 5 the authors rigorously prove the BPT formula. They chose to work from the beginning with infinite leads. A difficulty in that approach is that the one particle fermionic density matrix is no longer trace class, and one has to be careful when defining the currents. We manage to bypass this difficulty, by starting with the grand canonical density matrix in the associated Fock spaces for *finite* leads. Due to the absence of self-interactions, we manage to define one particle currents in a natural way. Then we let the lengths of the leads go to infinity, and finally we perform the adiabatic limit.

We note that Cohen in Ref. 13 investigates the connection between the BPT and Landauer formulas on one hand, and linear response theory on the other hand. By starting with the Kubo formalism, Cohen found expressions for both the dissipative and nondissipative parts of the response.

Application to pumping of the BPT formula can be traced back to several other authors. Probably the first one to use this tool was Brouwer.[9] Then Moskalets and Büttiker in Ref. 27 investigated dissipation and noise in adiabatic quantum pumps, while in Ref. 28 they extended the theory to nonadiabatic situations.

The paper is organized as follows. Section II sets notation and gives the main result, Section III presents some relevant spectral properties of our system, while Sec. IV contains the proof of our main theorem. Section V is devoted to a simple application of the formalism to the resonant transport through noninteracting quantum dots. Several technical tools are left to appendices.

II. PRELIMINARIES AND RESULTS

A. The model

We use the tight-binding approximation, and thus a discrete model, throughout the paper. The system, through which the current will run, is modeled by Γ, chosen to be a finite subset of $\mathbb{Z}^2$ (we can also identify it with a finite subset of $\mathbb{N}$). We couple Γ to several "one-dimensional" leads. The sites of each lead are modeled by $\mathcal{N}\subseteq\mathbb{N}$; when $\mathcal{N}=\mathbb{N}$ the lead is semi-infinite. In the sequel the finite system described by Γ will be named sample while the name "system" will be given to the whole structure consisting of "sample+leads."

The total one-particle Hilbert space is a direct sum of the space modeling the sample, and M spaces corresponding to the leads,

$$\mathcal{H} = l^2(\Gamma) \oplus l^2(\mathcal{N}) \oplus \cdots l^2(\mathcal{N}). \tag{2.1}$$

Let us describe the one-particle Hamiltonian. In the sample we may have any self-adjoint bounded operator H^S. For example, we can choose H^S to be the restriction of a Harper-type operator to $l^2(\Gamma)$ with Dirichlet boundary conditions,

$$H^S = \sum_{(m,n)\in\mathbb{Z}^2} (E_0|m,n\rangle\langle m,n| + t_1(e^{-i(Bm/2)}|m,n\rangle\langle m,n+1| + \text{H.c.}) + t_2(e^{-i(Bn/2)}|m,n\rangle\langle m+1,n| + \text{H.c.})). \tag{2.2}$$

Here H.c. means Hermitian conjugate, E_0 is the reference energy, B is a magnetic field, from which the magnetic phases appear (the symmetric gauge was used), while t_1 and t_2 are hopping integrals between nearest neighbor sites.

As for the leads, the dynamics in each of them is governed by the one-dimensional discrete Laplacian on $l^2(\mathcal{N})$ with Dirichlet boundary conditions (see Appendix A). The Hamiltonian on the leads will be ($t_L>0$ is the hopping integral on leads)

$$H^L = \sum_{\alpha=1}^{M} H^L_\alpha, \quad H^L_\alpha = \sum_{n_\alpha\in\mathcal{N}} t_L\cdot(|n_\alpha\rangle\langle n_\alpha+1| + \text{H.c.}), \tag{2.3}$$

acting on functions, which by convention are extended with value zero at the sites -1 and $N+1$.

The "coupling" between the sample and leads is described by the tunneling Hamiltonian,

$$H^T = \tau\sum_{\alpha=1}^{M} |0_\alpha\rangle\langle\mathcal{S}^\alpha| + \tau\sum_{\alpha=1}^{M} |\mathcal{S}^\alpha\rangle\langle 0_\alpha| =: H^{LS} + H^{SL}. \tag{2.4}$$

Here $\tau>0$ is the hopping integral between each lead and the sample, and simulates a quantum point constriction, or a tunneling barrier. Here $|0_\alpha\rangle$ is the first site on the lead α, and $|\mathcal{S}^\alpha\rangle$ is the site from the sample, through which the coupling with the lead α is realized.

Then the total one-particle Hamiltonian is the sum $H^S+H^L+H^T$, with obvious identifications. In the case when the leads are *semi-infinite*, we introduce a special notation for it,

$$K := H^S + \sum_{\alpha=1}^{M} H^L_\alpha + H^T = H^S + H^L + H^{LS} + H^{SL}. \tag{2.5}$$

B. Adiabatic currents and conductivity

Here we deal with electronic transport through the system. We first take the leads to be finite (i.e., each lead consists of $N<\infty$ sites), although their length can be arbitrarily large. However, the thermodynamic limit $N\to\infty$ is to be taken at a certain point in our argument.

We will only work in the grand canonical ensemble. This means that our system is in contact with a reservoir of energy and particles. Having this in mind, we will study the linear response of

a system of noninteracting fermions at temperature T and chemical potential μ subjected to a perturbation, which is switched on adiabatically (to insure that the system is at equilibrium at all times).

Let χ_η, $\eta>0$, be a smooth switching function $0\leqslant\chi_\eta(t)\leqslant 2$,

$$\chi_\eta(t)=\begin{cases} e^{\eta t} & \text{if } t\leqslant 0,\\ 1 & \text{if } t>1. \end{cases} \tag{2.6}$$

Then the perturbation is given by (i_α denotes the ith site on the lead α)

$$V(N,t) := \chi_\eta(t)\sum_{\alpha=1}^{M} V_\alpha \sum_{i_\alpha=0}^{N} |i_\alpha\rangle\langle i_\alpha|. \tag{2.7}$$

Notice that $V(N,t)$ models the adiabatic application of a constant voltage V_α on the lead α. This will generate a charge transfer between the leads via the sample.

The relevant one-particle Hamiltonians then are given by

$$H_0(N) := H^S + H^L(N) + H^T,$$

$$H(N,t) := H_0(N) + V(N,t). \tag{2.8}$$

Here $H^L(N)$ is the Hamiltonian acting on the finite leads, while $H_0(N)$ is the same operator as in (2.5), but the different notation indicates that it describes the initial equilibrium state for finite leads.

Now we are interested in deriving the current response of the system due to the perturbation. Since we work in the grand canonical ensemble, we have to consider all our operators in the second quantization, see Appendix B for further notation and properties.

At $t=-\infty$ our system is characterized by the Gibbs equilibrium state, and its corresponding statistical operator (density matrix) is the well known one [see (B2)]. The statistical operator describing the equilibrium state at time t for the sample coupled with the finite leads is denoted by $\hat{\rho}^{(N)}(t)$, and is defined as the (trace class) solution of the quantum Liouville equation

$$i\frac{\partial\hat{\rho}^{(N)}(t)}{\partial t}=[\mathrm{d}\Gamma(H(N,t)),\hat{\rho}^{(N)}(t)], \tag{2.9}$$

which satisfies the initial condition $\lim_{t\to-\infty}\hat{\rho}^{(N)}(t)=\hat{\rho}_0^{(N)}$, where $\hat{\rho}_0^{(N)}$ is as in (B2), but with $H_0(N)$ instead of H. We stress here the fact that if the leads are infinite, these operators are no longer of trace class.

Let us now write the perturbation in the "interaction picture,"

$$\tilde{V}(N,s) := e^{isH_0(N)}V(N,s)e^{-isH_0(N)}. \tag{2.10}$$

To describe the solution of the Liouville equation we consider the following equation:

$$\frac{\mathrm{d}W}{\mathrm{d}s}(s)=iW(s)\mathrm{d}\Gamma(\tilde{V}(N,s)),\quad W(-\infty)=\mathrm{Id},$$

where the unitary $W(s)$ is given by the usual Dyson series with respect to $\mathrm{d}\Gamma(\tilde{V}(N,s))$. By direct computation, and using (B5) for $\tilde{V}(N,s)$, one can verify that

$$\hat{\rho}^{(N)}(t)=e^{-it\ \mathrm{d}\Gamma(H_0(N))}W^*(t)\hat{\rho}_0^{(N)}W(t)e^{it\ \mathrm{d}\Gamma(H_0(N))} \tag{2.11}$$

is the unique solution to the Liouville equation, providing us with a positive operator of trace class. Expanding the Dyson series up to the first order, and using (B4) and (B5), a straightforward computation gives

$$\hat{\rho}^{(N)}(t) = \hat{\rho}_0^{(N)} - i\int_{-\infty}^{t} [\mathrm{d}\Gamma(e^{i(s-t)H_0(N)}V(N,s)e^{-i(s-t)H_0(N)}), \hat{\rho}_0^{(N)}]\mathrm{d}s + \mathcal{O}(V^2). \tag{2.12}$$

Let us introduce the one-particle charge operator in a given lead α (which is just minus the projection corresponding to the lead, the sign taking into account the fact that we deal with electrons)

$$Q_\alpha^{(N)} = -\sum_{i=0}^{N} |i_\alpha\rangle\langle i_\alpha|. \tag{2.13}$$

Denote by $\mathbf{Q}_\alpha^{(N)} = \mathrm{d}\Gamma(Q_\alpha^{(N)})$ its second quantization. Since we work in the grand canonical ensemble, the average charge in the lead α is given by

$$\mathcal{Q}_\alpha^{(N)}(t) := \mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}^{(N)}(t)\mathbf{Q}_\alpha^{(N)}). \tag{2.14}$$

Then the average charge is smooth in t, and we can define the current in the lead α as the charge transfer per unit of time, namely

$$\mathcal{I}_\alpha(t) := \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{Q}_\alpha(t). \tag{2.15}$$

We will see that at $t=0$, this current can be written as

$$\mathcal{I}_\alpha(0) = \sum_\beta g_{\alpha\beta}(T,\mu,\eta,N)V_\beta + \mathcal{O}(V^2), \tag{2.16}$$

where $g_{\alpha\beta}(T,\mu,\eta,N)$ are the so-called conductance coefficients.[15] At this stage they depend on the temperature, the chemical potential, the adiabatic coefficient, and the length of the leads. The point of this paper is then to study the connection between $g_{\alpha\beta}$ and the transmittance of the problem, defined below.

Let us stress once again, as we have already done it in the introduction, that the above current is derived in a linear response regime. As it is well known, this approach does not allow one to perform the adiabatic limit first, since the error in (2.16) is in fact $\mathcal{O}(V^2/\eta^2)$. Such a result would demand a different approach, as done, for example, in Avron *et al.*[5] Nevertheless, the linear response theory gives relevant results, if the amplitude of the external perturbation is weaker than its rate of adiabaticity.

For the mathematical treatment of linear response theory, together with an analysis of its physical applicability, we cite a recent paper by Bouclet *et al.*[7]

C. The transmittance

Now we briefly switch to an apparently unrelated scattering problem, associated with the pair of Hamiltonians (K,H_0), where $H_0=H^L$ and $K=H_0+W=H_0+H^S+H^T$. Thus the "free" system consists here of the *semi-infinite* leads, while the complete evolution is that of the coupled system (leads and sample).

The operator K is defined on the full space $\mathcal{H}$, see (2.1), and the operator H_0 is defined on the subspace $\mathcal{H}_0=\oplus_{\alpha=1}^{M} l^2(\mathbb{N})$. We denote by $J:\mathcal{H}_0\to\mathcal{H}$ the identification operator. We obviously have $J^*J=\mathrm{Id}$, the identity on $\mathcal{H}_0$. Note that H_0 has purely absolutely continuous spectrum. The operator $KJ-JH_0$ is of finite rank, hence the (two space) trace class scattering theory (see Refs. 30–32) implies that the wave operators

$$\Omega_\pm = s - \lim_{t\to\mp\infty} e^{itK}Je^{-itH_0} \tag{2.17}$$

exist and are asymptotically complete.

In the sequel we will return to the notation H^L, instead of H_0. It will be clear from the context, whether we regard it as an operator on $\mathcal{H}$, or on $\mathcal{H}_0$. The (normalized) generalized eigenfunctions of H^L on the semi-infinite leads are [here $k \in (0,\pi)$, $\lambda = 2t_L \cos(k)$, and $1 \leqslant \alpha \leqslant M$] given by

$$\Psi_\alpha(\lambda) = \sum_{m \geqslant 0} \Psi(\lambda;m)|m\rangle, \quad \Psi(\lambda;m) = \frac{\sin(k(m+1))}{\sqrt{\pi t_L \sin(k)}}.$$

The generalized Fourier transform associated to these eigenvectors is defined as

$$F: \overset{M}{\underset{\alpha=1}{\oplus}} l^2(\mathbb{N}) \to \overset{M}{\underset{\alpha=1}{\oplus}} L^2([-2t_L, 2t_L]), \tag{2.18}$$

$$[F(\Phi)]_\alpha(\lambda) = \langle \Psi_\alpha(\lambda), \Phi_\alpha \rangle_{l^2(\mathbb{N})} = \sum_{m \geqslant 0} \overline{\Psi(\lambda;m)} \Phi_\alpha(m). \tag{2.19}$$

Its adjoint is given by

$$F^*: \overset{M}{\underset{\alpha=1}{\oplus}} L^2([-2t_L, 2t_L]) \to \overset{M}{\underset{\alpha=1}{\oplus}} l^2(\mathbb{N}), \tag{2.20}$$

$$[F^*(\Xi)]_\alpha(m) = \int_{-2t_L}^{2t_L} \Xi_\alpha(\lambda) \Psi(\lambda;m) \mathrm{d}\lambda. \tag{2.21}$$

We see that F is a unitary operator, and that $FH^L F^*$ is just multiplication by λ, i.e.,

$$FH^L F^* = 2t_L \cos(k) \mathrm{Id}. \tag{2.22}$$

The scattering operator is unitary, and is given by $S = \Omega_-^* \Omega_+$. The T-operator is defined by $T := S - \mathrm{Id}$. In the spectral representation of H_0, the T-operator is a λ-dependent $M \times M$ matrix, the T-matrix. Thus [see (4.4)

$$\sum_\beta t_{\alpha\beta}(\lambda) \Xi_\beta(\lambda) = [F(S - \mathrm{Id}) F^* \Xi]_\alpha(\lambda). \tag{2.23}$$

The transmittance between the leads α and β at energy λ is finally defined as

$$\mathcal{T}_{\alpha\beta}(\lambda) := |t_{\alpha\beta}(\lambda)|^2. \tag{2.24}$$

D. The Landauer–Büttiker formula and the main theorem

We can finally give the main result of our paper.

Theorem 2.1: *Consider the conductance $g_{\alpha\beta}(T, \mu, \eta, N)$ between the leads α and β ($\alpha \neq \beta$), at temperature $T > 0$, chemical potential $\mu \in (-2t_L, 2t_L)$, adiabatic switch-on coefficient $\eta > 0$ and length of the leads $N < \infty$. Assume that the point spectrum of K [the one from (2.5), with $N = \infty$] is disjoint from the thresholds $-2t_L$ and $2t_L$. Then if we first take the limit $N \to \infty$, and after that $\eta \searrow 0$, we have*

$$g_{\alpha\beta}(T, \mu) := \lim_{\eta \searrow 0} [\lim_{N \to \infty} g_{\alpha\beta}(T, \mu, \eta, N)] = -\frac{1}{2\pi} \int_{-2t_L}^{2t_L} \mathrm{d}E \frac{\partial f_{\mathrm{FD}}(E)}{\partial E} \mathcal{T}_{\alpha\beta}(E), \tag{2.25}$$

where $\mathcal{T}_{\alpha\beta}(\cdot)$ is real analytic on $(-2t_L, 2t_L)$ and equal to zero outside this interval. The function f_{FD} is the usual Fermi–Dirac function [see (B3)]. If $T \to 0$ in (2.25) (limit taken at last), we obtain the Landauer formula

$$g_{\alpha\beta}(0_+,\mu) = \frac{1}{2\pi}\mathcal{T}_{\alpha\beta}(\mu). \tag{2.26}$$

III. THE FESHBACH FORMULA AND SPECTRAL ANALYSIS FOR THE SYSTEM WITH SEMI-INFINITE LEADS

We assume throughout this section that the leads are semi-infinite. We denote by $R^L(z)$ the resolvent of the leads as a block diagonal matrix in $\oplus_{\alpha=1}^{M} l^2(\mathbb{N})$. Some of its properties are given in Appendix A.

We use the Feshbach formula[19,29] in order to express the full resolvent in terms of an effective Hamiltonian, which describes the mesoscopic system in the presence of the leads.

If Π^S denotes the projection onto the subspace corresponding to the "system" $l^2(\Gamma)$, and $\Pi^L = \mathrm{Id} - \Pi^S$ denotes the projection onto the leads, then we can rewrite (2.1) as

$$\mathcal{H} = \Pi^S\mathcal{H} \oplus \Pi^L\mathcal{H}. \tag{3.1}$$

To simplify, we write

$$R^L(z) = (\Pi^L K \Pi^L - z\Pi^L)^{-1},$$

as an operator acting on $\Pi^L\mathcal{H}$.

The effective Hamiltonian is defined as

$$H_{\mathrm{eff}}(z) := H^S - H^{SL}R^L(z)H^{LS}, \quad z \in \mathbb{C}\setminus\mathbb{R}, \tag{3.2}$$

acting on $\Pi^S\mathcal{H}$. We abuse notation slightly, and write

$$R_{\mathrm{eff}}(z) = (H_{\mathrm{eff}}(z) - z)^{-1}$$

on this space.

Using the identity (A1) from Nenciu's paper,[29] the total resolvent reads in operator matrix notation [see also (2.5)],

$$R(z) = (K-z)^{-1} = \begin{bmatrix} R_{\mathrm{eff}}(z) & -R_{\mathrm{eff}}(z)H^{SL}R^L(z) \\ -R^L(z)H^{LS}R_{\mathrm{eff}}(z) & R^L(z) + R^L(z)H^{LS}R_{\mathrm{eff}}(z)H^{SL}R^L(z) \end{bmatrix}. \tag{3.3}$$

Using (2.4), the explicit expression for the matrix elements of $R^L(z)$ that we gave in (A1), and Proposition 6.1(iii), we can write

$$H_{\mathrm{eff}}(z) = H^S - \tau^2\sum_{\alpha=1}^{M} |\mathcal{S}^\alpha\rangle\langle 0_\alpha|R^L(z)|0_\alpha\rangle\langle\mathcal{S}^\alpha| = H^S - \frac{\tau^2}{t_L}\zeta_1(z)\sum_{\alpha=1}^{M}|\mathcal{S}^\alpha\rangle\langle\mathcal{S}^\alpha|. \tag{3.4}$$

The spectral problem for K is thus reduced to the spectral problem for H^L and H_{eff}. Note that $H_{\mathrm{eff}}(z)$ is not Hermitian. We also have

$$(H_{\mathrm{eff}}(z) - z)^{-1} = \Pi^S(K-z)^{-1}\Pi^S, \quad \mathrm{Im}\, z \neq 0, \tag{3.5}$$

again with a slight abuse of the notation Π^S.

We need some more notation. For $\epsilon > 0$, define the strip

$$\Omega_\epsilon := \{x + iy \in \mathbb{C} : -2t_L + \epsilon < x < 2t_L - \epsilon, |y| < 1/\epsilon\}. \tag{3.6}$$

Finally, introduce the orthogonal projection

$$\Pi^T := \sum_{\alpha=1}^{M} |\mathcal{S}^\alpha\rangle\langle\mathcal{S}^\alpha|. \tag{3.7}$$

We can then write

$$H_{\text{eff}}(z) = H^S - \frac{\tau^2}{t_L}\zeta_1(z)\Pi^T.$$

The main result of this section is stated as follows.

Proposition 3.1: Let $|S^\beta\rangle$ *and* $|S^\gamma\rangle$ *be the coupling points between the sample, and leads* β *and* γ. *Define*

$$u_{\beta\gamma}(z) = \langle\mathcal{S}^\beta, [H^S - z - (\tau^2/t_L)\zeta_1(z)\Pi^T]^{-1}\mathcal{S}^\gamma\rangle, \quad \text{Im } z > 0. \tag{3.8}$$

Then for all positive τ *and* ϵ, *the function* $u_{\beta\gamma}$ *admits a meromorphic extension* $u^+_{\beta\gamma}$ *to* $\mathbb{C}_+ \cup \Omega_\epsilon$, *and all its poles have negative imaginary part. In particular, the restriction of* $u^+_{\alpha\beta}$ *to the interval* $(-2t_L, 2t_L)$ *is real analytic.*

Proof: First note that $u^+_{\beta\gamma}$ is the key term appearing in the transmittance formula [see (4.6)]. Now introduce the notation [see (A4)]

$$H_+(z) := H^S - \frac{\tau^2}{t_L}\zeta_+(z)\Pi^T. \tag{3.9}$$

Then $u^+_{\beta\gamma}(z) = \langle\mathcal{S}^\beta, [H_+(z) - z]^{-1}\mathcal{S}^\gamma\rangle$ is the meromorphic extension we are looking for. Since $l^2(\Gamma)$ is finite dimensional, the set of poles is included in the set of solutions of $\det(H_+(z) - z) = 0$. Due to (3.5), the poles cannot be in the upper complex half-plane.

Now let us prove that the poles are neither on the real axis. If there are no solutions for $\det(H_+(z) - z) = 0$ in $(-2t_L, 2t_L)$, then we are done. Now assume that there exists $\lambda \in (-2t_L, 2t_L)$, such that $H_+(\lambda) - \lambda$ is not invertible. Then $H_+(\lambda) - \lambda$ is not injective. Denote by p_λ the orthogonal projection onto to the null space of $H_+(\lambda) - \lambda$. For every $\phi_\lambda \in \text{Ran}(p_\lambda)$ we have

$$(H^S - \lambda)\phi_\lambda - \frac{\tau^2}{t_L}\zeta_+(\lambda)\Pi^T\phi_\lambda = 0.$$

Taking the scalar product with ϕ_λ and estimating the imaginary part, we have [use (A4)]

$$\langle\phi_\lambda, \Pi^T\phi_\lambda\rangle = \|\Pi^T\phi_\lambda\|^2 = 0.$$

This implies that $\Pi^T\phi_\lambda = 0$, and thus ϕ_λ must also be an eigenfunction for H^S, corresponding to the eigenvalue λ. Notice that this does not say that all eigenvectors of H^S corresponding to λ are in the range of p_λ.

Because $p_\lambda\Pi^T = (\Pi^T p_\lambda)^* = 0$, and because $\text{Ran}(p_\lambda)$ is spanned by eigenvectors of H^S, it means that p_λ commutes with $H_+(z)$, and we can write (here $q_\lambda = \text{Id} - p_\lambda$)

$$H_+(z) - z = p_\lambda(H_+(z) - z)p_\lambda + q_\lambda(H_+(z) - z)q_\lambda = (\lambda - z)p_\lambda + q_\lambda(H_+(z) - z)q_\lambda. \tag{3.10}$$

The range of q_λ is generated by eigenvectors of H^S, which either correspond to other eigenvalues than λ, or correspond to λ but are orthogonal to $\text{Ran}(p_\lambda)$. Now $q_\lambda(H_+(\lambda) - \lambda)q_\lambda$ is one to one on $\text{Ran}(q_\lambda)$, thus invertible, and so is $q_\lambda(H_+(z) - z)q_\lambda$ for z close to λ (by simple perturbation theory and the Neumann series). Moreover, its inverse is holomorphic near λ. Therefore,

$$(H_+(z) - z)^{-1} - (\lambda - z)^{-1}p_\lambda \tag{3.11}$$

is holomorphic around λ. In conclusion, since $p_\lambda\mathcal{S}^\gamma = 0$,

$$u^{+}_{\beta\gamma}(z) = \langle \mathcal{S}^{\beta}, [H_{+}(z) - z]^{-1}\mathcal{S}^{\gamma} - (\lambda - z)^{-1} p_{\lambda}\mathcal{S}^{\gamma}\rangle \tag{3.12}$$

is also holomorphic near λ, and we are done. A similar reasoning gives a meromorphic extension to $\mathbb{C}_{-} \cup \Omega_{\epsilon}$, which we denote by $u^{-}_{\beta\gamma}$. It is also easy to see [use (3.5) and (3.8)] that

$$\overline{u^{+}_{\beta\gamma}(\overline{z})} = u^{-}_{\gamma\beta}(z). \tag{3.13}$$

■

Remark: The above proposition does not rule out real poles for the effective Hamiltonian. It only says that its eventual real poles are not singularities for functions like $u_{\beta\gamma}$. Notice that we allowed τ to be arbitrarily large.

Another important observation is that K cannot have an infinite number of discrete eigenvalues outside $[-2t_L, 2t_L]$. Assume the contrary. Then the equation $\det[H_{\text{eff}}(\lambda) - \lambda] = 0$ would have infinitely many solutions, which accumulate either at $-2t_L$, or at $2t_L$. Since the determinant is continuous at $\pm 2t_L$, it would mean that either $-2t_L$ or $2t_L$ is also a zero. This would imply that K has an eigenvalue at the thresholds, contradicting our hypothesis in Theorem 2.1.

IV. PROOF OF THE MAIN THEOREM

As we have already announced in the introduction, the strategy of the proof is to compute the conductance and transmittance separately, and then to show that they are related as in (2.25). Since the transmittance involves less work, we start with it.

A. A formula for the transmittance

We will use the notation introduced in Sec. II C. The scattering operator $S: \mathcal{H}^L \to \mathcal{H}^L$ can be written as

$$S = \Omega^{*}_{-}\Omega_{+} = \text{Id} + \frac{2i}{\pi}\int_{-2t_L}^{2t_L} \text{Im}[(H^L - x + i0)^{-1}]X(x + i0)\text{Im}[(H^L - x + i0)^{-1}]\text{d}x, \tag{4.1}$$

where we used the fact that H^L has purely absolutely continuous spectrum, and introduced

$$X(z) = J^{*}H^{LS}J - J^{*}H^{LS}(K - z)^{-1}H^{SL}J$$

with the usual abuse of notation. See Ref. 34 for a proof of this formula in general two space trace class scattering theory.

Note that $J^{*}H^{LS}J = 0$. Using the Feshbach formula we get

$$S = \text{Id} - \frac{2i\tau^2}{\pi}\sum_{\alpha,\beta=1}^{M}\int_{-2t_L}^{2t_L} (\text{Im}[(H^L - x + i0)^{-1}]|0_{\alpha}\rangle) \times \langle \mathcal{S}^{\alpha}, R_{\text{eff}}(x + i0)\mathcal{S}^{\beta}\rangle (\langle 0_{\beta}|\text{Im}[(H^L - x + i0)^{-1}])\text{d}x. \tag{4.2}$$

Take $\Xi \in \oplus_{\alpha=1}^{M} C_0^{\infty}((-2t_L, 2t_L))$. Using the formulas (2.22); (2.18), (2.20), and (3.8), we have

$$[F(S - \text{Id})F^{*}\Xi]_{\alpha}(\lambda) = -\frac{2i\tau^2}{\pi}\sum_{\beta=1}^{M}\int_{-2t_L}^{2t_L}\text{d}x(\text{Im}[(\lambda - x + i0)^{-1}]\Psi(\lambda;0))u^{+}_{\alpha\beta}(x) \times \left(\int_{-2t_L}^{2t_L}\text{Im}[(\lambda' - x + i0)^{-1}]\Psi(\lambda';0)\Xi_{\beta}(\lambda')\text{d}\lambda'\right). \tag{4.3}$$

Using twice Sohotsky's formula $1/(t + i0) = \text{P.V.}(1/t) - i\pi\delta$, we get

$$[F(S-\mathrm{Id})F^*\Xi]_\alpha(\lambda) = 2\pi\tau^2 i\sum_{\beta=1}^{M}|\Psi(\lambda;0)|^2 u^+_{\alpha\beta}(\lambda)\Xi_\beta(\lambda). \tag{4.4}$$

Therefore, the T-matrix in the spectral representation of H^L is given by the elements

$$t_{\alpha\beta}(\lambda) = \frac{2\tau^2}{t_L} i\sin(k)u^+_{\alpha\beta}(\lambda). \tag{4.5}$$

Then the transmittance between the leads α and β at energy $\mu =: 2t_L\cos(k_\mu)$ is [see (2.24)] expressed as

$$\mathcal{T}_{\alpha\beta}(\mu) = \frac{4\tau^4}{t_L^2}\sin^2(k_\mu)|u^+_{\alpha\beta}(\mu)|^2. \tag{4.6}$$

B. Conductivities via the linear response theory

We now concentrate on the left-hand side of (2.25). Our main goal here is to obtain a more detailed version of formula (2.16), and to put into evidence the conductivities $g_{\alpha\beta}$ between different leads. Then we perform the thermodynamic and adiabatic limits.

1. Deriving the linear response: a Kubo formula

Differentiating in (2.15), using the Liouville equation (2.9), trace properties [i.e., $\mathrm{Tr}([A,B]C) = -\mathrm{Tr}(B[A,C])$], and (B4), we have

$$\begin{aligned}\mathcal{I}_\alpha(t) &= \mathrm{Tr}_{\mathcal{F}_a}\left(\frac{\mathrm{d}\hat{\rho}^{(N)}(t)}{\mathrm{d}t}\mathbf{Q}^{(N)}_\alpha\right) = i\,\mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}^{(N)}(t)[\mathbf{H}(N,t),\mathbf{Q}^{(N)}_\alpha])\\ &= i\,\mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}^{(N)}(t)\mathrm{d}\Gamma([H(N,t),Q^{(N)}_\alpha])) = \mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}^{(N)}(t)\mathrm{d}\Gamma(j_\alpha(t))),\end{aligned} \tag{4.7}$$

where the one-particle current operator is

$$j_\alpha(t) =: i[H(N,t),Q^{(N)}_\alpha], \tag{4.8}$$

and has a simple explicit form, independent of time [because $Q^{(N)}_\alpha$ and $V(N,t)$ commute],

$$j_\alpha = i\tau(|0_\alpha\rangle\langle\mathcal{S}^\alpha| - |\mathcal{S}^\alpha\rangle\langle 0_\alpha|). \tag{4.9}$$

Note that j_α is a rank two operator. Notice also that even if the leads are semiinfinite, j_α is the *same*, this fact justifying the absence of N in its notation.

Now we continue to compute the current, using the decomposition (2.12). Introduce the notation [see also (2.8) and (B3), and set $t=0$]

$$\mathcal{I}^{(0)}(0) =: \mathrm{Tr}_{\mathcal{H}}(f_{\mathrm{FD}}(H_0(N))j_\alpha),$$

$$\mathcal{I}^{(1)}(0) =: i\int_{-\infty}^{0}\mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}^{(N)}_0[\mathrm{d}\Gamma(\tilde{V}(N,s)),\mathrm{d}\Gamma(j_\alpha)])\mathrm{d}s. \tag{4.10}$$

Inserting (2.12) in (4.7), and using (B6) for the first term and trace commutation properties for the second one, we obtain

$$\mathcal{I}_\alpha(0) = \mathcal{I}^{(0)}(0) + \mathcal{I}^{(1)}(0) + \mathcal{O}(V^2). \tag{4.11}$$

Introduce the notation

$$Q_\beta^{(N)}(-s) := e^{-isH_0(N)} Q_\beta^{(N)} e^{+isH_0(N)}. \tag{4.12}$$

We continue rewriting $\mathcal{I}^{(1)}(0)$ employing (B4)–(B6), which leads to

$$\begin{aligned}
\mathcal{I}^{(1)}(0) &= i\int_{-\infty}^{0} \mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}_0^{(N)}[\mathrm{d}\Gamma(e^{isH_0(N)}V(N,s)e^{-isH_0(N)}),\mathrm{d}\Gamma(j_\alpha)])\mathrm{d}s \\
&= -i\sum_\beta \int_0^\infty \chi_\eta(-s)\mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}_0^{(N)}[\mathrm{d}\Gamma(Q_\beta(-s),\mathrm{d}\Gamma(j_\alpha)])V_\beta\,\mathrm{d}s \\
&= -i\sum_\beta \int_0^\infty \mathrm{d}s\ \chi_\eta(-s)\mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}_0^{(N)}\,\mathrm{d}\Gamma[Q_\beta(-s),j_\alpha])V_\beta \\
&= -i\sum_\beta \int_0^\infty \mathrm{d}s\ \chi_\eta(-s)\mathrm{Tr}_{\mathcal{H}}(f_{\mathrm{FD}}(H_0(N))[Q_\beta(-s),j_\alpha])V_\beta.
\end{aligned}$$

Notice that the minus sign appears, because the charge is negative, and we replaced the projection on each lead with the corresponding charge operator. The average current at time $t=0$ then becomes

$$\begin{aligned}
\mathcal{I}_\alpha(0) = \mathcal{I}^{(0)}(0) + \mathcal{I}^{(1)}(0) + \mathcal{O}(V^2) &= \mathrm{Tr}_{\mathcal{H}}(f_{\mathrm{FD}}(H_0(N))j_\alpha) - i\sum_\beta \int_0^\infty \mathrm{d}s\ e^{-\eta s}\,\mathrm{Tr}_{\mathcal{H}}(f_{\mathrm{FD}}(H_0(N)) \\
&\quad \times[Q_\beta^{(N)}(-s),j_\alpha])V_\beta + \mathcal{O}(V^2).
\end{aligned} \tag{4.13}$$

If we compare this expression with the one announced in (2.16), we see that we are almost in place with the exception of the term $\mathcal{I}^{(0)}(0)$. This term represents the current in the equilibrium state when all V_α's are zero. Let us now prove that this term is always zero. Indeed,

$$\mathcal{I}^{(0)}(0) = i\,\mathrm{Tr}\{f_{\mathrm{FD}}(H_0(N))[H_0(N),Q_\alpha(N)]\} = i\,\mathrm{Tr}\{[f_{\mathrm{FD}}(H_0(N)),H_0(N)]Q_\alpha(N)] = 0. \tag{4.14}$$

Therefore, we have finally obtained an expression for the total current as it was announced in (2.16), where the conductivities are given by

$$g_{\alpha\beta}(T,\mu,\eta,N) := -i\int_0^\infty \mathrm{d}s\ e^{-\eta s}\,\mathrm{Tr}_{\mathcal{H}}(f_{\mathrm{FD}}(H_0(N))[Q_\beta^{(N)}(-s),j_\alpha]). \tag{4.15}$$

What we do in the next paragraphs is to perform the various limits required by Theorem 2.25.

2. Making the leads semi-infinite: N→∞

Define the quantity which is the natural candidate for the limit $N\to\infty$

$$g_{\alpha\beta}(T,\mu,\eta,\infty) := -i\int_0^\infty \mathrm{d}s\ e^{-\eta s}\,\mathrm{Tr}_{\mathcal{H}}(f_{\mathrm{FD}}(K)[Q_\beta^{(\infty)}(-s),j_\alpha]). \tag{4.16}$$

Notice that in the limit $N=\infty$, we have $H_0(\infty)=K$ [see (2.8) and (2.5)]. Neither $f_{\mathrm{FD}}(K)$ nor $Q_\beta^{(\infty)}\times(-s)$ are of trace class anymore, but since j_α is the same as in (4.9) (thus of rank two), the total operator is of trace class with trace uniformly bounded with respect to s. It is easy to see that $g_{\alpha\beta}(T,\mu,\eta,N)$ converges to (4.16), since $H_0(N)$ converges strongly to K, and j_α is trace class. The hard part is to say something about the rate of convergence.

The main result of this paragraph is contained in the following lemma, which states that the speed of convergence when N grows to infinity is faster than any inverse power of N.

Lemma 4.1: For every $J>0$, there exists $C>0$, which may depend on all other parameters but N, so that

$$|g_{\alpha\beta}(T,\mu,\eta,N) - g_{\alpha\beta}(T,\mu,\eta,\infty)| \leqslant CN^{-J}. \tag{4.17}$$

Proof: We will need the formula (3.3), where we replace H^L with $H^L(N)$ [see below (2.8) for the definition of $H^L(N)$]. We introduce the obvious notation $R^L(N,z)$ and $H_{\text{eff}}(N,z)$, to indicate that the leads have finite length. For future reference, formula (3.3) leads to

$$\langle \mathcal{S}^\alpha, (H_0(N)-z)^{-1}0_\alpha\rangle = -\langle \mathcal{S}^\alpha, (H_{\text{eff}}(N,z)-z)^{-1}\mathcal{S}^\alpha\rangle\langle 0_\alpha, R^L(N,z)0_\alpha\rangle = \langle 0_\alpha, (H_0(N)-z)^{-1}\mathcal{S}^\alpha\rangle. \tag{4.18}$$

We first reduce (4.15) to a form which is easier to work with. Replacing the expression for $Q_\beta^{(N)}(-s)$ [see (4.12) and (2.13)] we have (using trace commutation properties)

$$g_{\alpha\beta}(T,\mu,\eta,N) = -i\int_0^\infty \mathrm{d}s\, e^{-\eta s}\{\mathrm{Tr}(f_{\text{FD}}(H_0(N))e^{-isH_0(N)}Q_\beta^{(N)}e^{isH_0(N)}j_\alpha) - \mathrm{Tr}(f_{\text{FD}}(H_0(N))e^{isH_0(N)}j_\alpha e^{-isH_0(N)}Q_\beta^{(N)})\}. \tag{4.19}$$

It is clear that it is enough to prove an estimate as in (4.17) for just one of the terms in (4.19). Define

$$A_{\alpha\beta}(N) := \int_0^\infty e^{-\eta s}\,\mathrm{Tr}(f_{\text{FD}}(H_0(N))e^{-isH_0(N)}Q_\beta^{(N)}e^{isH_0(N)}j_\alpha)\mathrm{d}s. \tag{4.20}$$

Since $\|H_0(N)\| \leqslant \text{const}$ uniformly in N, it means that we can find an interval $[a,b]$, independent of N, which contains the spectrum of $H_0(N)$. Define the function $\phi_0 \in C_0^\infty(\mathbb{R})$, $0 \leqslant \phi_0 \leqslant 1$, $\mathrm{supp}(\phi_0) \subset (-1+a, b+1)$ and

$$\phi_0(x) = \frac{1}{e^{\beta(x-\mu)}+1}, \quad x \in (a,b). \tag{4.21}$$

Also define for every $s>0$ the function

$$\phi_s(x) := \phi_0(x)e^{-isx}. \tag{4.22}$$

Clearly, $f_{\text{FD}}(H_0(N))e^{-isH_0(N)} = \phi_s(H_0(N))$. Assume that $\tilde{\phi}_0$ is an almost analytic extension of ϕ_0, supported in the strip,

$$\mathrm{supp}(\tilde{\phi}_0) \subset (-1+a, b+1) \times (-\eta/2, \eta/2) \subset \mathbb{C}, \tag{4.23}$$

and such that

$$\sup_{-1+a\leqslant x\leqslant b+1} |\overline{\partial}\tilde{\phi}_0(x+iy)| \leqslant \text{const}\cdot|y|^P, \quad |y| \leqslant \eta/2, \tag{4.24}$$

where P is any previously given positive integer. Because e^{-isz} is entire as function of z, an almost analytic extension for ϕ_s is simply $\tilde{\phi}_s(z) := \tilde{\phi}_0(z)e^{-isz}$. The Helffer–Sjöstrand formula is the formula (see, for example, Ref. 16)

$$\phi_s(H_0(N)) = \frac{1}{\pi}\int_{\mathrm{supp}(\tilde{\phi}_0)} (\overline{\partial}\tilde{\phi}_0(x+iy))e^{-isx+sy}(H_0(N)-x-iy)^{-1}\,\mathrm{d}x\,\mathrm{d}y.$$

We will use the following technical result.

Proposition 4.2: Let $F:\mathbb{C}\to\mathbb{C}\backslash\mathbb{R}$ be smooth. Assume that for $x+iy$ in the support of $\tilde{\phi}_0$, we can find two positive integers $k_1 \leqslant P$ and $k_2 \leqslant P$, such that we have the estimate

$$|F(x+iy)| \leqslant \text{const}\cdot\frac{1}{N^{k_1}|y|^{k_2}}, \quad x+iy \in \mathrm{supp}(\tilde{\phi}_0), \quad y \neq 0. \tag{4.25}$$

Then

$$\int_{\mathrm{supp}(\tilde{\phi}_0)} |\overline{\partial\tilde{\phi}_0}(z)| \cdot |F(z)| \mathrm{d}x\, \mathrm{d}y \leqslant \mathrm{const} \cdot \frac{1}{N^{k_1}}. \tag{4.26}$$

Clearly, the proposition is immediately implied by (4.24) and (4.25) and it does not require further details.

We can introduce the expression of $\phi_s(H_0(N))$ in (4.20) and perform the integral with respect to s; the interchange of integrals is permitted because on the support of $\tilde{\phi}_0$ we have $|y| < \eta$. In order to simplify the writing, we denote $x+iy=z$ and $\mathrm{d}x\,\mathrm{d}y$ by d^2z. Then, up to constants, we have that $A_{\alpha\beta}(N)$ is proportional to

$$\int_{\mathrm{supp}(\tilde{\phi}_0)} \overline{\partial\tilde{\phi}_0}(z) \mathrm{Tr}((H_0(N)-z)^{-1} Q_\beta^{(N)} (H_0(N)-z+i\eta)^{-1} j_\alpha) \mathrm{d}^2 z. \tag{4.27}$$

Next we want to simplify the above trace, by expressing Q_β with the help of the current operator j_β. Let $z'=z-i\eta$. We have [see (4.8) and (4.9)]

$$j_\beta = -i[Q_\beta^{(N)}, H_0(N)] = -i(Q_\beta^{(N)}(H_0(N)-z') - (H_0(N)-z)Q_\beta^{(N)}) - i(z'-z)Q_\beta^{(N)},$$

then using obvious notation for the resolvents

$$R_0(N,z)Q_\beta^{(N)}R_0(N,z') = \frac{1}{z'-z}\{iR_0(N,z)j_\beta R_0(N,z') + Q_\beta^{(N)}R_0(N,z') - R_0(N,z)Q_\beta^{(N)}\}. \tag{4.28}$$

Inserting this back into (4.27), we have a number of terms, which must be treated separately. We only deal with one of them, namely the term given (up to constants) by

$$\int_{\mathrm{supp}(\tilde{\phi}_0)} \overline{\partial\tilde{\phi}_0}(z) \mathrm{Tr}(R_0(N,z) Q_\beta^{(N)} j_\alpha) \mathrm{d}^2 z. \tag{4.29}$$

Since $Q_\beta^{(N)} j_\alpha = -i\tau\delta_{\alpha\beta}|0_\alpha\rangle\langle\mathcal{S}^\alpha|$, introducing it back again and performing the trace, we obtain up to constants [see (4.18)]

$$\delta_{\alpha\beta}\int_{\mathrm{supp}(\tilde{\phi}_0)} \overline{\partial\tilde{\phi}_0}(z) \langle\mathcal{S}^\alpha, (H_{\mathrm{eff}}(N,z)-z)^{-1}\mathcal{S}^\alpha\rangle \langle 0_\alpha, R^L(N,z)0_\alpha\rangle \mathrm{d}^2 z. \tag{4.30}$$

The next step is to replace the quantities involving finite leads with the ones corresponding to semi-infinite leads. Let J be an arbitrarily large integer. We see that one term we have to look at in connection with (4.30) is

$$F_1(z) := \langle\mathcal{S}^\alpha, (H_{\mathrm{eff}}(N,z)-z)^{-1}\mathcal{S}^\alpha\rangle \cdot (\langle 0_\alpha, R^L(N,z)0_\alpha\rangle - \langle 0_\alpha, R^L(z)0_\alpha\rangle).$$

An application of (C3) and (C6) yields the estimate

$$|\langle 0_\alpha, R^L(N,z)0_\alpha\rangle - \langle 0_\alpha, R^L(z)0_\alpha\rangle| \leqslant \mathrm{const} \cdot \frac{1}{|\mathrm{Im}\, z|^2} e^{-2cN|\mathrm{Im}\, z|}, \tag{4.31}$$

uniformly in z on the support of $\tilde{\phi}_0$, with $\mathrm{Im}\, z \neq 0$. Notice that (3.5) is also true at finite N, and this gives an upper bound of order $1/|\mathrm{Im}\, z|$ on the first factor in $F_1(z)$. We finally obtain

$$|F_1(z)| \leqslant \mathrm{const} \cdot \frac{1}{|\mathrm{Im}\, z|^3} e^{-2cN|\mathrm{Im}\, z|}, \tag{4.32}$$

uniformly in z on the support of $\tilde{\phi}_0$, with $\mathrm{Im}\, z \neq 0$. But this implies

$$|F_1(z)| \leqslant \text{const} \cdot \frac{1}{|\text{Im } z|^{3+J}} N^{-J}. \tag{4.33}$$

Now choose $\tilde{\phi}_0$ to have a decay in y near the real axis with an exponent P larger than $J+3$ [see (4.24)]. Then (4.26) implies that the integral of F_1 times $\overline{\partial\tilde{\phi}_0}$ will decay at least like N^{-J}.

Another type of term one needs to estimate can be set into the form

$$F_2(z) := \langle 0_\alpha, R^L(z) 0_\alpha \rangle [\langle \mathcal{S}^\alpha (H_{\text{eff}}(N,z) - z)^{-1} \mathcal{S}^\alpha \rangle - \langle \mathcal{S}^\alpha (H_{\text{eff}}(z) - z)^{-1} \mathcal{S}^\alpha \rangle]. \tag{4.34}$$

Using the identity $A^{-1} - B^{-1} = A^{-1}(B-A)B^{-1}$, and the expression (3.2), which is valid for both effective Hamiltonians, we reduce the problem to the estimate from (4.31), but in addition we have some other terms which are each bounded from above by $1/|\text{Im } z|$. We eventually get the estimate

$$|F_2(z)| \leqslant \text{const} \cdot \frac{1}{|\text{Im } z|^5} e^{-2cN|\text{Im } z|}, \tag{4.35}$$

and then we argue as before.

Concluding, we proved that the difference between a term as in (4.30) at finite N, and a similar term "with infinite leads," decays faster than any inverse power of N. We consider that (4.17), thus the lemma, to be proven. ■

3. Taking the adiabatic limit: $\eta \searrow 0$

The next limit to be performed is the adiabatic limit. Thus we define

$$g_{\alpha\beta}(T,\mu) := \lim_{\eta \searrow 0} g_{\alpha\beta}(T,\mu,\eta,\infty), \tag{4.36}$$

where $g_{\alpha\beta}(T,\mu,\eta,\infty)$ is given by (4.16). The idea is again to use the resolvent properties, as we did in the preceding section, one important difference now being that we have to use Stone's formula instead of the Helffer–Sjöstrand formula. The computations will also be more involved in this case. From (4.16) we have

$$g_{\alpha\beta}(T,\mu,\eta,\infty) = -i \int_0^\infty \text{ds } e^{-\eta s} \text{Tr}_{\mathcal{H}} (f_{\text{FD}}(K) e^{-isK} Q_\beta e^{isK} j_\alpha - j_\alpha e^{-isK} Q_\beta e^{isK} f_{\text{FD}}(H)).$$

We note that in the above formula appears again $f_{\text{FD}}(K)e^{-isK}$ and its adjoint. We will express them using Stone's formula. Recall now that K can have point spectrum outside the interval $[-2t_L, 2t_L]$; we also assumed that $\pm 2t_L$ are not eigenvalues. This implies that K can only have a finite number of eigenvalues outside $[-2t_L, 2t_L]$ [see the remarks following (3.13)]. We will see in the next section that K might have embedded eigenvalues in $(-2t_L, 2t_L)$ (see Proposition 5.4).

Consider without loss of generality that there is only one eigenvalue E_1 outside $[-2t_L, 2t_L]$, P_1 being the corresponding projection. Then from Stone's formula one has

$$f_{\text{FD}}(K)e^{-isK} = \lim_{\varepsilon \to 0} \int_{-2t_L}^{2t_L} \text{d}E \, f_{\text{FD}}(E) e^{-isE} \frac{1}{\pi} \text{Im } R(E + i\varepsilon) + f_{\text{FD}}(E_1) e^{-isE_1} P_1. \tag{4.37}$$

Now we follow the same steps as in Sec. IV B 2, namely we perform the integrals over s and we get

$$g_{\alpha\beta}(T,\mu,\eta,\infty) = \frac{i}{2\pi} \lim_{\varepsilon \to 0} \int_{-2t_L}^{2t_L} \text{d}E \, f_{\text{FD}}(E) \, \text{Tr}_{\mathcal{H}} (M_{\alpha\beta}(E,\eta,\varepsilon)) + f_{\text{FD}}(E_1) \, \text{Tr}_{\mathcal{H}} (P_1 Q_\beta R(E_1 - i\eta) j_\alpha$$
$$+ j_\alpha R(E_1 + i\eta) Q_\beta P_1), \tag{4.38}$$

where we wrote

$$M_{\alpha\beta}(E,\eta,\varepsilon) := (R(E+i\varepsilon)-R(E-i\varepsilon))Q_\beta R(E-i\eta)j_\alpha + j_\alpha R(E+i\eta)Q_\beta(R(E+i\varepsilon)-R(E-i\varepsilon)). \tag{4.39}$$

We start with the terms arising from the eigenvalue E_1, and show that in the limit $\eta \searrow 0$ they give no contribution. First we use again a trick to introduce current operators instead of charge operators, namely we write

$$P_1 j_\beta R(E_1 - i\eta) = iP_1[K-(E_1-i\eta),Q_\beta]R(E_1-i\eta) = -\eta P_1 Q_\beta R(E_1-i\eta) - iP_1 Q_\beta,$$

from which we get

$$P_1 Q_\beta R(E_1-i\eta) = -\frac{1}{\eta}P_1 j_\beta R(E_1-i\eta) - \frac{i}{\eta}P_1 Q_\beta. \tag{4.40}$$

Then replacing $P_1 Q_\beta R(E_1 - i\eta)$ and its adjoint in the second term from (4.38) we obtain for the second term in this expression

$$-\mathrm{Tr}_{\mathcal{H}}(P_1 Q_\beta R(E_1-i\eta)j_\alpha + j_\alpha R(E_1+i\eta)Q_\beta P_1) = \frac{1}{\eta}\mathrm{Tr}_{\mathcal{H}}(j_\alpha R(E_1+i\eta)j_\beta P_1 + j_\alpha P_1 j_\beta R(E_1-i\eta) + i(P_1 Q_\beta j_\alpha - j_\alpha Q_\beta P_1)), \tag{4.41}$$

and we can see right away that the last term disappears, when $\alpha \neq \beta$.

The singularities appearing in resolvents can be isolated by writing

$$R(E_1 \pm i\eta) = \pm i\frac{P_1}{\eta} + \frac{1}{2\pi i}\int_{|z-E_1|=\epsilon}\frac{1}{z-(E_1\pm i\eta)}(K-z)^{-1}\,\mathrm{d}z \quad \text{with } \epsilon > \eta. \tag{4.42}$$

We also write P_1 as a Riesz integral,

$$P_1 = \frac{i}{2\pi}\int_{|z'-E_1|=\epsilon'} R(z')\mathrm{d}z' \quad \text{with } \epsilon' < \epsilon. \tag{4.43}$$

By looking at (4.41) we see that the singular term equal to

$$\frac{1}{\eta^2}\mathrm{Tr}_{\mathcal{H}}\{j_\alpha P_1 j_\beta P_1\}$$

is in fact identically zero, due to

$$P_1 j_\alpha P_1 = iP_1[K,Q_\alpha]P_1 = iP_1[K-E_1,Q_\alpha]P_1 = 0. \tag{4.44}$$

Thus we are only left with the regular part from (4.42). Substitute it into (4.41), together with P_1 expressed as in (4.43). We have

$$\frac{1}{\eta}\mathrm{Tr}_{\mathcal{H}}\{j_\alpha R(E_1+i\eta)j_\beta P_1 + j_\alpha P_1 j_\beta R(E_1-i\eta)\} = \frac{1}{4\pi^2\eta}\int_{|z-E_1|=\epsilon}\mathrm{d}z\int_{|z'-E_1|=\epsilon'}\mathrm{d}z'\,F_{\alpha\beta}(z,z',\eta), \tag{4.45}$$

where we used the notation

$$F_{\alpha\beta}(z,z',\eta) := \frac{1}{z-(E_1+i\eta)}\mathrm{Tr}_{\mathcal{H}}(j_\alpha R(z)j_\beta R(z')) + \frac{1}{z-(E_1-i\eta)}\mathrm{Tr}_{\mathcal{H}}(j_\alpha R(z')j_\beta R(z)). \tag{4.46}$$

To go further with the computations we need a technical lemma that gives a general expression for $\mathrm{Tr}_{\mathcal{H}}(j_\alpha R(z)j_\beta R(z'))$.

Lemma 4.3: Let $u_{\alpha\beta}(z)$ *be the function introduced in Proposition* 3.1. *Then the following identity holds* ($\alpha \neq \beta$):

$$\mathrm{Tr}_{\mathcal{H}}(j_\alpha R(z) j_\beta R(z')) = \frac{\tau^4}{t_L^2}(\zeta_1(z) - \zeta_1(z'))^2 u_{\alpha\beta}(z) u_{\beta\alpha}(z'). \tag{4.47}$$

Proof: Taking into account the explicit form of j_α and j_β, we have

$$\mathrm{Tr}_{\mathcal{H}}(j_\alpha R(z) j_\beta R(z')) = -\tau^2\{\langle \mathcal{S}^\alpha, R(z)0_\beta\rangle\langle \mathcal{S}^\beta, R(z')0_\alpha\rangle - \langle \mathcal{S}^\alpha, R(z)\mathcal{S}^\beta\rangle\langle 0_\beta, R(z')0_\alpha\rangle - \langle 0_\alpha, R(z)0_\beta\rangle \times\langle \mathcal{S}^\beta, R(z')\mathcal{S}^\alpha\rangle + \langle 0_\alpha, R(z)\mathcal{S}^\beta\rangle\langle 0_\beta, R(z')\mathcal{S}^\alpha\rangle\}.$$

Each term is then computed using the Feshbach formula for $R(z)$,

$$\langle \mathcal{S}^\alpha, R(z)0_\beta\rangle\langle \mathcal{S}^\beta, R(z')0_\alpha\rangle = \tau^2\langle \mathcal{S}^\alpha, R_{\mathrm{eff}}(z)\mathcal{S}^\beta\rangle\langle 0_\beta, R^L(z)0_\beta\rangle\langle \mathcal{S}^\beta, R_{\mathrm{eff}}(z')\mathcal{S}^\alpha\rangle\langle 0_\alpha, R^L(z')0_\alpha\rangle,$$

$$\langle \mathcal{S}^\alpha, R(z)\mathcal{S}^\beta\rangle\langle 0_\beta, R(z')0_\alpha\rangle = \tau^2\langle \mathcal{S}^\alpha, R_{\mathrm{eff}}(z)\mathcal{S}^\beta\rangle\langle 0_\beta, R^L(z')0_\beta\rangle\langle \mathcal{S}^\beta, R_{\mathrm{eff}}(z')\mathcal{S}^\alpha\rangle\langle 0_\alpha, R^L(z')0_\alpha\rangle,$$

$$\langle 0_\alpha, R(z)0_\beta\rangle\langle \mathcal{S}^\beta, R(z')\mathcal{S}^\alpha\rangle = \tau^2\langle 0_\alpha, R^L(z)0_\alpha\rangle\langle \mathcal{S}^\alpha, R_{\mathrm{eff}}(z)\mathcal{S}^\beta\rangle\langle 0_\beta, R^L(z)0_\beta\rangle\langle \mathcal{S}^\beta, R_{\mathrm{eff}}(z')\mathcal{S}^\alpha\rangle,$$

$$\langle 0_\alpha, R(z)\mathcal{S}^\beta\rangle\langle 0_\beta, R(z')\mathcal{S}^\alpha\rangle = \tau^2\langle 0_\alpha, R^L(z)0_\alpha\rangle\langle \mathcal{S}^\alpha, R_{\mathrm{eff}}(z)\mathcal{S}^\beta\rangle\langle 0_\beta, R^L(z')0_\beta\rangle\langle \mathcal{S}^\beta, R_{\mathrm{eff}}(z')\mathcal{S}^\alpha\rangle.$$

Moreover, we can also use the expression for the matrix elements of the resolvent R^L, which proves the lemma. ■

Now turning back to (4.46), and using the lemma above, we arrive at

$$\frac{t_L^2}{\tau^4}F_{\alpha\beta}(z,z',\eta) = \frac{1}{z-(E_1+i\eta)}(\zeta_1(z)-\zeta_1(z'))^2 u_{\alpha\beta}(z)u_{\beta\alpha}(z') + \frac{1}{z-(E_1-i\eta)} \times(\zeta_1(z)-\zeta_1(z'))^2 u_{\alpha\beta}(z')u_{\beta\alpha}(z).$$

Now we must handle the contour integrals in (4.45). Notice that $u_{\alpha\beta}(z)$ is singular around E_1. However, due to the equivalence (3.5) and relation (4.42), we have (with $\epsilon_1 > \epsilon$)

$$u_{\alpha\beta}(z) = \langle \mathcal{S}^\alpha, P_1\mathcal{S}^\beta\rangle\frac{1}{E_1-z} + \frac{1}{2\pi i}\int_{|z_1-E_1|=\epsilon_1} \mathrm{d}z_1 \frac{1}{z_1-z}\langle \mathcal{S}^\alpha, R(z_1)\mathcal{S}^\beta\rangle. \tag{4.48}$$

Remember that we have $\epsilon_1 > \epsilon > \epsilon'$. Substituting the u's in (4.46) we obtain a lot of terms. The most singular one is of the form (we omit the contours and constants for simplicity)

$$A_1 := \frac{1}{\eta}\int \mathrm{d}z \int \mathrm{d}z' \left(\frac{1}{z-(E_1+i\eta)} + \frac{1}{z-(E_1-i\eta)}\right)\frac{(\zeta_1(z)-\zeta_1(z'))^2}{(E_1-z)\cdot(E_1-z')}. \tag{4.49}$$

By the residue theorem

$$A_1 = \frac{(2\pi)^2 i}{\eta^2}((\zeta_1(E_1-i\eta)-\zeta_1(E_1))^2 - (\zeta_1(E_1+i\eta)-\zeta_1(E_1))^2).$$

Writing the Taylor series for $\zeta_1(E_1 \pm i\eta)$, one is left inside the parentheses with an expression of order η^3, and A_1 vanishes in the limit $\eta \to 0$.

Next, take one of the terms involving the singular part of $u_{\alpha\beta}(z)$ and the regular part of $u_{\alpha\beta}(z')$ (we omit for the moment the constants t_L, τ as well as the matrix elements of P_1),

$$A_2 = \frac{1}{\eta}\int \mathrm{d}z \int \mathrm{d}z' \frac{(\zeta_1(z)-\zeta_1(z'))^2}{z-(E_1+i\eta)} \cdot \frac{1}{E_1-z}\int \frac{\mathrm{d}z_1}{z_1-z'} u_{\alpha\beta}(z_1). \tag{4.50}$$

We see that the integral with respect to z' only involves analytic functions in the disk $|E_1-z'| < \epsilon'$, therefore the integral vanishes.

Another term coming from the singular part of $u_{\alpha\beta}(z')$ and the regular part of $u_{\alpha\beta}(z)$ is the following:

$$\begin{aligned} A_3 &:= \frac{1}{\eta}\int \mathrm{d}z \int \mathrm{d}z' \frac{(\zeta_1(z)-\zeta_1(z'))^2}{z-(E_1+i\eta)} \cdot \frac{1}{E_1-z'}\int \frac{\mathrm{d}z_1}{z_1-z} u_{\alpha\beta}(z_1) \\ &= -\frac{2\pi i}{\eta}\int \mathrm{d}z \frac{(\zeta_1(z)-\zeta_1(E_1))^2}{z-(E_1+i\eta)}\int \frac{\mathrm{d}z_1}{z_1-z} u_{\alpha\beta}(z_1), \end{aligned} \tag{4.51}$$

where in the second line we performed the integral with respect to z'. We can also perform the integral with respect to z and get up to constants the term

$$\frac{1}{\eta}(\zeta_1(E_1+i\eta)-\zeta_1(E_1))^2 \int \frac{\mathrm{d}z_1}{z_1-E_1} u_{\alpha\beta}(z_1).$$

Using again the Taylor series we see that $A_3 \sim \eta$, thus it will disappear as well. The same thing happens with all the other terms.

Looking back at (4.38), we continue with the contribution of $M_{\alpha\beta}$. Let us first bring $M_{\alpha\beta}(E,\eta,\varepsilon)$ to a suitable form. Using (4.28) it turns out that

$$M_{\alpha\beta}(E,\eta,\varepsilon) = M^{(1)}_{\alpha\beta}(E,\eta,\varepsilon) + M^{(2)}_{\alpha\beta}(E,\eta,\varepsilon), \tag{4.52}$$

where

$$\begin{aligned} M^{(1)}_{\alpha\beta}(E,\eta,\varepsilon) &:= \frac{1}{\eta-\varepsilon}(j_\alpha R(E-i\varepsilon) j_\beta R(E-i\eta) - j_\alpha R(E+i\eta) j_\beta R(E+i\varepsilon)) - \frac{1}{\eta+\varepsilon} \\ &\times (j_\alpha R(E+i\varepsilon) j_\beta R(E-i\eta) - j_\alpha R(E+i\eta) j_\beta R(E-i\varepsilon)), \end{aligned} \tag{4.53}$$

while $M^{(2)}_{\alpha\beta}$ includes all terms with only one resolvent. Since $\alpha \neq \beta$, and using the trace cyclicity, the trace of $M^{(2)}_{\alpha\beta}$ is zero and we are only left with $M^{(1)}_{\alpha\beta}$,

$$g_{\alpha\beta}(T,\mu) = \lim_{\eta \searrow 0}\lim_{\epsilon \searrow 0} \frac{i}{2\pi}\int_{-2t_L}^{2t_L} \mathrm{d}E f_{\mathrm{FD}}(E) \mathrm{Tr}_{\mathcal{H}}(M^{(1)}_{\alpha\beta}(E,\eta,\epsilon)). \tag{4.54}$$

Now we apply again the identity (4.47) and we use the meromorphic extensions of $u_{\alpha\beta}(z)$ (see Proposition 3.1), and the properties of $\zeta_1(z)$. The result is

$$g_{\alpha\beta}(T,\mu) = \lim_{\eta \searrow 0}\lim_{\epsilon \searrow 0} \frac{\tau^4}{t_L^2}\frac{i}{2\pi}\int_{-2t_L}^{2t_L} \mathrm{d}E\, f_{\mathrm{FD}}(E)\left(\frac{C_{\alpha\beta}(E,\eta,\epsilon)}{\eta-\epsilon} - \frac{D_{\alpha\beta}(E,\eta,\epsilon)}{\eta+\epsilon}\right), \tag{4.55}$$

with the following notation [see also (3.8) and (3.13)]

$$\begin{aligned} C_{\alpha\beta}(E,\eta,\epsilon) &:= (\zeta_-(E-i\epsilon)-\zeta_-(E-i\eta))^2 u^-_{\alpha\beta}(E-i\epsilon) u^-_{\beta\alpha}(E-i\eta) - (\zeta_+(E+i\eta)-\zeta_+(E+i\epsilon))^2 \\ &\times u^+_{\alpha\beta}(E+i\eta) u^+_{\beta\alpha}(E+i\epsilon), \end{aligned} \tag{4.56}$$

$$\begin{aligned} D_{\alpha\beta}(E,\eta,\epsilon) &:= (\zeta_+(E+i\epsilon)-\zeta_-(E-i\eta))^2 u^+_{\alpha\beta}(E+i\epsilon) u^-_{\beta\alpha}(E-i\eta) - (\zeta_+(E+i\eta)-\zeta_-(E-i\epsilon))^2 \\ &\times u^+_{\alpha\beta}(E+i\eta) u^-_{\beta\alpha}(E-i\epsilon). \end{aligned} \tag{4.57}$$

Since the $u^{\pm}(z)$ are smooth near the real axis, and the $\zeta_{\pm}$ have good behavior, one can take at once

the limit $\epsilon \searrow 0$ in (4.56) and (4.57). In the following we show that $C_{\alpha\beta}$ vanishes in the limit $\eta \searrow 0$. To see this we write, for example,

$$\zeta_+(E + i\eta) - \zeta_+(E) = -i\int_0^\eta (\partial_y \zeta_+(E + iy))\mathrm{d}y \tag{4.58}$$

and use the explicit form of ζ_+ to obtain the estimate

$$|\partial_y \zeta_+(E + iy)| \leqslant \text{const} \cdot \frac{1}{\sqrt{4t_L^2 - E^2}}, \tag{4.59}$$

which shows that $(1/\eta)C_{\alpha\beta} \sim \eta$ and the result follows.

The last step is to deal with

$$g_{\alpha\beta}(T,\mu) = -\lim_{\eta \searrow 0} \frac{\tau^4}{t_L^2}\frac{i}{2\pi}\int_{-2t_L}^{2t_L} f_{\mathrm{FD}}(E)\frac{D_{\alpha\beta}(E,\eta,0_+)}{\eta}\mathrm{d}E. \tag{4.60}$$

One notes that with the notation

$$F(E,\eta) := (\zeta_+(E + i\eta) - \zeta_-(E))^2 u^+_{\alpha\beta}(E + i\eta)u^-_{\beta\alpha}(E),$$

we have $D_{\alpha\beta}(E,\eta,0_+) = -2i\,\mathrm{Im}\,F(E,\eta)$ and

$$g_{\alpha\beta}(T,\mu) = -\lim_{\eta \searrow 0} \frac{\tau^4}{t_L^2}\frac{1}{\pi}\int_{-2t_L}^{2t_L} f_{\mathrm{FD}}(E)\frac{\mathrm{Im}\,F(E,\eta)}{\eta}\mathrm{d}E. \tag{4.61}$$

Using (3.13) and (A4) we see that $\mathrm{Im}\,F(E,i0_+) = 0$ and

$$\mathrm{Re}\,F(E,0_+) = -4[\mathrm{Im}\,\zeta_+(E)]^2 \cdot |u^+_{\alpha\beta}(E)|^2.$$

Taking the limit $\eta \searrow 0$, we obtain in the integral the term $(\partial_\eta \mathrm{Im}\,F)(E,0_+)$. Using the Cauchy–Riemann equations for u^+ and ζ_+, we get after some work that we can replace $(\partial_\eta \mathrm{Im}\,F)(E,0_+)$ by $(1/2)\times\partial_E \mathrm{Re}\,F(E,0_+)$. This also shows that F is not analytic.

Integrating by parts and noticing that $\zeta_+(\pm 2t_L) - \zeta_-(\pm 2t_L) = 0$ we proved the following lemma.

Lemma 4.4: The conductance coefficients $g_{\alpha\beta}(T,\mu)$ defined in (4.36) are given by the relation

$$g_{\alpha\beta}(T,\mu) = -\frac{4\tau^4}{t_L^2}\frac{1}{2\pi}\int_{-2t_L}^{2t_L} \mathrm{d}E\frac{\partial f_{\mathrm{FD}}(E)}{\partial E}(\mathrm{Im}\,\zeta_+(E))^2|u^+_{\alpha\beta}(E)|^2. \tag{4.62}$$

C. Completion of the proof of the main theorem

Before giving the final step in the proof of the Landauer–Büttiker formula, let us briefly review what we have done in this section. We started with the scattering problem associated to the semi-infinite leads case, the transmission between two leads being found in (4.6). The rest of the work has been done to obtain explicit expressions for the conductance coefficients given by the Kubo-type formula (4.15), when the thermodynamic and adiabatic limits are taken.

To finish the proof of Theorem 2.1 there is not much to be done. First, use the explicit expressions for $\zeta_\pm(\cdot)$, together with the definition of the Fermi "momentum," $E = 2t_L\cos(k_E)$, in (4.62). The result is

$$g_{\alpha\beta}(T,\mu) = -\frac{4\tau^4}{t_L^2}\frac{1}{2\pi}\int_{-2t_L}^{2t_L} \mathrm{d}E\frac{\partial f_{\mathrm{FD}}(E)}{\partial E}\sin^2(k_E)|u^+_{\alpha\beta}(E)|^2. \tag{4.63}$$

Now comparing (4.63) and (4.6) one obtains (2.25), and we are done. Notice that when $T \to 0$, we have $-\partial_E f_{\mathrm{FD}} \to \delta(E-\mu)$, and (2.26) follows.

The presence of $1/2\pi$ in those equations is not an accident. It makes more sense, if one carefully includes in computations the physical constants e and $\hbar$ (we have been working until now with the convention $e=\hbar=1$). Without giving details, we assure the reader that in the end the equality in (2.26) becomes

$$g_{\alpha\beta}(0_+,\mu)=\frac{e^2}{2\pi\hbar}\mathcal{T}_{\alpha\beta}(\mu)=\frac{e^2}{h}\mathcal{T}_{\alpha\beta}(\mu), \tag{4.64}$$

which is nothing but the well-known Landauer formula at zero temperature. Note that when the total particle density is fixed, then μ represents the Fermi energy of our system. When the leads become infinite, the sample does not contribute to the thermodynamic limit, thus the Fermi energy is fixed by the leads. The proof of Theorem 2.1 is completed. ■

V. RESONANT TRANSPORT IN A QUANTUM DOT

Up to now we allowed τ to be arbitrarily large, together with the assumption that the Hamilton operator for the system with semi-infinite leads K had no eigenvalues at $\pm 2t_L$. In this section we are interested in small coupling, i.e., the limit $\tau\to 0$.

We now assume that the sample Hamiltonian H^S *does not have eigenvalues* $\pm 2t_L$. This assumption implies, through a simple perturbation argument, and the explicit form of the effective Hamiltonian, that the full Hamiltonian K does not have eigenvalues $\pm 2t_L$, provided τ is sufficiently small.

Assume that H^S has $J\geqslant 1$ (possibly degenerate) eigenvalues, denoted by $\{E_1,\ldots,E_J\}$, such that

$$\sigma(H^S)\cap[-2t_L,2t_L]=\{E_1,\ldots,E_J\}\subset(-2t_L,2t_L). \tag{5.1}$$

We are not interested in possible eigenvalues outside $[-2t_L,2t_L]$, since for small τ they will still remain discrete eigenvalues for K, and we saw that they do not contribute to transport. Now we focus on the influence of $\{E_1,\ldots,E_J\}$ on the transport properties, when τ is small.

Let us give the main result of this section. We consider the transmittance [see (4.6)] between the leads β and γ. Assume that all eigenvalues $\{E_1,\ldots,E_J\}\subset(-2t_L,2t_L)$ of H^S are nondegenerate. The normalized eigenvector corresponding to E_j is denoted by ϕ_j.

Proposition 5.1: (i) *For every* $\lambda\in(-2t_L,2t_L)\backslash\{E_1,\ldots,E_J\}$ *we have*

$$\lim_{\tau\searrow 0}\mathcal{T}_{\beta\gamma}(\lambda,\tau)=0. \tag{5.2}$$

(ii) *Fix* $\lambda=E_j$. *If either* $\langle\mathcal{S}^\beta,\phi_j\rangle$ *or* $\langle\mathcal{S}^\gamma,\phi_j\rangle$ *is zero, then*

$$\lim_{\tau\searrow 0}\mathcal{T}_{\beta\gamma}(E_j,\tau)=0. \tag{5.3}$$

(iii) *Fix* $\lambda=E_j$. *If both* $\langle\mathcal{S}^\beta,\phi_j\rangle$ *and* $\langle\mathcal{S}^\gamma,\phi_j\rangle$ *are different from zero, then there exists a positive constant* $C(E_j)$ *such that*

$$\lim_{\tau\searrow 0}\mathcal{T}_{\beta\gamma}(E_j,\tau)=C(E_j)\left|\frac{\langle\mathcal{S}^\beta,\phi_j\rangle\cdot\langle\mathcal{S}^\gamma,\phi_j\rangle}{\sum_{\alpha=1}^{M}|\langle\mathcal{S}^\alpha,\phi_j\rangle|^2}\right|^2. \tag{5.4}$$

Remark: The physical significance of this proposition is quite transparent. It states that at small coupling, the following things happen: (i) If the energy of the incident electron is not close to the eigenvalues of H^S, it will not contribute to the current. (ii) If the incident energy is close to some eigenvalue E_j, but the eigenfunction ϕ_j is not localized around both coupling points $\mathcal{S}^\gamma$ and $\mathcal{S}^\beta$, then again there is no current. (iii) In order to have a peak in the current, it is necessary for H^S to have extended edge states, which couple several leads. A numerical analysis of the Harper operator on large domains with Dirichlet boundary conditions puts into evidence such extended

edge states, as well as the existence of bulk states concentrated in the middle of the dot (see Refs. 26 and 33).

Proof: We split the proof into several technical results. We will not assume that the E_j's are nondegenerate, unless stated otherwise.

Lemma 5.2: Consider $u_{\beta\gamma}$ given in (3.8), and $u^+_{\beta\gamma}$ its meromorphic extension. Then

$$\lim_{\tau\searrow 0}(\tau^2 \sup_{\lambda\in(-2t_L,2t_L)}|u^+_{\beta\gamma}(\lambda,\tau)|)<\infty.$$

Proof: The lemma roughly says that $u^+_{\beta\gamma}(\lambda)$ cannot blow up worse than $1/\tau^2$, when τ is small. In other words, its poles (if any) have an imaginary part of order τ^2, when τ is small.

Clearly, if τ is smaller than some $\delta_0>0$, then by the usual perturbation theory we get that for all λ located outside some small disks (with radii determined by δ_0) centered at $\{E_j\}_{j=1}^J$ (the eigenvalues of H^S), we have

$$\|(H_+(\lambda)-\lambda)^{-1}\|\leqslant C\max_{j\in\{1,\ldots,J\}}|E_j-\lambda|^{-1},$$

thus we only need to look at what happens in each interval of the form $(E_j-\epsilon,E_j+\epsilon)$.

Assume that E_j is n-fold degenerate. Denote by Π_j the n-dimensional projection corresponding to E_j. The operator $\Pi_j\Pi^T\Pi_j$ has a (possibly trivial) null space in $\mathrm{Ran}(\Pi_j)$. Let p_j be the projection onto this space. Let $\tilde{p}_j=\Pi_j-p_j$ be the projection onto the orthogonal complement of $\mathrm{Ran}(p_j)$ in $\mathrm{Ran}(\Pi_j)$. It is easy to see that there exists a positive constant C_j, such that

$$\tilde{p}_j\Pi^T\tilde{p}_j\geqslant C_j\tilde{p}_j^2. \tag{5.5}$$

Indeed, this is implied by the fact that the operator is non-negative, and with a trivial null space.

Let $q_j=\mathrm{Id}-p_j$. Since $\Pi^Tp_j=0$, and arguing as in (3.10), we have

$$(H_+(\lambda)-\lambda)^{-1}-(E_j-\lambda)^{-1}p_j=q_j[q_j(H_+(\lambda)-\lambda)q_j]^{-1}q_j.$$

Only the right-hand side will contribute to $u^+_{\beta\gamma}$, since $p_j\mathcal{S}^\gamma=0$. The proposition will be proven, if we can show the estimate [on $\mathrm{Ran}(q_j)$]

$$\|[q_j(H_+(\lambda)-\lambda)q_j]^{-1}\|\leqslant C/\tau^2 \tag{5.6}$$

for λ near E_j.

Notice that $q_j=\tilde{p}_j+(\mathrm{Id}-\Pi_j)$, i.e., it is the orthogonal sum of some part of Π_j and the projections corresponding to all other eigenvalues of H^S different from E_j. Let $A_j:=q_j(H_+(\lambda)-\lambda)q_j$.

Note further that $(\mathrm{Id}-\Pi_j)A_j(\mathrm{Id}-\Pi_j)$ is well-behaved when λ is close to E_j, because it essentially equals $(\mathrm{Id}-\Pi_j)(H^S-\lambda)(\mathrm{Id}-\Pi_j)$ plus a perturbation of order τ^2. Applying the Neumann series again, we get that on $\mathrm{Ran}(\mathrm{Id}-\Pi_j)$,

$$\|[(\mathrm{Id}-\Pi_j)A_j(\mathrm{Id}-\Pi_j)]^{-1}\|\leqslant\mathrm{const} \tag{5.7}$$

for λ close to E_j and τ small enough. Hence if $\tilde{p}_j=0$, this estimate implies

$$\|[q_j(H_+(\lambda)-\lambda)q_j]^{-1}\|\leqslant\mathrm{const}, \tag{5.8}$$

which implies (5.6), and we are done.

If $\tilde{p}_j\neq 0$, we again apply the Feshbach lemma for the operator A_j, intending to reduce the problem to the subspace $\mathrm{Ran}(\tilde{p}_j)$. Then A_j is invertible in $\mathrm{Ran}(q_j)$, if and only if the operator

$$X_j:=\tilde{p}_jA_j\tilde{p}_j-\tilde{p}_jA_j(\mathrm{Id}-\Pi_j)[(\mathrm{Id}-\Pi_j)A_j(\mathrm{Id}-\Pi_j)]^{-1}(\mathrm{Id}-\Pi_j)A_j\tilde{p}_j \tag{5.9}$$

is invertible in $\mathrm{Ran}(\tilde{p}_j)$, and their inverses will have the same estimate for their norm, when τ is small. It is not difficult to see that the second term in (5.9) is of order τ^4, when λ is near E_j. We can then write

$$X_j = \tilde{p}_j A_j \tilde{p}_j + \mathcal{O}(\tau^4). \tag{5.10}$$

But the operator

$$\tilde{p}_j A_j \tilde{p}_j = E_j - \lambda - (\tau^2/t_L)\zeta_+(\lambda)\tilde{p}_j \Pi^T \tilde{p}_j \tag{5.11}$$

is one to one (thus invertible), because for every $f \in \mathrm{Ran}(\tilde{p}_j)$ with norm one we have [see also (A4)]

$$\|\tilde{p}_j A_j \tilde{p}_j f\| \geqslant |\langle f, A_j f\rangle| \geqslant |\mathrm{Im}(\langle f, A_j f\rangle)| = (\tau^2/t_L)\sqrt{1-\lambda^2/(4t_L^2)}\langle f, \Pi^T f\rangle,$$

and using (5.5) we get

$$\|\tilde{p}_j A_j \tilde{p}_j f\| \geqslant (\tau^2/t_L)\sqrt{1-\lambda^2/(4t_L^2)}C_j,$$

which leads to

$$\|[\tilde{p}_j A_j \tilde{p}_j]^{-1}\| \leqslant \mathrm{const} \cdot 1/\tau^2.$$

Using this in (5.10) by employing again the Neumann series, we get that for τ small and λ near E_j we have

$$\|X_j^{-1}\| \leqslant \mathrm{const} \cdot 1/\tau^2,$$

thus (5.6) is proven, and so is the lemma. ■

Remark: We see that if $p_j \neq 0$, its range is spanned by eigenvectors of K corresponding to E_j. But they do not contribute in any way to $u^+_{\beta\gamma}$.

Corollary 5.3: We use the notation introduced in the previous lemma. Assume that E_j is n-fold degenerate.

(i) *For every $\lambda \in (-2t_L, 2t_L)$ with $\lambda \notin \{E_1, \ldots, E_J\}$ we have*

$$\lim_{\tau \searrow 0} \tau^2 |u^+_{\beta\gamma}(\lambda, \tau)| = 0. \tag{5.12}$$

(ii) *Fix $\lambda = E_j$. Assume $\tilde{p}_j = 0$. Then*

$$\lim_{\tau \searrow 0} \tau^2 |u^+_{\beta\gamma}(E_j, \tau)| = 0. \tag{5.13}$$

(iii) *Fix $\lambda = E_j$. Assume that $\tilde{p}_j \neq 0$. Then $\tilde{p}_j \Pi^T \tilde{p}_j$ is positive on* $\mathrm{Ran}(\tilde{p}_j)$ *and*

$$\lim_{\tau \searrow 0} \tau^2 |u^+_{\beta\gamma}(E_j, \tau)| = t_L |\langle \mathcal{S}^\beta, \tilde{p}_j [\tilde{p}_j \Pi^T \tilde{p}_j]^{-1} \tilde{p}_j \mathcal{S}^\gamma\rangle|. \tag{5.14}$$

Proof: (i) By regular perturbation theory, we see that $|u^+_{\beta\gamma}(\lambda, \tau)|$ remains bounded when τ tends to zero, while λ is fixed and away from the eigenvalues of H^S. Hence (5.12) is straightforward.

(ii) If $\tilde{p}_j = 0$ and $\lambda = E_j$, the estimate (5.8) implies again that $|u^+_{\beta\gamma}(E_j, \tau)|$ remains bounded when τ tends to zero, thus (5.13) follows.

(iii) If $\tilde{p}_j \neq 0$ and $\lambda = E_j$, we rely on the properties of the inverse on $\mathrm{Ran}(\tilde{p}_j)$ of the operator $\tilde{p}_j A_j \tilde{p}_j$ introduced in (5.11). A consequence of the arguments presented in the previous proposition is that for λ close to E_j we have

$$u^+_{\beta\gamma}(\lambda) - \langle \mathcal{S}^\beta, \tilde{p}_j [\tilde{p}_j A_j \tilde{p}_j]^{-1} \tilde{p}_j \mathcal{S}^\gamma\rangle = \mathcal{O}_\tau(1). \tag{5.15}$$

Then using (5.11) with $\lambda = E_j$, and the fact that $|\zeta_+(\lambda)| = 1$, the result follows easily. The corollary is proven. ■

Completing the proof of Proposition 5.1: The proof is easily obtained by replacing (5.12)–(5.14) in (4.6), in the nondegenerate case. Details are omitted.

We see that in the degenerate case it is not that simple to give clear criteria, for which the current is zero, or not, in the small coupling regime. Assume that E_j is n-fold degenerate. Denote by $\{\phi_j^{(s)}\}_{s=1}^n$ the normalized eigenvectors of H^S spanning the range of Π_j. A sufficient condition for the right-hand side of (5.14) to be zero for every β and γ, is Π_j to be orthogonal to Π^T. In other words, $\langle S^\alpha, \phi_j^{(r)}\rangle = 0$ for every $1 \leqslant \alpha \leqslant M$ and $1 \leqslant r \leqslant n$. Physically, this means no contact at all between the leads and the mode E_j. A necessary but not sufficient condition for the right-hand side of (5.14) to be different from zero is to have $\tilde{p}_j \neq 0$. The proposition is proven. ■

We continue this section with a result giving more information about the poles in the case, when τ is small, and we are near a nondegenerate eigenvalue of H^S.

Assume that the eigenvalue $E_1 \in (-2t_L, 2t_L)$ of H^S is nondegenerate. We denote the corresponding normalized eigenvector with ϕ_1, i.e., $H^S\phi_1 = E_1\phi_1$. It is clear that one of the following two alternatives is true:

(1) A_1, there exists $\alpha_1 \in \{1, \ldots, M\}$ such that $\langle \phi_1, \mathcal{S}^{\alpha_1}\rangle \neq 0$;
(2) A_2, for all $\alpha \in \{1, \ldots, M\}$ we have $\langle \phi_1, \mathcal{S}^{\alpha}\rangle = 0$.

If A_1 holds, then ϕ_1 is "coupled" with at least one lead. If A_2 holds, then the coupling is absent.

Define the projection $\Pi^L = \Sigma_{\alpha=1}^M |0_\alpha\rangle\langle 0_\alpha|$. By direct computation we have [see (3.8) and (3.3)]

$$\Pi^L(K-z)^{-1}\Pi^L = \frac{\zeta_1(z)}{t_L}\sum_{\alpha=1}^M |0_\alpha\rangle\langle 0_\alpha| + \frac{\zeta_1^2(z)}{t_L^2}\sum_{\alpha,\beta=1}^M |0_\alpha\rangle u_{\alpha\beta}(z)\langle 0_\beta|. \tag{5.16}$$

Then the weighted resolvent $\Pi^L(K-z)^{-1}\Pi^L$ admits a meromorphic extension to any domain of the form $\mathbb{C}_+ \cup \Omega_\epsilon$ [see (3.6)].

Proposition 5.4: (i) *For small enough τ, the weighted resolvent $\Pi^L(K-z)^{-1}\Pi^L$ has a simple pole near E_1* [*denoted by $\tilde{E}_1(\tau)$*].

(ii) *If A_1 holds true, then for $\tau > 0$ small enough the pole $\tilde{E}_j(\tau)$ is a resonance for K with*

$$\lim_{\tau \searrow 0}(\mathrm{Re}\,\tilde{E}_1(\tau) - E_1)/\tau^2 = -\frac{E_1}{2t_L^2}\sum_{\alpha=1}^M |\langle \phi_1, \mathcal{S}^\alpha\rangle|^2$$

and

$$\lim_{\tau \searrow 0}\mathrm{Im}\,\tilde{E}_1(\tau)/\tau^2 = -\frac{\sqrt{4t_L^2 - E_1^2}}{2t_L^2}\sum_{\alpha=1}^M |\langle \phi_1, \mathcal{S}^\alpha\rangle|^2.$$

(iii) *If A_2 holds for ϕ_1, then $\tilde{E}_1(\tau) = E_1$ and ϕ_1 remains an eigenvector for K, i.e., $K\phi_1 = \tilde{E}_1\phi_1$.*

Proof: Let us focus on what happens near E_1, when A_1 holds. Denote by P_1 the spectral projection of H^S corresponding to ϕ_1, and let $Q_1 = \mathrm{Id} - P_1$. The Feshbach lemma gives [using a compact notation, cf. (3.3)]

$$\begin{aligned}(H_+(z) - z)^{-1} = (Q_1H_+Q_1 - z)^{-1} + (1 - (Q_1H_+Q_1 - z)^{-1}Q_1H_+P_1)\\ \times (\tilde{H}_+(z) - z)^{-1} \cdot (1 - P_1H_+Q_1(Q_1H_+Q_1 - z)^{-1}),\end{aligned} \tag{5.17}$$

where the new effective Hamiltonian $\tilde{H}_+(z)$ is defined by

$$\tilde{H}_+(z) := P_1H_+(z)P_1 - P_1H_+Q_1(Q_1H_+Q_1 - z)^{-1}Q_1H_+P_1, \tag{5.18}$$

and lives in a one-dimensional space. With the notation

$$f_1(z,\tau) := \sum_{\alpha,\beta=1}^{M} \sum_{i,i'\neq 1} \frac{\tau^4}{t_L^2} \zeta_+^2(z) \langle \phi_1, \mathcal{S}^\alpha \rangle \langle \mathcal{S}^\alpha, \phi_i \rangle \times \langle \phi_i, (Q_1 H_+ Q_1 - z)^{-1} \phi_{i'} \rangle \langle \phi_{i'}, \mathcal{S}^\beta \rangle \langle \mathcal{S}^\beta, \phi_1 \rangle,$$

we have that for small enough τ, $H_+(z)-z$ is invertible, if and only if the function

$$F_1(z,\tau) := E_1 - z - \frac{\tau^2}{t_L} \zeta_+(z) \sum_{\alpha=1}^{M} |\langle \phi_j, \mathcal{S}^\alpha \rangle|^2 - f_1(z,\tau)$$

is different from zero. Notice that for τ small enough, and z near E_1, we have $f_1(z,\tau)=\mathcal{O}(\tau^4)$.

For small τ, and with z near E_1, the implicit function theorem provides us with a unique solution $\tilde{E}_1(\tau)$ to the equation $F_1(z,\tau)=0$.

If we define

$$\begin{aligned}\mathcal{T}_1(z,\tau) := &- (Q_1 H_+ Q_1 - z)^{-1} Q_1 H_+ P_1 - P_1 H_+ Q_1 (Q_1 H_+ Q_1 - z)^{-1} \\ &+ (Q_1 H_+ Q_1 - z)^{-1} Q_1 H_+ P_1 H_+ Q_1 (Q_1 H_+ Q_1 - z)^{-1},\end{aligned}$$

then we can write

$$(H_+ - z)^{-1} = \frac{1}{F_1(z,\tau)} [P_1 + \mathcal{T}_1] + (Q_1 H_+ Q_1 - z)^{-1}. \tag{5.19}$$

It is easy to see that $\mathcal{T}_1$ is analytic in z near E_1, and of order $\mathcal{O}(\tau^2)$. Now we must take the matrix elements $\langle \mathcal{S}^\alpha, (H_+(z)-z)^{-1} \mathcal{S}^\beta \rangle$ to obtain $u_{\alpha\beta}(z)$ in (5.16). It turns out that

$$\Pi^L (K-z)^{-1} \Pi^L = \text{bounded and analytic term} + \frac{\zeta_+^2(z)}{t_L^2} \sum_{\alpha,\beta=1}^{M} \left\{ \frac{\langle \mathcal{S}^\alpha, \psi_1 \rangle \langle \psi_1, \mathcal{S}^\beta \rangle + \langle \mathcal{S}^\alpha, \mathcal{T}_1 \mathcal{S}^\beta \rangle}{F_1(z,\tau)} \right\} |0_\alpha\rangle\langle 0_\beta|.$$

Moreover, since we can show that

$$F_1(z,\tau)/(E_1(\tau) - z) = 1 + \mathcal{O}(\tau^2)$$

for z in a small neighborhood of E_1, we conclude that

$$\begin{aligned}\Pi^L (K-z)^{-1} \Pi^L = &\text{ bounded and analytic term} + (1 + \mathcal{O}(\tau^2)) \frac{\zeta_+^2(z)}{t_L^2} \sum_{\alpha,\beta=1}^{M} \frac{\langle \mathcal{S}^\alpha, \psi_1 \rangle \langle \psi_1, \mathcal{S}^\beta \rangle + \mathcal{O}(\tau^2)}{\tilde{E}_1(\tau) - z} \\ &\times |0_\alpha\rangle\langle 0_\beta|.\end{aligned}$$

Therefore the second statement of the proposition is now proved up to a straightforward application of the implicit function theorem for the claimed properties of $\tilde{E}_1(\tau)$. The third statement is also straightforward. ■

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APPENDIX A: THE DISCRETE LAPLACIAN ON THE HALF-LINE

Denote by $\{|n\rangle\}_{n\geq 0}$ the standard basis in $l^2(\mathbb{N})$. For $t_L>0$, consider the operator H_α^L, which acts on $\psi \in l^2(\mathbb{N})$ as follows:

$$(H_\alpha^L \psi)(j) = t_L \psi(j+1) + t_L \psi(j-1), \quad j \geq 0, \quad \psi(-1) := 0.$$

It is well known that the spectrum of H_α^L is purely absolutely continuous, and moreover $\sigma(H_\alpha^L)=[-2t,2t]$. We are interested in the matrix elements of the resolvent of H_α^L. If $\mathrm{Im}\, z>0$, one can easily compute

$$\langle m,R_\alpha^L(z)n\rangle = \frac{1}{t_L(\zeta_2-\zeta_1)}(\zeta_1(z)^{|m-n|}-\zeta_1(z)^{m+n+2}), \tag{A1}$$

where $\zeta_{1,2}$ are solutions of the equation

$$t_L\zeta^2 - z\zeta + t = 0, \tag{A2}$$

and ζ_1 is chosen, such that $|\zeta_1|\sim 1/|z|$ at infinity (note that $\zeta_1\zeta_2=1$).

We give several explicit representations for ζ_1. By $\ln(x)=\ln(|x|)+i\arg(x)$ we understand the principal branch of the natural logarithm defined on $\mathbb{C}\backslash(-\infty,0]$, with $\arg(x)\in(-\pi,\pi)$. Thus $\sqrt{x}=\sqrt{|x|}e^{(i/2)\arg(x)}$.

Proposition 6.1: We have the following properties.

(i) *Assume that* $z\notin[-2t_L,2t_L]$. *Then*

$$\zeta_1(z) = \frac{z}{2t_L}(1-\sqrt{1-4t_L^2/z^2}). \tag{A3}$$

(ii) *Consider the holomorphic functions*

$$\zeta_\pm(z) = \frac{z}{2t_L} \mp i\sqrt{1-z^2/(4t_L^2)}, \quad z\notin(-\infty,-2t_L]\cup[2t_L,\infty). \tag{A4}$$

Then $\zeta_1(z)=\zeta_+(z)$ *if* $\mathrm{Im}\, z>0$, *and* $\zeta_1(z)=\zeta_-(z)$ *if* $\mathrm{Im}\, z<0$.

(iii) *We have* $\zeta_2(z)=1/\zeta_1(z)$.

Proof: We see that ζ_1 in (A3) solves the equation, and behaves like $1/z$ for large $|z|$. Furthermore, since ζ_1 and $\tilde{\zeta}_\pm$ are holomorphic, it is enough to verify their equality at points of the form $\pm it$ with $t>0$, which is trivial. ■

APPENDIX B: THE SECOND QUANTIZATION OF AN IDEAL FERMI GAS

The results in this section are well known, see for example Ref. 8. We recall the results to fix the notation.

Given a separable Hilbert space $\mathcal{H}$, the associated antisymmetric Fock space is given by

$$\mathcal{F}_a(\mathcal{H}) = \bigoplus_{n=0}^{\infty} \mathcal{H}^{\otimes_a n}, \quad \mathcal{H}^{\otimes_a 0} := \mathbb{C}.$$

Here the subscript a indicates the total antisymmetrization of the tensor products. Let $\mathcal{B}=\{e_k\}_{k\geqslant 1}$ be an orthonormal basis in $\mathcal{H}$. Then we can construct the "occupation number" basis in $\mathcal{F}_a(\mathcal{H})$ associated to $\mathcal{B}$. We denote a generic vector by $\Psi_{N_1,N_2,\ldots}$, where the N_k's are numbers (either 0 or 1) showing how many times e_k appears in the tensor products defining Ψ. For example, $\Psi_{0,0,\ldots}=1\in\mathbb{C}$ is the vacuum.

The annihilation operators associated with this particular basis are defined as

$$a_\alpha\Psi_{N_1,N_2,\ldots,N_\alpha=0,\ldots} = 0,$$

$$a_\alpha\Psi_{N_1,N_2,\ldots,N_\alpha=1,\ldots} = (-1)^{\Sigma_{\beta<\alpha}N_\beta}\Psi_{N_1,N_2,\ldots,N_\alpha=0,\ldots},$$

while their adjoints (the creation operators) are given by

$$a_\alpha^\dagger\Psi_{N_1,N_2,\ldots,N_\alpha=1,\ldots} = 0,$$

$$a_\alpha^\dagger \Psi_{N_1,N_2,\ldots,N_\alpha=0,\ldots} = (-1)^{\Sigma_{\beta<\alpha} N_\beta} \Psi_{N_1,N_2,\ldots,N_\alpha=1,\ldots}.$$

If A is a bounded linear operator in $\mathcal{H}$, its second quantization $\mathbf{A}=\mathrm{d}\Gamma(A)$ is the operator on $\mathcal{F}_a$, whose restriction to $\mathcal{H}^{\otimes_a n}$ is given by

$$A \otimes \mathrm{Id} \otimes \cdots \otimes \mathrm{Id} + \ldots + \mathrm{Id} \otimes \cdots \otimes \mathrm{Id} \otimes A,$$

where the above sum has n terms. Using the particular basis $\mathcal{B}$, we have

$$\mathbf{A} = \mathrm{d}\Gamma(A) = \sum_{k,j\geqslant 1} \langle e_k, Ae_j\rangle a_k^+ a_j. \tag{B1}$$

For example, the total Hamiltonian is $\mathbf{H}=\mathrm{d}\Gamma(H)$, and the number operator is $\mathbf{N}=\mathrm{d}\Gamma(\mathrm{Id})$.

Now assume that $\mathcal{H}$ is finite dimensional. The grand canonical partition function Ξ and the density matrix operator in the grand canonical ensemble $\hat{\rho}_0$ are defined as

$$\Xi := \mathrm{Tr}_{\mathcal{F}_a} e^{-\beta(\mathbf{H}-\mu\mathbf{N})}, \quad \hat{\rho}_0 := \frac{1}{\Xi} e^{-\beta(\mathbf{H}-\mu\mathbf{N})}. \tag{B2}$$

Finally, we define

$$f_{\mathrm{FD}}(x) = \frac{1}{e^{\beta(x-\mu)}+1}, \quad \rho_0 := f_{\mathrm{FD}}(H). \tag{B3}$$

The following proposition will be used extensively in Sec. III.

Proposition 6.2: Let A and B be bounded operators in $\mathcal{H}$. Denote by $[A,B]=AB-BA$ their commutator. Then

$$\mathrm{d}\Gamma([A,B]) = [\mathbf{A},\mathbf{B}], \tag{B4}$$

$$e^{\mathbf{A}}\mathbf{B}e^{-\mathbf{A}} = \mathrm{d}\Gamma(e^A B e^{-A}), \tag{B5}$$

$$\mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}_0 \mathbf{A}) = \mathrm{Tr}_{\mathcal{H}}(\rho_0 A). \tag{B6}$$

Proof: The first identity is easily proven using the anticommutation relations

$$\begin{aligned}[\mathbf{A},\mathbf{B}] &= \sum_{k,j,m,n} \langle e_k, Ae_j\rangle\langle e_m, Be_n\rangle [a_k^\dagger a_j a_m^\dagger a_n - a_m^\dagger a_n a_k^\dagger a_j] \\ &= \sum_{k,j,m,n} \langle e_k, Ae_j\rangle\langle e_m, Be_n\rangle [a_k^\dagger a_n \delta_{jm} - a_m^\dagger a_n \delta_{kn}] = \sum_{k,j} \langle e_k, (AB-BA)e_j\rangle = \mathrm{d}\Gamma([A,B]),\end{aligned}$$

while the second one is implied by the first equality, the Baker–Cambell–Hausdorff formula

$$e^{\mathbf{A}}\mathbf{B}e^{-\mathbf{A}} = \mathbf{B} + [\mathbf{A},\mathbf{B}] + \tfrac{1}{2}[\mathbf{B},[\mathbf{B},\mathbf{A}]] + \cdots,$$

and the linearity of $\mathrm{d}\Gamma(\cdot)$.

Concerning the third identity (see also Proposition 5.2.23 in Ref. 8) we first note that the trace is invariant with respect to the basis used, so we may assume that the basis $\mathcal{B}=\{e_k\}$ is the set of eigenvectors of H. We consider the occupation number basis derived from it. The eigenvalues of H are denoted by $\{\lambda_k\}$. Then

$$\Xi = \Pi_k (1 + e^{-\beta(\lambda_k-\mu)}) < \infty, \tag{B7}$$

and we can write

$$\mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}_0\mathbf{A}) = \sum_{N_1,N_2,\ldots\in\{0,1\}} \langle \Psi_{N_1,N_2,\ldots}, \hat{\rho}_0\mathbf{A}\Psi_{N_1,N_2,\ldots}\rangle.$$

Since

$$\hat{\rho}_0\Psi_{N_1,N_2,\ldots} = \frac{1}{\Xi}e^{-\beta\Sigma_j N_j(\lambda_j-\mu)}\Psi_{N_1,N_2,\ldots} = \frac{1}{\Xi}\Pi_j e^{-\beta N_j(\lambda_j-\mu)}\Psi_{N_1,N_2,\ldots},$$

and

$$\langle \Psi_{N_1,N_2,\ldots}, \mathbf{A}\Psi_{N_1,N_2,\ldots}\rangle = \sum_{k,m}\langle e_k, Ae_m\rangle \delta_{N_k,1}\delta_{N_m,1}\delta_{k,m},$$

we have

$$\mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}_0\mathbf{A}) = \sum_k \langle e_k, Ae_k\rangle \frac{1}{\Xi}\sum_{N_1,N_2,\ldots\in\{0,1\}} \Pi_j e^{-\beta N_j(\lambda_j-\mu)}\delta_{N_k,1}.$$

Note that

$$\sum_{N_1,N_2,\ldots\in\{0,1\}} \Pi_j e^{-\beta N_j(\lambda_j-\mu)}\delta_{N_k,1} = (1+e^{-\beta(\lambda_1-\mu)})(1+e^{-\beta(\lambda_2-\mu)})\cdots e^{-\beta(\lambda_k-\mu)}\cdots(1+e^{-\beta(\lambda_j-\mu)})\cdots, \tag{B8}$$

hence

$$\frac{1}{\Xi}\sum_{N_1,N_2,\ldots\in\{0,1\}} \Pi_j e^{-\beta N_j(\lambda_j-\mu)}\delta_{N_k,1} = f_{\mathrm{FD}}(\lambda_k),$$

and therefore

$$\mathrm{Tr}_{\mathcal{F}_a}(\hat{\rho}_0\mathbf{A}) = \sum_k \langle e_k, Ae_k\rangle f_{\mathrm{FD}}(\lambda_k) = \mathrm{Tr}_{\mathcal{H}}(\rho_0 A).$$

■

APPENDIX C: A DISCRETE KREIN FORMULA AND EXPONENTIAL DECAY

We now give a formula relating the resolvent of the discrete Laplacian defined on $l^2(\mathcal{N})$, $\mathcal{N}=\{0,1,\ldots,N\}$, with the resolvent of the Laplacian defined on $l^2(\mathbb{N})$; both operators are with Dirichlet boundary conditions. We denote by $r^L(N,z)$ the resolvent on the finite segment, and by $r^L(z)$ the resolvent on the semi-infinite lead. We use lower case letters to emphasize that we model only one lead. The operator itself is denoted by $h^L(N)$ when restricted to a segment, and by h^L on $l^2(\mathbb{N})$. The vector δ_m is the vector in $l^2(\mathcal{N})$ having 1 in the mth position, and 0 elsewhere. Define for every $z\in\mathbb{C}\backslash\mathbb{R}$ the "integral kernels"

$$g_{m,n}(N,z) = \langle \delta_m, r^L(N,z)\delta_n\rangle, \quad g_{m,n}(z) = \langle \delta_m, r^L(z)\delta_n\rangle. \tag{C1}$$

The Dirichlet boundary condition means

$$g_{-1,n}(N,z) = g_{N+1,n}(N,z) = g_{-1,n}(z) = 0, \tag{C2}$$

with analogous equalities for the second argument, due to the symmetry property $g_{m,n}(N,z) = \overline{g_{n,m}(N,\bar{z})}$.

Proposition 6.3: For all $0\leqslant m,n\leqslant N$ *we have the following Krein formula:*

$$g_{m,n}(N,z) - g_{m,n}(z) = t_L g_{m,N}(N,z) g_{N+1,n}(z). \tag{C3}$$

Proof: The proof is outlined here. For every fixed n, the vectors $g_{\cdot,n}(N,z)$ ($g_{\cdot,n}(z)$) are in $l^2(\mathcal{N})$ ($l^2(\mathbb{N})$). Then

$$[(h^L(N)-z)g_{\cdot,n}(N,z)](m)=\delta_{m,n},$$

$$[(h^L-z)g_{\cdot,n}(z)](m)=\delta_{m,n}. \tag{C4}$$

Using summation by parts, we get the identity [the scalar products are in $l^2(\mathcal{N})$]

$$\langle[(h^L(N)-\overline{z})g_{\cdot,m}(N,\overline{z})],g_{\cdot,n}(z)\rangle=\langle g_{\cdot,m}(N,\overline{z}),(h^L-z)g_{\cdot,n}(z)\rangle-t_L g_{m,N}(N,z)g_{N+1,n}(z), \tag{C5}$$

where we employed various symmetry properties of the kernels, together with (C2). The use of (C4) finishes the proof. ■

Finally, we need an exponential decay estimate for the resolvents.

Proposition 6.4: There exist constants $0<c<C$, *such that uniformly in* N *and* z *with* $0<|\mathrm{Im}\, z|<1$ *we have*

$$|g_{m,n}(N,z)|\leqslant\frac{C}{|\mathrm{Im}\, z|}\exp(-c|\mathrm{Im}\, z||m-n|), \tag{C6}$$

for all $m,n\in\mathcal{N}$. *The same estimate holds, when* $N=\infty$.

Proof: This proof is a discrete (and simpler) version of the usual Combes–Thomas argument (see Ref. 14), which leads to boundedness of resolvents between spaces with exponential weights. Define the discrete dilation for $\alpha>0$ by

$$(W_\alpha\psi)(n)=e^{\alpha n}\psi(n). \tag{C7}$$

Then, by a direct computation, the dilated Hamiltonian $H(\alpha)=W_\alpha H W_{-\alpha}$ is given by

$$\begin{aligned}(H(\alpha)\psi)(n)&=e^{-\alpha}\psi(n+1)+e^{\alpha}\psi(n-1)\\&=(H\psi)(n)+(e^{-\alpha}-1)\psi(n+1)+(e^{\alpha}-1)\psi(n-1)=((H+V(\alpha))\psi)(n),\end{aligned}$$

where the perturbation $V(\alpha):=(e^{-\alpha}-1)T_1+(e^{\alpha}-1)T_{-1}$, $T_{\pm1}$ being the shift operators. Noting that $V(\alpha)$ is of order $\mathcal{O}(\alpha)$. If c is a sufficiently small positive constant, and $\alpha\leqslant c|\mathrm{Im}\, z|$, we can write

$$(H(\alpha)-z)^{-1}=(H-z)^{-1}(1+V(\alpha)(H-z)^{-1})^{-1}, \tag{C8}$$

where the second part is invertible, and its norm is less than a chosen constant (for example, 2). Hence,

$$\|(H(\alpha)-z)^{-1}\|\leqslant\|(H-z)^{-1}\|\cdot\|(1+V(\alpha)(H-z)^{-1})^{-1}\|\leqslant\frac{2}{|\mathrm{Im}\, z|}. \tag{C9}$$

Define the following vectors in $l^2(\mathcal{N})$ (the exponential is in the mth position)

$$\Psi_{mn}=(0,0,\ldots,e^{i\arg(g_{mn}(N,z))},\ldots,0,0),\quad m\geqslant n. \tag{C10}$$

Then

$$\langle\Psi_{mn},W_\alpha(H-z)^{-1}W_{-\alpha}\delta_n\rangle=e^{\alpha(m-n)}|g_{mn}(N,z)|=\langle\Psi_{mn},(H(\alpha)-z)^{-1}\delta_n\rangle\leqslant\frac{C}{|\mathrm{Im}\, z|},$$

from which the claimed estimate follows. ■

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Moment operators of the Cartesian margins of the phase space observables

Jukka Kiukas[a)]
Department of Physics, University of Turku, FIN-20014 Turku, Finland

Pekka Lahti[b)]
Department of Physics, University of Turku, FIN-20014 Turku, Finland

Kari Ylinen[c)]
Department of Mathematics, University of Turku, FIN-20014 Turku, Finland

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The theory of operator integrals is used to determine the moment operators of the Cartesian margins of the phase space observables generated by the mixtures of the number states. The moments of the x-margin are polynomials of the position operator and those of the y-margin are polynomials of the momentum operator. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1851957]

I. INTRODUCTION

According to the theory developed in Ref. 7, each complex valued measurable function f and operator measure E determine a unique, possibly unbounded, linear operator $L(f,E)$, the operator integral of f with respect to E. In the case of real valued functions and phase space operator measures, a natural application of this theory is quantization.

In general, quantization means any procedure which associates a quantum mechanical observable to a given classical dynamical variable, the latter being represented by a real valued measurable function on the phase space $\mathbb{R}^{2n}$ of the classical system. Phase space quantization schemes are often realized by associating to a given classical variable f the operator $\int f(q,p)\Delta(q,p)\mathrm{d}q\,\mathrm{d}p$, where Δ is some operator valued phase space function and the integral is interpreted, e.g., in the weak or strong sense on a suitable domain (cf., e.g., Refs. 6, 10, and 13).

Consider the quantization determined by the operator density $(q,p)\mapsto\Delta(q,p):=(2\pi)^{-1}W(-q,p)TW(-q,p)^*$, where the $W(-q,p)$ are the Weyl operators acting in a separable Hilbert space and T is a state, i.e., a positive operator of trace one. Now the map $\mathcal{B}(\mathbb{R}^{2n})\ni B\mapsto E(B):=\int_B\Delta\in L(\mathcal{H})$ is a phase space observable, so that any classical variable f can be integrated with respect to it. On its natural domain, the operator integral $L(f,E)$ coincides with the (weak) quantization integral $\int f\Delta$. In this way, $L(f,E)$ can be interpreted as a quantization of the classical variable f. It can be noted that this approach differs from the Weyl quantization, which is obtained by replacing T in the above density $\Delta(q,p)$ by (a constant times) the parity operator in $L^2(\mathbb{R})$ (cf., e.g., Ref. 3, Sec. IV.1, Ref. 6, p. 199, and Ref. 10, pp. 140–141).

In this paper, we consider the phase space observables on $\mathbb{R}^2$ associated with certain pure states and their convex combinations, with the state vectors being taken from a fixed countable orthonormal basis of the separable Hilbert space. The moment operators of the Cartesian margins of these operator measures will be determined using the theory of operator integrals. The results sharpen and extend some of those obtained previously in Ref. 9.

[a)]Electronic mail: jukka.kiukas@utu.fi
[b)]Electronic mail: pekka.lahti@utu.fi
[c)]Electronic mail: kari.ylinen@utu.fi

II. OPERATOR INTEGRALS AND PHASE SPACE OBSERVABLES

A. The operator integral

In the following, we review the basic results of Ref. 7 on the theory of operator integrals and prove a proposition concerning integration with respect to sequences of positive operator measures.

Let $\mathcal{H}$ be a Hilbert space, with inner product $\langle\cdot|\cdot\rangle$, and $L(\mathcal{H})$ the set of bounded operators on $\mathcal{H}$. Let Ω be a nonempty set, $\mathcal{A}$ a σ-algebra of subsets of Ω, and $E:\mathcal{A}\to L(\mathcal{H})$ a positive operator measure (a positive operator valued set function σ-additive with respect to the strong, or, equivalently, the weak operator topology). For all φ, $\psi\in\mathcal{H}$, the map $\mathcal{A}\ni X\mapsto\langle\psi|E(X)\varphi\rangle\in\mathbb{C}$ is a complex measure, and it is denoted by $E_{\psi,\varphi}$. Let $f:\Omega\to\mathbb{C}$ be an $\mathcal{A}$-measurable function and let $D(f,E)$ be the set of those vectors $\varphi\in\mathcal{H}$ for which f is integrable with respect to the complex measure $E_{\psi,\varphi}$ for all $\psi\in\mathcal{H}$. The set $D(f,E)$ is a vector subspace of $\mathcal{H}$, and there is a unique linear operator $L(f,E)$ on the domain $D(f,E)$ such that

$$\langle\psi|L(f,E)\varphi\rangle=\int f\,\mathrm{d}E_{\psi,\varphi}$$

for all $\varphi\in D(f,E)$ and $\psi\in\mathcal{H}$ (cf. Ref. 7). We call $L(f,E)$ the *(operator) integral* of f with respect to E.

Let $\tilde{D}(f,E)$ be the set of those vectors $\varphi\in\mathcal{H}$ for which $|f|^2$ is integrable with respect to the positive measure $E_{\varphi,\varphi}$. We have the following results, proved in Ref. 7.

Theorem 1: (a) *$\tilde{D}(f,E)$ is a vector subspace of $D(f,E)$.* (b) *If $E(X)$ is a projection for all $X\in\mathcal{A}$, then $\tilde{D}(f,E)=D(f,E)$.* It is well known that, in case (b), the domain is dense.

Theorem 2: *If f is real valued, then $L(f,E)$ is a symmetric operator, that is, $\langle\psi|L(f,E)\varphi\rangle=\langle L(f,E)\psi|\varphi\rangle$ for all $\psi,\varphi\in D(f,E)$.* The following general lemma will be used in the proof of Proposition 1.

Lemma 1: Let $\mu_n:\mathcal{A}\to\mathbb{C}$ be a complex measure for each $n\in\mathbb{N}$ such that the series $\Sigma_{n\in\mathbb{N}}\mu_n$ converges absolutely in the total variation norm. Let μ and ν denote the measures $\Sigma_{n\in\mathbb{N}}\mu_n$ and $\Sigma_{n\in\mathbb{N}}|\mu_n|$, respectively. Here $|\cdot|$ stands for the total variation.

(a) *f is ν-integrable, if and only if $\Sigma_{n=1}^{\infty}\int|f|d|\mu_n|<\infty$.*
(b) *If f is ν-integrable, then f is integrable with respect to μ and all the measures μ_n, and*

$$\int f\,\mathrm{d}\mu=\sum_{n=1}^{\infty}\int f\,\mathrm{d}\mu_n.$$

Proof: (a) Assume that f is ν-integrable (i.e., $|f|$ is such). Since $|\mu_n(B)|\leqslant\nu(B)$ for all $B\in\mathcal{A}$ and $n\in\mathbb{N}$, $|f|$ is μ_n-integrable for each $n\in\mathbb{N}$. Now

$$\sum_{n=1}^{k}\int|f|d|\mu_n|=\int|f|d\left(\sum_{n=1}^{k}|\mu_n|\right)\leqslant\int|f|\mathrm{d}\nu$$

for each $k\in\mathbb{N}$, so that $\Sigma_{n=1}^{\infty}\int|f|d|\mu_n|<\infty$. The converse follows from Lemma A.5. of Ref. 7.

(b) Clearly μ and all the μ_n are ν-continuous. Let g and g_n be their Radon–Nikodým derivatives with respect to ν, respectively. Since

$$\left(\sum_{n=1}^{k}\mu_n-\mu\right)(B)=\int_B\left(\sum_{n=1}^{k}g_n-g\right)\mathrm{d}\nu$$

for all $B\in\mathcal{A}$ and $k\in\mathbb{N}$, we have

$$\lim_{k\to\infty}\int\left|\sum_{n=1}^{k}g_n-g\right|\mathrm{d}\nu=\lim_{k\to\infty}\left\|\sum_{n=1}^{k}\mu_n-\mu\right\|=0,$$

where $\|\cdot\|$ denotes the total variation norm. This means that the series $\Sigma_n g_n$ converges in $L^1(\nu)$ to the function g. Thus some subsequence $(\Sigma_{n=1}^{k_m}g_n)$ converges to g ν-almost everywhere. In addition, the monotone convergence theorem gives

$$\nu(B)=\sum_{n=1}^{\infty}\int_B|g_n|\mathrm{d}\nu=\int_B\left(\sum_n|g_n|\right)\mathrm{d}\nu$$

for all $B\in\mathcal{A}$, so that

$$\left|f(x)\sum_{n=1}^{k_m}g_n(x)\right|\leqslant|f(x)|\sum_n|g_n|=|f(x)| \tag{1}$$

for ν-almost all $x\in\Omega$.

Assume now that f is ν-integrable. Then by (a), f is μ_n-integrable for each $n\in\mathbb{N}$, and the series $\Sigma_{n=1}^{\infty}\int f\,\mathrm{d}\mu_n$ converges absolutely. Because of (1), the dominated convergence theorem implies that fg is ν-integrable, i.e., f is μ-integrable, and

$$\int f\,\mathrm{d}\mu=\int fg\,\mathrm{d}\nu=\lim_{m\to\infty}\sum_{n=1}^{k_m}\int fg_n\,\mathrm{d}\nu=\sum_{n=1}^{\infty}\int f\,\mathrm{d}\mu_n.$$

■

Proposition 1: Let $E^n:\mathcal{A}\to L(\mathcal{H})$ be a positive operator measure for each $n\in\mathbb{N}$ such that the range of E^n is bounded in norm by $M_n>0$, with $\Sigma_n M_n<\infty$. Then the norm limit $\Sigma_n E^n(B)$, $B\in\mathcal{A}$, defines a positive operator measure E, for which

$$L(f,E)|_{\tilde{D}(f,E)}\subset\sum_n L(f,E^n)|_{\tilde{D}(f,E^n)},$$

where the series is understood to converge in the weak sense to an operator, whose domain consists of those vectors $\varphi\in\cap_{n\in\mathbb{N}}\tilde{D}(f,E^n)$ for which the vector series $\Sigma_n L(f,E^n)\varphi$ converges weakly.

Proof: Let $\psi,\varphi\in\mathcal{H}$. Since $\|E^n_{\psi,\varphi}\|\leqslant 4\sup_{B\in\mathcal{A}}|E^n_{\psi,\varphi}(B)|\leqslant 4\|\psi\|\,\|\varphi\|M_n$, the series $\Sigma_n E^n_{\psi,\varphi}$ converges absolutely in the total variation norm. The above inequality also implies that for every $B\in\mathcal{A}$, the sesquilinear functional $(\varphi,\psi)\mapsto\Sigma_n E^n_{\psi,\varphi}(B)$ is bounded, so that there is a (clearly positive) operator $E(B)\in L(\mathcal{H})$, for which $\langle\psi|E(B)\varphi\rangle=\Sigma_n E^n_{\psi,\varphi}(B)$. Thus the map $B\mapsto E(B)$ is a positive operator measure, for which $E(B)=\Sigma_n E^n(B)$ in the operator norm and $E_{\psi,\varphi}=\Sigma_n E^n_{\psi,\varphi}$ in the total variation norm.

By applying Lemma 1 (b) to the finite positive measures $E^n_{\varphi,\varphi}$ and the function $|f|^2$, we see that if $\varphi\in\tilde{D}(f,E)$, then $\varphi\in\tilde{D}(f,E^n)$ for all $n\in\mathbb{N}$, and $\Sigma_n\int|f|^2\,\mathrm{d}E^n_{\varphi,\varphi}=\int|f|^2\,\mathrm{d}E_{\varphi,\varphi}<\infty$. Now let F^n denote the positive operator measure $M_n^{-1}E^n$. We have $\Sigma_n M_n\sqrt{\int|f|^2\,\mathrm{d}F^n_{\psi,\varphi}}\leqslant\Sigma_n M_n(1+\int|f|^2\,\mathrm{d}F^n_{\psi,\varphi})<\infty$. Using the inequality

$$\int|f|d|F^n_{\psi,\varphi}|\leqslant\|\psi\|\sqrt{\int|f|^2\,\mathrm{d}F^n_{\varphi,\varphi}}$$

from Ref. 7, we get $\Sigma_n\int|f|d|E^n_{\psi,\varphi}|=\Sigma_n M_n\int|f|d|F^n_{\psi,\varphi}|<\infty$, from which it follows by Lemma 1 (a) and (b) that

$$\langle\psi|L(f,E)\varphi\rangle = \sum_n \langle\psi|L(f,E^n)\varphi\rangle.$$

■

B. Phase space observables

We assume that the Hilbert space $\mathcal{H}$ is separable. For any $\varphi,\psi\in\mathcal{H}$, let $|\varphi\rangle\langle\psi|$ denote the operator $\xi\mapsto\langle\psi|\xi\rangle\varphi$. Let $\{|n\rangle|n\geqslant 0\}$ be a fixed orthonormal basis of $\mathcal{H}$. We call it the number basis. Let $A_+=\Sigma_{n\geqslant 0}\sqrt{n+1}|n+1\rangle\langle n|$ and $A_-=\Sigma_{n\geqslant 0}\sqrt{n+1}|n\rangle\langle n+1|$ be the raising and lowering operators associated with this basis. They are closed operators with the domain

$$\mathcal{D}(A_+)=\mathcal{D}(A_-)=\left\{\varphi\in\mathcal{H}\middle|\sum_k k|\langle\varphi|k\rangle|^2<\infty\right\},$$

and they satisfy the relation $A_+=A_-^*$. The symmetric operators $(1/\sqrt{2})(A_++A_-)$ and $(1/\sqrt{2})i(A_+-A_-)$ are essentially self-adjoint on $\mathcal{D}(A_+)$ and their closures Q and P are unitarily equivalent to the canonical position and momentum operators, respectively, acting in $L^2(\mathbb{R})$. The operators A_+ and A_- can be expressed in terms of Q and P according to

$$A_+=\frac{1}{\sqrt{2}}(Q-iP),\qquad A_-=\frac{1}{\sqrt{2}}(Q+iP) \tag{2}$$

(cf. Ref. 2, p. 283 and Ref. 12, p. 73). The number operator $N:=\Sigma_{n\geqslant 0}n|n\rangle\langle n|=A_+A_-$, with the domain

$$D(N)=\left\{\varphi\in\mathcal{H}\middle|\sum_k k^2|\langle\varphi|k\rangle|^2<\infty\right\},$$

is self-adjoint and satisfies

$$N+\tfrac{1}{2}I=\tfrac{1}{2}(Q^2+P^2). \tag{3}$$

[The last equality is a simple consequence of (2) and the fact that $D(N)=D(A_+A_-)=D(A_-A_+)$.]

The operators Q and P generate strongly continuous one parameter unitary groups $p\mapsto V(p):=e^{ipQ}$ and $q\mapsto \mathrm{U}(q):=e^{iqP}$ which satisfy the Weyl relation $\mathrm{U}(q)V(p)=e^{iqp}V(p)\mathrm{U}(q)$ for all $q,p\in\mathbb{R}$. The Weyl operators $W(q,p)$ are defined by $W(q,p)=e^{-(1/2)iqp}\mathrm{U}(q)V(p)$ for $q,p\in\mathbb{R}$. The map $(q,p)\mapsto W(-q,p)$ is a projective representation of $\mathbb{R}^2$.

Let T be a state operator. Then

$$I=\frac{1}{2\pi}\int_{\mathbb{R}^2} W(-q,p)TW(-q,p)^*\,\mathrm{d}q\,\mathrm{d}p,$$

and the map $E^T:\mathcal{B}(\mathbb{R}^2)\to L(\mathcal{H})$ defined by

$$E^T(B)=\frac{1}{2\pi}\int_B W(-q,p)TW(-q,p)^*\,\mathrm{d}q\,\mathrm{d}p$$

is a normalized positive operator measure, a phase space observable. Here $\mathcal{B}(\mathbb{R}^2)$ denotes the σ-algebra of Borel subsets of $\mathbb{R}^2$ and the integrals are understood in the weak sense. The construction of the operator measures E^T can be found for instance in Refs. 5 or 14. The operator measure E^T is covariant with respect to the projective representation $(q,p)\mapsto W(-q,p)$ in the sense that $E^T(B+(q_0,p_0))=W(-q_0,p_0)E^T(B)W(-q_0,p_0)^*$ for all $B\in\mathcal{B}(\mathbb{R}^2)$ and $(q,p)\in\mathbb{R}^2$.

The following characterization is obtained in Refs. 4 and 15: every normalized positive operator measure $E:\mathcal{B}(\mathbb{R}^2)\to L(\mathcal{H})$, which is covariant with respect to the representation $(q,p)\mapsto W(-q,p)$, is of the form E^T for some state T.

We let $E^{|s\rangle}$ denote the phase space observable associated with the number state $|s\rangle\langle s|$. Consider the mixed states

$$T=\sum_{n=0}^{\infty} w_n|n\rangle\langle n|, \tag{4}$$

where $w_n\geqslant 0$ and $\Sigma w_n=1$. These states are the ones for which the observable E^T is covariant also with respect to the phase shifts in the sense that

$$e^{i\theta N}E^T([0,\infty)\times X)e^{-i\theta N}=E^T([0,\infty)\times(X+\theta))$$

for all $\theta\in[0,2\pi)$ and $X\in\mathcal{B}([0,2\pi))$, where $\mathbb{R}^2=[0,\infty)\times[0,2\pi)$ and the sum $X+\theta$ is understood modulo 2π. (cf. Ref. 8).

Since $w_n\|E^{|n\rangle}(B)\|\leqslant w_n$ for all $n\in\mathbb{N}$ and $B\in\mathcal{B}(\mathbb{R}^2)$, Proposition 1 can be applied to the positive operator measures $w_nE^{|n\rangle}$. That the norm limit $\Sigma_n w_nE^{|n\rangle}(B)$ equals $E^T(B)$, follows from the identity

$$\langle\varphi|E^T(B)\varphi\rangle=\frac{1}{2\pi}\int_B\left(\sum_n w_n|\langle\varphi|W(-q,p)|n\rangle|^2\right)\mathrm{d}q\,\mathrm{d}p=\sum_n w_n\langle\varphi|E^{|n\rangle}(B)\varphi\rangle,$$

where $\varphi\in\mathcal{H}$ is arbitrary and the monotone convergence theorem has been used.

III. MOMENT OPERATORS OF THE CARTESIAN MARGINS OF THE PHASE SPACE OBSERVABLES ASSOCIATED WITH THE NUMBER STATES

Let x and y denote the functions $(q,p)\mapsto q$ and $(q,p)\mapsto p$, respectively. In Ref. 7, the moment operators $L((x\pm iy)^k,E^{|n\rangle})$ and $L((x^2+y^2)^k,E^{|n\rangle})$ were determined. In Ref. 9, these results were used to obtain the operator relations

$$\begin{aligned} L(x,E^{|n\rangle})&\subset Q,\\ L(y,E^{|n\rangle})&\subset P,\\ L(x^2,E^{|n\rangle})&\subset\left(n+\tfrac{1}{2}\right)I+Q^2,\\ L(y^2,E^{|n\rangle})&\subset\left(n+\tfrac{1}{2}\right)I+P^2. \end{aligned} \tag{5}$$

In this section, we determine directly the moment operators $L(x^k,E^T)$ and $L(y^k,E^T)$, where the state T is taken to be of the form $\Sigma_n w_n|n\rangle\langle n|$. The results show, among other things, that the inclusions (5) are in fact equalities.

A. The operators $L(x^k,E^{|n\rangle})$ and $L(y^k,E^{|n\rangle})$

Let $U:L^2(\mathbb{R})\to\mathcal{H}$ be the unitary operator which maps the Hermite function basis $\{h_n\}_{n\geqslant 0}$ of $L^2(\mathbb{R})$ onto the number basis of $\mathcal{H}$ according to the rule $Uh_n=|n\rangle$. The position and momentum operators in $L^2(\mathbb{R})$ correspond to the operators Q and P via the unitary transformation U, so that the operators $W_0(q,p)$, defined by $W_0(q,p)=U^{-1}W(q,p)U$, act in $L^2(\mathbb{R})$ according to the formula

$$(W_0(q,p)f)(t)=e^{i(1/2)qp}e^{ipt}f(t+q).$$

We need the following well-known result (see, e.g., Ref. 14, pp. 47 and 49).

Lemma 2: Let $F:L^2(\mathbb{R})\to L^2(\mathbb{R})$ denote the Fourier–Plancherel operator. Let $u\in L^2(\mathbb{R})$ be a

unit vector and $f \in L^2(\mathbb{R})$. *Then* $\overline{u}(\cdot - q)f \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ *for almost all* $q \in \mathbb{R}$ *and* $\overline{Fu}(\cdot - p)Ff \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ *for almost all* $p \in \mathbb{R}$. *In addition,*

$$\frac{1}{\sqrt{2\pi}}\langle W_0(-q,p)u|f\rangle = e^{i(1/2)qp}F(\overline{u}(\cdot - q)f)(p)$$

for almost all $q \in \mathbb{R}$ *and all* $p \in \mathbb{R}$, *and*

$$\frac{1}{\sqrt{2\pi}}\langle W_0(-q,p)u|f\rangle = e^{-i(1/2)qp}F^{-1}(\overline{Fu}(\cdot - p)Ff)(q)$$

for almost all $p \in \mathbb{R}$ *and all* $q \in \mathbb{R}$.

Proof: Since u, $f \in L^2(\mathbb{R})$, the function $\overline{u}(\cdot - q)f$ is integrable. Because $\|f\|^2 = \int |\overline{u}(t-q)f(t)|^2 \, dt \, dq$ by Fubini's theorem, $\overline{u}(\cdot - q)f \in L^2(\mathbb{R})$ for almost all q. Similarly, $\overline{Fu}(\cdot - p)Ff \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ for almost all $p \in \mathbb{R}$. The rest of the proof follows from straightforward calculations.

■

First we determine the square integrability domains corresponding to the functions x^k and y^k.

Lemma 3: $\tilde{D}(x^k, E^{|n\rangle}) = D(Q^k)$ *and* $\tilde{D}(y^k, E^{|n\rangle}) = D(P^k)$ *for all* $k \in \mathbb{N}$.

Proof: Let $k \in \mathbb{N}$ be fixed. Let $\varphi \in \mathcal{H}$ and $f = U^{-1}\varphi \in L^2(\mathbb{R})$. If $\varphi \in \tilde{D}(x^k, E^{|n\rangle})$, the function $(q,p) \mapsto q^{2k}|\langle f|W_0(-q,p)h_n\rangle|^2 = q^{2k}|\langle \varphi|W(-q,p)|n\rangle|^2$ is integrable over $\mathbb{R}^2$, and

$$\begin{aligned}
\int_{\mathbb{R}^2} q^{2k} \, dE^{|n\rangle}_{\varphi,\varphi}(q,p) &= \frac{1}{2\pi}\int q^{2k}\left(\int |\langle \varphi|W(-q,p)|n\rangle|^2 \, dp\right)dq \\
&= \int q^{2k}\left(\int |F(\overline{h_n}(\cdot - q)f)(p)|^2 \, dp\right)dq \\
&= \int q^{2k}\left(\int |h_n(t-q)|^2|f(t)|^2 \, dt\right)dq \\
&= \int \left(\int q^{2k}|h_n(t-q)|^2|f(t)|^2 \, dq\right)dt \\
&= \int\int (t-q)^{2k}|h_n(q)|^2|f(t)|^2 \, dq \, dt \\
&= \int\int (t-q)^{2k}|h_n(q)|^2|f(t)|^2 \, dt \, dq,
\end{aligned}$$

where Lemma 2, the unitarity of the Fourier–Plancherel operator, and Fubini's theorem have been used. The existence of the last integral implies that $t \mapsto (t-q)^{2k}|f(t)|^2$ is integrable over $\mathbb{R}$ for almost all $q \in \mathbb{R}$. Thus also $t \mapsto t^{2k}|f(t)|^2$ must be integrable. [In fact, take one $q \in \mathbb{R}$ for which $t \mapsto (t-q)^{2k}|f(t)|^2$ is integrable and use the fact that there exist positive constants A, B, M, such that $At^{2k} \leqslant (t-q)^{2k} \leqslant Bt^{2k}$ for $|t| \geqslant M$.] This means that f belongs to the domain of the kth power of the position operator in $L^2(\mathbb{R})$ and hence $\varphi = Uf \in D(Q^k)$. Conversely, if $\varphi = Uf \in D(Q^k)$, the functions $t \mapsto |t^l||f(t)|^2$ and $q \mapsto |q^l||h_n(q)|^2$ are integrable over $\mathbb{R}$ for all $l \leqslant 2k$ and hence $(t,q) \mapsto (t-q)^{2k}|h_n(q)|^2|f(t)|^2$ is integrable over $\mathbb{R}^2$. The preceding calculation now shows that $\varphi \in \tilde{D}(x^k, E^{|n\rangle})$. The equality $\tilde{D}(x^k, E^{|n\rangle}) = D(Q^k)$ is thus proved.

The results $\tilde{D}(y^k, E^{|n\rangle}) = D(P^k)$ is obtained in an analogous manner by using the fact that the position and momentum operators in $L^2(\mathbb{R})$ are unitarily equivalent via the Fourier–Plancherel operator F.

■

Now we can determine the operators $L(x^k, E^{|n\rangle})$ and $L(y^k, E^{|n\rangle})$.

Theorem 3: *$L(x^k, E^{|n\rangle}) = p_k^{|n\rangle}(Q)$ and $L(y^k, E^{|n\rangle}) = p_k^{|n\rangle}(P)$, where $p_k^{|n\rangle}: \mathbb{R} \to \mathbb{R}$ is the polynomial*

$$p_k^{|n\rangle}(t) = \langle n|(t-Q)^k|n\rangle = \sum_{l=0}^{k} \left(\binom{k}{l} (-1)^{k-l} \langle n|Q^{k-l}|n\rangle \right) t^l.$$

Proof: Since $p_k^{|n\rangle}$ is a polynomial of order k and Q is unitarily equivalent to the position operator in $L^2(\mathbb{R})$, the natural domain of the operator $p_k^{|n\rangle}(Q)$ [which is the set $D(Q^k) \cap D(Q^{k-1}) \cap \cdots D(Q)$] is equal to that of Q^k. Because Q and P are unitarily equivalent, also $D(p_k^{|n\rangle}(P)) = D(P^k)$. Thus by the preceding lemma, we have $D(p_k^{|n\rangle}(Q)) = D(Q^k) = \tilde{D}(x^k, E^{|n\rangle})$ and $D(p_k^{|n\rangle}(P)) = D(P^k) = \tilde{D}(y^k, E^{|n\rangle})$.

Let $\varphi,\ \psi \in \tilde{D}(x^k, E^{|n\rangle}) \subset D(x^k, E^{|n\rangle})$. Let $f = U^{-1}\varphi$, $g = U^{-1}\psi$. Since the function

$$(q,p) \mapsto q^k \langle \psi|W(-q,p)|n\rangle \overline{\langle \varphi|W(-q,p)|n\rangle}$$

is integrable over $\mathbb{R}^2$, we get

$$\begin{aligned}
\langle \psi|L(x^k, E^{|n\rangle})\varphi\rangle &= \int_{\mathbb{R}^2} q^k \, \mathrm{d}E^{|n\rangle}_{\psi,\varphi}(q,p) \\
&= \frac{1}{2\pi} \int q^k \left(\int \langle \psi|W(-q,p)|n\rangle \overline{\langle \varphi|W(-q,p)|n\rangle} \mathrm{d}p \right) \mathrm{d}q \\
&= \int q^k \left(\int \overline{F(\overline{h_n}(\cdot - q)g)(p)} F(\overline{h_n}(\cdot - q)f)(p) \mathrm{d}p \right) \mathrm{d}q \\
&= \int q^k \left(\int \overline{h_n(t-q)g(t)} h_n(t-q) f(t) \mathrm{d}t \right) \mathrm{d}q \\
&= \int \left(\int q^k |h_n(t-q)|^2 \mathrm{d}q \right) \overline{g(t)} f(t) \mathrm{d}t \\
&= \int \left(\int (t-q)^k |h_n(q)|^2 \mathrm{d}q \right) \overline{g(t)} f(t) \mathrm{d}t, \\
&= \int \langle n|(t-Q)^k|n\rangle \overline{g(t)} f(t) \mathrm{d}t \\
&= \langle \psi|p_k^{|n\rangle}(Q)\varphi\rangle.
\end{aligned}$$

The fifth equality follows from Fubini's theorem, since $(q,t) \mapsto q^k |h_n(t-q)|^2 \overline{g(t)} f(t)$ is integrable [because of the inequality

$$|q^k |h_n(t-q)|^2 \overline{g(t)} f(t)| \leqslant \tfrac{1}{2}(1 + q^{2k})(|f(t)|^2 + |g(t)|^2) |h_n(t-q)|^2$$

and the proof of Lemma 3]. The unitarity of F is also used. Since ψ was taken arbitrarily from the dense set $D(Q^k) = \tilde{D}(f, E^{|n\rangle})$, we have $p_k^{|n\rangle}(Q) \subset L(x^k, E^{|n\rangle})$.

The equality $p_k^{|n\rangle}(Q) = L(x^k, E^{|n\rangle})$ follows from the fact that being self-adjoint, the operator $p_k^{|n\rangle}(Q)$ cannot have a proper symmetric extension.

The statement $p_k^{|n\rangle}(P) = L(y^k, E^{|n\rangle})$ is obtained in the same manner, since $p_k^{|n\rangle}$ can also be written in the form $p_k^{|n\rangle}(t) = \langle n|(t-P)^k|n\rangle$ and $p_k^{|n\rangle}(P)$ is self-adjoint. ■

Remark: Since $\langle n|Q^m|n\rangle = 0$ for odd m, and $\langle n|Q^m|n\rangle > 0$ for even m, only the terms with even $k-l$ are present in the sum defining the polynomial $p_k^{|n\rangle}$, and the coefficients of the corresponding x^l are all strictly positive. In particular, $L(x^k, E^{|n\rangle}) \neq Q^k$ and $L(y^k, E^{|n\rangle}) \neq P^k$ for $k > 1$ and $n \geqslant 0$, reflecting the difference from the Weyl quantization (Ref. 6, p. 229), as well as the fact that the Cartesian margins of $E^{|n\rangle}$ are not the spectral measures of Q and P.

Using Theorem 3, all the operators $L(x^k, E^{|n\rangle})$ and $L(x^k, E^{|n\rangle})$ can be written in terms of Q and P, respectively. In particular, the first and second moment operators are the following:

$$\begin{aligned} L(x, E^{|n\rangle}) &= Q, \\ L(y, E^{|n\rangle}) &= P, \\ L(x^2, E^{|n\rangle}) &= \left(n + \tfrac{1}{2}\right) I + Q^2, \\ L(y^2, E^{|n\rangle}) &= \left(n + \tfrac{1}{2}\right) I + P^2. \end{aligned} \tag{6}$$

For the special case of $n=0$, these results were already obtained by formal computations in Ref. 1, pp. 28–29 (without addressing the question on the domains of the operators). A related result of Ref. 10, p. 140, however, seems to lack a constant term.

B. The operators $L(x^k, E^T)$ and $L(y^k, E^T)$ with $T=\Sigma_n w_n |n\rangle\langle n|$

In the next theorem, we need to consider the expressions $\langle n|Q^{2k}|n\rangle$. These integrals are well known and can be calculated, e.g., as instructed in Ref. 11, p. 60. We need here only the following fact.

Lemma 4: For $n \geqslant k$, the expression $\langle n|Q^{2k}|n\rangle$ can be written as a polynomial in n of order k.

Proof: Expressing Q in terms of A_+ and A_-, we get $\langle n|Q^{2k}|n\rangle = (1/2^k)\|(A_+ + A_-)^k|n\rangle\|^2$. Because $A_- A_+ = N + I$, we can write

$$(A_+ + A_-)^k |n\rangle = \sum_{m=0}^{k} a_m |n + k - 2m\rangle,$$

where $a_m|n+k-2m\rangle = A_+^{k-2m} q_m^+(N)|n\rangle$ for $0 \leqslant m \leqslant k/2$ and $a_m|n+k-2m\rangle = A_-^{2m-k} q_m^-(N)|n\rangle$ for $k/2 \leqslant m \leqslant k$, where $q_m^{\pm}$ are some polynomials with $2\deg(q_m^{\pm}) \pm (k-2m) \leqslant k$. Now $a_m^2 = (n+1)(n+2)\cdots(n+k-2m) q_m^+(n)^2$ for $0 \leqslant m \leqslant k/2$ and $a_m^2 = n(n-1)\cdots(n-(2m-k)+1) q_m^-(n)^2$ for $k/2 \leqslant m \leqslant k$, so that each a_m^2 is a polynomial in n of order at most k, with the coefficient of the highest power positive. Since $a_0^2 = (n+1)(n+2)\cdots(n+k)$, we see that $\langle n|Q^{2k}|n\rangle = (1/2^k)\Sigma_{m=0}^k a_m^2$ is a polynomial in n of order exactly k.

■

Theorem 4: *Let $T = \Sigma_n w_n |n\rangle\langle n|$ be a mixture of the number states and $k \in \mathbb{N}$. Let $p_k^{|n\rangle}$ denote the polynomials defined in Theorem 3, and define*

$$s_{kl} = \binom{k}{l} \sum_{n=0}^{\infty} w_n \langle n|Q^{k-l}|n\rangle (\leqslant \infty)$$

for $0 \leqslant l \leqslant k$.

(a) $\tilde{D}(x^k, E^T) \neq \{0\}$ *if and only if*

$$\sum_n n^k w_n < \infty, \tag{7}$$

in which case $s_{kl} < \infty$ for all $0 \leqslant l \leqslant k$, $D(x^k, E^T) = \tilde{D}(x^k, E^T) = D(Q^k)$, and

$$L(x^k, E^T) = \sum_{l=0}^{k} s_{kl} Q^l.$$

In particular, the operator $L(x^k, E^T)$ is then self-adjoint.

(b) *The statement (a) holds true when "x" and "Q" are replaced by "y" and "P."*

Proof: Let $k \in \mathbb{N}$ be fixed. According to Proposition 1, Lemma 3 and Theorem 3 we have

$$L(x^k,E^T)|_{\tilde{D}(x^k,E^T)} \subset \sum_n w_n L(x^k,E^{|n\rangle}) = \sum_n w_n p_k^{|n\rangle}(Q) \tag{8}$$

(where the series of operators are understood in the same sense as in Proposition 1). Let $\varphi \in D(Q^k) \supset D(\Sigma_n w_n p_k^{|n\rangle}(Q))$ and $\varphi \neq 0$. Let $A_{\varphi,\varphi}^{|n\rangle}$ be the density function of the positive measure $E_{\varphi,\varphi}^{|n\rangle}$. By the definition of the square integrability domain, $\varphi \in \tilde{D}(x^k,E^T)$ if and only if the function $x^{2k}\Sigma_n w_n A_{\varphi,\varphi}^{|n\rangle}$ is integrable. By the monotone convergence theorem, the latter statement is equivalent to

$$\sum_n w_n \int x^{2k}\, \mathrm{d}E_{\varphi,\varphi}^{|n\rangle} < \infty. \tag{9}$$

According to the proof of Lemma 3,

$$\begin{aligned}\int x^{2k}\, \mathrm{d}E_{\varphi,\varphi}^{|n\rangle} &= \int\int (t-q)^{2k}|h_n(q)|^2|(U^{-1}\varphi)(t)|^2\, \mathrm{d}t\, \mathrm{d}q \\ &= \sum_{l=0}^{2k}\binom{2k}{l}(-1)^{2k-1}\left(\int t^l|(U^{-1}\varphi)(t)|^2\, \mathrm{d}t\right)\langle n|Q^{2k-l}|n\rangle.\end{aligned}$$

Since $\langle n|Q^m|n\rangle = 0$ for odd $m \in \mathbb{N}$, only the terms with even l are present in the above sum. Because $U^{-1}\varphi \neq 0$, these terms are all strictly positive. Since $0 < \langle n|Q^{2l}|n\rangle \leqslant \int(1+q^{2k})|h_n(q)|^2\, \mathrm{d}q = 1 + \langle n|Q^{2k}|n\rangle$ for all $l \leqslant k$ and $\Sigma_n w_n = 1$, the convergence of the series $\Sigma_n w_n\langle n|Q^{2k}|n\rangle$ implies the convergence of each series $\Sigma_n w_n\langle n|Q^{2l}|n\rangle$ and s_{kl}, $l \leqslant k$. Thus, it follows that a nonzero vector in $D(Q^k)$ belongs to $\tilde{D}(x^k,E^T)$ if and only if the series

$$\sum_n w_n\langle n|Q^{2k}|n\rangle \tag{10}$$

converges. By the preceding lemma, this is equivalent to (7). Since $\tilde{D}(x^k,E^T) \subset D(Q^k)$ by (8), we have shown that $\tilde{D}(x^k,E^T) \neq \{0\}$ if and only if (7) holds, and in that case, $\tilde{D}(x^k,E^T) = D(Q^k)$ and $s_{kl} < \infty$ for $l \leqslant k$.

From the definition of the polynomials $p_k^{|n\rangle}$ we see that if (10) converges, then [using (8)] we get

$$\langle\psi|L(x^k,E^T)\varphi\rangle = \sum_n w_n\langle\psi|p_k^{|n\rangle}(Q)\varphi\rangle = \sum_{l=0}^{k} s_{kl}\langle\psi|Q^l\varphi\rangle$$

for each $\varphi \in D(Q^k)$ and $\psi \in \mathcal{H}$. Thus, $\Sigma_{l=0}^k s_{kl}Q^l \subset L(x^k,E^T)$ [now $D(\Sigma_{l=0}^k s_{kl}Q^l) = D(Q^k)$, because $s_{kk} = 1$]. Since the operator $\Sigma_{l=0}^k s_{kl}Q^l$ is self-adjoint and $L(x^k,E^T)$ is symmetric, the statement (a) has been proved.

The result (b) is obtained in the same manner, since

$$L(y^k,E^T)|_{\tilde{D}(y^k,E^T)} \subset \sum_n w_n L(y^k,E^{|n\rangle}) = \sum_n w_n p_k^{|n\rangle}(P),$$

$\langle n|Q^m|n\rangle = \langle n|P^m|n\rangle$ for all m, $n \geqslant 0$ and

$$\int y^{2k}\,\mathrm{d}E^{|n\rangle}_{\varphi,\varphi} = \int\int (t-p)^{2k}|Fh_n(p)|^2|(FU^{-1}\varphi)(t)|^2\,\mathrm{d}t\,\mathrm{d}p$$
$$= \sum_{l=0}^{2k}\binom{2k}{l}(-1)^{2k-l}\left(\int t^l|(FU^{-1}\varphi)(t)|^2\,\mathrm{d}t\right)\langle n|P^{2k-l}|n\rangle$$

for all $\varphi \in D(P^k)$. ∎

Remark: For each $k \in \mathbb{N}$, there are states T of the form (4) such that (7) does not converge [so that $\widetilde{D}(x^k,E^T)=\{0\}$], but all the series s_{kl} do. In that case, $\Sigma_{l=0}^k s_{kl}Q^l$ is still a well-defined self-adjoint operator with the domain $D(Q^k)$. An example of such a state for $k \in \mathbb{N}$ is given by $t_n = 1/(Sn^{k+1})$, where $S=\Sigma_n n^{-(k+1)}$. We do not know whether there are any nonzero vectors in the domain $D(x^k,E^T)$ then.

IV. OPERATOR INTEGRALS OF SOME POLYNOMIALS

In this last section, we use Theorem 3 to determine the operator integrals for certain types of polynomials. To that end, let h, h_1, h_2 be real polynomials defined by $h(t)=\Sigma_{l=0}^k a_l t^l$, $a_k \neq 0$, and $h_i(t)=\Sigma_{l=0}^{k_i} a_{i,l}t^l$, $a_{i,k_i}\neq 0$, $i=1,2$.

The operators $L(h\circ x,E^{|n\rangle})$ and $L(h\circ y,E^{|n\rangle})$: Let ψ, $\varphi \in \mathcal{H}$. There exist positive constants M, A, B such that $A|t^k| \leqslant |h(t)| \leqslant B|t^k|$ for $|t| \geqslant M$, which implies that the function $h\circ x$ [i.e., $(q,p)\mapsto h(q)$] is $E^{|n\rangle}_{\psi,\varphi}$-integrable if and only if x^k is such, and in that case, $\int h\circ x\,\mathrm{d}E^{|n\rangle}_{\psi,\varphi} = \Sigma_{l=0}^k a_l \int x^l\,\mathrm{d}E^{|n\rangle}_{\psi,\varphi}$. Since $D(x^k,E^{|n\rangle})=D(Q^k)\subset D(Q^l)=D(x^l,E^{|n\rangle})$ for $l\leqslant k$, it follows that $D(h\circ x,E^{|n\rangle})=D(Q^k)$, and

$$L(h\circ x,E^{|n\rangle}) = \sum_{l=0}^{k} a_l p_l^{|n\rangle}(Q). \tag{11}$$

Naturally, a similar result holds for the function $h\circ y$.

The operators $L(h_1\circ x+ih_2\circ y,E^{|n\rangle})$: Let ψ, $\varphi \in \mathcal{H}$. The function $h_1\circ x+ih_2\circ y$ is $E^{|n\rangle}_{\psi,\varphi}$-integrable if and only if both $h_1\circ x$ and $h_2\circ y$ are such, and in that case $\int(h_1\circ x+ih_2\circ y)\mathrm{d}E^{|n\rangle}_{\psi,\varphi} = \int h_1\circ x\,\mathrm{d}E^{|n\rangle}_{\psi,\varphi} + i\int h_2\circ y\,\mathrm{d}E^{|n\rangle}_{\psi,\varphi}$. Thus, we have $D(h_1\circ x+ih_2\circ y,E^{|n\rangle})=D(Q^{k_1})\cap D(P^{k_2})$, and

$$L(h_1\circ x + ih_2\circ y,E^{|n\rangle}) = \sum_{l=0}^{k_1} a_{1,l}p_l^{|n\rangle}(Q) + i\sum_{l=0}^{k_2} a_{2,l}p_l^{|n\rangle}(P). \tag{12}$$

The operators $L(h_1\circ x+h_2\circ y,E^{|n\rangle})$ with k_i even and $a_{i,k_i}>0$: Assume that k_i is even, and $a_{i,k_i}>0$, $i=1,2$. Then we can choose positive constants M, A_i, B_i such that $h_i(t)\geqslant 0$ and $A_i t^{k_i} \leqslant h_i(t) \leqslant B_i t^{k_i}$ for $|t|\geqslant M$ and $i=1,2$. This implies that the function $h_1\circ x+h_2\circ y$ is $E^{|n\rangle}_{\psi,\varphi}$-integrable for ψ, $\varphi \in \mathcal{H}$ if and only if both x^{k_1} and y^{k_2} are such. We get $D(h_1\circ x+h_2\circ y,E^{|n\rangle}) = D(Q^{k_1})\cap D(P^{k_2})$, and

$$L(h_1\circ x + h_2\circ y,E^{|n\rangle}) = \sum_{l=0}^{k_1} a_{1,l}p_l^{|n\rangle}(Q) + \sum_{l=0}^{k_2} a_{2,l}p_l^{|n\rangle}(P). \tag{13}$$

A note on the operators $L(x\pm iy,E^{|n\rangle})$ and $L(x^2+y^2,E^{|n\rangle})$: The above observations show that, in particular, $L((1/\sqrt{2})(x\pm iy),E^{|n\rangle})=(1/\sqrt{2})(Q\pm iP)$, and $L\left(\frac{1}{2}(x^2+y^2),E^{|n\rangle}\right)=\frac{1}{2}(Q^2+P^2)+\left(n+\frac{1}{2}\right)I$. These operator integrals have already been determined in Ref. 7 (using a different method) to be the following: $L((1/\sqrt{2})(x\pm iy),E^{|n\rangle})=A_{\mp}$ and $L\left(\frac{1}{2}(x^2+y^2),E^{|n\rangle}\right)=N+(n+1)I$. The fundamental operator equalities (2) and (3) now show that the results are indeed consistent.

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Initial states and decoherence of histories

Artur Scherer[a] and Andrei N. Soklakov
Department of Mathematics, Royal Holloway, University of London, Egham, Surrey, TW20 0EX, United Kingdom

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We study decoherence properties of arbitrarily long histories constructed from a fixed projective partition of a finite dimensional Hilbert space. We show that decoherence of such histories for all initial states that are naturally induced by the projective partition implies decoherence for arbitrary initial states. In addition we generalize the simple necessary decoherence condition [Scherer *et al.*, Phys. Lett. A **326**, 307 (2004)] for such histories to the case of arbitrary coarse graining. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1888030]

I. INTRODUCTION

In the Copenhagen interpretation of quantum mechanics all properties of a quantum system are defined with respect to measurements performed by an external observer using classical measuring devices. This interpretation, however, cannot be used in the case of closed quantum systems, such as the Universe as a whole. In this case any observer must be a part of the system itself. A self-contained theory of closed quantum systems that does not rely on either the external observer nor on the existence of classical devices is still under development. The decoherent histories approach[1–5] is probably the most promising candidate for such a theory. This approach predicts probabilities for quantum histories, i.e., ordered sequences of quantum-mechanical "propositions." Mathematically, these propositions are represented by projectors, the same projectors that would define a quantum measurement in the Copenhagen approach. In particular, an exhaustive set of mutually exclusive propositions corresponds to a complete set of mutually orthogonal projectors.

Due to quantum interference, one cannot always assign probabilities to a set of histories in a consistent way. For this to be possible, the set of histories must be decoherent. Whether the corresponding decoherence condition is fulfilled or not depends on the initial state, the unitary dynamics of the system and the propositions from which the histories are constructed. The dependence on the initial state is connected to one of the central questions in quantum cosmology, the question of how the classical features of our world evolve from the initial quantum state of the Universe. This question provides the main motivation for the research presented in this paper.

Here we consider histories that are constructed from a *fixed* exhaustive set of mutually exclusive propositions, $\{P_\mu\}$, and investigate the question of how the choice of the initial state affects decoherence of such histories. We show that decoherence of arbitrarily long histories for all initial states that are induced by the projectors $\{P_\mu\}$ via normalization implies the decoherence for arbitrary initial states. It is relevant to note that, unlike the set of all possible states, the set $\{P_\mu\}$ is discrete and may contain as few as just two elements (for "yes–no" propositions). As an additional result, we obtain a generalization of the simple necessary decoherence condition that was derived for fine-grained histories in Ref. 6. The condition is applicable to arbitrary coarse grainings.

The paper is organized as follows. After introducing our framework we present the mathematical content of our results in the form of a theorem. We prove the theorem, infer the results, and conclude with a short summary.

[a]Author to whom correspondence should be addressed, Electronic mail: artur.scherer@uni-konstanz.de

II. OUR FRAMEWORK

Definition 1: A set of projectors $\{P_\mu\}$ on a Hilbert space $\mathcal{H}$ is called a projective *partition* of $\mathcal{H}$, if $\forall \mu,\mu' : P_\mu P_{\mu'} = \delta_{\mu\mu'} P_\mu$ and $\Sigma_\mu P_\mu = \mathbb{1}_\mathcal{H}$. Here, $\mathbb{1}_\mathcal{H}$ denotes the unit operator. We call a projective partition *fine-grained* if all projectors are one dimensional, i.e., $\forall \mu$ $\dim(\mathrm{supp}(P_\mu))=1$,[7] and *coarse-grained* otherwise.

Definition 2: Given a projective partition $\{P_\mu\}$ of a Hilbert space $\mathcal{H}$, we denote by $\mathcal{K}[\{P_\mu\};k] := \{h_\alpha : h_\alpha = (P_{\alpha_1}, P_{\alpha_2}, \ldots, P_{\alpha_k}) \in \{P_\mu\}^k\}$ the corresponding exhaustive set of mutually exclusive histories of length k. Histories are thus defined to be ordered sequences of projection operators, corresponding to quantum-mechanical propositions. Note that we restrict ourselves to histories constructed from a *fixed* projective partition, the projectors P_{α_j} within the sequences are all chosen from the same partition for all "times" $j=1,\ldots,k$.

Definition 3: Given a Hilbert space $\mathcal{H}$ and a projective partition $\{P_\mu\}$ of $\mathcal{H}$, we denote by $\mathcal{S}$ the set of all density operators on $\mathcal{H}$ and by $\mathcal{S}_{\{P_\mu\}}$ the discrete set of "*partition states*" induced by the partition $\{P_\mu\}$ via normalization,

$$\mathcal{S}_{\{P_\mu\}} := \left\{ \frac{P_\nu}{\mathrm{Tr}[P_\nu]} : P_\nu \in \{P_\mu\} \right\}. \tag{1}$$

An initial state $\rho \in \mathcal{S}$ and a unitary dynamics generated by a unitary map $U:\mathcal{H}\to\mathcal{H}$ induce a probabilistic structure on the event algebra associated with $\mathcal{K}[\{P_\mu\};k]$, if certain consistency conditions are fulfilled. These are given in terms of properties of the *decoherence functional* $\mathcal{D}_{U,\rho}[\cdot,\cdot]$ on $\mathcal{K}[\{P_\mu\};k]\times\mathcal{K}[\{P_\mu\};k]$, defined by

$$\mathcal{D}_{U,\rho}[h_{\boldsymbol{\alpha}}, h_{\boldsymbol{\beta}}] := \mathrm{Tr}[C_{\boldsymbol{\alpha}} \rho C_{\boldsymbol{\beta}}^\dagger], \tag{2}$$

where

$$C_{\boldsymbol{\alpha}} := (U^{\dagger k} P_{\alpha_k} U^k)(U^{\dagger k-1} P_{\alpha_{k-1}} U^{k-1}) \cdots (U^\dagger P_{\alpha_1} U) = U^{\dagger k} P_{\alpha_k} U P_{\alpha_{k-1}} U \cdots P_{\alpha_2} U P_{\alpha_1} U. \tag{3}$$

The set $\mathcal{K}[\{P_\mu\};k]$ is said to be *decoherent* or *consistent* with respect to a given unitary map $U:\mathcal{H}\to\mathcal{H}$ and a given initial state $\rho\in\mathcal{S}$, if

$$\mathcal{D}_{U,\rho}[h_{\boldsymbol{\alpha}}, h_{\boldsymbol{\beta}}] \propto \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}} \equiv \prod_{j=1}^{k} \delta_{\alpha_j \beta_j} \tag{4}$$

for all $h_{\boldsymbol{\alpha}}, h_{\boldsymbol{\beta}} \in \mathcal{K}[\{P_\mu\};k]$. These are the consistency conditions. If they are fulfilled, probabilities may be assigned to the histories and are given by the diagonal elements of the decoherence functional, $p[h_{\boldsymbol{\alpha}}] = \mathcal{D}_{U,\rho}[h_{\boldsymbol{\alpha}}, h_{\boldsymbol{\alpha}}]$.

What we have just described is a slightly simplified version of the general decoherent histories formalism. In general, both the partition and the unitary may depend on the parameter $j=1,\ldots,k$. Our setting based on a fixed partition and a fixed unitary is motivated by the analogy with the classical symbolic dynamics.[6,8] Various generalizations of this setting will be addressed in forthcoming publications. In the literature several consistency conditions of different strength can be found.[9] The conditions given above are known as *medium decoherence*.[5] It has recently been shown that consideration of the weaker decoherence conditions is problematic.[10]

III. RESULTS

Theorem: *Let a projective partition $\{P_\mu\}$ of a finite dimensional Hilbert space $\mathcal{H}$ and a unitary map U on $\mathcal{H}$ be given. Then the following three statements are equivalent:*

(a) $\forall \rho \in \mathcal{S}_{\{P_\mu\}} \forall k \in \mathbb{N}\ \forall h_{\boldsymbol{\alpha}}, h_{\boldsymbol{\beta}} \in \mathcal{K}[\{P_\mu\};k] : \mathcal{D}_{U,\rho}[h_{\boldsymbol{\alpha}}, h_{\boldsymbol{\beta}}] \propto \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}}$,
(b) $\forall P_{\mu'}, P_{\mu''} \in \{P_\mu\} \forall n \in \mathbb{N} : [U^n P_{\mu'} (U^\dagger)^n, P_{\mu''}] = 0$,
(c) $\forall \rho \in \mathcal{S}\ \forall k \in \mathbb{N}\ \forall h_{\boldsymbol{\alpha}}, h_{\boldsymbol{\beta}} \in \mathcal{K}[\{P_\mu\};k] : \mathcal{D}_{U,\rho}[h_{\boldsymbol{\alpha}}, h_{\boldsymbol{\beta}}] \propto \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}}$.

Proof: We will prove the theorem by showing that (a) implies (b), (b) implies (c), and (c) implies (a). The last implication, (c)$\Rightarrow$(a), is trivial, and the second implication, (b)$\Rightarrow$(c), can be easily shown using the notation of Eq. (3). It remains to prove the implication (a)$\Rightarrow$(b).

The proof is constructed as follows. We first show that the proposition

$$\forall \rho \in \mathcal{S}_{\{P_\mu\}} \forall n \in \mathbb{N} \ \ \forall \mu_0, \mu', \mu'' \quad \text{with } \mu' \neq \mu'' : \mathrm{Tr}[P_{\mu''}(U^n P_{\mu_0} U^{\dagger n}) P_{\mu'}(U^n \rho U^{\dagger n}) P_{\mu''}] = 0 \tag{5}$$

is a necessary consequence of the decoherence condition (a) and then conclude that this proposition implies the commutativity condition (b) of the theorem.

The first part of the proof will be accomplished by contradiction, i.e., we will assume that (5) is not satisfied, and then show that this assumption contradicts the decoherence condition (a) of the theorem.

Assume condition (5) is not satisfied. This means there exist a partition state $\tilde{\rho} \in \mathcal{S}_{\{P_\mu\}}$, an integer $\tilde{n} \in \mathbb{N}$, and partition-element labels μ_0, μ', μ'', with $\mu' \neq \mu''$, such that

$$\mathrm{Tr}[P_{\mu''}(U^{\tilde{n}} P_{\mu_0} U^{\dagger \tilde{n}}) P_{\mu'}(U^{\tilde{n}} \tilde{\rho} U^{\dagger \tilde{n}}) P_{\mu''}] = c \neq 0. \tag{6}$$

This, as we will see, is in contradiction to decoherence condition (a). Written out, the decoherence condition (a) is

$$\mathrm{Tr}[P_{\alpha_k} U P_{\alpha_{k-1}} U \cdots P_{\alpha_1} U \rho_0 U^\dagger P_{\beta_1} \cdots P_{\beta_{k-1}} U^\dagger P_{\beta_k}] \propto \prod_{j=1}^{k} \delta_{\alpha_j \beta_j} \tag{7}$$

for all $k \in \mathbb{N}$, all initial states $\rho_0 \in \mathcal{S}_{\{P_\mu\}}$, and arbitrary histories $h_{\boldsymbol{\alpha}}, h_{\boldsymbol{\beta}}$. Since the length k of the histories is arbitrary, we may choose $k = q\tilde{n}$ with arbitrary $q \in \mathbb{N}$. By summing over $\alpha_1, \ldots, \alpha_{\tilde{n}-1}, \alpha_{\tilde{n}+1}, \ldots, \alpha_{q\tilde{n}-1}$ and $\beta_1, \ldots, \beta_{\tilde{n}-1}, \beta_{\tilde{n}+1}, \ldots, \beta_{q\tilde{n}-1}$, and using $\Sigma_\mu P_\mu = \mathbb{1}_{\mathcal{H}}$, we obtain

$$\mathrm{Tr}[P_{\alpha_{q\tilde{n}}} (U^{q-1})^{\tilde{n}} P_{\alpha_{\tilde{n}}} U^{\tilde{n}} \rho_0 U^{\dagger \tilde{n}} P_{\beta_{\tilde{n}}} (U^{\dagger q-1})^{\tilde{n}} P_{\beta_{q\tilde{n}}}] \propto \delta_{\alpha_{q\tilde{n}} \beta_{q\tilde{n}}} \delta_{\alpha_{\tilde{n}} \beta_{\tilde{n}}} \tag{8}$$

for all $q \in \mathbb{N}$, and $\rho_0 \in \mathcal{S}_{\{P_\mu\}}$, and arbitrary $\alpha_{\tilde{n}}, \beta_{\tilde{n}}, \alpha_{q\tilde{n}}, \beta_{q\tilde{n}}$. In order to proceed we will need the following lemma.[6]

Lemma: Let $\mathcal{H}$ be a finite dimensional Hilbert space and $U : \mathcal{H} \to \mathcal{H}$ any unitary map on $\mathcal{H}$. Then $\forall \epsilon > 0 \ \exists q \in \mathbb{N}$ such that $\|U^q - \mathbb{1}_{\mathcal{H}}\| < \epsilon$, $\|\cdot\|$ meaning the conventional operator norm, which is $\|A\| := \sup\{\|Av\| : v \in \mathcal{H}, \|v\| = 1\}$ for an operator A on $\mathcal{H}$.

According to this lemma, for any given arbitrarily small $\epsilon > 0$ we can always find a $q \in \mathbb{N}$ such that $U^q = \mathbb{1}_{\mathcal{H}} + \hat{\mathcal{O}}(\epsilon)$, where $\hat{\mathcal{O}}(\epsilon)$ is some operator whose norm is of order ϵ, $\|\hat{\mathcal{O}}(\epsilon)\| < \epsilon$. Using the submultiplicativity property of operator norms, we have

$$\|U^{-1}\hat{\mathcal{O}}(\epsilon)\| \leqslant \|U^{-1}\| \times \|\hat{\mathcal{O}}(\epsilon)\| = \|\hat{\mathcal{O}}(\epsilon)\| \tag{9}$$

and hence $U^{q-1} = U^{-1} + \hat{\mathcal{O}}'(\epsilon)$, where $\|\hat{\mathcal{O}}'(\epsilon)\| < \epsilon$.

Now we are in a position to derive a contradiction. We let our histories start with the initial state $\rho_0 = \tilde{\rho}$. Furthermore we choose $\alpha_{\tilde{n}} = \mu'$, $\beta_{\tilde{n}} = \mu''$, and $\alpha_{q\tilde{n}} = \beta_{q\tilde{n}} = \mu_0$. Since $\mu' \neq \mu''$, condition (8) becomes

$$\forall q \in \mathbb{N} : \mathrm{Tr}[P_{\mu_0} (U^{q-1})^{\tilde{n}} P_{\mu'} U^{\tilde{n}} \tilde{\rho} U^{\dagger \tilde{n}} P_{\mu''} (U^{\dagger q-1})^{\tilde{n}} P_{\mu_0}] = 0. \tag{10}$$

Choosing q such that $\|U^q - \mathbb{1}_{\mathcal{H}}\| < \epsilon$ for a given *arbitrarily small* $\epsilon > 0$, we get a situation where the expressions $(U^{q-1})^{\tilde{n}}$ and $(U^{\dagger q-1})^{\tilde{n}}$ in Eq. (10) can be replaced by $(U^\dagger + \hat{\mathcal{O}}'(\epsilon))^{\tilde{n}}$ and $(U + \hat{\mathcal{O}}'^\dagger(\epsilon))^{\tilde{n}}$, respectively. In the following it will be convenient to use the definition

$$A_{r_1,r_2,\ldots,r_{\tilde{n}}} := \prod_{i=1}^{\tilde{n}} (U^{\dagger r_i}(\hat{\mathcal{O}}'(\epsilon))^{1-r_i}), \tag{11}$$

where the operators inside the product are written out from left to right in the order of increasing index i. Using this definition we have

$$(U^\dagger + \hat{\mathcal{O}}'(\epsilon))^{\tilde{n}} = \sum_{r_1,\ldots,r_{\tilde{n}}\in\{0,1\}} A_{r_1,\ldots,r_{\tilde{n}}}. \tag{12}$$

This yields for the left-hand side of Eq. (10),

$$\begin{aligned}
&\mathrm{Tr}[P_{\mu_0}(U^{q-1})^{\tilde{n}}P_{\mu'}U^{\tilde{n}}\tilde{\rho}U^{\dagger\tilde{n}}P_{\mu''}(U^{\dagger q-1})^{\tilde{n}}P_{\mu_0}] \\
&\quad = \mathrm{Tr}\left[P_{\mu_0}\left(\sum_{r_1,\ldots,r_{\tilde{n}}\in\{0,1\}} A_{r_1,\ldots,r_{\tilde{n}}}\right)P_{\mu'}U^{\tilde{n}}\tilde{\rho}U^{\dagger\tilde{n}}P_{\mu''}\left(\sum_{s_1,\ldots,s_{\tilde{n}}\in\{0,1\}} A^\dagger_{s_1,\ldots,s_{\tilde{n}}}\right)P_{\mu_0}\right] \\
&\quad = \sum_{r_1,\ldots,r_{\tilde{n}}\in\{0,1\}}\ \sum_{s_1,\ldots,s_{\tilde{n}}\in\{0,1\}} \mathrm{Tr}[P_{\mu_0}A_{r_1,\ldots,r_{\tilde{n}}}P_{\mu'}U^{\tilde{n}}\tilde{\rho}U^{\dagger\tilde{n}}P_{\mu''}A^\dagger_{s_1,\ldots,s_{\tilde{n}}}P_{\mu_0}].
\end{aligned} \tag{13}$$

According to (10) the left-hand side of this equation must be zero. Hence we have

$$\begin{aligned}
&\mathrm{Tr}[P_{\mu_0}(U^\dagger)^{\tilde{n}}P_{\mu'}U^{\tilde{n}}\tilde{\rho}U^{\dagger\tilde{n}}P_{\mu''}U^{\tilde{n}}P_{\mu_0}] \\
&\quad = -\sum_{\substack{r_1,\ldots,r_{\tilde{n}}\in\{0,1\}\\ r_1+\cdots+r_{\tilde{n}}<\tilde{n}}}\ \sum_{\substack{s_1,\ldots,s_{\tilde{n}}\in\{0,1\}\\ s_1+\cdots+s_{\tilde{n}}<\tilde{n}}} \mathrm{Tr}[P_{\mu_0}A_{r_1,\ldots,r_{\tilde{n}}}P_{\mu'}U^{\tilde{n}}\tilde{\rho}U^{\dagger\tilde{n}}P_{\mu''}A^\dagger_{s_1,\ldots,s_{\tilde{n}}}P_{\mu_0}].
\end{aligned} \tag{14}$$

Using the cyclic permutation-invariance property of the trace and the triangle inequality, we obtain

$$\begin{aligned}
&|\mathrm{Tr}[P_{\mu''}(U^{\tilde{n}}P_{\mu_0}U^{\dagger\tilde{n}})P_{\mu'}(U^{\tilde{n}}\tilde{\rho}U^{\dagger\tilde{n}})P_{\mu''}]| \\
&\quad \leqslant \sum_{\substack{r_1,\ldots,r_{\tilde{n}}\in\{0,1\}\\ r_1+\cdots+r_{\tilde{n}}<\tilde{n}}}\ \sum_{\substack{s_1,\ldots,s_{\tilde{n}}\in\{0,1\}\\ s_1+\cdots+s_{\tilde{n}}<\tilde{n}}} |\mathrm{Tr}[A^\dagger_{s_1,\ldots,s_{\tilde{n}}}P_{\mu_0}A_{r_1,\ldots,r_{\tilde{n}}}P_{\mu'}U^{\tilde{n}}\tilde{\rho}U^{\dagger\tilde{n}}P_{\mu''}]|.
\end{aligned} \tag{15}$$

Utilizing the inequality $|\mathrm{Tr}[BT]| \leqslant \|B\|\mathrm{Tr}\sqrt{T^\dagger T}$ for bounded operators $B:\mathcal{H}\to\mathcal{H}$ and operators $T:\mathcal{H}\to\mathcal{H}$ with finite trace norm $\|T\|_1 := \mathrm{Tr}\sqrt{T^\dagger T}$, see Ref. 11, we deduce from Eq. (15),

$$|\mathrm{Tr}[P_{\mu''}(U^{\tilde{n}}P_{\mu_0}U^{\dagger\tilde{n}})P_{\mu'}(U^{\tilde{n}}\tilde{\rho}U^{\dagger\tilde{n}})P_{\mu''}]| \leqslant \sum_{\substack{r_1,\ldots,r_{\tilde{n}}\in\{0,1\}\\ r_1+\cdots+r_{\tilde{n}}<\tilde{n}}}\ \sum_{\substack{s_1,\ldots,s_{\tilde{n}}\in\{0,1\}\\ s_1+\cdots+s_{\tilde{n}}<\tilde{n}}} \|B^{s_1,\ldots,s_{\tilde{n}}}_{r_1,\ldots,r_{\tilde{n}}}\|\mathrm{Tr}\sqrt{T^\dagger T}, \tag{16}$$

where we defined

$$B^{s_1,\ldots,s_{\tilde{n}}}_{r_1,\ldots,r_{\tilde{n}}} := A^\dagger_{s_1,\ldots,s_{\tilde{n}}}P_{\mu_0}A_{r_1,\ldots,r_{\tilde{n}}}, \tag{17}$$

$$T := P_{\mu'}U^{\tilde{n}}\tilde{\rho}U^{\dagger\tilde{n}}P_{\mu''}. \tag{18}$$

Using the fact that $\|B^\dagger\| = \|B\|$ for any bounded operator B and it's adjoint $B^\dagger$,[12] we have $\|\hat{\mathcal{O}}'^\dagger(\epsilon)\| = \|\hat{\mathcal{O}}'(\epsilon)\| < \epsilon$. Utilizing the submultiplicativity property of operator norms we deduce that the norms of the operators $B^{s_1,\ldots,s_{\tilde{n}}}_{r_1,\ldots,r_{\tilde{n}}}$ are all bounded from above by ϵ, except in the case where all $s_1,\ldots,s_{\tilde{n}}$ and all $r_1,\ldots,r_{\tilde{n}}$ are equal 1, which is excluded from the sum on the right-hand side of Eq. (16). Indeed we have

$$\|B^{s_1,\ldots,s_{\tilde{n}}}_{r_1,\ldots,r_{\tilde{n}}}\| \leqslant \left(\prod_{i=1}^{\tilde{n}} \|U\|^{s_i}\|\hat{\mathcal{O}}'^{\dagger}(\epsilon))\|^{1-s_i}\right)\|P_{\mu_0}\|\left(\prod_{i=1}^{\tilde{n}} \|U^{\dagger}\|^{r_i}\|\hat{\mathcal{O}}'(\epsilon))\|^{1-r_i}\right)$$
$$\leqslant \left(\prod_{i=1}^{\tilde{n}} \epsilon^{1-s_i}\right)\left(\prod_{j=1}^{\tilde{n}} \epsilon^{1-r_j}\right) \leqslant \epsilon^2 < \epsilon, \quad \text{if } s_1 + \cdots + s_{\tilde{n}} < \tilde{n}, \quad r_1 + \cdots + r_{\tilde{n}} < \tilde{n}, \tag{19}$$

where we used $\|P_{\mu_0}\| = \|U\| = \|U^{\dagger}\| = 1$ and $\epsilon \ll 1$. With the definition $M := \mathrm{Tr}\sqrt{T^{\dagger}T}$ we finally conclude from Eq. (16),

$$|\mathrm{Tr}[P_{\mu''}(U^{\tilde{n}}P_{\mu_0}U^{\dagger\tilde{n}})P_{\mu'}(U^{\tilde{n}}\tilde{\rho}U^{\dagger\tilde{n}})P_{\mu''}]| < 2^{2\tilde{n}}M\epsilon. \tag{20}$$

Since c, $\tilde{n}$, and M are fixed constants, we can always arrange $2^{2\tilde{n}}M\epsilon < |c|$ by choosing a sufficiently small $\epsilon > 0$. This contradicts the assumption (6) and thus proves our proposition (5).

We are now in a position to derive the commutativity condition (b) of the theorem. It is a straightforward consequence of proposition (5) we have just proven. Taking condition (5) and choosing in it the state $\rho \in \mathcal{S}_{\{P_\mu\}}$ to be proportional to the projector sandwiched between U^n and $U^{\dagger n}$ within the first bracket,

$$\rho = \frac{P_{\mu_0}}{\mathrm{Tr}[P_{\mu_0}]}, \tag{21}$$

where P_{μ_0} is still arbitrary, we necessarily get the condition

$$\forall n \in \mathbb{N} \ \forall \mu_0, \mu', \mu'' \quad \text{with } \mu' \neq \mu'' : \mathrm{Tr}[P_{\mu''}(U^n P_{\mu_0} U^{\dagger n})P_{\mu'}(U^n P_{\mu_0} U^{\dagger n})P_{\mu''}] = 0. \tag{22}$$

With the definition $A := P_{\mu'}(U^n P_{\mu_0} U^{\dagger n})P_{\mu''}$ Eq. (22) becomes $\mathrm{Tr}[A^{\dagger}A] = 0$. Since $A^{\dagger}A$ is a positive operator, this is possible if and only if $A = 0$. Hence condition (22) is equivalent to

$$\forall n \in \mathbb{N} \ \forall \mu_0, \mu', \mu'' \quad \text{with } \mu' \neq \mu'' : P_{\mu'}(U^n P_{\mu_0} U^{\dagger n})P_{\mu''} = 0. \tag{23}$$

This condition implies

$$\sum_{\mu'} P_{\mu'}(U^n P_{\mu_0} U^{\dagger n})P_{\mu''} = P_{\mu''}(U^n P_{\mu_0} U^{\dagger n})P_{\mu''} \tag{24}$$

for any μ_0 and μ'', and arbitrary $n \in \mathbb{N}$. But since $\Sigma_{\mu'} P_{\mu'} = \mathbb{1}_{\mathcal{H}}$, the left-hand side of the last equation must be equal to $(UP_{\mu_0}U^{\dagger})P_{\mu''}$. Hence we obtain

$$P_{\mu''}(U^n P_{\mu_0} U^{\dagger n})P_{\mu''} = (U^n P_{\mu_0} U^{\dagger n})P_{\mu''} \tag{25}$$

on the one hand and by taking the adjoint of Eq. (25),

$$P_{\mu''}(U^n P_{\mu_0} U^{\dagger n})P_{\mu''} = P_{\mu''}(U^n P_{\mu_0} U^{\dagger n}) \tag{26}$$

on the other hand, for any $n \in \mathbb{N}$ and arbitrary μ_0 and μ''. Therefore

$$(U^n P_{\mu_0} U^{\dagger n})P_{\mu''} = P_{\mu''}(U^n P_{\mu_0} U^{\dagger n}) \tag{27}$$

for any $n \in \mathbb{N}$ and arbitrary μ_0, μ'', and so $[U^n P_{\mu_0} U^{\dagger n}, P_{\mu''}] = 0$ for any $n \in \mathbb{N}$ and all $P_{\mu_0}, P_{\mu''} \in \{P_\mu\}$. □

The implication (a) $\Rightarrow$ (c) of the theorem constitutes the main result of this paper: the decoherence of histories of arbitrary length for all initial states from the set $\mathcal{S}_{\{P_\mu\}}$ implies decoherence of such histories for arbitrary initial states $\rho \in \mathcal{S}$. It should be mentioned that the set $\mathcal{S}_{\{P_\mu\}}$ can be viewed as the smallest natural set of states that is associated with our framework. It is discrete and

may consist of just two elements (in the case of "yes–no" propositions). The set $\mathcal{S}$, on the other hand, contains the continuum of all possible states that are allowed in our framework.

In Ref. 6 the notion of classical states with respect to a partition $\{P_\mu\}$ was introduced.

Definition 4: A state represented by the density operator ρ is called *classical with respect to (w.r.t.) a partition* $\{P_\mu\}$ of the Hilbert space $\mathcal{H}$, if it is block-diagonal w.r.t. $\{P_\mu\}$, i.e., if $\rho = \Sigma_\mu P_\mu \rho P_\mu$. We denote by $\mathcal{S}^{\mathrm{cl}}_{\{P_\mu\}}$ the set of all density operators that are classical w.r.t. $\{P_\mu\}$.

In Ref. 6 it was shown that in the case of fine-grained partitions sets of histories of arbitrary length decohere for all classical initial states *only if* the unitary dynamics preserves the classicality of states, i.e., *only if*

$$\forall \rho \in \mathcal{S}^{\mathrm{cl}}_{\{P_\mu\}}: U\rho U^\dagger \in \mathcal{S}^{\mathrm{cl}}_{\{P_\mu\}}. \tag{28}$$

It is a single-iteration criterion, to verify that it holds for a particular unitary map U, only a single iteration of the map needs to be taken into account, which can be much easier than establishing decoherence directly by computing the off-diagonal elements of the decoherence functional. This is especially useful for studying chaotic quantum maps, for which typically only the first iteration is known in a closed analytical form.[13] Unfortunately, condition (28) fails to be necessary in the coarse-grained case. The following simple corollary of our theorem provides a necessary single-iteration condition that applies to arbitrary coarse grainings and is equivalent to (28) in the fine-grained case.

Corollary: Let a projective partition $\{P_\mu\}$ *of a finite dimensional Hilbert space* $\mathcal{H}$ *and a unitary map* U *on* $\mathcal{H}$ *be given. The medium decoherence condition is then satisfied for all classical initial states and arbitrarily long histories, i.e.,*

$$\forall \rho \in \mathcal{S}^{\mathrm{cl}}_{\{P_\mu\}}\ \forall k \in \mathbb{N}\ \ \forall h_{\boldsymbol{\alpha}}, h_{\boldsymbol{\beta}} \in \mathcal{K}[\{P_\mu\};k]: \mathcal{D}_{U,\rho}[h_{\boldsymbol{\alpha}}, h_{\boldsymbol{\beta}}] \propto \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}}, \tag{29}$$

only if the following necessary condition is fulfilled:

$$\forall P_{\mu'}, P_{\mu''} \in \{P_\mu\}: [UP_{\mu'}U^\dagger, P_{\mu''}] = 0. \tag{30}$$

Proof: Follow trivially from the implication (a)$\Rightarrow$(b) of the theorem, as $\mathcal{S}_{\{P_\mu\}} \subset \mathcal{S}^{\mathrm{cl}}_{\{P_\mu\}}$. □

IV. SUMMARY

We have investigated decoherence properties of sets of quantum histories constructed from a fixed projective partition $\{P_\mu\}$ of a finite dimensional Hilbert space. We have found that if decoherence is established for arbitrary history lengths and all initial states from $\mathcal{S}_{\{P_\mu\}}$, which is the smallest natural set induced by $\{P_\mu\}$, then any set of histories constructed from $\{P_\mu\}$ is decoherent for all possible initial states. In addition, we have provided a necessary single-iteration criterion for decoherence of arbitrarily long histories that generalizes the condition of Ref. 6 to the case of arbitrary coarse grainings.

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Improvement of uncertainty relations for mixed states

Yong Moon Park[a)]
Department of Mathematics, Yonsei University, Seoul 120-749, Korea

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We study a possible improvement of uncertainty relations. The Heisenberg uncertainty relation employs commutator of a pair of conjugate observables to set the limit of quantum measurement of the observables. The Schrödinger uncertainty relation improves the Heisenberg uncertainty relation by adding the correlation in terms of anti-commutator. However both relations are insensitive whether the state used is pure or mixed. We improve the uncertainty relations by introducing additional terms which measure the mixtureness of the state. For the momentum and position operators as conjugate observables and for the thermal state of quantum harmonic oscillator, it turns out that the equalities in the improved uncertainty relations hold. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1876874]

I. INTRODUCTION

Soon after Heisenberg and Schrödinger invented Quantum Mechanics around 1925, Heisenberg discovered the uncertainty relation in 1927.[1] The standard form of Heisenberg's uncertainty relation for any pair of observables A and B and a density matrix ρ is expressed as

$$\frac{1}{4}|\langle [A,B]\rangle_\rho|^2 \leqslant \mathrm{Var}_\rho(A)\mathrm{Var}_\rho(B), \tag{1.1}$$

where $\mathrm{Var}_\rho(A)=\mathrm{tr}(\rho A^2)-(\mathrm{tr}(\rho A))^2$ is the variance of A in the state defined by ρ, and $\mathrm{Var}_\rho(B)$ is defined analogously, $\langle [A,B]\rangle_\rho=\mathrm{tr}(\rho[A,B])$ is the expectation of the commutator $[A,B]=AB-BA$. The relation (1.1) states the fundamental limitation on quantum measurement for incompatible (noncommuting) observables and has played a fundamental role in quantum theory.

In 1930, Schrödinger[2] improved the uncertainty relation (1.1) by including the correlation between observables:

$$\frac{1}{4}|\langle [A,B]\rangle_\rho|^2+\frac{1}{4}|\langle \{A_0,B_0\}\rangle_\rho|^2 \leqslant \mathrm{Var}_\rho(A)\mathrm{Var}_\rho(B), \tag{1.2}$$

where $\langle \{A_0,B_0\}\rangle_\rho=\mathrm{tr}(\rho\{A_0,B_0\})$ denotes the expectation of anticommutator $\{A_0,B_0\}=A_0B_0+B_0A_0$ and $A_0=A-\langle A\rangle_\rho$, $B_0=B-\langle B\rangle_\rho$. The first term on the left-hand side of (1.2) encodes incompatibility, while the second term encodes correlation between observables A and B.

In recent years in the field of quantum computation and quantum information, the strong correlation, such as the phenomenon of entanglement, in the quantum world that cannot occur in classical mechanics, has been intensively studied.[3] Thus one expects that the Schrödinger uncertainty relation will play an important role in quantum theory.[4]

In this paper, we improved the uncertainty relations (1.1) and (1.2) by introducing additional terms in the lower bounds of (1.1) and (1.2), respectively. We will show that for any observables A and B, and any density matrix ρ, the following uncertainty relations hold:

a)Electronic mail: ympark@yonsei.ac.kr

$$\frac{1}{4}|\langle [A,B]\rangle_\rho|^2 + \mathrm{tr}(A_0\rho^{1/2}A_0\rho^{1/2})(\mathrm{tr}(B_0\rho^{1/2}B_0\rho^{1/2})) \leqslant \mathrm{Var}_\rho(A)\mathrm{Var}_\rho(B) \tag{1.3}$$

and

$$\frac{1}{4}|\langle [A,B]\rangle_\rho|^2 + \frac{1}{4}|\langle \{A_0,B_0\}\rangle_\rho|^2 + M(A_0,B_0;\rho) \leqslant \mathrm{Var}_\rho(A)\mathrm{Var}_\rho(B), \tag{1.4}$$

where the quantity $M(A_0,B_0;\rho)$ is defined in Theorem 2.2 explicitly. Notice that the relations (1.3) and (1.4) are improved versions of the relations (1.1) and (1.2), respectively. If the density matrix ρ is pure, then the second term on the left-hand side of (1.3) and the third term in (1.4) are vanished, and so (1.3) and (1.4) are reduced to the original relations (1.1) and (1.2), respectively.

It may be worth mentioning that for any observable A the functional,

$$\rho \mapsto \mathrm{tr}(A\rho^{1/2}A\rho^{1/2}),$$

is concave by Lieb's concavity theorem,[5] and so in a sense the values of additional terms in the above measure the mixturedness of ρ. We also note that the Wigner–Yanase skew information[6] is given by

$$I(\rho,A) = -\frac{1}{2}\mathrm{tr}([\rho^{1/2},A]^2) = \mathrm{tr}(\rho A^2) - \mathrm{tr}(A\rho^{1/2}A\rho^{1/2}), \tag{1.5}$$

and so the terms we introduced are related to the Wigner–Yanase information. See Sec. III for the details.

In order to show that the uncertainty relations (1.3) and (1.4) are optimal in some special situations, we consider the position and momentum operators as a pair of conjugate observables in $L^2(\mathbb{R})$, and choose the density operator ρ corresponding to the thermal state (quasi-free state) for a quantum harmonic oscillator. In this case, we show that the equalities in (1.3) and (1.4) hold. See Theorem 4.2.

Let us describe the main idea employed in this paper. Let A and B be self-adjoint operators (observables) acting on a separable Hilbert space. Let $\langle\cdot,\cdot\rangle$ be the Hilbert–Schmidt inner product defined on the class of Hilbert Schmidt operators:

$$\langle A,B\rangle := \mathrm{tr}(A^*B).$$

Then the left-hand side of (1.2) equals $|\langle A_0\rho^{1/2},B_0\rho^{1/2}\rangle|^2$. In order to make ρ play the same role as A and B, we introduce orthogonal decompositions:

$$\begin{aligned} A\rho^{1/2} &= A_{\rho,+} + A_{\rho,-}, \\ B\rho^{1/2} &= B_{\rho,+} + B_{\rho,-}, \end{aligned} \tag{1.6}$$

where

$$\begin{aligned} A_{\rho,+} &:= \frac{1}{2}(A\rho^{1/2} + \rho^{1/2}A), \\ A_{\rho,-} &:= \frac{1}{2}(A\rho^{1/2} - \rho^{1/2}A), \end{aligned} \tag{1.7}$$

and $B_{\rho,+}$ and $B_{\rho,-}$ are defined analogously. Notice that $\langle A_{\rho,-},A_{\rho,+}\rangle = 0$ and $\langle B_{\rho,-},B_{\rho,+}\rangle = 0$. One observes that

$$|\langle A_{\rho,+}, B_{\rho,-}\rangle| = |\langle A_{\rho,-}, B_{\rho,+}\rangle| = \frac{1}{4}|\langle [A,B]\rangle_\rho|.$$

The relation (1.3) will be followed from the above relation and the Schwarz inequality. See the proof of Theorem 2.1 in Sec. III. The proof of (1.4) is a little complicated. Let S be the subspace spanned by $B_{\rho,+}$ and $B_{\rho,-}$ and let P_S be the projection onto S. Denote by $\|\cdot\|_2$ the norm induced by $\langle\cdot,\cdot\rangle$. Notice that $\|P_S A\rho^{1/2}\|_2 \leqslant \|A\rho^{1/2}\|_2$. We will estimate $\|P_S A_\rho\|_2$ to prove the relation (1.4). See Sec. III for details.

There have been several proposals to quantify uncertainty by many authors. A prominent one is the Shanon entropy,[7,8] and another one is the Fisher information arising in Statistical Inference.[9,10] Recently Luo and Zhang[11] tried to characterize uncertainty relations by the Wigner–Yanase skew information.[6] Also, there are other families of uncertainty relations for mixed states. See Ref. 12 and the references therein. However, the results and the method used differ from those in this paper.

The paper is organized as follows: In Sec. II, we list our main results, Theorem 2.1 and Theorem 2.2. In Sec. III, we produce the proofs of main theorems by introducing the concept of orthogonal decompositions of $A\rho^{1/2}$ and $B\rho^{1/2}$. In Sec. IV, we give a brief discussion on the possible optimal improvement. Then, we give an example of a mixed state (and a pair of conjugate observables) for which the equalities in (1.3) and (1.4) hold.

II. IMPROVEMENT OF UNCERTAINTY RELATIONS: MAIN RESULTS

In this section we first list our main results, Theorem 2.1 and Theorem 2.2, and then give some remarks on the content of the results.

Let $\mathcal{H}$ be a separable Hilbert space. Denote by $\mathcal{L}(\mathcal{H})$ the algebra of all bounded linear operators on $\mathcal{H}$. An operator $T \in \mathcal{L}(\mathcal{H})$ is called Hilbert–Schmidt if $\mathrm{tr}(T^*T) < \infty$, where $\mathrm{tr}(T^*T)$ is the trace of T^*T. The class of all Hilbert–Schmidt operators is denoted by $\mathcal{L}_2(\mathcal{H})$.

We consider a pair of self-adjoint operators A and B acting on $\mathcal{H}$. Denote by $D(A)$ [resp., $D(B)$] the domain of A (resp., B). Let ρ be a density matrix (operator) on $\mathcal{H}$; $\rho \geqslant 0$ and $\mathrm{tr}(\rho) = 1$. In order to care for the domain problems arising from the unboundedness of A and B, we assume that the properties in the following assumption hold.

Assumption 2.1: Let A and B be self-adjoint operators acting on a separable Hilbert space $\mathcal{H}$ and let $\rho \in \mathcal{L}(\mathcal{H})$ be a density matrix. We assume that the following properties hold:

(a) *The inclusions* $\rho^{1/2}\mathcal{H} \subset \mathbf{(}D(A) \cap D(B)\mathbf{)}$, $A\rho^{1/2}\mathcal{H} \subset \mathbf{(}D(A) \cap D(B)\mathbf{)}$ *and* $B\rho^{1/2}\mathcal{H} \subset \mathbf{(}D(A) \cap D(B)\mathbf{)}$, *hold.*

(b) *The composition maps* $A\rho^{1/2}$, $B\rho^{1/2}$, $BA\rho^{1/2}$, $AB\rho^{1/2}$, $A^2\rho^{1/2}$, and $B^2\rho^{1/2}$ *define Hilbert–Schmidt operators on* $\mathcal{H}$.

(c) *There is a dense set* $D \subset \mathbf{(}D(A) \cap D(B)\mathbf{)}$ *such that the following inclusions hold:* $AD \subset \mathbf{(}D(A) \cap D(B)\mathbf{)}$ *and* $BD \subset \mathbf{(}D(A) \cap D(B)\mathbf{)}$.

We now list our main results. For notational simplicity, put

$$\langle T\rangle_\rho := \mathrm{tr}(T\rho), \quad \|T\|_\rho^2 = \mathrm{tr}(T^*T\rho),$$

for any (unbounded) operator, whenever the expressions in the above are well defined. Let $[A,B] := AB - BA$ and $\{A,B\} := AB + BA$ be the commutator and anticommutator of A and B, respectively. The following results are improved versions of the uncertainty relations (1.1) and (1.2):

Theorem 2.1: *Let A and B be self-adjoint operators acting on a separable Hilbert space $\mathcal{H}$ and let ρ be a density matrix. Under Assumption 2.1, the relation*

$$\frac{1}{4}|\langle [A,B]\rangle_\rho|^2 + \mathrm{tr}(A\rho^{1/2}A\rho^{1/2})\mathrm{tr}(B\rho^{1/2}B\rho^{1/2}) \leqslant \|A\|_\rho^2\|B\|_\rho^2 \tag{2.1}$$

holds.

Theorem 2.2: *Let A, B, and ρ be the operators as in Theorem 2.1. Under Assumption 2.1, the relation,*

$$\frac{1}{4}|\langle [A,B]\rangle_\rho|^2 + \frac{1}{4}|\langle \{A,B\}\rangle_\rho|^2 + M(A,B;\rho) \leqslant \|A_\rho\|^2\|B\|_\rho^2 \tag{2.2}$$

holds, where $M(A,B;\rho)=max\{M_1(A,B;\rho),M_1(B,A;\rho)\}$ *and* $M_1(A,B;\rho)$ *is given by*

$$M_1(A,B;\rho) := \frac{1}{4}\frac{(|\langle [A,B]\rangle_\rho|\mathrm{tr}(B\rho^{1/2}B\rho^{1/2}))^2}{\|B\|_\rho^4 - (\mathrm{tr}(B\rho^{1/2}B\rho^{1/2}))^2} \tag{2.3}$$

if $\mathrm{tr}(B\rho^{1/2}B\rho^{1/2}) < \|B\|_\rho^2$, *and* $M_1(A,B;\rho)=0$ *otherwise.*

Under Assumption 2.1, one can check that each term in the relations (2.1) and (2.2) is well defined. It may be possible to weaken Assumption 2.1 to get the relations (2.1) and (2.2). Put

$$A_0 := A - \langle A\rangle_0, \quad B_0 := B - \langle B\rangle_\rho.$$

If one replaces A and B by A_0 and B_0 in the relations (2.1) and (2.2), one can see that Theorem 2.1 and Theorem 2.2 are improvements of Heisenberg's uncertainty relation (1.1) and Schrödinger's uncertainty relation (1.2), respectively. Notice that if ρ is pure, $\mathrm{tr}(A_0\rho^{1/2}A_0\rho^{1/2})=\mathrm{tr}(B_0\rho^{1/2}B_0\rho^{1/2})=0$, and so the relations (2.1) and (2.2) are reduced to the relations (1.1) and (1.2), respectively, for any pure states.

It may be worth giving discussions on the content of Theorem 2.1 and Theorem 2.2 in more detail.

Remark 2.1: The Wigner–Yanase skew information[6] for any observable A and a density matrix ρ is defined by

$$I(\rho,A) := \frac{1}{2}\mathrm{tr}([\rho^{1/2},A][A,\rho^{1/2}]) = \mathrm{tr}(A^2\rho) - \mathrm{tr}(A\rho^{1/2}A\rho^{1/2}). \tag{2.4}$$

Thus, the terms we introduced in Theorem 2.1 and Theorem 2.2 are related to the above skew information. Since $0 \leqslant I(\rho,A)$, we see that $\mathrm{tr}(A\rho^{1/2}A\rho^{1/2}) \leqslant \|A\|_\rho^2$ and the equality holds if and only if $[\rho,A]=0$. If ρ commutes with either A or else B, then $\langle [A,B]\rangle_\rho=0$. Thus, if A and B are conjugate observables, there does not exist such a density matrix, and the strict inequalities $\mathrm{tr}(A\rho^{1/2}A\rho^{1/2}) < \|A\|_\rho^2$ and $\mathrm{tr}(B\rho^{1/2}B\rho^{1/2}) < \|B\|_\rho^2$ hold for any conjugate observables A and B.

Remark 2.2: The inequality (2.2) is not optimal. In fact, we discarded complicated non-negative terms in the derivation of (2.2). We will give a discussion on the optimal lower bound of (2.2). See Theorem 4.1 in Sec. IV.

Remark 2.3: As an application of the uncertainty relations (2.1) and (2.2), we considered the position and momentum operators on $L^2(\mathbb{R})$ as a pair of conjugate observables and the density matrix ρ corresponding to the thermal state for a quantum harmonic oscillator. We proved that the equalities in the uncertainty relations in (2.1) and (2.2) hold in this case. See Theorem 4.2.

III. PROOFS OF THEOREM 2.1 AND THEOREM 2.2

We produce the proofs of Theorem 2.1 and Theorem 2.2 in this section. Let A and B be self-adjoint operators and ρ a density matrix satisfying the properties in Assumption 2.1. For notational brevity, we write

$$A_\rho := A\rho^{1/2}, \quad B_\rho := B\rho^{1/2}. \tag{3.1}$$

We decompose A_ρ and B_ρ as

$$A_\rho = A_{\rho,+} + A_{\rho,-},$$

$$B_\rho = B_{\rho,+} + B_{\rho,-}, \tag{3.2}$$

where

$$\begin{aligned} A_{\rho,+} &:= \frac{1}{2}(A\rho^{1/2} + \rho^{1/2}A) = \frac{1}{2}\{A, \rho^{1/2}\}, \\ A_{\rho,-} &:= \frac{1}{2}(A\rho^{1/2} - \rho^{1/2}A) = \frac{1}{2}[A, \rho^{1/2}], \\ B_{\rho,+} &:= \frac{1}{2}(B\rho^{1/2} + \rho^{1/2}B) = \frac{1}{2}\{B, \rho^{1/2}\}, \\ B_{\rho,-} &:= \frac{1}{2}(B\rho^{1/2} - \rho^{1/2}B) = \frac{1}{2}[B, \rho^{1/2}]. \end{aligned} \tag{3.3}$$

Denote by $\langle T,S\rangle, T,S \in \mathcal{L}_2(\mathcal{H})$, the Hilbert–Schmidt inner product on $\mathcal{L}_2(\mathcal{H})$:

$$\langle T,S\rangle := \mathrm{tr}(T^*S), \quad \forall\, T,S \in \mathcal{L}_2(\mathcal{H}), \tag{3.4}$$

and $\|T\|_2$ the induced norm:

$$\|T\|_2^2 := \mathrm{tr}(T^*T). \tag{3.5}$$

Here we have used the norm $\|T\|_2$ to distinguish it from the operator norm $\|T\|$. In the sequel, we assume that the properties in Assumption 2.1 hold.

Lemma 3.1: (a) The composite maps $\rho^{1/2}A$, $\rho^{1/2}B$, $\rho^{1/2}AB$, $\rho^{1/2}BA$, $\rho^{1/2}A^2$, *and* $\rho^{1/2}B^2$ *are bounded on* D. *The bounded extensions of those operators, denoted by the same symbols, are adjoint operators of* $A\rho^{1/2}$, $B\rho^{1/2}$, $BA\rho^{1/2}$, $AB\rho^{1/2}$, $A^2\rho^{1/2}$, *and* $B^2\rho^{1/2}$, respectively.

(b) The equalities,

$$\rho^{1/2}(A^2\rho^{1/2}) = (\rho^{1/2}A)(A\rho^{1/2}), \quad \rho^{1/2}(B^2\rho^{1/2}) = (\rho^{1/2}B)(B\rho^{1/2}),$$

$$\rho^{1/2}(AB\rho^{1/2}) = (\rho^{1/2}A)(B\rho^{1/2}), \quad \rho^{1/2}(BA\rho^{1/2}) = (\rho^{1/2}B)(A\rho^{1/2}),$$

hold, where $\rho^{1/2}(A^2\rho^{1/2})$ *is the composite map (operator product) of* $\rho^{1/2}$ *and* $A^2\rho^{1/2}$, *and* $(\rho^{1/2}A)\times(A\rho^{1/2})$ *the composite map of* $\rho^{1/2}A$ *and* $A\rho^{1/2}$, *etc.*

(c) $\langle A_{\rho,+}, A_{\rho,-}\rangle = 0$ *and* $\langle B_{\rho,+}, B_{\rho,-}\rangle = 0$.

Proof: (a) By Assumption 2.1 (b)–(c), one has that for any $\varphi \in D$ and $\eta \in \mathcal{H}$,

$$(\varphi, A\rho^{1/2}\eta) = (\rho^{1/2}A\varphi, \eta),$$

and so $\rho^{1/2}A = (A\rho^{1/2})^*$ on D. Since D is dense, the relation extends to $\mathcal{H}$. The rest of the part (a) follows from a similar method used above.

(b) Those equalities follow from Assumption 2.1 (b) and the part (a) of the lemma.

(c) Part (c) of the lemma follows from the definitions of $A_{\rho,\pm}$ and $B_{\rho,\pm}$ in (3.3) and the trace property; $\mathrm{tr}(TS) = \mathrm{tr}(ST)$. □

It follows from Lemma 3.1 (c) that the decompositions in (3.2) are orthogonal decompositions. Also, Lemma 3.1 (a) shows that $A_{\rho,+}$ and $B_{\rho,+}$ are self-adjoint, and $(A_{\rho,-})^* = -A_{\rho,-}$ and $(B_{\rho,-})^* = -B_{\rho,-}$.

Lemma 3.2: The equalities,

$$\langle A_{\rho,\pm}, A_{\rho,\pm}\rangle = \frac{1}{2}\{\mathrm{tr}(A^2\rho) \pm \mathrm{tr}(A\rho^{1/2}A\rho^{1/2})\},$$

$$\langle B_{\rho,\pm}, B_{\rho,\pm}\rangle = \frac{1}{2}\{\mathrm{tr}(B^2\rho) \pm \mathrm{tr}(B\rho^{1/2}B\rho^{1/2})\},$$

$$\langle B_{\rho,\pm}, A_{\rho,\pm}\rangle = \frac{1}{4}\{\mathrm{tr}(\{A,B\}\rho) \pm 2\mathrm{tr}(B\rho^{1/2}A\rho^{1/2})\},$$

$$\langle B_{\rho,\pm}, A_{\rho,\mp}\rangle = \frac{1}{4}\{\mathrm{tr}([B,A]\rho)\ ,$$

hold.

Proof: The equalities follow from the definitions of $A_\pm$ and $B_\pm$ in (3.3) and direct computations. □

Notice that by the first and second equalities in Lemma 3.2, one has that

$$\|A_{\rho,\pm}\|_2^2 = \frac{1}{2}\{\|A\|_\rho^2 \pm \mathrm{tr}(A\rho^{1/2}A\rho^{1/2})\},$$

$$\|B_{\rho,\pm}\|_2^2 = \frac{1}{2}\{\|B\|_\rho^2 \pm \mathrm{tr}(B\rho^{1/2}B\rho^{1/2})\}. \tag{3.6}$$

Also one recognizes that the Wigner–Yanase skew information $I(\rho,A)$ and $\|A_{\rho,-}\|$ are related by

$$I(\rho,A) = 2\|A_{\rho,-}\|^2. \tag{3.7}$$

See the definition of $I(\rho,A)$ in (2.4).

We are now ready to prove Theorem 2.1 and Theorem 2.2. It follows from (3.1) that

$$\langle B_\rho, A_\rho\rangle = \mathrm{tr}(BA\rho) = \frac{1}{2}\mathrm{tr}(\{B,A\}\rho) + \frac{1}{2}\mathrm{tr}([B,A]\rho).$$

Since the first term on the rhs of the above is real and the second term is pure imaginary,

$$|\langle B_\rho, A_\rho\rangle|^2 = \frac{1}{4}|\mathrm{tr}(\{B,A\}\rho)|^2 + \frac{1}{4}|\mathrm{tr}([B,A]\rho)|^2, \tag{3.8}$$

and so by the Schwarz inequality, the Schrödinger uncertainty relation,

$$\frac{1}{4}(\mathrm{tr}([B,A]\rho)|^2 + \frac{1}{4}|\mathrm{tr}(\{B,A\}\rho)|^2 \leqslant \|A_\rho\|_2^2\|B_\rho\|_2^2, \tag{3.9}$$

holds. Recall that $\|A_\rho\|_2^2 = \|A\|_\rho^2$ and $\|B_\rho\|_2^2 = \|B\|_\rho^2$.

Proof of Theorem 2.1: It follows from the Schwarz inequality and (3.6) that

$$|\langle B_{\rho,+}, A_{\rho,-}\rangle|^2 \leqslant \|B_{\rho,+}\|_2^2\|A_{\rho,-}\|_2^2 = \frac{1}{4}(\|B\|_\rho^2 + \mathrm{tr}(B\rho^{1/2}A\rho^{1/2}))(\|A\|_\rho^2 - \mathrm{tr}(A\rho^{1/2}A\rho^{1/2})),$$

$$|\langle B_{\rho,-}, A_{\rho,+}\rangle|^2 \leqslant \|B_{\rho,-}\|_2^2\|A_{\rho,+}\|_2^2 = \frac{1}{4}(\|B\|_\rho^2 - \mathrm{tr}(B\rho^{1/2}A\rho^{1/2}))(\|A\|_\rho^2 + \mathrm{tr}(A\rho^{1/2}A\rho^{1/2})).$$

Thus, by the fourth equality in Lemma 3.2 and the above inequality. we have

$$\frac{1}{8}|\mathrm{tr}([B,A]\rho)|^2 = |\langle B_{\rho,+}, A_{\rho,-}\rangle|^2 + |\langle B_{\rho,-}, A_{\rho,+}\rangle|^2 \leqslant \frac{1}{2}\{\|B\|_\rho^2\|A\|_\rho^2 - \mathrm{tr}(B\rho^{1/2}B\rho^{1/2})\mathrm{tr}(A\rho^{1/2}A\rho^{1/2})\}.$$

The above relation equals that in Theorem 2.1. □.

Now, let us turn to the proof of Theorem 2.2. Recall that the class $\mathcal{L}_2(\mathcal{H})$ of the Hilbert–Schmidt operator is a Hilbert space with the Hilbert–Schmidt inner product $\langle\cdot,\cdot\rangle$ defined in (3.4). Denote by $\hat{A}_{\rho,\pm}$ and $\hat{B}_{\rho,\pm}$ the normalized vectors in $\mathcal{L}_2(\mathcal{H})$ in the direction of $A_{\rho,\pm}$ and $B_{\rho,\pm}$, respectively:

$$\hat{A}_{\rho,\pm} = A_{\rho,\pm}/\|A_{\rho,\pm}\|_2, \quad \hat{B}_{\rho,\pm} = B_{\rho,\pm}/\|B_{\rho,\pm}\|_2. \tag{3.10}$$

If $\|A_{\rho,-}\|_2=0$ (resp., $\|B_{\rho,-}\|_2=0$), we set $\hat{A}_{\rho,-}=0$ (resp., $\hat{B}_{\rho,-}=0$). By (3.2) and (3.10),

$$\begin{aligned} A_\rho &= \|A_{\rho,+}\|_2\hat{A}_{\rho,+} + \|A_{\rho,-}\|_2\hat{A}_{\rho,-}, \\ B_\rho &= \|B_{\rho,+}\|_2\hat{B}_{\rho,+} + \|B_{\rho,-}\|_2\hat{B}_{\rho,-}. \end{aligned} \tag{3.11}$$

We introduce vectors orthogonal to A_ρ and B_ρ by

$$\begin{aligned} A_\rho^\perp &= \|A_{\rho,-}\|_2\hat{A}_{\rho,+} - \|A_{\rho,+}\|_2\hat{A}_{\rho,-}, \\ B_\rho^\perp &= \|B_{\rho,-}\|_2\hat{B}_{\rho,+} - \|B_{\rho,+}\|_2\hat{B}_{\rho,-}. \end{aligned} \tag{3.12}$$

It is easy to check that

$$\begin{aligned} &\|A_\rho^\perp\|_2 = \|A_\rho\|_2, \quad \|B_\rho^\perp\|_2 = \|B_\rho\|_2, \\ &\langle A_\rho^\perp, A_\rho\rangle = 0, \quad \langle B_\rho^\perp, B_\rho\rangle = 0. \end{aligned} \tag{3.13}$$

Denote by $\tilde{S}$ and S the subspace of $\mathcal{L}_2(\mathcal{H})$ spanned by $\{\hat{A}_{\rho,+},\hat{A}_{\rho,-}\}$ and $\{\hat{B}_{\rho,+},\hat{B}_{\rho,-}\}$, respectively, and let P_S be the projection to S.

Proposition 3.1: The inequality,

$$|\langle B_\rho, A_\rho\rangle|^2 + |\langle B_\rho^\perp, A_\rho\rangle|^2 \leqslant \|B_\rho\|_2^2\|A_\rho\|_2^2,$$

holds.

Proof: Let $\hat{B}_\rho$ and $\hat{B}_\rho^\perp$ be normalized vectors in the directions of B_ρ and $B_\rho^\perp$, respectively:

$$\hat{B}_\rho = B_\rho/\|B_\rho\|_2, \quad \hat{B}_\rho^\perp = B_\rho^\perp/\|B_\rho\|_2.$$

Since $\{\hat{B}_\rho, \hat{B}_\rho^\perp\}$ is an orthonormal basis of S, we have

$$\|P_S A_\rho\|^2 = |\langle \hat{B}_\rho, P_S A_\rho\rangle|^2 + |\langle \hat{B}_\rho^\perp, P_S A_\rho\rangle|^2, \tag{3.14}$$

and so

$$|\langle \hat{B}_\rho, A_\rho\rangle|^2 + |\langle \hat{B}_\rho^\perp, A_\rho\rangle|^2 = \|P_S A_\rho\|_2^2 \leqslant \|A_\rho\|_2^2.$$

By multiplying $\|B_\rho\|_2^2$ to both sides of the above inequality, we proved the lemma. □

Lemma 3.3: The equality,

$$|\langle B_\rho^\perp, A\rangle|^2 = M_1(A,B;\rho) + M_2(A,B;\rho),$$

holds, where $M_1(A,B;\rho)$ is given by (2.3) in Theorem 2.2 and

$$M_2(A,B;\rho) = \frac{1}{4}(\|B_{\rho,+}\|_2\|B_{\rho,-}\|_2)^{-2}\left[\|B\|_\rho^2 \mathrm{tr}(B\rho^{1/2}A\rho^{1/2}) - \frac{1}{2}\langle\{B,A\}\rangle_\rho \mathrm{tr}(B\rho^{1/2}B\rho^{1/2})\right]^2, \tag{3.15}$$

if $\mathrm{tr}(B\rho^{1/2}B\rho^{1/2}) < \|B\|_\rho^2$, *and* $M_2(A,B;\rho)=0$ *otherwise.*

Proof: By the definition of $B_\rho^\perp$ in (3.12),

$$\begin{aligned}\langle B_\rho^\perp, A_\rho\rangle &= \langle \|B_{\rho,-}\|_2 \hat{B}_{\rho,+} - \|B_{\rho,+}\|_2 \hat{B}_{\rho,-}, A_{\rho,+} + A_{\rho,-}\rangle \\ &= \left\{ \frac{\|B_{\rho,-}\|_2}{\|B_{\rho,+}\|_2}\langle B_{\rho,+}, A_{\rho,+}\rangle - \frac{\|B_{\rho,+}\|_2}{\|B_{\rho,-}\|_2}\langle B_{\rho,-}, A_{\rho,-}\rangle \right\} \\ &\quad + \left\{ \frac{\|B_{\rho,-}\|_2}{\|B_{\rho,+}\|_2}\langle B_{\rho,+}, A_{\rho,-}\rangle - \frac{\|B_{\rho,+}\|_2}{\|B_{\rho,-}\|_2}\langle B_{\rho,-}, A_{\rho,+}\rangle \right\}.\end{aligned}$$

Since the first term on the rhs of the last equality in the above is real and the second term is pure imaginary, we have

$$|\langle B_\rho^\perp, A_\rho\rangle|^2 = M_1(A,B;\rho) + M_2(A,B;\rho),$$

where

$$M_1(A,B;\rho) = \left| \frac{\|B_{\rho,-}\|_2}{\|B_{\rho,+}\|_2}\langle B_{\rho,+}, A_{\rho,-}\rangle - \frac{\|B_{\rho,+}\|_2}{\|B_{\rho,-}\|_2}\langle B_{\rho,-}, A_{\rho,+}\rangle \right|^2,$$

$$M_2(A,B;\rho) = \left| \frac{\|B_{\rho,-}\|_2}{\|B_{\rho,+}\|_2}\langle B_{\rho,+}, A_{\rho,+}\rangle - \frac{\|B_{\rho,+}\|_2}{\|B_{\rho,-}\|_2}\langle B_{\rho,-}, A_{\rho,-}\rangle \right|^2. \tag{3.16}$$

By Lemma 3.2,

$$M_1(A,B;\rho) = \frac{1}{4^2}|\langle [B,A]\rangle_\rho|^2 (\|B_{\rho,+}\|_2 \|B_{\rho,-}\|_2)^{-2} (\|B_{\rho,-}\|_2^2 - \|B_{\rho,+}\|)^2.$$

Substituting (3.6) into the above expression, we proved that $M_1(A,B;\rho)$ in the above equals that in (2.3).

Next, we consider $M_2(A,B;\rho)$ in (3.16). $M_2(A,B;\rho)$ can be expressed as

$$M_2(A,B;\rho) = (\|B_{\rho,+}\|_2 \|B_{\rho,-}\|_2)^{-2} [\|B_{\rho,-}\|_2^2 \langle B_{\rho,+}, A_{\rho,-}\rangle - \|B_{\rho,+}\|_2^2 \langle B_{\rho,-}, A_{\rho,-}\rangle]^2.$$

Using Lemma (3.2) and (3.6), one can check that the above expression equals that in (3.15). Notice that, if $\|B_{\rho,-}\|_2 = 0$, then $B_\rho^\perp = 0$ by (3.12). Thus, $M_1(A,B;\rho) = M_2(A,B;\rho) = 0$ in this case. This proved the lemma completely. □

Proof of Theorem 2.2: Since $M_2(A,B;\rho) \geqslant 0$, Theorem 2.2 for $M_1(A,B;\rho)$ follows from Proposition 3.1, (3.8), and Lemma 3.3. By interchanging the role of A_ρ and B_ρ, we proved the theorem completely. □

IV. OPTIMAL IMPROVEMENT AND APPLICATION

We give a brief discussion on the optimal improvement of Theorem 2.2, which can be obtained by the method used in Sec. III. Then, as an application of Theorem 2.1 and Theorem 2.2, we consider the thermal states of a quantum harmonic oscillator.

A. Possible optimal improvement

Recall that S is the subspace of $\mathcal{L}_2(\mathcal{H})$ spanned by $\{\hat{B}_{\rho,+}, \hat{B}_{\rho,-}\}$ and P_S is the projection onto S. In the proof of Theorem 2.2, we have used the identity (3.14). The quantity $\|P_S A_\rho\|$ is the length of the projection of A_ρ onto S. Thus, it is clear that, in order to obtain the optimal improvement one has to find the vector X with $\|X\|_2 = \|A_\rho\|_2$ in the subspace $\tilde{S}$ spanned by $\{\hat{A}_{\rho,+}, \hat{A}_{\rho,-}\}$, which has the biggest component in S.

In order to find such a vector in $\tilde{S}$, put

$$X = \alpha A_\rho + \beta A_\rho^\perp,$$

where α and β are complex constants satisfying

$$|\alpha|^2 + |\beta|^2 = 1.$$

One has that

$$\|P_S X\|_2^2 = \alpha^2 \|P_S A_\rho\|_2^2 + \overline{\alpha}\beta\langle P_S A_\rho, P_S A_\rho^\perp\rangle + \alpha\overline{\beta}\langle P_S A_\rho^\perp, P_S A_\rho\rangle + |\beta|^2 \|P_S A_\rho^\perp\|_2^2.$$

One can choose α such that $\alpha \geqslant 0$. The first and last terms on the rhs of the above are non-negative. To make the other terms non-negative, we choose β as

$$\beta = \gamma\langle P_S A_\rho^\perp, P_S A_\rho\rangle / |\langle P_S A_\rho^\perp, P_S A_\rho\rangle|,$$

where $\gamma \geqslant 0$. We then have

$$\|P_S X\|_2^2 = \alpha^2 \|P_S A_\rho\|_2^2 + 2\alpha\gamma|\langle P_S A_\rho, P_S A_\rho^\perp\rangle| + \gamma^2 \|P_S A_\rho^\perp\|_2^2, \tag{4.1}$$

where α and γ are non-negative real numbers satisfying

$$\alpha^2 + \gamma^2 = 1. \tag{4.2}$$

Thus, the problem is to maximize (4.1) under the constraint (4.2). The problem can be solved by the method of the Lagrange multiplier.

We use the following notation:

$$a = \|P_S A_\rho\|_2^2,\ b = \|P_S A_\rho^\perp\|_2^2,\ c = |\langle P_S A_\rho, P_S A_\rho^\perp\rangle|. \tag{4.3}$$

Put

$$d = (a - b)/2c. \tag{4.4}$$

The method of the Lagrange multiplier implies that

$$a\alpha + c\gamma = \lambda\alpha,$$

$$b\gamma + c\alpha = \lambda\gamma,$$

where λ is the Lagrange multiplier. The above relations imply

$$\alpha^2 - 2d\alpha\gamma - \gamma^2 = 0. \tag{4.5}$$

Since $\alpha > 0$, one has that

$$\alpha = (d + \sqrt{d^2 + 1})\gamma. \tag{4.6}$$

From (4.2) and (4.6), α and γ can be solved explicitly. One may check that

$$\gamma^2 = 1/(1 + (d + \sqrt{d^2 + 1})^2) = 1/[2(d^2 + 1) + 2d\sqrt{d^2 + 1}]. \tag{4.7}$$

The relations (4.5) and (4.2) imply

$$\alpha\gamma = (1 - 2\gamma^2). \tag{4.8}$$

We substitute (4.7) and (4.8) into

$$\|P_S X\|_2^2 = a(1 - \gamma^2) + 2c\alpha\gamma + b\gamma^2$$

to obtain

$$\|P_S X\|_2^2 = a + c(\sqrt{d^2+1} - d) = a + \frac{1}{2}\{[(a-b)^2 + 4c^2]^{1/2} - (a-b)\}. \tag{4.9}$$

We leave that detailed derivation of (4.9) to the reader.

Let us denote by

$$m_3(A,B;\rho) := \frac{1}{2}\{[(a-b)^2 + 4c^2]^{1/2} - (a-b)\}, \tag{4.10}$$

where a, b, and c are given by (4.3). Put

$$M_3(A,B;\rho) := \|B\|_\rho^2 m_3(A,B;\rho). \tag{4.11}$$

We then obtain the following result.

Theorem 4.1: *The relation*

$$\frac{1}{4}|\langle [A,B]\rangle_\rho|^2 + \frac{1}{4}|\langle \{A,B\}\rangle_\rho|^2 + \tilde{M}(A,B;\rho) \leqslant \|A\|_\rho^2 \|B\|_\rho^2.$$

holds, where

$$\tilde{M}(A,B;\rho) = \max\left\{\sum_{k=1}^{3} M_k(A,B;\rho), \sum_{k=1}^{3} M_k(B,A;\rho)\right\},$$

and $M_1(A,B;\rho)$, $M_2(A,B;\rho)$ and $M_3(A,B;\rho)$ are given as in (2.3), (3.15), and (4.11), respectively.

Proof: It follows from (4.9) that

$$\|B\|_\rho^2 \|P_S A_\rho\|_2^2 + M_3(A,B;\rho) = \|B\|_\rho^2 \|P_S X\|_2^2 \leqslant \|B\|_\rho^2 \|X\|_2^2 = \|B\|_\rho^2 \|A\|_\rho^2. \tag{4.12}$$

We recall from the (3.14) and Lemma 3.3 that

$$\|B\|_\rho^2 \|P_S A_\rho\|_2^2 = |\langle B_\rho, A_\rho\rangle|^2 + M_1(A,B;\rho) + M_2(A,B;\rho). \tag{4.13}$$

Thus, the theorem follows from (4.12), (4.13), and (3.8) together with interchanging the role of A and B. □

Even if $M_3(A,B;\rho)$ can be expressed explicitly in terms of $\|A_{\rho,\pm}\|_2$, $\|B_{\rho,\pm}\|_2$, etc., the expression is complicated and so we do not present it here.

B. An Application

In $L^2(\mathbb{R})$, the momentum operator P and the position operator Q are represented by

$$P = i\frac{d}{dx}, \quad Q = x. \tag{4.14}$$

It is convenient to introduce the annihilation and creation operators that are defined as

$$a = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right), \quad a^* = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right).$$

Those operators satisfy the canonical commutation relations

$$[a,a^*] = 1, \quad [a,a] = [a,a^*] = 0, \tag{4.15}$$

and P and Q can be written as

$$P = \frac{i}{\sqrt{2}}(a - a^*), \quad Q = \frac{1}{\sqrt{2}}(a + a^*). \tag{4.16}$$

Let N be the number operator defined by

$$N = a^* a. \tag{4.17}$$

The Hamiltonian for quantum harmonic oscillator is given by

$$H = \frac{1}{2}(P^2 + Q^2) = N + \frac{1}{2}. \tag{4.18}$$

Let Ω be the ground state of H and let $\mathcal{F}_0$ be the dense subset consisting of finite linear combinations of vectors $\{(a^*)^n\Omega, n \in \mathbb{N}\}$. Then $\mathcal{F}_0$ is a common core for a, a^*, and N. For the details, we refer to Sec. 5.2 of Ref. 13.

The density operator ρ corresponding to the thermal state is given by

$$\rho = \frac{1}{Z}\exp(-\beta H) = \frac{1}{Z}\exp\left(-\beta\left(N + \frac{1}{2}\right)\right), \tag{4.19}$$

where $Z = \mathrm{tr}(\exp(-\beta H))$ and $\beta > 0$ the inverse of the temperature.

Theorem 4.2: *Let $A = P$ and $B = Q$ and let ρ be given by (4.19). Then the properties in Assumption 2.1 hold (with $D = \mathcal{F}_0$). Moreover each side of (2.1) and (2.2) equals* $\cosh^2(\beta/2))/4\sinh^2(\beta/2)$, *and so the equalities in the uncertainty relations in Theorem 2.1 and Theorem 2.2 hold.*

Proof: Let $a_k^{\#}$, $k = 1, 2, \ldots, n$, be either a^* or else a. It can be checked that

$$\left\| \prod_{k=1}^{n} a_k^{\#} \varphi \right\| \leqslant \|(N + n + 1)^{n/2}\varphi\|,$$

for any $\varphi \in \mathcal{F}_0$.[13] Thus $(\Pi_{k=1}^n a_k^{\#})(N+n+1)^{-n/2}$ is bounded operator for each n. Thus the properties (a) and (b) in Assumption 2.1 hold.

Notice that the equalities

$$a(N + 1) = (N + 2)a, \quad a^*(N + 2) = (N + 1)a^*,$$

hold on $\mathcal{F}_0$. The above equalities imply

$$(N + 2)^{-1}a = a(N + 1)^{-1}, \quad (N + 1)^{-1}a^* = a^*(N + 2)^{-1}.$$

Using the above relations repeatedly, one can check that property (c) in Assumption 2.1 holds. We leave the details to the reader.

Next, we compute each side of (2.1) and (2.2). A direct computation shows that

$$\langle a^* a\rangle_\rho = e^{-\beta}/(1 - e^{-\beta}). \tag{4.20}$$

It follows from (4.20) and the canonical commutation relations (4.15) that

$$\|Q\|_\rho^2 = \frac{1}{2}\mathrm{tr}((a + a^*)(a + a^*)\rho) = \frac{1}{2} + e^{-\beta}/(1 - e^{-\beta}) = \frac{1}{2}\cosh(\beta/2)/\sinh(\beta/2). \tag{4.21}$$

The method used in the above gives

$$\|P\|_\rho^2 = \frac{1}{2}\cosh(\beta/2)/\sinh(\beta/2). \tag{4.22}$$

It can be checked that

$$\rho^{1/2}a = e^{\beta/2}a\rho^{1/2}, \quad \rho^{1/2}a^* = e^{-\beta/2}a^*\rho^{1/2}. \tag{4.23}$$

We use (4.23) to obtain

$$\begin{aligned}\mathrm{tr}(Q\rho^{1/2}Q\rho^{1/2}) &= \frac{1}{2}\mathrm{tr}((a+a^*)(e^{\beta/2}a + e^{-\beta/2}a^*)\rho) = \frac{1}{2}\mathrm{tr}(e^{-\beta/2}aa^* + e^{\beta/2}a^*a) \\ &= \frac{1}{2}\{e^{-\beta/2} + (e^{\beta/2} + e^{-\beta/2})e^{-\beta}/(1-e^{-\beta})\} = 1/2\,\sinh(\beta/2),\end{aligned} \tag{4.24}$$

$$\mathrm{tr}(P\rho^{1/2}P\rho^{1/2}) = 1/2\,\sinh(\beta/2). \tag{4.25}$$

A direct computation yields

$$\langle\{P,Q\}\rangle_\rho = 0, \quad \mathrm{tr}(P\rho^{1/2}Q\rho^{1/2}) = 0. \tag{4.26}$$

Thus (4.21) and (4.22) imply

$$\|P\|_\rho^2\|Q\|_\rho^2 = \cosh^2(\beta/2)/4\,\sinh^2(\beta/2). \tag{4.27}$$

Since $[P,Q]=i$, (4.24) and (4.25) imply that

$$\text{lhs of (2.1)} = \frac{1}{4} + \frac{1}{4\,\sinh^2(\beta/2)} = \cosh^2(\beta/2)/4\,\sinh^2(\beta/2). \tag{4.28}$$

Next, we compute the lhs of (2.2). We use (4.21) and (4.24) to obtain

$$\begin{aligned}\|Q\|_\rho^4 - (\mathrm{tr}(Q\rho^{1/2}Q\rho^{1/2}))^2 &= \frac{1}{4}\left\{\frac{\cosh^2(\beta/2)}{\sinh^2(\beta/2)} - \frac{1}{\sinh^2(\beta/2)}\right\}, \\ &= \frac{1}{4},\end{aligned}$$

and so

$$M_1(P,Q;\rho) = (\mathrm{tr}(Q\rho^{1/2}Q\rho^{1/2}))^2 = 1/4\,\sinh^2(\beta/2).$$

Thus, we conclude that

$$\text{lhs of (2.2)} = \cosh^2(\beta/2)/4\,\sinh^2(\beta/2). \tag{4.29}$$

Combining (4.27)–(4.29), we complete the proof of Theorem 4.2. □

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Construction of the dual family of Gazeau–Klauder coherent states via temporally stable nonlinear coherent states

R. Roknizadeh[a] and M. K. Tavassoly[b]
Quantum Optics Group, Physics Department, University of Isfahan, Isfahan, Iran

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Using the *analytic representation* of the so-called Gazeau–Klauder coherent states (CSs), we shall demonstrate that how a new class of generalized CSs, namely the *family of dual states* associated with theses states, can be constructed through viewing these states as *temporally stable nonlinear CSs*. Also we find that the ladder operators, as well as the displacement type operator corresponding to these two pairs of generalized CSs, may be easily obtained using our formalism, without employing the *supersymmetric quantum mechanics* (SUSYQM) techniques. Then, we have applied this method to some physical systems with known spectrum, such as Pöschl–Teller, infinite well, Morse potential and hydrogenlike spectrum as some quantum mechanical systems. Finally, we propose the generalized form of the Gazeau–Klauder CS and the corresponding dual family. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1861276]

I. INTRODUCTION

Coherent states (CSs) play an important role in various fields of physics, quantum technologies and especially in quantum optics (see, for instance, Refs. 1–4). Therefore efforts along generalizations and applications have been appreciably increased in recent years.[5] Recently, Gazeau and Klauder have introduced an important class of generalized CSs, the so-called "*Gazeau–Klauder CSs*" have been denoted by $|J,\gamma\rangle$, corresponding to any arbitrary quantum mechanical system.[6,7] Keeping in mind that Gazeau–Klauder CSs are really CSs, we will refer to them as "*GK states*." These states have attracted much attention in literature (see, e.g., Refs. 8–13). More recently, along generalization of GK states, the vector CSs of the GK type have been constructed and some physical applications of them have been addressed.[14]

In another direction, a new way of generalization has been proposed to construct the so-called *family of the dual states* corresponding to some particular known classes of CSs such as nonlinear CSs.[15,16] In an extended framework we have recently studied this idea, rederived basically and well developed.[16] The construction of the dual pairs may be actually performed for all classes of generalized CSs, obtained by each of the three ways of generalizations; i.e., *algebraic*, *symmetric*, and *dynamics*. We have found that the canonical CSs are the only *self-dual* family (a useful check point for our future construction in this paper). Also we have already established the dual states associated with KPS,[17] PS,[18] and SU (1,1) group CSs successfully, of course, after demonstrating the nonlinearity nature of these states.[8] Unfortunately, as we have stated in earlier works, employing either our previous approaches in Ref. 16 or the formalism proposed in Ref. 15 for constructing the dual of GK state, do not lead to full consistent CSs with the Gazeau–Klauder criteria. For instance according to the proposition in Ref. 16 the $\hat{T}^{-1}$ operator, whose action on canonical CS

[a]Electronic mail: rokni@sci.ui.ac.ir
[b]Electronic mail: mk.tavassoly@sci.ui.ac.ir

yields $|J,\gamma\rangle$ may be obtained trivially. But when one acts the related $\hat{T}$-operator on the standard CS, the output state which was expected to be of the GK type (in fact the dual set of GK states), encounters some difficulties. For example, apart from the ill-definition of the $\hat{T}$ (and so $\hat{T}^{-1}$) operator, the obtained states do not fulfill *temporal stability*. Consequently, the important property of the GK states, *the action identity* evolves some problems. Therefore one must try some *radically different method* from the previous ones.

This paper is organized as follows: first, after imposing a *second modification* on the *modified* GK states $|z,\alpha\rangle$ (*to be distinguished from "GK states," by abuse of notation we shall call them as GKCSs*) introduced by El Kinani and Daoud,[11] we shall clarify the nonlinearity of these states. Second, in view of establishing the GKCS as an extension of "*KPS nonlinear CS*"[17] to "*temporally stable CS*," together with the fact that the dual family of KPS nonlinear CS has already been introduced appropriately, we attempt to find the dual of GKCS (we shall refer to it as DGKCS) through generalization of "the dual of KPS nonlinear CS" to state that it possesses the "*temporal stability*" characteristic. Upon generalizing this result, we shall introduce the $\hat{S}(\alpha)$-operator ($\alpha \in \mathbb{R}$) which transfers any generalized nonlinear CS, corresponding to a Hamiltonian with known spectrum (which does not preserve temporal stability) to a situation in which it nicely restores this property.

Additionally, a set of new interesting results such as the explicit form of annihilation, creation, and displacement type operators corresponding to each of the two generalized CSs (GKCSs and DGKCSs) will be obtained. Also, by using the dual family of GKCS, the even, odd, and Schrödinger cat CSs have been introduced. We then apply the method to some well-known solvable systems, i.e., harmonic oscillator, Pöschl–Teller, infinite well and Morse potential and hydrogenlike spectrum as some examples of quantum mechanical systems. Finally, we outline a scheme for *generalization of the GKCSs* as well as *DGKCSs*.

II. ANALYTICAL REPRESENTATIONS OF GAZEAU–KLAUDER CS AS NONLINEAR CS

In this section, we first revisit the analytical representations of GKCSs and then impose a second modification on them. At last, we establish their nonlinearity nature.

A. Analytical representations of GK states

The GK states, $|J,\gamma\rangle$, corresponding to any Hamiltonian with discrete (nondegenerate) eigenvalues $e_n \geqslant 0$, are defined as[6,7,19]

$$|J,\gamma\rangle \doteq \mathcal{N}(J)^{-1/2}\sum_{n=0}^{\infty}\frac{J^{n/2}e^{-i\gamma e_n}}{\sqrt{\rho(n)}}|n\rangle, \quad J \geqslant 0, \quad -\infty < \gamma < \infty, \tag{1}$$

where $\mathcal{N}$ is a normalization constant may be determined (for a new and interesting formalism related to degenerate Hamiltonian see Ref. 14). The orthonormal set $\{|n\rangle\}_{n=0}^{\infty}$ satisfy the eigenvalue equation

$$\hat{H}|n\rangle = E_n|n\rangle \equiv \hbar\omega e_n|n\rangle = e_n|n\rangle, \quad \hbar \equiv 1, \quad \omega \equiv 1. \tag{2}$$

The eigenvalues of the Hamiltonian $\hat{H}$ are such that

$$0 = e_0 < e_1 < e_2 < \cdots < e_n < e_{n+1} < \cdots . \tag{3}$$

These states should satisfy the following properties: (i) *continuity of labeling*, (ii) *resolution of the identity*, (iii) *temporal stability*, and (iv) *action identity*. The last two conditions require $\rho(n) = [e_n]!$.

Along the works on GK states, El Kinani and Daoud in a series of papers,[11–13] imposed a minor modification on these states via generalizing the Bargman representation for the standard harmonic oscillator.[20] The authors introduced the *analytical representations of GK states*, denoted by us as GKCSs,

$$|z,\alpha\rangle \doteq \mathcal{N}(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^n e^{-i\alpha e_n}}{\sqrt{\rho(n)}}|n\rangle, \quad z\in\mathbb{C}, \quad \alpha\in\mathbb{R}, \tag{4}$$

where the normalization constant and the function $\rho(n)$ are given by

$$\mathcal{N}(|z|^2)=\sum_{n=0}^{\infty}\frac{|z|^{2n}}{\rho(n)}, \quad \rho(n)=[e_n]!\,. \tag{5}$$

Briefly speaking, they replaced $-\infty<\gamma<\infty$ and $J>0$ in (1) by $\alpha\in\mathbb{R}$ and $z\in\mathbb{C}$, respectively. We must emphasize the main difference between the GKCSs presented in (4) and GK states in (1) in view of the significance and the role of γ and α, particularly in the integration procedure, in order to establish the resolution of unity. For this purpose, it is required to find an appropriate positive measure $\mathrm{d}\lambda(z)$ such that

$$\int_0^R |z,\alpha\rangle\langle z,\alpha|\mathrm{d}\lambda(z)=\sum_{n=0}^{\infty}|n\rangle\langle n|=\hat{I}, \quad 0<R\leqslant\infty. \tag{6}$$

Inserting (4) in (6), writing $z=xe^{i\theta}$ and expressing the measure as

$$\mathrm{d}\lambda(z)=\mathrm{d}\lambda(|z|^2)=\pi\mathcal{N}(x^2)\sigma(x^2)x\,\mathrm{d}x\,\mathrm{d}\theta, \tag{7}$$

performing the integration over $\theta\in[0,2\pi]$, the over-completeness relation (6) finally reduced to the following moment problem (see Ref. 17 and references therein)

$$\int_0^R x^n\sigma(x)\mathrm{d}x=\rho(n), \quad 0<R\leqslant\infty. \tag{8}$$

B. A discussion about the modification of GK states

As it is observed in the preceding section, in the modification imposed by El Kinani and Daoud on the GKCSs, the parameter α has been *implicitly* considered as a constant, whose presence in the exponential factor of the introduced CSs preserves the temporal stability requirement (it is not now an integration *variable*). Meanwhile, for the temporal stability of the states in (4) one reads

$$e^{-i\hat{H}t}|z,\alpha\rangle=|z,\alpha'\rangle, \quad \alpha'=\alpha+\omega t. \tag{9}$$

Upon a closer inspection, one can see that the latter relation is indeed inconsistent with the resolution of the identity. By this, we mean that when α is considered as a constant parameter, it really labels any over-complete set of GKCSs, $\{|z,\alpha\rangle\}$. But the time evolution operator in (9) maps the over-complete set of states $\{|z,\alpha\rangle\}$ to another over-complete set $\{|z,\alpha'\rangle\}$. These are two *distinct sets of CSs*, each of them labeled with a specific α, if one considers the El Kinani-Daoud formalism. But the temporal stability precisely means that under the chosen dynamics, the time evolution of a CS remains CS, *of the same family*. In this manner, the states introduced in (4) are not of the Gazeau–Klauder type, exactly.

To overcome this problem, we redefine the resolution of the identity as follows:

$$\lim_{\Gamma\to\infty}\frac{1}{2\Gamma}\int_{-\Gamma}^{\Gamma}\mathrm{d}\alpha\int_0^R |z,\alpha\rangle\langle z,\alpha|\mathrm{d}\lambda(z)=\sum_{n=0}^{\infty}|n\rangle\langle n|=\hat{I}, \quad 0<R\leqslant\infty. \tag{10}$$

We can simplify the left-hand side (LHS) of (10) which interestingly led us exactly to the LHS of (6). Indeed we have

$$\int_0^R |z,\alpha\rangle\langle z,\alpha| \mathrm{d}\lambda(z) = \lim_{\Gamma\to\infty} \frac{1}{2\Gamma} \int_{-\Gamma}^{\Gamma} \mathrm{d}\alpha \int_0^R |z,\alpha\rangle\langle z,\alpha| \mathrm{d}\lambda(z), \tag{11}$$

where $\mathrm{d}\lambda(z)$ is determined as in (7).

By this fact we want to conclude that both of the over-complete collection of states $\{|z,\alpha\rangle\}$ and $\{|z,\alpha'\rangle\}$, with *fixed* α and $\alpha' \equiv \alpha + \omega t$, belong to a large set of over-complete states with an arbitrary α,

$$\{|z,\alpha\rangle, z \in C, -\infty \leqslant \alpha \leqslant \infty\}. \tag{12}$$

Note that by replacing $\alpha \in R$ with $-\infty \leqslant \alpha \leqslant \infty$ in (12) we want to emphasize that the parameter α is relaxed from the constraint of being fixed. But we will encounter other difficulty, that is the *variability* of α destroys the well definition of the "*operator valued function*" $f(\alpha,\hat{n})$, which will be introduced later in (14), in addition to the deformed annihilation and creation operators $A = af(\alpha,\hat{n})$ and $A^\dagger = f^\dagger(\alpha,\hat{n})a^\dagger$. To overcome this difficulty we may bridge the gap between these two situations: variability and constancy of α. We define the set of operators $A = af(\alpha,\hat{n})$, $A^\dagger = f^\dagger(\alpha,\hat{n})a^\dagger$ and any other operator which explicitly depends on α, in each *sector* (*subspace*) $\mathfrak{H}_\alpha$, labeled by a specific α parameter, of the whole Hilbert space $\mathfrak{H}$ which contains all GKCSs $\{|z,\alpha\rangle\}$. Indeed, the whole Hilbert space foliates by each α (remember the continuity of α). Moreover, the action of the time evolution operator on any state on a specific sector, transfer it to another sector, both belong to a large Hilbert space. So, *when we deal with the operators that depend on the* α *parameter, it should necessarily be fixed, while this is not the case when we are dealing with the states*.

We notify here that taking α as a *constant* in somewhere and as a *variable* in another may be confused and seems to be problematic. However, it is similar to the case which one encounters in the contexts of general relativity and quantum field theory, where the covariant formulation of the theory is required. In these cases one considers in the whole space with the dimension n, the spacelike Cauchy hypersurface Σ is defined with the dimension $n-1$. Fixing α is similar to the so-called gauge fixing (e.g., a section in time). For instance by gauge fixing one may calculate the evolution of metric in solving the *Einstein equation* in general relativity or the commutation relation in quantum field theory. So in the present case, although the operators are typically true operators over the whole Hilbert space $\mathfrak{H}$, but the calculations and their commutation relations are done with a fixed α in the subspace $\mathfrak{H}_\alpha$.

C. The relation between nonlinear CS and GKCS

On the other hand, the notion of nonlinear CSs introduced in Refs. 21–23 has attracted much attention in the recent decade, especially in quantum optics. The realization of a special class of these states has been proposed in the quantized motion of a trapped ion in a Paul trap.[22,24] The nonlinear CS defined as eigenvector of the deformed annihilation operator has the following expansion over the Fock space:

$$|z\rangle_f = \mathcal{N}_f(|z|^2)^{-1/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n![f(n)]!}} |n\rangle, \quad [f(n)]! \doteq f(n)f(n-1)f(n-2)\cdots f(1), \tag{13}$$

where $f(0) \equiv 1$ and $\mathcal{N}_f$ in some appropriate normalization constant may be determined. We recall that by replacing $f(n)$ with $1/f(n)$ in the relation (13) one immediately gets the nonlinear CSs introduced in Ref. 15. We have called these states as the dual family of nonlinear CSs of Man'ko's type.[16]

Following the formalism given in Ref. 8 for the states expressed in (4) one may obtain

$$f_{\mathrm{GK}}(\alpha,\hat{n}) = e^{i\alpha(\hat{e}_n-\hat{e}_{n-1})}\sqrt{\frac{\rho(\hat{n})}{\hat{n}\rho(\hat{n}-1)}}, \quad \alpha, \quad \text{being fixed.} \tag{14}$$

where we have chosen the notation $\hat{e}_n \equiv \rho(\hat{n})/\rho(\hat{n}-1)$.

Moreover, we gain the opportunity to find raising and lowering operators in a safe manner

$$A_{\mathrm{GK}} = af_{\mathrm{GK}}(\alpha,\hat{n}), \quad A_{\mathrm{GK}}^{\dagger} = f_{\mathrm{GK}}^{\dagger}(\alpha,\hat{n})a^{\dagger}. \tag{15}$$

It is easy to verify that $A_{\mathrm{GK}}|z,\alpha\rangle = z|z,\alpha\rangle$. Obviously the commutation relation between these two (f-deformed) ladder operators obeys[23] the relation

$$\begin{aligned}[A_{\mathrm{GK}},A_{\mathrm{GK}}^{\dagger}] &= \frac{\rho(\hat{n}+1)}{\rho(\hat{n})} - \frac{\rho(\hat{n})}{\rho(\hat{n}-1)} \\ &= \hat{e}_{n+1} - \hat{e}_n. \end{aligned} \tag{16}$$

The special case $\rho(n)=n!$ recovers the standard bosonic commutation relation $[a,a^{\dagger}]=\hat{I}$. Using the "*normal-ordered*" form of the Hamiltonian as in Ref. 8 and taking $\hbar=1=\omega$, for the Hamiltonian of GKCSs we get

$$\hat{H}_{\mathrm{GK}} \equiv \hat{\mathcal{H}} = A_{\mathrm{GK}}^{\dagger}A_{\mathrm{GK}} = \hat{n}|f_{\mathrm{GK}}(\alpha,\hat{n})|^2 = \frac{\rho(\hat{n})}{\rho(\hat{n}-1)} = \hat{e}_n \tag{17}$$

which clearly shows that the dynamics of the system is independent of α.

III. THE DUAL FAMILY OF GKCS AS THE TEMPORALLY STABLE CS OF THE DUAL OF KPS CS

The KPS coherent states, introduced by Klauder, Penson, and Sixdeniers[17] have the following form:

$$|z\rangle_{\mathrm{KPS}} = \mathcal{N}_{\mathrm{KPS}}(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{\rho(n)}}|n\rangle, \quad z\in\mathbb{C}. \tag{18}$$

As demonstrated in Ref. 8, all of the various sets of CSs introduced in Ref. 17, constructed by diverse $\rho(n)$'s, are nonlinear CSs in nature. Also the appropriate nonlinearity function $f(n)$ as well as the deformed annihilation, creation, and Hamiltonian operators were introduced there. Especially, it is found that $\rho(n)$ in (18) must satisfy the relation $\rho(n)=[nf^2(n)]!=[e_n]!$, where e_n's are the eigenvalues of the associated factorized Hamiltonian. Taking into account the above results, comparing (18) with GKCS in (4) and keeping $\hbar$ and ω in the formulas, one may conclude that

$$e^{-i(\alpha/\hbar\omega)\hat{\mathcal{H}}}|z\rangle_{\mathrm{KPS}} = |z,\alpha\rangle, \quad 0\neq\alpha\in\mathbb{R}, \quad z\in\mathbb{C}. \tag{19}$$

While $|z\rangle_{\mathrm{KPS}}$ states are not temporally stable, $|z,\alpha\rangle$ states enjoy this property.

Now we may outline a relatively evident physical meaning to the arbitrary real α in (4) or (19) as $\alpha\equiv\omega t$, where by t we mean the time that the operator acts on the KPS coherent states. It should be mentioned that, in a sense this interpretation has been presented for the GKCSs in a compact form.[10] If so, then $|z,\alpha\rangle$ can be considered as the evolution of $|z\rangle_{\mathrm{KPS}}$. Therefore in a more general framework, we claim that the action of the evolution type operator

$$\hat{S}(\alpha) = e^{-i(\alpha/\hbar\omega)\hat{\mathcal{H}}}, \quad \hat{S}\hat{S}^{\dagger} = \hat{S}^{\dagger}\hat{S} = \hat{I}, \quad 0\neq\alpha\in\mathbb{R}, \tag{20}$$

on any nontemporally stable CSs, makes it temporally stable CSs. So, $\hat{S}(\alpha)$ *is a nice operator which transfers any generalized CS to a situation which it restores the temporal stability property*. Here, we stress the fact that in (20) the Hamiltonian, $\hat{\mathcal{H}}$, should satisfy $\hat{\mathcal{H}}|n\rangle=\hbar\omega e_n|n\rangle$.

At this point we are ready to find a suitable way to define the dual family of GKCS. First, we note that the dual family of KPS CSs introduced in (18) has already been established in Ref. 8, via the following exact form:

$$|\widetilde{z}\rangle_{\mathrm{KPS}} = \widetilde{\mathcal{N}}_{\mathrm{KPS}}(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{\mu(n)}}|n\rangle, \quad z \in \mathbb{C}, \tag{21}$$

where

$$\mu(n) \equiv \widetilde{\rho}(n) = \frac{(n\,!\,)^2}{\rho(n)}. \tag{22}$$

Hereafter, the sign "tilde" over the operators and states, assign them to the corresponding dual operators and states, respectively. For instance $\widetilde{\rho}(n)$ is dual correspondence of $\rho(n)$. Equation (22) expresses the relation between KPS and the associated dual CSs, in a simple way. Obviously $\mathcal{N}_{\mathrm{KPS}}$ and $\widetilde{\mathcal{N}}_{\mathrm{KPS}}$ in (18) and (21) are the normalization constants obtained. Employing the formalism led to (19), for "the dual of KPS states" in (21) naturally results in the following superposition of Fock states for the dual family of GKCSs (we shall refer to them as DGKCS):

$$\begin{aligned}\widetilde{\hat{S}}(\alpha)|\widetilde{z}\rangle_{\mathrm{KPS}} &= e^{-i(\alpha/\hbar\omega)\widetilde{\hat{H}}}|\widetilde{z}\rangle_{\mathrm{KPS}} \\ &= \widetilde{\mathcal{N}}(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^n e^{-i\alpha\varepsilon_n}}{\sqrt{\mu(n)}}|n\rangle = |\widetilde{z,\alpha}\rangle, \quad z \in \mathbb{C}, \quad 0 \neq \alpha \in \mathbb{R},\end{aligned} \tag{23}$$

where $\widetilde{\mathcal{N}}=\widetilde{\mathcal{N}}_{\mathrm{KPS}}$ [because of the unitarity of $\hat{S}(\alpha)$, which preserves the norm] is given by

$$\widetilde{\mathcal{N}}(|z|^2) = \sum_{n=0}^{\infty}\frac{|z|^{2n}}{\mu(n)}. \tag{24}$$

The special case of $\varepsilon_n=n$ in (23) recovers the canonical CSs, correctly. Note also that setting $\alpha=\omega t$ in (20) and (23) reduces the operators $\hat{S}(\alpha)$ and $\widetilde{\hat{S}}(\alpha)$ to the well-known *time evolution operators* $\mathcal{U}(t)$ and $\widetilde{\mathcal{U}}(t)$, respectively. The case $\alpha=0$ for the states in (4) and (23) recovers KPS and the corresponding dual CSs (which certainly are not temporally stable), respectively. The overlap between two states of the DGKCSs takes the following form:

$$\langle\widetilde{z,\alpha}|\widetilde{z',\alpha'}\rangle = \widetilde{\mathcal{N}}(|z|^2)^{-1/2}\widetilde{\mathcal{N}}(|z'|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{(z^*z')^n e^{-i\varepsilon_n(-\alpha+\alpha')}}{\mu(n)}, \tag{25}$$

which means that the states are essentially nonorthogonal.

It should be noticed that the produced states [$|\widetilde{z,\alpha}\rangle$ introduced in (23)] form a *new class of generalized CSs*, essentially different from $|z,\alpha\rangle$ in (4). Also, it is apparent that for our introduction of DGKCSs, we have obtained directly the analytic representation of DGKCS for any arbitrary quantum mechanical system. Using the formalism proposed in Ref. 8, one can deduce the nonlinearity function for the dual states in (23) as

$$\widetilde{f}_{\mathrm{GK}}(\alpha,\hat{n}) = e^{i\alpha(\hat{\varepsilon}_n-\hat{\varepsilon}_{n-1})}\sqrt{\frac{\mu(\hat{n})}{\hat{n}\mu(\hat{n}-1)}}, \quad \alpha \text{ being fixed}, \tag{26}$$

where we have used the notation $\hat{\varepsilon}_n \equiv \mu(\hat{n})/\mu(\hat{n}-1)$. Therefore, analogous to (17) the deformed annihilation and creation operators of the dual system may be expressed explicitly as

$$\widetilde{A}_{\mathrm{GK}} = a e^{i\alpha(\hat{\varepsilon}_n - \hat{\varepsilon}_{n-1})} \sqrt{\frac{\mu(\hat{n})}{\hat{n}\mu(\hat{n}-1)}}, \tag{27}$$

$$\widetilde{A}^{\dagger}_{\mathrm{GK}} = e^{-i\alpha(\hat{\varepsilon}_n - \hat{\varepsilon}_{n-1})} \sqrt{\frac{\mu(\hat{n})}{\hat{n}\mu(\hat{n}-1)}} a^{\dagger}. \tag{28}$$

The normal-ordered Hamiltonian of *dual oscillator* in the same manner stated in (17) is

$$\widetilde{\hat{\mathcal{H}}}_{\mathrm{GK}} \equiv \widetilde{\hat{\mathcal{H}}} = \widetilde{A}^{\dagger}_{\mathrm{GK}} \widetilde{A}_{\mathrm{GK}} = \frac{\mu(\hat{n})}{\mu(\hat{n}-1)} = \frac{\hat{n}^2}{\hat{e}_n}, \tag{29}$$

which is again independent of α. As a result

$$\widetilde{\hat{\mathcal{H}}}|n\rangle = \widetilde{\mathcal{E}}_n|n\rangle \equiv \hbar\omega\varepsilon_n|n\rangle = \varepsilon_n|n\rangle, \quad \varepsilon_n \equiv \widetilde{e}_n = \frac{n^2}{e_n}, \tag{30}$$

where again we have used the units $\omega = 1 = \hbar$. The first equation in (30) illustrates clearly the relation between the eigenvalues of the two mutual dual systems. Also, the DGKCSs are required to satisfy the following inequalities:

$$0 = \varepsilon_0 < \varepsilon_1 < \varepsilon_2 < \cdots < \varepsilon_n < \varepsilon_{n+1} < \cdots, \tag{31}$$

the same as that of e_n's in (3). At this point a question may have arisen: to what extent one may be sure that the DGKCSs in (23) are of the Gazeau–Klauder type? Let us briefly investigate this question.

(1) *Continuity of labeling*, it is clearly satisfied.
(2) *Resolution of unity*,

$$\int_0^{\widetilde{R}} |\widetilde{z,\alpha}\rangle\langle\widetilde{z,\alpha}| \mathrm{d}\lambda(z) = \sum_{n=0}^{\infty} |n\rangle\langle n| = \hat{I}, \quad 0 < \widetilde{R} \leqslant \infty, \tag{32}$$

where the measure $\mathrm{d}\lambda(z)$ is defined as in (7). The radius of convergence of DGKCS is determined as $\widetilde{R} = \lim_{n\to\infty} \sqrt[n]{\mu(n)}$ and $\mu(n)$ is defined as positive constants assumed to be appearing as moments of a probability distribution. Similar calculations that led to the result in (8) are needed to arrive at the new moment problem associated with the DGKCSs,

$$\mu(n) \equiv \widetilde{\rho}(n) = \int_0^{\widetilde{R}} x^n \widetilde{\sigma}(x) \mathrm{d}x, \quad 0 < \widetilde{R} \leqslant \infty, \tag{33}$$

which must be solved with the help of the previously mentioned techniques. As for the GKCSs, we assume that $\mu(0) = 1$ and $\mu(n) < \infty$ for all n.
(3) *Temporal stability*, using (23) and the relevant Hamiltonian (30) gives us

$$\begin{aligned} e^{-i\widetilde{\hat{\mathcal{H}}}t}|\widetilde{z,\alpha}\rangle &= \widetilde{\mathcal{N}}(|z|^2)^{-1/2} \sum_{n=0}^{\infty} \frac{z^n e^{-i\varepsilon_n(\alpha+\omega t)}}{\sqrt{\mu(n)}} |n\rangle \\ &= |z, \widetilde{\alpha+\omega t}\rangle, \end{aligned} \tag{34}$$

which illustrates that DGKCSs remain coherent, as time goes on.
(4) *Action identity:* from the condition (iii) we find that the time evolution of a CS is a map given by $(z,\alpha) \mapsto (z, \alpha+\omega t)$. The new states $|\widetilde{z,\alpha}\rangle$ satisfy the relation

$$\langle\widetilde{z,\alpha}|\widetilde{\hat{\mathcal{H}}}|\widetilde{z,\alpha}\rangle = \omega|z|^2, \tag{35}$$

in consistence with Gazeau–Klauder's criteria, which is the so-called action identity. This is a strong requirement which uniquely specifies the weights $\{\mu(n)\}_{n\geqslant 0}$ in the denominator of the expansion coefficients of the DGKCS. Using (23), (24), and (30) on the LHS of (35) we obtain

$$\sum_{n=0}^{\infty}\frac{\varepsilon_n|z|^{2n}}{\mu(n)} = |z|^2\sum_{n=0}^{\infty}\frac{|z|^{2n}}{\mu(n)}, \tag{36}$$

by which we arrive at the following condition;

$$\varepsilon_n = \frac{\mu(n)}{\mu(n-1)}. \tag{37}$$

By conventional choice of $\mu(0)\equiv 1$, we thus deduce

$$\mu(n) = \varepsilon_n\varepsilon_{n-1}\cdots\varepsilon_1 = \Pi_{k=1}^{n}\varepsilon_k \equiv [\varepsilon_n]\,!\,. \tag{38}$$

So, we have established that the DGKCSs in (23) are exactly of the Gazeau–Klauder type. It should be noted that the same arguments we presented in Sec. II B about the resolution of the identity (and the integration procedures), the α parameter (the states and the operators which depend on it) and the corresponding Hilbert spaces must also be considered for the DGKCSs have been built in the present section.

A. The introduction of temporally stable nonlinear CS

Let us now outline the main idea in a general framework. It is believed that the property of the temporal stability is intrinsic to the *harmonic oscillator* and the systems which are *unitarily equivalent* to it.[25] But in what follows we shall demonstrate how this important property can be restored by a redefinition of any generalized CSs which can be classified in the nonlinear CSs category. Recall that the nonlinear CSs we introduced in (13) do not generally have the temporal stability property.[23] So, by considering the results obtained in the previous work[8] and the above explanations, we want to proceed and introduce generally the notion of "*temporally stable nonlinear CSs*" as

$$|z,\alpha\rangle_f = \mathcal{N}_f(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^n e^{-i\alpha e_n}}{\sqrt{n!}[f(n)]!}|n\rangle, \quad e_n = nf^2(n), \quad 0\neq\alpha\in\mathbb{R}, \quad z\in\mathbb{C}. \tag{39}$$

We can also define the dual of the latter states by the following expression:

$$|\widetilde{z,\alpha}\rangle_f = \widetilde{\mathcal{N}}_f(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^n[f(n)]\,!\,e^{-i\alpha\varepsilon_n}}{\sqrt{n!}}|n\rangle, \quad \varepsilon_n = \frac{n}{f^2(n)}, \quad 0\neq\alpha\in\mathbb{R}, \quad z\in\mathbb{C}, \tag{40}$$

which are indeed the temporally stable version of the nonlinear CSs that have been introduced in Ref. 15. In both sets of the CSs given by (39) and (40), α is a real constant and the normalization factors are independent of α. Setting $\alpha=0$ in (39) and (40), we recover the old form of Man'ko's and Roy's nonlinear CSs, respectively, which clearly are not temporally stable.

B. Temporally stable CS of SU (1,1) group

An instructive example of the families of nonlinear CSs is provided by the Gilmore–Perelomov (GP)[26] and Barut–Girardello (BG) CSs[27], defined for the discrete series representations of the group SU (1,1). Using the results of Ref. 8 for GP states, and then imposing the proposed

formalism on them, the "*temporally stable CSs of GP type associated with SU* (1,1) *group*" can be defined as

$$|z,\alpha\rangle_{\mathrm{GP}}^{\mathrm{SU}(1,1)}=\mathcal{N}_{\mathrm{GP}}(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^n e^{-i\alpha[n/(n+2\kappa-1)]}}{[n\,!\,/\Gamma(n+2\kappa)]^{1/2}}|n\rangle,\quad |z|<1, \tag{41}$$

where $\mathcal{N}_{\mathrm{GP}}$ is a normalization factor and the parameter $\kappa=1,3/2,2,5/2,\ldots$, labels the SU (1,1) representation being used. Analogously, applying the presented extension to the BG type of CSs, gives immediately "*temporally stable CSs of BG type associated with SU* (1,1) *group*" as follows:

$$|z,\alpha\rangle_{\mathrm{BG}}^{\mathrm{SU}(1,1)}\equiv|\widetilde{z,\alpha}\rangle_{\mathrm{GP}}^{\mathrm{SU}(1,1)}=\mathcal{N}_{\mathrm{BG}}(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^n e^{-i\alpha n(n+2\kappa-1)}}{[n\,!\,\Gamma(n+2\kappa)]^{1/2}}|n\rangle,\quad z\in\mathbb{C}, \tag{42}$$

where once more, $\mathcal{N}_{\mathrm{BG}}$ is chosen by normalization of the states.

C. Temporally stable CS of Penson–Solomon type and its dual

As established in Ref. 8, the generalized CSs introduced by Penson and Solomon[18] as

$$|q,z\rangle=\mathcal{N}(q,|z|^2)\sum_{n=0}^{\infty}\frac{q^{n(n-1)/2}}{\sqrt{n!}}z^n|n\rangle, \tag{43}$$

are also nonlinear with $f(n)=q^{(1-n)}$ and therefore the factorized Hamiltonian reads $\hat{\mathcal{H}}_{\mathrm{PS}}=\hat{n}q^{2(1-\hat{n})}$. It is stated in Ref. 18 that under the action of $\exp(-i\hat{H}t)$ these states are temporally stable, where the Hamiltonian $\hat{H}=a^{\dagger}a=\hat{n}$ expresses the (shifted) quantum harmonic oscillator with the corresponding canonical CS. Seemingly to verify the invariance under time evolution operator, it may be more realistic to act the operator, $\exp(-i\hat{\mathcal{H}}_{\mathrm{PS}}t)$, on the PS states in (43), where $\hat{\mathcal{H}}_{\mathrm{PS}}|n\rangle=\hat{n}q^{2(1-\hat{n})}|n\rangle=nq^{2(1-n)}|n\rangle$. Clearly by such proposition these states are not temporally stable. But the presented formalism in this paper allows one to construct the temporally stable CS of PS type as follows:

$$|q,z,\alpha\rangle\equiv e^{-i(\alpha/\hbar\omega)\hat{\mathcal{H}}_{\mathrm{PS}}}|q,z\rangle=\mathcal{N}_{\mathrm{PS}}(q,|z|^2)\sum_{n=0}^{\infty}\frac{q^{n(n-1)/2}}{\sqrt{n!}}e^{-i\alpha e_n}z^n|n\rangle, \tag{44}$$

where $e_n=nq^{2(1-n)}$.

We have already introduced the dual family of the PS states of Eq. (43) $\widetilde{|q,z\rangle}$ in Ref. 8. So the temporally stable dual of these states may also be obtained immediately as

$$\widetilde{|q,z,\alpha\rangle}\equiv e^{-i(\alpha/\hbar\omega)\tilde{\hat{\mathcal{H}}}_{\mathrm{PS}}}\widetilde{|q,z\rangle}=\tilde{\mathcal{N}}_{\mathrm{PS}}(q,|z|^2)\sum_{n=0}^{\infty}\frac{q^{-n(n-1)/2}}{\sqrt{n!}}e^{-i\alpha\varepsilon_n}z^n|n\rangle, \tag{45}$$

where $\varepsilon_n=n/q^{2(1-n)}$.

D. Some remarkable points

We end this section with some remarkable points.

(i) First, one can prove that the f-deformed annihilation operator given by (14) is just the same as the one derived earlier in Ref. 10, denoted by $a(\alpha)$,

$$a(\alpha)=e^{-i\alpha\hat{H}(\hat{n})/\hbar\omega}\breve{a}e^{i\alpha\hat{H}(\hat{n})/\hbar\omega}, \tag{46}$$

or in terms of the introduced evolution operator $\hat{S}(\alpha)$,

$$a(\alpha) = \hat{S}(\alpha)\check{a}\hat{S}^{\dagger}(\alpha). \tag{47}$$

It must be noticed that $\check{a}$ and its adjoint $\check{a}^{\dagger}$ in Eqs. (46) and (47) have been defined as follows:

$$\check{a}|n\rangle = \sqrt{e_n}|n-1\rangle, \quad \check{a}^{\dagger}|n\rangle = \sqrt{e_{n+1}}|n+1\rangle. \tag{48}$$

Now using the relations $f^{\dagger}(\hat{n})a = af^{\dagger}(\hat{n}-1)$ and $\hat{n}a = a(\hat{n}-1)$, we have

$$e^{-i\alpha\hat{H}(\hat{n})/\hbar\omega}\check{a} = \check{a}e^{-i\alpha\hat{H}(\hat{n}-1)/\hbar\omega} = \check{a}e^{-i\alpha\hat{e}_{n-1}}, \tag{49}$$

where we have used Eq. (2) in the last step. Upon replacing (49) on the right-hand side (RHS) of (46) and taking into account (2) we are readily led to the equality $a(\alpha) \equiv A_{\mathrm{GK}} = af_{\mathrm{GK}}(\alpha, \hat{n})$.

(ii) In light of the presented explanations the annihilation operator eigenstate (algebraic definition) for GKCSs and DGKCS are such that

$$A_{\mathrm{GK}}|z,\alpha\rangle = z|z,\alpha\rangle, \quad \widetilde{A}_{\mathrm{GK}}|\widetilde{z,\alpha}\rangle = z|\widetilde{z,\alpha}\rangle. \tag{50}$$

The deformed annihilation and creation operators $\widetilde{A}_{\mathrm{GK}}$ and $\widetilde{A}^{\dagger}_{\mathrm{GK}}$ of the dual oscillator algebra, satisfy the following eigenvector equations:

$$\widetilde{A}_{\mathrm{GK}}|n\rangle = \sqrt{\varepsilon_n}e^{i\alpha(\varepsilon_n-\varepsilon_{n-1})}|n-1\rangle, \tag{51}$$

$$\widetilde{A}^{\dagger}_{\mathrm{GK}}|n\rangle = \sqrt{\varepsilon_{n+1}}e^{i\alpha(\varepsilon_{n+1}-\varepsilon_n)}|n+1\rangle, \tag{52}$$

$$[\widetilde{A}_{\mathrm{GK}}, \widetilde{A}^{\dagger}_{\mathrm{GK}}]|n\rangle = (\varepsilon_{n+1}-\varepsilon_n)|n\rangle, \tag{53}$$

$$[\widetilde{A}_{\mathrm{GK}}, \hat{n}] = \widetilde{A}_{\mathrm{GK}}, \quad [\widetilde{A}^{\dagger}_{\mathrm{GK}}, \hat{n}] = -\widetilde{A}^{\dagger}_{\mathrm{GK}}. \tag{54}$$

Upon looking on the actions defined in (51) and (52) one can interpret $\widetilde{A}_{\mathrm{GK}}$ and $\widetilde{A}^{\dagger}_{\mathrm{GK}}$ as the operators which correctly annihilate and create one quanta of *deformed photon*, respectively. A closer look at the basis of the involved Hilbert space $\mathfrak{H}_{\alpha}$ in each over-complete set $\{|z,\alpha\rangle\}$, shows that it is spanned by the vectors

$$|n,\alpha\rangle = \frac{(\widetilde{A}^{\dagger}_{\mathrm{GK}})^n e^{i\alpha\varepsilon_n}}{\sqrt{[e_n]!}}|0\rangle \equiv |n\rangle, \quad \widetilde{A}_{\mathrm{GK}}|0\rangle = 0. \tag{55}$$

Moreover, we have omitted the α parameter from the basis for simplicity. At last, we are able to introduce the generators of the deformed oscillator algebra[28] of Gazeau–Klauder and the corresponding dual family as $\{A_{\mathrm{GK}}, A^{\dagger}_{\mathrm{GK}}, \hat{\mathcal{H}}\}$ and $\{\widetilde{A}_{\mathrm{GK}}, \widetilde{A}^{\dagger}_{\mathrm{GK}}, \widetilde{\hat{\mathcal{H}}}\}$, respectively.

(iii) One may expect that the inequalities for ε_n given in (31) corresponding to any solvable system do not hold for DGKCSs [the restriction which also exists in (3) for GKCSs]. This generally may be true, but fortunately many cases—if not all—such as all physical systems considered in this paper are of this sort (both of ε_n and e_n are strictly increasing). So it must be mentioned that before making use of our formalism for dual states associated with any set of GKCSs one should be sure about the condition (31). If both of the inequalities in (3) and (31) hold simultaneously, then one has

$$1 > \frac{e_n}{e_{n+1}} > \frac{n^2}{(n+1)^2} \tag{56}$$

which can be expressed in terms of the nonlinearity function $f_{\mathrm{GK}}(\alpha, \hat{n})$ as follows:

$$\sqrt{\frac{n+1}{n}} > \sqrt{\left|\frac{f_{\mathrm{GK}}(\alpha,\hat{n})}{f_{\mathrm{GK}}(\alpha,\hat{n}+1)}\right|^2} > \sqrt{\frac{n}{n+1}}, \tag{57}$$

for all $n>0$.

(iv) As it may be clear, when one wants to work with one of the dual pairs singly, they can be considered on their relevant domains. But to deal with their mutual relation, calculations must be done only in the intersection of the domains of the pair of CSs (in this case GKCSs and DGKCSs); i.e., generally on a unit disk, unless the CS is defined on a finite dimensional Hilbert space. As we shall see later, the latter is the case for Morse potential.

(v) Finally, the probability distribution for the DGKCSs is defined as

$$\widetilde{\mathbf{P}}(n) = |\langle n|\widetilde{z,\alpha}\rangle|^2 = \widetilde{\mathcal{N}}(|z|^2)^{-1}\frac{|z|^{2n}}{\mu(n)}, \tag{58}$$

which is independent of the α parameter.

We terminate this section with recalling that there exists also a set of equations such as (51)–(54) related to GKCSs which may be obtained just by replacing $\widetilde{A}_{\mathrm{GK}}$, $\widetilde{A}^{\dagger}_{\mathrm{GK}}$, and ε_n with A_{GK}, $A^{\dagger}_{\mathrm{GK}}$, and e_n, respectively. The latter have been already derived by applying SUSYQM techniques,[12] but rederivation of them are very easy by our formalism. According to their results, the one-dimensional SUSYQM provides a mathematical tool to define ladder operators for an exactly solvable potential. But the authors did not express the *explicit* form of the ladder operators, and only the concerning actions were expressed there. Therefore besides the simplicity of our method, it is more complete in the sense that as we found the *explicit* form of the raising and lowering operators in terms of the standard bosonic creation and annihilation operators and the photon number (intensity of the field) have been found easily [see Eqs. (15), (27), and (28)].

IV. DISPLACEMENT OPERATORS ASSOCIATED WITH GKCS AND THE CORRESPONDING DUAL FAMILY

Now that we introduced the explicit form of the deformed annihilation operator and hence the annihilation operator definition for GKCSs and DGKCSs according to Eqs. (50), we are in the position to extract the CSs of Klauder–Perelomov type for an arbitrary quantum mechanical system. For this purpose, we introduce the following auxiliary operators related to GKCSs:

$$B_{\mathrm{GK}} = a\frac{1}{f_{\mathrm{GK}}(-\alpha,\hat{n})}, \quad B^{\dagger}_{\mathrm{GK}} = \frac{1}{f^{\dagger}_{\mathrm{GK}}(-\alpha,\hat{n})}a^{\dagger}, \tag{59}$$

and those for the dual families DGKCSs,

$$\widetilde{B}_{\mathrm{GK}} = a\frac{1}{\widetilde{f}_{\mathrm{GK}}(-\alpha,\hat{n})}, \quad \widetilde{B}^{\dagger}_{\mathrm{GK}} = \frac{1}{\widetilde{f}^{\dagger}_{\mathrm{GK}}(-\alpha,\hat{n})}a^{\dagger}. \tag{60}$$

Notice that the minus sign in the argument of the f-function is needed in both cases, since only in such cases we have $f^{\dagger}_{\mathrm{GK}}(-\alpha,\hat{n}) = f_{\mathrm{GK}}(\alpha,\hat{n})$.

The f-deformed operators given by (59) and (60) are canonically conjugate of the f-deformed creation and annihilation operators $(A_{\mathrm{GK}},A^{\dagger}_{\mathrm{GK}})$ and $(\widetilde{A}_{\mathrm{GK}},\widetilde{A}^{\dagger}_{\mathrm{GK}})$, respectively; i.e., they satisfy the algebras $[A_{\mathrm{GK}},B^{\dagger}_{\mathrm{GK}}]=[B_{\mathrm{GK}},A^{\dagger}_{\mathrm{GK}}]=\hat{I}$ and $[\widetilde{A}_{\mathrm{GK}},\widetilde{B}^{\dagger}_{\mathrm{GK}}]=[\widetilde{B}_{\mathrm{GK}},\widetilde{A}^{\dagger}_{\mathrm{GK}}]=\hat{I}$, respectively. Now we have all mathematical tools to construct the displacement operators for GKCS,

$$D_{\mathrm{GK}}(z,\alpha) = \exp(zB^{\dagger}_{\mathrm{GK}} - z^{*}A_{\mathrm{GK}}), \tag{61}$$

and for DGKCS,

$$\widetilde{D}_{\mathrm{GK}}(z,\alpha)=\exp(z\widetilde{B}^{\dagger}_{\mathrm{GK}}-z^{*}\widetilde{A}_{\mathrm{GK}}). \tag{62}$$

The actions of $D_{\mathrm{GK}}(z,\alpha)$ and $\widetilde{D}_{GK}(z,\alpha)$ on the vacuum state $|0\rangle$ yield the GKCSs and DGKCS, up to some normalization constant, respectively, as we demand. From the group theoretical point of view, one can see that the sets $\{A_{\mathrm{GK}},B^{\dagger}_{\mathrm{GK}},B^{\dagger}_{\mathrm{GK}},A_{\mathrm{GK}},\hat{I}\}$ and $\{\widetilde{A}_{\mathrm{GK}},\widetilde{B}^{\dagger}_{\mathrm{GK}},\widetilde{B}^{\dagger}_{\mathrm{GK}}\widetilde{A}_{\mathrm{GK}},\hat{I}\}$, which are, respectively, associated with GKCSs and DGKCSs, form the Lie algebra h_4 and the corresponding Lie group is the well-known Weyl–Heisenberg (WH) group. Also, the action of the latter operators in (61) and (62) on the vacuum state are the orbits of the projective *nonunitary* representations of the WH group.[16] It must be understood that as we pointed out earlier, we have applied neither the formalism in Ref. 16 nor the equivalent formalism of Ref. 15 for constructing the dual states, since the states obtained from the earlier formalisms were not completely consistent with the Gazeau–Klauder criteria. Indeed, we proposed a way, through viewing the GKCSs $|z,\alpha\rangle$ and its dual pair $|\widetilde{z,\alpha}\rangle$ as generalization of KPS nonlinear CSs $|z\rangle_{\mathrm{KPS}}$ and its dual $|\tilde{z}\rangle_{\mathrm{KPS}}$ to the two distinct temporally stable CSs, respectively. Speaking otherwise, the operators introduced in (61) and (62) do not have the relation $\widetilde{D}_{\mathrm{GK}}(-z,\alpha)=D_{\mathrm{GK}}(z,\alpha)=[D_{\mathrm{GK}}(z,\alpha)^{-1}]^{\dagger}$, which is the characteristic of the earlier formalisms. To this end, it is possible to build the following displacement type operators, $V_{\mathrm{GK}}(z,\alpha)=\exp(zA^{\dagger}_{\mathrm{GK}}-z^{*}B_{\mathrm{GK}})$ for GKCSs, and in a similar manner, $\widetilde{V}_{\mathrm{GK}}(z,\alpha)=\exp(z\widetilde{A}^{\dagger}_{\mathrm{GK}}-z^{*}\widetilde{B}_{\mathrm{GK}})$ for DGKCSs, whose actions on the vacuum state yield two new sets of states. But it is easy to investigate that none of them can be classified in the Gazeau–Klauder CSs.

V. THE CONSTRUCTION OF EVEN, ODD AND SCHRÖDINGER CAT COHERENT STATES FROM THE INTRODUCED DGKCS

Various superpositions of CSs may result in different nonclassical states of light. Recently, there has been much interest in the construction as well as generation of these states, in the regard of their applications in the context of quantum optics. Their different characteristics are due to the various quantum interference between summands. As an example, the even and odd CSs associated with canonical CSs as well as other classes of generalized CSs such as nonlinear CSs extensively studied in the literature[29] exhibit nonclassical features, such as squeezing, sub-Poissonian statistics (antibunching), and oscillatory number distribution. The symmetric (antisymmetric) combinations of GKCSs have been introduced in Ref. 11. Similarly, using the unnormalized DGKCSs we are led to the even (odd) CSs denoted by + (−),

$$\begin{aligned}|\widetilde{z,\alpha}\rangle_{\pm}&=\widetilde{\mathcal{N}'}_{\pm}(|z|^2)^{-1/2}(|\widetilde{z,\alpha}\rangle\pm|\widetilde{-z,\alpha}\rangle)\\&=\widetilde{\mathcal{N}'}_{\pm}(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{e^{-i\alpha\varepsilon_n}[z^n\pm(-z)^n]}{\sqrt{\mu(n)}}|n\rangle,\end{aligned} \tag{63}$$

where $z\in\mathbb{C}$ and $\alpha\in\mathbb{R}$. For the normalization factors we get

$$\widetilde{N'}_{\pm}(|z|^2)=2\left(\sum_{n=0}^{\infty}\frac{|z|^{2n}}{\mu(n)}+\sum_{n=0}^{\infty}\frac{(-1)^n|z|^{2n}}{\mu(n)}\right)^{-1}. \tag{64}$$

A few simplifications imposed on the states in (63) will clarify the name even (odd) associated with these states

$$|\widetilde{z,\alpha}\rangle_{+}=\widetilde{\mathcal{N}'}_{+}(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^{2n}e^{-i\alpha\varepsilon_{2n}}}{\sqrt{\mu(2n)}}|2n\rangle, \tag{65}$$

$$|\widetilde{z,\alpha}\rangle_- = \widetilde{\mathcal{N}'}_-(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^{2n+1}e^{-i\alpha\varepsilon_{2n+1}}}{\sqrt{\mu(2n+1)}}|2n+1\rangle. \tag{66}$$

Finally the (±) states in (65) and (66) satisfy the following eigenvalue equations:

$$(\tilde{A}_{\mathrm{GK}})^2|\widetilde{z,\alpha}\rangle_\pm = z^2|\widetilde{z,\alpha}\rangle_\pm. \tag{67}$$

The probability distributions for the even-DGKCS (+) and odd-DGKCS (−) are derived as

$$\tilde{\mathbf{P}}_\pm(n) = |\langle n|\widetilde{z,\alpha}\rangle_\pm|^2 = \widetilde{\mathcal{N}'}_\pm(|z|^2)^{-1}\frac{|z|^{2n}}{\mu(n)}, \tag{68}$$

which clearly are independent of the α parameter.

Now, we pay attention to another specific superposition of the DGKCSs $|\widetilde{z,\alpha}\rangle$, by which we may obtain the *real* (+) and *imaginary* (−) *Schrödinger cat states as*

$$|\widetilde{z,\alpha}\rangle_\pm^{\mathrm{Cat}} = \widetilde{\mathcal{N}''}_\pm(|z|^2)^{-1/2}(|\widetilde{z,\alpha}\rangle \pm |\widetilde{z^*,\alpha}\rangle), \tag{69}$$

where z^* is the complex conjugate of z. Inserting $z=re^{i\theta}$ in the last equations give us the following explicit forms:

$$|\widetilde{z,\alpha}\rangle_+^{\mathrm{Cat}} = \widetilde{\mathcal{N}''}_+(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{r^n\cos(n\theta)}{\sqrt{\mu(n)}}e^{-i\alpha\varepsilon_n}|n\rangle \tag{70}$$

and

$$|\widetilde{z,\alpha}\rangle_-^{\mathrm{Cat}} = \widetilde{\mathcal{N}''}_-(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{r^{n+1}\sin[(n+1)\theta]}{\sqrt{\mu(n+1)}}e^{-i\alpha\varepsilon_{n+1}}|n+1\rangle, \tag{71}$$

where the normalization constants would be

$$\widetilde{\mathcal{N}''}_+(|z|^2) = \sum_{n=0}^{\infty}\frac{r^{2n}\cos^2(n\theta)}{\mu(n)} \tag{72}$$

and

$$\widetilde{\mathcal{N}''}_-(|z|^2) = \sum_{n=0}^{\infty}\frac{r^{2(n+1)}\sin^2[(n+1)\theta]}{\mu(n+1)}. \tag{73}$$

The probability distribution for the real (+) and imaginary (−) Schrödinger cat CSs in (70) and (71) can be calculated as

$$\tilde{\mathbf{P}}_\pm^{\mathrm{Cat}}(n) = |\langle n|\widetilde{z,\alpha}\rangle_\pm^{\mathrm{Cat}}|^2 = \widetilde{\mathcal{N}''}_\pm(r^2)^{-1}\frac{r^{2n}(1\pm\cos(2n\theta))}{\mu(n)}, \tag{74}$$

which are again independent of α.

VI. SOME PHYSICAL APPLICATIONS OF THE DGKCS

In order to illustrate the presented idea in this paper, let us apply the formalism on some physical examples which the associated GKCSs have already been known. To economize in the space the complete form of DGKCSs have not been given in what follows and it will be enough for our intention to present ε_n, $\mu(n)$, and $\tilde{\mathcal{N}}(|z|^2)$, since substituting these quantities into (23) gives readily the explicit form of the DGKCSs, $|\widetilde{z,\alpha}\rangle$.

Example 1, harmonic oscillator: As the simplest example we apply the formalism to the

harmonic oscillator Hamiltonian, whose nonlinearity function is equal to 1, hence $\varepsilon_n=n=e_n$ which results in the moments as $\mu(n)=n!=\rho(n)$. Note that we have considered a shifted Hamiltonian to lower the zero-point energy to zero ($e_0=0=\varepsilon_0$). Eventually

$$|\widetilde{z,\alpha}\rangle_{\mathrm{CCS}}=e^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{z^n e^{-i\alpha n}}{\sqrt{n!}}|n\rangle=|z,\alpha\rangle_{\mathrm{CCS}} \tag{75}$$

ensures the *self-duality* of canonical CS. For this example all the Gazeau–Klauder's requirements are satisfied, trivially.

Example 2, Pöschl–Teller potential: The interest in this potential and its CSs is due to various applications in many fields of physics particularly in atomic and molecular physics. The usual GKCSs for the Pöschl–Teller potential have been demonstrated nicely by Antoine *et al.*[10] Their obtained results are as follows:

$$e_n=n(n+\nu),\quad \rho(n)=\frac{n!\,\Gamma(n+\nu+1)}{\Gamma(\nu+1)},\quad \nu>2 \tag{76}$$

with the radius of convergence $R=\infty$. Consequently using the equations given by (76) in (22) and (30) we are able to construct DGKCSs associated with this particular potential by the new quantities obtained as

$$\varepsilon_n=\frac{n}{n+\nu},\quad \mu(n)=\frac{n!\,\Gamma(\nu+1)}{\Gamma(n+\nu+1)},\quad \nu>2 \tag{77}$$

and for the normalization constant we obtain from (24),

$$\widetilde{\mathcal{N}}(|z|^2)=(1-|z|^2)^{-1-\nu}, \tag{78}$$

whose region of convergence is determined as the open unit disk. The overlap between two of these states when $\alpha=\alpha'$ is obtained from (25) as

$$\langle\widetilde{z,\alpha}|\widetilde{z',\alpha}\rangle=[(1-|z|^2)(1-|z'|^2)]^{(1+\nu)/2}(1-zz')^{(-1-\nu)}. \tag{79}$$

For these dual states we only investigate the resolution of the identity; since the other three requirements are obviously satisfied. As required, we must find $\widetilde{\sigma}(x)$ such that the moment integral

$$\int_0^1 x^n\widetilde{\sigma}(x)\mathrm{d}x=\frac{n!\,\Gamma(\nu+1)}{\Gamma(n+\nu+1)} \tag{80}$$

holds. It may be checked that the proper weight function $\widetilde{\sigma}(x)$ is determined as $\nu(1-x)^{\nu-1}$.

At this point we recall that e_n's in (76) denotes the eigenvalues of different Hamiltonians. The characteristics of the dynamical system has been shown by the parameter ν. For instance, the eigenvalues of the anharmonic (nonlinear) oscillator, well studied in literature and the related GKCSs and GK states have been discussed in Refs. 11 and 30 in detail, respectively. In the current example the parameter ν is related to two other parameters, namely λ and κ through the relation $\nu=\lambda+\kappa$, which determine the height and the depth of the well potential. However, when one deals with the nonlinear oscillator it has another meaning; e.g., we refer to Ref. 30, in which the interest was due to its usefulness in the study of laser light propagation in a *nonlinear Kerr medium*. In particular, ν in this case is related to the nonlinear susceptibility of the medium. So, the obtained results in (77) and (78) can be exactly used for the anharmonic oscillator, too. To this end, we shall see in the next example that the case of $\nu=2$ in (76) is the eigenvalues of the infinite well potential.

Example 3, infinite well potential: The GKCSs for the infinite well, have been established by Antoine *et al.* in Ref. 10. The related quantities are

$$e_n = n(n+2), \quad \rho(n) = \frac{n!\,(n+2)!}{2}, \tag{81}$$

with radius of convergence as $R=\infty$. Consequently inserting (81) in (22) and (30) one can construct the dual of these states by the quantities

$$\varepsilon_n = \frac{n}{n+2}, \quad \mu(n) = \frac{2}{(n+1)(n+2)}, \tag{82}$$

and the normalization factor can be obtained from (24) as

$$\widetilde{\mathcal{N}}(|z|^2) = (1-|z|^2)^{-3}, \tag{83}$$

whose region of convergence is determined as the open unit disk. The overlap between two of these states for the special case $\alpha=\alpha'$ is obtained from (25) as

$$\langle \widetilde{z,\alpha} | \widetilde{z',\alpha} \rangle = [(1-|z|^2)(1-|z'|^2)]^{3/2} \frac{1}{1-zz'}. \tag{84}$$

To clarify the fact that these dual states are actually CSs, we only investigate the resolution of the identity, since the other three requirements are satisfied straightforwardly. For this condition we must find $\tilde{\sigma}(x)$ such that the integral

$$\int_0^1 x^n \tilde{\sigma}(x)\mathrm{d}x = \frac{2}{(n+1)(n+2)} \tag{85}$$

holds. It is easy to verify that $\tilde{\sigma}(x)=2(1-x)$ is the solution.

Example 4, Morse potential: The GKCSs for the Morse potential, which is the simplest type of anharmonic oscillator and is useful in various problems in different fields of physics (for example, spectroscopy, diatomic, and polyatomic molecule vibrations and scattering), can be obtained using the related quantities given in Ref. 9:

$$e_n = \frac{n(M+1-n)}{M+2}, \quad \rho(n) = \frac{\Gamma(n+1)\Gamma(M+1)}{(M+2)^n \Gamma(M+1-n)}, \tag{86}$$

where $n=0,1,2,\ldots<(M+1)$. Therefore taking into account (86) in (22) and (30) the dual of these states can be produced by the following quantities:

$$\varepsilon_n = \frac{n(M+2)}{M-n+1}, \quad \mu(n) = \frac{(M+2)^n \Gamma(n+1)\Gamma(M-n+1)}{\Gamma(M+1)}. \tag{87}$$

For the normalization factor in this case one obtains

$$\widetilde{\mathcal{N}}(|z|^2) = \left[1 + \frac{|z|^2}{2+M}\right]^M, \tag{88}$$

where again Eq. (24) has been used. Noticing that the series led to $\widetilde{\mathcal{N}}(|z|^2)$ in (88) is finite, it is readily found that it is absolutely convergent. i.e., $x=\sqrt{|z|^2}\geqslant 0$, $z\in\mathbb{C}$. For evaluating the overlap between two of these states, when $\alpha=\alpha'$, the formula (25) is not useful and one must calculate especially the overlap between the Morse states for themselves, because of the upper bound of the summation

$$\langle \widetilde{z,\alpha}|\widetilde{z',\alpha}\rangle = \widetilde{\mathcal{N}}(|z|^2)^{-1/2}\widetilde{\mathcal{N}}(|z'|^2)^{-1/2}\sum_{n=0}^{M+1}\frac{(z^*z')^n}{\mu(n)}$$
$$= \left[\left(1+\frac{|z|^2}{2+M}\right)\left(1+\frac{|z'|^2}{2+M}\right)\right]^{-M/2}\left[\frac{2+M+zz'}{2+M}\right]^M. \tag{89}$$

We need only to verify the resolution of the identity. As before, we must find a function $\tilde{\sigma}(x)$ such that

$$\int_0^\infty x^n\tilde{\sigma}(x)\mathrm{d}x = \frac{(M+2)^n\Gamma(n+1)\Gamma(M-n+1)}{\Gamma(M+1)}. \tag{90}$$

Using the definition of Meijer's G-function and the inverse Mellin theorem, it follows that[31]

$$\int_0^\infty \mathrm{d}x\, x^{s-1}G_{p,q}^{m,n}\left(\alpha x\middle|\begin{matrix}a_1, & \ldots, & a_n, & a_{n+1}, & \ldots, & a_p\\ b_1, & \ldots, & b_m, & b_{m+1}, & \ldots, & b_q\end{matrix}\right)$$
$$= \frac{1}{\alpha^s}\frac{\Pi_{j=1}^m\Gamma(b_j+s)\Pi_{j=1}^n\Gamma(1-a_j-s)}{\Pi_{j=n+1}^p\Gamma(a_j+s)\Pi_{j=m+1}^q\Gamma(1-b_j-s)}. \tag{91}$$

Comparing (90) and (91), one can find the function $\tilde{\sigma}(x)$ needed in (90), in terms of the Meijer's G-function by the expression

$$\tilde{\sigma}(x) = (M+2)\Gamma(M+1)G_{0,0}^{1,1}\left(x(M+2)^{-1}\middle|\begin{matrix}-(M+1), & .\\ 0, & .\end{matrix}\right). \tag{92}$$

Example 5, hydrogenlike spectrum: As the final physical example, we choose the hydrogenlike spectrum where the corresponding CS has been a long-standing subject and discussed frequently in the literature. For instance in Refs. 6 and 32 the one-dimensional model of such a system with the Hamiltonian $\hat{H}=-\omega/(\hat{n}+1)^2$ and the eigenvalues $E_n=-\omega/(n+1)^2$ has been considered ($\omega=me^4/2$, and $n=0,1,2,\ldots$). But to be consistent with the GKCSs, as it has been done in Ref. 32, the energy levels should be shifted by a constant amount, such that after taking $\omega=1$ one has the eigenvalues e_n and therefore the functions $\rho(n)$ as follows:

$$e_n = 1-\frac{1}{(n+1)^2}, \quad \rho(n) = \frac{(n+2)}{2(n+1)} \tag{93}$$

with unit disk centered at the origin as the region of convergence, i.e., $R=1$. Therefore the related dual family of GKCSs for a bound state portion of the hydrogenlike atom can be constructed. For this purpose, we take into account (93) in (22) and (30), so the corresponding quantities for the DGKCSs can be easily obtained as

$$\varepsilon_n = \frac{n(n+1)^2}{n+2}, \quad \mu(n) = \frac{2n!\,(n+1)!}{n+2}. \tag{94}$$

In this case $\widetilde{R}=\infty$ as the radius of convergence. For the normalization factor, using Eq. (24) obtains

$$\widetilde{\mathcal{N}}(|z|^2) = \frac{1}{2\sqrt{|z|^2}}[2I_1(2\sqrt{|z|^2}) + \sqrt{|z|^2}I_2(2\sqrt{|z|^2})], \tag{95}$$

where $I_\nu(z)$ is the modified Bessel function of the first kind. Similar to the preceding examples, we only verify the resolution of the identity. In the present case we must find a function $\tilde{\sigma}(x)$ such that

$$\int_0^\infty x^n \tilde{\sigma}(x)\mathrm{d}x = 2\frac{n\,!\,(n+1)!}{n+2}. \tag{96}$$

The integral in (91) is again helpful, if we rewrite the RHS of (96) as $2n![(n+1)!]^2/(n+2)!$. The suitable measure is then found to be

$$\tilde{\sigma}(x) = G^{3,1}_{0,0}\left(x \left| \begin{matrix} 0,\ 1,\ 1,\ . \\ \qquad 2,\ . \end{matrix} \right.\right). \tag{97}$$

The overlap between these states for the special case $\alpha=\alpha'$ is obtained from (25) in the closed form

$$\langle\widetilde{z,\alpha}|\widetilde{z',\alpha}\rangle = \tilde{\mathcal{N}}(|z|^2)^{-1/2}\tilde{\mathcal{N}}(|z'|^2)^{-1/2}\frac{1}{2\sqrt{z^* z'}}(2I_1(2\sqrt{z^* z'}) + \sqrt{z^* z'}I_2(2\sqrt{z^* z'})), \tag{98}$$

where $\tilde{\mathcal{N}}(|z|^2)$ and $\tilde{\mathcal{N}}(|z'|^2)$ are determined by Eq. (95).

VII. INTRODUCING THE GENERALIZED GKCS AND THE ASSOCIATED DUAL FAMILY

In light of the above explanations we are now in a position to propose the generalized GKCSs, by which we may recover the GKCSs given by Eq. (4) (also the associated dual family, DGKCSs) and the nonlinear CSs given by Eq. (13) as some special cases. In the following scheme, the physical meaning of the α parameter which enters in the GKCS and DGKCS will be more clear, the case we have already mentioned [in the explanations after Eq. (19)] as $\alpha=\omega t$.

A. Time evolved CSs as the generalized GKCSs

Consider the Hamiltonian $\hat{H}$ whose eigenvectors and eigenvalues are $|\phi_n\rangle$ and e_n, respectively, such that

$$\hat{H} = \omega\sum_{n=0}^{\infty} e_n|\phi_n\rangle\langle\phi_n|, \quad \text{where} \quad \hat{H}|\phi_n\rangle = \omega e_n|\phi_n\rangle, \tag{99}$$

where ω is a constant with the dimension of energy (taking $\hbar=1$). Let $\mathfrak{H}$ be a separable, infinite dimensional and complex Hilbert space spanned by orthonormal set $\{|\phi_n\rangle\}_{n=0}^{\infty}$. Also suppose $0=e_0<e_1<e_2<\cdots<e_n<e_{n+1}<\cdots$, be such that the sum $\Sigma_{n=0}^{\infty}(x^n/[e_n]!)$ converges in some interval $0<x\leqslant L$. For $z\in\mathbb{C}$, such that $|z|^2<L\leqslant\infty$, we define the generalized CSs as follows:

$$|z\rangle \doteq \mathcal{N}(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{[e_n]!}}|\phi_n\rangle, \tag{100}$$

where $\mathcal{N}(|z|^2)$ is a normalization factor. As it is clear, these states known as nonlinear CSs, with the nonlinearity function $f(n)=\sqrt{e_n/n}$. Setting $z=re^{i\theta}$ with $r=J^{1/2}$, it is reasonable to write $|z\rangle \equiv |J,\theta\rangle$. Now if $\mathrm{d}\nu$ be a measure which solves the moment problem

$$\int_0^L J^n\,\mathrm{d}\nu(J) = [e_n]\,!\,, \quad \int_0^L \mathrm{d}\nu(J) = 1, \tag{101}$$

then these CSs satisfy the resolution of the identity

$$\int_0^L\left[\int_0^{2\pi}|J,\theta\rangle\langle J,\theta|\mathcal{N}(J)\frac{\mathrm{d}\theta}{2\pi}\right]\mathrm{d}\nu(J) = I_{\mathfrak{H}}. \tag{102}$$

The CSs in (100) evolve with time in the manner

$$|z,t\rangle = e^{-i\hat{H}t}|z\rangle = \mathcal{N}(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^n e^{-i\omega e_n t}}{\sqrt{[e_n]!}}|\phi_n\rangle, \tag{103}$$

or equivalently in terms of the new variables J and θ,

$$|J,\theta,t\rangle = e^{-i\hat{H}t}|J,\theta\rangle = \mathcal{N}(J)^{-1/2}\sum_{n=0}^{\infty}\frac{J^{n/2}e^{in\theta}e^{-i\omega e_n t}}{\sqrt{[e_n]!}}|\phi_n\rangle. \tag{104}$$

This larger set of GKCSs, we will call them "*generalized GKCSs*," defined for all t, satisfies the resolution of the identity,

$$\begin{aligned}
&\int_{\mathbb{R}}\left[\int_0^L\left\{\int_0^{2\pi}|J,\theta,t\rangle\langle J,\theta,t|\mathcal{N}(J)\frac{\mathrm{d}\theta}{2\pi}\right\}\mathrm{d}\nu(J)\right]\mathrm{d}\mu_{\mathcal{B}}\\
&\quad=\int_0^L\left[\int_0^{2\pi}|J,\theta,t\rangle\langle J,\theta,t|\mathcal{N}(J)\frac{\mathrm{d}\theta}{2\pi}\right]\mathrm{d}\nu(J)\\
&\quad=\int_{\mathbb{R}}\left[\int_0^L|J,\theta,t\rangle\langle J,\theta,t|\mathcal{N}(J)\mathrm{d}\nu(J)\right]\mathrm{d}\mu_{\mathcal{B}}\\
&\quad=\sum_{n=0}^{\infty}|\phi_n\rangle\langle\phi_n| = I_{\mathfrak{H}},
\end{aligned} \tag{105}$$

where $\mathrm{d}\mu_{\mathcal{B}}$ which is really a functional (not a measure) is referred to as the *Bohr measure*,

$$\langle\mu_{\mathcal{B}};f\rangle \doteq \lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}f(x)\mathrm{d}x = \int_{\mathbb{R}}f(x)\mathrm{d}\mu_{\mathcal{B}}(x), \tag{106}$$

and f is a suitably chosen function over $\mathbb{R}$. In particular, if $f(x)=1$ for all x, then $\langle\mu_{\mathcal{B}};f\rangle=1$, so that $\mu_{\mathcal{B}}$ resembles a probability measure. Therefore writing the Bohr measure as an integral has only a symbolic meaning.

Setting $t=0$ in the "generalized GKCSs" of Eq. (103), we shall recover the nonlinear CSs and for $\theta=0$, the generalized CSs of Eq. (104) reduce to the GKCSs $|J,\alpha\rangle$ in (1) with $\alpha\equiv\omega t$, which the latter states satisfy the resolution of the identity,

$$\int_{\mathbb{R}}\left[\int_0^L|J,\alpha\rangle\langle J,\alpha|\mathcal{N}(J)\mathrm{d}\nu(J)\right]\mathrm{d}\mu_{\mathcal{B}}(t) = I_{\mathfrak{H}}. \tag{107}$$

The generalized GKCSs $|J,\theta,t\rangle$ in (104) satisfy the temporal stability condition and the action identity, as well as the continuity in the labels and resolution of the identity,

$$e^{-i\hat{H}t'}|J,\theta,t\rangle = |J,\theta,t+t'\rangle, \quad \langle J,\theta,t|\hat{H}|J,\theta,t\rangle = \omega J, \tag{108}$$

and so do the states $|z,t\rangle$ in (103).

B. The dual family of the "generalized GKCS"

Let us now write $e_n=nf^2(n)$, so using our previous results in the present paper, there is a *dual set* of numbers $\tilde{e}_n\equiv\varepsilon_n=n/f^2(n)$, associated with the *dual Hamiltonian* $\tilde{\hat{H}}$. Correspondingly this Hamiltonian has eigenvectors $|\phi_n\rangle$ and eigenvalues ε_n, such that

$$\widetilde{\hat{H}} = \omega \sum_{n=0}^{\infty} \varepsilon_n |\phi_n\rangle\langle\phi_n|, \quad \text{where } \widetilde{\hat{H}}|\phi_n\rangle = \omega\varepsilon_n|\phi_n\rangle. \tag{109}$$

Also assume that $0=\varepsilon_0<\varepsilon_1<\varepsilon_2<\cdots<\varepsilon_n<\varepsilon_{n+1}<\cdots$, such that the sum $\Sigma_{n=0}^{\infty}(x^n/[\varepsilon_n]!)$ converges in some interval $0<x\leqslant\tilde{L}$. We can now define the *dual family* of generalized CSs introduced in (100) by

$$|\tilde{z}\rangle \doteq \tilde{\mathcal{N}}(|z|^2)^{-1/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{[\varepsilon_n]!}} |\phi_n\rangle, \tag{110}$$

which are the well-known (dual) nonlinear CSs of Ref. 15. The time evolution of these states reads as

$$\widetilde{|z,t\rangle} = e^{-i\hat{H}t}|\tilde{z}\rangle = \tilde{\mathcal{N}}(|z|^2)^{-1/2} \sum_{n=0}^{\infty} \frac{z^n e^{-i\omega\varepsilon_n t}}{\sqrt{[\varepsilon_n]!}} |\phi_n\rangle. \tag{111}$$

Again, setting $z=re^{i\theta}$ with $r=J^{\frac{1}{2}}$, we can write $|\tilde{z}\rangle \equiv \widetilde{|J,\theta\rangle}$. So, equivalently the states in (111) can be rewritten in terms of the new variables J and θ as

$$\widetilde{|J,\theta,t\rangle} = e^{-i\hat{H}t}\widetilde{|J,\theta\rangle} = \tilde{\mathcal{N}}(J)^{-1/2} \sum_{n=0}^{\infty} \frac{J^{n/2} e^{in\theta} e^{-i\omega\varepsilon_n t}}{\sqrt{[\varepsilon_n]!}} |\phi_n\rangle. \tag{112}$$

We call this large set of states as the "*dual of the generalized GKCS*." Setting $\theta=0$ in (112) will reduce it to the dual of the GKCSs we introduced in (23) with $\alpha=\omega t$. Provided the moment problem

$$\int_0^{\tilde{L}} J^n \, \mathrm{d}\tilde{\nu}(J) = [\varepsilon_n]\,!\,, \quad \int_0^{\tilde{L}} \mathrm{d}\tilde{\nu}(J) = 1, \tag{113}$$

has a solution, we also have expressions for the resolution of the identity of the type (102), (105), and (107). The GK criteria may immediately be verified for the dual of the generalized GKCS in Eq. (112), as it was down for the "generalized GKCSs" in Eq. (104).

C. Generalized creation and annihilation operators

We define two sets of the generalized annihilation operators

$$A|\phi_n\rangle = \sqrt{e_n}|\phi_{n-1}\rangle, \quad \tilde{A}|\phi_n\rangle = \sqrt{\varepsilon_n}|\phi_{n-1}\rangle, \tag{114}$$

and the corresponding generalized creation operators

$$A^\dagger|\phi_n\rangle = \sqrt{e_{n+1}}|\phi_{n+1}\rangle, \quad \tilde{A}^\dagger|\phi_n\rangle = \sqrt{\varepsilon_{n+1}}|\phi_{n+1}\rangle, \tag{115}$$

where $\varepsilon_n=\tilde{e}_n$. Therefore, the Hamiltonian of the system and its associated dual are

$$\hat{H} = \omega A^\dagger A, \quad \widetilde{\hat{H}} = \omega\tilde{A}^\dagger\tilde{A}. \tag{116}$$

Note that we have dropped the GK indices from all the operators in this last section because the discussion is exclusively related to the GK states. Then, for the states in (100) and (110) we have clearly

$$A|z\rangle = z|z\rangle, \quad \tilde{A}|\tilde{z}\rangle = z|\tilde{z}\rangle. \tag{117}$$

In the Heisenberg picture the generalized annihilation operators A and $\tilde{A}$ evolve in time as

$$A(t) = e^{i\hat{H}t}Ae^{-i\hat{H}t}, \quad \tilde{A}(t) = e^{i\tilde{\hat{H}}t}\tilde{A}e^{-i\tilde{\hat{H}}t}, \tag{118}$$

and similarly for the generalized creation operators. At any time t one may obtain,

$$A(t)|z,-t\rangle = z|z,-t\rangle, \quad \tilde{A}(t)\widetilde{|z,-t\rangle} = z\widetilde{|z,-t\rangle}. \tag{119}$$

D. Interpolating between generalized GKCSs and their dual

Following the approach proposed in Ref. 16 we can define the operator $\hat{T}$ on $\mathfrak{H}$ as

$$\hat{T} \doteq \sum_{n=0}^{\infty} \sqrt{\frac{[e_n]!}{[\varepsilon_n]!}}|\phi_n\rangle\langle\phi_n|, \tag{120}$$

with the action

$$\hat{T}|\phi_n\rangle = \sqrt{\frac{[e_n]!}{[\varepsilon_n]!}}|\phi_n\rangle, \quad n = 0,1,2\ldots . \tag{121}$$

Then, writing $\eta_z = \mathcal{N}(|z|^2)^{1/2}|z\rangle$ and similarly defining $\tilde{\eta}_z$, $\eta_{J,\theta,t}$, and $\tilde{\eta}_{J,\theta,t}$ as the unnormalized CSs, we have

$$\hat{T}\eta_z = \tilde{\eta}_z. \tag{122}$$

Since $\hat{T}$, $\hat{H}$, and $\tilde{\hat{H}}$ commute, we have the interpolation rule at any fixed time t; i.e., fixed α,

$$e^{-i(\tilde{\hat{H}}-\hat{H})t}\hat{T}\eta_{J,\theta,t} = \tilde{\eta}_{J,\theta,t}. \tag{123}$$

VIII. CONCLUDING REMARKS

Finally we present a summary of our results. After imposing a second modification on GK states, we showed that both the GKCSs and DGKCSs are essentially of the type of the so-called nonlinear (f-deformed) CSs. In each of the two cases the relevant nonlinearity function is an *operator valued function* which depends on the intensity of light ($\tilde{n}$), but is labeled by a constant real parameter (α). The introduced nonlinearity function which contains an intensity dependent phase factor, has not appeared in literature up to now. This feature originates from the temporal stability requirement imposed on GKCSs and DGKCSs. Meanwhile, using the two nonlinearity functions we constructed the raising and lowering operators, by which one can create and annihilate the *deformed photons*. After all, we proposed a general evolution operator $\hat{S}(\alpha)$, whose action on any generalized CS with known spectrum transforms it to a temporally stable CS. This *physically* makes the generalized CS more useful in practical experiments.

Adding the results presented in Sec. VI we show that, at least in most of the considered physical systems, i.e., when the CS deals with the whole Fock space $\{|n\rangle\}_{n=0}^{\infty}$, while the GKCSs is defined on the whole complex plane (unit disk) the DGKCSs are restricted to unit disk (whole plane), and vice versa. This situation does not hold for Morse potential in which there is a cutoff in the summation (finite dimensional Hilbert space: $\{|n\rangle\}_{n=0}^{M+1}$). So based on the results in Ref. 33 in which the authors relate the radius of convergence to the physical quantities, it can be concluded that GKCSs and DGKCSs can be produced under different physical conditions.

We emphasize the fact that the Hamiltonian involved in the operator $\hat{S}(\alpha)$ must be the one that expresses the dynamics of the system. Using this proposition we introduced the dual family of GKCS. Also it may be understood that the GKCSs can be rewritten in terms of the associated f_{GK} function, explicitly as

$$|z,\alpha\rangle_f = \mathcal{N}(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}[f_{\mathrm{GK}}(\alpha,\hat{n})]!}|n\rangle,$$

and similarly for the DGKCSs in terms of the same nonlinearity function $f_{\mathrm{GK}}(\alpha,\hat{n})$,

$$\widetilde{|z,\alpha\rangle}_f = \tilde{\mathcal{N}}(|z|^2)^{-1/2}\sum_{n=0}^{\infty}\frac{z^n[f_{\mathrm{GK}}(\alpha,\hat{n})]!}{\sqrt{n!}}|n\rangle.$$

Hence, we have established that the latter states are indeed a special class of nonlinear CSs which are temporally stable. This property is preserved, using a particular set of nonlinearity functions as introduced in (14) and (26). Also, the map

$$|z,\alpha\rangle \mapsto \widetilde{|z,\alpha\rangle}$$

may be obtained by the following map:

$$f_{\mathrm{GK}}(\alpha,\hat{n}) \mapsto \frac{1}{f_{\mathrm{GK}}(\alpha,\hat{n})}.$$

Note that this map converts even the normalization factor correctly. Keeping in mind the above explanation, a certain class of nonlinear CS and its dual, determined on a specified point of the phase space ($z \in \mathbb{C}$), including the fact that the standard CS is self-dual, may be similar to the image of a state by the map defined above. While the images of standard canonical CS are the same in any arbitrary point of the phase space, i.e., the usual CS does not destroy the flatness of the mirror (or the linearity of the medium), this is not so for the nonlinear CSs. It may be recognized that the operator f in the CSs affect the flatness of the mirror (or the linearity of the medium), and makes it to be curved (or nonlinear). As much as the state is far from the harmonic oscillator CSs, the effect of the f-function is more strong and the dual state (image) is far from the state itself. So the role of the nonlinearity in the nonlinear CSs may be related to the medium, instead of the source of light. In other words, corresponding to any nonlinear CSs there exist an equivalent situation, "a linear source (ordinary photon) with a *nonlinear optical medium*," such as Kerr medium. This particular interpretation of the nonlinear CSs has already been realized in Refs. 34 and 35.

Finally, we confined ourselves to the general introduction of the new type of Gazeau–Klauder CSs in this paper. Although it would be interesting for further applications in quantum optics to investigate in detail, minimization of Robertson–Schrödinger uncertainty equation, the intelligent states and the statistical properties, quadrature squeezing, etc., of DGKCSs and the special superpositions of them have been introduced associated with various exactly solvable quantum mechanical systems and compared with those of the old one (GKCSs type). Also it seems that the vector CSs of DGKCSs may be constructed, as it was done for GK states.[14] These matters are under consideration for future works.

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Estimates on Green functions of second order differential operators with singular coefficients

Z. Haba[a)]
Institute of Theoretical Physics, University of Wroclaw, 50-204 Wroclaw, Plac Maxa Borna 9, Poland

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We investigate the Green functions $G(x;x')$ of some second order differential operators on R^{d+1} with singular coefficients depending only on one coordinate x_0. We express the Green functions by means of the Brownian motion. Applying probabilistic methods we prove that when $x=(0,\mathbf{x})$ and $x'=(0,\mathbf{x}')$ (here $x_0=0$) lie on the singular hyperplanes, then $G(0,\mathbf{x};0,\mathbf{x}')$ is more regular than the Green function of operators with regular coefficients. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1855934]

I. INTRODUCTION

We discuss Green functions of some second order differential operators with singular coefficients appearing in quantum physics.

As a first example consider the Lagrangian for a scalar field in $(d+1)$-dimensions interacting with gravity

$$\mathcal{L} = g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi + (m^2 + \xi R)\phi^2, \tag{1}$$

where $g^{\mu\nu}$ is the metric tensor and R is the scalar curvature. Such a Lagrangian with $m=0$ and the minimal coupling $\xi=0$ appears also in the theory of structure formation (cosmological perturbations).[1] We discuss the Euclidean version of a spatially homogeneous metric [we write $x=(t,\mathbf{x})$ or $x=(x_0,\mathbf{x})$ depending on whether the first coordinate has an interpretation of time or space],

$$ds^2 = dt^2 + g_{jk}(t)dx^j dx^k.$$

The Laplace–Beltrami operator resulting from the bilinear form in Eq. (1) reads

$$\Delta_g = \tfrac{1}{2}g^{-1/2}\partial_\mu(g^{\mu\nu}g^{1/2}\partial_\nu) \tag{2}$$

[here $g=\det(g_{\mu\nu})$]. In cosmological models $g_{jk}\simeq t^{2\alpha}$ and $g^{jk}\simeq t^{-2\alpha}$ when $t\to 0$ with $\alpha>0$. Such a singular behavior can appear also in models describing collapse phenomena in general relativity.[2]

As a second example we consider quantum mechanics on a (topologically trivial) manifold with the Hamiltonian

$$H = -\Delta_g + U(x_0) \tag{3}$$

[in some global coordinates $x=(x_0,\mathbf{x})$].

The Green functions of (Euclidean) quantum scalar fields (1) with $m=0$ and the minimal coupling $\xi=0$ are solutions of the equation

a)Electronic mail: zhab@ift.uni.wroc.pl

$$-\Delta_g G = g^{-1/2}\delta. \tag{4}$$

These Green functions are also relevant for classical field theory because they describe a propagation of disturbances. In quantum mechanics (3) we are interested in the propagator kernels

$$\exp(-\tau H)(x_0,\mathbf{x};x_0',\mathbf{x}'), \tag{5}$$

where τ is purely imaginary.

In this paper we prove that if the coefficients of the Laplace–Beltrami operator have a power-law singularity at a certain point $t=t_0$, then the Green functions $G(t_0,\mathbf{x};t_0,\mathbf{x}')$ are more regular than the ones of operators with regular coefficients (for regular coefficients the Green function can be expressed by the geodesic distance[3,4]). In quantum field theory these Green functions have the meaning of expectation values of quantum fields at equal times. In quantum mechanics the propagator (5) will have an anomalous behavior in τ. The Green function (4) can be obtained from the propagator (5) by means of an integration over τ.

II. THE GREEN FUNCTIONS

Let us change coordinates

$$\frac{dt}{d\eta} = \sqrt{g}. \tag{6}$$

The Laplace–Beltrami operator (2) takes the form

$$2\Delta_g = g^{-1}\partial_\eta^2 + g^{jk}\partial_j\partial_k. \tag{7}$$

The bilinear form in Eq. (1) determines an operator $\mathcal{A}$ which is of the same form as H in quantum mechanics [Eq. (3)]:

$$\mathcal{A} = -\Delta_g + w. \tag{8}$$

Here, $w=\frac{1}{2}m^2+\frac{1}{2}\xi R$ for the scalar field and $w=U$ for quantum mechanics. The Green function of $\mathcal{A}$ is a solution of the equation

$$-(\partial_\eta^2 + gg^{jk}\partial_j\partial_k - W)G = 2\delta(\eta-\eta')\delta(\mathbf{x}-\mathbf{x}'), \tag{9}$$

where we write

$$W = gw. \tag{10}$$

Together with Eq. (9) we consider the differential equation

$$-\partial_\tau P_\tau = \mathcal{A}P_\tau \tag{11}$$

with the initial condition $P_0(\eta,\mathbf{x};\eta',\mathbf{x}')=\delta(\eta-\eta')\delta(\mathbf{x}-\mathbf{x}')$. Equation (11) defines the transition function of a stochastic process.[5]

We can formulate the problem of solving the equation

$$\mathcal{A}G = \delta \tag{12}$$

as a problem in the Hilbert space of square integrable functions $L^2(d\eta d\mathbf{x})$.[6] We assume that W is a non-negative function. The operator $\mathcal{A}$ can be considered as a self-adjoint non-negative operator in L^2 if gg^{jk} and W are locally integrable functions [then we can define the Friedrichs extension[6] of the symmetric differential operator (8)]. The transition function P_τ of Eq. (11) can be defined as the integral kernel of $\exp(-\tau\mathcal{A})$. Then, the kernel of the inverse

$$\mathcal{A}^{-1} = \int_0^\infty d\tau \exp(-\tau\mathcal{A})$$

is the solution of Eq. (9). It follows that the Fourier transform $\tilde{G}$ of G has the representation

$$\tilde{G}(\eta, \eta'; \mathbf{p}) = \int_0^\infty d\tau \tilde{P}_\tau(\eta, \eta', \mathbf{p}), \tag{13}$$

where $\tilde{P}$ is a solution of the equation

$$-\partial_\tau \tilde{P}_\tau = \tilde{\mathcal{A}}\tilde{P}_\tau \tag{14}$$

with the initial condition $\tilde{P}_0(\eta, \eta', \mathbf{p}) = \delta(\eta - \eta')$ (the fundamental solution). Here

$$\tilde{\mathcal{A}} = -\tfrac{1}{2}\partial_\eta^2 + \tfrac{1}{2}p_j g^{jk}(\eta)g(\eta)p_k + W \equiv -\tfrac{1}{2}\partial_\eta^2 + V(\eta) + W(\eta). \tag{15}$$

Equation (14) is a Schrödinger-type equation with the Hamiltonian $\tilde{\mathcal{A}}$ and the potential $V+W$ where

$$V(\eta) = \tfrac{1}{2}p_j g^{jk}(\eta)g(\eta)p_k \equiv \mathbf{p}\tilde{V}\mathbf{p}(\eta). \tag{16}$$

If the potentials V and W belong to $L^1_{loc}(d\eta)$, then $\tilde{\mathcal{A}}$ is a well-defined essentially self-adjoint operator in $L^2(d\eta)$.[7]

We can express the kernel $\tilde{P}$ by means of the Brownian motion b (the Feynman–Kac formula;[8] a discussion of the probabilistic representation for singular potentials can be found in Ref. 9):

$$\tilde{P}_\tau(\eta, \eta', \mathbf{p}) = E\left[\delta(\eta' - \eta - b(\tau))\exp\left(-\int_0^\tau V(\eta + b(s))ds - \int_0^\tau W(\eta + b(s))ds\right)\right], \tag{17}$$

where $E[.]$ denotes an average over the Brownian paths. Now, the kernel of $\exp(-\tau\mathcal{A})$ has the representation

$$P_\tau(\eta, \mathbf{x}, \eta', \mathbf{x}') = (2\pi)^{-d}\int d\mathbf{p}\, \exp(i\mathbf{p}(\mathbf{x}' - \mathbf{x})) \times E\left[\delta(\eta' - \eta - b(\tau))\exp\left(-\int_0^\tau V(\eta + b(s))ds - \int_0^\tau W(\eta + b(s))ds\right)\right]. \tag{18}$$

In order to eliminate the δ function in Eq. (17) it is useful to express the expectation value over the Brownian motion by means of an expectation value over the Brownian bridge γ. Let q be a path connecting η with η'

$$q\left(\frac{s}{\tau}\right) = \eta + (\eta' - \eta)\frac{s}{\tau} + \sqrt{\tau}\gamma\left(\frac{s}{\tau}\right), \tag{19}$$

where γ is the Gaussian process on the interval $[0, 1]$ (the Brownian bridge) starting from 0 and ending in 0 with the covariance

$$E[\gamma(s)\gamma(s')] = s'(1 - s)$$

for $s' \leqslant s$. Then, Eq. (17) can be rewritten in the form[8]

$$\widetilde{P}_\tau(\eta,\eta',\mathbf{p}) = (2\pi\tau)^{-1/2}\exp\left(-\frac{1}{2\tau}(\eta'-\eta)^2\right)E\left[\exp\left(-\tau\int_0^1 ds(V(q(s))+W(q(s))\right)\right]. \tag{20}$$

Applying the Jensen inequality (see Refs. 10 and 11) to the $E[..]$ integral we obtain the inequality

$$\widetilde{P}_\tau(\eta,\eta',\mathbf{p}) \geqslant (2\pi\tau)^{-1/2}\exp\left(-\frac{1}{2\tau}(\eta'-\eta)^2\right)\exp\left(-\tau\int_0^1 ds\, E[V(q(s))+W(q(s))]\right) \equiv \widetilde{P}^L. \tag{21}$$

This integral is

$$\widetilde{P}^L_\tau(\eta,\eta',\mathbf{p}) = (2\pi\tau)^{-1/2}\exp\left(-\frac{1}{2\tau}(\eta'-\eta)^2\right)\exp\left(-\tau\int_0^1 ds\int dy(2\pi s(1-s))^{-1/2}\exp\left(-\frac{y^2}{2s(1-s)}\right)\right.$$
$$\left.\times(V+W)(\eta+s(\eta'-\eta)+\sqrt{\tau}y)\right). \tag{22}$$

As a simple application of the inequality (21) we note that if

$$V+W \leqslant A'\mathbf{p}^2+B', \tag{23}$$

then

$$\widetilde{P}^L_\tau(\eta,\eta',\mathbf{p}) \geqslant (2\pi\tau)^{-1/2}\exp\left(-\frac{1}{2\tau}(\eta'-\eta)^2\right)\exp(-\tau A'\mathbf{p}^2-\tau B'). \tag{24}$$

Hence, we obtain a bound from below by the transition function for the d-dimensional Brownian motion.

On the other hand, we may apply the Jensen inequality in the opposite direction to the s-integral

$$\widetilde{P}_\tau(\eta,\eta',\mathbf{p}) \leqslant (2\pi\tau)^{-1/2}\exp\left(-\frac{1}{2\tau}(\eta'-\eta)^2\right)\int_0^1 ds\, E[\exp(-\tau V(q(s))-\tau W(q(s)))] \equiv \widetilde{P}^U. \tag{25}$$

This integral takes the form

$$\widetilde{P}^U_\tau(\eta,\eta',\mathbf{p}) = (2\pi\tau)^{-1/2}\exp\left(-\frac{1}{2\tau}(\eta'-\eta)^2\right)\int_0^1 ds\int dy(2\pi s(1-s))^{-1/2}\exp\left(-\frac{y^2}{2s(1-s)}\right)$$
$$\times\exp(-\tau(V+W)(\eta+s(\eta'-\eta)+\sqrt{\tau}y)). \tag{26}$$

If

$$V+W \geqslant A\mathbf{p}^2+B,$$

then

$$\widetilde{P}^U_\tau(\eta,\eta',\mathbf{p}) \leqslant (2\pi\tau)^{-1/2}\exp\left(-\frac{1}{2\tau}(\eta'-\eta)^2\right)\exp(-\tau A\mathbf{p}^2-\tau B). \tag{27}$$

Hence, we estimate the transition function from above by the Wiener transition function.

III. SCALE INVARIANT METRICS

We consider in this section a power-law cosmological expansion. Such an expansion is an exact solution of coupled Einstein equations for a metric and for the scalar field with an exponential self-interaction. Some consequences for a structure formation with such an expansion are discussed in Refs. 12 and 13. If $g_{jk}(t)$ has an isotropic power-law behavior, then V is scale invariant. Let us assume here that V and W are non-negative and scale invariant around $\eta=0$ [there is nothing special in the choice of $\eta=0$ as a singular point, see a discussion at Eq. (44)]:

$$\tilde{V}^{jk}(\lambda\eta) = \lambda^{2\nu}\tilde{V}^{jk}(\eta) \tag{28}$$

and

$$W(\lambda\eta) = \lambda^{2\sigma}W(\eta). \tag{29}$$

Let us denote $\theta=\tau^{-1/2}\eta$. We apply the scaling properties of the Brownian bridge (19). Then, for V of the form (28) and W in (29) we obtain

$$\tilde{P}_\tau(\eta,\eta',\mathbf{p}) = (2\pi\tau)^{-1/2}\exp\left(-\frac{1}{2\tau}(\eta'-\eta)^2\right)E\left[\exp\left(-\tau^{1+\nu}\int_0^1 \mathbf{p}\tilde{V}\mathbf{p}(\theta+s(\theta'-\theta)+\gamma(s))ds\right)\right.$$
$$\left.\times\exp\left[\left(-\tau^{1+\sigma}\int_0^1 W(\theta+s(\theta'-\theta)+\gamma(s))ds\right)\right]\right]. \tag{30}$$

The bounds (22) and (26) become simple if $\eta=\eta'=0$. Then, the bound (22) reads

$$\tilde{P}^L_\tau(0,0,\mathbf{p}) = (2\pi\tau)^{-1/2}\exp\left(-\tau^{1+\nu}\int_0^1 ds\int dy(2\pi s(1-s))^{-1/2}V(y)\exp\left(-\frac{y^2}{2s(1-s)}\right)\right.$$
$$\left.-\tau^{1+\sigma}\int_0^1 ds\int dy(2\pi s(1-s))^{-1/2}W(y)\exp\left(-\frac{y^2}{2s(1-s)}\right)\right)$$
$$= (2\pi\tau)^{-1/2}\exp\left(-\tau^{1+\nu}\mathbf{p}h\mathbf{p}\int_0^1 ds(s(1-s))^\nu - B\tau^{1+\sigma}\int_0^1 ds(s(1-s))^\sigma\right), \tag{31}$$

where the bilinear form h in $\mathbf{p}$ is defined by

$$\mathbf{p}h\mathbf{p} = (2\pi)^{-1/2}\int dy\exp\left(-\frac{y^2}{2}\right)\mathbf{p}\tilde{V}(y)\mathbf{p} \tag{32}$$

and the constant B in Eq. (31) is

$$B = (2\pi)^{-1/2}\int dy\exp\left(-\frac{y^2}{2}\right)W(y). \tag{33}$$

The integral (32) is finite if $\nu>-\frac{1}{2}$ and (33) is finite if $\sigma>-\frac{1}{2}$. In such a case the lower bound (31) is nontrivial. The upper bound (26) takes the form

$$\tilde{P}^U_\tau(0,0,\mathbf{p}) = (2\pi\tau)^{-1/2}\int_0^1 ds\int dy(2\pi s(1-s))^{-1/2}\exp\left(-\frac{y^2}{2s(1-s)}\right)\exp(-\tau^{1+\nu}V(y)-\tau^{1+\sigma}W(y)). \tag{34}$$

We are interested in the Green functions (9) of the operator $\mathcal{A}$ which according to Eqs. (13) and (18) are expressed by a τ integration upon P_τ. As the simplest example of the integral (13) let $V+W=A\mathbf{p}^2+B$. Then performing the τ integration upon the rhs of Eq. (13) we obtain

$$\widetilde{G}_0(0,0;\mathbf{p}) = (2A\mathbf{p}^2 + 2B)^{-1/2}. \tag{35}$$

This is the standard behavior of equal-time Green functions for the quantum free field.

In Eq. (31) let us first discuss the case $W=B=0$. Then, the integral over τ of Eq. (31) gives the lower bound on the Green function

$$\widetilde{G}(0,0;\mathbf{p}) \geqslant K_1(\mathbf{p}h\mathbf{p})^{-\omega}, \tag{36}$$

where

$$\omega = \frac{1}{2(1+\nu)}. \tag{37}$$

In order to estimate the upper bound (34) (for $W=0$) let us assume a lower bound $|\widetilde{V}|_0$ on $\widetilde{V}$, i.e., for $\mathbf{p}\neq 0$

$$\mathbf{p}\widetilde{V}\mathbf{p} \geqslant \mathbf{p}^2|\widetilde{V}|_0 > 0. \tag{38}$$

Now, we change variables in Eqs. (13) and (34), $(\tau,y)\to(\rho,u)$, where

$$\rho = \tau|\mathbf{p}|^{2/(1+\nu)}|\widetilde{V}(y)|_0^{1/(1+\nu)},$$

$$u = y(s(1-s))^{-1/2}.$$

Then, the upper bound takes the form

$$\widetilde{G}(0,0;\mathbf{p}) \leqslant |\mathbf{p}|^{-2\omega}\int_0^\infty d\rho(2\pi\rho)^{-1/2}\int_0^1 ds\int du(2\pi)^{-1/2}(s(1-s))^{-\nu/(1+\nu)}|\widetilde{V}(u)|_0^{-\omega}$$
$$\times\exp\left(-\frac{u^2}{2}\right)\exp(-\rho^{1+\nu}). \tag{39}$$

We can see that the integral on the rhs of Eq. (39) is finite if $-1<\nu<\infty$.

We can summarize our results as follows.

Theorem 1: Assume that $W=0$ and the potential V in Eq. (15) is non-negative and scale invariant with $\nu>-\frac{1}{2}$ [Eq. (28)]. Then, the operator $\widetilde{\mathcal{A}}$ is essentially self-adjoint and the integral kernel of $\exp(-\tau\widetilde{\mathcal{A}})$ has the probabilistic representation (20). The Green function G of Eq. (9) can be defined as an integral kernel of $\mathcal{A}^{-1}$. Assume that the potential V satisfies the lower bound (38). Then the Fourier transform $\widetilde{G}(\eta,\eta';\mathbf{p})$ of $G(\eta,\eta',\mathbf{x}-\mathbf{x}')$ at $\eta=\eta'=0$ for any $\mathbf{p}$ satisfies the inequalities

$$K_1(\mathbf{p}h\mathbf{p})^{-\omega} \leqslant \widetilde{G}(0,0;\mathbf{p}) \leqslant K_2|\mathbf{p}|^{-2\omega}, \tag{40}$$

where h is defined in Eq. (32) and K_1 and K_2 are some positive constants.

For $\nu<0$ the Fourier transform $\widetilde{G}$ is decaying to zero faster than the Green function for operators with constant coefficients. As a consequence G is less singular than the one for operators with constant coefficients [see Eq. (43) below].

In the configuration space, if $W=0$, then we can extract the τ dependence from V using its scale invariance. Then, changing the integration variable in Eq. (18), $\mathbf{p}=\tau^{-(1/2)(1+\nu)}\mathbf{k}$, we can conclude that P has the form

$$P_\tau(\eta,\mathbf{x},\eta',\mathbf{x}') = \tau^{-(1/2)(1+\nu)d-1/2}F(\tau^{-1/2}\eta,\tau^{-1/2}\eta',\tau^{-(1/2)(1+\nu)}(\mathbf{x}-\mathbf{x}')) \tag{41}$$

with a certain function F. Integration over τ with a rescaled $\tau=r|\mathbf{x}-\mathbf{x}'|^{2/(1+\nu)}$ brings the Green function at equal time to the form

$$G(\eta,\mathbf{x},\eta,\mathbf{x}') = |\mathbf{x}-\mathbf{x}'|^{-d+1/(1+\nu)} f(|\mathbf{x}-\mathbf{x}'|^{1/(1+\nu)}\eta, (\mathbf{x}-\mathbf{x}')|\mathbf{x}-\mathbf{x}'|^{-1}). \tag{42}$$

It follows

$$G(0,\mathbf{x},0,\mathbf{x}') = |\mathbf{x}-\mathbf{x}'|^{-d+1/(1+\nu)} f((\mathbf{x}-\mathbf{x}')|\mathbf{x}-\mathbf{x}'|^{-1}). \tag{43}$$

We obtain such a behavior in $|\mathbf{x}-\mathbf{x}'|$ if we apply the inverse Fourier transform to the functions on both sides of the inequalities (40).

Let us note that if V is singular at $\eta_0 \neq 0$ (e.g., $V \simeq |\eta-\eta_0|^{2\nu}$), then all our results concerning the transition functions and Green functions still hold true but instead of setting $\eta=\eta'=0$ we set $\eta=\eta'=\eta_0$ [this conclusion follows directly from Eq. (30)]. So, e.g., the formula (43) reads

$$G(\eta_0,\mathbf{x},\eta_0,\mathbf{x}') = |\mathbf{x}-\mathbf{x}'|^{-d+1/(1+\nu)} f((\mathbf{x}-\mathbf{x}')|\mathbf{x}-\mathbf{x}'|^{-1}). \tag{44}$$

We admit now $W \neq 0$

Theorem 2: Let $W \geqslant 0$ be scale invariant [Eq. (29)] and $\sigma > -\frac{1}{2}$. Then (under the assumptions of Theorem 1 concerning V) for any $\Lambda > 0$, if $|\mathbf{p}| > \Lambda$, then there exist positive constants K_1 and K_2 such that the inequalities (40) hold true.

Proof: Setting $W=0$ in Eq. (34) we obtain the upper bound (39). For the lower bound we note that the exponential in Eq. (31) is dominated by the term quadratic in the momenta. We change the integration variable in Eqs. (13) and (34):

$$\tau = r(\mathbf{p}h\mathbf{p})^{-1/(1+\nu)}.$$

Then, we can see that for any $\Lambda > 0$, if $|\mathbf{p}| > \Lambda$, then there exists a constant C such that in the exponential of Eq. (31) $B\tau^{1+\sigma} < Cr^{1+\sigma}$. Then

$$\int d\tau \, \tilde{P}^L_\tau(0,0,\mathbf{p}) \geqslant (\mathbf{p}h_2\mathbf{p})^{-\omega} \int dr (2\pi r)^{-1/2} \exp\left(- r^{1+\nu} \int_0^1 ds (s(1-s))^\nu - Cr^{1+\sigma} \int_0^1 ds (s(1-s))^\sigma \right).$$

From this lower bound and from the upper bound (39) we obtain the results of the theorem.

If $W > 0$, then the lower bound in Eq. (40) cannot be true for arbitrarily small $\mathbf{p}$ because as follows from Eq. (34) ($V=0$ for $\mathbf{p}=0$)

$$\tilde{G}(0,0,\mathbf{0}) \leqslant \int_0^\infty d\tau (2\pi\tau)^{-1/2} \int_0^1 ds \int dy (2\pi s(1-s))^{-1/2} \exp\left(- \frac{y^2}{2s(1-s)} \right) \exp(-\tau^{1+\sigma} W(y)) < \infty. \tag{45}$$

If we imposed the condition that $t \geqslant 0$ (which is quite artificial in the Euclidean framework), then we would need to impose boundary conditions at $\eta=0$ on the Brownian motion in the path integral (17). The Dirichlet boundary conditions can easily be imposed in the functional integration framework. We just insert the characteristic function of the positive real axis in the path integral (17), rejecting all the Brownian paths which leave the positive real axis. With the Dirichlet boundary conditions our estimates on the upper bound remain unchanged whereas the estimates on the lower bound require some minor modifications.

Let us consider an example of a three-dimensional space. By a change of coordinates we can diagonalize the matrix (g_{jk}):

$$g_{jk} = \delta_{jk} a_j^2. \tag{46}$$

Let $a = (a_1 a_2 a_3)^{1/3}$ and

$$\delta_j = a_j^{-1} a^{-2} \partial_\eta a_j,$$

$$\delta = a^{-3} \partial_\eta a,$$

$$Q = \frac{1}{18}\sum_{j<k} (\delta_j - \delta_k)^2.$$

Then, in the potential W of Eq. (9),[14]

$$gR = 6a^4(a^{-2}\partial_\eta \delta + \delta^2 + Q) \tag{47}$$

and

$$m^2 g = m^2 a^6. \tag{48}$$

We obtain a scale invariant V and W if a_j are scale invariant. Let us consider the simplest case when all a_j are equal, $t \in R$, and

$$a(t) = |t|^\alpha. \tag{49}$$

We have

$$\eta = (1 - 3\alpha)^{-1} t|t|^{-3\alpha}.$$

Note that for $\alpha > \frac{1}{3}$ the point $t=0$ corresponds to $\eta = -\infty$ and $t = \infty$ to $\eta = 0$.

Then

$$V(y) = \kappa \mathbf{p}^2 |y|^{2\nu},$$

where $\kappa > 0$ is a certain constant and

$$\nu = 2\alpha(1 - 3\alpha)^{-1}. \tag{50}$$

For a scale invariant metric

$$W = m^2 g(\eta) + \xi g R = C_1 m^2 |\eta|^{6\alpha/(1-3\alpha)} + \xi C_2 \eta^{-2}.$$

De Sitter space can be obtained as a limit $\alpha \to \infty$. Then, we have $V(\eta) = c\mathbf{p}^2|\eta|^{-4/3}$ and $m^2 g = c' \eta^{-2}$, hence $W(\eta) = \tilde{c}\eta^{-2}$. This is a singular perturbation which goes beyond our analysis. It can be treated by means of the path integral methods. However, in such a case W needs a regularization, then a renormalization and a subsequent removal of the regularization.[9] The η^{-2} singularity comes also from the term gR. Hence, the results of this section apply only to $\xi = 0$. Then, in Eq. (29) $\sigma = 3\alpha(1-3\alpha)^{-1}$. B in Eq. (33) is finite if $|\alpha| < \frac{1}{3}$.

In quantum mechanics x_0 is interpreted as a space variable. The metric takes the form ($d+1=3$)

$$ds^2 = dx_0^2 + |x_0|^{2\alpha}(dx_1^2 + dx_2^2).$$

Then, $\eta = (1-2\alpha)^{-1} x_0 |x_0|^{-2\alpha}$. The Hamiltonian (3) is symmetric in $L^2(\sqrt{g}dx)$. The change of coordinates $x_0 \to \eta$ associates with H the operator $\tilde{A} = g\tilde{H}$ which is symmetric in $L^2(d\eta d\mathbf{x})$,

$$\tilde{A} = -\partial_\eta^2 + V + W,$$

where

$$V(\eta) = C_1 \mathbf{p}^2 |\eta|^{2\alpha/(1-2\alpha)} \tag{51}$$

with $\mathbf{p}^2 = p_1^2 + p_2^2$ and

$$W = gU(\eta) = C_2 |\eta|^{4\alpha/(1-2\alpha)} U(\eta). \tag{52}$$

The anomalous behavior of $\tilde{P}_\tau$ has the following as a consequence.

Corollary 3: Let $\tilde{P}_\tau(\eta,\eta',\mathbf{p})$ be the fundamental solution of Eq. (14) with $W=0$ and V defined in Eq. (51). If $\nu=\alpha/(1-2\alpha)>-\frac{1}{2}$, then for any $\tau\geqslant 0$

$$\int d\mathbf{x}\, P_\tau(0,\mathbf{x},0,\mathbf{x}')|\mathbf{x}-\mathbf{x}'|^2=(-\Delta_{\mathbf{p}})\tilde{P}_\tau(0,0,\mathbf{p})_{|\mathbf{p}=0}=B_1\tau^{1/2+\nu} \tag{53}$$

and

$$\int d\mathbf{x}d\eta'\, P_\tau(0,\mathbf{x},\eta',\mathbf{x}')|\mathbf{x}-\mathbf{x}'|^2=\int d\eta'(-\Delta_{\mathbf{p}})\tilde{P}_\tau(0,\eta',\mathbf{p})_{|\mathbf{p}=0}=B_2\tau^{1+\nu}. \tag{54}$$

If $W(\eta)\geqslant 0$ defined in Eq. (52) belongs to $L^1_{loc}(d\eta)$, then instead of the equalities in Eqs. (53) and (54) we have bounds from above by $B_1\tau^{1/2+\nu}$ in Eq. (53) and $B_2\tau^{1+\nu}$ in Eq. (54).

Proof: We prove Eq. (54) [Eq. (53) is simpler and proved in a similar way]. Let us calculate

$$(-\Delta_{\mathbf{p}})\int d\eta'\,\tilde{P}_\tau(0,\eta',\mathbf{p})_{|\mathbf{p}=0}=\int d\eta'(2\pi\tau)^{-1/2}\exp\left(-\frac{1}{2\tau}(\eta')^2\right)$$
$$\times E\left[\tau^{1+\nu}\int_0^1 Tr\tilde{V}(s\tau^{-1/2}\eta'+\gamma(s))ds\right]=B_2\tau^{1+\nu}. \tag{55}$$

If $W\geqslant 0$, then instead of the expectation value (55) we have

$$\int d\eta'(2\pi\tau)^{-1/2}\exp\left(-\frac{1}{2\tau}(\eta')^2\right)E\left[\tau^{1+\nu}\int_0^1 Tr\tilde{V}(s\tau^{-1/2}\eta'+\gamma(s))ds\right.$$
$$\left.\times\exp\left(-\int_0^\tau W\left(s\tau^{-1}\eta'+\sqrt{\tau}\gamma\left(\frac{s}{\tau}\right)\right)ds\right)\right]\leqslant B_2\tau^{1+\nu},$$

where the inequality follows from $W\geqslant 0$.

Corollary 3 means that if $\nu<0$, then the sample paths of diffusions generated by operators with singular coefficients have worse continuity properties than the Brownian paths (for Brownian paths see Ref. 8).

IV. MORE GENERAL METRICS

We study the lower bound on G following from Eq. (22)

$$\tilde{G}^L(0,0,\mathbf{p})=\int_0^\infty d\tau(2\pi\tau)^{-1/2}\exp\left(-\tau\int_0^1 ds\int dy(2\pi s(1-s))^{-1/2}\exp\left(-\frac{y^2}{2s(1-s)}\right)\mathcal{V}(\sqrt{\tau}y)\right),$$

and the upper bound following from Eq. (26)

$$\tilde{G}^U(0,0,\mathbf{p})=\int_0^\infty d\tau(2\pi\tau)^{-1/2}\int_0^1 ds\int dy(2\pi s(1-s))^{-1/2}\exp\left(-\frac{y^2}{2s(1-s)}\right)\exp(-\tau\mathcal{V}(\sqrt{\tau}y))$$

for more general $\mathcal{V}$.

A generalization of Theorem 1 reads as follows.

Theorem 4: Let us consider $\mathcal{V}=\mathbf{p}\tilde{\mathcal{V}}\mathbf{p}$, which is not scale invariant but of the form

$$\tilde{\mathcal{V}}(\eta)=\tilde{V}(\eta)f(\eta)+l(\eta), \tag{56}$$

where $\tilde{V}$ is a matrix scale invariant function (28) satisfying the conditions of Theorem 1 with $-\frac{1}{2}<\nu<0$, f is a bounded function with a strictly positive lower bound, and l is a non-negative bounded matrix function. Assume in addition that

$$\int dy \exp\left(-\frac{y^2}{2}\right) f(y)\tilde{V}(y) \geqslant cI > 0, \tag{57}$$

where c is a positive number. Under our assumptions (56) and (57) for any $\Lambda > 0$, if $|\mathbf{p}| > \Lambda$, then there exist a positively definite bilinear form h_2 and constants K_1 and K_2 such that

$$K_1(\mathbf{p}h_2\mathbf{p})^{-\omega} \leqslant \tilde{G}(0,0;\mathbf{p}) \leqslant K_2|\mathbf{p}|^{-2\omega}. \tag{58}$$

If $\nu \geqslant 0$ for $\tilde{V}$ in Eq. (56), then for $|\mathbf{p}| > \Lambda$ the inequalities (58) hold true with $\omega = \frac{1}{2}$.

Proof: Our assumptions (56) on $\tilde{\mathcal{V}}$ mean that it satisfies the inequalities

$$\tau^{\nu}\mathbf{p}\tilde{V}_1(y)\mathbf{p} + \mathbf{p}l_1\mathbf{p} \leqslant \mathcal{V}(\sqrt{\tau}y) \leqslant \tau^{\nu}\mathbf{p}\tilde{V}_2(y)\mathbf{p} + \mathbf{p}l_2\mathbf{p} \tag{59}$$

with certain matrix functions $\tilde{V}_1$ and $\tilde{V}_2$ independent of τ and bilinear forms l_1 and l_2 (independent of y). It follows that the integral of $\tilde{P}_\tau$ satisfies the bounds

$$\int d\tau\, \tilde{P}_\tau^{L_2} \exp(-\tau\mathbf{p}l_2\mathbf{p}) \leqslant \int d\tau\, \tilde{P}_\tau \leqslant \int d\tau\, \tilde{P}_\tau^{U_1} \exp(-\tau\mathbf{p}l_1\mathbf{p}), \tag{60}$$

where in the lower bound $\tilde{P}^{L_2}$ the potential V_2 from the rhs of Eq. (59) is applied and in $\tilde{P}^{U_1}$ the one from the lhs of Eq. (59). The integral (57) defines h of Eq. (32) [and the h_2 from the upper bound (59)]. Let us change the integration variable $\tau = r(\mathbf{p}h_2\mathbf{p})^{-1/(1+\nu)}$ on the lhs of Eq. (60) and $\tau = \rho|\mathbf{p}|^{-4\omega}|\tilde{V}_1(y)|_0^{-2\omega}$ on the rhs. Then, the lower and upper bounds read [from Eqs. (31), (34), and (38)]

$$\begin{aligned}
&(\mathbf{p}h_2\mathbf{p})^{-\omega}\int_0^\infty dr(2\pi r)^{-1/2} \exp(-r^{1+\nu} - r(\mathbf{p}h_2\mathbf{p})^{-2\omega}\mathbf{p}l_2\mathbf{p}) \\
&\quad \leqslant \tilde{G}(0,0,\mathbf{p}) \leqslant |\mathbf{p}|^{-2\omega}\int_0^\infty d\rho(2\pi\rho)^{-1/2}\int_0^1 ds \int du(2\pi)^{-1/2}(s(1-s))^{-\nu/(1+\nu)}|\tilde{V}_1(u)|_0^{-\omega} \\
&\quad \times \exp\left(-\frac{u^2}{2}\right)\exp(-\rho^{1+\nu} - \rho|\mathbf{p}|^{-4\omega}|\tilde{V}_1(u\sqrt{s(1-s)})|_0^{-2\omega}\mathbf{p}l_1\mathbf{p}).
\end{aligned} \tag{61}$$

The condition (57) implies that the bilinear form h_2 is strictly positive. Hence, there exists a constant K such that

$$K\mathbf{p}h_2\mathbf{p} \geqslant \mathbf{p}l_2\mathbf{p}.$$

Then, for $-\frac{1}{2} < \nu < 0$ and $|\mathbf{p}| > \Lambda$, there exists c_1 such that

$$r(\mathbf{p}h_2\mathbf{p})^{-1/(1+\nu)}\mathbf{p}l_2\mathbf{p} < rc_1$$

in the exponential on the lhs of Eq. (61). The l_1 term can be set zero for the upper bound. In such a case for each $\Lambda > 0$ there exist constants c_1 and c_2 such that if $|\mathbf{p}| > \Lambda$, then the inequalities (61) take the form

$$\begin{aligned}
&(\mathbf{p}h_2\mathbf{p})^{-\omega}\int_0^\infty dr(2\pi r)^{-1/2} \exp(-r^{1+\nu} - rc_1) \\
&\quad \leqslant \tilde{G}(0,0,\mathbf{p}) \leqslant |\mathbf{p}|^{-2\omega}\int_0^\infty d\rho(2\pi\rho)^{-1/2}\int_0^1 ds \int du(2\pi)^{-1/2} \\
&\quad \times (s(1-s))^{-\nu/(1+\nu)}|\tilde{V}_1(u)|_0^{-\omega} \exp\left(-\frac{u^2}{2}\right)\exp(-\rho^{1+\nu}).
\end{aligned} \tag{62}$$

The inequalities (62) coincide with (58) because under our assumptions the integrals in Eq. (62) are finite. The last statement of Theorem 4 follows from the inequalities (60) because the behavior for large $\mathbf{p}$ follows from the behavior of $\tilde{P}_\tau$ for a small τ. If $\nu>0$, then in Eq. (60) $\tau^{1+\nu}<A\tau$ for any A and a sufficiently small τ. Hence, we obtain the same behavior of $\tilde{G}$ for large momenta as in the case $\tilde{V}=1$.

We would like to note that the restrictive form (56) of $\mathcal{V}$ is not necessary. As an example we could consider $\mathcal{V}$ which has singularities at several points, e.g.,

$$\mathcal{V}(\eta)=\mathbf{p}^2(a_0|\eta-\eta_0|^{2\nu_0}+\kappa|\eta|^{2\nu}) \tag{63}$$

with $|\nu_0|<|\nu|$ (only negative indices are nontrivial). An application of the lower and upper bounds (31) and (34) to the potential (63) leads to the conclusion that after an integration upon τ the inequalities (40) hold true for $|\mathbf{p}|>\Lambda$. Hence, the leading singularity ν determines the behavior at large momenta.

V. DISCUSSION AND SUMMARY

As we pointed out in the Introduction our results concerning the Green functions can find an application to quantum field theory in an expanding universe. The stronger damping in momenta [Eq. (40)] in the inflationary models ($\alpha>1$) at $\eta=\eta'=0$ indicates that it would be promising to start quantization at this time ($\eta=0$ corresponds to $t=\infty$ in cosmological models with $\alpha>\frac{1}{3}$). The exponential inflation can be obtained as a limit $\alpha\to\infty$ which corresponds to $\nu=-\frac{2}{3}$. This limit is beyond our rigorous approach but it could be treated by means of more sophisticated methods of Ref. 9. By a formal scaling argument we obtain again the behavior (40) which in inflationary cosmological models is known as the Harrison–Zeldovich spectrum of scalar fluctuations.[1,15] The Green functions can be applied in order to derive a solution of Einstein equations linearized around the homogeneous background.[12,13] In such a case in addition to the scalar Green function the tensor Green function must be studied as well. Further consequences of our estimates concerning the spectrum of $\tilde{G}$ for the complete theory still need to be explored. For this purpose a detailed dependence of the Green function on η and η' would be useful. It is much harder to derive such estimates than the ones for the time zero case. In the Appendix we investigate the upper bound G^U for general η. In particular, calculations performed there suggest that it is only the behavior of $\mathcal{V}(y)$ for small y which is relevant for Theorem 4 and that the upper bound is valid for all $\nu>-1+1/d$. For the lower bound G^L we can also obtain an integral representation. However, it is quite complicated.

Another motivation for a study of the $(d+1)$-dimensional Green functions comes from the problem of a dimensional reduction of quantum fields defined on a brane.[16] In such a case we restrict ourselves to a d-dimensional submanifold imposing the condition $\eta=\eta'=0$. We have proved here that if the metric has a power-law behavior, then the Green functions of the restricted quantum field theory are decaying faster in the momentum space than the standard $|\mathbf{p}|^{-1}$. In particular, for $\nu=-\frac{1}{2}$ we obtain the propagator $|\mathbf{p}|^{-2}$ in d-dimensions which is the same as the one of the Euclidean massless free field.

APPENDIX

We calculate the upper bound for the Green function $\tilde{G}$ following the form of Eqs. (26) and (13) in more detail. Set $u=\sqrt{\tau}y$ and let us perform the integration upon τ in Eq. (26) with $W=0$. Then

$$\tilde{G}^U(\eta,\eta',\mathbf{p})=2(2\pi)^{-1/2}\int_0^1 ds\int du(2\pi s(1-s))^{-1/2}K_0(\sqrt{2M\mathbf{p}\tilde{V}\mathbf{p}(u)}), \tag{A1}$$

where

$$M = (\eta' - \eta)^2 + (s(1-s))^{-1}(u - \eta - s(\eta' - \eta))^2 \tag{A2}$$

and K_ρ is the modified Bessel function of order ρ.[17]

The integral is simpler if $\eta = \eta'$

$$\tilde{G}^U(\eta, \eta, \mathbf{p}) = \pi^{-1} \int_0^1 ds \int du\, K_0(N\sqrt{2\mathbf{p}\tilde{V}\mathbf{p}(u)}), \tag{A3}$$

where

$$N = (s(1-s))^{-1/2}\eta - u. \tag{A4}$$

If $\eta' = \eta = 0$, then the integral (A1) further simplifies. If additionally V is scale invariant, then we can calculate it exactly as in Sec. III.

For arbitrary η and η' the behavior of $\tilde{G}^U$ is much more complicated because the decay of $\tilde{G}^U$ substantially depends on η. In the simplest case, when $\tilde{V} = \frac{1}{2}$

$$\tilde{G}(\eta, \eta', \mathbf{p}) = |\mathbf{p}|^{-1} \exp(-|\mathbf{p}||\eta' - \eta|). \tag{A5}$$

Let us consider an arbitrary V and assume that it behaves as

$$V(\lambda y) = \lambda^{2\nu} B_\lambda(y) \tag{A6}$$

when $\lambda \to 0$ with a certain B_λ, which as a function of λ is bounded from above and from below, i.e., $C_2(y) \geqslant B_\lambda(y) \geqslant C_1(y) > 0$ for a small λ. Let us change variables in Eq. (A1)

$$u = |\mathbf{p}|^{-1/(1+\nu)} y. \tag{A7}$$

Assume that $|\mathbf{p}| \to \infty$, $\eta \to 0$, and $\eta' \to 0$ in such a way that $\theta = |\mathbf{p}|^{1/(1+\nu)}\eta$ and $\theta' = |\mathbf{p}|^{1/(1+\nu)}\eta'$ remain finite. In such a case from Eq. (A1) we can conclude that

$$\tilde{G}(|\mathbf{p}|^{-1/(1+\nu)}\theta, |\mathbf{p}|^{-1/(1+\nu)}\theta', \mathbf{p}) \simeq |\mathbf{p}|^{-2\omega} \tag{A8}$$

for large $\mathbf{p}$ in agreement with Eqs. (40) and (A5) ($\nu = 0$ for a constant $\tilde{V}$).

Equations (A1)–(A4) give an integral representation of the upper bound which is expected to approximate the exact Green function $\tilde{G}$ for large $\mathbf{p}$. We suppose that the Fourier transform G^U of $\tilde{G}^U$ is a reliable approximation to G at short distances. After the Fourier transform of Eq. (26) with $W = 0$ we can calculate the τ integral in Eq. (13) exactly. We obtain

$$G^U(\eta, \mathbf{x}, \eta', \mathbf{x}') = (2\pi)^{-(d+2)/2} \int_0^1 ds (s(1-s))^{-1/2} \int dy (\det \tilde{V}(y))^{-1/2} ((\mathbf{x} - \mathbf{x}')\tilde{V}^{-1}(y)(\mathbf{x} - \mathbf{x}')$$
$$+ (\eta - \eta')^2 + (s(1-s))^{-1}(y - \eta - s(\eta' - \eta))^2)^{-d/2}. \tag{A9}$$

If $\tilde{V}^{ij}(y) = \delta^{ij} v(y)$, then the formula (A9) can be expressed in a simpler form

$$G^U(\eta, \mathbf{x}, \eta', \mathbf{x}') = (2\pi)^{-(d+2)/2} \int_0^1 ds (s(1-s))^{-1/2} \int dy (|\mathbf{x} - \mathbf{x}'|^2 + v(y)(\eta - \eta')^2$$
$$+ (s(1-s))^{-1} v(y)(y - \eta - s(\eta' - \eta))^2)^{-d/2}. \tag{A10}$$

If $v = 1$, then Eq. (A10) gives

$$(2\pi)^{-(d+1)/2}(|\mathbf{x} - \mathbf{x}'|^2 + (\eta - \eta')^2)^{-(d-1)/2}, \tag{A11}$$

as it should.

The integrals (A9) and (A10) suggest some generalizations of the theorems proved in the main part. First, assume that $V(y) \simeq |y|^{2\rho}$ for a large $|y|$. Then the integrals (A9) and (A10) are finite (for $|\mathbf{x}-\mathbf{x}'| \neq 0$) if $\rho > -1+1/d$. Next, it can be shown from Eq. (A10) that if $v(y) \simeq |y|^{2\nu}$ for $y \to 0$ and $\eta = \eta' = 0$, then

$$G^U(0,\mathbf{x},0,\mathbf{x}') \simeq |\mathbf{x}-\mathbf{x}'|^{-d+1/(1+\nu)}$$

for $\mathbf{x}-\mathbf{x}' \to 0$. The derivation of the result (44) based on Eq. (A10) suggests that for Theorem 4 only the behavior of $V(y)$ for a small y is relevant [assuming the integral (A10) is finite].

For general v and arbitrary $\mathbf{x}, \mathbf{x}', \eta$ and η' it is harder to obtain usable estimates. Let us mention some special cases. It follows directly from Eq. (41) that

$$G(\eta,\mathbf{x},0,\mathbf{x}) \simeq |\eta|^{-d(1+\nu)+1}$$

and

$$G(0,\mathbf{x},\eta',\mathbf{x}) \simeq |\eta'|^{-d(1+\nu)+1},$$

whereas from Eq. (A10) we obtain that if $v(\eta) \neq 0$, then

$$G^U(\eta,\mathbf{x},\eta,\mathbf{x}') \simeq v(\eta)^{-1/2}|\mathbf{x}-\mathbf{x}'|^{-d+1} \tag{A12}$$

when $\mathbf{x} \to \mathbf{x}'$.

If $V(y) \geqslant c|y|^{2\rho}$ with $c > 0$ and $\rho > -1+1/d$ for large y, then changing the integration variable $y = |\mathbf{x}-\mathbf{x}'|^{1/(1+\rho)}z$ we can show that for any η and η' there exists A such that if $|\mathbf{x}-\mathbf{x}'| \geqslant A$, then

$$G^U(\eta,\mathbf{x},\eta',\mathbf{x}') \leqslant K|\mathbf{x}-\mathbf{x}'|^{-d+1/(1+\rho)}. \tag{A13}$$

When $\rho > 0$, then Eq. (A13) gives a nontrivial estimate saying that the Green function has a stronger decay for large distances than the one for operators with constant coefficients. However, such a decay at large distances will be changed by most perturbations W whereas the behavior for short distances is remarkably stable with respect to perturbations.

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Mass renormalization in nonrelativistic quantum electrodynamics

Fumio Hiroshima[a)]
Department of Mathematics and Physics, Setsunan University, 572-8508, Osaka, Japan

Herbert Spohn[b)]
Zentrum Mathematik and Physik Department, TU München, D-80290, München, Germany

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In nonrelativistic quantum electrodynamics the charge of an electron equals its bare value, whereas the self-energy and the mass must be renormalized. In our contribution we study perturbative mass renormalization, including second order in the fine structure constant α, in the case of a single, spinless electron. As is well known, if m denotes the bare mass and m_{eff} the mass computed from the theory, to order α one has $m_{\mathrm{eff}}/m=1+(8\alpha/3\pi)\log(1+\frac{1}{2}(\Lambda/m))+O(\alpha^2)$ which suggests that $m_{\mathrm{eff}}/m=(\Lambda/m)^{8\alpha/3\pi}$ for small α. If correct, in order α^2 the leading term should be $\frac{1}{2}((8\alpha/3\pi)\log(\Lambda/m))^2$. To check this point we expand m_{eff}/m to order α^2. The result is $\sqrt{\Lambda/m}$ as leading term, suggesting a more complicated dependence of m_{eff} on m. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1852699]

I. INTRODUCTION

Nonperturbative renormalization in relativistic quantum electrodynamics (QED) remains as a mathematical challenge. Thus it is of interest to study simplified candidates, an obvious one being nonrelativistic QED. In this theory, with comparable little effort, one can start from a self-adjoint Hamiltonian operator and thus has a well-defined mathematical framework. As an additional simplification, there is no charge renormalization because of the absence of positrons. Nevertheless, even in nonrelativistic QED, energy and mass renormalization remain poorly understood. Our, admittedly modest, contribution is to study mass renormalization including order α^2.

Let us first explain the basic Hamiltonian. We consider a single, spinless free electron coupled to the quantized radiation field. We will use relativistic units and employ immediately the total momentum representation. Then the Hilbert space of states is the symmetric Fock space, $\mathcal{F}$, over the one-particle space $L^2(\mathbb{R}^3\times\{1,2\})$, i.e.,

$$\mathcal{F}=\oplus_{n=0}^{\infty}[\otimes_s^n L^2(\mathbb{R}^3\times\{1,2\})].$$

The inner product in $\mathcal{F}$ is denoted by $(\cdot,\cdot)$ and the Fock vacuum by Ω. On $\mathcal{F}$ we introduce the Bose field

$$a(f)=\sum_{j=1,2}\int f(k,j)^* a(k,j)\mathrm{d}k, \quad f\in L^2(\mathbb{R}^3\times\{1,2\}). \tag{1.1}$$

Operators $a(f)$ and $a(f)^*=a^*(f)$ are densely defined and satisfy the CCR,

$$[a(f),a^*(g)]=(f,g)_{L^2(\mathbb{R}^3\times\{1,2\})},$$

a)Electronic mail: hiroshima@mpg.setsunan.ac.jp
b)Electronic mail: spohn@ma.tum.de

$$[a(f),a(g)]=0,$$

$$[a^*(f),a^*(g)]=0.$$

The kinetic energy of the photon is given by

$$H_f=\sum_{j=1,2}\int \omega(k)a^*(k,j)a(k,j)\mathrm{d}k, \tag{1.2}$$

which is the second quantization of $\omega(k)=|k|$ considered as a multiplication operator on $L^2(\mathbb{R}^3)$. Similarly the momentum of the photon field is

$$P_f=\sum_{j=1,2}\int ka^*(k,j)a(k,j)\mathrm{d}k. \tag{1.3}$$

The coupling of the electron to the Maxwell field is mediated through the transverse vector potential $A_{\hat{\varphi}}$ defined by

$$A_{\hat{\varphi}}=\frac{1}{\sqrt{2}}(a(f_{\hat{\varphi}})+a^*(f_{\hat{\varphi}})), \tag{1.4}$$

where

$$f_{\hat{\varphi}}(k,j)=\frac{1}{\sqrt{\omega}}\hat{\varphi}(k)e(k,j),\quad k\in\mathbb{R}^3,\quad j=1,2, \tag{1.5}$$

with $k/|k|$, $e(k,1)$, $e(k,2)$ forming a right-handed dreibein in $\mathbb{R}^3$. $\hat{\varphi}$ is the form factor which, as a minimal assumption, satisfies

$$\int_{\mathbb{R}^3}|\hat{\varphi}(k)|^2(\omega(k)^{-2}+\omega(k))\mathrm{d}k<\infty. \tag{1.6}$$

Later on, we will make a more specific choice of $\hat{\varphi}$.

With these definitions the Hamiltonian under study is

$$H_{\hat{\varphi}}(p)=\tfrac{1}{2}:(p-P_f-eA_{\hat{\varphi}})^2:+H_f,\quad p\in\mathbb{R}^3, \tag{1.7}$$

where p is the total momentum, e the charge, to be definite $e\geqslant 0$, and $:X:$ denotes the Wick order of X. $H_{\hat{\varphi}}(p)$ with domain $D(H_f+\frac{1}{2}P_f^2)=D(H_f)\cap D(\frac{1}{2}P_f^2)$ is self-adjoint for e and p with $|e|<e_0$ and $|p|<p_0$ for some e_0 and p_0, provided (1.6) holds. The energy-momentum relation is defined as the bottom of the spectrum of $H_{\hat{\varphi}}(p)$,

$$E_{\hat{\varphi}}(p)=\inf\sigma(H_{\hat{\varphi}}(p)). \tag{1.8}$$

In (1.7) the bare mass m of the electron is still missing. It appears in two places. First the form factor depends on m. Let us assume a sharp ultraviolet cutoff Λ. Then

$$\hat{\varphi}(k)=\hat{\varphi}_0(mck/\Lambda),\quad \Lambda>0,$$

$$\hat{\varphi}_0(k)=\begin{cases}(2\pi)^{-3/2} & \text{for } |k|\leqslant 1,\\ 0 & \text{for } |k|>1,\end{cases} \tag{1.9}$$

with $1/mc$ the Compton wavelength. Second, energy is to be measured in units of mc^2 and momentum in units of mc. We henceforth set $c=1$ (and also $\hbar=1$). Thus the true energy-momentum relation of the Pauli–Fierz Hamiltonian is

$$E_{m,\Lambda}(p) = mE_{\hat{\varphi}}(p/m), \quad \hat{\varphi} \text{ of (1.9)}. \tag{1.10}$$

Note that equivalently $E_{m,\Lambda}(p)$ is given through

$$E_{m,\Lambda}(p) = \inf \sigma\left(\frac{1}{2m} :(p - P_f - eA_{\hat{\varphi}_0(\cdot/\Lambda)})^2: + H_f \right).$$

Removal of the ultraviolet cutoff Λ through mass renormalization means to find sequences

$$\Lambda \to \infty, \quad m \to 0 \tag{1.11}$$

such that $E_{m,\Lambda}(p) - E_{m,\Lambda}(0)$ has a nondegenerate limit. A convenient criterion for nondegeneracy is the curvature of $E_{m,\Lambda}(p)$ at $p=0$, in other words the inverse effective mass. Let us assume for a moment an infrared cutoff,

$$\hat{\varphi}(k) = 0 \quad \text{for } |k| < \kappa/m$$

with some $0 < \kappa$. Then it is known[1] that, for $|e| < e_*$, $|p| < p_*$ with suitable $e_* > 0$ and $p_* > 0$, $H_{\hat{\varphi}}(p)$ has a nondegenerate ground state $\psi_g(p)$ separated by a gap from the continuum, i.e.,

$$H_{\hat{\varphi}}(p)\psi_g(p) = E_{\hat{\varphi}}(p)\psi_g(p), \quad \psi_g(p) \in \mathcal{F},$$

has a unique solution. Let us set

$$E_{m,\Lambda}(p) - E_{m,\Lambda}(0) = \frac{1}{2m_{\text{eff}}} p^2 + \mathcal{O}(|p|^3) \tag{1.12}$$

for small p. Then, using second order perturbation theory in (1.10), one obtains

$$\frac{m}{m_{\text{eff}}} = 1 - \frac{2}{3} \sum_{\mu=1,2,3} \frac{(\psi_g(0), (P_f + eA_{\hat{\varphi}})_\mu (H_{\hat{\varphi}}(0) - E_{\hat{\varphi}}(0))^{-1} (P_f + eA_{\hat{\varphi}})_\mu \psi_g(0))}{(\psi_g(0), \psi_g(0))}. \tag{1.13}$$

We assume that this formula remains valid also when $\kappa = 0$.

On the basis of (1.13), mass renormalization can be discussed more precisely. From (1.13) it trivially follows that m/m_{eff} depends only on the ratio Λ/m. It is convenient to express this dependence in the form

$$\frac{m_{\text{eff}}}{m} = h(\Lambda/m). \tag{1.14}$$

Clearly $h \geqslant 1$ and $h(0) = 1$. Let us set

$$\lambda = \frac{\Lambda}{m}. \tag{1.15}$$

One expects that h is increasing in λ, because with increasing Λ more photons are bound to the electron which makes m_{eff} larger.

Let us distinguish several cases. If h has a finite limit as $\lambda \to \infty$, then the mass renormalization is finite,

$$m_{\text{eff}} = h(\infty)m.$$

Such kind of behavior occurs in the Nelson model.[2] Second, let us consider the case that $h(\lambda)$ increases linearly for large λ. We set

$$h(\lambda) = 1 + b_0\lambda$$

with $b_0 > 0$. Then

$$m_{\text{eff}} = m + b_0\Lambda. \tag{1.16}$$

Hence mass renormalization is additive. This behavior is found in the dipole approximation to the Pauli–Fierz Hamiltonian, e.g., Ref. 3, and in the classical Abraham model.[4] If $m_{\text{eff}} > 0$ is imposed, then as $\Lambda \to \infty$ necessarily $m \to -\infty$. As soon as $m < 0$, $mH_{\hat{\varphi}}(p/m)$ is not bounded from below. Therefore we regard the theory as not renormalizable. Thus the case of interest is when for large λ,

$$h(\lambda) \simeq b_0\lambda^{\gamma}, \quad b_0 > 0, \quad 0 < \gamma < 1, \tag{1.17}$$

which defines the scaling exponent γ and the amplitude b_0. γ depends on e, as does b_0. Inserting (1.17) in (1.14), one obtains for sufficiently large λ,

$$\frac{m_{\text{eff}}}{m} \simeq b_0\left(\frac{\Lambda}{m}\right)^{\gamma}. \tag{1.18}$$

Thus the choice

$$m = \Lambda^{-\gamma/(1-\gamma)} b_1^{1/(1-\gamma)} \tag{1.19}$$

yields

$$\lim_{\Lambda\to\infty} m_{\text{eff}}(\Lambda) = m^* = b_0 b_1. \tag{1.20}$$

Here b_0 is fixed by $h(\lambda)$ and b_1 is a parameter which can be adjusted to yield the experimentally determined mass of the electron.

Of course, the difficulty with our discussion is that, while the scaling function is well defined, at present we have no technique to find out its behavior for large λ. For that reason we turn to perturbative renormalization which, through the interchange of the limits $\Lambda \to \infty$ and $e \to 0$, tries to guess the proper value of γ. The details will be given in the following sections, but let us summarize briefly our findings. The fine structure constant is defined through

$$\alpha = \frac{e^2}{4\pi}. \tag{1.21}$$

To first order one finds

$$h(\lambda) = 1 + \frac{8\alpha}{3\pi}\log\left(1 + \frac{1}{2}\lambda\right) + \mathcal{O}(\alpha^2), \tag{1.22}$$

which suggests

$$h(\lambda) \simeq \lambda^{8\alpha/3\pi} \tag{1.23}$$

for sufficiently large λ and therefore

$$\gamma = \frac{8\alpha}{3\pi}, \quad \alpha \ll 1. \tag{1.24}$$

To have a control check, one assumes that to second order

$$h(\lambda) \simeq \lambda^{(8/3\pi)\alpha + b\alpha^2} \simeq 1 + \frac{8\alpha}{3\pi}\log\lambda + \frac{1}{2}\left(\frac{8\alpha}{3\pi}\log\lambda\right)^2 + b\alpha^2\log\lambda + \mathcal{O}(\alpha^3) \tag{1.25}$$

for small α. Therefore by expanding m_{eff}/m to order α^2, one should find a term $(\log\lambda)^2$ with an already determined prefactor and a term proportional to $\log\lambda$, together with lower order terms. As to explain, this guess is not confirmed. *Instead* we prove that

$$h(\lambda) = 1 + \frac{8\alpha}{3\pi}\log\left(1 + \frac{1}{2}\lambda\right) + c_0\alpha^2\sqrt{\lambda} + \mathcal{O}(\alpha^3), \quad c_0 > 0, \tag{1.26}$$

for $|\alpha|$ small enough *depending on* Λ, which could suggest $\gamma = \frac{1}{2}$ independent of e.

Note added in proof: Since the completion of this work, Hiroshima and Ito[5] extended the investigation to include the spin of the electron. The number of terms in the perturbation series up to the same order as studied here is then multiplied by a factor of 4. As a net result one finds that the leading divergence is proportional to λ^2, rather than $\lambda^{1/2}$. Because of the interaction with the quantized magnetic field the effective mass (at the order considered) is more strongly ultraviolet divergent when spin is included.

Some aspects of the effective mass and its renormalization have been studied before. Spohn[6] investigates the effective mass of the Nelson model[2] from a functional integral point of view. Lieb and Loss[7,8] study mass renormalization and binding energies for various models of matter coupled to the radiation field including the Pauli–Fierz model. Hainzl[9] and Hainzl and Seiringer[10] compute the leading order of the effective mass of the Pauli–Fierz Hamiltonian with spin $1/2$.

Our paper is organized in the following way. In Sec. II we review under which conditions $E_{\hat{\varphi}}(p) = E_{\hat{\varphi}}(p,e)$ is jointly analytic in p and e. In Sec. III we set up the perturbation theory for the effective mass and work out explicitly the terms including α^2. Their asymptotics with $\Lambda \to \infty$ is studied in Sec. IV.

II. GROUND STATE AND ITS ANALYTIC PROPERTIES

Throughout this paper we assume that

$$\hat{\varphi}(k) = \begin{cases} 0 & \text{for } |k| < \kappa/m, \\ (2\pi)^{-3/2} & \text{for } \kappa/m \leqslant |k| \leqslant \Lambda/m, \\ 0 & \text{for } |k| > \Lambda/m. \end{cases}$$

For notational convenience, we shall use notations $H(p)$, A, and $E(p)$ instead of $H_{\hat{\varphi}}(p)$, $A_{\hat{\varphi}}$, and $E_{\hat{\varphi}}(p)$, respectively. Let $\mathcal{F}_\kappa$ (respectively, $\mathcal{F}_{\kappa,0}$) be the symmetric Fock space over $L^2(\mathbb{R}^3_{\kappa/m} \times \{1,2\})$ [respectively, $L^2(\mathbb{R}^{3\perp}_{\kappa/m} \times \{1,2\})$], where $\mathbb{R}^3_{\kappa/m} = \{k \in \mathbb{R}^3 \| k| \geqslant \kappa/m\}$. Then it follows that

$$\mathcal{F} \cong \mathcal{F}_\kappa \otimes \mathcal{F}_{\kappa,0}. \tag{2.1}$$

It is seen that $\mathcal{F}_\kappa$ reduces $H(p)$ and, under the identification (2.1),

$$H(p) \cong \left(H(p)\lceil_{\mathcal{F}_\kappa}\right) \otimes 1 + 1 \otimes \left(H_f\lceil_{\mathcal{F}_{\kappa,0}}\right). \tag{2.2}$$

The bottom of the continuous spectrum of $H(p)\lceil_{\mathcal{F}_\kappa}$ is denoted by $E_c(p)$. Note that $\inf \sigma(H(p)\lceil_{\mathcal{F}_\kappa}) = E(p)$. The following lemma can be proven in the similar manner as in Ref. 11.

Lemma 2.1 (Ref. 11): There exists a constant $p_* > 0$ independent of e with $|e| < e_0$ such that for $p \in \mathbb{R}^3$ with $|p| < p_*$,

$$E_c(p) - E(p) > 0.$$

In particular there exists a ground state $\psi_{g,\kappa}(p) \in \mathcal{F}_\kappa$ of $H(p)\lceil_{\mathcal{F}_\kappa}$ for $p \in \mathbb{R}^3$ provided $|p| < p_*$.

By Lemma 2.1, we see that $H(p)$ has the ground state

$$\psi_g(p) = \psi_{g,\kappa}(p) \otimes \Omega_{\kappa,0}$$

for $p \in \mathbb{R}^3$ provided $|p| < p_*$, where $\Omega_{\kappa,0}$ denotes the vacuum of $\mathcal{F}_{\kappa,0}$. To have uniqueness, one proves that for any ground state $\psi_g(p)$, one has

$$(\psi_g(p), \Omega) > 0$$

provided $|p| < p_*$ and $|e| < e_*$ with some e^*.

Lemma 2.2 (Ref. 1): There exists a constant $e_* > 0$ such that for $(p,e) \in \mathbb{R}^3 \times \mathbb{R}$ with

$|p|<p_*$ *and* $|e|<e_*$, *the ground state of* $H(p)$ *is unique up to multiple constants.*

Remark 2.3: In the case $\kappa=0$ *and for sufficiently small* e, *Chen*[12] *proves the absence of a ground state of* $H(p)$ *in* $\mathcal{F}$ *for* $p\neq 0$ *and the existence of a ground state of* $H(0)$.

We also need the analytic properties of $\psi_g(p)=\psi_g(p,e)$ and $E(p)=E(p,e)$ with respect to $(p,e)\in\mathbb{R}^3\times\mathbb{R}$ in a neighborhood of $(0,0)\in\mathbb{R}^3\times\mathbb{R}$.

Lemma 2.4: There exists an open neighborhood $\mathcal{O}$ *of* $(0,0)\in\mathbb{R}^3\times\mathbb{R}$ *such that* $\psi_g(p,e)$ *is strongly analytic and* $E(p,e)$ *analytic on* $\mathcal{O}$.

Proof: Let $\psi_{g,\kappa}(p)\in\mathcal{F}_\kappa$ be the ground state of $H(p)\restriction_{\mathcal{F}_\kappa}$. Since $\psi_g(p)=\psi_{g,\kappa}(p)\otimes\Omega_{\kappa,0}$, it is enough to show that $\psi_{g,\kappa}(p)$ is strongly analytic on $\mathcal{O}$. We split $H(p)$ as

$$H(p)=H_0(p)+H_I(p), \tag{2.3}$$

where

$$H_0(p)=\tfrac{1}{2}(p-P_f)^2+H_f,$$

$$H_I(p)=-e(p-P_f)\cdot A+\frac{e^2}{2}{:}A^2{:}\,.$$

Then we obtain that

$$\|H_I(p)\Psi\|_{\mathcal{F}_\kappa}\leqslant c_4\|H_0(p)\Psi\|_{\mathcal{F}_\kappa}+c_5\|\Psi\|_{\mathcal{F}_\kappa} \tag{2.4}$$

for $\Psi\in D(H_0(p)\restriction_{\mathcal{F}_\kappa})=D(H_f)\cap D(P_f{}^2)\cap\mathcal{F}_\kappa$. Then $H(p)\restriction_{\mathcal{F}_\kappa}$ is an analytic family of type (A) for e near $e=0$ (see Ref. 13, p. 16). Thus by Ref. 13, Theorem XII.9, $H(p)\restriction_{\mathcal{F}_\kappa}$ is an analytic family in the sense of Kato, which implies that by Ref. 13, Theorem XII.8, together with Lemmas 2.1 and 2.2, $\psi_{g,\kappa}(p,e)$ is strongly analytic and $E(p,e)$ analytic for e near $e=0$. Alternatively we split $H(p)$ as

$$H(p)=H_0'+p\cdot H_I'+\tfrac{1}{2}p^2,$$

where

$$H_0'=\tfrac{1}{2}{:}(P_f+eA_{\hat{\varphi}})^2{:}+H_f,\quad H_I'=-(P_f+eA_{\hat{\varphi}}).$$

Then we have

$$\|H_I'\Psi\|_{\mathcal{F}_\kappa}\leqslant c_6\|H_0'\Psi\|_{\mathcal{F}_\kappa}+c_7\|\Psi\|_{\mathcal{F}_\kappa} \tag{2.5}$$

with some constants c_6 and c_7 for $\Psi\in D(H_f)\cap D(P_f{}^2)\cap\mathcal{F}_\kappa$. Thus $H(p)\restriction_{\mathcal{F}_\kappa}$ is an analytic family of type (A) for $p\in\mathbb{R}^3$ near $p=0$. We can see that $\psi_{g,\kappa}(p,e)$ is strongly analytic and $E(p,e)$ analytic for p near $p=0$ in the similar manner as for e. ■

III. EFFECTIVE MASS

A. Formulas

In what follows we assume that $(p,e)\in\mathcal{O}$. By the definition of $E(p,e)$, we have

$$\frac{m}{m_{\text{eff}}}=\frac{1}{3}\Delta_p E(p,e)\restriction_{p=0}. \tag{3.1}$$

Actually we can see in Ref. 1 that $H(p)$ is unitarily equivalent to $H(|p|n_z)$, where $n_z=(0,0,1)$. Thus $E(p,e)=\tilde{E}(|p|,e)=\inf\sigma(H(|p|n_z))$ and

$$\frac{m}{m_{\text{eff}}}=\partial_{|p|}^2\tilde{E}(|p|,e)\restriction_{|p|=0}.$$

Moreover we see that $\tilde{E}(-|p|,e)=\tilde{E}(|p|,e)$. Then

$$\partial p_\mu E(p,e)\big|_{p_\mu=0} = 0, \quad \mu = 1,2,3. \tag{3.2}$$

Since $E(p,e)$ also has the symmetry, $E(p,-e)=E(p,e)$, $E(p,e)$ is a function of e^2. In particular it follows that

$$\partial_e^{2m+1} E(p,e)\big|_{e=0} = 0, \quad m \geqslant 0. \tag{3.3}$$

Lemma 3.1: The ratio m/m_{eff} can be expressed as

$$\frac{m}{m_{\text{eff}}} = 1 - \frac{2}{3}\sum_{\mu=1,2,3} \frac{(\psi_g(0),(P_f+eA)_\mu (H(0)-E(0))^{-1}(P_f+eA)_\mu \psi_g(0))}{(\psi_g(0),\psi_g(0))}.$$

Proof: Since

$$(H(p)\Psi,\psi_g(p)) = E(p)(\Psi,\psi_g(p)),$$

for $\Psi \in D(H(p))$, taking a derivative with respect to p_μ on the both sides above, we have

$$(H'_\mu(p)\Psi,\psi_g(p)) + (H(p)\Psi,\psi'_{g_\mu}(p)) = E'_\mu(p)(\Psi,\psi_g(p)) + E(p)(\Psi,\psi'_{g_\mu}(p)) \tag{3.4}$$

and

$$\begin{aligned}(H''_\mu(p)\Psi,\psi_g(p)) + 2(H'_\mu(p)\Psi,\psi'_{g_\mu}(p)) + (H(p)\Psi,\psi''_{g_\mu}(p))\\ = E''_\mu(p)(\Psi,\psi_g(p)) + 2E'_\mu(p)(\Psi,\psi'_{g_\mu}(p)) + E(p)(\Psi,\psi''_{g_\mu}(p)).\end{aligned} \tag{3.5}$$

Here $E'_\mu(p)$ [respectively, $\psi'_{g_\mu}(p)$] denotes the derivative (respectively, strong derivative) in p_μ, and $H'_\mu(p)=(p-P_f-eA_{\hat{\varphi}})_\mu$, $H''_\mu(p)=1$. By (3.2) it follows that $E'_\mu(0)=0$, and by (3.4) with $p=0$,

$$(P_f+eA)_\mu \psi_g(0) \in D((H(0)-E(0))^{-1}),$$

and

$$\psi'_{g_\mu}(0) = (H(0)-E(0))^{-1}(P_f+eA)_\mu \psi_g(0).$$

Therefore, using (3.1) and (3.5), we have

$$\begin{aligned}\frac{m}{m_{\text{eff}}} &= \frac{1}{3}\sum_{\mu=1,2,3} \frac{(\psi_g(0),E''(0)_\mu \psi_g(0))}{(\psi_g(0),\psi_g(0))}\\ &= \frac{1}{3}\sum_{\mu=1,2,3}\left\{1 + \frac{(\psi_g(0),2H'_\mu(0)\psi'_{g_\mu}(0))}{(\psi_g(0),\psi_g(0))}\right\}\\ &= 1 - \frac{2}{3}\sum_{\mu=1,2,3} \frac{((P_f+eA)_\mu\psi_g(0),(H(0)-E(0))^{-1}(P_f+eA)_\mu\psi_g(0))}{(\psi_g(0),\psi_g(0))}.\end{aligned} \tag{3.6}$$

Thus the lemma follows. ■

From this lemma we obtain the following corollary.

Corollary 3.2: Let $|e|<e_*$. Then $m_{\text{eff}} \geqslant m$.

B. Perturbative expansions

Let

$$\psi_g(0) = \sum_{n=0}^{\infty} \frac{e^n}{n!}\varphi_n, \quad E(0) = \sum_{n=0}^{\infty} \frac{e^{2n}}{(2n)!}E_{2n}.$$

We want to get the explicit form of φ_n. Let

$$\mathcal{F}_{\rm fin} = \{\{\Psi^{(n)}\}_{n=0}^{\infty} \in \mathcal{F} | \Psi^{(m)} = 0 \quad \text{for } m \geqslant \ell \text{ with some } \ell\},$$

$$\mathcal{F}_0 = \{\Psi \in \mathcal{F}_{\rm fin} | ({\rm i}) \Psi^{(0)} = 0, ({\rm ii}) {\rm supp}_{k \in \mathbb{R}^{3n}} \Psi^{(n)}(k,j) \not\ni \{0\}, n \geqslant 1, j \in \{1,2\}^n\}.$$

Lemma 3.3: It follows that $\mathcal{F}_0 \subset D(H_0^{-1})$.

Proof: Let $\Psi = \{\Psi^{(n)}\}_{n=0}^{\infty} \in \mathcal{F}_0$. Since

$$(H_0^{-1}\Psi)^{(n)}(k_1, \ldots, k_n, j_1, \ldots, j_n) = \left[\frac{1}{2}(k_1 + \cdots + k_n)^2 + \sum_{i=1}^{n} \omega(k_i)\right]^{-1} \Psi^{(n)}(k_1, \ldots, k_n, j_1, \ldots, j_n),$$

and ${\rm supp}_{(k_1,\ldots,k_n) \in \mathbb{R}^{3n}} \Psi^{(n)}(k_1, \ldots, k_n, j_1, \ldots, j_n) \not\ni \{(0, \ldots, 0)\}$, we obtain that

$$\|H_0^{-1}\Psi\|_{\mathcal{F}}^2 = \sum_{n=1}^{\infty} \|(H_0^{-1}\Psi)^{(n)}\|_{\mathcal{F}^{(n)}}^2 < \infty$$

and the lemma follows. ■

We define A^- and A^+ by

$$A^- = \frac{1}{\sqrt{2}} a(f_{\hat{\varphi}}), \quad A^+ = \frac{1}{\sqrt{2}} a^*(f_{\hat{\varphi}}).$$

Then $A = A^+ + A^-$. Moreover A_μ^- and A_μ^+ are defined by A^- and A^+ with $e(k,j) = (e^1(k,j), e^2(k,j), e^3(k,j))$ replaced by $e^\mu(k,j)$. We split $H(0)$ as

$$H(0) = H_0 + eH_1 + \frac{e^2}{2} H_2,$$

where

$$H_0 = \tfrac{1}{2} P_f^2 + H_f,$$

$$H_1 = \tfrac{1}{2}(P_f \cdot A + A \cdot P_f) = P_f \cdot A = A \cdot P_f,$$

$$H_2 = :A^2: = A^+ \cdot A^+ + A^- \cdot A^- + 2A^+ \cdot A^-.$$

Lemma 3.4: It follows that $E_0 = E_2 = 0$, *and there exists a ground state* $\psi_g(0) = \Sigma_{n=0}^{\infty}(e^n/n!)\varphi_n$ *such that*

$$\varphi_0 = \Omega, \quad \varphi_1 = 0, \quad \varphi_2 = -H_0^{-1} H_2 \Omega, \quad \varphi_3 = 3H_0^{-1} H_1 H_0^{-1} H_2 \Omega. \tag{3.7}$$

In particular $\varphi_2 \in \mathcal{F}^{(2)}$ *and* $\varphi_3 \in \mathcal{F}^{(1)} \oplus \mathcal{F}^{(3)}$.

Proof: It is obvious that $E_0 = 0$. Let $\psi_g(0) = \Sigma_{n=0}^{\infty}(e^n/n!)\varphi_n$ be an arbitrary strongly analytic ground state of $H(0)$ with $(\varphi_0, \Omega) \neq 0$. Let $\rho(e) = \Sigma_{n=0}^{\infty}(e^n/n!)\rho_n$ be an analytic function on e and set $\psi_g^\rho = \rho(e)\psi_g(0)$. Then ψ_g^ρ is also a strongly analytic ground state of $H(0)$ and

$$\psi_g^\rho = \underbrace{\rho_1 \varphi_0}_{=\varphi_0^\rho} + \underbrace{e(\rho_0\varphi_1 + \rho_1\varphi_0)}_{=\varphi_1^\rho} + e^2 \frac{1}{2!} \underbrace{(\rho_0\varphi_2 + 2\rho_1\varphi_1 + \rho_2\varphi_0)}_{=\varphi_2^\rho}$$

$$+ e^3 \frac{1}{3!} \underbrace{(\rho_0\varphi_3 + 3\rho_1\varphi_2 + 3\rho_2\varphi_1 + \rho_3\varphi_0)}_{=\varphi_3^\rho} + \mathcal{O}(e^4).$$

Set

$$\rho_0 = 1/(\varphi_0,\Omega), \quad \rho_1 = -\rho_0(\varphi_1,\Omega)/(\varphi_0,\Omega),$$

$$\rho_2 = -\{\rho_0(\varphi_2,\Omega) + 2\rho_1(\varphi_1,\Omega)\}/(\varphi_0,\Omega),$$

$$\rho_3 = -\{\rho_0(\varphi_3,\Omega) + 3\rho_1(\varphi_2,\Omega) + 3\rho_2(\varphi_1,\Omega)\}/(\varphi_0,\Omega).$$

Then $\psi_g^\rho = \Sigma_{n=0}^\infty (e^n/n!)\varphi_n^\rho$ satisfies that

$$(\varphi_n^\rho,\Omega) = \delta_{0,n}, \quad n = 0,1,2,3. \tag{3.8}$$

We reset ψ_g^ρ (respectively, φ_n^ρ) with (3.8) as $\psi_g(0)$ (respectively, φ_n). Let us write $H(0)$, $E(0)$, and $\psi_g(0)$ as H, E, and ψ_g, respectively. Take derivative in e on the both sides of $(H\Psi,\psi_g) = E(\Psi,\psi_g)$, $\Psi \in D(H)$. Then we have

$$(H'\Psi,\psi_g) + (H\Psi,\psi_g') = E'(\Psi,\psi_g) + E(\Psi,\psi_g'), \tag{3.9}$$

$$(H''\Psi,\psi_g) + 2(H'\Psi,\psi_g') + (H\Psi,\psi_g'') = E''(\Psi,\psi_g) + 2E'(\Psi,\psi_g') + E(\Psi,\psi_g''), \tag{3.10}$$

$$3(H''\Psi,\psi_g') + 3(H'\Psi,\psi_g'') + (H\Psi,\psi_g''') = E'''(\Psi,\psi_g) + 3E''(\Psi,\psi_g') + 3E'(\Psi,\psi_g'') + E(\Psi,\psi_g'''), \tag{3.11}$$

where E' (respectively, ψ_g') denotes the derivative (respectively, strong derivative) in e, and $H' = P_f(P_f + eA)$ and $H'' = P_f \cdot A$. Set $\Psi = \Omega$ and $e = 0$ in (3.10). Then

$$0 = E_2(\Omega,\Omega), \tag{3.12}$$

which shows that $E_2 = 0$. From (3.9) with $e = 0$ it follows that

$$H_1\Omega + H_0\varphi_1 = 0,$$

from which it holds that $H_0\varphi_1 = 0$. Hence $\varphi_1 = b\Omega$ with some constant b. By (3.8) we have, however, $b = 0$. Then $\varphi_1 = 0$ follows. By (3.10) with $e = 0$, we have

$$H_2\Omega + H_0\varphi_2 = 0.$$

Since $H_2\Omega \in \mathcal{F}_0$, we see that by Lemma 3.3, $H_2\Omega \in D(H_0^{-1})$. Thus we have $\varphi_2 = -H_0^{-1}H_2\Omega + c\Omega$ with some constant c. Since $(-H_0^{-1}H_2\Omega,\Omega) = 0$, it follows that $c = 0$ from (3.8). From (3.11) it follows that in $e = 0$,

$$3H_1\varphi_2 + H_0\varphi_3 = 0.$$

Since $H_1\varphi_2 = -H_1H_0^{-1}H_2\Omega \in \mathcal{F}_0$, Lemma 3.3 ensures that $H_1\varphi_2 \in D(H_0^{-1})$. Hence $\varphi_3 = -3H_0^{-1}H_1\varphi_2 + d\Omega = 3H_0^{-1}H_1H_0^{-1}H_2\Omega + d\Omega$ with some constant d. Since $(3H_0^{-1}H_1H_0^{-1}H_2\Omega,\Omega) = 0$, it follows that $d = 0$ from (3.8). Then the lemma is proven. ■

In the similar manner as Lemma 3.4, we can prove the following proposition.

Proposition 3.5: There exists a ground state $\psi_g(0) = \Sigma_{n=0}^\infty (e^n/n!)\varphi_n$ such that

$$\varphi_{2m} = H_0^{-1}\left\{ -\sum_{j=1,2} \binom{2m}{j} H_1\varphi_{2m-j} + \sum_{j=2}^{m} \binom{2m}{2j} E_{2j}\varphi_{2m-2j} \right\}, \quad m \geqslant 2,$$

$$\varphi_{2m+1} = H_0^{-1}\left\{ -\sum_{j=1,2} \binom{2m+1}{j} H_j\varphi_{2m+1-j} + \sum_{j=2}^{m-1} \binom{2m+1}{2j} E_{2j}\varphi_{2m-2j+1} \right\}, \quad m \geqslant 2,$$

with $\varphi_{2m} \in \mathcal{F}^{(2)} \oplus \mathcal{F}^{(4)} \oplus \cdots \oplus \mathcal{F}^{(2m)}$ and $\varphi_{2m+1} \in \mathcal{F}^{(1)} \oplus \mathcal{F}^{(3)} \oplus \cdots \oplus \mathcal{F}^{(2m+1)}$, and E_{2m} is given by

$$E_{2m} = \binom{2m}{2}(\Omega, H_2\varphi_{2m-2}), \quad m \geqslant 2.$$

C. Effective mass up to order e^4

In this section we expand m/m_{eff} up to order e^4.

Lemma 3.6: The ratio m/m_{eff} can be expanded as

$$\begin{aligned}\frac{m}{m_{\text{eff}}} = 1 &- e^2\frac{2}{3}\sum_{\mu=1,2,3}(\Omega, A_\mu H_0^{-1}A_\mu\Omega) \\ &- e^4\frac{2}{3}\sum_{\mu=1,2,3}\Big\{2(\Psi_3^\mu, H_0^{-1}\Psi_1^\mu) + (\Psi_2^\mu, H_0^{-1}\Psi_2^\mu) - 2(\Psi_2^\mu, H_0^{-1}H_1H_0^{-1}\Psi_1^\mu) \\ &\qquad - \frac{1}{2}(\Psi_1^\mu, H_0^{-1}H_2H_0^{-1}\Psi_1^\mu) + (\Psi_1^\mu, H_0^{-1}H_1H_0^{-1}H_1H_0^{-1}\Psi_1^\mu)\Big\} + \mathcal{O}(e^6),\end{aligned} \tag{3.13}$$

where

$$\Psi_1^\mu = A_\mu\Omega,$$

$$\Psi_2^\mu = -\tfrac{1}{2}P_{f\mu}H_0^{-1}(A^+\cdot A^+)\Omega,$$

$$\Psi_3^\mu = \tfrac{1}{2}\big\{-A_\mu H_0^{-1}(A^+\cdot A^+)\Omega + \tfrac{1}{2}P_{f\mu}H_0^{-1}(P_f\cdot A + A\cdot P_f)H_0^{-1}(A^+\cdot A^+)\Omega\big\}.$$

Proof: Since by (3.6),

$$\frac{m}{m_{\text{eff}}} = 1 - \frac{2}{3}\sum_{\mu=1,2,3}\frac{((P_f+eA)_\mu\psi_g(0), \psi_{g_\mu}'(0))}{(\psi_g(0),\psi_g(0))}, \tag{3.14}$$

where $\psi_{g_\mu}'(0) = s\text{-}\partial_{p_\mu}\psi_g(p)\big|_{p=0}$, we expand $\psi_{g_\mu}'(0)$ and $\psi_g(0)$ in e. Assume that $\psi_g(0) = \sum_{n=0}^\infty (e^n/n!)\varphi_n$ satisfies (3.7), i.e., $\varphi_0 = \Omega$, $\varphi_1 = 0$, $\varphi_2 = -H_0^{-1}H_2\Omega$, and $\varphi_3 = 3H_0^{-1}H_1H_0^{-1}H_2\Omega$. We have

$$\begin{aligned}(P_f+eA)_\mu\psi_g(0) &= eA_\mu\Omega + e^2\big(\tfrac{1}{2}P_{f\mu}\varphi_2\big) + e^3\big(\tfrac{1}{2}A_\mu\varphi_2 + \tfrac{1}{6}P_{f\mu}\varphi_3\big) + \mathcal{O}(e^4) \\ &= e\Psi_1^\mu + e^2\Psi_2^\mu + e^3\Psi_3^\mu + \mathcal{O}(e^4).\end{aligned} \tag{3.15}$$

Note that by Proposition 3.5,

$$\varphi_0 \in \mathcal{F}^{(0)}, \quad \varphi_2 \in \mathcal{F}^{(2)}, \quad \varphi_3 \in \mathcal{F}^{(3)}\oplus\mathcal{F}^{(1)}, \quad \varphi_4 \in \mathcal{F}^{(4)}\oplus\mathcal{F}^{(2)}.$$

In particular

$$\frac{1}{(\psi_g,\psi_g)} = 1 - e^4(\frac{1}{2}\varphi_2, \frac{1}{2}\varphi_2) - e^4(\Omega, \frac{1}{24}\varphi_4) + \mathcal{O}(e^6) = 1 - e^4\frac{1}{4}(\varphi_2,\varphi_2) + \mathcal{O}(e^6). \tag{3.16}$$

Let

$$\psi_{g_\mu}'(0) = \sum_{n=0}^\infty \frac{e^n}{n!}\Phi_n^\mu. \tag{3.17}$$

Since

$$((H(0)-E(0))\Psi,\psi'_{g_\mu}(0))=((P_f+eA)_\mu\Psi,\psi_g(0)),\quad \Psi\in D(H(0)),\tag{3.18}$$

setting $e=0$ on the both sides of (3.18), we have

$$H_0\Phi_0^\mu=0.$$

Then

$$\Phi_0^\mu=b_0\Omega\tag{3.19}$$

with some constant b_0. From taking derivative of the both sides of (3.18) at $e=0$, we see that by (3.7),

$$H_0\Phi_1^\mu=A_\mu\Omega,$$

$$H_2\Phi_0^\mu+2H_1\Phi_1^\mu+H_0\Phi_2^\mu=P_{f\mu}\varphi_2,$$

$$3H_2\Phi_1^\mu+3H_1\Phi_2^\mu+H_0\Phi_3^\mu=3A_\mu\varphi_2+P_{f\mu}\varphi_3.$$

From them it follows that

$$\Phi_1^\mu=H_0^{-1}\Psi_1^\mu+b_1\Omega,\tag{3.20}$$

$$\begin{aligned}\Phi_2^\mu&=H_0^{-1}(2\Psi_2^\mu-2H_1\Phi_1^\mu-H_2\Phi_0^\mu)+b_2\Omega\\&=2H_0^{-1}(\Psi_2^\mu-H_1H_0^{-1}\Psi_1^\mu)+(-b_0H_0^{-1}H_2\Omega+b_2\Omega),\end{aligned}\tag{3.21}$$

$$\begin{aligned}\Phi_3^\mu&=H_0^{-1}(6\Psi_3^\mu-3H_1\Phi_2^\mu-3H_2\Phi_1^\mu)+b_3\Omega\\&=6H_0^{-1}\left\{\Psi_3^\mu-H_1H_0^{-1}\Psi_2^\mu+\left(H_1H_0^{-1}H_1H_0^{-1}-\tfrac{1}{2}H_2H_0^{-1}\right)\Psi_1^\mu\right\}\\&\quad+(3b_0H_0^{-1}H_1H_0^{-1}H_2\Omega-3b_1H_0^{-1}H_2\Omega+b_3\Omega),\end{aligned}\tag{3.22}$$

where b_1, b_2, b_3 are some constants. Here we used that $H_1\Omega=0$. By (3.14) (3.15) (3.16) and (3.17) we have

$$\begin{aligned}\frac{m}{m_{\text{eff}}}=1-\frac{2}{3}\sum_{\mu=1}^{3}\Bigg\{&e^2((\Psi_1^\mu,\Phi_1^\mu)+(\Psi_2^\mu,\Phi_0^\mu))\\&+e^4\left(\frac{1}{6}(\Psi_1^\mu,\Phi_3^\mu)+\frac{1}{2}(\Psi_2^\mu,\Phi_2^\mu)+(\Psi_3^\mu,\Phi_1^\mu)\right)\Bigg\}+\mathcal{O}(e^6).\end{aligned}\tag{3.23}$$

Substitute (3.20)–(3.22) into (3.23). No contribution of constants $b_0,\ldots,b_3$ exists, i.e., we can directly see that

$$e^2\{b_1(\Psi_1^\mu,\Omega)+b_0(\Psi_2^\mu,\Omega)\}=0$$

and

$$\begin{aligned}e^4\Bigg\{&\frac{1}{6}b_3(\Psi_1^\mu,\Omega)+\frac{1}{6}b_1(\Psi_1^\mu,-3H_0^{-1}H_2\Omega)+\frac{1}{6}b_0(\Psi_1^\mu,3H_0^{-1}H_1H_0^{-1}H_2\Omega)\\&+\frac{1}{2}b_2(\Psi_2^\mu,\Omega)+\frac{1}{2}b_0(\Psi_2^\mu,-H_0^{-1}H_2\Omega)+b_1(\Psi_3^\mu,\Omega)\Bigg\}=0.\end{aligned}$$

Then the lemma follows. ■

Remark 3.7: By Lemma 3.1 we have seen that

$$\frac{m}{m_{\text{eff}}} = 1 - \frac{2}{3}\sum_{\mu=1,2,3} \frac{((P_f + eA)_\mu \psi_g(0), (H(0) - E(0))^{-1}(P_f + eA)_\mu \psi_g(0))}{(\psi_g(0), \psi_g(0))}. \tag{3.24}$$

We "informally" expand $(H(0)-E(0))^{-1}$ *as*

$$\begin{aligned}(H(0) - E(0))^{-1} &= \sum_{n=0}^{\infty} \left(- H_0^{-1} \sum_{l=1}^{\infty} \frac{e^l}{l!} H_l \right)^n H_0^{-1} \\ &= \sum_{n=0}^{\infty} (-1)^n \sum_{k=n}^{\infty} e^k \sum_{\substack{l_1,\ldots,l_n=1 \\ l_1+\cdots+l_n=k}}^{k} \frac{1}{l_1! \cdots l_n!} H_0^{-1} H_{l_1} H_0^{-1} H_{l_2} \cdots H_0^{-1} H_{l_n} H_0^{-1}. \end{aligned} \tag{3.25}$$

Here we set

$$H_j = \begin{cases} H_j, & j = 1,2, \\ -E_j, & j \geqslant 3. \end{cases}$$

Then we have

$$\begin{aligned}(H(0) - E(0))^{-1} &= H_0^{-1} - eH_0^{-1} H_1 H_0^{-1} \\ &\quad + e^2 \left(-\tfrac{1}{2} H_0^{-1} H_2 H_0^{-1} + H_0^{-1} H_1 H_0^{-1} H_1 H_0^{-1} \right) + \mathcal{O}(e^3). \end{aligned} \tag{3.26}$$

Substitute (3.26) into (3.24). Then the result coincides with (3.13).

D. Explicit expressions

For each $k \in \mathbb{R}^3$ let us define the projection $Q(k)$ on $\mathbb{R}^3$ by

$$Q(k) = \sum_{j=1,2} |e_j(k)\rangle\langle e_j(k)|.$$

We also set

$$m = 1,$$

since it can easily be reintroduced at the end of the computation. We set

$$\hat{\varphi}_j = \hat{\varphi}(k_j), \quad \omega_j = \omega(k_j), \quad Q(k_j) = Q_j, \quad j = 1,2.$$

Let

$$\frac{1}{E_j} = \frac{1}{|k_j|^2/2 + \omega_j}, \quad j = 1,2,$$

$$\frac{1}{E_{12}} = \frac{1}{|k_1 + k_2|^2/2 + \omega_1 + \omega_2}, \quad k_1, k_2 \in \mathbb{R}^3,$$

$$\frac{1}{F_j} = \frac{1}{r_j^2/2 + r_j}, \quad j = 1,2,$$

$$\frac{1}{F_{12}} = \frac{1}{(r_1^2 + 2r_1 r_2 X + r_2^2)/2 + r_1 + r_2}, \quad r_1, r_2 \geqslant 0, \quad -1 \leqslant X \leqslant 1.$$

Lemma 3.8: It follows that

$$\frac{m}{m_{\mathrm{eff}}} = 1 - \alpha a_1(\Lambda,\kappa) - \alpha^2 a_2(\Lambda,\kappa) + \mathcal{O}(\alpha^3),$$

where

$$a_1(\Lambda,\kappa) = \frac{8}{3\pi}\log\left(\frac{\Lambda+2}{\kappa+2}\right) \tag{3.27}$$

and

$$\begin{aligned} a_2(\Lambda,\kappa) = (4\pi)^2\frac{2}{3}\int\int \mathrm{d}^3k_1\,\mathrm{d}^3k_2 \frac{|\hat{\varphi}_1|^2}{2\omega_1}\frac{|\hat{\varphi}_2|^2}{2\omega_2} \\ \times\Bigg\{-\left(\frac{1}{E_1}+\frac{1}{E_2}\right)\frac{1}{E_{12}}(1+s^2)+\left(\frac{1}{E_{12}}\right)^3\frac{|k_1+k_2|^2}{2}(1+s^2) \\ +\left(\frac{1}{E_1}+\frac{1}{E_2}\right)\left(\frac{1}{E_{12}}\right)^2(k_1\cdot k_2)(-1+s^2)-\frac{1}{E_1}\frac{1}{E_2}(1+s^2) \\ +\left(\frac{|k_1|^2}{E_1^2}+\frac{|k_2|^2}{E_2^2}\right)\frac{1}{E_{12}}(1-s^2)+\frac{1}{E_1}\frac{1}{E_2}\frac{1}{E_{12}}(k_1\cdot k_2)(-1+s^2)\Bigg\}, \end{aligned} \tag{3.28}$$

where $s=(\hat{k}_1,\hat{k}_2)$. *Changing variables to polar coordinates we also have*

$$\begin{aligned} a_2(\Lambda,\kappa) = \frac{(4\pi)^2}{(2\pi)^6}\frac{2}{3}\int_{-1}^{1}\mathrm{d}X\int_{\kappa}^{\Lambda}\mathrm{d}r_1\int_{\kappa}^{\Lambda}\mathrm{d}r_2\,2\pi^2 r_1 r_2 \\ \times\Bigg\{-\left(\frac{1}{F_1}+\frac{1}{F_2}\right)\frac{1}{F_{12}}(1+X^2)+\left(\frac{1}{F_{12}}\right)^3\frac{r_1^2+2r_1r_2X+r_2^2}{2}(1+X^2) \\ +\left(\frac{1}{F_1}+\frac{1}{F_2}\right)\left(\frac{1}{F_{12}}\right)^2 r_1r_2X(-1+X^2)-\frac{1}{F_1}\frac{1}{F_2}(1+X^2)+\left(\frac{r_1^2}{F_1^2}+\frac{r_2^2}{F_2^2}\right)\frac{1}{F_{12}}(1-X^2) \\ +\frac{1}{F_1}\frac{1}{F_2}\frac{1}{F_{12}}r_1r_2X(-1+X^2)\Bigg\}. \end{aligned} \tag{3.29}$$

Proof: Note that

$$\begin{aligned} a_1(\Lambda,\kappa) &= \frac{2}{3}(\sqrt{4\pi})^2(A_\mu^+\Omega, H_0^{-1}A_\mu^+\Omega) \\ &= \frac{2}{3}(\sqrt{4\pi})^2 2\int\frac{\hat{\varphi}(k)^2}{2\omega(k)}\frac{1}{|k|^2/2+|k|}\mathrm{d}^3k \\ &= \frac{2}{3}(\sqrt{4\pi})^2\frac{1}{(2\pi)^3}4\pi\int_{\kappa}^{\Lambda}\frac{1}{r/2+1}\mathrm{d}r \\ &= \frac{8}{3\pi}\log\left(\frac{\Lambda+2}{\kappa+2}\right). \end{aligned}$$

Thus (3.27) follows. To check $a_2(\Lambda,\kappa)$ we exactly compute the five terms on the right-hand side of (3.13) separately.

(1) We have

$$2(\Psi_3^\mu, H_0^{-1}\Psi_1^\mu) = (\Omega, -(A^-\cdot A^-)H_0^{-1}A_\mu H_0^{-1}A_\mu^+\Omega) + \tfrac{1}{2}(\Omega,(A^-\cdot A^-)H_0^{-1}(P_f\cdot A + A\cdot P_f)H_0^{-1}P_{f\mu}H_0^{-1}A_\mu^+\Omega). \tag{3.30}$$

Since $P_{f\mu}H_0^{-1}A_\mu\Omega = H_0^{-1}A_\mu P_{f\mu}\Omega = 0$, the second term of the right-hand side of (3.30) vanishes, we have

$$2(\Psi_3^\mu, H_0^{-1}\Psi_1^\mu) = -(\Omega,(A^-\cdot A^-)H_0^{-1}A_\mu^+H_0^{-1}A_\mu^+\Omega) = -\int\int \mathrm{d}^3k_1\,\mathrm{d}^3k_2 \frac{|\hat\varphi_1|^2}{2\omega_1}\frac{|\hat\varphi_2|^2}{2\omega_2}\frac{1}{E_{12}}\left(\frac{1}{E_1}+\frac{1}{E_2}\right)\mathrm{tr}(Q_1Q_2). \tag{3.31}$$

(2) We have

$$\begin{aligned}(\Psi_2^\mu, H_0^{-1}\Psi_2^\mu) &= \left(\frac{1}{2}\right)^2 (P_{f\mu}H_0^{-1}(A^+\cdot A^+)\Omega, H_0^{-1}P_{f\mu}H_0^{-1}(A^+\cdot A^+)\Omega)\\ &= \left(\frac{1}{2}\right)^2 (\Omega,(A^-\cdot A^-)(H_0^{-1})^3(P_f\cdot P_f)(A^+\cdot A^+)\Omega)\\ &= \left(\frac{1}{2}\right)^2 \int\int \mathrm{d}^3k_1\,\mathrm{d}^3k_2 \frac{|\hat\varphi_1|^2}{2\omega_1}\frac{|\hat\varphi_2|^2}{2\omega_2}\left(\frac{1}{E_{12}}\right)^3 |k_1+k_2|^2\,2\,\mathrm{tr}(Q_1Q_2).\end{aligned} \tag{3.32}$$

(3) We have

$$\begin{aligned}&-2(\Psi_2^\mu, H_0^{-1}H_1H_0^{-1}\Psi_1^\mu)\\ &= \frac{1}{2}(P_{f\mu}H_0^{-1}(A^+\cdot A^+)\Omega, H_0^{-1}(P_f\cdot A + A\cdot P_f)H_0^{-1}A_\mu^+\Omega)\\ &= \sum_{\nu=1,2,3}(\Omega,(A^-\cdot A^-)H_0^{-1}P_{f\mu}H_0^{-1}P_{f\nu}A_\nu^+H_0^{-1}A_\mu^+\Omega)\\ &= \int\int \mathrm{d}^3k_1\,\mathrm{d}^3k_2 \frac{|\hat\varphi_1|^2}{2\omega_1}\frac{|\hat\varphi_2|^2}{2\omega_2}\left(\frac{1}{E_{12}}\right)^2\left(\frac{1}{E_1}+\frac{1}{E_2}\right)(k_2, Q_1Q_2k_1).\end{aligned} \tag{3.33}$$

(4) We have

$$\begin{aligned}&-\frac{1}{2}(\Psi_1^\mu, H_0^{-1}H_2H_0^{-1}\Psi_1^\mu)\\ &= -\frac{1}{2}(A_\mu^+\Omega, H_0^{-1}((A^+\cdot A^+) + 2(A^+\cdot A^-) + (A^-\cdot A^-))H_0^{-1}A_\mu^+\Omega)\\ &= -(\Omega, A_\mu^- H_0^{-1}(A^+\cdot A^-)H_0^{-1}A_\mu^+\Omega)\\ &= -\int\int \mathrm{d}^3k_1\,\mathrm{d}^3k_2 \frac{|\hat\varphi_1|^2}{2\omega_1}\frac{|\hat\varphi_2|^2}{2\omega_2}\frac{1}{E_1}\frac{1}{E_2}\mathrm{tr}(Q_1Q_2).\end{aligned} \tag{3.34}$$

(5) We have

$$(\Psi_1^\mu, H_0^{-1}H_1H_0^{-1}H_1H_0^{-1}\Psi_1^\mu) = \left(\frac{1}{2}\right)^2 (A_\mu^+\Omega, H_0^{-1}(P_f\cdot A + A\cdot P_f)H_0^{-1}(P_f\cdot A + A\cdot P_f)H_0^{-1}A_\mu^+\Omega)$$
$$= (A_\mu^+\Omega, H_0^{-1}(P_f\cdot A)H_0^{-1}(P_f\cdot A)H_0^{-1}A_\mu^+\Omega)$$
$$= \sum_{\nu,\kappa=1,2,3} (A_\mu^+\Omega, H_0^{-1}P_{f\nu}A_\nu^+H_0^{-1}P_{f\kappa}A_\kappa^-H_0^{-1}A_\mu^+\Omega)$$
$$+ \sum_{\nu,\kappa=1,2,3} (A_\mu^+\Omega, H_0^{-1}P_{f\nu}A_\nu^-H_0^{-1}P_{f\kappa}A_\kappa^+H_0^{-1}A_\mu^+\Omega). \tag{3.35}$$

Since

$$P_{f\kappa}A_\kappa^-H_0^{-1}A_\mu^+\Omega = 0,$$

the first term on the last line in (3.35) vanishes. Then we have

$$(\Psi_1^\mu, H_0^{-1}H_1H_0^{-1}H_1H_0^{-1}\Psi_1^\mu) = \sum_{\nu,\kappa=1,2,3} (\Omega, A_\mu^-H_0^{-1}P_{f\nu}A_\nu^-H_0^{-1}P_{f\kappa}A_\kappa^+H_0^{-1}A_\mu^+\Omega)$$
$$= \int\int \mathrm{d}^3k_1\,\mathrm{d}^3k_2 \frac{|\hat\varphi_1|^2}{2\omega_1}\frac{|\hat\varphi_2|^2}{2\omega_2}\frac{1}{E_{12}}\left\{\left(\frac{1}{E_2}\right)^2 2(k_2, Q_1k_2) + \frac{1}{E_1}\frac{1}{E_2}(k_2, Q_1Q_2k_1)\right\}$$
$$= \int\int \mathrm{d}^3k_1\,\mathrm{d}^3k_2 \frac{|\hat\varphi_1|^2}{2\omega_1}\frac{|\hat\varphi_2|^2}{2\omega_2}\frac{1}{E_{12}}\left\{\left(\frac{1}{E_1}\right)^2 (k_1, Q_2k_1) + \left(\frac{1}{E_2}\right)^2 (k_2, Q_1k_2)\right\}$$
$$+ \int\int \mathrm{d}^3k_1\,\mathrm{d}^3k_2 \frac{|\hat\varphi_1|^2}{2\omega_1}\frac{|\hat\varphi_2|^2}{2\omega_2}\frac{1}{E_{12}}\frac{1}{E_1}\frac{1}{E_2}(k_2, Q_1Q_2k_1). \tag{3.36}$$

Equation (3.28) follows from Lemma 3.6, (3.31), (3.32), (3.33), (3.34), (3.36) and the facts

$$\mathrm{tr}[Q(k_1)Q(k_2)] = \sum_{j,j'=1,2} (e_j(k_1)e_{j'}(k_2))^2 = 1 + (\hat k_1, \hat k_2)^2,$$

$$(k_1, Q(k_2)Q(k_1)k_2) = (k_1, k_2)((\hat k_1, \hat k_2)^2 - 1),$$

$$(k_1, Q(k_2)k_1) = |k_1|^2(1 - (\hat k_1, \hat k_2)^2).$$

Thus the proof is complete. ■

IV. MAIN THEOREM

By (3.29) we can see that

$$a_2(\Lambda, \kappa) = \frac{(4\pi)^2}{(2\pi)^6}\frac{2}{3}\sum_{j=1}^{6} b_j(\Lambda), \tag{4.1}$$

where

$$b_1(\Lambda) = -\int_{-1}^{1}\mathrm{d}X(1+X^2)\int_\kappa^\Lambda \mathrm{d}r_1\int_\kappa^\Lambda \mathrm{d}r_2\, 2\pi^2 r_1r_2\left(\frac{1}{F_1}+\frac{1}{F_2}\right)\frac{1}{F_{12}},$$

$$b_2(\Lambda) = \int_{-1}^{1}\mathrm{d}X(1+X^2)\int_\kappa^\Lambda \mathrm{d}r_1\int_\kappa^\Lambda \mathrm{d}r_2\, 2\pi^2 r_1r_2\left(\frac{1}{F_{12}}\right)^3\frac{r_1^2+2r_1r_2X+r_2^2}{2},$$

$$b_3(\Lambda) = \int_{-1}^{1} \mathrm{d}X\, X(-1+X^2) \int_{\kappa}^{\Lambda} \mathrm{d}r_1 \int_{\kappa}^{\Lambda} \mathrm{d}r_2\, 2\pi^2 r_1^2 r_2^2 \left(\frac{1}{F_1} + \frac{1}{F_2}\right)\left(\frac{1}{F_{12}}\right)^2,$$

$$b_4(\Lambda) = -\int_{-1}^{1} \mathrm{d}X(1+X^2) \int_{\kappa}^{\Lambda} \mathrm{d}r_1 \int_{\kappa}^{\Lambda} \mathrm{d}r_2\, 2\pi^2 r_1 r_2 \frac{1}{F_1}\frac{1}{F_2},$$

$$b_5(\Lambda) = \int_{-1}^{1} \mathrm{d}X(1-X^2) \int_{\kappa}^{\Lambda} \mathrm{d}r_1 \int_{\kappa}^{\Lambda} \mathrm{d}r_2\, 2\pi^2 r_1 r_2 \left(\frac{r_1^2}{F_1^2} + \frac{r_2^2}{F_2^2}\right)\frac{1}{F_{12}},$$

$$b_6(\Lambda) = \int_{-1}^{1} \mathrm{d}X\, X(-1+X^2) \int_{\kappa}^{\Lambda} \mathrm{d}r_1 \int_{\kappa}^{\Lambda} \mathrm{d}r_2\, 2\pi^2 r_1^2 r_2^2 \frac{1}{F_1}\frac{1}{F_2}\frac{1}{F_{12}}.$$

Our main theorem is stated as follows.

Theorem 4.1: *There exist strictly positive constants c_1 and c_2 such that*

$$c_1 \leqslant \lim_{\Lambda\to\infty} \frac{a_2(\Lambda,\kappa)}{\sqrt{\Lambda}} \leqslant c_2.$$

To prove Theorem 4.1 we estimate the lower and upper bounds of $a_2(\Lambda,\kappa)/\sqrt{\Lambda}$ as $\Lambda\to\infty$ in what follows.

Let $\rho_\Lambda(\cdot,\cdot)$: $[0,\infty)\times[-1,1]\to\mathbb{R}$ be defined by

$$\rho_\Lambda = \rho_\Lambda(r,X) = r^2 + 2\Lambda r X + \Lambda^2 + 2r + 2\Lambda = (r + \Lambda X + 1)^2 + \Delta,$$

where

$$\Delta = \Lambda^2(1-X^2) + 2\Lambda(1-X) - 1. \tag{4.2}$$

Lemma 4.2: There exist constants C_1, C_2, C_3, and C_4 such that for sufficiently large $\Lambda > 0$,

$$(1)\ \int_{-1}^{1} \mathrm{d}X \int_{0}^{\Lambda} \mathrm{d}r \frac{1}{\rho_\Lambda(r,X)} \leqslant C_1 \frac{1}{\Lambda},$$

$$(2)\ \int_{-1}^{1} \mathrm{d}X \int_{0}^{\Lambda} \mathrm{d}r \left(\frac{1}{\rho_\Lambda(r,X)}\right)^2 \leqslant C_2 \frac{1}{\Lambda^{5/2}},$$

$$(3)\ \int_{-1}^{1} \mathrm{d}X \int_{0}^{\Lambda} \mathrm{d}r \frac{1}{\rho_\Lambda(r,X)}\frac{1}{r+2} \leqslant C_3 \frac{\log\Lambda}{\Lambda^2},$$

$$(4)\ \int_{-1}^{1} \mathrm{d}X \int_{0}^{\Lambda} \mathrm{d}r \left(\frac{1}{\rho_\Lambda(r,X)}\right)^2 (1-X^2) \leqslant C_4 \frac{1}{\Lambda^3}.$$

Proof: See Appendix A. ∎

A. Upper bounds

Lemma 4.3: There exists a constant $C_{\max}$ such that

$$\lim_{\Lambda\to\infty} \left| \frac{a(\Lambda,\kappa)}{\sqrt{\Lambda}} \right| < C_{\max}.$$

Proof: Note that for a continuous function f,

$$\frac{\mathrm{d}}{\mathrm{d}\Lambda}\int_\kappa^\Lambda \mathrm{d}r_1 \int_\kappa^\Lambda \mathrm{d}r_2\, f(r_1,r_2) = \int_\kappa^\Lambda f(\Lambda,r)\mathrm{d}r + \int_\kappa^\Lambda f(r,\Lambda)\mathrm{d}r. \tag{4.3}$$

In this proof, C denotes some sufficiently large constant and is not necessarily the same number.

(1) We have

$$\frac{\mathrm{d}}{\mathrm{d}\Lambda}b_1(\Lambda) = 16\pi^2\int_{-1}^1 \mathrm{d}X\int_\kappa^\Lambda \mathrm{d}r \frac{1}{\rho_\Lambda(r,X)}\left(\frac{\Lambda}{r+2}+\frac{r}{\Lambda+2}\right)(1+X^2).$$

Since by Lemma 4.2 (3) and (1),

$$\int_{-1}^1 \mathrm{d}X\int_\kappa^\Lambda \mathrm{d}r \frac{1}{\rho_\Lambda(r,X)}\frac{\Lambda}{r+2} \leqslant C\frac{\log\Lambda}{\Lambda},$$

$$\int_{-1}^1 \mathrm{d}X\int_\kappa^\Lambda \mathrm{d}r \frac{1}{\rho_\Lambda(r,X)}\frac{r}{\Lambda+2} \leqslant C\frac{1}{\Lambda},$$

we have

$$\left|\frac{\mathrm{d}}{\mathrm{d}\Lambda}b_1(\Lambda)\right| \leqslant C\frac{\log\Lambda}{\Lambda}. \tag{4.4}$$

(2) We see that by Lemma 4.2 (2),

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\Lambda}b_2(\Lambda) &= 16\pi^2\int_{-1}^1 \mathrm{d}X\int_\kappa^\Lambda \mathrm{d}r\left(\frac{1}{\rho_\Lambda(r,X)}\right)^3 r\Lambda(\Lambda^2+r^2+2\Lambda rX)(1+X^2)\\ &\leqslant 16\pi^2\int_{-1}^1 \mathrm{d}X\int_\kappa^\Lambda \mathrm{d}r\left(\frac{1}{\rho_\Lambda(r,X)}\right)^2 r\Lambda(1+X^2)\\ &\leqslant 16\pi^2\Lambda^2\int_{-1}^1 \mathrm{d}X\int_\kappa^\Lambda \mathrm{d}r\left(\frac{1}{\rho_\Lambda(r,X)}\right)^2 (1+X^2) \leqslant C\frac{1}{\sqrt{\Lambda}}.\end{aligned}$$

Hence

$$\left|\frac{\mathrm{d}}{\mathrm{d}\Lambda}b_2(\Lambda)\right| \leqslant C\frac{1}{\sqrt{\Lambda}}. \tag{4.5}$$

(3) We have

$$\left|\frac{\mathrm{d}}{\mathrm{d}\Lambda}b_3(\Lambda)\right| = 32\pi^2\left|\int_{-1}^1 \mathrm{d}X\int_\kappa^\Lambda \mathrm{d}r\, X(X^2-1)\left(\frac{1}{\rho_\Lambda(r,X)}\right)^2\left(\frac{\Lambda^2 r}{r+2}+\frac{r^2\Lambda}{\Lambda+2}\right)\right|.$$

Since by Lemma 4.2 (3) and (4),

$$\left|\int_{-1}^1 \mathrm{d}X\int_\kappa^\Lambda \mathrm{d}r\, X(X^2-1)\left(\frac{1}{\rho_\Lambda(r,X)}\right)^2\frac{\Lambda^2 r}{r+2}\right| \leqslant C\frac{1}{\Lambda},$$

$$\left|\int_{-1}^1 \mathrm{d}X\int_\kappa^\Lambda \mathrm{d}r\, X(X^2-1)\left(\frac{1}{\rho_\Lambda(r,X)}\right)^2\frac{r^2\Lambda}{\Lambda+2}\right| \leqslant C\frac{1}{\Lambda},$$

we have

$$\left|\frac{\mathrm{d}}{\mathrm{d}\Lambda}b_3(\Lambda)\right| \leqslant C\frac{1}{\Lambda}. \tag{4.6}$$

(4) It is trivial that

$$|b_4(\Lambda)| \leqslant C[\log \Lambda]^2. \tag{4.7}$$

(5) We have

$$\frac{\mathrm{d}}{\mathrm{d}\Lambda}b_5(\Lambda) = 32\pi^2\int_{-1}^{1}\mathrm{d}X\int_{\kappa}^{\Lambda}\mathrm{d}r\frac{1}{\rho_\Lambda(r,X)}(1-X^2)r\Lambda\left\{\left(\frac{1}{\Lambda+2}\right)^2+\left(\frac{1}{r+2}\right)^2\right\}.$$

Since by Lemma 4.2 (1),

$$\int_{-1}^{1}\mathrm{d}X\int_{\kappa}^{\Lambda}\mathrm{d}r\frac{1}{\rho_\Lambda(r,X)}(1-X^2)r\Lambda\left(\frac{1}{\Lambda+2}\right)^2 \leqslant C\frac{1}{\Lambda},$$

$$\int_{-1}^{1}\mathrm{d}X\int_{\kappa}^{\Lambda}\mathrm{d}r\frac{1}{\rho_\Lambda(r,X)}(1-X^2)r\Lambda\left(\frac{1}{r+2}\right)^2 \leqslant C\frac{1}{\Lambda},$$

we see that

$$\left|\frac{\mathrm{d}}{\mathrm{d}\Lambda}b_5(\Lambda)\right| \leqslant C\frac{1}{\Lambda}. \tag{4.8}$$

(6) We have by Lemma 4.2 (1)

$$\left|\frac{\mathrm{d}}{\mathrm{d}\Lambda}b_6(\Lambda)\right| = 32\pi^2\left|\int_{-1}^{1}\mathrm{d}X\int_{\kappa}^{\Lambda}\mathrm{d}r(X^2-1)X\frac{1}{\rho_\Lambda(r,X)}\frac{r}{r+2}\frac{\Lambda}{\Lambda+2}\right| \leqslant C\frac{1}{\Lambda}.$$

Then we have

$$\left|\frac{\mathrm{d}}{\mathrm{d}\Lambda}b_6(\Lambda)\right| \leqslant C\frac{1}{\Lambda}. \tag{4.9}$$

From (4.4)–(4.9) it follows that

$$|b_j(\Lambda)| \leqslant C[\log \Lambda]^2, \quad j=1,4,$$

$$|b_2(\Lambda)| \leqslant C\Lambda^{1/2}, \quad |b_j(\Lambda)| \leqslant C\log\Lambda, \quad j=3,5,6. \tag{4.10}$$

Then the lemma follows. ■

B. Lower bounds

Lemma 4.4: There exists a positive constant $C_{\min}>0$ *such that*

$$C_{\min} \leqslant \lim_{\Lambda\to\infty}\frac{b_2(\Lambda)}{\sqrt{\Lambda}}.$$

From this lemma and (4.10), i.e.,

$$\lim_{\Lambda\to\infty}\frac{b_j(\Lambda)}{\sqrt{\Lambda}} = 0, \quad j=1,3,4,5,6,$$

the following corollary follows.

Corollary 4.5: It follows that

$$C_{\min} \leqslant \lim_{\Lambda\to\infty} \frac{a_2(\Lambda,\kappa)}{\sqrt{\Lambda}}.$$

Proof of Lemma 4.4: We have

$$\frac{\mathrm{d}}{\mathrm{d}\Lambda} b_2(\Lambda) = 16\pi^2 \int_{-1}^{1} \mathrm{d}X \int_{\kappa}^{\Lambda} \mathrm{d}r (1+X^2) \left(\frac{1}{\rho_\Lambda(r,X)}\right)^3 (r^2 + 2r\Lambda X + \Lambda^2) r\Lambda, \tag{4.11}$$

where, recall that

$$\rho_\Lambda(r,X) = (r + \Lambda X + 1)^2 + \Delta,$$

$$\Delta = \Lambda^2(1-X^2) + 2\Lambda(1-X) - 1.$$

Note that $\Delta > 0$ for $X \leqslant 0$ and a sufficiently large Λ. Since the integrand of (4.11),

$$T_R(r) = \left(\frac{1}{\rho_\Lambda(r,X)}\right)^3 (r^2 + 2r\Lambda X + \Lambda^2) r\Lambda$$

is positive, it is enough to prove that

$$\lim_{\Lambda\to\infty} \sqrt{\Lambda} \frac{\mathrm{d}}{\mathrm{d}\Lambda} b_2(\Lambda) \geqq \lim_{\Lambda\to\infty} \sqrt{\Lambda} \int_{-1+(1/\Lambda)}^{0} \mathrm{d}X \int_{\kappa}^{\Lambda} \mathrm{d}r\, T_R(r)(1+X^2) > 0. \tag{4.12}$$

We simply set $\rho = \rho_\Lambda(r,X)$. Since

$$(r^2 + 2r\Lambda X + \Lambda^2) r\Lambda = \Lambda\{(r-2)\rho + (4 + 4\Lambda X - 2\Lambda) r + 2(\Lambda^2 + 2\Lambda)\},$$

we have

$$\begin{aligned}\int_{\kappa}^{\Lambda} \mathrm{d}r\, T_R(r) &= \Lambda \int_{\kappa}^{\Lambda} \mathrm{d}r \frac{r-2}{\rho^2} + \Lambda(4 + 4\Lambda X - 2\Lambda) \int_{\kappa}^{\Lambda} \mathrm{d}r \frac{r}{\rho^3} + 2\Lambda(\Lambda^2 + 2\Lambda) \int_{\kappa}^{\Lambda} \mathrm{d}r \frac{1}{\rho^3} \\ &= \Lambda \int_{\kappa}^{\Lambda} \mathrm{d}r \frac{r}{\rho^2} + \Lambda^2(4X - 2) \int_{\kappa}^{\Lambda} \mathrm{d}r \frac{r}{\rho^3} + 2\Lambda^3 \int_{\kappa}^{\Lambda} \mathrm{d}r \frac{1}{\rho^3} + t_1(\Lambda),\end{aligned}$$

where

$$t_1(\Lambda) = -2\Lambda \int_{\kappa}^{\Lambda} \mathrm{d}r \frac{1}{\rho^2} + 4\Lambda \int_{\kappa}^{\Lambda} \mathrm{d}r \frac{r}{\rho^3} + 2\Lambda^2 \int_{\kappa}^{\Lambda} \mathrm{d}r \frac{1}{\rho^3}.$$

Moreover since

$$\int_{\kappa}^{\Lambda} \mathrm{d}r \frac{r}{\rho^2} = -\frac{1}{2}\left[\frac{1}{\rho}\right]_{\kappa}^{\Lambda} - \int_{\kappa}^{\Lambda} \mathrm{d}r \frac{\Lambda X + 1}{\rho^2},$$

$$\int_{\kappa}^{\Lambda} \mathrm{d}r \frac{r}{\rho^3} = -\frac{1}{4}\left[\frac{1}{\rho^2}\right]_{\kappa}^{\Lambda} - \int_{\kappa}^{\Lambda} \mathrm{d}r \frac{\Lambda X + 1}{\rho^3},$$

we have

$$\int_\kappa^\Lambda \mathrm{d}r\, T_R(r) = -\Lambda^2 X \int_\kappa^\Lambda \mathrm{d}r \frac{1}{\rho^2} + \Lambda^3(2 - X(4X-2)) \int_\kappa^\Lambda \mathrm{d}r \frac{1}{\rho^3} + t_1(\Lambda) + t_2(\Lambda),$$

where

$$t_2(\Lambda) = \Lambda\left(-\frac{1}{2}\right)\left[\frac{1}{\rho}\right]_\kappa^\Lambda - \Lambda \int_\kappa^\Lambda \mathrm{d}r \frac{1}{\rho^2} + \Lambda^2(4X-2)\left(-\frac{1}{4}\right)\left[\frac{1}{\rho^2}\right]_\kappa^\Lambda - \Lambda^2(4X-2)\int_\kappa^\Lambda \mathrm{d}r \frac{1}{\rho^3}.$$

Note that

$$\int \frac{1}{(x^2+a^2)^{n+1}}\mathrm{d}x = \frac{1}{2na^2}\frac{x}{(x^2+a^2)^n} + \frac{2n-1}{2n}\frac{1}{a^2}\int \frac{1}{(x^2+a^2)^n}\mathrm{d}x, \quad n \geqslant 1.$$

Then

$$\int_\kappa^\Lambda \mathrm{d}r \frac{1}{\rho^2} = \left[\frac{r+\Lambda X+1}{2\Delta}\frac{1}{\rho}\right]_\kappa^\Lambda + \frac{1}{2\Delta^{3/2}}\left[\arctan\frac{r+\Lambda X+1}{\sqrt{\Delta}}\right]_\kappa^\Lambda,$$

$$\int_\kappa^\Lambda \mathrm{d}r \frac{1}{\rho^3} = \left[\frac{r+\Lambda X+1}{4\Delta}\frac{1}{\rho^2}\right]_\kappa^\Lambda + \frac{3}{8}\left[\frac{r+\Lambda X+1}{\Delta^2}\frac{1}{\rho}\right]_\kappa^\Lambda + \frac{3}{8}\frac{1}{\Delta^{5/2}}\left[\arctan\frac{r+\Lambda X+1}{\sqrt{\Delta}}\right]_\kappa^\Lambda.$$

Hence we have

$$\begin{aligned}\int_\kappa^\Lambda \mathrm{d}r\, T_R(r) = &-\Lambda^2 X \frac{1}{2\Delta^{3/2}}\left\{\left[\arctan\frac{r+\Lambda X+1}{\sqrt{\Delta}}\right]_\kappa^\Lambda + \left[\sqrt{\Delta}\frac{r+\Lambda X+1}{\rho}\right]_\kappa^\Lambda\right\} \\ &+ \frac{3}{8}\Lambda^3 2(2X+1)(1-X)\frac{1}{\Delta^{5/2}}\left\{\left[\arctan\frac{r+\Lambda X+1}{\sqrt{\Delta}}\right]_\kappa^\Lambda + \left[\sqrt{\Delta}\frac{r+\Lambda X+1}{\rho}\right]_\kappa^\Lambda\right\} \\ &+ t_1(\Lambda) + t_2(\Lambda) + t_3(\Lambda),\end{aligned}$$

where

$$t_3(\Lambda) = \Lambda^3 2(2X+1)(1-X)\left[\frac{r+\Lambda X+1}{4\Delta}\frac{1}{\rho^2}\right]_\kappa^\Lambda.$$

It is proven in Lemma B.1 of Appendix B that

$$\lim_{\Lambda\to\infty}\sqrt{\Lambda}\int_{-1+1/\Lambda}^0 (1+X^2)(t_1(\Lambda)+t_2(\Lambda)+t_3(\Lambda))\mathrm{d}X = 0. \tag{4.13}$$

From this it is enough to show that

$$\begin{aligned}\lim_{\Lambda\to\infty}\sqrt{\Lambda}\Lambda^2 \int_{-1+1/\Lambda}^0 \mathrm{d}X(1+X^2)\frac{1}{\Delta^{3/2}}&\left[\sqrt{\Delta}\frac{r+\Lambda X+1}{\rho}\right]_\kappa^\Lambda \\ &\times\frac{1}{4}\left\{-2X+3(1-X)(2X+1)\frac{\Lambda}{\Delta}\right\} \geqslant 0\end{aligned} \tag{4.14}$$

and that there exists a positive constant $\xi > 0$ such that

$$\lim_{\Lambda\to\infty}\sqrt{\Lambda}\int_{-1+1/\Lambda}^{0} dX(1+X^2)\left\{-\Lambda^2 X\frac{1}{2\Delta^{3/2}}\left[\arctan\frac{r+\Lambda X+1}{\sqrt{\Delta}}\right]_{\kappa}^{\Lambda}\right.$$
$$\left.+\frac{3}{8}\Lambda^3 2(2X+1)(1-X)\frac{1}{\Delta^{5/2}}\left[\arctan\frac{r+\Lambda X+1}{\sqrt{\Delta}}\right]_{\kappa}^{\Lambda}\right\}$$
$$=\lim_{\Lambda\to\infty}\sqrt{\Lambda}\Lambda^2\int_{-1+1/\Lambda}^{0} dX(1+X^2)\frac{1}{\Delta^{3/2}}\left[\arctan\frac{r+\Lambda X+1}{\sqrt{\Delta}}\right]_{\kappa}^{\Lambda}$$
$$\times\frac{1}{4}\left\{-2X+3(1-X)(2X+1)\frac{\Lambda}{\Delta}\right\}>\xi. \tag{4.15}$$

Changing variable X to $-y$, we shall prove (4.15), i.e.,

$$\lim_{\Lambda\to\infty}\sqrt{\Lambda}\Lambda^2\int_{0}^{1-(1/\Lambda)} dy(1+y^2)\frac{1}{\Delta^{3/2}}\left[\arctan\frac{r-\Lambda y+1}{\sqrt{\Delta}}\right]_{\kappa}^{\Lambda}\frac{1}{4}a_{\Lambda}(y)dy>\xi,$$

where

$$a_{\Lambda}(y)=2y+\frac{6}{\Lambda}+b_{\Lambda}(y),$$

$$b_{\Lambda}(y)=\frac{3}{\Lambda}\left(1+\frac{4}{\Lambda}\right)\frac{y+\dfrac{\Lambda^2+4\Lambda-2}{\Lambda(\Lambda+4)}}{\left(y-\dfrac{1}{\Lambda}\right)^2-\dfrac{\Lambda+2}{\Lambda}}.$$

The function $b_{\Lambda}(\cdot)$ satisfies the following properties.

(1) $b_{\Lambda}''(y)<0$ for $0\leqslant y\leqslant 1-1/\Lambda$, i.e., $b_{\Lambda}(y)$ is concave for $0\leqslant y\leqslant 1-1/\Lambda$.
(2) $\lim_{\Lambda\to\infty} b_{\Lambda}(1-1/\Lambda)=-1$.
(3) $\lim_{\Lambda\to\infty} b_{\Lambda}(y)=0$ for $y\neq 1$ and $\lim_{\Lambda\to\infty} b_{\Lambda}(1)=-3/2$.

By (1)–(3) we have

$$\inf_{0\leqslant y\leqslant 1-1/\Lambda} b_{\Lambda}(y)=\min\{b_{\Lambda}(0),b_{\Lambda}(1-1/\Lambda)\}$$

and then for sufficiently large Λ,

$$\inf_{0\leqslant y\leqslant 1-1/\Lambda} b_{\Lambda}(y)=b_{\Lambda}(1-1/\Lambda)>-\tfrac{7}{4}.$$

Hence

$$\inf_{15/16\leqslant y\leqslant 1-1/\Lambda} a_{\Lambda}(y)\geqslant \tfrac{15}{8}-\tfrac{7}{4}=\tfrac{1}{8}>0.$$

Moreover

$$\left[\arctan\frac{r-\Lambda y+1}{\sqrt{\Delta}}\right]_{\kappa}^{\Lambda}=\arctan\frac{(1-y)\Lambda+1}{\sqrt{\Delta}}-\arctan\frac{\kappa-\Lambda y+1}{\sqrt{\Delta}}>0,$$

$$\lim_{\Lambda\to\infty}\left[\arctan\frac{r-\Lambda y+1}{\sqrt{\Delta}}\right]_{\kappa}^{\Lambda}=\arctan\frac{1-y}{\sqrt{1-y^2}}+\arctan\frac{y}{\sqrt{1-y^2}}>0$$

for $0\leqslant y\leqslant 1$. Then

$$\delta = \inf_{\Lambda>1} \inf_{0\leqslant y\leqslant 1} \left[\arctan \frac{r-\Lambda y+1}{\sqrt{\Delta}} \right]_\kappa^\Lambda > 0.$$

Then we have

$$\begin{aligned}
&\lim_{\Lambda\to\infty} \sqrt{\Lambda}\Lambda^2 \int_0^{1-(1/\Lambda)} dy(1+y^2) \frac{1}{\Delta^{3/2}} \left[\arctan \frac{r-\Lambda y+1}{\sqrt{\Delta}} \right]_\kappa^\Lambda \frac{1}{4} a_\Lambda(y) \\
&\geqslant \lim_{\Lambda\to\infty} \sqrt{\Lambda}\Lambda^2 \int_{15/16}^{1-(1/\Lambda)} dy(1+y^2) \frac{1}{\Delta^{3/2}} \left[\arctan \frac{r-\Lambda y+1}{\sqrt{\Delta}} \right]_\kappa^\Lambda \frac{1}{4} a_\Lambda(y) \\
&\geqslant \frac{1}{8} \times \frac{1}{4} \times \delta \times \lim_{\Lambda\to\infty} \sqrt{\Lambda}\Lambda^2 \int_{15/16}^{1-(1/\Lambda)} dy \frac{1}{\Delta^{3/2}}.
\end{aligned}$$

Furthermore,

$$\begin{aligned}
&\lim_{\Lambda\to\infty} \sqrt{\Lambda}\Lambda^2 \int_{15/16}^{1-(1/\Lambda)} dy \frac{1}{\Delta^{3/2}} \\
&= \lim_{\Lambda\to\infty} \frac{1}{\sqrt{\Lambda}} \int_{15/16}^{1-(1/\Lambda)} dy \frac{1}{\left\{ (1-y^2) + \frac{2}{\Lambda}(1+y) - \frac{1}{\Lambda^2} \right\}^{3/2}} \\
&\geqslant \lim_{\Lambda\to\infty} \frac{1}{\sqrt{\Lambda}} \int_{15/16}^{1-(1/\Lambda)} dy \frac{1}{\left\{ (1-y) + \frac{2}{\Lambda} \right\}^{3/2}} \frac{1}{(1+y)^{3/2}} \\
&\geqslant \lim_{\Lambda\to\infty} \frac{1}{\sqrt{\Lambda}} \int_{15/16}^{1-(1/\Lambda)} dy \frac{1}{\left\{ (1-y) + \frac{2}{\Lambda} \right\}^{3/2}} \frac{1}{2^{3/2}} \\
&= \lim_{\Lambda\to\infty} \frac{1}{\sqrt{2}} \frac{1}{\sqrt{\Lambda}} \left(\frac{1}{\sqrt{3/\Lambda}} - \frac{1}{\sqrt{1/16+2/\Lambda}} \right) = \frac{1}{\sqrt{6}}.
\end{aligned}$$

Then we proved that

$$\lim_{\Lambda\to\infty} \sqrt{\Lambda} \frac{\mathrm{d}}{\mathrm{d}\Lambda} b_2(\Lambda) > 4\pi \times \tfrac{1}{8} \times \tfrac{1}{4} \times \tfrac{1}{\sqrt{6}} \times \delta = \frac{\pi\delta}{8\sqrt{6}} > 0.$$

Then (4.15) follows. We shall show (4.14). Since the left-hand side of (4.14) is

$$\lim_{\Lambda\to\infty} \sqrt{\Lambda}\Lambda^2 \int_0^{1-(1/\Lambda)} dy(1+y^2) \frac{1}{\Delta^{3/2}} \left[\sqrt{\Delta} \frac{r-\Lambda y+1}{\rho} \right]_\kappa^\Lambda \frac{1}{4} a_\Lambda(y) dy, \tag{4.16}$$

it is enough to show that $[\cdots]_\kappa^\Lambda$ in (4.16) is non-negative. We can directly see that

$$\left[\sqrt{\Delta} \frac{r-\Lambda y+1}{\rho} \right]_\kappa^\Lambda = \frac{\sqrt{\Delta} K}{\{(\Lambda+\Lambda X+1)^2+\Delta\}\{(\kappa+\Lambda X+1)^2+\Delta\}},$$

where, for $0\leqslant y\leqslant 1$,

$$K = (-2y^2+y+1)\Lambda^3 + (1+4y)\Lambda^2 - 2\Lambda + \kappa((y^2-2)\Lambda^2 + (-2y-2)\Lambda + 1) + \kappa^2((-y+1)\Lambda+1).$$

Since $K>0$ for a sufficiently large Λ, (4.14) follows. ■

Proof of Theorem 4.1: The theorem follows from Lemma 4.3 and Corollary 4.5. ■

Remark 4.6: (1) $a_2(\Lambda,\kappa)/\sqrt{\Lambda}$ *converges to a non-negative constant as* $\Lambda\to\infty$. *(2) By (4.1), we can define* $a_2(\Lambda,0)$ *since* $b_j(\Lambda)$ *with* $\kappa=0$ *are finite. Moreover* $a_2(\Lambda,0)$ *also satisfies Theorem 4.1.*

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APPENDIX A: PROOF OF LEMMA 4.2

Proof of Lemma 4.2: By the definition of Δ it follows that for sufficiently large Λ,

$$\frac{1}{\Delta}\leqslant\frac{1}{\Lambda}\quad\text{for } X\leqslant 0.$$

Let

$$\delta=\delta(k)=\frac{1}{\Lambda^k},\quad 0<k\leqslant 2.$$

Then for sufficiently large Λ,

$$\Delta\geqslant\Lambda^2(1-X^2)-1>0\quad\text{for } -1+\delta(k)<X\leqslant 0,\quad 0<k\leqslant 2.$$

In particular we obtain

$$\frac{1}{\Delta}\leqslant\frac{a}{\Lambda^2}\frac{1}{1-X^2}\quad\text{for } -1+\delta(k)\leqslant X\leqslant 0,\quad 0<k\leqslant 2,$$

with some constant a independent of Λ. In this proof C denotes some sufficiently large constant and it is not necessarily the same number. We divide $\int_{-1}^{1}\cdots dX$ as

$$\int_{-1}^{1}\cdots dX=\int_{0}^{1}+\int_{-1+\delta}^{0}+\int_{-1}^{-1+\delta}.$$

(1) It is trivial that $|\int_0^1\cdots dX|\leqslant C/\Lambda$. Note that

$$\left|\int_0^\Lambda dr\frac{1}{\rho_\Lambda(r,X)}\right|=\frac{1}{\sqrt{\Delta}}\left|\arctan\frac{\Lambda+\Lambda X+1}{\sqrt{\Delta}}-\arctan\frac{\Lambda X+1}{\sqrt{\Delta}}\right|\leqslant\pi\frac{1}{\sqrt{\Delta}}.$$

Let $\delta=\delta(1/2)=1/\sqrt{\Lambda}$. Hence we have

$$\left|\int_{-1+\delta}^{0}\cdots dX\right|\leqslant\frac{C}{\Lambda}\arcsin(1-\delta),$$

$$\left|\int_{-1}^{-1+\delta}\cdots dX\right|\leqslant\frac{C}{\sqrt{\Lambda}}\delta.$$

Thus (1) follows.

(2) It is trivial that $|\int_0^1\cdots dX|\leqslant C/\Lambda^3$. Note that

$$\left|\int_0^\Lambda \mathrm{d}r \frac{1}{\rho_\Lambda(r,X)^2}\right| = \frac{1}{2\Delta}\left|\int_0^\Lambda \frac{1}{\rho_\Lambda(r,X)}\mathrm{d}r + \left(\frac{\Lambda+\Lambda X+1}{(\Lambda+\Lambda X+1)^2+\Delta} - \frac{\Lambda X+1}{(\Lambda X+1)^2+\Delta}\right)\right|$$
$$\leqslant \begin{cases} \dfrac{C}{\Lambda^2}\left(\dfrac{1}{\Lambda(1-X^2)^{3/2}}+\dfrac{1}{\Lambda}\right), & -1+\delta \leqslant X \leqslant 0, \\ \dfrac{C}{\Lambda}\left(\dfrac{1}{\sqrt{\Lambda}}+\dfrac{1}{\Lambda}\right), & -1 \leqslant X \leqslant -1+\delta. \end{cases}$$

Let $\delta=\delta(1)=1/\Lambda$. Hence we have

$$\left|\int_{-1+\delta}^0 \cdots \mathrm{d}X\right| \leqslant \frac{C}{\Lambda^3}\int_{-1+\delta}^0 \mathrm{d}X\left(\frac{1}{(1-X^2)^{3/2}}+1\right) \leqslant \frac{C}{\Lambda^3}\left(\frac{1}{\sqrt{\delta}}+1\right),$$

$$\left|\int_{-1}^{-1+\delta} \cdots \mathrm{d}X\right| \leqslant \frac{C}{\Lambda}\left(\frac{1}{\sqrt{\Lambda}}+\frac{1}{\Lambda}\right)\delta.$$

Then (2) follows.

(3) We see that

$$\frac{1}{\rho_\Lambda(r,X)}\frac{1}{r+2} = \frac{\ell_1}{r+2} + \frac{\ell_2}{\rho_\Lambda(r,X)},$$

where

$$\ell_1 = \frac{1}{\Lambda^2}\frac{1}{(4X-1)/\Lambda-1}, \quad \ell_2 = \frac{1}{\Lambda^2}\frac{r+2\Lambda X}{(4X-1)/\Lambda-1}.$$

We have

$$\left|\int_{-1}^1 \mathrm{d}X\int_0^\Lambda \mathrm{d}r\frac{\ell_1}{r+2}\right| \leqslant \frac{\log(\Lambda+2)}{\Lambda^2}\int_{-1}^1 \mathrm{d}X\frac{1}{(4X-1)/\Lambda-1} \leqslant C\frac{\log\Lambda}{\Lambda^2},$$

$$\left|\int_{-1}^1 \mathrm{d}X\int_0^\Lambda \mathrm{d}r\frac{\ell_2}{\rho_\Lambda(r,X)}\right| \leqslant \frac{\Lambda}{\Lambda^2}\int_{-1}^1 \mathrm{d}X\int_0^\Lambda \frac{1}{\rho_\Lambda(r,X)}\frac{1+2X}{(4X-1)/\Lambda-1} \leqslant \frac{C}{\Lambda^2}.$$

Hence (3) follows.

(4) It is trivial that $|\int_0^1 \cdots \mathrm{d}X| \leqslant C/\Lambda^3$. Let $\delta=\delta(3/2)=1/\Lambda^{3/2}$. From the proof of (2) it follows that

$$\left|\int_{-1+\delta}^0 \cdots \mathrm{d}X\right| \leqslant \frac{C}{\Lambda^3}\int_{-1+\delta}^0 \mathrm{d}X\left\{\frac{(1-X^2)}{(1-X^2)^{3/2}}+(1-X^2)\right\} \leqslant \frac{C}{\Lambda^3}(\arcsin(1-\delta)+1),$$

$$\left|\int_{-1}^{-1+\delta} \cdots \mathrm{d}X\right| \leqslant \frac{C}{\Lambda}\left(\frac{1}{\sqrt{\Lambda}}+\frac{1}{\Lambda}\right)\delta.$$

Hence (4) follows. ■

APPENDIX B: PROOF OF (4.13)

Lemma B.1: It follows that

$$\lim_{\Lambda\to\infty}\sqrt{\Lambda}\int_{-1+1/\Lambda}^{0}(1+X^2)(t_1(\Lambda)+t_2(\Lambda)+t_3(\Lambda))\mathrm{d}X=0, \tag{B1}$$

where

$$t_1(\Lambda)=-2\Lambda\int_{\kappa}^{\Lambda}\mathrm{d}r\frac{1}{\rho^2}+4\Lambda\int_{\kappa}^{\Lambda}\mathrm{d}r\frac{r}{\rho^3}+2\Lambda^2\int_{\kappa}^{\Lambda}\mathrm{d}r\frac{1}{\rho^3},$$

$$t_2(\Lambda)=\Lambda\left(-\frac{1}{2}\right)\left[\frac{1}{\rho}\right]_{\kappa}^{\Lambda}-\Lambda\int_{\kappa}^{\Lambda}\mathrm{d}r\frac{1}{\rho^2},$$

$$t_3(\Lambda)=\Lambda^3 2(2X+1)(1-X)\left[\frac{r+\Lambda X+1}{4\Delta}\frac{1}{\rho^2}\right]_{\kappa}^{\Lambda}.$$

Proof: In this proof C also denotes some sufficiently large constant, which is not necessarily the same number. We have

$$\sqrt{\Lambda}\Lambda\left|\int_{-1+(1/\Lambda)}^{0}\mathrm{d}X\int_{\kappa}^{\Lambda}\mathrm{d}r\frac{1}{\rho^2}\right|\leqslant C\sqrt{\Lambda}\Lambda\frac{1}{\Lambda^{5/2}}=C\frac{1}{\Lambda},$$

$$\sqrt{\Lambda}\Lambda\left|\int_{-1+(1/\Lambda)}^{0}\mathrm{d}X\int_{\kappa}^{\Lambda}\mathrm{d}r\frac{r}{\rho^3}\right|\leqslant C\sqrt{\Lambda}\Lambda^2\frac{1}{\Lambda^{7/2}}=C\frac{1}{\Lambda},$$

$$\sqrt{\Lambda}\Lambda^2\left|\int_{-1+(1/\Lambda)}^{0}\mathrm{d}X\int_{\kappa}^{\Lambda}\mathrm{d}r\frac{1}{\rho^3}\right|\leqslant C\sqrt{\Lambda}\Lambda^2\frac{1}{\Lambda^{7/2}}=C\frac{1}{\Lambda}.$$

Then

$$\lim_{\Lambda\to\infty}\sqrt{\Lambda}\int_{-1+1/\Lambda}^{0}\mathrm{d}X(1+X^2)t_1(\Lambda)=0$$

follows. Next we shall show that

$$\lim_{\Lambda\to\infty}\sqrt{\Lambda}\int_{-1+1/\Lambda}^{0}\mathrm{d}X(1+X^2)t_2(\Lambda)=0. \tag{B2}$$

Note that

$$\left|\left[\frac{1}{\rho}\right]_{\kappa}^{\Lambda}\right|=\left|\frac{1}{(\Lambda+\Lambda X+1)^2+\Delta}-\frac{1}{(\kappa+\Lambda X+1)^2+\Delta}\right|\leqslant\frac{2}{\Delta}\leqslant\frac{2}{\Lambda^2}\frac{1}{1-X^2}.$$

Then

$$\left|\int_{-1+1/\Lambda}^{0}\mathrm{d}X\left[\frac{1}{\rho}\right]_{\kappa}^{\Lambda}\right|\leqslant C\frac{\log\Lambda}{\Lambda^2}.$$

Similarly we can see that

$$\left| \int_{-1+1/\Lambda}^{0} \mathrm{d}X \left[\frac{1}{\rho^2} \right]_\kappa^\Lambda \right| \leqslant C \frac{1}{\Lambda^3},$$

which implies that

$$\sqrt{\Lambda}\Lambda \left| \int_{-1+1/\Lambda}^{0} \mathrm{d}X \left[\frac{1}{\rho} \right]_\kappa^\Lambda \right| \leqslant C \frac{\log \Lambda}{\sqrt{\Lambda}},$$

$$\sqrt{\Lambda}\Lambda^2 \left| \int_{-1+1/\Lambda}^{0} \mathrm{d}X \left[\frac{1}{\rho^2} \right]_\kappa^\Lambda \right| \leqslant C \frac{1}{\sqrt{\Lambda}}.$$

Hence (B2) follows. Finally we shall show that

$$\lim_{\Lambda \to \infty} \sqrt{\Lambda} \int_{-1+1/\Lambda}^{0} \mathrm{d}X (1 + X^2) t_3(\Lambda) = 0. \tag{B3}$$

We divide $\int_{-1+1/\Lambda}^{0} \mathrm{d}X$ as

$$\int_{-1+1/\Lambda}^{0} \mathrm{d}X = \int_{-1+1/\Lambda}^{-1/2} \mathrm{d}X + \int_{-1/2}^{0} \mathrm{d}X.$$

Since

$$\frac{1}{\Delta} \leqslant \frac{1}{\Lambda^2} \frac{1}{1 - X^2} \leqslant \frac{1}{\Lambda^2} \frac{4}{3} \quad \text{for } -\frac{1}{2} \leqslant X \leqslant 0,$$

we see that

$$\sqrt{\Lambda}\Lambda^3 \left| \int_{-1/2}^{0} \mathrm{d}X \left[\frac{r + \Lambda X + 1}{\Delta} \frac{1}{\rho^2} \right]_\kappa^\Lambda \right| \leqslant C \sqrt{\Lambda}\Lambda^3 \frac{\Lambda}{\Lambda^2} \frac{1}{\Lambda^3} = C \frac{1}{\sqrt{\Lambda}}. \tag{B4}$$

On the other hand,

$$\left[\frac{r + \Lambda X + 1}{\Delta} \frac{1}{\rho^2} \right]_\kappa^\Lambda = \frac{\Lambda + \Lambda X + 1}{\Delta} \frac{1}{\{(\Lambda + \Lambda X + 1)^2 + \Delta\}^2} - \frac{\kappa + \Lambda X + 1}{\Delta} \frac{1}{\{(\kappa + \Lambda X + 1)^2 + \Delta\}^2}.$$

Since

$$\left| \frac{\Lambda + \Lambda X + 1}{\Delta} \right| \leqslant \frac{C}{\Lambda}, \quad \left| \frac{\kappa + \Lambda X + 1}{(\kappa + \Lambda X + 1)^2 + \Delta} \right| \leqslant \frac{C}{\Lambda},$$

we have

$$\left| \int_{-1+1/\Lambda}^{-1/2} \mathrm{d}X \left[\frac{r + \Lambda X + 1}{\Delta} \frac{1}{\rho^2} \right]_\kappa^\Lambda \right| \leqslant C \frac{1}{\Lambda} \int_{-1+1/\Lambda}^{-1/2} \frac{1}{\Delta^2} \leqslant C \frac{1}{\Lambda^4}.$$

Then we obtain that

$$\sqrt{\Lambda}\Lambda^3 \left| \int_{-1+1/\Lambda}^{-1/2} \mathrm{d}X \left[\frac{r + \Lambda X + 1}{\Delta} \frac{1}{\rho^2} \right]_\kappa^\Lambda \right| \leqslant C \frac{1}{\sqrt{\Lambda}}. \tag{B5}$$

Thus (B3) follows from (B4) and (B5). ■

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Existence of the semilocal Chern–Simons vortices

Dongho Chae[a)]
Department of Mathematics, Sungkyunkwan University, Suwon 440-746, Korea

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We consider the Bogomol'nyi equations of the Abelian Chern–Simons–Higgs model with $SU(N)_{global} \otimes U(1)_{local}$ symmetry. This is a generalization of the well-known Abelian Chern–Simons–Higgs model with $U(1)_{local}$ symmetry. We prove existence of both topological and nontopological multivortex solutions of the system on the plane. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1868858]

I. INTRODUCTION

The Abelian Chern–Simons–Higgs model with $SU(N)_{global} \otimes U(1)_{local}$ symmetry is defined by the Lagrangian,

$$\mathcal{L} = \frac{\kappa}{4}\epsilon^{\mu\nu\lambda}F_{\mu\nu}A_\lambda + (D_\mu\Phi)^\dagger(D^\mu\Phi) - \frac{1}{\kappa^2}|\Phi|^2(|\Phi|^2-1)^2,$$

where $A_\mu(\mu=0,1,2)$ is the gauge field on $\mathbb{R}^3$, $F_{\mu\nu}=(\partial/\partial x^\mu)A_\nu-(\partial/\partial x^\nu)A_\mu$ is the corresponding gauge curvature tensor, $D_\mu=(\partial/\partial x^\mu)-iA_\mu$ is the gauge covariant derivative, $\Phi=(\Phi_1,\Phi_2,\ldots,\Phi_N)$ is a $\mathbb{C}^N$ valued function on $\mathbb{R}^3$, called the Higgs multiplet, $\epsilon_{\mu\nu\rho}$ is the totally skewsymmetric tensor with $\epsilon_{012}=1$, and finally $\kappa>0$ is the Chern–Simons coupling constant. Our metric on $\mathbb{R}^3$ is $(g_{\mu\nu})=\mathrm{diag}(1,-1,-1)$. This model was suggested by Khare,[6] generalizing the original Abelian Chern–Simons–Higgs model, due to Hong–Kim–Pac[4] and Jackiw–Weinberg.[5] We also mention that there are also studies of the corresponding Abelian Higgs model with $SU(N)_{global} \otimes U(1)_{local}$ symmetry in Refs. 14 and 3. Similar to the case of Abelian Chern–Simons–Higgs model, in the static case, the following Bogomol'nyi system in $\mathbb{R}^2$ is obtained:[6]

$$(D_1 \pm iD_2)\Phi_k = 0, \quad \forall\, k=1,\ldots,N,$$

$$F_{12} = \pm\frac{2}{\kappa^2}|\Phi|^2(|\Phi|^2-1). \tag{1.1}$$

This system is equipped with one of the following boundary conditions: either

$$|\Phi(z)|^2 \to 1 \quad \text{as } |z|\to\infty, \tag{1.2}$$

or

$$|\Phi(z)|^2 \to 0 \quad \text{as } |z|\to\infty \tag{1.3}$$

Following the standard Jaffe–Taubes reduction procedure,[13] we introduce new variable $(u_1,\ldots,u_N)$ by

a)Electronic mail: chae@skku.edu

$$\Phi_k(z) = \exp\left[\frac{1}{2}u_k + i\sum_{j=1}^{M_k} \mathrm{Arg}(z - z_{k,j})\right], \quad z = x_1 + ix_2 \in \mathbb{C}^1 = \mathbb{R}^2,$$

where $\mathbb{Z}_k = \{z_{k,j}\}_{j=1}^{M_k}$ is the set of zeros of $\Phi_k(z)$. Then, the system (1.1) becomes the following semilinear elliptic system for $(u_1, \ldots, u_N)$ in $\mathbb{R}^2$:

$$\Delta u_k = \left(\sum_{j=1}^{N} e^{u_j}\right)\left(\sum_{j=1}^{N} e^{u_j} - 1\right) + 4\pi\sum_{j=1}^{M_k} \delta(z - z_{k,j}), \quad k = 1, \ldots, N, \tag{1.4}$$

where we set $\kappa = 2$ for simplicity. In terms of $(u_1, \ldots, u_N)$, the boundary condition (1.2) reads

$$e^{u_k} \to \sigma_k \quad \text{as } |z| \to \infty$$

$$\text{with } \sigma_k \geqslant 0 \quad \text{for all } k = 1, \ldots, N, \text{and} \sum_{k=1}^{N} \sigma_k = 1, \tag{1.5}$$

while (1.3) reads

$$e^{u_k} \to 0 \quad \text{as } |z| \to \infty \quad \text{for all } k = 1, \ldots, N. \tag{1.6}$$

The boundary condition (1.5) is called topological, while the boundary condition (1.6) is called nontopological. We observe that when $N = 1$, the system (1.4) reduces to the well-known (scalar) Chern–Simons equation, for which there are many studies for topological vortices,[11,15] nontopological vortices,[1,2,10] periodic vortex condensates,[9,8,12,16] respectively. We first consider the nontopological case. In the system (1.4) equipped with (1.3), without loss of generality, we assume $M_1 \geqslant M_k$ for all $k = 1, \ldots, N$. Let us define

$$f_k(z) = (M_k + 1)\prod_{j=1}^{M_k} (z - z_{k,j}), \quad F_k(z) = \int_0^z f_k(\xi)\mathrm{d}\xi. \tag{1.7}$$

Given $\varepsilon > 0$, $a = a_1 + ia_2 \in \mathbb{C}$, let us introduce the functions $\rho_{\varepsilon,a}^{(k)}(z)$ by

$$\rho_{\varepsilon,a}^{(k)}(z) = \frac{8\varepsilon^{2M_k+2}|f_k(z)|^2}{\left(1 + \varepsilon^{2M_1+2}\left|F_1(z) + \dfrac{a}{\varepsilon^{M_1+1}}\right|^2\right)^2}. \tag{1.8}$$

We note that for any $\varepsilon > 0$ and $a \in \mathbb{C}^1$, $\ln \rho_{\varepsilon,a}^{(1)}(z)$ is a solution of the Liouville equation,

$$\Delta \ln \rho_{\varepsilon,a}^{(1)}(z) = -\rho_{\varepsilon,a}^{(1)}(z) + 4\pi\sum_{j=1}^{M_1} \delta(z - z_{1,j}). \tag{1.9}$$

We state the existence theorem for the nontopological vortices.

Theorem 1.1 (Existence of nontopological vortices): *Let $N \geqslant 2$. For each $k = 1, \ldots, N$ let $M_k \in \mathbb{N}$ with $M_1 \geqslant M_k$ for all $k = 1, \ldots, N$, and let $\mathbb{Z}_1, \ldots, \mathbb{Z}_N$ be given with $\mathbb{Z}_k = \{z_{k,j}\}_{j=1}^{M_k} \in \mathbb{R}^2$. Then, there exists a constant $\varepsilon_1 > 0$ such that for any $\varepsilon \in (0, \varepsilon_1)$ there exists a family of solutions to (1.4) $(u_1, u_2, \ldots, u_N)$ equipped with the boundary condition (1.6). Moreover, the solutions we constructed have the following representations:*

$$u_1(z) = \ln \rho_{\varepsilon,a_\varepsilon^*}^{(1)}(z) + \varepsilon^2 w(\varepsilon|z|) + \varepsilon^2 v_\varepsilon^*(\varepsilon z), \tag{1.10}$$

$$u_k(z) = \ln \rho_{\varepsilon,a_\varepsilon^*}^{(k)}(z) + \varepsilon^2 w(\varepsilon|z|) + \varepsilon^2 v_\varepsilon^*(\varepsilon z) + \ln \varepsilon^4, \tag{1.11}$$

for all $k = 2, \ldots, N$.

In (1.10) and (1.11), the function $\varepsilon \mapsto a_\varepsilon^*$ *is continuous in a neighborhood of* 0, *and* $|a_\varepsilon^*| \to 0$ *as* $\varepsilon \to 0$. *The radial function w in (1.10) and (1.11) has the following asymptotic behavior:*

$$w(|z|) = -C_0 \ln|z| + O(1), \tag{1.12}$$

as $|z| \to \infty$ *with the constant* $C_0 > 0$ *defined by*

$$C_0 = \frac{4\pi M_1^2 (2M_1+1)^6}{15(M_1+1)^5 \sin\left(\frac{\pi M_1}{M_1+1}\right)}. \tag{1.13}$$

The function v_ε^* *in (1.10) and (1.11) satisfies*

$$\sup_{z\in\mathbb{R}^2} \frac{|v_\varepsilon^*(\varepsilon z)|}{\ln(1+|z|)} \leqslant o(1) \quad \text{as } \varepsilon \to 0. \tag{1.14}$$

Next, we consider the system (1.4) equipped with the topological boundary condition (1.5). Without loss of generality, we assume that for $m \in \{1, \ldots, N\}$,

$$e^{u_k} \to \sigma_k \quad \text{as } |z| \to \infty \quad \text{for } k = 1, \ldots, m, \tag{1.15}$$

$$e^{u_k} \to 0 \quad \text{as } |z| \to \infty \quad \text{for all } k = m+1, \ldots, N, \tag{1.16}$$

where $\Sigma_{k=1}^m \sigma_k = 1$, and $\sigma_k \in (0,1]$ for each $k = 1, \ldots, m$. The following is our second main theorem.

Theorem 1.2 (Existence of topological vortices): *In order to have solution to the system (1.4) equipped with (1.15) and (1.16), it is necessary that*

$$M_1 = M_2 = \cdots = M_m (\equiv M) \quad \text{and } M_k < M \quad \text{for all } k = m+1, \ldots, N. \tag{1.17}$$

If the condition (1.17) is satisfied, then there exists a solution $(u_1, \ldots, u_N)$ *to the problem. Moreover, the solutions we constructed have the following representations:*

$$u_k(z) = \ln\left(\sigma_k \prod_{j=1}^{M} \frac{|z - z_{k,j}|^2}{(\mu + |z - z_{1,j}|^2)} \right) + v \quad \text{for } k = 1, \ldots, m, \tag{1.18}$$

while

$$u_k(z) = \ln\left(\frac{\prod_{j=1}^{M_k} |z - z_{k,j}|^2}{\prod_{j=1}^{M} (\mu + |z - z_{1,j}|^2)} \right) + v \quad \text{for } k = m+1, \ldots, N \tag{1.19}$$

for a function $v \in \cap_{q=1}^{\infty} H^q(\mathbb{R}^2)$.

II. EXISTENCE OF NONTOPOLOGICAL VORTICES

In this section our aim is to prove Theorem 1.1. From the equation, $\Delta \ln|z - z_0|^2 = 4\pi\delta(z - z_0)$ in $\mathbb{R}^2$ we find that

$$\Delta\left(u_k - u_1 - \sum_{j=1}^{M_k} \ln|z - z_{k,j}|^2 + \sum_{j=1}^{M_1} \ln|z - z_{1,j}|^2 \right) = 0.$$

Hence, we obtain the relations between u_1 and u_k,

$$u_k = u_1 + \ln\left(\frac{\prod_{j=1}^{M_k}|z-z_{k,j}|^2}{\prod_{j=1}^{M_1}|z-z_{1,j}|^2}\right) + h_k(z) \tag{2.1}$$

for all $k=1,\dots,N$, where $h_k(z)$ is a harmonic function in $\mathbb{R}^2$. We choose

$$h_k(z) \equiv \ln \varepsilon^{4+2M_k-2M_1}.$$

Then, (2.1) becomes

$$u_k = u_1 + \ln\left(\frac{\varepsilon^{4+2M_k-2M_1}\prod_{j=1}^{M_k}|z-z_{k,j}|^2}{\prod_{j=1}^{M_1}|z-z_{1,j}|^2}\right). \tag{2.2}$$

We introduce $g^{(k)}_{\varepsilon,a}(z)$, $\rho_k(r)$, $k=1,\dots,N$ as follows:

$$g^{(k)}_{\varepsilon,a}(z) = \frac{1}{\varepsilon^2}\rho^{(k)}_{\varepsilon,a}\left(\frac{z}{\varepsilon}\right), \quad \rho_k(r) = \frac{8(M_k+1)^2 r^{2M_k}}{(1+r^{2M_1+2})^2} \quad \left[=\lim_{\varepsilon\to 0} g^{(k)}_{\varepsilon,0}(z)\right]. \tag{2.3}$$

Let us make a change of variables from u_1 to v by the following formula:

$$u_1(z) = \ln \rho^{(1)}_{\varepsilon,a}(z) + \varepsilon^2 w(\varepsilon|z|) + \varepsilon^2 v(\varepsilon x), \tag{2.4}$$

where $w(\cdot)$ is a radial function to be determined below. Then, after elementary computations we find that combination of (2.2) and (2.4) implies the following representation formula for u_k:

$$u_k(z) = \ln \rho^{(k)}_{\varepsilon,a}(z) + \varepsilon^2 w(\varepsilon|z|) + \varepsilon^2 v(\varepsilon x) + \ln \varepsilon^4 \tag{2.5}$$

for all $k=2,\dots,N$.

Then, the equation for u_1 in (1.4) can be written as the functional equation $P(v,a,\varepsilon)=0$, where

$$P(v,a,\varepsilon) = \Delta v + \frac{1}{\varepsilon^2} g^{(1)}_{\varepsilon,a}(z)(e^{\varepsilon^2(v+w)}-1) - [g^{(1)}_{\varepsilon,a}(z)]^2 e^{2\varepsilon^2(v+w)} + \varepsilon^2 \sum_{k=2}^{N} g^{(k)}_{\varepsilon,a}(z) e^{\varepsilon^2(v+w)} - \varepsilon^4 \sum_{k=2}^{N} g^{(1)}_{\varepsilon,a}(z) g^{(k)}_{\varepsilon,a}$$

$$\times(z) e^{2\varepsilon^2(v+w)} - \varepsilon^8 \sum_{k,l=2}^{N} g^{(l)}_{\varepsilon,a}(z) g^{(k)}_{\varepsilon,a}(z) e^{2\varepsilon^2(v+w)}. \tag{2.6}$$

Now we introduce the functions spaces introduced in Ref. 1. Let us fix $\alpha \in (0, \frac{1}{2})$ throughout this paper. Following Ref. 1, we introduce the Banach spaces X_α and Y_α as

$$X_\alpha = \left\{ u \in L^2_{\mathrm{loc}}(\mathbb{R}^2) \Big| \int_{\mathbb{R}^2} (1+|x|^{2+\alpha})|u(x)|^2 \, \mathrm{d}x < \infty \right\}$$

equipped with the norm $\|u\|^2_{X_\alpha} = \int_{\mathbb{R}^2}(1+|x|^{2+\alpha})|u(x)|^2 \, \mathrm{d}x$, and

$$Y_\alpha = \left\{ u \in W^{2,2}_{\mathrm{loc}}(\mathbb{R}^2) \Big| \|\Delta u\|^2_{X_\alpha} + \left\| \frac{u(x)}{1+|x|^{1+(\alpha/2)}} \right\|^2_{L^2(\mathbb{R}^2)} < \infty \right\}$$

equipped with the norm

$$\|u\|^2_{Y_\alpha} = \|\Delta u\|^2_{X_\alpha} + \left\| \frac{u(x)}{1+|x|^{1+(\alpha/2)}} \right\|^2_{L^2(\mathbb{R}^2)}.$$

We recall the following propositions proved in Ref. 1.

Proposition 2.1: Let Y_α be the function space introduced above. Then we have the followings:

(i) *If $v \in Y_\alpha$ is a harmonic function, then $v \equiv$ constant.*
(ii) *There exists a constant $C_1 > 0$ such that for all $v \in Y_\alpha$,*

$$|v(x)| \leqslant C_1 \|v\|_{Y_\alpha} \ln(e + |x|), \quad \forall\, x \in \mathbb{R}^2.$$

Proposition 2.2: Let $\alpha \in (0, \frac{1}{2})$, and let us set

$$L = \Delta + \rho_1 : Y_\alpha \to X_\alpha. \tag{2.7}$$

We have

$$\operatorname{Ker} L = \operatorname{Span}\{\varphi_+, \varphi_-, \varphi_0\}, \tag{2.8}$$

where we denoted

$$\varphi_+(r,\theta) = \frac{r^{M_1+1}\cos(M_1+1)\theta}{1 + r^{2M_1+2}}, \quad \varphi_-(r,\theta) = \frac{r^{M_1+1}\sin(M_1+1)\theta}{1 + r^{2M_1+2}}, \tag{2.9}$$

and

$$\varphi_0 = \frac{1 - r^{2M_1+2}}{1 + r^{2M_1+2}}. \tag{2.10}$$

Moreover, we have

$$\operatorname{Im} L = \left\{ f \in X_\alpha \,\middle|\, \int_{\mathbb{R}^2} f\varphi_\pm = 0 \right\}. \tag{2.11}$$

We can check easily that P is a well-defined continuous mapping from $B_{\varepsilon_0} \subset Y_\alpha \times \mathbb{C} \times \mathbb{R}_+$ into X_α, where $B_{\varepsilon_0} = \{\|v\|_{Y_\alpha} + |a| \leqslant \varepsilon < \varepsilon_0\}$ for sufficiently small ε_0. In order to have a continuous extension to $\varepsilon = 0$ of $P(\cdot)$ we require that $\lim_{\varepsilon \to 0} P(0,0,\varepsilon) = 0$, which implies the following equation for w:

$$\Delta w + \rho_1 w - \rho_1^2 = 0. \tag{2.12}$$

We first note the following lemma about asymptotic behaviors of the solutions $w \in Y_\alpha$, the proof of which is in the Appendix.

Lemma 2.1: Let C_0 be the number introduced in (1.13). Then, there exist radial solutions $w(|z|)$ of (2.12) belonging to Y_α, and satisfying the asymptotic formula in (1.12).

In order to obtain the linearized operator $P'_{(v,a)}(0,0,0) = \mathcal{A}$ we first compute,

$$\left.\frac{\partial g^{(k)}_{\varepsilon,a}(z)}{\partial a_1}\right|_{\varepsilon=0,a=0} = -4\rho_k\varphi_+, \qquad \left.\frac{\partial g^{(k)}_{\varepsilon,a}(z)}{\partial a_2}\right|_{\varepsilon=0,a=0} = -4\rho_k\varphi_-,$$

for all $k = 1, \ldots, N$, where ■ ■

Using these we find

$$\mathcal{A}[\nu,\beta] = L\nu - 4(\rho_1 w - 2\rho_1^2)(\varphi_+\beta_1 + \varphi_-\beta_2).$$

For the linearized operator $\mathcal{A}[\cdot]$ we need the following key lemma.

Lemma 2.2: The operator $\mathcal{A}: Y_\alpha \times \mathbb{R}^2 \to X^2_\alpha$ defined above is onto. Moreover, kernel of $\mathcal{A}$ is given by

$$\operatorname{Ker} A = \operatorname{Span}\{\varphi_+, \varphi_-, \varphi_0\} \times \{(0,0)\}. \tag{2.13}$$

Thus, if we decompose $Y_\alpha \times \mathbb{R}^2 = U_\alpha \oplus \operatorname{Ker}\mathcal{A}$, where we set $U_\alpha = (\operatorname{Ker}\mathcal{A})^\perp$, then $\mathcal{A}$ is an isomorphism from U_α onto X_α.

For the proof of Lemma 2.2 we need the following proposition, the proof of which is in the Appendix.

Proposition 2.3:

$$I_{\pm} := \int_{\mathbb{R}^2} (\rho_1 w - 2\rho_1^2)\varphi_{\pm}^2 \, dx \neq 0.$$

With Proposition 2.3 equipped, the proof of Lemma 2.2 is the same as the one in Ref. 1, since the linearized operator, $\mathcal{A}$ is the same as the one in it. We are now ready to prove our main theorem.

Proof of Theorem 1.1: Let us set

$$U_\alpha = (\mathrm{Ker}\, L)^{\perp} \times \mathbb{R}^2.$$

Then, Lemma 2.2 shows that $P'_{(v,\xi,\beta)}(0,0,0,0): U_\alpha \to X_\alpha \times X_\alpha$ is an isomorphism for $\alpha \in (0, \frac{1}{2})$. Then, the standard implicit function theorem (see, e.g., Ref. 17), applied to the functional $P: U_\alpha \times (-\varepsilon_0, \varepsilon_0) \to X_\alpha \times X_\alpha$, implies that there exists a constant $\varepsilon_1 \in (0, \varepsilon_0)$ and a continuous function $\varepsilon \mapsto \psi_\varepsilon^* := (v_\varepsilon^*, a_\varepsilon^*)$ from $(0, \varepsilon_1)$ into a neighborhood of 0 in U_α such that

$$P(v_\varepsilon^*, a_\varepsilon^*, \varepsilon) = 0 \quad \text{for all } \varepsilon \in (0, \varepsilon_1).$$

This completes the proof of Theorem 1.1. Since $M_1 \geqslant M_k$ for all $k = 1, \cdots, N$, the representation of solutions u_k, and the explicit form of

$$\ln[\rho^{(k)}_{\varepsilon, a_\varepsilon^*}(z)] = -[(4M_1 - 2M_k) + 4]\ln|z| + O(1)$$

as $|z| \to \infty$, together with the asymptotic behaviors of $w(\cdot)$ described in Lemma 2.1, the fact that $v_\varepsilon^* \in Y_\alpha$, combined with Proposition 2.1, implies that the solutions satisfy the boundary condition in (1.6). Now, from Proposition 2.1 we obtain that

$$|v_\varepsilon^*(z)| \leqslant C\|v_\varepsilon^*\|_{Y_\alpha}(\ln^+|z| + 1) \leqslant C\|\psi_\varepsilon\|_{U_\alpha}(\ln^+|z| + 1).$$

This implies then

$$|v_\varepsilon^*(\varepsilon x)| \leqslant C\|\psi_\varepsilon\|_{U_\alpha}(\ln^+|\varepsilon x| + 1) \leqslant C\|\psi_\varepsilon\|_{U_\alpha}(\ln^+|x| + 1). \tag{2.14}$$

From the continuity of the function $\varepsilon \mapsto \psi_\varepsilon$ from $(0, \varepsilon_0)$ into U_α and the fact $\psi_0^* = 0$ we have

$$\|\psi_\varepsilon\|_{U_\alpha} \to 0 \quad \text{as } \varepsilon \to 0. \tag{2.15}$$

The proof of (1.14) follows from (2.15) combined with (2.14). This completes the proof of Theorem 1.1. ■

III. EXISTENCE OF TOPOLOGICAL VORTICES

Our aim in this section is to prove Theorem 1.2.

Proof of Theorem 1.2: We first establish that in order to have existence of solution $(u_1, \cdots, u_N)$ satisfying (1.4) and (1.15) and (1.16), it is necessary to have (1.17). Without loss of generality we may assume $M_1 \geqslant M_k$ for all $k = 1, \cdots, m$. Suppose that there exists $M_k < M_1$ for some $k \in \{1, \cdots, m\}$. Then, from (1.4) we have

$$\Delta(u_k - u_1 - \sum_{j=1}^{M_k} \ln|z - z_{k,j}|^2 + \sum_{j=1}^{M_1} \ln|z - z_{l,j}|^2) = 0$$

and

$$u_k = u_1 + \ln\left(\frac{\prod_{j=1}^{M_k}|z-z_{k,j}|^2}{\prod_{j=1}^{M_1}|z-z_{l,j}|^2}\right) + h_k(z) \tag{3.1}$$

for some harmonic function $h_k(z)$. Since

$$u_k \to \ln\sigma_k, \quad u_1 \to \ln\sigma_1, \quad \ln\left(\frac{\prod_{j=1}^{M_k}|z-z_{k,j}|^2}{\prod_{j=1}^{M_1}|z-z_{l,j}|^2}\right) \to O((M_k - M_1)\ln|z|),$$

as $|z|\to\infty$, (3.1) implies $h_k \equiv C_k$ (constant), and provides an absurd relation. Hence, $M_1 = \cdots = M_m \equiv M$. Similarly, the relation (3.1) with $k=m+1,\cdots,N$ implies $M_k < M$ for all $k=m+1,\cdots,N$, since for all $k=m+1,\cdots,N$, $u_k \to -\infty$, while $u_1 \to \ln\sigma_1$ as $|z|\to\infty$.

Then, choosing $C_k = \ln(\sigma_k/\sigma_1)$ for all $k=1,\cdots,m$, (2.1) becomes

$$u_k = u_1 + \ln\left(\frac{\sigma_k}{\sigma_1}\prod_{j=1}^{M}\frac{|z-z_{k,j}|^2}{|z-z_{1,j}|^2}\right) \tag{3.2}$$

for $k=1,\cdots,N$. Let us set

$$\eta_k(z) = \begin{cases} \sigma_k\displaystyle\prod_{j=1}^{M}\frac{|z-z_{k,j}|^2}{(\mu+|z-z_{1,j}|^2)} & \text{for } k\in\{1,\cdots,m\}, \\ \dfrac{\prod_{j=1}^{M_k}|z-z_{k,j}|^2}{\prod_{j=1}^{M}(\mu+|z-z_{1,j}|^2)} & \text{for } k\in\{m+1,\cdots,N\}, \end{cases}$$

where $\mu>$ is a sufficiently large parameter. We introduce new unknown v by

$$u_1 = v + \ln\,\eta_1. \tag{3.3}$$

Then, (3.2) combined with (3.3) implies the representation for u_k, $k=1,\cdots,N$ by

$$u_k = v + \ln\,\eta_k.$$

We introduce

$$g(z) = \sum_{j=1}^{M}\frac{4\mu}{(\mu+|z-z_{1,j}|^2)^2}.$$

We note that

$$\Delta\ln\,\eta_1(z) = 4\pi\sum_{j=1}^{M}\delta(z-z_{1,j}) - g(z). \tag{3.4}$$

We also introduce the function u_0 defined by

$$\sum_{k=1}^{N}\eta_k = e^{u_0}. \tag{3.5}$$

Note that since $e^{u_0}\to\Sigma_{k=1}^{m}\sigma_k=1$, we have $u_0\to 0$ as $|z|\to\infty$.

Using (3.4) and (3.5), we can rewrite the equation for u_1 in (1.4) as follows:

$$\Delta v = e^{v+u_0}(e^{v+u_0}-1) + g,$$

which is the Euler–Lagrange equation of the functional

$$F(v)=\int_{\mathbb{R}^2}\left[\frac{1}{2}|\nabla v|^2+\frac{1}{2}(e^{u+u_0}-1)^2+gv\right]\mathrm{d}x. \tag{3.6}$$

After this step the arguments for the existence of solution by minimization of the functional $F(v)$ by showing the coercivity and the weak lower semicontinuity in $H^1(\mathbb{R}^2)$ for sufficiently large μ, is exactly the same as in Refs. 15 and 11 or 16 and we do not repeat them here. This finishes the proof of Theorem 1.2. ■

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APPENDIX

Here we prove Lemma 2.1 and Proposition 2.3. We begin with the following elementary integration lemma.

Lemma 4.1: Let $m\geqslant k+1$, then we have

$$\int_0^\infty \frac{r^{k(2N+2)-3}}{(1+r^{2N+2})^m}\mathrm{d}r=\frac{\pi\prod_{j=1}^{k-1}(Nj+j-1)\prod_{j=1}^{m-k}[Nj+j-1]}{2(m-1)!(N+1)^m\sin\left(\frac{\pi N}{N+1}\right)}. \tag{A1}$$

Proof:

$$\begin{aligned}\int_0^\infty \frac{r^{k(2N+2)-3}}{(1+r^{2N+2})^m}\mathrm{d}r&=\frac{1}{2N+2}\int_0^\infty \frac{t^{k-1-[1/(N+1)]}}{(1+t)^m}\mathrm{d}t \quad (\text{setting } t=r^{2N+2})\\ &=-\frac{1}{2N+2}\int_0^\infty \frac{t^{k-1-[1/(N+1)]}}{(m-1)}\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{(1+t)^{m-1}}\mathrm{d}t\\ &=\frac{1}{(2N+2)}\frac{1}{(m-1)}\left(k-1-\frac{1}{N+1}\right)\int_0^\infty \frac{t^{k-2-[1/(N+1)]}}{(1+t)^{m-1}}\mathrm{d}t=\cdots\\ &=\frac{\left(k-1-\frac{1}{N+1}\right)\left(k-2-\frac{1}{N+1}\right)\cdots\left(1-\frac{1}{N+1}\right)}{2(N+1)(m-1)(m-2)\cdots(m-k+1)}\int_0^\infty \frac{t^{-1/(N+1)}}{(1+t)^{m-k+1}}\mathrm{d}t.\end{aligned} \tag{A2}$$

Now we use the well-known formula from the Mellin transform (see, e.g., Ref. 7),

$$\int_0^\infty \frac{t^{a-1}}{(1+t)^n}\mathrm{d}t=\frac{\pi|(a-1)(a-2)\cdots(a-(n-1))|}{(n-1)!\sin(\pi a)},\quad a\in(0,1)$$

in order to evaluate

$$\int_0^\infty \frac{t^{-1/(N+1)}}{(1+t)^{m-k+1}}\mathrm{d}t=\int_0^\infty \frac{t^{a-1}}{(1+t)^{m-k+1}}\mathrm{d}t=\frac{\pi|(a-1)(a-2)\cdots(a-m+k)|}{(m-k)!\sin(\pi a)}, \tag{A3}$$

where we set $a=N/(N+1)$. Substituting (A3) into (A2), we obtain (A1). ■

Proof of Lemma 2.1: Let us set $f(r)=\rho_1(r)$. Then, it is found in Ref. 1 that the ordinary differential equation (with respect to r), $\Delta w+\rho_1 w=f(r)$ has a solution $w(r)\in Y_\alpha$ given by

$$w(r) = \varphi_0(r)\left\{ \int_0^r \frac{\phi_f(s) - \phi_f(1)}{(1-s)^2} \mathrm{d}s + \frac{\phi_f(1) r}{1-r} \right\} \tag{A4}$$

with

$$\phi_f(r) := \left(\frac{1 + r^{2M_1+2}}{1 - r^{2M_1+2}} \right)^2 \frac{(1-r)^2}{r} \int_0^r \varphi_0(t) t f(t) \mathrm{d}t,$$

where $\phi_f(1)$ and $w(1)$ are defined as limits of $\phi_f(r)$ and $w(r)$ as $r \to 1$. From the formula (A4) we find that

$$w(r) = \varphi_0(r) \int_2^r \left(\frac{1 + s^{2M_1+2}}{1 - s^{2M_1+2}} \right)^2 \frac{I(s)}{s} \mathrm{d}s + (\text{bounded function of } r) \tag{A5}$$

as $r \to \infty$, where

$$I(s) = \int_0^s \varphi_0(t) t \rho_1(t) \mathrm{d}t.$$

Since $\varphi_0(r) \to -1$ as $r \to \infty$, (1.12) follows if we show

$$I = I(\infty) = \int_0^\infty \varphi_0(r) r \rho_1(r) \mathrm{d}r = C_0.$$

We evaluate the integral,

$$\begin{aligned}
I &= \int_0^\infty \varphi_0(r) f(r) r \, \mathrm{d}r = \int_0^\infty \varphi_0(r) \rho_1(r)^2 r \, \mathrm{d}r = 64(M_1+1)^4 \int_0^\infty \frac{(1 - r^{2M_1+2}) r^{4M_1+1}}{(1 + r^{2M_1+2})^5} \mathrm{d}r \\
&= 64(M_1+1)^4 \left[\int_0^\infty \frac{r^{4M_1+1}}{(1 + r^{2M_1+2})^5} \mathrm{d}r - \int_0^\infty \frac{r^{6M_1+3}}{(1 + r^{2M_1+2})^5} \mathrm{d}r \right] \\
&= 64(M_1+1)^4 \left[\frac{\pi M_1^2 (2M_1+1)(3M_1+2)}{2 \times 4! (M_1+1)^5 \sin\left(\frac{\pi M_1}{M_1+1} \right)} - \frac{\pi M_1^2 (2M_1+1)^2}{2 \times 4! (M_1+1)^5 \sin\left(\frac{\pi M_1}{M_1+1} \right)} \right] \\
&= \frac{4\pi M_1^2 (2M_1+1)^6}{15(M_1+1)^5 \sin\left(\frac{\pi M_1}{M_1+1} \right)} = C_0,
\end{aligned}$$

where we used (A1) with $(k,m) = (2,5)$ and (3,5) in the fourth line. This completes the proof of Lemma 2.1. ■

Proof of Proposition 2.3: In order to transform the integral we use the formula

$$L\left[\frac{1}{16(1 + r^{2M_1+2})^2} \right] = \frac{(M_1+1)^2 r^{4M_1+2}}{(1 + r^{2M_1+2})^4},$$

which can be verified by an elementary computation. Using this, we have the following:

$$
\begin{aligned}
I_{\pm} &= \int_{\mathbb{R}^2} (\rho_1 w - 2\rho_1^2)\varphi_{\pm}^2 \, \mathrm{d}x = \int_0^{2\pi}\int_0^{\infty} (\rho_1 w - 2\rho_1^2) \frac{r^{2M_1+2}}{(1+r^{2M_1+2})^2} \begin{Bmatrix} \cos^2(M_1+1)\theta \\ \sin^2(M_1+1)\theta \end{Bmatrix} r \, \mathrm{d}r \, \mathrm{d}\theta \\
&= \pi \int_0^{\infty} \left[\frac{8(M_1+1)^2 r^{2M_1}}{(1+r^{2M_1+2})^2} w - 2\rho_1^2 \right] \frac{r^{2M_1+2}}{(1+r^{2M_1+2})^2} r \, \mathrm{d}r = \pi \int_0^{\infty} \left[\frac{1}{2} L \left\{ \frac{1}{(1+r^{2M_1+2})^2} \right\} w \right. \\
&\quad \left. - \frac{2\rho_1^2 r^{2M_1+2}}{(1+r^{2M_1+2})^2} \right] r \, \mathrm{d}r = \pi \int_0^{\infty} \left[\frac{1}{2} L w \cdot \frac{1}{(1+r^{2M_1+2})^2} - \frac{2\rho_1^2 r^{2M_1+2}}{(1+r^{2M_1+2})^2} \right] r \, \mathrm{d}r \\
&= \pi \int_0^{\infty} \left[\frac{\rho_1^2}{2(1+r^{2M_1+2})^2} - \frac{2\rho_1^2 r^{2M_1+2}}{(1+r^{2M_1+2})^2} \right] r \, \mathrm{d}r = \pi \int_0^{\infty} \left[\frac{5\rho_1^2}{2(1+r^{2M_1+2})^2} - \frac{2\rho_1^2}{(1+r^{2M_1+2})} \right] r \, \mathrm{d}r \\
&= 64\pi (M_1+1)^4 \int_0^{\infty} \left[\frac{5 r^{4M_1+1}}{2(1+r^{2M_1+2})^6} - \frac{2 r^{4M_1+1}}{(1+r^{2M_1+2})^5} \right] \mathrm{d}\, r \\
&= 64\pi (M_1+1)^4 \left[\frac{\pi M_1^2 (2M_1+1)(3M_1+2)(4M_1+3)}{4 \times 4! (M_1+1)^6 \sin\left(\dfrac{\pi M_1}{M_1+1} \right)} - \frac{\pi M_1^2 (2M_1+1)(3M_1+2)}{4! (M_1+1)^5 \sin\left(\dfrac{\pi M_1}{M_1+1} \right)} \right] \\
&= - \frac{2\pi^2 M_1^2 (2M_1+1)(3M_1+2)}{3(M_1+1)^2 \sin\left(\dfrac{\pi M_1}{M_1+1} \right)} < 0,
\end{aligned}
$$

where we used (A1) with $(k,m)=(2,6)$ and $(2,5)$, respectively, in order to evaluate the integrals in the seventh line. This completes the proof of the proposition. ■

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The topology of the electroweak interaction

Jürgen Tolksdorf[a)]
Max Planck Institute for Mathematics in the Sciences, Germany

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In this paper we show that the Higgs boson of the (minimal) standard model has at most three gauge inequivalent ground states. One of these states is related to ordinary electromagnetism and the other two to electromagnetism within magnetically charged vacua. If space–time is assumed to be rotationally symmetric then the charged electroweak vacua may be identified with Dirac monopoles of magnetic charge $g=\pm 1/2$. This offers a physical interpretation of magnetic monopoles and Dirac's quantization condition of electric charge in terms of the electroweak interaction. Moreover, in the case of the (minimal) standard model the three possible gauge inequivalent ground states of the Higgs boson are shown to fully determine the topological structure of the gauge bundle which underlies the electroweak interaction. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1883312]

I. INTRODUCTION

In this paper we discuss the topological structure that underlies the electroweak interaction as it is described by the (minimal) standard model. More specifically, we shall show that the topological structure of the principal $\mathrm{SU}(2)\times\mathrm{U}(1)$ bundle of the electroweak interaction is fully determined by the hypercharge of the Higgs boson.

In Ref. 15 it has been shown that the symmetry of electromagnetism under charge conjugation is equivalent to the triviality of the electroweak gauge bundle. The aim of this paper is to discuss the topology of the electroweak gauge bundle $\mathcal{P}$ over an arbitrary space–time $(\mathcal{M},g_{\mathrm{M}})$ when charge conjugation is not taken into account. We will show that the structure of $\mathcal{P}$ is fully determined by Dirac's famous quantization condition of electric charge. It follows that in the case of the (minimal) standard model the Higgs boson has at most three gauge inequivalent ground states, one of which corresponds to ordinary electromagnetism and the other two correspond to electromagnetism within a "magnetically charged vacuum." Thus, the latter spoil charge conjugation. The fact that there are two charged vacua corresponds to the $\mathbb{Z}_2$-grading of charge conjugation of ordinary electromagnetism. To prove this, we will first summarize the basic geometrical setup in the next section. In the third section we present the proof of the above statements and discuss some consequences. In the fourth section we propose a specific generalization of the moduli space of all electroweak vacua that has been introduced in Ref. 15 and discuss Dirac monopoles from the geometrical viewpoint presented in this paper. We finish with a summary of the results presented.

In the following we summarize the motivation and the physical terminology used in this paper (see also Ref. 15). This paper is part of a sequence of papers dealing with a globally geometrical analysis of spontaneously broken gauge theories. The discussion is based on a geometrical understanding of the "two shifts" usually performed in order to make perturbation theory on Minkowski space–time $\mathbb{R}^{1,3}$

$$d \mapsto d + A,$$

[a)]Electronic mail: juergen.tolksdorf@mis.mpg.de

$$\mathbf{z}_0 \mapsto \mathbf{z}_0 + \phi. \tag{1}$$

For example, in the semiclassical approximation ("tree-level") of the (minimal) standard model $A = B + W \in \Omega^1(\mathbb{R}^{1,3}, \mathbb{R} \oplus \mathbb{R}^3)$ denotes the electroweak gauge potential and $\phi \in \Omega^0(\mathbb{R}^{1,3}, \mathbb{C}^2)$ represents the Higgs boson. Moreover, the Higgs boson and the electroweak gauge boson are assumed to represent the following "particle multiplets:"

$$A = (A_{\mathrm{elm}}, W^{\pm}, Z^0),$$

$$\phi = (\phi_{\mathrm{G}}, \phi_{\mathrm{H,phys}}). \tag{2}$$

When "quantized" A_{elm} is identified with the photon and $W^{\pm}$ and Z^0 with the electroweak vector bosons; ϕ_{G} denotes the Goldstone boson and $\phi_{\mathrm{H,phys}}$ the physical Higgs boson.

In the unitary gauge the pair $(A, \phi_{\mathrm{H,phys}})$ is physically interpreted as a "fluctuation" of a ground state ("semiclassical vacuum") of the electroweak interaction. From a geometrical perspective such a ground state may be described as a particular "Yang–Mills–Higgs pair" $(d, \mathbf{z}_0)$, where "d" is considered as the exterior covariant derivative with respect to the trivial connection on $\mathbb{C}^2$. The chosen minimum $\mathbf{z}_0 \in \mathbb{C}^2$ of the Higgs potential V_{H} can be regarded as the canonical smooth mapping

$$\mathbf{z}_0 : \mathbb{R}^{1,3} \to \mathrm{orbit}(\mathbf{z}_0),$$

$$x \mapsto \mathbf{z}_0. \tag{3}$$

Here, the submanifold orbit $(\mathbf{z}_0) \subset \mathbb{C}^2$ is the orbit of $\mathbf{z}_0$ with respect to a unitary group action of $\mathrm{G} \equiv \mathrm{SU}(2) \times \mathrm{U}(1)$ on $\mathbb{C}^2$.

Of course, the decomposition (2) and the physical interpretation of $(A, \phi_{\mathrm{H,phys}})$ only makes sense if either the topology of space–time $(\mathcal{M}, g_{\mathrm{M}})$ or the topology of the underlying gauge bundle $\mathcal{P}$ is assumed to be trivial. But what do we know about the global properties of the respective spaces? And what kind of phenomena can we expect if the respective topologies are nontrivial? Usually, one argues that physics can only make local statements. Consequently, the above given interpretation may be considered as local relations for locally space–time and any (gauge) bundle are topologically trivial. Then, for example, the gauge classes of mappings (3) are known to be classified by $\pi_1(\mathrm{G}/\mathrm{H})$, where the closed subgroup $\mathrm{H} \subset \mathrm{G}$ is isomorphic to the isotropy group of $\mathbf{z}_0$. However, the notion of locality is physically meaningless in the context of gauge theories for the latter do not give rise to a scale (in contrast to gravity). Therefore, the mathematical fact that every bundle is locally trivial has no physical meaning. We are thus forced to consider a bundle as a global geometrical object. This holds true in particular with respect to a gauge bundle $\mathcal{P}$. Likewise, because of the local nature of our experiments it seems more appropriate to determine the topological structure of space–time only by physical reasoning and not by *a priori* assumptions.

The assumption that the topology of $(\mathcal{M}, g_{\mathrm{M}})$ and of $\mathcal{P}$ is quite general naturally rises the question about the moduli space of gauge classes of semiclassical vacua. This moduli space is related to the topology of space–time and the underlying gauge bundle. One may thus learn something about the global structure of the latter by investigating the moduli space of semiclassical vacua. Notice that the topological structure of space–time and of the gauge bundle also determines the global structure of every associated bundle (up to equivalence). That the moduli space of semiclassical vacua actually provides a good tool to study the possible topolological structure of $\mathcal{P}$ is demonstrated in this paper for the special case of the electroweak interaction. Although restricted to the semiclassical approximation the results presented may also have nontrivial consequences for quantizing the electroweak/electromagnetic interaction on curved space–time. Indeed, our discussion is also intended as a preliminary step towards a geometrical understanding of perturbation theory.

II. THE ELECTROWEAK INTERACTION AS A SPECIFIC YANG–MILLS–HIGGS GAUGE THEORY

For the convenience of the reader we summarize in this section the basic geometrical notions used to geometrically formulate the bosonic sector of the electroweak interaction as a specific Yang–Mills–Higgs (YMH) gauge theory. For the terminology used and the details we refer to Refs. 13 and 15. A corresponding discussion of fermions can be found in Ref. 14.

In what follows $(\mathcal{M},g_{\mathrm{M}})$ denotes a smooth orientable (semi-)Riemannian manifold of arbitrary signature and dimension. As a topological space, $\mathcal{M}$ is assumed to be paracompact, connected and Hausdorff. In addition we shall assume that either the cohomology of $\mathcal{M}$ is torsion free, or all cohomological statements presented are regarded "modulo torsion." Since we are mainly interested in the case where $(\mathcal{M},g_{\mathrm{M}})$ denotes a four dimensional Lorentzian manifold of signature -2, we call $\mathcal{M}$ "space–time." Likewise, by $\mathcal{P}$ we mean a smooth principal G bundle over space–time $\mathcal{M}$,

$$\pi_{\mathrm{P}}:\mathrm{P}\to\mathcal{M},$$

$$p\mapsto x, \tag{4}$$

with structure group $\mathrm{G}:=\mathrm{SU}(2)\times\mathrm{U}(1)$. We call $\mathcal{P}$ the "electroweak gauge bundle." Its topological structure is thought to be given but so-far arbitrary. We will show that the actual bundle structure is fully determined (up to equivalence) by physical reasoning.

We call $(\mathcal{P},\rho_{\mathrm{H}},V_{\mathrm{H}})$ the geometrical data which permit to describe the electroweak interaction as a specific YMH gauge theory. Here,

$$\rho_{\mathrm{H}}:\mathrm{G}\to\mathrm{GL}(2,\mathbb{C}),$$

$$g=(g_{(2)},g_{(1)})\mapsto g_{(2)}g_{(1)}^{\mathrm{y}}, \tag{5}$$

with $y\in\mathbb{Q}$ denoting the so-called "hypercharge;"

$$V_{\mathrm{H}}:\mathbb{C}^2\to\mathbb{R},$$

$$\mathbf{z}\mapsto\lambda|\mathbf{z}|^4-\mu^2|\mathbf{z}|^2 \tag{6}$$

is the well-known Higgs potential $(\lambda,\mu>0)$. Note that the unitary representation ρ_{H} is faithful and the Higgs potential is rotationally symmetric, i.e., $V_{\mathrm{H}}=f_{\mathrm{H}}\circ r$ with $r(\mathbf{z}):=|\mathbf{z}|$ the "radial function."

The "Higgs bundle" ξ_{H} and the "Yang–Mills bundle" $\xi_{\mathrm{YM}}:=\tau_{\mathrm{M}}^{*}\otimes\mathfrak{ad}(\mathcal{P})$ are naturally associated with the geometrical data $(\mathcal{P},\rho_{\mathrm{H}},V_{\mathrm{H}})$. The Higgs bundle is defined by

$$\pi_{\mathrm{H}}:E_{\mathrm{H}}:=\mathrm{P}\times_{\rho_{\mathrm{H}}}\mathbb{C}^2\to\mathcal{M},$$

$$\mathfrak{z}\equiv[(p,\mathbf{z})]\mapsto\pi_{\mathrm{P}}(p) \tag{7}$$

and the adjoint bundle $\mathfrak{ad}(\mathcal{P})$ is given by

$$\pi_{\mathrm{ad}}:\mathrm{ad}(\mathrm{P}):=\mathrm{P}\times_{\mathrm{ad}}\mathrm{Lie}(\mathrm{G})\to\mathcal{M},$$

$$\tau\equiv[(p,T)]\mapsto\pi_{\mathrm{P}}(p). \tag{8}$$

The latter is always considered as a real vector bundle of rank four. Also the Higgs bundle will be mainly regarded as a real vector bundle of rank four. The real vector bundle τ_{M}^{*} denotes the cotangent bundle of space–time $\mathcal{M}$.

Each minimum $\mathbf{z}_0\in\mathbb{C}^2$ of the Higgs potential induces a specific fiber sub-bundle $\xi_{\mathrm{orb}}\subset\xi_{\mathrm{H}}$, which we call the "orbit bundle" with respect to $\mathbf{z}_0$,

$$\pi_{\mathrm{orb}}:\mathrm{Orbit}(\mathbf{z}_0) := \mathrm{P}\times_{\rho_{\mathrm{orb}}} \mathrm{orbit}(\mathbf{z}_0) \to \mathcal{M}$$

$$\mathfrak{z} \equiv [(p,\mathbf{z})] \mapsto \pi_{\mathrm{P}}(p), \tag{9}$$

with $\rho_{\mathrm{orb}} := \rho_{\mathrm{H}}|_{\mathrm{orbit}(\mathbf{z}_0)}$. Note that in the case at hand the Higgs potential has only one orbit of minima. Also, for two different minima the corresponding orbit bundles are equivalent. We therefore refer to (9) as the orbit bundle with respect to the data $(\mathcal{P},\rho_{\mathrm{H}},V_{\mathrm{H}})$. For rotationally symmetric Higgs potentials the orbit bundle can be thought of as a sphere sub-bundle of the Higgs bundle.

Each section $\mathcal{V}\in\Gamma(\xi_{\mathrm{orb}})$ is in one-to-one correspondence with a smooth principal H bundle $\mathcal{Q}$ over $\mathcal{M}$

$$\pi_{\mathrm{Q}}:\mathrm{Q}\to\mathcal{M},$$

$$q\mapsto x. \tag{10}$$

The structure group $\mathrm{H}\equiv\mathrm{U}_{\mathrm{elm}}(1)$ of $\mathcal{Q}$ is isomorphic to the isotropy group $I(\mathbf{z}_0)\subset\mathrm{G}$ of the minimum $\mathbf{z}_0\in\mathbb{C}^2$

$$I(\mathbf{z}_0)\equiv\{\exp(\theta[T+iy])|T=T(\mathbf{z}_0)\in\mathrm{su}(2),\mathrm{tr}[(T+iy)^2]=-n^2,n\in\mathbb{N}\}. \tag{11}$$

Moreover, there is an equivariant embedding of principal bundles $\iota:\mathcal{Q}\hookrightarrow\mathcal{P}$, such that $(\iota,\mathcal{Q})$ is an H reduction of $\mathcal{P}$ (see, Ref. 9). For a discussion of spontaneously broken gauge theories in terms of bundle reductions see, for example, Refs. 4, 5, 12, and 17. We call the principal H bundle $\mathcal{Q}$ the "electromagnetic gauge bundle" with respect to the "vacuum section" $\mathcal{V}$. The relation between a section $\mathcal{V}$ of the orbit bundle and the appropriate H reduction $(\iota,\mathcal{Q})$ of $\mathcal{P}$ is given by $\mathcal{V}(x)=[(\iota(q),\mathbf{z}_0)]|_{q\in\pi_{\mathrm{Q}}^{-1}(x)}$ for all $x\in\mathcal{M}$.

Each $\mathcal{V}\in\Gamma(\xi_{\mathrm{orb}})$ gives rise to a distinguished subset of principal connections on $\mathcal{P}$. They are determined by the requirement

$$d_{\mathrm{A}}\mathcal{V}=0, \tag{12}$$

where $\mathcal{A}\in\mathcal{A}(\xi_{\mathrm{H}})$ is the corresponding associated connection on ξ_{H}. The connections on $\mathcal{P}$ which satisfy the condition (12) are called compatible with the vacuum section $\mathcal{V}$ [respectively, with the H reduction $(\iota,\mathcal{Q})$ of $\mathcal{P}$]. These connections have the crucial property that they are flat when restricted to the "physical space–time" $\mathcal{M}_{\mathrm{phys}}:=\mathcal{V}(\mathcal{M})\subset E_{\mathrm{H}}$.

A YMH pair $(\mathcal{A},\Phi)\in\mathcal{A}(\xi_{\mathrm{H}})\times\Gamma(\xi_{\mathrm{H}})$ is called a "vacuum (pair)" iff $\Phi=\mathcal{V}$ is a vacuum section and $\mathcal{A}=\Theta$ is associated with a flat connection on $\mathcal{P}$ which is compatible with $\mathcal{V}$. Each vacuum defines an absolute minimum of the energy functional (if globally defined) that is associated with the well-known YMH functional. The moduli space of gauge classes of vacua is denoted by $\mathfrak{M}_{\mathrm{vac}}$. The latter turns out to be nontrivial iff $\mathcal{P}$ is trivial. In this case, $\mathfrak{M}_{\mathrm{vac}}$ can be canonically identified with $\mathrm{H}^1_{\mathrm{deR}}(\mathcal{M})$. In other words, the moduli space of the electroweak vacua only depends on the topology of space–time. In particular, if $\mathcal{M}$ is simply connected then there is a natural vacuum (pair) $(\Theta_0,\mathcal{V}_0)$ which generates $\mathfrak{M}_{\mathrm{vac}}$. This vacuum corresponds to the vacuum usually introduced in perturbation theory via the "shift" (1).

Since $\mathfrak{M}_{\mathrm{vac}}=\emptyset$ for nontrivial $\mathcal{P}$, we have to appropriately generalize the notion of the moduli space of electroweak vacua. This will be achieved by use of the fact that $\mathfrak{M}_{\mathrm{vac}}\neq\emptyset$ iff electromagnetism is symmetric with respect to charge conjugation. Before we introduce a generalization of $\mathfrak{M}_{\mathrm{vac}}$, however, we shall prove in the next section that Dirac's quantization condition of electric charge fully determines the topological structure of the electroweak gauge bundle.

III. THE TOPOLOGY OF THE ELECTROWEAK GAUGE BUNDLE

When charge conjugation is taken into account the existence of vacuum sections is equivalent to the triviality of the electroweak gauge bundle. We therefore consider in this section the situation where charge conjugation is spoiled. Physically, this is the case if an absolute magnetic field exists which, for example, is generated by a magnetic monopole. We show that in the case of the standard model the Higgs boson may also provide such a state.

Proposition 3.1: Let $\mathcal{Q}$ be a principal H bundle over a smooth manifold $\mathcal{M}$ and let $\lambda:\mathrm{H}\hookrightarrow\mathrm{G}$ be a homomorphism which is also a smooth embedding of Lie groups. Up to isomorphism there is a unique principal G bundle $\mathcal{P}$ over $\mathcal{M}$ together with a smooth embedding $\iota:\mathcal{Q}\hookrightarrow\mathcal{P}$ such that $(\iota,\mathcal{Q})$ is an H reduction of $\mathcal{P}$.

Proof: For this let $\{(U_i,\varphi_i)\,|\,i\in\Lambda\}$ be a family of local trivializations of the principal H bundle $\mathcal{Q}:\pi_\mathrm{Q}:\mathrm{Q}\to\mathcal{M}$. That is, $U_i\subset\mathcal{M}$ is an open subset such that $\mathcal{M}\subset\cup_{i\in\Lambda}U_i$, and

$$\varphi_i:\pi_\mathrm{Q}^{-1}(U_i)\to U_i\times\mathrm{H},$$

$$p\mapsto(x:=\pi_\mathrm{Q}(q),h_i:=\varphi_{i,x}(q)) \tag{13}$$

is an equivariant diffeomorphism for all $i\in\Lambda$.

Accordingly, for $U_i\cap U_j\neq\emptyset$ we denote by the mappings

$$h_{ij}:U_i\cap U_j\to\mathrm{H},$$

$$x\mapsto\varphi_{i,x}(q)(\varphi_{j,x}(q))^{-1}, \tag{14}$$

the transition functions with respect to the local trivialization $\{(U_i,\varphi_i)\,|\,i\in\Lambda\}$.

For all $i,j\in\Lambda$ such that $U_i\cap U_j\neq\emptyset$ we define smooth mappings

$$g_{ij}:U_i\cap U_j\to\mathrm{G},$$

$$x\mapsto\lambda(h_{ij}(x)) \tag{15}$$

which satisfy the co-cycle condition $g_{ij}(x)g_{jk}(x)g_{ki}(x)=e$ for all $x\in U_i\cap U_j\cap U_k$. Therefore, up to equivalence there is a unique principal G bundle $\mathcal{P}:\pi_\mathrm{P}:\mathrm{P}\to\mathcal{M}$ with local trivialization $\{(U_i,\psi_i)\,|\,i\in\Lambda\}$ such that $g_{ij}(x)=\psi_{i,x}(p)(\psi_{j,x}(p))^{-1}$.

We define a smooth family $\{(U_i,\iota_i\,|\,i\in\Lambda)\}$ of mappings

$$\iota_i:\pi_\mathrm{Q}^{-1}(U_i)\to\pi_\mathrm{P}^{-1}(U_i),$$

$$q\mapsto\psi_i^{-1}\,(x,\lambda(\varphi_{i,x}(q)))|_{x=\pi_\mathrm{Q}(q)}. \tag{16}$$

Since λ is an embedding, these mappings have maximal rank and fulfill $\iota_i(q)=\iota_j(q)$ for all $q\in\pi_\mathrm{Q}^{-1}(U_i\cap U_j)$. Therefore, they define a global immersion $\iota:\mathrm{Q}\to\mathrm{P}$ which is a homeomorphism onto $\iota(\mathrm{Q})$. Moreover, since λ is a homomorphism, the embedding ι is equivariant and fulfill $\pi_\mathrm{P}\circ\iota=\pi_\mathrm{Q}$. Consequently, $(\iota,\mathcal{Q})$ is an H reduction of $\mathcal{P}$ and thus $\mathcal{P}$ a G extension of $\mathcal{Q}$. Any other G-extension $\mathcal{P}'$ must be equivalent to $\mathcal{P}$, for the structure functions of $\mathcal{P}'$ are equivalent to those of $\mathcal{P}$. □

Therefore, for given data $(\mathcal{Q},\mathrm{G},\lambda)$ there is (up to equivalence) a unique G-extension $\mathcal{P}$ of the principal H bundle $\mathcal{Q}$. Since every principal U(1) bundle is characterized by an integer we may apply the Proposition 3.1 to prove our main result.

Proposition 3.2: Let $(\mathcal{P},\rho_\mathrm{H},V_\mathrm{H})$ be the geometrical data which specifies the electroweak interaction of the (minimal) standard model as a YMH gauge theory. Up to equivalence the topological structure of the electroweak gauge bundle is fully determined by the hypercharge of the Higgs boson. Moreover, for a given hypercharge $y>0$ there are $2|n|+1$ gauge inequivalent sections of the orbit bundle where

$$y = \sqrt{\tfrac{1}{2}\left(n^2 - \tfrac{1}{2}\right)}, \quad n \in \mathbb{Z}^*. \tag{17}$$

Proof: To prove the statement we make use of the fact that every principal U(1) bundle is characterized by its Chern number $n \in \mathbb{Z}$, where $n=0$ corresponds to the trivial bundle (see Ref. 7). For a given hypercharge $y \in \mathbb{Q}$, the definition (11) of the isotropy group of a minimum $\mathbf{z}_0 \in \mathbb{C}^2$ of the Higgs potential V_{H} determines an integer $n \in \mathbb{Z}^* \equiv \mathbb{Z}\backslash\{0\}$ which is unique modulo $\mathbb{Z}_2$. For example, one may assume that $\mathbf{z}_0 = (0,0,0,r_0)$ with $r_0 := \sqrt{\mu^2/2\lambda}$ and $T(\mathbf{z}_0) = i\tau_3/2 \in \mathrm{su}(2)$ to prove the relation (17). In the case where $y<0$, we may replace y by $-|y|$ in the definition of the hypercharge. So, we may assume $y>0$ without loss of generality. The relation (17) is Dirac's quantization condition of electric charge in terms of the hypercharge of the Higgs boson. Modulo $\mathbb{Z}_2$, this condition fixes a specific principal $\mathrm{U}_{\mathrm{elm}}(1)$ bundle $\mathcal{Q}$ over $\mathcal{M}$, where $h \in \mathrm{U}_{\mathrm{elm}}(1)$ is given by $h = \det \exp(\theta[T+iy])$. Accordingly, the embedding λ reads

$$\lambda : U_{\mathrm{elm}}(1) \hookrightarrow \mathrm{SU}(2) \times \mathrm{U}(1),$$

$$h = \exp(in\theta) \mapsto (\exp(\theta T), \exp(i\theta y)). \tag{18}$$

Therefore, the structure of the electroweak gauge bundle $\mathcal{P}$ is fully determined by the hypercharge of the Higgs boson. Moreover, if the case $n=0$ is taken into account one obtains $2|n|+1$ $\mathrm{U}_{\mathrm{elm}}(1)$ reductions of the principal $\mathrm{SU}(2)\times\mathrm{U}(1)$ bundle $\mathcal{P}$. □

The case $n=0$ is special in several respects and has been thoroughly discussed in Ref. 15. For instance, as already mentioned, the corresponding electromagnetic gauge bundle equals the trivial principal $\mathrm{U}_{\mathrm{elm}}(1)$ bundle independently from the topology of space–time,

$$\mathrm{pr}_1 : \mathcal{M} \times \mathrm{U}_{\mathrm{elm}}(1) \to \mathcal{M},$$

$$q = (x,h) \mapsto x. \tag{19}$$

This electromagnetic gauge bundle is the only one which possesses a flat connection. Moreover, it has a natural flat connection that is induced by the Maurer–Cartan form on $\mathrm{U}_{\mathrm{elm}}(1)$. Since the electroweak gauge bundle is trivial too, the corresponding embedding $\iota : \mathcal{Q} \hookrightarrow \mathcal{P}$ is given by

$$\iota : \mathcal{M} \times \mathrm{U}_{\mathrm{elm}}(1) \hookrightarrow \mathcal{M} \times (\mathrm{SU}(2) \times \mathrm{U}(1)),$$

$$(x,h) \mapsto (x, \lambda(h)). \tag{20}$$

Accordingly, the vacuum section $\mathcal{V}_0$ reads

$$\mathcal{V}_0 : \mathcal{M} \to \mathcal{M} \times \mathrm{orbit}(\mathbf{z}_0),$$

$$x \mapsto (x, \mathbf{z}_0). \tag{21}$$

Indeed, it has been shown that, for the trivial electroweak gauge bundle, any other vacuum section $\mathcal{V}$ must be gauge equivalent to the canonical section $\mathcal{V}_0$. It follows that $\mathfrak{M}_{\mathrm{vac}} \simeq \mathrm{H}^1_{\mathrm{deR}}(\mathcal{M})$, which turns out to be equivalent to the existence of charge conjugation. Therefore, the case $n=0$ corresponds to ordinary electromagnetism generated by the ground state $\mathcal{V}_0$ of the Higgs boson.

Since for $n \neq 0$ the corresponding electromagnetic gauge bundles possess no flat connection, we call the appropriate ground states of the Higgs boson "magnetically charged." They spoil the symmetry of ordinary electromagnetism under charge conjugation like a magnetic monopole. However, the $\mathbb{Z}_2$ symmetry of charge conjugation is hidden in the two-to-one relation (17) between the Chern number and the hypercharge of the Higgs boson. Physically this means that it is possible

to absolutely distinguish between positive and negative electrically charged particles if we know the gauge class of the ground states of the Higgs boson. We stress that for $n \neq 0$ the electroweak gauge bundle $\mathcal{P}$ is nontrivial and possesses no flat connection.

When the Gell–Mann–Nishijima relation between the hypercharges and the electric charges of the fermions is taken into account, the hypercharge of the Higgs boson yields $y=1/2$ (cf., for instance, Refs. 1,11, or 20). Thus, in the case of the (minimal) standard model the Higgs boson has exactly three gauge inequivalent ground states, which are parametrized by the Chern numbers $n=0,\pm 1$. These ground states correspond to the lowest nonvanishing electric charge a particle may have.

Let $\mathcal{O} \in \Gamma(\xi_{\mathrm{H}})$ be the zero section and $\Gamma^*(\xi_{\mathrm{H}}) \equiv \Gamma(\xi_{\mathrm{H}}) \backslash \{\mathcal{O}\}$. Then, the Proposition 3.2 shows that the Higgs bundle ξ_{H} has at least $2|n|+1$ nonvanishing sections. Therefore, $\Gamma^*(\xi_{\mathrm{H}}) \neq \emptyset$, and for each $\Phi \in \Gamma^*(\xi_{\mathrm{H}})$ there is a unique $n \in \mathbb{Z}$ and a nonvanishing function $\varphi \in \mathcal{C}^\infty(\mathcal{M})$ such that

$$\Phi: \mathcal{M} \to E_{\mathrm{H}},$$

$$x \mapsto \varphi(x)\mathcal{V}(x). \tag{22}$$

Consequently, also for $n \neq 0$ every nonvanishing section of the Higgs bundle is fully determined by its length. This is but a geometrical variant of what is usually referred to as "unitary gauge." In fact, despite the chosen terminology the unitary gauge is not a choice of gauge (which may not exist globally). Instead, it refers to the moduli space of ground states of the Higgs boson.

IV. MAGNETICALLY CHARGED VACUA AND MONOPOLES

As discussed in the preceding section, ordinary electromagnetism corresponds to the $n=0$ ground states of the Higgs boson. Moreover, the moduli space of electroweak vacua is related to the topology of space–time via the isomorphism $\mathfrak{M}_{\mathrm{vac}} \simeq \mathrm{H}^1_{\mathrm{deR}}(\mathcal{M})$.

As we have already mentioned, in the case of $n \neq 0$ the electroweak gauge bundle possesses no flat connection and thus $\mathfrak{M}_{\mathrm{vac}} = \emptyset$. One may therefore ask for an appropriate generalization of $\mathfrak{M}_{\mathrm{vac}}$. For this we call a solution $F_{\mathrm{mag}} \in \Omega^2(\mathcal{M})$ of the Maxwell equations a "Dirac–Higgs (DH) monopole," provided it satisfies the following conditions: (a) $[F_{\mathrm{mag}}]/2\pi \in \mathrm{H}^2_{\mathrm{deR}}(\mathcal{M})$ is integral; (b) the Chern number n of the isomorphism class of principal U(1) bundles defined by F_{mag} is either zero or related to the hypercharge of the Higgs boson via Dirac's quantization condition (17); (c) for each $x \in \mathcal{M}$ there is a geodesic normal coordinate system (U,φ) such that $i_{\partial_t} F_{\mathrm{mag}} = 0$, where ∂_t is the (local) timelike vector field that is induced by (U,φ). In particular, for $n=0$ it is assumed that condition (c) holds true for every geodesic normal coordinate system. We let $\mathfrak{M}_{\mathrm{mag}}$ be the moduli space of all gauge classes of YMH pairs $(\mathcal{A},\mathcal{V}) \in \mathcal{A}(\xi_{\mathrm{H}}) \times \Gamma(\xi_{\mathrm{H}})$ such that $\mathcal{A}$ is associated with a connection on $\mathcal{P}$ which is compatible with the vacuum section $\mathcal{V}$ and whose curvature corresponds to F_{mag}.

The condition (c) physically means that there is always an inertial reference system (U,φ) such that with respect to this system F_{mag} is purely magnetic, $\imath_t^* F_{\mathrm{mag}} = B_t \in \Omega^2(\Sigma_t)$ with $\imath_t: \Sigma_t \hookrightarrow U \subset \mathcal{M}$ is defined by the local spacelike hypersurface $t=$const. Moreover, for $n=0$ we have $F_{\mathrm{mag}}=0$.

For $n \neq 0$ we call $\mathfrak{M}_{\mathrm{mag}}$ the "(magnetically) charged sector" of the moduli space of the electroweak vacua. Accordingly, for $n=0$ we call $\mathfrak{M}_{\mathrm{mag}} = \mathfrak{M}_{\mathrm{vac}}$ the "(magnetically) uncharged sector" of the electroweak vacua. Note that the charged sector of $\mathfrak{M}_{\mathrm{mag}}$ also depends on the geometry of space–time. (We would like to thank G. Naber for an appropriate hint).

To present an example which demonstrates the nontriviality of the magnetically charged sector of $\mathfrak{M}_{\mathrm{mag}}$ we consider the exterior Schwarzschild space–time $(\mathcal{M}, g_{\mathrm{M}})$. Here, $\mathcal{M} \simeq \mathbb{R} \times [r_0, \infty[\times S^2$ with $r_0 \in \mathbb{R}_+$ the Schwarzschild radius. Consequently, $\mathcal{M} \approx S^2$ where the latter is a spacelike submanifold of $(\mathcal{M}, g_{\mathrm{M}})$. Since the pull-back of g_{M} to this submanifold equals the Riemannian standard metric on $S^2 \subset \mathbb{R}^3$ it is straightforward to check that

$$F_{\mathrm{mag}} = \frac{n}{2} \sin\vartheta \, \mathrm{d}\vartheta \wedge \mathrm{d}\varphi \tag{23}$$

defines a Dirac–Higgs monopole provided $n \neq 0$ satisfies Dirac's quantization condition (17). The corresponding electromagnetic gauge bundle $(\mathcal{Q}, \iota)$ over $(\mathcal{M}, g_{\mathrm{M}})$ is equivalent to the (generalized) Hopf bundle (see, for instance, Refs. 10, 17, and 18 for a very readable approach)

$$\pi_n : S^3/\mathbb{Z}_n \to S^2, \tag{24}$$

where $\mathbb{Z}_n := \{e^{2k\pi i/n} \,|\, k = 0, 1, \ldots, n-1\} \subset \mathrm{U}(1)$ and π_n generalizes the famous Hopf map π_1 between spheres (cf. Ref. 8; for a recent discussion of the various physical meanings of the Hopf fibration see Ref. 19).

In classical electrodynamics the DH monopole field (23) is regarded as being created by a massive magnetically charged pointlike particle ("Dirac monopole") moving in Minkowski space–time $\mathbb{R}^{1,3}$. In this context the monopole field $F_{\mathrm{mag}} \in \Omega^2(\mathcal{M})$ is known as the Dirac monopole field on $\mathcal{M} := \mathbb{R}^{1,3} \backslash \Gamma$, where $\Gamma \subset \mathcal{M}$ denotes the worldline of the Dirac monopole, see Ref. 6. However, in the context of the standard model the physical interpretation of (23) is different. Notice that in either case $(g_{\mathrm{M}}, F_{\mathrm{mag}})$ is not a solution of the combined Einstein–Maxwell equations. Also notice that the DH monopole has finite energy since the Schwarzschild radius r_0 acts like an ultraviolet cutoff. Indeed, the energy-momentum current $\tau \in \Gamma(\mathrm{End}(\tau_{\mathrm{M}}))$ of the DH monopole field (23) reads $\tau = (n^2/2r^4)\mathrm{Id}_{\mathrm{TM}}$. Hence, the "vacuum energy" Λ is given by the magnetical analogue of the electrostatic energy of an electrically charged sphere

$$\Lambda = 4\pi \frac{g^2}{r_0}, \tag{25}$$

where $g \equiv n/2$ is the magnetic charge of the DH monopole. Notice that the vacuum energy either is zero or uniquely determined by the Schwarzschild radius and the hypercharge of the Higgs boson, i.e., by the topology of space–time and the electroweak gauge bundle. In particular, in the case of the standard model one has $\Lambda \in \{0, \pi/r_0\}$.

The given example of a DH monopole also demonstrates that the electroweak gauge bundle $\mathcal{P}$ is nontrivial in general. However, to determine the structure of the moduli space $\mathfrak{M}_{\mathrm{mag}}$ of electroweak vacua for more general space–times $(\mathcal{M}, g_{\mathrm{M}})$ is certainly a major challenge. The geometry of (static) monopoles (in Minkowski space–time) is thoroughly discussed, for example, in Refs. 2 and 3 (see also, in Ref. 16). However, the point here is to not regard magnetic monopoles as individual "classical (pointlike) particles" in space–time but instead to consider monopoles as specific ground states of the Higgs boson whose realizations depend on both the topology and the geometry of space–time. Indeed, the notion of a world line $\Gamma \subset \mathcal{M}$ is a purely classical concept which seems to make no sense within (quantum) field theory. Also, Dirac's famous quantization condition $qn \in \mathbb{Z}$ of electric charge $q \in \mathbb{Q}$ (again, when measured in appropriate units, see again Ref. 6) holds true only if the appropriate monopole bundle (which is characterized by $n \in \mathbb{Z}^*$) is identified with the electromagnetic gauge bundle. However, this is consistent with the standard model only if the monopole bundle is regarded as a specific $\mathrm{U}_{\mathrm{elm}}(1)$ reduction of the electroweak gauge bundle $\mathcal{P}$. That is, the monopole is identified with a specific gauge class of ground states of the Higgs boson which are not gauge equivalent to those considered in perturbation theory.

In Ref. 15 it has been shown that, with respect to any electroweak vacuum, the Yang–Mills bundle decomposes as

$$\xi_{\mathrm{YM}} = \xi_{\mathrm{elm}} \oplus \xi_{Z^0} \oplus \xi_{W^\pm}. \tag{26}$$

Here, respectively, ξ_{elm} and ξ_{Z^0} are trivial line bundles which geometrically represent an (asymptotically free) photon and an electrically neutral massive weak vector boson. In contrast, $\xi_{W^\pm} := \tau_{\mathrm{M}}^* \otimes \xi_W$, with $\xi_W \subset \mathfrak{ad}(\mathcal{P})$ denoting a rank two vector bundle, simultaneously represents both of the electrically charged and massive weak vector bosons $W^\pm$ iff electromagnetism is symmetric with respect to charge conjugation. Of course, one may expect that only electrically charged

particles permit a physical distinction between the magnetically charged and uncharged ground states of the Higgs boson. With respect to a magnetically charged vacuum, the (massive) vector bosons W^+ and W^- are no longer charge conjugate to each other due to their electromagnetic interaction with the corresponding DH monopole. Geometrically, this is expressed by the nontriviality of ξ_W and that the asymptotically free states of the $W^\pm$ bosons must satisfy the field equation (see also Eq. 35 in Ref. 15)

$$\delta_A d_A W^\pm + m_W^2 W^\pm = 0. \tag{27}$$

Here, respectively, d_A and δ_A is the exterior covariant derivative and its formal adjoint with respect to a DH monopole connection $\mathcal{A}$ and $W^\pm \in \Gamma(\xi_{W^\pm})$ is (the electrically charged part of) a smooth "fluctuation" of $\mathcal{A}$. Moreover, $m_W^2 \in \mathbb{R}_+$ is a nonvanishing eigenvalue of the Yang–Mills mass matrix (for the terminology used please see Ref. 15) $\mathcal{V}^* M_{\mathrm{YM}}^2 \in \Gamma(\mathrm{End}(\xi_{\mathrm{YM}}))$ with $[(\mathcal{A},\mathcal{V})] \in \mathfrak{M}_{\mathrm{mag}}$.

However, in the case of a magnetically charged vacuum the $\mathbb{Z}_2$ symmetry of charge conjugation is restored in the two-to-one correspondence between the charge of the vacuum and the hypercharge of the Higgs boson. Of course, it is interesting to also ask for appropriate physical effects which permit to distinguish between the gauge inequivalent ground states of the Higgs boson. Though we do not want to discuss this question here, we would like to stress again that such an interaction can only occur for a topologically nontrivial space–time. Moreover, such an interaction also depends on the space–time geometry, i.e., on the gravitational field. Consequently, appropriate physical effects caused by the interaction of the electrically charged weak vector bosons (respectively, fermions) with the electroweak vacuum may provide the possibility to gain some insight into the topology and the geometry of space–time.

V. CONCLUSION

We have shown that the topological structure of the electroweak gauge bundle either is trivial or fully determined by the hypercharge of the Higgs boson. This is a geometrical variant of Dirac's quantization condition within the realm of the electroweak interaction. For this it is crucial, however, that in the case of the (minimal) standard model "charge comes with mass." Indeed, it is a remarkable fact that no massless electrically charged particles are known to exist in nature. In general, the moduli space of the electroweak vacua consists of a magnetically charged and an uncharged sector. The uncharged sector corresponds to ordinary electromagnetism. It is determined by the assumption that the electrically charged massive weak vector bosons are charge conjugate to each other. The uncharged sector is fixed by the topology of space–time via the first de Rham cohomology group of $\mathcal{M}$. In contrast, a necessary condition for the existence of the charged sector (i.e., the existence of DH monopoles) is the nontriviality of the second de Rham cohomology group of space–time provided there is no (algebraic) torsion (the author thanks R. Vitolo for appropriate discussion on the occurrence of torsion) [e.g., $\mathrm{H}_1(\mathcal{M},\mathbb{Z})=0$]. Moreover, a charged ground state of the Higgs boson can only exist if it also fits with the geometry of space–time.

In the case of the (minimal) standard model the physical Higgs boson geometrically appears as a fluctuation of any of the three gauge inequivalent ground states of the Higgs boson which are characterized by the Chern numbers $n=0,\pm 1$. These ground states correspond to the lowest possible nonvanishing electric charge a particle may assume. However, the magnetically charged ground states $n=\pm 1$ can be realized only if space–time possesses a nontrivial topology as, for example, in the case of a rotationally symmetric space–time. In this case, the corresponding electromagnetic gauge bundles are equivalent to Hopf fibrations. The appropriate DH monopoles generalize the well-known Dirac monopoles of magnetic charge $g=\pm 1/2$ to the electroweak interaction within the (minimal) standard model. This example may also motivate the terminology of "magnetically charged electroweak vacua." In general, these topologically nontrivial ground states of the Higgs boson yield electric charge quantization analogous to ordinary Dirac monopoles. Clearly, whether these ground states of the Higgs boson can be actually realized for a

general space–time manifold $(\mathcal{M}, g_{\mathrm{M}})$ needs a more thorough analysis of the space of solutions $F_{\mathrm{mag}} \in \Omega^2(\mathcal{M})$ of the corresponding Maxwell equations. Moreover, like in the usual discussion of magnetic monopoles also the definition of DH monopoles does not refer to some field equation of gravity. Of course, this seems unsatisfying from a physical viewpoint. However, to mathematically discuss the structure of the correspondingly enlarged moduli space of electroweak vacua is obviously even more challenging. In any case, the geometrical viewpoint presented here with respect to the electroweak interaction of the (minimal) standard model suggests that the mechanism of spontaneous symmetry breaking may provide a better understanding of the link between topology and geometry.

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Integral equations for heat kernel in compound media

I. G. Pirozhenko[a] and V. V. Nesterenko[b]
Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, 141980 Dubna, Russia

M. Bordag[c]
Institute for Theoretical Physics, University of Leipzig, Augustusplatz 10/11, 04109 Leipzig, Germany

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By making use of the potentials of the heat conduction equation the integral equations are derived which determine the heat kernel for the Laplace operator $-a^2\Delta$ in the case of compound media. In each of the media the parameter a^2 acquires a certain constant value. At the interface of the media the conditions are imposed which demand the continuity of the temperature and the heat flows. The integration in the equations is spread out only over the interface of the media. As a result the dimension of the initial problem is reduced by 1. The perturbation series for the integral equations derived are nothing else as the multiple scattering expansions for the relevant heat kernels. Thus a rigorous derivation of these expansions is given. In the one dimensional case the integral equations at hand are solved explicitly (Abel equations) and the exact expressions for the regarding heat kernels are obtained for diverse matching conditions. Derivation of the asymptotic expansion of the integrated heat kernel for a compound media is considered by making use of the perturbation series for the integral equations obtained. The method proposed is also applicable to the configurations when the same medium is divided, by a smooth compact surface, into internal and external regions, or when only the region inside (or outside) this surface is considered with appropriate boundary conditions. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1870734]

I. INTRODUCTION

The heat kernel technique[1–5] is widely used for constructing the quantum field theory in gravitational background and with allowance for nontrivial boundary conditions. Of a particular interest is the asymptotic expansion of the heat kernel it terms of evolution parameter for its small values. The coefficients of this expansion pertain to divergences and anomalies in the relevant quantum field theory models. Proceeding from this one can develop the renormalization procedure needed.

For well posed spectral problems the heat kernel coefficients are expressed, in an polynomial way, through the local geometric characteristics of the manifold D and its boundary S. Not only the contributions of D and S are independent but the contributions of individual regions of D and S are also additive.

The spectral problem is well posed for the goal of constructing the heat kernel if the second oder elliptic differential operator in question is close to the Laplace operator defined on a smooth manifold with a smooth boundary, if any.

[a]Electronic mail: pirozhen@thsun1.jinr.ru
[b]Electronic mail: nestr@thsun1.jinr.ru
[c]Electronic mail: michael.bordag@itp.uni-leipzig.de

There are no universal methods for constructing the heat kernel and its asymptotic expansion. The development of different approaches to this problem is the subject of many works (see, for example, the reviews[1–5] and references therein).

The initial definition of the heat kernel is the Green function of the heat-conduction equation with an elliptic operator under study. In many physical problems it is worth going from the differential equation, defining the solution to be found or the relevant Green's function, to the equivalent integral equation. In the dynamical evolution problems the integral equations manifestly show the reason–consequence relations governing the physical process under study. Reducing the problem to the integral equation, as a rule, allows one to develop the method of successive approximations (perturbation theory).

Transforming the initial differential equation into the integral form is in the general case a nontrivial problem. Special attention should be paid here to incorporating the boundary conditions into the integral equation. When constructing the integral equations governing the Green's function of the heat equation we shall use the surface potentials for this equation. The volume potential and the potentials of single and double layers naturally arise in the theory of the Laplace equation. In this case they are referred to as the Newtonian (or electrostatic) potentials. This idea proved to be fruitful also in studies of the Helmholtz equation describing, for example, steady harmonic oscillations, the wave equation, and the heat-conduction equation. The potentials are particular solutions of these homogeneous equations, and they are constructed in a universal way in terms of the fundamental (or elementary) solution of the initial equation. The potential technique has turned out to be effective both for consideration of the general properties of the equations under study (for example, the prove of the solution uniqueness) and for deriving particular solutions with given properties and for obtaining the Green's functions.

This paper seeks to demonstrate the efficiency of using the heat potentials when constructing the integral equations for the heat kernel (Green functions) at first in the case of manifolds with boundary. It is worth noting that integration in these equations is spread out over the boundary only. As a result the dimensionality of the initial problem is reduced by co-dimension of the boundary S. Further this approach is extended to the compound media, where the principal part of the differential operator has a discontinuity at the interface between different media. A typical example here is the electrodynamics of continuous media.[6] The velocity of light has, in the general case, a jump discontinuity on the border between two media with different characteristics (for example, on the border between dielectric and vacuum). In the both media the Maxwell equations are well defined, and at the interface the matching conditions (or boundary conditions) should be satisfied. The concrete form of these conditions is determined by the physical content of the problem in question. In the same way the conduction of heat in compound media is treated.[7] As far as we are aware, the heat kernel for compound media is not investigated yet.[4]

The layout of the paper is as follows. In Sec. II the essentials of the potential theory are recalled first for the Laplace equation (Newtonian potentials) and then for the heat-conduction equation (heat potentials). By making use of the heat potentials the integral equation for the Green function (heat kernel) is derived for a compact region of Euclidean space bounded by a smooth surface. The perturbative series for this equation is developed which is nothing else as the multiple scattering expansion for the heat kernel. Thus a rigorous derivation of this expansion is presented. The convenience to use here the Laplace transform is shown. In Sec. III the integral equations are derived that determine the heat kernel for compound media. The efficiency of the approach proposed is demonstrated by deriving the t-small asymptotics of the first three terms of the perturbation series for the heat kernel in the case of compound media (Sec. IV). In Sec. V the heat kernel on an infinite line is constructed in an exact form for diverse matching conditions. In the Conclusion (Sec. VI) the obtained results are briefly summarized and the possibility of extending the approach proposed is discussed. In the Appendix the general conditions at the interface are found which result in self-adjoint boundary value problem for the Laplace operator considered in compound media.

II. HEAT POTENTIALS

In order to recall the basic facts from the potential theory, we first address the Laplace equation

$$\Delta u = 0 \tag{2.1}$$

considered in the d-dimensional Euclidean space $\mathbb{R}_d$, which is divided by a smooth closed surface S into a compact internal domain D_+ and external one D_-. On the surface S the relevant boundary conditions should be imposed, that depend on the physical content of the problem in question. For example, it may be a mathematical formulation of the electrostatic problem.[6] The surface S is supposed to possess the properties of smoothness needed. In the potential theory[8–11] this implies that S is the Lyapunov type surface. The points of Euclidean space $\mathbb{R}_d$ are denoted by $x,y,z,\ldots$, and r_{xy} is the Euclidean distance between x and y. At any point x on S there exists a unit normal n_x or $n(x)$. For definiteness we choose the inward directed normal. It is possible because we are dealing with closed surfaces S.

For a linear homogeneous differential equation the fundamental (or elementary) solution is defined, which is the Green function of this equation in an unbounded space. By definition, the fundamental solution obeys the initial equation with a δ-like source on its right-hand side. In the case of the Laplace equation in $\mathbb{R}_d$ the fundamental solution is

$$E_d(x;x') = -\frac{\Gamma(d/2)(r_{xx'})^{-d+2}}{(2d-4)\pi^{d/2}}, \quad d \geqslant 3, \quad E_3(x;x') = -\frac{1}{4\pi r_{xx'}} \tag{2.2}$$

with the properties

$$\Delta_x E_d(x;x') = \Delta_{x'} E_d(x;x') = \delta^{(d)}(x,x'), \quad E_d(x;x') = E_d(x';x). \tag{2.3}$$

The potentials for the Laplace equation are constructed by making use of the fundamental solution, namely, the volume potential

$$U(x) = -\frac{1}{4\pi}\int_D \frac{w(y)}{r_{xy}}\mathrm{d}y, \tag{2.4}$$

the single-layer potential

$$V(x) = -\frac{1}{4\pi}\int_S \frac{\nu(y)}{r_{xy}}\mathrm{d}S_y, \tag{2.5}$$

and the potential of a double layer

$$W(x) = -\frac{1}{4\pi}\int_S \mu(y)\frac{\partial}{\partial n_y}\frac{1}{r_{xy}}\mathrm{d}S_y. \tag{2.6}$$

These formulas are written for $\acute{d}=3$, and the following notations are used: $\mathrm{d}y$ and $\mathrm{d}S_y$ are, respectively, the elements of the volume and of the surface at the point $y, w(y), \mu(y)$, and $\nu(y)$ are the densities of these potentials. It is convenient to consider the densities $w(y), \mu(y)$, and $\nu(y)$ to be continuous functions.

All three potentials are solutions of the Laplace equation (2.1), namely, the volume potential (2.4) is harmonic outside $D, V(x)$, and $W(x)$ are harmonic outside S. The single-layer potential $V(x)$ is continuous everywhere in $\mathbb{R}_d$, specifically, on passing through S. The potential of a double layer $W(x)$ has a discontinuity on S, namely,

$$W_i(x) = W(x) - \tfrac{1}{2}\mu(x),$$

$$W_e(x) = W(x) + \tfrac{1}{2}\mu(x), \quad x \in S. \tag{2.7}$$

Here $W(x)$ is the value of the integral (2.6), when the point x belongs to S [$W(x)$ is a continuous function for x varying along S], $W_i(x)$ is the value of the double-layer potential (2.6), when the point x tends to S from D_+, and $W_e(x)$ is the same when the point x approaches at S from D_-.

In what follows we shall frequently use the derivative along the normal to the surface S at the point y, which belongs to S. This derivative acts on the function the argument of which is the distance r_{xy} between the points x and y, the point x being not obliged to lay on S. Simple calculation gives

$$\frac{\partial}{\partial n_y} r_{xy} = \cos\varphi, \tag{2.8}$$

where φ is the angle between the vector $\mathbf{r}_{xy}$, which starts at x and ends at y, and the normal $\mathbf{n}_y$. In the same way we have

$$\frac{\partial}{\partial n_y} f(r_{xy}) = f'(r_{xy})\cos\varphi, \quad \frac{\partial}{\partial n_y}\left(\frac{1}{r_{xy}}\right) = -\frac{\cos\varphi}{r_{xy}^2}. \tag{2.9}$$

Equations (2.8) and (2.9) are obviously valid for both inward and outward directed normals.

The application of the potentials (2.4)–(2.7) for transforming the boundary problems for the Laplace equation (2.1) to the integral equations can be found in many textbooks on mathematical physics.[8–10,12–15]

Let us proceed to consideration of the heat-conduction equation,

$$\frac{\partial u}{\partial t} - a^2\Delta u = 0. \tag{2.10}$$

The fundamental (or elementary) solution to this equation in $\mathbb{R}_d$ is

$$E_d(x,t;x',t') = \theta(t-t')K_0(x,t;x',t'), \tag{2.11}$$

where

$$K_0(x,t;x',t') = \frac{1}{(2a\sqrt{\pi(t-t')})^d}\exp\left[-\frac{r_{xx'}^2}{4a^2(t-t')}\right]. \tag{2.12}$$

The function $K_0(x,t;x',t')$ (the propagator[14] or the heat kernel) obeys the homogeneous heat equations,

$$\left(\frac{\partial}{\partial t} - a^2\Delta_x\right)K_0(x,t;x',t') = 0,$$

$$\left(\frac{\partial}{\partial t'} + a^2\Delta_{x'}\right)K_0(x,t;x',t') = 0, \tag{2.13}$$

and inhomogeneous initial condition

$$K_0(x,t;x',t') \to \delta^{(d)}(x-x'), \quad \text{when } t-t'. \tag{2.14}$$

This condition enables one to construct the solution of the Cauchy problem for the nonhomogeneous heat equation

$$\left(\frac{\partial}{\partial t} - a^2\Delta_x\right)u(x,t) = f(x,t) \tag{2.15}$$

considered in an unbounded space

$$u(x,t) = \int \mathrm{d}x'\, K_0(x,t;x',t')u_0(x') + \int_{t'}^{t}\mathrm{d}\theta \int \mathrm{d}x'\, K_0(x,t;x',\theta)f(x',\theta), \tag{2.16}$$

where $u_0(x)=u(x,t=t')$. In the classical mathematical physics[8] the representation (2.16) of the solution to the heat-conduction equation (2.15) is known as the Poisson formula. The last term in (2.16) can be considered as an analog of Eq. (2.4) defining the volume potential for the Laplace equation.

In a complete agreement with the definitions (2.5) and (2.6) the heat surface potentials are introduced, namely, the simple-layer potential,

$$V(x,t) = a^2\int_0^t \mathrm{d}\theta \int_S \mathrm{d}S_y\, K_0(x,t;y,\theta)\,\nu(y,\theta) \tag{2.17}$$

and the potential of a double layer,

$$W(x,t) = a^2\int_0^t \mathrm{d}\theta \int_S \mathrm{d}S_y \frac{\partial K_0}{\partial n_y}(x,t;y,\theta)\mu(y,\theta) = -\int_0^t \frac{\mathrm{d}\theta}{2(t-\theta)}\int_S \mathrm{d}S_y r_{xy}\cos\varphi\, K_0(x,t;y,\theta)\mu(y,\theta), \tag{2.18}$$

where the functions $\nu(y,\theta)$ and $\mu(y,\theta)$ are the surface densities of these potentials. By the construction the heat potentials $V(x,t)$ and $W(x,t)$ vanish at $t=0$.

For bounded density $\nu(x,t)$ the heat potential of a single layer $V(x,t)$ is continuous everywhere in $\mathbb{R}_d$, also on passing through the surface S, and satisfies the homogeneous heat-conduction equation (2.10) outside S, i.e., it is parabolic outside S. The normal derivatives of $V(x,t)$ have jump discontinuities on S. For continuous in S density $\nu(x,t)$ these discontinuities are given by

$$\left(\frac{\partial V(x,t)}{\partial n_x}\right)_i = \frac{\partial V(x,t)}{\partial n_x} - \frac{1}{2}\nu(x,t),$$

$$\left(\frac{\partial V(x,t)}{\partial n_x}\right)_e = \frac{\partial V(x,t)}{\partial n_x} + \frac{1}{2}\nu(x,t), \quad x \in S. \tag{2.19}$$

For bounded density $\mu(x,t)$ the heat potential of a double layer (2.18) is continuous everywhere outside of S (in $\mathbb{R}_d\backslash S$) and in S. Outside S the potential $W(x,t)$ is parabolic. On passing through S it has discontinuities. For continuous in S density $\mu(x,t)$ these discontinuities are given by $(d=3)$

$$W_i(x,t) = W(x,t) + \tfrac{1}{2}\mu(x,t),$$

$$W_e(x,t) = W(x,t) - \tfrac{1}{2}\mu(x,t), \quad x \in S. \tag{2.20}$$

The normal derivatives of the double-layer potential are continuous on passing through S.

The employment of the Newtonian and heat potentials for transforming the boundary-value problems for Laplace and heat equations into the integral ones is based on the discontinuity properties on the boundary of the double-layer potential and the normal derivatives of the single-layer potential. Let us consider a simple example, namely, construction of the solution to the Dirichlet problem for the heat equation in a compact domain D bounded by a smooth surface S,

$$\left(\frac{\partial}{\partial t} - a^2\Delta\right)u(x,t) = 0, \quad x \in D, \quad t > 0,$$

$$u(x,0) = 0, \quad x \in D,$$

$$u(x,t) = \psi(x,t), \quad x \in S, \quad t > 0, \tag{2.21}$$

where the function $\psi(x,t)$ specifies the temperature on the boundary S at different time instants t. We shall look for the solution $u(x,t)$ in terms of the heat potential of a double layer (2.18),

$$u(x,t) = W(x,t). \tag{2.22}$$

With account of Eq. (2.20) we have on the boundary S,

$$\frac{1}{2}\mu(x,t) = -a^2\int_0^t dt' \int_S dS_{x'} \frac{\partial K_0}{\partial n_{x'}}(x,t;x',t')\mu(x',t') + \psi(x,t), \quad x,x' \in S. \tag{2.23}$$

Thus, the problem under consideration is reduced to the solution of the linear integral equation of the second kind. With respect to the variable t these equations are of the Volterra type and with respect to the spatial variables x and x' they are of the Fredholm type, the variables x and x' ranging on the boundary S.

In an analogous way the integral equations for the Green's function of the heat equation can be deduced. Let us consider this technique in the case of the first boundary-value problem (the Dirichlet problem) for this equation. The Green function $K(x,t;x',t')$ is specified by the following conditions:[8] it should satisfy the homogeneous heat equation with respect to the first pair of its arguments

$$\left(\frac{\partial}{\partial t} - a^2\Delta_x\right)K(x,t;x',t') = 0, \tag{2.24}$$

it should obey the inhomogeneous initial condition

$$K(x,t;x',t) = \delta(x,x'), \quad t \geqslant 0, \tag{2.25}$$

and the homogeneous boundary condition

$$K(x,t;x',t') = 0, \quad x \in S. \tag{2.26}$$

Strictly speaking, the function $K(x,t;x',t')$ is the propagator of the heat equation. It should be multiplied by the step function $\theta(t-t')$ in order to get the Green function.[14] This point should be kept in mind when dealing with the parabolic equations.

We represent the Green function $K(x,t;x',t')$ as the sum of a free propagator and the heat potential of a double layer,

$$K(x,t;x',t') = K_0(x,t;x',t') + a^2\int_{t'}^t d\theta \int_S dS_y \frac{\partial K_0}{\partial n_y}(x,t;y,\theta)\mu(y,\theta;x',t'). \tag{2.27}$$

The right-hand side of this equation obviously satisfies Eq. (2.24). When $t=t'$ the double-layer potential in (2.27) (the second term) vanishes. The free propagator in this formula K_0 enables one to obey the initial condition (2.25). The density of the double-layer potential $\mu(y,\theta;x',t')$ is determined from the boundary condition (2.26). On substituting Eq. (2.27) into (2.26) the following integral equation is obtained for the potential density μ:

$$\frac{1}{2}\mu(x,t;x',t') = -K_0(x,t;x',t') - a^2\int_{t'}^{t} d\theta \int_S dS_y \frac{\partial K_0}{\partial n_y}(x,t;y,\theta)\mu(y,\theta;x',t'), \quad x \in S. \tag{2.28}$$

For Eq. (2.28) and consequently for Eq. (2.27) the method of successive approximations can be developed, as Eq. (2.28) is an integral equation of the second kind. It has been proved, that the series arising here is uniformly convergent.[16] The first terms of this series for Eq. (2.27) are

$$\begin{aligned} K(x,t;x',t') = {} & K_0(x,t;x',t') + (-2a^2)^1 \int_{t'}^{t} d\theta \int_S dS_y \frac{\partial K_0}{\partial n_y}(x,t;y,\theta)K_0(y,\theta;x',t') \\ & + (-2a^2)^2 \int_{t'}^{t} d\theta \int_S dS_y \frac{\partial K_0}{\partial n_y}(x,t;y,\theta) \int_{t'}^{\theta} d\theta_1 \int dS_{y_1} \frac{\partial K_0}{\partial n_{y_1}}(y,\theta;y_1,\theta_1) \\ & \times K_0(y_1,\theta_1;x',t') + \cdots . \end{aligned} \tag{2.29}$$

Obviously, this series is a result of successive approximations applied to the integral equation for the complete propagator

$$K(x,t;x',t') = K_0(x,t;x',t') - 2a^2 \int_{t'}^{t} d\theta \int_S dS_y \frac{\partial K_0}{\partial n_y}(x,t;y,\theta)K(y,\theta;x',t'). \tag{2.30}$$

The series (2.29) is nothing else as the multiple scattering expansion for the heat kernel in the problems under consideration.[17,18] Thus we have derived this expansion in a rigorous way.

By making use of the Laplace transform in Eq. (2.29) one can remove the integrations over the intermediate time variables θ's,

$$\begin{aligned} \overline{K}(x,x';p) = {} & \overline{K_0}(r_{xx'};p) + (-2a^2)^1 \int_S dS_y\, \overline{K_1}(r_{xy};p)\overline{K_0}(r_{yx'};p) \\ & + (-2a^2)^2 \int_S dS_y\, \overline{K_1}(r_{xy};p) \int_S dS_{y_1}\, \overline{K_1}(r_{yy_1};p)\overline{K_0}(r_{y_1x'};p) + \cdots , \end{aligned} \tag{2.31}$$

where

$$\overline{K}(x,x';p) = \int_0^{\infty} e^{-pt}K(x,t;x',0)dt, \tag{2.32}$$

$$\overline{K_0}(r_{xy};p) = \int_0^{\infty} e^{-pt}K_0(x,t;y,0)dt = \frac{1}{2\pi a^2}K_0\left(\frac{r_{xy}}{a}\sqrt{p}\right), \tag{2.33}$$

$$\overline{K_1}(r_{xy};p) = \int_0^{\infty} e^{-pt}\frac{\partial K_0}{\partial n_y}(x,t;y,0)dt = -\frac{\cos\varphi}{2\pi a^3}\sqrt{p}K_1\left(\frac{r_{xy}}{a}\sqrt{p}\right), \quad y \in S. \tag{2.34}$$

In Eq. (2.34) φ is the angle between the vectors $\mathbf{r}_{xy}$ and $\mathbf{n}_y$. The Laplace transforms $\overline{K_0}$ and $\overline{K_1}$ are calculated for $d=2$. They are expressed in terms of the modified Bessel functions[19] $K_0(z)$ and $K_1(z)$. We hope that our notations will not lead to confusion because the free propagator $K_0(x,t;x',t')$ and the Bessel function $K_0(z)$ have a different number of arguments. The series (2.31) is the perturbative solution to the following integral equation:

$$\overline{K}(x,x';p) = \overline{K}_0(r_{xx'};p) - 2a^2 \int_S \mathrm{d}S_y\, \overline{K}_1(r_{xy};p)\overline{K}(r_{yx'};p). \tag{2.35}$$

The series (2.29) or (2.31) contains complete information about the Green function (heat kernel) in the problem at hand. However, extracting it from here is not a simple task.

The second term on the right-hand side of Eq. (2.31) is responsible for one reflection from the boundary (the Born approximation). Its contribution into the heat kernel can be expressed in terms of the confluent hypergeometric function[19] $W_{\alpha\beta}$. By making use of the convolution theorem for the Laplace transform[7,19–21] we obtain

$$\overline{K}^{(1)}(x,x';p) = \frac{2a^2\sqrt{p}}{(2\pi)^2 a^5} \int_S \mathrm{d}S_y \cos\varphi\, K_0\left(\frac{r_{xy}}{a}\sqrt{p}\right) K_1\left(\frac{r_{yx'}}{a}\sqrt{p}\right). \tag{2.36}$$

The inverse Laplace transform gives[22]

$$K^{(1)}(x,x;t) = \frac{1}{2^{5/2}\pi^{3/2}a^2 t} \int_S \mathrm{d}S_y \frac{\cos\varphi}{r_{xy}} \exp\left(-\frac{r_{xy}^2}{2a^2 t}\right) W_{\frac{1}{2}\frac{1}{2}}\left(\frac{r_{xy}^2}{a^2 t}\right), \tag{2.37}$$

where φ is the angle between the vector $\mathbf{r}_{xy}$ and the inward directed normal to the boundary S at the point y.

The perturbation series (2.31) can be employed, for example, to find the asymptotic expansion of the heat kernel trace.

III. COMPOUND MEDIA

An important advantage of the heat potential technique for constructing the integral equations is the possibility of applying it to compound media. We show this by considering first the solution of the heat-conduction equation instead of the relevant Green's function.

Thus, in both the regions D_+ and D_- the heat equations are defined

$$\left(\frac{\partial}{\partial t} - a_+^2\Delta\right) u_+(x,t) \equiv \hat{T}_{tx}(a_+)u_+(x,t) = 0, \quad x \in D_+, \tag{3.1}$$

$$\left(\frac{\partial}{\partial t} - a_-^2\Delta\right) u_-(x,t) \equiv \hat{T}_{tx}(a_-)u_-(x,t) = 0, \quad x \in D_-, \tag{3.2}$$

with the matching conditions at the interface S, namely, when crossing S the following quantities should be continuous: temperature

$$u_+(x,t) = u_-(x,t), \quad x \in S \tag{3.3}$$

and heat current

$$\lambda_+ \frac{\partial u_+(x,t)}{\partial n_+(x)} + \lambda_- \frac{\partial u_-(x,t)}{\partial n_-(x)} = 0, \quad x \in S, \tag{3.4}$$

where $n_+(x)$ and $n_-(x)$ are inward normals to the surface S at the point x for the regions D_+ and D_-, respectively. These matching conditions imply, in particular, that there are no heat sources on S. The parameters a_+, a_-, λ_+, and λ_- specify the material characteristics of the media.

We shall look for the solution to this problem in terms of the heat potentials of single layer and double layer. Here the following feature proves to be important. If the solution $u_+(x,t)$ in the internal region D_+ is represented as the heat potential of a single layer,

$$u_+(x,t) = a_+^2 \int_0^t \mathrm{d}t' \int_S \mathrm{d}S_{x'}\, K_0^{(+)}(x,t;x',t')\,\nu(x',t'), \tag{3.5}$$

then the solution $u_-(x,t)$ in the external region D_- should be looked for in terms of the heat potential of a double layer,

$$u_-(x,t) = a_-^2 \int_0^t \mathrm{d}t' \int_S \mathrm{d}S_{x'} \frac{\partial K_0^{(-)}}{\partial n_-(x')}(x,t;x',t')\,\mu(x',t'), \tag{3.6}$$

where $K_0^{(+)}$ and $K_0^{(-)}$ are the fundamental solutions of the heat equations (3.1) and (3.2), which are defined by the formula (2.12) with $a=a_+$ and $a=a_-$, respectively.

Substituting Eqs. (3.5) and (3.6) into the first matching condition (3.3) we obtain

$$a_+^2 \int_0^t \mathrm{d}t' \int_S \mathrm{d}S_{x'}\, K_0^{(+)}(x,t;x',t')\,\nu(x',t') = \frac{1}{2}\mu(x,t) + a_-^2 \int_0^t \mathrm{d}t' \int_S \mathrm{d}S_{x'} \frac{\partial K_0^{(-)}}{\partial n_-(x')}(x,t;x',t')\,\mu(x',t'), \quad x,x' \in S. \tag{3.7}$$

The second matching condition (3.4) results in another integral equation,

$$\lambda_+ a_+^2 \int_0^t \mathrm{d}t' \int_S \mathrm{d}S_{x'} \frac{\partial K_0^{(+)}}{\partial n_+(x)}(x,t;x',t')\,\nu(x',t') - \frac{1}{2}\lambda_+\nu(x,t) + \lambda_- a_-^2 \int_0^t \mathrm{d}t' \int_S \mathrm{d}S_{x'} \frac{\partial^2 K_0^{(+)}}{\partial n_-(x)\,\partial n_-(x')}(x,t;x',t')\,\mu(x',t') = 0, \quad x,x' \in S. \tag{3.8}$$

Thus the problem under consideration is reduced to the solution of the system of two linear integral equations of the second kind (3.7) and (3.8). It is worth noting that we have obtained homogeneous equations, because there are not any heat sources in the problem under study. Hence, we are dealing here with the eigenfunctions only.

Let us proceed to the Green's function $K(x,t;x',t')$ in this problem. In what follows, it is convenient to represent this function in terms of the following four components depending on the range of the arguments:

$$K(x,t;x',t') = \begin{cases} K_{++}(x,t;x',t'), & x,x' \in D_+, \\ K_{+-}(x,t;x',t'), & x \in D_+, x' \in D_-, \\ K_{-+}(x,t;x',t'), & x \in D_-, x' \in D_+, \\ K_{--}(x,t;x',t'), & x,x' \in D_-. \end{cases} \tag{3.9}$$

The conditions, which specify the Green function $K(x,t;x',t')$, can be found in the following way. This function should provide the solution $\overline{u}(x,t)$ of the inhomogeneous boundary-value problem (3.1)–(3.4) with the heat source $f(x,t)$ in the form

$$\overline{u}(x,t) = -\,\theta(t-t') \int_{t'}^t \mathrm{d}\tau \int_{\mathbb{R}_d} K(x,t;\xi,\tau) f(\xi,\tau)\mathrm{d}\xi, \tag{3.10}$$

where $\theta(t-t')$ is the step function. The function $\overline{u}(x,t)$ will satisfy the inhomogeneous heat-conduction equation

$$f(x,t)=\begin{cases}\hat{T}_{tx}(a_+)\overline{u}(x,t), & x\in D_+,\\ \hat{T}_{tx}(a_-)\overline{u}(x,t), & x\in D_-,\end{cases} \tag{3.11}$$

if the Green function $K(x,t;x',t')$ obeys the corresponding homogeneous heat equations with respect to the first pair of its arguments

$$\hat{T}_{tx}(a_+)K(x,t;x',t')=0, \quad x\in D_+,$$

$$\hat{T}_{tx}(a_-)K(x,t;x',t')=0, \quad x\in D_-, \tag{3.12}$$

and the inhomogeneous initial condition (2.25) with respect to both pairs of its arguments. In terms of the components (3.9) the initial condition (2.25) acquires the form

$$K_{++}(x,t;x',t)=\delta(x,x'), \quad x,x'\in D_+, \tag{3.13}$$

$$K_{--}(x,t;x',t)=\delta(x,x'), \quad x,x'\in D_-, \tag{3.14}$$

$$K_{+-}(x,t;x',t)=K_{-+}(x,t;x',t)=0. \tag{3.15}$$

On the right-hand side of the initial conditions (3.15) the delta function $\delta(x,x')$ with $x,x'\in S$ is absent. Thus in our consideration we eliminate the treatment of heat sources at the interface. The point is such sources alter the matching conditions instead of the initial conditions. In the next section the solution to the heat-conduction equation, defined on a line, will be constructed for such a configuration by making use of the heat potential technique.

The matching conditions (3.3) and (3.4) are directly transformed into the conditions for the Green function $K(x,t;x',t')$ with respect to the first pair of its arguments,

$$K_{++}(x,t;x',t')=K_{-+}(x,t;x',t'), \tag{3.16}$$

$$\lambda_+\frac{\partial K_{++}}{\partial n_+(x)}(x,t;x',t')+\lambda_-\frac{\partial K_{-+}}{\partial n_-(x)}(x,t;x',t')=0, \tag{3.17}$$

$$K_{+-}(x,t;x',t')=K_{--}(x,t;x',t'), \tag{3.18}$$

$$\lambda_+\frac{\partial K_{+-}}{\partial n_+(x)}(x,t;x',t')+\lambda_-\frac{\partial K_{--}}{\partial n_-(x)}(x,t;x',t')=0, \tag{3.19}$$

$$x\in S.$$

It turns out that the heat equations (3.12), the initial conditions (3.13)–(3.15), and the matching conditions (3.16)–(3.19) are enough for construction of the Green function in the case of compound media in a unique way.

We shall look for the components of the Green function (3.9) in terms of the heat potentials of single and double layers with respect to the first pair of their arguments, the components K_{++} and K_{+-} being expressed through the heat potentials of single layers and the components K_{--} and K_{-+} through the heat potentials of double layers. In order to take into account the inhomogeneous initial conditions (3.13) and (3.14) for the components K_{++} and K_{--} we add to the chosen heat potentials (nonsingular part of the Green function) the free propagator $K_0^{(+)}$ or $K_0^{(-)}$ (singular part of this function)

$$K_{++}(x,t;x',t') = K_0^{(+)}(x,t;x',t') + a_+^2 \int_{t'}^{t} \mathrm{d}\theta \int_S \mathrm{d}S_y \, K_0^{(+)}(x,t;y,\theta)\, \nu_{++}(y,\theta;x',t'), \tag{3.20}$$

$$K_{+-}(x,t;x',t') = a_+^2 \int_{t'}^{t} \mathrm{d}\theta \int_S \mathrm{d}S_y \, K_0^{(+)}(x,t;y,\theta)\, \nu_{+-}(y,\theta;x',t'), \tag{3.21}$$

$$K_{--}(x,t;x',t') = K_0^{(-)}(x,t;x',t') + a_-^2 \int_{t'}^{t} \mathrm{d}\theta \int_S \mathrm{d}S_y \frac{\partial K_0^{(-)}}{\partial n_-(y)}(x,t;y,\theta)\, \nu_{--}(y,\theta;x',t'), \tag{3.22}$$

$$K_{-+}(x,t;x',t') = a_-^2 \int_{t'}^{t} \mathrm{d}\theta \int_S \mathrm{d}S_y \frac{\partial K_0^{(-)}}{\partial n_-(y)}(x,t;y,\theta)\, \nu_{-+}(y,\theta;x',t'). \tag{3.23}$$

The matching conditions (3.16) and (3.17) give

$$\begin{aligned} &K_0^{(+)}(x,t;x',t') + a_+^2 \int_{t'}^{t} \mathrm{d}\theta \int_S \mathrm{d}S_y \, K_0^{(+)}(x,t;y,\theta)\, \nu_{++}(y,\theta;x',t') \\ &\quad = \frac{1}{2}\nu_{-+}(x,t;x',t') + a_-^2 \int_{t'}^{t} \mathrm{d}\theta \int_S \mathrm{d}S_y \frac{\partial K_0^{(-)}}{\partial n_-(y)}(x,t;y,\theta)\, \nu_{-+}(y,\theta;x',t'), \end{aligned} \tag{3.24}$$

$$\begin{aligned} &\lambda_+ \frac{\partial K_0^{(+)}}{\partial n_+(x)}(x,t;x',t') + \lambda_+ a_+^2 \int_{t'}^{t} \mathrm{d}\theta \int_S \mathrm{d}S_y \frac{\partial K_0^{(+)}}{\partial n_+(x)}(x,t;y,\theta)\, \nu_{++}(y,\theta;x',t') - \frac{1}{2}\lambda_+ \nu_{++}(y,\theta;x',t') \\ &\quad + \lambda_- a_-^2 \int_{t'}^{t} \mathrm{d}\theta \int_S \mathrm{d}S_y \frac{\partial^2 K_0^{(-)}}{\partial n_-(x)\, \partial n_-(y)}(x,t;y,\theta)\, \nu_{-+}(y,\theta;x',t') = 0, \quad x \in S. \end{aligned} \tag{3.25}$$

In the same way we deduce from (3.18) and (3.19)

$$\begin{aligned} a_+^2 \int_{t'}^{t} \mathrm{d}\theta \int_S \mathrm{d}S_y \, K_0^{(+)}(x,t;y,\theta)\, \nu_{+-}(y,\theta;x',t') &= K_0^{(-)}(x,t;x',t') + \frac{1}{2}\nu_{--}(x,t;x',t') \\ &\quad + a_-^2 \int_{t'}^{t} \mathrm{d}\theta \int_S \mathrm{d}S_y \frac{\partial K_0^{(-)}}{\partial n_-(y)}(x,t;y,\theta)\, \nu_{--}(y,\theta;x',t'), \end{aligned} \tag{3.26}$$

$$\begin{aligned} &-\frac{1}{2}\lambda_+ \nu_{+-}(x,t;x',t') + \lambda_+ a_+^2 \int_{t'}^{t} \mathrm{d}\theta \int_S \mathrm{d}S_y \frac{\partial K_0^{(+)}}{\partial n_+(x)}(x,t;y,\theta)\, \nu_{+-}(y,\theta;x',t') \\ &\quad + \lambda_- a_-^2 \int_{t'}^{t} \mathrm{d}\theta \int_S \mathrm{d}S_y \frac{\partial^2 K_0^{(-)}}{\partial n_-(x)\, \partial n_-(y)}(x,t;y,\theta)\, \nu_{--}(y,\theta;x',t') + \lambda_- \frac{\partial K_0^{(-)}}{\partial n_-(x)}(x,t;x',t') = 0, \quad x \in S. \end{aligned} \tag{3.27}$$

The sets of integral equations of the second kind (3.24), (3.25) and (3.26), (3.27) define the heat kernel for compound media in full. With respect to spatial variables these equations are of Fredholm type while regarding time variable they are of Volterra type. It is essential that the integration over the spatial variables is restricted by the interface S only. Hence the dimension of the initial problem is reduced by 1. By making use of the Laplace transform one can remove the integration over the time variables in Eqs. (3.24)–(3.27) as it has been done in Sec. II.

Obviously the integral equations for the heat kernel derived here can be also applied when the surface S divides the same medium into the regions D_+ and D_+, i.e., when the constants a_+^2 and a_-^2 equal.

For constructing the solutions to the integral equations (3.24)–(3.27) the perturbation theory can be employed (see Sec. II). The expansion parameters in this case prove to be the constants $a_\pm^2$ and $\lambda_\pm$. The perturbation series generated here are nothing else as the multiple scattering expansion for the heat kernel.[17,18] Thus we have proposed a rigorous derivation of these expansions both for homogeneous media and compact regions and for compound media.

IV. ASYMPTOTIC EXPANSION OF HEAT KERNEL FROM PERTURBATION SERIES

In practical applications, especially in QFT, the asymptotic expansion of the integrated heat kernel when $t \to +0$ proves to be important.[1–4] It has the form

$$K(t) \equiv \int \mathrm{d}x\, K(x,t;x,0) = (4\pi t)^{-d/2} \sum_{n=0,1,2,\ldots}^{\infty} t^{n/2} B_{n/2} + \mathrm{ES}. \tag{4.1}$$

In this expansion d is the dimension of the configuration space and ES stands for the exponentially small corrections as $t \to +0$. We show how to derive this expansion proceeding from the perturbation series for the integral equations (3.24)–(3.27). The functions K_{-+} and K_{+-} do not contribute to integrated heat kernel (see Sec. V C), thus we must consider only K_{++} and K_{--}.

For our purposes it is convenient to use such coordinates that in the vicinity of the surface S the metric is $g_{ij}\,\mathrm{d}x^i\,\mathrm{d}x^j = (\mathrm{d}x^3)^2 + g_{ab}\,\mathrm{d}x^a\,\mathrm{d}x^b$ where x^3 is a coordinate on the normal to S, $x^3=0$ on S. In view of the exact form of the free propagator (2.12), one can infer that in each term of the perturbation series for integral equations (3.24)–(3.27) the power in t contributions are given only at the following conditions: when evaluating the heat kernel trace, the integration over dx should be spread over the region immediately adjacent to the boundary S and in the course of the multiple integration over the boundary S the respective distances $r_{yy'}$ should be also small. Therefore in the vicinity of S we may replace the squared distance $(x-z)^2$ by several terms of its expansion in powers of the corresponding geodesic distance σ on the surface S,

$$(x-z)^2 = (x_3-z_3)^2 + \sigma^2\{1-(x_3+y_3)k_1 + x_3 z_3(k_1^2+k_2^2)\} + \sigma^3\left\{-\tfrac{1}{3}(2z_3+x_3)k_1' + x_3 z_3(k_1 k_1' + k_2 k_2')\right\} + \cdots,$$

$$k_1 = L_{ab}\xi^a\xi^b, \quad k_2 = \frac{1}{2}(\varepsilon_{ac}L_b^c + \varepsilon_{bc}L_a^c)\xi^a\xi^b, \quad \varepsilon_{ac} = -\varepsilon_{ca}, \quad k_1' \equiv \frac{\mathrm{d}k_1}{\mathrm{d}\sigma}, \quad k_2' \equiv \frac{\mathrm{d}k_2}{\mathrm{d}\sigma}. \tag{4.2}$$

The surface area element is $\mathrm{d}S_z = \left(1-\frac{1}{12}R_{ab}\xi^a\xi^b\sigma^2+\cdots\right)\sigma\,\mathrm{d}\sigma\,\mathrm{d}\Omega$, Ω parametrizes a unit sphere, L_{ab} is the second fundamental form on S, R_{ab} is intrinsic Ricci curvature, ξ is a unit tangent vector at x to the geodesics with the length σ joining z to x on S (see, for example, Ref. 23).

Here we present the first three terms of the perturbation series under consideration when $t \to +0 (d=3)$,

$$K^{(0)}(t) = K_{++}^{(0)}(t) + K_{--}^{(0)}(t) = \frac{t^{-3/2}}{(4\pi a_+^2)^{3/2}}D_+ + \frac{t^{-3/2}}{(4\pi a_-^2)^{3/2}}D_-,$$

$$K_{++}^{(1)}(t) = \frac{t^{-1}S}{8\pi a_+^2} + \frac{t^{-1/2}}{8\pi^{3/2}a_+}\int_S \mathrm{d}S\, L_a^a + \frac{t^0}{2^8\pi}\int_S \mathrm{d}S\left[5(L_a^a)^2 + L_a^b L_b^a - \frac{2}{3}R_a^a\right] + \cdots,$$

$$K_{++}^{(2)}(t) = -\frac{t^{-1}}{8\pi}\frac{\lambda_-}{\lambda_+}\frac{S}{a_+^2} - \frac{1}{8\pi^{3/2}}\frac{\lambda_-}{\lambda_+}\frac{t^{-1/2}}{a_+}\int_S dS\, L_a^a + \frac{t^0}{32\pi}\left\{ a_-\frac{\lambda_-}{\lambda_+}\frac{(a_+ + 2a_-)}{(a_+ + a_-)^2}\int_S dS\left[-(L_a^a)^2 + 4L_a^b L_b^a - \frac{1}{3}R_a^a\right] + \left[\frac{1}{8} - \frac{\lambda_-}{\lambda_+}\frac{1}{(a_+ + a_-)^3}\left(\frac{35}{12}a_-^3 + \frac{11}{4}a^2 a_+ + 2a_+^2 a_- + \frac{2}{3}a_+^3 + \frac{9}{4}\frac{a_-^4}{a_+} + \frac{3}{4}\frac{a_-^5}{a_+^2}\right)\right]\int_S dS[(L_a^a)^2 + 2L_a^b L_b^a]\right\} + \cdots . \tag{4.3}$$

To obtain $K_{--}^{(1)}(t)$ and $K_{--}^{(2)}(t)$ one should replace $a_+ \leftrightarrow a_-, \lambda_+ \leftrightarrow \lambda_-, L_a^b \to -L_a^b$. The asymptotics of the subsequent terms of perturbation series may be found in a similar way. After that all factors appearing with the same powers of t are added up to give the heat kernel coefficients. The latter are expressed through the integrals of the surface geometric invariants. The asymptotics (4.3) were presented in Ref. 24 without considering the derivation of the relevant integral equations.

V. HEAT KERNEL ON A LINE

In this section we demonstrate the efficiency of our approach based on integral equations for constructing the heat kernel on a line. In this case the interface between the media reduces to a point. As a result we are dealing with the Volterra integral equations in respect of one (time) variable. These equations are of a special type (Abel equations), and their solutions can be found in an exact form.

A. Homogeneous media with gluing conditions

By making use of the heat potential technique we construct here, in an exact form, the heat kernel $K(x,y;t)$ for the Laplace operator on an infinite line for homogeneous medium with a nonstandard gluing conditions at the origin (these conditions will be specified below). From the physical point of view $K(x,y;t)$ is the temperature at the point x which is generated by a unit instantaneous heat source placed at the point y at the moment $t=0$.

As in the preceding sections we first formulate the conditions that define the heat kernel in the problem under consideration. With respect to the first argument $K(x,y;t)$ should satisfy the one-dimensional heat-conduction equation

$$\left(\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}\right)K(x,y;t) = 0, \quad t > 0, \quad -\infty < x < \infty \tag{5.1}$$

and special conditions at the interface $x=0$

$$lK(-0,y;t) = l^{-1}K(+0,y;t), \tag{5.2}$$

$$l^{-1}\frac{\partial}{\partial x}K(x,y;t)\bigg|_{x=-0} = l\frac{\partial}{\partial x}K(x,y;t)\bigg|_{x=+0}, \tag{5.3}$$

where l is a dimensionless parameter. We shall refer to these conditions as to gluing ones. In the Appendix it is shown that such conditions lead to a self-adjoint spectral problem for the Laplace operator in any dimension. The initial condition for $K(x,y;t)$ involves its both space arguments

$$K(x,y;0) = \delta(x,y). \tag{5.4}$$

We shall seek for $K(x,y;t)$ in terms of free heat kernel and single-layer heat potentials. The solution is decomposed in four components related to different positions of the heat source and the observer

$$K_{-+}(x,y;t) = \int_0^t \mathrm{d}\tau\, K_0(x,0;t-\tau)\alpha_1(\tau,y), \quad x<0, \quad y>0, \tag{5.5}$$

$$K_{++}(x,y;t) = K_0(x,y;t) + \int_0^t \mathrm{d}\tau\, K_0(x,0;t-\tau)\alpha_2(\tau,y), \quad x,y>0, \tag{5.6}$$

$$K_{+-}(x,y;t) = \int_0^t \mathrm{d}\tau\, K_0(x,0;t-\tau)\alpha_3(\tau,y), \quad x>0, \quad y<0, \tag{5.7}$$

$$K_{--}(x,y;t) = K_0(x,y;t) + \int_0^t \mathrm{d}\tau\, K_0(x,0;t-\tau)\alpha_4(\tau,y), \quad x,y<0, \tag{5.8}$$

where $K_0(x,y;t)$ is the free heat kernel (propagator) on an infinite line

$$K_0(x,y;t) = \frac{1}{2\sqrt{\pi t}} e^{-[(x-y)^2/4t]}. \tag{5.9}$$

In multi-dimensional problems we may also choose single-layer potential for internal region and double-layer potential for external region. However when $d=1$ such a choice may lead to divergent integrals.

First we substitute Eqs. (5.5) and (5.6) into the gluing conditions (5.2) and (5.3). Then we take into account that the single-layer potential changes smoothly across the boundary, while the normal derivative of this potential undergoes a jump

$$K_{-+}(-0,y;t) = \frac{1}{2\sqrt{\pi}} \int_0^t \mathrm{d}\tau\, \frac{\alpha_1(y,\tau)}{\sqrt{t-\tau}}, \tag{5.10}$$

$$K_{++}(+0,y;t) = K_0(0,y;t) + \frac{1}{2\sqrt{\pi}} \int_0^t \mathrm{d}\tau\, \frac{\alpha_2(y,\tau)}{\sqrt{t-\tau}}, \tag{5.11}$$

$$\frac{\partial}{\partial x} K_{-+}(x,y;t)\bigg|_{x=-0} = -\frac{1}{2}\alpha_1(y,t), \tag{5.12}$$

$$\frac{\partial}{\partial x} K_{++}(x,y;t)\bigg|_{x=+0} = -\frac{1}{2}\alpha_2(y,t) + \frac{\partial}{\partial x} K_0(x,y;t)\bigg|_{x=0}. \tag{5.13}$$

Inserting Eqs. (5.10) and (5.11) into Eq. (5.2) one obtains the Abel integral equation

$$\frac{1}{2\sqrt{\pi}} \int_0^t \frac{\mathrm{d}\tau}{\sqrt{t-\tau}} [l^2\alpha_1(y,\tau) - \alpha_2(y;\tau)] = K_0(0,y;t) \tag{5.14}$$

with the solution

$$\alpha_1(y,t) - l^{-2}\alpha_2(y;t) = \frac{2}{l^2\sqrt{\pi}} \frac{d}{\mathrm{d}t} \int_0^t \frac{K_0(0,y;\tau)}{\sqrt{t-\tau}} \mathrm{d}\tau = \frac{1}{2\sqrt{\pi} l^2} \frac{y}{t^{3/2}} \exp\left(-\frac{y^2}{4t}\right). \tag{5.15}$$

When considering the gluing conditions the use of the single-layer potentials leads to the exactly solvable (no iterations needed) Abel equation only in one-dimensional case. The substitution of Eqs. (5.12) and (5.13) into Eq. (5.3) gives

$$\alpha_1(y,t) = -l^2\alpha_2(y,t) + \frac{l^2}{2\sqrt{\pi}}\frac{y}{t^{3/2}}e^{-y^2/4t}. \tag{5.16}$$

From (5.15) and (5.16) it follows that

$$\alpha_1(y,t) = \frac{l^2}{l^4+1}\frac{y}{\sqrt{\pi}t^{3/2}}e^{-y^2/4t}, \quad \alpha_2(y,t) = \frac{l^4-1}{l^4+1}\frac{y}{2\sqrt{\pi}t^{3/2}}e^{-y^2/4t}. \tag{5.17}$$

And finally

$$K_{-+}(x,y;t) = \frac{l^2}{l^4+1}\frac{1}{\sqrt{\pi t}}e^{-[(x-y)^2/4t]}, \tag{5.18}$$

$$K_{++}(x,y;t) = \frac{1}{2\sqrt{\pi t}}e^{-[(x-y)^2/4t]} + \frac{l^4-1}{l^4+1}\frac{1}{2\sqrt{\pi t}}e^{-[(x+y)^2/4t]}. \tag{5.19}$$

In a similar way one gets

$$K_{+-}(x,y;t) = \frac{l^2}{l^4+1}\frac{1}{\sqrt{\pi t}}e^{-[(x-y)^2/4t]}, \tag{5.20}$$

$$K_{--}(x,y;t) = \frac{1}{2\sqrt{\pi t}}e^{-[(x-y)^2/4t]} - \frac{l^4-1}{l^4+1}\frac{1}{2\sqrt{\pi t}}e^{-[(x+y)^2/4t]}. \tag{5.21}$$

These formulas are in complete agreement with the result of a combined employment of the Lemma 5.2 argued in Ref. 25 and Lemma 4.1 from Ref. 26,

$$K_{++}(x,y;t) = \cos^2\theta K_N(x,y;t) + \sin^2\theta K_D(x,y;t), \tag{5.22}$$

$$K_{--}(x,y;t) = \sin^2\theta K_N(x,y;t) + \cos^2\theta K_D(x,y;t), \tag{5.23}$$

$$K_{+-}(x,y;t) = \sin\theta\cos\theta[K_N(x,y;t) - K_D(x,y;t)], \tag{5.24}$$

where

$$\cos^2\theta = \frac{l^4}{l^4+1}, \quad \sin^2\theta = \frac{1}{l^4+1},$$

and $K_D(x,y;t)$ and $K_N(x,y;t)$ are the heat kernels for Dirichlet and Neumann boundary conditions, respectively.

B. Dielectriclike conditions on a line

We construct here the heat kernel for the Laplace operator defined on an infinite line with dielectriclike matching conditions at the origin $x=0$. The heat kernel is defined by the heat-conduction equation

$$\left(\frac{\partial}{\partial t} - a^2(x)\frac{\partial^2}{\partial x^2}\right)K(x,y;t) = 0, \quad t>0, \quad -\infty < x < +\infty, \quad x \neq 0, \tag{5.25}$$

where

$$a^2(x) = \begin{cases} a_-^2, & x < 0, \\ a_+^2, & x > 0, \end{cases}$$

a_+^2 and a_-^2 being positive constants. At the interface of dielectric media the matching conditions

$$K(-0,y;t) = K(+0,y;t), \tag{5.26}$$

$$\lambda_- \frac{\partial}{\partial x} K(x,y;t)\Big|_{x=-0} = \lambda_+ \frac{\partial}{\partial x} K(x,y;t)\Big|_{x=+0} \tag{5.27}$$

should be met. As usual, the initial condition for $K(x,y;t)$ is given by (5.4).

We call the boundary conditions (5.26) and (5.27) the dielectriclike conditions. The use of this term requires some explanations. When two dielectric media D_+ and D_- possessing different characteristics are separated by the interface S of an arbitrary form then in Maxwell theory we have on the surface S the set of coupled boundary conditions involving all the components of the electromagnetic potential $A_\mu(t,\mathbf{x})$, $\mu = 0,\cdots,d$. If one disregards the vector character of the electromagnetic field and confine oneself to oscillations described by a sole scalar potential (for example, sound waves which are described by a scalar velocity potential) then at the interface between different media the conditions (5.26) and (5.27) should be satisfied. In other words, these boundary conditions hold in the theory of scalar "photons" in compound media.

Again we seek for the solution in terms of a relevant free propagator and single-layer heat potentials,

$$K_{-+}(x,y;t) = a_-^2 \int_0^t d\tau\, K_0(x,0;a_-^2(t-\tau))\beta_1(\tau,y), \quad x<0, \quad y>0, \tag{5.28}$$

$$K_{++}(x,y;t) = K_0(x,y;a_+^2 t) + a_+^2 \int_0^t d\tau\, K_0(x,0;a_+^2(t-\tau))\beta_2(\tau,y), \quad x,y>0, \tag{5.29}$$

$$K_{+-}(x,y;t) = a_+^2 \int_0^t d\tau\, K_0(x,0;a_+^2(t-\tau))\beta_3(\tau,y), \quad x>0, \quad y<0, \tag{5.30}$$

$$K_{--}(x,y;t) = K_0(x,y;a_-^2 t) + a_-^2 \int_0^t d\tau\, K_0(x,0;a_-^2(t-\tau))\beta_4(\tau,y), \quad x,y<0. \tag{5.31}$$

First we insert Eqs. (5.28) and (5.29) into the matching conditions (5.26) and (5.27). The single-layer potential changes smoothly across the boundary, while its normal derivative undergoes a jump,

$$K_{-+}(-0,y;t) = \frac{a_-}{2\sqrt{\pi}} \int_0^t d\tau \frac{\beta_1(y,\tau)}{\sqrt{t-\tau}}, \tag{5.32}$$

$$K_{++}(+0,y;t) = K_0(0,y;a_+^2 t) + \frac{a_+}{2\sqrt{\pi}} \int_0^t d\tau \frac{\beta_2(y,\tau)}{\sqrt{t-\tau}}, \tag{5.33}$$

$$\frac{\partial}{\partial x} K_{-+}(x,y;t)\Big|_{x=-0} = -\frac{1}{2}\beta_1(y,t), \tag{5.34}$$

$$\frac{\partial}{\partial x}K_{++}(x,y;t)\bigg|_{x=+0} = -\frac{1}{2}\beta_2(y,t) + \frac{\partial}{\partial x}K_0(x,y;a_+^2t)\bigg|_{x=0}. \tag{5.35}$$

Substituting Eqs. (5.32) and (5.33) into Eq. (5.26) one obtains the Abel integral equation,

$$\frac{1}{2\sqrt{\pi}}\int_0^t \frac{\mathrm{d}\tau}{\sqrt{t-\tau}}[a_-\beta_1(y,\tau) - a_+\beta_2(y;\tau)] = K_0(0,y;a_+^2t) \tag{5.36}$$

with the solution

$$a_-\beta_1(y,t) - a_+\beta_2(y;t) = \frac{2}{\sqrt{\pi}}\frac{d}{\mathrm{d}t}\int_0^t \frac{\mathrm{d}\tau}{\sqrt{t-\tau}}K_0(0,y;a_+^2\tau) = \frac{1}{2\sqrt{\pi}}\frac{y}{a_+^2t^{3/2}}\exp\left(-\frac{y^2}{4a_+^2t}\right). \tag{5.37}$$

The substitution of Eqs. (5.34) and (5.35) into Eq. (5.27) gives

$$\lambda_-\beta_1(y,t) = -\lambda_+\beta_2(y,t) + \lambda_+\frac{1}{2\sqrt{\pi}}\frac{y}{a_+^3t^{3/2}}e^{-(y^2/4a_+^2t)}. \tag{5.38}$$

From Eqs. (5.37) and (5.38) it follows that

$$\beta_1(y,t) = \frac{\frac{\lambda_+}{a_+}}{\frac{\lambda_+}{a_+}+\frac{\lambda_-}{a_-}}\frac{y}{\sqrt{\pi}a_+^3t^{3/2}}e^{-y^2/4a_+^2t}, \quad \beta_2(y,t) = \frac{\frac{\lambda_+}{a_+}-\frac{\lambda_-}{a_-}}{\frac{\lambda_+}{a_+}+\frac{\lambda_-}{a_-}}\frac{y}{2\sqrt{\pi}a_+^3t^{3/2}}e^{-y^2/4a_+^2t}. \tag{5.39}$$

And finally

$$K_{-+}(x,y;t) = \frac{\frac{\lambda_+}{a_+}}{\frac{\lambda_+}{a_+}+\frac{\lambda_-}{a_-}}\frac{1}{\sqrt{\pi a_+^2t}}e^{-[(x-y\ a_-/a_+)^2/4a_-^2t]}, \tag{5.40}$$

$$K_{++}(x,y;t) = \frac{1}{2\sqrt{\pi\ a_+^2t}}e^{-[(x-y)^2/4\ a_+^2t]} + \frac{\frac{\lambda_+}{a_+}-\frac{\lambda_-}{a_-}}{\frac{\lambda_+}{a_+}+\frac{\lambda_-}{a_-}}\frac{1}{2\sqrt{\pi\ a_+^2t}}e^{-[(x+y)^2/4\ a_+^2t]}. \tag{5.41}$$

In a similar way one gets

$$K_{+-}(x,y;t) = \frac{\frac{\lambda_-}{a_-}}{\frac{\lambda_-}{a_-}+\frac{\lambda_+}{a_+}}\frac{1}{\sqrt{\pi\ a_-^2t}}e^{-[(x-ya_+/a_-)^2/4\ a_+^2t]}, \tag{5.42}$$

$$K_{--}(x,y;t) = \frac{1}{2\sqrt{\pi\ a_-^2t}}e^{-[(x-y)^2/4\ a_-^2t]} + \frac{\frac{\lambda_-}{a_-}-\frac{\lambda_+}{a_+}}{\frac{\lambda_-}{a_-}+\frac{\lambda_+}{a_+}}\frac{1}{2\sqrt{\pi\ a_-^2t}}e^{-[(x+y)^2/4\ a_-^2t]}. \tag{5.43}$$

The solution obtained here exactly reproduces the results obtained in this problem by other methods.[7,27]

C. δ-like heat source at the interface

In the preceding considerations we excluded the configuration when the δ-like heat source is placed at the interface of the media $y=0$. For completeness we have to check whether this configuration contributes to the trace $\int_{-\infty}^{\infty}K(x,x;t)\mathrm{d}x$. To this end we use the approach of Ref. 28. The idea is to modify the boundary conditions (5.26) and (5.27) so that they allow for the heat source placed at the interface

$$K_-(-0;t) = K_+(+0;t), \tag{5.44}$$

$$\lambda_- \frac{\partial}{\partial x} K_-(x;t)\bigg|_{x=-0} - \lambda_+ \frac{\partial}{\partial x} K_+(x;t)\bigg|_{x=+0} = Q\ \delta(t). \tag{5.45}$$

The condition (5.45) means that the heat Q instantly generated by the source is divided into two flows which are proportional to λ_- and λ_+. We represent the solution in the form

$$K_-(x;t) = a_-^2 \int_0^t \mathrm{d}\tau\, K_0(x,0;a_-^2(t-\tau))\beta_1(\tau), \quad x<0, \tag{5.46}$$

$$K_+(x;t) = a_+^2 \int_0^t \mathrm{d}\tau\, K_0(x,0;a_+^2(t-\tau))\beta_2(\tau), \quad x>0. \tag{5.47}$$

The functions $\beta_1(\tau)$ and $\beta_2(\tau)$ can be determined by making use of the Laplace transform. We denote by $\overline{K}(x;s)$ the transform of $K(x;t)$, i.e.,

$$\overline{K}(x;p) = \int_0^\infty \mathrm{d}t\, e^{-p\ t} K(x;t).$$

Transforming (5.45) and (5.47) we obtain

$$\overline{K}_-(x;p) = a_-\overline{\beta}_-(p)\sqrt{\pi/p}\,\exp(-x\sqrt{p}/a_-), \tag{5.48}$$

$$\overline{K}_+(x;p) = a_+\overline{\beta}_+(p)\sqrt{\pi/p}\,\exp(-x\sqrt{p}/a_+). \tag{5.49}$$

Then Eq. (5.44) leads to the relation between the Laplace transforms $\overline{\beta}_-$ and $\overline{\beta}_+$,

$$a_-\overline{\beta}_-(p) - a_+\overline{\beta}_+(p) = 0. \tag{5.50}$$

The substitution of Eqs. (5.46) and (5.47) into Eq. (5.45) gives

$$\lambda_-\beta_-(t) + \lambda_+\beta_+(t) = 2\ Q\ \delta(t). \tag{5.51}$$

After the Laplace transform one arrives at the second relation between $\overline{\beta}_1$ and $\overline{\beta}_2$,

$$\lambda_1\overline{\beta}_-(p) + \lambda_2\beta_+(p) = 2\ Q\ \overline{\delta}(p). \tag{5.52}$$

How to apply the Laplace transform to the singular δ function can be found in appropriate handbooks.[20,21] The essence of the matter comes to defining the integration rule

$$\int_0^\infty f(t)\delta(t)\mathrm{d}t = f(0),$$

whence it follows in particular

$$\overline{\delta}(p) = \int_0^\infty e^{-pt}\delta(t)\mathrm{d}t = 1.$$

In the problems treated by the integral Laplace transform the semiaxis $t>0$ (or $t>t_0$) is usually considered. Therefore the δ-function should be defined here in a nonsymmetric way, for example, as the limit when $\varepsilon \to +0$ of the function

$$\delta_\varepsilon(t) = \begin{cases} 0, & t<0, \quad t>\varepsilon, \\ 1/\varepsilon, & 0<t<\varepsilon. \end{cases}$$

The solution of the system (5.50) and (5.52) is

$$\overline{\beta}_-(p) = \frac{2\,a_+Q\,\overline{\delta}(p)}{\lambda_+a_- + \lambda_-a_+}, \quad \overline{\beta}_+(p) = \frac{2\,a_-Q\,\overline{\delta}(p)}{\lambda_+a_- + \lambda_-a_+}. \tag{5.53}$$

By the inverse Laplace transform we find from (5.53)

$$\beta_-(t) = \frac{2\,a_+Q\,\delta(t)}{\lambda_+a_- + \lambda_-a_+}, \quad \beta_+(t) = \frac{2\,a_-Q\,\delta(t)}{\lambda_+a_- + \lambda_-a_+}. \tag{5.54}$$

Having inserted (5.54) into (5.46) and (5.47) we derive

$$K_-(x;t) = \frac{1}{\sqrt{\pi t}} e^{-x^2/4a_-^2 t} \frac{Q}{\frac{\lambda_+}{a_+} + \frac{\lambda_-}{a_-}}, \quad x < 0, \tag{5.55}$$

$$K_+(x;t) = \frac{1}{\sqrt{\pi t}} e^{-x^2/4a_+^2 t} \frac{Q}{\frac{\lambda_+}{a_+} + \frac{\lambda_-}{a_-}}, \quad x > 0. \tag{5.56}$$

These formulas show that for $t>0$ the heat kernel is finite notwithstanding the δ-like heat source situated at the interface between two media. Therefore the neighborhood of the point $x=0$ gives no contribution to the heat kernel trace $\int_{-\infty}^{\infty} K(x,x;t)\mathrm{d}x$.

VI. CONCLUSION

For a broad set of boundary conditions the finding of the heat kernel is reduced to the solution of integral equations defined on the boundary (or at the interface) of the manifolds. As a result the dimension of the initial problem is brought down by 1. Remarkably this technique is applicable to compound media where the standard methods for the investigation of heat kernel do not work because in this case the principal part of the elliptic operator in question is not smooth.

The perturbation series for the integral equations derived are nothing else as the multiple scattering expansions for the relevant heat kernels. Thus a rigorous derivation of these expansions both for homogeneous media and compact regions and for compound media has been done.

The efficiency of this approach is convincingly demonstrated by constructing, in an exact form, the heat kernel on an infinite line with diverse matching conditions and by deriving the first terms of the asymptotic expansion for integrated heat kernel in the case of three-dimensional compound media.

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APPENDIX : SELF-ADJOINTNESS OF BOUNDARY VALUE PROBLEMS FOR COMPOUND MEDIA

Often it is helpful to use the spectral representation for the Green's function of the heat-conduction equation (2.10),

$$K(x,t;x',0) = \sum_k e^{-\omega_k t} f_k(x) f_k^*(x'), \tag{A1}$$

where $f_k(x)$ are the eigenfunctions of the spectral problem at hand

$$-a^2\Delta f_k(x) = \omega_k f_k(x), \quad x \in D \tag{A2}$$

obeying the relevant boundary conditions on S. Apparently, the representation (A1) is well defined if the spectral problem (A2) is Hermitian and positive definite. In this connection it is worth

elucidating the boundary conditions for compound media that lead to the self-adjoint spectral problem [see Eqs. (3.1)–(3.4)]. In this case we have instead of (A2),

$$-a^2(x)\Delta f_k(x) = \omega_k f_k(x), \tag{A3}$$

where

$$a^2(x) = \begin{cases} a_+^2, & x \in D_+, \\ a_-^2, & x \in D_-, \end{cases} \tag{A4}$$

a_+^2 and a_-^2 being constants. At the interface S the natural modes $f_k(x)$ obey the dielectriclike conditions

$$f_{k+}(x) = f_{k-}(x),$$

$$\lambda_+ \frac{\partial f_{k+}(x)}{\partial n_+(x)} + \lambda_- \frac{\partial f_{k-}(x)}{\partial n_-(x)} = 0,$$

$$x \in S. \tag{A5}$$

Here we are using the same notations as in Eqs. (3.1)–(3.4).

Since the outer region D_- is not bounded the spectrum ω_k is continuous. For example, we can assume that at the spatial infinity $|\mathbf{x}| \to \infty$ the natural modes $f_k(x)$ satisfy the scattering problem conditions and decrease sufficiently fast. The explicit form of these conditions will not be needed below.

The differential operator in Eq. (A3) apparently coincides with its adjoint

$$[-a^2(x)\Delta]\dagger = \begin{cases} -a_+^2\Delta, & x \in D_+, \\ -a_-^2\Delta, & x \in D_-. \end{cases} \tag{A6}$$

The boundary value problem with the operator $-a^2(x)\Delta$ will be self-adjoint when the integral for two sufficiently smooth functions $u(x)$ and $v(x)$,

$$I = \int_{D_+ \cup D_-} \mathrm{d}x\, a^2(x)(v\Delta u - u\Delta v) \tag{A7}$$

vanishes. Applying the Green integral formula for the domains D_+ and D_- separately we obtain

$$I = \int_S \mathrm{d}S \left[a_+^2 \left(u_+ \frac{\partial v_+}{\partial n_+} - v_+ \frac{\partial u_+}{\partial n_+} \right) + a_-^2 \left(u_- \frac{\partial v_-}{\partial n_-} - v_- \frac{\partial u_-}{\partial n_-} \right) \right]. \tag{A8}$$

The functions $u(x)$ and $v(x)$ are assumed to diminish at the infinity in such a way that the region $|\mathbf{x}| \to \infty$ does not contribute to the integral (A8). The integral I is equal to zero, for example, for the following conditions at the interface S:

$$u_+(x) = u_-(x),$$

$$a_+^2 \frac{\partial u_+(x)}{\partial n_+(x)} + a_-^2 \frac{\partial u_-(x)}{\partial n_-(x)} = 0, \quad x \in S. \tag{A9}$$

The function $v(x)$ should satisfy the same boundary conditions on S. Thus the dielectriclike conditions (A5) lead to self-adjoint boundary value problem if

$$\frac{\lambda_+}{a_+^2} = \frac{\lambda_-}{a_-^2}.$$

Of course, conditions (A9) do not exhaust all the cases when the boundary value problem under consideration is self-adjoint. Let the surface S divides the same medium into the domains D_+ and D_-, i.e., $a_+^2 = a_-^2$. We get the self-adjoint spectral problem if we impose at the interface S the following gluing conditions:

$$lu_+(x) = l^{-1}u_-(x),$$

$$l^{-1}\frac{\partial u_+(x)}{\partial n_+(x)} + l\frac{\partial u_-(x)}{\partial n_-(x)} = 0, \quad x \in S, \tag{A10}$$

where l is a dimensionless constant. The one-dimensional version of this problem has been considered in Sec. V.

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Universality in a class of Q-ball solutions: An analytic approach

T. A. Ioannidou[a)]
Mathematics Division, School of Technology, University of Thessaloniki, Thessaloniki 54124, Greece

A. Kouiroukidis[b)] and N. D. Vlachos[c)]
Physics Department, University of Thessaloniki, Thessaloniki 54124, Greece

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The properties of Q-balls in the general case of a sixth order potential have been studied using analytic methods. In particular, for a given potential, the initial field value that leads to the soliton solution has been derived and the corresponding energy and charge have been explicitly evaluated. The proposed scheme is found to work reasonably well for all allowed values of the model parameters. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1851972]

I. INTRODUCTION

A scalar field theory with a spontaneously broken U(1) symmetry may contain stable nontopological solitons, the so-called Q-balls.[1,2] Q-balls are coherent states of complex scalar fields that carry a global U(1) charge and can be understood as bound states of scalar particles which appear as stable classical solutions carrying a rotating time dependent internal phase. They are characterized by a conserved nontopological charge Q (Noether charge) that ensures existence and stability.[3,4]

The concepts associated with these solutions are quite general and occur in a wide variety of physical contexts.[5] Q-balls are allowed in supersymmetric extensions of the standard model that allow flat directions in the scalar potential. Flat directions in the minimal supersymmetric standard model (MSSM)[6] have been shown to exist. The conserved charge is associated with the U(1) symmetries of baryons and leptons, while, the relevant U(1) fields correspond to either squark or slepton particles. Thus, Q-balls can be thought of as condensates of a large number of either squark or slepton particles which can affect baryogenesis via the Affleck–Dine mechanism[7] during the post-inflationary period of the early universe. The Q-ball stability is cosmologically important since if stable Q-balls are formed in the early universe they can contribute to its dark matter content. These can be huge balls with charges of order 10^{20}; however, very small Q-balls can also be considered as dark matter constituents.[8] Decaying Q-balls can also be of crucial cosmological significance. If Q-balls decay after the electroweak phase transition, they can protect baryons from the erasure of baryon number due to sphaleron transitions. Furthermore, the Q-ball decay may contribute to dark matter production in the form of the lightest supersymmetric particle, explaining the baryon to dark matter ratio of the universe.[9]

Consider the U(1) Goldstone model Lagrangian describing a single complex scalar field ϕ in three spatial dimensions given by

[a)]Electronic mail: ti3@gen.auth.gr
[b)]Electronic mail: kouirouki@astro.auth.gr
[c)]Electronic mail: vlachos@physics.auth.gr

$$\mathcal{L} = \tfrac{1}{2}\partial_\mu \phi \partial^\mu \overline{\phi} - \mathrm{U}(|\phi|). \tag{1}$$

$\mathrm{U}(|\phi|)$ has a single minimum at $\phi=0$ which is equivalent of stating that there is a sector of scalar particles (mesons) carrying U(1) charge with mass equal to $\sqrt{\frac{1}{2}\mathrm{U}''(0)}$. The corresponding energy functional is given by

$$E = \int \left(\frac{1}{2}|\dot{\phi}|^2 + \frac{1}{2}|\nabla \phi|^2 + \mathrm{U}(|\phi|) \right) \mathrm{d}^3x \tag{2}$$

while the conserved Noether current [due to the global U(1) symmetry] is

$$J_\mu = \frac{1}{2i}(\overline{\phi}\partial_\mu \phi - \phi \partial_\mu \overline{\phi}) \tag{3}$$

with charge given by

$$Q = \frac{1}{2i} \int (\overline{\phi}\partial_t \phi - \phi \partial_t \overline{\phi}) \mathrm{d}^3x. \tag{4}$$

The stationary Q-ball solution can be obtained by assuming that

$$\phi = e^{i\omega t} f(r), \tag{5}$$

where $f(r)$ is a real radial profile function that satisfies the ordinary differential equation,

$$\frac{\mathrm{d}^2 f}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}f}{\mathrm{d}r} = -\omega^2 f + \mathrm{U}'(f), \tag{6}$$

with boundary conditions $f(\infty)=0$ and $f'(0)=0$. In each case, the effective potential is defined as $\mathrm{U}_{\mathrm{eff}}(f) = \omega^2 f^2/2 - \mathrm{U}(f)$, while, the existence of Q-ball solutions leads to constraints on the potential $\mathrm{U}(f)$ and the frequency ω, (i) the effective mass of f must be negative, so, by assuming that $\mathrm{U}(0)=\mathrm{U}'(0)=0$ and $\mathrm{U}''(0)=\omega_+^2>0$ one can deduce that $\omega<\omega_+$. (ii) The minimum of $\mathrm{U}(f)/f^2$ must be attained at some positive value of f (say $0<f_0<\infty$) and existence of the solution requires that $\omega>\omega_-$ where $\omega_-^2 = 2\mathrm{U}(f_0)/f_0^2$. Hence, Q-balls exist for all ω in the range $\omega_- < |\omega| < \omega_+$.

The charge (4) and energy (2) of a stationary Q-ball solution (5) take the simple form

$$Q = 4\pi\omega \int r^2 f^2(r) \mathrm{d}r, \tag{7}$$

$$E = \frac{1}{2}\omega^2 Q^2 + 4\pi \int \left(\frac{f'^2}{2} + \mathrm{U}(f) \right) r^2 \mathrm{d}r. \tag{8}$$

Numerical and analytical methods have shown that when the internal frequency is close to the minimal value ω_- the profile function is almost constant, implying that the charge (7) is large (thin-wall approximation). On the other hand, when the internal frequency approaches the maximal value ω_+ the profile function falls off very quickly (thick-wall approximation). In the thick-wall approximation the behavior of Q depends on the particular form of the potential and the number of dimensions.[10]

The choice of the potential is not unique since the only requirement is that the ratio $\mathrm{U}(f)/f^2$ has a local minimum at some value of f different from zero. There are several natural types to be considered, two of which are shown below,

$$\text{(I)} \quad U(f) = \frac{m_1^2}{2} f^2 - \lambda_1 f^4 + \mu_1 f^6,$$

$$\text{(II)} \quad U(f) = m_3 f^2 (1 - K \log(\lambda_3 f^2)) + \mu_3 f^{2p}. \tag{9}$$

In each case, two of the parameters can be removed by rescaling, thus, the potentials of type I have one free parameter while potentials of type II have two for fixed p. The type I potential is the simplest allowed one which is a polynomial in f^2, while type II mimics the D-flat direction in MSSM. Here, $p \geqslant 6$ is some integer that ensures the growth of the potential for large f, but does not destroy the flatness property for intermediate values of f. None of these types are the kind which might be associated with a renormalizable quantum field theory, but, they are typical of effective theories incorporating radiative or finite temperature corrections to a bare potential. In this paper, we shall be dealing with type I potentials only, for which $\omega_+ = m_1$ and $\omega_- = \sqrt{(2m_1^2\mu_1 - \lambda_1^2)/2\mu_1}$. Stable Q-balls exist for $\sqrt{(2m_1^2\mu_1 - \lambda^2)/2\mu_1} < \omega < m_1$. The equation of motion (6) is

$$\frac{d^2 f}{dr^2} + \frac{2}{r}\frac{df}{dr} = \alpha^2 f - 4\lambda_1 f^3 + 6\mu_1 f^5, \tag{10}$$

where we have defined $\alpha^2 = m_1^2 - \omega^2$.

Q-balls can be studied either analytically,[1,10,11] or numerically.[3–10,12–14] In a recent work,[15,16] we employed analytic arguments in order to construct an approximate profile function of the symmetrized Woods–Saxon type, expected to be valid in the thin-wall limit. This approximate profile led to an explicit energy-charge relation which, to our surprise, was found to yield valid results for a region far exceeding the expected limits of the thin-wall approximation. The calculation was carried out for a specific form of type I potential, i.e., $\lambda_1 = 2$, $\mu_1 = 1$, and $m = 2$. In this paper, the aforementioned work is being extended to include the general case of type I potentials (where the parameters are taken to be arbitrary) in *both* regimes, thin-wall and thick-wall, respectively. This way, the soliton energy and charge as well as the initial field value $f(0)$ can be accurately derived as functions of α for the whole allowed range of the model parameters.

II. POTENTIAL ENERGY

From a mechanical point of view, a Q-ball solution describes the motion of a particle moving with friction in the potential

$$U_{\text{eff}}(f) = -\tfrac{1}{2}\alpha^2 f^2 + \lambda_1 f^4 - \mu_1 f^6, \quad \lambda_1, \mu_1 > 0. \tag{11}$$

The corresponding equation of motion is given by (10). Upon rescaling $r \to r/\alpha$ and letting $f(r) = f(0)\psi(ar)$ for $\psi(0) = 1$, Eq. (10) transforms to

$$\frac{d^2\psi}{dr^2} + \frac{2}{r}\frac{d\psi}{dr} = \psi - 4\lambda\psi^3 + 6\mu\psi^5, \tag{12}$$

where $\lambda = \lambda_1 f(0)^2/\alpha^2$ and $\mu = \mu_1 f(0)^4/\alpha^2$ and the effective potential (11) becomes

$$U(\psi) = -\tfrac{1}{2}\psi^2 + \lambda\psi^4 - \mu\psi^6. \tag{13}$$

After some algebra, it can be shown that Eq. (12) implies that

$$\int_0^\infty r^{n-1}\left(\frac{d\psi}{dr}\right)^2 dr = \frac{2n}{4-n}\int_0^\infty r^{n-1}\left(-\frac{1}{2}\psi^2 + \lambda\psi^4 - \mu\psi^6\right)dr, \quad n \neq 0. \tag{14}$$

For the special cases $n = 3$ and $n = 0$, we get that

$$\frac{1}{2}\int_0^\infty r^2\left(\frac{\mathrm{d}\psi}{\mathrm{d}r}\right)^2 \mathrm{d}r = 3\int_0^\infty r^2\left(-\frac{1}{2}\psi^2 + \lambda\psi^4 - \mu\psi^6\right)\mathrm{d}r, \tag{15}$$

$$2\int_0^\infty r^{-1}\left(\frac{\mathrm{d}\psi}{\mathrm{d}r}\right)^2 \mathrm{d}r = -\frac{1}{2}\psi(0)^2 + \lambda\psi(0)^4 - \mu\psi(0)^6 \equiv \mathrm{U}(1). \tag{16}$$

The first condition is Derrick's (or virial) theorem which states that, for a three-dimensional model, the kinetic energy equals three times the potential energy; the second condition describes the energy dissipation of the mechanical system.

The mechanical analogue imposes several constraints on U(1). Consider a particle initially located at the point $\psi(0)=1$ which starts rolling down the potential wall to eventually stop at the point $\psi(\infty)=0$. (Here r corresponds to the time variable). Then, the potential energy (13) at the origin $\mathrm{U}(1)=-\frac{1}{2}+\lambda-\mu$ must be consumed by the friction term $(2/r)(\mathrm{d}\psi/\mathrm{d}r)$, therefore U(1) must be bounded both from below and above, since for U(1) large the particle will overshoot the top point while for U(1) small it will not reach it.

The initial potential energy U(1) must be positive implying that

$$\mu \leqslant \lambda - \tfrac{1}{2} \tag{17}$$

and, also, $\mathrm{U}'(1)$ must be positive (attractive "force") leading to

$$\mu \leqslant \tfrac{1}{6}(4\lambda - 1). \tag{18}$$

These conditions are satisfied for $\lambda > 1$ when (18) holds while for $1/2 < \lambda < 1$ when (17) holds. Note that for $\lambda < 1$ no Q-ball solutions can be found. Depending on the shape of the potential (i.e., the actual values of λ and μ) the following two distinct cases occur.

(I) *Thin-wall approximation:* In this case, $\psi(0)$ lies near the maximum of the effective potential which is deep. Then $\mathrm{U}'(1)=-1+4\lambda-6\mu\approx 0$ must be positive and close to zero (slow roll) while $\mathrm{U}''(1)$ is negative (convex region) and of order unity. The Q-ball solutions lie approximately on the line

$$\mu = \tfrac{1}{6}(4\lambda - 1) \tag{19}$$

and the initial potential energy depends linearly on λ,

$$\mathrm{U}(1) = \tfrac{1}{3}(\lambda - 1), \quad \lambda > 1. \tag{20}$$

(II) *Thick-wall approximation:* Here, the potential is shallow and the maxima are high up while $\mathrm{U}''(1)$ is positive and large (concave region) and μ is small. The initial potential energy U(1) increases with λ and reaches its maximal value when $\mu \to 0$. This value can be determined numerically and is found to be $\lambda_{\max} \simeq 4.701\,37$. The actual functional dependence of U(1) on λ however, is unknown and needs to be determined.

To that end, let us assume a leading power law behavior

$$\mathrm{U}(1) = \kappa\lambda^n. \tag{21}$$

Then, (13) implies that the Q-ball solutions lie on the line

$$\mu = -\tfrac{1}{2} + \lambda - \kappa\lambda^n \tag{22}$$

which determines κ in terms of $\lambda_{\max}$ [since $\mu(\lambda_{\max})=0$],

$$\kappa = \frac{2\lambda_{\max} - 1}{2\lambda_{\max}^n}. \tag{23}$$

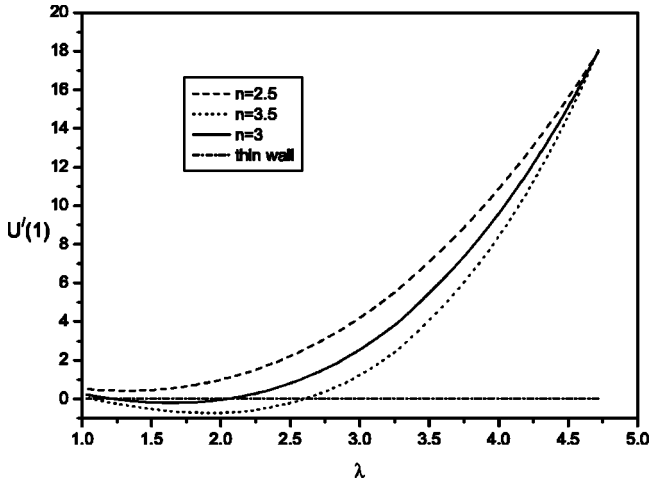

FIG. 1. The potential energy gradient in terms of λ for different values of n.

In order to determine the value of n in (21), we require that the transition from the thick-wall region to the thin-wall one be smooth implying that, $U'(1)$ is small for small values of λ ($\simeq 1$), i.e.,

$$U'(1) = 2(1-\lambda) + 6\kappa\lambda^n \approx 0. \tag{24}$$

Its minimum value occurs at the point $\lambda_{\min} = (3n\kappa)^{1/(1-n)}$. Substituting $\lambda_{\min}$ in (24) one gets that $U'(1)$ vanishes for $n = 2.821\,87$ in which case $\lambda_{\min} = 1.548\,89$ (in agreement to our hypothesis). Assuming that n can only take integer or half-integer values (otherwise the structure of the model on the complex plane would be very complicated), Fig. 1 shows that for $n=3$, the transition is indeed satisfactorily smooth. For this case, we get that $\kappa = 1/24.75$. This way, we get the $\mu(\lambda)$ relation for the thin-wall (19) and thick-wall (22) limits depicted in Fig. 2 against numerical data.

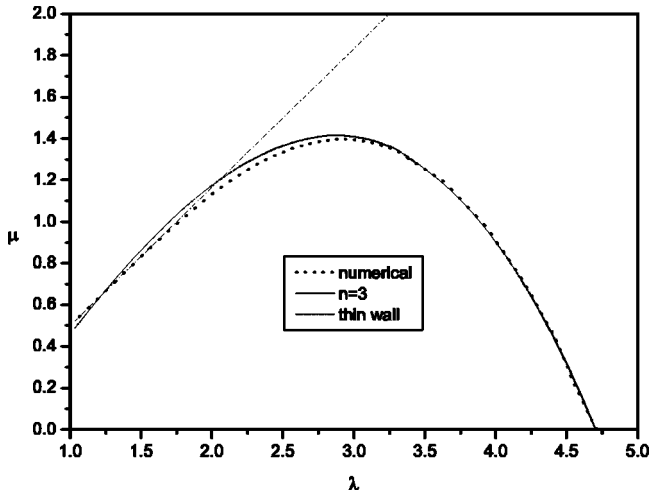

FIG. 2. The $\mu(\lambda)$ relation for $n=3$ against numerical data.

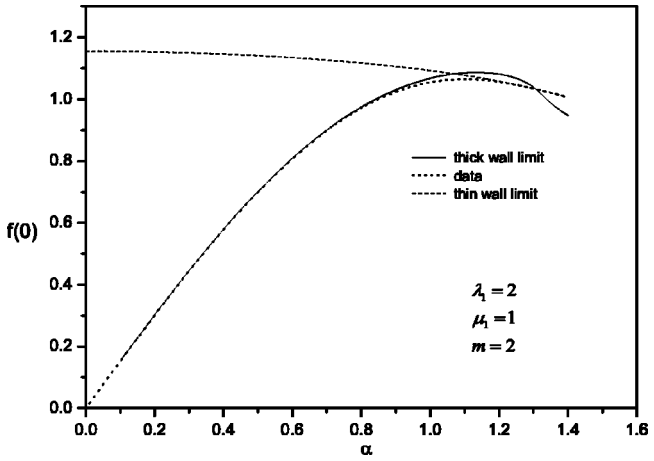

FIG. 3. Predicted initial field values $f(0)$ against numerical data.

III. PROPERTIES OF Q-BALLS

Using the rescaling formulas of the preceding section, the α dependence of the functions E, Q, and $f(0)$ can now be analytically determined. The initial field value $f(0)$ that leads to a Q-ball solution is given by

$$f(0) = \alpha\sqrt{\frac{\lambda}{\lambda_1}}, \quad \alpha = \sqrt{\frac{\mu}{\mu_1}}\frac{\lambda_1}{\lambda}. \tag{25}$$

Figure 3 depicts predicted values of $f(0)$ in terms of α against numerically calculated ones for sample values $\lambda_1=2$, $\mu_1=1$, $m=2$ (as in Ref. 16).

The corresponding charge (7) and energy (8) functionals are given by

$$Q = \frac{4\pi\omega}{\alpha}\frac{\lambda}{\lambda_1}\int_0^\infty \psi^2 r^2\,\mathrm{d}r, \tag{26}$$

$$E = \frac{\alpha^2+2\omega^2}{2\omega}Q + 4\pi\alpha\frac{\lambda}{\lambda_1}\int_0^\infty \left(\frac{1}{2}\psi'^2 - \lambda\psi^4 + \mu\psi^6\right)r^2\,\mathrm{d}r. \tag{27}$$

It was shown in Ref. 16 that a trial function satisfying the boundary conditions and having the right asymptotic behavior, is the symmetrized Woods–Saxon profile

$$\phi(r) = \frac{c}{\sqrt{1+c_1\cosh(br)}}. \tag{28}$$

This function satisfies the exact differential equation

$$\phi'' = \frac{b^2}{4}\phi - \frac{b^2}{c^2}\phi^3 + \frac{3}{4}\frac{b^2}{c^4}(1-c_1^2)\phi^5 \tag{29}$$

and the approximate one

$$\phi'' + \frac{2}{r}\phi' = \frac{b^2}{4}\left(1-\frac{4}{br}\right)\phi - \frac{b^2}{c^2}\left(1-\frac{1}{br}\right)\phi^3 + \frac{3b^2}{4c^4}\left((1-c_1^2)+\frac{2}{3}\frac{c_1^2}{br}\right)\phi^5 + O(\phi^7). \tag{30}$$

Here, c, c_1, and b are arbitrary parameters which need to be determined in order that (28) fits the exact profile function $\psi(r)$ in the best possible way. Note that only two of the three parameters in

(28) are independent since the initial condition $\phi(0)=1$ implies that $c=\sqrt{1+c_1}$.

First note that (28) satisfies the following relations:

$$\phi'^2=\frac{b^2}{4}\phi^2-\frac{1}{2}\frac{b^2}{c^2}\phi^4+\frac{1}{4}\frac{b^2}{c^4}(1-c_1^2)\phi^6,$$

$$\phi^4=c^2\phi^2+c^2c_1\frac{\mathrm{d}}{\mathrm{d}c_1}\phi^2, \tag{31}$$

$$\phi^6=c^4\phi^2+2c^4c_1\frac{\mathrm{d}}{\mathrm{d}c_1}\phi^2+\frac{1}{2}c^4c_1^2\frac{\mathrm{d}^2}{\mathrm{d}c_1^2}\phi^2,$$

in terms of which the charge (26) and energy (27) functionals can be explicitly evaluated,

$$Q=\frac{4\pi\omega}{\alpha}\frac{\lambda}{\lambda_1}\frac{c^2}{3b^3}i_0, \tag{32}$$

$$E=4\pi\frac{c^2}{3b^3}\sqrt{\frac{\mu}{\mu_1}}\left\{\left(\frac{(m^2+\omega^2)}{2\alpha}\frac{\lambda}{\lambda_1}\sqrt{\frac{\mu_1}{\mu}}+\mu c^4-\lambda c^2-\frac{1}{8}b^2c_1^2\right)i_0+\left(2\mu c^4-\lambda c^2-\frac{1}{4}b^2c_1^2\right)c_1\frac{\mathrm{d}i_0}{\mathrm{d}c_1}\right.$$
$$\left.+\frac{1}{2}\left(\mu c^4+\frac{1}{8}b^2(1-c_1^2)\right)c_1^2\frac{\mathrm{d}^2i_0}{\mathrm{d}c_1^2}\right\}. \tag{33}$$

Here i_0 is a function of c_1 given by

$$i_0(c_1)=\frac{1}{\sqrt{1-c_1^2}}\operatorname{arccosh}\left(\frac{1}{c_1}\right)\left[\pi^2+\operatorname{arccosh}\left(\frac{1}{c_1}\right)^2\right],\quad \text{for } c_1<1. \tag{34}$$

Note that λ_1, μ_1, m are fixed external parameters, λ varies continuously between 1 and 4.701 37 and μ is a known function of λ given by (19) and (22) depending on the regime.

The profile parameters b and c_1 can be determined by imposing the conditions (15) and (16) on $\phi(r)$, that is

$$\frac{1}{2}b^2c_1^2c^2\int_0^\infty\frac{\mathrm{d}r}{r}\frac{\sinh^2 r}{(1+c_1\cosh r)^3}=\mathrm{U}(1), \tag{35}$$

$$\left(\frac{1}{2}-\lambda c^2+\mu c^4-\frac{b^2c_1^2}{24}\right)i_0+\left(2\mu c^4-\frac{b^2c_1^2}{12}-\lambda c^2\right)c_1\frac{\mathrm{d}i_0}{\mathrm{d}c_1}+\frac{c_1^2}{2}\left(\mu c^4+\frac{b^2}{24}(1-c_1^2)\right)\frac{\mathrm{d}^2i_0}{\mathrm{d}c_1^2}=0. \tag{36}$$

Equation (35) can be written in a compact form

$$b=\frac{1}{c_1c}\sqrt{\frac{2\mathrm{U}(1)}{i_1}}, \tag{37}$$

where

$$i_1=\int_0^\infty\frac{\mathrm{d}r}{r}\frac{\sinh^2 r}{(1+c_1\cosh r)^3} \tag{38}$$

in terms of which (36) becomes

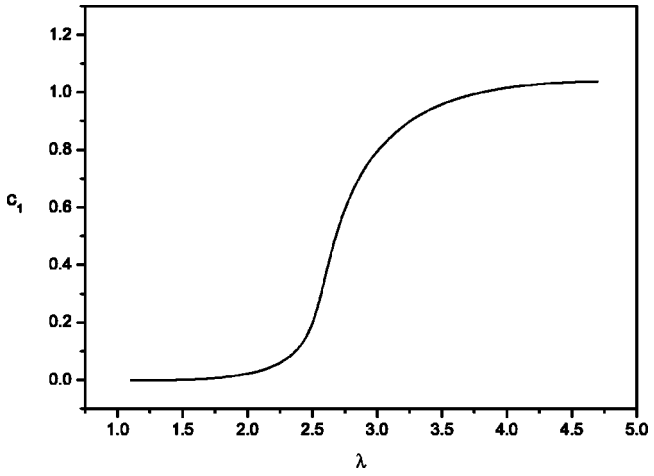

FIG. 4. The $c_1(\lambda)$ relation obtained from (39).

$$\left(\frac{1}{2}-\lambda c^2+\mu c^4-\frac{1}{12c^2}\frac{\mathrm{U}(1)}{i_1}\right)i_0+\left(2\mu c^4-\frac{1}{6c^2}\frac{\mathrm{U}(1)}{i_1}-\lambda c^2\right)c_1\frac{\mathrm{d}i_0}{\mathrm{d}c_1}+\frac{c_1^2}{2}\left(\mu c^4+\frac{(1-c_1^2)}{12c_1^2c^2}\frac{\mathrm{U}(1)}{i_1}\right)\frac{\mathrm{d}^2 i_0}{\mathrm{d}c_1^2}=0. \tag{39}$$

Equation (39) determines c_1 in terms of λ and is depicted in Fig. 4. Note that the values of c_1 and b obtained this way are universal since they do not depend on the geometrical parameters of the potential. Nevertheless, the values of the energy and charge do depend on the specific form of the potential, i.e., the values of λ_1, μ_1, and m. These values tend to infinity in both limits since (i) in the thin-wall limit $c_1\to 0$ while (ii) in the thick-wall limit $\alpha\to 0$.

Figures 5 and 6 present the α dependence of the charge (32) and energy (33) against values obtained numerically, for $\lambda_1=2$, $\mu_1=1$, $m=2$. It is interesting to realize that the range of validity of the thick-wall approximation is very wide and gives satisfactory results even in the thin-wall region. It appears that in this class of theories the Q-balls prefer to be "thick."

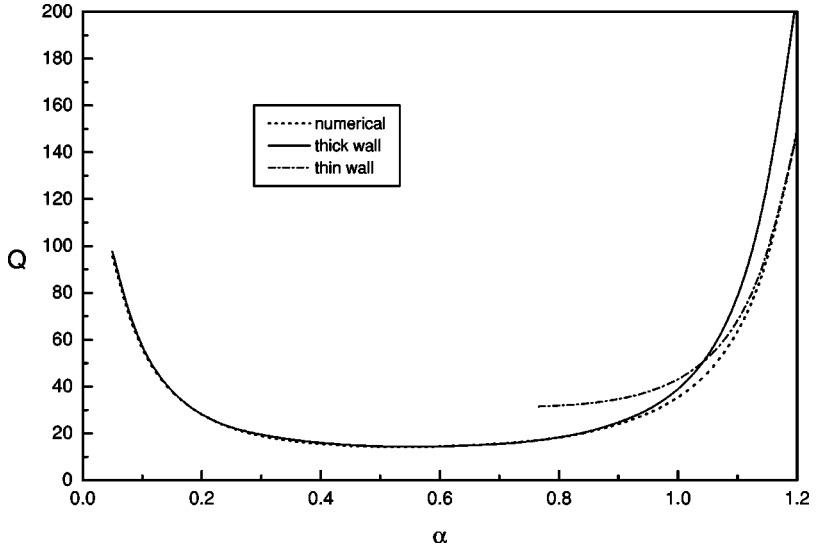

FIG. 5. The α dependence of Q given by (32).

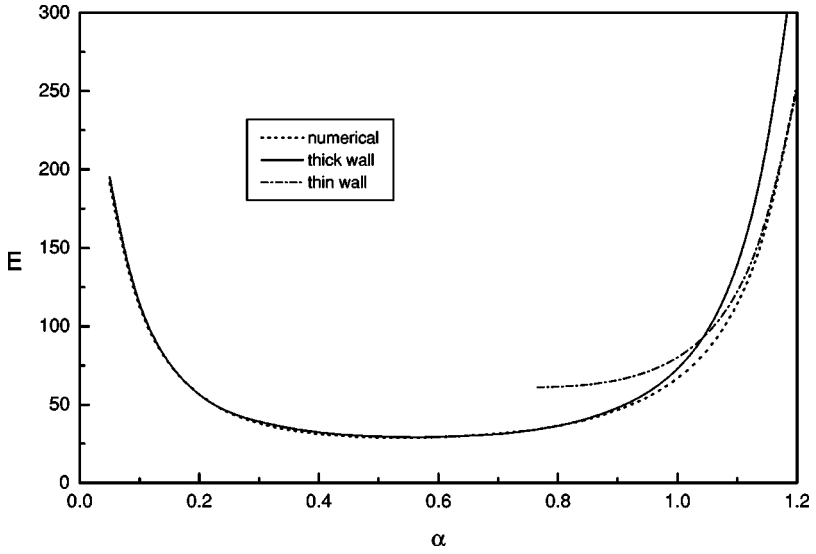

FIG. 6. The α dependence of E given by (33).

IV. CONCLUSIONS

In this paper we have extended our earlier work[16] and investigated phenomenologically relevant properties of Q-balls in a universal way. In particular, we have addressed the following problem: Given the geometrical characteristics of the scalar potential find the initial field value that will lead to a Q-ball solution as well as the corresponding charge and energy of the soliton. For a particular class of potentials (sixth order polynomials), after parameter rescaling, the problem can be tackled in a universal way. The Q-ball profile can be accurately approximated by means of a two-parameter symmetrized Woods–Saxon function which can be analytically calculated in all cases. This scheme is found to yield satisfactory results in the whole parameter region so that we do not have to rely on approximations like thin-wall or thick-wall. The soliton energy and charge can subsequently be analytically calculated and compared against numerically calculated values taken from an earlier work.[15]

We believe that a similar line of argument can be applied to study the profile function and the energy-charge dependence in all types of potentials.

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Relation between generalized Bogoliubov and Bogoliubov–de Gennes approaches including Nambu–Goldstone mode

M. Mine[a)]
Department of Physics, Waseda University, Tokyo 169-8555, Japan

M. Okumura[b)]
Department of Applied Physics, Waseda University, Tokyo 169-8555, Japan

Y. Yamanaka[c)]
Department of Materials Science and Engineering, Waseda University, Tokyo 169-8555, Japan

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The two approaches of consistent quantum field theory for systems of the trapped Bose–Einstein condensates are known, one is the Bogoliubov–de Gennes approach and the other is the generalized Bogoliubov approach. In this paper, we investigate the relation between the two approaches and show that they are formally equivalent to each other. To do this one must carefully treat the Nambu–Goldstone mode which plays a crucial role in the condensation. It is emphasized that the choice of vacuum is physically relevant. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1865322]

I. INTRODUCTION

The Bose–Einstein condensation is associated with the appearance of the Nambu–Goldstone (NG) mode[1] which is gapless. This is because the phenomenon is a manifestation of a spontaneous breakdown of a global phase (gauge) symmetry in quantum field theory (QFT) and then the Goldstone theorem requires that there must be a gapless mode. The NG mode plays a crucial role in creating and maintaining an ordered state such as the Bose–Einstein condensate (BEC).

For systems of the trapped BECs,[2–4] there are two approaches in QFT involving the NG mode explicitly. They are called the Bogoliubov–de Gennes (BdG)[5,6] and the generalized Bogoliubov (GB)[7,8] approaches. Both seem to offer consistent formulations in the sense that the canonical commutation relations are respected and that the unperturbed Hamiltonian is diagonalized. The purpose of this paper is to study the relation between them. We can prove that they are formally equivalent to each other, finding the explicit linear transformation in operators from one to the other. The treatment of the NG mode is subtle. We will clarify this point.

After the formal equivalence of the two approaches are established, we emphasize that the choice of vacuum is relevant physically while the choice of approach is not.

The paper is organized as follows. In Sec. II, the model action and Hamiltonian are given. An artificial breaking term is introduced there. Sections III and IV are devoted to reviews of the GB and BdG approaches, respectively. Section V is a central part of this paper, in which first the equivalence in the excitation modes is proved and then the correspondence between the NG modes in the two approaches is established. It will be found that the two sets of the NG modes are related through a squeezing transformation. In Sec. VI, we give a summary and discuss implications of

[a)]Electronic mail: mine@toki.waseda.jp
[b)]Electronic mail: okumura@aoni.waseda.jp
[c)]Electronic mail: yamanaka@waseda.jp

our conclusion. Finally we comment that the two different types of vacua lead to different observable results. In the Appendix, we give expressions for free propagators when the unperturbed vacuum associated with quantum coordinates is chosen.

II. MODEL ACTION AND HAMILTONIAN

We start with the following action to describe the trapped BEC of neutral atoms:

$$S = \int \mathrm{d}t\, \mathrm{d}^3x \left[\psi^\dagger(x)(T - K - V + \mu)\psi(x) - \frac{g}{2}\psi^\dagger(x)\psi^\dagger(x)\psi(x)\psi(x) \right], \tag{1}$$

where

$$T = i\frac{\partial}{\partial t}, \tag{2a}$$

$$K = -\frac{1}{2m}\nabla^2, \tag{2b}$$

$$V = \tfrac{1}{2}m\omega^2(x^2 + y^2 + z^2). \tag{2c}$$

with the chemical potential μ and the coupling constant g. Here we assumed for simplicity the isotropic trapping potential with its frequency ω, but the essences of the present paper are not lost even in anisotropic trapping potentials. Throughout this paper $\hbar$ is set to unity. This action is invariant under the global phase transformation,

$$\psi(x) \to e^{i\eta}\psi(x) \quad \text{and} \quad \psi^\dagger(x) \to e^{-i\eta}\psi^\dagger(x), \tag{3}$$

where η is an arbitrary constant phase.

When a continuous symmetry is broken spontaneously and the NG mode is present, one usually needs an artificial breaking interaction to control an infrared behavior of the system. In the system of the BEC, we add

$$\Delta S = \varepsilon\overline{\epsilon}\int \mathrm{d}t\, \mathrm{d}^3x [e^{-i\theta}v(\mathbf{x})\psi(x) + e^{i\theta}v(\mathbf{x})\psi^\dagger(x)] \tag{4}$$

to the original action (1),[8]

$$S_\varepsilon = S + \Delta S. \tag{5}$$

Here ε is an infinitesimal dimensionless parameter which is taken to be vanishing at the final stage of calculation, and $\overline{\epsilon}$ is a typical energy scale of the system given by ω. As we will see below, such a breaking term is necessary for the GB formalism, while it seems that the BdG formalism can be formulated without it.

Let us divide the original field $\psi(x)$ into the classical and quantum parts as

$$\psi(x) = e^{i\theta}v(\mathbf{x}) + e^{i\theta}\varphi(x), \tag{6}$$

where it is assumed that the c-number real function $v(\mathbf{x})$, whose square is a distribution function of condensed particle, is time independent, and that θ is real, time and space independent, corresponding to the situation without vortices. We factorize $e^{i\theta}$ in $\varphi(x)$ so that there appears no phase factor in the following formulations. Equation (6) is substituted into Eq. (5), which is rewritten in terms of $v(\mathbf{x})$ and $\varphi(x)$ as follows:

$$S_\varepsilon = S_0 + S_1 + S_2 + S_{3,4}, \tag{7}$$

where

$$S_0 = \int \mathrm{d}t\, \mathrm{d}^3x \left[v(\mathbf{x})(-K - V + \mu + 2\varepsilon\overline{\epsilon})v(\mathbf{x}) - \frac{g}{2}v^4(x) \right], \tag{8a}$$

$$S_1 = \int \mathrm{d}t\, \mathrm{d}^3x \{v(\mathbf{x})[-K - V + \mu - gv^2(\mathbf{x}) + \varepsilon\overline{\epsilon}]\varphi(x) + \varphi^\dagger(x)[-K - V + \mu - gv^2(\mathbf{x}) + \varepsilon\overline{\epsilon}]v(\mathbf{x})\}, \tag{8b}$$

$$S_2 = \int \mathrm{d}t\, \mathrm{d}^3x \left\{ \varphi^\dagger(x)[T - K - V + \mu]\varphi(x) - \frac{g}{2}v^2(\mathbf{x})[4\varphi^\dagger(x)\varphi(x) + \varphi^2(x) + \varphi^{\dagger 2}(x)] \right\}, \tag{8c}$$

$$S_{3,4} = \int \mathrm{d}t\, \mathrm{d}^3x \left\{ -gv(\mathbf{x})[\varphi^\dagger(x)\varphi^\dagger(x)\varphi(x) + \varphi^\dagger(x)\varphi(x)\varphi(x)] - \frac{g}{2}\varphi^\dagger(x)\varphi^\dagger(x)\varphi(x)\varphi(x) \right\}. \tag{8d}$$

At the tree level, the c-number function $v(\mathbf{x})$ satisfies

$$[K + V - \mu + gv^2(\mathbf{x}) - \varepsilon\overline{\epsilon}]v(\mathbf{x}) = 0, \tag{9}$$

which, at the limit of vanishing ε, is reduced to the Gross–Pitaevskii (GP) equation:[9]

$$[K + V - \mu + gv^2(\mathbf{x})]v(\mathbf{x}) = 0. \tag{10}$$

We rewrite $v(\mathbf{x})$ as

$$v(\mathbf{x}) = \sqrt{N_c} f_\varepsilon(\mathbf{x}), \tag{11}$$

since the condensate particle number N_c is given by

$$N_c = \int \mathrm{d}^3x\, v^2(\mathbf{x}), \tag{12}$$

and $f_\varepsilon(\mathbf{x})$ can be normalized to unity,

$$\int \mathrm{d}^3x\, f_\varepsilon^2(\mathbf{x}) = 1. \tag{13}$$

The suffix ε in $f_\varepsilon(\mathbf{x})$ is put to remind us that it is ε-dependent, which will be relevant in later sections.

The total Hamiltonian of the system is now written as

$$\hat{H} = \hat{H}_0 + \hat{H}_{\mathrm{int}}, \tag{14}$$

where

$$\hat{H}_0 = \int \mathrm{d}^3x \left\{ \hat{\varphi}^\dagger(x)(K + V - \mu)\hat{\varphi}(x) + \frac{gN_c}{2} f_\varepsilon^2(\mathbf{x})[4\hat{\varphi}^\dagger(x)\hat{\varphi}(x) + \hat{\varphi}^2(x) + \hat{\varphi}^{\dagger 2}(x)] \right\}, \tag{15}$$

$$H_{\mathrm{int}} = \int \mathrm{d}^3x \left\{ g\sqrt{N_c} f_\varepsilon(\mathbf{x})[\hat{\varphi}^\dagger(x)\hat{\varphi}^\dagger(x)\hat{\varphi}(x) + \hat{\varphi}^\dagger(x)\hat{\varphi}(x)\hat{\varphi}(x)] + \frac{g}{2}\hat{\varphi}^\dagger(x)\hat{\varphi}^\dagger(x)\hat{\varphi}(x)\hat{\varphi}(x) \right\}. \tag{16}$$

It is emphasized that the canonical commutation relations

$$[\hat{\varphi}(\mathbf{x},t), \hat{\varphi}^\dagger(\mathbf{x}',t)] = \delta^3(\mathbf{x} - \mathbf{x}') \tag{17}$$

and $[\hat{\varphi}(\mathbf{x},t), \hat{\varphi}(\mathbf{x}',t)] = [\hat{\varphi}^\dagger(\mathbf{x},t), \hat{\varphi}^\dagger(\mathbf{x}',t)] = 0$, must hold for consistent QFT.

III. GENERALIZED BOGOLIUBOV APPROACH

First let us review the GB approach, in which the field operator $\hat{\varphi}(x)$ and $\hat{\varphi}^\dagger(x)$ are expanded as

$$\hat{\varphi}(x) = \sum_{n=0}^{\infty} \hat{a}_n(t) w_n^{(\varepsilon)}(\mathbf{x}), \tag{18a}$$

$$\hat{\varphi}^\dagger(x) = \sum_{n=0}^{\infty} \hat{a}_n^\dagger(t) w_n^{(\varepsilon)}(\mathbf{x}), \tag{18b}$$

where the complete orthonormal set of real functions $\{w_n^{(\varepsilon)}(\mathbf{x})\}$,

$$\int \mathrm{d}^3x w_n^{(\varepsilon)}(\mathbf{x}) w_m^{(\varepsilon)}(\mathbf{x}) = \delta_{nm}, \tag{19}$$

$$\sum_{n=0}^{\infty} w_n^{(\varepsilon)}(\mathbf{x}) w_n^{(\varepsilon)}(\mathbf{x}') = \delta^3(\mathbf{x}-\mathbf{x}'), \tag{20}$$

is obtained from the following eigenequation:

$$(\mathcal{L}-\mathcal{M}) w_n^{(\varepsilon)}(\mathbf{x}) = (\epsilon_n + \varepsilon\overline{\epsilon}) w_n^{(\varepsilon)}(\mathbf{x}). \tag{21}$$

For later convenience, we have introduced the abbreviated notations of

$$\mathcal{L} = K + V - \mu + 2gN_c f_\varepsilon^2(\mathbf{x}), \tag{22a}$$

$$\mathcal{M} = gN_c f_\varepsilon^2(\mathbf{x}), \tag{22b}$$

and the index (ε) in $\{w_n^{(\varepsilon)}(\mathbf{x})\}$ indicates that they are ε-dependent, and $\{w_n^{(\varepsilon)}(\mathbf{x})\}$ are expanded as

$$w_n^{(\varepsilon)}(\mathbf{x}) = w_n^{(0)}(\mathbf{x}) + \varepsilon w_n^{(1)}(\mathbf{x}) + \cdots . \tag{23}$$

So in the limit $\varepsilon \to 0$, the functions $\{w_n^{(\varepsilon)}(\mathbf{x})\}$ reduce to $\{w_n^{(0)}(\mathbf{x})\}$, which are the solutions of the eigenequations

$$(\mathcal{L}-\mathcal{M}) w_n^{(0)}(\mathbf{x}) = \epsilon_n w_n^{(0)}(\mathbf{x}). \tag{24}$$

The eigenequation (21) with $n=0$ is identical with the (ε-modified) GP equation (9), and $w_0^{(\varepsilon)}(\mathbf{x})$ is nothing but $f_\varepsilon(\mathbf{x})$ defined in Eq. (11). Hereafter the index (ε) in $\{w^{(\varepsilon)}(\mathbf{x})\}$ is omitted otherwise mentioned.

For the operators $\hat{a}_n(t)$ and $\hat{a}_n^\dagger(t)$ the following commutation relations are assumed:

$$[\hat{a}_n(t), \hat{a}_m^\dagger(t)] = \delta_{nm} \tag{25}$$

and $[\hat{a}_n(t), \hat{a}_m(t)] = [\hat{a}_n^\dagger(t), \hat{a}_m^\dagger(t)] = 0$. Combining these with the completeness condition in Eq. (20), one can reproduce the canonical commutation relations of Eq. (17). In the formulation under the "Bogoliubov" approximation, meaning that the term $\hat{a}_0 w_n(\mathbf{x})$ is absent in the expansion of Eq. (18), the canonical commutation relations are violated as

$$[\hat{\varphi}(\mathbf{x},t), \hat{\varphi}^\dagger(\mathbf{x}',t)] = \delta^3(\mathbf{x}-\mathbf{x}') - w_0(\mathbf{x}) w_0(\mathbf{x}'). \tag{26}$$

Substituting Eq. (18) into Eq. (15), we rewrite $\hat{H}_0$ in terms of the $\hat{a}$-operators,

$$\hat{H}_0 = \sum_{n=0}^{\infty} \epsilon_n \hat{a}_n^\dagger \hat{a}_n + \sum_{n,m=0}^{\infty} [2\hat{a}_n^\dagger U_{nm} \hat{a}_m + \hat{a}_n U_{nm} \hat{a}_m + \hat{a}_n^\dagger U_{nm} \hat{a}_m^\dagger], \tag{27}$$

where

$$U_{nm} = \frac{gN_c}{2} \int \mathrm{d}^3x \, f_\varepsilon^2(\mathbf{x}) w_n(\mathbf{x}) w_m(\mathbf{x}). \tag{28}$$

This Hamiltonian can be diagonalized by introducing the generalized Bogoliubov transformation,

$$\hat{b}_n = \sum_{m=0}^{\infty} (C_{nm} \hat{a}_m + S_{nm} \hat{a}_m^\dagger), \tag{29a}$$

$$\hat{b}_n^\dagger = \sum_{m=0}^{\infty} (C_{nm} \hat{a}_m^\dagger + S_{nm} \hat{a}_m), \tag{29b}$$

and

$$\hat{H}_0 = \sum_{n=0}^{\infty} [E_{G,n} \hat{b}_n^\dagger \hat{b}_n + (\text{c-numbers})]. \tag{30}$$

Here the real matrices C and S in the matrix notation are given by

$$C = \tfrac{1}{2}(E_G^{1/2} \mathcal{O} \boldsymbol{\epsilon}^{-1/2} + E_G^{-1/2} \mathcal{O} \boldsymbol{\epsilon}^{1/2}), \tag{31a}$$

$$S = \tfrac{1}{2}(E_G^{1/2} \mathcal{O} \boldsymbol{\epsilon}^{-1/2} - E_G^{-1/2} \mathcal{O} \boldsymbol{\epsilon}^{1/2}), \tag{31b}$$

with

$$(E_G)_{nm} = E_{G,n} \delta_{nm}, \tag{32a}$$

$$(\boldsymbol{\epsilon})_{nm} = (\epsilon_n + \varepsilon \overline{\epsilon}) \delta_{nm}, \tag{32b}$$

and the orthogonal matrix $\mathcal{O}$ diagonalizes the real symmetric matrix W with eigenvalues of $E_{G,n}^2 (n = 0, 1, 2, \ldots)$,

$$\mathcal{O} W \mathcal{O}^T = E_G^2, \tag{33}$$

where

$$W = \begin{pmatrix} 4(\varepsilon \overline{\epsilon}) U_{00} + O(\varepsilon^2) & \sqrt{\varepsilon \overline{\epsilon}} u'^T + O(\varepsilon^{3/2}) \\ \sqrt{\varepsilon \overline{\epsilon}} u' + O(\varepsilon^{3/2}) & W' + O(\varepsilon) \end{pmatrix}, \tag{34}$$

with

$$u' = \begin{pmatrix} 4\sqrt{\epsilon_1} U_{10} \\ 4\sqrt{\epsilon_2} U_{20} \\ \vdots \end{pmatrix}, \tag{35a}$$

$$W'_{nm} = \epsilon_n^2 \delta_{nm} + 4\sqrt{\epsilon_n} U_{nm} \sqrt{\epsilon_m} \; (n, m = 1, 2, \ldots). \tag{35b}$$

We use the following notations for matrices such as A and A': A' stands for a matrix A_{nm} with $n, m = 1, 2, \ldots$ while A does for one with $n, m = 0, 1, 2, \ldots$. And we notice that when we investigate

the leading order behavior of ε, it does not matter if we use $\{w_n^{(0)}(\mathbf{x})\}$ for U_{nm} instead of $\{w_n^{(\varepsilon)}(\mathbf{x})\}$ [see Eq. (28)].

One can easily check the properties of C and S from Eq. (31),

$$\sum_{m=0}^{\infty}(C_{nm}C_{n'm}-S_{nm}S_{n'm})=\delta_{nn'}, \tag{36a}$$

$$\sum_{m=0}^{\infty}(C_{nm}S_{n'm}-S_{nm}C_{n'm})=0. \tag{36b}$$

The above expressions are expanded with respect to the infinitesimal parameter ε. We note that the zeroth eigenvalue,

$$E_{G,0}=\sqrt{\varepsilon\epsilon}\sqrt{\overline{E_0}}+O(\varepsilon^{3/2}), \tag{37a}$$

$$\overline{E_0}\equiv 4U_{00}-u'^{T}W'^{-1}u', \tag{37b}$$

approaches zero as it should be, but is kept nonvanishing due to ε, which enables us to diagonalize $\hat{H}_0$.

The matrix $\mathcal{O}$ is obtained explicitly as

$$\mathcal{O}=\begin{pmatrix}1-\frac{1}{2}(\varepsilon\overline{\epsilon})u'^{T}W'^{-2}u'+O(\varepsilon^2) & -\sqrt{\varepsilon\overline{\epsilon}}u'^{T}W'^{-1}\mathcal{O}'^{T}+O(\varepsilon^{3/2})\\ \sqrt{\varepsilon\overline{\epsilon}}\mathcal{O}'W'^{-1}u'+O(\varepsilon^{3/2}) & \mathcal{O}'+O(\varepsilon)\end{pmatrix}, \tag{38}$$

where $\mathcal{O}'$ is an orthogonal matrix diagonalizing the matrix W',

$$\mathcal{O}'W'\mathcal{O}'^{T}=E_G'^{2}, \tag{39}$$

with the diagonal matrix

$$(E_G'^{2})_{nm}=E_{G,n}^2\delta_{nm}+O(\varepsilon^{1/2})\quad(n,m=1,2,\dots). \tag{40}$$

Thus the mixing among $\hat{a}_n$ $(n=1,2,\dots)$ is regular with respect to ε, only the mixing between $\hat{a}_0$ and other $\hat{a}_n$'s gives rise to a singularity.

Thus the field operators in the GB approach are expanded in terms of $\hat{b}$-operators diagonalizing the unperturbed Hamiltonian as

$$\hat{\varphi}(\mathbf{x})=\sum_{n=0}^{\infty}[\hat{b}_n w_{Cn}(\mathbf{x})-\hat{b}_n^{\dagger}w_{Sn}(\mathbf{x})], \tag{41a}$$

$$\hat{\varphi}^{\dagger}(\mathbf{x})=\sum_{n=0}^{\infty}[\hat{b}_n^{\dagger}w_{Cn}(\mathbf{x})-\hat{b}_n w_{Sn}(x)] \tag{41b}$$

with

$$w_{Cn}(\mathbf{x})=\sum_{m=0}^{\infty}C_{nm}w_m(\mathbf{x}), \tag{42a}$$

$$w_{Sn}(\mathbf{x})=\sum_{m=0}^{\infty}S_{nm}w_m(\mathbf{x}). \tag{42b}$$

IV. BOGOLIUBOV–DE GENNES APPROACH

Next we review the BdG approach. The parameter ε is set to be zero throughout this section, so all the quantities are those of $\varepsilon=0$.

One sets up the coupled eigenequations,

$$\mathcal{L}u_n(\mathbf{x}) - \mathcal{M}v_n(\mathbf{x}) = E_{B,n}u_n(\mathbf{x}), \tag{43a}$$

$$\mathcal{L}v_n(\mathbf{x}) - \mathcal{M}u_n(\mathbf{x}) = -E_{B,n}v_n(\mathbf{x}), \tag{43b}$$

where the notations in Eq. (22) are used and we assume the functions $u_n(\mathbf{x})$ and $v_n(\mathbf{x})$ to be real. The orthonormal condition reads as

$$\int \mathrm{d}^3x[u_n(\mathbf{x})u_m(\mathbf{x}) - v_n(\mathbf{x})v_m(\mathbf{x})] = \delta_{nm}, \tag{44a}$$

$$\int \mathrm{d}^3x[u_n(\mathbf{x})v_m(\mathbf{x}) - v_n(\mathbf{x})u_m(\mathbf{x})] = 0. \tag{44b}$$

Several authors have already made remarks on states with zero eigenvalue for Eq. (43).[10–12] It is easy to see that $u_0(\mathbf{x})=v_0(\mathbf{x})=f(\mathbf{x})$ [the normalized solution of GP equation, see Eqs. (10) and (11)] are eigenfunctions with $E_B=0$. However, the set of $f(\mathbf{x})$ and $\{u_n(\mathbf{x}),v_n(\mathbf{x})\}$ with $E_{B,n}\neq 0$ is not complete. One needs one more state denoted by $h(\mathbf{x})$ for the completeness,[12] which is a solution of

$$(\mathcal{L}+\mathcal{M})h(\mathbf{x}) = \frac{1}{I}f(\mathbf{x}), \tag{45}$$

where I is a positive constant. The orthonormal properties are, in addition to Eqs. (13) and (44) for eigenfunctions of nonzero eigenvalues,

$$0 = \int \mathrm{d}^3x[\{u_n(\mathbf{x}) - v_n(\mathbf{x})\}f(\mathbf{x})], \tag{46a}$$

$$0 = \int \mathrm{d}^3x[\{u_n(\mathbf{x}) + v_n(\mathbf{x})\}h(\mathbf{x})], \tag{46b}$$

$$\tfrac{1}{2} = \int \mathrm{d}^3x\, f(\mathbf{x})h(\mathbf{x}). \tag{46c}$$

The last line fixes the value of I. The completeness condition now reads as

$$\sum_{n=1}^{\infty}[u_n(\mathbf{x})u_n(\mathbf{x}') - v_n(\mathbf{x})v_n(\mathbf{x}')] + [f(\mathbf{x})h(\mathbf{x}') + h(\mathbf{x})f(\mathbf{x}')] = \delta^3(\mathbf{x}-\mathbf{x}'), \tag{47a}$$

$$\sum_{n=1}^{\infty}[u_n(\mathbf{x})v_n(\mathbf{x}') - v_n(\mathbf{x})u_n(\mathbf{x}')] + [f(\mathbf{x})h(\mathbf{x}') - h(\mathbf{x})f(\mathbf{x}')] = 0. \tag{47b}$$

Consider the field operators. We introduce the oscillator-operators $\hat{\alpha}_n(t)=\hat{\alpha}_n e^{-iE_{B,n}t}$ and $\hat{\alpha}_n^{\dagger}(t) = \hat{\alpha}_n^{\dagger}e^{iE_{B,n}t}$ associated with $u_n(\mathbf{x})$ and $v_n(\mathbf{x})$, respectively, and also a set of canonical variables $\{\hat{\mathcal{Q}}(t),\hat{\mathcal{P}}(t)\}$ for $f(\mathbf{x})$ and $h(\mathbf{x})$,

$$[\hat{\alpha}_n, \hat{\alpha}_m^\dagger] = \delta_{nm}, \tag{48}$$

$$[\hat{\mathcal{Q}}(t), \hat{\mathcal{P}}(t)] = i, \tag{49}$$

and other vanishing commutation relations. Then the field operators are expanded as

$$\hat{\varphi}(x) = \hat{\mathcal{P}}(t)h(\mathbf{x}) - i\hat{\mathcal{Q}}(t)f(\mathbf{x}) + \sum_{n=1}^{\infty} [\hat{\alpha}_n(t)u_n(\mathbf{x}) - \hat{\alpha}_n^\dagger(t)v_n(\mathbf{x})], \tag{50a}$$

$$\hat{\varphi}^\dagger(x) = \hat{\mathcal{P}}(t)h(\mathbf{x}) + i\hat{\mathcal{Q}}(t)f(\mathbf{x}) + \sum_{n=1}^{\infty} [\hat{\alpha}_n^\dagger(t)u_n(\mathbf{x}) - \hat{\alpha}_n(t)v_n(\mathbf{x})]. \tag{50b}$$

It is easy to check that the canonical commutation relations are derived from these expressions and the completeness condition in Eq. (47). Also the substitution of Eq. (50) into the $\hat{H}_0$ in Eq. (15) leads to

$$\hat{H}_0 = \frac{\hat{\mathcal{P}}^2}{2I} + \sum_{n=1}^{\infty} [E_{B,n}\hat{\alpha}_n^\dagger\hat{\alpha}_n + (c\text{-numbers})], \tag{51}$$

where we have employed the orthonormal conditions, (13), (44), and (46). Important observations here are that the canonical commutation relations would be violated without introducing $h(\mathbf{x})$ and that we have the term $\hat{\mathcal{P}}^2/(2I)$ in the Hamiltonian as a result of the existence of the NG mode.

V. RELATION BETWEEN GENERALIZED BOGOLIUBOV AND BOGOLIUBOV–DE GENNES APPROACHES

We have reviewed the GB and BdG approaches in the preceding two sections. Both of them seem to be consistent canonical theories in which the NG mode is taken account of properly.

On the other hand, the two approaches follow different procedures. For example, one sees in the BdG approach the appearance of canonical variables $\hat{\mathcal{P}}$ and $\hat{\mathcal{Q}}$, while one does not in the GB approach. Furthermore, in the BdG approach one apparently sees no problem of infrared divergence associated with the NG modes, while one encounters it in the GB approach.

Then arises a natural question whether the two approaches are equivalent. In this section, we first show that these two approaches are equivalent in the excitation modes. After that, we find a correspondence in the zero-mode eigenspaces of the two approaches, investigating the functions $f(\mathbf{x})$ and $h(\mathbf{x})$ in the BdG approach in terms of $w_n(\mathbf{x})$ in the GB one. Then the limit of $\varepsilon \to 0$ in the GB approach must be taken carefully.

First, let us deal with the following simultaneous equations for excited states with $n \geqslant 1$, equivalent to Eq. (43),[13]

$$(\mathcal{L} - \mathcal{M})u_{+,n}(\mathbf{x}) = E_{B,n}u_{-,n}(\mathbf{x}), \tag{52a}$$

$$(\mathcal{L} + \mathcal{M})u_{-,n}(\mathbf{x}) = E_{B,n}u_{+,n}(\mathbf{x}), \tag{52b}$$

where

$$u_{\pm,n}(\mathbf{x}) = u_n(\mathbf{x}) \pm v_n(\mathbf{x}). \tag{53}$$

Then we have

$$(\mathcal{L} + \mathcal{M})(\mathcal{L} - \mathcal{M})u_{+,n}(\mathbf{x}) = E_{B,n}^2 u_{+,n}(\mathbf{x}) \tag{54a}$$

$$(\mathcal{L} - \mathcal{M})(\mathcal{L} + \mathcal{M})u_{-,n}(\mathbf{x}) = E_{B,n}^2 u_{-,n}(\mathbf{x}). \tag{54b}$$

Suppose that the eigenfunctions $u_{\pm,n}(\mathbf{x})$ $(n=1,2,\ldots)$ in the BdG approach can be expanded in terms of $w_n^{(\varepsilon)}(\mathbf{x})$ $(n=0,1,\ldots)$ in the GB approach,

$$u_{\pm,n}(\mathbf{x}) = \sum_{m=0}^{\infty} R_{\pm,nm} w_m^{(\varepsilon)}(\mathbf{x}). \tag{55}$$

Substitute Eq. (55) into Eq. (52), apply Eq. (21), multiply $w_{n'}^{(\varepsilon)}(\mathbf{x})$ from the left and integrate over $\mathbf{x}$, then we derive the matrix equations

$$R_+ \boldsymbol{\epsilon} = E_B R_-, \tag{56a}$$

$$R_-(\boldsymbol{\epsilon} + 4U) = E_B R_+, \tag{56b}$$

where the matrix notations are $(E_B)_{nm}=E_{B,nm}$ and $(U)_{nm}=U_{nm}$ in Eq. (28), and $(\boldsymbol{\epsilon})_{nm}$ is defined in Eq. (32). Remark that the indices of $(R_\pm)_{nm}$ run from $n=1$ and $m=0$. From these equations derive the equations,

$$R_+ \boldsymbol{\epsilon}(\boldsymbol{\epsilon} + 4U) = E_B^2 R_+, \tag{57a}$$

$$R_-(\boldsymbol{\epsilon} + 4U)\boldsymbol{\epsilon} = E_B^2 R_-. \tag{57b}$$

One can easily find the solutions for $R_\pm$ by using $\mathcal{O}$ satisfying Eq. (33), that is,

$$R_+ = H_+ \mathcal{O} \boldsymbol{\epsilon}^{-1/2}, \tag{58a}$$

$$R_- = H_- \mathcal{O} \boldsymbol{\epsilon}^{1/2}, \tag{58b}$$

where $H_\pm$ are arbitrary matrices $(n=1,2,\ldots;m=0,1,2,\ldots)$ whose off-diagonal elements are vanishing. In fact we have from Eqs. (31)–(33),

$$R_+ \boldsymbol{\epsilon}(\boldsymbol{\epsilon} + 4U) = E_G^2 R_+, \tag{59a}$$

$$R_-(\boldsymbol{\epsilon} + 4U)\boldsymbol{\epsilon} = E_G^2 R_-, \tag{59b}$$

where $(E_G')_{nm}=E_{G,n}\delta_{nm}$ $(n,m=1,2,\ldots)$. The comparison of Eqs. (57) and (59) clearly shows that the energy spectra E_B and E_G are identical for excited states, so let us denote them simply by E. If we take

$$H_+ = E^{1/2}, \tag{60a}$$

$$H_- = E^{-1/2}, \tag{60b}$$

we can find in the limit of $\varepsilon \to 0$ from arguments in Sec. IV that

$$u_n(\mathbf{x}) = w_{Cn}^{(0)}(\mathbf{x}), \tag{61a}$$

$$v_n(\mathbf{x}) = w_{Sn}^{(0)}(\mathbf{x}). \tag{61b}$$

Thus it has been proved that the two approaches are essentially equivalent to each other in the excited modes.

Next, in order to include the zero-mode eigenspace, we introduce a new function $h_\varepsilon(\mathbf{x})$, corresponding to Eq. (45), through the relation,

$$(\mathcal{L}+\mathcal{M})h_\varepsilon(\mathbf{x})=\frac{1}{I_\varepsilon}f_\varepsilon(\mathbf{x}). \tag{62}$$

Here $f_\varepsilon(\mathbf{x})$ is defined in Eq. (11) with Eq. (9), and the constant I_ε is determined from the condition

$$\frac{1}{2}=\int \mathrm{d}^3x\, f_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}). \tag{63}$$

It is clear from their definitions that the functions $f_\varepsilon(\mathbf{x})$ and $h_\varepsilon(\mathbf{x})$ and the constant I_ε reduce to $f(\mathbf{x})$, $h(\mathbf{x})$, and I, respectively, as ε goes to zero.

We attempt to expand $h_\varepsilon(\mathbf{x})$ in terms of $\{w_n^{(\varepsilon)}\}$,

$$h_\varepsilon(\mathbf{x})=\sum_{n=0}^{\infty}k_n w_n^{(\varepsilon)}(\mathbf{x}). \tag{64}$$

Remark that $w_0^{(\varepsilon)}(\mathbf{x})$ is included in this summation. Substitute this into Eq. (45),

$$(\mathcal{L}+\mathcal{M})h_\varepsilon(\mathbf{x})=\sum_{n=0}^{\infty}k_n[(\epsilon_n+\varepsilon\overline{\epsilon})+2\mathcal{M}]w_n^{(\varepsilon)}(\mathbf{x})=\frac{1}{I_\varepsilon}f_\varepsilon(\mathbf{x}), \tag{65}$$

and multiply it by $\int \mathrm{d}^3x\, w_m^{(\varepsilon)}(\mathbf{x})$, one obtains in the matrix notation

$$[\boldsymbol{\epsilon}+4U]k=\frac{1}{I_\varepsilon}e_0, \tag{66}$$

with $(e_0)_n=\delta_{0n}$ and $(k)_n=k_n$. We manipulate this as

$$[\boldsymbol{\epsilon}^2+4\boldsymbol{\epsilon}^{1/2}U\boldsymbol{\epsilon}^{1/2}]\boldsymbol{\epsilon}^{-1/2}k=W\boldsymbol{\epsilon}^{-1/2}k=\frac{1}{I_\varepsilon}\boldsymbol{\epsilon}^{1/2}e_0, \tag{67}$$

where W is defined in Eq. (34), and we have

$$k=\frac{1}{I_\varepsilon}\boldsymbol{\epsilon}^{1/2}W^{-1}\boldsymbol{\epsilon}^{1/2}e_0. \tag{68}$$

We remark that $(\boldsymbol{\epsilon})_{nm}$ should be interpreted not as $\epsilon_n\delta_{nm}$ but as $(\epsilon_n+\varepsilon\overline{\epsilon})\delta_{nm}$. Since $\mathcal{O}W^{-1}\mathcal{O}^T=E_G^{-2}$ from Eq. (33) and $C-S=E_G^{-1/2}\mathcal{O}\boldsymbol{\epsilon}^{1/2}$ from Eq. (31), Eq. (68) reduces to

$$k=\frac{1}{I_\varepsilon}(C-S)^TE_G^{-1}(C-S)e_0. \tag{69}$$

The behaviors of the matrices E_G^{-1}, $(C-S)$, and $(C+S)=E_G^{1/2}\mathcal{O}\boldsymbol{\epsilon}^{-1/2}$ with respect to ε can be estimated from Sec. III,

$$E_G^{-1}=\begin{pmatrix}O(\varepsilon^{-1/2}) & 0\\ 0 & O(\varepsilon^0)\end{pmatrix} \tag{70a}$$

$$C-S=\begin{pmatrix}O(\varepsilon^{1/4}) & O(\varepsilon^{1/4})\\ O(\varepsilon) & O(\varepsilon^0)\end{pmatrix} \tag{70b}$$

$$C+S=\begin{pmatrix}O(\varepsilon^{-1/4}) & O(\varepsilon^{3/4})\\ O(\varepsilon^0) & O(\varepsilon^0)\end{pmatrix}, \tag{70c}$$

where the first rows and columns correspond to $n=0$, and the second ones to $n=1,2,\ldots$. Therefore, up to the leading order of ε, we have after some manipulations

$$E_G^{-1}(C-S)e_0 = \overline{E_0}^{-3/4}(\varepsilon\overline{\epsilon})^{-1/4}e_0 + O(\varepsilon). \tag{71}$$

Recall the definition of Eq. (37) for $\overline{E_0}$ which is independent of ε. Finally k becomes

$$k = \frac{1}{I_\varepsilon}\overline{E_0}^{-3/4}(\varepsilon\overline{\epsilon})^{-1/4}(C-S)^T e_0 + O(\varepsilon), \tag{72}$$

implying that

$$\begin{aligned} h_\varepsilon(\mathbf{x}) &= \frac{1}{I_\varepsilon}(\overline{E_0})^{-3/4}(\varepsilon\overline{\epsilon})^{-1/4}(w_{C0}^{(\varepsilon)}(\mathbf{x}) - w_{S0}^{(\varepsilon)}(\mathbf{x})) + O(\varepsilon) \\ &= \frac{1}{I_\varepsilon}\overline{E_0}^{-1}\left[w_0^{(\varepsilon)}(\mathbf{x}) - \sum_{n=1}^{\infty}(u'^T W'^{-1})_n \epsilon_n^{1/2} w_n^{(\varepsilon)}(\mathbf{x}) \right] + O(\varepsilon^{1/2}). \end{aligned} \tag{73}$$

The constant I_ε can be evaluated from Eq. (73), Eq. (63), and $f_\varepsilon(\mathbf{x}) = w_0^{(\varepsilon)}(\mathbf{x})$,

$$I_\varepsilon = \frac{2}{\overline{E_0}} + O(\varepsilon^{1/2}). \tag{74}$$

Then we have an explicit form of $h_\varepsilon(\mathbf{x})$ as

$$h_\varepsilon(\mathbf{x}) = \frac{1}{2}\left[w_0^{(0)}(\mathbf{x}) - \sum_{n=1}^{\infty}(u'^T W'^{-1})_n \epsilon_n^{1/2} w_n^{(0)}(\mathbf{x}) \right] + O(\varepsilon^{1/2}). \tag{75}$$

We rewrite the function $f_\varepsilon(\mathbf{x})$, which is $w_0^{(0)}(\mathbf{x})$ in the limit of $\varepsilon \to 0$, as

$$f_\varepsilon(\mathbf{x}) = w_0^{(\varepsilon)}(\mathbf{x}) = (\overline{E_0})^{-1/4}(\varepsilon\overline{\epsilon})^{1/4}[(w_{C0}(\mathbf{x}) + w_{S0}(\mathbf{x})) + O(\varepsilon^{1/2})], \tag{76}$$

since then the completeness condition becomes evident [see Eqs. (20) and (47) with Eq. (61)],

$$\begin{aligned} \delta^3(\mathbf{x}-\mathbf{x}') &= \sum_{n=0}^{\infty} w_n^{(\varepsilon)}(\mathbf{x}) w_n^{(\varepsilon)}(\mathbf{x}') \\ &= \sum_{n=1}^{\infty}[w_{Cn}^{(\varepsilon)}(\mathbf{x}) w_{Cn}^{(\varepsilon)}(\mathbf{x}') - w_{Sn}^{(\varepsilon)}(\mathbf{x}) w_{Sn}^{(\varepsilon)}(\mathbf{x}')] + [f_\varepsilon(\mathbf{x}) h_\varepsilon(\mathbf{x}') + h_\varepsilon(\mathbf{x}) f_\varepsilon(\mathbf{x}')]. \end{aligned} \tag{77}$$

This way it has been confirmed that $f_\varepsilon(\mathbf{x})$ and $h_\varepsilon(\mathbf{x})$ thus defined in the GB approach correspond to $f(\mathbf{x})$ and $h(\mathbf{x})$ in the BdG approach in the limit of $\varepsilon \to 0$.

As the next step, we rewrite the oscillatorlike operator $\hat{b}_0$ by a new set of canonical operators $\{\hat{\mathcal{Q}}_b, \hat{\mathcal{P}}_b\}$,

$$\hat{b}_0 = \frac{1}{\sqrt{2}}(\hat{\mathcal{P}}_b - i\hat{\mathcal{Q}}_b), \tag{78a}$$

$$\hat{b}_0^\dagger = \frac{1}{\sqrt{2}}(\hat{\mathcal{P}}_b + i\hat{\mathcal{Q}}_b), \tag{78b}$$

with

$$[\hat{\mathcal{Q}}_b, \hat{\mathcal{P}}_b] = i \tag{79}$$

and

$$[\hat{\mathcal{Q}}_b, \hat{\mathcal{Q}}_b] = [\hat{\mathcal{P}}_b, \hat{\mathcal{P}}_b] = 0. \tag{80}$$

Using Eqs. (73), (76), and (75) one can express the field operator in the GB approach as

$$\hat{\varphi}(x) = \hat{b}_0(t) w_{C0}^{(\varepsilon)}(\mathbf{x}) - \hat{b}_0^\dagger(t) w_{S0}^{(\varepsilon)}(\mathbf{x}) + \hat{\varphi}_{\mathrm{exc}}(x) = \xi \hat{\mathcal{P}}_b(t) h_\varepsilon(\mathbf{x}) - i\xi^{-1} \hat{\mathcal{Q}}_b(t) f_\varepsilon(\mathbf{x}) + \hat{\varphi}_{\mathrm{exc}}(x) + O(\varepsilon^{1/2}), \tag{81}$$

where

$$\xi = \sqrt{2}\overline{E_0}^{-1/4} (\varepsilon \overline{\epsilon})^{1/4}, \tag{82}$$

$$\hat{\varphi}_{\mathrm{exc}}(x) = \sum_{n=1}^{\infty} [\hat{b}_n(t) w_{Cn}^{(\varepsilon)}(\mathbf{x}) - \hat{b}_n^\dagger(t) w_{Sn}^{(\varepsilon)}(\mathbf{x})]. \tag{83}$$

Recall Eq. (74) and that $\varphi_{\mathrm{exc}}(x)$ is common, which has been proved in the first part of this section, and we see that Eqs. (81) and (50) become identical to each other in the limit of $\varepsilon \to 0$, if we identify

$$\hat{\mathcal{P}} = \xi \hat{\mathcal{P}}_b, \tag{84a}$$

$$\hat{\mathcal{Q}} = \xi^{-1} \hat{\mathcal{Q}}_b. \tag{84b}$$

Namely, the field operators in the GB approach may be expressed as

$$\hat{\varphi}(x) = \hat{\mathcal{P}}(t) h_\varepsilon(\mathbf{x}) - i \hat{\mathcal{Q}}(t) f_\varepsilon(\mathbf{x}) + \hat{\varphi}_{\mathrm{exc}}(x) + O(\varepsilon^{1/2}), \tag{85a}$$

$$\hat{\varphi}^\dagger(x) = \hat{\mathcal{P}}(t) h_\varepsilon(\mathbf{x}) + i \hat{\mathcal{Q}}(t) f_\varepsilon(\mathbf{x}) + \hat{\varphi}_{\mathrm{exc}}^\dagger(x) + O(\varepsilon^{1/2}). \tag{85b}$$

The Hamiltonian (30) in the GB approach is in terms of $\hat{\mathcal{P}}$ and $\hat{\mathcal{Q}}$,

$$\begin{aligned} \hat{H}_0 &= \frac{1}{2I_\varepsilon} \xi^2 \hat{\mathcal{P}}_b^2 + (\varepsilon \overline{\epsilon}) \xi^{-2} \hat{\mathcal{Q}}_b^2 + \sum_{n=1}^{\infty} E_n \hat{b}_n^\dagger \hat{b}_n + (c\text{-numbers}) \\ &= \frac{1}{2I_\varepsilon} \hat{\mathcal{P}}^2 + (\varepsilon \overline{\epsilon}) \hat{\mathcal{Q}}^2 + \sum_{n=1}^{\infty} E_n \hat{b}_n^\dagger \hat{b}_n + (c\text{-numbers}) \to \frac{1}{2I} \hat{\mathcal{P}}^2 + \sum_{n=1}^{\infty} E_n \hat{b}_n^\dagger \hat{b}_n + (c\text{-numbers}), \end{aligned} \tag{86}$$

which is the same as Eq. (51).

Thus Eqs. (78), (82), and (84) reveal the correspondence between the two sets of operators representing the NG modes in the two approaches, $\{\hat{b}_0, \hat{b}_0^\dagger\}$ and $\{\hat{\mathcal{P}}, \hat{\mathcal{Q}}\}$, in the limit of $\varepsilon \to 0$.

VI. SUMMARY AND DISCUSSIONS

It was shown explicitly in this paper that in the unperturbed representation for systems of the trapped BECs (i) the operators of excitation modes in the GB and BdG approaches are identical, and (ii) the operators $\hat{b}_0$ and $\hat{b}_0^\dagger$ of the NG mode in the GB approach are related to the quantum coordinates $\hat{\mathcal{P}}$ and $\hat{\mathcal{Q}}$ in the BdG approach through the linear relations (78) and (84) with Eq. (82). The introduction of the breaking term in Eq. (4) and the parameter ε in the GB is very important to find the relations. The formal equivalence of the two approaches is established since the operators turned out to be related to each other linearly.

We note that the scale transformation [see Eq. (84)],

$$\hat{\mathcal{P}}_b \to \hat{\mathcal{P}} = \xi \hat{\mathcal{P}}_b, \tag{87a}$$

$$\hat{\mathcal{Q}}_b \to \hat{\mathcal{Q}} = \xi^{-1} \hat{\mathcal{Q}}_b, \tag{87b}$$

which is canonical, corresponds to the squeezing, although it is singular as ξ^{-1} diverges in the limit of $\varepsilon \to 0$.

Let us discuss on vacuum states. Because of the result (i), the vacuum structures with respect to the excitation modes are identical in the two approaches, we simply require

$$\hat{b}_n |\Omega_{\text{exc}}\rangle = 0 \quad (n \geqslant 1). \tag{88}$$

But there are two ways to determine the vacuum structure in the NG mode sector. One is a prescription, naturally adopted in the GB approach, to have the vacuum defined by

$$\hat{b}_0 |\Omega_0\rangle = 0. \tag{89}$$

Here the operator $\hat{b}_0$ is treated as a gapless mode. The other is to have no unique vacuum but a quantum mechanical state associated with the quantum coordinates $\{\hat{\mathcal{P}}, \hat{\mathcal{Q}}\}$, denoted by $|Q\rangle$. Although this state must satisfy

$$\langle Q|\hat{\mathcal{Q}}|Q\rangle = \langle Q|\hat{\mathcal{P}}|Q\rangle = 0, \tag{90}$$

due to the condition

$$\langle \Omega|\hat{\varphi}(x)|\Omega\rangle = 0, \tag{91}$$

where $|\Omega\rangle$ is the total vacuum, it cannot be determined completely from general considerations. As an example, one may take for it a Gaussian wave function, centered at $Q=0$. Here Q is a quantum number associated with the operator $\hat{\mathcal{Q}}$.

In summary, we have the two types of total vacuum, depending on whether the NG mode is treated as a gapless mode or as quantum coordinates,

$$|\Omega\rangle = \begin{cases} |\Omega_0\rangle \otimes |\Omega_{\text{exc}}\rangle & \text{(as gapless mode)}, \\ |Q\rangle \otimes |\Omega_{\text{exc}}\rangle & \text{(as quantum coordinate)}. \end{cases} \tag{92}$$

One should not confuse the choice of approach and that of vacuum. We can develop in the GB approach a consistent formulation with the vacuum $|Q\rangle \otimes |\Omega_{\text{exc}}\rangle$ as quantum coordinates, guided by the relations (78) and (84) with Eq. (82). What matters physically is the choice of vacuum but not that of approach. We are discussing the unperturbed representation in this paper. The choice of unperturbed vacuum affects the unperturbed (free) propagator and inevitably all of the higher order effects. The corrections at one-loop level to the original GP equation have been evaluated when the vacuum $|\Omega_0\rangle \otimes |\Omega_{\text{exc}}\rangle$ is chosen.[8] We have reported the evaluation of the same corrections with the choice of $|Q\rangle \otimes |\Omega_{\text{exc}}\rangle$ in Ref. 14. The expressions for free propagators with $|Q\rangle \otimes |\Omega_{\text{exc}}\rangle$ are given in the Appendix, while those with $|\Omega_0\rangle \otimes |\Omega_{\text{exc}}\rangle$ are found in Ref. 8.

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APPENDIX: PROPAGATORS USING QUANTUM COORDINATES

In this Appendix, we construct unperturbed (free) propagators with $|Q\rangle\otimes|\Omega_{\rm exc}\rangle$. These are necessary to calculate quantum and thermal corrections.

The time dependence of $\hat{\mathcal{Q}}$ and $\hat{\mathcal{P}}$ are governed by the Hamiltonian (86),

$$\hat{\mathcal{Q}}(t)=\cos(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\hat{\mathcal{Q}}+\frac{1}{\sqrt{\varepsilon\bar{\mathcal{E}}I_\varepsilon}}\sin(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\hat{\mathcal{P}}, \tag{A1a}$$

$$\hat{\mathcal{P}}(t)=\cos(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\hat{\mathcal{P}}-(\sqrt{\varepsilon\bar{\mathcal{E}}I_\varepsilon})\sin(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\hat{\mathcal{P}}, \tag{A1b}$$

where $\bar{\mathcal{E}}=\sqrt{\bar{\epsilon}\bar{E}_0}+O(\varepsilon)$.

We substitute Eq. (A1) into the field operators in Eq. (85),

$$\hat{\varphi}(x)=[\cos(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\hat{\mathcal{P}}-\sqrt{\varepsilon\bar{\mathcal{E}}I_\varepsilon}\sin(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\hat{\mathcal{Q}}]h_\varepsilon(\mathbf{x})-i\left[\cos(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\hat{\mathcal{Q}}+\frac{1}{\sqrt{\varepsilon\bar{\mathcal{E}}I_\varepsilon}}\sin(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\hat{\mathcal{P}}\right]f_\varepsilon(\mathbf{x})$$
$$+\hat{\varphi}_{\rm exc}(x)+O(\varepsilon), \tag{A2a}$$

$$\hat{\varphi}^\dagger(x)=[\cos(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\hat{\mathcal{P}}-\sqrt{\varepsilon\bar{\mathcal{E}}I_\varepsilon}\sin(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\hat{\mathcal{Q}}]h_\varepsilon(\mathbf{x})+i\left[\cos(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\hat{\mathcal{Q}}+\frac{1}{\sqrt{\varepsilon\bar{\mathcal{E}}I_\varepsilon}}\sin(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\hat{\mathcal{P}}\right]f_\varepsilon(\mathbf{x})$$
$$+\hat{\varphi}^\dagger_{\rm exc}(x)+O(\varepsilon). \tag{A2b}$$

When the limit $\varepsilon\to 0$ is taken, they are

$$\hat{\varphi}(x)=\hat{\mathcal{P}}h(\mathbf{x})-i\left(\hat{\mathcal{Q}}+\frac{1}{I}\hat{\mathcal{P}}t\right)f(\mathbf{x})+\hat{\varphi}_{\rm exc}(x), \tag{A3a}$$

$$\hat{\varphi}^\dagger(x)=\hat{\mathcal{P}}h(\mathbf{x})+i\left(\hat{\mathcal{Q}}+\frac{1}{I}\hat{\mathcal{P}}t\right)f(\mathbf{x})+\hat{\varphi}^\dagger_{\rm exc}(x). \tag{A3b}$$

These representations are the same as in Ref. 12.

Next, let us construct the propagators with Eq. (A2) and the vacuum $|Q\rangle\otimes|\Omega_{\rm exc}\rangle$. The 2×2-matrix propagator is derived as

$$\mathbf{G}_Q(\mathbf{x},\mathbf{x}';t,t')=\begin{pmatrix}G_{Q,11}(\mathbf{x},\mathbf{x}';t,t') & G_{Q,12}(\mathbf{x},\mathbf{x}';t,t')\\ G_{Q,21}(\mathbf{x},\mathbf{x}';t,t') & G_{Q,22}(\mathbf{x},\mathbf{x}';t,t')\end{pmatrix}, \tag{A4}$$

where

$$G_{Q,11}(\mathbf{x},\mathbf{x}';t,t')\equiv\langle\Omega|\mathcal{T}[\hat{\varphi}(x)\hat{\varphi}^\dagger(x')]|\Omega\rangle=\Bigg[\cos(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\cos(\sqrt{\varepsilon\bar{\mathcal{E}}}t')h_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}')$$
$$+\left(\frac{1}{\sqrt{\varepsilon\bar{\mathcal{E}}I_\varepsilon}}\right)^2\sin(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\sin(\sqrt{\varepsilon\bar{\mathcal{E}}}t')f_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}')$$
$$+i\frac{1}{\sqrt{\varepsilon\bar{\mathcal{E}}I_\varepsilon}}\cos(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\sin(\sqrt{\varepsilon\bar{\mathcal{E}}}t')h_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}')$$
$$-i\frac{1}{\sqrt{\varepsilon\bar{\mathcal{E}}I_\varepsilon}}\sin(\sqrt{\varepsilon\bar{\mathcal{E}}}t)\cos(\sqrt{\varepsilon\bar{\mathcal{E}}}t')f_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}')\Bigg]\langle Q|\hat{\mathcal{P}}^2|Q\rangle$$

$$
\begin{aligned}
&+ [\cos(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') + (\sqrt{\varepsilon\mathcal{E}}I_\varepsilon)^2\sin(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}') \\
&+ i(\sqrt{\varepsilon\mathcal{E}}I_\varepsilon)\cos(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}') \\
&- i(\sqrt{\varepsilon\mathcal{E}}I_\varepsilon)\sin(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}')]\langle Q|\hat{\mathcal{Q}}^2|Q\rangle \\
&+ \left\{\theta(t-t')\left[-(\sqrt{\varepsilon\mathcal{E}}I_\varepsilon)\cos(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}')\right.\right. \\
&+ \frac{1}{\sqrt{\varepsilon\mathcal{E}}I_\varepsilon}\sin(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') + i\sin(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}') \\
&\left.+ i\cos(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}')\right] + \theta(t'-t) \\
&\times\left[-(\sqrt{\varepsilon\mathcal{E}}I_\varepsilon)\sin(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}')\right. \\
&+ \frac{1}{\sqrt{\varepsilon\mathcal{E}}I_\varepsilon}\cos(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') - i\sin(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') \\
&\left.\left.- i\cos(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}')\right]\right\}\langle Q|\hat{\mathcal{P}}\hat{\mathcal{Q}}|Q\rangle \\
&+ \left\{\theta(t-t')\left[-(\sqrt{\varepsilon\mathcal{E}}I_\varepsilon)\sin(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}')\right.\right. \\
&+ \frac{1}{\sqrt{\varepsilon\mathcal{E}}I_\varepsilon}\cos(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') - i\cos(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}') \\
&\left.- i\sin(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}')\right] + \theta(t'-t) \\
&\times\left[-(\sqrt{\varepsilon\mathcal{E}}I_\varepsilon)\cos(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}')\right. \\
&+ \frac{1}{\sqrt{\varepsilon\mathcal{E}}I_\varepsilon}\sin(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') + i\cos(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') \\
&\left.\left.+ i\sin(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}')\right]\right\}\langle Q|\hat{\mathcal{Q}}\hat{\mathcal{P}}|Q\rangle \qquad \text{(A5)}
\end{aligned}
$$

$$
G_{Q,22}(\mathbf{x},\mathbf{x}';t,t') = G_{Q,11}(\mathbf{x}',\mathbf{x};t',t), \qquad \text{(A6)}
$$

$$
\begin{aligned}
G_{Q,12}(\mathbf{x},\mathbf{x}';t,t') \equiv \langle\Omega|T[\hat{\varphi}(\mathbf{x})\hat{\varphi}(x')]|\Omega\rangle = &\left[\cos(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}')\right. \\
&+ \left(\frac{1}{\sqrt{\varepsilon\mathcal{E}}I_\varepsilon}\right)^2\sin(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}')
\end{aligned}
$$

$$
\begin{aligned}
&- i\frac{1}{\sqrt{\varepsilon\mathcal{E}I_\varepsilon}}\cos(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') \\
&- i\frac{1}{\sqrt{\varepsilon\mathcal{E}I_\varepsilon}}\sin(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}')\Big]\langle Q|\hat{\mathcal{P}}^2|Q\rangle \\
&+ [\cos(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') + (\sqrt{\varepsilon\mathcal{E}I_\varepsilon})^2\sin(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}') \\
&+ i(\sqrt{\varepsilon\mathcal{E}I_\varepsilon})\cos(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}') \\
&+ i(\sqrt{\varepsilon\mathcal{E}I_\varepsilon})\sin(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}')]\langle Q|\hat{\mathcal{Q}}^2|Q\rangle \\
&+ \Bigg\{\theta(t-t')\Bigg[-(\sqrt{\varepsilon\mathcal{E}I_\varepsilon})\cos(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}') \\
&+ \frac{1}{\sqrt{\varepsilon\mathcal{E}I_\varepsilon}}\sin(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') + i\sin(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}') \\
&- i\cos(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}')\Bigg] + \theta(t'-t) \\
&\times\Bigg[-(\sqrt{\varepsilon\mathcal{E}I_\varepsilon})\sin(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}') \\
&+ \frac{1}{\sqrt{\varepsilon\mathcal{E}I_\varepsilon}}\cos(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') + i\sin(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') \\
&- i\cos(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}')\Bigg]\Bigg\}\langle Q|\hat{\mathcal{P}}\hat{\mathcal{Q}}|Q\rangle \\
&+ \Bigg\{\theta(t-t')\Bigg[-(\sqrt{\varepsilon\mathcal{E}I_\varepsilon})\sin(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}') \\
&+ \frac{1}{\sqrt{\varepsilon\mathcal{E}I_\varepsilon}}\cos(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') - i\cos(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}') \\
&+ i\sin(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}')\Bigg] + \theta(t'-t) \\
&\times\Bigg[-(\sqrt{\varepsilon\mathcal{E}I_\varepsilon})\cos(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}') \\
&+ \frac{1}{\sqrt{\varepsilon\mathcal{E}I_\varepsilon}}\sin(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') - i\cos(\sqrt{\varepsilon\mathcal{E}}t)\cos(\sqrt{\varepsilon\mathcal{E}}t')h_\varepsilon(\mathbf{x})f_\varepsilon(\mathbf{x}') \\
&+ i\sin(\sqrt{\varepsilon\mathcal{E}}t)\sin(\sqrt{\varepsilon\mathcal{E}}t')f_\varepsilon(\mathbf{x})h_\varepsilon(\mathbf{x}')\Bigg]\Bigg\}\langle Q|\hat{\mathcal{Q}}\hat{\mathcal{P}}|Q\rangle \qquad \text{(A7)}
\end{aligned}
$$

$$
G_{Q,21}(\mathbf{x},\mathbf{x}';t,t') = G_{Q,12}(\mathbf{x}',\mathbf{x};t',t). \qquad \text{(A8)}
$$

In the above definitions, we use the notation for propagators without NG mode,

$$
G_{\mathrm{exc},11}(\mathbf{x},\mathbf{x}';t-t') \equiv \langle\Omega_{\mathrm{exc}}|T[\hat{\varphi}_{\mathrm{exc}}(x)\hat{\varphi}^\dagger_{\mathrm{exc}}(x')]|\Omega_{\mathrm{exc}}\rangle, \qquad \text{(A9a)}
$$

$$G_{\mathrm{exc},12}(\mathbf{x},\mathbf{x}';t-t') \equiv \langle \Omega_{\mathrm{exc}}|T[\hat{\varphi}_{\mathrm{exc}}(\mathbf{x})\hat{\varphi}_{\mathrm{exc}}(\mathbf{x}')]|\Omega_{\mathrm{exc}}\rangle, \tag{A9b}$$

$$G_{\mathrm{exc},21}(\mathbf{x},\mathbf{x}';t-t') \equiv \langle \Omega_{\mathrm{exc}}|T[\hat{\varphi}^{\dagger}_{\mathrm{exc}}(\mathbf{x})\hat{\varphi}^{\dagger}_{\mathrm{exc}}(x')]|\Omega_{\mathrm{exc}}\rangle, \tag{A9c}$$

$$G_{\mathrm{exc},22}(\mathbf{x},\mathbf{x}';t-t') \equiv \langle \Omega_{\mathrm{exc}}|T[\hat{\varphi}^{\dagger}_{\mathrm{exc}}(x)\hat{\varphi}_{\mathrm{exc}}(x')]|\Omega_{\mathrm{exc}}\rangle. \tag{A9d}$$

One can find their explicit forms in Ref. 8.

In the limit of $\varepsilon \to 0$, the propagators become

$$\begin{aligned} G_{Q,11}(\mathbf{x},\mathbf{x}';t,t') = & \left[h(\mathbf{x})h(\mathbf{x}') + f(\mathbf{x})f(\mathbf{x}')\left(\frac{t}{I}\right)\left(\frac{t'}{I}\right) + ih(\mathbf{x})f(\mathbf{x}')\left(\frac{t'}{I}\right) - if(\mathbf{x})h(\mathbf{x}')\left(\frac{t}{I}\right)\right]\langle Q|\hat{\mathcal{P}}^2|Q\rangle \\ & + f(\mathbf{x})f(\mathbf{x}')\langle Q|\hat{\mathcal{Q}}^2|Q\rangle + \left\{ \theta(t-t')\left[f(\mathbf{x})f(\mathbf{x}')\left(\frac{t}{I}\right) + ih(\mathbf{x})f(\mathbf{x}')\right] + \theta(t'-t)\right. \\ & \left.\times\left[f(\mathbf{x})f(\mathbf{x}')\left(\frac{t'}{I}\right) - if(\mathbf{x})h(\mathbf{x}')\right]\right\}\langle Q|\hat{\mathcal{P}}\hat{\mathcal{Q}}|Q\rangle + \left\{ \theta(t-t')\left[f(\mathbf{x})f(\mathbf{x}')\left(\frac{t'}{I}\right)\right.\right. \\ & \left.\left. - if(\mathbf{x})h(\mathbf{x}')\right] + \theta(t'-t)\left[f(\mathbf{x})f(\mathbf{x}')\left(\frac{t}{I}\right) + ih(\mathbf{x})f(\mathbf{x}')\right]\right\}\langle Q|\hat{\mathcal{Q}}\hat{\mathcal{P}}|Q\rangle \\ & + G_{\mathrm{exc},11}(\mathbf{x},\mathbf{x}';t-t'), \end{aligned} \tag{A10}$$

$$G_{Q,22}(\mathbf{x},\mathbf{x}';t,t') = G_{Q,11}(\mathbf{x}',\mathbf{x};t',t), \tag{A11}$$

$$\begin{aligned} G_{Q,12}(\mathbf{x},\mathbf{x}';t,t') = & \left[h(\mathbf{x})h(\mathbf{x}') + f(\mathbf{x})f(\mathbf{x}')\left(\frac{t}{I}\right)\left(\frac{t'}{I}\right) - ih(\mathbf{x})f(\mathbf{x}')\left(\frac{t'}{I}\right) - if(\mathbf{x})h(\mathbf{x}')\left(\frac{t}{I}\right)\right]\langle Q|\hat{\mathcal{P}}^2|Q\rangle \\ & + f(\mathbf{x})f(\mathbf{x}')\langle Q|\hat{\mathcal{Q}}^2|Q\rangle + \left\{ \theta(t-t')\left[f(\mathbf{x})f(\mathbf{x}')\left(\frac{t}{I}\right) - ih(\mathbf{x})f(\mathbf{x}')\right] + \theta(t'-t)\right. \\ & \left.\times\left[f(\mathbf{x})f(\mathbf{x}')\left(\frac{t'}{I}\right) - if(\mathbf{x})h(\mathbf{x}')\right]\right\}\langle Q|\hat{\mathcal{P}}\hat{\mathcal{Q}}|Q\rangle + \left\{ \theta(t-t')\left[f(\mathbf{x})f(\mathbf{x}')\left(\frac{t'}{I}\right)\right.\right. \\ & \left.\left. - if(\mathbf{x})h(\mathbf{x}')\right] + \theta(t'-t)\left[f(\mathbf{x})f(\mathbf{x}')\left(\frac{t}{I}\right) - ih(\mathbf{x})f(\mathbf{x}')\right]\right\}\langle Q|\hat{\mathcal{Q}}\hat{\mathcal{P}}|Q\rangle \\ & + G_{\mathrm{exc},12}(\mathbf{x},\mathbf{x}';t-t'), \end{aligned} \tag{A12}$$

$$G_{Q,21}(\mathbf{x},\mathbf{x}';t,t') = G_{Q,12}(\mathbf{x}',\mathbf{x};t',t). \tag{A13}$$

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On extensions of superconformal algebras

Jasbir Nagi[a)]
DAMTP, University of Cambridge, Cambridge CB3 0WA, United Kingdom

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Starting from vector fields that preserve a differential form on a Riemann sphere with Grassmann variables, one can construct a superconformal algebra by considering central extensions of the algebra of vector fields. In this paper, the $N=4$ case is analyzed closely, where the presence of weight zero operators in the field theory forces the introduction of noncentral extensions. How this modifies the existing field theory, representation theory, and Gelfand–Fuchs constructions is discussed. It is also discussed how graded Riemann sphere geometry can be used to give a geometrical description of the central charge in the $N=1$ theory. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1863652]

I. INTRODUCTION

Two-dimensional conformal symmetry in quantum field theory has, over the last 30 years, touched many parts of mathematics and theoretical physics. A quantum field theory that is conformally invariant is called a conformal field theory (CFT), and in this paper, only the case of two dimensions is examined. Lying at the heart of CFT is understanding how to treat the infinite conformal symmetry on the quantum level, and understanding the representation theory of the algebra. If one wants a nontrivial, unitary representation of the symmetry algebra (known as the DeWitt algebra), then a central extension must be introduced into the algebra, yielding the Virasoro algebra.[3] Hence, when considering any algebra which has the Virasoro algebra as a subalgebra, the understanding of how and what extensions can be added is of crucial importance. Two-dimensional CFTs present an example of a quantum field theory where there is a rich interplay between the geometry of the theory and the quantum theory. As a result, many aspects of the quantum theory can be described elegantly by the geometry. This is a point of view that this paper will use repeatedly.

In this paper, the case of the conformal symmetries of a Riemann sphere and graded Riemann sphere are examined. In Ref. 7 it was found that a graded Riemann sphere is a sensible space on which to try and construct a superconformal field theory (SCFT). On this space many results can be obtained, and primary fields (fields that "generate" the space of states) can be built in a natural manner associated to the geometry of the space. These spaces give rise to lie graded algebras of vector fields that contain the DeWitt algebra. Much work has been done on the extensions of these algebras in Ref. 6. Here, the $N=4$ case is revisited, with particular attention paid to the weight 0 fields that arise in the theory. These fields give unusual behavior, giving logarithms in the super OPE, and exhibiting some Jordan block structure in the adjoint representation. The structure, however, turns out to be quite manageable, since the behavior turns out to be quite similar to that of a free boson. The understanding of how to construct bosonic primary fields geometrically, as sections of a line bundle is extremely well covered in the CFT literature. However, it is also known, in the bosonic theory, how to construct central extensions geometrically.[10] Here, this is extended to the $N=1$ case, and is discussed how this might extend to higher N.

In Sec. II, the vector fields for the $N=4$ case are found, and extensions of the algebra considered, using just the graded Jacobi identity. In particular, it is found that if the algebra is not

[a)]Electronic mail: j.s.nagi@damtp.cam.ac.uk

reduced to its simple subalgebra, then the Jacobi identity implies that algebra must be extended by noncentral elements, if it is to contain the Virasoro algebra with nontrivial central charge. Section III examines how this fits into the operator formalism of CFT, where the starting point is usually an operator product expansion. There the subtlety arises from understanding what mode expansions to take for operators, and how to treat logarithms in the operator product expansion. Section IV looks at how the usual representation theory of the $N=4$ algebra will be altered with the noncentral extension found. Section V then considers how the algebra obtained fits into the formalism of Gelfand–Fuchs extensions, and how superspace techniques can be used to write them. Section VI then looks at the $N=1$ Gelfand–Fuchs cocycle, i.e., the $N=1$ central charge, and considers how to realize the cocycle as a geometric object on a graded Riemann sphere.

II. THE ALGEBRA OF VECTOR FIELDS

On a Riemann sphere, one obtains the DeWitt algebra by looking at the vector fields that preserve the one-form dz, a basis of which is given by

$$l_n = -z^{n+1}\frac{\partial}{\partial z}. \tag{1}$$

Calculating the commutation relations given by the lie bracket yields the DeWitt algebra

$$[l_n, l_m] = (n-m)l_{n+m}. \tag{2}$$

Similarly, on a graded Riemann sphere, with $N=4$ and the usual one-form $\omega = \mathrm{d}z + \Sigma_{i=1}^{4}\theta_i\,\mathrm{d}\theta_i$, one finds a basis of vector fields that preserve ω (Ref. 6),

$$l_n = -z^n\left(z\partial + \tfrac{1}{2}(n+1)\,\theta_i\partial_i\right),$$

$$g_r^j = z^{r+1/2}\left(\theta_j\partial - \partial_j + \frac{\left(r+\frac{1}{2}\right)}{z}\theta_j\theta_k\partial_k\right),$$

$$t_n^{ml} = z^n\left(\theta_l\partial_m - \theta_m\partial_l + \frac{n}{z}\theta_m\theta_l\theta_p\partial_p\right), \tag{3}$$

$$\psi_r^k = -z^{r-1/2}\left(\tfrac{1}{6}\epsilon_{kpqr}\theta_p\theta_q\theta_r\partial + \frac{\left(r-\frac{1}{2}\right)}{z}\theta_1\theta_2\theta_3\theta_4\partial_k + \tfrac{1}{2}\epsilon_{kpqr}\theta_p\theta_q\partial_r\right),$$

$$u_n = -z^{n-1}\left(\theta_1\theta_2\theta_3\theta_4\partial + \tfrac{1}{12}\epsilon_{ijkl}\theta_i\theta_j\theta_k\partial_l\right).$$

These vector fields give rise to the graded commutation relations under the graded Lie bracket,

$$[l_n, l_m] = (n-m)l_{m+n}, \quad [l_n, g_r^j] = \left(\frac{n}{2} - r\right)g_{n+r}^j, \quad [l_n, t_m^{pq}] = -mt_m^{pq},$$

$$[l_n, \psi_r^k] = \left(-\frac{n}{2} - r\right)\psi_{n+r}^k, \quad [l_n, u_m] = -(n+m)u_{m+n},$$

$$\begin{gathered}[g_r^j, g_s^k] = 2\delta_{jk}l_{r+s} + (s-r)t_{r+s}^{jk}, \quad [t_n^{ml}, g_r^j] = \delta_{mj}g_{n+r}^l - \delta_{lj}g_{n+r}^m + n\epsilon_{mljk}\psi_{n+r}^k, \\ [g_r^j, \psi_s^k] = \delta_{jk}2(r+s)u_{r+s} + \tfrac{1}{2}\epsilon_{jkpq}t_{r+s}^{pq}, \quad [g_r^j, u_n] = -\tfrac{1}{2}\psi_{n+r}^j,\end{gathered} \tag{4}$$

$$[t_n^{ml}, t_r^{pq}] = \delta_{mq} t_{n+r}^{pl} + \delta_{mp} t_{n+r}^{lq} + \delta_{lq} t_{n+r}^{mp} + \delta_{lp} t_{n+r}^{qm}, \quad [t_n^{ml}, u_p] = 0,$$

$$[t_n^{ml}, \psi_r^k] = \delta_{mk} \psi_{n+r}^l - \delta_{kl} \psi_{n+r}^m, \quad [\psi_r^k, \psi_s^j] = 0, \quad [\psi_r^k, u_n] = 0, \quad [u_m, u_n] = 0.$$

Note that this algebra is not simple, and that $[\mathfrak{g}, \mathfrak{g}] = \mathfrak{g}/\langle u_o \rangle$ (quotient taken in the vector space sense) is simple. This simple algebra is the large $N=4$ algebra, without its three central elements. The t_n^{ml} form an so(4) loop algebra. This loop algebra may be written explicitly as so(4) = su(2) $\oplus$ su(2) by the change of basis

$$t_m^1 = \tfrac{1}{2}(t_m^{12} + t_m^{34}), \quad t_m^2 = \tfrac{1}{2}(t_m^{13} - t_m^{24}), \quad t_m^3 = \tfrac{1}{2}(t_m^{14} + t_m^{23}),$$

$$\overline{t}_m^1 = \tfrac{1}{2}(t_m^{34} - t_m^{12}), \quad \overline{t}_m^2 = \tfrac{1}{2}(-t_m^{13} - t_m^{24}), \quad \overline{t}_m^3 = \tfrac{1}{2}(t_m^{23} - t_m^{14}).$$

These su(2)s can then be centrally extended, to affine currents, with extension c and $\overline{c}$. Defining $c^+ = c + \overline{c}$ and $c^- = c - \overline{c}$, one finds the modified commutation relation,

$$[t_n^{ml}, t_r^{pq}] = \delta_{mq} t_{n+r}^{pl} + \delta_{mp} t_{n+r}^{lq} + \delta_{lq} t_{n+r}^{mp} + \delta_{lp} t_{n+r}^{qm} + (\delta_{mp}\delta_{lq} - \delta_{mq}\delta_{lp}) c^+ n \delta_{n+r,0} + \epsilon_{mlpq} c^- n \delta_{n+r,0}.$$

The c^- also modifies, by the Jacobi identity, the relations

$$[g_r^j, \psi_s^k] = \delta_{jk} 2(r+s) u_{r+s} + \tfrac{1}{2} \epsilon_{jkpq} t_{r+s}^{pq} + c^- \left(r + \tfrac{1}{2}\right) \delta_{jk} \delta_{r+s,0},$$

$$[l_n, u_m] = -(n+m) u_{m+n} - \frac{c^-}{4} (n+1) \delta_{m+n,0}.$$

The c^+ also modifies, by the Jacobi identity, the relations

$$[l_m, l_n] = (m-n) l_{m+n} - \frac{c^+}{4} m(m^2-1) \delta_{m+n,0},$$

$$[g_r^j, g_s^k] = 2\delta_{jk} l_{r+s} + (s-r) t_{r+s}^{jk} - c^+ \left(r^2 - \tfrac{1}{4}\right) \delta_{jk} \delta_{r+s,0},$$

$$[\psi_r^k, \psi_s^j] = c^+ \delta_{jk} \delta_{r+s,0}, \quad [u_m, u_n] = -\frac{c^+}{4m} \delta_{m+n,0} \quad \text{for } m \neq 0.$$

As it stands, the $\{g_r^j, \psi_s^j, u_0\}$ Jacobi identity implies $c^+ = 0$. This offending Jacobi identity is usually bypassed by working in $[\mathfrak{g}, \mathfrak{g}]$ rather than in $\mathfrak{g}$, but this is not the route that will be taken here. Nonzero c^+ can be obtained by adding another extension, denoted v_0. From the $[l_n, u_m]$ commutator, it can be seen that the u_m form a current of weight zero. This current can be deformed to include a logarithmic term, so that $u(z) = -\Sigma_n u_n z^{-n} + v_0 \log z$. This then modifies the commutation relations,

$$\begin{aligned} [l_n, u_m] &= -(m+n) u_{m+n} - v_0 \delta_{m+n,0}, \\ [g_r^j, \psi_s^k] &= 2\delta_{jk}((r+s) u_{r+s} + v_0 \delta_{r+s,0}) + \tfrac{1}{2} \epsilon_{jkpq} t_{r+s}^{pq}. \end{aligned} \tag{5}$$

Using the Jacobi identity, one can see that v_0 commutes with all elements, except u_0. The $\{g_r^j, \psi_s^j, u_0\}$ Jacobi identity now yields $[u_0, v_0] = c^+/4$. This algebra now realizes centrally extended $K'(4)$ (also known as large $N=4$) with the u_0 operator put back in. Note that in $K'(4)$, v_0 is a central extension.[6] The behavior of the u_m, v_0 is very similar to that of the modes of a free boson, identifying v_0 with momentum and u_0 with position. The commutation relations then become

$$[l_m,l_n]=(m-n)l_{m+n}-\frac{c^+}{4}m(m^2-1)\delta_{m+n,0},\quad [l_n,g_r^j]=\left(\frac{n}{2}-r\right)g_{n+r}^j,$$

$$[l_n,\psi_r^k]=\left(-\frac{n}{2}-r\right)\psi_{n+r}^k,\quad [l_n,u_m]=-(n+m)u_{m+n}-\left(\frac{c^-}{4}(n+1)+v_0\right)\delta_{m+n,0},$$

$$[g_r^j,g_s^k]=2\delta_{jk}l_{r+s}+(s-r)t_{r+s}^{jk}-c^+\left(r^2-\tfrac{1}{4}\right)\delta_{jk}\delta_{r+s,0},\quad [l_n,t_m^{pq}]=-mt_m^{pq},$$

$$[t_n^{ml},g_r^j]=\delta_{mj}g_{n+r}^l-\delta_{lj}g_{n+r}^m+n\epsilon_{mljk}\psi_{n+r}^k,\quad [g_r^j,u_n]=-\tfrac{1}{2}\psi_{n+r}^j,$$

$$[g_r^j,\psi_s^k]=\delta_{jk}2(r+s)u_{r+s}+\tfrac{1}{2}\epsilon_{jkpq}t_{r+s}^{pq}+\left(c^-\left(r+\tfrac{1}{2}\right)+2v_0\right)\delta_{jk}\delta_{r+s,0}, \tag{6}$$

$$[t_n^{ml},t_r^{pq}]=\delta_{mq}t_{n+r}^{pl}+\delta_{mp}t_{n+r}^{lq}+\delta_{lq}t_{n+r}^{mp}+\delta_{lp}t_{n+r}^{qm}+(\delta_{mp}\delta_{lq}-\delta_{mq}\delta_{lp})c^+n\delta_{n+r,0}+\epsilon_{mlpq}c^-n\delta_{n+r,0},$$

$$[t_n^{ml},u_p]=0,\quad [t_n^{ml},\psi_r^k]=\delta_{mk}\psi_{n+r}^l-\delta_{kl}\psi_{n+r}^m,\quad [\psi_r^k,\psi_s^j]=c^+\delta_{jk}\delta_{r+s,0},$$

$$[\psi_r^k,u_n]=0,\quad [u_m,u_n]=-\frac{c^+}{4m}\delta_{m+n,0},\quad [u_0,v_0]=\frac{c^+}{4}$$

with $c^{\pm}$ central, and v_0 has only one nontrivial commutator, namely $[u_0,v_0]$. Thus, while u_0,v_0 can both be considered to be operators at level 0, they cannot both be in the Cartan subalgebra. If v_0 is nonzero, one can choose it to be in the Cartan subalgebra. Usually, in a conformal field theory, one finds that the space of operators at level zero can be identified with the Cartan subalgebra. This is not the case here, and can potentially lead to Jordan blocks. In this sense, the $N=4$ theory can be thought of as a logarithmic theory, with the logarithmic character coming from $u(z)$. The usual large algebra comes from looking at the simple subalgebra obtained from identifying $u_0 \sim 0$, i.e., considering the field $\partial u(z)$ as fundamental rather than $u(z)$. To see where the logarithms actually come in, one must look at the operator formalism.

III. THE OPERATOR APPROACH

The super operator product expansion of the super Virasoro operator with a primary superfield for the $N=4$ case is given by[5]

$$\begin{aligned}\mathbb{T}(Z_1)\Phi(Z_2)\sim{}&\frac{h\theta_{12,1}\theta_{12,2}\theta_{12,3}\theta_{12,4}}{Z_{12}^2}\Phi(Z_2)+\frac{\theta_{12,1}\theta_{12,2}\theta_{12,3}\theta_{12,4}}{Z_{12}}\partial\Phi(Z_2)\\&+\frac{1}{12}\frac{\epsilon_{ijkl}\theta_{12,i}\theta_{12,j}\theta_{12,k}}{Z_{12}}D_l\Phi(Z_2)+\frac{1}{4}\frac{\epsilon_{ijkl}\theta_{12,i}\theta_{12,j}J^{kl}}{Z_{12}}\Phi(Z_2)+p\log(Z_{12})\Phi(Z_2),\end{aligned} \tag{7}$$

where $Z_1=(w,\chi_i)$, $Z_2=(z,\theta_i)$, $\theta_{12,i}=(\chi_i-\theta_i)$, $Z_{12}=(w-z-\chi_i\theta_i)$,

$$\mathbb{T}(Z_2)=\theta_1\theta_2\theta_3\theta_4L(z)+\tfrac{1}{12}\epsilon_{ijkl}\theta_i\theta_j\theta_kG^l(z)+\tfrac{1}{8}\epsilon_{ijkl}\theta_i\theta_jT^{kl}(z)+\tfrac{1}{2}\theta_k\psi^k(z)-U(z) \tag{8}$$

and the J^{ab} form an so (4) algebra with commutation relations given by $\frac{1}{2}t_0^{ab}$. $\log(Z_{12})$ is defined by

$$\log(Z_{12})=\log(w-z)-\sum_{p=1}^{4}\frac{1}{p}\left(\frac{\chi_i\theta_i}{(w-z)}\right)^p. \tag{9}$$

The χ_i components of each side can be taken, giving

$$L(w)\Phi(Z_2)\sim\left(\frac{h}{(w-z)^2}+\frac{1}{(w-z)}\partial+\frac{1}{2(w-z)^2}\theta_i\partial_i-\frac{\theta_i\theta_jJ^{ij}}{(w-z)^2}-\frac{6\theta_1\theta_2\theta_3\theta_4}{(w-z)^4}p\right)\Phi(Z_2),$$

$$\frac{1}{2}G^i(w)\Phi(Z_2)\sim\left(\frac{-h\theta_i}{(w-z)^2}-\frac{\theta_i\partial}{2(w-z)}+\frac{\partial_i}{2(w-z)}-\frac{\theta_i\theta_j\partial_j}{2(w-z)^2}+\frac{\theta_i\theta_j\theta_kJ^{jk}}{(w-z)^3}+\frac{\theta_jJ^{ji}}{(w-z)^2}-\frac{\epsilon_{ijkl}\theta_j\theta_k\theta_l}{3(w-z)^3}p\right)\Phi(Z_2),$$

$$\frac{1}{2}T^{ab}(w)\Phi(Z_2)\sim\left(\frac{h\theta_a\theta_b}{(w-z)^2}+\frac{\theta_b\partial_a-\theta_a\partial_b}{2(w-z)}+\frac{\theta_a\theta_b\theta_j\partial_j}{2(w-z)^2}-\frac{\theta_1\theta_2\theta_3\theta_4}{(w-z)^3}\epsilon_{abjk}J^{jk}+\frac{1}{(w-z)^2}(\theta_a\theta_jJ^{bj}-\theta_b\theta_jJ^{aj})+\frac{1}{(w-z)}J^{ab}+\frac{\epsilon_{abjk}\theta_j\theta_k}{2(w-z)^2}p\right)\Phi(Z_2),\tag{10}$$

$$\frac{1}{2}\psi^k(w)\Phi(Z_2)\sim\left(\frac{-h\epsilon_{klmn}\theta_l\theta_m\theta_n}{6(w-z)^2}+\frac{\epsilon_{klmn}\theta_l\theta_m\theta_n}{12(w-z)}\partial+\frac{\theta_1\theta_2\theta_3\theta_4}{2(w-z)^2}\partial_k+\frac{\epsilon_{klmn}\theta_l\theta_m}{4(w-z)}\partial_n-\frac{\epsilon_{klmn}\theta_l}{2(w-z)}J^{mn}+\frac{\theta_k\epsilon_{lmnp}\theta_l\theta_m}{4(w-z)^2}J^{np}-\frac{\theta_k}{(w-z)}p\right)\Phi(Z_2),$$

$$-U(w)\Phi(Z_2)\sim\left(\frac{h\theta_1\theta_2\theta_3\theta_4}{(w-z)^2}-\frac{\theta_1\theta_2\theta_3\theta_4}{(w-z)}\partial-\frac{\epsilon_{klmn}\theta_k\theta_l\theta_m}{12(w-z)}\partial_n+\frac{\epsilon_{klmn}\theta_k\theta_l}{4(w-z)}J^{mn}+\log(w-z)p\right)\Phi(Z_2)$$

from which the vector fields of (3) can be recovered. Note that logarithms only appear in OPEs containing $U(z)$. Clearly, in this last OPE, a contour integral can only be taken if $\partial U(w)\Phi(z)$ is considered. Taking $U(z)=\Sigma_nU_nz^{-n}+V_0\log z$, it can be shown that $[V_0,\Phi]=p\Phi$. Allowing V_0 to annihilate the vacuum[11] then yields $V_0|\Phi\rangle=p|\Phi\rangle$. The $[V_0,\Phi]$ commutator is unusual, in that it contains no differential operators. Hence, it is not obvious how to associate a conformal vector field of the form of (3) to V_0. The logarithm in the last OPE of (10) prevents one from obtaining an action from U_0. If one looks at a representation where $V_0=0$, then it can be seen that $p=0$ and that the w contour integral in $U(w)\Phi(z)$ can be performed, to give

$$[U_0,\Phi(Z)]\sim\left(\frac{h\theta_1\theta_2\theta_3\theta_4}{z^2}+\frac{\theta_1\theta_2\theta_3\theta_4\partial}{z}+\frac{\epsilon_{klmn}\theta_k\theta_l\theta_m\partial_n}{12z}-\frac{\epsilon_{klmn}\theta_k\theta_lJ^{mn}}{4z}\right)\Phi(Z).$$

However, its action on the highest weight from this approach is unclear, and a more careful approach to the representation theory is warranted.

The logarithmic character can also be examined by looking at the $\mathbb{T}(Z_1)\mathbb{T}(Z_2)$ OPE, given by

$$\mathbb{T}(Z_1)\mathbb{T}(Z_2)\sim\frac{c^+\log(Z_{12})}{4}-\frac{c^-\theta_{12,1}\theta_{12,2}\theta_{12,3}\theta_{12,4}}{4Z_{12}^2}+\frac{\theta_{12,1}\theta_{12,2}\theta_{12,3}\theta_{12,4}}{Z_{12}}\partial\mathbb{T}(Z_2)+\frac{1}{12}\frac{\epsilon_{ijkl}\theta_{12,i}\theta_{12,j}\theta_{12,k}}{Z_{12}}D_l\mathbb{T}(Z_2).\tag{11}$$

Using (9), one can see that the only term involving logarithms is the term,

$$U(w)U(z)\sim\frac{c^+}{4}\log(w-z).\tag{12}$$

Therefore, if $c^+\neq0$, $U(z)$ must have a logarithmic component in its mode expansion. This can easily be verified by taking the contour integrals in (12) to get the commutation relations. If there is no logarithmic component in $U(z)$, then from the computation one can deduce that $c^+=0$, the

same result found when using the Jacobi identity in the preceding section. The field $U(z)$ behaves in a very similar way to a free boson. In particular, $[V_0, U_0] = c^+/4$, and hence they are not mutually diagonalizable, as was reflected by the above manipulations of the last OPE in (10).

One can ask if the field, $U(z)$, can be written in a logarithmic form[1]

$$L(w)D(z) \sim \frac{hD(z) + E(z)}{(z-w)^2} + \frac{\partial D(z)}{(w-z)},$$

$$L(w)E(z) \sim \frac{hE(z)}{(z-w)^2} + \frac{\partial E(z)}{(w-z)}.$$

From (11) one can read off the $L(w)U(z)$ OPE to find

$$L(w)U(z) \sim \frac{\partial U(z)}{(w-z)} - \frac{c^-}{4(w-z)^2}. \tag{13}$$

Regarding $-c^-/4$ as a constant field of weight zero, one then gets the desired form. While the V_0 operator gives rise to an eigenvalue, this analysis does not yield a conformal transformation associated to V_0. The previous analysis shows that v_0 had to be introduced as an extension of the algebra. This suggests that rather than thinking of the p eigenvalue as being associated to a primary field, one should instead think of the V_0 operator as appearing in a similar way to a central extension.

IV. A LITTLE REPRESENTATION THEORY

A closer look at the level zero operators is warranted. These are normally defined as those operators with $\mathrm{ad}l_0$ eigenvalue being zero. Considering the commutation relations (6), one can see that clearly $\{l_0, t_0^{ml}, v_0, c^{\pm}\}$ fall into this category. However, u_0 has a strange action under $\mathrm{ad}l_0$, namely

$$[l_0, u_0] = -\left(\frac{c^-}{4} + v_0\right).$$

If one were to define a basis $e_1 = -(c^-/4) - v_0$, $e_2 = u_0$ and write down the matrix for $\mathrm{ad}l_0$ with respect to this basis, one would find the Jordan block

$$(\mathrm{ad}l_0) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

In this manner, u_0 can be considered as an operator at level zero that is not in the Cartan subalgebra.

The algebra here differs slightly from the usual large $N=4$ algebra, by the mode u_0. This affects the representation theory. The Fock space will be enlargened, due to the presence of polynomials in u_0 acting on the highest weight. Using the analogy of v_0 as momentum, and u_0 as position, instead of considering the states $u_0^n|h\rangle$, the "momentum" eigenstates $|k,h\rangle = e^{-ku_0}|h\rangle$ can be considered. From the fact that the only nontrivial commutators u_0 has are with l_n, g_r^j, v_0, one can show

$$v_0|k,h\rangle = \left(\frac{c^+k}{4} + p\right)|k,h\rangle, \quad g_r^j|k,h\rangle = e^{-ku_0}g_r^j|h\rangle + \frac{k}{2}\psi_r^j|k,h\rangle,$$
$$l_n|k,h\rangle = \begin{cases} e^{-ku_0}l_n|h\rangle + knu_n|k,h\rangle, & n \neq 0, \\ \left(h + k\left(\frac{c^-}{4} + p\right) + k^2\frac{c^+}{8}\right)|k,h\rangle, & n = 0 \end{cases} \tag{14}$$

from which it can be seen that $|k,h\rangle$ obeys highest weight conditions, with potentially different v_0 and l_0 eigenvalues from $|h\rangle$. In analogy with a free boson, the u_n. $n>0$ annihilate the vacuum and the highest weight state and v_0 annihilates the vacuum. For nonzero c^+, u_0 annihilates neither.

V. GELFAND–FUCHS 2-COCYCLES

For an algebra of vector fields, where a function can be associated to each vector field, it is often useful to construct central extensions by considering Gelfand–Fuchs 2-cocycles.[4] Here, superfield formalisms are used, which yield similar results to Ref. 4. For instance, in the bosonic case, one has[10]

$$l_m = -z^{m+1}\frac{\partial}{\partial z}, \quad l(z) = z^{m+1}, \text{ then}$$
$$c(l_m,l_n) = \frac{1}{24\pi i}\oint_0 \mathrm{d}z\left(\frac{\partial^3}{\partial z^3}z^{m+1}\right)z^{n+1} = \frac{c}{12}m(m^2-1)\delta_{m+n,0} \tag{15}$$

or for a general polynomial $l(z)$

$$c(l_{(1)},l_{(2)}) = \frac{1}{24\pi i}\oint_0 \mathrm{d}z\, l'''_{(1)}l_{(2)}, \tag{16}$$

where the contour is a closed loop around the origin, say the unit circle, beginning and ending at $z=1$. Since the extensions are known for the $N=1$, 2,3,4 algebras, they can be set in Gelfand–Fuchs 2-cocycle form. For the $N=1$ case

$$l_n = -z^n\left(z\partial_z + \tfrac{1}{2}(n+1)\theta\partial_\theta\right), \quad l(z) = z^{n+1},$$
$$g_r = z^{r+1/2}(\partial_\theta - \theta\partial_z), \quad g(z) = z^{r+1/2}. \tag{17}$$

Defining the graded field $X_{(i)} = \frac{1}{2}l_{(i)} + \theta g_{(i)}$ with l and g graded even polynomials in z, z^{-1}, one finds the central extension is given by the 2-cocycle,

$$c(X_{(1)},X_{(2)}) = \frac{1}{6\pi i}\oint_0 \mathrm{d}z\,\mathrm{d}\theta(DX''_{(1)})X_{(2)}, \tag{18}$$

where $D = \partial_\theta + \theta\partial_z$, and, as usual, $\int \mathrm{d}\theta$ really means $\partial/\partial\theta$. Similarly, for $N=2$, the vector fields and associated fields are

$$l_n = -z^n\left(z\partial_z + \tfrac{1}{2}(n+1)\theta_i\partial_{\theta_i}\right), \quad l(z) = z^{m+1},$$
$$g_r^i = z^{r-1/2}\left(z\theta_i\partial_z - z\partial_{\theta_i} + \left(r+\tfrac{1}{2}\right)\theta_i\theta_j\partial_{\theta_j}\right), \quad g^i(z) = z^{r+1/2}, \tag{19}$$
$$t_m = -z^m(\theta_2\partial_{\theta_1} - \theta_1\partial_{\theta_2}), \quad t(z) = z^m.$$

Introducing the graded field,

$$X_{(i)} = \tfrac{1}{2} l_{(i)} + \theta_j g^j_{(i)} + \theta_1\theta_2 t_{(i)} \tag{20}$$

the 2-cocycle is given by

$$c(X_{(1)},X_{(2)}) = \frac{1}{6\pi i}\oint_0 \mathrm{d}z\, \mathrm{d}\theta_2\, \mathrm{d}\theta_1 (D_1 D_2 X'_{(1)}) X_{(2)}, \tag{21}$$

where $D_i = \partial_{\theta_i} + \theta_i \partial_z$. For $N=3$,

$$\begin{gathered}
l_n = -z^n\left(z\partial_z + \tfrac{1}{2}(n+1)\theta_i\partial_{\theta_i}\right), \quad l(z) = z^{m+1}, \\
g^i_r = z^{r-1/2}\left(z\theta_i\partial_z - z\partial_{\theta_i} + \left(r+\tfrac{1}{2}\right)\theta_i\theta_j\partial_{\theta_j}\right), \quad g^i(z) = z^{r+1/2}, \\
t^i_m = z^{m-1}(z\epsilon_{ijk}\theta_j\partial_{\theta_k} - m\theta_1\theta_2\theta_3\partial_{\theta_i}), \quad t^i(z) = z^m, \\
\psi_r = -z^{r-1/2}\left(\theta_1\theta_2\theta_3\partial_z + \tfrac{1}{2}\epsilon_{ijk}\theta_i\theta_k\partial_{\theta_k}\right), \quad \psi(z) = z^{r-1/2},
\end{gathered} \tag{22}$$

$$X_{(i)} = \tfrac{1}{2} l_{(i)} + \theta_j g^j_{(i)} + \tfrac{1}{2}\epsilon_{klm}\theta_k\theta_l t^m_{(i)} + \theta_1\theta_2\theta_3\psi_{(i)}, \tag{23}$$

$$c(X_{(1)},X_{(2)}) = \frac{1}{6\pi i}\oint_0 \mathrm{d}z\, \mathrm{d}\theta_3\, \mathrm{d}\theta_2\, \mathrm{d}\theta_1 (D_1 D_2 D_3 X_{(1)}) X_{(2)}. \tag{24}$$

Now, for $N=4$, $X_{(i)}$ is given by

$$X_{(i)} = \tfrac{1}{2} l_{(i)} + \theta_j g^j_{(i)} + \tfrac{1}{2}\theta_a\theta_b t^{ab}_{(i)} - \tfrac{1}{6}\epsilon_{abcd}\theta_a\theta_b\theta_c\psi^d_{(i)} - \theta_1\theta_2\theta_3\theta_4 \tfrac{1}{2} u_{(i)}, \tag{25}$$

where $u_{(i)} = z^{n-1}$ corresponds to the vector u_m in (3), and similarly for the other fields in $X_{(i)}$. In the cases so far, given an $X_{(i)}$, a conformal vector field can be obtained. It is worth considering what $X_{(i)}$ means in the operator approach. To this end, recall the super stress-energy tensor $\mathbb{T}$ from (8). From the OPE (11), it can be shown that $L(z)$ scales like a field of weight 2, and hence expansion $L(z) = \Sigma_m L_m z^{-m-2}$. Similarly, the other operators have scaling dimensions-G^i is $\frac{3}{2}$, T^{ij} is 1, ψ^j is $\frac{1}{2}$ and U is 0. In fact, the G^i, T^{ij}, ψ^j are primary fields. Now, rather than obtain the vector field associated to $X_{(i)}$, the operator associated to it can be obtained by computing

$$\frac{1}{\pi i}\oint_0 \mathrm{d}z\, \mathrm{d}\theta_4\, \mathrm{d}\theta_3\, \mathrm{d}\theta_2\, \mathrm{d}\theta_1\, X_{(i)}\mathbb{T}. \tag{26}$$

A similar formula[12] holds for the smaller N. Since V_0 is a part of $\mathbb{T}$, one can ask how to obtain the operator V_0 from the above integral, and see if it sheds light on how the $[u_0, v_0] = c^+/4$ commutator might be obtained. To this end, consider the logarithmic part of

$$\begin{aligned}
\frac{1}{\pi i}\int_{1+i\epsilon}^{1-i\epsilon} \mathrm{d}z \frac{1}{2} u(z) U(z) &= \frac{1}{\pi i}\int_{1+i\epsilon}^{1-i\epsilon} \mathrm{d}z \frac{1}{2} u(z) V_0 \log(z) \\
&= -\frac{1}{2\pi i}\int_{1+i\epsilon}^{1-i\epsilon} \mathrm{d}z \frac{1}{z} V_0 \int u + \frac{1}{2\pi i} V_0 \left[\log(z)\int u\right]_{1+i\epsilon}^{1-i\epsilon}.
\end{aligned} \tag{27}$$

Concentrating on the first part of the expression, it seems very suggestive to associate the constant part of $\int u$, which arises as an integration constant, to the algebra element v_0 (assuming $\int u$ is single valued around the origin, i.e., u has no $1/z$ term). This turns out to be precisely what is needed to obtain the c^+ 2-cocycle,

$$c^+(X_{(1)},X_{(2)}) = \frac{-1}{2\pi i}\oint_0 \mathrm{d}z\,\mathrm{d}\theta_4\,\mathrm{d}\theta_3\,\mathrm{d}\theta_2\,\mathrm{d}\theta_1\left(D_1D_2D_3D_4\int X_{(1)}\right)X_{(2)} \tag{28}$$

assuming the integrand is single valued around the origin. On expanding out the $X_{(i)}$ and applying all the superderivatives, the only component of $X_{(1)}$ that is actually integrated in $D_1D_2D_3D_4\int X_{(1)}$ is the $u_{(1)}$ component. This essentially means that $c^+(u_0,u_0)$ cannot be explicitly obtained, since the integrand would have logs in it. This, however, is not a problem, since $[u_0,u_0]=0$ by antisymmetry of the commutator. Also, $c^+(v_0,v_0)$ is not obtained, but by the same argument is clearly zero. Most importantly, if the integration constant is taken to be 1, then one can obtain $c^+(v_0,u_0)=-\frac{1}{4}$. The c^- cocycle can also be found,

$$c^-(X_{(1)},X_{(2)}) = -\frac{1}{2\pi i}\oint_0 \mathrm{d}z\,\mathrm{d}\theta_4\,\mathrm{d}\theta_3\,\mathrm{d}\theta_2\,\mathrm{d}\theta_1 X'_{(1)}X_{(2)} \tag{29}$$

as well as an expression for the v_0 extension,

$$v_0(X_{(1)},X_{(2)}) = \frac{2}{\pi i}\oint_0 \mathrm{d}z\,\mathrm{d}\theta_4\,\mathrm{d}\theta_3\,\mathrm{d}\theta_2\,\mathrm{d}\theta_1\left(\frac{1}{z}\left(1-\tfrac{1}{2}\theta_i\partial_{\theta_i}\right)X_{(1)}\right)X_{(2)}. \tag{30}$$

All of the extensions here for all N are consistent with the operator formalism. Apart from c^+ in $N=4$, which has a problem with logs, all the extensions can be obtained from the super OPE by calculating

$$-\frac{1}{4\pi}\oint_0 \mathrm{d}z\,\mathrm{d}\theta_N\cdots\mathrm{d}\theta_1\oint_z \mathrm{d}w\,\mathrm{d}\chi_N\cdots\mathrm{d}\chi_1\,X_{(1)}(Z_1)X_{(2)}(Z_2)\mathbb{T}(Z_1)\mathbb{T}(Z_2) \tag{31}$$

and give rise to the same formulas. The formulas also suggest that the extensions should be described by a map from two vector fields into something proportional to the volume form

$$C:\mathcal{D}^1\mathcal{A}_N\times\mathcal{D}^1\mathcal{A}_N\to \mathrm{d}z\otimes_i\frac{\partial}{\partial\theta_i}. \tag{32}$$

VI. *N*=1 GELFAND–FUCHS 2-COCYCLE

In (17), a parametrization of a vector field in terms of a field was written. One can try and explore how these fields are related to a graded Riemann sphere. First, redefine $X=\frac{1}{2}f(z)+g(z)\theta$, where now f and g need not have a defined parity, i.e., they are each a sum of an even part and an odd part. Now, introduce the map

$$l:X\mapsto -\left(f(z)\frac{\partial}{\partial z}+\frac{1}{2}f'(z)\theta D\right)-g(z)\left(2\theta\frac{\partial}{\partial z}-D\right). \tag{33}$$

Under this identification, (18) holds. In components (18) now reads

$$c(X_{(1)},X_{(2)}) = \frac{1}{6\pi i}\oint \mathrm{d}z\left(\frac{1}{4}f'''_{(1)}f_{(2)}+(-1)^{g_{(2)}}g''_{(1)}g_{(2)}\right), \tag{34}$$

where[13] $(-1)^{g_{(2)}}g_{(2)}=(-1)^{g_{(2)0}}g_{(2)0}+(-1)^{g_{(2)1}}g_{(2)1}=g_{(2)0}-g_{(2)1}$ with $g_{(2)0}$ and $g_{(2)1}$ being, respectively, the even and odd parts of $g_{(2)}$. Recall that any invertible superconformal transformation can be parametrized by $\Phi:(z,\theta)\mapsto(w,\pi)$,

$$w = w_0 + \theta w_1 (w_0')^{1/2},$$

$$\chi = w_1 + \theta (w_0' + w_1 w_1')^{1/2}, \tag{35}$$

where $w_0 = w_0(z)$ is even and with body, and $w_1 = w_1(z)$ is odd. Restricting to invertible transformations, and using the superconformal condition $Dw = \chi D\chi$, one can show that

$$\Phi^* \begin{pmatrix} \frac{\partial}{\partial w} \\ D_\chi \end{pmatrix} = \begin{pmatrix} (D_\theta \chi)^{-2} & -\left(\frac{\partial \chi}{\partial z}\right)(D_\theta \chi)^{-3} \\ 0 & (D_\theta \chi)^{-1} \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial z} \\ D_\theta \end{pmatrix}. \tag{36}$$

Plugging in the parametrization (35), and looking at the pull-pack of the vector field $l(X)$, one finds the induced transformation law for X,

$$X(w, \chi) \mapsto (D_\theta \chi)^{-2} (X \circ \Phi)(z, \theta) =: \hat{X}(z, \theta) \tag{37}$$

showing that X can in fact be identified with components of sections of the locally rank one sheaf ω^{-1},[7,9] where $\omega = \mathrm{d}z + \theta\, \mathrm{d}\theta$. Thus, in local coordinates, it reads as the tensor $\mathbf{X} = X\omega^{-1}$, yielding the transformation law

$$\Phi^*(X(w, \chi)\omega^{-1}) = (X \circ \Phi)(z, \theta)\omega^{-1}(D_\theta \chi)^{-2} = \hat{X}(z, \theta)\omega^{-1}. \tag{38}$$

A bracket can be introduced on $\Gamma(\omega^{-1})$[6]as

$$[X_{(1)}, X_{(2)}] = -2X_{(1)}X_{(2)}' + 2X_{(1)}'X_{(2)} - (-1)^{X_{(1)}}(DX_{(1)})(DX_{(2)}). \tag{39}$$

The bracket represents graded antisymmetric and obeys the graded Jacobi identity, and hence defines a Lie graded algebra structure. The map $l: \Gamma(\omega^{-1}) \to \Gamma(\mathcal{D}^1 \mathcal{A}_1)$ is then a Lie graded algebra homomorphism, with the brackets on vector fields given by the usual Lie bracket. Equation (18) can be rewritten as

$$c(X_{(1)}, X_{(2)}) = \frac{1}{12\pi i} \oint_0 \mathrm{d}z\, \mathrm{d}\theta ((DX_{(1)}'')X_{(2)} - (-1)^{X_{(1)}X_{(2)}}(DX_{(2)}'')X_{(1)}). \tag{40}$$

The integration measure, transforms, according to the Berezinian as

$$\Phi^* \left[\mathrm{d}w \frac{\partial}{\partial \chi} \right] = \left[\mathrm{d}z \frac{\partial}{\partial \theta} \right] (D_\theta \chi). \tag{41}$$

Knowing how X transforms from (37), one can compute

$$\begin{aligned} \Phi^*((D_\chi X_{(1)}'')X_{(2)} - (-1)^{X_{(1)}X_{(2)}}(D_\chi X_{(2)}'')X_{(1)}) = (D_\theta \chi)^{-1} &((D_\theta \hat{X}_{(1)}'')\hat{X}_{(2)} - (-1)^{X_{(1)}X_{(2)}}(D_\theta \hat{X}_{(2)}'')\hat{X}_{(1)} \\ &+ 2\{\chi, \theta\}[\hat{X}_{(1)}, \hat{X}_{(2)}] + D_\theta(\{\chi, \theta\}((D_\theta \hat{X}_{(1)}'')\hat{X}_{(2)} \\ &- (-1)^{X_{(1)}X_{(2)}}(D_\theta \hat{X}_{(2)}'')\hat{X}_{(1)})\ ), \end{aligned} \tag{42}$$

where the primes on the left-hand side are derivatives with respect to w, and on the right-hand side with respect to z. Also, $(-1)^X \hat{X} = (-1)^{\hat{X}} \hat{X}$ on virtue of $D_\theta \chi$ being even and

$$\{\chi, \theta\} = \frac{\chi''}{D_\theta \chi} - 2\frac{\chi' D_\theta \chi'}{(D_\theta \chi)^2} \tag{43}$$

is the $N = 1$ Schwarzian.[8] Notice that the last term in (42) is a total derivative in D_θ, and hence will vanish under the integral. Hence, it is most useful to look at sections of $\mathrm{d}z \otimes \partial/\partial\theta$ modulo exact derivatives. More explicitly,

$$\oint_0 \mathrm{d}z\, \mathrm{d}\theta (f_0 + f_1\theta) = (-1)^{f_1} \oint_0 \mathrm{d}z\, f_1 \tag{44}$$

and modulo exact derivatives means that if f_1 has an antiderivative, then $(f_0+f_1\theta)\sim 0$. In particular, this means

$$f_0 + f_1\theta = f_0 + F_1'\theta = D_\theta((-1)^{F_1}F_1 + (-1)^{f_0}f_0\theta) \sim 0 \tag{45}$$

as required.

Given $\Phi:(z,\theta)\mapsto(w,\chi)$, a contravariant map can be defined as

$$U_{\chi,\theta}:\begin{pmatrix} \frac{c}{6}((D_\chi X''_{(1)})X_{(2)} - (-1)^{X_{(1)}X_{(2)}}(D_\chi X''_{(2)})X_{(1)}) \\ [X_{(1)},X_{(2)}] \end{pmatrix} \mapsto \begin{pmatrix} \frac{c}{6}((D_\theta \hat{X}''_{(1)})\hat{X}_{(2)} - (-1)^{X_{(1)}X_{(2)}}(D_\theta \hat{X}''_{(2)})\hat{X}_{(1)}) \\ [\hat{X}_{(1)},\hat{X}_{(2)}] \end{pmatrix} \tag{46}$$

by

$$\begin{aligned} &U_{\chi,\theta}\begin{pmatrix} \frac{c}{6}((D_\chi X''_{(1)})X_{(2)} - (-1)^{X_{(1)}X_{(2)}}(D_\chi X''_{(2)})X_{(1)}) \\ [X_{(1)},X_{(2)}] \end{pmatrix} \\ &= \begin{pmatrix} (D_\theta\chi) & -\frac{c}{3}\{\chi,\theta\}(D_\theta\chi)^{-2} \\ 0 & (D_\theta\chi)^{-2} \end{pmatrix} \Phi^* \begin{pmatrix} \frac{c}{6}((D_\chi X''_{(1)})X_{(2)} - (-1)^{X_{(1)}X_{(2)}}(D_\chi X''_{(2)})X_{(1)}) \\ [X_{(1)},X_{(2)}] \end{pmatrix}, \end{aligned} \tag{47}$$

recalling that the first term is only defined up to exact derivatives. Given, in addition, a map $\Psi:(w,\chi)\mapsto(u,\rho)$, and using the property of the Schwarzian $\{\rho,\theta\}=\{\rho,\chi\}(D_\theta\chi)^3+\{\chi,\theta\}$ which can be deduced from (43), one can show

$$U_{\chi,\theta}\circ U_{\rho,\chi} = U_{\rho,\theta}. \tag{48}$$

Associating the necessary open sets to the maps Φ and Ψ then realizes (48) as the requirement on restriction maps. This then, locally, represents a nontrivial extension of

$$\left[\mathrm{d}z\frac{\partial}{\partial\theta}\right] \oplus \omega^{-1} \tag{49}$$

modulo exact derivatives in the first slot and for $c\neq 0$. If $c=0$, the extension becomes trivial. The graded Lie brackets can then be defined on sections of this extension as

$$\left[\begin{pmatrix} \lambda \\ X_{(1)} \end{pmatrix},\begin{pmatrix} \mu \\ X_{(2)} \end{pmatrix}\right] = \begin{pmatrix} \frac{c}{6}((D_\chi X''_{(1)})X_{(2)} - (-1)^{X_{(1)}}X_{(1)}(D_\chi X''_{(2)})) \\ [X_{(1)},X_{(2)}] \end{pmatrix}, \tag{50}$$

where the grade is given by the lower component. Note that, although it looks like the top component has a different parity to the bottom component, after performing the $\int \mathrm{d}z\, \mathrm{d}\theta$ integral to get the central charge, it will have the same parity. The graded Jacobi identity is already satisfied by the lower component, it remains to verify the upper component.

$$(-1)^{X_{(1)}X_{(3)}}\left[\left[\begin{pmatrix} \lambda \\ X_{(1)} \end{pmatrix},\begin{pmatrix} \mu \\ X_{(2)} \end{pmatrix}\right],\begin{pmatrix} \sigma \\ X_{(3)} \end{pmatrix}\right] + \text{cyclic} = \begin{pmatrix} U \\ 0 \end{pmatrix} \tag{51}$$

has top component

$$
\begin{aligned}
U = {} & (-1)^{X_{(1)}X_{(3)}}((-(DX_{(1)})X'''_{(2)} + (-1)^{X_{(1)}}X'''_{(1)}(DX_{(2)}) - 3(-1)^{X_{(1)}}X'_{(1)}(DX''_{(2)}) + 3(DX''_1)X'_2 \\
& - 2(-1)^{X_{(1)}}X_1(DX'''_2) + 2(DX'''_{(1)})X_{(2)})X_3 + (-1)^{X_{(1)}+X_{(2)}}(2X_{(1)}X'_{(2)} - 2X'_{(1)}X_{(2)} \\
& + (-1)^{X_{(1)}}(DX_{(1)}DX_{(2)})))(DX''_3) + \text{cyclic} \\
= {} & (-1)^{X_{(1)}X_{(3)}}\partial(2(DX'_{(1)})X'_{(2)}X_{(3)} - 2(DX'_{(1)})X_{(2)}X'_{(3)} + 2(-1)^{(X_1)}X_{(1)}(DX'_{(2)})X'_{(3)} \\
& - 2(-1)X_{(1)}(DX'_{(2)})X_{(3)} + 2(-1)^{X_{(1)}+X_{(2)}}X'_{(1)}X_{(2)}(DX'_{(3)}) - 2(-1)^{X_{(1)}+X_{(2)}}X_{(1)}X'_{(2)}(DX'_{(3)}) \\
& - (-1)^{X_{(2)}}\partial((DX_{(1)})(DX_{(2)})(DX_{(3)}))) + (-1)^{X_{(1)}X_{(3)}}D(2(-1)^{X_{(1)}}(DX'_{(1)}) \\
& - 2(-1)^{X_{(1)}+X_{(2)}}(DX'_{(1)})X_{(2)}(DX'_{(3)}) + 2(-1)^{X_{(2)}}X_{(1)}(DX'_{(2)})(DX'_{(3)}) + (-1)^{X_{(1)}}(DX''_{(1)})(DX_{(2)})X_{(3)} \\
& - (-1)^{X_{(1)}+X_{(2)}}(DX''_{(1)})X_{(2)}(DX_{(3)}) + (-1)^{X_{(1)}}(DX_{(1)})(DX''_{(2)})X_{(3)} + (-1)^{X_{(2)}}X_{(1)}(DX''_{(2)})(DX_{(3)}) \\
& + (-1)^{X_{(2)}}X_{(1)}(DX_{(2)})(DX''_{(3)}) - (-1)^{X_{(1)}+X_{(2)}}(DX_{(1)})X_{(2)}(DX''_{(3)})) \sim 0, \qquad (52)
\end{aligned}
$$

where the equivalence follows since the term is a total derivative (recall $\partial = D^2$), and the brackets obey the graded Jacobi identity. Hence, the algebra of conformal vector fields admits an extension on the graded Riemann sphere to accommodate the central charge, which realizes a map of the form (32) using (18). The construction precisely mirrors that done for the bosonic case in Ref. 10. Given the list of Schwarzians in Ref. 8, it should be possible to extend the construction to all $N \leqslant 4$.

VII. CONCLUSIONS

If one wishes to study all of the conformal symmetries on an $N=4$ graded Riemann sphere at the quantum level, and not neglect any symmetries, then one is forced to look at adding noncentral extensions to the algebra. If the u_0 symmetry is neglected, then all of the extensions are central. To the author's knowledge, this has not been observed before, and the author is unaware of the $N=4$ algebra given by (6) having appeared previously in the literature. It was found that this extension was completely consistent with the usual CFT treatments of the quantum theory, i.e., with the operator product expansions of the $N=4$ theory, and in fact explained why the logarithms appeared in the OPE. The effect on the representation theory was discussed, as was the description of the Gelfand–Fuchs extensions for $N=1,\ldots,4$, given by the superfield formalism. There, it was found that the extra extension explained the appearance of the indefinite integral inside the contour integral in (28). It was then described for the $N=1$ case how the central extension arises from the geometry of an $N=1$ graded Riemann sphere, and how it might be expected that the central extensions for the higher N might be obtained.

As well as exploiting graded Riemann sphere geometry to describe extensions of superconformal algebras, these calculations also shed some light on how one might try to treat noncentral extensions in a CFT. In this case, the field theory exhibited an, albeit mild, logarithmic behavior, not unrelated to the manner in which zero modes are modified in Ref. 2. For higher N, the requirement of having a Virasoro subalgebra with nonzero central extension could force noncentral extensions to appear that enrich the zero mode structure. $N=5$ would have a graded odd weight $-\frac{1}{2}$ field whose zero mode structure might give unavoidable Jordan cells in the representation theory. In the $N=4$ case, the modified zero mode structure was reflected by the appearance of indefinite integrals in the Gelfand–Fuchs extensions.

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[11] If $U(z)|0\rangle$ is to be regular at $z=0$, then V_0 must annihilate $|0\rangle$.
[12] For example, in the $N=0$ case $(1/\pi i)\oint_0 dz\, X_{(i)}\mathbb{T}=(1/2\pi i)\oint_0 dz\, l_{(i)}L(z)$. The vector l_n is parametrized by $l_{(i)}=z^{n+1}$. Then $(1/2\pi i)\oint_0 dz\, l_{(i)}L(z)=(1/2\pi i)\oint_0 z^{n+1}\Sigma_m L_m z^{-m-2}=L_n$.
[13] More generally, $(-1)^{\Pi_i X_{(i)}}\Pi_i X_{(i)}=\Sigma_{n_i\in\{0,1\}}(-1)^{\Pi_i X_{(i)n_i}}\Pi_i X_{(i)n_i}$.

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Functional determinants for the Dirac equation with mixed pseudodifferential boundary conditions over finite cylinders

Paul Loya[a)]
Department of Mathematics, Binghamton University, Vestal Parkway East, Binghamton, New York 13902

Jinsung Park[b)]
Mathematisches Institut, Universität Bonn, Beringstrasse 1, D-53115 Bonn, Germany

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In this note, we explicitly compute the functional determinant of a Dirac Laplacian with nonlocal *pseudodifferential* boundary conditions over a finite cylinder in terms of the ζ-function of the Dirac operator on the cross section and the pseudodifferential operators defining the boundary conditions. In particular, this result reduces to our previous formula [J. Phys. A **37**, 7381 (2004)] for the special case of generalized Atiyah–Patodi–Singer conditions. To prove our main result, we use the gluing and comparison formulas established by the present authors in Refs 14 and 15.
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I. INTRODUCTION

Recent advances in quantum field theory have necessitated the explicit evaluation of functional determinants of Dirac operators over a variety of space–time configurations. In fact, at the one-loop order, any such theory can be reduced to the theory of determinants. We refer the reader to the works of Dowker and Critchley[1] and Hawking.[2] See also Elizalde *et al.*,[3] Kirsten,[4] and Scott and Wojciechowski,[5] for recent reviews. Because of their increasingly important role in mathematical physics, over the past several years there has been intense research to compute functional ζ-determinants of Dirac Laplacians. Of great significance is the Dirac Laplacian with spectral pseudodifferential boundary conditions; the Atiyah–Patodi–Singer (henceforth APS) boundary conditions being the most well-known example. Such boundary conditions arise in, for instance, one-loop quantum cosmology,[6–8] spectral branes,[9] and the study of Dirac fields in the background of a magnetic flux.[10]

However, only recently was the open problem of explicitly computing the ζ-determinant of a Dirac Laplacian with APS conditions over a finite cylinder solved.[11] One reason this problem withstood the efforts of existing mathematical methods is that it is impossible to find explicit formulas for the eigenvalues of such a Dirac operator. For this reason, we had to attack the problem using the method of *adiabatic decomposition* pioneered by Douglas and Wojciechowski[12] for the eta invariant and by the second author and Wojciechowski[13] for the ζ-determinant. The purpose of this current paper is twofold. First, we extend the result of Ref. 11 to a general class of pseudodifferential conditions that generalize the APS condition up to operators of *arbitrary* finite rank. To compute the ζ-determinant in this generalized framework, which in some sense possesses eigenvalues that are even more enigmatic, we use the gluing and comparison formulas for ζ-determinants proved by the authors in Refs. 14 and 15 to break up this general framework into tangible parts which can be explicitly computed. The second purpose of this paper is to elucidate

[a)]Electronic mail: paul@math.binghamton.edu
[b)]Electronic mail: jpark@math.uni.bonn.de

the effectiveness of these gluing and comparison formulas to compute ζ-determinants that have eluded explicit evaluations due to the perplexity of their eigenvalues. This also exemplifies the aim of gluing and comparison formulas: Breaking up complex problems into simpler more tractable ones.

We now describe our setup. Fix $R>0$ and let $\mathcal{D}:C^\infty(N_R,S)\to C^\infty(N_R,S)$ be a Dirac type operator where $N_R=[-R,R]\times Y$ is a finite cylinder with $R>0$, Y a closed compact Riemannian manifold (of arbitrary dimension), and S a Clifford bundle over N_R. We assume that $\mathcal{D}$ is of product form

$$\mathcal{D}=G(\partial_u+D_Y), \tag{1.1}$$

where G is a unitary bundle isomorphism of S and D_Y is a Dirac operator acting on $C^\infty(Y,S)$ such that $G^2=-\mathrm{Id}$ and $GD_Y=-D_YG$. Furthermore, we assume that

$$\dim(\ker(G+i)\cap\ker(D_Y))=\dim(\ker(G-i)\cap\ker(D_Y)). \tag{1.2}$$

Let Π_+,Π_-, and Π_0 denote the orthogonal projections onto the positive, negative, and zero eigenspaces of D_Y. Since N_R has boundaries, we have to impose boundary conditions. Let $\mathrm{Gr}^*_\infty(D_Y)$ denote the space of pairs $(\mathcal{P}_1,\mathcal{P}_2)$, where $\mathcal{P}_1$ and $\mathcal{P}_2$ are orthogonal pseudodifferential projections on $L^2(Y,S)$ such that

$$\mathcal{P}_1-\Pi_+,\quad \mathcal{P}_2-\Pi_-\ \text{are smoothing operators},$$

and for $i=1,2$,

$$\mathcal{P}_iG=G(\mathrm{Id}-\mathcal{P}_i),\quad D_Y\mathcal{P}_i=\mathcal{P}_iD_Y.$$

An important class of such boundary conditions are the renowned generalized APS spectral conditions,[16] which are defined as follows. Let σ_1,σ_2 be involutions (that is, $\sigma_i^2=\mathrm{Id}$) over $\ker(D_Y)$ such that $\sigma_1G=-G\sigma_1$ and $\sigma_2G=-G\sigma_2$. Note that such involutions exist because of the assumption (1.2). Then

$$\Pi_+^{\sigma_1}:=\Pi_++\frac{1+\sigma_1}{2}\Pi_0,\quad \Pi_-^{\sigma_2}:=\Pi_-+\frac{1+\sigma_2}{2}\Pi_0 \tag{1.3}$$

are called *generalized APS spectral projections*, and $(\Pi_+^{\sigma_1},\Pi_-^{\sigma_2})\in\mathrm{Gr}^*_\infty(D_Y)$. These generalized APS boundary conditions were considered in our paper (Ref. 11), but elements of $\mathrm{Gr}^*_\infty(D_Y)$ are much more general and can differ from APS projections by operators of *arbitrary* finite rank. Let $P=(\mathcal{P}_1,\mathcal{P}_2)\in\mathrm{Gr}^*_\infty(D_Y)$ and impose boundary conditions for $\mathcal{D}$ at $\{-R\}\times Y$ and $\{R\}\times Y$ via

$$\mathcal{P}_1\quad\text{at}\ \{-R\}\times Y,\quad \mathcal{P}_2\quad\text{at}\ \{R\}\times Y.$$

We denote by $\mathcal{D}_P$ the resulting operator with these boundary conditions, that is,

$$\mathcal{D}_P:=\mathcal{D}:\mathrm{dom}(\mathcal{D}_P)\to L^2(N_R,S), \tag{1.4}$$

where

$$\mathrm{dom}(\mathcal{D}_P):=\{\phi\in H^1(N_R,S)\,|\,\mathcal{P}_1(\phi|_{u=-R})=0,\quad \mathcal{P}_2(\phi|_{u=R})=0\}.$$

By the fundamental work of Seeley,[17,18] the spectrum of the Dirac operator $\mathcal{D}_P$ consists of discrete real eigenvalues $\{\lambda_k\}$. The ζ-function of $\mathcal{D}_P^2$ is defined by

$$\zeta_{\mathcal{D}_P^2}(s)=\sum_{\lambda_k\neq0}\lambda_k^{-2s},$$

which is *a priori* defined for $\Re(s)\gg0$, and by the work of Grubb[19,20] and Wojciechowski[21] (cf. Lei[22] and Loya and Park[15]), has a meromorphic extension to $\mathbb{C}$ with 0 as a regular point. The ζ-determinant of $\mathcal{D}_P^2$ is defined by

$$\det_\zeta \mathcal{D}_P^2 := \exp(-\zeta'_{\mathcal{D}_P^2}(0)).$$

This definition first appeared in Ray and Singer's seminal paper[23] on the analytic torsion. Since we imposed nonlocal pseudodifferential boundary conditions, it is impossible to compute the eigenvalues $\{\lambda_k\}$ of $\mathcal{D}_P$ explicitly, so there is no direct way to compute the ζ-determinant $\det_\zeta \mathcal{D}_P^2$ from the eigenvalues. However, we shall give two derivations of the formula for $\det_\zeta \mathcal{D}_P^2$:

(1) Using the gluing formula proved in Ref. 14.
(2) Using the comparison/relative invariant formula proved in Ref. 15.

See Sec. II for more on these results. The formula for $\det_\zeta \mathcal{D}_P^2$ is described as follows. Since the $\mathcal{P}_i$'s are orthogonal projectors such that $\mathcal{P}_i G = G(\mathrm{Id} - \mathcal{P}_i)$ by assumption, with respect to the decomposition

$$L^2(Y,S) = L^2(Y,S^+) \oplus L^2(Y,S^-) \tag{1.5}$$

with $S^\pm$ denoting the $(\pm i)$-eigenspaces of G in S (recall that $G^2 = -\mathrm{Id}$), we can write

$$\mathcal{P}_i = \frac{1}{2}\begin{pmatrix} \mathrm{Id} & \kappa_i^{-1} \\ \kappa_i & \mathrm{Id} \end{pmatrix},$$

where $\kappa_i : L^2(Y,S^+) \to L^2(Y,S^-)$ are corresponding isometries. In particular,

$$U_P := -\kappa_1 \kappa_2^{-1} : L^2(Y,S^-) \to L^2(Y,S^-)$$

is a unitary operator. Let $\hat{U}_P$ denote the restriction of U_P to the orthogonal complement of its (-1)-eigenspace. Let $W := \mathrm{Im}(\mathrm{Id} - \mathcal{P}_1) \cap \mathrm{Im}(\mathrm{Id} - \mathcal{P}_2)$. Then our assumptions on $(\mathcal{P}_1, \mathcal{P}_2)$ imply that W is a finite-dimensional vector space and that $D_Y : \mathrm{Im}(\mathcal{P}_i) \to \mathrm{Im}(\mathcal{P}_i)$ and $D_Y : \mathrm{Im}(\mathrm{Id} - \mathcal{P}_i) \to \mathrm{Im}(\mathrm{Id} - \mathcal{P}_i)$. We define a map T_P over W by

$$T_P := \begin{cases} \frac{\sinh(2RD_Y)}{D_Y} & \text{on } W \cap \ker(D_Y)^\perp, \\ 2R & \text{on } W \cap \ker(D_Y). \end{cases}$$

We also define $T_{\mathcal{P}_1}$ and $T_{\mathcal{P}_2}$ over the finite-dimensional vector spaces $\mathrm{Im}(\Pi_+) \cap \mathrm{Im}(\mathrm{Id} - \mathcal{P}_1)$ and $\mathrm{Im}(\Pi_+) \cap \mathrm{Im}(\mathcal{P}_2)$, respectively, by

$$T_{\mathcal{P}_1} := e^{4RD_Y}, \quad T_{\mathcal{P}_2} := e^{4RD_Y}.$$

The following theorem is the main result of this note.

Theorem 1.1. *The following equality holds:*

$$\det_\zeta \mathcal{D}_P^2 = e^{2CR} 2^{\zeta_{D_Y^2}(0) + h_Y} \frac{(\det T_P)^2}{(\det T_{\mathcal{P}_1})^2 (\det T_{\mathcal{P}_2})^2} \cdot \det_F\left(\frac{2\,\mathrm{Id} + \hat{U}_P + \hat{U}_P^{-1}}{4} \right),$$

where $C = (\Gamma(s)^{-1} \zeta_{D_Y^2}(s - 1/2))'(0)$ *with* $\zeta_{D_Y^2}(s)$ *the* ζ*-function of* D_Y^2, $h_Y = \dim \ker(D_Y)$ *and* $\det_F$ *denotes the Fredholm determinant.*

More explicitly, if we let E_μ denote the eigenspace of D_Y associated to the eigenvalue $\mu \in \mathrm{spec}(D_Y)$, then we can write

$$\det{}_\zeta \mathcal{D}_P^2 = e^{2CR} 2^{\zeta_{D_Y^2}(0)+h_Y} \left(\prod_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\neq 0}} e^{-4\mu R} \right) \cdot \left(\prod_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathcal{P}_2)\neq 0}} e^{-4\mu R} \right)$$
$$\cdot \left(\prod_{\substack{\mu \in \mathrm{spec}(D_Y) \\ E_\mu \cap W \neq 0}} \frac{\sinh^2(2\mu R)}{\mu^2} \right) \cdot \det{}_F \left(\frac{2\mathrm{Id} + \hat{U}_P + \hat{U}_P^{-1}}{4} \right), \tag{1.6}$$

where if $\mu=0$ in the product in the second line, we replace $[\sinh^2(2\mu R)]/\mu^2$ by its limit as $\mu \to 0$, that is, $(2R)^2$. In particular, when $\mathcal{P}_1=\Pi_+^{\sigma_1}$ and $\mathcal{P}_2=\Pi_-^{\sigma_2}$, the generalized APS spectral projectors in (1.3), then Theorem 1.1 reduces to the main result of Ref. 11.

$$\det{}_\zeta \mathcal{D}^2_{\Pi_+^{\sigma_1},\Pi_-^{\sigma_2}} = e^{2CR} 2^{\zeta_{D_Y^2}(0)+h_Y} (2R)^{2h} \det{}^* \left(\frac{2\mathrm{Id} - (\sigma_1\sigma_2)_- - (\sigma_1\sigma_2)_-^{-1}}{4} \right), \tag{1.7}$$

where $(\sigma_1\sigma_2)_-$ is the restriction of the unitary map $\sigma_1\sigma_2$ to $L^2(Y,S^-) \cap \ker(D_Y)$, h is the number of $(+1)$-eigenvalues of $(\sigma_1\sigma_2)_-$, and where $\det^*(L)$ denotes the determinant of $(L|_{\ker(L)^\perp})$ for an operator L over a finite-dimensional vector space.

The structure of this paper is as follows. In Sec. II, we review the gluing formula from Ref. 14 and the comparison/relative invariant formula from Ref. 15, which we shall use in the subsequent sections. In Sec. III, we derive new formulas for ζ-determinant ratios of Dirac Laplacians with boundary conditions of special types. Finally, in Sec. IV we combine these special ζ-determinant ratios and the gluing and comparison formulas from Refs. 14 and 15 to derive our main Theorem 1.1.

II. THE GLUING AND COMPARISON FORMULAS FROM REFS. 14 and 15

In this section we review the gluing formula from Ref. 14 and the comparison/relative invariant formula from Ref. 15.

Let $\mathcal{D}$ be a Dirac type operator acting on $C^\infty(M,S)$ where M is a closed compact Riemannian manifold of arbitrary dimension and S is a Clifford bundle over M. Suppose that $M=M_- \cup M_+$ is partitioned into a union of manifolds with a common boundary $Y=\partial M_-=\partial M_+$. We assume that all geometric structures are of product type over a tubular neighborhood N of Y where $\mathcal{D}$ takes the product form (1.1). By restriction of $\mathcal{D}$, we obtain Dirac type operators $\mathcal{D}_\pm$ over $M_\pm$. We impose the boundary conditions given by the orthogonalized Calderón projectors $\mathcal{C}_\pm$ for $\mathcal{D}_\pm$ and we denote by $\mathcal{D}_{\mathcal{C}_\pm}$ the resulting operators,

$$\mathcal{D}_{\mathcal{C}_\pm} = \mathcal{D}_\pm : \mathrm{dom}(\mathcal{D}_{\mathcal{C}_\pm}) := \{\phi \in H^1(M_\pm,S) | \mathcal{C}_\pm(\phi|_Y) = 0\} \to L^2(M_\pm,S).$$

Here, we recall that the Calderón projectors $\mathcal{C}_\pm$ are the projectors defined intrinsically as the unique orthogonal projectors onto the closures in $L^2(Y,S)$ of the infinite-dimensional *Cauchy data spaces* of $\mathcal{D}_\pm$:

$$\{\phi|_Y | \phi \in C^\infty(M_\pm,S), \quad \mathcal{D}_\pm\phi = 0\} \subset C^\infty(Y,S).$$

The *gluing problem* for the ζ-determinant is to describe the "defect"

$$\frac{\det_\zeta \mathcal{D}^2}{\det_\zeta \mathcal{D}^2_{\mathcal{C}_+} \cdot \det_\zeta \mathcal{D}^2_{\mathcal{C}_-}} = \boxed{?}$$

in terms of recognizable data. To describe the solution in Ref. 14, we need to introduce some notations. With respect to the decomposition as in (1.5), the Calderón projectors $\mathcal{C}_\pm$ have the matrix forms

$$\mathcal{C}_\pm = \frac{1}{2}\begin{pmatrix} \mathrm{Id} & \kappa_\pm^{-1} \\ \kappa_\pm & \mathrm{Id} \end{pmatrix}, \tag{2.1}$$

where the maps $\kappa_\pm : L^2(Y,S^+) \to L^2(Y,S^-)$ are corresponding isometries, so that $\mathcal{U} := -\kappa_- \kappa_+^{-1}$ is a unitary operator over $L^2(Y,S^-)$. Furthermore, $\mathcal{U}$ is of Fredholm determinant class. We denote by $\hat{\mathcal{U}}$ the restriction of $\mathcal{U}$ to the orthogonal complement of its (-1)-eigenspace. We also put

$$\mathcal{L} := \sum_{k=1}^{h_M} \gamma U_k \otimes \gamma U_k : \gamma \ker(\mathcal{D}) \to \gamma \ker(\mathcal{D}),$$

where $h_M = \dim \ker(\mathcal{D})$, γ is the restriction map from M to Y, and $\{U_k\}$ is an orthonormal basis of $\ker(\mathcal{D})$. Then $\mathcal{L}$ is a positive operator on the finite-dimensional vector space

$$\gamma \ker(\mathcal{D}) \equiv \mathrm{Im}(\mathcal{C}_-) \cap \mathrm{Im}(\mathcal{C}_+).$$

We now have all the ingredients to state the following *gluing formula*:[14]

$$\frac{\det_\zeta \mathcal{D}^2}{\det_\zeta \mathcal{D}^2_{\mathcal{C}_-} \cdot \det_\zeta \mathcal{D}^2_{\mathcal{C}_+}} = 2^{-\zeta_{D_Y^2}(0)-h_Y} (\det \mathcal{L})^{-2} \det_F\left(\frac{2\mathrm{Id} + \hat{\mathcal{U}} + \hat{\mathcal{U}}^{-1}}{4}\right), \tag{2.2}$$

where $h_Y = \dim \ker(D_Y)$ and $\det_F$ denotes the Fredholm determinant. There is a similar formula for manifolds with cylindrical ends.[24]

We now explain the comparison/relative invariant formula proved in Ref. 15 for $(M_-, \mathcal{D}_-)$. To this end, we consider the space $\mathrm{Gr}^*_\infty(\mathcal{D}_-)$, which consists of orthogonal projections $\mathcal{P}$ such that $\mathcal{P} - \mathcal{C}_-$ are smoothing operators and $G\mathcal{P} = (\mathrm{Id} - \mathcal{P})G$. Let us fix $\mathcal{P} \in \mathrm{Gr}^*_\infty(\mathcal{D}_-)$ and let $\kappa_\mathcal{P} : L^2(Y,S^+) \to L^2(Y,S^-)$ be the map that determines $\mathcal{P}$ as $\kappa_\pm$ does $\mathcal{C}_\pm$ in (2.1). Let $\mathcal{D}_\mathcal{P}$ denote the operator $\mathcal{D}_-$ on M_- with the boundary condition given by $\mathcal{P}$. Let P_W be the orthogonal projection of $L^2(Y,S)$ onto the finite-dimensional vector space

$$W := \gamma \ker(\mathcal{D}_\mathcal{P}) \equiv \mathrm{Im}(\mathcal{C}_-) \cap \mathrm{Im}(\mathrm{Id} - \mathcal{P}).$$

Then we introduce a linear map

$$L := -P_W G \mathcal{R}^{-1} G P_W : \gamma \ker(\mathcal{D}_\mathcal{P}) \to \gamma \ker(\mathcal{D}_\mathcal{P}), \tag{2.3}$$

where $\mathcal{R}$ is the sum of the Dirichlet to Neumann maps on an extension of M_- defined as follows. Fix *any* invertible extension $\widetilde{\mathcal{D}}$ of $\mathcal{D}$ to a manifold $\widetilde{M}$ that contains M_-. (The *double* of $\mathcal{D}$ would do nicely.) Then for any $\varphi \in C^\infty(Y,S)$, there are unique $\phi_1 \in C^\infty(M_-,S)$ and $\phi_2 \in C^\infty(\widetilde{M} \setminus M_-, S)$ that are continuous at Y with value φ such that $\widetilde{\mathcal{D}}^2 \phi_i = 0$, $i = 1, 2$, off of Y. Then

$$\mathcal{R}\varphi := \partial_u \phi_1|_Y - \partial_u \phi_2|_Y. \tag{2.4}$$

In Ref. 15, we prove that L is a positive operator so that $\det L$ is a positive real number. Now the main result of Ref. 15 states that

$$\frac{\det_\zeta \mathcal{D}^2_\mathcal{P}}{\det_\zeta \mathcal{D}^2_{\mathcal{C}_-}} = (\det L)^2 \cdot \det_F\left(\frac{2\mathrm{Id} + \hat{U} + \hat{U}^{-1}}{4}\right), \tag{2.5}$$

where $\hat{U}$ is the restriction of $U := \kappa_- \kappa_\mathcal{P}^{-1}$ to the orthogonal complement of its (-1)-eigenspace. The formula (2.5) extends the work of Scott[25] for the invertible case (cf. Scott and Wojciechowski[26]), and has recently been further extended to noncompact manifolds whose boundaries are manifolds with multi-cylindrical ends.[27]

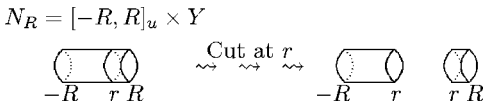

FIG. 1. Cutting N_R at r into two pieces.

III. THE ζ-DETERMINANT FOR SPECIAL BOUNDARY CONDITIONS

If $(\mathcal{P}_1,\mathcal{P}_2)\in \mathrm{Gr}^*_\infty(D_Y)$, then for the sake of clarity we shall denote the operator $\mathcal{D}_P$ in the introduction with these boundary conditions by $\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2}$. Thus, over $N_R=[-R,R]\times Y$ we impose boundary conditions at $\{-R\}\times Y$ and $\{R\}\times Y$ via

$$\mathcal{P}_1 \text{ at } \{-R\}\times Y, \quad \mathcal{P}_2 \text{ at } \{R\}\times Y,$$

and $\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2}$ is the operator with domain

$$\mathrm{dom}(\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2}) := \{\phi\in H^1(N_R,S)\,|\,\mathcal{P}_1(\phi|_{u=-R})=0,\quad \mathcal{P}_2(\phi|_{u=R})=0\}. \tag{3.1}$$

Let $\mathcal{P}$ be a projection on $L^2(Y,S)$ with $(\mathcal{P},\mathrm{Id}-\mathcal{P})\in \mathrm{Gr}^*_\infty(D_Y)$. By definition of $\mathrm{Gr}^*_\infty(D_Y)$, the image of $\mathcal{P}\Pi_0$ is a Lagrangian subspace in $\mathrm{Im}(\Pi_0)=\ker(D_Y)$. Let σ be the involution over $\mathrm{Im}(\Pi_0)$ such that $[(1+\sigma)/2]\Pi_0=\mathcal{P}\Pi_0$. Recalling $\Pi^\sigma_+:=\Pi_+ +[(\mathrm{Id}+\sigma)/2]\Pi_0$, it follows that $(\mathcal{P},\mathrm{Id}-\Pi^\sigma_+)\in \mathrm{Gr}^*_\infty(D_Y)$. Recall that we can write

$$\mathcal{P}=\frac{1}{2}\begin{pmatrix}\mathrm{Id} & \kappa_{\mathcal{P}}^{-1}\\ \kappa_{\mathcal{P}} & \mathrm{Id}\end{pmatrix},\quad \Pi^\sigma_+=\frac{1}{2}\begin{pmatrix}\mathrm{Id} & \kappa_{\sigma}^{-1}\\ \kappa_{\sigma} & \mathrm{Id}\end{pmatrix}$$

for corresponding isometries $\kappa_{\mathcal{P}},\kappa_\sigma: L^2(Y,S^+)\to L^2(Y,S^-)$, and define $\hat{U}_{\mathcal{P}}$ as the restriction of $U_{\mathcal{P}}:=\kappa_{\mathcal{P}}\kappa_\sigma^{-1}$ over $L^2(Y,S^-)$ to the orthogonal complement of its (-1)-eigenspace. Note that $-\kappa_{\mathcal{P}}$ and $-\kappa_\sigma$ are the isometries corresponding to $\mathrm{Id}-\mathcal{P}$ and $\mathrm{Id}-\Pi^\sigma_+$, respectively. We begin by computing the following ratio.

Lemma 3.1: We have

$$\frac{\det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\Pi^\sigma_+}}{\det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\mathcal{P}}}=\left(\prod_{\substack{\mu>0\\ E_\mu\cap \mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}}\frac{e^{4\mu R}\sinh^2(2\mu R)}{\mu^2}\right)\cdot \det_F\left(\frac{2\mathrm{Id}+\hat{U}_{\mathcal{P}}+\hat{U}_{\mathcal{P}}^{-1}}{4}\right),$$

where E_μ denotes the eigenspace of D_Y associated to the eigenvalue $\mu\in\mathrm{spec}(D_Y)$.

Proof: We give two proofs, first using the gluing formula (2.2) then using the comparison formula (2.5), in order to demonstrate the effectiveness of these formulas.

Gluing proof of Lemma 3.1: Let us decompose N_R into two parts $[-R,r]\times Y$ and $[r,R]\times Y$ as shown in Fig. 1. Then the restrictions of $\mathcal{D}_{\mathcal{P},\mathrm{Id}-\Pi^\sigma_+}$ over the decomposed parts $[-R,r]\times Y$ and $[r,R]\times Y$ define two Dirac type operators with boundary conditions given by $\mathcal{P}$ at $\{-R\}\times Y$ and $\mathrm{Id}-\Pi^\sigma_+$ at $\{R\}\times Y$. It is easy to check that the Calderón projections of these two operators are, respectively, just $\mathcal{C}_-=\mathrm{Id}-\mathcal{P}$ and $\mathcal{C}_+=\Pi^\sigma_+$ over $\{r\}\times Y$. We denote the operators over the decomposed parts $[-R,r]\times Y$ and $[r,R]\times Y$, with the new boundary conditions given by these Calderón projectors over $\{r\}\times Y$, by $\mathcal{D}_{\mathcal{P},\mathrm{Id}-\mathcal{P}}(r)$ and $\mathcal{D}_{\Pi^\sigma_+,\mathrm{Id}-\Pi^\sigma_+}(r)$, respectively. Applying the gluing formula (2.2) to this situation, we obtain

$$\frac{\det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\Pi^\sigma_+}}{\det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\mathcal{P}}(r)\cdot \det_\zeta \mathcal{D}^2_{\Pi^\sigma_+,\mathrm{Id}-\Pi^\sigma_+}(r)}=2^{-\zeta_{D_Y^2}(0)-h_Y}(\det \mathcal{L}_r)^{-2}\det_F\left(\frac{2\,\mathrm{Id}+\hat{U}_{\mathcal{P}}+\hat{U}_{\mathcal{P}}^{-1}}{4}\right), \tag{3.2}$$

where $\zeta_{D_Y^2}(s)$ is the ζ-function of D_Y^2 and $h_Y=\dim\ker(D_Y)$, where we used that the $\hat{\mathcal{U}}$ in (2.2) for this situation is $-(-\kappa_{\mathcal{P}})(\kappa_\sigma^{-1})=\kappa_{\mathcal{P}}\kappa_\sigma^{-1}=:\hat{U}_{\mathcal{P}}$, and where

$$\mathcal{L}_r := \sum_{k=1}^{h_{\mathcal{P}}} \gamma_r U_k \otimes \gamma_r U_k : \gamma_r \ker(\mathcal{D}_{\mathcal{P},\mathrm{Id}-\Pi_+^\sigma}) \to \gamma_r \ker(\mathcal{D}_{\mathcal{P},\mathrm{Id}-\Pi_+^\sigma}),$$

where $h_{\mathcal{P}}=\dim \ker(\mathcal{D}_{\mathcal{P},\mathrm{Id}-\Pi_+^\sigma})$, γ_r is the restriction map from N_R to $\{r\}\times Y$, and $\{U_k\}$ is an orthonormal basis of $\ker(\mathcal{D}_{\mathcal{P},\mathrm{Id}-\Pi_+^\sigma})$. From the main result of Ref. 11 [that is, the formula (1.7)], we have

$$\det{}_\zeta \mathcal{D}^2_{\Pi_+^\sigma,\mathrm{Id}-\Pi_+^\sigma}(r) = e^{C(R-r)} 2^{\zeta_{D_Y^2}(0)+h_Y},$$

where $C=(\Gamma(s)^{-1}\zeta_{D_Y^2}(s-1/2))'(0)$. Thus, $\det_\zeta \mathcal{D}^2_{\Pi_+^\sigma,\mathrm{Id}-\Pi_+^\sigma}(r) \to 2^{\zeta_{D_Y^2}(0)+h_Y}$ as $r\to R$, so taking $r\to R$ in (3.2), we see that

$$\frac{\det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\Pi_+^\sigma}}{\det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\mathcal{P}}} = (\det \mathcal{L}_R)^{-2} \det{}_F\left(\frac{2\,\mathrm{Id} + \hat{U}_{\mathcal{P}} + \hat{U}_{\mathcal{P}}^{-1}}{4}\right).$$

It remains to compute $(\det \mathcal{L}_R)^{-2}$. To do so, we note that

$$\ker(\mathcal{D}_{\mathcal{P},\mathrm{Id}-\Pi_+^\sigma}) \equiv \mathrm{Im}(\mathrm{Id}-\mathcal{P}) \cap \mathrm{Im}(\Pi_+^\sigma) = \mathrm{Im}(\mathrm{Id}-\mathcal{P}) \cap \mathrm{Im}(\Pi_+),$$

since $\mathrm{Im}(\mathrm{Id}-\mathcal{P})$ and $\mathrm{Im}(\Pi_+^\sigma)$ have zero intersection in $\ker(D_Y)$ by definition of σ. Let $\{\psi_\mu\}$ be an orthonormal basis of $\mathrm{Im}(\mathrm{Id}-\mathcal{P})\cap\mathrm{Im}(\Pi_+)$ where $\psi_\mu \in E_\mu$. (Here, we recall that $D_Y\mathcal{P}=\mathcal{P}D_Y$, so D_Y preserves $\mathrm{Im}(\mathrm{Id}-\mathcal{P})$ and obviously $\mathrm{Im}(\Pi_+)$ as well. It follows that D_Y can be diagonalized within the finite-dimensional space $\mathrm{Im}(\mathrm{Id}-\mathcal{P})\cap\mathrm{Im}(\Pi_+)$. This elementary fact will be used quite often in the sequel.) Then $\phi_\mu = e^{-\mu u}\psi_\mu \in \ker(\mathcal{D}_{\mathcal{P},\mathrm{Id}-\Pi_+^\sigma})$ and

$$\|\phi_\mu\|^2 = \int_{-R}^{R} e^{-2\mu u} du = \frac{e^{2\mu R} - e^{-2\mu R}}{2\mu} = \frac{\sinh(2\mu R)}{\mu}.$$

It follows that

$$\mathcal{L}_R = \sum_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}} \frac{\phi_\mu(R)}{\|\phi_\mu\|} \otimes \frac{\phi_\mu(R)}{\|\phi_\mu\|} = \sum_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}} \frac{e^{-2\mu R}}{\|\phi_\mu\|^2} \psi_\mu \otimes \psi_\mu.$$

Hence,

$$(\det \mathcal{L}_R)^{-2} = \prod_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}} \left(\frac{e^{-2\mu R}}{\|\phi_\mu\|^2}\right)^{-2} = \prod_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}} e^{4\mu R} \frac{\sinh^2(2\mu R)}{\mu^2}.$$

This completes the Gluing proof of Lemma 3.1.

Comparison proof of Lemma 3.1: We shall apply the comparison formula (2.5) to the pair $(\mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\Pi_+^\sigma}, \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\mathcal{P}})$. Here we regard $\mathrm{Id}-\mathcal{P}$ as the Calderón projector at the boundary $\{R\}\times Y$ of the operator

$$D : \mathrm{dom}(D) \to L^2(N_R, S),$$

where

$$\mathrm{dom}(D) := \left\{\phi \in H^1(N_R,S) \,|\, \mathcal{P}(\phi|_{u=-R}) = 0\right\}.$$

Then $D_{\mathrm{Id}-\Pi_+^\sigma} = \mathcal{D}_{\mathcal{P},\mathrm{Id}-\Pi_+^\sigma}$ and $D_{\curvearrowright} = \mathcal{D}_{\mathcal{P},\mathrm{Id}-\mathcal{P}}$, so by the comparison formula (2.5),

$$\frac{\det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\Pi^\sigma_+}}{\det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\mathcal{P}}} = (\det L)^2 \cdot \det_F\left(\frac{2\,\mathrm{Id} + \hat{U}_\mathcal{P} + \hat{U}_\mathcal{P}^{-1}}{4}\right),$$

where we used that the U in (2.5) for this situation is $(-\kappa_\mathcal{P})(-\kappa_\sigma^{-1}) = \kappa_\mathcal{P}\kappa_\sigma^{-1} =: U_\mathcal{P}$, and where L is the map over $\{R\}\times Y$ defined in (2.3):

$$L = -P_W G \mathcal{R}^{-1} G P_W : W \to W$$

with

$$W := \gamma_R \ker(\mathcal{D}_{\mathcal{P},\mathrm{Id}-\Pi^\sigma_+}) \equiv \mathrm{Im}(\mathrm{Id}-\mathcal{P}) \cap \mathrm{Im}(\Pi^\sigma_+) = \mathrm{Im}(\mathrm{Id}-\mathcal{P}) \cap \mathrm{Im}(\Pi_+).$$

To determine $(\det L)^2$, we need to find $\mathcal{R}$. An invertible extension $\tilde{D}$ of D is just $G(\partial_u + D_Y)$ over $[-R,2R]\times Y$ with boundary condition $\mathcal{P}$ at $-R$ and $\mathrm{Id}-\mathcal{P}$ at $2R$. Let $\{\psi_\mu\}$ be an orthonormal basis of $W = \mathrm{Im}(\mathrm{Id}-\mathcal{P}) \cap \mathrm{Im}(\Pi_+)$ where $\psi_\mu \in E_\mu$, and for each such μ, define $\varphi_\mu := G\psi_\mu \in GW$. Since $GD_Y = -D_Y G$ and $\mathcal{P}G = G(\mathrm{Id}-\mathcal{P})$, it follows that $\varphi_\mu = G\psi_\mu \in E_{-\mu} \cap \mathrm{Im}(\mathcal{P})$. Using this, it is straightforward to check that

$$\phi_1 := \frac{\sinh(\mu(u+R))}{\sinh(2\mu R)}\varphi_\mu \quad \text{over} \quad [-R,R]\times Y,$$

and

$$\phi_2 := e^{\mu(u-R)}\varphi_\mu \quad \text{over} \quad [R,2R]\times Y,$$

are continuous at $u=R$ with value φ_μ and satisfy $\tilde{D}^2\phi_i = 0$, $i=1,2$. Thus, by the definition of $\mathcal{R}$ in (2.4), we have

$$\mathcal{R}\varphi_\mu := \partial_u\phi_1|_{u=R} - \partial_u\phi_2|_{u=R} = \left(\mu\frac{\cosh(2\mu R)}{\sinh(2\mu R)} - \mu\right)\varphi_\mu = \frac{\mu e^{-2\mu R}}{\sinh(2\mu R)}\varphi_\mu.$$

Therefore,

$$-G\mathcal{R}G\psi_\mu = -G\mathcal{R}\varphi_\mu = -G\frac{\mu e^{-2\mu R}}{\sinh(2\mu R)}\varphi_\mu = \frac{\mu e^{-2\mu R}}{\sinh(2\mu R)}\psi_\mu.$$

It follows that

$$L = -P_W G \mathcal{R}^{-1} G P_W = \sum_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}} \frac{e^{2\mu R}\sinh(2\mu R)}{\mu}\psi_\mu \otimes \psi_\mu.$$

Hence,

$$(\det L)^2 = \prod_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}} e^{4\mu R}\frac{\sinh^2(2\mu R)}{\mu^2},$$

which completes the Comparison proof of Lemma 3.1. □

Next, we compute a related ζ-determinant ratio.

Lemma 3.2: With the notations above, the following equality holds:

$$\frac{\det_\zeta \mathcal{D}^2_{\Pi^\sigma_+,\mathrm{Id}-\mathcal{P}}}{\det_\zeta \mathcal{D}^2_{\Pi^\sigma_+,\mathrm{Id}-\Pi^\sigma_+}} = \left(\prod_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}} \frac{e^{-4\mu R}\sinh^2(2\mu R)}{\mu^2}\right) \cdot \det_F\left(\frac{2\,\mathrm{Id} + \hat{U}_\mathcal{P} + \hat{U}_\mathcal{P}^{-1}}{4}\right).$$

Proof: Observe that $\mathrm{Id}-\Pi_+^\sigma$ is the Calderón projector at $\{R\}\times Y$ of the operator

$$D:\mathrm{dom}(D)\to L^2(N_R,S),$$

where

$$\mathrm{dom}(D):=\{\phi\in H^1(N_R,S)\,|\,\Pi_+^\sigma(\phi|_{u=-R})=0\}.$$

Then $D_{\mathrm{Id}-\mathcal{P}}=\mathcal{D}_{\Pi_+^\sigma,\mathrm{Id}-\mathcal{P}}$ and $D_{\mathcal{C}_-}=\mathcal{D}_{\Pi_+^\sigma,\mathrm{Id}-\Pi_+^\sigma}$, so the comparison formula (2.5) applied to this situation gives us

$$\frac{\det_\zeta\mathcal{D}^2_{\Pi_+^\sigma,\mathrm{Id}-\mathcal{P}}}{\det_\zeta\mathcal{D}^2_{\Pi_+^\sigma,\mathrm{Id}-\Pi_+^\sigma}}=(\det L)^2\cdot\det_F\left(\frac{2\,\mathrm{Id}+\hat{U}_{\mathcal{P}}^{-1}+\hat{U}_{\mathcal{P}}}{4}\right),$$

where we used that the U in (2.5) for this situation is $(-\kappa_\sigma)(-\kappa_{\mathcal{P}}^{-1})=\kappa_\sigma\kappa_{\mathcal{P}}^{-1}=(\kappa_{\mathcal{P}}\kappa_\sigma^{-1})^{-1}=U_{\mathcal{P}}^{-1}$, and where L is the map over $\{R\}\times Y$ defined in (2.3):

$$L:=-P_W G\mathcal{R}^{-1}GP_W:W\to W$$

with

$$W:=\gamma_R\ker(\mathcal{D}_{\Pi_+^\sigma,\mathrm{Id}-\mathcal{P}})\equiv\mathrm{Im}(\mathrm{Id}-\Pi_+^\sigma)\cap\mathrm{Im}(\mathcal{P})=\mathrm{Im}(\mathcal{P})\cap\mathrm{Im}(\Pi_-).$$

To compute $(\det L)^2$ for this example, we proceed in much the same way as for the Comparison proof of Lemma 3.1. An invertible extension $\tilde{D}$ of D is just $G(\partial_u+D_Y)$ over $[-R,2R]\times Y$ with boundary condition Π_+^σ at $-R$ and $\mathrm{Id}-\Pi_+^\sigma$ at $2R$. Let $\{\psi_\nu\}$ be an orthonormal basis of $W=\mathrm{Im}(\mathcal{P})\cap\mathrm{Im}(\Pi_-)$ where $\psi_\nu\in E_\nu$. It is important to note that, in contrast to the Comparison proof of Lemma 3.1, the ν's are *negative* (rather than positive) and that $\psi_\nu\in E_\nu\cap\mathrm{Im}(\mathcal{P})$ [rather than $\mathrm{Im}(\mathrm{Id}-\mathcal{P})$]. Following the Comparison proof of Lemma 3.1 almost verbatim, it is straightforward to check that

$$L=-P_W G\mathcal{R}^{-1}GP_W=\sum_{\substack{\nu<0\\ E_\nu\cap\mathrm{Im}(\mathcal{P})\neq 0}}\frac{e^{2\nu R}\sinh(2\nu R)}{\nu}\psi_\nu\otimes\psi_\nu,$$

so

$$(\det L)^2=\prod_{\substack{\nu<0\\ E_\nu\cap\mathrm{Im}(\mathcal{P})\neq 0}}e^{4\nu R}\frac{\sinh^2(2\nu R)}{\nu^2}.$$

Finally, using that G maps $E_\nu\cap\mathrm{Im}(\mathcal{P})$ isomorphically onto $E_{-\nu}\cap\mathrm{Im}(\mathrm{Id}-\mathcal{P})$, where we used that $GD_Y=-D_YG$ and $\mathcal{P}G=G(\mathrm{Id}-\mathcal{P})$, we finally get

$$(\det L)^2=\prod_{\substack{\mu>0\\ E_\mu\cap\mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}}e^{4(-\mu)R}\frac{\sinh^2(-2\mu R)}{(-\mu)^2}=\prod_{\substack{\mu>0\\ E_\mu\cap\mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}}e^{-4\mu R}\frac{\sinh^2(2\mu R)}{\mu^2},$$

which completes our proof. □

We are now ready to prove the following

Lemma 3.3: With the notations above, the following equality holds:

$$\det_\zeta\mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\mathcal{P}}=e^{2CR}2^{\zeta_{D_Y^2}(0)+h_Y}\cdot\left(\prod_{\substack{\mu>0\\ E_\mu\cap\mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}}e^{-8\mu R}\right),$$

where $C=(\Gamma(s)^{-1}\zeta_{D_Y^2}(s-1/2))'(0)$ *with* $\zeta_{D_Y^2}(s)$ *the* ζ*-function of* D_Y^2 *and* $h_Y=\dim\ker(D_Y)$.

Proof: Solving for $\det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\mathcal{P}}$ in Lemma 3.1, we obtain

$$\det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\mathcal{P}} = \det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\Pi^\sigma_+} \cdot \left(\prod_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}} \frac{e^{-4\mu R}\mu^2}{\sinh^2(2\mu R)} \right) \cdot \det_F \left(\frac{2\,\mathrm{Id} + \hat{U}_\mathcal{P} + \hat{U}_\mathcal{P}^{-1}}{4} \right)^{-1}. \tag{3.3}$$

On the other hand, from Lemma 3.2, we know that

$$\frac{\det_\zeta \mathcal{D}^2_{\Pi^\sigma_+,\mathrm{Id}-\mathcal{P}}}{\det_\zeta \mathcal{D}^2_{\Pi^\sigma_+,\mathrm{Id}-\Pi^\sigma_+}} = \left(\prod_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}} \frac{e^{-4\mu R}\sinh^2(2\mu R)}{\mu^2} \right) \cdot \det_F \left(\frac{2\,\mathrm{Id} + \hat{U}_\mathcal{P} + \hat{U}_\mathcal{P}^{-1}}{4} \right)$$

and from the main result of Ref. 11 [see formula (1.7)], we also have

$$\det_\zeta \mathcal{D}^2_{\Pi^\sigma_+,\mathrm{Id}-\Pi^\sigma_+} = e^{2CR} 2^{\zeta_{D_Y^2}(0)+h_Y}.$$

Hence,

$$\det_\zeta \mathcal{D}^2_{\Pi^\sigma_+,\mathrm{Id}-\mathcal{P}} = e^{2CR} 2^{\zeta_{D_Y^2}(0)+h_Y} \left(\prod_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P})\neq 0}} \frac{e^{-4\mu R}\sinh^2(2\mu R)}{\mu^2} \right) \cdot \det_F \left(\frac{2\mathrm{Id} + \hat{U}_\mathcal{P} + \hat{U}_\mathcal{P}^{-1}}{4} \right).$$

Substituting this expression into (3.3), using that

$$\det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\Pi^\sigma_+} = \det_\zeta \mathcal{D}^2_{\Pi^\sigma_+,\mathrm{Id}-\mathcal{P}}, \tag{3.4}$$

concludes the proof of our result once we show that (3.4) holds. In fact, (3.4) holds in the more general setting: $\det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\mathcal{Q}} = \det_\zeta \mathcal{D}^2_{\mathcal{Q},\mathrm{Id}-\mathcal{P}}$ for all $(\mathcal{P},\mathrm{Id}-\mathcal{Q}) \in \mathrm{Gr}^*_\infty(D_Y)$. To prove this, we simply observe that

$$G(\partial_u + D_Y)\phi = \lambda\phi, \quad \mathcal{P}\phi(-R) = 0, \quad (\mathrm{Id}-\mathcal{Q})\phi(R) = 0$$

if and only if $\psi(u) := G\phi(-u)$ satisfies

$$G(\partial_u + D_Y)\psi = -\lambda\psi, \quad (\mathrm{Id}-\mathcal{P})\psi(R) = 0, \quad \mathcal{Q}\psi(-R) = 0,$$

where we used that $G^2 = -\mathrm{Id}$, $GD_Y = -D_Y G$, $\mathcal{P}G = G(\mathrm{Id}-\mathcal{P})$, and $\mathcal{Q}G = G(\mathrm{Id}-\mathcal{Q})$. It follows that $\mathrm{spec}(\mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\mathcal{Q}}) = \mathrm{spec}(\mathcal{D}^2_{\mathcal{Q},\mathrm{Id}-\mathcal{P}})$, which implies that $\det_\zeta \mathcal{D}^2_{\mathcal{P},\mathrm{Id}-\mathcal{Q}} = \det_\zeta \mathcal{D}^2_{\mathcal{Q},\mathrm{Id}-\mathcal{P}}$. □

IV. PROOF OF THEOREM 1.1

As we already mentioned, in order to demonstrate the effectiveness of the gluing formula (2.2) and the comparison formula (2.5), we shall give separate proofs of Theorem 1.1 exploiting both formulas.

Gluing proof of Theorem 1.1: Recall that the operator $\mathcal{D}_P$ as defined in (1.4) written using the notation (3.1) is

$$\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2} := \mathcal{D}:\mathrm{dom}(\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2}) \to L^2(N_R,S),$$

where

$$\mathrm{dom}(\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2}) := \{\phi \in H^1(N_R,S) | \mathcal{P}_1(\phi|_{u=-R}) = 0, \quad \mathcal{P}_2(\phi|_{u=R}) = 0\}.$$

Let us decompose N_R into two parts $[-R,0]\times Y$ and $[0,R]\times Y$ as shown in Fig. 2. Then the restrictions of $\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2}$ over the decomposed parts define two Dirac type operators with boundary

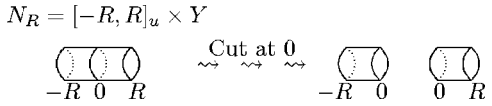

FIG. 2. Cutting N_R at 0 into two pieces.

conditions given by $\mathcal{P}_1$ at $\{-R\}\times Y$ and $\mathcal{P}_2$ at $\{R\}\times Y$. It is easy to check that the Calderón projections of these operators are, respectively, just $\mathrm{Id}-\mathcal{P}_1$ and $\mathrm{Id}-\mathcal{P}_2$ over $\{0\}\times Y$. We denote the operators over the decomposed parts $[-R,0]\times Y$ and $[0,R]\times Y$ with the new boundary conditions given by these Calderón projectors over $\{0\}\times Y$ by $D_{\mathcal{P}_1,\mathrm{Id}-\mathcal{P}_1}$ and $D_{\mathrm{Id}-\mathcal{P}_2,\mathcal{P}_2}$, respectively. Now applying the gluing formula (2.2) to this situation, we obtain

$$\frac{\det_\zeta \mathcal{D}^2_{\mathcal{P}_1,\mathcal{P}_2}}{\det_\zeta D^2_{\mathcal{P}_1,\mathrm{Id}-\mathcal{P}_1}\cdot \det_\zeta D^2_{\mathrm{Id}-\mathcal{P}_2,\mathcal{P}_2}} = 2^{-\zeta_{D_Y^2}(0)-h_Y}(\det \mathcal{L})^{-2}\det_F\left(\frac{2\,\mathrm{Id}+\hat{U}_P+\hat{U}_P^{-1}}{4}\right), \tag{4.1}$$

where the $\hat{\mathcal{U}}$ in (2.2) for this situation is the restriction of $-(-\kappa_1)(-\kappa_2^{-1})=-\kappa_1\kappa_2^{-1}=:U_P$ over $L^2(Y,S^-)$ to the orthogonal complement of its (-1)-eigenspace, noting that $-\kappa_i$ is the isometry corresponding to $\mathrm{Id}-\mathcal{P}_i$ for $i=1$, 2, and where

$$\mathcal{L} := \sum_{k=1}^{h_P} \gamma_0 U_k \otimes \gamma_0 U_k : \gamma_0 \ker(\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2}) \to \gamma_0 \ker(\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2}), \tag{4.2}$$

where $h_P=\dim\ker(\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2})$, γ_0 is the restriction map from N_R to $\{0\}\times Y$, and $\{U_k\}$ is an orthonormal basis of $\ker(\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2})$. By Lemma 3.3 (here we need to replace R with $R/2$ since the lengths of $[-R,0]$ and $[0,R]$ are half that of $[-R,R]$, which is the interval considered in Lemma 3.3),

$$\det_\zeta D^2_{\mathcal{P}_1,\mathrm{Id}-\mathcal{P}_1} = e^{CR}2^{\zeta_{D_Y^2}(0)+h_Y}\cdot\left(\prod_{\substack{\mu>0\\ E_\mu\cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\neq 0}} e^{-4\mu R}\right),$$

and

$$\det_\zeta D^2_{\mathrm{Id}-\mathcal{P}_2,\mathcal{P}_2} = e^{CR}2^{\zeta_{D_Y^2}(0)+h_Y}\cdot\left(\prod_{\substack{\mu>0\\ E_\mu\cap \mathrm{Im}(\mathcal{P}_2)\neq 0}} e^{-4\mu R}\right).$$

Now to complete the Gluing proof of Theorem 1.1, it remains to compute $(\det\mathcal{L})^{-2}$ over $\gamma_0\ker(\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2})\equiv \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\cap\mathrm{Im}(\mathrm{Id}-\mathcal{P}_2)$. To do so, we note that

$$\ker(\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2}) \equiv \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\cap\mathrm{Im}(\mathrm{Id}-\mathcal{P}_2) := W.$$

Let $\{\psi_\mu\}$ be an orthonormal basis of W where $\psi_\mu\in E_\mu$. Then $\phi_\mu := e^{-\mu u}\psi_\mu \in \ker(\mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2})$ and

$$\|\phi_\mu\|^2 = \int_{-R}^{R} e^{-2\mu u}du = \frac{\sinh(2\mu R)}{\mu},$$

where if $\mu=0$, then we replace $[\sinh(2\mu R)]/\mu$ by its limit as $\mu\to 0$, that is, $2R$. It follows that

$$\mathcal{L} = \sum_{\substack{\mu\in\mathrm{spec}(D_Y)\\ E_\mu\cap W\neq 0}} \frac{\phi_\mu(0)}{\|\phi_\mu\|}\otimes\frac{\phi_\mu(0)}{\|\phi_\mu\|} = \sum_{\substack{\mu\in\mathrm{spec}(D_Y)\\ E_\mu\cap W\neq 0}} \frac{1}{\|\phi_\mu\|^2}\psi_\mu\otimes\psi_\mu.$$

Hence,

$$(\det \mathcal{L})^{-2} = \prod_{\substack{\mu \in \operatorname{spec}(D_Y) \\ E_\mu \cap W \neq 0}} \left(\frac{1}{\|\phi_\mu\|^2} \right)^{-2} = \prod_{\substack{\mu \in \operatorname{spec}(D_Y) \\ E_\mu \cap W \neq 0}} \frac{\sinh^2(2\mu R)}{\mu^2}.$$

This completes the Gluing proof of Theorem 1.1.

Comparison proof of Theorem 1.1: We now prove Theorem 1.1 using the comparison formula (2.5) applied to the pair $(\mathcal{D}^2_{\mathcal{P}_1,\mathcal{P}_2}, \mathcal{D}^2_{\mathcal{P}_1,\mathrm{Id}-\mathcal{P}_1})$. Here we regard $\mathrm{Id}-\mathcal{P}_1$ as the Calderón projector at the boundary $\{R\}\times Y$ of the operator

$$D{:}\operatorname{dom}(D) \to L^2(N_R, S),$$

where

$$\operatorname{dom}(D) := \{\phi \in H^1(N_R, S) | \mathcal{P}(\phi|_{u=-R}) = 0\}.$$

Then $D_{\mathcal{P}_2} = \mathcal{D}_{\mathcal{P}_1,\mathcal{P}_2}$ and $D_{c_-} = \mathcal{D}_{\mathcal{P}_1,\mathrm{Id}-\mathcal{P}_1}$, so applying the comparison formula (2.5) to this situation, we obtain

$$\frac{\det_\zeta \mathcal{D}^2_{\mathcal{P}_1,\mathcal{P}_2}}{\det_\zeta \mathcal{D}^2_{\mathcal{P}_1,\mathrm{Id}-\mathcal{P}_1}} = (\det L)^2 \cdot \det_F\left(\frac{2\mathrm{Id} + \hat{U}_P + \hat{U}_P^{-1}}{4} \right), \tag{4.3}$$

where we used that the U in (2.5) for this situation is $(-\kappa_1)\kappa_2^{-1} =: U_P$ noting that $-\kappa_1$ corresponds to $\mathrm{Id}-\mathcal{P}_1$, and where L is the operator defined in (2.3) for this situation, which we will investigate in detail soon. Now, by Lemma 3.3,

$$\det_\zeta \mathcal{D}^2_{\mathcal{P}_1,\mathrm{Id}-\mathcal{P}_1} = e^{2CR} 2^{\zeta_{D_Y^2}(0)+h_Y} \cdot \left(\prod_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\neq 0}} e^{-8\mu R} \right),$$

therefore by (4.3),

$$\det_\zeta \mathcal{D}^2_{\mathcal{P}_1,\mathcal{P}_2} = e^{2CR} 2^{\zeta_{D_Y^2}(0)+h_Y} \left(\prod_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\neq 0}} e^{-8\mu R} \right) \cdot (\det L)^2 \cdot \det_F\left(\frac{2\mathrm{Id} + \hat{U}_P + \hat{U}_P^{-1}}{4} \right).$$

To compute $\det L$, we use almost the exact same argument found in Lemma 3.2 to show that with $W := \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1) \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_2)$,

$$(\det L)^2 = \prod_{\substack{\mu \in \operatorname{spec}(D_Y) \\ E_\mu \cap W \neq 0}} e^{4\mu R} \frac{\sinh^2(2\mu R)}{\mu^2},$$

where in the product, when $\mu = 0$ we replace $[\sinh^2(2\mu R)]/\mu^2$ by its limit as $\mu \to 0$, that is, $(2R)^2$. Therefore,

$$\begin{aligned} \det_\zeta \mathcal{D}^2_{\mathcal{P}_1,\mathcal{P}_2} = e^{2CR} 2^{\zeta_{D_Y^2}(0)+h_Y} & \left(\prod_{\substack{\mu>0 \\ E_\mu \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\neq 0}} e^{-8\mu R} \right) \cdot \left(\prod_{\substack{\mu \in \operatorname{spec}(D_Y) \\ E_\mu \cap W \neq 0}} e^{4\mu R} \right) \\ & \cdot \left(\prod_{\substack{\mu \in \operatorname{spec}(D_Y) \\ E_\mu \cap W \neq 0}} \frac{\sinh^2(2\mu R)}{\mu^2} \right) \cdot \det_F\left(\frac{2\mathrm{Id} + \hat{U}_P + \hat{U}_P^{-1}}{4} \right). \end{aligned} \tag{4.4}$$

Since $W = \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1) \cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_2)$, we have

$$\prod_{\substack{\mu\in\mathrm{spec}(D_Y)\\ E_\mu\cap W\neq 0}} e^{4\mu R} = \left(\prod_{\substack{\mu>0\\ E_\mu\cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\cap\mathrm{Im}(\mathrm{Id}-\mathcal{P}_2)\neq 0}} e^{4\mu R}\right)\cdot\left(\prod_{\substack{\mu<0\\ E_\mu\cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\cap\mathrm{Im}(\mathrm{Id}-\mathcal{P}_2)\neq 0}} e^{4\mu R}\right)$$

$$= \left(\prod_{\substack{\mu>0\\ E_\mu\cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\neq 0}} e^{4\mu R}\right)\cdot\left(\prod_{\substack{\mu>0\\ E_\mu\cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\cap\mathrm{Im}(\mathcal{P}_2)\neq 0}} e^{-4\mu R}\right)$$

$$\cdot\left(\prod_{\substack{\mu<0\\ E_\mu\cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\cap\mathrm{Im}(\mathrm{Id}-\mathcal{P}_2)\neq 0}} e^{4\mu R}\right).$$

Since $D_Y G=-GD_Y$ and $\mathcal{P}_i G=G(\mathrm{Id}-\mathcal{P}_i)$, we have

$$E_\mu\cap\mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\cap\mathrm{Im}(\mathrm{Id}-\mathcal{P}_2)\neq 0\Leftrightarrow E_{-\mu}\cap\mathrm{Im}(\mathcal{P}_1)\cap\mathrm{Im}\mathcal{P}_2\neq 0,$$

as G maps the first space isomorphically onto the second space, therefore

$$\prod_{\substack{\mu\in\mathrm{spec}(D_Y)\\ E_\mu\cap W\neq 0}} e^{4\mu R} = \left(\prod_{\substack{\mu>0\\ E_\mu\cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\neq 0}} e^{4\mu R}\right)\cdot\left(\prod_{\substack{\mu>0\\ E_\mu\cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\cap\mathrm{Im}(\mathcal{P}_2)\neq 0}} e^{-4\mu R}\right)$$

$$\cdot\left(\prod_{\substack{\mu>0\\ E_\mu\cap \mathrm{Im}(\mathcal{P}_1)\cap\mathrm{Im}(\mathcal{P}_2)\neq 0}} e^{-4\mu R}\right)$$

$$= \left(\prod_{\substack{\mu>0\\ E_\mu\cap \mathrm{Im}(\mathrm{Id}-\mathcal{P}_1)\neq 0}} e^{4\mu R}\right)\cdot\left(\prod_{\substack{\mu>0\\ E_\mu\cap \mathrm{Im}(\mathcal{P}_2)\neq 0}} e^{-4\mu R}\right).$$

Putting this expression into (4.4) completes the Comparison proof of Theorem 1.1.

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Nontopological bare solutions in the relativistic self-dual Maxwell–Chern–Simons–Higgs model

Jongmin Han[a] and Jaeduk Jang[b]
Department of Mathematics, Hankuk University of Foreign Studies, 89 Wangsan-ri Mohyun, Yongin, Kyounggi-do 449-791, Korea

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In this paper we prove the existence of the radially symmetric nontopological bare solutions in the relativistic self-dual Maxwell–Chern–Simons–Higgs model. We also verify the Chern–Simons limit for those solutions. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1861277]

I. INTRODUCTION

In this paper we are concerned with the relativistic Maxwell–Chern–Simons–Higgs model (MCSH).[1] Consider $(2+1)$-dimensional Minkowski space $\mathbb{R}^{1,2}$ with the metric $\mathrm{diag}(1,-1,-1)$. The metric is used to raise or lower indices. The Lagrangian density of the relativistic MCSH is given by

$$\mathcal{L} = (D_\alpha\phi)\overline{(D^\alpha\phi)} - \frac{1}{4}F_{\alpha\beta}F^{\alpha\beta} + \frac{\kappa}{4}\epsilon^{\alpha\beta\gamma}A_\alpha F_{\beta\gamma} + \frac{1}{2}\partial_\alpha N\partial^\alpha N - q^2|\phi|^2N^2 - \frac{1}{2}(q|\phi|^2 + \kappa N - q)^2, \tag{1.1}$$

where all the greek indices run over 0,1,2. Here $q>0$ is the charge of electron, $\kappa>0$ is the Chern–Simons coupling constant, $\phi:\mathbb{R}\times\mathbb{R}^2\to\mathbb{C}$ is the Higgs field, $A_\alpha:\mathbb{R}\times\mathbb{R}^2\to\mathbb{R}$ is the gauge field, $N:\mathbb{R}\times\mathbb{R}^2\to\mathbb{R}$ is the neutral scalar field, $D_\alpha=\partial_\alpha-iqA_\alpha$ is the covariant derivative with $i=\sqrt{-1}$, and $F_{\alpha\beta}=\partial_\alpha A_\beta-\partial_\beta A_\alpha$ is the field strength.

We say that (ϕ,A_α) is gauge equivalent to (ψ,B_α), if there exists a function χ such that

$$(\psi,B_\alpha) = (e^{i\chi}\phi, A_\alpha + \partial_\alpha\chi).$$

It is easily verified that the $\mathcal{L}$ and its Euler–Lagrange equations are invariant under the gauge transformation.

We consider the stationary solutions of the Euler–Lagrange equations for (1.1). The variational equation for A_0, often called the Gauss constraint equation, gives

$$-\Delta A_0 + 2q^2|\phi|^2A_0 = -\kappa F_A. \tag{1.2}$$

Using this equation, we can write the static MCSH energy functional as

$$\mathcal{E}(\phi,A,N) = \int_{\mathbb{R}^2} |D_A\phi|^2 + \frac{1}{2}|F_A|^2 + q^2|\phi|^2A_0^2 + \frac{1}{2}|\nabla A_0|^2 + q^2|\phi|^2N^2 + \frac{1}{2}|\nabla N|^2 + \frac{1}{2}(q|\phi|^2 + \kappa N - q)^2. \tag{1.3}$$

Here we used the notations as follows: $A=(A_1,A_2)$, $D_A\phi=\nabla\phi-iq\phi A$, and $F_A=\partial_1A_2-\partial_2A_1$.

Using (1.2) and integrating by parts, we obtain

[a]Electronic mail: jmhan@hufs.ac.kr
[b]Electronic mail: jdjang@hufs.ac.kr

$$\mathcal{E}(\phi,A,N)=\int_{\mathbb{R}^2}\Big(|D_1\phi\pm iD_2\phi|^2+q^2|\phi|^2|A_0\pm N|^2+\frac{1}{2}|\nabla A_0\pm\nabla N|^2$$
$$+\frac{1}{2}|F_A\pm(q|\phi|^2+\kappa N-q)|^2\Big)\mathrm{d}x\pm\Lambda,$$

where

$$\Lambda=q\int_{\mathbb{R}^2}F_A\,\mathrm{d}x. \tag{1.4}$$

If Λ is positive (negative), then choose the upper (lower) sign. This yields the lower bound of the energy functional,

$$\mathcal{E}(\phi,A,N)\geqslant|\Lambda|,$$

which is saturated by the following system of self-dual equations:

$$D_1\phi\pm iD_2\phi=0, \tag{1.5}$$

$$A_0\pm N=0, \tag{1.6}$$

$$F_A\pm(q|\phi|^2+\kappa N-q)=0. \tag{1.7}$$

Since the solutions of (1.5)–(1.7) are the global minimizer of $\mathcal{E}$ over a suitable function space,[2] they are solutions of the Euler–Lagrange equations of the Lagrangian $\mathcal{L}$. It is not yet proved whether the converse is true, i.e., the self-dual equations (1.5)–(1.7) are equivalent to the Euler–Lagrange equations.

The boundary conditions are given by the finite energy condition of (1.3) as $|x|\to\infty$, either

$$|\phi|\to1\quad\text{and }N\to0,$$

or

$$|\phi|\to0\quad\text{and }N\to\frac{q}{\kappa}.$$

The former is called topological, while the latter nontopological.

Let us take the upper signs in (1.5)–(1.7). The lower sign case can be obtained by the conjugate transformation $(\phi,A,N)\to(\overline{\phi},-A,N)$. To examine the self-dual equations further, we use the classical Jaffe–Taubes arguments.[3] In fact, Eq. (1.5) implies that ϕ is holomorphic up to a nonvanishing multiple factor and has exactly m zeros allowing multiplicities. Thus we may assume that ϕ takes the form

$$\phi(z)=\exp\left(\frac{1}{2}u(x)+i\sum_{j=1}^{k}n_j\arg(x-p_j)\right), \tag{1.8}$$

where the points $p_1,\ldots,p_k$, called the vortex points, are the distinct zeros of ϕ with multiplicities $n_1,\ldots,n_k$, respectively. Clearly, $n_1+\cdots+n_k=m$. We observe that the arbitrary choice on the imaginary part of ϕ merely reflects the gauge invariance of (1.2)–(1.7). Now the equations (1.2), (1.6), and (1.7) are transformed into

$$\Delta u=2q^2(e^u-1)+2\kappa qN+4\pi\sum_{j=1}^{k}n_j\delta_{p_j},\quad\text{in }\mathbb{R}^2, \tag{1.9}$$

$$\Delta N = \kappa q(e^u - 1) + (\kappa^2 + 2q^2 e^u)N \quad \text{in } \mathbb{R}^2. \tag{1.10}$$

The boundary conditions are rewritten as

$$\text{topological}, \quad u \to 0 \quad \text{and } N \to 0, \tag{1.11}$$

$$\text{nontopological}, \quad u \to -\infty \quad \text{and } N \to \frac{q}{\kappa}, \tag{1.12}$$

as $|x| \to \infty$. Conversely, once we find a solution (u, N) of (1.9) and (1.10), we may recover A and A_0 from (1.5) and (1.6) by the formula

$$qA_1 + iqA_2 = -2i\overline{\partial} \ln \phi,$$

where $\overline{\partial} = (\partial_1 + i\partial_2)/2$.

It was proved that the equations (1.9) and (1.10) allow both topological[4] and nontopological[5] solutions. On the other hand, one can consider the self-dual equations (1.5)–(1.7) on the 't Hooft type periodic domain, of which solutions are called condensate solutions. There has been several results for the condensate solutions.[6–8]

It is an interesting question that there exists a radially symmetric solution to (1.9) and (1.10) if $k=0$ or 1. Such a radial solution has been studied in several self-dual gauge models.[9,10] Concerning the Maxwell–Chern–Simons–Higgs model, if $k=0$, then the only solution of (1.9) and (1.10) with the topological boundary condition (1.11) is proved to be $u \equiv N \equiv 0$ by the maximum principle, while there is no result for the nontopological solution. For the case $k=1$, every topological solution is radially symmetric about the only vortex point.[11] Although the existence of nontopological multivortex solutions was established by Chae–Imanuvilov,[5] their solutions are not radially symmetric about the vortex point for the case $k=1$. In this context, when $k=0$ or $k=1$, it is an interesting problem to consider nontopological solutions which is radially symmetric about a point. In this paper we are interested in the radially symmetric nontopological solutions when there are no vortex points, i.e., $k=0$. In this case, the solutions are called bare solutions.[12] For the case $k=1$, we postpone the study of nontopological radial solutions to a forthcoming paper.

From now on we assume $m=0$ and let us rewrite (1.9) as

$$\Delta u = 2q^2(e^u - 1) + 2\kappa q N. \tag{1.13}$$

Our first result in this paper is to establish the radial solutions of (1.10) and (1.13) as follows.

Theorem 1.1: *For any $x_0 \in \mathbb{R}^2$ and $a<0$, there exists a unique number $b=b(a) \in (0, q/\kappa)$ such that the equations (1.10) and (1.13) with the boundary condition (1.12) admit a unique solution which is radially symmetric about x_0. The corresponding solution (ϕ, A, N) of the self-dual equations (1.5)–(1.7) is of finite energy. Furthermore, we have the following.*

(i) *There exists a constant $\gamma = \gamma(a) > 4$ such that*

$$\mathcal{E}(\phi, A, N) = \pi\gamma.$$

(ii) *(ϕ, A, N) is radially symmetric about x_0.*

(iii) *ϕ has no zeros in $\mathbb{R}^2$.*

(iv) $\max_{x \in \mathbb{R}^2} |\phi(x)|^2 = |\phi(x_0)|^2 = e^a, \quad \min_{x \in \mathbb{R}^2} N(x) = N(x_0) = b.$

(v) $|\phi(x)|^2, \quad q - \kappa N(x) = O(|x|^{-\gamma}).$

On the other hand, if we set

$$\kappa = 0, \quad q = 1/\sqrt{2}, \quad N \equiv 0, \tag{1.14}$$

then the equations (1.9) and (1.10) reduce to

$$\Delta u = e^u - 1 + 4\pi \sum_{j=1}^{k} n_j \delta_{p_j},$$

which is the self-dual equation of the Abelian–Higgs model.[13] Similarly, if we set

$$\kappa = \mu q^2, \quad \mu > 0, \quad N = q(1 - e^u)/\kappa, \quad q \to \infty, \tag{1.15}$$

then the equations (1.9) and (1.10) tend formally to

$$\Delta u = \frac{1}{\mu^2} e^u (e^u - 1) + 4\pi \sum_{j=1}^{k} n_j \delta_{p_j}, \tag{1.16}$$

which is the self-dual equation of the Chern–Simons–Higgs model.[14,15] Therefore, one can formally consider the Maxwell–Chern–Simons–Higgs model as a unification of the Abelian–Higgs model and the Chern–Simons–Higgs model.[1] The first limit is called the Maxwell limit (or Abelian–Higgs limit), while the second one the Chern–Simons limit. There have been several results about the mathematically rigorous proof for the convergence of the topological solutions[4] and the condensate[6–8] solutions. See Ref. 2 for the Chern–Simons limit of the solutions of the Euler–Lagrange equations on a bounded domain. However, there have been no results about the verification of the limits for the nontopological solutions on $\mathbb{R}^2$, as far as we know. For the nontopological solutions on $\mathbb{R}^2$, only the Chern–Simons limit is meaningful because the self-dual equations of the Abelian–Higgs model permits only the topological boundary conditions at infinity. In the following theorem we verify the Chern–Simons limit for the radially symmetric nontopological bare solutions, which is the main contribution of the present paper.

Theorem 1.2 (Chern–Simons limit): *Let $a<0$ be fixed and set $\kappa=\mu q^2$. Let (u_q, N_q) be the unique solution of the equations (1.10) and (1.13) with the boundary condition (1.12) which is radially symmetric about a point $x_0 \in \mathbb{R}^2$ with $u(x_0)=a$ and $N(x_0)=b(a)$. Let $\tilde{N}_q = qN_q$. Then, as $q \to \infty$, $(u_q, \tilde{N}_q)$ converges to (u_*, N_*) such that (u_*, N_*) satisfies*

$$\Delta u_* = \frac{1}{\mu^2} e^{u_*}(e^{u_*} - 1), \quad u(x_0) = a, \quad u_* \to -\infty \quad \text{as } |x| \to \infty, \tag{1.17}$$

and $N_* = (1 - e^{u_*})/\mu$. More precisely, for any $R>0$,

$$\|u_q - u_*\|_{C^2(B_R)} = O(q^{-2}), \quad \|\tilde{N}_q - N_*\|_{C^0(B_R)} = O(q^{-2}).$$

The solutions of the equation (1.17) are well known.[10] In fact, every solution of (1.17) is radially symmetric about a point $x_0 \in \mathbb{R}^2$ with the property $u<0$ on $\mathbb{R}^2$, and for each $a<0$ (1.17) allows a unique radial solution with $u(x_0)=a$. In this point of view it is an interesting question whether every nontopological bare solution of (1.10) and (1.13) is radially symmetric about a point.

In the next two sections, we will prove Theorems 1.1 and 1.2.

II. EXISTENCE OF RADIAL SOLUTIONS

In this section we prove Theorem 1.1 following the argument in Refs. 9 and 10, which was used to prove the existence of several kind of self-dual equations of nontopological type. We will develop the argument in Refs. 9 and 10 into a system of equations. We begin with the following lemma.

Lemma 2.1: Let (u, N) be a solution of (1.10) and (1.13) with the boundary, condition (1.12). Then

$$0 < N < \frac{q}{\kappa}(1 - e^u). \tag{2.1}$$

Proof: Although this lemma is well known,[6] we provide a proof for the sake of completeness.

We first show that $N \geqslant 0$. Suppose that x_0 is a negative minimum point of N. Then by the maximum principle,

$$0 > N(x_0) > \frac{\kappa q(1 - e^{u(x_0)})}{\kappa^2 + 2q^2 e^{u(x_0)}}.$$

In particular, $u(x_0) > 0$, and hence if x_1 is a maximum point of u, then $u(x_1) > 0$. Again the maximum principle implies,

$$N(x_1) < q(1 - e^{u(x_1)}).$$

Combining these two inequalities, we obtain

$$\frac{\kappa^2}{\kappa^2 + 2q^2 e^{u(x_0)}}(1 - e^{u(x_0)}) < (1 - e^{u(x_0)}).$$

Since $u(x_0) > 0$, this lead us to a contradiction.

Now let $v = q(e^u - 1) + \kappa N$. A short computation gives

$$\Delta v - (4q^2 e^u + \kappa^2)v = 2\kappa q^2 e^u N + qe^u |\nabla u|^2 > 0.$$

Since $v \to 0$ as $|x| \to \infty$, the maximum principle implies (2.1). ■

We will study solutions of (1.10) and (1.13) which is radially symmetric about a point $x_0 \in \mathbb{R}^2$, say $x_0 = 0$. If we set $r = |x|$, $u = u(r)$, and $N = N(r)$, then (1.10) and (1.13) become

$$u_{rr} + \frac{1}{r}u_r = 2q^2(e^u - 1) + 2\kappa qN, \quad r > 0, \tag{2.2}$$

$$N_{rr} + \frac{1}{r}N_r = \kappa q(e^u - 1) + (\kappa^2 + 2q^2 e^u)N, \quad r > 0, \tag{2.3}$$

$$u(0) = a, \quad N(0) = b. \tag{2.4}$$

Furthermore, if we make a change of variables $t = \ln r$, then with $u = u(t)$ and $N = N(t)$, we obtain

$$u'' = 2q^2 e^{2t}(e^u - 1) + 2\kappa qe^{2t}N, \quad t \in \mathbb{R}, \tag{2.5}$$

$$N'' = \kappa qe^{2t}(e^u - 1) + (\kappa^2 + 2q^2 e^u)e^{2t}N, \quad t \in \mathbb{R}, \tag{2.6}$$

$$u(t) = a + o(1), \quad N(t) = b + o(1) \text{ near } -\infty. \tag{2.7}$$

Here, prime denotes the derivative with respect to the variable t.

In view of Lemma 2.1, a necessary condition of the existence of a global solution to (2.5)–(2.7) with the boundary condition (1.12) is

$$0 < b < \frac{q}{\kappa}(1 - e^a). \tag{2.8}$$

In particular, $a < 0$. Moreover, we can rewrite (2.5) and (2.6) as

$$u'' = 2q^2 e^{2t} f(u) + 2\kappa qe^{2t}N \equiv e^{2t}\Phi(u, N), \tag{2.9}$$

$$N'' = \kappa q e^{2t} f(u) + (\kappa^2 + 2q^2 g(u)) e^{2t} N \equiv e^{2t} \Psi(u, N), \tag{2.10}$$

where $f(u) = e^u - 1$ and $g(u) = e^u$ for $u \leqslant 0$, and both f and g are smoothly defined for $u > 0$ in such a way that

$$\alpha = \sup_{u \in \mathbb{R}} (1 + |f(u)| + |f'(u)| + |g(u)| + |g'(u)|) < \infty.$$

We observe that both Φ and Ψ are increasing in u and N, and $\Phi < 2q\Psi/\kappa$ for $N > 0$. This fact plays an important role on the analysis of the above equations with the following identity:

$$u'' = \frac{2q}{\kappa} N'' - \frac{4q^3}{\kappa} e^{2t} e^u N. \tag{2.11}$$

We also define a number

$$\beta = \max\{1, \kappa, q\}.$$

Lemma 2.2: For $a < 0$ and $b > 0$, the equations (2.9) and (2.10) admits a unique solution satisfying

$$\lim_{t \to -\infty} u(t) = a, \quad \lim_{t \to -\infty} N(t) = b. \tag{2.12}$$

Proof: It is easy to show that (u, N) is a solution of (2.9) and (2.10) satisfying (2.12) if and only if (u, N) verifies

$$u(t) = a + \int_{-\infty}^{t} (t - s) e^{2s} \Phi(u(s), N(s)) \mathrm{d}s, \tag{2.13}$$

$$N(t) = b + \int_{-\infty}^{t} (t - s) e^{2s} \Psi(u(s), N(s)) \mathrm{d}s. \tag{2.14}$$

Let $T \in \mathbb{R}$ be a constant satisfying

$$e^{2T}(\beta^2 + \alpha\beta^2 + \beta^2 b + \alpha\beta^2 b) < \min\left\{\tfrac{1}{2}, b\right\}.$$

In order to find a solution in the interval $(-\infty, T]$, we construct a Picard iterative sequence (u_j, N_j) with the initial data $u_0 = a$, and $N_0 = b$,

$$u_j(t) = a + \int_{-\infty}^{t} (t - s) e^{2s} \Phi(u_{j-1}(s), N_{j-1}(s)) \mathrm{d}s,$$

$$N_j(t) = b + \int_{-\infty}^{t} (t - s) e^{2s} \Psi(u_{j-1}(s), N_{j-1}(s)) \mathrm{d}s.$$

Inductively, for $t \in (-\infty, T]$,

$$|N_j(t)| \leqslant b + (\kappa q \sup_{\mathbb{R}} |f| + (\kappa^2 + 2q^2 \sup_{\mathbb{R}} |g|) \sup_{(-\infty, T]} |N_{j-1}|) \int_{-\infty}^{T} (T - s) e^{2s} \, \mathrm{d}s \leqslant b$$

$$+ \frac{1}{4} e^{2T} (\alpha\beta^2 + 2b(\beta^2 + 2\alpha\beta^2)) \leqslant 2b.$$

Now for $t \in (-\infty, T]$,

$$|u_{j+1}(t)-u_j(t)| \leqslant \tfrac{1}{4}e^{2T}(2q^2 \sup_{\mathbb{R}}|f'| \cdot \sup_{(-\infty,T]}|u_j-u_{j-1}| + 2\kappa q \sup_{(-\infty,T]}|N_j-N_{j-1}|)$$
$$\leqslant \tfrac{1}{2}e^{2T}(\beta^2+\alpha\beta^2)(\sup_{(-\infty,T]}|u_j-u_{j-1}| + \sup_{(-\infty,T]}|N_j-N_{j-1}|),$$

and, since $|N_{j-1}(t)| \leqslant 2b$,

$$|N_{j+1}(t)-N_j(t)| \leqslant \tfrac{1}{4}e^{2T}(\alpha\beta^2 \sup_{(-\infty,T]}|u_j-u_{j-1}| + \beta^2 \sup_{(-\infty,T]}|N_j-N_{j-1}|) + \int_{-\infty}^{t} 2q^2e^{2s}(t-s)[g(u_j)(N_j$$
$$-N_{j-1}) + (g(u_j)-g(u_{j-1}))N_{j-1}]\mathrm{d}s \leqslant \tfrac{1}{4}e^{2T}((\alpha\beta^2+4\alpha\beta^2b) \sup_{(-\infty,T]}|u_j-u_{j-1}| + (\beta^2$$
$$+2\alpha\beta^2) \sup_{(-\infty,T]}|N_j-N_{j-1}|).$$

Consequently,

$$\sup_{(-\infty,T]}(|u_{j+1}-u_j| + |N_{j+1}-N_j|) \leqslant \tfrac{1}{4}e^{2T}(3\beta^2+4\alpha\beta^2+4\alpha\beta^2b)) \sup_{(-\infty,T]}(|u_j-u_{j-1}| + |N_j-N_{j-1}|)$$
$$\leqslant \tfrac{1}{2} \sup_{(-\infty,T]}(|u_j-u_{j-1}| + |N_j-N_{j-1}|),$$

and thus we obtain a solution on $(-\infty,T]$. Since $\alpha<\infty$, the solution can be extended in $\mathbb{R}$. Moreover, it is easily verified that the solution is unique on $(-\infty,T]$, and hence in $\mathbb{R}$. ■

Given $a<0$ and $b\in(0,q/\kappa)$, let us denote by $(u(t,a,b),N(t,a,b))$ the solutions of (2.9) and (2.10) constructed in Lemma 2.2. For $a<0$, let us define

$$\mathcal{S}^+(a)=\{b\in(0,q/\kappa): N(t_0,a,b)>q/\kappa \text{ for some } t_0\},$$

$$\mathcal{S}^0(a)=\{b\in(0,q/\kappa): 0\leqslant N(t,a,b)\leqslant q/\kappa,\ \forall\, t\in\mathbb{R}\},$$

$$\mathcal{S}^-(a)=\{b\in(0,q/\kappa): N(t,a,b)\leqslant q/\kappa\ \forall\, t \text{ and } N(t_0,a,b)<0 \text{ for some } t_0\}.$$

From now on let $a<0$ be fixed and set

$$b_1(a)\equiv\frac{\kappa q}{\kappa^2+2q^2e^a}(1-e^a),\quad b_2(a)\equiv\frac{q}{\kappa}(1-e^a). \tag{2.15}$$

We note that $\Phi(a,b_2)=0$ and $\Psi(a,b_1)=0$.

Lemma 2.3: (i) *If* $b\in(0,b_1)$, *then* $b\in\mathcal{S}^-(a)$. (ii) *If* $b\in(b_2,q/\kappa)$, *then* $b\in\mathcal{S}^+(a)$. (iii) $\mathcal{S}^-(a)$ *and* $\mathcal{S}^+(a)$ *are open*. (iv) $\mathcal{S}^0(a)$ *is a closed nonempty set.*

Proof: Note that

$$u'(t)=\int_{-\infty}^{t} e^{2s}\Phi(u(s),N(s))\mathrm{d}s, \tag{2.16}$$

$$N'(t)=\int_{-\infty}^{t} e^{2s}\Psi(u(s),N(s))\mathrm{d}s. \tag{2.17}$$

We observe that if $b\in(0,b_1)$, then $\Phi(a,b)<0$ and $\Psi(a;b)<0$. Hence there exists $T\in\mathbb{R}$ such that $u'',u',N'',N'<0$ for all $t>T$. Since $\Phi(u,N)$ and $\Psi(u,N)$ are monotone increasing in both $u<0$ and N, it holds that $u'',u',N'',N'<0$ for all $t\in\mathbb{R}$, which implies that $b\in\mathcal{S}^-(a)$. This establishes (i).

On the other hand, it is easy to check that if $b \in (b_2, q/\kappa)$, then $\Phi(a,b)>0$ and $\Psi(a,b)>0$. Then by the same argument as above, it remains that $u'', u', N'', N' > 0$ until the graph of u touches the t-axis. Once $u(t)>0$, we see that $u''(t)>0$ by the definition of Φ, and hence $u'', u', N'', N' > 0$ for all $t \in \mathbb{R}$. Thus $b \in \mathcal{S}^+(a)$, which proves (ii).

The assertion (iii) comes from the continuous dependence of solutions on b. Finally, the statement (iv) is derived from the fact that

$$\left(0, \frac{q}{\kappa}\right) = \mathcal{S}^-(a) \cup \mathcal{S}^0(a) \cup \mathcal{S}^+(a).$$

■

Lemma 2.4: There exist two numbers $b^-(a)$ and $b^+(a)$ satisfying $b^- \geqslant b_1$ and $b^+ \leqslant b_2$ such that

$$\mathcal{S}^-(a) = (0, b^-), \quad \mathcal{S}^0(a) = [b^-, b^+], \quad \mathcal{S}^+(a) = (b^+, q/\kappa).$$

Proof: We notice from Lemma 2.3 (i) and (ii) that

$$\{b:(0,b] \subset \mathcal{S}^-(a)\} \neq \emptyset, \quad \{b:[b, q/\kappa) \subset \mathcal{S}^+(a)\} \neq \emptyset.$$

We claim that

$$b \in \mathcal{S}^-(a)(b \in \mathcal{S}^+(a), \text{resp.}) \Rightarrow (0,b] \subset \mathcal{S}^-(a)([b, q/\kappa) \subset \mathcal{S}^+(a), \text{resp.}). \tag{2.18}$$

Then the numbers defined by

$$b^-(a) = \sup\{b:(0,b] \subset \mathcal{S}^-(a)\}, \quad b^+(a) = \inf\{b:[b, q/\kappa) \subset \mathcal{S}^+(a)\}$$

satisfy the assertion.

It remains to prove (2.18). Since $\mathcal{S}^-(a)$ is open, it suffices to show that if $(d_1, d_2] \subset \mathcal{S}^-(a)$, then $d_1 \in \mathcal{S}^-(a)$. Suppose that $d_1 \notin \mathcal{S}^-(a)$. Since $\mathcal{S}^-(a)$ and $\mathcal{S}^+(a)$ are open, $d_1 \in \mathcal{S}^0(a)$ and thus $N(t) \geqslant 0$ for all $t \in \mathbb{R}$. Let $u_i(t) = u(t, a, d_i)$ and $N_i(t) = N(t, a, d_i)$ for $i = 1, 2$. Note that $\Phi(a, d_1) < \Phi(a, d_2)$ and $\Psi(a, d_1) < \Psi(a, d_2)$. Since $\Phi(u, N)$ and $\Psi(u, N)$ are increasing functions of u and N, $u_1(t) < u_2(t)$ and $N_1(t) < N_2(t)$ for all $t \ll -1$ by the formulas (2.13) and (2.14). On the other hand, since $d_1 \in \mathcal{S}^0(a)$ and $d_2 \in \mathcal{S}^-(a)$, there exists $T \in \mathbb{R}$ such that $N_1(T) = N_2(T)$ and $N_1(t) < N_2(t)$ for all $t < T$.

We claim that $u_1(t) < u_2(t)$ for all $t < T$. Otherwise, there would exist a number $T_1 < T$ such that $u_1(T_1) = u_2(T_1)$ and $u_1(t) < u_2(t)$ for all $t < T_1$. Hence $(u_2 - u_1)''(t) < 0$ for all $t < T_1$ by the monotonicity of $\Phi(u, N)$ in u and N. Consequently, $u_2(T_1) - u_1(T_1) > u_2(-\infty) - u_1(-\infty) = 0$, a contradiction. Now, since $u_1(t) < u_2(t)$ and $N_1(t) < N_2(t)$ for all $t < T$, we conclude that $(N_2 - N_1)'' > 0$ for $t < T$, and hence $N_1(T) < N_2(T)$, which violates the fact that $N_1(T) = N_2(T)$. This completes the proof of the lemma. ■

Lemma 2.5: If $b \in \mathcal{S}^0(a)$, then a and b satisfy (2.8). Furthermore,

$$N'(t) \geqslant 0, \quad u'(t) \leqslant 0, \quad \forall\, t \in \mathbb{R}, \tag{2.19}$$

$$\lim_{t \to \infty} u(t) = -\infty, \quad \lim_{t \to \infty} N(t) = \frac{q}{\kappa}. \tag{2.20}$$

In addition, N'' changes signs only once, from $+$ to $-$.

Proof: Let $b \in \mathcal{S}^0(a)$. Then $0 \leqslant N(t) \leqslant q/\kappa$ for all $t \in \mathbb{R}$. Since $b_1 \leqslant b \leqslant b_2$, it holds that $\Phi(a,b) \leqslant 0$ and $\Psi(a,b) \geqslant 0$. We split the proof into three steps.

Step 1: If $b \in \mathcal{S}^0(a)$, then (2.19) holds.

We have three cases, $b_1 < b < b_2$, $b = b_2$, and $b = b_1$. If $b_1 < b < b_2$, then $\Phi(a,b) < 0$ and $\Psi(a,b) > 0$. Hence there exists $T_0 \in \mathbb{R}$ such that $u'(t) < 0$, $u''(t) < 0$, $N''(t) > 0$, and $N'(t) > 0$ for all $t < T_0$. Therefore if $N'(T) < 0$ for some T, then there exist two numbers T_1 and T_2 such that $N'(t) < 0$ and $N''(t) < 0$ on (T_1, T_2). We note from (2.11) that

$$u'(t) = \frac{2q}{\kappa}N'(t) - \int_{-\infty}^{t} \frac{4q^3}{\kappa}e^{u(s)}N(s)\mathrm{d}s.$$

Hence $u'(t)<0$ and $u''(t)<0$ on (T_1,T_2). Consequently, the monotonicity of Φ and Ψ implies that $b\in\mathcal{S}^-(a)$, a contradiction. Therefore, $N'(t)>0$ for all $t\in\mathbb{R}$. On the other hand, if $u'>0$ at some point, since $u',u''<0$ near $-\infty$, there exists an interval (T_3,T_4) such that $u',u''>0$ on (T_3,T_4). This would imply that $N',N''>0$ on (T_3,T_4), and thus $b\in\mathcal{S}^+(a)$. Hence $u'(t)\leqslant 0$ for all $t\in\mathbb{R}$. This proves (2.19).

We now turn to the second case, $b=b_2$. Since $\Phi(a,b)=0$ and $\Psi(a,b)>0$, we have $N'',N'>0$ near $-\infty$. Thus $u'',u'\leqslant 0$ near $-\infty$, otherwise $b\in\mathcal{S}^+(a)$. Now the similar argument as above shows (2.19).

Finally if $b=b_1$, then $\Phi(a,b)<0$ and $\Psi(a,b)=0$. By a similar argument as the second case, we arrive at (2.19).

Step 2: (2.20) holds.

Let $\lambda=\limsup\{N(t):t\in\mathbb{R}\}\leqslant q/\kappa$. Since $N'(t)\geqslant 0$ for all $t\in\mathbb{R}$,

$$\lambda = \lim_{t\to\infty} N(t), \quad \lim_{t\to\infty} N''(t) = 0. \tag{2.21}$$

If $\tau=\liminf\{u(t):t\in\mathbb{R}\}>-\infty$, by (2.19),

$$\tau = \lim_{t\to\infty} u(t), \quad \lim_{t\to\infty} u''(t) = 0.$$

Thus $\Phi(\tau,\lambda)=\Psi(\tau,\lambda)=0$ and this implies that $\lambda e^{\tau}=0$, which is absurd. In the sequel, the first part of (2.20) is proved. The second identity is now the consequence of (2.21).

Step 3: N'' changes signs only once, from $+$ to $-$.

Since (u,N) is a solution of (2.5)–(2.7) satisfying (2.20), it comes from (2.1) that $\Phi(a,b)<0$, namely, a and b satisfy (2.8). Since $\Psi(a,b)>0$, $N''>0$ for all $t\ll -1$. Moreover, since $N'\geqslant 0$ and $N(t)$ is convergent as $t\to\infty$, $N''(t)<0$ for all $t\gg 1$. If N'' changes signs twice, there exist two numbers $T_1<T_2$ such $u'',u',N'',N'<0$ on (T_1,T_2), which means $b\in\mathcal{S}^-(a)$, a contradiction. This completes the proof. ■

It follows from (2.8) and (2.20) that $b_2\notin\mathcal{S}^0(a)$, namely, $b^+<b_2$.

Lemma 2.6: $\mathcal{S}^0(a)$ consists of only one point.

Proof: Suppose that $d_1,d_2\in\mathcal{S}^0(a)$ with $d_1<d_2$. Let (u_i,N_i) be the unique solutions of (2.5)–(2.7) corresponding to d_i, $i=1,2$. Since $\Phi(u,N)$ and $\Psi(u,N)$ are increasing functions of u and N, there exists $T\in\mathbb{R}$ such that $u_1(t)<u_2(t)$ and $N_1(t)<N_2(t)$ for all $t\leqslant T$.

We claim that $u_1<u_2$ for all $t\in\mathbb{R}$. Assume the contrary. Then there exists a number $T_1\in\mathbb{R}$ such that $u_1(T_1)=u_2(T_1)$ and $u_1(t)<u(t)$ for all $t<T_1$. We note that $N_1(t)<N_2(t)$ for all $t<T_1$. Otherwise there would be a number $T_2<T_1$ such that $N_1(T_2)=N_2(T_2)$ and $N_1(t)<N_2(t)$ for all $t<T_2$, which implies that $(N_2-N_1)''(t)>0$ for all $t<T_2$ by the monotonicity of $\Psi(u,N)$ with respect to u and N. Consequently, $N_2(T_2)-N_1(T_2)>d_2-d_1>0$, a contradiction. Since $N_1(t)<N_2(t)$ for all $t<T_1$, we conclude that $(u_2-u_1)''>0$ for $t<T_1$, and hence $u_1(T_1)<u_2(T_1)$, a contradiction. Thus the claim follows.

It now follows that $N_1(t)<N_2(t)$ for all $t\in\mathbb{R}$ by a similar argument as above. However, this implies that

$$(N_2-N_1)''(t)>0 \quad \forall\, t\in\mathbb{R}, \quad \lim_{t\to\infty}(N_2-N_1)=0,$$

a contradiction. ■

It follows from Lemma 2.5 and Lemma 2.6 that for each $a<0$, there exists a unique $b=b(a)\in(0,q/\kappa)$ such that the equations (2.5)–(2.7) satisfying (2.20). Moreover, $b\in(b_1,b_2)$ by Lemma 2.4. Hereafter let $(u(t,a),N(t,a))$ be the unique solution to (2.5)–(2.7) with the boundary condition (1.12).

Lemma 2.7: There exists a constant $\gamma=\gamma(a)>4$ such that

$$\lim_{t\to\infty} u'(t) = -\gamma. \tag{2.22}$$

Proof: Since $u''<0$ by Lemma 2.1, there exists a constant $\gamma\in(0,\infty]$ such that $u'(t)\to-\gamma$ as $t\to\infty$. If $\gamma=\infty$, then there is a number T satisfying that $u'(t)<-3$ for all $t>T$. Thus $u(t)<-3t+C$ for all $t>T$, and

$$\int_{-\infty}^{\infty} e^{2s}e^{u(s)}\,\mathrm{d}s<\infty.$$

Since $b<N(t)<q/\kappa$ for all $t\in\mathbb{R}$ and $\lim_{t\to\infty}N'(t)=0$, we see from (2.11) that

$$\lim_{t\to\infty} u'(t) = \frac{2q}{\kappa}\lim_{t\to\infty}N'(t) - \frac{4q^3}{\kappa}\int_{-\infty}^{\infty} e^{2s}e^{u(s)}N(s)\mathrm{d}s \geqslant -\frac{4q^4}{\kappa^2}\int_{-\infty}^{\infty} e^{2s}e^{u(s)}\,\mathrm{d}s > -\infty,$$

a contradiction. Hence $\gamma<\infty$.

Set $w=u-2qN/\kappa$. Then

$$w'' = -\frac{4q^3}{\kappa}e^{2t}e^{u}N, \quad \lim_{t\to\infty} w'(t) = -\gamma. \tag{2.23}$$

Since $u''<0$ and

$$\gamma = \frac{4q^3}{\kappa}\int_{-\infty}^{\infty} e^{2s}e^{u(s)}N(s)\mathrm{d}s<\infty, \tag{2.24}$$

we conclude that $\gamma>2$ and thus $e^{2t+u}\to 0$ as $t\to\infty$. Using this fact and integrating by parts after multiplication of (2.23) by w', we are led to

$$\frac{\gamma^2}{2}-2\gamma = \frac{4q^3}{\kappa}\int_{-\infty}^{\infty} e^{2t+u}N'\left(1+\frac{2q}{\kappa}N\right)\mathrm{d}t>0. \tag{2.25}$$

Hence $\gamma>4$. ■

We are now in a position to prove Theorem 1.1. We have constructed a unique solution (u,N) of the equations (2.5)–(2.7) satisfying (2.20). In terms of $r=e^t$ variable, (u,N) is a solution of (2.2)–(2.4) with the boundary condition (1.12). Then we can recover the nontopological solution (u,A,N) of (1.5)–(1.7) as mentioned in the Introduction. In other words, we have proved the statements (ii)–(iv) of Theorem 1.1. To complete the proof of Theorem 1.1, it remains to show that (u,A,N) is a finite energy solution and verify the statements (i) and (v).

It follows from (2.22) that

$$\lim_{t\to\infty}\frac{u(t)}{t} = \lim_{t\to\infty} u'(t) = -\gamma.$$

Hence $u(x)=O(-\gamma\ln|x|)$ near ∞, which proves the first part of (v). We also observe that

$$\Delta N = e^u(\kappa q + 2q^2N) - \kappa(q-\kappa N)\to 0$$

as $|x|\to\infty$. This proves the second part of (v).

Next, we show that (u,A,N) is a finite energy solution. Using the self-dual equations (1.6) and (1.7), we can rewrite (1.3) as

$$\mathcal{E}(\phi,A,N) = \int_{\mathbb{R}^2} |D_A\phi|^2 + (q|\phi|^2+\kappa N-q)^2 + 2q^2|\phi|^2N^2 + |\nabla N|^2.$$

Since $ru_r=u_t=O(1)$, we have $u_r=O(r^{-1})$. Then

$$|D_A\phi|^2 = \tfrac{1}{2}|u_r|^2 e^u = O(r^{-\gamma-2}) \in L^1(\mathbb{R}^2),$$

$$(q|\phi|^2 + \kappa N - q)^2 = O(r^{-2\gamma}) \in L^1(\mathbb{R}^2),$$

$$2q^2|\phi|^2 N^2 = O(r^{-\gamma}) \in L^1(\mathbb{R}^2).$$

Meanwhile, multiplying (1.10) by N and integrating by parts, we are led to

$$\|\nabla N\|_{L^2} \leqslant C(\|e^u\|_{L^1} + \|q - \kappa N\|_{L^1}) < \infty.$$

Consequently, (u,A,N) is of finite energy.

Finally, we prove the statement (i). By means of (1.7), the magnetic flux given by (1.4) is computed as

$$\Lambda = -q\int_{\mathbb{R}^2}(q|\phi|^2 + \kappa N - q)\mathrm{d}x = -2\pi q\int_{-\infty}^{\infty} e^{2t}(qe^u + \kappa N - q)\mathrm{d}t = -\pi u'(\infty) = \pi\gamma.$$

Here we used the $t=\ln r$ variable. Since (ϕ,A,N) satisfies the self-dual equations, we conclude that

$$\mathcal{E}(\phi,A,N) = \Lambda = \pi\gamma.$$

This completes the proof of Theorem 1.1.

In the remaining part of this section, we make an observation of γ given by (2.22). We are going to prove that the lower bound of γ in Lemma 2.7 is optimal. In fact, we show that there exists a solution of (2.5)–(2.7) satisfying (2.20) such that the corresponding γ is arbitrarily close to 4. We begin with the following lemma.

Lemma 2.8: $b=b(a)$ is a continuous decreasing function such that

$$\lim_{a\to 0} b = 0, \quad \lim_{a\to-\infty} b = \frac{q}{\kappa}. \tag{2.26}$$

Proof: If $a_k \to a_0 < 0$, then up to a subsequence $b(a_k) \to b_0$. It follows from the continuous dependence of solutions to the initial data that $(u(t,a_0),N(t,a_0))$ is the unique solution of (2.5) and (2.6) with the boundary condition (2.20) satisfying $u(-\infty,a_0)=a_0$ and $N(-\infty,a_0)=b_0$. By virtue of the uniqueness result of Lemma 2.6, $b_0=b(a_0)$ and hence $b(a)$ is a continuous function.

The decreasing property of $b=b(a)$ follows from similar arguments of the proof of Lemma 2.6. Indeed, if $a_1<a_2$ and $b(a_1)\leqslant b(a_2)$, then we arrive at a contradiction by virtue of the monotonicity of $\Phi(u,N)$ and $\Psi(u,N)$ as in the proof of Lemma 2.6.

Finally, it is easily seen from (2.15) that

$$\lim_{a\to 0} b_1(a) = \lim_{a\to 0} b_2(a) = 0, \quad \lim_{a\to-\infty} b_1(a) = \lim_{a\to-\infty} b_2(a) = \frac{q}{\kappa}.$$

Since $b_1 \leqslant b \leqslant b_2$, this implies (2.26). ■

Proposition 2.9: $\gamma=\gamma(a)$ is a continuous function and

$$\lim_{a\to-\infty} \gamma(a) = 4. \tag{2.27}$$

Proof: We first show the continuity of $\gamma(a)$. For $a<0$, let $a_k \to a$. Let T_0 be such that $u'(T_0,a) = -7/2$. Since $u'(t,a)$ is continuous in a, we may assume that $u'(T_0,a_k) < -3$ for all k. Since u' is decreasing, we deduce that $u'(t,a_k) < -3$ for all $t > T_0$. Thus for $t \geqslant T_0$,

$$u(t,a_k) < u(T_0,a_k) - 3(t-T_0) \leqslant a_k - 3(t-T_0).$$

Now

$$\int_{-\infty}^{\infty} e^{2t}e^{u(t,a_k)}N(t,a_k)\mathrm{d}t \leqslant \frac{q}{\kappa}e^{a_k}\int_{-\infty}^{T_0} e^{2t}\,\mathrm{d}t + \frac{q}{\kappa}e^{a_k+3T_0}\int_{T_0}^{\infty} e^{-t}\,\mathrm{d}t = \frac{q}{2\kappa}e^{\alpha_k}e^{2T_0} + \frac{q}{\kappa}e^{a_k}e^{2T_0} \leqslant C$$

as $a_k \to a$. Since γ is given by the formula (2.24), it comes from the Lebesgue convergence theorem that $\gamma(a_k)\to\gamma(a)$. This implies the continuity of $\gamma(a)$.

To show (2.27), we observe from (2.25) that

$$\gamma^2(a) - 4\gamma(a) \leqslant C_1\int_{-\infty}^{\infty} e^{2t}e^{u(t,a)}N'(t,a)\mathrm{d}t, \quad C_1 = \frac{8q^3}{\kappa}\left(1+\frac{2q^2}{\kappa^2}\right). \tag{2.28}$$

Let $h(t,a)=N'(t,a)$. A simple calculation gives

$$h'' - (\kappa^2 + 2q^2e^u)h = (\kappa q + 2q^2N)e^u u'.$$

We recall that $h>0$. Let $T_1=T_1(a)$ be the positive maximum point of $h(t,a)$. Since $u'(t)>-\gamma$ for all $t\in\mathbb{R}$, we have

$$h(T_1;a) \leqslant \left(\frac{\kappa q + 2q^2N}{\kappa^2 + 2q^2e^u}e^u(-u')\right)(T_1,a) \leqslant \frac{1}{\kappa^2}\left(\kappa q + \frac{2q^3}{\kappa}\right)e^a\gamma(a) = C_2e^a\gamma(a)$$

as $a\to-\infty$. Thus by (2.28),

$$\gamma^2(a) - 4\gamma(a) \leqslant C_1C_2e^a\gamma(a)\int_{-\infty}^{\infty} e^{2t}e^{u(t,a)}\,\mathrm{d}t$$

as $a\to-\infty$. On the other hand, it comes from (2.24) and (2.26) that

$$\int_{-\infty}^{\infty} e^{2t}e^{u(t,a)}\,\mathrm{d}t \leqslant \frac{1}{b}\int_{-\infty}^{\infty} e^{2t}e^{u(t,a)}N(t,a)\mathrm{d}t = \left(\frac{\kappa^2}{4q^4} + o(1)\right)\gamma(a)$$

as $a\to-\infty$. In the sequel,

$$\gamma^2(a) - 4\gamma(a) \leqslant Ce^a\gamma^2(a),$$

and hence $\gamma(a)-4=o(1)$ as $a\to-\infty$. This establishes (2.27). ■

III. CHERN–SIMONS LIMIT

This section is devoted to the proof of Theorem 1.2. Throughout this section, let $a<0$ be fixed. Let (u_q,N_q) be the unique solution of (2.5)–(2.7) satisfying (2.20) corresponding to $(\kappa,q)=(\mu q^2,q)$ such that $b_q=\lim_{t\to-\infty}N_q(t)$ is uniquely determined by a and q. Set

$$\widetilde{N}_q = qN_q, \quad \widetilde{b}_q = qb_q, \quad w_q = u_q + \frac{2}{\mu q^2}\left(\frac{1}{\mu} - \widetilde{N}_q\right).$$

We notice that

$$\widetilde{N}_q < \mu^{-1}, \quad \|w_q - u_q\|_{L^\infty(\mathbb{R})} = O(q^{-2}), \quad w_q'' = -\frac{4}{\mu}e^{2t}e^{u_q}\widetilde{N}_q < 0. \tag{3.1}$$

Since w_q' is decreasing, it follows from (2.22) that $w_q' \searrow -\gamma_q$ with $\gamma_q>4$ as $t\to\infty$.

On the other hand, we recall from Lemma 2.4 that

$$\frac{\kappa q}{\kappa^2 + 2q^2e^a}(1-e^a) \leqslant b_q \leqslant \frac{q}{\kappa}(1-e^a).$$

Hence

$$b_* \equiv \lim_{q\to\infty} \tilde{b}_q = \frac{1}{\mu}(1-e^a) > 0.$$

It was proved[10] that every solution of (1.17) is radially symmetric about a point $x_0 \in \mathbb{R}^2$, say $x_0=0$, with the property $u<0$. In addition, for each $a<0$, there exists a unique radial solution such that $u(x_0)=a$. Let us rewrite (1.17) in the t variable as

$$u'' = \frac{4}{\mu^2} e^{2t} e^u (e^u - 1), \quad t \in \mathbb{R}. \tag{3.2}$$

Let u_* be the unique solution satisfying $u_*(t)=a+o(1)$ near $-\infty$. Then we can write

$$u_*(t) = a + \frac{4}{\mu^2}\int_{-\infty}^{t} (t-s) e^{2s} e^{u_*(s)} (e^{u_*(s)} - 1) \mathrm{d}s.$$

In this section we will prove that u_q converges to u_* as $q\to\infty$.

Lemma 3.1: γ_q is uniformly bounded in q.

Proof: Let $T_1=T_1(q)$ be the number such that $w_q'(T_1)=-2$. We claim that $\{T_1(q)\}$ is bounded above for all large q. Suppose that $T_1>0$. It follows that $w_q(t)+2t>w(0)$ for $t\in(0,T_1)$. Thus for all large q,

$$2 > \int_0^{T_1} w'' \,\mathrm{d}t = \frac{4}{\mu}\int_0^{T_1} e^{2t} e^{u_q} \tilde{N}_q \,\mathrm{d}t > \frac{4\tilde{b}_q}{\mu}\int_0^{T_1} e^{2t} e^{u_q}\,\mathrm{d}t > \frac{2\tilde{b}_q}{\mu}\int_0^{T_1} e^{2t+w_q}\,\mathrm{d}t > \frac{2\tilde{b}_q}{\mu} e^{w_q(0)} T_1.$$

Hence if q is large enough, then $T_1 < \mu \tilde{b}_q^{-1} e^{-w_q(0)}$. Let $z_q(t)=\mu^{-2}e^{2t}-a+w_q(t)$. Then $z_q''=4\mu^{-1}e^{2t}(\mu^{-1}-e^{u_q}\tilde{N}_q)>0$. Since $z_q(-\infty)>0$ and $z_q'(-\infty)=0$, it is seen that $z_q(0)>0$. As a consequence, we conclude that $T_1 \leqslant C$.

Set $T_2=T_2(q)=(w_q')^{-1}(-3)$. Then for $t>T_2$,

$$-w_q'(t) - 3 = -\int_{T_2}^{t} w_q''(s)\mathrm{d}s \leqslant \frac{4}{\mu^2}\int_{T_2}^{t} e^{2s} e^{u_q(s)}\,\mathrm{d}s \leqslant \frac{4}{\mu^2}\int_{T_2}^{t} e^{2s+w_q(s)}\,\mathrm{d}s.$$

Since $-w_q'(t)>3$ for $t>T_2$, it follows that $w_q(t)<-3(t-T_2)+w_q(T_2)$. Hence for $t>T_2$,

$$-w_q'(t) - 3 < \frac{4}{\mu^2}\int_{T_2}^{t} e^{-s+3T_2+w_q(T_2)}\,\mathrm{d}s.$$

Letting $t\to\infty$, we find that $\gamma_q<3+4\mu^{-2}e^{2T_2+w_q(T_2)}$. Since $-w_q'(t)>2$ for $t>T_1$, it follows that $2t+w_q(t)<2T_1+w_q(T_1)$. Since $T_1<T_2$, we obtain

$$\gamma_q < 3 + 4\mu^{-2} e^{2T_1+w_q(T_1)} \leqslant C.$$

■

Lemma 3.2: As $q\to\infty$, we have

$$e^{u_q} - 1 + \mu\tilde{N}_q = O(q^{-2}). \tag{3.3}$$

Proof: We first observe from (2.16) that $|u'(t)| \leqslant Cq^2 e^{2t}$ for all $t\in\mathbb{R}^2$. In particular,

$$e^{-2t}|u'(t)| \leqslant Cq^2 \tag{3.4}$$

for all $t\in\mathbb{R}$. Let us write $u_q''=2e^{2t}v_q$, where $v_q=q^2(e^{u_q}-1+\mu\tilde{N}_q)$. Then $v_q<0$ and

$$v_q'' - e^{2t}v_q(2q^2e^{u_q}+\mu^2q^4) = q^2e^{u_q}|u_q'|^2 + 2\mu q^4 e^{2t} e^{u_q}\tilde{N}_q.$$

If $T_3=T_3(q)$ is a minimum point of v_q, then by Lemma 3.1 and (3.4),

$$0 > v_q(T_3) \geqslant -\frac{e^{-2t}|u_q'|^2 e^{u_q} + 2\mu q^2 e^{u_q}\tilde{N}_q}{2e^{u_q} + \mu^2 q^2}(T_3) \geqslant -\frac{Cq^2\gamma_q e^{u_q} + 2\mu q^2 e^{u_q}\tilde{N}_q}{2e^{u_q} + \mu^2 q^2}(T_3) \geqslant -C$$

for some positive constant. This finishes the proof. ■

Lemma 3.3: For any $T \in \mathbb{R}$, we have

$$\sup_{t\leqslant T}|u_q - u_*| = O(q^{-2}), \quad \sup_{t\leqslant T}|\tilde{N}_q - N_*| = O(q^{-2}), \tag{3.5}$$

where $N_* = \mu^{-1}(1-e^{u_*})$.

Proof: Let $T \in \mathbb{R}$ be fixed. It comes from (3.3) that

$$w_q'' = \frac{4}{\mu^2}e^{2t}e^{u_q}(e^{u_q}-1) - \frac{4}{\mu^2}e^{2t}e^{u_q}(e^{u_q}-1+\mu\tilde{N}_q) = \frac{4}{\mu^2}e^{2t}e^{u_q}(e^{u_q}-1) + O(q^{-2})\cdot e^{2t} \tag{3.6}$$

as $q\to\infty$. Let $T_0 \leqslant T$. For any $t \leqslant T_0$, by (3.1) and (3.6),

$$\begin{aligned}|w_q(t) - u_*(t)| &\leqslant O(q^{-2}) + \int_{-\infty}^{t} e^{2t}(t-s)\left(\frac{4}{\mu^2}|e^{u_q}(e^{u_q}-1) - e^{u_*}(e^{u_*}-1)| + O(q^{-2})\right)ds \\ &\leqslant Ce^{2T_0}\sup_{t\leqslant T_0}|u_q - u_*| + Cq^{-2}e^{2T_0} + O(q^{-2}) \\ &\leqslant Ce^{2T_0}\sup_{t\leqslant T_0}|w_q - u_*| + Cq^{-2}e^{2T_0} + O(q^{-2}).\end{aligned}$$

Hence if T_0 is small enough, then

$$\sup_{t\leqslant T_0}|w_q - u_*| = O(q^{-2}).$$

Applying the standard continuation argument, we obtain

$$\sup_{t\leqslant T}|w_q - u_*| = O(q^{-2}),$$

and thus by (3.1), we have

$$\sup_{t\leqslant T}|u_q - u_*| = O(q^{-2}).$$

Finally for $t \leqslant T$, by (3.3),

$$|\tilde{N}_q - N_*| = \frac{1}{\mu}|e^{\mu_q} - e^{u_*}| + O(q^{-2}) = O(q^{-2}).$$

■

Lemma 3.4: As $q\to\infty$, we have

$$\mu q^2(e^{u_q} - 1 + \mu\tilde{N}_q) + 2e^{u_q}\tilde{N}_q = O(q^{-2}). \tag{3.7}$$

Proof: Let us write $\tilde{N}_q'' = e^{2t}h_q$, where

$$h_q = q^2[\mu q^2(e^{u_q} - 1 + \mu\tilde{N}_q) + 2e^{u_q}\tilde{N}_q].$$

It suffice to show that $\|h_q(t)\|_{L^\infty(\mathbb{R})} \leqslant C$ as $q\to\infty$. A simple calculation yields that

$$h_q'' - q^2e^{2t}h_q(\mu^2q^2 + 2e^{u_q}) = \mu q^4 e^{u_q}|u_q'|^2 + 2\mu q^4 e^{2t}e^{u_q}v_q + 2q^2e^{u_q}|u_q'|^2\tilde{N}_q + 4q^2e^{2t}e^{u_q}\tilde{N}_q v_q + 4q^2u_q'e^{u_q}\tilde{N}_q'.$$

Here v_q is defined by $v_q = q^2(e^{u_q} - 1 + \mu\tilde{N}_q)$ as in the proof of Lemma 3.2. Since $v_q < 0$, if $T_4 = T_4(q)$ is a positive maximum point of h_q, then

$$0 < h_q(T_4) \leqslant -\frac{2\mu q^2 e^{u_q}v_q + 4e^{u_q}\tilde{N}_q v_q + 4e^{-2t}\tilde{N}_q'u_q'e^{u_q}}{\mu^2q^2 + 2e^{u_q}}(T_4).$$

We observe from (2.17) and (3.3) that $|\tilde{N}_q'(t)| \leqslant Cq^2e^{2t}$ for all $t \in \mathbb{R}$. Combining this and Lemma 3.1 with the above inequality, we conclude that $h_q(T_4) \leqslant C$.

Similarly, if $T_5 = T_5(q)$ is a negative minimum point of h_q, then

$$0 > h_q(T_5) \geqslant -\frac{\mu q^2 e^{-2t}e^{u_q}|u_q'|^2 + 2e^{-2t}e^{u_q}|u_q'|^2\tilde{N}_q}{\mu^2q^2 + e^{u_q}}(T_5). \tag{3.8}$$

We claim that T_5 is bounded below. On the contrary, suppose that $T_5 \to -\infty$. We recall from Lemma 2.5 that $\tilde{N}_q''$ changes signs only once, from $+$ to $-$. Let $T_6 = T_6(q)$ be the unique zero of h_q. Then $h_q > 0$ for $t < T_6$ and $h_q < 0$ for $t > T_6$. Thus $T_6 \to -\infty$. Fix $T_0 \in \mathbb{R}$ such that $T_6 < T_0$ for all large q. For $t \geqslant T_0$,

$$0 < \tilde{N}_q'(t) = \int_{-\infty}^{t} e^{2t}h_q(t)\mathrm{d}t \leqslant \int_{-\infty}^{T_6} e^{2t}h_q(t)\mathrm{d}t \leqslant \frac{1}{2}h_q(T_4)e^{2T_6}.$$

Integrating this inequality on (T_0, t), we have

$$\tilde{N}_q(t) - \tilde{N}_q(T_0) = \tfrac{1}{2}h_q(T_4)e^{2T_6}(t - T_0).$$

Letting $q \to \infty$, we have $N_*(t) = N_*(T_0)$ for all $t \geqslant T_0$. Since T_0 was arbitrary, N_* is a constant, which gives a contradiction.

Now since T_6 is bounded below, it follows from Lemma 3.1 and (3.8) that $0 > h_q(T_5) \geqslant -C$. This completes the proof. ■

Lemma 3.5: For any $T \in \mathbb{R}^2$, we have

$$\sup_{t \leqslant T}|u_q'' - u_*''| = O(q^{-2}). \tag{3.9}$$

Proof: Fix $T \in \mathbb{R}^2$. Combining (3.2) and (3.6) with (3.5), we obtain

$$\sup_{t \leqslant T}|w_q'' - u_*''| \leqslant Ce^{2T}\sup_{t \leqslant T}|u_q - u_*| + O(q^{-2}) \cdot e^{2T} = O(q^{-2}) \cdot e^{2T}.$$

Since $\sup_{t \leqslant T}\tilde{N}_q'' \leqslant C$ by (3.7), we are led to

$$\sup_{t \leqslant T}|u_q'' - u_*''| \leqslant \sup_{t \leqslant T}|u_q'' - u_*''| + \sup_{t \leqslant T}|w_q'' - u_*''| \leqslant Cq^{-2}\sup_{t \leqslant T}\tilde{N}_q'' + O(q^{-2}) \cdot e^{2T} = O(q^{-2}),$$

and thus the proof is complete. ■

It now follows from (3.5) and (3.9) that for any $T \in \mathbb{R}^2$,

$$\|u_q - u_*\|_{C^2(-\infty,T]} = O(q^{-2}).$$

This finishes the proof of Theorem 1.2.

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Quantum averaging and resonances: Two-level atom in a one-mode quantized field

M. Amniat-Talab[a)]
Laboratoire de Physique, UMR CNRS 5027, Université de Bourgogne, B.P. 47870, F-21078 Dijon, France, and Physics Department, Faculty of Sciences, Urmia University, P.B. 165, Urmia, Iran

S. Guérin[b)] and H. R. Jauslin[c)]
Laboratoire de Physique, UMR CNRS 5027, Université de Bourgogne, B.P. 47870, F-21078 Dijon, France

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We construct a nonperturbative approach based on quantum averaging combined with resonant transformations to detect the resonances of a given Hamiltonian and to treat them. This approach, which generalizes the rotating-wave approximation, takes into account the resonances at low field and also at high field (nonlinear resonances). This allows us to derive effective Hamiltonians that contain the qualitative features of the spectrum, i.e., crossings and avoided crossings, as a function of the coupling constant. At a second stage the precision of the spectrum can be improved quantitatively by standard perturbative methods like contact transformations. We illustrate this method by determining the spectrum of a two-level atom interacting with a single-mode quantized field. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1864252]

I. INTRODUCTION

Some important features of classical and quantum systems are determined by resonances of the system which cannot be treated by perturbative approaches. In the vicinity of resonances the perturbative formulas display small denominators that lead to the divergence of the perturbative expansions. A widely used model that incorporates a one-photon resonance is the Jaynes-Cummings Hamiltonian extracted from the full dressed Hamiltonian that describes a two-level system coupled with a single mode of a quantized field.[1] Its counterpart for an interaction with a semiclassical laser field is the RWA Hamiltonian (rotating-wave approximation).[2]

In this article we give a systematic method that allows us to construct effective Hamiltonians and determine their spectrum by treating the resonances with an adaptation of resonant transformations that were introduced in Ref. 3 in the context of laser-driven quantum systems in the Floquet representation. The semiclassical model with several incommensurate frequencies[4] has been treated by different methods in Refs. 5–8.

The goal is to obtain the spectrum for a whole interval of values of a parameter like the coupling constant. This is needed, e.g., in applications where the coupling changes adiabatically,[9] corresponding, e.g., to envelopes of laser pulses or to transversal spatial profiles of cavity fields. The method is based on the detection of resonances by a projector derived from quantum averaging. We illustrate it on the problem of a two-level atom interacting with a quantized field and show that a treatment of all the relevant resonances of the system in a given range of parameters allows us to reproduce with good accuracy the spectrum of this system. The treatment of the resonances yields the qualitative structure of the spectrum—the crossings and avoided

[a)]Electronic mail: amniyatm@u-bourgogne.fr
[b)]Electronic mail: sguerin@u-bourgogne.fr
[c)]Electronic mail: jauslin@u-bourgogne.fr

crossings—as a function of the coupling constant. Once this main structure is obtained, one can systematically improve the quantitative accuracy of the spectrum by applying perturbative methods. We use contact transformations with a Kolmogorov-Arnold-Moser (KAM) iteration,[3] which are particularly efficient due to its superconvergent properties.

The paper is structured as follows. In Sec. II, we describe the method of resonance analysis and the construction of effective Hamiltonians. Section III contains the presentation of the model and some preliminary considerations. In Sec. IV, taking into account the resonances of this model in the weak-coupling regime, we extract the effective Hamiltonians by quantum averaging techniques and resonant transformations. In the weak-coupling regime we have to iterate this procedure several times to derive the essential structure of the spectrum in larger ranges of the coupling constant. In Sec. V we extract the effective Hamiltonians in the strong-coupling regime where the qualitative properties of the spectrum can be globally obtained by some preliminary unitary transformations and one resonant transformation which treats the zero-field resonances. We obtain an accurate approximation valid for all values of the coupling constant that contains all the qualitative structures. Finally, in Sec. VI we give some conclusions.

II. PRINCIPLE OF THE METHOD

We consider a Hamiltonian $H=H_0+\epsilon V$, where H_0 is the reference (unperturbed) Hamiltonian, ϵV is the perturbation, and ϵ is an ordering parameter. The first analysis of this problem is in terms of perturbation theory: we look for a KAM-type unitary transformation $e^{\epsilon W}$ close to the identity that allows us to reduce the order of the perturbation from ϵ to ϵ^2:

$$e^{-\epsilon W}He^{\epsilon W}=H_0+\epsilon D+\epsilon^2V_2. \tag{1}$$

ϵD is a remaining term of order ϵ that satisfies $[H_0,D]=0$. The unknown W and D are solutions of the following equations:[3,10]

$$[H_0,W]+V=D, \tag{2a}$$

$$[H_0,D]=0. \tag{2b}$$

The remaining perturbation of order ϵ^2 is given by

$$\epsilon^2V_2=\sum_{m=2}^{\infty}\frac{\epsilon^m}{m!}((m-1)L_W^{m-1}V+L_W^{m-1}D), \tag{3}$$

where L_W is defined as

$$L_WB=[B,W]. \tag{4}$$

The solutions of Eqs. (2) can be written in terms of averaging:[3,11]

$$D=\overline{V}\equiv\Pi_{H_0}V:=\lim_{\tau\to\infty}\frac{1}{\tau}\int_0^{\tau}dse^{-iH_0s}Ve^{iH_0s}=\sum_{\nu,j,j'}|\nu,j\rangle\langle\nu,j|V|\nu,j'\rangle\langle\nu,j'|, \tag{5a}$$

$$W=\lim_{\tau\to\infty}\frac{-i}{\tau}\int_0^{\tau}ds\int_0^{s}ds'e^{-iH_0s'}(V-\Pi_{H_0}V)e^{iH_0s'}=-\sum_{\nu,j,j',\nu'\neq\nu}\frac{|\nu,j\rangle\langle\nu,j|V|\nu',j'\rangle\langle\nu',j'|}{E_\nu^{(0)}-E_{\nu'}^{(0)}}, \tag{5b}$$

where ν labels the different eigenvalues $E_\nu^{(0)}$ of H_0, and j is a degeneracy index which distinguishes different basis vectors $|\nu,j\rangle$ of the degeneracy eigenspace. The operator Π_{H_0} is the projector on the kernel of the application $A\mapsto[H_0,A]$. We remark that the integral representation of D,W in Eqs. (5) can be also well defined in cases where H_0 has a continuum spectrum. We can

iterate the KAM procedure taking $H_0+\epsilon D$ as the new reference Hamiltonian and $\epsilon^2 V_2$ as the new perturbation. The units are chosen such that $\hbar=1$. In the following discussion, we do not write explicitly the ordering parameter ϵ.

A *resonance* is defined as a degeneracy of an eigenvalue $E_\nu^{(0)}$ of H_0 and is said to be *active* if the perturbation V has nonzero matrix elements in the degeneracy subspace of $E_\nu^{(0)}$: $\langle \nu,j|V|\nu,j'\rangle \neq 0$ for some j,j'. Otherwise the resonance is called *passive* or *mute*. Equation (5b) shows that in the case of quasi-resonance (as opposed to exact resonance) where the denominator would be different from zero but very small with respect to the numerator, W can be very large, and thus the expansion cannot be expected to converge. The method we present here is a construction designed to avoid such divergences. We remark that the concept of resonance is defined intrinsically for H_0, while the distinction between active and passive depends on the relation between H_0 and V. The analysis of the resonances thus involves three aspects:

- Decomposition of the Hamiltonian into $H=H_0+V$. Different decompositions can be considered for different regimes of the parameters of H.
- Determination of degenerate eigenvalues of H_0.
- Detection of the *resonant terms* in the perturbation V that couple these degenerate eigenstates.

The resonant terms of V can be detected by projectors of type Π_{H_0} that extract a block-diagonal part of V relative to H_0, where the blocks are generated by the degeneracy subspaces. In the absence of active resonances, when all the eigenvalues of H_0 are nondegenerate or when the resonances are mute, the matrix representation of $\Pi_{H_0}V$ is in fact diagonal in the eigenbasis of H_0. In the presence of active resonances, the block-diagonal effective Hamiltonian that takes into account the considered resonance of the original Hamiltonian can be written as

$$H^{\text{eff}} = H_0 + \Pi_{H_0} V. \tag{6}$$

We will call the transformation that diagonalizes H^{eff} *resonant transformation* (RT). The Hamiltonian $H=H^{\text{eff}}+(V-\Pi_{H_0}V)$ is transformed under RT (denoted $\mathcal{R}$) as follows:

$$H_1 = \mathcal{R}^\dagger H \mathcal{R} = \mathcal{R}^\dagger H^{\text{eff}} \mathcal{R} + \mathcal{R}^\dagger (V - \Pi_{H_0} V)\mathcal{R} =: H_1^{(0)} + V_1, \tag{7}$$

where $H_1^{(0)}$ is defined as the new renormalized reference Hamiltonian and V_1 is the new perturbation. The effect of $\Pi_{H_0}V$ in (6) is to lift the degeneracy of H_0. This can happen in two ways: either the active resonance is transformed into a passive one (e.g., in the case of zero-field resonances) or the resonance disappears completely (when a crossing is transformed into an avoided crossing). The new Hamiltonian H_1 can, however, have other resonances at different values of the coupling parameter. If $H_1^{(0)}+V_1$ does not have any other active resonance in the considered range of the coupling constant, we can, at a second stage, improve the spectrum by a KAM-type perturbative expansion which is expected to converge. If there are other active resonances, we have to iterate the renormalization procedure by applying another RT. We remark that there are cases of multiphoton resonances where the active resonances appear only after applying one or several contact transformations.

III. DESCRIPTION OF THE MODEL AND PRELIMINARY CONSIDERATIONS

We consider as an illustration a two-level atom interacting with a single mode of a quantized field described by

$$H = \omega(a^\dagger a + 1/2) \otimes \mathbb{1}_2 + \frac{\omega_0}{2}\mathbb{1} \otimes \sigma_z + g(a + a^\dagger) \otimes \sigma_x, \tag{8}$$

where a, $a^\dagger$ are the annihilation and creation operators for the field mode with the commutation relation $[a,a^\dagger]=\mathbb{1}=\Sigma_{n=0}^{\infty}|n\rangle\langle n|$, σ_z,σ_x are Pauli matrices, and $\mathbb{1}_2$ is the 2×2 identity matrix. Here ω is the frequency of the field mode, ω_0 is the energy difference of the two atomic states, and g is the

dipole-coupling between the field mode and the atom. This Hamiltonian acts on the Hilbert space $\mathcal{K}=\mathcal{F}\otimes\mathcal{H}$ where $\mathcal{H}=\mathbb{C}^2$ is the Hilbert space of the atom generated by $|\pm\rangle$ (eigenvectors of σ_z) and $\mathcal{F}$ is the Fock space of the field mode generated by the orthonormal basis $\{|n\rangle; n=0,1,2,\ldots\}$, n being the photon number of the field.

For this system there is a parity operator

$$P = e^{i\pi a^\dagger a} \otimes \sigma_z = \sum_{n=0}^{\infty} (-1)^n |n\rangle\langle n| \otimes \sigma_z, \tag{9}$$

with the properties

$$[P,H] = 0, \quad P = P^\dagger, \quad P^2 = \mathbb{1}_{\mathcal{K}} \equiv \mathbb{1} \otimes \mathbb{1}_2. \tag{10}$$

As a consequence, the eigenstates of H can be separated into two symmetry classes, even or odd, under P:

$$P|\phi_{n,\pm}\rangle = \pm|\phi_{n,\pm}\rangle, \quad H|\phi_{n,\pm}\rangle = E_{n,\pm}|\phi_{n,\pm}\rangle. \tag{11}$$

The parity operator also commutes with any operator that depends only on $N=a^\dagger a$ and σ_z.

In spite of the simple form of (8), its exact solutions are not known. This can be related to the fact that the classical limit of this model is nonintegrable.[12] This model is of great interest as a physical model in quantum optics[13–16] and quantum chaos.[17,18] Some approximate solutions of this model have been studied among many others in Refs. 19 and 20 using different formalisms.

The conceptual framework for the solution of this system based on the construction of unitary transformations can be described as follows: First, we decompose the Hamiltonian in two terms as $H=H_0+V$. Depending on the considered ranges of the parameters of the system, different decompositions may be considered. H_0 is *a priori* an operator that is a regular function exclusively of the operators N and σ_z. The operators N and σ_z can be considered in the present model as quantum analogs of classical *global actions*,[21] and H_0 can be labeled *integrable*. The perturbation V contains functions that involve also the other operators $a, a^\dagger, \sigma_x, \sigma_y$. The goal is to determine a unitary transformation U, which should be expressed in terms of well-behaved regular functions of $a, a^\dagger, \sigma_x, \sigma_y, \sigma_z$, such that

$$U^\dagger(H_0(N,\sigma_z) + V(a,a^\dagger,\sigma_x,\sigma_y,\sigma_z))U = H'(N,\sigma_z), \tag{12}$$

where H' is a regular function f exclusively of the action operators N, σ_z: $H'(N,\sigma_z)=f(N,\sigma_z)$. With this transformation the eigenvectors of H can be expressed as $|\phi_{n,\pm}\rangle = U(|n\rangle\otimes|\pm\rangle)$ and the corresponding eigenvalues as $E_{n,\pm}=f(n,\pm1)$ where $N|n\rangle=n|n\rangle$ and $\sigma_z|\pm\rangle=\pm|\pm\rangle$.

We remark that in our context the important property for singling out the operators N, σ_z is that they commute with each other and their spectrum and eigenvectors are explicitly available. The question of whether for a given model there exists a regular unitary transformation U that accomplishes the above requirement is, to our knowledge, an open problem.

Most of the perturbative approaches can be interpreted as methods to find approximations of the transformation U. The presence of resonances is one of the central difficulties in the construction of U, as will be made precise below. In this paper we discuss an iterative approach that consists of constructing first some approximations of U that take into account the dominating effects of a certain number of resonances. The transformations involved in this stage are far from the identity and have a clearly nonperturbative character. Once we have a transformation that takes into account the main effect of a set of resonances that are relevant in a considered interval of the coupling constant g, a perturbative approach (like the KAM, Van Vleck, or other types of the contact transformation) can be applied to improve the approximation quantitatively. The transformations involved in this second stage can be considered as deformations of the identity, since they can be written in the form e^W. This stage cannot be implemented if the resonances are not taken care of beforehand. Indeed the perturbative formulations diverge close to resonances due to the appearance of *small denominators* as can be seen in Eq. (5b).

As in classical mechanics, the construction of the transformation U leading to a Hamiltonian that contains only action variables can often be considered in two steps: $U=U_1U_2$. In the first step, which is called *reduction*, the Hamiltonian is transformed by U_1 into a form that contains functions of $\sigma_z, \sigma_x, \sigma_y$ and N, but not of a and $a^\dagger$. The degree of freedom of the field is made trivial and the number of nontrivial degrees of freedom is thus reduced by one. When we apply this reduction to the effective Hamiltonian (6), we obtain a *reduced effective Hamiltonian*. We remark that in the literature, this "reduced effective Hamiltonian" is often called simply "effective Hamiltonian." In the second step, the reduced Hamiltonian is transformed under U_2 into a form that contains functions of only N and σ_z. For the model (8), the reduction step corresponds to diagonalization in the Fock space and the second step corresponds to diagonalization in the atomic Hilbert space which in this case is trivial. The construction of the RT is based on this reduction procedure.

IV. EFFECTIVE HAMILTONIANS IN THE WEAK-COUPLING REGIME

In this section we consider the Hamiltonian (8) at resonance $\omega_0=\omega$ in the weak coupling regime, so that H can be decomposed as follows:

$$H = H_0 + V,$$

$$H_0(N,\sigma_z) = \omega(N+1/2)\otimes \mathbb{1}_2 + \frac{\omega_0}{2}\mathbb{1}\otimes\sigma_z, \tag{13}$$

$$V(a,a^\dagger,\sigma_x,g) = g(a+a^\dagger)\otimes\sigma_x.$$

The eigenvalues and eigenvectors of H_0 are

$$E^{(0)}_{n,\pm} = \omega(n+1/2) \pm \frac{\omega_0}{2},$$

$$|\phi^{(0)}_{n,\pm}\rangle = |n,\pm\rangle = |n\rangle\otimes|\pm\rangle, \tag{14}$$

$$|n,+\rangle = \begin{pmatrix} |n\rangle \\ 0 \end{pmatrix}, \quad |n,-\rangle = \begin{pmatrix} 0 \\ |n\rangle \end{pmatrix}.$$

For $\omega_0=\omega$ there is a one photon resonance which corresponds to the degeneracies $E^{(0)}_{n,+}=E^{(0)}_{n+1,-}$. The degeneracy eigenspaces are spanned by the vectors $|\phi^{(0)}_{n,+}\rangle$ and $|\phi^{(0)}_{n+1,-}\rangle$. The resonant part of V is obtained by (5a):

$$V_{res} := \Pi_{H_0}V = \sum_{n=0}^{\infty}\left(|n,+\rangle\langle n,+|V|n+1,-\rangle\langle n+1,-| + |n+1,-\rangle\langle n+1,-|V|n,+\rangle\langle n,+|\right)$$
$$= g\begin{pmatrix} 0 & a \\ a^\dagger & 0 \end{pmatrix}, \tag{15}$$

where we have used the relations

$$a = \sum_{n=0}^{\infty}\sqrt{n+1}|n\rangle\langle n+1|, \quad a^\dagger = \sum_{n=0}^{\infty}\sqrt{n+1}|n+1\rangle\langle n|. \tag{16}$$

The effective Hamiltonian containing the one-photon resonance is the so-called Jaynes-Cummings Hamiltonian that can be written as

$$H_0^{\text{eff}} = H_{JC} = H_0 + \Pi_{H_0} V = \omega(N + 1/2) \otimes \mathbb{1}_2 + \frac{\omega}{2}\mathbb{1} \otimes \sigma_z + g\begin{pmatrix} 0 & a \\ a^\dagger & 0 \end{pmatrix}. \tag{17}$$

H_{JC} is a good approximation of (8) for low energies in the limit $g \ll \omega_0, |\omega - \omega_0| \ll \omega_0$. In this limit, the so-called counter-rotating terms $g\left(\begin{smallmatrix} 0 & a^\dagger \\ a & 0 \end{smallmatrix}\right)$ can be discarded (rotating-wave approximation). H can thus be written as $H = H_0^{\text{eff}}(N, a, a^\dagger, \sigma_x, \sigma_y; g) + (V - \Pi_{H_0} V)$. Next we transform H_0^{eff} by a resonant transformation $\mathcal{R}_1$ to a regular function of exclusively the action operators N, σ_z. Every resonant transformation is performed in two steps. To diagonalize H_0^{eff} in the Fock space (the reduction step of the RT denoted R_1) we define a transformation in such a way that the following condition is satisfied:

$$R_1^\dagger V_{res} R_1 = f(N) \otimes \sigma_x, \tag{18}$$

where f is a regular function of N which has to be determined. We require furthermore that $R_1^\dagger H_0 R_1$ stays a function of only N and σ_z. A suitable transformation satisfying these conditions is

$$R_1 := \begin{pmatrix} (aa^\dagger)^{-1/2} a & 0 \\ 0 & \mathbb{1} \end{pmatrix} \equiv \begin{pmatrix} \sum_{n=0}^{\infty} |n\rangle\langle n+1| & 0 \\ 0 & \mathbb{1} \end{pmatrix}. \tag{19}$$

This transformation is not unitary but *isometric*:[22]

$$R_1 R_1^\dagger = \mathbb{1}_{\mathcal{K}}, \quad R_1^\dagger R_1 = \mathbb{1}_{\mathcal{K}} - \begin{pmatrix} |0\rangle\langle 0| & 0 \\ 0 & 0 \end{pmatrix}, \tag{20}$$

where we have used the identity $a^\dagger (N+1)^{-1} a = \mathbb{1} - |0\rangle\langle 0|$. Applying this transformation on the resonant term gives

$$R_1^\dagger V_{res} R_1 = g a^\dagger (aa^\dagger)^{-1/2} a \otimes \sigma_x = g\sqrt{N} \otimes \sigma_x \tag{21}$$

and H is transformed under R_1 as

$$H_{R_1} = R_1^\dagger H R_1 = \omega N \otimes \mathbb{1}_2 + g\sqrt{N} \otimes \sigma_x + g\begin{pmatrix} 0 & A^\dagger \\ A & 0 \end{pmatrix}, \tag{22}$$

where

$$A = a(aa^\dagger)^{-1/2} a = \sum_{n=0}^{\infty} \sqrt{n+1} |n\rangle\langle n+2|, \tag{23}$$

with the properties

$$AA^\dagger = aa^\dagger, \quad A^\dagger A = a^\dagger a - \mathbb{1} + |0\rangle\langle 0|. \tag{24}$$

To each eigenvector $|\phi\rangle$ of H corresponds an eigenvector $R_1^\dagger|\phi\rangle$ of H_{R_1}, since

$$H_{R_1} R_1^\dagger |\phi\rangle = R_1^\dagger H R_1 R_1^\dagger |\phi\rangle = \lambda R_1^\dagger |\phi\rangle. \tag{25}$$

We remark that $R_1^\dagger|\phi\rangle \neq 0 \ \forall |\phi\rangle \in \mathcal{K}$. Every eigenvalue of the original Hamiltonian H is also an eigenvalue of the transformed Hamiltonian H_{R_1}. However, since $R_1|0,+\rangle = 0$, there is a difference in the spectrum between H and H_{R_1}: H_{R_1} has an extra zero eigenvalue with eigenvector $|0,+\rangle$. The spurious eigenvalue can be detected and eliminated after applying the transformation. Indeed, since $|0,+\rangle$ is not coupled to any vector in its orthogonal complement, one can eliminate it from the rest of the calculation by taking the projection of H_{R_1} into the orthogonal complement $H_{R_1,\perp(0,+)} = P_{\perp(0,+)} H_{R_1} P_{\perp(0,+)}$ with $P_{\perp(0,+)} = \mathbb{1}_{\mathcal{K}} - |0,+\rangle\langle 0,+|$. This difference between unitary and

isometric transformations was not taken into account in Ref. 23 in diagonalizing the Jaynes-Cummings Hamiltonian.

The second step of the RT is the diagonalization of $R_1^\dagger H_0^{\text{eff}} R_1 = \omega N \otimes \mathbb{1}_2 + \sqrt{N} \otimes \sigma_x$ in the atomic Hilbert space. This can be performed by a $\pi/2$ rotation around the y-axis:

$$T = e^{-i(\pi/4)\sigma_y} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \tag{26}$$

with the properties

$$T^\dagger \sigma_x T = \sigma_z, \quad T^\dagger \sigma_z T = -\sigma_x. \tag{27}$$

However, since the spurious eigenvector $|0,+\rangle$ can be separated and $|0,-\rangle$ is already an eigenvector of $R_1^\dagger H_0^{\text{eff}} R_1$, the transformation T must be applied only on the subspace with $n \geqslant 1$ photons. The complete transformation (denoted T_1) reads thus

$$T_1 = P_0 \otimes \mathbb{1}_2 + P_{\perp 0} \otimes T, \tag{28}$$

where

$$P_0 = |0\rangle\langle 0|, \quad P_{\perp 0} = \sum_{n=1}^{\infty} |n\rangle\langle n|. \tag{29}$$

Applying T_1 gives

$$H_1 := T_1^\dagger R_1^\dagger H R_1 T_1 = H_1^{(0)}(N, \sigma_z; g) + V_1(a, a^\dagger, \sigma_z, \sigma_x, \sigma_y; g), \tag{30}$$

with

$$H_1^{(0)} = \omega N \otimes \mathbb{1}_2 + g\sqrt{N} \otimes \sigma_z,$$

$$V_1 = \frac{g}{2} \begin{pmatrix} A_{\perp 0} + A_{\perp 0}^\dagger & -A_{\perp 0} + A_{\perp 0}^\dagger \\ A_{\perp 0} - A_{\perp 0}^\dagger & -A_{\perp 0} - A_{\perp 0}^\dagger \end{pmatrix} + \frac{g}{\sqrt{2}} \begin{pmatrix} 0 & |2\rangle\langle 0| \\ |0\rangle\langle 2| & -|2\rangle\langle 0| - |0\rangle\langle 2| \end{pmatrix}, \tag{31}$$

where

$$A_{\perp 0} = P_{\perp 0} A P_{\perp 0} = \sum_{n=1}^{\infty} \sqrt{n+1}\, |n\rangle\langle n+2|, \tag{32}$$

and use has been made of the relations

$$AP_0 = P_0 A^\dagger = 0, \quad P_0 A P_{\perp 0} = |0\rangle\langle 2|. \tag{33}$$

The first RT is thus the combination of $R_1 T_1$. Since the transformation R_1 dresses the upper atomic state by (-1) photon,[15] $\mathcal{R}_1 = R_1 T_1$ can be called a one-photon RT.

$H_1^{(0)}$ is in fact the diagonalized Jaynes-Cummings Hamiltonian in the resonant case with the eigenvalues

$$E_{1,(n,\pm)}^{(0)}(g) = \omega n \pm g\sqrt{n}, \quad n = 0, 1, 2, \ldots . \tag{34}$$

The eigenvalues and therefore the degeneracies of $H_1^{(0)}$ depend on the coupling constant g. For small enough g and low energies, $H_1^{(0)}$ does not have other degeneracies besides the ones at $g = 0$ for which the new perturbation V_1 does not have resonant terms, and we can apply a finite number of KAM-type transformations to improve quantitatively the precision of the spectrum by iteration. We apply a finite number of KAM-type transformations with a cutoff in energy to improve iteratively the precision of the spectrum at small energies. This iteration cannot be

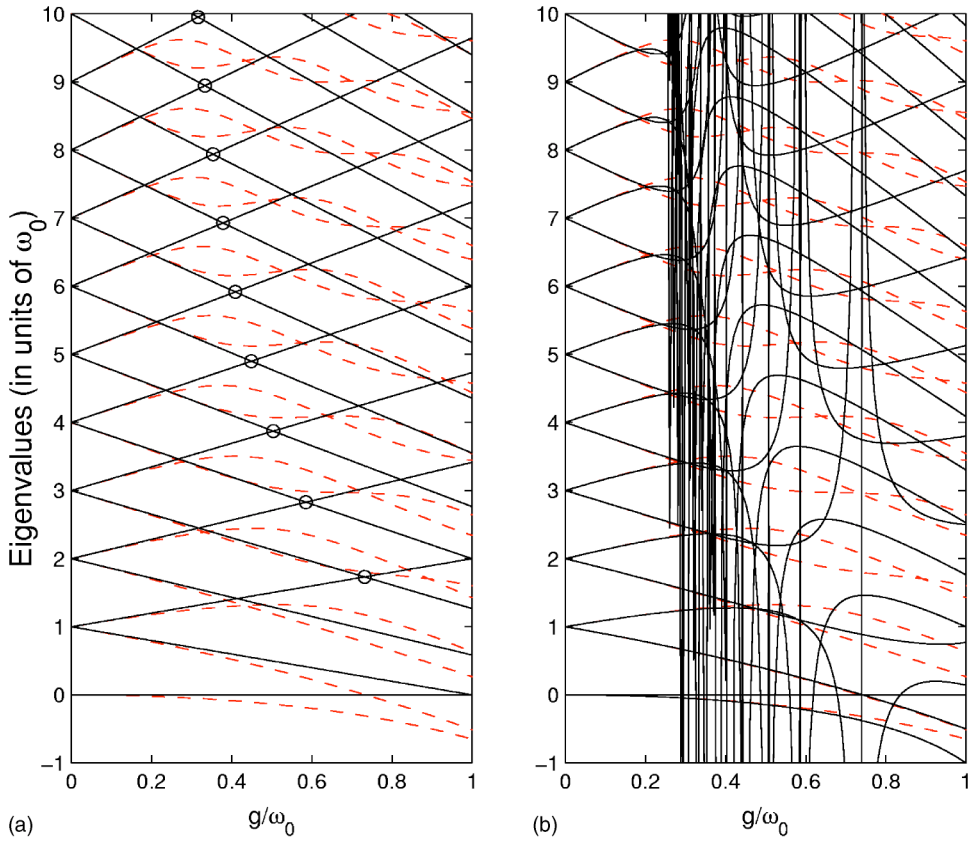

FIG. 1. Comparison of exact numerical eigenvalues (dashed lines) of (8) for one-photon resonance $\omega=\omega_0$ with the approximate ones (solid lines) obtained after (a) one one-photon RT given by (34) and (b) one one-photon RT plus one iteration of KAM-type perturbative expansion. The divergence observed around $g/\omega_0=0.3$ in panel (b) is due to the active nonlinear resonances of $H_1^{(0)}$ that occurred at the degeneracies marked by circles in panel (a). One can see clearly that the locations of these resonances depend on n according to Eq. (35).

expected to converge for all values of g in an interval $[0,g_0]$, because of the presence of a countable number of resonances at high energies at arbitrarily small values of g. A single KAM transformation (which is essentially equivalent to second-order perturbation theory) already gives quite good precision, as shown in Fig. 1(b) for $g/\omega_0<0.25$ for energies smaller than $10\omega_0$. If we take large enough g or larger energies, we encounter new resonances which appear at some specific finite values of g. These resonances are called *field-induced resonances* or *nonlinear resonances*. For larger values of the coupling $[g/\omega_0\approx 0.3$ for the shown energy interval in Fig. 1(b)], where we encounter nonlinear resonances, the KAM iteration diverges. The eigenvalues of $H_1^{(0)}$ are degenerate at $g_n=\omega/(\sqrt{n}+\sqrt{n+1})$ as $E^{(0)}_{1,(n,+)}(g_n)=E^{(0)}_{1,(n+1,-)}(g_n)$. But the corresponding resonant terms in V_1 are zero due to parity (mute resonances). The next degeneracies appear at

$$g_n = 2\omega/(\sqrt{n}+\sqrt{n+2}), \tag{35}$$

as

$$E^{(0)}_{1,(n,+)}(g_n) = E^{(0)}_{1,(n+2,-)}(g_n), \tag{36}$$

which have been marked by circles in Fig. 1(a). All the other resonances are mute. There is an infinite family of nonlinear resonances located at different values of the coupling g_n. We observe from (35) that for higher energies the nonlinear resonances appear for arbitrary small coupling $(\lim_{n\to\infty} g_n=0)$. We can extract the resonant terms corresponding to the whole family in a single

step by working with the combined projector $\Sigma_n \Pi_{H_1^{(0)}(g_n)}$. The resonant terms in V_1 corresponding to the degeneracies (36) are

$$\sum_n \Pi_{H_1^{(0)}(g_n)} V_1 = -\frac{g}{2}\begin{pmatrix} 0 & A_{\perp 0} \\ A_{\perp 0}^\dagger & 0 \end{pmatrix} - \frac{g}{\sqrt{2}}\begin{pmatrix} 0 & 0 \\ 0 & |2\rangle\langle 0| + |0\rangle\langle 2| \end{pmatrix}, \tag{37}$$

and the new effective Hamiltonian is thus

$$H_1^{\text{eff}} = \omega N \otimes \mathbb{1}_2 + g\sqrt{N} \otimes \sigma_z + \sum_n \Pi_{H_1^{(0)}(g_n)} V_1. \tag{38}$$

To diagonalize H_1^{eff}, it can be decomposed according to three orthogonal subspaces:

$$H_1^{\text{eff}} = P_{(0,2,-)} H_1^{\text{eff}} P_{(0,2,-)} + P_{(0,+)} H_1^{\text{eff}} P_{(0,+)} + P_\perp H_1^{\text{eff}} P_\perp = H_1^{\text{eff}} P_{(0,2,-)} + H_1^{\text{eff}} P_{(0,+)} + H_1^{\text{eff}} P_\perp, \tag{39}$$

where the projectors, which commute with H_1^{eff}, are defined by

$$P_{(0,2,-)} = \begin{pmatrix} 0 & 0 \\ 0 & |0\rangle\langle 0| + |2\rangle\langle 2| \end{pmatrix}, \quad P_{(0,+)} = \begin{pmatrix} |0\rangle\langle 0| & 0 \\ 0 & 0 \end{pmatrix},$$

$$P_\perp = \mathbb{1}_{\mathcal{K}} - P_{(0,2,-)} - P_{(0,+)} = \begin{pmatrix} \sum_{n=1}^{\infty} |n\rangle\langle n| & 0 \\ 0 & \sum_{n=1,\neq 2}^{\infty} |n\rangle\langle n| \end{pmatrix}, \tag{40}$$

which leads to

$$H_1^{\text{eff}} P_{(0,+)} = 0, \quad H_1^{\text{eff}} P_{(0,2,-)} = \left[(2\omega - g\sqrt{2})|2\rangle\langle 2| - \frac{g}{\sqrt{2}}(|2\rangle\langle 0| + |0\rangle\langle 2|) \right] \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

$$H_1^{\text{eff}} P_\perp = \omega \begin{pmatrix} \sum_{n=1}^{\infty} n|n\rangle\langle n| & 0 \\ 0 & + \sum_{n=1,n\neq 2}^{\infty} n|n\rangle\langle n| \end{pmatrix} + g \begin{pmatrix} \sum_{n=1}^{\infty} \sqrt{n}|n\rangle\langle n| & 0 \\ 0 & \sum_{n=1,n\neq 2}^{\infty} \sqrt{n}|n\rangle\langle n| \end{pmatrix}$$
$$- \frac{g}{2}\begin{pmatrix} 0 & A_{\perp 0} \\ A_{\perp 0}^\dagger & 0 \end{pmatrix}. \tag{41}$$

$H_1^{\text{eff}} P_{(0,2,-)}$ can be directly diagonalized by

$$R_{(0,2,-)} = P_{(0,2,-)} \begin{pmatrix} 0 & 0 \\ 0 & \cos\theta(|2\rangle\langle 2| - |0\rangle\langle 0|) - \sin\theta(|2\rangle\langle 0| + |0\rangle\langle 2|) \end{pmatrix} P_{(0,2,-)}, \tag{42}$$

where the angle θ is defined by the relation

$$\tan 2\theta = \frac{g\sqrt{2}}{2\omega - g\sqrt{2}}, \quad 0 \leqslant \theta < \frac{\pi}{2}, \tag{43}$$

and the corresponding eigenvalues are

$$E^{\text{eff}}_{1,(0,+)} = 0, \quad E^{\text{eff}}_{1,(n=0,2,-)} = \omega - \frac{g}{\sqrt{2}} \pm \frac{1}{2}\sqrt{(2\omega - g\sqrt{2})^2 + 2g^2}. \tag{44}$$

The reduction step of the second RT to diagonalize $H_1^{\text{eff}} P_\perp$ in the Fock space can be defined as

$$R_{2,\perp} := P_\perp \begin{pmatrix} (A_{\perp 0} A_{\perp 0}^\dagger)^{-1/2} A_{\perp 0} & 0 \\ 0 & \mathbb{1} \end{pmatrix} P_\perp = \begin{pmatrix} \sum_{n=1}^{\infty} |n\rangle\langle n+2| & 0 \\ 0 & \sum_{n=1,\neq 2}^{\infty} |n\rangle\langle n| \end{pmatrix} \tag{45}$$

with the properties

$$R_{2,\perp} R_{2,\perp}^\dagger = P_\perp, \quad R_{2,\perp}^\dagger R_{2,\perp} = P_\perp - \begin{pmatrix} |1\rangle\langle 1| + |2\rangle\langle 2| & 0 \\ 0 & 0 \end{pmatrix}. \tag{46}$$

Equation (45) shows that $R_{2,\perp}$ dresses the upper atomic state by (-2) photons. Therefore $\mathcal{R}_{2,\perp}$ can be called a two-photon RT. Since $R_{2,\perp}|1,+\rangle = 0 = R_{2,\perp}|2,+\rangle$, the spectrum of $R_{2,\perp}^\dagger H_1^{\text{eff}} P_\perp R_{2,\perp}$ has two extra zero eigenvalues relative to the spectrum of $H_1^{\text{eff}} P_\perp$. Applying $R_{2,\perp}$ gives

$$R_{2,\perp}^\dagger H_1^{\text{eff}} P_\perp R_{2,\perp} = \omega \begin{pmatrix} \sum_{n=3}^{\infty} (n-2)|n\rangle\langle n| & 0 \\ 0 & \sum_{n=1,\neq 2}^{\infty} n|n\rangle\langle n| \end{pmatrix} + g \begin{pmatrix} \sum_{n=3}^{\infty} \sqrt{n-2}|n\rangle\langle n| & 0 \\ 0 & -\sum_{n=1,\neq 2}^{\infty} \sqrt{n}|n\rangle\langle n| \end{pmatrix}$$
$$- g/2 \sum_{n=3}^{\infty} \sqrt{n-1}|n\rangle\langle n| \otimes \sigma_x. \tag{47}$$

Combining the transformations on the different subspaces we can write the transformation that diagonalizes H_1^{eff} in the Fock space as

$$R_2 = R_{2,\perp} + R_{(0,2,-)} + P_{(0,+)}. \tag{48}$$

At the right-hand side of (47), the three matrices have entries that commute with each other so we can diagonalize the sum of them in the atomic Hilbert space (the second step of $\mathcal{R}_{2,\perp}$) as if they had scalar entries. The eigenvalues of $R_{2,\perp}^\dagger H_1^{\text{eff}} P_\perp R_{2,\perp}$ are thus

$$E^{\text{eff}}_{1,(n=1,-)} = \omega - g, \quad E^{\text{eff}}_{1,(n=1,+)} = 0, \quad E^{\text{eff}}_{1,(n=2,+)} = 0,$$

$$E^{\text{eff}}_{1,(n\geqslant 3,\pm)} = \omega(n-1) + \frac{g}{2}(\sqrt{n-2} - \sqrt{n}) \pm \frac{1}{2}[(-2\omega + g(\sqrt{n-2} + \sqrt{n}))^2 + g^2(n-1)]^{1/2}. \tag{49}$$

As it can be seen from (49), there are two extra zero eigenvalues which have been added by $R_{2,\perp}$ to the spectrum of H_1^{eff}.

Figures 2(a) and 2(b) compare respectively the exact spectrum of H calculated numerically with the spectrum of $H_0^{\text{eff}} = H_{JC}$ given by (34) and of H_1^{eff} given by (49) and (44). The crossings of the exact spectrum are all among the eigenvalues with different parities. It is found that the spectrum of H_0^{eff} coincides with the exact one only in the range of quite small coupling. The spectrum of H_1^{eff} has been modified with respect to the one of H_0^{eff} by transforming the encircled crossings between eigenvalues with the same parity into avoided crossings in the small g region. This procedure to treat resonances can be iterated to take into account other resonances appearing at larger values of g. Figures 2(a)–2(e) show how the combination of a one-photon RT and

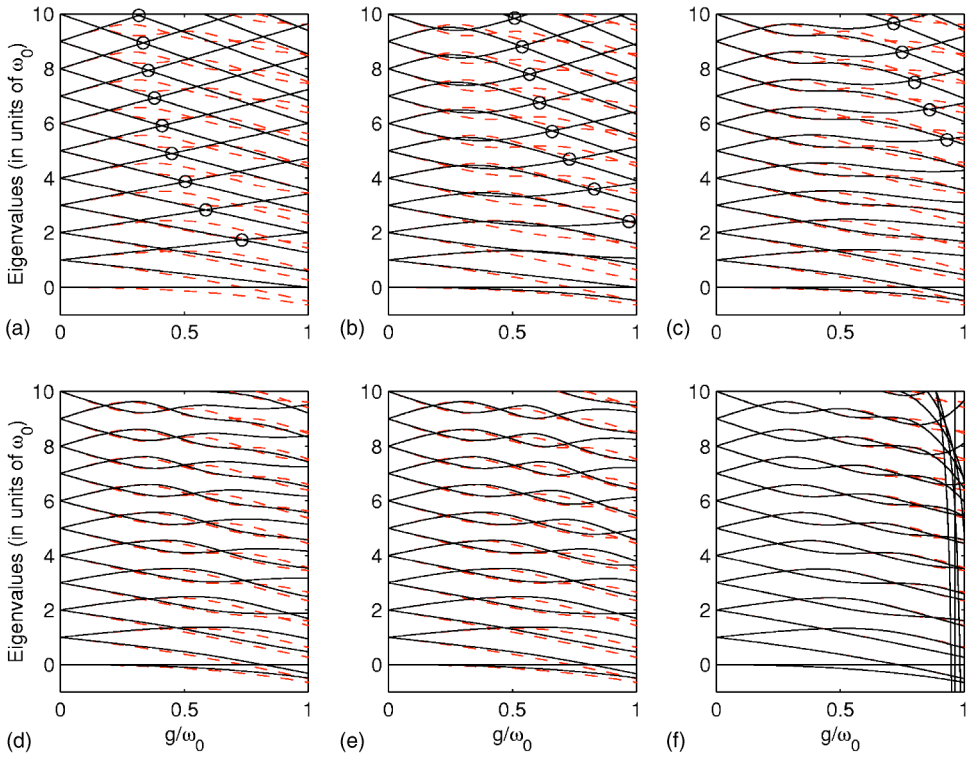

FIG. 2. Comparison of the exact numerical eigenvalues (dashed lines) of (8) for one-photon resonance $\omega=\omega_0$ with the approximate ones (solid lines) obtained respectively after (a) one one-photon RT given by (34), (b) one one-photon RT plus one two-photon RTs given by (49), (c) one one-photon RT plus two two-photon RTs, (d) one one-photon RT plus three two-photon RTs, (e) one one-photon RT plus four two-photon RTs, (f) one one-photon RT plus four two-photon RTs plus one iteration of KAM-type perturbative expansion. The divergence of the KAM transformation observed close to $g/\omega_0=1$ in panel (f) is due to the presence of active resonances at larger values of g.

consecutive two-photon RTs lift the artificial degeneracies (marked by circles) of the effective Hamiltonians. The successive steps, which we have implemented numerically, transform eigenvalue crossings into avoided crossings. We observe that these RTs also produce an improvement of the approximations of the spectrum. Figure 2(f) shows the effect of a KAM transformation after the fourth two-photon RT which improves quantitatively the result of Fig. 2(e). The divergence of the KAM transformation close to $g=1$ in Fig. 2(e) is due to the presence of active resonances at larger values of g.

V. EFFECTIVE HAMILTONIANS IN THE STRONG-COUPLING REGIME

In this section we use quantum averaging techniques and RT to obtain the effective Hamiltonians of (8) by starting the analysis from the strong-coupling regime. We derive a formula that reproduces the spectrum quite accurately in the whole range of g and for all energies. We consider an alternative decomposition of the Hamiltonian (8) in a way suggested by the strong coupling regime $g \gg \omega_0 > 0$,

$$H = H_0 + V,$$

$$H_0 = \omega(N + 1/2) \otimes \mathbb{1}_2 + g(a + a^\dagger) \otimes \sigma_x, \tag{50}$$

$$V = \frac{\omega_0}{2}\mathbb{1} \otimes \sigma_z$$

which can be interpreted as the system of a quantized field plus the coupling term perturbed by the two-level atom. We will use this decomposition as an alternative starting point. As it will be seen later, this approach will allow us to obtain the spectral data for the whole range of values of the coupling $g \in [0,\infty)$. We remark that in this decomposition, H_0 contains all the unbounded operators of the complete model and that the perturbation V is a bounded operator. In this case $H_0(N,a,a^\dagger,\sigma_z,\sigma_x;g)$ is integrable since we can explicitly transform it into a form involving a regular function exclusively of the action operators N,σ_z [given below in Eq. (55)]. To transform H_0 to a function of action operators, first we diagonalize the term $g(a+a^\dagger)\otimes\sigma_x$ in the atomic Hilbert space by the transformation (26):

$$T^\dagger H T = \omega(N + 1/2) \otimes \mathbb{1}_2 + g(a + a^\dagger) \otimes \sigma_z - \frac{\omega_0}{2}\mathbb{1} \otimes \sigma_x. \tag{51}$$

Next we apply a second unitary transformation,

$$U = \begin{pmatrix} e^{-(g/\omega)(a^\dagger - a)} & 0 \\ 0 & e^{(g/\omega)(a^\dagger - a)} \end{pmatrix}, \tag{52}$$

to transform $\omega(N+1/2)\otimes\mathbb{1}_2+g(a+a^\dagger)\otimes\sigma_z$ into a function of only N,σ_z (in this case only of N):

$$H_1 := U^\dagger T^\dagger H T U = \left[\omega(N + 1/2) - \frac{g^2}{\omega}\right] \otimes \mathbb{1}_2 - \frac{\omega_0}{2}\begin{pmatrix} 0 & e^{2(g/\omega)(a^\dagger - a)} \\ e^{-2(g/\omega)(a^\dagger - a)} & 0 \end{pmatrix}, \tag{53}$$

where use has been made of the commutation relations among a, $a^\dagger$, N, and the Hausdorff formula:

$$e^B C e^{-B} = C + [B,C] + \frac{1}{2!}[B,[B,C]] + \cdots. \tag{54}$$

We decompose H_1 as

$$H_1 = H_1^{(0)} + V_1,$$

$$H_1^{(0)} = U^\dagger T^\dagger H_0 T U = \left[\omega(N + 1/2) - \frac{g^2}{\omega}\right] \otimes \mathbb{1}_2, \tag{55}$$

$$V_1 = -\omega_0/2\begin{pmatrix} 0 & e^{2(g/\omega)(a^\dagger - a)} \\ e^{-2(g/\omega)(a^\dagger - a)} & 0 \end{pmatrix}.$$

The effective Hamiltonian of the system for strong-coupling regime can thus be written as

$$H_1^{\text{eff}} = H_1^{(0)} + \Pi_{H_1^{(0)}} V_1. \tag{56}$$

The eigenvalues of $H_1^{(0)}$ have a twofold degeneracy for every value of n as

$$E^{(0)}_{1,(n,\pm)} = \omega(n + 1/2) - \frac{g^2}{\omega}. \tag{57}$$

The average of V_1 relative to $H_1^{(0)}$ is thus

$$\begin{aligned}\Pi_{H_1^{(0)}} V_1 &= \sum_{n=0}^{\infty} \{|n,+\rangle\langle n,+|V_1|n,-\rangle\langle n,-| + |n,-\rangle\langle n,-|V_1|n,+\rangle\langle n,+|\} \\ &= -\frac{\omega_0}{2}\sum_{n=0}^{\infty} f_n |n\rangle\langle n| \otimes \sigma_x,\end{aligned} \tag{58}$$

with

$$\begin{aligned}f_n &= \langle n|e^{(-2g/\omega)(a^\dagger - a)}|n\rangle = \langle n|e^{(+2g/\omega)(a^\dagger - a)}|n\rangle = e^{-2g^2/\omega^2}\langle n|e^{(-2g/\omega)a^\dagger}e^{(+2g/\omega)a}|n\rangle \\ &= e^{-2g^2/\omega^2}\left(\sum_{j=0}^{n}\frac{(-2g/\omega)^j}{j!}\sqrt{\frac{n!}{(n-j)!}}\langle n-j|\right)\left(\sum_{i=0}^{n}\frac{(+2g/\omega)^i}{i!}\sqrt{\frac{n!}{(n-i)!}}|n-i\rangle\right) \\ &= e^{-2g^2/\omega^2}\sum_{j=0}^{n}\frac{(2g/\omega)^{2j}(-1)^j}{(j!)^2}\frac{n!}{(n-j)!} = e^{-2g^2/\omega^2}L_n\left(\frac{4g^2}{\omega^2}\right)\end{aligned} \tag{59}$$

where the L_n are the Laguerre polynomials. We remark that in the limit of a large photon number $(n\to\infty)$, f_n can be expressed as a zeroth-order Bessel function $J_0(4g\sqrt{n}/\omega)$.[15] H_1 can be reorganized as

$$H_1 = H_1^{\text{eff}} + (V_1 - \Pi_{H_1^{(0)}} V_1),$$

$$H_1^{\text{eff}} = \left(\omega(N + 1/2) - \frac{g^2}{\omega}\right)\otimes 1_2 - \frac{\omega_0}{2}F \otimes \sigma_x, \tag{60}$$

$$(V_1 - \Pi_{H_1^{(0)}} V_1) = -\frac{\omega_0}{2}\begin{pmatrix} 0 & G - F \\ G^\dagger - F & 0\end{pmatrix},$$

where

$$G = e^{(+2g/\omega)(a^\dagger - a)}, \quad F = \sum_{n=0}^{\infty} f_n |n\rangle\langle n|. \tag{61}$$

H_1^{eff} can easily be diagonalized by applying the transformation (26) that diagonalizes σ_x:

$$H_2 := T^\dagger H_1 T = H_2^{(0)} + V_2, \tag{62}$$

with

$$H_2^{(0)} = T^\dagger H_1^{\text{eff}} T = \left(\omega(N + 1/2) - \frac{g^2}{\omega}\right)\otimes 1_2 - \frac{\omega_0}{2}F \otimes \sigma_z, \tag{63}$$

and

$$V_2 = T^\dagger(V_1 - \Pi_{H_1^{(0)}} V_1)T = -\omega_0/4\begin{pmatrix} G + G^\dagger - 2F & G - G^\dagger \\ -G + G^\dagger & -G - G^\dagger + 2F\end{pmatrix}. \tag{64}$$

The eigenvalues of $H_2^{(0)}$ are therefore

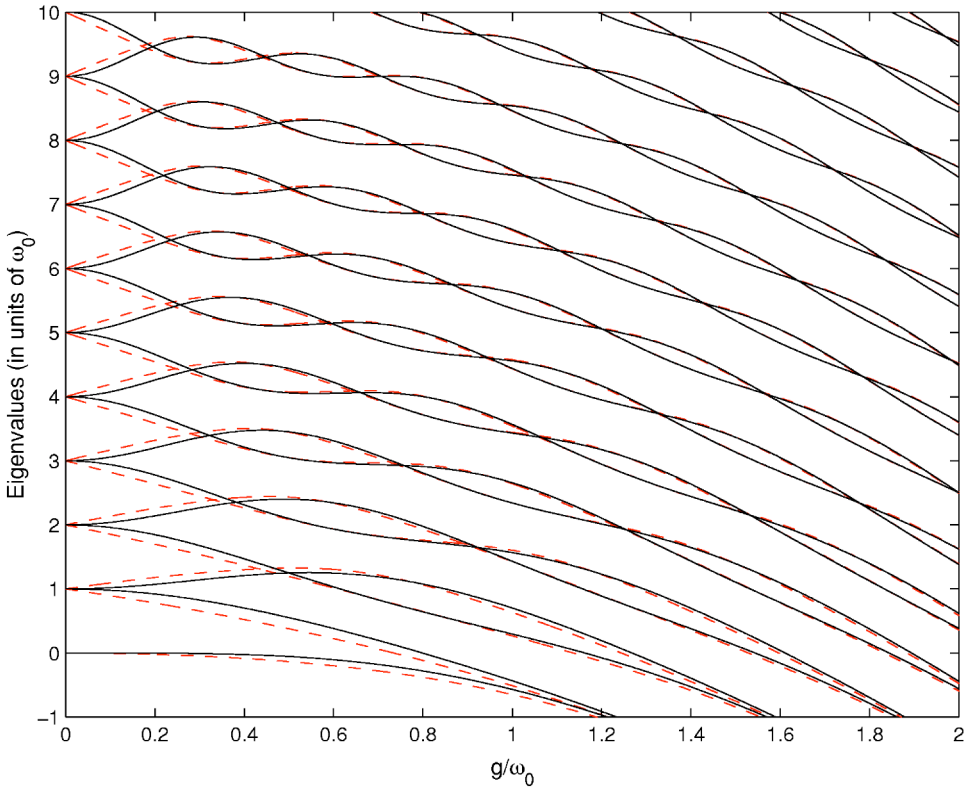

FIG. 3. Comparison of exact numerical eigenvalues (dashed lines) of (8) as a function of the coupling constant in the resonant case ($\omega=\omega_0$), with the approximate eigenvalues (solid lines) obtained from (65).

$$E^{(0)}_{2,(n,\pm)} = \omega(n+1/2) - \frac{g^2}{\omega} \mp \frac{\omega_0}{2} e^{-2g^2/\omega^2} L_n\left(\frac{4g^2}{\omega^2}\right), \tag{65}$$

which is the same result obtained in Refs. 17, 19, and 20 by other methods. Figure 3 compares the exact numerical spectrum of (8) with the approximation (65) for the resonant case $\omega=\omega_0$. One can see that for large enough g, the formula (65) reproduces the spectrum well. It is not very accurate for small values of g because of the presence of the one-photon zero-field resonances that we analyze as follows. In the limit $g\to 0$, we have

$$H_2^{(0),g\to 0} \rightsquigarrow \omega(N+1/2)\otimes \mathbb{1}_2 - \frac{\omega}{2}\mathbb{1}\otimes\sigma_z,$$

$$V_2^{g\to 0} \rightsquigarrow g\begin{pmatrix} 0 & a-a^\dagger \\ -(a-a^\dagger) & 0 \end{pmatrix}. \tag{66}$$

Thus degeneracies of $H_2^{(0),g\to 0}$ occur as

$$E^{(0),g\to 0}_{2,(n,+)} = E^{(0),g\to 0}_{2,(n-1,-)}. \tag{67}$$

They are made active by the resonant terms of $V_2^{g\to 0}$:

$$V_{2,res}^{g\to 0} = \Pi_{H_2^{(0)}}^{g\to 0} V_2^{g\to 0} = -g\begin{pmatrix} 0 & a^\dagger \\ a & 0 \end{pmatrix}. \tag{68}$$

The transformation (the reduction step of the RT) which transforms this resonant term to a regular function of N is

$$R_1 := \begin{pmatrix} \mathbb{1} & 0 \\ 0 & (aa^\dagger)^{-1/2}a \end{pmatrix} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \sum_{n=0}^{\infty} |n\rangle\langle n+1| \end{pmatrix}, \tag{69}$$

with the properties

$$R_1 R_1^\dagger = \mathbb{1}_{\mathcal{K}}, \quad R_1^\dagger R_1 = \mathbb{1}_{\mathcal{K}} - \begin{pmatrix} 0 & 0 \\ 0 & |0\rangle\langle 0| \end{pmatrix}. \tag{70}$$

We remark that the definition of R_1 depends on the type of resonant terms. The reduction step of the RT presented here is different from (19). The Hamiltonian transformed under this RT has an extra zero eigenvalue corresponding to spurious eigenvector $|0, -\rangle$, while for the Hamiltonian transformed under (19), the extra zero eigenvalue corresponds to $|0, +\rangle$. Applying R_1 on H_2 gives

$$\begin{aligned} H_3 := R_1^\dagger H_2 R_1 &= \left(\omega N - \frac{g^2}{\omega}\right) \otimes \mathbb{1}_2 + R_1^\dagger V_2 R_1 \\ &+ \begin{pmatrix} \frac{\omega}{2}\left(1 - \sum_{n=0}^{\infty} f_n |n\rangle\langle n|\right) & 0 \\ 0 & -\frac{\omega}{2}\left(1 - \sum_{n=1}^{\infty} f_{n-1}|n\rangle\langle n|\right) - \left(\frac{\omega}{2} + \frac{g^2}{\omega}\right)|0\rangle\langle 0| \end{pmatrix}. \end{aligned} \tag{71}$$

Next, we take $H_3^{(0)} = \omega N \otimes \mathbb{1}_2$ and the rest of H_3 as V_3. Since $H_3^{(0)}$ has a twofold degeneracy as $E_{3,(n,+)}^{(0)} = E_{3,(n,-)}^{(0)}$, the average of V_3 relative to $H_3^{(0)}$ is thus

$$\Pi_{H_3^{(0)}} V_3 = \begin{pmatrix} \frac{\omega}{2} - \frac{g^2}{\omega} - \frac{\omega}{2}\sum_{n=0}^{\infty} f_n |n\rangle\langle n| & \sum_{n=1}^{\infty} -\frac{g}{\sqrt{n}} e^{-2g^2/\omega^2} L_{n-1}^{(1)}\left(\frac{4g^2}{\omega^2}\right)|n\rangle\langle n| \\ \sum_{n=1}^{\infty} -\frac{g}{\sqrt{n}} e^{-2g^2/\omega^2} L_{n-1}^{(1)}\left(\frac{4g^2}{\omega^2}\right)|n\rangle\langle n| & -\left(\frac{\omega}{2} + \frac{g^2}{\omega}\right)(1 - |0\rangle\langle 0|) + \frac{\omega}{2}\sum_{n=1}^{\infty} f_{n-1}|n\rangle\langle n| \end{pmatrix}, \tag{72}$$

where we have used the relation[16]

$$\langle m|e^{\pm(2g/\omega)(a^\dagger - a)}|n\rangle = \sqrt{\frac{n!}{m!}}\left(\frac{\pm 2g}{\omega}\right)^{m-n} e^{-(2g^2/\omega^2)} L_n^{(m-n)}\left(\frac{4g^2}{\omega^2}\right), \tag{73}$$

with $L_n^{(m-n)}(x)$ the associated Laguerre polynomials and $m \geqslant n$. The new effective Hamiltonian can thus be written as

$$H_3^{\text{eff}} = \omega N \otimes \mathbb{1}_2 + \Pi_{H_3^{(0)}} V_3. \tag{74}$$

Since all the entries of H_3^{eff} commute with N, it can be diagonalized in the atomic Hilbert space as if its entries were scalars. The eigenvalues of H_3^{eff} are thus

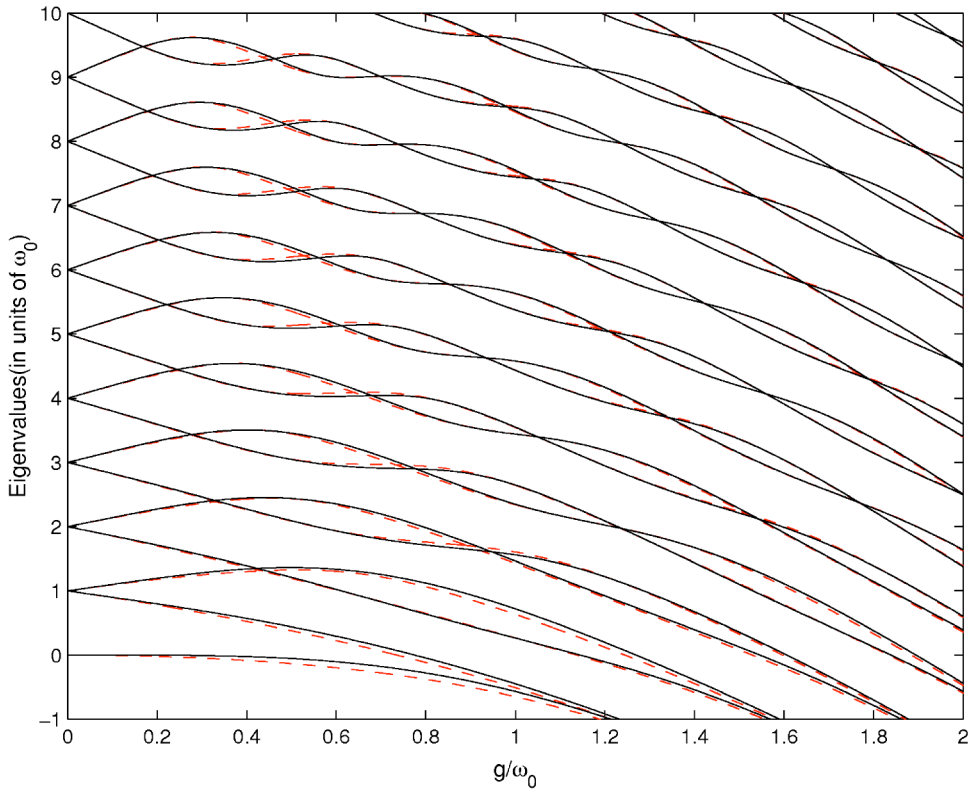

FIG. 4. Comparison of exact numerical spectrum of (8) (dashed lines) as a function of the coupling constant in the resonant case ($\omega=\omega_0$), with the quite accurate result (75) which has treated the zero-field resonances by a RT (solid lines).

$$E^{\mathrm{eff}}_{3,(0,-)}=0,\quad E^{\mathrm{eff}}_{3,(0,+)}=\frac{\omega}{2}-\frac{g^2}{\omega}-\frac{\omega}{2}e^{-2g^2/\omega^2},$$

$$E^{\mathrm{eff}}_{3,(n\geqslant 1,\pm)}=n\omega-\frac{g^2}{\omega}-\frac{\omega}{4}e^{-2g^2/\omega^2}\left(L_n\left(\frac{4g^2}{\omega^2}\right)-L_{n-1}\left(\frac{4g^2}{\omega^2}\right)\right)$$
$$\pm\frac{1}{2}\left[\left(\omega-\frac{\omega}{2}e^{-2g^2/\omega^2}\left(L_n\left(\frac{4g^2}{\omega^2}\right)+L_{n-1}\left(\frac{4g^2}{\omega^2}\right)\right)\right)^2+\frac{4g^2}{n}e^{-4g^2/\omega^2}\left(L^{(1)}_{n-1}\left(\frac{4g^2}{\omega^2}\right)\right)^2\right]^{1/2}. \tag{75}$$

The zero eigenvalue is the extra spurious one that has been added by the RT to the spectrum. Figure 4 compares the exact numerical spectrum of (8) and the approximation (75) which has treated the zero-field resonances by a RT. The figure shows that treating all the active resonances of the system allows us to obtain all the qualitative features of the spectrum in the whole range of the coupling constant and for all energies. At a second stage, since we have treated all the active resonances, we can improve further this spectrum quantitatively by a KAM-type perturbative iteration.

VI. CONCLUSIONS

We have presented a nonperturbative method based on the quantum averaging technique to determine the spectral properties of systems containing resonances. It consists in the construction of unitary or isometric transformations that leads to an effective reduced Hamiltonian. These transformations are composed of two qualitatively distinct stages. The first one consists of non-

perturbative transformations (RTs) that are adapted to the structure of the resonances. Their role is to construct a first effective Hamiltonian that contains the main qualitative features of the spectrum—crossings and avoided crossings—in a given range of the coupling parameter. The diagonalized form of this effective Hamiltonian, which depends parametrically on the coupling constant, is then taken as a new reference Hamiltonian around which one can apply perturbative techniques to improve the quantitative accuracy of the spectrum. We formulate the perturbative approach in terms of a KAM-type iteration of contact transformations. Similar results can be obtained with other formulations of perturbation theory.

We have illustrated the method with a model of a two-level atom interacting with a single mode of a quantized field. The method can be applied to more general systems with several field modes. It can also be adapted to the treatment of semiclassical models in which the field is described as a time-dependent function.

We have analyzed the resonances in two regimes of weak and strong coupling. The results we obtained in the weak-coupling regime can be expected to be applicable to quite general models. The analysis of the strong-coupling regime of this model leads to results that are valid for all values of the coupling and for all energies. The possibility to obtain such a global result is due to a particular property of the model, and one cannot expect to obtain it for general models. The particular property is that the part we selected as the reference Hamiltonian H_0 in the strong-coupling regime contains all the unbounded operators of the complete model and is explicitly solvable. The term that was left to be treated by RT and perturbation theory is a bounded operator.

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An abstract interface to higher spin gauge field theory

A. K. H. Bengtsson[a)]
School of Engineering, University College of Borås, Allégatan 1, S-50190 Borås, Sweden

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A comprehensive approach to the theory of higher spin gauge fields is proposed. By explicitly separating out details of implementation from general principles, it becomes possible to focus on the bare minimum of requirements that such a theory must satisfy. The abstraction is based on a survey of the progress that has been achieved since relativistic wave equations for higher spin fields were first considered in the 1930s. As a byproduct, a formalism is obtained that is abstract enough to describe a wide class of classical field theories. The formalism, viewed as syntax, can then be semantically mapped to a category of strongly homotopy Lie algebras, thus showing that the theory in some sense exists, at least as an abstract mathematical structure. Still, a concrete physicslike, implementation remains to be constructed. Lacking deep physical insight into the problem, an implementation in terms of generalized vertex operators is set up within which a brute force iterative determination of the first few orders in the interaction can be attempted. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1867976]

I. INTRODUCTION

On a very high level of abstraction, the theory of self-interacting higher spin gauge fields becomes either trivial or void. This might seem like a preposterous statement about a problem, the solution of which has eluded theoretical physics since the 1970s, when the problem was first explicitly raised.[1] In this paper, we will try to explain the intuition behind this claim.

Theoretical physics in general, and high energy physics in particular, rest on a tremendous body of knowledge about reality. The nature of this knowledge is manifold, one aspect is the general principles like the relativity principle, the equivalence principle, various gauge principles and the quantum paradigm. Another aspect is the many elaborate calculational schemes employed in particular models, realistic or of the toy variant. This is the nuts and bolts of the science. Whereas the principles are lofty and beautiful to contemplate, the nuts and bolts are often ugly and boring to struggle with. Of course, this is a matter of taste and outlook. But in the end, the nuts and bolts must be there in the right place in order to make contact with experiment, and ensure eventual mathematical consistency.

In computer science, we also find this division between a high level abstract approach to problems, and a low level nuts and bolts code grinding. But in computer science the division is more explicitly pronounced. The complexity of modern software development has forced an approach where one must get the principles right first.

One purpose of the present paper is to adopt this mode of working with respect to the problem of introducing self-interactions for higher spin massless gauge fields. Substantial progress notwithstanding, the problem is still not completely solved, and far less understood. It is not even clear how to recognize or evaluate a purported solution. Massless higher spin fields appear in many contexts related to string theory, membrane theory and M-theory and theories deriving from these.

a)Electronic mail: anders.bengtsson@hb.se

This makes it interesting to find out if higher spin gauge fields can stand on their own, without crutches, so to speak, from circumstantial theoretical constructs. Furthermore, a problem so simple to formulate, but so difficult to solve, is intriguing in itself.

We will approach the problem by formulating an as general as possible *interface* to higher spin gauge field theory. In the process, specifications that the theory must meet, will be cataloged. The interface will then turn out to be quite trivial. Then comes the question of implementing the interface. This is where the nuts and bolts enters. Perhaps there is no implementation, in which case the theory is void.

Now, what do we gain by adopting this strategy? First, we get a framework where we can discuss the general aspects of the theory without worrying at the same time whether they can be implemented or not. We do not have to fix space–time dimension or signature, or worry about background geometry and coupling to gravity. Indeed, we do not have to worry about space–time at all. Second, it might be possible to separate the issue of existence from the issue of construction. Third, if the theory exists, there might be several, in some sense different implementations, thus avoiding the so common pattern of thinking in terms of uniqueness. Fourth, it might be possible to implement the theory computationally in some set of abstract data types. (In that case, considerations of finite definition enters, but that can presumably be taken care of relying on lazy evaluation, thus effectively allowing enumerably infinite data structures.) And last, and perhaps not completely independent of the previous points, we can separate physics from mathematics. The problem is so difficult that we cannot *a priori* know if all our cherished physical principles can be retained. Better then to keep an open mind and treat the problem purely mathematically.

There is one further point to be made. When solving hard problems in theoretical physics, it is natural to search through mathematics in the hope of finding a pre-existing structure that can be used. However, one could imagine a physics problem for which there is no mathematical structure available as yet. That this situation could be encountered in fundamental physics is not at all unthinkable. It seems to me that computer science has tools to tackle this situation, or at least to formulate it. Thus, again borrowing from computer science, the approach to higher spin theory proposed here can also be viewed as an attempt to provide a *syntax* for the problem. Then implementation corresponds to providing the syntactical model with *semantics*. Now syntax and semantics are concepts normally applied to programming languages, or formal languages in general, so we use the concepts in a slightly transferred sense. Continuing this train of thought, of the different semantical schemes, *denotational* semantics, where the syntactical structures are mapped to mathematical objects in a pre-existing (and well understood) semantical domain,[2] seems to be the most appropriate. If a semantical domain cannot be found, then research should perhaps be directed towards inventing new mathematics, rather than trying to solve a theoretical physics problem. If the domain exists, we might be able to target this mathematical structure more precisely. This is one reason for adopting computer science inspired thinking rather than working directly within a mathematical structure from the outset.

If it seems strange to use computer science concepts in high energy physics, one should consider the fact that the subject of theoretical computer science is, in essence, *data* and *processes* in general, and therefore it can be useful in various scientific contexts where one must deal with complex systems.

Parts of the discussion in this paper are quite elementary. That is inherent in the formal, syntactic approach. We want to focus on the abstract and general issues involved, not taking, at least not consciously so, to much pre-existing mathematics on board. But as the present work is mainly conceptual and in a creative phase, the formalization will not be pushed to far. A pure syntactic approach would almost certainly obscure the main idea. In order to communicate, we will compromise by using a somewhat unprincipled mix of syntax, semantics, and mathematics. If the approach is fruitful, an exact formulation can be set up later.

Perhaps a simple example helps to further explicate this point of view. Consider the real numbers. The axioms for this structure are well known and used almost subconsciously in everyday calculating. When working in calculus or real analysis, for example solving differential equations, these axioms and the theorems are used throughout. We never worry about their relevance

or their truth. But of course, if there was no implementation of the axioms, the exercise would be void, i.e., just formal manipulations. Now we know that there are different implementations of the real numbers in terms of, for example, Dedekind cuts or limits of Cauchy sequences. These implementations are in their turn based on implementations of the rational numbers in terms of the natural numbers. The story is well known. But one more point can be made. If numerical calculations must be done, then a detailed implementation of the real numbers in terms of floating point numbers is necessary.

Now, we never start with a completely blank mind. We have some knowledge about the problem at hand and we often have more or less strong intuitions. There might also be folklore on the subject, but in my opinion, folklore is often too prejudiced to be useful in a creative way.

The first step will be to abstract from what we already know. The scope of the present paper is to set up a general enough framework within which the problem of self-interactions can be analyzed, while allowing for various forms for the free theory and allowing for different implementational ideas as regards interactions.

Two other sources of ideas for the present paper should be mentioned. One is string field theory,[3,4] in particular the nonpolynomial closed string field theory,[5,6] and the other is the mathematical theory of higher homotopy Lie algebras (see Ref. 7 for further references). Classical string field theory can be seen as an implementation of the framework presented here, although we have actually worked the other way, abstracting what is nonparticular to strings. The various algebraic structures, on the other hand, can be considered as (themselves quite abstract, but understood) semantical domains for the syntax presented here. In fact, there is an enormous amount of mathematics that might be relevant. We do not understand higher spin gauge fields well enough to target the appropriate mathematics with precision yet, although it seems possible to semantically map to higher homotopy Lie algebras. Still we need a concrete, physics like, implementation. Thus, we envisage a four-tier structure: syntactic formulation of the theory $\rightarrow$semantical map into a known mathematical structure$\rightarrow$concrete physicslike implementation $\rightarrow$computational implementation.

II. NOTES ON THE FREE FIELD THEORY

The free field theory of higher spin gauge fields is a simple generalization of the lower spin gauge theories for spin 1 and spin 2. There are many variations, developed and proposed during the last five decades.[8–14] Indeed, the literature on higher spin fields is enormous, and we will not attempt to review it. However, it seems to be that certain approaches stand out as particularly simple and, perhaps for that reason, suited as a basis for interactions. One is the original formulation[15–18] in terms of field equations and Lagrangians for symmetric tensor fields, perfected by Fronsdal.[9] Another is the formulation of Freedman and deWit[12] in terms of generalized Christoffel symbols (see also Ref. 19). A third is the BRST approach developed by Siegel and Zwiebach,[20] Ouvry and Stern,[21] and independently by the author.[22] This approach was inspired by and adapted from the, at that time, very active work on string field theory. The reader is referred to the review[4] for a list of references. The BRST approach has been rediscovered[23–26] several times during the years since it was first written down in 1986. Then there is the light-front formulation,[27–29] which, in a way, is the simplest formulation of all, if not for the intricate mixing of gauge symmetry with Poincaré symmetry which makes higher order interactions untractable. Then we have the approach of Vasiliev[13] which has lead to a dramatic progress on interactions in an AdS background geometry. See Refs. 30 and 31 for recent reviews and further references, as well as a view on the higher spin problem that is complementary to the one given in the present paper. For completeness, the twistor approach should be noted.[8,32]

A detailed discussion of the BRST formulation of the free field theory, suitable for our present purposes, can be found in Ref. 33. Here, the notation that will be needed when discussing the BRST implementation will be reviewed.

Consider a phase space spanned by bosonic variables (x_μ, p_μ) and $(\alpha_\mu, \alpha_\mu^\dagger)$ and ghost variables (c^+, b_+), (c^-, b_-), and (c^0, b_0) with commutation relations

$$[x_\mu, p_\nu] = i\eta_{\mu\nu}, \quad [\alpha_\mu, \alpha_\nu^\dagger] = \eta_{\mu\nu}, \tag{1}$$

$$\{c^+, b_+\} = \{c^-, b_-\} = \{c^0, b_0\} = 1. \tag{2}$$

The ghosts have the following properties under Hermitian conjugation

$$(c^-)^\dagger = c^+, \quad (b_-)^\dagger = b_+, \quad (c^0)^\dagger = c^0, \quad (b_0)^\dagger = b_0. \tag{3}$$

The vacuum is degenerate

$$\alpha_\mu|+\rangle = \alpha_\mu|-\rangle = 0, \tag{4}$$

$$\langle +|-\rangle = \langle -|+\rangle = 1, \tag{5}$$

$$\langle +|+\rangle = \langle -|-\rangle = 0, \tag{6}$$

with properties

$$b_0|+\rangle = 0, \quad b_0|-\rangle = |+\rangle, \tag{7}$$

$$c^0|-\rangle = 0, \quad c^0|+\rangle = |-\rangle, \tag{8}$$

$$c^-|+\rangle = c^-|-\rangle = 0, \tag{9}$$

$$b_+|+\rangle = b_+|-\rangle = 0. \tag{10}$$

The ghost variables are Grassmann odd, while the bosonic are Grassmann even. The equations $b_0|-\rangle = |+\rangle$ and $c^0|+\rangle = |-\rangle$ relating the vacua, then implies that either one of the two vacua must be odd. Here, we will choose $|-\rangle$ Grassmann even and $|+\rangle$ Grassmann odd. A peculiar consequence is that $\langle +|-\rangle$ becomes odd.

Ghost numbers, gh, are assigned according to

$$\begin{gathered} x_\mu, p_\mu, \alpha_\mu, \alpha_\mu^\dagger \quad 0 \\ c^0, c^+, c^- \quad 1 \\ b_0, b_+, b_- \quad -1 \\ |+\rangle \quad -1/2 \\ |-\rangle \quad 1/2. \end{gathered} \tag{11}$$

The higher spin fields are collected into the ket $|\Phi\rangle$ with expansion

$$|\Phi\rangle = \Phi(p)|+\rangle + F(p)c^+b_-|+\rangle + H(p)b_-|-\rangle, \tag{12}$$

where $\Phi(p)$ contains the symmetric higher spin gauge fields, and $F(p)$ and $H(p)$ are certain auxiliary fields. These fields are further expanded in terms of the oscillators

$$\Phi = \Phi_0 + i\Phi^\mu\alpha_\mu^\dagger + \Phi^{\mu\nu}\alpha_\mu^\dagger\alpha_\nu^\dagger + \cdots, \tag{13}$$

$$F = F_0 + iF^\mu\alpha_\mu^\dagger + F^{\mu\nu}\alpha_\mu^\dagger\alpha_\nu^\dagger + \cdots, \tag{14}$$

$$H = H_0 + iH^{\mu}\alpha_{\mu}^{\dagger} + H^{\mu\nu}\alpha_{\mu}^{\dagger}\alpha_{\nu}^{\dagger} + \cdots . \tag{15}$$

The gauge parameters are expanded as

$$|\Xi\rangle = (\xi_0 - i\xi^{\mu}\alpha_{\mu}^{\dagger} + \xi^{\mu\nu}\alpha_{\mu}^{\dagger}\alpha_{\nu}^{\dagger} + \cdots)b_{-}|+\rangle. \tag{16}$$

Note that the field $|\Phi\rangle$ is odd while the $|\Xi\rangle$ is even. The Grassmann properties are carried by the vacua. When abstracting the free theory, the vacua will be dropped, and the Grassmann properties of Φ and Ξ will be interchanged. They can be defined either way in the abstract theory.

The BRST operator Q is expressed in terms of the generators

$$G_0 = \tfrac{1}{2}p^2, \quad G_{-} = \alpha \cdot p, \quad G_{+} = \alpha^{\dagger} \cdot p, \tag{17}$$

spanning the simple algebra

$$[G_{-}, G_{+}] = 2G_0, \tag{18}$$

with all other commutators zero.

In terms of these generators, the BRST operator reads (signs are chosen so that the component field actions works out as in Ref. 34)

$$Q = c^0 G_0 - c^{+}G_{+} - c^{-}G_{-} - 2c^{+}c^{-}b_0. \tag{19}$$

The action

$$A = \langle\Phi|Q|\Phi\rangle, \tag{20}$$

is invariant under the gauge transformations,

$$\delta_{\Xi}|\Phi\rangle = Q|\Xi\rangle, \tag{21}$$

as is the field equation

$$Q|\Phi\rangle = 0. \tag{22}$$

There is one, somewhat puzzling aspect, of this theory. When expanding the equations (20)–(22), everything works out nicely for the component fields, except the fact that the theory contains auxiliary fields which cannot be solved for without introducing a further constraint. This constraint is applied to both the field and the gauge parameter

$$T|\Phi\rangle = 0, \quad T|\Xi\rangle = 0, \tag{23}$$

where T is the operator

$$T = \frac{1}{2}\alpha \cdot \alpha + b_{+}c^{-}. \tag{24}$$

When expanded, the constraint equation yields the double tracelessness constraint for component fields of spin $s \geqslant 4$ and the tracelessness constraint for the corresponding component gauge parameters. The free field theory is still gauge invariant without imposing these constraints, but the constraints are needed in order to get the correct number of physical degrees of freedom. These questions are discussed in Ref. 33.

So the bottom line of the BRST treatment of the free field theory is that the action can be written as $\langle\Phi|Q|\Phi\rangle$ with Q a nilpotent kinetic operator and $|\Phi\rangle$ a certain expansion over internal and ghost degrees of freedom. Below, when discussing an abstract approach to the theory, we will not use this notation, instead inventing a new syntax. The reason is to keep bra and ket vectors, oscillators, and commutator brackets, etc., where they belong, namely in the implementation.

It is neither particularly difficult, nor very interesting at the present stage of investigation to write down more complicated free field theories than the one reviewed here. For our present purpose, it suffices to consider this particular free theory, which is presumable the simplest one, as an example to abstract.

A note on units: Working in mass units, i.e., with dimensionality $\mathrm{d}(p)=1$, all configuration space fields have $\mathrm{d}(\Phi(x))=(D-2)/2$ where D is the space–time dimension, while momentum space fields have $\mathrm{d}(\Phi(p))=-(D+2)/2$. All in all we get dimensionalities d according to

$$\begin{array}{ll} p,c^{+},c^{-} & 1 \\ \alpha,\alpha^{\dagger},c^{0},b^{0} & 0 \\ |+\rangle,|-\rangle & 0 \\ x,b^{+},b^{-} & -1. \end{array} \tag{25}$$

Consequently, $\mathrm{d}(|\Phi\rangle)=-(D+2)/2$ and $\mathrm{d}(Q)=2$.

III. NOTES ON SELF-INTERACTIONS

There is a large amount of work on interactions for higher spin gauge fields. We will certainly not try to review the full body of knowledge on the matter. Instead, we will outline a few salient features that we think are significant with respect to the self-interaction problem. We will do this based on a brief overview of the subject, well aware of the prejudices this might entail. (In particular, we will leave out all references to work on coupling point particles to background higher spin gauge fields, not because the topic is uninteresting, but because it lies somewhat outside the main thrust of the present paper. The same comment goes for all occurrences of massless higher spin fields in string theory and its descendants).

As far as we know, the question of introducing self-interactions (electromagnetic and gravitational interactions will be briefly discussed at the end of this section) for higher spin massless fields was first published in Ref. 1, reviewing the so named Gupta program. This program belongs to the attempts to quantize gravity in terms of an interacting spin 2 field.[35,36] It can be approached via two paths, either by linearizing Einstein gravity, or by starting with a free spin 2 field and attempting to introduce self-consistent interactions in an iterative way. This latter approach soon acquired immediacy of its own, more or less independent of the quantization problem. Indeed, the question of self-coupling a free spin 2 field into a nonlinear theory can be studied as a problem in classical field theory. Some of the often cited early works on this subject are Refs. 37–40.

That general relativity can be derived from requiring a consistent self-interacting theory of spin 2 fields, was shown by Deser in Ref. 41 (see also Ref. 42). In that paper, it is shown that the Einstein and Yang–Mills theories can both be derived from the requirement of self-interaction in just one iterative step. The resulting theories are cubic in the first order form, i.e., where pairs of independent fields $(g^{\mu\nu},\ \Gamma^{\alpha}_{\mu\nu})$ and $(A_{\mu},\ F_{\mu\nu})$ are used, respectively. In this approach, the further nonlinearities of the theories are hidden in the choice of first order field variables, since upon relating to the standard formulation, the field $\Gamma^{\alpha}_{\mu\nu}$ must be solved in terms $g^{\mu\nu}$, and $F_{\mu\nu}$ in terms of A_{μ} in the well known way. This derivation uses only the Abelian local gauge invariance of the free theory, and the full non-Abelian local gauge invariance is a result rather than an input.

But in the course of this work on Yang–Mills theory and gravity, it became apparent that gauge invariance is a crucial concept. By iteratively adding nonlinear terms to the free spin 2 action and Abelian gauge transformations, it could be proved[1] that a consistent, gauge invariant theory of self-interacting spin 2 fields can be constructed that is equivalent to Einstein gravity. This derivation relied on starting from Minkowski space–time, and a free spin 2 field $h_{\mu\nu}$ propagating in this flat background. That the condition of a Minkowski background can be lifted was shown in Ref. 43.

It was only natural then to try and extend the program to spin 3 fields and higher. The general idea behind this approach is to take a free field theory and its Abelian gauge symmetry and then *deform* it into a nonlinear theory. The problem was from the outset[1] put in a deformation theoretic context.[44] Most authors express the hope that the so constructed nonlinear theory, if it exists, will turn out to be unique. A first requirement for this method to succeed is that a general enough ansatz for the nonlinear theory can be written down. This is a nontrivial problem in general. As soon as we go beyond spin 2, the problem explodes in a potential complexity of fields, multiplets, background manifolds, dimensions, symmetry groups, etc., and any ansatz runs the risk of being to restrictive.

Returning to the historical path, at roughly the same time, another approach to gravity appeared, more closely modeled on Yang–Mills theory. The Yang–Mills interaction of spin 1 fields was introduced by gauging of a global symmetry algebra like SU (N) in the well-known way.[45] A natural question was whether gravity could likewise be obtained by gauging an appropriate global space–time symmetry. The candidate global space–time symmetries are the Lorentz or Poincaré symmetries. It turns out that gravity can indeed be obtained by gauging the Poincaré group using techniques of vierbeins and spin connections.[46–50] The gauging approach is different from the deformation approach in that the gauge algebra is fixed, but it is promoted from being global to becoming local. In deformation theory, the algebra is already local, but it is promoted from being Abelian to becoming non-Abelian. The question then is whether the two approaches yield the same result. In the case of spin 1 the answer is definitely positive.[51,52] In the case of spin 2, there are conceptual problems involved, at least if one is strongly prejudiced towards a geometrical view, but barring this, the results agree.

The subsequent work on the higher spin problem followed these two paths, either deforming the free theory Abelian gauge group, or gauging a global (but non-Abelian) symmetry algebra. The impressive work of Vasiliev falls in the second category. The far less advanced BRST program falls in the first category, as does the light-front approach and the approach of Berends, Burgers, and van Dam referred to below. Note also that these methods have been extensively used for obtaining various supergravity theories (for reviews, see Refs. 53 and 54).

As regards higher spin gauge field interactions, the first positive result was the light-front construction of cubic interaction terms for arbitrary spin.[27] When going from spin 1 and spin 2 in the light-front approach to higher spin, nothing strange happens. Quite to the contrary, the generalization seems very natural. In four dimensions, where each and every integer spin gauge field has just two physical helicity degrees of freedom, parametrized by a natural number λ, the cubic interaction term can be written

$$g\int \mathrm{d}^4x\sum_{n=0}^{\lambda}(-1)^n\binom{\lambda}{n}(\partial^+)^\lambda\phi\left[\frac{\partial}{\partial^+}\right]^{(\lambda-n)}\bar{\phi}\left[\frac{\partial}{\partial^+}\right]^n\bar{\phi}+\text{complex conjugate}, \tag{26}$$

where the two components of the complex field $(\phi,\bar{\phi})$ correspond to the two helicities λ and $-\lambda$, and where $(\partial,\bar{\partial})$ are complex transverse partial derivatives. The interaction is essentially a binominal expansion. In the case of odd λ, the fields entering the interaction term carry an index contracted into an antisymmetric symbol f_{abc} reminiscent of the situation for spin 1. How this generalizes to higher orders in the interaction is not known, since the quartic interaction term has resisted attempts at construction.

From the cubic interaction term, we can read the following information:

(i) There are λ transverse derivatives.
(ii) The coupling constant g has mass dimension $1-\lambda$.
(iii) The odd spin fields carry an antisymmetrized index.

The covariant spin 3 vertex constructed in Ref. 55 is consistent with these general properties. Furthermore, fixing the light-front gauge in the covariant cubic interaction for spin 3 yields precisely the light-front cubic interaction term for spin 3.[56]

In a way, the light-front result is a bit odd. If it turns out, as claimed by Vasiliev, that higher spin interactions require an anti-deSitter background, then why does the nonlinear Minkowski Poincaré algebra allow this term? Is it just a coincidence, and the theory breaks down at the quartic level? We do not know. Note, though, that there are other cubic interaction terms on the light-front, involving fields of different helicities.[29] Whether any of these terms describe higher spin interaction with gravity to lowest order in the spin 2 field, is at least to my knowledge, not known. The same situation occurs in covariant approach of Berends, Burgers, and van Dam.[55]

These latter authors found that upon commuting two spin 3 gauge transformations, the commutator did not close on spin 3, but produced terms that could be interpreted as gauge transformations for fields of spin >3. This is a clear hint that once one goes beyond spin 2, an infinite tower of higher spin fields will be needed (see also Refs. 57 and 58). Berends, Burgers, and van Dam[59,60] furthermore made an extensive analysis of the higher spin problem that is still highly relevant. Their analysis is within the deformation approach and is based on the original formulation of the free field theory mentioned in Sec. II.

Higher spin fields in electromagnetic and gravitational backgrounds: Self-interactions was not the first type of interaction discussed for higher spin fields. Rather, it was electromagnetic and gravitational interactions. To begin with, massive higher spin fields, i.e., matter, in particular spin $3/2$, was studied. Later the discussion included massless higher spin gauge fields. There is a huge literature on this subject, and here we will just point out a list of original references (hopefully not to incomplete) as well as some recent papers that might be helpful to the reader wishing to pursue this topic.

To make a long story short, minimally coupling higher spin gauge fields to gravity violates the higher spin gauge invariances. In the special case of supergravity, nonminimal terms can be added that saves the theory. But in general, higher spin fields coupled to gravity suffer from a consistency problem that cannot be alleviated by nonminimal couplings. Similar problems arise in attempts to couple higher spin fields to electromagnetism. There thus seems to be no consistent way of introducing higher spin fields into a pre-existing spin 1 and 2 system. The problem was first noted already by Fierz and Pauli,[16] and there exist a long series of papers discussing these problems.[61–72] A modern reference is Ref. 73.

In view of these discouraging results it is reasonable to ask if it is at all useful to pursue investigations into higher spin gauge field interactions. The authors' own point of view is based on the following three observations, being well aware of the fact that this is a weak spot; (i) negative (so-called no-go results) have been circumvented before, (ii) as soon as spin 2 is passed, all spins must be included, and presumably all be treated on a common ground, and it is not clear what happens then, (iii) all negative results derived within a space–time setting, this might be misguided if higher spins play any fundamental role at all.

The reader should note that the present paper does not purport to solve these problems, but rather proposes a way to work around them, by setting up a framework with as few as possible restrictions.

IV. ABSTRACTING DYNAMICS

Physics concerns itself with the dynamics of physical systems. A physical system is a part of the universe with a well-defined interface towards the rest of the universe which becomes the environment. One of the standard paradigms of dynamics is to describe the system in terms of an action. The action in its turn depends on a set of dynamical variables. Often the action possess symmetries, i.e., parameter dependent variations of the variables that leave the action essentially invariant. Equations of motion are obtained by varying the action with respect to the dynamical variables. The scheme is well known to every physicist, and clearly, it can be formalized. Here we will choose a moderate level of formalization, sufficient as a backdrop to the formalization we will need for higher spin gauge fields.

Thus, abstract dynamics can be described as follows.

Let the description of the system be in terms of a set of variables $\{\phi_i\}$ where the index i runs

over an index set $\mathcal{I}$. Dynamics is governed by the action A. The action is a function $A(\{\phi_i\})$ of the set of variables $\{\phi_i\}$. The equations of motion follows from varying the action with respect to the variables. Formally we have

$$\forall j \in \mathcal{I}:(\delta_{\phi_j} A(\{\phi_i\}) = 0 \rightarrow \exists\, W_j : W_j(\{\phi_i\}) = 0). \tag{27}$$

Here, W denotes the equations of motion,

$$\forall j \in \mathcal{I}: W_j(\{\phi_i\}) = 0. \tag{28}$$

Defining the variation δ_{ϕ_j} requires some care, but we will rely on the standard application of this operation.

Invariance of the action under symmetry transformations

$$\delta_\xi \phi = f(\{\phi_n\}, \xi), \tag{29}$$

is the demand that the variation of the action evaluates to zero

$$\delta_\xi A = 0. \tag{30}$$

We also demand that the transformation close and form an algebra, possibly modulo the field equations,

$$[\delta_{\xi_1}, \delta_{\xi_2}]\phi = f(\{\delta_{\xi_1}\phi_n\}, \xi_2) - f(\{\delta_{\xi_2}\phi_n\}, \xi_1) = \delta_{\xi(\{\phi_n\},\xi_1,\xi_2)}\phi (\text{mod } W). \tag{31}$$

The algebra can be field dependent, as signaled by the field dependent gauge parameter $\xi(\{\phi_n\}, \xi_1, \xi_2)$ in the commutator of two gauge transformations.

V. ABSTRACTING THE FREE FIELD THEORY

All higher spin gauge fields, as well as auxiliary fields, are packaged into one master field Φ. Let such a field be called an HS field. The explicit representation is left to the implementation. However, we need a way to extract the component fields. Let us write this formally as

$$\textbf{get}(\Phi, s) \rightarrow \phi_s, \tag{32}$$

where we can think of **get** as either an operator acting on Φ or as a function call in the case that the theory is implemented computationally. **get** applied to the field equation for Φ should yield the component field equations. In practice, in order to make contact with conventional field theory, the component fields will be ordinary symmetric tensors, so that

$$\phi_s(p) = \phi_{\mu_1\mu_2\cdots\mu_s}(p). \tag{33}$$

Here, p denotes a momentum space coordinate and the indices μ are space–time indices. It should be kept in mind, though, that there might be situations where we want to hide the space–time representation, or where we want to extract an entirely different representation. There is also the possibility that there is no space–time representation. (A deep reason for the severe problems in constructing interactions might be that space–time is not the proper arena for higher spins. Assuming that the very concept of spin can be given a reasonable definition independent of a background space–time geometry, such a representation is currently under investigation.)

Furthermore, we need a way to distinguish different fields. Here we will build in one piece of classical field theory. Fields depend on variables, in general space–time coordinates and possibly extra variables. All these will be collected into one indexed symbol σ_i, which as already noted, need not be related to space–time at all. Thus we will write HS fields as $\Phi(\sigma_i)$, sometimes abbreviated to Φ_i for convenience.

Implicit in the above discussion on the HS fields is that they belong to some set $\mathcal{H}$. Eventually $\mathcal{H}$ might be a Hilbert space, but we need not presuppose that as yet. We write $\Phi :: \mathcal{H}$. One can think of this equation as stating the *type* of Φ.

Furthermore, to the extent to which we need to be able to multiply fields by numbers and add them, we may assume that the set $\mathcal{H}$ of HS fields is a vector space. The scalars of the vector space can be complex numbers of even or odd Grassmann parity. The fields might carry a Grassmann parity $\varrho(\Phi) \in \{0,1\}$, so that

$$\Phi_1\Phi_2 = (-)^{\varrho(\Phi_1)\varrho(\Phi_2)}\Phi_2\Phi_1. \tag{34}$$

The product involved here is just a direct product $\otimes$. This equation could also be regarded as a purely textual ordering of symbols. It will be used subsequently when a proper field product is defined.

A minimum requirement in order to write down a free field theory action is that we can write a real bilinear form containing some kind of kinetic operator K. Contemplating this, it becomes clear that we need to enforce the structure of an inner product $\mathbf{in}(\cdot,\cdot)$ on the vector space,

$$\mathbf{in}(\cdot,\cdot) :: \mathcal{H}^2 \to \mathrm{C}. \tag{35}$$

Finally, we need a structure of linear operators acting on the fields. Let K be one such operator

$$K :: \mathcal{H} \to \mathcal{H}, \tag{36}$$

then the free field theory action is written

$$A(\Phi) = \mathbf{in}(\Phi, K\Phi). \tag{37}$$

It is clearly interesting to analyze what is the weakest possible structure that needs to be introduced. The above assumptions are more based on intuition than on a systematic study. As already noted in the introduction, a pure syntactic formulation should presumably be pursued, but it is not useful at the present exploratory stage of investigation.

In this context, it can be discussed how general the equation (37) for the free action is. It is clearly an abstraction of the $\langle\Phi|Q|\Phi\rangle$ action in the BRST approach. However, that the free action should be a bilinear in the abstract field Φ is hard to dispute. Furthermore, the field equations should involve some operators, differential (or momentum) in a space–time description, so it is hard to escape some linear operator K acting on Φ and in some way extracting a concrete kinetic operator acting on the component fields. But the reader must judge for herself/himself.

VI. ABSTRACTING INTERACTIONS

In any field theory, interactions between different fields enter the field equations with nonlinear terms, corresponding to nonquadratic contributions to the action. To accommodate this in our scheme, we need a way to form products between fields. It is immediately clear that ordinary naive school products are insufficient in the general case. That only works in scalar polynomial theories like the ϕ^3-model. All other field theories, electrodynamics, gravity, string field theory, etc., requires more elaborate schemes. For example, the Yang–Mills three field interaction term reads

$$g f_{abc} A^a_\mu(x) A^b(x) \cdot \partial A(x)^{c\mu}. \tag{38}$$

Superficially, the three fields seem to enter the interaction term in an unsymmetric way. But if the term is transformed to momentum space, it can be written as

$$g f_{abc} A^a(p_1) \cdot A^b(p_2)(p_1 - p_2) \cdot A^c(p_3) + \text{cyclic permutations}. \tag{39}$$

The configuration space interaction term is local in space–time, whereas in momentum space, the fields entering the interaction term carry their own momenta. This is the form of interaction that we want to abstract, since then each field carries a unique label encoded in σ_i.

A product of n HS fields is a multilinear map $\mathbf{pr} :: \mathcal{H}^{\otimes n} \to \mathrm{H}$,

$$\Phi(\sigma_{n+1}) = \mathbf{pr}(\Phi(\sigma_1), \Phi(\sigma_2), \ldots, \Phi(\sigma_n)). \tag{40}$$

A priori, this product has no symmetries, an issue to which we will return below. A shorthand notation is useful when the field arguments are not needed

$$\mathbf{pr}(\Phi^n) \equiv \mathbf{pr}(\Phi(\sigma_1),\Phi(\sigma_2),\ldots,\Phi(\sigma_n)) \equiv \mathbf{pr}(\Phi_1,\ldots,\Phi_n). \tag{41}$$

We will also need expressions like $\mathbf{pr}(\Phi^k,\Psi^l)$, which are naturally expanded as need be

$$\mathbf{pr}(\Phi^k,\Psi^l) = \mathbf{pr}(\Phi_1,\ldots,\Phi_k,\Psi_1,\ldots,\Psi_l). \tag{42}$$

Multilinearity entails

$$\begin{aligned}\mathbf{pr}(\Phi_1,\ldots,a_n\Phi_n + b_n\Psi_n,\ldots,\Phi_m) = a_n(-)^{\iota(a_n,n)}\mathbf{pr}(\Phi_1,\ldots,\Phi_n,\ldots,\Phi_m)\\ + b_n(-)^{\iota(b_n,n)}\mathbf{pr}(\Phi_1,\ldots,\Psi_n,\ldots,\Phi_m),\end{aligned} \tag{43}$$

where

$$\iota(a_n,n) = \varrho(a_n)(\varrho(\Phi_1) + \cdots + \varrho(\Phi_{n-1}) \ . \tag{44}$$

Upon reordering adjacent fields in the product, there might be a sign flip in the case where they anticommute,

$$\mathbf{pr}(\Phi_1,\ldots,\Phi_n,\Psi_{n+1},\ldots,\Phi_m) = (-)^{\varrho(\Phi_n)\varrho(\Psi_{n+1})}\mathbf{pr}(\Phi_1,\ldots,\Psi_{n+1},\Phi_n,\ldots,\Phi_m). \tag{45}$$

The HS fields themselves can be chosen as Grassmann even, as seen from the free field theory (where the odd parity derives from the vacuum). But we need this generality, taking grading into account, since the gauge parameters are odd, and there will occur odd operators like Q. This also derives from the BRST free theory. The product itself is assumed to carry no intrinsic Grassmann parity.

Now, flipping the order of adjacent fields in the product, all permutations of the fields can be reached. In the case of Grassmann even fields, the product is therefore independent of the particular order in which the fields are written, and the product is strictly commutative. This might sound confusing, since we certainly do not expect an Abelian theory. However, noncommutativity enters when one considers the nested products that appear when studying gauge invariance and commutators of gauge transformations. Furthermore, associativity is not an issue at this stage. Here we are considering primitive n-ary products, and associativity only enters upon discussing, for example, expressing a product of three factors in terms of successive products of two factors.

It should be clear that in order for this product to serve as a basis for introducing interactions, it must have further properties. This is precisely the subject of our study. The bare minimum of such properties will be derived from the requirement of gauge invariance of the action.

The low indices $n=0$ and $n=1$ merit simplified notation. Thus we define

$$\mathbf{pr}(\Phi^0) \equiv \mathbf{pr}(\ ) = 0, \tag{46}$$

where Φ^0 is defined to be a void argument, and

$$\mathbf{pr}(\Phi) = K\Phi. \tag{47}$$

Since for $n=1$, **pr** is of type $\mathcal{H}\to\mathcal{H}$, it makes sense to define it as linear transformation. If any of the fields is identically zero for all values of the labels σ_i, then the product is zero.

We now have the abstract tools for writing interactions. By taking the product between $n-1$ HS fields and then the inner product with an nth field, a candidate for an n-field interaction term can be written

$$\mathbf{in}(\Phi_n,\mathbf{pr}(\Phi_1,\Phi_2,\ldots,\Phi_{n-1})). \tag{48}$$

It makes sense to introduce a special notation for this expression

$$\mathbf{vx}(\Phi_1,\Phi_2,\ldots,\Phi_n) = \mathbf{in}(\Phi_n,\mathbf{pr}(\Phi_1,\Phi_2,\ldots,\Phi_{n-1})) \tag{49}$$

so that **vx** is a multilinear map $\mathbf{vx} :: \mathcal{H}^{\otimes n} \to C$.

Just as the product (40), **vx** has no *a priori* symmetries. However, if this is to be useful in an interaction term, it must at least be cyclic symmetric in the field [compare to the Yang–Mills three field interaction term above (39)]. This can be fixed by explicitly summing over all permutations of the fields. Alternatively, one could just sum over all cyclic permutations. It turns out, though, that summing over all permutations leads to simpler formulas. Computationally, it is inefficient to sum over all permutations. However, in actual implementations, the permutation symmetries will be explicit, and the combinatorial sums collapse into at most $\mathcal{O}(n^2)$ terms.

To that end, let $\pi[0..n]$ denote the set of all permutations of the list $[0..n]$ of natural numbers between 0 and n. Then $\Sigma_{\pi[n]}$ will denote a sum over permutations.

This finishes setting up of the basic syntax of the theory. In the following sections, we will perform calculations within this syntax. That might seem a bit strange, since we have not defined any rules of calculation or rewrite rules. However, close scrutiny of the manipulations that follow shows that we only need to do substitutions and rearrangements of sums. This is a weak form of equational reasoning that we certainly want to do in any formalism, but strictly speaking, rewrite rules, belong to semantics.

VII. THE ACTION AND GAUGE INVARIANCE

Since we are working within the deformation tradition it makes sense to write an ansatz for the action as a formal power series in the polymorphic map **vx**. The action then reads

$$A(\Phi) = \sum_{i=2}^{\infty} \frac{g^{i-2}}{i!} \sum_{\pi[i]} \mathbf{vx}(\Phi_1, \Phi_2, \ldots, \Phi_i). \tag{50}$$

To clean up notation, introduce a new summation symbol $\Sigma^{\infty}_{\pi(i=m)} \equiv \Sigma^{\infty}_{i=m} \Sigma_{\pi[i]}$.

The action can written, highlighting the kinetic term explicitly and expanding **vx**, in the form

$$\begin{aligned} A(\Phi) &= \mathbf{in}(\Phi, K\Phi) + \sum_{\pi(i=3)}^{\infty} \frac{g^{i-2}}{i!} \mathbf{in}(\Phi_i, \mathbf{pr}(\Phi_1, \Phi_2, \ldots, \Phi_{i-1}) \\ &= \mathbf{in}(\Phi, K\Phi) + \sum_{\pi(i=3)}^{\infty} \frac{g^{i-2}}{i!} \mathbf{in}(\Phi, \mathbf{pr}(\Phi^{i-1})), \end{aligned} \tag{51}$$

where

$$\mathbf{in}(\Phi, K\Phi) = \tfrac{1}{2}(\mathbf{in}(\Phi_1, K_2\Phi_2) + \mathbf{in}(\Phi_2, K_1\Phi_1)). \tag{52}$$

The gauge transformation will also be written as a formal power series. At this stage we have a choice either to introduce a new abstract product $\mathbf{pr}_\mathbf{g}$ (renaming the previously introduced product $\mathbf{pr}_\mathbf{a}$), or use the same product as the one used for the action. This is one of the points where one is confronted with a dilemma as to the generality of the ansatz. We will be conservative here and use the same product. The gauge transformation then reads

$$\delta_\Xi \Phi = \sum_{\pi(i=0)}^{\infty} \frac{g^i}{i!} \mathbf{pr}(\Phi^i, \Xi) = K\Xi + \sum_{\pi(i=1)}^{\infty} \frac{g^i}{i!} \mathbf{pr}(\Phi^i, \Xi). \tag{53}$$

Gauge invariance of the action to all orders of interaction amounts to

$$\delta_\Xi A(\Phi) = 0. \tag{54}$$

By demanding this to be true, we can derive the requisite demands on the maps **in**, **pr**, and **vx**. We must go through this calculation meticulously as we must note all steps where required properties of the maps must be recorded. To that aim, apply δ_Ξ to the action (50),

$$\delta_\Xi A(\Phi) = \sum_{i=2}^{\infty} \frac{g^{i-2}}{i!} \delta_\Xi \sum_{\pi[i]} \mathbf{vx}(\Phi^i). \tag{55}$$

We immediately run into the problem of how to perform this operation. However, by analyzing how the operation of varying the action is normally done in standard field theories, we see that this can be done by just textually substituting $\delta_\Xi\Phi$ for all the occurences of Φ one at a turn so to speak. Indeed

$$\begin{aligned}\delta_\Xi \mathbf{vx}(\Phi_1, \Phi_2, \ldots, \Phi_i) = \mathbf{vx}(\delta_\Xi\Phi_1, \Phi_2, \ldots, \Phi_i) + \mathbf{vx}(\Phi_1, \delta_\Xi\Phi_2, \ldots, \Phi_i) \\ + \cdots + \mathbf{vx}(\Phi_1, \Phi_2, \ldots, \delta_\Xi\Phi_i),\end{aligned} \tag{56}$$

so that we get

$$\delta_\Xi \sum_{\pi[n]} \mathbf{vx}(\Phi^n) = n \sum_{\pi[n]} \mathbf{vx}(\delta_\Xi\Phi, \Phi^{n-1}). \tag{57}$$

Thus continuing the calculation (55), we get

$$\delta_\Xi A(\Phi) = \sum_{\pi(i=2)}^{\infty} \frac{g^{i-2}}{(i-1)!} \mathbf{vx}(\delta_\Xi\Phi, \Phi^{i-1}). \tag{58}$$

Then, upon substituting (53) for $\delta_\Xi\Phi$ and shifting the i-sum, $i \to i-1$,

$$\sum_{\pi(i=1)}^{\infty} \frac{g^{i-1}}{i!} \sum_{\pi(j=0)}^{\infty} \frac{g^j}{j!} \mathbf{vx}(\mathbf{pr}(\Phi^j, \Xi), \Phi^i). \tag{59}$$

Here, we can use the definition (49) of **vx**,

$$\sum_{\pi(i=1)}^{\infty} \sum_{\pi(j=0)}^{\infty} \frac{g^{i+j-1}}{i!j!} \mathbf{in}(\mathbf{pr}(\Phi^j, \Xi), \mathbf{pr}(\Phi^i)). \tag{60}$$

No harm is done by extending the i-sum to start at $i=0$. Assuming that it is allowed to rearrange the double sum, it can be written as

$$\sum_{i=0}^{\infty} \sum_{\substack{\pi(k=0) \\ \pi(l=0)}}^{k+l=i} \frac{g^{i-1}}{k!l!} \mathbf{in}(\mathbf{pr}(\Phi^k, \Xi), \mathbf{pr}(\Phi^l)), \tag{61}$$

i.e., we are summing order by order in the total power of the field, corresponding to how an order by order checking of invariance would be performed. Thus, for any fixed $i=n$, study

$$\sum_{\substack{\pi(k=0) \\ \pi(l=0)}}^{k+l=n} \frac{g^{n-1}}{k!l!} \mathbf{in}(\mathbf{pr}(\Phi^k, \Xi), \mathbf{pr}(\Phi^l)) = \sum_{\substack{\pi(k=0) \\ \pi(l=0)}}^{k+l=n} \frac{g^{n-1}}{k!l!} \mathbf{in}(\mathbf{pr}(\Phi^l), \mathbf{pr}(\Phi^k, \Xi)). \tag{62}$$

Again using the definition (49) of **vx**,

$$\sum_{\substack{\pi(k=0) \\ \pi(l=0)}}^{k+l=n} \frac{g^{n-1}}{k!l!} \mathbf{vx}(\mathbf{pr}(\Phi^l), \Phi^k, \Xi) = \sum_{\substack{\pi(k=0) \\ \pi(l=0)}}^{k+l=n} \frac{g^{n-1}}{k!l!} \mathbf{vx}(\Xi, \Phi^k, \mathbf{pr}(\Phi^l)) = \sum_{\substack{\pi(k=0) \\ \pi(l=0)}}^{k+l=n} \frac{g^{n-1}}{k!l!} \mathbf{in}(\Xi, \mathbf{pr}(\Phi^k, \mathbf{pr}(\Phi^l))). \tag{63}$$

Normally, invariance should not depend on the gauge parameter Ξ, so in order for this sum to vanish, we must require for all $n \in N$,

$$\sum_{\substack{\pi(k=0)\\ \pi(l=0)}}^{k+l=n} \frac{1}{k!l!}\mathbf{pr}(\Phi^k,\mathbf{pr}(\Phi^l)) = 0. \tag{64}$$

This is a nontrivial demand on the map **pr**. The other demands can be considered as part of the syntax, but this one involves the semantics of the theory. We will refer to this requirement as the *product identity*.

Low level special cases of the product identity: The first four levels, i.e., values of n, are of immediate importance.

When $n=0$ the identity trivializes to

$$\mathbf{pr}(\mathbf{pr}(\,)) = \mathbf{pr}(0) = 0. \tag{65}$$

The case $n=1$ becomes

$$\mathbf{pr}(\Phi,\mathbf{pr}(\,)) + \mathbf{pr}(\mathbf{pr}(\Phi)) = KK\Phi = 0. \tag{66}$$

This equation expresses gauge invariance for the free theory.

When $n=2$, taking permutations into account and noting that $\mathbf{pr}(\Phi_1,\Phi_2)$ is actually symmetric, we get

$$\mathbf{pr}(\mathbf{pr}(\Phi_1,\Phi_2)) + \mathbf{pr}(\Phi_1,\mathbf{pr}(\Phi_2)) + \mathbf{pr}(\Phi_2,\mathbf{pr}(\Phi_1)) = 0, \tag{67}$$

or

$$K\mathbf{pr}(\Phi_1,\Phi_2) + \mathbf{pr}(\Phi_1,K\Phi_2) + \mathbf{pr}(K\Phi_1,\Phi_2) = 0. \tag{68}$$

This equation expresses gauge invariance of the cubic interaction term. Granting that we already know how to implement the $n=1$ equation in terms of an appropriate field and a kinetic operator, the $n=2$ equation is the first nontrivial equation to implement. It involves the two-product $\mathbf{pr}(\cdot,\cdot)$ which so far is undefined. This is the product that was partially studied in Ref. 33.

The next level, $n=3$ involves the quartic interaction term

$$\begin{aligned} &K\mathbf{pr}(\Phi_1,\Phi_2,\Phi_3) + \mathbf{pr}(K\Phi_1,\Phi_2,\Phi_3) + \mathbf{pr}(\Phi_1,K\Phi_2,\Phi_3) + \mathbf{pr}(\Phi_1,\Phi_2,K\Phi_3) + \mathbf{pr}(\Phi_1,\mathbf{pr}(\Phi_2,\Phi_3))\\ &\quad + \mathbf{pr}(\Phi_2,\mathbf{pr}(\Phi_3,\Phi_1)) + \mathbf{pr}(\Phi_3,\mathbf{pr}(\Phi_1,\Phi_2)) = 0. \end{aligned} \tag{69}$$

This equation expresses gauge invariance up to the quartic level. In order to solve it, the full two-product $\mathbf{pr}(\cdot,\cdot)$ must have been obtained first. Clearly, it can then be seen as a differential equation for the three-product $\mathbf{pr}(\cdot,\cdot,\cdot)$ with K acting as differential operator.

It follows that a necessary condition for the interaction to be cubic is that the two-product satisfies a Jacobi identity. In the cubic case, the three-product $\mathbf{pr}(\cdot,\cdot,\cdot)$ is zero, and the first four terms in (69) vanishes.

The field equations: Varying the action (50) with respect to the field Φ yields the field equation

$$\delta_\Phi A(\Phi) = \sum_{\pi(i=2)}^{\infty} \frac{g^{i-2}}{(i-1)!}\mathbf{vx}(\delta_\Phi,\Phi^{i-1}) = \mathbf{in}\left(\delta_\Phi, \sum_{\pi(i=1)}^{\infty} \frac{g^{i-1}}{i!}\mathbf{pr}(\Phi^i)\right). \tag{70}$$

According to the abstract dynamics, we get the field equation

$$W(\Phi) = \sum_{\pi(i=1)}^{\infty} \frac{g^{i-1}}{i!}\mathbf{pr}(\Phi^i) = 0, \tag{71}$$

thus expressing the basic intuition that the product captures the interactions.

VIII. THE GAUGE ALGEBRA

In order to examine the gauge algebra, we do the standard calculation,

$$\begin{aligned}
[\delta_{\Xi_1},\delta_{\Xi_2}]\Phi &= \delta_{\Xi_1}\delta_{\Xi_2}\Phi - (1\leftrightarrow 2)\\
&= \delta_{\Xi_1}\left(\sum_{\pi(i=0)}^{\infty}\frac{g^i}{i!}\mathbf{pr}(\Phi^i,\Xi_2)\right) - (1\leftrightarrow 2)\\
&= \sum_{\pi(i=1)}^{\infty}\frac{g^i}{(i-1)!}\mathbf{pr}(\delta_{\Xi_1}\Phi,\Phi^{i-1},\Xi_2) - (1\leftrightarrow 2)\\
&= \sum_{\pi(i=0)}^{\infty}\sum_{\pi(j=0)}^{\infty}\frac{g^{i+j+1}}{i!j!}\mathbf{pr}(\mathbf{pr}(\Phi^j,\Xi_1),\ \Phi^i,\Xi_2)) - (1\leftrightarrow 2)\\
&= \sum_{i=0}^{\infty}\sum_{\substack{\pi(k=0)\\ \pi(l=0)}}^{k+l=i}\frac{g^{k+l+1}}{k!l!}\mathbf{pr}(\Phi^k,\Xi_1,\mathbf{pr}(\Phi^l,\Xi_2)) - (1\leftrightarrow 2).
\end{aligned} \tag{72}$$

This is as far as we can get without invoking semantics for the product. Experience with field theory, shows that the commutator of two gauge transformations should close on a new, possibly field dependent gauge transformation, possibly modulo the field equations.

The form of Eq. (72) suggests considering

$$\mathbf{pr}(\Phi^k,\mathbf{pr}(\Xi_1,\Xi_2,\Phi^l)). \tag{73}$$

If we could establish the following identity,

$$\begin{aligned}
&\sum_{\substack{\pi(k=0)\\ \pi(l=0)}}^{k+l=i}\frac{g^{k+l+1}}{k!l!}\{\mathbf{pr}(\Phi^k,\mathbf{pr}(\Xi_1,\Xi_2,\Phi^l)) + \mathbf{pr}(\Phi^k,\Xi_1,\Xi_2,\mathbf{pr}(\Phi^l)) + \mathbf{pr}(\Phi^k,\Xi_1,\mathbf{pr}(\Xi_2,\Phi^l))\\
&\quad - \mathbf{pr}(\Phi^k,\Xi_2,\mathbf{pr}(\Xi_1,\Phi^l))\} = 0,
\end{aligned} \tag{74}$$

then the calculation (72) could be continued with

$$\begin{aligned}
&-\sum_{n=0}^{\infty}\sum_{\substack{\pi(k=0)\\ \pi(l=0)}}^{k+l=n}\frac{g^{k+l+1}}{k!l!}(\mathbf{pr}(\Phi^k,\mathbf{pr}(\Xi_1,\Xi_2,\Phi^l)) + \mathbf{pr}(\Phi^k,\Xi_1,\Xi_2,\mathbf{pr}(\Phi^l)\ )\\
&= -\sum_{\pi(k=0)}^{\infty}\frac{g^k}{k!}\mathbf{pr}\left(\Phi^k,\sum_{\pi(l=0)}^{\infty}\frac{g^{l+1}}{l!}\mathbf{pr}(\Xi_1,\Xi_2,\Phi^l)\right) - \sum_{\pi(k=0)}^{\infty}\frac{g^k}{k!}\mathbf{pr}\left(\Phi^k,\Xi_1,\Xi_2,\sum_{\pi(l=0)}^{\infty}\frac{g^{l+1}}{l!}\mathbf{pr}(\Phi^l)\right).
\end{aligned} \tag{75}$$

The first term can be recognized as a field dependent gauge transformation and the second as being proportional to the field equations, thus

$$[\delta_{\Xi_1},\delta_{\Xi_2}]\Phi = \delta_{\Xi(\Phi,\Xi_1,\Xi_2)}\Phi - g^2\sum_{\pi(k=0)}^{\infty}\frac{g^k}{k!}\mathbf{pr}(\Phi^k,\Xi_1,\Xi_2,W(\Phi)), \tag{76}$$

where the new gauge parameter is

$$\Xi(\Phi,\Xi_1,\Xi_2) = -\sum_{\pi(l=0)}^{\infty}\frac{g^{l+1}}{l!}\mathbf{pr}(\Xi_1,\Xi_2,\Phi^l). \tag{77}$$

We can now record the required properties of the product. Apart from being able to make substitutions, add and compare equal terms, i.e., use standard equational reasoning, the product identity (64) is the only nontrivial demand on **pr**. The equation (74) that is needed in the gauge algebra calculation, can be subsumed in a generalization of the product identity (64). Let us see how this can be done.

The product identity was derived under the assumption that all the fields were Grassmann even, and that the only odd object was the gauge parameter. Therefore, the Grassmann properties could be ignored. We must generalize (64) to include the case of fields with even and odd parities. To that end, let $\{\Gamma_i\}$ denote a set of n fields with $\varrho(\Gamma_i) \in \{0,1\}$.

The sum in the product identity runs over all permutations just for convenience. The different terms are cyclic permutations of the split of the string of fields $\Phi_1 \cdots \Phi_n$ into two strings with k and l fields, respectively, and the factor $1/k!l!$ is cancelled against the number of equal permutations in each split. Therefore (64) can be written as

$$\sum_{\substack{k=0,l=0 \\ \text{cycl.perm.}}}^{k+l=n} \mathbf{pr}(\Phi^k, \mathbf{pr}(\Phi^l)) = 0. \tag{78}$$

Another way to express this is to consider the index set $\{1,\ldots,n\}$ as split into the two sets $\{i_1,\ldots,i_k\}$ and $\{j_1,\ldots,j_l\}$.

Denote the split $\{\{i_1,\ldots,i_k\},\{j_1,\ldots,j_l\}\}$ by $\chi(k,l)$. The sum then runs over all different such splits

$$\sum_{\substack{k=0,l=0 \\ \chi(k,l)}}^{k+l=n} \mathbf{pr}(\Phi_{i_1} \cdots \Phi_{i_k}, \mathbf{pr}(\Phi_{j_1} \cdots \Phi_{j_l})) = 0. \tag{79}$$

The order of the indices does not matter when all the fields are Grassmann even. When arbitrary parities are involved, we need a convention as to the order. Instead of sets $\{i_1,\ldots,i_k\}$ and $\{j_1,\ldots,j_l\}$ we use ordered lists $[i_1..i_k]$ and $[j_1..j_l]$. This pair of ordered lists is denoted by $\pi(k,l)$. It is a particular permutation of the index set into two lists with $i_1 < \cdots < i_k$ and $j_1 < \cdots < j_l$.

If the fields carry arbitrary Grassmann parity, the weakest generalization is to record a sign picked up when the order of the fields $\Gamma_{i_1} \cdots \Gamma_{i_k} \cdots \Gamma_{j_1} \cdots \Gamma_{j_l}$ are reordered lexicographically into $\Gamma_1 \Gamma_2 \cdots \Gamma_n$. Denote this sign by $\epsilon(\pi(k,l))$.

We must sum over all such splittings, keeping track of the signs

$$\sum_{\substack{k=0,l=0 \\ \pi(k,l)}}^{k+l=n} \epsilon(\pi(k,l)) \mathbf{pr}(\Gamma_{i_1} \cdots \Gamma_{i_k}, \mathbf{pr}(\Gamma_{j_1} \cdots \Gamma_{j_l})) = 0. \tag{80}$$

We can then return to the equation (74) that governs the closure of the gauge algebra. Consider first the last expression of the commutator calculation (72). Expanding the permutations we have

$$\sum_{\substack{k=0,l=0 \\ \text{cycl.perm.}}}^{k+l=n} \mathbf{pr}(\Phi^k, \Xi_1, \mathbf{pr}(\Phi^l, \Xi_2)) - (1 \leftrightarrow 2). \tag{81}$$

Consider applying the identity (80) to the string of fields $\Gamma^n = \Phi^{k'} \Xi_1 \Xi_2 \Phi^{l'}$. Of the terms in the sum, there are terms where both Ξ_1 and Ξ_2 are in the first list, both Ξ_1 and Ξ_2 in the second list, and terms where $\Xi_1(\Xi_2)$ is in the first and $\Xi_2(\Xi_1)$ in the second. Writing this out explicitly yields

$$\sum_{\substack{k=0,l=0\\ \chi(k,l)}}^{k+l=n} \{\mathbf{pr}(\Phi^k,\mathbf{pr}(\Xi_1,\Xi_2,\Phi^l)) + \mathbf{pr}(\Phi^k,\Xi_1,\Xi_2,\mathbf{pr}(\Phi^l)) + \mathbf{pr}(\Phi^k,\Xi_1,\mathbf{pr}(\Xi_2,\Phi^l)) - \mathbf{pr}(\Phi^k,\Xi_2,\mathbf{pr}(\Xi_1,\Phi^l))\} = 0. \tag{82}$$

Thus, the identity (74) we used in the gauge algebra calculation follows from the generalized product identity (80) taking Grassmann parities into account.

Therefore, given a particular type of free gauge fields Φ, gauge parameter Ξ, a kinetic operator K and the inner product **in**, construction of the map **pr** satisfying (80) is the only nontrivial task.

In this way, the vaguely defined problem of introducing interactions for higher spin gauge fields, has been focused on implementing the product map **pr** satisfying the product identity (80). Since very little has been assumed as to the particulars of such an implementation, we are quite free to explore various implementational schemes. These vary from finding pre-existing mathematical domains to setting up concrete data structures within which computerized explorations can be performed. In the last two paragraphs, we will outline examples of these two extreme approaches.

IX. STRONGLY HOMOTOPY LIE ALGEBRAS

The product identities we have found are similar to the defining identities for strongly homotopy Lie algebras (sh-Lie algebras or L_∞ algebras).[74,75] This opens the possibility to map the syntax set up here onto such an algebra. Furthermore, in a recent paper[76] it is shown that if the gauge algebra of the Lagrangian higher spin field theory of Berends, Burgers, and van Dam[59] actually exists, then it has the structure of an sh-Lie algebra. The approach of the present paper is more direct in that the gauge algebra falls into an sh-Lie algebra pattern without further analysis. In both these approaches, the problem is that we do not know which particular algebra to choose. Or phrased differently, we do not know if the deformed gauge algebra of the interacting fields exist, starting from the gauge field theory of the free fields.

There are a few variants of the basic definitions of strongly homotopy Lie algebras in the literature, but the following, mildly technical, is sufficient for our purpose to bring out the similarity to the product identity.

Definition: Consider a $\mathbf{Z_2}$ graded vector space $V=V_0\oplus V_1$ over some number field, and denote the elements by x. The grading is given by ϱ with $\varrho(x)=0$ if $x\in V_0$ and $\varrho(x)=1$ if $x\in V_1$. V is supposed to carry a sequence of n-linear products denoted by brackets. The graded n-linearity is expressed by

$$[x_1,\ldots,x_n,x_{n+1},\ldots,x_m] = (-)^{\varrho(x_n)\varrho(x_{n+1})}[x_1,\ldots,x_{n+1},x_n,\ldots,x_m], \tag{83}$$

$$[x_1,\ldots,a_nx_n+b_nx_n'\ldots,x_m] = a_n(-)^{\iota(a_n,n)}[x_1,\ldots,x_n,\ldots,x_m] + b_n(-)^{\iota(b_n,n)}[x_1,\ldots,x_n',\ldots,x_m], \tag{84}$$

where $\iota(a_n,n)=\varrho(a_n)(\varrho(x_1)+\cdots+\varrho(x_{n-1})$.

The defining identities for the algebra are, for all $n\in N$,

$$\sum_{\substack{k=0\\ l=0}}^{k+l=n} \sum_{\pi(k,l)} \epsilon(\pi(k,l))[[x_{\pi(1)},\ldots,x_{\pi(k)}],x_{\pi(k+1)},\ldots,x_{\pi(k+l)}] = 0, \tag{85}$$

where $\pi(k,l)$ stands for (k,l)-unshuffles. A (k,l)-unshuffle is a permutation π of the indices $1,2,\ldots,k+l$ such that $\pi(1)<\cdots<\pi(k)$ and $\pi(k+1)<\cdots<\pi(k+l)$. $\epsilon(\pi(k,l))$ is the sign picked up during the unshuffle as the points x_i with indices $0\leqslant i\leqslant k$ are taken through the points x_j with indices $k+1\leqslant j\leqslant l$. This is just the normal procedure in superalgebras.

The low index, $n=0$ and $n=1$ brackets are treated separately, thus

$$[\cdot] = 0, \tag{86}$$

$$[x] = \partial x, \tag{87}$$

with ∂ a derivation.

This is a definition. Given that such algebras do exist, it is clear that they provide a possible semantic target for abstract higher spin gauge field theory. It is obvious that the image of a field Φ_n is a point x_n, and that the products $\mathbf{pr}(\cdot)$ map into the brackets $[\cdot]$. A technical detail is that in order for the mapping to be complete, the sh-Lie algebra must be supplied with an inner product.

The details of setting up this mapping would require some care, but it should be essentially straightforward. The problem lies elsewhere, we still do not know which particular algebra to map to. Had we known the correct concrete algebra, then we would have had a solution to the higher spin problem.

A way out of this dilemma is to, as a first step, map the corresponding categories instead. By formalizing the syntax given here, a category of interacting fields, say **IField** is set up. The same is done for strongly homotopy Lie algebras, denoted by **shLie**. The interpretation map $[|\cdot|]$ is then a functor from the interacting fields to the sh-Lie algebras.

$$[|\cdot|] :: \mathbf{IField} \to \mathbf{shLie}.$$

Clearly, there is much work to done here and many technical details to work out. It should be noted that category theory can in fact be used in denotational semantics for programming languages.[77] Given that a programming language is just an example of a formal language, and that abstract field theory also can be formulated as a formal language, it should be clear that this point of view is feasible. Whether it helps in the quest to obtain a concrete physicslike implementation remains to be seen. At least, we are able to put interacting higher spin gauge fields in a context where models can be systematically searched for.

From a physics point of view it is clear that the abstract view given here must be supplemented by physical insight into the problem. That is, what are higher spin gauge fields? What kind of physics do they describe? What is the proper context to set them in? Lacking that understanding, we will in the next section set up a framework for a concrete implementation within which the problem can at least be pursued by brute force computerized calculation.

X. VERTEX IMPLEMENTATION

With the free field theory implemented using the BRST technique briefly reviewed in Sec. II, it is natural to try to implement the interacting field products in terms of vertex operators. This is how string field theory is done. Taking the open string as an example, the three string vertex is a product of a bosonic vertex and a ghost vertex. The bosonic vertex is

$$|V_3\rangle = \exp\left(\frac{1}{2}\sum_{r,s=1}^{3}\sum_{n,m=0}^{\infty}\alpha_{-n}^{\mu,r}N_{nm}^{rs}\alpha_{-m}^{\mu,s}\right)|-\rangle_3,$$

in terms of bosonic string oscillators $\alpha_{-n}^{\mu,r}$ and the Neumann function matrices N_{nm}^{rs}. There has been attempts to use this form of three vertex for higher spin gauge fields, but that fails since such a vertex do not reproduce the spin 1 Yang–Mills cubic interaction term.[78]. It is known from the light-front form of the cubic interaction term[29] that the vertex must at least contain terms of the generic form $\alpha^\dagger\alpha^\dagger\alpha^\dagger p$ (indices suppressed), i.e., with three oscillators and one momentum label. Such a covariant vertex was partially determined in Ref. 33 and it correctly reproduces the Yang–Mills cubic interaction term. Further progress was halted by a lack of an effective way of calculating higher order terms in the three vertex. In this section, higher spin vertices will be discussed from the point of view of the abstract approach presented here.

The intention is to define the field products in terms of vertex operators. An n-vertex operator is an object that takes $n-1$ fields, labeled by $\{\sigma_i\}_1^{n-1}$ and outputs a new field, labeled by σ_n. Each field $\Phi(\sigma_i)$ is represented as a ket vector $|\Phi(\sigma_i)\rangle$ in the oscillator and ghost Fock space corresponding to the label σ_i as in Eqs. (12)–(15). The product is defined in terms of the n-vertex $|V(\sigma_1,\ldots,\sigma_{n-1},\sigma_n)\rangle$ by

$$\mathbf{pr}(\Phi(\sigma_1),\ldots,\Phi(\sigma_{n-1})) \equiv \langle\Phi(\sigma_1)|\cdots\langle\Phi(\sigma_{n-1})||V(\sigma_1,\ldots,\sigma_{n-1},\sigma_n)\rangle. \tag{88}$$

The notation makes it explicit that the product evaluates to a ket field $|\Phi(\sigma_n)\rangle$, or

$$\langle\Phi(\sigma_1)|\cdots\langle\Phi(\sigma_{n-1})||V(\sigma_1,\ldots,\sigma_{n-1},\sigma_n)\rangle \to |\Phi(\sigma_n)\rangle. \tag{89}$$

Note that the fields $|\Phi\rangle$ are now Grassmann odd due to the vacuum $|+\rangle$, whereas the gauge parameters are Grassmann even. As will be seen below, the vertex can be built from Grassmann even objects, so that it has full permutational symmetry in all the n field labels.

Likewise the map **vx** is represented by

$$\mathbf{vx}(\Phi(\sigma_1),\ldots,\Phi(\sigma_n)) \equiv \langle\Phi(\sigma_1)|\cdots\langle\Phi(\sigma_n)||V(\sigma_1,\ldots,\sigma_n)\rangle, \tag{90}$$

which evaluates to a combination of component fields and momentum labels. In the abstract action, **vx** is summed over all permutations of the fields. If we allow ourselves the trick of moving all the $\langle+|_n$ vacua to the left, we get

$$\begin{aligned}\frac{1}{n!}\sum_{\pi[1..n]}\mathbf{vx}(\Phi(\sigma_1),\ldots,\Phi(\sigma_n)) &= \frac{1}{n!}(\otimes_{i=1}^n\langle+|_i)\Big(\sum_{\pi[1..n]}\Phi(\sigma_1)\cdots\Phi(\sigma_n)\Big)|V(\sigma_1,\ldots,\sigma_n)\rangle \\ &= \langle\Phi(\sigma_1)|\cdots\langle\Phi(\sigma_n)||V(\sigma_1,\ldots,\sigma_n)\rangle,\end{aligned} \tag{91}$$

i.e., one term, in that particular order. With ${}_{1\cdots n}\langle+|$ as a shorthand for $\otimes_{i=1}^n\langle+|_i$, this can also be written keeping all the vacua to the left,

$${}_{1\cdots n}\langle+|\Phi(\sigma_1)\cdots\Phi(\sigma_n)|V(\sigma_1,\ldots,\sigma_n)\rangle, \tag{92}$$

a form that is convenient for explicit calculations.

When implementing the abstract gauge transformation, some care is needed considering the permutations. The vertex implementation of the gauge transformation becomes

$$\delta_\Xi|\Phi(\sigma_n)\rangle = Q(n)|\Phi(\sigma_n)\rangle + \frac{n}{2}\sum_{\substack{\text{cycl.perm}\\ [\sigma_1..\sigma_{n-1}]}}{}_{1\cdots n}\langle+|\Phi(\sigma_1)\cdots\Phi(\sigma_{n-2})\Xi(\sigma_{n-1})|V(\sigma_1,\ldots,\sigma_{n-1},\sigma_n)\rangle, \tag{93}$$

where the coefficient $n/2$ is an artefact of the permutations.

When evaluating expressions such as (88), (90), and (93), the explicit oscillator and ghost representations of Sec. II is used.

In order for the vertex to encode nontrivial interaction information, we introduce an n-ary function $\mathcal{F}$ of the labels $\{\sigma_i\}_1^n$. Then we write the vertex as

$$|V(\sigma_1,\ldots,\sigma_n)\rangle = \mathcal{F}(\sigma_1,\ldots,\sigma_n)\int \mathrm{d}^Dp_1|-\rangle_1\cdots\int \mathrm{d}^Dp_n|-\rangle_n\delta^D(\Sigma_{i=1}^n p_i), \tag{94}$$

where $\delta^D(\Sigma_{i=1}^n p_i)$ enforces momentum conservation.

For notational convenience, write

$$|-\rangle_{1\cdots n} = \int \mathrm{d}^Dp_1|-\rangle_1\cdots\int \mathrm{d}^Dp_n|-\rangle_n\delta^D(\Sigma_{i=1}^n p_i). \tag{95}$$

The n-order interaction term can now be written

$$g^{n-2}\langle\Phi|^{\otimes n}\mathcal{F}_n|-\rangle_{1\cdots n}. \tag{96}$$

With this form for the vertex, mass dimensions and ghost number counting should work out correctly. It is natural to demand $\mathrm{gh}(\mathcal{F})=0$, i.e., the ghost number is zero, but it must carry mass dimension, as will be calculated shortly.

The ghost number count works out

$$\mathrm{gh}(\langle\Phi|^{\otimes n}) + \mathrm{gh}(|-\rangle_{1\cdots n}) = n\left(-\frac{1}{2}\right) + \frac{n}{2} = 0.$$

The mass dimension count yields

$$(n-2)\mathrm{d}(g) + \mathrm{d}(\mathcal{F}_n) + n\left(-\frac{D+2}{2}\right) + nD - D = 0. \tag{97}$$

There is no compelling reason to let g carry nonzero dimensionality, thus we set $\mathrm{d}(g)=0$, so that

$$\mathrm{d}(\mathcal{F}_n) = D + n - \frac{nD}{2} \tag{98}$$

in four dimensions, the dimension is simply $4-n$.

Ansatz for the vertex function: The ansatz for the vertex function $\mathcal{F}_n$ is based on the following clauses:

(i) $\mathrm{gh}(\mathcal{F}_n)=0$,
(ii) $\mathcal{F}_n$ does not contain annihilators c^0, c^-, b_+ or α_μ,
(iii) $\mathcal{F}_n$ is a space–time scalar,
(iv) $\mathrm{d}(\mathcal{F}_n)=\frac{1}{2}(2D+2n-nD)$.

The first three clauses imply that $\mathcal{F}_n$ can be built from the following bilinears:

$$\alpha_r^\dagger\cdot\alpha_s^\dagger, \quad \alpha_r^\dagger\cdot p_s, \quad c_r^+ b_{s-}, \quad c_r^+ b_{s0},$$

where the indices r,s label HS fields. The fourth clause requires that we introduce at least one-dimensional constant κ to balance the dimensions for the second and last bilinear. Choose $\mathrm{d}(\kappa)=-1$. Introduce a symbol η_{rs}^a to denote the dimensionless bilinears according to

$$\eta_{rs}^1 = \alpha_r^\dagger\cdot\alpha_s^\dagger, \quad \eta_{rs}^2 = \kappa\alpha_r^\dagger\cdot p_s, \quad \eta_{rs}^3 = c_r^+ b_{s-}, \quad \eta_{rs}^4 = \kappa c_r^+ b_{s0}. \tag{99}$$

As already noted, the higher spin vertices cannot be built out of these bilinears alone, rather, powers of the bilinears must be considered. To that end, introduce a symbol Δ_{2m}^n where n denotes the order of the vertex and m denotes the homogenous power of bilinears,

$$\Delta_{2m}^n = {}^nY_{a_1\cdots a_m}^{r_1 s_1\cdots r_m s_m}\eta_{r_1 s_1}^{a_1}\cdots\eta_{r_m s_m}^{a_m}, \tag{100}$$

where there are implicit summations according to

(i) all r_i and s_i, $i\in[1..m]$ are summed over the list $[1..n]$,
(ii) all a_i, $i\in[1..m]$ are summed over the list $[1..4]$,

and where the coefficients ${}^nY_{a_1\cdots a_m}^{r_1 s_1\cdots r_m s_m}$ are algebraic numbers to be determined.

Finally, $\mathcal{F}_n$ can be synthesized as

$$\mathcal{F}_n = \sum_m^\infty \kappa^{[(nD/2)-D-n]}\Delta_{2m}^n. \tag{101}$$

In this framework, the countable set of functions $\{\mathcal{F}_n\}_{n=3}^{\infty}$, if they exist, encode the full interacting theory of higher spin gauge fields. The same information can therefore also be considered as encoded into the countable set of numbers $\{{}^nY^{r_1s_1\cdots r_ms_m}_{a_1\cdots a_m}\}$.

Summarizing, we have the action

$$A = \langle\Phi|Q|\Phi\rangle + \sum_{n=2}^{\infty} g^{n-2}\langle\Phi|^{\otimes n}\mathcal{F}_n|-\rangle_{1\cdots n}, \tag{102}$$

and the gauge transformations

$$\delta_{\Xi}|\Phi\rangle = Q|\Xi\rangle + \sum_{n=3}^{\infty}\frac{n}{2}g^{n-2}\sum_{\text{cycl.perm}}{}_{1\cdots n}\langle+|\Phi^{\otimes(n-2)}\Xi\mathcal{F}_n|-\rangle_{1\cdots n}. \tag{103}$$

It is clear that when formulated in this manner, the gauge invariance of the action can be checked order by order by computerized calculation. At least it should be possible to work out the quartic vertex up to and including spin 3 fields. This would make it possible to compare with the known spin 1 and spin 2 cubic and quartic interaction terms, and with the covariant cubic interaction term for spin 3 derived by Berends, Burgers, and van Dam.[55] Furthermore, it is likely that any obstructions that might make the theory inconsistent should crop up beyond the cubic term.

In order to organize such a calculation a few more points need clarifying. These are the issues of field redefinitions, global symmetries and the tracelessness constraints. A brief discussion of these points can be found in Ref. 33. Setting up the concrete data structures can be done in a functional language like Haskell. But the details of this belong to a computer science journal rather then a physics journal. Therefore this paper defers a thorough discussion to a more appropriate context.

XI. CONCLUSIONS AND OUTLOOK

It is clear that the framework constructed here is not specific to higher spin gauge fields. Higher spin gauge fields enter in the specifications of the fields Φ and the kinetic BRST operator Q, thus essentially in the free field theory. The rest of the abstract structure is independent of the detailed form of Φ and Q. Whether there is an implementation of the structure or not, depends, consequently, on the form of the free theory.

In particular, the abstract structure is silent on the question of multiplet structure, global symmetries, group theory factors, etc. The free field theory contemplated in Sec. II is special in that it contains just one component field of each integer spin s. This is perhaps the most simple situation to envision. We do not know yet if the interacting theory can be constructed in this case. It might be that more complicated multiplet structures are needed, perhaps accompanied by supersymmetry.

There is one peculiarity about the theory outlined here. What is the role of the spin 2 gauge field that appears in the free field theory? The question is connected to the role of gravity and space–time background. Presumably, the free field theory can be cast in any fixed spacetime background. The kinetic operator Q is known in Minkowski space and in AdS space.

The author is reluctant at the moment to speculate on a fundamental role for higher spin gauge fields. But one line of thought seems appropriate to air in the present context. The ubiquity of gravity at all scales of physics is one of the standard tenets of fundamental physics. In particular, this is one of the motivations behind the many attempts to quantize gravity and unify gravity with the spin 1 Yang–Mills forces. On the other hand, there is something glaringly macroscopic about gravity. The force is weak and long range. It is fair to say that we do not know much about gravity on extreme submicroscopic scales. There is a strand of research based on the assumption that gravity is not a fundamental force at all, but just an effective force that manifests itself above submicroscopic scales. Furthermore, as is clear from the cited work on deriving the gravitational equations either by deforming the free field theory, or by gauging the Poincaré group, that the nonlinearities can be understood without building it on a geometrical interpretation. This squares

well with the present day folklore that space–time breaks down at the Planck scale. But if space–time breaks down, then so does physical geometry. This emphasizes the intuition that arithmetic is more fundamental than geometry. Arithmetic is completely scale independent, and since the abstraction of arithmetic is algebra, it can be argued that an algebraic approach to the fundamental theory is more natural than a geometric. Should it furthermore turn out that there is a fundamentally discrete substructure to reality, we think physical geometry is out at the most minute scales.

There are no-go theorems[79,80,34] to the effect that massless fields of spin greater than 2 cannot generate long range forces. This is also consistent with everyday experience. One, admittedly sweeping, scenario would be that in a theory containing massless fields of all integer (and perhaps half-integer) spin, all the fields with spin $s>2$ just generate extreme submicroscopic forces, while the spin 2 field gets effectively self-coupled to generate gravity, and the spin 1 fields generate the standard model forces, one of them surviving as long-range electrodynamics.

Related to the issues discussed here, there is one advantage of the abstract approach to higher spin fields. It makes it very natural to reconsider, as already noted, the higher spin problem in a non-space–time context.

To conclude, there is at least three areas where research is needed. First, the semantic mapping into generalized Lie algebras need to be clarified. Second, a brute force calculation within the vertex implementation should be undertaken for experimental reasons. And third, physical insight into the significance of higher spin gauge fields is badly needed.

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New spherically symmetric monopole and regular solutions in Einstein–Born–Infeld theories

D. J. Cirilo Lombardo[a)]
Bogoliubov Laboratory of Theoretical Physics, Joint Institute of Nuclear Research, Dubna, Moscow Region, 141980, Russia

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In this work a new asymptotically flat solution of the coupled Einstein–Born–Infeld equations for a static spherically symmetric space–time is obtained. When the intrinsic mass is zero the resulting space–time is regular everywhere, in the sense given by Hoffmann and Infeld in 1937, and the Einstein–Born–Infeld theory leads to the identification of the gravitational with the electromagnetic mass. This means that the metric, the electromagnetic field, and their derivatives do not have discontinuities in all the manifold. In particular, there are not conical singularities at the origin, in contrast to the well-known monopole solution studied by Hoffmann in 1935. The lack of uniqueness of the action function in nonlinear electrodynamics is discussed. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1862308]

I. INTRODUCTION AND RESULTS

The four-dimensional solutions with spherical symmetry of the Einstein equations coupled to Born–Infeld fields have been well studied in the literature.[1–4] In particular, the electromagnetic field of the Born–Infeld monopole, in contrast to Maxwell's counterpart, contributes to the ADM mass of the system (it is the four momentum of asymptotic flat manifolds). Hoffmann was the first to study such static solutions in the context of general relativity with the idea of obtaining consistent particle-like model.[2] Unfortunately, these static Einstein–Born–Infeld (EBI) models generate conical singularities at the origin[2,3] that cannot be removed as in global monopoles or other nonlocalized defects of the space–time.[5,6] With the existence of these types of singularities in the space–time of the monopole we cannot identify the gravitational with the electromagnetic mass. In this work a *new* static spherically symmetric solution with Born–Infeld charge is obtained. The new metric, when the intrinsic mass of the system is zero, is *regular* everywhere in the sense that was given by Hoffmann and Infeld[3] in 1937 and the EBI theory leads to identification of the gravitational with the electromagnetic mass. This means that the metric, the electromagnetic field, and their derivatives do not have singularities and discontinuities in all the manifold. The fundamental feature of this solution is the lack of conical singularities at the origin. A distant observer will associate with this solution an electromagnetic mass that is twice the mass of the electromagnetic geon found by Demianski[4] in 1986. The energy–momentum tensor and the electric field are both regular with zero value at the origin and new parameters appear, given to the new metric surprising behaviors. The convention[7,8] used is the *spatial* of Landau and Lifshitz (1962), with signatures of the metric, Riemann, and Einstein tensors all positives $(+++)$.

The plan of this paper is as follows: in Sec. II we give a short introduction to the Born–Infeld theory: properties and principal features. In Sec. III the regularity condition as was given by Hoffmann and Infeld[3] in 1937. Sections IV–VII are devoted to finding the new solution and analyzing its properties. Finally, the conclusion and comments of the results are presented in Sec. VIII.

[a)]Electronic mail: diego@thsun1.jinr.ru

II. THE BORN–INFELD THEORY

The most significant nonlinear theory of electrodynamics is, by excellence, the Born–Infeld theory.[1,9] Among its many special properties is an exact SO(2) electric-magnetic duality invariance. The Lagrangian density describing Born–Infeld theory (in arbitrary space–time dimensions) is

$$\mathcal{L}_{\mathrm{BI}} = \sqrt{-g}L_{\mathrm{BI}} = \frac{b^2}{4\pi}\{\sqrt{-g} - \sqrt{|\det(g_{\mu\nu} + b^{-1}F_{\mu\nu})|}\}, \tag{1}$$

where b is a fundamental parameter of the theory with field dimensions. In open superstring theory,[10] for example, loop calculations lead to this Lagrangian with $b^{-1}=2\pi\alpha'$ ($\alpha' \equiv$ inverse of the string tension). In four space–time dimensions the determinant in (1) may be expanded out to give

$$L_{\mathrm{BI}} = \frac{b^2}{4\pi}\left\{1 - \sqrt{1 + \frac{1}{2}b^{-2}F_{\mu\nu}F^{\mu\nu} - \frac{1}{16}b^{-4}(F_{\mu\nu}\widetilde{F}^{\mu\nu})^2}\right\}, \tag{2}$$

which coincides with the usual Maxwell Lagrangian in the weak field limit.

It is useful to define the second rank tensor $P^{\mu\nu}$ by

$$P^{\mu\nu} = -\frac{1}{2}\frac{\partial L_{\mathrm{BI}}}{\partial F_{\mu\nu}} = \frac{F^{\mu\nu} - \frac{1}{4}b^{-2}(F_{\rho\sigma}\widetilde{F}^{\rho\sigma})\widetilde{F}^{\mu\nu}}{\sqrt{1 + \frac{1}{2}b^{-2}F_{\rho\sigma}F^{\rho\sigma} - \frac{1}{16}b^{-4}(F_{\rho\sigma}\widetilde{F}^{\rho\sigma})^2}} \tag{3}$$

(so that $P^{\mu\nu} \approx F^{\mu\nu}$ for weak fields) satisfying the electromagnetic equations of motion

$$\nabla_\mu P^{\mu\nu} = 0, \tag{4}$$

which are highly nonlinear in $F_{\mu\nu}$. The energy–momentum tensor may be written as

$$T_{\mu\nu} = \frac{1}{4\pi}\left\{\frac{F_\mu{}^\lambda F_{\nu\lambda} + b^2\left[\mathbb{R} - 1 - \frac{1}{2}b^{-2}F_{\rho\sigma}F^{\rho\sigma}\right]g_{\mu\nu}}{\mathbb{R}}\right\},$$
$$\mathbb{R} \equiv \sqrt{1 + \tfrac{1}{2}b^{-2}F_{\rho\sigma}F^{\rho\sigma} - \tfrac{1}{16}b^{-4}(F_{\rho\sigma}\widetilde{F}^{\rho\sigma})^2}. \tag{5}$$

Although it is by no means obvious, it may be verified that Eqs. (3)–(5) are invariant under electric-magnetic rotations of duality $F \leftrightarrow *G$. We can show that the SO(2) structure of the Born–Infeld theory is more easily seen in quaternionic form,[11,12]

$$\frac{1}{R}(\sigma_0 + i\sigma_2\overline{\mathbb{P}})L = \mathbb{L},$$

$$\frac{\mathbb{R}}{(1+\overline{\mathbb{P}^2})}(\sigma_0 - i\sigma_2\overline{\mathbb{P}})\mathbb{L} = L,$$

$$\overline{\mathbb{P}} \equiv \frac{\mathbb{P}}{b},$$

where we defined

$$L = F - i\sigma_2\widetilde{F},$$

$$\mathbb{L} = P - i\sigma_2\widetilde{P},$$

the pseudoescalar of the electromagnetic tensor $F^{\mu\nu}$,

$$\mathbb{P} = -\tfrac{1}{4}F_{\mu\nu}\widetilde{F}^{\mu\nu},$$

and σ_0, σ_2 the well-known Pauli matrix.

In flat space, and for purely electric configurations, the Lagrangian (2) reduces to

$$L_{\mathrm{BI}} = \frac{4\pi}{b^2}\{1 - \sqrt{1 - b^{-2}\vec{E}^2}\}$$

so there is an upper bound on the electric field strength $\vec{E}$,

$$|\vec{E}| \leqslant b. \tag{6}$$

III. THE REGULARITY CONDITION

The new field theory initiated in 1934 by Born[9] introduces in the classical equations of the electromagnetic field a characteristic length r_0 representing the radius of the elementary particle through

$$r_0 = \sqrt{\frac{e}{b}},$$

where e is the elementary charge and b the fundamental field strength entering in a nonlinear Lagrangian function. It was originally thought that the Lagrangian (1) was the simplest choice which would lead to a finite energy for an electric particle. This is, however, not the case. It is possible to find an infinite number of quite different action functions, each giving simple algebraic relations between the fields and each leading to a finite energy for an electric particle.

In 1937 Hoffmann and Infeld[3] introduced a regularity condition on the new field theory of Born[9] with the main idea to solve the lack of uniqueness of the function action. They had already seen that the condition of regularity of the field gives the restriction in the spherically symmetric electrostatic case $E_r = 0$ for $r = 0$.

In the general theory they applied the regularity condition not only to the $F_{\mu\nu}$ field but also to the $g_{\mu\nu}$ field. The regularity condition for the general theory was that:

Only those solutions of the fields equations may have physical meaning for which space–time is everywhere regular and for which the $F_{\mu\nu}$ and the $g_{\mu\nu}$ fields and those of their derivatives which enter in the field equations and the conservation laws exist everywhere.

In the general theory of relativity the spherically symmetric solution of the purely gravitational field equations is given by the Schwarzschild line element

$$\mathrm{d}s^2 = -A\,\mathrm{d}t^2 + A^{-1}\mathrm{d}r^2 + r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\varphi^2),$$

$$A \equiv 1 - \frac{2M}{r},$$

where $(-2M)$ is a constant of integration M having the significance of the gravitational mass of the body source of the field (we take the gravitational constant $G = 1$). This line element has an essential singularity at $r = 0$ and does not satisfy the regularity condition.

In the general relativity form of the original new field theory the requirement that there be no infinities in the $g_{\mu\nu}$ forces the identification of gravitational with electromagnetic mass. In Ref. 3 Hoffmann and Infeld have used for such identification the line element of the well-known monopole solution studied by Hoffmann[2] in 1935,

$$A \equiv 1 - \frac{8\pi}{r}\int_0^r [(r^4+1)^{1/2} - r^2]\mathrm{d}r,$$

which is originated by an Einstein–Born–Infeld action as in Eq. (1). This line element approximates the Schwarzschild form for r greater than the electronic radius but avoids the infinities of that line element for $r=0$. However it is still a singularity of conical type at the pole. When $r \to 0$ the above expression for A gives

$$A \to (1 - 8\pi) \equiv \beta$$

so $\mathrm{d}s^2$ becomes

$$\mathrm{d}s^2 = -\beta\,\mathrm{d}t^2 + \beta^{-1}\,\mathrm{d}r^2 + r^2(\mathrm{d}\theta^2 + \sin^2\theta \mathrm{d}\varphi^2).$$

Thus the radius of the circumference to the radius of a small circle having its center at the pole is, in the limit, $2\pi\beta$ and not 2π. Therefore the origin (it is at $r=0$) is a conical point and not regular. Note that because of the conical point no coordinate can be introduced which will be nonsingular at $r=0$ and derivatives are actually undefined at this point.

This problem with the conical singularities at $r=0$, which destroys the regularity condition, makes that in Ref. 3 change the action of the Born–Infeld form as in Eq. (1) for other nonlinear Lagrangian of logarithmic type. The new logarithmic action does not present such difficulties at $r=0$, and makes many people change the very nice form of the Einstein–Born–Infeld action (1) for other nonlinear Lagrangians that solved the problem of the self-energy of the electron and the regularity condition given above.

In this work we present an *exact* spherically symmetric solution of the Einstein–Born–Infeld equations. The metric, when the intrinsic mass of the system is zero, is *regular* everywhere in the sense that was given by Hoffmann and Infeld[3] in 1937, and the EBI theory leads to identification of the gravitational with the electromagnetic mass. In this manner we also show that stronger conditions are needed to solve the problem of lack of uniqueness of the function action.

IV. STATEMENT OF THE PROBLEM

We propose the following line element for the static Born–Infeld monopole:

$$\mathrm{d}s^2 = -e^{2\Lambda}\,\mathrm{d}t^2 + e^{2\Phi}\mathrm{d}r^2 + e^{2F(r)}\mathrm{d}\theta^2 + e^{2G(r)}\sin^2\theta\,\mathrm{d}\varphi^2, \tag{7}$$

where the components of the metric tensor are

$$g_{tt} = -e^{2\Lambda}, \quad g^{tt} = -e^{-2\Lambda},$$

$$g_{rr} = e^{2\Phi}, \quad g^{rr} = e^{-2\Phi},$$

$$g_{\theta\theta} = e^{2F}, \quad g^{\theta\theta} = e^{-2F},$$

$$g_{\varphi\varphi} = \sin^2\theta e^{2G}, \quad g^{\varphi\varphi} = \frac{e^{-2G}}{\sin^2\theta}. \tag{8}$$

For the obtention of the Einstein–Born-Infeld equation system we use Cartan's structure equations method,[13] which is most powerful and direct where we work with differential forms and in an orthonormal frame (tetrad). The line element (7) in the one-forms basis takes the following form:

$$\mathrm{d}s^2 = -(\omega^0)^2 + (\omega^1)^2 + (\omega^2)^2 + (\omega^3)^2, \tag{9}$$

where the forms are

$$\omega^0 = e^{\Lambda}\mathrm{d}t \Rightarrow \mathrm{d}t = e^{-\Lambda}\omega^0,$$

$$\omega^1 = e^{\Phi}\mathrm{d}r \Rightarrow \mathrm{d}r = e^{-\Phi}\omega^1,$$

$$\omega^2 = e^{F(r)}\mathrm{d}\theta \Rightarrow \mathrm{d}\theta = e^{-F(r)}\omega^2, \tag{10}$$

$$\omega^3 = e^{G(r)}\sin\theta\,\mathrm{d}\varphi \Rightarrow \mathrm{d}\varphi = e^{-G(r)}(\sin\theta)^{-1}\omega^3.$$

Now, following the standard procedure of the structure equations (Appendix) to obtain easily the components of the Riemann tensor, we can construct the Einstein equations

$$G^1{}_2 = -e^{-(F+G)}\frac{\cos\theta}{\sin\theta}\partial_r(G-F), \tag{11}$$

$$G^0{}_0 = e^{-2\Phi}\Psi - e^{-2F},$$

$$\Psi \equiv [\partial_r\partial_r(F+G) - \partial_r\Phi\partial_r(F+G) + (\partial_r F)^2 + (\partial_r G)^2 + \partial_r F\partial_r G], \tag{12}$$

$$G^1{}_1 = e^{-2\Phi}[\partial_r\Lambda\partial_r(F+G) + \partial_r F\partial_r G] - e^{-2F}, \tag{13}$$

$$G^2{}_2 = e^{-2\Phi}[\partial_r\partial_r(\Lambda+G) - \partial_r\Phi\partial_r(\Lambda+G) + (\partial_r\Lambda)^2 + (\partial_r G)^2 + \partial_r\Lambda\partial_r G], \tag{14}$$

$$G^3{}_3 = e^{-2\Phi}[\partial_r\partial_r(F+\Lambda) - \partial_r\Phi\partial_r(F+\Lambda) + (\partial_r\Lambda)^2 + (\partial_r F)^2 + \partial_r F\partial_r\Lambda], \tag{15}$$

$$G^1{}_3 = G^2{}_3 = G^0{}_3 = G^0{}_2 = G^0{}_1 = 0. \tag{16}$$

In the tetrad defined by (10), the energy–momentum tensor of Born–Infeld takes a diagonal form, its components being the following:

$$-T_{00} = T_{11} = \frac{b^2}{4\pi}\left(\frac{\mathbb{R}-1}{\mathbb{R}}\right), \tag{17}$$

$$T_{22} = T_{33} = \frac{b^2}{4\pi}(1-\mathbb{R}), \tag{18}$$

where

$$\mathbb{R} \equiv \sqrt{1-\left(\frac{F_{01}}{b}\right)^2}. \tag{19}$$

In this manner, one can see from the Einstein equation (11) the characteristic property of the spherically symmetric space–times,[14]

$$G^1{}_2 = -e^{-(F+G)}\frac{\cos\theta}{\sin\theta}\partial_r(G-F) = 0 \Rightarrow G = F. \tag{20}$$

Notice that for the interval to be a spherically symmetric one, the functions $F(r)$ and $G(r)$ must be equal. As we saw in the precedent paragraph the components of the energy–momentum tensor of BI assures this condition is in a natural form. Also it is interesting to see from Eqs. (17) and (18) that the energy–momentum tensor of Born–Infeld has the same form as the energy–momentum tensor of an anisotropic fluid.

V. EQUATIONS FOR THE ELECTROMAGNETIC FIELDS OF BORN–INFELD IN THE TETRAD

The equations that describe the dynamic of the electromagnetic fields of Born–Infeld in a curved space–time are

$$\nabla_a \mathbb{F}^{ab} = \nabla_a \left[\frac{F^{ab}}{\mathbb{R}} + \frac{P}{b^2 \mathbb{R}} \widetilde{F}^{ab} \right] = 0 \quad \text{(field equations)}, \tag{21}$$

$$\nabla_a \widetilde{F}^{ab} = 0 \quad \text{(Bianchi's identity)}, \tag{22}$$

where

$$P \equiv -\tfrac{1}{4} F_{\alpha\beta} \widetilde{F}^{\alpha\beta}, \tag{23}$$

$$S \equiv -\tfrac{1}{4} F_{\alpha\beta} F^{\alpha\beta}, \tag{24}$$

$$\mathbb{R} \equiv \sqrt{1 - \frac{2S}{b^2} - \left(\frac{P}{b^2} \right)^2}. \tag{25}$$

The above equations can be solved explicitly giving the follow result:

$$F_{01} = A(r), \tag{26}$$

$$\mathbb{F}_{01} = f e^{-2G}, \tag{27}$$

where f is a constant. We can see from Eqs. (19) and (21) that

$$\mathbb{F}_{01} = \frac{F_{01}}{\sqrt{1 - (\overline{F}_{01})^2}},$$

where we obtain the following form for the electric field of the self-gravitating BI monopole:

$$F_{01} = \frac{b}{\sqrt{\left(\frac{b}{f} e^{2G} \right)^2 + 1}}. \tag{28}$$

We can associate[1]

$$f = b r_0^2 \equiv Q \Rightarrow F_{01} = \frac{b}{\sqrt{\left(\frac{e^G}{r_0} \right)^4 + 1}}, \tag{29}$$

where r_0 is a constant with units of longitude that in Ref. 1 were associated with the radius of the electron. Finally the components of the energy–momentum tensor of BI takes its explicit form reemplacing the F_{01} that was found in Eq. (29) in expressions (17) and (18)

$$-T_{00} = T_{11} = \frac{b^2}{4\pi} \left(1 - \sqrt{\left(\frac{r_0}{e^G} \right)^4 + 1} \right), \tag{30}$$

$$T_{22} = T_{33} = \frac{b^2}{4\pi}\left(1 - \frac{1}{\sqrt{\left(\frac{r_0}{e^G}\right)^4 + 1}}\right). \tag{31}$$

Expressions (11)–(16) together with (30), (31), and (20) are the full set of Einstein equations in explicit form.

VI. REDUCTION AND SOLUTIONS OF THE SYSTEM OF EINSTEIN–BORN–INFELD EQUATIONS

Of the above-noted expressions, we can see that $G^0{}_0 = G^1{}_1$ then

$$\partial_r\partial_r G + (\partial_r G)^2 - \partial_r G\partial_r(\Phi + \Lambda) = 0. \tag{32}$$

In order to reduce Eq. (32) we will proceed as follows. First we make

$$\partial_r G \equiv \xi \tag{33}$$

with this change of variables, in Eq. (32) we have first derivatives only

$$\partial_r\xi + \xi^2 - \xi\partial_r(\Phi + \Lambda) = 0. \tag{34}$$

Dividing expression (34) by ξ and making the substitution

$$\chi \equiv \ln \xi \tag{35}$$

we obtain the following inhomogeneous equation:

$$\partial_r\chi + e^{\chi} = \partial_r(\Phi + \Lambda). \tag{36}$$

The homogeneous part of the last equation is easy to integrate,

$$\chi_h = -\ln r. \tag{37}$$

Now, as usual, we make the following substitution in Eq. (36):

$$\chi = \chi_h + \chi_p = -\ln r + \ln \mu = -\ln r + \ln(1 + \eta). \tag{38}$$

Then

$$\partial_r \ln(1 + \eta) + \frac{\eta}{r} = \partial_r(\Phi + \Lambda) \Rightarrow \partial_r[\ln(1 + \eta) + \mathcal{F}(r) - (\Phi + \Lambda)] = 0 \tag{39}$$

$$\ln(1 + \eta) + \mathcal{F}(r) - (\Phi + \Lambda) = cte = 0,$$

where $d\mathcal{F}(r)/dr \equiv \eta(r)/r$. The constant must be put equal to zero to obtain the correct limit. Finally the form of the exponent G is

$$G = \ln r + \mathcal{F}(r). \tag{40}$$

The next step is to put Φ in function of Λ and G in expression (13). After tedious but straightforward computations and integrations, we obtain

$$e^{2\Lambda} = 1 + a_0 e^{-G} + e^{2G}\frac{2b^2}{3} - 2b^2 e^{-G}\int^{Y(r)} \sqrt{Y^4 + (r_0)^4}\,dY, \tag{41}$$

where we define

$$Y(r) = e^{G}$$

and $a(0)$ is an integration constant.

Hitherto, we know that $\mathcal{F}$ is an arbitrary function of the radial coordinate r, but to be sure of it, we must introduce the function Λ given for the above equation in the Einstein equations (14) and (15) and verify that $G_{22}=G_{33}$. This equality is verified successfully and the functions Λ, Φ, and G remain mathematically determinate. In this manner the line element of our problem (7) takes the following form:

$$ds^2 = -e^{2\Lambda}dt^2 + e^{2\mathcal{F}(r)}[e^{-2\Lambda}(1 + r\partial_r\mathcal{F}(r))^2 dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)]. \tag{42}$$

A. Analysis of the function $\mathcal{F}(r)$ from the physical point of view

The function $\mathcal{F}(r)$ must, to have the behavior in the form of the electric field of the configuration, obey the following requirements to give a regular solution in the sense that was given by Hoffmann and Infeld,[3]

$$F_{01}|_{r=r_0} < b, \tag{43}$$

$$F_{01}|_{r=0} = 0, \tag{44}$$

$$F_{01}|_{r\to\infty} = 0 \quad \text{asymptotically Coulomb} \tag{45}$$

the simplest function $\mathcal{F}(r)$ that obey the above conditions is of the type

$$e^{2\mathcal{F}(r)} = \left[1 - \left(\frac{r_0}{a|r|}\right)^n\right]^{2m}, \tag{46}$$

where a is an arbitrary constant, and the exponents n and m will obey the following relation:

$$mn > 1 \quad (m,n \in \mathbb{N}) \tag{47}$$

with

$$0 < a < 1 \text{ or } -1 < a < 0$$

depending on whether $m(n)$ is even or odd and

$$a \neq 0$$

that ensure a consistent regularization condition not only for the electric (magnetic) field but for the energy-momentum tensor (30) and (31) and the line element (42).

The analysis of the Riemann tensor indicates to us that it is regular everywhere and its components go faster than $1/r^3$ when $r\to\infty$. With all these considerations, the metric solution to the problem is

$$ds^2 = -e^{2\Lambda}dt^2 + \left[1 - \left(\frac{r_0}{a|r|}\right)^n\right]^{2m}\left\{e^{-2\Lambda}dr^2\left[\frac{1 - \left(\frac{r_0}{a|r|}\right)^n (mn-1)}{\left[1 - \left(\frac{r_0}{a|r|}\right)^n\right]}\right]^2 + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)\right\} \tag{48}$$

and the electric field takes the form

$$F_{01} = \frac{b}{\sqrt{1 + \left[1 - \left(\frac{r_0}{a|r|}\right)^n\right]^{4m} \left(\frac{r}{r_0}\right)^4}}. \tag{49}$$

It is interesting to note that if we violate condition (43) taking $a=1$ and $F_{01}|_{r=r_0}=b$ (limit value for the electric field in BI theory) the energy momentum diverges automatically at $r=r_0$. Strictly, the regularity conditions for the energy–momentum tensor (without divergences and discontinuities in the neighborhood of r_0, physical radius of the spherical source of the nonlinear electromagnetic field) are

$$T_{ab}|_{r=r_0} = \text{finite} \Rightarrow -1 < a < 0 \text{ or } 0 < a < 1$$

depending on parity of m, n; and

$$T_{ab}|_{r=0} \to 0 \Rightarrow \mathbb{R} \to 1.$$

For the magnetic monopole case the line element is as expression (48) with the following obvious definition for the magnetic charge,

$$br_0^2 \equiv Q_m.$$

The magnetic field takes the following form:

$$F_{23} = \frac{b}{\left[1 - \left(\frac{r_0}{a|r|}\right)^n\right]^{2m} \left(\frac{r}{r_0}\right)^2} = \frac{Q_m}{\left[1 - \left(\frac{r_0}{a|r|}\right)^n\right]^{2m} r^2}$$

and considerations concerning the regularity conditions on the energy momentum tensor are as in the electric monopole case.

B. Interesting cases for particular values of *n* and *m*

Because

$$\exp 2\mathcal{F}(r) = \left[1 - \left(\frac{r_0}{a|r|}\right)^n\right]^{2m}$$

it is easy to see that for $m=0$,

$$e^G = r.$$

We obtain the spherically symmetric line element of Hoffmann,[2] the electric field F_{01}, and the energy–momentum tensor T_{ab} takes the form of the well-known EBI solution for the electromagnetic geon of Demiánski.[4]

On the other hand, in the *limit* when: $a \to 1$, $n \to 4$, and $m \to \frac{1}{4}$ we have

$$F_{01} \to \frac{b}{\sqrt{1 + \left[1 - \left(\frac{r_0}{|r|}\right)^4\right] \left(\frac{r}{r_0}\right)^4}} = \frac{Q}{r^2},$$

where (as is usually taken) $br_0^2 \equiv Q$. How we see, we obtain as solution in the *limit* the Maxwellian linear field. Note that the values of a and the exponents m and n are restricted by conditions (47).

VII. ANALYSIS OF THE METRIC

We have the metric (42)

$$ds^2 = -e^{2\Lambda}dt^2 + e^{2\mathcal{F}(r)}[e^{-2\Lambda}(1 + r\partial_r\mathcal{F}(r))^2dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)]$$

if we make the substitution

$$Y \equiv re^{\mathcal{F}(r)},$$

and differentiating it

$$dY \equiv e^{\mathcal{F}(r)}(1 + r\partial_r\mathcal{F}(r))dr$$

the interval (7) takes the form

$$ds^2 = -e^{2\Lambda}dt^2 + e^{-2\Lambda}dY^2 + Y^2(d\theta^2 + \sin^2\theta\, d\varphi^2)$$

we can see that the metric (in particular the g_{tt} coefficient), in the new coordinate $Y(r)$, takes the similar form like a Demianski solution for the Born–Infeld monopole space–time:

$$e^{2\Lambda} = 1 - \frac{2M}{Y} - \frac{2b^2r_0^4}{3(\sqrt{Y^4 + r_0^4} + Y^2)} - \frac{4}{3}b^2r_{02}^2F_1\left[1/4, 1/2, 5/4; -\left(\frac{Y}{r_0}\right)^4\right].$$

Here M is an integration constant, which can be interpreted as an intrinsic mass, and ${}_2F_1$ is the Gauss hypergeometric function.[15] We have pass

$$g_{rr} \to g_{YY}, \quad g_{tt}(r) \to g_{tt}(Y).$$

Specifically, for the form of the $\mathcal{F}(r)$ given by (46), Y is

$$Y^2 \equiv \left[1 - \left(\frac{r_0}{a|r|}\right)^n\right]^{2m} r^2.$$

Now, with the metric coefficients fixed to an asymptotically Minkowskian form, one can study the asymptotic behavior of our solution. A regular, asymptotically flat solution with the electric field and energy–momentum tensor both regular, in the sense of Hoffmann and Infeld, is when the exponent numbers of $Y(r)$ take the following particular values:

$$n = 3, \quad m = 1.$$

In this case, and for $r \gg r_0/a$, we have the following asymptotic behavior for $Y(r)$ and $-g_{tt}$, which does not depend on the a parameter

$$Y(r) \to r \quad \left(r \gg \frac{r_0}{a}\right),$$

$$e^{2\Lambda} \simeq 1 - \frac{2M}{r} - \frac{8b^2r_0^4K(1/2)}{3r_0r} + 2\frac{b^2r_0^4}{r^2} + \cdots.$$

A distant observer will associate with this solution a total mass

$$M_{\text{eff}} = M + \frac{4b^2r_0^4K(1/2)}{3r_0}$$

and total charge

$$Q^2 = 2b^2 r_0^2.$$

Notice that when the intrinsic mass M is zero the line element is regular everywhere, the Riemann tensor is also regular everywhere and hence the space–time is singularity free. The electromagnetic mass

$$M_{\mathrm{el}} = \frac{4b^2 r_0^4 K(1/2)}{3r_0} \tag{50}$$

and the charge Q are *twice* that of the electromagnetic charge and mass of the Demianski solution[4] for the static electromagnetic geon. Notice that the M_{el} is necessarily positive, which was not the case in the Schwarzschild line element. The other important reason for us to take the constant $M=0$ is that we must regard the quantity (let us restore for one moment the gravitational constant G)

$$4\pi G \int_{Y(r=0)}^{Y(r)} T_0^0(Y) Y^2 \mathrm{d}Y$$

as the *gravitational mass* causing the field at coordinate distance r from the pole. In our case T_0^0 is given by expression (30). This quantity is precisely (in gravitational units) M_{el} given by (50), the *total electromagnetic mass* within the sphere having its center at $r=0$ and coordinate r. We will take $M=0$ in the rest of the analysis.

On the other hand, the function $Y(r)$ for the values of the m and n parameters given above has the following behavior near the origin:

$$\text{for } a<0 \quad \text{when } r\to 0, Y(r)\to\infty,$$

$$\text{for } a>0 \quad \text{when } r\to 0, Y(r)\to -\infty.$$

Notice that the case $a>0$ will be excluded because in any value $r_0 \to Y(r_0)=0$, the electric field takes the limit value b and condition (43) is violated. For $M=0$ and $a<0$, expanding the hypergeometric function, we can see that the $-g_{tt}$ coefficient has the following behavior near the origin:

$$e^{2\Lambda} \simeq 1 - \frac{8b^2 r_0^4 K(1/2)}{3r_0} r^2 \left(\frac{|a|}{r_0}\right)^3 + 2b^2 r_0^4 r^4 \left(\frac{|a|}{r_0}\right)^6 + \cdots .$$

The metric (see figures) and the energy–momentum tensor *both* remain regulars at the origin (it is: $g_{tt}\to -1$, $T_{\mu\nu}\to 0$ for $r\to 0$). It is not very difficult to check that (for $m=1$ and $n=3$) the maximum of the electric field (see the figures) is not in $r=0$, but in the *physical border* of the spherical configuration source of the electromagnetic fields (this point is located around $r_B = 2^{1/3} r_0/|a|$). It means that $Y(r)$ maps correctly the internal structure of the source in the same form as the quasiglobal coordinate of Ref. 16 for the global monopole in general relativity. The lack of conical singularities at the origin is due to the very good description of the manifold in the neighborhood of $r=0$ given by $Y(r)$.

Because the metric is regular ($g_{tt}=-1$, at $r=0$ and at $r=\infty$), its derivative must change sign. In the usual gravitational theory of general relativity the derivative of g_{tt} is proportional to the gravitational force which would act on a test particle in the Newtonian approximation. In Einstein–Born–Infeld theory with this new static solution, it is interesting to note that although this force is attractive for distances of the order $r_0 \ll r$, it is actually a repulsion for very small r. For r greater than r_0, the line element closely approximates to the Schwarzschild form. Thus the regularity condition shows that the electromagnetic and gravitational mass are the same and, as in the Newtonian theory, we now have the result that the attraction is zero in the center of the spherical configuration source of the electromagnetic field.

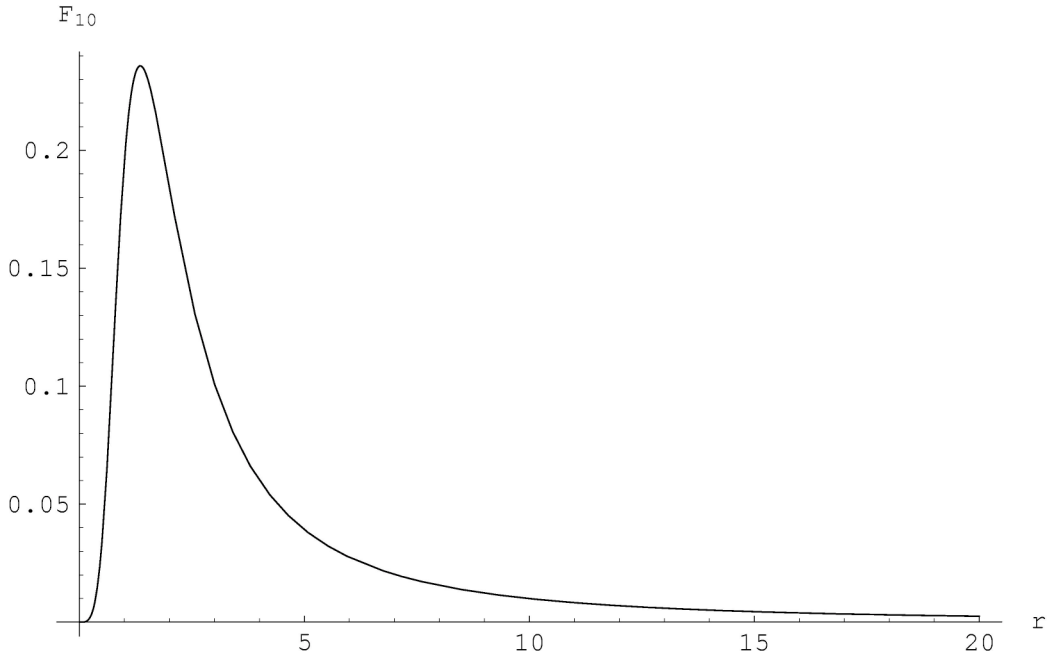

FIG. 1. Electric field F_{10} of the EBI - monopole in function of r, for $M=0$, $r_0=1$, $m=1$, $n=3$ and $a=-0.9$

VIII. CONCLUSIONS

In this report a *new* exact solution of the Einstein–Born–Infeld equations for a static spherically symmetric monopole is presented. The general behavior of the geometry is strongly modified according to the value that r_0 takes (Born–Infeld radius[1,9]) and three new parameters: a, m, and n.

The fundamental feature of this solution is the lack of conical singularities at the origin when $-1<a<0$ or $0<a<1$ (depends on parity of m and n) and $mn>1$. In particular, for $m=1$ and $n=3$, with the parameter a in the range given above and the intrinsic mass of the system M being zero, the strong regularity conditions given by Hoffmann and Infeld in Ref. 3 hold in all the space–time. For the set of values for the above-given parameters, the solution is asymptotically flat, free of singularities in the electric field, metric, energy–momentum tensor and their derivatives (with derivative values zero for $r\to 0$); and the electromagnetic mass (ADM) of the system is twice that of the electromagnetic mass of other well-known[2,4] solutions for the Einstein–Born–Infeld monopole. The electromagnetic mass M_{el} asymptotically is necessarily positive, which was not the case in the Schwarzschild line element (See Figs. 1 and 2).

This solution has a surprising similitude with the metric for the global monopole in general relativity given in Refs. 16 and 17 in the sense that the physics of the problem has a correct description only by means of a new radial function $Y(r)$.

Because the metric is regular ($g_{tt}=-1$, at $r=0$ and at $r=\infty$), its derivative (that is proportional to the force in Newtonian approximation) must change sign. In Einstein–Born–Infeld theory with this new static solution, it is interesting to note that although this force is attractive for distances of the order $r_0 \lll r$, it is actually repulsive for very small r.

With this new regular solution, we also show that stronger conditions are needed to solve the problem of the lack of uniqueness of the function action in nonlinear electrodynamics.

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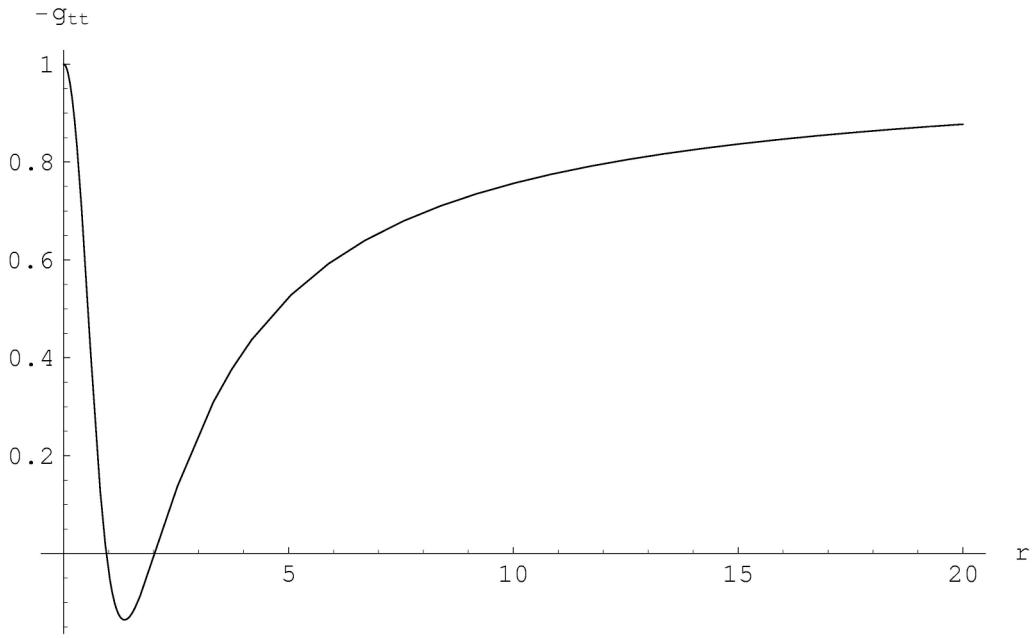

FIG. 2. Coefficient $-g_{tt}$ of the EBI - monopole in function of r, for $M=0$, $r_0=1$, $m=1$, $n=3$ and $a=-0.9$

APPENDIX: CONNECTIONS AND CURVATURE FORMS FROM THE GEOMETRICAL CARTAN'S FORMULATION

The standard procedure of Cartan has its start point in the following:

$$\mathrm{d}\omega^{\alpha} = -\,\omega^{\alpha}{}_{\beta} \wedge \omega^{\beta}, \tag{A1}$$

$$\mathcal{R}^{\alpha}{}_{\beta} = d\omega^{\alpha}{}_{\beta} + \omega^{\alpha}{}_{\lambda} \wedge \omega^{\lambda}{}_{\beta}. \tag{A2}$$

These are denominated *the structure equations*. The procedure to obtain the Einstein equations is as follows.

(i) Making the exterior derivatives of ω^{α} we compute the connection one-forms $\omega^{\alpha}{}_{\beta}$:

$$\omega^{0}{}_{1} = \omega^{1}{}_{0} = e^{-\Phi}\partial_r \Lambda \omega^{0},$$

$$\omega^{2}{}_{1} = -\,\omega^{1}{}_{2} = e^{-\Phi}\partial_r F(r)\omega^{2},$$

$$\omega^{3}{}_{1} = -\,\omega^{1}{}_{3} = e^{-\Phi}\partial_r G(r)\omega^{3}, \tag{A3}$$

$$\omega^{3}{}_{2} = -\,\omega^{2}{}_{3} = \frac{\cos\theta}{\operatorname{sen}\theta} e^{-F(r)}\omega^{3}.$$

(ii) Making the exterior derivatives of $\omega^{\alpha}{}_{\beta}$ we compute the curvature two-forms $\mathcal{R}^{\alpha}{}_{\beta}$:

$$\mathcal{R}^{0}{}_{1} = e^{-2\Phi}(\partial_r\partial_r\Lambda - \partial_r\Phi\partial_r\Lambda + (\partial_r\Lambda)^2)\omega^{1} \wedge \omega^{0},$$

$$\mathcal{R}^{2}{}_{1} = e^{-2\Phi}(\partial_r\partial_r F - \partial_r\Phi\partial_r F + (\partial_r F)^2)\omega^{1} \wedge \omega^{2},$$

$$\mathcal{R}^3{}_2 = e^{-(F+\Phi)}\partial_r(G-F)\frac{\cos\theta}{\operatorname{sen}\theta}\omega^1\wedge\omega^3 + (e^{-2\Phi}\partial_r G\partial_r F - e^{-2F})\omega^2\wedge\omega^3,$$

$$\mathcal{R}^3{}_1 = e^{-2\Phi}(\partial_r\partial_r G - \partial_r\Phi\partial_r G + (\partial_r G)^2)\omega^1\wedge\omega^3 + e^{-(F+\Phi)}\partial_r(G-F)\frac{\cos\theta}{\operatorname{sen}\theta}\omega^2\wedge\omega^3, \tag{A4}$$

$$\mathcal{R}^0{}_2 = -e^{-2\Phi}\partial_r\Lambda\partial_r F\omega^0\wedge\omega^2,$$

$$\mathcal{R}^0{}_3 = -e^{-2\Phi}\partial_r\Lambda\partial_r G\omega^0\wedge\omega^3.$$

(iii) The components of the Riemann tensor are easily obtained from the well-know geometrical relation of Cartan:

$$\mathcal{R}^\alpha{}_\beta = R^\alpha{}_{\beta\rho\sigma}\omega^\rho\wedge\omega^\sigma,$$

where we obtain explicitly

$$R^0{}_{110} = e^{-2\Phi}(\partial_r\partial_r\Lambda - \partial_r\Phi\partial_r\Lambda + (\partial_r\Lambda)^2),$$

$$R^2{}_{112} = e^{-2\Phi}(\partial_r\partial_r F - \partial_r\Phi\partial_r F + (\partial_r F)^2),$$

$$R^3{}_{113} = e^{-2\Phi}(\partial_r\partial_r G - \partial_r\Phi\partial_r G + (\partial_r G)^2),$$

$$R^3{}_{213} = e^{-(F+\Phi)}\partial_r(G-F)\frac{\cos\theta}{\sin\theta},$$

$$R^3{}_{123} = e^{-(F+\Phi)}\partial_r(G-F)\frac{\cos\theta}{\sin\theta}, \tag{A5}$$

$$R^3{}_{223} = e^{-2\Phi}\partial_r G\partial_r F - e^{-2F},$$

$$R^0{}_{330} = e^{-2\Phi}\partial_r\Lambda\partial_r G,$$

$$R^0{}_{220} = e^{-2\Phi}\partial_r\Lambda\partial_r F,$$

from which we can construct the Einstein equations of the usual manner.

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Conformal symmetries of Einstein's field equations and initial data

Ramesh Sharma[a)]
Department of Mathematics, University of New Haven, West Haven, Connecticut 06516

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This paper examines the initial data for the evolution of the space–time solution of Einstein's equations admitting a conformal symmetry. Under certain conditions on the extrinsic curvature of the initial complete spacelike hypersurface and sectional curvature of the space–time with respect to sections containing the normal vector field, we have shown that the initial hypersurface is conformally diffeomorphic to a sphere or a flat space or a hyperbolic space or the product of an open real interval and a complete 2-manifold. It has been further shown that if the initial hypersurface is compact, then it is conformally diffeomorphic to a sphere. Finally, the conformal symmetries of a generalized Robertson–Walker space–time have been described. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1868372]

I. INTRODUCTION

Most of the known solutions of Einstein's field equations (that are highly nonlinear) are based on the assumption that they admit one or more Killing vector fields (infinitesimal isometries) or homothetic vector fields. These solutions provide many clues and insights into astrophysical and cosmological questions. However, it would be interesting to analyze space–time solutions with weaker symmetries, such as, conformal symmetries. This would be further supported by the fact that Robertson–Walker space–times (which provide a satisfactory cosmological model) do admit a G_6 of Killing vectors and a G_9 of conformal Killing vector fields (see Maartens and Maharaj[14]). One may also note that conformal symmetries preserve the causal character of space–times. One little drawback with conformal symmetries lies in the fact that unlike isometries and homotheties, conformal symmetries do not leave Einstein tensor invariant, and in this respect, may be regarded unnatural or accidental. Nevertheless, some solutions with conformal symmetries are known (for details we refer to Duggal and Sharma[6]). We note that the existence of a proper conformal symmetry places severe restrictions on the space–times, as indicated by the results proven by Collinson and French,[5] Garfinkle and Tian,[10] and Sharma.[17] The work reported in this paper is primarily intrigued by the following significant result of Eardley, Isenberg, Marsden, and Moncrief:[8] "*Let* (M,g) *be a globally hyperbolic spacetime which (a) satisfies the Einstein equations for a stress tensor T obeying the mixed energy condition and the dominant energy condition; (b) admits a homothetic Killing vector field* ξ *of g*; *and (c) admits a compact hypersurface of constant mean curvature (CMC). Then either* (M,g) *is an expanding hyperbolic model with T vanishing everywhere, or* ξ *is Killing*." In this paper we characterize a space–time solution of Einstein's equation with a conformal symmetry, in terms of a spacelike hypersurface as an initial data. *As this is a formidable task, we have assumed a curvature condition on the space–time*. This assumption is motivated by the fact that this holds on a generalized Robertson–Walker space–time (in particular, Robertson–Walker space–time) as indicated in Example (1) of Sec. II. First we derive the constraint and evolution equations for a conformal Killing vector (CKV) field on the space–time solution of Einstein's equations. Assuming that the space–time solution M admits a proper CKV field ξ, and is evolved out of a spacelike hypersurface Σ such that (a) Σ is complete

a)Electronic mail: rsharma@newhaven.edu

and totally umbilical in M, (b) the normal sectional curvature of the space–time is independent of the normal section at each point of Σ, and (c) the normal component of ξ is nonvanishing and nonconstant on Σ, we prove that such a hypersurface is conformally diffeomorphic to one of the following: (i) sphere S^3, (ii) Euclidean space E^3, (iii) hyperbolic space H^3, (iv) the Riemannian product of a real open interval and a complete 2-manifold. Then we prove the main result of this paper, i.e., if a space–time solution M of Einstein's equation admits a CKV field ξ and is evolved out of a compact spacelike CMC hypersurface Σ such that (a) ξ is nowhere tangential and nonvanishing on Σ, (b) the normal component of ξ is nonconstant over Σ, and (c) the normal sectional curvature of M is independent of the normal section at each point of Σ, then Σ is totally umbilical in M, and conformally diffeomorphic to a 3-sphere. Finally we describe CKV fields on a generalized Robertson–Walker space–time (see example (1) under Sec. II).

II. PRELIMINARIES AND NOTATIONS

We would like to follow the ADM 3+1 splitting formalism due to Arnowitt, Deser, and Misner[2] that slices the space–time (M,g) into a one-parameter family of spacelike hypersurfaces and considers that the space–time geometry evolve out of an initial spacelike hypersurface $\Sigma(t=\text{constant})$ with initial data as its Riemannian metric γ and the second fundamental form (extrinsic curvature) k. Let us denote arbitrary vector fields tangential to Σ by X,Y,Z,W, and the timelike unit vector field normal to Σ by N. Then the Gauss and Weingarten formulas are

$$\bar{\nabla}_X Y = \nabla_X Y + k(X,Y)N, \quad \bar{\nabla}_X N = KX, \tag{1}$$

where K is the Weingarten (shape) operator of Σ defined by $k(X,Y)=\langle KX,Y\rangle$ ($\langle,\rangle$ denotes the inner product with respect to the 3-metric γ of Σ as well as the space–time metric g), and $\bar{\nabla},\nabla$ the Levi–Civita connections of the metrics g,γ, respectively. We write the Gauss and Codazzi equations as

$$\langle \bar{R}(X,Y)Z,W\rangle = \langle R(X,Y)Z,W\rangle + k(Y,Z)k(X,W) - k(X,Z)k(Y,W), \tag{2}$$

$$\langle \bar{R}(X,Y)N,Z\rangle = (\nabla_X k)(Y,Z) - (\nabla_Y k)(X,Z), \tag{3}$$

where $\bar{R}$ and R denote curvature tensors of g and γ, respectively. Let $(e_a)(a=1,2,3)$ denote a local orthonormal frame on an open neighborhood $\mathcal{O}$ in Σ. Then (e_a,N) is a local orthonormal basis of the tangent space of M at each point of $\mathcal{O}$. Contracting (2) and (3) with respect to this basis one gets

$$\overline{\mathrm{Ric}}(X,Y) + \langle \bar{R}(N,X)Y,N\rangle = \mathrm{Ric}(X,Y) + \tau\langle KX,Y\rangle - \langle KX,KY\rangle, \tag{4}$$

$$\overline{\mathrm{Ric}}(X,N) = (\mathrm{div}\, K)X - X\tau, \tag{5}$$

where $\overline{\mathrm{Ric}}$ and Ric are the Ricci tensors of g and γ, respectively, and $\tau=\mathrm{Tr}\,K=3$ times the mean curvature of Σ. Denoting the scalar curvature and the energy-momentum tensor of the space–time solution of the Einstein's field equations

$$\overline{\mathrm{Ric}} - \frac{\bar{r}}{2}g = 8\pi T \tag{6}$$

by $\bar{r}$ and T, respectively, and using (4)–(6) yields the constraint equations

$$r + \frac{2\tau^2}{3} - |L|^2 = 16\pi T_{nn}, \tag{7}$$

$$(\operatorname{div} L)X - \tfrac{2}{3}X\tau = 8\pi T(X,N), \tag{8}$$

where r is the scalar curvature of γ, $\|$ the norm operator with respect to γ, $L=K-(\tau/3)I$ and $T_{nn}=T(N,N)$.

At this point we assume that (M,g) admits a conformal Killing vector field ξ, i.e.,

$$\mathfrak{L}_{\xi} g = \sigma g \tag{9}$$

for a sufficiently smooth function σ on (M,g), and decompose ξ along Σ as

$$\xi = V + \rho N, \tag{10}$$

where V is the tangential component of ξ. A straightforward calculation using Eqs. (1), (9), and (10) provides

$$\mathfrak{L}_V \gamma = \sigma\gamma - 2\rho k. \tag{11}$$

Next, differentiating $\rho=-g(\xi,N)$ twice along Σ, and following the procedure given on p. 103 of Ref. 18, we obtain

$$(\nabla\,\nabla\,\rho)(X,Y) = \frac{N\sigma}{2}\langle X,Y\rangle + \langle \bar{R}(V,X)Y,N\rangle + \rho\langle \bar{R}(N,X)Y,N\rangle + \frac{\sigma}{2}k(X,Y) - \langle \nabla_Y V, KX\rangle - \rho\langle KX,KY\rangle - \langle \nabla_X KV, Y\rangle. \tag{12}$$

The use of (3) and (4) in the above equation shows

$$\langle (\mathfrak{L}_V K)X,Y\rangle = -(\nabla\,\nabla\,\rho)(X,Y) + \frac{N\sigma}{2}\langle X,Y\rangle - \left(\frac{\sigma}{2} - \rho\tau\right)\langle KX,Y\rangle + \rho\,\mathrm{Ric}(X,Y) - \rho\,\overline{\mathrm{Ric}}(X,Y). \tag{13}$$

Going back to the Einstein's Eqs. (6) we observe that $\bar{r}=8\pi(T_{nn}-T^m_m)$, where $T^m_m=\langle Te_m,e_m\rangle$. The use of (6) in (13) gives rise to

$$(\mathfrak{L}_V K)X = -\nabla_X D\rho + \frac{N\sigma}{2}X + \left(\rho\tau - \frac{\sigma}{2}\right)KX + \rho QX - 8\pi\rho TX + 4\pi\rho(T^m_m - T_{nn})X, \tag{14}$$

where D is the spatial gradient operator, and Q is the Ricci operator of γ, and $\nabla^2=\nabla^a\nabla_a$ (a summed over 1,2,3). Equations (7), (11), and (14) provide the following evolution equations:

$$(\mathfrak{L}_V\gamma)(X,Y) = \sigma\gamma(X,Y) - 2\rho\langle LX,Y\rangle - \frac{2\rho\tau}{3}\gamma(X,Y), \tag{15}$$

$$(\mathfrak{L}_V L)X = -\left(\nabla_X D\rho - \frac{\nabla^2\rho}{3}X\right) - 8\pi\rho\left(TX - \frac{T^m_m}{3}X\right) + \left(\rho\tau - \frac{\sigma}{2}\right)LX + \rho\left(QX - \frac{r}{3}X\right), \tag{16}$$

$$\mathfrak{L}_V\tau = \frac{3N\sigma}{2} - \frac{\sigma\tau}{2} - \nabla^2\rho + \rho\left[\frac{\tau^2}{3} + |L|^2 + 4\pi(T^m_m + T_{nn})\right]. \tag{17}$$

These evolution equations were derived in Ref. 8 through a different approach using Berger's trick[4] that sets the evolution vector field equal to the CKV field.

Let us now define the concept of normal sectional curvature of the space–time with respect to a normal section. A normal section of (M,g) at a point p of a spacelike hypersurface Σ is the timelike plane section spanned by the normal N and a tangential vector, say X, at p. The normal sectional curvature $\bar{K}(N,X)$ of M at a point p and along a unit tangent vector X of Σ is defined as $\langle \bar{R}(N,X)N,X\rangle$ (see p. 331 of Ref. 3 for the definition of sectional curvature of a timelike plane

section). If $\bar{K}(N,X)$ is independent of the choice of X at each point of Σ, then it follows that $\bar{R}(N,X)N=fN$ for some smooth function f and arbitrary vector field X tangent to Σ. This normal sectional curvature condition is a weakening of constant curvature condition for M, and holds when M is Minkowski, de Sitter, anti-de Sitter, and Robertson–Walker space–times. The normal sectional curvature has been termed a principal sectional curvature of the Robertson–Walker space–time by O'Neill (p. 345 of Ref. 16). Next we provide three examples of space–times satisfying this condition.

Example 1: The normal sectional curvature condition holds for generalized Robertson–Walker (GRW) space–times defined by Alias, Romero, and Sanchez in Ref. 1 as the warped product $I\times_f\Sigma$ of the timeline I with an *arbitrary* three-dimensional Riemannian manifold (Σ,γ) through the warping function $f>0$ on I such that the metric of the warped product space–time (M,g) is

$$ds^2=-dt^2+(f(t))^2\gamma_{ab}\,dx^a\,dx^b,$$

where $x^a(a=1,2,3)$ are the coordinates on the fiber Σ. Note that, when (Σ,γ) is of constant curvature; the GRW space–time reduces to the Robertson–Walker space–time. Here $N=\partial/\partial t$. For the GRW space–time, it is known (see p. 210 of Ref. 16) that $\bar{R}(X,N)N$ is a multiple of X, where $\bar{R}$ denotes the curvature tensor of g and X is an arbitrary vector field on the fiber Σ. Each slice $t=$constant, is homothetic to the fiber Σ, and totally umbilical in (M,g).

Example 2: Consider a conformally flat perfect fluid solution of Einstein's equations, admitting a spacelike hypersurface Σ orthogonal to the 4-velocity. In this case the 4-velocity vector is N, the energy-momentum tensor is $T=(\mu+p)N^*N^*+pg$, where N^* denotes the 1-form metrically (g) equivalent to N, and μ,p denote, respectively, the energy density and pressure of the perfect fluid. It turns out, after a straightforward calculation, that $\langle\bar{R}(N,X)N,X\rangle=-(4\pi/3)(\mu+3p)$ for an arbitrary unit vector field X tangent to Σ.

Example 3: Classically, we know that the shape operator K of an (orientable) hypersurface of a space–time of constant curvature (Minkowski, de Sitter, and anti-de Sitter) is a Codazzi tensor, i.e., satisfies $(\nabla_X K)Y=(\nabla_Y K)X$ [which follows from the Codazzi Eq. (3)]. This need not be true for a general ambient space–time. A hypersurface Σ of a space–time (M,g) is said to be Codazzi if its shape tensor is Codazzi. A totally umbilical CMC hypersurface of M is obviously Codazzi. One can also verify that if a three-dimensional space Σ of constant curvature c is a hypersurface of (M,g) with $K=cfI+\nabla Df$ for a smooth function f on Σ, and where D denotes the gradient operator of Σ, then Σ is Codazzi in (M,g). However, the converse holds only locally, i.e., if K is a Codazzi tensor on a space of constant curvature c, then locally, $K=cfI+\nabla Df$, for a smooth function f (see Ref. 9). Now let (M,g) denote a space–time with a closed CKV field ξ, and a spacelike hypersurface Σ such that Σ is Codazzi in (M,g) and ξ is nowhere tangential to Σ. We then have $\bar{\nabla}_{\bar{X}}\xi=\sigma\bar{X}$ for a smooth function σ and arbitrary vector field $\bar{X}$ on M. A straightforward computation shows

$$\bar{R}(\bar{X},\bar{Y})\xi=(\bar{X}\sigma)\bar{Y}-(\bar{Y}\sigma)\bar{X}$$

for arbitrary vector fields $\bar{X}$, $\bar{Y}$ on M. Substituting $\bar{X}=N$, $\bar{Y}=Y$(an arbitrary vector field tangent to Σ), and using the orthogonal splitting $\xi=\rho N+V$ (V being the tangential component of ξ) we have

$$\rho\bar{R}(N,Y)N+\bar{R}(N,Y)V=(N\sigma)Y-(Y\sigma)N$$

on Σ. Taking its inner product with an arbitrary tangent vector field X on Σ, and noting

$$g(\bar{R}(N,Y)V,X)=g(\bar{R}(V,X)N,Y)=0$$

(in view of Codazzi equation and the assumption that Σ is a Codazzi hypersurface), we find

$$\rho g(\bar{R}(N,Y)N,X) = (N\sigma)g(X,Y).$$

As per our assumption, ρ vanishes nowhere on Σ. Hence $\bar{R}(N,Y)N=(N\sigma/\rho)Y$, i.e., the normal sectional curvature of M is independent of the choice of the arbitrary vector field Y at each point of Σ.

III. RESULTS AND THEIR PROOFS

From a cosmological point of view, it makes sense to assume that space–time is spatially homogeneous (e.g., Robertson–Walker, Bianchi I, and Taub-NUT space–times are so) and since a homogeneous Riemannian manifold is complete (see p. 127 of Ref. 3), one may assume that space–time is spatially complete. Recently, Duggal and Sharma[7] considered the Example 3 of the preceding section, with Σ as a totally umbilical CMC hypersurface and proved "*Let* (M,g) *be a space–time evolved out of a complete initial hypersurface* Σ *that is totally umbilical and has nonzero CMC. If M admits a closed CKV field* ξ *nonvanishing on* Σ*, then either* ξ *is orthogonal to* Σ*, or* Σ *is conformally diffeomorphic to* E^3, S^3, H^3*, or the Riemannian product of an open interval and a complete Riemannian 2-manifold*." This result assumes that the CKV field is closed, which implies in view of Example 3, that the normal sectional curvature condition holds. We would like to consider the case when the CKV is not necessarily closed, but the normal sectional curvature condition holds. Omitting the CMC condition, and assuming completeness of Σ we state our first result.

Theorem 1: *Let* (M,g) *be a space–time solution of Einstein's field equations admitting a CKV field* ξ *and be evolved out of a complete spacelike hypersurface* Σ *such that (a)* Σ *is totally umbilical in M, (b) the normal component* ρ *of* ξ *is nonconstant on* Σ*, and (c) the normal sectional curvature of M is independent of the tangential direction at each point of* Σ*. Then* Σ *is conformally diffeomorphic to (i) a 3-sphere* S^3*, or (ii) Euclidean space* E^3*, or (iii) hyperbolic space* H^3*, or (iv) the Riemannian product of a complete two-dimensional manifold and an open real interval. If* Σ *is compact, then only (i) holds.*

Proof: By hypothesis,we have that $\bar{R}(N,X)N=fX$ for some function f and any vector field X tangent to Σ, at each point of Σ. This implies, upon contraction, that $f=(-1/3)\overline{\mathrm{Ric}}(N,N)$. Also, as Σ is totally umbilical, Eq. (4) assumes the form

$$\overline{\mathrm{Ric}}(X,Y) = \mathrm{Ric}(X,Y) + \frac{1}{3}\left(\frac{2\tau^2}{3} - \overline{\mathrm{Ric}}(N,N)\right)\langle X,Y\rangle. \tag{18}$$

Contracting this one gets

$$\bar{r} + 2\,\overline{\mathrm{Ric}}(N,N) = r + \frac{2\tau^2}{3}.$$

Further, (6) implies

$$\bar{r} + 2\,\overline{\mathrm{Ric}}(N,N) = 16\pi T_{nn}.$$

Using (6) in (18) we have

$$8\pi TX = QX + \left(\frac{2\tau^2}{9} - 8\pi T_{nn} + \frac{2\,\overline{\mathrm{Ric}}(N,N)}{3}\right)X.$$

Its trace-free part is

$$8\pi\left(TX - \frac{T_m^m}{3}X\right) = QX - \frac{r}{3}X. \tag{19}$$

By hypothesis, $L=0$, and hence we have from (16) that

$$\nabla_X D\rho = \frac{\nabla^2\rho}{3} X. \tag{20}$$

Now we recall the following result of Kuehnel (pp. 133 and 135 of Ref. 13) "Let (Σ, g) be a complete connected n-dimensional Riemannian manifold admitting a nonconstant solution ρ of $\nabla\nabla\rho = (\nabla^2\rho/n)g$. Then the number of critical points of ρ is $N \leqslant 2$, and Σ is conformally diffeomorphic to (i) the sphere (S^n, g_1) if $N=2$, (ii) the Euclidean space (E^n, g_0) or hyperbolic space (H^n, g_{-1}) if $N=1$, and (iii) the Riemannian product of an $(n-1)$-dimensional Riemannian manifold and an open real interval, if $N=0$. In case when Σ is compact, only (i) holds." According to our hypothesis, ρ is nonconstant. Since ρ satisfies Eq. (20), the above result is applicable and therefore applying it completes the proof.

Our next result assumes the existence of a compact spacelike CMC hypersurface. This is well motivated because such hypersurfaces have been shown to exist in a Lorentzian manifold by Gerhardt.[11] Before stating our next result we state the following lemma.

Lemma: Let (M, g) be a space–time manifold admitting a CKV field ξ and be evolved out of a compact spacelike CMC hypersurface Σ such that the normal vector field to Σ is an eigenvector of the Ricci tensor of M, at each point of Σ and ξ is nonvanishing and nowhere tangent to Σ. Then Σ is totally umbilical in M.

This lemma is the Lorentzian analog and a slight extension of the corresponding result of Katsurada[12] for an Einstein Riemannian (M, g), and its proof is similar to that of the Riemannian case.

Before stating our main theorem we would like to recall the following notions. The geometrodynamic field momentum dynamically conjugate to the geometrodynamic field coordinate g_{ab} is defined as $\pi^{ab} = \gamma^{1/2}(K^{ab} - \tau\gamma^{ab})$. The supermomentum in the ADM formalism is defined as $\mathcal{H}^a = 2\nabla_b[\sqrt{\gamma}(\tau\gamma^{ab} - K^{ab})]$, where γ is the determinant of the 3-metric γ_{ab} and ∇ acts a covariant derivative of a tensor density (see p. 521 of Ref. 15 for details). Our main result is as follows.

Theorem 2: *Let (M, g) be a space–time solution of Einstein's equations admitting a CKV field ξ and evolved out of a compact spacelike CMC hypersurface Σ such that (i) the supermomentum $\mathcal{H}^a$ vanishes on Σ, (ii) the normal component ρ of ξ is nonvanishing and nonconstant on Σ, and (iii) the normal sectional curvature of M is independent of the tangential direction at each point of Σ. Then Σ is totally umbilical in M, and conformally diffeomorphic to the 3-sphere.*

Proof: As $\mathcal{H}^a = 0$ on Σ, it follows that

$$\nabla_a\tau - \nabla_b K^b_a = 0.$$

In view of this and Eq. (5) we observe that N is an eigenvector of the Ricci tensor of (M, g) at each point of Σ. Hence the lemma stated above is applicable here and hence Σ is totally umbilical. Now Theorem 1 becomes applicable and hence Σ being compact, is conformally diffeomorphic to S^3. This completes the proof.

Remark: The metrics of Σ in the conclusions of Theorems 1 and 2 can be expressed as

$$du^2 + (\rho'(u))^2\, d\psi^2,$$

globally for case (iv), and except at critical points of ρ for cases (i), (ii), and (iii); where $d\psi^2$ denotes the metric of the complete two-dimensional space orthogonal to $\partial/\partial u$ (for details see Ref. 13). Also, one may note that Σ is quasi-Einstein, because the Ricci tensor of $d\psi^2$ (which is the metric of a two-dimensional Riemannian manifold S) is just a scalar multiple of its metric.

IV. CONFORMAL SYMMETRIES OF GRW SPACE–TIMES.

Let ξ be a CKV field on a generalized Robertson–Walker space–time (M, g), as described in Example 1. Setting $\xi = \rho\,\partial/\partial t + V^a\,\partial/\partial x^a$ (where x^a are the coordinates on the fiber Σ), and decomposing the CKV equations into normal–normal components [note that $\partial/\partial t$ is the unit timelike vector normal to spacelike slice $\Sigma_t(t = \text{constant})$] we find that

$$\sigma = 2\,\partial\rho/\partial t. \tag{21}$$

Similarly, decomposing the CKV equation into tangential–normal, and tangential–tangential components gives

$$\partial\rho/\partial x^a = f^2(\partial V^b/\partial t)\gamma_{ab}, \tag{22}$$

$$\mathfrak{L}_V\gamma_{ab} = \left(\sigma - 2\frac{\rho}{f}\,\partial f/\partial t\right)\gamma_{ab}. \tag{23}$$

If $V=0$, i.e., ξ is orthogonal to the slices Σ_t, then from (22) ρ is a function of only t and from (21) we have $\sigma=2\dot{\rho}$, where an overdot means derivative with respect to t. Using this expression of σ in (23), and noting that $V=0$, shows $\dot{\rho}=(\dot{f}/f)\rho$. Integrating it provides $\rho=cf$ for an arbitrary constant c, and hence we obtain $\xi=cf\,\partial/\partial t$. This is the well known[14] timelike CKV normal to the slices Σ_t of a Robertson–Walker space–time. On the other hand, if $\rho=0$, i.e., ξ is tangent to each slice Σ_t, then from Eq. (21) it follows that $\sigma=0$, i.e., ξ is Killing on (M,g). *This generalizes the fact* (see Ref. 14) *that the CKV fields that are tangential to the constant curvature slices* Σ_t *of a Robertson–Walker space–time, are Killing*. More generally, if ρ is a function of only spatial coordinates x^a, then (21) implies $\sigma=0$ and hence ξ is Killing, though ξ is not tangential to Σ_t. Now suppose that ρ is a function of only t, i.e., constant on each slice Σ_t. Then Eq. (22) shows that V^a are functions of only x^a, and hence Eqs. (21) and (23) show that $\dot{\rho}-(\dot{f}/f)\rho=c_1$(a constant). Solving this linear equation provides

$$\rho = f(t)\left(c_1\int_{t_0}^{t}\frac{1}{f(\tau)}\mathrm{d}\tau + c_2\right), \tag{24}$$

where c_2 is an arbitrary constant. The value of σ is gotten by using this expression of ρ in (21). *If* ρ *is a nonvanishing function of all the four coordinates* t,x^a, *then from Theorem 1 (note that all the hypotheses of Theorem 1 are satisfied by GRW space–times) it follows that each slice is conformally diffeomorphic to one of the model spaces mentioned in the conclusion of Theorem 1, and has the line element* $du^2+(\rho'(u))^2\,d\psi^2$ *where* $d\psi^2$ *is the 2-metric orthogonal to* $\partial/\partial u$. *This does compare with the line element of the spatial slice of the Robertson–Walker space–time where the 2-metric* $d\psi^2$ *is the standard metric of the unit 2-sphere*. Finally we note that if the GRW space–time admits a maximal conformal group G_{15}, then it is conformally flat, and hence Σ has constant curvature, i.e., GRW space–time reduces to Robertson–Walker space–time.

V. CONCLUDING REMARKS

In the hypotheses of Theorems 1 and 2, we have assumed that the normal component ρ of the CKV field ξ is nonvanishing and nonconstant on Σ. If we just assume that (M,g) is a space–time admitting a CKV field ξ and a spacelike hypersurface Σ such that ρ is zero, i.e., ξ is everywhere tangential to Σ, then we observe from Eqs. (11) and (16) that V is conformal on Σ and L is preserved by V up to the factor $-\sigma/2$. Next, suppose that a space–time solution (M,g) of Einstein's equations admits a CKV field ξ and a totally umbilical spacelike hypersurface Σ such that the normal component ρ of ξ is a nonzero constant on Σ. Then one can show using Eqs. (3), (9), and (12) that $\langle\bar{R}(N,X)N,X\rangle=-4\pi/3(T_{nn}+T^m_m)$ for any unit tangent vector field X on Σ, i.e., the normal sectional curvature of M is independent of the tangential direction at each point of Σ. Conversely, this consequence need not imply that ρ is constant on Σ. This intrigued us to include this normal sectional curvature condition as a hypothesis in Theorems 1 and 2. This is further motivated by the fact that the normal sectional curvature condition holds for GRW space–times.

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Exact solutions with noncommutative symmetries in Einstein and gauge gravity

Sergiu I. Vacaru[a)]
Instituto de Matematicas y Fisica Fundamental, Consejo Superior de Investigaciones Cientificas, Calle Serrano 123, Madrid 28006, Spain

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We present new classes of exact solutions with noncommutative symmetries constructed in vacuum Einstein gravity (in general, with nonzero cosmological constant), five-dimensional (5D) gravity and (anti) de Sitter gauge gravity. Such solutions are generated by anholonomic frame transforms and parametrized by generic off-diagonal metrics. For certain particular cases, the new classes of metrics have explicit limits with Killing symmetries but, in general, they may be characterized by certain anholonomic noncommutative matrix geometries. We argue that different classes of noncommutative symmetries can be induced by exact solutions of the field equations in commutative gravity modeled by a corresponding moving real and complex frame geometry. We analyze two classes of black ellipsoid solutions (in the vacuum case and with cosmological constant) in four-dimensional gravity and construct the analytic extensions of metrics for certain classes of associated frames with complex valued coefficients. The third class of solutions describes 5D wormholes which can be extended to complex metrics in complex gravity models defined by noncommutative geometric structures. The anholonomic noncommutative symmetries of such objects are analyzed. We also present a descriptive account how the Einstein gravity can be related to gauge models of gravity and their noncommutative extensions and discuss such constructions in relation to the Seiberg–Witten map for the gauge gravity. Finally, we consider a formalism of vielbeins deformations subjected to noncommutative symmetries in order to generate solutions for noncommutative gravity models with Moyal (star) product. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1869538]

I. INTRODUCTION

In the last 15 years much effort has been made to elaborate a consistent formulation of noncommutative gravity theory generalizing the standard Einstein theory but up to now the problem is quite difficult to approach (see, for instance, Refs. 1–8 for details related to existing models). The proposed theories are for the spaces with Euclidean signatures, and, in general, result in models of complex gravity in noncommutative spaces provided with complex and/or nonsymmetric metrics and anholonomic frames. There were also derived some effective noncommutative gravity models from string/brane theory, by considering quantum group structures and/or by proposing noncommutative gaugelike generalizations of gravity.

In this paper, we pursue the idea that noncommutative geometric structures are present in the Einstein, five-dimensional (in brief, 5D) gravity and gauge gravity models. Such noncommutative symmetries are emphasized if the anholonomic moving frames[9–12] are introduced into consideration. This hidden noncommutativity is nontrivial for various classes of generic off-diagonal metrics admitting effective diagonalizations by anholonomic transforms with associated nonlinear connection structure.[13–19] The metrics may be subjected to the condition to define exact solutions

[a)]Electronic mail: vacaru@imaff.cfmac.csic.es and sergiu_vacaru@yahoo.com

of the vacuum field equations with certain possible extensions to matter sources. The noncommutative anhlonomic geometries can be derived even from the commutative general relativity theory and admit a natural embedding into different models of complex noncommutative gravity. The metric and frame (vielbein) coefficients corresponding to off-diagonal solutions depend on two, three or four variables and define space–times with associated noncommutative symmetries. Such classes of exact solutions are very different from the well-known examples of metrics with Killing symmetry (like the Schwarzschild or Kerr–Newmann solutions; see a detailed analysis in Ref. 20).

Our aim is to prove, by constructing and analyzing three classes of exact solutions, that certain noncommutative geometric structures can be defined in the framework of the Einstein (in general, with the cosmological term) and 5D gravity. We emphasize classes of anholonomic real and complex deformations of metrics possessing associated noncommutative symmetries. Contrary to other approaches to noncommutative gravity and field interactions theory elaborated by substituting the commutative algebras of functions with noncommutative algebras and/or by postulating any complex noncommutative relations for coordinates, we try to derive noncommutative structures from associated symmetries of metrics and frames subjected to anholonomy relations. We shall propose a classification of such space–times and state a method of complexification of exact solutions preserving the noncommutative symmetry for black hole and wormhole metrics in real and complex gravity.

The study of anholonomic noncommutative symmetries of gravitational field interactions is more involved in the moving frame formalism conventionally adapted to equivalent redefinitions of the Einstein equations as Yang–Mills equations for nonsemisimple gauge groups like in the Poincare gauge gravity.[21,22] This construction has direct generalizations to various type of gauge gravity models with nondegenerate metrics in the total bundle spaces, in both commutative and noncommutative forms.[23–29,6] The connection between the general relativity theory and gauge gravity models is emphasized in order to apply and compare with a set of results from noncommutative gauge theory.

Among our static solutions we find geometries having a structure as have Schwarzschild, Reissner–Nordstrem, and (anti) de Sitter spaces but with the coefficients redefined (with certain polarization constants) with respect to anholonomic real/complex frames which make possible definition of such objects in noncommutative models of gravity. There are equally interesting applications to black hole physics, quantum gravity, and string gravity.

Next, the emerged anholonomic noncommutative symmetries of off-diagonal metrics prescribe explicit rules of deformation the solutions on small noncommutative parameters and connect the results to quantum deformations of gravity and gauge models. So, even a generally accepted version of noncommutative gravity theory has been not yet formulated, we know how to generate particular classes of real and complex stable metrics with noncommutative symmetries and possessing properties very similar to the usual black hole and wormhole solutions. In particular, we present a systematic procedure for constructing exact solutions both in commutative and noncommutative gravity models, to define black hole and wormhole objects with noncommutative symmetries and quantum corrections. We are able to investigate the physical properties of such objects subjected to certain classes of anholonomic and/or quantum deformations.

The paper is organized as follows.

We begin in Sec. II with a brief introduction into the geometry of space–times provided with anholonomic frame structure and associated nonlinear connections. Such geometries are characterized by corresponding anholonomy relations induced by nonlinear connection coefficients related to certain off-diagonal metric components. This also induces a corresponding noncommutative space–time structure.

In Sec. III, we illustrate that such noncommutative anholonomic geometries can be associated even to real space–times and that a simple realization holds within the algebra for complex matrices. We emphasize that a corresponding noncommutative differential calculus can be derived from the anholonomy coefficients deforming the structure constants of the related Lie algebras.

Section IV is devoted to a rigorous analysis of two classes of static black ellipsoid solutions [the first and second type metrics defining, respectively, four-dimensional (4D) vacuum Einstein

and induced by cosmological constant configurations]. We prove that such metrics can be complexified in order to admit associated complex frame/nonlinear connection structures inducing noncommutative matrix geometries and show how analytic extensions of such real and complexified space–times can be constructed.

In Sec. V, a class of 5D wormhole solutions with anisotropic elliptic polarizations is considered for the 5D gravity. We argue that such generic off-diagonal metrics may be also complexified as to preserve the wormhole configurations being additionally characterized by complex valued coefficients for the associated nonlinear connection. Such objects possess the same noncommutative symmetry for both types of real and complex solutions.

Section VI is a discussion of how the Einstein gravity and its higher dimension extensions can be incorporated naturally into commutative and noncommutative gauge models. A new point is that the proposed geometric formalism is elaborated in order to include anholonomic complex vielbeins.

In Sec. VII, we define the Seiberg–Witten map for the de Sitter gauge gravity and state a prescription how the exact solutions possessing anholonomic noncommutative symmetries can be adapted to deformations via star products with noncommutative relations for coordinates.

We conclude and discuss the results in Sec. VIII. For convenience, we summarize the necessary results from Refs. 13–19 and 30–32 in Appendixes A–C and state some definitions on "star" products and enveloping algebras in Appendix D.

II. OFF-DIAGONAL METRICS AND ANHOLONOMIC FRAMES

We consider a $(n+m)$-dimensional space–time manifold V^{n+m} provided with a (pseudo) Riemannian metric $\mathbf{g}=\{g_{\mu\nu}\}$ and denote the local coordinates $u=(x,y)$, or in component form, $u^{\alpha}=(x^i,y^a)$, where the greek indices are conventionally split into two subsets, $x=\{x^i\}$ and $y=\{y^a\}$, labelled, correspondingly, by italic indices of type $i,j,k,\ldots=1,2,\ldots,n$, and $a,b,\ldots=1,2,\ldots,m$. In general, the geometric objects on such space–times may possess some nontrivial Killing symmetries (the Killing case is emphasized by the condition $L_X\mathbf{g}=0$, where L_X is the Lie derivative with respect to a vector field X on V^{n+m}, see, for instance, Ref. 20) or some deformations of such symmetries, for instance, by frame transforms. The space–times may have some additional frame structures with associated nonlinear connection, bundle structure, and even nontrivial torsions being adapted to the frame structure.

We shall define our constructions for a general metric ansatz of type

$$\mathbf{g}=g_{\mu\nu}\delta u^{\mu}\otimes\delta u^{\nu}=g_{ij}(x^k)\mathrm{d}x^i\otimes\mathrm{d}x^j+h_{ab}(x^k,v)\delta y^a\otimes\delta y^b \tag{1}$$

with respect to a locally adapted basis $[\mathrm{d}x^i,\delta y^a]$, where the Einstein's summation rule is applied and by v we emphasize the dependence on a so-called anisotropic coordinate from the set $\{y^a\}$. The local basis

$$e^{\mu}_{[N]}=\delta^{\mu}=\delta u^{\mu}=[\mathrm{d}x^i,\delta y^a]=[\mathrm{d}x^i,\mathrm{d}y^a=\mathrm{d}y^a+N^a_i(x^k,v)\mathrm{d}x^i] \tag{2}$$

(called to be N-elongated; we shall provide an additional index $[N]$ if necessary to distinguish such objects) is dual to the local basis

$$e^{[N]}_{\alpha}=\delta_a=\frac{\delta}{\delta u^a}=\left[\frac{\delta}{\partial x^i}=\frac{\partial}{\partial x^i}-N^a_i(x^k,v)\frac{\partial}{\partial y^a},\frac{\partial}{\partial y^b}\right]. \tag{3}$$

We consider an off-diagonal metric ansatz for (1) having the components

$$\hat{g}_{\alpha\beta}=\begin{bmatrix} g_{ij}+N^a_iN^b_jh_{ab} & N^e_jh_{ae} \\ N^e_ih_{be} & h_{ab}\end{bmatrix}. \tag{4}$$

So, we can write equivalently $\mathbf{g}=\hat{g}_{\alpha\beta}\,\mathrm{d}u^{\alpha}\,\mathrm{d}u^{\beta}$ if the metric is rewritten with respect to the local dual coordinate basis $\mathrm{d}u^{\mu}=[\mathrm{d}x^i,\mathrm{d}y^a]$, the dual to $\partial/\partial u^{\alpha}=[\partial/\partial x^i,\partial/\partial y^b]$ (defined correspondingly by usual partial derivatives and differentials).

A very surprising fact is that the off-diagonal metric ansatz (4) for dimensions $n+m=3,4,5$ and certain imbedding of such configurations in extra dimension (super) spaces results in completely integrable systems of partial differential equations (see details in Refs. 13–19 with a review of results in Refs. 30 and 31 and Theorems 1–3 in Appendix B). In this paper, we shall consider that any metric (4), or equivalently (1) and frames (vielbeins) (2) and (3), parametrizes an exact solution of the Einstein equations in a commutative gravity theory.

Let us state the main geometric properties of space–times provided with off-diagonal metrics which can be effectively diagonalized with respect to the *N*-elongated frames (2) and (3).

(1) Such space–times are characterized by certain anholonomic frame relations (anholonomy conditions)

$$e_{\alpha}^{[N]}e_{\beta}^{[N]}-e_{\beta}^{[N]}e_{\alpha}^{[N]}=w_{\alpha\beta}^{[N]\gamma}e_{\gamma}^{[N]} \tag{5}$$

with some nontrivial anholonomy coefficients $w_{\alpha\beta}^{[N]\gamma}$ computed as

$$w^{k}{}_{ij}=0,\ w^{k}{}_{aj}=0,\quad w^{k}{}_{ab}=0,\ w^{c}{}_{ab}=0,$$

$$w^{a}{}_{bj}=-w^{a}{}_{jb}=\partial_{b}N_{j}^{a},\quad w^{a}{}_{ij}=-\Omega_{ij}^{a}=\delta_{i}N_{j}^{a}-\delta_{j}N_{i}^{a} \tag{6}$$

(we shall omit the label $[N]$ if this will not result in any confusion; as a matter of principle, we can consider arbitrary anholonomy coefficients not related to any off-diagonal metric terms). If the values $w_{\alpha\beta}^{[N]\gamma}$ do not vanish, it is not possible to diagonalize the metric (4) by any coordinate transforms: such space–times are generic off diagonal. The holonomic frames (in particular the coordinate ones) consist of a subclass of vielbeins with vanishing anholonomy coefficients.

(2) To any frame (vielbein) transform defined by the coefficients of $e_{\alpha}^{[N]}$ decomposed with respect to usual coordinate frames, we can associate a nonlinear connection structure (in brief, *N* connection) **N** with the coefficients $\{N_{j}^{a}\}$ [in global form the *N* connection was defined in Ref. 33 by developing previous ideas from Finsler geometry,[9–12,34–36] investigated in details for vector bundle spaces in Refs. 37 and 38; see also Refs. 13–19 and 30–32 on definition of such objects in (pseudo) Riemannian and Riemann–Cartan–Weyl geometry or on superspaces]. Here we note that the *N*-connection structure is characterized by its curvature (*N* curvature) $\Omega=\{\Omega_{ij}^{a}\}$ with the coefficients computed as in (6). The well-known class of linear connections is to be distinguished as a particular case when $N_{j}^{a}(x,y)=\Gamma_{jb}^{a}(x)y^{b}$. On (pseudo) Riemannian spaces, the *N* connection is a geometric object completely defined by anholonomic frames when the vielbein transforms $e_{\alpha}^{[N]}$ are parametrized explicitly via certain values $(N_{i}^{a},\delta_{i}^{j},\delta_{b}^{a})$, where δ_{i}^{j} and δ_{b}^{a} are the Kronecker symbols, like in (3).

(3) The *N* coefficients define a conventional global horizontal–vertical (in brief, $h-v$) splitting of space–time V^{n+m} into holonomic–anholonomic subsets of geometrical objects labeled by *h* components with indices $i,j,\ldots$ and *v* components with indices $a,b,\ldots$; see details in Refs. 13–19 and 30–32. The necessary formulas for the $h-v$ decompositions of the curvature, Ricci and Einstein tensors are contained in Appendix A.

(4) Such generic "off-diagonal" space–times may be characterized by the so-called canonical *N*-adapted linear connection $\Gamma^{[c]}=\{L^{i}{}_{jk},L^{a}{}_{bk},C^{i}{}_{jc},C^{a}{}_{bc}\}$ satisfying the metricity condition $D_{\gamma}^{[c]}g_{\alpha\beta}=0$ and being adapted to the $h-v$ distribution. The coefficients of $\Gamma^{[c]}$ are

$$L^{i}{}_{jk}=\tfrac{1}{2}g^{in}(\delta_{k}g_{nj}+\delta_{j}g_{nk}-\delta_{n}g_{jk}),$$

$$L^{a}{}_{bk}=\partial_{b}N_{k}^{a}+\tfrac{1}{2}h^{ac}(\delta_{k}h_{bc}-h_{dc}\partial_{b}N_{k}^{d}-h_{db}\partial_{c}N_{k}^{d}), \tag{7}$$

$$C^i_{jc} = \tfrac{1}{2} g^{ik} \partial_c g_{jk}, \quad C^a_{bc} = \tfrac{1}{2} h^{ad} (\partial_c h_{db} + \partial_b h_{dc} - \partial_d h_{bc}),$$

where $\delta_k = \delta / \partial x^k$ and $\partial_c = \partial / \partial y^a$; they are constructed from the coefficients (and their partial derivatives) of the metric and N connection. This connection is an anholonomic deformation (by N coefficients) of the Levi–Civita connection.

(5) The torsion of the connection $\Gamma^{[c]}$ is defined (for simplicity, we omit the label $[c]$)

$$T^\alpha_{\beta\gamma} = \Gamma^\alpha_{\beta\gamma} - \Gamma^\alpha_{\gamma\beta} + w^\alpha_{\beta\gamma}, \tag{8}$$

with $h-v$ components

$$T^i_{.jk} = T^i_{jk} = L^i_{jk} - L^i_{kj} = 0 \quad \text{in the canonical case,}$$

$$T^a_{.bc} = S^a_{.bc} = C^a_{bc} - C^a_{cb} = 0 \quad \text{in the canonical case,} \tag{9}$$

$$T^i_{.ja} = 0, \quad T^i_{ja} = -T^i_{aj} = -C^i_{ja}, \quad T^a_{.ij} = -\Omega^a_{ij}, \quad T^a_{.bi} = -T^a_{.bi} = \partial_b N^a_i - L^a_{.bi}.$$

The nonvanishing components of torsion are induced as an anholonomic frame effect which is obtained by vielbien transforms (2) and (3) even for a (pseudo) Riemannian metric (4). In this paper, we shall also consider some nontrivial torsion structures existing in extra dimension gravity.

(6) By straightforward calculations with respect to the frames (2) and (3) (see for instance, Refs. 39 and 40) we can compute the coefficients of the Levi–Civita connection ∇, i.e., $\Gamma^{[\nabla]}_{\alpha\beta\gamma} = g(e^{[N]}_\alpha, \nabla_\gamma e^{[N]}_\beta) = g_{\alpha\tau} \Gamma^{[\nabla]\tau}_{\beta\gamma}$, satisfying the metricity condition $\nabla_\gamma g_{\alpha\beta} = 0$ for $g_{\alpha\beta} = (g_{ij}, h_{ab})$,

$$\Gamma^{[\nabla]}_{\alpha\beta\gamma} = \tfrac{1}{2} (e^{[N]}_\beta g_{\alpha\gamma} + e^{[N]}_\gamma g_{\beta\alpha} - e^{[N]}_\alpha g_{\gamma\beta} + g_{\alpha\tau} w^\tau{}_{\gamma\beta} + g_{\beta\tau} w^\tau{}_{\alpha\gamma} - g_{\beta\tau} w^\tau{}_{\beta\alpha}).$$

Using the values (6) and (3), we can write

$$\Gamma^{[\nabla]\tau}_{\beta\gamma} = \left\{ L^i_{jk}, L^a_{bk} + \frac{\partial N^a_k}{\partial y^b}, C^i_{jc} + \frac{1}{2} g^{ik} \Omega^a_{jk} h_{ca}, C^a_{bc} \right\}. \tag{10}$$

Comparing the coefficients of $\Gamma^{[c]}$ and $\Gamma^{[\nabla]}$, we conclude that both connections have the same coefficients with respect to the N-adapted frames (2) and (3) if and only if $\partial N^a_k / \partial y^b = 0$ and $\Omega^a_{jk} = 0$.

(7) The ansatz of type (4) have been largely used in Kaluza–Klein theories (see, for instance, Refs. 41–43). For the corresponding compactifications, the coefficients N^a_i may be associated to the potential of certain gauge fields but, in general, they belong to some noncompactified metric and vielbein gravitational fields. There were elaborated general methods for constructing exact solutions without compactification and arbitrary N^a_i in various types of gravity models.[13–19]

Any ansatz of type (4) with the components satisfying the conditions of the Theorems 1–3 from Appendix B define a new class of exact solutions, vacuum and nonvacuum ones, in three- through five-dimensional gravity parametrized by generic off-diagonal metrics with the coefficients depending on two, three or even four variables. These solutions can be constructed in explicit form by using corresponding boundary and symmetry conditions following the so-called anholonomic frame method elaborated and developed in Refs. 13–19, 30, and 31 (for instance, they can describe black elipsoid/tori configurations, two- through three-dimensional solitonic–spinor–dilaton interactions, polarized wormhole/flux tube solutions, locally anisotropic Taub NUT space–times and so on).

Perhaps, by using the anholonomic frame method, we can construct the most general known class of exact solutions in Einstein gravity and its extra dimension and string generalizations. From a formal point of view, we can use superpositions of anholonomic maps in order to construct integral varieties of the Einstein equations with the metric/frame coefficients being functions of necessary smooth class depending on arbitrary number of variables but parametrized as products

of functions depending on one, two, three, and four real, or some complex, variables with real and complex valued functions. The physical meaning of such classes of solutions should be stated following explicit physical models. We note that the bulk of the well-known black hole and cosmological solutions (for instance, the Schwarzschild, Kerr–Newman, Reissner–Nordström, and Friedmann–Roberston–Walker solutions) are with metrics being diagonalizable by coordinate transforms and depending only on one variable (radial or timelike), with imposed spherical or cylindrical symmetries and subjected to the conditions of Killing symmetry being asymptotically flat.

In general, the solutions with anholonomic configurations do not possess Killing symmetries (for instance, they are not restricted by "black hole uniqueness theorems," proved for Killing space–times satisfying corresponding asymptotic conditions, see details and references in Ref. 20) but have new properties like the (1)–(7) stated above. There is a subclass of off-diagonal solutions resulting in corresponding limits into the well-known asymptotically flat space–times, or with (anti) de Sitter symmetries.[13–19,30,31] We are interested to investigate possible symmetries of such non-Killing exact solutions.

The purpose of the next section is to prove that the space–times with a nontrivial anholonomic and associated N-connection structure possess a natural noncommutative symmetry.

III. ANHOLONOMIC NONCOMMUTATIVE STRUCTURES

We shall analyze two simple realizations of noncommutative geometry of anholonomic frames within the algebra of complex $k\times k$ matrices, $M_k(\mathrm{IC},u^\alpha)$ depending on coordinates u^α on space–time V^{n+m} connected to complex Lie algebras SL (k,IC) and SU_k. We shall consider matrix valued functions of a necessary smooth class derived from the anholonomic frame relations (5) (being similar to the Lie algebra relations) with the coefficients (6) induced by off-diagonal metric terms in (4) and by N-connection coefficients N_i^a. We shall use algebras of complex matrices in order to have the possibility for some extensions to complex solutions. Usually, for commutative gravity models, the anholonomy coefficients $w_{\alpha\beta}^{[N]\gamma}$ are real functions but in Sec. VII we shall consider also complex space–times related to noncommutative gravity.[3–5]

We start with the basic relations for the simplest model of noncommutative geometry realized with the algebra of complex $(k\times k)$ noncommutative matrices,[44], $M_k(\mathrm{IC})$. An element $M\in M_k(\mathrm{IC})$ can be represented as a linear combination of the unit $(k\times k)$ matrix I and (k^2-1) Hermitian traceless matrices $q_{\underline{\alpha}}$ with the underlined index $\underline{\alpha}$ running values $1,2,\ldots,k^2-1$, i.e.,

$$M=\alpha I+\sum\beta^{\underline{\alpha}}q_{\underline{\alpha}}$$

for some constants α and $\beta^{\underline{\alpha}}$. It is possible to choose the basis matrices $q_{\underline{\alpha}}$ satisfying the relations

$$q_{\underline{\alpha}}q_{\underline{\beta}}=\frac{1}{k}\rho_{\underline{\alpha}\underline{\beta}}I+Q_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}q_{\underline{\gamma}}-\frac{i}{2}f^{\underline{\gamma}}{}_{\underline{\alpha}\underline{\beta}}q_{\underline{\gamma}}, \tag{11}$$

where $i^2=-1$ and the real coefficients satisfy the properties

$$Q_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}=Q_{\underline{\beta}\underline{\alpha}}^{\underline{\gamma}},\quad Q_{\underline{\gamma}\underline{\beta}}^{\underline{\gamma}}=0,\quad f^{\underline{\gamma}}{}_{\underline{\alpha}\underline{\beta}}=-f^{\underline{\gamma}}{}_{\underline{\beta}\underline{\alpha}},\quad f^{\underline{\gamma}}{}_{\underline{\gamma}\underline{\alpha}}=0$$

with $f^{\underline{\gamma}}{}_{\underline{\alpha}\underline{\beta}}$ being the structure constants of the Lie group SL (k,IC) and the Killing–Cartan metric tensor $\rho_{\underline{\alpha}\underline{\beta}}=f^{\underline{\tau}}{}_{\underline{\alpha}\underline{\gamma}}f^{\underline{\gamma}}{}_{\underline{\tau}\underline{\beta}}$. The interior derivatives $\hat{\partial}_{\underline{\gamma}}$ of this algebra can be defined as

$$\hat{\partial}_{\underline{\gamma}}q_{\underline{\beta}}=ad(iq_{\underline{\gamma}})q_{\underline{\beta}}=i[q_{\underline{\gamma}},q_{\underline{\beta}}]=f^{\underline{\alpha}}{}_{\underline{\gamma}\underline{\beta}}q_{\underline{\alpha}}. \tag{12}$$

Following the Jacobi identity, we obtain

$$\hat{\partial}_{\underline{\alpha}}\hat{\partial}_{\underline{\beta}}-\hat{\partial}_{\underline{\beta}}\hat{\partial}_{\underline{\alpha}}=f^{\underline{\gamma}}{}_{\underline{\alpha}\underline{\beta}}\hat{\partial}_{\underline{\gamma}}. \tag{13}$$

Our idea is to construct a noncommutative geometry starting from the anholonomy relations of frames (5) by adding to the structure constants $f^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}$ the anholonomy coefficients $w^{[N]\tau}_{\alpha\gamma}$ (6). Such deformed structure constants consist from N-connection coefficients N^a_i and their first partial derivatives, i.e., they are induced by some off-diagonal terms in the metric (4) being a solution of the gravitational field equations. We note that there is a rough analogy between formulas (13) and (5) because the anholonomy coefficients do not satisfy, in general, the condition $w^{[N]\tau}_{\tau\alpha}=0$. There is also another substantial difference, the anholonomy relations are defined for a manifold of dimension $n+m$, with greek indices $\alpha,\beta,\ldots$ running values from 1 to $n+m$ but the matrix noncommutativity relations are stated for traceless matrices labeled by underlined indices $\underline{\alpha},\underline{\beta}$, running values from 1 to k^2-1. It is not possible to satisfy the condition $k^2-1=n+m$ by using integer numbers for arbitrary $n+m$. We suggest to extend the dimension of space–time from $n+m$ to any $n'\geqslant n$ and $m'\geqslant m$ when the condition $k^2-1=n'+m'$ can be satisfied by a trivial embedding of the metric (4) into higher dimension, for instance, by adding the necessary number of unities on the diagonal by writing

$$\hat{g}_{\underline{\alpha}\underline{\beta}}=\begin{bmatrix} 1 & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 1 & 0 & 0 \\ 0 & \cdots & 0 & g_{ij}+N^a_iN^b_jh_{ab} & N^e_jh_{ae} \\ 0 & \cdots & 0 & N^e_ih_{be} & h_{ab} \end{bmatrix}$$

and $e^{[N]}_{\underline{\alpha}}=\delta_{\underline{\alpha}}=(1,1,\ldots,e^{[N]}_{\alpha})$, where, for simplicity, we preserve the same type of underlined greek indices, $\underline{\alpha},\underline{\beta},\ldots=1,2,\ldots,k^2-1=n'+m'$. The anholonomy coefficients $w^{[N]\gamma}_{\alpha\beta}$ can be extended with some trivial zero components and for consistency we rewrite them without labeled indices, $w^{[N]\gamma}_{\alpha\beta}\to W^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}$. The set of anholonomy coefficients $w^{[N]\gamma}_{\alpha\beta}$ (6) may result in degenerated matrices, for instance for certain classes of exact solutions of the Einstein equations. Nevertheless, we can consider an extension $w^{[N]\gamma}_{\alpha\beta}\to W^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}$ when the coefficients $w^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}(u^{\underline{\tau}})$ for any fixed value $u^{\underline{\tau}}=u^{\underline{\tau}}_{[0]}$ would be some deformations of the structure constants of the Lie algebra SL (k,IC), like

$$W^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}=f^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}+w^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}, \tag{14}$$

being nondegenerate.

Instead of the matrix algebra $M_k(\mathrm{IC})$, constructed from constant complex elements, we shall consider dependencies on coordinates $u^{\underline{\alpha}}=(0,\ldots,u^{\alpha})$, for instance, like a trivial matrix bundle on $V^{n'+m'}$, and denote this space $M_k(\mathrm{IC},u^{\underline{\alpha}})$. Any element $B(u^{\underline{\alpha}})\in M_k(\mathrm{IC},u^{\underline{\alpha}})$ with a noncommutative structure induced by $W^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}$ is represented as a linear combination of the unit $(n'+m')\times(n'+m')$ matrix I and the $[(n'+m')^2-1]$ Hermitian traceless matrices $q_{\underline{\alpha}}(u^{\underline{\tau}})$ with the underlined index $\underline{\alpha}$ running values $1,2,\ldots,(n'+m')^2-1$,

$$B(u^{\underline{\tau}})=\alpha(u^{\underline{\tau}})I+\sum\beta^{\underline{\alpha}}(u^{\underline{\tau}})q_{\underline{\alpha}}(u^{\underline{\tau}})$$

under condition that the following relation holds:

$$q_{\underline{\alpha}}(u^{\underline{\tau}})q_{\underline{\beta}}(u^{\underline{\gamma}})=\frac{1}{n'+m'}\rho_{\underline{\alpha}\underline{\beta}}(u^{\underline{\nu}})+Q^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}q_{\underline{\gamma}}(u^{\underline{\mu}})-\frac{i}{2}W^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}q_{\underline{\gamma}}(u^{\underline{\mu}})$$

with the same values of $Q^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}$ from the Lie algebra for SL (k,IC) but with the Killing–Cartan-type metric tensor defined by anholonomy coefficients, i.e., $\rho_{\underline{\alpha}\underline{\beta}}(u^{\underline{\nu}})=W^{\underline{\tau}}_{\underline{\alpha}\underline{\gamma}}(u^{\underline{\alpha}})W^{\underline{\gamma}}_{\underline{\tau}\underline{\beta}}(u^{\underline{\alpha}})$. For complex space–times, we shall consider that the coefficients $N^{\underline{a}}_{\underline{i}}$ and $W^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}$ may be some complex valued functions of necessary smooth (in general, with complex variables) class. In result, the Killing–Cartan-type metric tensor $\rho_{\underline{\alpha}\underline{\beta}}$ can also be complex.

We rewrite (5) as

$$e_{\underline{\alpha}}e_{\underline{\beta}} - e_{\underline{\beta}}e_{\underline{\alpha}} = W^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}e_{\underline{\gamma}} \tag{15}$$

being equivalent to (13) and defining a noncommutative anholonomic structure (for simplicity, we use the same symbols $e_{\underline{\alpha}}$ as for some N-elongated partial derivatives, but with underlined indices). The analogs of derivation operators (12) are stated by using $W^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}$,

$$e_{\underline{\alpha}}q_{\underline{\beta}}(u^{\underline{\gamma}}) = ad[iq_{\underline{\alpha}}(u^{\underline{\gamma}})]q_{\underline{\beta}}(u^{\underline{\gamma}}) = i[q_{\underline{\alpha}}(u^{\underline{\gamma}})q_{\underline{\beta}}(u^{\underline{\gamma}})] = W^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}q_{\underline{\gamma}}. \tag{16}$$

The operators (16) define a linear space of anholonomic derivations satisfying the conditions (15), denoted Ader $M_k(\mathrm{IC}, u^{\underline{\alpha}})$, elongated by N connection and distinguished into irreducible h and v components, respectively, into $e_{\underline{i}}$ and $e_{\underline{b}}$, like $e_{\underline{\alpha}}=(e_{\underline{i}}=\partial_{\underline{i}}-N^{\underline{a}}_{\underline{i}}e_{\underline{a}}, e_{\underline{b}}=\partial_{\underline{b}})$. The space Ader $M_k(\mathrm{IC}, u^{\underline{\alpha}})$ is not a left module over the algebra $M_k(\mathrm{IC}, u^{\underline{\alpha}})$ which means that there is a substantial difference with respect to the usual commutative differential geometry where a vector field multiplied on the left by a function produces a new vector field.

The duals to operators (16), $e^{\underline{\mu}}$, found from $e^{\underline{\mu}}(e_{\underline{\alpha}})=\delta^{\underline{\mu}}_{\underline{\alpha}}I$, define a canonical basis of 1-forms $e^{\underline{\mu}}$ connected to the N-connection structure. By using these forms, we can span a left module over $M_k(\mathrm{IC}, u^{\underline{\alpha}})$ following $q_{\underline{\alpha}}e^{\underline{\mu}}(e_{\underline{\beta}})=q_{\underline{\alpha}}\delta^{\underline{\mu}}_{\underline{\beta}}I=q_{\underline{\alpha}}\delta^{\underline{\mu}}_{\underline{\beta}}$. For an arbitrary vector field

$$Y = Y^{\alpha}e_{\alpha} \to Y^{\underline{\alpha}}e_{\underline{\alpha}} = Y^{\underline{i}}e_{\underline{i}} + Y^{\underline{a}}e_{\underline{a}},$$

it is possible to define an exterior differential (in our case being N elongated), starting with the action on a function φ (equivalent, a 0-form),

$$\delta\varphi(Y) = Y\varphi = Y^{\underline{i}}\delta_{\underline{i}}\varphi + Y^{\underline{a}}\delta_{\underline{a}}\varphi$$

when

$$(\delta I)(e_{\underline{\alpha}}) = e_{\underline{\alpha}}I = ad(ie_{\underline{\alpha}})I = i[e_{\underline{\alpha}}, I] = 0, \quad \text{i.e.,}\ \delta I = 0,$$

and

$$\delta q_{\underline{\mu}}(e_{\underline{\alpha}}) = e_{\underline{\alpha}}(e_{\underline{\mu}}) = i[e_{\underline{\mu}}, e_{\underline{\alpha}}] = W^{\underline{\gamma}}_{\underline{\alpha}\underline{\mu}}e_{\underline{\gamma}}. \tag{17}$$

Considering the nondegenerated case, we can invert (17) as to obtain a similar expression with respect to $e^{\underline{\mu}}$,

$$\delta(e_{\underline{\alpha}}) = W^{\underline{\gamma}}_{\underline{\alpha}\underline{\mu}}e_{\underline{\gamma}}e^{\underline{\mu}}, \tag{18}$$

from which a very important property follows by using the Jacobi identity, $\delta^2=0$, resulting in a possibility to define a usual Grassman algebra of p-forms with the wedge product $\wedge$ stated as

$$e^{\underline{\mu}} \wedge e^{\underline{\nu}} = \tfrac{1}{2}(e^{\underline{\mu}} \otimes e^{\underline{\nu}} - e^{\underline{\nu}} \otimes e^{\underline{\mu}}).$$

We can write (18) as

$$\delta(e^{\underline{\alpha}}) = -\tfrac{1}{2}W^{\underline{\alpha}}_{\underline{\beta}\underline{\mu}}e^{\underline{\beta}}e^{\underline{\mu}}$$

and introduce the canonical 1-form $e=q_{\underline{\alpha}}e^{\underline{\alpha}}$ being coordinate independent and adapted to the N-connection structure and satisfying the condition $\delta e + e\wedge e = 0$.

In a standard manner, we can introduce the volume element induced by the canonical Cartan–Killing metric and the corresponding star operator $\star$ (Hodge duality). We define the volume element σ by using the complete antisymmetric tensor $\epsilon_{\underline{\alpha}_1\underline{\alpha}_2\cdots\underline{\alpha}_{k^2-1}}$ as

$$\sigma = \frac{1}{[(n'+m')^2-1]!}\epsilon_{\underline{\alpha}_1\underline{\alpha}_2\cdots\underline{\alpha}_{n'+m'}} e^{\underline{\alpha}_1}\wedge e^{\underline{\alpha}_2}\wedge\cdots\wedge e^{\underline{\alpha}_{n'+m'}}$$

to which any (k^2-1)-form is proportional $(k^2-1=n'+m')$. The integral of such a form is defined as the trace of the matrix coefficient in the form σ and the scalar product introduced for any couple of p-forms ϖ and ψ,

$$(\varpi,\psi) = \int (\varpi\wedge\star\psi).$$

Let us analyze how a noncommutative differential form calculus (induced by an anholonomic structure) can be developed and related to the Hamiltonian classical and quantum mechanics and Poisson bracket formalism.

For a p-form $\varpi^{[p]}$, the antiderivation i_Y with respect to a vector field $Y\in \mathrm{Ader}\, M_k(\mathrm{IC},u^{\underline{\alpha}})$ can be defined as in the usual formalism,

$$i_Y\varpi^{[p]}(X_1,X_2,\ldots,X_{p-1}) = \varpi^{[p]}(Y,X_1,X_2,\ldots,X_{p-1}),$$

where $X_1,X_2,\ldots,X_{p-1}\in \mathrm{Ader}\, M_k(\mathrm{IC},u^{\underline{\alpha}})$. By a straightforward calculus we can check that for a 2-form $\Xi=\delta e$ one holds

$$\delta\Xi = \delta^2 e = 0 \quad \text{and } L_Y\Xi = 0,$$

where the Lie derivative of forms is defined as $L_Y\varpi^{[p]}=(i_Y\ \delta+\delta\ i_Y)\varpi^{[p]}$.

The Hamiltonian vector field $H_{[\varphi]}$ of an element of algebra $\varphi\in M_k(\mathrm{IC},u^{\underline{\alpha}})$ is introduced following the equality $\Xi(H_{[\varphi]},Y)=Y\varphi$ which holds for any vector field. Then, we can define the Poisson bracket of two functions (in a quantum variant, observables) φ and χ, $\{\varphi,\chi\}=\Xi(H_{[\varphi]},H_{[\chi]})$ when

$$\{e_{\underline{\alpha}},e_{\underline{\beta}}\} = \Xi(e_{\underline{\alpha}},e_{\underline{\beta}}) = i[e_{\underline{\alpha}},e_{\underline{\beta}}].$$

This way, a simple version of noncommutative classical and quantum mechanics (up to a factor like the Planck constant, $\hbar$) is proposed, being derived by anholonomic relations for a certain class of exact off-diagonal solutions in commutative gravity.

We note that by using the Lie algebra SU (k,IC) we can elaborate an alternative noncommutative calculus related to the special unitary group SU_k in k dimensions when the anholonomic coefficients

$$W^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}} = p^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}} + w^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}} \tag{19}$$

induce a linear connection in the associated noncommutative space (noncommutative geometries with $p^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}$ being the structure constants of SU_k were investigated in Refs. 44–49 and 8).

Let us state the main formulas for such realization of anholonomic noncommutativity: In this case, the matrix basis $q_{\underline{\alpha}}$ consists from anti-Hermitian (and not Hermitian) matrices and the relations (11) are stated in a different form

$$q_{\underline{\alpha}}q_{\underline{\beta}} = -\frac{1}{k}\rho_{\underline{\alpha}\underline{\beta}}I + Z^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}q_{\underline{\gamma}} + \frac{1}{2}p^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}q_{\underline{\gamma}}, \tag{20}$$

where $\rho_{\underline{\alpha}\underline{\gamma}}Z^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}$ is trace free and symmetric in all pairs of indices and $\rho_{\underline{\alpha}\underline{\beta}}=p^{\underline{\tau}}_{\underline{\alpha}\underline{\gamma}}p^{\underline{\gamma}}_{\underline{\tau}\underline{\beta}}$. We consider dependencies of matrix coefficients on coordinates $u^{\underline{\alpha}}=(0,\ldots,u^{\alpha})$, i.e., we work in the space $M_k(\mathrm{IC},u^{\underline{\alpha}})$, and introduce the anholonomic derivations $e_{\underline{\alpha}}$,

$$e_{\underline{\alpha}}\varphi = [q_{\underline{\alpha}}, \varphi],$$

for arbitrary matrix function $\varphi \in M_k(\mathrm{IC}, u^{\underline{\alpha}})$ defining a basis for the Lie algebra of derivations $\mathrm{Der}[M_k(\mathrm{IC}, u^{\underline{\alpha}})]$ of $M_k(\mathrm{IC}, u^{\underline{\alpha}})$. In this case, we generalize (20) to

$$q_{\underline{\alpha}}(u^{\underline{\tau}})q_{\underline{\beta}}(u^{\underline{\tau}}) = -\frac{1}{k}\rho_{\underline{\alpha}\underline{\beta}}(u^{\underline{\tau}})I + Z^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}q_{\underline{\gamma}}(u^{\underline{\tau}}) + \frac{1}{2}W^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}(u^{\underline{\tau}})q_{\underline{\gamma}}(u^{\underline{\tau}}),$$

with an effective (of N-anholonomy origin) metric $\rho_{\underline{\alpha}\underline{\beta}}(u^{\underline{\lambda}}) = W^{\underline{\tau}}_{\underline{\alpha}\underline{\gamma}}(u^{\underline{\lambda}})W^{\underline{\gamma}}_{\underline{\tau}\underline{\beta}}(u^{\underline{\lambda}})$ being an anholonomic deformation of the Killing metric of SU_k.

In order to define the algebra of forms $\Omega^*[M_k(\mathrm{IC}, u^{\underline{\alpha}})]$ over $M_k(\mathrm{IC}, u^{\underline{\alpha}})$ we set $\Omega^0 = M_k$ and write

$$\delta\varphi(e_{\underline{\alpha}}) = e_{\underline{\alpha}}(\varphi)$$

for every matrix function $\varphi \in M_k(\mathrm{IC}, u^{\underline{\alpha}})$. As a particular case, we have

$$\delta q^{\underline{\alpha}}(e_{\underline{\beta}}) = -W^{\underline{\alpha}}_{\underline{\beta}\underline{\gamma}}q^{\underline{\gamma}},$$

where indices are raised and lowered with the anholonomically deformed metric $\rho_{\underline{\alpha}\underline{\beta}}(u^{\underline{\lambda}})$. This way, we can define the set of 1-forms $\Omega^1[M_k(\mathrm{IC}, u^{\underline{\alpha}})]$ to be the set of all elements of the form $\varphi\delta\beta$ with φ and β belonging to $M_k(\mathrm{IC}, u^{\underline{\alpha}})$. The set of all differential forms define a differential algebra $\Omega^*[M_k(\mathrm{IC}, u^{\underline{\alpha}})]$ with the couple $(\Omega^*[M_k(\mathrm{IC}, u^{\underline{\alpha}})], \delta)$ said to be a differential calculus in $M_k(\mathrm{IC}, u^{\underline{\alpha}})$ induced by the anholonomy of certain exact solutions (with off-diagonal metrics and associated N connections) in a gravity theory.

We can also find a set of generators $e^{\underline{\alpha}}$ of $\Omega^1[M_k(\mathrm{IC}, u^{\underline{\alpha}})]$, as a left/right module completely characterized by the duality equations $e^{\underline{\mu}}(e_{\underline{\alpha}}) = \delta^{\underline{\mu}}_{\underline{\alpha}}I$ and related to $\delta q^{\underline{\alpha}}$,

$$\delta q^{\underline{\alpha}} = W^{\underline{\alpha}}_{\underline{\beta}\underline{\gamma}}q^{\underline{\beta}}q^{\underline{\gamma}} \quad \text{and } e^{\underline{\mu}} = q_{\underline{\gamma}}q^{\underline{\mu}}\delta q^{\underline{\gamma}}.$$

Similarly to the formalism presented in details in Ref. 8, we can elaborate a differential calculus with derivations by introducing a linear torsionless connection

$$\mathcal{D}e^{\underline{\mu}} = -\omega^{\underline{\mu}}_{\ \underline{\gamma}} \otimes e^{\underline{\gamma}}$$

with the coefficients $\omega^{\underline{\mu}}_{\ \underline{\gamma}} = -\frac{1}{2}W^{\underline{\mu}}_{\ \underline{\gamma}\underline{\beta}}e^{\underline{\gamma}}$, resulting in the curvature 2-form,

$$\mathcal{R}^{\underline{\mu}}_{\ \underline{\gamma}} = \tfrac{1}{8}W^{\underline{\mu}}_{\ \underline{\gamma}\underline{\beta}}W^{\underline{\beta}}_{\ \underline{\alpha}\underline{\tau}}e^{\underline{\alpha}}e^{\underline{\tau}}.$$

So, even the anholonomy coefficients (6) of a solution, for instance, in string gravity, has nontrivial torsion coefficients, (9), the associated linear connection induced by the anholonomy coefficients in the associated noncommutative space of symmetries of the solution can be defined to be torsionless but to have a specific metrics and curvature being very different from the space–time curvature tensor. This is a surprising fact that commutative curved space–times provided with off-diagonal metrics and associated anholonomic frames and N connections may be characterized by a noncommutative shadow space with a Lie algebralike structure induced by the frame anholonomy. We argue that such metrics possess anholonomic noncommutative symmetries.

Finally, in this section, we conclude that for the holonomic solutions of the Einstein equations, with vanishing $w^{\underline{\gamma}}_{\underline{\alpha}\underline{\beta}}$, any associated noncommutative geometry or SL (k, IC), or SU_k type, decouples from the off-diagonal (anholonomic) gravitational background and transforms into a trivial one defined by the corresponding structure constants of the chosen Lie algebra. The anholonomic noncommutativity and the related differential geometry are induced by the anholonomy coefficients. All such structures reflect a specific type of symmetries of generic off-diagonal metrics and associated frame/N-connection structures. Considering exact solutions of the gravitational field equations, we can assert that we constructed a class of vacuum or nonvacuum metrics

possessing a specific noncommutative symmetry instead, for instance, of any usual Killing symmetry. In general, we can introduce a new classification of space–times following anholonomic noncommutative aglebraic properties of metrics and vielbein structures.

IV. BLACK ELLIPSOIDS WITH NONCOMMUTATIVE SYMMETRY

In this section, we shall analyze two classes of black ellipsoid solutions of the Einstein and (anti) de Sitter gravity (with arbitrary cosmological term) possessing hidden noncommutative symmetries. Such off-diagonal metrics will be constructed as to generate also exact solutions in complex gravity, with respect to complex N-elongated vielbeins (for simplicity, we shall consider the metric coefficients to be real with respect to such complex frames) which must be considered if any noncommutativity of coordinates with complex parameters and/or Wick-type rotations to Euclidean signatures are introduced. Such metrics are stable for certain configurations with complex off-diagonal terms (a rigorous proof may be performed by generalizing to complex spaces the results from Refs. 18 and 19).

A. Anholonomic complex deformations of the Schwarzschild solution

We consider a 4D off-diagonal metric ansatz [a complex generalization of (4), or equivalently, of (1) with complex frames (vielbeins) (2) and (3), see also the ansatz (C2) in Appendix C],

$$\delta s^2 = -\left(1-\frac{2m}{r}+\frac{\varepsilon}{r^2}\right)^{-1} dr^2 - r^2\gamma(r)d\theta^2 - \eta_3(r,\varphi)r^2\sin^2\theta\, d\varphi^2 + \eta_4(r,\varphi)\left(1-\frac{2m}{r}+\frac{\varepsilon}{r^2}\right)\delta t^2. \tag{21}$$

for usual local spherical and timelike coordinates $u=\{u^\alpha=(u^2=r,u^3=\theta,u^4=\varphi,u^5=t)\}$. In order to have compatibility with notations from Appendixes B and C, in this section, we consider that 4D greek indices run from 2 to 5 where the "polarization" functions $\eta_{3,4}$ are decomposed on a small parameter $\varepsilon, 0<|\varepsilon|\ll 1$,

$$\eta_4(r,\varphi) = \eta_{4[0]}(r,\varphi) + \varepsilon\lambda_4(r,\varphi) + \varepsilon^2\gamma_4(r,\varphi) + \cdots,$$

$$\eta_5(r,\varphi) = 1 + \varepsilon\lambda_5(r,\varphi) + \varepsilon^2\gamma_5(r,\varphi) + \cdots, \tag{22}$$

$\gamma(r)$ is a necessary smooth class function satisfying $\gamma(r)=1$ if $\varepsilon\to 0$ (it will be defined below) and

$$\delta t = dt + n_2(r,\varphi)dr \tag{23}$$

for $n_2=n_2^{[re]}+in_2^{[im]}\sim\varepsilon\cdots+\varepsilon^2$ terms being, in general, a complex valued function. In the particular case, when n_2 is real, i.e., when $n_2=n_2^{[re]}$ and $n_2^{[im]}=0$, the labels [re] and [im] being used, respectively, for the real and imaginary parts, the metric (21) was investigated in connection to the definition of static and nonstatic black ellipsoid configurations in Refs. 13–19, 30, and 31. The functions $\eta_{4,5}(r,\varphi)$ and $n_2(r,\varphi)$ will be found as the metric will define a solution of the vacuum Einstein equations (A6) [see Appendixes A–C for the explicit form of field equations (B3)–(B6) written for the 4D ansatz (C2)]. By introducing certain complex components of metric generated by small deformations of the spherical static symmetry on a small positive parameter ε (in the limits $\varepsilon\to 0$ and $\eta_{4,5}\to 1$ we have just the Schwarzschild solution for a point particle of mass m) we show here that it is possible to extend the results of Refs. 18 and 19 with respect to complex anholonomic structures (2) with a nontrivial component $N_2^5=n_2(r,\varphi)$ given by N elongation (23).

A more interesting class of exact solutions with an effective electric charge q induced from the complex/noncommutative/anholonomic gravity may be constructed if we state that the parameter of anholonomic deformations is of type $\varepsilon=(iq)^2$ for a real q and imaginary i. In this case the metric (21) will have real coefficients in the first order of ε, being very similar to those from the well-known Reissner–Nordström metric with, in our case effective, electric charge q. For convenience, in our further calculations we shall use both small parameters ε and/or q.

The set of η, λ and γ functions from (22) define arbitrary anholonomic (in our case with certain complexity) deformations of the Schwarzschild metric. As a particular case, we can consider the condition of vanishing of the metric coefficient before δt^2,

$$\eta_5(r,\varphi)\left(1-\frac{2m}{r}+\frac{\varepsilon}{r^2}\right)=1-\frac{2m}{r}+\varepsilon\frac{\Phi_5}{r^2}+\varepsilon^2\Theta_5=0,$$

$$\Phi_5=\lambda_4(r^2-2mr)+1, \tag{24}$$

$$\Theta_5=\gamma_4\left(1-\frac{2m}{r}\right)+\lambda_4,$$

defining a rotation ellipsoid configuration when

$$\lambda_5=\left(1-\frac{2m}{r}\right)^{-1}\left(\cos\varphi-\frac{1}{r^2}\right) \quad \text{and} \quad \gamma_5=-\lambda_5\left(1-\frac{2m}{r}\right)^{-1}.$$

Really, in the first order on ε, one follows a zero value for the coefficient before δt^2 if

$$r_+=\frac{2m}{1-q^2\cos\varphi}=2m[1+q^2\cos\varphi], \tag{25}$$

which is the equation for a three-dimensional (3D) ellipsoidlike hypersurface with a small eccentricity q^2. In general, we can consider arbitrary pairs of functions $\lambda_5(r,\theta,\varphi)$ and $\gamma_5(r,\theta,\varphi)$ [for φ-anisotropies, $\lambda_5(r,\varphi)$ and $\gamma_5(r,\varphi)$] which may be singular for some values of r, or on some hypersurfaces $r=r(\theta,\varphi)$ [$r=r(\varphi)$]. Such a configuration may define a static black ellipsoid object (a Schwarzschild-type static solution with the horizon slightly deformed to an ellipsoidal hypersurface[18,19]).

In general, not being restricted only to ellipsoidal configurations, the simplest way to analyze the condition of vanishing of the metric coefficient before δt^2 is to choose γ_5 and λ_5 as to have $\Theta=0$. In this case we find from (24),

$$r_\pm=m\pm m\sqrt{1-\varepsilon\frac{\Phi}{m^2}}\simeq m\left[1\pm\left(1+q^2\frac{\Phi_5}{2m^2}\right)\right], \tag{26}$$

where $\Phi_5(r,\varphi)$ is taken for $r=2m$.

Let us introduce a new radial coordinate

$$\xi=\int \mathrm{d}r\sqrt{\left|1-\frac{2m}{r}-\frac{q^2}{r^2}\right|} \tag{27}$$

and define

$$h_4=-\eta_4(\xi,\varphi)r^2(\xi)\sin^2\theta, \quad h_5=1-\frac{2m}{r}-q^2\frac{\Phi_5}{r^2}. \tag{28}$$

For $r=r(\xi)$ found as the inverse function after integration in (27), we can write the metric (21) as

$$\mathrm{d}s^2=-\mathrm{d}\xi^2-r^2(\xi)\gamma(\xi)\mathrm{d}\theta^2+h_4(\xi,\theta,\varphi)\delta\varphi^2+h_5(\xi,\theta,\varphi)\delta t^2,$$

$$\delta t=\mathrm{d}t+n_2(\xi,\varphi)\mathrm{d}\xi, \tag{29}$$

where the coefficient n_2 is taken to solve the Eq. (B6) and to satisfy the condition $\Omega^a_{jk}=0$ which states that we fix the canonical N-adapted connection (7) to coincide with the Levi–Civita connection (10), i.e., to consider a complexlike Einstein but not Einstein–Cartan theory, which to-

gether with the condition $r^2(\xi)\gamma(\xi)=\xi^2$ will be transformed into the usual Schwarzschild metric for $\varepsilon\to 0$.

Let us define the conditions when the coefficients of metric (21) define solutions of the vacuum Einstein equations (such solutions exists in the real case following Theorems 1–3 from Appendix B, in our case we only state a generalization for certain complex valued metric coefficients). For $g_2=-1$, $g_3=-r^2(\xi)\gamma(\xi)$ and arbitrary $h_4(\xi,\theta,\varphi)$ and $h_5(\xi,\theta)$, we get solutions of Eqs. (B3)–(B5). If h_5 depends on anisotropic variable φ, Eq. (B4) may be solved if

$$\sqrt{|\eta_4|}=\eta_0(\sqrt{|\eta_5|})^* \tag{30}$$

for $\eta_0=$const. Considering decompositions of type (22) we set $\eta_0=\eta/|\varepsilon|$, where the constant η is taken as to have $\sqrt{|\eta_3|}=1$ in the limits

$$\frac{(\sqrt{|\eta_4|})^*\to 0}{|\varepsilon|\to 0}\to\frac{1}{\eta}=\text{const}. \tag{31}$$

These conditions are satisfied if the functions $\eta_{4[0]}$, $\lambda_{4,5}$, and $\gamma_{4,5}$ are related via relations

$$\sqrt{|\eta_{4[0]}|}=\frac{\eta}{2}\lambda_5^*,\quad \lambda_5=\eta\sqrt{|\eta_{4[0]}|}\gamma_5^*$$

for arbitrary $\gamma_4(r,\varphi)$. In this paper we select only such solutions which satisfy the conditions (30) and (31) being a complex variant of the conditions (B16), see Appendix B. Similar classes of solutions were selected also in Refs. 18 and 19, for static black ellipsoid metrics for the (noncomplex) Einstein gravity with real ε parameter.

The next step is to construct the solution of (B6) which in general real form is (B18). To consider linear infinitesimal extensions on ε of the Schwarzschild metric, we may write the solution of (B6) as

$$n_2=\varepsilon\hat{n}_2(\xi,\varphi),$$

where

$$\hat{n}_2(\xi,\varphi)=n_{2[1]}(\xi)+n_{2[2]}(\xi)\int \mathrm{d}\varphi\, n_4(\xi,\varphi)/(\sqrt{|\eta_5(\xi,\varphi)|})^3,\quad \eta_5^*\neq 0=n_{2[1]}(\xi)+n_{2[2]}$$
$$\times(\xi)\int \mathrm{d}\varphi\,\eta_4(\xi,\varphi),\quad \eta_5^*=0=n_{2[1]}(\xi)+n_{2[2]}(\xi)\int \mathrm{d}\varphi/(\sqrt{|\eta_5(\xi,\varphi)|})^3,\quad \eta_4^*=0, \tag{32}$$

with the functions $n_{2[1,2]}(\xi)$ may be complex valued and must be stated by boundary conditions.

The data

$$g_1=-1,\quad g_2=-1,\quad g_3=-r^2(\xi)\gamma(\xi),$$

$$h_4=-\eta_4(\xi,\varphi)r^2(\xi)\sin^2\theta,\quad h_5=1-\frac{2m}{r}+\varepsilon\frac{\phi_5}{r^2}, \tag{33}$$

$$w_{2,3}=0,\quad n_2=\varepsilon\hat{n}_2(\xi,\varphi),\quad n_3=0,$$

for the metric (21) written in variables (ξ,θ,φ,t) define a class of solutions of the complex vacuum Einstein equations with nontrivial polarization function η_4 and extended on parameter ε up to the second order (the polarization functions being taken as to make zero the second order coefficients). Such solutions are generated by small complex deformations (in particular cases of rotation ellipsoid symmetry) of the Schwarzschild metric. It is possible to consider some particular

parametrizations of N coefficients resulting in Hermitian metrics and frames, or another type of complex configurations. Such constructions do not affect the stability properties of solutions elaborated in this paper.

We can relate our complex exact solutions (33) with some small deformations of the Schwarzschild metric to a Reissner–Nordström-type metric with the "electric" charge induced effectively from the anholonomic complex gravity, as well we can satisfy the asymptotically flat condition, if we choose such functions $n_{k[1,2]}(x^i)$ as $n_k \to 0$ for $\varepsilon \to 0$ and $\eta_4 \to 1$. These functions must also be selected as to vanish far away from the horizon, for instance, like $\sim 1/r^{1+\tau}$, $\tau > 0$, for long distances $r \to \infty$. We get a static metric with effective "electric" charge induced by a small, quadratic on ε, off-diagonal metric extension. Roughly, we can say that we have constructed a Reissner–Nordström-type world "living" in a slightly complexified frame which induced both an effective electric charge and certain polarizations of the metric coefficients via the functions $h_{4[0]}$, $\eta_{4,5}$, and n_5. Another very important property is that the deformed metric was stated to define a vacuum solution which differs substantially from the usual Reissner–Nördstrom metric being an exact static solution of the Einstein–Maxwell equations. For $\varepsilon \to 0$ and $h_{4[0]} \to 1$ and for $\gamma = 1$, the metric (21) transforms into the usual Schwarzschild metric. A solution with ellipsoid symmetry can be selected by a corresponding condition of vanishing of the coefficient before δt which defines an ellipsoidal hypersurfacelike for the Kerr metric, but in our case the metric is nonrotating.

B. Analytic extensions of ellipsoid complex metrics

In order to understand that the construction in this section of exact solution of vacuum complex gravity really defines black-hole-like objects we must analyze it's analytic extensions, horizon, and geodesic behavior and stability.

The metric (21) has a singular behavior for $r = r_{\pm}$, see (26) like the usual Reissner–Nördstrom one. Our aim is to prove that we have constructed a solution of the vacuum complex Einstein equations with a static "anisotropic" horizon being a small deformation on parameter ε of the Schwarzschild's solution horizon. We may analyze the anisotropic horizon's properties for some fixed "direction" given in a smooth vicinity of any values $\varphi = \varphi_0$ and $r_+ = r_+(\varphi_0)$. The final conclusions will be some general ones for arbitrary φ when the explicit values of coefficients will have a parametric dependence on angular coordinate φ. Of course, in order to avoid singularities induced by integration of Eq. (B6) we must choose such solutions (32) as the associated anholonomic frames with necessary smooth class, without singularities.

The metrics (21) and (29) are regular in the regions I ($\infty > r > r_+^{\Phi}$), II ($r_+^{\Phi} > r > r_-^{\Phi}$), and III ($r_-^{\Phi} > r > 0$). As in the Schwarzschild, Reissner–Nordström, and Kerr cases these singularities can be removed by introducing suitable coordinates and extending the manifold to obtain a maximal analytic extension.[50,51] We have similar regions as in the Reissner–Nördstrom space–time, but with just only one possibility $\varepsilon < 1$ instead of three relations for static electro-vacuum cases ($q^2 < m^2, q^2 = m^2, q^2 > m^2$; where q and m are correspondingly the electric charge and mass of the point particle in the Reissner–Nordström metric). This property holds for both types of anholonomic deformations, real or complex ones. So, we may consider the usual Penrose's diagrams as for a particular case of the Reissner–Nördstrom space–time but keeping in mind that such diagrams and horizons have an additional parametrization on an angular coordinate and that the frames have some complex coefficients.

We can construct the maximally extended manifold step by steps like in the Schwarzschild case (see details, for instance, in Ref. 52) by supposing that the complex valued coefficients of metrics and frame are of necessary smooth class as real and complex valued functions (for simplicity, we consider the simplest variant when the space–time is provided with a complex valued metric but admits covering by real coordinates which after certain coordinate transform may be also complex). We introduce a new coordinate

$$r^{\|} = \int \mathrm{d}r\left(1 - \frac{2m}{r} - \frac{q^2}{r^2}\right)^{-1}$$

for $r > r_+^1$ and find explicitly the coordinate

$$r^{\|} = r + \frac{(r_+^1)^2}{r_+^1 - r_-^1}\ln(r - r_+^1) - \frac{(r_-^1)^2}{r_+^1 - r_-^1}\ln(r - r_-^1), \tag{34}$$

where $r_\pm^1 = r_\pm^\Phi$ with $\Phi = 1$. If r is expressed as a function on ξ, than $r^{\|}$ can be also expressed as a function on ξ depending additionally on some parameters.

Defining the advanced and retarded coordinates, $v = t + r^{\|}$ and $w = t - r^{\|}$, with corresponding elongated differentials

$$\delta v = \delta t + \mathrm{d}r^{\|} \quad \text{and} \quad \delta w = \delta t - \mathrm{d}r^{\|}, \tag{35}$$

which are N-adapted frames like (2) but complex one, the metric (29) takes the form

$$\delta s^2 = -r^2(\xi)\gamma(\xi)\mathrm{d}\theta^2 - \eta_3(\xi,\varphi_0)r^2(\xi)\sin^2\theta\,\delta\varphi^2 + \left(1 - \frac{2m}{r(\xi)} - q^2\frac{\Phi_4(r,\varphi_0)}{r^2(\xi)}\right)\delta v\,\delta w,$$

where (in general, in nonexplicit form) $r(\xi)$ is a function of type $r(\xi) = r(r^{\|}) = r(v,w)$. Introducing new coordinates (v'', w'') by

$$v'' = \arctan\left[\exp\left(\frac{r_+^1 - r_-^1}{4(r_+^1)^2}v\right)\right], \quad w'' = \arctan\left[-\exp\left(\frac{-r_+^1 + r_-^1}{4(r_+^1)^2}w\right)\right] \tag{36}$$

and multiplying the last term on the conformal factor we obtain

$$\delta s^2 = -r^2\gamma(r)\mathrm{d}\theta^2 - \eta_4(r,\varphi_0)r^2\sin^2\theta\delta\varphi^2 + 64\frac{(r_+^1)^4}{(r_+^1 - r_-^1)^2}\left[1 - \frac{2m}{r(\xi)} - q^2\frac{\Phi_5(r,\varphi_0)}{r^2(\xi)}\right]\delta v''\,\delta w'', \tag{37}$$

where r is defined implicitly by

$$\tan v''\tan w'' = -\exp\left[\frac{r_+^1 - r_-^1}{2(r_+^1)^2}r\right]\sqrt{\frac{r - r_+^1}{(r - r_-^1)\chi}}, \quad \chi = \left(\frac{r_+^1}{r_-^1}\right)^2, \tag{38}$$

where the functions tan and exp should be considered as the complex functions. As particular cases, we may choose $\eta_5(r,\varphi)$ as the condition of vanishing of the metric coefficient before $\delta v''\,\delta w''$ will describe a horizon parametrized by a resolution ellipsoid hypersurface.

The metric (37) is very similar to that analyzed in Refs. 18 and 19 but the coordinate transforms defined by (35)–(38) involve complex coordinate transforms, so $\delta v''\,\delta w''$ is a product defined by complexified N-adapted frames.

The maximal extension of the Schwarzschild metric deformed by a small parameter ε, i.e., the extension of the metric (21), is defined by taking (37) as the metric on the maximal manifold (which for corresponding coordinate transforms can be considered as a real one but with complex valued coefficients of the metric and moving frames) on which this metric is of smooth class C^2. The Penrose diagram of this static but locally anisotropic space–time, for any fixed angular value φ_0 is similar to the Reissner–Nördstrom solution, for the case $q^2 \to \varepsilon$ and $q^2 < m^2$ (see, for instance, Ref. 52). There are an infinite number of asymptotically flat regions of type I, connected by intermediate regions II and III, where there is still an irremovable singularity at $r = 0$ for every region III. We may travel from a region I to another one by passing through the wormholes made by anisotropic deformations (ellipsoid off diagonality of metrics, or anholonomy) like in the Reissner–Nordström universe because $\sqrt{\varepsilon} \sim q$ may model an effective electric charge. One cannot turn back in such travel because the complex frames "do not allow us."

It should be noted that the metric (37) is analytic everywhere except at $r=r_{-}^{1}$ (we must use the term analytic as real functions for the metric coefficients in the lower approximations on ε and analytic as complex functions for the higher approximations of the metric coefficients and for all terms contained in the vielbein coefficients). We may eliminate this coordinate degeneration by introducing other new complex coordinates

$$v'''=\arctan\left[\exp\left(\frac{r_{+}^{1}-r_{-}^{1}}{2n_0(r_{+}^{1})^2}v\right)\right],\quad w'''=\arctan\left[-\exp\left(\frac{-r_{+}^{1}+r_{-}^{1}}{2n_0(r_{+}^{1})^2}w\right)\right],$$

where the integer $n_0\geqslant(r_{+}^{1})^2/(r_{-}^{1})^2$ and complex functions. In these coordinates, the metric is (in general, complex) analytic everywhere except at $r=r_{+}^{1}$ where it is degenerate. This way the space–time manifold can be covered by an analytic atlas by using coordinate carts defined by (v'',w'',θ,φ) and $(v''',w''',\theta,\varphi)$. We also note that the analytic extensions of the deformed metrics were performed with respect to anholonomic complex frames which distinguish such constructions from those dealing only with holonomic and/or real coordinates, like for the usual Reissner–Nördstrom and Kerr metrics.

A more rigorous analysis of the metric (21) should involve a computation of its curvature and investigation of singularity properties. We omit here this cumbersome calculus by emphasizing that anholonomic deformations of the Schwarzschild solution defined by a small real or complex parameter ε cannot remove the bulk singularity of such space–times; there are deformations of the horizon, frames, and specific polarizations of constants.

The metric (21) and its analytic extensions do not possess Killing symmetries being deformed by anholonomic transforms. Nevertheless, we can associate to such solutions certain noncommutative symmetries following the procedure described in Sec. III. Taking the data (33) and formulas (6), we compute the corresponding nontrivial anholonomy coefficients

$$w_{42}^{[N]5}=-w_{24}^{[N]5}=\partial n_2(\xi,\varphi)/\partial\varphi=n_2^{*}(\xi,\varphi) \tag{39}$$

with n_2 defined by (32). Our vacuum solution is for 4D, so for $n+m=4$, the condition $k^2-1=n+m$ cannot be satisfied in integer numbers. We may trivially extend the dimensions like $n'=6$ and $m'=m=2$ and for $k=3$ to consider the Lie group SL (3, IC) noncommutativity with corresponding values of $Q_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}$ and structure constants $f_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}$, see (11). An extension $w_{\alpha\beta}^{[N]\gamma}\to W_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}$ may be performed by stating the N-deformed "structure" constants (14), $W_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}=f_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}+w_{\underline{\alpha}\underline{\beta}}^{[N]\underline{\gamma}}$, with only two nontrivial values of $w_{\underline{\alpha}\underline{\beta}}^{[N]\underline{\gamma}}$ given by (39).

The associated anholonomic noncommutative symmetries of the black ellipsoid solutions can be alternatively defined as in the trivial anholonomy limit they will result in a certain noncommutativity for the Lie group SU_3. In this case, we must consider a N deformation of the group structure constants $p_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}$, like in (19), $W_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}=p_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}+w_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}$. This variant of deformations can be related directly with the "de Sitter nonlinear gauge gravity model of (non)commutative gravity"[6] and the $SU_k[SO(k)]$ models of noncommutative gravity[7] by considering complex vielbeins.

C. Black ellipsoids and the cosmological constant

We can generalize the vacuum equations to the gravity with cosmological constant λ,

$$R_{\mu'\nu'}=\lambda g_{\mu'\nu'}, \tag{40}$$

where $R_{\mu'\nu'}$ is the Ricci tensor (A3), in general with anholonomic variables and the indices take values $i',k'=1,2$ and $a',b'=3,4$.

For an ansatz of type (C5),

$$\delta s^2=g_1(\mathrm{d}x^1)^2+g_2(\mathrm{d}x^2)^2+h_3(x^{i'},y^3)(\delta y^3)^2+h_4(x^{i'},y^3)(\delta y^4)^2,$$

$$\delta y^3 = \mathrm{d}y^3 + w_{i'}(x^{k'}, y^3)\mathrm{d}x^{i'}, \quad \delta y^4 = \mathrm{d}y^4 + n_{i'}(x^{k'}, y^3)\mathrm{d}x^{i'}, \tag{41}$$

the Einstein equations (40) are written [see Refs. 30, 31, and 13–19 for details on computation; this is a particular case of source of type (C14), see Appendix B]

$$R_1^1 = R_2^2 = -\frac{1}{2g_1g_2}\left[\ddot{g_2} - \frac{\dot{g_1}\dot{g_2}}{2g_1} - \frac{(\dot{g_2})^2}{2g_2} + g_1'' - \frac{g_1'g_2'}{2g_2} - \frac{(g_1')^2}{2g_1}\right] = \lambda, \tag{42}$$

$$R_3^3 = R_4^4 = -\frac{\beta}{2h_3h_4} = \lambda, \tag{43}$$

$$R_{3i'} = -w_{i'}\frac{\beta}{2h_4} - \frac{\alpha_{i'}}{2h_4} = 0, \tag{44}$$

$$R_{4i'} = -\frac{h_4}{3h_3}[n_{i'}^{***} + \gamma n_{i'}^{*}] = 0. \tag{45}$$

The coefficients of Eqs. (42)–(45) are given by

$$\alpha_i = \partial_i h_4^* - h_4^* \partial_i \ln\sqrt{|h_3h_4|}, \quad \beta = h_4^{***} - h_4^*[\ln\sqrt{|h_3h_4|}]^*, \quad \gamma = \frac{3h_4^*}{2h_4} - \frac{h_3^*}{h_3}. \tag{46}$$

The various partial derivatives are denoted as $a^{\cdot} = \partial a/\partial x^1$, $a' = \partial a/\partial x^2$, $a^* = \partial a/\partial y^3$. This system of equations can be solved by choosing one of the ansatz functions [e.g., $g_1(x^i)$ or $g_2(x^i)$] and one of the ansatz functions [e.g., $h_3(x^i, y^3)$ or $h_4(x^i, y^3)$] to take some arbitrary, but physically interesting form (see Theorem 3 in Appendix B). Then, the other ansatz functions can be analytically determined up to an integration in terms of this choice. In this way we can generate a loss of different solutions, but we impose the condition that the initial, arbitrary choice of the ansatz functions is "physically interesting" which means that one wants to make this original choice so that the generated final solution yields a well-behaved metric.

In Ref. 19 (see also the preceding section), we proved that for

$$g_1 = -1, \quad g_2 = r^2(\xi)q(\xi),$$

$$h_3 = -\eta_3(\xi,\varphi)r^2(\xi)\sin^2\theta, \tag{47}$$

$$h_4 = n_4(\xi,\varphi)h_{4[0]}(\xi) = 1 - \frac{2\mu}{r} + \varepsilon\frac{\Phi_4(\xi,\varphi)}{2\mu^2},$$

with coordinates $x^1 = \xi = \int \mathrm{d}r\sqrt{1 - 2m/r + \varepsilon/r^2}$, $x^2 = \theta$, $y^3 = \varphi$, $y^4 = t$ [the (r, θ, φ) being usual radial coordinates], the ansatz (41) is a vacuum solution with $\lambda = 0$ of the equations (40) which defines a black ellipsoid with mass μ, eccentricity ε, and gravitational polarizations $q(\xi)$, $\eta_3(\xi,\varphi)$, and $\Phi_4(\xi,\varphi)$. Such black holes are certain deformations of the Schawarzschild metrics to static configurations with ellipsoidal horizons which is possible if generic off-diagonal metrics and anholonomic frames are considered. A complex generalization of this solution is given by the values (33). In this section we show that the data (47) and/or (33) can be extended as to generate exact black ellipsoid solutions, defined correspondingly with respect to real or complex N frames, with nontrivial cosmological constant $\lambda = 1/4$ which can be imbedded in string theory.

At the first step, we find a class of solutions with $g_1 = -1$ and $g_2 = g_2(\xi)$ solving Eq. (42), which under such parametrizations transforms to

$$\ddot{g_2} - \frac{(\dot{g_2})^2}{2g_2} = 2g_2\lambda.$$

With respect to the variable $Z=(g_2)^2$ this equation is written as

$$\ddot{Z} + 2\lambda Z = 0$$

which can be integrated in explicit form, $Z=Z_{[0]}\sin(\sqrt{2\lambda}\xi+\xi_{[0]})$, for some constants $Z_{[0]}$ and $\xi_{[0]}$ which means that

$$g_2 = -Z^2_{[0]}\sin^2(\sqrt{2\lambda}\xi+\xi_{[0]}) \tag{48}$$

parametrize in real string gravity a class of solution of (42) for the signature $(-,-,-,+)$. For $\lambda\to 0$ we can approximate $g_2=r^2(\xi)$, $q(\xi)=-\xi^2$, and $Z^2_{[0]}=1$ which has compatibility with the data (47). The solution (48) with cosmological constant (of string or nonstring origin) induces oscillations in the "horizontal" part of the metric written with respect to *N*-adapted frames.

The next step is to solve Eq. (43),

$$h_4^{**} - h_4^{*}[\ln\sqrt{|h_3h_4|}]^{*} = -2\lambda h_3h_4.$$

For $\lambda=0$ a class of solution is given by any $\hat{h}_3$ and $\hat{h}_4$ related as

$$\hat{h}_3 = \eta_0[(\sqrt{|\hat{h}_4|})^{*}]^2$$

for a constant η_0 chosen to be negative in order to generate the signature $(-,-,-,+)$. For nontrivial λ, we may search the solution as

$$h_3 = \hat{h}_3(\xi,\varphi)f_3(\xi,\varphi) \quad \text{and } h_4 = \hat{h}_4(\xi,\varphi), \tag{49}$$

which solves (43) if $f_3=1$ for $\lambda=0$ and

$$f_3 = \frac{1}{4\lambda}\left[\int \frac{\hat{h}_3\hat{h}_4}{\hat{h}_4^{*}}d\varphi\right]^{-1} \quad \text{for } \lambda\neq 0.$$

Now it is easy to write down the solutions of equations (44) (being a linear equation for $w_{i'}$) and (45) (after two integrations of $n_{i'}$ on φ),

$$w_{i'} = \varepsilon\hat{w}_{i'} = -\alpha_{i'}/\beta, \tag{50}$$

where $\alpha_{i'}$ and β are computed by setting (49) into corresponding values from (46) (we choose the initial conditions as $w_{i'}\to 0$ for $\varepsilon\to 0$) and

$$n_1 = \varepsilon\hat{n}_1(\xi,\varphi),$$

where the coefficients

$$\hat{n}_1(\xi,\varphi) = n_{1[1]}(\xi) + n_{1[2]}(\xi)\int d\varphi\ \eta_3(\xi,\varphi)/(\sqrt{|\eta_4(\xi,\varphi)|})^3, \quad \eta_4^{*}\neq 0 = n_{1[1]}(\xi) + n_{1[2]}$$
$$\times(\xi)\int d\varphi\ \eta_3(\xi,\varphi), \quad \eta_4^{*}=0 = n_{1[1]}(\xi) + n_{1[2]}(\xi)\int d\varphi/(\sqrt{|\eta_4(\xi,\varphi)|})^3, \quad \eta_3^{*}=0, \tag{51}$$

being stated to be real or complex valued for a corresponding model of real or complex gravity, with the functions $n_{k[1,2]}(\xi)$ to be stated by boundary conditions.

We conclude that the set of data $g_1=-1$, with nontrivial $g_2(\xi)$, h_3, h_4, $w_{i'}$, and n_1 stated, respectively, by (48)–(51) we can define a black ellipsoid solution with explicit dependence on

cosmological constant λ, i.e., a metric (41). The stability of such static black ellipsoids in (anti) de Sitter space can be proven exactly as it was done in Ref. 19 for the real case vanishing cosmological constant.

The analytic extension of black ellipsoid solutions with cosmological constant can be performed similarly as in the preceding section when for the real/complex solutions we are dealing with real/complex values of $\hat{n}_1(\xi,\varphi)$ defining some components of N-adapted frames. We note that the solution from string theory contains a frame induced torsion with the components (9) (in general, with complex coefficients) computed for nontrivial $N^3_{i'}=-\alpha_{i'}/\beta$ [see (50)] and $N^4_1=\varepsilon\hat{n}_1(\xi,\varphi)$ [see (51)]. This is an explicit example illustrating that the anholonomic frame method is also powerful for generating exact solutions in models of gravity with nontrivial torsion, induced by anholonomic frame transforms. For such solutions we may elaborate corresponding analytic extension and Penrose diagram formalisms if the constructions are considered with respect to N-elongated vielbeins.

Finally, we analyze the structure of noncommutative symmetries associated to the (anti) de Sitter black ellipsoid solutions. The metric (41) with real and/or complex coefficients defining the corresponding solutions and its analytic extensions also do not possess Killing symmetries being deformed by anholonomic transforms. For this solution, we can associate certain noncommutative symmetries following the same procedure as for the Einstein real/complex gravity but with additional nontrivial coefficients of anholonomy and even with nonvanishing coefficients of the nonlinear connection curvature, $\Omega^3_{12}=\delta_1N^3_2-\delta_2N^3_1$. Taking the data (50) and (51) and formulas (6), we compute the corresponding nontrivial anholonomy coefficients

$$w^{[N]4}_{31}=-w^{[N]4}_{13}=\partial n_1(\xi,\varphi)/\partial\varphi=n^*_2(\xi,\varphi),$$
$$w^{[N]4}_{12}=-w^{[N]4}_{21}=\delta_1(\alpha_2/\beta)-\delta_2(\alpha_1/\beta) \tag{52}$$

for $\delta_1=\partial/\partial\xi-w_1\partial/\partial\varphi$ and $\delta_2=\partial/\partial\theta-w_2\partial/\partial\varphi$, with n_1 defined by (32) and $\alpha_{1,2}$ and β computed by using the formula (46) for the solutions (49). Our exact solution, with nontrivial cosmological constant, is for 4D, like in the preceding section. So, for $n+m=4$, the condition $k^2-1=n+m$ cannot be satisfied by any integer numbers. We may similarly trivially extend the dimensions like $n'=6$ and $m'=m=2$ and for $k=3$ to consider the Lie group SL (3, IC) noncommutativity with corresponding values of $Q^{\gamma}_{\underline{\alpha}\underline{\beta}}$ and structure constants $f^{\gamma}_{\underline{\alpha}\underline{\beta}}$, see (11). An extension $w^{[N]\gamma}_{\alpha\beta}\to W^{\gamma}_{\underline{\alpha}\underline{\beta}}$ may be performed by stating the N-deformed "structure" constants (14), $W^{\gamma}_{\underline{\alpha}\underline{\beta}}=f^{\gamma}_{\underline{\alpha}\underline{\beta}}+w^{[N]\gamma}_{\underline{\alpha}\underline{\beta}}$, with nontrivial values of $w^{[N]\gamma}_{\underline{\alpha}\underline{\beta}}$ given by (52). In a similar form, we can consider anholonomic deformations of the SU_k structure constants, see (19).

V. NONCOMMUTATIVE COMPLEX WORMHOLES

The black ellipsoid solutions defined by real and certain complex metrics elaborated in the preceding section were for the 4D Einstein gravity, in general, with nontrivial cosmological constant. In this section we construct and analyze an exact 5D solution which can be also complexified by using complex anholonomic transforms as well they can be provided with associated noncommutative structure. For such configurations we can apply directly the formulas stated in Appendix B. The metric ansatz (1) is taken in the form

$$\delta s^2=g_1(\mathrm{d}x^1)^2+g_2(\mathrm{d}x^2)^2+g_3(\mathrm{d}x^3)^2+h_4(\delta y^4)^2+h_5(\delta y^5)^2,$$
$$\delta y^4=\mathrm{d}y^4+w_{k'}(x^{i'},v)\mathrm{d}x^{k'},\quad \delta y^5=\mathrm{d}y^5+n_{k'}(x^{i'},v)\mathrm{d}x^{k'},\quad i',k'=1,2,3, \tag{53}$$

where

$$g_1=1,\quad g_2=g_2(r),\quad g_3=-a(r),$$

$$h_4 = \hat{h}_4 = \hat{\eta}_4(r,\theta,\varphi)h_{4[0]}(r), \quad h_5 = \hat{h}_5 = \hat{\eta}_5(r,\theta,\varphi)h_{5[0]}(r,\theta) \tag{54}$$

for the parametrization of coordinate of type

$$x^1 = t, \quad x^2 = r, \quad x^3 = \theta, \quad y^4 = v = \varphi, \quad y^5 = p = \chi, \tag{55}$$

where t is the time coordinate, (r,θ,φ) are spherical coordinates, χ is the fifth coordinate; φ is the anholonomic coordinate; for this ansatz there is not considered the dependence of metric coefficients on the second anholonomic coordinate χ. Following similar approximations as in Sec. IV C for deriving the equations (40), we can write the gravity equations with cosmological constant as a system of 5D Einstein equations with constant diagonal source (the related details on computing the Ricci tensors with anholonomic variables and possible sources are given in Appendix B):

$$\frac{1}{2}R_1^1 = R_2^2 = R_3^3 = -\frac{1}{2g_2g_3}\left[\ddot{g_3} - \frac{\dot{g_2}\dot{g_3}}{2g_2} - \frac{(\dot{g_3})^2}{2g_3} + g_2'' - \frac{g_2'g_3'}{2g_3} - \frac{(g_2')^2}{2g_2}\right] = \lambda, \tag{56}$$

$$R_4^4 = R_5^5 = -\frac{\beta}{2h_4h_5} = \lambda, \tag{57}$$

$$R_{4i'} = -w_{i'}\frac{\beta}{2h_5} - \frac{\alpha_{i'}}{2h_5} = 0, \tag{58}$$

$$R_{5i'} = -\frac{h_5}{2h_4}[n_{i'}^{**} + \gamma n_{i'}^{*}] = 0, \tag{59}$$

where $i' = 1,2,3$. The coefficients of the equations are given by

$$\alpha_{i'} = \partial_i h_5^* - h_5^*\partial_{i'}\ln\sqrt{|h_4h_5|}, \quad \beta = h_5^{**} - h_5^*[\ln\sqrt{|h_4h_5|}]^*, \quad \gamma = \frac{3h_5^*}{2h_5} - \frac{h_4^*}{h_4}. \tag{60}$$

The various partial derivatives are denoted as $a^{\cdot} = \partial a/\partial x^2$, $a' = \partial a/\partial x^3$, $a^* = \partial a/\partial v$.

The system of equations (56)–(59) can be solved by choosing one of the ansatz functions [e.g., $h_4(x^{i'},v)$ or $h_5(x^{i'},v)$] to take some arbitrary, but physically interesting form. Then the other ansatz functions can be analytically determined up to an integration in terms of this choice. In this way one can generate many solutions, but the requirement that the initial, arbitrary choice of the ansatz functions be "physically interesting" means that one wants to make this original choice so that the final solution generated in this way yield a well-behaved solution. To satisfy this requirement we start from well-known solutions of Einstein's equations and then use the above procedure to deform this solution in a number of ways as to include it in a string theory, for instance, as a gravity model with cosmological constant.

The data

$$g_1 = 1, \quad \hat{g}_2 = -1, \quad g_3 = -a(r),$$

$$h_{4[0]}(r) = -r_0^2 e^{2\psi(r)}, \quad \eta_4 = 1/\kappa_r^2(r,\theta,\varphi), \quad h_{5[0]} = -a(r)\sin^2\theta, \quad \eta_5 = 1,$$

$$w_1 = \hat{w}_1 = w(r), \quad w_2 = \hat{w}_2 = 0, \quad w_3 = \hat{w}_3 = n\cos\theta/\kappa_n^2(r,\theta,\varphi),$$

$$n_1 = \hat{n}_1 = 0, \quad n_{2,3} = \hat{n}_{2,3} = n_{2,3[1]}(r,\theta) \int \ln|\kappa_r^2(r,\theta,\varphi)|\mathrm{d}\varphi \tag{61}$$

for some constants r_0 and n and arbitrary functions $a(r)$, $\psi(r)$ and arbitrary vacuum gravitational polarizations $\kappa_r(r,\theta,\varphi)$ and $\kappa_n(r,\theta,\varphi)$ define an exact vacuum 5D solution of Kaluza–Klein gravity[14] describing a locally anisotropic wormhole with elliptic gravitational vacuum polarization of charges,

$$\frac{q_0^2}{4a(0)\kappa_r^2} + \frac{Q_0^2}{4a(0)\kappa_n^2} = 1,$$

where $q_0 = 2\sqrt{a(0)}\sin\alpha_0$ and $Q_0 = 2\sqrt{a(0)}\cos\alpha_0$ are, respectively, the electric and magnetic charges and $2\sqrt{a(0)}\kappa_r$ and $2\sqrt{a(0)}\kappa_n$ are ellipse's axes.

The first aim in this section is to prove that following the ansatz (53) we can construct locally anisotropic wormhole metrics in (anti) de Sitter gravity, in general complexified by a certain class of anholonomic frame transforms as solutions of the system of Eqs. (56)–(59) with redefined coordinates as in (55). For simplicity, we select such solutions when only the coefficients n_i can be real or complex valued functions. Having the vacuum data (61), we may try to generalize the solution for a nontrivial cosmological constant by supposing that the new solutions may be represented as

$$h_4 = \hat{h}_4(x^{i'},v)q_4(x^{i'},v) \quad \text{and } h_5 = \hat{h}_5(x^{i'},v), \tag{62}$$

with $\hat{h}_{4,5}$ taken as in (54) which solves (57) if $q_4 = 1$ for $\lambda = 0$ and

$$q_4 = \frac{1}{4\lambda}\left[\int \frac{\hat{h}_5(r,\theta,\varphi)\hat{h}_4(r,\theta,\varphi)}{\hat{h}_5^*(r,\theta,\varphi)}\mathrm{d}\varphi\right]^{-1} \quad \text{for } \lambda \neq 0.$$

This q_4 can be considered as an additional polarization to η_4 induced by the cosmological constant λ. We state $g_2 = -1$ but

$$g_3 = -\sin^2(\sqrt{2\lambda}\theta + \xi_{[0]}),$$

defining a solution of (56) with signature $(+,-,-,-,-)$ being different from the solution (18). A nontrivial q_4 results in modification of coefficients (60),

$$\alpha_{i'} = \hat{\alpha}_{i'} + \alpha_{i'}^{[q]}, \quad \beta = \hat{\beta} + \beta^{[q]}, \quad \gamma = \hat{\gamma} + \gamma^{[q]},$$

$$\hat{\alpha}_{i'} = \partial_i \hat{h}_5^* - \hat{h}_5^* \partial_{i'} \ln\sqrt{|\hat{h}_4\hat{h}_5|}, \quad \hat{\beta} = \hat{h}_5^{**} - \hat{h}_5^*[\ln\sqrt{|\hat{h}_4\hat{h}_5|}]^*, \quad \hat{\gamma} = \frac{3\hat{h}_5^*}{2\hat{h}_5} - \frac{\hat{h}_4^*}{\hat{h}_4},$$

$$\alpha_{i'}^{[q]} = -h_5^* \partial_{i'} \ln\sqrt{|q_4|}, \quad \beta^{[q]} = -h_5^*[\ln\sqrt{|q_4|}]^*, \quad \gamma^{[q]} = -\frac{q_4^*}{q_4},$$

which follow formulas (58) and (59) result in additional terms to the *N*-connection coefficients, i.e.,

$$w_{i'} = \hat{w}_{i'} + w_{i'}^{[q]} \quad \text{and } n_{i'} = \hat{n}_{i'} + n_{i'}^{[q]}, \tag{63}$$

with $w_{i'}^{[q]}$ and $n_{i'}^{[q]}$ computed by using, respectively, $\alpha_{i'}^{[q]}$, $\beta^{[q]}$, and $\gamma^{[q]}$.

The simplest way to generate complex solutions is to consider that $\hat{n}_{i'}$ from the data (61) and (63) can be complex valued functions, for instance, with complex valued coefficients $n_{2,3[1]} \times (r,\theta)$ resulting from integration. In this case the metric (53) has real coefficients describing

wormhole solutions with polarized constants but such metric coefficients are defined with respect to anholonomic frames being N elongated by some real and complex functions.

Having nontrivial values of (63), we can associate certain noncommutative symmetries following the same procedure as for real/complex black ellipsoids. The wormhole cases are described by a more general set of nontrivial coefficients of anholonomy $w_{\underline{\alpha}\underline{\beta}}^{[N]\underline{\gamma}}$, computed by using formulas (6) and (15) (for simplicity, we omit such cumbersome expressions), and a nontrivial nonlinear connection curvature, in our case $\Omega_{i'k'}^{a}=\delta_{i'}N_{k'}^{a}-\delta_{k'}N_{i'}^{a}$ with $N_{k'}^{4}=w_{k'}$ and $N_{k'}^{5}=n_{k'}$. Such coefficients depend on variables (r,θ,φ), in general, being complex valued functions. We must extend trivially the dimensions. We must extend the dimensions like $n=5\to n'=6$ and $m'=m=2$ and for $k=3$ if we want to associate a Lie group SL (3, IC) like noncommutativity with the corresponding values of $Q_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}$ and structure constants $f_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}$, see (11). An extension $w_{\alpha\beta}^{[N]\gamma}\to W_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}$ may be similarly performed by introducing N-deformed "structure" constants (14), $W_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}=f_{\underline{\alpha}\underline{\beta}}^{\underline{\gamma}}+w_{\underline{\alpha}\underline{\beta}}^{[N]\underline{\gamma}}$, with nontrivial values of $w_{\underline{\alpha}\underline{\beta}}^{[N]\underline{\gamma}}$ defined by (63).

VI. NONCOMMUTATIVE SYMMETRIES AND GAUGE GRAVITY

We start with discussing the results of Refs. 6 and 7 concerning noncommutative gauge models of gravity.

The basic idea of Ref. 6 was to use a geometrical result[21,22] that the Einstein gravity can be equivalently represented as a gauge theory with a specific connection in the bundle of affine frames. Such gauge theories are with nonsemisimple structure gauge groups, i.e., with degenerated metrics in the total spaces. Using an auxiliary symmetric form for the typical fiber, any such model can be transformed into a variational one. There is an alternative way to construct geometrically a usual Yang–Mills theory by applying a corresponding set of absolute derivations and dualities defined by the Hodge operator. For both such approaches, there is a projection formalism reducing the geometric field equations on the base space to be exactly the Einstein equations from the general relativity theory.

For more general purposes, it was suggested to consider also extensions to a nonlinear realization with the (anti) de Sitter gauge structural group.[23] The constructions with nonlinear group realizations are very important because they prescribe a consistent approach of distinguishing the frame indices and coordinate indices subjected to different rules of transformation. This approach to gauge gravity (of course, after a corresponding generalizations of the Seiberg–Witten map) may include, in general, quadratic on curvature and torsion terms (as it is stated in Ref. 6) being correlated to the results on gravity on noncommutative D-branes.[53] At the first step, it was very important to suggest an idea how to include the general relativity into a gauge model being more explicitly developed in noncommutative form[1,2,45] (see recent developments in Refs. 54–60).

A. Nonlinear gauge models for the (anti) de Sitter group

There were elaborated some alternative approaches to the noncommutative gauge gravity models in Ref. 7 [by deforming the Einstein gravity based on gauging the commutative inhomogeneous Lorentz group ISO (3,1) using the Seiberg–Witten map] and 60 [by considering some simplest noncommutative deformations of the gauge theory U (2,2) and of the Lorentz algebra SO (1,3)]. Such theories reduce to the general relativity if certain constraints and brocking symmetries are imposed. Perhaps, only some experimental data would emphasize a priority of a theory of noncommutative gravity with a proper prescription how the vielbeins and connection from "commutative" gravity must be combined into components of a linear/nonlinear realizations of a noncommutative gauge potentials defined by corresponding Seiberg–Witten maps. At the present state of elaboration of noncommutative geometry and physics, we have to analyze the physical consequences of different classes of models of noncommutative gravity.

We introduce vielbein decompositions of (in general) complex metrics (4),

$$\hat{g}_{\alpha\beta}(u)=e_{\alpha}{}^{\alpha'}(u)e_{\beta}{}^{\beta'}(u)\,\eta_{\alpha'\beta'},$$

$$e_{\alpha}^{\ \alpha'}e^{\beta}_{\ \alpha'}=\delta_{\alpha}^{\beta} \quad \text{and } e_{\alpha}^{\ \alpha'}e^{\alpha}_{\ \beta'}=\delta_{\beta'}^{\alpha'},$$

where $\eta_{\alpha'\beta'}$ is a constant diagonal matrix [for real space–times we can consider it as the flat Minkowski metric, for instance, $\eta_{\alpha'\beta'}=\mathrm{diag}(-1,+1,\ldots,+1)$] and δ_{α}^{β} and $\delta_{\beta'}^{\alpha'}$ are Kronecker's delta symbols. The vielbiens with an associated N-connection structure $N_i^a(x^j,y^a)$, being real or complex valued functions, have a special paramtrization

$$e_{\alpha}^{\ \alpha'}(u)=\begin{bmatrix} e_i^{\ i'}(x^j) & N_i^c(x^j,y^a)e_c^{\ b'}(x^j,y^a) \\ 0 & e_e^{\ e'}(x^j,y^a) \end{bmatrix} \tag{64}$$

and

$$e^{\alpha}_{\ \alpha'}(u)=\begin{bmatrix} e^i_{\ i'}(x^j) & -N_i^c(x^j,y^a)e^i_{\ i'}(x^j) \\ 0 & e^c_{\ c'}(x^j,y^a) \end{bmatrix} \tag{65}$$

with $e_i^{\ i'}(x^j)$ and $e_c^{\ b'}(x^j,y^a)$ generating the coefficients of metric (1) with the coefficients defined with respect to anholonmic frames,

$$g_{ij}(x^j)=e_i^{\ i'}(x^j)e_j^{\ j'}(x^j)n_{i'j'} \quad \text{and } h_{ab}(x^j,y^c)=e_a^{\ a'}(x^j,y^c)e_b^{\ b'}(x^j,y^c)\eta_{a'b'}. \tag{66}$$

By using vielbeins and metrics of type (64) and (65) and, respectively, (66), we can model in a unified manner various types of (pseudo) Riemannian, Einstein–Cartan, Riemann–Finsler and vector/covector bundle nonlinear connection commutative and noncommutative geometries in effective gauge and string theories (it depends on the parameterization of $e_i^{\ i'}$, $e_c^{\ b'}$, and N_i^c on coordinates and anholonomy relations, see details in Refs. 24–28).

We consider the de Sitter space Σ^4 as a hypersurface defined by the equations $\eta_{AB}u^Au^B=-l^2$ in the four-dimensional flat space enabled with diagonal metric η_{AB}, $\eta_{AA}=\pm 1$ (in this section $A,B,C,\ldots=1,2,\ldots,5$), where $\{u^A\}$ are global Cartesian coordinates in $\mathbb{R}^5$; $l>0$ is the curvature of de Sitter space (for simplicity, we consider here only the de Sitter case; the anti-de Sitter configuration is to be stated by a hypersurface $\eta_{AB}u^Au^B=l^2$). The de Sitter group $S_{(\eta)}=\mathrm{SO}_{(\eta)}(5)$ is the isometry group of Σ^5-space with six generators of Lie algebra $\mathrm{so}_{(\eta)}(5)$ satisfying the commutation relations

$$[M_{AB},M_{CD}]=\eta_{AC}M_{BD}-\eta_{BC}M_{AD}-\eta_{AD}M_{BC}+\eta_{BD}M_{AC}. \tag{67}$$

We can decompose the capital indices $A,B,\ldots$ as $A=(\alpha',5)$, $B=(\beta',5),\ldots,$, and the metric η_{AB} as $\eta_{AB}=(\eta_{\alpha'\beta',\eta_{55}})$. The operators (67) M_{AB} can be decomposed as $M_{\alpha'\beta'}=\mathcal{F}_{\alpha'\beta'}$ and $P_{\alpha'}=l^{-1}M_{5\alpha'}$ written as

$$[\mathcal{F}_{\alpha'\beta'},\mathcal{F}_{\gamma'\delta'}]=\eta_{\alpha'\gamma'}\mathcal{F}_{\beta'\delta'}-\eta_{\beta'\gamma'}\mathcal{F}_{\alpha'\delta'}-\eta_{\beta'\delta'}\mathcal{F}_{\alpha'\gamma'}-\eta_{\alpha'\delta'}\mathcal{F}_{\beta'\gamma'},$$

$$[P_{\alpha'},P_{\beta'}]=-l^{-2}\mathcal{F}_{\alpha'\beta'}, \tag{68}$$

$$[P_{\alpha'},\mathcal{F}_{\beta'\gamma'}]=\eta_{\alpha'\beta'}P_{\underline{\gamma}}-\eta_{\alpha'\gamma'}P_{\beta'},$$

where the Lie algebra $\mathrm{so}_{(\eta)}(5)$ is split into a direct sum, $\mathrm{SO}_{(\eta)}(5)=\mathrm{SO}_{(\eta)}(4)\oplus V_4$ with V_4 being the vector space stretched on vectors $P_{\underline{\alpha}}$. We remark that $\Sigma^4=S_{(\eta)}/L_{(\eta)}$, where $L_{(\eta)}=\mathrm{SO}_{(\eta)}(4)$. For $\eta_{AB}=\mathrm{diag}(-1,+1,+1,+1)$ and $S_{10}=\mathrm{SO}(1,4)$, $L_6=\mathrm{SO}(1,3)$ is the group of Lorentz rotations.

The generators $I^{\underline{a}}$ and structure constants $f_{\underline{t}}^{\underline{sp}}$ of the de Sitter–Lie group can be parameterized in a form distinguishing the de Sitter generators and commutations (68). The action of the group $S_{(\eta)}$ may be realized by using 4×4 matrices with a parameterization distinguishing the subgroup $L_{(\eta)}$,

$$B = bB_L, \tag{69}$$

where

$$B_L = \begin{pmatrix} L & 0 \\ 0 & 1 \end{pmatrix},$$

$L \in L_{(\eta)}$ is the de Sitter bust matrix transforming the vector $(0,0,\ldots,\rho) \in \mathbb{R}^5$ into the arbitrary point $(V^1,V^2,\ldots,V^5) \in \Sigma^5_\rho \subset \mathcal{R}^5$ with curvature ρ ($V_A V^A = -\rho^2, V^A = \tau^A \rho$), and the matrix b is expressed

$$b = \begin{pmatrix} \delta^{\alpha'}{}_{\beta'} + \dfrac{\tau^{\alpha'}\tau_{\beta'}}{(1+\tau^5)} & \tau^{\alpha'} \\ \tau_{\beta'} & \tau^5 \end{pmatrix}.$$

The de Sitter gauge field is associated with a $\mathrm{so}_{(\eta)}(5)$-valued connection 1-form,

$$\widetilde{\Omega} = \begin{pmatrix} \omega^{\alpha'}{}_{\beta'} & \widetilde{\theta}^{\alpha'} \\ \widetilde{\theta}_{\beta'} & 0 \end{pmatrix}, \tag{70}$$

where $\omega^{\alpha'}{}_{\beta'} \in \mathrm{SO}(4)_{(\eta)}$, $\widetilde{\theta}^{\alpha'} \in \mathcal{R}^4$, $\widetilde{\theta}_{\beta'} \in \eta_{\beta'\alpha'}\widetilde{\theta}^{\alpha'}$.

The actions of $S_{(\eta)}$ mix the components of the matrix $\omega^{\alpha'}{}_{\beta'}$ and $\widetilde{\theta}^{\alpha'}$ fields in (70). Because the introduced parameterization is invariant on action on $\mathrm{SO}_{(\eta)}(4)$ group, we cannot identify $\omega^{\alpha'}{}_{\beta'}$ and $\widetilde{\theta}^{\alpha'}$, respectively, with the connection $\Gamma^{[c]}$ and the 1-form e^α defined by a N-connection structure like in (2) with the coefficients chosen as in (64) and (65). To avoid this difficulty we can consider nonlinear gauge realizations of the de Sitter group $S_{(\eta)}$ by introducing the nonlinear gauge field

$$\Gamma = b^{-1}\widetilde{\Omega}b + b^{-1}\,\mathrm{d}b = \begin{pmatrix} \Gamma^{\alpha'}{}_{\beta'} & \theta^{\alpha'} \\ \theta_{\beta'} & 0 \end{pmatrix}, \tag{71}$$

where

$$\Gamma^{\alpha'}{}_{\beta'} = \omega^{\alpha'}{}_{\beta'} - (\tau^{\alpha'} D\tau_{\beta'} - \tau_{\beta'} D\tau^{\alpha'})/(1+\tau^5),$$

$$\theta^{\alpha'} = \tau^5\widetilde{\theta}^{\alpha'} + D\tau^{\alpha'} - \tau^{\alpha'}(\mathrm{d}r^5 + \widetilde{\theta}_{\gamma'}\tau^{\gamma'})/(1+\tau^5),$$

$$D\tau^{\alpha'} = \mathrm{d}\tau^{\alpha'} + \omega^{\alpha'}{}_{\beta'}\tau^{\beta'}.$$

The action of the group $\mathrm{S}(\eta)$ is nonlinear, yielding the transformation rules

$$\Gamma' = L'\Gamma(L')^{-1} + L'd(L')^{-1}, \quad \theta' = L\theta,$$

where the nonlinear matrix-valued function

$$L' = L'(\tau^\alpha, b, B_T)$$

is defined from $B_b = b'B_{L'}$ [see the parametrization (69)]. The de Sitter "nonlinear" algebra is defined by generators (68) and nonlinear gauge transforms of type (71).

B. de Sitter nonlinear gauge gravity and general relativity

We generalize the constructions from Refs. 23 and 6 to the case when the de Sitter nonlinear gauge gravitational connection (71) is defined by the viebeins (64) and (65) and the linear connection (7) $\Gamma^{[c]\alpha}{}_{\beta\mu}=\{\Gamma^{\alpha}{}_{\beta\mu}\}$,

$$\Gamma=\begin{pmatrix}\Gamma^{\alpha'}{}_{\beta'} & l_0^{-1}e^{\alpha'}\\ l_0^{-1}e_{\beta'} & 0\end{pmatrix}, \tag{72}$$

where

$$\Gamma^{\alpha'}{}_{\beta'}=\Gamma^{\alpha'}{}_{\beta'\mu}\delta u^{\mu}, \tag{73}$$

for

$$\Gamma^{\alpha'}{}_{\beta'\mu}=e_{\alpha}{}^{\alpha'}e^{\beta}{}_{\beta'}\Gamma^{\alpha}{}_{\beta\mu}+e_{\alpha}{}^{\alpha'}\delta_{\mu}e^{\alpha}{}_{\beta'},$$

$$e^{\alpha'}=e_{\mu}{}^{\alpha'}\delta u^{\mu}, \tag{74}$$

and l_0 being a dimensional constant.

The matrix components of the curvature of the connection (72),

$$\mathcal{R}^{(\Gamma)}=\mathrm{d}\Gamma+\Gamma\wedge\Gamma,$$

can be written

$$\mathcal{R}^{(\Gamma)}=\begin{pmatrix}\mathcal{R}^{\alpha'}{}_{\beta'}+l_0^{-1}\pi^{\alpha'}_{\beta'} & l_0^{-1}T^{\alpha'}\\ l_0^{-1}T^{\beta'} & 0\end{pmatrix}, \tag{75}$$

where

$$\pi^{\alpha'}_{\beta'}=e^{\alpha'}\wedge e_{\beta'},\quad \mathcal{R}^{\alpha'}{}_{\beta'}=\tfrac{1}{2}\mathcal{R}^{\alpha'}{}_{\beta'\mu\nu}\,\delta u^{\mu}\wedge\delta u^{\nu},$$

and

$$\mathcal{R}^{\alpha'}{}_{\beta'\mu\nu}=e^{\beta}{}_{\beta'}e_{\alpha}{}^{\alpha'}R^{\alpha}{}_{\beta\mu\nu}$$

with the coefficients $R^{\alpha}{}_{\beta\mu\nu}$ defined with $h-v$-invariant components, see (A2) in Appendix A.

The de Sitter gauge group is semisimple, we are able to construct a variational gauge gravitational theory with the Lagrangian

$$L=L_{(g)}+L_{(m)}, \tag{76}$$

where the gauge gravitational Lagrangian is defined

$$L_{(g)}=\frac{1}{4\pi}\mathrm{Tr}(\mathcal{R}^{(\Gamma)}\wedge *_G\mathcal{R}^{(\Gamma)})=\mathcal{L}_{(G)}|g|^{1/2}\delta^4u,$$

for

$$\mathcal{L}_{(g)}=\frac{1}{2l^2}T^{\alpha'}{}_{\mu\nu}T_{\alpha'}{}^{\mu\nu}+\frac{1}{8\lambda}\mathcal{R}^{\alpha'}{}_{\beta'\mu\nu}\mathcal{R}^{\beta'}{}_{\alpha'}{}^{\mu\nu}-\frac{1}{l^2}(\overleftarrow{R}(\mathrm{T})-2\lambda_1),$$

with δ^4u being the volume element, $|g|$ is the determinant computed the metric coefficients (1) stated with respect to N-elongated frames, the curvature scalar $\overleftarrow{R}(\Gamma)$ is computed as in (A4), $T^{\alpha'}{}_{\mu\nu}=e^{\alpha'}{}_{\alpha}T^{\alpha}{}_{\mu\nu}$ (the gravitational constant l^2 satisfies the relations $l^2=2l_0^2\lambda$, $\lambda_1=-3/l_0$), Tr denotes

the trace on α', β' indices. The matter field Lagrangian from (76) is defined

$$L_{(m)} = -\tfrac{1}{2}\mathrm{Tr}(\Gamma \wedge *_g \mathcal{I}) = \mathcal{L}_{(m)}|g|^{1/2}\,\delta^n u,$$

with the Hodge operator derived by $|g|$ and $|h|$, where

$$\mathcal{L}_{(m)} = \tfrac{1}{2}\Gamma^{\alpha'}{}_{\beta'\mu}S^{\beta'}{}_{\alpha'}{}^{\mu} - t^{\mu}{}_{\alpha'}l^{\alpha'}{}_{\mu}.$$

The matter field source $\mathcal{J}$ is obtained as a variational derivation of $\mathcal{L}_{(m)}$ on Γ and is parameterized in the form

$$\mathcal{J} = \begin{pmatrix} S^{\alpha'}{}_{\beta} & -l_0\tau^{\alpha'} \\ -l_0\tau_{\beta'} & 0 \end{pmatrix}$$

with $\tau^{\alpha'} = \tau^{\alpha'}{}_{\mu}\delta u^{\mu}$ and $S^{\alpha'}{}_{\beta'} = S^{\alpha'}{}_{\beta'\mu}\delta u^{\mu}$ being, respectively, the canonical tensors of energy momentum and spin density.

Varying the action

$$S = \int \delta^4 u(\mathcal{L}_{(g)} + \mathcal{L}_{(m)})$$

on the Γ-variables (72), we obtain the gauge-gravitational field equations,

$$d(*\mathcal{R}^{(\Gamma)}) + \Gamma \wedge (*\mathcal{R}^{(\Gamma)}) - (*\mathcal{R}^{(\Gamma)}) \wedge \Gamma = -\lambda(*\mathcal{J}), \tag{77}$$

where the Hodge operator $*$ is used. This equations can be alternatively derived in geometric form by applying the absolute derivation and dual operators.

Distinguishing the variations on Γ and e-variables, we rewrite (77),

$$\hat{\mathcal{D}}(*\mathcal{R}^{(\Gamma)}) + \frac{2\lambda}{l^2}(\hat{\mathcal{D}}(*\pi) + e \wedge (*T^T) - (*T) \wedge e^T) = -\lambda(*S),$$

$$\hat{\mathcal{D}}(*T) - (*\mathcal{R}^{(\Gamma)}) \wedge e - \frac{2\lambda}{l^2}(*\pi) \wedge e = \frac{l^2}{2}\left(*t + \frac{1}{\lambda} * \mathfrak{s}\right),$$

e^T being the transposition of e, where

$$T^t = \left\{T_{\alpha'} = \eta_{\alpha'\beta'}T^{\beta'}, T^{\beta'} = \tfrac{1}{2}T^{\beta'}{}_{\mu\nu}\delta u^{\mu} \wedge \delta u^{\nu}\right\},$$

$$e^T = \{e_{\alpha'} = \eta_{\alpha'\beta'}e^{\beta'}, e^{\beta'} = e^{\beta'}{}_{\mu}\delta u^{\mu}\}, \quad \hat{\mathcal{D}} = \delta + \hat{\Gamma}$$

($\hat{\Gamma}$ acts as $\Gamma^{\alpha'}{}_{\beta'\mu}$ on indices $\gamma', \delta', \ldots$ and as $\Gamma^{\alpha}{}_{\beta\mu}$ on indices $\gamma, \delta, \ldots$). The value $\mathfrak{s}$ defines the energy-momentum tensor of the gauge gravitational field $\hat{\Gamma}$,

$$\mathfrak{s}_{\mu\nu}(\hat{\Gamma}) = \tfrac{1}{2}\mathrm{Tr}\left(\mathcal{R}_{\mu\alpha}\mathcal{R}^{\alpha}{}_{\nu} - \tfrac{1}{4}\mathcal{R}_{\alpha\beta}\mathcal{R}^{\alpha\beta}G_{\mu\nu}\right).$$

Equations (77) make up the complete system of variational field equations for nonlinear de Sitter gauge gravity. We note that we can obtain a nonvariational Poincaré gauge gravitational theory if we consider the contraction of the gauge potential (72) to a potential $\Gamma^{[P]}$ with values in the Poincaré–Lie algebra

$$\Gamma = \begin{pmatrix} \Gamma^{\alpha'}{}_{\beta'} & l_0^{-1} e^{\alpha'} \\ l_0^{-1} e_{\beta'} & 0 \end{pmatrix} \to \Gamma^{[P]} = \begin{pmatrix} \Gamma^{\alpha'}{}_{\beta'} & l_0^{-1} e^{\alpha'} \\ 0 & 0 \end{pmatrix}. \tag{78}$$

A similar gauge potential was considered in the formalism of linear and affine frame bundles on curved space–times by Popov and Dikhin.[21,22] They considered the gauge potential (78) to be just the Cartan connection form in the affine gaugelike gravity and proved that the Yang–Mills equations of their theory are equivalent, after projection on the base, to the Einstein equations.

Let us give an example how an exact vacuum solution of the Einstein equations, with associated noncommutative symmetry, can be included as to define an exact solution in gauge gravity. Using the data (33) defining a 4D black ellipsoid solution, we write the nontrivial vielbein coefficients (64) as

$$e_2{}^{2'} = 1, \quad e_3{}^{3'} = \sqrt{|g_3|}, \quad e_4{}^{4'} = \sqrt{|h_4|}, \quad e_5{}^{5'} = \sqrt{|h_5|}, \quad N_2^5 = n_2 \tag{79}$$

for the diagonal Minkowski metric $\eta_{\alpha'\beta'} = (-1,-1,-1,1)$ with the tetrad and coordinate indices running, respectively, the values $\alpha', \beta', \ldots = 2,3,4,5$ and $\alpha, \beta, \ldots = 2,3,4,5$. The connection coefficients $\Gamma^{\alpha'}{}_{\beta'\mu}$, see formula (74), are computed by using the values $e_\alpha{}^{\alpha'}$ and (7) and used for definition of the potential $\Gamma^{[P]}$ (78) which defines a gauge gravity model with the Yang–Mills equations (77) being completely equivalent to the Einstein equations even the frames are anholonomic (see details in Refs. 21, 22, and 24–28). *N* coefficients, for instance, a complex $N_2^5 = n_2$ we can construct both complex Einstein and gauge gravity vacuum configurations which are stable and define anholonomically deformed black hole solutions with associated noncommutative symmetries.

Finally, we emphasize that in a similar manner, by extending the dimensions of spaces and gauge groups and introducing the cosmological constant, we can include the solutions for the (anti) de Sitter black ellipsoids and wormholes, with real or complex anholonomic structures (constructed, respectively, in Secs. IV C and V), into a gauge gravity theory [Einstein and Poincaré types, or as a degenerated configuration in the nonlinear (anti) de Sitter gravity].

VII. NONCOMMUTATIVE GAUGE DEFORMATIONS OF GRAVITY

The noncommutative gravity theories are confronted with the problem of definition of noncommutative variants of pseudo-Eucliedean and pseudo-Riemannian metrics. This is connected with another problem when the generation of noncommutative metric structures via the Moyal product and the Seiberg–Witten map[45] results in complex and noncommutative metrics for, in general, nonstable and/or unphysical gravitational vacua. In order to avoid the mentioned difficulties, we elaborated a model of noncommutative gauge gravity starting from a variant of gauge gravity being equivalent to the Einstein gravity and emphasizing in such approach the vielbein (frame) and connection structures, but not the metric configuration (see Refs. 6 and 61). The metric for such theories is induced by an anholonomic (in general) frame transform.

For explicit constructions, we follow the method of restricted enveloping algebras[62] and construct gauge gravitational theories by stating corresponding structures with semisimple or nonsemisimple Lie algebras and their extensions. We use power series of generators for the affine and nonlinearly realized de Sitter gauge groups and compute the coefficient functions of all the higher powers of the generators of the gauge group which are functions of the coefficients of the first power. Such constructions are based on the Seiberg–Witten map and on the formalism of $*$-product formulation of the algebra[45,63–69] when for functional objects, being functions of commuting variables, there are associated some algebraic noncommutative properties encoded in the $*$-product. Here we note that an approach to the gauge theory on noncommutative spaces was introduced geometrically[70] by defining the covariant coordinates without speaking about derivatives. This formalism was also developed for quantum planes.[71,72]

In this section, we shall prove the existence for noncommutative spaces of gauge models of gravity which agrees with usual gauge gravity theories being equivalent, or extending, the general

relativity theory in the limit of commuting spaces. We shall show how it is possible to adapt mutually the Seiberg–Witten map and anholonomic frame transforms in order to generate solutions of the gauge gravity preserving noncommutative symmetries even in the classical limit of commutative Einstein gravity.

A. Enveloping algebras for gauge gravity connections

We define the gauge fields on a noncommutative space as elements of an algebra $\mathcal{A}_u$ that form a representation of the generator I algebra for the de Sitter gauge group and the noncommutative space is modeled as the associative algebra of IC. This algebra is freely generated by the coordinates modulo ideal $\mathcal{R}$ generated by the relations (one accepts formal power series) $\mathcal{A}_u = \mathrm{IC}[[\hat{u}^1, \ldots, \hat{u}^N]]/\mathcal{R}$. A variational gauge gravitational theory can be formulated by using a minimal extension of the affine structural group $\mathcal{A}f_{3+1}(\mathbb{R})$ to the de Sitter gauge group $S_{10} = \mathrm{SO}(4+1)$ acting on $\mathbb{R}^{4+1}$ space. (See Refs. 73–78.)

Let now us consider a noncommutative space (see Appendix D for a brief outline of necessary concepts). The gauge fields are elements of the algebra $\hat{\psi} \in \mathcal{A}_I^{(\mathrm{dS})}$ that form the nonlinear representation of the de Sitter algebra $\mathrm{so}_{(\eta)}$ (5) (the whole algebra is denoted $\mathcal{A}_z^{(\mathrm{dS})}$). The elements transform

$$\delta\hat{\psi} = i\hat{\gamma}\hat{\psi}, \quad \hat{\psi} \in \mathcal{A}_u, \quad \hat{\gamma} \in \mathcal{A}_z^{(dS)'},$$

under a nonlinear de Sitter transformation. The action of the generators (68) on $\hat{\psi}$ is defined as the resulting element will form a nonlinear representation of $\mathcal{A}_I^{(\mathrm{dS})}$ and, in consequence, $\delta\hat{\psi} \in \mathcal{A}_u$ despite $\hat{\gamma} \in \mathcal{A}_z^{(\mathrm{dS})}$. We emphasize that for any representation the object $\hat{\gamma}$ takes values in enveloping de Sitter algebra but not in a Lie algebra as would be for commuting spaces.

We introduce a connection $\hat{\Gamma}^\nu \in \mathcal{A}_z^{(\mathrm{dS})}$ in order to define covariant coordinates,

$$\hat{U}^\nu = \hat{u}^\nu + \hat{\Gamma}^\nu.$$

The values $\hat{U}^\nu\hat{\psi}$ transform covariantly, i.e., $\delta\hat{U}^\nu\hat{\psi} = i\hat{\gamma}\hat{U}^\nu\hat{\psi}$, if and only if the connection $\hat{\Gamma}^\nu$ satisfies the transformation law of the enveloping nonlinear realized de Sitter algebra,

$$\delta\hat{\Gamma}^\nu\hat{\psi} = -i[\hat{u}^\nu, \hat{\gamma}] + i[\hat{\gamma}, \hat{\Gamma}^\nu],$$

where $\delta\hat{\Gamma}^\nu \in \mathcal{A}_z^{(\mathrm{dS})}$.

The enveloping algebra-valued connection has infinitely many component fields. Nevertheless, all component fields can be induced from a Lie algebra-valued connection by a Seiberg–Witten map[45,62] and, for $\mathrm{SO}(n)$ and $\mathrm{Sp}(n)$, see Ref. 79. Here, we show that similar constructions can be performed for nonlinear realizations of de Sitter algebra when the transformation of the connection is considered

$$\delta\hat{\Gamma}^\nu = -i[u^\nu, * \hat{\gamma}] + i[\hat{\gamma}, * \hat{\Gamma}^\nu].$$

We treat in more detail the canonical case with the star product (D4). The first term in the variation $\delta\hat{\Gamma}^\nu$ gives

$$-i[u^\nu, * \hat{\gamma}] = \theta^{\nu\mu}\frac{\partial}{\partial u^\mu}\gamma.$$

Assuming that the variation of $\hat{\Gamma}^\nu = \theta^{\nu\mu}Q_\mu$ starts with a linear term in θ, we have

$$\delta\hat{\Gamma}^\nu = \theta^{\nu\mu}\delta Q_\mu, \quad \delta Q_\mu = \frac{\partial}{\partial u^\mu}\gamma + i[\hat{\gamma}, * Q_\mu].$$

We expand the star product (D4) in θ but not in g_a and find up to first order in θ that

$$\gamma = \gamma^1_{\underline{a}} I^{\underline{a}} + \gamma^1_{\underline{ab}} I^{\underline{a}} I^{\underline{b}} + \cdots, \quad Q_\mu = q^1_{\mu,\underline{a}} I^{\underline{a}} + q^2_{\mu,\underline{ab}} I^{\underline{a}} I^{\underline{b}} + \cdots, \tag{80}$$

where $\gamma^1_{\underline{a}}$ and $q^1_{\mu,\underline{a}}$ are of order zero in θ and $\gamma^1_{\underline{ab}}$ and $q^2_{\mu,\underline{ab}}$ are of second order in θ. The expansion in $I^{\underline{b}}$ leads to an expansion in g_a of the $*$-product because the higher order $I^{\underline{b}}$ derivatives vanish. For the de Sitter case, we take the generators $I^{\underline{b}}$ (68), see commutators (D3), with the corresponding de Sitter structure constants $f^{\underline{bc}}_{\underline{d}} \simeq f^{\underline{\alpha\beta}}_{\underline{\beta}}$ (in our further identifications with space–time objects like frames and connections we shall use greek indices). The result of calculation of variations of (80), by using g_a to the order given in (D2), is

$$\delta q^1_{\mu,\underline{a}} = \frac{\partial \gamma^1_{\underline{a}}}{\partial u^\mu} - f^{\underline{bc}}_{\underline{a}} \gamma^1_{\underline{b}} q^1_{\mu,\underline{c}}, \quad \delta Q_\tau = \theta^{\mu\nu} \partial_\mu \gamma^1_{\underline{a}} \partial_\nu q^1_{\tau,\underline{b}} I^{\underline{a}} I^{\underline{b}} + \cdots,$$

$$\delta q^2_{\mu,\underline{ab}} = \partial_\mu \gamma^2_{\underline{ab}} - \theta^{\nu\tau} \partial_\nu \gamma^1_{\underline{a}} \partial_\tau q^1_{\mu,\underline{b}} - 2 f^{\underline{bc}}_{\underline{a}} \{ \gamma^1_{\underline{b}} q^2_{\mu,\underline{cd}} + \gamma^2_{\underline{bd}} q^1_{\mu,\underline{c}} \}.$$

Let us introduce the objects ε, taking the values in de Sitter Lie algebra and W_μ, taking values in the enveloping de Sitter algebra, i.e.,

$$\varepsilon = \gamma^1_{\underline{a}} I^{\underline{a}} \quad \text{and } W_\mu = q^2_{\mu,\underline{ab}} I^{\underline{a}} I^{\underline{b}},$$

with the variation δW_μ satisfying the equation

$$\delta W_\mu = \partial_\mu (\gamma^2_{\underline{ab}} I^{\underline{a}} I^{\underline{b}}) - \tfrac{1}{2} \theta^{\tau\lambda} \{ \partial_\tau \varepsilon, \partial_\lambda q_\mu \} + i[\varepsilon, W_\mu] + i[(\gamma^2_{\underline{ab}} I^{\underline{a}} I^{\underline{b}}), q_\nu].$$

This equation can be solved[70,45] in the form

$$\gamma^2_{\underline{ab}} = \tfrac{1}{2} \theta^{\nu\mu} (\partial_\nu \gamma^1_{\underline{a}}) q^1_{\mu,\underline{b}}, \quad q^2_{\mu,\underline{ab}} = -\tfrac{1}{2} \theta^{\nu\tau} q^1_{\nu,\underline{a}} (\partial_\tau q^1_{\mu,\underline{b}} + R^1_{\tau\mu,\underline{b}}).$$

The values

$$R^1_{\tau\mu,\underline{b}} = \partial_\tau q^1_{\mu,\underline{b}} - \partial_\mu q^1_{\tau,\underline{b}} + f^{\underline{ec}}_{\underline{d}} q^1_{\tau,\underline{e}} q^1_{\mu,\underline{e}}$$

could be identified with the coefficients $\mathcal{R}^{\underline{\alpha}}{}_{\underline{\beta}\mu\nu}$ of de Sitter nonlinear gauge gravity curvature [see formula (75)] if in the commutative limit

$$q^1_{\mu,\underline{b}} \simeq \begin{pmatrix} \Gamma^{\underline{\alpha}}{}_{\underline{\beta}} & l_0^{-1} \chi^{\underline{\alpha}} \\ l_0^{-1} \chi_{\underline{\beta}} & 0 \end{pmatrix}$$

[see (72)].

We note that the below presented procedure can be generalized to all the higher powers of θ. As an example, we compute the first order corrections to the gravitational curvature.

B. Noncommutative covariant gauge gravity dynamics

The constructions from the preceding section can be summarized by a conclusion that the de Sitter algebra valued object $\varepsilon = \gamma^1_{\underline{a}}(u)\, I^{\underline{a}}$ determines all the terms in the enveloping algebra

$$\gamma = \gamma^1_{\underline{a}} I^{\underline{a}} + \frac{1}{4} \theta^{\nu\mu} \partial_\nu \gamma^1_{\underline{a}} q^1_{\mu,\underline{b}} (I^{\underline{a}} I^{\underline{b}} + I^{\underline{b}} I^{\underline{a}}) + \cdots.$$

and the gauge transformations are defined by $\gamma^1_{\underline{a}}(u)$ and $q^1_{\mu,\underline{b}}(u)$, when

$$\delta_{\gamma^1} \psi = i \gamma(\gamma^1, q^1_\mu) * \psi.$$

Applying the formula (D4) we calculate

$$[\gamma, * \zeta] = i\gamma^1_{\underline{a}}\zeta^1_{\underline{b}}f^{\underline{ab}}_{\underline{c}}I^{\underline{c}} + \frac{i}{2}\theta^{\nu\mu}\{\partial_v(\gamma^1_{\underline{a}}\zeta^1_{\underline{b}}f^{\underline{ab}}_{\underline{c}})q_{\mu,\underline{c}} + (\gamma^1_{\underline{a}}\partial_v\zeta^1_{\underline{b}} - \zeta^1_{\underline{a}}\partial_v\gamma^1_{\underline{b}})q_{\mu,\underline{b}}f^{\underline{ab}}_{\underline{c}} + 2\partial_v\gamma^1_{\underline{a}}\partial_\mu\zeta^1_{\underline{b}}\}I^{\underline{d}}I^{\underline{c}},$$

where we used the properties that, for the de Sitter enveloping algebras, one holds the general formula for compositions of two transformations,

$$\delta_\gamma\delta_\varsigma - \delta_\varsigma\delta_\gamma = \delta_{i(\varsigma*\gamma-\gamma*\varsigma)}.$$

This is also true for the restricted transformations defined by γ^1,

$$\delta_{\gamma^1}\delta_{\varsigma^1} - \delta_{\varsigma^1}\delta_{\gamma^1} = \delta_{i(\varsigma^1*\gamma^1-\gamma^1*\varsigma^1)}.$$

Such commutators could be used for definition of tensors

$$\hat{S}^{\mu\nu} = [\hat{U}^\mu, \hat{U}^\nu] - i\hat{\theta}^{\mu\nu}, \tag{81}$$

where $\hat{\theta}^{\mu\nu}$ is, respectively, stated for the canonical, Lie and quantum plane structures. Under the general enveloping algebra one holds the transform

$$\delta\hat{S}^{\mu\nu} = i[\hat{\gamma}, \hat{S}^{\mu\nu}].$$

For instance, the canonical case is characterized by

$$S^{\mu\nu} = i\theta^{\mu\tau}\partial_\tau\Gamma^\nu - i\theta^{\nu\tau}\partial_\tau\Gamma^\mu + \Gamma^\mu * \Gamma^\nu - \Gamma^\nu * \Gamma^\mu = \theta^{\mu\tau}\theta^{\nu\lambda}\{\partial_\tau Q_\lambda - \partial_\lambda Q_\tau + Q_\tau * Q_\lambda - Q_\lambda * Q_\tau\}.$$

We introduce the gravitational gauge strength (curvature)

$$R_{\tau\lambda} = \partial_\tau Q_\lambda - \partial_\lambda Q_\tau + Q_\tau * Q_\lambda - Q_\lambda * Q_\tau, \tag{82}$$

which could be treated as a noncommutative extension of de Sitter nonlinear gauge gravitational curvature (75), and calculate

$$R_{\tau\lambda,\underline{a}} = R^1_{\tau\lambda,\underline{a}} + \theta^{\mu\nu}\Big\{R^1_{\tau\mu,\underline{a}}R^1_{\lambda\nu,\underline{b}} - \tfrac{1}{2}q^1_{\mu,\underline{a}}[(D_\nu R^1_{\tau\lambda,\underline{b}}) + \partial_\nu R^1_{\tau\lambda,\underline{b}}]\Big\}I^{\underline{b}},$$

where the gauge gravitation covariant derivative is introduced,

$$(D_\nu R^1_{\tau\lambda,\underline{b}}) = \partial_\nu R^1_{\tau\lambda,\underline{b}} + q_{\nu,\underline{c}}R^1_{\tau\lambda,\underline{d}}f^{\underline{cd}}_{\underline{b}}.$$

Following the gauge transformation laws for γ and q^1 we find

$$\delta_{\gamma^1}R^1_{\tau\lambda} = i[\gamma, {}^*R^1_{\tau\lambda}]$$

with the restricted form of γ. Such formulas were proved in Ref. 45 for usual gauge (nongravitational) fields. Here we reconsidered them for the gravitational gauge fields.

One can formulate gauge covariant gravitational dynamics of noncommutative spaces following the nonlinear realization of de Sitter algebra and the $*$-formalism and introducing derivatives in such a way that one does not obtain new relations for the coordinates. In this case, a Leibniz rule can be defined that

$$\hat{\partial}_\mu\hat{u}^\nu = \delta^\nu_\mu + d^{\nu\tau}_{\mu\sigma}\hat{u}^\sigma\hat{\partial}_\tau,$$

where the coefficients $d^{\nu\tau}_{\mu\sigma} = \delta^\nu_\sigma\delta^\tau_\mu$ are chosen to not have new relations when $\hat{\partial}_\mu$ acts again to the right-hand side. One holds the $*$-derivative formulas

$$\partial_\tau * f = \frac{\partial}{\partial u^\tau}f + f * \partial_\tau, \quad [\partial_l, {}^*(f * g)] = ([\partial_l, {}^*f]) * g + f * ([\partial_l, {}^*g])$$

and the Stokes theorem

$$\int [\partial_l, f] = \int d^N u [\partial_l, {}^* f] = \int d^N u \frac{\partial}{\partial u^l} f = 0,$$

where, for the canonical structure, the integral is defined,

$$\int \hat{f} = \int d^N u f(u^1, \ldots, u^N).$$

An action can be introduced by using such integrals. For instance, for a tensor of type (81), when

$$\delta \hat{L} = i[\hat{\gamma}, \hat{L}],$$

we can define a gauge invariant action

$$W = \int d^N u \, \mathrm{Tr}\, \hat{L}, \quad \delta W = 0,$$

where the trace must be taken for the group generators.

For the nonlinear de Sitter gauge gravity a proper action is

$$L = \tfrac{1}{4} R_{\tau\lambda} R^{\tau\lambda},$$

where $R_{\tau\lambda}$ is defined by (82) [in the commutative limit we shall obtain the connection (72)]. In this case the dynamic of noncommutative space is entirely formulated in the framework of quantum field theory of gauge fields. In general, we are dealing with anisotropic gauge gravitational interactions. The method works for matter fields as well to restrictions to the general relativity theory.

C. Noncommutative symmetries and star product deformations

The aim of this section is to prove that there are possible extensions of exact solutions from the Einstein and gauge gravity possessing hidden noncommutative symmetries without introducing new fields. For simplicity, we present the formulas including decompositions up to the second order on noncommutative parameter $\theta^{\alpha\beta}$ for vielbeins, connections, and curvatures which can be arranged to result in different models of noncommutative gravity. We give the data for the SU $(1, n+m-1)$ and SO $(1, n+m-1)$ gauge models containing, in general, complex N-elongated frames, modeling some exact solutions, for instance, those derived in Secs. IV and V. All data can be considered for extensions with nonlinear realizations into a bundle of affine or de Sitter frames (in this case, one generates noncommutative gauge theories of the type considered in Ref. 6 or to impose certain constraints and breaking of symmetries (in order to construct other models[7,60]).

In the preceding sections we considered noncommutative geometric structures introduced by frame anholonomic relations (5), or (15). The standard approaches to noncommutative geometry also contain certain noncommutative relations for coordinates,

$$[u^\alpha, u^\beta] = u^\alpha u^\beta - u^\beta u^\alpha = i\theta^{\alpha\beta}(u^\gamma), \tag{83}$$

where, in the simplest models, the commutator $[u^\alpha, u^\beta]$ is approximated to be constant, but there were elaborated approaches for general manifolds with the noncommutative parameter $\theta^{\alpha\beta}$ treated as functions on u^γ in Ref. 68. We define the star (Moyal) product to include possible N-elongated partial derivatives (3) and a quantum constant $\hbar$,

$$f * \varphi = f\varphi + \frac{\hbar}{2} B^{\underline{\alpha}\underline{\beta}}(\delta_{\underline{\alpha}} f \delta_{\underline{\beta}}\varphi + \delta_{\underline{\beta}} f \delta_{\underline{\alpha}}\varphi) + \hbar^2 B^{\underline{\alpha}\underline{\beta}} B^{\underline{\gamma}\underline{\mu}}[\delta_{(\underline{\alpha}}\delta_{\underline{\gamma})} f][\delta_{(\underline{\beta}}\delta_{\underline{\mu})}\varphi]$$

$$+ \frac{2}{3}\hbar^2 B^{\underline{\alpha}\underline{\beta}} \delta_{\underline{\beta}} B^{\underline{\gamma}\underline{\mu}}\{[\delta_{(\underline{\alpha}}\delta_{\underline{\gamma})} f]\delta_{\underline{\mu}}\varphi + [\delta_{(\underline{\alpha}}\delta_{\underline{\gamma})}\varphi]\delta_{\underline{\mu}} f\} + O(\hbar^3), \tag{84}$$

where, for instance, $\delta_{(\mu}\delta_{\nu)} = (1/2)(\delta_\mu\delta_\nu + \delta_\nu\delta_\mu)$,

$$B^{\underline{\alpha}\underline{\beta}} = \frac{\theta^{\alpha\beta}}{2}(\delta_\alpha u^{\underline{\alpha}} \delta_\beta u^{\underline{\beta}} + \delta_\beta u^{\underline{\alpha}} \delta_\alpha u^{\underline{\beta}}) + O(\hbar^3) \tag{85}$$

is defined for new coordinates $u^{\underline{\alpha}} = u^{\underline{\alpha}}(u^\alpha)$ inducing a suitable Poisson bi-vector field $B^{\underline{\alpha}\underline{\beta}}(\hbar)$ being related to a quantum diagram formalism [we shall not consider details concerning geometric quantization in this paper by investigating only classical deformations related to any anholonomic frame and coordinate (83) noncommutativity origin]. The formulas (84) and (85) transform into the usual ones with partial derivatives ∂_α and $\partial_{\underline{\alpha}}$ from Refs. 68 and 7 considered for vanishing anholonomy coefficients. We can define a star product being invariant under diffeomorphism transforms, $* \to *^{[-]}$, adapted to the *N*-connection structure (in a vector bundle provided with *N*-connection configuration, we use the label $[-]$ in order to emphasize the dependence on coordinates $u^{\underline{\alpha}}$ with "overlined" indices), by introducing the transforms

$$f^{[-]}(\hbar) = \Theta f(\hbar),$$

$$f^{[-]} *^{[-]} \varphi^{[-]} = \Theta(\Theta^{-1} f^{[-]} * \Theta^{-1})\varphi^{[-]}$$

for $\Theta = 1 + \Sigma_{[k=1]}\hbar^k \Theta_{[k]}$, for simplicity, computed up to the squared order on $\hbar$,

$$\Theta = 1 - 2\hbar^2 \theta^{\mu\nu}\theta^{\rho\sigma}\{[\delta_{(\mu}\delta_{\nu)} u^{\underline{\alpha}}][\delta_{(\rho}\delta_{\sigma)} u^{\underline{\beta}}]\delta_{(\underline{\alpha}}\delta_{\underline{\beta})} + [\delta_{(\mu}\delta_{\rho)} u^{\underline{\alpha}}](\delta_\nu u^{\underline{\beta}})(\delta_\sigma u^{\underline{\gamma}})[\delta_{(\underline{\alpha}}\delta_{\underline{\beta}}\delta_{\underline{\gamma})}]\} + O(\hbar^4),$$

where $\delta_{(\underline{\alpha}}\delta_{\underline{\beta}}\delta_{\underline{\gamma})} = (1/3!)(\delta_{\underline{\alpha}}\delta_{\underline{\beta}}\delta_{\underline{\gamma}} + \text{all } \textit{symmetric permutations})$. In our further constructions we shall omit the constant $\hbar$ considering that $\theta \sim \hbar$ is a small value by writing the necessary terms in the approximation $O(\theta^3)$ or $O(\theta^4)$.

We consider a noncommutative gauge theory on a space with *N*-connection structure stated by the gauge fields $\hat{A}_\mu = (\hat{A}_i, \hat{A}_a)$ when "hats" on symbols will be used for the objects defined on spaces with coordinate noncommutativity. In general, the gauge model can be with different types of structure groups like SL(k,IC), SU$_k$, U$_k$, SO($k-1,1$) and their nonlinear realizations. For instance, for the U($n+m$) gauge fields there are satisfied conditions $\hat{A}^+_\mu = -\hat{A}_\mu$, where "+" is the Hermitian conjugation. It is useful to present the basic geometric constructions for a unitary structural group containing the SO (4, 1) as a particular case if we want to consider noncommutative extensions of 4D exact solutions.

The noncommutative gauge transforms of potentials are defined by using the star product

$$\hat{A}^{[\varphi]}_\mu = \hat{\varphi} * \hat{A}_\mu \hat{\varphi}^{-1}_{[*]} - \hat{\varphi} * \delta_\mu \hat{\varphi}^{-1}_{[*]},$$

where the *N*-elongated partial derivatives (3) are used $\hat{\varphi} * \hat{\varphi}^{-1}_{[*]} = 1 = \hat{\varphi}^{-1}_{[*]} * \hat{\varphi}$. The matrix coefficients of fields will be distinguished by "underlined" indices, for instance, $\hat{A}_\mu = \{\hat{A}^{\underline{\alpha}\underline{\beta}}_\mu\}$, and for commutative values, $A_\mu = \{A^{\underline{\alpha}\underline{\beta}}_\mu\}$. Such fields are subjected to the conditions

$$(\hat{A}^{\underline{\alpha}\underline{\beta}}_\mu)^+(u,\theta) = -\hat{A}^{\underline{\beta}\underline{\alpha}}_\mu(u,\theta) \quad \text{and} \quad \hat{A}^{\underline{\alpha}\underline{\beta}}_\mu(u,-\theta) = -\hat{A}^{\underline{\beta}\underline{\alpha}}_\mu(u,\theta).$$

There is a basic assumption[45] that the noncommutative fields are related to the commutative fields by the Seiberg–Witten map in a manner that there are not new degrees of freedom being satisfied by the equation

$$\hat{A}^{\underline{\alpha\beta}}_{\mu}(A) + \Delta_{\hat{\lambda}}\hat{A}^{\underline{\alpha\beta}}_{\mu}(A) = \hat{A}^{\underline{\alpha\beta}}_{\mu}(A + \Delta_{\hat{\lambda}}A), \tag{86}$$

where $\hat{A}^{\underline{\alpha\beta}}_{\mu}(A)$ denotes a functional dependence on commutative field $A^{\underline{\alpha\beta}}_{\mu}$, $\hat{\varphi}=\exp\hat{\lambda}$, and the infinitesimal deformations $\hat{A}^{\underline{\alpha\beta}}_{\mu}(A)$ and of $A^{\underline{\alpha\beta}}_{\mu}$ are given, respectively, by

$$\Delta_{\hat{\lambda}}\hat{A}^{\underline{\alpha\beta}}_{\mu} = \delta_{\mu}\hat{\lambda}^{\underline{\alpha\beta}} + \hat{A}^{\underline{\alpha\gamma}}_{\mu} * \hat{\lambda}^{\underline{\gamma\beta}} - \hat{\lambda}^{\underline{\alpha\gamma}} * \hat{A}^{\underline{\gamma\beta}}_{\mu}$$

and

$$\Delta_{\lambda}A^{\underline{\alpha\beta}}_{\mu} = \delta_{\mu}\lambda^{\underline{\alpha\beta}} + A^{\underline{\alpha\gamma}}_{\mu} * \lambda^{\underline{\gamma\beta}} - \lambda^{\underline{\alpha\gamma}} * A^{\underline{\gamma\beta}}_{\mu},$$

where instead of partial derivatives ∂_{μ} we use the N-elongated ones, δ_{μ} and sum on index $\underline{\gamma}$.

Solutions of the Seiberg–Witten equations for models of gauge gravity are considered, for instance, in Refs. 6 and 7 (there are discussed procedures of deriving expressions on θ to all orders). Here we present only the first order on θ for the coefficients $\hat{\lambda}^{\underline{\alpha\beta}}$ and the first and second orders for $\hat{A}^{\underline{\alpha\beta}}_{\mu}$ including anholonomy relations and not depending on model considerations,

$$\hat{\lambda}^{\underline{\alpha\beta}} = \lambda^{\underline{\alpha\beta}} + \frac{i}{4}\theta^{\nu\tau}\{(\delta_{\nu}\lambda^{\underline{\alpha\gamma}})A^{\underline{\gamma\beta}}_{\mu} + A^{\underline{\alpha\gamma}}_{\mu}(\delta_{\nu}\lambda^{\underline{\gamma\beta}})\} + O(\theta^2)$$

and

$$\begin{aligned}
\hat{A}^{\underline{\alpha\beta}}_{\mu} = {} & A^{\underline{\alpha\beta}}_{\mu} - \frac{i}{4}\theta^{\nu\tau}\{A^{\underline{\alpha\gamma}}_{\mu}(\delta_{\tau}A^{\underline{\gamma\beta}}_{\nu} + R^{\underline{\gamma\beta}}{}_{\tau\nu}) + (\delta_{\tau}A^{\underline{\alpha\gamma}}_{\mu} + R^{\underline{\alpha\gamma}}{}_{\tau\mu})A^{\underline{\gamma\beta}}_{\nu}\} + \tfrac{1}{32}\theta^{\nu\tau}\theta^{\rho\sigma}\{[2A^{\underline{\alpha\gamma}}_{\rho}(R^{\underline{\gamma\varepsilon}}{}_{\sigma\nu}R^{\underline{\varepsilon\beta}}{}_{\mu\tau} \\
& + R^{\underline{\gamma\varepsilon}}{}_{\mu\tau}R^{\underline{\varepsilon\beta}}{}_{\sigma\nu}) + 2(R^{\underline{\alpha\varepsilon}}{}_{\sigma\nu}R^{\underline{\varepsilon\gamma}}{}_{\mu\tau} + R^{\underline{\alpha\varepsilon}}{}_{\mu\tau}R^{\underline{\varepsilon\gamma}}{}_{\sigma\nu})A^{\underline{\gamma\beta}}_{\rho}] - [A^{\underline{\alpha\gamma}}_{\nu}(D_{\tau}R^{\underline{\gamma\beta}}{}_{\sigma\mu} + \delta_{\tau}R^{\underline{\gamma\beta}}{}_{\sigma\mu}) \\
& + (D_{\tau}R^{\underline{\alpha\gamma}}{}_{\sigma\mu} + \delta_{\tau}R^{\underline{\alpha\gamma}}{}_{\sigma\mu})A^{\underline{\gamma\beta}}_{\nu}] - \delta_{\sigma}[A^{\underline{\alpha\gamma}}_{\nu}(\delta_{\tau}A^{\underline{\gamma\beta}}_{\mu} + R^{\underline{\gamma\beta}}{}_{\tau\mu}) + (\delta_{\tau}A^{\underline{\alpha\gamma}}_{\mu} + R^{\underline{\alpha\gamma}}{}_{\tau\mu})A^{\underline{\gamma\beta}}_{\nu}] \\
& + [(\delta_{\nu}A^{\underline{\alpha\gamma}}_{\rho})(2\delta_{(\tau}\delta_{\sigma)}A^{\underline{\gamma\beta}}_{\mu} + \delta_{\tau}R^{\underline{\gamma\beta}}{}_{\sigma\mu}) + (2\delta_{(\tau}\delta_{\sigma)}A^{\underline{\alpha\gamma}}_{\mu} + \delta_{\tau}R^{\underline{\alpha\gamma}}{}_{\sigma\mu})(\delta_{\nu}A^{\underline{\gamma\beta}}_{\rho})] - [A^{\underline{\alpha\varepsilon}}_{\nu}(\delta_{\tau}A^{\underline{\varepsilon\gamma}}_{\rho} + R^{\underline{\varepsilon\gamma}}{}_{\tau\rho}) \\
& + (\delta_{\tau}A^{\underline{\alpha\varepsilon}}_{\rho} + R^{\underline{\alpha\varepsilon}}{}_{\tau\rho})A^{\underline{\varepsilon\gamma}}_{\nu}](\delta_{\sigma}A^{\underline{\gamma\beta}}_{\mu} + R^{\underline{\gamma\beta}}{}_{\sigma\mu}) - (\delta_{\sigma}A^{\underline{\alpha\gamma}}_{\mu} + R^{\underline{\alpha\gamma}}{}_{\sigma\mu})[A^{\underline{\gamma\varepsilon}}_{\nu}(\delta_{\tau}A^{\underline{\varepsilon\beta}}_{\rho} + R^{\underline{\varepsilon\beta}}{}_{\tau\rho}) \\
& + (\delta_{\tau}A^{\underline{\gamma\varepsilon}}_{\rho} + R^{\underline{\gamma\varepsilon}}{}_{\tau\rho})A^{\underline{\varepsilon\beta}}_{\nu}] + O(\theta^3),
\end{aligned} \tag{87}$$

where the curvature is defined $R^{\underline{\alpha\beta}}{}_{\tau\nu} = e^{\underline{\alpha}}_{\alpha}e^{\beta\beta}R_{\beta}{}^{\alpha}{}_{\tau\nu}$ with $R_{\beta}{}^{\alpha}{}_{\tau\nu}$ computed as in Appendix A, see formula (A1), when $\Gamma \to A$, and for the gauge model of gravity, see (75) and (82). By using the star product, we can write symbolically the solution (87) in general form,

$$\Delta\hat{A}^{\underline{\alpha\beta}}_{\mu}(\theta) = -\frac{i}{4}\theta^{\nu\tau}[\hat{A}^{\underline{\alpha\gamma}}_{\mu} * (\delta_{\tau}\hat{A}^{\underline{\gamma\beta}}_{\nu} + \hat{R}^{\underline{\gamma\beta}}{}_{\tau\nu}) + (\delta_{\tau}\hat{A}^{\underline{\alpha\gamma}}_{\mu} + \hat{R}^{\underline{\alpha\gamma}}{}_{\tau\mu}) * \hat{A}^{\underline{\gamma\beta}}_{\nu}],$$

where $\hat{R}^{\underline{\gamma\beta}}{}_{\tau\nu}$ is defined by the same formulas as $R^{\underline{\alpha\beta}}{}_{\tau\nu}$ but with the star products, like $AA \to A*A$.

There is a problem how to determine the dependence of the noncommutative vielbeins $\hat{e}^{\underline{\alpha}}_{\alpha}$ on commutative ones $e^{\underline{\alpha}}_{\alpha}$. If we consider the frame fields to be included into a (anti) de Sitter gauge gravity model with the connection (72), the vielbein components should be treated as certain coefficients of the gauge potential with specific nonlinear transforms for which the results of Ref. 6 are found. The main difference (considered in this work) is that the frames are in general with anholonomy induced by a N-connection field. In order to derive in such model the Einstein gravity we must analyze the reduction (78) to a Poincaré gauge gravity. An explicit calculus of the curvature of such gauge potential (see details in Refs. 21, 22, and 24–28), show that the coefficients of the curvature of the connection (78), obtained as a reduction from the SO (4, 1) gauge group is given by the coefficients (75) with vanishing torsion and constraints of type $\hat{A}^{\underline{\gamma 5}}_{\nu} = \epsilon\hat{e}^{\underline{\gamma}}_{\nu}$ and $\hat{A}^{\underline{55}}_{\nu} = \epsilon\hat{\phi}_{\nu}$ with $\hat{R}^{\underline{55}}{}_{\tau\nu} \sim \epsilon$ vanishing in the limit $\epsilon \to 0$ like in Ref. 7 (we obtain the same formulas for the vielbein and curvature components derived for the inhomogeneous Lorentz group but gener-

alized to N-elongated derivatives and with distinguishing into $h-v$ components). The result for $\hat{e}^{\underline{\mu}}_{\mu}$ in the limit $\epsilon \to 0$ generalized to the case of canonical connections (7) defining the covariant derivatives D_{τ} and corresponding curvatures (A1) is

$$\hat{e}^{\underline{\mu}}_{\mu} = e^{\underline{\mu}}_{\mu} - \frac{i}{4}\theta^{\nu\tau}[A^{\underline{\mu}\underline{\gamma}}_{\nu}\delta_{\tau}e^{\underline{\gamma}}_{\mu} + (\delta_{\tau}A^{\underline{\mu}\underline{\gamma}}_{\mu} + R^{\underline{\mu}\underline{\gamma}}{}_{\tau\mu})e^{\underline{\gamma}}_{\nu}] + \tfrac{1}{32}\theta^{\nu\tau}\theta^{\beta\sigma}\{2(R^{\underline{\mu}\underline{\varepsilon}}{}_{\sigma\nu}R^{\underline{\varepsilon}\underline{\gamma}}{}_{\mu\tau} + R^{\underline{\mu}\underline{\varepsilon}}{}_{\mu\tau}R^{\underline{\varepsilon}\underline{\gamma}}{}_{\sigma\nu})e^{\underline{\gamma}}_{\beta}$$
$$- A^{\underline{\mu}\underline{\gamma}}_{\beta}(D_{\tau}R^{\underline{\gamma}\underline{\beta}}{}_{\sigma\mu} + \delta_{\tau}R^{\underline{\gamma}\underline{\beta}}{}_{\sigma\mu})e^{\underline{\beta}}_{\beta} - [A^{\underline{\mu}\underline{\gamma}}_{\nu}(D_{\tau}R^{\underline{\gamma}\underline{\beta}}{}_{\sigma\mu} + \delta_{\tau}R^{\underline{\gamma}\underline{\beta}}{}_{\sigma\mu}) + (D_{\tau}R^{\underline{\mu}\underline{\gamma}}{}_{\sigma\mu} + \delta_{\tau}R^{\underline{\mu}\underline{\gamma}}{}_{\sigma\mu})A^{\underline{\gamma}\underline{\beta}}_{\nu}]e^{\underline{\beta}}_{\beta}$$
$$- e^{\underline{\beta}}_{\beta}\delta_{\sigma}[A^{\underline{\mu}\underline{\gamma}}_{\nu}(\delta_{\tau}A^{\underline{\gamma}\underline{\beta}}_{\mu} + R^{\underline{\gamma}\underline{\beta}}{}_{\tau\mu}) + (\delta_{\tau}A^{\underline{\mu}\underline{\gamma}}_{\mu} + R^{\underline{\mu}\underline{\gamma}}{}_{\tau\mu})A^{\underline{\gamma}\underline{\beta}}_{\nu}] + 2(\delta_{\nu}A^{\underline{\mu}\underline{\gamma}}_{\beta})\delta_{(\tau}\delta_{\sigma)}e^{\underline{\gamma}}_{\mu} - A^{\underline{\mu}\underline{\gamma}}_{\beta}\delta_{\sigma}[A^{\underline{\gamma}\underline{\beta}}_{\nu}\delta_{\tau}e^{\underline{\beta}}_{\mu}$$
$$+ (\delta_{\tau}A^{\underline{\gamma}\underline{\beta}}_{\mu} + R^{\underline{\gamma}\underline{\beta}}{}_{\tau\mu})e^{\underline{\beta}}_{\nu}] - (\delta_{\nu}e^{\underline{\gamma}}_{\beta})\delta_{\tau}(\delta_{\sigma}A^{\underline{\mu}\underline{\gamma}}_{\mu} + R^{\underline{\mu}\underline{\gamma}}{}_{\sigma\mu}) - [A^{\underline{\mu}\underline{\gamma}}_{\nu}(\delta_{\tau}A^{\underline{\gamma}\underline{\beta}}_{\beta} + R^{\underline{\gamma}\underline{\beta}}{}_{\tau\beta}) + (\delta_{\tau}A^{\underline{\mu}\underline{\gamma}}_{\beta}$$
$$+ R^{\underline{\mu}\underline{\gamma}}{}_{\tau\beta})A^{\underline{\gamma}\underline{\beta}}_{\nu}]\delta_{\sigma}e^{\underline{\beta}}_{\mu} - (\delta_{\sigma}A^{\underline{\mu}\underline{\gamma}}_{\mu} + R^{\underline{\mu}\underline{\gamma}}{}_{\sigma\mu})[A^{\underline{\gamma}\underline{\beta}}_{\mu}(\delta_{\nu}e^{\underline{\beta}}_{\beta}) + e^{\underline{\beta}}_{\nu}(\delta_{\sigma}A^{\underline{\gamma}\underline{\beta}}_{\mu} + R^{\underline{\gamma}\underline{\beta}}{}_{\sigma\mu})]\} + O(\theta^3). \quad (88)$$

Having the decompositions (88), we can define the inverse vielbein $\hat{e}^{\mu}_{*\underline{\mu}}$ from the equation

$$\hat{e}^{\mu}_{*\underline{\mu}} * \hat{e}^{\underline{\nu}}_{\mu} = \delta^{\underline{\nu}}_{\underline{\mu}}$$

and consequently compute θ-deformations of connections, curvatures, torsions, and any type of actions and field equations (for simplicity, we omit such cumbersome formulas being certain analogies to those computed in Ref. 7 but with additional N deformations).

The main result of this section consists in formulation of a procedure allowing to map exact solutions of a commutative gravity model into a corresponding noncommutative model without introducing new fields. For instance, we can take the data (33) and (79) and construct the θ deformation of the exact solution defining a static black ellipsoid (a similar prescription works in transforming both real and complex wormholes from Sec. V). The analysis presented in Secs. IV B and IV C illustrates a possibility to preserve the black ellipsoid stability for a certain class of extensions of solutions to noncommutative/complex gravity with complexified N frames. In another turn, if we consider arbitrary noncommutative relations for coordinates (θ noncommutativity) (83) the resulting θ deformation of stable solution will be, in general, unstable because arbitrary decompositions of type (88) will induce arbitrary complex terms in the metric, connection, and curvature coefficients, i.e., will result in complex terms in the "inverse Schrödinger problem" and related instability (see Refs. 18 and 19). Perhaps, a certain class of stable θ-deformed solutions can be defined if we constrain the θ-noncommutativity (83) to be dual to the so-called anholonomic frame noncommutativity (5), or (15), by connecting the nontrivial values of $\theta^{\alpha\beta}$ to certain complex N^a_i resulting in stable noncommutative configurations, or (in the simplest case) to say that the noncommutative extensions are modeled only by N fields $N^a_i \sim \hbar\theta$. The resulting noncommutative extensions could be defined as to preserve stability at least in the first order of $(\hbar\theta)$ terms.

VIII. DISCUSSION AND CONCLUSIONS

With this paper we begin the investigation of space–times with anholonomic noncommutative symmetry. The exact solutions we find are parametrized by generic off-diagonal metric ansatz and anholonomic frame (vielbein) structures with associated nonlinear connections (defining nontrivial anholonomy relations and inducing natural matrix noncommutative differential geometries). Their noncommutative symmetries are derived from exact solutions of the field equations in the Einstein gravity theory and their extra dimension and gauge like generalizations.

We analyzed the geometric and physical properties of new classes of exact solutions with hidden noncommutativity describing specific nonperturbative vacuum and nonvacuum gravitational configurations. Such space–times with generic off-diagonal metrics are very different, for instance, from those possessing Killing symmetries. We also addressed a particular class of solutions with noncommutative symmetries defining static black ellipsoid space–times which are not

prohibited by the uniqueness black hole theorems (proved for metrics with Killing symmetries and satisfying asymptotic flat conditions) because the generic anholonomic noncommutative configurations are very different from the Killing ones.

Let us comment on the difference between our approach and the former elaborated ones: In the so-called Connes–Lot models,[1,2] the gravitational models with Euclidean signature were elaborated from a spectral analysis of Dirac operators connected to the noncommutative geometry. This type of noncommutative geometry was constructed by replacing the algebra of smooth function on a manifold with a more general associative but noncommutative algebra. The fundamental matter field interactions and Riemannian gravity were effectively derived from a corresponding spectral calculus. In an alternative approach, the noncommutative geometry, as a low energy noncommutativity of coordinates, can be obtained in string theory because of presence of the so-called *B* fields. A number of models of gravity were proposed in order to satisfy certain noncommutativity relations for coordinates and frames (of Lie group, or quantum group type, or by computing some effective actions from string/brane theory and noncommutative gauge generalizations of gauge, Kaluza–Klein, and Einstein gravity), see Refs. 3–5 and 8. All mentioned noncommutative theories suppose that that the noncommutative geometry transforms into a commutative one in some limits to the Einstein theory and its extra dimension generalizations. In our approach we argue that the existence of hidden noncommutative structures suggests a natural way for constructing noncommutative models of gravitational interactions.

Our strategy explained in Sec. III is quite different from the previous attempts to construct the noncommutative gravity theory. We give a proof and analyze some explicit examples illustrating that there are some specific hidden noncommutative geometric structures even in the classical Einstein and gauge gravity models. This fact can be of fundamental importance in constructing more general models of noncommutative gravity with complex and nonsymmetric metrics.

Of course, there are two different notions of noncommutativity: The first one is related to the space–time deformations via Seiberg–Witten transforms with noncommutative coordinates and the second one is associated to noncommutative algebra modeled by anholonomic vielbeins. In general, the result of such deformations and frame maps cannot be distinguished exactly on a resulting complex space–time because there is a "mixture" of coordinate, gauge and frame transforms in the case of noncommutative geometry. Nevertheless, there are certain types of gravitational configurations possessing Lie type (noncommutative) symmetries which "survive" in the limit of commutative coordinates and real valued metrics. We say that such type of solutions of the gravitational field equations possess hidden noncommutative symmetries and describe a generic off-diagonal class of metrics and anholonomic frame transforms. It is a very difficult task to get exact solutions of the deformed gravity. In this work, we succeeded to do this by generating such gravitational configurations which are adapted both to the Seiberg–Witten-type deformations and to the vielbein transforms. In Sec. VII C we proved that there are possible extensions (on deformation parameters) of exact solutions from the Einstein and gauge gravity possessing hidden noncommutative symmetries without introducing new fields.

In this work, from a number of results following from application of Seiberg–Witten maps and related anholonomic vielbein transforms, we selected only those which allow us to define classes of solutions as noncommutative generalizations of some commutative ones of special physical interest. Such metrics with hidden noncommutative symmetry are described by a general off-diagonal ansatz for the metric and vielbein coefficients. The solutions can be extended to complex metrics by allowing that some subsets of vielbein coefficients (with associated nonlinear connection structure) may be complex valued. With respect to adapted frames, such metrics have real coefficients describing vacuum black ellipsoid or wormhole configurations (there were elaborated procedures of their analytical extensions and proofs of stability). The new types of metrics may be considered as certain exact solutions in complex gravity which must be considered if some noncommutative relations for coordinates are introduced. Such configurations may play an important role in the further understanding of vacua of noncommutative gauge and gravity theories and investigation of their quantum variants.

The anholonomic noncommutative symmetry of exact solutions of four-dimensional vacuum

Einstein equations positively does not violate the local (real) Lorentz symmetry. This symmetry may be preserved in a specific form even by anholonomic complex vielbein transforms mapping the 4D real Einstein's metrics into certain complex ones for noncommutative gravity. Such frames may be defined as the generated new solutions will be a formal analogy with their real (diagonal) pedigrees, to be stable with well-defined geodesic and horizon properties, like it was concluded for black ellipsoid solutions in general relativity.[18,19] By complex frame transforms with noncommutative symmetries we demonstrated that we may deform the horizon of the Schwarzshild solution to a static ellipsoid configuration as well to induce an effective electric charge of complex noncommutative origin.

We compare the generated off-diagonal ellipsoidal (in general, complex) metrics possessing anholonomic noncommutative symmetries with those describing the distorted diagonal black hole solutions (see the vacuum case in Refs. 80 and 81 and an extension to the case of nonvanishing electric fields in Ref. 82). In the complex ellipsoidal cases the space–time distortion is caused by some anisotropic off-diagonal terms being nontrivial in some regions but in the case of "pure diagonal" distortions one treats such effects following the fact that the vacuum Einstein equations are not satisfied in some regions because of presence of matter. Alternatively, the complex ellipsoid solutions may be described as in a real world with real metric coefficients but defined with respect to complex frames.

Here we emphasize that the off-diagonal gravity may model some gravity–matter-like interactions (for instance, in the Kaluza–Klein theory by emphasizing some very particular metric's configurations and topological compactifications) but, in general, the off-diagonal vacuum gravitational dynamics cannot be associated to any effective matter dynamics in a holonomic gravitational background. So, we may consider that the anholonomic ellipsoidal deformations of the Schwarzschild metric defined by real and/or complex anholonomic frame transforms generate some kind of anisotropic off-diagonal distortions modeled by certain vacuum gravitational fields with the distortion parameters (equivalently, vacuum gravitational polarizations) depending both on radial, angular and extra dimension coordinates. For complex valued nonlinear connection coefficients, we obtain a very specific complex space–time distortion instead of matter type distortion. We note that both classes of off-diagonal anisotropic and "pure" diagonal distortions (like in Refs. 80 and 81) result in solutions which in general are not asymptotically flat. However, it is possible to find asymptotically flat extensions, as it was shown in this paper and in Refs. 18 and 19, even for ellipsoidal configurations by introducing the corresponding off-diagonal terms. The asymptotic conditions for the diagonal distortions are discussed in Ref. 82 where it was suggested that to satisfy such conditions one must include some additional matter fields in the exterior portion of space–time. For ellipsoidal real/complex metrics, we should consider that the off-diagonal metric terms have a corresponding behavior as to result far away from the horizon in the Minkowski metric.

The deformation parameter ε effectively seems to put an "electric charge" on the black hole which is of gravitational off-diagonal/anholonomic origin. For complex metrics such "electric charges" may be induced by complex values of off-diagonal metric/anholonomic frame coefficients. It can describe effectively both positive and negative gravitational polarizations (even some repulsive gravitational effects). The polarization may have very specific nonlinearities induced by complex gravity terms. This is not surprising because the coefficients of an anisotropic black hole are similar to those of the Reissner–Nördstrom solution only with respect to corresponding anholonomic complex/real frames which are subjected to some constraints (anholonomy conditions).

Applying the method of anholonomic frame transforms elaborated and developed in Refs. 13–19 and 24–31, we can construct off-diagonal ellipsoidal extensions of the already diagonally disturbed Schwarzschild metric [see the metric (3.7) from Ref. 82]. Such anholonomic deformations would contain in the diagonal limit configurations with $\varepsilon \to 0$ but $\eta_3 \neq 1$ [see (47) and/or (33) and (51)] for such configurations where the function η_3 must be related in the corresponding limits with the values $\overline{\gamma}_D$, $\overline{\psi}_D$, and A from Ref. 82. We remark that there are different classes of ellipsoidal deformations of the Schwarzschild metric which result in real or complex vacuum

configuration. The conditions $\varepsilon \to 0$ and $q,\ \eta_3=1$ and $\lambda \to 0$ select just the limit of the usual radial Schwarzschild asymptotics without any (also possible) additional diagonal distortions. For nontrivial values of $q,\ \eta_3$, and η_4 we may obtain diagonal distortions.

In the case of ellipsoidal metrics with the Schwarzschild asymptotics, the ellipsoidal character could result in some observational effects in the vicinity of the horizon. For instance, scattering of particles on a static ellipsoid can be computed. We can also model anisotropic matter accretion effects on an ellipsoidal black hole put in the center of a galactic being of ellipsoidal, toroidal or another configuration. Even in 4D the nonspheric topology of horizons seem to be prohibited in the general relativity theory[52,83–86,20] following some general differential geometry and censorship theorems, such objects can be induced from extra dimensions and can exist in theories with cosmological constant,[87–89] nontrivial torsion or induced by anholonomic frames.[13–19,30,31] We can consider black torus/ellipsoid solutions as a background for potential tests for existence of extra dimensions and of general relativity. A point of further investigations could be the anisotropic ellipsoidal collapse when both the matter and space–time are of ellipsoidal generic off-diagonal symmetry (former theoretical and computational investigations were performed only for rotoids with anisotropic matter and particular classes of perturbations of the Schwarzshild solutions[90]). It is interesting to elaborate collapse scenaria with respect to compexified anholonomic frames. For very small eccentricities, we may not have any observable effects like perihelion shift or light bending if we restrict our investigations only to the Schwarzschild–Newton asymptotics but some kind of dissipation can be considered for complex metrics.

We also present some comments on mechanics and thermodynamics of ellipsoidal black holes. For the static black ellipsoids/tori with flat asymptotics, we can compute the area of the ellipsoidal horizon, associate an entropy and develop corresponding black ellipsoid thermodynamics. But this is a rough approximation because, in general, we are dealing with off-diagonal metrics depending anisotropically on two/three coordinates. Such solutions are with anholonomically deformed Killing horizons, or with anholonomic noncommutative symmetries, and should be described by a thermodynamics (in general, both nonequilibrium and irreversible) of black ellipsoids/tori self-consistently embedded into an off-diagonal anisotropic gravitational vacuum with potential dissipation described by some complex metric and frame coefficients. This forms a ground for numerous new conceptual issues to be developed and related to anisotropic black holes and the anisotropic kinetics and thermodynamics[29] as well to a framework of isolated anisotropic horizons,[91–93] defined in a locally anistoropic/noncommutative/complex background with wormhole real and/or complex configurations which is a matter of our further investigations.

Finally, we note that we elaborated a general formalism of generating noncommutative solutions starting from exact vacuum solutions with anholonomic noncommutativity, but we do not know how to extend our solutions via star (Moyal) product as to preserve their stability because of induced general complex terms in the metrics. For some particular duality relations between the coordinate and frame noncommutativity it seems possible to get stability at least in the first approximation of noncommutative deformation parameter but an arbitrary noncommutative coordinate relation results in less defined physical configurations. A better understanding of the physical relevance of the anholonomic noncommutative configurations completed also to general coordinate noncommutativity is an interesting open question which we leave for the future.

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APPENDIX A: EINSTEIN EQUATIONS AND *N* CONNECTIONS

For convenience, we present in this Appendix a selection of necessary results from Refs. 13–19, 30, and 31.

The curvature tensor of a connection $\Gamma^{[c]}$ with $h-v$ components (7) induced by anholonomic frames (2) and (3) with associated N-connection structure is defined $R(\delta_\tau, \delta_\gamma)\delta_\beta = R_\beta{}^\alpha{}_{\gamma\tau}\delta_\alpha$, where

$$R_{\beta}{}^{\alpha}{}_{\gamma\tau} = \delta_{\tau}\Gamma^{\alpha}{}_{\beta\gamma} - \delta_{\gamma}\Gamma^{\alpha}{}_{\beta\tau} + \Gamma^{\varphi}{}_{\beta\gamma}\Gamma^{\alpha}{}_{\varphi\tau} - \Gamma^{\varphi}{}_{\beta\tau}\Gamma^{\alpha}{}_{\varphi\gamma} + \Gamma^{\alpha}{}_{\beta\varphi}w^{\varphi}{}_{\gamma\tau}, \tag{A1}$$

splits into irreducible $h-v$ components $R_{\beta}{}^{\alpha}{}_{\gamma\tau}=\{R^{i}_{h.jk}, R^{a}_{b.jk}, P^{i}_{j.ka}, P^{c}_{b.ka}, S^{i}_{j.bc}, S^{a}_{b.cd}\}$, with

$$R^{i}_{h.jk} = \delta_k L^{i}_{.hj} - \delta_j L^{i}_{.hk} + L^{m}_{.hj}L^{i}_{mk} - L^{m}_{.hk}L^{i}_{mj} - C^{i}_{.ha}\Omega^{a}_{.jk},$$

$$R^{a}_{b.jk} = \delta_k L^{a}_{.bj} - \delta_j L^{a}_{.bk} + L^{c}_{.bj}L^{a}_{.ck} - L^{c}_{.bk}L^{a}_{.cj} - C^{a}_{.bc}\Omega^{c}_{.jk},$$

$$P^{i}_{j.ka} = \partial_a L^{i}_{.jk} + C^{i}_{.jb}T^{b}_{.ka} - (\delta_k C^{i}_{.ja} + L^{i}_{.lk}C^{l}_{.ja} - L^{l}_{.jk}C^{i}_{.la} - L^{c}_{.ak}C^{i}_{.jc}),$$

$$P^{c}_{b.ka} = \partial_a L^{c}_{.bk} + C^{c}_{.bd}T^{d}_{.ka} - (\delta_k C^{c}_{.ba} + L^{c}_{.dk}C^{d}_{.ba} - L^{d}_{.bk}C^{c}_{.da} - L^{d}_{.ak}C^{c}_{.bd}),$$

$$S^{i}_{j.bc} = \partial_c C^{i}_{.jb} - \partial_b C^{i}_{.jc} + C^{h}_{.jb}C^{i}_{.hc} - C^{h}_{.jc}C^{i}_{hb},$$

$$S^{a}_{b.cd} = \partial_d C^{a}_{.bc} - \partial_c C^{a}_{.bd} + C^{e}_{.bc}C^{a}_{.ed} - C^{e}_{.bd}C^{a}_{.ec}, \tag{A2}$$

where we omitted the label $[c]$ in formulas. The Ricci tensor $R_{\beta\gamma}=R_{\beta}{}^{\alpha}{}_{\gamma\alpha}$ has the irreducible $h-v$ components

$$R_{ij} = R^{k}_{i.jk}, \quad R_{ia} = -{}^{2}P_{ia} = -P^{k}_{i.ka},$$

$$R_{ai} = {}^{1}P_{ai} = P^{b}_{a.ib}, \quad R_{ab} = S^{c}_{a.bc}. \tag{A3}$$

This tensor is nonsymmetric, ${}^{1}P_{ai} \neq {}^{2}P_{ia}$ (this could be with respect to anholonomic frames of reference). The scalar curvature of the metric d connection, $\overleftarrow{R}=g^{\beta\gamma}R_{\beta\gamma}$, is computed

$$\overleftarrow{R} = G^{\alpha\beta}R_{\alpha\beta} = \hat{R} + S, \tag{A4}$$

where $\hat{R}=g^{ij}R_{ij}$ and $S=h^{ab}S_{ab}$.

By substituting (A3) and (A4) into the 5D Einstein equations,

$$R_{\alpha\beta} - \tfrac{1}{2}g_{\alpha\beta}R = \kappa\Upsilon_{\alpha\beta},$$

where κ and $\Upsilon_{\alpha\beta}$ are, respectively, the coupling constant and the energy-momentum tensor, we obtain the $h-v$ decomposition of the Einstein equations,

$$R_{ij} - \tfrac{1}{2}(\hat{R} + S)g_{ij} = \kappa\Upsilon_{ij},$$

$$S_{ab} - \tfrac{1}{2}(\hat{R} + S)h_{ab} = \kappa\Upsilon_{ab}, \tag{A5}$$

$${}^{1}P_{ai} = \kappa\Upsilon_{ai}, \quad {}^{2}P_{ia} = \kappa\Upsilon_{ia}.$$

The vacuum 5D gravitational field equations, in invariant $h-v$ components, are written

$$R_{ij} = 0, \quad S_{ab} = 0, \quad {}^{1}P_{ai} = 0, \quad {}^{2}P_{ia} = 0. \tag{A6}$$

The main trick of the anholonomic frames method of integrating the Einstein equations in general relativity and various (super) string and higher/lower dimension gravitational theories consist in a procedure of definition of such coefficients N^{a}_{j} such that the block matrices g_{ij} and h_{ab} are diagonalized. This substantially simplifies computations but we must apply N-elongated partial derivatives.

APPENDIX B: MAIN THEOREMS FOR 5D

We restrict our considerations to a five-dimensional (in brief, 5D) space–time provided with a generic off-diagonal (pseudo) Riemannian metric and labeled by local coordinates $u^{\alpha}=(x^i,y^4=v,y^5)$, for $i=1,2,3$. We state the condition when exact solutions of the Einstein equations depending on holonomic variables x^i and on one anholonomic (equivalently, anisotropic) variable $y^4=v$ can be constructed in explicit form. Every coordinate from a set u^{α} may be timelike, 3D spacelike, or extra dimensional. For simplicity, the partial derivatives will be denoted as $a^{\times}=\partial a/\partial x^1$, $a^{\cdot}=\partial a/\partial x^2$, $a'=\partial a/\partial x^3$, $a^{*}=\partial a/\partial v$.

The 5D quadratic line element is chosen

$$ds^2=g_{\alpha\beta}(x^i,v)du^{\alpha}\,du^{\beta} \tag{B1}$$

when the metric components $g_{\alpha\beta}$ are parametrized with respect to the coordinate dual basis by an off-diagonal matrix (ansatz),

$$\begin{bmatrix} g_1+w_1{}^2h_4+n_1{}^2h_5 & w_1w_2h_4+n_1n_2h_5 & w_1w_3h_4+n_1n_3h_5 & w_1h_4 & n_1h_5 \\ w_1w_2h_4+n_1n_2h_5 & g_2+w_2{}^2h_4+n_2{}^2h_5 & w_2w_3h_4+n_2n_3h_5 & w_2h_4 & n_2h_5 \\ w_1w_3h_4+n_1n_3h_5 & w_2w_3h_4+n_2n_3h_5 & g_3+w_3{}^2h_4+n_3{}^2h_5 & w_3h_4 & n_3h_5 \\ w_1h_4 & w_2h_4 & w_3h_4 & h_4 & 0 \\ n_1h_5 & n_2h_5 & n_3h_5 & 0 & h_5 \end{bmatrix}, \tag{B2}$$

with the coefficients being some necessary smooth class functions of type

$$g_1=\pm 1,\quad g_{2,3}=g_{2,3}(x^2,x^3),\quad h_{4,5}=h_{4,5}(x^i,v),$$

$$w_i=w_i(x^i,v),\quad n_i=n_i(x^i,v),$$

where the N coefficients from (3) and (2) are parametrized $N_i^4=w_i$ and $N_i^5=n_i$.

By straightforward calculation, we can prove[30,31] the following.

Theorem 1: *The nontrivial components of the 5D vacuum Einstein equations, $R_{\alpha}^{\beta}=0$ [see (A6) in the Appendix A] for the metric (1) defined by the ansatz (B2), computed with respect to anholonomic frames (2) and (3) can be written in the form*

$$R_2^2=R_3^3=-\frac{1}{2g_2g_3}\left[\ddot{g_3}-\frac{\dot{g_2}\dot{g_3}}{2g_2}-\frac{(\dot{g_3})^2}{2g_3}+g_2''-\frac{g_2'g_3'}{2g_3}-\frac{(g_2')^2}{2g_2}\right]=0, \tag{B3}$$

$$S_4^4=S_5^5=-\frac{\beta}{2h_4h_5}=0, \tag{B4}$$

$$R_{4i}=-w_i\frac{\beta}{2h_5}-\frac{\alpha_i}{2h_5}=0, \tag{B5}$$

$$R_{5i}=-\frac{h_5}{2h_4}[n_i^{**}+\gamma n_i^{*}]=0, \tag{B6}$$

where

$$\alpha_i=\partial_i h_5^{*}-h_5^{*}\partial_i\ln\sqrt{|h_4h_5|},\quad \beta=h_5^{**}-h_5^{*}[\ln\sqrt{|h_4h_5|}]^{*},\quad \gamma=3h_5^{*}/2h_5-h_4^{*}/h_4. \tag{B7}$$

Following this theorem, (1) we can define a function $g_2(x^2,x^3)$ for a given $g_3(x^2,x^3)$, or inversely, to define a function $g_2(x^2,x^3)$ for a given $g_3(x^2,x^3)$, from Eq. (B3); (2) we can define a function $h_4(x^1,x^2,x^3,v)$ for a given $h_5(x^1,x^2,x^3,v)$, or inversely, to define a function $h_5(x^1,x^2,x^3,v)$ for a given $h_4(x^1,x^2,x^3,v)$, from Eq. (B4); (3) and (4) having the values of h_4 and

h_5, we can compute the coefficients (B7) which allow to solve the algebraic equations (B5) and to integrate two times on v the equation (B6) which allows to find, respectively, the coefficients $w_i(x^k,v)$ and $n_i(x^k,v)$.

We can generalize the construction by introducing a conformal factor $\Omega(x^i,v)$ and additional deformations of the metric via coefficients $\zeta_{\hat{i}}(x^i,v)$ (here, the indices with a "hat" take values like $\hat{i}=1,2,3,5$), i.e., for metrics of type

$$ds^2=\Omega^2(x^i,v)\hat{g}_{\alpha\beta}(x^i,v)du^\alpha\, du^\beta, \tag{B8}$$

where the coefficients $\hat{g}_{\alpha\beta}$ are parametrized by the ansatz

$$\begin{bmatrix} g_1+(w_1{}^2+\zeta_1{}^2)h_4+n_1{}^2h_5 & (w_1w_2+\zeta_1\zeta_2)h_4+n_1n_2h_5 & (w_1w_3+\zeta_1\zeta_3)h_4+n_1n_3h_5 & (w_1+\zeta_1)h_4 & n_1h_5 \\ (w_1w_2+\zeta_1\zeta_2)h_4+n_1n_2h_5 & g_2+(w_2{}^2+\zeta_2{}^2)h_4+n_2{}^2h_5 & (w_2w_3+\zeta_2\zeta_3)h_4+n_2n_3h_5 & (w_2+\zeta_2)h_4 & n_2h_5 \\ (w_1w_3+\zeta_1\zeta_3)h_4+n_1n_3h_5 & (w_2w_3+\zeta_2\zeta_3)h_4+n_2n_3h_5 & g_3+(w_3{}^2+\zeta_3{}^2)h_4+n_3{}^2h_5 & (w_3+\zeta_3)h_4 & n_3h_5 \\ (w_1+\zeta_1)h_4 & (w_2+\zeta_2)h_4 & (w_3+\zeta_3)h_4 & h_4 & 0 \\ n_1h_5 & n_2h_5 & n_3h_5 & 0 & h_5+\zeta_5h_4 \end{bmatrix}. \tag{B9}$$

Such 5D metrics have a second order anisotropy[32,37,38] when the N coefficients are parametrized in the first order anisotropy like $N_i^4=w_i$ and $N_i^5=n_i$ (with three anholonomic, x^i, and two anholonomic, y^4 and y^5, coordinates) and in the second order anisotropy [on the second "shell," with four anholonomic (x^i,y^5), and one anholonomic, y^4, coordinates] with $N_{\hat{i}}^5=\zeta_{\hat{i}}$, in this work we state, for simplicity, $\zeta_5=0$. For trivial values $\Omega=1$ and $\zeta_{\hat{i}}=0$, the squared line interval (B8) transforms into (B1).

The Theorem 1 can be extended as to include the generalization to the second ansatz (B8).

Theorem 2: *The nontrivial components of the 5D vacuum Einstein equations, $R_\alpha^\beta=0$ [see (A6) in Appendix A] for the metric (B8) consist from the system (B3)–(B6) with the additional conditions that*

$$\hat{\delta}_i h_4=0 \quad \textit{and}\ \hat{\delta}_i\Omega=0 \tag{B10}$$

for $\hat{\delta}_i=\partial_i-(w_i+\zeta_i)\partial_4+n_i\partial_5$ when the values $\zeta_{\hat{i}}=(\zeta_i,\zeta_5=0)$ are to be found as to be a solution of (B10); for instance, if

$$\Omega^{q_1/q_2}=h_4 \quad (q_1 \textit{ and } q_2 \textit{ are integers}), \tag{B11}$$

ζ_i satisfy the equations

$$\partial_i\Omega-(w_i+\zeta_i)\Omega^*=0. \tag{B12}$$

The proof of Theorem 2 consists from a straightforward calculation of the components of the Ricci tensor (A3) as it is outlined in the Appendix A. The simplest way is to use the calculus for Theorem 1 and then to compute deformations of the canonical connection (7). Such deformations induce corresponding deformations of the Ricci tensor (A3). The condition that we have the same values of the Ricci tensor for the (B2) and (B9) results in Eqs. (B10) and (B12) which are compatible, for instance, if $\Omega^{q_1/q_2}=h_4$. There are also other possibilities to satisfy the condition (B10), for instance, if $\Omega=\Omega_1\Omega_2$, we can consider that $h_4=\Omega_1^{q_1/q_2}\Omega_2^{q_3/q_4}$ for some integers q_1, q_2, q_3, and q_4.

A very surprising result is that we are able to construct exact solutions of the 5D vacuum Einstein equations for both types of the ansatz (B2) and (B9).

Theorem 3: *The system of second order nonlinear partial differential equations (B3)–(B6) and (B12) can be solved in general form if there are given some values of functions $g_2(x^2,x^3)$ [or $g_3(x^2,x^3)$], $h_4(x^i,v)$ [or $h_5(x^i,v)$], and $\Omega(x^i,v)$.*

(i) *The general solution of Eq. (B3) can be written in the form*

$$\varpi = g_{[0]} \exp[a_2 \tilde{x}^2(x^2,x^3) + a_3 \tilde{x}^3(x^2,x^3)], \tag{B13}$$

where $g_{[0]}$, a_2, and a_3 are some constants and the functions $\tilde{x}^{2,3}(x^2,x^3)$ define any coordinate transforms $x^{2,3} \to \tilde{x}^{2,3}$ for which the 2D line element becomes conformally flat, i.e.,

$$g_2(x^2,x^3)(\mathrm{d}x^2)^2 + g_3(x^2,x^3)(\mathrm{d}x^3)^2 \to \varpi[(\mathrm{d}\tilde{x}^2)^2 + \epsilon(\mathrm{d}\tilde{x}^3)^2]. \tag{B14}$$

(ii) *The equation (B4) relates two functions $h_4(x^i,v)$ and $h_5(x^i,v)$ following two possibilities:*

(a) *to compute*

$$\sqrt{|h_5|} = h_{5[1]}(x^i) + h_{5[2]}(x^i) \int \sqrt{|h_4(x^i,v)|}\mathrm{d}v, \quad h_4^*(x^i,v) \neq 0 = h_{5[1]}(x^i) + h_{5[2]}(x^i)v,$$

$$h_4^*(x^i,v) = 0, \tag{B15}$$

for some functions $h_{5[1,2]}(x^i)$ stated by boundary conditions;

(b) *or, inversely, to compute h_4 for a given $h_5(x^i,v)$, $h_5^* \neq 0$,*

$$\sqrt{|h_4|} = h_{[0]}(x^i)(\sqrt{|h_5(x^i,v)|})^*, \tag{B16}$$

with $h_{[0]}(x^i)$ given by boundary conditions.

(iii) *The exact solutions of (B5) for $\beta \neq 0$ is*

$$w_k = \partial_k \ln[\sqrt{|h_4 h_5|}/|h_5^*|]/\partial_v \ln[\sqrt{|h_4 h_5|}/|h_5^*|], \tag{B17}$$

with $\partial_v = \partial/\partial v$ and $h_5^* \neq 0$. If $h_5^* = 0$, or even $h_5^* \neq 0$ but $\beta = 0$, the coefficients w_k could be arbitrary functions on (x^i,v). For vacuum Einstein equations this is a degenerated case which imposes the the compatibility conditions $\beta = \alpha_i = 0$, which are satisfied, for instance, if the h_4 and h_5 are related as in the formula (B6) but with $h_{[0]}(x^i) = const$..

(iv) *The exact solution of (B6) is*

$$n_k = n_{k[1]}(x^i) + n_{k[2]}(x^i) \int [h_4/(\sqrt{|h_5|})^3]\mathrm{d}v, \quad h_5^* \neq 0,$$

$$= n_{k[1]}(x^i) + n_{k[2]}(x^i) \int h_4 \, \mathrm{d}v, \quad h_5^* = 0, \tag{B18}$$

$$= n_{k[1]}(x^i) + n_{k[2]}(x^i) \int [1/(\sqrt{|h_5|})^3]\mathrm{d}v, \quad h_4^* = 0,$$

for some functions $n_{k[1,2]}(x^i)$ stated by boundary conditions.

(v) *The exact solution of (B12) is given by some arbitrary functions $\zeta_i = \zeta_i(x^i,v)$ if both $\partial_i \Omega = 0$ and $\Omega^* = 0$, we choose $\zeta_i = 0$ for $\Omega = const$, and*

$$\zeta_i = -w_i + (\Omega^*)^{-1}\partial_i \Omega, \quad \Omega^* \neq 0,$$

$$= (\Omega^*)^{-1}\partial_i \Omega, \quad \Omega^* \neq 0, \quad \textit{for vacuum solutions}. \tag{B19}$$

We note that a transform (B14) is always possible for 2D metrics and the explicit form of solutions depends on the chosen system of 2D coordinates and on the signature $\epsilon = \pm 1$. In the simplest case the equation (B3) is solved by arbitrary two functions $g_2(x^3)$ and $g_3(x^2)$. The equation (B4) is satisfied by arbitrary pairs of coefficients $h_4(x^i,v)$ and $h_{5[0]}(x^i)$.

The proof of Theorem 3, following from a direct integration of (B3)–(B6) and (B12) is given in the Appendix B of Ref. 30.

There are some important consequences of the Theorems 1–3.

Corollary 1: The nontrivial diagonal components of the Einstein tensor, $G^{\alpha}_{\beta}=R^{\alpha}_{\beta}-\frac{1}{2}R\delta^{\alpha}_{\beta}$, for the metric (1), given with respect to N frames, are

$$G^1_1=-(R^2_2+S^4_4),\quad G^2_2=G^3_3=-S^4_4,\quad G^4_4=G^5_5=-R^2_2 \tag{B20}$$

imposing the condition that the dynamics is defined by two values R^2_2 and S^4_4. The rest of the nondiagonal components of the Ricci (Einstein tensor) are compensated by fixing corresponding values of N coefficients.

The formulas (B20) are obtained following the relations for the Ricci tensor (B3)–(B6).

Corollary 2: We can extend the system of 5D vacuum Einstein equations (B3)–(B6) by introducing matter fields for which the coefficients of the energy-momentum tensor $\Upsilon_{\alpha\beta}$ given with respect to N frames satisfy the conditions

$$\Upsilon^1_1=\Upsilon^2_2+\Upsilon^4_4,\quad \Upsilon^2_2=\Upsilon^3_3,\quad \Upsilon^4_4=\Upsilon^5_5. \tag{B21}$$

We note that, in general, the tensor $\Upsilon_{\alpha\beta}$ for the nonvacuum Einstein equations,

$$R_{\alpha\beta}-\tfrac{1}{2}g_{\alpha\beta}R=\kappa\Upsilon_{\alpha\beta},$$

is not symmetric because with respect to anholonomic frames there are imposed constraints which makes nonsymmetric the Ricci and Einstein tensors [the symmetry conditions may be defined explicitly only with respect to holonomic, coordinate frames; for details see Appendix A and the formulas (A5)].

For simplicity, in our investigations we can consider only diagonal matter sources, given with respect to *N* frames, satisfying the conditions

$$\kappa\Upsilon^2_2=\kappa\Upsilon^3_3=\Upsilon_2,\quad \kappa\Upsilon^4_4=\kappa\Upsilon^5_5=\Upsilon_4,\quad \text{and } \Upsilon_1=\Upsilon_2+\Upsilon_4, \tag{B22}$$

where κ is the gravitational coupling constant. In this case the equations (B3) and (B4) are, respectively, generalized to

$$R^2_2=R^3_3=-\frac{1}{2g_2g_3}\left[\ddot{g_3}-\frac{\dot{g_2}\dot{g_3}}{2g_2}-\frac{(\dot{g_3})^2}{2g_3}+g_2''-\frac{g_2'g_3'}{2g_3}-\frac{(g_2')^2}{2g_2}\right]=-\Upsilon_4 \tag{B23}$$

and

$$S^4_4=S^5_5=-\frac{\beta}{2h_4h_5}=-\Upsilon_2. \tag{B24}$$

Corollary 3: An arbitrary solution of the system of equations (B3)–(B6) and (B12) is defined for a canonical connection (7) containing, in general, nontrivial torsion coefficients. This can be effectively applied in order to construct exact solutions, for instance, in string gravity containing nontrivial torsion. We can select solutions corresponding to the Levi–Civita connection (10) for a generic off-diagonal (pseudo) Riemannian metric if we impose the condition that the coefficients $N^4_i=w_i(x^k,v)$, $N^5_i=n_i(x^k,v)$, and $N^5_{\hat{i}}=\zeta_{\hat{i}}$ are fixed to result in a zero N curvature, $\Omega^a_{jk}=0$, on all "shells" of anisotropy. Such selections are possible by fixing corresponding boundary conditions and selecting corresponding classes of functions like $n_{k[1,2]}(x^i)$, obtained after a general integration, in formulas (B17)–(B19).

The above presented results are for generic 5D off-diagonal metrics, anholonomic transforms and nonlinear field equations. Reductions to a lower dimensional theory are not trivial in such cases. We emphasize here some specific points of this procedure (see details in Ref. 30).

APPENDIX C: REDUCTION FROM 5D TO 4D

The simplest way to construct a 5D$\to$4D reduction for the ansatz (B2) and (B9) is to eliminate from formulas the variable x^1 and to consider a 4D space [parametrized by local coordinates

(x^2,x^3,v,y^5)] being trivially embedded into 5D space [parametrized by local coordinates (x^1,x^2,x^3,v,y^5) with $g_{11}=\pm 1$, $g_{1\hat{\alpha}}=0$, $\hat{\alpha}=2,3,4,5$] with further possible 4D conformal and anholonomic transforms depending only on variables (x^2,x^3,v). We suppose that the 4D metric $g_{\hat{\alpha}\hat{\beta}}$ could be of arbitrary signature. In order to emphasize that some coordinates are stated just for such 4D space we underline the greek indices, $\hat{\alpha},\hat{\beta},\ldots$ and the italic indices from the middle of alphabet, $\hat{i},\hat{j},\ldots=2,3$, where $u^{\hat{\alpha}}=(x^{\hat{i}},y^a)=(x^2,x^3,y^4,y^5)$.

In result, the analogs, Theorems 1–3 and Corollaries 1–3 can be reformulated for 4D gravity with mixed holonomic–anholonomic variables. We outline here the most important properties of such reduction.

(i) The line element (B1) with ansatz (B2) and the line element (B1) with (B9) are, respectively, transformed on 4D space to the values.

The first type 4D quadratic line element is taken

$$ds^2 = g_{\hat{\alpha}\hat{\beta}}(x^{\hat{i}},v)du^{\hat{\alpha}}\,du^{\hat{\beta}} \tag{C1}$$

with the metric coefficients $g_{\hat{\alpha}\hat{\beta}}$ parametrized

$$\begin{bmatrix} g_2+w_2{}^2h_4+n_2{}^2h_5 & w_2w_3h_4+n_2n_3h_5 & w_2h_4 & n_2h_5 \\ w_2w_3h_4+n_2n_3h_5 & g_3+w_3{}^2h_4+n_3{}^2h_5 & w_3h_4 & n_3h_5 \\ w_2h_4 & w_3h_4 & h_4 & 0 \\ n_2h_5 & n_3h_5 & 0 & h_5 \end{bmatrix}, \tag{C2}$$

where the coefficients are some necessary smooth class functions of type

$$g_{2,3}=g_{2,3}(x^2,x^3),\quad h_{4,5}=h_{4,5}(x^{\hat{k}},v),$$

$$w_{\hat{i}}=w_{\hat{i}}(x^{\hat{k}},v),\quad n_{\hat{i}}=n_{\hat{i}}(x^{\hat{k}},v),\quad \hat{i},\hat{k}=2,3.$$

The anholonomically and conformally transformed 4D line element is

$$ds^2=\Omega^2(x^{\hat{i}},v)\hat{g}_{\hat{\alpha}\hat{\beta}}(x^{\hat{i}},v)du^{\hat{\alpha}}\,du^{\hat{\beta}}, \tag{C3}$$

where the coefficients $\hat{g}_{\hat{\alpha}\hat{\beta}}$ are parametrized by the ansatz

$$\begin{bmatrix} g_2+(w_2{}^2+\zeta_2{}^2)h_4+n_2{}^2h_5 & (w_2w_3+\zeta_2\zeta_3)h_4+n_2n_3h_5 & (w_2+\zeta_2)h_4 & n_2h_5 \\ (w_2w_3+\zeta_2\zeta_3)h_4+n_2n_3h_5 & g_3+(w_3{}^2+\zeta_3{}^2)h_4+n_3{}^2h_5 & (w_3+\zeta_3)h_4 & n_3h_5 \\ (w_2+\zeta_2)h_4 & (w_3+\zeta_3)h_4 & h_4 & 0 \\ n_2h_5 & n_3h_5 & 0 & h_5+\zeta_5h_4 \end{bmatrix}, \tag{C4}$$

where $\zeta_{\hat{i}}=\zeta_{\hat{i}}(x^{\hat{k}},v)$ and we shall restrict our considerations for $\zeta_5=0$.

(ii) We have a quadratic line element (1) which can be written

$$\delta s^2=g_2(dx^2)^2+g_3(dx^3)^2+h_4(\delta v)^2+h_5(\delta y^5)^2, \tag{C5}$$

with respect to the anholonomic coframe $(dx^{\hat{i}},\delta v,\delta y^5)$, where

$$\delta v=dv+w_{\hat{i}}\,dx^{\hat{i}}\quad\text{and}\quad \delta y^5=dy^5+n_{\hat{i}}\,dx^{\hat{i}} \tag{C6}$$

is the dual of $(\delta_{\hat{i}},\partial_4,\partial_5)$, where

$$\delta_{\hat{i}} = \partial_{\hat{i}} + w_{\hat{i}}\partial_4 + n_{\hat{i}}\partial_5. \tag{C7}$$

(iii) In the conditions of the 4D variant of the Theorem 1 we have the same equations (B3)–(B6) where we must set $h_4 = h_4(x^{\hat{k}}, v)$ and $h_5 = h_5(x^{\hat{k}}, v)$. As a consequence we have that $\alpha_i(x^k, v) \to \alpha_{\hat{i}}(x^{\hat{k}}, v)$, $\beta = \beta(x^{\hat{k}}, v)$, and $\gamma = \gamma(x^{\hat{k}}, v)$ which result that $w_{\hat{i}} = w_{\hat{i}}(x^{\hat{k}}, v)$ and $n_{\hat{i}} = n_{\hat{i}}(x^{\hat{k}}, v)$.

(iv) The 4D line element with conformal factor (B8) subjected to an anholonomic map with $\zeta_5 = 0$ transforms into

$$\delta s^2 = \Omega^2(x^{\hat{i}}, v)[g_2(\mathrm{d}x^2)^2 + g_3(\mathrm{d}x^3)^2 + h_4(\hat{\delta}v)^2 + h_5(\delta y^5)^2], \tag{C8}$$

given with respect to the anholonomic coframe $(\mathrm{d}x^{\hat{i}}, \hat{\delta}v, \delta y^5)$, where

$$\delta v = \mathrm{d}v + (w_{\hat{i}} + \zeta_{\hat{i}})\,\mathrm{d}x^{\hat{i}} \quad \text{and} \quad \delta y^5 = \mathrm{d}y^5 + n_{\hat{i}}\,\mathrm{d}x^{\hat{i}} \tag{C9}$$

is dual to the frame $(\hat{\delta}_{\hat{i}}, \partial_4, \hat{\partial}_5)$ with

$$\hat{\delta}_{\hat{i}} = \partial_{\hat{i}} - (w_{\hat{i}} + \zeta_{\hat{i}})\partial_4 + n_{\hat{i}}\partial_5, \quad \hat{\partial}_5 = \partial_5. \tag{C10}$$

(v) The formulas (B10) and (B12) from Theorem 2 must be modified into a 4D form

$$\hat{\delta}_{\hat{i}} h_4 = 0 \quad \text{and} \quad \hat{\delta}_{\hat{i}}\Omega = 0 \tag{C11}$$

and the values $\zeta_{\hat{i}} = (\zeta_{\hat{i}}, \zeta_5 = 0)$ are found as to be a unique solution of (B10); for instance, if

$$\Omega^{q_1/q_2} = h_4 \quad (q_1 \text{ and } q_2 \text{ are integers}),$$

$\zeta_{\hat{i}}$ satisfy the equations

$$\partial_{\hat{i}}\Omega - (w_{\hat{i}} + \zeta_{\hat{i}})\Omega^* = 0. \tag{C12}$$

(vi) One holds the same formulas (B15)–(B18) from the Theorem 3 on the general form of exact solutions with that difference that their 4D analogs are to be obtained by reductions of holonomic indices, $\hat{i} \to i$, and holonomic coordinates, $x^i \to x^{\hat{i}}$, i.e., in the 4D solutions there is not contained the variable x^1.

(vii) The formulas (B20) for the nontrivial coefficients of the Einstein tensor in 4D stated by the Corollary 1 are written

$$G_2^2 = G_3^3 = -S_4^4, \quad G_4^4 = G_5^5 = -R_2^2. \tag{C13}$$

(viii) For symmetries of the Einstein tensor (C13), we can introduce a matter field source with a diagonal energy momentum tensor, like it is stated in the Corollary 2 by the conditions (B21), which in 4D are transformed into

$$\Upsilon_2^2 = \Upsilon_3^3, \quad \Upsilon_4^4 = \Upsilon_5^5. \tag{C14}$$

APPENDIX D: STAR-PRODUCTS, ENVELOPING ALGEBRAS AND NONCOMMUTATIVE GEOMETRY

For a noncommutative space the coordinates $\hat{u}^i$ $(i = 1, \ldots, N)$ satisfy some noncommutative relations

$$[\hat{u}^i,\hat{u}^j]=\begin{cases} i\theta^{ij}, & \theta^{ij}\in \mathrm{IC}, \quad \text{canonical structure},\\ if_k^{ij}\hat{u}^k, & f_k^{ij}\in \mathrm{IC}, \quad \text{Lie structure},\\ iC_{kl}^{ij}\hat{u}^k\hat{u}^l, & C_{kl}^{ij}\in \mathrm{IC}, \quad \text{quantum plane}, \end{cases} \tag{D1}$$

where IC denotes the complex number field.

The noncommutative space is modeled as the associative algebra of IC; this algebra is freely generated by the coordinates modulo ideal $\mathcal{R}$ generated by the relations (one accepts formal power series) $\mathcal{A}_u=\mathrm{IC}[[\hat{u}^1,\ldots,\hat{u}^N]]/\mathcal{R}$. One restricts attention[94] to algebras having the (so-called, Poincaré–Birkhoff–Witt) property that any element of $\mathcal{A}_u$ is defined by its coefficient function and vice versa,

$$\hat{f}=\sum_{L=0}^{\infty} f_{i_1,\ldots,i_L}{:}\hat{u}^{i_1}\cdots\hat{u}^{i_L}{:} \quad \text{when } \hat{f}\sim\{f_i\},$$

where: $\hat{u}^{i_1}\cdots\hat{u}^{i_L}$: denotes that the basis elements satisfy some prescribed order (for instance, the normal order $i_1\leqslant i_2\leqslant\cdots\leqslant i_L$, or, another example, are totally symmetric). The algebraic properties are all encoded in the so-called diamond ($\diamondsuit$) product which is defined by

$$\hat{f}\hat{g}=\hat{h}\sim\{f_i\}\diamondsuit\{g_i\}=\{h_i\}.$$

In the mentioned approach to every function $f(u)=f(u^1,\ldots,u^N)$ of commuting variables $u^1,\ldots,u^N$ one associates an element of algebra $\hat{f}$ when the commuting variables are substituted by anticommuting ones,

$$f(u)=\sum f_{i_1,\ldots,i_L}u^1\cdots u^N\to\hat{f}=\sum_{L=0}^{\infty} f_{i_1,\ldots,i_L}{:}\hat{u}^{i_1}\cdots\hat{u}^{i_L}{:}$$

when the $\diamondsuit$ product leads to a bilinear $*$-product of functions (see details in Ref. 70)

$$\{f_i\}\diamondsuit\{g_i\}=\{h_i\}\sim(f*g)(u)=h(u).$$

The $*$-product is defined, respectively, for the cases (D1);

$$f*g=\begin{cases} \exp\left[\dfrac{i}{2}\dfrac{\partial}{\partial u^i}\theta^{ij}\dfrac{\partial}{\partial u'^j}\right]f(u)g(u')|_{u'\to u},\\ \exp\left[\dfrac{i}{2}u^k g_k\left(i\dfrac{\partial}{\partial u'},i\dfrac{\partial}{\partial u''}\right)\right]f(u')g(u'')|_{u''\to u}^{u'\to u},\\ q^{1/2[-u'(\partial/\partial u')v(\partial/\partial v)+u(\partial/\partial u)v'(\partial/\partial v')]}f(u,v)g(u',v')|_{v'\to v}^{u'\to u}, \end{cases}$$

where there are considered values of type

$$e^{ik_n\hat{u}^n},\quad e^{ip_n\hat{u}^n}=e^{i\{k_n+p_n+1/2g_n(k,p)\}\hat{u}^n},$$

$$g_n(k,p)=-k_ip_jf_n^{ij}+\tfrac{1}{6}k_ip_j(p_k-k_k)f_m^{ij}f_n^{mk}+\cdots, \tag{D2}$$

$$e^Ae^B=e^{A+B+1/2[A,B]+1/12([A,[A,B]]+[B,[B,A]])}+\cdots,$$

and for the coordinates on quantum (Manin) planes one holds the relation $uv=qvu$.

A non-Abelian gauge theory on a noncommutative space is given by two algebraic structures, the algebra $\mathcal{A}_u$ and a non-Abelian–Lie algebra $\mathcal{A}_I$ of the gauge group with generators $I^1,\ldots,I^S$ and the relations

$$[I^{\underline{s}},I^{\underline{p}}]=if^{\underline{sp}}_{\underline{t}}I^{\underline{t}}. \tag{D3}$$

In this case both algebras are treated on the same footing and one denotes the generating elements of the big algebra by $\hat{u}^{i}$,

$$\hat{z}^{\underline{i}}=\{\hat{u}^{1},\ldots,\hat{u}^{N},I^{1},\ldots,I^{S}\},\quad \mathcal{A}_{z}=\mathrm{IC}[[\hat{u}^{1},\ldots,\hat{u}^{N+S}]]/\mathcal{R}$$

and the $*$-product formalism is to be applied for the whole algebra $\mathcal{A}_{z}$ when there are considered functions of the commuting variables u^{i} $(i,j,k,\ldots=1,\ldots,N)$ and $I^{\underline{s}}$ $(s,p,\ldots=1,\ldots,S)$.

For instance, in the case of a canonical structure for the space variables u^{i} we have

$$(F*G)(u)=\exp\left[\frac{i}{2}\left(\theta^{ij}\frac{\partial}{\partial u'^{i}}\frac{\partial}{\partial u''^{j}}+t^{s}g_{s}\left(i\frac{\partial}{\partial t'},i\frac{\partial}{\partial t''}\right)\right)\times F(u',t')G(u'',t'')\Big|^{u'\to u,u''\to u.}_{t'\to t,t''\to t}\right]. \tag{D4}$$

This formalism was developed in Ref. 90 for general Lie algebras.

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Two-spinor curvature structures for a class of conformally flat space–times

J. G. Cardoso
Department of Mathematics, Centre for Technological Sciences-UDESC, Joinville 89223-100 SC, Brazil

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A well-known class of conformally flat space–times which admit decomposable Christoffel connexions is considered. It is shown that the corresponding spin-affine configurations can be constructed within the framework of Infeld–van-der-Waerden's γ-formalism only if a specific constancy property is imposed on one of the densities borne by the expression for a typical metric function. Explicit expressions for the gravitational spinors of those space–times are then derived. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1876871]

I. INTRODUCTION

The present paper can be looked upon as an application of Infeld–van-der-Waerden's γ-formalism[1–5] that may be of a cosmological interest. Our procedures take up a work carried out originally by Penrose and Rindler,[6,7] which involves the utilization of a decomposable Christoffel connexion along with a particular spin-affine pattern for describing some properties of a class of conformally flat space–times. We establish that the consistency of the overall situation will be ensured only if the independent entry of any γ-metric spinor is taken to bear a specialized world-gauge form. In fact, this prescription automatically entails ascribing a specific symmetry property to the relevant spin-affine connexions, and likewise suggests a simple mechanism that allows one to keep track of all strongly required world behaviors[3] in a natural way. We deduce the conformal-flatness property by showing explicitly that the corresponding wave functions for gravitons vanish identically. It appears, in addition, that one of Infeld's expressions for Ricci scalars[2] becomes completely recoverable when the case of a real γ-metric function is effectively allowed for.

The world-spinor-index notation of Ref. 6 will be adopted throughout the work. Vertical bars surrounding an index block will mean that the indices singled out are not to partake of a symmetry operation. Space–time coordinates and a typical covariant world-metric tensor are denoted as x^a and g_{ab}, with

$$\partial_a \doteq \frac{\partial}{\partial x^a}.$$

One of the γ-metric spinors is set as

$$(\gamma_{AB}) = \begin{pmatrix} 0 & \gamma \\ -\gamma & 0 \end{pmatrix}, \quad \gamma = |\gamma| \exp(i\Phi),$$

where $(|\gamma|, \Phi)$ stands for a pair of differentiable real-valued world invariants. The Hermitian connecting objects for the γ-formalism are presumably taken as the elements of

$$\{\sigma_{aBB'}, \sigma^{a}_{BB'}, \sigma_{a}^{BB'}, \sigma^{aBB'}\},$$

while an appropriate unprimed-index spin connexion for it is written as $\gamma_{aB}{}^{C}$. For the eigenvalue occurring in the equation (see Ref. 5)

$$\partial_a \gamma_{AB} = \alpha_a \gamma_{AB},$$

we have the identification $\alpha_a = iK_a - \theta_a$, with

$$\theta_a = \partial_a \log|\gamma|^{-1}, \quad K_a \doteqdot \partial_a \Phi.$$

Some further conventions will be explained in due course.

We have outlined the paper as follows. All the specific metric and affine prescriptions are obtained in Sec. II. It will be expedient to build up in Sec. III some partial-derivative computational devices. The pertinent curvature structures are exhibited in Sec. IV. We shall make a few remarks on our work in Sec. V.

II. METRIC AND AFFINE PRESCRIPTIONS

Within the framework of the γ-formalism, the key metric prescription is written as[5]

$$|\gamma|^4 = \mu(-\mathfrak{g})^{1/2}, \tag{1}$$

where μ amounts to a real spin-scalar density of world weight -1 and absolute weight $+4$, which is defined by

$$\partial_a \log \mu = \sigma_b^{BB'} \partial_a \sigma_{BB'}^b. \tag{2}$$

These structures yield at once the expression

$$(-4)\theta_a = \partial_a \log[\mu(-\mathfrak{g})^{1/2}]. \tag{3}$$

Equation (3) can be specialized to the case wherein μ is identified with a density c that particularly bears ∂-constancy in a given world frame, namely

$$\sigma_b^{BB'} \partial_a \sigma_{BB'}^b = 0, \tag{4}$$

and, consequently, θ_a takes the noncovariant form

$$(-4)\theta_a = \partial_a \log[c(-\mathfrak{g})^{1/2}] = \Gamma_a. \tag{5}$$

Indeed, the required world covariance of γ_{aBC} and its complex conjugate[1] is simply recovered from the coordinate-transformation law (our Jacobian functional determinant Δ_W is the inverse of that used in Ref. 8)

$$c' = (\Delta_W)^{-1} c, \tag{6}$$

which also guarantees the world invariance of $|\gamma|$. The constancy of μ in the former world frame can be thought of as playing a "catalytic" role in the construction of a covariant vector θ_a from a metric expression of the form (3). Obviously, the affine relationship borne by Eq. (5) applies only to one of the frames of each character being eventually dealt with, while the law (6) ensures that the world behavior of the standard correlation[5]

$$\Gamma_{AA'BB'CC'} + \sigma_{sCC'} \partial_{AA'} \sigma_{BB'}^s = \gamma_{AA'BC} \gamma_{B'C'} + \gamma_{AA'B'C'} \gamma_{BC}, \tag{7}$$

will remain appropriately specified when Eq. (5) is actually called for.

To effectively derive the explicit affine expressions associated to the specialization (4), we initially make use of the eigenvalue equation

$$\partial_a(\gamma_{BC}\gamma_{B'C'}) = (-2\theta_a)\gamma_{BC}\gamma_{B'C'}, \tag{8}$$

together with its upper-spinor-index version, and implement configurations of the type

$$\sigma_b^{BB'}\partial_a\sigma_{BB'}^b = \sigma_b^{BB'}\partial_a(\sigma^{bCC'}\gamma_{CB}\gamma_{C'B'}). \tag{9}$$

Such a procedure leads us to the equations

$$\partial_a\sigma^{bBB'} = \left(-\tfrac{1}{2}\right)\Gamma_a\sigma^{bBB'}, \quad \partial_a\sigma_{bBB'} = \tfrac{1}{2}\Gamma_a\sigma_{bBB'}, \tag{10}$$

which immediately imply that

$$\partial_a g^{bc} = \left(-\tfrac{1}{2}\right)\Gamma_a g^{bc}, \quad \partial_a g_{bc} = \tfrac{1}{2}\Gamma_a g_{bc}. \tag{11}$$

We are then led to the constancy properties

$$\partial_a\sigma_b^{BB'} = 0, \quad \partial_a\sigma_{BB'}^b = 0, \tag{12}$$

along with the affine relationships[5]

$$\Gamma_{A(BC)A'(B'C')} = 0, \quad \tfrac{1}{2}\Gamma_{A(BC)A'D'}{}^{D'} = \theta_{A'(B}\,\gamma_{C)A} = \gamma_{AA'(BC)}, \tag{13}$$

which clearly satisfy

$$\gamma_{A'(ABC)} = 0. \tag{14}$$

It follows that we can write down the expansion[6]

$$\gamma_{AA'BC} = \theta_{BA'}\gamma_{CA} - i\Phi_{AA'}\gamma_{BC}, \tag{15}$$

from which we get the world expression

$$\Gamma_{abc} = \tfrac{1}{2}\sigma_c^{BB'}\sigma_{B'(a}^{A}\,\sigma_{b)B}^{A'}\Gamma_{AA'}, \tag{16}$$

with the quantity Φ_a being taken (the expansion given in Ref. 6 differs from ours by an overall "minus" sign) as a covariant world vector that bears a well-specified physical meaning (for further details, see Refs. 3 and 5). Hence, working out the index configuration of Eq. (16) produces the structures

$$\Gamma_{AA'BB'CC'} = \tfrac{1}{2}[\sigma_{CC'}^{h}(\partial_{BB'}\sigma_{hAA'} + \partial_{AA'}\sigma_{hBB'}) - \sigma_{BB'}^{h}\partial_{CC'}\sigma_{hAA'}] \tag{17}$$

and

$$\Gamma_{abc} = \tfrac{1}{2}\Gamma_{(a}\,g_{\,b)c} - \tfrac{1}{4}g_{ab}\Gamma_c. \tag{18}$$

We should observe that the first of Eqs. (13) amounts to the same thing as saying that the trace-free part of $\Gamma_{a(bc)}$ equals zero.

It will be established later in Sec. IV that world affinities of the type prescribed by Eq. (18) give rise to identically vanishing Weyl tensors, and thus specify parallel displacements in conformally flat space–times. In any such case, we can write down the derivatives

$$\nabla_{AA'}w_{BB'} = \partial_{AA'}w_{BB'} + \theta_{BA'}w_{AB'} + \theta_{AB'}w_{BA'} \tag{19}$$

and

$$\nabla_{AA'}u^{BB'} = \partial_{AA'}u^{BB'} - 2\theta_{AA'}u^{BB'} + \theta_A^B u_A^{B'} + \theta_A^{B'}u_{A'}^B, \tag{20}$$

which can therefore be reset as

$$\nabla_a w_b = \partial_a w_b + \tfrac{1}{4}g_{ab}(\Gamma^c w_c) - \tfrac{1}{2}\Gamma_{(a}\,w_{\,b)} \tag{21}$$

and

$$\nabla_a u^b = \partial_a u^b + \tfrac{1}{4}[(\Gamma_c u^c)\delta_a{}^b + \Gamma_a u^b - g_{ac}\Gamma^b u^c], \tag{22}$$

with $\Gamma^a \doteq g^{ab}\Gamma_b$.

III. ∂-DEVICES

Equations (12) make it legitimate to account for the spinor commutator

$$[\partial_{AA'}, \partial_{BB'}] = \sigma^a_{AA'}\sigma^b_{BB'}[\partial_a, \partial_b] = 0. \tag{23}$$

Transvecting (23) with γ^{AB} and $\gamma^{A'B'}$ provides us with the commutativity property

$$\partial^A_{(A'}\,\partial_{B')A} = 0 \Rightarrow \partial^A_{A'}\partial_{B'A} = \partial^A_{[A'}\,\partial_{B']A}, \tag{24}$$

along with its complex conjugate. Then, using either of the relations

$$\partial^A_{(A'}\,\partial_{B')A} = \partial^A_{(A'}\,(\gamma_{|BA|}\partial^B_{B')}), \quad \partial^A_{(A'}\,\partial_{B')A} = \gamma^{AB}\partial_{B(A'}\,\partial_{B')A}, \tag{25}$$

yields the derivative-order lowering device

$$\partial_{A(A'}\,\partial^A_{B')} = (-1)\alpha_{A(A'}\,\partial^A_{B')}, \tag{26}$$

together with the formal bivector splittings (henceforth, the symbol "c.c." will stand for an overall complex-conjugate piece),

$$[\partial_{AA'}, \partial_{BB'}] = (-1)(\gamma_{AB}\partial^C_{(A'}\,\partial_{B')C} + \text{c.c.}), \tag{27}$$

and

$$[\partial_{AA'}, \partial_{BB'}] = \gamma_{AB}(\partial_{C(A'}\,\partial^C_{B')} + \alpha_{C(A'}\,\partial^C_{B')}) + \text{c.c.} \tag{28}$$

It should be pointed out that the only ∂-prescriptions for manipulating adequately skew two-covariant-index structures are supplied by the rules

$$\partial_{A'[A}\,\partial_{B]B'} = \tfrac{1}{2}\gamma_{BA}\partial^C_{A'}\partial_{B'C} = \tfrac{1}{2}\partial_{A'C}(\gamma_{AB}\partial^C_{B'}), \tag{29}$$

and their complex conjugates. We thus have the useful relations

$$\partial_{AA'}\partial_{BB'} = \partial_{(A(A'}\,\partial_{B')B)} + \tfrac{1}{4}\gamma_{AB}\gamma_{A'B'}g^{ch}\partial_c\partial_h, \tag{30}$$

$$2(\partial_{AA'} + \alpha_{AA'})\partial^A_{B'} = 2(\partial_{A[A'} + \alpha_{A[A'})\partial^A_{B']} = \gamma_{A'B'}(\alpha^h\partial_h - \partial^{C'}_A\partial^A_{C'}), \tag{31}$$

and

$$\gamma^{AB}\partial^{C'}_D(\gamma_{AB}\partial^D_{C'}) = (-2)\partial^{CC'}\partial_{CC'} = \gamma^{A'B'}\partial^C_{D'}(\gamma_{A'B'}\partial^{D'}_C). \tag{32}$$

Therefore, we can utilize the configurations

$$\partial_{CA'}\partial^C_{B'} + \alpha_{CA'}\partial^C_{B'} = (-1)\partial^C_{A'}\partial_{CB'} \tag{33}$$

and

$$2(\partial_{AA'} + \alpha_{AA'})\partial^A_{B'} = \gamma_{A'B'}\partial^{CC'}\partial_{CC'}. \tag{34}$$

A remarkable feature of the upper-spinor-index version of Eq. (23) is the fact that a relation formally similar to (26) can also be derived, but now *no* zero operator actually arises. This result

reflects the noncommutativity of the partial-derivative operators that carry upper-world indices, namely

$$\partial^a \doteq g^{ab}\partial_b, \quad [\partial^a,\partial^b] = 2(\partial^{[a}\, g^{\,b]c})\partial_c = 4\theta^{[a}\,\partial^{\,b]}. \tag{35}$$

As regards the last equality of (35), it is worth observing that

$$g^{c[a}\, g^{\,b]h}\partial_c\partial_h = g^{a[c}\, g^{\,h]b}\partial_c\partial_h = 0. \tag{36}$$

We also remark that Eqs. (12) guarantee the applicability of the relations

$$\partial^{\mathcal{C}}\partial_c = \partial^{CC'}\partial_{CC'}, \quad \partial_c\partial^{\mathcal{C}} = \partial_{CC'}\partial^{CC'}. \tag{37}$$

A short calculation then gives the spinor relationships

$$\partial^{C'(A}\,\partial^{\,B)}_{C'} = \theta^{C'(A}\,\partial^{\,B)}_{C'} - iK^{C'(A}\,\partial^{\,B)}_{C'} \tag{38}$$

and

$$\partial^{(A'}_{C}\,\partial^{\,B')C} = 2\,\theta^{(A'}_{C}\,\partial^{\,B')C}, \tag{39}$$

as well as their complex conjugates. We thus have the structures

$$\gamma_{AC}\gamma_{BD}\partial^{C'(C}\,\partial^{\,D)}_{C'} = (-1)\,\alpha^{C'}_{(A}\,\partial_{\,B)C'}, \tag{40}$$

and

$$\gamma_{A'C'}\gamma_{B'D'}\partial^{(C'}_{C}\,\partial^{\,D')C} = (-2)(\mathrm{Re}\;\alpha^h)\sigma_{hC(A'}\,\partial^{C}_{\,B')}, \tag{41}$$

which, when worked out explicitly, turn out to agree with Eqs. (25) and (26). We notice that the contravariant counterparts of the devices (29) must be written as

$$\partial^{A'[A}\,\partial^{\,B]B'} = \tfrac{1}{2}\gamma^{AB}\partial^{A'}_{C}\,\partial^{B'C} = \tfrac{1}{2}\partial^{A'C}(\gamma^{BA}\partial^{B'}_{C}), \tag{42}$$

and, consequently, we can likewise put into practice the upper-primed-index version of the correlation (33), namely

$$\partial^{A'}_{C}\partial^{B'C} + \alpha^{A'}_{C}\,\partial^{B'C} = (-1)\partial^{CA'}\partial^{B'}_{C}. \tag{43}$$

Accordingly, the contravariant bivector configuration may be set as

$$[\partial^{AA'},\partial^{BB'}] = \gamma^{AB}\partial^{(A'}_{M}\,\partial^{\,B')M} + \gamma^{A'B'}\partial^{(A}_{M'}\partial^{\,B)M'}. \tag{44}$$

For some differentiable object χ_a, we particularly have the device

$$\partial_{AA'}\chi^{A}_{B'} + \alpha_{AA'}\chi^{A}_{B'} = (-1)\partial^{A}_{A'}\chi_{AB'}. \tag{45}$$

In case $\chi_a = \partial_a f$, with f being some adequate numerical function, Eq. (24) will immediately supply the skew-symmetry relation

$$\partial^{A}_{A'}\chi_{AB'} = \partial^{A}_{[A'}\,\chi_{\,B']A}. \tag{46}$$

Thus, on the basis of Eqs. (11) and (29), we can implement the statements

$$(-2)\partial^{A}_{[A'}\,\chi_{\,B']A} = \gamma_{A'B'}\partial^h\chi_h = \gamma_{A'B'}\Omega_h\chi^h \tag{47}$$

and

$$\partial_{A(A'}\,\chi^{A}_{\ B')} = (-1)\alpha_{A(A'}\,\chi^{A}_{\ B')}, \tag{48}$$

with $\Omega_h \doteq \partial_h - 2\theta_h$. Moreover, since θ_a and K_a are both expressed as ∂-derivatives, we can spell out the eigenvalue equations

$$\partial_{A(A'}\,\theta^{A}_{\ B')} = (-i)K_{A(A'}\,\theta^{A}_{\ B')}, \tag{49}$$

and

$$\partial_{A(A'}\,K^{A}_{\ B')} = \theta_{A(A'}\,K^{A}_{\ B')}, \tag{50}$$

along with their complex conjugates. Equations (47) and (48) will play a significant role in the development of Sec. IV.

IV. CURVATURE STRUCTURES

There are two essentially equivalent procedures for expressing in terms of explicit spin-affine pieces the curvature spinors of the connexion given as Eq. (15). One consists in working out the bivector configurations that arise out of the implementation of generalized covariant spinor commutators,[3,5] while the other just involves the spinor translation of the classical world expression for the Riemann tensor $R_{abc}^{\ \ d}$ of the Christoffel connexion (18). We will adopt the latter procedure here insofar the legitimacy of the work of the preceding section may automatically afford a verification of the curvature formulas for the class of space–times at issue. An identically vanishing Weyl spinor will thus emerge, but the point regarding the admissibility of its symmetries[6,9,10] will be illustrated. The configurations arising at this stage coincide with the cosmological ones afforded by Ref. 11.

To start with, let us consider the contribution

$$\begin{aligned} 2\partial_{[AA'}\,\Gamma_{\ BB']CC'}^{\ \ \ \ \ \ DD'} &= 2\gamma_{C'}^{\ \ D'}\partial_{[AA'}\,\gamma_{\ BB']C}^{\ \ \ D} + \text{c.c.} \\ &= \gamma^{D'}_{\ \ C'}(\gamma_{AB}\partial^{M}_{(A'}\,\gamma_{\ B')MC}^{\ \ \ \ D} + \gamma_{A'B'}\partial^{M'}_{(A}\,\gamma_{\ B)M'C}^{\ \ \ \ D}) + \text{c.c.}, \end{aligned} \tag{51}$$

where the square brackets accordingly mean skew-symmetrization over the index pairs. It is useful to implement the splittings

$$\partial^{M}_{(A'}\,\gamma_{\ B')MC}^{\ \ \ \ D} = \partial^{M}_{(A'}\,[\gamma^{DS}(\gamma_{\ B')M(CS)} + \gamma_{\ B')M[CS]})] \tag{52}$$

and

$$\partial^{M'}_{(A}\,\gamma_{\ B)M'C}^{\ \ \ \ D} = \partial^{M'}_{(A}[\gamma^{DS}(\gamma_{\ B)M'(CS)} + \gamma_{\ B)M'[CS]})], \tag{53}$$

together with their complex conjugates. The overall *CS*-skew contribution of (51) is proportional to

$$\begin{aligned} (\gamma_{AB}\partial^{M}_{(A'}\,\gamma_{\ B')ML}^{\ \ \ \ L} + \gamma_{A'B'}\partial^{M'}_{(A}\,\gamma_{\ B)M'L}^{\ \ \ \ L}) + \text{c.c.} &= (-1)[\gamma_{AB}(\partial^{M}_{(A'}\,\theta_{\ B')M} + 2i\partial^{M}_{(A'}\,\Phi_{\ B')M}) \\ &\quad + \gamma_{A'B'}(\partial^{M'}_{(A}\,\theta_{\ B)M'} + 2i\partial^{M'}_{(A}\,\Phi_{\ B)M'})] + \text{c.c.} \end{aligned} \tag{54}$$

Each of the $\partial\theta$ pieces of Eq. (54) vanishes because of the property (24), whereas each $\partial\Phi$ piece involved explicitly is cancelled by the complex-conjugate contribution. Calling upon the expansion (15), we perform the following calculation [one should notice that $\partial_a\gamma^{AB} = (-\alpha_a)\gamma^{AB}$] for the symmetric parts of Eqs. (52) and (53):

$$\gamma_{AB}\partial^{M}_{(A'}(\gamma^{DS}\gamma_{B')M(CS)}) + \gamma_{A'B'}\partial^{M'}_{(A}(\gamma^{DS}\gamma_{B)M'(CS)}) = \gamma^{DS}[\gamma_{AB}(\partial^{M}_{(A'}\gamma_{B')M(CS)} - \alpha^{M}_{(A'}\gamma_{B')M(CS)}) + \gamma_{A'B'}(\partial^{M'}_{(A}\gamma_{B)M'(CS)} - \alpha^{M'}_{(A}\gamma_{B)M'(CS)})] = \gamma^{DS}(\gamma_{A'B'}\gamma_{(C|(A}\partial^{M'}_{B)|}\theta_{S)M'} - \gamma_{AB}\partial_{(C(A'}\theta_{B')S)}). \tag{55}$$

In order to make up the expression for the left-hand side of (51), we invoke the complex-conjugate version of Eqs. (47) and (48), to obtain

$$\gamma_{(C|(A}\partial^{M'}_{B)|}\theta_{S)M'} = \left(-\tfrac{1}{2}\right)\gamma_{C(A}\gamma_{B)S}\Omega_h\theta^h. \tag{56}$$

Thus, the overall $\partial\Gamma$-contribution reads

$$2\partial_{[AA'}\Gamma_{BB']CC'}{}^{DD'} = \gamma_{C'}{}^{D'}\gamma^{DS}\left(\tfrac{1}{2}\gamma_{A'B'}\gamma_{C(A}\gamma_{B)S}\Omega_h\theta^h + \gamma_{AB}\partial_{(C(A'}\theta_{B')S)}\right) + \text{c.c.} \tag{57}$$

The relevant quadratic Γ term is written out as the bivector configuration

$$2\Gamma_{MM'[AA'}{}^{DD'}\Gamma_{BB']CC'}{}^{MM'} = [\gamma_{AB}(\gamma^{D'}{}_{(A'}\gamma_{B')SC}{}^{M}\gamma_{MC'}{}^{SD} + \gamma^{D'}{}_{(A'}\gamma_{B')SC'}{}^{M'}\gamma_{CM'}{}^{SD}) + \gamma_{A'B'}(\gamma_{MC'(A}{}^{D}\gamma^{D'}_{B)C}{}^{M} + \gamma_{CM'(A}{}^{D}\gamma^{D'}_{B)C'}{}^{M'})] + \text{c.c.} \tag{58}$$

Manipulating the indices of Eqs. (15) and (58) gives

$$2\Gamma_{MM'[AA'}{}^{DD'}\Gamma_{BB']CC'}{}^{MM'} = [\gamma_{AB}(\gamma^{D'}{}_{(A'}\theta_{B')C}\theta^{D}_{C'} - \gamma^{D'}{}_{(A'}\theta^{M}_{B')}\theta_{MC'}\gamma^{D}{}_{C}) + \gamma_{A'B'}(\theta^{D'}_{(A}\theta_{B)C'}\gamma_{C}{}^{D} - \gamma^{D}{}_{(A}\theta_{B)C'}\theta^{D'}_{C})] + \text{c.c.} \tag{59}$$

Hence, lowering the indices DD' of (57) and (59), after rearranging conjugate pieces and implementing the computational results

$$\gamma_{C'D'}\gamma_{D(A}\theta^{M'}_{B)}\theta_{CM'} + \gamma_{D(A}\theta_{B)C'}\theta_{CD'} + \gamma_{CD}\theta_{D'(A}\theta_{B)C'} + \theta_{CD'}\theta_{C'(A}\gamma_{B)D} = \gamma_{CD}\theta_{(C'(A}\theta_{B)D')} + \gamma_{C'D'}\theta_{M'(A}\gamma_{B)(C}\theta^{M'}_{D)} \tag{60}$$

and

$$\theta_{M'(A}\gamma_{B)(C}\theta^{M'}_{D)} = \left(-\tfrac{1}{2}\right)\gamma_{C(A}\gamma_{B)D}\theta_h\theta^h, \tag{61}$$

we arrive at the irreducible expression

$$R_{AA'BB'CC'DD'} = \gamma_{A'B'}\left[\gamma_{CD}(\partial_{(C'(A}\theta_{B)D')} + \theta_{(C'(A}\theta_{B)D')}) + \tfrac{1}{2}\gamma_{C'D'}\gamma_{C(A}\gamma_{B)D}(\Omega_h\theta^h - \theta_h\theta^h)\right] + \text{c.c.} \tag{62}$$

We emphasize that the Riemann spinor (62) bears world invariance. In essence, this comes from the fact that the operator Ω_h can be expressed covariantly as $(\nabla_h + 2\theta_h)$ upon acting on θ^h.

To carry through our main procedure, we simply apply to the left-hand side of Eq. (62) the formal definitions

$$\mathrm{X}_{ABCD} \doteqdot \tfrac{1}{4}M^{A'B'}M^{C'D'}R_{AA'BB'CC'DD'} \tag{63}$$

and

$$\Xi_{CA'DB'} \doteqdot \tfrac{1}{4}M^{AB}M^{C'D'}R_{AA'BB'CC'DD'}, \tag{64}$$

which amount to the gravitational spinors of $\gamma_{aB}{}^{C}$. We thus readily obtain the structures

$$\mathrm{X}_{ABCD} = \tfrac{1}{2}(\partial_h \theta^h - 3\theta_h \theta^h)\gamma_{C(A}\,\gamma_{B)D} = \tfrac{1}{2}(\nabla_h \theta^h + \theta_h \theta^h)\gamma_{C(A}\,\gamma_{B)D} \tag{65}$$

and

$$\Xi_{CA'DB'} = \partial_{(C(A'}\,\theta_{B')D)} + \theta_{(C(A'}\,\theta_{B')D)}, \tag{66}$$

which exhibit all the characteristic symmetries. (The most natural procedure for fixing the symmetries of the $X\Xi$ spinors is provided in Ref. 5.) Evidently, the X-spinor (65) bears a purely cosmological character, that is to say,

$$\mathrm{X}_{(ABCD)} \doteq \Psi_{ABCD} \equiv 0, \tag{67}$$

while the Ricci tensor of the connexion (18) appears to be associated to the configuration

$$R_{AA'BB'} = \left(-\tfrac{3}{2}\right)(\nabla_h \theta^h + \theta_h \theta^h)\gamma_{AB}\gamma_{A'B'} - 2(\partial_{(A(A'}\,\theta_{B')B)} + \theta_{(A(A'}\,\theta_{B')B)}), \tag{68}$$

which promptly yields the cosmological expressions

$$\lambda = \tfrac{3}{2}(3\theta_h \theta^h - \partial_h \theta^h) = \left(-\tfrac{3}{2}\right)(\nabla_h \theta^h + \theta_h \theta^h), \tag{69}$$

where λ is the so-called cosmological constant.[6,12]

The structures exhibited previously give rise to an expression for a Ricci scalar that coincides in the case of a real eigenvector α_a with a formula given much earlier by Infeld.[2] An easy way of deducing this result involves first implementing the relation

$$\partial_a \theta^a = \partial^A_{A'}\partial^{A'}_A \log|\gamma| - \alpha_a \theta^a, \tag{70}$$

and then performing the calculation

$$R = 6(3\theta_a \theta^a - \partial_a \theta^a) = 6[2\theta_a \theta^a + (iK_a \theta^a - \partial^A_{A'}\partial^{A'}_A \log|\gamma|)] = 3\left[4\theta_a \theta^a + 2iK_a \theta^a - \partial^A_{A'}\left(\frac{1}{|\gamma|^2}\partial^{A'}_A |\gamma|^2\right)\right]$$

$$= 3\left(2iK_a \theta^a - \frac{1}{|\gamma|^2}\partial^A_{A'}\partial^{A'}_A |\gamma|^2\right). \tag{71}$$

V. CONCLUSIONS AND OUTLOOK

The work we have presented above sheds some light on the spinor description of conformally flat space–times that bear affine structures having the form specified by Eq. (18). It thereby clarifies once and for all the situation concerning the geometric significance of the choice (14). We believe that it would be worthwhile to derive a set of pertinent world-transformation laws. It can be shown that, under the circumstances stipulated in Sec. II, any properties like those exhibited as Eqs. (12) must behave invariantly under the action of manifold mapping groups. We will probably elaborate upon these matters elsewhere.

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A note on positive energy theorem for spaces with asymptotic SUSY compactification

Xianzhe Dai
Mathematics, University of California Santa Barbara, Santa Barbara, California 93106

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We extend the higher dimensional positive mass theorem in [Dai, X., Commun. Math. Phys. **244**, 335–345 (2004)] to the Lorentzian setting. This includes the original higher dimensional positive energy theorem whose spinor proof is given in [Witten, E., Commun. Math. Phys. **80**, 381–402 (1981)] and [Parker, T., and Taubes, C., Commun. Math. Phys. **84**, 223–238 (1982)] for dimension 4 and in [Zhang, X., J. Math. Phys. **40**, 3540–3552 (1999)] for dimension 5. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1862095]

I. INTRODUCTION AND STATEMENT OF THE RESULT

In this note, we formulate and prove the Lorentzian version of the positive mass theorem in Ref. 4. There we prove a positive mass theorem for spaces of any dimension which asymptotically approach the product of a flat Euclidean space with a compact manifold which admits a nonzero parallel spinor (such as a Calabi–Yau manifold or any special honolomy manifold except the quaternionic Kähler manifold). This is motivated by string theory, especially the recent work in Ref. 7. The application of the positive mass theorem of Ref. 4 to the study of stability of Ricci flat manifolds is discussed in Ref. 5.

In general relativity, a space–time is modelled by a Lorentzian 4-manifold (N,g) together with an energy-momentum tensor T satisfying Einstein equation

$$R_{\alpha\beta} - \tfrac{1}{2} g_{\alpha\beta} R = 8\pi T_{\alpha\beta}. \tag{1.1}$$

The positive energy theorem[11,14] says that an isolated gravitational system with non-negative local matter density must have non-negative total energy, measured at spatial infinity. More precisely, one considers a complete oriented spacelike hypersurface M of N satisfying the following two conditions.

(a) *M is asymptotically flat*, that is, there is a compact set K in M such that $M-K$ is the disjoint union of a finite number of subsets $M_1,\ldots,M_k$ and each end M_l is diffeomorphic to $\mathbb{R}^3 - B_R(0)$. Moreover, under this diffeomorphism, the metric of M_l is of the form

$$g_{ij} = \delta_{ij} + O(r^{-\tau}), \quad \partial_k g_{ij} = O(r^{-\tau-1}), \quad \partial_k \partial_l g_{ij} = O(r^{-\tau-2}). \tag{1.2}$$

Furthermore, the second fundamental form h_{ij} of M in N satisfies

$$h_{ij} = O(r^{-\tau-1}), \quad \partial_k h_{ij} = O(r^{-\tau-2}). \tag{1.3}$$

Here $\tau > 0$ is the asymptotic order and r is the Euclidean distance to a base point.

(b) *M has non-negative local mass density*: for each point $p \in M$ and for each timelike vector e_0 at p, $T(e_0,e_0) \geqslant 0$ and $T(e_0,\cdot)$ is a nonspacelike covector. This implies the dominant energy condition

$$T^{00} \geqslant |T^{\alpha\beta}|, \quad T^{00} \geqslant (-T_{0i}T^{0i})^{1/2}. \tag{1.4}$$

The total energy (the ADM mass) and the total (linear) momentum of M can then be defined as follows[1,10] [for simplicity we suppress the dependence here on l (the end M_l)]:

$$E = \lim_{R\to\infty} \frac{1}{4\omega_n} \int_{S_R} (\partial_i g_{ij} - \partial_j g_{ii}) * \mathrm{d}x_j,$$
$$P_k = \lim_{R\to\infty} \frac{1}{4\omega_n} \int_{S_R} 2(h_{jk} - \partial_{jk} h_{ii}) * \mathrm{d}x_j. \tag{1.5}$$

Here $x_1, \ldots, x_n$ are the Euclidean coordinates on the end; $*$ denotes the Hodge star operator; ω_n denotes the volume of the $n-1$ sphere and S_R the Euclidean sphere with radius R centered at the base point. When the asymptotic order $\tau > (n-2)/2$, these quantities are finite and independent of the asymptotic coordinates. [Here $n=3$.]

Theorem 1.1: (Refs. 12–14): *With the assumptions as above and assuming that M is spin, one has*

$$E - |P| \geqslant 0$$

on each end M_l. Moreover, if $E=0$ for some end M_l, then M has only one end and N is flat along M.

Now, according to string theory,[2] our universe is really 10-dimensional, modelled on $\mathbb{R}^{3,1} \times X$ where X is a Calabi–Yau threefold. This is the so-called Calabi–Yau compactification[6] which motivates the spaces we now consider.

Thus we consider a Lorentzian manifold N [with signature $(-, +, \cdots, +)$] of $\dim N = n+1$, with a energy-momentum tensor satisfying the Einstein equation. Then let M be a complete oriented spacelike hypersurface in N. Further, assume that the Riemannian manifold (M^n, g) with g induced from the Lorentzian metric decomposes $M = M_0 \cup M_1 \cup \cdots \cup M_s$, where M_0 is compact as before but now each of the ends $M_l \simeq (\mathbb{R}^k - B_R(0)) \times X_l$ for some radius $R > 0$ and X_l a compact simply connected spin manifold which admits a nonzero parallel spinor. Moreover the metric on each M_l satisfies

$$g = \mathring{g} + u, \quad \mathring{g} = g_{\mathbb{R}^k} + g_X, \quad u = O(r^{-\tau}), \quad \mathring{\nabla} u = O(r^{-\tau-1}), \quad \mathring{\nabla}\mathring{\nabla} u = O(r^{-\tau-2}), \tag{1.6}$$

and the second fundamental form h of M in N satisfies

$$h = O(r^{-\tau-1}), \quad \mathring{\nabla} h = O(r^{-\tau-2}). \tag{1.7}$$

Here $\mathring{\nabla}$ is the Levi–Civita connection of $\mathring{g}$ (extended to act on all tensor fields), r the Euclidean distance in the Euclidean factor, and $\tau > 0$ is the asymptotical order.

The total energy and total momentum for each end M_l can then be defined by (again we suppress the dependence on l here)

$$E = \lim_{R\to\infty} \frac{1}{4\omega_k vol(X)} \int_{S_R\times X} (\partial_i g_{ij} - \partial_j g_{aa}) * \mathrm{d}x_j \, \mathrm{d}vol(X),$$
$$P_k = \lim_{R\to\infty} \frac{1}{4\omega_k vol(X)} \int_{S_R\times X} 2(h_{jk} - \partial_{jk} h_{ii}) * \mathrm{d}x_j \, \mathrm{d}vol(X). \tag{1.8}$$

Here the $*$ operator is the one on the Euclidean factor, the index i, j run over the Euclidean factor and g_{aa} is the trace of the metric g on the manifold M.

Then we have the following.

Theorem 1.2: *Assuming that M is spin and $\tau > (k-2)/2$, $k \geqslant 2$, one has*

$$E - |P| \geqslant 0$$

on each end M_l. Moreover, if $E=0$ for some end M_l, then M has only one end and N is flat along M.

In particular, this result includes the original positive energy theorem whose spinor proof is given in Refs. 14 and 10 for dimension 4 and in Ref. 15 for dimension 5. The dimension specific nature in these work is due to the use of special isomorphisms of low dimensional spin groups. Here we construct the desired metrics directly using the Clifford algebra .

Remark: If M is globally a product $\mathbb{R}^k \times X$ topologically, then the compact factor X need not be simply connected. The simply connected condition is imposed to guarantee that the spin structure on the ends coincides with the one obtained by restricting the spin structure from the inside.

II. THE HYPERSURFACE DIRAC OPERATOR

We will adapt Witten's spinor method[14] to our situation. For that, we follow the presentation and notations of Ref. 10. The crucial ingredient here is the hypersurface Dirac operator on M, acting on the (restriction of the) spinor bundle of N. Let S be the spinor bundle of N and still denote by the same notation its restriction (or rather, pullback) to M. Denote by ∇ the connection on S induced by the Lorentzian metric on N. The Lorentzian metric on N also induces a Riemannian metric on M, whose Levi–Civita connection gives rise to another connection, $\overline{\nabla}$ on S. The two, of course, differ by a term involving the second fundamental form.

There are two choices of metrics on S, which is another subtlety here. Since part of the treatment in Ref. 10 is special to dimension 4, we will give a construction directly using the Clifford algebra Ref. 8.

Let $\mathrm{SO}(n,1)$ denote the identity component of the groups of orientation preserving isometries of the Minkowski space $\mathbb{R}^{n,1}$. A choice of a unit timelike covector e^0 gives rise to injective homomorphisms α, $\hat{\alpha}$, and a commutative diagram

$$\begin{array}{rccc} \alpha\colon & \mathrm{SO}(n) & \rightarrow & \mathrm{SO}(n,1) \\ & \uparrow & & \uparrow \\ \hat{\alpha}\colon & \mathrm{Spin}(n) & \rightarrow & \mathrm{Spin}(n,1). \end{array} \tag{2.1}$$

We now fix a choice of unit timelike normal covector e^0 of M in N. Let $F(N)$ denote the $\mathrm{SO}(n,1)$ frame bundle of N and $F(M)$ the $\mathrm{SO}(n)$ frame bundle of M. Then $i^*F(N)=F(M)\times_\alpha \mathrm{SO}(n,1)$, where $i\colon M\hookrightarrow N$ is the inclusion. If N is spin, then we have a principal $\mathrm{Spin}(n,1)$ bundle $P_{\mathrm{Spin}(n,1)}$ on N, whose restriction on M is then $i^*P_{\mathrm{Spin}(n,1)}=P_{\mathrm{Spin}(n)}\times_{\hat{\alpha}}\mathrm{Spin}(n,1)$, where $P_{\mathrm{Spin}(n)}$ is the principal $\mathrm{Spin}(n)$ bundle of M. Thus, even if N is not spin, $i^*P_{\mathrm{Spin}(n,1)}$ is still well-defined as long as M is spin.

Similarly, when N is spin, the spinor bundle S on N is the associated bundle $P_{\mathrm{Spin}(n,1)}\times_{\rho_{n,1}}\Delta$, where $\Delta=\mathbb{C}^{2^{[(n+1)/2]}}$ is the complex vector space of spinors and

$$\rho_{n,1}\colon \mathrm{Spin}(n,1)\rightarrow \mathrm{GL}(\Delta) \tag{2.2}$$

is the spin representation. Its restriction to M is given by $i^*P_{\mathrm{Spin}(n,1)}\times_{\rho_{n,1}}\Delta=P_{\mathrm{Spin}(n)}\times_{\rho_n}\Delta$ with

$$\rho_n\colon \mathrm{Spin}(n)\overset{\hat{\alpha}}{\hookrightarrow}\mathrm{Spin}(n,1)\xrightarrow{\rho_{n,1}}\mathrm{GL}(\Delta). \tag{2.3}$$

Again, the restriction is still well defined as long as M is spin.

Let e^0, e^i be an orthonormal basis of the Minkowski space $\mathbb{R}^{n,1}$ such that $|e^0|^2=-1$ (in this section the indices i and j range from 1 to n).

Lemma 2.1: There is a positive definite Hermitian inner product $\langle,\rangle$ on Δ which is Spin(n)-invariant. Moreover, $(s,s')=\langle e^0\cdot s,s'\rangle$ defines a Hermitian inner product which is also Spin(n)-invariant but not positive definite. In fact

$$(v\cdot s,s')=(s,v\cdot s')$$

for all $v\in\mathbb{R}^{n,1}$.

Proof: Detailed study via Γ matrices (Ref. 3, pp. 10 and 11) shows that there is a positive definite Hermitian inner product $\langle,\rangle$ on Δ with respect to which e^i is skew-Hermitian while e^0 is Hermitian. It follows then that $\langle,\rangle$ is Spin(n)-invariant. We now show that $(s,s')=\langle e^0\cdot s,s'\rangle$ defines a Spin(n)-invariant Hermitian inner product. Since e^0 is Hermitian with respect to $\langle,\rangle$, $(,)$ is clearly Hermitian. To show that $(,)$ is Spin(n)-invariant, we take a unit vector v in the Minkowski space, $v=a_0e^0+a_ie^i$, a_0, $a_i\in\mathbb{R}$, and $-a_0^2+\Sigma_{i=1}^n a_i^2=1$. Then

$$\begin{aligned}(vs,vs')&=\langle e^0vs,vs'\rangle=a_0^2\langle e^0e^0s,e^0s'\rangle+a_ia_0\langle e^0e^is,e^0s'\rangle+a_0a_i\langle e^0e^0s,e^is'\rangle+a_ia_j\langle e^0e^is,e^js'\rangle\\&=a_0^2\langle s,e^0s'\rangle-a_ia_j\langle e^je^0e^is,s'\rangle=a_0^2\langle e^0s,s'\rangle+a_ia_j\langle e^0e^je^is,s'\rangle\\&=a_0^2\langle e^0s,s'\rangle-a_i^2\langle e^0s,s'\rangle=-(s,s').\end{aligned}$$

Consequently, $(,)$ is Spin(n)-invariant. The above computation also implies that $v\cdot$ acts as Hermitian operator on Δ with respect to $(,)$. ■

Thus the spinor bundle S restricted to M inherits an Hermitian metric $(,)$ and a positive definite metric $\langle,\rangle$. They are related by the equation

$$(s,s')=\langle e^0\cdot s,s'\rangle. \tag{2.4}$$

Now the hypersurface Dirac operator is defined by the composition

$$\mathcal{D}:\Gamma(M,S)\xrightarrow{\nabla}\Gamma(M,T^*M\otimes S)\xrightarrow{c}\Gamma(M,S), \tag{2.5}$$

where c denotes the Clifford multiplication. In terms of a local orthonormal basis $e_1,e_2,\ldots,e_n$ of TM,

$$\mathcal{D}\psi=e^i\cdot\nabla_{e_i}\psi,$$

where e^i denotes the dual basis.

The two most important properties of hypersurface Dirac operator are the self-adjointness with respect to the metric $\langle,\rangle$ and the Bochner–Lichnerowicz–Weitzenbock formula.[14,10]

Lemma 2.2: Define a $(n-1)$*-form on* M *by* $\omega=\langle\phi,e^i\cdot\psi\rangle\mathrm{int}(e_i)\mathrm{d}vol$*, where* $\mathrm{d}vol$ *is the volume form of the Riemannian metric* g *and* $\mathrm{int}(e_i)$ *is the interior multiplication by* e_i*. We have*

$$[\langle\phi,\mathcal{D}\psi\rangle-\langle\mathcal{D}\phi,\psi\rangle]\mathrm{d}vol=\mathrm{d}\omega.$$

Thus $\mathcal{D}$ *is formally self-adjoint with respect to the* L^2 *metric defined by* $\langle,\rangle$ *and* $\mathrm{d}vol$*.*

Proof: Since ω is independent of the choice of the orthonormal basis, we do our computation locally using a preferred basis. For any given point $p\in M$, choose a local orthonormal frame e_i of TM near p such that $\overline{\nabla e_i}=0$ at p. Extend e_0, e_i to a neighborhood of p in N by parallel translating along e_0 direction. Then, at p, $\nabla_{e_i}e^j=-h_{ij}e^0$ and $\nabla_{e_i}e^0=-h_{ij}e^j$. Therefore (again at p),

$$\begin{aligned}\mathrm{d}\omega&=\nabla_{e_i}\langle\phi,e^i\cdot\psi\rangle\mathrm{d}vol\\&=[((\nabla_{e_i}e^0)\cdot\phi,e^i\cdot\psi)+(e^0\cdot\nabla_{e_i}\phi,e^i\cdot\psi)+(e^0\cdot\phi,(\nabla_{e_i}e^i)\cdot\psi)+(e^0\cdot\phi,e^i\cdot\nabla_{e_i}\psi)]\mathrm{d}vol\\&=[-h_{ij}(e^j\cdot\phi,e^i\cdot\psi)+(e^i\cdot e^0\cdot\nabla_{e_i}\phi,\psi)-h_{ii}(e^0\cdot\phi,e^0\cdot\psi)+\langle\phi,\mathcal{D}\psi\rangle]\mathrm{d}vol\\&=[-h_{ij}(e^i\cdot e^j\cdot\phi,\psi)-\langle\mathcal{D}\phi,\psi\rangle-h_{ii}(e^0\cdot\phi,e^0\cdot\psi)+\langle\phi,\mathcal{D}\psi\rangle]\mathrm{d}vol\\&=[-\langle\mathcal{D}\phi,\psi\rangle+\langle\phi,\mathcal{D}\psi\rangle]\mathrm{d}vol.\end{aligned}$$

■

The second property we need is the Bochner–Lichnerowicz–Weitzenbock formula. For a proof, see Ref. 10.

Lemma 2.3: One has

$$\mathcal{D}^2 = \nabla^* \nabla + \mathcal{R},$$
$$\mathcal{R} = \tfrac{1}{4}(R + 2R_{00} + 2R_{0i}e^0 \cdot e^i \cdot) \in \mathrm{End}(S). \tag{2.6}$$

Here the adjoint ∇^* is with respect to the metric $\langle,\rangle$.

III. PROOF OF THE THEOREM

By the Einstein equation,

$$\mathcal{R} = 4\pi(T_{00} + T_{0i}e^0 \cdot e^i \cdot).$$

It follows then from the dominant energy condition (1.4) that

$$\mathcal{R} \geqslant 0. \tag{3.1}$$

Now, for $\phi \in \Gamma(M,S)$ and a compact domain $\Omega \subset M$ with smooth boundary, the Bochner–Lichnerowicz–Weitzenbock formula yields

$$\int_\Omega [|\nabla \phi|^2 + \langle \phi, \mathcal{R}\phi\rangle - |\mathcal{D}\phi|^2]\mathrm{d}vol(g) = \int_{\partial\Omega} \sum \langle (\nabla_{e_a} + e_a \cdot \mathcal{D})\phi, \phi\rangle \mathrm{int}(e_a)\mathrm{d}vol(g) \tag{3.2}$$

$$= \int_{\partial\Omega} \sum \langle (\nabla_\nu + \nu \cdot \mathcal{D})\phi, \phi\rangle \mathrm{d}vol(g|_{\partial\Omega}), \tag{3.3}$$

where e_a is an orthonormal basis of g and ν is the unit outer normal of $\partial\Omega$.

Now without loss of generality, assume that M has only one end. That is, let the manifold $M = M_0 \cup M_\infty$ with M_0 compact and $M_\infty \simeq (\mathbb{R}^k - B_R(0)) \times X$, and (X, g_X) a compact Riemannian manifold with nonzero parallel spinors. Moreover, the metric g on M satisfies (1.6). Let e_a^0 be the orthonormal basis of $\mathring{g}$ which consists of $\partial/\partial x_i$ followed by an orthonormal basis f_α of g_X. Orthonormalizing e_a^0 with respect to g gives rise an orthonormal basis e_a of g. Moreover,

$$e_a = e_a^0 - \tfrac{1}{2}u_{ab}e_b^0 + O(r^{-2\tau}). \tag{3.4}$$

This gives rise to a gauge transformation

$$A: \mathrm{SO}(\mathring{g}) \ni e_a^0 \to e_a \in \mathrm{SO}(g)$$

which identifies the corresponding spin groups and spinor bundles.

We now pick a unit norm parallel spinor ψ_0 of $(\mathbb{R}^k, g_{\mathbb{R}^k})$ and a unit norm parallel spinor ψ_1 of (X, g_X). Then $\phi_0 = A(\psi_0 \otimes \psi_1)$ defines a spinor of M_∞. We extend ϕ_0 smoothly inside. Then $\nabla^0\phi_0 = 0$ outside the compact set.

Lemma 3.1: If a spinor ϕ is asymptotic to ϕ_0: $\phi = \phi_0 + O(r^{-\tau})$, then we have

$$\lim_{R\to\infty} \Re \int_{S_R \times X} \sum \langle (\nabla_{e_a} + e_a \cdot D)\phi, \phi\rangle \mathrm{int}(e_a)\mathrm{d}vol(g) = \omega_k vol(X)\langle \phi_0, E\phi_0 + P_k\, \mathrm{d}x^0 \cdot \mathrm{d}x^k \cdot \phi_0\rangle,$$

where $\Re$ means taking the real part.

Proof. Recall that $\overline{\nabla}$ denote the connection on S induced from the Levi–Civita connection on M. We have

$$\nabla_{e_a}\psi = \overline{\nabla}_{e_a}\psi - \tfrac{1}{2}h_{ab}e^0 \cdot e^b \cdot \psi. \tag{3.5}$$

By the Clifford relation,

$$\langle(\nabla_{e_a}+e_a\cdot D)\phi,\phi\rangle=-\tfrac{1}{2}\langle[e^a\cdot,e^b\cdot]\nabla_{e_b}\phi,\phi\rangle.$$

Hence

$$\begin{aligned}\int_{S_R\times X}\sum\langle(\nabla_{e_a}+e_a\cdot D)\phi,\phi\rangle\mathrm{int}(e_a)\mathrm{d}vol(g)\\ =-\frac{1}{2}\int_{S_R\times X}\langle[e^a\cdot,e^b\cdot]\overline{\nabla}_{e_b}\phi,\phi\rangle\mathrm{int}(e_a)\mathrm{d}vol(g)\\ +\frac{1}{4}\int_{S_R\times X}\sum\langle[e^a\cdot,e^b\cdot]h_{bc}e^0\cdot e^c\cdot\phi,\phi\rangle\mathrm{int}(e_a)\mathrm{d}vol(g).\end{aligned}$$

Using (3.4) and the asymptotic conditions (1.7), the second term on the right-hand side can be easily seen to give us

$$\lim_{R\to\infty}\frac{1}{4}\int_{S_R\times X}\langle 2(h_{ac}-\delta_{ac}h_{bb})e^0\cdot e^c\cdot\phi,\phi\rangle\mathrm{int}(e_a)\mathrm{d}vol(g)=\omega_k vol(X)\langle\phi_0,P_k\,\mathrm{d}x^0\cdot\mathrm{d}x^k\cdot\phi_0\rangle.$$

The first term is computed in Ref. 4 to limit

$$\omega_k vol(X)\langle\phi_0,E\phi_0\rangle.$$

■

The following lemma is standard, see Refs. 10 and 14.

Lemma 3.2: If

$$\langle\phi_0,E\phi_0+P_k\,\mathrm{d}x^0\cdot\mathrm{d}x^k\cdot\phi_0\rangle\geqslant 0$$

for all constant spinors ϕ_0*, then*

$$E-|P|\geqslant 0.$$

As usual, the trick to get the positivity now is to find a harmonic spinor ϕ asymptotic to ϕ_0.

Lemma 3.3: There exists a harmonic spinor ϕ *on* (M,g) *which is asmptotic to the parallel spinor* ϕ_0 *at infinity,*

$$\mathcal{D}\phi=0,\quad \phi=\phi_0+O(r^{-\tau}).$$

Proof: The proof is essentially the same as in Ref. 4 [Cf. Refs. 6 and 9]. We use the Fredholm property of $\mathcal{D}$ on a weighted Sobolev space and $\mathcal{R}\geqslant 0$ to show that it is an isomorphism. The harmonic spinor ϕ can then be obtained by setting $\phi=\phi_0+\xi$ and solving $\xi\in O(r^{-\tau})$ from the equation $\mathcal{D}\xi=-\mathcal{D}\phi_0$. ■

Thus, with the choice of harmonic spinor as above, the left-hand side of (3.4) will be nonnegative since $\mathcal{R}\geqslant 0$. Taking the limit as $R\to 0$ and using Lemma 3.1 and Lemma 3.2 then give us the desired result.[4,9,10,14]

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Fractional boundary for the Gott-Hiscock string

J. P. Krisch
Department of Physics, University of Michigan, Ann Arbor, Michigan 48109

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A fractional boundary condition is used to join the Gott-Hiscock string to a Levi-Civita vacuum. The use of a fractional derivative generates Israel boundary layers whose density depends on the order of the fractional derivative. Variable boundary layers for the same two bounding space–times can be studied. The string angular deficit depends on the order of the fractional deficit. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1863692]

I. INTRODUCTION

The Gott-Hiscock[1,2] solution describes a constant density string matched to a vacuum Levi-Civita space–time with angular deficit. Two of the most common boundary matching conditions for non-null boundaries are due to Lichnerowicz and Darmois. These conditions have been discussed by Bonnor and Vickers.[3] Both conditions involve matching a metric and some metric derivatives across the boundary. The Darmois condition matches the metric and its second fundamental forms on the boundary while the Lichnerowicz condition matches the metric and its first derivatives on the boundary. The resulting space–time exterior to the string has an angular deficit related to the mass per unit length of the string interior. For general space—times, if a derivative, or extrinsic curvature, match is not possible, the most common procedure is to use the Israel[4] formalism, defining a surface boundary layer stress energy through the jump in the extrinsic curvature between space–times on either side of the boundary. Other space–times, whose extrinsic curvature was not continiuous across the boundary, could have been used for the exterior match, creating an Israel layer on the string boundary.

The Israel technique provides information about the stress energy content of the bounding surface layer. While the Israel surface layer can be used to describe the jump in the extrinsic curvature across a space–time boundary, it will not distinguish surface layers of different densities or structures that might bound the same two spacetimes. Within the Israel formalism, the only way of varying the boundary layer properties is to vary the bounding space–times.

One way of modifying the boundary conditions to include different kinds of boundary surfaces for the same bounding space–times is to generalize the Lichnerowicz boundary conditions to a fractional derivative matching and then to use the Israel formalism to describe the resulting surface layer. This creates boundary layers whose stress energy content depends on the order of the fractional derivative and allows the study of variable boundary structures between the same two space–times. In the next section, we apply this fractional matching method to the Gott-Hiscock string. The hallmark of string behavior, the angular deficit, also depends on the order of the fractional derivative. The change in the angular deficit introduced by the fractional match is discussed.

II. FRACTIONAL BOUNDARY CONDITION

A. The metrics

Consider a string oriented along the z axis with constant stress energy content

$$T_t^t = T_z^z = -\varepsilon. \tag{1}$$

From the field equations, the interior metric[2] is

$$ds^2 = -dt^2 + d\rho^2 + dz^2 + \rho^{*2}\sin^2\left(\frac{\rho}{\rho^*}\right)d\varphi^2, \tag{2}$$

where $\rho^* = (8\pi\epsilon)^{-1/2}$ and the string is assumed to be flat at $\rho = 0$.

The exterior vacuum space–time is

$$ds^2 = -dT^2 + dr^2 + dZ^2 + a^2r^2d\varphi^2. \tag{3}$$

B. The nonfractional boundary match

The metric match at $\rho = \rho_o$, $r = r_o$ provides the condition

$$ar_o = \rho^* \sin\left(\frac{\rho_o}{\rho^*}\right).$$

The extrinsic curvature is defined as[5]

$$K_{ij} = n_{(\alpha;\beta)}e_i^\alpha e_j^\beta,$$

where the e_i^α are the tangents to the boundary hypersurface with normal vector n_α. Calculating the extrinsic curvatures one finds in the interior

$$K_{\varphi\varphi} = \rho^* \sin\left(\frac{\rho_o}{\rho^*}\right)\cos\left(\frac{\rho_o}{\rho^*}\right). \tag{4}$$

In the exterior the extrinsic curvatures are

$$K_{tt} = 0,$$

$$K_{\varphi\varphi} = a^2r_o, \tag{5}$$

$$K_{zz} = 0.$$

The difference in the extrinsic curvatures across the boundary is

$$\langle K_{\phi\phi}\rangle = K_{\phi\phi}(\text{vacuum}) - K_{\phi\phi}(\text{interior}) = \left(a^2r_o - \rho^* \sin\left(\frac{\rho_o}{\rho^*}\right)\cos\left(\frac{\rho_o}{\rho^*}\right)\right),$$

$$\langle K\rangle = K_\varphi^\varphi(\text{vacuum}) - K_\varphi^\varphi(\text{interior}) = \frac{1}{r_o} - \frac{1}{\rho^*}\frac{\cos(\rho_o/\rho^*)}{\sin(\rho_o/\rho^*)} = \frac{1}{r_o} - \frac{1}{a}\frac{\cos(\rho_o/\rho^*)}{r_o}.$$

In the Israel formalism,[4] the stress energy of the boundary layer is

$$8\pi S_{ab} = -\{\langle K_{ab}\rangle - h_{ab}\langle K_c^c\rangle\},$$

$$8\pi S_{tt} = \langle K\rangle h_{oo} = \frac{\cos(\rho_o/\rho^*) - a}{ar_o},$$

$$8\pi S_{zz} = \frac{a - \cos(\rho_o/\rho^*)}{ar_o},$$

$$8\pi S_{\varphi\varphi} = 0. \tag{6}$$

If the extrinsic curvatures match, there is no stress energy in the boundary. The match of the extrinsic curvature provides the same condition as a match of the $g_{\phi\phi}$ derivatives across the string boundary,

$$a = \cos\left(\frac{\rho_o}{\rho^*}\right).$$

C. The fractional match

In the fractional boundary match, the metric matching conditions are the same as in the smooth boundary match:

$$ar_o = \rho^* \sin\left(\frac{\rho_o}{\rho^*}\right). \tag{7}$$

Instead of a match of the extrinsic curvatures, a fractional derivative match is used with the regular partial derivative, ∂_i replaced by an (α) order Caputo fractional derivative as described in the Appendix.

1. Fractional derivatives for the interior metric

In the interior, since the Caputo derivative of a constant is zero, the only function to consider is $f=\rho^{*2}\sin^2(\rho/\rho^*)$. Using α as the fractional index we have that the αth fractional derivative is

$$D^{(\alpha)}_{\rho,L}\left(\rho^{*2}\sin^2\left(\frac{\rho}{\rho^*}\right)\right) = \rho^* S_{\rho_o}(\alpha,\rho^*,\rho_o).$$

The form of the function $S_{\rho_o}(\alpha,\rho^*,\rho_o)$ depends on the range of the fractional derivative order. For $\alpha<1$ we have

$$S_{\rho_o}(\alpha,\rho^*,\rho_o) = \frac{(\rho^*/2)^{1-\alpha}}{\Gamma(1-\alpha)}\left[\sin\left(\frac{2\rho_o}{\rho^*}\right)\int_0^{2\rho_o/\rho^*} z^{-\alpha}\cos(z)dz - \cos\left(\frac{2\rho_o}{\rho^*}\right)\int_0^{2\rho_o/\rho^*} z^{-\alpha}\sin(z)dz\right]. \tag{8}$$

For $\alpha>1$ the function is

$$S_{\rho_o}(\alpha,\rho^*,\rho_o) = \frac{(\rho^*/2)^{1-\alpha}}{\Gamma(2-\alpha)}\left[\sin\left(\frac{2\rho_o}{\rho^*}\right)\int_0^{2\rho_o/\rho^*} z^{1-\alpha}\sin(z)dz + \cos\left(\frac{2\rho_o}{\rho^*}\right)\int_0^{2\rho_o/\rho^*} z^{1-\alpha}\cos(z)dz\right]. \tag{9}$$

The two can be related by an integration by parts and the use of a gamma function recursion relation. For $\alpha=1$, the usual first derivative is recovered.

2. Fractional derivatives for the exterior metric

In the exterior it is the right-handed derivative which should be applied. The exterior fractional derivative of the metric function is

$$D^{(\alpha)}_{r,R}(a^2r^2) = \frac{\Gamma(3)}{\Gamma(3-\alpha)}a^2r^{2-\alpha}. \tag{10}$$

TABLE I. Values of the function $h(\alpha,\rho_o/\rho^*)=\cos(\rho_o/\rho^*)-a$ as α and ρ_o/ρ^* vary. ρ_o is the radius of the string in the internal metric. $\rho^*=(8\pi\epsilon)^{(-1/2)}$ where ϵ is the constant internal energy density of the string. Complex values are indicated by C. When $\alpha=1$, $h(\alpha,\rho_o/\rho^*)=0$, providing the usual derivative matching condition.

	α					
ρ_o/ρ^*	0.1	0.3	0.7	0.9	1.1	1.2
0.1π	−0.013	−0.011	−0.006	−0.002	0.002	0.005
0.2π	−0.051	−0.043	−0.023	−0.008	0.010	0.021
0.3π	−0.113	−0.097	−0.052	−0.02	0.023	0.05
0.4π	−0.199	−0.172	−0.095	−0.038	0.047	0.107
0.45π	−0.25	−0.218	−0.125	−0.051	0.069	C
0.5π	−0.31	−0.272	−0.163	−0.071	C	C

3. The boundary match

The equation for the boundary match is

$$\frac{\Gamma(3)}{\Gamma(3-\alpha)}a^2 r_o^{2-\alpha}=\rho^* S_{\rho_o}(\alpha,\rho^*,\rho_o).$$

For $\alpha=1$ the usual derivative is obtained, leading to the original derivative matching result

$$a=\cos\left(\frac{\rho_o}{\rho^*}\right). \tag{11}$$

For $\alpha\neq 1$ there is a boundary layer which can be described by the Israel[4] formalism.

III. BOUNDARY STRESS ENERGY

The boundary stress energy, Eq. (6), involves the function

$$h\left(\alpha,\frac{\rho_o}{\rho^*}\right)=\cos\left(\frac{\rho_o}{\rho^*}\right)-a.$$

The two fractional matching equations, Eqs. (7) and (10), can be combined to give an equation for the parameter "*a*,"

$$\alpha<1{:}a^\alpha=\frac{\Psi(\alpha,\rho_o/\rho^*)}{\Gamma(1-\alpha)}\left[\sin\left(\frac{2\rho_o}{\rho^*}\right)\int_0^{2\rho_o/\rho^*}z^{-\alpha}\cos(z)dz-\cos\left(\frac{2\rho_o}{\rho^*}\right)\int_0^{2\rho_o/\rho^*}z^{-\alpha}\sin(z)dz\right], \tag{12}$$

$$\alpha>1{:}a^\alpha=\frac{\Psi(\alpha,\rho_o/\rho^*)}{\Gamma(2-\alpha)}\left[\sin\left(\frac{2\rho_o}{\rho^*}\right)\int_0^{2\rho_o/\rho^*}z^{1-\alpha}\sin(z)dz+\cos\left(\frac{2\rho_o}{\rho^*}\right)\int_0^{2\rho_o/\rho^*}z^{1-\alpha}\cos(z)dz\right], \tag{13}$$

where $\Psi(\alpha,\rho_o/\rho^*)=[\Gamma(3-\alpha)\sin^{\alpha-2}(\rho_o/\rho^*)]/2^{2-\alpha}$. For a smooth match, $h(\alpha,\rho_o/\rho^*)$ should be zero. Using Eq. (12), Eq. (13), and MAPLE, $h(\alpha,\rho_o/\rho^*)$ was evaluated for a range of ρ_o/ρ^* and fractional indices. The results are in Table I.

Examining Table I, one sees in all cases that, as $\alpha=1$ is approached, the stress energy of the layer approaches zero. For $\alpha<1$ the boundary layer has negative density and positive *z*-stress. As ρ_o/ρ^* moves above $\pi/2$, the values become complex. For $\alpha>1$, the boundary layer density is positive and the stress is a *z*-tension. For $\alpha>1$ complex values occur for values of $\rho_o/\rho^*<\pi/2$.

TABLE II. Values of the angular deficit factor "a" as a function of α and ρ_o/ρ^*. ρ_o is the radius of the string in the internal metric. $\rho^*=(8\pi\epsilon)^{(-1/2)}$ where ϵ is the constant internal energy density of the string. Complex values are indicated by C.

	α					
ρ_o/ρ^*	0.1	0.3	0.7	1	1.1	1.2
0.1π	0.964	0.962	0.957	0.951	0.949	0.946
0.2π	0.86	0.852	0.832	0.809	0.799	0.788
0.3π	0.701	0.684	0.639	0.588	0.565	0.538
0.4π	0.507	0.48	0.404	0.309	0.263	0.202
0.5π	0.308	0.272	0.163	0	C	C

The string angular deficit, the cut in the range of the ϕ coordinate due to the presence of the parameter "a" in the exterior metric, is a hallmark of cosmic string behavior. The angular deficit depends on the energy density of the string.[2] When a fractional boundary condition is used, the internal stress energy of the string does not change but the energy density of the boundary layer affects the angular deficit since it must be included in the total energy density of the string. The angular deficit can be defined by

$$\delta\varphi = 2\pi[1 - a]. \tag{14}$$

The values of "a" for various α and ρ_o/ρ^* were calculated and are found in Table II. In Table II, the $\alpha=1$ column values are calculated from the standard nonfractional match. The linear density of the string is not affected by the boundary layer but the angular deficit is, increasing in value as α increases. For $\alpha<1$, the angular deficit is less than the zero-boundary-layer, $\alpha=1$, value because the negative boundary layer density is decreasing the overall mass density of the string. For $\alpha>1$ the deficit is larger than the zero-boundary-layer value because the positive boundary layer mass increases the string density.

One possible way to interpret the variation of the parameter "a" and the surface energy density is through a packing fraction. The packing fraction is normally defined as the ratio of the area covered by a tiling to the total area being tiled. Adapting this to the surface layer we can consider the ratio of the $\alpha\neq 1$ surface area to the $\alpha=1$ surface area which is just the ratio of the "a" values in each row of Table II to the "a" value for $\alpha=1$:

$$pf(\alpha) = \frac{2\pi a(\alpha\neq 1)Lr_o}{2\pi a(\alpha=1)Lr_o} = \frac{a(\alpha\neq 1)}{a(\alpha=1)}.$$

For $\alpha<1$, the layer with its negative density matter seems overpacked. For $\alpha>1$ this ratio can be used to make some qualitative comments about the energy distribution. From Table II, generally one notes that the packing fraction decreases as α increases for a given ρ_o/ρ^* and that the packing fraction decreases as the ρ_o/ρ^* increases. The latter effect can be simply explained by examining cylinders of constant radius and varying internal energy density. As the internal energy density decreases and the ratio ρ_o/ρ^* goes up, the packing fraction decreases as there is less energy to distribute over the surface. The first effect is more difficult to motivate. One possible explanation comes from assuming a specific tiling mechanism for the boundary layer and then using the packing fraction variation to motivate differences within the tiling. For example, if the surface layer is tiled with an Apollonian packing,[6,7] circles with increasing smaller circles packed in the interstitial regions, the packing fraction is given roughly by

$$pf = 1 - (r(\min)/r(\max))^{2-d}$$

where $r(\max)$ is the radius of the largest circle in the packing, $r(\min)$ is the smallest circle in the tiling, and $d\sim 1.3$ is the fractal dimension[8] of the tiling in flat space. Using this, the variation in

the packing fraction as a function of α can be explained as a variation in the range of granule sizes making up the surface layer.

IV. DISCUSSION

In this note, we have suggested using a Caputo space fractional derivative to generate variable density Israel surface layers on the Gott-Hiscock string bounded by a Levi-Civita vacuum. The method generates, for $\alpha>1$, a family of positive energy, increasingly dense boundary layers between the constant density string interior and the vacuum exterior. For $\alpha<1$, the energy density is negative. The Caputo derivatives can be more restrictive than the Riemann-Liouville forms since the derivatives of the matching metric functions must exist to use the Caputo definition. The Riemann-Liouville form would give an additional nonzero matching condition for the constant metric functions which would identify r_o and ρ_o.

When joining many hypersurfaces, it is common practice to match extrinsic curvatures. Since the extrinsic curvature is a Lie derivative, it can be calculated from simple partial derivatives and can be fractionally generalized. Because the string boundary, as defined in the bounding space–time, had a well-defined unit normal and derivatives, a simple fractional extrinsic curvature matching would have given the same result as the fractional derivative matching. However, null surfaces, for example, do not have a well-defined extrinsic curvature and junction conditions outside of an extrinsic curvature matching have been developed.[9–11] Mars and Senovilla[12] have discussed junction conditions using a rigged metric connection for general hypersurfaces. Hayward[13] has discussed an action for nonsmooth boundaries. Using fractional derivatives as a method for generating variable density boundary layers apart from the second fundamental form might instead be a way of giving physical meaning to possible fractional extrinsic curvature definitions.

A smooth boundary with well-defined derivatives is not a necessary condition for the use of a fractional derivative matching. The Riemann-Liouville derivatives can be applied to functions which themselves do not have a well defined derivatives. For example, using the Riemann-Liouville form, Rocco and West[14] showed that the continuous but nondifferentiable Wierstrass function had a well-defined fractional derivative. Kolwankar and Gangal[15] also discussed the fractional derivatives of the Weierstrass function. Fractional derivatives have seen increasing use in the development of fractional kinetics,[16] particularly in discussions of anomalous transport processes.[17] While the method presented in this note generates a family of surface layers of varying densities between the same two bounding static space–times, the use of fractional derivatives in boundary matching could reflect an underlying boundary matter structure that was built by an anomalous transport process. A single tiling was used as an example of the relation between possible matter distributions and the order of the fractional derivative. The results from other tilings or sums over tilings is an interesting question for investigation.

APPENDIX: FRACTIONAL OPERATIONS

The idea of a fractional derivative arose in 1695 when L'Hopital[18] asked Leibniz about the meaning of $d^n y/dx^n$ for $n=\frac{1}{2}$. The ideas of fractional calculus have attracted the attention of many of the same people that are associated with the development of physics: Lagrange, Laplace, Fourier, Liouville, Riemann, and Weyl, among others.[19] Since the first conference on fractional calculus in 1974, the applications to physics have grown enormously, describing phenomena such as the modeling of viscoelastic phenomena[20] and fractional matter transport.[17] There have been many definitions of fractional operations because of the diverse array of applications. Some of the fractional differentiation definitions are (a) the left-handed Riemann-Liouville form,[18]

$$D_a^\nu f(x) = \frac{d^m}{dx^m}\left\{ \frac{1}{\Gamma(m-\nu)} \int_a^x f(y)(x-y)^{m-\nu-1} dy \right\},$$

and (b) the right-handed Riemann-Liouville form,[18]

$$ {}_bD^{\nu}f(x) = \frac{d^m}{dx^m}\left\{ \frac{(-1)^m}{\Gamma(m-\nu)} \int_x^b f(y)(y-x)^{m-\nu-1} dy \right\}, $$

where, in both cases, m is the smallest integer bigger than ν. One very interesting thing about this form of the fractional derivative is that the derivative of a constant is not zero. For example, the left-handed derivative of "1" is

$$ D_a^{\nu}[1] = \frac{d^2}{dx^2}\left\{ \frac{1}{\Gamma(2-\nu)} \int_0^x (x-y)^{1-\nu} dy \right\} = \frac{x^{-\nu}\Gamma(1)}{\Gamma(1-\nu)}, $$

where the definition of the beta function,

$$ B(z,w) = \int_0^1 x^{z-1}(1-x)^{w-1} dx = \frac{\Gamma(z)\Gamma(w)}{\Gamma(z+w)}, $$

and the recursion relation for the gamma function have been used. There are other fractional forms, with modified definitions. The Caputo[19] fractional derivatives are similar to the Riemann-Liouville derivatives except that the derivative appears inside of the integral; $f^{(m)}(y)$ is the mth derivative of $f(x)$. The left-hand Caputo[19] derivative is

$$ {}_CD^{\nu}{}_a[f(x)] = \frac{1}{\Gamma(m-\nu)} \int_a^x (x-y)^{m-\nu-1} f^{(m)}(y) dy. $$

The right-hand derivative is similar. Butzer and Westphal[21] credit Liouville with the definition. In this paper we shall use the Caputo form.

The notation that we will use is

$$ \partial_i -> D_{iL}^{(\nu)}, $$

$$ \partial_i -> D_{iR}^{(\nu)}, $$

where ν the fractional order, has been placed in parentheses to distinguish it from a tensor index, i is the index of the coordinate derivative, and L, R denote the left- or right-hand derivatives.

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On quadratic Poisson brackets

Ali Ulas Özgür Kisisel[a)]
Department of Mathematics, Middle East Technical University, 06531, Ankara, Turkey

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In this paper, we present a method for constructing large families of quadratic Poisson brackets on a manifold using more elementary brackets on a different manifold. The method is then applied to several examples of completely integrable systems. One can recover several known brackets for systems such as the Toda lattice or the open discrete KP hierarchy. New brackets for a doubly periodic discrete KP hierarchy are also constructed. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1866221]

I. INTRODUCTION

Poisson brackets are classical limits of commutators in deformation quantization, and play a key role in the theory of completely integrable systems. The so-called quadratic or second Poisson brackets carry a homogeneity property distinguishing them. It is possible to prove that many systems are completely integrable by exhibiting two compatible Poisson brackets one of which is quadratic; this was an idea which originated in Ref. 17 and evolved much further.

The aim of this paper is to present a systematic method for constructing quadratic Poisson brackets, and to apply it to several examples. The method is some sort of a hybrid of the Miura transform which involves factorizing the Lax operator noncommutatively and then using a reduction (see Refs. 1, 6, 7, and 16), and the method described in the paper[19] of Suris which involves starting from Poisson brackets satisfying r-matrix like conditions on $g\oplus g\oplus\cdots\oplus g$ to produce new r-matrix brackets on g. Our construction is different in the sense that we do not require any r-matrix like conditions, but rather start from a set of so-called simple brackets (to be defined) on a subspace of $g\oplus g\oplus\cdots\oplus g$, again to produce new, nonsimple brackets on g. In this context, the classical r-matrix brackets would be self-inducing (see Ref. 20).

The second section explains this construction. In the third section we work it out in detail for the smallest nontrivial example. In the fourth section, first we explain how the second bracket of the (A-series) Toda hierarchy can be obtained by this method. Afterwards, we demonstrate how the (known) quadratic Poisson bracket for the Kadomtsev-Petviashvili (KP) hierarchy, discrete in both space directions can be obtained. Finally, we show that a quadratic Poisson bracket for a doubly periodic discrete KP hierarchy can be tailor-made, and in a sense uniquely, using the general construction, if the two periods M and N are relatively prime. To our knowledge, these last brackets are new. Commutation of conserved quantities holds for these brackets, but is not proved in this paper. For this, we refer the reader to Ref. 12 or Ref. 13.

II. SIMPLE BRACKETS AND DESCENT PROPERTIES

Let M be a smooth manifold. Recall that a Poisson structure on M is a skew symmetric bilinear map from $C^\infty(M)\times C^\infty(M)$ to $C^\infty(M)$ which satisfies the Leibniz rule and the Jacobi identity. M equipped with a Poisson structure is called a Poisson manifold. A smooth map $f:M\to N$ between two Poisson manifolds is called a Poisson map if the naturally induced ring homomorphism $f^*:C^\infty(N)\to C^\infty(M)$ defined as $f^*(g)=g\circ f$ commutes with the brackets, i.e., $\{f^*(u),f^*(v)\}_M=f^*\{u,v\}_N$ for all u,v. Suppose that $A(M)$ is a graded subring of $C^\infty(M)$ closed

a)Electronic mail: akisisel@metu.edu.tr

under the bracket operation. [A typical example is where M is an algebraic variety, $A(M)$ denotes the ring of regular functions on M, and $\{,\}$ is defined by polynomial expressions, taking pairs of homogenous polynomials to homogenous polynomials. We also remark that more generally one can consider sheaves of rings rather than global functions on M.] We call a Poisson structure on M quadratic if $\deg(\{u,v\})=\deg(u)+\deg(v)$ for all homogenous $u,v\in A(M)$. (This name refers to the case when u,v have degree 1 and thus the degree of $\{u,v\}$ is 2.) In this paper quadratic Poisson brackets will be the main objects of our concern. For more general information about Poisson manifolds, please see Refs. 3 and 22.

Definition 1: Suppose that M, $A(M)$ and $\{,\}$ are as above. Say $\{x_1,\ldots,x_n\}$ is a set of generators for the ring $A(M)$. Assume that there exist constants $\mu_{i,j}$ such that $\mu_{i,j}=-\mu_{j,i}$ and

$$\{x_i,x_j\}=\mu_{i,j}x_ix_j$$

for all i,j. Then we will say that $\{,\}$ is simple (or diagonal, or diagonalized) with respect to this set of generators.

It is straightforward to check that for any choice of constants $\mu_{i,j}$ subject to the condition $\mu_{i,j}=-\mu_{j,i}$, the resulting bracket satisfies the Jacobi identity.

We remark that in a paper by Dufour and Haraki[5] it is shown that simple brackets are in some sense generic among all quadratic brackets. This is done as follows. It is well known that specifying a Poisson bracket is equivalent to specifying a bivector field π satisfying $[\pi,\pi]=0$ where $[,]$ denotes the Schouten bracket.[3] They associate π a vector field $D(\pi)$, called its curl. One proves that $[D(\pi),\pi]=0$. Then if $D(\pi)$ is diagonalizable and its eigenvalues avoid a certain finite set of identities, this relation forces π to be diagonalizable. This certainly is a generic condition among possible Jordan forms of $D(\pi)$, however there are new components in the parameter space of all quadratic brackets, which consist in π Schouten commuting with the nongeneric $D(\pi)$. Quadratic brackets of many familiar integrable systems, such as the Toda lattice, are not diagonalizable by a linear change of coordinates, even though they have a diagonalizable curl; hence they fall into this second class.

We also remark that the sum of any two simple brackets is a simple bracket. Thus any two members of the family of simple brackets form a compatible pair (equivalently, their Schouten bracket is 0).

We will describe a method through which some nonsimple brackets may be constructed using simple brackets. In the later sections we will show that the quadratic brackets of several well-known integrable systems arise in this way. We also use this method to construct a highly nonlocal quadratic bracket for an integrable system for which such a bracket was formerly unknown. Our setting is as follows: Let a be an associative algebra, g an affine or vector subspace of a, and $\mathbf{h}$ an affine or vector subspace of $a\oplus a\oplus\cdots\oplus a$ (M times) for some positive integer M.

Assume that the image of the map f on $\mathbf{h}$ defined by $f(L^{(1)},\ldots,L^{(M)})=L^{(1)},\ldots,L^{(M)}$ is equal to g. Then the induced map $f^*:C^\infty(g)\to C^\infty(\mathbf{h})$ is injective. Since f is a polynomial map f^* also induces a map from $A(g)$ to $A(\mathbf{h})$ where these denote the rings of polynomial functions on g and $\mathbf{h}$, respectively.

Next, choose a set of generators for $A(\mathbf{h})$ and consider the set of all simple Poisson brackets with respect to this set of generators. By the remarks above, this set of brackets is itself a vector space, and we will denote it by $\mathcal{S}(\mathbf{h})$.

Theorem 1: *Say $\{,\}_h$ is a Poisson bracket on $\mathbf{h}$. Suppose that for every $u,v\in A(g)$ there exists $w\in A(g)$ such that $\{f^*(u),f^*(v)\}_h=f^*(w)$. Then w is the unique element of $A(g)$ having this property, and the bracket defined by $\{u,v\}_g=w$ is a Poisson bracket on g.*

Proof: The uniqueness of w follows from the injectivity of f^*, and makes $\{,\}_g$ well defined. The bilinearity and the Jacobi identity for $\{,\}_g$ follow from the bilinearity and the Jacobi identity for $\{,\}_{\mathbf{h}}$ and the fact that f^* is a ring homomorphism. ■

We will say that a bracket on $\mathbf{h}$ satisfying the hypothesis of the previous theorem "descends" to a bracket on g.

Corollary 1: The set $\mathcal{D}(\mathbf{h})$ of simple quadratic brackets on $\mathbf{h}$ which descend to a bracket on g is a vector subspace of $\mathcal{S}(\mathbf{h})$.

Proof: It only remains to check that a linear combination of two elements of $\mathcal{D}(\mathbf{h})$ is in $\mathcal{D}(\mathbf{h})$. But this easily follows since f^* is an injective homomorphism. ■

There are at least two nice features of $\mathcal{D}(\mathbf{h})$ which in our opinion make it worthwhile to study. First, it is relatively easy to determine $\mathcal{D}(\mathbf{h})$ or some of its subspaces explicitly for concrete examples. Second, the induced brackets by this family on g give us a rich source of not necessarily simple brackets on g, among which one can find the quadratic brackets of many familiar integrable systems, along with new quadratic brackets for certain nonlocal systems.

III. EXAMPLE: M(2)

We will work out the general construction of the last section in detail for the example of $g=M(2)$ (over $\mathbb{R}$ or $\mathbb{C}$), the associative algebra of 2×2 matrices, $M=2$, and $\mathbf{h}=L(2)\oplus U(2)$ where $L(2)$ is the vector space of lower triangular 2×2 matrices, and $U(2)$ the vector space of upper triangular 2×2 matrices. Let $f:\mathbf{h}=L(2)\oplus U(2)\to g$ be given by $f(A,B)=AB$. Let a,b,c,d be coordinate functionals dual to the entries on g; x,y,z dual to those on $L(2)$ and u,v,w dual to those on $U(2)$ in the orders such that f^* is given by

$$\begin{bmatrix} x & 0 \\ y & z \end{bmatrix}\begin{bmatrix} u & v \\ 0 & w \end{bmatrix} \leftarrow \begin{bmatrix} a & b \\ c & d \end{bmatrix},$$

i.e., $f^*(a)=xu$, $f^*(b)=xv$, $f^*(c)=yu$, and $f^*(d)=yv+zw$. Consider an arbitrary simple bracket $\{,\}_{\mathbf{h}}$ on $\mathbf{h}$. Denote $\{x,y\}_{\mathbf{h}}=\mu_{x,y}xy$, $\{x,u\}_{\mathbf{h}}=\mu_{x,u}xu$ and so on. Recall that $\mu_{i,j}=-\mu_{j,i}\,\forall\, i,j$. An elementary computation gives

$$\{f^*(a),f^*(b)\}_{\mathbf{h}}=(\mu_{x,v}+\mu_{u,v}+\mu_{u,x})f^*(ab),$$

$$\{f^*(a),f^*(c)\}_{\mathbf{h}}=(\mu_{x,y}+\mu_{x,u}+\mu_{u,y})f^*(ac),$$

$$\{f^*(b),f^*(c)\}_{\mathbf{h}}=(\mu_{x,y}+\mu_{x,u}+\mu_{v,y}+\mu_{v,u})f^*(bc),$$

$$\begin{aligned}\{f^*(a),f^*(d)\}_{\mathbf{h}}&=(\mu_{x,y}+\mu_{x,v}+\mu_{u,y}+\mu_{u,v})xuyv+(\mu_{x,z}+\mu_{x,w}+\mu_{u,z}+\mu_{u,w})xuzw\\&=(\mu_{x,y}+\mu_{x,v}+\mu_{u,y}+\mu_{u,v}-\mu_{x,z}-\mu_{x,w}-\mu_{u,z}-\mu_{u,w})f^*(bc)+(\mu_{x,z}+\mu_{x,w}+\mu_{u,z}\\&\quad+\mu_{u,w})f^*(ad),\end{aligned}$$

$$\{f^*(b),f^*(d)\}_{\mathbf{h}}=(\mu_{x,y}+\mu_{x,v}+\mu_{v,y})xv^2y+(\mu_{x,z}+\mu_{x,w}+\mu_{v,z}+\mu_{v,w})xvzw,$$

$$\{f^*(c),f^*(d)\}_{\mathbf{h}}=(\mu_{y,v}+\mu_{u,y}+\mu_{u,v})y^2uv+(\mu_{y,z}+\mu_{y,w}+\mu_{u,z}+\mu_{u,w})yuzw.$$

This implies that a necessary and sufficient condition for $\{,\}_{\mathbf{h}}$ to descend on g is

$$\mu_{x,y}+\mu_{x,v}+\mu_{v,y}=\mu_{x,z}+\mu_{x,w}+\mu_{v,z}+\mu_{v,w} \tag{1}$$

and

$$\mu_{y,v}+\mu_{u,y}+\mu_{u,v}=\mu_{y,z}+\mu_{y,w}+\mu_{u,z}+\mu_{u,w}. \tag{2}$$

Therefore $\mathcal{D}(\mathbf{h})$ is a 13-dimensional subspace of the 15-dimensional vector space $\mathcal{S}(\mathbf{h})$. On the other hand, the linear transformation sending each element of $\mathcal{D}(\mathbf{h})$ to the associated bracket $\{,\}_g$ over g has a large kernel. To determine exactly what it is, set $\mu_{a,b}=\mu_{x,v}+\mu_{u,v}+\mu_{u,x}$, $\mu_{a,c}=\mu_{x,y}+\mu_{x,u}+\mu_{u,y}$, $\mu_{b,c}=\mu_{x,y}+\mu_{x,u}+\mu_{v,y}+\mu_{v,u}$, $l=\mu_{x,z}+\mu_{x,w}+\mu_{u,z}+\mu_{u,w}$, $k=\mu_{x,y}+\mu_{x,v}+\mu_{u,y}+\mu_{u,v}$, $\mu_{b,d}=\mu_{x,y}+\mu_{x,v}+\mu_{v,y}$, $\mu_{c,d}=\mu_{y,v}+\mu_{u,y}+\mu_{u,v}$. After a row reduction, and taking equations (1) and (2) into account, we have

$$\mu_{a,b} = k - \mu_{a,c}, \quad \mu_{b,c} = \mu_{a,c} - \mu_{c,d}, \quad \mu_{b,d} = k - \mu_{c,d}$$

and, the set $\{k, l, \mu_{a,c}, \mu_{c,d}\}$ is linearly independent considered as linear functions on $\mathcal{D}(\mathbf{h})$. Thus we obtain a complete description of all quadratic brackets on g which descend from simple brackets of $\mathbf{h}$,

$$\{a,b\}_g = (k - \mu_{a,c})ab, \quad \{a,c\}_g = \mu_{a,c}ac, \quad \{b,c\}_g = (\mu_{a,c} - \mu_{c,d})bc,$$

$$\{a,d\}_g = lad + (k - l)bc, \quad \{b,d\}_g = (k - \mu_{c,d})bd, \quad \{c,d\}_g = \mu_{c,d}cd.$$

This is a four-dimensional linear space of compatible brackets. Notice that such a bracket is simple on g if and only if $k=l$, hence those lie in a codimension 1 locus (thus the six-dimensional vector space of simple brackets on g meets the four-dimensional vector space of descended brackets in a three-dimensional subspace).

For $\mu_{a,c}=\mu_{c,d}=1, k=2, l=0$ one gets

$$\{a,b\}_g = ab, \quad \{a,c\}_g = ac, \quad \{b,c\}_g = 0,$$

$$\{a,d\}_g = 2bc, \quad \{b,d\}_g = bd, \quad \{c,d\}_g = cd$$

which is the r-matrix Poisson bracket on M(2) associated to $r=\pi_+ - \pi_-$ (Ref. 20, Example 5). For another example, set $\mu_{a,c}=\mu_{c,d}=k=0, l=-1$. The only nonzero bracket then is $\{a,d\}_g = bc - ad$. The submanifold given by $b=c$ is a Poisson submanifold for this bracket, and the resulting bracket on this submanifold is the example given in Ref. 18. It was shown here that this bracket does not come from a classical r-matrix.

Considering applications to integrable systems, one interesting question is the following: For which values of the constants do a set of given functions Poisson commute? As an example, let us take the trace and determinant functionals, $f_1 = a + d$ and $f_2 = ad - bc$. (This is a natural choice since for a system where the 2×2 matrix is one of the two matrices of the Lax pair, and the flows are the isospectral flows of L, f_1 and f_2 clearly have to be conserved quantities.) A calculation gives

$$\{f_1, f_2\}_g = -l(abc) + l(bcd).$$

Thus we deduce that $\{f_1, f_2\}_g = 0 \Leftrightarrow l = 0$.

The general question of which quadratic Poisson brackets can be obtained from any such descent process is unanswered at the moment. But for the current example, we note the following result.

Theorem 2: *Suppose that we have a quadratic Poisson bracket on g of the form*

$$\{a,b\}_g = \mu_{a,b}ab, \quad \{a,c\}_g = \mu_{a,c}ac, \quad \{b,c\}_g = \mu_{b,c}bc,$$

$$\{a,d\}_g = lad + rbc, \quad \{b,d\}_g = \mu_{b,d}bd, \quad \{c,d\}_g = \mu_{c,d}cd.$$

Then, either the bracket is simple, or, up to a linear change of coordinates $\{,\}_g$ *descends from a quadratic Poisson bracket on* $\mathbf{h}$ *as above.*

Proof: From the identity $\{a,\{c,d\}_g\}_g + \{d,\{a,c\}_g\}_g + \{c,\{d,a\}_g\}_g = 0$ we obtain

$$r(\mu_{c,d} - \mu_{a,c} + \mu_{b,c})bc^2 = 0.$$

Assume that the bracket is not simple. Therefore $r \neq 0$, so $\mu_{b,c} = \mu_{a,c} - \mu_{c,d}$. Next, using the identity $\{a,\{b,d\}_g\}_g + \{d,\{a,b\}_g\}_g + \{b,\{d,a\}_g\}_g = 0$ we obtain

$$r(\mu_{b,d} - \mu_{a,b} - \mu_{b,c})b^2c = 0.$$

Thus $\mu_{b,d} - \mu_{a,b} = \mu_{a,c} - \mu_{c,d}$. Now set $a' = ta$. Then $\{a',b\} = t\{a,b\} = t\mu_{a,b}ab = \mu_{a,b}a'b$, similarly $\{a',c\} = \mu_{a,c}a'c$ but $\{a',d\} = t\{a,d\} = tlad + trbc = la'd + trbc$. So the effect of this transformation on the bracket is to replace r with tr. Taking

$$t = \frac{\mu_{a,b} + \mu_{a,c} - l}{r}$$

and setting $k = l + tr$ we obtain that $\mu_{a,b} = k - \mu_{a,c}$, thus $\mu_{b,d} = k - \mu_{c,d}$, therefore the proof is complete. ■

IV. THE TODA AND DISCRETE KP HIERARCHIES

In what follows, let $\hat{\mathrm{M}}(\infty)$ denote the associative algebra of infinite matrices L having the property that $\exists n$ such that $L_{ij} = 0$ if $|i-j| > n$. (The last condition makes it possible to form ordinary matrix products of these matrices.)

The open Toda lattice equations (for the A series of Lie algebras) are given by

$$\dot{a}_i = 2(b_{i+1}^2 - b_i^2),$$

$$\dot{b}_i = b_i(a_i - a_{i-1}),$$

where $i \in \mathbb{Z}$ (Ref. 4) (please note the difference in notation from this paper). We obtain the finite Toda lattice of length N if $a_i = 0$ for $i \leqslant 0$ and for $i > N$, and $b_i = 0$ for $i \leqslant 1$ and for $i > N$. Similarly, we obtain the periodic Toda lattice of period N if $a_{i+N} = a_i$ and $b_{i+N} = b_i$ for all i (see Ref. 10).

Let g be the vector subspace of $\hat{\mathrm{M}}(\infty)$ consisting in symmetric tridiagonal matrices (i.e., $L_{ij} = 0$ if $|i-j| > 1$, and $L_{ij} = L_{ji}$). Also let $\mathbf{h}$ be the subspace of $\hat{\mathrm{M}}(\infty) \oplus \hat{\mathrm{M}}(\infty)$ consisting in pairs (K, K^t) such that $K_{ij} = 0$ unless $i = j$ or $i = j-1$. Define $f: \mathbf{h} \to g$ by $f(K, K^t) = KK^t$. Suppose that a_i, b_i are coordinate functionals on g and x_i, y_i coordinates on $\mathbf{h}$ in the way that f^* is given by

$$\begin{bmatrix} \cdots & \cdots & & & & & \\ & y_1 & x_1 & & & & \\ & & y_2 & x_2 & & & \\ & & & \cdots & \cdots & & \\ & & & & y_N & x_N & \\ & & & & & \cdots & \end{bmatrix} \begin{bmatrix} \cdots & & & & & & \\ x_0 & y_1 & & & & & \\ & x_1 & y_2 & & & & \\ & & \cdots & \cdots & & & \\ & & & x_{N-1} & y_N & & \\ & & & & \cdots & \cdots & \end{bmatrix} \leftarrow \begin{bmatrix} \cdots & \cdots & & & & & \\ b_1 & a_1 & b_2 & & & & \\ & b_2 & a_2 & b_3 & & & \\ & & \cdots & \cdots & \cdots & & \\ & & & b_N & a_N & b_{N+1} & \\ & & & & \cdots & \cdots & \end{bmatrix}. \tag{3}$$

In other words,

$$f^*(a_i) = x_i^2 + y_i^2, \quad f^*(b_i) = x_{i-1} y_i.$$

The following quadratic Poisson bracket on g is well known:

$$\{a_i, a_{i+1}\} = 2b_{i+1}^2, \quad \{a_i, b_i\} = -a_i b_i,$$

$$\{a_i, b_{i+1}\} = a_i b_{i+1} \quad \{b_i, b_{i+1}\} = \tfrac{1}{2} b_i b_{i+1}. \tag{4}$$

An important property of this bracket is the following: Denote the rightmost matrix in 3 by L. Then the coefficients of the characteristic polynomial of L commute with respect to this bracket.

Remark: For the infinite Toda lattice, one may define the kth coefficient of the characteristic polynomial of L as the coefficient of $\lambda^{\infty - k}$ in $\det(L - \lambda I)$. That is, let it be the formal sum, of monomials in a_i's and b_i's containing all but k of the λ's, over all permutations of $\mathbb{Z}$. Poisson brackets of such formal sums make sense here (as a formal sum again) because the bracket 4 is local.

Proposition 1: The bracket 4 is induced by the following simple bracket on **h**:

$$\{x_i, y_i\} = -\tfrac{1}{2} x_i y_i, \quad \{x_i, y_{i+1}\} = \tfrac{1}{2} x_i y_{i+1}.$$

Proof: This is a straightforward computation. ■

For our next class of examples, let a be the affine subalgebra of $\hat{\mathrm{M}}(\infty)$ consisting in lower unipotent matrices (i.e., $L \in a$ if $L_{ii}=1\ \forall i$, $L_{ij}=0$ if $j>i$, and $\exists n$ such that $L_{ij}=0$ if $i-j>n$). For a given positive integer M, let g_M be the affine subspace of a consisting in L such that $L_{ij}=0$ if $i-j>M$. Set $\mathbf{h}=g_1\oplus g_1\oplus\cdots\oplus g_1$ (M times) and let $f:\mathbf{h}\to g_M$ be the usual map, $f(L^{(1)},\ldots,L^{(M)})=L^{(1)},\ldots,L^{(M)}$. It is easy to see that f is surjective.

Let $u_j^{(i)}, i=1,\ldots,M, j\in\mathbb{Z}$ be coordinate functionals on $\mathbf{h}$ and v_{ij}, $i,j\in\mathbb{Z}, i>j, i-j\leqslant M$ be coordinate functionals on g_m so that f^* is given by

$$\begin{bmatrix} \cdots & & & & \\ \cdots & 1 & & & \\ & u_2^{(1)} & 1 & & \\ & & u_3^{(1)} & 1 & \\ & & & \cdots & \cdots \end{bmatrix} \cdots \begin{bmatrix} \cdots & & & & \\ \cdots & 1 & & & \\ & u_2^{(M)} & 1 & & \\ & & u_3^{(M)} & 1 & \\ & & & \cdots & \cdots \end{bmatrix} \leftarrow \begin{bmatrix} \cdots & & & & \\ \cdots & 1 & & & \\ \cdots & v_{21} & 1 & & \\ \cdots & v_{31} & v_{32} & 1 & \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix}. \tag{5}$$

Denote these matrices by $I+U^{(1)},\ldots,I+U^{(M)}$ and V, respectively. Then this equation can be written as $f^*(V)=(I+U^{(1)})\cdots(I+U^{(M)})$.

One can verify by induction that

$$f^*(v_{ij})=\sum_{k_1<k_2<\cdots<k_{i-j}\leqslant M} u_i^{(k_1)}u_{i-1}^{(k_2)}\cdots u_{j+1}^{(k_{i-j})}.$$

Theorem 3: *Consider the following simple Poisson bracket on* $\mathbf{h}$:

$$\{u_i^{(k)},u_j^{(l)}\}_{\mathbf{h}}=(\delta_{i,j+1}-\delta_{i,j})u_i^{(k)}u_j^{(l)} \quad \text{if } k<l,$$

$$\{u_i^{(k)},u_j^{(l)}\}_{\mathbf{h}}=(\delta_{i,j}-\delta_{i,j-1})u_i^{(k)}u_j^{(l)} \quad \text{if } k>l.$$

$$\{u_i^{(k)},u_j^{(k)}\}_{\mathbf{h}}=0.$$

The bracket descends on g_m *to a bracket given by*

$$\{v_{ij},v_{nm}\}_{g_m}=0 \quad \text{if } n>i \text{ and } m<j, \text{or if } n<j,$$

$$\{v_{ij},v_{jm}\}_{g_m}=v_{im},$$

$$\{v_{kj},v_{ij}\}_{g_m}=v_{kj}v_{ij} \quad \text{if } k>i,$$

$$\{v_{ij},v_{ik}\}_{g_m}=v_{ij}v_{ik} \quad \text{if } j>k,$$

$$\{v_{ij},v_{kl}\}_{g_m}=v_{ij}v_{kl}+v_{kj}v_{il} \quad \text{if } i>k>j>l.$$

The resulting bracket is an r-matrix Poisson bracket, therefore a proof of this theorem can in principle be obtained using the method described in Ref. 19. We give an independent proof in the Appendix.

The bracket of theorem 3 is an element of $\mathcal{D}(\mathbf{h})$, and the bracket it induces on g_m is a quadratic Poisson bracket for the open and finite discrete KP hierarchies (see Refs 2 and 11). To be precise, the name "KP hierarchy" is usually attached to the completely integrable system associated to the pseudodifferential operator $L=\partial+v_{-1}\partial^{-1}+v_2\partial^{-2}+\cdots$ (see Refs. 8, 14, and 15). Above, the Lax operator is $V=S^0+V^{(1)}S^{-1}+V^{(2)}S^{-2}+\cdots+V^{(M)}S^{-M}$ where S is the finite difference analog of ∂, i.e.,

a subdiagonal matrix consisting of 1's, and $V^{(i)}$ the diagonal matrix such that $V^{(i)}_{jj}=V_{jj-i}$. It is a nontrivial theorem that the conserved quantities of these systems commute under this bracket.

For the discrete KP hierarchy periodic in one spatial direction (namely, $\exists N$ such that $v_{ij}=v_{i+Nj+N}\forall i,j$), the bracket produces a Hamiltonian interpretation in the same manner (Refs. 14 and 21): Assume the same periodicity on the $u^{(k)}_i$, i.e., set $u^{(k)}_{i+N}=u^{(k)}_i\forall i,k$ and modify the bracket above such that

$$\{u^{(k)}_i,u^{(l)}_j\}_{\mathbf{h}}=\left(\sum_{n=-\infty}^{\infty}(\delta_{i,j+1+nN}-\delta_{i,j+nN})\right)u^{(k)}_iu^{(l)}_j \quad \text{if } k<l,$$

$$\{u^{(k)}_i,u^{(l)}_j\}_{\mathbf{h}}=\left(\sum_{n=-\infty}^{\infty}(\delta_{i,j+nN}-\delta_{i,j-1+nN})\right)u^{(k)}_iu^{(l)}_j \quad \text{if } k>l,$$

$$\{u^{(k)}_i,u^{(k)}_j\}_{\mathbf{h}}=0.$$

Theorem 3 is valid for this simple bracket without much change.

Considering the presence of two space variables in the KP equation, it is natural to ask for a further symmetry in the system corresponding to periodicity in a second spatial direction. Such a system was considered in Ref. 9 for instance. For the purposes of this paper, let us only assume that we want to find a Poisson bracket such that the dependence of $\{u^{(k)}_i,u^{(l)}_j\}_{\mathbf{h}}$ on k and l is only via the value of $k-l$ in $\mathbb{Z}/M\mathbb{Z}$, and in particular does not depend on whether $k<l$ or $k>l$. The bracket $\{,\}_{\mathbf{h}}$ of Theorem 3 does not satisfy this condition.

Assume that M and N are relatively prime. Make a change of indexing by setting $w^{(k)}_i=u^{(k)}_{i-k}$. Below, we will construct another element of $\mathcal{D}(\mathbf{h})$ such that when added to the bracket of 3, we obtain a doubly periodic bracket on $w^{(k)}_i$'s.

We start from some general results. Recall the following notation: Say $A=(a_{ij})$ and $B=(b_{ij})$ where a_{ij},b_{ij} are C^∞ functions on a Poisson manifold. Define $\{A^{\otimes},B\}$ to be the matrix obtained in the same way as taking a Kronecker product, but where each product of a pair of functions is replaced by their Poisson brackets. It is easy to see that the matrix Leibniz rule holds, i.e., $\{AB^{\otimes},C\}=(A\otimes I)\{B^{\otimes},C\}+\{A^{\otimes},C\}(B\otimes I)$. Here I is the identity matrix.

Let us return to the setting of the Poisson manifolds $\mathbf{h}$ and g_m above. Suppose that S is a set of positive integers, and let t be a non-negative integer. Let E^t_S denote the matrix which is the tth elementary symmetric function in the matrices $U^{(i)}$ with $i\in S$. (Since $U^{(i)}$ do not commute, the order of products appearing in this symmetric function is important. In each case, we order the $U^{(i)}$ with respect to increasing order in i.) Notice that $f^*(V)=I+\Sigma_{t=1}^n E^t_{1,\ldots,m}$.

Lemma 1: Let c be a positive integer. For any fixed integer t such that $0\leqslant t\leqslant c$,

$$\sum_{i=1}^{m}E^t_{1,\ldots,i-1}U^{(i)}E^{c-t}_{i+1,\ldots,m}=E^{c+1}_{1,\ldots,m}.$$

Proof: Consider an arbitrary monomial of the form $U^{(j_1)}\cdots U^{(j_{c+1})}$ such that $j_1<\cdots<j_{c+1}$. We claim that this occurs once in both sides of the sum above. This is clear for the right-hand side, and for the left-hand side it is obtained for $i=j_{t+1}$. ■

Let $F\in\hat{\mathrm{M}}(\infty)\otimes\hat{\mathrm{M}}(\infty)$ be a diagonal matrix, i.e., $F_{ij,kl}=0$ unless $i=j$ and $k=l$. The formula $\{U^{(k)\otimes},U^{(l)}\}_{\mathbf{h}}=F(U^{(k)}\otimes U^{(l)})$, explicitly written, means

$$\{u^{(k)}_i,u^{(l)}_j\}=F_{i+1i+1,j+1j+1}u^{(k)}_iu^{(l)}_j.$$

Therefore this defines a simple quadratic Poisson bracket on $\mathbf{h}$ if and only if the antisymmetry condition is satisfied, which happens if and only if $F_{ii,jj}=-F_{jj,ii}$ for all i,j. Notice that this class of brackets does not include any brackets that depend on k or l, and in particular the bracket of Theorem 3.

Define $F^{a,b}$ to be the diagonal matrix such that $F^{a,b}_{ij,kl}=F_{i-aj-a,k-bl-b}$, i.e., F shifted a blocks downwards along the diagonal, and b entries within each block. Notice that $(U^{(i)}\otimes I)F=F^{1,0}(U^{(i)}\otimes I)$ and $(I\otimes U^{(i)})F=F^{0,1}(I\otimes U^{(i)})$.

Theorem 4: *Let $F\in\hat{\mathrm{M}}(\infty)\otimes\hat{\mathrm{M}}(\infty)$ be a diagonal matrix satisfying the antisymmetry condition above. Define a Poisson bracket on* $\mathbf{h}$ *via the formula $\{U^{(k)\otimes},U^{(l)}\}_{\mathbf{h}}=F(U^{(k)}\otimes U^{(l)})$ for all i,j. Then $\{,\}_{\mathbf{h}}\in\mathcal{D}(\mathbf{h})$.*

Proof: Compute $\{f^*(V)^{\otimes},f^*(V)\}_{\mathbf{h}}$,

$$\begin{aligned}\{f^*(V)^{\otimes},f^*(V)\}_{\mathbf{h}}&=\left\{\prod_{i=1}^{m}(I+U^{(i)})\otimes\prod_{i=1}^{m}(I+U^{(i)})\right\}_{\mathbf{h}}\\&=\sum_{i,j}\left(\prod_{k=1}^{i-1}(I+U^{(k)})\otimes\prod_{n=1}^{j-1}(I+U^{(n)})\right)F(U^{(i)}\otimes U^{(j)})\\&\quad\times\left(\prod_{k=i+1}^{m}(I+U^{(k)})\otimes\prod_{n=j+1}^{m}(I+U^{(n)})\right)\\&=\sum_{i,j,t,s,c_1,c_2}(E^{t}_{1,\ldots,i-1}\otimes E^{s}_{1,\ldots,j-1})F(U^{(i)}\otimes U^{(j)})(E^{c_1-t}_{i+1,\ldots,m}\otimes E^{c_2-s}_{j+1,\ldots,m})\\&=\sum_{i,j,t,s,c_1,c_2}F^{t,s}(E^{t}_{1,\ldots,i-1}\otimes E^{s}_{1,\ldots,j-1})(U^{(i)}\otimes U^{(j)})(E^{c_1-t}_{i+1,\ldots,m}\otimes E^{c_2-s}_{j+1,\ldots,m})\\&=\sum_{c_1,c_2}\left(\sum_{t=0}^{c_1}\sum_{s=0}^{c_2}F^{t,s}\right)E^{c_1+1}_{1,\ldots,m}\otimes E^{c_2+1}_{1,\ldots,m}.\end{aligned}$$

In the last step we used Lemma 1 for each fixed (t,s). This finishes the proof since each $E^{c}_{1,\ldots,m}$ is a diagonal of $f^*(V)$. ∎

Notice that in the proof we obtained, as a bonus, a formula for the descent bracket on g_m. We remark that this new bracket is simple on g_m as well.

Adding the bracket obtained from all possible F's of the type discussed above to the bracket of Theorem 3, we obtain the following set of simple brackets on $\mathbf{h}$:

$$\{u^{(k)}_i,u^{(l)}_j\}_{\mathbf{h}}=(F_{i+1i+1,j+1j+1}+\delta_{i,j+1}-\delta_{i,j})u^{(k)}_iu^{(l)}_j\quad\text{if } k<l,\text{and}$$

$$\{u^{(k)}_i,u^{(l)}_j\}_{\mathbf{h}}=(F_{i+1i+1,j+1j+1}+\delta_{i,j}-\delta_{i,j-1})u^{(k)}_iu^{(l)}_j\quad\text{if } k>l.$$

$$\{u^{(k)}_i,u^{(k)}_j\}_{\mathbf{h}}=F_{i+1i+1,j+1j+1}u^{(k)}_iu^{(l)}_j.$$

We assume that $F=F^{m,m}$ for all m. This implies that the bracket depends on $j-i$, but not on i and j separately. Notice that the bracket already depends on k and l via $l-k$ only. In order to do the same for the bracket periodic in one direction, it is enough to ensure F also produces periodic terms with the same period. For this we assume $F_{ii,jj}=F_{ii,j+Nj+N}\,\forall\, i,j$. The combined bracket is

$$\{u^{(k)}_i,u^{(l)}_j\}_{\mathbf{h}}=\left(F_{i+1i+1,j+1j+1}+\sum_{n=-\infty}^{\infty}(\delta_{i,j+1+nN}-\delta_{i,j+nN})\right)u^{(k)}_iu^{(l)}_j\quad\text{if } k<l,$$

and

$$\{u_i^{(k)},u_j^{(l)}\}_{\mathbf{h}}=\left(F_{i+1i+1,j+1j+1}+\sum_{n=-\infty}^{\infty}(\delta_{i,j+nN}-\delta_{i,j-1+nN})\right)u_i^{(k)}u_j^{(l)}\quad\text{if } k>l,$$

$$\{u_i^{(k)},u_j^{(k)}\}_{\mathbf{h}}=F_{i+1i+1,j+1j+1}u_i^{(k)}u_j^{(l)}.$$

Expressing this bracket in terms of the variables $w_i^{(k)}=u_{i-k}^{(k)}$, we obtain

$$\{w_i^{(k)},w_j^{(l)}\}_{\mathbf{h}}=\left(F_{i-k+1i-k+1,j-l+1j-l+1}+\sum_{n=-\infty}^{\infty}(\delta_{i-k,j-l+1+nN}-\delta_{i-k,j-l+nN})\right)w_i^{(k)}w_j^{(l)}$$

if $k<l$, and

$$\{w_i^{(k)},w_j^{(l)}\}_{\mathbf{h}}=\left(F_{i-k+1i-k+1,j-l+1j-l+1}+\sum_{n=-\infty}^{\infty}(\delta_{i-k,j-l+nN}-\delta_{i-k,j-l-1+nN})\right)w_i^{(k)}w_j^{(l)}$$

if $k>l$.

$$\{w_i^{(k)},w_j^{(k)}\}_{\mathbf{h}}=F_{i-k+1i-k+1,j-l+1j-l+1}w_i^{(k)}w_j^{(l)}.$$

This bracket is still simple, and let us denote the coefficient of $w_i^{(k)}w_j^{(l)}$ in $\{w_i^{(k)},w_j^{(k)}\}_{\mathbf{h}}$ above by κ_{j-i}^{l-k}, noting again that it depends only on $j-i$ and $l-k$, and not separately on the four variables. The indexing makes the formulas look very complicated, but observing the following properties of the function κ_b^a, where $b\in\mathbb{Z}, a\in\{1-k,\ldots,M-k\}$ results in considerable simplification:

$$\kappa_0^0=0,$$

$$\kappa_{b+N}^a=\kappa_b^a\quad\text{for all } a,b,(\text{so assume } b\in\mathbb{Z}/N\mathbb{Z} \text{ for the rest}),$$

$$\kappa_b^a-\kappa_{b-1}^{a-1}=\delta_{a,1}\delta_{b,0}-\delta_{a,1}\delta_{b,1}-\delta_{a,0}\delta_{b,1}+\delta_{a,0}\delta_{b,0}\quad\text{for all } b\in\mathbb{Z}/N\mathbb{Z},$$

and $a\in\{2-k,\ldots,M-k\}$

Finally, we want to select F above, equivalently κ, such that the bracket above becomes doubly periodic. This happens if and only if we can extend κ to all $a\in\mathbb{Z}$ such that $\kappa_b^{a+M}=\kappa_b^a$, and the conditions above are satisfied for all a,b. We prove the following.

Theorem 5: *If M and N are relatively prime positive integers, there exists a unique function κ on $\mathbb{Z}/N\mathbb{Z}\times\mathbb{Z}/M\mathbb{Z}$ such that $\kappa_0^0=0$ and*

$$\kappa_b^a-\kappa_{b-1}^{a-1}=\delta_{a,1}\delta_{b,0}-\delta_{a,1}\delta_{b,1}-\delta_{a,0}\delta_{b,1}+\delta_{a,0}\delta_{b,0}\quad \textit{for all } b\in\mathbb{Z}/N\mathbb{Z} \textit{ and } a\in\mathbb{Z}/M\mathbb{Z}.$$

Proof: Since M and N are relatively prime, $(1,1)$ is a generator for the group $\mathbb{Z}/N\mathbb{Z}\times\mathbb{Z}/M\mathbb{Z}$. Hence the difference equation and the initial value $\kappa_0^0=0$ determines κ uniquely if it exists. To prove existence, consider the sequence $(1,1),(2,2),\ldots$. The two elements $(1,0)$ and $(-1,0)$ of $\mathbb{Z}/N\mathbb{Z}\times\mathbb{Z}/M\mathbb{Z}$ appear in some order in this sequence. If $(1,0)$ appears first, then set

$$\kappa_1^1=\kappa_2^2=\cdots=\kappa^{0,-1}=-1,$$

$$\kappa_{-1}^{-1}=\kappa_{-2}^{-2}=\cdots=\kappa^{0,1}=1,$$

and $\kappa_b^a=0$ otherwise.

If the alternative happens, i.e., if $(-1,0)$ appears before $(1,0)$ then set

$$\kappa_1^1 = \kappa_2^2 = \cdots = \kappa^{-1,0} = -1,$$

$$\kappa_{-1}^{-1} = \kappa_{-2}^{-2} = \cdots = \kappa^{1,0} = 1,$$

and $\kappa_b^a = 0$ otherwise.

It is easy to check that in both cases the difference equation is satisfied. ■

Thus there exists a choice for F making the combined bracket doubly periodic, and we showed that if F is subject the requirements above, it is unique.

Remarks: The proof of the last theorem shows that there are two combinatorially distinct cases depending on M and N. One can check that the alternative which is realized depends on the parity of the number of steps in the Euclidean algorithm for N and M.

The system in Ref. 9 can be equipped with a quadratic Poisson bracket along these lines. However there, the variables on which periodicity is imposed are coordinate functionals in $(I + U_{2i+1})(I + U_{2i+2})$, i.e., the matrices are lumped in pairs. It is also true that the conserved quantities Poisson commute under the bracket obtained. For this computation, and more on the Hamiltonian properties of these systems see Ref. 12 or Ref. 13.

V. CONCLUSION

In this paper we presented a method for producing quadratic Poisson brackets from a family of brackets which are easy to construct (simple brackets), and applied this method to several examples. It is possible to produce large families of Poisson brackets using this method, and then one can seek for a particular element of the family satisfying further requirements, such as commutation of conserved quantities, or periodicity, etc. The method can produce nonlocal brackets which are sometimes indispensable (as in the doubly periodic KP hierarchy above).

We believe the following questions are worthy of further investigation: Given an algebra g, it is unclear at the moment what the locus of brackets obtainable by such a method in the moduli space of all quadratic brackets is. Also, understanding the interplay of conserved quantities with the descent process requires further work (e.g., can one characterize those brackets among descent brackets admitting a large set of commuting quantities?). In a different direction, it might be worthwhile to ask if these brackets can be used in the ways r-matrix brackets are used in geometry, such as in producing link invariants.

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APPENDIX: PROOF OF THEOREM 3

We will prove Theorem 3. Recall the formula

$$f^*(v_{ij}) = \sum_{k_1<k_2<\ldots<k_{i-j}\leqslant M} u_i^{(k_1)} u_{i-1}^{(k_2)} \ldots u_{j+1}^{(k_{i-j})}.$$

Lemma 2: Suppose $i>j>m$ Then

$$\{v_{ij}, v_{jm}\}_{g_m} = v_{im}.$$

Also, if $k<j$ then $\{v_{ij}, v_{kl}\}_{g_m} = 0$

Proof: Using the formula above, we can express the bracket in terms of $u_j^{(i)}$'s,

$$\{v_{ij},v_{jm}\}_{g_m}=\left\{\sum_{k_1<k_2<\ldots<k_{i-j}\leqslant M}u_i^{(k_1)}u_{i-1}^{(k_2)}\ldots u_{j+1}^{(k_{i-j})},\sum_{l_1<l_2<\ldots<l_{j-m}\leqslant M}u_j^{(l_1)}u_{j-1}^{(l_2)}\ldots u_{m+1}^{(l_{j-m})}\right\}_{\mathbf{h}}.$$

When the bracket above is expanded using the Leibniz rule, all brackets except those of type $\{u_{j+1}^{(k_{i-j})},u_j^{(l_1)}\}_{\mathbf{h}}$ with $k_{i-j}<l_1$ are zero. Thus we obtain

$$\{v_{ij},v_{jm}\}_{g_m}=\sum_{k_1<\cdots<k_{i-j}<l_1<\cdots<l_{j-m}\leqslant M}u_i^{(k_1)}\cdots u_{j+1}^{(k_{i-j})}u_j^{(l_1)}\cdots u_{m+1}^{(l_{j-m})}=v_{im}.$$

The second part of the assertion is clear, since in that case there are no pairs of terms that give a nonzero bracket. ■

Lemma 3: (i) $\{v_{ii-1},v_{jm}\}_{g_m}=0$ *if* $j>i$ *and* $m<i-1$, (ii) $\{v_{ii-1},v_{im}\}_{g_m}=v_{ii-1}v_{im}$ *if* $m<i-1$, (iii) $\{v_{ii-1},v_{ji-1}\}_{g_m}=-v_{ii-1}v_{ji-1}$ *if* $j>i$.

Proof:

$$\{v_{ii-1},v_{jm}\}_{g_m}=\left\{\sum_{k\leqslant M}u_i^{(k)},\sum_{l_1<\cdots<l_{j-m}\leqslant M}u_j^{(l_1)}\cdots u_{m+1}^{(l_{j-m})}\right\}_{\mathbf{h}}.$$

Consider brackets of pairs of monomials. $u_i^{(k)}$ may have nonzero brackets only with the three terms $u_{i+1}^{(l_a)},u_i^{(l_b)}$ and $u_{i-1}^{(l_c)}$ of a monomial $\mathbf{m}$ in v_{jm}. For part (i), note that by the hypothesis $j>i>m+1$, each monomial $\mathbf{m}$ of v_{jm} contains all three terms. For convenience, $\mathbf{m}$ will be indexed as $\mathbf{m}_{l_a,l_b,l_c}$. If $k\leqslant l_a$, $l_c\leqslant k$ or $k=l_b$, one checks that $\{u_i^{(k)},\mathbf{m}_{l_a,l_b,l_c}\}_{\mathbf{h}}=0$. If $l_a<k<l_b$, then $\{u_i^{(k)},\mathbf{m}_{l_a,l_b,l_c}\}_{\mathbf{h}}=-\{u_i^{(l_b)},\mathbf{m}_{l_a,k,l_c}\}_{\mathbf{h}}$. Therefore the sum vanishes because of pairwise cancellation, and (i) is proven.

To prove (ii), note that $u_i^{(l_b)}$ and $u_{i-1}^{(l_c)}$, but not $u_{i+1}^{(l_a)}$ occur in each monomial $\mathbf{m}$ of v_{im} (hence, denoted by $\mathbf{m}_{l_b,l_c}$). If $k<l_b$, $\{u_i^{(k)},\mathbf{m}_{l_b,l_c}\}_{\mathbf{h}}=0$, if $l_b<k<l_c$, $\{u_i^{(k)},\mathbf{m}_{l_b,l_c}\}_{\mathbf{h}}=2u_i^{(k)}\mathbf{m}_{l_b,l_c}$. Therefore for $k<l_b$, $\{u_i^{(k)},\mathbf{m}_{l_b,l_c}\}_{\mathbf{h}}+\{u_i^{(l_b)},\mathbf{m}_{k,l_c}\}_{\mathbf{h}}=2u_i^{(k)}\mathbf{m}_{l_b,l_c}$. For $k=l_b$ and $k\geqslant l_c$ one gets $\{u_i^{(k)},\mathbf{m}_{l_b,l_c}\}_{\mathbf{h}}=u_i^{(k)}\mathbf{m}_{l_b,l_c}$. Therefore, the sum of all the terms gives $v_{ii-1}v_{im}$. (iii) is similar to (ii). ■

Lemma 4: $\{v_{ij},v_{nm}\}_{g_m}=0$ *if* $n>i$ *and* $m<j$.

Proof: Do induction on $i-j$. For $i-j=1$, the statement reduces to (i) of Lemma 3. Notice that by Lemma 2 $v_{ij}=\{v_{ij+1},v_{j+1j}\}_{g_m}$. Then

$$\{v_{ij},v_{nm}\}_{g_m}=\{\{v_{ij+1},v_{j+1j}\}_{g_m},v_{nm}\}_{g_m}=-\{\{v_{nm},v_{ij+1}\}_{g_m},v_{j+1j}\}_{g_m}-\{\{v_{j+1j},v_{nm}\}_{g_m},v_{ij+1}\}_{g_m}=0$$

by the Jacobi identity and the induction hypothesis. ■

Lemma 5: (i) $\{v_{kj},v_{ij}\}_{g_m}=v_{kj}v_{ij}$ *if* $k>i$. (ii) $\{v_{ij},v_{ik}\}_{g_m}=v_{ij}v_{ik}$ *if* $j>k$.

Proof: The two parts are similar, so we will only prove (i). Again, do induction on $i-j$. Notice $v_{ij}=\{v_{ij+1},v_{j+1j}\}_{g_m}$,

$$\begin{aligned}\{v_{kj},v_{ij}\}_{g_m}&=\{v_{kj},\{v_{ij+1},v_{j+1j}\}\}_{g_m}\\&=-\{v_{j+1j},\{v_{kj},v_{ij+1}\}_{g_m}\}_{g_m}-\{v_{ij+1},\{v_{j+1j},v_{kj}\}_{g_m}\}_{g_m}\\&=-\{v_{j+1j},0\}_{g_m}+\{v_{ij+1},v_{j+1j}v_{kj}\}_{g_m}\\&=\{v_{ij+1},v_{j+1j}\}_{g_m}v_{kj}+\{v_{ij+1},v_{kj}\}_{g_m}v_{j+1j}\\&=v_{ij}v_{kj}.\end{aligned}$$

■

Lemma 6: Suppose $i>k>j>l$. *Then* $\{v_{ij},v_{kl}\}_{g_m}=v_{ij}v_{kl}+v_{kj}v_{il}$.

Proof: We know that $v_{kl}=\{v_{kj},v_{jl}\}_{g_m}$. Then,

$$
\begin{aligned}
\{v_{ij},v_{kl}\}_{g_m} &= \{v_{ij},\{v_{kj},v_{jl}\}_{g_m}\}_{g_m} \\
&= -\{v_{jl},\{v_{ij},v_{kj}\}_{g_m}\}_{g_m} - \{v_{kj},\{v_{jl},v_{ij}\}_{g_m}\}_{g_m} \\
&= -\{v_{jl},v_{ij}v_{kj}\}_{g_m} + \{v_{kj},v_{il}\}_{g_m} \\
&= -\{v_{jl},v_{ij}v_{kj}\}_{g_m} \\
&= -\{v_{jl},v_{ij}\}_{g_m}v_{kj} - \{v_{jl},v_{kj}\}_{g_m}v_{ij} \\
&= v_{il}v_{kj} + v_{kl}v_{ij}.
\end{aligned}
$$

■

Thus the proof is complete.

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On deformations of standard *R*-matrices for integrable infinite-dimensional systems

Błażej M. Szablikowski[a] and Maciej Błaszak[b]
Institute of Physics, A. Mickiewicz University, Poznań, Poland

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Simple deformations, with a parameter ϵ, of classical R-matrices which follow from decomposition of appropriate Lie algebras, are considered. As a result nonstandard Lax representations for some well-known integrable systems are presented and integrable evolution equations are constructed. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1868373]

I. INTRODUCTION

In the theory of nonlinear evolutionary systems one of the most important problems is construction of integrable systems. By integrable systems we understand those which have infinite hierarchy of commuting symmetries. It is well known that a very powerful tool, called the classical R-matrix formalism, can be used for systematic construction of field and lattice integrable dispersive systems (soliton systems) as well as dispersionless integrable field systems (see Refs. 1–10 and the references therein).

The crucial point of the formalism is the observation that integrable systems can be obtained from Lax equations. Let $\mathfrak{g}$ be a Lie algebra, equipped with the Lie bracket $[\cdot,\cdot]$. A linear map $R:\mathfrak{g}\to\mathfrak{g}$, such that the bracket $[a,b]_R:=[Ra,b]+[a,Rb]$ is a second Lie product on $\mathfrak{g}$, is called the classical R-matrix. Assume that R satisfies a Yang–Baxter equation YB(α): $[Ra,Rb]-R[a,b]_R+\alpha[a,b]=0$, which is a sufficient condition for R to be an R-matrix. Then, powers of L generate mutually commuting vector fields

$$L_{t_n}=[R(L^n),L]. \tag{1}$$

For fixed n the remaining systems are considered as its symmetries. In this sense (1) represents a hierarchy of integrable dynamical systems.

In this paper the deformation method for systems (1), preserving the integrability, is presented. It has been done on the level of their Lax representations through simple deformations, with parameter ϵ, of classical R-matrices. It is shown that such a procedure leads to the construction of nonstandard Lax representations for some well-known integrable systems as well as to the construction of new integrable evolution equations.

II. DEFORMATIONS OF STANDARD *R*-MATRICES

To construct the simplest R-structure let us assume that the Lie algebra $\mathfrak{g}$ can be split into a direct sum of Lie subalgebras $\mathfrak{g}_+$ and $\mathfrak{g}_-$, i.e., $\mathfrak{g}=\mathfrak{g}_+\oplus\mathfrak{g}_-$, where $[\mathfrak{g}_\pm,\mathfrak{g}_\pm]\subset\mathfrak{g}_\pm$. Denoting the projections onto these subalgebras by $P_\pm$, we define the R-matrix as

$$R=\tfrac{1}{2}(P_+-P_-). \tag{2}$$

Straightforward calculation shows that (2) solves YB$\left(\frac{1}{4}\right)$. The classical R-matrices constructed in this way we understand as standard ones.

[a]Electronic mail: bszablik@amu.edu.pl
[b]Electronic mail: blaszakm@amu.edu.pl

Let us consider the following deformation of (2):

$$R'(a) = R(a) + \epsilon r(a), \tag{3}$$

where ϵ is an arbitrary constant playing the role of a deformation parameter and r is a linear deformation operator. First, assume that r satisfies the following two relations:

$$[ra,b_+] \in \mathfrak{g}_+, \quad [ra,b_-] \in \mathfrak{g}_-, \quad a \in \mathfrak{g}, \quad b_+ \in \mathfrak{g}_+, \quad b_- \in \mathfrak{g}_-. \tag{4}$$

So, the question arises when the deformed R preserves the property of being R-matrix. Once again, straightforward calculation shows that (3) solves $\mathrm{YB}(\frac{1}{4})$ when the following condition is fulfilled:

$$r[a,b]_R + \epsilon r[a,b]_r - \epsilon[ra,rb] = 0, \tag{5}$$

where $[a,b]_r = [ra,b] + [a,rb]$.

III. DISPERSIONLESS SYSTEMS

Let A be the algebra of formal Laurent series (Lax polynomials) in p (Ref. 6),

$$A = \left\{ L = \sum_{i \in Z} u_i(x) p^i \right\}, \tag{6}$$

where the coefficients $u_i(x)$ are smooth functions of x. Poisson brackets on A can be introduced in infinitely many ways as

$$[f,g] \equiv \{f,g\}_s := p^s \left(\frac{\partial f}{\partial p}\frac{\partial g}{\partial x} - \frac{\partial f}{\partial x}\frac{\partial g}{\partial p} \right), \quad s \in \mathbb{Z}. \tag{7}$$

Then, fixing s, A is the Poisson algebra with an appropriate bracket (7). We construct the standard R-matrix, through a decomposition of A into a direct sum of Lie subalgebras. For a fixed s let $A_{\geqslant -s+k} = \{\Sigma_{i \geqslant -s+k} u_i(x) p^i\}$ and $A_{<-s+k} = \{\Sigma_{i<-s+k} u_i(x) p^i\}$. Then, $A_{\geqslant -s+k}$, $A_{<-s+k}$ are Lie subalgebras in the following cases:

(1) $s=0$, $k=0$,
(2) $s \in \mathbb{Z}$, $k=1,2$,
(3) $s=2$, $k=3$.

So, fixing s we fix the Lie algebra structure with k numbering the standard R-matrices given in the following form:

$$R = \tfrac{1}{2}(P_{\geqslant -s+k} - P_{<-s+k}) = P_{\geqslant -s+k} - \tfrac{1}{2} = \tfrac{1}{2} - P_{<-s+k}, \tag{8}$$

where P are appropriate projections. The Lax hierarchy (1) can be represented by two equivalent representations,

$$L_{t_q} = \{(L^q)_{\geqslant -s+k}, L\}_s = -\{(L^q)_{<-s+k}, L\}_s. \tag{9}$$

Notice that different schemes are interrelated. Under the transformation

$$x' = x, \quad p' = p^{-1}, \quad t' = t \tag{10}$$

the Lax hierarchy (9) defined by k, s, and L transforms into the Lax hierarchy (9) defined by $k' = 3-k$, $s' = 2-s$, and $L' = L$, i.e.,

$$L \text{ for } k, \quad s \quad \Leftrightarrow \quad L' = L \quad \text{for } k' = 3-k, \quad s' = 2-s. \tag{11}$$

In such a situation it is enough to consider the cases of $k=0$ and $k=1$.

We are interested in extracting closed systems for a finite number of fields. To obtain a consistent Lax equation, the Lax operator L must form a proper submanifold of the full Poisson algebra A, i.e., the left- and right-hand sides of expression (9) must coincide. They are given in the form[7]

$$s=0, \quad k=0, \quad L=p^N+u_{N-2}p^{N-2}+u_{N-3}p^{N-3}+\cdots+u_1p+u_0, \tag{12}$$

$$s\in\mathbb{Z}, \quad k=1, \quad L=p^N+u_{N-1}p^{N-1}+\cdots+u_{1-m}p^{1-m}+u_{-m}p^{-m}, \tag{13}$$

where u_i are dynamical fields. Notice, that powers of L, in general fractional, can be calculated by expanding them around poles, for (12) around ∞ and for (13) around ∞ and 0. So, for $k=0$ we construct one Lax hierarchy and for $k=1$ we construct, in general, two mutually commuting Lax hierarchies.

We are looking for a simple deformation of (8) in the form

$$r=p^{\alpha}P_{\beta}, \quad P_{\beta}(L)=[L]_{\beta}=u_{\beta} \tag{14}$$

which will satisfy (4) and (5) for arbitrary ϵ. By some straightforward calculations, we find them in the form

$$r=p^{-s+k}P_{k-1} \quad \text{for} \begin{cases} (1) & s=0, \quad k=0, \\ (2) & s=0, \quad k=1, \\ (3) & s=1, \quad k=1 \end{cases} \tag{15}$$

and

$$r=p^{-s+k-1}P_{k-2} \quad \text{for} \begin{cases} (4) & s=1, \quad k=2, \\ (5) & s=2, \quad k=2, \\ (6) & s=2, \quad k=3. \end{cases} \tag{16}$$

We see that deformations of (8) given by the form (3) and (14), exist only for distinguished values of s and k. Nevertheless, for particular fixed values of ϵ and fixed s (i.e., fixed Lie algebra) there exist other deformations of the form (14), but they are trivial in the sense that they relate standard R-matrices (8) with different k. Moreover, deformations (16) are constructed from (15) by using transformation (10) and (11). Hence, the only relevant deformations are (15) and so further we will consider only them. The deformed R-matrices for the cases in (15) take the form

$$R'=P_{\geqslant -s+k}-\tfrac{1}{2}+\epsilon p^{-s+k}P_{k-1}=\tfrac{1}{2}-P_{<-s+k}+\epsilon p^{-s+k}P_{k-1}. \tag{17}$$

The case: $s=0$, $k=0$.

The Lax hierarchy for a deformed R-matrix is

$$L_{t_q}=\{(L^q)_{\geqslant 0}+\epsilon[L^q]_{-1},L\}_0=-\{(L^q)_{<0}-\epsilon[L^q]_{-1},L\}_0. \tag{18}$$

Consistent Lax equations are obtained for Lax operators of the form

$$L=p^N+u_{N-1}p^{N-1}+u_{N-2}p^{N-2}+\cdots+u_1p+u_0, \tag{19}$$

where u_i are dynamical fields. From (18) it follows that

$$\begin{aligned} (u_{N-1})_{t_q}&=-\epsilon N([L^q]_{-1})_x, \\ (u_{N-2})_{t_q}&=N([L^q]_{-1})_x-\epsilon(N-1)u_{N-1}([L^q]_{-1})_x, \\ &\cdots \quad . \end{aligned} \tag{20}$$

So, for $\epsilon=0$ the field u_{N-1} becomes time independent and without losing the generality we can

assume that it is zero. Then, Lax operator becomes a standard Lax operator (12) for the case with nondeformed R-matrix. From (20) the following relation between u_{N-1} and u_{N-2} results:

$$u_{N-2} = -\frac{1}{\epsilon}u_{N-1} + \frac{N-1}{2N}(u_{N-1})^2 \tag{21}$$

so we can eliminate one of them. Eliminating u_{N-2} we will consider constrained Lax operator in the form

$$L = p^N + u_{N-1}p^{N-1} + \left(-\frac{1}{\epsilon}u_{N-1} + \frac{N-1}{2N}(u_{N-1})^2\right)p^{N-2} + u_{N-3}p^{N-3} + \cdots + u_1 p + u_0. \tag{22}$$

Reparametrizing (22), $u_{N-1} \mapsto -\epsilon u_{N-2}$ and then taking the limit $\epsilon \to 0$ it becomes the standard Lax operator (12).

Lemma 3.1: For arbitrary ϵ the Lax hierarchy (18) and (22) *is equivalent to the Lax hierarchy* (9) and (12) *with* $s=k=0$.

The sketch of the proof is as follows. We are looking for transformations that will relate fields from (22) and fields from (12). We postulate the following form of these relations:

$$u_{N-1} \mapsto -\epsilon u_{N-2},$$

$$u_i \mapsto u_i + f_i(u_{N-2}, u_{N-3}, \ldots, u_{i+1}) \quad \text{for } N-3 \geqslant i \geqslant 0. \tag{23}$$

Then, we construct functions f_i in such a way, that hierarchy (18) will lead to the same evolution system as (9) for $s=k=0$. We compare the first nontrivial systems from these hierarchies. Functions f_i are recursively constructed comparing evolution expressions for u_{i+1t}. Such a procedure guarantees that the expressions for the fields will be the same only for components $u_{N-2_t}, \ldots, u_{1_t}$. So, the equality between both evolution expressions for u_0 must be argued. The systems for Lax operators (12) and (22) both can be understood as the reduction of infinite-field systems for Lax operators of the form $L' = a_1 p + a_0 + a_{-1}p^{-1} + \ldots$, given by constraint $L = L'^N$. The equivalence between the hierarchies considered, constructed from L', can be shown by explicit infinite recurrence form (23). Now, reducing them to finite-field systems one finds the appropriate transformation between finite-field systems, including the evolution for u_0. So, the Lax hierarchy (18) and (22) is a new representation of well-known integrable dispersionless hierarchies. The form of transformation (23), relating both systems, guarantees that it is an invertible transformation.

Example 3.2: Dispersionless KdV: $N=2$.

For $L = p^2 + up + v$ *and* $L_{t_i} = \{(L^{i/2})_{\geqslant 0} + \epsilon[L^{i/2}]_{-1}, L\}_0$ *we find*

$$\begin{pmatrix} u \\ v \end{pmatrix}_{t_1} = \begin{pmatrix} \frac{1}{2}\epsilon u u_x - \epsilon v_x \\ \frac{1}{4}(\epsilon u - 2)(u u_x - 2v_x) \end{pmatrix},$$

$$\begin{pmatrix} u \\ v \end{pmatrix}_{t_3} = \begin{pmatrix} -\frac{3}{16}\epsilon(u^2 - 4v)(u u_x - 2v_x) \\ -\frac{3}{32}\epsilon(\epsilon u - 2)(u^2 - 4v)(u u_x - 2v_x) \end{pmatrix}, \tag{24}$$

$$\cdots.$$

In the limit $\epsilon \to 0$ *and* $u=0$ *it becomes the standard dispersionless KdV hierarchy. Notice, that fields* u and v *are not independent. According to* (21) $v = -(1/\epsilon)u + \frac{1}{4}u^2$ *and the hierarchy* (24) *is equivalent to the one*

$$u_{t_1} = u_x, \quad u_{t_3} = -\frac{3}{2\epsilon}u u_x, \quad \cdots, \tag{25}$$

i.e., reparametrized dispersionless KdV. The transformation to the standard form of dispersionless

KdV is given by $u\mapsto -\epsilon u$. *The hierarchy* (25) *is generated from* $L=p^2+up+\frac{1}{4}u^2-(1/\epsilon)u$.

Example 3.3: Dispersionless Boussinesq: $N=3$.

Here we present only the result for the constrained Lax operator (22) $L=p^3+up^2+\left[\frac{1}{3}u^2-(1/\epsilon)u\right]p+w$. *Then, the first nontrivial system from the hierarchy is*

$$L_{t_2}=\{(L^{\frac{2}{3}})_{\geqslant 0}+\epsilon[L^{\frac{2}{3}}]_{-1},L\}_0 \Leftrightarrow \begin{pmatrix} u \\ w \end{pmatrix}_{t_2} = \begin{pmatrix} \frac{2}{9}(\epsilon u-6)uu_x-2\epsilon w_x \\ \frac{2}{81\epsilon^2}(\epsilon u-3)(\epsilon u(\epsilon u-9)+9)uu_x-\frac{2}{9}(\epsilon u-6)uw_x \end{pmatrix}.$$

Eliminating the field w *we obtain the reparametrized dispersionless Boussinesq,* $u_{tt}=(2/3\epsilon)\times(u^2)_{xx}$. *The transformation* (23) *to the standard form of the dispersionless Boussinesq system is given by* $u\mapsto -\epsilon u$, $w\mapsto w-\frac{1}{3}\epsilon u^2-\frac{1}{27}\epsilon^3u^3$.

The case: $s=0$, $k=1$.

The Lax hierarchy for the deformed R-matrix (17) is

$$L_{t_q}=\{(L^q)_{\geqslant 1}+\epsilon[L^q]_0p,L\}_0=-\{(L^q)_{<1}-\epsilon[L^q]_0p,L\}_0. \tag{26}$$

Appropriate Lax operators are of the form

$$L=u_Np^N+u_{N-1}p^{N-1}+\cdots+u_{1-m}p^{1-m}+u_{-m}p^{-m}. \tag{27}$$

From (26) one finds that $(u_N)_t=\epsilon(u_N)_x[L^q]_0-\epsilon Nu_N([L^q]_0)_x$. Hence, in the limit of $\epsilon=0$ the field u_N becomes a time-independent field c_N. Fixing $c_N=1$ the Lax operator becomes a standard Lax operator (13) for $s=0$, $k=1$. Moreover, there is no constraint contrary to the previous case. Hence, the Lax hierarchy (27) and (26) leads to new integrable dispersionless systems, at least to the best of our knowledge. Notice that the zero power of L always leads to the space translation symmetry, $L_{t_0}=\epsilon L_x$.

Example 3.4: Extended dispersionless Benney, $N=m=1$.

Let $L=up+v+wp^{-1}$, *then for* $L_{t_i}=\{(L^i)_{\geqslant 1}+\epsilon[L^i]_0p,L\}_0$ *we find*

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_{t_0} = \epsilon\begin{pmatrix} u_x \\ v_x \\ w_x \end{pmatrix},$$

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_{t_1} = \begin{pmatrix} \epsilon u_xv-\epsilon uv_x \\ uv_x+\epsilon vv_x \\ u_xw+uw_x+\epsilon v_xw+\epsilon vw_x \end{pmatrix},$$

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_{t_2} = \begin{pmatrix} \epsilon u_xv^2-2\epsilon uvv_x-2\epsilon u^2w_x \\ 2uu_xw+2uvv_x+2u^2w_x+\epsilon v^2v_x+2\epsilon uv_xw \\ 2u_xvw+2uv_xw+2uvw_x+2\epsilon u_xw^2+2\epsilon vv_xw+\epsilon v^2w_x+4\epsilon uww_x \end{pmatrix},$$

$$\cdots.$$

In the limit $\epsilon\to 0$ *and* $u=1$ *we obtain the standard dispersionless Benney system.*

Example 3.5: Two field system, $N=0$, $m=1$.

Consider $L=v+wp^{-1}$. *Then* $[L^i]_0=v^i$ *and* $(L^i)_{\geqslant 1}=0$ *for* $i=0,1,2,\ldots$. *Hence we obtain the system*

$$L_{t_i}=\{\epsilon[L^i]_0p,L\}_0 \Leftrightarrow \begin{pmatrix} v \\ w \end{pmatrix}_{t_i} = \begin{pmatrix} \epsilon v^iv_x \\ \epsilon(v^iw)_x \end{pmatrix} \tag{28}$$

which does not have any standard counterpart.

The case: $s=1$, $k=1$.

The Lax hierarchy is

$$L_{t_q} = \{(L^q)_{\geqslant 0} + \epsilon[L^q]_0, L\}_1 = -\{(L^q)_{<0} - \epsilon[L^q]_0, L\}_1 \tag{29}$$

and appropriate Lax operators take the form

$$L = u_N p^N + u_{N-1} p^{N-1} + \cdots + u_{1-m} p^{1-m} + u_{-m} p^{-m}. \tag{30}$$

From (29) it follows that

$$(u_N)_t = -\epsilon N u_N([L^q]_0)_x, \quad \cdots, \quad (u_{-m})_t = (1+\epsilon) m u_{-m}([L^q]_0)_x. \tag{31}$$

So, we find that the highest and lowest fields are related by

$$u_N^{(1+\epsilon)m} = u_{-m}^{-\epsilon N}.$$

For $\epsilon=0$ the field u_N becomes a time-independent field c_N (let $c_N=1$), then the Lax operator (30) becomes a standard Lax operator (13) for $s=k=1$. For $\epsilon=-1$ the field u_{-m} becomes time independent and the Lax operator becomes a standard Lax operator for $s=1$, $k=2$. This last case follows from the fact that for $s=1$, $k=1$, and $\epsilon=-1$ the deformed R-matrix (17) becomes the standard R-matrix (8) for $s=1$, $k=2$. Eliminating u_N field the Lax operator takes the form

$$L = u_{-m}^{-[\epsilon N/(1+\epsilon)m]} p^N + u_{N-1} p^{N-1} + \cdots + u_{1-m} p^{1-m} + u_{-m} p^{-m}. \tag{32}$$

In the limit $\epsilon \to 0$ it becomes the standard Lax operator (13) for $s=k=1$.

Lemma 3.6: For arbitrary ϵ*, the Lax hierarchy* (29) and (30) *is equivalent to the Lax hierarchy* (9) and (13) *with* $s=k=1$.

To show this let us make the following transformation:

$$u_i \mapsto u_i u_N^{i/N}, \quad p \mapsto u_N^{-1/N} p \quad \text{for } N-1 \geqslant i > -m. \tag{33}$$

The Poisson bracket (7) for $s=1$ is invariant under (33). Moreover, the Lax operators (30) transform into (13) one. Then, after the transformation of coordinates (33)

$$L_t \mapsto L_t + \frac{1}{N} u_N^{-1} (u_N)_t p L_p \overset{\text{by (31)}}{=} L_t - \epsilon([L^q]_0)_x p L_p = L_t + \{\epsilon[L^q]_0, L\}_1.$$

Hence, the hierarchy (29) turns into (9) one with $s=k=1$.

Example 3.7: Extended dispersionless Toda, $N=m=1$.

For Lax operator $L=up+v+wp^{-1}$ *from* $L_{t_1}=\{(L)_{\geqslant 0}+\epsilon[L]_0, L\}_0$ *we find*

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_{t_1} = \begin{pmatrix} -\epsilon u v_x \\ u_x w + u w_x \\ (1+\epsilon) v_x w \end{pmatrix}.$$

In the limit $\epsilon=0$ *and* $u=1$ *we obtain the standard dispersionless Toda system. In the limit* $\epsilon=-1$ and $w=1$ *we obtain the reparametrized dispersionless Toda system. The transformation* (33) *to the standard case is given by* $v \mapsto v$, $w \mapsto u^{-1} w$. *Eliminating field* u, *for* $L = w^{-[\epsilon/(1+\epsilon)]} p + v + w p^{-1}$, *we get*

$$\begin{pmatrix} v \\ w \end{pmatrix}_{t_1} = \begin{pmatrix} \dfrac{1}{1+\epsilon} w^{-[\epsilon/1+\epsilon]} w_x \\ (1+\epsilon) v_x w \end{pmatrix}.$$

For $\epsilon=0$ *or by the transformation* $v \mapsto v$, $w \mapsto w^{1+\epsilon}$ *it becomes the standard dispersionless Toda system.*

Notice that for some dispersionless systems it is possible to construct their integrable dispersive counterparts, field and lattice soliton systems. Actually, one can do it on the level of their Lax representation through Weyl-Moyal-type deformation quantization procedure[10] of the dispersionless case. The idea relies on the deformation of the usual multiplication in A (6) to the new associative but noncommutative product,

$$f\star g = f\exp(\hbar p^s\partial_p \otimes \partial_x)g = \sum_{i\geqslant 0}\frac{\hbar^i}{i!}(p^s\partial_p)^i f\cdot\partial_x^i g, \quad f,g\in A \tag{34}$$

called $\star$-product. It depends on the formal deformation parameter $\hbar$. The Lie algebra structure is defined by the commutator $\{f,g\}_\star^s=(1/\hbar)(f\star g-g\star f)$. Then, the $\star$-product (34) in the limit $\hbar\to 0$ reduces to the standard multiplication and the commutator reduces to the Poisson bracket (7) for fixed s. To construct integrable dispersive systems one must split the algebra A with the $\star$-product into a direct sum of its Lie subalgebras and then construct the standard R-matrices. It can be done only for $s=0,1,2$. But, the case $s=2$ is equivalent to the case $s=0$. The algebra A with $\star$-product (34) for $s=0$ is isomorphic to the Lie algebra of pseudodifferentials operators (35), while for $s=1$ is isomorphic to the Lie algebra of shift operators (47) ($\mathcal{E}=\exp\hbar\partial_x$). The first case leads to the construction of field soliton systems, and the second one leads to the construction of lattice soliton systems. Obviously, integrable dispersionless systems can be constructed from integrable dispersive systems in the so-called quasiclassical (dispersionless) limit, $\partial_t\mapsto\hbar\partial_t$, $\partial_x\mapsto\hbar\partial_x$, and $\hbar\to 0$.

IV. FIELD SOLITON SYSTEMS

Let $\mathfrak{g}$ be the algebra of pseudodifferential operators[2]

$$\mathfrak{g}=\left\{L=\sum_{i\in\mathbf{Z}}u_i(x)\partial_x^i\right\}, \tag{35}$$

where the multiplication of two such operators uses the generalized Leibniz rule $\partial^m u=\sum_{s\geqslant 0}\binom{m}{s}u_{sx}\partial_x^{m-s}$. The Lie algebra structure of $\mathfrak{g}$ is given by the commutator $[L_1,L_2]=L_1L_2-L_2L_1$. We consider decomposition of $\mathfrak{g}$ in the form $\mathfrak{g}_{\geqslant k}=\{\sum_{i\geqslant k}u_i(x)\partial_x^i\}$ and $\mathfrak{g}_{<k}=\{L=\sum_{i<k}u_i(x)\partial_x^i\}$, which are Lie subalgebras for $k=0,1,2$. In this case the standard R-matrices are given by

$$R=\tfrac{1}{2}(P_{\geqslant k}-P_{<k})=P_{\geqslant k}-\tfrac{1}{2}=\tfrac{1}{2}-P_{<k}.$$

So, the Lax hierarchy has the form

$$L_{t_q}=[(L^q)_{\geqslant k},L]=-[(L^q)_{<k},L]. \tag{36}$$

Consistent Lax equations are obtained for Lax operators of the form[3]

$$k=0,\quad L=\partial_x^N+u_{N-2}\partial_x^{N-2}+\cdots+u_1\partial_x+u_0, \tag{37}$$

$$k=1,\quad L=\partial_x^N+u_{N-1}\partial_x^{N-1}+\cdots+u_0+\partial_x^{-1}u_{-1}, \tag{38}$$

$$k=2,\quad L=u_N\partial_x^N+u_{N-1}\partial_x^{N-1}+\cdots+u_0+\partial_x^{-1}u_{-1}+\partial_x^{-2}u_{-2}, \tag{39}$$

where u_i are dynamical fields. Comparing Lax operators (37)–(39) with those for the dispersionless case (12) and (13) for $s=0$ we see that not all dispersionless systems have dispersive counterparts.

The simple deformations satisfying (4) and (5) are the following ones:

$$r = P_{k-1}(\cdot)\partial_x^k \quad \text{for } k = 0,1.$$

Note, that the first case has been considered, in a little bit of a different manner, earlier in Ref. 4. Hence, the deformed R-matrices have the form

$$R' = P_{\geqslant k} - \tfrac{1}{2} + \epsilon P_{k-1}(\cdot)\partial_x^k = \tfrac{1}{2} - P_{<k} + \epsilon P_{k-1}(\cdot)\partial_x^k.$$

The case: $k=0$.

The Lax hierarchy is

$$L_{t_q} = [(L^q)_{\geqslant 0} + \epsilon[L^q]_{-1}, L] = -[(L^q)_{<0} - \epsilon[L^q]_{-1}, L] \tag{40}$$

and the appropriate Lax operators are given in the form

$$L = \partial_x^N + u_{N-1}\partial_x^{N-1} + u_{N-2}\partial_x^{N-2} + \cdots + u_1\partial_x + u_0. \tag{41}$$

From (40) one finds

$$(u_{N-1})_{t_q} = -\epsilon N([L^q]_{-1})_x,$$

$$(u_{N-2})_{t_q} = N([L^q]_{-1})_x - \epsilon(N-1)u_{N-1}([L^n]_{-1})_x - \epsilon\frac{N(N-1)}{2}([L^q]_{-1})_{2x}, \tag{42}$$

$$\cdots.$$

Hence, for $\epsilon=0$ the field u_{N-1} becomes the time-independent c_{N-1} one (let $c_{N-1}=0$), then Lax operator becomes a standard Lax operator (37). Expression (42) implies the relation between fields u_{N-1}, u_{N-2},

$$u_{N-2} = -\frac{1}{\epsilon}u_{N-1} + \frac{N-1}{2N}(u_{N-1})^2 + \frac{N-1}{2}(u_{N-1})_x.$$

We eliminate the field u_{N-2} and as a result the Lax operators take the form

$$L = \partial_x^N + u_{N-1}\partial_x^{N-1} + \left(-\frac{1}{\epsilon}u_{N-1} + \frac{N-1}{2N}(u_{N-1})^2 + \frac{N-1}{2}(u_{N-1})_x\right)\partial_x^{N-2} + \cdots + u_0. \tag{43}$$

In the dispersionless limit (43) reduces to (22). Reparametrizing (43), $u_{N-1} \mapsto -\epsilon u_{N-2}$ and then taking limit $\epsilon \to 0$ we obtain the standard Lax operator (37).

Lemma 4.1: For arbitrary ϵ *the Lax hierarchy* (40) and (43) *is equivalent to the Lax hierarchy* (36) and (37).

We are looking for relations between fields from Lax operators (43) and (37), respectively. They are given in the following form:

$$u_{N-1} \mapsto -\epsilon u_{N-2},$$

$$u_i \mapsto u_i + f_i[u_{N-2}, u_{N-3}, \ldots, u_{i+1}] \quad \text{for } N-3 \geqslant i \geqslant 0. \tag{44}$$

The square brackets in (44) mean that functions f_i, in opposite to the case (23), depend not only on u_i, but also on the derivatives $(u_i)_x, (u_i)_{xx}, \ldots$. Functions f_i are constructed in such a way that hierarchy (40) will lead to the same evolution system as hierarchy (36) for $k=0$. Argumentation that this equality indeed holds is of the same nature as in Sec. III, the paragraph $s=k=0$.

Example 4.2: KdV, $N=2$.

For the constrained Lax operator (43) *of the form* $L=\partial_x^2+u\partial_x+\frac{1}{4}u^2-(1/\epsilon)u+\frac{1}{2}u_x$ *we find reparametrized KdV,*

$$L_{t_3} = [(L^{3/2})_{\geqslant 0} + \epsilon[L^{3/2}]_{-1}, L] \Leftrightarrow u_{t_3} = \frac{1}{4}u_{3x} - \frac{3}{2\epsilon}uu_x.$$

The transformation to the standard form of KdV is given by $u \mapsto -\epsilon u$.

Example 4.3: Deformed Boussinesq, $N=3$.

Let $L = \partial_x^3 + u\partial_x^2 + \left[\frac{1}{3}u^2 - (1/\epsilon)u + u_x\right]\partial_x + w$ *then*

$$L_{t_2} = [(L^{2/3})_{\geqslant 0} + \epsilon[L^{2/3}]_{-1}, L] \Leftrightarrow$$

$$u_{t_2} = -\frac{4}{3}uu_x - u_{2x} + \frac{2}{9}\epsilon u^2 u_x + \frac{2}{3}\epsilon u_x^2 + \frac{2}{3}\epsilon uu_{2x} + \frac{2}{3}\epsilon u_{3x} - 2\epsilon w_x,$$

$$\begin{aligned} w_{t_2} = &-\frac{2}{3\epsilon}uu_x + \frac{8}{9\epsilon}u^2u_x + \frac{2}{3\epsilon}u_x^2 + \frac{4}{3\epsilon}uu_{2x} + \frac{2}{3\epsilon}u_{3x} - \frac{8}{27}u^3u_x - \frac{14}{9}uu_x^2 + \frac{4}{3}uw_x - \frac{10}{9}u^2u_{2x} - \frac{8}{3}u_xu_{2x} \\ &+ w_{2x} - \frac{14}{9}uu_{3x} - \frac{2}{3}u_{4x} + \frac{2}{81}\epsilon u^4u_x + \frac{8}{27}\epsilon u^2u_x^2 + \frac{10}{27}\epsilon u_x^3 - \frac{2}{9}\epsilon u^2w_x - \frac{2}{3}\epsilon u_xw_x + \frac{4}{27}\epsilon u^3u_{2x} \\ &+ \frac{4}{3}\epsilon uu_xu_{2x} + \frac{2}{3}\epsilon u_{2x}^2 - \frac{2}{3}\epsilon uw_{2x} + \frac{10}{27}\epsilon u^2u_{3x} + \frac{10}{9}\epsilon u_xu_{3x} - \frac{2}{3}\epsilon w_{3x} + \frac{4}{9}\epsilon uu_{4x} + \frac{2}{9}\epsilon u_{5x}. \end{aligned}$$

Eliminating the field w we obtain reparametrized Boussinesq, $u_{tt} = \left[(2/3\epsilon)u^2 - \frac{1}{3}u_{xx}\right]_{xx}$. *The transformation* (44) *to the standard form of the Boussinesq system is given by* $u \mapsto -\epsilon u$, $w \mapsto w - \frac{1}{3}\epsilon u^2 - \frac{1}{27}\epsilon^3 u^3 + \frac{1}{3}\epsilon^2 uu_x - \frac{1}{3}\epsilon u_{2x}$.

The case: $k=1$.

The Lax hierarchy becomes

$$L_{t_q} = [(L^q)_{\geqslant 1} + \epsilon[L^q]_0\partial_x, L] = -[(L^q)_{<1} - \epsilon[L^q]_0\partial_x, L] \tag{45}$$

and the appropriate Lax operators have the form

$$L = u_N\partial_x^N + u_{N-1}\partial_x^{N-1} + \cdots + u_0 + \partial_x^{-1}u_{-1}. \tag{46}$$

From (45) one finds that $(u_N)_t = \epsilon(u_N)_x[L^q]_0 - \epsilon N u_N([L^q]_0)_x$. Hence in the limit $\epsilon = 0$ the field u_N becomes a time-independent c_N one (let $c_N = 1$), then Lax operator becomes a standard Lax operator (46). There is no constraint contrary to the previous case. The Lax operators (45) with (46) lead to the construction of new integrable soliton systems, at least to the best of our knowledge. Again the zero power of L always leads to the space translation symmetry, $L_{t_0} = \epsilon L_x$.

Example 4.4: Extended Kaup–Broer, $N=1$.

Let $L = u\partial_x + v + \partial_x^{-1}w$, *then for* $L_{t_i} = [(L^i)_{\geqslant 1} + \epsilon[L^i]_0\partial_x, L]$ *we find*

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_{t_0} = \epsilon\begin{pmatrix} u_x \\ v_x \\ w_x \end{pmatrix},$$

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_{t_1} = \begin{pmatrix} \epsilon u_x v - \epsilon u v_x \\ uv_x + \epsilon v v_x \\ u_x w + uw_x + \epsilon v_x w + \epsilon v w_x \end{pmatrix},$$

$$u_{t_2} = \epsilon u_x v^2 - 2\epsilon uvv_x - 2\epsilon u^2 w_x - \epsilon u^2 v_{2x},$$

$$v_{t_2} = 2uu_x w + 2uvv_x + 2u^2 w_x + uu_x v_x + u^2 v_{2x} + \epsilon v^2 v_x + 2\epsilon uv_x w + \epsilon uv_x^2,$$

$$w_{t_2} = 2u_x vw + 2uv_x w + 2uvw_x - u_x^2 w - 3uu_x w_x - uu_{2x} w - u^2 w_{2x} + 2\epsilon u_x w^2 + 2\epsilon vv_x w + \epsilon u_x v_x w + \epsilon v^2 w_x + 4\epsilon uww_x + \epsilon uv_x w_x + \epsilon uv_{2x} w,$$

$$\cdots .$$

It is dispersive counterpart of the hierarchy from Example 3.4. In the limit $\epsilon \to 0$ *and* $u=1$ *we obtain the standard Kaup–Broer system.*

Example 4.5: Two field system, $N=0$.

For $L=v+w\partial_x^{-1}$ *we have* $[L^i]_0=v^i$ *and* $(L^i)_{\geqslant 1}=0$, *where* $i=0,1,2,\ldots$. *Then, we obtain for* $L_{t_i}=[\epsilon[L^i]_0\partial_x, L]$ *again the dispersionless hierarchy* (28).

V. LATTICE SOLITON SYSTEMS

Let $\mathfrak{g}$ be the algebra of shift operators[9]

$$\mathfrak{g} = \left\{ L = \sum_{i\in\mathbf{Z}} u_i(x)\mathcal{E}^i \right\}, \tag{47}$$

where $\mathcal{E}$ is the shift operator such that $\mathcal{E}^m u(x) = u(x+m)\mathcal{E}^m$. The Lie algebra structure of $\mathfrak{g}$ is given by the commutator $[L_1, L_2] = L_1L_2 - L_2L_1$. We consider simple decomposition of $\mathfrak{g}$ in the form $\mathfrak{g}_{\geqslant k} = \{\Sigma_{i\geqslant k} u_i\mathcal{E}^i\}$ and $\mathfrak{g}_{<k} = \{\Sigma_{i<k} u_i\mathcal{E}^i\}$, which are Lie subalgebras for $k=0,1$. In these cases the standard R-matrix is given by

$$R = \tfrac{1}{2}(P_{\geqslant k} - P_{<k}) = P_{\geqslant k} - \tfrac{1}{2} = \tfrac{1}{2} - P_{<k}.$$

The Lax hierarchy is

$$L_{t_q} = [(L^q)_{\geqslant k}, L] = -[(L^q)_{<k}, L], \quad k = 0,1. \tag{48}$$

Notice that these two cases are related by simple transformation $\mathcal{E} \mapsto \mathcal{E}^{-1}$ and $u_i(x-m) \mapsto u_{-i}(x+m)$. Then, $k=0$ goes to $k=1$ and vice versa. So, it is enough to consider only the first case. For $k=0$, the appropriate Lax operators are of the form[9]

$$L = \mathcal{E}^N + u_{N-1}(x)\mathcal{E}^{N-1} + \cdots + u_{1-m}(x)\mathcal{E}^{1-m} + u_{-m}(x)\mathcal{E}^{-m}. \tag{49}$$

The powers of L are in general fractional and can be constructed in two ways, for $L^{1/N} = a_1\mathcal{E} + a_0 + a_{-1}\mathcal{E}^{-1} + \cdots$ by requiring $(L^{1/N})^N = L$ and for $L^{1/m} = \cdots + a_1\mathcal{E} + a_0 + a_{-1}\mathcal{E}^{-1}$ by requiring $(L^{1/m})^m = L$. Then, in (48) we use $L^{i/N}$ and $L^{i/m}$ for $i=0,1,2,\ldots$. The Lax hierarchies (48) for $k=0,1$ are dispersive counterparts of the dispersionless hierarchies (9) for $s=1$, $k=1$ and $s=1$, $k=2$, respectively.

The simple deformations satisfying (4) and (5) are of the form

$$k = 0,1, \quad r = P_0.$$

But for the same reason as above it is enough to consider the case $k=0$.

The case: $k=0$.

The deformed R-matrix is given by

$$R = P_{\geqslant 0} - \tfrac{1}{2} + \epsilon P_0 = \tfrac{1}{2} - P_{<0} + \epsilon P_0.$$

Hence

$$L_{t_q} = [(L^q)_{\geqslant 0} + \epsilon[L^q]_0, L] = -[(L^q)_{<0} + \epsilon[L^q]_0, L]. \tag{50}$$

The appropriate Lax operators are of the form

$$L = u_N(x)\mathcal{E}^N + u_{N-1}(x)\mathcal{E}^{N-1} + \cdots + u_{1-m}(x)\mathcal{E}^{1-m} + u_{-m}(x)\mathcal{E}^{-m}. \tag{51}$$

From (50) it follows that

$$u_N(x)_t = \epsilon u_N(x)(1-E^N)[L^q]_0, \quad \cdots, \; u_{-m}(x)_t = (1+\epsilon)u_{-m}(x)(1-E^{-m})[L^q]_0. \tag{52}$$

As a result we find that the highest and lowest field are interrelated in the following way:

$$\left(\frac{u_N(x)}{u_N(x-m)}\right)^{1+\epsilon} = \left(\frac{u_{-m}(x)}{u_{-m}(x+N)}\right)^{\epsilon}. \tag{53}$$

For $\epsilon=0$ the field u_N becomes a time-independent c_N one (let $c_N=1$), then the Lax operator (51) becomes a standard Lax operator (49) for $k=0$. For $\epsilon=-1$ the field u_{-m} becomes time independent and the Lax operator becomes a standard Lax operator for $k=1$. It is so, because for $k=0$ and $\epsilon=-1$ the deformed R-matrix becomes the standard R-matrix for $k=1$.

Lemma 5.1: For arbitrary ϵ, the Lax hierarchy (50) and (51) *is equivalent to the Lax hierarchy* (48) and (49) *for* $k=0$.

Consider the following transformations:

$$\mathcal{E}'^N = u_N(x)\mathcal{E}^N \Leftrightarrow \mathcal{E}' = a(x)\mathcal{E},$$

$$u_i'(x) = \begin{cases} \dfrac{u_i(x)}{a(x)a(x+1)\cdot\cdots\cdot a(x+i-1)} & \text{for } N-1 \geqslant i > 0, \\ u_0(x) & \text{for } i=0, \\ u_i(x)a(x-1)a(x-2)\cdot\cdots\cdot a(x-i) & \text{for } 0 > i > -m, \end{cases} \tag{54}$$

and $t'=t$, where $a(x)$ is given by the following relation:

$$u_N(x) = a(x)a(x+1)\cdot\cdots\cdot a(x+N-1). \tag{55}$$

It transforms the Lax operators (51) into the Lax operators (49) with $u_i'(x)$ components. From (54) it follows that

$$(\mathcal{E}'^i)_t = \Pi_i(\ln a(x))_t \mathcal{E}'^i, \tag{56}$$

where

$$\Pi_i = \begin{cases} 1+E+\cdots+E^{i-1} & \text{for } i \geqslant 1, \\ 0 & \text{for } i=0, \\ -E^{-1}-E^{-2}-\cdots-E^{i} & \text{for } i \leqslant -1. \end{cases}$$

One finds also from (55), that

$$(\ln a(x))_t = (\Pi_N)^{-1}(\ln u_N(x))_t \overset{\text{by (52)}}{=} \epsilon(\Pi_N)^{-1}(1-E^N)[L^q]_0.$$

Then, using relation $(1-E^N)\Pi_i=(1-E^i)\Pi_N$ which is valid for arbitrary N, $i>0$, we have

$$L_t = L_{t'} + \sum_{i=-m}^{N} u_i'(x)(\mathcal{E}'^i)_t \overset{\text{by (56)}}{=} L_{t'} + \epsilon\sum_{i=-m}^{N} u_i'(x)(1-E^N)\Pi_i(\Pi_N)^{-1}[L^q]_0\mathcal{E}'^i = L_{t'} + \epsilon\sum_{i=-m}^{N} u_i'(x)(1-E^i)$$
$$\times[L^q]_0\mathcal{E}'^i = L_{t'} + [\epsilon[L^q]_0, L],$$

where $u_N'(x)=1$. Hence, the hierarchy (50) becomes (48) with $k=0$.

Example 5.2: Extended Toda, $k=0$.

For the Lax operator $L=u(x)\mathcal{E}+v(x)+w(x)\mathcal{E}^{-1}$ and $L_{t_1}=[(L)_{\geqslant 0}+\epsilon[L]_0, L]$ we find

$$\begin{pmatrix} u(x) \\ v(x) \\ w(x) \end{pmatrix}_{t_1} = \begin{pmatrix} -\epsilon u(x)[v(x+1)-v(x)] \\ u(x)w(x+1)-u(x-1)w(x) \\ (1+\epsilon)[v(x)-v(x-1)]w(x) \end{pmatrix}. \tag{57}$$

Again, in the limit $\epsilon \to 0$ *and* $u(x)=1$ *or by the transformation* (54), $v(x)\mapsto v(x)$, $w(x)\mapsto w(x)/u(x-1)$ *we obtain the standard Toda system. In the limit* $\epsilon=-1$ *and* $w(x)=1$ *we obtain the reparametrized Toda system. The fields* $u(x)$ *and* $v(x)$ *in* (57) *according to* (53) *are related by* $u(x-1)^{1+\epsilon}=w(x)^{-\epsilon}$.

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Solving the quantum nonlinear Schrödinger equation with δ-type impurity

V. Caudrelier[a)]
Laboratoire de Physique Théorique LAPTH,[b)] LAPP, BP 110, F-74941 Annecy-le-Vieux Cedex, France

M. Mintchev[c)]
INFN and Dipartimento di Fisica, Universitá di Pisa, Via Buonarroti 2, 56127 Pisa, Italy

E. Ragoucy[d)]
Laboratoire de Physique Théorique LAPTH,[b)] LAPP, BP 110, F-74941 Annecy-le-Vieux Cedex, France

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We establish the exact solution of the nonlinear Schrödinger equation with a delta-function impurity, representing a pointlike defect which reflects and transmits. We solve the problem both at the classical and the second quantized levels. In the quantum case the Zamolodchikov–Faddeev algebra, familiar from the case without impurities, is substituted by the recently discovered reflection-transmission (RT) algebra, which captures both particle–particle and particle–impurity interactions. The off-shell quantum solution is expressed in terms of the generators of the RT algebra and the exact scattering matrix of the theory is derived. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1842353]

I. INTRODUCTION

Impurity problems arise in different areas of quantum field theory and are essential for understanding a number of phenomena in condensed matter physics. At the experimental side, the recent interest in pointlike impurities (defects) is triggered by the great progress in building nanoscale devices.

The interaction of quantum fields with impurities represents in general a hard and yet unsolved problem, but there are relevant achievements[1–11] in the case of integable systems in $1+1$ space–time dimensions. The study[12–19] of the special case of purely reflecting impurities (boundaries) indicates factorized scattering theory[20–24] as the most efficient method for dealing with this kind of problem. The method provides on-shell information about the system and allows to derive the exact scattering matrix. The goal of the present paper is to extend this framework, exploring the possibility to recover off-shell information and to reconstruct the quantum fields, generating the above scattering matrix. We test this possibility on one of the most extensively studied integrable systems—the nonlinear Schrödinger (NLS) model.[25–32] More precisely, we are concerned below with the NLS model coupled to a delta-function impurity. The basic tool of our investigation is a specific exchange algebra,[6,7] called reflection-transmission (RT) algebra. The RT algebra is a generalization of the Zamolodchikov–Faddeev (ZF)[21,23] algebra used in the case without defects. The RT algebra is originally designed for the construction of the total scattering operator from the fundamental scattering data, namely the two-body bulk scattering matrix and the reflec-

[a)]Electronic mail: caudreli@lapp.in2p3.fr
[b)]UMR 5108 du CNRS, associée à l'Université de Savoie.
[c)]Electronic mail: mintchev@mail.df.unipi.it
[d)]Electronic mail: ragoucy@lapp.in2p3.fr

tion and transmission amplitudes of a single particle interacting with the defect. In what follows we demonstrate that in the NLS model the same algebra allows to reconstruct the corresponding off-shell quantum field as well. Being the first exactly solvable example with nontrivial bulk scattering matrix, the NLS model sheds some light on the interplay between pointlike impurities, integrability, and symmetries. In this respect our solution clarifies a debated question about the Galilean invariance of the bulk scattering matrix.

After introducing the model in Sec. II, we establish the solution, both at the classical (Sec. II B) and second-quantized (Sec. III) levels. We do this in detail, clarifying the basic properties of the solution. In Sec. IV we derive from the off-shell quantum field the total scattering matrix of the model, showing that it coincides with the one obtained directly from factorized scattering. In Sec. V we indicate some generalizations. Our conclusions and ideas about further developments are also collected there. Appendixes A and B are devoted to the proofs of some technical results.

We present below the analysis of the so-called δ-type impurity. A wider class of defects, interacting with the NLS model and preserving its integrability, can be treated in a similar way.[33] We have chosen to focus here on the particular δ-type defect in order to keep the length of the proofs reasonable, referring to Ref. 33 for a more physically oriented treatment of the general case (without detailed proofs).

II. INTRODUCING AN IMPURITY IN THE NLS MODEL

We start by recalling some well-known results about the NLS model without impurity. The reason for this is twofold: first, because this is a good guide to tackle the problem with impurity and second, because the central piece of the solution of the NLS model, the Rosales expansion,[34,35] can be adapted to the impurity case.

A. The model to solve

The field theoretic version of NLS is described by a classical complex field $\Phi(t,x)$ whose equation of motion reads

$$(i\partial_t + \partial_x^2)\Phi(t,x) = 2g|\Phi(t,x)|^2\Phi(t,x). \tag{2.1}$$

The corresponding action takes the form

$$\mathcal{A}_{\mathrm{NLS}} = \int_{\mathbb{R}} \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x (i\bar{\Phi}(t,x)\partial_t\Phi(t,x) - |\partial_x\Phi(t,x)|^2 - g|\Phi(t,x)|^4), \tag{2.2}$$

and, being in particular invariant under time translation, ensures the conservation of the energy

$$\mathcal{E}_{\mathrm{NLS}} = \int_{\mathbb{R}} \mathrm{d}x (|\partial_x\Phi(t,x)|^2 + g|\Phi(t,x\ |^4). \tag{2.3}$$

The latter is non-negative for $g \geqslant 0$.

It is well-known that this is a nonrelativistic integrable model[36] (see also Ref. 30 for a review) and an explicit solution for the field was given by Rosales in Ref. 34,

$$\Phi(t,x) = \sum_{n=0}^{\infty} (-g)^n \Phi^{(n)}(t,x), \tag{2.4}$$

where

$$\Phi^{(n)}(t,x)=\int_{\mathbb{R}^{2n+1}}\prod_{\substack{i=1\\ j=0}}^{n}\frac{\mathrm{d}p_i}{2\pi}\frac{\mathrm{d}q_j}{2\pi}\overline{\lambda}(p_1)\cdots\overline{\lambda}(p_n)\lambda(q_n)\cdots\lambda(q_0)\frac{e^{i\Sigma_{j=0}^{n}(q_jx-q_j^2t)-i\Sigma_{i=1}^{n}(p_ix-p_i^2t)}}{\prod_{i=1}^{n}(p_i-q_{i-1})(p_i-q_i)} \tag{2.5}$$

and the overbar denotes complex conjugation.

The level $n=0$ is the linear part of the field corresponding to the free Schrödinger equation. It was argued in Ref. 32 that this solution is well-defined for a large class of functions λ [containing the Schwarz space $\mathcal{S}(\mathbb{R})$] and an upper bound for g was given for the series (2.4) to converge uniformly in x. It also represents a physical field since it vanishes as $x\to\pm\infty$. In the same paper, the authors considered NLS on the half-line $\mathbb{R}^+$, which can be seen as the model on the whole line in the presence of a purely reflecting impurity sitting at the origin. Therefore, the latter represents a particular case of the model with transmitting and reflecting impurity at $x=0$ we wish to contemplate in this paper. They gave the following action:

$$\mathcal{A}_R=\int_{\mathbb{R}}\mathrm{d}t\int_{\mathbb{R}^+}\mathrm{d}x(i\overline{\Phi}(t,x)\partial_t\Phi(t,x)-|\partial_x\Phi(t,x)|^2-g|\Phi(t,x)|^4)-\eta\int_{\mathbb{R}}\mathrm{d}t|\Phi(t,0)|^2,$$

where $\eta\in\mathbb{R}$ is the parameter controlling the boundary condition

$$\lim_{x\to0^+}(\partial_x-\eta)\Phi(t,x)=0. \tag{2.6}$$

In our case, since the impurity is allowed to reflect and transmit, we must take the $\mathbb{R}^-$ part into account and we are led to work with the following action:

$$\mathcal{A}_{\mathrm{RT}}=\mathcal{A}_+ +\mathcal{A}_- +\mathcal{A}_0, \tag{2.7}$$

where

$$\mathcal{A}_\pm=\int_{\mathbb{R}}\mathrm{d}t\int_{\mathbb{R}^\pm}\mathrm{d}x(i\overline{\Phi}(t,x)\partial_t\Phi(t,x)-|\partial_x\Phi(t,x)|^2-g|\Phi(t,x)|^4), \tag{2.8}$$

$$\mathcal{A}_0=-2\eta\int_{\mathbb{R}}\mathrm{d}t|\Phi(t,0)|^2. \tag{2.9}$$

The form of $\mathcal{A}_{\mathrm{RT}}$ shows the particular status of the origin $x=0$ where the impurity sits. Again, the invariance of the action under time translations ensures the conservation of the energy,

$$\mathcal{E}_{\mathrm{RT}}=\int_{\mathbb{R}^-\oplus\mathbb{R}^+}\mathrm{d}x(|\partial_x\Phi(t,x)|^2+g|\Phi(t,x)|^4)+2\eta|\Phi(t,0)|^2. \tag{2.10}$$

It is positive for $g\geqslant0$, $\eta\geqslant0$, which is what we assume in the rest of this paper. We will see that η characterizes the transmission and reflection properties of the impurity. Using the variational principle, one deduces the equation of motion and the boundary conditions for the field: $\Phi(t,x)$ must be the solution of NLS on $\mathbb{R}^-$ and $\mathbb{R}^+$, continuous at $x=0$ and satisfy a "jump condition" at the origin. It must also vanish at infinity as a physical field.

Definition 2.1: The nonlinear Schrödinger model with a transmitting and reflecting impurity at the origin is described by the following boundary problem for the field $\Phi(t,x)$:

$$(i\partial_t+\partial_x^2)\Phi(t,x)-2g|\Phi(t,x)|^2\Phi(t,x)=0,\quad x\neq0, \tag{2.11}$$

$$\lim_{x\to0^+}\{\Phi(t,x)-\Phi(t,-x)\}=0, \tag{2.12}$$

$$\lim_{x\to 0^+}\{(\partial_x\Phi)(t,x)-(\partial_x\Phi)(t,-x)\}-2\eta\Phi(t,0)=0, \tag{2.13}$$

$$\lim_{x\to\pm\infty}\Phi(t,x)=0. \tag{2.14}$$

B. Explicit solution

As announced, the Rosales solution[34] can be adapted suitably to solve the problem of definition 2.1. Since (2.4) is a solution of NLS on $\mathbb{R}$, it is easy to devise a solution for (2.11). Starting from two copies of (2.4) and (2.5), one based on a function λ_+ and the other on a function λ_-, denoted $\Phi_+(t,x)$ and $\Phi_-(t,x)$, respectively, we define

$$\Phi(t,x)=\begin{cases}\Phi_+(t,x), & x>0,\\ \Phi_-(t,x), & x<0,\\ \frac{1}{2}(\Phi_+(t,0)+\Phi_-(t,0)), & x=0.\end{cases} \tag{2.15}$$

It is clearly solution of (2.11) for $x\neq 0$ and from the vanishing of $\Phi_\pm(t,x)$ as $x\to\pm\infty$, (2.14) is also satisfied. However, there is no reason why, in general, $\Phi(t,x)$ so defined should satisfy the boundary conditions (2.12) and (2.13). In order to satisfy these conditions, we parametrize λ_+, λ_- as follows:

$$\begin{pmatrix}\lambda_+(p)\\ \lambda_-(p)\end{pmatrix}=\begin{pmatrix}1 & T(p)\\ T(-p) & 1\end{pmatrix}\begin{pmatrix}\mu_+(p)\\ \mu_-(p)\end{pmatrix}+\begin{pmatrix}R(p) & 0\\ 0 & R(-p)\end{pmatrix}\begin{pmatrix}\mu_+(-p)\\ \mu_-(-p)\end{pmatrix}, \tag{2.16}$$

where

$$T(p)=\frac{p}{p+i\eta},\quad R(p)=\frac{-i\eta}{p+i\eta},\quad p\in\mathbb{R}, \tag{2.17}$$

and $\mu_\pm(p)$ are arbitrary Schwarz test functions. Then, the functions $\lambda_\pm(p)$ satisfy

$$\lambda_\pm(p)=T(\pm p)\lambda_\mp(p)+R(\pm p)\lambda_\pm(-p),\quad \forall\, p\in\mathbb{R} \tag{2.18}$$

which follows from the identities

$$R(p)R(-p)+T(p)T(-p)=1\quad\text{and}\quad T(p)R(-p)+R(p)T(-p)=0,\quad \forall\, p\in\mathbb{R}. \tag{2.19}$$

These relations plus a particular choice for the form of $\mu_\pm$ will be essential in the proof of the theorem 2.2 below.

Anticipating the quantum case, if we interpret λ_+ (respectively, λ_-) as a wave packet, (2.18) shows that each wave packet in $\mathbb{R}^+$ (respectively, $\mathbb{R}^-$) is equivalent to the superimposition of a transmitting part coming from $\mathbb{R}^-$ (respectively, $\mathbb{R}^+$) and a reflected part in $\mathbb{R}_+$ (respectively, $\mathbb{R}_-$). This physical interpretation will show up in the next section when we construct a Fock representation of the creation and annihilation operators.

We are now in position to state the main result of this section whose lengthy proof we defer until Appendix A.

Theorem 2.2: Let μ_+, μ_- *be given by*

$$\mu_\pm(k)=\pm\frac{\mu_0(\pm k)+(k\mp i\eta)\mu_1(k)}{k\mp i\eta+1}, \tag{2.20}$$

where μ_0, μ_1 *are arbitrary Schwartz functions,* μ_1 *being even and let* $\Phi_+(t,x)$, $\Phi_-(t,x)$ *be given by the Rosales expansion (2.4) and (2.5) with* λ *replaced by* λ_+ *and* λ_-, *respectively. Then,* $\Phi(t,x)$ *as defined in (2.15) satisfies the boundary conditions (2.12) and (2.13), i.e.,*

$$\lim_{x\to 0^+}\{\Phi(t,x)-\Phi(t,-x)\}=0,$$

$$\lim_{x\to 0^+}\{(\partial_x\Phi)(t,x)-(\partial_x\Phi)(t,-x)\}-2\eta\Phi(t,0)=0.$$

With this result, we can say that $\Phi(t,x)$ rewritten as

$$\Phi(t,x)=\theta(x)\Phi_+(t,x)+\theta(-x)\Phi_-(t,x), \tag{2.21}$$

where $\theta(x)$ is the Heaviside function defined here to be $\frac{1}{2}$ at $x=0$, is the classical solution of the nonlinear Schrödinger model with impurity as given in definition 2.1.

We want to emphasize that these boundary conditions decouple for the nonlinear part of the field (as shown in Appendix A) and this is due to the reflection-transmission property (2.18) satisfied by λ_+ and λ_-. This already gives a good hint that the construction of a local field from the quantum counterparts of λ_+, λ_- is achievable, as we now explain.

III. QUANTIZATION OF THE SYSTEM

In this section, we move on to the construction and resolution of the quantized version of NLS with impurity. As we mentioned earlier, the crucial ingredient is the RT algebra which encodes the properties of the impurity.

A. Reflection-transmission algebra

Here we rely on the constructions developed in Ref. 7 and recast them in the particular context of the scalar nonlinear Schrödinger model (no internal degrees of freedom, special form of the exchange matrix and of the generators, see also Ref. 11).

We consider the associative algebra with identity element **1** and two sets of generators, $\{a_\alpha(p),a_\alpha^\dagger(p);p\in\mathbb{R},\alpha=\pm\}$ and $\{r(p),t(p);p\in\mathbb{R}\}$, called the bulk and defect (reflection and transmission) generators. The label $\alpha=\pm$ refers to the half-line $\mathbb{R}^\pm$ with respect to the impurity (in practice it will indicate where the particle is created or annihilated). Introducing the measurable function $S:\mathbb{R}\times\mathbb{R}\to\mathbb{C}$ defined by

$$S(p)=\frac{p-ig}{p+ig} \tag{3.1}$$

the $\mathcal{S}$-matrix is defined in our context by

$$\mathcal{S}=\sum_{\alpha_1,\alpha_2=\pm}\mathcal{S}_{\alpha_1\alpha_2}(p_1,p_2)E_{\alpha_1\alpha_1}\otimes E_{\alpha_2\alpha_2}, \tag{3.2}$$

where $\mathcal{S}_{\alpha_1\alpha_2}(p_1,p_2)=S(\alpha_1p_1-\alpha_2p_2)$ and $(E_{\alpha\beta})_{\sigma\gamma}=\delta_{\alpha\sigma}\delta_{\beta\gamma}$. It is easy to check that $\mathcal{S}$ satisfies the unitarity condition and the quantum Yang–Baxter equation

$$\mathcal{S}_{12}(p_1,p_2)\mathcal{S}_{21}(p_2,p_1)=\mathbb{1}\otimes\mathbb{1}, \tag{3.3}$$

$$\mathcal{S}_{12}(p_1,p_2)\mathcal{S}_{13}(p_1,p_3)\mathcal{S}_{23}(p_2,p_3)=\mathcal{S}_{23}(p_2,p_3)\mathcal{S}_{13}(p_1,p_3)\mathcal{S}_{12}(p_1,p_2). \tag{3.4}$$

Our defect generators $r(p)$, $t(p)$ are related to $r_\alpha^\beta(p)$, $t_\alpha^\beta(p)$ defined in Ref. 7 by

$$r_\alpha^\beta(p)=\delta_\alpha^\beta r(\alpha p)\quad\text{and } t_\alpha^\beta(p)=\epsilon_\alpha^\beta t(\alpha p)\text{ with }\epsilon=\begin{pmatrix}0&1\\1&0\end{pmatrix}. \tag{3.5}$$

All this setup gives rise to a particular RT algebra whose defining relations then read as follows.

(i) Bulk exchange relations,

$$a_{\alpha_1}(p_1)a_{\alpha_2}(p_2) - S(\alpha_2 p_2 - \alpha_1 p_1)a_{\alpha_2}(p_2)a_{\alpha_1}(p_1) = 0, \tag{3.6}$$

$$a^\dagger_{\alpha_1}(p_1)a^\dagger_{\alpha_2}(p_2) - S(\alpha_2 p_2 - \alpha_1 p_1)a^\dagger_{\alpha_2}(p_2)a^\dagger_{\alpha_1}(p_1) = 0, \tag{3.7}$$

$$\begin{aligned} a_{\alpha_1}(p_1)a^\dagger_{\alpha_2}(p_2) - S(\alpha_1 p_1 - \alpha_2 p_2)a^\dagger_{\alpha_2}(p_2)a_{\alpha_1}(p_1) &= 2\pi\delta(p_1 - p_2)[\delta^{\alpha_2}_{\alpha_1}\mathbf{1} + \epsilon^{\alpha_2}_{\alpha_1}t(\alpha_1 p_1)] \\ &+ 2\pi\delta(p_1 + p_2)\delta^{\alpha_2}_{\alpha_1}r(\alpha_1 p_1). \end{aligned} \tag{3.8}$$

(ii) Defect exchange relations,

$$[r(p_1), r(p_2)] = 0, \tag{3.9}$$

$$[t(p_1), t(p_2)] = 0, \tag{3.10}$$

$$[t(p_1), r(p_2)] = 0. \tag{3.11}$$

(iii) Mixed exchange relations,

$$a_{\alpha_1}(p_1)r(p_2) = S(p_2 - p_1)S(p_2 + p_1)r(p_2)a_{\alpha_1}(p_1), \tag{3.12}$$

$$r(p_1)a^\dagger_{\alpha_2}(p_2) = S(p_1 - p_2)S(p_1 + p_2)a^\dagger_{\alpha_2}(p_2)r(p_1), \tag{3.13}$$

$$a_{\alpha_1}(p_1)t(p_2) = S(p_2 - p_1)S(p_2 + p_1)t(p_2)a_{\alpha_1}(p_1), \tag{3.14}$$

$$t(p_1)a^\dagger_{\alpha_2}(p_2) = S(p_1 - p_2)S(p_1 + p_2)a^\dagger_{\alpha_2}(p_2)t(p_1). \tag{3.15}$$

(iv) Finally, the defect generators are required to satisfy unitarity conditions,

$$t(p)t(-p) + r(p)r(-p) = \mathbf{1}, \tag{3.16}$$

$$t(p)r(-p) + r(p)t(-p) = 0, \tag{3.17}$$

which amount to implement the physical energy conservation when reflection and transmission occur.

Since we aim at second quantize a physical system, we now turn to the Fock representation of this algebraic setup as it is presented in Ref. 7. What we need is to represent the generators $\{a_\alpha(p), a^\dagger_\alpha(p), r(p), t(p), p \in \mathbb{R}\}$ as operator-valued distributions acting on a common invariant subspace of a Hilbert space, $\mathcal{F}$, to be defined. We should also identify a normalizable vacuum state Ω annihilated by a_α and cyclic with respect to $a^\dagger_\alpha$. Applying the general construction of Ref. 7, we know that each such Fock representation is characterized by two numerical matrices $\mathcal{T}(p)$ and $\mathcal{R}(p)$. Here we take

$$\mathcal{T}(p) = \begin{pmatrix} 0 & T(p) \\ T(-p) & 0 \end{pmatrix}, \quad \mathcal{R}(p) = \begin{pmatrix} R(p) & 0 \\ 0 & R(-p) \end{pmatrix} \tag{3.18}$$

with T, R given in (2.17). Now consider

$$\mathcal{L} = \bigoplus_{\alpha=\pm} L^2(\mathbb{R}) \tag{3.19}$$

endowed with the usual scalar product

$$\langle \varphi, \psi \rangle = \int_{\mathbb{R}} \mathrm{d}p \sum_{\alpha=\pm} \overline{\varphi}_\alpha(p) \psi_\alpha(p), \tag{3.20}$$

which makes it a Hilbert space for the associated norm denoted $\|\cdot\|$. Then, the n-particle subspace $\mathcal{H}^{(n)}$ is the subspace of the n-fold tensor product $\mathcal{L}^{\otimes n}$ defined as follows. If $\varphi^{(n)} \in \mathcal{L}^{\otimes n}$, we identify it with the column whose entries are $\varphi^{(n)}_{\alpha_1,\ldots,\alpha_n}$. Then explicitly, $\mathcal{H}^{(0)}=\mathcal{C}$ and for $n \geqslant 1$, $\varphi^{(n)} \in \mathcal{H}^{(n)}$ if and only if

$$\varphi^{(n)} \in \mathcal{L}^{\otimes n},$$

$$\varphi^{(n)}_{\alpha_1 \cdots \alpha_n}(p_1, \ldots, p_n) = T(\alpha_n p_n) \varphi^{(n)}_{\alpha_1 \cdots \alpha_{n-1}, -\alpha_n}(p_1, \ldots, p_{n-1}, p_n) + R(\alpha_n p_n) \varphi^{(n)}_{\alpha_1 \cdots \alpha_{n-1} \alpha_n}(p_1, \ldots, p_{n-1}, -p_n), \tag{3.21}$$

$$\begin{aligned} n > 1,\ \varphi^{(n)}_{\alpha_1 \cdots \alpha_i \alpha_{i+1} \cdots \alpha_n}(p_1, \ldots, p_i, p_{i+1}, \ldots, p_n) &= S(\alpha_i p_i - \alpha_{i+1} p_{i+1}) \\ &\times \varphi^{(n)}_{\alpha_1 \cdots \alpha_{i+1} \alpha_i \cdots \alpha_n}(p_1, \ldots, p_{i+1}, p_i, \ldots, p_n), \quad 1 < i < n-1. \end{aligned} \tag{3.22}$$

The Fock space is $\mathcal{F}=\oplus_{n=0}^{\infty} \mathcal{H}^{(n)}$ and the common invariant subspace is the finite particle space $\mathcal{D}$ spanned by the linear combination of sequences $\varphi=(\varphi^{(0)}, \varphi^{(1)}, \ldots, \varphi^{(n)}, \ldots)$ with $\varphi^{(n)} \in \mathcal{H}^{(n)}$ and $\varphi^{(n)}=0$ for n large enough. $\mathcal{D}$ is dense in $\mathcal{F}$. We extend the scalar product, again denoted by $\langle \cdot, \cdot \rangle$, to $\mathcal{F}$,

$$\begin{aligned} \forall \varphi, \psi \in \mathcal{F}, \quad \langle \varphi, \psi \rangle &= \sum_{n=0}^{\infty} \langle \varphi^{(n)}, \psi^{(n)} \rangle \\ &= \sum_{n=0}^{\infty} \int_{\mathbb{R}^n} \mathrm{d}p_1 \cdots \mathrm{d}p_n \sum_{\alpha_1, \ldots, \alpha_n = \pm} \overline{\varphi}_{\alpha_1 \cdots \alpha_n}(p_1, \ldots, p_n) \psi_{\alpha_1 \cdots \alpha_n}(p_1, \ldots, p_n). \end{aligned}$$

The unit norm vacuum state is $\Omega=(1,0,\ldots,0,\ldots)$ and belongs to $\mathcal{D}$.

Now, we can define the action of the smeared bulk operators $\{a(\mathfrak{f}), a^\dagger(\mathfrak{f}); \mathfrak{f} \in \oplus_{\alpha=\pm} C_0^\infty(\mathbb{R})\}$ on $\mathcal{D}$ as follows:

$$a(\mathfrak{f})\Omega = 0, \tag{3.23}$$

and for any $\varphi^{(n)} \in \mathcal{H}^{(n)}$,

$$[a(\mathfrak{f})\varphi]^{(n-1)}_{\alpha_1 \cdots \alpha_{n-1}}(p_1, \ldots, p_{n-1}) = \sqrt{n} \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} \sum_{\alpha=\pm} \overline{\mathfrak{f}}_\alpha(p) \varphi^{(n)}_{\alpha \alpha_1 \cdots \alpha_{n-1}}(p, p_1, \ldots, p_{n-1}), \tag{3.24}$$

$$[a^\dagger(\mathfrak{f})\varphi]^{(n+1)}_{\alpha_1 \cdots \alpha_{n+1}}(p_1, \ldots, p_{n+1}) = \sqrt{n+1} [P^{(n+1)} \mathfrak{f} \otimes \varphi^{(n)}]_{\alpha_1 \cdots \alpha_{n+1}}(p_1, \ldots, p_{n+1}), \tag{3.25}$$

where $P^{(n)}$ is the orthogonal projector in $\mathcal{L}^{\otimes n}$ defined in Ref. 7. For completeness, the explicit form of (3.25) is given in Appendix B. These operators are bounded on each $\mathcal{H}^{(n)}$,

$$\forall \varphi \in \mathcal{H}^{(n)}, \quad \|a(\mathfrak{f})\varphi\| \leqslant \sqrt{n} \|\mathfrak{f}\| \, \|\varphi\|, \quad \|a^\dagger(\mathfrak{f})\varphi\| \leqslant \sqrt{n+1} \|\mathfrak{f}\| \, \|\varphi\|. \tag{3.26}$$

In particular, they are continuous in the smearing function $\mathfrak{f}$. Finally, they satisfy

$$\forall \varphi, \psi \in \mathcal{D}, \quad \langle \varphi, a(\mathfrak{f})\psi \rangle = \langle a^\dagger(\mathfrak{f})\varphi, \psi \rangle. \tag{3.27}$$

The defect generators are represented as multiplicative operators on $\mathcal{D}$, preserving the bulk particle number,

$$[r(p)\varphi]^{(n)}_{\alpha_1\cdots\alpha_n}(p_1,\ldots,p_n) = S(p-\alpha_1 p_1)\cdots S(p-\alpha_n p_n)R(p)S(\alpha_n p_n+p)\cdots S(\alpha_1 p_1+p) \times \varphi^{(n)}_{\alpha_1\cdots\alpha_n}(p_1,\ldots,p_n), \tag{3.28}$$

$$[t(p)\varphi]^{(n)}_{\alpha_1\cdots\alpha_n}(p_1,\ldots,p_n) = S(p-\alpha_1 p_1)\cdots S(p-\alpha_n p_n)T(p)S(\alpha_n p_n+p)\cdots S(\alpha_1 p_1+p) \times \varphi^{(n)}_{\alpha_1\cdots\alpha_n}(p_1,\ldots,p_n). \tag{3.29}$$

It follows then that r and t have nonvanishing vacuum expectation values

$$\langle\Omega, r(p)\Omega\rangle = R(p), \quad \langle\Omega, t(p)\Omega\rangle = T(p). \tag{3.30}$$

Introducing finally the operator-valued distributions $a_\alpha(p)$, $a^\dagger_\alpha(p)$ as

$$a(\mathfrak{f}) = \int_{\mathbb{R}} \frac{dp}{2\pi} \sum_{\alpha=\pm} \overline{\mathfrak{f}}_\alpha(p) a_\alpha(p), \quad a^\dagger(\mathfrak{f}) = \int_{\mathbb{R}} \frac{dp}{2\pi} \sum_{\alpha=\pm} a^\dagger_\alpha(p)\mathfrak{f}_\alpha(p) \tag{3.31}$$

one can check that the defining relations of the RT algebra are satisfied on $\mathcal{D}$. The operators $a, a^\dagger$ will be referred to as annihilation and creation operators, respectively. Implementing the automorphism ϱ defined in Ref. 7 for which we know that it is realized by the identity operator for any Fock representation, we get the quantum analog of the reflection-transmission property (2.18)

$$a_\alpha(p) = \epsilon^\beta_\alpha t(\alpha p) a_\beta(p) + \delta^\beta_\alpha r(\alpha p) a_\beta(-p), \tag{3.32}$$

$$a^\dagger_\alpha(p) = \epsilon^\alpha_\beta a^\dagger_\beta(p) t(\beta p) + \delta^\alpha_\beta a^\dagger_\beta(-p) r(-\beta p). \tag{3.33}$$

B. The question of operator domains

From the above it appears that the natural domain to start with is $\mathcal{D}$. Actually, it is much too big for practical calculations and we would like to work on a dense subspace of $\mathcal{D}$ which would play the role of the standard formal "state space," a basis of which is usually denoted by $|k_1,\ldots,k_n\rangle$, $k_1>\cdots>k_n$. As a first step, we define

$$\mathcal{D}_0^0 = \mathbb{C},$$

$$\mathcal{D}_0^n = \{a^\dagger_{\alpha_1}(\mathfrak{f}_1)\cdots a^\dagger_{\alpha_n}(\mathfrak{f}_n)\Omega; \mathfrak{f}_i \in C_0^\infty(\mathbb{R}), \quad \alpha_i = \pm, i=1,\ldots,n\}, \quad n \geqslant 1. \tag{3.34}$$

One can check that $\mathcal{D}_0^n$ is dense in $\mathcal{H}^{(n)}$, i.e., Ω is cyclic with respect to $a^\dagger_\alpha$. The corresponding domain $\mathcal{D}_0$, dense in $\mathcal{D}$, is the linear space of sequences $\varphi=(\varphi^{(0)},\varphi^{(1)},\ldots,\varphi^{(n)},\ldots)$ with $\varphi^{(n)} \in \mathcal{D}_0^n$ and $\varphi^{(n)}=0$ for n large enough. $\mathcal{D}_0$ is stable under the action of $a_\alpha(\mathfrak{f})$ and $a^\dagger_\alpha(\mathfrak{f})$. Finally, since T, R, and S are bounded, C^∞-functions, $\mathcal{D}_0^n \subset C_0^\infty(\mathbb{R}^n)$. Now in order to formulate the desired properties of the quantum field in the next paragraph, we introduce a partial ordering relation on $C_0^\infty(\mathbb{R})$ by

$$f \succ g \Leftrightarrow \forall\, x \in \mathrm{supp}(f), \quad \forall\, y \in \mathrm{supp}(g), \quad |x| > |y|, \tag{3.35}$$

which extends naturally to $C_0^\infty(\mathbb{R}^\alpha)$, $\alpha=\pm$. Let us introduce

$$\tilde{a}^\dagger_\alpha(t,x) = \int_{\mathbb{R}} \frac{dp}{2\pi} a^\dagger_\alpha(p) e^{-ipx+ip^2 t}, \quad (t,x) \in \mathbb{R}^2,$$

$$\tilde{a}^{\dagger}_{\alpha}(t,f) = \int_{\mathbb{R}} \mathrm{d}x\, \tilde{a}^{\dagger}_{\alpha}(t,x) f(x), \quad f \in C_0^{\infty}(\mathbb{R}). \tag{3.36}$$

Now, fix $t \in \mathbb{R}$ and $\alpha_1, \ldots, \alpha_n$ and define (vect standing for "linear span of") $\tilde{\mathcal{D}}_0^0 = \mathbb{C}$ and for $n \geqslant 1$,

$$\tilde{\mathcal{D}}^n_{0,\alpha_1\cdots\alpha_n} = \mathrm{vect}\{\tilde{a}^{\dagger}_{\alpha_1}(t,f_{1,\alpha_1})\cdots\tilde{a}^{\dagger}_{\alpha_n}(t,f_{n,\alpha_n})\Omega;\ f_{1,\alpha_1} \succ \cdots \succ f_{n,\alpha_n}, f_{i,\alpha_i} \in C_0^{\infty}(\mathbb{R}^{\alpha_i}),$$
$$0 \notin \mathrm{supp}(f_{i,\alpha_i}),\ i = 1, \ldots, n\} \tag{3.37}$$

then the following theorem holds.

Theorem 3.1: $\forall t \in \mathbb{R}$, $\forall \alpha_1, \ldots, \alpha_n = \pm$, $\tilde{\mathcal{D}}^n_{0,\alpha_1\cdots\alpha_n}$ *is dense in* $\mathcal{H}^{(n)}$.

Proof: We only need to consider $n \geqslant 1$. The proof relies on two known results of standard analysis. First, the Fourier transform of a C^{∞}-function with compact support is real analytic (i.e., a Gevrey class 1 function). Second, a real analytic function vanishing on a given open subset U of an open connected set O, vanishes on the whole of O (see, e.g., Ref. 37).

Here, it suffices to show that $\tilde{\mathcal{D}}^n_{0,\alpha_1\cdots\alpha_n}$ is dense in $\mathcal{D}_0^n$ for any $t \in \mathbb{R}$ so let us consider the matrix element

$$\tilde{A}_{t,\varphi,\alpha_1\cdots\alpha_n}(x_1, \ldots, x_n) = \langle \varphi^{(n)}, \tilde{a}^{\dagger}_{\alpha_1}(t,x_1)\cdots\tilde{a}^{\dagger}_{\alpha_n}(t,x_n)\Omega\rangle, \tag{3.38}$$

where $\varphi^{(n)} \in \mathcal{D}_0^n$ is arbitrary. To prove the statement, we now have to show that

$$\tilde{A}_{t,\varphi,\alpha_1\cdots\alpha_n}(x_1, \ldots, x_n) = 0, \quad \forall\, |x_1| > \cdots > |x_n| > 0, \quad x_i \in \mathbb{R}^{\alpha_i}, \quad i = 1, \ldots, n \tag{3.39}$$

implies $\varphi^{(n)} = 0$. From (3.36), we get

$$\tilde{A}_{t,\varphi,\alpha_1\cdots\alpha_n}(x_1, \ldots, x_n) = \int_{\mathbb{R}^n} \prod_{j=1}^{n} \frac{\mathrm{d}p_j}{2\pi} e^{-ip_jx_j + itp_j^2} \langle \varphi^{(n)}, a^{\dagger}_{\alpha_1}(p_1)\cdots a^{\dagger}_{\alpha_n}(p_n)\Omega\rangle, \tag{3.40}$$

which shows that $\tilde{A}_{t,\varphi,\alpha_1\cdots\alpha_n}$ is the Fourier transform of a C^{∞}-function with compact support and is therefore real analytic. Condition (3.39) amounts to saying that $\tilde{A}_{t,\varphi,\alpha_1\cdots\alpha_n}$ vanishes on the set

$$U_{\alpha_1\cdots\alpha_n} = \{x \in \mathbb{R}^n\, s.t.\, |x_1| > \cdots > |x_n| > 0,\ x_i \in \mathbb{R}^{\alpha_i},\ i = 1, \ldots, n\}. \tag{3.41}$$

$U_{\alpha_1\cdots\alpha_n}$ being an open subset of (the open and connected space) $\mathbb{R}^n$, we conclude that $\tilde{A}_{t,\varphi,\alpha_1\cdots\alpha_n}$ vanishes on $\mathbb{R}^n$. This gives in turn that

$$\langle \varphi^{(n)}, a^{\dagger}_{\alpha_1}(p_1)\cdots a^{\dagger}_{\alpha_n}(p_n)\Omega\rangle = 0, \quad \forall\, p_j \in \mathbb{R}, \quad j = 1, \ldots, n, \tag{3.42}$$

or, equivalently, from the cyclicity of Ω with respect to $a^{\dagger}$

$$\varphi^{(n)}_{\alpha_1\cdots\alpha_n}(p_1, \ldots, p_n) = 0, \quad \forall\, p_j \in \mathbb{R}, \quad j = 1, \ldots, n. \tag{3.43}$$

Now using the properties (3.21) and (3.22) satisfied by $\varphi^{(n)}$, we get

$$\varphi^{(n)}_{\alpha_1\cdots\alpha_n}(p_1, \ldots, p_n) = 0, \quad \forall\, p_j \in \mathbb{R}, \quad \forall\, \alpha_j = \pm, \quad j = 1, \ldots, n \tag{3.44}$$

that is $\varphi^{(n)} = 0$. ■

This theorem will prove to be fundamental in the sequel to derive the required properties of the quantum field operator. Indeed, it will be enough to perform all calculations only on states in

$$\tilde{\mathcal{D}}_0^{n,\alpha} = \tilde{\mathcal{D}}^n_{0,\underbrace{\alpha\cdots\alpha}_{n}} \quad \text{with } \alpha = \pm \tag{3.45}$$

and conclude for the whole domain $\mathcal{D}$ by a continuity argument.

Lemma 3.2: Let $f_{1,\alpha_1} \succ \cdots \succ f_{n,\alpha_n}$ *and* $h_{1,\beta_1} \succ \cdots \succ h_{n,\beta_n}$, *then*

$$\langle \tilde{a}^\dagger_{\alpha_1}(t,f_{1,\alpha_1}) \cdots \tilde{a}^\dagger_{\alpha_n}(t,f_{n,\alpha_n})\Omega, \tilde{a}^\dagger_{\beta_1}(t,h_{1,\beta_1}) \cdots \tilde{a}^\dagger_{\beta_n}(t,h_{n,\beta_n})\Omega\rangle = \prod_{j=1}^{n} \delta_{\alpha_j\beta_j}\langle f_{j,\alpha_j}, h_{j,\beta_j}\rangle. \tag{3.46}$$

In particular, for $\varphi \in \tilde{D}^n_{0,\alpha_1\cdots\alpha_n}$ *represented as*

$$\varphi = \sum_{\beta\in B} \tilde{a}^\dagger_{\alpha_1}(t,f^\beta_{1,\alpha_1}) \cdots \tilde{a}^\dagger_{\alpha_n}(t,f^\beta_{n,\alpha_n}), \quad f^\beta_{1,\alpha_1} \succ \cdots \succ f^\beta_{n,\alpha_n}, \quad \forall\, \beta \in B, \tag{3.47}$$

where B *is a finite set, one has* $\|\varphi\| = \|\Sigma_{\beta\in B} f^\beta_{1,\alpha_1} \otimes \cdots \otimes f^\beta_{n,\alpha_n}\|$.

Proof: To get (3.46), one uses an induction on n and combines (3.36), (3.27), (3.8), and (3.23) together with the support conditions on the smearing functions. Using a contour integral argument, these support conditions imply that all the contributions arising from the RT algebra vanish except for the usual δ- term producing the right-hand side. Equation (3.47) is a mere consequence of (3.46). ■

Remark: It is important to realize that the n particle space $\mathcal{H}^{(n)}$ is the central piece in this construction and that, on this space, any operation we have considered (scalar product, creation operator, Fourier transform) is continuous in the smearing functions. Since $C_0^\infty(\mathbb{R})$ is dense in $\mathcal{S}(\mathbb{R})$, the Schwarz space, we can extend the above (especially the definition of $\mathcal{D}_0^n$) to smearing functions in $\mathcal{S}(\mathbb{R})$.

C. Quantum field

We start by defining $\Phi(t,f)$ as

$$\Phi(t,f) = \int_{\mathbb{R}} dx \sum_{\alpha=\pm} \overline{f_\alpha}(x)\Phi_\alpha(t,x), \quad f \in \mathcal{C} \text{ where } \mathcal{C} = \bigoplus_{\alpha=\pm} C_0^\infty(\mathbb{R}^\alpha). \tag{3.48}$$

f is viewed as a column vector $f = \binom{f_+}{f_-}$ with $f_\alpha \in C_0^\infty(\mathbb{R}^\alpha)$ and $0 \notin \mathrm{supp}(f_\alpha)$. Following the standard argument of Ref. 29, we replace $\lambda_\alpha(p), \overline{\lambda_\alpha}(p)$ in the Rosales expansion of the classical field (2.4) and (2.5) by the operators $a_\alpha(p), a^\dagger_\alpha(p)$ in order to define

$$\Phi_\alpha(t,x) = \sum_{n=0}^{\infty} (-g)^n \Phi^{(n)}_\alpha(t,x), \quad g > 0 \tag{3.49}$$

and

$$\Phi^{(n)}_\alpha(t,x) = \int_{\mathbb{R}^{2n+1}} \prod_{\substack{i=1\\ j=0}}^{n} \frac{dp_i}{2\pi}\frac{dq_j}{2\pi} a^\dagger_\alpha(p_1)\cdots a^\dagger_\alpha(p_n)a_\alpha(q_n)\cdots a_\alpha(q_0) \frac{e^{i\Sigma_{j=0}^n (q_j x - q_j^2 t) - i\Sigma_{i=1}^n (p_i x - p_i^2 t)}}{\prod_{i=1}^{n} (p_i - q_{i-1} - i\alpha\varepsilon)(p_i - q_i - i\alpha\varepsilon)}, \tag{3.50}$$

where we used an $i\varepsilon$ prescription depending on $\alpha = \pm$.

We now have several requirements to meet for our quantum theory to be well defined. We must give a precise meaning to $\Phi_\alpha(t,x)$, show that the canonical commutation relations as well as the boundary conditions (2.12) and (2.13) hold in a sense we shall make precise and that $\Phi_\alpha(t,x)$ is indeed the quantum solution we look for.

We start by associating $\Phi_\alpha(t,x)$ with the quadratic form defined on $\mathcal{D}\times\mathcal{D}$ by

$$(\varphi,\psi)\mapsto\langle\varphi,\Phi_\alpha(t,x)\psi\rangle, \tag{3.51}$$

$\mathcal{D}$ containing only finite particle vectors, it is enough to investigate $\langle\varphi,\Phi_\alpha^{(n)}(t,x)\psi\rangle$ for arbitrary n.

Proposition 3.3: $\forall\ n\geqslant 0$, $\forall\ \varphi,\psi\in\mathcal{D}$, $(t,x)\mapsto\langle\varphi,\Phi_\alpha^{(n)}(t,x)\psi\rangle$ *is a* C^∞ *function.*

Proof: The proof is the same as in Ref. 32. ■

We define the conjugate $\Phi_\alpha^\dagger(t,x)$ again as a quadratic form on $\mathcal{D}\times\mathcal{D}$ by

$$\langle\varphi,\Phi_\alpha^\dagger(t,x)\psi\rangle=\langle\Phi_\alpha(t,x)\varphi,\psi\rangle. \tag{3.52}$$

It has the same smoothness properties and from (3.27), we get

$$\Phi_\alpha^{\dagger(n)}(t,x)=\int_{\mathbb{R}^{2n+1}}\prod_{\substack{i=1\\ j=0}}^{n}\frac{\mathrm{d}p_i}{2\pi}\frac{\mathrm{d}q_j}{2\pi}a_\alpha^\dagger(q_0)\cdots a_\alpha^\dagger(q_n)a_\alpha(p_n)\cdots a_\alpha(p_1)$$
$$\times\frac{e^{-i\Sigma_{j=0}^n(q_jx-q_j^2t)+i\Sigma_{i=1}^n(p_ix-p_i^2t)}}{\prod_{i=1}^n(p_i-q_{i-1}+i\alpha\varepsilon)(p_i-q_i+i\alpha\varepsilon)}. \tag{3.53}$$

Defining the smeared version

$$\Phi^\dagger(t,f)=\int_{\mathbb{R}}\mathrm{d}x\sum_{\alpha=\pm}\Phi_\alpha^\dagger(t,x)f_\alpha(x),\quad f\in\mathcal{C} \tag{3.54}$$

we conclude that $\Phi(t,f)$ and $\Phi^\dagger(t,f)$ are understood as quadratic forms on the domain $\mathcal{D}$ and are related by

$$\langle\varphi,\Phi_\alpha^\dagger(t,f)\psi\rangle=\langle\Phi_\alpha(t,f)\varphi,\psi\rangle. \tag{3.55}$$

To get true quantum fields, we need to show that these quadratic forms give rise to operators on $\mathcal{D}$. This requires the following two lemmas.

Lemma 3.4: $\forall\ \varphi,\psi\in\mathcal{D}$,

(i) *For* $h_{1,\alpha}\succ\cdots\succ h_{n,\alpha}$,

$$\langle\varphi,\Phi_\alpha(t,f_\alpha)\tilde{a}_\alpha^\dagger(t,h_{1,\alpha})\cdots\tilde{a}_\alpha^\dagger(t,h_{n,\alpha})\Omega\rangle=\sum_{j=1}^n\langle f_\alpha,h_{j,\alpha}\rangle$$
$$\times\langle\varphi,\tilde{a}_\alpha^\dagger(t,h_{1,\alpha})\cdots\widehat{\tilde{a}_\alpha^\dagger(t,h_{j,\alpha})}\cdots\tilde{a}_\alpha^\dagger(t,h_{n,\alpha})\Omega\rangle, \tag{3.56}$$

where the hatted symbol is omitted.

(ii) *For* $h_\alpha\succ f_\alpha$,

$$\langle\varphi,\Phi_\alpha^\dagger(t,f_\alpha)\tilde{a}_\alpha^\dagger(t,h_\alpha)\psi\rangle=\langle\varphi,\tilde{a}_\alpha^\dagger(t,h_\alpha)\Phi_\alpha^\dagger(t,f_\alpha)\psi\rangle. \tag{3.57}$$

(iii) *For* $f_\alpha\succ h_{j,\alpha}$, $j=1,\ldots,n$,

$$\langle\varphi,\Phi_\alpha^\dagger(t,f_\alpha)\tilde{a}_\alpha^\dagger(t,h_{1,\alpha})\cdots\tilde{a}_\alpha^\dagger(t,h_{n,\alpha})\Omega\rangle=\langle\varphi,\tilde{a}_\alpha^\dagger(t,f_\alpha)\tilde{a}_\alpha^\dagger(t,h_{1,\alpha})\cdots\tilde{a}_\alpha^\dagger(t,h_{n,\alpha})\Omega\rangle. \tag{3.58}$$

Proof: One just has to apply the order by order technique developed in Ref. 29. The latter heavily relied on the ZF algebra satisfied by the creation and annihilation operators. Here, one must take care in addition of the many contributions of the defect generators but it is remarkable that the RT algebra satisfied by the bulk and defect operators leads to the same results (using the support requirements of the smearing functions and the conditions $g\succ 0$, $\eta\succ 0$, all the defect contributions vanish). One realizes in these manipulations, especially in (3.58), that the contribu-

tions of Φ, $\Phi^\dagger$ on $\tilde{\mathcal{D}}_0^{n,\alpha}$ are carried by the zeroth order corresponding to the linear problem (it is the Fourier transform of a, $a^\dagger$). ■

Lemma 3.5: Given $\varphi_\alpha \in \tilde{\mathcal{D}}_0^{n,\alpha}$, $\psi_\alpha \in \tilde{\mathcal{D}}_0^{n+1,\alpha}$ *and* $f_\alpha \in C_0^\infty(\mathbb{R}^\alpha)$, *the quadratic form (3.51) satisfies the following boundedness condition:*

$$|\langle \varphi_\alpha, \Phi_\alpha(t,f_\alpha)\psi_\alpha\rangle| \leqslant (n+1)\|f_\alpha\|\,\|\varphi_\alpha\|\,\|\psi_\alpha\|. \tag{3.59}$$

Proof: The proof is similar to that given in Ref. 32 and uses lemmas 3.2 and 3.4(i). ■

From the Riesz lemma and theorem 3.1, we conclude that $\Phi_\alpha(t,f_\alpha):\mathcal{H}^{(n+1)}\to\mathcal{H}^{(n)}$ is a bounded operator for any $n\geqslant 0$. Thus, it defines an operator on the common invariant domain $\mathcal{D}$. The same holds for $\Phi_\alpha^\dagger(t,f_\alpha)$, $\mathcal{H}^{(n)}\to H^{(n+1)}$ by (3.55). We can therefore collect our results in the following theorem.

Theorem 3.6: $\Phi(t,f)$, $\Phi^\dagger(t,f):\mathcal{D}\to\mathcal{D}$ *are Hermitian conjugate, linear operators and satisfy*

$$\Phi(t,f)\Omega = 0, \quad \Phi^\dagger(t,f)\Omega = \tilde{a}^\dagger(t,f)\Omega. \tag{3.60}$$

Finally, we will have a *nonrelativistic quantum field* if we prove the canonical commutation relations for Φ, $\Phi^\dagger$.

Theorem 3.7: $\{\Phi(t,f),\Phi^\dagger(t,f), f\in\mathcal{C}\}$ *realize a Fock representation of the equal time canonical commutation relations on* $\mathcal{D}$,

$$[\Phi(t,f_1),\Phi(t,f_2)] = 0 = [\Phi^\dagger(t,f_1),\Phi^\dagger(t,f_2)], \tag{3.61}$$

$$[\Phi(t,f_1),\Phi^\dagger(t,f_2)] = \langle f_1,f_2\rangle. \tag{3.62}$$

Proof: We know that it suffices to compute the commutators on $\tilde{\mathcal{D}}_0^{n,+}$ or $\tilde{\mathcal{D}}_0^{n,-}$ for arbitrary n and then extend the results by continuity to $\mathcal{H}^{(n)}$ and by linearity to $\mathcal{D}$. From theorem 3.6, we get that (i)–(iii) of lemma 3.4 hold as operator equalities. Let us start with the first commutator. It is made out of four parts,

$$\begin{aligned}[\Phi(t,f_1),\Phi(t,f_2)] = {}& [\Phi_+(t,f_{1,+}),\Phi_+(t,f_{2,+})] + [\Phi_+(t,f_{1,+}),\Phi_-(t,f_{2,-})] + [\Phi_-(t,f_{1,-}),\Phi_+(t,f_{2,+})] \\ & + [\Phi_-(t,f_{1,-}),\Phi_-(t,f_{2,-})].\end{aligned} \tag{3.63}$$

The first and fourth parts of the right-hand side are easily seen to be zero from (i) of lemma 3.4 One has for $\alpha=\pm$,

$$\begin{aligned}\Phi_\alpha(t,f_{1,\alpha})\Phi_\alpha(t,f_{2,\alpha})\tilde{a}_\alpha^\dagger(t,h_{1,\alpha})\cdots\tilde{a}_\alpha^\dagger(t,h_{n,\alpha})\Omega = {}& \sum_{j=1}^{n}\sum_{\substack{k=1\\k\neq j}}^{n}\langle f_{2,\alpha},h_{j,\alpha}\rangle\langle f_{1,\alpha},h_{k,\alpha}\rangle\tilde{a}_\alpha^\dagger(t,h_{1,\alpha})\cdots \\ & \times\widehat{\tilde{a}_\alpha^\dagger(t,h_{j,\alpha})}\cdots\widehat{\tilde{a}_\alpha^\dagger(t,h_{k,\alpha})}\cdots\tilde{a}_\alpha^\dagger(t,h_{n,\alpha})\Omega,\end{aligned} \tag{3.64}$$

which is symmetric under the exchange of f_1 and f_2 implying the vanishing of the commutators. As for the mixed terms, one can check that

$$\Phi_\alpha(t,f_{i,\alpha})\tilde{a}_{-\alpha}^\dagger(t,h_{1,-\alpha})\cdots\tilde{a}_{-\alpha}^\dagger(t,h_{n,-\alpha})\Omega = 0, \quad i=1,2 \tag{3.65}$$

implying the vanishing of the second and third commutators on $\tilde{\mathcal{D}}_0^{n,-\alpha}$ and hence on $\mathcal{D}$. Now the vanishing of $[\Phi^\dagger(t,f_1),\Phi^\dagger(t,f_2)]$ on $\mathcal{D}$ is obtained by Hermitian conjugation. This proves (3.61).

Equation (3.62) is obtained as follows. Again, we split the commutator into four parts. Now given a state in $\tilde{\mathcal{D}}_0^{n,\alpha}$, we assume $h_{k,\alpha}\succ f_{2,\alpha}\succ h_{k+1,\alpha}$ for some k and using lemma 3.4, we compute for $\alpha=\pm$,

$$\Phi_\alpha(t,f_{1,\alpha})\Phi_\alpha^\dagger(t,f_{2,\alpha})\tilde{a}_\alpha^\dagger(t,h_{1,\alpha})\cdots\tilde{a}_\alpha^\dagger(t,h_{n,\alpha})\Omega=\langle f_{1,\alpha},f_{2,\alpha}\rangle\tilde{a}_\alpha^\dagger(t,h_{1,\alpha})\cdots\tilde{a}_\alpha^\dagger(t,h_{n,\alpha})\Omega+\mathfrak{S} \tag{3.66}$$

and

$$\Phi_\alpha^\dagger(t,f_{2,\alpha})\Phi_\alpha(t,f_{1,\alpha})\tilde{a}_\alpha^\dagger(t,h_{1,\alpha})\cdots\tilde{a}_\alpha^\dagger(t,h_{n,\alpha})\Omega=\mathfrak{S}, \tag{3.67}$$

where $\mathfrak{S}$ is

$$\sum_{j=1}^{n}\langle f_{1,\alpha},h_{j,\alpha}\rangle\tilde{a}_\alpha^\dagger(t,h_{1,\alpha})\cdots\widehat{\tilde{a}_\alpha^\dagger(t,h_{j,\alpha})}\cdots\tilde{a}_\alpha^\dagger(t,h_{k,\alpha})\tilde{a}_\alpha^\dagger(t,f_{2,\alpha})\tilde{a}_\alpha^\dagger(t,h_{k+1,\alpha})\cdots\tilde{a}_\alpha^\dagger(t,h_{n,\alpha})\Omega.$$

This gives

$$[\Phi_+(t,f_{1,+}),\Phi_+^\dagger(t,f_{2,+})]+[\Phi_-(t,f_{1,-}),\Phi_-^\dagger(t,f_{2,-})]=\langle f_{1,+},f_{2,+}\rangle+\langle f_{1,-},f_{2,-}\rangle=\langle f_1,f_2\rangle, \tag{3.68}$$

i.e., the desired contribution. It is then straightforward using (3.65) to verify that the mixed terms do not contribute

$$[\Phi_+(t,f_{1,+}),\Phi_-^\dagger(t,f_{2,-})]=[\Phi_-(t,f_{1,-}),\Phi_+^\dagger(t,f_{2,+})]=0.$$

■

Now we prove that Ω is cyclic with respect to $\Phi^\dagger$ and that $\Phi(t,x)$ is the solution of the quantum nonlinear Schrödinger equation with impurity. Extending the partial ordering $\succ$ to functions in $\mathcal{C}$ as follows:

$$\text{for } f,g\in\mathcal{C},\quad f\succ g\Leftrightarrow f_\alpha\succ g_\alpha,\quad \alpha=\pm, \tag{3.69}$$

one can prove the following theorems.

Theorem 3.8: *The space*

$$\mathcal{H}_0^{(n)}=\text{vect}\{\Phi^\dagger(t,f_1)\cdots\Phi^\dagger(t,f_n)\Omega;\quad f_i\in\mathcal{C},\quad i=1,\ldots,n,\quad f_n\succ\ldots\succ f_1\} \tag{3.70}$$

is dense in $\mathcal{H}^{(n)}$.

Proof: Let $\varphi^{(n)}\in\mathcal{H}^{(n)}$ and suppose

$$\langle\varphi^{(n)},\Phi^\dagger(t,f_1)\cdots\Phi^\dagger(t,f_n)\Omega\rangle=0,\quad \forall f_n\succ\cdots\succ f_1.$$

Then, it is true in particular for $f_{i,-}=0$, $i=1,\ldots,n$ but in that case, we have

$$\Phi^\dagger(t,f_1)\cdots\Phi^\dagger(t,f_n)\Omega=\tilde{a}_+^\dagger(t,f_{n,+})\cdots\tilde{a}_+^\dagger(t,f_{1,+})\Omega$$

which implies $\varphi^{(n)}=0$ since $\tilde{\mathcal{D}}_0^{n,+}$ is dense in $\mathcal{H}^{(n)}$. ■

Theorem 3.9: *The quantum field* Φ *is solution of the quantum nonlinear Schrödinger equation with impurity, i.e., it satisfies*

$$(i\partial_t+\partial_x^2)\langle\varphi,\Phi(t,x)\psi\rangle=2g\langle\varphi,{:}\Phi\Phi^\dagger\Phi{:}(t,x)\psi\rangle \tag{3.71}$$

and the following boundary conditions:

$$\lim_{x\to0^+}\langle\varphi,\{\Phi_+(t,x)-\Phi_-(t,-x)\}\psi\rangle=0, \tag{3.72}$$

$$\lim_{x\to0^+}\partial_x\langle\varphi,\{\Phi_+(t,x)+\Phi_-(t,-x)\}\psi\rangle=2\eta\lim_{x\to0}\langle\varphi,\Phi(t,x)\psi\rangle, \tag{3.73}$$

$$\lim_{x\to\pm\infty}\langle\varphi,\Phi(t,x)\psi\rangle=0, \tag{3.74}$$

for any $\varphi, \psi \in \mathcal{D}$.

Proof: Inspired by the classical case, we split the field as follows:

$$\Phi(t,x) = \theta(x)\Phi_+(t,x) + \theta(-x)\Phi_-(t,x). \tag{3.75}$$

The main difficulty here is to specify a normal ordering prescription for the analog of the cubic term. We adopt the prescription detailed in Ref. 32 for the normal ordering denoted $:\cdots:$ and apply it to Φ_α, $\alpha=\pm$. Then following Ref. 32 (theorem 5), one gets that the quantum field Φ_α is solution of the nonlinear Schrödinger equation on the half-line $\mathbb{R}^\alpha$: for all $\varphi, \psi \in \mathcal{D}$,

$$(i\partial_t + \partial_x^2)\langle \varphi, \Phi_\alpha(t,x)\psi\rangle = 2g\langle \varphi, :\Phi_\alpha \Phi_\alpha^\dagger \Phi_\alpha:(t,x)\psi\rangle. \tag{3.76}$$

The situation is now similar to the classical case and we have to check the quantum analog of (2.12)–(2.14). The idea lies again in realizing that Eqs. (3.72)–(3.74) can be cast into a zeroth-order/linear problem. Following the line of argument of Ref. 32 (theorem 6), one shows that given $\varphi, \psi \in \mathcal{D}$, there exists $\chi \in \mathcal{H}^{(1)}$ such that $\langle \varphi, \Phi(t,f)\psi\rangle = \langle \Omega, \Phi(t,f)\chi\rangle$ and χ is independent of f. This gives in particular $\langle \varphi, \Phi_\alpha(t,f_\alpha)\psi\rangle = \langle \Omega, \Phi_\alpha(t,f_\alpha)\chi\rangle$, $\alpha=\pm$ and we can compute

$$\langle \varphi, \Phi_\alpha(t,x)\psi\rangle = \langle \tilde{a}_\alpha^\dagger(t,x)\Omega, \chi\rangle = \int_{\mathbb{R}} \frac{dp}{2\pi} e^{ipx - ip^2 t}\chi_\alpha(p). \tag{3.77}$$

Then, Eqs. (3.72) and (3.73) are easily obtained using the property (3.21) satisfied by χ. Finally, since $\chi_\alpha \in L^2(\mathbb{R})$, $\langle \varphi, \Phi_\alpha(t,x)\psi\rangle$ as a function of x is also in $L^2(\mathbb{R})$ and therefore vanishes at infinity. Noting that $\lim_{x\to\pm\infty}\langle \varphi, \Phi(t,x)\psi\rangle = \lim_{x\to\pm\infty}\langle \varphi, \Phi_\pm(t,x)\psi\rangle$, we get (3.74). ■

We have finally achieved the goal of this section: we have explicitly constructed off-shell local fields for the quantum nonlinear Schrödinger system on the line in the presence of a transmitting and reflecting impurity. As mentioned in Ref. 7, this remained a challenging open problem for which we brought an answer here. In other words, the quantum inverse scattering method remains valid in the presence of an impurity provided that the ZF algebra is replaced by the RT algebra.

IV. SCATTERING THEORY

Scattering theory in the presence of an impurity was studied on general grounds in Ref. 7 by introducing the RT algebra which, being a generalization of the ZF and boundary algebras, is believed to prove fundamental also in the study of off-shell correlations functions and symmetries for $1+1$-dimensional integrable systems with impurity.

In this section, we aim at giving some credit to this in the context of the nonlinear Schrödinger model. Indeed from the above results, we can get some insight in the correlations functions of the theory. The correlations functions vanish unless they involve the same number of Φ and $\Phi^\dagger$ and for a given $2n$-point function, we need at most the first $(n-1)$-order terms in the Rosales expansion of the field. This reads

$$\begin{aligned}&\langle \Omega, \Phi(t_1,x_1)\cdots\Phi(t_n,x_n)\Phi^\dagger(t_{n+1},x_{n+1})\cdots\Phi^\dagger(t_{2n},x_{2n})\Omega\rangle \\ &\quad = \sum_{\substack{K\leqslant n-1 \\ L\leqslant n-1}} g^{K+L}\langle \Omega, \Phi^{(k_1)}(t_1,x_1)\cdots\Phi^{(k_n)}(t_n,x_n)\Phi^{\dagger(l_1)}(t_{n+1},x_{n+1})\cdots\Phi^{\dagger(l_n)}(t_{2n},x_{2n})\Omega\rangle,\end{aligned} \tag{4.1}$$

where $K=\sum_{i=1}^n k_i$ and $L=\sum_{i=1}^n l_i$ and the sum runs over all n-uplets $(k_1,\ldots,k_n)$, $(l_1,\ldots,l_n)\in\mathbb{Z}_+^n$ such that $K,L\leqslant n-1$.

One has, for example (with $t_{12}=t_1-t_2$, $x_{12}=x_1-x_2$, and $\tilde{x}_{12}=x_1+x_2$),

$$\langle\Omega,\Phi(t_1,x_1)\Phi^*(t_2,x_2)\Omega\rangle = \int_{-\infty}^{+\infty}\frac{\mathrm{d}p}{2\pi}e^{-ip^2t_{12}}\{\theta(x_1)\theta(x_2)[e^{ipx_{12}}+R(p)e^{ip\tilde{x}_{12}}]+\theta(-x_1)\theta(-x_2)[e^{ipx_{12}} + \overline{R}(p)e^{ip\tilde{x}_{12}}]+\theta(x_1)\theta(-x_2)T(p)e^{ipx_{12}}+\theta(-x_1)\theta(x_2)\overline{T}(p)e^{ipx_{12}}\}. \tag{4.2}$$

More importantly, using the Haag–Ruelle approach suitably, we can relate off-shell and asymptotic theories and, doing so, fill the gap of our quantum field theory. Indeed, on the one hand, we know from Ref. 7 that the Fock representation of the RT algebra generates the asymptotic states of a general integrable theory with impurity with corresponding *S*-matrix. On the other hand, in this paper we constructed off-shell local time-dependent fields whose behavior as $t\to\pm\infty$ we would like to know.

A. Asymptotic theory

The first step is to characterize wave packets for the free Schrödinger equation which take into account the presence of the impurity at $x=0$. We adopt the following setup. For $\mathfrak{f}\in C_0^\infty(\mathbb{R})$, we define

$$f^t(x) = \int_{\mathbb{R}}\frac{\mathrm{d}p}{2\pi}\mathfrak{f}(p)e^{ipx-ip^2t}. \tag{4.3}$$

We transpose the partial ordering (3.35) to functions of the variable p.

Definition 4.1: Given $n,m\geqslant 1$, consider two sets of functions

$$\mathfrak{H}_n=\{\mathfrak{h}_{i,\alpha_i}\in C_0^\infty(\mathbb{R}^{\alpha_i}),\quad i=1,\ldots,n\}\quad\text{and}\quad \mathfrak{G}_m=\{\mathfrak{g}_{i,\beta_i}\in C_0^\infty(\mathbb{R}^{-\beta_i}),\quad i=1,\ldots,m\}, \tag{4.4}$$

where the functions obey the following order prescriptions:

$$\mathfrak{h}_{1,\alpha_1}\succ\cdots\succ\mathfrak{h}_{n,\alpha_n},\quad \mathfrak{g}_{m,\beta_m}\succ\cdots\succ\mathfrak{g}_{1,\beta_1}. \tag{4.5}$$

We also define

$$h^\theta_{i,\alpha_i}(x)=\theta(\alpha_i x)h^t_{i,\alpha_i}(x),\quad g^\theta_{i,\beta_i}(x)=\theta(\beta_i x)g^t_{i,\beta_i}(x). \tag{4.6}$$

By construction, $h^\theta_{i,\alpha_i}(x)$ represent wave packets in $\mathbb{R}^{\alpha_i}$ moving away from the impurity towards $\alpha_i\infty$ while $g^\theta_{i,\beta_i}(x)$ represent wave packets in $\mathbb{R}^{\beta_i}$ moving towards the impurity. One already understands that they will be relevant for the so-called "out" and "in" states, respectively. In fact, this is the main theorem of this section for which we need some preliminary results.

From the preceding section, we know the exchange and commutation properties of $\Phi^\dagger$ and $\tilde{a}^\dagger$ smeared with ordered functions in the variable x. Here, our wave packets were constructed from ordered functions in p but we made no assumption as to their ordering in x. Therefore, we must include all the possibilities and this requires the use of the permutation group of n elements $\mathfrak{S}_n$. For $\sigma\in\mathfrak{S}_n$, $\pi\in\mathfrak{S}_m$, $n,m\geqslant 2$, we introduce

$$\theta^\sigma_h(\alpha_1x_1,\ldots,\alpha_nx_n)=\prod_{\substack{i,j=1\\ i<j}}^{n}\theta(\alpha_{\sigma_i}x_{\sigma_i}-\alpha_{\sigma_j}x_{\sigma_j}), \tag{4.7}$$

$$\theta^\pi_g(\beta_1x_1,\ldots,\beta_mx_m)=\prod_{\substack{i,j=1\\ i>j}}^{m}\theta(\beta_{\pi_i}x_{\pi_i}-\beta_{\pi_j}x_{\pi_j}), \tag{4.8}$$

satisfying

$$\sum_{\sigma\in\mathfrak{S}_n}\theta_h^\sigma(\alpha_1x_1,\ldots,\alpha_nx_n)=1=\sum_{\pi\in\mathfrak{S}_m}\theta_g^\pi(\beta_1x_1,\ldots,\beta_mx_m). \tag{4.9}$$

Lemma 4.2: Given any two sets of functions in $\mathfrak{H}_n$ and $\mathfrak{G}_m$,

(i) *The following limits hold:*

$$\lim_{t\to+\infty}\|h^\theta_{1,\alpha_1}\otimes\cdots\otimes h^\theta_{n,\alpha_n}-h^t_{1,\alpha_1}\otimes\cdots\otimes h^t_{n,\alpha_n}\|=0,$$

$$\lim_{t\to-\infty}\|g^\theta_{1,\beta_1}\otimes\cdots\otimes g^\theta_{m,\beta_m}-g^t_{1,\beta_1}\otimes\cdots\otimes g^t_{m,\beta_m}\|=0. \tag{4.10}$$

(ii) *Let e_n be the identity of $\mathfrak{S}_n$ and let us define*

$$H^\sigma_{\alpha_1\cdots\alpha_n}(x_1,\ldots,x_n)=h^\theta_{1,\alpha_1}(x_1)\cdots h^\theta_{n,\alpha_n}(x_n)\theta_h^\sigma(\alpha_1x_1,\ldots,\alpha_nx_n),$$

$$G^\pi_{\beta_1\cdots\beta_m}(x_1,\ldots,x_m)=g^\theta_{1,\beta_1}(x_1)\cdots g^\theta_{m,\beta_m}(x_m)\theta_g^\pi(\beta_1x_1,\ldots,\beta_mx_m). \tag{4.11}$$

Then

$$\lim_{t\to+\infty}\|H^\sigma_{\alpha_1\cdots\alpha_n}\|=0,\quad \lim_{t\to-\infty}\|G^\pi_{\beta_1\cdots\beta_m}\|=0\quad \textit{for all } \sigma\neq e_n,\quad \pi\neq e_m. \tag{4.12}$$

(iii) *The following estimate is valid for any $F\in L^2(\mathbb{R}^n)$,*

$$\left\|\int_{\mathbb{R}^n}\mathrm{d}x_1\cdots\mathrm{d}x_nF(x_1,\ldots,x_n)\tilde a^\dagger_{\alpha_1}(t,x_1)\cdots\tilde a^\dagger_{\alpha_n}(t,x_n)\right\|\leqslant\sqrt{n!}\|F\|. \tag{4.13}$$

Proof: The ideas are the same as those detailed in Ref. 32 from theorem 7 onwards and rest especially on the use of the weak limit

$$\lim_{t\to\pm\infty}\frac{e^{itk}}{k\pm i\varepsilon}=0. \tag{4.14}$$

We just stress again that in our case all the above holds thanks to the use of the RT algebra and by paying careful attention to the support conditions encoded in (4.5). ■

We are now in position to identify the asymptotic behavior of the field as $t\to\pm\infty$.

Theorem 4.3: *The following limits hold in the strong sense in the Fock space $\mathcal{F}$*:

$$\lim_{t\to+\infty}\Phi^\dagger(t,h^\theta_{1,\alpha_1})\cdots\Phi^\dagger(t,h^\theta_{n,\alpha_n})\Omega=a^\dagger_{\alpha_1}(\mathfrak{h}_{1,\alpha_1})\cdots a^\dagger_{\alpha_n}(\mathfrak{h}_{n,\alpha_n})\Omega, \tag{4.15}$$

$$\lim_{t\to-\infty}\Phi^\dagger(t,g^\theta_{1,\beta_1})\cdots\Phi^\dagger(t,g^\theta_{m,\beta_m})\Omega=a^\dagger_{\beta_1}(\mathfrak{g}_{1,\beta_1})\cdots a^\dagger_{\beta_m}(\mathfrak{g}_{m,\beta_m})\Omega. \tag{4.16}$$

Proof: We note first that from (3.75) one gets $\Phi^\dagger(t,h^\theta_{i,\alpha_i})=\Phi^\dagger_{\alpha_i}(t,h^\theta_{i,\alpha_i})$ and $\Phi^\dagger(t,g^\theta_{i,\beta_i})=\Phi^\dagger_{\beta_i}(t,g^\theta_{i,\beta_i})$ so that

$$\Phi^\dagger(t,h^\theta_{i,\alpha_i})\Omega=\tilde a^\dagger_{\alpha_i}(t,h^\theta_{i,\alpha_i})\Omega\quad\text{and }\Phi^\dagger(t,g^\theta_{i,\beta_i})\Omega=\tilde a^\dagger_{\beta_i}(t,g^\theta_{i,\beta_i})\Omega. \tag{4.17}$$

Moreover, for $\mathfrak{f}_\alpha\in C_0^\infty(\mathbb{R}^\alpha)$, one has

$$a^\dagger_\alpha(\mathfrak{f}_\alpha)=\tilde a^\dagger_\alpha(t,f^t_\alpha). \tag{4.18}$$

Collecting all this, theorem 4.3 is proved for $n=m=1$ using (i), and (iii) of lemma (4.2),

$$\|\Phi^\dagger(t,f^\theta_\alpha)\Omega - a^\dagger_\alpha(\mathfrak{f}_\alpha)\Omega\| = \|\tilde{a}^\dagger_\alpha(t,f^\theta_\alpha)\Omega - \tilde{a}^\dagger_\alpha(t,f^t_\alpha)\Omega\| \leqslant \|f^\theta_\alpha - f^t_\alpha\|, \tag{4.19}$$

$\mathfrak{f}$ playing the role of $\mathfrak{h}$ or $\mathfrak{g}$. Now we want to compute the left-hand sides of Eqs. (4.15) and (4.16) for $n,m \geqslant 2$. We give details for Eq. (4.15),

$$\begin{aligned}\Phi^\dagger(t,h^\theta_{1,\alpha_1})\cdots\Phi^\dagger(t,h^\theta_{n,\alpha_n})\Omega &= \sum_{\sigma\in\mathfrak{S}_n}\int_{\mathbb{R}^n} dx_1\cdots dx_n\, H^\sigma_{\alpha_1\cdots\alpha_n}(x_1,\ldots,x_n)\Phi^\dagger_{\alpha_1}(t,x_1)\cdots\Phi^\dagger_{\alpha_n}(t,x_n)\Omega\\ &= \sum_{\sigma\in\mathfrak{S}_n}\int_{\mathbb{R}^n} dx_1\cdots dx_n\, H^\sigma_{\alpha_1\cdots\alpha_n}(x_1,\ldots,x_n)\tilde{a}^\dagger_{\alpha_{\sigma_1}}(t,x_{\alpha_{\sigma_1}})\cdots\tilde{a}^\dagger_{\alpha_{\sigma_n}}(t,x_{\alpha_{\sigma_n}})\Omega\\ &= \tilde{a}^\dagger_{\alpha_1}(t,h^\theta_{1,\alpha_1})\cdots\tilde{a}^\dagger_{\alpha_n}(t,h^\theta_{n,\alpha_n})\Omega + \sum_{\substack{\sigma\in\mathfrak{S}_n\\ \sigma\neq e_n}}\int_{\mathbb{R}^n} dx_1\cdots dx_n\, H^\sigma_{\alpha_1\cdots\alpha_n}(x_1,\ldots,x_n)\\ &\quad\times\{\tilde{a}^\dagger_{\alpha_{\sigma_1}}(t,x_{\alpha_{\sigma_1}})\cdots\tilde{a}^\dagger_{\alpha_{\sigma_n}}(t,x_{\alpha_{\sigma_n}})\Omega - \tilde{a}^\dagger_{\alpha_1}(t,h^\theta_{1,\alpha_1})\cdots\tilde{a}^\dagger_{\alpha_n}(t,h^\theta_{n,\alpha_n})\Omega\},\end{aligned} \tag{4.20}$$

where we used point (iii) of lemma 3.4 and (3.61) for $\Phi^\dagger$ in the second equality. Applying (4.13) then gives

$$\begin{aligned}\|\Phi^\dagger(t,h^\theta_{1,\alpha_1})\cdots\Phi^\dagger(t,h^\theta_{n,\alpha_n})\Omega - a^\dagger_{\alpha_1}(\mathfrak{h}_{1,\alpha_1})\cdots a^\dagger_{\alpha_n}(\mathfrak{h}_{n,\alpha_n})\Omega\| &\leqslant \sqrt{n!}\|h^\theta_{1,\alpha_1}\otimes\cdots\otimes h^\theta_{n,\alpha_n} - h^t_{1,\alpha_1}\otimes\cdots\\ &\otimes h^t_{n,\alpha_n}\| + 2\sqrt{n!}\sum_{\substack{\sigma\in\mathfrak{S}_n\\ \sigma\neq e_n}}\|H^\sigma_{\alpha_1\cdots\alpha_n}\|,\end{aligned} \tag{4.21}$$

implying (4.15) by points (i)–(ii) of lemma 4.2 Similar computations give

$$\begin{aligned}\|\Phi^\dagger(t,g^\theta_{1,\beta_1})\cdots\Phi^\dagger(t,g^\theta_{m,\beta_m})\Omega - a^\dagger_{\beta_1}(\mathfrak{g}_{1,\beta_1})\cdots a^\dagger_{\beta_m}(\mathfrak{g}_{m,\beta_m})\Omega\| &\leqslant \sqrt{m!}\|g^\theta_{1,\beta_1}\otimes\cdots\otimes g^\theta_{m,\beta_m} - g^t_{1,\beta_1}\\ &\otimes\cdots\otimes g^t_{m,\beta_m}\| + 2\sqrt{m!}\sum_{\substack{\pi\in\mathfrak{S}_m\\ \neq e_m}}\|G^\pi_{\beta_1\cdots\beta_m}\|,\end{aligned} \tag{4.22}$$

proving (4.16). ■

B. Scattering matrix

Now that we have identified the natural "free" dynamics approached by our interacting field as $t\to\pm\infty$, we are left with the verification of asymptotic completeness allowing the construction of a unitary S-matrix. We emphasize here that our "in" and "out" spaces are slightly different from those exhibited in Ref. 7 because of our ordering involving absolute values, so that we must recheck their properties.

Proposition 4.4: Let

$$\mathcal{F}^{\text{in}} = \text{vect}\{\Omega, a^\dagger_{\beta_1}(\mathfrak{g}_{1,\beta_1})\cdots a^\dagger_{\beta_m}(\mathfrak{g}_{m,\beta_m})\Omega,\ \beta_i = \pm,\ i=1,\ldots,m,\ m\geqslant 1\}, \tag{4.23}$$

$$\mathcal{F}^{\text{out}} = \text{vect}\{\Omega, a^\dagger_{\alpha_1}(\mathfrak{h}_{1,\alpha_1})\cdots a^\dagger_{\alpha_n}(\mathfrak{h}_{n,\alpha_n})\Omega,\ \alpha_i = \pm,\ i=1,\ldots,n,\ n\geqslant 1\}, \tag{4.24}$$

where $\mathfrak{h}_{i,\alpha_i}$ *and* $\mathfrak{g}_{j,\beta_j}$ *run over* $\mathfrak{H}_n$ *and* $\mathfrak{G}_m$.

Then, $\mathcal{F}^{\text{in}}$ *and* $\mathcal{F}^{\text{out}}$ *are separately dense in* $\mathcal{F}$.

Proof: We deal with $\mathcal{F}^{\text{in}}$. Again, it is sufficient to consider the matrix element,

$$A_{t,\varphi,\beta_1\cdots\beta_p}(p_1,\ldots,p_m)=\langle\varphi^{(n)},a^\dagger_{\beta_1}(t,p_1)\cdots a^\dagger_{\beta_m}(t,p_m)\Omega\rangle, \tag{4.25}$$

where $\varphi^{(n)}\in\mathcal{H}^{(n)}$ is arbitrary and to show that

$$A_{t,\varphi,\beta_1\cdots\beta_p}(p_1,\ldots,p_m)=0,\quad \forall\,|p_1|<\cdots<|p_m|,\quad p_i\in\mathbb{R}^{-\beta_i},\quad \beta_i=\pm,\quad i=1,\ldots,m \tag{4.26}$$

implies $\varphi^{(n)}=0$. From the cyclicity of Ω with respect to $a^\dagger$, (4.26) gives

$$\varphi^{(n)}_{\beta_1\cdots\beta_p}(p_1,\ldots,p_m)=0,\quad \forall\,|p_1|<\cdots<|p_m|,\quad p_i\in\mathbb{R}^{-\beta_i},\quad \beta_i=\pm,\quad i=1,\ldots,m \tag{4.27}$$

and in view of the properties of $\varphi^{(n)}\in\mathcal{H}^{(n)}$, this implies in turn

$$\varphi^{(n)}_{\beta_1\cdots\beta_p}(p_1,\ldots,p_m)=0,\quad \forall\,p_i\in\mathbb{R},\quad \beta_i=\pm,\quad i=1,\ldots,m, \tag{4.28}$$

i.e., $\varphi^{(n)}=0$. The case of $\mathcal{F}^{\text{out}}$ is similar. ■

We turn to the definition of the scattering operator **S** of our theory.

Proposition 4.5: Take functions in $\mathfrak{H}_n$ and let $\mathbf{S}$: $\mathcal{F}^{\text{out}}\to\mathcal{F}^{\text{in}}$ *act as follows:*

$$\mathbf{S}\Omega=\Omega\quad \textit{and}\quad \mathbf{S}{:}\,a^\dagger_{\alpha_1}(\mathfrak{h}_{1,\alpha_1})\cdots a^\dagger_{\alpha_n}(\mathfrak{h}_{n,\alpha_n})\Omega\mapsto a^\dagger_{\alpha_n}(\hat{\mathfrak{h}}_{n,\alpha_n})\cdots a^\dagger_{\alpha_1}(\hat{\mathfrak{h}}_{1,\alpha_1})\Omega \tag{4.29}$$

$$\textit{where}\quad \hat{\mathfrak{h}}_{i,\alpha_i}(p)=\mathfrak{h}_{i,\alpha_i}(-p)\in\mathfrak{G}_n. \tag{4.30}$$

Then **S** *is invertible and* $\mathbf{S}$, $\mathbf{S}^{-1}$ *are unitary operators acting on* $\mathcal{F}$.

Proof: From the definitions (4.29) and (4.30), one deduces immediately that $\mathbf{S}^{-1}$ is well defined. Then, it is straightforward, albeit lengthy, to check that

$$\begin{aligned}&\langle\mathbf{S}a^\dagger_{\alpha_1}(\mathfrak{h}_{1,\alpha_1})\cdots a^\dagger_{\alpha_n}(\mathfrak{h}_{n,\alpha_n})\Omega,\mathbf{S}a^\dagger_{\gamma_1}(\mathfrak{f}_{1,\gamma_1})\cdots a^\dagger_{\gamma_n}(\mathfrak{f}_{n,\gamma_n})\Omega\rangle\\&\quad=\langle a^\dagger_{\alpha_1}(\mathfrak{h}_{1,\alpha_1})\cdots a^\dagger_{\alpha_n}(\mathfrak{h}_{n,\alpha_n})\Omega,a^\dagger_{\gamma_1}(\mathfrak{f}_{1,\gamma_1})\cdots a^\dagger_{\gamma_n}(\mathfrak{f}_{n,\gamma_n})\Omega\rangle.\end{aligned} \tag{4.31}$$

In evaluating the left-hand side, one just has to notice that all the contributions coming from the defect generators vanish due to the support properties of the smearing functions and one is left with what would be obtained by using the ZF algebra. Then, it is just a matter of changing the variables into their opposite to get the right-hand side.

Next, following the line of argument given in Ref. 19, one extends **S** to $\mathcal{F}^{\text{out}}$ by linearity, preserving unitarity. This gives rise to bounded linear operators which one can uniquely extend by continuity to the whole of $\mathcal{F}$. We note that this last step is allowed by the asymptotic completeness property satisfied by $\mathcal{F}^{\text{out}}$ and $\mathcal{F}^{\text{in}}$ (cf. Proposition 4.4). The case of $\mathbf{S}^{-1}$ is similar. ■

Refering now to Ref. 7 we finish the description of our scattering theory by defining the correspondence between in and out states and the asymptotic states identified in theorem 4.3 (correspondence already anticipated in our calling $\mathcal{F}^{\text{out}}$ and $\mathcal{F}^{\text{in}}$ the "in" and "out" spaces),

$$|\mathfrak{g}_{1,\beta_1};\ldots;\mathfrak{g}_{m,\beta_m}\rangle^{\text{in}}=a^\dagger_{\beta_1}(\mathfrak{g}_{1,\beta_1})\cdots a^\dagger_{\beta_m}(\mathfrak{g}_{m,\beta_m})\Omega, \tag{4.32}$$

$$|\mathfrak{h}_{1,\alpha_1};\ldots;\mathfrak{h}_{n,\alpha_n}\rangle^{\text{out}}=a^\dagger_{\alpha_1}(\mathfrak{h}_{1,\alpha_1})\cdots a^\dagger_{\alpha_n}(\mathfrak{h}_{n,\alpha_n})\Omega. \tag{4.33}$$

Transition amplitudes are therefore easily computable from

$$ {}^{\text{out}}\langle \mathfrak{h}_{1,\alpha_1};\ldots;\mathfrak{h}_{n,\alpha_n}|\mathfrak{g}_{1,\beta_1};\ldots;\mathfrak{g}_{m,\beta_m}\rangle^{\text{in}} = \langle a^\dagger_{\alpha_1}(\mathfrak{h}_{1,\alpha_1})\cdots a^\dagger_{\alpha_n}(\mathfrak{h}_{n,\alpha_n})\Omega, a^\dagger_{\beta_1}(\mathfrak{g}_{1,\beta_1})\cdots a^\dagger_{\beta_m}(\mathfrak{g}_{m,\beta_m})\Omega\rangle \tag{4.34} $$

and using (3.27), (3.8), (3.13), (3.15), and (3.23). One recovers for transition amplitudes that they vanish unless $n=m$ as expected for an integrable system where particle production does not occur. As an example, we derive in our context the one and two particle transition amplitudes obtained in Ref. 6. We start with the computation of the correlators,

$$ \langle a^\dagger_\alpha(p)\Omega, a^\dagger_\beta(q)\Omega\rangle = \delta^\beta_\alpha\delta(p-q) + \epsilon^\beta_\alpha\delta(p-q)T(\alpha p) + \delta^\beta_\alpha\delta(p+q)R(\alpha p) \tag{4.35} $$

and

$$ \begin{aligned}
&\langle a^\dagger_{\alpha_1}(p_1)a^\dagger_{\alpha_2}(p_2)\Omega, a^\dagger_{\beta_1}(q_1)a^\dagger_{\beta_2}(q_2)\Omega\rangle \\
&\quad = S(\alpha_1p_1-\beta_1q_1)[\delta^{\beta_1}_{\alpha_2}+\epsilon^{\beta_1}_{\alpha_2}T(\alpha_2p_2)][\delta^{\beta_2}_{\alpha_1}+\epsilon^{\beta_2}_{\alpha_1}T(\alpha_1p_1)] \\
&\qquad \times \delta(p_2-q_1)\delta(p_1-q_2) + S(\alpha_1p_1-\beta_1q_1)[\delta^{\beta_1}_{\alpha_2}R(\alpha_2p_2)][\delta^{\beta_2}_{\alpha_1}+\epsilon^{\beta_2}_{\alpha_1}T(\alpha_1p_1)] \\
&\qquad \times \delta(p_2+q_1)\delta(p_1-q_2) + S(\alpha_1p_1-\beta_1q_1)[\delta^{\beta_1}_{\alpha_2}+\epsilon^{\beta_1}_{\alpha_2}T(\alpha_2p_2)][\delta^{\beta_2}_{\alpha_1}R(\alpha_1p_1)]\delta(p_2-q_1)\delta(p_1+q_2) \\
&\qquad + S(\alpha_1p_1-\beta_1q_1)[\delta^{\beta_1}_{\alpha_2}R(\alpha_2p_2)][\delta^{\beta_2}_{\alpha_1}R(\alpha_1p_1)]\delta(p_2+q_1)\delta(p_1+q_2) \\
&\qquad + [\delta^{\beta_1}_{\alpha_1}+S(\alpha_1p_1-\beta_2q_2)S(\alpha_1p_1+\beta_2q_2)\epsilon^{\beta_1}_{\alpha_1}T(\alpha_1p_1)][\delta^{\beta_2}_{\alpha_2}+\epsilon^{\beta_2}_{\alpha_2}T(\alpha_2p_2)]\delta(p_1-q_1)\delta(p_2-q_2) \\
&\qquad + S(\alpha_1p_1-\beta_2q_2)S(\alpha_1p_1+\beta_2q_2)[\delta^{\beta_1}_{\alpha_1}R(\alpha_1p_1)][\delta^{\beta_2}_{\alpha_2}+\epsilon^{\beta_2}_{\alpha_2}T(\alpha_2p_2)]\delta(p_1+q_1)\delta(p_2-q_2) \\
&\qquad + [\delta^{\beta_1}_{\alpha_1}+S(\alpha_1p_1-\beta_2q_2)S(\alpha_1p_1+\beta_2q_2)\epsilon^{\beta_1}_{\alpha_1}T(\alpha_1p_1)][\delta^{\beta_2}_{\alpha_2}R(\alpha_2p_2)]\delta(p_1-q_1)\delta(p_2+q_2) \\
&\qquad + S(\alpha_1p_1-\beta_2q_2)S(\alpha_1p_1+\beta_2q_2)[\delta^{\beta_1}_{\alpha_1}R(\alpha_1p_1)][\delta^{\beta_2}_{\alpha_2}R(\alpha_2p_2)]\delta(p_1+q_1)\delta(p_2+q_2)
\end{aligned} \tag{4.36} $$

We note that the result for the two-particle correlator differs from that obtained in Ref. 6 by the appearance of two S coefficients in the four last terms. This is due to the fact that we started with a more general RT algebra where the defect generators do not necessarily obey the linear relations used in Ref. 6. For the one-particle amplitudes, there are two possibilities according to the relative signs of the in and out states

$$ {}^{\text{out}}\langle \mathfrak{h}_\pm, \mathfrak{g}_\pm\rangle^{\text{in}} = \begin{cases} \displaystyle\int_0^\infty \frac{dp}{2\pi}\overline{\mathfrak{h}}_+(p)R(p)\mathfrak{g}_+(-p), \\ \displaystyle\int_{-\infty}^0 \frac{dp}{2\pi}\overline{\mathfrak{h}}_-(p)R(-p)\mathfrak{g}_-(-p), \end{cases} \tag{4.37} $$

$$ {}^{\text{out}}\langle \mathfrak{h}_\pm|\mathfrak{g}_\mp\rangle^{\text{in}} = \begin{cases} \displaystyle\int_0^\infty \frac{dp}{2\pi}\overline{\mathfrak{h}}_+(p)T(p)\mathfrak{g}_-(p), \\ \displaystyle\int_{-\infty}^0 \frac{dp}{2\pi}\overline{\mathfrak{h}}_-(p)T(-p)\mathfrak{g}_+(p). \end{cases} \tag{4.38} $$

One clearly sees the particle-impurity interaction through the reflection coefficient R for a final and an initial state on the same half-line and through the transmission coefficient T otherwise, as expected. The particle–particle interaction through the bulk interaction coefficient S shows up in the 2^4 different two-particle amplitudes. As an illustration, we compute four such amplitudes gathered into two generic expressions:

$$
{}^{\text{out}}\langle \mathfrak{h}_{1,\pm};\mathfrak{h}_{2,\pm}|\mathfrak{g}_{1,\pm};\mathfrak{g}_{2,\pm}\rangle^{\text{in}} = \int_{\mathbb{R}^\pm}\frac{dp_1}{2\pi}\int_{\mathbb{R}^\pm}\frac{dp_2}{2\pi}(\overline{\mathfrak{h}}_{1,\pm}(p_1)\overline{\mathfrak{h}}_{2,\pm}(p_2)R(\pm p_2)S(\pm p_1 \pm p_2)R(\pm p_1)\mathfrak{g}_{1,\pm}(-p_2)
$$

$$
\times\mathfrak{g}_{2,\pm}(-p_1) + \overline{\mathfrak{h}}_{1,\pm}(p_1)\overline{\mathfrak{h}}_{2,\pm}(p_2)R(\pm p_1)S(\pm p_1 \pm p_2)S(\pm p_1 \mp p_2)R(\pm p_2)
$$

$$
\times\mathfrak{g}_{1,\pm}(-p_1)\mathfrak{g}_{2,\pm}(-p_2)) \tag{4.39}
$$

and

$$
{}^{\text{out}}\langle \mathfrak{h}_{1,\pm};\mathfrak{h}_{2,\pm}|\mathfrak{g}_{1,\pm};\mathfrak{g}_{2,\mp}\rangle^{\text{in}} = \int_{\mathbb{R}^\pm}\frac{dp_1}{2\pi}\int_{\mathbb{R}^\pm}\frac{dp_2}{2\pi}(\overline{\mathfrak{h}}_{1,\pm}(p_1)\overline{\mathfrak{h}}_{2,\pm}(p_2)R(\pm p_2)S(\pm p_1 \pm p_2)T(\pm p_1)
$$

$$
\times\mathfrak{g}_{1,\pm}(-p_2)\mathfrak{g}_{2,\mp}(p_1) + \overline{\mathfrak{h}}_{1,\pm}(p_1)\overline{\mathfrak{h}}_{2,\pm}(p_2)R(\pm p_1)
$$

$$
\times S(\pm p_1 \pm p_2)S(\pm p_1 \mp p_2)T(\pm p_2)\mathfrak{g}_{1,\pm}(-p_1)\mathfrak{g}_{2,\mp}(p_2)). \tag{4.40}
$$

More complex transition amplitudes contain the same building blocks namely R, T, and S, which shows that the corresponding processes involve a succession of particle-impurity and particle–particle interactions as expected from the factorized scattering occurring in this integrable model.

V. DISCUSSION AND CONCLUSIONS

We have analyzed above the NLS model interacting with a δ-type impurity, establising the exact classical and quantum solutions. We have shown that an appropriate RT algebra and its Fock representation allow to construct not only the scattering operator, but also the off-shell quantum field $\Phi(t,x)$. As already mentioned in the introduction, these results can be extended[33] to a whole class of point-like defects, substituting (3.72) and (3.73) by the impurity boundary conditions

$$
\lim_{x\downarrow 0}\begin{pmatrix} \langle\varphi,\Phi(t,x)\psi\rangle \\ \partial_x\langle\varphi,\Phi(t,x)\psi\rangle \end{pmatrix} = \alpha\begin{pmatrix} a & b \\ c & d \end{pmatrix}\lim_{x\uparrow 0}\begin{pmatrix} \langle\varphi,\Phi(t,x)\psi\rangle \\ \partial_x\langle\varphi,\Phi(t,x)\psi\rangle \end{pmatrix}, \tag{5.1}
$$

where

$$
\{a,\ldots,d\in\mathbb{R},\ \alpha\in\mathbb{C}: ad-bc=1,\ \overline{\alpha}\alpha=1,\}. \tag{5.2}
$$

In absence of impurity bound states, namely in the domain

$$
a+d+\sqrt{(a-d)^2+4}\leqslant 0, \quad b<0,
$$

$$
c(a+d)^{-1}\geqslant 0, \quad b=0, \tag{5.3}
$$

$$
a+d-\sqrt{(a-d)^2+4}\geqslant 0, \quad b>0,
$$

one can treat the model closely following the δ-impurity case, because the corresponding reflection and transmission matrices $\mathcal{R}$ and $\mathcal{T}$ have the same analytic properties as (3.18).

We would like to comment finally on the symmetry content of the solution derived in the paper. It is quite obvious that impurities break down Galilean (Lorentz) invariance of the *total* scattering matrix **S**. However, since the *bulk* scattering matrix $\mathcal{S}$ describes the scattering away from the impurity, some authors[1–5] have assumed that $\mathcal{S}$ preserves these symmetries and that the breaking in **S** is generated exclusively by the reflection and transmission coefficients $\mathcal{R}$ and $\mathcal{T}$. This assumption however, combined with the conditions of factorized scattering, implies[1,5] that $\mathcal{S}$ is constant, which is too restrictive. In fact, one is left with a few systems of limited physical interest. In order to avoid this negative result, a consistent factorized scattering theory was developed in Refs. 6 and 7, which does not necessarily assume that $\mathcal{S}$ is Galilean (Lorentz) invariant. Since the impurity NLS model considered above is the first concrete application of this framework with nontrivial bulk scattering, the lesson from it is quite instructive. Focusing on $\mathcal{S}$ (3.2), we see

that Galilean invariance is broken by the entries which describe the scattering of two incoming particles localized for $t\to-\infty$ on the different half-lines $\mathbb{R}_-$ and $\mathbb{R}_+$ respectively. Indeed, these entries depend on k_1+k_2 and not on k_1-k_2. An intuitive explanation for this breaking is that before such particles scatter, one of them must necessarily cross the impurity. The nontrivial transmission is therefore the origin of the symmetry breaking in $\mathcal{S}$. This conclusion agrees with the observation that in systems which allow only reflection (e.g., models on the half-line), one can have[14–19] both Galilean (Lorentz) invariant and nonconstant bulk scattering matrices.

The issue of internal symmetries in the presence of impurities has been partially addressed in Refs. 8 and 11. In particular, the role of the reflection and transmission elements of the RT algebra as symmetry generators has been established. However, this question deserves further investigation. It will be interesting in this respect to extend the analysis[38] of the SU(N)–NLS model on the half-line to the impurity case. Work is in progress on this aspect.

Let us conclude by observing that the concept of RT algebra indeed represents a powerful tool for solving the NLS model with impurities. We are currently exploring the possibility to apply this algebraic framework also to the quantization of other integrable systems with defects.

APPENDIX A: PROOF OF THEOREM 2.2

First, notice that (2.12) and (2.13) translate into

$$\lim_{x\to0^+}\{\Phi_+(t,x)-\Phi_-(t,-x)\}=0, \tag{A1}$$

$$\lim_{x\to0^+}\{(\partial_x\Phi_+)(t,x)-(\partial_x\Phi_-)(t,-x)\}-2\eta\Phi(t,0)=0, \tag{A2}$$

which we are going to check order by order in the Rosales expansion. The idea is to introduce the one-to-one correspondence

$$\beta_\pm(p)=\tfrac{1}{2}\{\lambda_+(p)\pm\lambda_-(-p)\},\quad p\in\mathbb{R} \tag{A3}$$

and it is not difficult to check that

$$\beta_\alpha(p)=B_\alpha(p)\beta_\alpha(-p),\quad \text{with } B_\alpha(p)=\alpha\frac{p-i\alpha\eta}{p+i\eta},\quad \alpha=\pm. \tag{A4}$$

Take $n=0$ corresponding to the linear problem. One gets

$$\lim_{x\to0^+}\{\Phi_+^{(0)}(t,x)-\Phi_-^{(0)}(t,-x)\}=\int_{\mathbb{R}}\frac{dp}{2\pi}\beta_-(p)e^{-ip^2t},$$

$$\lim_{x\to0^+}\{(\partial_x\Phi_+^{(0)})(t,x)-(\partial_x\Phi_-^{(0)})(t,-x)\}-2\eta\Phi^{(0)}(t,0)=\int_{\mathbb{R}}\frac{dp}{2\pi}(ip-\eta)\beta_+(p)e^{-ip^2t},$$

which vanish using the properties (A4). It is interesting to note that the time-dependent phase e^{-ip^2t}, being even in p, does not play any role in the vanishing of the previous expressions. It will be the same in the following as we shall see.

For $n\geqslant1$, we start by changing variables in the Rosales expansion according to $(p_1,\ldots,p_n,q_n,\ldots,q_0)\to(k_1,\ldots,k_{2n-1},-k_{2n}\ldots,-k_0)$ and we use the one-to-one correspondence (A3) to rewrite the left-hand side of (A1) as

$$\lim_{x\to 0^+}\{\Phi_+^{(n)}(0,x)-\Phi_-^{(n)}(0,-x)\}=\sum_{\alpha_0,\ldots,\alpha_{2n}=\pm}\left(1-\prod_{i=0}^{2n}\alpha_i\right)\int_{\mathbb{R}^{2n+1}}\prod_{i=0}^{2n}\frac{dk_i}{2\pi}\overline{\beta}_{\alpha_1}(k_1)\cdots\overline{\beta}_{\alpha_{2n-1}}(k_{2n-1})$$
$$\times\beta_{\alpha_{2n}}(-k_{2n})\cdots\beta_{\alpha_0}(-k_0)\frac{e^{-i\Sigma_{j=0}^{2n}k_j^2t}}{\prod_{j=1}^{2n}(k_j+k_{j-1})}. \tag{A5}$$

In view of the linear case, we "B_α-symmetrize" the integrand of the previous integral for each k_i. Introducing

$$B_\alpha^\sigma(p)=\begin{cases}1 & \text{for } \sigma=+,\\ B_\alpha(p) & \text{for } \sigma=-,\end{cases} \tag{A6}$$

this reads

$$\frac{1}{2^{2n+1}}\sum_{\sigma_0,\ldots,\sigma_{2n}=\pm}\frac{B_{\alpha_1}^{\sigma_1}(k_1)\cdots B_{\alpha_{2n-1}}^{\sigma_{2n-1}}(k_{2n-1})B_{\alpha_{2n}}^{\sigma_{2n}}(-k_{2n})\cdots B_{\alpha_0}^{\sigma_0}(-k_0)}{\prod_{j=1}^{2n}(\sigma_jk_j+\sigma_{j-1}k_{j-1})}\overline{\beta}_{\alpha_1}(k_1)\cdots\overline{\beta}_{\alpha_{2n-1}}(k_{2n-1})$$
$$\times\beta_{\alpha_{2n}}(-k_{2n})\cdots\beta_{\alpha_0}(-k_0)e^{-i\Sigma_{j=0}^{2n}k_j^2t}$$

which we rewrite as

$$\frac{1}{2^{2n+1}}\sum_{\sigma_0,\ldots,\sigma_{2n}=\pm}B_{\alpha_1}^{\sigma_1}(k_1)\cdots B_{\alpha_{2n-1}}^{\sigma_{2n-1}}(k_{2n-1})B_{\alpha_{2n}}^{\sigma_{2n}}(-k_{2n})\cdots B_{\alpha_0}^{\sigma_0}(-k_0)\prod_{j=1}^{2n}(\sigma_{j-1}k_{j-1}-\sigma_jk_j)$$
$$\times\frac{\overline{\beta}_{\alpha_1}(k_1)\cdots\overline{\beta}_{\alpha_{2n-1}}(k_{2n-1})\beta_{\alpha_{2n}}(-k_{2n})\cdots\beta_{\alpha_0}(-k_0)}{\prod_{j=1}^{2n}(k_{j-1}^{2n}-k_j^2)}e^{-i\Sigma_{j=0}^{2n}k_j^2t}.$$

Let us concentrate on the part depending on the σ's. Developing explicitly the sum over σ_{2n}, one gets

$$\frac{1}{2^{2n+1}}\sum_{\sigma_0,\ldots,\sigma_{2n-1}=\pm}B_{\alpha_1}^{\sigma_1}(k_1)\cdots B_{\alpha_{2n-1}}^{\sigma_{2n-1}}(k_{2n-1})B_{\alpha_{2n-2}}^{\sigma_{2n-2}}(-k_{2n-2})\cdots B_{\alpha_0}^{\sigma_0}(-k_0)\prod_{j=1}^{2n-1}(\sigma_{j-1}k_{j-1}-\sigma_jk_j)$$
$$\times\left(\delta_{\alpha_{2n},+}\frac{2k_{2n}}{k_{2n}+i\eta}-\delta_{\alpha_{2n},-}2k_{2n}\right)$$

Collecting all the pieces depending on k_{2n}, one gets a function proportional to

$$\frac{k_{2n}}{k_{2n-2}^2-k_{2n}^2}\left(\frac{\beta_+(-k_{2n})}{k_{2n}+i\eta}-\beta_-(-k_{2n})\right). \tag{A7}$$

Now taking μ_+,μ_- as in (2.20) it is not hard to see that the function in parentheses in (A7) is identically zero, implying the vanishing of (A5).

The case of the jump condition is treated in complete analogy. Indeed, in evaluating the term proportional to η in (A2) in terms of $\beta_\pm$, all one must do is to replace $(1-\Pi_{i=0}^{2n}\alpha_i)$ in (A5) by $(1+\Pi_{i=0}^{2n}\alpha_i)$. The rest of the argument implies therefore that

$$\Phi^{(n)}(0,0)=0, \quad n\geqslant 1. \tag{A8}$$

As for the term involving derivatives of the field, an analogous treatment produces the following integrand:

$$\frac{1}{2^{2n+1}}\sum_{\sigma_0,\ldots,\sigma_{2n}=\pm} B^{\sigma_1}_{\alpha_1}(k_1)\cdots B^{\sigma_{2n-1}}_{\alpha_{2n-1}}(k_{2n-1})B^{\sigma_{2n}}_{\alpha_{2n}}(-k_{2n})\cdots B^{\sigma_0}_{\alpha_0}(-k_0)\prod_{j=1}^{2n}(\sigma_{j-1}k_{j-1}-\sigma_j k_j)$$
$$\times\left(\sum_{j=0}^{2n} i\sigma_j k_j\right)\frac{\overline{\beta}_{\alpha_1}(k_1)\cdots\overline{\beta}_{\alpha_{2n-1}}(k_{2n-1})\beta_{\alpha_{2n}}(-k_{2n})\cdots\beta_{\alpha_0}(-k_0)}{\prod_{j=1}^{2n}(k_{j-1}^2-k_j^2)}e^{-i\Sigma_{j=0}^{2n}k_j^2 t}.$$

This time, one must develop the sum for σ_{2n} and σ_{2n-1}. This produces the function (A7) but in the variable k_{2n-1} and we know it vanishes. This leads to

$$\lim_{x\to 0^+}\{(\partial_x\Phi_+^{(n)})(0,x)-(\partial_x\Phi_-^{(n)})(0,-x)\}=0, \quad n\geqslant 1. \tag{A9}$$

As already mentioned, we see that the continuity and the jump condition of the field hold for any time t. Put another way, they are conserved in time and this is due to the dispersion relation of the free Schrödinger equation (being quadratic in k_j, it is not affected by all the symmetrizations $k_j\to -k_j$ involved in the proof).

It is remarkable that the jump condition actually decouples for the nonlinear terms ($n\geqslant 1$) as seen from (A8) and (A9). This is also true for the continuity which, combined with (A8) shows that

$$\Phi_-^{(n)}(0,0)=\Phi_+^{(n)}(0,0)=0, \quad n\geqslant 1.$$

■

APPENDIX B: EXPLICIT FORM OF THE ACTION OF THE CREATION OPERATOR

The projector $P^{(n)}$ is constructed in Ref. 7 in terms of the generators of the Weyl group associated to the root system of the classical Lie algebra B_n and of their representation on $\mathcal{L}^{\otimes n}$. In our context, we get for $f\in\mathcal{C}$ and $\varphi^{(n-1)}\in\mathcal{H}^{(n-1)}$,

$$[a^\dagger(f)\varphi]^{(n)}_{\alpha_1\cdots\alpha_n}(p_1,\ldots,p_n)=\frac{1}{2\sqrt{n}}\sum_{k=1}^{n}S(\alpha_{k-1}p_{k-1}-\alpha_k p_k)\cdots S(\alpha_1 p_1-\alpha_k p_k)(f_{\alpha_k}(p_k)$$
$$+C_k(\alpha_1 p_1,\ldots,\alpha_n p_n)[T(\alpha_k p_k)f_{-\alpha_k}(p_k)+R(\alpha_k p_k)f_{\alpha_k}(-p_k)])$$
$$\times\varphi^{(n-1)}_{\alpha_1\cdots\hat{\alpha_k}\cdots\alpha_n}(p_1,\ldots,p_n), \tag{B1}$$

where we have defined

$$C_k(p_1,\ldots,p_n)=S(p_k-p_1)\cdots S(\widehat{p_k-p_k})\cdots S(p_k-p_n)S(p_n+p_k)\cdots S(\widehat{p_k+p_k})\cdots S(p_1+p_k).$$

All the hatted symbols must be omitted.

One recognizes the reflected and transmitted structure inside the square brackets of (B1) which, combined with all the S matrices, ensures the properties (3.21) and (3.22) required for the functions of $\mathcal{H}^{(n)}$.

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On the local and nonlocal Camassa–Holm hierarchies

Paolo Casati,[a] Paolo Lorenzoni,[b] and Giovanni Ortenzi[c]
Dipartimento di Matematica e Applicazioni, II, Università di Milano Bicocca-Ed. U5, via R. Cozzi 53, I-20125 Milano, Italy

Marco Pedroni[d]
Dipartimento di Ingegneria Gestionale e dell'Informazione, Università di Bergamo, Viale Marconi 5, I-24044 Dalmine (BG), Italy

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We construct the local and nonlocal conserved densities for the Camassa–Holm equation by solving a suitable Riccati equation. We also define a Kadomtsev–Petviashvili extension for the local Camassa–Holm hierarchy. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1888568]

I. INTRODUCTION

Since its introduction in Ref. 1 as a model for shallow water waves, the Camassa–Holm equation

$$u_t - u_{xxt} = 6u_x u - 4u_{xx}u - 2uu_{xxx} \tag{1}$$

has been the subject of a great number of papers. In particular, some of them (Refs. 4,7, and 9, just to cite a few) have been devoted to investigate its bi-Hamiltonian structure and its relation with other nonlinear partial differential equations living on the same phase space, namely the Korteweg–de Vries (KdV) equation, the Hunter–Saxton equation,[3] and the Harry–Dym (HD) equation.[5] It is well known how to use the bi-Hamiltonian structure of the KdV equation to construct the whole corresponding hierarchy (see, e.g., Ref. 8). This structure has been used in Ref. 2 to relate in a geometrical way the KdV hierarchy with the celebrated Kadomtsev–Petviashvili (KP) hierarchy. [In this paper by "KP hierarchy" we mean the Sato form, in terms of pseudodifferential operators, of the KP hierarchy. This is a hierarchy of $(1+1)$ evolution equations for infinitely many fields.] The same results have been found in Ref. 11 for the HD equation, recovering in this way the KP extension of the Harry–Dym hierarchy presented in Ref. 10.

The aim of this paper is to develop an analogous theory for the CH equation as well. More precisely, we show how the bi-Hamiltonian approach to the CH allows us to write a Riccati equation whose solutions give rise to the conserved densities of the CH equation. As it is well known, there are two hierarchies of such conserved quantities. The first one contains the Camassa–Holm equation, and its Hamiltonian densities are nonlocal, while the other one is formed by local densities. (To the best of our knowledge, and according to Ref. 6, there is no sound proof of the existence of an infinite number of members of the nonlocal hierarchy. In this paper we give such a proof.) Moreover we show that the local CH hierarchy can be embedded in a wider hierarchy in an infinite number of fields, exactly like the KdV equation can be included in the KP hierarchy.

The paper is organized as follows. In the next section we use the bi-Hamiltonian method to find a Riccati equation that allows us to construct the two above-mentioned hierarchies of con-

[a]Electronic mail: paolo.casati@unimib.it
[b]Electronic mail: paolo.lorenzoni@unimib.it
[c]Electronic mail: giovanni.ortenzi@unimib.it
[d]Electronic mail: marco.pedroni@unibg.it

served quantities. In the third and last section we show—using the technique of the Faà di Bruno polynomials—how the local CH hierarchy can be framed in a more general hierarchy which plays the same role that the KP hierarchy does in the KdV case.

II. THE CONSERVED DENSITIES

It is well known that the CH equation (1) is a bi-Hamiltonian system on the infinite dimensional space $C^\infty(S^1,\mathbb{R})$ of C^∞ functions from the circle to the real line, with respect to the Poisson tensors,

$$P_0 = \tfrac{1}{2}\partial_x - \tfrac{1}{2}\partial_x^3, \quad P_1 = -(m\partial_x + \partial_x m),$$

where m is defined by $m=(1-\partial_x^2)u$. In this section we construct the positive and negative CH hierarchies using the so-called method of the Casimir of the Poisson pencil. This means that we look for Casimirs of the Poisson pencil $P_\lambda = P_0 - \lambda P_1$, i.e., for functionals $H(\lambda)$ whose differentials $v(\lambda)$ belong to the kernel of P_λ. The coefficients of the Laurent expansion of any such Casimir $H(\lambda)=\Sigma_{k=-\infty}^{+\infty} H_k \lambda^{-k}$ provide indeed a set of functionals satisfying the Lenard–Magri recursion relation

$$P_0\, \mathrm{d}H_k = P_1\, \mathrm{d}H_{k+1}$$

and thus in involution with respect to both Poisson structures (see, e.g., Ref. 8).

The key point to determine $v(\lambda)$ is to notice that

$$vP_\lambda v = v\left(\tfrac{1}{2}v_x - \tfrac{1}{2}v_{xxx} + 2\lambda m v_x + \lambda m_x v\right) = \left(\tfrac{1}{4}v^2 - \tfrac{1}{2}v_{xx}v + \tfrac{1}{4}v_x^2 + \lambda m v^2\right)_x. \tag{2}$$

This result is a direct consequence of the fact that $\int vP_\lambda v$ is the antisymmetric action of the 2-tensor P_λ on the pair (v,v). The condition $P_\lambda v(\lambda)=0$ is thus equivalent to

$$\tfrac{1}{4}v^2 - \tfrac{1}{2}v_{xx}v + \tfrac{1}{4}v_x^2 + \lambda m v^2 = f(m,\lambda), \tag{3}$$

where $f(m,\lambda)$ satisfies $f_x=0$. It turns out that v is an exact 1-form if f does not depend on m. Without loss of generality, we can set $f(\lambda)=\lambda/4$. Then Eq. (3) can be set in the useful Riccati form

$$h_x + h^2 = \tfrac{1}{4} + z^2 m \tag{4}$$

through the transformation

$$-v_x + 2vh = z, \tag{5}$$

where $z^2=\lambda$. Let us verify that $v(\lambda)$ is an exact 1-form:

$$\langle v, \dot{m}\rangle \overset{(4)}{=} \int_{S^1} v z^{-2}(\dot{h}_x + 2h\dot{h})\mathrm{d}x \overset{(5)}{=} \frac{1}{z^2}\int_{S^1}(-v_x + 2vh)\dot{h}\,\mathrm{d}x = \frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}t}\int_{S^1} h\,\mathrm{d}x, \tag{6}$$

so that the potential of $v(\lambda)$ is given by $H=z^{-1}\int_{S^1} h\,\mathrm{d}x$. In the next two sections we will solve the Riccati equation (4) using a formal development for the function h. We will find a first solution of the form $h(z)=\Sigma_{i=-1}^{\infty} h_i z^{-i}$, where the h_i are functions of m and its x derivatives. This solution gives rise to the local (often called also negative) CH hierarchy, starting from a Casimir of P_1. The second solution has the form $k(z)=\Sigma_{i=0}^{\infty} k_i z^{-i}$, where the k_i are now nonlocal densities. They constitutes the usual (nonlocal, positive) CH hierarchy, which the CH equation belongs to. In other words, we will deal with two possible different choices of the essential singularity of the solutions of the Riccati equation (4).

A. The local CH hierarchy

In this case the Laurent expansion of the density of Hamiltonians is

$$h(z) = h_{-1}z + h_0 + \frac{h_1}{z} + \frac{h_2}{z^2} + \cdots = h_{-1}z + h_0 + \sum_{i=1}^{\infty} \frac{h_i}{z^i}, \tag{7}$$

where the maximum degree of the positive term is established by (4).

If we substitute this expansion in (4) we get

$$\sum_{i=-2}^{\infty} \left(\left(h_{i_x} + \sum_{j=-1}^{i+1} h_{i-j}h_j \right) \frac{1}{z^i} \right) = \frac{1}{4} + z^2 m. \tag{8}$$

Then the obtained system can be solved in a purely algebraic way by equating the terms with the same degree in z,

$$z^2, \quad h_{-1}^2 = m, \quad h_{-1} = \sqrt{m},$$

$$z^1, \quad h_{-1x} + 2h_0h_{-1} = 0, \quad h_0 = (\ln(m^{-1/4}))_x,$$

$$z^0, \quad h_{0x} + h_0^2 + 2h_1h_{-1} = \tfrac{1}{4}, \quad h_1 = \frac{1}{8\sqrt{m}} - \frac{1}{8}\frac{m_{xx}}{\sqrt{m^3}} + \frac{5}{32}\frac{m_x^2}{\sqrt{m^5}},$$

$$z^{-1}, \quad h_{1x} + 2h_0h_1 + 2h_2h_{-1} = 0, \quad h_2 = \left(-\frac{1}{16m} + \frac{1}{16}\frac{m_{xx}}{m^2} + \frac{5}{64}\frac{m_x^2}{m^3} \right)_x,$$

and so on. It can be shown that the even densities are x derivatives, so that $H = z^{-1}\int_{S^1} h\, \mathrm{d}x$ is actually a Laurent series in λ:

$$H(\lambda) = \sum_{i=0}^{+\infty} H_{2i}\lambda^{-i}.$$

If j is even, we call X_j the Hamiltonian vector field associated with $H_j = \int_{S^1} h_{j-1}\, \mathrm{d}x$ by means of the Poisson operator P_0. By construction, X_j is the Hamiltonian vector field associated with H_{j+2} by means of P_1. The first nontrivial equation of the hierarchy, corresponding to X_0, is

$$\frac{\partial m}{\partial t_0} = P_0\, \mathrm{d}H_0 = (\partial_x - \partial_x^3)\frac{1}{4\sqrt{m}} = -\frac{1}{8}\frac{m_x}{\sqrt{m^3}} - \frac{1}{8}\frac{m_{xxx}}{\sqrt{m^3}} + \frac{9}{16}\frac{m_{xx}m_x}{\sqrt{m^5}} - \frac{15}{32}\frac{m_x^3}{\sqrt{m^7}} = P_1\, \mathrm{d}H_2. \tag{9}$$

B. The nonlocal CH hierarchy

In this case the Laurent expansion of the solution $k(z)$ of the Riccati equations (4) is

$$k(z) = k_0 + k_{-1}z + k_{-2}z^2 + k_{-3}z^3 + \cdots = \sum_{i=0}^{+\infty} k_{-i}z^i. \tag{10}$$

Substituting it in (4), we obtain

$$\sum_{i=0}^{\infty} \left(\left(k_{-i_x} + \sum_{j=0}^{i} k_{-j}k_{j-1} \right) z^i \right) = \frac{1}{4} + z^2 m. \tag{11}$$

Exactly as before, we can find a recursive solution of (11) comparing the terms of the same degree on both sides of the equation. However, in the present case this requires to solve at any step a differential equation. This fact is responsible for the presence of nonlocal quantities. The first equation to be considered is that related to the coefficient of z^0,

$$k_{0x} + k_0^2 = \tfrac{1}{4}.$$

It is easily checked that the only periodic solutions of this equation are the constant solutions $k_0 = \pm\frac{1}{2}$. Let us choose the positive constant solution. Next, the coefficient of z^1 gives

$$k_{-1x} + 2k_0 k_{-1} = 0$$

or, using $k_0 = \frac{1}{2}$,

$$(1 + \partial_x)k_{-1} = 0.$$

This linear equation is solved by $k_{-1} = c\exp(-x)$, where c is a constant. But again among them the only solution which lies in $C^\infty(S^1, \mathbb{R})$ is the trivial one, $k_{-1} = 0$. More generally, the operator $1 + \partial_x$ is invertible in $C^\infty(S^1, \mathbb{R})$. The unique solution of

$$(1 + \partial_x)k = f(x)$$

of period 1 is indeed explicitly given by

$$k(x) = \int_0^x e^{y-x} f(y)\mathrm{d}y + \frac{1}{e-1}\int_0^1 e^{y-x} f(y)\mathrm{d}y.$$

From $k_{-1} = 0$ one can immediately show that $k_{-2n-1} = 0$ for all $n \geqslant 0$. In fact, k_{-2n-1} appears for the first time in the coefficient of z^{n+1},

$$k_{-2n-1_x} + k_{-2n-1} + 2\sum_{i=1}^{n} k_{-2i}k_{-2(n-i)-1} = 0,$$

and this allows us to prove by recursion that all the odd terms in the Laurent series $k(z)$ are zero. Using the remaining equations,

$$z^2, \quad k_{-2x} + 2k_0 k_{-2} + k_{-1}^2 = m,$$

$$z^4, \quad k_{-4x} + 2k_0 k_{-4} + 2k_{-1}k_{-3} + k_{-2}^2 = 0,$$

$$z^6, \quad k_{-6x} + 2k_0 k_{-6} + 2k_{-1}k_{-5} + k_{-3}^2 + 2k_{-2}k_{-4} = 0,$$

$$\cdots, \quad \cdots,$$

it is now simple to find the even terms,

$$k_{-2} = (1 + \partial_x)^{-1} m,$$

$$k_{-4} = -(1 + \partial_x)^{-1}((1 + \partial_x)^{-1} m)^2,$$

$$k_{-6} = 2(1 + \partial_x)^{-1}((1 + \partial_x)^{-1} \cdot ((1 + \partial_x)^{-1} m)^2 (1 + \partial_x)^{-1} m)$$

$$\cdots = \cdots.$$

Thanks to the invertibility of the operator $1 + \partial_x$ in the space of C^∞ periodic functions, we can conclude that there is an infinite sequence of (increasingly nonlocal) densities k_{-2i}, giving rise to a set of functionals in involution with respect to both Poisson brackets. More precisely, let $K(\lambda) = \int_{S^1} k\, ax$ be the Casimir of the Poisson pencil constructed with k. Then $K(\lambda) = \frac{1}{4} + \sum_{j=1}^{\infty} K_{-2j}\lambda^j$, with $K_{-2j} = \int_{S^1} k_{-2j}\, \mathrm{d}x$. We call X_j the Hamiltonian vector field associated with K_j by means of the

Poisson operator P_1. By construction, X_j is the Hamiltonian vector field associated with K_{j-2} by means of P_0.

Since $k_{-2x}+k_{-2}=m$, we have that $K_{-2}=\int_{S^1}k_{-2}\,dx=\int_{S^1}m\,dx$, so that the first equation of the hierarchy is $m_{t_{-2}}=P_1\,dK_{-2}=-m_x$. In order to write the second vector field, we recall that $k_{-4x}+k_{-4}+k_{-2}^2=0$ and therefore

$$K_{-4}=\int_{S^1}k_{-4}\,dx=-\int_{S^1}k_{-2}^2\,dx=-\int_{S^1}((1+\partial_x)^{-1}m)^2\,dx.$$

This functional becomes local after the usual change of variables $m=u-u_{xx}$, that is invertible in the space of C^∞ periodic functions because it is the composition of $1+\partial_x$ and $1-\partial_x$. Its inverse is explicitly given by

$$u(x)=\int_0^x m(y)\sinh(y-x)dy+\frac{1}{2\sinh\frac{1}{2}}\int_0^1 m(y)\cosh\left(y-x-\frac{1}{2}\right)dy.$$

In terms of u we have that $K_{-4}=-\int_{S^1}(u^2+u_x^2)dx$, so that

$$\frac{\partial m}{\partial t_{-4}}=P_1\,dK_{-4}=-(m\partial_x+\partial_x m)(1-\partial_x^2)^{-1}(-2u+2u_{xx})=4mu_x+2m_xu, \tag{12}$$

that is, with $t_{-4}=t$,

$$u_t-u_{xxt}=6u_xu-4u_{xx}u_x-2uu_{xxx}, \tag{13}$$

which is the standard Camassa–Holm equation with null critical velocity term. The next symmetry of the hierarchy is related to the Hamiltonian $K_{-6}=\int_{S^1}k_{-6}=2\int_{S^1}(u^3+uu_x^2)dx$, which, using (5) to compute dK_{-6}, gives

$$\frac{\partial m}{\partial t_{-6}}=P_1\,dK_{-6}=-(m\partial_x+\partial_x m)(1-\partial_x^2)^{-1}(6u^2-2u_x^2-4uu_{xx}).$$

We remark that, due to the Lenard–Magri recursion relations, the equation (13) can be obtained also as $\partial m/\partial t_{-4}=P_0\,dK_{-6}$.

III. KP EXTENSION OF THE LOCAL CH HIERARCHY

In Ref. 2 it has been shown how to generate, from a bi-Hamiltonian viewpoint, the KP hierarchy starting from the KdV hierarchy. The same procedure has been performed in Ref. 11, where the KP extension of the Harry–Dym hierarchy (already found in Ref. 10) has been recovered. The idea is quite simple and can be successfully applied to the local CH hierarchy, as we do in this section.

In Sec. II A we have found a map $m\mapsto h(m)$, where $h(m)$ is the unique solution of the Riccati equation (4) with the asymptotic expansion (7). Since the coefficients of $h(m)$ are the densities of the Hamiltonians of the hierarchy, the time derivatives of $h(m)$ must be an x derivative, that is,

$$\frac{\partial h}{\partial t_s}=\partial_x H^{(s)},\quad s=0,2,\ldots,$$

for suitable currents $H^{(s)}$. They can be explicitly constructed after noticing that the vector fields of the hierarchy are not only bi-Hamiltonian, but they are Hamiltonian with respect to every Poisson structure of the pencil. Indeed, one can immediately see that

$$\frac{\partial h}{\partial t_{2s}} = P_\lambda(\lambda^s \, \mathrm{d}H(\lambda))_{\mathrm{reg}} = P_\lambda\left(\sum_{r=0}^{s} \mathrm{d}H_{2r}\lambda^{s-r}\right), \tag{14}$$

where "reg" stands for the regular part in the Laurent expansion. Moreover, using (4) the Poisson pencil P_λ can be factorized in the following way:

$$P_\lambda = -\tfrac{1}{2}(\partial_x + 2h)\partial_x(\partial_x - 2h).$$

Substituting it in the derivative with respect to t_{2s} of (4), we obtain

$$\lambda^{-1}(\partial_x + 2h)h_{t_{2s}} = -\tfrac{1}{2}(\partial_x + 2h)\partial_x(\partial_x - 2h)(\lambda^s \, \mathrm{d}H(\lambda))_{\mathrm{reg}}.$$

From the previous equation, due to the particular form of the z development of h, it follows that the continuity equation

$$\frac{\partial h}{\partial t_{2s}} = \partial_x\left(-\frac{\lambda}{2}(\partial_x - 2h)(\lambda^s \, \mathrm{d}H(\lambda))_{\mathrm{reg}}\right) \tag{15}$$

holds true. Therefore, the currents $H^{(2s)}$ we are looking for are given by

$$H^{(2s)} = -\frac{\lambda}{2}(\partial_x - 2h)(\lambda^s \, \mathrm{d}H(\lambda))_{\mathrm{reg}} = -\frac{\lambda}{2}(\lambda^s v(\lambda)_x)_{\mathrm{reg}} + h\lambda(\lambda^s v(\lambda))_{\mathrm{reg}}. \tag{16}$$

The next step is to realize that the currents $H^{(s)}$, where s is even, can be obtained directly from a Laurent series h of the form (7), without using the Riccati equation (4). We start with the preliminary consideration that they can be written in two equivalent ways,

$$H^{(s)} = \sum_{i=0}^{s}\left(-\frac{1}{2}v_{i,x}(z^{s-i+2}) + v_i(z^{s-i+2}h)\right) \tag{17}$$

and

$$\begin{aligned} H^{(s)} &= -\frac{1}{2}(\partial_x - 2h)(z^{s+2} \, \mathrm{d}H(z) - z^2(z^s \, \mathrm{d}H(z))_{\mathrm{sing}}) = \frac{1}{2}z^{s+2}(-v_x + 2hv) - \frac{z^2}{2}(\partial_x - 2h)(z^s v)_{\mathrm{sing}} \\ &\overset{(5)}{=} \frac{1}{2}z^{s+3} - \frac{z^2}{2}(\partial_x - 2h)(z^s v)_{\mathrm{sing}}, \end{aligned} \tag{18}$$

where with "sing" we mean the singular part of the expansion in z. Equation (18), using (4), gives the regular asymptotic behavior of the currents, that is, $(H^{(s)})_{\mathrm{reg}} = \frac{1}{2}z^{s+3} + O(z)$. On the other hand, Eq. (17) implies that the currents belong to a particular vector space H_h, which can be constructed using only the Hamiltonian density h. It is defined as the linear span over the functions $C^\infty(S^1, \mathbb{R})$ of the Faà di Bruno polynomials $h^{(n)} = (\partial_x + h)^n z^2$, with $n \geqslant 0$, $h^{(0)} = z^2$.

Proposition 3.1: The currents $H^{(2s)}$, with $s \geqslant 0$, are elements of H_h.

Proof: Thanks to the representation (17), it suffices to show that z^{2i} and $z^{2i}h$ are elements of H_h for all $i \geqslant 1$. First of all, $z^2 = h^{(0)} \in H_h$ and $z^2 h = h^{(1)} \in H_h$ by definition of H_h. Moreover, the Riccati equation multiplied by z^2,

$$z^2(h_x + h^2) = \frac{z^2}{4} + z^4 m, \tag{19}$$

shows that $z^4 = (1/m)\left(h^{(2)} - \frac{1}{4}h^{(0)}\right) \in H_h$. Now, acting with $(\partial_x + h)$ on both sides of (19), we can show that $z^4 h \in H_h$. More generally, acting with $(\partial_x + h)^n$, we prove that $z^2(H_h) \subset H_h$, and this concludes the proof. □

At this point it is not difficult to see that the current $H^{(s)}$ can be characterized in a unique way by the following properties:

(1) $H^{(s)}=\frac{1}{2}z^{s+3}+O(z)$,
(2) $H^{(s)}\in H_h$.

Therefore, we can assume that h is an arbitrary Laurent series of the form

$$h(z)=h_{-1}z+\sum_{i=0}^{+\infty}\frac{h_i}{z^i}, \tag{20}$$

where the coefficients h_i are not constrained by the Riccati equation, and we can define the currents $H^{(s)}$, for all $s\geqslant 0$, imposing the two above-mentioned properties. Then we define the s-th equation of the *local KP–CH hierarchy* as

$$\frac{\partial h}{\partial t_s}=\partial_x H^{(s)},\quad s\geqslant 0. \tag{21}$$

It is an evolution equation in an infinite number of fields given by the coefficients $h_{-1},h_0,h_1,\ldots$ of h.

In order to write these equations one must compute the first Faà di Bruno polynomials,

$$h^{(0)}=z^2,$$

$$h^{(1)}=h_{-1}z^3+h_0z^2+h_1z+\cdots,$$

$$h^{(2)}=(h_{-1}^2)z^4+(h_{-1x}+2h_{-1}h_0)z^3+(h_{0x}+h_0^2+2h_{-1}h_1)z^2+(h_{1x}+2h_{-1}h_2+2h_0h_1)z+\cdots,$$

$$h^{(3)}=\cdots.$$

Then the first currents are given by

$$H^{(0)}=\frac{1}{2h_{-1}}h^{(1)}-\frac{h_0}{2h_{-1}}h^{(0)}=\frac{1}{2}z^3+\frac{h_1}{2h_{-1}}z+\cdots,$$

$$\begin{aligned}H^{(1)}&=\frac{1}{2h_{-1}^2}h^{(2)}-\left(\frac{h_{-1x}}{2h_{-1}^3}+\frac{h_0}{h_{-1}^2}\right)h^{(1)}-\left(\frac{h_{0x}}{2h_{-1}^2}+\frac{h_0^2}{2h_{-1}^2}+\frac{h_1}{h_{-1}}-\frac{h_{-1x}h_0}{2h_{-1}^3}-\frac{h_{-1}h_0^2}{h_{-1}^3}\right)h^{(0)}\\&=\frac{1}{2}z^4+\left(\frac{h_{-1x}}{2h_{-1}^2}+\frac{h_2}{h_{-1}}+\frac{h_1h_0}{h_{-1}^2}-\frac{h_{-1x}h_1}{2h_{-1}^3}-\frac{h_0h_1}{h_{-1}^2}\right)z+\cdots,\end{aligned}$$

$$H^{(2)}=\cdots.$$

To recover the local CH hierarchy, one must impose on h the constraint given by the Riccati equation (4). It entails that all the fields h_i can be written in terms of m and its x derivatives. Thus the local KP–CH hierarchy (21) reduces to the local CH hierarchy. This reduction can be interpreted, like in the KdV and HD cases, as a stationary reduction. Indeed, the Riccati equation and the very definition of the currents imply that the current $H^{(1)}$ is equal to $z^4/2$ and therefore that t_1 is a stationary time. From Proposition 3.1 it also follows that all the odd times are stationary.

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Variable-separation theory for the null Hamilton–Jacobi equation

S. Benenti, C. Chanu, and G. Rastelli
Dipartimento di Matematica, Università di Torino, Via Carlo Alberto 10, 10123 Torino, Italy

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The theory of the separation of variables for the null Hamilton–Jacobi equation $\mathcal{H}=0$ is systematically revisited and based on Levi–Civita separability conditions with Lagrangian multipliers. The separation of the null equation is shown to be equivalent to the ordinary separation of the image of the original Hamiltonian under a generalized Jacobi–Maupertuis transformation. The general results are applied to the special but fundamental case of the orthogonal separation of a natural Hamiltonian with a fixed value of the energy. The separation is then related to conditions which extend those of Stäckel and Kalnins and Miller (for the null geodesic case) and it is characterized by the existence of conformal Killing two-tensors of special kind. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1862325]

I. INTRODUCTION

The aim of this paper is to propose a general approach to the theory of variable separation for the *null* Hamilton–Jacobi equation (HJE)

$$\mathcal{H}(\underline{q},\underline{p})=0, \quad \underline{q}=(q^i), \quad \underline{p}=(p_i), \quad p_i=\frac{\partial W}{\partial q^i}.$$

This approach is based on a suitable definition of separation (Sec. II), whose geometrical content (Sec. III) is related to special integrable Lagrangian distributions on the cotangent bundle T^*Q, of coordinates $(\underline{q},\underline{p})$. By the Hadamard lemma, the integrability conditions of these special distributions lead in Sec. IV to *Levi–Civita separability conditions with Lagrangian multipliers* (Theorem 4.1), which are a natural extension of the classical Levi–Civita conditions,[24] and from which we derive two characterizations of the separation of the null HJE. The first one (Theorem 4.2) asserts that the separation occurs in a given coordinate system if and only if the ordinary Levi–Civita equations are satisfied on the surface $\mathcal{H}=0$; the second one (Theorem 4.3) asserts that the separation occurs if and only if there exists a function $\Lambda(\underline{q},\underline{p})\neq 0$ such that the ordinary Levi–Civita equations are satisfied by the *conformal Hamiltonian* $\mathcal{H}/\Lambda$. The passage from a Hamiltonian $\mathcal{H}$ to a conformal Hamiltonian $\mathcal{H}/\Lambda$ is an extension of the so-called *Jacobi* (or *Maupertuis*) *transformation* for natural Hamiltonians,[9,16,23,28,31,33] recalled and discussed in Sec. VI.

We apply these general results to the analysis of particular cases of Hamiltonians. In Sec. V we consider the so-called *homogeneous formalism* in time-dependent mechanics and get a rigorous proof of a known property of the separation in the time-dependent HJE.[15] In Sec. VI we consider a natural Hamiltonian in orthogonal coordinates, $H=\frac{1}{2}g^{ii}p_i^2+V(\underline{q})$ and the corresponding HJE with a fixed value E of the energy,

$$\mathcal{H}(\underline{q},\underline{p}) \doteq \tfrac{1}{2}g^{ii}p_i^2+V(\underline{q})-E=0.$$

From a general theorem (Theorem 6.1) concerned with the separation of this equation, we derive three theorems (Theorems 6.3, 6.4, and 6.5) characterizing the separation for the following three special cases,

$$V=0, \quad E\neq 0, \quad \text{non-null geodesics},$$

$$V=0, \quad E=0, \quad \text{null geodesics},$$

$$V-E\neq 0, \quad \text{dynamical trajectories with total energy } E.$$

The case of null geodesics occurs, of course, for indefinite metric tensors. In Sec. VII we analyze the intrinsic framework of the theorems stated in Sec. VI, by considering special kinds of conformal Killing tensors and by introducing the notion of conformal involution. The first integrals and the separated equations are examined in Sec. VIII. In Sec. IX we consider the two-dimensional case. We renounce here to deal with the nonorthogonal separation for natural Hamiltonians, which is currently under investigation within the general framework presented in this paper. All this work is also made in the perspective of application to the theory of the ordinary multiplicative separation and of the *R*-separation for the second-order differential equations of mathematical physics (Laplace, Helmholtz, Poisson, Schrödinger equations).[20,22] As possible applications of the present theory we mention: (i) The integration of the equations of the null geodesics in general relativity theory,[11] (ii) The integration of dynamical systems which are Hamiltonian only on single hypersurfaces of the phase space.

II. DEFINITION OF SEPARATED COMPLETE SOLUTION OF THE NULL HJE

Let Q be a real n-dimensional differentiable manifold and $\mathcal{H}$ be a smooth real-valued function on the cotangent bundle T^*Q. Let $\underline{q}=(q^i)$ be local coordinates on an open subset $U\subseteq Q$ and $(\underline{q},\underline{p})=(q^i,p_i)$ the corresponding standard canonical coordinates on T^*Q. In the following, ∂_i and ∂^i will denote the partial derivative with respect to q^i and p_i, respectively.

We restrict our analysis to the open set $\mathcal{O}\subseteq T^*U\subseteq T^*Q$, where $\partial^i\mathcal{H}\neq 0$ for all $i=1,\ldots,n$, assuming that it is not empty. In this open set we have $\mathrm{d}\mathcal{H}\neq 0$, so that any equation of the kind $\mathcal{H}(\underline{q},\underline{p})=h$, $h\in\mathbb{R}$, defines a set $\mathcal{E}_h$ that, if not empty, is a submanifold of codimension 1. In particular, we focus on the submanifold $\mathcal{E}_0$ described by equation $\mathcal{H}=0$.

We consider the HJE for $h=0$,

$$\mathcal{H}\left(\underline{q},\frac{\partial W}{\partial \underline{q}}\right)=0, \tag{2.1}$$

and two definitions of complete solution.

Definition 2.1: An *internal complete solution* of the HJE (2.1) is a solution $W^I(\underline{q},c_\alpha)$ depending on $n-1$ parameters (c_α) such that the following completeness condition is satisfied:

$$\operatorname{rank}\left[\frac{\partial^2 W^I}{\partial q^i\,\partial c_\alpha}\right]=n-1. \tag{2.2}$$

An *extended complete solution* of the HJE (2.1) is a function $W^E(\underline{q},\underline{c})$ depending on n real parameters $\underline{c}=(c_i)$ satisfying the completeness condition

$$\det\left[\frac{\partial^2 W^E}{\partial q^i\,\partial c_j}\right]\neq 0 \tag{2.3}$$

for all admissible values of $(\underline{q},\underline{c})$, and satisfying Eq. (2.1) for all $\underline{c}$ belonging to a suitable $n-1$-dimensional submanifold of $\mathbb{R}^n$ (see Remark 2.1 below) or (up to a transformation of $\underline{c}$) for $c_n=0$.

The geometrical meaning of these two definitions is the following. An internal complete solution W^I defines a Lagrangian foliation $\mathcal{L}^I$ of the submanifold $\mathcal{E}_0$, Fig. 1(a), via equations $p_i=\partial_i W^I$. Each Lagrangian submanifold $L_{(c_\alpha)}\in\mathcal{L}^I$ is parametrized by the value of the $n-1$ parameters (c_α).

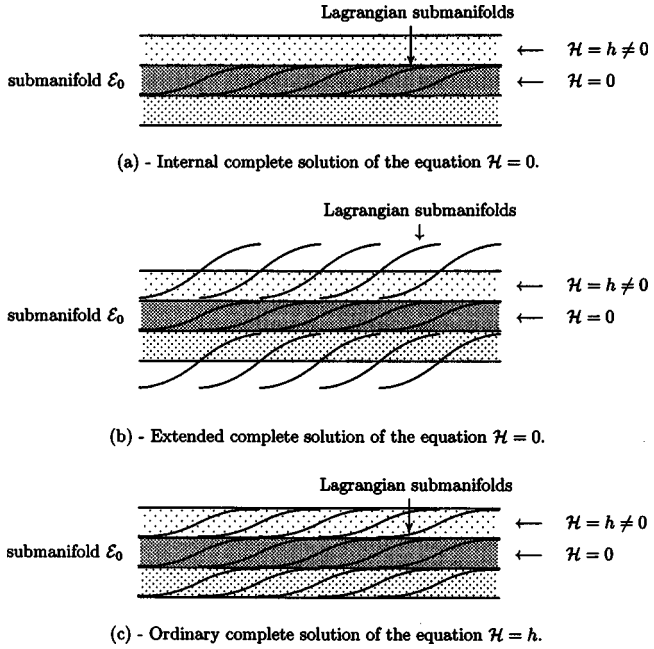

FIG. 1. The geometry of the three definitions of complete solution.

An extended complete solution W^E defines a Lagrangian foliation $\mathcal{L}^E$ on an open neighborhood of T^*Q via equations $p_i = \partial_i W^E$. Each Lagrangian submanifold $L_{(c_i)} \in \mathcal{L}^E$ is parametrized by the value of the n parameters $\underline{c} = (c_i)$. This foliation is compatible with the submanifold $\mathcal{E}_0$, in the sense that it is reducible to a foliation of $\mathcal{E}_0$, Fig. 1(b).

Remark 2.1: The quotient set $\mathcal{C}$ of the foliation $\mathcal{L}^E$ is locally a n-dimensional manifold with coordinates (c_i). The restriction $\mathcal{L}^I$ of $\mathcal{L}^E$ to $\mathcal{E}_0$ is a submanifold $\mathcal{S} \subset \mathcal{C}$ of dimension $n-1$. Then $\mathcal{S}$ is locally defined by an equation $h(c_i) = 0$ with $\mathrm{d}h \,|\, \mathcal{S} \neq 0$. Up to a transformation $(c_i) \leftrightarrow (c_i')$ we can find coordinates adapted to $\mathcal{S}$ such that equation $h(c_i) = 0$ is replaced by $c_n' = 0$. This means that for a suitable choice of the parameters appearing in a W^E equation (2.1) is satisfied for $c_n = 0$.

Remark 2.2: In general, the foliation generated by a W^E may be not reducible to the submanifolds $\mathcal{E}_h$ with $h \neq 0$. When it is reducible to each $\mathcal{E}_h$, then we have an *ordinary complete solution*, Fig. 1(c), of the HJE

$$\mathcal{H}\left(\underline{q}, \frac{\partial W}{\partial \underline{q}}\right) = h. \tag{2.4}$$

The following proposition shows that the two definitions of internal and extended complete solutions are, in a sense, equivalent.

Proposition 2.1: Equation (2.1) *admits an internal complete solution* W^I *if and only if it admits an extended complete solution* W^E.

Proof: Let W^I be an internal complete solution. By the completeness condition (2.2), we know that there exist $n-1$ linearly independent columns in the matrix $\partial^2 W^I / \partial q^i \partial c_\alpha$. Thus, we can assume without loss of generality that

$$\det\left[\frac{\partial^2 W^I}{\partial q^\beta \partial c_\alpha}\right] \neq 0, \quad \alpha, \beta = 1, \ldots, n-1.$$

Then, the function

$$W^E(\underline{q},\underline{c}) = W^I(\underline{q},c_\alpha) + c_n q^n, \quad \underline{c} = (c_i) = (c_\alpha, c_n) \tag{2.5}$$

is an extended complete solution: the completeness condition (2.3) is satisfied. Conversely, if W^E is an extended complete solution, then the function $W^I = W^E|_{c_n=0}$ is an internal complete solution. ■

Now we adapt the above-given definitions to a particular class of complete solutions:

Definition 2.2: An *internal separated solution* of the HJE (2.1) is an internal complete solution $W^I(\underline{q},c_\alpha)$ of the form

$$W^I(\underline{q},c_\alpha) = \sum_{i=1}^{n} W_i^I(q^i,c_\alpha). \tag{2.6}$$

An *extended separated solution* of the HJE (2.1) is an extended complete solution $W^E(\underline{q},\underline{c})$ of the form

$$W^E(\underline{q},\underline{c}) = \sum_{i=1}^{n} W_i^E(q^i,\underline{c}). \tag{2.7}$$

It is obvious that the additive separation is preserved in the passage from a W^E to a W^I. However, it is remarkable that it is also preserved in the inverse passage, from a W^I to a W^E, due to the particular form of formula (2.5). Hence, from Proposition 2.1 it follows that

Proposition 2.2: Equation (2.1) *admits an internal separated solution* W^I *in a coordinate system* $\underline{q}=(q^i)$ *if and only if it admits an extended separated solution* W^E *in the same coordinates.*

The equivalence proved in Proposition 2.2 leads to the following definition of separability for $\mathcal{H}=0$:

Definition 2.3: The null HJE (2.1) is *separable* in the coordinates $\underline{q}=(q^i)$ if it admits an internal separated solution or, equivalently, if it admits an extended separated solution.

Remark 2.3: The definition of *internal separated solution* given here, i.e., depending on $n-1$ constant parameters satisfying the completeness condition (2.2), is that commonly adopted in the literature. See, e.g., Ref. 17, p. 107. However, the use of a second, although equivalent, definition of separation (Proposition 2.2) is essential for a complete development of the present theory. Indeed, as will be shown in Sec. IV, the definition of *extended separated solution* allows the characterization of the separability for the null HJE (2.1) by means of Lagrangian multipliers.

III. SPECIAL DISTRIBUTIONS RELATED TO THE SEPARATION

In order to give necessary and sufficient conditions for the existence of separated solutions it is convenient to give a geometrical interpretation of the separation in terms of complete integrability of a special kind of first-order differential systems. This interpretation is related to the concept of separated connection on a cotangent bundle.[5]

With a coordinate system $\underline{q}=(q^i)$ on Q we associate n differential operators on functions on T^*Q of the kind

$$D_i = \partial_i + R_i(\underline{q},\underline{p})\partial^i, \tag{3.1}$$

where R_i are assigned functions on T^*Q. The vector fields D_i on T^*Q are pointwise independent and transversal to the fibers. Thus, they span a regular distribution $\Delta \subset TT^*U$ of rank n transversal to the fibers: this means that at each point $x \in T^*U$ they span an n-dimensional subspace $\Delta_x \subset T_x(T^*U)$ which is transversal to the vertical vectors of TT^*U. We say that the vector fields D_i are the generators of Δ.

With the same functions R_i entering (3.1) we associate the first-order normal differential system

$$\partial_i p_j = \delta_{ij} R_i(\underline{q},\underline{p}) \tag{3.2}$$

and we remark as follows,

(i) Any integral manifold L of Δ, i.e., a submanifold $L \subset T^*U$ such that $T_x L = \Delta_x$ for all $x \in L$, is locally described by equations

$$p_i = \varphi_i(\underline{q}), \tag{3.3}$$

where the functions φ_i are solutions of system (3.2). Indeed, since Δ is transversal to the fibers, any integral manifold L of Δ is an n-dimensional submanifold transversal to the fibers, thus locally described by equations of the kind (3.3). Moreover, by definition of integral manifold, the generators D_i are tangent to L, so that equations $D_j(p_i - \varphi_i(\underline{q})) = 0$ are satisfied on L. This implies $0 = D_j(p_i - \varphi_i(\underline{q})) = (\partial_j + R_j\partial^j)(p_i - \varphi_i(\underline{q})) = -\partial_j\varphi_i + R_j\delta_{ij}$. This shows that the functions (3.3) satisfy the differential system (3.2).

(ii) Any integral manifold L is a Lagrangian submanifold, since the distribution Δ spanned by D_i is Lagrangian with respect to the canonical symplectic form $\omega = \mathrm{d}p_k \wedge \mathrm{d}q^k$. Indeed, we have

$$\omega(D_i,D_j) = (\mathrm{d}p_k \wedge \mathrm{d}q^k)(D_i,D_j) = \langle D_i, \mathrm{d}p_k\rangle\langle D_j, \mathrm{d}q^k\rangle - \langle D_j, \mathrm{d}p_k\rangle\langle D_i, \mathrm{d}q^k\rangle = R_i\delta_j^i - R_j\delta_i^j = 0.$$

This shows that Δ is an isotropic distribution. Being of rank n, it is a Lagrangian distribution.

(iii) Any Lagrangian submanifold L transversal to the fibers of T^*Q admits local generating functions, i.e., functions $W(\underline{q})$ such that L is described by equations $p_i = \partial_i W$. If L is an integral manifold of the distribution Δ, then $p_i = \partial_i W$ must be a solution of system (3.2). It follows that for $i \neq j$, $\partial_i\partial_j W = 0$, i.e.,

$$W(\underline{q}) = \sum_{i=1}^{n} W_i(q^i). \tag{3.4}$$

(iv) The Lie brackets of the generators D_i are vertical vectors, i.e., vectors tangent to the fibers of T^*Q. Indeed,

$$\begin{aligned}[D_i,D_j] &= [\partial_i + R_i\partial^i, \partial_j + R_j\partial^j] \\ &= \partial_i\partial_j + \partial_i R_j\partial^j + R_j\partial_i\partial^j + R_i\partial^i\partial_j + R_i\partial^i R_j\partial^j + R_i R_j\partial^i\partial^j - \partial_j\partial_i - \partial_j R_i\partial^i - R_i\partial_j\partial^i - R_j\partial^j\partial_i \\ &\quad - R_j\partial^j R_i\partial^i - R_j R_i\partial^j\partial^j = (\partial_i R_j + R_i\partial^i R_j)\partial^j - (\partial_j R_i + R_j\partial^j R_i)\partial^i.\end{aligned}$$

It follows that

$$[D_i,D_j] = D_i R_j\partial^j - D_j R_i\partial^i, \tag{3.5}$$

being

$$\partial_i R_j + R_i\partial^i R_j = D_i R_j. \tag{3.6}$$

Hence, Δ is completely integrable if and only if the generators commute, $[D_i,D_j] = 0$, i.e., if and only if

$$D_i R_j = 0, \quad i \neq j. \tag{3.7}$$

So far we have no links with the HJE $\mathcal{H} = 0$. Now we introduce the function $\mathcal{H}$.

(v) The distribution Δ, when restricted to the points of $\mathcal{E}_0$, gives rise to a distribution Δ_0 on $\mathcal{E}_0$ if and only if the generators are tangent to $\mathcal{E}_0$, and this happens if and only if

$$D_i\mathcal{H}|_{\mathcal{E}_0} = (\partial_i\mathcal{H} + R_i\partial^i\mathcal{H})|_{\mathcal{E}_0} = 0. \tag{3.8}$$

In this case we say that Δ is reducible to $\mathcal{E}_0$ and a well-known property of the Lie bracket tells us that

$$[D_i|\mathcal{E}_0, D_j|\mathcal{E}_0] = [D_i, D_j]|\mathcal{E}_0. \tag{3.9}$$

It follows that the reduced distribution Δ_0 is integrable if and only if

$$D_i R_j|\mathcal{E}_0 = 0, \quad i \neq j. \tag{3.10}$$

Theorem 3.1: *The HJE* (2.1) *admits an extended separated solution in the coordinate system* $\underline{q}$ *if and only if there exist n functions* $R_i(\underline{q},\underline{p})$ *satisfying one of the following equivalent conditions:* (a) *The distribution* Δ *spanned by the generators* (3.1) *is completely integrable and reducible to a distribution* Δ_0 *on* $\mathcal{E}_0$. (b) *Conditions* (3.7) and (3.8) *are satisfied*:

$$\partial_i R_j + R_i \partial^i R_j = 0, \quad i \neq j, \quad (\partial_i \mathcal{H} + R_i \partial^i \mathcal{H})|_{\mathcal{E}_0} = 0. \tag{3.11}$$

Proof: Conditions (a) and (b) are clearly equivalent because of the remarks above. Let $W^E(\underline{q},\underline{c})$ be an extended separated solution. The completeness condition (2.3) means that $(\underline{q},\underline{c})$ are local noncanonical coordinates of T^*Q. Thus, the functions $R_i = \partial_i^2 W^E(\underline{q},\underline{c})$ are well defined on an open subset of T^*Q. Then we consider the separable connection Δ with generators

$$D_i = \partial_i + \partial_i^2 W^E \partial^i.$$

The integral manifolds of Δ are locally described by equations $p_i = \partial_i W^E(\underline{q},\underline{c})$ and, due to the completeness condition (2.3), we get the complete integrability of Δ. Moreover, since for $c_n = 0$, W^E is a solution of (2.1), the generators are tangent to $\mathcal{E}_0$. Conversely, assume that functions R_i exist satisfying (3.11). Then the distribution Δ is completely integrable and the integral manifolds are generated by a separated solution $W^E(\underline{q},\underline{c})$ parametrized by n parameters $\underline{c} = (c_i)$. Since the integral manifolds form a foliation, there is only one integral manifold $L_{\underline{c}}$ containing a given point. This means that equations $p_i = \partial_i W^E$ must be solvable with respect to $\underline{c}$. This is equivalent to the completeness condition (2.3). ■

Theorem 3.2: *The HJE* (2.1) *admits an internal separated solution in the coordinate system* $\underline{q}$ *if and only if there exist functions* $R_i(\underline{q},\underline{p})$ *such that* (a) *the distribution* Δ *spanned by the generators* (3.1) *is reducible to a distribution* Δ_0 *on* $\mathcal{E}_0$ *and this reduced distribution is completely integrable, i.e., such that* (b) *conditions* (3.8) and (3.10) *are satisfied*:

$$(\partial_i \mathcal{H} + R_i \partial^i \mathcal{H})|_{\mathcal{E}_0} = 0, \quad (\partial_i R_j + R_i \partial^i R_j)|_{\mathcal{E}_0} = 0, \quad i \neq j \tag{3.12}$$

Proof: The equivalence between conditions (a) and (b) follows from the above remarks. Let W^I be an internal separated solution. Then, by Proposition 2.2, we can construct an extended separated solution W^E in the same coordinates. Hence, by Theorem 3.1, there exist functions R_i satisfying (3.11). It is clear that these functions R_i satisfy (3.12). Conversely, we consider functions R_i satisfying (3.12) which are associated with a distribution Δ reducible to a completely integrable distribution Δ_0 on $\mathcal{E}_0$. The integral manifolds of Δ_0 are generated by a separated solution $W^I(\underline{q},c_\alpha)$ parametrized by $n-1$ parameters (c_α). Since they form a foliation $\mathcal{L}^I \subseteq \mathcal{E}_0$, there is only one integral manifold containing a given point $p \in \mathcal{E}_0$. This means that equations $p_i = \partial_i W^I$ are solvable with respect to c_α so that the completeness condition (2.2) holds. ■

Remark 3.1: We know from Proposition 2.2 that the existence of a separated solution W^I is equivalent to the existence of a separated solution W^E. However, this does not mean that the functions R_i entering Theorem 3.1 and Theorem 3.2 are the same functions. Indeed, it is obvious that functions R_i satisfying (3.11) also satisfy (3.12); but functions R_i satisfying (3.12) may not satisfy (3.11).

IV. THE LEVI–CIVITA SEPARABILITY CONDITIONS WITH LAGRANGIAN MULTIPLIERS

The ordinary separation of the HJE $\mathcal{H} = h$ (2.4) is characterized by the Levi–Civita equations,[24]

$$\partial_i\mathcal{H}\partial_j\mathcal{H}\partial^i\partial^j\mathcal{H} + \partial^i\mathcal{H}\partial^j\mathcal{H}\partial_i\partial_j\mathcal{H} - \partial_i\mathcal{H}\partial^j\mathcal{H}\partial^i\partial_j\mathcal{H} - \partial^i\mathcal{H}\partial_j\mathcal{H}\partial_i\partial^j\mathcal{H} = 0, \quad i \neq j. \tag{4.1}$$

We want to write similar differential equations characterizing the separation of the null HJE $\mathcal{H}=0$ (2.1). For this reason, we look for differential systems equivalent to the conditions (3.11) and (3.12), respectively. Since these conditions are differential conditions restricted to a submanifold, we base our approach on the Hadamard lemma (cf. Ref. 1, for the one-dimensional case).

Lemma 4.1: Let $f(\underline{x},y)$ *be a smooth* (C^∞) *function on an open subset* U of $\mathbb{R}^{m+1}$ *such that* $f(\underline{x},0)=0$. *Then there exists a smooth function* $\lambda(\underline{x},y)$ *such that* $f(\underline{x},y)=y\lambda(\underline{x},y)$.

Proof: The function $\lambda(\underline{x},y)$ is defined by

$$\lambda(\underline{x},y) = \int_0^1 \frac{\partial f}{\partial y}(\underline{x},ty)\mathrm{d}t. \tag{4.2}$$

Indeed we have

$$y\int_0^1 \frac{\partial f}{\partial y}(\underline{x},ty)\mathrm{d}t = \int_0^1 \frac{\partial f}{\partial y}(\underline{x},ty)y\ \mathrm{d}t = \int_0^y \frac{\partial f}{\partial y}(\underline{x},u)\mathrm{d}u = f(\underline{x},y) - f(\underline{x},0) = f(\underline{x},y).$$

The function defined by (4.2) is smooth. ■

We use Hadamard's lemma in the following form.

Lemma 4.2: A smooth function F *on* T^*Q *which vanishes on the submanifold* $\mathcal{E}_0$ *defined by equation* $\mathcal{H}=0$ *is of the form*

$$F = \mathcal{H}\lambda, \tag{4.3}$$

where λ *is a suitable function on* T^*Q.

Proof: Since $\mathcal{E}_0$ is a submanifold of codimension 1, and $\mathrm{d}\mathcal{H}\neq 0$, we can consider local coordinates $(\underline{x},y)$ on T^*Q, such that $\mathcal{E}_0$ is locally defined by equation $y=\mathcal{H}=0$. Then, by applying Lemma 4.1 to the function $F=F(\underline{x},y)$, there exists a smooth function $\lambda(\underline{x},y)$ such that $F=y\lambda$, i.e., a smooth function $\lambda(\underline{q},\underline{p})$ such that (4.3) holds. ■

Due to Lemma 4.2, and recalling our assumption $\partial^i\mathcal{H}\neq 0$, we can reformulate Theorems 3.1 and 3.2 as follows.

Proposition 4.1: The HJE (2.1) *admits an extended separated solution in the coordinates* $\underline{q}=(q^i)$ *if and only if there exist* n *functions* $\lambda_i(\underline{q},\underline{p})$ *such that equations*

$$\partial_i R_j + R_i\partial^i R_j = 0, \quad i \neq j, \tag{4.4}$$

are satisfied for

$$R_i \doteq -\frac{\partial_i\mathcal{H} - \lambda_i\mathcal{H}}{\partial^i\mathcal{H}}. \tag{4.5}$$

Proof: It is sufficient to examine the second equation (3.11). Due to Lemma 4.2, this is equivalent to the existence of functions λ_i on T^*Q such that

$$\partial_i\mathcal{H} + R_i\partial^i\mathcal{H} = \lambda_i\mathcal{H}. \tag{4.6}$$

Then we get for R_i the expression (4.5). ■

Proposition 4.2: The HJE (2.1) *admits an internal separated solution in the coordinates* $\underline{q}=(q^i)$ *if and only if there exist functions* $\lambda_i(\underline{q},\underline{p})$ *and* $\mu_{ij}(\underline{q},\underline{p})$ *such that equations*

$$\partial_i R_j + R_i\partial^i R_j = \mu_{ij}\mathcal{H}, \quad i \neq j, \tag{4.7}$$

are satisfied for R_i *given by* (4.5),

$$R_i \doteq -\frac{\partial_i\mathcal{H} - \lambda_i\mathcal{H}}{\partial^i\mathcal{H}}.$$

Proof: By recalling the proof of Proposition 4.1, the first equation (3.12) means that R_i must have the form (4.5). Moreover, due to Lemma 4.2, the second equation (3.12) is equivalent to the existence of functions μ_{ij} on T^*Q such that (4.7) holds

.■

We remark that the additional functions λ_i and μ_{ij} play the role of Lagrangian multipliers. Now we are able to state three effective criteria for the separability (Definition 2.3) of the null HJE.

Theorem 4.1: The HJE $\mathcal{H}=0$ (2.1) *is separable in the coordinates* $\underline{q}=(q^i)$ *if and only if there exist n functions* $\underline{\lambda}=(\lambda_k)$ *on* T^*Q *such that equations*

$$L_{ij}(\mathcal{H};\underline{\lambda}) \doteq L_{ij}(\mathcal{H}) + \mathcal{H}[\lambda_i(\partial^j\mathcal{H}\partial^i\partial_j\mathcal{H} - \partial_j\mathcal{H}\partial^i\partial^j\mathcal{H}) + \lambda_j(\partial^j\mathcal{H}\partial_i\partial^j\mathcal{H} - \partial^i\partial^j\mathcal{H}\partial_i\mathcal{H}) + \lambda_i\lambda_j(\mathcal{H}\partial^i\partial^j\mathcal{H} - \partial^i\mathcal{H}\partial^j\mathcal{H}) - \partial_j\lambda_i\partial^i\mathcal{H}\partial^j\mathcal{H} + \partial^j\lambda_i(\partial_j\mathcal{H}\partial^i\mathcal{H} - \lambda_j\mathcal{H}\partial^i\mathcal{H})] = 0 \quad (4.8)$$

are satisfied for $i \neq j$, *where*

$$L_{ij}(\mathcal{H}) \doteq \partial_i\mathcal{H}\partial_j\mathcal{H}\partial^i\partial^j\mathcal{H} + \partial^i\mathcal{H}\partial^j\mathcal{H}\partial_i\partial_j\mathcal{H} - \partial_i\mathcal{H}\partial^j\mathcal{H}\partial^i\partial_j\mathcal{H} - \partial^i\mathcal{H}\partial_j\mathcal{H}\partial_i\partial^j\mathcal{H}. \quad (4.9)$$

We call equations (4.8), $L_{ij}(\mathcal{H},\underline{\lambda})=0$, the *Levi–Civita conditions with Lagrangian multipliers.*

Proof: By Proposition 4.1, the HJE (2.1) is separable if and only if there exist functions λ_i on T^*Q such that equations (4.4) and (4.5) hold. Due to the expression of R_i given by (4.5), the left-hand side D_iR_j of (4.4) becomes

$$D_iR_j = -\frac{1}{\partial^j\mathcal{H}(\partial^j\mathcal{H})^2}L_{ij}(\mathcal{H};\underline{\lambda}), \quad (4.10)$$

so that equations (4.4) are equivalent to equations (4.8). ■

Remark 4.1: For all $\lambda_i=0$, the expression (4.5) reduces to

$$R_i = -\frac{\partial_i\mathcal{H}}{\partial^i\mathcal{H}}, \quad (4.11)$$

and (4.8) become the usual Levi–Civita conditions (4.1). Conditions (4.8) are more general than (4.1). Indeed, equations (4.1) are satisfied if and only if for R_i given by (4.11) we have $D_iR_j=0$, i.e., if and only if the associated distribution Δ is completely integrable on an open subset of T^*Q and reducible to every $\mathcal{E}_h$, that is if and only if there exists an ordinary complete solution of equation $\mathcal{H}=h$ (2.4).

Remark 4.2: Equations (4.8) can be written in the form $L_{ij}(\mathcal{H})=P_{ij}(\underline{q},\underline{p})\mathcal{H}$. This is just a special case [corresponding to a first order PDE $\mathcal{H}(\underline{q},\underline{p})=0$] of a general equation written by Kalnins and Miller in their theory of the variable separation for partial differential equations [Eq. (1.25) of Ref. 26, or Eq. (1.17) of Ref. 21]. In fact, equation $L_{ij}(\mathcal{H})=\mathcal{H}P_{ij}$ is considered as a *definition* of a so-called regular separation of equation $\mathcal{H}=0$. Instead, in our approach it is a consequence of the definitions of separation given in Sec. II and rigorously proved by means of the Hadamard lemma, as shown by the following.

Theorem 4.2: *The HJE* $\mathcal{H}=0$ (2.1) *is separable in the coordinates* $\underline{q}=(q^i)$ *if and only if the Levi–Civita conditions* $L_{ij}(\mathcal{H})=0$ *are satisfied for* $\mathcal{H}=0$, *that is on the submanifold* $\mathcal{E}_0$,

$$L_{ij}(\mathcal{H})|_{\mathcal{E}_0} = 0. \quad (4.12)$$

Proof: The Levi–Civita conditions with Lagrangian multipliers (4.8) obviously imply $L_{ij}(\mathcal{H})=0$ for $\mathcal{H}=0$. Conversely, assume that (4.12) holds. Then, by Lemma 4.2, there exist functions ν_{ij} such that $L_{ij}(\mathcal{H})=\nu_{ij}\mathcal{H}$. If we set

$$\mu_{ij} = -\frac{1}{\partial^i \mathcal{H}(\partial^j \mathcal{H})^2}\nu_{ij},$$

and $\lambda_i = 0$, then due to (4.10) we get that equations (4.5) and (4.7) are satisfied, and due to Proposition 4.2 the HJE admits an internal separated solution. ■

We remark that conditions (4.12) do not involve Lagrangian multipliers.

Remark 4.3: When the functions R_i are given by (4.5), the generators D_i become

$$D_i = \partial_i - \frac{\partial_i \mathcal{H} - \lambda_i \mathcal{H}}{\partial^j \mathcal{H}}\,\partial^i. \tag{4.13}$$

Then, the Levi–Civita conditions with Lagrangian multipliers (4.8) can be written in the form

$$L_{ij}(\mathcal{H};\lambda_k) = L_{ij}(\mathcal{H}) + \mathcal{H}[\lambda_i(\partial^j \mathcal{H}\partial^i\partial_j \mathcal{H} - \partial_j \mathcal{H}\partial^i\partial^j \mathcal{H}) + \lambda_j(\partial^i \mathcal{H}\partial_i\partial^j \mathcal{H} - \partial^i\partial^j \mathcal{H}\partial_i \mathcal{H}) + \lambda_i\lambda_j(\mathcal{H}\partial^i\partial^j \mathcal{H} - \partial^i \mathcal{H}\partial^j \mathcal{H}) - D_j\lambda_i\partial^i \mathcal{H}\partial^j \mathcal{H}] = 0. \tag{4.14}$$

It is a remarkable fact that the Levi–Civita separability conditions with Lagrangian multipliers λ_i are equivalent to differential conditions involving a single undetermined function Λ on T^*Q and that these new conditions are the ordinary Levi–Civita separability conditions, but with respect to a modified Hamiltonian, $\mathcal{J} = \mathcal{H}/\Lambda$.

Theorem 4.3: *The HJE* $\mathcal{H} = 0$ (2.1) *is separable in the coordinates* $\underline{q} = (q^i)$ *if and only if there exists a nowhere vanishing function* $\Lambda = \Lambda(\underline{q}, \underline{p})$ *such that for any* $i \neq j$,

$$L_{ij}\left(\frac{\mathcal{H}}{\Lambda}\right) = 0. \tag{4.15}$$

Proof: The Levi–Civita equations with Lagrangian multipliers (4.14) are not symmetric in the indices (i,j), due to the last term. By taking their skew-symmetric part, we obtain equations

$$\partial^i \mathcal{H}\partial^j \mathcal{H} D_j\lambda_i = \partial^i \mathcal{H}\partial^j \mathcal{H} D_i\lambda_j, \tag{4.16}$$

which are necessary conditions for the solvability of (4.14). Since D_i and D_j commute, it follows that (4.16) are locally equivalent to the existence of a function $F(\underline{q}, \underline{p})$ such that

$$\lambda_i = D_i F. \tag{4.17}$$

Indeed, the commutation condition $[D_i, D_j] = 0$ is equivalent to the existence of local coordinates (x^i, y^j) such that $D_i = \partial/\partial y^i$. Hence, equations (4.16) become equivalent to $\partial\lambda_i/\partial y^j = \partial\lambda_j/\partial y^i$. By considering the coordinates (x^i) as independent parameters, this is locally equivalent to the existence of a function $F(\underline{x}, \underline{y})$ such that $\lambda_i = \partial F/\partial y^i$, and we get (4.17). However, it turns out to be more convenient to replace the function F in (4.17) with $F = \ln|\Lambda|$, where $\Lambda(\underline{q}, \underline{p})$ is a nowhere vanishing function, so that

$$\lambda_i = \tfrac{1}{\Lambda} D_i \Lambda. \tag{4.18}$$

Then, by inserting (4.18) in (4.5), we obtain

$$R_i = -\frac{\partial_i \mathcal{H}}{\partial^j \mathcal{H}} + \frac{1}{\Lambda} D_i \Lambda \frac{\mathcal{H}}{\partial^j \mathcal{H}},$$

and, by (4.13),

$$R_i = -\frac{\partial_i \mathcal{H}}{\partial^j \mathcal{H}} + \frac{1}{\Lambda}(\partial_i \Lambda + R_i \partial^j \Lambda)\frac{\mathcal{H}}{\partial^j \mathcal{H}}.$$

By solving this equation with respect to R_i, we find

$$R_i = -\frac{\Lambda\partial_i\mathcal{H} - \mathcal{H}\partial_i\Lambda}{\Lambda\partial^i\mathcal{H} - \mathcal{H}\partial^i\Lambda}, \tag{4.19}$$

that is

$$R_i = -\frac{\partial_i(\mathcal{H}/\Lambda)}{\partial^i(\mathcal{H}/\Lambda)}. \tag{4.20}$$

Hence, for the functions (4.20) the complete integrability conditions (4.4) become the Levi–Civita conditions (4.15) for the new Hamiltonian $\mathcal{J}=\mathcal{H}/\Lambda$. ■

Remark 4.4: The explicit expression of the n Lagrangian multipliers λ_i in terms of Λ is

$$\lambda_i = \frac{\{\mathcal{H},\Lambda\}_i}{\Lambda\partial^i\mathcal{H} - \mathcal{H}\partial^i\Lambda}, \tag{4.21}$$

where $\{\mathcal{H},\Lambda\}_i \doteq \partial^i\mathcal{H}\partial_i\Lambda - \partial^i\Lambda\partial_i\mathcal{H}$. Indeed, by (4.20), the generators D_i become

$$D_i = \partial_i - \frac{\partial_i(\mathcal{H}/\Lambda)}{\partial^i(\mathcal{H}/\Lambda)}\partial^i.$$

In particular, using (4.19), the Lagrangian multipliers (4.18) become

$$\lambda_i = \frac{\partial^i\mathcal{H}\partial_i\Lambda - \partial^i\Lambda\partial_i\mathcal{H}}{\Lambda\partial^i\mathcal{H} - \mathcal{H}\partial^i\Lambda},$$

that is (4.21).

We call the function

$$\mathcal{J} = \frac{\mathcal{H}}{\Lambda} \tag{4.22}$$

the *conformal Hamiltonian* associated to $\mathcal{H}$ and the function Λ the conformal factor. The link between the two Hamiltonian vector fields $\mathbf{X}_\mathcal{H}$ and $\mathbf{X}_\mathcal{J}$ generated by the Hamiltonians $\mathcal{H}$ and $\mathcal{J}$, respectively, is given by the following.

Proposition 4.3: On the submanifold $\mathcal{E}_0$ the vector fields $\mathbf{X}_\mathcal{H}$ and $\mathbf{X}_\mathcal{J}$ are parallel and differ by the factor Λ,

$$(\Lambda X_\mathcal{J})|_{\mathcal{E}_0} = X_\mathcal{H}|_{\mathcal{E}_0} \tag{4.23}$$

so that the corresponding affine parameters t and $\bar{t}$ are related by equation

$$\mathrm{d}\bar{t} = \Lambda\,\mathrm{d}t. \tag{4.24}$$

Proof: Let ω be the symplectic form on T^*Q. Then,

$$i_{\mathbf{X}_\mathcal{J}}\omega = -\,\mathrm{d}\mathcal{J} = \tfrac{1}{\Lambda^2}\mathcal{H}\,\mathrm{d}\Lambda - \tfrac{1}{\Lambda}\mathrm{d}\mathcal{H}, \quad i_{\mathbf{X}_\mathcal{H}}\omega = -\,\mathrm{d}\mathcal{H}. \tag{4.25}$$

By eliminating $\mathrm{d}\mathcal{H}$ in these two equations we get the single equation $\Lambda i_{\mathbf{X}_\mathcal{J}}\omega - d\ln|\Lambda|\mathcal{H} = i_{\mathbf{X}_\mathcal{H}}\omega$, which is equivalent to

$$i_{(\mathbf{X}_\mathcal{H}-\Lambda\mathbf{X}_\mathcal{J})}\omega = \frac{\mathcal{H}}{\Lambda}\mathrm{d}\Lambda. \tag{4.26}$$

By (4.26), for $\mathcal{H}=0$ the Hamiltonian vector field $(\mathbf{X}_\mathcal{H}-\Lambda\mathbf{X}_\mathcal{J})$ vanishes and we get (4.23). If t and $\bar{t}$ are the affine parameters of $\mathbf{X}_\mathcal{H}$ and $\mathbf{X}_\mathcal{J}$, respectively, then by (4.23), we find that (4.24) holds on $\mathcal{E}_0$. ■

Theorem 4.4: *If we know a complete solution of the HJE $\mathcal{J}=h$ for the conformal Hamiltonian*

(4.22), *then for* $h=0$ *we get the orbits on* $\mathcal{E}_0$ *of the Hamiltonian vector field* $\mathbf{X}_{\mathcal{H}}$.

Proof: According to Proposition 4.3, on $\mathcal{E}_0$, the integral curves of the vector fields $\mathbf{X}_{\mathcal{H}}$ and $\mathbf{X}_{\mathcal{J}}$ coincide, up to the reparametrization given by (4.24). Since $\mathcal{H}=0$ means $\mathcal{J}=0$, by inserting the condition $h=0$ in a complete solution of the HJE $\mathcal{J}=h$, we get the orbits of the field $\mathbf{X}_{\mathcal{H}}$ on the hypersurface $\mathcal{H}=0$. ■

Remark 4.5: We recall that a first integral of a Hamiltonian $\mathcal{H}$ is a function F on T^*Q which is constant on the integral curves of $\mathbf{X}_{\mathcal{H}}$ and that this is equivalent to the condition $\mathbf{X}_{\mathcal{H}}F=0$ or $\{\mathcal{H},F\}=0$. We call isoenergetic first integral of a function $\mathcal{H}$ any function F which is constant on all the integral curves contained in a submanifold $\mathcal{H}=h$ for some values of $h\in\mathbb{R}$. Due to the Hadamard lemma, this is equivalent to the existence of a function ϕ such that $\{\mathcal{H},F\}=\phi(\mathcal{H}-h)$. Of course, any ordinary first integral is a special kind of isoenergetic first integral. If $h=0$ we call F a *null first integral* of $\mathcal{H}$: it is characterized by equation

$$\{\mathcal{H},F\}=\phi\mathcal{H}. \tag{4.27}$$

By (4.23), it follows that any first integral F of $\mathbf{X}_{\mathcal{J}}$ is a null first integral of $\mathbf{X}_{\mathcal{H}}$. In Sec. VIII we shall use this definition.

Remark 4.6: Let the Hamiltonian $\mathcal{H}$ be of the form $\mathcal{H}=H+\Lambda$. In this case we can consider a particular conformal Hamiltonian $J=H/\Lambda$. We call the Hamiltonian J the *generalized Jacobi transform* of $\mathcal{H}$. According to Theorem 4.4, we get that the orbits of $\mathcal{H}$ on the hypersurface $\mathcal{H}=0$ coincide with the orbits of J on $J=1$. Moreover, by (4.24), the generalized Jacobi transform can be considered[33] as a transformation on the cotangent bundle $T^*\overline{Q}$ of the extended configuration manifold $\overline{Q}=\mathbb{R}\times Q$ which is a canonical transformation only on the hypersurface $p_0+\mathcal{H}=0$.

V. A FIRST APPLICATION: THE SEPARATION FOR TIME-DEPENDENT HAMILTONIANS

Let $H(t,q)$ be a time-dependent Hamiltonian, that is a function on the $(n+1)$-dimensional manifold $\overline{Q}=\mathbb{R}\times Q$ (the extended configuration manifold). The well-known HJE associated with a time-dependent system is

$$\frac{\partial W}{\partial t}+H\left(t,q^i,\frac{\partial W}{\partial q^i}\right)=0. \tag{5.1}$$

In the so-called homogeneous formalism, this is equivalent to consider on the cotangent bundle $T^*\overline{Q}$, with coordinates $(q^A,p_A)=(q^0,q^i,p_0,p_i)$, the function

$$\mathcal{H}(q^A,p_A)=p_0+H(q^A,p_i), \tag{5.2}$$

whose corresponding equation $\mathcal{H}=0$ is (5.1) (with $q^0=t$). We have the separation of variables of (5.1) on the hypersurface $\mathcal{H}=0$ if and only if the Levi–Civita conditions $L_{AB}(\mathcal{H})=0 (A\neq B=0,\ldots,n)$ are satisfied on $\mathcal{E}_0$, that is for

$$p_0=-H(q^A,p_i). \tag{5.3}$$

The Levi–Civita equations $L_{AB}(\mathcal{H})=0$ for the Hamiltonian (5.2) become

$$L_{ij}(\mathcal{H})=L_{ij}(H),\quad L_{i0}(\mathcal{H})=\partial^j H\partial_i\partial_0 H-\partial_i H\partial^j\partial_0 H\quad (i,j=1,\ldots,n). \tag{5.4}$$

It is remarkable the fact that, due to (5.3) and since equations (5.4) do not contain p_0, we have

$$L_{AB}(\mathcal{H})|\mathcal{E}_0=0\quad\Leftrightarrow\quad L_{AB}(\mathcal{H})=0.$$

Thus, in this case we have the perfect equivalence between the separation of the HJE $\mathcal{H}=h$ of the kind (2.4) and the separation of variables for the single equation $\mathcal{H}=0$ of the kind (2.1). Then, in order to have the separability for the HJE (5.1) we need that the following conditions be satisfied:

$$L_{ij}(H)=0,\quad \partial^j H\partial_i\partial_0 H-\partial_i H\partial^j\partial_0 H=0\quad (i\ \text{n.s.}). \tag{5.5}$$

Remark 5.1: Equations (5.5) implies that the T^*Q-Poisson bracket of the functions H and $\partial_0 H$ vanishes,

$$\{H, \partial_0 H\}_{T^*Q} = \partial^i H \partial_i \partial_0 H - \partial_i H \partial^i \partial_0 H = 0.$$

Remark 5.2: If conditions (5.5) hold, then the Levi–Civita conditions with $n+1$ Lagrangian multipliers $L_{AB}(\mathcal{H}; \lambda_C) = 0$ are satisfied for $\lambda_C = 0 (C = 0, \ldots, n)$ or, equivalently, conditions (4.15) hold for $\Lambda = 1$.

Remark 5.3: Equations (5.5) are the Levi–Civita separability conditions for the time-dependent case proposed by Forbat.[15] However, the proof given by Forbat is unsatisfactory. Indeed, it is based on the fact that, assuming that the equation (5.1) admits a complete solution of the form $W = W_0(t, \underline{c}) + \Sigma_i W_i(q^i, \underline{c})$, by differentiating (5.1) with respect to a coordinate q^i, we get equations

$$\partial^i H \partial_i p_i + \partial_i H = 0 \tag{5.6}$$

(no summation on the index i). By solving (5.6) with respect to $\partial_i p_i$, we obtain the system

$$\partial_j p_i = \delta_{ij} R_i, \quad R_i = -\frac{\partial_i H}{\partial^i H}, \tag{5.7}$$

whose integrability conditions are (5.5). However, equations (5.6) are derivable also from equation $\mathcal{H} = h$, where h is any constant, not only from equation $\mathcal{H} = 0$. In other words, in considering the integrability conditions of system (5.7) one is actually considering the separation of all equations $\mathcal{H} = h = \text{const}$, which is not in general equivalent to the separation of the single equation $\mathcal{H} = 0$, as we have seen in the preceding sections.

VI. THE ORTHOGONAL SEPARATION FOR NATURAL HAMILTONIANS

Let us apply the general theory so far developed to the special but fundamental case of a natural Hamiltonian $H = G + V$ in orthogonal coordinates,

$$H(\underline{q}, \underline{p}) = \tfrac{1}{2} g^{ii} p_i^2 + V(\underline{q}).$$

With an orthogonal metric $\mathbf{G} = (g^{ii})$ we associate differential operators $S_{ij}(A)$ on functions $A(\underline{q})$,

$$S_{ij}(A) \doteq \partial_i \partial_j A - \partial_j \ln|g^{ii}| \partial_i A - \partial_i \ln|g^{jj}| \partial_j A = \partial_i \partial_j A - \frac{1}{g^{ii}} \partial_j g^{ii} \partial_i A - \frac{1}{g^{jj}} \partial_i g^{jj} \partial_j A,$$

which we call *Stäckel operators*. The indices (i, j) are assumed to be distinct and not summed (n.s.). In the following the condition "$i \neq j$ n.s." referred to an operator S_{ij} will be understood. We know (see, e.g., Ref. 3) that g^{kk} is a Stäckel metric if and only if

$$S_{ij}(g^{kk}) = 0, \tag{6.1}$$

and that a potential V is separable in these coordinates if and only if $S_{ij}(V) = 0$. Indeed, for a natural Hamiltonian in orthogonal coordinates the Levi–Civita equations become

$$L_{ij}(H) = g^{ii} g^{jj} p_i p_j \left(\tfrac{1}{2} S_{ij}(g^{kk}) p_k^2 + S_{ij}(V) \right) = 0, \tag{6.2}$$

and they are satisfied if and only if $\frac{1}{2} S_{ij}(g^{kk}) p_k^2 + S_{ij}(V) = 0$. For the operators S_{ij} the following rules hold:

$$S_{ij}(c) = 0, \quad c \in \mathbb{R},$$

$$S_{ij}(A + B) = S_{ij}(A) + S_{ij}(B),$$

$$S_{ij}(AB) = AS_{ij}(B) + BS_{ij}(A) + \partial_i A \partial_j B + \partial_j A \partial_i B,$$

$$S_{ij}(A^{-1}) = 2A^{-3}\partial_i A \partial_j A - A^{-2}S_{ij}(A). \tag{6.3}$$

The Stäckel operators $\bar{S}_{ij}$ corresponding to a conformal orthogonal metric $\bar{g}^{ii}=(1/\sigma)g^{ii}$ obey rules (6.3) and

$$\bar{S}_{ij}(A) = S_{ij}(A) - \sigma^{-3}(\partial_i \sigma \partial_j A + \partial_i A \partial_j \sigma),$$

$$\bar{S}_{ij}(\bar{g}^{kk}) = \sigma^{-1}S_{ij}(g^{kk}) - g^{kk}\sigma^{-2}S_{ij}(\sigma) = \frac{g^{kk}}{\sigma}\left(\frac{1}{g^{kk}}S_{ij}(g^{kk}) - \frac{1}{\sigma}S_{ij}(\sigma)\right). \tag{6.4}$$

Remark 6.1: From the second equation (6.4), by setting $\sigma=g^{11},\ldots,g^{nn}$, we derive the following theorem due to Kalnins and Miller, Ref. 20, Lemma 1: *If* (g^{ii}) *is a Stäckel metric then all metrics* $(g^{ii}/g^{11}),\ldots,(g^{ii}/g^{nn})$ *are Stäckel metrics*. We recall also Lemma 2 of Ref. 20: *An orthogonal metric* (g^{ii}) *is conformal to a Stäckel metric if and only if* g^{ii}/g^{jj}*, for any fixed value of the index* j*, is a Stäckel metric*. Indeed, this follows from Lemma 1 and the fact that for any conformal metric $\bar{g}^{ii}$ we have $\bar{g}^{ii}/\bar{g}^{ij}=g^{ii}/g^{jj}$. Note that equation (6.1) are equivalent to equations

$$\partial_{ij}^2 \ln|g_{ii}| - \partial_i \ln|g_{kk}|\partial_j \ln|g_{ii}| + \partial_i \ln|g_{jj}|\partial_j \ln|g_{kk}| + \partial_j \ln|g_{ii}|\partial_i \ln|g_{kk}| = 0.$$

With the substitution $g_{ii}=e_i H_i^2$, $e_i=\pm 1$, they coincide with the equations given by Eisenhart (Ref. 14, Appendix 13).

Let us apply the results of Sec. IV to the function

$$\mathcal{H} = \tfrac{1}{2}g^{ii}p_i^2 + V - E, \quad E \in \mathbb{R}.$$

Theorem 6.1: *The HJE*

$$\tfrac{1}{2}g^{ii}p_i^2 + V - E = 0, \tag{6.5}$$

is separable in the orthogonal coordinates (q^i)*, for a fixed value* $E\in\mathbb{R}$*, if and only if equations*

$$\frac{1}{g^{hh}}S_{ij}(g^{hh}) = \frac{1}{g^{kk}}S_{ij}(g^{kk}), \quad S_{ij}(V) = \frac{V-E}{g^{hh}}S_{ij}(g^{hh}), \tag{6.6}$$

are satisfied for all indices h*,* k *and* $i\neq j$.

Proof: Due to Theorem 4.2, a necessary and sufficient condition for the separation of $\mathcal{H}=0$ is that the Levi–Civita conditions be satisfied when restricted to the submanifold $\mathcal{E}_0$, that is for $\mathcal{H}=0$. By (6.5), equation $\mathcal{H}=0$ is equivalent to

$$p_1^2 = -\sum_{k=2}^{n}\frac{g^{kk}}{g^{11}}p_k^2 + \frac{2}{g^{11}}(E-V). \tag{6.7}$$

Thus, by (6.2) and (6.7), we get

$$L_{ij}(\mathcal{H})|_{\mathcal{E}_0} = g^{ii}g^{jj}p_i p_j\left(\frac{1}{2}\sum_{k=2}^{n}S_{ij}(g^{kk})p_k^2 + S_{ij}(V) - \frac{1}{2}S_{ij}(g^{11})\sum_{k=2}^{n}\frac{g^{kk}}{g^{11}}p_k^2 + \frac{S_{ij}(g^{11})}{g^{11}}(E-V)\right). \tag{6.8}$$

Functions (6.8) vanish if and only if

$$\frac{1}{2}\sum_{k=2}^{n}\left[S_{ij}(g^{kk})-\frac{g^{kk}}{g^{11}}S_{ij}(g^{11})\right]p_k^2-S_{ij}(E-V)-\frac{S_{ij}(g^{11})}{g^{11}}(E-V)=0. \tag{6.9}$$

Since conditions (6.9) must be satisfied for all values of $p_2,\ldots,p_n$, they are equivalent to

$$S_{ij}(g^{kk})-\frac{g^{kk}}{g^{11}}S_{ij}(g^{11})=0,\quad S_{ij}(E-V)-\frac{E-V}{g^{11}}S_{ij}(g^{11})=0,$$

hence to (6.6). ■

The first equations (6.6) mean that the functions $(1/g^{hh})S_{ij}(g^{hh})$ do not depend on the choice of the index h. This is a necessary condition for the separability of equation (6.5), which has the following equivalent formulation.

Theorem 6.2: *The necessary condition for the separability of the HJE* (6.5)

$$\frac{1}{g^{hh}}S_{ij}(g^{hh})=\frac{1}{g^{kk}}S_{ij}(g^{kk})\quad \textit{for all indices } h,\ k \textit{ and } i\neq j, \tag{6.10}$$

is equivalent to the existence of a function $\sigma\neq 0$ *such that the conformal metric* $\bar{g}^{ii}=g^{ii}/\sigma$ *is a Stäckel metric,*

$$\bar{S}_{ij}(\bar{g}^{kk})=0. \tag{6.11}$$

Proof: (i) If such a function σ exists, then by the second equation (6.4) we derive $(1/g^{kk})S_{ij}(g^{kk})=(1/\sigma)S_{ij}(\sigma)$. Hence, (6.10) follows. (ii) Conversely, assume that (6.10) holds. If we choose $\sigma=g^{11}$ then from the second equation (6.4) we get $\bar{S}_{ij}(\bar{g}^{kk})=0$. ■

Remark 6.2: From this proof it follows that condition (6.10) is verified if and only if (6.11) is satisfied with $\sigma=g^{jj}$ for any arbitrary choice of the index j.

This theorem suggests the following.

Definition 6.1: We call *conformal separable coordinates* orthogonal coordinates $\underline{q}=(q^i)$ for which conditions (6.10) or (6.11) hold.

Remark 6.3: A special class of orthogonal conformal separable coordinates is that for which $g^{ii}=c^i\sigma(\underline{q})$, $c^i\in\mathbb{R}$. In this case the components of the orthogonal conformal metric are $c^i=g^{ii}/\sigma$ = constant; hence, they are obviously of the Stäckel type. Up to a rescaling of the coordinates we can reduce to the case $g^{ii}=\pm\sigma$, according to the signature of the metric. Note that in this case the original metric (g^{ii}) is conformally flat. Orthogonal coordinates for which $g^{ii}=g^{jj}$ are called isothermal.

Now we apply Theorem 6.1 to the following three special cases:

$V=0,\quad E\neq 0,$	non-null geodesics,
$V=0,\quad E=0,$	null geodesics,
$V-E\neq 0,$	dynamical trajectories with total energy E.

The results for the null geodesics case date back to Stäckel[32] (see also Ref. 20).

Theorem 6.3: *The HJE* $\frac{1}{2}g^{ii}p_i^2=E$ *with a fixed value* $E\neq 0$, *is separable in orthogonal coordinates* (q^i) *if and only if* (g^{ii}) *is a Stäckel metric, i.e., if and only if it is separable in the ordinary sense for all values of* E.

Proof: For $V=0$ the second equation (6.6) gives $S_{ij}(g^{kk})=0$. ■

Theorem 6.4: *The HJE of the null geodesics*

$$g^{ii}p_i^2=0 \tag{6.12}$$

is separable in the orthogonal coordinates (q^i) *if and only if these coordinates are conformal separable.*

Proof: For $V=0$ and $E=0$ the second equations (6.6) are trivially satisfied, so that only the first equations characterize the separation. ■

Theorem 6.5: *The HJE*

$$\tfrac{1}{2}g^{ii}p_i^2 + V - E = 0 \quad (V - E \neq 0), \tag{6.13}$$

is separable if and only if the conformal metric

$$\bar{g}^{ii} = \frac{1}{E - V}g^{ii} \tag{6.14}$$

is a Stäckel metric, or equivalently, if and only if for all indices h, k and $i \neq j$,

$$\frac{1}{g^{kk}}S_{ij}(g^{kk}) = \frac{1}{V - E}S_{ij}(V). \tag{6.15}$$

This means that the coordinates are conformal separable, according to Definition 6.1, but the conformal factor σ must be equal to the function $V-E$.

Proof: For $V-E \neq 0$ system (6.6) is equivalent to (6.15). Moreover, let us consider the conformal metric (6.14) and the associated Stäckel operators $\bar{S}_{ij}$. From the second formula (6.4) with $\sigma = E - V$, we get

$$\bar{S}_{ij}(\bar{g}^{kk}) = \frac{1}{E - V}S_{ij}(g^{kk}) - \frac{g^{kk}}{(E - V)^2}S_{ij}(E - V).$$

Thus, $\bar{S}_{ij}(\bar{g}^{kk}) = 0$ is equivalent to (6.15). ■

Remark 6.4: The metric $\bar{g}^{ii} = (E-V)^{-1}g^{ii}$ is called the *Jacobi metric* or action metric (see, e.g., Ref. 33 and the references cited therein) of the natural Hamiltonian $H = G + V$ for the fixed value E of the total energy. Then, Theorem 6.5 can be reformulated as follows

Theorem 6.6: *The HJE* (6.13) *is separable if and only if the corresponding Jacobi metric is a Stäckel metric.*

We adapt to the Jacobi metric the considerations about the conformal Hamiltonians stated in Proposition 4.3 and Theorem 4.4.

With a natural Hamiltonian $H = G + V = \frac{1}{2}g^{ij}p_ip_j + V$ and a fixed value of the energy $E \in \mathbb{R}$ we associate two Hamiltonians,

$$H_E = \tfrac{1}{2}g^{ij}p_ip_j + V - E, \quad J_E = \tfrac{1}{2}\frac{g^{ij}}{E-V}p_ip_j.$$

The passage from the natural Hamiltonian $H = G + V$ to the geodesic Hamiltonian J_E is called Jacobi transformation[16,28,30] or Maupertuis transformation.[9,33]

Let $\mathbf{X}_H$ be the Hamiltonian vector field generated by H (it coincides with that generated by H_E) and $\mathbf{X}_J$ the Hamiltonian vector field generated by J_E. Adapting to these cases Proposition 4.3, Theorem 4.4, and Remark 4.5, we get the following.

Theorem 6.7: *Assume that equation $H_E = 0$ (i.e., $J_E = 1$) defines a regular hypersurface of T^*Q. Then* (i) *on this hypersurface the Hamiltonian vector fields $\mathbf{X}_H$ and $\mathbf{X}_J$ are parallel,*

$$(E - V)\mathbf{X}_J = \mathbf{X}_H, \tag{6.16}$$

and outside this surface the difference $(E-V)\mathbf{X}_J - \mathbf{X}_H$ is a vertical vector field. (ii) *On $H_E = 0$ the integral curves of the vector fields $\mathbf{X}_H$ and $\mathbf{X}_J$ coincide, up to a reparametrization, and the affine parameters t and $\bar{t}$ of $\mathbf{X}_H$ and $\mathbf{X}_J$, respectively, are related by $\mathrm{d}\bar{t} = (E-V)\mathrm{d}t$.* (iii) *Any first integral F of $\mathbf{X}_J$ is constant along the integral curves of $\mathbf{X}_H$ contained on $H_E = 0$.* (iv) *If a complete solution of the geodesic HJE $J_E = h$ is known, then for $h = 1$ we get the orbits of the field $\mathbf{X}_H$ on the hypersurface $H_E = 0$.*

Proof: By (4.23), we get (6.16). Moreover, due to (4.26), we have that $\mathbf{X}_H - (E-V)\mathbf{X}_J$ is vertical outside the hypersurface $H_E = 0$, since it is generated by the function $\Lambda = E - V$ which is constant along the fibers. ■

Hence, as a corollary of Theorem 6.6, we have the following.

Theorem 6.8: *The orthogonal separation (in the ordinary sense) of the geodesic HJE $J_E=h$ is equivalent to the orthogonal separation of the HJE $H_E=0$ for a fixed value E of the energy. For $h=1$ we get the orbits corresponding to the integral curves of $\mathbf{X}_H$ with total energy E.*

Remark 6.5: Equation (6.15) shows that $S_{ij}(V)=0$ if and only if $S_{ij}(g^{kk})=0$. These two conditions characterize the orthogonal Stäckel separation for a natural Hamiltonian. In this case the Jacobi metric is a Stäckel metric for all values of E. From (6.15) it follows also that if the conformal Jacobi metric (6.14) is a Stäckel metric for two distinct values $E_1 \neq E_2$ of the energy, then it is a Stäckel metric for all values of E. Indeed, from (6.15) written for $E=E_1$ and $E=E_2$ it follows that

$$\frac{1}{V-E_1}S_{ij}(V) = \frac{1}{V-E_2}S_{ij}(V).$$

Thus, $S_{ij}(V)=0$, so that also $S_{ij}(g^{kk})=0$. As a consequence, we have the following.

Theorem 6.9: *The HJE* (6.13) *is separable for two distinct values of the energy E if and only if it is separable in the ordinary sense.*

Remark 6.6: According to Theorem 6.9, we have that if a natural Hamiltonian $H=G+V$ is not separable in the ordinary sense, then there exists at most one value of the energy E such that $H=E$ is separable.

Remark 6.7: For a natural Hamiltonian in orthogonal coordinates the Lagrangian multipliers λ_i or the function Λ, involved in Theorems 4.1 and 4.3, respectively, which in general are functions on T^*Q, are necessarily constant along the fibers, i.e., they reduce in this case to functions on Q.

We conclude this section with the formulation of Theorems 6.2 and 6.3 in terms of Stäckel matrices. We recall that an orthogonal metric is a Stäckel metric if and only if it is a row of the inverse of a Stäckel matrix $\mathbf{S}=[\varphi_i^{(j)}(q^i)]$. By applying this definition to the general conformal metric $\overline{g}^{ii}=g^{ii}/\sigma$ and to the Jacobi metric (6.14) we get the following.

Theorem 6.10: (i) *Coordinates (q^i) are conformal separable if and only if there exists a Stäckel matrix $\mathbf{S}=[\varphi_i^{(j)}(q^i)]$ such that*

$$\frac{g^{ii}}{\varphi^i_{(n)}} = \frac{g^{jj}}{\varphi^j_{(n)}}, \tag{6.17}$$

where $[\varphi^i_{(j)}]=\mathbf{S}^{-1}$. (ii) *The Jacobi metric* (6.14) *is a Stäckel metric if and only if there exists a Stäckel matrix $\mathbf{S}=[\varphi_i^{(j)}(q^i)]$ such that* (6.17) *holds and moreover,*

$$E - V = \sum_i \varphi_i^{(n)} g^{ii}. \tag{6.18}$$

Proof: We have

$$\exists \sigma \left| \frac{g^{ii}}{\sigma} = \varphi^i_{(n)} \Leftrightarrow \frac{g^{ii}}{\varphi^i_{(n)}} = \frac{g^{jj}}{\varphi^j_{(n)}}, \right.$$

$$\frac{g^{ii}}{E-V} = \varphi^i_{(n)} \Leftrightarrow \frac{g^{ii}}{\varphi^i_{(n)}} = \frac{g^{jj}}{\varphi^j_{(n)}} \wedge E - V = \sum_i \varphi_i^{(n)} g^{ii}. \qquad \blacksquare$$

Remark 6.8: Let us denote by M^i_j the cofactor of $\varphi^{(i)}_j$. We have $\det \mathbf{S} = \Sigma_i \varphi_i^{(n)} M_i^n$ and

$$\varphi^i_{(n)} = \frac{M_i^n}{\det \mathbf{S}}.$$

Hence, (6.17) is equivalent to

$$\frac{g^{ii}}{M_i^n} = \cdots = \frac{g^{jj}}{M_j^n}.$$

We observe that in these conditions, only the first $n-1$ columns of the Stäckel matrix are involved, while the last column is involved only in the expression (6.18) of $E-V$. Hence, in the characterization of the null geodesic separation only a rectangular $n\times(n-1)$ Stäckel matrix is involved,

$$\begin{bmatrix} \varphi_1^{(1)} & \cdots & \varphi_1^{(n-1)} \\ \vdots & \vdots & \vdots \\ \varphi_n^{(1)} & \cdots & \varphi_n^{(n-1)} \end{bmatrix}.$$

VII. THE INTRINSIC CHARACTERIZATION OF THE ORTHOGONAL SEPARATION

Theorems 6.4 and 6.5 show that the separation of variables of the HJE for the null geodesics and for a fixed value of the energy is equivalent to the ordinary complete orthogonal separation of a conformal (contravariant) metric

$$\overline{\mathbf{G}} = \frac{1}{\sigma}\mathbf{G},$$

where $\overline{\mathbf{G}}=(\overline{g}^{ii})$, $\mathbf{G}=(g^{ii})$ and σ is a nowhere vanishing function on Q. In these two cases we have, respectively,

$$\sigma = \text{a suitable function on } Q \quad \text{for the null geodesics},$$

$$\sigma = E - V \quad \text{for the Jacobi metric}.$$

Since the ordinary geodesic separation can be characterized by means of Killing tensors (KT's), in both cases we are led to consider KT's of a conformal metric. A basic well known property is the following.

Proposition 7.1: A symmetric two-tensor $\mathbf{K}$ *is a KT for the conformal metric* $\overline{\mathbf{G}}=(1/\sigma)\mathbf{G}$ *i.e.*,

$$[\overline{\mathbf{G}},\mathbf{K}] = 0 \ (\Leftrightarrow \{P_{\overline{\mathbf{G}}}, P_{\mathbf{K}}\} = 0), \tag{7.1}$$

if and only if

$$[\mathbf{G},\mathbf{K}] = -\frac{2}{\sigma}\mathbf{K}\nabla\,\sigma\odot\mathbf{G} \quad \left(\Leftrightarrow \{P_{\mathbf{G}}, P_{\mathbf{K}}\} = -\frac{2}{\sigma}P_{\mathbf{K}\nabla\sigma}P_{\mathbf{G}}\right). \tag{7.2}$$

Notation: Here we denote by $[\cdot,\cdot]$ the Lie–Schouten bracket of contravariant symmetric tensors and by $\odot$ the symmetric tensor product. If we consider the homogeneous polynomial functions $P_{\mathbf{K}}$ on T^*Q associated with contravariant symmetric tensors $\mathbf{K}=(K^{i\cdots j})$ on Q, then this bracket is defined by $P_{[\mathbf{K}_1,\mathbf{K}_2]}=\{P_{\mathbf{K}_1}, P_{\mathbf{K}_2}\}$ and the symmetric product by $P_{\mathbf{K}_1\odot\mathbf{K}_2}=P_{\mathbf{K}_1}P_{\mathbf{K}_2}$. We say that $\mathbf{K}_1$ and $\mathbf{K}_2$ are in involution if $[\mathbf{K}_1,\mathbf{K}_2]=0$. We denote by $\mathbf{KX}$ the image of a vector field $\mathbf{X}$ by $\mathbf{K}$ interpreted as a (1,1) tensor.

Proof of Proposition 7.1: The equivalence of (7.1) and (7.2) is proved by the following calculation:

$$[\overline{\mathbf{G}},\mathbf{K}] = \left[\frac{1}{\sigma}\odot\mathbf{G},\mathbf{K}\right] = \frac{1}{\sigma}\odot[\mathbf{G},\mathbf{K}] + \left[\frac{1}{\sigma},\mathbf{K}\right]\odot\mathbf{G}$$
$$= \frac{1}{\sigma}[\mathbf{G},\mathbf{K}] - 2\mathbf{K}\nabla\frac{1}{\sigma}\odot\mathbf{G} = \frac{1}{\sigma}\left([\mathbf{G},\mathbf{K}] + \frac{2}{\sigma}\mathbf{K}\nabla\,\sigma\odot\mathbf{G}\right). \qquad \blacksquare$$

A symmetric two-tensor **K** is a conformal Killing tensor (CKT) if there exists a vector field **C** such that

$$[\mathbf{G},\mathbf{K}] = 2\mathbf{C}\odot\mathbf{G} \ (\Leftrightarrow\{P_{\mathbf{G}},P_{\mathbf{K}}\} = 2P_{\mathbf{C}}P_{\mathbf{G}}). \tag{7.3}$$

We say that **K** is a CKT of *gradient type* if there exists a function U such that $\mathbf{C}=\nabla U$. We say that **K** is a CKT of *self-gradient type* if $\mathbf{C}=\mathbf{K}\nabla U$.

We remark that in Proposition 7.1 the tensor **K** is a CKT of self-gradient type with respect to the metric **G** with $U=-\ln|\sigma|$.

Remark 7.1: The eigenvectors of **K** in Proposition 7.1 are the same with respect both metrics $\overline{\mathbf{G}}$ and **G**. If $\overline{\rho}^i$ are the eigenvalues of **K** with respect to $\overline{\mathbf{G}}$, then the eigenvalues with respect to **G** are

$$\rho^i = \frac{\overline{\rho}^i}{\sigma}. \tag{7.4}$$

If the eigenvalues are simple with respect to $\overline{\mathbf{G}}$, then they are also simple with respect to **G**.

Remark 7.2: Tensors of the kind $f\mathbf{G}$ are at the same time CKT's of gradient type (with $\mathbf{C}=\nabla f$, i.e., $U=f$) and of self-gradient type (with $\mathbf{C}=f\mathbf{G}\nabla \ln f$, i.e., $U=\ln f$).

Definition 7.1: Two CKT's **K** and $\mathbf{K}'$ are said to be *equivalent* if $\mathbf{K}'=\mathbf{K}+f\mathbf{G}$ for some function f.

Equivalent CKT's have the same eigenvectors. We shall be interested in equivalence classes of this kind. In any equivalence class there exists a trace-free representative, so that only trace-free CKT's are considered by some authors.[20,29,34]

As shown by the following proposition, in some special case a CKT **K** is equivalent to a tensor $\mathbf{K}'$ of self-gradient type (hence, a KT of a conformal metric).

Proposition 7.2: (i) *A CKT* **K** *which is diagonalized in orthogonal coordinates is equivalent to a CKT* $\mathbf{K}'$ *of self-gradient type.* (ii) *For any given orthogonal coordinate system there exists a function U such that any CKT* **K** *diagonalized in these coordinates is equivalent to a CKT* $\mathbf{K}'$ *of self-gradient type such that* $[\mathbf{G},\mathbf{K}']=2\mathbf{K}'\nabla U\odot\mathbf{G}$, *i.e., to a KT of the conformal metric* $\overline{\mathbf{G}}=e^U\mathbf{G}$. (iii) *The n functions* $U_k=-\ln|g^{kk}|$ *satisfy item (ii).*

Proof: If $g^{ij}=0$ and $K^{ij}=0$ for $i\neq j$, then $K^{ii}=\rho^i g^{ii}$ and Eq. (7.3) is equivalent to

$$\partial_i\rho^j = (\rho^i-\rho^j)\partial_i \ln g^{jj} + \partial_i\rho^i, \quad C_i = \partial_i\rho^i. \tag{7.5}$$

Let us take the tensor $\mathbf{K}'=\mathbf{K}-\rho^n\mathbf{G}$ with eigenvalues $\rho'^i=\rho^i-\rho^n$. By using (7.5) we get

$$\partial_i\rho'^j = (\rho'^i-\rho'^j)\partial_i \ln|g^{jj}| - \rho'^i\partial_i \ln|g^{nn}|.$$

This shows that $\mathbf{K}'$ is a CKT with $C'_i=-\rho'^i\partial_i\ln|g^{nn}|$, hence of self-gradient type with $U=-\ln|g^{nn}|$ and a KT for the conformal metric $\mathbf{G}/g^{nn}$. We remark that U does not depend on **K** but only on the given coordinates. ■

In the following two sections we give intrinsic versions of Theorems 6.4 and 6.5, respectively, for the case considered in Theorem 6.3 the intrinsic characterizations are just that of the ordinary orthogonal separation.[4,18] We shall use the following.

Definition 7.2: A (conformal) Killing two-tensor with simple eigenvalues and normal eigenvectors is called *characteristic (conformal) Killing tensor*.

A. The orthogonal separation of the null geodesics

A first characterization is related to the existence of a single CKT.

Theorem 7.1: *The HJE* (6.12) *for the null geodesics is separable in orthogonal coordinates if and only if on Q there exists a characteristic CKT* **K**.

Proof: According to the intrinsic characterization of the orthogonal separation of a geodesic Hamiltonian,[4,18] a metric $\overline{\mathbf{G}}$ is orthogonally separable if and only if it admits a KT **K**, $[\overline{\mathbf{G}},\mathbf{K}]=0$, with simple eigenvalues and normal eigenvectors. Since $\overline{\mathbf{G}}=\mathbf{G}/\sigma$, due to Proposition 7.1, this

is equivalent to the existence of a characteristic CKT satisfying equation (7.2). Proposition 7.2 shows that this is equivalent to the existence of a characteristic CKT without any other condition. ■

Remark 7.3: Theorem 7.1 was first stated by Kalnins and Miller (Ref. 20, Theorem 1, Sec. II with a different proof, not involving the use of self-gradient CKT's.

A second characterization is related to n CKT's.

Theorem 7.2: *The HJE* (6.12) *for the null geodesics is separable in orthogonal coordinates if and only if on Q there exist n CKT's* $(\mathbf{K}_i)=(\mathbf{K}_1,\mathbf{K}_2,\ldots,\mathbf{K}_n)$, (i) *pointwise independent,* (ii) *with common eigenvectors,* (iii) *in involution.*

Proof: By Theorem 8.8 of Ref. 7 the common eigenvectors are normal. There exists orthogonal coordinate systems in which all the tensors are diagonalized. Then, the pointwise independence implies the existence of a linear combination (with constant coefficients) $\mathbf{K}=c^i\mathbf{K}_i$ with simple eigenvalues. This is a conformal characteristic tensor. Then we apply Theorem 7.1. Conversely, since the separation of (6.12) is equivalent to the ordinary separation of a conformal metric $\overline{\mathbf{G}}=\mathbf{G}/\sigma$, there exist n KT's $\mathbf{K}_i$ for the conformal metric satisfying (i), (ii), (iii). Due to Proposition 7.1, these tensors are CKT's for $\mathbf{G}$. ■

Remark 7.4: In the intrinsic characterization of the ordinary orthogonal separation in terms of n independent KT's (in involution), the metric $\mathbf{G}$ may be one of them. On the contrary, in Theorem 7.2 none CKT's $\mathbf{K}_i$ can be the metric. Indeed, if one of the $\mathbf{K}_i$ is the metric, then condition (iii) implies that all $\mathbf{K}_i$ are KT's and we reduce to the ordinary orthogonal separation. In other words, the metric cannot belong to the linear space generated by the $\mathbf{K}_i$ (by linear combinations with constant coefficients). However,

Proposition 7.3: Given, n CKT's $\mathbf{K}_i$ *with common normal eigenvectors, there exist a linear combination with constant coefficients and a function f such that* $c^i\mathbf{K}_i=f\mathbf{G}$.

Proof: We apply the second part of Proposition 7.2. Then, there are equivalent CKT's of self-gradient type $\mathbf{K}_i'=\mathbf{K}_i+f_i\mathbf{G}$ with the same function U. They are KT's of the metric $e^U\mathbf{G}=\overline{\mathbf{G}}$ with common normal eigenvectors. Thus, there exists a linear combination with constant coefficients such that $c^i\mathbf{K}_i'=\overline{\mathbf{G}}$. It follows that $c^i\mathbf{K}_i=-c^if_i\mathbf{G}+e^U\mathbf{G}=f\mathbf{G}$ with $f=e^U-c^if_i$.■

A third characterization of the separability for (6.12) involves $n-1$ CKT's.

Theorem 7.3: *The HJE* (6.12) *for the null geodesics is separable in orthogonal coordinates if and only if on Q there exist* $n-1$ *CKT's* $(\mathbf{K}_\alpha)=(\mathbf{K}_1,\mathbf{K}_2,\ldots,\mathbf{K}_{n-1})$ *with* (i) *common normal eigenvectors (i.e., all simultaneously diagonalizable in orthogonal coordinates) and such that* (ii) $\mathbf{G},\mathbf{K}_1,\mathbf{K}_2,\ldots,\mathbf{K}_{n-1}$ *are pointwise independent.*

Proof: Due to the pointwise independence of the tensors, there exists a linear combination with constant coefficients having distinct eigenvalues, i.e., which is a characteristic CKT and by Theorem 7.1 we have the separation of variables for (6.12) Conversely, if (6.12) is separable, then the conformal metric $\overline{\mathbf{G}}$ is separable and there exists $n-1$ tensors $(\mathbf{K}_\alpha)$ which are (a) KT's with respect to $\overline{\mathbf{G}}$, (b) with common normal eigenvectors, and such that (c) $(\overline{\mathbf{G}},\mathbf{K}_1,\mathbf{K}_2,\ldots,\mathbf{K}_{n-1})$ are pointwise independent. Hence, $\mathbf{K}_\alpha$ satisfy (i), (ii), and (iii). ■

This theorem is a slightly modified version of Theorem 2, Sec. II of Ref. 20. In general, a set of tensors $(\mathbf{K}_\alpha)$ satisfying the hypotheses of Theorem 7.3 may not be in involution. However,

Proposition 7.4: The tensors $(\mathbf{K}_\alpha)$ *in Theorem 7.3 are equivalent to CKT's in involution.*

Proof: First of all we remark that also the tensors $\mathbf{K}_\alpha+f_\alpha\mathbf{G}$ satisfy the hypotheses of Theorem 7.3, for any choice of the $n-1$ nonzero functions f_α. By using equations (7.5), we see that two CKT's $\mathbf{K}_\alpha$, $\mathbf{K}_\beta$ (diagonalized in orthogonal coordinates) are in involution if and only if for all indices i,

$$\frac{C_{\alpha i}}{\rho_\alpha^i}=\frac{C_{\beta i}}{\rho_\beta^i}\quad(\alpha,\beta\in\{1,\ldots,n-1\}),\tag{7.6}$$

where ρ_α^i are the eigenvalues of $\mathbf{K}_\alpha$ and $C_{\alpha i}$ are the covariant components of the vector fields $\mathbf{C}_\alpha$ satisfying $[\mathbf{G},\mathbf{K}_\alpha]=2\mathbf{C}_\alpha\odot\mathbf{G}$. Condition (7.6) is not preserved by replacing the tensors by equivalent ones. Moreover, by Proposition 7.2 (ii), $\mathbf{K}_\alpha$ are equivalent to CKT's $\mathbf{K}_\alpha'$ of self-gradient type

with the same function U. By Proposition 7.1, $\mathbf{K}'_\alpha$ are KT's of the conformal metric $e^U\mathbf{G}$, having common normal eigenvectors. Hence, they are in involution. ■

There is an alternative formulation of Theorem 7.3, still involving $n-1$ CKT's, due to Kalnins and Miller (Ref. 20, Theorem 4, Sec. II):

Theorem 7.4: *The HJE* (6.12) *for the null geodesics is separable in orthogonal coordinates if and only if on Q there exist* $n-1$ *CKT's* $(\mathbf{K}_\alpha)=(\mathbf{K}_1,\mathbf{K}_2,\ldots,\mathbf{K}_{n-1})$ (i) *with common eigenvectors,* (ii) *in involution and such that* (iii) $\mathbf{G},\mathbf{K}_1,\mathbf{K}_2,\ldots,\mathbf{K}_{n-1}$ *are pointwise independent.*

We give here a proof which is based on the following general characterization of the integrability of frames, which is an extension of that given in Ref. 7, Theorem 8, Sec. VIII.

Theorem 7.5: *Let* $(\mathbf{X}_i)$ *a frame on Q. Let* $(\mathbf{K}_a)$ *be n contravariant symmetric two-tensors* (i) *pointwise independent,* (ii) *simultaneously diagonalized in the frame* $(\mathbf{X}_i)$ *and such that* (iii) *for each* $a\neq b$ *there exists a vector field* $\mathbf{C}_{ab}$ *and a symmetric two tensor* $\mathbf{M}_{ab}$ *diagonalized in the frame* $(\mathbf{X}_i)$ *such that*

$$\{P(\mathbf{K}_a),P(\mathbf{K}_b)\}=2P(\mathbf{C}_{ab})P(\mathbf{M}_{ab}). \tag{7.7}$$

Then, the frame is integrable and all the two-tensors are simultaneously diagonalized in a same coordinate system.

We recall (cf. Ref. 7) that (I) a frame is called *integrable* if for each index i the distribution Δ_i spanned by the vectors $(\mathbf{X}_1,\ldots,\mathbf{X}_{i-1},\mathbf{X}_{i+1},\ldots,\mathbf{X}_n)$ is completely integrable; (II) a frame is integrable if and only if the distributions Δ_{ij} spanned by pairs of vectors $(\mathbf{X}_i,\mathbf{X}_j)$ are completely integrable; (III) a frame is integrable if and only if there exist local coordinates (q^i) such that $\mathbf{X}_i=f_i\partial/\partial q^i$, where f_i are nowhere vanishing functions.

Proof: Let us set $[\mathbf{X}_i,\mathbf{X}_j]=\Omega_{ij}^h\mathbf{X}_h$, $\Omega_{ij}^h=-\Omega_{ji}^h$, $P(\mathbf{X}_i)=x_i$, so that $\{x_i,f\}=\langle\mathbf{X}_i,\mathrm{d}f\rangle$, $\{x_i,x_j\}=P([\mathbf{X}_i,\mathbf{X}_j])=\Omega_{ij}^hx_h$. Assumptions (ii) and (iii) mean that $\mathbf{K}_a=K_a^i\mathbf{X}_i\odot\mathbf{X}_i$, $\mathbf{M}=M^i\mathbf{X}_i\odot\mathbf{X}_i$. By recalling the calculation of Ref. 7, Sec. VIII, we have

$$\{P(\mathbf{K}_a),P(\mathbf{K}_b)\}=2\big(2K_a^iK_b^h\Omega_{ih}^j+(K_a^i\langle\mathbf{X}_i,\mathrm{d}K_b^k\rangle-K_b^i\langle\mathbf{X}_i,\mathrm{d}K_a^k\rangle)\delta_k^h\delta_k^j\big)x_ix_hx_j.$$

Being $2P(\mathbf{C}_{ab})P(\mathbf{M}_{ab})=2C_{ab}^kx_kM_{ab}^lx_l^2=2C_{ab}^kM_{ab}^lx_kx_l^2$, from Eq. (7.7) it follows that

$$\big(2K_a^iK_b^h\Omega_{ih}^j+(K_a^i\langle\mathbf{X}_i,\mathrm{d}K_b^k\rangle-K_b^i\langle\mathbf{X}_i,\mathrm{d}K_a^k\rangle-C_{ab}^iM_{ab}^k)\delta_k^h\delta_k^j\big)x_ix_hx_j=0.$$

This is a homogeneous polynomial equation which must be identically satisfied for all values of the variables (p_k), i.e., for all values of the variables (x_i), since $x_i=P(\mathbf{X}_i)=X_i^kp_k$, and $\det[X_i^k]\neq0$. Thus, all coefficients vanish. In particular, the coefficient of $x_1x_2x_3$ (as well as for all possible choices of three distinct indices) gives rise to equation

$$K_a^1K_b^2\Omega_{12}^3+K_a^1K_b^3\Omega_{13}^2+K_a^2K_b^3\Omega_{23}^1+K_a^2K_b^1\Omega_{21}^3+K_a^3K_b^1\Omega_{31}^2+K_a^3K_b^2\Omega_{32}^1=0.$$

From now on the proof is the same of Theorem 8.8 of Ref. 7. ■

Proof of Theorem 7.4: The tensors $(\mathbf{K}_a)=(\mathbf{G},\mathbf{K}_\alpha)$ fulfill the assumptions of Theorem 7.5. In particular, Eqs. (7.7) become

$$\{P(\mathbf{K}_\alpha),P(\mathbf{K}_\beta)\}=0,\quad \{P(\mathbf{K}_\alpha),P(\mathbf{G})\}=2P(\mathbf{C}_\alpha)P(\mathbf{G}).$$

Hence, the common eigenvectors are normal. ■

A final important remark is that Theorems 7.2 and 7.4 can be derived from more general statements.

Definition 7.2: We say that two symmetric two-tensors $\mathbf{K}_1$ and $\mathbf{K}_2$ on a Riemannian manifold are in conformal involution if there exists a vector field $\mathbf{C}_{12}$ such that

$$[\mathbf{K}_1,\mathbf{K}_2]=2\mathbf{C}_{12}\odot\mathbf{G}\quad(\Leftrightarrow\{P_{\mathbf{K}_1},P_{\mathbf{K}_2}\}=2P_{\mathbf{C}_{12}}P_{\mathbf{G}}). \tag{7.8}$$

Theorem 7.6: *The HJE* (6.12) *for the null geodesics is separable in orthogonal coordinates if and only if on Q there exist n CKT's* $(\mathbf{K}_i)=(\mathbf{K}_0,\mathbf{K}_1,\ldots,\mathbf{K}_{n-1})$ (i) *pointwise independent,* (ii) *with common eigenvectors and* (iii) *in conformal involution.*

Proof: The common eigenvectors are normal, since equation (7.8) is a particular case of (7.7). Item (i) implies the existence of a linear combination $\mathbf{K}=c^i\mathbf{K}_i$ with simple eigenvalues. Then we apply Theorem 7.1. Conversely, due to Theorem 7.2, the separation implies the existence of independent CKT's $\mathbf{K}_i$ satisfying (7.8) with $\mathbf{C}_{ij}=0$. ■

Remark 7.5: Theorem 7.6 is in perfect analogy with the intrinsic characterization of the ordinary orthogonal separation in terms of *n* independent KT's in involution: it is enough to cancel the word "conformal." This shows that the notion of conformal involution is a natural and useful extension of the ordinary involution.

Proposition 7.5: All CKT's diagonalized in orthogonal coordinates (q^i) *are in conformal involution.*

Proof: According to Proposition 7.2, two tensors $\mathbf{K}_1$, $\mathbf{K}_2$ diagonalized in (q^i) are equivalent to two KT's $\mathbf{K}_1'=\mathbf{K}_1-\rho_1^n\mathbf{G}$, $\mathbf{K}_2'=\mathbf{K}_2-\rho_2^n\mathbf{G}$ of the conformal metric $\overline{\mathbf{G}}=\mathbf{G}/g^{nn}$. Two simultaneously diagonalized KT's are in involution (Ref. 4, Sec. II). Hence,

$$[\mathbf{K}_1,\mathbf{K}_2]=[\mathbf{K}_1'+\rho_1^n\mathbf{G},\mathbf{K}_2'+\rho_2^n\mathbf{G}]=2(\mathbf{K}_1\nabla\rho_2^n-\mathbf{K}_2\nabla\rho_1^n)\odot\mathbf{G}.$$

■

Remark 7.6: As a consequence of this proposition, for two CKT's simultaneously diagonalized in orthogonal coordinates equation (7.7), $[\mathbf{K}_1,\mathbf{K}_2]=2\mathbf{C}_{12}\odot\mathbf{M}_{12}$, implies $\mathbf{M}_{12}=\mathbf{G}$, thus the conformal involution (7.8). In other words, in Theorem 7.6 by replacing the conformal involution conditions (iii), $[\mathbf{K}_i,\mathbf{K}_j]=2\mathbf{C}_{ij}\odot\mathbf{G}$ with $[\mathbf{K}_i,\mathbf{K}_j]=2\mathbf{C}_{ij}\odot\mathbf{M}_{ij}$ we do not get an extension of the theorem.

Remark 7.7: The CKT's $\mathbf{K}_i$ of Theorem 7.6 generate an *n*-dimensional space $\mathcal{K}$ of CKT's in conformal involution which are simultaneously diagonalized in orthogonal coordinates. We call such a space a *conformal Killing–Stäckel space* (CKS space). The existence of such a space is necessary and sufficient for the orthogonal separation of the null geodesic HJE. However, since properties (i), (ii), and (iii) in this theorem are invariant with respect to the equivalence transformations $\mathbf{K}_i\rightarrow\mathbf{K}_i'=\mathbf{K}_i+f_i\mathbf{G}$, there are infinitely many CKS-spaces $\mathcal{K}'$ associated with $\mathcal{K}$, corresponding to any choice of the functions f_i, having the same properties and diagonalized in the same coordinates. We remark that (I) each CKS space contain a tensor of the kind $f\mathbf{G}$ (i.e., a symmetric tensor with *n* coinciding eigenvalues). (II) There exists a CKS space which contains the metric tensor $\mathbf{G}$. Property (I) follows from Proposition 7.3. To prove (II), starting from the given $\mathbf{K}_i$, according to Proposition 7.3, we can find a linear combination such that $c^i\mathbf{K}_i=f\mathbf{G}$. Thus, if $c^0\neq 0$, we replace $\mathbf{K}_0$ by the equivalent tensor $\mathbf{K}_0'=\mathbf{K}_0+[(1-f)/c^0]\mathbf{G}$. Then the CKS space generated by $(\mathbf{K}_0',\mathbf{K}_1,\ldots,\mathbf{K}_{n-1})$ contains the metric $\mathbf{G}=c^0\mathbf{K}_0'+c^1\mathbf{K}_1+\cdots+c^{n-1}\mathbf{K}_{n-1}$. A consequence of these remarks is that we can reformulate Theorem 7.6 assuming that the metric tensor $\mathbf{G}$ is one of the $\mathbf{K}_i$. This shows that Theorem 7.4 follows from Theorem 7.6.

B. The orthogonal separation for $E-V\neq 0$

Theorem 7.7: *The HJE* (6.13) *for a fixed value E of the energy and for* $E-V\neq 0$ *is separable in orthogonal coordinates if and only if on Q there exists a characteristic CKT* $\mathbf{K}$ *such that*

$$[\mathbf{G},\mathbf{K}]=\frac{2}{E-V}\mathbf{K}\nabla V\odot\mathbf{G} \tag{7.9}$$

or, equivalently, if and only if there exist a function f and a characteristic CKT $\mathbf{K}'$ *such that*

$$[\mathbf{G},\mathbf{K}']=\frac{2}{E-V}(\mathbf{K}'\nabla V+\nabla f)\odot\mathbf{G}. \tag{7.10}$$

Proof: The proof of the first part of this statement follows the same pattern of that of Theorem 7.1, with $\sigma=E-V$. Moreover, if we find a characteristic CKT $\mathbf{K}'$ satisfying (7.10), then the equivalent tensor $\mathbf{K}=\mathbf{K}'-[f/(E-V)]\mathbf{G}$ satisfies condition (7.9). ■

Theorem 7.8: *The HJE (6.13) for a fixed value E of the energy and for* $E-V\neq 0$ *is separable*

in orthogonal coordinates if and only if on Q there exist n CKT's $(\mathbf{K}_i)=(\mathbf{K}_0,\mathbf{K}_1,\ldots,\mathbf{K}_{n-1})$ *(i) pointwise independent, (ii) with common eigenvectors, (iii) in conformal involution and such that*

$$[\mathbf{G},\mathbf{K}_i]=\frac{2}{E-V}(\mathbf{K}_i\nabla V+\nabla f_i)\odot\mathbf{G} \tag{7.11}$$

with suitable functions f_i.

Proof: Due to Theorem 7.5 and item (iii) the common eigenvectors are normal. Items (i) and (ii) imply the existence of a CKT with simple eigenvalues satisfying (7.10). Then we apply Theorem 7.7. Conversely, if (6.13) is separable, then the Jacobi metric $\overline{\mathbf{G}}=\mathbf{G}/(E-V)$ is separable. This means that there exists n KT's $\mathbf{K}_i$ for $\overline{\mathbf{G}}$, pointwise independent, with common eigenvectors, in involution, hence in conformal involution. Recalling Proposition 7.1, we have

$$[\mathbf{G},\mathbf{K}_i]=\tfrac{2}{E-V}\mathbf{K}_i\nabla V\odot\mathbf{G}.$$

This is a particular case of (7.11). ■

Remark 7.8: This theorem shows that, in other words, the orthogonal separation of the Jacobi metric is equivalent to the existence of a CKS space satisfying the additional condition (7.11). We observe that we can always modify the basis $(\mathbf{K}_i)$ in order to include the metric tensor $\mathbf{G}$. Due to Proposition 7.2, there exist a function f and n real numbers c^i not all equal to zero, such that $f\mathbf{G}=\Sigma_i c^i\mathbf{K}_i$. Up to a reordering of the tensors, we can suppose that $c^0\neq 0$. Then, $(\mathbf{G},\mathbf{K}_\alpha)=(\mathbf{G},\mathbf{K}_1,\ldots,\mathbf{K}_{n-1})$ satisfy items (ii), (iii) and are pointwise independent,

$$\det\begin{bmatrix} g^{ii} \\ K^{ii}_\alpha \end{bmatrix}=\frac{1}{f}\det\begin{bmatrix} c^jK^{ii}_j \\ K^{ii}_\alpha \end{bmatrix}=\sum_{\beta=1}^{n-1}\frac{c^\beta}{f}\det\begin{bmatrix} K^{ii}_\beta \\ K^{ii}_\alpha \end{bmatrix}+\frac{c^0}{f}\det\begin{bmatrix} K^{ii}_0 \\ K^{ii}_\alpha \end{bmatrix}=\frac{c^0}{f}\det[K^{ii}_j]\neq 0.$$

VIII. SEPARATED EQUATIONS

Summarizing the results of Sec. VII A, we have five intrinsic characterizations of the orthogonal separation of the null geodesic HJE: Theorem 7.1 (involving a single characteristic CKT), Theorem 7.2 (involving n CKT's in involution), Theorem 7.3 (involving $n-1$ simultaneously diagonalized CKT's), Theorem 7.4 (involving $n-1$ CKT's in involution), and Theorem 7.6 (involving n CKT's in conformal involution). We show how, for each one of these characterizations, we can reduce the HJE to separated ordinary differential equations. This reduction involves the use of Stäckel matrices. As shown in Ref. 2, we can state the following.

Lemma 8.1: Let $(F_i)=(F_1,\ldots,F_n)$ *be n independent functions of the form* $F_i=\varphi^j_{(i)}p_j^2$. *They are in involution if and only if the matrix* $[\varphi^j_{(i)}]$ *is the inverse of a Stäckel matrix* $\mathbf{S}=[\varphi^{(j)}_i]$.

Proof: We prove this statement in a direct way, without any reference with the known links between Stäckel matrices and the orthogonal separation. The condition

$$\{F_i,F_h\}=2(\varphi^k_{(i)}\partial_k\varphi^j_{(h)}-\varphi^k_{(h)}\partial_k\varphi^j_{(i)})p_kp_j^2=0$$

is equivalent to equations

$$\varphi^k_{(i)}\partial_k\varphi^j_{(h)}=\varphi^k_{(h)}\partial_k\varphi^j_{(i)},\quad k\ \text{n.s.} \tag{8.1}$$

(i) Multiplying by $\varphi^{(i)}_l$ and summing over i, we get the equivalent system $\delta^k_l\partial_k\varphi^{(h)}_j=-\varphi^k_{(h)}\Sigma_i\varphi^j_{(i)}\partial_k\varphi^{(i)}_l$. For $k\neq l$, $\varphi^k_{(h)}\Sigma_i\varphi^j_{(i)}\partial_k\varphi^{(i)}_l=0$. For any fixed index k there always exists an index h such that $\varphi^k_{(h)}\neq 0$. It follows that $\Sigma_i\varphi^j_{(i)}\partial_k\varphi^{(i)}_l=0$. And this is equivalent to $\partial_k\varphi^{(i)}_l=0$, for $k\neq l$. (ii) Conversely, let $[\varphi^{(j)}_i]$ be a Stäckel matrix. By applying ∂_k to equation $\varphi^i_{(h)}\varphi^{(l)}_i=\delta^l_h$, we get $\Sigma_i(\varphi^{(l)}_i\partial_k\varphi^i_{(h)})+\varphi^k_{(h)}\partial_k\varphi^{(l)}_k=0$. Let us multiply by $\varphi^j_{(l)}$ and sum over the index l; we get $\partial_k\varphi^j_{(h)}-\varphi^k_{(h)}\Sigma_l\varphi^{(l)}_k\partial_k\varphi^j_{(l)}=0$. If we multiply by $\varphi^k_{(i)}$ without summing over k, then we find $\varphi^k_{(i)}\partial_k\varphi^j_{(h)}=\varphi^k_{(i)}\varphi^k_{(h)}\Sigma_l\varphi^{(l)}_k\partial_k\varphi^j_{(l)}$. This shows that $\varphi^k_{(i)}\partial_k\varphi^j_{(h)}$ is symmetric with respect to the indices (i,h). Thus,

(8.1) is proved. ■

Case of Theorem 7.2: Let $(\mathbf{K}_i)$ be n CKT's satisfying the conditions of this theorem. The functions $F_i = K_i^{jj} p_j^2$ fulfill Lemma 8.1. Hence, $\varphi^j_{(i)} \doteq K_i^{jj}$ form the inverse $\mathbf{S}^{-1}$ of a Stäckel matrix. Moreover, since they are CKT's, see (7.3), we have $\{P_{\mathbf{G}}, F_i\} = 2P_{\mathbf{C}_i} P_{\mathbf{G}}$, where $P_{\mathbf{G}} = g^{ii} p_i^2$. This shows that F_i *are null first integrals* of the null geodesics [cf. (4.27)]. Since F_i are independent and in involution, equations

$$F_i(\underline{q}, \underline{p}) \doteq K_i^{jj} p_j^2 = c_i \tag{8.2}$$

describe a Lagrangian foliation on an open subset of T^*Q which is compatible with the submanifold of equation $g^{ii} p_i^2 = 0$ (see Sec. II). This foliation is the geometrical counterpart of an extended complete solution of the null HJE. This complete solution is separable. Indeed, by solving equations (8.2), $\varphi^j_{(i)} p_j^2 = c_i$, we get the separated equations

$$p_j^2 = \varphi_j^{(i)} c_i. \tag{8.3}$$

Case of Theorem 7.3: Let $(\mathbf{K}_\alpha) = (\mathbf{K}_1, \ldots, \mathbf{K}_{n-1})$ be $n-1$ CKT's satisfying the conditions of this theorem. They are diagonalized in orthogonal coordinates. Let us consider the diagonalized tensors $\mathbf{K}'_\alpha = \mathbf{K}_\alpha - \rho_\alpha^n \mathbf{G}$, where ρ_α^n are the last eigenvalues of $\mathbf{K}_\alpha$. Since $\rho_\alpha^n = K_\alpha^{nn}/g^{nn}$, the diagonal components of $\mathbf{K}'_\alpha$ are

$$K_\alpha^{jj} - K_\alpha^{nn} \frac{g^{jj}}{g^{nn}}. \tag{8.4}$$

By recalling the proof of Proposition 7.2, all $\mathbf{K}'_\alpha$ are KT's of the conformal metric $\mathbf{G}/g^{nn}$, simultaneously diagonalized, hence in involution. As a consequence, the $n-1$ functions

$$F_\alpha \doteq \left(K_\alpha^{jj} - K_\alpha^{nn} \frac{g^{jj}}{g^{nn}} \right) p_j^2$$

are null first integrals in involution of the null geodesics. Moreover, the function

$$F_n \doteq \frac{g^{jj}}{g^{nn}} p_j^2$$

is a further null first integral in involution. These n first integrals in involution are independent because of item (ii) of Theorem 7.3. Thus, due to Lemma 8.1, the functions

$$\varphi^j_{(\alpha)} \doteq K_\alpha^{jj} - K_\alpha^{nn} \frac{g^{jj}}{g^{nn}}, \quad \varphi^j_{(n)} \doteq \frac{g^{jj}}{g^{nn}},$$

form the inverse of a Stäckel matrix. It follows that equations

$$F_\alpha = \varphi^j_{(\alpha)} p_j^2 = c_\alpha, \quad F_n = \varphi^j_{(n)} p_j^2 = 0, \tag{8.5}$$

define a Lagrangian foliation of the submanifold $g^{ii} p_i^2 = 0$, which is the geometrical counterpart of an internal complete solution of the null HJE. This complete solution is separable. Indeed, by solving equations (8.5), $\varphi^j_{(i)} p_j^2 = c_i$, with $c_n = 0$, we get separated equations of the kind (8.3), but with $n-1$ constant parameters (c_α),

$$p_j^2 = \varphi_j^{(\alpha)} c_\alpha. \tag{8.6}$$

This result is in agreement with Remark 6.8.

Case of Theorem 7.4: The procedure is the same as for the case of Theorem 7.3.

Case of Theorem 7.6: Let $(\mathbf{K}_i)$ be n CKT's satisfying the conditions of this theorem. By recalling Remark 7.7, we can always find a linear (constant coefficients) combination such that $a^i \mathbf{K}_i = f\mathbf{G}$. When the constants a^i and the function f are determined, assuming (up to a reordering)

that $a^0 \neq 0$, we can replace $\mathbf{K}_0$ by $\mathbf{G}$, and we are in the case of Theorem 7.3.

Case of Theorem 7.1: We point out that Theorem 7.1 is convenient for characterizing the separation, since it involves only a single CKT. However, in order to get separated equations (involving a Stäckel matrix) we need to know $n-1$ CKT's. Let ρ^i be the eigenvalues of the given characteristic CKT $\mathbf{K}$. According to Proposition 7.2, the tensor $\widetilde{\mathbf{K}}=\mathbf{K}-\rho^n\mathbf{G}$ is a characteristic KT for the conformal metric $\overline{\mathbf{G}}=\mathbf{G}/g^{nn}$ (instead of the last one n, we can choose any other index). As it is well known, any characteristic KT generates a n-space of KT's simultaneously diagonalized in orthogonal coordinates, whose eigenvalues $\overline{\rho}^i$ with respect to the metric $\overline{\mathbf{G}}$ satisfy the Killing–Eisenhart equations

$$\partial_i \overline{\rho}^j = (\overline{\rho}^i - \overline{\rho}^j)\partial_i \ln \overline{g}^{jj} \tag{8.7}$$

which form a complete integrable system. Since $\overline{\rho}^j=(\rho^j-\rho^n)g^{nn}$, we observe that for the given tensor $\widetilde{\mathbf{K}}$ we have $\overline{\rho}^n=0$. We observe that, following Kalnins and Miller,[20] if we set $\mu^i=\rho^i-\rho^n$, then from (8.7) we obtain equations

$$\partial_i \mu^j = (\mu^i - \mu^j)\partial_i \ln g^{jj} - \mu^i \partial_i \ln g^{nn},$$

which summarize Eqs. (2.8) of Ref. 20. Let us take n independent solutions $\overline{\rho}_i^j$ of system (8.7) with $\overline{\rho}_n^j=1$ for all j. The corresponding tensors $\mathbf{K}_i$ of components $K_i^{jj}=\overline{\rho}_i^j g^{jj}/g^{nn}$ are independent KT's for $\overline{\mathbf{G}}$ such that $\mathbf{K}_n=\overline{\mathbf{G}}$. This means that

$$\varphi_{(i)}^j = K_i^{jj} = \overline{\rho}_i^j g^{jj}/g^{nn}$$

form the inverse of a Stäckel matrix and equations $\varphi_{(i)}^j p_j^2 = c_i$ are equivalent to the separated equations $p_j^2=\varphi_j^{(i)}c_i$. This gives an extended separated solution. For $c_n=0$ we get the null geodesics.

Finally, let us consider the case of $E-V\neq 0$.

Case of Theorem 7.8: Let $(\mathbf{K}_i)=(\mathbf{K}_0,\ldots,\mathbf{K}_{n-1})$ be n CKT's satisfying the conditions of this theorem. By recalling the proof of Theorem 7.7, if we perform the equivalence transformation $\widetilde{\mathbf{K}}_i=\mathbf{K}_i-[f_i/(E-V)]\mathbf{G}$ we get n KT's of the Jacobi metric $\overline{\mathbf{G}}=\mathbf{G}/(E-V)$, characterizing its orthogonal separation. Then the functions $\varphi_{(i)}^j=K_i^{jj}-f_i/(E-V)$ form the inverse of a Stäckel matrix. By solving equations $\varphi_{(i)}^j p_j^2=c_i$, we get the separated equations

$$p_j^2 = \varphi_j^{(i)} c_i \tag{8.8}$$

thus, a complete separated solution of the HJE,

$$(E-V)^{-1} g^{ii} p_i^2 = 2h. \tag{8.9}$$

The separated solution following from (8.8) is an extended separated solution of the HJE $\frac{1}{2}g^{ii}p_i^2 = E-V$ with the fixed value E of the energy. By substituting in (8.9) the expressions of p_j given by (8.8), we get an equation of the kind $h=h(c_i)$. It follows that for $h=1$ we get equation $h(c_i)=1$. When the constants c_i satisfy this equation we get an internal separated solution of the HJE for the given value E of the energy.

Case of Theorem 7.7: If we have a characteristic CKT tensor $\mathbf{K}'$ satisfying (7.10), then $\mathbf{K}=\mathbf{K}'-[f/(E-V)]\mathbf{G}$ is characteristic KT of the Jacobi metric $\overline{\mathbf{G}}=\mathbf{G}/(E-V)$. System (8.7) with $\overline{g}^{jj}=g^{jj}/(E-V)$ is completely integrable and provides n independent solutions $\overline{\rho}_i^j$ with $\overline{\rho}_n^j=1$ for all j. With such a solution we define the inverse of a Stäckel matrix by setting $\varphi_{(i)}^j=\overline{\rho}_i^j g^{jj}/(E-V)$. Then, by solving equations $\varphi_{(i)}^j p_j^2=c_i$ we get separated equations which define an extended separated solution. By setting $c_n=1$ we get an internal separated solution. We remark that in both cases the Stäckel matrices depend on the value E.

IX. THE TWO-DIMENSIONAL CASE

A two-dimensional Riemannian manifold is always conformally flat. The link between the conformal separation in two dimensions, the analytical functions and the CKT's is examined in Ref. 28, and used for generalizing a result of Ref. 25. We show here how some known results follow from the general theory developed in the preceding sections.

We can write the most general 2×2 Stäckel matrix in two variables in the form

$$\mathbf{S}=\begin{bmatrix}\phi_1(q^1) & \psi_1(q^1)\\ \phi_2(q^2) & \psi_2(q^2)\end{bmatrix},\quad \phi_1\psi_2-\phi_2\psi_1\neq 0. \tag{9.1}$$

The inverse matrix is

$$\mathbf{S}^{-1}=\frac{1}{\phi_1\psi_2-\phi_2\psi_1}\begin{bmatrix}\psi_2 & -\psi_1\\ -\phi_2 & \phi_1\end{bmatrix}. \tag{9.2}$$

The components $\bar{g}^{ii}$ of a separable orthogonal metric $\overline{\mathbf{G}}$ and of the associated KT $\mathbf{K}$ are given by the second and the first line of $\mathbf{S}^{-1}$,

$$[\bar{g}^{11},\bar{g}^{22}]=\frac{1}{\phi_1\psi_2-\psi_1\phi_2}[-\phi_2,\phi_1],\quad [K^{11},K^{22}]=\frac{1}{\phi_1\psi_2-\psi_1\phi_2}[\psi_2,-\psi_1].$$

Then Theorem 6.10 implies the following.

Theorem 9.1: (i) *The HJE of the null geodesics* (6.12) *is separable in the orthogonal coordinates* (q^1,q^2) *if and only if there exist two nowhere vanishing functions* $\xi_1(q^1)$ *and* $\xi_2(q^2)$ *such that*

$$\frac{g^{11}}{g^{22}}=\frac{\xi_1}{\xi_2}. \tag{9.3}$$

(ii) *The HJE* (6.13), *for a fixed value of* E *and for* $E-V\neq 0$, *is separable in the orthogonal coordinates* (q^1,q^2) *if and only if there exist four functions* $(\xi_1(q^1),\xi_2(q^2),\psi_1(q^1),\psi_2(q^2))$, *with*

$$\frac{\psi_2}{\xi_1}+\frac{\psi_1}{\xi_2}\neq 0, \tag{9.4}$$

such that (9.3) *holds and moreover*,

$$E-V=\psi_1 g^{11}+\psi_2 g^{22}. \tag{9.5}$$

Proof: From (6.17) and (9.2) it follows that there exist functions $\phi_1(q^1)$ and $\phi_2(q^2)$ such that $g^{11}/g^{22}=-\phi_2/\phi_1$. The functions ξ_i of the statement are then given by $\xi_1=1/\phi_1$ and $\xi_2=-1/\phi_2$. Formula (9.5) follows from (6.18) and (9.1). Condition (9.4) is the regularity condition of the Stäckel matrix (9.1). ■

From Theorem 9.1 it follows that on a two-dimensional Riemannian manifold, orthogonal coordinates (q^1,q^2) are conformal separable coordinates if and only if the ratio g^{11}/g^{22} has the form (9.3), which is equivalent to say that g^{11}/g^{22} is a product of two functions depending only on q^1 and q^2, respectively. In Remark 6.3 we have seen that coordinates satisfying $g^{ii}=c^i\sigma(\underline{q})$ $(c^i\in\mathbb{R})$ are conformal separable. The following theorem shows that in fact any two-dimensional conformal separable system is of this kind.

Theorem 9.2: *On a two-dimensional manifold an orthogonal coordinate system is conformal separable if and only if, up to a rescaling,*

$$g^{11}=\pm g^{22}. \tag{9.6}$$

Proof: According to Remark 6.3, if (9.6) holds, then the coordinates are conformal separable. Conversely, assume that (9.3) holds. Then $g_{11}=\rho/\xi_1$, $g_{22}=\rho/\xi_2$, and

$$ds^2 = g_{11}(dq^1)^2 + g_{22}(dq^2)^2 = \rho\left(\frac{(dq^1)^2}{\xi_1} + \frac{(dq^2)^2}{\xi_2}\right).$$

In the coordinates $(\tilde{q}^i)$ defined by the rescaling $d\tilde{q}^i = |\xi_i|^{-1/2}\, dq^i$ we have $ds^2 = \rho(e_1(d\tilde{q}^1)^2 + e_2(d\tilde{q}^2)^2)$, where $e_i = \mathrm{sign}(\xi_i)$. It follows that $\tilde{g}_{ii} = \rho e_i$. ■

Remark 9.1: If (9.6) holds, from (9.3) and (9.5) it follows that $\xi_2 = \pm\xi_1 = \text{constant}$ and $E - V = (\psi_1 \pm \psi_2)g^{11}$. Then the Stäckel matrix (9.1) and its inverse (9.2) have the form

$$\mathbf{S} = \begin{bmatrix} c & \psi_1(q^1) \\ \mp c & \psi_2(q^2) \end{bmatrix}, \quad \psi_2 \pm \psi_1 \neq 0, \quad \mathbf{S}^{-1} = \frac{1}{c(\psi_2 \pm \psi_1)} \begin{bmatrix} \psi_2 & -\psi_1 \\ \pm c & c \end{bmatrix}.$$

Let us consider the particular case of the Euclidean plane $\mathbb{E}_2$, with Cartesian coordinates (x,y). We recall the following (see, e.g., Ref. 28).

Proposition 9.1: *If $f(z) = u(x,y) + iv(x,y)$, $z = x + iy$, is a non constant analytic function, then in the open domain where $\nabla u \neq 0$ the real and the imaginary parts define conformal separable coordinates $q^1 = u(x,y)$ and $q^2 = v(x,y)$ such that $g^{11} = g^{22}$.*

Proof: From the Cauchy–Riemann conditions

$$u_x = v_y, \quad u_y = -v_x \tag{9.7}$$

(the suffixes denote the partial derivatives) it follows that

$$g^{12} = u_x v_x + u_y v_y = 0, \quad g^{11} = (u_x)^2 + (u_y)^2 = (v_y)^2 + (v_x)^2 = g^{22}. \tag{9.8}$$

Then we apply Remark 9.1. The coordinate transformation is singular at those points where the partial derivatives (9.7) vanish, since

$$\det\begin{bmatrix} u_x & v_x \\ u_y & v_y \end{bmatrix} = u_x v_y - v_x u_y = (u_x)^2 + (u_y)^2 .$$ ■

By applying Theorem 9.2, we prove the converse of Proposition 9.1.

Proposition 9.2: *Up to a rescaling, every conformal separable system of the Euclidean plane is generated by a nonconstant analytic function.*

*Proof:*According to Theorem 9.2, we can rescale a conformal separable coordinate system in order to have $g^{11} = g^{22}$ and such that the corresponding coordinate transformation satisfies (9.8). The solutions of (9.8) are

$$\begin{aligned} u_x &= v_y, & u_x &= -v_y, \\ u_y &= -v_x, & u_y &= v_x, \end{aligned}$$

which are the Cauchy–Riemann conditions for $f = u(x,y) + iv(x,y)$ or $\tilde{f} = v(x,y) + iu(x,y)$. Hence the coordinates are generated by an analytic function. ■

Remark 9.2: The real and imaginary part of a given analytic function are both harmonic functions on $\mathbb{R}^2$, i.e., solutions of the Laplace equation in the plane $\Delta u = 0$. Conversely, each harmonic function $u(x,y)$ can be chosen as real part of an analytic function. The corresponding imaginary part $v(x,y)$ is determined up to an additive constant.

Remark 9.3: It is possible to associate with every harmonic function a class of potentials, depending on two real parameters a, b, which are separable for a single value of the energy. The conformal separable coordinates and the suitable value of E depend on (a,b). Let $u(x,y)$ be a harmonic function. Then, the functions $\tilde{u} = u + ax + by$, $a,b \in \mathbb{R}$ are harmonic. According to Remark 9.2, we construct a coordinate transformation

$$q^1 = q^1(x,y) = \tilde{u}, \quad q^2 = q^2(x,y) = \tilde{v},$$

with $\tilde{v}$ such that $\tilde{u} + i\tilde{v}$ is analytic. For these coordinates we have

$$g^{11} = g^{22} = \left(\frac{\partial \tilde{u}}{\partial x}\right)^2 + \left(\frac{\partial \tilde{u}}{\partial y}\right)^2.$$

Hence, (q^1, q^2) are conformal separable coordinates compatible with a natural Hamiltonian $H = G + V$ for a fixed value of the energy E if and only if

$$E - V = (\psi_1(q^1) + \psi_2(q^2))g^{11}. \tag{9.9}$$

In particular, the case $E - V = g^{11}$ is satisfied by choosing $E = a^2 + b^2$ and

$$V(x,y) = \left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2 + 2a\frac{\partial u}{\partial x} + 2b\frac{\partial u}{\partial y}. \tag{9.10}$$

In the following example we consider a dynamical system with a scalar potential depending on a single parameter a, which is a special case of the potential (9.10) obtained by considering $b = 0$ in the preceding discussion.

Example 9.1: In $\mathbb{E}_2$ let us consider the potential

$$V(x,y) = -\frac{2ax + 1}{x^2 + y^2},$$

where (x,y) are Cartesian coordinates and a is a real parameter. By examining the separability condition

$$\mathrm{d}(\mathbf{K}\,\mathrm{d}V) = 0, \tag{9.11}$$

where $\mathbf{K}$ is a generic KT of the Euclidean plane (see Ref. 6 for the details of this technique), we find that, for $a \neq 0$, (9.11) is satisfied only for $\mathbf{K} = \mathbf{G}$ (the metric tensor). Thus, for $a \neq 0$, V is not separable in $\mathbb{E}_2$. However, for any value of $a \neq 0$ there is a suitable value of the energy E, such that the HJE $G + V - E = 0$ is separable in a conformal coordinate system depending on a. Let us consider

$$q^1 = \log\sqrt{x^2 + y^2} + ax = \log \varrho + a\varrho \cos \vartheta, \quad q^2 = \arctan\left(\frac{y}{x}\right) + k\pi + ay = \vartheta + a\varrho \sin \theta.$$

With respect to these coordinates we have

$$g^{11}(q^1,q^2) = g^{22}(q^1,q^2) = \frac{x^2}{(x^2 + y^2)^2} + a^2 + \frac{2ax}{x^2 + y^2} + \frac{y^2}{(x^2 + y^2)^2} = \frac{2ax + 1}{x^2 + y^2} + a^2.$$

Thus, (q^1, q^2) are conformally separable. Moreover, since for $E = a^2$ we get $E - V = g^{11}$, which is of the form (9.9), we have the separation of variables for the fixed value of the energy $E = a^2$. Now we solve the HJE and the corresponding dynamical system. We construct the Stäckel matrix $\mathbf{S}$ associated with (q^1, q^2). By applying to this special case (9.3), (9.4), and (9.9), we have

$$\xi_1 = 1 = \xi_2, \quad \psi_1 = 1, \quad \psi_2 = 0,$$

so that the Stäckel matrix and its inverse are

$$\mathbf{S} = \begin{bmatrix} 1 & 1 \\ -1 & 0 \end{bmatrix}, \quad \mathbf{S}^{-1} = \begin{bmatrix} 0 & -1 \\ 1 & 1 \end{bmatrix}.$$

A basis of the conformal Killing–Stäckel space is

$$\mathbf{G} = \frac{\partial}{\partial q^1} \otimes \frac{\partial}{\partial q^1} + \frac{\partial}{\partial q^2} \otimes \frac{\partial}{\partial q^2}, \quad \mathbf{K} = \frac{\partial}{\partial q^2} \otimes \frac{\partial}{\partial q^2}.$$

With respect to the new coordinates, the natural Hamiltonian

$$\mathcal{H} = \frac{1}{2}p_x^2 + \frac{1}{2}p_y^2 - \frac{2ax+1}{x^2+y^2} - a^2$$

becomes the geodesic Hamiltonian $J_E = \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2$. The quadratic first integral is $H_K = \frac{1}{2}p_2^2$. The separated equations are given by the system

$$\begin{array}{ll} J_E = h, & \\ H_K = c, & \end{array} \Leftrightarrow \begin{array}{l} \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 = h, \\ \frac{1}{2}p_2^2 = c, \end{array} \Leftrightarrow \begin{array}{l} p_1^2 = 2(h-c), \\ p_2^2 = 2c. \end{array}$$

The constants have to fulfill the conditions $0 \leqslant c \leqslant h$. The integral curves of the Hamilton equations are

$$p_1 = \pm\sqrt{2(h-c)}, \quad p_2 = \pm\sqrt{2c}, \quad q^1 = \pm\sqrt{2(h-c)}t + q_0^1, \quad q^2 = \pm\sqrt{2c}t + q_0^2,$$

and their orbits are described by the equation

$$q^1 - q_0^1 = \pm\sqrt{\frac{h-c}{c}}(q^2 - q_0^2).$$

For $h=1$, we have the orbits of $\mathcal{H}=0$, i.e., of the natural Hamiltonian with potential V and energy $E=a^2$, parametrized by $c \in (0,1)$. In Cartesian coordinates the orbits are given by

$$\log\sqrt{x^2+y^2} + ax = \pm\sqrt{\frac{1-c}{c}}\left[\arctan\left(\frac{y}{x}\right) + k\pi + ay\right] + d$$

and in polar coordinates (ϱ, ϑ) by

$$\log\varrho + a\varrho\cos\vartheta = \pm\sqrt{\frac{1-c}{c}}(\vartheta + a\varrho\sin\theta) + d,$$

where $d = q_0^1 \pm \sqrt{[1-c/c]}q_0^2$ is a constant depending on the initial point.

Remark 9.4: For $n>2$ it is no longer possible to relate conformal separable coordinates with analytic functions, as for the case $n=2$. However, it can be seen that the orthogonal coordinate systems which allow the R-separation of the Laplace equation in n-dimensional manifolds with constant curvature, obtained by different methods,[8,10,17,19,27] and known in the Euclidean three-space as confocal cyclides[12,13] are all conformal separable coordinates according to our Definition 6.1. This fact exhibits the deep relation between the R-separation and the separation of the HJE with a fixed value of the energy developed in this paper. Indeed, both conformal separable and R-separable coordinates are characterized by CKT's (see, e.g., Ref. 20). A further analysis of this link is in progress.

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Magnetic hydrodynamics with asymmetric stress tensor

Yuly Billig[a)]
School of Mathematics and Statistics, Carleton University, Ottawa, Canada K1S 5B6

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In this paper we study equations of magnetic hydrodynamics with a stress tensor. We interpret this system as the generalized Euler equation associated with an Abelian extension of the Lie algebra of vector fields with a nontrivial 2-cocycle. We use the Lie algebra approach to prove the energy conservation law and the conservation of cross-helicity. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1857065]

I. INTRODUCTION

Magnetic hydrodynamics (MHD) describes evolution of a fluid or plasma, carrying a magnetic field. This theory is used to model the processes in the Solar corona,[22] as well as to design tokamaks.[14] There are numerous books treating various aspects of the subject, see e.g., Refs. 9 and 20.

The MHD equations are derived from the Euler equation of motion of an incompressible fluid and the Maxwell's electrodynamics equations, and describe evolution of a fluid with the velocity vector field $\mathbf{v}$ and the magnetic field $\mathbf{B}$,

$$\frac{\partial \mathbf{v}}{\partial t} = -(\mathbf{v}\cdot\nabla)\mathbf{v} + (\mathbf{B}\cdot\nabla)\mathbf{B} - \nabla p,$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\{\mathbf{v},\mathbf{B}\},$$

$$\operatorname{div}(\mathbf{v}) = 0, \quad \operatorname{div}(\mathbf{B}) = 0. \tag{1.1}$$

In this paper we study another system of PDEs, where we add extra terms into the evolution equation for the velocity,

$$\frac{\partial \mathbf{v}}{\partial t} = -(\mathbf{v}\cdot\nabla)\mathbf{v} + (\mathbf{B}\cdot\nabla)\mathbf{B} + \sum_{i,j} \frac{\partial B_i}{\partial x_j}\nabla\frac{\partial v_j}{\partial x_i} - \nabla p. \tag{1.2}$$

The additional terms here are of the third degree in derivatives and one can draw certain parallels between (1.2) and the Korteweg–de Vries equation,

$$u_t = uu_x + u_{xxx}. \tag{1.3}$$

We interpret the extra terms in (1.2) as a contribution of a stress tensor,

$$T_{ki} = \sum_j \frac{\partial B_i}{\partial x_j}\frac{\partial v_j}{\partial x_k}. \tag{1.4}$$

This stress tensor is not symmetric, which indicates that the particles of the fluid should possess electric or magnetic momentum.

[a)]Electronic mail: billig@math.carleton.ca

In spite of the additional higher-order terms, the new system of PDEs retains many features of the original system. In particular, we show that it still admits the Alfvén wave solutions.

We follow an approach developed by Arnold to give an interpretation of the MHD equations with the stress tensor as a generalized Euler equation. A generalized Euler equation is an equation for the geodesics on a (possibly infinite-dimensional) Lie group supplied with a Riemannian structure. This equation describes the evolution of a tangent vector of the geodesic in the Lie algebra of the Lie group (see Sec. III for details).

The Lie algebra that corresponds to the MHD equations with the stress tensor is an Abelian extension $\mathfrak{g}(\tau)$ of the Lie algebra of the divergence zero vector fields twisted with a nontrivial 2-cocycle τ. This Lie algebra was studied in the framework of the representation theory of the toroidal Lie algebras and the cocycle plays a prominent role there.

Infinite-dimensional groups associated with Abelian extensions of the Lie algebra of vector fields are discussed in Ref. 8.

The Lie algebra $\mathfrak{g}(\tau)$ has nice properties and this translates into nice properties of the PDEs. In particular we establish the energy conservation law and the cross-helicity conservation for MHD with the stress tensor.

Ovsienko and Khesin showed in Ref. 21 that the generalized Euler equation for the Lie algebra of vector fields on a circle yields the nonlinear wave equation $u_t = uu_x$, while incorporation of the Virasoro cocycle into the Lie algebra leads to the Korteweg–de Vries equation (1.3). In a way, the present paper may be viewed as a higher-dimensional generalization of Ref. 21.

The paper is organized as follows: in Sec. II we discuss the properties of the system (1.2), derive the expression for the stress tensor, list the conservation laws and describe the Alfvén wave solutions. In Sec. III we review the generalized Euler equation for an arbitrary Lie algebra and we apply this method in Sec. IV to an Abelian extension of the Lie algebra of the divergence zero vector fields, deriving (1.2), and establishing the conservation laws in a purely algebraic way.

II. MAGNETIC HYDRODYNAMICS WITH A STRESS TENSOR AND ITS PROPERTIES

Evolution of an incompressible fluid carrying a magnetic field is given by the equations of magnetic hydrodynamics (MHD),

$$\frac{\partial \mathbf{v}}{\partial t} = -(\mathbf{v}\cdot\nabla)\mathbf{v} + (\mathbf{B}\cdot\nabla)\mathbf{B} - \nabla p,$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\{\mathbf{v},\mathbf{B}\},$$

$$\operatorname{div}(\mathbf{v}) = 0, \quad \operatorname{div}(\mathbf{B}) = 0. \tag{2.1}$$

Here $\mathbf{B}$ is the magnetic field, $\mathbf{v}$ is the velocity vector field of the fluid, and p (pressure) is an auxiliary function which is chosen in such a way that the equation $\operatorname{div}(\mathbf{v})=0$ is satisfied. The formal dot product $\mathbf{v}\cdot\nabla$ represents the differential operator

$$\mathbf{v}\cdot\nabla = \sum_j v_j \frac{\partial}{\partial x_j}.$$

The Poisson (Lie) bracket $\{\mathbf{v},\mathbf{B}\}$ of two vector fields $\mathbf{v}=\Sigma_j v_j(x)(\partial/\partial x_j)$ and $\mathbf{B}=\Sigma_j B_j(x)(\partial/\partial x_j)$ is given by

$$\{\mathbf{v},\mathbf{B}\} = \operatorname{ad}(\mathbf{v})\mathbf{B} = (\mathbf{v}\cdot\nabla)\mathbf{B} - (\mathbf{B}\cdot\nabla)\mathbf{v} = \sum_j \left(v_j \frac{\partial \mathbf{B}}{\partial x_j} - B_j \frac{\partial \mathbf{v}}{\partial x_j} \right).$$

In the three-dimensional space, the first equation in (2.1) may be also written as

$$\frac{\partial \mathbf{v}}{\partial t} = \mathbf{v} \times \operatorname{curl}(\mathbf{v}) + \operatorname{curl}(\mathbf{B}) \times \mathbf{B} - \nabla p.$$

For a conducting medium, the curl of the magnetic field is equal to the electric current (Ampère's law), and so the expression curl $(\mathbf{B}) \times \mathbf{B}$ represents the Lorentz force, with which the magnetic field acts on the current.

The configuration space for a flow of an incompressible fluid is the group of volume-preserving diffeomorphisms. In his remarkable paper,[2] Arnold interpreted the Euler equation for an ideal fluid as the geodesic equation on this Lie group. The geodesic equation describes the evolution of the tangent vector of the geodesic curve, and this tangent vector belongs to the Lie algebra, which is the Lie algebra SVect of the divergence zero vector fields, in case of the group of volume preserving diffeomorphisms.

Using Arnold's method, Vishik and Dolzhanskii[24] (see also Ref. 17) showed that the MHD equations (2.1) also may be interpreted as a geodesic equation for a certain infinite-dimensional Lie group. The Lie algebra that is used to write this equation is the semidirect product

$$\mathrm{SVect} \oplus \Omega^1/\mathrm{d}\Omega^0$$

of the Lie algebra of divergence zero vector fields SVect with its dual space—the factor $\Omega^1/\mathrm{d}\Omega^0$ of the differential 1-forms modulo the exact 1-forms. We review this construction in detail in Sec. III.

The Lie algebra that is associated with the MHD equations,

$$\mathfrak{g} = \mathrm{SVect} \oplus \Omega^1/\mathrm{d}\Omega^0,$$

has recently attracted much interest in representation theory. It turns out that representations of $\mathfrak{g}$ may be used for constructing modules for toroidal Lie algebras (see, e.g., Refs. 5, 6, and 11). It was also discovered that this Lie algebra has an important deformation—the Lie bracket in $\mathfrak{g}$ may be twisted with a Virasoro-like 2-cocycle τ. The twisted Lie algebra $\mathfrak{g}(\tau)$ still has nice properties, and its representation theory is even better than for $\mathfrak{g}$ itself.

In this paper we study the system of PDEs that comes from the geodesic equation for $\mathfrak{g}(\tau)$. In Sec. IV we show that this Lie algebra yields the following system of PDEs:

$$\frac{\partial \mathbf{v}}{\partial t} = -(\mathbf{v} \cdot \nabla)\mathbf{v} + (\mathbf{B} \cdot \nabla)\mathbf{B} + \sum_{i,j} \frac{\partial B_i}{\partial x_j} \nabla \frac{\partial v_j}{\partial x_i} - \nabla p,$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\{\mathbf{v}, \mathbf{B}\},$$

$$\operatorname{div}(\mathbf{v}) = 0, \quad \operatorname{div}(\mathbf{B}) = 0. \tag{2.2}$$

Let us discuss the properties of this system of PDEs.

First of all, we note that the new term

$$\sum_{i,j} \frac{\partial B_i}{\partial x_j} \nabla \frac{\partial v_j}{\partial x_i} = \sum_{i,j} \frac{\partial^2}{\partial x_i \, \partial x_j} (B_i \nabla v_j) \tag{2.3}$$

can also be written as

$$-\sum_{i,j} \frac{\partial v_j}{\partial x_i} \nabla \frac{\partial B_i}{\partial x_j}, \tag{2.3$'$}$$

since the difference of the two expressions is the gradient of $\Sigma_{i,j}(\partial v_j/\partial x_i)(\partial B_i/\partial x_j)$ and may be absorbed into ∇p.

It is curious to note here that in the one-dimensional case the passage from the Lie algebra of vector fields to the Virasoro algebra leads to the transition from the nonlinear wave equation

$$u_t = uu_x$$

to the Korteweg–de Vries equation

$$u_t = uu_x + u_{xxx},$$

as shown by Ovsienko and Khesin in Ref. 21.

Just like the dispersion term u_{xxx} in the KdV, the new term $\Sigma_{i,j}(\partial B_i/\partial x_j)\nabla(\partial v_j/\mathrm{d}x_i)$ that we get in (2.2) has a triple derivative in x.

Next we are going to show that (2.2) describes magnetic hydrodynamics with a *stress tensor*. Indeed, for a stress tensor T_{ki}, the equations on the velocity field in (2.1) will become (see, e.g., Sec. 1.7 in Ref. 23)

$$\frac{\partial v_k}{\partial t} = -(\mathbf{v}\cdot\nabla)v_k + (\mathbf{B}\cdot\nabla)B_k + \sum_i \frac{\partial T_{ki}}{\partial x_i} - \frac{\partial p}{\partial x_k}. \tag{2.4}$$

Proposition 1: The system (2.2) describes magnetic hydrodynamics with a stress tensor. The stress tensor T_{ki} may be written as

$$T_{ki} = \sum_j \frac{\partial B_i}{\partial x_j}\frac{\partial v_j}{\partial x_k} \tag{2.5}$$

or as

$$T'_{ki} = -\sum_j \frac{\partial v_i}{\partial x_j}\frac{\partial B_j}{\partial x_k} \tag{2.5$'$}$$

or as a linear combination $\alpha T_{ki} + \beta T'_{ki}$ with $\alpha+\beta=1$.

Proof: We will prove the statement of the Proposition for tensor T_{ki} given by (2.5). We write the contribution in (2.4) from the stress tensor (2.5),

$$\sum_i \frac{\partial T_{ki}}{\partial x_i} = \sum_{i,j} \frac{\partial^2 B_i}{\partial x_i\,\partial x_j}\frac{\partial v_j}{\partial x_k} + \sum_{i,j}\frac{\partial B_i}{\partial x_j}\frac{\partial^2 v_j}{\partial x_i\,\partial x_k}.$$

Since $\mathrm{div}(\mathbf{B})=0$, the first term on the right-hand side vanishes, and we get precisely the first equation from (2.2).

The stress tensor (2.5′) will yield the additional term written in the form (2.3′). The proof in this case is completely analogous.

We point out that the stress tensors we obtain here are not symmetric, $T_{ki}\neq T_{ik}$. In a typical situation in hydrodynamics, stress tensor is symmetric. The derivation of the symmetry of a stress tensor is based on the consideration of the angular momentum for an infinitesimal region of the fluid. Provided that the external force does not cause angular acceleration of individual particles of the fluid, the stress tensor must be symmetric. However, this need not to be the case if there is a force acting on polarized fluid particles (see discussion in Sec. 1.3 in Ref. 4 or Chap. 8 in Ref. 23). The asymmetry of stress tensor (2.5) indicates that the particles of the fluid are polar, i.e., possess electric or magnetic momentum. The derivation of the stress tensor from the first principles is rather delicate (see, e.g., Chap. 7 in Ref. 23), and this paper does not describe precisely the physical situations when the stress tensors (2.5) and (2.5′) would occur.

Introduction of the term (2.3) which has the third order in derivatives, into the equations will clearly change the behavior of the solutions in a substantial way. It is quite surprising that the conservation laws of magnetic hydrodynamics still hold for the system (2.2).

Our next goal is to study the conservation laws for magnetic hydrodynamics with the stress tensor (2.2). However before we do that, let us discuss the class of solutions that we consider here.

We require that the functions $v_i(x), B_i(x)$ are defined in a domain $D \subset \mathbb{R}^n$ and belong to the intersection of the Sobolev spaces $\cap_{k=1}^{\infty} H_0^k(D)$. We recall that the space $H_0^k(D)$ is the closure in the Sobolev space $H^k(D)$ of the functions of class C^k with compact support (see, e.g., Ref. 1). This will ensure that all functions and their partial derivatives of all orders are square-integrable [belong to $L^2(D)$] and satisfy the vanishing conditions on the boundary of D (if D is unbounded this means that at infinity the functions go to zero faster than the inverse of any polynomial). Choosing this class of functions will allow us to carry out integration by parts with the boundary term vanishing.

Alternatively, we may consider periodic boundary conditions, as it is often done in turbulence theory.

There are several conserved quantities for the MHD system—mass, momentum, magnetic helicity, as well as energy and cross-helicity. It turns out that all of these are also conserved for the MHD with the stress tensor. Since we consider the case of an incompressible fluid, the conservation of mass (volume) holds trivially. The derivation of the conservation of magnetic helicity involves only the evolution equation on magnetic field **B**, and is exactly the same for both systems. Let us prove the conservation of momentum for the new system.

Proposition 2: The total momentum is a conserved quantity for the MHD system with the stress tensor (2.2),

$$\int_D \mathbf{v}(x) \mathrm{d}V \equiv \text{const}.$$

Proof: With the help of Proposition 1, we can write the first equation using the divergence operator,

$$\frac{\partial v_k}{\partial t} = \sum_i \frac{\partial}{\partial x_i}(-v_i v_k + B_i B_k + T_{ki} - p\delta_{ki}).$$

By the divergence theorem, we get

$$\frac{\partial}{\partial t}\int_D v_k(x) \mathrm{d}V = \oint_{\partial D} R_{ki} \mathbf{e}_i \cdot \mathrm{d}\mathbf{n},$$

where R is a 2-tensor

$$R_{ki} = -v_i v_k + B_i B_k + T_{ki} - p\delta_{ki},$$

n denotes the unit outward normal vector, and $\mathbf{e}_i$'s are the standard basis vectors. Since the vector fields we consider vanish on the boundary of D, the last integral is zero.

Next we state the corresponding theorem for the conservation of energy and the cross-helicity conservation.

Theorem 3: The system (2.2) of magnetic hydrodynamics with stress tensor (2.5) in a domain $D \subset \mathbb{R}^n$ with appropriate boundary conditions (see discussion above) has the following two first integrals:

$$\int_D \sum_i v_i(x)^2 + \sum_i B_i(x)^2 \, \mathrm{d}V \equiv \text{const} \quad \text{(energy conservation)} \tag{2.6}$$

and

$$\int_D \sum_i v_i(x) B_i(x) \mathrm{d}V \equiv \text{const (cross-helicity conservation)}. \tag{2.7}$$

We will give the proof of this theorem in Sec. IV. These conservation laws will be derived from the properties of the Lie algebra $\mathfrak{g}(\tau)$.

It is interesting to note that unlike the case of the Navier–Stokes equation, introduction of the stress tensor in (2.2) does not lead to the dissipation of energy, and the energy conservation law still holds.

For the topological interpretation of helicity and cross-helicity, see Refs. 18 and 19.

In the conclusion of this section we show that system (2.2) admits Alfvén wave solutions.

Alfvén waves solutions are obtained as a perturbation of a steady-state constant solution $\mathbf{v}(x)=0, \mathbf{B}(x)=\mathbf{B}_0$. If we take an expansion $\mathbf{v}=\tilde{\mathbf{v}}(x), \mathbf{B}=\mathbf{B}_0+\tilde{\mathbf{B}}(x)$ near this equilibrium state, we will get the following system:

$$\frac{\partial \tilde{\mathbf{v}}}{\partial t} = -(\tilde{\mathbf{v}}\cdot\nabla)\tilde{\mathbf{v}} + (\mathbf{B}_0\cdot\nabla)\tilde{\mathbf{B}} + (\tilde{\mathbf{B}}\cdot\nabla)\tilde{\mathbf{B}} + \sum_{i,j}\frac{\partial \tilde{B}_i}{\partial x_j}\nabla\frac{\partial \tilde{v}_j}{\partial x_i} - \nabla p,$$

$$\frac{\partial \tilde{\mathbf{B}}}{\partial t} = -(\tilde{\mathbf{v}}\cdot\nabla)\tilde{\mathbf{B}} + (\mathbf{B}_0\cdot\nabla)\tilde{\mathbf{v}} + (\tilde{\mathbf{B}}\cdot\nabla)\tilde{\mathbf{v}},$$

$$\operatorname{div}(\tilde{\mathbf{v}}) = 0, \quad \operatorname{div}(\tilde{\mathbf{B}}) = 0. \tag{2.8}$$

Next we set $\tilde{\mathbf{B}}=\tilde{\mathbf{v}}$. In this case the term $\Sigma_{i,j}(\partial\tilde{B}_i/\partial x_j)\nabla(\partial\tilde{v}_j/\partial x_i)$ is a gradient of $\Sigma_{i,j}(\partial\tilde{v}_i/\partial x_j)\times(\partial\tilde{v}_j/\partial x_i)$, and we can eliminate it by setting

$$p = \sum_{i,j}\frac{\partial \tilde{v}_i}{\partial x_j}\frac{\partial \tilde{v}_j}{\partial x_i}. \tag{2.9}$$

Now the first two equations in (2.8) reduce to a single equation

$$\frac{\partial \tilde{\mathbf{v}}}{\partial t} = (\mathbf{B}_0\cdot\nabla)\tilde{\mathbf{v}}. \tag{2.10}$$

Finally, by taking an arbitrary divergence zero vector field $\mathbf{w}(x)$, we can construct a solution of (2.8),

$$\tilde{\mathbf{v}}(x,t) = \mathbf{w}(x+\mathbf{B}_0 t).$$

This traveling wave solution is called the Alfvén wave. The only difference with the classical MHD system (2.1) is the change of the pressure term (2.9).

III. GENERALIZED EULER EQUATION

In this section we are going to review the geodesic equation approach to hydrodynamics developed by Arnold. In the key paper,[2] Arnold gave an interpretation of the Euler equation for an incompressible ideal fluid

$$\frac{\partial \mathbf{v}}{\partial t} = -(\mathbf{v}\cdot\nabla)\mathbf{v} - \nabla p,$$

$$\operatorname{div}(\mathbf{v}) = 0, \tag{3.1}$$

from the perspective of infinite-dimensional Lie groups. He showed that the Euler equation may be interpreted as the geodesic equation on the group of diffeomorphisms, where the Riemannian structure on the group is given by the energy functional.

We will describe this approach here following Ref. 3.

Let G be a Lie group (possibly infinite-dimensional), and let $\mathfrak{g}$ be its Lie algebra. Consider a map from $\mathfrak{g}$ to its dual

$$A\colon \mathfrak{g} \to \mathfrak{g}^* \quad \text{(inertia operator)},$$

such that it defines a positive-definite symmetric bilinear form on $\mathfrak{g}$,

$$\langle X|Y\rangle = \tfrac{1}{2}A(X)Y + \tfrac{1}{2}A(Y)X, \quad X,Y \in \mathfrak{g}.$$

The corresponding quadratic form $\langle X|X\rangle = A(X)X$ is called the energy functional.

The Lie algebra $\mathfrak{g}$ acts on its dual space via the coadjoint action,

$$(\mathrm{ad}^*(X)u)(Y) = -u([X,Y]) \quad \text{for } X,Y \in \mathfrak{g},\ u \in \mathfrak{g}^*.$$

We assume that the space $A(\mathfrak{g})$ is invariant under the coadjoint action, and we make a convention that in what follows $\mathfrak{g}^*$ stands for $A(\mathfrak{g})$ [this is a slight abuse of notations since in the infinite-dimensional case $A(\mathfrak{g})$ is typically smaller than the formal dual of $\mathfrak{g}$]. Since the kernel of A is trivial [otherwise, the quadratic form $\langle X|X\rangle = A(X)X$ is not positive-definite], then with the above convention the operator A is invertible.

The bilinear form $\langle\cdot|\cdot\rangle$ may be left-translated from $\mathfrak{g} = T_e(G)$ to the tangent spaces at all points of G. This gives a Riemannian structure on G, and allows us to consider the geodesics on this group.

Next we are going to write the equation for the geodesics on G, which describes the evolution of the tangent vector $X \in \mathfrak{g}$ to the geodesic curve. It turns out however, that it is easier to write the evolution equation for the covector $u = A(X) \in \mathfrak{g}^*$ rather than for X itself. The generalized Euler equation is the evolution equation for $u = A(X)$ which is written using the coadjoint action [see (6.4) in Ref. 3]

$$u_t = -\mathrm{ad}^*(A^{-1}u)u. \tag{3.2}$$

When $G = \mathrm{SO}(3)$ this equation turns into the equations of motion of a rigid body with a fixed point.

Let us discuss equation (3.2) in the context of fluid dynamics. Evolution of an incompressible fluid in domain $D \subset \mathbb{R}^n$ from time 0 to time t is given by a volume-preserving diffeomorphism of D. Thus the group of the volume preserving diffeomorphisms $G = \mathrm{SDiff}(D)$ is the configuration space for this motion. The Lie algebra of the group $\mathrm{SDiff}(D)$ is the Lie algebra of the divergence zero vector fields $\mathrm{SVect}(D)$. As the energy functional we take the kinetic energy,

$$\left\langle \sum_i v_i(x)\ \frac{\partial}{\partial x_i} \middle| \sum_i v_i(x)\frac{\partial}{\partial x_i} \right\rangle = \int_D \sum_i v_i(x)^2\, \mathrm{d}V. \tag{3.3}$$

The dual space for the divergence zero vector fields is the factor space of differential 1-forms of D by exact 1-forms,

$$\mathrm{SVect}(D)^* = \Omega^1(D)/\mathrm{d}\Omega^0(D).$$

The pairing between $\mathrm{SVect}(D)$ and $\Omega^1(D)/\mathrm{d}\Omega^0(D)$ is given by the integral

$$\sum_j w_j(x)\mathrm{d}x_j\left(\sum_i v_i(x)\frac{\partial}{\partial x_i}\right) = \int_D \sum_j w_j(x)v_j(x)\mathrm{d}V. \tag{3.4}$$

It is easy to check that exact 1-forms vanish on the divergence zero vector fields, and so the value of the integral on the right-hand side is independent of the choice of a representative in a class of 1-forms modulo $\mathrm{d}\Omega^0(D)$.

The inertia operator

$$A\colon \mathrm{SVect}(D) \to \Omega^1(D)/\mathrm{d}\Omega^0(D)$$

that corresponds to the energy functional (3.3) is written as follows:

$$A\left(\sum_i v_i(x)\frac{\partial}{\partial x_i}\right)=\sum_i v_i(x)\mathrm{d}x_i.$$

It is possible to check that in these settings, Eq. (3.2) turns into the Euler equations of motion of an ideal fluid.

Ebin and Marsden[10] used this interpretation of the Euler equations to prove existence of solutions for the motion of an ideal fluid for small times. A variational approach to the generalized Euler equation is presented in Ref. 16.

The equations of the magnetic hydrodynamics (2.1) can also be obtained as a special case of the generalized Euler equation (3.2). To construct the corresponding Lie algebra we take the Lie algebra SVect(D) together with its dual space,

$$\mathfrak{g}=\mathrm{SVect}(D)\oplus\Omega^1(D)/\mathrm{d}\Omega^0(D).$$

The Lie bracket of two 1-forms is set to be zero. The Lie bracket of two vector fields is defined in the usual way,

$$\left[\sum_i v_i(x)\frac{\partial}{\partial x_i},\sum_j w_j(x)\frac{\partial}{\partial x_j}\right]=\sum_{i,j} v_i\frac{\partial w_j}{\partial x_i}\frac{\partial}{\partial x_j}-w_j\frac{\partial v_i}{\partial x_j}\frac{\partial}{\partial x_i},\tag{3.5}$$

and the Lie bracket of a vector field with a 1-form is given by the Lie derivative,

$$\left[\sum_i v_i(x)\frac{\partial}{\partial x_i},\sum_j w_j(x)\mathrm{d}x_j\right]=\sum_{i,j} v_i\frac{\partial w_j}{\partial x_i}\mathrm{d}x_j+\sum_j w_j\mathrm{d}(v_j).\tag{3.6}$$

It is easy to see that the space $\mathrm{d}\Omega^0(D)$ is invariant under the Lie derivative action, so the above formula may be taken modulo $\mathrm{d}\Omega^0(D)$.

The Lie algebra $\mathfrak{g}$ is a semidirect product of SVect(D) with its module $\Omega^1(D)/\mathrm{d}\Omega^0(D)$. The space $\Omega^1(D)/\mathrm{d}\Omega^0(D)$ forms an Abelian ideal in $\mathfrak{g}$.

A really important feature of the Lie algebra $\mathfrak{g}$ is the existence of an invariant symmetric nondegenerate bilinear form. In contrast, the Lie algebra SVect does not possess such a form. The invariant form on $\mathfrak{g}$ is defined as follows [cf. (3.4)]:

$$\left(\sum_i v_i(x)\ \ \frac{\partial}{\partial x_i}\middle|\sum_j w_j(x)\mathrm{d}x_j\right)=\int_D\sum_i v_i(x)w_i(x)\mathrm{d}V,$$

$$\left(\sum_i v_i(x)\ \ \frac{\partial}{\partial x_i}\middle|\sum_j w_j(x)\frac{\partial}{\partial x_j}\right)=0,\quad\left(\sum_i v_i(x)\mathrm{d}x_i\middle|\sum_j w_j(x)\mathrm{d}x_j\right)=0.\tag{3.7}$$

One can verify that the bilinear form (3.7) satisfies the invariance property,

$$([X,Y]|Z)=(X|[Y,Z])\quad\text{for all } X,Y,Z\in\mathfrak{g}.$$

We can use this form to identify each element $X\in\mathfrak{g}$ with a linear functional $(X|\cdot)$ in $\mathfrak{g}^*$. It is well known that when the bilinear form that is used to identify $\mathfrak{g}^*$ with $\mathfrak{g}$, is invariant and nondegenerate, the coadjoint action becomes isomorphic to the adjoint action. In this case the generalized Euler equation takes the following form:

$$X_t=-\mathrm{ad}(A^{-1}X)X,\tag{3.8}$$

where now $X\in\mathfrak{g}$ and the inertia operator A now maps $\mathfrak{g}$ to $\mathfrak{g}$.

The generalized Euler equation (3.8) yields the equations of magnetic hydrodynamics (2.1) if we choose A to be the following involution on $\mathfrak{g}$:

$$A\left(\sum_i v_i(x)\frac{\partial}{\partial x_i}\right) = \sum_i v_i(x)\mathrm{d}x_i,$$

$$A\left(\sum_i w_i(x)\mathrm{d}x_i\right) = \sum_i w_i(x)\frac{\partial}{\partial x_i}. \tag{3.9}$$

Note that in the second equality we choose a (unique) representative in a class modulo $\mathrm{d}\Omega^0$ satisfying $\Sigma_i(\partial w_i/\partial x_i)=0$, so that the right-hand side is a divergence zero vector field.

We see that the inertia operator (3.9) satisfies $A^{-1}=A$, and the energy functional $(AX|X)$ for $X=\Sigma_i v_i(x)(\partial/\partial x_i)+\Sigma_i w_i(x)\mathrm{d}x_i \in \mathfrak{g}$ is given by the integral

$$\int_D \sum_i v_i(x)^2 + \sum_i w_i(x)^2 \,\mathrm{d}V. \tag{3.10}$$

The Lie algebra

$$\mathfrak{g} = \mathrm{Svect} \oplus \Omega^1/\mathrm{d}\Omega^0$$

appears in the study of toroidal Lie algebras (Refs. 5–7, 11, and 15). The representations of $\mathfrak{g}$ are an essential ingredient for constructing the representation theory of toroidal Lie algebras. It was discovered however that $\mathfrak{g}$ admits a nontrivial deformation with a $\Omega^1/\mathrm{d}\Omega^0$-valued 2-cocycle on SVect, and one gets a better representation theory for the deformed algebra than for $\mathfrak{g}$ itself.

In the next section we will describe this deformation of $\mathfrak{g}$ and study the associated generalized Euler equation.

IV. ABELIAN EXTENSIONS OF THE LIE ALGEBRA OF VECTOR FIELDS

In the preceding section we have constructed a semidirect product $\mathfrak{g}$ of the Lie algebra of divergence zero vector fields with $\Omega^1/\mathrm{d}\Omega^0$. It turns out that on the same vector space

$$\mathfrak{g} = \mathrm{Svect} \oplus \Omega^1/\mathrm{d}\Omega^0$$

we may deform the Lie bracket in a nontrivial way. When we define the Lie bracket of two vector fields, we are going to add to the right-hand side of (3.5) a correction term which has value in $\Omega^1(D)/\mathrm{d}\Omega^0(D)$,

$$\left[\sum_i v_i(x)\frac{\partial}{\partial x_i}, \sum_j w_j(x)\frac{\partial}{\partial x_j}\right] = \sum_{i,j}\left(v_i\frac{\partial w_j}{\partial x_i}\frac{\partial}{\partial x_j} - w_j\frac{\partial v_i}{\partial x_j}\frac{\partial}{\partial x_i}\right) + \tau\left(\sum_i v_i(x)\frac{\partial}{\partial x_i}, \sum_j w_j(x)\frac{\partial}{\partial x_j}\right). \tag{4.1}$$

In order to get a Lie bracket, τ must be a 2-cocycle on $\mathrm{SVect}(D)$ with values in $\Omega^1(D)/\mathrm{d}\Omega^0(D)$.

The following cocycle plays an important role in the representation theory:

$$\tau\left(\sum_i v_i(x)\frac{\partial}{\partial x_i}, \sum_j w_j(x)\frac{\partial}{\partial x_j}\right) = \sum_{i,j}\frac{\partial v_i}{\partial x_j}\mathrm{d}\left(\frac{\partial w_j}{\partial x_i}\right). \tag{4.2}$$

This cocycle may be viewed as a higher-dimensional generalization of the Virasoro cocycle. Just as the Virasoro cocycle, it has a triple derivative in x, and in fact (4.2) reducès to the Virasoro cocycle for the Lie algebra of vector fields on a circle.

The cocycle τ can be constructed using Gelfand–Fuks cohomology.[12,13] In its explicit form it first appeared in Ref. 11 in the context of the representation theory of toroidal Lie algebras.

We will denote the Lie algebra with the Lie bracket deformed by the cocycle τ by $\mathfrak{g}(\tau)$. Note that

$$\mathfrak{g}(\tau) = \mathrm{Svect}(D) \oplus \Omega^1(D)/\mathrm{d}\Omega^0(D)$$

is no longer a semidirect product, but the subspace $\Omega^1(D)/\mathrm{d}\Omega^0(D)$ still forms an Abelian ideal. As before, the action of $\mathrm{Svect}(D)$ on $\Omega^1(D)/\mathrm{d}\Omega^0(D)$ is given by the Lie derivative formula (3.6).

Proposition 4: The bilinear form on $\mathfrak{g}(\tau)$ given by (3.7) is invariant.

Proof: We need to establish the invariance property,

$$([X,Y]|Z) = (X|[Y,Z]).$$

There are three nontrivial cases to be considered,

(i) $X, Y \in \mathrm{Svect}(D), Z \in \Omega^1(D)/\mathrm{d}\Omega^0(D)$,
(ii) $X, Z \in \mathrm{SVect}(D), Y \in \Omega^1(D)/\mathrm{d}\Omega^0(D)$,
(iii) $X, Y, Z \in \mathrm{SVect}(D)$.

We will verify the invariance only for the last case, since only this case will involve the cocycle τ, and leave the first two cases as an exercise to the reader.

Suppose

$$X = \sum_i u_i \frac{\partial}{\partial x_i}, \quad Y = \sum_j v_j \frac{\partial}{\partial x_j}, \quad Z = \sum_k w_k \frac{\partial}{\partial x_k}.$$

Since $(\mathrm{SVect}|\mathrm{SVect}) = 0$, then we get that $([X,Y]|Z) = (\tau(X,Y)|Z)$ and $(X|[Y,Z]) = (X|\tau(Y,Z))$.

We have

$$([X,Y]|Z) = \left(\sum_{i,j,s} \frac{\partial u_i}{\partial x_j} \frac{\partial^2 v_j}{\partial x_i \partial x_s} \mathrm{d}x_s \middle| \sum_k w_k \frac{\partial}{\partial x_k} \right) = \int_D \sum_{i,j,k} w_k \frac{\partial u_i}{\partial x_j} \frac{\partial^2 v_j}{\partial x_i \partial x_k} \mathrm{d}V.$$

Integrating by parts and using the fact that $\Sigma_i (\partial u_i / \partial x_i) = 0$, we get

$$([X,Y]|Z) = -\int_D \sum_{i,j,k} \frac{\partial w_k}{\partial x_i} \frac{\partial u_i}{\partial x_j} \frac{\partial v_j}{\partial x_k} \mathrm{d}V.$$

On the other hand,

$$(X|\tau(Y,Z)) = \left(\sum_i u_i \frac{\partial}{\partial x_i} \middle| \sum_{j,k,s} \frac{\partial v_j}{\partial x_k} \frac{\partial^2 w_k}{\partial x_j \mathrm{d}x_s} \mathrm{d}x_s \right) = \int_D \sum_{i,j,k} u_i \frac{\partial v_j}{\partial x_k} \frac{\partial^2 w_k}{\partial x_j \mathrm{d}x_i} \mathrm{d}V = -\int_D \sum_{i,j,k} \frac{\partial u_i}{\partial x_j} \frac{\partial v_j}{\partial x_k} \frac{\partial w_k}{\partial x_i} \mathrm{d}V.$$

This proves the invariance property $([X,Y]|Z) = (X|[Y,Z])$ in case (iii).

Now we are going to prove the following theorem.

Theorem 5: The generalized Euler equation

$$X_t = -[AX, X] \tag{4.3}$$

for the Lie algebra $\mathfrak{g}(\tau)$ with the inertia operator A given by (3.9) yields the equations of magnetic hydrodynamics with asymmetric stress tensor (2.2).

Proof: We write

$$X = \sum_i B_i \frac{\partial}{\partial x_i} + \sum_j v_j \, \mathrm{d}x_j.$$

We will fix representatives of classes of 1-forms modulo $\mathrm{d}\Omega^0(D)$ by imposing a condition $\Sigma_j (\partial v_j / \partial x_j) = 0$. Then we have

$$AX = \sum_j v_j \frac{\partial}{\partial x_j} + \sum_i B_i \, \mathrm{d}x_i$$

and

$$[X,AX] = \sum_{i,j} B_i \frac{\partial v_j}{\partial x_i} \frac{\partial}{\partial x_j} - \sum_{i,j} v_j \frac{\partial B_i}{\partial x_j} \frac{\partial}{\partial x_i} + \sum_{i,j,k} \frac{\partial B_i}{\partial x_j} \frac{\partial^2 v_j}{\partial x_i \partial x_k} \mathrm{d}x_k + \sum_{i,j} B_i \frac{\partial B_j}{\partial x_i} \mathrm{d}x_j + \sum_i B_i d(B_i)$$
$$- \sum_{i,j} v_i \frac{\partial v_j}{\partial x_i} \mathrm{d}x_j - \sum_i v_i d(v_i).$$

Note that the terms $B_i d(B_i) = \frac{1}{2} d(B_i^2)$ and $v_i d(v_i) = \frac{1}{2} d(v_i^2)$ are full differentials and thus may be dropped.

Substituting the obtained expression into the generalized Euler equation (4.3) and collecting terms at $\mathrm{d}x_j, \partial/\partial x_j$, and taking into account that equality of 1-forms is taken modulo $\mathrm{d}\Omega^0(D)$, we get the following system of PDEs:

$$\frac{\partial v_j}{\partial t} = - \sum_i v_i \frac{\partial v_j}{\partial x_i} + \sum_i B_i \frac{\partial B_j}{\partial x_i} + \sum_{i,k} \frac{\partial B_i}{\partial x_k} \frac{\partial^2 v_k}{\partial x_i \partial x_j} - \frac{\partial p}{\partial x_j},$$

$$\frac{\partial B_j}{\partial t} = - \sum_i \left(v_i \frac{\partial B_j}{\partial x_i} - B_i \frac{\partial v_j}{\partial x_i} \right),$$

$$\sum_j \frac{\partial v_j}{\partial x_j} = 0, \quad \sum_j \frac{\partial B_j}{\partial x_j} = 0.$$

Rewriting this system in a vector form with the vector fields we get (2.2).

Finally let us prove Theorem 3 and establish the energy and the cross-helicity conservation laws for MHD equations with the stress tensor (2.2). We will in fact obtain Theorem 3 as a corollary of the following.

Theorem 6: Let $\mathfrak{g}$ be a Lie algebra with a nondegenerate symmetric invariant bilinear form $(\cdot|\cdot)$. Let A be an involution of $\mathfrak{g}$ preserving the invariant form

$$A\colon \mathfrak{g} \to \mathfrak{g}, \quad A^2 = \mathrm{Id}, \quad (AX|AY) = (X|Y) \quad \text{for all } X, Y \in \mathfrak{g}.$$

Then the generalized Euler equation $X_t = -[AX, X]$ has the following two first integrals:

$$(AX|X) \equiv \mathrm{const} \tag{4.4}$$

and

$$(X|X) \equiv \mathrm{const}. \tag{4.5}$$

Proof: Let us evaluate $(\partial/\partial t)(AX|X)$,

$$\frac{\partial}{\partial t}(AX|X) = (AX_t|X) + (AX|X_t).$$

Taking into account that $(X|Y) = (AX|AY)$ and $A^2 = \mathrm{Id}$, we get that $(AX_t|X) = (A^2 X_t|AX) = (X_t|AX)$. Thus

$$\frac{\partial}{\partial t}(AX|X) = 2(AX|X_t).$$

Substituting the right-hand side of the generalized Euler equation for X_t we obtain

$$\frac{\partial}{\partial t}(AX|X) = -2(AX|[AX,X]).$$

By invariance of the form we get

$$(AX|[AX,X]) = ([AX,AX]|X) = 0.$$

Thus $(\partial/\partial t)(AX|X)=0$ and (4.4) is established.

The second conservation law (4.5) is obtained in a similar way,

$$\frac{\partial}{\partial t}(X|X) = 2(X_t|X) = -2([AX,X]|X) = -2(AX|[X,X]) = 0.$$

This completes the proof of Theorem 6.

Note that for (4.5) we may drop the requirements that A preserves the invariant form and is an involution.

We obtain Theorem 3 as an immediate corollary to the previous theorem, noting that the bilinear form (3.7) on $\mathfrak{g}(\tau)$ is invariant by Proposition 4 and the inertia operator (3.9) is an involution and preserves this form.

We can see that for

$$X = \sum_i B_i \frac{\partial}{\partial x_i} + \sum_j v_j \, \mathrm{d}x_j,$$

the first integral (4.4) becomes the energy conservation law

$$(AX|X) = \int_D \sum_i v_i(x)^2 + \sum_i B_i(x)^2 \, \mathrm{d}V \equiv \text{const},$$

and (4.5) becomes the cross-helicity conservation,

$$(X|X) = 2\int_D \sum_i v_i(x) B_i(x) \mathrm{d}V \equiv \text{const}.$$

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A special class in vanishing helicity ideal flows

Homayoon Eshraghi[a)]
Institute for Studies in Theoretical Physics and Mathematics (IPM), P. O. Box 19395-5531, Tehran, Iran

Yousefali Abedini
Physics Department of Zanjan University, P. O. Box 313, Zanjan, Iran

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The derivation of a Lagrangian invariant so-called *spirality* is reviewed through the Lagrangian coordinates. The value of the spirality is fixed up to a gauge transformation. The helicity conservation follows directly from this invariant. Among all ideal flows with zero helicity in a domain of flow frozen into the fluid motion, a special class is introduced. This special topological class has the possibility to transform its spirality to be identically zero everywhere in the domain. For those simply connected domains of motion, a necessary and a sufficient condition is presented for these zero spirality flows. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1860592]

I. INTRODUCTION

Hydrodynamics has been a very nice laboratory to observe many interesting physical and mathematical phenomena. Various mathematical theories such as PDEs, dynamical systems, turbulence, functional analysis, geometry, topology, etc., are being widely extended to give as complete as possible description for fluid dynamics equations.

Among these topics, the geometrical study, especially for ideal flows, is a very useful tool to analyze fluid flows. In this approach the invariants of the fluid motion have been found to highly simplify the complicated behavior of nonlinear flows. (see, for example, Moffatt, 1990). Perhaps the most ramifications of topological investigations nest in vortex dynamics in ideal fluids as well as magnetic fields in conductor plasmas. The conservation of the helicity is a fine topological character of motions. This constant was first understood and interpreted in vortex and magnetic fields by Moffatt (1969). However, the conservation of helicity was known even by Kelvin from the 19th century (see Moffatt, 1990).

The helicity is practically a measure for the wrapping and winding of field lines inside each other. This quantity is concerned with the so-called writhing number or linking number of two closed curves in three-space. Historically, as cited by Cantarella *et al.* (2001), Gauss in 1833 discussed the linking number of two separate closed curves. Later, Woltjer (1958, Calugareanu in 1959–1961), Moffatt in (1969), and Fuller in (1971) developed this subject (see these references in Cantarella *et al.* 2000, 2001). Further progressions in this material within various points of view were achieved by many people such as Arnold (1974), Berger and Field (1984), Yoshida and Giga (1990), Freedman and He (1991), Laurence and Avellaneda (1991), Moffatt and Ricca (1992), Ricca and Moffatt (1992), Chui and Moffatt (1995), and Cantarella *et al.* (2000–2002).

Vortex Lagrangian invariants reveal a number of special symmetries in ideal fluids. Here the purpose of the present article is concentrated on the helicity. For other kinds of symmetries and invariants the reader can, for instance, refer to Lamb (1932), Tagor and Treve (1982), Salmon

[a)]Electronic mail: eshraghi@theory.ipm.ac.ir

(1988), Sagdeef, Tur, and Yanovsky (1990), and references therein), Troshkin (1995), Zakharov and Kuznetsov (1997), Kuznetsov and Ruban (1998, 2000), Arnold and Khesin (1998), and Kuznetsov (2002).

The conservation of helicity is a result of a Lagrangian invariant named *Spirality*. A nonrelativistic version of spirality for incompressible flow can be found in the book of Marchioro and Pulvirenti (1994), although this fact has been studied both analytically (Tur and Yanovsky, 1993) and numerically (see, for example, Russo and Smereca, 1999, and many references therein). A more detailed derivation for the spirality in relativistic fluids is presented by the first author (see Eshraghi, 2003). We will review this invariant in this paper in Lagrangian description to give the helicity conservation. The aim of this paper is to notice the important relation of spirality with the topology of vortex field. We will consider a zero helicity flow in a volume surrounded by a surface everywhere tangent to vortex lines. The sustained vanishing helicity as will be shown can naturally result in the existence of a special class of such flows. In this special class the invariant spirality can be chosen to be *identically zero* among the moving (with fluid) volume.

There is a feeling (even not so clear) that this invariant may play some role in the difficult debate of "finite time singularity" in vortex dynamics. It seems that the singularity cannot happen by any arbitrary initial conditions. Only some of the initial flows may result in a singularity at a finite future time. In other words, the singularity is probably hidden in the topology of the initial flow. We still have no obvious clue, but hope that the study of spirality may help us to discover a topological (invariant) character of initially smooth flows that possess the potential of creating singularity in later times.

II. SPIRALITY AND HELICITY CONSERVATION

Let us recall the Lagrangian coordinates which are suitable for invariance properties in ideal fluids. Although many solutions of hydrodynamic systems are mostly explained in terms of Eulerian variables, there exist some interesting solutions requesting a Lagrangian description (see Yakubovich and Zenkovich, 2001). If a fluid particle at time t is at the position $\mathbf{X}$ while initially (at $t=0$) was at the position $\mathbf{a}$, one can take $\mathbf{X}$ as a function of $\mathbf{a}$ and t and vice versa. Hence

$$\mathbf{X} = \mathbf{X}(\mathbf{a}, t), \qquad \dot{\mathbf{X}} = \mathbf{v}, \tag{1}$$

where $\mathbf{v}$ is the fluid velocity. In an isentropic (where entropy is constant), or barotropic (where the pressure is only function of density), or incompressible flow, the equation of motion reads

$$\dot{\mathbf{v}} = \ddot{\mathbf{X}} = -\nabla w, \quad \nabla = \left(\frac{\partial}{\partial X_1}, \frac{\partial}{\partial X_2}, \frac{\partial}{\partial X_3}\right). \tag{2}$$

The function w is the enthalpy or heat function per unit mass of the fluid element. For the incompressible case w must be simply replaced by $P/\rho_\circ$ where P and $\rho_\circ$ are the pressure and the constant density, respectively.

Consider now the jth component of Eq. (1) and multiply it by $(\partial X_j/\partial a_i)$ and sum over j. It is easily obtained that

$$\left(\frac{\partial \mathbf{u}}{\partial t}\right)_{\mathbf{a}} = \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = -\nabla_{\mathbf{a}}(w - v^2/2), \tag{3}$$

where

$$u_i \equiv v_j \frac{\partial X_j}{\partial a_i}, \quad \nabla_{\mathbf{a}} = \left(\frac{\partial}{\partial a_1}, \frac{\partial}{\partial a_2}, \frac{\partial}{\partial a_3}\right). \tag{4}$$

A formal solution for Eq. (3) is

$$\mathbf{u}(\mathbf{a},t) = \mathbf{u}_\circ(\mathbf{a}) + \nabla_\mathbf{a}\varphi, \tag{5}$$

with

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = -(w - v^2/2) + f(t).$$

Here $f(t)$ is an arbitrary function of time only which we can put to zero. So

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = v^2/2 - w, \tag{6}$$

with the assumed initial condition

$$\varphi_{t=0} \equiv 0. \tag{7}$$

An inverse transformation of Eq. (5) yields

$$\mathbf{v} = u_{\circ j}(\mathbf{a})\,\boldsymbol{\nabla}\, a_j + \boldsymbol{\nabla}\,\varphi, \quad (\mathbf{a} = \mathbf{a}(\mathbf{X},t))$$

or we define a vector function $\boldsymbol{\gamma}$,

$$\boldsymbol{\gamma} \equiv \mathbf{v} - \boldsymbol{\nabla}\,\varphi = u_{\circ j}(\mathbf{a})\,\boldsymbol{\nabla}\, a_j. \tag{8}$$

Then

$$\boldsymbol{\nabla} \times \boldsymbol{\gamma} = \boldsymbol{\nabla} \times \mathbf{v} \equiv \boldsymbol{\omega}.$$

The vector $\boldsymbol{\gamma}$ in Eq. (8) is the same as the impulse density function corresponding to the geometrical gauge introduced in the literature (see, for example, Russo and Smereca, 1999).

It follows from Eq. (8) that

$$\boldsymbol{\gamma}\cdot\boldsymbol{\omega} = \boldsymbol{\gamma}\cdot\boldsymbol{\nabla} \times \boldsymbol{\gamma} = (u_{\circ i}\,\boldsymbol{\nabla}\, a_i)\cdot[\boldsymbol{\nabla} u_{\circ j} \times \boldsymbol{\nabla}\, a_j] = \boldsymbol{\gamma}\cdot\boldsymbol{\omega} = \det\left(\frac{\partial a_m}{\partial X_n}\right) u_{\circ i}\frac{\partial u_{\circ j}}{\partial a_k}\epsilon_{ikj}.$$

By use of the well-known relation $\det(\partial a_m/\partial X_n) = \rho/\rho_\circ$ we obtain a Lagrangian invariant so-called "spirality" which we denote by "Sp:"

$$\mathrm{Sp}(\mathbf{a}) \equiv \frac{\boldsymbol{\gamma}\cdot\boldsymbol{\omega}}{\rho} = \rho_\circ^{-1}(\mathbf{a})\epsilon_{ikj}u_{\circ i}(\mathbf{a})\frac{\partial u_{\circ j}(\mathbf{a})}{\partial a_k}. \tag{9}$$

The invariance of the spirality is also easily visible through the Eulerian variables which we do not review it here. The reader can find it in Marchioro and Pulvirenti (1994).

Now let us realize the relation between spirality and helicity. Consider a fluid volume Ω_t frozen into the fluid motion. This volume contains a constant amount of mass. At $t=0$ this domain was $\Omega_\circ$. If its boundary $\partial\Omega_\circ$ was everywhere tangent to vortex lines $\boldsymbol{\omega}_\circ(\mathbf{a})$, it remains so for any future time t because of the frozenness of vortex lines in ideal flows. Therefore

$$\boldsymbol{\omega}\cdot\mathbf{n}\big|_{\partial\Omega_t} = 0, \tag{10}$$

where $\mathbf{n}$ is the unit vector normal to the surface $\partial\Omega_t$.

The conservation of the helicity $\mathcal{H}$ of the domain Ω_t easily follows from Eqs. (8) and (10) and the fact that $\boldsymbol{\nabla}\cdot\boldsymbol{\omega}=0$. Hence,

$$\mathcal{H} \equiv \int_{\Omega_t} \boldsymbol{\omega}\cdot\mathbf{v}\mathrm{d}^3X = \int_{\Omega_t} \boldsymbol{\omega}\cdot\boldsymbol{\gamma}\mathrm{d}^3X = \int_{\Omega_\circ} \mathrm{Sp}(\mathbf{a})\rho_\circ(\mathbf{a})\mathrm{d}^3a = \mathrm{const}. \tag{11}$$

Equation (6) admits a simple gauge transformation

$$\varphi \to \tilde{\varphi} = \varphi + \varphi_\circ(\mathbf{a}), \tag{12}$$

where $\varphi_\circ(\mathbf{a})$ is an arbitrary differentiable function of $\mathbf{a}$ only. This transformation clearly changes the value of the spirality at each point but does not change the helicity which is the result of the frozenness of vortex lines

$$\frac{\boldsymbol{\omega}}{\rho} = \left(\frac{\boldsymbol{\omega}_\circ}{\rho_\circ} \cdot \boldsymbol{\nabla}_\mathbf{a}\right)\mathbf{X}.$$

The new (invariant) spirality $\widetilde{\mathrm{Sp}}(\mathbf{a})$ after the gauge transformation (12) is

$$\widetilde{\mathrm{Sp}}(\mathbf{a}) = \frac{\boldsymbol{\omega}}{\rho} \cdot (\mathbf{v} - \boldsymbol{\nabla}\tilde{\varphi}) = \frac{\boldsymbol{\omega}_\circ}{\rho_\circ} \cdot (\mathbf{v}_\circ - \boldsymbol{\nabla}_\mathbf{a}\varphi_\circ), \tag{13}$$

in which Eq. (7) and the invariance of spirality were taken. Thus, by the gauge transformation (12) the helicity remains unchanged while the spirality takes new invariant values. In the next section, the case of zero helicity will be studied.

III. SPECIAL TOPOLOGY DUE TO ZERO SPIRALITY

Assume the helicity in Ω_t vanishes,

$$\mathcal{H} = \int_{\Omega_t} \boldsymbol{\omega} \cdot (\mathbf{v} - \boldsymbol{\nabla}\varphi)\mathrm{d}^3X = \int_{\Omega_\circ} \boldsymbol{\omega}_\circ \cdot (\mathbf{v}_\circ - 0)\mathrm{d}^3a = 0. \tag{14}$$

The total spirality also vanishes according to Eq. (11). As was shown, the transformation (12) leaves the total spirality and so the helicity unchanged. A natural question arises here: *For what kinds of flows one can find a suitable function* $\varphi_\circ(\mathbf{a})$ *such that the new spirality* $\widetilde{\mathrm{Sp}}$ *identically vanishes throughout* $\Omega_\circ$ *and so* Ω_t*?* In other words, we want to reveal a special class of zero helicity in which the spirality can be brought to zero identically:

$$\widetilde{\mathrm{Sp}}(\mathbf{a}) \equiv 0, \tag{15}$$

with $\widetilde{\mathrm{Sp}}(\mathbf{a})$ given by Eq. (13). It is enough to study this property in the initial configuration in $\Omega\circ$. In this paper we want to notice to the topological meaning of the property (15) which imposes a strong restriction among all zero-helicity flows. Although a complete description of the problem seems to be difficult and complicated, in some special cases there exist some viable statements.

Before starting the topological study we would like to mention an important point. The property (15) may contain a significant relation with finite time singularity. In this singularity the vorticity $\boldsymbol{\omega}$ is supposed to become infinite at some finite point and finite time while initially it was smooth. Due to the invariance of the spirality since it can be transformed to zero by Eq. (15), everywhere $\boldsymbol{\gamma}$ can be perpendicular to the vorticity. It means that in this case there is more freedom for $\boldsymbol{\gamma}$, i.e., there is no restriction on its singularity or smoothness. If the spirality cannot be transformed to zero, then it must have a finite invariant value by initial conditions. Starting from a smooth initial point and following the fluid trajectory, assume at a finite point and time a singularity occurs, i.e., $\boldsymbol{\omega}$ becomes infinite. In this case the component of $\boldsymbol{\gamma}$ which is parallel to $\boldsymbol{\omega}$ must necessarily go to zero in order to compensate the singularity of vorticity. This means that we have some restriction on $\boldsymbol{\gamma}$. To conclude we say that if the spirality can be *identically* transformed to zero everywhere, then the possibility of a singularity occurring at some point seems to be increased compared with the case when the spirality cannot be globally zero.

Let us come back to our geometrical consideration. We restrict our consideration to a *simply connected domain* for $\Omega_\circ$. In this geometry one may find a *necessary* condition and also a *sufficient* condition separately for Eq. (15). We emphasize that we still do not know a complete geometrical description for this property and only give one necessary and one sufficient condition which must be studied very carefully.

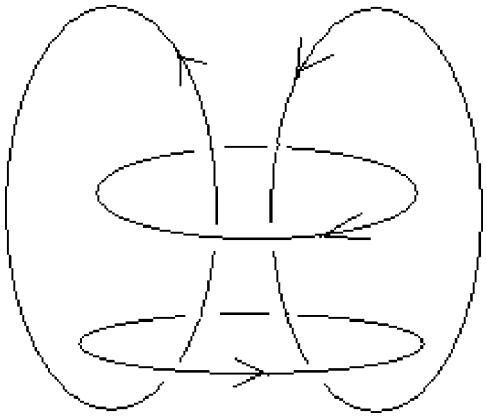

FIG. 1. Four nonzero vortex rings with zero helicity and zero spirality.

A necessary condition. Assume in the simply connected set $\Omega_\circ$ some closed vortex lines of $\boldsymbol{\omega}_\circ$ exist such that everywhere on these lines vorticity does not vanish. Let the closed curve $C_\circ$ be such a field line of $\boldsymbol{\omega}_\circ$, i.e.,

$$|\boldsymbol{\omega}_\circ(\mathbf{a})|_{C_\circ} \neq 0, \quad \frac{\boldsymbol{\omega}_\circ}{|\boldsymbol{\omega}_\circ|} = \frac{\mathrm{d}\mathbf{l}}{|\mathrm{d}\mathbf{l}|} \text{ on } C_\circ. \tag{16}$$

Let us substitute the right side of Eq. (13) into Eq. (15) and then divide it by $|\boldsymbol{\omega}_\circ(\mathbf{a})|$ for points on the closed curve $C_\circ$. The integration over this curve yields

$$\oint_{C_\circ} \mathbf{v}_\circ \cdot \mathrm{d}\mathbf{l} = \oint_{C_\circ} (\boldsymbol{\nabla}_\mathbf{a}\varphi_\circ) \cdot \mathrm{d}\mathbf{l} = 0. \tag{17}$$

By the use of Stokes theorem for a surface $\Sigma_\circ$ surrounded by $C_\circ$ (entirely inside $\Omega_\circ$) we obtain

$$\int_{\Sigma_\circ} \boldsymbol{\omega}_\circ \cdot \mathrm{d}\mathbf{S} = 0. \tag{18}$$

Therefore, if the spirality vanishes everywhere then the "total flux" of vortex lines across any closed nonzero vortex line must vanish. Of course this does not imply that the closed vortex lines have no link inside each other. They wrap inside one another but for each such closed curve, various links cancel provided the total link (flux) is zero. This fact is consistent with the zero helicity but, of course, the inverse is not necessarily true: If the helicity is zero, one can imagine some of closed vortex lines having nonzero fluxes inside but the sum of all these nonzero fluxes must be zero. To feel this difference in topologies, we consider only four nonzero vortex rings such that their helicity is zero. If Eq. (15) holds then necessarily Eq. (18) holds across each of these four nonzero vortex rings. The situation is shown in Fig. 1. We see that across each vortex ring, two opposite vortex lines pass and so the total flux of vorticity passing through each vortex ring is zero and also the helicity is zero. On the other hand, in Fig. 2 these four vortex rings have again zero helicity but the flux across each ring is not zero. It means that Eq. (18) imposes a significant restriction on the topology of vortex rings. However the general situation is much more complicated and requests a careful study.

It is very vital here to recall that the problem of the existence of a function $\varphi_\circ$ is a *global* existence and not a local one. Indeed, "locally" one can "always" use the Clebsh variables λ, μ, and $\tilde{\varphi}$ such that

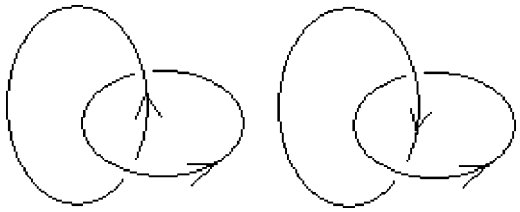

FIG. 2. Four nonzero vortex rings with zero helicity but nonzero spirality.

$$\mathbf{v} = \frac{\lambda}{\rho}\nabla\mu + \nabla\tilde{\varphi}, \tag{19}$$

from which Eq. (15) follows (but only locally). If there is no closed vortex lines in $\Omega_\circ$ (and so in Ω_t) the Clebsh variables globally exist and so the spirality can be chosen to be identically zero.

A sufficient condition. Again consider the simply connected domain $\Omega_\circ$. According to the "decomposition theorem," any smooth vector field defined on $\Omega_\circ$ can be represented as the sum of a divergence free and tangent to the boundary vector field, and a gradient field (i.e., the field which is the gradient of some smooth scalar function). See, for example, Marchioro and Pulvirenti (1994) or Gallavotti (2002). A more general decomposition applicable even for nonsimply connected domains is the "Hodge decomposition theorem" accessible, for example, in Cantarella *et al.* (2000–2002) or Schwarz (1995).

Let us apply the decomposition theorem to the initial velocity field $\mathbf{v}_\circ$. This field can be *uniquely* decomposed as

$$\mathbf{v}_\circ(\mathbf{a}) = \mathbf{w}_\circ(\mathbf{a}) + \nabla_{\mathbf{a}}\phi_\circ(\mathbf{a}), \tag{20}$$

where the unique vector $\mathbf{w}_\circ(\mathbf{a})$ satisfies

$$\begin{aligned} \nabla_{\mathbf{a}}\cdot\mathbf{w}_\circ &= 0 \quad \text{in } \Omega_\circ, \\ \mathbf{w}_\circ\cdot\mathbf{n}_\circ &= 0 \quad \text{on } \partial\Omega_\circ \end{aligned} \tag{21}$$

and $\phi_\circ$ is unique up to a constant.

A sufficient condition for Eq. (15) is then to have

$$\mathbf{w}_\circ\cdot\nabla_{\mathbf{a}}\times\mathbf{w}_\circ = \mathbf{w}_\circ\cdot\boldsymbol{\omega}_\circ = 0. \tag{22}$$

If the above condition is found in the initial velocity field, then it is enough to put

$$\varphi_\circ = \phi_\circ. \tag{23}$$

The condition (22) is equivalent to the *local* integrability of the vector field $\mathbf{w}_\circ$. This is the result of the "Frobenius theorem" (see Arnold, 1988, or more generally Yang, 1992). It is valuable to emphasize the feature of "local" integrability of $\mathbf{w}_\circ$. This means that if one looks for some surfaces everywhere normal to $\mathbf{w}_\circ$, i.e.,

$$\mathbf{w}_\circ\cdot d\mathbf{a} = 0, \tag{24}$$

then the above equation is integrable and there exists locally a surface $\mu=0$ on which Eq. (24) holds. This means that locally one can write

$$\mathbf{w}_\circ = \frac{\lambda}{\rho}(\mathbf{a})\boldsymbol{\nabla}_\mathbf{a}\mu, \tag{25}$$

which is the consequence of the Lagrangian invariance of the local Clebsh variables λ/ρ and μ. Since according to Eqs. (4), (5), and (7) we have $\mathbf{u}_\circ = \mathbf{v}_\circ$, then, regarding Eqs. (25), (20), and (23) one finds

$$\mathbf{u}_\circ = \frac{\lambda}{\rho}(\mathbf{a})\boldsymbol{\nabla}_\mathbf{a}\mu + \nabla_\mathbf{a}\varphi_\circ. \tag{26}$$

The first term on the right-hand side of the above equation holds "locally" while the last term is valid "globally" throughout $\Omega_\circ$. Indeed, since the vector field $\mathbf{w}_\circ$ is divergence free, its field lines may become closed curves. We know that topologically for a smooth closed curve like $\mathbf{w}_\circ$ we cannot find any "global" scalar function which its level surfaces are everywhere normal to $\mathbf{w}_\circ$. Hence, in this case there is not any "global" scalar function $\mu(\mathbf{a})$ on the entire domain of $\Omega_\circ$ such that the surface $\mu(\mathbf{a}) = \text{const}$ be everywhere normal to $\mathbf{w}_\circ$. Finally substitution of Eq. (26) into Eq. (8) reproduces the Clebsh representation (19).

We summarize our sufficient condition, Eq. (22), in a global sense or equivalently, Eq. (25) in a local sense only. If this is fulfilled, then the spirality can "globally" (identically) transformed to zero [Eq. (15) holds] provided the gauge transformation (12) is based on the unique "global" function $\varphi_\circ = \phi_\circ$.

IV. SUMMARY

In the present note we reviewed a nonfamous Lagrangian invariant so-called spirality. This invariant, which depends on the Bernoulli's potential and Weber transformation, may have significant geometrical and topological features. In particular, we hope the spirality may be helpful in understanding those topological invariants which may have the potential to create singularity in future finite times. It seems that if the spirality can be globally zero, the possibility for the creation of a singularity will increase relative to the other case.

The conservation of helicity, which is a well-known law, can also be obtained by the invariance of the spirality mentioned in Marchioro and Pulvirenti (1994) and also Eshraghi (2003). A gauge transformation for the spirality was given which leaves the helicity unchanged. Then, in the case of vanishing helicity in a co-moving domain of fluid motion whose boundary was tangent to vortex lines, we studied a special class of zero spirality. In other words, we tried to discover the geometrical meaning of such a flow in which one can change the spirality to be identically zero inside the mentioned domain. We considered a simply connected domain of fluid motion with zero helicity. For such a domain a necessary and a sufficient condition for the possibility of zero spirality was introduced.

The necessary condition says that across any closed nonzero vortex line (if any) inside the domain, the total flux (link) of other vortex lines must vanish. This means that there can exist some links or wrapping of vortex lines around each other but for any of them all links cancel and the total link vanishes.

The sufficient condition was derived through the global nature of the decomposition theorem. By this theorem we could decompose the initial velocity field as the sum of a unique global divergence free and tangent to the boundary plus a unique global gradient field. It was shown that if the divergence free field is locally integrable, then the spirality can globally be brought to zero everywhere.

However, the spirality "locally," always can become zero. This is the direct result of the Clebsh variables. We saw under the situation of the sufficient condition that the local invariant Clebsh variables λ/ρ and μ can also represent the divergence free (and tangent to the boundary) component of the initial velocity field. Hence, in this case the invariant Clebsh variables λ/ρ and μ are only local while $\tilde{\varphi}$ turns out to be global.

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A Bethe Ansatz study of free energy and excitation spectrum for even spin Fateev–Zamolodchikov model

Subhankar Ray[a)]
Department of Physics, Jadavpur University, Calcutta 700 032, India and C. N. Yang Institute for Theoretical Physics, Stony Brook, New York 11794

J. Shamanna
Department of Physics, Visva Bharati University, Santiniketan 731235, India

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A Bethe–Ansatz study of a self-dual Z_N spin model is undertaken for even spin system. One must solve a coupled system of Bethe–Ansatz equations (BAE) involving zeroes of two families of transfer matrices. A numerical study on finite size lattices is done for identification of elementary excitations over the ferromagnetic and antiferromagnetic ground states. The free energies for both ferromagnetic and antiferromagnetic ground states and dispersion relation for elementary excitations are found. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1847708]

I. INTRODUCTION

The present model was first proposed in 1982 by Fateev and Zamolodchikov[1] as a two-dimensional self-dual Z_N lattice model with nearest neighbor spin-spin interaction. Baxter, Bazhanov, and Perk[2] discovered a set of functional equations involving families of chiral Potts (CP) transfer matrices. Fateev–Zamolodchikov model (FZM) was shown to be a nonchiral self-dual limit of chiral Potts.[3,4] The chiral Potts transfer matrix functional equations were used to obtain transcendental equations (Bethe Ansatz equations)[5] for the zeroes of the transfer matrices for the present problem.[3,4] In the general FZM model the Bethe Ansatz equations (BAE) are coupled involving two automorphically connected families of transfer matrices as in the CP case.[2] In the odd spin case these families are connected by simple transformations and the BAEs greatly simplify and decouple requiring us to solve only one set of equations.[4] For this odd spin case alone, Albertini obtained the ferromagnetic ground state.[6] A unified treatment for the ground state of odd and even spin FZM can be found in a previous work.[4] For $N=4$ FZM a comprehensive study has been done. This includes determination of exact energy values and central charge,[7] and completeness and classification of Bethe states.[8] The present work demonstrates the study of these Bethe equations in both ferromagnetic and antiferromagnetic cases for finding the free energy and elementary excitations.

In a generic situation for the Fateev–Zamolodchikov model (to be specific we shall use the even spin case) we obtained coupled Bethe–Ansatz equations,

$$\prod_{k=1}^{L_{Uq}} \frac{\sinh(\lambda_j - \overline{\lambda_k} - i\gamma)}{\sinh(\lambda_j - \overline{\lambda_k} + i\gamma)} = (-1)^{M+1}\left[\frac{\sinh 2(\lambda_j + is\gamma)}{\sinh 2(\lambda_j - is\gamma)}\right]^{2M}, \tag{1}$$

a)Electronic mail: subho@juphys.ernet.in

$$\prod_{k=1}^{L_q} \frac{\sinh(\overline{\lambda_j} - \lambda_k - i\gamma)}{\sinh(\overline{\lambda_j} - \lambda_k + i\gamma)} = (-1)^{M+1}, \tag{2}$$

where $\{\lambda_j\}$ and $\{\overline{\lambda_j}\}$ are the spectral variables for transfer matrices T_q and T_{U_q}, respectively and $\gamma = \pi/2N$ and $s = \frac{1}{2}$.

The first equation is quite similar to the generic case of the Bethe equation. However it involves zeroes of two different transfer matrices $(\lambda, \overline{\lambda})$ that are coupled further by a second equation whose form is quite unique.

The generic case of the most commonly encountered Bethe Ansatz equation looks like

$$\prod_{k=1}^{L} \frac{\sinh(\lambda_j - \lambda_k - i\gamma)}{\sinh(\lambda_j - \lambda_k + i\gamma)} = (-)^{M+1} \left[\frac{\sinh(\lambda_j - iS\gamma)}{\sinh(\lambda_j + iS\gamma)} \right]^{2M},$$

where S is the spin and γ is the anisotropy parameter of the model. In Bethe's original paper,[5] he studied the case $\gamma \to \infty$, where the hyperbolic functions reduce to rational ones. Note that in the generic case we have only one type of λ_j as opposed to two species of λ_j and $\overline{\lambda_j}$ as they appear in the present problem.

The standard procedure of calculating the physical quantities, e.g., the energy spectrum, dispersion curves, free energy, is to assume that the solutions for the Bethe equation are given by the string hypothesis. Starting with the work of Bethe there has been a great deal of study in these complex solutions of BAE. They appear in the form,

$$\lambda_{\alpha,k}^{(n,\nu)} = \lambda_{\alpha}^{(n,\nu)} + \frac{\gamma}{2}(n + 1 - 2k)i + \frac{(1-\nu)\pi}{4}i + \delta_{\alpha,k}^{(n,\nu)}, \quad k = 1, 2, \ldots, n,$$

where $\lambda_{\alpha}^{(n,\nu)}$ is the real part, n is its length, k runs from 0 through n labelling the root. The coefficient ν takes on the value (+1) (positive parity) or (−1) (negative parity); $\delta_{\alpha,k}^{(n,\nu)}$ vanishes regularly as $M \to \infty$.

However Bethe himself realized that for large M not all solutions of BAE are of the form (above) with $\lim_{M\to\infty} \mathrm{Im}(\delta) = 0$. Modern work for the case of $\lim_{M\to\infty} \mathrm{Im}(\delta) \neq 0$ was initiated by Destri and Lowenstein and Woynarovich who introduced the definition of narrow pairs for $\lim_{M\to\infty} \mathrm{Im}(\delta) < 0$ and wide pairs for $\lim_{M\to\infty} \mathrm{Im}(\delta) > 0$ and was furthered by Avdeev and Dörfel[9,10] who introduced three classes for $\lim_{M\to\infty} \mathrm{Im}(\delta)$. It is clear that none of the existing approaches to BAE for S integer or half-integer is sufficiently refined to answer the reality or completeness question for the Hamiltonian.

In the general spin hypothesis framework one obtains equations for the centers of the strings by multiplying the Bethe Ansatz equations over different members of the same string and then taking the logarithm of the resulting equation. This yields

$$\frac{1}{2\pi}\Theta_j^{(1)}(\lambda_\alpha^j) - \frac{1}{2\pi M}\sum_k \sum_{\beta=1}^{M^{(k)}} \Theta_{jk}^{(2)}(\lambda_\alpha^{(j)} - \lambda_\beta^{(k)}) = \frac{I_\alpha^{(j)}}{M},$$

where $M^{(k)}$ is the number of k-strings and

$$\Theta_j^{(1)}(\lambda) = 2\sum_{\ell=1}^{n_j} \phi(\lambda, n_j + 2s - 2\ell + 1, \nu_j),$$

$$\Theta_{jk}(\lambda) = \phi(\lambda, n_j + n_k, \nu_j\nu_k) + \phi(\lambda, |n_j - n_k|, \nu_j\nu_k) + \sum_{\ell=1}^{\min(n_j,n_k)-1} 2\phi(\lambda, |n_j - n_k| + 2\ell, \nu_j\nu_k),$$

and

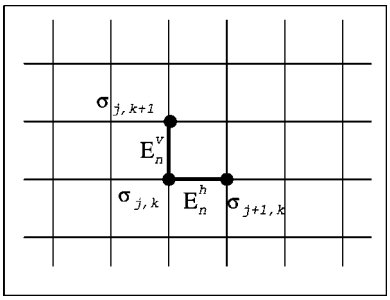

FIG. 1. Fateev–Zamolodchikov model on a square lattice.

$$\phi(\lambda,n,\nu)=\begin{cases}2\nu\arctan\left(\cot\left(\dfrac{n\gamma}{2}\right)^{\nu}\tanh(\lambda)\right),\\ 0 \text{ if } n\gamma=q\pi, \quad q\in Z.\end{cases}$$

In certain cases, e.g., δ-function Bose gas, it can be proved that the solutions are real, and no such multiplying of string components is necessary.[11] In such cases, the integers designating the branches of logarithms uniquely characterize the states and may be viewed as quantum numbers for the states. A monotonic relation is shown to exist between the integers and the values of the spectral variable $\lambda_{\alpha}^{(n,v)}$. In almost all subsequent work in the field this unique characterization of states by integers and their monotonic relation to solutions have been assumed. In few cases some counting argument is attempted[5,12–15] to justify this assumption. In the $N\to\infty$ limit, after introducing the concept of density of string centers, one obtains a coupled set of integral equations. These equations are manipulated to calculate the energies of the ground state and low lying excited states. For the spin 4 system, complete classification of Bethe states, and exact calculation for finite and infinite systems is already known.[7,8]

In the present problem, we had to deal with a doubly coupled set of integral equations; two sets of coupled equations both involving zeroes of two types of transfer matrices. However linearity of the equations made it possible to solve for the ground state and elementary excitations by the Fourier transform method. A study of the classification of roots is undertaken. However one must keep track of the added complexity of having to handle T_q and T_{U_q} simultaneously. One can identify the ground state and elementary excitations on the basis of this numerical study. The excitation spectrum and dispersion relations can hence be calculated.

II. FATEEV–ZAMOLODCHIKOV MODEL

Fateev and Zamolodchikov proposed in 1982 a two-dimensional self-dual Z_N lattice spin model with nearest neighbor interaction. They obtained this model as the self-dual[16] solution of the star-triangle relations.[17]

A general Z_N model can be defined as follows. On a two-dimensional rectangular lattice the lattice sites are occupied by a spin variable z which takes its values in the group Z_N $[z^N=1]$. If one designates the sites on the lattice by a two-dimensional integer-valued vector x, one can write down the partition function of the statistical Z_N model with nearest neighbor interaction as

$$Z=\sum_{\{z\}}\prod_{\mathbf{x}}\prod_{\sigma=\pm}w^{(\sigma)}(z(\mathbf{x}),z(\mathbf{x}+\boldsymbol{\epsilon}_{\delta})), \tag{3}$$

where the sum runs over all values of the variable z in every site of the lattice. The functions w^{σ}, $(\sigma=\pm1)$ are the weight functions corresponding to the interaction between spins on the neighboring sites of the lattice in horizontal $(\sigma=1)$ and vertical $(\sigma=-1)$ directions, respectively. The vectors $\boldsymbol{\epsilon}_1=(1,0)$ and $\boldsymbol{\epsilon}_{-1}=(0,1)$ are the basis vectors of the lattice (see Fig. 1).

In the absence of external fields, the most general interaction between two neighboring spins after appropriate normalization is given by

$$w^{(\sigma)}(z_1,z_2) = 1 + \sum_{i=1}^{N-1} x_i^{(\sigma)} \cdot (z_1 z_2^{\star})^i, \tag{4}$$

where superscript * denotes complex conjugate. Reality of $w^{(\sigma)}(z_1,z_2)$ imposes on the parameters the following restriction:

$$x_i^{(\sigma)} = x_{N-i}^{(\sigma)}. \tag{5}$$

The dual transformation of the statistical weights are given by

$$\tilde{x}_i^{(\sigma)} = \left(1 + \sum_{k=1}^{N-1} x_k^{(-\sigma)} \omega^{ki}\right)\left(1 + \sum_{k=1}^{N-1} x_k^{(-\sigma)}\right)^{-1}, \tag{6}$$

where $\omega = \exp(2\pi i/N)$. The region of self-duality is then given by

$$\tilde{x}_i^{(\sigma)} = x_i^{(\sigma)}. \tag{7}$$

Let the parameters $x_i^{(\sigma)}$ be represented by a family of functions $W_i(\alpha)$ of auxiliary parameter $\alpha \in \mathcal{C}$,

$$x_i^{(1)} = W_i(\alpha), \quad x_i^{(-1)} = W_i(\pi - \alpha). \tag{8}$$

The star-triangle relation[18,19] on $x_i(\alpha)$,

$$\sum_{k=0}^{N-1} W_{n_1-k}(\alpha) W_{n_2-k}(\pi - \alpha - \alpha') W_{n_3-k}(\alpha') = c(\alpha,\alpha') W_{n_2-n_3}(\pi - \alpha) W_{n_1-n_3}(\alpha + \alpha') W_{n_1-n_2}(\pi - \alpha'). \tag{9}$$

The particular solution of Eq. (9) that possesses the self-duality property, e.g., Eq. (7), is given by

$$W_0 = 1, \quad W_n(\alpha) = \prod_{k=0}^{n-1} \frac{\sin[\pi k/N + \alpha/2N]}{\sin[\pi(k+1)/N - \alpha/2N]}. \tag{10}$$

Denoting $x_n^{(1)} = W(n|u)$ and $x_n^{(-1)} = \bar{W}(n|u)$ we get

$$\frac{W(n|u)}{W(0|u)} = \prod_{j=1}^{n} \frac{\sin(\pi j/N - \pi/2N - u)}{\sin(\pi j/N - \pi/2N + u)}, \tag{11}$$

$$\frac{\bar{W}(n|u)}{\bar{W}(0|u)} = \prod_{j=1}^{n} \frac{\sin(\pi j/N - \pi/N + u)}{\sin(\pi j/N - u)}. \tag{12}$$

We adopt the normalization $W(0|u) = \bar{W}(0|u) = 1$. The "physical region" defined by non-negative real Boltzmann weights (BW), is given by $u \in [0, \pi/2N[$. For $N=2,3$ Eq. (11) and Eq. (12) simply reduce to the self-dual critical Potts model. For $N=4$ it gives a particular case of critical Ashkin–Teller model. Fateev and Zamolodchikov propose that for $N=5,7$ the solution describes the critical bifurcation points in the phase diagram of Alcaraz and Koberle.[20]

III. CHIRAL–POTTS MODEL AND CONNECTION TO FZM

On the sites of a two-dimensional lattice of size $\mathcal{M} \times \mathcal{N}$ denoted by two-dimensional vector (j,k) with integer entries, we place Z_N spins $\sigma_{j,k}$. The spins $\sigma_{j,k}$ are classical variables satisfying

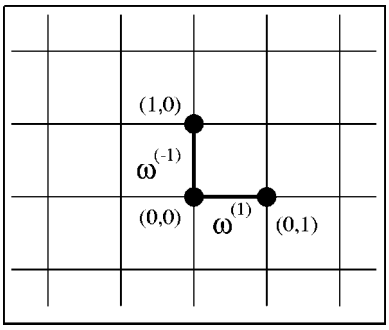

FIG. 2. Square lattice chiral Potts model.

$$\sigma_{j,k}^{N} = 1,$$

i.e., $\sigma_{j,k} = \omega^{\nu}$, $\nu \in \{0,1,2,\ldots,N-1\}$ where ω is the complex Nth root of unity with the minimum argument,

$$\omega = e^{2\pi i/N}.$$

The energy corresponding to a given configuration of spins $\{\sigma_{j,k}\}$ is

$$\mathcal{E} = -\sum_{\{j,k\}} \sum_{n=1}^{N-1} \{E_n^h \cdot (\sigma_{j,k}\sigma_{j,k+1}^{\star})^n + E_n^v \cdot (\sigma_{j,k}\sigma_{j+1,k}^{\star})^n\}.$$

Row index j runs over 1 to $\mathcal{M}$ and column index k runs over 1 to $\mathcal{N}$ with periodic boundary condition in both directions implied (see Fig. 2).

In chiral Potts a subspace of the coupling parameters (E_n^h, E_n^v) is chosen which has a built-in handedness, or phase. The energy of a nearest neighbor pair is chosen as

$$\mathcal{E}_{\text{pair}}^{h,v}(\sigma_1,\sigma_2) = -\sum_{n=1}^{N-1} E_n^{h,v} \cdot (\sigma_1\sigma_2^{\star})^n,$$

where $E_n^{h,v} = |E_n^{h,v}| \cdot e^{i\delta_n}$. The local Boltzmann weights (BW) can now be easily defined as

$$W^{h,v}(n) = e^{(1/k_B T)\sum_{j=1}^{N-1} E_j^{h,v}\omega^{jn}}.$$

Let us denote two adjacent row configurations by $\{l\}$ and $\{l'\}$ (l corresponds to the lower row), where

$$\{l\} = \{\omega^{l_j} | j = 1(1)\mathcal{N} \text{ and } l_j \in 0,1,\ldots,N-1\}.$$

The row to row transfer matrix is given by

$$T_{\{l\},\{l'\}} = \prod_{j=1}^{\mathcal{N}} W^h(l_j - l'_{j+1}) \cdot W^v(l_j - l'_j).$$

It has been shown by several authors[1,21–23] that the transfer matrices corresponding to the interaction parameters belonging to the chiral Potts submanifold commute,

$$[T, T'] = 0.$$

The self-dual chiral Potts model is given by BWs,

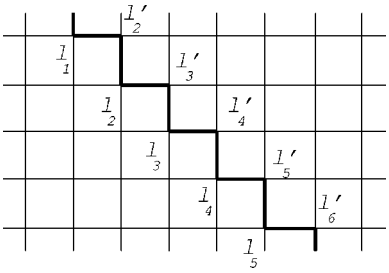

FIG. 3. Transfer matrix $T_{\{l\},\{l'\}}$.

$$\frac{W_{pq}(n)}{W_{pq}(0)} = \prod_{j=1}^{n} \frac{b_q - \omega^j a_p}{b_p - \omega^j a_q}, \tag{13}$$

$$\frac{\overline{W}_{pq}(n)}{\overline{W}_{pq}(0)} = \prod_{j=1}^{n} \frac{\omega a_p - \omega^j a_q}{b_q - \omega^j b_p}, \tag{14}$$

where $\omega = \exp(2\pi i/N)$ and the paired complex variables $(a,b) \in \mathcal{C}^2$ satisfy the constraint

$$a_x^N + b_x^N = \kappa, \tag{15}$$

$\kappa \in [0,1]$, and $x = p$ or q. In the nonchiral limit, when $\kappa = 0$, we can parametrize (a_x, b_x) in Eq. (15) as

$$a_x = e^{2ix}, \quad b_x = \omega^{1/2} e^{2ix}. \tag{16}$$

Defining $u = q - p$ Eq. (13) and Eq. (14) reduce to Eq. (11) and Eq. (12). However we retain suffixes (p,q) in the Boltzmann weights $W_{pq}(n|u)$ and $\overline{W}_{pq}(n|u)$ to signify that these BWs are obtained from the chiral Potts BWs defined in terms of p and q variables.

The transfer matrix for the FZM can be constructed from the BWs as

$$T_{p,q}^{\mathrm{n},\mathrm{n}'}(u) = \prod_{k=1}^{M} \overline{W}_{pq}(n_k - n_k'|u) W_{pq}(n_k - n_{k+1}'|u), \tag{17}$$

where M is the number of sites in each row and periodic boundary condition is implied (see Fig. 3). These transfer matrices for different spectral variable u form a commuting set. This can be argued from the fact that these transfer matrices come as a limit of CP transfer matrix, which are known to be commuting. A more direct argument would be that Fateev and Zamolodchikov obtained FZM BWs as solutions of star-triangle relation, and hence the transfer matrix constructed out of them should commute,

$$[T(u), T(u')] = 0 \ \forall \ u, u' \in C. \tag{18}$$

Transfer matrix $T(u)$ reduces to identity operator for $u \to 0$. An expansion of $T(u)$ gives us the associated spin chain Hamiltonian H,

$$T(u) = 1 - Mu \sum_{n=1}^{N-1} \frac{1}{\sin(n\pi/N)} - uH + O(u^2), \tag{19}$$

$$H = -\sum_{k=1}^{M}\sum_{n=1}^{N-1}\frac{1}{\sin(n\pi/N)}(X_k^n + Z_k^n Z_{k+1}^{-n}), \tag{20}$$

where X and Z are defined as

$$X_k|n_1\cdots n_k\cdots n_M\rangle = |n_1\cdots n_k+1\cdots n_M\rangle \bmod N,$$

$$Z_k|n_1\cdots n_k\cdots n_M\rangle = \omega^{n_k}|n_1\cdots n_k\cdots n_M\rangle.$$

Equations (19) and (20) imply that each Hamiltonian commutes with all the transfer matrices and their associated Hamiltonians. Thus it has an infinite set of conserved charges in involution. However only a subset of them, whose number is equal to the degrees of freedom of the system, are independent.

In order to obtain the zeros of the eigenvalues of the transfer matrix T_q, we will use functional equations connecting T_q with its automorphically conjugate partners. Thus it is important to understand the relevant automorphisms of the constraint Eq. (15). It has been claimed in the preceding section that the transfer matrices constructed out of CP BWs, Eq. (13) and Eq. (14), commute as long as they satisfy Eq. (15). For any $(a,b)\in\mathcal{C}^2$ satisfying the above relations there exist other complex pairs connected to them which satisfy the same relation. Two such automorphic relations of importance are

$$R(a,b) = (b,\omega a), \quad U(a,b) = (\omega a, b). \tag{21}$$

It is rather straightforward to check

$$a_{Rx}^N + b_{Rx}^N = \kappa, \quad a_{Ux}^N + b_{Ux}^N = \kappa$$

from the relation

$$a_x^N + b_x^N = \kappa.$$

If one makes an attempt to go over from CP BWs to FZM BWs through a limiting process, one gets the following relations for W_{pRq}, $\overline{W}_{pRq}$, W_{pUq}, and $\overline{W}_{pUq}$:

$$\frac{W_{pRq}(n|u)}{W_{pRq}(0|u)} = \prod_{k=1}^{n}\frac{\sin(\pi k/N - \pi/N - u)}{\sin(\pi k/N + u)}, \tag{22}$$

$$\frac{\overline{W}_{pRq}(n|u)}{\overline{W}_{pRq}(0|u)} = \prod_{k=1}^{n}\frac{\sin(\pi k/N - \pi/2N + u)}{\sin(\pi k/N - \pi/2N - u)}, \tag{23}$$

$$\frac{W_{pUq}(n|u)}{W_{pUq}(0|u)} = e^{-\imath\pi n/N}\prod_{k=1}^{n}\frac{\sin(\pi k/N - \pi/2N - u)}{\sin(\pi k/N + \pi/2N + u)}, \tag{24}$$

$$\frac{\overline{W}_{pUq}(n|u)}{\overline{W}_{pUq}(0|u)} = e^{\imath\pi n/N}\prod_{k=1}^{n}\frac{\sin(\pi k/N + u)}{\sin(\pi k/N - u)}. \tag{25}$$

Thus in the nonchiral limit, $T_q \to T_q(u)$ and $T_{Rq} \to T_q(u+\pi/2N)$. There is no simple relation between T_q and T_{Uq} though. However, we do feel that there must exist some nontrivial mapping between T_q and T_{Uq} whose understanding will unravel the connection between the zeroes of T_q and T_{U_q} and will give the satisfactory derivation of completeness of states.

IV. BETHE ANSATZ TYPE EQUATIONS FOR THE EVEN *N* FZM

We define the normalized transfer matrices by removing their denominators,

$$T_q^N(u) = [g_q(u)\overline{g_q}(u)]^M T_q(u),$$

where

$$g_q(u) = \prod_{j=1}^{N/2} \sin\left(\frac{\pi j}{N} - \frac{\pi}{2N} + u\right), \quad \overline{g_q}(u) = \prod_{j=1}^{N/2} \sin\left(\frac{\pi j}{N} - u\right).$$

One must note that the superscript in T_q^N denotes "normalize" and is not related to the spin quantum number N. Each entry of $T_q^N(u)$ is a product of NM sines and it has the general form

$$\prod_{k=1}^{NM} (c_k^{(1)} e^{iu} + c_k^{(2)} e^{-iu}).$$

The calculation of this section goes in the same spirit as that of odd N case. Hence we only quote the results,

$$\Lambda_{Q=0}(u) = \left[\frac{g_q(0)\overline{g_q}(0)}{g_q(u)\overline{g_q}(u)}\right]^M \prod_{k=1}^{L} \frac{\sin(u - v_k)}{\sin v_k},$$
$$L = A + B = NM. \tag{26}$$

The normalization has been fixed by $T_q(0) = 1_{id}$.

The momentum (P) is given by

$$e^{iP} = \Lambda_Q\left(u = \frac{\pi}{2N}\right) = \left[\frac{g_q(0)\overline{g_q}(0)}{g_q\left(\frac{\pi}{2N}\right)\overline{g_q}\left(\frac{\pi}{2N}\right)}\right]^M \prod_{k=1}^{L} \frac{\sin\left(\frac{\pi}{2N} - v_k\right)}{\sin v_k}. \tag{27}$$

Now we turn to the sectors $Q \neq 0$, and the symmetry under charge conjugation allows us to consider the sectors $Q = 1, 2, \ldots, (N-1)/2$ only. While we have not been able to obtain a proof like the one given above, one can show that, in the sector Q,

$$\text{(a) } A, B \leqslant \frac{NM}{2} - Q, \quad Q = 1, 2, \cdots, \frac{N}{2},$$

$$\text{(b) } A, B \geqslant \frac{NM}{2} - \frac{N}{2}.$$

Following similar argument as before, we arrive at

$$A = B = \frac{NM}{2} - Q.$$

The reader must be warned that this conclusion lacks rigor just like in the case of N odd. The factorization in terms of sines can be carried out without the appearance of a phase $(e^{2iu})^{\pm(B-A)}$. We assume this to be true also for the others Q sectors, and arrive at the general form

$$\Lambda_Q(u) = \left[\frac{g_q(0)\overline{g_q}(0)}{g_q(u)\overline{g_q}(u)}\right]^M \prod_{k=1}^{L} \frac{\sin(u-v_k)}{\sin v_k},$$
$$L = NM - 2Q, \quad Q = 0,1,\cdots\frac{N}{2}, \quad \Lambda_{N-Q}(u) = \Lambda_Q(u). \tag{28}$$

From this, the eigenvalue of H is easily found to be

$$E = \sum_{k=1}^{L} \cot v_k - 2M\sum_{j=1}^{N/2} \cot(\pi j/N). \tag{29}$$

The momentum (P) is given by

$$e^{iP} = \Lambda_Q\left(u = \frac{\pi}{2N}\right) = \left[\frac{g_q(0)\overline{g_q}(0)}{g_q\left(\frac{\pi}{2N}\right)\overline{g_q}\left(\frac{\pi}{2N}\right)}\right]^M \prod_{k=1}^{L} \frac{\sin\left(\frac{\pi}{2N} - v_k\right)}{\sin v_k}. \tag{30}$$

We shall use the set of functional equations for the eigenvalues of transfer matrices of chiral Potts derived by Baxter, Bazhanov, and Perk.[2,24] This functional relation appears in Ref. 2 as Eq. (4.40) and has the following form:

$$\widetilde{T}_{\overline{q}} = \sum_{m=0}^{N-1} c_{m,q} T^{-1}_{U^m q} T_q T^{-1}_{U^{m+1}q} X^{-m-1}, \tag{31}$$

where $\widetilde{T} = TS$, $\overline{q} = (a_{\overline{q}}, b_{\overline{q}}) = UR^{-1}(a_q, b_q)$, and

$$c_{m,q} = \left(\left(\prod_{j=0}^{m-1} \frac{b_p - \omega^{j+1}a_q}{a_p - \omega^j a_q}\right)\cdot\left(\prod_{j=m+1}^{N-1} \frac{\omega(a_p - \omega^j a_q)}{b_p - \omega^{j+1}a_q}\right)\cdot\left(\frac{N(b_q - b_p)(b_p - a_q)}{a_p b_p - \omega^m a_q b_q}\right)\right)^M,$$

$$\widetilde{T}_{\overline{q}} = \sum_{s=0}^{(N/2)-1} (c_{2s,q} T^{-1}_{U^{2s}q} T_q T^{-1}_{U^{2s+1}q} X^{-2s-1}) + \sum_{s=0}^{(N/2)-1} (c_{2s+1,q} T^{-1}_{U^{2s+1}q} T_q T^{-1}_{U^{2s+2}q} X^{-2s-2})$$
$$= \sum_{s=0}^{(N/2)-1} \left(\frac{c_{2s,q}}{A_{s,q}A_{s,q'}} \cdot T^{-1}_{R^{2s}q} T_q T^{-1}_{R^{2s}(Uq)} X^{-1} + \frac{c_{2s+1,q}}{A_{s,q'}A_{s+1,q}} \cdot T^{-1}_{R^{2s}(Uq)} T_q T^{-1}_{R^{2s+2}q} X^{-1}\right).$$

Define

$$p_{2s} = \frac{c_{2s,q}}{A_{s,q}A_{s,q'}}, \quad d_{2s+1} = \frac{c_{2s+1,q}}{A_{s,q'}A_{s+1,q}}.$$

The independent inverse factors of $T_{R^{2s}q}$ and $T_{R^{2s}(Uq)}$ are considered, and both sides of the above equation are multiplied by the appropriate common factor so as to get rid of inverses of transfer matrix. The appropriate factor is

$$X\prod_{j=1}^{N/2} T_{R^{2j}q} \prod_{j=0}^{(N/2)-1} T_{R^{2j}(Uq)}. \tag{32}$$

After multiplying we get

$$X\cdot\tilde{T}_{\bar{q}}\cdot\prod_{j=1}^{N/2}T_{R^{2j}q}T_{R^{2(j-1)}(Uq)}=\sum_{s=0}^{(N/2)-1}\left(p_{2s}\prod_{\substack{j=0\\ j\neq s}}^{N/2}T_{R^{2j}q}\cdot\prod_{\substack{j=0\\ j\neq s}}^{(N/2)-1}T_{R^{2j}(Uq)}+d_{2s+1}\prod_{\substack{j=0\\ j\neq (s+1)}}^{N/2}T_{R^{2j}q}\cdot\prod_{\substack{j=0\\ j\neq s}}^{(N/2)-1}T_{R^{2j}(Uq)}\right). \tag{33}$$

If one expresses $T_{p,q}$ and $T_{p,Uq}$ in terms of a complex parameter u, where $u=q-p$ as $k\to 0$,

$$\begin{gathered}T_q\to T_q,\quad T_{Uq}\to T_{Uq}(u),\\ T_{R^{2k}q}\to T_q\left(u+\frac{k\pi}{N}\right),\quad T_{R^{2k}(Uq)}\to T_{(Uq)}\left(u+\frac{k\pi}{N}\right),\end{gathered} \tag{34}$$

with this parametrization we get

$$X\cdot\tilde{T}_{\bar{q}}\cdot\prod_{j=1}^{N/2}T_q\left(u+\frac{\pi j}{N}\right)\cdot\prod_{j=0}^{(N/2)-1}T_{Uq}\left(u+\frac{\pi j}{N}\right)=\sum_{s=0}^{(N/2)-1}\left(p_{2s}\prod_{\substack{j=0\\ j\neq s}}^{N/2}T_q\left(u+\frac{\pi j}{N}\right)\prod_{\substack{j=0\\ j\neq s}}^{(N/2)-1}T_{Uq}\left(u+\frac{\pi j}{N}\right)+d_{2s+1}\prod_{\substack{j=0\\ j\neq s+1}}^{N/2}T_q\left(u+\frac{\pi j}{N}\right)\prod_{\substack{j=0\\ j\neq s}}^{(N/2)-1}T_{Uq}\left(u+\frac{\pi j}{N}\right)\right). \tag{35}$$

Let v be a zero of T_q, i.e., $T_q(v)=0$, then whenever $u=v-\pi k/N$, $T_q(u+\pi k/N)=0$. Thus for $u=v-\pi k/N\ k\in\{1,2,\ldots,(N/2)-1\}$ all but two terms vanish,

$$p_{2k}\prod_{\substack{j=0\\ j\neq k}}^{N/2}T_q\left(u+\frac{\pi j}{N}\right)\prod_{\substack{j=0\\ j\neq k}}^{(N/2)-1}T_{Uq}\left(u+\frac{\pi j}{N}\right)+d_{2k-1}\prod_{\substack{j=0\\ j\neq k}}^{N/2}T_q\left(u+\frac{\pi j}{N}\right)\prod_{\substack{j=0\\ j\neq k-1}}^{(N/2)-1}T_{Uq}\left(u+\frac{\pi j}{N}\right)=0. \tag{36}$$

Cancelling the common factors we get

$$p_{2k}(u)\cdot T_{Uq}\left(u+\frac{\pi k}{N}-\frac{\pi}{N}\right)+d_{2k-1}(u)\cdot T_{Uq}\left(u+\frac{\pi k}{N}\right)=0 \tag{37}$$

whence

$$\frac{T_{Uq}(v)}{T_{Uq}\left(v-\frac{\pi}{N}\right)}=-\frac{p_{2k}\left(v-\frac{\pi k}{N}\right)}{d_{2k-1}\left(v-\frac{\pi k}{N}\right)}. \tag{38}$$

Recalling the expression for T_{Uq},

$$\prod_{j=1}^{L_{Uq}}\frac{\sin(v_i-\bar{v_j})}{\sin\left(v_i-\bar{v_j}-\frac{\pi}{N}\right)}=-\left(\frac{g_{Uq}(v_i)\cdot\bar{g}_{Uq}(v_i)}{g_{Uq}\left(v_i-\frac{\pi}{N}\right)\cdot\bar{g}_{Uq}\left(v_i-\frac{\pi}{N}\right)}\right)^M\cdot\frac{p_{2k}\left(v_i-\frac{\pi k}{N}\right)}{d_{2k-1}\left(v_i-\frac{\pi k}{N}\right)}. \tag{39}$$

The ratio of g_{Uq}'s can be obtained as

$$g_{Uq}(v_i) = \prod_{j=1}^{(N/2)-1} \sin\left(\frac{\pi j}{N} + \frac{\pi}{2N} + v_i\right), \quad g_{Uq}\left(v_i - \frac{\pi}{N}\right) = \prod_{j=0}^{(N/2)-2} \sin\left(\frac{\pi j}{N} + \frac{\pi}{2N} + v_i\right),$$

$$\frac{g_{Uq}(v_i)}{g_{Uq}\left(v_i - \frac{\pi}{N}\right)} = \frac{\sin\left(\frac{\pi}{2} - \frac{\pi}{N} + \frac{\pi}{2N} + v_i\right)}{\sin\left(0 + \frac{\pi}{2N} + v_i\right)} = \frac{\cos\left(v_i - \frac{\pi}{2N}\right)}{\sin\left(v_i + \frac{\pi}{2N}\right)}. \tag{40}$$

Similarly the ratios of $\overline{g}_{Uq}$ is found as

$$\overline{g}_{Uq}(v_i) = \prod_{j=1}^{(N/2)-1} \sin\left(\frac{\pi j}{N} - v_i\right), \quad \overline{g}_{Uq}\left(v_i - \frac{\pi}{N}\right) = \prod_{j=2}^{N/2} \sin\left(\frac{\pi j}{N} - v_i\right),$$

$$\frac{\overline{g}_{Uq}(v_i)}{\overline{g}_{Uq}\left(v_i - \frac{\pi}{N}\right)} = \frac{\sin\left(\frac{\pi}{N} - v_i\right)}{\sin\left(\frac{\pi}{2} - v_i\right)} = (-1) \cdot \frac{\sin\left(v_i + \frac{\pi}{N}\right)}{\cos(v_i)}. \tag{41}$$

Using these results for the ratios of g_{Uq} and those of (p_{2k}/d_{2k-1}) we finally get the Bethe equations[5]

$$\prod_{j=1}^{L_{Uq}} \frac{\sin(v_i - \overline{v_j})}{\sin\left(v_i - \overline{v_j} - \frac{\pi}{N}\right)} = (-1)^{M+1}\left[\frac{\sin 2\left(v_i - \frac{\pi}{2N}\right)}{\sin(2v_i)}\right]^{2M}. \tag{42}$$

Let $\overline{v}$ be a zero of T_{Uq}, i.e., $T_{Uq}(\overline{v})=0$, then whenever $u=\overline{v}-\pi k/N$, $T_q(u+\pi k/N)=0$. For $u=\overline{v}-\pi k/N$ $k \in \{1,2,\ldots,(N/2)-1\}$ all but two terms vanish

$$p_{2k} \prod_{\substack{j=0 \\ j \neq k}}^{N/2} T_q\left(u + \frac{\pi j}{N}\right) \prod_{\substack{j=0 \\ j \neq k}}^{(N/2)-1} T_{Uq}\left(u + \frac{\pi j}{N}\right) + d_{2k+1} \prod_{\substack{j=0 \\ j \neq k+1}}^{N/2} T_q\left(u + \frac{\pi j}{N}\right) \prod_{\substack{j=0 \\ j \neq k}}^{(N/2)-1} T_{Uq}\left(u + \frac{\pi j}{N}\right) = 0. \tag{43}$$

Cancelling the common factors we get

$$p_{2k}(u) \cdot T_q\left(u + \frac{\pi k}{N} + \frac{\pi}{N}\right) + d_{2k+1}(u) \cdot T_q\left(u + \frac{\pi k}{N}\right) = 0,$$

$$\frac{T_q(\overline{v})}{T_q\left(\overline{v} + \frac{\pi}{N}\right)} = -\frac{p_{2k}\left(\overline{v} - \frac{\pi k}{N}\right)}{d_{2k+1}\left(\overline{v} - \frac{\pi k}{N}\right)}. \tag{44}$$

The ratios of g_q's can be obtained as

$$g_q(\overline{v_i}) = \prod_{j=1}^{N/2} \sin\left(\frac{\pi j}{N} - \frac{\pi}{2N} + \overline{v_i}\right), \quad g_q\left(\overline{v_i} + \frac{\pi}{N}\right) = \prod_{j=2}^{(N/2)+1} \sin\left(\frac{\pi j}{N} - \frac{\pi}{2N} + \overline{v_i}\right),$$

$$\frac{g_q(\overline{v_i})}{g_q\left(\overline{v_i} + \frac{\pi}{N}\right)} = \frac{\sin\left(\frac{\pi}{N} - \frac{\pi}{2N} + \overline{v_i}\right)}{\sin\left(\frac{\pi}{N} + \frac{\pi}{N} + \overline{v_i}\right)} = \frac{\sin\left(\overline{v_i} + \frac{\pi}{2N}\right)}{\cos\left(\overline{v_i} + \frac{\pi}{2N}\right)}. \tag{45}$$

Similarly the ratios of $\overline{g_q}$'s is found as

$$\overline{g_q}(\overline{v_i}) = \prod_{j=1}^{N/2} \sin\left(\frac{\pi j}{N} - \overline{v_i}\right), \quad \overline{g_q}\left(\overline{v_i} + \frac{\pi}{N}\right) = \prod_{j=0}^{(N/2)-1} \sin\left(\frac{\pi j}{N} - \overline{v_i}\right),$$

$$\frac{\overline{g_q}(\overline{v_i})}{\overline{g_q}\left(\overline{v_i} + \frac{\pi}{N}\right)} = \frac{\sin\left(\frac{\pi}{2} - \overline{v_i}\right)}{\sin(0 - v_i)} = (-1) \cdot \frac{\cos(\overline{v_i})}{\sin(\overline{v_i})}. \tag{46}$$

Using these results for the ratios of g_q and those of p_{2k}/d_{2k+1} we finally get

$$\prod_{j=1}^{L_q} \frac{\sin(\overline{v_i} - v_j)}{\sin\left(\overline{v_i} - v_j + \frac{\pi}{N}\right)} = (-1)^{M+1}.$$

In order to cast the BAE's for the even case in a simpler (and standard) form, we make a change of variables.

$$v_j = i\lambda_j + \frac{\pi}{4N}, \quad \overline{v_j} = i\overline{\lambda_j} - \frac{\pi}{4N}. \tag{47}$$

The BAE's in terms of these new variables are

$$\prod_{k=1}^{L_{Uq}} \frac{\sinh(\lambda_j - \overline{\lambda_k} - i\gamma)}{\sinh(\lambda_j - \overline{\lambda_k} + i\gamma)} = (-1)^{M+1}\left[\frac{\sinh 2(\lambda_j + is\gamma)}{\sinh 2(\lambda_j - is\gamma)}\right]^{2M}, \tag{48}$$

$$\prod_{k=1}^{L_q} \frac{\sinh(\overline{\lambda_j} - \lambda_k - i\gamma)}{\sinh(\overline{\lambda_j} - \lambda_k + i\gamma)} = (-1)^{M+1}, \tag{49}$$

where $\gamma = \pi/2N$ and $s = \frac{1}{2}$. From the numerical study for even spin BAE's, it was found that λ_j's are related to one another. In fact

$$\forall \lambda_j \, \exists \, \lambda_j + i\pi/2 \bmod(\pi). \tag{50}$$

This allows us to group λ_j such that $\lambda_j \in [-\pi/4, \pi/4]$. Using transformation rules for the hyperbolic functions one can rewrite the expressions in terms of a new variable $\chi_j = 2\lambda_j$. The left-hand side (LHS) of BAE(1) becomes

$$\prod_{k=1}^{L_{Uq}/2} \frac{\sinh(\lambda_j - \overline{\lambda}_k - i\gamma)}{\sinh(\lambda_j - \overline{\lambda}_k + i\gamma)} \cdot \frac{\sinh\left(\lambda_j - \overline{\lambda}_k - i\gamma - \frac{i\pi}{2}\right)}{\sinh\left(\lambda_j - \overline{\lambda}_k + i\gamma - \frac{i\pi}{2}\right)} = \prod_{k=1}^{L_{Uq}/2} \frac{\sinh 2(\lambda_j - \overline{\lambda}_k - i\gamma)}{\sinh 2(\lambda_j - \overline{\lambda}_k + i\gamma)}$$

$$= \prod_{k=1}^{L_{Uq}/2} \frac{\sinh(\chi_j - \overline{\chi}_k - 2i\gamma)}{\sinh(\chi_j - \overline{\chi}_k + 2i\gamma)}. \tag{51}$$

The right-hand side (RHS) of BAE(1) is rewritten in terms of variables χ_j,

$$(-1)^{M+1}\left(\frac{\sinh(\chi_j + 2is\gamma)}{\sinh(\chi_j - 2is\gamma)}\right)^{2M} = (-1)^{M+1}\left(\frac{\sinh(\chi_j + i\gamma)}{\sinh(\chi_j - i\gamma)}\right)^{2M}, \quad \text{since } s = \tfrac{1}{2}. \tag{52}$$

A similar transformation is done for BAE(2). Hence the BAE equations become

$$\prod_{k=1}^{L_{Uq}/2} \frac{\sinh(\chi_j - \overline{\chi}_k - 2i\gamma)}{\sinh(\chi_j - \overline{\chi}_k + 2i\gamma)} = (-1)^{M+1}\left(\frac{\sinh(\chi_j + i\gamma)}{\sinh(\chi_j - i\gamma)}\right)^{2M}, \tag{53}$$

$$\prod_{k=1}^{L_q/2} \frac{\sinh(\overline{\chi}_j - \chi_k - 2i\gamma)}{\sinh(\overline{\chi}_j - \chi_k + 2i\gamma)} = (-1)^{M+1}. \tag{54}$$

The eigenvalues $\Lambda_Q(u)$ of the transfer matrix are given in terms of these zeroes χ_j's as[3]

$$\Lambda_Q(u) = \left[\frac{g_q(0)\overline{g}_q(0)}{g_q(u)\overline{g}_q(u)}\right]^M \prod_{k=1}^{L/2} \frac{\sin\left(2u - i\chi_k - \frac{\pi}{2N}\right)}{\sin\left(i\chi_k + \frac{\pi}{2N}\right)}, \tag{55}$$

where

$$g_q(u) = \prod_{j=1}^{N/2} \sin\left(\frac{\pi j}{N} - \frac{\pi}{2N} + u\right), \quad \overline{g}_q(u) = \prod_{j=1}^{N/2} \sin\left(\frac{\pi j}{N} - u\right). \tag{56}$$

V. STUDY OF FINITE SIZE SYSTEMS

The BAE in the present model differs from the standard form. The sign in front of γ on the right hand side of BAE(1) is reversed. That is to say that the RHS is equal to the inverse of what usually is known to be the RHS. The second of the coupled pair, BAE(2) is even more striking. Though the LHS is still coupled, the RHS is independent of the spectral variable. Understanding the real significance of these peculiarities can help enormously in solving the problem.

The transfer matrix for the FZM is constructed from the FZM Boltzmann weights (BW) as

$$T_q^{\mathbf{n},\mathbf{n}'}(u) = T_{p,q}^{\mathbf{n},\mathbf{n}'}(u) = \prod_{k=1}^{M} \overline{W}_{pq}(n_k - n'_k|u)W_{pq}(n_k - n'_{k+1}|u), \tag{57}$$

where M is the number of sites in each row and periodic boundary condition is implied. These transfer matrices for different spectral variable u form a commuting family. Transfer matrix acts on vectors defined in terms of spin indices along a row (or diagonal)[3] or the spin configuration $\mathbf{n} = |n_1, n_2, \ldots, n_M\rangle$.

There is an associated transfer matrix $T_{p,Uq}$ which corresponds to a conjugate set of Boltzmann weights,[4]

$$T_{Uq}^{\mathbf{n},\mathbf{n}'}(u) = T_{p,Uq}^{\mathbf{n},\mathbf{n}'}(u) = \prod_{k=1}^{M} \overline{W}_{pUq}(n_k - n'_k|u)W_{pUq}(n_k - n'_{k+1}|u). \tag{58}$$

The shift or translation operator $\hat{S}$ is defined by its action on a state function or spin configuration $\mathbf{n}=|n_1,n_2,\ldots,n_M\rangle$.

$$\hat{S}|n_1,n_2,n_3,\ldots,n_M\rangle = |n_M,n_1,n_2,\ldots,n_{M-1}\rangle. \tag{59}$$

Momentum P is defined in terms of the shift operator as

$$e^{iP} = \hat{S}^{-1}.$$

The z-component of spin operator $\hat{Z}_k$ and spin raising operator $\hat{X}_k$ corresponding to a given lattice site (k) are defined by their action on a state function or spin configuration as $\mathbf{n}=|n_1,n_2,\ldots,n_M\rangle$, $n_k=0,1,\ldots,N-1$.

$$\hat{X}_k|n_1\cdots n_k\cdots n_M\rangle = |n_1\cdots n_k+1\cdots n_M\rangle \mathrm{mod}(N),$$

$$\hat{Z}_k|n_1\cdots n_k\cdots n_M\rangle = \omega^{n_k}|n_1\cdots n_k\cdots n_M\rangle.$$

The global spin raising operator is given by

$$\hat{X} = \prod_{k=1}^{M} \hat{X}_k.$$

The spin Q is defined in terms of $\hat{X}$ as

$$e^{iQ} = \hat{X}^{-1}.$$

$T_{p,q}(u)$ and $T_{p,Uq}(u)$ commute with $\hat{S}$, $\hat{Z}_k$, and $\hat{X}$. Hence it is possible to make a spin and momentum sectorwise study of the problem.

The roots of the BAE are studied by computing the eigenvalues of the transfer matrices as meromorphic functions of $x=e^{\lambda}$. Since the transfer matrices with different spectral parameter λ commute, their eigenvectors are independent of the spectral parameter. Hence by taking a specific value of the spectral parameter one can determine the eigenvectors numerically by diagonalizing the finite size transfer matrix. From the definition of the eigenvalue equation one can express the eigenvalues as meromorphic functions of x, as the entries of transfer matrix are polynomials in x and the eigenvectors are vectors with numerical (independent of x) entries.

However the problem being coupled, one needs to simultaneously diagonalize T_q and T_{Uq} or in other words find the eigenvalues corresponding to simultaneous eigenvectors of T_q and T_{Uq}. This fact by itself introduces a significantly higher level of difficulty over other numerical simulation of similar type (noncoupled eqns.), e.g., chiral Potts.[25] Coupled BAE and any simultaneous eigenvalue problem (eigenvalues corresponding to simultaneous eigenvectors) results in the same generic problem in computer algorithm. One must develop efficient optimized codes for tackling this.

A detailed numerical study for chains of length $M \leqslant 8$ was done in Ref. 3. The main observations of this numerical study are as follows:

(i) 1-string with both parities, $(1,v)$, $v=(\pm 1)$,
(ii) even length strings with positive parities, $(n,+)$, $n=2,4,\ldots,N$,
(iii) nonstring solutions $\mathrm{Im}(\lambda) \sim \pm \pi/3$.

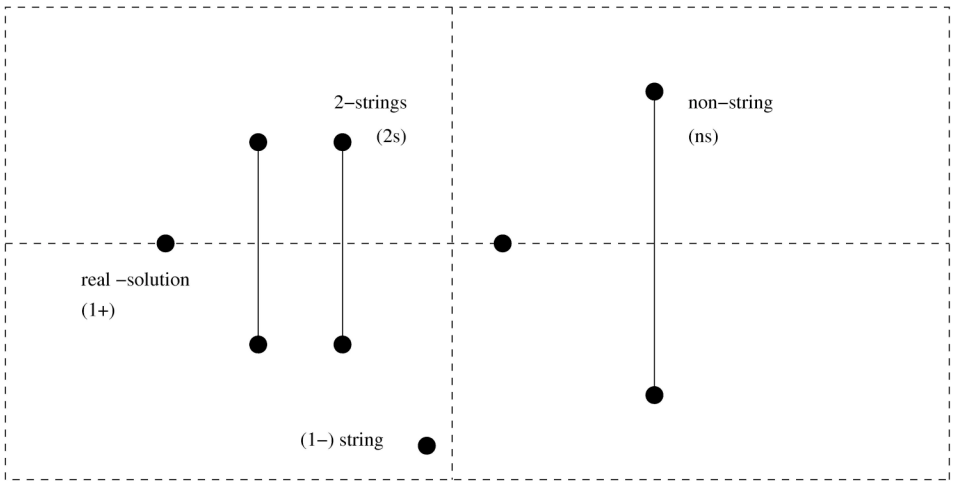

FIG. 4. String and nonstring solutions for BAE.

The ferromagnetic ground state is a filled band of 2-strings, and the excitations consist of $(1+)$, $(1-)$, etc. The antiferromagnetic ground state on the other hand is a filled band of $(1,\pm)$ and excitations are 2-strings with positive parity (see Fig. 4).

It is remarkable that a good deal of insight into the nature of string solutions can be obtained from finite systems of rather small size. The 2-strings are easily identified as having imaginary parts close to $\pi/4$. One can also identify the real roots and roots with negative parity $\mathrm{Im}(\lambda)=\pi/2$. There are roots whose imaginary parts are not well approximated by $\pi/2$ or $\pi/4$. These roots do not seem to systematically approach the 2-string value as $M\to\infty$. These roots are classified as nonstrings. For space limitation $M=2$ and $M=3$ figures are presented in this paper. The imaginary parts of the nonstring (ns) roots are

$M=2$	$P=0$	$-0.321\,982\,35\pi i$
		$0.321\,982\,35\pi i$
$M=3$	$P=0$	$-0.297\,309\,02\pi i$
		$0.297\,309\,02\pi i$
	$P=1$	$0.179\,912-0.330\,545\pi i$
		$0.179\,912+0.330\,545\,15\pi i$
	$P=2$	$-0.179\,912-0.330\,545\pi i$
		$-0.179\,912+0.330\,545\,15\pi i$
$M=4$	$P=0$	$-0.337\,809\,88\pi i$
		$0.337\,809\,88\pi i$
		$-0.348\,355-0.342\,016\pi i$
		$-0.348\,355+0.342\,016\,21\pi i$
		$0.348\,355-0.342\,016\pi i$
		$0.348\,355+0.342\,016\,21\pi i$
		$-0.283\,248\,74\pi i$
		$0.283\,248\,74\pi i$
	$P=1$	$-0.258\,619-0.387\,940\,57\pi i$
		$-0.258\,619+0.387\,940\,57\pi i$

Tables I and II show the classification of roots for spin-4, for lattice sizes 2, 3 and 4 in the $Q=0$ sector. The first column shows the momentum P. The second column gives the roots of the

TABLE I. Classification of roots and integers for $M=2$.

P	$\lambda_k=\ln x_k$	Content	I_k	Energy
	$-0.216\,337-0.227\,395\pi i$	$(2s)$	0.5	
	$-0.216\,337+0.227\,394\,69\pi i$			
	$0.216\,337-0.227\,395\pi i$	$(2s)$	-0.5	
0	$0.216\,337+0.227\,394\,69\pi i$			$-6.246\,22$
	$-0.265\,319$	$(1+)$	-0.5	
	$-0.321\,982\,35\pi i$	(ns)	0	
	$0.321\,982\,35\pi i$			
0	$0.265\,319$	$(1+)$	0.5	4
	$-0.440\,687$	$(1+)$	-1	
	0	$(1+)$	0	
	$-0.5\pi i$	$(1-)$	0	
1	0.440 687	$(1+)$	1	8

BAE in the variable χ. The content or the type of root is identified in column three. Column four gives the corresponding integer that appears in the BAE. In column five the energy calculated for the corresponding eigenvalue for transfer matrix is given.

VI. FREE ENERGY IN THE FERROMAGNETIC CASE FOR *N* EVEN

From the numerical study one can identify that the ferromagnetic (FM) ground state corresponds to a filled band of $N/2$ strings of positive parity for T_q and a filled band of 1-string of negative parity for T_{Uq}. This vector always falls in the $P=0$ sector as is expected. A further study up to eight sites reveals that this remains true.

The LHS of the first of Bethe Ansatz equations, BAE(1), is given by

$$\prod_{k=1}^{L_{Uq/2}} \frac{\sinh(\chi_j-\overline{\chi_k}-2i\gamma)}{\sinh(\chi_j-\overline{\chi_k}+2i\gamma)} = (-1)^{M+1}\left[\frac{\sinh(\chi_j+\gamma i)}{\sinh(\chi_j-\gamma i)}\right]^{2M}. \tag{60}$$

For the ferromagnetic case we made the assumption that the ground state corresponds to $N/2$ strings with positive parity for T_q and 1-strings of negative parity for T_{Uq},

$$\chi_{\alpha,v}^{n,l} = \chi_\alpha^n + 2\gamma(n+1-2l)i, \tag{61}$$

$$\overline{\chi}_{\alpha,v}^{n,l} = \overline{\chi}_\alpha^n - \frac{i\pi}{2}. \tag{62}$$

Define x and $\overline{x}$ by $\chi=2\gamma x$ and $\overline{\chi}=2\gamma\overline{x}$. If $M^{(n)}$ denotes the number of n-strings, we get for the left-hand side (LHS) of the BAE(1),

$$\prod_{l=1}^{n} \frac{\sinh 2\gamma(x_\alpha^n-\overline{x_\beta}+(n+1-2l)i-i-p_0 i)}{\sinh 2\gamma(x_\alpha^n-\overline{x_\beta}+(n+1-2l)i+i-p_0 i)} = \frac{\sinh 2\gamma(x_\alpha^n-\overline{x_\beta}-ni-p_0 i)}{\sinh 2\gamma(x_\alpha^n-\overline{x_\beta}+ni-p_0 i)}.$$

Taking product over the string elements of χ_α the first BAE becomes decoupled and is given in terms of the variables for T_q alone,

TABLE II. Classification of roots and integers for $M=3$.

P	$\lambda_k=\ln x_k$	Content	I_k	Energy
	$-0.325\,636-0.228\,897\pi i$	$(2s)$	1	
	$-0.325\,636+0.228\,896\,64\pi i$			
	$-0.239\,862\,44\pi i$	$(2s)$	0	
	$0.239\,862\,44\pi i$			
	$0.325\,636-0.228\,897\pi i$	$(2s)$	-1	
0	$0.325\,636+0.228\,896\,64\pi i$			$-8.369\,45$
	$-0.388\,991$	$(1+)$	-1	
	$-0.267\,718\pi i$	$(2s)$	0	
	$0.267\,718\pi i$			
	$-0.297\,309\,02\pi i$	(ns)	0	
	$0.297\,309\,02\pi i$			
0	0.388 991	$(1+)$	1	$-1.656\,86$
	$-0.570\,869$	$(1+)$	-1.5	
	$-0.213\,538-0.5\pi i$	$(1-)$	0	
	$-0.149\,008$	$(1+)$	-0.5	
	0.087 3277	$(1+)$	0.5	
	$0.423\,044-0.242\,196\pi i$	$(2s)$	-1.5	
0	$0.423\,044+0.242\,196\,19\pi i$			8
	$-0.768\,026$	$(1+)$	-2	
	$-0.241\,758$	$(1+)$	-1	
	$-0.249\,498\,65\pi i$	$(2s)$	0	
	$0.249\,498\,65\pi i$			
	0.241 758	$(1+)$	1	
0	0.768 026	$(1+)$	2	4.486 83
	$-0.353\,241-0.236\,642\pi i$	$(2s)$	1	
	$-0.353\,241+0.236\,642\,31\pi i$			
	$-0.013\,2479$	$(1+)$	0	
	$0.179\,912-0.330\,545\pi i$	(ns)	0	
	$0.179\,912+0.330\,545\,15\pi i$			
1	0.359 907	$(1+)$	1	3.371 55
	$-0.540\,092$	$(1+)$	-1.5	
	$-0.129\,032$	$(1+)$	-0.5	
	$-0.072\,5776-0.5\pi i$	$(1-)$	0	
	$0.117\,714-0.250\,431\pi i$	$(2s)$	-0.5	
	$0.117\,714+0.250\,430\,57\pi i$			
1	0.506 275	$(1+)$	1.5	3.101 02
	$-0.692\,847$	$(1+)$	-2	
	$-0.209\,487-0.250\,419\pi i$	$(2s)$	1	
	$-0.209\,487+0.250\,418\,75\pi i$			
	0.021 7873	$(1+)$	0	
	0.2683	$(1+)$	1	
1	0.821 734	$(1+)$	2	6.828 43
	$-0.856\,212$	$(1+)$	-2	
	$-0.287\,304$	$(1+)$	-1	
	$-0.506\,275$	$(1+)$	-1.5	
	$-0.117\,714-0.250\,431\pi i$	$(2s)$	0.5	

TABLE II. (*Continued.*)

P	$\lambda_k = \ln x_k$	Content	I_k	Energy
	$-0.117\,714 + 0.250\,430\,57\pi i$			
	$0.072\,5776 - 0.5\pi i$	$(1-)$	0	
	0.129 032	$(1+)$	0.5	
2	0.540 092	$(1+)$	1.5	3.101 02
	$-0.539\,776 - 0.247\,284\pi i$	$(2s)$	1	
	$-0.539\,776 + 0.247\,284\,22\pi i$			
	−0.163 49	$(1+)$	−1	
	0.053 5889	$(1+)$	0	
	0.304 098	$(1+)$	1	
2	0.885 356	$(1+)$	2	11.4569
	−0.620 538	$(1+)$	−2	
	$-0.375\,937 - 0.5\pi i$	$(1-)$	0.5	
	−0.185 678	$(1+)$	−1	
	0.038 6368	$(1+)$	0	
	0.287 304	$(1+)$	1	
2	0.856 212	$(1+)$	2	12.899
	−0.821 734	$(1+)$	−2	
	−0.2683	$(1+)$	−1	
	−0.021 7873	$(1+)$	0	
	$0.209\,487 - 0.250\,419\pi i$	$(2s)$	−1	
	$0.209\,487 + 0.250\,418\,75\pi i$			
2	0.692 847	$(1+)$	2	6.828 43

$$(-1)^{(M+1)n}\left[\prod_{l=1}^{n}\frac{\sinh 2\gamma\left(x_\alpha^n+\left(n+1-2l+\frac{1}{2}\right)i\right)}{\sinh 2\gamma\left(x_\alpha^n-\left(n+1-2l+\frac{1}{2}\right)i\right)}\right]^{2M}=(-1)^{M+1}. \tag{63}$$

After multiplying for the elements of a string, the second BAE becomes

$$\prod_{k=1}^{L_q/2}\prod_{l=1}^{n}\frac{\sinh 2\gamma(\overline{x_\alpha}-x_\beta^n-(n+1-2l)i-i-p_0 i)}{\sinh 2\gamma(\overline{x_\alpha}-x_\beta^n-(n+1-2l)i+i-p_0 i)}=(-1)^{(M+1)+(nL_q/2)}. \tag{64}$$

Thus we have only one set of BAE which involves the zeros of the transfer matrix T_q. From the above equation taking natural logarithm of both sides we get

$$2M\sum_{l=1}^{n} i\cdot\ln\left(\frac{\sinh\left(\chi_\alpha+2\gamma\left(n+1-2l+\frac{1}{2}\right)\right)}{\sinh\left(\chi_\alpha-a\gamma\left(n+1-2l+\frac{1}{2}\right)\right)}\right)=\pi I_\alpha.$$

Defining the density of string centers for the zeros of T_q by

$$\rho(\chi)=\lim_{M\to\infty}\frac{1}{M(\chi_{k+1}-\chi_k)} \tag{65}$$

we get

$$\rho(\chi)=\frac{1}{\pi}\Theta_{(N/2,+)}^{(1)'}(\chi), \tag{66}$$

where

$$\Theta^{(1)}_{(N/2,+)}(\chi) \doteq \sum_{l=1}^{n} 2\phi\left(\chi, n+\frac{1}{2}-2l, +\right)$$

and prime on $\Theta^{(1)}_{(N/2,+)}(\chi)$ denotes differentiation with respect to the variable χ. Here the function ϕ, as defined by Takahashi and Suzuki[26] is

$$\phi(x,n,v) \doteq i\cdot\ln(g(x,n,v)), \quad g(x,n,v) \doteq \frac{\sinh 2\gamma(x+ni+p_0 i)}{\sinh 2\gamma(x-ni+p_0 i)}.$$

Evaluating the sum over l in the Fourier space,

$$\tilde{\Theta}^{(1)'}_{(N/2,+)}(k) = 2\pi\frac{\sinh\left(\frac{\pi k}{2}-\frac{\pi k}{2N}\right)}{\sinh\left(\frac{\pi k}{N}\right)}, \tag{67}$$

$$\tilde{\rho}(k) = 4\frac{\sinh\left(\frac{\pi k}{2}-\frac{\pi k}{2N}\right)}{\sinh\left(\frac{\pi k}{N}\right)}. \tag{68}$$

By inverse Fourier transform we get

$$\rho(\chi) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}k\, e^{-ik\chi}\tilde{\rho}(k).$$

The free energy for the ferromagnetic ground state is defined as

$$f_0(u) \doteq \lim_{M\to\infty}\left(-\frac{1}{M}\ln\Lambda_0(u)\right) = \prod_{\alpha=1}^{M^{N/2}}\prod_{l=1}^{N/2}\frac{\sin(2u-i\chi_\alpha+x(l))}{\sin(i\chi_\alpha-x(l))}.$$

Replacing the summation by an integral over the symmetrically placed string centers,

$$f_0(u) = -\frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}\chi\,\rho(\chi)\sum_{l=1}^{N/2}\ln\left(\frac{\cosh(2\chi)-\cos(4u+2x(l))}{\cosh(2\chi)-\cos(2x(l))}\right). \tag{69}$$

Transforming to the Fourier space and utilizing the expression and properties of $\tilde{\rho}(k)$ we get

$$f_0(u) = \int_{-\infty}^{\infty}\frac{4\mathrm{d}k}{k}\frac{\sinh\left(k\pi-\frac{k\pi}{N}\right)\sinh(2ku)\sinh\left(2ku-k\pi-\frac{k\pi}{N}\right)}{\sinh^2\left(\frac{2k\pi}{N}\right)}. \tag{70}$$

VII. EXCITATION ON FM GROUND STATE

We have seen in the preceding section that the FM ground state is given by a filled band of $(2s)$ strings. Consider the $Z_{(2s)}(\chi)$ function. In the general case it should look like

$$Z_{(2s)}(\chi) = \frac{1}{2\pi}\Theta^{(1)}_{(2s)}(\chi) - \frac{1}{2\pi M}\sum_k\sum_{\beta=1}^{M^{(k)}}\Theta^{(2)}_{(2s,k)}(\chi-\chi^k_\beta). \tag{71}$$

The density of $(2s)$ vacancies is given by

$$\sigma_{(2s)}(\chi) \doteq -Z'_{(2s)}(\chi). \tag{72}$$

The vacancy density and the density of $(2s)$ particles is related by

$$\sigma_{(2s)}(\chi) = \rho_{(2s)}(\chi) + \frac{1}{M}\sum_{\beta=1}^{M_h^{(2s)}} \delta(\chi - \chi_\beta^{(2s)h}), \tag{73}$$

where $\chi_\beta^{(2s)h}$ are the position of the holes.

Thus

$$-\sigma_{(2s)}(\chi) = \frac{1}{2\pi}\Theta'^{(1)}_{(2s)}(\chi) - \frac{1}{2\pi M}\sum_{k\neq(2s)}\sum_{\beta=1}^{M^{(k)}} \Theta'^{(2)}_{(2s,k)}(\chi - \chi_\beta^k) - \frac{1}{2\pi}\int \Theta'^{(2)}_{(2s,2s)}(\chi-\mu)\mathrm{d}\mu$$
$$+ \frac{1}{2\pi M}\sum_{h=1}^{M_h^{(2s)}} \Theta'^{(2)}_{(2s,2s)}(\chi - \chi_\beta^{(2s)h}). \tag{74}$$

The above equation can be interpreted as a collection of terms contributing to $(2s)$-ground state, $(2s)$-holes and excited particles $\sigma_{(2s)} = \sigma^{(0)}_{(2s)} + \sigma^{(h)}_{(2s)} + \Sigma_j \sigma^{(j)}_{(2s)}$ where $\sigma^{(0)}_{(2s)}$ is the same as $\rho_{(2s)}$ of the last section.

The expressions for energy (E) and momentum (P) are

$$E = \sum_{k=1}^{L/2} \cot\left(i\chi_k + \frac{\pi}{2N}\right) - 2M\sum_{k=1}^{N/2} \cot\left(\frac{\pi k}{N}\right), \tag{75}$$

$$e^{iP} = \prod_{k=1}^{L/2} \frac{\sinh\left(\chi_k + \frac{i\pi}{2N}\right)}{\sinh\left(\chi_k - \frac{i\pi}{2N}\right)}. \tag{76}$$

We obtain the energy of a state designated by a given set of strings

$$E = \sum_{\substack{k \\ \text{strings}}} \sum_{\beta=1}^{M^{(k)}} \epsilon_k(\chi_\beta^{(k)}) = \int \mathrm{d}\chi\, \sigma_{(2s)}(\chi)\epsilon_{(2s)}(\chi) - \sum_{\beta=1}^{M_h^{(2s)}} \epsilon_{(2s)}(\chi_\beta^{(2s)h}) + \sum_{\substack{k \\ k\neq(2S)}} \sum_{\beta=1}^{M^{(k)}} \epsilon(\chi_\beta^{(k)}). \tag{77}$$

The bare energies for n-string with parity v is easily obtained

$$\epsilon_{(n,v)}(\chi_\alpha) = \sum_{k=1}^{n} \cot\left(i\chi_{k,\alpha}^{(n,v)} + \frac{\pi}{2N}\right) = \sum_{k=1}^{n} \cot\left(i\chi_\alpha^{(n,v)} - 2\gamma(n+1-2k) - \frac{\pi}{4}(1-v) + \frac{\pi}{2N}\right)$$
$$= \sum_{k=1}^{n} \tan\left(\frac{\pi}{2} - i\chi_\alpha^{(n,v)} + 2\gamma(n+1-2k) + \frac{\pi}{4}(1-v) - \frac{\pi}{2N}\right).$$

One can separate the real and imaginary parts of this expression. This helps in determining whether we require additional constraints on rapidities χ_j to ensure reality of the total energy.

Numerical study showed that there exist several spurious solutions and only a subset of them, corresponding to a specific choice of counting numbers $I_\alpha^{(j)}$, is admissible. Nonstring solutions exist, however they are not as numerous. From the numerical study we make the assumption that the elementary excitations over the FM [a sea of $(2s)$-strings] are (a) a pair of $(1+)$ strings, and (b) $(1+)$ and $(1-)$ strings.

The FM ground state is a filled band of $(2s)$ strings. The density of ground state energy is

$$e_0 = \lim_{M\to\infty} \frac{E_0}{M} = \int d\chi\, \rho_{(2s)}(\chi)\epsilon_{(2s)}(\lambda) - 2\sum_{k=1}^{(N-1)/2} \cot\left(\frac{\pi k}{N}\right). \tag{78}$$

The observed correlation between the integers suggest that the rapidities corresponding to $(2s)$ and (a) should be connected allowing cancellation of the imaginary part of the total energy,

$$\mathrm{Im}[\epsilon_{(2s)}] = \mathrm{Im}[\epsilon_{(a)}]. \tag{79}$$

It can be shown that, $\mathrm{Im}[\epsilon_{(2s)}]=\mathrm{Im}[\epsilon_{(a)}]$ and $\mathrm{Re}[\epsilon_{(2s)}]=-\mathrm{Re}[\epsilon_{(a)}]$.

$$\mathrm{Re}[\epsilon_{(a)}(\chi)] = \frac{4}{\cosh(4\chi)}. \tag{80}$$

Similar argument holds for (b)-type excitations, where $\mathrm{Im}[\epsilon_{(2s)}]=\mathrm{Im}[\epsilon_{(b)}]$ and $\mathrm{Re}[\epsilon_{(2s)}]=-\mathrm{Re}[\epsilon_{(b)}]$.

$$\mathrm{Re}[\epsilon_{(b)}(\chi)] = \frac{4}{\cosh(4\chi)}. \tag{81}$$

One should note that the dressed energy and bare energy are equal since the function coupling the ground state density to excited states $\Theta^{(2)}_{(j,k)}$ is zero for $j=(2s)$. Thus we arrive at

$$E = E_0 + \sum_{\beta=1}^{M^{(a)}} 2\epsilon_{(a)}(\chi^{(a)}_\beta) + \sum_{\beta=1}^{M^{(b)}} 2\epsilon_{(b)}(\chi^{(b)}_\beta), \tag{82}$$

where E_0 is the ground state energy.

We now turn to the calculation of momentum. The momentum associated with a string of length j and parity v is found to be

$$p_{(1+)}(\chi) = -\tfrac{1}{2}\Theta^{(1)}_{(1+)}(\chi),$$

$$p_{(j)}(\chi) = -\tfrac{1}{2}\Theta^{(1)}_{(j)}(\chi) \quad \text{for } j \neq (1+), \tag{83}$$

whence

$$p_{(a)}(\chi) = p_{(b)}(\chi) = 2\arctan\left(\tanh\left(\frac{\chi}{2}\right)\right) + \pi. \tag{84}$$

These expressions are similar to the ones for nonstring excitations in the anti-ferromagnetic case for odd spin FZM. We get the dispersion relations for elementary excitations over the ferromagnetic ground state as

$$\epsilon_{(a)}(p) = 4\sin\left(\frac{p}{2}\right),$$

$$\epsilon_{(b)}(p) = 4\sin\left(\frac{p}{2}\right). \tag{85}$$

VIII. FREE ENERGY IN THE ANTIFERROMAGNETIC CASE FOR *N* EVEN

From the numerical study for finite lattices it was apparent that the antiferromagnetic (AFM) ground-state corresponds to a filled band of real roots for both T_q and T_{Uq}. In other words the AFM ground state is a filled sea of $(1,+)$ strings for both families of transfer matrices.

The AFM ground state corresponds to real roots for both families of transfer matrices. Hence we consider the natural logarithm of both sides of BAE's. From BAE(1) we get

$$\sum_{k=1}^{L_{Uq}/2} i \ln\left(\frac{\sinh(\chi_j - \overline{\chi_k} - 2i\gamma)}{\sinh(\chi_j - \overline{\chi_k} + 2i\gamma)}\right) = 2M \cdot i \ln\left(\frac{\sinh(\chi_j + i\gamma)}{\sinh(\chi_j - i\gamma)}\right) + 2\pi I_j \tag{86}$$

with standard definition of $\rho_1(\chi)$ and $\rho_2(\chi)$,

$$\rho_1(\chi_\alpha) = \frac{1}{\pi}\Theta_1^{(1)'}(\chi_\alpha) - \frac{1}{2M\pi}\sum_{\beta=1}^{\overline{M}} \Theta_1^{(2)'}(\chi_\alpha - \overline{\chi_\beta}) = \frac{1}{\pi}\Theta_1^{(1)'}(\chi_\alpha) - \frac{1}{2M\pi}\int_{-\infty}^{+\infty} d\overline{\mu}\Theta_1^{(2)'}(\chi - \overline{\mu})\rho_1(\overline{\mu}). \tag{87}$$

From BAE(2) we get

$$\sum_{k=1}^{L_q/2} i \ln\left(\frac{\sinh(\overline{\chi_j} - \chi_k - 2i\gamma)}{\sinh(\overline{\chi_j} - \chi_k + 2i\gamma)}\right) = 2\pi\overline{I_j}. \tag{88}$$

In the continuum limit $M \to \infty$ we get

$$\rho_2(\overline{\chi}) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\mu\, \Theta_2^{(2)'}(\overline{\chi_\alpha} - \mu)\rho_1(\mu). \tag{89}$$

The above pair of BAE is solved as before by the Fourier transform method,

$$\tilde{\rho}_1(k) = \frac{1}{\pi}\tilde{\Theta}_1^{(1)'}(k) - \frac{1}{2\pi}\tilde{\Theta}_1^{(2)'}(k)\tilde{\rho}_2(k), \tag{90}$$

$$\tilde{\rho}_2(k) = \frac{1}{2\pi}\tilde{\Theta}_2^{(2)'}(k)\tilde{\rho}_1(k). \tag{91}$$

From the above two equations,

$$\tilde{\rho}_1(k) = \frac{\sinh\left(\frac{\pi k}{2}\right) \cdot \sinh\left(\frac{\pi k}{2} - \frac{\pi k}{2N}\right)}{\sinh\left(\frac{\pi k}{N}\right) \cdot \sinh\left(\pi k + \frac{\pi k}{N}\right)}. \tag{92}$$

Following a similar procedure as shown in detail in the ferromagnetic case, the free energy for the antiferromagnetic case is obtained as

$$f = \frac{1}{2}\int_{-\infty}^{+\infty} \frac{dk}{k}\frac{\tilde{\rho}_1(2k)}{\sinh(\pi k)}\left[\cosh k\left(\pi - 4u - \frac{\pi}{N}\right) - \cosh k\left(\pi - \frac{\pi}{N}\right)\right]. \tag{93}$$

Substituting for $\tilde{\rho}_1(2k)$,

$$f = \frac{1}{2}\int_{-\infty}^{+\infty} \frac{dk}{k} \frac{\sinh\left(\pi k - \frac{\pi k}{N}\right)}{\sinh\left(\frac{2\pi k}{N}\right) \cdot \sinh\left(2\pi k + \frac{2\pi k}{N}\right)} \cdot \cosh k\left(\pi - 4u - \frac{\pi}{N}\right)$$

$$- \int_{-\infty}^{+\infty} \frac{dk}{k} \frac{\sinh\left(\pi k - \frac{\pi k}{N}\right)}{\sinh\left(\frac{2\pi k}{N}\right) \cdot \sinh\left(2\pi k + \frac{2\pi k}{N}\right)} \cdot \cosh k\left(\pi - \frac{\pi}{N}\right). \tag{94}$$

IX. EXCITATION ON AFM GROUND STATE

In the case of AFM, the ground state is a filled band of $(1+)$. The results of the preceding section suggest that excitations appear as $(2s)$ strings when a hole is created in the $(1+)$ sea. Consider the $Z_{(1+)}(\chi)$ function. In the general case it should look like

$$Z_{(1+)}(\chi) = \frac{1}{2\pi}\Theta^{(1)}_{(1+)}(\chi) - \frac{1}{2\pi M}\sum_k \sum_{\beta=1}^{M^{(k)}} \Theta^{(2)}_{(1+,k)}(\chi - \chi^k_\beta). \tag{95}$$

The density of $(1+)$ vacancies is given by

$$\sigma_{(1+)}(\chi) \doteq - Z'_{(1+)}(\chi). \tag{96}$$

The vacancy density $\sigma_{(1+)}(\chi)$ and the density of $(1+)$ particles $\rho_{(1+)}(\chi)$ is related by

$$\sigma_{(1+)}(\chi) = \rho_{(1+)}(\chi) + \frac{1}{M}\sum_{\beta=1}^{M_h^{(1+)}} \delta(\chi - \chi^{(1+)h}_\beta), \tag{97}$$

where $\chi^{(1+)h}_\beta$ are the position of the holes.

Thus

$$- \sigma_{(1+)}(\chi) = \frac{1}{2\pi}\Theta^{(1)\prime}_{(1+)}(\chi) - \frac{1}{2\pi M}\sum_{k\neq(1+)} \sum_{\beta=1}^{M^{(k)}} \Theta^{(2)\prime}_{(1+,k)}(\chi - \chi^k_\beta) - \frac{1}{2\pi}\int \Theta^{(2)\prime}_{(1+,1+)}(\chi - \mu)d\mu$$

$$+ \frac{1}{2\pi M}\sum_{\beta=1}^{M_h^{(1+)}} \Theta^{(2)\prime}_{(1+,1+)}(\chi - \chi^{(1+)h}_\beta). \tag{98}$$

The above equation can be interpreted as a collection of terms contributing to $(1+)$ ground state, $(1+)$ holes and excited particles over the ground state sea of $(1+)$ string. $\sigma_{(1+)} = \sigma^{(0)}_{(1+)} + \sigma^{(h)}_{(1+)} + \Sigma_j \sigma^{(j)}_{(1+)}$, where $\sigma^{(0)}_{(1+)}$ is the same as $\rho_{(1+)}$ of the last section.

We obtain the energy of a state designated by a given set of strings $\{k\}$, having $M^{(k)}$ strings of type (k) with string centers at $\chi^{(k)}_\beta$,

$$E = \sum_{\substack{k \\ \text{strings}}} \sum_{\beta=1}^{M^{(k)}} \epsilon_k(\chi^{(k)}_\beta) = \int d\chi\, \sigma_{(1+)}(\chi)\epsilon_{(1+)}(\chi) - \sum_{\beta=1}^{M_h^{(1+)}} \epsilon_{(1+)}(\chi^{(1+)h}_\beta) + \sum_{\substack{k \\ k\neq(1+)}} \sum_{\beta=1}^{M^{(k)}} \epsilon(\chi^{(k)}_\beta). \tag{99}$$

From the numerical study we can make the assumption that the elementary excitations over the AFM ground state, which is a sea of $(1+)$-strings, is given by a set of $(2s)$ strings.

The density of ground state energy for the AFM case is given by

$$e_0 = \lim_{M\to\infty} \frac{E_0}{M} = \int d\chi\, \rho_{(1+)}(\chi)\epsilon_{(1+)}(\lambda) - 2\sum_{k=1}^{(N-1)/2} \cot\left(\frac{\pi k}{N}\right). \tag{100}$$

Total energy is real since the imaginary part of the energy contribution from holes cancel the imaginary part of the energy of excitation, i.e., $\mathrm{Im}[\epsilon_{(2s)}]=\mathrm{Im}[\epsilon_{(1+)}]$. The real parts are given by

$$\mathrm{Re}[\epsilon_{(2s)}(\chi)] = \mathrm{Re}[\epsilon_{(1+)h}(\chi)]. \tag{101}$$

In this case also, the dressed energy equals the bare energy. As before, we will denote by $\epsilon_{(2s)} \times(\chi_\beta^{(2s)})$ its real part. The total energy is given by

$$E = E_0 + \sum_{\beta=1}^{M^{(2s)}} 2\epsilon_{(2s)}(\chi_\beta^{(2s)}), \tag{102}$$

where E_0 is the ground state energy.

We now turn to the calculation of momentum. The momentum associated with a string of length j and parity v is found to be

$$p_{(1+)}(\chi) = -\tfrac{1}{2}\Theta_{(1+)}^{(1)}(\chi), \tag{103}$$

$$p_{(j)}(\chi) = -\tfrac{1}{2}\Theta_{(j)}^{(1)}(\chi) \quad \text{for } j \neq (1+), \tag{104}$$

whence

$$p_{(2s)}(\chi) = 2\arctan\left(\tanh\left(\frac{\chi}{2}\right)\right). \tag{105}$$

If one keeps in mind the fact that the correlation of χ's demand an additional π for the creation of $(1+)$ hole, we can derive the dispersion relation

$$\epsilon_{(2s)}(p) = 4\sin\left(\frac{p}{2}\right). \tag{106}$$

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Diagrammatic Young projection operators for U(n)

Henriette Elvang
Department of Physics, UCSB, Santa Barbara, California 93106

Predrag Cvitanović
Center for Nonlinear Science, Georgia Institute of Technology, Atlanta, Georgia 30332-0430

Anthony D. Kennedy
School of Physics, JCMB, King's Buildings, University of Edinburgh, Edinburgh EH9 3JZ, Scotland

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We utilize a diagrammatic notation for invariant tensors to construct the Young projection operators for the irreducible representations of the unitary group U(n), prove their uniqueness, idempotency, and orthogonality, and rederive the formula for their dimensions. We show that all U(n) invariant scalars ($3n-j$ coefficients) can be constructed and evaluated diagrammatically from these U(n) Young projection operators. We prove that the values of all U(n) $3n-j$ coefficients are proportional to the dimension of the maximal representation in the coefficient, with the proportionality factor fully determined by its S_k symmetric group value. We also derive a family of new sum rules for the $3-j$ and $6-j$ coefficients, and discuss relations that follow from the negative dimensionality theorem. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1832753]

I. INTRODUCTION

Symmetries are beautiful, and theoretical physics is replete with them, but there comes a time when a calculation must be done. Innumerable calculations in high-energy physics, nuclear physics, atomic physics, and quantum chemistry require construction of irreducible many-particle states (irreps), decomposition of Kronecker products of such states into irreps, and evaluations of group theoretical weights (Wigner $3n-j$ symbols, reduced matrix elements, quantum field theory "vacuum bubbles"). At such times effective calculational methods gain in appreciation.

In his 1841 fundamental paper[1] on the determinants today known as "Jacobians," Jacobi initiated the theory of irreps of the symmetric group S_k. Schur used the S_k irreps to develop the representation theory of GL($n;\mathbb{C}$) in his 1901 dissertation,[2] and already by 1903 the Young tableaux[3,4] came into use as a powerful tool for reduction of both S_k and GL($n;\mathbb{C}$) representations. In quantum theory the group of choice[5] is the unitary group U(n), rather than the general linear group GL($n;\mathbb{C}$). Today this theory forms the core of the representation theory of both discrete and continuous groups, described in many excellent textbooks.[6–17]

Here we transcribe the theory of the Young projection operators into a form particularly well suited to particle physics calculations, and show that the diagrammatic methods of Ref. 18 can be profitably employed in explicit construction of U(n) multiparticle states, and evaluation of the associated $3n-j$ coefficients.

In diagrammatic notation tensor objects are manipulated without any explicit indices. Diagrammatic evaluation rules are intuitive and relations between tensors can often be grasped visually. Take as an example the reduction of a two-index tensor T_{ij} into symmetric and antisymmetric parts, $T=(S+A)T$, where

$$ST_{ij} = \tfrac{1}{2}(\mathbb{I} + (12))T_{ij}$$

$$AT_{ij} = \tfrac{1}{2}(\mathbb{I} - (12))T_{ij},$$

and $\mathbb{I}$ and (12) denote the identity and the index transposition. Diagrammatically, the two projection operators are drawn as

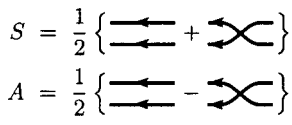

(1)

It is clear at a glance that S symmetrizes and A antisymmetrizes the two tensor indices. Here we shall construct such projection operator for tensors of any rank.

Penrose's papers are the first (known to the authors) to cast the Young projection operators into a diagrammatic form. Here we use Penrose diagrammatic notation for symmetrization operators,[19] Levi–Civita tensors[20] and "strand networks."[21] For several specific, few-particle examples, diagrammatic Young projection operators were constructed by Canning,[22] Mandula,[23] and Stedman.[24] A diagrammatic construction of the U(n) Young projection operators for *any* Young tableau was outlined in Ref. 25, without proofs. Here we present the method in detail, as well as the proof that the Young projection operators so constructed are unique.[26] The other new results are a proof that every U(n) $3n-j$ coefficient is proportional to the dimension of the largest irrep within the $3n-j$ diagram, and several sum rules for U(n) $3-j$ and $6-j$ coefficients.

The paper is organized as follows. The diagrammatic notation for tensors is reviewed in Sec. II and the Young tableaux in Sec. III. This material is standard and the reader is referred to any of the above cited monographs for further details. In Sec. IV we construct diagrammatic Young projection operators for U(n), and give formulas for the normalizations and the dimensions of U(n) irreps. In Sec. V we recast the Clebsch–Gordan recoupling relations into a diagrammatic form, and show that—somewhat surprisingly—the values of all U(n) $3n-j$ coefficients follow from the representation theory for the symmetric group S_k alone. The $3n-j$ coefficients for U(n) are constructed from the Young projection operators and evaluated by diagrammatic methods in Sec. V B. We derive a family of new sum rules for U(n) $3n-j$ coefficients in Sec. V C. In Sec. VI we briefly discuss the case of SU(n) and mixed multiparticle antiparticle states. In Sec. VII we state and prove the negative dimensionality theorem for U(n). Not only does this proof provide an example of the power of diagrammatic methods, but the theorem also simplifies certain group theoretic calculations. We summarize our results in Sec. VIII.

The key, but lengthy original result presented in this paper, the proof of the uniqueness, completeness, and orthogonality of the Young projection operators[26] is relegated to the appendix.

II. DIAGRAMMATIC NOTATION

In the diagrammatic notation[18] an invariant tensor is drawn as a "blob" with a leg representing each index. An arrow indicates whether it is an upper or lower index; lower index arrows always point away from the blob whereas upper index arrows point into the blob. The index legs are ordered in the counterclockwise direction around the blob, and if the indices are not cyclic there must be an indication of where to start, for example,

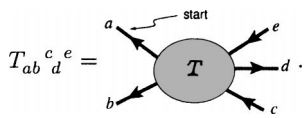

An internal line in a diagram implies a sum over the corresponding index: matrix multiplication is drawn as

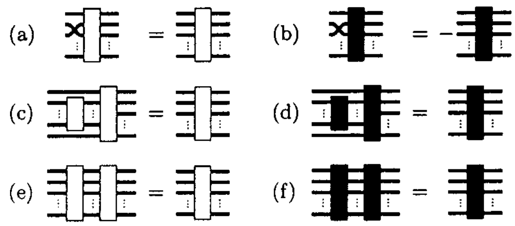

FIG. 1. Properties of the diagrammatic symmetrization and antisymmetrization operators.

where the index b can be omitted, as indeed can all other "dummy" indices. The Kronecker delta is drawn as

$$\delta^a_b = b \longleftarrow a \quad a,b = 1,2,\ldots,n,$$

and its trace—the dimension of the representation—is drawn as a closed loop,

$$= \delta^a_a = n\,. \tag{2}$$

Index permutations can be drawn in terms of Kronecker deltas. For example, the symmetric group S_2 acting on two indices consists of the identity element $\mathbb{I}_{ab}{}^{cd} = \delta^d_a \delta^c_b$ and the transposition $(12)\,_{ab}{}^{cd} = \delta^c_a \delta^d_b$. In the diagrammatic notation these operators are drawn as

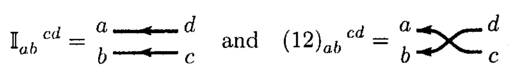

Symmetrization of p indices is achieved by adding all permutations σ of p indices, $S = (1/p!)\Sigma_{\sigma\in S_p}\, \delta^{a_1}_{\sigma(b1}\ldots\delta^{a_p}_{b_p)}$. Similarly, the operator$A = (1/p!)\Sigma_{\sigma\in S_p} \operatorname{sgn}(\sigma)\; \delta^{a_p}_{\sigma(b_1}\ldots\delta^{a_1}_{b_p)}$ (with a minus − for odd permutations) antisymmetrizes p indices. Combinations of symmetrizers S and antisymmetrizers A are collectively referred to as *symmetry operators*.

In the diagrammatic notation we write the symmetrizers and the antisymmetrizers of *length p* as[19]

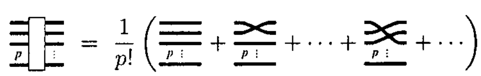

(3)

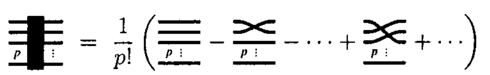

(4)

In order to streamline the notation we shall neglect the arrows whenever this leads to no confusion. Basic properties of the symmetry operators are listed in Fig. 1: A symmetrizer is invariant under any permutation of its legs, rule (a). The antisymmetrizer changes sign under odd permutations, rule (b). A symmetrizer connected by more than one line to an antisymmetrizer is zero by rules (a) and (b),

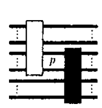

$$= 0, \quad p \geq 2\,. \tag{5}$$

Recursive identities for the (anti)symmetrizers are given in (A5) and (A4).

III. YOUNG TABLEAUX

Partition k identical boxes into D subsets, and let λ_m, $m=1,2,\ldots,D$, be the number of boxes in the subsets ordered so that $\lambda_1 \geqslant \lambda_2 \cdots \geqslant \lambda_D \geqslant 1$. Then the partition $\lambda=[\lambda_1,\lambda_2,\cdots,\lambda_D]$ fulfills $\Sigma_{m=1}^{D}\lambda_m=k$. The diagram obtained by drawing the D rows of boxes on top of each other, left aligned, starting with λ_1 at the top, is called a *Young diagram* Y.

Inserting each number from the set $\{1,\ldots,k\}$ into a box of a Young diagram Y in such a way that numbers increase when reading a column from top to bottom and numbers do not decrease when reading a row from left to right yields a *Young tableau* Y_a. The subscript a labels different tableaux derived from a given Young diagram, i.e., different admissible ways of inserting the numbers into the boxes. A *standard tableau* is a k-box Young tableau constructed by inserting the numbers $1,\ldots,k$ according to the above rules, but using each number exactly once.

As an example, three distinct standard tableaux,

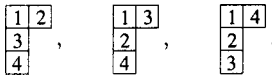

are obtained from the four-box Young diagram with partition $\lambda=[2,1,1]$.

A. Symmetric group S_k

Young diagrams label the irreps of the symmetric group S_k. A k-box Young diagram Y corresponds to an irrep of S_k, and Δ_λ, the dimension of the irrep λ, is the number of standard tableaux Y_a that can be constructed from the Young diagram Y. From the above example we see that the irrep $\lambda=[2,1,1]$ of S_4 is three dimensional. The formula for the dimension Δ_Y of the irrep of S_k corresponding to the Young diagram Y is

$$\Delta_Y = \frac{k!}{|Y|}. \tag{6}$$

The number $|Y|$ is computed using a "hook" rule: Enter into each box of the Young diagram the number of boxes below and to the left of the box, including the box itself. Then $|Y|$ is the product of the numbers in all the boxes. For instance,

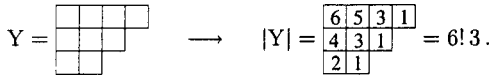

The hook rule (6) was first proved surprisingly late, in 1954, by Frame, de B. Robinson, and Thrall.[27] Various proofs can be found in Refs.[15,16,28–31]; in particular, see Sagan[32] and references therein.

B. Representations of U(n)

While every Young diagram labels an irrep of S_k, every standard tableau labels an irrep of U(n). The dimension d_Y of an irrep labeled by the Young diagram Y equals the number of Young tableaux Y_a that can be obtained from Y by inserting numbers from the set $\{1,2,\ldots,n\}$ such that the numbers increase in each column and do not decrease in each row.

For example, for SU (2) the partition [2] corresponds to a three-dimensional irrep with tableaux $\boxed{1}\boxed{1}$, $\boxed{1}\boxed{2}$, and $\boxed{2}\boxed{2}$, and the partition [1, 1] corresponds to a one-dimensional irrep with one tableau, $\begin{array}{|c|}\hline 1\\\hline 2\\\hline\end{array}$. Similarly, one can check that for SU (3), the partition [2] is six dimensional and the partition [1, 1] is three dimensional. We shall derive the dimension formula for any irrep of U(n) in Sec. IV C.

IV. YOUNG PROJECTION OPERATORS

We now present a diagrammatic method for construction of Young projection operators. A combinatorial version of these operators was given by van der Waerden,[33] who credited von Neumann. There are many other versions in the literature, all of them illustrating the fundamental theorem of 't Hooft and Veltman:[34] combinatorics cannot be taught. What follows might aid those who think visually.

A. The group algebra

Our goal is to construct the projection operators such as (1) for any irrep of S_k. We need to construct a basis set of invariant tensors, multiply them by scalars, add and subtract them, and multiply a tensor by another tensor. The necessary framework is provided by the notion of *group algebra*.

The elements $\sigma \in S_k$ of the symmetric group S_k form a basis of a $k!$-dimensional vector space V of elements

$$s = \sum_{\sigma \in S_k} s_\sigma \sigma \in V, \tag{7}$$

where s_σ are the components of the vector s in the given basis. If s, $t \in V$ have components (s_σ) and (t_σ), we define the product of s and t as the vector st in V with components $(st)_\sigma = \Sigma_{\tau \in S_k} s_\tau t_{\tau^{-1}\sigma}$. This multiplication is associative because it relies on the associative group operation. Since V is closed under the multiplication the elements of V form an associative algebra—the *group algebra* of S_k. Acting on an element $s \in V$ with any group element maps s to another element in the algebra, hence this map gives a $k!$-dimensional matrix representation of the group algebra, the *regular representation*. Note that the matrices of any representation μ of the group is also a basis for representation of the algebra: Let $D^\mu(\sigma)$ denote a (possibly reducible) representation of S_k. The group algebra of S_k in the representation μ then consists of elements

$$D^\mu(\mathrm{s}) = \sum_{\sigma \in S_k} \mathrm{s}_\sigma D^\mu(\sigma) \in V,$$

where s is given by (7). The minimal left-ideals V_λ of the group algebra (i.e., $sV_\lambda = V_\lambda$ for all $s \in V$, and V_λ has no proper subideals) are the proper invariant subspaces corresponding to the irreps of the symmetric group S_k.

The regular representation is reducible and each irrep appears Δ_λ times in the reduction, where Δ_λ is the dimension of the subspace V_λ corresponding to the irrep λ. This gives the well-known relation between the order of the symmetric group $|S_k| = k!$ (the dimension of the regular representation) and the dimensions of the irreps,

$$|S_k| = \sum_{\text{irreps } \lambda} \Delta_\lambda^2.$$

Using (6) and the fact that the Young diagrams label the irreps of S_k, we have

$$1 = k! \sum_{(k)} \frac{1}{|\mathrm{Y}|^2}, \tag{8}$$

where the sum is over all Young diagrams with k boxes. We shall use this relation to determine the normalization of Young projection operators in the Appendix.

The reduction of the regular representation of S_k gives a completeness relation

$$\mathbb{I} = \sum_{(k)} P_{\mathrm{Y}}$$

into projection operators

$$P_{\mathrm{Y}} = \sum_{\mathrm{Y}_a \in \mathrm{Y}} P_{\mathrm{Y}_a}.$$

The sum is over all Young tableaux derived from the Young diagram Y. Each P_{Y_a}. projects onto the corresponding invariant subspace V_{Y_a}. For each Y there are Δ_{Y} such projection operators (corresponding to the Δ_{Y} possible standard arrangements of the diagram) and each of these project onto one of the Δ_{Y} invariant subspaces V_{Y} of the reduction of the regular representation. It follows that the projection operators are orthogonal and that they constitute a complete set.

B. Diagrammatic Young projection operators

We now generalize (1), the S_2 projection operators expressed in terms of Kronecker deltas, to Young projection operator for any S_k.

The Kronecker delta is invariant under unitary transformations, $\delta^b_a = (U^\dagger)_a{}^{a'} \delta^{b'}_{a'} U_{b'}{}^b$, $U \in \mathrm{U}(n)$, and so is any combination of Kronecker deltas, such as the symmetrizers of Fig. 1. Since these operators constitute a complete set, any U(n) invariant tensor built from Kronecker deltas can be written in terms of symmetrizers and antisymmetrizers. In particular, the invariance of the Kronecker delta under U(n) transformations implies that the same symmetry group operators which project the irreps of S_k also yield the irreps of U(n).

The simplest examples of Young projection operators are those associated with the Young tableaux consisting of either one row or one column. The corresponding Young projection operators are simply the symmetrizers (3) or the antisymmetrizers (4), respectively. As projection operators for S_k, the symmetrizer projects onto the one-dimensional subspace corresponding to the fully symmetric representation, and the antisymmetrizer projects onto the alternating representation.

A Young projection operator for a mixed symmetry Young tableau will here be constructed by first antisymmetrizing subsets of indices, and then symmetrizing other subsets of indices; which subsets are dictated by the form of the Young tableau, as will be explained shortly. Schematically,

$P_{\mathrm{Y}_a} = \alpha_{\mathrm{Y}}$ 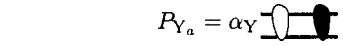 ,

where α_{Y} is a normalization constant (defined below) ensuring that the operators are idempotent, $P_{\mathrm{Y}_a} P_{\mathrm{Y}_b} = \delta_{ab} P_{\mathrm{Y}_a}$. This particular form of projection operators is by no means unique—Young projection operators symmetric under transposition are constructed in Ref. 18—but is particularly convenient for explicit computations

Let Y_a be a k-box standard tableau. Arrange a set of symmetrizers corresponding to the rows in Y_a, and to the right of this arrange a set of antisymmetrizers corresponding to the columns in Y_a. For a Young diagram Y with s rows and t columns we label the rows $\mathrm{S}_1, \mathrm{S}_2, \ldots, \mathrm{S}_s$ and to the columns $\mathrm{A}_1, \mathrm{A}_2, \ldots, \mathrm{A}_t$. Each symmetry operator in P_{Y_a} is associated with a row/column in Y_a, hence we label a symmetry operator after the corresponding row/column, for example

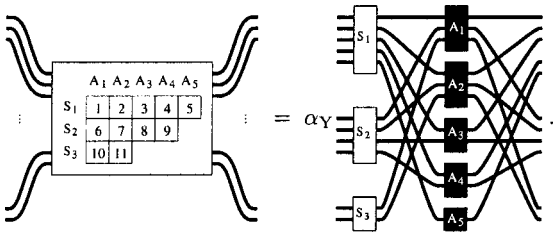

Let the lines numbered 1 to k enter the symmetrizers as described by the numbers in the boxes in the standard tableau and connect the set of symmetrizers to the set of antisymmetrizers in a nonvanishing way, avoiding multiple intermediate lines prohibited by (5). Finally, arrange the lines coming out of the antisymmetrizers such that if the lines all passed straight through the symmetry operators, they would exit in the same order as they entered.

We shall denote by Δ_Y the dimensions of irreps of S_k, and by d_Y the dimensions of irreps of U(n). Let $|S_i|$ or $|A_i|$ denote the number of boxes within a row or column, respectively. Thus $|A_i|$ also denotes the number of lines entering the antisymmetrizer A_i, and similarly for the symmetrizers. The normalization constant α_Y is given by

$$\alpha_Y = \frac{\Pi_{i=1}^{s}|S_i|!\Pi_{j=1}^{t}|A_j|!}{|Y|},$$

where $|Y|$ is related through (6) to Δ_Y, the dimension of irrep Y of S_k, and is a hook rule S_k combinatoric number. The normalization depends only on the shape of the Young diagram, not the particular tableau. The Young projection operators

(1) are *idempotent*, $P_Y^2 = P_Y$;
(2) are *orthogonal*: if Y and Z are two distinct standard tableaux, then $P_Y P_Z = P_Z P_Y = 0$; and
(3) constitute a *complete set*, $\mathbb{I} = \Sigma P_Y$, where the sum is over all standard tableaux Ywith k boxes.

The projections are unique up to an overall sign. By construction, the identity element always appears as a term in the expansion of the symmetry operators of the Young projection operators—the overall sign is fixed by requiring that the identity element comes with a positive coefficient. The diagrammatic proof that the above rules indeed assign a unique projection operator to each standard tableaux is the central result of this paper; as it would impede the flow of our argument at this point, it is placed in the Appendix.

Example: The Young diagram corresponding to the partition $[3,1]$ tells us to use one symmetrizer of length three, one of length one, one antisymmetrizer of length two, and two of length one. There are three distinct standard tableaux, each corresponding to a projection operator

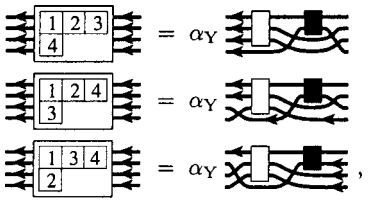

where α_Y is the normalization constant. The symmetry operators of unit width need not be drawn explicitly. We have $|Y| = 8$, $|S_1| = 3$, $|S_2| = 1$, $|A_1| = 2$, etc., yielding the normalization $\alpha_Y = 3/2$.

C. Dimensions of U(n) irreps

The dimension d_Y of a U(n) irrep is computed by taking the trace of the corresponding Young projection operator, $d_Y = \mathrm{tr}\, P_Y$. The trace can be evaluated by expanding the symmetry operators using (3) and (4). By (2), each closed line is worth n, so d_Y is a polynomial in n of degree k.

Example: The dimension of a three-index Young projection operator,

d_Y = 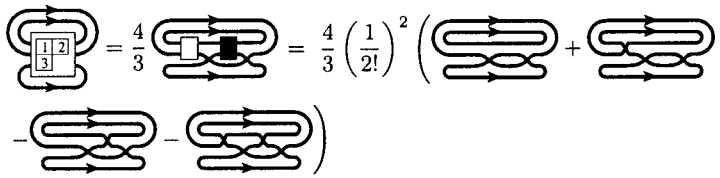 (9)

$$= \frac{1}{3}(n^3 + n^2 - n^2 - n) = \frac{n(n^2-1)}{3}. \tag{10}$$

Such brute expansion is unnecessarily laborious: The dimension of the irrep labeled by Y is

$$d_Y = \frac{f_Y(n)}{|Y|}, \tag{11}$$

where $f_Y(n)$ is the polynomial in n obtained from the Young diagram Y by multiplying the numbers written in the boxes of Y, according to the following rules: (A) The upper left box contains an n. (B) The numbers in a row increase by 1 when reading from left to right. (C) The numbers in a column decrease by 1 when reading from top to bottom. Hence, if k is the number of boxes in Y, $f_Y(n)$ is a polynomial in n of degree k. The dimension formula (11) is well known, see for instance Ref. 11.

In the example (10), we have $f_Y(n)=n(n-1)(n+1)$ and $|Y|=3$, giving $d_Y=n(n^2-1)/3$.

Example: For $Y=[4,2,1]$ we have

$$d_Y = \begin{array}{|c|c|c|c|} \hline n & n+1 & n+2 & n+3 \\ \hline n-1 & n & & \\ \cline{1-2} n-2 & & & \\ \cline{1-1} \hline 6 & 4 & 2 & 1 \\ \hline 3 & 1 & & \\ \cline{1-2} 1 & & & \\ \cline{1-1} \end{array} = \frac{n^2(n^2-1)(n^2-4)(n+3)}{144}.$$

A diagrammatic proof of the U(n) dimension formula (11) is given in the Appendix.

Diagrammatically, the number $f_Y(n)$ is the number of n-color colorings of the strand network corresponding to tr P_Y, see, for example, Ref. 18.

D. Examples

We present examples to illustrate decomposition of reducible representation into irreps using the diagrammatic projection operators.

The Young diagram $\square$ corresponds to the fundamental n-dimensional irrep of U(n). As we saw in (1), the direct product of two of these n-dimensional representations is a n^2-dimensional reducible representation,

$\square \otimes \square$ = 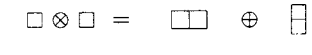 (12)

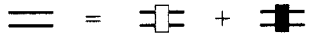 (13)

$$n^2 = \frac{n(n+1)}{2} + \frac{n(n-1)}{2}. \tag{14}$$

Equation (12) shows the decomposition of the reducible representation in terms of Young diagrams, and (13) gives the corresponding projection operators. Tracing (13) yields the dimensions (14) of the irreps.

The first nontrivial example is the reduction of the three-index tensor Young projection operators, listed in Fig. 2. Further examples can be found in Ref. 18.

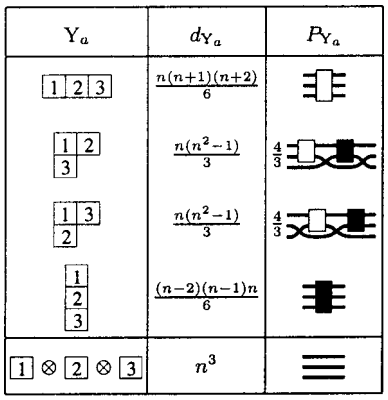

FIG. 2. Reduction of a three-index tensor. Bottom row; the direct product of three unit tableaux, the sum of dimensions, and the projection operators completeness sum.

The four projectors are orthogonal by inspection. In order to verify the completeness, expand first the two three-index projection operators of mixed symmetry,

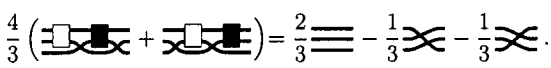

(15)

In the sum of the fully symmetric and the fully antisymmetric tensors all the odd permutations cancel, and we are left with

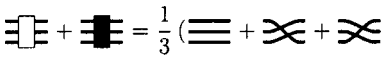

(16)

Adding (15) and (16) we find

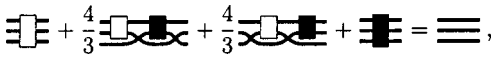

verifying the completeness relation.

Acting with any permutation on the fully symmetric or antisymmetric projection operators gives ± 1 times the projection operator (see Fig. 1). For projection operators of mixed symmetry the action of a permutation is not as simple, because the permutations will mix the spaces corresponding to the different tableaux. Here we shall need only the action of a permutation within a $3n-j$ coefficient, and, as we shall show below, in this case the result will again be simple, a factor ± 1 or 0.

V. RECOUPLING RELATIONS

In the spirit of Feynman diagrams, group theoretic weights with all indices contracted can be drawn as "vacuum bubbles." We now show that for U(n) any such vacuum bubble can be evaluated diagrammatically, either directly, as a $3n-j$ coefficient, or following a reduction to $3-j$ and $6-j$ coefficients. The exposition of this section follows closely Ref. 18; the reader can find there more details, as well as the precise relationship between our $3-j$ and $6-j$ coefficients, and the Wigner $3-j$ and $6-j$ symbols.[35]

The decomposition of a many-particle state can be implemented sequentially, decomposing two-particle states at each step. The Clebsch–Gordan coefficients for $X \otimes Z \rightarrow Y$ can be drawn as *3-vertices*,

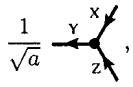

(17)

where $1/\sqrt{a}$ is an (arbitrary) normalization constant. The projection operators for $X\otimes Z\to Y\to X\otimes Z$ can be drawn as

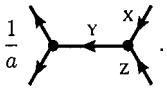

The orthogonality of irreps implies W=Y in

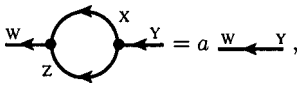

(18)

and the completeness relation can be drawn as

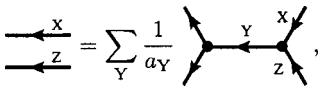

(19)

where the sum is over all irreps contained in $X\otimes Z$.

The normalization constant a can be computed by tracing (18),

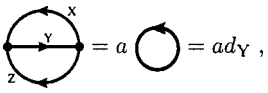

where d_Y is the dimension of the representation Y. The vacuum bubble on the left-hand side is called a $3-j$ coefficient. More generally, vacuum bubbles with n lines are called $n-j$ coefficients.

Let particles in representations U and V interact by exchanging a particle in the representation W, with the final state particles in the representations X and Z,

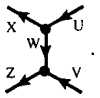

Applying the completeness relation (19) repeatedly yields

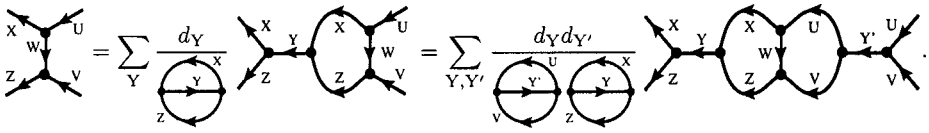

By the orthogonality of irreps $Y=Y'$, and we obtain the *recoupling relation*

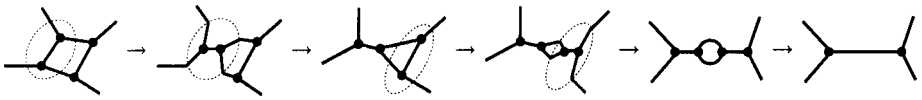

FIG. 3. A reduction of a 4-vertex loop to a sum of "tree" tensors, weighted by products of $3-j$ and $6-j$ coefficients.

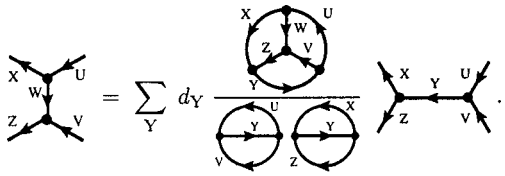

(20)

The "Mercedes" vacuum bubbles in the numerators are called $6-j$ coefficients. *Any* arbitrarily complicated vacuum bubble can be reduced to $3-j$ and $6-j$ coefficients by recursive use of the recoupling relation (20). For instance, a four-vertex loop can be reduced to a two-vertex loop by repeated application of the recoupling relations as sketched in Fig. 3.

Another, more explicit example of a sequence of recouplings, is the following step-by-step reduction of a five-particle state:

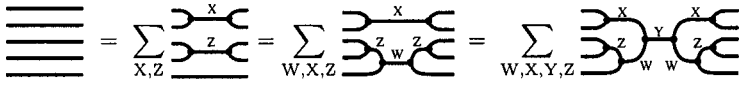

(for brevity we omit the normalization factors here). Taking the trace of both sides leads to $12-j$ coefficients of the form

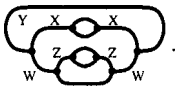

(21)

A. U(n) recoupling relations

Due to the overall particle number conservation (we consider no "antiparticle" states here), for U(n) the above five-particle recoupling flow takes a very specific form in terms of Young projection operators,

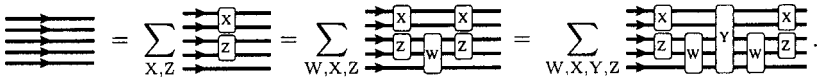

More generally, we can visualize any sequence of U(n) pairwise Clebsch–Gordan reductions as a flow with lines joining into thicker and thicker projection operators, always ending in a maximal P_Y which spans across all lines.

In the trace (21) we can use the idempotency of the projection operators to double the maximal Young projection operator P_Y, and sandwich by it all smaller projection operators,

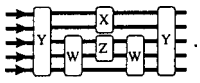

(22)

From uniqueness of the connection between the symmetry operators (see the Appendix I) we have for any permutation $\sigma \in S_k$

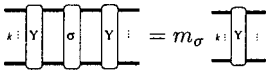

(23)

where $m_\sigma = 0, \pm 1$. Expressions like (22) can be evaluated by expanding the projection operators

P_W, P_X, P_Z and determining the value of m_σ of (23) for each permutation σ of the expansion. The result is

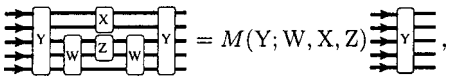

where the factor $M(\mathrm{Y};\mathrm{W},\mathrm{X},\mathrm{Z})$ *does not depend* on n and is determined by a purely symmetric group calculation. Several examples follow.

B. Evaluation of 3*n*-*j* coefficients

Let X, Y, and Z be irreps of U(n). In terms of the Young projection operators P_X, P_Y, and P_Z, a U(n) three-vertex (17) is obtained by tying together the three Young projection operators,

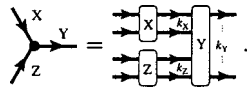

(24)

The number of particles is conserved (the multiparticle states constructed here consist only of particles, no "antiparticles"): $k_X+k_Z=k_Y$. A $3-j$ coefficient constructed from the vertex (24) is then

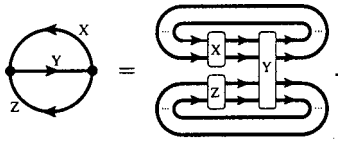

(25)

As an example, take

$$\mathrm{X}=\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}\,,\quad \mathrm{Y}=\begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3&5&6\\\cline{1-3}\end{array}\,,\qquad \text{and}\qquad \mathrm{Z}=\begin{array}{|c|c|}\hline 4&5\\\hline 6\\\cline{1-1}\end{array}\,.$$

Then

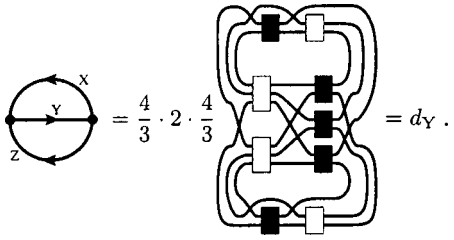

(26)

In principle the value of such $3-j$ coefficient can be computed by expanding out all symmetry operators, but that is not recommended as the number of terms in such expansions grows combinatorially with the total number of boxes in the Young diagram Y. Instead, the answer—in this case $d_Y=(n^2-1)n^2(n+1)(n+2)/144$— is obtained as follows.

In general, the $3-j$ coefficients (25) can be evaluated by expanding the projections P_X and P_Z and determing the value of m_σ in (23) for each permutation σ of the expansion.

As an example, consider the $3-j$ coefficient (26). With P_Y as in (26) we find

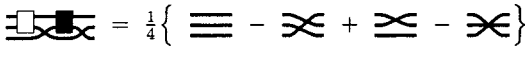

$$m_\sigma(P_X): \quad +1 \quad 0 \quad +1 \quad -1$$

$$m_\sigma(P_Z): \quad +1 \quad -1 \quad 0 \quad -1\,,$$

hence

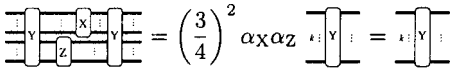

and the value of the $3-j$ is d_{Y} as claimed in (26). That the eigenvalue happens to be 1 is an accident—in tabulations of $3-j$ coefficients[26] it takes a range of values.

The relation (23) implies that the value of any U(n) $3-j$ coefficient (25) is $M(\mathrm{Y};\mathrm{X},\mathrm{Z})d_{\mathrm{Y}}$, where d_{Y} is the dimension of the maximal irrep Y.

A $6-j$ coefficient is composed of the three-vertex (17) and the other three-vertex in the projection operator (24), with all arrows reversed. A general U(n) $6-j$ coefficient has the form

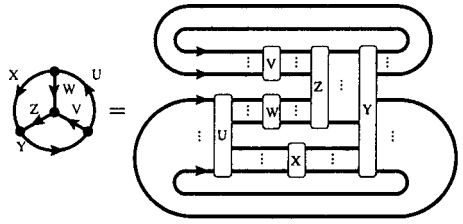

(27)

Using the relation (23) we immediately see that

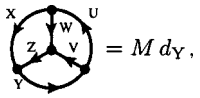

(28)

where M is a pure symmetric group $S_{k\mathrm{Y}}$ number, independent of U(n); it is surprising that the only vestige of U(n) is the fact that the value of a $6-j$ coefficient is proportional to the dimension d_{Y} of its largest projection operator.

Example: Consider the $6-j$ constructed from the Young tableaux,

$$\mathrm{U}=\begin{array}{|c|c|}\hline 2&3\\\hline 4\\\cline{1-1}\end{array},\quad \mathrm{V}=\begin{array}{|c|}\hline 1\\\cline{1-1}\end{array},\quad \mathrm{W}=\begin{array}{|c|}\hline 2\\\cline{1-1}\end{array},$$

$$\mathrm{X}=\begin{array}{|c|}\hline 3\\\hline 4\\\cline{1-1}\end{array},\quad \mathrm{Y}=\begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}4\\\cline{1-1}\end{array},\quad \mathrm{Z}=\begin{array}{|c|}\hline 1\\\hline 2\\\cline{1-1}\end{array}.$$

Using the idempotency we can double the projection P_{Y} and sandwich the other operators, as in (22). Several terms cancel in the expansion of the sandwiched operator, and we left with

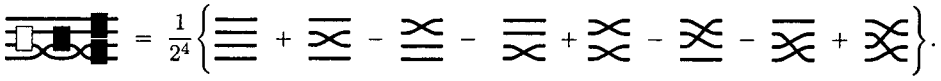

m_σ : +1 0 −1 0 0 −1 0 +1

We have listed the symmetry factors m_σ of (23) for each of the permutations σ sandwiched between the projection operators P_{Y}. We find that in this example the symmetric group factor M of (28) is

$$M=\frac{4}{2^4}\alpha_{\mathrm{U}}\alpha_{\mathrm{V}}\alpha_{\mathrm{W}}\alpha_{\mathrm{X}}\alpha_{\mathrm{Z}}=\frac{1}{3},$$

so the value of the $6-j$ is

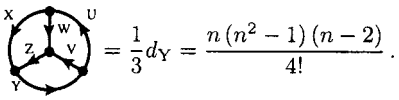

The method generalizes to evaluations of any $3n-j$ coefficients of U(n).

C. Sum rules

Let Y be a standard tableau with k_Y boxes, and let Λ be the set of all standard tableaux with one or more boxes (exclude the trivial $k=0$ representation). Then the $3-j$ coefficients obey the sum rule

$$\sum_{X,Z\in\Lambda}$$  $$= (k_Y-1)d_Y. \tag{29}$$

The sum is finite, because the $3-j$ is nonvanishing only if the number of boxes in X and Z add up to k_Y, and this happens only for a finite number of tableaux.

To prove (29), recall that the Young projection operators constitute a complete set, $\Sigma_{X\in\Lambda_k}P_X=\mathbb{I}$, where $\mathbb{I}$ is the $k\times k$ unit matrix and Λ_k the set of all standard tableaux of Young diagrams with k boxes. Hence

$$\sum_{X,Z\in\Lambda}$$  $$= \sum_{k_X=1}^{k_Y-1} \sum_{\substack{X\in\Lambda_{k_X}\\ Z\in\Lambda_{k_Y-k_X}}}$$ 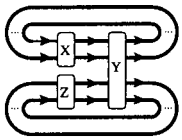

$$= \sum_{k_X=1}^{k_Y-1}$$ 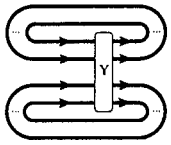 $$= \sum_{k_X=1}^{k_Y-1} d_Y = (k_Y-1)d_Y\,.$$

This sum rule offers a useful cross-check on tabulations of $3-j$ values, see for instance Ref. 26.

There is a similar sum rule for the $6-j$ coefficients,

$$\sum_{X,Z,U,V,W\in\Lambda}$$  $$= \frac{1}{2}(k_Y-1)(k_Y-2)\,d_Y\,. \tag{30}$$

Referring to the $6-j$ (27), let k_U be the number of boxes in the Young diagram U, k_X be the number of boxes in X, etc., and let k_Y be given. From (27) we see that k_X takes values between 1 and k_Y-2 and k_Z takes values between 2 and k_Y-1, subject to the constraint $k_X+k_Z=k_Y$. We now sum over all tableaux U, V, and W keeping k_Y, k_X, and k_Z fixed. Note that k_V can take values 1,…, k_Z-1. Using completeness we find

$$\sum_{U,V,W\in\Lambda}$$  $$= \sum_{k_V=1}^{k_Z-1} \sum_{V\in\Lambda_{k_V}} \sum_{W\in\Lambda_{k_Z-k_V}} \sum_{U\in\Lambda_{k_Y-k_V}}$$

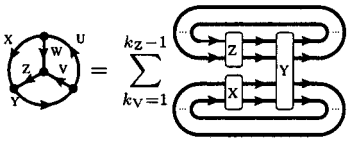 $$= (k_Z-1)$$  .

Now sum over all tableaux X and Z to find

$$\sum_{X,Z,U,V,W\in\Lambda}$$  $$= \sum_{k_Z=2}^{k_Y-1}(k_Z-1) \sum_{Z\in\Lambda_{k_Z}} \sum_{X\in\Lambda_{k_Y-k_Z}}$$  $$= \frac{1}{2}(k_Y-1)(k_Y-2)\,d_Y$$

verifying the sum rule (30) for $6-j$ coefficients.

VI. SU(N) AND ITS ADJOINT REPRESENTATION

The SU(n) group elements satisfy det U=1, so SU(n) has an additional invariant, the Levi–Civita tensor

$$\epsilon_{a_1 a_2 \cdots an} = U_{a_1}{}^{a_1'} U_{a_2}{}^{a_2'} \cdots U_{a_n}{}^{a_n'} \epsilon_{a_1' a_2' \cdots a_n'}.$$

In the diagrammatic notation the Levi–Civita tensors can be drawn as[20]

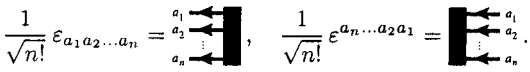

They satisfy

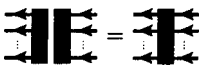

(31)

(Levi–Civita projects an n-particle state onto a single, one-dimensional, singlet representation), and are correctly normalized,

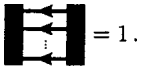

The Young diagrams for SU(n) cannot contain more than n rows, since at most n indices can be antisymmetrized. By contraction with the Levi-Civita tensor, a column with k boxes can be converted into a column of $n-k$ boxes: this operation associates to each irrep the *conjugate* irrep. The Young diagram corresponding to the irrep is the *conjugate* Young diagram constructed from the missing pieces needed to complete the rectangle of n rows. For example, the conjugate of the irrep corresponding to the partition [4, 2, 2, 1] of SU(6) has the partition [4, 4, 3, 2, 2]:

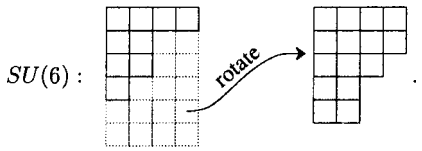

The Levi–Civita tensor converts an antisymmetrized collection of $n-1$ "in" indices, an ($n-1$)-particle state, into 1 "out" index: a single antiparticle state $\overline{\square}$, the conjugate of the fundamental representation $\square$ single particle state. The corresponding Young diagram is a single column of $n-1$ boxes. The product of the fundamental representation and the conjugate representation of SU(n) decomposes into a singlet and the adjoint representation,

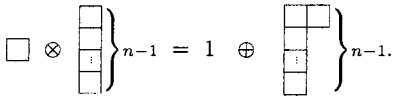

In the notation introduced in Sec. IV, the Young projection operator for the adjoint representation A is drawn as

$$P_A = \frac{2(n-1)}{n}$$

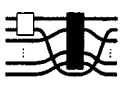

Using P_A and the definition (24) of the three-vertex, SU(n) group theory weights involving quarks, antiquarks, and gluons can be calculated by expansion of the symmetry operators or by application of the recoupling relation. When the adjoint representation plays a key role, as it does in gauge theories, it is wisest to abandon the above construction of all irreps by Clebsch–Gordan reductions of multiparticle states, and build the theory by taking a single particle and a single antiparticle as the fundamental building blocks. A much richer theory, beyond the scope of this paper follows,

leading to a diagrammatic construction of representations of all simple Lie groups, the classical as well as the exceptional. The reader is referred to Ref. 18 for the full exposition.

VII. NEGATIVE DIMENSIONS

We conclude by a brief discussion of implications of the $n \to -n$ duality[18,36] of U(n) invariant scalars.

Any SU(n) invariant tensor is built from Kronecker deltas and Levi–Civita tensors. A scalar is a tensor object with all indices contracted, so in the diagrammatic notation a scalar is a diagram with no external legs, a vacuum bubble. Thus, in scalars Levi–Civita tensors can appear only in pairs (the lines must end somewhere), and by (31) the Levi–Civita tensors combine to antisymmetrizers. Consequently both U(n) and SU(n) invariant scalars are all built only from symmetrizers and antisymmetrizers.

Expanding all symmetry operators in a U(n) vacuum bubble gives a sum of entangled loops. Each loop is worth n, so each term in the sum is a power of n, and therefore a U(n) invariant scalar is a polynomial in n.

The negative dimensionality theorem[18,36] for U(n) states that interchanging symmetrizers and antisymmetrizers in U(n) invariant scalar is equivalent (up to an overall sign) to substituting $n \to -n$ in the polynomial, which is the value of the scalar. We write this

$$\overline{\mathrm{U}(n)} = \mathrm{U}(-n).$$

The bar symbolizes the interchange of symmetrizers and antisymmetrizers.

The terms in the expansion of all symmetry operators in a U(n) vacuum bubble can be arranged in pairs that only differ by one crossing,

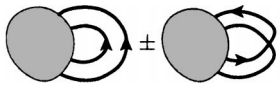

(32)

with $\pm$ depending on whether the crossing is due to symmetrization $(+)$ or antisymmetrization $(-)$. The gray blobs symbolize the tangle of lines common to the two terms.

If the two arcs outside the gray blob of the first term of (32) belong to separate loops, then in the second term they will belong to the same loop. The two terms thus differ only by a factor of n: schematically,

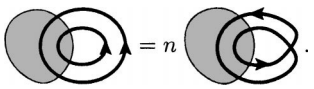

Likewise, if the arcs in the first term belong to the same loop then in the second term they will belong to two separate loops. In this case the first term is $1/n$ times the second term. In either case the ratio of the two terms is an odd power of n. Interchanging symmetrizers and antisymmetrizers in a U(n) vacuum bubble changes the sign in (32). Up to an overall sign the result is the same as substituting $n \to -n$. This proves the theorem.

Consider now the implications for the dimension formulas and the values of $3n-j$ coefficients. The dimension of an irrep of U(n) is the trace of the Young projection operator, a vacuum bubble diagram built from symmetrizers and antisymmetrizers. Applying the negative dimensionality theorem we get $d_{Y^t}(n) = d_Y(-n)$, where Y^t is the *transpose* Y^t of the standard Young tableau Y obtained by interchanging rows and columns (reflection across the diagonal). For instance [3, 1] is the transpose of [2, 1, 1],

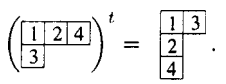

As an example, note the $n \to -n$ dualities in the dimension formulas of Fig. 2.

Now for standard tableaux X, Y, and Z, compare the diagram of the $3-j$ constructed from X, Y, and Z to that constructed from X^t, Z^t, and Y^t. The diagrams are related by a reflection in a vertical line, reversal of all the arrows on the lines, and interchange of symmetrizers and antisymmetrizers. The first two operations do not change the value of the diagram, hence the values of the two diagrams are again related by $n \leftrightarrow -n$ (and possibly an overall sign; this sign is fixed by requiring that the highest power of n comes with a positive coefficient). Hence in tabulation it is sufficient to calculate approximately half of all $3-j$'s. The $3-j$ sum rule (29) provides a cross-check.

The two $6-j$ coefficients

are related by a reflection in a vertical line, reversal of all the arrows on the lines, and interchange of symmetrizers and antisymmetrizers—this can be seen by writing out the $6-j$ coefficients in terms of the Young projection operators as in (27). By the negative dimensionality theorem, the values of the two $6-j$ coefficients are therefore again related by $n \leftrightarrow -n$.

VIII. SUMMARY

We have presented a diagrammatic method for construction of correctly normalized Young projection operators for U(n). These projection operators in diagrammatic form are useful for explicit evaluation of group theoretic quantities such as the $3n-j$ coefficients. Using the recoupling relations, all U(n) invariant scalars can be reduced to expressions involving only terms of $3-j$ and $6-j$ coefficients and the dimensionalities of the representations. Our main results are as follows:

(i) Diagrammatic Young projection operators for tensors (multiparticle states) with given symmetry properties; a diagrammatic proof of their uniqueness, completeness, and orthogonality.
(ii) U(n) invariant scalars may be expressed in terms of the Young projection operators, and their values computed by diagrammatic expansions.
(iii) U(n) $3-j$ and $6-j$ coefficients constructed from the three-vertex defined in (24) have simple n-dependencies: they are proportional to the dimension of the maximal irrep projection operator that spans over all multiparticle indices.
(iv) The negative dimensionality theorem applies to all U(n) invariant scalars, in particular the $3n-j$ coefficients and the dimensions of the irreps of U(n).
(v) The sum rules (29) and (30) for $3-j$ and $6-j$ coefficients afford useful cross-checks of $3n-j$ tabulations.

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APPENDIX: DIAGRAMMATIC YOUNG PROJECTION OPERATORS: THE PROOFS

In this appendix we prove the properties of the Young projection operators stated above in Sec. IV.

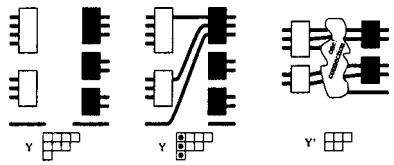

FIG. 4. There is a unique (up to an overall sign) connection between the symmetrizers and the antisymmetrizers, so the Young projection operators are well defined by the construction procedure explained in the text. The figure shows the principles of the proof. The dots on the middle Young diagram mark boxes that correspond to contracted lines.

Uniqueness

We show that the Young projection operators P_{Y} are well defined by proving the existence and uniqueness (up to an overall sign) of a nonvanishing connection between the symmetrizers and antisymmetrizers in P_{Y}.

The proof is by induction over the number of columns t in the Young diagram Y; the principles are illustrated in Fig. 4. For $t=1$ the Young projection operator consists of one antisymmetrizer of length s and s symmetrizers of length 1, and clearly the connection can only be made in one way, up to an overall sign, see Fig. 1(b).

Assume the result to hold for Young projection operators derived from Young diagrams with $t-1$ columns. Let Y be a Young diagram with t columns. The lines from A_1 in P_{Y} must connect to different symmetrizers for the connection to be nonzero. Since there are exactly $|\mathrm{A}_1|$ symmetrizers in P_{Y}, this can be done in essentially one way, since which line goes to which symmetrizer is only a matter of an overall sign, and where a line enters a symmetrizer is irrelevant due to Fig. 1(a).

After having connected A_1, connecting the symmetry operators in the rest of P_{Y} is the problem of connecting symmetrizers to antisymmetrizers in the Young projection operator $P_{\mathrm{Y}'}$, where Y′ is the Young diagram obtained from Y by slicing off the first column. Thus Y′ has $k-1$ columns, so by the induction hypothesis the rest of the symmetry operators in P_{Y} can be connected in exactly one nonvanishing way (up to an overall sign).

Orthogonality

If Y_a and Y_b denote standard tableaux derived from the same Young diagram Y, then $P_{\mathrm{Y}_a}P_{\mathrm{Y}_b}=P_{\mathrm{Y}_b}P_{\mathrm{Y}_a}=\delta_{ab}P^2_{\mathrm{Y}_a}$, since there is a permutation of the lines connecting the symmetry operators of Y with those of Z and by uniqueness of the nonzero connection the result is either $P^2_{\mathrm{Y}_a}$ (if $\mathrm{Y}_a=\mathrm{Y}_b$) or (if $\mathrm{Y}_a\neq\mathrm{Y}_b$).

Next, consider two different Young diagrams Y and Z with the same number of boxes. Since at least one column must be bigger in (say) Y than in Z and the p lines from the corresponding antisymmetrizer must connect to different symmetrizers, it is not possible to make a nonzero connection between the antisymmetrizers of P_{Y_a} to the symmetrizers in P_z, where subscripts a and b denote any standard tableaux of Y and Z. Hence $P_{\mathrm{Y}_a}P_{\mathrm{Z}_b}=0$, and by a similar argument $P_{\mathrm{Z}_b}P_{\mathrm{Y}_a}=0$.

Normalization and completeness

We now derive the formula for the normalization factor α_{Y} such that the Young projection operators are idempotent, $P^2_{\mathrm{Y}_a}=P_{\mathrm{Y}_a}$. By the normalization of the symmetry operators, Young projection operators corresponding to fully symmetric or antisymmetric Young tableaux will be idempotent with $\alpha_{\mathrm{Y}}=1$.

Diagrammatically $P^2_{\mathrm{Y}a}$ is simply P_{Y_a} connected to P_{Y_a}, hence it may be viewed as a set of *outer* symmetry operators connected by a set of *inner* symmetry operators. Expanding all the inner symmetry operators and using the uniqueness of the nonzero connection between the symmetrizers and antisymmetrizers of the Young projection operators, we find that each term in the expansion is

either 0 or a copy of P_{Y_a}. For a Young diagram with s rows and t columns there will be a factor of $1/|S_i|!(1/|A_j|!)$ from the expansion of each inner (anti)symmetrizer, so we find

$$P_{Y_a}^2 = \alpha_{Y_a}^2$$
$$= \frac{\alpha_{Y_a}^2}{\prod_{i=1}^{s}|S_i|!\prod_{j=1}^{t}|A_j|!}\sum_{\sigma}\sigma$$
$$= \alpha_{Y_a}\frac{\kappa_Y}{\prod_{i=1}^{s}|S_i|!\prod_{j=1}^{t}|A_j|!}P_{Y_a},$$

where the sum is over permutation σ from the expansion of the inner symmetry operators. Note that by the uniqueness of the connection between the symmetrizers and antisymmetrizers, the constant κ_Y is independent of which tableau gives rise to the projection, and consequently the normalization constant α_Y depends only on the Young diagram and not the tableau.

For a given k, consider the Young projection operators P_{Y_a} corresponding to all the k-box Young tableaux. Since the operators P_{Y_a} are orthogonal and in one-to-one correspondence with the Young tableaux, it follows from the discussion in Sec. IV A that there are no other operators of k lines orthogonal to this set. Hence the P_{Y_a}'s form a complete set, so that

$$\mathbb{I} = \sum_{Y_a} P_{Y_a}. \tag{A1}$$

Expanding the projections the identity appears only once, so we have

$$P_{Y_a} = \alpha_Y \frac{1}{\prod_{i=1}^{s}|S_i|!\prod_{j=1}^{t}|A_j|!}\left(\underline{\equiv}_{p} + \ldots\right),$$

and using this, equation (A1) states

$$\underline{\equiv}_{p} = \left(k!\sum_{Y}\frac{\alpha_Y/|Y|}{\prod_{i=1}^{s}|S_i|!\prod_{j=1}^{t}|A_j|!}\right)\underline{\equiv}_{p} \tag{A2}$$

since all permutation different from the identity must cancel. When changing the sum from a sum over the tableaux to a sum over the Young diagrams we use that α_Y depends only on the diagram and that there are $\Delta_Y = k!/|Y|$ k-standard tableaux for a given diagram. Choosing

$$\alpha_Y = \frac{\Pi_{i=1}^{s}|S_i|!\Pi_{j=1}^{t}|A_j|!}{|Y|}, \tag{A3}$$

the factor on the right-hand side of (A2) is 1 by (8).

Since the choice of normalization (A3) gives the completeness relation (A1), it follows that it also gives idempotent operators, multiplying by P_{Z_b} on both sides of (A1) and using orthogonality, we find $P_{Z_b} = P_{Z_b}^2$ for any Young tableau Z_b.

Dimensionality

To prove the dimension formula (11) we need the identities

$$\underline{\equiv}_{p}\,| = \frac{1}{p}\left(\underline{\equiv}_{p-1}| + (p-1)\,\underline{\equiv}_{p-1}\right) \tag{A4}$$

and

$$\underline{\equiv}_{p}\,| = \frac{1}{p}\left(\underline{\equiv}_{p-1}| - (p-1)\,\underline{\equiv}_{p-1}\right) \tag{A5}$$

given in Ref. 18. For Young tableaux with a single row or column, the dimension formula can be derived directly using the relations (A4) and (A5).

Let Y be a standard tableau with k boxes, and Y′ the standard Young tableau obtained from it by removing the box containing k. Draw the Young projection operators corresponding to Y and Y′ and note that P_{Y} with the "last" line traced is proportional to $P_{\mathrm{Y}'}$.

Quite generally the contraction of the last line will look like

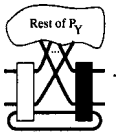

(A6)

Using (A4) and (A5) we have

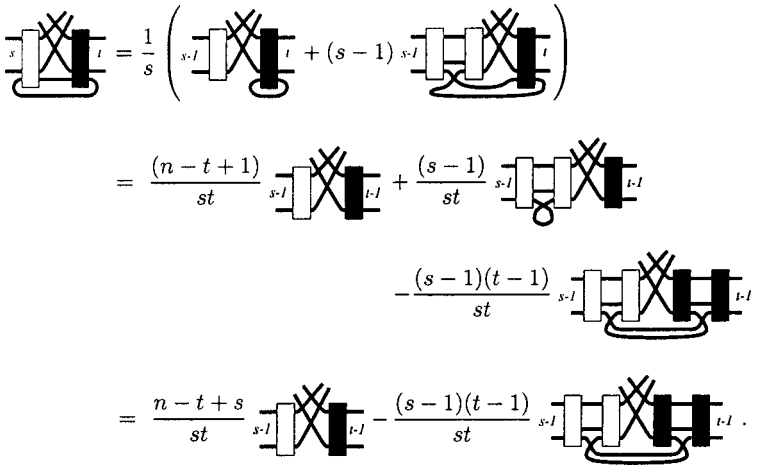

Inserting this into (A6) we see that the first term is proportional to the projection operator $P_{\mathrm{Y}'}$

The second term vanishes,

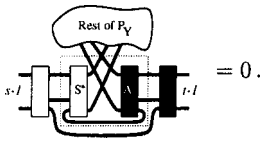

If we ignore the internal structure within the dotted box we see that this is exactly of the form of $P_{\mathrm{Y}'}$, except that the "last" symmetrizers and antisymmetrizers are connected by a line. There is a unique nonvanishing way of connecting the symmetrizers and antisymmetrizers in $P_{\mathrm{Y}'}$, and the "last" symmetrizer and antisymmetrizer are not connected in this, as they correspond to a row and column with no common box in the Young tableau. Therefore every term obtained from the expansion of the dotted box must vanish.

The dimensionality formula follows by induction on the number of boxes in the Young diagrams with the dimension of a single box Young diagram being n. Let Y be a Young diagram with p boxes. We assume that the dimensionality formula is valid for any Young diagram with $p-1$ boxes. With $P_{\mathrm{Y}'}$ obtained from P_{Y} as above, we have (using the above calculation and writing D_{Y} for the diagrammatic part of P_{Y})

$$\dim P_{\mathrm{Y}} = \alpha_{\mathrm{Y}}\ \mathrm{tr}\ D_{\mathrm{Y}} = \frac{n-t+s}{st}\alpha_{\mathrm{Y}}\ \mathrm{tr}\ D_{\mathrm{Y}'} = (n-t+s)\alpha_{Y'}\frac{|\mathrm{Y}'|}{|\mathrm{Y}|}\mathrm{tr}\ D_{\mathrm{Y}'} = (n-t+s)\frac{f_{\mathrm{Y}'}}{|\mathrm{Y}|} = \frac{f_{\mathrm{Y}}}{|\mathrm{Y}|}.$$

This completes the proof of the dimensionality formula (11).

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Hierarchy of conservation laws of diffusion-convection equations

Roman O. Popovych[a] and Nataliya M. Ivanova[b]
Institute of Mathematics of National Academy of Sciences of Ukraine,
3 Tereshchenkivska Str., Kyiv-4, 01601, Ukraine

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We introduce notions of equivalence of conservation laws with respect to Lie symmetry groups for fixed systems of differential equations and with respect to equivalence groups or sets of admissible transformations for classes of such systems. We also revise the notion of linear dependence of conservation laws and define the notion of local dependence of potentials. To construct conservation laws, we develop and apply the most direct method which is effective to use in the case of two independent variables. Admitting possibility of dependence of conserved vectors on a number of potentials, we generalize the iteration procedure proposed by Bluman and Doran-Wu for finding nonlocal (potential) conservation laws. As an example, we completely classify potential conservation laws (including arbitrary order local ones) of diffusion-convection equations with respect to the equivalence group and construct an exhaustive list of locally inequivalent potential systems corresponding to these equations. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1865813]

I. INTRODUCTION

After Noether's remarkable paper[30] had become well known, a number of authors[21,31,38,40] searched for conservation laws using the symmetry approach based on the Noether's results. In view of the generalized Noether's theorem,[31] there exists one-to-one correspondence between the nontrivial generalized variational symmetries of some functional and the nontrivial conservation laws of the associated Euler–Lagrange equations, and any such symmetry is a generalized symmetry of the Euler–Lagrange equations.

The Noether's approach has a number of advantages. It reduces construction of conservation laws to finding symmetries for which there exist a number of well-developed methods, and complete description of necessary symmetry properties is known for a lot of systems of differential equations. However, this approach can be applied only to Euler–Lagrange equations that form normal systems and admit symmetry groups satisfying an additional "variational" property of leaving the variational integral invariant in some sense.[31] The latter requirements lead to restriction of class of systems that could be investigated in such way.

At the same time, the definition of conservation laws itself gives rise to a method of finding conservation laws. Technique of calculations used in the framework of this method is similar to the classical Lie method yielding symmetries of differential equations.[20] As mentioned in the above reference, such algorithmic possibility was first employed by Laplace[27] for derivation of the well-known Laplace vector of the two-body Kepler problem. Following tradition from group analysis of differential equations, we may call this method *direct* and distinguish four versions of it, depending on the way of taking into account systems under investigation. (See, e.g., Refs. 4, 5, 8, and 23 and Sec. IV of this paper for more details as well as Ref. 44 for comparison of the

[a]Electronic mail: rop@imath.kiev.ua
[b]Electronic mail: ivanova@imath.kiev.ua

versions and their realizations in computer algebra programs.) In the present paper we use the most direct version based on immediate solving of determining equations for conserved vectors of conservations laws on the solution manifolds of investigated systems.

Let us note that there exist other approaches for construction of conservation laws which differ from the Noether's or above direct ones, are based on exploitation of symmetry properties of differential equations and can be applied to non-Lagrangian systems. Thus, Fushchych and Nikitin[17] proposed to calculate directly bilinear combinations of solutions of motion equations, which are conserved in time by virtue of symmetries of these equations. It is possible in such way to find conservation laws corresponding to nongeometric symmetries. In the recent work[2] a purely algebraic formula has been derived for generating conservation laws of systems of differential equations that possess a scaling invariance.

To classify conservation laws, instead of the usual equivalence relation on their set (more exactly, on the set of conserved vectors) we propose to use the natural and more general notions of equivalences of conservation laws with respect to Lie symmetry groups for fixed systems of differential equations and with respect to equivalence groups or sets of admissible point (or contact) transformations for classes of such systems. Results of classification up to these equivalences are more comprehensible, especially, if a whole class of systems is studied and blend with the framework of group analysis.

Bluman and Doran-Wu[8] proposed an ingenious procedure of branching iterations for finding nonlocal (potential) conservation laws of diffusion equations. Namely, on each iteration they use a conservation law from the previous iteration (one conservation law for one iteration) to introduce a potential and to construct the extended potential system. Then they study local conservation laws of the potential system, which are, generally speaking, nonlocal (potential) conservation laws for the initial equation. To the best of our knowledge, it was the first paper where the idea of hierarchy of potential systems and associated conservation laws is presented in an explicit form.

We generalize the iteration procedure by Bluman and Doran-Wu, admitting dependence of conserved vectors on different number (from one to the maximum possible that) of new potentials on each iteration. The idea of a similar approach was adduced by Wahlquist and Estabrook[43] and was formalized in the form of notion of *universal Abelian covering* of differential equations.[10,36,42] Such approach naturally results in the questions on some independence of employed potentials. That is why, in this paper we consider definition of linear dependence of conservation laws in detail and define the notion of local dependence of potentials.

Therefore, in the first part of the paper we propose some technique and discuss the classification problem for conservation laws in general. The ultimate goal of the second part is to present an exhaustive classification of potential conservation laws in a quite difficult and interesting case. As an illustration of the proposed technique, we choose the class of diffusion-convection equations

$$u_t = (A(u)u_x)_x + B(u)u_x, \tag{1}$$

where $A=A(u)$ and $B=B(u)$ are arbitrary smooth functions of u, $A(u)\neq 0$. Symmetry properties of (1) were considered by a number of authors,[13,32,45] however the complete and strong group classification of (1) was first presented in our recent work[34] [see also references therein for more details about symmetry analysis of classes intersecting class (1)].

Studying conservation laws of equations (1) was started from linear equations.[38] Dorodnitsyn and Svirshchevskii[12] (see also Ref. 20) completely investigated the local conservation laws for reaction-diffusion equations $u_t=(A(u)u_x)_x+C(u)$. The first-order local conservation laws of equations (1) were constructed by Kara and Mahomed.[24] Developing results of Bluman and Doran-Wu[8] obtained for the case $B=0$, Ivanova[22] classified the first-order local conservation laws for equations (1) with respect to the equivalence group and constructed potential conservation laws of the first level. Namely, she made two steps of the iteration procedure, looking, in the second step, for the first-order local conservation laws of the potential systems obtained after the first step.

In the present work we exhaustively classify, with respect to the corresponding equivalence group, the local conservation laws of an arbitrary order, find the simplest and general potential

conservation laws and construct locally inequivalent potential systems of equations (1). All possible steps of the branching iterations procedure are done, and admission of dependence of conserved vectors on a number of potentials is of fundamental importance for completing iterations. We obtain the following eight inequivalent cases of equations (1) having different sets of potential conservation laws:

(i) the general case (the parameter-functions A and B are arbitrary);
(ii) three cases with an arbitrary value of A and a special value of B ($B=0; B=A; B=\int A\,\mathrm{d}u + uA$);
(iii) three corresponding linearizable equations ($A=u^{-2}, B=0; A=B=u^{-2}; A=1, B=2u$) and
(iv) the linear heat equation ($A=1, B=0$).

The latter case takes on special significance in our consideration since investigation of the linearizable equations having infinite series of potential conservation laws is reduced to this case and the nonlinearizable equations from class (1) have at the most two independent conservation laws.

Our paper is organized as follows. First (Sec. II) we give a basic theoretical background, following the spirit of Olver's book.[31] We recall the notions of equivalence of conserved vectors and characteristics with respect to the triviality relation and discuss properties of the space of conserved vectors and the space of characteristics. This naturally results in the notions of linear dependence of conservation laws and local dependence of potentials (Secs. IV and V). In Sec. III we introduce the notions of equivalence of conservation laws with respect to Lie symmetry groups for fixed systems of differential equations and equivalence groups or sets of admissible point (or contact) transformations for classes of such systems. We emphasize the possibility of solving classification problems for conservation laws with respect to the above equivalences similarly to usual group classification problems for differential equations. In Sec. IV we adduce different versions of the direct method of construction of conservation laws, emphasizing the most direct one and combining it with classification up to symmetry or equivalence groups. Since the two-dimensional case is special for construction of potential systems we describe it in more detail in Sec. V.

Then we apply the theoretical background given in the previous sections to investigation of diffusion-convection equations from class (1). The local conservation laws of (1) are classified with respect to the corresponding equivalence group in Sec. VI. In Sec. VII we construct simplest potential conservation laws and analyze connections between them using potential equivalence transformations. The subject of Sec. VIII is the description of general potential conservation laws of the linear heat equation. In Sec. IX we complete studying potential conservation laws of diffusion-convection equations and adduce the hierarchy of conservation laws obtained in our framework. In the same section we give an exhaustive list of locally inequivalent potential systems of equations (1). The obtained results can be interpreted as construction of universal Abelian covering for the whole class of diffusion-convection equations.

II. BASIC DEFINITIONS AND STATEMENTS

Let $\mathcal{L}$ be a system $L(x,u_{(\rho)})=0$ of l differential equations $L^1=0,\dots,L^l=0$ for m unknown functions $u=(u^1,\dots,u^m)$ of n independent variables $x=(x_1,\dots,x_n)$. Here $u_{(\rho)}$ denotes the set of all the derivatives of the functions u with respect to x of order no greater than ρ, including u as the derivatives of the zero order. Let $\mathcal{L}_{(k)}$ denote the set of all algebraically independent differential consequences that have, as differential equations, orders no greater than k. We identify $\mathcal{L}_{(k)}$ with the manifold determined by $\mathcal{L}_{(k)}$ in the jet space $J^{(k)}$.

Definition 1: A *conservation law* of the system $\mathcal{L}$ is a divergence expression $\mathrm{Div}\,F:=D_iF^i$ which vanishes for all solutions of $\mathcal{L}$: $\mathrm{Div}\,F|_{\mathcal{L}}=0$. The n-tuple $F=(F^1(x,u_{(r)}),\dots,F^n(x,u_{(r)}))$ is called a *conserved vector* of this (local) conservation law.

In Definition 1 and below $D_i=D_{x_i}$ denotes the operator of total differentiation with respect to the variable x_i, i.e., $D_i=\partial_{x_i}+u^a_{\alpha,i}\partial_{u^a_\alpha}$, where u^a_α and $u^a_{\alpha,i}$ stand for the variables in jet spaces, which

correspond to derivatives $\partial^{|\alpha|}u/\partial x_1^{\alpha_1}\cdots\partial x_n^{\alpha_n}$ and $\partial u^a_\alpha/\partial x_i$, $\alpha=(\alpha_1,\dots,\alpha_n)$, $\alpha_i\in\mathbb{N}\cup\{0\}$, $|\alpha|:=\alpha_1+\cdots+\alpha_n$. We use the summation convention for repeated indices and assume any function as its zero-order derivative. The notation $V|_{\mathcal{L}}$ means that values of V are considered only on solutions of the system $\mathcal{L}$.

Definition 2: A conserved vector F is called *trivial* if

$$F^i=\hat{F}^i+\check{F}^i,\quad i=\overline{1,n},$$

where $\hat{F}^i$ and $\check{F}^i$ are, likewise F^i, functions of x and derivatives of u (i.e., differential functions), $\hat{F}^i$ vanish on the solutions of $\mathcal{L}$ and the n-tuple $\check{F}=(\check{F}^1,\dots,\check{F}^n)$ is a null divergence (i.e., its divergence vanishes identically).

The triviality concerning the vanishing conserved vectors on solutions of the system can be easily eliminated by confining on the manifold of the system, taking into account all its necessary differential consequences.

A characterization of all null divergences is given by the following lemma (see, e.g., Ref. 31).

Lemma 1: The n-tuple $F=(F^1,\dots,F^n)$, $n\geqslant 2$, *is a null divergence* ($\mathrm{Div}\,F\equiv 0$) *iff there exist smooth functions* v^{ij} $(i,j=\overline{1,n})$ *of x and derivatives of u, such that* $v^{ij}=-v^{ji}$ *and* $F^i=D_jv^{ij}$.

The functions v^{ij} are called *potentials* corresponding to the null divergence F. If $n=1$ any null divergence is constant.

Definition 3: Two conserved vectors F and F' are called *equivalent* if the vector-function $F'-F$ is a trivial conserved vector.

By the latter definition any trivial conserved vector is equivalent to the vanishing one. For any system $\mathcal{L}$ of differential equations the set $\mathrm{CV}(\mathcal{L})$ of conserved vectors of its conservation laws is a linear space, and the subset $\mathrm{CV}_0(\mathcal{L})$ of trivial conserved vectors is a linear subspace in $\mathrm{CV}(\mathcal{L})$. The factor space $\mathrm{CL}(\mathcal{L})=\mathrm{CV}(\mathcal{L})/\mathrm{CV}_0(\mathcal{L})$ coincides with the set of equivalence classes of $\mathrm{CV}(\mathcal{L})$ with respect to the equivalence relation adduced in Definition 3. We can identify elements of $\mathrm{CL}(\mathcal{L})$ with conservation laws and call $\mathrm{CL}(\mathcal{L})$ also as *the space of conservation laws* of $\mathcal{L}$ (see, e.g., Ref. 46). That is why we assume description of the set of conservation laws as finding $\mathrm{CL}(\mathcal{L})$ that is equivalent to construction of either a basis if $\dim\mathrm{CL}(\mathcal{L})<\infty$ or a system of generatrices in the infinite dimensional case, and we will additionally identify elements from $\mathrm{CL}(\mathcal{L})$ with their representatives in $\mathrm{CV}(\mathcal{L})$. In contrast to the order r_F of a conserved vector F as the maximal order of derivatives explicitly appearing in F, the *order of a conservation law* as an element $\mathcal{F}$ from $\mathrm{CL}(\mathcal{L})$ is called $\min\{r_F\,|\,F\in\mathrm{CV}(\mathcal{L})\text{corresponds to }\mathcal{F}\}$. Under linear dependence of conservation laws we understand linear dependence of corresponding elements in $\mathrm{CL}(\mathcal{L})$.

Definition 4: Conservation laws of a system $\mathcal{L}$ are called *linearly dependent* if a linear combination of them has a trivial conserved vector.

Note 1: Sometimes other definitions of equivalence of conservation laws are used.[16]

Let the system $\mathcal{L}$ be totally nondegenerate.[31] Then application of the Hadamard lemma to the definition of conservation law and integrating by parts imply that the left-hand side of any conservation law of $\mathcal{L}$ can always be presented up to the equivalence relation as a linear combination of left-hand side of independent equations from $\mathcal{L}$ with coefficients λ^μ being functions on a suitable jet space $J^{(k)}$,

$$\mathrm{Div}\,F=\lambda^\mu L^\mu. \tag{2}$$

Here the order k is determined by $\mathcal{L}$ and the allowable order of conservation laws, $\mu=\overline{1,l}$.

Definition 5: Formula (2) and the l-tuple $\lambda=(\lambda^1,\dots,\lambda^l)$ are called the *characteristic form* and the *characteristic* of the conservation law $\mathrm{Div}\,F=0$ correspondingly.

The characteristic λ is *trivial* if it vanishes for all solutions of $\mathcal{L}$. Since $\mathcal{L}$ is nondegenerate, the characteristics λ and $\tilde{\lambda}$ satisfy (2) for the same F and, therefore, are called *equivalent* iff $\lambda-\tilde{\lambda}$ is a trivial characteristic. Similarly to conserved vectors, the set $\mathrm{Ch}(\mathcal{L})$ of characteristics corresponding to conservation laws of the system $\mathcal{L}$ is a linear space, and the subset $\mathrm{Ch}_0(\mathcal{L})$ of trivial characteristics is a linear subspace in $\mathrm{Ch}(\mathcal{L})$. The factor space $\mathrm{Ch}_f(\mathcal{L})=\mathrm{Ch}(\mathcal{L})/\mathrm{Ch}_0(\mathcal{L})$ coincides

with the set of equivalence classes of $\mathrm{Ch}(\mathcal{L})$ with respect to the above characteristic equivalence relation.

The following result[31] forms the cornerstone for the methods of studying conservation laws, which are based on formula (2), including the Noether theorem and the direct method by Anco and Bluman.[4,5]

Theorem 1: (Ref. 31) *Let $\mathcal{L}$ be a normal, totally nondegenerate system of differential equations. Then representation of conservation laws of $\mathcal{L}$ in the characteristic form (2) generates a one-to-one linear mapping between* $\mathrm{CL}(\mathcal{L})$ *and* $\mathrm{Ch}_f(\mathcal{L})$.

Using properties of total divergences, we can exclude the conserved vector F from (2) and obtain a condition for the characteristic λ only. Namely, a differential function f is a total divergence, i.e., $f=\mathrm{Div}\,F$ for some n-tuple F of differential functions iff $\mathsf{E}(f)=0$. Hereafter the Euler operator $\mathsf{E}=(\mathsf{E}^1,\dots,\mathsf{E}^m)$ is the m-tuple of differential operators

$$\mathsf{E}^a=(-D)^\alpha\partial_{u^a_\alpha},\quad a=\overline{1,m},$$

where $\alpha=(\alpha_1,\dots,\alpha_n)$ runs the multi-indices set $(\alpha_i\in\mathbb{N}\cup\{0\})$, $(-D)^\alpha=(-D_1)^{\alpha_1}\cdots(-D_m)^{\alpha_m}$. Therefore, action of the Euler operator on (2) results to the equation

$$\mathsf{E}(\lambda^\mu L^\mu)=\mathsf{D}^*_\lambda(L)+\mathsf{D}^*_L(\lambda)=0, \tag{3}$$

which is a necessary and sufficient condition on characteristics of conservation laws for the system $\mathcal{L}$. The matrix differential operators D^*_λ and D^*_L are the adjoints of the Fréchet derivatives D_λ and D_L, i.e.,

$$\mathsf{D}^*_\lambda(L)=\left((-D)^\alpha\left(\frac{\partial\lambda^\mu}{\partial u^a_\alpha}L^\mu\right)\right),\quad \mathsf{D}^*_L(\lambda)=\left((-D)^\alpha\left(\frac{\partial L^\mu}{\partial u^a_\alpha}\lambda^\mu\right)\right).$$

Since $\mathsf{D}^*_\lambda(L)=0$ automatically on solutions of $\mathcal{L}$ then Eq. (3) implies a necessary condition for λ to belong to $\mathrm{Ch}(\mathcal{L})$:

$$\mathsf{D}^*_L(\lambda)|_{\mathcal{L}}=0. \tag{4}$$

Condition (4) can be considered as adjoint to the criteria $\mathsf{D}_L(\eta)|_{\mathcal{L}}=0$ for infinitesimal invariance of $\mathcal{L}$ with respect to evolutionary vector field having the characteristic $\eta=(\eta^1,\dots,\eta^m)$. That is why solutions of (4) are sometimes called *cosymmetries*[7,36] or *adjoint symmetries*.[5]

By writing $\mathcal{L}$ in Cauchy–Kovalevskaya form (which is always possible since $\mathcal{L}$ is normal), system (3) can be split on the solution manifold of $\mathcal{L}$ to get determining equations for λ^μ formulated entirely on the solution manifold of $\mathcal{L}$. These equations include the adjoint symmetry condition (4) and certain adjoint-linearization equations.[5] As stated in Ref. 2, one only needs to find adjoint symmetries of $\mathcal{L}$ [i.e., solutions of (4)] in order to obtain conservation laws whenever $\mathcal{L}$ possesses a scaling symmetry.

III. EQUIVALENCE OF CONSERVATION LAWS

We can essentially simplify and order classification of conservation laws, taking into account additionally symmetry transformations of a system or equivalence transformations of a whole class of systems. Such problem is similar to one of group classification of differential equations.

Proposition 1: Any point transformation g maps a class of equations in the conserved form into itself. More exactly, the transformation g: $\tilde{x}=x_g(x,u)$, $\tilde{u}=u_g(x,u)$ prolonged to the jet space $J^{(r)}$ transforms the equation $D_iF^i=0$ to the equation $D_iF^i_g=0$. The transformed conserved vector F_g is determined by the formula

$$F^i_g(\tilde{x},\tilde{u}_{(r)})=\frac{D_{x_j}\tilde{x}_i}{|D_x\tilde{x}|}F^j(x,u_{(r)}),\quad \text{i.e., } F_g(\tilde{x},\tilde{u}_{(r)})=\frac{1}{|D_x\tilde{x}|}(D_x\tilde{x})F(x,u_{(r)}) \tag{5}$$

in the matrix notions. Here $|D_x\tilde{x}|$ is the determinant of the matrix $D_x\tilde{x}=(D_{x_j}\tilde{x}_i)$.

Note 2: In the case of one dependent variable ($m=1$) g can be a contact transformation: $\tilde{x}=x_g(x,u_{(1)})$, $\tilde{u}_{(1)}=u_{g(1)}(x,u_{(1)})$. Similar notes are also true for the statements below.

Definition 6: Let G be a symmetry group of the system $\mathcal{L}$. Two conservation laws with the conserved vectors F and F' are called *G-equivalent* if there exists a transformation $g\in G$ such that the conserved vectors F_g and F' are equivalent in the sense of Definition 3.

Any transformation $g\in G$ induces a linear one-to-one mapping g_* in $\mathrm{CV}(\mathcal{L})$, transforms trivial conserved vectors only to trivial ones [i.e., $\mathrm{CV}_0(\mathcal{L})$ is invariant with respect to g_*] and therefore induces a linear one-to-one mapping g_f in $\mathrm{CL}(\mathcal{L})$. It is obvious that g_f preserves linear (in)dependence of elements in $\mathrm{CL}(\mathcal{L})$ and maps a basis (a set of generatrices) of $\mathrm{CL}(\mathcal{L})$ in a basis (a set of generatrices) of the same space. In such way we can consider the G-equivalence relation of conservation laws as well determined on $\mathrm{CL}(\mathcal{L})$ and use it to classify conservation laws.

Proposition 2: If the system $\mathcal{L}$ admits a one-parameter group of transformations then the infinitesimal generator $X=\xi^i\partial_i+\eta^a\partial_{u^a}$ of this group can be used for construction of new conservation laws from known ones. Namely, differentiating Eq. (5) with respect to the parameter ε and taking the value $\varepsilon=0$, we obtain the new conserved vector

$$\tilde{F}^i=-X_{(r)}F^i+(D_j\xi^j)F^j-(D_j\xi^j)F^i. \tag{6}$$

Here $X_{(r)}$ denotes the rth prolongation[31,33] of the operator X.

Note 3: Formula (6) can be directly extended to generalized symmetry operators (see, for example, Refs. 6 and 24). A similar statement for generalized symmetry operators in evolutionary form ($\xi^i=0$) was known earlier.[19,31] It was used by Khamitova[25] to introduce a notion of basis of conservation laws as a set which generates a whole set of conservation laws with action of generalized symmetry operators and operation of linear combination.

Proposition 3: Any point transformation g between systems $\mathcal{L}$ and $\tilde{\mathcal{L}}$ induces a linear one-to-one mapping g_* from $\mathrm{CV}(\mathcal{L})$ into $\mathrm{CV}(\tilde{\mathcal{L}})$, which maps $\mathrm{CV}_0(\mathcal{L})$ into $\mathrm{CV}_0(\tilde{\mathcal{L}})$ and generates a linear one-to-one mapping g_f from $\mathrm{CL}(\mathcal{L})$ into $\mathrm{CL}(\tilde{\mathcal{L}})$.

Corollary 1: Any point transformation g between systems $\mathcal{L}$ and $\tilde{\mathcal{L}}$ induces a linear one-to-one mapping $\hat{g}_f$ from $\mathrm{Ch}_f(\mathcal{L})$ into $\mathrm{Ch}_f(\tilde{\mathcal{L}})$.

It is possible to obtain an explicit formula for correspondence between characteristics of $\mathcal{L}$ and $\tilde{\mathcal{L}}$. Let $\tilde{\mathcal{L}}^\mu=\Lambda^{\mu\nu}\mathcal{L}^\nu$, where $\Lambda^{\mu\nu}=\Lambda^{\mu\nu\alpha}D^\alpha$, $\Lambda^{\mu\nu\alpha}$ are differential functions, $\alpha=(\alpha_1,\dots,\alpha_n)$ runs the multi-indices set ($\alpha_i\in\mathbb{N}\cup\{0\}$), $\mu,\ \nu=\overline{1,l}$. Then

$$\lambda^\mu=\Lambda^{\nu\mu*}(|D_x\tilde{x}|\tilde{\lambda}^\nu).$$

Here $\Lambda^{\nu\mu*}=(-D)^\alpha\cdot\Lambda^{\mu\nu\alpha}$ is the adjoint to the operator $\Lambda^{\nu\mu}$. For a number of cases, e.g., if $\mathcal{L}$ and $\tilde{\mathcal{L}}$ are single partial differential equations ($l=1$), the operators $\Lambda^{\mu\nu}$ are simply differential functions (i.e., $\Lambda^{\mu\nu\alpha}=0$ for $|\alpha|>0$) and, therefore, $\Lambda^{\nu\mu*}=\Lambda^{\mu\nu}$.

Consider the class $\mathcal{L}|_S$ of systems $L(x,u_{(\rho)},\theta(x,u_{(\rho)}))=0$ parametrized with the parameter-functions $\theta=\theta(x,u_{(\rho)})$. Here L is a tuple of fixed functions of x, $u_{(\rho)}$ and θ. θ denotes the tuple of arbitrary (parametric) functions $\theta(x,u_{(\rho)})=(\theta^1(x,u_{(\rho)}),\dots,\theta^k(x,u_{(\rho)}))$ satisfying the condition $S(x,u_{(\rho)},\theta_{(q)}(x,u_{(\rho)}))=0$. This condition consists of differential equations on θ, where x and $u_{(\rho)}$ play the role of independent variables and $\theta_{(q)}$ stands for the set of all the partial derivatives of θ of order no greater than q. In what follows we call the functions θ arbitrary elements. Denote the local transformations group preserving the form of systems from $\mathcal{L}|_S$ as $G^\sim=G^\sim(L,S)$.

Consider the set $P=P(L,S)$ of all pairs each of which consists of a system from $\mathcal{L}|_S$ and a conservation law of this system. In view of Proposition 3, action of transformations from $G^\sim$ together with the pure equivalence relation of conserved vectors naturally generates an equivalence relation on P. Classification of conservation laws with respect to $G^\sim$ will be understood as classification in P with respect to the above equivalence relation. This problem can be investigated in the way that is similar to group classification in classes of systems of differential equations. Namely, we construct first the conservation laws that are defined for all values of the arbitrary

elements. (The corresponding conserved vectors may depend on the arbitrary elements.) Then we classify, with respect to the equivalence group, arbitrary elements for each of that the system admits additional conservation laws.

In an analogous way we also can introduce an equivalence relation on P generated by all admissible point or contact transformations (called also form-preserving ones[26]) in pairs of equations from $\mathcal{L}|_S$.

Note 4: It can be easily shown that all the above equivalences are indeed equivalence relations.

IV. DIRECT ITERATION METHOD OF FINDING CONSERVATION LAWS

To construct conservation laws of a system $\mathcal{L}$ of differential equations, we iterate a modification of the most *direct method* based on Definition 1. More precisely, the algorithm is as follows.

Zeroth iteration: At first we construct local conservation laws of $\mathcal{L}$. We fix an (arbitrary) order r of conserved vectors under consideration. Then we introduce local coordinates ("unconstrained variables") on the manifold $\mathcal{L}_{(r+1)}$ determined by the system $\mathcal{L}$ and its differential consequences in $J^{(r+1)}$. The other ("constrained") variables of $J^{(r+1)}$ are expressed via unconstrained ones by means of using the equations of $\mathcal{L}_{(r+1)}$. We substitute the expressions for constrained variables into a conservation law and split the obtained condition with respect to the unconstrained variables. This procedure results in a first-order linear system of determining equations for conserved vectors. Solving the determining equations up to the usual equivalence relation on $\mathrm{CV}(\mathcal{L})$, we obtain complete description of local conservation laws of $\mathcal{L}$. To classify conservation laws in easier and more systematic way (especially for classes of systems of differential equations), instead of usual equivalence we use the introduced above equivalence with respect to symmetry or equivalence transformations. (See Sec. VI for examples.)

First iteration: After applying Lemma 1 to constructed conservation laws on the set of solutions of $\mathcal{L}=\mathcal{L}^0$, we introduce potentials as additional dependent variables and attach the equations connecting the potentials with components of corresponding conserved vectors to $\mathcal{L}^0$. (If $n>2$ the attached equations of such kind form an underdetermined system with respect to the potentials. Therefore, we can also attach gauge conditions on the potentials to $\mathcal{L}^0$. See discussion on gauge freedom in potential systems and necessity of gauge conditions in paper.[3])

We must use linear independent conservation laws since otherwise the introduced potentials will be *dependent* in the following sense: there exists a linear combination of the potential tuples, which is, for some $r' \in \mathbb{N}$, a tuple of functions of x and $u_{(r')}$ only.

Then we exclude the unnecessary equations (i.e., the equations that are dependent on equations of $\mathcal{L}^0$ and attached equations simultaneously) from the extended (potential) system $\mathcal{L}^1$ which will be called a *potential system of the first level*. Any conservation law of $\mathcal{L}^0$ is one of $\mathcal{L}^1$. We iterate the above procedure of the direct method for $\mathcal{L}^1$ to find its conservation laws which are linear independent with ones from the previous iteration and will be called *potential conservation laws of the first level*.

Further iterations: We make iterations while it is possible [i.e., the iteration procedure has to be stopped if all the conservation laws of a *potential system* $\mathcal{L}^{k+1}$ *of the* $(k+1)$*th level* are linear dependent with the ones of $\mathcal{L}^k$] or construct infinite chains of conservation laws by means of induction. This process may yield *purely potential* conservation laws of the initial system $\mathcal{L}$, which are linear independent with local conservation laws and, therefore, depend explicitly on potential variables.

Any conservation law from the previous step of iteration procedure will be a conservation law for the next step and vice versa; conservation laws which are obtained on the next step and depend only on variables of the previous step are linear dependent with conservation laws from the previous step. It is also obvious that the conservation laws used for construction of a potential system of the next level are trivial on the manifold of this system.

Since gauge conditions on potentials can be chosen in many different ways, exhaustive realization of iterations is improbable in the case $n>2$.

The procedure of exclusion of constrained variables (which are described above in detail only for the zeroth iteration) is called in classical group analysis as "confining to the manifold of $\mathcal{L}$." Taking into account $\mathcal{L}$ in the above way, we automatically eliminate the ambiguity connected with vanishing conserved vectors on the solutions of $\mathcal{L}$. However, the second kind of ambiguity arising via existence of null divergences is preserved, and it is the main reason of difficulties in realization of this algorithm with symbolic computation systems.[44]

To find conservation laws on each step of iteration procedure, one can apply other methods which are based on the characteristic form (2) or its consequences (3) and (4). These methods are also called as direct.[4,5] Following Ref. 44, for convenience we will numerate them as the second, third, and fourth versions of the direct method in contrast to the above first one. They are close to the symmetry group method by Noether since in the case of Euler–Lagrange equations the coefficients λ^a are nothing else than Noether's characteristics. Taking into account the equivalence relation on $\mathrm{Ch}(\mathcal{L})$, one can assume during calculations that characteristics depend only on unconstrained variables.

In the second version of the direct method the representation (2) is regarded as an equation defined on an open subset of $J^{(k)}$ with respect to conserved vectors and characteristics simultaneously.

In the framework of the third version, sought quantities are characteristics only. Determining Eq. (3) is defined on an open subset of $J^{(k)}$. Conserved vectors are reconstructed from known characteristics via explicit integral formulas. An algorithm of this (third) version of the direct method was developed for Cauchy–Kovalevskaya systems by Anco and Bluman[4,5] (see also Refs. 31 and 46 for a theoretical background).

The fourth version is based on Eq. (4) which is defined on the manifold $\mathcal{L}$ and is only a necessary condition on characteristic of conservation laws. Therefore, one has to choose characteristics from the set of adjoint symmetries using additional conditions. Such approach was used by Bluman and Doran-Wu[8] for studying conservation laws of diffusion equations.

Each from four above versions of the direct method has its advantages and disadvantages. A detailed comparative analysis of all the versions and their realizations in computer algebra programs are given by Wolf.[44]

Prototypes and sources of a number of above ideas can be found in Ref. 28.

V. TWO-DIMENSIONAL CASE

The case of two independent variables is singular, in particular, with respect to possible (constant) indeterminacy after introduction of potentials and high effectiveness of application of potential symmetries. That is why we consider some notions connected with conservation laws in this case separately. We denote independent variables as t (the time variable) and x (the space one). Any local conservation law has the form

$$D_t F(t,x,u_{(r)}) + D_x G(t,x,u_{(r)}) = 0. \tag{7}$$

Here D_t and D_x are the operators of the total differentiation with respect to t and x. F and G are called the *conserved density* and the *flux* of the conservation law correspondingly.

Two conserved vectors (F,G) and (F',G') are *equivalent* if there exist such functions $\hat{F}$, $\hat{G}$, and H of t, x, and derivatives of u that $\hat{F}$ and $\hat{G}$ vanish on $\mathcal{L}_{(k)}$ for some k and

$$F' = F + \hat{F} + D_x H, \quad G' = G + \hat{G} - D_t H. \tag{8}$$

Any conservation law (7) of $\mathcal{L}$ allows us to deduce the new dependent (potential) variable v by means of the equations

$$v_x = F, \quad v_t = -G. \tag{9}$$

To construct a number of potentials in one step, we must use a set of linear independent conservation laws (see the preceding section) since otherwise the potentials will be dependent in the

following sense: there exists a linear combination of the potentials, which is, for some $r' \in \mathbb{N}$, a function of t, x, and $u_{(r')}$ only.

In the case of two independent variables we can also introduce the more general notion of potential dependence.

Definition 7: The potentials $v^1, \dots, v^p$ are called *locally dependent on the set of solution of the system* $\mathcal{L}$ (or, briefly speaking, *dependent*) if there exist $r' \in \mathbb{N}$ and a function H of the variables t, x, $u_{(r')}, v^1, \dots, v^p$ such that $H(t,x,u_{(r')},v^1,\dots,v^p)=0$ for any solution $(u,v^1,\dots,v^p)$ of the united system determining the set of potentials $v^1,\dots,v^p$.

Proof of local dependence or independence of potentials for general classes of differential equations is difficult since it is closely connected with precise description of possible structure of conservation laws. An example of such proof for diffusion-convection equations is presented below.

In the case of single equation $\mathcal{L}$, equations of form (9) combine into the complete potential system since $\mathcal{L}$ is a differential consequence of (9). As a rule, systems of such kind admit a number of nontrivial symmetries and so they are of great interest.

Equations (5) and (9) imply the following statement.

Proposition 4: Any point transformation connecting two systems $\mathcal{L}$ and $\widetilde{\mathcal{L}}$ of PDEs with two independent variables generates a one-to-one mapping between the sets of potential systems, which correspond to $\mathcal{L}$ and $\widetilde{\mathcal{L}}$. Generation is made via trivial prolongation on the space of introduced potential variables, i.e., we can assume that the potentials are not transformed.

Corollary 2: The Lie symmetry group of a system $\mathcal{L}$ *of differential equations generates an equivalence group on the set of potential systems corresponding to* $\mathcal{L}$.

Corollary 3: Let $\hat{\mathcal{L}}|_S$ *be the set of all potential systems constructed for systems from the class* $\mathcal{L}|_S$ *with their construction laws. Action of transformations from* $G^{\sim}(L,S)$ *together with the equivalence relation of potentials naturally generates an equivalence relation on* $\hat{\mathcal{L}}|_S$.

Note 5: Proposition 4 and its corollaries imply that the equivalence group for a class of systems or the symmetry group for single system can be prolonged to potential variables for any step of the direct iteration procedure. It is natural the prolonged equivalence groups are used to classify possible conservation laws and potential systems in each iteration. Additional equivalences which exist in some subclasses of the class or arise after introducing potential variables can be used for deeper analysis of connections between conservation laws.

VI. LOCAL CONSERVATION LAWS OF DIFFUSION-CONVECTION EQUATIONS

To classify the conservation laws of equations from class (1) we have to start our investigation from finding equivalence transformations. Application of the direct method to class (1) allows us to find the complete equivalence group $G^{\sim}$ including the both continuous and discrete transformations. The following statement is true.

Theorem 2: (Refs. 34 and 35) *Any transformation from* $G^{\sim}$ *has the form*

$$\tilde{t} = \varepsilon_4 t + \varepsilon_1, \quad \tilde{x} = \varepsilon_5 x + \varepsilon_7 t + \varepsilon_2, \quad \tilde{u} = \varepsilon_6 u + \varepsilon_3, \quad \tilde{A} = \varepsilon_4^{-1}\varepsilon_5^2 A, \quad \tilde{B} = \varepsilon_4^{-1}\varepsilon_5 B - \varepsilon_7,$$

where $\varepsilon_1,\dots,\varepsilon_7$ *are arbitrary constants,* $\varepsilon_4\varepsilon_5\varepsilon_6 \neq 0$.

The kernel of Lie symmetry group of equations from class (1) is the group of the transformations which are common for all of these equations. We denote it as G^{ker}. Via trivial prolongation on the arbitrary elements A and B, G^{ker} is isomorphic to a normal subgroup of $G^{\sim}$.

Theorem 3: G^{ker} *is formed by the transformations*

$$\tilde{t} = t + \varepsilon_1, \quad \tilde{x} = x + \varepsilon_2, \quad \tilde{u} = u,$$

where ε_1 *and* ε_2 *are arbitrary constants*.

First we search the conservation laws of equations from class (1) in the form (7).

Lemma 2: Any local conservation law of any equation from class (1) *has the first order.*

Moreover, up to equivalence on conserved vectors one can assume that the density depending on t, x, and u and the flux depending on t, x, u, and u_x.

Proof: Considering conservation laws on the manifold of Eq. (1) and its differential consequences, we can assume that F and G depend only on t, x, and $u_k=\partial^k u/\partial x^k$, $k=\overline{0,r'}$, where $r' \leqslant 2r$. We expand the total derivatives in (7) and take into account differential consequences of the form $u_{tj}=D_x^{j+2}\int A+D_x^{j+1}\int B$, where $\int A=\int A(u)\mathrm{d}u$, $\int B=\int B(u)\mathrm{d}u$, $j=\overline{0,r'}$. As a result we obtain the following condition:

$$F_t+F_{u_j}\left(D_x^{j+2}\int A+D_x^{j+1}\int B\right)+G_x+G_{u_j}u_{j+1}=0. \tag{10}$$

Let us decompose (10) with respect to the highest derivatives u_j. So, the coefficients of $u_{r'+2}$ and $u_{r'+1}$ give the equations $F_{u_{r'}}=0$, $G_{u_{r'}}+AF_{u_{r'-1}}=0$ that result in

$$F=\hat{F},\quad G=-Au_{r'}\hat{F}_{u_{r'-1}}+\hat{G},$$

where $\hat{F}$ and $\hat{G}$ are functions of $t,x,u,u_1,\dots,u_{r'-1}$. Then, after selecting the terms containing $u_{r'}^2$, we obtain that $-A\hat{F}_{u_{r'-1}u_{r'-1}}=0$. It yields that $\hat{F}=\check{F}^1u_{r'-1}+\check{F}^0$, where $\check{F}^1$ and $\check{F}^0$ depend only on $t,x,u,u_1,\dots,u_{r'-2}$.

Consider the conserved vector with the density $\widetilde{F}=F-D_xH$ and the flux $\widetilde{G}=G+D_tH$, where $H=\int\check{F}^1\mathrm{d}u_{r'-2}$. This conserved vector is equivalent to the initial one, and

$$\widetilde{F}=\widetilde{F}(t,x,u,u_1,\dots,u_{r'-2}),\quad \widetilde{G}=\widetilde{G}(t,x,u,u_1,\dots,u_{r'-1}).$$

Iterating this procedure a necessary number of times, we obtain the lemma statement. ■

Note 6: A similar statement is true for an arbitrary $(1+1)$-dimensional evolution equation $\mathcal{L}$ of the even order $r=2\overline{r},\overline{r}\in\mathbb{N}$.[1,19] For example,[19] for any conservation law of $\mathcal{L}$ we can assume up to equivalence of conserved vectors that F and G depend only on t, x and derivatives of u with respect to x, and the maximal order of derivatives in F is not greater than $\overline{r}$.

Lemma 2 gives a stronger result for a more restricted class of equations. In the above proof we specially use the most direct method to demonstrate its effectiveness in quite general cases. This proof can be easily extended to other classes of $(1+1)$-dimensional evolution equations of odd orders and potential systems corresponding to equations from class (1) (see the proof of Lemma 3).

Theorem 4: *Any equation from class* (1) *has the conservation law* (7) *where*

$$(1)\quad F=u,\quad G=-Au_x-\int B. \tag{11}$$

A complete list of $G^{\sim}$-inequivalent equations (1) *having additional* [*i.e., linear independent with* (11)] *conservation laws is exhausted by the following ones:*

$$(2)\quad \forall A,\quad B=0:\quad F=xu,\quad G=\int A-xAu_x, \tag{12}$$

$$(3)\quad \forall A,\quad B=A:\quad F=(e^x+\varepsilon)u,\quad G=-(e^x+\varepsilon)Au_x-\varepsilon\int A, \tag{13}$$

$$(4)\quad A=1,\quad B=0:\quad F=\alpha u,\quad G=\alpha_x u-\alpha u_x, \tag{14}$$

where $\varepsilon\in\{0,\pm1\}\bmod G^{\sim}$, $\int A=\int A(u)\mathrm{d}u$, $\int B=\int B(u)\mathrm{d}u$, $\alpha=\alpha(t,x)$ is an arbitrary solution of the linear heat equation $\alpha_t+\alpha_{xx}=0$. (*Together with values A and B we also adduce complete lists of densities and the fluxes of additional conservation laws.*)

Proof: In view of Lemma 2, we can assume at once that $F=F(t,x,u)$ and $G=G(t,x,u,u_x)$. Let us substitute the expression for u_t deduced from (1) into (7) and decompose the obtained equation with respect to u_{xx}. The coefficient of u_{xx} gives the equation $AF_u+G_{u_x}=0$, therefore $G=-AF_u u_x+G^1(t,x,u)$. Taking into account the latter expression for G and splitting the rest of Eq. (7) with respect to the powers of u_x, we obtain the system of PDEs on the functions F and G^1 of the form

$$F_{uu}=0, \quad BF_u-AF_{ux}+G^1_u=0, \quad F_t+G^1_x=0. \tag{15}$$

Solving the first two equations of (15) yields

$$F=F^1(t,x)u+F^0(t,x), \quad G^1=F^1_x\int A-F^1\int B+G^0(t,x). \tag{16}$$

In further consideration the major role is played by the equation $AF_{uxx}-BF_{ux}+F_{ut}=0$ that is a differential consequence of system (15) and can be rewritten as

$$AF^1_{xx}-BF^1_x+F^1_t=0.$$

Indeed, it is the unique classifying condition for this problem. There exist four different possibilities for values A and B. In all cases we obtain the equation $F^0_t+G^0_x=0$. Therefore, up to conservation laws equivalence we can assume $F^0=G^0=0$. Moreover, the function $F^1=\text{const}$ is a solution of the classifying condition in the general case. This solution corresponds to the conservation laws of case 1. Only conservation laws of such kind exist for all admissible values of arbitrary elements A and B. Then we classify special values of A and B for which Eq. (1) possesses additional conservation laws.

(1) $B\notin\langle A,1\rangle$. Then $F^1_x=0$, $F^1_t=0$ that gives contradiction with the assumption $F^1\neq\text{const}$.
(2) $A\notin\langle 1\rangle$, $B\in\langle 1\rangle$. Then $B=0 \bmod G^\sim$ and $F^1_{xx}=0$, $F^1_t=0$, i.e., $F^1=x \bmod G^\sim$ (case 2).
(3) $B\in\langle A,1\rangle$, $A,B\notin\langle 1\rangle$. Then $B=A \bmod G^\sim$ and $F^1_{xx}+F^1_x=0$, $F^1_t=0$, i.e., $F^1=e^x+\varepsilon \bmod G^\sim$, where $\varepsilon\in\{0,\pm 1\}$ (case 3).
(4) A, $B\in\langle 1\rangle$. Therefore, $A=1$, $B=0 \bmod G^\sim$, and $F^1_t+F^1_{xx}=0$ (case 4). ■

Note 7: It follows from the proof that we can assume $(A,B)\neq\text{const}$ in cases 1, 2, and 3. [If $(A,B)=\text{const}$ cases 1, 2, and 3 are included in case 4 for different values of α.]

Using the conservation laws adduced in Theorem 4, we can introduce potentials for different values of the parameter functions A and B and construct the corresponding potential systems (cases 1–4 of Table I). The important question for our consideration is whether the introduced potentials are locally independent in the sense of Definition 7. If we know the precise structure of conservation laws the answer is almost obvious.

Theorem 5: *For any equation* (1) *potentials are locally dependent on the equation manifold iff the corresponding conservation laws are linear dependent.*

Proof: Since the direct statement of the theorem is obvious (see Sec. V), we prove only the inverse statement, using the rule of contraries. Suppose that potentials $v^0,\dots,v^p$ introduced with (independent) conservation laws of cases 1–4 are locally dependent. The vanishing p means local triviality of v^0 as a potential, i.e., v^0 can be expressed in terms of local variables and the corresponding conservation law is trivial. That is why it is sufficient to investigate only the special cases when the number of independent conservation laws is greater than 1. Therefore, $p=1$ if either $B=0$ or $B=A$ and $p\in\mathbb{N}/\{0\}$ for the linear heat equation.

Without loss of generality we can assume that there exist $r\in\mathbb{N}$ and a fixed function V of $t,x,\overline{v}=(v^1,\dots,v^p)$ and $u_{(r)}$ that $v^0=V(t,x,\overline{v},u_{(r)})$ for any solution of the united system determining the whole set of potentials $v^0,\dots,v^p$. Taking into account equation (1) and its differential consequences, we can assume that V depends only on t, x, $\overline{v}$, and $u_k=\partial^k u/\partial x^k$, $k=\overline{0,r'}$, where $r'\leqslant 2r$. Let us apply the operator D_x to the condition $v^0=V(t,x,\overline{v},u,u_1,\dots,u_{r'})$: $v^0_x=V_x+V_{v^s}v^s_x+V_{u^k}u_{k+1}$. (Hereafter the index s takes the values from 1 to p.) Since in any case under consideration $v^s_x=f^s u$ for some functions f^s of t and x, we can split the differentiated condition with respect

TABLE I. Conservation laws and potential systems of convection-diffusion equations.[a]

N	A	B	F	G	Potential system
1	$\forall$	$\forall$	u	$-Au_x-\int B$	$v_x=u,\ v_t=Au_x+\int B$
1.1	$\forall$	0	v	$-\int A$	$v_x=u,\ w_x=v,\ w_t=\int A$
1.2	$\forall$	A	$e^x v$	$-e^x\int A$	$v_x=u,\ w_x=e^x v,\ w_t=e^x\int A$
1.3	$\forall$	$\int A+uA$	e^v	$-e^v\int A$	$v_x=u,\ w_x=e^v,\ w_t=e^v\int A$
1.4	u^{-2}	0	σ	$\sigma_v u^{-1}$	$v_x=u,\ w_x=\sigma,\ w_t=-\sigma_v u^{-1}$
1.5	u^{-2}	u^{-2}	σe^x	$\sigma_v u^{-1}e^x$	$v_x=u,\ w_x=\sigma e^x,\ w_t=-\sigma_u u^{-1}e^x$
1.6	1	$2u$	αe^v	$\alpha_x e^v-\alpha u e^v$	$v_x=u,\ w_x=\alpha e^v,\ w_t=\alpha u e^v-\alpha_x e^v$
2	$\forall$	0	xu	$\int A-xAu_x$	$v_x=xu,\ v_t=xAu_x-\int A$
2.1	$\forall$	0	$x^{-2}v$	$-x^{-1}\int A$	$v_x=xu,\ w_x=x^{-2}v,\ w_t=x^{-1}\int A$
3	$\forall$	A	$(e^x+\varepsilon)u$	$-(e^x+\varepsilon)Au_x-\varepsilon\int A$	$v_x=(e^x+\varepsilon)u,\ v_t=(e^x+\varepsilon)Au_x+\varepsilon\int A$
3.1	$\forall$	A	$e^x(e^x+\varepsilon)^{-2}v$	$-e^x(e^x+\varepsilon)^{-1}\int A$	$v_x=(e^x+\varepsilon)u,\ w_x=e^x(e^x+\varepsilon)^{-2}v,$ $w_t=e^x(e^x+\varepsilon)^{-1}\int A$
4	1	0	αu	$\alpha_x u-\alpha u_x$	$v_x=\alpha u,\ v_t=\alpha u_x-\alpha_x u$
4.1	1	0	$(\beta/\alpha)_x v$	$-\alpha(\beta/\alpha)_x u-(\beta/\alpha)_t v$	$v_x=\alpha u,$ $w_x=(\beta/\alpha)_x v,\ w_t=\alpha(\beta/\alpha)_x u+(\beta/\alpha)_t v$

[a]Here $\varepsilon\in\{0,\pm1\}$, $\int A=\int A(u)\mathrm{d}u$, $\int B=\int B(u)\mathrm{d}u$; $\alpha(t,x)$, $\beta(t,x)$, and $\alpha(t,v)$ are arbitrary solutions of the linear heat equation $(\alpha_t+\alpha_{xx}=0,\beta_t+\beta_{xx}=0,\sigma_t+\sigma_{vv}=0)$. In case 1.3 we assume $\int B=u\int A$ for a conservation law to have the adduced form.

to u_k step-by-step in the reverse sequence, beginning with the major derivative. As a result, we obtain $V_{u^k}=0$, $V_x=0$, and $f^0=V_{v^s}f^s$, i.e., the functions $f^0,\dots,f^p$ are linear dependent. This gives a contradiction with the supposition that the conservation laws are independent. ■

VII. SIMPLEST POTENTIAL CONSERVATION LAWS OF DIFFUSION-CONVECTION EQUATIONS

Let us investigate local conservation laws of potential systems 1–4 from Table I, which have the form

$$D_t F(t,x,u_{(r)},v_{(r)})+D_x G(t,x,u_{(r)},v_{(r)})=0. \tag{17}$$

These laws can be considered as nonlocal (*potential*) conservation laws of equations from class (1). We assume them as simplest potential conservation laws since the corresponding potential systems are constructed from the initial equation (1) with one conservation law only.

We classify conservation laws up to the equivalence relation with respect to the transformation group $G^{\sim}_{\mathrm{pr}}$ which is a result of the trivial prolongation of the group $G^{\sim}$ from Theorem 2 to the space of the potential v.

Lemma 3: Any conservation law of form (17) *for each of systems* 1–4 *from Table I has the zero order, i.e., it is equivalent to a law with a conserved density F and a flux G that are independent on the (nonzero order) derivatives of u and v.*

Proof: Consider any from the systems 1–4. Taking it and its differential consequences into account, we can exclude dependence of F and G on all (nonzero order) derivatives of v and the derivatives of u containing differentiation with respect to t. The remaining part of the proof is completely similar to the one of Lemma 2. ■

In an analogous to proof of Theorem 4 and more cumbersome way we prove the following statement.

Theorem 6: *A complete set of* $G^{\sim}_{\mathrm{pr}}$*-inequivalent conservation laws of form* (17) *for equations from class* (1) *is presented in Table I with a double numeration of cases.*

Note 8: To prove Theorem 6 we use all independent differential consequences of correspondent potential systems. In Table I for the double numerated potential systems we omit equations containing v_t since they are only differential consequences of equations of these systems.

Let us analyze connections between conservation laws and ones between potential systems, which arise due to additional (including purely potential) equivalence transformations in some special cases. Below we assume $A \notin \{1, u^{-2}\}$ mod $G^{\sim}$ as a general value of A.

General case: Equation (1) in the general case has the unique linear independent local conservation law (case 1) with the conserved vectors $(F^1, G^1) = (u, -Au_x)$. All conservation laws of the corresponding potential system

$$v^1_x = u, \quad v^1_t = Au_x + \int B, \tag{18}$$

are trivial, i.e., in our framework equation (1) of the general form admits only trivial potential conservation laws.

$B=0$: Any equation of such form has two linear independent local conservation laws (cases 1 and 2) with the conserved vectors $(F^1, G^1) = (u, -Au_x)$ and $(F^2, G^2) = (xu, \int A - xAu_x)$, and any conservation law is G^{ker}-equivalent to one of them. Using these conservation laws, we can introduce two potentials v^1 and v^2, where

$$v^1_x = u, \quad v^1_t = Au_x, \tag{19}$$

$$v^2_x = xu, \quad v^2_t = xAu_x - \int A. \tag{20}$$

Equations (19) and (20) considered separately form two potential systems for equation (1) with vanishing B in unknown functions (u, v^1) and (u, v^2) correspondingly. The third potential system is formed by Eqs. (19) and (20) simultaneously, and three functions u, v^1, and v^2 are assumed as unknown. Each from systems (19) and (20) has one linear independent local conservation law (cases 1.1 and 2.1). These conservation laws with conserved vectors $(F^{11}, G^{11}) = (v^1, -\int A)$ and $(F^{21}, G^{21}) = (x^{-2}v^2, -x^{-1}\int A)$ are simplest potential conservation laws for Eq. (1) with vanishing B and allow us to introduce "second-level" potentials w^1 and w^2. As a result, we obtain two potential systems of the next level,

$$v^1_x = u, \quad w^1_x = v^1, \quad w^1_t = \int A, \tag{21}$$

$$v^2_x = xu, \quad w^2_x = x^{-2}v^2, \quad w^2_t = x^{-1}\int A. \tag{22}$$

At the same time, the simplest potential conservation laws are trivial on the solution manifold of the united system (19) and (20) since

$$F^{11} = D_x(xv^1 - v^2), \quad G^{11} = -D_t(xv^1 - v^2),$$

$$F^{21} = D_x(v^1 - x^{-1}v^2), \quad G^{21} = -D_t(v^1 - x^{-1}v^2).$$

Moreover $w^1 = xv^1 - v^2$, $w^2 = v^1 - x^{-1}v^2$, i.e., system (21), system (22), and united system (19) and (20) are point equivalent. It implies that really system (19) and (20) is generated by only three independent equations. (We can choose, e.g., the equation $v^1_x = u$, $v^2_x = xu$, $xv^1_t - v^2_t = \int A$.) Although system (21) formally belongs to the second level, it is the most convenient for further investigation since it has the simplest form.

$B=A$: This case is analyzed in the similar way to the previous one. Any equation with $B=A$ has the two-dimensional space of local conservation laws. Up to G^{ker}-equivalence, we have two possibilities for conserved vectors (cases 1 and 3),

$$(F^1,G^1)=\left(u,-Au_x-\int A\right)\quad\text{and}\quad(F^3,G^3)=\left((e^x+\varepsilon)u,-(e^x+\varepsilon)Au_x-\varepsilon\int A\right).$$

Using these conservation laws, we can introduce two potentials v^1 and v^3, where

$$v^1_x=u,\quad v^1_t=Au_x+\int A, \tag{23}$$

$$v^3_x=(e^x+\varepsilon)u,\quad v^3_t=(e^x+\varepsilon)Au_x+\varepsilon\int A. \tag{24}$$

Equations (23) and (24) considered separately form two potential systems for Eq. (1) with $B=A$ in unknown functions (u,v^1) and (u,v^3) correspondingly. The third potential system is formed by Eqs. (23) and (24) simultaneously, and three functions u, v^1, and v^3 are assumed as unknown. Each from systems (23) and (24) has one linear independent local conservation law (cases 1.2 and 3.1). These conservation laws with conserved vectors

$$(F^{12},G^{12})=\left(e^xv^1,-e^x\int A\right)$$

and

$$(F^{31},G^{31})=\left(\frac{e^x}{(e^x+\varepsilon)^2}v^3,-\frac{e^x}{e^x+\varepsilon}\int A\right)$$

are simplest potential conservation laws for Eq. (1) with $B=A$ and allow us to introduce "second-level" potentials w^1 and w^3. As a result, we obtain two potential systems of the next level,

$$v^1_x=u,\quad w^1_x=e^xv^1,\quad w^1_t=e^x\int A, \tag{25}$$

$$v^3_x=(e^x+\varepsilon)u,\quad w^3_x=\frac{e^x}{(e^x+\varepsilon)^2}v^3,\quad w^3_t=\frac{e^x}{e^x+\varepsilon}\int A. \tag{26}$$

At the same time, the simplest potential conservation laws are trivial on the solution manifold of the united system (23) and (24) since

$$F^{12}=D_x((e^x+\varepsilon)v^1-v^3),\quad G^{12}=-D_t((e^x+\varepsilon)v^1-v^3),$$

$$F^{31}=D_x\left(v^1-\frac{v^3}{e^x+\varepsilon}\right),\quad G^{31}=-D_t\left(v^1-\frac{v^3}{e^x+\varepsilon}\right).$$

Moreover

$$w^1=(e^x+\varepsilon)v^1-v^3,\quad w^3=v^1-\frac{v^3}{e^x+\varepsilon},$$

i.e., system (25), system (26), and united system (23) and (24) are point equivalent. It implies that really system (23) and (24) is generated by only three independent equations. [We can choose, e.g., the equation $v^1_x=u$, $v^3_x=(e^x+\varepsilon)u$, $(e^x+\varepsilon)v^1_t-v^3_t=e^x\int A$.] Although system (25) formally belongs to the second level, it is the most convenient for further investigation since it has the simplest form.

$B=\int A+uA$: The initial potential system in case 1.3 is reduced to case 1.2 by means of the hodograph transformation

$$\tilde{t} = t, \quad \tilde{x} = v, \quad \tilde{v} = x, \quad \tilde{u} = u^{-1}, \quad \tilde{A} = u^{-2}A, \tag{27}$$

and the conservation law 1.3 is transformed to the local one of case 3 where $\varepsilon = 0$. The same transformation extended to the potential w as $\tilde{w} = -w + ve^x$ also reduces the potential system 1.3 to 1.2.

Linearizable equations: It is well known[9,11,14,15,18,39,41] that equations (1) $G^{\sim}$-equivalent to ones of cases 1.4, 1.5, and 1.6 are linearized by a nonlocal (so-called potential equivalence[29,35]) transformations to the linear heat equation. That is why these equations stand out against the other diffusion-convection equations with having an infinite number of linear independent purely potential conservation laws.

The u^{-2}-diffusion equation $u_t = (u^{-2}u_x)_x$ is reduced to the linear heat equation[9] by the hodograph transformation (27). More exactly, (27) is a local transformation between the corresponding potential systems $v_x = u$, $v_t = u^{-2}u_x$ and $v_x = u$, $v_t = u_x$ constructed by means of using the "common" conservation law (case 1). The u^{-2}-diffusion equation has, as a subcase of the case $B = 0$, two linear independent local conservation laws with the conserved vectors

$$F^1 = u, \quad G^1 = -u^{-2}u_x, \tag{28}$$

$$F^2 = xu, \quad G^2 = -xu^{-2}u_x - u^{-1} \tag{29}$$

(cases 1 and 2 of Table I) and the infinite series of potential conservation laws (case 1.4) additionally. Under the action of hodograph transformation (27) the conservation law with conserved vector (28) is transformed to the trivial one of the linear heat equation with the conserved vector (1, 0). And vice versa, the conservation law of the linear heat equation corresponding to the value $\alpha = 1$ (case 4) is transformed by (27) to the trivial one of the u^{-2}-diffusion equation with the conserved vector (1, 0). The conservation law with conserved vector (29) is trivial on the manifold of potential system constructed by means of (28), is equivalent to the one from case 1.4 with $\sigma = 1$ and is transformed to case 4.1, where $\alpha = 1$ and $\beta = x$. Case 1.4 is reduced by (27) to case 4, where $\alpha = \sigma$.

Since the equation $u_t = (u^{-2}u_x)_x + u^{-2}u_x$ is reduced to the u^{-2}-diffusion equation by the local transformation $\tilde{t} = t$, $\tilde{x} = e^x$, $\tilde{u} = e^{-x}u$, its conservation laws are connected with ones of the linear heat equation in a way which is similar to the previous case.

The potential systems $\tilde{v}_{\tilde{x}} = \tilde{u}$, $\tilde{v}_{\tilde{t}} = \tilde{u}_{\tilde{x}} + \tilde{u}^2$, and $v_x = u$, $v_t = u_x$ constructed with the "common" conservation law for the Burgers equation $u_t = u_{xx} + 2uu_x$ and the linear heat equation $u_t = u_{xx}$ are connected via the transformation $t = \tilde{t}$, $x = \tilde{x}$, $u = \tilde{u}e^{\tilde{v}}$, $v = e^{\tilde{v}}$. (Here the tilde variables correspond to the Burgers equation.) Let us note that really the famous Cole–Hopf transformation[11,18] (first found in Ref. 15) linearizes the Burgers equation to the "potential" heat equation $v_t = v_{xx}$.[29,35] The Burgers equation has the "common" local conservation law (case 1) and the infinite series of simplest potential conservation laws (case 1.6). The above transformation between the potential systems induces the one-to-one mapping preserving α between the infinite series 1.6 and the one 4 of the "potential" heat equation $v_t = v_{xx}$. Then, the conservation law of form 4 with the function $\tilde{\alpha}$ for the "potential" heat equation $v_t = v_{xx}$ is equivalent to the one with the function α for the heat equation $u_t = u_{xx}$, where $\tilde{\alpha} = \alpha_x$. The conservation law of case 1 for the Burgers equation is trivial on the manifold of the corresponding potential system and is mapped to trivial one of the system $v_x = u$, $v_t = u_x$.

Linear heat equation: The linear heat equation $u_t = u_{xx}$ has an infinite dimensional space of local conservation laws,[12] which is generated by conserved vectors of the form $(F^\alpha, G^\alpha) = (\alpha u, \alpha_x u - \alpha u_x)$, where $\alpha = \alpha(t,x)$ is an arbitrary solution of the backward linear heat equation $\alpha_t + \alpha_{xx} = 0$. Using a fixed conservation law of such form, we can introduce the potential v^α, where

$$v^\alpha_x = \alpha u, \quad v^\alpha_t = \alpha u_x - \alpha_x u. \tag{30}$$

System (30) has one infinite series of conservation laws (case 4.1) with conserved vectors

$$(F^{\alpha\beta},G^{\alpha\beta})=\left(\left(\frac{\beta}{\alpha}\right)_x v^\alpha,-\alpha\left(\frac{\beta}{\alpha}\right)_x u-\left(\frac{\beta}{\alpha}\right)_t v^\alpha\right), \tag{31}$$

where $\beta=\beta(t,x)$ is an arbitrary solution of the backward linear heat equation $\beta_t+\beta_{xx}=0$. These conservation laws are simplest potential ones for the linear heat equation and allow us to introduce "second-level" potentials $w^{\alpha\beta}$. As a result, we obtain potential systems of the next level,

$$v^\alpha_x=\alpha u,\quad w^{\alpha\beta}_x=\left(\frac{\beta}{\alpha}\right)_x v^\alpha,\quad w^{\alpha\beta}_t=\alpha\left(\frac{\beta}{\alpha}\right)_x u+\left(\frac{\beta}{\alpha}\right)_t v^\alpha. \tag{32}$$

Consider the system

$$v^\alpha_x=\alpha u,\quad v^\alpha_t=\alpha u_x-\alpha_x u,\quad v^\beta_x=\beta u,\quad v^\beta_t=\beta u_x-\beta_x u \tag{33}$$

that is the union of two potential systems of form (30) corresponding to the local conservation laws with the conserved vectors (F^α,G^α) and (F^β,G^β). In a similar way to the previous cases we can state that the second-level potential conservation law with conserved vector (31) is trivial on the solution manifold of system (33) since

$$F^{\alpha\beta}=D_x\left(\frac{\beta}{\alpha}v^\alpha-v^\beta\right)\quad\text{and}\quad G^{\alpha\beta}=-D_t\left(\frac{\beta}{\alpha}v^\alpha-v^\beta\right).$$

Moreover, systems (32) and (33) are connected via the local substitution

$$w^{\alpha\beta}=\frac{\beta}{\alpha}v^\alpha-v^\beta.$$

It implies that really system (33) is generated by only three independent equations. We can choose, e.g., the equations

$$v^\alpha_x=\alpha u,\quad v^\beta_x=\beta u,\quad \frac{\beta}{\alpha}v^\alpha_t-v^\beta_t=\alpha\left(\frac{\beta}{\alpha}\right)_x u.$$

As a result of our analysis, we can formulate the following statement.

Theorem 7: *For any nonlinearized equation* (1) *and the linear heat equation the potential systems of the second level, which are constructed by means of using single conservation law of the simplest potential systems, are equivalent to first-level potential systems obtained with pairs of conservation laws.*

VIII. POTENTIAL CONSERVATION LAWS OF LINEAR HEAT EQUATION

With respect to $G^{\sim}$-equivalence the linear heat equation is the unique linear equation in class (1). Investigation of its general potential conservation laws plays the major role in classification of potential conservation laws for linearizable equations in class (1) and, therefore, for whole class (1). (The simplest potential conservation laws are studied in the preceding section.)

As proved in Theorem 4, the linear heat equation has the infinite series of local conservation laws. Fixing an arbitrary $p\in\mathbb{N}$ and choosing p linear independent solutions $\overline{\alpha}=(\alpha^1,\dots,\alpha^p)$ of the backward linear heat equation, we obtain p linear independent conservation laws with the conserved vectors $(F^s,G^s)=(\alpha^s u,\alpha^s_x u-\alpha^s u_x)$. (Hereafter $s=\overline{1,p}$.) In view of Theorem 5 the potentials $\overline{v}=(v^1,\dots,v^p)$ introduced with these conservation laws by the formulas

$$v^s_x=\alpha^s u,\quad v^s_t=\alpha^s u_x-\alpha^s_x u \tag{34}$$

are independent in the sense of Definition 7.

For the linear heat equation the complete set of first level potential conservation laws is indeed the union set of conservation laws of systems (34) corresponding to all possible values of p and p-tuples $\overline{\alpha}$. The following theorem is true.

Theorem 8: *Any local conservation law of system* (34) *is equivalent on the manifold of system* (34) *to a local conservation law of the linear heat equation.*

Corollary 4: For the linear heat equation potential conservation laws of any level are equivalent to local ones on the manifolds of the corresponding potential systems, and potentials of any level are locally expressed via local variables t, x, $u_{(r)}$ *(for some* r*) and potentials of the first lèvel only.*

We present the proof of Theorem 8 as the chain of simple and nice lemmas.

Lemma 4: Any local conservation law of system (34) *is equivalent to that with the conserved vector* $(Ku, K_x u - Ku_x)$ *where the function* $K=K(t,x,\overline{v})$ *is determined by the system*

$$K_t + K_{xx} = 0, \quad \alpha^s K_{xv^s} - \alpha^s_x K_{v^s} = 0. \tag{35}$$

Proof: Consider a local conservation law of system (34) in the most general form, where the conserved vector is a vector-function of t, x and derivatives of the functions u and v^s from the zero order up to some finite one. Taking into account system (34) and its differential consequences, we can exclude dependence of the conserved vector on all (nonzero order) derivatives of v^s and the derivatives of u containing differentiation with respect to t. Similarly to Lemma 2 we can prove that the reduced conserved vector (F,G) does not depend on (nonzero order) derivatives of u and, moreover, $F=F(t,x,\overline{v})$, $G=-\alpha^s F_{v^s}(t,x,\overline{v})u+G^0(t,x,\overline{v})$. The functions F and G^0 satisfy the system

$$\alpha^s \alpha^{s'} F_{v^s v^{s'}} = 0, \quad \alpha^s G^0_{v^s} = 2\alpha^s_x F_{v^s} + \alpha^s F_{xv^s}, \quad F_t + G^0_x = 0.$$

Let us pass on to the equivalent conserved vector $(\widetilde{F},\widetilde{G})$, where $\widetilde{F}=F+D_x H$, $\widetilde{G}=G-D_t H$, and $H=H(t,x,\overline{v})$ is a solution of the equations $H_x=-F$, $H_t=G$. (The variables v^s is assumed as parameters in the latter equations.) Then $\widetilde{F}=Ku$, $\widetilde{G}=K_x u-Ku_x$. The function $K=\alpha^s H_{v^s}$ depends on t, x, and $\overline{v}$ and satisfies system (35). ■

Lemma 5: Let the solutions $\alpha^s=\alpha^s(t,x)$ *and* $\beta^s=\beta^s(t,x)$ *of the (backward) linear heat equation satisfy the additional condition* $\alpha^s_x\beta^s-\alpha^s\beta^s_x=0$. *Then for any* $i,j\in\mathbb{N}$,

$$\alpha^s_i\beta^s_j - \alpha^s_j\beta^s_i = 0. \tag{36}$$

Hereafter the subscripts i *and* j denote the *ith and jth order derivatives with respect to* x.

Proof: We make the proof by means of mathematical induction with respect to the value $i+j$. Equation (36) is trivial for $i+j=0$, coincides with the additional condition for $i+j=1$ and is obtained from this condition by means of differentiation with respect to x if $i+j=2$. Let us suppose that the lemma's statement is true if $i+j=m-1$ and $i+j=m$ and prove it for $i+j=m+1$. Acting on Eq. (36) where $i+j=m-1$ with the operator $\partial_t+\partial_{xx}$ and taking into account the conditions $\alpha^s_t+\alpha^s_{xx}=0$ and $\beta^s_t+\beta^s_{xx}=0$, we obtain the equation $\alpha^s_{i+1}\beta^s_{j+1}-\alpha^s_{j+1}\beta^s_{i+1}=0$. Therefore, the statement is true for $i'+j'=m+1$, $1\leqslant i',j'\leqslant m$ $(i'=i+1, j'=j+1)$. It remains to perform the proof in the case $i'=m+1$, $j'=0$ (or equivalently $i'=0$, $j'=m+1$). For these values of i' and j' the statement is produced by subtracting the induced above equation $\alpha^s_m\beta^s_1-\alpha^s_1\beta^s_m=0$ from the results of differentiation of Eq. (36) where $i=m$, $j=0$ with respect to x. ■

Let $W(\varphi^1,\dots,\varphi^l)$ denotes the Wronskian of the functions $\varphi^1,\dots,\varphi^l$ with respect to the variable x, i.e., $W(\varphi^1,\dots,\varphi^l)=\det(\varphi^j_i)^l_{i,j=1}$.

Lemma 6: The solutions $\varphi^1=\varphi^1(t,x),\dots,\varphi^l=\varphi^l(t,x)$ *of a linear evolution equation* $L\varphi=0$ *are linear dependent iff* $W(\varphi^1,\dots,\varphi^l)=0$.

Proof: Since the equation $L\varphi=0$ is linear and evolution the operator L is the sum of ∂_t and linear differential operator with respect to x with the coefficients depending on t and x. If the functions $\varphi^1,\dots,\varphi^l$ are linear dependent then the equality $W(\varphi^1,\dots,\varphi^l)=0$ is obvious. Let us prove the inverse statement.

In the case $l=2$ the condition $W(\varphi^1,\varphi^2)=0$ implies $\varphi^2=C\varphi^1$, where C is a smooth function of t. Acting on the latter equality with the operator L, we obtain $C_t\varphi^1=0$, i.e., $C=\text{const}$ or $\varphi^1=0$. In any case the functions φ^1 and φ^2 are linear dependent.

Suppose $W(\varphi^1,\dots,\varphi^l)=0$. Without loss of generality we can assume $W(\varphi^1,\dots,\varphi^{l-1})\neq 0$. (Otherwise we consider a less value of l.) Then $\varphi^l=C^k\varphi^k$, where C^k are smooth functions of t and the superscript k runs from 1 to $l-1$. Action of the operator L on the latter equality results in the equation $C^k_t\varphi^k=0$ that implies, in view of the condition $W(\varphi^1,\dots,\varphi^{l-1})\neq 0$, $C^k=\text{const}$. It gives the Lemma's statement. ■

Lemma 7: If $\alpha^s_i\beta^s_j-\alpha^s_j\beta^s_i=0$ *for* $0\leqslant i<j\leqslant p$ *then* $W(\alpha^1,\dots,\alpha^p,\beta^{s'})=0$ *for any* s'.

Proof: Let $M^{s'}_{ij}$ denote the $(p-1)$th order minor of $W(\overline{\alpha},\beta^{s'})$, which is obtained by means of deletion of s'th and $(p+1)$th columns corresponding to the functions $\alpha^{s'}$ and $\beta^{s'}$ and ith and jth rows. Let us multiply the equation $\alpha^s_i\beta^s_j-\alpha^s_j\beta^s_i=0$ by $(-1)^{i+j+s'+p+1}M^{s'}_{ij}$ and convolve with respect to the indices i and j. In view of the Laplace theorem on determinant expansion we obtain $W(\overline{\alpha}|_{\alpha^s\rightsquigarrow\alpha^{s'}},\beta^s)=0$. Here the sign "$\rightsquigarrow$" means that the function α^s is substituted instead of the function $\alpha^{s'}$ and we have summation over the index s. The lemma's statement easily follows from the latter equation since for any fixed $s\neq s'$ we have $W(\overline{\alpha}|_{\alpha^s\rightsquigarrow\alpha^{s'}},\beta^s)=0$. ■

Lemma 8: The general solution of system (35) *can be presented in the form*

$$K=\alpha^sH_{v^s}+\beta^0, \tag{37}$$

where H *is an arbitrary smooth function of* $\overline{v}$, $\beta^0=\beta^0(t,x)$ *is an arbitrary solution of the backward linear heat equation.*

Proof: In view of Lemma 4 the functions α^s and $\beta^s=K_{v^s}$ satisfy the conditions of Lemma 5 and, therefore, the ones of Lemma 7, and the variables $\overline{v}$ are assumed as parameters. Since α^s are linear independent it implies $K_{v^\sigma}=C^{\sigma s}\alpha^s$, where $C^{\sigma s}$ are smooth functions of the variables $\overline{v}$ only. Hereafter the indices s, σ, and ς run from 1 to p. The expressions for the cross derivatives $K_{v^\sigma v^\varsigma}=C^{\sigma s}_{v^\varsigma}\alpha^s=C^{\varsigma s}_{v^\sigma}\alpha^s$ result in the equation $C^{\sigma s}_{v^\varsigma}=C^{\varsigma s}_{v^\sigma}$ which can be easily integrated, $C^{\sigma s}=P^s_{v^\sigma}$ for some smooth function P^s of the variables $\overline{v}$. Substituting the expressions for $C^{\sigma s}$ in the equations on K and integrating, we obtain $K=\alpha^sP^s+\beta^0$, where $\beta^0=\beta^0(t,x)$ is a solution of the backward heat equation. The latter equality and the equation $\alpha^sK_{xv^s}-\alpha^s_xK_{v^s}=0$ together imply the equation $(\alpha^\sigma_x\alpha^\varsigma-\alpha^\sigma\alpha^\varsigma_x)(P^\varsigma_{v^\sigma}-P^\sigma_{v^\varsigma})=0$. Analogously to Lemma 7 we can state for any $i,j\in\mathbb{N}$

$$(\alpha^\sigma_i\alpha^\varsigma_j-\alpha^\sigma_j\alpha^\varsigma_i)(P^\varsigma_{v^\sigma}-P^\sigma_{v^\varsigma})=0. \tag{38}$$

Let $M^{\sigma'\varsigma'}_{ij}$ denote the $(p-2)$th order minor of $W(\overline{\alpha})$, which is obtained by means of deletion of σ'th and ς'th columns corresponding to the functions $\alpha^{\sigma'}$ and $\alpha^{\varsigma'}$ and ith and jth rows. Let us multiply the Eq. (38) by $(-1)^{i+j+\sigma'+\varsigma'}M^{\sigma'\varsigma'}_{ij}$ and convolve with respect to the indices i and j. In view of the Laplace theorem on determinant expansion we obtain

$$W(\overline{\alpha}|_{\alpha^\sigma\rightsquigarrow\alpha^{\sigma'},\alpha^\varsigma\rightsquigarrow\alpha^{\varsigma'}})(P^\varsigma_{v^\sigma}-P^\sigma_{v^\varsigma})=0. \tag{39}$$

Here the sign "$\rightsquigarrow$" means that the functions α^σ and α^ς is substituted instead of the function $\alpha^{\sigma'}$ and α^ς correspondingly and we have summation over the indices σ and ς. For any fixed $\sigma\neq\sigma'$ and $\varsigma\neq\varsigma'$ we have $W(\overline{\alpha}|_{\alpha^\sigma\rightsquigarrow\alpha^{\sigma'},\alpha^\varsigma\rightsquigarrow\alpha^{\varsigma'}})=0$. Since $W(\overline{\alpha})\neq 0$ in view of linear independence of the functions α^s, Eq. (39) implies $P^{\varsigma'}_{v^{\sigma'}}-P^{\sigma'}_{v^{\varsigma'}}=0$, i.e., $P^s=H_{v^s}$ for some smooth function H of $\overline{v}$. ■

In view of Lemma 8 the conserved vector (Ku,K_xu-Ku_x) from Lemma 4 has the form $(\beta^0u+D_xH,\beta^0_xu-\beta^0u_x-D_tH)$.

The proof of Theorem 8 is completed.

IX. POTENTIAL CONSERVATION LAWS OF NONLINEAR DIFFUSION-CONVECTION EQUATIONS

More general potential conservation laws than simplest ones are admissible only if the investigated system has

(i) either more than one linear independent local conservation laws (and, therefore, we can introduce a number of different potentials for the first iteration step),

(ii) or nontrivial simplest potential conservation laws.

As shown in Sec. VII, it is possible in class (1) only for special values of the parameter functions A and B. In view of results of Sec. VII for the linearizable equations and Theorem 8, we can formulate the following statement.

Theorem 9: *For any linearizable equation from class* (1) *all potential conservation laws of the second level are equivalent on the manifold of the corresponding potential systems to potential conservation laws of the first level.*

To investigate completely the potential conservation laws of equations from class (1), it remains to study the subclasses with $B=0$ and $B=A$, equations from which have two independent local conservation laws, and the subclass $B=\int A+uA$ reduced to $B=A$ by means of potential equivalence transformations.

Theorem 10: *All potential conservation laws of any equation from class* (1) *with* $B=0$ *or* $B=A$ *are trivial on the manifold of the united potential system* (19), (20) *and united potential system* (23), (24) *constructed with pairs of independent local conservation laws.*

Proof: Consider the united system (19) and (20) [or (23) and (24)]. (Below we write down the differences of the second case with the first one in brackets.) Similarly to Lemma 3, we can assume without loss of generality that $F=F(t,x,v^1,v^2)$ and $G=G(t,x,u,v^1,v^2)$. Let us split the equation $D_tF+D_xG=0$ on the manifold determining by the united system. Integration of one from the obtained equations results in the following expression for the flux G: $G=-(QF)\int A+G^0$, where $G^0=G^0(t,x,v^1,v^2)$ and $Q=\partial_{v^1}+x\partial_{v^2}$ $(Q=\partial_{v^1}+e^x\partial_{v^2})$. The other equations form the system on the functions F and G^0,

$$Q^2F=0, \quad QG^0=0, \quad F_t+G^0_x=0, \quad (QF)_x+F_{v^2}=0 \quad [(QF)_x-F_{v^1}=0].$$

Therefore, $F=F^1v^1+F^0$, and F^1, F^0, and G^0 are functions of t, $y=x$ and $\omega=xv^1-v^2$ $(\omega=e^xv^1-v^2)$ for which $F^0_\omega=F^1_y$, $F^1_t=-G^0_\omega$, $F^0_t=-G^0_y$. The latter system implies existence of such function $H=H(t,y,\omega)$ that $F^1=H_\omega$ $(F^1=e^xH_\omega)$, $F^0=H_y$, $G^0=-H_t$. Then, $F=D_xH$, $G=-D_tH$, i.e., the conservation law is trivial. ■

As shown above, there exists the following chain of local transformations between potential systems: $1.3\leftrightarrow 1.2\leftrightarrow$ (23) and (24), i.e., system 1.3 is locally equivalent to system (23) and (24). In view of this fact and Theorem 10 we obtain the following statement.

Theorem 11: *On the manifold of the potential system 1.3 all potential conservation laws of any equation from class* (1) *with* $B=\int A+uA$ *are trivial.*

Summarizing the above results, we note that up to $G^{\sim}$-equivalence the hierarchy of conservation laws (including local ones) for diffusion-convection equations (1) has the following form:

(i) the "common" local conservation law (case 1) for arbitrary values of the parameter functions A and B;
(ii) two independent local conservation laws if $B=0$ (cases 1 and 2) or $B=A$ (cases 1 and 3);
(iii) one "common" local conservation law (case 1) and one simplest potential that (case 1.3) if $B=\int A+uA$;
(iv) the infinite series of local conservation laws (case 4) for the linear heat equation;
(v) one "common" local conservation law (case 1) and the infinite series of simplest potential conservation laws (case 1.6) for the Burgers equation;
(vi) two independent local conservation laws for the u^{-2}-diffusion equation (cases 1 and 2) and the equation $u_t=(u^{-2}u_x)_x+u^{-2}u_x$ (cases 1 and 3) as subcases of $B=0$ and $B=A$ and the infinite series of simplest potential conservation laws (cases 1.4 and 1.5) additionally.

Note 9: Above we did not consider in an explicit form action of transformations from Lie symmetry groups on conservation laws of corresponding equations or potential systems. For the majority of cases this action is quite trivial. For example, we use translations with respect to x to normalize the constant ε in case 3. In case 2 the same translations result in adding the "common" conservation law to the special one of this case.

A nonobvious connection between independent conservation laws can be established only for

$A=u^{-4/3}$, $B=0$ (case 1 and case 2) by means of the transformation $\tilde{t}=t$, $\tilde{x}=1-x^{-1}$, $\tilde{u}=x^3u$ from the Lie symmetry group of the corresponding equation. This fact was first discovered in Ref. 24 in the framework of the "operator" approach. It should be mentioned that the values $A=u^{-4/3}$, $B=0$ give rise to the equation which distinguishes from nonlinear diffusion-convection equations (1) by singular Lie symmetry properties.

The Lie symmetry group $\mathcal{G}_-$ of the linear heat equation contains infinite dimensional normal subgroup $\mathcal{G}_-^0$ formed by the linear superposition transformations $\tilde{u}=u+f(t,x)$, where $f=f(t,x)$ is an arbitrary solution of the same equation. Up to the equivalence relation, transformations from $\mathcal{G}_-^0$ act identically on the set of conservation laws of case 4. Action of the finite dimensional factor group $\mathcal{G}_-/\mathcal{G}_-^0$ on this set induces the analogous factor group $\mathcal{G}_+/\mathcal{G}_+^0$ on the set of solutions of the backward linear heat equation, which is varied over by the parameter-function α.

The hierarchy of conservation laws generates the complete set of locally inequivalent potential systems for the class under consideration:

(i) "common" potential system (18) (case 1);
(ii) additional simplest potential systems (20) (case 2) or (24) (case 3) if $B=0$ or $B=A$ correspondingly;
(iii) second level potential systems (21) (case 1.1) and (25) (case 1.2) (which are really equivalent to the united potential systems of the first level) if $B=0$ or $B=A$ correspondingly;
(iv) system (34) with arbitrary number of locally independent potentials for the linear heat equation.

Potential symmetries arising for equations (1) from cases 1 and 1.1 of Table I were studied by Sophocleous.[37] Complete investigation of the potential system (18) (case 1) with the symmetry point of view was carried out in Ref. 35.

X. CONCLUSION

The notions and methods proposed in the paper are simple and effective tools for investigation of both local and pure potential conservation laws. They can be applied to a wide range of physically interesting systems of differential equations. At the same time, there exist a number of unresolved problems, in particular, on determining the number of necessary iterations for construction of an exhaustive list of independent potential conservation laws or on connections of our framework with Wahlquist–Estabrook prolongation structures.[43] We hope to consider these problems in the near future.

The adduced results for diffusion-convection equations can be developed and generalized in a number of directions. So, studying different kinds of symmetries (Lie, nonclassical, generalized ones) of constructed potential systems, we may obtain the corresponding kinds of potential symmetries (usual potential, nonclassical potential, generalized potential ones). Let us note that investigation of generalized symmetries is natural for potential systems, since potentials introduced with equivalent conservation laws are related, in general, via transformations depending on derivatives of local dependent variables. Analogously, local equivalence transformations between potential systems constructed for different initial equations result in nonlocal (potential) equivalence transformations for the class under consideration. In such way it is possible to find new connections between well-studied diffusion-convection equations.[35] We believe that the same approach can be used for investigation of wider classes of differential equations, e.g., variable coefficient diffusion-convection equations. We also plan to study conservation laws of more general structure (e.g., ones with pseudopotentials).

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The spectral action for Moyal planes

Victor Gayral[a),b)] and Bruno Iochum[a),c)]
Centre de Physique Théorique, CNRS-Luminy, Case 907, 13288 Marseille Cedex 9, France[d)]

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Extending a result of Vassilevich, we obtain the asymptotic expansion for the trace of a spatially regularized heat operator $L^{\Theta}(f)e^{-t\Delta^{\Theta}}$, where Δ^{Θ} is a generalized Laplacian defined with Moyal products and $L^{\Theta}(f)$ is Moyal left multiplication. The Moyal planes corresponding to any skewsymmetric matrix Θ being spectral triples, the spectral action introduced in noncommutative geometry by Chamseddine and Connes is computed. This result generalizes the Connes–Lott action previously computed by Gayral for symplectic Θ. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1855401]

I. INTRODUCTION

Since few years, the interest in noncommutative field theory has been renewed in many works. The noncommutative space is quite often of Moyal type, involving either noncommutative tori or Moyal planes (see Refs. 19 and 33 for recent reviews).

Historically, Moyal[39] has tried to build quantum mechanics with a statistical point of view using a phase space approach. Actually, his idea was that the formalism of quantum theory allows to derive the phase space distributions $F(p,q)$ when a theory of functions of noncommuting observables is specified conversely. This type of consideration was initiated by Wigner[54] with a formula for $F(p,q)$ using Fourier transform and for canonical conjugate coordinates and momenta by Weyl[52] with group theoretical motivations. A noncommutative star product was previously explicitly given by Groenewold.[29] In fact, the use of quantification by deformation[1,42] has been intensively investigated since it yields a continuous path between classical and quantum mechanics. In the meantime, the Weyl–Wigner quantification process was also interesting for the pseudodifferential operators theory.[22] The Seiberg–Witten[44] map allows to go from ordinary to noncommutative gauge field theory and the replacement of the ordinary commutative product of functions by the Moyal noncommutative one is now ubiquitous in string theory where the effective low energy theory of D-branes with B-field background lives in a noncommutative space.

The mathematical background of these different developments for quantization within noncommutative geometry[8,9,28,48] where noncommutative tori[7,41] play an important role,[12] includes the construction of new spectral triples,[3,13,14,16,24] and more generally the theory of pseudodifferential operators,[18,45] the construction of star product,[26,34] integrable systems, etc. For reviews on these topics, see Refs. 9, 28, 35, 37, and 38.

It has been proposed for a long time[46,55] that the noncommutative space–time is a quantum effect of gravity and that this could provide some hints for the regularization of quantum field theory. Naturally, many types of action have been proposed and here we choose the spectral action introduced by Chamseddine and Connes[5,6] in a proper noncommutative geometry setting. Since a similar action was derived in Refs. 23 and 24 following a prescription by Connes and Lott,[15] it is

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[a)]Also at Université de Provence.
[b)]Electronic mail: gayral@cpt.univ-mrs.fr
[c)]Electronic mail: iochum@cpt.univ-mrs.fr
[d)]UMR 6207, Unité Mixte de Recherche du CNRS et des Universités Aix-Marseille I, Aix-Marseille II et de l'Université du Sud Toulon-Var, Laboratoire affilié à la FRUMAM—FR 2291.

interesting to quote the differences. In Ref. 6, the idea is to recover the usual action of the standard model of particle physics from purely gravitational considerations; more precisely to define the bosonic action by $\mathrm{Tr}(\phi(\mathcal{D}^2/\Lambda^2))$ while the fermionic action is simply $\langle\psi,\mathcal{D}\psi\rangle$ where $\mathcal{D}$ is the Dirac operator, Λ is an energy scale cutoff and ϕ is a smooth positive function. So Chamseddine and Connes recovered the Einstein plus Yang–Mills and Weyl actions including of course the spin 1 bosons, but also the part induced by the Higgs fields of spin 0. The action functional computed in Refs. 23 and 24 is defined by $\mathrm{Tr}^+(F^2\mathcal{D}^{-d})$ where F is the field strength curvature of a vector potential and Tr^+ is a Dixmier trace which pins down the leading term of logarithmic divergence in the usual trace of F^2.

Here we choose for the manifold the Moyal plane $\mathbb{R}^{2m}$ with flat curvature, technically viewed as an algebra $(\mathcal{S}(\mathbb{R}^{2m}),\star_\theta)$ for the Moyal product $\star_\theta$ ($\mathcal{S}$ is the Schwartz space) and as Dirac operator, the usual one $-i(\partial_\mu+L^\Theta(\omega_\mu))\otimes\gamma^\mu$ but where the connection ω acts by Moyal left multiplication $L^\Theta(\omega)$ on the usual Hilbert space of L^2-sections of the trivial spinor bundle spinors $\mathcal{H}=L^2(\mathbb{R}^{2m})\otimes\mathbb{C}^{2^m}$. In Ref. 24, this algebra and one of its unitizations is proved to be a real spectral triple of spectral dimension $2m$. So this case completely fits the requirements and the computation of $\mathrm{Tr}(\phi(\mathcal{D}/\Lambda))$ is possible using a standard heat kernel technique. The not so surprisingly result is that one recovers the usual commutative action where all commutative products have been replaced by the Moyal ones.

Despite the fact that this computation is made here in Euclidean signature and with no real gravity, the main interest is that all the algebraic and analytical difficulties are overcome and that it is the first example of spectral action for a not almost commutative spectral triple. Since the Dirac operator has a noncompact resolvent, a spatial regularization by the multiplication of a function f in the algebra is introduced to get the tracability of $L^\Theta(f)e^{-t\Delta^\Theta}$ where Δ^Θ is the generalized Moyal Laplacian. Of course, the choice of a regularization is arbitrary and one could prefer for instance a soliton one,[36] when one wants to avoid, before the limit, the renormalization problems set in by UV/IR mixing.

After some reminders on the role of the Moyalology for spectral triples in Sec. II, we establish the main result, and then, give the important technical details on the heat kernel computation in Sec. III. Section IV is just an application to the case of Moyal planes which ends with a few remarks on the difficulties with nonflat cases.

II. MOYAL SPECTRAL TRIPLES AND SPECTRAL ACTION

A. Moyal analysis

In this section, the very basic tools on Moyal analysis are recalled and we refer to Ref. 24 for a review. The Moyal product comes from the phase space formulation of flat quantum mechanics, that is a deformation of the associative algebra structure of a suitable family of functions on $\mathbb{R}^{2m}$ with pointwise product in the direction of the flat Poisson bracket $\{.,.\}_P$. More precisely, if we denote by W the Weyl map which assigns Schwartz functions on $\mathbb{R}^{2m}$ say, to bounded operators on $L^2(\mathbb{R}^m)$, the Moyal product $\star_\theta$ is constructed in order to obtain a $*$-algebra homomorphism

$$W:\mathcal{S}(\mathbb{R}^{2m})\to\mathcal{L}(L^2(\mathbb{R}^m)),\quad W(f\star_\theta g)=W(f)W(g).$$

This leads us to

$$(f\star_\theta g)(x):=(\pi\theta)^{-2m}\int\int_{\mathbb{R}^{2m}\times\mathbb{R}^{2m}} f(y)g(z)e^{(2i/\theta)(x-y)\cdot S(x-z)}d^{2m}yd^{2m}z, \tag{1}$$

where

$$S := \begin{pmatrix} 0 & 1_m \\ -1_m & 0 \end{pmatrix}$$

comes from the canonical symplectic structure of $\mathbb{R}^{2m} = T^*\mathbb{R}^m$ and $\theta \in \mathbb{R}_+^*$ is the deformation parameter.

Actually, one can define Moyal products on $\mathcal{S}(\mathbb{R}^n)$, n even or odd, independently of any symplectic structure. In those cases, it is any real skewsymmetric matrix Θ which defines the deformation directions. Generic Moyal products are then defined by

$$(f \star_\Theta g)(x) := (2\pi)^{-n} \int_{\mathbb{R}^n \times \mathbb{R}^n} e^{i\xi(x-y)} f\left(x - \tfrac{1}{2}\Theta\xi\right) g(y) d^n y d^n \xi. \tag{2}$$

To fix notations and avoid to refer to the odd or even case, n will be an integer equal to the plane dimension and m will be the integer part of $n/2$.

This formula shows that the theory of pseudodifferential operators on $\mathbb{R}^n$ (Refs. 31 and 45) is suitable for the analysis of left and right Moyal multiplication operators $L^\Theta(f)$ and $R^\Theta(f)$ defined by $L^\Theta(f)\psi := f \star_\theta \psi$ and $\mathbb{R}^\Theta(f)\psi := \psi \star_\theta f$. In particular their symbols are

$$\sigma[L^\Theta(f)](\xi, x) = f\left(x - \tfrac{1}{2}\Theta\xi\right), \quad \sigma[R^\Theta(f)](\xi, x) = f\left(x + \tfrac{1}{2}\Theta\xi\right). \tag{3}$$

On coordinate functions x^μ, $\mu = 1, \ldots, n$, generic Moyal products formally define a generalized Heisenberg Lie algebra structure,

$$[x^\mu, x^\nu]_{\star_\Theta} = i\Theta^{\mu\nu} 1.$$

This equality can have a precise analytical meaning if we work with Moyal products on some tempered distribution spaces,[27,47] and is obvious from the asymptotic expansion of Moyal products,

$$f \star_\Theta g \sim \sum_{\alpha \in \mathbb{N}^n} \left(\frac{i}{2}\right)^{|\alpha|} \frac{1}{\alpha!} \frac{\partial f}{\partial x^\alpha} \frac{\partial g}{\partial (\Theta x)^\alpha}. \tag{4}$$

This expansion can be heuristically derived from (2) by a Taylor expansion of $\sigma[L^\Theta(f)](\xi, x)$ "near" x, for a more rigorous approach see Ref. 20. Moyal products satisfy a few useful algebraic equalities (see Ref. 24 for a review); in particular the Leibniz rule is satisfied, the integral is a faithful trace and the complex conjugation is an involution,

$$\partial^\mu (f \star_\Theta g) = \partial^\mu f \star_\Theta g + f \star_\Theta \partial^\mu g, \tag{5}$$

$$\int (f \star_\Theta g)(x) d^n x = \int f(x) g(x) d^n x, \tag{6}$$

$$(f \star_\Theta g)^* = g^* \star_\Theta f^*. \tag{7}$$

These properties allow to prove that $\mathcal{B}_\Theta := (\mathcal{S}(\mathbb{R}^n), \star_\theta)$ is an associative and involutive Fréchet algebra with a jointly continuous product.

For Θ symplectic, hence $n = 2m$, it is proved in Refs. 27 and 47 that $(L^2(\mathbb{R}^{2m}), \star_\theta)$ is an associative Banach algebra, and we have shown in Ref. 24 that $(\mathcal{D}_{L^2}(\mathbb{R}^{2m}), \star_\theta)$ is also an *-algebra with a jointly continuous product, $\mathcal{D}_{L^2}(\mathbb{R}^{2m})$ being the space of smooth functions, having all their derivatives in $L^2(\mathbb{R}^{2m})$ endowed with the Fréchet topology of L^2-convergence for all derivatives. For the nonunital spectral triple point of view (see below), one needs also to choose a unitization for these algebras. Reference 24 it is studied that unital *-algebra $(\mathcal{O}_0(\mathbb{R}^{2m}), \star_\theta)$, where $\mathcal{O}_0(\mathbb{R}^{2m})$ consists in smooth bounded functions with bounded derivatives, with the topology given by the family of seminorms $\{p_\alpha\}_{\alpha \in \mathbb{N}^{2N}}$, $p_\alpha(f) := \|\partial^\alpha f\|_\infty$.

For generic Moyal products, $(\mathcal{S}(\mathbb{R}^n),\star_\theta)$, $(\mathcal{D}_{L^2}(\mathbb{R}^n),\star_\theta)$, $(\mathcal{O}_0(\mathbb{R}^n),\star_\theta)$ are also Fréchet algebras. Actually this statement comes from the algebra structure of $\mathcal{S}(\mathbb{R}^n)$, $\mathcal{D}_{L^2}(\mathbb{R}^n)$, $\mathcal{O}_0(\mathbb{R}^n)$ with pointwise product as well as with Moyal one, and because any Moyal product splits into a symplectic Moyal product and a pointwise one denoted by a point (Ref. 42, Proposition 2.7 and Corollary 2.8): Namely, $f\star_\theta g(x)=f(x).g(x)$ when $\Theta=0$, so if the matrix Θ is decomposed as the direct sum of a symplectic one θ of dimension $2m$ and the zero matrix of dimension $n-2m$, then $(\mathcal{S}(\mathbb{R}^n),\star_\theta)\cong(\mathcal{S}(\mathbb{R}^{2m}),\star_\theta)\hat{\otimes}(\mathcal{S}(\mathbb{R}^{n-2m}),.)$. Remark in particular that $\mathcal{S}(\mathbb{R}^n)$ and $\mathcal{O}_0(\mathbb{R}^n)$ are algebras for pointwise product while for $\mathcal{D}_{L^2}(\mathbb{R}^n)$ this is a consequence of the inclusion $\mathcal{D}_{L^2}(\mathbb{R}^n)\subset\mathcal{O}_0(\mathbb{R}^n)$.[43]

A *spectral triple* $(\mathcal{A},\tilde{\mathcal{A}},\mathcal{H},\mathcal{D},J,\chi)$ (a noncommutative generalization of a Riemannian spin manifold) consists of an algebra $\mathcal{A}$, a suitable one of its unitizations $\tilde{\mathcal{A}}\supset\mathcal{A}$ (for the analog of the noncompact case) both faithfully represented by bounded operators on a separable Hilbert space $\mathcal{H}$ (the representation is denoted by π), together with an unbounded self-adjoint operator $\mathcal{D}$ such that $\pi(a)(\mathcal{D}+\lambda)^{-1}$ is a compact operator for all $a\in\mathcal{A}$ and λ in the resolvent of $\mathcal{D}$ and such that the commutators $[\mathcal{D},\pi(a)]$ for all $a\in\tilde{\mathcal{A}}$ extend to bounded operators. J and χ are, respectively, antiunitary and unitary operators with commutation relations depending on the dimension of the triple. These data must moreover fulfill a set of axioms (see Refs. 10 and 24).

It is shown in Ref. 24 that symplectic Moyal planes yield nonunital spectral triples if we choose $\mathcal{A}=(\mathcal{D}_{L^2}(\mathbb{R}^{2m}),\star_\theta)$, $\tilde{\mathcal{A}}=(\mathcal{O}_0(\mathbb{R}^{2m}),\star_\theta)$, represented by the diagonal left regular representation $\pi^\theta(f):=L^\theta(f)\otimes 1_{2^m}$ on the Hilbert space of L^2-sections of the trivial spinor bundle $\mathcal{H}=L^2(\mathbb{R}^{2m})\otimes\mathbb{C}^{2^N}$, and for $\mathcal{D}$, the flat Dirac operator $\not{\partial}:=-i\partial_\mu\otimes\gamma^\mu$ where γ^μ are the Clifford matrices associated to $(\mathbb{R}^{2m},\eta)$ with η the standard Euclidean metric of $\mathbb{R}^{2m}$.

B. Main result

The *action functional* or Connes–Lott action[15] associated with this spectral triple gives the noncommutative Yang–Mills action for symplectic Moyal products,

$$\mathrm{YM}(\alpha)=c\int F^{\mu\nu}\star_\theta F_{\mu\nu}d^{2m}x, \tag{8}$$

where α is a universal represented connection,

$$\alpha\in\tilde{\pi}^\theta(\{a_0\delta a_1:a_0,a_1\in\mathcal{B}_\theta\})=\{\pi^\theta(a_0)[\not{\partial},\pi^\theta(a_1)]:a_0,a_1\in\mathcal{B}_\theta\},$$

and F is its curvature, $F^{\mu\nu}=\partial^\mu A^\nu-\partial^\nu A^\mu+[A^\mu,A^\nu]_{\star_\theta}$ and A^μ being defined by $\alpha=L^\theta(A_\mu)\otimes\gamma^\mu$. This result comes from the Junk computation[23] and the following result.[24]

Theorem 2.1: *For $f\in\mathcal{S}(\mathbb{R}^{2m})$, the compact operator $\pi^\theta(f)(\not{D}^2+\varepsilon^2)^{-m}$ lies in $\mathcal{L}^{(1,\infty)}(\mathcal{H})$ and any of its Dixmier traces Tr_ω is independent of the positive number ε. More precisely we have,*

$$\mathrm{Tr}_\omega(\pi^\theta(f)(\not{D}^2+\varepsilon^2)^{-m})=\frac{2^m\Omega_{2m}}{2m(2\pi)^{2m}}\int f(x)d^{2m}x, \tag{9}$$

where $\mathcal{L}^{(1,\infty)}(\mathcal{H})$ is the ideal of compact operators whose kth singular values satisfy $\mu_k(T)=O(k^{-1})$ and Ω_{2m} is the hyper-area of the unit sphere in $\mathbb{R}^{2m}$.

For generic Moyal products, $[(\mathcal{D}_{L^2}(\mathbb{R}^n),\star_\theta),(\mathcal{O}_0(\mathbb{R}^n),\star_\theta),L^2(\mathbb{R}^n)\otimes\mathbb{C}^{2^m},\not{\partial}]$ yields also a nonunital spectral triple, but the Connes–Lott action computation is not obvious because the computation of (8) was basis dependent.

Let Δ^Θ be a *noncommutative generalized Laplacian* associated with Moyal products,

$$\Delta^\Theta:=-(\eta^{\mu\nu}(\partial_\mu+L^\Theta(\omega_\mu))(\partial_\nu+L^\Theta(\omega_\nu))+L^\Theta(E))\otimes 1_{2^m},$$

$$\Delta^{\Theta} =: \Delta_r^{\Theta} \otimes 1_{2^m} \tag{10}$$

acting on the Hilbert space $\mathcal{H}=L^2(\mathbb{R}^n)\otimes\mathbb{C}^{2^m}:=\mathcal{H}_r\otimes\mathbb{C}^{2^m}$, where $\omega_\mu^*=-\omega_\mu$ and E are in $\mathcal{O}_0(\mathbb{R}^n)$. From now on, let $\mathcal{B}_\Theta:=(\mathcal{S}(\mathbb{R}^n),\star_\theta)$ acting on $\mathcal{H}$ by the diagonal left regular representation $\pi^\Theta(.):=L^\Theta(.)\otimes 1_{2^m}$.

For $f\in\mathcal{B}_\Theta$, $L^\Theta(f)e^{-t\Delta^\Theta}$ will be called *spatially regularized heat operator* associated with the generalized Laplacian Δ^Θ.

The following is the main result.

Theorem 2.2: *Let* Δ^θ *be as in* (10) *and* $f\in\mathcal{B}_\Theta$. *Then* $\mathrm{Tr}(\pi^\Theta(f)e^{-t\Delta^\Theta})$ *has an asymptotic expansion*

$$\mathrm{Tr}(\pi^\Theta(f)e^{-t\Delta^\Theta}) \underset{t\to 0}{\sim} 2^m\left(\frac{1}{4\pi t}\right)^{n/2}\sum_{l\in\mathbb{N}} t^l\int_{\mathbb{R}^n} f(x)\tilde{a}_{2l}(x)d^nx, \tag{11}$$

where

$$\tilde{a}_0(x)=1,$$

$$\tilde{a}_2(x)=E(x),$$

$$\tilde{a}_4(x)=\tfrac{1}{2}E\star_\Theta E(x)+\tfrac{1}{6}\eta^{\mu\nu}E_{;\mu\nu}(x)+\tfrac{1}{12}\Omega^{\mu\nu}\star_\Theta\Omega_{\mu\nu}(x),$$

$$\begin{aligned}\tilde{a}_6(x)=&\tfrac{1}{6}E\star_\Theta E\star_\Theta E(x)+\tfrac{1}{12}\eta^{\mu\nu}E_{;\mu}\star_\Theta E_{;\nu}(x)+\tfrac{1}{6}\eta^{\mu\nu}E\star_\Theta E_{;\mu\nu}(x)+\tfrac{1}{60}\eta^{\mu\nu}\eta^{\rho\sigma}E_{;\mu\nu\rho\sigma}(x)\\&+\tfrac{1}{12}E\star_\Theta\Omega^{\mu\nu}\star_\Theta\Omega_{\mu\nu}(x)+\tfrac{1}{45}\eta^{\rho\sigma}\Omega^{\mu\nu}_{;\rho}\star_\Theta\Omega_{\mu\nu;\sigma}(x)+\tfrac{1}{180}\eta^{\rho\sigma}\Omega^{\mu\nu}_{;\nu}\star_\Theta\Omega_{\mu\rho;\sigma}(x)\\&+\tfrac{1}{30}\eta^{\rho\sigma}\Omega^{\mu\nu}\star_\Theta\Omega_{\mu\nu;\rho\sigma}-\tfrac{1}{30}\Omega^{\mu\nu}\star_\Theta\Omega_{\nu\rho}\star_\Theta\Omega^\rho_\mu(x),\end{aligned}$$

where $g_{;\mu}:=\partial_\mu g+[\omega_\mu,g]_{\star_\theta}$ *and* $\Omega_{\mu\nu}:=\partial_\mu\omega_\nu-\partial_\nu\omega_\mu+[\omega_\mu,\omega_\nu]_{\star_\theta}$ *is the curvature of the connection* ω.

III. HEAT KERNEL EXPANSION FOR MOYAL GENERALIZED LAPLACIANS

We will first discuss the heat kernel expansion for Laplace type operators associated with Moyal products, for NC planes as well as for NC tori. This section generalizes Vassilevich's result[50] in two directions: first the Moyal products are defined by their integral form as opposed to differential or formal Moyal products (4) and second they are taken over the whole plane $\mathbb{R}^n$ and not only on NC tori. This noncompact situation generates some analytical difficulties.

We use the standard one-parameter semigroup theory of e^{-tA} where A is a positive (unbounded) operator and $t\in\mathbb{R}^+$. Let $\mathcal{H}$ be a separable Hilbert space. We denote by $\mathcal{B}(\mathcal{H})$ the set of bounded operators on $\mathcal{H}$, by $\mathcal{K}(\mathcal{H})$ the compact one's and by $\mathcal{L}^p(\mathcal{H})$ the pth Schatten class.

If we assume that A is a non-negative self-adjoint operator on $\mathcal{H}$, then e^{-zA} is holomorphic for $\Re(z)>0$ and $\|e^{-zA}\|\leqslant 1$ (Ref. 32, Example 1.25, p. 493).[56] With $\mathcal{R}_A(z):=(z-A)^{-1}$ denoting the resolvent of A, one can use the holomorphic functional calculus,

$$e^{-tA}=\frac{1}{2i\pi}\int_\Gamma e^{-tz}\mathcal{R}_A(z)\mathrm{d}z, \tag{12}$$

where Γ is a positively oriented (possibly infinite) closed curve containing the spectrum of A.

Lemma 3.1: Let B be a bounded operator and A be a non-negative densely defined generator of a holomorphic semigroup such that $B\mathcal{R}_A(z)^l\in\mathcal{L}^1(\mathcal{H})$ *for some* $z\notin\mathrm{Spect}(A)$. *Then for* $t>0$, Be^{-tA} *is trace-class*.

Proof: For some $z_0\notin\mathrm{Spect}(A)$, the semigroup property together with the first resolvent equation and (12) gives

$$Be^{-tA} = B(e^{-(t/l)A})^l = B\mathcal{R}_A(z_0)^l\left(\frac{1}{2i\pi}\int_\Gamma e^{-(t/l)z}(1+(z-z_0)\mathbb{R}_A(z))\mathrm{d}z\right)^l.$$

This concludes the proof because $\|\mathcal{R}_A(z)\| \leqslant M/|z|$ for all z with $\Re(z)>0$, thus

$$\int_\Gamma e^{-(t/l)\Re(z)}(1+|z-z_0|\|\mathcal{R}_A(z)\|)|\mathrm{d}z| < \infty.$$

■

Since we are interested in the small t-asymptotic expansion of $\mathrm{Tr}(Be^{-tA})$, recall the following definition.

Let $\{f_n\}_n$ be a sequence of functions such that $f_n(t)\neq 0$ for $t\neq 0$ and $f_{n+1}(t)=o(f_n(t))$ as $t\to 0$. A function f has the *asymptotic expansion* $f(t)\sim_{t\to 0}\Sigma_{n=0}^{\infty}a_n f_n(t)$, when for each $k\in\mathbb{N}$, $f(t)=\Sigma_{n=0}^{k}a_n f_n(t)+O(f_{k+1}(t))$ as $t\to 0$.

A. Heat kernel expansion for Moyal planes

We will first show that $L^\Theta(f)e^{-t\Delta_r^\Theta}$ is trace-class for $t\in\mathbb{R}_+^*$, then we will show that its trace has a small t-asymptotic expansion:

$$\mathrm{Tr}(L^\Theta(f)e^{-t\Delta_r^\Theta})\sim_{t\to 0}\left(\frac{1}{4\pi t}\right)^{n/2}\sum_{l\in\mathbb{N}}t^l\int_{\mathbb{R}^n}f(x)\tilde{a}_{2l}(x)d^nx,$$

where the local invariants $\tilde{a}_l$ are built from the universal (represented) connection ω_μ, the (non-local) endomorphism E and their covariant derivative (in the adjoint representation) $\partial_\mu+L^\Theta(\omega_\mu)-R^\Theta(\omega_\mu)$.

We will prove that $L^\Theta(f)e^{-t\Delta_r^\Theta}$ is trace-class by two approaches. The first uses semigroup theory results while the second will be based on pseudodifferential operator (ΨDO) techniques, which is more in the spirit of Ref. 24.

Theorem 3.2: *Let $f\in\mathcal{S}(\mathbb{R}^n)$, ω_μ, $E\in\mathcal{O}_0(\mathbb{R}^n)$ with $\omega_\mu^*=-\omega_\mu$ and $E=-g^*\star_\theta g$ for some $g\in\mathcal{O}_0(\mathbb{R}^n)$. Then, for all $t>0$ the spatially regularized heat operator associated with Δ^Θ defined in* (10) *is trace-class.*

First proof of Theorem 3.2: Because $(L^\Theta(g))^*=L^\Theta(g^*)$, $\Im(g)=0$ implies $L^\Theta(g)$ is self-adjoint, so Δ^Θ is positive. Thanks to Lemma 3.1, it is enough to prove that $L^\Theta(f)R_{\Delta_r^\Theta}(z)^l$ is trace-class for $l>n/2$.

Let us anticipate further notations to see that Δ^Θ is a squared covariant Dirac operator:

$$\Delta^\Theta = \not{\partial}_\omega^2 - B,$$

$$\not{\partial}_\omega := -i(\partial_\mu + L^\Theta(\omega_\mu))\otimes\gamma^\mu,$$

and $B := L^\Theta(E)\otimes 1_{2^m} - L^\Theta(\partial_\mu(\omega_\nu)-\omega_\mu\star_\theta\omega_\nu)\otimes(\eta^{\mu\nu}1_{2^m}-\gamma^\nu\gamma^\mu)$ is bounded.

Assume first that $l=1$, $z=-1$, $B=0$. Using the notations $\pi^\Theta(\omega):=L^\Theta(\omega_\mu)\otimes\gamma^\mu$, $\pi^\Theta(\not{\partial}(f)) := L^\Theta(\partial_\mu f)\otimes\gamma^\mu$ and the fact that all $f\in\mathcal{S}(\mathbb{R}^n)$ factorizes as $f=f_1\star_\theta f_2$, for some $f_1, f_2\in\mathcal{S}(\mathbb{R}^n)$ (Ref. 24, Proposition 2.7), one gets

$$\begin{aligned}\pi^\Theta(f)\mathcal{R}_{\Delta^\Theta}(-1) &= -\pi^\Theta(f)\frac{1}{\not{\partial}-i}\left(1-\pi^\Theta(\omega)\frac{1}{\not{\partial}_\omega-i}\right)\frac{1}{\not{\partial}_\omega+i}\\ &= -\pi^\Theta(f_1)\frac{1}{\not{\partial}-i}\pi^\Theta(f_2)\left(1-\pi^\Theta(\omega)\frac{1}{\not{\partial}_\omega-i}\right)\frac{1}{\not{\partial}_\omega+i}\\ &\quad -\pi^\Theta(f_1)\frac{1}{\not{\partial}-i}\pi^\Theta(\not{\partial}(f_2))\frac{1}{\not{\partial}-i}\left(1-\pi^\Theta(\omega)\frac{1}{\not{\partial}_\omega-i}\right)\frac{1}{\not{\partial}_\omega+i}\end{aligned}$$

$$= -\pi^{\Theta}(f_1)\frac{1}{\not\partial - i}\pi^{\Theta}(f_2)\frac{1}{\not\partial + i}\left(1 - \pi^{\Theta}(\omega)\frac{1}{\not\partial_{\omega} + i}\right)$$
$$+ \pi^{\Theta}(f_1)\frac{1}{\not\partial - i}\pi^{\Theta}\ (f_2)\star_{\Theta}\omega)\frac{1}{\not\partial - i}\left(1 - \pi^{\Theta}(\omega)\frac{1}{\not\partial_{\omega} - i}\right)\frac{1}{\not\partial_{\omega} + i}$$
$$- \pi^{\Theta}(f_1)\frac{1}{\not\partial - i}\pi^{\Theta}(\not\partial(f_2)\star_{\Theta}\omega)\frac{1}{\not\partial - i}\left(1 - \pi^{\Theta}(\omega)\frac{1}{\not\partial_{\omega} - i}\right)\frac{1}{\not\partial_{\omega} + i}.$$

By (Ref. 24, Lemmata 4.5 and 4.14), $\pi^{\Theta}(g)\mathcal{R}_{\not\partial}(i)\pi^{\Theta}(h)\mathcal{R}_{\not\partial}(i) \in \mathcal{L}^p(\mathcal{H})$ whenever $g, h \in \mathcal{S}(\mathbb{R}^n)$ and $p > n/2$. The boundness of $\pi^{\Theta}(\omega)$ and $\mathcal{R}_{\not\partial_{\omega}}(z)$ then yields $\pi^{\Theta}(f)\mathcal{R}_{\Delta^{\Theta}}(-1) \in \mathcal{L}^p(\mathcal{H})$ for the same p. For $l \geqslant 1$, repeat this algorithm using $(A+C)^{-1} = A^{-1}(1 - CA^{-1}(\cdots(1 - C(A+C)^{-1})\cdots))$ up to order l.

The case with nonzero B is obtained using the same trick,

$$\pi^{\Theta}(f)\mathcal{R}_{\Delta^{\Theta}}(-1) = \pi^{\Theta}(f)\mathcal{R}_{\not\partial^2_{\omega}}(-1)(1 - B\mathcal{R}_{\Delta^{\Theta}}(-1)).$$

The first resolvent equation implies the same result for any z instead of -1 in the resolvent set of $\mathrm{Spect}(\Delta^{\Theta})$. ■

The second proof, which is based on a functional calculus for ΨDO,[18] needs the following definition of ΨDO classes relevant for Moyal analysis (Shubin[45] or GLS[30] symbol classes).

Definition 3.3: Let $S^{\rho,\lambda}$ be the Shubin or GLS symbol class

$$S^{\rho,\lambda} := \{\sigma \in \mathcal{C}^{\infty}(\mathbb{R}^{2n}) : \forall\ \alpha, \beta \in \mathbb{N}^n,\ \exists\ C_{\alpha\beta} \in \mathbb{R}^+ | \partial_x^{\alpha}\partial_{\xi}^{\beta}\sigma(\xi, x)|,$$

$$\leqslant C_{\alpha,\beta}(1 + |x|^2)^{(\rho - |\alpha|)/2}(1 + |\xi|^2)^{(\lambda - |\beta|)/2}$$

and let $\Psi^{\rho,\lambda} := \{A \in \Psi\mathrm{DO} : \sigma[A] \in S^{\rho,\lambda}\}$ be the associated ΨDO class.

Actually, $S^{\rho,\lambda}$ fits into the general Hörmander symbol classes (see Ref. 31, Chap. XVIII) $S(m, g)$ with order function $m(\xi, x) = (1 + |x|^2)^{\rho/2}(1 + |\xi|^2)^{\lambda/2}$ and slowly varying metric $g_{\xi,x} = (1 + |\xi|^2)^{-1}|\mathrm{d}\xi|^2 + (1 + |x|^2)^{-1}|\mathrm{d}x|^2$.

Second proof of Theorem 3.2: First, Eq. (3) and the product formula for ΨDOs allows us to compute the symbol of Δ_r^{θ},

$$\sigma[\Delta_r^{\theta}](\xi, x) = \eta^{\mu\nu}\xi_{\mu}\xi_{\nu} + 2i\omega_{\mu}\left(x - \tfrac{1}{2}\Theta\xi\right)\xi_{\nu} - \partial_{\mu}\omega_{\nu}\left(x - \tfrac{1}{2}\Theta\xi\right) - \omega_{\nu}\star_{\Theta}\omega_{\nu}\left(x - \tfrac{1}{2}\Theta\xi\right) - E\left(x - \tfrac{1}{2}\Theta\xi\right),$$

and because $\omega_{\mu}, E \in \mathcal{O}_0(\mathbb{R}^n)$, Δ_r^{θ} lies in $\Psi^{0,2}$.

Let $\{f_N\}_{N\in\mathbb{N}}$ be the family of smooth compactly supported functions defined by $f_N(x) := \chi_N(x)e^{-x}$, where $0 \leqslant \chi_N \leqslant 1$, $\chi_N \in \mathcal{C}_c^{\infty}(\mathbb{R})$ with $\chi_N(x) = 0$ for $x \in]-\infty, -\epsilon] \cup [N, +\infty[$ for a fixed $\epsilon > 0$ and $\chi_N(x) = 1$ for $x \in [0, N - \epsilon]$. First, Ref. 18, Theorem 8.7 yields $f_N(t\Delta_r^{\theta}) \in \Psi^{0,-\infty}$, and basic estimates (see Ref. 24, Sec. 2.4 for details) gives $L^{\Theta}(f) \in \Psi^{-\infty,0}$ for all $f \in \mathcal{S}(\mathbb{R}^n)$. Then, by Ref. 31 Lemma 18.4.3 one obtains $L^{\Theta}(f)f_N(t\Delta_r^{\Theta}) \in \Psi^{-\infty,-\infty}$ and its symbol is in $\mathcal{S}(\mathbb{R}^{2n})$. Therefore,

$$C := \sum_{|\alpha|+|\beta|\leqslant 2n+1} \|\partial_x^{\alpha}\partial_{\xi}^{\beta}\sigma[L^{\Theta}(f)f_N(t\Delta_r^{\Theta})]\|_1$$

$$\leqslant \sum_{|\alpha|+|\beta|\leqslant 2n+1} C_{\alpha,\beta}\int (1 + |x|^2)^{(-l-|\alpha|)/2}(1 + |\xi|^2)^{(-k-|\beta|)/2} d^n x d^n \xi,$$

for some $C_{\alpha,\beta} < \infty$ and all $l, k \in \mathbb{N}$, hence $C < \infty$. Finally, Ref. 18, Theorem 9.4 shows $L^{\Theta}(f)f_N(t\Delta_r^{\Theta})$ is trace-class for all $N \in \mathbb{N}$. Looking at the estimates in the proof of Ref. 18, Theorem 8.7, one can find constants $C_{\alpha,\beta}$ independent of N (because e^{-x} is rapidly decreasing when $x \to +\infty$, the right support of f_N plays no role), therefore one obtains that $L^{\Theta}(f)f_N(t\Delta_r^{\Theta})$ is trace-class uniformly in N.

To finish the proof, it remains to show that s-lim $L^{\Theta}(f)f_N(t\Delta_r^{\Theta}) = L^{\Theta}(f)e^{-t\Delta_r^{\Theta}}$, because Ref. 17, Proposition 2 will ensure that $L^{\Theta}(f)e^{-t\Delta_r^{\Theta}}$ is trace-class for all $t > 0$.

Let $\phi \in \mathcal{H}$ and E_λ be the spectral family of Δ_r^Θ, then

$$\|(\chi_N(\Delta_r^\Theta)-1)\phi\|_2^2 = \langle\phi|(\chi_N(\Delta_r^\Theta)-1)^2\phi\rangle$$
$$= \int_{\mathrm{Spect}(\Delta_r^\Theta)} (\chi_N(\lambda)-1)^2 d\langle\phi|E_\lambda\phi\rangle \leqslant \int_{\mathrm{Spect}(\Delta_r^\theta)} d\langle\phi|E_\lambda\phi\rangle = \langle\phi|\phi\rangle.$$

Hence by dominated convergence and with $\phi = e^{-t\Delta_r^\Theta}\psi$,

$$\lim_{N\to\infty}\|(\chi_N(\Delta_r^\Theta)-1)e^{-t\Delta_r^\Theta}\psi\|_2^2 = \lim_{N\to\infty}\int_{\mathrm{Spect}(\Delta_r^\Theta)} (\chi_N(\lambda)-1)^2 d\langle e^{-t\Delta_r^\Theta}\psi, E_\lambda e^{-t\Delta_r^\Theta}\psi\rangle$$
$$= \int_{\mathrm{Spect}(\Delta_r^\theta)} \lim_{N\to\infty}(\chi_N(\lambda)-1)^2 d\langle e^{-t\Delta_r^\Theta}\psi, E_\lambda e^{-t\Delta_r^\Theta}\psi\rangle = 0,$$

where the last equality comes from $\mathrm{Spect}(\Delta_r^\Theta)\subset\mathbb{R}^+$. ∎

We now come to the computation of the exponential of Δ^Θ following a Vassilevich's idea.[50]

Proof of Theorem 2.2: Let

$$X := 2L^\Theta(\omega_\mu)\partial^\mu + L^\Theta(\partial_\mu\omega^\mu) + L^\Theta(\omega_\mu \star_\Theta \omega^\mu) + L^\Theta(E)$$

$$Y := -\partial_\mu\partial^\mu,$$

so $\Delta_r^\Theta = Y - X$ and the Baker–Campbell–Hausdorff (BCH) formula

$$e^T e^S = e^{T+S+1/2[T,S]+1/12[T,[T,S]]+1/12[S,[S,T]]-1/48[T,[S,[T,S]]]+\cdots},$$

allows to write

$$e^{-t\Delta_r^\Theta} = e^{tX+1/2t^2[X,Y]+1/12t^3[X,[X,Y]]-1/6t^3[Y,[X,Y]]-1/48t^4[X,[Y,[X,Y]]]+1/48t^4[Y,[Y,[X,Y]]]+\cdots}e^{-tY}.$$

In order to obtain a power expansion when t goes to zero, the strategy is to expand the first exponential, to compute the commutators, to reorganize the sequence and finally to write down the explicit symbol of those ΨDO's. The trace will be simply taken by integrating them with respect to $(\xi,x)\in\mathbb{R}^{2n}$. Actually, the reorganization in homogeneous terms in powers of t is slightly more elaborate than a simple exponential expansion. All the operators coming from this expansion are of the type $L^\Theta(g)\partial^\alpha$, $\alpha\in\mathbb{N}^n$, for some $g\in\mathcal{B}_\Theta$. Some terms will give no contributions to the trace since $\int\xi_1^{\alpha_1}\cdots\xi_n^{\alpha_n}e^{-t|\xi|^2}d^n\xi = \Pi_i^n\frac{1}{2}(1+(-1)^{\alpha_i})\Gamma[(n+1)/2]t^{-(\alpha_i+1)/2}$ is zero when at least one of the α_i is odd, and when they are all even, $|\alpha| = \Sigma_i^n\alpha_i = 2l$ is even and we get

$$\int_{\mathbb{R}^n}\xi_{\mu_1}\cdots\xi_{\mu_{2l}}e^{-t|\xi|^2}d^n\xi = \left(\frac{\pi}{t}\right)^{n/2}(2t)^{-l}\sum_{\sigma\in S_{2l}}\frac{1}{2^l l!}\delta_{\sigma(\mu_1)\sigma(\mu_2)}\cdots\delta_{\sigma(\mu_{2l-1})\sigma(\mu_{2l})},$$

where σ runs over the permutation group S_{2l} of $2l$ elements. So, in the reorganization of the power series, we must keep in mind that $t^l L^\Theta(g)\partial^\alpha$ is effectively a term of order $t^{l-|\alpha|/2}$ [independently of the $(\pi/t)^{n/2}$ term]. Moreover, to obtain the asymptotic expansion up to order l say, we must use the BCH formula up to order $2l-1$. The order of the BCH formula is defined as the number of commutators in the expansion. The term with higher degree derivatives coming from the BCH formula at order l is

$$[t\partial^2,[t\partial^2,\ldots,[t\partial^2,tL^\Theta(g)\partial]\cdots]] \propto t^{l+1}L^\Theta(h)\partial^{l+1},$$

for some $h\in\mathcal{B}_\Theta$, which yields a term of order $t^{(l+1)/2}$.

Let us show how it works up to order one. We must use the BCH formula up to order one also, $e^{-t\Delta_r^\Theta} = e^{tX-tY} = e^{tX+\frac{1}{2}[tX,tY]+\cdots}e^{-tY}$, and

$$
\begin{aligned}
[tX,tY] &= t^2[\partial_\nu\partial^\nu, 2L^\Theta(\omega_\mu)\partial^\mu + L^\Theta(\partial_\mu\omega^\mu) + L^\Theta(\omega_\mu \star_\Theta \omega^\mu) + L^\Theta(E)] \\
&= t^2(2L^\Theta(\partial_\nu\partial^\nu\omega_\mu)\partial^\mu + 4L^\Theta(\partial_\nu\omega_\mu)\partial^\mu\partial^\nu + L^\Theta(\partial_\nu\partial^\nu\partial_\mu\omega^\mu) + 2L^\Theta(\partial_\nu\partial_\mu\omega^\mu)\partial^\nu \\
&\quad + L^\Theta(\partial_\nu\partial^\nu(\omega_\mu\star_\Theta\omega^\mu)) + 2L^\Theta(\partial_\nu(\omega_\mu\star_\Theta\omega^\mu))\partial^\nu + L^\Theta(\partial_\nu\partial^\nu E) + 2L^\Theta(\partial_\nu E)\partial^\nu) \\
&= 4t^2L^\Theta(\partial_\nu\omega_\mu)\partial^\mu\partial^\nu + O(t^2),
\end{aligned}
$$

hence

$$
\begin{aligned}
L^\Theta(f)e^{-t\Delta_r^\Theta} &= L^\Theta(f)e^{t(2L^\Theta(\omega_\mu)\partial^\mu + L^\Theta(\partial_\mu\omega^\mu) + L^\Theta(\omega_\mu\star_\Theta\omega^\mu) + L^\Theta(E)) + 2t^2L^\Theta(\partial_\nu\omega_\mu)\partial^\mu\partial^\nu + \cdots}e^{t\partial_\mu\partial^\mu} \\
&= L^\Theta(f)(1 + t(2L^\Theta(\omega_\mu)\partial^\mu + L^\Theta(\partial_\mu\omega^\mu) + L^\Theta(\omega_\mu\star_\Theta\omega^\mu) + L^\Theta(E)) \\
&\quad + 2t^2(L^\Theta(\partial_\nu\omega_\mu)\partial^\mu\partial^\nu + L^\Theta(\omega_\mu\star_\Theta\omega_\nu)\partial^\mu\partial^\nu) + O(t^2))e^{t\partial_\mu\partial^\mu},
\end{aligned}
$$

where the last t^2-term comes from e^{tX}. So, by (3),

$$
\begin{aligned}
\sigma[L^\Theta(f)e^{-t\Delta_r^\Theta}](\xi,x) &= \Big(f\Big(x-\tfrac{1}{2}\Theta\xi\Big) + t\Big(2f\star_\Theta\omega_\mu\Big(x-\tfrac{1}{2}\Theta\xi\Big)(-i\xi)^\mu + f\star_\Theta\partial_\mu\omega^\mu\Big(x-\tfrac{1}{2}\Theta\xi\Big) \\
&\quad + f\star_\Theta\omega_\mu\star_\Theta\omega^\mu\Big(x-\tfrac{1}{2}\Theta\xi\Big) + f\star_\Theta E\Big(x-\tfrac{1}{2}\Theta\xi\Big)\Big) + 2t^2\Big(f\star_\Theta\partial_\nu\omega_\mu\Big(x-\tfrac{1}{2}\Theta\xi\Big) \\
&\quad \times(-i\xi)^\mu(-i\xi)^\nu + f\star_\Theta\omega_\mu\star_\Theta\omega_\nu\Big(x-\tfrac{1}{2}\Theta\xi\Big)(-i\xi)^\mu(-i\xi)^\nu\Big) + O(t^2)\Big)e^{-t\xi_\mu\xi^\mu}.
\end{aligned}
$$

Finally, it remains to integrate $\sigma[L^\Theta(f)e^{-t\Delta_r^\Theta}](\xi,x)$. By the translation $x\to x+\frac{1}{2}\Theta\xi$, one obtains,

$$
\begin{aligned}
\mathrm{Tr}(L^\Theta(f)e^{-t\Delta_r^\Theta}) &= (2\pi)^{-n}\int\int (f(x) + t(2f\star_\Theta\omega_\mu(x)(-i\xi)^\mu + f\star_\Theta\partial_\mu\omega^\mu(x) + f\star_\Theta\omega_\mu\star_\Theta\omega^\mu(x) \\
&\quad + f\star_\Theta E(x)) + 2t^2(f\star_\Theta\partial_\nu\omega_\mu(x)(-i\xi)^\mu(-i\xi)^\nu + f\star_\Theta\omega_\mu\star_\Theta\omega_\nu(x) \\
&\quad \times(-i\xi)^\mu(-i\xi)^\nu))e^{-t\xi_\mu\xi^\mu}d^nxd^n\xi + O(t^{(n/2)+2}) \\
&= (4\pi t)^{-n/2}\int f(x)(1 + t(\partial_\mu\omega^\mu(x) + \omega_\mu\star_\Theta\omega^\mu(x) + E(x) - \partial_\mu\omega^\mu(x) \\
&\quad - \omega_\mu\star_\Theta\omega^\mu(x)))d^nx + O(t^{-(n/2)+2}) \\
&= (4\pi t)^{-n/2}\int f(x)(1 + tE(x))d^nx + O(t^{-n/2+2}).
\end{aligned}
$$

The higher order terms can be obtained by similar computations, that is to say, one generically gets

$$
L^\Theta(f)e^{-t\Delta_r^\Theta} \sim_{t\to 0} L^\Theta(f)\Bigg(\sum_{l\in\mathbb{N}} t^l \sum_{\alpha\in\mathbb{N}^n,|\alpha|\leqslant l} L^\Theta(g_{\alpha,l})t^{|\alpha|/2}\partial^\alpha\Bigg)e^{t\partial_\mu\partial^\mu},
$$

for some $g_{\alpha,l}\in\mathcal{B}_\Theta$, and where we have corrected the power series in t by the order of derivatives, with respect to the previous discussion. Here $\sim$ means asymptotic expansion with respect to the trace-norm topology,

$$
\Bigg\| L^\Theta(f)e^{-t\Delta_r^\Theta} - L^\Theta(f)\Bigg(\sum_{l\leqslant N} t^l \sum_{\alpha\in\mathbb{N}^n,|\alpha|\leqslant l} L^\Theta(g_{\alpha,l})t^{|\alpha|/2}\partial^\alpha\Bigg)e^{t\partial_\mu\partial^\mu}\Bigg\|_1 = O(t^{N+1}),
$$

convergence of the sequence being warranted by Theorem 3.2.

This concludes the proof of Theorem 2.2 since in (11) we get the coefficient $\mathrm{Tr}(1_{\mathbb{C}^{2^m}})$. ■

Remark 3.4: This systematic computation also yields that the other coefficients $\tilde{a}_{2l}$, $l>3$ have the same canonical form, that is Moyal products replace pointwise ones everywhere.

We will use this asymptotic expansion to compute the spectral action, but it can also be used to compute counterterms and anomalies in noncommutative quantum field theory [see the recent review (Ref. 51) and the quoted references].

B. Heat kernel expansion for NC tori in Moyal (re)presentation

Let $\mathcal{A}_\Theta$ be the smooth algebra of Schwartz (rapidly decreasing) linear combination of the plane waves $\{e^{ik.x}\}_{k\in\mathbb{Z}^n}$ endowed with Moyal product,

$$\mathcal{A}_\Theta = \left(\left\{\sum_{k\in\mathbb{Z}^n} c_k e^{ik.x} : (c_k) \in \mathcal{S}(\mathbb{Z}^n)\right\}, \star_\Theta\right).$$

$\mathcal{A}_\Theta$ closes to an algebra and represents the NC n-tori,

$$e^{ik.x}\star_\Theta e^{iq.x} = e^{-ik.\Theta q} e^{iq.x}\star_\Theta e^{ik.x}, \tag{13}$$

this canonical commutation relation of the NC n-tori coming from the straightforward computation (here Fourier modes are viewed as tempered distributions):

$$e^{ik.x}\star_\Theta e^{iq.x} = (2\pi)^{-n}\int\int_{\mathbb{R}^n\times\mathbb{R}^n} e^{i\xi.(x-y)} e^{ik.(x-1/2\Theta\xi)} e^{iq.y} d^n\xi d^n y = e^{-i1/2k.\Theta q} e^{i(k+q).x}.$$

One can build a unital spectral triple associated to this algebra,[11,28] with $\mathcal{H}=L^2(\mathbb{T}^n)\otimes\mathbb{C}^{2^m}$ the squared integrable sections of the trivial spinor bundle over $\mathbb{T}^n$, and $\mathcal{D}=\partial\!\!\!/$ the flat Dirac operator. $\mathcal{A}_\Theta$ is again represented on bounded operators by the left regular representation $\pi^\Theta(a)\psi = L^\Theta(a)\otimes 1_{2^m}\psi = a\star_\Theta\psi$, for $a\in\mathcal{A}_\Theta$, $\psi\in\mathcal{H}$. Actually, this construction is equivalent to the GNS representation associated to the state given by the canonical trace τ of $\mathcal{A}_\Theta$: when $a(x)=\Sigma_{k\in\mathbb{Z}^n} c_k e^{ik.x} \in \mathcal{A}_\Theta$,

$$\tau(a) := c_0 = \int_{\mathbb{T}^n} a(x) d^n x.$$

Let again Δ^Θ be the noncommutative generalized Laplacian defined in (10) acting now on $\mathcal{H} := L^2(\mathbb{T}^n)\otimes\mathbb{C}^{2^m}$, where $\omega_\mu^* = -\omega_\mu$ and $E\leqslant 0$ are in $\mathcal{A}_\Theta$.

We will first show that in the NC-tori cases, $e^{-t\Delta^\Theta}$ is trace-class for $t\in\mathbb{R}_+^*$ is a direct consequence of the compactness of $\mathcal{R}_\Delta^\Theta(z) := (\Delta^\Theta - z)^{-1}$. Then, thanks to the preceding section, it will be straightforward to show that its trace has a small-t asymptotic expansion (11) where the local invariants $\tilde{a}_l$ are the same as in the Moyal plane case, but with $f=1$.

Theorem 3.5: *Let Δ^Θ be as in (10), then $e^{-t\Delta^\Theta}$ is trace-class for all $t\in\mathbb{R}_+^*$.*

Proof: The proof is simpler than for the Moyal plane. Clearly, $\mathcal{R}_\theta(z)\in\mathcal{L}^p(\mathcal{H})$, $p>n$, and so $\mathcal{R}_{\Delta\Theta}(z)\in\mathcal{L}^{p/2}(\mathcal{H})$ (use the same trick as in the proof of Theorem 3.2). Then Theorem 3.1 yields $e^{-t\Delta^\Theta} = (e^{-t(2/p)\Delta^\Theta})^{p/2} \in \mathcal{L}^1(\mathcal{H})$. ∎

For the computation of the small-t expansion, because all algebraic properties (mainly Leibniz rule) used in the preceding section work as well as for the tori, we also obtain

$$e^{-t\Delta^\Theta} \underset{t\to 0}{\sim} \sum_{l\in\mathbb{N}} t^l \left(\sum_{\alpha\in\mathbb{N}^n, |\alpha|\leqslant l} L^\Theta(g_{\alpha,l}) t^{|\alpha|/2}\partial^\alpha\right) e^{t\partial_\mu\partial^\mu},$$

where $g_{\alpha,l}\in\mathcal{A}_\Theta$ are the same as for the Moyal plane case except that now $f=1$. So the trace has the small-t expansion,

$$\begin{aligned}\mathrm{Tr}(e^{-t\Delta^\Theta}) &= 2^m(2\pi)^{-n}\int_{\mathbb{T}^n} d^n x \int_{\mathbb{R}^n} \sigma[e^{-t\Delta^\Theta}](\xi,x) d^n\xi \\ &\underset{t\to 0}{\sim} \frac{2^m}{(2\pi)^n}\int_{\mathbb{T}^n} d^n x \int_{\mathbb{R}^n} \sum_{l\in\mathbb{N}} t^l \left(\sum_{\alpha\in\mathbb{N}^n, |\alpha|\leqslant l} g_{\alpha,l}\left(x - \frac{1}{2}\Theta\xi\right) t^{|\alpha|/2}(-i\xi)^\alpha\right) e^{-t|\xi|^2} d^n\xi.\end{aligned}$$

Now, expanding $g_{\alpha,l}$ in Fourier modes and using

$$\int_{\mathbb{T}^n} e^{ik(x-(1/2)\Theta\xi)} d^n x = e^{-ik1/2\Theta\xi}\delta_{k,0} = \delta_{k,0},$$

we directly obtain the following result.

Theorem 3.6: *Let* Δ^{Θ} *be as in (10), then*

$$\mathrm{Tr}(e^{-t\Delta^{\Theta}}) \underset{t\to 0}{\sim} 2^m \left(\frac{1}{4\pi t}\right)^{n/2} \sum_{l\in\mathbb{N}} t^l \int_{\mathbb{T}^n} \tilde{a}_{2l}(x) d^n x,$$

where the $\tilde{a}_{2l}(x)$ *are given in Theorem 2.2.*

IV. THE SPECTRAL ACTION

A. Spectral action for nonunital spectral triples

For a unital spectral triple $(\mathcal{A},\mathcal{H},\mathcal{D})$, Chamseddine and Connes[5,6] proposed a definition of a physical action which depends only on the spectrum of the covariant $\mathcal{D}$-operator (the spectral action principle),

$$S(\mathcal{D},A) := \mathrm{Tr}(\phi(\mathcal{D}_A^2/\Lambda^2)), \tag{14}$$

where $\mathcal{D}_A$ is the covariant "Dirac" operator $\mathcal{D}_A := \mathcal{D}+A+\epsilon JAJ^{-1}$, A is a universal represented 1-form $A\in\tilde{\pi}(\Omega^1\mathcal{A})$, $\tilde{\pi}$ being the lifted representation on the whole differential algebra $\Omega^{\cdot}\mathcal{A}$ $(\tilde{\pi}(a_0\delta a_1\cdots\delta a_p) := \pi(a_0)[\mathcal{D},\pi(a_1)]\cdots[\mathcal{D},\pi(a_p)], a_i\in\mathcal{A}, i=1,\ldots,p)$, J is the real structure of the triple (the charge conjugation for spinors in the commutative case), ϕ a suitable cutoff function, Λ a mass scale and $\epsilon\in\{+1,-1\}$ depending upon the dimension. Any positive smooth function ϕ mimicking the step function $\chi_{[0,1]}$ was initially used in Refs. 5 and 6 and in Ref. 21, sufficient conditions on ϕ have been detailed. Since in the unital case, $\mathcal{D}$ has compact resolvent and likewise for the perturbed $\mathcal{D}_A$ by Theorem 3.5, $\phi(\mathcal{D}_A^2/\Lambda^2)$ is trace-class as long as ϕ decreases fast enough; for instance $r^{n-1}\phi(r^2)\in L^1(\mathbb{R}^+)$ is a sufficient condition for a spectral triple with spectral dimension equal to n.

Let us be more explicit about the covariant "Dirac" operator $\mathcal{D}_A$. The starting point is the analogy between the invariance group of a gauge theory on a Riemannian manifold M coupled with general relativity, $G=U\rtimes\mathrm{Diff}(M)$ and the group of automorphism of an algebra $\mathcal{A}$ which splits into its inner and outer part $\mathrm{Aut}(\mathcal{A})=\mathrm{Int}(\mathcal{A})\rtimes\mathrm{Out}(\mathcal{A})$, with the following exact (group) sequence:

$$1\to U\to G\to \mathrm{Diff}(M)\to 1,$$

$$1\to \mathrm{Int}(\mathcal{A})\to \mathrm{Aut}(\mathcal{A})\to \mathrm{Out}(\mathcal{A})\to 1.$$

In particular, if we choose $\mathcal{A}=\mathcal{C}^\infty(M,M_n(\mathbb{C}))\cong\mathcal{C}^\infty(M)\otimes M_n(\mathbb{C})$, $n>1$, the two constructions coincide: $\mathrm{Out}(\mathcal{A})=\mathrm{Diff}(M)$, $\mathrm{Int}(\mathcal{A})=\mathcal{C}^\infty(M,\mathrm{SU}_n/\mathbb{Z}_n)$. The natural invariance group for an action defined on a spectral triple must be the automorphism group of the algebra. In order to retrieve a gauge theory with spin matter when $\mathcal{A}$ is almost commutative that is $\mathcal{A}=\mathcal{C}^\infty(M)\otimes A_F$ [where A_F is a finite algebra such as $\mathbb{H}\oplus\mathbb{C}\oplus M_3(\mathbb{C})$ for the standard model of particle physics (Refs. 2, 5, and 6)], we must represent $\mathrm{Aut}(\mathcal{A})$ in the fermionic Hilbert space $\mathcal{H}$. In particular, we must lift $\mathrm{Int}(\mathcal{A})$ to the unitary group $\mathcal{U}(\mathcal{H})$ of the bounded operators on $\mathcal{H}$,

$$\mathcal{U}(\mathcal{A})\ni u\mapsto \sigma(u)=\pi(u)J\pi(u)J^{-1}\in\mathcal{U}(\mathcal{H}).$$

For NC tori, Moyal planes and some almost-commutative geometries, this is the adjoint representation, $\pi(u)J\pi(u)J^{-1}\psi = u\star_\Theta\psi\star_\Theta u^*$, $\psi\in\mathcal{H}$. Under this transformation, $\mathcal{D}$ transforms as

$$\mathcal{D} \to \sigma(u)\mathcal{D}\sigma(u)^{-1} = \mathcal{D} + \pi(u)[\mathcal{D}, \pi(u^*)] + \epsilon J\pi(u)[\mathcal{D}, \pi(u^*)]J^{-1}, \tag{15}$$

where ϵ comes from commutation relations $\mathcal{D}J = \epsilon J\mathcal{D}$, $\epsilon \in \{+1, -1\}$ [(see Refs. 10 and 28 for a table of signs)]. The sign ϵ in Eq. (15) is actually wrong in most of the literature, however the computations linked with physics models are unaffected because $\epsilon = 1$ in the zero and four-dimensional cases. Hence $\mathcal{D}_A \to \mathcal{D}_{A'}$ with $A' = \pi(u)A\pi(u^*) + \pi(u)[\mathcal{D}, \pi(u^*)]$ transforms covariantly.

For almost commutative geometry $\mathcal{C}^\infty(M) \otimes A_F$, in particular for the standard model, with $\mathcal{D} = \not{D} \otimes 1_{\mathcal{H}_F}$ and the curved Dirac operator $\not{D} = -ie^\mu{}_a \gamma^a(\partial_\mu + \omega_\mu)$, ω being the spin connection on M, $S(\mathcal{D}, A)$ is asymptotically computable by heat kernel techniques. We may note that $\not{D}_A^2$ can be written as a generalized Laplacian, $\not{D}_A^2 = P$ with $P = -(g^{\mu\nu}(\partial_\mu + \omega_\mu)(\partial_\nu + \omega_\nu) + E)$, where $g^{\mu\nu}$ is the metric tensor, now ω_μ is a connection containing spin and Yang–Mills part and E is an endomorphism of the fiber bundle, on whose sections P acts. One can formally show,[5,6] expanding ϕ in Taylor series, that $S(\mathcal{D}, A)$ is linked to the Seeley–DeWitt coefficients $a_k(P, x)$ of the trace of the heat operator on a n-dimensional manifold,

$$\mathrm{Tr}(e^{-tP}) \underset{t \to 0}{\sim} (4\pi)^{-n/2} \sum_{l \in \mathbb{N}} t^{(l-n)/2} \int_M a_l(P, x)\mathrm{dvol}(x), \tag{16}$$

where $\mathrm{dvol}(x)$ is the Riemannian volume form, by the relation between zeta function and trace of the heat operator[25]

$$\zeta_P(s) := \mathrm{Tr}(P^{-s}) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1}\, \mathrm{Tr}(e^{-tP})\mathrm{d}t. \tag{17}$$

On a manifold without boundary $a_l(P, x) = 0$, l odd, therefore in the four-dimensional case, this yields,

$$S(\not{D} \otimes 1_{A_F}, A) = (4\pi)^{-2} \sum_{l=0}^{2} \Lambda^{4-2l} \phi_{2l} \int_M a_{2l}(P, x)\mathrm{dvol}(x) + O(\Lambda^{-2}), \tag{18}$$

where

$$\phi_0 = \int_0^\infty \phi(t)t\, \mathrm{d}t, \quad \phi_2 = \int_0^\infty \phi(t)\mathrm{d}t, \quad \phi_{2(2l+2)} = (-1)^l \phi^{(l)}(0), \quad l \geqslant 0. \tag{19}$$

A less formal, derivation of this relation with precise constraints on ϕ can be found in Refs. 21 and 40. For M still four dimensional and $A_F = \mathbb{H} \oplus \mathbb{C} \oplus M_3(\mathbb{C})$, the spectral action yields a unification of the Einstein plus Weyl gravity and the standard model including the Higgs sector and its spontaneous symmetry breaking (see Refs. 2, 5, and 6). There is no restriction for an arbitrary dimension but the coefficients (19) will be slightly different, as we will see below for the Moyal plane.

Remark 4.1: The relation (17), links also the Dixmier trace with the heat kernel expansion, and therefore the Connes–Lott action (8) with the spectral action as explained in Sec. IV C.

For the nonunital case, since $\mathcal{D}$ has no longer a compact resolvent, we invoke a *spatial regularization* ρ to define the spectral action. Like the energy regularization ϕ, ρ is a positive function rapidly decreasing, in the almost commutative case, and must be generically an element of the algebra $\mathcal{A}$.

Definition 4.2: For a nonunital spectral triple $(\mathcal{A}, \tilde{\mathcal{A}}, \mathcal{H}, \mathcal{D})$ of spectral dimension n, the *spectral action* is

$$S(\mathcal{D}, A, \rho) := \mathrm{Tr}_{\mathcal{H}}(\pi(\rho)\phi(\mathcal{D}_A^2/\Lambda^2)), \tag{20}$$

where as in the unital case, $\mathcal{D}_A = \mathcal{D} + A + \epsilon JAJ^{-1}$ ($\epsilon \in \{+1, -1\}$ depending on n), and $A \in \Omega^1_{\mathcal{D}}(\tilde{\mathcal{A}})$ is now a represented self-adjoint 1-form of the unitized algebra, $A = \Sigma_{i \in I} \pi(b_0^i)[\mathcal{D}, \pi(b_1^i)]$, for I a

finite set, b_0^i, $b_1^i \in \tilde{\mathcal{A}}$, $0 \leqslant \rho \in \mathcal{A}$ and moreover $0 \leqslant \phi$, Λ are as in the unital case.

Remark 4.3: (i) This definition gives more importance to the choice of the unitization. The 1-form A is now constructed from $\tilde{\mathcal{A}}$, and all the symmetry considerations discussed previously occur now for the unitized algebra. This is important because unitaries in the algebra are necessary to express gauge invariance, $S(\mathcal{D},A,\rho)$ is gauge invariant that is invariant under the lifted inner automorphism implemented by the unitary operator $\pi(u)J\pi(u)J^{-1}$ and now the regularization ρ transforms also

$$A \to uAu^* + u[\mathcal{D},u^*],$$

$$\rho \to u\rho u^*.$$

(ii) The positivity of ρ and ϕ is necessary in order to get a positive action.

(iii) Other regularizations are possible. For instance, $\phi(\mathcal{D}_A^2\pi(\rho)^{-1})$ where $\rho \in \mathcal{S}$ is a strictly positive function also give rise to trace-class operators for Moyal planes, but the asymptotic expansion is still unmanageable.

Let us show how it works for an almost commutative geometry associated with a boundaryless noncompact smooth manifold M. In this case, we still work with $\mathcal{A}=\mathcal{C}_c^\infty(M)\otimes A_F$. The operator ρe^{-tP}, $t \in \mathbb{R}_+^*$, is trace-class, for $\rho \in \mathcal{C}_c^\infty(M)$ viewed as a pointwise multiplication operator and P being a generalized Laplacian (ΨDO operator of order two with metric tensor as coefficient of the leading symbol). In this case the formula (17) has an analog,

$$\zeta_{\rho,P}(s) := \mathrm{Tr}(\rho P^{-s}) = \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\,\mathrm{Tr}(\rho e^{-tP})\mathrm{d}t, \tag{21}$$

one obtains, for $P=(\not{D}+A+\epsilon JAJ^{-1})^2$,

$$S(\not{D}\otimes 1_{A_F},A) = (4\pi)^{-n/2}\sum_{l=0}^{m}\Lambda^{n-2l}\phi_{2l}\int_M a_{2l}(P,x)\rho(x)\mathrm{dvol}(x) + O(\Lambda^{n-2(m+1)}),$$

where a_{2l} are still the Seeley–DeWitt coefficients which are now only locally integrable while $a_{2l}(P,x)\rho(x)$ are globally integrable (see Ref. 49). The coefficients ϕ_{2l} have the form (19) in the four-dimensional case, and their values in any dimension n is now computed for Moyal planes.

B. The case of the Moyal plane

Actually, the relation (21) is quite general, that is for any bounded operator S and any operator T such that ST^{-s} is trace-class, we have

$$\zeta_{S,T}(s) := \mathrm{Tr}(ST^{-s}) = \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\,\mathrm{Tr}(Se^{-tT})\mathrm{d}t. \tag{22}$$

With this relation and the result of Sec. III, one can derive the spectral action for Moyal planes. However in order to obtain more directly the form of the coefficients ϕ_{2k} in any dimension, we will derive it by Laplace transform techniques such as in Ref. 40 (see Ref. 53 for details on Laplace transform). We assume that the function ϕ has the following property:

$$\phi \in \mathcal{C}^\infty(\mathbb{R}^+) \text{ is the Laplace transform of } \hat{\psi} \in \mathcal{S}(\mathbb{R}^+) := \{g \in \mathcal{S}: g(x) = 0, x \leqslant 0\}. \tag{23}$$

Thus, any function with this property has necessarily an analytic extension on the right complex plane and is a Laplace transform. Consequently, any m-differentiable function ψ such that $\psi^{(m)} = \phi$ is the Laplace transform of a function $\hat{\psi}$ and by differentiation, it satisfies

$$\phi(z) = \psi^{(m)}(z) = (-1)^m \int_0^\infty e^{-sz} s^m \hat{\psi}(s)\mathrm{d}s, \quad \Re z > 0.$$

With Δ^Θ defined in (10), using $\phi(\Delta_r^\Theta) = (-1)^m \int_0^\infty e^{-s\Delta_r^\Theta} s^m \hat{\psi}(s)\mathrm{d}s$ and the positivity of $\rho = g^* \star_\Theta g$, $g \in \mathcal{B}_\Theta$, we get

$$\mathrm{Tr}(L^\Theta(\rho)\phi(\Delta_r^\Theta/\Lambda^2)) = (-1)^m \,\mathrm{Tr}\left(L^\Theta(g) \int_0^\infty e^{-t\Delta_r^\Theta/\Lambda^2} t^m \hat{\psi}(t)\mathrm{d}t \, L^\Theta(g^*) \right).$$

Let $\{\Phi_p\}_{p\in\mathbb{N}}$ be any orthonormal basis of $\mathcal{H}_r$ and let $0 \leqslant B_t := L^\Theta(g) e^{-t\Delta_r^\Theta/\Lambda^2} L^\Theta(g^*)$, then

$$\mathrm{Tr}(L^\Theta(\rho)\phi(\Delta_r^\Theta/\Lambda^2)) = \lim_{N\to\infty} \int_0^\infty \sum_{p\leqslant N} \langle \Phi_p, B_t \Phi_p \rangle t^m \hat{\psi}(t)\mathrm{d}t \leqslant \lim_{N\to\infty} \int_0^\infty \|B_t\|_1 t^m \hat{\psi}(t)\mathrm{d}t = \int_0^\infty \|B_t\|_1 t^m \hat{\psi}(t)\mathrm{d}t.$$

Let us estimate $\|B_t\|_1$. For $t > \epsilon$ with a fixed arbitrary small ϵ, we have

$$\|B_t\|_1 = \|L^\Theta(g) e^{-t\Delta_r^\Theta/2\Lambda^2}\|_2^2 \leqslant \|L^\Theta(g) e^{-\epsilon\Delta_r^\Theta/2\Lambda^2}\|_2^2 \|e^{-(t-\epsilon)\Delta_r^\Theta/2\Lambda^2}\|.$$

But, $(t-\epsilon)\Delta_r^\Theta$ being positive, we have $\|e^{-(t-\epsilon)\Delta_r^\Theta/2\Lambda^2}\| \leqslant 1$. Hence for $t > \epsilon$, $\|B_t\|_1 \leqslant C$ uniformly in t. For $t \leqslant \epsilon$, our previous computation shows that $\|B_t\|_1 = O(t^{-n/2})$. Hence $\mathrm{Tr}(\int_0^\infty B_t t^m \hat{\psi}(t)\mathrm{d}t) < \infty$, so by dominated convergence one obtains

$$\begin{aligned}
\mathrm{Tr}(L^\Theta(\rho)\phi(\Delta_r^\Theta/\Lambda^2)) &= (-1)^m \int_0^\infty \mathrm{Tr}(L^\Theta(\rho) e^{-t\Delta_r^\Theta/\Lambda^2}) t^m \hat{\psi}(t)\mathrm{d}t \\
&= (-1)^m (4\pi)^{-n/2} \int_0^\infty \sum_{l=0}^m \Lambda^{n-2l} t^{m+l-n/2} \hat{\psi}(t)\mathrm{d}t \int_{\mathbb{R}^n} \rho \star_\Theta \tilde{a}_{2l}(x) d^n x + O(\Lambda^{n-2(m+1)}) \\
&= (4\pi)^{-n/2} \sum_{l=0}^m \Lambda^{n-2l} \phi_{2l} \int_{\mathbb{R}^n} \rho \star_\Theta \tilde{a}_{2l}(x) d^n x + O(\Lambda^{n-2(m+1)}),
\end{aligned}$$

where ϕ_{2l} is now defined by

$$\phi_{2l} := (-1)^m \int_0^\infty t^{m+l-n/2} \hat{\psi}(t)\mathrm{d}t. \tag{24}$$

When $n = 2m$ is even, ϕ_{2l} has the more familiar form of (19),

$$\phi_{2l} = \begin{cases} \dfrac{1}{\Gamma(m-l)} \displaystyle\int_0^\infty \phi(t) t^{m-1-l}\,\mathrm{d}t & \text{for } l = 0, \ldots, m-1, \\ (-1)^l \phi^{(l-m)}(0) & \text{for } l = m, \ldots, n. \end{cases} \tag{25}$$

For n odd, the coefficients ϕ_{2l} have less explicit forms because they invoke fractional derivatives of ϕ, so in this case, it is better to stick to definition (24).

Let us summarize.

Theorem 4.4: *Let $\rho \in \mathcal{S}(\mathbb{R}^n)$, $A = -iL^\Theta(A_\mu) \otimes \gamma^\mu$, $A_\mu^* = -A_\mu \in \mathcal{O}_0(\mathbb{R}^n)$, $\phi \in \mathcal{C}^\infty(\mathbb{R}^+)$ be a positive function satisfying condition (23) and $\not{b}_A = \not{b} + A$. Then $L^\Theta(\rho)\phi(\not{b}_A^2/\Lambda^2)$ is trace-class. Moreover, the following expansion of the spectral action holds:*

$$S(\not{b}, A, \rho) = 2^m (4\pi)^{-n/2} \sum_{l=0}^m \Lambda^{n-2l} \phi_{2l} \int_{\mathbb{R}^n} \rho(x) \tilde{a}_{2l}(x) d^n x + O(\Lambda^{n-2(m+1)}),$$

where the ϕ_{2l} are defined in (24) or (25) depending on the dimension and the $\tilde{a}_{2l}(x)$ are given in Theorem 2.2 with the following replacement in (10):

$$L^{\Theta}(\omega_{\mu}) \to L^{\Theta}(A_{\mu}),$$

$$L^{\Theta}(E) \otimes 1_{2^m} \to (L^{\Theta}(\partial_{\mu}A_{\nu}) + L^{\Theta}(A_{\mu} \star_{\Theta} A_{\nu})) \otimes \tfrac{1}{2}(\gamma^{\mu}\gamma^{\nu} - \gamma^{\nu}\gamma^{\mu}).$$

Moreover, all terms in $\tilde{a}_{2l}$ linear in E are zero.

Proof: This follows from $\gamma^{\mu}\gamma^{\nu} = \eta^{\mu\nu} + \frac{1}{2}(\gamma^{\mu}\gamma^{\nu} - \gamma^{\nu}\gamma^{\mu})$, so all linear terms in E are of zero trace. ■

Remark 4.5: When the Dirac operator is symmetrized, $\mathcal{D}_A = \mathcal{D} + A + \epsilon JAJ^{-1}$, one must replace $L^{\Theta}(A_{\mu})$ by $L^{\Theta}(A_{\mu}) - R^{\Theta}(A_{\mu})$ since $\epsilon J(L^{\Theta}(A_{\mu}) \otimes \gamma^{\mu})J^{-1} = R^{\Theta}(A_{\mu}^{*}) \otimes \gamma^{\mu}$. So, the behavior in t of different terms like $\mathrm{Tr}(L^{\Theta}(f)R^{\Theta}(g)(-i\partial)^{\alpha}e^{t\partial_{\mu}\partial^{\mu}})$ must be computed. More precisely, since

$$\sigma[L^{\Theta}(f)R^{\Theta}(g)](\xi, x) = (2\pi)^{-n} \int e^{i(\eta-\xi).(x-y)} f\left(x - \tfrac{1}{2}\Theta\eta\right) g\left(y + \tfrac{1}{2}\Theta\xi\right) d^n y d^n \eta,$$

we have

$$\begin{aligned}\mathrm{Tr}(L^{\Theta}(f)R^{\Theta}(g)(-i\partial)^{\alpha}e^{t\partial_{\mu}\partial^{\mu}}) &= \int \sigma[L^{\Theta}(f)R^{\Theta}(g)(-i\partial)^{\alpha}e^{t\partial_{\mu}\partial^{\mu}}](\xi, x) d^n x d^n \xi \\ &= \int f\left(x - \tfrac{1}{2}\Theta\xi\right) g\left(x + \tfrac{1}{2}\Theta\xi\right) \xi^{\alpha} e^{-t|\xi|^2} d^n x d^n \xi,\end{aligned}$$

the translation invariance $x \to x + \frac{1}{2}\Theta\xi$ crucially used in the proof of Theorem 2.2 now fails. This point is related to the UV/IR mixings and must be clarified.

C. Connes–Lott versus Chamseddine–Connes actions

In order to compare this result with the Connes–Lott action computation of the four-dimensional Moyal plane,[23] up to negative order terms with respect to the mass scale Λ, we obtain

$$S(\phi, A, \rho) = \frac{1}{4\pi^2}\left(\Lambda^4 \phi_0 \int_{\mathbb{R}^4} \rho(x) d^4x + \frac{\phi(0)}{6} \int_{\mathbb{R}^4} \rho(x) F^{\mu\nu} \star_{\Theta} F_{\mu\nu}(x) d^4x\right) + O(\Lambda^{-2}),$$

where $F^{\mu\nu} := \partial^{\mu}A^{\nu} - \partial^{\nu}A^{\mu} + [A^{\mu}, A^{\nu}]_{\star_{\Theta}}$.

If we choose the characteristic function $\rho = \chi_V$ of a bounded subset $V \subset \mathbb{R}^4 (\chi_V \notin \mathcal{S}(\mathbb{R}^4))$, property (6) yields

$$S(\phi, A, \chi_V) = \frac{1}{4\pi^2}\left(\Lambda^4 \phi_0 \int_V d^4x + \frac{\phi(0)}{6} \int_V F^{\mu\nu} \star_{\Theta} F_{\mu\nu}(x) d^4x\right) + O(\Lambda^{-2}), \tag{26}$$

which, modulo a cosmological term, is the spatially localized noncommutative Yang–Mills action. This expression must be compared with the four-dimensional Connes–Lott one (8) for Θ symplectic, hence $\star_{\Theta} = \star_{\Theta}$,

$$\mathrm{YM}(\alpha) = -\frac{1}{4g^2} \int F^{\mu\nu} \star_{\Theta} F_{\mu\nu}(x) d^4x.$$

This action is slightly different from (26), because property (6), together with the absence of ρ gives

$$\mathrm{YM}(\alpha) = -\frac{1}{4g^2} \int F^{\mu\nu}(x) F_{\mu\nu}(x) d^4x.$$

For the noncommutative tori, we have also a similar result, with the spectral action in the unital case ($\rho = 1$),

$$S(\not{b},A)\sim_{\Lambda\to\infty}2^m(4\pi)^{-n/2}\sum_{k\in\mathbb{N}}\Lambda^{n-2k}\phi_{2k}\int_{\mathbb{T}^n}\tilde{a}_{2k}(x)d^nx,$$

which also yields for $n=4$,

$$S(\not{b},A)=\frac{1}{4\pi^2}\left(\Lambda^4\phi_0+\frac{\phi(0)}{6}\int_{\mathbb{T}^4}F^{\mu\nu}\star_\Theta F_{\mu\nu}(x)d^4x\right)+O(\Lambda^{-2}).$$

D. Towards a gravitational degree of freedom

One can ask about adding gravitational degrees of freedom for Moyal planes or NC tori. For instance, the results of Sec. III also work with a nonconstant metric $g^{\mu\nu}(x)$. More precisely, Theorem 3.2 is still true if we replace in (10), Δ^Θ by the square of

$$-ie_a^\mu(\partial_\mu+\omega_\mu+L^\Theta(A_\mu))\otimes\gamma^a,$$

where e_a^μ and ω_μ are bounded functions. Here, the pointwise and Moyal products are mixed, but in this case, computation of the trace of its regularized semigroup can be done, at least in principle, with the same techniques but it will be highly less easy.

However, this construction is meaningless from a spectral triple point of view. A nonflat Dirac operator over $\mathbb{R}^n$, $\not{D}=-ie_a^\mu(x)\gamma^a(\partial_\mu+\omega_\mu(x))$, ω_μ being the spin connection, will violate most of the axioms describing spectral triples, for instance,

$$[\not{D},\pi^\Theta(f)]=-i\gamma^a([e_a^\mu\omega_\mu,\pi^\Theta(f)]+e_a^\mu\pi^\Theta(\partial_\mu f)+[e_a^\mu,\pi^\Theta(f)]\partial_\mu).$$

So, for $f\in\mathcal{B}_\Theta$, $[\not{D},\pi^\Theta(f)]$ can be extended to a bounded operator only if $[e_a^\mu,\pi^\Theta(f)]=0$. This condition can be satisfied for instance by a n-dimensional Riemannian manifold (M,g) endowed with an isometric action of $\mathbb{R}^l$, $l\geqslant 2$ (periodic or not). This is actually the Connes–Landi isospectral deformations.[13,14] Those cases, admit nontrivial fluctuations of the metric (in some sense for the untwisted directions). Since the only invariant metric on $\mathbb{R}^n$ or $\mathbb{T}^n$ by the natural action of $\mathbb{R}^n$ is the flat one and this is the geometrical obstruction to deal with nonflat Moyal planes (see Ref. 4).

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Dirichlet series and the integrability of multilinear differential equations

A. Pickering[a] and J. Prada
Departamento de Matemáticas, Universidad de Salamanca, Plaza de la Merced 1, 37008 Salamanca, Spain

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We explore the relationship between the integrability of nonsemilinear partial differential equations and formal Dirichlet series solutions. To this end we consider a variety of integrable and nonintegrable differential equations. We also demonstrate that such series solutions are a natural extension to the nonlinear case of those obtained by basic solution techniques for linear ordinary differential equations. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1879083]

I. INTRODUCTION

One class of completely integrable partial differential equations (PDEs) that has long been of interest is that of nonsemilinear PDEs; see for example Refs. 1–4. However, nonsemilinear PDEs, when compared with other classes of PDE, present certain problems. One is that many such equations, even if completely integrable, fail the Painlevé test.[5] In other words, there is no simple test of integrability that can be applied directly to such PDEs.

In two recent papers[6,7] it has been suggested that, instead of classifiying equations using Painlevé expansions, a classification using Dirichlet series might be used. It was noted that, for two particular classes of nonsemilinear PDEs, the only equations admitting such series solutions are transformable back onto the only known completely integrable PDEs within those classes. One aim of the present paper is to explore these ideas still further, and to this end we consider a variety of nonsemilinear PDEs, both integrable and nonintegrable, in $1+1$ and multidimensions. For a discussion of integrability in multidimensions, see e.g., Refs. 8 and 9.

However, despite the apparent link between Dirichlet series and integrability—at least in the case of particular examples, or for certain classes of equations—it would be imprudent to claim a hard and fast connection. Indeed, we show here that the existence of Dirichlet series solutions is not sufficient for integrability; the question of necessity remains open. A precise description of the uncertainties in the current state of the art can be found in the concluding Secs. VII and VIII.

A second aim of the present paper is to provide an understanding of our technique as a method of constructing series solutions. We find that instead of a comparison with Painlevé analysis, it is more profitable to consider a comparison with solution techniques for linear ordinary differential equations (ODEs). It turns out that the important feature is that of having multilinear terms that are dominant over other terms in the equation. We explain our ideas within the context not only of the PDEs considered but also using ODE examples which help to make clear the connection between Dirichlet series solutions for nonlinear equations and basic solution techniques for linear ODEs. We note that Dirichlet series solutions for nonlinear ODEs have been considered before (see, e.g., Ref. 10), although this connection with the linear case does not seem to have been remarked upon.

[a]Address from 1 October 2004: Area de Matemática Aplicada, ESCET, Universidad Rey Juan Carlos, C/Tulipán s/n, 28933 Móstoles, Madrid, Spain.

II. DIRICHLET SERIES: AN ODE EXAMPLE

In this section we recall some basic facts about Dirichlet series, and illustrate our ideas using a simple ODE example. A Dirichlet series is a series of the form

$$\sum_{j=0}^{\infty} a_j e^{-\lambda_j x}, \tag{1}$$

where $\{\lambda_j\}$ is a strictly monotonic increasing sequence of real numbers (only a finite number of which are negative), unbounded above, and $x, a_j \in \mathbb{C}$. We recall that a Dirichlet series, if convergent for $x=x_0$, is then also convergent for all x with $\mathrm{Re}(x) > \mathrm{Re}(x_0)$, and uniformly convergent for all x with $|\arg(x-x_0)| \leqslant \theta$, for any fixed θ, $0 < \theta < \pi/2$. That is, in general, convergence is in right half-planes, and uniform convergence is in sectors. For further details, see e.g., Ref. 11. Clearly, $x \to -x$ allows us to define Dirichlet-type series convergent in left half-planes; more generally, a rotation $x \to e^{i\varphi} x$ $(-\pi < \varphi \leqslant \pi)$ allows us to define Dirichlet-type series convergent in skewed half-planes,

$$\sum_{j=0}^{\infty} a_j e^{\mu_j x}, \tag{2}$$

where $\mu_j = -\lambda_j e^{i\varphi}$ is a sequence of points lying on a half-line in the complex plane. We will refer to any series of the form (2) as a Dirichlet series, or standard Dirichlet series when we wish to distinguish between a series (2) and generalizations thereof.

We note that Dirichlet series appear to be used little in the study of solutions of differential equations. The reason for this is presumably that, in comparison to power series (Taylor or Laurent), relatively few functions, and so also relatively few solutions of differential equations, can be expressed as Dirichlet series; there is in fact no reason why a given function should have such an expression. Thus, in general, in order to represent solutions of differential equations, Dirichlet series need modification, and those cases where this is not necessary are therefore very special. Indeed, in any half-plane of convergence, a Dirichlet series sums to an analytic function of x. We return to these considerations later (see Sec. VI).

We now illustrate the basic ideas underlying our approach using as an example the ODE,

$$B[V] \equiv VV_{xxx} + 2V_x V_{xx} - 3VV_x + V - V_{xx} = 0. \tag{3}$$

We first seek a leading order term for our Dirichlet series,

$$V \sim V_0 e^{px}, \quad V_0 \neq 0, \quad \text{constant}. \tag{4}$$

Substituting into the dominant (quadratic) terms gives

$$VV_{xxx} + 2V_x V_{xx} - 3VV_x \sim 3p(p^2-1)V_0^2 e^{2px}, \tag{5}$$

and so we may take $p = \pm 1$ or $p = 0$. However in this last case the quadratic terms are not dominant over the linear terms, and so we are left with $p = \pm 1$.

We take $p = -1$, and seek to determine which coefficients in our putative Dirichlet series will be arbitrary, using a substitution of the form

$$V \sim V_0 e^{-x} + V_j e^{(j-1)x}, \tag{6}$$

which allows us to determine the coefficient of V_j in the recursion relation by which the coefficients of our Dirichlet series are determined. We thus obtain that this recursion relation is of the form

$$j(j-2)(j-3)V_j = R_j(V_{j-1}, V_{j-2}, \ldots, V_0), \tag{7}$$

for some function R_j, and so we have arbitrary coefficients at $j=0,2,3$. We therefore seek a solution of our ODE as

$$V = e^{-x}\sum_{j=0}^{\infty} V_j e^{jx}, \tag{8}$$

where all V_j are constant. We note in passing that if instead of x in the series (8), we write $x-\tilde{x}$, for some constant $\tilde{x}$, we can always absorb the factor $e^{-j\tilde{x}}$ into the coefficient V_j.

Substitution of the series (8) into our ODE yields

$$B[V] = e^{-2x}\sum_{j=0}^{\infty} B_j e^{jx} = 0, \tag{9}$$

and so a sequence of equations $B_j=0$ for the coefficients V_j. Here,

$$B_0 = 0, \tag{10}$$

$$B_1 = 2V_0V_1, \tag{11}$$

$$B_2 = V_1, \tag{12}$$

$$B_3 = -2V_1V_2, \tag{13}$$

$$B_4 = 8V_0V_4 + 2V_1V_3 - 3V_3. \tag{14}$$

Thus we see that V_0 is left arbitrary and that, at $j=1$, since we assume $V_0 \neq 0$, V_1 is determined as $V_1=0$. At $j=2$, V_2 is not determined, and we have the compatibility condition $R_2=0$ (i.e., $B_2=0$), satisfied since $V_1=0$. Similarly at $j=3$, where V_3 is left undetermined, we must have $R_3=0$ (i.e., $B_3=0$), again satisfied since $V_1=0$. The equations $B_j=0$, $j\geqslant 4$, then determine all subsequent coefficients V_j, $j=4,5,6,\ldots$, in terms of V_0, V_2, and V_3. Our ODE therefore admits, at least formally, a Dirichlet series solution. We note that, if one of the conditions at $j=2$ or $j=3$ had not been satisfied, then we would have had to modify the series solution by the inclusion of powers of x. Examples of differential equations where such modifications are needed will be presented later.

We note that for the choice $p=1$, the fact that we have a Dirichlet series solution of the form

$$V = e^{x}\sum_{j=-\infty}^{0} \tilde{V}_j e^{jx}, \tag{15}$$

with $\tilde{V}_0$, $\tilde{V}_{-2}$, and $\tilde{V}_{-3}$ arbitrary, follows immediately from the observation that our ODE admits the discrete symmetry $(V,x)\rightarrow(-V,-x)$.

Thus our ODE admits formal Dirichlet series solutions. These are constructed by first identifying a leading order, determined by the terms of highest nonlinearity, and then checking that compatibility conditions—which arise when coefficients are left arbitrary—are satisfied. It is the construction of such series solutions that we will explore in later sections. We will also consider variations of our approach, i.e., series solutions of a more general form than the standard Dirichlet series (2).

The above ODE example, however, also ties in with the other main theme of our paper, which is integrability: the ODE (3) is integrable, having the Lax pair

$$\phi_{xx} = \tfrac{1}{4}[1-\mu(V_{xx}-V)]\phi, \tag{16}$$

$$\phi_\mu = \left(\frac{V}{\mu} - \frac{2}{\mu^2}\right)\phi_x - \frac{1}{2}\frac{V_x}{\mu}\phi. \tag{17}$$

It was the existence of Dirichlet series solutions for integrable PDEs that motivated the work in Refs. 6 and 7. Here we have an integrable ODE which also admits formal Dirichlet series solutions. In fact the ODE (3) can be obtained from the classification in Ref. 7. It can also be obtained[12] as a similarity reduction of the now famous Fuchsteiner–Fokas–Camassa–Holm (FFCH) equation,[13,14]

$$UU_{xxx} + 2U_xU_{xx} - 3UU_x + U_{xxt} - U_t - 2\kappa U_x = 0. \tag{18}$$

It is to this question of integrability to which we now turn. We consider Dirichlet series solutions for PDEs, as well as modifications of such for equations where compatibility conditions are not satisfied. Perhaps the best way to begin is to summarize briefly the results of Refs. 6 and 7. This we now do.

III. DIRICHLET SERIES FOR PDEs

In Ref. 12, the Painlevé analysis of the class of nonsemilinear PDEs

$$F \equiv F_1 + F_2 = 0, \tag{19}$$

where

$$F_1 = UU_{xxx} + \beta U_xU_{xx} - p^2(\beta + 1)UU_x, \tag{20}$$

$$F_2 = \epsilon U_{xxt} - U_t - 2\kappa U_x, \tag{21}$$

was considered. It was shown that no equation in this class survived the combination of the Painlevé ODE (Ref. 15) and PDE (Ref. 16) tests. In particular, since the FFCH equation is contained in this class, the drawbacks of Painlevé analysis for certain classes of equations—as first observed by Weiss for the Dym equation[5]—were confirmed. It also led to the question, posed in Ref. 12, of how many other equations in this class are actually integrable, in spite of not passing the Painlevé tests.

Remarkably, it turns out that the class of equations (19) does contain another completely integrable PDE, namely the Degasperis–Procesi (DP) equation,[17]

$$UU_{xxx} + 3U_xU_{xx} - 4UU_x + U_{xxt} - U_t = 0. \tag{22}$$

Further, as is clear from the results presented in Ref. 12, this PDE also fails to survive the Painlevé tests: in fact, this PDE admits the weak Painlevé expansion

$$U = -\psi'(t) + \phi^{1/2}(x,t)\sum_{j=0}^{\infty} U_{j/2}(t)\phi^{j/2}(x,t), \quad \phi(x,t) = x + \psi(t), \tag{23}$$

where ψ, U_0, and U_1 are three arbitrary functions of t. This then highlights the need for some simple and directly applicable test—analogous to the Painlevé tests—capable of identifying completely integrable differential equations in such a class.

We note that a partial answer to the question of which PDEs in the class (19) are completely integrable has been given in Ref. 18, as follows. First we observe that in the case $p \neq 0$ we may assume, without loss of generality, that $p=1$ (in the later sections of this paper we prefer to include the parameter p—as did the authors of Ref. 12—so that the known equations in the class (19) can be taken in standard form). That is, when $p \neq 0$, an appropriate rescaling yields

$$UU_{xxx} + \beta U_x U_{xx} - (\beta + 1)UU_x + \hat{\epsilon} U_{xxt} - U_t - 2\kappa U_x = 0, \tag{24}$$

where $\hat{\epsilon} = p^2 \epsilon$. If in addition we have $(\beta+1)\hat{\epsilon} \neq 1$, we may use a Galilean transformation to set $\kappa = 0$.[12] Of the resulting equations,

$$UU_{xxx} + \beta U_x U_{xx} - (\beta + 1)UU_x + \hat{\epsilon} U_{xxt} - U_t = 0, \tag{25}$$

it was shown in Ref. 18 that in the special case $\hat{\epsilon} = 1$, only those having $\beta = 2$ or $\beta = 3$ are completely integrable. This relied on a quasilocal extension of the symmetry approach, so that in this case $\hat{\epsilon} = 1$, (25) is expressed in evolution form using the operator $\Delta = (1 - \partial^2/\partial x^2)^{-1}$, with higher symmetries containing nestings of Δ. The case $\beta = 2$ corresponds to the FFCH equation, and $\beta = 3$ to the DP equation.

However, as indicated above, one of our aims here is to explore the relationship between a simple property of solutions, easily testable for a much wider class of equations, i.e., their expression as formal Dirichlet series, and integrability. It was with this aim in mind that in Refs. 6 and 7 the following class of equations was considered:

$$E \equiv E_1 + E_2 = 0, \tag{26}$$

where

$$E_1 = UU_{xxx} + \beta U_x U_{xx} - (\beta + 1)UU_x \tag{27}$$

and

$$\begin{aligned} E_2 = {} & a(t) + b(t)U + c_0(t)U_x + c_1(t)U_t + d_0(t)U_{xx} + d_1(t)U_{xt} + d_2(t)U_{tt} \\ & + e_0(t)U_{xxx} + e_1(t)U_{xxt} + e_2(t)U_{xtt} + e_3(t)U_{ttt}, \end{aligned} \tag{28}$$

i.e., where E_1 consists of quadratic terms equivalent to those of (19) for $p \neq 0$, and E_2 consists of all possible linear terms up to and including third derivatives.

Motivated by the observation that not only does the FFCH equation (18) admit the exact solution[12]

$$U = f(t)e^{-x} - \kappa + g(t)e^{x}, \tag{29}$$

but also a generalization having the form of a Dirichlet series,

$$U = e^{-x} \sum_{j=0}^{\infty} U_j(t) e^{jx}, \tag{30}$$

where U_0, U_2, and U_3 are three arbitrary functions of t, it was shown in Refs. 6 and 7 that for each of the choices $\beta = 2$ and $\beta = 3$ in (26), the only equations admitting Dirichlet series solutions can be transformed back onto the only known integrable equation within that class (FFCH and DP, respectively). These results suggest a connection between Dirichlet series solutions and certain classes of integrable equations.

We note that the construction of a Dirichlet series solution such as (30), here for the FFCH equation, proceeds in the same way as in the ODE case: we have dominant and nondominant terms (E_1 and E_2, respectively), the former determining the leading order behavior and also which coefficients are left arbitrary. We then have compatibility conditions to be satisfied, in order that our solution remains a series in powers of exponentials only. When a compatibility condition is not satisfied the series has to be modified by the inclusion of powers of x (higher and higher powers for higher powers of e^x). We also note that if instead of x in (30) we have $x - \eta(t)$, we can always absorb the factor $e^{-j\eta(t)}$ into the coefficient $U_j(t)$.

In order to explore the connection between Dirichlet series solutions and integrability, we consider the construction of Dirichlet series solutions for a wide variety of PDEs. We begin in Sec. IV with various examples of PDEs in the class (19). For example, we will see in Sec. IV A that the

Fornberg–Whitham equation[21] does not admit Dirichlet series solutions, and so this PDE differs in this respect from the integrable FFCH and DP equations; this example also allows us to illustrate the modification of a putative Dirichlet series solution with powers of x in the case of failed compatibility conditions. We will also see that in the case $\hat{\epsilon}=1$, all equations in the class (25) admit Dirichlet series solutions for all integer $\beta \geqslant 2$, and thus while there is indeed a strong connection between Dirichlet series solutions and integrability, the admission of Dirichlet series solutions is not sufficient for integrability. In Sec. V we give further examples of integrable PDEs, but in multidimensions rather than 1+1, that admit Dirichlet series solutions. In Sec. VI we consider some technical points, such as convergence, and the connection between our approach and basic solution techniques for linear ODEs; we also consider more general Dirichlet-type series, but find that even integrable equations may require that such nonstandard Dirichlet series solutions be modified by including powers of x. We return to a discussion of the connection between integrability and Dirichlet series solutions in Sec. VII; a summary of our conclusions is given in Sec. VIII.

IV. EXAMPLES IN 1+1 DIMENSIONS

A. The Fornberg–Whitham equation

In this section we consider the Fornberg–Whitham (FW) equation,[19–21]

$$G[U] \equiv UU_{xxx} + 3U_xU_{xx} - UU_x + U_{xxt} - U_t - U_x = 0, \tag{31}$$

which corresponds to the parameter choice $(\epsilon, p^2, \beta, \kappa) = \left(1, \frac{1}{4}, 3, \frac{1}{2}\right)$ in Eq. (19).

We begin by seeking a leading order term for our Dirichlet series,

$$U \sim U_0(t)e^{px}, \quad U_0(t) \neq 0. \tag{32}$$

Substitution into the quadratic terms of the equation gives

$$UU_{xxx} + 3U_xU_{xx} - UU_x \sim p(4p^2 - 1)U_0^2 e^{2px} \tag{33}$$

and so we have the possible leading order (dominant) behaviors $U \sim U_0(t)e^{\pm(1/2)x}$. Corresponding to these leading order behaviors we obtain the recursion relations

$$j(j \pm 1)(j \pm 2)U_j = R_j, \tag{34}$$

for the coefficients of our Dirichlet series, where R_j is now a function not only of previous coefficients but also of their derivatives. Thus, corresponding respectively to the cases $p=-\frac{1}{2}$ and $p=\frac{1}{2}$, we seek solutions of the form

$$U = e^{-(1/2)x}\sum_{2j=0}^{\infty} U_j(t)e^{jx} = e^{-(1/2)x}(U_0(t) + U_{1/2}(t)e^{1/2x} + U_1(t)e^{x} + \cdots), \tag{35}$$

where the coefficients U_0, U_1, and U_2 will be left arbitrary, and

$$U = e^{1/2x}\sum_{2j=-\infty}^{0} U_j(t)e^{jx} = e^{1/2x}(U_0(t) + U_{-(1/2)}(t)e^{-(1/2)x} + U_{-1}(t)e^{-x} + \cdots), \tag{36}$$

where the coefficients U_0, U_{-1}, and U_{-2} will be left arbitrary.

Here we consider the case $p=-\frac{1}{2}$. Substitution of (35) into (31) yields

$$G[U] = e^{-x}\sum_{2j=0}^{\infty} G_j e^{jx} = 0, \tag{37}$$

where

$$G_0 = 0, \tag{38}$$

$$G_{1/2} = \tfrac{1}{8}(4U_0 + 3U_0U_{1/2} - 6U_0'), \tag{39}$$

$$G_1 = -U_{1/2}', \tag{40}$$

$$G_{3/2} = -\tfrac{1}{8}(4U_1 + 3U_{1/2}U_1 + 3U_0U_{3/2} + 6U_1'), \tag{41}$$

$$G_2 = -U_{3/2}, \tag{42}$$

and $'$ is used to denote derivatives with respect to t. We see that U_0 is left arbitrary, and that $U_{1/2}$ is determined by the equation $G_{1/2}=0$ as

$$U_{1/2} = -\frac{4}{3} + 2\frac{U_0'}{U_0}. \tag{43}$$

The equation $G_1=0$ does not determine U_1, which is left arbitrary. However, we have the compatibility condition $U_{1/2}'=0$, a condition not satisfied for arbitrary U_0. Moreover, we see that even if we were to have a satisfied compatibility condition at $j=1$, we would still have another compatibility condition to be satisfied at $j=2$. That is, the FW equation does not admit Dirichlet series solutions of the form (35).

The series (35), in order to satisfy the FW equation, needs to be modified by the inclusion of powers of x. Thus, instead of (35), we seek a solution of the form

$$\begin{aligned} U = e^{-(1/2)x}&(U_0 + U_{1/2}e^{(1/2)x} + (U_{1,0} + U_{1,1}x)e^{x} + (U_{3/2,0} + U_{3/2,1}x)e^{(3/2)x} \\ &+ (U_{2,0} + U_{2,1}x + U_{2,2}x^2)e^{2x} + (U_{5/2,0} + U_{5/2,1}x + U_{5/2,2}x^2)e^{(5/2)x} + \cdots), \end{aligned} \tag{44}$$

where as before all coefficients are functions of t. Substitution into (31) then gives

$$G[U] = e^{-x}\sum_{2j=0}^{\infty} \tilde{G}_j e^{jx} = 0, \tag{45}$$

where each $\tilde{G}_j$ is now polynomial in x:

$$\tilde{G}_0 = 0, \tag{46}$$

$$\tilde{G}_{1/2} = \tfrac{1}{8}(4U_0 + 3U_0U_{1/2} - 6U_0'), \tag{47}$$

$$\tilde{G}_1 = -U_0U_{1,1} - U_{1/2}', \tag{48}$$

$$\begin{aligned} \tilde{G}_{3/2} = &-\tfrac{1}{8}[4U_1 + 3U_{1/2}U_{1,0} + 8U_{1,1} + 2U_{1/2}U_{1,1} + 3U_0U_{3/2,0} + 2U_0U_{3/2,1} \\ &+ 6U_{1,0}' - 8U_{1,1}'] - \tfrac{1}{8}[4U_{1,1} + 3U_{1/2}U_{1,1} + 3U_0U_{3/2,1} + 6U_{1,1}']x, \end{aligned} \tag{49}$$

$$\begin{aligned} \tilde{G}_2 = &[2U_{1,0}U_{1,1} + 3U_{1,1}^2 - U_{3/2,0} - U_{3/2,1} + 2U_{1/2}U_{3/2,1} + 2U_0U_{2,1} \\ &+ 6U_0U_{2,2} + 2U_{3/2,1}'] + [2U_{1,1}^2 - U_{3/2,1} + 4U_0U_{2,2}]x, \end{aligned} \tag{50}$$

with $\tilde{G}_{5/2}$ being quadratic in x.

We see, as before, that U_0 is arbitrary, and that $U_{1/2}$ is determined by $\tilde{G}_{1/2}=0$ to be as given in (43). However at $j=1$, $U_{1,0}$ is left arbitrary, and $\tilde{G}_1=0$ determines the coefficient $U_{1,1}$. At j

$=3/2$, the equation $\tilde{G}_{3/2}=0$ determines both $U_{3/2,1}$ and $U_{3/2,0}$. Then at $j=2$, $U_{2,0}$ is left arbitrary and the equation $\tilde{G}_2=0$ determines $U_{2,2}$ and $U_{2,1}$. The equation $\tilde{G}_{5/2}=0$ determines the three coefficients $U_{5/2,2}$, $U_{5/2,1}$, and $U_{5/2,0}$. Our modified series therefore contains three arbitrary coefficients, U_0, $U_{1,0}$, and $U_{2,0}$. We thus see how a putative Dirichlet series needs to be modified in the case of failed compatibility conditions, so that the modified series satisfies the PDE/ODE and contains the predicted number of arbitrary coefficients. In Sec. VI we explain this modification process in terms of basic solution techniques for linear ODEs.

We now briefly remark on an alternative procedure which allows us to obtain a solution of the FW equation of the form (35), albeit not containing three arbitrary functions of t. This can be done by insisting that the compatibility conditions (40) and (42) be satisfied: (40) requires that $(\log(U_0))''=0$, and so $U_0=ae^{bt}$ for some arbitrary $a,b\in\mathbb{C}$; (42) then requires that $(\log(U_1))'=-b$, and so $U_1=ce^{-bt}$ for some arbitrary $c\in\mathbb{C}$. Thus for these choices of U_0 and U_1 we have a solution of the form (35) containing one arbitrary function of t, namely U_2. In the special case $U_2=0$ this infinite series becomes finite to give the exact solution $U=ae^{-(1/2)(x-2bt)}+\left(2b-\frac{4}{3}\right)+ce^{(1/2)(x-2bt)}$, as obtained in Ref. 12.

B. The Rosenau–Hyman equation

We now consider the Rosenau–Hyman (RH) equation,[22]

$$H[U]\equiv UU_{xxx}+3U_xU_{xx}+UU_x-U_t=0, \tag{51}$$

which corresponds to the parameter choice $(\epsilon,p^2,\beta,\kappa)=\left(0,-\frac{1}{4},3,0\right)$ in Eq. (19).

Proceeding as for the FW equation, we obtain the leading order or dominant behaviors $U\sim U_0(t)e^{\pm(i/2)x}$, and the corresponding recursion relations

$$j(j\pm i)(j\pm 2i)U_j=R_j \tag{52}$$

for the coefficients of our Dirichlet series, where R_j is a function of previous coefficients and their derivatives. Thus, corresponding respectively to the cases $p=-(i/2)$ and $p=i/2$, we seek solutions of the form

$$U=e^{-(i/2)x}\sum_{2k=0}^{\infty}U_k(t)e^{kix}=e^{-(i/2)x}(U_0(t)+U_{1/2}(t)e^{(i/2)x}+U_1(t)e^{ix}+\cdots), \tag{53}$$

where U_0, U_1, and U_2 (corresponding to $j=0,i,2i$) will be left arbitrary, and

$$U=e^{(i/2)x}\sum_{2k=-\infty}^{0}U_k(t)e^{kix}=e^{(i/2)x}(U_0(t)+U_{-(1/2)}(t)e^{-(i/2)x}+U_{-1}(t)e^{-ix}+\cdots), \tag{54}$$

where U_0, U_{-1}, and U_{-2} (corresponding to $j=0,-i,-2i$) will be left arbitrary.

Here we consider the case $p=-(i/2)$. Substitution of (53) into (51) yields

$$H[U]=e^{-ix}\sum_{2k=0}^{\infty}H_ke^{kix}=0, \tag{55}$$

where

$$H_0=0, \tag{56}$$

$$H_{1/2}=-\tfrac{1}{8}i(3U_0U_{1/2}-8iU_0'), \tag{57}$$

$$H_1=-U_{1/2}', \tag{58}$$

$$H_{3/2} = \tfrac{1}{8} i(3U_{1/2}U_1 + 3U_0U_{3/2} + 8iU_1'), \tag{59}$$

$$H_2 = -U_{3/2}'. \tag{60}$$

Thus U_0 is left arbitrary, and $U_{1/2}$ is determined by the equation $H_{1/2}=0$ as

$$U_{1/2} = \frac{8}{3} i \frac{U_0'}{U_0}. \tag{61}$$

Then U_1 is left arbitrary, with compatibility condition $H_1=0$, or $U_{1/2}'=0$; this condition is not satisfied for arbitrary U_0. Further—as for the FW equation—even if this condition at $j=i$ were to be satisfied, we would still have another compatibility condition, $H_2=0$, to be satisfied at $j=2i$. Thus we see that the RH equation does not admit Dirichlet series solutions of the form (53).

The series (53), in order to satisfy the RH equation, needs to be modified by the inclusion of powers of x. Thus, instead of (53), we seek a solution of the form

$$\begin{aligned} U = e^{-(i/2)x}(U_0 + U_{1/2}e^{i/2x} + (U_{1,0} + U_{1,1}x)e^{ix} + (U_{3/2,0} + U_{3/2,1}x)e^{(3i/2)x} \\ + (U_{2,0} + U_{2,1}x + U_{2,2}x^2)e^{2ix} + (U_{5/2,0} + U_{5/2,1}x + U_{5/2,2}x^2)e^{(5i/2)x} + \cdots), \end{aligned} \tag{62}$$

where as before all coefficients are functions of t. Substituting into (51), we find that U_0, $U_{1,0}$, and $U_{2,0}$ are left arbitrary with all other coefficients in our series determined in terms of these three.

Once again, as for the FW equation, we can also obtain a solution of the RH equation of the form (53) but depending on less than three arbitrary functions of t, by insisting that the compatibility conditions (58) and (60) be satisfied. Condition (58) requires that $(\log(U_0))''=0$, and so $U_0=ae^{bt}$ for some arbitrary $a,b\in\mathbb{C}$. Then condition (60) requires that $U_1''-b^2U_1=0$, and so $U_1=ce^{-bt}+de^{bt}$ for some arbitrary $c,d\in\mathbb{C}$. For these choices of U_0 and U_1 we have a solution of the form (53) containing one arbitrary function of t, U_2. In the special case $U_2=0$ and $d=0$ this infinite series self-truncates to give the exact solution $U=ae^{-(i/2)(x+2bit)}+\frac{8}{3}bi+ce^{(i/2)(x+2bit)}$, as obtained in Ref. 12.

C. A further example in 1+1 dimensions

In Secs. IV A and IV B we have seen that the FW and RH equations fail to admit Dirichlet series solutions. In this they therefore differ from the completely integrable FFCH and DP equations. Of course, in general, the integrability of a nonsemilinear PDE not admitting (standard) Dirichlet series solutions remains an open question.

In this section we will see that it is not always the case that a nonintegrable equation fails to admit Dirichlet series solutions. That is, the admission of Dirichlet series solutions is not sufficient for integrability. In order to show this we will consider in this section a special case of the class of equations (19), namely those that can be put in the form (25) with $\hat{\epsilon}=1$, and in addition with β an integer $\geqslant 2$,

$$K[U] \equiv UU_{xxx} + \beta U_xU_{xx} - (\beta+1)UU_x + U_{xxt} - U_t = 0. \tag{63}$$

We know from Ref. 18 that only those equations (63) having $\beta=2$ or $\beta=3$ are completely integrable. However, as we will see, all equations (63) admit Dirichlet series solutions. We note that the FW and RH equations are not included in the class (63): for the FW equation, we cannot remove the U_x term, and in any case—as also for the RH equation—we do not have $\hat{\epsilon}=p^2\epsilon=1$ (see Sec. III).

Seeking a leading order behavior for a possible Dirichlet series solution of (63) leads to $U \sim U_0(t)e^{\pm x}$, with corresponding recursion relations

$$j(j\pm 2)(j\pm\beta\pm 1)U_j = R_j, \tag{64}$$

where R_j is a function of previous coefficients and their derivatives.

Here we consider the case $U \sim U_0(t)e^{-x}$. We claim that each equation in the class (63) has a Dirichlet series solution of the form

$$U = U_0(t)e^{-x} + U_2(t)e^{x} + \sum_{j=\beta+1}^{\infty} U_j(t)e^{(j-1)x}, \tag{65}$$

with U_0, U_2, and $U_{\beta+1}$ arbitrary. In order to show this, we substitute (65) into (63) to obtain

$$K[U] = e^{-2x}\sum_{j=0}^{\infty} K_j e^{jx} = 0, \tag{66}$$

and show that each K_j, for $j \leqslant \beta+1$, is identically zero. That is, we need to prove that (66) is in fact

$$K[U] = e^{-2x}\sum_{j=\beta+2}^{\infty} K_j e^{jx} = 0. \tag{67}$$

If this is so, then for $j \geqslant \beta+2$, each equation $K_j=0$ will determine U_j in terms of U_0, U_2, and $U_{\beta+1}$.

Our discussion of this example is simplified by the fact that all equations in class (63) can be written in the factorized form,[12]

$$K[U] = \left(U\frac{\partial}{\partial x} + \beta U_x + \frac{\partial}{\partial t}\right)(U_{xx} - U) = 0. \tag{68}$$

Setting

$$U = U_0(t)e^{-x} + U_2(t)e^{x} + U_{\beta+1}(t)e^{\beta x} + U_{\beta+2}(t)e^{(\beta+1)x} + \cdots, \tag{69}$$

we therefore calculate

$$U_{xx} - U = (\beta^2 - 1)U_{\beta+1}(t)e^{\beta x} + (\beta^2 + 2\beta)U_{\beta+2}(t)e^{(\beta+1)x} + \cdots, \tag{70}$$

and thus obtain

$$K[U] = [(\beta^2 + 2\beta)U_0(t)U_{\beta+2}(t) + (\beta^2 - 1)U'_{\beta+1}(t)]e^{\beta x} + \cdots = K_{\beta+2}e^{\beta x} + \cdots, \tag{71}$$

as required [compare with (67)].

Thus we see that all equations in the class (63) admit formal Dirichlet series solutions of the form (65). It then follows, using the discrete symmetry $(x,t) \to (-x,-t)$ of (63), that these equations also admit formal Dirichlet series of the form

$$U = \widetilde{U}_0(t)e^{x} + \widetilde{U}_{-2}(t)e^{-x} + \sum_{j=-\infty}^{-(\beta+1)} \widetilde{U}_j(t)e^{(j+1)x} \tag{72}$$

$$= \widetilde{U}_0(t)e^{x} + \widetilde{U}_{-2}(t)e^{-x} + \widetilde{U}_{-(\beta+1)}e^{-\beta x} + \widetilde{U}_{-(\beta+2)}e^{-(\beta+1)x} + \cdots, \tag{73}$$

where $\overline{U_0}(t)$, $\widetilde{U}_{-2}(t)$, and $\widetilde{U}_{-(\beta+1)}$ are arbitrary, and where all other coefficients in the series are determined in terms of these three.

V. EXAMPLES IN MULTIDIMENSIONS

A. The Kraenkel–Zenchuk system

We now turn to an example of a completely integrable PDE in multidimensions, namely the Kraenkel–Zenchuk (KZ) system,[23–25]

$$L_1 \equiv -m_t + um_x + 2mu_x = 0, \tag{74}$$

$$L_2 \equiv mu_y + u_x - u_{xx} - 2p_x = 0, \tag{75}$$

$$L_3 \equiv m^2 p_y + mp_x + mp_{xx} - pm_x - p_x m_x = 0, \tag{76}$$

which constitutes an extension of the FFCH equation to $2+1$ dimensions. This system fails the Painlevé PDE test: in fact it admits weak Painlevé expansions.[26] It thus behaves similarly to the FFCH and DP equations (see, respectively, Ref. 12 and Sec. III). Here we see that this system admits Dirichlet series solutions.

For this system, we find corresponding to the leading order behavior

$$u \sim u_0(y,t)e^{-x}, \quad m \sim m_0(y,t)e^{2x}, \quad p \sim p_0(y,t)e^{-x}, \tag{77}$$

where $p_0 = u_0$, and u_0 and m_0 are arbitrary, the recursion relation

$$\mathbf{J}\begin{pmatrix} u_j \\ m_j \\ p_j \end{pmatrix} \equiv \begin{pmatrix} 2jm_0 & ju_0 & 0 \\ -(j-2)(j-1) & 0 & -2(j-1) \\ 0 & 0 & j(j-3)m_0 \end{pmatrix}\begin{pmatrix} u_j \\ m_j \\ p_j \end{pmatrix} = \begin{pmatrix} R_{1j} \\ R_{2j} \\ R_{3j} \end{pmatrix}, \tag{78}$$

where R_{1j}, R_{2j}, and R_{3j} are functions of previous coefficients and their derivatives. Arbitrary coefficients will enter our expansions at values of j satisfying

$$\det \mathbf{J} = 0, \quad \text{i.e.,} \quad j^2(j-1)(j-2)(j-3) = 0. \tag{79}$$

At $j=0$, the two arbitrary coefficients are u_0 and m_0, as noted previously.

We therefore seek a Dirichlet series solution of the KZ system of the form

$$u = e^{-x}\sum_{j=0}^{\infty} u_j e^{jx}, \quad m = e^{2x}\sum_{j=0}^{\infty} m_j e^{jx}, \quad p = e^{-x}\sum_{j=0}^{\infty} p_j e^{jx}, \tag{80}$$

with $p_0 = u_0$. Substitution into the KZ system yields

$$L_1 = e^{x}\sum_{j=0}^{\infty} L_{1j}e^{jx} = 0, \quad L_2 = e^{-x}\sum_{j=0}^{\infty} L_{2j}e^{jx} = 0, \quad L_3 = e^{x}\sum_{j=0}^{\infty} L_{3j}e^{jx} = 0, \tag{81}$$

where L_{10}, L_{20}, and L_{30} are identically zero, and where of course for $j \geqslant 1$ [compare (78)], we have $(L_{1j}, L_{2j}, L_{3j})^T = \mathbf{J}(j)(u_j, m_j, p_j)^T - (R_{1j}, R_{2j}, R_{3j})^T$.

At $j=1$, we see from (78) that one of the coefficients u_1 or m_1 will be left arbitrary, and that we have as corresponding compatibility condition $L_{21}=0$. This compatibility condition is satisfied. We then use the equation $L_{31}=0$ to determine p_1, and $L_{11}=0$ to determine m_1, leaving u_1 arbitrary. At $j=2$, we see from (78) that one of u_2 or m_2 will be left arbitrary, and that the corresponding compatibility condition is $m_0 L_{22} - L_{32} = 0$. This condition is satisfied. We then use the equation $L_{32}=0$ to determine p_2, and $L_{12}=0$ to determine m_2, leaving u_2 arbitrary. At $j=3$, we see that one of the coefficients u_3, m_3, or p_3 will be left arbitrary, and that the corresponding compatibility condition is $L_{33}=0$. Again, the compatibility condition is satisfied. We then use the equation $L_{23}=0$ to determine p_3, and $L_{13}=0$ to determine m_3, leaving u_3 arbitrary. All coefficients in the series (81) are then determined in terms of the five arbitrary coefficients u_0, m_0, u_1, u_2, and u_3. This number of arbitrary coefficients is consistent with the order of the KZ system (see also Ref. 26). Thus we see that we have another example of a weak Painlevé but completely integrable system which admits Dirichlet series solutions.

B. A further example in 2+1 dimensions

Here we consider an alternative generalization of the FFCH equation to $2+1$ dimensions, one based on a nonisospectral scattering problem: discussions of such scattering problems can be found for example in Refs. 27–29, as well as in Refs. 8 and 9. This completely integrable equation,

$$M[U] \equiv \tfrac{1}{2}U_{xxxx}U_y + U_{xxx}U_{xy} - \tfrac{1}{2}U_{xx}U_y - U_{xy}U_x + U_{xxxt} - U_{xt} = 0, \tag{82}$$

was given in Ref. 30. The reduction

$$U(x,y,t) = W(z,\tau), \quad z = x + y, \quad \tau = \tfrac{1}{2}t, \tag{83}$$

yields the FFCH equation in W_z, with $\kappa = 0$ (which is anyway equivalent to the case $\kappa \neq 0$; see Sec. III).

We note in passing that Eq. (82) admits a solution in the form of a weak Painlevé expansion,

$$U = U_{(-5/3)} - \frac{1}{\psi_y}(2\psi_t + U_{(-5/3),y})\phi + \phi^{5/3}\sum_{j=0}^{\infty} U_{j/3}\phi^{j/3}, \tag{84}$$

where all coefficients $U_{(-5/3)}, U_0, U_{1/3}, U_{2/3}, \ldots$ are functions of (y,t), and $\phi = x + \psi(y,t)$.

The expansion (84) contains four arbitrary functions $(U_{(-5/3)}, \psi, U_0, U_{2/3})$ of (y,t), corresponding to the resonances $-5/3, -1, 0, 2/3$, respectively. We note that for this equation the negative resonance at $-5/3$ can be catered for by introducing an extra coefficient at constant level (i.e., at level ϕ^0); for a further example where this can be done we refer to Ref. 26. We also remark that the term at level ϕ in (84) is an additional lower order term which corrects the balancing of terms in the leading order analysis. Further examples of the use of such an additional term, although at constant level rather than level ϕ, can be found in Ref. 12, as well as in Refs. 26 and 31; see also the weak Painlevé expansion for the DP equation given in Sec. III.

We now turn to the construction of Dirichlet series solutions for Eq. (82). Proceeding as in previous sections, we obtain for Eq. (82) the leading order behaviors $U \sim U_0(y,t)e^{\pm x}$, with corresponding recursion relations

$$j(j \pm 1)(j \pm 2)(j \pm 3)U_j = R_j, \tag{85}$$

where R_j is a function of previous coefficients and their derivatives.

Let us consider the case $U \sim U_0(y,t)e^{-x}$, corresponding to which we seek a Dirichlet series solution

$$U = e^{-x}\sum_{j=0}^{\infty} U_j(y,t)e^{jx}, \tag{86}$$

where the coefficients U_0, U_1, U_2, and U_3 will be left arbitrary. Substitution of (86) into (82) yields

$$M[U] = e^{-2x}\sum_{j=0}^{\infty} M_j e^{jx}, \tag{87}$$

where M_0, M_1, M_2, and M_3 are all identically zero. Thus we see that all compatibility conditions are satisfied, and that Eq. (82) does indeed admit formal Dirichlet series solutions of the form (86), with U_0, U_1, U_2, and U_3 arbitrary, and all other coefficients determined in terms of these four.

It then follows, using the discrete symmetry $(x,t) \to (-x,-t)$ of Eq. (82), that this equation also admits formal Dirichlet series solutions of the form

$$U = e^x \sum_{j=-\infty}^{0} \tilde{U}_j(y,t) e^{jx}. \tag{88}$$

Thus Eq. (82) provides a further example of a completely integrable PDE, again in $2+1$ dimensions, which admits formal Dirichlet series solutions.

VI. TECHNICAL CONSIDERATIONS

In previous sections we have considered the construction of formal Dirichlet series solutions of a certain form, with coefficients determined recursively by linear algebraic equations (thus in the present paper we do not consider series having coefficients determined by a sequence of differential equations), for a wide variety of differential equations. We now turn to some technical points related to such series solutions, including how our approach can be understood as an extension of basic solution techniques for linear ODEs.

A. Convergence

We have not, for the examples presented in earlier sections, considered the convergence or otherwise of the Dirichlet series solutions constructed. Here—rather than considering general approaches to proving convergence—we present a simple ODE example which shows us that such series solutions can be convergent, in which case they do give meaningful information about the behavior of solutions. In particular, we see that a Dirichlet series solution may indeed turn out to represent a solution which is analytic in some half-plane (see comments in Sec. II). This is in turn related to a second motivation behind the discussion in this section, which is the question of whether Dirichlet series are not, for certain equations, better suited to the representation of solutions than Painlevé expansions.

We consider the ODE

$$N[U] \equiv UU_{xx} - 2U_x^2 + UU_x = 0, \tag{89}$$

for which we obtain the leading order behaviors $U \sim U_0 e^{px}$ (U_0 constant), with $p=1$ or $p=0$. We note that here, in the absence of any additional linear terms, the choice $p=0$ is allowed.

Corresponding to $p=1$, i.e., $U \sim U_0 e^x$, we obtain the recursion relation

$$j(j-1)U_j = R_j \tag{90}$$

for the coefficients of our Dirichlet series, where R_j is a function of previous coefficients. In this case we therefore seek a Dirichlet series solution

$$U = e^x \sum_{j=0}^{\infty} U_j e^{jx}. \tag{91}$$

Substitution into (89) yields

$$N[U] = e^{2x} \sum_{j=0}^{\infty} N_j e^{jx}, \tag{92}$$

where N_0 and N_1 are identically zero. Thus we obtain a formal Dirichlet series solution (91), with U_0 and U_1 arbitrary and all other coefficients determined in terms of these two.

Meanwhile, for the case $p=0$, i.e. $U \sim \tilde{U}_0$, we obtain the recursion relation

$$j(j+1)\tilde{U}_j = R_j \tag{93}$$

for the coefficients of our Dirichlet series, R_j being a function of previous coefficients. We now therefore seek a Dirichlet series solution

$$U = \sum_{j=-\infty}^{0} \tilde{U}_j e^{jx}. \tag{94}$$

Substitution into our Eq. (89) yields

$$N[U] = \sum_{j=-\infty}^{0} \tilde{N}_j e^{jx}, \tag{95}$$

where $\tilde{N}_0$ and $\tilde{N}_{-1}$ are identically zero. We therefore obtain a formal Dirichlet series solution (94), with $\tilde{U}_0$ and $\tilde{U}_{-1}$ arbitrary, and all other coefficients determined in terms of these two.

Each of the series solutions (91) and (94) is in fact summable. The ODE (89) has the general solution

$$U = \frac{Ae^x}{B - e^x}, \tag{96}$$

where A, $B \in \mathbb{C}$ are two arbitrary constants of integration. This function can be represented by the Dirichlet series

$$U = e^x \sum_{j=0}^{\infty} \left(\frac{A}{B^{j+1}} \right) e^{jx}, \tag{97}$$

for $\mathrm{Re}(x) < \log|B|$, and also by the Dirichlet series

$$U = \sum_{j=-\infty}^{0} \left(\frac{-A}{B^j} \right) e^{jx}, \tag{98}$$

for $\mathrm{Re}(x) > \log|B|$. We can identify (97) with (91), with $U_0 = A/B$ and $U_1 = A/B^2$, and thus conclude that (91) is convergent to a solution analytic in the left half-plane $\mathrm{Re}(x) < \log|U_0/U_1|$. Similarly, we can identify (98) with (94), with $\tilde{U}_0 = -A$ and $\tilde{U}_{-1} = -AB$. Thus we see that (94) is convergent to a solution analytic in the right half-plane $\mathrm{Re}(x) > \log|\tilde{U}_{-1}/\tilde{U}_0|$.

The function (96) is of course analytic except for simple poles spaced at intervals of 2π along the line $\mathrm{Re}(x) = \log|B|$. The general solution of the ODE (89) therefore has no movable branched singularities, and so has the Painlevé property. We note that since these poles are at $x = \log|B| + i \arg B$, their locations depend on the value of (one of) the constants of integration, and so they are movable. The two Dirichlet series represent the function (96) on either side of this line of poles. Thus our Dirichlet series solutions seem to be much more suited to the representation of the general solution of this ODE than the usual Painlevé expansion, which would only give a solution convergent in a punctured disk of radius 2π, centered at a pole (although it is this last that gives information about the nature of the singularities).

B. Linear and multilinear differential equations

We have developed a method of seeking solutions in the form of Dirichlet series for differential equations having a set of constant-coefficient multilinear terms, illustrated using examples where these terms are quadratic, or bilinear; we use these terms to determine possible leading orders. However, the simplest example where our approach can be applied is that of the constant-coefficient linear ODE,

$$\left(\prod_{j=1}^{N} (D - \mu_j)^{n_j} \right) U = f(x), \quad D = \frac{d}{dx}, \tag{99}$$

where $n_j \in \mathbb{N}$ and $\mu_j \in \mathbb{C}$, and where for our purposes it is sufficient to assume that

$$f(x) = \sum_{j=1}^{N} P_j(x) e^{\mu_j x}, \tag{100}$$

for some polynomials P_j of x. In the case where all $n_j = 1$ and all $P_j(x) \equiv 0$, the general solution of this ODE consists of a linear combination of terms $e^{\mu_j x}$,

$$U = \sum_{j=1}^{N} A_j e^{\mu_j x}, \quad A_j \in \mathbb{C}. \tag{101}$$

If the constants μ_j lie on a line in the complex plane [of course, since the equation is linear, the general solution (101) can always be decomposed into a sum of solutions U_k, where this is true for each U_k], this solution can be understood as a *finite* Dirichlet series [compare (2)]. Such a Dirichlet series, when some $n_j > 1$, or some $P_j(x) \not\equiv 0$, needs, in order to give the general solution of the ODE, to be modified by the inclusion of powers of x; in the language used earlier, we would say that in the case where some $P_j(x) \not\equiv 0$ we have a failed compatibility condition at the resonance μ_j. The use of infinite Dirichlet series represents the extension of such basic solution techniques for linear ODEs to nonlinear differential equations.

C. Doubly infinite series

Here we simply comment that Dirichlet-type series of a more general form than the standard Dirichlet series (2) may be used to represent solutions of differential equations. For example, the ODE

$$P[U] \equiv U_{xx} + 3e^x U U_x - U_x + e^{2x} U^3 = 0 \tag{102}$$

has the general solution

$$U = \frac{1}{e^x - A} + \frac{1}{e^x - B}, \tag{103}$$

which—assuming $|A| < |B|$—can be represented by the series

$$U = e^{-x} \sum_{j=-\infty}^{\infty} U_j e^{jx} \tag{104}$$

for $\log|A| < \mathrm{Re}(x) < \log|B|$, where

$$U_j = \begin{cases} 1/A^j & j \leqslant 0, \\ -1/B^j, & j > 0. \end{cases} \tag{105}$$

Thus we have a representation of the general solution of the ODE (102) as a doubly infinite series, which is convergent in the strip $\log|A| < \mathrm{Re}(x) < \log|B|$, rather than in a half-plane.

The general solution (103) of Eq. (102) is analytic except for simple poles, and so this equation has the Painlevé property. There are two families of simple poles, spaced at intervals of 2π along the lines $\mathrm{Re}(x) = \log|A|$ and $\mathrm{Re}(x) = \log|B|$; since the locations of these poles, at $x = \log|A| + i \arg A$ and $x = \log|B| + i \arg B$, depend on the constants of integration, they are movable. The series (104) provides a representation of the general solution in the strip between these two lines of poles. Clearly, in addition to (104), we also have the Dirichlet series solutions

$$U = \sum_{j=0}^{\infty} \left(-\frac{1}{A^{j+1}} - \frac{1}{B^{j+1}} \right) e^{jx} \tag{106}$$

and

$$U = e^{-x} \sum_{j=-\infty}^{0} \left(\frac{1}{A^j} + \frac{1}{B^j} \right) e^{jx}, \tag{107}$$

convergent for $\mathrm{Re}(x) < \log|A|$ and $\mathrm{Re}(x) > \log|B|$, respectively. Together, the three series solutions given above provide representations of the general solution of Eq. (102) in all the complex plane except on the two lines $\mathrm{Re}(x) = \log|A|$ and $\mathrm{Re}(x) = \log|B|$. As with our previous example discussed in Sec. VI A, such series solutions appear to be much more suited to representing the general solution of this ODE than would be the usual Painlevé expansion. Of course, this is because of the form of the general solution; as remarked in Sec. I, there is no reason why the general solution of any given ODE should admit such a representation. However, for this ODE, such series seem more appropriate than Taylor or Laurent series. We also note that this example demonstrates the possibility of seeking Dirichlet-type series solutions when we have nonautonomous dominant terms.

D. A perturbative technique

In all of our examples so far, except for the ODE discussed in Sec. VI A, we have excluded from consideration the leading order behavior $p=0$, on the grounds that the terms of highest nonlinearity are then no longer dominant over the other terms in the equation. However, the possibility of $p=0$ occurring as a leading order behavior is one that needs to be taken into account. Here we consider two examples, one an ODE and one a PDE: we find that even for integrable differential equations it may happen that series solutions in terms of exponentials require modification by the inclusion of power of x. Our results are obtained using a perturbative approach.

1. An ODE example

Here we consider the ODE

$$Q[U] \equiv UU_{xxx} + 2U_xU_{xx} - 3UU_x = 0, \tag{108}$$

which consists of the quadratic terms of the FFCH equation, and also of the ODE (3). As mentioned in Sec. II, $p=0$ occurs as a possible leading order behavior of solutions of this ODE (in addition to $p=\pm 1$ and corresponding to these the series obtained from those of FFCH via the reduction $\partial/\partial t=0$ and $\kappa=0$). For this choice $p=0$, we obtain the recursion relation

$$j(j^2-3)U_j = R_j, \tag{109}$$

and so we have resonances at $j=0, \pm\sqrt{3}$. Corresponding to this leading order behavior, we find that we can construct a Dirichlet series solution of the form

$$U = U_0 + U_{\sqrt{3}}e^{\sqrt{3}x} + U_{2\sqrt{3}}e^{2\sqrt{3}x} + U_{3\sqrt{3}}e^{3\sqrt{3}x}\cdots, \tag{110}$$

where U_0 and $U_{\sqrt{3}}$ are arbitrary constants, and with all remaining coefficients (constants) being determined in terms of these two. It then follows, from the discrete symmetry $x \to -x$ of the ODE (3), that we also have a Dirichlet series solution

$$U = U_0 + U_{-\sqrt{3}}e^{-\sqrt{3}x} + U_{-2\sqrt{3}}e^{-2\sqrt{3}x} + U_{-3\sqrt{3}}e^{-3\sqrt{3}x} + \cdots, \tag{111}$$

this having the same coefficients as the Dirichlet series solution (110).

However, in order to construct a solution of our third order ODE containing three arbitrary constants—one for each resonance—a different approach needs to be used. Thus we consider a perturbation about the constant solution $U=U_0$,

$$U = U_0 + \epsilon V + \epsilon^2 W + \epsilon^3 Z + \cdots, \tag{112}$$

which then gives a sequence of ODEs, the first three of which are

$$U_0(V_{xxx} - 3V_x) = 0, \tag{113}$$

$$U_0(W_{xxx} - 3W_x) = 3VV_x - 2V_xV_{xx} - VV_{xxx}, \tag{114}$$

$$U_0(Z_{xxx} - 3Z_x) = 3WV_x + 3W_xV - 2W_{xx}V_x - 2W_xV_{xx} - WV_{xxx} - W_{xxx}V. \tag{115}$$

As a solution of (113) we take

$$V = V_{-\sqrt{3}}e^{-\sqrt{3}x} + V_{\sqrt{3}}e^{\sqrt{3}x}, \tag{116}$$

where $V_{-\sqrt{3}}$ and $V_{\sqrt{3}}$ are two arbitrary constants corresponding to the resonances $j=\pm\sqrt{3}$ (we already have an arbitrary constant corresponding to the resonance $j=0$ at order ϵ^0). For this choice of V, we then take as solution of Eq. (114)

$$W = W_{-2\sqrt{3}}e^{-2\sqrt{3}x} + W_{2\sqrt{3}}e^{2\sqrt{3}x}, \tag{117}$$

where $W_{-2\sqrt{3}}$ and $W_{2\sqrt{3}}$ are determined as

$$W_{-2\sqrt{3}} = -\frac{1}{3}\frac{(V_{-\sqrt{3}})^2}{U_0}, \quad W_{2\sqrt{3}} = -\frac{1}{3}\frac{(V_{\sqrt{3}})^2}{U_0}, \tag{118}$$

and where, since we already have three arbitrary coefficients in (112), we do not include any further such here. Then as a solution of Eq. (115) we take

$$Z = Z_{-3\sqrt{3}}e^{-3\sqrt{3}x} + Z_{-\sqrt{3}}xe^{-\sqrt{3}x} + Z_{\sqrt{3}}xe^{\sqrt{3}x} + Z_{3\sqrt{3}}e^{3\sqrt{3}x}, \tag{119}$$

whose four coefficients, determined in terms of U_0, $V_{-\sqrt{3}}$ and $V_{\sqrt{3}}$, are in the general case nonzero. We note that, formally, since at each order of ϵ we need to introduce higher powers of $e^{\pm\sqrt{3}x}$, our perturbation results in a doubly infinite series. We see from the above that, at order ϵ^3, we need to introduce powers of x into (112).

2. A PDE example

We now consider the following nonsemilinear PDE:

$$R[U] \equiv U_{xxxx}U_t + 2U_{xxx}U_{xt} - U_{xx}U_t - 2U_xU_{xt} = 0, \tag{120}$$

which corresponds to the reduction $\partial/\partial t=0$ (with y then relabelled as t) of Eq. (82). In the absence of additional linear terms, in addition to $p=\pm 1$ and the corresponding series obtained by reduction from those in Sec. V B, $p=0$ is a possible leading order behavior. Corresponding to this choice $p=0$, we obtain the recursion relation

$$j^2(j^2-1)U_j = R_j, \tag{121}$$

and so the resonances $j=0,0,\pm 1$. Proceeding as in the previous section, we take

$$U = U_0 + \epsilon V + \epsilon^2 W + \cdots, \tag{122}$$

i.e., we make a perturbation about the solution $U=U_0(t)$. We thus obtain a sequence of PDEs, the first two of which are

$$U_0'(V_{xxxx} - V_{xx}) = 0, \tag{123}$$

$$U_0'(W_{xxxx} - W_{xx}) = -V_{xxxx}V_t - 2V_{xxx}V_{xt} + V_{xx}V_t + 2V_xV_{xt}. \tag{124}$$

As solution of the first of the above, we take

$$V = V_{-1}(t)e^{-x} + V_0(t)x + V_1(t)e^{x}, \tag{125}$$

where V_{-1}, V_0, and V_1 are three arbitrary functions of t, and as solution of the second

$$W = W_{-1}(t)xe^{-x} + W_0(t)x^2 + W_1(t)xe^{x}, \tag{126}$$

where

$$W_{-1} = \frac{V_0 V_{-1}'}{U_0'}, \quad W_0 = -\frac{V_0 V_0'}{U_0'}, \quad W_1 = \frac{V_0 V_1'}{U_0'}. \tag{127}$$

Thus we have four arbitrary functions of t (U_0, V_{-1}, V_0, and V_1), one corresponding to each of the resonances $j=0,0,\pm 1$. We see that for this example, consideration of the case $p=0$ leads to the introduction of powers of x in our perturbation expansion, basically because of the double resonance at $j=0$. Given that the PDE (120) is completely integrable—it has the Lax pair

$$\psi_{xx} = \tfrac{1}{4}[1 - \lambda(U_{xxx} - U_x)]\psi, \tag{128}$$

$$\psi_t = \tfrac{1}{2}\lambda U_t \psi_x - \tfrac{1}{4}\lambda U_{xt}\psi, \tag{129}$$

—this then implies that needing to modify such a formal series solution with powers of x is not enough to claim non-integrability. However, as we will see in Sec. VII, for some PDEs we can establish a direct link between needing to modify a (standard) Dirichlet series solution in this way and their apparent nonintegrability.

VII. DISCUSSION: DIRICHLET SERIES AND INTEGRABILITY

One of the main aims of this paper has been to explore, for nonsemilinear PDEs, the connection between integrability and Dirichlet series solutions. Our motivation was the work in Refs. 6 and 7 where not only was it observed that the FFCH and DP equations admit standard Dirichlet series solutions, but also that, for certain classes of PDEs, the only equations admitting such solutions were transformable back onto the only known completely integrable PDEs within those classes. Here we have given other examples of completely integrable nonsemilinear PDEs, both in $1+1$ and multidimensions, which admit standard Dirichlet series solutions.

However, we have also seen that nonintegrable PDEs may admit Dirichlet series solutions; that is, the admission of Dirichlet series solutions is not sufficient for integrability. This result might be as expected, since such series—even if convergent—provide only partial information about the behavior of solutions. Thus, the techniques explored here should be regarded as being *complementary* to known techniques (e.g., Painlevé analysis, and the use of hodograph transformations). [The ODE (3), for example, while admitting standard Dirichlet series solutions, also has branched solutions; we have the weak Painlevé expansion $V=(x-x_0)^{2/3}\Sigma_{j=0}^{\infty}V_{j/3}(x-x_0)^{j/3}$, where x_0, V_0, and $V_{2/3}$ are arbitrary. Consideration of the function

$$U = \frac{1}{(e^x - A)^{1/2}}$$

is also instructive.]

We have also seen, using a perturbative approach, that generalized Dirichlet series solutions of integrable PDEs may require modification by the inclusion of powers of x; examples include Eq. (120), as well as, by implication from the results of Sec. VI D 1, the FFCH equation. Strictly speaking, this tells us that the admission of Dirichlet series solutions (allowing here, as we should, such more general formulations within our definition) is not a necessary condition for integrability. Of course, there is no reason to expect a simple relationship between integrability and Dirichlet series, especially given the well known problems that equations of the type being considered here present for other integrability tests, e.g. for the Painlevé tests. However, it may also be that we should, as in the previous papers on classification using Dirichlet series,[6,7] restrict our attention to

standard Dirichlet series; it is certainly the case that in Refs. 6 and 7 the use of standard Dirichlet series isolated what were essentially the FFCH and DP equations. (Of course, a complete classification of integrable equations in the classes considered in Refs. 6 and 7 remains an open problem.)

We conclude this section with an example where modification by powers of x of a standard Dirichlet series solution can be directly related to the apparent nonintegrability of a PDE, although of course in general the integrability of a nonsemilinear PDE not admitting such Dirichlet series solutions remains an open question. This PDE is the x-derivative of the FFCH equation,

$$S[U] \equiv (UU_{xxx} + 2U_xU_{xx} - 3UU_x + U_{xxt} - U_t - 2\kappa U_x)_x = 0, \tag{130}$$

and has for the leading order behaviors $U \sim U_0(t)e^{\pm x}$ the recursion relations

$$j(j \pm 2)^2(j \pm 3)U_j = R_j, \tag{131}$$

and so resonances $j = 0, \mp 2, \mp 2, \mp 3$. We know from our results for the FFCH equation that, corresponding to the leading order behavior $U \sim U_0(t)e^{-x}$, the PDE (130) has a standard Dirichlet series solution

$$U = e^{-x}\sum_{j=0}^{\infty} U_j(t)e^{jx}, \tag{132}$$

with U_0, U_2, and U_3 arbitrary. However, because of the double resonance at $j=2$, this solution needs to be modified. As a solution of Eq. (130) we therefore obtain

$$\begin{aligned} U = e^{-x}(&U_0(t) + U_1(t)e^x + (U_{2,0}(t) + U_{2,1}(t)x)e^{2x} + (U_{3,0}(t) + U_{3,1}(t)x)e^{3x} \\ &+ (U_{4,0}(t) + U_{4,1}(t)x)e^{4x} + (U_{5,0}(t) + U_{5,1}(t)x + U_{5,2}(t)x^2)e^{5x} + \cdots), \end{aligned} \tag{133}$$

where now U_0, $U_{2,0}$, $U_{2,1}$, and $U_{3,0}$ are arbitrary. Thus we see that we need to modify our standard Dirichlet series solution by including powers of x. [Similarly for the series corresponding to the leading order behavior $U \sim U_0(t)e^x$; alternatively we may use in (133) the discrete symmetry $(x,t) \to (-x,-t)$ of Eq. (130).]

The extra resonance at $j=2$, when compared to the leading order behavior $U \sim U_0(t)e^{-x}$ of the FFCH equation, arises because of the overall x-derivative in Eq. (130). Meanwhile, the travelling wave reduction $U(x,t) = W(z) - m$, $z = x + mt$, yields the ODE

$$WW_{zzz} + 2W_zW_{zz} - 3WW_z - \alpha W_z + \beta = 0, \tag{134}$$

where the constant α is defined as $\alpha = 2\kappa - 2m$, and β is a constant of integration. A nonlinear time transformation (following Ref. 32) then yields an ODE which does not have the Painlevé property, in contrast to the case of the FFCH equation itself discussed in Ref. 32. This is then suggestive of the nonintegrability of Eq. (130); for details see Ref. 31, where a $2+1$-dimensional version of this PDE is considered. The reason why the ODE obtained from Eq. (134) does not have the Painlevé property is because of the constant of integration β, which arises precisely because of the overall x-derivative in Eq. (130). Thus we see that the inclusion of powers of x in the standard Dirichlet series solution (132)—to obtain the modified Dirichlet series solution (133)—can be directly related to the apparent nonintegrability of the PDE (130). It is worth recalling here that the x-derivative of the completely integrable modified Korteweg–de Vries equation, $(U_t - U_{xxx} + 6U^2U_x)_x = 0$, fails the Weiss–Tabor–Carnevale Painlevé test,[16] and so is presumably nonintegrable.

VIII. CONCLUSIONS

Our main conclusions are as follows:

(1) For certain classes of equations, there is a strong connection between standard Dirichlet series solutions and integrability. This follows from Refs. 6 and 7, and from our results for the integrable and nonintegrable equations discussed here.
(2) This connection is, however, difficult to unravel: standard Dirichlet series solutions are not sufficient for integrability and, despite the results presented here, we remain at this stage reluctant to claim necessity.
(3) For some equations, Dirichlet-type series give useful representations of solutions. However, information about singularities enters such series in a nontrivial way. Thus we regard our approach as complementary to known techniques, e.g., Painlevé analysis (to study singularities) or hodograph transformations.

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The dynamics of one-dimensional Bloch electrons in constant electric fields

F. Bentosela and P. Duclos
Centre de Physique Théorique UMR 6207—Unité Mixte de Recherche du CNRS et des Universités Aix-Marseille I, Aix-Marseille II et de l' Université du Sud Toulon-Var—Laboratoire Affilié à la FRUMAM, F-13288 Marseille Cedex 9, France

V. Moldoveanu
Group of Theoretical Physics, National Institute of Materials Physics, P.O. Box MG-7, 76900—Bucharest, Romania

G. Nenciu
Department of Theoretical Physics, University of Bucharest, P.O. Box MG 11, 76900—Bucharest, Romania and Institute of Mathematics of the Romanian Academy, P.O. Box 1-764, RO70700 Bucharest, Romania

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We study the dynamics of a one-dimensional Bloch electron subjected to a constant electric field. The periodic potential is supposed to be less singular than the δ-like potential (Dirac comb). We give a rigorous proof of Ao's result that for a large class of initial conditions (high momentum regime) there is no localization in momentum space. The proof is based on the mathematical substantiation of the two simplifying assumptions made in physical literature: the transitions between far away bands can be neglected and the transitions at the quasicrossing can be described by Landau–Zener-type formulas. Using the connection between the above model and the driven quantum ring (DQR) shown by Avron and Nemirovski, our results imply the increase of energy for weakly singular such DQR and appropiate initial conditions. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1870732]

I. INTRODUCTION

The dynamics of Bloch electrons (i.e., electrons subjected to a periodic potential) in the presence of a homogeneous electric field is among those topics that appeared since the beginning of the quantum theory of the solid state physics but are still alive today for both mathematical and physical reasons; in particular the emergence of superlattices leads to interesting physics (see, e.g., Ref. 31).

The dynamics of an electron in one dimension subjected to a periodic potential $V_{\mathrm{per}}(x)$ and a constant electric field $E=-eF$ is described by the time-dependent Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t}(x,t)=H^{\mathrm{SW}}\psi(x,t)=\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-eFx+V_{\mathrm{per}}(x)\right)\psi(x,t), \tag{1.1}$$

where H^{SW} is the so-called Stark–Wannier Hamiltonian.

There is a large body of mathematically oriented literature about spectral properties of the Stark–Wannier Hamiltonian (especially concerning the Stark–Wannier ladder problem; see Refs. 8,9,10,22,24 and references therein). In particular the spectrum has been proved to be absolutely continuous for twice differentiable potentials[7] and recently, results about the nature of the spectrum were obtained for more singular potentials.[4,13,16,17,26]

On the contrary, at the rigorous level there are by far fewer results concerning the dynamics generated by H^{SW}. Of course, as well known, the results about spectral properties of H^{SW} lead to results about dynamics but they either concern finite (albeit long) intervals of time[24,25] or are only qualitative. As an example we mention the results of Avron and Nemirovski[5] on driven quantum

rings. They first proved the nice result that there is a close connection between driven quantum rings and Stark–Wannier Hamiltonians. Then, using this connection and the fact mentioned above that the spectrum of H^{SW} is absolutely continuous for twice differentiable potentials they proved that the energy of a smoothly driven quantum ring grows indefinitely as $t\to\infty$ for arbitrary initial conditions.

At the physical level the dynamics generated by H^{SW} has been thoroughly studied (using the temporal gauge representation) both by analytical and numerical methods. Due to the difficulty of the problem two main assumptions are made.

(1) The only interband transitions considered are the ones between neighboring bands (the so-called Zener tunneling process[33] through avoided crossings); all the others are considered sufficiently small to be neglected.
(2) The transition probabilities can be computed approximatively via Landau–Zener type formulae.

Based on earlier developements,[12] the consequences of these assumptions were exhaustively discussed by Ao.[2] More precisely, writing the evolution at arbitrary times as a product of evolutions over half Bloch periods and using for the last ones the "scattering matrix" between adjacent bands given by Blatter and Browne[12] he reduced the original problem to a discrete dynamics, amenable to numerical and analytical study. The main result coming from his analysis is that for potentials more regular than the Dirac comb and a large class of initial conditions there is a propagating front for the Bloch electron (in other words it will escape at infinity). The Dirac comb is a critical border, one could have either propagation or localization (respectively, pure point, continuous spectrum spectrum or even mixed cases) depending upon the electric field strength and some resonance conditions.

At the rigorous level the existence of a propagating front (with quantitative estimates) for a large class of initial conditions as well as some spectral consequences has been recently proved in Ref. 3 for potentials more regular than the L^2_{loc} class.

The aim of this paper is to provide a rigorous justification of the simplifying assumptions (1) and (2) above in order to substantiate from the mathematical point of view at least a part of Ao's analysis. We do it for a class of periodic potentials whose Fourier coefficients, $\hat{V}(n)$, satisfy $|\hat{V}(n)|<\mathrm{const}|n|^{-r}$ for all $r>0$. Notice however that the results of Secs. III and IV are even valid for $r>-\frac{1}{2}$.

The need for a rigorous control comes from the fact that even if the errors involved in the assumptions (1) and (2) are "small" over a half Bloch period they acummulate during a long time evolution to the point of making irrelevant the approximate computation based on the discrete dynamics.

The problem turned out to be fairly complex for two reasons. First we are dealing with singular periodic potentials which leads to a definition in the form sense of the gauged Hamiltonian $\tilde{H}^{\mathrm{SW}}$ and second, we want to control the evolution over infinite intervals of time which demands a very good control of the errors involved.

The results in this paper allows us to prove the existence of a propagating front (which in turn implies the existence of continuous spectrum for H^{SW}) up to the Dirac comb [which corresponds to $\hat{V}(n)=1$ and is known as notoriously difficult]. Actually the Dirac comb case remains open, although it is not clear for us whether the present approach could provide as well some results in this case.

The plan of the paper is as follows. Section II contains the preliminaries: the direct integral representation of the Stark–Wannier Hamiltonian in the temporal gauge, the periodicity in time properties of the fiber Hamiltonian and the reduction to the one Bloch period. All that is done for $\tilde{H}^{\mathrm{SW}}$ defined as a quadratic form sum. Section II contains in addition a key technical estimate (Lemma 2.3) used many times in the following sections. Since the proof is technical and somehow long it was moved to the Appendix.

Section III contains the first main result of our paper (Theorem 3.1) saying that the transitions

over a half Bloch period, between far-away bands [neglected by assumption (1) in the physical literature] can be controlled by adiabatic techniques. The idea is that in adiabatic perturbation theory the relevant parameter is ε/Δ, where ε is the slowness parameter and Δ is the spectral gap. In our case it is the gap that grows with energy making thus the adiabatic machinery effective.

After the far-away decoupling in Sec. III we come to the "in-band" dynamics, i.e., to Zener transitions through quasicrossings at high energies. The task of computing this dynamics has been taken again and again in the physical literature. It consists in solving a 2×2 system of first order ordinary differential equations over a finite interval of time. There are two problems here. The first is that the coefficients are taken as given by a low order almost degenerate pertubation theory without any control of the reminder. Second, the obtained "Zener model" is solved over an infinite period of time. We cope with the first problem by using the reduction theory in Sec. IV to obtain an effective Hamiltonian (Theorem 4.1). Then we integrate the system over one-half period by the use of Dyson series; we compute the first two terms in Sec. V and estimate the remainder in the Appendix. The resulting "transfer matrix" is given in Theorem 5.1. We expect the results mentioned above to give a lot of information on spectral and dynamical properties of the Stark–Wannier (SW) and driven quantum ring models for fairly singular potentials. As an example in Sec. VI the results in the preceding sections are assembled to prove the Ao's statement about the the existence of a propagating front. As direct side consequences we obtain (see Corollary 6.4) that for $r>0$ the continuous spectrum of H^{SW} is not empty (see however the recent paper of Perelman[26] for a better result in this direction), that for a large class of initial conditions the energy of the DQR increases like t^2 (see Corollary 6.5) and that there is no localization in momentum space (see Corollary 6.6).

In the Appendix we state for convenience the Sz-Nagÿ transformation matrix. In order to make the reading of the paper easier we start each section by simply stating the theorems and lemmas, their proofs being provided later.

II. PRELIMINARIES

As already said in the introduction we are interested in the evolution given by the Stark–Wannier operator. For simplicity we normalize $e=\hbar=2m=1$. Moreover since the results we are going to prove along the paper do not depend upon the electric field strength, we set $F=1$. Accordingly the Stark–Wannier Hamiltonian writes

$$H^{\mathrm{SW}} = -\frac{d^2}{\mathrm{d}x^2} - x + V_{\mathrm{per}}, \tag{2.1}$$

where V_{per} is a real periodic potential with periodicity $a=2\pi$. Under these assumptions the quantity $2\pi\hbar/aF$, the so-called Bloch period, is equal to 1.

Let us define

$$\tilde{U}^{\mathrm{SW}}(t,s) := G(t)e^{-i(t-s)H^{\mathrm{SW}}}G(s)^*, \tag{2.2}$$

where $G(t)$ is the temporal gauge,

$$G(t)\psi(x,t) := e^{-ixt}\psi(x,t) =: \tilde{\psi}(x,t). \tag{2.3}$$

Actually $G(t)$ has the role of a boost to a free falling frame that eliminates the field. Then using (2.2) and (2.3) one has by direct computation,

$$i\frac{d}{\mathrm{d}t}\tilde{U}^{\mathrm{SW}}(t,s) = \left(\left(-i\frac{d}{\mathrm{d}x}+t\right)^2 + V_{\mathrm{per}}(x)\right)\tilde{U}^{\mathrm{SW}}(t,s) =: \tilde{H}^{\mathrm{SW}}(t)\tilde{U}^{\mathrm{SW}}(t,s).$$

As is well known the periodicity of V_{per} allows a direct integral representation for $\tilde{H}^{\mathrm{SW}}(t)$ via the Fourier–Bloch transform[28] which maps unitarily the space $L^2(\mathbb{R})$ onto $L^2([0,1),\mathrm{d}k,l^2(\mathbb{Z}))$,

$$(S\psi)(k,n) = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} e^{-inx}\left\{\sum_{\gamma\in\mathbb{Z}} e^{-ik(x+2\pi\gamma)}\psi(x+2\pi\gamma)\right\}\mathrm{d}x. \tag{2.4}$$

Note that $(S\psi)(k,n)=(\mathcal{F}\psi)(k+n)$ where $\mathcal{F}$ is the Fourier transform. In this representation $\tilde{H}^{\mathrm{SW}}(t)$ reads as

$$S\tilde{H}^{\mathrm{SW}}(t)S^* = \int_{[0,1)}^{\oplus} H(k,t)\mathrm{d}k, \tag{2.5}$$

with the fiber Hamiltonian

$$H(k,t) \coloneqq H_0(k,t) + V. \tag{2.6}$$

We remark that $H(0,t)$ coincide with the Hamiltonian of the DQR when written in the Fourier representation (see, e.g., Ref. 5) so all the results below on the evolution $U(t,s)$, generated by $H(0,t)$ apply (see the Corollary 6.5 below) to the DQR problem. The unperturbed Hamiltonian $H_0(k,t)$ has a simple spectral representation

$$H_0(k,t) = \sum_{n\in\mathbb{Z}} E_{n,0}(k,t)P_{n,0}(k), \tag{2.7}$$

where

$$E_{n,0}(k,t) = (n+k+t)^2 \tag{2.8}$$

and $P_{n,0}(k)\coloneqq P_{n,0}$ is the projection on the nth vector, φ_n, from the canonical basis in $l^2(\mathbb{Z})$,

$$\varphi_{n,0}(m) = \delta_{n,m}. \tag{2.9}$$

The perturbation V is given by the following convolution in $l^2(\mathbb{Z})$:

$$(V\phi)(k,m) = \sum_{n\in\mathbb{Z}} \hat{V}(m-n)\phi(k,n), \tag{2.10}$$

$\hat{V}(n)$ being the Fourier coefficients of V_{per}. Since V_{per} is real we have $\hat{V}(n)=\overline{\hat{V}}(-n)$. Moreover we can choose $\hat{V}(0)=0$ (this amounts for a shift in the energy scale). We characterize different classes of perturbations by the norm

$$\|V\|_r \coloneqq \sup_{n\in\mathbb{Z}}\langle n\rangle^r|\hat{V}(n)| < \infty, \quad \langle n\rangle \coloneqq \sqrt{1+n^2} \quad r\in\mathbb{R}. \tag{2.11}$$

Notice that when r gets smaller and smaller, $\hat{V}(n)$ are allowed to decrease slower hence $V_{\mathrm{per}}(x)$ is more and more singular. Actually $V_{\mathrm{per}}(x)$ is to be considered as a tempered distribution on the one-dimensional torus $\mathbb{T}$ such that its Fourier series satisfies $\|V\|_r<\infty$. For $r>0$, $V_{\mathrm{per}}(x)$ is realized as an usual function while $r=0$ corresponds to δ-like potentials. For $r>\frac{1}{2}$, $V_{\mathrm{per}}(x)$ is square integrable over the unit cell, and then as well known,[28] V is $H_0(k,t)$ bounded with relative bound zero. As a consequence, by the Kato–Rellich theorem,[28] $H(k,t)$ is self-adjoint on the (time independent) domain of $H_0(k,t)$:

$$\mathcal{D}(H_0(k,t)) = \mathcal{H}^2 = \{\phi(n)|\langle n\rangle^2\phi(n) \in l^2(\mathbb{Z})\}. \tag{2.12}$$

In addition, the existence of a strongly continuous evolution $U(k;t,s)$, generated by $H(k,t)$ is assured by standard results (see Ref. 32 and Theorem X.70 in Ref. 27). We are mainly interested in the case of more singular potentials corresponding to $r\leqslant\frac{1}{2}$ and here the problem is more involved since as one can easily see [take, for example, $\hat{V}(n)=\langle n\rangle^{-1/2}$] V is no more $H_0(k,t)$ bounded. Notice that the time independent form domain of $H_0(k,t)$ is $\mathcal{Q}(H_0(k,t))=\mathcal{H}^1$

$=\{\phi(n)\,|\,\langle n\rangle\phi(n)\in l^2(\mathbb{Z})\}$. Then one can use the theory of Hamiltonians defined as quadratic forms.[27] More precisely, from

$$R_0(z,k,t) := \sum_{n\in\mathbb{Z}} \frac{P_{n,0}}{E_{n,0}(k,t)-z} \tag{2.13}$$

let us define

$$|R_0(z,k,t)|^{1/2} = \sum_{n\in\mathbb{Z}} \frac{P_{n,0}}{|E_{n,0}(k,t)-z|^{1/2}} \tag{2.14}$$

and

$$R_0(z,k,t)^{1/2} = \sum_{n\in\mathbb{Z}} \frac{\mathrm{sgn}(E_{n,0}(k,t)-z)P_{n,0}}{|E_{n,0}(k,t)-z|^{1/2}}. \tag{2.15}$$

Then $R_0(z,k,t)=R_0(z,k,t)^{1/2}|R_0(z,k,t)|^{1/2}$. The following operator, defined for $z\notin\sigma(H_0(k,t))$ will appear many times along the paper:

$$K(z,k,t) := |R_0(z,k,t)|^{1/2} V R_0(z,k,t)^{1/2}. \tag{2.16}$$

The fact that V is $H_0(k,t)$-bounded in the form sense with relative bound zero is implied by the following lemma.

Lemma 2.1: Let $r>-\frac{1}{2}$. Then uniformly in t and k,

$$\lim_{a\to\infty}\|K(-a^2,k,t)\| = 0. \tag{2.17}$$

As a consequence one can use the KLMN theorem[27] to define $H(k,t)$ as a form sum with form domain $\mathcal{H}^1$. The associated quadratic form is

$$\mathcal{H}^1 \ni \phi \to \sum_n |(n+k+t)\phi(k,n)|^2 + \sum_{m,n\in\mathbb{Z}} \hat{V}(m-n)\overline{\phi}(k,m)\phi(k,n). \tag{2.18}$$

Due to Lemma 2.1 one can write a useful formula for $R(z,k,t):=(H(k,t)-z)^{-1}$. Indeed, for sufficiently large a

$$R(-a^2,k,t) = R_0(-a^2,k,t)^{1/2}(1+K(-a^2,k,t))^{-1}|R_0(-a^2,k,t)|^{1/2}, \tag{2.19}$$

one has by analytic continuation

$$R(z,k,t) = R_0(z,k,t)^{1/2}(1+K(z,k,t))^{-1}|R_0(z,k,t)|^{1/2}. \tag{2.20}$$

Since $|R_0(z,k,t)|^{1/2}$ is compact, it follows from (2.19) that $R(z,k,t)$ is compact which implies (see Ref. 28) that the spectrum of $H(k,t)$ is discrete. In what concerns the evolution $U(k,s,t)$ generated by $H(k,t)$, as a corollary of Theorem 2.27 in Ref. 29 one has the following result assuring the existence of $U(k;s,t)$ in the weak sense.

Lemma 2.2: Let $\mathcal{H}^{-1}$ denote the space of continuous linear forms on $\mathcal{H}^1$. Then for every $\phi(k,0)\in H^1$ it exists a unique function $\phi(k,\cdot):\mathbb{R}\to H^1$ such that

(i) *$\mathbb{R}\ni t\to(\phi(k,t),\psi)$ is continuous for any $\psi\in H^{-1}$,*

(ii) *for every $f\in\mathcal{H}^1$,*

$$\frac{1}{i}\frac{d}{dt}(\phi(k,t),f) + (\phi(k,t),H(k,t)f) = 0.$$

(iii) *The map $U(k,t,s):\phi(k,s)\to\phi(k,t)$ is isometric and its extension by continuity is unitary in $l^2(\mathbb{Z})$.*

From (2.2) and (2.5) and Lemma 2.2 we can write the following formula for the Stark–Wannier evolution

$$e^{-i(t-s)H^{\mathrm{SW}}} = G(t)^* S^* \int_{[0,1)}^{\oplus} U(k,t,s)\mathrm{d}k\, SG(s), \tag{2.21}$$

so the study of $e^{-i(t-s)H^{\mathrm{SW}}}$ is reduced to the study of the family of evolutions $U(k,t,s)$ in $l^2(\mathbb{Z})$ generated by $H(k,t)$, and the rest of the paper will be devoted to this problem. From (2.6)–(2.10) it follows that $H(k,t)=H(0,k+t)$ and then

$$U(k,t,s) = U(0,k+t,k+s), \tag{2.22}$$

which means that one can restrict the analysis to the fiber $k=0$, and from now on we omit to write k when it is taken to be zero, e.g., $H(k=0,t)=H(t)$, $E_{n,0}(k=0,t)=E_{n,0}(t)$, etc. The next remark is that although $H(t)$ is not periodic in t there is a hidden periodicity. More precisely if T is the shift operator in $l^2(\mathbb{Z})$,

$$(T\psi)(n) = \psi(n-1) \tag{2.23}$$

then by direct computation one can see that

$$TH(k,t+1)T^* = H(k,t), \tag{2.24}$$

which in turn implies

$$U(t+1,s+1) = T^* U(t,s) T. \tag{2.25}$$

The analysis of $U(t,s)$ can be restricted to one period. We take the basic period to be the union of two half-periods,

$$t \in I_0 \cup I_1, \quad I_0 = \left[-\tfrac{1}{4},\tfrac{1}{4}\right), \quad I_1 = \left[\tfrac{1}{4},\tfrac{3}{4}\right). \tag{2.26}$$

Let us consider now in more detail the spectral properties of $H_0(t)$ and $H(t)$. We remark that when $t \in I_0 \cup I_1$, $H_0(t)$ has degeneracies at the points $t=0$ and $t=\frac{1}{2}$. Actually the splitting of one period into two half-periods is due to the existence of two points per period where $H_0(t)$ has degeneracies. Since the latter play a key role in the dynamics (due to the Zener transitions) the above structure suggests to describe $\sigma(H_0(t))$ inside I_l, $l=0,1$ as a union of pairs of eigenvalues that cross at $t=0$ and $t=\frac{1}{2}$. We define (see Fig. 1)

$$\sigma_{m,0}(t) \coloneqq E_{m-1,0}(t) \cup E_{-(m-1),0}(t) \quad \text{for } m \geqslant 1, \quad t \in I_0, \tag{2.27}$$

$$\tilde{\sigma}_{m,0}(t) \coloneqq E_{m-1,0}(t) \cup E_{-m,0}(t) \quad \text{for } m \geqslant 1, \quad t \in I_1, \tag{2.28}$$

so that $\sigma(H_0(t))=\cup_{m\geqslant 1}\sigma_{m,0}(t)$, $\sigma(H_0(t))=\cup_{m\geqslant 1}\tilde{\sigma}_{m,0}(t)$ on I_0 and I_1, respectively. An alternative way of labelling the eigenvalues of $H_0(t)$ is to count them in the increasing order

$$E_1^0(t) \leqslant E_2^0(t) \leqslant E_3^0(t) \cdots, \quad t \in \mathbb{R}. \tag{2.29}$$

Of course the two labellings are related, for a fixed α and a given t there exists an $n_\alpha(t)$ such that

$$E_\alpha^0(t) = E_{n_\alpha(t),0}(t) \quad \text{and } P_\alpha^0(t) = P_{n_\alpha(t),0}. \tag{2.30}$$

Let $t \in \left[-\frac{1}{2},0\right)+(N/2)$ with $N=0,1,2,\ldots$. Then the correspondence between α and $n_\alpha(t)$ is given as follows:

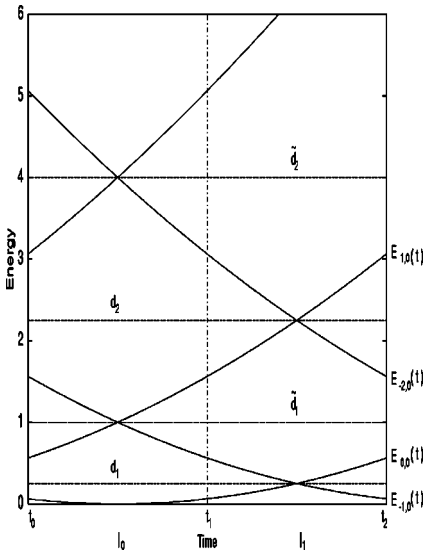

FIG. 1. The first eigenvalues of the free Hamiltonian $H_0(t)$ as a function of time and the horizontal lines $d_m, \tilde{d}_m$ used in Lemma 2.3. The intervals I_0 and I_1 are also marked.

$$n_\alpha(t) = \begin{cases} \dfrac{\alpha - N}{2} & \text{if } N \text{ and } \alpha \text{ have the same parity,} \\ -\dfrac{\alpha + N - 1}{2} & \text{if } N \text{ and } \alpha \text{ have different parities.} \end{cases} \tag{2.31}$$

With this labelling one has

$$\sigma_{1,0}(t) = E_1^0(t), \quad \sigma_{m,0}(t) = E_{2m-2}^0 \cup E_{2m-1}^0 \quad \text{for } t \in I_0, \tag{2.32}$$

$$\tilde{\sigma}_{m,0}(t) = E_{2m-1}^0 \cup E_{2m}^0 \quad \text{for } t \in I_1. \tag{2.33}$$

The spectral projections of $H_0(t)$ corresponding to $\sigma_{m,0}(t)$ and $\tilde{\sigma}_{m,0}(t)$ are denoted $Q_{m,0}$ and $\tilde{Q}_{m,0}$,

$$Q_{1,0} = P_{0,0}, \quad Q_{m,0} = P_{m-1,0} + P_{-(m-1),0} \quad \text{for } t \in I_0, \tag{2.34}$$

$$\tilde{Q}_{m,0} = P_{m-1,0} + P_{-m,0} \quad \text{for } t \in I_1. \tag{2.35}$$

By construction, for any $m = 1, 2, \ldots$ and $t \in I_0$, $\sigma_{m,0}(t)$ are well separated. Similarly, for $t \in I_1$ $\tilde{\sigma}_{m,0}(t)$ are well separated,

$$\inf_{t \in I_0} \operatorname{dist}(\sigma_{m,0}(t), \sigma_{m+1,0}(t)) = m - \tfrac{1}{2},$$

$$\inf_{t \in I_1} \operatorname{dist}(\tilde{\sigma}_{m,0}(t), \tilde{\sigma}_{m+1,0}(t)) = m. \tag{2.36}$$

Moreover, at the end of the interval I_0, the two eigenvalues composing $\sigma_{m,0}(t)$ [with the exception of $\sigma_{1,0}(t)$ which consists in just one eigenvalue] are well separated, e.g.,

$$E^0_{2m-1}\left(-\tfrac{1}{4}\right) - E^0_{2m-2}\left(-\tfrac{1}{4}\right) = m - 1. \tag{2.37}$$

The same is true for the two eigenvalues composing $\tilde{\sigma}_{m,0}(t)$. We come now to the spectral properties of $H(t)$.

Since $K\left(n+\frac{1}{2},t\right)$ tends to zero as n tends to infinity, uniformly with respect to t the analytic perturbation theory of type *B*, see Ref. 15, Chap. VII, works here as long as $r > -\frac{1}{2}$. More precisely if we label the eigenvalues of $H(t)$ in increasing order $E_\alpha(t)$, $\alpha = 1,\ldots$ then $\lim_{\alpha\to\infty}(E_\alpha(t) - E^0_\alpha(t)) = 0$. In addition for $t \neq 0, \frac{1}{2}$, when all the eigenvalues are nondegenerate the corresponding spectral projections $P_\alpha(t)$ are close the unperturbed ones, $\lim_{\alpha\to\infty}\|P_\alpha(t) - P^0_\alpha(t)\| = 0$. In the following $\varphi_\alpha(t)$ denotes the eigenfunction of $H(t)$ corresponding to the eigenvalue $E_\alpha(t)$.

Let

$$\Gamma_m = \left\{\left(m - \tfrac{1}{2}\right)^2 + iy | y \in \mathbb{R}\right\}, \quad \tilde{\Gamma}_m = \{m^2 + iy | y \in \mathbb{R}\} \quad m = 1,2,\ldots \tag{2.38}$$

be vertical lines in the energy plane. In what follows, each time a quantity will be bounded from above by a positive constant, this will be denoted by C, while for the lower bounds we denote it c.

The main estimates, used many times along the paper are contained in the following.

Lemma 2.3: Let $A < \infty$. Then for each $r > -\frac{1}{2}$ there exists a constant C_V independent of m and a positive integer N_r such that for any $m > N_r$ the following estimate holds:

$$\sup_{t\in I_0}\left(\sup_{z\in\Gamma_m}\|K(z,t)\| + \int_{\Gamma_m}\|R_0(z,t)\|\cdot\|K(z,t)\|dy\right) + \sup_{t\in I_1}\left(\sup_{z\in\tilde{\Gamma}_m}\|K(z,t)\| + \int_{\tilde{\Gamma}_m}\|R_0(z,t)\|\cdot\|K(z,t)\|dy\right)$$
$$+ \max_{t=-1/4,1/4}\left(\sup_{z\in\Gamma_m\cup\tilde{\Gamma}_m}\|K(z,t)\| + \int_{\Gamma_m\cup\tilde{\Gamma}_m}\|R_0(z,t)\|\cdot\|K(z,t)\|dy\right) \leqslant C_V b(m), \tag{2.39}$$

where

$$b(m) := \frac{\log^2\langle 4m-1\rangle}{\langle m\rangle^{1+\min\{0,2r\}}}. \tag{2.40}$$

Also one has

$$\lim_{y\to\infty}\sup_{t\in I_0}\sup_{x\leqslant A}\|K(x+iy,t)\| = 0. \tag{2.41}$$

Let $m > 1$, $d_m := \left(m-\frac{1}{2}\right)^2$, $\tilde{d}_m := m^2$ and γ_m, $\tilde{\gamma}_m$ be closed finite contours that intersect the real axis in and only in d_m, d_{m-1} and $\tilde{d}_m$, $\tilde{d}_{m-1}$ [for example, γ_m can be a square of length $8(m-1)$]. Then there exist an absolute constant C such that

$$\sup_{t\in I_0}\sup_{z\in\gamma_m}\|K(z,t)\| \leqslant C\|K(d_m,0)\|, \tag{2.42}$$

$$\sup_{t\in I_1}\sup_{z\in\tilde{\gamma}_m}\|K(z,t)\| \leqslant C\|K(\tilde{d}_m,0)\|. \tag{2.43}$$

Due to the above lemma we are able to give upper bounds of the type $(C_V\langle b(m)\rangle)^N$. In the following we shall say that a quantity A is of order $(\mathcal{O}_r(\langle b(m)\rangle)^N)$ if it obeys the estimate $\|A\| \leqslant (C_V\langle b(m)\rangle)^N$. The subscript r reminds us the dependence on $\|V\|_r$. We notice that the third line in (2.39) follows at once from the estimates of the first and the second lines. As we have said, the proof of the lemma is postponed to the Appendix.

Now we are ready to spell the spectral properties of $H(t)$. We shall consider only $t \in I_0$; the results and the proofs for $t \in I_1$, with the appropiate identifications, are the same. The first remark

is that there exists an m^* such that for any $m>m^*$ the norm of $K(z,t)$ is smaller than $\frac{1}{2}$. Second, for all $t\in I_0$ $d_m\in\rho(H(t))$ and for all $t\in I_1$ $\tilde{d}_m\in\rho(H(t))$. Moreover, $\tilde{d}_m\in\rho(H(-\frac{1}{4}))$.

Corollary 2.4: Let $m>m^*$. Then

$$\min\{\inf_{t\in I_0}\operatorname{dist}(d_m,\sigma(H(t))),\inf_{t\in I_1}\operatorname{dist}(\tilde{d}_m,\sigma(H(t)))\}\geqslant cm. \tag{2.44}$$

Let $Q_m(t)$ the spectral projection associated to $\sigma_m(t)=(d_{m-1},d_m)\cap\sigma(H(t))$. Then one has the following.

Corollary 2.5: For m sufficiently large or V small enough

$$\sup_{t\in I_0}\|Q_m(t)-Q_{m,0}\|\leqslant C_V b(m). \tag{2.45}$$

Let for $\alpha=2m-2,2m-1$ [see (2.31)],

$$P_\alpha^0\left(-\tfrac{1}{4}\right)=P_{n_\alpha(-1/4),0},\quad \varphi_\alpha^0\left(-\tfrac{1}{4}\right)=\varphi_{n_\alpha(-1/4),0}, \tag{2.46}$$

and $P_{2m-2}\left(-\frac{1}{4}\right)$, $P_{2m-1}\left(-\frac{1}{4}\right)$ the spectral projections of $H\left(-\frac{1}{4}\right)$ corresponding to the intervals $(d_{m-1},\tilde{d}_{m-1})$ and $(\tilde{d}_{m-1},d_m)$, respectively. Then the following estimate holds.

Corollary 2.6: Let $\alpha=2m-2,2m-1$. Then for $m>m^*$,

$$\left\|P_\alpha\left(-\tfrac{1}{4}\right)-P_\alpha^0\left(-\tfrac{1}{4}\right)\right\|\leqslant C_V b(m). \tag{2.47}$$

For sufficiently large m, by Sz-Nagÿ lemma (see the Appendix), $P_\alpha\left(-\frac{1}{4}\right)$ and $P_\alpha^0\left(-\frac{1}{4}\right)$ are unitarily equivalent so that $H\left(-\frac{1}{4}\right)$ has nondegenerate eigenvalues in $(d_{m-1},\tilde{d}_{m-1})$ and $(\tilde{d}_{m-1},d_m)$, respectively. They are denoted by $E_{2m-2}\left(-\frac{1}{4}\right)$ and $E_{2m-1}\left(-\frac{1}{4}\right)$. Moreover, if $N_\alpha\left(-\frac{1}{4}\right)$ is the Sz-Nagÿ transformation corresponding to the pair $P_\alpha\left(-\frac{1}{4}\right)$, $P_\alpha^0\left(-\frac{1}{4}\right)$ then

$$\varphi_\alpha\left(-\tfrac{1}{4}\right)=N_\alpha\left(-\tfrac{1}{4}\right)\varphi_\alpha^0\left(-\tfrac{1}{4}\right) \tag{2.48}$$

are eigenvectors of $H\left(-\frac{1}{4}\right)$ corresponding to $E_\alpha\left(-\frac{1}{4}\right)$. We say that an eigenbasis $\{\varphi_\alpha\left(-\frac{1}{4}\right)\}_{\alpha=1}^\infty$ of $H\left(-\frac{1}{4}\right)$ is a canonical one if for sufficiently large α (such that all the above construction works) $\varphi_\alpha\left(-\frac{1}{4}\right)$ is given by (2.48). In the same way one constructs canonical bases for $t=\frac{1}{4}$. For $t_l:=-\frac{1}{4}+(l/2)$, $l=2,3,\ldots$ the canonical bases are provided by [see (2.24)]

$$T\varphi_\alpha(t_l+1)=\varphi_\alpha(t_l). \tag{2.49}$$

Before going to the proofs let us write the reduction to one period formula (2.25) in the canonical basis.

Lemma 2.7: Let l be even, $t_0=-\frac{1}{4}$, $t_l=t_0+(l/2)$. Then for α and β sufficiently large

$$\langle\varphi_\alpha(t_l+1),U(t_l+1,t_l)\varphi_\beta(t_l)\rangle=\langle\varphi_\alpha(t_2),U(t_2,t_0)\varphi_\beta(t_0)\rangle. \tag{2.50}$$

Now we present the proofs for the lemmas and corollaries given above.

Proof of Lemma 2.1: We estimate the Hilbert–Schmidt norm of $K(-a^2,k,t)$,

$$\begin{aligned}\|K(-a^2,k,t)\|^2\leqslant\|K(-a^2,k,t)\|_{\mathrm{HS}}^2&\leqslant\|V\|_r^2\sum_{m,n\in\mathbb{Z}}\frac{1}{(m+k+t)^2+a^2}\langle m-n\rangle^{-2r}\frac{1}{(n+k+t)^2+a^2}\\&\leqslant\|V\|_r^2\left(\frac{\sqrt{5}}{2}\right)^{\max\{-2r,0\}}\sum_{m\in\mathbb{Z}}\frac{\langle m\rangle^{\max\{-2r,0\}}}{(m+k+t)^2+a^2},\end{aligned}$$

where in the last line we used the inequality

$$\langle m-n\rangle^{-2r} \leqslant \left(\frac{\sqrt{5}}{2}\langle m\rangle\langle n\rangle\right)^{\max\{-2r,0\}}. \tag{2.51}$$

Then the above series is convergent for $r>-\frac{1}{2}$ and the lemma is proved using the Lebesque dominated convergence theorem. □

Proof of Corollary 2.4: $R(d_m,t)$ can be written as

$$R(d_m,t) = |R_0(d_m,t)|^{\frac{1}{2}}(1+K(d_m,t))^{-1}R_0(d_m,t)^{\frac{1}{2}}. \tag{2.52}$$

Taking into account that $\mathrm{dist}(d_m,\sigma(H_0(t))) \geqslant cm$ one obtains from (2.52),

$$\|R(d_m,t)\| \leqslant 2\||R_0(d_m,t)|^{1/2}\|\cdot\|R_0(d_m,t)^{1/2}\| = 2\|R_0(d_m,t)\| \leqslant 2(Cm)^{-1}, \tag{2.53}$$

which implies $\inf_{t\in I_0}\mathrm{dist}(d_m,\sigma(H(t))) \geqslant cm$. The proof of the inequality $\mathrm{dist}\left(\tilde{d}_m,\sigma\left(H\left(-\frac{1}{4}\right)\right)\right) \geqslant Cm/2$ is similar. □

Proof of Corollary 2.5: By perturbation theory

$$Q_m(t)-Q_{m,0} = -\frac{i}{2\pi}\int_{\gamma_m} R_0(z,t)^{1/2}K(z,t)(1+K(z,t))^{-1}|R_0(z,t)|^{1/2}\,\mathrm{d}z.$$

Taking the norms, using that $\oint_{\gamma_m}\|R_0(z,t)\|\mathrm{d}z \leqslant C$ the estimate (2.45) follows from (2.42) and (2.39).

Proof of Corollary 2.6: Similar to the proof of Corollary 2.5. □

Proof of Lemma 2.7: Direct computation using (2.25), (2.48), and (2.49). □

III. THE ADIABATIC THEOREM

As already said in the introduction our first task is to show that at high energies the most important "interband transitions" during a half Bloch period are the so-called Zener transitions, namely the ones between neighboring bands [e.g., on I_0 between $E_{2m-2}(t)$ and $E_{2m-1}(t)$]. This is nothing else but to claim that for $t,s\in I_0$ the subspace $Q_m(t)\mathcal{H}$ is almost invariant under the evolution $U(t,s)$. In this section we construct adiabatic evolutions $U_m^A(t,t_0)$ and $\tilde{U}_m^A(t,t_1)$ on I_0 and I_1, respectively, satisfying

$$U_m^A(t,t_0)Q_m(t_0)\mathcal{H} = Q_m(t)\mathcal{H}, \quad t\in I_0, \tag{3.1}$$

$$\tilde{U}_m^A(t,t_1)\tilde{Q}_m(t_1)\mathcal{H} = \tilde{Q}_m(t)\mathcal{H}, \quad t\in I_1, \tag{3.2}$$

and prove that they are close to $U(t,t_0)$ and $U(t,t_1)$, respectively. We consider first the half Bloch period I_0 and at the end indicate the changes for I_1. Let

$$Q_m^+(t) := \sum_{j=m+1}^{\infty} Q_j(t), \quad Q_m^-(t) := \sum_{j=1}^{m-1} Q_j(t), \quad t\in I_0, \tag{3.3}$$

and define $H_m^A(t)$ by

$$H_m^A(t) := H(t)-X_m(t) =: H(t) - iQ_m^+(t)\dot{Q}_m^+(t) - iQ_m(t)\dot{Q}_m(t) - iQ_m^-(t)\dot{Q}_m^-(t). \tag{3.4}$$

It turns out (see the proof of Lemma 3.4 below) that $X_m(t)$ are bounded hence $H_m^A(t)$ are self-adjoint on $\mathcal{D}(H(t))$. The adiabatic evolution $U_m^A(t,t_0)$ generated by $H_m^A(t)$ will be defined as the solution (in the weak sense, as in Lemma 2.2) of the equation

$$i\frac{d}{dt}U_m^A(t,t_0) = H_m^A(t)U_m^A(t,t_0), \quad U_m^A(t_0,t_0) = 1. \tag{3.5}$$

As in the case of standard adiabatic theorem of quantum mechanics, $U_m^A(t,t_0)$ has the intertwining property

$$Q_m(t) = U_m^A(t,t_0)Q_m(t_0)U_m^A(t,t_0)^*, \quad Q_m^{\pm}(t) = U_m^A(t,t_0)Q_m^{\pm}(t_0)U_m^A(t,t_0)^*, \tag{3.6}$$

i.e., the families of subspaces $Q_m(t)\mathcal{H}$, $Q_m^{\pm}(t)\mathcal{H}$ are invariant under $U_m^A(t,t_0)$. The proof is standard (Krein–Kato lemma[15,18,23]). For $t \in I_1$ one constructs in a similar way $\tilde{U}_m^A(t,t_1)$ by replacing $Q_j(t)$ by $\tilde{Q}_j(t)$. The main result of this section is to show that $U_m^A(t,t_0)$ and $U(t,t_0)$ are close.

Theorem 3.1: *For any $r > -\frac{1}{2}$ and m sufficiently large or $\|V\|_r$ small enough it holds,*

$$\sup_{t\in I_0}\|U(t,t_0) - U_m^A(t,t_0)\| \leqslant C_V b(m)\langle m\rangle^{-1}, \tag{3.7}$$

$$\sup_{t\in I_1}\|U(t,t_1) - \tilde{U}_m^A(t,t_1)\| \leqslant C_V b(m)\langle m\rangle^{-1}, \tag{3.8}$$

where C_V is a constant that depends on V and $b(m)$ was introduced in Lemma 2.3.

The basic steps of the proof are the standard ones but we must check the relevant estimates. Define

$$\Omega_m(t,t_0) := U_m^A(t,t_0)^* U(t,t_0), \tag{3.9}$$

and notice that $\|\Omega_m(t,t_0)-1\| = \|U_m^A(t,t_0) - U(t,t_0)\|$, so one is left with the estimation of $\|\Omega_m(t,t_0)-1\|$. Since a direct estimation of

$$i(\Omega_m(t,t_0) - 1) = \int_{t_0}^{t} \mathrm{d}s\; U_m^A(s,t_0)^* X_m(s) U_m^A(s,t_0)\Omega_m(s,t_0) \tag{3.10}$$

would give (see Lemma 3.4) a bound of order $\mathcal{O}_r(b(m))$, which is not accurate enough for the error estimates in the long time behavior we must follow the proof of the standard adiabatic theorem[6] and make "an integration by parts." More precisely we have the following.

Lemma 3.2: $X_m(t)$ can be written in the form (we omit for simplicity the time dependence),

$$X_m = [H, Y_m], \tag{3.11}$$

with

$$Y_m = \frac{1}{2\pi}\oint_{\gamma_m^-} \mathrm{d}z\, R(z)\{Q_m^- \dot{Q}_m^- - Q_m^+ \dot{Q}_m^+ Q_m^-\}R(z) + \frac{1}{2\pi}\oint_{\gamma_m} \mathrm{d}z\, R(z)\{Q_m \dot{Q}_m - Q_m^+ \dot{Q}_m^+ Q_m\}R(z). \tag{3.12}$$

Here γ_m^- is a closed contour around $\sigma(Q_m^- H(t))$. Now the integration by parts will give $\|\Omega_m(t,t_0)-1\|$ in terms of Y_m.

Lemma 3.3: If t belongs to I_0 the following estimate holds:

$$\|\,\Omega_m(t,t_0) - 1)\| \leqslant \|Y_m(t)\| + \|Y_m(t_0)\| + \int_{t_0}^{t} \mathrm{d}s(\|X_m(s)Y_m(s)\| + \|\dot{Y}_m(s)\|), \tag{3.13}$$

so we are left with verifying (3.11)–(3.13) and to estimate the norms in (3.13). The basic estimation is contained in the following.

Lemma 3.4: For m sufficiently large

$$\sup_{t\in I_0}(\|\dot{Q}_m(t)\| + \|\dot{Q}_m^-(t)\| + \|\dot{Q}_m^+(t)\|) \leqslant C_V b(m). \tag{3.14}$$

Notice that since $Q_m^+(t)=1-Q_m(t)-Q_m^-(t)$, we must only estimate $\|\dot{Q}_m(t)\|$ and $\|\dot{Q}_m^-(t)\|$. Taking Lemma 3.4 for granted we give now the proofs of Lemmas 3.2 and 3.3.

Proof of Lemma 3.2: Since by Lemma 3.4 $X_m(t)$ is bounded

$$\sup_{t\in I_0}\|X_m(t)\| \leqslant C_V b(m) \tag{3.15}$$

and in addition [remember that for an orthogonal projection valued function $E(t)$ $E(t)\dot{E}(t)E(t)=0$] $X_m(t)$ is off-diagonal with respect to the decomposition $\mathcal{H}=Q_m^+(t)\mathcal{H}\oplus Q_m\mathcal{H}\oplus Q_m^-\mathcal{H}$ one obtains $Y_m(t)$ as the solution of the commutator equation (3.11) by using Theorem 9.3 in Ref. 11. Actually one can verify that (3.12) solves (3.11) by straightforward computation. □

Proof of Lemma 3.3: We omit for simplicity the index m and the time dependence. Using the identity [see (3.11)]

$$i\frac{d}{dt}(U^{A^*}YU^A) = U^{A^*}\{i\dot{Y} - X + [X,Y]\}U^A$$

and replacing $U^{A^*}XU^A$ in (3.10) one has

$$\begin{aligned} i(\Omega-1) &= \int_{t_0}^t ds\left\{-i\frac{d}{ds}(U^{A^*}YU^A) + U^{A^*}[X,Y]U^A + iU^{A^*}\dot{Y}U^A\right\}\Omega \\ &= \int_{t_0}^t ds\left\{-i\frac{d}{ds}(U^{A^*}YU^A\Omega) + iU^{A^*}YU^A\dot{\Omega} + U^{A^*}[X,Y]U^A\Omega + iU^{A^*}\dot{Y}U^A\Omega\right\} \\ &= -iU^{A^*}YU^A\Omega|_{t_0}^t + \int_{t_0}^t ds\, U^{A^*}\{XY + i\dot{Y}\}U^A\Omega \end{aligned}$$

which in norm gives the claimed result. □

Proof of Lemma 3.4: We give detailed calculations only for $\dot{Q}_m^-(t)$. Computing Q_m perturbatively, using the identity $\dot{R}(z,t)=-R(z,t)\dot{H}(t)R(z,t)$ one has

$$\dot{Q}_m^-(t) = \frac{i}{2\pi}\oint_{\gamma_m^-} dz\{R_0(z)\dot{H}_0R_0(z)VR(z) + R_0(z)VR(z)\dot{H}R(z)\},$$

where we omited the explicit t dependence. To go further with the estimates we deform first γ_m^- to $\gamma_m^-(L) := \gamma_{m-1}(L)\cup\gamma'_{m-1}(L)\cup\gamma''_{m-1}(L)\cup\gamma_0(L)$ with

$$\gamma_{m-1}(L) := \{d_{m-1} + iy | y\in[-L,L]\}, \tag{3.16}$$

$$\gamma'_{m-1}(L) := \{x + iL | x\in[-L,d_{m-1}]\}, \tag{3.17}$$

$$\gamma''_{m-1}(L) := \{x - iL | x\in[-L,d_{m-1}]\}, \tag{3.18}$$

$$\gamma_0(L) := \{-L + iy | y\in[-L,L]\}, \tag{3.19}$$

and then use the estimate (2.41) to show that the only integral that survives from γ_m^- in the limit $L\to\infty$ is the one on Γ_{m-1} [notice that $\lim_{L\to\infty}\gamma_{m-1}(L)=\Gamma_{m-1}$]. Using the polar decomposition of $R_0(z)$ and the resolvent equation for $R(z)$ it follows that

$$\|\dot{Q}_m^-(t)\| \leqslant \frac{1}{2\pi}\oint_{\Gamma_{m-1}} |\mathrm{d}z|\|R_0(z)\|\|K(z)\| \cdot \||R_0(z)|^{1/2}\dot{H}_0 R_0(z)^{1/2}\| \cdot \|(1+K(z))^{-1}\| + \frac{1}{2\pi}\oint_{\Gamma_{m-1}} |\mathrm{d}z|\|R_0(z)\|$$
$$\times \|K(z)\| \cdot \||R_0(z)|^{1/2}\dot{H}_0 R_0(z)^{1/2}\| \cdot \|(1+K(z))^{-1}\|^2.$$

We note that the quantity $|R_0(z,t)^{1/2}|\dot{H}_0(t)R_0(z,t)^{1/2}$ is uniformly bounded on Γ_{m-1} (namely this quantity is bounded in norm by a constant). Indeed,

$$\sup_{t\in I_0}\sup_{z\in\Gamma_{m-1}} \|R_0(z,t)^{1/2}\dot{H}_0(t)|R_0(z,t)|^{1/2}\| = \sup_{t\in I_0}\sup_{y\in\mathbb{R}}\sup_{m'\in\mathbb{Z}} \left|\frac{2(m'+t)}{(m'+t)^2 - d_{m-1} - iy}\right| \leqslant C.$$

Then using Lemma 2.3 and the inequality $\|(1+K)\|^{-1} \leqslant (1-\|K\|)^{-1}$ one obtains

$$\sup_{t\in I_0}\|\dot{Q}_m^-(t)\| \leqslant C_V b(m-1). \tag{3.20}$$

Since $b(m-1) \leqslant Cb(m)$ we proved the claimed result on $\dot{Q}_m^-(t)$. The estimate of $\dot{Q}_m(t)$ goes along the same line, by deforming the closed contour around $\sigma(Q_m(t)H)$, γ_m, to $\Gamma_{m-1}\cup\Gamma_m$. The lemma is now proved. □

We turn now to the estimations of the norms in the right-hand side (rhs) of (3.13). For $X_m(t)$ Lemma 3.4 gives

$$\sup_{t\in I_0}\|X_m(t)\| \leqslant C_V b(m), \tag{3.21}$$

while for $Y_m(t)$ we write

$$\|Y_m(t)\| \leqslant \frac{1}{2\pi}(\|\dot{Q}_m^-(t)\| + \|\dot{Q}_m^+(t)\|)\int_{\Gamma_{m-1}} \mathrm{d}z\|R(z,t)\|^2 + \frac{1}{2\pi}(\|\dot{Q}_m(t)\| + \|\dot{Q}_m^+(t)\|)\int_{\Gamma_{m-1}\cup\Gamma_m} \mathrm{d}z\|R(z,t)\|^2. \tag{3.22}$$

Now for example [use again the estimate of $K(z,t)$ on $\Gamma_{m-1}\cup\Gamma_m$]

$$\sup_{t\in I_0}\int_{\Gamma_{m-1}\cup\Gamma_m} |\mathrm{d}z|\|R(z,t)\|^2 \leqslant C\sup_{t\in I_0}\int_{\Gamma_{m-1}\cup\Gamma_m} |\mathrm{d}z|\|R_0(z,t)\|^2 = \sup_{t\in I_0}\sup_{m'\in\mathbb{Z}}\int_{-\infty}^{\infty}\left\{\frac{\mathrm{d}y}{[E_{m',0}(t)-d_{m-1}]^2+y^2}\right.$$
$$\left. + \frac{\mathrm{d}y}{[E_{m',0}(t)-\mathrm{d}_m]^2+y^2}\right\} \leqslant C\langle m\rangle^{-1},$$

which together with Lemma 3.4 gives

$$\sup_{t\in I_0}\|Y_m(t)\| \leqslant C_V b(m)\langle m\rangle^{-1}. \tag{3.23}$$

Obviously, $Y_m(t_0)$ satisfies the same estimate. To estimate $\|\dot{Y}_m(t)\|$ one observes first that it involves estimates on $\ddot{Q}_m^-(t)$, $\ddot{Q}_m^+(t)$, and $\ddot{Q}_m(t)$. In what concerns $\ddot{Q}_m^-(t)$, we perform all the derivatives involved and estimate the various terms that appear. After a long but straightforward calculation one can check that the estimates for these terms involve only powers of $(1+K(z,t))^{-1}$, $R_0(z,t)^{1/2}\dot{H}_0(t)|R_0(z,t)|^{1/2}$, and the integral of $\|R_0(z,t)^{1/2}\|^2 \cdot \|K(z,t)\|$ on Γ_{m-1} which was already estimated in Lemma 2.3. The result is

$$\sup_{t\in I_0}\|\ddot{Q}_m^-(t)\| \leqslant C_V b(m). \tag{3.24}$$

The same estimate is satisfied by $\ddot{Q}_m(t)$ and then

$$\sup_{t\in I_0}\|\dot{Y}(t)\| \leqslant C_V b(m)\langle m\rangle^{-1}. \tag{3.25}$$

The last term to be considered is $X_m(t)Y_m(t)$ which gives a better estimate

$$\sup_{t\in I_0}\|X_m(t)Y_m(t)\| \leqslant C_V^2 b(m)^2\langle m\rangle^{-1}. \tag{3.26}$$

Collecting (3.13), (3.21), (3.23), (3.25), and (3.26) one obtains the first estimate from Theorem 3.1. For $\tilde{U}_m^A(t,t_0)$ the computations and estimations are similar as above, the only difference being that the contour of integration $\tilde{\Gamma}_m$ is slightly different, i.e., it is shifted upwards with $\frac{1}{2}$ with respect to Γ_m. As a consequence all the estimations will be improved with $\frac{1}{2}$, in the sense that $b(m) \to b\left(m+\frac{1}{2}\right)$. Thus there is no loss if we write

$$\sup_{t\in I_1}\|U(t,t_0) - \tilde{U}_m^A(t,t_0)\| \leqslant C_V b(m)\langle m\rangle^{-1}. \tag{3.27}$$

The proof of Theorem 3.1 is done. □

IV. THE ADIABATIC EVOLUTION. THE EFFECTIVE HAMILTONIAN

As shown in Theorem 3.1 the true evolution over the half-periods I_0 and I_1 is well approximated, in the limit of large m, by the adiabatic evolutions U_m^A and $\tilde{U}_m^A$. The next step is to compute, up to small controllable errors, U_m^A when restricted to $Q_m(t)\mathcal{H}$ and $\tilde{U}_m^A$ when restricted to $\tilde{Q}_m(t)\mathcal{H}$. In what follows we consider explicitly only U_m^A over I_0 and give the similar results for $\tilde{U}_m^A$ over I_1.

Before entering the computation of U_m^A let us show that, when restricted to $Q_m(t)\mathcal{H}$, U_m^A is nothing but the simplified dynamics in Ref. 2 obtained by keeping only the couplings between almost touching bands. Indeed, consider an initial wave function $\psi_m(s) \in Q_m(s)\mathcal{H}$, $s \in I_0$. Then, as far as $t \in I_0$, the adiabatic vector $\psi_m^A(t) := U_m^A(t,s)\psi_m(s) \in Q_m(t)\mathcal{H}$ and it can be written as

$$\psi_m^A(t) = \sum_{j=1}^{2} c_j(t)\varphi_{\alpha_j}(t), \quad \alpha_1 = 2m-2, \quad \alpha_2 = 2m-1, \tag{4.1}$$

where $\varphi_{\alpha_j}(t)$ are eigenfunctions of $H(t)$ corresponding to the eigenvalues from $\sigma(H(t))$ [one can assume that for $t=t_0$ or $t=t_1$, $\varphi_{\alpha_j}(t)$ coincide with the canonical eigenfunctions constructed in Sec. II]. Plugging the decomposition (4.1) into the Schrödinger equation for $\psi_m^A(t)$ (see Sec. III),

$$i\frac{d}{dt}\psi_m^A(t) = H_m^A(t)\psi_m^A(t) = (H(t) - X_m(t))\psi_m^A(t), \tag{4.2}$$

taking the scalar product with $\varphi_{\alpha_l}(t)$ and using the fact that $X_m(t)$ is off diagonal i.e., $Q_m(t)X_m(t)Q_m(t)=0$, one obtains

$$i\frac{d}{dt}c_l(t) = c_l(t)E_{\alpha_l}(t) + \sum_{j=1}^{2}\chi_{l,j}(t)c_j(t), \tag{4.3}$$

where

$$\chi_{l,j}(t) := -i\left\langle \varphi_{\alpha_l}(t), \frac{d}{dt}\varphi_{\alpha_j}(t)\right\rangle \tag{4.4}$$

which is nothing but the equation given in Ao's paper.

To compute U_m^A amounts then to solve the 2×2 system (4.3) and this problem has been considered many times (see Refs. 2,12,19,20 and references therein) in the physical literature. The trouble with (4.3) is that $\chi_{l,j}(t)$ are not easy to compute up to a controlled error in the limit $m \to \infty$ since due to the existence of quasicrossings one must deal with almost degenerate perturba-

tion theory. To our knowledge the earlier papers take for $\chi_{l,j}(t)$ a low order perturbation theory formula, but never controlled the rest. We avoid this difficulty by using the reduction theory which is the standard tool in analytic perturbation theory[15] and was as well extended to other contexts, in particular for adiabatic perturbation theory (see, e.g., Refs. 21,23 and references therein). More precisely, for m sufficiently large (see Corollary 2.2) $\|Q_m(t)-Q_{m,0}\|<1$ and then (see the Appendix) one can write the Sz-Nagÿ transformation matrix corresponding to the pair $Q_m(t), Q_{m,0}$,

$$Q_m(t) = W_m(t)Q_{m,0}W_m(t)^*. \tag{4.5}$$

Then if one defines for $t,s \in I_0$,

$$\mathcal{U}_m(t,s) := W_m(t)^* U_m^A(t,s)W_m(s), \tag{4.6}$$

it can be checked by straightforward calculation that

$$i\frac{\mathrm{d}\mathcal{U}_m(t,s)}{\mathrm{d}t} = (i\dot{W}_m(t)^* W_m(t) + W_m(t)^* H_m^A(t)W_m(t))\mathcal{U}_m(t,s) \tag{4.7}$$

and that

$$[Q_{m,0},\mathcal{U}_m(t,s)] = 0. \tag{4.8}$$

As a consequence if by definition

$$\mathcal{U}_{\mathrm{eff},m}(t,s) := Q_{m,0}\mathcal{U}_m(t,s)Q_{m,0} \tag{4.9}$$

then $\mathcal{U}_{\mathrm{eff},m}(t,s)$ satisfies (as operators in $Q_{m,0}\mathcal{H}$) the equation of motion

$$i\frac{d\mathcal{U}_{\mathrm{eff},m}(t,s)}{\mathrm{d}t} = Q_{m,0}(i\dot{W}_m(t)^* W_m(t) + W_m(t)^* H(t)W_m(t))Q_{m,0}\mathcal{U}_{\mathrm{eff},m}(t,s) =: H_{\mathrm{eff},m}(t)\mathcal{U}_{\mathrm{eff},m}(t,s). \tag{4.10}$$

Going backwards, once $\mathcal{U}_{\mathrm{eff},m}(t,s)$ is known one can recover $U_m^A(t,s)$ when restricted to $Q_m(t_0)\mathcal{H}$,

$$U_m^A(t,t_0)Q_m(t_0) = W_m(t)\mathcal{U}_{\mathrm{eff},m}(t,t_0)W_m(t_0)^* Q_m(t_0). \tag{4.11}$$

The point of the reduction theory outlined above is that we can compute $H_{\mathrm{eff},m}(t)$ up to a controlled error.

Theorem 4.1: *For sufficiently large m,*

$$H_{\mathrm{eff},m}(t) = Q_{m,0}(H_0(t)+V)Q_{m,0} + \tfrac{1}{2}Q_{m,0}(\hat{E}_{m,1}(t)V + V\hat{E}_{m,1}(t))Q_{m,0} + \Delta H_{\mathrm{eff},m}(t), \tag{4.12}$$

where

$$\hat{E}_{m,1}(t) := \frac{1}{2\pi i}\oint_{\gamma_m} \mathrm{d}z\, R_0(z,t)VR_0(z,t) \tag{4.13}$$

and

$$\sup_{t\in I_0}\|\Delta H_{\mathrm{eff},m}(t)\| \leqslant C_V\langle m\rangle b(m)^3. \tag{4.14}$$

We prove the theorem in a few lemmas, each lemma giving an estimate for different terms that appear in $H_{\mathrm{eff},m}(t)$. In the proofs we shall use several results of the perturbation theory. As well known, $Q_m(t)$ has the following expansion:

$$Q_m(t) = \sum_{j=0}^{N} \hat{E}_{m,j}(t) + E_{m,N+1}(t), \tag{4.15}$$

with

$$\hat{E}_{m,j}(t) := \frac{(-1)^j i}{2\pi} \oint_{\gamma_m} \mathrm{d}z\, R_0(z,t)(VR_0(z,t))^j, \tag{4.16}$$

$$E_{m,j}(t) := \frac{(-1)^j i}{2\pi} \oint_{\gamma_m} \mathrm{d}z (R_0(z,t)V)^j R(z,t). \tag{4.17}$$

Using the identity $Q_m(t) = (Q_m(t))^2$ one can easily check the following relations:

$$Q_{m,0}\hat{E}_{m,1}(t)Q_{m,0} = 0, \tag{4.18}$$

$$Q_{m,0}\hat{E}_{m,2}(t)Q_{m,0} = -Q_{m,0}\hat{E}^2_{m,1}(t)Q_{m,0}, \tag{4.19}$$

$$[H_0(t), \hat{E}_{m,1}(t)] = -[V, Q_{m,0}]. \tag{4.20}$$

Moreover, $E_{m,j}(t)$ and its derivatives obey the estimates

$$\sup_{t\in I_0} \|E_{m,j}(t)\| \leqslant C_V(b(m))^j, \tag{4.21}$$

$$\sup_{t\in I_0} \|\dot{E}_{m,j}(t)\| \leqslant C_V(j+1)(b(m))^j. \tag{4.22}$$

To see (4.21) we deform the contour γ_m into $\Gamma_{m-1} \cup \Gamma_m$ and write

$$\begin{aligned}\sup_{t\in I_0} \|E_{m,j}(t)\| &= \frac{1}{2\pi} \sup_{t\in I_0} \left\| \int_{\Gamma_{m-1}\cup\Gamma_m} \mathrm{d}z |R_0(z,t)|^{1/2} (K(z,t))^j (1+K(z,t))^{-1} R_0(z,t)^{1/2} \right\| \\ &\leqslant \frac{2}{2\pi} \sup_{t\in I_0} \sup_{z\in\Gamma_{m-1}\cup\Gamma_m} \|(K(z,t))^{j-1}\| \int_{\Gamma_{m-1}\cup\Gamma_m} |\mathrm{d}z| \|R_0(z,t)^{1/2}\|^2 \|K(z,t)\| \leqslant C_V(b(m))^j,\end{aligned}$$

where in the last line we used Lemma 2.3. The estimate (4.22) is obtained in the same way. We remark without giving details that $\hat{E}_{m,j}$ and $\dot{\hat{E}}_{m,j}$ verify the same estimates as $E_{m,j}$ and $\dot{E}_{m,j}$. Now we list the estimates for the various term appearing in $H_{\mathrm{eff},m}$.

Lemma 4.2: The first term in the effective Hamiltonian obeys the following estimate:

$$\sup_{t\in I_0} \|Q_{m,0}\dot{W}_m(t)^* W_m(t) Q_{m,0}\| \leqslant C_V \langle m\rangle b(m)^3. \tag{4.23}$$

Lemma 4.3: The second term is estimated as follows:

$$Q_0 W_m^*(t) H_0(t) W_m(t) Q_0 = Q_0 H_0(t) Q_0 - \tfrac{1}{2}\{Q_0 V \hat{E}_{m,1}(t) Q_0 + Q_0 \hat{E}_{m,1}(t) V Q_0\} + \mathcal{O}_r(\langle m\rangle b(m)^3). \tag{4.24}$$

Lemma 4.4: The last term gives

$$Q_0 W(t)^*_m V W_m(t) Q_0 = Q_0 V Q_0 + Q_0(V\hat{E}_{m,1}(t) + \hat{E}_{m,1}(t)V)Q_0 + \mathcal{O}_r(\langle m\rangle (b(m))^3). \tag{4.25}$$

Combining now Lemmas 4.2, 4.3, and 4.4 one obtains the explicit form of the effective Hamiltonian as given in Theorem 4.1. When proving the lemmas we skip for simplicity the index m and the time dependence of $W_m(t)$, $E_{m,1}(t)$, $Q_m(t)$, and other related quantities.

Proof of Lemma 4.2: We shall use the fact that E_1, $\hat{E}_1$, and E_2 are symmetric hence in particular $\partial_t(1-E_1^2)^{-1/2}$ is also symmetric. As we have said it is easy to see that

$$E_1 = \mathcal{O}_r(b(m)), \quad \hat{E}_1 = \mathcal{O}_r(b(m)), \quad E_2 = \mathcal{O}_r(b^2(m)).$$

Denoting $L := (1-E_1^2)^{-1/2} =: 1+M := 1+E_1^2F$ one has

$$WQ_0 = LQQ_0, \quad Q_0\dot{W}^* = Q_0\dot{Q}L + Q_0Q\dot{L}$$

and

$$M = \mathcal{O}_r(b^2(m)).$$

Actually by writing $L^2 = 1+\tilde{N}$ we obtain

$$Q_0\dot{W}^*WQ_0 = \tfrac{1}{2}Q_0(\dot{W}^*W - W^*\dot{W})Q_0 = \tfrac{1}{2}Q_0(\dot{Q}L^2Q - QL^2\dot{Q})Q_0 + \tfrac{1}{2}Q_0Q[\dot{L},L]QQ_0 = \tfrac{1}{2}Q_0[\dot{Q},Q]Q_0$$
$$+ \tfrac{1}{2}Q_0(\dot{Q}\tilde{N}Q - Q\tilde{N}\dot{Q})Q_0 + \tfrac{1}{2}Q_0Q[\dot{\tilde{N}},\tilde{N}]QQ_0 = \tfrac{1}{2}Q_0[\dot{Q},Q]Q_0 + \mathcal{O}_r(b^3(m))$$

where we used that $\tilde{N}$ and $\dot{\tilde{N}}$ are of $\mathcal{O}_r(b^2(m))$ and $\dot{Q} = \mathcal{O}_r(b(m))$. Now one should use the expansion $Q = Q_0 + \hat{E}_1 + E_2$ and the property $Q_0\hat{E}_1Q_0 = 0$,

$$Q_0[\dot{Q},Q]Q_0 = Q_0[\dot{\hat{E}}_1 + \dot{E}_2, Q_0 + \hat{E}_1 + E_2]Q_0 = Q_0[\dot{\hat{E}}_1, \hat{E}_1]Q_0 + \mathcal{O}_r(b^3(m)).$$

The last thing to be done is to show that $Q_0[\dot{\hat{E}}_1, \hat{E}_1]Q_0 = 0$. This follows by writing explicitly $\hat{E}_1$ (that is, by using residue theorem) and by direct calculation. □

Proof of Lemma 4.3: The idea behind the proof is to write

$$Q_0W^*H_0WQ_0 = Q_0W^*\hat{H}_0WQ_0 + (m-1)^2Q_0 \tag{4.26}$$

with $\hat{H}_0 := H_0 - (m-1)^2Q_0$ and to estimate the first term. As $W = (1+E_1^2F)(QQ_0 + (1-Q)(1-Q_0))$ then

$$WQ_0 = QQ_0 + E_1^2FQQ_0 \tag{4.27}$$

from where

$$Q_0W^*\hat{H}_0WQ_0 = Q_0Q\hat{H}_0QQ_0 + Q_0Q(\hat{H}_0E_1^2F + \text{h.c.}) + Q_0QFE_1^2\hat{H}_0E_1^2FQQ_0.$$

We start by estimating the last term

$$\sup_{t\in I_0}\|FE_1^2\hat{H}_0E_1^2F\| \leqslant \text{ct}\|E_1^2\| \cdot \|E_1\hat{H}_0E_1\|, \tag{4.28}$$

which requires an estimate on $E_1\hat{H}_0E_1$. To obtain it we shall use

$$\sup_{t\in I_0}\sup_{z,z'\in\Gamma_{m-1}\cup\Gamma_m}\|R_0(z',t)^{1/2}\hat{H}_0R_0(z,t)^{1/2}\| \leqslant C. \tag{4.29}$$

It follows from this that

$$\sup_{t\in I_0}\|E_1\hat{H}_0E_1\| = \sup_{t\in I_0}\Big\|\frac{1}{2\pi^2}\oint_{\gamma_m}\oint_{\gamma_m} \mathrm{d}z\,\mathrm{d}z' R_0(z,t)^{1/2}(1+K(z,t))^{-1}K(z,t)$$
$$\cdot |R_0(z,t)|^{1/2}\hat{H}_0|R_0(z',t)|^{1/2}K(z',t)(1+K(z',t))^{-1}|R_0(z',t)|^{1/2}$$
$$\leqslant C\oint_{\gamma_m}|\mathrm{d}z|\|R_0(z,t)^{1/2}\|\|K(z,t)\|\cdot\oint_{\gamma_m}|\mathrm{d}z'|\|R_0(z',t)^{1/2}\|\|K(z',t)\|\leqslant C_V\langle m\rangle b(m)^2.$$

Then the term $FE_1^2\hat{H}_0E_1^2F$ turns out to be of order $\mathcal{O}_r(\langle m\rangle b(m)^4)$ and can be disregarded. We continue the estimations with $Q_0QFE_1^2\hat{H}_0QQ_0$ using the perturbation theory up to E_1 (i.e., $Q=Q_0+E_1$):

$$Q_0QFE_1^2\hat{H}_0QQ_0 = Q_0FE_1^2\hat{H}_0Q_0 + Q_0FE_1^2\hat{H}_0E_1Q_0 + Q_0E_1FE_1^2\hat{H}_0E_1Q_0 + Q_0E_1FE_1^2\hat{H}_0Q_0.$$

The second and the third terms in the above equation are simply estimated using the bounds on E_1 and $E_1\hat{H}_0E_1$. For the fourth term we have to estimate instead $Q_0\hat{H}_0E_1$. Following the same steps as in the estimation of $E_1\hat{H}_0E_1$ we arrive at

$$\sup_{t\in I_0}\|Q_0\hat{H}_0E_1(t)\| = \sup_{t\in I_0}\left\|\frac{1}{2\pi^2}\oint_{\gamma_m}\oint_{\gamma_m}\mathrm{d}z\,\mathrm{d}z'\,R_0(z,t)\hat{H}_0(t)R_0\,(z',t)V(z',t))R(z',t)\right\|\leqslant C_V\langle m\rangle b(m). \tag{4.30}$$

In the similar way one can prove a more general result that will be used below, namely

$$\sup_{t\in I_0}\|Q_0\hat{H}_0E_j\|\leqslant C_V\langle m\rangle(b(m))^j. \tag{4.31}$$

It follows then from (4.30) that

$$\sup_{t\in I_0}\|Q_0E_1FE_1^2\hat{H}_0Q_0\|\leqslant C\|E_1\|^2\|E_1\hat{H}_0Q_0\|\leqslant C_V\langle m\rangle(b(m))^3.$$

Hence a preliminar result is

$$Q_0W^*\hat{H}_0WQ_0 = Q_0Q\hat{H}_0QQ_0 + Q_0Q(FE_1^2\hat{H}_0 + \hat{H}_0E_1^2F)QQ_0 + \mathcal{O}_r(\langle m\rangle(b(m))^3). \tag{4.32}$$

To go further we shall use that $F=\frac{1}{2}+E_1^2G$ (G and its derivatives being again uniformly bounded). Then

$$Q_0QFE_1^2\hat{H}_0QQ_0 = \tfrac{1}{2}Q_0QE_1^2\hat{H}_0QQ_0 + Q_0QE_1^2GE_1^2\hat{H}_0QQ_0$$

and the last term is of order $\mathcal{O}_r(\langle m\rangle(b(m))^4)$. In what concerns $Q_0QE_1^2\hat{H}_0QQ_0$ one should use the perturbation theory up to E_1,

$$Q_0QE_1^2\hat{H}_0QQ_0 = Q_0E_1^2\hat{H}_0Q_0 + \mathcal{O}_r(\langle m\rangle(b(m))^3) \tag{4.33}$$

so finally

$$Q_0W^*\hat{H}_0WQ_0 = Q_0\hat{H}_0Q_0 + Q_0(\hat{H}_0E_1 + E_1\hat{H}_0)Q_0 + \tfrac{1}{2}Q_0(\hat{H}_0E_1^2 + E_1^2\hat{H}_0)Q_0$$
$$+ Q_0E_1\hat{H}_0E_1Q_0 + \mathcal{O}_r(\langle m\rangle(b(m))^3).$$

In the following we shall use the expansion $E_1=\hat{E}_1+\cdots+\hat{E}_N+E_{N+1}$ for suitable N and the estimate (4.31), in such a way that the terms containing E_{N+1} are small. It turns out that in order to estimate the third and the fourth terms it is sufficient to go up to E_2. When plugging this expansion in $Q_0\hat{H}_0E_1^2Q_0$ and $Q_0E_1\hat{H}_0E_1Q_0$ several new terms will appear ($Q_0\hat{H}_0\hat{E}_1E_2Q_0$, $Q_0\hat{E}_1\hat{H}_0E_2$, and

$Q_0E_2\hat{H}_0E_2$). All of them are easily estimated in the same way as before and the result is

$$Q_0\hat{H}_0E_1^2Q_0 = Q_0\hat{H}_0\hat{E}_1^2Q_0 + \mathcal{O}_r(\langle m\rangle(b(m))^3),$$

$$Q_0E_1\hat{H}_0E_1Q_0 = Q_0\hat{E}_1\hat{H}_0\hat{E}_1 + \mathcal{O}_r(\langle m\rangle(b(m))^3). \tag{4.34}$$

For the first term we must go up to E_3 with the expansion. Using (4.31) and the identity (4.18) we arrive at

$$Q_0\hat{H}_0E_1Q_0 = Q_0\hat{H}_0\hat{E}_2Q_0 + \mathcal{O}_r(\langle m\rangle(b(m))^3). \tag{4.35}$$

Moreover, using (4.19) we can replace $Q_0\hat{E}_2Q_0$ and write

$$\begin{aligned} Q_0W^*H_0WQ_0 &= Q_0\hat{H}_0 + Q_0(n_0-1)^2 - \tfrac{1}{2}Q_0(\hat{H}_0\hat{E}_1^2 + \hat{E}_1^2\hat{H}_0)Q_0 + \tfrac{1}{2}(Q_0\hat{E}_1\hat{H}_0\hat{E}_1Q_0 + Q_0\hat{E}_1\hat{H}_0\hat{E}_1Q_0) \\ &\quad + \mathcal{O}_r(\langle m\rangle(b(m))^3) = Q_0H_0 + \tfrac{1}{2}(Q_0[\hat{E}_1,\hat{H}_0]\hat{E}_1Q_0 + Q_0\hat{E}_1[\hat{H}_0,\hat{E}_1]) + \mathcal{O}_r(\langle m\rangle(b(m))^3) \\ &= Q_0H_0Q_0 - \tfrac{1}{2}\{Q_0V\hat{E}_1Q_0 + Q_0\hat{E}_1VQ_0\} + \mathcal{O}_r(\langle m\rangle(b(m))^3). \end{aligned} \tag{4.36}$$

In the last line we used (4.20). The lemma is now proved. □

Proof of Lemma 4.4: Using (4.27) and $Q=Q_0+E_1$ it results

$$\begin{aligned} Q_0W(t)^*VW(t)Q_0 &= Q_0VQ_0 + Q_0(E_1V+VE_1)Q_0 + Q_0E_1VE_1Q_0 + Q_0(Q_0+E_1)(VE_1^2F + FE_1^2V)(Q_0 \\ &\quad + E_1)Q_0 + Q_0(Q_0+E_1)FE_1(E_1VE_1)E_1F(Q_0+E_1)Q_0. \end{aligned}$$

Let us first show that the last three terms are small. To see this we need estimates on E_1VE_1 and Q_0VE_1. For E_1VE_1 one has

$$\begin{aligned} E_1VE_1 = -\frac{1}{2\pi^2}\oint_{\gamma_m}\oint_{\gamma_m} \mathrm{d}z\,\mathrm{d}z'\, R_0(z,t)^{1/2}K(z,t)(1+K(z,t))^{-1}\cdot|R_0(z,t)|^{1/2}VR_0(z',t)^{1/2} \\ \times K(z',t)(1+K(z',t))^{-1}|R_0(z',t)|^{1/2}. \end{aligned} \tag{4.37}$$

Now observe that

$$\sup_{t\in I_0}\sup_{z\in\gamma_m}\sup_{z'\in\gamma_m}\||R_0(z,t)|^{1/2}VR_0(z',t)^{1/2}\| \leqslant C_Vb(m). \tag{4.38}$$

Then using the fact that $l(\gamma_m)\sim\langle m\rangle$,

$$\sup_{t\in I_0}\|E_1VE_1\| \leqslant C_V\langle m\rangle(b(m))^3. \tag{4.39}$$

In what concerns Q_0VE_1 we have

$$\sup_{t\in I_0}\|Q_0VE_1\| = \frac{1}{2\pi}\left\|\oint_{\gamma_m}\oint_{\gamma_m}\mathrm{d}z\,\mathrm{d}z'\,R_0(z,t)VR_0(z',t)VR(z',t)\right\| \leqslant C_V\langle m\rangle(b(m))^2. \tag{4.40}$$

The estimates (4.39) and (4.40) used in $Q_0W(t)^*VW(t)Q_0$ suffices to prove that the last three terms are of order $\mathcal{O}_r(\langle m\rangle(b(m))^3)$. We arrived thus at

$$Q_0W^*VWQ_0 = Q_0VQ_0 + Q_0(VE_1+E_1V)Q_0 + \mathcal{O}_r(\langle m\rangle(b(m))^3).$$

As for the remaining term $Q_0E_1VQ_0$ we shall write it more carefully by writing

$$Q_0E_1VQ_0 = Q_0(\hat{E}_1+E_2)VQ_0. \tag{4.41}$$

Finally, $Q_0E_2VQ_0$ is found to be of order $\mathcal{O}_r(\langle m\rangle(b(m))^3)$ and the lemma is finished. □

For $\tilde{H}_{\mathrm{eff},m}$ the computations and estimations are similar as above the difference appearing again due to the different integration contour. We can then conclude that

$$\tilde{H}_{\mathrm{eff},m}(t) = \tilde{Q}_{m,0}(H_0(t) + V)\tilde{Q}_{m,0} + \tfrac{1}{2}\tilde{Q}_{m,0}(\hat{E}_{m,1}(t)V + V\hat{E}_{m,1}(t))\tilde{Q}_{m,0} + \Delta\tilde{H}_{\mathrm{eff},m}(t),$$

where $\hat{E}_{m,1}(t)$ is now the first order term from the pertubative expansion for $\tilde{Q}_m(t)$ and the remainder $\Delta\tilde{H}_{\mathrm{eff},m}(t)$ is of the same order as in Theorem 4.2.

V. THE ADIABATIC EVOLUTION. THE TRANSITION AMPLITUDES

We shall use now the effective Hamiltonian obtained in the preceding section to compute $U_m^A(t_1,t_0)$ and $\tilde{U}_m^A(t_2,t_1)$ when restricted to $Q_m(t_0)\mathcal{H}$ and $\tilde{Q}_m(t_1)\mathcal{H}$, respectively, up to an error which remains small after taking the sum over m from some sufficiently large n_0 to infinity. This amounts to the computation of the 2×2 transfer matrices $\mathcal{S}^m(t_1,t_0): Q_m(t_0)\mathcal{H} \to Q_m(t_1)\mathcal{H}$ and $\tilde{\mathcal{S}}^m(t_2,t_1): \tilde{Q}_m(t_1)\mathcal{H} \to \tilde{Q}_m(t_2)\mathcal{H}$ (remember that $t_0=-\frac{1}{4}$, $t_1=\frac{1}{4}$, $t_2=\frac{3}{4}$). They are in turn related to the effective evolutions $U_{\mathrm{eff},m}$ and $\tilde{U}_{\mathrm{eff},m}$ (see Sec. IV) by the unitary transformations that rotate the proper basis of $Q_m(t)\mathcal{H}$ and $\tilde{Q}_m(t)\mathcal{H}$ to the canonical ones in $Q_{m,0}\mathcal{H}$ and $\tilde{Q}_{m,0}\mathcal{H}$. The coefficients of these transformations are easily estimated thus one is left with the calculation of the effective evolutions. The strategy goes as follows: We start from the effective Hamiltonians introduced in Sec. IV and use Dyson techniques. Along the Dyson expansions new effective Hamiltonians appear as well as additional error terms which we carefully count. The final Hamiltonian has a nice simple structure: it decomposes into a free diagonal time-dependent part and an off-diagonal time independent perturbation. Its associated evolution leads to the Landau–Zener formulas similar to the ones obtained by Browne and Lenstra. The rigorous form of the above discussion is the main result of this section and is contained in the following.

Theorem 5.1: *Let $r>-\frac{1}{2}$, m sufficiently large and define the transfer matrices*

$$\mathcal{S}^m(t_1,t_0) = \begin{pmatrix} \mathcal{S}^m_{2m-1,2m-2}(t_1,t_0) & \mathcal{S}^m_{2m-1,2m-1}(t_1,t_0) \\ \mathcal{S}^m_{2m-2,2m-2}(t_1,t_0) & \mathcal{S}^m_{2m-2,2m-1}(t_1,t_0) \end{pmatrix}, \tag{5.1}$$

$$\tilde{\mathcal{S}}^m(t_2,t_1) = \begin{pmatrix} \tilde{\mathcal{S}}^m_{2m,2m-1}(t_2,t_1) & \tilde{\mathcal{S}}^m_{2m,2m}(t_2,t_1) \\ \tilde{\mathcal{S}}^m_{2m-1,2m-1}(t_2,t_1) & \tilde{\mathcal{S}}^m_{2m-1,2m}(t_2,t_1) \end{pmatrix}, \tag{5.2}$$

with

$$\mathcal{S}^m_{i,j}(t_1,t_0) := \langle \varphi_i(t_1), U_m^A(t_1,t_0)\varphi_j(t_0)\rangle, \quad i,j = 2m-2, 2m-1 \tag{5.3}$$

$$\tilde{\mathcal{S}}^m_{i,j}(t_2,t_1) := \langle \varphi_i(t_2), \tilde{U}_m^A(t_2,t_1)\varphi_j(t_1)\rangle, \quad i,j = 2m-1, 2m. \tag{5.4}$$

Then

$$\mathcal{S}^m(t_1,t_0) = e^{-i\theta_m(t_1,t_0)}\begin{pmatrix} \alpha_{2m-2}(t_1,t_0) & -\overline{\beta}_{2m-2}(t_1,t_0) \\ \beta_{2m-2}(t_1,t_0) & \alpha'_{2m-2}(t_1,t_0) \end{pmatrix} + \mathcal{R}_{\mathrm{eff},m}, \tag{5.5}$$

$$\tilde{\mathcal{S}}^m(t_2,t_1) = e^{-i\tilde{\theta}_m(t_2,t_1)}\begin{pmatrix} \tilde{\alpha}_{2m-1}(t_2,t_1) & -\bar{\tilde{\beta}}_{2m-1}(t_2,t_1) \\ \tilde{\beta}_{2m-1}(t_2,t_1) & \tilde{\alpha}'_{2m-1}(t_2,t_1) \end{pmatrix} + \mathcal{R}_{\mathrm{eff},m}, \tag{5.6}$$

with

$$\mathcal{R}_{\mathrm{eff},m} = \mathcal{O}_r\left(\frac{\log^8\langle m\rangle}{\langle m\rangle^{\min\{2+8r,3/2+5r,3/2+r,2\}}}\right) \quad \text{as } m\to\infty \tag{5.7}$$

and the following notations (we list below only the quantities related to $\mathcal{S}^m$; the ones corresponding to $\widetilde{\mathcal{S}}^m$ are discussed at the end of this section):

$$\alpha_{2m-2}(t_1,t_0) := 1 - \frac{|\hat{V}(2(m-1))|^2}{m-1} c_{2,m}(t_1,t_0) - i\omega_{1,m}(t_1,t_0), \tag{5.8}$$

$$\alpha'_{2m-2}(t_1,t_0) := 1 - \frac{|\hat{V}(2(m-1))|^2}{m-1} c_{2,m}(t_1,t_0) - i\omega_{2,m}(t_1,t_0), \tag{5.9}$$

$$\beta_{2m-2}(t_1,t_0) := \frac{\overline{\hat{V}(2(m-1))}}{\sqrt{m-1}} c_{1,m}(t_1,t_0) - i\lambda_m(t_1,t_0) - \frac{\overline{2\hat{V}(2(m-1))}}{m-1}, \tag{5.10}$$

$$c_{1,m}(t_1,t_0) := -(i+1)\frac{\sqrt{\pi}}{2} e^{i(m-1)/8} \operatorname{erf}\left(\frac{i+1}{4}\sqrt{m-1}\right), \tag{5.11}$$

$$c_{2,m}(t_1,t_0) := \frac{\pi}{4}\left|\operatorname{erf}\left(\frac{i-1}{4}\sqrt{m-1}\right)\right|^2, \tag{5.12}$$

$$\theta_m(t_1,t_0) := \int_{t_0}^{t_1} \mathrm{d}s((m-1)^2 + s^2),$$

$$\lambda_m(t_1,t_0) := \int_{t_0}^{t_1} \mathrm{d}s\, \overline{\Delta}_m(s) e^{-2i(m-1)(s^2-t_0^2)}, \tag{5.13}$$

$$\omega_{1,m}(t_1,t_0) := \int_{t_0}^{t_1} \mathrm{d}s \frac{1}{2}\langle \varphi_{m-1,0}, (V\hat{E}_1(t) + \hat{E}_1(t)V)\varphi_{m-1,0}\rangle =: \int_{t_0}^{t_1} \mathrm{d}s\, \gamma_{1,m}(s) \tag{5.14}$$

$$\omega_{2,m}(t_1,t_0) := \int_{t_0}^{t_1} \mathrm{d}s \frac{1}{2}\langle \varphi_{-(m-1),0}, (V\hat{E}_1(t) + \hat{E}_1(t)V)\varphi_{-(m-1),0}\rangle =: \int_{t_0}^{t_1} \mathrm{d}s\, \gamma_{2,m}(s), \tag{5.15}$$

$$\Delta_m(t) := \tfrac{1}{2}\langle \varphi_{m-1,0}, (V\hat{E}_1(t) + \hat{E}_1(t)V)\varphi_{-(m-1),0}\rangle. \tag{5.16}$$

Here $\operatorname{erf}(z)$ *is the error function (see Ref. 1):*

$$\operatorname{erf}(z) := \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2}\, \mathrm{d}t. \tag{5.17}$$

Remark: Although the above estimates are valid for $r > -\frac{1}{2}$ the bound on the error terms gets small as m tends to infinity only for $r > -\frac{1}{4}$ and is summable with respect to m only for $r > -\frac{1}{10}$ (these facts can be noticed from the behavior of the error term $\mathcal{R}_{\mathrm{eff},m}$).

Proof: We shall consider only $S^m_{i,j}$; the proof for $\widetilde{S}^m_{i,j}$ is similar. From (2.48) and (4.11):

$$S^m_{i,j}(t_1,t_0) = \sum_{k,l=2m-2,2m-1} \overline{c}^m_{k,i}(t_1)\mathcal{U}_{\mathrm{eff},m;k,l}(t_1,t_0)c^m_{l,j}(t_0), \tag{5.18}$$

where $\varphi^0_\alpha(t_\beta) = \varphi_{n_\alpha,0}(t_\beta)$ [see (2.30)] and we introduced the coefficients

$$c^m_{i,k}(t_p) := \langle \varphi^0_i(t_p), W_m(t_p)^* N_k(t_p) \varphi^0_k(t_p) \rangle, \quad p = 0,1 \tag{5.19}$$

and

$$\mathcal{U}_{\mathrm{eff},m;k,l}(t_1,t_0) := \langle \varphi^0_k(t_1), \mathcal{U}_{\mathrm{eff},m}(t_1,t_0) \varphi^0_l(t_0) \rangle. \tag{5.20}$$

The estimation of the coefficients $c^m_{i,k}(t_p)$ is easy and reads as follows.

Lemma 5.2: For m large enough and $r > -\frac{1}{2}$ *one has*

$$c^m_{\alpha,\beta}(t_p) = \delta_{\alpha,\beta} + \frac{\langle \varphi^0_\alpha(t_p), V\varphi^0_\beta(t_p) \rangle}{E^0_\beta(t_p) - E^0_\alpha(t_p)} (1 - \delta_{\alpha,\beta}) + \mathcal{O}_r(b^2(m)) \quad \text{as } m \to \infty. \tag{5.21}$$

The estimation of $\mathcal{U}_{\mathrm{eff},m}$ is more involved and the result is summarized in the following.

Lemma 5.3: For m large enough and $r > -\frac{1}{2}$ *the effective evolution is given by*

$$\mathcal{U}_{\mathrm{eff},m;i,j}(t_1,t_0) = \mathcal{S}^m_{ij}(t_1,t_0) + e^{-i\theta_m(t_1,t_0)} v_m + \mathcal{R}_{\mathrm{eff},m} \quad \text{as } m \to \infty \tag{5.22}$$

with

$$v_m := \begin{pmatrix} 0 & -\dfrac{2\hat{V}(2(m-1))}{m-1} \\ \dfrac{2\hat{V}(2(m-1))}{m-1} & 0 \end{pmatrix}. \tag{5.23}$$

The proof of Theorem 5.1 requires only straightforward calculations using (5.18), (5.21), and (5.22).

Proof of Lemma 5.2: Write [see (4.16) and (4.17)]

$$Q_m(t_p) - Q^0_m(t_p) = \hat{E}_{m,1}(t_p) + E_{m,2}(t_p), \tag{5.24}$$

and in the same way

$$P_\alpha(t_p) - P^0_\alpha(t_p) = -\frac{i}{2\pi} \int_{C_\alpha} \mathrm{d}z\, R_0(z,t_p) V R_0(z,t_p) + \frac{i}{2\pi} \int_{C_\alpha} \mathrm{d}z\, R_0(z,t_p) V R(z,t_p) V R_0(z,t_p) =: \hat{e}_{\alpha,1}(t_p) + e_{\alpha,2}(t_p), \quad p = 0,1 \tag{5.25}$$

with $C_{2m-2} = \Gamma_{m-1} \cup \tilde{\Gamma}_{m-1}$ and $C_{2m-1} = \tilde{\Gamma}_{m-1} \cup \Gamma_m$, i.e., C_α is a countour which contains only one eigenvalue of $H_0(t_p)$ namely $E^0_\alpha(t_p)$. By Lemma 2.3 (see also Sec. IV) one has

$$\|\hat{E}_{m,1}(t_p)\| + \|\hat{e}_{\alpha,1}(t_p)\| \leqslant C_V b(m), \tag{5.26}$$

$$\|E_{m,2}(t_p)\| + \|e_{\alpha,2}(t_p)\| \leqslant C_V b(m)^2. \tag{5.27}$$

Then using the expansion in the Sz-Nagÿ formula, (5.26) and (5.27), and the fact that for $\alpha = 2m-2$, $2m-1$ we have $Q_{m,0} P^0_\alpha(t_p) = P^0_\alpha(t_p) Q_{m,0} = P^0_\alpha(t_p)$ and $P^0_\alpha(t_p) \varphi^0_\alpha(t_p) = \varphi^0_\alpha(t_p)$ it follows that up to errors of order $\mathcal{O}_r b(m)^2$,

$$c^m_{\alpha,\beta}(t_p) = \langle \varphi^0_\alpha(t_p), (1 + \hat{E}_{m,1}(t_p) + \hat{e}_{\beta,1}(t_p)) \varphi^0_\beta(t_p) \rangle. \tag{5.28}$$

Since $Q_{m,0} \hat{E}_{m,1}(t_p) Q_{m,0} = P^0_\beta(t_p) \hat{e}_{\beta,1}(t_p) P^0_\beta(t_p) = 0$ one gets finally

$$|c^m_{\alpha,\beta}(t_p) - \delta_{\alpha,\beta} - \langle \varphi^0_\alpha(t_p), \hat{e}_{\beta,1}(t_p) \varphi^0_\beta(t_p) (1 - \delta_{\alpha,\beta}) \rangle| \leqslant C_V b(m)^2 \tag{5.29}$$

and computing the third term on the left-hand side (lhs) of (5.29) by residues theorem we obtain the needed result. □

Proof of Lemma 5.3: First remark that due to Theorem 4.1 one can write

$$H_{\mathrm{eff},m}(t) = h_{\mathrm{eff},m}(t) + \Delta H_{\mathrm{eff},m}(t), \tag{5.30}$$

where

$$h_{\mathrm{eff},m}(t) = Q_{m,0}(H_0(t) + V)Q_{m,0} + \tfrac{1}{2}Q_{m,0}(\hat{E}_{m,1}(t)V + V\hat{E}_{m,1}(t))Q_{m,0}. \tag{5.31}$$

Denote then by $\mathcal{U}^0_{\mathrm{eff},m}(t,t_0)$ the evolution associated to $h_{\mathrm{eff},m}(t)$ having the equation of motion

$$i\frac{d}{dt}\mathcal{U}^0_{\mathrm{eff},m}(t,t_0) = h_{\mathrm{eff},m}(t)\mathcal{U}^0_{\mathrm{eff},m}(t,t_0), \quad \mathcal{U}^0_{\mathrm{eff},m}(t_0,t_0) = 1. \tag{5.32}$$

The usual estimation for $\Omega_{\mathrm{eff},m}(t,t_0) := \mathcal{U}^0_{\mathrm{eff},m}(t,t_0)^*\mathcal{U}_{\mathrm{eff},m}(t,t_0)$ gives

$$\sup_{t\in I_0}\|\Omega_{\mathrm{eff},m}(t,t_0) - 1\| \leqslant \frac{1}{2}\sup_{t\in I_0}\|\Delta H_{\mathrm{eff},m}(s)\| \leqslant C_V\langle m\rangle b(m)^3.$$

Hence

$$\mathcal{U}_{\mathrm{eff},m}(t,t_0) = \mathcal{U}^0_{\mathrm{eff},m}(t,t_0) + \mathcal{O}_r(\langle m\rangle b(m)^3) \quad \text{as } m\to\infty. \tag{5.33}$$

We continue the computation of $\mathcal{U}^0_{\mathrm{eff},m}(t,t_0)$ by further decomposing $h_{\mathrm{eff},m}(t)$ into a "free" part

$$H_{P,m}(t) := Q_{m,0}(H_0(t) + V)Q_{m,0} \tag{5.34}$$

and a perturbation

$$B_m(t) := \tfrac{1}{2}Q_{m,0}(\hat{E}_{m,1}(t)V + V\hat{E}_{m,1}(t))Q_{m,0}. \tag{5.35}$$

Remark first that $H_{P,m}(t)$ has a simple matrix form in the eigenbasis of $H_0(t)$ that can be explicitly written taking into account that $Q_{m,0} = P_{m-1,0} + P_{-(m-1),0}$. Second one notes that it is possible to eliminate a diagonal term from $H_{P,m}(t)$ by writing

$$\mathcal{U}^0_{\mathrm{eff},m}(t_1,t_0) := \exp\left(-i\int_{t_0}^{t_1}((m-1)^2 + s^2)\mathrm{d}s\right)\hat{\mathcal{U}}_{\mathrm{eff},m}(t_1,t_0), \tag{5.36}$$

where $\hat{\mathcal{U}}_{\mathrm{eff},m}(t,t_0)$ satisfies the equation

$$i\frac{d}{dt}\hat{\mathcal{U}}_{\mathrm{eff},m}(t,t_0) = (\hat{H}_{P,m}(t) + B_m(t))\hat{\mathcal{U}}_{\mathrm{eff},m}(t,t_0), \quad \hat{\mathcal{U}}_{\mathrm{eff},m}(t_0,t_0) = 1, \tag{5.37}$$

and

$$\hat{H}_{P,m}(t) = \begin{pmatrix} 2(m-1)t & \hat{V}(2(m-1)) \\ \hat{V}(2(m-1)) & -2(m-1)t \end{pmatrix}. \tag{5.38}$$

Now let $\hat{\mathcal{U}}_{P,m}(t,t_0)$ be the evolution generated by $\hat{H}_{P,m}(t)$ and

$$\hat{\Omega}_{P,m}(t_1,t_0) = \hat{\mathcal{U}}_{P,m}(t_1,t_0)^*\hat{\mathcal{U}}_{m,\mathrm{eff}}(t_1,t_0). \tag{5.39}$$

We write the Dyson expansion for $\hat{\Omega}_{P,m}$ with the remainder of order 2,

$$\hat{\Omega}_{P,m}(t_1,t_0) = 1 + (-i)\int_{t_0}^{t_1} \mathrm{d}s_1\, B_m^{\mathrm{int}}(s_1) + (-i)^2 \int_{t_0}^{t_1} \mathrm{d}s_1\, B_m^{\mathrm{int}}(s_1) \int_{t_0}^{s_1} \mathrm{d}s_2\, B_m^{\mathrm{int}}(s_2)\hat{\Omega}_{P,m}(s_2,t_0), \tag{5.40}$$

where $B_m^{\mathrm{int}}(t) = \hat{\mathcal{U}}_{P,m}(t,t_0)^* B_m(t)\hat{\mathcal{U}}_{P,m}(t,t_0)$. Observe first that $\sup_{t\in I_0} B_m(t) = \mathcal{O}_r(\langle m\rangle b(m)^2)$ as $m \to \infty$ [this follows from the estimate on $Q_{m,0}V\hat{E}_1(t)$ which is the same as the one from Eq. (4.40)]. Then

$$\sup_{t\in I_0} \left\| \int_{t_0}^{t_1} \mathrm{d}s_1\, B_m^{\mathrm{int}}(s_1) \int_{t_0}^{s_1} \mathrm{d}s_2\, B_m^{\mathrm{int}}(s_2)\hat{\Omega}_{P,m}(s_2,t_0) \right\| \leqslant \frac{1}{4}(\sup_{t\in I_0}\|B_m(t)\|)^2 = \mathcal{O}_r((\langle m\rangle b(m)^2)^2) \quad \text{as } m \to \infty. \tag{5.41}$$

In conclusion, at this level of approximation from (5.39) we have

$$\hat{\mathcal{U}}_{\mathrm{eff},m}(t_1,t_0) = \hat{\mathcal{U}}_{P,m}(t_1,t_0)\left[1 - i\int_{t_0}^{t_1} \mathrm{d}s\, B_m^{\mathrm{int}}(s)\right] + \mathcal{O}_r((\langle m\rangle b(m)^2)^2) \quad \text{as } m \to \infty. \tag{5.42}$$

Thus we have reduced the problem at hand to the computation of $\hat{\mathcal{U}}_{P,m}(t_1,t_0)$ and of the contribution of B_m^{int}. Now we write $\hat{H}_{P,m}(t)$ in the form $\hat{H}_{P,m}(t) = \hat{H}_{P,m}^0(t) + \hat{V}_P$, where

$$\hat{H}_{P,m}^0(t) = \begin{pmatrix} 2(m-1)t & 0 \\ 0 & -2(m-1)t \end{pmatrix}, \quad \hat{V}_P = \begin{pmatrix} 0 & \hat{V}(2(m-1)) \\ \overline{\hat{V}(2(m-1))} & 0 \end{pmatrix}.$$

Let $\hat{\mathcal{U}}_{P,m}^0$ be the evolution generated by $\hat{H}_{P,m}^0$,

$$\hat{\mathcal{U}}_{P,m}^0(t,t_0) = \begin{pmatrix} e^{-i(m-1)(t^2-t_0^2)} & 0 \\ 0 & e^{i(m-1)(t^2-t_0^2)} \end{pmatrix}. \tag{5.43}$$

By defining all the "effective" Hamiltonians above we ended with a time-independent perturbation $\hat{V}_P$ (which is precisely the one considered in the physical literature[2,12]). Writing the Dyson expansion with the remainder of order 3 for $\hat{\Omega}_{P,m}^0(t_1,t_0) = \hat{\mathcal{U}}_{P,m}^0(t_1,t_0)^*\hat{\mathcal{U}}_{P,m}(t_1,t_0)$,

$$\begin{aligned}\hat{\Omega}_{P,m}^0(t_1,t_0) &= 1 + (-i)\int_{t_0}^{t_1} \mathrm{d}s_1\, \hat{V}_P(s_1) + (-i)^2 \int_{t_0}^{t_1} \mathrm{d}s_1\, \hat{V}_P(s_1) \int_{t_0}^{s_1} \mathrm{d}s_2\, \hat{V}_P(s_2) \\ &\quad + (-i)^3 \int_{t_0}^{t_1} \mathrm{d}s_1\, \hat{V}_P(s_1) \int_{t_0}^{s_1} \mathrm{d}s_2\, \hat{V}_P(s_2) \int_{t_0}^{s_2} \mathrm{d}s_3\, \hat{V}_P(s_3)\hat{\Omega}_{P,m}^0(s_3,t_0) \\ &:= 1 + \hat{\Omega}_{P,m}^{0,(1)}(t_1,t_0) + \hat{\Omega}_{P,m}^{0,(2)}(t_1,t_0) + \mathcal{R}_3, \end{aligned} \tag{5.44}$$

where $\hat{V}_P(t) = \hat{\mathcal{U}}_{P,m}^0(t,t_0)^*\hat{V}_P\hat{\mathcal{U}}_{P,m}^0(t,t_0)$. We compute explicitely the first and second order terms while the remainder $\mathcal{R}_3$ is estimated using Eq. (A28) from the Appendix. That is, we use (A45) for $p=3$ which gives, with m large enough

$$\|\mathcal{R}_3\| \leqslant C_{m_0}\|V\|_r^3 \frac{\log^2\langle m\rangle}{\langle m\rangle^{3/2+3r}}. \tag{5.45}$$

As for the first two terms in the Dyson expansion by direct computation we have

$$\sum_{k=0}^{2}\hat{\Omega}_{P,m}^{0,(k)}(t_1,t_0)=\begin{pmatrix}1-\dfrac{|\hat{V}(2(m-1))|^2}{m-1}c_{2,m}(t_1,t_0) & -\dfrac{\hat{V}(2(m-1))}{\sqrt{m-1}}\overline{c_{1,m}(t_1,t_0)}\\ \dfrac{\overline{\hat{V}(2(m-1))}}{\sqrt{m-1}}c_{1,m}(t_1,t_0) & 1-\dfrac{|\hat{V}(2(m-1))|^2}{m-1}c_{2,m}(t_1,t_0)\end{pmatrix}, \tag{5.46}$$

with $c_{1,m}(t_1,t_0)$ and $c_{2,m}(t_1,t_0)$ as introduced in Theorem 5.1.

The expression (5.46) together with the estimate (5.45) allow to compute approximately $\hat{\mathcal{U}}_{P,m}$ with the help of the following formula for $B_m(t)$ [see (5.35) and (5.14)–(5.16)]:

$$B_m(t)=\begin{pmatrix}\gamma_{1,m}(t) & \Delta_m(t)\\ \overline{\Delta}_m(t) & \gamma_{2,m}(t)\end{pmatrix}. \tag{5.47}$$

Later on we shall need the the following expansion of B_m^{int}:

$$B_m^{\mathrm{int}}(t)=\hat{\mathcal{U}}_{P,m}(t,t_0)^*B_m(t)\hat{\mathcal{U}}_{P,m}(t,t_0)=\left(\hat{\mathcal{U}}_{P,m}^0(t,t_0)\left(1+(-i)\int_{t_0}^{t}\mathrm{d}s\ \hat{V}_P(s)\hat{\Omega}_{P,m}^0(s,t_0)\right)\right)^*B_m(s)\hat{\mathcal{U}}_{P,m}^0(t,t_0)$$
$$\times\left(1+(-i)\int_{t_0}^{t}\mathrm{d}s\ \hat{V}_P(s)\hat{\Omega}_{P,m}^0(s,t_0)\right).$$

The term $(-i)\int_{t_0}^{t}\mathrm{d}s\ \hat{V}_P(s)\hat{\Omega}_{P,m}^0(s,t_0)$ is actually the remainder of order 1 from the Dyson expansion of $\hat{\Omega}_{P,m}^0(s,t_0)$. Consequently we denote this quantity $\mathcal{R}_1$ and estimate it by (A45) (for m large enough) as

$$\|\mathcal{R}_1\|\leqslant C_{m_0}\|V\|_r\frac{\log\langle m\rangle}{\langle m\rangle^{1/2+r}}. \tag{5.48}$$

Using that $B_m(t)=\mathcal{O}_r((b(m))^2\langle m\rangle)$ and (5.48) we have

$$B_m^{\mathrm{int}}(t)=\hat{\mathcal{U}}_{P,m}^0(t,t_0)^*B_m(t)\hat{\mathcal{U}}_{P,m}^0(t,t_0)+\mathcal{O}_r\left(\frac{\log^5\langle m\rangle}{\langle m\rangle^{\min\{3/2+r,3/2+5r\}}}\right)\quad\text{as } m\to\infty. \tag{5.49}$$

To write down $\mathcal{U}_{\mathrm{eff},m}(t_1,t_0)$ we use (5.33), (5.36), (5.39), (5.41), (5.43), (5.44), (5.46), and (5.49),

$$\mathcal{U}_{\mathrm{eff},m}(t_1,t_0)=e^{-i\theta_m(t_1,t_0)}\begin{pmatrix}1-\dfrac{|\hat{V}(2(m-1))|^2}{m-1}c_{2,m}(t_1,t_0) & -\dfrac{\hat{V}(2(m-1))}{\sqrt{m-1}}\overline{c_{1,m}(t_1,t_0)}\\ \dfrac{\overline{\hat{V}(2(m-1))}}{\sqrt{m-1}}\overline{c_{1,m}}(t_1,t_0) & 1-\dfrac{|\hat{V}(2(m-1))|^2}{m-1}c_{2,m}(t_1,t_0)\end{pmatrix}$$
$$-i\begin{pmatrix}\omega_{1,m} & \overline{\lambda_m}\\ \lambda_m & \omega_{2,m}\end{pmatrix}+\mathcal{R}_{\mathrm{eff},m}. \tag{5.50}$$

The remainder $\mathcal{R}_{\mathrm{eff},m}$ takes into account all the errors involved during the computation of the effective evolution in the subspace $Q_m\mathcal{H}$,

$$\|\mathcal{R}_{\mathrm{eff},m}\|\leqslant 2\|\mathcal{R}_1\|\cdot\|B_m\|+\|\mathcal{R}_3\|+\|\ B_m)\|^2+\|\Delta H_{\mathrm{eff},m}\|=\mathcal{O}_r\left(\frac{\log^8\langle m\rangle}{\langle m\rangle^{\min\{2+8r,3/2+5r,3/2+r,2\}}}\right). \tag{5.51}$$

Making the necessary identifications in (5.50) one finds that this expression coincides with the one given in Lemma 5.3 which is now proven. □

Remark 5.4: Let us justify why we kept explicitly the matrix elements of $B_m(t)$ in the effective

evolution. First we point out, without giving details, that one can obtain sharp estimates on Δ_m and γ's as in Eqs. (10) and (11) from Ref. 3, namely ($j=1,2$)

$$\sup_{t\in I_0}|\Delta_m(t)| \leqslant \frac{C\|V\|_r^2}{\langle m\rangle^{1+r}}, \quad \sup_{t\in I_0}|\gamma_{j,m}(t)| \leqslant \frac{C\|V\|_r^2}{\langle m\rangle^{\min\{2,1+2r\}}}. \tag{5.52}$$

Second, observe that from these estimates one cannot conclude that the diagonal contribution of $B_m(t)$ is smaller that the second terms from the Landau–Zener coefficients α_{2m-2}, α'_{2m-2}.

To obtain $\tilde{\mathcal{U}}_{\mathrm{eff},m}(t_2,t_1)$ we must follow the same steps as above, using the effective Hamiltonian $\tilde{H}_{\mathrm{eff},m}$. Without giving explicit calculations we summarize the results and the notations. Up to errors of order $\mathcal{O}_r(\langle m\rangle^{\min\{2,2+8r\}})$ as $m\to\infty$,

$$\tilde{\mathcal{U}}_{\mathrm{eff},m}(t_2,t_1) = e^{-i\tilde{\theta}_m(t_2,t_1)}\begin{pmatrix} 1-\dfrac{|\hat{V}(2m-1)|^2}{m-\frac{1}{2}}\tilde{c}_{2,m}(t_2,t_1) & -\dfrac{\hat{V}(2m-1)}{\sqrt{m-\frac{1}{2}}}\,\overline{\tilde{c}_{1,m}(t_2,t_1)}) \\ \dfrac{\overline{\hat{V}(2m-1)}}{\sqrt{m-\frac{1}{2}}}\tilde{c}_{1,m}(t_2,t_1) & 1-\dfrac{|\hat{V}(2m-1)|^2}{m+\frac{1}{2}}\tilde{c}_{2,m}(t_2,t_1) \end{pmatrix} - ie^{-i\tilde{\theta}_m(t_2,t_1)} \times \begin{pmatrix} \tilde{\omega}_{1,m}(t_2,t_1) & \overline{\tilde{\lambda}_m(t_2,t_1)} \\ \tilde{\lambda}_m(t_2,t_1) & \tilde{\omega}_{2,m}(t_2,t_1) \end{pmatrix} \tag{5.53}$$

the phase $\tilde{\theta}_m$ coeficients $\tilde{c}_i(m)$ being related to the ones of $\mathcal{U}_{\mathrm{eff},m}(t_1,t_0)$ by the relations

$$\tilde{\theta}_m(t_2,t_1) = \theta_{m+1/2}(t_1,t_0), \tag{5.54}$$

$$\tilde{c}_{i,m}(t_2,t_1) = c_{i,m+1/2}(t_1,t_0), \quad i=1,2. \tag{5.55}$$

$\tilde{\lambda}_m(t_2,t_1)$ and $\tilde{\gamma}_{1,m}(t)$ are to be computed in the same way as $\lambda_m(t_1,t_0)$ and $\gamma_m(t_1,t_0)$ [replace $\varphi_{-(m-1),0}$ with $\varphi_{-m,0}$ and $\hat{E}_{m,1}(t)$ with $\tilde{\hat{E}}_{m,1}(t)$ associated to $\tilde{Q}_m(t)$]. Finally,

$$\tilde{\alpha}_{2m-1}(t_2,t_1) := 1-\frac{|\hat{V}(2m-1)|^2}{m-\frac{1}{2}}\tilde{c}_{2,m}(t_2,t_1) - i\tilde{\omega}_{1,m}(t_2,t_1), \tag{5.56}$$

$$\tilde{\beta}_{2m-1} := \frac{\overline{\hat{V}(2m-1)}}{\sqrt{m-\frac{1}{2}}}\tilde{c}_{1,m}(t_2,t_1) - i\tilde{\lambda}_m(t_2,t_1). \tag{5.57}$$

The proof of Theorem 5.1 is finished. □

VI. THE LONG TIME BEHAVIOR. SPECTRAL PROPERTIES

The last part of this work is concerned with the long time behavior of the Bloch electron. Suppose that at the time $t_0=-\frac{1}{4}$ the electron is in a given band [say $E_{2n_0-2}(t_0)$ for n_0 fixed] and its wave function $\psi(t_0)=\varphi_{2n_0-2}(t_0)$ [let us recall that $\varphi_i(t)$ is the eigenfunction of $H(t)$ which corresponds to the eigenvalue $E_i(t)$]. We are interested in obtaining some quantitative information about $\psi(t_N)=U(t_N,t_0)\psi(t_0)$ where $t_N=t_0+(N/2)$, particular attention being payed to the case when N goes to infinity.

To answer these questions we proceed as follows: the complete evolution $U(t_N,t_0)$ is written as a product of one-period evolutions $U(t_l+1,t_l)$ each of them being then reduced to the first period $I_0\cup I_1$ by using (2.25). Then we use Theorem 3.1 to approximate the one-period evolution by the adiabatic evolutions which were written explicitly (in suitable subspaces) in Theorem 5.1. As pointed out by Ao it is of particular interest to establish how far the electron goes in the energy

space, otherwise stated, to say up to what band it is accelerated by the electric field. Because in the neighbor band approximation the electron can jump during one-half period only up to the next band it is clear that after N-half periods the uppermost reachable band is $E_{2n_0-2+N}(t_N)$. Its eigenfunction $\varphi_{2n_0-2+N}(t_N)$ is related to $\varphi_{2n_0-2+N}(t_0)$ by the shift operator T [see (2.49)]. The long time behavior of the Bloch electron is described in the following theorem.

Theorem 6.1: *Let $r>0$ and n_0 sufficiently large. Define the so-called propagating front,*[2]

$$\mathcal{P}(N) := |\langle \varphi_{2n_0-2+N}(t_N), U(t_N,t_0)\varphi_{2n_0-2}(t_0)\rangle|^2. \tag{6.1}$$

Then

$$\liminf_{N\to\infty} \mathcal{P}(N) = \exp\left\{ -2\sum_{l=0}^{\infty} \frac{|\hat{V}(2n_0+l-2)|^2}{n_0+(l/2)-1} c_{2,n_0+(l/2)}(t_1,t_0) \right\} \times (1+\mathcal{R}), \tag{6.2}$$

with

$$|\mathcal{R}| \leqslant \sum_{l=0}^{\infty} \frac{C_V}{\left\langle n_0 + l - \frac{1}{2}\right\rangle^{1+2r}} + \frac{C_V \log^8\langle n_0\rangle}{\langle n_0\rangle^{\min\{1+8r,1/2+5r,1/2+r,1\}}} \exp\left(\sum_{l=0}^{\infty} \frac{C_V}{\langle n_0+(l/2)-1\rangle^{1+2r}} \right). \tag{6.3}$$

As one may guess we need first a more explicit form for the scalar product in Eq. (6.1). Consequently a preliminary result is the following.

Lemma 6.2: For $r>-\frac{1}{10}$, n_0 sufficiently large and N even one gets

$$\langle \varphi_{2n_0+N-2}(t_N), U(t_N,t_0)\varphi_{2n_0-2}(t_0)\rangle = \prod_{l=0}^{(N/2)-1} e^{-i(\tilde{\theta}_{n_0+l}(t_2,t_1)+\theta_{n_0+l}(t_1,t_0))} \tilde{\alpha}_{2(n_0+l)-1}(t_2,t_1)\alpha_{2(n_0+l)-2}(t_1,t_0) + \mathcal{R}(N), \tag{6.4}$$

where the remainder $\mathcal{R}(N)$ satisfy the estimate

$$|\mathcal{R}(N)| \leqslant \frac{C_V \log^8\langle n_0\rangle}{\langle n_0\rangle^{\min\{1+8r,1/2+5r,1/2+r,1\}}}. \tag{6.5}$$

A similar expression holds for N odd.

Proof: The idea is to factorize $U(t_N,t_0)$ into one-period evolutions and to use the adiabatic theorem for a suitable index m of the two-dimensional projector $Q_m(t)$ or $\tilde{Q}_m(t)$. By the telescoping sum rule,

$$\prod_{l=0}^{n} a_l - \prod_{l=0}^{n} b_l = \sum_{l'=0}^{n} \prod_{l=l'+1}^{n} a_l (a_{l'} - b_{l'}) \prod_{l=0}^{l'-1} b_l$$

one has

$$U(t_N,t_0) = \prod_{l=0}^{(N/2)-1} U(t_{2l+2},t_{2l+1})U(t_{2l+1},t_{2l}) =: \prod_{l=0}^{(N/2)-1} \tilde{U}^A_{n_0+l}(t_{2l+2},t_{2l+1})U^A_{n_0+l}(t_{2l+1},t_{2l}) + \mathcal{R}_{\mathrm{ad}}(N). \tag{6.6}$$

The property $T^* U(t,s)T = U(t+1,s+1)$ leads to

$$\mathcal{R}_{\mathrm{ad}}(N) := \sum_{l=0}^{(N/2)-1} U(t_N,t_{2l+2})(T^*)^l(\ U(t_2,t_0)) - \tilde{U}^A_{n_0+l}(t_2,t_1)U^A_{n_0+l}(t_1,t_0))T^l \times \prod_{k=0}^{l-1}(T^*)^k\tilde{U}^A_{n_0+k}(t_2,t_1)U^A_{n_0+k}(t_1,t_0)T^k.$$

We pass now to the estimation of $\mathcal{R}_{\mathrm{ad}}(N)$. Clearly due to the presence of many unitarities one gets at once from the adiabatic theorem,

$$\|\mathcal{R}_{\mathrm{ad}}(N)\| \leqslant \sum_{l=0}^{(N/2)-1} \|U(t_2,t_0) - \tilde{U}^A_{n_0+l}(t_2,t_1)U^A_{n_0+l}(t_1,t_0)\| \leqslant \sum_{l=0}^{(N/2)-1} \|U(t_2,t_1) - \tilde{U}^A_{n_0+l}(t_2,t_1)\| + \|U(t_1,t_0) - U^A_{n_0+l}(t_1,t_0)\| \leqslant \sum_{l=0}^{(N/2)-1} 2C_V b(n_0+l)\langle n_0+l\rangle^{-1}.$$

We concentrate on the following term:

$$\begin{aligned}
&\prod_{l=0}^{(N/2)-1} \tilde{U}^A_{n_0+l}(t_{2l+2},t_{2l+1})U^A_{n_0+l}(t_{2l+1},t_{2l})P_{2n_0-2}(t_0)\\
&\quad= \sum_{j_{N/2}=1}^{\infty} P_{j_{N/2}}(t_N) \prod_{l=0}^{(N/2)-1} \left(\tilde{U}^A_{n_0+l}(t_{2l+2},t_{2l+1}) \sum_{\tilde{j}_l=1}^{\infty} P_{\tilde{j}_l}(t_{2l+1})U^A_{n_0+l}(t_{2l+1},t_{2l}) \sum_{j_l=1}^{\infty} P_{j_l}(t_{2l}) \right) P_{2n_0-2}(t_0)\\
&\quad= \sum_{j_{N/2},j_{(N/2)-1},\tilde{j}_{(N/2)-1},\ldots,j_0,\tilde{j}_0} P_{j_{N/2}}(t_N)\\
&\qquad\times \left(\prod_{l=0}^{(N/2)-1} \tilde{U}^A_{n_0+l}(t_{2l+2},t_{2l+1})P_{\tilde{j}_l}(t_{2l+1})U^A_{n_0+l}(t_{2l+1},t_{2l})P_{j_l}(t_{2l}) \right) P_{2n_0-2}(t_0),
\end{aligned}$$

where all the j indices run for the moment from 1 to ∞. However since U^A_n and $\tilde{U}^A_n$ leave invariant Ran Q_n and Ran $\tilde{Q}_n$ and since for any $l \in \mathbb{Z}$

$$Q_n(t_l) = P_{2n-2}(t_l) + P_{2n-1}(t_l),$$

$$\tilde{Q}_n(t_l) = P_{2n-1}(t_l) + P_{2n}(t_l),$$

we know that the only indices which contribute are the ones of the set J_{2n_0-2} where we define J_n as follows:

$$J_n := \{(j_{N/2},\tilde{j}_{(N/2)-1},j_{(N/2)-1},\ldots,\tilde{j}_0,j_0),\quad j_0 = 2n_0-2,\quad \forall\, l,\quad \tilde{j}_l = j_l \text{ or } j_l+1;\quad j_{l+1} = \tilde{j}_l \text{ or } \tilde{j}_l+1\}.$$

Then (we drop the times variables in U^A and $\tilde{U}^A$ since their values are clear from the context)

$$\left(\prod_{l=0}^{(N/2)-1} \tilde{U}^A_{n_0+l}U^A_{n_0+l} \right) P_{2n_0-2} = \sum_{J_{2n_0-2}} P_{j_{N/2}} \prod_{l=0}^{(N/2)-1} \tilde{U}^A_{n_0+l}P_{\tilde{j}_l}U^A_{n_0+l}P_{j_l}.$$

Clearly if we force $j_{N/2}$ to be equal to $2n_0+N-2$ by multiplying on the left by P_{2n_0+N-2} it remains only one "path" in this sum. Using (2.25), (2.49), (5.3), and (5.4) one may write

$$\begin{aligned}
&\left\langle \varphi_{2n_0+N-2}(t_N),\ \prod_{l=0}^{(N/2)-1} \tilde{U}^A_{n_0+l}(t_{2l+2},t_{2l+1})U^A_{n_0+l}(t_{2l+1},t_{2l})\varphi_{2n_0-2}(t_0)\right\rangle = \left\langle \varphi_{2n_0+N-2}(t_N), P_{2n_0+N-2}(t_N)\right.\\
&\quad\left.\times \prod_{l=0}^{(N/2)-1} \tilde{U}^A_{n_0+l}(t_{2l+2},t_{2l+1})P_{2n_0+2l-1}(t_{2l+1})U^A_{n_0+l}(t_{2l+1},t_{2l})P_{2n_0+2l-2}(t_{2l})\varphi_{2n_0-2}(t_0)\right\rangle\\
&= \left\langle \varphi_{2n_0+N-2}(t_2), T^{(N/2)-1}P_{2n_0+N-2}(t_N)\right.\\
&\quad\left.\times \prod_{l=0}^{(N/2)-1} (T^*)^l\tilde{U}^A_{n_0+l}(t_2,t_1)P_{2n_0+2l-1}(t_1)U^A_{n_0+l}(t_1,t_0)P_{2n_0+2l-2}(t_0)T^l\varphi_{2n_0-2}(t_0)\right\rangle\\
&= \prod_{l=0}^{(N/2)-1} \tilde{S}^{n_0+l}_{2n_0+2l,2n_0+2l-1}(t_2,t_1)S^{n_0+l}_{2n_0+2l-1,2n_0+2l-2}(t_1,t_0)\\
&=: \prod_{l=0}^{(N/2)-1} e^{-i\tilde{\theta}_{n_0+l}(t_2,t_1)}\tilde{\alpha}_{2n_0+2l-1}(t_2,t_1)e^{-i\theta_{n_0+l}(t_1,t_0)}\alpha_{2n_0+2l-2}(t_1,t_0) + \mathcal{R}_{\mathrm{eff}}(N),
\end{aligned}$$

where

$$\begin{aligned}
|\mathcal{R}_{\mathrm{eff}}(N)| &\leqslant \sum_{l=0}^{(N/2)-1} (2|\mathcal{R}_{\mathrm{eff},n_0+l}| + |R_{\mathrm{eff},n_0+l}|^2) \leqslant \sum_{l=0}^{\infty} (2|\mathcal{R}_{\mathrm{eff},n_0+l}| + |\mathcal{R}_{\mathrm{eff},n_0+l}|^2)\\
&= \frac{C_V \log^8\langle n_0\rangle}{\langle n_0\rangle^{\min\{1+8r,1/2+5r,1/2+r,1\}}}.
\end{aligned}$$

Defining

$$\mathcal{R}(N) := \mathcal{R}_{\mathrm{eff}}(N) + \langle \varphi_{2n_0+N-2}, \mathcal{R}_{\mathrm{ad}}(N)\varphi_{2n_0-2}\rangle \tag{6.7}$$

the lemma follows immediately from the estimates of $\mathcal{R}_{\mathrm{ad}}(N)$ and $\mathcal{R}_{\mathrm{eff}}(N)$. □

Proof of Theorem 6.1: Let

$$\mathcal{A}(N) := \prod_{l=0}^{(N/2)-1} e^{-i(\tilde{\theta}_{n_0+l}(t_2,t_1)+\theta_{n_0+l}(t_1,t_0))}\tilde{\alpha}_{2n_0+2l-1}(t_2,t_1)\alpha_{2n_0+2l-2}(t_1,t_0). \tag{6.8}$$

Then by Lemma 6.2 the propagating front reads as

$$\mathcal{P}(N) = |\mathcal{A}(N)|^2 \cdot \left|1 + \frac{\mathcal{R}(N)}{\mathcal{A}(N)}\right|^2. \tag{6.9}$$

Replacing $\alpha_{2m-2}(t_1,t_0)$ and $\tilde{\alpha}_{2m-1}(t_2,t_1)$ for $m=n_0+k$ it follows that (we omit the time arguments for the simplicity of writing)

$$\begin{aligned}
|\mathcal{A}(N)| = \prod_{l=0}^{(N/2)-1} |\tilde{\alpha}_{2n_0+2l-1}\alpha_{2n_0+2l-2}| &= \prod_{l=0}^{(N/2)-1} \left(\left(1 - \frac{|\hat{V}(2n_0+2l-1)|^2}{n_0+l-\frac{1}{2}}\tilde{c}_{2,n_0+l}\right)^2 + \tilde{\omega}^2_{1,n_0+l}\right)^{1/2}\\
&\quad\times \left(\left(1 - \frac{|\hat{V}(2(n_0+l-1))|^2}{n_0+l-1}c_{2,n_0+l}\right)^2 + \omega^2_{1,n_0+l}\right)^{1/2}\\
&= \exp\left\{\frac{1}{2}\sum_{l=0}^{(N/2)-1} \log\left(\left(1 - \frac{|\hat{V}(2n_0+2l-1)|^2}{n_0+l-\frac{1}{2}}\tilde{c}_{2,n_0+l}\right)^2 + \tilde{\omega}^2_{1,n_0+l}\right)\right\}
\end{aligned}$$

$$\times \exp\left\{\frac{1}{2}\sum_{l=0}^{(N/2)-1}\log\left(\left(1-\frac{|\hat{V}(2(n_0+l-1))|^2}{n_0+l-1}c_{2,n_0+l}\right)^2+\omega_{1,n_0+l}^2\right)\right\}$$

$$=\exp\left\{-\sum_{l=0}^{N-1}\frac{|\hat{V}(2n_0+l-2)|^2}{n_0+\frac{l}{2}-1}c_{2,n_0+(l/2)}\right\}$$

$$\times\left(1+\mathcal{O}\left(\sum_{l=0}^{\infty}\frac{1}{\langle n_0+l-\frac{1}{2}\rangle^{1+2r}}\right)\right),$$

where we used estimates of the following type (similar bounds are found for the sums containing ω_{1,n_0+l}^2 and $\tilde{\omega}_{1,n_0+l}^2$) and the relation $\tilde{c}_{i,m}(t_2,t_1)=c_{i,m+1/2}(t_1,t_0)$:

$$\sum_{l=0}^{(N/2)-1}\left|\frac{|\hat{V}(2n_0+2l-1)|^2}{n_0+l-\frac{1}{2}}\tilde{c}_{2,n_0+l}\right|\leqslant\sum_{l=0}^{\infty}\left|\frac{C_V}{\langle n_0+l-\frac{1}{2}\rangle^{1+2r}}\right|.$$

Thus

$$\lim_{N\to\infty}\left|\frac{\mathcal{R}(N)}{\mathcal{A}(N)}\right|=:|\mathcal{R}|\leqslant\frac{C_V\log^8\langle n_0\rangle}{\langle n_0\rangle^{\min\{1+8r,1/2+5r,1/2+r,1\}}}\exp\left(\sum_{l=0}^{\infty}\frac{C_V}{\langle n_0+(l/2)-1\rangle^{1+2r}}\right).$$

The proof of the theorem is done. □

Remark 6.3: Since as long as $r>0$ the series that appears in Eq. (6.2) both in the exponential and in the error term converges the propagating front does not vanish in the limit $N\to\infty$. This means that the electron is always accelerated and it escapes at infinity *in the energy space*, provided that it is initially prepared in a band with sufficient energy. Thus we recovered rigorously the Ao's result. We end the paper with a result on the spectral properties of the Stark–Wannier operator.

Corollary 6.4: For $r>0$ one has $\sigma_{\mathrm{cont}}(H^{\mathrm{SW}})\neq\emptyset$.

Proof of Corollary 6.4: Let $\phi\in\mathcal{H}_{\mathrm{pp}}(H^{\mathrm{SW}})$ and Π_N a family of bounded operators that goes strongly to zero when $N\to\infty$. Then it is known (see Ref. 14) that

$$\lim_{N\to\infty}\sup_{\pm t>0}\left\|\Pi_N e^{-itH^{\mathrm{SW}}}\phi\right\|=0.$$

In particular, for $t_N:=t_0+(N/2)$,

$$\lim_{N\to\infty}\left\|\Pi_N e^{-i(t_N-t_0)H^{\mathrm{SW}}}\phi\right\|=0. \tag{6.10}$$

The strategy of the proof consists in writing $\Pi_N e^{-i(t_N-t_0)H^{\mathrm{SW}}}\phi$ in the Fourier–Bloch representation and then to express the result in terms of the propagating front $\mathcal{P}(N)$ which was computed in Theorem 6.1. Using (2.21), writing [see (2.22)]

$$U(k,t_N,t_0)=U(0,t_N+k,t_0+k)=:U(t_N+k,t_0+k)=U(t_N+k,t_N)U(t_N,t_0)U(t_0,t_0+k)$$

and choosing

$$\phi:=e^{it_0X}S^*\left(\int_{[0,1)}^{\oplus}\mathrm{d}k\,U(t_0,t_0+k)\varphi_{2n_0-2}(t_0)\right) \tag{6.11}$$

one has

$$\|\Pi_N e^{-i(t_N-t_0)H^{\mathrm{SW}}}\phi\| = \left\| Se^{-it_N X}\Pi_N e^{it_N X}S^*\left(\int_{[0,1)}^{\oplus} \mathrm{d}k\, U(t_N+k,t_N)U(t_N,t_0)\varphi_{2n_0-2}(t_0)\right)\right\|.$$

Now we choose Π_N such that

$$Se^{-it_N X}\Pi_N e^{it_N X}S^*\left(\int_{[0,1)}^{\oplus} \mathrm{d}k\, U(t_N+k,t_N)\right) = \left(\int_{[0,1)}^{\oplus} \mathrm{d}k\, P_{2n_0-2+N}(t_N)\right). \tag{6.12}$$

Let us show that Π_N goes strongly to zero as N goes to infinity. Using the identity

$$Se^{-inX}S^* = \mathrm{id}\otimes T^{-n}, \quad \forall\, n\in\mathbb{Z} \tag{6.13}$$

it turns out that Π_N is given by

$$\Pi_N := e^{it_N X}S^*\left(\int_{[0,1)}^{\oplus} \mathrm{d}k\, P_{2n_0-2+N}(t_N)U(t_N,t_N+k)\right)Se^{-it_N X} = e^{it_0 X}S^*\left(\int_{[0,1)}^{\oplus} \mathrm{d}k\, T^{N/2}P_{2n_0-2+N}(t_N)U(t_N,t_N+k)T^{-(N/2)}\right)Se^{-it_0 X} = e^{it_0 X}S^*\left(\int_{[0,1)}^{\oplus} \mathrm{d}k\, P_{2n_0-2+N}(t_0)U(t_0,t_0+k)\right)Se^{-it_0 X}.$$

Then clearly

$$s-\lim_{N\to\infty}\Pi_N = 0.$$

Finally observe that from (6.11) and (6.12)

$$\|\Pi_N e^{-i(t_N-t_0)H^{\mathrm{SW}}}\phi\|^2 = \|P_{2n_0-2+N}(t_N)U(t_N,t_0)\varphi_{2n_0-2}(t_0)\|^2 = \mathcal{P}(N).$$

However, from Theorem 6.1 we know that for n_0 sufficiently large and $r>0$ the propagating front $\mathcal{P}(N)$ does not vanish when $N\to\infty$ so ϕ must have a part in $\mathcal{H}_{\mathrm{cont}}(H^{\mathrm{SW}})$. □

When applied to the driven quantum ring problem the existence of a propagating front gives the following at once.

Corollary 6.5: Let $r>0$ and $\varphi\left(t_0=-\frac{1}{4}\right)=\varphi_{2n_0-2}(t_0)$, $\varphi[t_N=t_0+(N/2)]=U(t_N,t_0)\varphi(t_0)$. Then

$$\langle\varphi(t_N),H(t)\varphi(t_N)\rangle \geqslant \left(1+\mathcal{O}_r\left(\frac{1}{\langle n_0\rangle^r}\right)\right)\cdot t^2. \tag{6.14}$$

We end this section of applications by showing that there is no localization in momentum space for appropriate initial conditions.

Corollary 6.6: Let $F_D(I)$ be the spectral projection of $D:=-i\partial_x$ on the interval $I:=[n_0,n_0+1)$. Then for all V such that $r>0$ one has

$$\lim_{n_0\to\infty}\lim_{N\to\infty}\|F_D(I+t_N)e^{-i(t_n-t_0)H^{\mathrm{SW}}}F_D(I+t_0)\| = 1.$$

Proof: One can check that SDS^* is simply the multiplication by $k+n$; thus $SF_D(I)S^*=1\otimes P_{n_0,0}$. One has successively

$$\|F_D(I+t_N)e^{-i(t_N-t_0)H^{\mathrm{SW}}}F_D(I+t_0)\| = \left\| F_D(I+t_N)e^{it_N X}S^*\int_{[0,1)}^{\oplus}\mathrm{d}k\, U(t_N+k,t_0+k)Se^{-it_0 X}F_D(I+t_0)\right\| \quad [\text{see (2.21)}]$$

$$= \left\| Se^{-it_N X}F_D(I+t_N)e^{it_N X}S^*\int_{[0,1)}^{\oplus}\mathrm{d}k\, U(t_N+k,t_0+k)Se^{-it_0 X}F_D(I$$

$$
\begin{aligned}
&+ t_0)e^{it_0X}S^*\Big\| \\
&= \left\| SF_D(I)S^\star \int_{[0,1)}^{\oplus} \mathrm{d}k\, U(t_N + k, t_0 + k) SF_D(I)S^\star \right\| \\
&= \left\| 1 \otimes P_{n_0,0} \int_{[0,1)}^{\oplus} \mathrm{d}k\, U(t_N + k, t_0 + k) 1 \otimes P_{n_0,0} \right\| = \sup_{k\in[0,1)} \\
&\quad \times \| \times P_{n_0,0} U(t_N + k, t_0 + k) P_{n_0,0} \| \geqslant \| P_{n_0,0} U(t_N, t_0) P_{n_0,0} \| \\
&= \| P^0_{2n_0+N}(t_N) U(t_N, t_0) P^0_{2n_0+N}(t_0) \| \quad [\text{see (2.30)}] \\
&= \| P_{2n_0+N}(t_N) U(t_N, t_0) P_{2n_0+N}(t_0) \| + \mathcal{O}_r(b(n_0 + 1)) \\
&\quad (\text{see Corollary 2.6}) \\
&= \mathcal{P}(N + 1) + \mathcal{O}_r(b(n_0 + 1)).
\end{aligned}
$$

Using Theorem 6.1, the rest is now clear. □

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APPENDIX

The key estimate

Proof of Lemma 2.3: In the following we shall use the notation $\alpha := \max\{0, -r\}$. We start by estimating $\sup_{t\in I_0} \sup_{z\in\Gamma_m} \|K((d_m + iy), t)\|$,

$$
\begin{aligned}
\sup_{t\in I_0} \sup_{z\in\Gamma_m} \|K((d_m + iy), t)\|_{\mathrm{HS}} &\leqslant \|V\|_r \left(\frac{\sqrt{5}}{2}\right)^{\alpha} \sup_{t\in I_0} \sum_{n\in\mathbb{Z}} \frac{\langle n\rangle^{2\alpha}}{|(n + t)^2 - d_m - iy|} \\
&\leqslant \|V\|_r \left(\frac{\sqrt{5}}{2}\right)^{\alpha} \sup_{t\in I_0} \sum_{n\in\mathbb{Z}} \frac{\langle n\rangle^{2\alpha}}{|(n + t)^2 - d_m|} \leqslant 4\|V\|_r \left(\frac{\sqrt{5}}{2}\right)^{\alpha} \sum_{n\in\mathbb{Z}} \frac{\langle n\rangle^{2\alpha}}{|n^2 - d_m|} \\
&= \|V\|_r \left(\frac{\sqrt{5}}{2}\right)^{\alpha} \left\{ \frac{1}{d_m} + 2 \sum_{n\geqslant 1} \frac{\langle n\rangle^{2\alpha}}{|n^2 - d_m|} \right\} \qquad \text{(A1)}
\end{aligned}
$$

where the time dependence of $K((d_m + iy), t)$ was eliminated by using the inequality (proved below)

$$
\sup_{t\in I_0} |(n + t)^2 - d_m| \geqslant \tfrac{1}{4}|n^2 - d_m|. \qquad \text{(A2)}
$$

The next step is to estimate the sum from the rhs of (A1). Let us assume that $m > 1$ (the particular case $m = 1$ will be discussed separately). Then approximating the sum with integrals one has

$$\sum_{n\geqslant 1}\frac{\langle m\rangle^{2\alpha}}{|n^2-d_m|}\leqslant\int_1^{m-1}\frac{\langle x\rangle^{2\alpha}}{d_m-x^2}\mathrm{d}x+\frac{\langle m-1\rangle^{2\alpha}}{\frac{1}{2}\left(2m-\frac{3}{2}\right)}+\frac{\langle m\rangle^{2\alpha}}{m-\frac{1}{4}}+\int_m^{\infty}\frac{\langle x\rangle^{2\alpha}}{x^2-d_m}=:S_1+S_2+S_3+S_4. \tag{A3}$$

Since $\langle x\rangle$ is an increasing function we can estimate the term S_1 as follows:

$$S_1\leqslant\langle m-1\rangle^{2\alpha}\int_1^{m-1}\frac{\mathrm{d}x}{d_m-x^2}=\frac{\langle m-1\rangle^{2\alpha}}{2\sqrt{d_m}}\log\left(\frac{\sqrt{d_m}+m-1}{\sqrt{d_m}-(m-1)}\cdot\frac{\sqrt{d_m}-1}{\sqrt{d_m}+1}\right)\leqslant\frac{\langle m\rangle^{2\alpha}}{2\sqrt{d_m}}\log\left(\frac{m+\sqrt{d_m}}{m-\sqrt{d_m}}\right). \tag{A4}$$

To obtain the last line we used the following estimate (valid for $m\geqslant 2$):

$$\frac{\sqrt{d_m}+m-1}{\sqrt{d_m}-(m-1)}\cdot\frac{\sqrt{d_m}-1}{\sqrt{d_m}+1}=\frac{2m-\frac{3}{2}}{\frac{1}{2}}\cdot\frac{m-\frac{3}{2}}{m+\frac{1}{2}}\leqslant\frac{2m-\frac{1}{2}}{\frac{1}{2}}=\frac{m+\sqrt{d_m}}{m-\sqrt{d_m}}.$$

The next two terms are easier,

$$S_2\leqslant\frac{12}{5\log 7}\cdot\frac{\langle m\rangle^{2\alpha}}{2\sqrt{d_m}}\cdot\log\left(\frac{m+\sqrt{d_m}}{m-\sqrt{d_m}}\right), \tag{A5}$$

$$S_3\leqslant\frac{12}{7\log 7}\cdot\frac{\langle m\rangle^{2\alpha}}{2\sqrt{d_m}}\cdot\log\left(\frac{m+\sqrt{d_m}}{m-\sqrt{d_m}}\right). \tag{A6}$$

We give some details only for S_2. First we write

$$S_2=\frac{\langle m-1\rangle^{2\alpha}}{\frac{1}{2}\left(2m-\frac{3}{2}\right)}\leqslant\frac{\langle m\rangle^{2\alpha}}{\frac{1}{2}\left(2m-\frac{3}{2}\right)}\cdot\frac{\log\left(\frac{m+\sqrt{d_m}}{m-\sqrt{d_m}}\right)}{2\sqrt{d_m}}\cdot\frac{2\sqrt{d_m}}{\log\left(\frac{m+\sqrt{d_m}}{m-\sqrt{d_m}}\right)}.$$

Then use

$$\frac{2\sqrt{d_m}}{\frac{1}{2}\left(2m-\frac{3}{2}\right)}=\frac{4\left(m-\frac{1}{2}\right)}{2m-\frac{3}{2}}=2\cdot\frac{m-\frac{1}{2}}{m-\frac{3}{4}}\leqslant\frac{12}{5}$$

and

$$\frac{1}{\log\left(\frac{m+\sqrt{d_m}}{m-\sqrt{d_m}}\right)}=\frac{1}{\log\left(\frac{2m-\frac{1}{2}}{\frac{1}{2}}\right)}\leqslant\frac{1}{\log 7}.$$

To estimate S_4 we make an integration by parts,

$$\begin{aligned}S_4=\int_m^{\infty}\frac{(1+x^2)^{\alpha}}{x^2-d_m}&=\left[\frac{(1+x^2)^{\alpha}}{2\sqrt{d_m}}\log\left(\frac{x-\sqrt{d_m}}{x+\sqrt{d_m}}\right)\right]_m^{\infty}-\frac{\alpha}{\sqrt{d_m}}\int_m^{\infty}\mathrm{d}x\,x(1+x^2)^{\alpha-1}\log\left(\frac{x-\sqrt{d_m}}{x+\sqrt{d_m}}\right)\\&\leqslant\frac{\langle m\rangle^{2\alpha}}{2\sqrt{d_m}}\log\left(\frac{m+\sqrt{d_m}}{m-\sqrt{d_m}}\right)+\frac{\alpha}{\sqrt{d_m}}\left(\sup_{x\geqslant m}x\log\left(\frac{x+\sqrt{d_m}}{x-\sqrt{d_m}}\right)\right)\int_m^{\infty}x^{2(\alpha-1)}\,\mathrm{d}x.\end{aligned}$$

The supremum above is computed by simply noticing that the function $f(x):=x\log[(x+a)/(x-a)]$ is decreasing on (a,∞). Indeed, its first two derivatives are given by

$$f'(x) = \log\left(\frac{x+a}{x-a}\right) + \frac{2xa}{a^2-x^2} \to 0 \quad \text{if } x \to \infty,$$

$$f''(x) = \frac{4a^3}{(a^2-x^2)^2}.$$

Hence

$$S_4 \leqslant \frac{\langle m\rangle^{2\alpha}}{2\sqrt{d_m}} \log\left(\frac{m+\sqrt{d_m}}{m-\sqrt{d_m}}\right) + \frac{\alpha}{1-2\alpha}\frac{\langle m\rangle^{2\alpha}}{\sqrt{d_m}} \log\left(\frac{m+\sqrt{d_m}}{m-\sqrt{d_m}}\right) = \frac{1}{2(1-2\alpha)} \cdot \frac{\langle m\rangle^{2\alpha}}{2\sqrt{d_m}} \cdot \log\left(\frac{m+\sqrt{d_m}}{m-\sqrt{d_m}}\right). \tag{A7}$$

Now taking into account that

$$\frac{1}{d_m} \leqslant \frac{4}{3\log 7} \frac{\langle m\rangle^{2\alpha}}{2\sqrt{d_m}} \log\left(\frac{m+\sqrt{d_m}}{m-\sqrt{d_m}}\right), \tag{A8}$$

and that $2\sqrt{d_m} \geqslant (3/\sqrt{5})\langle m\rangle$ we collect all the estimates (A4)–(A7) and plug them into (A1)

$$\sup_{t\in I_0}\sup_{z\in\Gamma_m} \|K((d_m+iy),t)\| \leqslant \|V\|_r \frac{4\sqrt{5}}{3}\left(\frac{\sqrt{5}}{2}\right)^{\alpha} \cdot \frac{9-6\alpha}{1-2\alpha} \frac{\log(4m-1)}{\langle m\rangle^{1-2\alpha}} := C_V \frac{\log(4m-1)}{\langle m\rangle^{1+\min\{0,2r\}}}. \tag{A9}$$

Note that the constant C_V depends on r and has a pathological behavior at $r=-\frac{1}{2}$. We treat now the case $m=1$. This term contains actually only the terms of the type S_3 and S_4, so that

$$\sup_{t\in I_0}\sup_{z\in\Gamma_1} \|K((d_1+iy),t)\| \leqslant \|V\|_r \left(\frac{\sqrt{5}}{2}\right)^{\alpha} \left\{ \frac{1}{d_1} + 2\sum_{n\geqslant 1} \frac{\langle 1\rangle^{2\alpha}}{|n^2-d_1|} \right\}$$

and

$$\sum_{n\geqslant 1}^{\infty} \frac{\langle n\rangle^{2\alpha}}{\left|n^2-\frac{1}{4}\right|} \leqslant \frac{4\langle 1\rangle^{2\alpha}}{3} + \int_2^{\infty} \frac{\langle x\rangle^{2\alpha}}{x^2-\frac{1}{4}}.$$

This leads to

$$\sup_{t\in I_0}\sup_{z\in\Gamma_1} \|K((d_1+iy),t)\| \leqslant \|V\|_r \left(\frac{\sqrt{5}}{2}\right)^{\alpha} \left(4 + \frac{8\langle 1\rangle^{2\alpha}}{3} + \frac{\langle 1\rangle^{2\alpha}}{1-2\alpha}\log 3\right) \leqslant C_V \frac{\log 3}{\langle 1\rangle^{1+\min\{0,2r\}}}. \tag{A10}$$

Inspecting (A9) and (A10) it is clear that one has for any $m \geqslant 1$,

$$\sup_{t\in I_0}\sup_{z\in\Gamma_m} \|K((d_m+iy),t)\| \leqslant C_V \frac{\log(4m-1)}{\langle m\rangle^{1+\min\{0,2r\}}}. \tag{A11}$$

From this estimate one can identify m^* such that for any $m > m^*$ we have $\sup_{t\in I_0}\sup_{z\in\Gamma_m}\|K((d_m+iy),t)\| \leqslant 1$.

Now we turn to the estimation of $\sup_{t\in I_0}\int_{\Gamma_m}\|R_0(z,t)\|\cdot\|K(z,t)\|\mathrm{d}y$. The resolvent is easily estimated as

$$\|R_0(z,t)\| \leqslant \frac{1}{\sqrt{A^2+y^2}}, \tag{A12}$$

where we introduced the notation $A := (m-\frac{1}{2})^2-(m-\frac{3}{4})^2$. Since $\sup_{t\in I_0}\|K(z,t)\| \leqslant 4\|K(z,0)\|_{\mathrm{HS}}$ we have

$$\begin{aligned}
\sup_{t\in I_0}\int_{\Gamma_m}\|R_0(z,t)\|\cdot\|K(z,t)\|\mathrm{d}y &\leqslant 4\|V\|_r\left(\frac{\sqrt{5}}{2}\right)^{\alpha}\int_{-\infty}^{\infty}\mathrm{d}y\frac{1}{\sqrt{A^2+y^2}}\left(\sum_{n_1\in\mathbb{Z}}\frac{\langle n_1\rangle^{2\alpha}}{\sqrt{B_{n_1}^2+y^2}}\cdot\sum_{n_2\in\mathbb{Z}}\frac{\langle n_2\rangle^{2\alpha}}{\sqrt{B_{n_2}^2+y^2}}\right)^{1/2}\\
&\leqslant 4\|V\|_r\left(\frac{\sqrt{5}}{2}\right)^{\alpha}\left(\int_{-\infty}^{\infty}\mathrm{d}y\sum_{n_1\in\mathbb{Z}}\frac{\langle n_1\rangle^{2\alpha}}{\sqrt{A^2+y^2}\sqrt{B_{n_1}^2+y^2}}\right)^{1/2}\\
&\quad\cdot\left(\int_{-\infty}^{\infty}\mathrm{d}y\sum_{n_2\in\mathbb{Z}}\frac{\langle n_2\rangle^{2\alpha}}{\sqrt{A^2+y^2}\sqrt{B_{n_2}^2+y^2}}\right)^{1/2}\quad\text{by Cauchy – Schwartz}\\
&= 4\|V\|_r\left(\frac{\sqrt{5}}{2}\right)^{\alpha}\sum_{n\in\mathbb{Z}}\langle n\rangle^{2\alpha}\int_{-\infty}^{\infty}\frac{\mathrm{d}y}{\sqrt{A^2+y^2}\sqrt{B_n^2+y^2}}\\
&:= 4\|V\|_r\left(\frac{\sqrt{5}}{2}\right)^{\alpha}\sum_{n\in\mathbb{Z}}\langle n\rangle^{2\alpha}I(A,B_n).
\end{aligned}$$

In the above calculation we used as well the notation

$$B_n := n^2 - d_m. \tag{A13}$$

The integral $I(A,B_n)$ is estimated as follows (in our case $B_n > A$ always):

$$\begin{aligned}
I(A,B_n) &\leqslant \frac{1}{B_n^{1-\delta}}\int_{-\infty}^{\infty}\mathrm{d}y\frac{1}{\sqrt{A^2+y^2}\cdot(A^2+y^2)^{\delta/2}} = \frac{1}{A^{\delta}B_n^{1-\delta}}\int_{-\infty}^{\infty}\mathrm{d}p\frac{1}{(1+p^2)^{(1+\delta)/2}}\\
&= \frac{1}{A^{\delta}B_n^{1-\delta}}\cdot\frac{\sqrt{\pi}\Gamma(\delta/2)}{\Gamma((1+\delta)/2)} = \frac{C_{\delta}}{A^{\delta}B_n^{1-\delta}},
\end{aligned}$$

where we made the substitution $p=y/A$. On the other hand, B_n obeys the following estimate:

$$B_n = |n^2 - d_m| \leqslant \max\{n^2, d_m\} \leqslant \max\{\langle n\rangle^2, \langle d_m\rangle^2\} \leqslant \langle n\rangle^2\langle d_m\rangle^2 \tag{A14}$$

from where

$$I(A,B_n) \leqslant C_{\delta}\frac{\langle n\rangle^{2\delta}\langle d_m\rangle^{2\delta}}{A^{\delta}B_n}. \tag{A15}$$

Using the fact that the function $g(m) := \langle d_m\rangle^2/A\langle n\rangle$ is decreasing so that $\max_{m\in\mathbb{Z}} g(m) = g(0) = 4$ one has $\langle d_m\rangle^{2\delta}/A^{\delta} \leqslant 4\langle m\rangle^{2\delta}$. Thus

$$\sup_{t\in I_0}\int_{\Gamma_m}\|R_0(z,t)\|\cdot\|K(z,t)\|\mathrm{d}y \leqslant 16\|V\|_r\left(\frac{\sqrt{5}}{2}\right)^{\alpha}C_{\delta}\langle m\rangle^{2\delta}\sum_{n\in\mathbb{Z}}\frac{\langle n\rangle^{2(\alpha+\delta)}}{|n^2-d_m|} \leqslant C_V C_{\delta}\frac{\langle m\rangle^{4\delta}\log(4m-1)}{\langle m\rangle^{1+\min\{0,2r\}}},$$

$$0 < \delta < \frac{1}{4} - \frac{\alpha}{2}. \tag{A16}$$

The last condition on δ assures that the rhs vanishes in the limit $m\to\infty$. We further optimize the result by using the inequality

$$C(\delta) \leqslant \frac{3}{\delta} \tag{A17}$$

and taking

$$\delta = \frac{1}{4\log\langle m\rangle} < \frac{1}{4} - \frac{\alpha}{2}, \tag{A18}$$

from where it follows that $\langle m\rangle \geqslant e^{1/(1-2\alpha)}$ and

$$\delta^{-1}\langle m\rangle^{4\delta} = 4e\log\langle m\rangle. \tag{A19}$$

Then

$$\sup_{t\in I_0}\int_{\Gamma_m}\|R_0(z,t)\|\cdot\|K(z,t)\|\mathrm{d}y \leqslant C_V\frac{\log^2(4m-1)}{\langle m\rangle^{\min\{1,1+2r\}}}. \tag{A20}$$

The estimates (A11) and (A20) lead to

$$\sup_{t\in I_0}\left(\sup_{z\in\tilde{\Gamma}_m}\|K(z,t)\| + \int_{\Gamma_m}\|R_0(z,t)\|\cdot\|K(z,t)\|\mathrm{d}y\right) \leqslant C_V\frac{\log^2\langle 4m-1\rangle}{\langle m\rangle^{\min\{1,1+2r\}}}. \tag{A21}$$

In what concerns the estimates on $\tilde{\Gamma}_m$ one must follow the same steps as above, the result being that m is pushed to $m+\frac{1}{2}$. Since $\langle m+\frac{1}{2}\rangle \leqslant \sqrt{2}\langle m\rangle$ and $\log(4m+1) \leqslant 2\log(4m-1)$ one can work only with $b(m)$. To prove (2.41) and (2.42) one must use the first resolvent identity,

$$\|K(z,t)\| \leqslant \|K(d_m,t)\|\cdot\left\|\frac{R_0(z,t)}{R_0(d_m,t)}\right\| \leqslant \|K(d_m,t)\|\left(1+\frac{|z-d_m|}{\inf_{z\in\gamma_m}\mathrm{dist}(z,\sigma(H_0(t)))}\right).$$

Since

$$\sup_{z\in\gamma_n}|z-d_m| = \sqrt{5}(m-1)$$

$$\inf_{t\in I_0}\inf_{z\in\gamma_m}\mathrm{dist}(z,\sigma(H_0(t))) \leqslant \tfrac{1}{4}\left(2m-\tfrac{11}{4}\right)$$

from where (2.42) follows. Finally let us prove (A2),

$$\begin{aligned}
\inf_{t\in I_0}\inf_{n\in\mathbb{Z}}\left|\frac{(n+t)^2-d_m}{n^2-d_m}\right| &= \inf_{t\in I_0}\inf_{n\in\mathbb{Z}}\left|\frac{(n+t)-\sqrt{d_m}}{n-\sqrt{d_m}}\right|\left|\frac{(n+t)+\sqrt{d_m}}{n+\sqrt{d_m}}\right| \\
&\geqslant \inf_{t\in I_0}\inf_{n\in\mathbb{Z}}\left|\frac{(n+t)-\sqrt{d_m}}{n-\sqrt{d_m}}\right|\inf_{t\in I_0}\inf_{n\in\mathbb{Z}}\left|\frac{(n+t)+\sqrt{d_m}}{n+\sqrt{d_m}}\right| \\
&= \inf_{t\in I_0}\inf_{n\in\mathbb{Z}}\left|1+\frac{t}{n-\sqrt{d_m}}\right|\inf_{t\in I_0}\inf_{n\in\mathbb{Z}}\left|1+\frac{t}{n+\sqrt{d_m}}\right| \\
&\geqslant \left(1-\sup_{t\in I_0}\sup_{n\in\mathbb{Z}}\left|\frac{t}{n-\sqrt{d_m}}\right|\right)\left(1-\sup_{t\in I_0}\sup_{n\in\mathbb{Z}}\left|\frac{t}{n+\sqrt{d_m}}\right|\right) \\
&\geqslant \left(1-\sup_{n\in\mathbb{Z}}\left|\frac{\frac{1}{4}}{n-\sqrt{d_m}}\right|\right)\left(1-\sup_{n\in\mathbb{Z}}\left|\frac{\frac{1}{4}}{n+\sqrt{d_m}}\right|\right) = \left(1-\frac{1}{4\,\mathrm{dist}(\sqrt{d_m},\mathbb{Z})}\right)^2 = \frac{1}{4}.
\end{aligned}$$

The proof of Lemma 2.3 is finished. □

The Sz-Nagÿ transformation

For convenience we give here the well known[15,30] Sz-Nagÿ lemma on unitary equivalence of orthogonal projections.

Lemma 7.2.1: Let P,Q be orthogonal projections in a Hilbert space $\mathcal{H}$ satisfying

$$\|P-Q\|<1 \tag{A22}$$

If U is defined by

$$U=(1-(P-Q)^2)^{-1/2}(PQ+(1-P)(1-Q)), \tag{A23}$$

then

$$U^*=U^{-1} \tag{A24}$$

and

$$P=UQU^*. \tag{A25}$$

Notice also that

$$(1-(P-Q)^2)^{-1/2}=1+\sum_{j\geqslant 1}\frac{(2j-1)!!}{j!2^j}(P-Q)^{2j}. \tag{A26}$$

The remainder of order *p* for the Dyson series

In this section we review a method to estimate the remainder of order p for the Dyson series of $\hat{\Omega}_{P,m}$ encountered in Sec. V. Let $\mathcal{E}$ be the space of C^∞ operator-valued functions on I_0 taking values in $\mathcal{B}(\mathbb{C}^2)$. Thus $\forall X\in\mathcal{E}$, $\forall l\in\mathbb{N}$

$$\|X\|_\infty := \sup_{t\in I_0}\|\partial_t^l X(t)\|<\infty, \tag{A27}$$

since I_0 is compact and $t\to\partial_t^l X(t)$ is continuous. We define the operator $K:\mathcal{E}\to\mathcal{E}$ by the following relation:

$$(KX)(t) := -i\int_{t_0}^{t}\hat{V}_P(s)X(s)\mathrm{d}s,\quad \hat{V}_P(t) := \begin{pmatrix}0 & b(t)\\ \overline{b(t)} & 0\end{pmatrix}, \tag{A28}$$

where $b(t):=\hat{V}(2(m-1))e^{2i(m-1)(t^2-t_0^2)}$. The Dyson series with remainder of order p reads as

$$\hat{\Omega}^0_{P,m}(t_1,t_0)=\sum_{k=0}^{m-1}K^k(t)\mathrm{id}+K^m(t)\hat{\Omega}^0_{P,n_0}(t_1,t_0). \tag{A29}$$

Here K^k denotes $K\circ K\circ\cdots\circ K$ k times. We start by proving a technical lemma.

Lemma 7.3.1: Let $a:=m-1$. Then for all $X\in\mathcal{E}$ it holds

$$\|KX\|_\infty\leqslant\frac{|b|}{\sqrt{a}}2\sqrt{6}\|X\|_\infty+|b|\frac{\log\left(\frac{\sqrt{a}}{2\sqrt{6}}\vee 1\right)}{a}\|\dot{X}\|_\infty, \tag{A30}$$

where we used the notation $m\vee n:=\max\{m,n\}$.

Proof: We shall use the canonical basis in $\mathcal{B}(\mathbb{C}^2)$ which reads as follows:

$$\Pi_{1,1} := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \Pi_{2,2} := \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \Pi_{1,2} := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \Pi_{2,1} := \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{A31}$$

Also, let χ_-, χ_0 et χ_+ be the characteristic functions corresponding to the intervals $[-\frac{1}{4}, -\varepsilon]$, $[-\varepsilon, \varepsilon]$ and $[\varepsilon, \frac{1}{4}]$ where $0 < \varepsilon < \frac{1}{4}$. Then we have

$$KX = K\chi_- X + K\chi_0 X + K\chi_+ X. \tag{A32}$$

One gets immediately

$$\|K\chi_0 X\|_\infty \leqslant 2\varepsilon |b| \|X\|_\infty. \tag{A33}$$

For $K\chi_\pm X$ we use the identity $K\chi_\pm X = K\chi_\pm \Pi_{1,1} X + K\chi_\pm \Pi_{2,2} X$. We shall treat in detail only the term $K\chi_- \Pi_{2,2} X$, the estimates for the remaining parts being completely similar. Then with the notation $m \wedge n := \min\{m, n\}$ we have

$$(K\chi_- \Pi_{2,2} X)(t) = -i \int_{t_0}^{t\wedge -\varepsilon} b(s) \Pi_{1,2} X(s) \mathrm{d}s = -\int_{t_0}^{t\wedge -\varepsilon} 4ias b(s) \frac{\Pi_{1,2} X(s)}{4as} \mathrm{d}s = -\left[\frac{b(s) \Pi_{1,2} X(s)}{4as} \right]_{t_0}^{t\wedge -\varepsilon} + \int_{t_0}^{t\wedge -\varepsilon} b(s) \partial_s \left(\frac{\Pi_{1,2} X(s)}{4as} \right) \mathrm{d}s,$$

since $\dot{b}(s) = 4ias b(s)$. The first term is estimated as follows:

$$\left\| \left[b(s) \frac{\Pi_{1,2} X(s)}{4as} \right]_{t_0}^{t\wedge -\varepsilon} \right\| \leqslant \frac{|b|}{2a\varepsilon} \|\Pi_{1,2} X\|_\infty. \tag{A34}$$

For the second term,

$$\int_{t_0}^{t\wedge -\varepsilon} b(s) \partial_s \left(\frac{\Pi_{1,2} X(s)}{4as} \right) \mathrm{d}s = \int_{t_0}^{t\wedge -\varepsilon} b(s) \left(-\frac{\Pi_{1,2} X(s)}{4as^2} + \frac{\Pi_{1,2} \dot{X}(s)}{4as} \right) \mathrm{d}s, \tag{A35}$$

and consequently

$$\left\| \int_{t_0}^{t\wedge -\varepsilon} b(s) \partial_s \left(\frac{\Pi_{1,2} X(s)}{4as} \right) \mathrm{d}s \right\| \leqslant \|\Pi_{1,2} X\|_\infty \int_{t_0}^{-\varepsilon} \frac{|b|}{4as^2} \mathrm{d}s + \|\Pi_{1,2} \dot{X}\|_\infty \int_{t_0}^{-\varepsilon} \frac{|b|}{4a|s|} \mathrm{d}s \leqslant \frac{|b|}{4a\varepsilon} \|\Pi_{1,2} X\|_\infty - \frac{|b| \log(4\varepsilon)}{4a} \|\Pi_{1,2} \dot{X}\|_\infty.$$

Finally we find

$$\|KX\|_\infty \leqslant |b| \left(\left(2\varepsilon + \frac{1}{a\varepsilon} \right) \|X\|_\infty - \frac{\log(4\varepsilon)}{a} \|\dot{X}\|_\infty \right) \tag{A36}$$

and choosing $\varepsilon = \sqrt{3}(2a)^{-1/2} \wedge \frac{1}{4}$ we arrive at the announced result. □

Using Lemma 7.3.1 and the identity $(d/\mathrm{d}t)(K^{p-1}X)(t) = \hat{V}(t)(K^{p-2}X)(t)$ one can get the general result,

$$\text{if } p \geqslant 2, \quad \|K^p X\|_\infty \leqslant \frac{|b|}{\sqrt{a}} c \|K^{p-1} X\|_\infty + |b| \frac{\log \frac{\sqrt{a}}{c}}{a} \|\hat{V} K^{p-2} X\|_\infty \leqslant A \|K^{p-1} X\|_\infty + B \|K^{p-2} X\|_\infty, \tag{A37}$$

with the notations

$$c = 2\sqrt{6}, \quad A := \frac{|b|}{\sqrt{a}}c, \quad B = |b|^2 \frac{\log \frac{\sqrt{a}}{c} \vee 1}{a}.$$

By looking at the expansion of $\Omega^0_{P,m}(t_1,t_0)$ it is clear that we must solve (A37) in the case $X = \Omega^0_{P,m}$. However, in order to estimate as well $\hat{\Omega}^{0,(p)}_{P,m}$ the case $X=1$ would be also usual. We consider then the following two sequences for $\forall p \geqslant 2$:

$$x_p^{(k)} = Ax_{p-1}^{(k)} + Bx_{p-2}^{(k)} \quad \text{with} \quad x_0^{(k)} = 1 \quad \text{and} \quad x_1^{(k)} \text{ given}. \tag{A38}$$

Here $k=1,2$ labels the considered case, namely $x_p^{(1)} = \|K^p\|$ and $x_p^{(2)} = \|K_p \hat{\Omega}^0_{P,m}\|$. We know that x_p is a linear combination of two geometric series $p \to r_\pm^p$. More explicitly $x_p = \alpha_+ r_+^p + \alpha_- r_-^p$ where $r_\pm$ are the solutions of the characteristic equation $r^2 - Ar - B = 0$. Denoting with $\Delta := \sqrt{A^2+4B}$ one finds

$$r_\pm = \frac{A \pm \sqrt{\Delta}}{2}. \tag{A39}$$

The coefficients of the linear combination $\alpha_\pm$ are solutions of the equation

$$\begin{pmatrix} 1 & 1 \\ r_+ & r_- \end{pmatrix} \begin{pmatrix} \alpha_+ \\ \alpha_- \end{pmatrix} = \begin{pmatrix} x_0 \\ x_1 \end{pmatrix} \Leftrightarrow \alpha_\pm = \pm \frac{x_1 - r_\mp x_0}{\sqrt{\Delta}}. \tag{A40}$$

Now for the case 1 we have by direct calculation $\alpha_\pm^{(1)} = r_\pm / \sqrt{\Delta}$ and then

$$x_p^{(1)} = \frac{r_+^{p+1} - r_-^{p+1}}{\sqrt{\Delta}} = \sum_{k=0}^{p} r_+^k r_-^{p-k} = r_+^p \sum_{k=0}^{p} \left(\frac{r_-}{r_+}\right)^{p-k}.$$

For the second case we use the superposition principle. Let y the sequence defined by the relation as x with the initial conditions $y_0 = 0$ et $y_1 = B$. Then we have $x^{(2)} = x^{(1)} + y$. Since $y_p = \beta_+ r_+^p + \beta_- r_-^p$ with $\beta_\pm = \pm B\Delta^{-1/2}$ one has

$$x_p^{(2)} = x_p^{(1)} + \frac{B}{\sqrt{\Delta}}(r_+^p - r_-^p) = x_p^{(1)} + B\sum_{k=0}^{p-1} r_+^k r_-^{p-k}.$$

We proceed to the estimates by noticing that $|r_-| < r_+$ which allows to write

$$\left| \sum_{k=0}^{p} r_+^k r_-^{p-k} \right| = \left| r_+^p \sum_{k=0}^{p} \left(\frac{r_-}{r_+}\right)^{p-k} \right| \leqslant r_+^p \frac{1}{1 - \frac{|r_-|}{r_+}} = \frac{r_+^{p+1}}{r_+ - |r_-|} = \frac{r_+^{p+1}}{A}$$

and consequently

$$|x_p^{(1)}| \leqslant \frac{r_+^{p+1}}{A}, \quad |x_p^{(2)}| \leqslant \frac{r_+^{p+1}}{A} + \frac{B}{A} r_+^p. \tag{A41}$$

Using these results we obtain

$$\|K^p \,\mathrm{id}\| \leqslant \frac{r_+}{A} r_+^p \leqslant \left(1 + \frac{\sqrt{B}}{A}\right) B^{p/2} \left(1 + \frac{A}{\sqrt{B}}\right)^p, \tag{A42}$$

where

$$\frac{\sqrt{B}}{A} = \frac{1}{4\sqrt{3}}\left(\log\left(\frac{a}{24}\vee 1\right)\right)^{1/2}.$$

The estimate on $x_p^{(2)}$ gives

$$\|K^p\hat{\Omega}^0_{P,m}\| \leqslant \frac{r_+^{p+1}}{A} + \frac{B}{A}r_+^p \leqslant \left(1+\frac{\sqrt{B}}{A}+\frac{B}{A}\right)B^{p/2}\left(1+\frac{A}{\sqrt{B}}\right), \tag{A43}$$

where

$$\frac{B}{A} = \frac{1}{4\sqrt{6}}\frac{|b|}{\sqrt{a}}\log\left(\frac{a}{24}\vee 1\right).$$

Therefore we have proved the following.

Theorem 7.3.2: *Let $\hat{\mathcal{U}}_{P,m}$ and $\hat{\mathcal{U}}^0_{P,m}$ as defined in Sec. V $a=m-1$ and $b=\hat{V}(2(m-1))$. Then there exists m_0 and a constant C_{m_0} such that the Dyson series for $\hat{\Omega}^0_{P,m}(t,t_0)=\hat{\mathcal{U}}^0_{P,m}(t,t_0)^*\hat{\mathcal{U}}^0_{P,m}$ converges uniformly with respect to t for every $t\in I_0$ and that for any $m>m_0$ one has the following estimate:*

$$\|\hat{\Omega}^{0,(p)}_{P,m}\|_\infty \leqslant C_{m_0}|b|^p\sqrt{\log a}\left(\frac{\log a}{a}\right)^{p/2}. \tag{A44}$$

The remainder of order p satisfy the estimate

$$\|K^p\hat{\Omega}^0_{P,m}\|_\infty \leqslant 2C_{m_0}|b|^p\sqrt{\log a}\left(\frac{\log a}{a}\right)^{p/2}. \tag{A45}$$

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Inverse variational problem and canonical structure of Burgers equations

B. Talukdar[a)]
Department of Physics, Visva-Bharati University, Santiniketan 731235, India

S. Ghosh
Patha-Bhavana, Visva-Bharati, University, Santiniketan 731235, India

U. Das
Abhedananda Mahavidyalaya, Sainthia 731234, India

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It is demonstrated that Burgers equations, which are often believed to describe dissipative systems, are non-Lagrangian. Following Bateman's analysis of damped harmonic oscillator an action is defined to look for a Lagrangian representation for equations in the Burgers hierarchy. The associated higher-order Lagrangian densities are found to be degenerate such that the Hamiltonian structure could be studied by a repackaging of Ostrogradski formalism and Dirac's theory of constraints. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1852700]

The Burgers equation

$$u_t = u_{xx} + 2uu_x, \quad u = u(x,t) \tag{1}$$

represents the simplest nonlinear evolution equation that can be regarded as a one-dimensional reduction of the Navier–Stokes equation.[1] This equation is dissipative and does not support soliton solutions. However, it appears in many applicative contexts including the study of acoustics and shock waves.[2] Its solvability was discovered before the introduction of the spectral transform method.[3] For example, the Cole–Hopf transformation[4]

$$u = \frac{\phi_x}{\phi}, \quad \phi = \phi(x,t) \tag{2}$$

was found to map the equation in (1) into the integrable linear diffusion equation

$$\phi_t = \phi_{xx}. \tag{3}$$

It is of interest to note that (1) represents the first nontrivial flow of the hierarchy written as[5]

$$u_{t_{n+1}} = \partial(\partial + u)^n u, \quad \partial = \frac{\partial}{\partial x} \tag{4}$$

with t_{n+1}, the commutative time. For (4), an equation similar to that in (3) is given by

$$\phi_{t_{n+1}} = \partial^{n+1}\phi. \tag{5}$$

Taflin[6] first observed that (1) can be written in the Hamiltonian form[7] and that it has an infinite number of constants of the motion in involution. A similar study was carried out by Tasso[8] for the third-order Burgers equation. In each of these studies the canonical structure was derived with particular attention to the linear equation as given in (5). Moreover, there was no explicit reference

[a)]Electronic mail: binoy123@sancharnet.in

to Lagrangians to construct the Hamiltonian densities. The object of the present work is to provide an *ab initio* approach for the canonical or Hamiltonian structure of Burgers equations. We shall present all results with particular emphasis on the third-order equation. This is however, no loss of generalization because the method derived by us is applicable to any equation in the hierarchy. We shall begin by solving the inverse problem of variational calculus to construct an appropriate Lagrangian and then Hamiltonize this equation to get the relevant Poisson structure. The following gives a brief outline for the inverse variational problem as given by Helmholtz.[9]

Let $P[\zeta]=P(x,\zeta^n)\epsilon\mathcal{A}^r$ be an r-tuple of differential functions. The Fréchet derivative of P is the differential operator $D_P:\mathcal{A}^q\rightarrow\mathcal{A}^r$ and is defined as

$$D_P(Q) = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} P[\zeta + \epsilon Q(\zeta)] \tag{6}$$

for any $Q\epsilon\mathcal{A}^q$. The Helmholtz condition[9] asserts that P is the Euler–Lagrange expression for some variational problem if D_P is self-adjoint. Once the existence of a Lagrangian is guaranteed, the expression for it can be constructed by using a homotopy formula.[10] The solution given by Helmholtz is very neat, from the wider perspective of determining which systems of differential equations arise from variational principle. However, there are situations where the Helmholtz solution may turn out to be somewhat unsatisfactory. For example, if D_P is not self-adjoint for a system of differential equations, we have to stop by inferring that the system is non-Lagrangian. In the following, we first show that Burgers equation does not satisfy the Helmholtz condition and then try to construct a Lagrangian by taking recourse to the celebrated work of Bateman.[11]

The third-order equation is given by

$$u_t = u_{3x} + 3u^2u_x + 3uu_{2x} + 3u_x^2, \quad u = u(x,t). \tag{7}$$

To study the inverse problem for nonlinear evolution equations it is convenient to work with an integral of u

$$w(x,t) = \int_x^\infty \mathrm{d}y\, u(y,t) \tag{8}$$

rather than u itself; w is often called a potential function. In terms of this dependent variable, (7) reads

$$w_{xt} = w_{4x} + 3w_x^2w_{2x} - 3w_{2x}^2 - 3w_xw_{3x}. \tag{9}$$

Equivalently,

$$w_t = w_{3x} + w_x^3 - 3w_xw_{2x}. \tag{10}$$

For (9) we write the Euler–Lagrange expression as

$$P[w] = w_{4x} + 3w_x^2w_{2x} - 3w_{2x}^2 - 3w_xw_{3x}. \tag{11}$$

From (6) and (11)

$$D_P = D_{4x} + 6w_xw_{2x}D_x + 3w_x^2D_{2x} - 3w_xD_{3x} - 3w_{3x}D_x - 6w_{2x}D_{2x},$$
$$D_{nx} = \left(\frac{d}{dx}\right)^n. \tag{12}$$

To construct the adjoint operator D_P^* corresponding to (12) we write D_P as

$$D_P = \sum_{j=1}^{4} P_j(w) D_{jx} \tag{13}$$

and make use of the definition

$$D_P^* = \sum_{j=1}^{4} (-D)_{jx} P_j(w). \tag{14}$$

This gives

$$D_P^* = D_{4x} + 6w_x w_{2x} D_x + 3w_x^2 D_{2x} + 3w_{2x} D_{2x} + 3w_x D_{3x}. \tag{15}$$

From (12) and (15) we see that $D_P \neq D_P^*$. This tells us that the Burgers equation (7) or (10) is non-Lagrangian. The same is true for any member of the hierarchy. Thus it remains an interesting curiosity to find a Lagrangian from which we could get the Burgers equation using an action principle. To achieve this, we remember that, being weakly nonlinear the equations of the Burgers hierarchy are dissipative. In particle dynamics Bateman[11] allowed for an additional equation of motion to write an explicitly time independent Lagrangian for the damped harmonic oscillator. In particular, the Lagrangian

$$L = \dot{x}\dot{y} + \tfrac{1}{2}\lambda(x\dot{y} - \dot{x}y) - w^2 xy \tag{16}$$

was found to give two equations of motion

$$\ddot{x} + \lambda\dot{x} + w^2 x = 0 \quad \text{and } \ddot{y} - \lambda\dot{y} + w^2 y = 0, \tag{17}$$

where w is the natural frequency of the oscillator and λ, the damping constant. Therefore, following Bateman, we introduce an ansatz,

$$\mathcal{L} = \frac{1}{2}(w_t v_x + w_x v_t) + (w_{2x} \quad F_1 \quad F_2 \quad \cdots \quad F_{m-1}) \begin{pmatrix} (-1)^{n-1} v_{(n-1)x} \\ G_1 \\ G_2 \\ \cdots \\ G_{m-1} \end{pmatrix} \tag{18}$$

with $v = v(x,t)$ and $G_i = -v_x$, $i = 1, 2, \ldots, m-1$ to define a Lagrangian density $\mathcal{L}$. In writing (18), we assumed that the nth equation in the Burgers hierarchy written in terms of $w(x,t)$ can be expressed as

$$w_t = w_{nx} + \sum_{i=1}^{m-1} F_i. \tag{19}$$

We demand that the Lagrangian density in (18) should satisfy the following lemmas.

Lemma 1: $\mathcal{L}$ *via* an appropriate action principle gives equations in the Burgers hierarchy.

Lemma 2: $\mathcal{L}$ introduces a set of new equations coupled with the original Burgers equations.

Proof of Lemma 1: The potential function w and v which enter in (18) can be used to obtain equations of the Burgers hierarchy from an action principle. For this purpose, we consider

$$\delta I = 0, \quad I = \int \mathcal{L}\, dx\, dt. \tag{20}$$

To make the proof transparent we consider the third order equation. Comparing (10) and (19) we have

$$F_1 = w_x^3 \quad \text{and } F_2 = -3w_x w_{2x}, \tag{21}$$

such that

$$\mathcal{L} = \tfrac{1}{2}(w_t v_x + w_x v_t) + w_{2x} v_{2x} - w_x^3 v_x + 3w_x w_{2x} v_x. \tag{22}$$

The Euler–Lagrange equation from (20) can be written in the form

$$\frac{\delta \mathcal{L}}{\delta \psi} - \frac{d}{\mathrm{d}t}\left(\frac{\partial \mathcal{L}}{\partial \psi_t}\right) = 0 \tag{23}$$

with the variational derivative

$$\frac{\delta}{\delta \psi} = \frac{\partial}{\partial \psi} - \frac{d}{\mathrm{d}x}\frac{\partial}{\partial \psi_x} + \frac{d^2}{\mathrm{d}x^2}\frac{\partial}{\partial \psi_{2x}} - \cdots . \tag{24}$$

For the Lagrangian in (22), the function $\psi(x,t)$ is either $v(x,t)$ or $w(x,t)$. Choosing $\psi(x,t) = v(x,t)$ we get from (22) and (23) the third order Burgers equation in (10). This is true for any member of the hierarchy.

Proof of Lemma 2: For $\psi(x,t) = w(x,t)$, the Euler–Lagrange equation gives

$$v_t = v_{3x} + 3w_x^2 v_x + 3w_x v_{2x}. \tag{25}$$

This equation is coupled with (10) verifying our demand in Lemma 2. An equation similar to (25) can be obtained for each member of the hierarchy.

We shall now recast the equation of the Burgers hierarchy into canonical form and obtain an explicit expression for the exact Hamiltonian. We do this with particular emphasis on the Lagrangian in (22). This Lagrangian density is first order in time and higher order in the space variable. In the context of particle dynamics similar Lagrangians are often called higher-order Lagrangians. Euler[12] first investigated the variational problem in which the integral implied in the definition of action depends on higher derivatives of the generalized coordinates. The standard procedure for Hamiltonizing a higher-order Lagrangian is due to Ostrogradaski[13] who proceeded by introducing a set of new variables such that one could finally work with an effective first-order action to arrive at the canonical structure. We closely follow this procedure to deal with the Lagrangian density in (22).

In view of the above, we rewrite (22) using

$$w_{2x} v_{2x} = (w_x v_{2x} + v_x w_{2x})_x - w_{2x} v_{2x} - w_x v_{3x} - v_x w_{3x} \tag{26}$$

such that

$$\mathcal{L} = \tfrac{1}{2}(w_t v_x + v_t w_x) - w_{2x} v_{2x} - w_x v_{3x} - v_x w_{3x} - w_x^3 v_x - 3w_x w_{2x} v_x. \tag{27}$$

Here, we have omitted the trivial gauge term $(w_x v_{2x} + v_x w_{2x})_x$. We reduce the action to first order by introducing a set of constraints

$$\theta - w_{2x} = 0 \quad \text{and } \eta - v_{2x} = 0. \tag{28}$$

From (27) and (28) we have

$$\mathcal{L} = \tfrac{1}{2}(w_t v_x + v_t w_x) - \eta\theta - w_x \eta_x - v_x \theta_x - w_x^3 v_x - 3w_x v_x \theta. \tag{29}$$

The Lagrangian density in (29) is degenerate because the associated Hessian is zero. Degenerate Lagrangians are Hamiltonized by using the Dirac's machinery[14] which is supposed to introduce a set of new constraints to consistently define the Hamiltonian density. To pass from the Lagrangian to the Hamiltonian formulation of the problem we introduce the canonical momentum densities

$$\pi_w = \frac{\partial \mathcal{L}}{\partial w_t} = \frac{1}{2} v_x,$$

$$\pi_v = \frac{\partial \mathcal{L}}{\partial v_t} = \frac{1}{2} w_x,$$

$$\pi_\theta = \frac{\partial \mathcal{L}}{\partial \theta_t} = 0, \tag{30}$$

$$\pi_\eta = \frac{\partial \mathcal{L}}{\partial \eta_t} = 0.$$

These momenta cannot be inverted for velocities. This represents a characteristic feature of degenerate Lagrangians. In the Dirac's machinery one proceeds by defining the primary constraints through the weak equations

$$c_1 = \pi_w - \tfrac{1}{2} v_x \approx 0,$$

$$c_2 = \pi_v - \tfrac{1}{2} w_x \approx 0,$$

$$c_3 = \pi_\theta \approx 0, \tag{31}$$

$$c_4 = \pi_\eta \approx 0.$$

These equations play a role in the Poisson bracket formalism of Hamiltonian mechanics. The sign "$\approx$" implies that we should not use these constraints before working out the Poisson brackets chracterizing the dynamical evolution of the system. In other words, all Poisson brackets occurring in the theory must be worked out before we make use of (31). In Dirac's theory, the total Hamiltonian of the system is given by

$$H = \int \mathcal{H}\, dx, \quad \mathcal{H} = \mathcal{H}_0 + \mathcal{H}', \tag{32}$$

where $\mathcal{H}_0$ is the free part of the Hamiltonian density determined by the usual Legendre transformation and we have

$$\mathcal{H}_0 = \eta\theta + w_x \eta_x + v_x \theta_x + w_x^3 v_x + 3 w_x v_x \theta. \tag{33}$$

The interaction part $\mathcal{H}'$ is an arbitrary linear combination of the constraints such that the total Hamiltonian could give the correct equations of motion with the usual Poisson brackets. Thus, we write

$$\mathcal{H}' = \beta c_1 + \gamma c_2 + \sigma c_3 + \rho c_4, \tag{34}$$

where β, γ, σ, and ρ are undetermined multipliers. In order for the Hamiltonian formulation of dynamics to be consistent it is not only necessary that the positions and momenta evolve in a manner which respects the constraints, but it is also necessary that the constraints themselves have dynamics. Thus one must require that

$$\frac{dc_i}{dt} = [c_i, H] \approx 0 \tag{35}$$

and this requirement will determine the multipliers provided there are no further constraints in the problem.

Using the canonical Poisson brackets of the w, v, θ, and η fields written as

$$\begin{aligned} [w(x), \pi_w(x')] &= \delta(x - x'), \\ [v(x), \pi_v(x')] &= \delta(x - x'), \\ [\theta(x), \pi_\theta(x')] &= \delta(x - x'), \\ [\eta(x), \pi_\eta(x')] &= \delta(x - x') \end{aligned} \tag{36}$$

we have found the following Poisson brackets given by

$$\begin{aligned} [c_1, H] &= [\gamma - \eta_x - 3w_x^2 v_x - 3v_x\theta]_x, \\ [c_2, H] &= -[\beta + \theta_x + 3w_x\theta + w_x^3]_x, \\ [c_3, H] &= [\eta - v_{2x} + 3w_x v_x], \\ [c_4, H] &= [\theta - w_{2x}]. \end{aligned} \tag{37}$$

It is clear that the last two Poisson brackets in (37) cannot be made to vanish by any choice of the multipliers. This implies that there are secondary constraints in the theory. We introduce these constraints as

$$\begin{aligned} c_5 &= \eta - v_{2x} + 3w_x v_x \approx 0, \\ c_6 &= \theta - w_{2x} \approx 0. \end{aligned} \tag{38}$$

The constraints c_5 and c_6 must be incorporated in the total Hamiltonian to get the correct dynamics of the system. Thus we replace (34) by

$$\mathcal{H}' = \beta c_1 + \gamma c_2 + \sigma c_3 + \rho c_4 + \mu c_5 + \xi c_6 \tag{39}$$

with μ and ξ as additional multipliers. In order to check that if there are further constraints in the problem we have again calculated the following Poisson brackets:

$$\begin{aligned} [c_1, H] &= [\gamma - 3\mu v_x - \xi_x - \eta_x - w_x^2 v_x - 3v_x\theta]_x, \\ [c_2, H] &= -[\beta + \mu_x + 3w_x\mu + \theta_x + 3w_x\theta + w_x^3]_x, \\ [c_3, H] &= [\xi + \eta - v_{2x} + 3w_x v_x], \\ [c_4, H] &= [\mu + \theta - w_{2x}], \\ [c_5, H] &= [(\gamma_x + 3v_x\beta + 3w_x\gamma)_x - \rho], \end{aligned} \tag{40}$$

$$[c_6, H] = [\beta_{2x} - \sigma].$$

These Poisson brackets can be made to vanish by choosing the Lagrange's multipliers

$$\begin{aligned}
\beta &= -(w_{3x} + 3w_x w_{2x} + w_x^3), \\
\gamma &= (v_{3x} + w_x^2 v_x - 3w_x v_{2x}), \\
\sigma &= (w_{3x} + 3w_x w_{2x} + w_x^3)_{xx}, \\
\rho &= (v_{4x} - 3w_{2x}v_{2x} - 3w_{3x}v_x - 7w_x w_{2x} v_x - 8w_x^2 v_{2x}), \\
\mu &= (w_{2x} - \theta), \\
\xi &= (v_{2x} - \eta - 3w_x v_x).
\end{aligned} \tag{41}$$

Equations (41) indicate that $c_1 - c_6$ exhaust all constraints of the problem. Thus from (31), (33), (38), (39), and (41) we write the total Hamiltonian density in the form

$$\begin{aligned}
\mathcal{H} = {} & 2w_{2x}\eta - 2w_{2x}v_{2x} + \tfrac{15}{2} w_x w_{2x} v_x - \eta\theta + 2v_{2x}\theta - 3w_x v_x \theta + w_x \eta_x + v_x \theta_x + w_x^3 v_x + \tfrac{1}{2} w_{3x} v_x - \tfrac{1}{2} w_x v_{3x} \\
& + \tfrac{3}{2} w_x^2 v_{2x} - (w_{3x} + 3w_x w_{2x} + w_x^3)\pi_w + (v_{3x} + w_x^2 v_x - 3w_x v_{2x})\pi_v - (w_{3x} + 3w_x w_{2x} + w_x^3)_{xx}\pi_\theta \\
& + (v_{4x} - 3w_{2x}v_{2x} - 3w_{3x}v_x - 7w_x w_{2x} v_x - 8w_x^2 v_{2x})\pi_\eta.
\end{aligned} \tag{42}$$

It is straightforward to verify that each Poisson brackets $[\pi_\omega, H]$, $[\pi_v, H]$, $[\pi_\theta, H]$, and $[\pi_\eta, H]$, reproduces the Burgers equation in (10).

Let us now identify those constraints that are physically important for the dynamics of the system. In order that we must divide the constraints into first and second class irrespective of whether they are primary, secondary or tertiary. The constraints are called first class if they have vanishing Poisson brackets with all the rest, that is

$$[c_i, c_j] = 0, \quad i, j = 1, \cdots, 6 \tag{43}$$

otherwise the constraints are called second class. The first-class constraints are related, at least to some extent, to the gauge properties of the system while the second-class constraints are associated with the appearance of unphysical degrees of freedom in the theory. Thus, it is clear that these two classes play a fundamentally distinct role in the canonical analysis. We have found that the Poisson brackets involving all c's are zero except for $[c_i, c_j]$, $i=1, j=2,5$; $[c_i, c_j]$, $i=2, j=5$; $[c_i, c_j]$, $i=3, j=6$; and $[c_i, c_j]$, $i=4, j=5$. The existence of these nonvanishing Poisson brackets can be used to see that all constraints of the problem are second class. Moreover, by introducing Dirac brackets to write the equation of motion one can eventually eliminate all second-class constraints from the theory. This means that all weak equations now becomes strong, such that all c's are now strong zeros. This is precisely, the reason why the zero-order Hamiltonian when substituted in the canonical equation of Zakharov and Faddeev, and Gardner[7] gives the equation of motion. In the present case, we can make use of

$$\omega_t = \frac{\delta \mathcal{H}_0}{\delta v_x} \quad \text{and} \quad v_t = \frac{\delta \mathcal{H}_0}{\delta \omega_x} \tag{44}$$

to get (10) and (25). We conclude by noting the following.

The heat equation in (2) is an instructive case of an integrable equation since it is easier to find a Lagrangian structure[15] for this equation. Moreover, using the Cole–Hopf coordinate transformation, one can map structures (Lagrangian or Hamiltonian) of the heat equation into those of the potential Burgers equation. This viewpoint has been advocated by Hojman and his collaborators in

a number of publications.[16] However, the results cannot be applied directly to investigate the canonical structure. In the present work we exploited the similarity between physical effects described by Burgers equations and equations of the damped harmonic oscillator to define an action that gives an uncomplicated expression for a degenerate Lagrangian density $\mathcal{L}$ which is first order in time. Faddeev and Jackiw[17] found that one must refrain from viewing a Lagrangian that is linear in first order time derivatives as necessarily describing a constrained system. Despite that we used Dirac's machinery to derive the Hamiltonian structure presumably because our Lagrangian analytically represents a set of coupled equations which might also follow from a Lagrangian which is nonlinear in the first derivatives in time.[18]

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Conditional expectations associated with quantum states

Gerd Niestegge
Zillertalstrasse 39, D-81373 Muenchen, Germany

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An extension of the conditional expectations (those under a given subalgebra of events and not the simple ones under a single event) from the classical to the quantum case is presented. In the classical case, the conditional expectations always exist; in the quantum case, however, they exist only if a certain weak compatibility criterion is satisfied. This compatibility criterion was introduced among others in a recent paper by the author. Then, state-independent conditional expectations and quantum Markov processes are studied. A classical Markov process is a probability measure, together with a system of random variables, satisfying the Markov property and can equivalently be described by a system of Markovian kernels (often forming a semigroup). This equivalence is partly extended to quantum probabilities. It is shown that a dynamical (semi)group can be derived from a given system of quantum observables satisfying the Markov property, and the group generators are studied. The results are presented in the framework of Jordan operator algebras, and a very general type of observables (including the usual real-valued observables or self-adjoint operators) is considered. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1861275]

I. INTRODUCTION

A classical Markov process is a probability measure together with a system of random variables, satisfying the Markov property (which characterizes a certain memorilessness of the process). A classical Markov process can equivalently be described by a system of Markovian kernels forming a semigroup when the process is stationary.

The quantum analogues of probability measures, random variables and Markovian kernels are the states, observables and unital positive linear maps. A quantum Markov process is usually modeled as a semigroup of unital positive linear maps on a W^*-algebra (von Neumann algebra). The major result of the present paper is the derivation of such a semigroup from a stochastic process given as a quantum state together with a system of observables, satisfying a certain directed weak compatibility criterion, the Markov property and the stationarity criterion. This partly extends the classical equivalence between stationary Markov processes and semigroups of Markovian kernels to the quantum case. As in the classical case, the major tools are the Radon–Nikodym theorem and conditional expectations, the extension of which to the quantum case is a major result of the present paper.

The quantum probabilities are considered in the general framework of Jordan operator algebras, particularly the so-called JBW algebras. A justification for this is given in Ref. 10. An observable then becomes a homomorphism between such algebras. A classical random variable can be considered an observable on a classical space with values in a classical space. A real-valued quantum observable (spectral measure of a self-adjoint operator) can be considered an observable on a nonclassical quantum space with values in a classical space (the real numbers). This paper, however, uses the most general type, i.e., an observable on a nonclassical quantum space with values in a nonclassical quantum space; this is a homomorphism between two nonassociative Jordan operator algebras.

A *Jordan algebra* [4] is a linear space $\mathcal{A}$ equipped with a (nonassociative) commutative product $\circ$ satisfying $X\circ(Y\circ X^2)=(X\circ Y)\circ X^2$ for all $X,Y\in\mathcal{A}$. A *JB algebra* [4] is a real Jordan algebra $\mathcal{A}$ that

is a Banach space with a norm satisfying $\|X\circ Y\|\leqslant\|X\|\,\|Y\|$, $\|X^2\|=\|X\|^2$, and $\|X^2\|\leqslant\|X^2+Y^2\|$ for all $X,Y\in\mathcal{A}$. The subset $\mathcal{A}_+:=\{X^2|X\in\mathcal{A}\}$ of a JB algebra $\mathcal{A}$ is a closed convex cone, and a partial ordering is defined via $X\leqslant Y\Leftrightarrow Y-X\in\mathcal{A}_+$. For idempotent elements E and F, $E\leqslant F$ is equivalent to $E\circ F=E$. A linear functional $\mu:\mathcal{A}\to\mathbb{R}$ is called *positive* if $\mu(X)\geqslant 0$ for $X\in\mathcal{A}_+$. A positive linear functional μ is bounded with $\|\mu\|=\mu(\mathbb{I})$ and is called a *state* if $\mu(\mathbb{I})=1$; μ is *faithful* means that $\mu(X)=0$ with $X\geqslant 0$ implies that $X=0$. A linear map V from a JB algebra $\mathcal{A}$ to another JB algebra is *positive* if $V(X)\geqslant 0$ for $X\geqslant 0$. A JB algebra which is the dual of a Banach space is a *JBW algebra*. [4] A JBW algebra has a unit denoted by $\mathbb{I}$ and is generated by its idempotent elements called *events*; the event $E':=\mathbb{I}-E$ is the *negation* of the event E. Two events E and F are *orthogonal* if $E\circ F=0$. The spectral decomposition theorem each element of a JBW algebra.

The *conditional probability* $\mu(F|E)$ of an event F under another event E in a state μ with $\mu(E)>0$ has been introduced in Ref. 9, where it has been shown that $\mu(F|E)=\mu(\{E,F,E\})/\mu(E)$. Note that the *triple product* $\{\ ,\ ,\ \}$ in a Jordan algebra is defined as follows: $\{X,Y,Z\}=X\circ(Y\circ Z)-Y\circ(Z\circ X)+Z\circ(X\circ Y)$. For some pairs of events E and F, the conditional probability $\mu(F|E)$ does not depend on the underlying state μ and is then denoted by $\mathbb{P}(F|E)$.

Generally, the equation $\mu(F)=\mu(F|E)\mu(E)+\mu(F|E')\mu(E')$ or the equivalent equation $\mu(\{E,F,E\})=\mu(E\circ F)$ does not hold; if it does, we write $E\underset{\mu}{\to}F$. This is a weak state-dependent directed compatibility criterion that has been introduced in Ref. 11 and is always fulfilled in classical probability theory. Several stronger forms of compatibility exist, e.g., the event E and F are called *compatible* if $E\underset{\mu}{\to}F$ and$F\underset{\mu}{\to}F$ both hold for all states μ; in this case, E and F *operator-commute*. [4] With a JBW subalgebra $\mathcal{A}_1$ of $\mathcal{A}$, we write $\mathcal{A}_1\underset{\mu}{\to}F$ if $E\underset{\mu}{\to}F$ holds for each event E in $\mathcal{A}_1$, and with two JBW subalgebras $\mathcal{A}_1$ and $\mathcal{A}_2$ of $\mathcal{A}$, we write $\mathcal{A}_1\underset{\mu}{\to}\mathcal{A}_2$ if $E\underset{\mu}{\to}F$ each event E in $\mathcal{A}_1$ and each event F in $\mathcal{A}_2$. We shall later see that the condition $\mathcal{A}_1\underset{\mu}{\to}F$ ensures the existence of a reasonable conditional expectation of F under $\mathcal{A}_1$ in the state μ. This condition is satisfied, e.g., when $\mathcal{A}_1$ and F operator-commute, or when $\mathcal{A}$ is the tensor product [11] of $\mathcal{A}_1$ and $\mathcal{A}_2$ with $F\in\mathcal{A}_2$, or when μ is a trace state.[13]

A linear map (state, homomorphism, observable) on a JBW algebra $\mathcal{A}$ is called *normal* if it is continuous with respect to the weak topology on $\mathcal{A}$ generated by its predual. Normal linear maps are completely additive for any orthogonal family of events. The paper restricts to the study of normal states and normal observables although it would be desirable to include σ-additive states and standard observables that are σ-additive and not necessarily normal, but then some methods needed from the theory of JBW algebras would not apply (see also Sec. VII).

The paper is organized as follows: In Secs. II and III, some results that are well known for C^*-/W^*-algebras are extended to the Jordan operator algebras for later use; these are Kadison's generalized Schwarz inequality and Sakai's Radon–Nikodym theorem. The extension of conditional expectations and Markov processes to the quantum case is introduced in Secs. IV and V, respectively. It is shown that a semigroup of positive linear maps is associated with each such Markov process. Finally the generator of this semigroup is studied in Sec. VI.

Although the motivation for the work presented here primarily stems from a quantum probability model proposed in Refs. 9–11, the paper is written in such a way that most of it can be understood without knowledge of that quantum probability model. However, some knowledge of Jordan operator algebras is required, and the monograph Ref. 4 is recommended as an excellent reference.

II. THE GENERALIZED SCHWARZ INEQUALITY

The following lemma will be needed to prove the generalized Schwarz inequality for positive linear maps between JB algebras.

Lemma 2.1: *Let* $X_1,\ldots,X_n$ *be n positive elements in a JB algebra* $\mathcal{A}$ *with unit* $\mathbb{I}$ *such that* $\Sigma_{k=1}^n X_k\leqslant\mathbb{I}$ *and* $s_1,\ldots,s_n\in\mathbb{R}$. *Then*

$$\left(\sum_{k=1}^{n} s_k X_k\right)^2 \leqslant \sum_{k=1}^{n} s_k^2 X_k.$$

Proof: Let φ be a state on $\mathcal{A}$. On the direct sum of n copies of $\mathcal{A}$ we consider the positive–semidefinite inner product

$$\langle Y|Z\rangle := \sum_{k=1}^{n} \varphi(\{Y_k, X_k, Z_k\})$$

for $Y = Y_1 \oplus \cdots \oplus Y_n$ and $Z = Z_1 \oplus \cdots \oplus Z_n$ with $Y_k, Z_k \in \mathcal{A}$. Then the Cauchy–Schwarz inequality holds (note that $\{Y_k, X_k, Y_k\} \geqslant 0$ for $Y_k, X_k \in \mathcal{A}$ with $X_k \geqslant 0$) and, selecting $Y_k := s_k \mathbb{I}$ for $k = 1, \ldots, n$ and

$$Z_1 := \cdots := Z_n := \sum_{k=1}^{n} s_k X_k,$$

we get

$$\left(\varphi\left(\left(\sum_{k=1}^{n} s_k X_k\right)^2\right)\right)^2 = \langle Y|Z\rangle^2 \leqslant \langle Y|Y\rangle\langle Z|Z\rangle = \varphi\left(\sum_{k=1}^{n} s_k^2 X_k\right)\varphi\left(\left\{Z_1, \sum_{k=1}^{n} X_k, Z_1\right\}\right)$$
$$\leqslant \varphi\left(\sum_{k=1}^{n} s_k^2 X_k\right)\varphi(Z_1^2) = \varphi\left(\sum_{k=1}^{n} s_k^2 X_k\right)\varphi\left(\left(\sum_{k=1}^{n} s_k X_k\right)^2\right).$$

Hence

$$\varphi\left(\left(\sum_{K=1}^{n} s_k X_k\right)^2\right) \leqslant \varphi\left(\sum_{K=1}^{n} s_k^2 X_k\right)$$

and, since this every state φ, the lemma is proved.

The following proposition now provides the extension of Kadison's generalized Schwarz inequality for positive maps between C*-algebras[5] to the more general case of positive maps between JB algebras.

Proposition 2.2: *Let V be a positive linear map from a unital JB algebra $\mathcal{M}$ to a unital JB algebra $\mathcal{N}$ with $V(\mathbb{I}) = \mathbb{I}$. Then $(V(X))^2 \leqslant V(X^2)$ for every $X \in \mathcal{M}$.*

Proof: First, we assume that $\mathcal{M}$ is a JBW algebra[4] and that X has the shape $X = \Sigma_{k=1}^{n} s_k E_k$ with pairwise orthogonal idempotent elements $E_1, \ldots, E_n \in \mathcal{A}$ and $s_1, \ldots, s_n \in \mathbb{R}$. Then $0 \leqslant V(E_k)$ for $k = 1, \ldots, n$ and $\Sigma V(E_k) \leqslant \mathbb{I}$ such that we can apply Lemma 2.1 obtaining

$$(V(X))^2 = \left(\sum_{k=1}^{n} s_k V(E_k)\right)^2 \leqslant \sum_{k=1}^{n} s_k^2 V(E_k) = V\left(\sum_{k=1}^{n} s_k^2 E_k\right) = V(X^2).$$

Since, due to the spectral theorem, every $X \in \mathcal{M}$ can be approximated in the norm topology by a sequence of elements having the above special shape and since a positive linear map is automatically norm continuous, $(V(X))^2 \leqslant V(X^2)$ every $X \in \mathcal{M}$.

We now assume that $\mathcal{M}$ is a JB algebra. Then the double dual spaces $\mathcal{M}^{**}$ and $\mathcal{N}^{**}$ are JBW algebras containing $\mathcal{M}$ and $\mathcal{N}$, respectively, as subalgebras,[4] such that Proposition 2.2 follows by applying the above to the map $V^{**}: \mathcal{M}^{**} \to \mathcal{N}^{**}$.

Corollary 2.3: *Let V be a bijective positive linear map from a unital JB algebra $\mathcal{M}$ to a unital JB algebra $\mathcal{N}$ with $V(\mathbb{I}) = \mathbb{I}$ such that V^{-1} is positive as well. Then V is a muliplicative homomorphism.*

Proof: $(V(X))^2 \leqslant V(X^2)$ for every $X \in \mathcal{M}$ and $(V^{-1}(Y))^2 \leqslant V^{-1}(Y^2)$ for every $Y \in \mathcal{N}$. Hence with $Y = V(X): X^2 \leqslant V^{-1}((V(X)^2)$. Then, since V is positive, $V(X^2) \leqslant (V(X))^2$. Therefore, $V(X^2) = (V(X))^2$.

The identity $2A\circ B=(A+B^2)-A^2-B^2$ for $A,B\in\mathcal{M}$ finally implies that V is multiplicative.

III. THE RADON–NIKODYM THEOREM

We shall now extend one of Sakai's Radon–Nikodym theorems[14] from W^*-algebras to JBW algebras. Since all methods needed for the proof of the W^*-case are available in the JBW case as well, the proofs are quite similar in these two cases.

Theorem 3.1: *Let $\mathcal{A}$ be a JBW algebra and let ν, μ be two positive normal linear functionals on $\mathcal{A}$ with $\nu\leqslant\mu$. Then, there is an element $Y\in\mathcal{A}$ with $0\leqslant Y\leqslant\mathbb{I}$ such that $\nu(Z)=\mu(Y\circ Z)$ all $Z\in\mathcal{A}$.*

Proof: For $X\in\mathcal{A}$ we define μ_X via $\mu_X(Z):=\mu(X\circ Z)$ for $Z\in\mathcal{A}$ and consider the set $K:\{\mu_X|X\in\mathcal{A},0\leqslant X\leqslant\mathbb{I}\}$ which is a nonempty convex subset of the predual $\mathcal{A}_*$ of $\mathcal{A}$. Moreover, K is compact with respect to the weak topology on $\mathcal{A}_*$ that is generated by $\mathcal{A}$. Note that $\{X\in\mathcal{A},0\leqslant X\leqslant\mathbb{I}\}$ is compact and that the multiplication operation with one element fixed is continuous with respect to the weak topology on $\mathcal{A}$ generated by $\mathcal{A}_*$.

All we must show is that $\nu\in K$. We assume that $\nu\notin K$. From the Hahn–Banach theorem it then follows that there is an element $A\in\mathcal{A}$ and a real number r such that $\nu(A)>r$ and $\mu_X(A)\leqslant r$ for $X\in\mathcal{A}$ with $0\leqslant X\leqslant\mathbb{I}$. Now let F be the support of the positive part A_+ of A; these are defined as follows: with $A=\int\lambda\ dE_\lambda$ being the spectral decomposition of A, $A_+:=\int_{[0,\infty]}\lambda\ dE_\lambda$ and $F:=\int_{[0,\infty]}dE_\lambda$. Then $r\geqslant\mu_F(A)=\mu(F\circ A)=\mu(A_+)\geqslant\nu(A_+)\geqslant\nu(A)$, which contradicts $\nu(A)>r$.

IV. CONDITIONAL EXPECTATIONS

Let $\mathcal{A}$ be a JBW algebra and $\mathcal{A}_0$ a JBW subalgebra of $\mathcal{A}$ with $\mathbb{I}\in\mathcal{A}_0$. Let μ be a normal state on $\mathcal{A}$ and $X\in\mathcal{A}$ with $0\leqslant X\leqslant\mathbb{I}$.

Definition 4.1: *An element $Y\in\mathcal{A}_0$ such that $\mu(\{E,X,E\})=\mu(Y\circ E)$ all events E in $\mathcal{A}_0$ is called a conditional expectation of X under $\mathcal{A}_0$ in the state μ.*

If F is an event in $\mathcal{A}$ and if Y is a conditional expectation of F under $\mathcal{A}_0$ in the state μ, we get that $\mu(F|E)\mu(E)=\mu(Y\circ E)$ all events E in $\mathcal{A}_0$.

Lemma 4.2: *If a conditional expectation exists for $X\in\mathcal{A}$ with $0\leqslant X\leqslant\mathbb{I}$, then there is a least one conditional expectation Y with $0\leqslant Y\leqslant\mathbb{I}$.*

Proof: Let $Z\in\mathcal{A}_0$ be a conditional expectation with $Z=\int\lambda\ dE_\lambda$ being its spectral decomposition, and define

$$Z_-:=-\int_{(-\infty,0)}\lambda\ dE_\lambda,\quad Y:=\int_{[0,\infty]}\lambda\ dE_\lambda,\quad \text{and } E_0:=\int_{(-\infty,0)}dE_\lambda.$$

Then $Z_-,Y,E_0\in\mathcal{A}_0$. Hence $0\leqslant\mu(\{E_0,X,E_0\})=\mu(Z\circ E_0)=-\mu(Z_-)\leqslant 0$, i.e., $\mu(Z_-)=0$. Since $0\leqslant Z_-$, we get $\mu(Z_-^2)=0$, and the Cauchy–Schwarz inequality for states implies that $\mu(Z_-\circ E)=0$ for all events E in $\mathcal{A}_0$. Therefore $\mu(\{E,X,E\})=\mu(Z\circ E)=\mu((Z_-+Y)\circ E)=\mu(Y\circ E)$ for all events E in $\mathcal{A}_0$, i.e., Y is a positive conditional expectation of X. Repeating now the same procedure for the conditional expectation $\mathbb{I}-Y$ of $\mathbb{I}-X$ finally yields a conditional expectation Y with $0\leqslant Y\leqslant\mathbb{I}$.

Theorem 4.3: (i) *A conditional expectation of X under $\mathcal{A}_0$ in the state μ exists if and only if $\mathcal{A}_0\underset{\mu}{\rightarrow}X$ holds* [*i.e., $\mu(\{E,X,E\}=\mu(E\circ X))$ for all events $E\in\mathcal{A}_0$*].

(ii) If $\mathcal{A}_0\underset{\mu}{\rightarrow}X$ *holds and if the restriction of μ to $\mathcal{A}_0$ is faithful, then there is one and only one conditional expectation of X under $\mathcal{A}_0$ in the state μ* [*which shall be denoted by $\mu(X|\mathcal{A}_0)$ in the remaining part of this paper*].

Proof: (i) Let Y be a conditional expectation of X under $\mathcal{A}_0$ in the state μ, and let E be an event in $\mathcal{A}_0$. Then $\mu(X)=\mu(Y)=\mu(Y\circ E)+\mu(Y\circ E')=\mu(\{E,X,E\})+\mu(\{E',X,E'\})=\mu(X)-2\mu(X\circ E)+2\mu(\{E,X,E\})$, where the last equality follows from the identity $\{E',X,E'\}=X-2X\circ E+\{E,X,E\}$. Therefore $\mu(\{E,X,E\})=\mu(X\circ E)$.

Now let $\mathcal{A}_0\underset{\mu}{\rightarrow}X$ hold. We then define $\nu(Z):=\mu(X\circ Z)$ for $Z\in\mathcal{A}_0$; ν is a normal linear functional on $\mathcal{A}_0$. Due to the condition $\mathcal{A}_0\underset{\mu}{\rightarrow}X$, we have $0\leqslant\nu(E)\leqslant\mu(E)$ for all events E in $\mathcal{A}_0$.

Therefore $0 \leqslant \nu \leqslant \mu$ on $\mathcal{A}_0$. From the Radon–Nikodym theorem we get an element $Y \in \mathcal{A}_0$ with $0 \leqslant Y \leqslant \mathbb{I}$ such that $\nu(Z) = \mu(Y \circ Z)$ for all $Z \in \mathcal{A}_0$. Finally, we get that $\mu(Y \circ E) = \mu(X \circ E) = \mu(\{E,X,E\})$ the events E in $\mathcal{A}_0$, where we have again used the assumption $\mathcal{A}_0 \underset{\mu}{\rightarrow} X$. Thus, Y is a conditional expectation of X under $\mathcal{A}_0$ in the state μ.

(ii) Now let μ be faithful on $\mathcal{A}_0$ and $Y_1, Y_2 \in \mathcal{A}_0$ with $0 \leqslant Y_1, Y_2 \leqslant \mathbb{I}$ such that $\mu(\{E,X,E\}) = \mu(Y_1 \circ E) = \mu(Y_2 \circ E)$ for all events $E \in \mathcal{A}_0$. Then $\mu((Y_1 - Y_2) \circ E) = 0$ for all events $E \in \mathcal{A}_0$ and, since $\mathcal{A}_0$ is the closed linear hull of its events, we get $\mu((Y_1 - Y_2) \circ Z) = 0$ for all $Z \in \mathcal{A}_0$. Hence $\mu((Y_1 - Y_2)^2) = 0$. The faithfulness now implies that $(Y_1 - Y_2)^2 = 0$. Therefore $Y_1 = Y_2$.

Let the restriction of μ to $\mathcal{A}_0$ be faithful, and let $\mathcal{A}_0 \underset{\mu}{\rightarrow} X, X_1, X_2$ hold with $X, X_1, X_2 \in \mathcal{A}, 0 \leqslant X, X_1, X_2 \leqslant \mathbb{I}$. Lemma 4.2 implies that $0 \leqslant \mu(X|\mathcal{A}_0) \leqslant \mathbb{I}$. Obviously we have $\mu(0|\mathcal{A}_0) = 0$, $\mu(\mathbb{I}|\mathcal{A}_0) = \mathbb{I}$, and $\mu(\alpha X_1 + (1-\alpha)X_2|\mathcal{A}_0) = \alpha\mu(X_1|\mathcal{A}_0) + (1-\alpha)\mu(X_2|\mathcal{A}_0)$ for $0 \leqslant \alpha \leqslant 1$. Moreover, $\mu(\mu(X|\mathcal{A}_0)|\mathcal{A}_1) = \mu(X|\mathcal{A}_1)$ holds for any other JBW subalgebra $\mathcal{A}_1 \subseteq \mathcal{A}_0$ with $\mathcal{A}_1 \underset{\mu}{\rightarrow} \mu(X|\mathcal{A}_0)$.

The faithfulness of μ on $\mathcal{A}_0$ is not really a strong restriction; moving over from $\mathcal{A}$ to the JBW algebra $\{D,\mathcal{A},D\}$ with D being the support of μ, one could even assume that μ is faithful on $\mathcal{A}$. Note that the support is the smallest event E with $\mu(E) = 1$, which exists for normal states.

We are now in a position to extend the concept of the state-independent conditional probabilities [$\mathbb{P}(F|E)$; see Ref. 9] to the conditional expectations. If $\mu(X|\mathcal{A}_0) = \nu(X|\mathcal{A}_0)$ all normal states μ, ν on $\mathcal{A}$, which are faithful on $\mathcal{A}_0$ and satisfy $\mathcal{A}_0 \underset{\mu}{\rightarrow} X$ and $\mathcal{A}_0 \underset{\nu}{\rightarrow} X$, respectively, and if at least one such state exists, this state-independent conditional expectation is denoted by $\mathbb{E}(X|\mathcal{A}_0)$. The conditional expectations $\mu(F|\mathcal{A}_0)$ and $\mathbb{E}(F|\mathcal{A}_0)$ are elements in $\mathcal{A}_0$ while $\mu(F|E)$ and $\mathbb{P}(F|E)$ are real numbers for events E and F in $\mathcal{A}$. If E_n is a finite or infinite sequence of mutually orthogonal events in $\mathcal{A}$ with $\Sigma E_n = \mathbb{I}$ and $0 < \mu(E_n) < 1$ for each n, if $\mathcal{A}_0$ is the subalgebra generated by the E_n, and if $\mathcal{A}_0 \underset{\mu}{\rightarrow} F$ holds, we get $\mu(F|\mathcal{A}_0) = \Sigma\mu(F|E_n)E_n$. If, moreover, the E_n are atoms,[9] $\mathbb{E}(F|\mathcal{A}_0)$ exists and $\mathbb{E}(F|\mathcal{A}_0) = \Sigma\mathbb{P}(F|E_n)E_n$.

With $R: \mathcal{M} \rightarrow \mathcal{A}$ being a normal observable, i.e., a JBW-homomorphism from another JBW algebra $\mathcal{M}$ to $\mathcal{A}$, $R(\mathcal{M})$ is a JBW subalgebra of $\mathcal{A}$. If $R(\mathcal{M}) \underset{\mu}{\rightarrow} X$ and if μ is faithful on $R(\mathcal{M})$, $\mu(X|R(\mathcal{M})) \in R(\mathcal{M})$ is also denoted by $\mu(X|R)$ [or by $\mathbb{E}(X|R)$ in the case of independence of the particular state]. If R is injective, there is one and only one element $V_{R,\mu}(X) \in \mathcal{M}$ with $\mu(X|R) = RV_{R,\mu}(X)$. Then $0 \leqslant V_{R,\mu}(X) \leqslant \mathbb{I}$.

We now assume that $\mathcal{A}_1$ is a further subalgebra of $\mathcal{A}$ such that $\mathcal{A}_0 \underset{\mu}{\rightarrow} \mathcal{A}_1$ (i.e., $E \underset{\mu}{\rightarrow} X$ all events E in $\mathcal{A}_0$ and all $X \in \mathcal{A}_1$) or $R(\mathcal{M}) \underset{\mu}{\rightarrow} \mathcal{A}_1$. Then the maps $X \rightarrow \mu(X|\mathcal{A}_0), X \rightarrow \mu(X|R)$, and $X \rightarrow V_{R,\mu}(X)$ [possibly also $X \rightarrow \mathbb{E}(X|\mathcal{A}_0)$ and $X \rightarrow \mathbb{E}(X|R)$] are convex normal maps from the positive unit ball of $\mathcal{A}_1$ to the positive unit ball of $\mathcal{A}_0, R(\mathcal{M})$, and $\mathcal{M}$, respectively. Therefore, each of these maps has a unique extension to a positive normal linear map from $\mathcal{A}_1$ to $\mathcal{A}_0$, $R(\mathcal{M})$, and $\mathcal{M}$, respectively. Thus, $\mu(X|\mathcal{A}_0), \mu(X|R)$, and $V_{R,\mu}(X)$ [possibly also $\mathbb{E}(X|\mathcal{A}_0)$ and $\mathbb{E}(X|R)$] are defined for all $X \in \mathcal{A}_1$.

Differing from the notation used here, a positive linear map $\pi: \mathcal{A} \rightarrow \mathcal{A}_0, X \rightarrow \pi(X)$ with $\mathcal{A}_0 \subseteq \mathcal{A}_1$, $\pi = \pi^2$ and $\pi(\mathbb{I}) = \mathbb{I}$ is sometimes called a conditional expectation (e.g., Refs. 2 and 14); in Ref. 4, it is shown that then $\pi(X \circ Y) = \pi(X) \circ Y$ for $X \in \mathcal{A}$ and $Y \in \mathcal{A}_0$. If $\mathcal{A}$ is a JBW algebra with a faithful trace state (e.g., a JBW algebra with a finite dimension, or a type II_1 factor), then it follows from Theorem 4.3 that a positive linear map $\pi: \mathcal{A} \rightarrow \mathcal{A}$ with $\pi = \pi^2$, $\pi(\mathbb{I}) = \mathbb{I}$, and $\pi(\mathcal{A}) = \mathcal{A}_0$ exists for each JBW subalgebra $\mathcal{A}_0 \subseteq \mathcal{A}$; note that, with μ being a trace state, $E \underset{\mu}{\rightarrow} F$ all events E and F in $\mathcal{A}$, and define $\pi(X) := \mu(X|\mathcal{A}_0)$ for $X \in \mathcal{A}$.

V. THE MARKOV PROCESS

Let $\mathcal{A}$ be a JBW algebra. Let $R_s: \mathcal{M}_s \rightarrow \mathcal{A} (s \in S)$ be a family of normal observables with $\mathcal{M}_s$ being further JBW algebras. Typical examples of the index set S are intervals, e.g., $[0,\infty]$ or $[-\infty,\infty]$, the integers or the non-negative integers $\{0,1,2,\ldots\}$. The JBW subalgebra of $\mathcal{A}$ that is generated by $\cup_{s' \leqslant s} R_{s'}(\mathcal{M}_{s'})$ is denoted by $\mathcal{A}_{\leqslant s}$ for $s \in S$.

Definition 5.1: *The family of normal observables* $R_s (s \in S)$ *together with a faithful normal*

state μ on $\mathcal{A}$ is now called a normal Markov process if

(i) $\mathcal{A}_{\leqslant s} \underset{\mu}{\rightarrow} R_{s'}(\mathcal{M}_{s'})$ *for* $s<s'$, *and*

(ii) $\mu(X|\mathcal{A}_{\leqslant s})=\mu(X|R_s)$ *for* $s<s'$ *and* $X \in R_{s'}(\mathcal{M}_{s'})$ *both hold.*

Condition (i) is a weak directed compatibility criterion for the family of observables $R_s(s \in S)$ under the fixed state μ. Within classical probability theory, it is meaningless, since generally holding. Condition (ii) is the Markov property, meaning that a Markov process is memoryless; the future behavior of the process after time s depends only on its behavior at time s and not on the process history before time s.

We now assume a normal Markov process with each $R_s(s \in S)$ being injective; then $V_{R_s,\mu}(R_{s'}(Y)) \in \mathcal{M}_s$ for $Y \in \mathcal{M}_{s'}$ and $s<s'$ (see Sec. IV). Hence, the composition $V_{s,s'}:=V_{R_s,\mu}R_{s'}$ is a positive normal map $\mathcal{M}_{s'} \rightarrow \mathcal{M}_s$ with $V_{s,s'}(\mathbb{I})=\mathbb{I}$. Keep in mind that the $V_{s,s'}$ depend on the underlying state μ, although this is not shown in the nomenclature.

Theorem 5.2:(i) $\mu^{R_s}(V_{s,s'}(Y))=\mu^{R_{s'}}(Y)$ *for* $Y \in \mathcal{M}_{s'}$ and $s<s'$; *i.e., $V_{s,s'}$ transfers the probability distribution of R_s on $\mathcal{M}_s$ into the one of $R_{s'}$ on $\mathcal{M}_{s'}$. Note that μ^R with $\mu^R(E):=\mu(R(E))$ is the distribution of the observable R in the state μ.* (ii) $V_{s,s'}V_{s',s''}=V_{s,s''}$ for $s,s',s'' \in S$ with $s<s'<s''$.

Proof: (i) $\mu^{R_s}(V_{s,s'}(Y))=\mu((R_sV_{R_s,\mu}R_{s'})(Y))=\mu(\mu(R_{s'}(Y)|R_s))=\mu(R_{s'}(Y))=\mu^{R_{s'}}(Y)$. (ii) Let $X \in R_{s''}(\mathcal{M}_{s''})$. Note that $\mathcal{A}_{\leqslant s} \underset{\mu}{\rightarrow} \mu(X|R_{s'})=\mu(X|A_{\leqslant s'})$. Therefore $\mu(X|R_s)=\mu(X|\mathcal{A}_{\leqslant s})=\mu(\mu(X|\mathcal{A}_{\leqslant s'})|\mathcal{A}_{\leqslant s})=\mu(\mu(X|R_{s'})|\mathcal{A}_{\leqslant s})=\mu(\mu(X|R_{s'})|R_s)$, where the Markov property has been applied several times. With $X=R_{s''}(Y)$ we get $(R_sV_{R_s,\mu}R_{s''})(Y)=(R_sV_{R_s,\mu}R_{s'}V_{R_{s'},\mu}R_{s''})(Y)$ for all $Y \in M_{s''}$ and, due to the injectivity of R_s, $V_{R_s,\mu}R_{s''}=V_{R_s,\mu}R_{s'}V_{R_{s'},\mu}R_{s''}$. The left-hand side of this last equation is identical with $V_{s,s''}$ and the right-hand side is identical with $V_{s,s'}V_{s',s''}$.

Part (ii) of the theorem is the quantum version of the Chapman–Kolmogorov equation in classical probability theory. It holds if the Markov property is satisfied. Part (i) is valid more generally [i.e., if $R_s(\mathcal{M}_s) \rightarrow \mu\ R_{s'}(\mathcal{M}_{s'})$ is satisfied for $s<s'$]. The approach to Markov processes, presented here, is very similar to the one in classical mathematical probability theory (e.g., Ref. 8). The adaptation to the quantum case becomes possible due to the compatibility criterion (i) in Definition 5.1. The faithfulness of the underlying state μ and the injectivity of the R_s are technical assumptions to avoid the difficulties involved with the μ-almost-everywhere equivalence classes that are used in mathematical probability theory. Some further discussion of the assumptions will follow in the concluding remarks.

We call a Markov process *reversible*, if each $V_{s,s'}$ has an inverse $V_{s,s'}^{-1}$, and if this inverse is a positive map. Then $V_{s,s'}^{-1}$ transfers the probability distribution of $R_{s'}$ on $\mathcal{M}_{s'}$ into the one of R_s on $\mathcal{M}_s$. Without $V_{s,s'}^{-1}$ being positive, it would not transfer states to states, but to linear functionals that are not necessarily positive. The generalized Schwarz inequality (Corollary 2.3) implies that the $V_{s,s'}$ are multiplicative isomorphisms in the case of a reversible Markov process.

VI. THE DYNAMICAL GROUP AND ITS GENERATOR

We now assume a Markov process such that each $R_s(s \in S)$ is injective and $\mathcal{M}_s=\mathcal{M}$ for all s. Let $\mathrm{Aut}(\mathcal{M})$ denote the automorphism group of $\mathcal{M}$ and let $\mathrm{Pos}(\mathcal{M})$ be the set of all positive normal linear maps from $\mathcal{M}$ to $\mathcal{M}$ that map the unit element to itself; $\mathrm{Pos}(\mathcal{M})$ is a semigroup, but an inverse need not exist for an element of $\mathrm{Pos}(\mathcal{M})$. The $V_{s,s'}$ now lie in $\mathrm{Pos}(\mathcal{M})$, and if the Markov process is reversible, they lie in $\mathrm{Aut}(\mathcal{M})$.

With the index set S being one of the sets $(-\infty,\infty)$, $[0,\infty)$, $\{0,1,2,\ldots\}$ or $\{\ldots,-1,0,1,2\ldots\}$ and with $\mathcal{M}_s=\mathcal{M}$ for all $s \in S$, we call a Markov process *stationary*, if $\mu(R_{s'}(Y)|R_s)=\mu(R_{t'}(Y)|R_t)$ for $s'-s=t'-t$ ($s,t \in S$, $s<s'$, $t<t'$, and $Y \in \mathcal{M}$). Then $V_{s,s'}=V_{t,t'}$ for $s'-s=t'-t$, and we can define $V_{t,t'}=:V_{t'-t}$. For these V_t we have $V_sV_t=V_{s+t}$. Note that $V_{s,s}(s=s')$ as well as $V_0(t=0)$ have not been defined so far, and we now define $V_{s,s}$ and V_0 to be the identity map on $\mathcal{M}$. Thus, with $S=[0,\infty)$ and a stationary Markov process, the V_t form a dynamical semigroup in

$\mathrm{Pos}(\mathcal{M})$; with $S=(-\infty,\infty)$ and a stationary and reversible Markov process, the V_t form a dynamical group in $\mathrm{Aut}(\mathcal{M})$.

We shall now briefly consider the generators of such groups, but will not go into the technical details of the different kinds of convergence, since most of it is well known—if not for JBW algebras, then at least for the C^*-/W^*-algebras. If

$$L:\ \frac{d}{dt}V_t\bigg|_{t=0}$$

exists (convergence in some sense assumed) for a stationary Markov process, L is a linear operator $\mathcal{M}\to\mathcal{M}$ (or possibly defined only on a dense subset of $\mathcal{M}$) and the following differential equation holds:

$$\frac{d}{dt}V_t = LV_t.$$

Then $V_t=\exp(tL)$. L is called the *generator* of the dynamical (semi)group V_t. From the generalized Schwarz inequality we get for $Y\in\mathcal{M}$,

$$V_t(Y^2)-Y^2 \geqslant (V_t(Y))^2-Y^2 = (V_t(Y)+Y)\circ(V_t(Y)-Y)$$

and therefore (note that V_0 is the identity)

$$L(Y^2)=\frac{d}{dt}V_t(Y^2)\bigg|_{t=0}=\lim_{t\downarrow 0}\frac{1}{t}(V_t(Y^2)-Y^2)\geqslant\lim_{t\downarrow 0}(V_t(Y)+Y)\circ\lim_{t\downarrow 0}\frac{1}{t}(V_t(Y)-Y)=2Y\circ L(Y).$$

In the reversible case, each "$\geqslant$" can be replaced by "=" (Corollary 2.3). Then $L(Y^2)=2Y\circ L(Y)$ for $Y\in\mathcal{M}$. Linear maps L satisfying this equation are called *derivations*. We call a linear map L satisfying $L(Y^2)\geqslant 2Y\circ L(Y)$ for $Y\in\mathcal{M}$ a *dissipation*.

Thus, we have shown that the generator of the dynamical group associated with a stationary Markov process is a dissipation, and is a derivation if the Markov process is stationary and reversible. With $\mathcal{M}$ being the self-adjoint part of a W^*-algebra and with the inner derivation $L(X):=i[H,X]$ for $X\in\mathcal{M}$ [with some $H\in\mathcal{M}$], we get

$$\frac{d}{dt}V_t(X)=i[H,V_t(X)] \text{ and } V_t(X)=e^{itH}Xe^{-itH}.$$

This provides the Schrödinger equation and its solution as a very special case of a more general approach.

Derivations on C^*-algebras are studied in Refs. 2 and 1. The above definition of a dissipation differs from the dissipations studied in Refs. 1 and 3. In Ref. 1, a linear map δ on a *-subalgebra $\mathcal{A}_0$ of a C^*-algebra, satisfying $\delta(X^*X)\leqslant\delta(X^*)X+X^*\delta(X)$ for $X\in\mathcal{A}_0$, is called a dissipation. This implies, but is not equivalent to $\delta(X^2)\leqslant\delta(X)X+X\delta(X)=2X\circ\delta(X)$ for all self-adjoint X in $\mathcal{A}_0$. Other authors use the reversed inequality $\delta(X^*X)\geqslant\delta(X^*)X+X^*\delta(X)$ for the definition of a dissipation. Note that our definition is based on this reversed inequality which, moreover, is required to hold for the self-adjoint elements only (which form the JB algebra).

Note that other authors immediately define a quantum Markov process as a pair consisting of a W^*-algebra and a dynamical semigroup of (completely) positive normal maps on this W^*-algebra, without starting from a stochastic process given as a family of observables and implicitly assuming the stationarity.

VII. CONCLUDING REMARKS

The concept of the classical conditional expectations has been extended to the quantum case, using the framework of Jordan operator algebras. An important condition for the existence of the conditional expectations is given by a certain weak compatibility criterion that was introduced

earlier in Ref. 11. With these concepts, it has been possible to partly extend the classical equivalence between two different ways of describing a Markov process to the quantum case. Starting from a Markov process given as a family of observables, we have derived the positive maps $V_{s,s'}$. In classical probability theory, the reverse is also possible; a Markov process consisting of a family of random variables can be reconstructed from a system of Markovian kernels by using the concept of product σ-algebras. The problem of finding a satisfying analogue of these product σ-algebras for the quantum case has been addressed, but only partly been solved in Ref. 11.

The appropriate framework for this approach to quantum Markov processes are Jordan operator algebras, but neither the only norm-complete JB algebras nor the weakly complete JBW algebras are really satisfying. The JB algebras do not contain sufficiently many idempotent elements (quantum events). If the theory is based upon JBW algebras (as here in this paper), an important example, the algebra consisting of the measurable real-valued functions on a measurable space (the real-valued random variables of classical probability theory) is ruled out. This algebra can be embedded in a JBW algebra (even in a W^*-algebra,[7]) however, one is rather reluctant to work with this abstractly constructed JBW algebra instead of the well-understood algebra of measurable real functions. What is needed is a theory of monotone-sequentially complete JB algebras, similar to the one of the monotone-sequentially complete C^*-algebras studied by Kadison,[6] Kehlet,[7] and Pedersen.[12] This theory must include a Gleason-type theorem and a Radon–Nikodym theorem for σ-additive states. The Gleason-type theorem is needed for proving that unique conditional probabilities exist for σ-additive states defined on the system of events (as done for the JBW case in Ref. 9), and the Radon–Nikodym theorem is required for showing that the conditional expectations exist for the σ-additive states.

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Constructing and exploring wells of energy landscapes

Jean-Pierre Aubin[a)]
Réseau de Recherche Viabilité, Jeux, Contrôle, 14 rue Domat, F-75005 Paris

Annick Lesne[b)]
Laboratoire de Physique Théorique des Liquides, Case 121, Université Pierre et Marie Curie, 4 place Jussieu, F-75252 Paris

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Landscape paradigm is ubiquitous in physics and other natural sciences, but it has to be supplemented with both quantitative and qualitatively meaningful tools for analyzing the topography of a given landscape. We here consider dynamic explorations of the relief and introduce as basic topographic features "wells of duration T and altitude y." We determine an intrinsic exploration mechanism governing the evolutions from an initial state in the well up to its rim in a prescribed time, whose finite-difference approximations on finite grids yield a constructive algorithm for determining the wells. Our main results are thus (i) a quantitative characterization of landscape topography rooted in a dynamic exploration of the landscape, (ii) an alternative to stochastic gradient dynamics for performing such an exploration, (iii) a constructive access to the wells, and (iv) the determination of some bare dynamic features inherent to the landscape. The mathematical tools used here are not familiar in physics: They come from set-valued analysis (differential calculus of set-valued maps and differential inclusions) and viability theory (capture basins of targets under evolutionary systems) that have been developed during the last two decades; we therefore propose a minimal Appendix exposing them at the end of this paper to bridge the possible gap. © *2005 American Institute of Physics.*
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I. INTRODUCTION

A. The landscape paradigm in natural sciences

The general notion of landscape is encountered in many different domains, for instance in physics, neural networks (Hopfield nets[22]) and learning processes, molecular biology,[13,19] ecology and evolutionary biology,[23] or optimization problems, to cite but a few. From the mathematical viewpoint, a *landscape* is simply a function $V: X \mapsto \mathbb{R} \cup \{+\infty\}$ (more precisely, an extended[30] function since it might take infinite values $+\infty$) associating a real value $V(x)$ to each state $x \in X$ of the system. From a physical viewpoint, the status and definition of V strongly depend on the scale at which the system is described, reflecting in the choice of the space of states X.

Let us give some examples to sustain our exposition. In statistical physics and molecular biology, $V(x)$ can be the *energy landscape* if x is the (high-dimensional) microscopic configuration of the considered system: atomic coordinates in a glass,[15] spin orientations in a spin glass,[17] tridimensional conformation of the hundred or more amino acids forming a protein,[18] spatial positions of bead centers in a granular medium.[16] It can also be a (mesoscopic) *free energy landscape* if x is the value of a (low-dimensional) order parameter describing the global state of the system: spatially average density, overall magnetization, conformational parameter(s) for a macromolecule (as, for instance, its radius of gyration). At a still more macroscopic level, x can be

a)Electronic mail: J.P.Aubin@wanadoo.fr
b)Electronic mail: lesne@lptl.jussieu.fr

a reaction coordinate measuring the progress along a path representing some transformation of the system and inscribed on an *effective energy landscape*. In quite different contexts, cost functions encountered in optimization problems are close analogs to energy landscapes,[2] whereas fitness landscapes encountered in ecology and evolutionary biology can be cast in the frame of free or effective energy landscapes, up to a sign change (namely, by considering the opposite of the fitness). (See Ref. 28 for an introductory review.)

Energy or free energy landscapes are currently exploited in stochastic gradient methods accounting for the interplay between thermal motion and interaction forces (effective forces in the case of a free energy landscape) deriving from the potential $x \mapsto V(x)$. In complex systems (glasses, spin glasses, proteins, for instance) the landscape V typically presents a large number of local optima around which the solution of a stochastic gradient method is trapped and travels a long time before going away and visiting other local minima. This dynamical behavior has been advocated by Giorgio Parisi to encapsulate a meaning of complexity and rugged landscapes are often seen as a mark of complex systems. (See, for instance, Ref. 25.)

Although the landscape $V(x)$ is thus endowed with different status and interpretations in varying contexts, understanding and controlling the system behavior requires in any case a quantitative knowledge of the landscape topography. It is thus of the utmost importance to design efficient tools allowing a dynamical analysis of local minima of such a function $x \mapsto V(x)$. We emphasize that it is not just an academic issue since actual energy or free energy landscapes of real systems are available through either of the following:

(i) a *theoretical access* from first principles (e.g., molecular interactions, spin–spin interactions) and/or modeling hypotheses, allowing us to write an explicit formula for $V(x)$;
(ii) an *experimental access*, for instance, for proteins (indirect kinetic or spectral measurements) (Ref. 19);
(iii) a *numerical access*, either through molecular dynamics at an atomic scale, yielding the energy landscape, either through Monte Carlo sampling of the configuration space according to the Boltzmann distribution, yielding free energy landscapes for the relevant order parameter(s) of the system.[20]

B. Dynamical analysis of a landscape topography

Here we propose a theoretical and algorithmic analysis allowing us to determine quantitatively the landscape relief of a function V, e.g., location of wells, location and heights of the barriers associated with a given dynamics for exploring the landscape.[31] It gives access to a hierarchical picture of the landscape and allows us to determine the nesting of wells and barriers at different scales.

Given a dynamic exploration mechanism (such as a stochastic gradient dynamics), we define the "wells of velocity λ, duration T, and altitude y" as the sets of initial states $x \in X$ "below the level y," i.e., $V(x) \leqslant y$, from which at least one evolution governed by the exploration mechanism, and of velocity bounded by λ, reaches the rim y of the well at the prescribed time T. When the well is not empty, we then evidence intrinsic dynamics governing the evolutions from an initial state of the well up to its rim y at prescribed time T. This intrinsic exploration mechanism is characterized from *the time derivative of the well, regarded as a set-valued map associated with the prescribed duration T and the altitude y the elements of the well*. Both the wells and their intrinsic exploration mechanism can be approximated by finite-difference approximations on finite grids, *which allows us to implement a constructive algorithm*.

In this study we offer an alternative to stochastic gradient-type exploration mechanisms. In quite a similar way of thought, second-order exploration mechanisms of the graph of an energy landscape function has been proposed in Ref. 1. Here we suggest starting the landscape exploration with a universal mechanism, independent of the energy function, allowing us to look at any possible velocity with prescribed norm λ and retaining its intrinsic exploration dynamics as a good candidate for a dynamical system exploring the given energy landscape. The stochastic gradient

method is thus replaced by a differential inclusion involving the time derivative of the well, but allowing in the same spirit the system state to escape the trap of local minima, while being quantitatively influenced by their depth.

The mathematical tools we use are quite novel in physics: They come from set-valued analysis (differential calculus of set-valued maps and differential inclusions) and viability theory (capture basins of targets under evolutionary systems) that have been developed during the last two decades.

The resulting quantitative topographic description by wells rooted in a constructive dynamic exploration of the landscape and the associated determination of the statistical properties of its relief can then be exploited for the following:

(1) *performing a quantitative characterization of the landscape*, for comparison or classification purposes. It allows us to investigate bifurcations, more currently called phase transitions in many-particle systems (Ref. 24);
(2) *providing a quantitative access to the landscape hierarchical structure* and allowing us to estimate its ruggedness, which yields a tentative measure of the system complexity;
(3) *defining macrostates and macroscopic variables* to be used in coarse-grained descriptions of the system. The relevance of such an approach is to provide an intrinsic determination of macrostates, founded upon the identification of macroscopic features with slow modes and slowly evolving properties (Ref. 21).

Outline of the paper. In Sec. II, we shall define wells, introduce some mathematical features of their relief, and reformulate their characterization in terms of the "capture basin of a target," a key concept of viability theory that finds here an unexpected, yet natural, application. In Sec. III, we present the algorithm allowing us to construct explicitly these wells and the intrinsic exploration mechanism on which it is based. In Sec. IV, we introduce the notion of complete wells, matching more closely with physical landscape features. After a conclusive summary in Sec. V, the essential notions of viability theory needed for this paper are presented in an Appendix. ■

II. WELLS OF AN ENERGY LANDSCAPE

A. An efficient alternative to stochastic exploration

In order to provide both a quantitatively meaningful and quantitative topographic analysis of a landscape V on a space X, we introduce "wells of duration T and depth y." Given a dynamical system, allowing upward steps of velocity bounded by a parameter λ, these wells are the sets $\mathbf{P}_V(\lambda;t,y)$ of initial states "below the level y" [i.e., of states $x \in X$ such that $V(x) \leqslant y$] from which at least one[32] evolution reaches the upper level y (what we call the *rim of the well*) at time T. In other words, given some tolerance λ allowing upwards exploration, and some level y, the wells and their depth might be dynamically (the experimentally meaningful and operational way) determined according to the trapping time T.

For exploratory purposes, here we implement an alternative to stochastic gradient dynamics and replace stochastic differential equations encountered in physics by differential inclusions of the form[33]

$$\forall t \geqslant 0, \quad x'(t) \in F(\lambda;x(t)),$$

where $x \rightsquigarrow F(\lambda;x(t))$ is some set-valued function on X [i.e., $F(\lambda;x)$ is a subset of X] parametrized by a parameter $\lambda \in \mathbb{R}$. Compared to a differential equation, the solution of a differential inclusion is less constrained since the full specification of the derivative $x'(t)$ at each time t is replaced by a constraint on the region $F(\lambda;x(t))$, where it has to lie. Such a tolerance is highly valuable and quite realistic in the modeling of an actual system, since the experimentally available knowledge about its dynamics generally provides only bounds (or more generally viability constraints) on the kinetic rates, rather than explicit pointwise expressions of these rates as a function of the system state. These bounds might nevertheless vary with the system state $x(t)$, hence defining a specific

set $F(\lambda; x(t))$at each time t. For instance, in the case when the function V is differentiable, a close analog to stochastic gradient dynamics is provided by

$$x'(t) \in -\nabla V(x(t)) + \lambda B,$$

where B denotes the unit ball of the finite-dimensional vector space X. Indeed, the gradient dynamics $x'(t) = -\nabla V(x(t))$ governs evolutions decreasing along the function V, but stopping at the first encountered local minimum. To overcome this stalling situation, a natural idea is to perturb the gradient equation either by a stochastic noise, as currently implemented in simulated annealing methods, or, as we suggest here, by a "*tychastic*" one. Indeed, differential inclusion $x'(t) \in -\nabla V(x(t)) + \lambda B$ is the "tychastic version" of the stochastic differential equation $dx = -\nabla V(x(t))dt + \lambda\, dW(t)$ (see Ref. 8 for the links between stochastic and tychastic viability).

However, we have to overcome the fact that the function V is usually not differentiable, if obtained through experimental measures or simulations and no longer analytically defined. Hence the concept of gradient disappears (when the observable or simulated configuration space is discrete), or has to be approximated by gradients of functions interpolating in one way or another the experimental data. Any method allowing to bypass these obstacles and to deal with graphs of such functions may be worthy of being investigated.

Another suggestion is to leave open the choice of the directions of exploration by looking for any way to climb the landscape V to reach a given level y at a given time T. For that purpose, we can choose $F(\lambda; x) := \lambda B$, stating that any velocity of norm λ is *a priori* an eligible candidate to apply for such a mission. We shall provide below the way of further selecting the most efficient (subset of) velocity(ies), i.e., achieving the most thoroughly and the most efficiently from a numerical viewpoint the quantitative exploration of the landscape relief. The same type of strategy has been used in previous works for constructing an algorithm that is also of relevance for landscapes. This so-called Montagnes Russes Algorithm converges to global minima of an extended function jumping over local minima, which amounts to using the gradient algorithm to the smallest of the exponential Lyapunov functions above the energy function for the differential inclusion $x'(t) \in \lambda B$. (See Refs. 10 and 11.) But whereas this algorithm was devoted to the search of global minima, we are here looking for exploratory tools providing a complete hierarchical picture of the landscape.

B. Definition and characterization of wells

From now on, we assume that the set-valued map $x \rightsquigarrow F(\lambda; x)$ governing the exploration dynamics is given. We denote by $y \in \mathbb{R}$ the altitude of the well we wish to study. $y = 0$ is set through the (arbitrary) choice of a base level (or, if known and finite, by the lower bound on V). Usually, the relevant altitudes are the values of the *local maxima* or *saddle points* of the function V. We shall associate with it the concept of well $\mathbf{P}(\lambda; T, y)$ of duration T and altitude y defined as follows.

Definition II.1: Consider an extended function $V: X \mapsto \mathbb{R} \cup \{+\infty\}$ and a differential inclusion

$$\forall\, t \geqslant 0, \quad x'(t) \in F(\lambda; x(t)).$$

Denote by

$$\mathbf{S}(V, y) := \{x \in X \text{ such that } V(x) \leqslant y\} \text{ and } \mathbf{S}_0(V, y) := \{x \in X \text{ such that } V(x) = y\}$$

the level sets of the function V and by $\mathcal{S}_\lambda(x)$ the set of solutions to the above differential inclusion starting at x. The well $\mathbf{P}_V(\lambda; T, y) \subset \mathbf{S}(V; y)$ of duration T and altitude y of the function V is defined by the set of initial states $x \in \mathbf{S}(V; y)$ such that there exists at least one solution $x_\lambda(\cdot) \in \mathcal{S}_\lambda(x)$ such that

$$\text{(i) } V(x_\lambda(T)) = y,$$

$$\text{(ii)}\ \ \forall\, t \in [0,T], \quad V(x_\lambda(t)) \leqslant y.$$

We observe that $\mathbf{P}_V(\lambda;0,y)=\mathbf{S}_0(V,y):=\{x\in X \text{ such that } V(x)=y\}$. In other words, the well $\mathbf{P}_V(\lambda;T,y)$ is the set of initial conditions x in the well from which there exists at least one evolution $x_\lambda(\cdot)$ staying below the level y during a duration T and reaching the level y at exactly time T. This does not exclude the fact that for some earlier time $t^*\leqslant T$ (or some later time $t^*\geqslant T$), the evolution reaches the level y. This just means that x belongs to the intersection $\mathbf{P}_V(\lambda;T,y)\cap\mathbf{P}_V(\lambda;t^*,y)$ of wells of several durations. This point can be made more explicit: considering the initial state x of the system as a variable and the time to reach the level y as the result, we can define the *reaching function* $(\lambda,x,y)\mapsto\xi(\lambda,x,y)$ by

$$\xi(\lambda,x,y) := \inf_{x\in\mathbf{P}_V(\lambda;T,y)} T,$$

providing the first instant when one evolution starting from x reaches the level y.

We can also regard the same object by introducing the set-valued map $(\lambda;T,x)\rightsquigarrow\mathbf{P}_V^{-1}(\lambda;T,x)$ associated with the parameter λ, the duration T, and the initial state x the altitude y of the well, the rim of which can be reached at time T by at least one evolution governed by differential inclusion $x'(t)\in F(\lambda;x(t))$.

Turning back to the initial definition, the *maximal depth* $\delta_V(\lambda;T,y)$ of the well $\mathbf{P}_V(\lambda;T,y)$ is defined by

$$\delta_V(\lambda;T,y) := \sup_{x\in\mathbf{P}_V(\lambda;T,y)} (y - V(x)).$$

The knowledge of the wells provides some physical characteristics of the landscape V, thus bridging the above mathematical definitions with a more traditional description of landscapes. We observe, for instance, that $\xi(\lambda,x,y)$ is the *escape time* for the given dynamics, also called the *first passage time*, from above a barrier of top y when the velocity is bounded by λ. Its inverse $[\xi(\lambda,x,y)]^{-1}$ has the meaning of a kinetic constant.

Denoting $\Omega_V(\lambda;T,y)$ the number of the connected components of well $\mathbf{P}_V(\lambda;T,y)$, its logarithm is the *configurational entropy*. (See Refs. 29 and 16 for its meaning and use in physics, respectively, for glasses and granular media):

$$\sigma_V(\lambda;T,y) := \log(\Omega_V(\lambda;T,y)).$$

In summary, what we are basically looking for is the subset of (x,y,λ,T) such that either $x\in\mathbf{P}_y(\lambda;T,y)$ or $T>\xi(\lambda;x,y)$ or $y\in\mathbf{P}_V^{-1}(\lambda;T,x)$. As detailed in the next section, we shall give a mathematical characterization of this set as a "capture basin of a target under an auxiliary system," allowing us to implement a constructive algorithm. We choose here the representation of this set through the above concept of well $x\in\mathbf{P}_V(\lambda;T,y)$.

C. Viability characterization of wells

The next step of our investigation is to translate the above topographically meaningful features in terms of capture basins for which many properties have been established and constructive algorithms are available (See the Appendix and for further details, Refs. 3–6.)

Proposition II.2: Consider an extended function $V:X\mapsto\mathbb{R}\cup\{+\infty\}$ and a differential inclusion

$$\forall\, t\geqslant 0, \quad x'(t)\in F(\lambda;x(t)).$$

We associate with it the auxiliary system of differential inclusions

$$\text{(i)}\ x'(t)\in F(\lambda(t);x(t)),$$

$$\text{(ii)}\ y'(t)=0,$$

$$\text{(iii)}\ \lambda'(t) = 0,$$

$$\text{(iv)}\ \tau'(t) = -1 \tag{1}$$

the constrained set $\mathcal{K}$ and the target $\mathcal{C}$ defined by

$$\mathcal{K} := \mathcal{E}_p(V) \times \mathbb{R}_+ \times \mathbb{R}_+ \text{ and } \mathcal{C} := \text{Graph}(V) \times \mathbb{R}_+ \times \{0\},$$

where Graph(V) and $\mathcal{E}p(V) \subset X \times \mathbb{R} \cup \{+\infty\}$ are, respectively, the graph and epigraph of V (see the Appendix for a precise definition). Then

$$\mathbf{P}_V(\lambda; T, y) = \{x \in X \text{ such that } (x, y, \lambda, T) \in \text{Capt}_{(1)}(\mathcal{K}, \mathcal{C})\},$$

where $\text{Capt}_{(1)}(\mathcal{K}, \mathcal{C})$ is the capture basin of the target $\mathcal{C}$ under evolutionary system (1) and under the constraint of remaining in $\mathcal{K}$ (see Definition A.2 below).

Proof: Indeed, to say that $(x, y, \lambda, T) \in \text{Capt}_{(1)}(\mathcal{K}, \mathcal{C})$ amounts to saying that there exist one evolution $x_\lambda(\cdot) \in \mathcal{S}_\lambda(x)$ and a time $t^\star \geqslant 0$ such that the associated auxiliary evolution,

$$t \to (x(t), y(t); \lambda(t); \tau(t)) = (x(t), y, \lambda, T - t),$$

starting from (x, y, λ, T) at $t=0$, reaches the target $\mathcal{C}$ at time $t^\star$ while staying meanwhile in $\mathcal{K}$:

$$\text{(i)}\ (x(t^\star), y, \lambda, T - t^\star) \in \mathcal{C},$$

$$\text{(ii)}\ \forall\, t \in [0, t^\star], \quad (x(t), \lambda, y, T - t) \in \mathcal{K}.$$

The first condition is equivalent to both equations $t^\star = T$ and $V(x(T)) = y$. The second equation means that for every $t \in [0, T]$, $V(x(t)) \leqslant y$. These are the very properties stating that x belongs to the well $\mathbf{P}_V(\lambda; T, y)$, or, equivalently, that $\xi(\lambda; x, y) \leqslant T$. ■

Therefore, the graph of the set-valued map $(\lambda, T, y) \rightsquigarrow \mathbf{P}_V(\lambda; T, y)$ inherits the properties of capture basins. For instance, it can be shown (using Theorem A.6 given in the Appendix) that the well satisfies a kind of dynamical programming principle that can be stated in the following way:

Proposition II.3: The set-valued map $\mathbf{P}_V$ is the unique set-valued map $(\lambda, T, y) \rightsquigarrow \mathbf{P}(\lambda; T, y)$ satisfying the initial condition

$$\mathbf{P}(\lambda; 0, y) := \mathbf{S}_0(V, y) := \{x \in X \text{ such that } V(x) = y\}$$

the constraints

$$\mathbf{P}(\lambda; T, y) \subset \mathbf{S}(V; y)$$

and the "tracking property:" for any $x \in \mathbf{P}(\lambda; T, y)$, any evolution $x_\lambda(\cdot) \in \mathcal{S}_\lambda(x)$ starting from x at time 0 climbing the well until it reaches the rim at time T satisfies

$$\text{(i)}\ \forall\, t \in [0, T], \quad x(t) \in \mathbf{P}(\lambda; T - t, y),$$

$$\text{(ii)}\ \forall\, s \geqslant T \text{ such that } \forall\, t \in [T, s], \quad V(x(t)) \leqslant y, \quad \text{then } x(t) \in \mathbf{P}(\lambda; t - T, y).$$

D. Time derivative of the well as an *a posteriori* exploratory dynamical system

Since we have related the well of a landscape function to capture basins, the basic viability theorems provide tangential characterization of the wells, allowing us to find the underlying dynamical system governing the evolutions of differential inclusion climbing the wells up to their rims. This can be done to the price of using differential calculus of set-valued maps (invented in

the beginning of the 1980s for this purpose): Knowing the "derivatives" with respect to time of the set-valued map $t \rightsquigarrow \mathbf{P}_V(\lambda;t,y)$ (see Definition A.10 for a rigorous definition), we obtain an intrinsic exploration mechanism of the well.

Proposition II.4: For any $x \in \mathbf{P}_V(\lambda;T,y)$, those evolutions $x_\lambda(\cdot) \in \mathcal{S}_\lambda(x)$ starting at x and climbing the well $\mathbf{P}_V(\lambda;T,y)$ in the sense that $V(x_\lambda(t)) \leqslant y$ for any $t \in [0,T]$ and $V(x_\lambda(T)) = y$ are governed by differential inclusion

$$x'(t) \in -\frac{\partial \mathbf{P}_V(\lambda;T-t,y)}{\partial t} \cap F(\lambda;x(t)).$$

In particular, taking for initial exploration mechanism the set-valued map $F(\lambda;x) := \lambda B$ independent of the energy function V instead of exploration mechanisms $F(\lambda;x) := -\nabla V(x(t)) + \lambda B$ already dependent of V, we obtain a more intrinsic exploration mechanism.

Theorem A.12 stated in the Appendix gives a technically precise meaning to this symbolic statement. In other words, the underlying dynamical system governing the evolutions climbing the wells up to their rims is the set of velocities $v \in F(\lambda;x)$ pointing to the time derivative of the well in order to climb it from $-T$ to 0 in order to reach the rim of the well at altitude y. The associated mathematical problem to comfort this intuitive result starts with the definition of the time derivative and the proof of this result is based on results of viability theory. Let us just mention the following informal version of Theorem A.12 stated in the Appendix:

Proposition II.5: The set-valued map $\mathbf{P}_V$ is the unique "Frankowska solution to the partial differential inclusion"

$$\forall t > 0, x \in \mathbf{P}(\lambda;T,y), \quad 0 \in \frac{\partial \mathbf{P}(\lambda;T,y)}{\partial t} + F(\lambda;x)$$

satisfying the initial condition

$$\mathbf{P}(\lambda;0,y) := \mathbf{S}_0(V,y) := \{x \in X \text{ such that } V(x) = y\}$$

and the constraints

$$\mathbf{P}(\lambda;T,y) \subset \mathbf{S}(V;y).$$

We propose now to check the same statement in the discrete case, which allows us to define an algorithm providing the wells under discrete dynamics and the exploratory mechanisms.

III. THE SAINT-PIERRE CAPTURE BASIN ALGORITHM

The Saint-Pierre Capture Basin Algorithm provides both the set-valued map $\mathbf{P}_V$ and for any $x \in \mathbf{P}_V(\lambda;T,y)$, the evolutions climbing the well up to its rim under a given duration.

Let us consider any discrete time approximation $\Phi(\lambda;x)$ of $F(\lambda;x)$ governing the evolution of sequences $\vec{x} \in \vec{\mathcal{S}}_\lambda(x)$, governed by

$$x_{n+1} \in \Phi(\lambda;x_n).$$

[For instance, $\Phi(x): x + hF_h(\lambda;x)$, where h is a time step and F_h is an approximation of F in the sense that the graph of F_h converges to the graph of F in the Painlevé–Kuratowski sense]. The discrete version of a well defined by Definition II.1 for continuous time systems becomes as follows:

Definition III.1: Consider an extended function $V: X \mapsto \mathbb{R} \cup \{+\infty\}$ and a set-valued map $(\lambda,x) \rightsquigarrow \Phi(\lambda;x)$. The discrete time well $\vec{\mathbf{P}}_V(\lambda;N,y) \subset \mathbf{S}(V;y)$ of duration T and depth y of the function V is the subset of initial states $x \in \mathbf{S}(V;y)$ such that there exists one sequence $\vec{x} \in \mathcal{S}_\lambda(x)$ such that

$$\text{(i) } V(x_N) = y,$$

$$\text{(ii)}\ \ \forall\, n \in \{0,N\}, \quad V(x_n) \leqslant y.$$

In the discrete time, we obtain the intrinsic exploration mechanism under mere inspection:

Proposition III.2: Knowing the well $\vec{\mathbf{P}}_V$, the discrete dynamical system

$$x_{n+1} \in \Phi(\lambda; x_n) \cap \vec{\mathbf{P}}_V(\lambda; N-n, y)$$

governs the evolutions starting from $x \in \vec{\mathbf{P}}_V(\lambda; N, y)$ and arriving at step N at some $x_N \in \vec{\mathbf{P}}_V(\lambda; 0, y) = \mathbf{S}_0(V, y)$ of the rim of the well $\vec{\mathbf{P}}_V(\lambda; N, y)$.

In the discrete case, the discrete well is obtained by the Capture Basin Algorithm:

Proposition III.3: The Saint-Pierre Capture Basin Algorithm yields the discrete well as the intersection of the following subsets defined recursively by

$$\text{(i)}\ \vec{\mathbf{P}}_V(\lambda; 0, y) = \mathbf{S}_0(V, y),$$

$$\text{(ii)}\ \ \forall\, N \geqslant 0, \quad \vec{\mathbf{P}}_V(\lambda; N+1, y) = \Phi(\lambda; \cdot)^{-1}(\vec{\mathbf{P}}_V(\lambda; N, y)) \cap \mathbf{S}(V, y).$$

When $\Phi(\lambda; x) := x + \lambda B$, this algorithm can be written

$$\text{(i)}\ \vec{\mathbf{P}}_V(\lambda; 0, y) = \mathbf{S}_0(V, y),$$

$$\text{(ii)}\ \ \forall\, N \geqslant 0, \quad \vec{\mathbf{P}}_V(\lambda; N+1, y) = (\vec{\mathbf{P}}_V(\lambda; N, y) + \lambda B) \cap \mathbf{S}(V, y).$$

Proof: Indeed, we introduce the auxiliary system Ψ by

$$\Psi(x, y, \lambda, \tau) := \Phi(\lambda, x) \times \{y\} \times \{\lambda\} \times \{\tau - 1\},$$

governing the evolution of the sequence:

$$\begin{aligned} &\text{(i)}\ x_{n+1} \in \Phi(\lambda; x_n), \\ &\text{(ii)}\ y_{n+1} = y_n, \\ &\text{(iii)}\ \lambda_{n+1} = \lambda_n, \\ &\text{(iv)}\ \tau_{n+1} = \tau_n - 1, \end{aligned} \tag{2}$$

and the constrained set $\mathcal{K}$ and the target $\mathcal{C}$ defined by

$$\mathcal{K} := \mathcal{E}p(V) \times \mathbb{R}_+ \times \mathbb{R}_+ \quad \text{and} \quad \mathcal{C} := \text{Graph}(V) \times \mathbb{R}_+ \times \{0\}.$$

Then one can prove as in the continuous time case that

$$\vec{\mathbf{P}}_V(\lambda; N, y) = \{x \in X, \quad \text{such that} \quad (x, y, \lambda, N) \in \text{Capt}_{(2)}(\mathcal{K}, \mathcal{C})\},$$

where the subscript (2) in $\text{Capt}_{(2)}(\mathcal{K}, \mathcal{C})$ refers to the discrete evolutionary system (2).

The capture basin algorithm defines recursively a sequence of subsets $\mathcal{C}_n$ starting at $\mathcal{C}_0$ by

$$\mathcal{C}_{n+1} := \mathcal{K} \cap (\mathcal{C}_n \cup \Psi^{-1}(\mathcal{C}_n)),$$

which converges to the capture basin $\text{Capt}_{(2)}(\mathcal{K}, \mathcal{C})$. ■

One can prove that whenever the discrete map $x \rightsquigarrow \Phi_h(x) := x + hF_h(\lambda; x)$ is a time discretization of the differential inclusion $x'(t) \in F(\lambda; x(t))$, the graph of the discrete well converges to the graph of the well in the Kuratowski–Painlevé sense (see Refs. 26 and 27 and see Ref. 14, among other references).

IV. COMPLETE WELLS

The concept of well we proposed in Definition II.1 is not restrictive enough to match its physical counterpart, in the sense that it does not require that all evolutions starting from a point of a well $\mathbf{P}_V(\lambda;T,y)$ to remain below the rim of the well before time T while one of them at least reaches its rim at time T.

Definition IV.1: Consider an extended function $V:X\mapsto\mathbb{R}\cup\{+\infty\}$ and a differential inclusion

$$\forall t\geqslant 0,\quad x'(t)\in F(\lambda;x(t)).$$

The complete well $\mathbf{W}_V(\lambda;T,y)\subset\mathbf{P}(V;y)$ of duration T and depth y of the function V is defined by the set of initial states $x\in\mathbf{S}(V;y)$ such that

(i) all solutions $x_\lambda(\cdot)\in\mathcal{S}_\lambda(x)$ satisfy

$$\forall t\in[0,T],\quad V(x_\lambda(t))\leqslant y$$

(ii) at least one solution $x_\lambda(\cdot)\in\mathcal{S}_\lambda(x)$ satisfies

$$V(x_\lambda(T))=y.$$

The complete wells can be characterized in terms of absorption and capture basins. (See, for instance, Refs. 3–6.)

Proposition IV.2: Consider an extended function $V:X\mapsto\mathbb{R}\cup\{+\infty\}$ and a differential inclusion

$$\forall t\geqslant 0,\quad x'(t)\in F(\lambda;x(t)).$$

We associate with it the auxiliary system of differential inclusions (1). The constrained set $\mathcal{K}$ and the targets $\mathcal{C}$ and $\mathcal{D}$ are defined by

$$\mathcal{K}:=\mathcal{E}_p(V)\times\mathbb{R}_+\times\mathbb{R}_+ \text{ and } \mathcal{C}:=\mathrm{Graph}(V)\times\mathbb{R}_+\times\{0\}$$

and

$$\mathcal{D}:=\mathcal{E}_p(V)\times\mathbb{R}_+\times\{0\}.$$

Then

$$\mathbf{W}_V(\lambda;T,y)=\{x\in X \text{ such that } (x,y,\lambda,T)\in\mathrm{Capt}_{(1)}(\mathcal{K},\mathcal{C})\cap\mathrm{Abs}_{(1)}(\mathcal{K},\mathcal{D})\}.$$

Proof: Indeed, to say that $(x,y,\lambda,T)\in\mathrm{Capt}_{(1)}(\mathcal{K},\mathcal{C})\cap\mathrm{Abs}_{(1)}(\mathcal{K},\mathcal{D})$ amounts to saying the following:

(1) $(x,y,\lambda,T)\in\mathrm{Capt}_{(1)}(\mathcal{K},\mathcal{C})$, and thus, as we have seen, that $x\in\mathbf{P}_V(\lambda;T,y)$.

(2) $(x,y,\lambda,T)\in\mathrm{Abs}_{(1)}(\mathcal{K},\mathcal{D})$ means that for all evolutions $x_\lambda(\cdot)\in\mathcal{S}_\lambda(x)$, there exists a time $t^\star\geqslant 0$ such that the associated auxiliary evolutions,

$$t\rightarrow(x(t),y(t);\lambda(t);\pi(t))=(x(t),y,\lambda,T-t),$$

starting from (x,y,λ,T) at $t=0$ reaches the target $\mathcal{D}$ at time $t^\star$ while staying, meanwhile, in $\mathcal{K}$:

$$\text{(i) } (x(t^\star),y,\lambda,T-t^\star)\in\mathcal{D},$$

$$\text{(ii) } \forall\, t\in[0,t^\star],\quad (x(t),\lambda,y,T-t)\in\mathcal{K}.$$

The first condition is equivalent to both equation $t^\star=T$ and inequality $V(x(T))\leqslant y$. The second equation means that for every $t\in[0,T]$, $V(x(t))\leqslant y$.

These are the two properties stating that x belongs to the well $\mathbf{W}_V(\lambda;T,y)$. ■

V. CONCLUSIONS

Our objective in this investigation was to build exploration dynamics of a landscape V associating with a bound λ on the velocities of the exploration mechanism, a duration T, and an altitude y:

(1) The set $\mathbf{P}_V(\lambda;T,y)$ of initial states x below altitude y from which starts at least one evolution climbing the landscape in order to reach the altitude y at exactly the prescribed time T; altitude y might be either a reference level, thus providing access to the depth of the well, or chosen among the values of local maxima of the landscape function, thus providing access to the height of the barriers separating the well from the other ones.

(2) An underlying dynamical system governing the evolutions climbing the wells up to their rims the velocities of the exploration mechanism are consistently chosen among

$$x'(t) \in -\frac{\partial \mathbf{P}_V(\lambda;T-t,y)}{\partial t}.$$

Hence, the exploration mechanism is no longer an external stochastic modification of the gradient equation, but an intrinsic set-valued method involving the time derivative of the well.

This dynamic description of landscape topography has then been reformulated in the framework of viability theory, which provides a constructive algorithm to characterize quantitatively the landscape, built as an intrinsic exploration mechanism of energy landscapes; this mechanism could be either a perturbed gradient method or a universal mechanism independent of the energy function. The more refined notion of complete well, introduced in Sec. IV, allows us to bridge still more our mathematical definitions and exploration with the current landscape paradigm. As discussed in the Introduction (Sec. I B), our results can then be exploited for taxinomic purposes, to investigate phase transitions, to quantify the landscape hierarchical structure. It also proposes an alternative to standard stochastic gradient methods, namely differential inclusions, in modeling dynamics associated with an experimentally determined landscape.

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APPENDIX: ELEMENTS OF VIABILITY THEORY

Let X be a finite-dimensional vector space. A *set-valued map* $F:X \rightsquigarrow X$ associates to any $x \in X$ a subset $F(x) \subset X$. The set-valued map F generates the evolutionary system $\mathcal{S}_F:X \rightsquigarrow \mathcal{C}(0,\infty;X)$ associating with any initial state $x_0 \in X$ the set $\mathcal{S}_F(x_0) \subset \mathcal{C}(0,\infty;X)$ of solutions to *differential inclusion* $x'(t) \in F(x(t))$ starting at x_0. We denote by

$$\mathrm{Graph}(F) := \{(x,y) \in X \times Y | y \in F(x)\} \subset X \times Y,$$

the *graph* of a set-valued map $F:X \rightsquigarrow Y$ and $\mathrm{Dom}(F) := \{x \in X | F(x) \neq \emptyset\}$ its *domain*.

We shall say that a subset $K \subset X$ *is locally viable under* F (or under $\mathcal{S}_F$) if from every $x \in K$ starts *at least one* solution $x(\cdot)$ to the differential inclusion $x' \in F(x)$ *viable in* K on the nonempty interval $[0,T_x[$ in the sense

$$\forall\, t \in [0,T_x[, \quad x(t) \in K,$$

and that K is *viable* if we can take $T_x = +\infty$ for any $x \in K$. Most of the results of viability theory are true whenever we assume that the dynamics are Marchaud:

Definition A.1: We shall say that the set-valued map $F:X \rightsquigarrow Y$ is a Marchaud map if

(i) the graph of F is closed in $X \times Y$,
(ii) the values of $F(x)$ of F are convex subsets of Y,
(iii) the growth of F is linear: $\exists c > 0 \,|\, \forall x \in X,\ \|F(x)\| := \sup_{v \in F(x)} \|v\| \leqslant c(\|x\| + 1)$.

We shall say that F is λ-Lipschitz if (set-valued extension of the standard Lipschitz property)

$$\forall x, x' \in X, \quad F(x) \subset F(x') + \lambda \|x - x'\| B,$$

where B is the unit ball in Y.

We shall also need some other prerequisites from the Viability Theory: among which capture and absorption basins.

Definition A.2: Let $C \subset K \subset X$ be two subsets, C being regarded as a target, K as a constrained set. The subset $\mathrm{Capt}_F(K, C)$ of initial states $x_0 \in K$ such that C is reached in finite time, without leaving K, by at least one solution $x(\cdot) \in \mathcal{S}_F(x_0)$ starting at x_0 is called the viable-capture basin of C in K (the solution might eventually leave K, but only after having reached C). The subset $\mathrm{Abs}_F(K, C)$ of initial states $x_0 \in K$ such that ***all evolutions*** $x(\cdot) \in \mathcal{S}_F(x_0)$ starting at x_0 are viable in K until they reach C in finite time is called the absorption basin of K with target C.

Obviously $\mathrm{Abs}_F(K, C) \subset \mathrm{Capt}_F(K, C)$. We recall the following result (Ref. 7) of bilateral fixed point property:

Theorem A.3: The viable-capture basin $\mathrm{Capt}(K, C)$ of a target C viability being with respect to the constrained set K) is the unique subset D satisfying $C \subset D \subset K$ and

$$D = \mathrm{Capt}_F(K, D) = \mathrm{Capt}_F(D, C)$$

and the absorption basin of K with target C is the unique subset A satisfying $C \subset A \subset K$ and

$$A = \mathrm{Abs}_F(A, C) = \mathrm{Abs}_F(K, A).$$

We also recall backward invariance:

Definition A.4: The subset K is locally backward invariant under F if for every $t_0 \in]0, +\infty[$, $x \in K$, for all solutions $x(\cdot)$ to the differential inclusion $x' \in F(x)$ arriving at x at time t_0, there exists a time $s \in [0, t_0[$ (depending on the solution) such that $x(\cdot)$ is viable in K on the interval $[s, t_0]$. The subset K is backward invariant under F if we can take $s = 0$ for all solutions.

It is straightforward to check that backward evolutions $\theta \to z(\theta) = x(t_0 - \theta)$ are solutions of the differential inclusion $z'(\theta) \in -F(z(\theta))$ with initial condition $z(0) = x(t_0)$; we call them *backward solutions* (starting from $x(t_0)$ at time $\theta = 0$). It is noted that the (local) backward invariance of K is stronger than (local) viability of K under this backward evolution, since *all* solutions starting in a backward invariant subset K remain in K for a finite time (depending on each considered solution in case of the local version of the property), whereas the (local) viability of K only requires that for each point $x \in K$, at least *one* solution is (locally) viable in K.

We also introduce a weaker notion: A subset $D \subset K$ is *locally backward invariant relatively* to K if all backward solutions starting from D and viable in K (i.e. remaining in K for a finite time) are actually viable in D (i.e., remain in D for a finite time).

Definition A.5: A subset $R \subset X$ is a repeller under F if all solutions starting from R leave R in finite time.

Hence, R is not viable, but this does not exclude local viability. It is, moreover, obvious that any subset of a repeller is itself a repeller.

We can derive the following characterization of capture basin (see Ref. 4):

Theorem A.6: Let us assume that F is Marchaud and that the subsets $C \subset K$ and K are closed. If $K \backslash C$ is a repeller (this is for instance the case when K itself is a repeller), then the viable-capture basin $\mathrm{Capt}_F(K, C)$ of the target C under F is the unique closed subset D satisfying $C \subset D \subset K$ and[34]

(i) $D \backslash C$ is locally viable under F,
(ii) D is locally backward invariant relatively to K.

Definition A.7: The contingent cone $T_L(x)$ to $L \subset X$ at $x \in L$ is the set (obviously a closed cone)

of directions $v \in X$ such that there exist sequences $h_n > 0$ converging to 0 and v_n converging to v satisfying $x + h_n v_n \in L$ for every n (see, for instance, Ref. 9).

For instance, if L is a differentiable manifold in X, $T_L(x)$ coincides with the tangent space to L at point x. If the interior of L is nonempty, then $T_L(x) = X$ for any $x \in \mathrm{Int}(L)$.

We introduce the following Frankowska property that we need for deriving the system of Hamilton–Jacobi–Bellman equations of which the well is a solution:

Definition A.8: Let us consider a set-valued map $F: X \rightsquigarrow X$ and two subsets $C \subset K$ and K. We shall say that a subset D between C and K (i.e., $C \subset D \subset K$) satisfies the Frankowska property with respect to F if

$$\text{(i)} \quad \forall\, x \in D \setminus C, \quad F(x) \cap T_D(x) \neq \emptyset,$$

$$\text{(ii)} \quad \forall\, x \in D \text{ such that (Ref. 35) } -F(x) \cap T_K(x) \neq \emptyset \text{ then } -F(x) \subset T_D(x). \tag{A1}$$

When K is assumed further to be locally backward invariant (then $-F(x) \subset T_K(x)$ for any $x \in K$) the above conditions (A1) boil down to

$$\text{(i)} \quad \forall\, x \in D \setminus C, \quad F(x) \cap T_D(x) \neq \emptyset,$$

$$\text{(ii)} \quad \forall\, x \in D, \quad -F(x) \subset T_D(x) \tag{A2}$$

[The minus sign in front of F arises when considering backward evolution, governed by the differential inclusion, $z'(\theta) \in -F(z(\theta))$.]

Theorem A.6 and the Viability[36] and Invariance Theorems imply

Theorem A.9: Let us assume that F is Marchaud, that K and $C \subset K$ are closed subsets, and that $K \setminus C$ is a repeller. Then the capture basin $\mathrm{Capt}_F(K, C)$ is

(1) the largest closed subset D satisfying $C \subset D \subset K$ and

$$\forall x \in D \setminus C, \quad F(x) \cap T_D(x) \neq \emptyset. \tag{A3}$$

Furthermore, the evolutions $x(\cdot) \in \mathcal{S}_F(x)$ viable in K until they reach C are governed by the differential inclusion

$$x'(t) \in F(x(t)) \cap T_D(x(t)).$$

(It roughly means that these trajectories point into D or are taugent to D at any point where they reach the boundary of D, thus ensuring their viability until they reach C.)

(2) if F is Lipschitz, the unique closed subset D satisfying the Frankowska property (A1).

The absorption basin $\mathrm{Abs}_F(K, C)$ is the largest closed subset D satisfying $C \subset D \subset K$ and

$$\forall x \in D \setminus C, \quad F(x) \subset T_D(x). \tag{A4}$$

We shall apply Theorem A.9 to the case when subsets $K := \mathrm{Graph}(F)$ and $C := \mathrm{Graph}(H)$ are graphs of set-valued maps from X to X and when we decide to regard D as the graph of a set-valued map $G: \mathbb{R} \times X \rightsquigarrow Y$. We then interpret the contingent cone to the graph as the graph of the contingent derivative. We obtain set-valued solutions to systems of Hamilton–Jacobi inclusions that this unknown function G should satisfy in order that its graph yields the desired capture basin. We refer to Refs. 5 and 6, Ref. 12, and their references for more details on this topic. Here, we recall the definition of contingent derivative of a set-valued map and translate Theorem A.9 in the framework of wells.

Definition A.10: Let us consider a set-valued map $G: \mathbb{R} \times X \rightsquigarrow Y$. The graph of the contingent derivative $DG(t, x, y)$ (a set-valued map defined from $\mathbf{R} \times X$ to Y) at a point $(t, x, y) \in \mathrm{Graph}(G)$ is equal to the contingent cone to the graph of G at (t, x, y):

$$T_{\mathrm{Graph}(G)}(t, x, y) = \mathrm{Graph}(DG(t, x, y)).$$

Consequently, to say that $w \in Y$ belongs to the contingent derivative $DG(t,x,y)(\pm 1,v)$ of G at (t,x,y) in the direction $(\pm 1,v) \in \mathbf{R} \times X$ means that

$$\liminf_{h \to 0+, v' \to v} d\left(w, \frac{G(t \pm h, x + hv') - y}{h}\right) = 0,$$

where d is any distance in Y. Since the contingent cone is a closed subset, the graph of a contingent derivative is always closed and positively homogeneous (this is what remains of the required linearity of the derivative in classical analysis, but, fortunately, we can survive pretty well without linearity).

When $g: \mathbf{R} \times X \mapsto Y$ is single-valued, we set $Dg(t,x) := Dg(t,x,g(t,x))$. We see at once that $Dg(t,x)(\pm 1,v) = \pm \partial g(t,x)/\partial t + \partial g(t,x)/\partial x \cdot v$ whenever g is differentiable at (t,x). The above definition (A.10) generalizes to set-valued maps a property obviously valid for differentiable maps, hence provides a consistent extension of the differentiation to set-valued maps, coinciding with the plain notion for smooth single-valued maps. Moreover, it is to note that when g is Lipschitz on a neighborhood of (t,x) and when the dimension of X is finite, the domain of $Dg(t,x)$ is not empty. Furthermore, the Rademacher Theorem stating that a locally Lipschitz single-valued map is almost everywhere differentiable implies that $x \rightsquigarrow Dg(t,x)$ is almost everywhere single valued. However, in this case, equality $Dg(t,x)(-1,-v) = -Dg(t,x)(1,v)$ is not true in general. We refer to Ref. 9 for more details.

Remark: This is how Fermat defined in 1637 the derivative of a function as the slope of the tangent to its graph. Leibniz and Newton provided the characterization in terms of limits of difference quotients. Here, too, *the graph of the contingent derivative* $DG(t,x,y)$ *is the upper Painlevé–Kuratowski limit of the graphs of difference quotients* $\nabla_h G(t,x,y)$ of G at $(t,x,y) \in \mathrm{Graph}(G)$, defined by

$$(\lambda, v) \mapsto \nabla_h G(t,x,y)(\lambda, v) := \frac{G(t + \lambda h, x + hv) - y}{h}.$$

Indeed, we observe that

$$\mathrm{Graph}(\nabla_h G(t,x,y)) = \frac{\mathrm{Graph}(G) - (t,x,y)}{h} (\subset \mathbf{R} \times X \times Y),$$

so that the contingent cone to the graph of G, being the upper limit of the graphs of the difference quotients, is equal by definition to the graph of the upper graphical limit of the difference quotients.

The strong requirement of pointwise convergence of differential quotients involved in the usual derivatives can be weakened in (at least) two ways, each way sacrificing different groups of properties of these usual derivatives.

(i) *Distributional derivatives:* Fix the direction v and take the limit of the function $x \mapsto \nabla_h g(x)(v)$ in the weaker sense of distributions. The limit $D_v g$ may then be a distribution, and no longer a single-valued map. However, it coincides with the usual limit $(D_v g(x) = Dg(x) \cdot v)$ when g is Gâteaux differentiable. Moreover, one can define difference quotients of distributions, take their limit, and thus, differentiate distributions.
Distributions are no longer functions or maps defined on $\mathbf{R}^n$, so these distributional derivatives lose the pointwise character of functions and maps; on the other hand, this generalization retains the linearity of the operator $g \mapsto D_v g$, mandatory for using the theory of linear operator for solving partial differential equations.

(ii) *Graphical derivatives:* Fix the point x and take the limit of the function $v \mapsto \nabla_h g(x)(v)$ in the weaker sense of graphical convergence (the graph of the graphical limit being by definition the Painlevé–Kuratowski upper limit of the graphs). The limit $Dg(x)$ may then be a set-valued map, and no longer a single-valued map. However, it coincides with the usual limit when g is Gâteaux differentiable. Moreover, one can define difference quotients of

set-valued maps, take their graphical limit, and thus differentiate set-valued maps. These graphical derivatives keep the pointwise character of functions and maps, mandatory for implementing the Fermat Rule, proving inverse function theorems under constraints or using Lyapunov functions, for instance, but lose the linearity of the map $g \mapsto Dg(x)$.

In both cases, the approaches are similar: They use (different) convergences *weaker than the pointwise convergence* for increasing the possibility for the difference quotients to converge. But the price to pay is the loss of some properties by passing to these weaker limits (the pointwise character for distributional derivatives, the linearity of the differential operator for graphical derivatives). ■

Proposition II.2 related the graph of the well to the capture basin $P_v(\lambda;T,y) = \{x \in X \text{ such that } (x,y,\lambda,T) \in \text{Capt}_1(\mathcal{KC})\}$ under system (A1):

$$\begin{aligned} &\text{(i) } x'(t) \in F(\lambda(t);x(t)),\\ &\text{(ii) } y'(t) = 0,\\ &\text{(iii) } \lambda'(t) = 0,\\ &\text{(iv) } \tau'(t) = -1. \end{aligned} \tag{A1'}$$

At this point, we need to introduce the concepts of epigraph and epiderivative of extended numerical functions:

Definition A.11: Let $V: X \mapsto \mathbb{R} \cup \{+\infty\}$ be an extended function. Its epigraph $\mathcal{E}p(V)$ is the set of pairs $(x,y) \in X \times \mathbb{R}$ satisfying $V(x) \leqslant y$ [thus $\mathcal{E}p(V) \subset X \times \mathbf{R}$]. The contingent epiderivative $D_\uparrow V(x): X \mapsto \overline{\mathbb{R}}$ is defined through the relation

$$\mathcal{E}p(D_\uparrow V(x)) := T_{\mathcal{E}p(V)}(x, V(x)).$$

We can check that $D_\uparrow V(x)$ consistently coincide with the usual derivative $DV(x)$ when V is differentiable in x, and that for any $v \in X$,

$$D_\uparrow V(x)(v) = \liminf_{h \to 0+, v' \to v} \frac{V(x+hv') - V(x)}{h}$$

is a generalized limit of differential quotients.

We deduce from Proposition II.2 and Theorem A.9 the following characterization of the well as the unique solution to an initial-value problem of a partial differential inclusion satisfying viability constraints:

Theorem A.12: Assume that the set-valued map F is Marchaud and that the function V is continuous. Then the well $\mathbf{P}_V: \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R} \rightsquigarrow X$ is the largest set-valued map $\mathbf{P}: \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R} \rightsquigarrow X$ solution to the partial differential inclusion

$$\forall x \in \mathbf{P}(\lambda;T,y), \quad F(\lambda;x) \cap D\mathbf{P}(\lambda;T,y,x)(0,-1,0) \neq \emptyset$$

the initial condition

$$\mathbf{P}(\lambda;0,y) = \mathbf{S}_0(V,y)$$

and the viability constraint

$$\mathbf{P}(\lambda;T,y) \subset \mathbf{S}(V,y).$$

Furthermore, if F is Lipschitz, this solution is the unique solution satisfying

(i) $\forall x \in \mathbf{P}(\lambda;T,y)$, $F(\lambda;x) \cap D\mathbf{P}(\lambda;T,y,x)(0,-1,0) \neq \emptyset$,

(ii) $\forall x \in \mathbf{P}(\lambda;T,y)$ such that $\inf_{v \in F(\lambda;x)} D_{\uparrow}V(x)(-v) \leqslant 0$ then $-F(\lambda;x) \subset D\mathbf{P}(\lambda;T,y,x)(0,+1,0)$.

Proof: Theorem A.9 implies that the graph of the well $\mathbf{P}_V : \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R} \rightsquigarrow X$, once transformed by the permutation $(\lambda,\tau,y,x) \to (x,y,\lambda,\tau)$ of the coordinates, is the largest subset $\mathcal{D}$ between $\mathcal{C}$ and $\mathcal{K}$ (i.e., $\mathcal{C} \subset \mathcal{D} \subset \mathcal{K} \subset X \times \mathbb{R} \times \mathbb{R}_+ \times \mathbb{R}_+$), such that

$$\forall (x,y,\lambda,\tau), \quad (F(\lambda;x) \times \{0\} \times \{0\} \times \{-1\}) \cap T_{\mathcal{D}}(x,y,\lambda,\tau) \neq \emptyset.$$

This amounts to saying that the well $\mathbf{P}_V$ is the largest set-valued map $\mathbf{P}$ satisfying the initial condition $\mathbf{P}(\lambda;0,y) = \mathbf{S}_0(V,y)$, the constraint $\mathbf{P}(\lambda;T,y) \subset \mathbf{S}(V,y)$, and the contingent solution to the partial differential inclusion,

$$\forall x \in \mathbf{P}(\lambda;T,y), \quad F(\lambda;x) \cap D\mathbf{P}(\lambda;T,y,x)(0,-1,0) \neq \emptyset,$$

and that the evolutions $[t \mapsto (\lambda, T-t, y, x(t))]$ viable in the well until they reach its rim are governed by the differential inclusion

$$(0,-1,0,x'(t)) \in (\{0\} \times \{-1\} \times \{0\} \times F(\lambda;x(t))) \cap \mathrm{Graph}(D\mathbf{P}_V(\lambda;T-t,y,x(t))(0,-1,0)).$$

This can be written as

$$x'(t) \in F(\lambda;x(t)) \cap D\mathbf{P}_V(\lambda;T-t,y,x(t))(0,-1,0).$$

This is what we meant symbolically above as

$$x'(t) \in F(\lambda;x(t)) \cap -\frac{\partial \mathbf{P}_V(\lambda;T-t,y)}{\partial t}.$$

When F is Lipschitz [this is the case when $F(\lambda;x) := \lambda B$ (where B is the unit ball in X)], the graph of the well $\mathbf{P}_V$ (after permutation of the coordinates as above) is the unique subset $\mathcal{D}$, satisfying

$$\forall (x,y,\lambda,\tau), \quad (F(\lambda;x) \times \{0\} \times \{0\} \times \{-1\}) \cap T_{\mathcal{D}}(x,y,\lambda,\tau) \neq \emptyset,$$

and, whenever $(-F(\lambda;x) \times \{0\} \times \{0\} \times \{+1\}) \cap T_{\mathcal{K}}(x,y,\lambda,\tau) \neq \emptyset$, then

$$(-F(\lambda;x) \times \{0\} \times \{0\} \times \{+1\}) \subset T_{\mathcal{D}}(x,y,\lambda,\tau).$$

Thanks to the definition of the contingent epiderivative and the fact that $\mathcal{K} := \mathcal{E}p(V) \times \mathbb{R}_+ \times \mathbb{R}_+$, we infer that

$$(-v,0,0,+1) \in T_{\mathcal{D}}(x,y,\lambda,\tau),$$

if and only if $D_{\uparrow}V(x)(-v) \leqslant 0$. This concludes the proof. ■

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[30] We call V an "extended function" in the sense that it can take the value $+\infty$. This allows us to encapsulate state constraints $x \in K$ [where K is the subset of "viable" (acceptable, feasible) states] in the definition of the extended function, equal to $+\infty$ outside K. A well-known example in physics is hard-core interaction potential.
[31] Care has to be taken not to confuse exploration mechanism (valid whatever the interpretation of V is) and actual evolution (whose modeling is indissociable from the status and definition of V). We here mainly consider exploration dynamics. Only at the end of the paper, it is suggested that the intrinsic exploration mechanism determined in Sec. III could be a relevant alternative to stochastic gradient dynamics for modeling actual dynamic features of the system.
[32] or, if needed, all evolutions.
[33] At odds with stochastic models currently used in physics, differential inclusions provide another way to translate uncertainty in mathematical terms. A full corpus of results have been steadily accumulated since their introduction in the early 1930s by Marchaud and Zaremba, and next, by the Polish and Russian schools, around Ważewski and Filippov, who laid the foundations of the mathematical theory of differential inclusions after the 1950s. The confrontation of evolutions governed by differential inclusion and viability constraints for reaching targets in finite time began in the early 1980s to provide regulation maps and feedbacks. Their use for translating mathematically uncertainty "against nature" as an alternative to stochastic differential equations began at the same period, but is taking a new start when it was realized recently that they yield much more general results than the stochastic paradigm: Differential inclusions allow us to represent uncertainty by state-dependent maps. As a name needed to refer to such a viewpoint and to underline its difference with stochastic differential equations, we called these *tychastic systems* when the velocities depend upon both the state and a parameter that is called "tyche" [meaning "chance" in classical Greek, from the Goddess Tyche of (good and bad) fortune], which play the role of perturbations or disturbances on which actors and decision makers have no control. Tyches could in fact have been more plainly called "random variables" if this vocabulary were not already confiscated by probabilists. This is why we borrow the term of *tychastic evolution* to the American philosopher Charles Peirce who introduced it in a paper published in 1893 *under the title "Evolutionary love:" "Three modes of evolution have thus been brought before us: evolution by fortuitous variation, evolution by mechanical necessity, and evolution by creative love. We may term them tychastic evolution, or tychasm, anancastic evolution, or anancasm, and agapastic evolution, or agapasm.*
[34] The subset $K \backslash C$ denotes the intersection of K and the complement of C, i.e., is the set of elements of K that do not belong to C.
[35] This is always satisfied when $x \in \mathrm{Int}(K)$.
[36] See for instance Theorems 3.2.4, 3.3.2 and 3.5.2 of Ref. 3.

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Partial fractions expansions and identities for products of Bessel functions

Mathew D. Rogers
Department of Mathematics, University of British Columbia, Vancouver, BC, Canada V6T-1Z2

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We derive several partial fractions expansions for products of Bessel functions, and use them to prove algebraic relationships between infinite series involving squares of Bessel functions. We also give formulas for the Taylor series coefficients of the zeros of Bessel functions, when the zeros are regarded as functions of the order x of $J_x(y)$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1866222]

I. INTRODUCTION

In this paper we derive several partial fractions expansions for products of Bessel functions, the simplest of which is given by

$$J_x(y)J_{-x}(y)\frac{\pi}{\sin(\pi x)} = \sum_{n=-\infty}^{\infty} \frac{J_n^2(y)}{n+x}.$$

These formulas, which are presented in Sec. II, allow us to easily characterize $J_x(y)J_{-x}(y)$ as a function of x. Surprisingly, these sorts of identities are generally overlooked in the modern literature on Bessel functions.

We can apply these formulas to study the zeros of Bessel functions. Let $\nu_k(x)$ denote the kth zero of $J_x(y)$. In Sec. IV we recursively compute the Taylor series coefficients of $\nu_k(x)$ at the half-integers. In Sec. V we discuss computing the Taylor series at zero and the positive integers. The form that we give for the coefficients is interesting because they are expressed as polynomials in functions defined by series of squares of Bessel functions.

Besides appearing in the Taylor series coefficients of $\nu_k(x)$, functions like

$$\mu_k(y) = \sum_{n=1}^{\infty} \frac{J_n^2(y)}{n^k}, \quad \beta_k(y) = \sum_{n=-\infty}^{\infty} \frac{J_n^2(y)}{(2n+1)^k},$$

obey a bewildering variety of identities and algebraic relations. In Secs. IV, V, and VII we prove many interesting formulas involving these functions. We also present several associated open problems at the end of Secs. IV–VI.

Throughout this paper we will assume the usual differentiation and addition formulas for Bessel functions,

$$2\frac{x}{y}J_x(y) = J_{x-1}(y) + J_{x+1}(y),$$

$$2\frac{d}{dy}J_x(y) = J_{x-1}(y) - J_{x+1}(y).$$

We will also employ a standard Wronskian relation,

$$J_{x-1}(y)J_{-x}(y) + J_{1-x}(y)J_x(y) = \frac{2\sin(\pi x)}{\pi y}.$$

II. IDENTITIES AND PARTIAL FRACTIONS EXPANSIONS FOR BESSEL FUNCTIONS

The Bessel function of the first kind of order x is defined by the infinite series

$$J_x(y) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\Gamma(n+x+1)}\left(\frac{y}{2}\right)^{2n+x}, \tag{2.1}$$

where $\Gamma(x)$ is the usual gamma function.

We will use the following three partial fractions expansions throughout this paper.

Proposition 2.1: The following formulas hold for all $y \in \mathbf{C}$ and for all $x \notin \mathbf{Z}$,

$$J_x(y) = \frac{\left(\frac{y}{2}\right)^x}{\Gamma(x)} \sum_{n=0}^{\infty} \frac{J_n(y)}{n!} \frac{\left(\frac{y}{2}\right)^n}{n+x}, \tag{2.2}$$

$$J_x(y)J_{-x}(y)\frac{\pi}{\sin(\pi x)} = \sum_{n=-\infty}^{\infty} \frac{J_n^2(y)}{n+x}, \tag{2.3}$$

$$J_x(y)J_{1-x}(y)\frac{\pi}{\sin(\pi x)} = \sum_{n=-\infty}^{\infty} \frac{J_n(y)J_{n+1}(y)}{n+x}. \tag{2.4}$$

Equation (2.2) has a long history. It appears in several 19th century and 20th century books, including Lommel,[2] Schafheitlin,[4] and Watson (Ref. 5, p.143). From (2.2) one can easily derive Lommel's expression for $Y_0(z)$,

$$Y_0(z) = \frac{2}{\pi}(\log(z/2) + \gamma)J_0(z) + \frac{2}{\pi}\sum_{n=1}^{\infty} \frac{J_n(z)}{n!} \frac{\left(\frac{z}{2}\right)^n}{n}. \tag{2.5}$$

The function $Y_0(z)$ is a Bessel function of the second kind (Ref. 5, p.64).

Equations (2.3) and (2.4) seem to be omitted from the modern literature, as well as all of the easily accessible 19th century books. Considering their relative simplicity, it seems unlikely that 19th century mathematicians would have missed them. In fact, the following integral (Ref. 1, p.756)

$$\int_0^{\pi/2} \cos(2xu)J_0(2y\cos(u))\mathrm{d}u = \frac{\pi}{2}J_x(y)J_{-x}(y) \tag{2.6}$$

is exactly equivalent to Eq. (2.3).

We have found a particularly simple way to prove formulas (2.3) and (2.4) that is worth relating.

Proof: Lommel proves Eq. (2.2) in Ref. 2. We can also prove this result by applying the following elementary partial fractions expansion to Eq. (2.1):

$$\frac{n!}{x(x+1)(x+2)\cdots(x+n)} = \sum_{j=0}^{n} \frac{(-1)^j}{j+x}\binom{n}{j}.$$

To prove Eq. (2.4) we will use the reflection formula for the gamma function,

$$\Gamma(x)\Gamma(1-x)=\frac{\pi}{\sin(\pi x)},$$

and we will apply formula (2.2) several times. Proceeding with the proof,

$$J_x(y)J_{1-x}(y)\frac{\pi}{\sin(\pi x)}=(J_x(y)\Gamma(x))(J_{1-x}(y)\Gamma(1-x))=\left(\sum_{n=0}^{\infty}\frac{J_n(y)}{n!}\frac{\left(\frac{y}{2}\right)^{n+x}}{n+x}\right)\left(\sum_{m=0}^{\infty}\frac{J_m(y)}{m!}\frac{\left(\frac{y}{2}\right)^{m+1-x}}{m+1-x}\right)$$

$$=\sum_{n\geqslant 0,m\geqslant 0}^{\infty}\frac{J_n(y)J_m(y)}{n!m!}\frac{\left(\frac{y}{2}\right)^{n+m+1}}{(n+x)(m+1-x)}$$

$$=\sum_{n\geqslant 0,m\geqslant 0}^{\infty}\frac{J_n(y)J_m(y)}{n!m!}\frac{\left(\frac{y}{2}\right)^{n+m+1}}{n+m+1}\left(\frac{1}{n+x}+\frac{1}{m+1-x}\right).$$

Next split the sum into two pieces, then rearrange the order of summation to get

$$=\sum_{n=0}^{\infty}\frac{J_n(y)}{n!(n+x)}\left(\sum_{m=0}^{\infty}\frac{J_m(y)}{m!}\frac{\left(\frac{y}{2}\right)^{n+m+1}}{n+m+1}\right)+\sum_{m=0}^{\infty}\frac{J_m(y)}{m!(m+1-x)}\left(\sum_{n=0}^{\infty}\frac{J_n(y)}{n!}\frac{\left(\frac{y}{2}\right)^{n+m+1}}{n+m+1}\right).$$

Observe that the two nested sums in the preceding equation are just special cases of Eq. (2.2). Substituting the appropriate expressions we have

$$=\sum_{n=0}^{\infty}\frac{J_n(y)}{n!(n+x)}\Gamma(n+1)J_{n+1}(y)+\sum_{m=0}^{\infty}\frac{J_m(y)}{m!(m+1-x)}\Gamma(m+1)J_{m+1}(y)$$

$$=\sum_{n=0}^{\infty}\frac{J_n(y)J_{n+1}(y)}{n+x}+\sum_{m=0}^{\infty}\frac{J_m(y)J_{m+1}(y)}{m+1-x}.$$

Now let $m+1=-n$, and change the indices of summation on the right-hand sum to get

$$=\sum_{n=0}^{\infty}\frac{J_n(y)J_{n+1}(y)}{n+x}+\sum_{n=-1}^{-\infty}\frac{J_{-n-1}(y)J_{-n}(y)}{-n-x}.$$

Finally, recall that if $m\in\mathbf{Z}$ then $J_{-m}(y)=(-1)^m J_m(y)$. Substituting this relation into the preceding equation yields

$$=\sum_{n=0}^{\infty}\frac{J_n(y)J_{n+1}(y)}{n+x}+\sum_{n=-1}^{-\infty}\frac{J_n(y)J_{n+1}(y)}{n+x}=\sum_{n=-\infty}^{\infty}\frac{J_n(y)J_{n+1}(y)}{n+x},$$

completing the proof of (2.4).

The proof of Eq. (2.3) is nearly identical to the above proof, except that slightly more care must be taken when combining the partial fractions expansions for $J_x(y)$ and $J_{-x}(y)$. ■

Proposition 2.2: The infinite sums appearing in Proposition 2.1 are related as follows:

$$\left(\sum_{n=-\infty}^{\infty}\frac{J_n^2(y)}{n+x}\right)\left(\sum_{n=-\infty}^{\infty}\frac{J_n^2(y)}{n+1-x}\right)=\frac{2}{y}\left(\sum_{n=-\infty}^{\infty}\frac{J_n(y)J_{n+1}(y)}{n+x}\right)-\left(\sum_{n=-\infty}^{\infty}\frac{J_n(y)J_{n+1}(y)}{n+x}\right)^2,\qquad(2.7)$$

$$\sum_{n=-\infty}^{\infty} \frac{J_n(y)J_{n+1}(y)}{n+x} = \sum_{n=-\infty}^{\infty} \frac{J_n(y)J_{n+1}(y)}{n+1-x}, \tag{2.8}$$

$$\left(\sum_{n=0}^{\infty} \frac{J_n(y)}{n!}\frac{\left(\frac{y}{2}\right)^n}{n+x}\right)\left(\sum_{n=0}^{\infty} \frac{J_n(y)}{n!}\frac{\left(\frac{y}{2}\right)^{n+1}}{n+1-x}\right) = \sum_{n=-\infty}^{\infty} \frac{J_n(y)J_{n+1}(y)}{n+x}, \tag{2.9}$$

$$\left(\sum_{n=0}^{\infty} \frac{J_n(y)}{n!}\frac{\left(\frac{y}{2}\right)^n}{n+x}\right)\left(\sum_{n=0}^{\infty} \frac{J_n(y)}{n!}\frac{\left(\frac{y}{2}\right)^n}{n-x}\right) = \frac{-1}{x}\sum_{n=-\infty}^{\infty} \frac{J_n^2(y)}{n+x}. \tag{2.10}$$

Proof: Equations (2.8)–(2.10) follow trivially from Proposition 2.1.

Equation (2.7) is a simple consequence of the Wronskian relation for Bessel functions,

$$J_{x-1}(y)J_{-x}(y) + J_{1-x}(y)J_x(y) = \frac{2\sin(\pi x)}{\pi y}.$$

We will prove (2.7) as follows. Observe from Proposition 2.1 that the left-hand side (LHS) of Eq. (2.7) is given by

$$\text{LHS} = J_x(y)J_{1-x}(y)J_{x-1}(y)J_{-x}(y)\left(\frac{\pi}{\sin(\pi x)}\right)^2,$$

and the right-hand side (RHS) is given by

$$\text{RHS} = J_x(y)J_{1-x}(y)\left(\frac{\pi}{\sin(\pi x)}\right)^2\left(\frac{2\sin(\pi x)}{\pi y} - J_x(y)J_{1-x}(y)\right).$$

Apply the Wronskian relation to the RHS to see that LHS=RHS, which establishes (2.7). ■

Of course these are not the only partial fractions expansions available for Bessel functions. There are multitudes of ways to generalize these results. We state several generalizations in the next proposition.

Proposition 2.3: If x, y, and z are complex numbers such that $x \notin \mathbf{Z}$, *then*

$$\frac{\pi}{\sin(\pi x)}J_{z-x}(y)J_{x-z}(y) = \sum_{n=-\infty}^{\infty} (-1)^n \frac{J_{z+n}(y)J_{-z-n}(y)}{x+n}, \tag{2.11}$$

$$\frac{\pi}{\sin(\pi x)}J_x(y)J_{-x}(z) = \sum_{n=-\infty}^{\infty} \frac{J_n(y)J_n(z)}{n+x}\left(\frac{y}{z}\right)^{n+x}, \tag{2.12}$$

$$\frac{\pi}{\sin(\pi x)}J_x(y)J_{1-x}(z) = \sum_{n=-\infty}^{\infty} \frac{J_n(y)J_{n+1}(z)}{n+x}\left(\frac{y}{z}\right)^{n+x}. \tag{2.13}$$

Suppose that $x_1+x_2+x_3=1$, *then*

$$J_{x_1}(y)J_{x_2}(y)J_{x_3}(y)\Gamma(x_1)\Gamma(x_2)\Gamma(x_3) = \sum_{n\geq 0, m\geq 0} J_n(y)J_m(y)J_{n+m+1}(y)\binom{n+m}{m}\left(\frac{1}{(n+x_1)(m+x_2)} + \frac{1}{(n+x_1)(m+x_3)} + \frac{1}{(n+x_2)(m+x_3)}\right). \tag{2.14}$$

Letting $x_1=x_2=x_3=\frac{1}{3}$ in Eq. (2.14) yields an interesting double series for $(J_{1/3}(y))^3$,

$$(J_{1/3}(y))^3 = \frac{1}{\Gamma^3(4/3)} \sum_{n\geqslant 0, m\geqslant 0}^{\infty} \frac{J_n(y)J_m(y)J_{n+m+1}(y)}{(3n+1)(3m+1)} \binom{n+m}{m}. \tag{2.15}$$

III. PROPERTIES OF THE FUNCTION $\nu_k(x)$

We will give a brief description of the function $\nu_k(x)$, and then prove a new form for the differential equation that $\nu_k(x)$ satisfies. Throughout this section we will assume that $x \in \mathbf{R}$.

It is well known that $J_x(y)$ has infinitely many real zeros, and a finite number of complex zeros. We can regard the zeros of $J_x(y)$ as functions of the order x.

Definition 3.1: Let $\nu_k(x)$ *denote the* kth *real zero of* $J_x(y)$ *to the right of* x. *Then* $J_x(\nu_k(x)) = 0$ *for all* x.

It can be shown that $\nu_k(x)$ is continuous and differentiable for all $x \in \mathbf{R}\backslash\{-1,-2,\ldots\}$. In fact, it is well known that $\nu_k(x)$ satisfies transcendental differential equations. Nicholson's differential equation (Ref. 5, p. 508) is given by

$$\nu_k'(x) = -2\nu_k(x)\int_0^{\infty} K_0(2\nu_k(x)\sinh(t))e^{-2xt}\,dt, \tag{3.1}$$

and is valid provided that $x \notin \{-1,-2,\ldots\}$. The negative integers must be excluded from the domain of $\nu_k(x)$, because $\nu_k(x)$ is discontinuous at each of these points. These discontinuities occur because new solution curves of $J_x(y)=0$ come into existence when $x \in \{-1,-2,\ldots\}$. Watson provides a nice illustration (Ref. 5, p. 510) of this phenomenon.

The form of the differential equation that we are interested in follows almost directly from formula (2.3). Proposition 3.2 will allow us to express derivatives of $\nu_k(x)$ in terms of infinite series that obey interesting algebraic relations [see Theorem 4.7 and Eq. (4.24)].

Proposition 3.2: If $x \notin \{-1,-2,\ldots\}$, *then* $\nu_k(x)$ *satisfies the differential equation*

$$\nu_k'(x) = \frac{\nu_k(x)}{2} \sum_{n=-\infty}^{\infty} \frac{J_n^2(\nu_k(x))}{(n+x)^2}. \tag{3.2}$$

Proof: This proof is quite standard (Ref. 5, p. 507). By the definition of $\nu_k(x)$, and by formula (2.3) we have

$$0 = \sum_{n=-\infty}^{\infty} \frac{J_n^2(\nu_k(x))}{n+x}.$$

Now assume that x is not a negative integer, and take the derivative of each side to show that

$$0 = -\sum_{n=-\infty}^{\infty} \frac{J_n^2(\nu_k(x))}{(n+x)^2} + \nu_k'(x)\frac{d}{d\nu}\sum_{n=-\infty}^{\infty} \frac{J_n^2(\nu_k(x))}{(n+x)}.$$

Substituting Eq. (2.3) for the sum on the right-hand side we find that

$$0 = -\sum_{n=-\infty}^{\infty} \frac{J_n^2(\nu_k(x))}{(n+x)^2} + \nu_k'(x)\frac{\pi}{\sin(\pi x)}\frac{d}{d\nu}(J_x(\nu_k(x))J_{-x}(\nu_k(x))). \tag{3.3}$$

Now expand and simplify $d/d\nu(J_x(\nu_k(x))J_{-x}(\nu_k(x)))$ as follows:

$$\frac{\mathrm{d}}{\mathrm{d}\nu}(J_x(\nu_k(x))J_{-x}(\nu_k(x))) = \frac{J_{x-1}(\nu_k(x)) - J_{x+1}(\nu_k(x))}{2}J_{-x}(\nu_k(x)) + J_x(\nu_k(x))\frac{\mathrm{d}}{\mathrm{d}\nu}(J_{-x}(\nu_k(x)))$$

$$= \frac{J_{x-1}(\nu_k(x)) - J_{x+1}(\nu_k(x))}{2}J_{-x}(\nu_k(x)) + 0.$$

If $\nu_k(x) \neq 0$, then the Bessel function addition formula shows that $J_{x+1}(\nu_k(x)) = -J_{x-1}(\nu_k(x))$. Since the only x values for which we may have $\nu_k(x) = 0$ are the negative integers (Ref. 5, p. 510), the initial assumption that $x \notin \{-1, -2, \ldots\}$ satisfies this condition. Therefore we obtain

$$\frac{\mathrm{d}}{\mathrm{d}\nu}(J_x(\nu_k(x))J_{-x}(\nu_k(x))) = J_{x-1}(\nu_k(x))J_{-x}(\nu_k(x)).$$

The Wronskian relation shows that

$$J_{x-1}(\nu_k(x))J_{-x}(\nu_k(x)) = \frac{2\sin(\pi x)}{\pi\nu_k(x)},$$

which allows us to evaluate $(\mathrm{d}/\mathrm{d}\nu)(J_x(\nu_k(x))J_{-x}(\nu_k(x)))$ in a simple form,

$$\frac{\mathrm{d}}{\mathrm{d}\nu}(J_x(\nu_k(x))J_{-x}(\nu_k(x))) = \frac{2\sin(\pi x)}{\pi\nu_k(x)}.$$

Substituting this final result into Eq. (3.3) completes the proof. ■

For more technical results about the zeros of Bessel functions, Muldoon's paper[3] provides an excellent list of references.

IV. THE TAYLOR SERIES FOR $\nu_k(x)$ AT THE HALF-INTEGERS

In this section we will give a recursive formula for computing the derivatives of $\nu_k(x)$ at the half-integers. The resulting Taylor series converge relatively slowly, however the form that we give for the coefficients is very interesting. We show that the Taylor coefficients can always be expressed in terms of polynomials of entire functions. The entire functions in question are defined by summations of reciprocal powers of integers, with squares of Bessel functions in the numerators.

Definition 4.1: Let k be an integer, and define $\beta_k(y)$ and $d_k(y)$ by

$$\beta_k(y) = \sum_{n=-\infty}^{\infty} \frac{J_n^2(y)}{(2n+1)^k},$$

$$d_k(y) = \sum_{n=-\infty}^{\infty} \frac{J_n(y)J_{n+1}(y)}{(2n+1)^k}.$$

Also define the more general function

$$\beta_k^{(a,b)}(y) = \sum_{n=-\infty}^{\infty} \frac{J_{n+a}(y)J_{n+b}(y)}{(2n+1)^k}.$$

Proposition 4.2: The functions $\beta_k(y)$ and $d_k(y)$ have the following elementary properties:

$$\beta_0(y) = 1, \tag{4.1}$$

$$\beta_1(y) = \frac{\sin(2y)}{2y}, \tag{4.2}$$

$$\beta_2(y) = \frac{1}{2y}\int_0^{2y} \frac{\sin(z)}{z} dz, \tag{4.3}$$

$$d_{2k}(y) = 0 \quad \text{if } k \geqslant 0 \text{ is an integer}, \tag{4.4}$$

$$d_1(y) = \frac{1-\cos(2y)}{2y}. \tag{4.5}$$

Since (4.5) will be used later, we note that it follows from (2.4).

As a simple corollary to Proposition 4.2 we can obtain formulas for $1/\pi$. Here are two examples,

$$\frac{1}{\pi} = \frac{1}{2}\sum_{n=-\infty}^{\infty} \frac{J_n^2\left(\frac{\pi}{4}\right)}{2n+1}, \tag{4.6}$$

$$\frac{1}{\pi} = \frac{4}{9}\sum_{n=-\infty}^{\infty} \frac{J_n\left(\frac{\pi}{3}\right)J_{n+1}\left(\frac{\pi}{3}\right)}{2n+1}. \tag{4.7}$$

Proposition 4.3: Let $k \geqslant 1$ be an integer, then $\beta_k^{(a,b)}(y)$ has the following elementary properties for every pair $(a,b) \in \mathbf{Z}^2$:

$$\beta_k^{(a,b)}(y) = \frac{1}{y}\beta_{k-1}^{(a-1,b)}(y) + \frac{2a-3}{y}\beta_k^{(a-1,b)}(y) - \beta_k^{(a-2,b)}(y), \tag{4.8}$$

$$\beta_k^{(a,b)}(y) = \beta_k^{(b,a)}(y), \tag{4.9}$$

$$\beta_0^{(a,b)}(y) = \begin{cases} 1 & \text{if } a = b, \\ 0 & \text{if } a \neq b, \end{cases} \tag{4.10}$$

$$\beta_k^{(0,0)}(y) = \beta_k(y), \tag{4.11}$$

$$\beta_k^{(0,1)}(y) = d_k(y), \tag{4.12}$$

$$\beta_k^{(1,1)}(y) = (-1)^k \beta_k(y). \tag{4.13}$$

Proposition 4.3 establishes linear dependencies between $\beta_k^{(a,b)}(y)$, $\beta_k(y)$, and $d_k(y)$ for all $(a,b) \in \mathbf{Z}^2$. To express $\beta_k^{(a,b)}(y)$ in terms of $d_m(y)$'s and $\beta_m(y)$'s, use the recursion formula (4.8) while applying formula (4.10) as many times as necessary. For example, we can show that

$$\beta_k^{(-1,-1)}(y) = \left(\frac{1}{y^2} + (-1)^k\right)\beta_k(y) - \frac{2}{y^2}\beta_{k-1}(y) + \frac{1}{y^2}\beta_{k-2}(y) - \frac{2}{y}d_{k-1}(y) + \frac{2}{y}d_k(y). \tag{4.14}$$

The next proposition shows that $d_k(y)$ can always be written as a polynomial in $\beta_m(y)$'s for $m \leqslant k$, and the elementary functions. As a result we can always express $\beta_k^{(a,b)}(y)$ as a polynomial in $\beta_2(y), \beta_3(y), \ldots, \beta_k(y)$, and elementary functions.

Proposition 4.4: We can calculate $d_{2n+1}(y)$ recursively using the following formula:

$$\frac{\cos(2y)}{y}d_{2n+1}(y)=\sum_{k=1}^{2n-1}d_{k+1}(y)d_{2n+1-k}(y)+\sum_{k=0}^{2n}(-1)^k\beta_{k+1}(y)\beta_{2n+1-k}(y). \tag{4.15}$$

Proof: We will use Eq. (2.7) to prove this result. First observe that a slight rearrangement of (2.7) yields

$$\left(\sum_{n=-\infty}^{\infty}\frac{J_n^2(y)}{n+x}\right)\left(\sum_{n=-\infty}^{\infty}\frac{J_n^2(y)}{n+1-x}\right)=\frac{1}{y^2}-\left(\frac{1}{y}-\sum_{n=-\infty}^{\infty}\frac{J_n(y)J_{n+1}(y)}{n+x}\right)^2. \tag{4.16}$$

If $|x-\frac{1}{2}|<\frac{1}{2}$, then we can expand each infinite series about $x=1/2$ to obtain

$$\sum_{n=-\infty}^{\infty}\frac{J_n^2(y)}{n+x}=\sum_{k=0}^{\infty}(-1)^k2^{k+1}\beta_{k+1}(y)(x-1/2)^k,$$

$$\sum_{n=-\infty}^{\infty}\frac{J_n^2(y)}{n+1-x}=\sum_{k=0}^{\infty}2^{k+1}\beta_{k+1}(y)(x-1/2)^k,$$

$$\sum_{n=-\infty}^{\infty}\frac{J_n(y)J_{n+1}(y)}{n+x}=\sum_{k=0}^{\infty}2^{2k+1}d_{2k+1}(y)(x-1/2)^{2k}.$$

Substituting these formulas into (4.16), then collecting the series coefficients on each side of the equality proves Eq. (4.15). ■

Applying Proposition 4.4 yields the following evaluations of $d_3(y)$ and $d_5(y)$:

$$d_3(y)=\tan(2y)\beta_3(y)-\frac{y}{\cos(2y)}\beta_2^2(y), \tag{4.17}$$

$$d_5(y)=\tan(2y)\beta_5(y)-\frac{2y}{\cos(2y)}\beta_4(y)\beta_2(y)+\frac{y}{\cos^3(2y)}\beta_3^2(y)-2y^2\frac{\sin(2y)}{\cos^3(2y)}\beta_3(y)\beta_2^2(y)$$
$$+\frac{y^3}{\cos^3(2y)}\beta_2^4(y). \tag{4.18}$$

Now that we have shown how to write $d_k(y)$ and $\beta_k^{(a,b)}(y)$ in terms of $\beta_k(y)$, it is necessary to justify the claim that all of these functions are entire. Considering the fact that formula (4.17) contains multiple terms involving $1/\cos(2y)$, this claim is not obvious.

Theorem 4.5: *The functions $\beta_k(y)$, $d_k(y)$, and $\beta_k^{(a,b)}(y)$ are entire functions for all $k\geqslant 0$, and for all $(a,b)\in\mathbf{Z}^2$.*

Proof: Let $E_k(y)$ denote the kth Euler polynomial. Recall that $E_k(y)$ is a kth degree polynomial with generating function

$$\frac{2e^{yt}}{e^t+1}=\sum_{k=0}^{\infty}E_k(y)\frac{t^k}{k!}.$$

Then for all $k\geqslant 0$, and for all $(a,b)\in\mathbf{Z}^2$, we have the following representation of $\beta_{k+1}^{(a,b)}(y)$:

$$\beta_{k+1}^{(a,b)}(y)=(-1)^a\frac{\pi^k}{k!}\int_0^{\pi/2}\cos\left((a+b-1)z+\frac{\pi k}{2}\right)J_{b-a}(2y\cos z)E_k\left(\frac{1}{2}+\frac{z}{\pi}\right)dz. \tag{4.19}$$

Equation (4.19) expresses $\beta_k^{(a,b)}(y)$ as a finite integral of entire functions, so we conclude that $\beta_k^{(a,b)}(y)$ is entire for all $k \geqslant 1$ and for all $(a,b) \in \mathbf{Z}^2$. The $k=0$ case is clear from Eq. (4.10). This also proves that $\beta_k(y)$ and $d_k(y)$ are entire, since they are just special cases of $\beta_k^{(a,b)}(y)$. Recall that $\beta_k(y) = \beta_k^{(0,0)}(y)$ and $d_k(y) = \beta_k^{(0,1)}(y)$.

The proof of Eq. (4.19) is an exercise that we will leave to the reader. ■

The next proposition shows that $(d/dy)\beta_k(y)$ and $(d/dy)d_k(y)$ are just linear combinations of $d_k(y)$, $\beta_k(y)$, and $\beta_{k-1}(y)$ (with coefficients involving y and $1/y$). While Proposition 4.4 allows us to eliminate the notation $d_k(y)$, the convenience of working with linear differential equations justifies its continued use.

Proposition 4.6: The derivatives of $\beta_k(y)$ and $d_k(y)$ are related as follows:

$$\frac{\mathrm{d}}{\mathrm{d}y}(y\beta_k(y)) = \beta_{k-1}(y) - (1-(-1)^k)yd_k(y),$$

$$\frac{\mathrm{d}}{\mathrm{d}y}(yd_k(y)) = (1-(-1)^k)y\beta_k(y). \tag{4.20}$$

Proposition 4.6 allows us to reformulate our study of $\beta_k(y)$ and $d_k(y)$ from a differential equations perspective. By substituting the appropriate formulas for $d_k(y)$ into Eq. (4.20), we can express derivatives of $y\beta_k(y)$ as polynomials in $\beta_2(y), \beta_3(y), \ldots, \beta_k(y)$ and the elementary functions. For example, if we plug (4.17) into (4.20) we find

$$\frac{\mathrm{d}}{\mathrm{d}y}(y\beta_3(y)) = \beta_2(y) - 2\tan(2y)y\beta_3(y) + 2\sec(2y)(y\beta_2(y))^2. \tag{4.21}$$

Solving this resulting system of nonlinear differential equations will naturally lead to some very complicated integrals. To solve Eq. (4.21) for $\beta_3(y)$, multiply each side by $\sec(2y)$ and collect the terms involving $\beta_3(y)$ to get

$$\frac{\mathrm{d}}{\mathrm{d}y}\left(\frac{y\beta_3(y)}{\cos(2y)}\right) = \frac{\beta_2(y)}{\cos(2y)} + 2\left(\frac{y\beta_2(y)}{\cos(2y)}\right)^2. \tag{4.22}$$

Now integrate each side from 0 to y, restricting $|y| < \pi/4$ to avoid the poles of $\sec(2y)$. Therefore if $|y| < \pi/4$,

$$\beta_3(y) = \frac{\cos(2y)}{y}\int_0^y \frac{\beta_2(u)}{\cos(2u)} + 2\left(\frac{u\beta_2(u)}{\cos(2u)}\right)^2 \mathrm{d}u. \tag{4.23}$$

It might be of some interest to try to generalize the system of linear differential equations presented in (4.20). For example, can we perturb the coefficients, but still find a reduction to a first order system of equations? It appears (after some effort) that the equations in (4.20), combined with the initial conditions $\{\beta_0(y)=1, d_0(y)=0, \beta_k(0)=1, d_k(0)=0\}$ are not easily generalized.

Next we will establish a recursive formula for generating the Taylor series coefficients of $\nu_k(x)$ about $x = r+1/2$ where $r \in \mathbf{Z}$.

Theorem 4.7: *Let r be any integer, then we may compute the Taylor series for $\nu_k(x)$ about $x=r+1/2$. The derivatives of $\nu_k(x)$ can be computed recursively using*

$$\nu_k^{(n+1)}(r+1/2) = \sum_{m=0}^{n} 2^{m+1}(m+1)!\binom{n}{m}\frac{\mathrm{d}^{n-m}}{\mathrm{d}x^{n-m}}\left[\nu_k(x)\beta_{m+2}^{(r+1,r+1)}(\nu_k(x))\right]_{x=r+1/2}.$$

Since $J_{r+1/2}(y)$ can always be written in terms of elementary functions, $\nu_k(r+1/2)$ is always the root of an elementary function. The selection of k determines which zero of $J_x(y)$ that $\nu_k(x)$ will pass through.

TABLE I. Table of the first five positive zeros of $J_0(y)$. The approximations were calculated using Eq. (4.24).

Zero number	Exact zero	Approximate zero
1	2.4048…	2.4094…
2	5.5200…	5.5217…
3	8.6537…	8.6545…
4	11.7915…	11.7919…
5	14.9309…	14.9312…

To compute the Taylor series for $\nu_k(x)$ about $x=1/2$, apply Theorem 4.7 with $r=0$. Since $J_{1/2}(y)=(2/\pi y)^{\frac{1}{2}}\sin(y)$, the kth zero of $J_{1/2}(y)$ to the right-hand side of $x=1/2$ is just πk, therefore $\nu_k(1/2)=\pi k$. Computing the first few terms in our series, we get

$$\nu_k(x)=\pi k+2\pi k\beta_2(\pi k)(x-1/2)-8\pi k\beta_3(\pi k)\frac{(x-1/2)^2}{2!}+(48\pi k\beta_4(\pi k)-64\pi^3k^3\beta_2^3(\pi k)$$
$$-24\pi k\beta_2^2(\pi k))\frac{(x-1/2)^3}{3!}+\cdots. \tag{4.24}$$

Since $\nu_k(x)$ is not analytic at $x=-1$, Eq. (4.24) converges for $-1<x<2$. We can approximate the first few zeros of $J_0(y)$ using (4.24). As Table I illustrates, this series converges very slowly.

We will pose three open problems to conclude this section.

Open question 1: It is easy to see that if $m\geqslant 0$ is an integer, then $\nu_k^{(m)}(1/2)$ is a polynomial in the elements $\pi k,\beta_2(\pi k),\beta_3(\pi k),\ldots,\beta_{m+1}(\pi k)$. Thus $\nu_k^{(m)}(1/2)$ can be expressed as a polynomial in πk and the derivatives of $J_x(\pi k)J_{-x}(\pi k)[\pi/\sin(\pi x)]$ at $x=1/2$. Based on this evidence, we might conjecture the existence of a "nice" function $f(x,y,z)$, such that

$$\nu_k(x)=f\left(x,\pi k,\frac{\pi}{\sin(\pi x)}J_x(\pi k)J_{-x}(\pi k)\right). \tag{4.25}$$

It would be highly desirable to prove the existence of such a function, as it would give an exact solution of $J_x(y)=0$.

Open question 2: Are the elements of the set $\{y,\cos(2y),\beta_2(y),\beta_3(y),\ldots\}$ algebraically independent? For example, can $\beta_3(y)$ be expressed in terms of $\beta_2(y)$ and trigonometric functions?

This is not a trivial question. Using Eq. (4.17) we easily see that if $n\geqslant 0$ is an integer,

$$\beta_3\left((2n+1)\frac{\pi}{4}\right)=(-1)^n(2n+1)\frac{\pi}{4}\beta_2^2\left((2n+1)\frac{\pi}{4}\right). \tag{4.26}$$

This shows that $\beta_3(y)$ can be expressed in terms of $\beta_2(y)$ at certain discrete points. Whether or not this indicates more general algebraic relations remains unanswered.

Open question 3: Is it possible to simplify the recurrence relation given in Theorem 4.7? In other words, can we generate $\nu_k^{(m)}(1/2)$ in a way that does not involve taking derivatives?

V. THE TAYLOR SERIES FOR $\nu_k(x)$ AT THE INTEGERS

In general, calculating the Taylor series for $\nu_k(x)$ at the integers is far more challenging than computing the Taylor series at the half-integers. Recall that $\nu_k(x)$ is discontinuous when $x\in\{-1,-2,\}$, so it only makes sense to calculate a Taylor series for $x\in\{0,1,2,\ldots\}$. The main difficulty lies in the fact that

$$\nu_k'(x) = \frac{\nu_k(x)}{2} \sum_{n=-\infty}^{\infty} \frac{J_n^2(\nu_k(x))}{(n+x)^2}$$

has removable singularities at $x=0,1,2,\ldots$. This gives rise to polynomial rather than linear relationships between derivatives of $\nu_k(x)$. To illustrate this point, we will calculate the first Taylor polynomial of $\nu_k(x)$ at zero.

Proposition 5.1: The first Taylor polynomial of $\nu_k(x)$ at zero is given by

$$\nu_k(x) = \nu_k(0) + \frac{x}{2\nu_k(0)J_1^2(\nu_k(0))} + O(x^2). \tag{5.1}$$

Proof: We simply need to show that $\nu_k'(0)$ has the correct form, and consequently Eq. (5.1) really is the first Taylor polynomial of $\nu_k(x)$ at zero.

Applying Proposition 3.2, we obtain the following relation for $\nu_k'(0)$:

$$\frac{\nu_k'(0)}{\nu_k(0)} = \frac{1}{2}\lim_{x\to 0}\left(\frac{J_0^2(\nu_k(x))}{x^2}\right) + \frac{1}{2}\sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} \frac{J_n^2(\nu_k(0))}{n^2} = \frac{1}{2}J_1^2(\nu_k(0))(\nu_k'(0))^2 + \sum_{n=1}^{\infty} \frac{J_n^2(\nu_k(0))}{n^2}.$$

We will use Eq. (5.4) to simplify this expression. By letting $y \to \nu_k(0)$ in (5.4), we can show that

$$\sum_{n=1}^{\infty} \frac{J_n^2(\nu_k(0))}{n^2} = \frac{1}{2\nu_k^2(0)J_1^2(\nu_k(0))}. \tag{5.2}$$

Eliminating this infinite series and solving the resulting quadratic equation for $\nu_k'(0)$, we arrive at the simple formula

$$\nu_k'(0) = \frac{1}{2\nu_k(0)J_1^2(\nu_k(0))}. \tag{5.3}$$

The fact that we can use Eq. (5.2) to prove such a simple expression for $\nu_k'(0)$ is a minor miracle. The fact that we must solve a quadratic equation for $\nu_k'(0)$ illustrates why we should not expect to find a simple recursive formula like that in Theorem 4.7 to compute $\nu_k^{(m)}(0)$. ■

When we are computing higher derivatives of $\nu_k(x)$ at integer points, we will encounter the following three functions:

$$\mu_k(y) = \sum_{n=1}^{\infty} \frac{J_n^2(y)}{n^k},$$

$$\eta_k(y) = \sum_{n=1}^{\infty} \frac{J_{n+1}^2(y)}{n^k},$$

$$\rho_k(y) = \sum_{n=1}^{\infty} \frac{J_n(y)J_{n+1}(y)}{n^k}.$$

In Proposition 4.4 we showed that $d_k(y)$ is expressible in terms of $\beta_j(y)$'s and the elementary functions. Unfortunately such strong relationships are probably not possible between $\mu_k(y)$, $\eta_k(y)$, and $\rho_k(y)$. The strongest relationships that we have found allow us to eliminate $\rho_k(y)$ if k is even. It is not too difficult to show that

$$\rho_2(y) = -\frac{(J_0^2(y)-1)^2}{4y^2J_0(y)J_1(y)} + \frac{\mu_1(y)}{y} - \frac{J_0(y)}{J_1(y)}\frac{\rho_1(y)}{y} + \frac{1}{2}\frac{J_1(y)}{J_0(y)}\mu_2(y) + \frac{1}{2}\frac{J_0(y)}{J_1(y)}\eta_2(y). \tag{5.4}$$

Equation (5.4) was critical in our computation of the first Taylor polynomial of $\nu_k(x)$ at $x=0$. We will state the more general case in the next proposition.

Proposition 5.2: Define a_n, b_n, and c_n *as follows:*

$$a_n = \begin{cases} J_0(y)J_1(y) & \text{if } n=-1, \\ -\dfrac{J_0^2(y)}{y} & \text{if } n=0, \\ \dfrac{2}{y}\mu_n(y) - (1-(-1)^n)\rho_{n+1}(y) & \text{if } n \geqslant 1, \end{cases}$$

$$b_n = \begin{cases} J_0^2(y) & \text{if } n=-1, \\ -(1-(-1)^n)\mu_{n+1}(y) & \text{if } n \geqslant 0, \end{cases}$$

$$c_n = \begin{cases} -J_1^2(y) & \text{if } n=-1, \\ \dfrac{2}{y}J_0(y)J_1(y) & \text{if } n=0, \\ (1-(-1)^n)\eta_{n+1}(y) + \dfrac{4}{y^2}\mu_{n-1}(y) - \dfrac{4}{y}\rho_n(y) & \text{if } n \geqslant 1. \end{cases}$$

Then for $n=0,1,2\ldots$,

$$\sum_{k=-1}^{n+1} c_k b_{n-k} = \frac{\delta_{n0}}{y^2} - \sum_{k=-1}^{n+1} a_k a_{n-k}, \tag{5.5}$$

where

$$\delta_{n0} = \begin{cases} 1 & \text{if } n=0, \\ 0 & \text{otherwise}. \end{cases}$$

If n is odd, then Eq. (5.5) is trivial. When n is even, we obtain nontrivial relationships between $\eta_j(y)$*'s,* $\rho_j(y)$*'s, and* $\mu_j(y)$*'s. The case where* $n=0$ *yields Eq. (5.4).*

If we let $n=2$, Eq. (5.5) yields the complicated formula

$$\begin{aligned} 0 = {} & \frac{2}{y^2}\mu_1^2(y) - 2\left(\frac{1-J_0^2(y)}{y^2}\right)\mu_2(y) + 2\frac{J_0(y)J_1(y)}{y}\mu_3(y) + J_1^2(y)\mu_4(y) - 2\mu_2(y)\eta_2(y) + J_0^2(y)\eta_4(y) \\ & + \frac{4}{y}\mu_2(y)\rho_1(y) - \frac{4}{y}\mu_1(y)\rho_2(y) + 2\rho_2^2(y) - 2\frac{J_0^2(y)}{y}\rho_3(y) - 2J_0(y)J_1(y)\rho_4(y). \end{aligned} \tag{5.6}$$

To conclude this section, we will list a couple of interesting open questions about $\mu_k(y)$, $\eta_k(y)$, and $\rho_k(y)$.

Open question 4: Is it possible to find explicit expressions for $\mu_1(y)$, $\eta_1(y)$, and $\rho_1(y)$ in terms of known functions? It seems likely that these functions are somehow related to Bessel functions of the first and second kinds. Formulas similar to Eq. (4.2) and (4.5) would be desirable.

Open question 5: Do more nontrivial algebraic relations exist between $\mu_k(y)$, $\eta_k(y)$, and $\rho_k(y)$? This question is probably very hard, given the difficulty of working with these particular functions.

VI. A CONNECTION TO THE RIEMANN ZETA FUNCTION, AND FURTHER REMARKS ABOUT SERIES OF SQUARES OF BESSEL FUNCTIONS

The functions that we have considered so far, $\{\beta_k(y), d_k(y), \beta_k^{(a,b)}(y), \mu_k(y), \eta_k(y), \rho_k(y)\}$, are particularly nice. Besides their various algebraic relations and differentiation formulas, they are sums over products of Bessel functions of integer order. As a result, integrals like

$$\frac{1}{2} = \int_0^\infty J_n(y)J_{n+1}(y)\mathrm{d}y \quad \text{if } n \in \mathbf{Z} \text{ and } n \geqslant 0, \tag{6.1}$$

naturally connect them to the Riemann zeta function (Ref. 1, p. 1102).

Applying formula (6.1) to $d_k(y)$, it is easy to see that for $k=1,2,3,\ldots$,

$$\left(1 - \frac{1}{2^{2k+1}}\right)\zeta(2k+1) = \int_0^\infty d_{2k+1}(y)\mathrm{d}y. \tag{6.2}$$

Setting $k=1$ gives the following integral for $\zeta(3)$:

$$\frac{7}{8}\zeta(3) = \int_0^\infty d_3(y)\mathrm{d}y = \int_0^\infty (\tan(2y)\beta_3(y) - y\sec(2y)\beta_2^2(y))\mathrm{d}y.$$

A simple integration by parts generates another nontrivial integral for $\zeta(3)$. In general we can use the algebraic relations between our functions to find many complicated integrals for π and the odd values of the Riemann zeta function. Perhaps additional knowledge about the $\beta_k(y)$'s will yield some useful information about $\zeta(3), \zeta(5), \ldots$ (unfortunately this is probably too much to hope for).

Since the entire paper (up to this point) discusses functions defined by infinite series of squares of Bessel functions, we pose the following general question: What functions can be expressed in such a form?

As an example, we evaluated $\beta_2(y)$ in terms of the sine integral in formula (4.3). This expansion converges rapidly, and provides an example of a useful special function expressible by a series of squares of Bessel functions. We can also derive a similar expression for the cosine integral,

$$\int_0^{2y} \frac{1-\cos(z)}{z}\mathrm{d}z = 4\sum_{n=1}^{\infty} J_n^2(y)\sum_{k=0}^{n-1}\frac{1}{2k+1}. \tag{6.3}$$

Proof: We can prove (6.3) by showing that the derivatives of each side of the equation are equal, and by showing that the equation holds when $y=0$.

It is trivial to show that (6.3) holds when $y=0$, since both sides of the equation vanish. Therefore we just have to show that

$$\frac{1-\cos(2y)}{y} = 4\frac{d}{\mathrm{d}y}\left(\sum_{n=1}^{\infty} J_n^2(y)\sum_{k=0}^{n-1}\frac{1}{2k+1}\right).$$

Observe that this sum converges uniformly whenever $y \in \mathbf{R}$, so we may interchange summation and differentiation. Therefore if $y \in \mathbf{R}$,

$$\begin{aligned} 4\frac{d}{\mathrm{d}y}\left(\sum_{n=1}^{\infty} J_n^2(y)\sum_{k=0}^{n-1}\frac{1}{2k+1}\right) &= 4\sum_{n=1}^{\infty}\frac{d}{\mathrm{d}y}(J_n^2(y))\sum_{k=0}^{n-1}\frac{1}{2k+1} \\ &= 4\sum_{n=1}^{\infty}(J_{n-1}(y)J_n(y) - J_n(y)J_{n+1}(y))\sum_{k=0}^{n-1}\frac{1}{2k+1}. \end{aligned}$$

Now break the sum into two pieces, and combine the two pieces so that the inner sums telescope,

$$
\begin{aligned}
&= 4\sum_{n=1}^{\infty} J_{n-1}(y)J_n(y)\sum_{k=0}^{n-1}\frac{1}{2k+1} - 4\sum_{n=1}^{\infty} J_n(y)J_{n+1}(y)\sum_{k=0}^{n-1}\frac{1}{2k+1} \\
&= 4\sum_{n=0}^{\infty} J_n(y)J_{n+1}(y)\sum_{k=0}^{n}\frac{1}{2k+1} - 4\sum_{n=1}^{\infty} J_n(y)J_{n+1}(y)\sum_{k=0}^{n-1}\frac{1}{2k+1} \\
&= 4\sum_{n=0}^{\infty} J_n(y)J_{n+1}(y)\left(\sum_{k=0}^{n}\frac{1}{2k+1} - \sum_{k=0}^{n-1}\frac{1}{2k+1}\right) = 4\sum_{n=0}^{\infty}\frac{J_n(y)J_{n+1}(y)}{2n+1}.
\end{aligned}
$$

Using the fact that $J_{-n}(y) = (-1)^n J_n(y)$ [as in the proof of Eq. (2.4)], this becomes

$$
2\sum_{n=-\infty}^{\infty}\frac{J_n(y)J_{n+1}(y)}{2n+1} = \frac{1-\cos(2y)}{y}
$$

by Eq. (4.5). ■

In the next theorem we state Gegenbauer's result from the 1870s, namely that any even function with a Taylor series at zero can be written as a sum of squares of Bessel functions (Ref. 5, p. 525). The form that we give for this theorem is slightly different from Watson's statement, but is sufficient for our purposes.

Theorem 6.1: *(Gegenbauer) Suppose that $f(z)$ is an even function that is analytic at zero, or equivalently suppose that $f(z)$ is even and has a Taylor series at zero. Let*

$$
f(z) = \sum_{n=0}^{\infty}\frac{f^{(2n)}(0)}{(2n)!}z^{2n}.
$$

Then the following representation holds for $f(z)$:

$$
f(z) = \sum_{n=0}^{\infty} a_n J_n^2(z),
$$

where a_n is given by

$$
a_n = \begin{cases} f(0) & \text{if } n = 0, \\ 2n\displaystyle\sum_{k=0}^{n}\frac{\binom{n+k}{2k}}{n+k}\frac{2^{2k}}{\binom{2k}{k}}f^{(2k)}(0) & \text{if } n \geqslant 1. \end{cases}
$$

This formula relating a_n and $f^{(2n)}(0)$ can be inverted to give

$$
f^{(2n)}(0) = \frac{(-1)^n}{2^{2n}}\binom{2n}{n}\sum_{k=0}^{n}(-1)^k a_k\binom{2n}{n+k}.
$$

If we apply Theorem 6.1 to appropriately chosen hypergeometric functions, we can obtain a variety of "nice" series of squares of Bessel functions. Examples include

$$
\sum_{n=0}^{\infty}(-1)^n\frac{(2n)!}{n!^3}\frac{\left(\frac{y}{2}\right)^{2n}}{(x)_n} = J_0^2(y) + 2\sum_{n=1}^{\infty}(-1)^n\frac{(1-x)_n}{(x)_n}J_n^2(y), \tag{6.4}
$$

$$\sum_{n=0}^{\infty}(-1)^n\binom{2n}{n}\binom{2n-x}{n-x}\frac{\left(\frac{y}{2}\right)^{2n}}{(2n)!}=\sum_{n=0}^{\infty}\frac{(x)_n}{n!}J_n^2(y), \tag{6.5}$$

where $(x)_n=x(x+1)\cdots(x+n-1)$.

Open question 6: An interesting question associated with Theorem 6.1 is to find a "nice" expression for the Taylor series coefficients of $\mu_k(y)$ when k is an odd integer. It is easy to show that the Taylor series coefficients of $\beta_k(y)$, $d_k(y)$, and $\mu_{2k}(y)$ can always be expressed in terms of harmonic numbers. If we let

$$\lambda_n^{(j)}=\sum_{m=0}^{n}\frac{1}{(2m+1)^j},\quad H_n^{(j)}=\sum_{m=1}^{n}\frac{1}{m^j},$$

then we can obtain series expansions including

$$\beta_3(y)=\sum_{n=0}^{\infty}(-1)^n\lambda_n^{(2)}\frac{(2y)^{2n}}{(2n+1)!}, \tag{6.6}$$

$$\mu_4(y)=\sum_{n=1}^{\infty}(-1)^{n+1}\left(\frac{H_n^{(4)}+(H_n^{(2)})^2}{4}\right)\binom{2n}{n}\frac{\left(\frac{y}{2}\right)^{2n}}{n!^2}, \tag{6.7}$$

$$d_5(y)=\sum_{n=0}^{\infty}(-1)^n\left(\frac{\lambda_n^{(4)}+(\lambda_n^{(2)})^2}{2}\right)\frac{(2y)^{2n}}{(2n+2)!}. \tag{6.8}$$

A simple application of Theorem 6.1 shows that trying to find nice Taylor series coefficients for $\{\mu_3(y),\mu_5(y),\ldots\}$ is equivalent to reducing

$$r_n^{(j)}=\sum_{m=1}^{n}\frac{(-1)^{m+1}}{m^j}\binom{2n}{n+m},$$

into "some nice form" when $j>1$ is an odd integer.

In the case of $\mu_1(y)$, we can show that if A_n is the alternating harmonic series,

$$A_n=\sum_{k=1}^{n}\frac{(-1)^{k+1}}{k},$$

then we must have

$$\mu_1(y)=\sum_{n=1}^{\infty}(-1)^{n+1}A_{2n}\binom{2n}{n}\frac{\left(\frac{y}{2}\right)^{2n}}{n!^2}. \tag{6.9}$$

Generalizing this result has proven surprisingly difficult.

VII. MORE REPRESENTATIONS OF $\beta_k(y)$ AND $d_k(y)$ IN TERMS OF INFINITE SERIES

The functions $\beta_k(y)$ and $d_k(y)$ possess many representations in terms of infinite integrals and infinite series. Since $\beta_k(y)$ and $d_k(y)$ are just the derivatives with respect to order of products of Bessel functions, every one of the legions of representations for Bessel functions will yield formulas for $\beta_k(y)$ and $d_k(y)$. In this section we will present a few of the most visually appealing and useful formulas that we have encountered.

Our first formula expresses $d_k(y)$ in terms of sums running over the Bessel functions of half-integer order. This is noteworthy since the Bessel functions of half-integer order reduce to polynomials in $1/\pi$ whenever $y \to \pi k$.

Let $\alpha_n(y)$ be defined by

$$\alpha_n(y) = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^n} J_{1/2+k}(y) J_{1/2-k}(y), \tag{7.1}$$

and let B_j denote the Bernoulli numbers (Ref. 1, p. 1107). Then for $n \geqslant 1$,

$$d_{2n-1}(y) = \frac{4(4^n-1)}{(2n)!}|B_{2n}|\pi^{2n-2}\frac{\sin^2(y)}{y} + \frac{1}{4^{n-1}}\sum_{j=1}^{n-1}\frac{4^j(4^j-1)}{(2j)!}|B_{2j}|\pi^{2j-1}\alpha_{2n-2j}(y). \tag{7.2}$$

Equation (7.2) yields the following relation when $n=2$:

$$d_3(y) = \frac{\pi^2}{12}\frac{\sin^2(y)}{y} + \frac{\pi}{4}\alpha_2(y). \tag{7.3}$$

A second family of formulas can be obtained from Eqs. (2.9) and (2.10). We can decompose $\beta_k(y)$ and $d_k(y)$ in terms of two sets of functions defined by a modified Neumann series. Define $g_k(y)$ and $h_k(y)$ by

$$g_k(y) = \sum_{n=0}^{\infty} \frac{J_n(y)\left(\frac{y}{2}\right)^n}{n!(2n+1)^k}, \tag{7.4}$$

$$h_k(y) = \sum_{n=0}^{\infty} \frac{J_{n+1}(y)\left(\frac{y}{2}\right)^n}{n!(2n+1)^k}. \tag{7.5}$$

It is easy to see from Eq. (2.2) that $g_k(y)$ and $h_k(y)$ can be written compactly as

$$g_k(y) = \frac{(-1)^{k-1}}{2^k(k-1)!}\frac{\mathrm{d}^{k-1}}{\mathrm{d}x^{k-1}}\left[\left(\frac{2}{y}\right)^x \Gamma(x)J_x(y)\right]_{x=1/2} \quad \text{if } k \geqslant 1, \tag{7.6}$$

$$h_k(y) = \frac{-1}{2^k(k-1)!}\frac{\mathrm{d}^{k-1}}{\mathrm{d}x^{k-1}}\left[\left(\frac{2}{y}\right)^{1-x} \Gamma(1-x)J_{-x}(y)\right]_{x=1/2} \quad \text{if } k \geqslant 2. \tag{7.7}$$

We can prove the following formulas for $\beta_k(y)$ and $d_k(y)$:

$$d_{2n+1}(y) = 2h_{2n+1}(y) - y\sum_{m=0}^{2n}(-1)^m h_{m+1}(y)h_{2n+1-m}(y), \tag{7.8}$$

$$d_{2n+1}(y) = y\sum_{m=0}^{2n}(-1)^m g_{m+1}(y)g_{2n+1-m}(y), \tag{7.9}$$

$$\beta_n(y) = g_n(y) - y\sum_{m=0}^{n}(-1)^m h_{m+1}(y)g_{n-m}(y). \tag{7.10}$$

By combining these three formulas we can find a wide variety of relations between $\beta_k(y)$, $d_k(y)$, $h_k(y)$, and $g_k(y)$. We will use the following elementary evaluations of $g_0(y)$, $g_1(y)$, $h_0(y)$, and $h_1(y)$,

$$g_0(y) = 1, \quad g_1(y) = \frac{\sin(y)}{y}, \tag{7.11}$$

$$h_0(y) = \frac{y}{2}, \quad h_1(y) = \frac{1 - \cos(y)}{y}. \tag{7.12}$$

Examples of identities include

$$h_2(y)\sin(y) + g_2(y)\cos(y) = \beta_2(y), \tag{7.13}$$

$$h_3(y)\sin(y) + g_3(y)\cos(y) = \frac{1}{\sin(2y)}(d_3(y) + 2y\cos(y)g_2(y)\beta_2(y) - y\beta_2^2(y)), \tag{7.14}$$

$$h_4(y)\sin(y) + g_4(y)\cos(y) = \beta_4(y) + y(g_2(y)h_3(y) - h_2(y)g_3(y)). \tag{7.15}$$

Unfortunately, it seems to be impossible to express $g_k(y)$ or $h_k(y)$ only in terms of $\beta_k(y)$'s. This is not especially surprising, since we would not intuitively expect to find strong relationships between the derivatives of $J_x(y)$ and the derivatives of $J_x(y)J_{-x}(y)$. Interestingly enough however, it may be possible to express $g_k(y)$ in terms of $\beta_k(y)$'s at certain arguments. An example follows easily from Eq. (7.13),

$$g_2(\pi k) = (-1)^k \beta_2(\pi k) \quad \text{for } k \in \mathbf{Z}. \tag{7.16}$$

A third class of identities can be derived from Eqs. (2.12) and (2.13). While we have not explored this avenue in depth, we have derived a few noteworthy formulas. If we let

$$F_k(y,z) = \sum_{n=-\infty}^{\infty} \frac{J_n(y)J_n(z)}{(2n+1)^k}\left(\frac{y}{z}\right)^n,$$

$$G_k(y,z) = \sum_{n=-\infty}^{\infty} \frac{J_n(y)J_{n+1}(z)}{(2n+1)^k}\left(\frac{y}{z}\right)^n,$$

then examples of identities include

$$d_3(y) = -\left(\frac{\pi}{2}\right)^2 \beta_2^2\left(\frac{\pi}{2}\right)\frac{\sin^2(y)}{y} - yG_2^2\left(y, \frac{\pi}{2}\right) + 2\sin(y)G_3\left(y, \frac{\pi}{2}\right), \tag{7.17}$$

$$\frac{\sin(2z)}{2z}\beta_2(y) + \frac{\sin(2y)}{2y}\beta_2(z) = \frac{\sin(z)}{z}\cos(y)F_2(y,z) + \frac{\sin(y)}{y}\cos(z)F_2(z,y). \tag{7.18}$$

VIII. CONCLUSION

It would be particularly nice to see solutions to some of the open problems presented in this paper. A solution of question 4 could potentially yield a rapidly converging series for $Y_0(z)$, while a solution for question 3 would simplify Theorem 4.7. Such results would be quite useful.

It might also be interesting to generalize the results of Secs. II, IV, and V to other special functions. For example, while it is possible to generate a differential equation similar to Eq. (3.2) for the zeros of ${}_2F_1\left(\begin{matrix}a,1-a\\c\end{matrix}\middle| x\right)$, it is not immediately clear that this will yield a nice series similar to Eq. (4.24) for the zeros of this hypergeometric function.

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The multicomponent generalized Kaup–Newell hierarchy and its multicomponent integrable couplings system with two arbitrary functions

Tiecheng Xia[a)]
Department of Mathematics, Tianjin University, Tianjin 300072, People's Republic of China, Department of Mathematics, Bohai University, Jinzhou 121000, People's Republic of China and Department of Mathematics, Shanghai University, Shanghai 200436, People's Republic of China

Engui Fan[b)]
Institute of Mathematics, Fudan University, Shanghai 200433, People's Republic of China

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We devise a new simple loop algebra $\tilde{G}_M$ and an isospectral problem. By making use of the Tu scheme, the multicomponent generalized Kaup–Newell hierarchy is obtained. Furthermore, an expanding loop algebra $\tilde{F}_M$ of the loop algebra $\tilde{G}_M$ is presented. Based on $\tilde{F}_M$, the multicomponent integrable couplings system with two arbitrary functions of the multicomponent generalized Kaup–Newell hierarchy are worked out. The method can be applied to other nonlinear evolution equations hierarchy. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1866220]

I. INTRODUCTION

Searching for new integrable hierarchies of soliton equations is an important and interesting topic in soliton theory. Various efficient approaches have been developed to get many integrable systems such as AKNS hierarchy, Kaup–Newell hierarchy, Schrödinger system, and so on.[1–24] As far as the multicomponent integrable hierarchies are concerned, there have been developments such as in Refs. 13 and 14. Ma and Zhou once also gave the multicomponent AKNS hierarchies by using generalized Tu scheme in Ref. 15. In Refs. 16–18, a simple and efficient method for generating multicomponent integrable hierarchies was proposed. Constructing a new simple loop algebra and designing an isospectral problem of multicomponent hierarchy of soliton equations become a key step in this method. Although using the loop algebra in Refs. 16–18 can produce many multicomponent integrable hierarchies, it is not suitable for seeking the multicomponent generalized Kaup–Newell hierarchy.[10,11] In this paper, a new loop algebra $\tilde{G}_M$ is first constructed, and then an isospectral problem is designed. By employing Tu scheme,[6–19] the multicomponent generalized Kaup–Newell hierarchy is worked out. In addition, an expanding loop algebra $\tilde{F}_M$ of the loop algebra $\tilde{G}_M$ is presented, which is devoted to deducing the integrable couplings of the multicomponent generalized Kaup–Newell hierarchy.

In Refs. 10 and 11, we investigated the isospectral problem,

[a)]Electronic mail: xiatc@yahoo.com.cn
[b)]Electronic mail: faneg@fudan.edu.cn

$$\varphi_x = U\varphi, \quad U = \begin{pmatrix} -\lambda^2 + \beta qr & \lambda q \\ \lambda r & \lambda^2 - \beta qr \end{pmatrix}, \quad \lambda_t = 0. \tag{1}$$

Where β is an arbitrary constant. When $\beta=0$, problem (1) reduces to the Kaup–Newell spectral problem. We obtained the generalized Kaup–Newell hierarchy and established its multi-Hamiltonian structure by using Tu scheme,

$$u_t = \begin{pmatrix} q \\ r \end{pmatrix}_t = J\frac{\delta H_n}{\delta u} = JL\frac{\delta H_{n-1}}{\delta u} = JL^n\frac{\delta H_0}{\delta u}, \quad n = 1,2, \ldots .$$

It is interesting the hierarchy is related to seven well-known nonlinear evolution equations such as Kaup–Newell equations, Chen–Lee–Liu equations, Gerdjikov equation and Kundu type equation, etc.[11,12] In this paper, we would like to extend the hierarchy to the multicomponent generalized Kaup–Newell integrable hierarchy in the Lax sense. Finally, we shall obtain the multicomponent integrable couplings with two arbitrary functions of the multicomponent generalized Kaup–Newell integrable hierarchy based on a new loop algebra $\tilde{F}_M$.

II. A NEW LOOP ALGEBRA

If $G_M=\{a=(a_{ij})_{M\times 3}=(a_1,a_2,a_3)\}$ denotes a set of matrices, where M is a positive integer, $a_i(i=1,2,3)$ is the ith column of the matrix a. Then G_M is a linear space.

Let $\alpha=(\alpha_1,\alpha_2,\ldots,\alpha_M)^T$, $\beta=(\beta_1,\beta_2,\ldots,\beta_M)^T$, and define their product $\alpha*\beta=\beta*\alpha=(\alpha_1\beta_1,\alpha_2\beta_2,\ldots,\alpha_M\beta_M)^T$. If $a=(a_1,a_2,a_3)$, $b=(b_1,b_2,b_3)\in\tilde{G}_M$, a commutation operation for G_M is defined as

$$[a,b] = (a_2 * b_3 - a_3 * b_2, 2(a_1 * b_2 - a_2 * b_1), 2(a_3 * b_1 - a_1 * b_3)), \tag{2}$$

It is easy to verify that the operation (2) is linear and antisymmetric. For $\forall a,b,c\in G_M$, we can also verify that

$$[[a,b],c] + [[b,c],a] + [[c,a],b] = 0, \tag{3}$$

i.e., Jacobian identity holds. Therefore, G_M with the operation (2) becomes a Lie algebra. A corresponding loop algebra $\tilde{G}_M$ is defined as

$$\tilde{G}_M = \{a\lambda^n, a \in G_M, n = 0, \pm 1, \pm 2, \ldots\},$$

with a commutation operation defined as

$$[a\lambda^m, b\lambda^n] = [a,b]\lambda^{m+n}, \quad \forall\, a,b \in \tilde{G}_M. \tag{4}$$

Since $\tilde{G}_1$ is equal to $\tilde{A}_1$ in Refs. 21 and 22, we conclude that $\tilde{G}_M$ is an extension of the loop algebra $\tilde{A}_1$. We also find that $\tilde{G}_M$ has two features, (i) the commutation operation is simple and straightforward, as that in the loop algebra $\tilde{A}_1$; (ii) by means of $\tilde{G}_M$, we proceed to a simple calculation to be able to obtain various multicomponent integral systems.

Considering linear is spectral problem as follows:

$$\phi_x = [U,\phi], \quad \lambda_t = 0, \phi, U, \quad V \in \tilde{G}_M,$$

$$\phi_t = [V,\phi], \tag{5}$$

whose compatibility gives rise to

$$\phi_{xt} = [U_t,\phi] + [U,[V,\phi]] = \phi_{tx} = [V_x,\phi] + [V,[U,\phi]],$$

that is

$$[U_t,\phi]-[V_x,\phi]+[U,[V,\phi]]+[V,[U,\phi]]=0. \tag{6}$$

By employing (3), the formula (5) can be written as

$$[U_t,\phi]-[V_x,\phi]+[[U,V],\phi]=0. \tag{7}$$

Since ϕ is arbitrary, a condition of (7) holds if and only if the following equation does:

$$U_t-V_x+[U,V]=0. \tag{8}$$

Hence, the compatibility of (7) leads to a zero-curvature equation (8).

III. THE MULTICOMPONENT GENERALIZED KAUP–NEWELL HIERARCHY

We consider an is spectral problem

$$\phi_x=[U,\phi],\quad \lambda_t=0,\quad U=(-\lambda^2 I_M+\beta q*r,\lambda q*I_M,\lambda r*I_M), \tag{9}$$

where

$$I_M=\begin{pmatrix}1\\1\\\cdots\\1\end{pmatrix}_{M\times 1},\quad q=(q_1,q_2,\ldots,q_M)^T,\quad r=(r_1,r_2,\ldots r_M)^T.$$

Let

$$V=\sum_{m=0}^{\infty}(a(0,m),\lambda b(1,m),\lambda c(1,m))\lambda^{-2m},$$

where $a(0,m)=(a_{m1}^{(0)},\ldots,a_{mM}^{(0)})^T$, $b(1,m)=(b_{m1}^{(1)},\ldots,b_{mM}^{(1)})^T$, $c(1,m)=(c_{m1}^{(1)},\ldots,c_{mM}^{(1)})^T$. Solving the stationary zero curvature equation

$$V_x=[U,V], \tag{10}$$

gives

$$\begin{aligned}
&a_x(0,m)=q*c(1,m+1)-r*b(1,m+1),\\
&b_x(1,m)=-2b_m(1,m+1)+2\beta q*r*b(1,m)-2q*a(0,m),\\
&c_x(1,m)=2r*a(0,m)+2c(1,m+1)-2\beta q*r*c(1,m),\\
&a(1,m+1)=b(0,m)=c(0,m)=0,\\
&b(1,0)=c(1,0)=0,a(0,0)=\alpha=(\alpha_1,\alpha_2,\ldots,\alpha_M)\neq 0,\\
&c(1,1)=-\alpha*r,b(1,1)=-\alpha*q.
\end{aligned} \tag{11, 12}$$

Where $\alpha_i(i=1,2,\ldots,M)$ are constants.

Denoting $V_+^{(n)}=\Sigma_{m=0}^{n}(a(0,m),\lambda b(1,m),\lambda c(1,m))\lambda^{2n-2m}$, $V_-^{(n)}=\lambda^{2n}V-V_+^{(n)}$, then Eq. (7) can be written as

$$-V_{+x}^{(n)}+[U,V_+^{(n)}]=V_{-x}^{(n)}-[U,V_-^{(n)}]. \tag{13}$$

A direct calculation reads

$$-V_{+x}^{(n)}+[U,V_{+}^{(n)}]=(a_x(0,n+1),b_x(1,n+1)-2\beta q*r*b(1,n+1),c_x(1,n+1)+2\beta q*r*c(1,n+1))$$

Again taking

$$\Delta_n=(\beta(\partial^{-1}q*c_x(1,n+1)+r*b_x(1,n+1))+2\beta^2\partial^{-1}q*r*(q*c(1,n+1)-r*b(1,n+1)),0,0),$$

$$V^{(n)}=V_{+}^{(n)}+\Delta_n,$$

the zero curvature equation

$$U_t-V_x^{(n)}+[U,V^{(n)}]=0,$$

gives rise to the Lax integrable hierarchy

$$u_t=\begin{pmatrix}q\\r\end{pmatrix}_t=J'L'^{n-1}\begin{pmatrix}-\alpha*r\\-\alpha*q\end{pmatrix},\tag{14}$$

with

$$J'=\begin{pmatrix}J_{11}&J_{12}\\J_{21}&J_{22}\end{pmatrix},$$

where

$$J_{11}=2\beta q*\partial^{-1}q*\partial+4\beta^2q*\partial^{-1}q^2*r*,$$

$$J_{12}=\partial-2\beta q*r*+2\beta q*\partial^{-1}r*\partial-4\beta^2q*\partial^{-1}q*r^2*,$$

$$J_{21}=\partial+2\beta q*r*-2\beta r*\partial^{-1}q*\partial-4\beta^2r*\partial^{-1}r*q^2*,$$

$$J_{22}=-2\beta r*\partial^{-1}r*\partial-4\beta^2r*\partial^{-1}q*r^2*,$$

$$L'=\frac{1}{2}\begin{pmatrix}L_{11}&L_{12}\\L_{21}&L_{22}\end{pmatrix},$$

$$L_{11}=\partial-2\beta r*\partial^{-1}q^2*r*-r*\partial^{-1}q*\partial+2\beta q*r*,$$

$$L_{12}=2\beta r*\partial^{-1}q*r^2*-r*\partial^{-1}r*\partial,$$

$$L_{21}=-2\beta q*\partial^{-1}q^2*r*-q*\partial^{-1}q*\partial,$$

$$L_{22}=-\partial+2\beta q*\partial^{-1}q*r^2*-q*\partial^{-1}r*\partial+2\beta q*r*.$$

Let us see some special cases of our multicomponent hierarchy (14).

When $M=1$, the system (14) is just the the generalized Kaup–Newell hierarchy.[10,11] When $M>1$, the system (14) is the multicomponent generalized Kaup–Newell hierarchy.

The first system ($m=1$, $\alpha=-1$) in hierarchy (14) is the following coupled system:

$$q_t=b(1,n+1)_x-2\beta qrb(1,n+1)+2q\Delta_n,$$

$$r_t = c(1,n+1)_x - 2\beta qrc(1,n+1) - 2r\Delta_n. \tag{15}$$

Where Δ_n is given by

$$\Delta_n = (\beta(\partial^{-1}qc_x(1,n+1) + rb_x(1,n+1)) + 2\beta^2\partial^{-1}qr(qc(1,n+1) - rb(1,n+1)),0,0).$$

$$c(1,2) = \tfrac{1}{2}r_x - \tfrac{1}{2}(1-2\beta)r^2q; b(1,2) = -\tfrac{1}{2}q_x - \tfrac{1}{2}(1-2\beta)q^2r.$$

Taking $n=1$ and substituting $c(1,2)$, $b(1,2)$, Δ_n into system (15), we have

$$q_t = -\tfrac{1}{2}q_{xx} - \tfrac{1}{2}(q^2r)_x - 2\beta q(qr)_x - \tfrac{1}{2}\beta q^3r^2,$$

$$r_t = \tfrac{1}{2}r_{xx} - \tfrac{1}{2}(r^2q)_x - 2\beta r(qr)_x - \tfrac{1}{2}\beta q^2r^3,$$

which is just a generalized coupled derivative Schrödinger system in Ref. 11. Other kinds of equations can be obtained from system (15) in the cases when $n=2,\ldots$, we just omit them here.

IV. THE MULTICOMPONENT INTEGRABLE COUPLINGS SYSTEM

Set

$$F_M = \{a = (a_{ij})_{M\times 5} = (a_1,a_2,a_3,a_4,a_5)\}, \tag{16}$$

with a commutation operation defined as

$$[a,b] = (a_2 * b_3 - a_3 * b_2, 2(a_1 * b_2 - a_2 * b_1), 2(a_3 * b_1 - a_1 * b_3)), a_1 * b_4 - a_4 * b_1 + a_1 * b_5 - a_5 * b_1,$$

$$a_1 * b_5 - a_5 * b_1 + a_4 * b_1 - a_1 * b_4). \tag{17}$$

Then F_M is a Lie algebra. A corresponding loop algebra $\tilde{F}_M$ is defined as

$$\tilde{F}_M = \{a\lambda^n, a \in F_M, n = 0, \pm 1, \pm 2, \ldots\}, \tag{18}$$

with a commutation operation defined as

$$[a\lambda^m, b\lambda^n] = [a,b]\lambda^{m+n}, \forall\, a,b \in F_M. \tag{19}$$

Denote

$$\tilde{F}_M(1) = \{(a_1,a_2,a_3,0,0)\lambda^n\},$$

$$\tilde{F}_M(2) = \{(0,0,0,a_4,a_5)\lambda^n\},$$

then (i) $\tilde{F}_M = \tilde{F}_M(1) \oplus \tilde{F}_M(2)$, $\tilde{F}_M(1) \cong \tilde{G}_M$; (ii) $[\tilde{F}_M(1), \tilde{F}_M(2)] \subset \tilde{F}_M(2)$. Based on $\tilde{F}_M$, we consider an isospectral problem,

$$\phi_x = [U,\phi], \lambda_t = 0, U = (-\lambda^2 I_M + \beta u_1 * u_2, \lambda u_1 * I_M, \lambda u_2 * I_M, \lambda u_3 * I_M, \lambda u_4 * I_M), \tag{20}$$

where $u_i = (u_{i1}, u_{i2}, \ldots, u_{iM})^T$, $i=1,2,3,4$. Let $V = \Sigma_{m=0}^{n}(a_m, b_m, c_m, d_m, f_m)\lambda^{-2m}$. Solving the equation similar to (10) gives

$$a_x(0,m) = u_1 * c(1,m+1) - u_2 * b(1,m+1),$$

$$b_x(1,m) = -2b_m(1,m+1) + 2\beta * u_1 * u_2 * b(1,m) - 2u_1 * a(0,m),$$

$$c_x(1,m) = 2u_2 * a(0,m) + 2c(1,m+1) - 2\beta u_1 * u_2 * c(1,m),$$

$$d_x(1,n) = -d(1,n+1) + \beta * u_1 * u_2 * d(1,n) + \beta * u_1 * u_2 * f(1,n) - u_3 * a(0,n) - f(1,n+1) - u_4 * a(0,n),$$

$$f_x(1,n) = -f(1,n+1) + \beta * u_1 * u_2 * f(1,n) - \beta * u_1 * u_2 * d(1,n) - u_4 * a(0,n) + d(1,n+1) + u_3 * a(0,n),$$

$$a(1,m+1) = b(0,m) = c(0,m) = d(0,m) = f(0,m) = 0,$$

$$b(1,0) = c(1,0) = 0,\ a(0,0) = \alpha = (\alpha_1, \alpha_2, \ldots, \alpha_M) \neq 0,$$

$$c(1,1) = -\alpha * u_2,\ b(1,1) = -\alpha * u_1,\ d(1,1) = -\alpha * u_3,\ f(1,1) = -\alpha * u_4. \tag{21}$$

Taking

$$\Delta_n = (\beta * (\partial^{-1} u_1 * c_x(1,n+1) + u_2 * b_x(1,n+1)) + 2\beta^2 \partial^{-1} u_1 * u_2 * (u_1 * c(1,n+1) - u_2 * b(1,n+1)), 0, 0, \delta_{1n}, \delta_{2n}),$$

$$V^{(n)} = V_+^{(n)} + \Delta_n, \tag{22}$$

where δ_{1n}, δ_{2n} are arbitrary multicomponent functions of $u_i (i=1,2,3,4)$, therefore according to the zero curvature equation, we have following multicomponent integrable couplings of hierarchy of the multicomponent generalized Kaup–Newell hierarchy with two arbitrary functions:

$$u_t = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}_{t_n} = \begin{pmatrix} J_{11} * c(1,n+1) + J_{12} * b(1,n+1) \\ J_{21} * c(1,n+1) + J_{22} * b(1,n+1) \\ H_1 * \\ H_2 * \end{pmatrix}, \tag{23}$$

where

$$J_{11} = 2\beta * u_1 * \partial^{-1} u_1 * \partial + 4\beta^2 * u_1 * \partial^{-1} u_1^2 * u_2,$$

$$J_{12} = \partial - 2\beta * u_1 * u_2 + 2\beta * u_1 * \partial^{-1} r * \partial - 4\beta^2 u_1 * \partial^{-1} u_1 * u_2^2,$$

$$J_{21} = \partial + 2\beta * u_1 * u_2 - 2\beta * u_2 * \partial^{-1} u_1 * \partial - 4\beta^2 u_2 * \partial^{-1} u_2 * u_1^2,$$

$$J_{22} = -2\beta * u_2 * \partial^{-1} u_2 * \partial - 4\beta^2 * u_2 * \partial^{-1} u_1 * u_2^2,$$

$$H_1 = d_x(1,n+1) - \beta * u_1 * u_2 * d(1,n+1) - \beta * u_1 * u_2 * f(1,n+1) + (u_3 + u_4) * \Delta_n + \delta_{1nx} - \beta * u_1 * u_2 * \delta_{1n} - \beta * u_1 * u_2 * \delta_{2n},$$

$$H_2 = f_x(1,n+1) - \beta * u_1 * u_2 * f(1,n+1) + \beta * u_1 * u_2 * d(1,n+1) + (u_4 - u_3) * \Delta_n + \delta_{2nx} + \beta * u_1 * u_2 * \delta_{1n} - \beta * u_1 * u_2 * \delta_{2n}. \tag{24}$$

which have the Lax pair,

$$\phi_x = U\phi, \quad \phi_{t_n} = V^{(n)}\phi, \tag{25}$$

where U and $V^{(n)}$ satisty (9) and (22), respectively.

In particular, when taking $\delta_{1n}=\delta_{2n}=0$, from (23), we have

$$u_t = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}_t = \begin{pmatrix} J_{11}* & J_{12}* & 0 & 0 \\ J_{21}* & J_{22}* & 0 & 0 \\ J_{31}* & J_{32}* & \partial-\beta*u_1*u_2* & -\beta*u_1*u_2* \\ J_{41}* & J_{42}* & \beta*u_1*u_2* & \partial-\beta*u_1*u_2* \end{pmatrix} \begin{pmatrix} c(1,n+1) \\ b(1,n+1) \\ d(1,n+1) \\ f(1,n+1) \end{pmatrix} = J \begin{pmatrix} c(1,n+1) \\ b(1,n+1) \\ d(1,n+1) \\ f(1,n+1) \end{pmatrix}, \tag{26}$$

where $J_{ij}(i,j=1,2)$ comes from Eq. (24),

$$J_{31} = (u_3+u_4)*(\beta*\partial^{-1}u_1*\partial+2\beta^2*\partial^{-1}u_1^2*u_2),$$

$$J_{32} = (u_3+u_4)*(\beta*\partial^{-1}u_2*\partial-2\beta^2*\partial^{-1}u_2^2*u_1),$$

$$J_{41} = (u_4-u_3)*(\beta*\partial^{-1}u_1*\partial+2\beta^2*\partial^{-1}u_1^2*u_2),$$

$$J_{42} = (u_4-u_3)*(\beta*\partial^{-1}u_2*\partial-2\beta^2*\partial^{-1}u_2^2*u_1).$$

From (21), a recurrence operator is presented

$$L = \begin{pmatrix} L_{11}* & L_{12}* & 0 & 0 \\ L_{21}* & L_{22}* & 0 & 0 \\ L_{31}* & L_{32}* & \beta*u_1*u_2*-\frac{1}{2}\partial & \frac{1}{2}\partial \\ L_{41}* & L_{42}* & \beta*u_1*u_2*-\frac{1}{2}\partial & -\frac{1}{2}\partial \end{pmatrix},$$

with

$$L_{11} = \partial-2\beta*u_2*\partial^{-1}u_1^2*u_2-u_2*\partial^{-1}u_1*\partial+2\beta*u_1*u_2,$$

$$L_{12} = 2\beta*u_2*\partial^{-1}u_1*u_2^2-u_2*\partial^{-1}r*\partial,$$

$$L_{21} = -2\beta*u_1*\partial^{-1}u_1^2*u_2-u_1*\partial^{-1}u_1*\partial,$$

$$L_{22} = -\partial+2\beta*u_1*\partial^{-1}u_1*u_2^2-u_1*\partial^{-1}u_2*\partial+2\beta*u_1*u_2,$$

$$L_{31} = -u_3\partial^{-1}\left(\beta*u_1^2*u_2+\tfrac{1}{2}u_1*\partial\right),$$

$$L_{32} = -u_3\partial^{-1}\left(-\beta*u_2^2*u_1+\tfrac{1}{2}u_2*\partial\right),$$

$$L_{41} = -u_4\partial^{-1}\left(\beta*u_1^2*u_2+\tfrac{1}{2}u_1*\partial\right),$$

$$L_{42} = -u_4\partial^{-1}\left(-\beta*u_2^2*u_1+\tfrac{1}{2}u_2*\partial\right).$$

Thus, Eq. (23) can be written as

$$u_t = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}_t = JL^n \begin{pmatrix} -\alpha * u_2 \\ -\alpha * u_1 \\ -\alpha * u_3 \\ -\alpha * u_4 \end{pmatrix}. \tag{27}$$

When $M=1$, the system (27) is the integrable coupling of the generalized Kaup–Newell hierarchy.[10] When $M>1$, the (27) is the multicomponent integrable coupling of the multicomponent generalized Kaup–Newell hierarchy.

V. CONCLUSION AND REMARK

In this paper, a new loop algebra $\tilde{F}_M$ and Tu scheme are proposed to construct a multicomponent integrable couplings with two arbitrary functions of the multicomponent generalized Kaup–Newell hierarchy. It was shown that the obtained integrable couplings is integrable in the Lax sense and contains two arbitrary functions of old potentials (u_1,u_2) and new potentials (u_3,u_4) which are different from those in Refs. 16–18. Searching for new and multicomponent integrable systems is an important and difficult topic in integrable theory. It is obvious that the proposed method in this paper provides an efficient approach and a guideline to find new and multicomponent integrable systems. The loop algebra presented here can be used to other known integrable hierarchies of soliton equation for generating the multicomponent systems. But there are two open problems. How to improve the loop algebra $\tilde{F}_M$ such that the obtained multicomponent hierarchies are Liouville integrable and possess Hamiltonian structures? How to extend the proposed method for constructing integrable couplings of nonisospectral problem and corresponding evolution equation hierarchy? These problems are worthwhile studying in the future.

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On toric geometry, Spin(7) manifolds, and type II superstring compactifications

Adil Belhaj[a)]
Instituto de Física Teórica, C-XVI, Universidad Autónoma de Madrid, E-28049-Madrid, Spain

Jørgen Rasmussen[b)]
Centre de Recherches Mathématiques, Université de Montréal, C.P. 6128, Succursale Centre-ville, Montréal, PQ, Canada H3C 3J7

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We consider type II superstring compactifications on the singular Spin(7) manifold constructed as a cone on SU(3)/U(1). Based on a toric realization of the projective space $\mathbb{C}\mathbf{P}^2$, we discuss how the manifold can be viewed as three intersecting Calabi–Yau conifolds. The geometric transition of the manifold is then addressed in this setting. The construction is readily extended to higher dimensions where we speculate on possible higher-dimensional geometric transitions. Armed with the toric description of the Spin(7) manifold; we discuss a brane/flux duality in both type II superstring theories compactified on this manifold. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1873038]

I. INTRODUCTION

Calabi–Yau conifold transitions in superstring compactifications have been studied intensively over the last couple of years. These transitions have become a standard tool in understanding large N dualities. An example of such a duality is the equivalence of the SU(N) Chern–Simons theory on $\mathbf{S}^3$ for large N, and the closed topological strings on the resolved conifold.[1] A further example has been obtained by embedding these results in type IIA superstring theory.[2] In particular, the scenario with N $D6$-branes wrapped around the $\mathbf{S}^3$ of the deformed conifold $T^*\mathbf{S}^3$ for large N has been found to be equivalent to type IIA superstrings on the resolved conifold with N units of $R-R$ two-form fluxes through $\mathbf{S}^2$. The latter thus gives the strong-coupling description of the weak-coupling physics of the former.[1] This result has been lifted to the 11-dimensional M-theory[3] where it corresponds to a so-called flop duality in M-theory compactified on a manifold with G_2 holonomy, for short, a G_2 manifold.

Quite recently, similar studies have been done in three dimensions using either type IIA superstring compactification on a G_2 manifold,[4,5] or M-theory compactified on a Spin(7) manifold.[5] This Spin(7) manifold is constructed as a cone on SU(3)/U(1). Upon reduction of the M-theory case to 10 dimensions, the original geometric transition involving a collapsing $\mathbf{S}^5$ and a growing $\mathbb{C}\mathbf{P}^2$ may be interpreted as a transition between two phases described by wrapped $D6$-branes or $R-R$ fluxes, respectively.

An objective of the present work is to continue the study of geometric transitions and brane/flux dualities in lower dimensions. We shall thus consider type II superstrings propagating on the same Spin(7) manifold as above. By comparison with the known results for the Calabi–Yau conifold transition, in particular, we conjecture new brane/flux dualities in two dimensions. The type IIA and type IIB superstrings are treated separately, and we find that the resulting gauge theories in two dimensions have only one supercharge each, so that $\mathcal{N}=1/2$ in both cases.

a)Electronic mail: adil.belhaj@uam.es
b)Electronic mail: rasmusse@crm.umontreal.ca

The present study utilizes a toric geometry description of the Spin(7) manifold. We find that the manifold can be viewed as three intersecting Calabi–Yau conifolds associated to a triangular toric diagram. This result offers a picture for understanding the topology-changing transition of the Spin(7) manifold. It also allows us to discuss the aforementioned brane/flux transition based on an analysis of type II superstrings on the individual Calabi–Yau conifolds.

Our toric description of the Spin(7) manifold may be extended to higher-dimensional manifolds thus suggesting that (generalized) geometric transitions may play a role in higher dimensions as well. We propose an explicit hierarchy of pairs of geometries related by such transitions.

The remaining part of this paper is organized as follows. In Sec. II, we use toric geometry to discuss the Calabi–Yau conifold transition and its extension to the Spin(7) manifold, and speculate on a further generalization to higher dimensions. We then turn to compactifications of superstrings in Sec. III. Since our analysis is based on the toric description of the Spin(7) manifold, our results are deduced from similar results on compactifications on Calabi–Yau conifolds. The associated brane/flux dualities are discussed separately for type IIA and type IIB superstring propagations. Section IV contains some concluding remarks.

II. TORIC GEOMETRY AND GEOMETRIC TRANSITIONS

A. Projective spaces and odd-dimensional spheres

As a description of projective spaces in terms of toric geometry lies at the heart of our study of superstring compactifications, we shall review it here. Odd-dimensional (real) spheres are equally important in our analysis and are therefore also discussed here.

The simplest (complex) projective space is $\mathbb{C}\mathbf{P}^1$ with a toric U(1) action having two fixed points, v_1 and v_2, corresponding to the North and South poles, respectively, of the (real) two-sphere $\mathbf{S}^2 \sim \mathbb{C}\mathbf{P}^1$. In this way, $\mathbb{C}\mathbf{P}^1$ may be viewed as the interval $[v_1, v_2]$,

$$v_1 \text{———} v_2 \tag{1}$$

referred to as the toric diagram, with a circle on top which vanishes at the endpoints v_1 and v_2.

Embedded in $\mathbb{C}^3$, $\mathbb{C}\mathbf{P}^2$ may be described as the space of three complex numbers (z_1, z_2, z_3) not all zero, modulo the identification $(z_1, z_2, z_3) \sim (\lambda z_1, \lambda z_2, \lambda z_3)$ for all nonzero $\lambda \in \mathbb{C}$. Alternatively, $\mathbb{C}\mathbf{P}^2$ is the (complex) two-dimensional space with a toric $U(1)^2$ action with three fixed points, v_1, v_2, and v_3. Its toric diagram is the triangle $(v_1 v_2 v_3)$

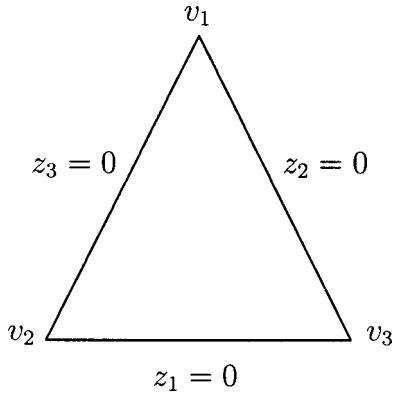

(2)

describing the intersection of three $\mathbb{C}\mathbf{P}^1$'s. Each of the three edges, $[v_1, v_2]$, $[v_2, v_3]$, and $[v_3, v_1]$, is characterized by the vanishing of one of the homogeneous coordinates, $z_3 = 0$, $z_1 = 0$ or $z_2 = 0$, respectively. Each edge is stable under the action of a subgroup of $U(1)^2$—two of them being the two U(1) factors, while the third subgroup is the diagonal one. This toric realization of $\mathbb{C}\mathbf{P}^2$ can be viewed as the triangle $(v_1 v_2 v_3)$ with a torus, $\mathbf{T}^2$, on top which collapses to a circle at an edge and to a point at a vertex.

This representation is readily extended to the n-dimensional projective space $\mathbb{C}\mathbf{P}^n$ where we have a $\mathbf{T}^n$ fibration over an n-dimensional simplex (regular polytope), see Ref. 6, for example. In

this case, the $\mathbf{T}^n$ collapses to a $\mathbf{T}^{n-1}$ on each of the n faces of the simplex, and to a $\mathbf{T}^{n-2}$ on each of the $(n-2)$-dimensional intersections of these faces, etc. We recall that $\mathbb{C}\mathbf{P}^n$ is defined similarly to $\mathbb{C}\mathbf{P}^2$ in terms of $n+1$ homogeneous coordinates modulo the identification $(z_1,\ldots,z_{n+1}) \sim (\lambda z_1,\ldots,\lambda z_{n+1})$.

The odd-dimensional (real) spheres admit a similar description. The one-sphere, for example, is trivially realized as a $\mathbf{T}^1 \sim \mathbf{S}^1$ over the zero-simplex—a point. The three-sphere may be realized as a $\mathbf{T}^2$ over a one-simplex—a line segment as the one in (1). This may be extended to the $(2n+1)$-dimensional sphere $\mathbf{S}^{2n+1}$ which may be described as a $\mathbf{T}^{n+1}$ over an n-simplex. Of particular interest is the five-sphere $\mathbf{S}^5$ which in this way may be realized as the triangle (2) with a $\mathbf{T}^3$ on top (whereas $\mathbb{C}\mathbf{P}^2$ had a $\mathbf{T}^2$ on top). It is stressed that it is for $n=1$ only that the even-dimensional sphere $\mathbf{S}^{2n}$ is equivalent to $\mathbb{C}\mathbf{P}^n$.

To illustrate this toric description of odd-dimensional spheres, let us add a couple of comments on $\mathbf{S}^5$ realized as a $\mathbf{T}^3$ over a triangle. As in (2), an edge of the triangle corresponds to the vanishing of one of the three complex coordinates of the embedding space $\mathbb{C}^3$. Each edge of the triangle (2) is stable under the action of one of the three U(1) factors of $\mathrm{U}(1)^3$ associated to $\mathbf{T}^3$. The three-torus itself collapses to a two-torus $\mathbf{T}^2$ at an edge and to a circle at a vertex. We may thus view $\mathbf{S}^5$ as three intersecting three-spheres over the triangle (2). As opposed to the toric description of $\mathbb{C}\mathbf{P}^2$ as a $\mathbf{T}^2$ over a triangle, the diagonal U(1) of $\mathrm{U}(1)^3$ in the $\mathbf{S}^5$ description has no fixed points. This is natural from the realization of $\mathbb{C}\mathbf{P}^2$ as $\mathbf{S}^5$ modulo U(1).

B. Calabi–Yau conifold

We shall also make use of the noncompact Calabi–Yau threefold defined in $\mathbb{C}^4$ by the equation

$$uv - xy = 0. \tag{3}$$

It may be viewed as the singular cone on the five-dimensional base $\mathbf{S}^2 \times \mathbf{S}^3$ and is therefore referred to as the Calabi–Yau conifold. The singularity is located at the origin and may be turned into a regular point by blowing it up. There are basically two ways of doing that, referred to as resolution and deformation, respectively. Resolving the singularity consists in replacing the singular point by a $\mathbb{C}\mathbf{P}^1$. In this way, the local geometry is given by an $O(-1)+O(-1)$ bundle over $\mathbb{C}\mathbf{P}^1$. The smooth manifold thus obtained is called the resolved conifold and is of topology $\mathbb{R}^4 \times \mathbb{C}\mathbf{P}^1$. In the case of complex deformation, the conifold singularity is removed by modifying the defining algebraic equation (3) by introducing the complex parameter μ,

$$uv - xy = \mu, \tag{4}$$

while keeping the Kähler structure. The origin is thereby replaced by $\mathbf{S}^3$, and the local geometry is given by $T^*\mathbf{S}^3$ of topology $\mathbb{R}^3 \times \mathbf{S}^3$. This is called the deformed conifold and is related to the resolved conifold by the so-called conifold transition.

This conifold transition admits a representation in toric geometry, where it can be understood as an enhancement or breaking, respectively, of the toric circle actions. On the one hand, the $O(-1)+O(-1)$ bundle over $\mathbb{C}\mathbf{P}^1$ has only one toric U(1) action, identified with the toric action on $\mathbb{C}\mathbf{P}^1$ itself, while the deformed conifold $T^*\mathbf{S}^3$ has a toric $\mathrm{U}(1)^2$ action since the spherical part can be viewed as a $\mathbf{T}^2$ over a line segment. Referring to (4), the torus is generated by the two U(1) actions

$$(u,v) \to (e^{i\theta_1}u, e^{-i\theta_1}v), \quad (x,y) \to (e^{i\theta_2}x, e^{-i\theta_2}y) \tag{5}$$

with θ_i real. Thus, the blown-up $\mathbf{S}^3$ may be described by the complex interval $[0,\mu]$ with the two circles parametrized by θ_i on top, where $\mathbf{S}^1(\theta_1)$ collapses to a point at μ while $\mathbf{S}^1(\theta_2)$ collapses to a point at 0. The transition occurs when one of these circles refrains from collapsing while the other one collapses at both interval endpoints. This breaks the toric $\mathrm{U}(1)^2$ action to U(1), and the missing U(1) symmetry has become a real line (over $\mathbb{C}\mathbf{P}^1$). The resulting geometry is thus the resolved conifold. The following picture may help to illustrate this transition which can go in both directions:

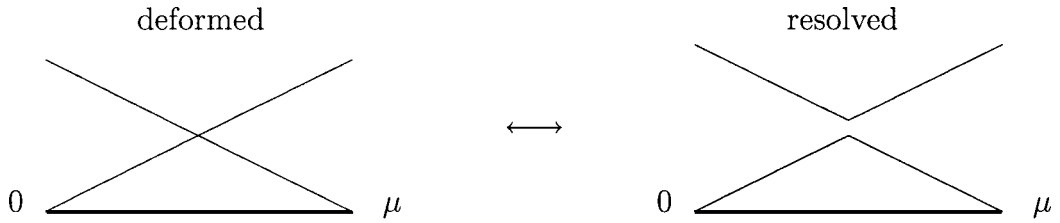

(6)

The top, thin and piecewise straight line in the resolved part of (6) corresponds to the extra $\mathbb{R}$ while the remaining three thin lines (the two straight lines in the deformed part, and the lower, thin and piecewise straight line segment in the resolved part) indicate the U(1)'s. The two thick line segments represent the underlying interval.

A somewhat pragmatic way of viewing the conifold transition is based on the conical structure of the conifold itself as a cone on $\mathbf{S}^2 \times \mathbf{S}^3$. As described in Ref. 4, an n-dimensional cone on an $(n-1)$-dimensional compact space Y with metric $\mathrm{d}\Omega^2$ has metric

$$\mathrm{d}s^2 = \mathrm{d}r^2 + r^2\,\mathrm{d}\Omega^2. \tag{7}$$

It has a singularity at the origin unless $Y = \mathbf{S}^{n-1}$ and $\mathrm{d}\Omega^2$ is the standard round metric. In that case the cone corresponds to $\mathbb{R}^n$. Now, the deformed conifold is obtained by pulling the conical structure off of the $\mathbf{S}^3$ factor in the base, while maintaining it on the $\mathbf{S}^2$ factor. The latter is then equivalent to $\mathbb{R}^3$ and we have recovered the $\mathbb{R}^3 \times \mathbf{S}^3$ structure of the deformed conifold. The resolved conifold is obtained in a similar way by pulling off the conical structure of the $\mathbf{S}^2$ factor.

C. Spin(7) manifolds

Here we shall present a picture for understanding the topology-changing geometric transition of the Spin(7) manifold discussed in Ref. 5 and alluded to in Sec. I. First we recall that a Spin(7) manifold is a real eight-dimensional Riemannian manifold with holonomy group Spin(7). As in the case of Calabi–Yau and G_2 manifolds, there are several such geometries.[7] The example we shall be interested in may be described as a singular real cone over the seven-dimensional Aloff–Wallach (coset) space SU(3)/U(1). It was argued in Ref. 5 that there are two ways of blowing up the singularity, replacing the singularity by either $\mathbb{C}\mathbf{P}^2$ or $\mathbf{S}^5$. The resulting smooth Spin(7) manifolds have topologies,

$$\text{resolution,} \quad \text{Spin}(7){:}\mathbb{R}^4 \times \mathbb{C}\mathbf{P}^2 \quad (\text{Calabi} - \text{Yau,} \quad \mathbb{R}^4 \times \mathbb{C}\mathbf{P}^1) \tag{8}$$

and

$$\text{deformation,} \quad \text{Spin}(7){:}\mathbb{R}^3 \times \mathbf{S}^5 \quad (\text{Calabi} - \text{Yau,} \quad \mathbb{R}^3 \times \mathbf{S}^3), \tag{9}$$

and are referred to as resolution and deformation, respectively, due to the similarity with the Calabi–Yau conifold discussed above [and indicated in (8) and (9)].

Our aim here is to re-address the transition between these two manifolds using toric geometry. As described in the following, the basic idea is to view the singular Spin(7) manifold [the real cone on SU(3)/U(1)] as three intersecting Calabi–Yau conifolds associated to the triangular toric diagram (2). To reach this picture, we first recall that a deformed Spin(7) manifold is obtained by blowing up an $\mathbf{S}^5$, while a resolved Spin(7) manifold is obtained by blowing up a $\mathbb{C}\mathbf{P}^2$. Deformed and resolved conifolds, on the other hand, are obtained by blowing up an $\mathbf{S}^3$ or a $\mathbb{C}\mathbf{P}^1$, respectively. Since an $\mathbf{S}^5$ may be represented by three intersecting three-spheres, while $\mathbb{C}\mathbf{P}^2$ may be represented by three intersecting two-spheres, we thus see that the deformed and resolved Spin(7) manifolds correspond to three intersecting conifolds being deformed or resolved, respectively.

To recapitulate this, let us consider $\mathbb{C}^3$ parametrized by (z_1, z_2, z_3). A five-sphere is obtained by imposing the constraint

$$|z_1|^2 + |z_2|^2 + |z_3|^2 = r \tag{10}$$

(with r real and positive), while the additional identification

$$(z_1, z_2, z_3) \sim (e^{i\theta} z_1, e^{i\theta} z_2, e^{i\theta} z_3) \tag{11}$$

(with θ real) will turn it into a $\mathbb{C}\mathbf{P}^2$. In either case, r measures the size. With both conditions imposed, we can obtain the three resolved Calabi–Yau conifolds

$$\mathbb{R}^4 \times \mathbb{C}\mathbf{P}^1 (z_k = 0), \quad k = 1,2,3 \tag{12}$$

embedded in $\mathbb{R}^4 \times \mathbb{C}^3$, simply by setting one of the coordinates equal to 0. With reference to the triangle (2), this means that the resolution of the Spin(7) singularity reached by blowing up a $\mathbb{C}\mathbf{P}^2$ may be described by three intersecting resolved conifolds over the triangle (2). Likewise, the deformation of the Spin(7) singularity constructed by blowing up an $\mathbf{S}^5$ may be realized as three intersecting deformed Calabi–Yau conifolds

$$\mathbb{R}^3 \times \mathbf{S}^3 (z_k = 0), \quad k = 1,2,3 \tag{13}$$

over the same triangle. This description is thus based on our toric representation of $\mathbf{S}^5$ as a $\mathbf{T}^3$ over a triangle. As already mentioned, this construction collapses to a $\mathbf{T}^2$ over an edge for $z_k = 0$ where $k = 1$, 2 or 3, and it is recalled that the resulting $\mathbf{T}^2$ over a line segment corresponds to $\mathbf{S}^3$.

Since the basic intersection of the deformed or resolved conifolds is governed by the constituent three- or two-spheres, one may describe the intersection of the conifolds by the intersection matrices associated to $\mathbf{S}^5$ or $\mathbb{C}\mathbf{P}^2$, respectively. They read

$$M_{\text{def}} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad M_{\text{res}} = \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}. \tag{14}$$

We emphasize that the Spin(7) transition in our picture is accompanied by Calabi–Yau conifold transitions. In the transition from the resolved Spin(7) manifold (8) to the deformed one (9), for example, this indicates that the collapsing $\mathbb{C}\mathbf{P}^2$ and its constituent two-spheres are replaced by $\mathbf{S}^5$ and its constituent three-spheres. This is at the core of the dualities in the phase transition of the compactified superstrings to be discussed below.

One may attempt to illustrate the geometric transitions of Spin(7) manifolds by generalizing (6). The following proposal extends readily to higher dimensions (see below), and reads

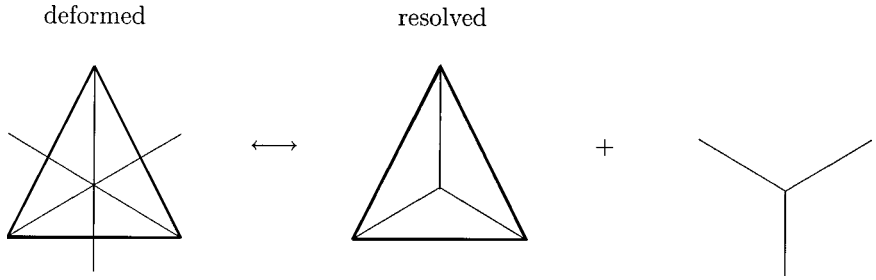

(15)

The configuration to the left is a representation of the $\mathbf{S}^5$ part of the deformed Spin(7) manifold, in which the three thin lines represent the three U(1) factors. The counting is less obvious to the right of the arrow, as the triangular part represents the $\mathbb{C}\mathbf{P}^2$ part of the resolved Spin(7) manifold. The inscribed three-vertex in thin line segments thus corresponds to two U(1) factors only. The three-vertex to the far right represents the extra $\mathbb{R}$ in the resolved scenario (8).

The Spin(7) transition may be viewed as taking place when passing a particular point while moving along a particular curve in the moduli space of Spin(7) manifolds. The point corresponds to the singular Spin(7) manifold, whereas the remaining points on the curve are associated to the deformed and resolved Spin(7) manifolds. In one direction away from the singular point, the

points correspond to the deformed manifolds with the size r of the blown-up $\mathbf{S}^5$ parametrizing that part of the curve. Likewise, the other direction away from the singular point is parametrized by the size r of the blown-up $\mathbb{C}\mathbf{P}^2$ in the resolved Spin(7) manifold. The singular point is shared as it is reached from either side when the relevant r vanishes, $r=0$.

In the interpretation of the Spin(7) manifold as three intersecting Calabi–Yau manifolds over a triangle, we see that the Spin(7) transition corresponds to all three Calabi–Yau manifolds undergoing simultaneous conifold transitions. We find it an interesting problem to understand the geometries associated to individual conifold transitions and hope to report on it elsewhere. Our graphic representation (15) [and (6)] does not seem to shed light on this as it is based on the transition of the full blow-ups, i.e., $\mathbf{S}^5$ and $\mathbb{C}\mathbf{P}^2$, and not on their constituent three- and two-spheres.

D. On possible extensions

It seems possible to extend our previous analysis of the Spin(7) manifold in terms of intersecting Calabi–Yau manifolds to higher dimensions. To this end, let us consider the complex $(n+1)$-dimensional space $\mathbb{C}^{n+1}$ parametrized by $(z_1,\ldots,z_{n+1})$. A $(2n+1)$-dimensional sphere is obtained by imposing the constraint

$$\sum_{j=1}^{n+1} |z_j|^2 = r \tag{16}$$

(with r real and positive), while the additional identification

$$(z_1,\ldots,z_{n+1}) \sim (e^{i\theta}z_1,\ldots,e^{i\theta}z_{n+1}) \tag{17}$$

(with θ real) will turn it into $\mathbb{C}\mathbf{P}^n$. In either case, r measures the size of the resulting space. Since $\mathbf{S}^{2n+1}$ can be described as a $\mathbf{T}^{n+1}$ over an n-simplex it supports a toric $\mathrm{U}(1)^{n+1}$ action whereas $\mathbb{C}\mathbf{P}^n$ (which may be realized as a $\mathbf{T}^n$ over an n-simplex) admits a toric $\mathrm{U}(1)^n$ action. The additional U(1) is the one used in the identification (17). As in the picture (6), we are thus expecting that a geometric transition can take place, replacing a U(1) by the one-dimensional real line $\mathbb{R}$. Since the U(1) is associated to one of the $\mathbf{S}^1$ factors of $\mathbf{T}^{n+1}$, the transition essentially amounts to replacing $\mathbf{T}^{n+1}$ by $\mathbf{T}^n\times\mathbb{R}$. Our interest is in real fibrations over the spaces $\mathbf{S}^{2n+1}$ and $\mathbb{C}\mathbf{P}^n$ so the relevant geometric transitions would read

$$\text{(deformed)}\quad \mathbb{R}^m\times\mathbf{S}^{2n+1} \leftrightarrow \mathbb{R}^{m+1}\times\mathbb{C}\mathbf{P}^n \quad \text{(resolved)}. \tag{18}$$

With $m=3$, we expect to be able to describe the transition (18) in terms of Calabi–Yau conifolds. Using arguments similar to the Spin(7) example above, this generalized geometric transition should be related to $\frac{1}{2}n(n+1)$ intersecting conifolds over the n-simplex, where the number of conifolds is equal to the number of one-dimensional edges of the simplex. One should also expect to be able to describe the transition in terms of $\frac{1}{6}n(n^2-1)$ intersecting Spin(7) manifolds over the n-simplex, where the number of them is equal to the number of two-dimensional faces of the simplex. We hope to address this further elsewhere.

The extension of the transition picture (15) to higher dimensions is based on $\mathbb{C}\mathbf{P}^n$ and $\mathbf{S}^{2n+1}$ admitting descriptions as $\mathbf{T}^n$ and $\mathbf{T}^{n+1}$ fibrations, respectively, over an n-simplex. One chooses an extra point different from the $n+1$ vertices of the n-simplex in such a way that any subset of $q<n+2$ nodes out of the total of $n+2$ points gives rise to a $(q-1)$-simplex. A natural choice is the center of the original (regular) n-simplex. To represent $\mathbf{S}^{2n+1}$, one then draws thin lines from the vertices through this extra point, where the thin lines represent the U(1) factors of $\mathrm{U}(1)^{n+1}$, cf. (15). The projective counterpart, $\mathbb{C}\mathbf{P}^n$, is represented by ending these thin lines at the common point, resulting in an $(n+1)$-vertex inscribed in the n-simplex. This inscribed vertex corresponds to $\mathrm{U}(1)^n$. Finally, the real line $\mathbb{R}$ may be represented by a free $(n+1)$-vertex, and the graphical representation of the transition (18) is a higher-dimensional version of (15).

The conifold analysis based on the toric variety $\mathbb{C}\mathbf{P}^2$ could alternatively be extended by blowing up some generic points. With the number of points restricted as $k=1,2,3$, this defines a so-called toric del Pezzo surface denoted dP_k. The blowing up consists in replacing a point by $\mathbb{C}\mathbf{P}^1$ with a line segment as its toric diagram. The full del Pezzo surface will thus have a polygon with $k+3$ legs as its toric diagram.

III. TYPE II SUPERSTRING COMPACTIFICATIONS

A. Compactification on conifold

Based on the Calabi–Yau conifold transition discussed above, Gopakumar and Vafa have argued that the SU(N) Chern–Simons theory on $\mathbf{S}^3$ for large N is dual to topological strings on the resolved conifold.[1] In this way, the 't Hooft expansion of the Chern–Simons free energy has been shown to be in agreement, for all genera, with the topological string amplitudes on the resolved conifold. This duality has subsequently been embedded in type IIA superstring theory,[2] where it was proposed that N $D6$-branes wrapped around the three-sphere of the deformed conifold is equivalent (for large N) to type IIA superstrings on the resolved conifold with the $D6$-branes replaced by N units of $R-R$ two-form fluxes through the two-sphere ($\mathbf{S}^2\sim\mathbb{C}\mathbf{P}^1$) in the resolved conifold. This duality thus offers a way of understanding the same physics at strong coupling.

The mirror version in type IIB superstring theory of this duality states that the scenario with N $D5$-branes wrapped around the two-sphere in the resolved conifold, is equivalent (for large N) to three-form fluxes through the $\mathbf{S}^3$ of the deformed conifold. This has been generalized to other Calabi–Yau threefolds where the blown-up geometries involve several $\mathbb{C}\mathbf{P}^1$'s.[8–14]

The large N duality in type IIA superstring theory has also been lifted to M-theory[3,4] (see also Ref. 15) where it is known to give a so-called flop duality. Unlike the duality in string theory, the phase transition here is smooth and does not correspond to a topology-changing geometric transition.

B. Compactification on Spin(7) manifold and brane/flux duality

Based on the results on superstrings compactified on Calabi–Yau threefolds and our toric description of the geometric transition of the Spin(7) manifolds, we now consider the two-dimensional gauge theories obtained by compactifying type II superstrings on these Spin(7) manifolds. The idea is to study the consequences of adding N wrapped D-branes to the setup before letting the manifold undergo the geometric transition. In the transition from the resolved to the deformed Spin(7) manifold, we initially have D-branes wrapping $\mathbb{C}\mathbf{P}^2$ (and its constituent two-spheres). We conjecture that they are replaced, under the transition, by $R-R$ fluxes through $\mathbf{S}^5$ (and its constituent three-spheres). Similarly in the transition from deformed to resolved Spin(7) manifolds, we conjecture that D-branes wrapped around $\mathbf{S}^5$ (and its constituent three-spheres) are replaced by $R-R$ fluxes through $\mathbb{C}\mathbf{P}^2$ (and its constituent two-spheres). The kind of D-branes involved and the more detailed phase transition depend on which type II superstrings are propagating on the Spin(7) manifolds. In the following we shall therefore consider type IIA and type IIB separately. We find that they lead to different brane/flux dualities.

1. Duality in type IIB superstring theory

We start by considering type IIB superstrings on the resolved Spin(7) manifold (8). Since the type IIB theory does not support four-forms, one considers $D5$-branes wrapped around $\mathbb{C}\mathbf{P}^2$. A two-dimensional U(N) gauge model can be obtained by wrapping N $D5$-branes on $\mathbb{C}\mathbf{P}^2$. The volume of $\mathbb{C}\mathbf{P}^2$ described by r (10) is proportional to the inverse of the gauge coupling squared. This two-dimensional model has only one supercharge so $\mathcal{N}=1/2$. Now, when the manifold undergoes the geometric transition to the deformed Spin(7) manifold (9), the N $D5$-branes disappear and we expect a dual physics with N units of $R-R$ three-fluxes through the compact three-cycles, $\mathbf{S}^3$, in the intersecting Calabi–Yau threefolds. These fluxes could be accompanied by some

NS–NS fluxes through the noncompact dual three-cycles in the six-dimensional deformed conifolds. In order to handle the associated divergent integrals, one would have to introduce a cutoff to regulate the infinity.[9]

2. Duality in type IIA superstring theory

Here we start with type IIA superstrings on the deformed Spin(7) manifold (9). In this case, a two-dimensional U(N) gauge theory can be obtained by wrapping N $D6$-branes around $\mathbf{S}^5$. As above, this gauge model has only one supercharge, so again $\mathcal{N}=1/2$. At the transition point, the $D6$-branes disappear and are replaced by $R-R$ two-form fluxes through the two-spheres embedded in $\mathbb{C}\mathbf{P}^2$ in the resolved Spin(7) manifold (8).

One could wonder if there is an M-theory interpretation of this type IIA transition. Let us therefore consider a nine-dimensional manifold X_9 with a U(1) isometry. M-theory compactified on X_9 is then equivalent to type IIA superstrings compactified on $X_9/\mathrm{U}(1)$. We start with the resolved Spin(7) manifold (8) and identify the extra eleventh compact dimension of M-theory with the $\mathbf{S}^1$ that generates (11). In this way, the extra M-theory circle becomes the fiber in the definition of $\mathbf{S}^5$ as an $\mathbf{S}^1$ fibration over $\mathbb{C}\mathbf{P}^2$. We thus end up with an $\mathbb{R}^4$ bundle over $\mathbf{S}^5$ as the compactification space in M-theory. As a consequence, the moduli space of M-theory on such a background is parametrized by the real parameter r defining the volume of $\mathbf{S}^5$ (10), and cannot be complexified by the C field. Starting with the resolved Spin(7) manifold, on the other hand, the eleventh M-theory dimension is obtained by extending $\mathbb{R}^3$ to $\mathbb{R}^4$ with the isometry being a trivial U(1) action on the fiber $\mathbb{R}^4$. Using arguments similar to those in Ref. 3, we conjecture that this lift to M-theory gives rise to a (smooth) flop transition in the $\mathbb{R}^4$ bundle over $\mathbf{S}^5$ where a five-sphere collapses and is replaced by a five-sphere. In our scenario, however, the physics resulting from the type IIA superstring compactification undergoes a singular phase transition.

IV. DISCUSSION

Based on toric geometry, we have studied geometric transitions of Spin(7) manifolds. Our framework allowed us to discuss extensions to higher dimensions. It also made it possible to address straightforwardly type II superstring compactifications on Spin(7) manifolds, from which some brane/flux dualities were extrapolated.

Our work opens up for further studies. One interesting problem is to understand better the geometries involved in our proposal for higher-dimensional geometric transitions. Another question is related to the toric description of the Spin(7) manifolds as intersecting Calabi–Yau threefolds over a triangle where the Spin(7) transition corresponds to three simultaneous conifold transitions. A natural question concerns the geometries associated to individual conifold transitions. Of potential importance to superstring and M-theory compactifications, one should then study what the physical implications of such transitions would be. It would also be interesting to understand the link between our results and the ones in Ref. 16 based on string compactifications on Calabi–Yau fourfolds. One approach to this problem could be to consider the Spin(7) manifold as a Calabi–Yau fourfold modulo an involution, thus ensuring the same number of supersymmetries. We hope to report elsewhere on these open problems.

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On a classification of irreducible almost commutative geometries, a second helping

Jan-Hendrik Jureit[a),b)] and Christoph A. Stephan[a),c)]
Centre de Physique Théorique, CNRS-Luminy, Case 907
13288 Marseille Cedex 9, France

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We complete the classification of almost commutative geometries from a particle physics point of view given by Iochum, Schücker, and Stephan, J. Math. Phys. (to be published). Four missing Krajewski diagrams will be presented after a short introduction into irreducible, nondegenerate spectral triples. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1876873]

I. INTRODUCTION

Alain Connes' noncommutative geometry[1–4] allows in an elegant way to unify gravity and the standard model of particle physics. A central role in this formalism is played by almost commutative spectral triples $(\mathcal{A},\mathcal{H},\mathcal{D})$ which decompose into an external and an internal, finite dimensional component. The external part encodes a compact four-dimensional Euclidian space–time and the internal one corresponds to a discrete 0-dimensional Kaluza–Klein space, determining the particle content of the theory. Via the spectral action[5] one recovers the Einstein–Hilbert action combined with the bosonic action of a Yang–Mills–Higgs (YMH) theory. Since the set of allowed YMH theories is determined by the possible internal, finite dimensional spectral triples, we will restrict ourselves to this part. The standard model of particle physics is the most prominent example in this context.

Real, finite dimensional spectral triples have been completely classified by Krajewski[6] and Paschke and Sitarz.[7] A classification of almost commutative geometries from a physical point of view was given in Ref. 8. The spectral triples were required to be irreducible and nondegenerate, in the sense that the Hilbert space was chosen to be as small as possible with nondegenerate fermion masses. Heavy use was made of Krajewski's diagrammatic method, which will be described briefly below. The main obstacle in finding all physically relevant almost commutative spectral triples is the sheer mass of diagrams which must be considered. Since this is a purely combinatorial problem it is convenient to let a computer do the tedious task. The cases of one and two matrix algebras can still be done by hand. But already three algebras produce hundreds of diagrams and one easily loses sight.

Therefore we developed an algorithm to calculate these diagrams and used the known results from Ref. 8 to test and calibrate the program. The main goal was to extend the calculations to more than three algebras, where we expect thousands of possible irreducible spectral triples. During the calibration it turned out that four diagrams were overlooked in the case of three algebras. To complete the proof we will present these four missing diagrams and their models in this paper. The algorithm to compute the diagrams and the results for the case of four algebras will be presented elsewhere.

[a)]Also at Université de Provence and Universität Kiel.
[b)]Electronic mail:jureit@cpt.univ-mrs.fr
[c)]Electronic mail: stephan@cpt.univ-mrs.fr

In Sec. II we give some basic definitions and briefly introduce Krajewski diagrams and irreducible, nondegenerate spectral triples. The missing diagrams for three algebras are presented in Sec. III.

II. BASIC DEFINITIONS, IRREDUCIBILITY, AND NONDEGENERACY

In this section we give the necessary basic definitions for a classification of almost commutative geometries from a particle physics point of view. As mentioned above only the 0-dimensional part will be taken into account, so we restrict ourselves to real, S^0-real, finite spectral triples $(\mathcal{A},\mathcal{H},\mathcal{D},J,\epsilon,\chi)$. The algebra $\mathcal{A}$ is a finite sum of matrix algebras $\mathcal{A}=\oplus_{i=1}^{N} M_{n_i}(\mathbb{K}_i)$ with $\mathbb{K}_i=\mathbb{R}$, $\mathbb{C}$, $\mathbb{H}$, where $\mathbb{H}$ denotes the quaternions. A faithful representation ρ of $\mathcal{A}$ is given on the finite dimensional Hilbert space $\mathcal{H}$. The Dirac operator $\mathcal{D}$ is a self-adjoint operator on $\mathcal{H}$ and plays the role of the fermionic mass matrix. J is an antiunitary involution, $J^2=1$, and is interpreted as the charge conjugation operator of particle physics. The S^0-real structure ϵ is a unitary involution, $\epsilon^2=1$. Its eigenstates with eigenvalue +1 are the particle states, eigenvalue −1 indicates antiparticle states. The chirality χ as well is a unitary involution, $\chi^2=1$, whose eigenstates with eigenvalue $+1(-1)$ are interpreted as right (left) particle states. These operators are required to fulfill Connes' axioms for spectral triples:

(i)
$$[J,\mathcal{D}]=[J,\chi]=[\epsilon,\chi]=[\epsilon,\mathcal{D}]=0, \quad \epsilon J=-J\epsilon, \quad \mathcal{D}\chi=-\chi\mathcal{D},$$

$$[\chi,\rho(a)]=[\epsilon,\rho(a)]=[\rho(a),J\rho(b)J^{-1}]=[[\mathcal{D},\rho(a)],J\rho(b)J^{-1}]=0,\ \forall\, a,b\in\mathcal{A}.$$

(ii) The chirality can be written as a finite sum $\chi=\Sigma_i\rho(a_i)J\rho(b_i)J^{-1}$. This condition is called *orientability*.

(iii) The intersection form $\cap_{ij}:=\mathrm{tr}(\chi\rho(p_i)J\rho(p_j)J^{-1})$ is nondegenerate, $\det\cap\neq 0$. The p_i are minimal rank projections in $\mathcal{A}$. This condition is called *Poincaré duality*.

Now the Hilbert space $\mathcal{H}$ and the representation ρ decompose with respect to the eigenvalues of ϵ and χ into left and right, particle and antiparticle spinors and representations,

$$\mathcal{H}=\mathcal{H}_L\oplus\mathcal{H}_R\oplus\mathcal{H}_L^c\oplus\mathcal{H}_R^c, \quad \rho=\rho_L\oplus\rho_R\oplus\overline{\rho_L^c}\oplus\overline{\rho_R^c}.$$

In this representation the Dirac operator has the form

$$\mathcal{D}=\begin{pmatrix} 0 & \mathcal{M} & 0 & 0 \\ \mathcal{M}^* & 0 & 0 & 0 \\ 0 & 0 & 0 & \overline{\mathcal{M}} \\ 0 & 0 & \overline{\mathcal{M}^*} & 0 \end{pmatrix},$$

where $\mathcal{M}$ is the fermionic mass matrix connecting the left-handed and the right-handed fermions.

Connes' axioms, the decomposition of the Hilbert space, the representation and the Dirac operator allow a diagrammatic dipiction. As was shown in Refs. 6,8 this can be boiled down to simple arrows, which encode the intersection form and the fermionic mass matrix. From this information all the ingredients of the spectral triple can be recovered. For our purpose a simple arrow and a double arrow are sufficient. The arrows always point from right fermions (positive chirality) to left fermions (negative chirality). We may also restrict ourselves to the particle part, since the information of the antiparticle part is included by transposing the particle part. We will adopt the conventions of Ref. 8.

The *fluctuation* ${}^f\mathcal{D}$ of the Dirac operator $\mathcal{D}$ is given by a finite collection f of real numbers r_j and algebra automorphisms $\sigma_j\in\mathrm{Aut}(\mathcal{A})^e$ lifted to the Hilbert space $\mathcal{H}$ such that

$$^f\mathcal{D} := \sum_j r_j L(\sigma_j)\mathcal{D}L(\sigma_j)^{-1}, \quad r_j \in \mathbb{R}, \quad \sigma_j \in \mathrm{Aut}(\mathcal{A})^e,$$

where the Lift is given by

$$L(\sigma) = \rho(u)J\rho(u)J^{-1}.$$

The spectral action of this almost commutative spectral triple reduced to the finite part is a functional on the vector space of all fluctuated, finite Dirac operators,

$$V(^f\mathcal{D}) = \lambda\ \mathrm{tr}\left[(^f\mathcal{D})^4\right] - \frac{\mu^2}{2}\ \mathrm{tr}\left[(^f\mathcal{D})^2\right],$$

where λ and μ are positive constants.[1,9] Our task is to find the minima $\hat{}^f\mathcal{D}$ of this action and their spectra.

To classify the almost commutative spectral triples we will impose some extra conditions as in Ref. 8. We will require the spectral triples to be irreducible and nondegenerate according to the following definitions.

Definition 2.1: (i) A spectral triple $(\mathcal{A},\mathcal{H},\mathcal{D})$ is *degenerate* if the kernel of $\mathcal{D}$ contains a nontrivial subspace of the complex Hilbert space $\mathcal{H}$ invariant under the representation ρ on $\mathcal{H}$ of the real algebra $\mathcal{A}$.

(ii) A nondegenerate spectral triple $(\mathcal{A},\mathcal{H},\mathcal{D})$ is *reducible* if there is a proper subspace $\mathcal{H}_0 \subset \mathcal{H}$ invariant under the algebra $\rho(\mathcal{A})$ such that $(\mathcal{A},\mathcal{H}_0,\mathcal{D}|_{\mathcal{H}_0})$ is a nondegenerate spectral triple. If the triple is real, S^0-real and even, we require the subspace $\mathcal{H}_0$ to also be invariant under the real structure J, the S^0-real structure ϵ and under the chirality χ such that the triple $(\mathcal{A},\mathcal{H}_0,\mathcal{D}|_{\mathcal{H}_0})$ is again real, S^0-real and even.

Definition 2.2: The irreducible spectral triple $(\mathcal{A},\mathcal{H},\mathcal{D})$ is *dynamically nondegenerate* if all minima $\hat{}^f\mathcal{D}$ of the action $V(^f\mathcal{D})$ define a nondegenerate spectral triple $(\mathcal{A},\mathcal{H},\hat{}^f\mathcal{D})$ and if the spectra of all minima have no degeneracies other than the three kinematical degeneracies: left–right, particle–antiparticle, and color. Of course in the massless case there is no left–right degeneracy. We also suppose that the color degeneracies are protected by the little group. By this we mean that all eigenvectors of $\hat{}^f\mathcal{D}$ corresponding to the same eigenvalue are in a common orbit of the little group (and scalar multiplication and charge conjugation).

In physicists' language nondegeneracy excludes all models with pairwise equal fermion masses up to color degeneracy. Irreducibility tells us that the Krajewski diagrams, which we must find must not contain more arrows than strictly necessary to satisfy Connes' axioms, especially the Poincaré duality. The last requirement of Definition 2.2 means noncommutative color groups are unbroken. It ensures that the corresponding mass degeneracies are protected from quantum corrections.

III. THE MISSING DIAGRAMS

In this section we will present the diagrams missing in the proof for three algebras in Ref. 8. For every diagram only one representative model will be given. All the other models can be obtained by simply exchanging left with right and particles with antiparticles. On the diagrammatic side this is equivalent to changing the directions of all arrows or reflecting the diagram on its diagonal. Permutations of the algebras in the diagrams are neglected as well, since they lead to the same physical models with a different order of the particles. For every diagram there are several ways to connect the algebras by arrows in accordance with the consistency conditions of Table 1 in Ref. 6. With respect to this, the four diagrams are all computed in the same way and they all fall in the same way. The possibilities of complex conjugating an algebra representation are limited and yield no essentially new models. It should be obvious from the diagrams whether the matrix algebras are complex, real, or quaternionic. In all other cases the choice of the field will

not affect the calculations, so we will not specify the algebras explicitly. For the four missing diagrams, $\mathcal{A}_1$, $\mathcal{A}_2$, $\mathcal{A}_3$ denote the algebras, a, b, c their generic elements and k, ℓ, p the respective size of the matrices.

Diagram 1 yields the representation

$$\rho_L(a,b,c)=\begin{pmatrix} b\otimes 1_k & 0 & 0\\ 0 & c\otimes 1_k & 0\\ 0 & 0 & b\otimes 1_p\end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} \overline{a}\otimes 1_k & 0 & 0\\ 0 & \overline{b}\otimes 1_k & 0\\ 0 & 0 & a\otimes 1_p\end{pmatrix},$$

$$\rho_L^c(a,b,c)=\begin{pmatrix} 1_\ell\otimes a & 0 & 0\\ 0 & 1_p\otimes a & 0\\ 0 & 0 & 1_\ell\otimes \overline{c}\end{pmatrix},\quad \rho_R^c(a,b,c)=\begin{pmatrix} 1_k\otimes a & 0 & 0\\ 0 & 1_\ell\otimes a & 0\\ 0 & 0 & 1_p\otimes \overline{c}\end{pmatrix}.$$

The mass matrix is

$$\mathcal{M}=\begin{pmatrix} M_1\otimes 1_k & 0 & 0\\ 0 & M_2\otimes 1_k & 0\\ 0 & 0 & M_3\otimes 1_p\end{pmatrix},\quad M_1,M_3\in M_{k\times\ell}(\mathbb{C}),\quad M_2\in M_{p\times\ell}(\mathbb{C}),$$

where all three algebras are $M_n(\mathbb{C})$. The fluctuations are

$${}^fM_1=\sum_j r_j v_j M_1 \overline{u_j}^{-1},\quad u_j\in U(\mathcal{A}_1),\quad v_j\in U(\mathcal{A}_2),$$

$${}^fM_2=\sum_j r_j w_j M_2 \overline{v_j}^{-1},\quad w_j\in U(\mathcal{A}_3),$$

$${}^fM_3=\sum_j r_j v_j M_3 u_j^{-1},$$

and the action $V(C_1,C_2,C_3)$ is, with $C_i:={}^fM_i^*{}^fM_i$ equal to

$$4k\left[\lambda\,\mathrm{tr}(C_1)^2-\tfrac{1}{2}\mu^2\,\mathrm{tr}(C_1)\right]+4k\left[\lambda\,\mathrm{tr}(C_2)^2-\tfrac{1}{2}\mu^2\,\mathrm{tr}(C_2)\right]+4p\left[\lambda\,\mathrm{tr}(C_3)^2-\tfrac{1}{2}\mu^2\,\mathrm{tr}(C_3)\right].$$

Counting neutrinos and imposing broken color to be commutative leaves only one case, $k=\ell=p=1$. The fluctuations decouple the ${}^fM_i$ so it is always possible to reach the absolute minimum of the Higgs potential and the triple is degenerate.

Diagram 2 falls in the same way.

Diagram 3 is degenerate in the commutative case and exhibits mass relations in the noncommutative case. The calculation runs along the lines of diagram 8 in Ref. 8.

Diagram 4 yields the representation

$$\rho_L(a,b,c)=\begin{pmatrix} c\otimes 1_k & 0\\ 0 & a\otimes 1_\ell\end{pmatrix},\quad \rho_R(a,b,c)=\begin{pmatrix} \overline{b}\otimes 1_k & 0 & 0\\ 0 & \overline{b}\otimes 1_k & 0\\ 0 & 0 & c\otimes 1_\ell\end{pmatrix},$$

$$\rho_L^c(a,b,c)=\begin{pmatrix} 1_p\otimes a & 0\\ 0 & 1_k\otimes b\end{pmatrix},\quad \rho_R^c(a,b,c)=\begin{pmatrix} 1_\ell\otimes a & 0 & 0\\ 0 & 1_\ell\otimes a & 0\\ 0 & 0 & 1_p\otimes b\end{pmatrix},$$

with possible complex conjugations here and there. The mass matrix is

$$\mathcal{M} = \begin{pmatrix} M_1 \otimes 1_k & M_2 \otimes 1_k & 0 \\ 0 & 0 & M_3 \otimes 1_\ell \end{pmatrix}, \quad M_1, M_2 \in M_{p\times\ell}(\mathbb{C}), \quad M_3 \in M_{k\times p}(\mathbb{C}).$$

The fluctuations are

$$^fM_1 = \sum_j r_j w_j M_1 \overline{v_j}^{-1}, \quad w_j \in U(\mathcal{A}_3), \quad v_j \in U(\mathcal{A}_2),$$

$$^fM_2 = \sum_j r_j w_j M_2 \overline{v_j}^{-1},$$

$$^fM_3 = \sum_j r_j u_j M_3 w_j^{-1}, \quad u_j \in U(\mathcal{A}_1),$$

and the action is

$$V(C_1, C_2, C_3) = 4k\left[\lambda\ \mathrm{tr}(C_1 + C_2)^2 - \tfrac{1}{2}\mu^2\ \mathrm{tr}(C_1 + C_2)\right] + 4p\left[\lambda\ \mathrm{tr}(C_3)^2 - \tfrac{1}{2}\mu^2\ \mathrm{tr}(C_3)\right].$$

The neutrino count and broken color imply $k=\ell=1$ and $p=1$ or $p=2$. The case $k=\ell=p=1$ is obviously degenerate.

For $k=\ell=1$, $p=2$ we have one neutrino. $^fM_3$ fluctuates independently and can be pushed into the absolute minimum of the Higgs potential. Let us set $^fM_1$ and $^fM_2$ into one matrix

$$^fM_{1,2} = \sum_j r_j w_j (M_1, M_2) \begin{pmatrix} \overline{v_j}^{-1} & 0 \\ 0 & \overline{v_j}^{-1} \end{pmatrix}.$$

Since the $\overline{v_j}^{-1} \in \mathbb{C}$ they commute with (M_1, M_2) and so

$$^fM_{1,2} = C(M_1, M_2),$$

where $C \in M_{2\times 2}(\mathbb{C})$ is an arbitrary matrix. M_1 must be linearly independent of M_2 because otherwise they would produce a second neutrino. It follows that (M_1, M_2) is invertible and we can choose C to be its inverse. In this way we reach the absolute minimum of the Higgs potential and the triple is degenerate.

IV. CONCLUSION

The new models discovered with help of the computer complete the proof for up to three algebras given in Ref. 8. We did not find anything of interest from the particle physics point of view but we gained confidence in our algorithm and it seems sensible to compute the case with four algebras.

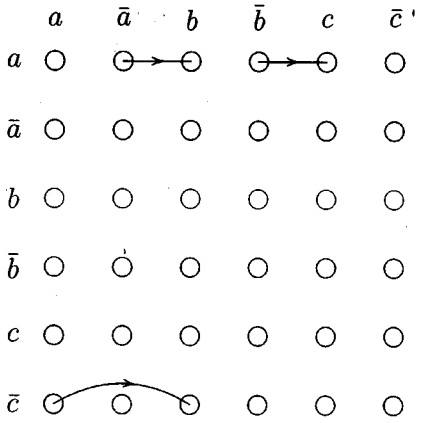

diag. 1

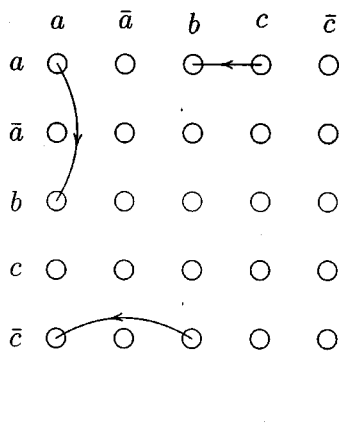

diag. 2

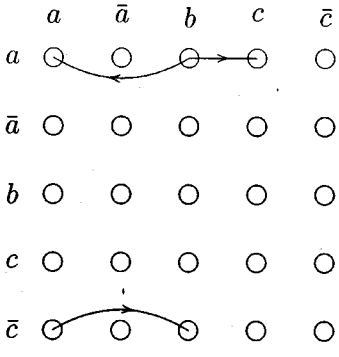

diag. 3

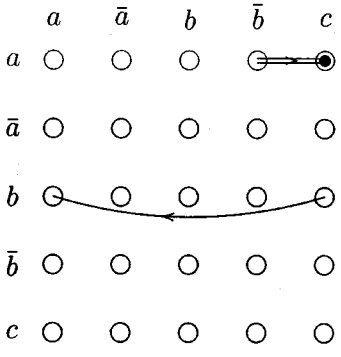

diag. 4

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Spherical functions on homogeneous superspaces

R. B. Zhang[a)]
University of Sydney, School of Mathematics and Statistics, Sydney, NSW 2006, Australia

Y. M. Zou[b)]
University of Wisconsin, Department of Mathematical Sciences, Milwaukee, Wisconsin 53201

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Homogeneous superspaces arising from the general linear supergroup are studied within a Hopf algebraic framework. Spherical functions on homogeneous superspaces are introduced, and the structures of the superalgebras of the spherical functions on classes of homogeneous superspaces are described explicitly. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1868859]

I. INTRODUCTION

We study spherical functions on homogeneous superspaces arising from the complex general linear supergroup. This is the first part of our endeavour to develop a theory of spherical functions on Lie supergroups[8,13] and quantum supergroups.[12,28] The theory of spherical functions on ordinary Lie groups has long reached its maturity (see, e.g., Ref. 26). There also exists extensive literature on spherical functions[9,18,14,3,17] on quantum symmetric spaces.[10,17,3,4,11] However, little seems to be known about spherical functions on Lie supergroups, let alone those on quantum supergroups. On the other hand, supersymmetry and its quantum analogue have become an integral part of modern mathematical physics, and have also permeated many areas of pure mathematics. A good understanding of spherical functions on Lie supergroups and quantum supergroups should facilitate practical means for studying the dynamics of physical systems with classical or quantum supersymmetries.

We choose to work within a Hopf superalgebraic framework to study homogeneous superspaces, as it can incorporate both the Lie supergroup (as defined by Kostant[8]) and quantum supergroup[12,28] cases. Our methodology is similar to that adopted in the literature on quantum homogeneous spaces.[10,17,3,4,11] The starting point is the universal enveloping algebra $\mathrm{U}(\mathfrak{g})$ of the general linear superalgebra $\mathfrak{g}=\mathfrak{gl}(m|n,\mathbb{C})$, which is a cocommutative Hopf superalgebra.[15] A $\mathbb{Z}_2$-graded subalgebra $\mathbb{C}(G)$ (see Definition 3.1) of the dual of the universal enveloping algebra acquires a Hopf superalgebra structure, from which the general linear supergroup can be reconstructed[21] in a manner similar to the Tanakan–Krein theory for compact Lie groups. The universal enveloping algebra admits many Hopf $*$-superalgebra structures, each corresponding to a real form $\mathfrak{g}^{\sigma,\sqrt{i}}$ (see Sec. IV A for definition) of $\mathfrak{g}$. Each Hopf $*$-superalgebra structure θ of $\mathrm{U}(\mathfrak{g})$ induces a Hopf $*$-superalgebraic structure on $\mathbb{C}(G)$. We fix the θ corresponding to one of the compact real forms of $\mathfrak{g}$ [see Eq. (4.3)]. Let $\mathfrak{p}\subset\mathfrak{g}$ be a parabolic subalgebra with Levi factor $\mathfrak{l}$, and let $\mathfrak{k}=\mathfrak{l}\cap\mathfrak{g}^{\sigma,\sqrt{i}}$ be the real form of $\mathfrak{l}$. Then the $*$-subalgebra $\mathbb{C}(K\backslash G)$ of $\mathbb{C}(G)$ invariant with respect to $\mathfrak{k}$ under the left translation defines a homogeneous superspace[12] in the spirit of noncommutative geometry.[2] We shall call this superalgebra the superalgebra of functions on the homogeneous superspace. Next we consider the subspace $\mathbb{C}(K\backslash G/K)$ of $\mathbb{C}(K\backslash G)$ consisting of elements that are

a)Electronic mail: rzhang@maths.usyd.edu.au
b)Electronic mail: ymzou@uwm.edu

invariant with respect to $\mathfrak{k}$ under the right translation. It can be shown that $\mathbb{C}(K\backslash G/K)$ forms a $*$-superalgebra, which will be referred to as the superalgebra of spherical functions on the homogeneous superspace.

Our aim in the present paper is to understand the structures of the superalgebras $\mathbb{C}(K\backslash G)$ and $\mathbb{C}(K\backslash G/K)$. The main results obtained are Theorem 4.2, Lemma 4.5, and Lemma 4.6, which give explicit descriptions of the superalgebra of functions on the homogeneous superspace and the superalgebra of spherical functions. In the case of a homogeneous superspace associated to a maximal rank reductive subgroup of a compact real form of the general linear supergroup, the superalgebra of spherical functions is either the polynomial algebra in one variable or a quotient thereof (Theorems 5.1 and 5.2).

Recall that the space of functions on an ordinary Lie group has another natural algebraic structure with the multiplication defined by convolution. In this context, the counter parts of $\mathbb{C}(K\backslash G)$ and $\mathbb{C}(K\backslash G/K)$ form subalgebras under convolution, where the analogue of $\mathbb{C}(K\backslash G/K)$ is the celebrated Hecke algebra.[26] The Hecke algebras associated with Riemannian symmetric spaces are commutative, and their elements provide the invariant integral operators acting on functions on the symmetric spaces. It is an important problem to develop a theory for such Hecke algebras in the Lie supergroup context, and to investigate properties of supersymmetric spaces from the viewpoint of Hecke algebras. We plan to do this in a future publication, as the problem requires in-depth investigations into the analytical theory of Lie supergroups.

The organization of the paper is as follows. In Sec. II we provide some preliminary material on the complex general linear superalgebra and its invariant theory. In Sec. III we discuss the Hopf superalgebra of functions on the general linear supergroup, and explain how the general linear supergroup itself can be extracted from this Hopf superalgebra.[21] The material in this section is not all new, but it forms the basis for the study of homogeneous superspaces and spherical functions in later sections. Sections IV and V contain the main results of the paper. In Sec. IV A we discuss real forms of the complex general linear superalgebra and general linear supergroup from a Hopf algebraic point of view. The material presented here is largely new, and we believe it to be interesting in its own right. In Sec. IV B we explain the notion of homogeneous superspaces in a Hopf algebraic setting, and in Sec. IV C we investigate the superalgebras of spherical functions on the homogeneous superspaces. In Sec. V we analyze in detail the superalgebras of spherical functions on the projective superspace and other symmetric superspaces arising from maximal rank subgroups of real forms of the general linear supergroup.

II. PRELIMINARIES ON $\mathfrak{gl}(m|n,\mathbb{C})$

We present some background material on the universal enveloping superalgebra of the general linear Lie superalgebra, which will be used later. General references are Refs. 6 and 19.

We shall work on the complex number field $\mathbb{C}$ for simplicity. Let W be a superspace, i.e., a $\mathbb{Z}_2$-graded vector space $W=W_{\bar{0}}\oplus W_{\bar{1}}$, where $W_{\bar{0}}$ and $W_{\bar{1}}$ are the even and odd subspaces, respectively. The elements of $W_{\bar{0}}\cup W_{\bar{1}}$ will be called homogeneous. Define a map $[\ ]: W_{\bar{0}}\cup W_{\bar{1}}\to\mathbb{Z}_2$ by $[w]=\alpha$ if $w\in W_\alpha$. (Quite generally, whenever a symbol like $[w]$ appears in the sequel, it is tacitly assumed that the element w is homogeneous.) The dual superspace ($\mathbb{Z}_2$-graded dual vector space) of W will be denoted by W^*, and the dual space pairing $W^*\otimes W\to\mathbb{C}$ by $\langle,\rangle$.

Denote by $\mathfrak{g}$ the Lie superalgebra $\mathfrak{gl}(m|n,\mathbb{C})$. A standard basis for $\mathfrak{g}$ is $\{E_{ab}|a,b\in\mathbf{I}\}$, where $\mathbf{I}=\{1,2,\ldots,m+n\}$ The element E_{ab} belongs to $\mathfrak{g}_{\bar{1}}$ if $a\leqslant m<b$, or $b\leqslant m<a$, and belongs to $\mathfrak{g}_{\bar{0}}$ otherwise. For convenience, we define the map

$$[\ ]:\mathbf{I}\to\mathbb{Z}_2 \text{ by } [a]=\begin{cases}\bar{0} & \text{if } a\leqslant m,\\ \bar{1} & \text{if } a>m.\end{cases}$$

Then $[E_{ab}]=[a]+[b]$. The supercommutation relations of the Lie superalgebra are given for the basis elements by

$$[E_{ab},E_{cd}] = E_{ad}\delta_{bc} - (-1)^{([a]-[b])([c]-[d])}E_{cb}\delta_{ad}.$$

As usual, we choose the Cartan subalgebra $\mathfrak{h} = \oplus_a \mathbb{C}E_{aa}$. Let $\{\epsilon_a | a \in \mathbf{I}\}$ be the basis of $\mathfrak{h}^*$ such that $\epsilon_a(E_{bb}) = \delta_{ab}$. The space h^* is equipped with a bilinear form $(,):\mathfrak{h}^* \times \mathfrak{h}^* \to \mathbb{C}$ such that $(\epsilon_a, \epsilon_b) = (-1)^{[a]}\delta_{ab}$. The roots of $\mathfrak{g}$ are $\epsilon_a - \epsilon_b$, $a \neq b$, where $\epsilon_a - \epsilon_b$ is even if $[a]+[b]=\overline{0}$ and odd otherwise. We choose as positive roots the elements of $\{\epsilon_a - \epsilon_b | a < b\}$, and as simple roots the elements of $\{\epsilon_a - \epsilon_{a+1} | a < m+n\}$.

The enveloping algebra $\mathrm{U}(\mathfrak{gl}(m|n,\mathbb{C}))$ of $\mathfrak{gl}(m|n,\mathbb{C})$ will be denoted by $\mathrm{U}(\mathfrak{g})$. We shall always regard $\mathfrak{g}$ as embedded in $\mathrm{U}(\mathfrak{g})$ in the natural way. As is well known, $\mathrm{U}(\mathfrak{g})$ forms a $\mathbb{Z}_2$-graded cocommutative Hopf algebra (i.e., a Hopf superalgebra) in the sense of Ref. 15, with

$$\text{comultiplication, } \Delta : \mathrm{U}(\mathfrak{g}) \to \mathrm{U}(\mathfrak{g}) \otimes \mathrm{U}(\mathfrak{g}), \quad \Delta(X) = X \otimes 1 + 1 \otimes X, \quad X \in \mathfrak{g},$$

$$\text{counit, } \quad \epsilon : \mathrm{U}(\mathfrak{g}) \to \mathbb{C}, \quad \epsilon(X) = 0, \quad X \in \mathfrak{g},$$

$$\text{antipode, } \quad S : \mathrm{U}(\mathfrak{g}) \to \mathrm{U}(\mathfrak{g}), \quad S(X) = -X, \quad X \in \mathfrak{g}.$$

In particular, this Hopf superalgebra structure allows us to introduce a natural left $\mathrm{U}(\mathfrak{g})$-module structure on the dual superspace W^* of any left $\mathrm{U}(\mathfrak{g})$-module W, with the $\mathrm{U}(\mathfrak{g})$-action given by

$$U(\mathfrak{g}) \otimes W^* \to W^*, \quad x \otimes \overline{w} \mapsto x\overline{w},$$

$$\langle x\overline{w}, v\rangle := (-1)^{[x][w]}\langle \overline{w}, S(x)v\rangle, \quad \forall\, v \in W.$$

As it stands, the last equation only makes sense for homogeneous $\overline{w} \in W^*$ and homogeneous $x \in \mathrm{U}(\mathfrak{g})$, but it can be extended to all elements of W^* and $\mathrm{U}(\mathfrak{g})$ linearly.

We shall denote by L_λ the irreducible left $\mathrm{U}(\mathfrak{g})$-module with highest weight $\lambda \in \mathfrak{h}^*$. The module L_λ is finite-dimensional if and only if λ is dominant,[7,19] i.e.,

$$2(\lambda, \epsilon_a - \epsilon_{a+1})/(\epsilon_a - \epsilon_{a+1}, \epsilon_a - \epsilon_{a+1}) \in \mathbb{Z}_+ \quad \forall\, a \neq m. \tag{2.1}$$

A basic problem in the representation theory of Lie superalgebras is to understand the weight space decompositions of the finite dimensional irreducible representations. However, the problem turned out to be unexpectedly difficult, resisting solution for some 20 years. Only a few years ago, Serganova[22] succeeded in developing an algorithm to compute formal characters of irreducible representations.

Of particular importance to us here is the contravariant vector module $V = L_{\epsilon_1}$ of $\mathfrak{g}$. It has the standard basis $\{v_a | a \in \mathbf{I}\}$ such that $E_{ab}v_c = \delta_{bc}v_a$, where v_a is even if $a \leqslant m$, and odd otherwise. The dual module V^* of V is the covariant vector module with highest weight $-\epsilon_{m+n}$. It has a basis $\{\overline{v_a} | a \in \mathbf{I}\}$ dual to the standard basis of V, i.e., $\langle \overline{v_a}, v_b\rangle = \delta_{ab}$. The action of $\mathfrak{g}$ on V^* is given by

$$E_{ab}\overline{v_c} = -(-1)^{[a]+[a][b]}\delta_{ac}\overline{v_b}. \tag{2.2}$$

As the antipode of $\mathrm{U}(\mathfrak{g})$ is of order two, there is a $\mathrm{U}(\mathfrak{g})$-module isomorphism between V and its double dual $V^{**} := (V^*)^*$,

$$V \cong V^{**}, \quad v \mapsto v^{**},$$

$$\langle v^{**}, \overline{w}\rangle = (-1)^{[v]}\langle \overline{w}, v\rangle, \quad \forall\, \overline{w} \in V^*.$$

Remark 2.1: (Reference 27) For all $d > 0$, $V^{\otimes d}$ is a semisimple $\mathrm{U}(\mathfrak{g})$-module, which does not contain any one-dimensional submodule.

Let $\mathfrak{S}_d$ be the symmetric group on d letters. There exists a natural action ρ_d of $\mathfrak{S}_d$ on $V^{\otimes d}$ defined in the following way. Let s_i denote the permutation $(i, i+1)$. Then

$$\rho_d(s_i)(v_{a_1} \otimes \cdots \otimes v_{a_{i-1}} \otimes v_{a_i} \otimes v_{a_{i+1}} \otimes v_{a_{i+2}} \cdots \otimes v_{a_d})$$
$$= (-1)^{[a_i][a_{i+1}]} v_{a_1} \otimes \cdots \otimes v_{a_{i-1}} \otimes v_{a_{i+1}} \otimes v_{a_i} \otimes v_{a_{i+2}} \cdots \otimes v_{a_d}.$$

Let us denote by t^d the representation of $\mathrm{U}(\mathfrak{g})$ in $V^{\otimes d}$, and denote by $\mathbb{C}\mathfrak{S}_d$ the group algebra of $\mathfrak{S}_d$. The following result was first proven by Sergeev[24,25] (see Ref. 1 for a detailed treatment).

Theorem 2.1: *The superalgebras* $t^d(\mathrm{U}(\mathfrak{g}))$ *and* $\rho_d(\mathbb{C}\mathfrak{S}_d)$ *are mutual centralizers in* $\mathrm{End}_{\mathbb{C}}(V^{\otimes d})$.

Let W be a finite dimensional $\mathrm{U}(\mathfrak{g})$-module. Let $\pi: \mathrm{U}(\mathfrak{g}) \to \mathrm{End}_{\mathbb{C}}(\mathrm{W})$ be the $\mathrm{U}(\mathfrak{g})$-representation furnished by W. Then $\mathrm{End}_{\mathbb{C}}(\mathrm{W})$ acquires a natural $\mathrm{U}(\mathfrak{g})$-module structure under the action

$$\mathrm{U}(\mathfrak{g}) \otimes \mathrm{End}_{\mathbb{C}}(\mathrm{W}) \to \mathrm{End}_{\mathbb{C}}(\mathrm{W}), \quad x \otimes \phi \mapsto \mathrm{Ad}_x(\phi),$$

$$\mathrm{Ad}_x(\phi) := \sum_{(x)} (-1)^{[x_{(2)}][\phi]} \pi(x_{(1)}) \phi \pi(S(x_{(2)})) \ ,$$

where we have used Sweedler's notation $\Delta(x) = \Sigma_{(x)} x_{(1)} \otimes x_{(2)}$ for the comultiplication of $x \in \mathrm{U}(\mathfrak{g})$. There exists the natural isomorphism $j: W \otimes W^* \cong \mathrm{End}_{\mathbb{C}}(\mathrm{W})$ of $\mathrm{U}(\mathfrak{g})$ modules defined, for any $u \otimes \overline{v} \in W \otimes W^*$ and $w \in W$, by

$$j(u \otimes \overline{v})(w) = \langle \overline{v}, w \rangle u.$$

For any $\mathrm{U}(\mathfrak{g})$-module M, we use the notation $(M)^{\mathrm{U}(\mathfrak{g})}$ to denote the invariant submodule

$$(M)^{\mathrm{U}(\mathfrak{g})} := \{w \in M | xw = \epsilon(x)w, \quad \forall\, x \in \mathrm{U}(\mathfrak{g})\}.$$

We have

$$(W \otimes W^*)^{\mathrm{U}(\mathfrak{g})} \cong \mathrm{End}_{\mathrm{U}(\mathfrak{g})}(\mathrm{W}) := \{\phi \in \mathrm{End}_{\mathbb{C}}(W) | \mathrm{Ad}_x(\phi) = \epsilon(x)\phi, \forall\, x \in \mathrm{U}(\mathfrak{g})\}. \tag{2.3}$$

Consider $V^{\otimes k} \otimes (V^*)^{\otimes \ell}$ as a $\mathrm{U}(\mathfrak{g})$-module, where the $\mathrm{U}(\mathfrak{g})$-action is defined by using the comultiplication. The element $Z = \Sigma_a E_{aa}$ acts on $V^{\otimes k} \otimes (V^*)^{\otimes \ell}$ by $(k-\ell)\mathrm{id}$. This immediately shows that

$$(V^{\otimes k} \otimes (V^*)^{\otimes \ell})^{\mathrm{U}(\mathfrak{g})} = \{0\} \quad \text{if } k \neq \ell. \tag{2.4}$$

As $(V^{\otimes d})^* \cong (V^*)^{\otimes d}$, we have the $\mathrm{U}(\mathfrak{g})$-module isomorphism

$$j: V^{\otimes d} \otimes (V^*)^{\otimes d} \to \mathrm{End}_{\mathbb{C}}(V^{\otimes d}).$$

It follows from Theorem 2.1 that the even subspace of $(V^{\otimes d} \otimes (V^*)^{\otimes d})^{\mathrm{U}(\mathfrak{g})}$ is isomorphic to $j^{-1} \circ \rho_d(\mathbb{C}\mathfrak{S}_d)$. Let $\mathfrak{g}_{\overline{0}} = \mathfrak{gl}(m) \oplus \mathfrak{gl}(n)$ be the maximal even subalgebra of $\mathfrak{g}$. Both V and V^* naturally restrict to $\mathfrak{g}_{\overline{0}}$-modules. By using Weyl's first fundamental theorem for the invariant theory of the general linear group,[5] we easily prove that $(V^{\otimes d} \otimes (V^*)^{\otimes d})^{\mathrm{U}(\mathfrak{g}_{\overline{0}})}$ is contained in the even subspace of $V^{\otimes d} \otimes (V^*)^{\otimes d}$. Since

$$(V^{\otimes d} \otimes (V^*)^{\otimes d})^{\mathrm{U}(\mathfrak{g}_{\overline{0}})} \supset (V^{\otimes d} \otimes (V^*)^{\otimes d})^{\mathrm{U}(\mathfrak{g})},$$

we have

$$(V^{\otimes d} \otimes (V^*)^{\otimes d})^{\mathrm{U}(\mathfrak{g})} = j^{-1} \circ \rho_d(\mathbb{C}\mathfrak{S}_d). \tag{2.5}$$

This result may be stated more explicitly as follows.

Theorem 2.2: (Reference 25) *The vector space* $(V^{\otimes d} \otimes (V^*)^{\otimes d})^{\mathrm{U}(\mathfrak{g})}$ *is spanned by the following elements:*

$$\sum_{a_1,\ldots,a_d} \mathrm{sgn}(\sigma, a_1, \ldots, a_d) \otimes v_{a_{\sigma(1)}} \otimes v_{a_{\sigma(2)}} \otimes \ \ldots \ \otimes v_{a_{\sigma(d)}} \otimes \overline{v}_{a_d} \otimes \overline{v}_{a_{d-1}} \otimes \ \ldots \overline{v}_{a_1}, \quad \forall\, \sigma \in \mathfrak{S}_d, \tag{2.6}$$

where $\mathrm{sgn}(\sigma,a_1,\ldots,a_d)$ *is a sign factor which is determined by the restriction of* σ *on the subset of odd indices in* $\{a_1,\ldots,a_d\}$ *in such a way that if the restriction is even then* $\mathrm{sgn}(\sigma,a_1,\ldots,a_d)$ *is* 1 *and* -1 *otherwise*.

We shall refer to both Theorems 2.1 and 2.2 as the first fundamental theorem of the invariant theory of the general linear supergroup.

III. SUPERALGEBRAS OF FUNCTIONS ON THE GENERAL LINEAR SUPERGROUP

We examine properties of the Hopf superalgebra of regular functions on the general linear supergroup in this section. The material presented here is of critical importance for setting up the framework for studying spherical functions. Some of the material can be extracted from Refs. 20 and 21.

Let $\mathrm{U}(\mathfrak{g})^0 := \{f \in \mathrm{U}(\mathfrak{g})^* \,|\, \ker f$ contains a cofinite $\mathbb{Z}_2$- graded ideal of $\mathrm{U}(\mathfrak{g})\}$ be the finite dual[16] of the universal enveloping algebra $\mathrm{U}(\mathfrak{g})$ of $\mathfrak{g}$. Standard Hopf algebra theory[15,16] asserts that the Hopf superalgebra structure of $\mathrm{U}(\mathfrak{g})$ induces a Hopf superalgebra structure on $\mathrm{U}(\mathfrak{g})^0$. Denote by $m_\circ$, $\Delta_\circ$, $\epsilon_\circ$, and $S_\circ$ the multiplication, comultiplication, counit, and antipode of $\mathrm{U}(\mathfrak{g})^0$, respectively. The maps are defined for all $f,\ \mathfrak{g} \in \mathrm{U}(\mathfrak{g})^0$, and $a,\ b \in \mathrm{U}(\mathfrak{g})$, by

$$\langle m_\circ(f \otimes g), a\rangle = \langle f \otimes g, \Delta(a)\rangle,$$

$$\langle \Delta_\circ(f), a \otimes b\rangle = \langle f, ab\rangle,$$

$$\langle S_\circ(f), a\rangle = \langle f, S(a)\rangle,$$

and $\mathbb{1}_{\mathrm{U}(\mathfrak{g})^0} = \epsilon$, $\epsilon_\circ = \mathbb{1}_{\mathrm{U}(\mathfrak{g})}$. Because $\mathrm{U}(\mathfrak{g})$ is supercocommutative, $\mathrm{U}(\mathfrak{g})^0$ is supercommutative. Recall that $S^2 = \mathrm{id}$ and hence also $S_\circ^2 = \mathrm{id}$. For convenience, we shall drop the subscript 0 from the notations for the multiplication, comultiplication, and antipode of $\mathrm{U}(\mathfrak{g})^0$.

Let π be a $\mathrm{U}(\mathfrak{g})$-representation of dimension $d < \infty$. Now for any $x \in \mathrm{U}(\mathfrak{g})$, $\pi(x)$ is a $d \times d$-matrix. We define a set of elements $\pi_{ij} \in \mathrm{U}(\mathfrak{g})^*$, $i,j = 1,2,\ldots,d$, by

$$\pi(x) = (\pi_{ij}(x))_{i,j=1}^{d}, \quad \forall\, x \in \mathrm{U}(\mathfrak{g}).$$

The π_{ij} will be called the matrix elements of π. It is easy to see that the matrix elements of every finite-dimensional representation of $\mathrm{U}(\mathfrak{g})$ belong to $\mathrm{U}(\mathfrak{g})^0$. Conversely, $\mathrm{U}(\mathfrak{g})^0$ is spanned by the matrix elements of all the finite-dimensional representations of $\mathrm{U}(\mathfrak{g})$. To see this, we only need to consider an arbitrary nonzero element $f \in \mathrm{U}(\mathfrak{g})^0$. Let Ker be a graded cofinite ideal of $\mathrm{U}(\mathfrak{g})$ contained in the kernel of f. Then $\mathrm{U}(\mathfrak{g})/\mathrm{Ker}$ forms a left $\mathrm{U}(\mathfrak{g})$-module,

$$\mathrm{U}(\mathfrak{g}) \otimes \mathrm{U}(\mathfrak{g})/\mathrm{Ker} \to \mathrm{U}(\mathfrak{g})/\mathrm{Ker},$$

$$y \otimes (x + \mathrm{Ker}) \mapsto yx + \mathrm{Ker}.$$

Let $\{x_i + \mathrm{Ker}\}$ be a basis of $\mathrm{U}(\mathfrak{g})/\mathrm{Ker}$, and denote by f_{ij} the matrix elements of the associated representation relative to this basis. Choose a set of complex numbers $c_i \in \mathbb{C}$ such that $\mathbb{1}_{\mathrm{U}(\mathfrak{g})} + \mathrm{Ker} = \Sigma_i c_i x_i + \mathrm{Ker}$, where the set $\mathbb{1}_{\mathrm{U}(\mathfrak{g})} + \mathrm{Ker}$ is not contained in the kernel of f since $f \neq 0$. Then $f = \Sigma_{i,j} c_i \langle f, x_j\rangle f_{ji}$.

We denote by t the $\mathrm{U}(\mathfrak{g})$-representation associated with the contravariant vector module $V = L_{\epsilon_1}$ in the standard basis, and denote its matrix elements by $t_{ab} \in \mathrm{U}(\mathfrak{g})^0$, $a,b \in \mathbf{I}$, where t_{ab} is even if $[a]+[b] = \overline{0}$, and odd otherwise. Note that

$$t_{ab}(E_{cd}) = \delta_{ac}\delta_{bd}.$$

Denote by $\overline{t}$ the covariant vector representation of $\mathrm{U}(\mathfrak{g})$ relative to the basis $\{\overline{v_a} \,|\, a \in \mathbf{I}\}$. Let $\overline{t_{ab}} \in \mathrm{U}(\mathfrak{g})^0$, $a,b \in \mathbf{I}$, be the matrix elements of $\overline{t}$. Then

$$\overline{t}_{ab}(E_{cd}) = -(-1)^{[a][b]+[b]}\delta_{bc}\delta_{ad}.$$

Note that $\overline{t}_{ab}$ is even if $[a]+[b]=\overline{0}$, and odd otherwise.

Definition 3.1: (Reference 20) Let $\mathbb{C}(G)$ be the subsuperalgebra of $\mathrm{U}(\mathfrak{g})^0$ generated by $\{t_{ab}, \overline{t}_{ab} | a, b \in \mathbf{I}\}$.

The following relations hold in $\mathbb{C}(G)$:

$$\sum_c t_{ac}\overline{t}_{bc}(-1)^{[c][a]+[b]} = \delta_{ab}, \quad \sum_c \overline{t}_{ca}t_{cb}(-1)^{[b][c]+[c]} = \delta_{ab}, \tag{3.1}$$

because t and $\overline{t}$ are dual representations of $\mathrm{U}(\mathfrak{g})$. More precisely, the first relation states that the canonical tensor $\Sigma_c v_c \otimes \overline{v}_c \in V \otimes V^*$ is $\mathrm{U}(\mathfrak{g})$-invariant, while the second relation means that the dual pairing $\langle , \rangle$: $V^* \otimes V \to \mathbb{C}$ is a $\mathrm{U}(\mathfrak{g})$-module homomorphism.

$\mathbb{C}(G)$ has a bisuperalgebra structure, with the comultiplication defined by

$$\Delta(t_{ab}) = \sum_{c \in \mathbf{I}} (-1)^{([c]-[a])([c]-[b])} t_{ac} \otimes t_{cb},$$

$$\Delta(\overline{t}_{ab}) = \sum_{c \in \mathbf{I}} (-1)^{([c]-[a])([c]-[b])} \overline{t}_{ac} \otimes \overline{t}_{cb}.$$

Let us also denote by S the antipode of $\mathrm{U}(\mathfrak{g})^0$. By using the definition of dual modules we can show that

$$S(t_{ab}) = (-1)^{[a][b]+[a]}\overline{t}_{ba}, \quad S(\overline{t}_{ab}) = (-1)^{[a][b]+[b]} t_{ba}. \tag{3.2}$$

The following result was proven in Ref. 20.

Proposition 3.1: (Reference 20) *(1)* $\mathbb{C}(G)$ *forms a Hopf sub-superalgebra of* $\mathrm{U}(\mathfrak{g})^0$. *(2)* $\mathbb{C}(G)$ *is dense in* $\mathrm{U}(\mathfrak{g})^*$ *in the following sense: for every nonzero element* $x \in \mathrm{U}(\mathfrak{g})$, *there exists some* $f \in \mathbb{C}(G)$ *such that* $\langle f, x \rangle \neq 0$.

Let Λ denote a finite-dimensional Grassmann algebra. Recall that the general linear supergroup $\mathrm{GL}(m|n, \Lambda)$ over Λ is the group of even invertible $(m+n)\times(m+n)$-matrices with entries in Λ. It was shown in Ref. 21 that $\mathrm{GL}(m|n, \Lambda)$ can be reconstructed from $\mathbb{C}(G)$ in the following way. The $\mathbb{Z}_2$-graded vector space $\mathrm{Hom}_{\mathbb{C}}(\mathbb{C}(G), \Lambda)$ has a natural superalgebra structure, with the multiplication defined for any ϕ and ψ by

$$(\phi\psi)(f) \coloneqq \sum_{(f)} (-1)^{[f_{(1)}][\psi]} \phi(f_{(1)}) \psi(f_{(2)}), \quad \forall f \in \mathbb{C}(G), \tag{3.3}$$

where we have used Sweedler's notation expressing the comultiplication $\Delta(f)$ of any $f \in \mathbb{C}(G)$ by $\Sigma_{(f)} f_{(1)} \otimes f_{(2)}$.

Theorem 3.1: (Reference 21) *Let* $G_{\mathbb{C}} \coloneqq \{$*superalgebra homomorphisms* $\mathbb{C}(G) \to \Lambda\}$. *Then with the multiplication defined by (3.3), the set* $G_{\mathbb{C}}$ *forms a group, which is isomorphic to* $\mathrm{GL}(m|n, \Lambda)$.

We shall not repeat the proof of the theorem here, but merely point out that the inverse α^{-1} of any element $\alpha \in G_{\mathbb{C}}$ is given by $\alpha^{-1}(f) = \alpha(S(f))$, for all $f \in \mathbb{C}(G)$.

We shall refer to the elements of $\mathbb{C}(G)$ as the regular functions on the general linear supergroup. We now consider their properties. Note that there exists two natural left actions dR and dL of $\mathrm{U}(\mathfrak{g})$ on $\mathbb{C}(G)$, respectively, corresponding to the left and right translations. For all $x \in \mathrm{U}(\mathfrak{g})$, $f \in \mathbb{C}(G)$,

$$\mathrm{d}R_x(f) = \sum_{(f)} (-1)^{[x][f]} f_{(1)} \langle f_{(2)}, x \rangle,$$

$$\mathrm{d}L_x(f) = \sum_{(f)} (-1)^{[x]} \langle f_{(1)}, S(x) \rangle f_{(2)}. \tag{3.4}$$

Equivalently, the equations in (3.4) can be rewritten in the form

$$\langle \mathrm{d}R_x(f), y \rangle = (-1)^{[x]([f]+[y])} \langle f, yx \rangle, \quad \langle \mathrm{d}L_x(f), y \rangle = (-1)^{[x][f]} \langle f, S(x)y \rangle, \tag{3.5}$$

for all $x, y \in \mathrm{U}(\mathfrak{g})$ and $f \in \mathbb{C}(G)$. Straightforward calculations show that each of $\mathrm{d}L$ and $\mathrm{d}R$ indeed converts $\mathbb{C}(G)$ into a (graded) left $\mathrm{U}(\mathfrak{g})$-module. With respect to this module structure the product map of $\mathbb{C}(G)$ is a $\mathrm{U}(\mathfrak{g})$-module homomorphism, and the unit element of $\mathbb{C}(G)$ is $\mathrm{U}(\mathfrak{g})$-invariant. Take $\mathrm{d}L$ as an example, we have

$$\sum_{(x)} (-1)^{[x_{(2)}][f]} \mathrm{d}L_{x_{(1)}}(f) \otimes \mathrm{d}L_{x_{(1)}}(g) \mapsto \mathrm{d}L_x(fg), \quad \forall\, f, g \in \mathrm{U}(\mathfrak{g})^0, \quad x \in \mathrm{U}(\mathfrak{g}),$$

$$\mathrm{d}L_x(\epsilon) = \epsilon(x)\epsilon, \quad \forall\, x \in \mathrm{U}(\mathfrak{g}). \tag{3.6}$$

This is saying that each of the actions $\mathrm{d}L$ and $\mathrm{d}R$ converts $\mathbb{C}(G)$ into a left $\mathrm{U}(\mathfrak{g})$-module superalgebra.[16] The two actions supercommute as can be easily checked. Thus $\mathbb{C}(G)$ forms a left $\mathrm{U}(\mathfrak{g}) \otimes \mathrm{U}(\mathfrak{g})$-module algebra, with the action

$$(x \otimes y) f = \mathrm{d}L_x\, \mathrm{d}R_y(f), \quad \forall\, x, y \in \mathrm{U}(\mathfrak{g}), \quad f \in \mathbb{C}(G).$$

The fact that the product map in $\mathbb{C}(G)$ is a module homomorphism means that the operators $\mathrm{d}R_x$ and $\mathrm{d}L_x$ behave as some sort of generalized superderivations. In particular, if $x \in \mathfrak{g}$, they are superderivations.

To better understand the structure of $\mathbb{C}(G)$, we let $X = V \otimes V^*$ and $\overline{X} = V^* \otimes V$. Using the standard bases of V and V^* we manufacture the bases $\{x_{ab} := v_b \otimes \overline{v_a}\}$ and $\{\overline{x_{ab}} := \overline{v_b} \otimes v_a\}$ for X and $\overline{X}$, respectively. Denote by $\mathbb{C}[X, \overline{X}]$ the $\mathbb{Z}_2$-graded symmetric algebra of $X \oplus \overline{X}$. Then $\mathbb{C}[X, \overline{X}]$ as an associative superalgebra can be described more explicitly as generated by x_{ab}, $\overline{x_{ab}}$, $a, b \in \mathbf{I}$, subject to the relations

$$x_{ab} x_{cd} = (-1)^{([b]-[a])([d]-[c])} x_{cd} x_{ab},$$

$$x_{ab} \overline{x_{cd}} = (-1)^{([b]-[a])([c]-[d])} \overline{x_{cd}} x_{ab},$$

$$\overline{x_{ab}}\, \overline{x_{cd}} = (-1)^{([a]-[b])([c]-[d])} \overline{x_{cd}}\, \overline{x_{ab}}.$$

The generators x_{ab} and $\overline{x_{ab}}$ are even if $[a]+[b]=\overline{0}$, and odd otherwise. Stated differently, the $2(m^2+n^2)$ even generators generate a polynomial algebra, the $4mn$ odd generators generate a Grassmann algebra with the standard grading, and $\mathbb{C}[X, \overline{X}]$ is the tensor product of the two. Let $\mathcal{J}$ be the (graded) ideal of $\mathbb{C}[X, \overline{X}]$ generated by the following elements:

$$\sum_c x_{ac} \overline{x_{bc}} (-1)^{[c][a]+[b]} - \delta_{ab}, \quad \sum_c \overline{x_{ca}} x_{cb} (-1)^{[b][c]+[c]} - \delta_{ab}, \quad a, b \in \mathbf{I}. \tag{3.7}$$

We have the following theorem.

Theorem 3.2: (Reference 20) *The assignments* $x_{ab} \mapsto t_{ab}$, $\overline{x_{ab}} \mapsto \overline{t_{ab}}$, $a, b \in \mathbf{I}$ *specify a well-defined superalgebra isomorphism* $j: \mathbb{C}[X, \overline{X}]/\mathcal{J} \to \mathbb{C}(G)$.

Define two left $\mathrm{U}(\mathfrak{g})$-actions on $X \oplus \overline{X}$,

$$\Phi: \mathrm{U}(\mathfrak{g}) \otimes (X \oplus \overline{X}) \to X \oplus \overline{X}, \quad u \otimes w \mapsto \Phi(u) w,$$

$$\Psi: \mathrm{U}(\mathfrak{g}) \otimes (X \oplus \overline{X}) \to X \oplus \overline{X}, \quad u \otimes w \mapsto \Psi(u)w,$$

by

$$\Phi(u)(v_b \otimes \overline{v_a}) = (-1)^{[u]} uv_b \otimes \overline{v_a},$$

$$\Psi(u)(v_b \otimes \overline{v_a}) = (-1)^{[u][b]} v_b \otimes u\overline{v_a},$$

$$\Phi(u)(\overline{v_b} \otimes v_a) = (-1)^{[u]} u\overline{v_b} \otimes v_a,$$

$$\Psi(u)(\overline{v_b} \otimes v_a) = (-1)^{[u]([u]+[b])} \overline{v_b} \otimes uv_a, \quad u \in \mathrm{U}(\mathfrak{g}).$$

These actions supercommute, and can both be extended to left $\mathrm{U}(\mathfrak{g})$-actions on $\mathbb{C}[X, \overline{X}]$ by

$$\Phi(x)(p_1 p_2) = \sum (-1)^{[x_{(2)}][p_1]} (\Phi(x_{(1)})p_1)(\Phi(x_{(2)})p_2),$$

$$\Psi(x)(p_1 p_2) = \sum (-1)^{[x_{(2)}][p_1]} (\Psi(x_{(1)})p_1)(\Psi(x_{(2)})p_2),$$

where $p_1, p_2 \in \mathbb{C}[X, \overline{X}]$ and $x \in \mathrm{U}(\mathfrak{g})$. This gives rise to a $\mathrm{U}(\mathfrak{g}) \otimes \mathrm{U}(\mathfrak{g})$-module algebra structure on $\mathbb{C}[X, \overline{X}]$. Note that the $\mathrm{U}(\mathfrak{g}) \otimes \mathrm{U}(\mathfrak{g})$-action leaves the ideal $\mathcal{J}$ invariant. Thus we have the following proposition.

Proposition 3.2: *The map* $j: \mathbb{C}[X, \overline{X}]/\mathcal{J} \to \mathbb{C}(G)$ *of Theorem 2 is a* $\mathrm{U}(\mathfrak{g}) \otimes \mathrm{U}(\mathfrak{g})$*-module algebra isomorphism, with*

$$j((\Psi(x) \otimes \Phi(y))p) = (\mathrm{d}L_x \otimes \mathrm{d}R_y) j(p), \quad \forall\, x, y \in \mathrm{U}(\mathfrak{g}), \quad p \in \mathbb{C}[X, \overline{X}].$$

IV. HOMOGENEOUS SUPERSPACES AND SPHERICAL FUNCTIONS

Recall the following well-known fact in the context of classical homogeneous spaces: if H is a compact semisimple Lie group, and $H_{\mathbb{C}}$ is its complexification, then for any parabolic subgroup Q of $H_{\mathbb{C}}$, we have $H_{\mathbb{C}}/Q = H/R$, where R is the intersection of the Levi factor of Q with H. We shall imitate this construction in the algebraic setting for Lie supergroups. For this we need to discuss real forms of the complex general linear superalgebra and the general linear supergroup.

A. Real forms

Let us begin by briefly discussing the notion of Hopf $*$-superalgebras.[28] A $*$-superalgebraic structure on an associative superalgebra A is a conjugate linear anti-involution θ: $A \to A$: for all $x, y \in A$, $c, c' \in \mathbb{C}$,

$$\theta(cx + c'y) = \overline{c}\theta(x) + \overline{c'}\theta(y), \quad \theta(xy) = \theta(y)\theta(x), \quad \theta^2(x) = x.$$

Note that the second equation does not involve any sign factors as one would normally expect of superalgebras. We shall sometimes use the notation (A, θ) for the $*$-superalgebra A with the $*$-structure θ. Let (B, θ_1) be another associative $*$-superalgebra. Now $A \otimes B$ has a natural superalgebra structure, with the multiplication defined for any $a, a' \in A$ and $b, b' \in B$ by

$$(a \otimes b)(a' \otimes b') = (-1)^{[b][a']} aa' \otimes bb',$$

where $(-1)^{[b][a']}$ is the usual sign factor required for exchanging positions of odd elements. Furthermore, the following conjugate linear map,

$$\theta\star\theta_1: a\otimes b \mapsto (1\otimes\theta_1(b))(\theta(a)\otimes 1) = (-1)^{[a][b]}\theta(a)\otimes\theta_1(b), \tag{4.1}$$

defines a $*$-superalgebraic structure on $A\otimes B$.

Let us assume that A is a Hopf superalgebra with comultiplication Δ, counit ϵ and antipode S. If the $*$-superalgebraic structure θ satisfies

$$(\theta\star\theta)\Delta = \Delta\theta, \quad \theta\epsilon = \epsilon\theta,$$

then A is called a Hopf $*$-superalgebra. Now

$$\sigma := S\theta$$

satisfies $\sigma^2 = id_A$, as follows from the definition of the antipode.

Let A^0 denote the finite dual of A, which has a natural Hopf superalgebraic structure. We shall still use Δ and S to, respectively, denote the comultiplication and antipode of A^0, but write its counit as ϵ_o. If A is a Hopf $*$-superalgebra with the Hopf $*$-superalgebraic structure θ, then $\sigma = S\theta$ induces a map $\omega: A^0\to A^0$ defined for any $f\in A^0$ by

$$\langle\omega(f),x\rangle = \overline{\langle f,\sigma(x)\rangle}, \quad \forall\, x\in A. \tag{4.2}$$

Lemma 4.1: The map $\omega: A^0\to A^0$ defined by (4.2) gives rise to a Hopf $*$-superalgebraic structure on A^0.

Proof: It is clear that ω is conjugate linear. Also, $\sigma^2 = \mathrm{id}_A$ implies $\omega^2 = \mathrm{id}_{A^0}$. For all $f,g\in A^0$, $x,y\in A$, we have

$$\begin{aligned}\langle\omega(fg),x\rangle &= \overline{\langle fg,\sigma(x)\rangle} = \overline{\langle f\otimes g,(S\otimes S)(\theta\star\theta)\Delta'(x)\rangle}\\ &= (-1)^{[f][g]}\langle\omega(f)\otimes\omega(g),\Delta'(x)\rangle = \langle\omega(g)\omega(f),x\rangle,\end{aligned}$$

that is, $\omega(fg)=\omega(g)\omega(f)$. Define $\omega\star\omega$ as in (4.1), we have

$$\begin{aligned}\langle(\omega\star\omega)\Delta(f),x\otimes y\rangle &= (-1)^{[x][y]}\overline{\langle\Delta(f),\sigma(x)\otimes\sigma(y)\rangle} = \overline{\langle f,\sigma(xy)\rangle}\\ &= \langle\omega(f),xy\rangle = \langle\Delta\omega(f),x\otimes y\rangle,\end{aligned}$$

that is $(\omega\star\omega)\Delta(f)=\Delta\omega(f)$. It is easy to show that ω also satisfies all the other minor requirements to qualify as a Hopf $*$-superalgebraic structure on A^0. ■

The universal enveloping algebra of the general linear superalgebra admits many Hopf $*$-superalgebraic structures. Let us fix one Hopf $*$-superalgebraic structure θ: $\mathrm{U}(\mathfrak{g})\to\mathrm{U}(\mathfrak{g})$ here. As $\mathfrak{g}$ is canonically embedded in $\mathrm{U}(\mathfrak{g})$, the restriction of θ to $\mathfrak{g}$ defines a conjugate anti-involution of the Lie superalgebra. Let $\mathfrak{g}_0^{\sigma}$ and $\mathfrak{g}_1^{\sigma}$ be the fixed point sets of $\mathfrak{g}_0$ and $\mathfrak{g}_1$ under σ, respectively. Let $\mathfrak{g}^{\sigma,\sqrt{i}}\subset\mathfrak{g}$ be the real span of $\mathfrak{g}_0^{\sigma}\cup\sqrt{i}\mathfrak{g}_1^{\sigma}$. Then $\mathfrak{g}^{\sigma,\sqrt{i}}$ forms a real Lie superalgebra, which is a real form of $\mathfrak{g}$. However, note that the σ-invariants of $\mathfrak{g}$ do not form a real subalgebra of $\mathfrak{g}$ if $\mathfrak{g}_1^{\sigma}$ is nontrivial. This is the reason for us to consider $\mathfrak{g}^{\sigma,\sqrt{i}}$ instead.

Denote by $\mathrm{U}^{\mathbb{R}}(\mathfrak{g}^{\sigma,\sqrt{i}})$ the real universal enveloping algebra of $\mathfrak{g}^{\sigma,\sqrt{i}}$, which is embedded in $\mathrm{U}(\mathfrak{g})$ in the natural way. Furthermore,

$$\mathrm{U}(\mathfrak{g}) = \mathbb{C}\otimes_{\mathbb{R}}\mathrm{U}^{\mathbb{R}}(\mathfrak{g}^{\sigma,\sqrt{i}}).$$

By Lemma 4.1, the Hopf $*$-superalgebraic structure θ induces a Hopf $*$-superalgebraic structure ω: $\mathbb{C}(G)\to\mathbb{C}(G)$ on $\mathbb{C}(G)$. By using the embedding of the real associative superalgebra $\mathrm{U}^{\mathbb{R}}(\mathfrak{g}^{\sigma,\sqrt{i}})$ in $\mathrm{U}(\mathfrak{g})$, we can see that $f\in\mathbb{C}(G)$ vanishes if and only if $\langle f,x\rangle=0$, for all $x\in\mathrm{U}^{\mathbb{R}}(\mathfrak{g}^{\sigma,\sqrt{i}})$. Therefore elements of $\mathbb{C}(G)$ can be considered as complex valued functionals on the real superalgebra $\mathrm{U}^{\mathbb{R}}(\mathfrak{g}^{\sigma,\sqrt{i}})$. From this point of view, we should interpret $\mathbb{C}(G)$ as the $*$-superalgebra of functions on some real supergroup G. Now let us make this discussion more precise.

Let Λ be the complex Grassmann algebra introduced in Sec. III. Let $^-: \Lambda\to\Lambda$ be a complex conjugation operation on supernumbers [i.e., $(\Lambda, ^-)$ is a $*$-superalgebra]. Theorem 3.1 shows that

all the superalgebra homomorphisms $\mathbb{C}(G)\to\Lambda$ form a supergroup G_{C}, which is isomorphic to $\mathrm{GL}(m|n,\Lambda)$. A homomorphism α: $\mathbb{C}(G)\to\Lambda$ will be called a $*$-superalgebra homomorphism if it preserves the $*$-superalgebraic structures in the sense that $\alpha(\omega(f))=\overline{\alpha(f)}$, for all $f\in\mathbb{C}(G)$. The following result can be easily proven.

Lemma 4.2: If an element α of G_{C} is a $*$-superalgebra homomorphism, then its inverse is also a $*$-superalgebra homomorphism. The product of any two $*$-superalgebra homomorphisms in G_{C} is again a $*$-superalgebra homomorphism.

Proof: We shall prove the first statement only. The second one can be shown in a similar way. Recall that the inverse of $\alpha\in G_{\mathrm{C}}$ is defined by

$$\langle\alpha^{-1},f\rangle=\langle\alpha,S(f)\rangle,\quad\forall\, f\in\mathbb{C}(G).$$

Now if α is a $*$-superalgebra homomorphism, then for all $f\in\mathbb{C}(G)$,

$$\langle\alpha^{-1},\omega(f)\rangle=\langle\alpha,S\omega(f)\rangle=\overline{\langle\alpha,S(f)\rangle}=\overline{\langle\alpha^{-1},f\rangle}.$$

This shows that α^{-1} is indeed a $*$-superalgebra homomorphism. ■

Introduce the map $\check{\theta}$: $G_{\mathrm{C}}\to G_{\mathrm{C}}$ defined by

$$\langle\check{\theta}(\alpha),f\rangle=\overline{\langle\alpha,\omega S(f)\rangle},\quad\forall\, f\in\mathbb{C}(G).$$

We need to show that the image of $\check{\theta}$ indeed lies in G_{C}. For any $f,g\in\mathbb{C}(G)$, we have

$$\begin{aligned}\langle\check{\theta}(\alpha),fg\rangle&=(-1)^{[f][g]}\overline{\langle\alpha,\omega S(f)\omega S(g)\rangle}\\&=(-1)^{[f][g]}\overline{\langle\alpha\otimes\alpha,\omega S(f)\otimes\omega S(g)\rangle}\\&=(-1)^{[f][g]}\overline{\langle\alpha,\omega S(f)\rangle\langle\alpha,\omega S(g)\rangle}\\&=\overline{\langle\alpha,\omega S(g)\rangle\langle\alpha,\omega S(f)\rangle}\\&=\overline{\langle\alpha,\omega S(f)\rangle}\cdot\overline{\langle\alpha,\omega S(g)\rangle}\\&=\langle\check{\theta}(\alpha),f\rangle\langle\check{\theta}(\alpha),g\rangle.\end{aligned}$$

Therefore, $\check{\theta}(\alpha)$ is a superalgebra homomorphism from $\mathbb{C}(G)$ to Λ, thus is indeed an element of G_{C}.

Definition 4.1: $G:=\{*\text{-superalgebra homomorphism }\mathbb{C}(G)\to\Lambda\}$.

Theorem 4.1: *G forms a subgroup of G_{C}. Furthermore, $\check{\theta}(\alpha)=\alpha^{-1}$ for all $\alpha\in G$.*

Proof: The fact that G forms a subgroup immediately follows from the above lemma. If $\alpha\in G$, we have

$$\begin{aligned}\langle\check{\theta}(\alpha),f\rangle&=\overline{\langle\alpha,\omega S(f)\rangle}=\langle\alpha,S(f)\rangle\\&=\langle\alpha^{-1},S(f)\rangle,\quad\forall\, f\in\mathbb{C}(G).\end{aligned}$$

This confirms the second claim. ■

B. Spherical functions on homogeneous superspaces

Hereafter we fix a Hopf $*$-superalgebraic structure θ for $\mathrm{U}(\mathfrak{g})$, which is defined for all the generators by

$$\theta:E_{ab}\mapsto E_{ba}.\tag{4.3}$$

The associated real form $\mathfrak{gl}(m|n;\mathbb{C})^{\sigma,\sqrt{i}}$ of the general linear superalgebra is one of the compact real forms of the general linear superalgebra, which probably deserves the notation $\mathfrak{u}(m|n)$ because it contains the maximal even subalgebra $\mathfrak{u}(m)\oplus\mathfrak{u}(n)$. (The unitarizable representations of this compact real form comprise the tensor powers of the natural representation, while the unita-

rizable representations of the other compact real form are the duals of these representations.[27]) Direct calculations can show that the Hopf $*$-superalgebraic structure on $\mathbb{C}(G)$ induced by θ is given by

$$\omega(t_{ab}) = (-1)^{[b]([a]+[b])}\overline{t_{ab}}, \quad \omega(\overline{t_{ab}}) = (-1)^{[b]([a]+[b])}t_{ab}. \tag{4.4}$$

The real supergroup G has body $\mathrm{U}(m)\times\mathrm{U}(n)$.

Let $\mathfrak{p}$ be a parabolic subalgebra of $\mathfrak{g}$ with Levi factor $\mathfrak{l}$. Let $\mathfrak{k}=\mathfrak{l}^{\sigma,\sqrt{i}}$ be the real form of $\mathfrak{l}$, which is a subalgebra of $\mathfrak{g}^{\sigma,\sqrt{i}}$. Denote by $\mathrm{U}^{\mathbb{R}}(\mathfrak{k})$ the universal enveloping algebra of $\mathfrak{k}$ over $\mathbb{R}$. Note that $\mathrm{U}^{\mathbb{R}}(\mathfrak{g}^{\sigma,\sqrt{i}})$ inherits a real Hopf superalgebra structure from $\mathrm{U}(\mathfrak{g})$, and $\mathrm{U}^{\mathbb{R}}(\mathfrak{k})$ inherits a real Hopf superalgebra structure from $\mathrm{U}^{\mathbb{R}}(\mathfrak{g}^{\sigma,\sqrt{i}})$. Let us introduce the following definition.

Definition 4.2:

$$\mathbb{C}(K\backslash G) := \{f \in \mathbb{C}(G) | \mathrm{d}L_k(f) = \epsilon(k)f, \forall\, k \in \mathrm{U}^{\mathbb{R}}(\mathfrak{k})\}. \tag{4.5}$$

Note the following obvious fact, which will be used immediately below:

$$\mathbb{C}(K\backslash G) := \{f \in \mathbb{C}(G) | \mathrm{d}L_k(f) = \epsilon(k)f, \forall\, k \in \mathrm{U}(\mathfrak{l})\}. \tag{4.6}$$

We have the following lemma.

Lemma 4.3: $\mathbb{C}(K\backslash G)$ *forms a* $*$*-subalgebra of* $\mathbb{C}(G)$*, which is also a left coideal of* $\mathbb{C}(G)$.

Proof: Since $\mathrm{U}(\mathfrak{l})$ is a Hopf subalgebra of $\mathrm{U}(\mathfrak{g})$, we have $\Delta(k)=\Sigma_{(k)}k_{(1)}\otimes k_{(2)} \in \mathrm{U}(\mathfrak{l})\otimes\mathrm{U}(\mathfrak{l})$ for all $k\in\mathrm{U}(\mathfrak{l})$. If $a,b\in\mathbb{C}(K\backslash G)$, then by (4.6),

$$\begin{aligned}
\mathrm{d}L_k(ab) &= \sum (-1)^{[a_{(2)}][b_{(1)}]+[k]}\langle a_{(1)}b_{(1)}, S(k)\rangle a_{(2)}b_{(2)} \\
&= \sum (-1)^{[a_{(2)}][k_{(1)}]+[k]}\langle a_{(1)}, S(k_{(2)})\rangle b_{(1)}, S(k_{(1)})a_{(2)}b_{(2)} \\
&= \sum (-1)^{[k]}\epsilon(k_{(1)})\langle a_{(1)}, S(k_{(2)})\rangle a_{(2)}b = \epsilon(k)ab, \quad \forall\, k \in \mathrm{U}(\mathfrak{l}).
\end{aligned}$$

Thus $ab\in\mathbb{C}(K\backslash G)$.

Given any $f\in\mathbb{C}(K\backslash G)$, we have $\mathrm{d}L_k(\omega(f))=\omega(\mathrm{d}L_{\theta(k)}(f))(-1)^{[k]([k]+[f])}$ for all $k\in\mathrm{U}(\mathfrak{l})$. As $\mathrm{U}(\mathfrak{l})$ is θ invariant, we have $\mathrm{d}L_{\theta(k)}(f)=\overline{\epsilon(k)}f$. Thus

$$\mathrm{d}L_k(\omega(f)) = \epsilon(k)\omega(f), \quad \forall\, k \in \mathrm{U}(\mathfrak{l}).$$

Also, a straightforward calculation shows that

$$(\mathrm{d}L_k \otimes \mathrm{id})\Delta(f) = \epsilon(k)\Delta(f), \quad \forall\, k \in \mathrm{U}(\mathfrak{l}).$$

Thus $\mathbb{C}(K\backslash G)$ is a left coideal. This completes the proof. ■

The subalgebra $\mathbb{C}(K\backslash G)$ consists of the elements of $\mathbb{C}(G)$ which are invariant with respect to $\mathrm{U}^{\mathbb{R}}(\mathfrak{k})$ under left translation. Following the general philosophy of noncommutative geometry,[2] we may take the viewpoint that $\mathbb{C}(K\backslash G)$ defines an algebraic homogeneous superspace.[12] We shall refer to $\mathbb{C}(K\backslash G)$ as the superalgebra of functions on the homogeneous superspace. Also a word about the notation $\mathbb{C}(K\backslash G)$: here K is used to indicate some real subsupergroup of G with Lie superalgebra $\mathfrak{k}$.

Remark 4.1: Since $\mathbb{C}(G)$ and $\mathbb{C}(K\backslash G)$ are all $*$-superalgebras, their elements are in general not holomorphic functions on the supergroup. This is a particularly welcome fact, as it indicates that our construction can lead to analogues of compact complex super manifolds like projective superspaces. As is well known from the Gelfand–Naimark theorem, the continuous functions on a compact manifold determine the manifold completely, even when the manifold is complex, where all the holomorphic functions are constants.

Remark 4.2: In the quantum group context, one usually considers left or right coideal subalgebras of the algebra of functions[10,17,3,11] in the place of $\mathbb{C}(K\backslash G)$. By Lemma 4.3 $\mathbb{C}(K\backslash G)$ forms a left coideal subalgebra of $\mathbb{C}(G)$.

Because the two left actions dR and dL of U($\mathfrak{g}$) on $\mathbb{C}(G)$ supercommute, the subalgebra $\mathbb{C}(K\backslash G)$ of $\mathbb{C}(G)$ forms a left module algebra over U($\mathfrak{g}$) under the action dR. We shall study the dR(U$^{\mathbb{R}}(\mathfrak{k})$)-invariant subspace of $\mathbb{C}(K\backslash G)$. Let us first generalize the definition of zonal spherical functions[26] to the supergroup setting. We shall refer to elements of the following space as spherical functions on the homogeneous superspace.

Definition 4.3:

$$\mathbb{C}(K\setminus G/K) := \{f \in \mathbb{C}(K\setminus G) \big| \mathrm{d}R_k(f) = \epsilon(k) f, \quad \forall\, k \in \mathrm{U}^{\mathbb{R}}(\mathfrak{k})\}. \tag{4.7}$$

Similar arguments as those in the proof of Lemma 4.3 show the following.

Lemma 4.4: The subspace $\mathbb{C}(K\backslash G/K)$ *forms a* $*$*-subalgebra of* $\mathbb{C}(K\backslash G)$. Obviously

$$\mathbb{C}(K\setminus G/K) = \{f \in \mathbb{C}(K\setminus G) \big| \mathrm{d}R_x(f) = \epsilon(x) f, \forall\, x \in \mathrm{U}(\mathfrak{l})\}, \tag{4.8}$$

where $\mathfrak{l}$ is the complexification of $\mathfrak{k}$. The fact will be used in the next section to prove Theorem 4.2.

C. Structure of superalgebra of spherical functions

Let $\mathfrak{l}$ be a reductive subalgebra of $\mathfrak{g}$ generated by E_{aa}, $a \in \mathbf{I}$, and $E_{c,c+1}$, $E_{c+1,c}$ with c belonging to some proper subset of $\mathbf{I}\backslash\{m+n\}$. As in the last section, we let

$$\mathfrak{k} = \mathfrak{l}^{\sigma,\sqrt{i}}.$$

See Remark 4.3 for further discussions on this choice of $\mathfrak{k}$. The main result here is Theorem 4.2, which enables us to obtain the superalgebras $\mathbb{C}(K\backslash G)$ and $\mathbb{C}(K\backslash G/K)$ from the invariants of $\mathbb{C}[X,\overline{X}]$. An explicit description of the generators of these superalgebras will also be given in Lemmas 4.5 and 4.6.

Theorem 4.2: *When* $\mathfrak{k}=\mathfrak{l}^{\sigma,\sqrt{i}}$, *we have*

$$\begin{aligned} \mathbb{C}(K\setminus G) &= \{j(p) \big| p \in \mathbb{C}[X,\overline{X}]^{\Psi(\mathrm{U}(\mathfrak{l}))}\}, \\ \mathbb{C}(K\setminus G/K) &= \{j(p) \big| p \in \mathbb{C}[X,\overline{X}]^{\Psi(\mathrm{U}(\mathfrak{l}))\otimes\Phi(\mathrm{U}(\mathfrak{l}))}\}. \end{aligned} \tag{4.9}$$

The remainder of this section is devoted to the proof of Theorem 4.2. The proof is carried out in two steps. We first show that the theorem holds when $\mathfrak{l}=\mathfrak{k}_{\mathbb{C}}$ is even, that is, when $\mathfrak{l}$ is a reductive Lie subalgebra of $\mathfrak{g}$. Then we use this fact to prove the general case. In the process of proving the theorem, we also establish Lemmas 4.5 and 4.6. We mention that Eqs. (4.6) and (4.8) will be used repeatedly in the proof without further warning.

1. Proof of Theorem 4.2 for $\mathfrak{l}$ *even*

In this case we can find a set of positive integers k_i, $i=1,2,\ldots,r,r+1,\ldots,s$ such that $\Sigma_{i=1}^{r}k_i=m$, $\Sigma_{j=r+1}^{s}k_j=n$, and $\mathfrak{l}=\oplus_{i=1}^{s}\mathfrak{gl}(k_i)$. More explicitly,

$$\mathfrak{l} = \left\{ \begin{pmatrix} A_1 & & 0 \\ & \ddots & \\ 0 & & A_s \end{pmatrix} \Big| A_i \in \mathfrak{gl}(k_i) \right\} \subset \mathfrak{g}.$$

Proposition 3.2 implies the following short exact sequence:

$$0 \to \mathcal{J} \to \mathbb{C}[X,\overline{X}] \xrightarrow{\mathcal{J}} \mathbb{C}(G) \to 0$$

in the category of U($\mathfrak{l}$)$\otimes$U($\mathfrak{l}$)-module superalgebras. Since the various U($\mathfrak{l}$) and U($\mathfrak{l}$)$\otimes$U($\mathfrak{l}$) actions on $\mathcal{J}$, $\mathbb{C}[X,\overline{X}]$ and $\mathbb{C}(G)$ are all semisimple, we have the following short exact sequences of U($\mathfrak{l}$)$\otimes$U($\mathfrak{l}$)-modules:

$$0 \to \mathcal{J}^{\Psi(\mathrm{U}(\mathfrak{l}))} \to \mathbb{C}[X,\overline{X}]^{\Psi(\mathrm{U}(\mathfrak{l}))} \to \mathbb{C}(G)^{\mathrm{d}L_{\mathrm{U}(\mathfrak{l})}} \to 0, 0 \to \mathcal{J}^{\Psi(\mathrm{U}(\mathfrak{l}))\otimes\Phi(\mathrm{U}(\mathfrak{l}))} \to \mathbb{C}[X,\overline{X}]^{\Psi(\mathrm{U}(\mathfrak{l}))\otimes\Phi(\mathrm{U}(\mathfrak{l}))}$$
$$\to \mathbb{C}(G)^{\mathrm{d}L_{\mathrm{U}(\mathfrak{l})}\otimes\mathrm{d}R_{\mathrm{U}(\mathfrak{l})}} \to 0,$$

where $\mathbb{C}(K\backslash G)=\mathbb{C}(G)^{\mathrm{d}L_{\mathrm{U}(\mathfrak{l})}}$ and $\mathbb{C}(K\backslash G/K)=\mathbb{C}(G)^{\mathrm{d}L_{\mathrm{U}(\mathfrak{l})}\otimes\mathrm{d}R_{\mathrm{U}(\mathfrak{l})}}$. These are also short exact sequences of $\mathrm{U}(\mathfrak{l})\otimes\mathrm{U}(\mathfrak{l})$-module algebras, thus they imply the claims of Theorem 4.2 in the case under consideration.

Let us now describe the algebras $\mathbb{C}(K\backslash G)$ and $\mathbb{C}(K\backslash G/K)$ more carefully. Set $l_i=\Sigma_{t=1}^{i}k_t$. Recall that $\mathbb{C}[X,\overline{X}]$ is the symmetric algebra in $X\oplus\overline{X}$ where $X=V\otimes\overline{V}$ and $\overline{X}=\overline{V}\otimes V$. Restricted to a $\mathrm{U}(\mathfrak{l})$-module, V decomposes into

$$V=\oplus_{i=1}^{s}V_i^{(k_i)}.$$

The ideal $\mathfrak{gl}(k_i)$ of $\mathfrak{l}$ acts on $V_i^{(k_i)}$ by the natural representation, and acts on all other submodules trivially. There is also an analogous decomposition of the restriction of $\overline{V}$ to a $\mathrm{U}(\mathfrak{l})$-module. By applying the first fundamental theorem of the invariant theory of the general linear group,[5] we obtain that the subalgebra $\mathbb{C}[X,\overline{X}]^{\Psi(\mathrm{U}(\mathfrak{l}))}$ of $\mathbb{C}[X,\overline{X}]$ is generated by

$$\hat{C}_{ab}^{(i)} := \sum_{c=1+l_{i-1}}^{l_i} x_{ca}\overline{x_{cb}}, \quad i=1,2,\ldots,s, \quad a,b\in\mathbf{I}.$$

It then immediately follows that $\mathbb{C}(K\backslash G)$ is generated by

$$C_{ab}^{(i)} := j(\hat{C}_{ab}^{(i)}) = \sum_{c=1+l_{i-1}}^{l_i} t_{ca}\overline{t_{cb}}, \quad i=1,2,\ldots,s, \quad a,b\in\mathbf{I}.$$

Note that the $C_{ab}^{(i)}$ are not algebraically independent, for example, for $a,b\in\mathbf{I}$ the following hold:

$$\sum_{i=1}^{s} C_{ab}^{(i)}(-1)^{[l_i]}=\delta_{ab}, \quad \sum_{a=1}^{m+n} C_{ab}^{(i)}=k_i. \tag{4.10}$$

Thus the elements of the set $\{C_{ab}^{(i)}\,|\,i\neq s; a,b\in\mathbf{I}\}$ can also generate $\mathbb{C}(K\backslash G)$. By using the fact that t_{ab} and $\overline{t_{cd}}$ supercommute, one can verify the following proposition easily.

Proposition 4.1: We have

$$C_{ab}^{(i)}C_{cd}^{(j)}=(-1)^{([a]+[b])([c]+[d])}C_{cd}^{(j)}C_{ab}^{(i)}, \tag{4.11}$$

in particular, if $[a]+[b]=1$ *then* $(C_{ab}^{(i)})^2=0$. *Thus for fixed i, there is an onto algebra homomorphism* $\mathbb{C}[X]\to\langle C_{ab}^{(i)}\,|\,a,b\in\mathbf{I}\rangle$, *where* $\mathbb{C}[X]$ *is the subalgebra of* $\mathbb{C}[X,\overline{X}]$ *generated by X, and* $\langle C_{ab}^{(i)}\,|\,a,b\in\mathbf{I}\rangle$ *is the subalgebra of* $\mathbb{C}(K\backslash G)$ *generated by* $\{C_{ab}^{(i)}\,|\,a,b\in\mathbf{I}\}$.

In a similar way we can show that $\mathbb{C}[X,\overline{X}]^{\Psi(\mathrm{U}(\mathfrak{l}))\otimes\Phi(\mathrm{U}(\mathfrak{l}))}$ is generated by

$$\hat{C}^{(i,j)} := \sum_{a=1+l_{j-1}}^{l_j}\sum_{c=1+l_{i-1}}^{l_i} x_{ca}\overline{x_{ca}}, \quad i,j=1,2,\ldots,s,$$

and $\mathbb{C}(K\backslash G/K)$ is generated by

$$C^{(i,j)} := j(\hat{C}^{(i,j)}) = \sum_{a=1+l_{j-1}}^{l_j}\sum_{c=1+l_{i-1}}^{l_i} t_{ca}\overline{t_{ca}}, \quad i,j=1,2,\ldots,s.$$

Again, the $C^{(i,j)}$ are not algebraically independent, for example,

$$\sum_{i=1}^{s} C^{(i,j)}(-1)^{[l_i]} = k_j, \quad \sum_{j=1}^{s} C^{(i,j)}(-1)^{[l_j]} = k_i. \tag{4.12}$$

Thus the elements of the set $\{C^{(i,j)} | i, j \neq r\}$ generate $\mathbb{C}(K\backslash G/K)$.

2. Proof of Theorem 4.2 for generic $\mathfrak{l}$

The most general form of $\mathfrak{l}$ is as follows. There exists a set of positive integers k_i as in the last section such that

$$\mathfrak{l} = (\oplus_{i=1}^{r-1} \mathfrak{gl}(k_i)) \oplus \mathfrak{gl}(k_r|k_{r+1}) \oplus (\oplus_{j=r+2}^{s} \mathfrak{gl}(k_j)).$$

More explicitly, we have

$$\mathfrak{l} = \left\{ \begin{pmatrix} \ddots & & & & 0 \\ & A_{r-1} & & & \\ & & B & & \\ & & & A_{r+2} & \\ 0 & & & & \ddots \\ & & & & & A_s \end{pmatrix} \middle| \begin{array}{lcl} A_i & \in & \mathfrak{gl}(k_i), \\ B & \in & \mathfrak{gl}(k_r|k_{r+1}) \end{array} \right\}.$$

Note that $\mathfrak{l}$ contains the maximal even subalgebra $\mathfrak{l}_0 = \oplus_{i=1}^{s} \mathfrak{gl}(k_i)$.

We first consider the subalgebra $\mathbb{C}(G)^{\mathrm{d}L_{\mathrm{U}(\mathfrak{l}_0)}}$ of $\mathbb{C}(G)$. By using results of the last section, we can immediately see that $\mathbb{C}(G)^{\mathrm{d}L_{\mathrm{U}(\mathfrak{l}_0)}}$ is generated by the elements of $\{C_{ab}^{(i)} | i \neq r; a, b \in \mathbf{I}\}$. Now

$$\mathbb{C}(K \setminus G) = \{f \in \mathbb{C}(G)^{\mathrm{d}L_{\mathrm{U}(\mathfrak{l}_0)}} | \mathrm{d}L_{E_{mm+1}}(f) = \mathrm{d}L_{E_{m+1,m}}(f) = 0\}.$$

We shall show that $\mathbb{C}(K\backslash G)$ is generated by $\{C_{ab}^{(i)} | i \neq r, r+1; a, b \in \mathbf{I}\}$.

Note that all the elements of $\{C_{ab}^{(i)} | i \neq r; a, b \in \mathbf{I}\}$ are annihilated by $\mathrm{d}L_{E_{mm+1}}$ and $\mathrm{d}L_{E_{m+1,m}}$ except for $C_{ab}^{(r+1)}$, for which we have

$$\mathrm{d}L_{E_{mm+1}}(C_{ab}^{(r+1)}) = -(-1)^{[a]+[b]} t_{m+1,a} \overline{t}_{mb}, \tag{4.13}$$

$$\mathrm{d}L_{E_{m+1,m}}(C_{ab}^{(r+1)}) = -(-1)^{[a]+[b]} t_{ma} \overline{t}_{m+1,b}, \quad a, b \in \mathbf{I}. \tag{4.14}$$

Note that as a $\mathrm{U}(\mathfrak{g})$-module, $\mathbb{C}(G)$ has a filtration defined by the degrees of the polynomials in the t_{ab} and the $\overline{t}_{ab}$, and the filtration on the $\mathrm{U}(\mathfrak{l}_0)$-module $\mathbb{C}(G)^{\mathrm{d}L_{\mathrm{U}(\mathfrak{l}_0)}}$ defined by the degrees of the polynomials in the $\{C_{ab}^{(i)} | i \neq r; a, b \in \mathbf{I}\}$ is compatible with this filtration. Thus in order to find those $f \in \mathbb{C}(G)^{\mathrm{d}L_{\mathrm{U}(\mathfrak{l}_0)}}$ such that $\mathrm{d}L_{E_{mm+1}}(f) = L_{E_{m+1,m}}(f) = 0$, by passing through to the associated graded modules defined by these filtrations if necessary, we may assume that f is homogeneous of degree μ in the elements of $\{C_{ab}^{(i)} | i \neq r; a, b \in \mathbf{I}\}$. We consider an element $f \in \mathbb{C}(G)^{\mathrm{d}L_{\mathrm{U}(\mathfrak{l}_0)}}$ as a polynomial in $\{C_{ab}^{(r+1)} | a, b \in \mathbf{I}\}$ with coefficients being polynomials in $\{C_{ab}^{(i)} | i \neq r, r+1; a, b \in \mathbf{I}\}$. Set $C_{ab} = C_{ab}^{(r+1)}$ $(a, b \in \mathbf{I})$. Then by Proposition 4.1, the subalgebra $\langle C_{ab} | a, b \in \mathbf{I}\rangle$ has a basis consists of elements of the form

$$C_{a_1 b_1}^{p_1} \cdots C_{a_s b_s}^{p_s} C_{c_1 d_1} \cdots C_{c_t d_t}, \tag{4.15}$$

with $[a_i] + [b_i] = 0 (1 \leqslant i \leqslant s)$, $[c_j] + [d_j] = 1 (1 \leqslant j \leqslant t)$, and $p_i \geqslant 0 (1 \leqslant i \leqslant s)$ are integers. Extend such a basis of $\langle C_{ab} | a, b \in I\rangle$ to a homogeneous basis $\mathbf{B}$ of $\mathbb{C}(G)^{\mathrm{d}L_{\mathrm{U}(\mathfrak{l}_0)}}$, so that the elements of $\mathbf{B}$ are of the form

$$CC_{a_1b_1}^{p_1}\cdots C_{a_sb_s}^{p_s}C_{c_1d_1}\cdots C_{c_td_t}, \tag{4.16}$$

where C is a monomial in $\{C_{ab}^{(i)}|i\neq r,r+1;a,b\in\mathbf{I}\}$. Now let us write $f=\Sigma_{0\leqslant k\leqslant\mu}f_k$, where f_k is a linear combination of the basis elements of (4.16) such that $\Sigma_i p_i+t=k$ and $\deg(C)+k=\deg(f)$. The action of E_{mm+1} (similarly for E_{m+1m}) on the elements of (4.5) can be computed by using (4.13), and we have

$$\begin{aligned}\mathrm{d}L_{E_{mm+1}}(C_{a_1b_1}^{p_1}\cdots C_{a_sb_s}^{p_s}C_{c_1d_1}\cdots C_{c_td_t}) &= -\sum_{i=1}^{s}(-1)^t p_i C_{a_1b_1}^{p_1}\cdots C_{a_ib_i}^{p_i-1}\cdots C_{a_sb_s}^{p_s}C_{c_1d_1}\cdots C_{c_td_t}t_{m+1a_i}\overline{t}_{mb_i}\\ &\quad + C_{a_1b_1}^{p_1}\cdots C_{a_sb_s}^{p_s}\sum_{j=1}^{t}(-1)^j C_{c_1d_1}\cdots\hat{C}_{c_jd_j}\cdots C_{c_td_t}t_{m+1c_j}\overline{t}_{md_j}.\end{aligned} \tag{4.17}$$

Since the product map of $\mathbb{C}(G)$ is a $\mathrm{U}(\mathfrak{g})$-module homomorphism [see (3.6)], by (4.17) the action of E_{mm+1} on the elements of (4.16) is given by

$$\begin{aligned}&\mathrm{d}L_{E_{mm+1}}(CC_{a_1b_1}^{p_1}\cdots C_{a_sb_s}^{p_s}C_{c_1d_1}\cdots C_{c_td_t})\\ &\quad=-(-1)^{[C]}C\sum_{i=1}^{s}(-1)^t p_i C_{a_1b_1}^{p_1}\cdots C_{a_ib_i}^{p_i-1}\cdots C_{a_sb_s}^{p_s}C_{c_1d_1}\cdots C_{c_td_t}t_{m+1a_i}\overline{t}_{mb_i}\\ &\quad+(-1)^{[C]}CC_{a_1b_1}^{p_1}\cdots C_{a_sb_s}^{p_s}\sum_{j=1}^{t}(-1)^j C_{c_1d_1}\cdots\hat{C}_{c_jd_j}\cdots C_{c_td_t}t_{m+1c_j}\overline{t}_{md_j},\end{aligned} \tag{4.18}$$

where $\hat{C}_{c_jd_j}$ means that the factor $C_{c_jd_j}$ is omitted.

For an element x of the form (4.16), let $x'(ab)$ be

$$CC_{a_1b_1}^{p_1}\cdots C_{a_{i-1}b_{i-1}}^{p_{i-1}}C_{a_ib_i}^{p_i-1}C_{a_{i+1}b_{i+1}}^{p_{i+1}}\cdots C_{a_sb_s}^{p_s}C_{c_1d_1}\cdots C_{c_td_t},$$

or

$$CC_{a_1b_1}^{p_1}\cdots C_{a_sb_s}^{p_s}C_{c_1d_1}\cdots\hat{C}_{c_jd_j}\cdots C_{c_td_t},$$

depending on whether $(ab)=(a_ib_i)$ or $(ab)=(c_jd_j)$.

Let us make some observations. First note that since

$$\langle m_\circ(h\otimes g),a\rangle=\langle h\otimes g,\Delta(a)\rangle,\quad h,g\in U(\mathfrak{g})^0,\quad a\in U(\mathfrak{g}),$$

if $\{b_i|1\leqslant i\leqslant\ell\}\subset\mathbb{C}(G)$ is a set of linearly independent functions which are constants on $U(\mathfrak{k}_0)$ and $\{t_{m+1a}\overline{t}_{mb}|a,b\in\mathbf{J}\subset\mathbf{I}\}$ is linearly independent, then the set $\{b_it_{m+1a}\overline{t}_{mb}|1\leqslant i\leqslant\ell,a,b\in\mathbf{J}\}$ is linearly independent. Then note that if $S_{cd}\subset\mathbf{B}$ with C_{cd} appearing in every element for a fixed pair c and d, then the set

$$S'_{cd}=\{x'(cd)|x\in S_{cd}\}$$

is linearly independent. In fact the elements of S_{cd} and $C_{cd}S'_{cd}$ are the same up to signs. Finally note that the only relation among the elements in $\{t_{m+1a}\overline{t}_{mb}|a,b\in\mathbf{I}\}$ is [see (3.1)]

$$\sum_{a\in I}t_{m+1a}\overline{t}_{ma}(-1)^{[a]}=\sum_{1\leqslant a\leqslant m}t_{m+1a}\overline{t}_{ma}-\sum_{m+1\leqslant a\leqslant m+n}t_{m+1a}\overline{t}_{ma}=0,$$

and this relation can only come from (via the map $\mathrm{d}L_{E_{mm+1}}$)

$$\sum_{1\leqslant a\leqslant m} C_{aa} - \sum_{m+1\leqslant a\leqslant m+n} C_{aa} = \sum_{1\leqslant a\leqslant m} \sum_{c=m+1}^{l_{r+1}} t_{ca}\overline{t_{ca}} - \sum_{m+1\leqslant a\leqslant m+n} \sum_{c=m+1}^{l_{r+1}} t_{ca}\overline{t_{ca}} = -k_{r+1},$$

i.e., a constant.

These observations together with (4.18) imply that $\mathrm{d}L_{E_{mm+1}}(f)=\mathrm{d}L_{E_{m+1,m}}(f)=0$ if and only if $f=f_0$, i.e., f is independent of $C_{ab}^{(r+1)}(a,b\in\mathbf{I})$. Therefore, we have the following.

Lemma 4.5: $\mathbb{C}(K\backslash G)$ *is generated by the elements of*

$$\{C_{ab}^{(i)} | i\neq r,r+1;a,b\in\mathbf{I}\}. \tag{4.19}$$

By Theorem 2.1 and the first fundamental theorem of the invariant theory of the general linear group, $\mathbb{C}[X,\overline{X}]^{\Psi(\mathrm{U}(\mathfrak{l}))}$ is generated by $\hat{C}_{ab}^{(i)}(i\neq r,r+1;a,b\in\mathbf{I})$, and $\hat{C}_{ab}^{(r)}-\hat{C}_{ab}^{(r+1)}(a,b\in\mathbf{I})$. We have $j(\hat{C}_{ab}^{(i)})=C_{ab}^{(i)}(i\neq r,r+1;a,b\in\mathbf{I})$, which yield all the elements of (4.19). This establishes the short exact sequence

$$0\rightarrow\mathcal{J}^{\Psi(\mathrm{U}(\mathfrak{l}))}\rightarrow\mathbb{C}[X,\overline{X}]^{\Psi(\mathrm{U}(\mathfrak{l}))}\rightarrow\mathbb{C}(K\setminus G)\rightarrow 0$$

of $\mathrm{U}(\mathfrak{l})\otimes\mathrm{U}(\mathfrak{l})$-module algebras, thus proves the first claim of Theorem 4.2.

Let us now consider the subalgebra $\mathbb{C}(K\backslash G)^{\mathrm{d}R_{\mathrm{U}(\mathfrak{l}_0)}}$ of $\mathbb{C}(K\backslash G)$, which is generated by the elements of the set $\{C^{(i,j)}|i\neq r,r+1;j\neq r\}$, as follows from results of the last section. Among all the elements of this set, only $C^{(i,r+1)}$ are not annihilated by $\mathrm{d}R_{E_{mm+1}}$ and $\mathrm{d}R_{E_{m+1,m}}$. Thus similar to the case of the left action, we can prove that $f\in\mathbb{C}(K\backslash G)^{\mathrm{d}R_{\mathrm{U}(\mathfrak{l}_0)}}$ satisfies $\mathrm{d}R_{E_{mm+1}}(f)=0$ and $\mathrm{d}R_{E_{m+1,m}}(f)=0$ if and only if it is independent of the $C^{(i,r+1)}(i\neq r,r+1)$. Observe that

$$\mathbb{C}(K\setminus G/K)=\{f\in\mathbb{C}(K\setminus G)^{\mathrm{d}R_{\mathrm{U}(\mathfrak{l}_0)}}|\mathrm{d}R_{E_{mm+1}}(f)=\mathrm{d}R_{E_{m+1,m}}(f)=0\}.$$

We have

Lemma 4.6: $\mathbb{C}(K\backslash G/K)$ *is generated by the elements of*

$$\{C^{(i,j)}|i,j\neq r,r+1\}. \tag{4.20}$$

By Theorem 2.1 and the first fundamental theorem of the invariant theory of the general linear group, $\mathbb{C}[X,\overline{X}]^{\Psi(\mathrm{U}(\mathfrak{l}))\otimes\Phi(\mathrm{U}(\mathfrak{l}))}$ is generated by

$$\hat{C}^{(i,j)},\hat{C}^{(r,j)}-\hat{C}^{(r+1,j)},\hat{C}^{(i,r)}-\hat{C}^{(i,r+1)},\quad i,j\neq r,r+1,\quad a,b\in\mathbf{I},$$

and since

$$j(\{\hat{C}^{(i,j)}|i,j\neq r,r+1\})=\{C^{(i,j)}|i,j\neq r,r+1\},$$

we have the following short exact sequence of $\mathrm{U}(\mathfrak{l})\otimes\mathrm{U}(\mathfrak{l})$-module algebras:

$$0\rightarrow\mathcal{J}^{\Psi(\mathrm{U}(\mathfrak{l}))\otimes\Phi(\mathrm{U}(\mathfrak{l}))}\rightarrow\mathbb{C}[X,\overline{X}]^{\Psi(\mathrm{U}(\mathfrak{l}))\otimes\Phi(\mathrm{U}(\mathfrak{l}))}\rightarrow\mathbb{C}(K\setminus G/K)\rightarrow 0,$$

which is equivalent to the second claim of Theorem 4.2.

Remark 4.3: Geometric homogeneous superspaces have been studied since the 1970s, see, for example, Refs. 8 and 13. Symmetric superspaces were also classified by Serganova in Ref. 23 at the level of Lie superalgebras. In relation to our algebraic definition of homogeneous superspaces, one may ask the following question. Let P be the parabolic subgroup of $\mathrm{GL}(m|n,\Lambda)$ with Lie superalgebra $\mathfrak{p}$. We have the homogeneous superspace $\mathrm{GL}(m|n,\Lambda)/P$ (understood as a left coset of P). Now let $\mathfrak{l}$ be the Levi factor of $\mathfrak{p}$ and take $\mathfrak{k}=\mathfrak{l}^{\sigma,\sqrt{\tilde{i}}}$, with θ being the Hopf $*$-superalgebraic structure of $\mathrm{U}(\mathfrak{g})$ corresponding to the compact real form of the general linear superalgebra [defined by (4.3)]. Then the question is whether the homogeneous superspace determined by $\mathbb{C}(K\backslash G)$ is the same as $\mathrm{GL}(m|n,\Lambda)/P$ in some appropriate sense. We expect the answer to be

affirmative, but have not been able to locate a reference, which addresses any form of the question, in the literature on supergeometry.

V. SPHERICAL FUNCTIONS ON $\mathbb{C}(K\backslash G)$ WITH MAXIMAL RANK K

We keep notations from the last section. In particular, we fix the $*$-structure θ of $\mathrm{U}(\mathfrak{g})$ given by (4.3), which corresponds to the real form $\mathfrak{u}(m|n)$ for the general linear superalgebra. We use $\mathfrak{l}$ to denote the Levi factor of a parabolic subalgebra of $\mathfrak{g}$, and set $\mathfrak{k}=\mathfrak{l}^{\sigma,\sqrt{i}}$. The homogeneous superspaces studied in this section are all examples of symmetric superspaces in the sense of Ref. 22 (see Tables 2 and 3 in Ref. 23).

A. The case with $\mathfrak{k}=\mathfrak{u}(m|n-1)\oplus\mathfrak{u}(1)$

We first examine in some detail the spherical functions on the homogeneous superspace corresponding to $\mathfrak{k}=\mathfrak{u}(m|n-1)\oplus\mathfrak{u}(1)$, where the complexification $\mathfrak{l}$ of $\mathfrak{k}$ is the subalgebra of $\mathfrak{g}$ spanned by the elements E_{ij}, $i,j\in\mathbf{I}\backslash\{m+n\}$, and $E_{m+n,m+n}$. But before discussing the superalgebra $\mathbb{C}(K\backslash G)$, let us introduce the following superalgebra.

Definition 5.1: $\mathbb{C}(\mathbb{S}^{2n-1|2m}):=\mathbb{C}(G)^{\mathrm{d}L_{\mathrm{U}^{\mathbb{R}}(\mathfrak{u}(m|n-1))}}$ relative to $\mathfrak{u}(m|n-1)\subset\mathfrak{k}$.

More explicitly,

$$\mathbb{C}(\mathbb{S}^{2n-1|2m})=\{f\in\mathbb{C}(G)|\mathrm{d}L_k(f)=\epsilon(k)f,\ \forall\, k\in\mathrm{U}^{\mathbb{R}}(\mathfrak{u}(m|n-1))\}.$$

We can modify the analysis of Sec. IV C to construct $\mathbb{C}(\mathbb{S}^{2n-1|2m})$. With the help of Theorem 2.1 for $\mathfrak{gl}(m|n-1)$, we can show that $\mathbb{C}(\mathbb{S}^{2n-1|2m})$ is generated by

$$z_a:=t_{m+n,a},\quad \overline{z_a}:=\overline{t}_{m+n,a},$$

$$Q_{ab}:=\sum_{c<m+n}\overline{t}_{ca}t_{cb}(-1)^{[b][c]+[c]},\quad a\in\mathbf{I},$$

where z_a and $\overline{z_a}$ are odd if $a\leqslant m$, and even otherwise. The defining relations of $\mathbb{C}(G)$ imply $Q_{ab}=\delta_{ab}\mathbb{1}-z_a\overline{z}_b(-1)^{[b]}$. Thus the z_a and $\overline{z_a}$ generate $\mathbb{C}(\mathbb{S}^{2n-1|2m})$ by themselves. We have the following result.

Lemma 5.1: The subalgebra of $\mathbb{C}(\mathbb{S}^{2n-1|2m})$ *of* $\mathbb{C}(G)$ *is generated by* z_a, $\overline{z_a}$, $a\in\mathbf{I}$, *which satisfy the following relation:*

$$\sum_{a\in\mathbf{I}}\overline{z_a}z_a=\mathbb{1}. \tag{5.1}$$

Remark 5.1: The notation suggests $\mathbb{C}(\mathbb{S}^{2n-1|2m})$ be the superalgebra of functions on the supersphere. This can be understood as follows. Under the $*$-map ω defined by (4.4), we have

$$\omega(z_a)=\overline{z_a},\quad \omega(\overline{z_a})=z_a.$$

Thus we may interpret $\overline{z_a}$ as the complex conjugate of z_a, and this indeed makes perfect sense when z_a and $\overline{z_a}$ are regarded as functions on G (see Sec. IV A). Thus Eq. (5.1) defines a supersphere in analogy with the embedding of a supersphere $\mathbb{S}^{2n-1|2m}$ in $\mathbb{C}^{n|m}$. This also indicates the importance of the $*$-structure in determining the underlying supermanifold of $\mathbb{C}(K\backslash G)$.

Remark 5.2: When $\mathfrak{k}=\mathfrak{u}(m|n-1)\oplus\mathfrak{u}(1)$, we have $\mathbb{C}(K\backslash G)=\mathbb{C}(\mathbb{S}^{2n-1|2m})^{\mathrm{d}L_{\mathfrak{u}(1)}}$. This superalgebra embedding $\mathbb{C}(K\backslash G)\hookrightarrow\mathbb{C}(\mathbb{S}^{2n-1|2m})$ corresponds to a projection from $\mathbb{S}^{2n-1|m}$ to the symmetric superspace, which is the supergeneralization of the Hopf map $\mathbb{S}^{2n-1}\to\mathbb{CP}^{n-1}$. Therefore, we shall regard the symmetric superspace associated with $\mathbb{C}(K\backslash G)$ as an algebraic analogue of the projective superspace $\mathbb{CP}^{n-1|m}$.

We denote $\mathbb{C}(K\backslash G)$ by $\mathbb{C}(\mathbb{P}^{n-1|m})$ when $\mathfrak{k}=\mathfrak{u}(m|n-1)\oplus\mathfrak{u}(1)$. Lemma 5.1 immediately leads to the following result.

Lemma 5.2: The superalgebra $\mathbb{C}(\mathbb{P}^{n-1|m})$ *is the* $*$*-subalgebra of* $\mathbb{C}(\mathbb{S}^{2n-1|2m})$ *generated by the quadratic elements* $z_a\overline{z_b}$, $a,b\in\mathbf{I}$.

Proof: Since for all a, $\mathrm{d}L_{E_{m+n,m+n}}z_a=z_a$, and $\mathrm{d}L_{E_{m+n,m+n}}\overline{z_a}=-\overline{z_a}$, any $\mathrm{d}L_{\mathfrak{u}(1)}$-invariant element of $\mathbb{C}(\mathbb{S}^{2n-1|2m})$ must be a polynomial in $z_a\overline{z_b}$, $a,b\in\mathbf{I}$. This result can also be obtained in a more direct way by using Theorem 4.2. ■

Remark 5.3: We should emphasize that elements of $\mathbb{C}(\mathbb{P}^{n-1|m})$ are functions on the projective superspace that are not holomorphic in general because $\mathbb{C}(\mathbb{P}^{n-1|m})$ is a $*$-superalgebra.

Now we use Theorem 4.2 to extract the algebra $\mathbb{C}(\mathbb{P}^{n-1|m})^{\mathrm{d}R_{\mathrm{U}^{\mathrm{R}}(\mathfrak{k})}}$ of spherical functions on the projective superspace. Let $z:=z_{m+n}$ and $\overline{z}=\overline{z_{m+n}}$. We have the following.

Theorem 5.1: *The algebra of the spherical functions on the projective superspace is generated by* $r:=z\overline{z}$ *as a* $*$*-subalgebra of* $\mathbb{C}(\mathbb{P}^{n-1|m})$. *When* $n>1$, *the spherical functions form a polynomial algebra in one variable. When* $n=1$, *we have* $(1-r)^{m+1}=0$.

Proof: It is an immediate consequence of Theorem 4.2 that the algebra $\mathbb{C}(\mathbb{P}^{n-1|m})^{\mathrm{d}R_{\mathrm{U}^{\mathrm{R}}(\mathfrak{k})}}$ of the spherical functions on the projective superspace is indeed generated by the single element r.

When $n=1$, all the z_c, $\overline{z_c}$, $c\leqslant m$, are odd. Thus the $(m+1)$th power of $1-r=\Sigma_{c\leqslant m}z_c\overline{z_c}$ vanishes identically.

To study the case with $n>1$, we first analyze $\mathbb{C}[\mathrm{GL}_n]$, the algebra generated by the matrix elements of the contravariant and covariant vector representations of $\mathfrak{gl}(n)$. Let $\mathfrak{q}=\mathfrak{gl}(n-1)\oplus\mathfrak{gl}(1)$ be the subalgebra of $\mathfrak{gl}(n)$ embedded block diagonally. Set $A=\mathbb{C}[\mathrm{GL}_n]^{\mathrm{d}L_{\mathrm{U}(\mathfrak{q})}\otimes\mathrm{d}R_{\mathrm{U}(\mathfrak{q})}}$. Recall that $\mathbb{C}[\mathrm{GL}_n]$ is semisimple as a left module $\mathrm{U}(\mathfrak{q})$-module under the action $\mathrm{d}L_{\mathrm{U}(\mathfrak{q})}\otimes\mathrm{d}R_{\mathrm{U}(\mathfrak{q})}$. There exists a surjective $\mathrm{d}L_{\mathrm{U}(\mathfrak{q})}\otimes\mathrm{d}R_{\mathrm{U}(\mathfrak{l})}$-module map $\psi:\mathbb{C}[\mathrm{GL}_n]\to\mathrm{A}$. Let $\psi^*,(\mathrm{id}-\psi)^*:\mathrm{U}(\mathfrak{gl}(n))\to\mathrm{U}(\mathfrak{gl}(n))$ be vector space maps defined by

$$\langle f,(\mathrm{id}-\psi)^*(u)\rangle=\langle(\mathrm{id}-\psi)(f),u\rangle,$$

$$\langle f,\psi^*(u)\rangle=\langle\psi(f),u\rangle,\quad\forall\, u\in\mathfrak{gl}(n),\ f\in\mathbb{C}[\mathrm{GL}_n].$$

Since the dual space pairing between $\mathbb{C}[\mathrm{GL}_n]$ and $\mathrm{U}(\mathfrak{gl}(n))$ is nondegenerate, there is a nondegenerate pairing between A and $\psi^*(\mathrm{U}(\mathfrak{gl}(n)))$. Now as vector spaces,

$$\psi^*(\mathrm{U}(\mathfrak{gl}(n)))\cong\mathrm{U}(\mathfrak{gl}(n))/(\mathfrak{q}\mathrm{U}(\mathfrak{gl}(n))+\mathrm{U}(\mathfrak{gl}(n))\mathfrak{q}),$$

where the right-hand side is clearly infinite dimensional. This in particular implies that the subalgebra A of $\mathbb{C}[\mathrm{GL}_n]$ is infinite dimensional.

Let $\zeta:\mathbb{C}(\mathbb{P}^{n-1|m})^{\mathrm{d}R_{\mathrm{U}^{\mathrm{R}}(\mathfrak{k})}}\to\mathbb{C}[\mathrm{GL}_n]$ be the map defined for any $f\in\mathbb{C}(\mathbb{P}^{n-1|m})^{\mathrm{d}R_{\mathrm{U}^{\mathrm{R}}(\mathfrak{k})}}$ and $u\in\mathrm{U}(\mathfrak{gl}(n))$ by $\langle\zeta(f),u\rangle=\langle\zeta(f),i(u)\rangle$, where i is the canonical embedding $\mathrm{U}(\mathfrak{gl}(n))\subset\mathrm{U}(\mathfrak{g})$. Then ζ is an algebra homomorphism, and we have

$$\zeta(\mathbb{C}(\mathbb{P}^{n-1|m})^{\mathrm{d}R_{\mathrm{U}^{\mathrm{R}}(\mathfrak{e})}})=A.$$

If there existed a nontrivial polynomial $P(r)$ in r which was identically zero as an element of $\mathbb{C}(\mathbb{P}^{n-1|m})$, then $\mathbb{C}(\mathbb{P}^{n-1|m})^{\mathrm{d}R_{\mathrm{U}^{\mathrm{R}}(\mathfrak{k})}}$ would have to be finite dimensional over $\mathbb{C}$. This contradicts the fact that A is an infinite dimensional algebra. ■

Let us now study the action of a generalized Laplacian operator on the spherical functions. Recall that the quadratic Casimir of $\mathrm{U}(\mathfrak{g})$ can be expressed as $c=\Sigma_{a,b=1}^{m+n}(-1)^{[b]}E_{ab}E_{ba}$. For any $f\in\mathbb{C}(K\backslash G/K)$, we have $\mathrm{d}R_X\,\mathrm{d}R_c(f)=\mathrm{d}R_c\,\mathrm{d}R_X(f)=0$, $\forall X\in\mathfrak{l}$. That is $\mathrm{d}R_c(f)\in\mathbb{C}(K\backslash G/K)$. Consider the following generalized Laplacian operator on the homogeneous superspace:

$$\nabla^2=-\sum_{i=1}^{m+n-1}E_{i,m+n}E_{m+n,i}.$$

Then the actions of $\mathrm{d}R_{\nabla^2}$ and $\frac{1}{2}\mathrm{d}R_c$ coincide on $\mathbb{C}(K\backslash G/K)$. Thus $\mathrm{d}R_{\nabla^2}$ also maps $\mathbb{C}(K\backslash G/K)$ to itself.

In the case of the projective superspace, we can show that

$$\mathrm{d}R_{\nabla^2}(r^k) = kr^{k-1}[(m-n-k+1)r+k], \quad k=0,1,\ldots . \tag{5.2}$$

Let us now consider eigenfunctions of $\mathrm{d}R_{\nabla^2}$ in $\mathbb{C}(\mathbb{P}^{n-1|m})^{\mathrm{d}R_{\mathrm{U}^{\mathbb{R}}(\mathfrak{k})}}$. Things turn out to be quite different for $m-n+1\leqslant 0$ and $m-n+1>0$.

(1) If $m-n+1\leqslant 0$, there exists an eigenfunction $\theta_k \in \mathbb{C}(\mathbb{P}^{n-1|m})^{\mathrm{d}R_{\mathrm{U}^{\mathbb{R}}(\mathfrak{k})}}$ of $\mathrm{d}R_{\nabla^2}$ for each $k\in\mathbb{Z}_+$ with $\mathrm{d}R_{\nabla^2}(\theta_k)=k(m-n-k+1)\theta_k$, where

$$\theta_k = \sum_{i=0}^{k} (-1)^i \binom{n-m+2k-2}{i} \binom{k}{i}^2 (i!)^2 r^{k-i}. \tag{5.3}$$

Furthermore, the θ_k, $k\in\mathbb{Z}_+$, span $\mathbb{C}(\mathbb{P}^{n-1|m})^{\mathrm{d}R_{\mathrm{U}^{\mathbb{R}}(\mathfrak{k})}}$.

(2) If $m-n+1>0$, we let $L=m-n+1$, and denote by $[L/2]$ the largest integer $\leqslant L/2$. Then there exists an eigenfunction $\theta_k \in \mathbb{C}(\mathbb{P}^{n-1|m})^{\mathrm{d}R_{\mathrm{U}^{\mathbb{R}}(\mathfrak{k})}}$ of $\mathrm{d}R_{\nabla^2}$ for each non-negative integer k satisfying either $k\leqslant[L/2]$ or $k>L$ with $\mathrm{d}R_{\nabla^2}$-eigenvalue $k(L-k)$, where the θ_k are still given by (5.3). However, the θ_k's do not span $\mathbb{C}(\mathbb{P}^{n-1|m})^{\mathrm{d}R_{\mathrm{U}^{\mathbb{R}}(\mathfrak{k})}}$.

Note that if $m-n+1>0$, the operator $\mathrm{d}R_{\nabla^2}$ is not diagonalizable over $\mathbb{C}(K\backslash G/K)$. The simplest illustration comes from the case with $L=1$, where $\mathbb{C}(K\backslash G/K)$ is the direct sum of $\{a+br \,|\, a,b\in\mathbb{C}\}$ and $\oplus_{k>1}\mathbb{C}\theta_k(r)$. While acting diagonally on the latter subspace, $\mathrm{d}R_{\nabla^2}$ acts on the former subspace by $\mathrm{d}R_{\nabla^2}(a+br)=b$.

Remark 5.4: $\mathbb{C}(G)$ is not semisimple with respect to $\mathrm{d}R_{\mathrm{U}(\mathfrak{g})}$. There exist $\mathrm{d}R_{\mathrm{U}(\mathfrak{g})}$-submodules of $\mathbb{C}(G)$ on which $\mathrm{d}R_c$ cannot be diagonalized. Therefore, $\mathrm{d}R_{\nabla^2}$ is not diagonalizable on $\mathbb{C}(K\backslash G/K)$ in general, and case (2) shows this fact.

B. The other maximal rank *K* cases

We assume that both m and n are greater than 2 in this section, and consider the maximal rank K's that correspond to the subalgebras $\mathfrak{k}_{n,k}:=\mathfrak{l}_{n,k}^{\sigma,\sqrt{\imath}}$ and $\mathfrak{k}_{m,k}:=\mathfrak{l}_{m,k}^{\sigma,\sqrt{\imath}}$, where

$$\mathfrak{l}_{n,k} = \mathfrak{gl}(m|n-k)\oplus\mathfrak{gl}(k), \quad 0<k\leqslant n,$$

$$\mathfrak{l}_{m,k} = \mathfrak{gl}(k)\oplus\mathfrak{gl}(m-k|n), \quad 0<k\leqslant m.$$

For the subalgebra $\mathfrak{k}_{n,k}$, by Theorem 4.1, the corresponding homogeneous superspace $\mathbb{C}(K_{n,k}\backslash G)$ is generated by

$$C_{ab} = \sum_{c=m+n-k+1}^{m+n} t_{ca}\overline{t_{cb}}, \quad a,b\in\mathbf{I}.$$

Note that $[c]=1$. As in Theorem 5.1, we can show that $\mathbb{C}[C_{ab}]$ forms a polynomial algebra in one variable if $[a]=[b]=1$; and if $[a]=[b]=0$, then $(C_{ab})^{k+1}=0$ and $(C_{ab})^k\neq 0$. Recall that by Proposition 4.1, we always have $(C_{ab})^2=0$ if $[a]+[b]=1$. The subalgebra of spherical functions $\mathbb{C}[K_{n,k}\backslash G/K_{n,k}]$ is generated by

$$C = \sum_{c,a=m+n-k+1}^{m+n} t_{ca}\overline{t_{ca}},$$

and forms a polynomial algebra in one variable. Similarly, for $\mathfrak{k}_{m,k}$, the symmetric superspace $\mathbb{C}(K_{m,k}\backslash G)$ is generated by

$$C_{ab} = \sum_{c=1}^{k} t_{ca}\overline{t_{cb}}, \quad a,b \in \mathbf{I}.$$

If $[a]=[b]=0$, then $\mathbb{C}[C_{ab}]$ forms a polynomial algebra in one variable, and if $[a]=[b]=1$, then $(C_{ab})^{k+1}=0$ and $(C_{ab})^{k}\neq 0$. The subalgebra of spherical functions $\mathbb{C}(K_{m,k}\backslash G/K_{m,k})$ is generated by

$$C = \sum_{c,a=1}^{k} t_{ca}\overline{t_{ca}},$$

as a polynomial algebra. To summarize, we have

Theorem 5.2: (1) *If $m\leqslant n$, then there is an onto algebra homomorphism,*

$$\phi:\mathbb{C}(K_{n,k}\backslash G) \rightarrow \mathbb{C}(K_{m,k}\backslash G)$$

which induces an isomorphism $\mathbb{C}(K_{n,k}\backslash G/K_{n,k})\rightarrow\mathbb{C}(K_{m,k}\backslash G/K_{m,k})$.

(2) *For each $1\leqslant k<n$, there is an onto algebra homomorphism,*

$$\phi_{k+1,k}:\mathbb{C}(K_{n,k+1}\backslash G) \rightarrow \mathbb{C}(K_{m,k}\backslash G)$$

which induces an isomorphism $\mathbb{C}(K_{n,k+1}\backslash G/K_{n,k+1})\rightarrow\mathbb{C}(K_{n,k}\backslash G/K_{n,k})$.

Proof: For (1), we just need to note that any relation among the C_{ab} holds for both algebras by symmetry. For (2), let the generators of $\mathbb{C}(K_{n,k}\backslash G)$ described above be $C_{ab}(k)$ $(a,b\in\mathbf{I}, 1\leqslant k\leqslant n)$, and define $\phi_{k+1,k}:\mathbb{C}(K_{n,k+1}\backslash G)\rightarrow\mathbb{C}(K_{m,k}\backslash G)$ by $\phi_{k+1,k}(C_{ab}(k+1))=[(k+1)/k]C_{ab}(k)$. ■

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Scattering amplitude and scattering phase for the Schrödinger equation with strong magnetic field

Laurent Michel[a)]
Institut Gallilée, Département de Mathématiques, Universite Paris XIII, 93430 Villetaneuse, France

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In this paper we consider the Schrödinger equation with constant magnetic field of strength $b>0$ in all dimension. We study the behavior of the scattering amplitude and the scattering phase when the parameter b goes to infinity and the energy is far from the Landau levels. © *2005 American Institute of Physics.*
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I. INTRODUCTION

In this paper, we are interested in the Schrödinger equation with magnetic field

$$i\partial_t\psi = H(b)\psi,$$

where $H(b)=H_0(b)+V(x)$ with $V\in L^\infty(\mathbb{R}^n)$ and

$$H_0(b) = |i\nabla_x - bA(x)|^2. \tag{1}$$

Here, $A:\mathbb{R}^n\to\mathbb{R}^n$ is the magnetic potential and b is a strictly positive real parameter. Our aim is to study the scattering matrix associate to the pair $(H(b),H_0(b))$. In order to lighten the notations we drop the parameter b and write H instead of $H(b)$. There is a wide literature dealing with the Schrödinger equation with magnetic field (see for instance Refs. 2, 7, and 14 for general properties dealing with our problem). In this paper, we consider the case where the magnetic field is constant. More precisely, denoting $A(x)=(A_1(x),\dots,A_n(x))$ with $A_j:\mathbb{R}^n\to\mathbb{R}$, $j=1,\dots,n$, the magnetic field B can be identified with the antisymmetric matrix $B(x)=(\partial_{x_i}A_j(x)-\partial_{x_j}A_i(x))_{i,j}$. Here, we consider the case where the magnetic field $B(x)$ does not depend on x. Regarding B as an antisymmetric linear map on $\mathbb{R}^n$, we set $2d=\dim \mathrm{Ran}\, B$ and $k=n-2d=\dim \mathrm{Ker}\, B$. As we are interested in the case where $B\neq 0$, we suppose that $d\neq 0$. On the other hand, as we study scattering problems we do not consider the case $n=2d$ where the spectrum of H_0 is pure point. Hence, we suppose that $k=n-2d\neq 0$. Under this assumption there exists Cartesian coordinates in which the reference Hamiltonian takes the form

$$H_0 = \sum_{j=1}^{d}\left[(i\partial_{x_{2j-1}} - b\mu_j x_{2j})^2 + (i\partial_{x2j} + b\mu_j x_{2j-1})^2\right] - \Delta_{x\|},$$

where $x=(x_1,x_2,\dots,x_{2d-1},x_{2d},x_\|)=(x_\perp,x_\|)\in\mathbb{R}^{2d}\times\mathbb{R}^{n-2d}$ and $\mu_1,\dots,\mu_d$ are strictly positive real numbers (see Ref. 14 for details). Under suitable assumptions on V, it is well known (see Ref. 2) that the scattering operator $\mathbf{S}=\mathbf{S}(b)$ associated to the pair (H_0,H) is well defined. Our aim is to describe this operator when the parameter b goes to infinity.

Before going further, let us recall some works concerning such problems. First, we would like to mention some results concerning the scattering matrix in the case where $A(x)$ is a long range potential [i.e., $A(x)$ decreases faster than $|x|^{-\rho}$ for some $\rho>0$ when $|x|$ goes to infinity]. In that

a)Electronic mail: michel@math.univ-paris13.fr

case, there is a scattering theory for the pair $(H,-\Delta)$ (cf. Refs. 10, 13, 16, and 18) and it is possible to describe the behavior of the scattering amplitude in the high energy limit (cf. the work of Nicoleau[12]).

On the other hand, there are some recent works of Bruneau–Pushnitski–Raikov[5] and Bruneau–Dimassi,[4] concerning the Schrödinger equation with constant magnetic field. In Ref. 5, the authors study the spectral shift function associate to this equation in dimension 3 and they describe its behavior in several asymptotic regimes. In particular, they investigate deeply the case where b goes to infinity and the distance from the energy to the set of Landau levels behaves as b. There are also some works of Kostrykin–Kvitsinsky–Mekuyriev,[8] where the authors study partial scattering matrix in dimension 3 near the Landau levels (b being fixed). Moreover, in Ref. 8 the authors make some symmetry assumption on the potential V. Here, we would like to treat the case of general potential in dimension n in the asymptotic regime considered in Ref. 5.

First, we need to give an exact definition of the scattering amplitude in the present situation. Let us consider the Schrödinger operator with constant magnetic field in dimension $2d$,

$$\hat{H}_0 = \sum_{j=1}^{d} [(i\partial_{x_{2j-1}} - b\mu_j x_{2j})^2 + (i\partial_{x_{2j}} + b\mu_j x_{2j-1})^2] \tag{2}$$

acting on $L^2(\mathbb{R}^{2d})$. As $\mu_1 \cdots \mu_d \neq 0$, it is well known that the spectrum of $\hat{H}_0$ is pure point.[2] For $q=(q_1,\ldots,q_d)\in\mathbb{N}^d$ we denote $\Lambda_q=(2_{q1}+1)\mu_1+\cdots+(2q_d+1)\mu_d$, so that the spectrum of $\hat{H}_0$ is given by the sequence of Landau levels

$$\mathbb{L} = \sigma(\hat{H}_0) = \sigma_{pp}(\hat{H}_0) = \{b\Lambda_q, q \in \mathbb{N}^d\}.$$

In particular, the bottom of the spectrum is given by $b\Lambda_0=b(\mu_1+\cdots+\mu_d)$. Let us denote by $\Upsilon_q \subset L^2(\mathbb{R}^{2d})$ the eigenspace associated to the eigenvalue $b\Lambda_q$ and $\Pi_q: L^2(\mathbb{R}^{2d}) \to \Upsilon_q$ the corresponding projector. Denoting $L^2_\alpha(\mathbb{R}^{n-2d})=\{f\in L^2(\mathbb{R}^{n-2d}); \langle x_\parallel\rangle^\alpha f \in L^2(\mathbb{R}^{n-2d})\}$; we define $\tilde{\mathcal{F}}_0(\lambda): L^2_\alpha(\mathbb{R}^{n-2d}) \to L^2(S^{n-2d-1})$ by

$$\tilde{\mathcal{F}}_0(\lambda)\varphi(\xi) = \frac{\lambda^{(n-2d-2)/4}}{\sqrt{2}(2\pi)^{(n-2d)/2}} \int_{\mathbb{R}^{n-2d}} e^{-i\sqrt{\lambda}\langle x,\xi\rangle}\varphi(a)\mathrm{d}x,$$

and we set

$$\mathcal{F}_0(\lambda): L^2(\mathbb{R}^{2d}, L^2_\alpha(\mathbb{R}^{n-2d})) \to L^2(\mathbb{R}^{2d}\times S^{n-2d-1}),$$

$$\varphi \mapsto \sum_{b\Lambda_q \leqslant \lambda} \Pi_q \otimes \tilde{\mathcal{F}}_0(\lambda - b\Lambda_q)\varphi.$$

Let us introduce the space

$$L^\infty_\alpha(\mathbb{R}^n) = \{u: \mathbb{R}^n \to \mathbb{R}, \langle x_\parallel\rangle^\alpha u \in L^\infty(\mathbb{R}^n)\}$$

and for $u\in L^\infty_\alpha(\mathbb{R}^n)$ let us set $\|u\|_{\infty,\alpha}=\|\langle x_\parallel\rangle^\alpha u\|_{L^\infty}$. The assumption that we make on the potential V is the following.

Assumption 1: We assume that $V(x_\parallel,x_\perp)=V^\infty(x_\parallel)+W(x_\parallel,x_\perp)$ with V^∞ and W in $L^\infty_\rho(\mathbb{R}^n)$ for some $\rho>1$, $V^\infty \geqslant 0$ and $\sup\{|W(n)|, 1\times 1 \geqslant R\} \to 0$ when $R\to+\infty$.

It follows from the general results of Ref. 2 that under this assumption the wave operators associated to the pair (H_0,H) exist and are complete. Therefore, the scattering operator $\mathbf{S}(b)$ is well defined and by the mean of $\mathcal{F}_0$, we can define the scattering matrix. More precisely, recall that the absolute continuous spectrum of H_0 is $\sigma_{ac}(H_0)=]b\Lambda_0,+\infty[$. Then for all $\lambda > b\Lambda_0$ there exists

$$S(\lambda,b): L^2(\mathbb{R}^{2d}\times S^{n-2d-1}) \to L^2(\mathbb{R}^{2d}\times S^{n-2d-1})$$

such that

$$S(\lambda,b)\mathcal{F}_0(\lambda) = \mathcal{F}_0(\lambda)\mathbf{S}(b).$$

Let us denote $\mathcal{H}_\alpha = L^2(\mathbb{R}^n, \langle x_\| \rangle^\alpha \, dx)$ and $\|\cdot\|_{\mathcal{H}_\alpha}$ the corresponding norm. Our first result gives a representation formula for the scattering matrix very similar to that obtained for the Schrödinger equation.[1]

Theorem 1: *Suppose that Assumption 1 is satisfied and denote by $\sigma_{pp}(H)$ the point spectrum of H. Then, for all $\lambda \in]b\Lambda_0, +\infty[\setminus (L \cup \sigma_{pp}(H))$, one has*

$$S(\lambda,b) - Id = -2i\pi\mathcal{F}_0(\lambda)V(x)\mathcal{F}_0(\lambda)^* + 2i\pi\mathcal{F}_0(\lambda)V(x)R(\lambda+i0)V(x)\mathcal{F}_0(\lambda)^*, \tag{3}$$

where

$$R(\lambda+i0) = \lim_{\mu\to 0^+} (H-\lambda-i\mu)^{-1}$$

exists in the space $\mathcal{L}(\mathcal{H}_\alpha, \mathcal{H}_{-\alpha})$ for $\alpha > 1/2$.

Remark 1.1: In the case where the potential V is compactly supported with respect to the variable $x_\|$, the scattering matrix takes a form that could be interesting for other applications. More precisely, suppose that $V \in L^\infty(\mathbb{R}^n)$ and there exists a compact $K \subset \mathbb{R}^{n-2d}$ such that $\forall x_\| \notin K$, $V(.,x_\|) = 0$. Let χ_1, $\chi_2 \in C_0^\infty(\mathbb{R}^{n-2d})$ such that $\chi_1 = 1$ in a neighborhood of K and $\chi_2 = 1$ on supp χ_1. *Then, using some ingrations by parts, it is not hard to prove that*

$$S(\lambda,b) - Id = -2i\pi\mathcal{F}_0(\lambda)[\Delta_{x_\|}, \chi_1]R(\lambda+i0)[\Delta_{x_\|}, \chi_2]\mathcal{F}_0(\lambda)^*.$$

Using Theorem 1, we can describe the behavior of $S(\lambda,b)$. Let us set $T(\lambda,b) = S(\lambda,b) - Id$, then $T(\lambda,b)$ has a kernel

$$(\omega,\omega') \in S^{n-2d-1} \times S^{n-2d-1} \mapsto T(\omega,\omega',\lambda,b) \in \mathcal{L}(L^2(R^{2d})).$$

Denote by $\hat{V}^\|$ the partial Fourier transform of V with respect to the variable $x_\|$. We need to introduce two additional assumptions.

Assumption 2: We suppose that $V \in L^\infty_\rho(\mathbb{R}^n)$ for some $\rho > n - 2d$, and that $\hat{V}^\| \in L^\infty_r(\mathbb{R}^n)$ for some $r > 0$.

Assumption 3: We suppose that $\hat{V}^\| \in C^1(\mathbb{R}^n)$ and that $\sup_{\mathbb{R}^n} |\partial_{x_\perp} \hat{V}^\|| < \infty$.

Now we are in position to state our main result on the scattering amplitude. In the following we denote

$$\tilde{\mathbb{L}} = \{\Lambda_q, q \in \mathbb{N}^d\} = b^{-1}\mathbb{L}.$$

and

$$\tilde{Q}(\mathcal{E}) = \{q \in \mathbb{N}^d; \Lambda_q \leqslant \mathcal{E}\},$$

which is a finite set, thanks to the fact that $\mu_1, \ldots, \mu_d > 0$. In this paper we denote by $\|\cdot\|$ the L^2 norm and the norm on the space of linear bounded operators on L^2. We have the following theorem.

Theorem 2: *Suppose that Assumptions 1 and 2 are satisfied and let $\lambda > b\Lambda$.*

(i) *Denote $\delta := dist(\lambda, \mathbb{L})$ and suppose that $\delta > \|V\|_{\infty,\rho}$, then*

$$\sup_{(\omega,\omega')\epsilon S^{n-2d-1}\times S^{n-2d-1}} \left\| T(\omega,\omega',\lambda,b) + \frac{i}{2(2\pi)^{n-2d+1}} \sum_{b\Lambda_q \leqslant \lambda} (\lambda - b\Lambda_q)^{(n-2d-2)/2} \Pi_q \hat{V}^{\|}(x_\perp, \sqrt{\lambda - b\Lambda_q} \times(\omega-\omega'))\Pi_q \right\| \leqslant C\lambda b^{-1} \delta^{[n-2d-2-\min(1,r)]/2}, \tag{4}$$

where C depends only on $\|\hat{V}^{\|}\|_{\infty,r}$ *and* $\|V\|_{\infty,\rho}$.

(ii) *We suppose additionally that Assumption 3 is satisfied. Let* $\mathcal{E} \in]\Lambda_0, +\infty[\setminus \tilde{\mathbb{L}}$ *and* $\Delta \subset \mathbb{R}$ *be a bounded interval. When b tends to infinity, one has*

$$\sup_{(\omega,\omega')\epsilon S^{n-2d-1}\times S^{n-2d-1}} \sup_{\lambda\in\Delta} \left\| T(\omega,\omega',\mathcal{E}b+\lambda,b) + \frac{ib^{(n-2d-2)/2}}{2(2\pi)^{n-2d+1}} \sum_{q\in\tilde{Q}(\mathcal{E})} \beta_q^{n-2d-2} \hat{V}^{\|}(x_\perp, b^{1/2}\beta_q(\omega - \omega'))\Pi_q \right\| \leqslant C b^{[n-2d-2-\min(1,r)]/2}, \tag{5}$$

where

$$\beta_q = (\mathcal{E} - \Lambda_q)^{1/2} = (\mathcal{E} - \mu_1 q_1 - \cdots - \mu_d q_d)^{1/2}. \tag{6}$$

From this theorem we can also deduce the following inverse scattering result.

Corollary 1.2: Suppose that V_1, V_2 *satisfy Assumptions* 1, 2, *and* 3. *Assume that the associate scattering operators* S_1 *and* S_2 *are equal. Then* $V_1 = V_2$.

We can also use the representation formula of Theorem 1 to study the scattering phase $s(\lambda,b)$ associate to the pair (H,H_0). Let us recall briefly how to define this function. Assume that the operator $T(\lambda,b)$ is trace class. Then the determinant $\det(I+T(\lambda,b))$ is well defined. Moreover, $S(\lambda,b)$ being unitary, this determinant is of modulus 1 so that the function $s(.,b)$ can be defined modulo 2π by

$$\det S(\lambda,b) = e^{-2i\pi s(\lambda,b)}. \tag{7}$$

Assume additionally that for b large enough, $\|T(\lambda,b)\| < 1$ uniformly with respect to λ. Then $s(\lambda,b) = (-1/2i\pi)\ln \det S(\lambda,b)$ can be determined uniquely by the following process. Consider the function

$$f{:}\sigma \in [0,1] \mapsto \det(I+\sigma T) \in \mathbb{C}$$

which is holomorphic with respect to σ. From the assumption $\|T\| < 1$ we deduce that the spectrum of T is contained in $]-1,1[$ and the function f is nonvanishing. Therefore, the function $\ln(f)$ such that $\ln(f)(0) = 0$ is uniquely defined and it follows that $s = \ln(f)(1) = (1/2i\pi)\ln \det(I+T)$ is well defined. Moreover, by construction, we have

$$2i\pi s(\lambda,b) = \int_0^1 \frac{\mathrm{d}}{\mathrm{d}\sigma} \ln(\det(Id + \sigma T(\lambda,b)))\mathrm{d}\sigma = \int_0^1 \mathrm{tr}\,(T(\lambda,b)(Id+\sigma T(\lambda,b))^{-1})\mathrm{d}\sigma. \tag{8}$$

Before we state our results, let us recall the link between the scattering phase $s(\lambda,b)$ and the spectral shift function $\xi(\lambda,b)$ (in short SSF). Assume that the difference $(H+\lambda_0)^{-\gamma} - (H_0+\lambda_0)^{-\gamma}$ is trace class for some $\lambda_0, \gamma > 0$ large enough [for instance, if $\langle x\rangle^{\delta/2} V \in L^2(\mathbb{R}^n)$ with $\delta > n$, this assumption is satisfied in view of Theorem XI.21 of Ref. 15 and the diamagnetic inequality]. Therefore, the spectral shift function can be defined (see Refs. 17 and 9) in the sense of distribution by:

$$\langle \xi'(.,b)\,.\,f\rangle = \mathrm{tr}(f(H) - f(H_0)), \quad \forall\, f \in C_0^\infty(\mathbb{R})$$

and $\xi(\lambda,b)=0$ for λ below the infimum spectrum of H. Moreover, we know from the Birman–Krein theory (see Refs. 3 and 17) that

$$\det S(\lambda,b) = e^{-2i\pi\xi(\lambda,b)}. \tag{9}$$

Comparing Eqs. (9) and (7), it follows that $\xi(\lambda,b)=s(\lambda,b)+c(\lambda,b)$ with $c(\lambda,b)\in\mathbb{Z}$. In Ref. 5, Bruneau, Pushnitski, and Raikov studied the asymptotics of $\xi(\lambda,b)$ far from the Landau levels. In the two next theorems we lead such a study for the scattering phase.

Theorem 3: *Suppose that Assumption 1 is satisfied and that* $V\in L^1(\mathbb{R}^n)$. *Let* $\mathcal{E}\in\,]\Lambda_0, +\infty[\backslash\widetilde{\mathbb{L}}$ *and* $\Delta\subset\mathbb{R}$ *be a bounded interval. When* $b\to+\infty$, *one has* $\sup_{\lambda\in\Delta}\|T(\mathcal{E}b+\lambda)\|\leqslant Cb^{-1/2}$ *and the scattering phase defined by (8) satisfies*

$$\sup_{\lambda\in\Delta}\left| s(\mathcal{E}b+\lambda,b) + b^{(n-2)/2}\frac{mes(S^{n-2d-1})}{2(2\pi)^{n-2d+1}}\sum_{q\in\widetilde{Q}(\mathcal{E})}\beta_q^{n-2d-1}\int_{\mathbb{R}^n}V(x)\mathrm{d}x\right| = \mathcal{O}(b^{(n-3)/2}), \tag{10}$$

where β_q *is given by (6) and* $mes(S^{n-2d-1})$ *denotes the Lebesgue measure of* S^{n-2d-1}.

Let us remark that in the asymptotic regime that we consider the scattering phase and the spectral shift function differ from a constant independent on λ and b. Indeed, it is clear that these functions are continuous far from the Landau levels. Hence, for $\mathcal{E}\in\,]\Lambda_0,+\infty[\backslash\widetilde{\mathbb{L}}$, the function $c(\mathcal{E}b+\lambda,b)$ is continuous with respect to $(\lambda,b)\in\Delta\times\,]b_0,+\infty[$ for b_0 large enough. As it takes its values in $\mathbb{Z}$ it follows that c is constant. Therefore, it follows from (10) that under the preceding assumptions we have

$$\sup_{\lambda\in\Delta}\left| \xi(\mathcal{E}b+\lambda,b) + b^{(n-2)/2}\frac{mes(S^{n-2d-1})}{2(2\pi)^{n-2d+1}}\sum_{q\in\widetilde{Q}(\mathcal{E})}\beta_q^{n-2d-1}\int_{\mathbb{R}^n}V(x)\mathrm{d}x\right| = \mathcal{O}(b^{(n-3)/2}).$$

Remark that this result generalizes Theorem 2.1 of Ref. 5 in several directions. First it holds in all dimension whereas Bruneau, Pushnitski, and Raikov work in dimension 3. Moreover, it needs less regularity on the potential. Let us also remark that the method we use to prove it is completely different from that of Ref. 5 as it stands on the study of the scattering phase. However, we can notice that for $n=3$, we obtain the same asymptotics than in Ref. 5.

Using this representation, we can also give a complete asymptotics expansion of scattering phase. For a sake of simplicity, we formulate the theorem only in the case $n=3$ (and hence we can suppose that $\mu_1=1$), but the proof is the same in the case where $n=2d+1$. We also prove the Theorem for V in the Schwartz class whereas it certainly holds for more general C^∞ potentials going to zero at infinity as well as their derivatives.

Theorem 4: *Suppose that* $V\in\mathcal{S}(\mathbb{R}^3)$. *Let* $\mathcal{E}\in\mathbb{R}_+^*\backslash\{2q+1, q\in\mathbb{N}\}$ *and* $\Delta\subset\mathbb{R}$ *be a bounded interval. There exists a sequence of coefficients* $(a_j(\lambda,\mathcal{E},V))_{j\in\mathbb{N}}$ *such that one has the following expansion when* $b\to+\infty$:

$$\sup_{\lambda\in\Delta}\left| s(\mathcal{E}b+\lambda,b) - b^{\frac{1}{2}}\sum_{j=0}^{\infty}a_j(\lambda,\mathcal{E},V)b^{-j}\right| = \mathcal{O}(b^{-\infty}). \tag{11}$$

Moreover, the coefficients a_j *can be computed explicitly. Setting* $\gamma_j(\mathcal{E})=\sum_{q=1}^{[(\varepsilon-1)]/2}(\mathcal{E}-2q-1)^{-\frac{1}{2}-j}$, *one has*

$$a_0(\lambda,\mathcal{E},V) = -\frac{\gamma_0(\mathcal{E})}{4\pi^2}\int_{\mathbb{R}^3}V(x)\mathrm{d}x,$$

$$a_1(\lambda,\mathcal{E},V)=\frac{\gamma_1(\mathcal{E})}{16\pi^2}\left(2\lambda\int_{\mathbb{R}^3}V(x)\mathrm{d}x-\int_{\mathbb{R}^3}V(x)^2\,\mathrm{d}x\right).$$

The plan of the paper is the following. In the next section we use the spectral resolution of H_0 to obtain a representation formula for the scattering matrix. In Sec. III, we study the scattering amplitude whereas the results concerning the scattering phase are proved in Sec. IV.

II. REPRESENTATION OF THE SCATTERING MATRIX

In this section, we recall some basic facts on the spectral resolution of H_0 and the limiting absorption principle and we prove Theorem 1. Let us denote $\partial\widetilde{E}_0/\partial\lambda:L^2(\mathbb{R}^{n-2d})\to L^2(\mathbb{R}^{n-2d})$ the spectral resolution of $-\Delta_{x_\parallel}$ on $\mathbb{R}^{n-2d}$. Then, it is well known that the spectral resolution of H_0 is given by

$$\frac{\partial E_0}{\partial\lambda}=\sum_{b\Lambda_q\leqslant\lambda}\Pi_q\otimes\frac{\partial\widetilde{E}_0}{\partial\lambda}(\lambda-\Lambda_q). \tag{12}$$

Moreover, one knows that $\partial\widetilde{E}_0/\partial\lambda=\widetilde{\mathcal{F}}_0(\lambda)^*\widetilde{\mathcal{F}}_0(\lambda)$ so that (12) yields

$$\frac{\partial E_0}{\partial\lambda}=\mathcal{F}_0(\lambda)^*\mathcal{F}_0(\lambda). \tag{13}$$

For $z\in\mathbb{C}$ with $\mathrm{Im}\,z\neq 0$, we set $R_0(z)=(H_0-z)^{-1}$ and $R(z)=(H-z)^{-1}$ which are holomorphic with respect to $z\in\mathbb{C}\backslash\mathbb{R}$. We denote by $\sigma_{pp}(H)$, the point spectrum of H. The following proposition gives the limiting absorption principle for the operators H_0 and H.

Proposition 2.1: (i) *Assume that* $\lambda\in]b\Lambda_0,+\infty[\backslash\mathbb{L}$, *then the following limit exists in the space of bounded operators* $\mathcal{L}(\mathcal{H}_\alpha,\mathcal{H}_{-\alpha})$ *for any* $\alpha>1/2$:

$$R_0(\lambda\pm i0)=\lim_{\mu\to0^+}R_0(\lambda\pm i\mu).$$

(ii) *Suppose that Assumption* 1 *is satisfied and that* $\lambda\in\mathbb{R}_+^*\backslash(\sigma_{pp}(H)\cup\mathbb{L})$, *then there exists*

$$R(\lambda\pm i0)=\lim_{\mu\to0^+}R(\lambda\pm i\mu)$$

in $\mathcal{L}(\mathcal{H}_\alpha,\mathcal{H}_{-\alpha})$ *for any* $\alpha>1/2$.

Proof: Using (12), it is clear that for all $z\in\mathbb{C}\backslash\mathbb{R}$, one has

$$R_0(z)=\sum_{q\in\mathbb{N}^d}\Pi_q\otimes(-\Delta_{x_\parallel}-(z-b\Lambda_q))^{-1}, \tag{14}$$

where the series converges in $\mathcal{L}(\mathcal{H}_\alpha,\mathcal{H}_{-\alpha})$ for any $\alpha>1/2$. Assume that $\lambda\in]b\Lambda_0,+\infty[\backslash\mathbb{L}$, then

$$R_0(\lambda\pm i\mu)=\sum_{b\Lambda_q\leqslant\lambda}\Pi_q\otimes(-\Delta_{x_\parallel}-(\lambda\pm i\mu-b\Lambda_q))^{-1}+W(\lambda\pm i\mu),$$

with

$$\|W(\lambda\pm i\mu)-W(\lambda\pm i\mu')\|^2\leqslant C|\mu-\mu'|^2\sum_{b\Lambda_q\geqslant\lambda}\|\Pi_q\otimes Id\|^2\leqslant C|\mu-\mu'|^2. \tag{15}$$

Moreover, using the limiting absorption principle for the free Laplacian on $\mathbb{R}^{n-2d}$ it is clear that for any $\lambda\in]b\Lambda_0,+\infty[\backslash\mathbb{L}$, there exists

$$\lim_{\mu\to 0^+}\sum_{b\Lambda_q\leqslant\lambda}\Pi_q\otimes(-\Delta_{x_\parallel}-(\lambda\pm i\mu-b\Lambda_q))^{-1}$$

and the proof of (i) is complete.

The proof of (ii) is very close to the proof of Agmon[1] for Schrödinger operator. For $\mathrm{Im}\, z>0$, let us denote $R_\infty(z)=(H_0+V^\infty-z)^{-1}$. The potential V^∞ being independent on $x_\perp$, it commutes with the projectors Π_q so that

$$\forall\,\mathrm{Im}\, z>0,\ R_\infty(z)=\sum_{q\in\mathbb{N}^d}\Pi_q\otimes(-\Delta_{x_\parallel}+V^\infty(x_\parallel)-(z-b\Lambda_q))^{-1}.$$

As V^∞ is non negative the spectrum of $-\Delta_{x_\parallel}+V^\infty$ is contained in $\mathbb{R}^+$ and we deduce from the limiting absorption principle for the Schrödinger operator that for any $\lambda\in]b\Lambda_0,+\infty[\backslash\mathbb{L}$,

$$R_\infty(\lambda\pm i0)=\lim_{\mu\to 0+}R_\infty(\lambda\pm i\mu)=\sum_{b\Lambda_q\leqslant\lambda}\Pi_q\otimes(-\Delta_{x_\parallel}+V^\infty-(\lambda\pm i0-b\Lambda_q))^{-1}$$

exists in $\mathcal{L}(\mathcal{H}_\alpha,\mathcal{H}_{-\alpha})$. Now for $\mathrm{Im}\ z>0$ we can write

$$R(z)=R_\infty(z)(Id+WR_\infty(z))^{-1}$$

As in Ref. 1, the only thing we have to check is that for all $z\in\mathbb{C}$ with $\mathrm{Im}\,(z)\geqslant 0$, $K(z)=W(x)R_\infty(z)$ is compact from $\mathcal{H}_\alpha$ into $\mathcal{H}_\alpha$ for some $\alpha>1/2$. On the other hand,

$$K(z)=W(x)R_0(z)(Id-V^\infty R_\infty(z))$$

and it follows from the limiting absorption principle for $R^\infty(z)$ that $(Id-V^\infty R_\infty(z))$ can be continued to $\mathrm{Im}\, z\geqslant 0$ into a bound operator on $\mathcal{H}_\alpha$ for $1/2<\alpha<\rho/2$. Hence the proof is reduced to show that $W R_0(z)$ is compact from $\mathcal{H}_\alpha$ into $\mathcal{H}_\alpha$. Using the diamagnetic inequality (see Ref. 14, Lemma 2.1), the compactness of $K(z)$ is a straightforward consequence of the same property for the Schrödinger operator.

In the next proposition we recall some estimates of the resolvent proved in Ref. 5.

Proposition 2.2: (i) *Assume that* $\lambda\in]b\Lambda_0,+\infty[\backslash\mathbb{L}$, *then*

$$\|\langle x_\parallel\rangle^{-\alpha}R_0(\lambda\pm i0)\langle x_\parallel\rangle^{-\alpha}\|\leqslant\frac{C}{dist(\lambda,\mathbb{L})^{1/2}},\ \forall\ \alpha>1/2.$$

(ii) *Suppose that Assumption 1 is verified and that* $\lambda\in]b\Lambda_0,+\infty[$ *satisfies* $dist(\lambda,\mathbb{L})>\|V\|_{\infty,\rho}$. *Then* $\lambda\notin\sigma_{pp}(H)$ *and*

$$\|\langle x_\parallel\rangle^{-\alpha}R(\lambda\pm i0)\langle x_\parallel\rangle^{-\alpha}\|\leqslant\frac{C}{dist(\lambda,\mathbb{L})^{1/2}},\ \forall\ 1/2<\alpha<\rho/2.$$

Proof: The point (i) is a direct consequence of the well-known high-energy estimates of the resolvent of the Schrödinger equation. The claim (ii) follows easily from Birman–Schwinger principle and from the following formula:

$$R(\lambda\pm i0)=R_0(\lambda\pm i0)(Id+V\,R_0(\lambda\pm i0))^{-1}.$$

■

Now, we are in position to give the proof of Theorem 1 which is an adaptation of the demonstration given in the case of the Schrödinger operator (cf. Ref. 6). We start with a simple lemma.

Lemma 2.3: Suppose that $\lambda\in]b\Lambda_0,+\infty[\backslash\mathbb{L}$, *then*

$$R_0(\lambda+i0)-R_0(\lambda-i0)=2i\pi\mathcal{F}_0(\lambda)^*\mathcal{F}_0(\lambda).$$

Proof: The proof is based on the fact that this result holds for the Schrödinger operator,

$$\forall \lambda > 0, (-\Delta_{x_\parallel} - \lambda - i0)^{-1} - (-\Delta_{x_\parallel} - \lambda + i0)^{-1} = 2i\pi \tilde{\mathcal{F}}_0(\lambda)^* \tilde{\mathcal{F}}_0(\lambda). \tag{16}$$

On the other hand, for $\lambda \in]b\Lambda_0, +\infty[\backslash \mathbb{L}$, it follows from (15) that

$$R_0(\lambda + i0) - R_0(\lambda - i0) = \sum_{b\Lambda_q \leqslant \lambda} (-\Delta_{x_\parallel} - \lambda + b\Lambda_q - i0)^{-1} \otimes \Pi_q - (-\Delta_{x_\parallel} - \lambda + b\Lambda_q + i0)^{-1} \otimes \Pi_q.$$

Using (16), we obtain

$$R_0(\lambda + i0) - R_0(\lambda - i0) = 2i\pi \sum_{b\Lambda_q \leqslant \lambda} \tilde{\mathcal{F}}_0(\lambda)^* \tilde{\mathcal{F}}_0(\lambda) \otimes \Pi_q = 2i\pi \mathcal{F}_0(\lambda)^* \mathcal{F}_0(\lambda),$$

and the proof is complete. ■

Using this lemma, we can prove Theorem 1. Let us denote $W_\pm$ the wave operators for the pair (H, H_0) and take f, g in the absolute continuous subspace of H_0. Then

$$\begin{aligned}\langle (\mathbf{S} - Id) f, g\rangle &= \langle (W_- - W_+) f, W_+ g\rangle \\ &= -i \int_{-\infty}^{+\infty} \langle e^{itH} V(x) e^{-itH_0} f, W_+ g\rangle \mathrm{d}t = -i \int_{-\infty}^{+\infty} \langle V(x) e^{-itH_0} f, W_+ e^{-itH_0} g\rangle \mathrm{d}t.\end{aligned}$$

Moreover, one knows that

$$W_+ - Id = i \int_0^{+\infty} e^{i\sigma H} V(x) e^{-i\sigma H_0} \mathrm{d}\sigma.$$

Therefore,

$$\begin{aligned}\langle (\mathbf{S} - Id) f, g\rangle &= i \int_0^{+\infty} i \int_{-\infty}^{+\infty} \langle V(x) e^{-i\tau H_0} f, e^{i\sigma H} V(x) e^{-i(\sigma+\tau)H_0} g\rangle \mathrm{d}\tau \, \mathrm{d}\sigma - i \int_{-\infty}^{+\infty} \langle V(x) e^{-itH_0} f, e^{-itH_0} g\rangle \mathrm{d}t \\ &= \lim_{\mu, \mu' \to 0^+} i \int_0^{+\infty} e^{-\mu\sigma} i \int_{-\infty}^{+\infty} e^{-\mu'|\tau|} \langle e^{i(\sigma+\tau)H_0} V(x) e^{-i\sigma H} V(x) e^{-i\tau H_0} f, g\rangle \mathrm{d}\tau \\ &\quad \times \mathrm{d}\sigma - i \int_{-\infty}^{+\infty} e^{-\mu'|\tau|} \langle V(x) e^{-itH_0} f, e^{-itH_0} g\rangle \mathrm{d}t \\ &= \lim_{\mu, \mu' \to 0} i \int_0^{+\infty} e^{-\mu\sigma} i \int_{-\infty}^{+\infty} e^{-\mu'|\tau|} \int_{b\Lambda_0}^{+\infty} \langle \mathcal{F}_0(\lambda) V(x) e^{-i\sigma(H-\lambda)} V(x) e^{-i\tau(H_0-\lambda)} f, \mathcal{F}_0(\lambda) g\rangle \, \mathrm{d}\lambda \\ &\quad \times \mathrm{d}\tau \, \mathrm{d}\sigma - i \int_{-\infty}^{+\infty} e^{-\mu'|\tau|} \int_{b\Lambda_0}^{+\infty} \langle \mathcal{F}_0(\lambda) V(x) e^{-it(H_0-\lambda)} f, \mathcal{F}_0(\lambda) g\rangle \mathrm{d}\lambda \, \mathrm{d}t \\ &= \lim_{\mu' \to 0^+} i \int_{-\infty}^{+\infty} e^{-\mu'|\tau|} \int_{b\Lambda_0}^{+\infty} \langle \mathcal{F}_0(\lambda) V(x) R(\lambda + i0) V(x) e^{-i\tau(H_0-\lambda)} f, \mathcal{F}_0(\lambda) g\rangle \mathrm{d}\lambda \, \mathrm{d}\tau \\ &\quad - i \int_{-\infty}^{+\infty} e^{-\mu'|\tau|} \int_{b\Lambda_0}^{+\infty} \langle \mathcal{F}_0(\lambda) V(x) e^{-it(H_0-\lambda)} f, \mathcal{F}_0(\lambda) g\rangle \mathrm{d}\lambda \, \mathrm{d}t \\ &= \int_{b\Lambda_0}^{+\infty} \langle \mathcal{F}_0(\lambda) V(x) R(\lambda + i0) V(x) (R_0(\lambda + i0) - R_0(\lambda - i0)) f, \mathcal{F}_0(\lambda) g\rangle \mathrm{d}\lambda \, \mathrm{d}\tau \\ &\quad - \int_{b\Lambda_0}^{+\infty} \langle \mathcal{F}_0(\lambda) V(x) (R_0(\lambda + i0) - R_0(\lambda - i0)) f, \mathcal{F}_0(\lambda) g\rangle \mathrm{d}\lambda \, \mathrm{d}t.\end{aligned}$$

Using Lemma 2.3, we obtain

$$\langle(\mathbf{S}-Id)f,g\rangle = 2i\pi\int_{b\Lambda_0}^{+\infty}\langle\mathcal{F}_0(\lambda)V(x)R(\lambda+i0)V(x)\mathcal{F}_0(\lambda)^*\mathcal{F}_0(\lambda)f,\mathcal{F}_0(\lambda)g\rangle \mathrm{d}\lambda\ \mathrm{d}\tau$$
$$-2i\pi\int_{b\Lambda_0}^{+\infty}\langle\mathcal{F}_0(\lambda)V(x)\mathcal{F}_0(\lambda)^*\mathcal{F}_0(\lambda)f,\mathcal{F}_0(\lambda)g\rangle \mathrm{d}\lambda\ \mathrm{d}t$$

and the proof of Theorem 1 is complete. ■

III. SCATTERING AMPLITUDE IN STRONG MAGNETIC FIELD

In this section, we prove Theorem 2. The first step is to write the scattering amplitude under a convenient form. Let us denote by $\langle .,.\rangle_{L^2(\mathbb{R}^{n-2d})}$ the scalar product on $L^2(\mathbb{R}^{n-2d})$. From Theorem 1 and Assumption 2, it is clear that for $\lambda\in]b\Lambda_0,+\infty[\setminus(\mathbb{L}\cup\sigma_{pp}(H))$, $T(\omega,\omega',\lambda,b)$ can be decomposed into $T=T_1+T_2$ with

$$T_1(\omega,\omega',\lambda,b) = -\frac{i\pi}{(2\pi)^{n-2d}}\sum_{b\Lambda_p\leqslant\lambda}\sum_{b\Lambda_p\leqslant\lambda}(\lambda-b\Lambda_q)^{(n-2d-2)/4}(\lambda-b\Lambda_p)^{(n-2d-2)/4}$$
$$\times\Pi_p\langle V(x_{\perp},.)e^{i\sqrt{\lambda-b\Lambda_q}\langle .,\omega'\rangle},e^{i\sqrt{\lambda-b\Lambda_p}\langle .,\omega\rangle}\rangle_{L^2(\mathbb{R}^{n-2d})}\Pi_q$$

and

$$T_2(\omega,\omega',\lambda,b) = \frac{i\pi}{(2\pi)^{n-2d}}\sum_{b\Lambda_p\leqslant\lambda}\sum_{b\Lambda_q\leqslant\lambda}(\lambda-b\Lambda_q)^{(n-2d-2)/4}(\lambda-b\Lambda_p)^{(n-2d-2)/4}$$
$$\times\int_{\mathbb{R}^{n-2d}}\Pi_p V(x_{\perp},x_{\|})e^{-i\sqrt{\lambda-b\Lambda_p}\langle x_{\|},\omega\rangle}R(\lambda+i0)V(x_{\perp},x_{\|})e^{i\sqrt{\lambda-b\Lambda_q}\langle x_{\|},\omega'\rangle}\Pi_q\mathrm{d}x_{\|},$$

where the last integral converges in the space of bounded operator on $L^2(\mathbb{R}^{2d})$. From Proposition 2.2, it follows that for $\delta>\|V\|_{\infty,\rho}$,

$$\|T_2(\omega,\omega',\lambda,b)\|\leqslant C\delta^{-1/2}\sum_{b\Lambda_q\leqslant\lambda}(\lambda-b\Lambda_q)^{(n-2d-2)/2}\|V\|_{\infty,\rho}^2\leqslant C\lambda\|V\|_{\infty,\rho}^2 b^{-1}\delta^{(n-2d-3)/2},$$

where the constant C does not depend on ω and ω'. It remains to treat the term T_1. Suppose that $p\neq q$. As $\hat{V}^{\|}\in L^{\infty}_r(\mathbb{R}^n)$, then

$$\sup_{(\omega,\omega')\in S^{n-2d-1}\times S^{n-2d-1}}\left|\langle V(x_{\perp},.)e^{i\sqrt{\lambda-b\Lambda_q}\langle .,\omega'\rangle},e^{i\sqrt{\lambda-b\Lambda_p}\langle .,\omega\rangle}\rangle_{L^2(\mathbb{R}^{n-2d})}\right|$$
$$=\sup_{(\omega,\omega')\in S^{n-2d-1}\times S^{n-2d-1}}\left|\hat{V}^{\|}(x_{\perp},\sqrt{\lambda-b\Lambda_p}\omega-\sqrt{\lambda-b\Lambda_q}\omega')\right|$$
$$\leqslant C\|\hat{V}^{\|}\|_{\infty,r}\sup_{(\omega,\omega')\in S^{n-2d-1}\times S^{n-2d-1}}\left|\sqrt{\lambda-b\Lambda_p}\omega-\sqrt{\lambda-b\Lambda_q}\omega'\right|^{-r}\leqslant C\|\hat{V}^{\|}\|_{\infty,r}\delta^{-r/2}. \tag{17}$$

Therefore,

$$\sup_{(\omega,\omega')\in S^{n-2d-1}\times S^{n-2d-1}}\left\|T_1(\omega,\omega',\lambda,b)+\frac{i\pi}{(2\pi)^{n-2d}}\sum_{b\Lambda_q\leqslant\lambda}(\lambda-b\Lambda_q)^{(n-2d-2)/2}\Pi_q\hat{V}^{\|}(x_{\perp},\sqrt{\lambda-b\Lambda_q}(\omega\right.$$
$$\left.-\omega'))\Pi_q\right\|\leqslant C\|\hat{V}^{\|}\|_{\infty,r}\lambda b^{-1}\delta^{[n-2d-2-\min(1,r)]/2} \tag{18}$$

and the proof of (i) is complete.

Let us prove (ii). Starting from (4) at the energy $\mathcal{E}b+\lambda$, we get

$$T(\omega,\omega',\mathcal{E}b+\lambda,b)=\frac{-i\pi}{(2\pi)^{n-2d}}b^{(n-2d-2)/2}\sum_{q\in\tilde{Q}(\mathcal{E})}\beta_q^{n-2d-2}\Pi_q\hat{V}^{\|}\Big(x_\perp,b^{\frac{1}{2}}\beta_q(\omega-\omega')\Big)\Pi_q + \mathcal{O}(b^{[n-2d-2-\min(1,r)]})/2.$$

On the other hand, we know from Lemma 9.1 in Ref. 5 that

$$\|(1-\Pi_q)\hat{V}^{\|}\Big(.,b^{\frac{1}{2}}\beta_q(\omega-\omega')\Big)\Pi_q\|\leqslant Cqb^{-1/2}\sup_{x\in\mathbb{R}^n}|\partial_{x_\perp}\hat{V}^{\|}|.$$

Combining these estimates, we obtain the result claimed in (ii).

Finally, let us give the proof of Corollary 1.2. Suppose that $S_1=S_2$, then $T_1=T_2$ and for all $\mathcal{E}\notin\tilde{\mathbb{L}}$, $b>0$ and $(\omega,\omega')\in S^{n-2d-1}\times S^{n-2d-1}$, we have

$$T_1(\omega,\omega',\mathcal{E}b,b)=T_2(\omega,\omega',\mathcal{E}b,b).$$

It follows from Theorem 2 that

$$\sum_{q\in\tilde{Q}(\mathcal{E})}\beta_q^{n-2d-2}\hat{W}^{\|}(x_\perp,b^{1/2}\beta_q(\omega-\omega'))\Pi_q=\mathcal{O}(b^{-[\min(1,r)]/2}),$$

where $W=V_1-V_2$. Now, let $\xi\in\mathbb{R}^{n-2d}$, then for all $b>0$ there exists $\omega,\omega'\in S^{n-2d-1}$ such that $b^{1/2}(\omega-\omega')=\xi$. Therefore,

$$\sum_{q\in\tilde{Q}(\mathcal{E})}\beta_q^{n-2d-2}\hat{W}^{2}(x_\perp,\beta_q\xi)\Pi_q=\mathcal{O}(b^{-[\min(1,r)]/2}),$$

and taking the limit when b tends to infinity, we obtain

$$\sum_{q\in\tilde{Q}(\mathcal{E})}\beta_q^{n-2d-2}\hat{W}^{2}(x_\perp,\beta_q\xi)\Pi_q=0.$$

Moreover, this equality holds for all $\mathcal{E}\notin\tilde{\mathbb{L}}$, so that for all $q\in\mathbb{N}^d$, the map $x_\perp\mapsto\hat{W}^{\|}(x_\perp,-\beta_q\xi)$ belongs to $(\mathrm{Im}\,\Pi_q)^\perp$. As $L^2(\mathbb{R}^{2d})=\oplus_{q\in\mathbb{N}^d}\mathrm{Im}\,\Pi_q$, it follows that $\hat{W}^{\|}$ vanishes identically and the proof is complete. ■

IV. ASYMPTOTICS OF THE SCATTERING PHASE

In this section, we prove Theorems 3 and 4. Starting from formula (8), we must show that the operator $T=T(\mathcal{E}b+\lambda,b)$, $\mathcal{E}\notin\tilde{\mathbb{L}}$ is trace class and to obtain convenient estimates on $\|T\|$. For this purpose, we recall that

$$T(\mathcal{E}b+\lambda,b)=-2i\pi\mathcal{F}_0(\mathcal{E}b+\lambda)V(x)\mathcal{F}_0(\mathcal{E}b+\lambda)^*+2i\pi\mathcal{F}_0(\mathcal{E}b+\lambda)V(x)\times R(\mathcal{E}b+\lambda+i0)V(x)\mathcal{F}_0(\mathcal{E}b+\lambda)^*.$$

Moreover, as $\mathcal{E}\notin\tilde{\mathbb{L}}$, Proposition 2.2 shows that $\|\langle x_\|\rangle^{-\alpha}R_0(\mathcal{E}b+\lambda+i0)\langle x_\|\rangle^{-\alpha}\|$ is bounded by $b^{-1/2}$. Using Assumption 1, the resolvent

$$R(\mathcal{E}b+\lambda+i0)=R_0(\mathcal{E}b+\lambda+i0)(Id+V\,R_0(\mathcal{E}b+\lambda+i0))^{-1}$$

can expand in powers of $V\,R_0$. Combining this argument with the formula giving $\mathcal{F}_0$, it follows that for $L\in\mathbb{N}$,

$$T(\mathcal{E}b+\lambda,b)=\sum_{l=0}^{L}\sum_{q\in\tilde{Q}(\mathcal{E})}T_{q,l}(\mathcal{E}b+\lambda,b)+\mathcal{O}(\|T_{q,L+1}(\mathcal{E}b+\lambda,b)\|_1), \tag{19}$$

where for $l\in\mathbb{N}$ we have defined

$$T_{q,l}(\mathcal{E}b+\lambda,b)=(-1)^{l+1}2i\pi\mathcal{F}_{q,0}(\mathcal{E}b+\lambda)(V(x)R_0(\mathcal{E}b+\lambda+i0))^lV(x)\mathcal{F}_{q,0}(\mathcal{E}b+\lambda)^* \tag{20}$$

and

$$\forall E>b\Lambda_q,\quad \mathcal{F}_{q,0}(E)=\Pi_q\otimes\tilde{\mathcal{F}}_0(E-b\Lambda_q). \tag{21}$$

Let us denote by S^1 the space of trace class operators on $L^2(\mathbb{R}^{2d}\times S^{n-2d-1})$ and by $\|.\|_1$ the corresponding norm. For $A\in S^1$, we denote by tr A the trace of A. With these notations, we have the following lemma.

Lemma 4.1: Suppose that V satisfies Assumption 1. Let $\mathcal{E}\in]\Lambda_0+\infty[\setminus\tilde{\mathbb{L}}$ *and* $\Delta\subset\mathbb{R}$ *be a bounded interval. When b tends to infinity, one has*

(i) $\forall\epsilon>0$,

$$\sup_{\lambda\in\Delta}\|T_{q,l}(\mathcal{E}b+\lambda,b)\|_{L^2(\mathbb{R}^{2d}\times S^{n-2d-1}),L^2(\mathbb{R}^{2d}\times S^{n-2d-1})}\leqslant Cb^{-\frac{3}{4}-\frac{1}{2}+\epsilon},$$

$$\sup_{\lambda\in\Delta}\|T(\mathcal{E}b+\lambda,b)\|_{L^2(\mathbb{R}^{2d}\times S^{n-2d-1}),L^2(\mathbb{R}^{2d}\times S^{n-2d-1})}\leqslant Cb^{-\frac{3}{4}+\epsilon}.$$

(ii) *Suppose additionally that* $V\in L^1(\mathbb{R}^n)$. For *b large enough,* $T_{q,l}(\mathcal{E}b+\lambda,b)$ *and* $T(\mathcal{E}b+\lambda,b)$ *are trace class and*

$$\sup_{\lambda\in\Delta}\|T_{q,l}(\mathcal{E}b+\lambda,b)\|_1\leqslant Cb^{(n-2-l)/2},\quad \sup_{\lambda\in\Delta}\|T(\mathcal{E}b+\lambda,b)\|_1\leqslant Cb^{(n-2)/2}.$$

Proof: Let us start with the point (i). We start by estimating the operator $\mathcal{F}^*_{q,0}(\mathcal{E}b+\lambda)$ which is bounded from $L^2(S^{n-2d-1}\times\mathbb{R}^{2d})$ into $L^2_{-\beta}(\mathbb{R}^{n-2d},L^2(\mathbb{R}^{2d}))$ for all $\beta>\frac{1}{2}$. Moreover, for all $\beta>\frac{1}{2}$ and $\varphi\in L^2(S^{n-2d-1})$, we have

$$\begin{aligned}\|\tilde{\mathcal{F}}_0(\lambda)^*\varphi\|^2_{L^2_{-\beta}}&=\lambda^{(n-2d-2)/2}\int_{\mathbb{R}^{n-2d}}\langle x\rangle^{-\beta}\left|\int_{S^{n-2d-1}}e^{i\sqrt{\lambda}x\omega}\mathrm{d}\omega\right|^2\mathrm{d}x\\&=\lambda^{-1}\int_{\mathbb{R}^{n-2d}}\langle\lambda^{-1/2}x\rangle^{-\beta}\left|\int_{S^{n-2d-1}}e^{ix\omega}d\omega\right|^2\mathrm{d}x\leqslant C\lambda^{(\beta/2)-1}\|\mathcal{F}_0(1)^*\varphi\|^2_{L^2_{-\beta}}\\&\leqslant C\lambda^{(\beta/2)-1}\|\varphi\|^2_{L^2(S^{n-2d-1})}.\end{aligned}$$

From this estimate, one deduces easily that for all $\beta>1/2$,

$$\begin{aligned}\|\mathcal{F}_{q,0}(\mathcal{E}b+\lambda)\|_\beta&:=\|\mathcal{F}_{q,0}(\mathcal{E}b+\lambda)\|_{L^2_\beta(\mathbb{R}^{n-2d},L^2(\mathbb{R}^{2d})),L^2(S^{n-2d-1}\times\mathbb{R}^{2d})}\\&=\|\mathcal{F}_{q,0}(\mathcal{E}b+\lambda)^*\|_{L^2(S^{n-2d-1}\times\mathbb{R}^{2d}),L^2_{-\beta}(\mathbb{R}^{n-2d},L^2(\mathbb{R}^{2d}))}\\&\leqslant C(\mathcal{E}b+\lambda-b\Lambda_q)^{(\beta-2)/4}.\end{aligned} \tag{22}$$

It follows from this estimate, Assumption 1, formula (20) and Proposition 2.2 that for $\epsilon>0$,

$$\begin{aligned}\|T_{q,l}(b)\|_{L^2(\mathbb{R}^{2d}\times S^{n-2d-1}),L^2(\mathbb{R}^{2d}\times S^{n-2d-1})}&\\ \leqslant C\|\mathcal{F}_{q,0}(\mathcal{E}b+\lambda)\|^2_{1/2+\epsilon}\times\|V(R_0(\mathcal{E}b+\lambda)V)^l\|_{L^2_{-1/2-\epsilon}(\mathbb{R}^{n-2d},L^2(\mathbb{R}^{2d})),L^2_{1/2+\epsilon}(\mathbb{R}^{n-2d},L^2(\mathbb{R}^{2d}))}&\\ \leqslant b^{-\frac{3}{4}-\frac{1}{2}+\epsilon}.&\end{aligned}\tag{23}$$

This achieves to prove the first estimate of (i). The second one then follows by Eq. (19).

Let us prove (ii). Thanks to the resolvent estimates of Proposition 2.2, it suffices to show that the operator $|V|^{\frac{1}{2}}\mathcal{F}_{q,0}(\lambda)^*: L^2(S^{n-2d-1}\times\mathbb{R}^{2d})\to L^2(\mathbb{R}^{2n})$ belongs to the Hilbert–Schmidt class and that

$$\||V|^{\frac{1}{2}}\mathcal{F}_{q,0}(\mathcal{E}b+\lambda)\|_2\leqslant Cb^{(n-2)/4},\tag{24}$$

where $\|.\|_2$ denotes the Hilbert–Schmidt norm. For $q=(q_1,\ldots,q_d)\in\mathbb{N}^d$, let us denote by $K_q(y_\perp,x_\perp)$ the kernel of Π_q and by $\sigma(.,.)$ the symplectic form on $\mathbb{R}^{2d}$. We have

$$K_q(y_\perp,x_\perp)=\frac{b^d}{2\pi}\exp\left(-\frac{b}{4}[|y_\perp-x_\perp|^2+2i\sigma(y_\perp,x_\perp)]\right)L_q(y_\perp,x_\perp,b),\tag{25}$$

with

$$L_q(y_\perp,x_\perp,b)=\prod_{j=1}^d\tilde{L}_{q_j-1}\left(\frac{b}{2}|y_{\perp,j}-x_{\perp,j}|^2\right),$$

where for $s\in\mathbb{N}$, $\tilde{L}_s$ is the Laguerre polynomial of order s (see Ref. 14 for more details). With these notations, the kernel $N(x_\perp,x_\parallel,x'_\perp,\omega)$ of $|V|^{\frac{1}{2}}\mathcal{F}_{q,0}(\lambda)^*$ satisfies

$$\begin{aligned}N(x_\perp,x_\parallel,x'_\perp,\omega)&=(\mathcal{E}b+\lambda-b\Lambda_q)^{(n-2d-2)/4}|V|^{\frac{1}{2}}K_q(x_\perp,x'_\perp)e^{-i\sqrt{\mathcal{E}b+\lambda-b\Lambda_q}\langle x_\parallel,\omega\rangle}\\&=\mathcal{O}(b^{(n-2d-2)/4})|V|^{\frac{1}{2}}K_q(x_\perp,x'_\perp)e^{-i\sqrt{\mathcal{E}b+\lambda-b\Lambda_q}\langle x_\parallel,\omega\rangle}\end{aligned}$$

and

$$\begin{aligned}\|N\|^2_{L^2(\mathbb{R}^n\times\mathbb{R}^{2d}\times S^{n-2d-1})}&=\mathcal{O}(b^{(n+2d-2)/2})\int_{\mathbb{R}^{2d}\times\mathbb{R}^{n-2d}\times\mathbb{R}^{2d}\times S^{n-2d-1}}|V(x_\perp,x_\parallel)|e^{-(b/2)|x_\perp-x'_\perp|^2}\\&\quad\times\left|L_q\left(\frac{b}{2}|x_\perp-x'_\perp|^2\right)\right|^2\mathrm{d}x_\perp\mathrm{d}x_\parallel\mathrm{d}x'_\perp\mathrm{d}\omega\\&\leqslant Cb^{(n+2d-2)/2}\int_{\mathbb{R}^{2d}\times\mathbb{R}^{n-2d}\times\mathbb{R}^{2d}}|V(x_\perp,x_\parallel)|e^{-(b/2)|x_\perp-x'_\perp|^2}\\&\quad\times\left|L_q\left(\frac{b}{2}|x_\perp-x'_\perp|^2\right)\right|^2\mathrm{d}x'_\perp\mathrm{d}x_\parallel\mathrm{d}x_\perp.\end{aligned}$$

By change of variable, it comes

$$\begin{aligned}\|N\|^2_{L^2(\mathbb{R}^n\times\mathbb{R}^{2d}\times S^{n-2d-1})}&\leqslant Cb^{(n+2d-2)/2}\int_{\mathbb{R}^{2d}\times\mathbb{R}^{n-2d}\times\mathbb{R}^{2d}}|V(x_\perp,x_\parallel)|e^{-b|x_\perp-x'_\perp|^2}\mathrm{d}x'_\perp\mathrm{d}x_\parallel\mathrm{d}x_\perp\\&\leqslant Cb^{(n+2d-2)/2}\int_{\mathbb{R}^n}|V(x)|\mathrm{d}x\int_{\mathbb{R}^{2d}}e^{-|x'_\perp|^2}\mathrm{d}x'_\perp\leqslant Cb^{(n-2)/2}\end{aligned}$$

which proves (24). Using (24) and Proposition 2.2, it comes

$$\|T_{q,l}(\mathcal{E}b+\lambda)\|_1 \leqslant Cb^{(n-2-l)/2}$$

and the proof of (ii) is complete. ■

From this lemma, we know that $\|T(\mathcal{E}b+\lambda,b)\|<1$ and by Taylor expansion, we deduce from (8) that for $N\in\mathbb{N}$

$$2i\pi s(\mathcal{E}b+\lambda,b)=\sum_{k=0}^{N}\frac{(-1)^k}{k+1}\mathrm{tr}(T(\mathcal{E}b+\lambda,b)^{k+1})+\mathcal{O}(\|T(\mathcal{E}b+\lambda,b)^{N+2}\|_1). \tag{26}$$

Hence, we must show that for $k\in\mathbb{N}$, $\mathrm{tr}(T(\mathcal{E}b+\lambda,b)^k)$ admits an expansion in powers of $b^{1/2}$. Using the fact that for $p\neq q$, $\Pi_p\Pi_q=0$, we deduce from Eq. (19) that

$$\mathrm{tr}(T(\mathcal{E}b+\lambda,b)^k)=\sum_{q\in\tilde{Q}(\mathcal{E})}\mathrm{tr}\left(\sum_{l=0}^{L}T_{q,l}(\mathcal{E}b+\lambda,b)\right)^k+\mathcal{O}(\|T_{q,L+1}^k(\mathcal{E}b+\lambda,b)\|_1). \tag{27}$$

At this point of the calculus, we can either continue the expansion to get a complete asymptotics or we can stop the expansion at the first order to prove Theorem 3. Indeed, it follows from Lemma 4.1 that the remainder terms in Eqs. (26) and (27) satisfy

$$\|T_{q,L+1}^N(\mathcal{E}b+\lambda,b)\|_1=\mathcal{O}(b^{[n-1-N(L+2)]/2}) \text{ and } \|T(\mathcal{E}b+\lambda,b)^{N+2}\|_1=\mathcal{O}(b^{(n-N-3)/2}).$$

Therefore, Eqs. (26) and (19) yield

$$s(\mathcal{E}b+\lambda,b)=\frac{1}{2i\pi}\sum_{q\in\tilde{Q}(\mathcal{E})}\mathrm{tr}(T_{q,0}(\mathcal{E}b+\lambda,b))+\mathcal{O}(b^{(n-3)/2}). \tag{28}$$

On the other hand, a standard calculation shows that the kernel $N_{q,0}$ of $T_{q,0}(\mathcal{E}b+\lambda,b)$ is given by

$$N_{q,0}(\omega',x_\perp',\omega,x_\perp)=-\frac{i\pi}{(2\pi)^{n-2d}}(\mathcal{E}b+\lambda-b\Lambda_q)^{(n-2d-2)/2}K_q(x_\perp,x_\perp')\hat{V}^{\|}(x_\perp,\sqrt{\mathcal{E}b+\lambda-b\Lambda_q}(\omega-\omega')).$$

Using (25), it follows that

$$\begin{aligned}\mathrm{tr}(T_{q,0}(\mathcal{E}b+\lambda,b))&=\int_{S^{n-2d-1}\times\mathbb{R}^{2d}}N_{q,0}(\omega,x_\perp,\omega,x_\perp)\mathrm{d}x_\perp\mathrm{d}\omega\\&=-\frac{i\pi}{(2\pi)^{n-2d+1}}b^d(\mathcal{E}b+\lambda-b\Lambda_q)^{(n-2d-2)/2}\int_{S^{n-2d-1}\times\mathbb{R}^{2d}}\hat{V}^{\|}(x_\perp,0)\mathrm{d}x_\perp\mathrm{d}\omega\\&=-\frac{i\pi\ mes(S^{n-2d-1})}{(2\pi)^{n-2d+1}}\int_{\mathbb{R}^n}V(x)\mathrm{d}x(b^{(n-2)/2}(\mathcal{E}-\Lambda_q)^{(n-2d-2)/2}+\mathcal{O}(b^{(n-4)/2})).\end{aligned}$$

Combining this equation with (28), we obtain the result claimed in Theorem 3.

The end of the paper is devoted to the proof of Theorem 4. We must show that for all $N\in\mathbb{N}^*$ and all $(l_1,\ldots,l_N)\in\mathbb{N}^N,(k_1,\ldots,k_N)\in\mathbb{N}^N$,

$$\mathrm{tr}(T_{q,l_1}^{k_1}\cdots T_{q,l_N}^{k_N})$$

admits an asymptotic expansion in powers of $b^{1/2}$. For this purpose, we work directly on the kernel of these operators that we expand with respect to b. For $V\in\mathcal{S}(\mathbb{R})$, let us denote $\hat{V}$ its Fourier transform. The two next lemmas permit us to obtain an expansion of the kernel of $T_{q,l_1}^{k_1}\cdots T_{q,l_N}^{k_N}$ by mean of the expansion of each term of the product.

Lemma 4.2. Let V_1, $V_2\in\mathcal{S}(\mathbb{R})$ *and for* ω, $\omega'\in\{\pm1\}$, $\lambda>0$ *let*

$$W(\lambda,\omega,\omega') = \sum_{\theta\in\{\pm 1\}} \hat{V}_1(\sqrt{\lambda}(\omega-\theta))\hat{V}_2(\sqrt{\lambda}(\theta-\omega')).$$

Then, there exists $V\in\mathcal{S}(\mathbb{R})$ *such that*

$$W(\lambda,\omega,\omega') = \hat{V}(\sqrt{\lambda}(\omega-\omega')) + \mathcal{O}(\lambda^{-\infty}),$$

when $\lambda\to+\infty$.

Proof: From the properties of the Fourier transform, it is clear that

$$W(\lambda,\omega,\omega') = \begin{cases} (\int V_1(x)\mathrm{d}x)(\int V_2(x)\mathrm{d}x) + \mathcal{O}(\lambda^{-\infty}) & \text{if} \quad \omega=\omega', \\ \mathcal{O}(\lambda^{-\infty}) & \text{if} \quad \omega\neq\omega'. \end{cases}$$

Let us set

$$V(x) = \left(\int V_2(y)\mathrm{d}y\right)V_1(x),$$

then it is clear that

$$W(\lambda,\omega,\omega') = \hat{V}(\sqrt{\lambda}(\omega-\omega')) + \mathcal{O}(\lambda^{-\infty}).$$

■

Lemma 4.3: Let $V\in\mathcal{S}(\mathbb{R})$ *and for* $l\in\mathbb{N}^*$, $\omega,\omega'\in\{\pm 1\}$, $\lambda>0$ *let*

$$W(\lambda,\omega,\omega') = \int e^{i\sqrt{\lambda}(|x_1-x_2|+\ldots+|x_l-x_{l+1}|+x_{l+1}\omega-x_1\omega')}V(x_1)\cdots V(x_{l+1})\mathrm{d}x_1\cdots\mathrm{d}x_{l+1}.$$

Then, there exists a sequence $(V_j)_{j\in\mathbb{N}}$ *of potentials in* $\mathcal{S}(\mathbb{R})$ *such that*

$$W(\lambda,\omega,\omega') = \sum_{j=0}^{+\infty}(i\sqrt{\lambda})^{-j}\hat{V}_j(\sqrt{\lambda}(\omega-\omega')).$$

Proof: The integral being absolutely convergent, we have

$$W(\lambda,\omega,\omega') = \int_{\mathbb{R}} e^{i\sqrt{\lambda}(\omega-\omega')y}V(y)\tilde{V}(y)\mathrm{d}y,$$

with

$$\tilde{V}(y) = \int_{\mathbb{R}} e^{i\sqrt{\lambda}(|x|-x\omega')}V(x+y)\mathrm{d}x.$$

Moreover,

$$\begin{aligned}\tilde{V}(y) &= \int_0^{+\infty} V(\omega' x+y)\mathrm{d}x + \int_{-\infty}^0 e^{-2i\sqrt{\lambda}x}V(\omega' x+y)\mathrm{d}x \\ &= V_0(y) - \frac{1}{2i\sqrt{\lambda}}[e^{-2i\sqrt{\lambda}x}V(\omega' x+y)]_{x=-\infty}^{x=0} + \frac{\omega'}{2i\sqrt{\lambda}}\int_{-\infty}^0 e^{-2i\sqrt{\lambda}x}V'(\omega' x+y)\mathrm{d}y \\ &= \tilde{V}_0(y) + \lambda^{-1/2}\tilde{V}_1(y) + \frac{\omega'}{2i\sqrt{\lambda}}\int_{-\infty}^0 e^{-2i\sqrt{\lambda}x}V'(\omega' x+y)\mathrm{d}y,\end{aligned}$$

with $\tilde{V}_0(y)=\int_0^{+\infty}V(\omega' x+y)\mathrm{d}x$ and $\tilde{V}_1(y)=(i/2)V(y)$. In particular, $\tilde{V}_0$ and $\tilde{V}_1$ are C^∞ functions whose derivatives are bounded at all orders. Integrating by parts N times, we obtain

$$\tilde{V}(y) = \tilde{V}_0(y) + \sum_{j=1}^{N} \lambda^{-j/2} \frac{\omega'^{j-1}}{(2i)^j} V^{(j-1)}(y) + \mathcal{O}(\lambda^{-N-1}).$$

Let us set $\tilde{V}_j(y) = [\omega'^{j-1}/(2i)^j] V^{(j-1)}(y)$, then

$$W(\lambda, \omega, \omega') = \sum_{j=0}^{N} \lambda^{-j/2} \int_{\mathbb{R}} e^{i\sqrt{\lambda}(\omega-\omega')y} V(y) \tilde{V}_j(y) \mathrm{d}y + \mathcal{O}(\lambda^{-N-1}) = \sum_{j=0}^{N} \lambda^{-j/2} \hat{V}_j(\sqrt{\lambda}(\omega - \omega')) + \mathcal{O}(\lambda^{-N-1}),$$

with $V_j(y) = V(y)\tilde{V}_j(y)$. As $V \in \mathcal{S}(\mathbb{R})$ and for $j \geqslant 0$, $\tilde{V}_j$ and their derivatives are bounded, it is clear that $V_j \in \mathcal{S}(\mathbb{R})$ and the proof is complete. ■

Now, we give the proof of Theorem 4. Thanks to Eqs. (26) and (27), it suffices to prove that for all $N \in \mathbb{N}^*$ and all $l = (l_1, \ldots, l_N) \in \mathbb{N}^N$, $k = (k_1, \ldots, k_N) \in \mathbb{N}^N$,

$$\mathrm{tr}(T_{q,l_1}^{k_1} \cdots T_{q,l_N}^{k_N})$$

admits an asymptotic expansion in powers of $b^{1/2}$. For this purpose, we will simply show that the kernel of $T_{q,l_1}^{k_1} \cdots T_{q,l_N}^{k_N}$ admits such an expansion. Let us start with $T_{q,l_j}^{k_j}$, $j \in \{1, \ldots, N\}$. Recall that

$$T_{q,l_j}(\mathcal{E}b + \lambda, b) = (-1)^{l_j+1} 2i\pi \mathcal{F}_{q,0}(\mathcal{E}b + \lambda)(V(x)R_0(\mathcal{E}b + \lambda + i0))^{l_j} V(x) \mathcal{F}_{q,0}(\mathcal{E}b + \lambda)^*.$$

Moreover, it is well known (see Ref. 11) that for $E > 0$, the resolvent $[-(\mathrm{d}^2/\mathrm{d}x^2) - E - i0]^{-1}$ has a kernel $N_0(x, y)$ given by

$$N_0(x, y) = \frac{1}{2i\sqrt{E}} e^{i\sqrt{E}|x-y|}.$$

Therefore, the kernel of T_{q,l_j} takes the form

$$N_{q,l_j}(\omega, \omega', x_\perp, x'_\perp) = \frac{(-1)^{l_j+1}}{(2i\sqrt{\mathcal{E}b + \lambda - b\Lambda_q})^{l_j+1}} K_q(x_\perp, x'_\perp) \int e^{i\sqrt{\mathcal{E}b+\lambda-b\Lambda_q}(|x_1-x_2|+\cdots+|x_{l_j}-x_{l_j+1}|+x_{l_j+1}\omega-x_1\omega')} \times V(x_\perp, x_1) \cdots V(x_\perp, x_{l_j+1}) \mathrm{d}x_1 \cdots \mathrm{d}x_{l_j+1}. \tag{29}$$

By Lemma 4.3 applied in the variable $x_\parallel$, we obtain the following expansion:

$$N_{q,l_j}(\omega, \omega', x_\perp, x'_\perp) = K_q(x_\perp, x'_\perp)(i\sqrt{b})^{-l_j-1} \sum_{m=0}^{+\infty} (i\sqrt{b})^{-m} \hat{V}^{\parallel}_{m,q,l_j}(x_\perp, \sqrt{\mathcal{E}b + \lambda - b\Lambda_q}(\omega - \omega')),$$

with $V_{m,q,lj} \in \mathbf{S}(\mathbb{R}^3)$. Using Lemma 4.2, it comes that the kernel N_{q,l_j,k_j} of $T_{q,l_j}^{k_j}$ has the expansion

$$N_{q,l_j,k_j}(\omega, \omega', x_\perp, x'_\perp) = K_q(x_\perp, x'_\perp)(i\sqrt{b})^{-l_j-1} \sum_{m=0}^{+\infty} (i\sqrt{b})^{-m} \hat{V}^{\parallel}_{m,q,l,k}(x_\perp, \sqrt{\mathcal{E}b + \lambda - b\Lambda_q}(\omega - \omega')),$$

with $V_{m,q,l_j,k_j} \in \mathbf{S}(\mathbb{R}^3)$. Next, using again Lemma 4.2, it follows by induction that $T_{q,l_1}^{k_1} \cdots T_{q,l_N}^{k_N}$ has a kernel $N_{q,l,k}(\omega, \omega', x_\perp, x'_\perp)$ which admits an expansion in powers of $ib^{-1/2}$,

$$N_{q,l,k}(\omega, \omega', x_\perp, x'_\perp) = (i\sqrt{b})^{-|l|-N} \sum_{m=0}^{+\infty} (i\sqrt{b})^{-m} \hat{V}^{\parallel}_{m,q,l,k}(x_\perp, \sqrt{\mathcal{E}b + \lambda - b\Lambda_q}(\omega - \omega')) K_q(x_\perp, x'_\perp),$$

where $|l| := l_1 + \cdots + l_N$. Hence, we get

$$\mathrm{tr}(T_{q,l_1}^{k_1}\dots T_{q,l_N}^{k_N}) = \sum_{\omega=\pm1}\int_{\mathbb{R}^2} N_{q,l,k}(\omega,\omega,x_\perp,x_\perp)\mathrm{d}x_\perp = 2(i\sqrt{b})^{-|l|-N}\sum_{m=0}^{+\infty}(i\sqrt{b})^{-m}\int_{\mathbb{R}^2}\hat{V}^{\|}_{m,q,l,k}(x_\perp,0)\mathrm{d}x_\perp$$

$$= 2(i\sqrt{b})^{-|l|-N}\sum_{m=0}^{+\infty}(i\sqrt{b})^{-m}\int_{\mathbb{R}^3} V_{m,q,l,k}(x)\mathrm{d}x$$

and the proof of Theorem 4 is almost complete. Indeed, we have shown that there exists a sequence $(\alpha_j)_{j\in\mathbb{N}}$ of real numbers such that

$$s(\mathcal{E}b+\lambda,b) = \frac{1}{2i\pi}b^{(n-2)/2}\sum_{j=0}^{+\infty}\alpha_j(\mathcal{E},\lambda)(i\sqrt{b})^{-j}.$$

Hence, we must prove that for $j\in\mathbb{N}$, $\alpha_{2j}=0$. For this purpose, let us remark that $S(\lambda,b)$ being unitary, $s(\mathcal{E}b+\lambda,b)$ is real valued. Therefore, the coefficients α_{2j}, $j\in\mathbb{N}$ vanish and the proof of expansion (11) is complete.

It remains to compute the coefficients a_0 and a_1. From Eqs. (26) and (27) and Lemma 4.1 we deduce that

$$s(\mathcal{E}b+\lambda,b) = \frac{1}{2i\pi}\sum_{q=0}^{[(\mathcal{E}-1)/2]}\sum_{k=0}^{2}\frac{(-1)^k}{k+1}\mathrm{tr}\left(\sum_{l=0}^{2}T_{q,l}(\mathcal{E}b+\lambda,b)\right)^{k+1}+\mathcal{O}(b^{-1}).$$

Using again Lemma 4.1, we obtain

$$s(\mathcal{E}b+\lambda,b) = \frac{1}{2i\pi}\sum_{q=0}^{[(\mathcal{E}-1)/2]}\left(\mathrm{tr}\,T_{q,0}+\mathrm{tr}\,T_{q,1}+\mathrm{tr}\,T_{q,2}-\frac{1}{2}\mathrm{tr}\,T_{q,0}^2-\mathrm{tr}\,T_{q,0}T_{q,1}+\frac{1}{3}\mathrm{tr}\,T_{q,0}^3\right)+\mathcal{O}(b^{-1}), \tag{30}$$

and we must compute all the terms of the sum. From the proof of Theorem 3 with $n=3$, $d=1$, we deduce that

$$\mathrm{tr}(T_{q,0}(\mathcal{E}b+\lambda,b)) = -\frac{2i\pi}{4\pi^2}\int_{\mathbb{R}^3}V(x)\mathrm{d}x\left(b^{\frac{1}{2}}(\mathcal{E}-2q-1)^{-\frac{1}{2}}-\frac{\lambda}{2}b^{-\frac{1}{2}}(\mathcal{E}-2q-1)^{-\frac{3}{2}}\right)+\mathcal{O}\left(b^{-\frac{3}{2}}\right).$$

By similar computations, we prove that

$$\mathrm{tr}(T_{q,0}^2(\mathcal{E}b+\lambda,b)) = -\frac{1}{4\pi(\mathcal{E}-2q-1)}\left(\int V(x)\mathrm{d}x\right)^2+\mathcal{O}(b^{-1})$$

and

$$\mathrm{tr}(T_{q,0}^3(\mathcal{E}b+\lambda,b)) = \frac{i(\mathcal{E}-2q-1)^{-3/2}}{8\pi}b^{-1/2}\left(\int V(x)\mathrm{d}x\right)^3+\mathcal{O}(b^{-1}).$$

Let us compute $\mathrm{tr}(T_{q,1})$. It follows from Eq. (29) that

$$\mathrm{tr}(T_{q,1}(\mathcal{E}b+\lambda,b)) = \frac{-b}{8\pi(\mathcal{E}b+\lambda-b\Lambda_q)}\sum_{\omega=\pm1}\int e^{i\sqrt{\mathcal{E}b+\lambda-b\Lambda_q}(|x_1-x_2|+\omega(x_1-x_2))}V(x_\perp,x_1)V(x_\perp,x_2)\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_\perp$$

$$= \frac{-1}{8\pi(\mathcal{E}-2q-1)}\int(1+e^{2i\sqrt{\mathcal{E}b+\lambda-b\Lambda_q}(|x_1-x_2|)})V(x_\perp,x_1)V(x_\perp,x_2)\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_\perp$$

$$+\mathcal{O}(b^{-1}) = \frac{-1}{8\pi(\mathcal{E}-2q-1)}\left(\int V(x)\mathrm{d}x\right)^2$$

$$-\frac{2}{8\pi(\mathcal{E}-2q-1)}\int_{x_1\leqslant x_2} e^{2i\sqrt{\mathcal{E}b+\lambda-1\Lambda_q}(x_2-x_1)}V(x_\perp,x_1)V(x_\perp,x_2)\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_\perp$$
$$+\mathcal{O}(b^{-1}).$$

Integrating by parts with respect to x_1, we obtain

$$\mathrm{tr}(T_{q,1}(\mathcal{E}b+\lambda,b)) = \frac{-1}{8\pi(\mathcal{E}-2q-1)}\left(\left(\int V(x)\mathrm{d}x\right)^2+\frac{i}{\sqrt{\mathcal{E}b+\lambda-b\Lambda_q}}\int V(x)^2\mathrm{d}x\right)+\mathcal{O}(b^{-1})$$
$$= \frac{-1}{8\pi(\mathcal{E}-2q-1)}\left(\left(\int V(x)\mathrm{d}x\right)^2-\frac{ib^{-1/2}}{8\pi(\mathcal{E}-2q-1)^{3/2}}\int V(x)^2\mathrm{d}x\right)+\mathcal{O}(b^{-1}).$$

The computations of $\mathrm{tr}(T_{q,2})$ and $\mathrm{tr}(T_{q,0}T_{q,1})$ are similar to the preceding ones. We find

$$\mathrm{tr}(T_{q,0}(\mathcal{E}b+\lambda,b)T_{q,1}(\mathcal{E}b+\lambda,b)) = \frac{i(\mathcal{E}-2q-1)^{-3/2}}{16\pi}b^{-1/2}\left(\int V(x)\mathrm{d}x\right)^3+\mathcal{O}(b^{-1})$$

and

$$\mathrm{tr}(T_{q,2}(\mathcal{E}b+\lambda,b)) = \frac{i(\mathcal{E}-2q-1)^{-3/2}}{48\pi}b^{-1/2}\left(\int V(x)\mathrm{d}x\right)^3+\mathcal{O}(b^{-1}).$$

Combining these equations with (30), we obtain

$$s(\mathcal{E}b+\lambda,b) = -\frac{\gamma_0(\mathcal{E})}{4\pi^2}b^{1/2}\left(\int V(x)\mathrm{d}x\right)+\frac{\lambda\gamma_1(\mathcal{E})}{8\pi^2}b^{-1/2}\left(\int V(x)\mathrm{d}x\right)$$
$$-\frac{\gamma_1(\mathcal{E})}{16\pi^2}b^{-1/2}\left(\int V(x)^2\mathrm{d}x\right)+\mathcal{O}(b^{-1})$$

with

$$\gamma_j(\mathcal{E}) = \sum_{q=0}^{[(\mathcal{E}-1)/2]}(\mathcal{E}-2q-1)^{-1/2-j}.$$

This completes the proof of Theorem 4. ■

To conclude, let us notice that Theorem 4 could be generalized to the case $n-2d>1$ by using stationary phase method in the variable $x_\parallel$. Nevertheless, there are some difficulties due to degenerate phases.

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Stochastic heat and Burgers equations and their singularities. II. Analytical properties and limiting distributions

Ian M. Davies[a] and Aubrey Truman[b]
Department of Mathematics, University of Wales Swansea, Singleton Park, Swansea, SA2 8PP, Wales, United Kingdom

Huaizhong Zhao[c]
Department of Mathematical Sciences, Loughborough University, Loughborough, Leicestershire, LE11 3TU, England, United Kingdom

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We study the inviscid limit, $\mu \to 0$, of the stochastic viscous Burgers equation, for the velocity field $v^\mu(x,t)$, $t>0$, $x \in \mathbb{R}^d$, $(\partial v^\mu/\partial t)+(v^\mu \cdot \nabla)v^\mu = -\nabla c(x,t) - \epsilon \nabla k(x,t)\dot{W}_t + (\mu^2/2)\Delta v^\mu$, for small ϵ, with $v^\mu(x,0) \equiv \nabla S_0(x)$ for some given S_0, $\dot{W}_t$ representing white noise. Here we use the Hopf–Cole transformation, $v^\mu = -\mu^2 \nabla \ln u^\mu$, where u^μ satisfies the stochastic heat equation of Stratonovich-type and the Feynmac–Kac Truman–Zhao formula for u^μ, where $\mathrm{d}u_t^\mu(x) = [(\mu^2/2)\Delta u_t^\mu(x) + \mu^{-2}c(x,t)u_t^\mu(x)]\mathrm{d}t + \epsilon\mu^{-2}k(x,t)u_t^\mu(x) \circ \mathrm{d}W_t$, with $u_0^\mu(x) = T_0(x) \times \exp(-S_0(x)/\mu^2)$, S_0 as before and T_0 a smooth positive function. In an earlier paper, Davies, Truman, and Zhao [J. Math. Phys. **43**, 3293 (2002)], an exact solution of the stochastic viscous Burgers equation was used to show how the formal "blow-up" of the Burgers velocity field occurs on *random shockwaves* for the $v^{\mu=0}$ solution of Burgers equation coinciding with the caustics of a corresponding Hamiltonian system with classical flow map Φ. Moreover, the $u^{\mu=0}$ solution of the stochastic heat equation has its *wavefront* determined by the behavior of the Hamilton principal function of the corresponding stochastic mechanics. This led in particular to the level surface of the minimizing Hamilton–Jacobi function developing cusps at points corresponding to points of intersection of the corresponding prelevel surface with the precaustic, "pre" denoting the preimage under Φ determined algebraically. These results were primarily of a geometrical nature. In this paper we consider small ϵ and derive the shape of the random shockwave for the inviscid limit of the stochastic Burgers velocity field and also give the equation determining the random wavefront for the stochastic heat equation both correct to first order in ϵ. In the case $c(x,t) = \frac{1}{2}x^T\Omega^2 x$, $\nabla k(x,t) = -a(t)$, we obtain the exact random shockwave and prove that its shape is unchanged by the addition of noise, it merely being displaced by a random Brownian vector $N(t)$. By exploiting the Jacobi fields for this problem we obtain the large time limit of the distribution of the Burgers fluid velocity for noises which have infinite time averages, such as almost periodic ones. Here resonance with the underlying $\epsilon = 0$ classical problem has an important effect. Imitating these results for the case of a periodic underlying classical problem perturbed by small noise, arming ourselves with some detailed estimates for Green's functions enables us to make generalizations. In the stochastic case we have also the possibility of "infinitely rapid" changes in the number of cusps on the minimizing level surface of the Hamilton–Jacobi function. This will engender stochastic turbulence in the Burgers velocity field and, due to its stochasticity, may be of an "intermittent" nature. There is no analog of this in the deterministic case. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1850836]

I. INTRODUCTION

Stochastic Burgers equations have attracted a considerable amount of attention in recent years, e.g., Refs. 2, 4, 7, 11, 12, 16, 20–24, 35, 41, 37, and 39. See also Refs. 3, 5, 18, and 30 for related works. Burgers equations have been used to give models of turbulence (see especially Ref. 11) and to model the large scale structure of the universe.[34] Here we shall be interested in what has come to be called Burgulence. Primarily we show how a knowledge of Jacobi fields, and the geometry of the level surfaces of a Hamilton–Jacobi function and the associated caustic surface can be used in determining the behavior of the velocity field of the viscous Burgers fluid in the inviscid limit. The presence of viscosity provides access to a range of powerful analytical methods.

Consider the stochastic viscous Burgers equation for the velocity field $v^\mu = v^\mu(x,t)$, $x \in \mathbb{R}^d$, $t > 0$, small $\epsilon \in \mathbb{R}$,

$$\frac{\partial v^\mu}{\partial t} + (v^\mu \cdot \nabla) v^\mu = \frac{\mu^2}{2}\Delta v^\mu - \nabla c(x) - \epsilon \nabla k(x,t)\dot{W}_t,$$

with initial velocity $v^\mu(x,0) = \nabla S_0(x) + O(\mu^2)$ where μ^2 is the coefficient of viscosity. Here c, k, and S_0 are C^2 functions and W_t is a Wiener process on the probability space $\{\Omega, \mathcal{F}, P\}$. The corresponding heat equation for $u^\mu = u^\mu(x,t)$ is the Stratonovich equation

$$\frac{\partial u^\mu}{\partial t} = \frac{\mu^2}{2}\Delta u^\mu + \frac{1}{\mu^2}c(x)u^\mu + \frac{\epsilon}{\mu^2}k(x,t)u^\mu \circ \dot{W}_t,$$

$$u^\mu(x,0) = T_0(x)\exp(-S_0(x)/\mu^2),$$

where T_0 is a smooth positive function, the square root of the initial Burgers fluid density.

The connection between u^μ and v^μ is the Hopf–Cole logarithmic transformation $v^\mu = -\mu^2 \nabla \ln u^\mu$. Our studies are driven by an interest in the blow-up of $v^0(x,t)$ where

$$v^0(x,t) = \lim_{\mu \to 0} v^\mu(x,t).$$

We seek an understanding of the advent of discontinuities in v^0 and the large time limit of its probability density. In particular we show how for small, almost periodic noise resonating with the underlying classical problem there is no invariant measure.

It is this correspondence with the stochastic heat equation that enables us to appeal to asymptotic methods in our study of the viscous Burgers fluid. Moreover, these methods highlight the importance of the stochastic dynamical flow and the stochastic Hamilton–Jacobi function in determining the behavior of solutions. With this in mind we would expect, from the work of Donsker, Freidlin *et al.*,[19,17,41] that we have as $\mu \to 0$,

$$-\mu^2 \ln u^\mu(x,t) \to \inf_{x_0}[A(x_0,x,t) + S_0(x_0)] = S(x,t), \tag{1.1}$$

with

$$A(x_0,x,t) = \inf_{\substack{X(s) \\ X(0)=x_0 \\ X(t)=x}} A[X],$$

where $A[X]$ is the stochastic action

[a]Electronic mail: i.m.davies@swansea.ac.uk
[b]Electronic mail: a.truman@swansea.ac.uk
[c]Electronic mail: h.zhao@lboro.ac.uk

$$A[X] = \frac{1}{2}\int_0^t |\dot{X}^2(s)|\mathrm{d}s - \int_0^t c(X(s))\mathrm{d}s - \epsilon\int_0^t k(X(s),s)\mathrm{d}W_s$$

and

$$\mathcal{A}(x_0,x,t) = A(x_0,x,t) + S_0(x_0).$$

We shall assume that $\tilde{x}_0(x,t)$ the minimizer of $\mathcal{A}(x_0,x,t)$ is unique. Note that we require absolute continuity of X (cf. Davies and Truman[9] and references therein) and we will have $\dot{X}$ continuous almost surely. Then $S(x,t)$ is the minimizing solution of the stochastic Hamilton–Jacobi equation

$$\mathrm{d}S_t + \frac{|\nabla S|^2}{2}\mathrm{d}t + c(x)\mathrm{d}t + \epsilon k(x,t)\mathrm{d}W_t = 0, \quad S(x,0) = S_0(x).$$

So $S(x,t)$ is Hamilton's principal function for a stochastic classical mechanical path $X(s)$, satisfying the second order stochastic differential equation

$$\mathrm{d}\dot{X}(s) + \nabla c(X(s))\mathrm{d}s + \epsilon\nabla k(X(s),s)\mathrm{d}W_s = 0, \quad s \in (0,t),$$

with

$$X(0) = x_0, \quad \dot{X}(0) = \nabla S_0(x_0),$$

where $x_0 = x_0(x,t)$ is determined by the boundary condition $X(t) = x$. Here we finally have to set $x_0 = \tilde{x}_0(x,t)$ to get the minimizing S.

When $x_0(x,t)$ above is unique, the solutions of the stochastic heat equation and the viscous stochastic Burgers equation, cf. Ref. 41, for each $m \geqslant 0$ are, respectively,

$$u_t^\mu(x) = \exp\left\{-\mu^{-2}\sum_{j=0}^{m}\mu^{2j}S_j(x,t)\right\}\mathbb{E}\exp\left\{-\frac{\mu^{2m}}{2}\int_0^t \Delta S_m(y_s^\mu, t-s)\mathrm{d}s\right.$$
$$\left. + \frac{1}{2}\sum_{j=m+1}^{2m}\mu^{2(j-1)}\sum_{\substack{0\leqslant i_1,i_2\leqslant m\\ i_1+i_2=j}}\int_0^t \nabla S_{i_1}\cdot\nabla S_{i_2}(y_s^\mu, t-s)\mathrm{d}s\right\},$$

$$v^\mu(x,t) = \sum_{j=0}^{m}\mu^{2j}v_j(x,t) - \mu^2\nabla\ln\mathbb{E}\left\{\exp\left\{-\frac{\mu^{2m}}{2}\int_0^t \nabla\cdot v_m(y_s^\mu, t-s)\mathrm{d}s\right.\right.$$
$$\left.\left. + \frac{1}{2}\sum_{j=m+1}^{2m}\mu^{2(j-1)}\sum_{\substack{0\leqslant i_1,i_2\leqslant m\\ i_1+i_2=j}}\int_0^t v_{i_1}\cdot v_{i_2}(y_s^\mu, t-s)\mathrm{d}s\right\}\right\},$$

where $v_j(x,t) = \nabla S_j(x,t)$ is known explicitly for $j = 0,1,2,\ldots$ (see Truman and Zhao[41]).

Note that each second factor in the expectation is of the form $(1+O(\mu^{2m}))$ and the first factor gives the expansion up to μ^{2m-2} for each m. The S_j satisfy the stochastic Hamilton–Jacobi equations

$$\frac{\partial S_j}{\partial t} + \frac{1}{2} \sum_{\substack{i_1, i_2 \geqslant 0 \\ i_1 + i_2 = j}} \nabla S_{i_1} \cdot \nabla S_{i_2} = \frac{1}{2} \Delta S_{j-1},$$

for $j=0,1,2,\ldots$, with the convention $\frac{1}{2}\Delta S_{-1} = -c - \epsilon k \dot{W}_t$, $\dot{W}_t$ being white noise and the Nelson diffusion process y_s^μ satisfying

$$\mathrm{d}y_s^\mu = \mu \mathrm{d}B_s - \nabla \sum_{j=0}^{m} \mu^{2j} S_j(y_s^\mu, t-s)\mathrm{d}s, \quad y_0^\mu = x, \quad B_s \text{ is BM}.$$

It is important to note that S_1, and hence all S_j, are T_0 dependent, cf. Ref. 41. Formally, we are using $S^\mu \sim \Sigma_{j=0}^{\infty} \mu^{2j} S_j$ where S^μ is the solution of the viscous stochastic Hamilton–Jacobi equation,

$$\mathrm{d}S^\mu + \tfrac{1}{2} |\nabla S^\mu|^2 \, \mathrm{d}t + c \, \mathrm{d}t + \epsilon k \, \mathrm{d}W_t = \tfrac{1}{2} \mu^2 \Delta S^\mu \, \mathrm{d}t.$$

Changes in the degree of nonuniqueness of $x_0(x,t)$ is associated with discontinuities in $v^0(x,t)$ and $u^0(x,t)$ and this occurs when infinitely many paths $X(s)$ focus in zero volume centered at x. For nondegenerate critical paths $X(\cdot)$, when the multiplicity of $x_0(x,t)$, $n=n(x,t)$, is finite so that for a given x and t the set of possible initial positions x_0 is $\{x_0^1(x,t), x_0^2(x,t), \ldots, x_0^n(x,t)\}$, we can deduce that

$$u^\mu(x,t) \sim \sum_{i=1}^{n} \theta_i \exp\{-S_0^i(x,t)/\mu^2\},$$

where

$$S_0^i(x,t) = S_0(x_0^i(x,t)) + A(x_0^i(x,t), x, t)$$

for $i=1,2,\ldots,n$ and θ_i is an asymptotic series in μ^2 associated with $x_0^i(x,t)$ as above. (The detailed structure of θ_i may be developed by drawing on the papers of Davies and Truman,[8,9] Ellis and Rosen[13–15] and Truman and Zhao.[41]) Needless to say the dominant term in the above comes from $\tilde{x}_0(x,t)$ the minimizing $x_0(x,t)$ so that

$$S(x,t) = \min_{i=1,2,\ldots,n} S_0^i(x,t)$$

in line with the results of Freidlin *et al.*[19,17] Here we assume, unless stated otherwise, that the minimizer $\tilde{x}_0(x,t)$ is unique. The caustic, where the focusing of the paths $X(s)$ occurs, is important since $u^0(x,t)$ can switch discontinuously from being exponentially large to exponentially small as we cross parts of the caustic. This is because two of the $x_0^i(x,t)$ can coalesce and then disappear causing the minimizing S_0^i to disappear.

In this paper we develop inequalities showing how closely related the stochastic caustic and wavefront are to their classical dynamical counterparts for small noise. Once again the classical dynamical structures guide the arguments and we state our results for the caustic in terms of the classical path X^0, the stochastic path X^ϵ and their near neighbor $\tilde{X}^\epsilon$. We also derive inequalities relating ∇X^0, ∇X^ϵ, and $\nabla \tilde{X}^\epsilon$. For small noise, the stochastic wavefront is shown to lie within an ϵ neighborhood of the classical wavefront by utilizing the solution of the matrix Jacobi equation, the Green's function, to construct the appropriate estimates. Our main theorems (3.5 and 4.6) relate to the nonexistence of an invariant measure for the small noise stochastic Burgers equation when there is resonance between the underlying classical mechanical problem and the almost periodic noise. It is here that we use the detailed properties of Jacobi fields, developed by imitating more or less standard results for the linear harmonic oscillator.

II. STOCHASTIC DYNAMICS, H_t AND C_t

We now define our main structures and state without proof some of the key results from our earlier paper.[10] The familiar objects from classical dynamics are easily recognizable.

Define $A(x_0,p_0,t)$, the stochastic action, to be

$$\frac{1}{2}\int_0^t |\dot{X}(s)|^2\,\mathrm{d}s - \int_0^t [c(X(s))\mathrm{d}s + \epsilon k(X(s),s)\mathrm{d}W_s], \quad \text{a.s.},$$

with $X(s)=X(s,x_0,p_0)$ satisfying

$$\mathrm{d}\dot{X}(s) = -\nabla c(X(s))\mathrm{d}s - \epsilon\nabla k(X(s),s)\mathrm{d}W_s,$$

$s\in[0,t]$, $X(0)=x_0$, $\dot{X}(0)=p_0$, x_0, $p_0\in\mathbb{R}^d$. We shall assume that the minimizing $X(s)$ satisfying $X(t)=x$ and $\dot{X}(0)=\nabla S_0(X(0))$ is unique in any space with $\dot{X}$ continuous, where we assume as usual that $X(s)$ is $\mathcal{F}_s$ measurable. Later on we must consider Poisson brackets $\{X(s),X(u)\}_{x_0,p_0}$ with respect to x_0, p_0 variables which we suppress. We also allow for p_0 to be an as yet unspecified function of x_0 such as $\nabla S_0(x_0)$.

Then, for ∇c, ∇k Lipschitz, with Hessians $\nabla^2 c$, $\nabla^2 k$ and all second derivatives with respect to space variables of c and k bounded, according to Kunita,[27] $\partial X(s)/\partial x_0^\alpha$ satisfies

$$\frac{d}{\mathrm{d}s}\left(\frac{\partial X(s)}{\partial x_0^\alpha}\right) = \frac{\partial \dot{X}(0)}{\partial x_0^\alpha} - \int_0^s \left[\nabla^2 c(X(r))\frac{\partial X(r)}{\partial x_0^\alpha}\mathrm{d}r + \epsilon\nabla^2 k(X(r),r)\frac{\partial X(r)}{\partial x_0^\alpha}\mathrm{d}W_r\right].$$

Moreover,

$$\dot{X}(s) = \dot{X}(0) - \int_0^s [\nabla c(X(r))\mathrm{d}r + \epsilon\nabla k(X(r),r)\mathrm{d}W_r]. \tag{2.1}$$

Define the random map $\Phi_s:\mathbb{R}^d\to\mathbb{R}^d$ corresponding to the classical flow by the second order stochastic differential equation

$$d_s\dot{\Phi}_s = -\nabla c(\Phi_s)\mathrm{d}s - \epsilon\nabla k(\Phi_s,s)\mathrm{d}W_s,$$

with $\Phi_0=I$ and $\dot{\Phi}_0=\nabla S_0$.

We then have $X(s)=\Phi_s\Phi_t^{-1}x$, where we accept that $x_0(x,t)=\Phi_t^{-1}x$ may not be necessarily unique. Given some regularity, the global inverse function theorem gives a caustic time $T(\omega)$ $\times(>0)$ such that, for $s<T(\omega)$, Φ_s is a random diffeomorphism.[40] So for $t<T(\omega)$, $x_0(x,t)$ is unique. Therefore, as we shall see,

$$v^0(x,t) = \dot{\Phi}_t\Phi_t^{-1}x = \nabla S(x,t)$$

is a formal solution of Burgers equation with $\mu=0$, which is well defined up to the caustic time $T(\omega)$.

Lemma 2.1: Assume S_0, $c\in C^2$ and $k\in C^{2,0}$, ∇c, ∇k are Lipschitz, with Hessians $\nabla^2 c$, $\nabla^2 k$ and all second derivatives with respect to space variables of c and k bounded. If $\dot{X}(s)$ satisfies Eq. (2.1) *and we have p_0, possibly x_0 dependent, then almost surely*

$$\frac{\partial A}{\partial x_0^\alpha}(x_0,p_0,t) = \dot{X}(t)\cdot\frac{\partial X(t)}{\partial x_0^\alpha} - \dot{X}_\alpha(0).$$

Remark 2.1: Observe that, if we fix $X(t)$ independently of x_0, we obtain almost surely

$$\frac{\partial A}{\partial x_0^\alpha}(x_0,p_0,t) = -\dot{X}_\alpha(0),$$

for $\alpha=1,2,\ldots,d$.

Let $X(s,x_0,x)=X(s,x_0,p_0)|_{p_0=p(x_0,x,t)}$ where $p_0=p(x_0,x,t)$ is the (assumed unique) random minimizer of $A(x_0,p_0,t)$ with $X(t,x_0,p_0)=x$.

Remark 2.2: Here we need the maps $\mathbb{R}^d \to \mathbb{R}^d$ defined by $p_0 \mapsto X(x_0,p_0,t)$, for fixed t, for each $x_0 \in \mathbb{R}^d$ to be onto with probability one (cf. Kolokoltsov *et al.*[26,25]).

Set $A(x_0,x,t)=A(x_0,p_0,t)|_{p_0=p(x_0,x,t)}$ and define Hamilton's principal function corresponding to the initial momentum $\nabla S_0(x_0)$ to be

$$\mathcal{A}(x_0,x,t) = A(x_0,x,t) + S_0(x_0).$$

Then

$$\frac{\partial \mathcal{A}}{\partial x_0^\alpha}(x_0,x,t) = 0 \quad \text{for } \alpha = 1,2,\ldots,d \Rightarrow \dot{X}(0) = \nabla S_0(X(0))$$

which defines the classical flow map Φ.

We define a prelevel surface of Hamilton's principal function for real constant c by eliminating x between the equations

$$\mathcal{A}(x_0,x,t) = c \quad \text{and} \quad \frac{\partial \mathcal{A}}{\partial x_0^\alpha}(x_0,x,t) = 0,$$

$\alpha=1,2,\ldots,d$, and a level surface H_t by eliminating x_0. We denote the prelevel surface by $\Phi_t^{-1}H_t$. Similarly we define the caustic C_t and the precaustic $\Phi_t^{-1}C_t$ by eliminating x_0 or x between

$$\mathrm{Det}\left(\frac{\partial^2 \mathcal{A}}{\partial {x_0}^2}(x_0,x,t)\right) = 0 \quad \text{and} \quad \frac{\partial \mathcal{A}}{\partial x_0^\alpha}(x_0,x,t) = 0,$$

$\alpha=1,2,\ldots,d$.

Remark 2.3: Note that $\Phi_t^{-1}H_t$ (and $\Phi_t^{-1}C_t$) are determined by taking algebraic inverse images, i.e., by eliminating x above. Those are not necessarily the same as the topological inverse images $\Phi_t^{-1}(H_t)$ and $\Phi_t^{-1}(C_t)$. In fact as we shall demonstrate $\Phi_t^{-1}C_t \neq \Phi_t^{-1}(C_t)$.

We shall need.

Lemma 2.2: The classical flow map $x=\Phi_t(x_0)$ is a differentiable map from $\Phi_t^{-1}H_t$ to H_t with Fréchet derivative

$$D\Phi_t(x_0) = \left(-\frac{\partial^2 \mathcal{A}}{\partial x\, \partial x_0}(x_0,x,t)\right)^{-1}\left(\frac{\partial^2 \mathcal{A}}{\partial {x_0}^2}(x_0,x,t)\right),$$

if $\mathcal{A}$ is C^3 in space derivatives.

In the next section we investigate the linear harmonic oscillator case in detail. This will provide us with the main ideas for the proofs of our general results.

III. HARMONIC OSCILLATOR WELLS WITH NOISE

The stochastic harmonic oscillator was studied by Albeverio *et al.*,[1] Markus and Weerasinghe,[28] and McKean.[29] The stochastic Mehler formula was first obtained by Truman and Zhao[38–40] and later using different techniques by Truman and Zastawniak.[36]

Consider $v=v(x,t)$, $x \in \mathbb{R}^d$, $t \in \mathbb{R}^+$, satisfying

$$dv + (v \cdot \nabla)v\ dt = -\Omega^2 x\ dt - \epsilon \nabla k(x,t) dW_t, \tag{3.1}$$

with $v(x,0) = \nabla S_0(x)$, i.e., v is Burgers velocity field for the perturbed harmonic oscillator potential

$$c(x) = \tfrac{1}{2} x^T \Omega^2 x,$$

where Ω^2 is a positive definite, real, symmetric matrix. Here the perturbing potential is the white noise term $k_t(x)\dot{W}_t$, with real valued $k_t(x) = k(x,t) \in C^{2,1}(\mathbb{R}^d, \mathbb{R}^+)$ and W_t is one-dimensional Brownian motion on the probability space $\{\Omega, \mathcal{F}, P\}$. The corresponding stochastic mechanics is

$$d_s \dot{X}^\epsilon(s) + \Omega^2 X^\epsilon(s) ds = -\epsilon \nabla k(X^\epsilon(s), s) dW_s, \tag{3.2}$$

with

$$X^\epsilon(0)(x_0) = x_0,$$

$$\dot{X}^\epsilon(0)(x_0) = \nabla S_0(x_0).$$

Here x_0 must be chosen such that

$$X^\epsilon(t)(x_0) = x,$$

for fixed t and x in $v^\mu(x,t)$ and to minimize $\mathcal{A}(x_0, x, t)$, the choice being unique.

When $\epsilon = 0$, we have a harmonic oscillator, which defines the classical flow map Φ_s^0,

$$X^0(s) = \Phi_s^0 x_0 = \cos(\Omega s) x_0 + \sin(\Omega s) \Omega^{-1} \nabla S_0(x_0), \tag{3.3}$$

Ω being the obvious positive square root of Ω^2.

Note that the solution $X^\epsilon(s)$ of (3.2) can be found explicitly as follows: provided $\nabla k(\cdot, s) = -a(s)$, is independent of spatial variables. We obtain in matrix notation

$$X^\epsilon(s) = \cos(\Omega s) x_0 + \sin(\Omega s) \Omega^{-1} \nabla S_0(x_0) + \epsilon \int_0^s \sin(\Omega(s-u)) \Omega^{-1} a(u) dW_u. \tag{3.4}$$

It therefore turns out that

$$X^\epsilon(s) - \epsilon \int_0^s \sin(\Omega(s-u)) \Omega^{-1} a(u) dW_u = \Phi_s^0 x_0. \tag{3.5}$$

The following simple result for shockwaves in a random environment is an easy corollary of the above computations.

Theorem 3.1: *At time t, let* $\Delta_t^0(x_0) = \mathrm{Det}(\partial X^0(t) / \partial x_0) = \mathrm{Det}(\nabla_{x_0} \Phi_t^0 x_0) = 0$ *be the equation of the precaustic in* x_0*, where* Φ_t^0 *is the classical flow map for the harmonic oscillator without noise and let* $x = \Phi_t x_0$*. Eliminating* y_0*, let the corresponding equation at time t in* $y = \Phi_t y_0$ *be*

$$\Delta_t^0((\Phi_t^0)^{-1}(y)) = 0.$$

Then, if $\nabla k(x,t) = -a(t)$*, independent of x, the random shockwave in the presence of noise at time t has equation*

$$\Delta_t^0((\Phi_t^0)^{-1}(y + \epsilon N(t))) = 0,$$

where $N(t)$ *is the random vector*

$$N(t) = \int_0^t \Omega^{-1} \sin(\Omega(t-s)) a(s) dW_s.$$

Remark 3.1: In this case the noise leaves the shape of the shockwaves unchanged merely displacing them by a random vector $-N(t)$.

Remark 3.2: Needless to say $N(t)$ satisfies the second order stochastic differential equation

$$\mathrm{d}\dot{N}_t + \Omega^2 N_t \,\mathrm{d}t = a(t)\mathrm{d}W_t,$$

where $N(0)=0$, $\dot{N}(0)=0$.

We need the following lemma, a simple one-dimensional result.

Lemma 3.2: Let $a(\cdot)\in C^1(\mathbb{R}^+)$ be bounded, with $\lim_{t\to\infty} t^{-1/2}a(t)=0$, and let the infinite time average

$$\lim_{t\to\infty} t^{-1}\int_0^t a^2(u)\mathrm{d}u = M(a^2) > 0.$$

Then, if $d(a^2(u))/\mathrm{d}u \in L^1(\mathbb{R}^+)$, the leading behavior of the noise term

$$N(t) = \int_0^t \Omega^{-1}\sin(\Omega(t-s))a(s)\mathrm{d}W_s,$$

as $t\to\infty$ is given almost surely by

$$N(t) \sim \Omega^{-1}M^{\frac{1}{2}}(a^2)(\sin(\Omega t)B^c(t) - \cos(\Omega t)B^s(t)),$$

where B^c and B^s are normalized $BM(\mathbb{R})$ processes B, with $\mathbb{E}(B^2(t))=t$, correlated by

$$\mathbb{E}(B^c(t)B^s(u)) = \int_0^{\tau_c(t)\wedge\tau_s(u)} a^2(r)\cos(\Omega r)\sin(\Omega r)\mathrm{d}r,$$

with

$$\tau_c(t) = \inf\left\{ s>0 : \int_0^s a^2(u)\cos^2(\Omega u)\mathrm{d}u = t \right\},$$

$$\tau_s(t) = \inf\left\{ s>0 : \int_0^s a^2(u)\sin^2(\Omega u)\mathrm{d}u = t \right\}.$$

Proof: We need McKean's result on time changed Brownian motion (see p. 29 of McKean[29]). Now

$$\int_0^t a^2(u)\cos^2(\Omega u)\mathrm{d}u = \frac{1}{2}\int_0^t (1+\cos(2\Omega u))a^2(u)\mathrm{d}u$$

and

$$t^{-1}\int_0^t \cos(2\Omega u)a^2(u)\mathrm{d}u = \frac{1}{2\Omega t}\left(a^2(t)\sin(2\Omega t) - \int_0^t \sin(2\Omega u)\frac{d}{\mathrm{d}u}(a^2(u))\mathrm{d}u \right) \to 0,$$

as $t\to\infty$. ∎

If we now work in Cartesian axes relative to which Ω is diagonal, $\Omega_{ij}=\Omega_i\delta_{ij}$, $\Omega_i>0$, for $i,j=1,2,\ldots,d$, we can deduce a vector version of the last lemma.

Lemma 3.3: Working in coordinates in which Ω is diagonal and $N(t)=(N_1(t),\ldots,N_d(t))$, we obtain the behavior as $t\to\infty$,

$$N_i(t) \sim \Omega_i^{-1}M^{\frac{1}{2}}(a_i^2)(\sin(\Omega_i t)B^{c_i}(t) - \cos(\Omega_i t)B^{s_i}(t)),$$

for $i=1,\ldots,d$, *where the* B^{c_i}, B^{s_i} *are normalized correlated* $BM(\mathbb{R})$ *processes with*

$$\mathbb{E}(B^{c_i}(t)B^{s_j}(u)) = \int_0^{\tau_{c_i}(t)\wedge\tau_{s_j}(u)} a_i(r)a_j(r)\cos(\Omega_i r)\sin(\Omega_j r)\mathrm{d}r,$$

together with similar results for $\mathbb{E}(B^{c_i}(t)B^{c_j}(u))$ *and* $\mathbb{E}(B^{s_i}(t)B^{s_j}(u))$.

Remark 3.3: The above results hold for any finite value of ϵ, no matter how large. This gives the leading behavior of $N(t)$ as $t\to\infty$ in terms of the Jacobi fields of the zero noise problem and thence the large time behavior of $v^0(x,t)$ and $X^\epsilon(x,t)$ and their sample paths. The Jacobi fields are also important in understanding the small noise processes, as we see in the next section.

Example: We now illustrate the development of the semicubical parabolic shockwave with respect to time for the velocity field of a Burgers' fluid with initial velocity $(xy, x^2/2)$ in a harmonic well with $V(x,y)=(x^2+\omega^2y^2)/2$. The effect of noise here is to superimpose on the deterministic movement of the cusp caustic a Brownian motion. Let us just consider the deterministic case. It is easy to see

$$\Phi_t\begin{pmatrix}x_0\\ y_0\end{pmatrix} = \begin{pmatrix} x_0\cos t + x_0y_0\sin t \\ y_0\cos\omega t + \dfrac{1}{2\omega}x_0^2\sin\omega t\end{pmatrix}. \tag{3.6}$$

So

$$\Delta_t^0(x_0,y_0) = \det\begin{pmatrix}\cos t + y_0\sin t, & x_0\sin t\\ \omega^{-1}x_0\sin\omega t, & \cos\omega t\end{pmatrix} = \cos\omega t\cos t + y_0\cos\omega t\sin t - \omega^{-1}x_0^2\sin t\sin\omega t. \tag{3.7}$$

The precaustic is then given by $\Delta_t^0(x_0,y_0)=0$. The caustic is obtained by mapping the precaustic under the map Φ_t. If ω is rational then the deterministic motion of the cusp is periodic as is the deterministic part of v_t^0. The equation is then given by

$$8(y\csc\omega t + \cot t\cot\omega t)^3\omega = 27x^2\cot^2\omega t\csc^2 t. \tag{3.8}$$

The periodic motion of the cusp can be seen in Fig. 1 where we plot a succession of caustics for the case $\omega=3/2$. Time increases from left to right and top to bottom. Many more illustrations of this periodic behavior can be found in the Ph.D. thesis of Reynolds.[31]

We continue to investigate Burgers equation in $\mathbb{R}^d$, Eqs. (3.1) and (3.2), where $\nabla k(x,u) = -a(u)$ is independent of x and $\int_0^t |a(u)|^2\,\mathrm{d}u<\infty$. The key elementary lemma here is the following.

Lemma 3.4: *Let* $\dot X^\epsilon(t)-\dot X^0(t)=\dot N(t)=\epsilon\int_0^t\cos[\Omega(t-u)]a(u)\mathrm{d}W_u$. *Then, working in a coordinate system in which* Ω^2 *is diagonal,* $\dot N(t)$ *has mean zero and is Gaussian with covariance,*

$$\begin{aligned}A_{ij}^{-1}(t) &= \mathbb{E}[\dot N_i(t)\dot N_j(t)]\\ &= \frac{\epsilon^2}{4}\sum_{\pm}\left\{\cos((\Omega_i\pm\Omega_j)t)\int_0^t\cos((\Omega_i\pm\Omega_j)u)a_i(u)a_j(u)\mathrm{d}u\right.\\ &\quad\left.+\sin((\Omega_i\pm\Omega_j)t)\int_0^t\sin((\Omega_i\pm\Omega_j)u)a_i(u)a_j(u)\mathrm{d}u\right\},\quad t>0.\end{aligned}$$

Proof: The point is that, if $0=s_0<s_1<\cdots<s_{n+1}=t$ is a partition of $[0,t]$,

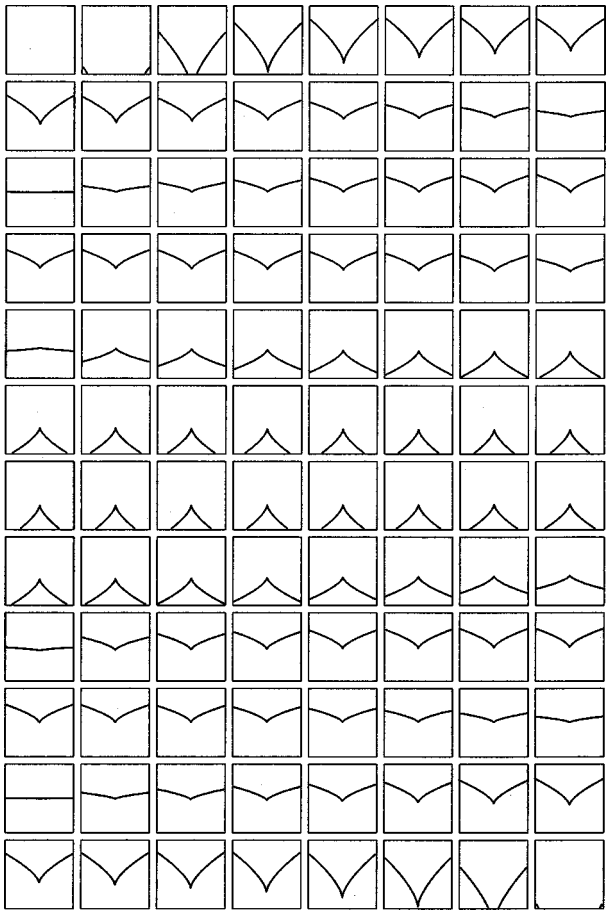

FIG. 1. Periodic motion of caustic.

$$\dot{N}_i(t) = \lim \sum_j \cos[\Omega_i(t - s_j)] a_i(s_j)[W(s_{j+1}) - W(s_j)]$$

exhibits $\dot{N}(t)$ as the limit of a sum of independent Gaussians. So for each t $\dot{N}(t)$ is Gaussian with mean and covariance as above. ■

A strikingly simple result emerges if we assume that $a(\cdot)$ is almost periodic in the sense that in our coordinate system $a(s)=(a_1(s),a_2(s),\ldots,a_d(s))$, where each a_j is almost periodic. [The class of almost periodic functions is a natural generalization of periodic functions in that they can be realized as uniform limits of trigonometric polynomials and if f is almost periodic $\lim_{t\uparrow\infty} t^{-1}\int_{t_0}^{t_0+t} f(s)\mathrm{d}s = M(f)$ exists, the class being closed under addition and multiplication.] When $a(\cdot)$ is almost periodic in our setup we refer to almost periodic white noise forces. The possibility of resonance between the almost periodic noise and the restraining harmonic oscillator force affects the long time behavior of the Burgers fluid.

Theorem 3.5: *For almost periodic white noise forces, for underlying harmonic oscillator potentials, the inviscid limit of Burgers fluid velocity* $v^0(x,t)$ *satisfies*

$$\mathbb{E}(v^0(x,t)) = \dot{X}^0(x,t) = \cos(\Omega t)\tilde{x}_0(x,t) + \Omega^{-1} \sin(\Omega t)\, \nabla S_0(\tilde{x}_0(x,t)),$$

where $\tilde{x}_0(x,t)$ *is the minimizer (assumed to be unique) of the deterministic* $\mathcal{A}(x_0,x,t)$. *Moreover,*

$$\mathbb{P}((v^0(x,t) - \dot{X}^0(x,t)) \in \mathrm{d}v) = \exp\left(-\frac{v^T A(t) v}{2}\right)(2\pi)^{-d/2}(\det A)^{-1/2}\, \mathrm{d}v,$$

where the matrix $A^{-1}(t)$ is specified above. In particular as $t\sim\infty$ we obtain

$$t^{-1}A_{ij}^{-1}(t) = t^{-1}\mathbb{E}[(v_i^0(x,t) - \dot{X}_i^0(x,t))(v_j^0(x,t) - \dot{X}_j^0(x,t))]$$
$$\sim \frac{\epsilon^2}{4}\sum_{\pm}\{\cos((\Omega_i \pm \Omega_j)t)M[\cos((\Omega_i \pm \Omega_j)\cdot)a_i(\cdot)a_j(\cdot)]$$
$$+ \sin((\Omega_i \pm \Omega_j)t)M[\sin((\Omega_i \pm \Omega_j)\cdot)a_i(\cdot)a_j(\cdot)]\},$$

where M denotes the infinite time average.

Proof: The proof is a simple consequence of the properties of almost periodic functions.[6] ■

Remark 3.4: (i) The ensemble average of the Burgers fluid velocity $\mathbb{E}(v^0(x,t))$ inherits the singularity structure of $\dot{X}^0(x,t)$ with caustics depending on the initial velocity field ∇S_0.

(ii) The distribution of Burgers fluid velocity depends only on the forces in this harmonic oscillator case.

(iii) Evidently, if there is resonance between the noise and the harmonic oscillator forces, there is no invariant measure for this problem as expected.

We emphasize here that the above results are true for any value of $\epsilon > 0$. We see in the next section to what extent the above results generalize to the nonlinear setting for small noise. Our main results will require new detailed estimates for this problem.

IV. GENERAL POTENTIALS WITH SMALL NOISE PERTURBATION

Having considered a special case in the preceding section we now demonstrate for small noise the closeness of the stochastic X_t, C_t, and H_t to their deterministic counterparts for more general potentials. Let X^ϵ, with ϵ highlighted, satisfy

$$d\dot{X}^\epsilon(x_0,s) = -\nabla c(X^\epsilon(x_0,s))ds - \epsilon\nabla k(X^\epsilon(x_0,s))dW_s, \tag{4.1}$$

with $X^\epsilon(x_0,0)=x_0$ and $\dot{X}^\epsilon(x_0,0)=\nabla S_0(x_0)$, for $0<s<t$. Abusing notation, let $X^0(x_0,s)=\Phi_s x_0$ be the deterministic version, where $\epsilon=0$, and let $\mathcal{G}$ be given by $\mathcal{G}_{ij}(x_0,s,u)=\{X_i^0(u),X_j^0(s)\}\theta(s-u)$, the first term being the Poisson bracket, the second a Heaviside function. The following elementary lemma is key.

Lemma 4.1: With X^0 defined as above, $\mathcal{G}$ satisfies the matrix Jacobi equation

$$\left(\frac{d^2}{ds^2} + \nabla^2 c(X^0(x_0,s))\right)\mathcal{G} = 0, \mathcal{G}(x_0,s_+,s) = 0, \quad \frac{d\mathcal{G}}{ds}(x_0,s,u)\bigg|_{s=u_+} = I.$$

Furthermore, $(\partial/\partial x_0^i)\mathcal{G}(x_0,s,u)$ satisfies

$$\frac{d^2}{ds^2}\frac{\partial}{\partial x_0^i}\mathcal{G}(x_0,s,u) + \sum_{j=1}^{n}\frac{\partial}{\partial X_j^0}\nabla^2 c(X^0(x_0,s))\left(\frac{\partial}{\partial x_0^i}X_j^0(x_0,s)\right)\mathcal{G}(x_0,s,u) + \nabla^2 c(X^0(x_0,s))\frac{\partial}{\partial x_0^i}\mathcal{G}(x_0,s,u) = 0 \tag{4.2}$$

and

$$\nabla_{x_0^i}\mathcal{G}(x_0,s_+,s) = 0, \qquad \frac{d}{ds}\nabla_{x_0^i}\mathcal{G}(x_0,s,u)\bigg|_{s=u_+} = 0. \tag{4.3}$$

Proof: A trivial computation using the properties of Poisson brackets. ■

We now come to one of our main results.

Theorem 4.2: *Subject to certain conditions on the continuity and boundedness of c and k and their derivatives, define*

$$\tilde{X}^{\epsilon}(x_0,s) = \Phi_s x_0 - \epsilon \int_0^s \mathcal{G}(x_0,s,u)\, \nabla\, k(\Phi_u x_0) \mathrm{d}W_u,$$

for $s \in [0,t]$. *Then there exists a constant* $M>0$ *such that for any* $\delta>0$ *and sufficiently small* $\epsilon>0$,

$$P\{\epsilon^{-\frac{3}{2}} |X^{\epsilon}(x_0,s) - \tilde{X}^{\epsilon}(x_0,s)| > \delta, \quad some \quad s \in [0,t]\} < \frac{M\epsilon^2}{\delta^4}, \tag{4.4}$$

and

$$P\{\epsilon^{-\frac{3}{2}} |\nabla X^{\epsilon}(x_0,s) - \nabla \tilde{X}^{\epsilon}(x_0,s)| > \delta, \quad \text{some} \quad s \in [0,t]\} < \frac{M\epsilon}{\delta^2}. \tag{4.5}$$

We have $X^{\epsilon}(x_0,s) - \tilde{X}^{\epsilon}(x_0,s) = o(\epsilon^{3/2})$, $\nabla X^{\epsilon}(x_0,s) - \nabla \tilde{X}^{\epsilon}(x_0,s) = \circ(\epsilon^{3/2})$ *as* $\epsilon \to 0$ *in probability.*

Proof: (i) We first prove (4.4). From the definition of $\tilde{X}^{\epsilon}(x_0,s)$ and Lemma 4.1, it is easy to see

$$\dot{\tilde{X}}^{\epsilon}(x_0,s) = \dot{\Phi}_s x_0 - \epsilon \int_0^s \frac{\partial}{\partial s} \mathcal{G}(x_0,s,u)\, \nabla\, k(\Phi_u x_0) \mathrm{d}W_u, \quad s \in [0,t].$$

Differentiating with respect to s again we have

$$\begin{aligned}
\mathrm{d}\dot{\tilde{X}}^{\epsilon}(x_0,s) &= -\, \nabla\, c(\Phi_s x_0)\mathrm{d}s - \epsilon \nabla\, k(\Phi_s x_0)\mathrm{d}W_s - \epsilon \int_0^s \frac{\partial^2}{\partial s^2} \mathcal{G}(x_0,s,u)\, \nabla\, k(\Phi_u x_0)\mathrm{d}W_u\, \mathrm{d}s \\
&= -\, \nabla\, c(\Phi_s x_0)\mathrm{d}s + \left(\nabla^2 c(\Phi_s x_0)\epsilon \int_0^s \mathcal{G}(x_0,s,u)\, \nabla\, k(\Phi_u x_0)\mathrm{d}W_u \right)\mathrm{d}s - \epsilon \nabla\, k(\Phi_s x_0)\mathrm{d}W_s.
\end{aligned}$$

It turns out that by Taylor's theorem, there exist ξ_1 and ξ_2 such that for $0 \leqslant s \leqslant t$,

$$\begin{aligned}
\mathrm{d}\dot{\tilde{X}}^{\epsilon}(x_0,s) = &-\, \nabla\, c\left(\Phi_s x_0 - \epsilon \int_0^s \mathcal{G}(x_0,s,u)\, \nabla\, k(\Phi_u x_0)\mathrm{d}W_u \right)\mathrm{d}s \\
&- \epsilon \nabla\, k\left(\Phi_s x_0 - \epsilon \int_0^s \mathcal{G}(x_0,s,u)\, \nabla\, k(\Phi_u x_0)\mathrm{d}W_u \right)\mathrm{d}W_s + \epsilon^2 \sum_{i,j=1}^{d} \frac{\partial^2}{\partial \xi_1^i \xi_1^j}\, \nabla\, c(\xi_1) \\
&\times \left(\int_0^s \mathcal{G}(x_0,s,u)\, \nabla\, k(\Phi_u x_0)\mathrm{d}W_u \right)_i \left(\int_0^s \mathcal{G}(x_0,s,u)\, \nabla\, k(\Phi_u x_0)\mathrm{d}W_u \right)_j \mathrm{d}s + \epsilon^2 \nabla^2 k(\xi_2) \\
&\times \left(\int_0^s \mathcal{G}(x_0,s,u)\, \nabla\, k(\Phi_u x_0)\mathrm{d}W_u \right)\mathrm{d}W_s \\
= &-\, \nabla\, c(\tilde{X}^{\epsilon}(x_0,s))\mathrm{d}s - \epsilon \nabla_{\tilde{X}^0} k(\tilde{X}^{\epsilon}(x_0,s))\mathrm{d}W_s + \epsilon^2 N_1(s)\mathrm{d}s + \epsilon^2 N_2(s)\mathrm{d}W_s.
\end{aligned}$$

Here N_1 and N_2 are given by

$$\begin{aligned}
N_1(s) &= \sum_{i,j=1}^{d} \frac{\partial^2}{\partial \xi_1^i \xi_1^j}\, \nabla\, c(\xi_1) \left(\int_0^s \mathcal{G}(x_0,s,u)\, \nabla\, k(\Phi_u x_0)\mathrm{d}W_u \right)_i \left(\int_0^s \mathcal{G}(x_0,s,u)\, \nabla\, k(\Phi_u x_0)\mathrm{d}W_u \right)_j, \\
N_2(s) &= \nabla^2 k(\xi_2) \int_0^s \mathcal{G}(x_0,s,u) \nabla_{X^0} k(\Phi_u x_0)\mathrm{d}W_u.
\end{aligned} \tag{4.6}$$

Now it is easy to see that

$$\begin{aligned}\tilde{X}^{\epsilon}(x_0,s) &= x_0 - s\,\nabla S_0(x_0) - \int_0^s \int_0^r \nabla c(\tilde{X}^{\epsilon}(x_0,u))\mathrm{d}u\ \mathrm{d}r - \epsilon \int_0^s \int_0^r \nabla k(\tilde{X}^{\epsilon}(x_0,u))\mathrm{d}W_u\ \mathrm{d}r \\ &\quad + \epsilon^2 \int_0^s \int_0^r N_1(u)\mathrm{d}u\ \mathrm{d}r + \epsilon^2 \int_0^s \int_0^r N_2(u)\mathrm{d}W_u\ \mathrm{d}r \\ &= x_0 - s\,\nabla S_0(x_0) - \int_0^s (s-r)\,\nabla c(\tilde{X}^{\epsilon}(x_0,r))\mathrm{d}r - \epsilon \int_0^s (s-r)\,\nabla k(\tilde{X}^{\epsilon}(x_0,r))\mathrm{d}W_r \\ &\quad + \epsilon^2 \int_0^s (s-r)N_1(r)\mathrm{d}r + \epsilon^2 \int_0^s (s-r)N_2(r)\mathrm{d}W_r. \end{aligned} \tag{4.7}$$

On the other hand, the solution of (4.1) can be represented by

$$X^{\epsilon}(x_0,s) = x_0 - s\,\nabla S_0(x_0) - \int_0^s (s-r)\,\nabla c(X^{\epsilon}(x_0,r))\mathrm{d}r - \epsilon \int_0^s (s-r)\,\nabla k(X^{\epsilon}(x_0,r))\mathrm{d}W_r. \tag{4.8}$$

Therefore it turns out that there exists $M_1 > 0$ such that

$$\begin{aligned}|\tilde{X}^{\epsilon}(x_0,s) - X^{\epsilon}(x_0,s)|^4 &= \Bigg| - \int_0^s (s-r)(\nabla c(\tilde{X}^{\epsilon}(x_0,r)) - \nabla c(X^{\epsilon}(x_0,r)))\mathrm{d}r - \epsilon \int_0^s (s-r)(\nabla k(\tilde{X}^{\epsilon}(x_0,r)) \\ &\quad - \nabla k(X^{\epsilon}(r)))\mathrm{d}W_r + \epsilon^2 \int_0^s (s-r)N_1(r)\mathrm{d}r + \epsilon^2 \int_0^s (s-r)N_2(r)\mathrm{d}W_r \Bigg|^4 \\ &\leqslant M_1 \Big| \int_0^s (s-r)(\nabla c(\tilde{X}^{\epsilon}(x_0,r)) - \nabla c(X^{\epsilon}(x_0,r)))\mathrm{d}r\Big|^4 + M_1\epsilon^4 \Big| \int_0^s (s-r) \\ &\quad \times (\nabla k(\tilde{X}^{\epsilon}(x_0,r)) - \nabla k(X^{\epsilon}(x_0,r)))\mathrm{d}W_r\Big|^4 + M_1\epsilon^8 \Big| \int_0^s (s-r)N_1(r) \\ &\quad \times \mathrm{d}r\Big|^4 + M_1\epsilon^8 \Big| \int_0^s (s-r)N_2(r)\mathrm{d}W_r\Big|^4. \end{aligned} \tag{4.9}$$

Now using Hölder's inequality, $E(\int_0^s f(r)\mathrm{d}W_r)^4 \leqslant M_2 s \int_0^s Ef^4(r)\mathrm{d}r$ for a constant $M_2 > 0$, and the Lipschitz continuity we have

$$\begin{aligned}E \sup_{0\leqslant s\leqslant t} |\tilde{X}^{\epsilon}(x_0,s) - X^{\epsilon}(x_0,s)|^4 &\leqslant M_1 \left(\int_0^s (s-r)^{\frac{4}{3}}\mathrm{d}r \right)^3 E \int_0^s \sup_{0\leqslant r\leqslant s} |\nabla c(\tilde{X}^{\epsilon}(x_0,r)) - \nabla c(X^{\epsilon}(x_0,r))|^4\ \mathrm{d}r \\ &\quad + M_1 M_2 \epsilon^4 s \int_0^s (s-r)^4 E \sup_{0\leqslant r\leqslant s} |\nabla k(\tilde{X}^{\epsilon}(x_0,r)) - \nabla k(X^{\epsilon}(r))|^4\ \mathrm{d}r \\ &\quad + M_1\epsilon^8 \left(\int_0^s (s-r)^{\frac{4}{3}}\ \mathrm{d}r \right)^3 \int_0^s E \sup_{0\leqslant r\leqslant s} |N_1(r)|^4\ \mathrm{d}r + M_1 M_2 \epsilon^8 s \\ &\quad \times \int_0^s (s-r)^4 E \sup_{0\leqslant r\leqslant s} |N_2(r)|^4\ \mathrm{d}r \\ &\leqslant M_3 s^7 L^4 \int_0^s E \sup_{0\leqslant r\leqslant s} |\tilde{X}^{\epsilon}(x_0,r) - X^{\epsilon}(x_0,r)|^4\ \mathrm{d}r + M_3 s^4 \epsilon^4 L^4 \end{aligned}$$

$$\times \int_0^s E \sup_{0\leqslant r\leqslant s} |\tilde{X}^\epsilon(x_0,r) - X^\epsilon(r)|^4 \, \mathrm{d}r + M_3 \epsilon^8 s^7 \int_0^s E \sup_{0\leqslant r\leqslant s} |N_1(r)|^4 \mathrm{d}r$$

$$+ M_3 s^4 \epsilon^8 \int_0^s E \sup_{0\leqslant r\leqslant s} |N_2(r)|^4 \, \mathrm{d}r. \tag{4.10}$$

Here L is a Lipschitz constant of ∇c and ∇k and M_3 is a constant. But using inequality $E(\int_0^s f(r)\mathrm{d}W_r)^8 \leqslant M_4 s^{4/3} \int_0^s E(f(r))^8 \mathrm{d}r$ for a $M_4 > 0$, and taking $M_5 = n \max_{l,\xi_1,\xi_2}\{|\text{eigenvalue of the Hessian}(\nabla^2(\nabla_l c(\xi_1)))|, |\text{ eigenvalue of the Hessian } (\nabla^2(k(\xi_2)))|\}$, then

$$E \sup_{0\leqslant s\leqslant t} |N_1(r)|^4 \leqslant M_4 M_5 r^{\frac{4}{3}} \int_0^r \sup_{0\leqslant r\leqslant s} < \mathcal{G}(x_0,s,u) \nabla k(\Phi_u x_0), \mathcal{G}(x_0,s,u) \nabla k(\Phi_u x_0) >^4 \, \mathrm{d}u \leqslant M_6 r^{\frac{4}{3}}, \tag{4.11}$$

and

$$E \sup_{0\leqslant s\leqslant t} (N_2(r))^4 = M_4 M_2 r \int_0^r \sup_{0\leqslant r\leqslant s} < \mathcal{G}(x_0,s,u) \nabla k(\Phi_u x_0), G(x_0,s,u) \nabla k(\Phi_u x_0) >^2 \, \mathrm{d}u \leqslant M_6 r. \tag{4.12}$$

Here $M_6 > 0$ is a constant.

It follows from (4.10) that there exists $M_7 > 0$ such that

$$E \sup_{0\leqslant s\leqslant t} (\tilde{X}^\epsilon(x_0,s) - X^\epsilon(x_0,s))^4 \leqslant M_3 s^7 L^4 \int_0^s E \sup_{0\leqslant r\leqslant s} (\tilde{X}^\epsilon(x_0,r) - X^\epsilon(x_0,r))^4 \, \mathrm{d}r$$

$$+ M_3 s^4 \epsilon^4 L^4 \int_0^s E \sup_{0\leqslant r\leqslant s} (\tilde{X}^\epsilon(x_0,r) - X^\epsilon(x_0,r))^4 \, \mathrm{d}r + M_7 s^{\frac{28}{3}} \epsilon^8 + M_7 s^6 \epsilon^8. \tag{4.13}$$

By using the Gronwall inequality we know that for $0 \leqslant s \leqslant t$,

$$E \sup_{0\leqslant s\leqslant t} (\tilde{X}^\epsilon(x_0,s) - X^\epsilon(x_0,s))^4 \leqslant M \epsilon^8, \tag{4.14}$$

for a constant $M > 0$. Then (4.4) follows from the Chebyshev inequality. Following a similar method, one can prove that $0 \leqslant s \leqslant t$,

$$E \sup_{0\leqslant s\leqslant t} (X(x_0,s))^4 \leqslant M, \tag{4.15}$$

for a constant $M > 0$.

(ii) Now we prove (4.5). Denote $\nabla_i = \partial / \partial x_0^i$. From the definition of $\tilde{X}^\epsilon(x_0,s)$ we know

$$\nabla_i \tilde{X}^\epsilon(x_0,s) = \nabla_i \Phi_s x_0 - \epsilon \int_0^s \mathcal{G}(x_0,s,u) \nabla^2 k(\Phi_u x_0) \nabla_i \Phi_u x_0 \, \mathrm{d}W_u - \epsilon \int_0^s \nabla_i \mathcal{G}(x_0,s,u) \nabla k(\Phi_u x_0) \mathrm{d}W_u.$$

Thus, applying Lemma 4.1 again we have

$$\frac{d}{\mathrm{d}s}\nabla_i\tilde{X}^{\epsilon}(x_0,s) = \nabla_i\dot{\Phi}_s x_0 - \epsilon\int_0^s \frac{\partial}{\partial s}\mathcal{G}(x_0,s,u)\nabla^2 k(\Phi_u x_0)\nabla_i\Phi_u x_0\ \mathrm{d}W_u$$

$$-\epsilon\int_0^s \frac{\partial}{\partial s}\nabla_i\mathcal{G}(x_0,s,u)\ \nabla\, k(\Phi_u x_0)\mathrm{d}W_u.$$

Then differentiating again and using Lemma 4.1 we have

$$\begin{aligned}
d\frac{d}{\mathrm{d}s}\nabla_i\tilde{X}^{\epsilon}(x_0,s) &= -\nabla^2 c(\Phi_s x_0)(\nabla_i\Phi_s x_0)\mathrm{d}s - \epsilon\nabla^2 k(\Phi_s x_0)(\nabla_i\Phi_s x_0)\mathrm{d}W_s \\
&\quad -\epsilon\int_0^s \frac{\partial^2}{\partial s^2}\mathcal{G}(x_0,s,u)\nabla^2 k(\Phi_u x_0)\nabla_i\Phi_u x_0\ \mathrm{d}W_u\ \mathrm{d}s \\
&\quad -\epsilon\int_0^s \left(\frac{\partial^2}{\partial s^2}\nabla_i\mathcal{G}(x_0,s,u)\right)\nabla\, k(\Phi_u x_0)\mathrm{d}W_u\ \mathrm{d}s \\
&= -\nabla^2 c(\Phi_s x_0)(\nabla_i\Phi_s x_0)\mathrm{d}s + \nabla^2 c(\Phi_s x_0)\epsilon\int_0^s \mathcal{G}(x_0,s,u)\nabla^2 k(\Phi_u x_0)\nabla_i\Phi_u x_0 \\
&\quad \times\mathrm{d}W_u\ \mathrm{d}s + \sum_{j=1}^{d}\frac{\partial}{\partial X_j}\nabla^2 c(\Phi_s x_0)(\nabla_i\Phi_s^j x_0)\epsilon\int_0^s \mathcal{G}(x_0,s,u)\ \nabla\, k(\Phi_u x_0)\mathrm{d}W_u\ \mathrm{d}s \\
&\quad + \nabla^2 c(\Phi_s x_0)\epsilon\int_0^s (\nabla_i\mathcal{G}(x_0,s,u))\ \nabla\, k(\Phi_u x_0)\mathrm{d}W_u\ \mathrm{d}s - \epsilon\nabla^2 k(\Phi_s x_0)(\nabla_i\Phi_s x_0)\mathrm{d}W_s \\
&= -\nabla^2 c(\Phi_s x_0)\nabla_i\tilde{X}^{\epsilon}(x_0,s)\mathrm{d}s + \sum_{j=1}^{d}\frac{\partial}{\partial X_j}\nabla^2 c(\Phi_s x_0)(\nabla_i\Phi_s^j x_0)\epsilon \\
&\quad \times\int_0^s \mathcal{G}(x_0,s,u)\ \nabla\, k(\Phi_u x_0)\mathrm{d}W_u\ \mathrm{d}s - \epsilon\nabla^2 k(\Phi_s x_0)(\nabla_i\Phi_s x_0)\mathrm{d}W_s.
\end{aligned}$$

Now using Taylor's theorem we know that there exist ξ_3 and ξ_4 such that

$$\begin{aligned}
d\frac{d}{\mathrm{d}s}\nabla_i\tilde{X}^{\epsilon}(x_0,s) &= -\nabla^2 c\left(\Phi_s x_0 - \epsilon\int_0^s \mathcal{G}(x_0,s,u)\ \nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)\nabla_i\tilde{X}^{\epsilon}(x_0,s)\mathrm{d}s \\
&\quad -\epsilon\nabla^2 k\left(\Phi_s x_0 - \epsilon\int_0^s \mathcal{G}(x_0,s,u)\ \nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)\nabla_i\tilde{X}^{\epsilon}(x_0,s)\mathrm{d}W_s \\
&\quad -\epsilon^2\sum_{j=1}^{d}\frac{\partial}{\partial X_j}\nabla^2 c(\Phi_s x_0)\left[\int_0^s \mathcal{G}(x_0,s,u)\nabla^2 k(\Phi_u x_0)\nabla_i X^0(x_0,u)\mathrm{d}W_u\right. \\
&\quad \left.+\int_0^s \nabla_i\mathcal{G}(x_0,s,u)\ \nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right]\times\left(\int_0^s \mathcal{G}(x_0,s,u)\ \nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)_j\mathrm{d}s \\
&\quad +\epsilon^2\sum_j\sum_l (\nabla_{\xi_3^j}\nabla_{\xi_3^l}\nabla^2 c(\xi_3))\left(\int_0^s \mathcal{G}(x_0,s,u)\ \nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)_j \\
&\quad \times\left(\int_0^s \mathcal{G}(x_0,s,u)\ \nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)_l\nabla_i\tilde{X}^{\epsilon}(x_0,s)\mathrm{d}s - \epsilon^2\sum_j \nabla_{\xi_4^j}\nabla^2 k(\xi_4) \\
&\quad \times\left(\int_0^s \mathcal{G}(x_0,s,u)\ \nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)_j\nabla_i(\tilde{X}^{\epsilon}(x_0,s))\mathrm{d}W_s \\
&= -\nabla^2 c(\tilde{X}^{\epsilon}(x_0,s))\nabla_i\tilde{X}^{\epsilon}(x_0,s)\mathrm{d}s - \epsilon\nabla^2 k(\tilde{X}^{\epsilon}(x_0,s))\nabla_i\tilde{X}^{\epsilon}(x_0,s)\mathrm{d}W_s
\end{aligned}$$

$$+ \epsilon^2 N_3(s)\mathrm{d}s + \epsilon^2 N_4(s)\mathrm{d}W_s, \quad s \in [0,t].$$

Here N_3 and N_4 are given by

$$\begin{aligned} N_3(s) = &- \sum_{j=1}^{d} \frac{\partial}{\partial X_j} \nabla^2 c(\Phi_s x_0) \Bigg[\int_0^s \mathcal{G}(x_0,s,u) \nabla^2 k(\Phi_u x_0) \nabla_i X^0(x_0,u) \mathrm{d}W_u \\ &+ \int_0^s \nabla_i \mathcal{G}(x_0,s,u) \nabla k(\Phi_u x_0) \mathrm{d}W_u \Bigg] \Bigg(\int_0^s \mathcal{G}(x_0,s,u) \nabla k(\Phi_u x_0) \mathrm{d}W_u \Bigg)_j + \sum_j \sum_l (\nabla_{\xi_3^{lj}} \nabla_{\xi_3^{jl}} c''(\xi_3)) \\ &\times \Bigg(\int_0^s \mathcal{G}(x_0,s,u) \nabla k(\Phi_u x_0) \mathrm{d}W_u \Bigg)_j \Bigg(\int_0^s \mathcal{G}(x_0,s,u) \nabla k(\Phi_u x_0) \mathrm{d}W_u \Bigg)_l \nabla_i \tilde{X}^\epsilon(x_0,s), \\ N_4(s) = &- \sum_j \nabla_{\xi_4^{jj}} \nabla^2 k(\xi_4) \Bigg(\int_0^s \mathcal{G}(x_0,s,u) \nabla k(\Phi_u x_0) \mathrm{d}W_u \Bigg)_j \nabla_i \tilde{X}^\epsilon(x_0,s). \end{aligned} \tag{4.16}$$

Using the Fubini theorem, it is easy to see that

$$\begin{aligned} \nabla_i \tilde{X}^\epsilon(x_0,s) &= e_i - s\nabla_i \nabla S_0(x_0) - \int_0^s \int_0^r \nabla^2 c(\tilde{X}^\epsilon(x_0,u))\mathrm{d}u \nabla_i \tilde{X}^\epsilon(x_0,r)\mathrm{d}r - \epsilon \int_0^s \int_0^r \nabla^2 k(\tilde{X}^\epsilon(x_0,u)) \\ &\quad \times \mathrm{d}W_u \nabla_i \tilde{X}^\epsilon(x_0,r)\mathrm{d}r + \epsilon^2 \int_0^s \int_0^r N_3(u)\mathrm{d}u \, \mathrm{d}r + \epsilon^2 \int_0^s \int_0^r N_4(u)\mathrm{d}W_u \, \mathrm{d}r \\ &= e_i - s\nabla_i \nabla S_0(x_0) - \int_0^s (s-r)\nabla^2 c(\tilde{X}^\epsilon(x_0,r)) \nabla_i \tilde{X}^\epsilon(x_0,r)\mathrm{d}r \\ &\quad - \epsilon \int_0^s (s-r)\nabla^2 k(\tilde{X}^\epsilon(x_0,r)) \nabla_i \tilde{X}^\epsilon(x_0,r)\mathrm{d}W_r \\ &\quad + \epsilon^2 \int_0^s (s-r) N_3(r)\mathrm{d}r + \epsilon^2 \int_0^s (s-r) N_4(r)\mathrm{d}W_r. \end{aligned} \tag{4.17}$$

Here $e_i = (0,0,\ldots,0,1,0,\ldots,0)$.

On the other hand, differentiating (4.8) we have

$$\begin{aligned} \nabla_i X^\epsilon(x_0,s) &= e_i - s\nabla_i \nabla S_0(x_0) - \int_0^s (s-r)\nabla^2 c(X^\epsilon(x_0,r))(\nabla_i X^\epsilon(x_0,r))\mathrm{d}r - \epsilon \int_0^s (s-r)\nabla^2 k(X^\epsilon(x_0,r)) \\ &\quad \times (\nabla_i X^\epsilon(x_0,r))\mathrm{d}W_r. \end{aligned} \tag{4.18}$$

Note here $\nabla_i \nabla S_0, \nabla^2 c, \nabla^2 k$ are bounded. So it is easy to prove there exists $M_1 > 0$ such that

$$E \sup_{0\leqslant s\leqslant t} |\nabla_i X^\epsilon(x_0,s)|^4 \leqslant M_1. \tag{4.19}$$

Therefore it turns out that

$$\begin{aligned}|\nabla_i \tilde{X}^\epsilon(x_0,s) - \nabla_i X^\epsilon(x_0,s)|^2 = \Bigg| &- \int_0^s (s-r)(\nabla^2 c(X^\epsilon(x_0,r)) - \nabla^2 c(\tilde{X}^\epsilon(x_0,r)))\nabla_i X^\epsilon(x_0,r)\mathrm{d}r - \int_0^s (s-r) \\ &\times (\nabla^2 c(\tilde{X}^\epsilon(x_0,r))(\nabla_i X^\epsilon(x_0,r) - \nabla_i \tilde{X}^\epsilon(x_0,r))\mathrm{d}r - \epsilon \int_0^s (s-r)(\nabla^2 k(X^\epsilon(x_0,r)) \\ &- \nabla^2 k(\tilde{X}^\epsilon(x_0,r)))\nabla_i X^\epsilon(x_0,r)\mathrm{d}W_r - \epsilon \int_0^s (s-r)\nabla^2 k(\tilde{X}^\epsilon(x_0,r)(\nabla_i X^\epsilon(x_0,r)) \\ &- \nabla_i \tilde{X}^\epsilon(x_0,r))\mathrm{d}W_r + \epsilon^2 \int_0^s (s-r)N_3(r)\mathrm{d}r + \epsilon^2 \int_0^s (s-r)N_4(r)\mathrm{d}W_r \Bigg|^2. \end{aligned} \tag{4.20}$$

This leads to, for any $0\leqslant s\leqslant t$,

$$\begin{aligned}E \sup_{0\leqslant s\leqslant t} |\nabla_i \tilde{X}^\epsilon(x_0,s) - \nabla_i X^\epsilon(x_0,s)|^2 \leqslant\ & 6E \sup_{0\leqslant s\leqslant t} \left| \int_0^s (s-r)(\nabla^2 c(\tilde{X}^\epsilon(x_0,r)) - \nabla^2 c(X^\epsilon(x_0,r)))\nabla_i X^\epsilon(x_0,r)\mathrm{d}r \right|^2 \\ &+ 6E \sup_{0\leqslant s\leqslant t} \left| \int_0^s (s-r)(\nabla^2 c(\tilde{X}^\epsilon(x_0,r))(\nabla_i X^\epsilon(x_0,r) - \nabla_i \tilde{X}^\epsilon(x_0,r))\mathrm{d}r \right|^2 \\ &+ 6\epsilon^2 E \sup_{0\leqslant s\leqslant t} \Bigg| \int_0^s (s-r)(\nabla^2 k(\tilde{X}^\epsilon(x_0,r)) \\ &- \nabla^2 k(X^\epsilon(r)))\nabla_i X^\epsilon(x_0,r)\mathrm{d}W_r \Bigg|^2 + 6\epsilon^2 E \sup_{0\leqslant s\leqslant t} \Bigg| \int_0^s (s \\ &- r)\nabla^2 k(\tilde{X}^\epsilon(x_0,r))(\nabla_i X^\epsilon(x_0,r) - \nabla_i X^\epsilon(x_0,r))\mathrm{d}W_r \Bigg|^2 \\ &+ 6\epsilon^4 E \sup_{0\leqslant s\leqslant t} \left| \int_0^s (s-r)N_3(r)\mathrm{d}r \right|^2 + 6\epsilon^4 E \sup_{0\leqslant s\leqslant t} \Bigg| \int_0^s (s \\ &- r)N_4(r)\mathrm{d}W_r \Bigg|^2. \end{aligned} \tag{4.21}$$

Denote by $M_2 = \sup_{x\in\mathbb{R}^d}\{|\text{eigenvalue of } \nabla^2 c(x))|, |\text{eigenvalue of } \nabla^2 k(x))|\}$ and by L the Lipschitz constant of $\nabla^2 c$ and $\nabla^2 k$. So by the Hölder inequality and the Lipschitz continuity we have

$$\begin{aligned}&E \sup_{0\leqslant s\leqslant t} |\nabla_i \tilde{X}^\epsilon(x_0,s) - \nabla_i X^\epsilon(x_0,s)|^2 \\ &\quad\leqslant 6E \sup_{0\leqslant s\leqslant t} \int_0^s (s-r)^2 |\nabla^2 c(\tilde{X}^\epsilon(x_0,r)) - \nabla^2 c(X^\epsilon(x_0,r))|^2 \mathrm{d}r \\ &\quad\quad\times \int_0^s |\nabla_i X^\epsilon(x_0,r)|^2\ \mathrm{d}r + 6E \sup_{0\leqslant s\leqslant t} \int_0^s (s-r)^2\ \mathrm{d}r \\ &\quad\quad\times \int_0^s |\nabla^2 c(\tilde{X}^\epsilon(x_0,r))(\nabla_i X^\epsilon(x_0,r) - \nabla_i \tilde{X}^\epsilon(x_0,r))|^2\ \mathrm{d}r + 6\epsilon^2 E \sup_{0\leqslant s\leqslant t} \int_0^s (s-r)^2 |\nabla^2 k(\tilde{X}^\epsilon(x_0,r))\end{aligned}$$

$$
\begin{aligned}
&- \nabla^2 k(X^\epsilon(r)))\nabla_i X^\epsilon(x_0,r)^2\,\mathrm{d}r + 6\epsilon^2 E \sup_{0\leqslant s\leqslant t}\int_0^s (s-r)^2 |\nabla^2 k(\widetilde{X}^\epsilon(x_0,r))(\nabla_i X^\epsilon(x_0,r) - \nabla_i \widetilde{X}^\epsilon(x_0,r))|^2\,\mathrm{d}r \\
&+ 6\epsilon^4 E \sup_{0\leqslant s\leqslant t}\int_0^s (s-r)^2\,\mathrm{d}r \int_0^s |N_3(r)|^2\,\mathrm{d}r + 6\epsilon^4 E \sup_{0\leqslant s\leqslant t}\int_0^s (s-r)^2 |N_4(r)|^2\,\mathrm{d}r \leqslant 6\Bigg\{ E \sup_{0\leqslant s\leqslant t}\Bigg(\int_0^s (s \\
&- r)^2 |\nabla^2 c(\widetilde{X}^\epsilon(x_0,r)) - \nabla^2 c(X^\epsilon(x_0,r))|^2\,\mathrm{d}r\Bigg)^2\Bigg\}^{1/2} \times \Bigg\{ E \sup_{0\leqslant s\leqslant t}\Bigg(\int_0^s (\nabla_i X^\epsilon(x_0,r))^2\,\mathrm{d}r\Bigg)^2\Bigg\}^{1/2} \\
&+ 2M_2 s^3 \int_0^s E \sup_{0\leqslant r\leqslant s} |\nabla_i X^\epsilon(x_0,r) - \nabla_i X^\epsilon(x_0,r)|^2\,\mathrm{d}r + 6\epsilon^2 \\
&\times \int_0^s (s-r)^2 \{E \sup_{0\leqslant r\leqslant s} (\nabla^2 k(\widetilde{X}^\epsilon(x_0,r)) - \nabla^2 k(X^\epsilon(r)))^4\}^{1/2} \{E \sup_{0\leqslant r\leqslant s} (\nabla_i X^\epsilon(x_0,r))^4\}^{1/2}\,\mathrm{d}r \\
&+ 6\epsilon^2 M_2 s^2 E \int_0^s E \sup_{0\leqslant r\leqslant s} (\nabla_i X^\epsilon(x_0,r) - \nabla_i \widetilde{X}^\epsilon(x_0,r))^2\,\mathrm{d}r + 2\epsilon^4 s^3 \int_0^s E \sup_{0\leqslant r\leqslant s} |N_3(r)|^2\,\mathrm{d}r \\
&+ 6s^2\epsilon^4 \int_0^s E \sup_{0\leqslant r\leqslant s} |N_4(r)|^2\,\mathrm{d}r. \qquad (4.22)
\end{aligned}
$$

This leads to

$$
\begin{aligned}
E \sup_{0\leqslant s\leqslant t} |\nabla_i \widetilde{X}^\epsilon(x_0,s) - \nabla_i X^\epsilon(x_0,s)|^2 \leqslant 6L^2 &\Bigg\{ \int_0^s (s-r)^4\,\mathrm{d}r \int_0^s E \sup_{0\leqslant r\leqslant s} |\widetilde{X}^\epsilon(x_0,r) - X^\epsilon(x_0,r)|^4\,\mathrm{d}r \Bigg\}^{1/2} \\
&\times \Bigg\{ \int_0^s E \sup_{0\leqslant r\leqslant s} |\nabla_i X^\epsilon(x_0,r)|^4\,\mathrm{d}r \Bigg\}^{1/2} + 6L^2\epsilon^2 \int_0^s (s-r)^2 \\
&\times \{E \sup_{0\leqslant r\leqslant s} |\widetilde{X}^\epsilon(x_0,r) - X^\epsilon(r)|^4\}^{1/2} \times \{E \sup_{0\leqslant r\leqslant s} |\nabla_i X^\epsilon(x_0,r)|^4\}^{1/2}\,\mathrm{d}r \\
&+ 2M_2 s^3 \int_0^s E|\nabla_i X^\epsilon(x_0,r) - \nabla_i \widetilde{X}^\epsilon(x_0,r)|^2\,\mathrm{d}r \\
&+ 6\epsilon^2 M_2 s^2 \int_0^s E \sup_{0\leqslant r\leqslant s} |\nabla_i X^\epsilon(x_0,r) - \nabla_i \widetilde{X}^\epsilon(x_0,r))^2\,\mathrm{d}r \\
&+ 2\epsilon^4 s^3 \int_0^s E \sup_{0\leqslant r\leqslant s} |N_3(r)|^2\,\mathrm{d}r + 6s^2\epsilon^4 \int_0^s E \sup_{0\leqslant r\leqslant s} |N_4(r)|^2\,\mathrm{d}r. \qquad (4.23)
\end{aligned}
$$

Note (4.19). Similar to the estimate of N_1 and N_2, we can prove that there exists $M_3 > 0$ such that

$$
E \sup_{0\leqslant s\leqslant t} |N_3(r)|^2 \leqslant M_3 < \infty \qquad (4.24)
$$

and

$$
E \sup_{0\leqslant s\leqslant t} |N_4(r)|^2 \leqslant M_3 < \infty. \qquad (4.25)
$$

It follows from (4.14) and (4.23)–(4.25) that there exists $M_4 > 0$ such that

$$E \sup_{0\leqslant s\leqslant t} |\nabla_i \tilde{X}^\epsilon(x_0,s) - \nabla_i X^\epsilon(x_0,s)|^2 \leqslant M_4 s^3 \int_0^s E \sup_{0\leqslant r\leqslant s} |\nabla_i \tilde{X}^\epsilon(x_0,r) - \nabla_i X^\epsilon(x_0,r)|^2 \, dr + M_4 \epsilon^2 \int_0^s E \sup_{0\leqslant r\leqslant s} |\nabla_i \tilde{X}^\epsilon(x_0,r) - \nabla_i X^\epsilon(x_0,r)|^2 \, dr + M_4 \epsilon^4. \tag{4.26}$$

By using the Gronwall inequality we know that

$$E \sup_{0\leqslant s\leqslant t} |\nabla_i \tilde{X}^\epsilon(x_0,s) - \nabla_i X^\epsilon(x_0,s)|^2 \leqslant M\epsilon^4, \tag{4.27}$$

for a constant $M>0$. Then (4.5) follows from Chebyshev inequality. ■

A. Behavior of the caustic

Define for any given $0\leqslant T<\infty$,

$$\Omega_0 = \{\omega \in \Omega: \epsilon^{-\frac{3}{2}} \sup_{x_0\in\mathbb{R}^d} |\nabla X^\epsilon(x_0,s) - \nabla \tilde{X}^\epsilon(x_0,s)| < \delta \text{ for all } s \in [0,T]\}.$$

Then from Theorem 4.2

$$P\{\Omega_0\} > 1 - \frac{M\epsilon}{\delta^2}.$$

Now we define for each $\omega \in \Omega_0$.

In the case of the caustic C_t we define

$$\mathcal{D}^\epsilon_{\text{pre}} = \{(t,x_0): \text{Det } \nabla_{x_0} X^\epsilon_t(x_0) \neq 0, 0 \leqslant t \leqslant T\},$$

$$\mathcal{D}_{\text{pre}} = \{(t,x_0): \text{Det } \nabla_{x_0} \Phi_t x_0 \neq 0, 0 \leqslant t \leqslant T\}.$$

Lemma 4.3: As $\epsilon\to 0$, $[0,T]\times\mathbb{R}^d - \mathcal{D}^\epsilon_{\text{pre}} \to [0,T]\times\mathbb{R}^d - \mathcal{D}_{\text{pre}}$ *in probability for any given* $T>0$. *That is to say the precaustic surface of the stochastic dynamics converges to the precaustic surface of the classical mechanics as* $\epsilon\to 0$ *in probability*.

Proof: From Lemma 4.1, *it is easy to see that for each* $\omega \in \Omega_0$,

$$\nabla_{x_0} X^\epsilon(x_0,s) = \nabla \Phi_s x_0 - \epsilon \int_0^s \mathcal{G}(x_0,s,u) \nabla^2 k(\Phi_u x_0) \nabla_{x_0} \Phi_u x_0 \, dW_u + o(\epsilon).$$

So if $\text{Det}(\nabla\Phi_s x_0) \neq 0$, then for sufficiently small ϵ, $\text{Det}(\nabla X^\epsilon(x_0,s)) \neq 0$. That is to say, $D^\epsilon_{\text{pre}} \to D_{\text{pre}}$ as $\epsilon\to 0$ in probability. So as $\epsilon\to 0$, $[0,T]\times\mathbb{R}^d - \mathcal{D}^\epsilon_{\text{pre}} \to [0,T]\times\mathbb{R}^d - \mathcal{D}_{\text{pre}}$ in probability. ■

Theorem 4.4: *Denote for any given* $T>0$,

$$\mathcal{D}^\epsilon = \{(t,x): \text{Det } (\nabla (X^\epsilon)^{-1}_t x) \neq 0, 0 \leqslant t \leqslant T\},$$

$$\mathcal{D} = \{(t,x): \text{Det}(\nabla \Phi^{-1}_t x) \neq 0, 0 \leqslant t \leqslant T\}.$$

Then $[0,T]\times\mathbb{R}^d - \mathcal{D}^\epsilon \to [0,T]\times\mathbb{R}^d - \mathcal{D}$, *as* $\epsilon\to 0$. *That is to say the caustic surface of the stochastic dynamics with noise converges in probability to the caustic surface of the classical mechanics without noise as* $\epsilon\to 0$.

Proof: Denote by $\mathcal{D}^\epsilon_{\text{pre}}(s)$ a projection of $\mathcal{D}^\epsilon_{\text{pre}}$ on $\mathbb{R}^d$ such that $(s, \mathcal{D}^\epsilon_{\text{pre}}(s)) \subset \mathcal{D}^\epsilon_{\text{pre}}$. So

$$\mathcal{D}^\epsilon = \{(s, X_s^\epsilon(\mathcal{D}_{\text{pre}}^\epsilon(s)), \text{all } s\}. \tag{4.28}$$

But

$$X_s^\epsilon(\mathcal{D}_{\text{pre}}^\epsilon(s)) = X_s(\mathcal{D}_{\text{pre}}^\epsilon(s)) + (X_s^\epsilon(\mathcal{D}_{\text{pre}}^\epsilon(s)) - X_s(\mathcal{D}_{\text{pre}}^\epsilon(s))). \tag{4.29}$$

But from Lemma 4.1 and Lemma 4.3, as $\epsilon \to 0$ in probability,

$$X_s(\mathcal{D}_{\text{pre}}^\epsilon(s)) \to X_s(\mathcal{D}_{\text{pre}}(s)) \tag{4.30}$$

and

$$X_s^\epsilon(\mathcal{D}_{\text{pre}}^\epsilon(s)) - X_s(\mathcal{D}_{\text{pre}}^\epsilon(s)) \to 0. \tag{4.31}$$

Therefore $X_s^\epsilon(\mathcal{D}_{\text{pre}}^\epsilon(s)) \to X_s(\mathcal{D}_{\text{pre}}^\epsilon(s))$, i.e., $\mathcal{D}^\epsilon(s) \to \mathcal{D}(s)$. So $\mathcal{D}^\epsilon \to \mathcal{D}$. ■

B. Behavior of the wavefront

To characterize the wavefront H_t we must consider the Hamilton principal function $S^\epsilon(x,t)$ where we have, once again, emphasized the ϵ dependence.

Theorem 4.5: *Let ϕ_s be the minimizer of*

$$\frac{1}{2}\int_0^t |\dot{\phi}_s|^2 \, \mathrm{d}s + S_0(\phi_t) - \int_0^t c(\phi_s)\mathrm{d}s,$$

satisfying $\phi_t = x$ and ϕ_s^ϵ be the minimizer of $\frac{1}{2}\int_0^t |\dot{\phi}_s^\epsilon|^2 \, \mathrm{d}s + S_0(\phi_t^\epsilon) - \int_0^t c(\phi_s^\epsilon)\mathrm{d}s - \epsilon\int_0^t k(\phi_s^\epsilon)\mathrm{d}W_s$, satisfying $\phi_t^\epsilon = x$ for almost all $\omega \in \Omega$. Then we have for almost all $\omega \in \Omega$

$$S(x,t) - \epsilon\int_0^t k(\phi_s^\epsilon)\mathrm{d}W_s \leqslant S^\epsilon(x,t) \leqslant S(x,t) - \epsilon\int_0^t k(\phi_s)\mathrm{d}W_s. \tag{4.32}$$

In particular, as $\epsilon \to 0$, $S^\epsilon(x,t) \to S(x,t)$ a.s.

Furthermore, for the classical mechanics, assume there exists a unique x_0 for fixed t and x such that $\Phi_t x_0 = x$. The random wavefront for the heat equation has (x,t) equation

$$S^0(x,t) = \epsilon\int_0^t k(\Phi_s x_0)\mathrm{d}W_s + o(\epsilon),$$

where $S^0(x,t)$ is Hamilton's principal function for the path $X^0(x,t)(s)$.

Proof: By the definition of ϕ_s and ϕ_s^ϵ, it is easy to see for almost all ω,

$$\frac{1}{2}\int_0^t |\dot{\phi}_s^\epsilon|^2 \, \mathrm{d}s + S_0(\phi_t^\epsilon) - \int_0^t c(\phi_s^\epsilon)\mathrm{d}s \geqslant \frac{1}{2}\int_0^t |\dot{\phi}_s|^2 \, \mathrm{d}s + S_0(\phi_t) - \int_0^t c(\phi_s)\mathrm{d}s, \tag{4.33}$$

and

$$\begin{aligned}\frac{1}{2}\int_0^t |\dot{\phi}_s|^2 \, \mathrm{d}s + S_0(\phi_t) - \int_0^t c(\phi_s)\mathrm{d}s - \epsilon\int_0^t k(\phi_s)\mathrm{d}W_s \\ \geqslant \frac{1}{2}\int_0^t |\dot{\phi}_s^\epsilon|^2 \, \mathrm{d}s + S_0(\phi_t^\epsilon) - \int_0^t c(\phi_s^\epsilon)\mathrm{d}s - \epsilon\int_0^t k(\phi_s^\epsilon)\mathrm{d}W_s.\end{aligned} \tag{4.34}$$

It turns out that

$$\frac{1}{2}\int_0^t |\dot{\phi}_s|^2 \, \mathrm{d}s + S_0(\phi_t) - \int_0^t c(\phi_s)\mathrm{d}s - \epsilon \int_0^t k(\phi_s)\mathrm{d}W_s$$
$$\geqslant \frac{1}{2}\int_0^t |\dot{\phi}^\epsilon_s|^2 \, \mathrm{d}s + S_0(\phi^\epsilon_t) - \int_0^t c(\phi^\epsilon_s)\mathrm{d}s - \epsilon \int_0^t k(\phi^\epsilon_s)\mathrm{d}W_s$$
$$\geqslant \frac{1}{2}\int_0^t |\dot{\phi}_s|^2 \, \mathrm{d}s + S_0(\phi_t) - \int_0^t c(\phi_s)\mathrm{d}s - \epsilon \int_0^t k(\phi^\epsilon_s)\mathrm{d}W_s. \tag{4.35}$$

That is (4.32). Denote

$$\Omega_1 = \left\{ \omega \in \Omega : \epsilon \sup_{0\leqslant t\leqslant T} \left| \int_0^t k(\phi_s)\mathrm{d}W_s \right| \leqslant \delta \right\}, \tag{4.36}$$

and

$$\Omega_2 = \left\{ \omega \in \Omega : \epsilon \sup_{0\leqslant t\leqslant T} \left| \int_0^t k(\phi^\epsilon_s)\mathrm{d}W_s \right| \leqslant \delta \right\}. \tag{4.37}$$

But it is easy to see that

$$P\{\Omega_1\} \geqslant P\left\{ \epsilon \int_0^t k(\phi_s)\mathrm{d}W_s - \frac{\delta\epsilon^2}{2\epsilon^2 \max_x k^2(x)T} \int_0^t k^2(\phi_s)\mathrm{d}s \leqslant \frac{1}{2}\delta \right\} \geqslant 1 - e^{-[\delta^2/2\epsilon^2 \max_x k^2(x)T]}. \tag{4.38}$$

Similarly

$$P\{\Omega_2\} \geqslant 1 - e^{-[\delta^2/2\epsilon^2 \max_x k^2(x)T]}. \tag{4.39}$$

So for $\omega \in \Omega_1 \cap \Omega_2$,

$$S(x,t) - \delta \leqslant S^\epsilon(x,t) \leqslant S(x,t) + \delta. \tag{4.40}$$

From this, it is easy to conclude as $\epsilon \to 0$, $S^\epsilon(x,t) \to S(x,t)$ almost surely. Now we assume that there exists a unique minimizer $x_0 = x_0(x,t)$ for fixed t and x such that $\Phi_t x_0 = x$. Consider the solution of the Hamilton–Jacobi equation for $\mathcal{L}(q,\dot{q}) = \dot{q}^2/2 + c(q)$,

$$S(x,t) = S_0(x_0(x,t)) + \int_0^t \mathcal{L}(q(s),\dot{q}(s))\mathrm{d}s|_{q=q_0},$$

where q_0 is $X_0(s) = \Phi_s x_0(x,t)$. Here S satisfies the Hamilton–Jacobi equation

$$\frac{\partial S}{\partial t} + \frac{1}{2}|\nabla S|^2 + c(x) = 0 \text{ and } S(x,0) = S_0(x). \tag{4.41}$$

Consider

$$\delta q(s) = \Phi_s x_0(x + \epsilon \int_0^t \mathcal{G}(x_0,t,u) \, \nabla \, k(\Phi_u x_0)\mathrm{d}W_u, t) - \epsilon \int_0^s \mathcal{G}(x_0,s,u) \, \nabla \, k(\Phi_u x_0)\mathrm{d}W_u - \Phi_s x_0(x,t).$$

By Taylor's theorem, there exists ξ such that

$$\delta q(s) = \left(\frac{\partial}{\partial x_0}\Phi_s x_0\right)\frac{\partial}{\partial x}x_0(x,t)\left(\epsilon\int_0^t \mathcal{G}(x_0,t,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)$$
$$+\sum_{i,j,l=1}^{d}\left[\sum_{k=1}^{d}(\nabla_k\nabla_l\Phi_s x_0(\xi,t))\frac{\partial}{\partial\xi_i}x_0^k(\xi,t)\frac{\partial}{\partial\xi_j}x_0^l(\xi,t)+(\nabla_l\Phi_s x_0(\xi,t))\frac{\partial^2}{\partial\xi_i\xi_j}x_0^l(\xi,t)\right]$$
$$\times\left(\epsilon\int_0^t \mathcal{G}(x_0,t,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)_i\left(\epsilon\int_0^t \mathcal{G}(x_0,t,u)\,\nabla\, k(\Phi_u x_0)dW_u\right)_j$$
$$-\epsilon\int_0^s \mathcal{G}(x_0,s,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u,$$

and computing $\dot{q}(s)$ gives

$$\delta\dot{q}(s) = \left(\frac{\partial}{\partial x_0}\right)\dot{\Phi}_s x_0\frac{\partial}{\partial x}x_0(x,t)\left(\epsilon\int_0^t \mathcal{G}(t,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)$$
$$+\sum_{i,j,l=1}^{d}\left[\sum_{k=1}^{d}(\nabla_k\nabla_l\dot{\Phi}_s x_0(\xi,t))\frac{\partial}{\partial\xi_i}x_0^k(\xi,t)\frac{\partial}{\partial\xi_j}x_0^l(\xi,t)+(\nabla_l\dot{\Phi}_s x_0(\xi,t))\frac{\partial^2}{\partial\xi_i\xi_j}x_0^l(\xi,t)\right]$$
$$\times\left(\epsilon\int_0^t \mathcal{G}(x_0,t,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)_i\left(\epsilon\int_0^t \mathcal{G}(x_0,t,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)_j$$
$$-\epsilon\int_0^s \frac{\partial}{\partial s}\mathcal{G}(x_0,s,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u.$$

Therefore, as required,

$$\delta\dot{q}(s) = \frac{d}{\mathrm{d}s}\delta q(s). \tag{4.42}$$

We see by definition that

$$\delta q(t) = 0, \tag{4.43}$$

$$\delta q(0) = x_0\left(x+\epsilon\int_0^t \mathcal{G}(x_0,t,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u, t\right) - x_0(x,t). \tag{4.44}$$

Define

$$\Omega_3 = \left\{\sup_{\substack{x_0\in\mathbb{R}^d\\ 0\leqslant s\leqslant t}}\epsilon^{1/2}\left|\int_0^s \mathcal{G}(x_0,s,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right| \leqslant \delta\right\}. \tag{4.45}$$

It is easy to see that

$$P\{\Omega_3\} > 1 - e^{-[\delta^2/2\epsilon\sup_{x_0\in\mathbb{R}^d}\int_0^T(\mathcal{G}(x_0,s,u)\,\nabla\, k(\Phi_u x_0))^2\ \mathrm{d}u]}. \tag{4.46}$$

Then for each $\omega\in\Omega_3$ there exists ξ_1 such that,

$$\delta q(0) = \frac{\partial}{\partial x} x_0(x,t)\left(\epsilon \int_0^t \mathcal{G}(x_0,s,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right) + \sum_{i,j=1}^{d} \frac{\partial^2}{\partial \xi_i\, \partial\, \xi_j} x_0(\xi_1,t)$$
$$\times\left(\epsilon \int_0^t \mathcal{G}(x_0,s,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)_i \left(\epsilon \int_0^t \mathcal{G}(x_0,s,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)_j$$
$$= \frac{\partial}{\partial x} x_0(x,t)\left(\epsilon \int_0^t \mathcal{G}(x_0,s,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right) + o(\epsilon). \tag{4.47}$$

Now we have

$$\delta S = \left\langle \left(\frac{\partial}{x_0} S_0\right), \left(\frac{\partial x_0}{\partial x}\right)\left(\epsilon \int_0^t \mathcal{G}(x_0,s,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)\right\rangle + \delta A. \tag{4.48}$$

And,

$$\delta A \epsilon \int_0^t k(\Phi_s x_0)\mathrm{d}W_s + \int_0^t \mathcal{L}(q_0+\delta q_0, \dot{q}_0 + \delta\dot{q}_0)\mathrm{d}s - \int_0^t \mathcal{L}(q_0,\dot{q}_0)\mathrm{d}s$$
$$= \epsilon \int_0^t k(\Phi_s x_0)\mathrm{d}W_s + \int_0^t \left(\frac{\partial \mathcal{L}}{\partial q}\delta q_0 + \frac{\partial \mathcal{L}}{\partial \dot{q}}\delta\dot{q}_0\right)\mathrm{d}s$$
$$= \epsilon \int_0^t k(\Phi_s x_0)\mathrm{d}W_s + \left[\frac{\partial \mathcal{L}}{\partial \dot{q}}\delta q_0\right]_{s=0}^{s=t} + \int_0^t \left(\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{\mathrm{d}s}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}}\right)\right)\delta q_0\ \mathrm{d}s$$
$$= \epsilon \int_0^t k(\Phi_s x_0)\mathrm{d}W_s - \langle \dot{q}(0), \delta q(0)\rangle. \tag{4.49}$$

It turns out that for each $\omega \in \Omega_3$,

$$\delta A = \epsilon \int_0^t k(\Phi_s x_0)\mathrm{d}W_s - \left\langle \nabla S_0(x_0), \frac{\partial}{\partial x} x_0(x,t)\left(\epsilon \int_0^t \mathcal{G}(x_0,s,u)\,\nabla\, k(\Phi_u x_0)\mathrm{d}W_u\right)\right\rangle + o(\epsilon). \tag{4.50}$$

Therefore for each $\omega \in \Omega_3$,

$$\delta S = \epsilon \int_0^t k(\Phi_s x_0)\mathrm{d}W_s + o(\epsilon). \tag{4.51}$$

The wavefront, for each $\omega \in \Omega_3$, satisfies

$$S(x,t) = \epsilon \int_0^t k(\Phi_s x_0)\mathrm{d}W_s + o(\epsilon). \tag{4.52}$$

■

C. Large time behavior for almost periodic small noise

Our Theorem 4.2 shows that for small noise $\dot{\tilde{X}}^\epsilon(x,t)$ is close to the actual solution of our problem in the inviscid limit. Also, we have an exact expression for $\tilde{X}^\epsilon$ in terms of the Jacobi fields for $\tilde{X}^0$, If we now assume that $\nabla k(x,s) = -a(s)$ is independent of x, we can define $\dot{\tilde{X}}^\epsilon(x,t)$ and

$\tilde{X}^{\epsilon}(x,t)$ in the same way as we did for the harmonic oscillator and, since we are working only to first order in ϵ, the $x^0(x,t)$'s are just the deterministic ones. It is therefore not surprising that there is an analog of Theorem 3.5.

Theorem 4.6: *Assume that* $\tilde{X}^0(x,t)$ *is periodic together with its Jacobi fields* $\partial\tilde{X}^0/\partial\gamma_0^{\alpha}$, $\alpha = 1,2,\ldots,2d$ *where* $\gamma_0=(x_0,p_0)^T$. *Then, if* $\int_0^t |a(s)|^2\,\mathrm{d}s<\infty$, *dropping* $\sim$, *the ensemble average is given by*

$$\mathbb{E}(\dot{\tilde{X}}^{\epsilon}(x,t)) = \dot{\tilde{X}}^0(x,t) = \dot{X}^0(x,t).$$

Moreover,

$$\mathbb{P}((\dot{\tilde{X}}^{\epsilon}(x,t) - \dot{X}^0(x,t)) \in \mathrm{d}v) = \exp\left(-\frac{v^T A(t) v}{2}\right)(2\pi)^{-d/2}(\det A)^{-1/2}\,\mathrm{d}v,$$

where the $d\times d$ *matrix* $A^{-1}(t)$ *is given by*

$$A^{-1}_{ii'}(t) = \epsilon^2 \int_0^t \frac{\partial X_i^0(u)}{\partial \gamma_0^{\alpha}} a_j(u) \frac{\partial X_{i'}^0(u)}{\partial \gamma_0^{\alpha'}} a_{j'}(u)\mathrm{d}u\; J_{\alpha\beta} J_{\alpha'\beta'} \frac{\partial \dot{X}_j^0(t)}{\partial \gamma_0^{\beta}} \frac{\partial \dot{X}_{j'}^0(t)}{\partial \gamma_0^{\beta'}},$$

$i,i'=1,2,\ldots,d$, *where* J *is the complex structure and the summation convention is enforced. In particular, if* $a(\cdot)$ *is almost periodic, with the above product almost periodic uniformly in* (x_0,p_0) *in a compact set* K,

$$t^{-1}A^{-1}_{ii'}(t) \sim \epsilon^2 M\left(\frac{\partial X_i^0}{\partial \gamma_0^{\alpha}} a_j \frac{\partial X_{i'}^0}{\partial \gamma_0^{\alpha'}} a_{j'}\right) J_{\alpha\beta} J_{\alpha'\beta'} \frac{\partial \dot{X}_j^0(t)}{\partial \gamma_0^{\beta}} \frac{\partial \dot{X}_{j'}^0(t)}{\partial \gamma_0^{\beta'}},$$

where M *denotes the infinite time average.*

Proof: This is a simple rewrite of the proof of Theorem 3.5. We need uniform almost periodicity because at the last step we must set $p_0=\nabla S_0(x_0)$ and $x_0=\tilde{x}_0(x,t)$ the minimizer (assumed unique) of $\mathcal{A}(x_0,x,t)$. We tacitly assume that $(\tilde{x}_0(x,t), \nabla S_0(\tilde{x}_0(x,t))) \in K$, our compact set. ■

Remark 4.1: The remarks after Theorem 3.5 are all relevant here save that the distribution of the Burgers fluid velocity now depends on the initial conditions. This distribution is in fact discontinuous across the cool part of the caustic because $\tilde{x}_0(x,t)$ jumps as we cross this part of the caustic, making the Jacobi fields jump here as well. The periodic behavior is in $\partial\dot{X}_j^0(t)/\partial\gamma_0^{\beta}$ and the resonance which is relevant is that between the zero noise Jacobi fields $\partial X_i^0/\partial\gamma_0^{\alpha}$ and the almost periodic noise term a. As expected the resonance destroys any possibility of an invariant measure existing. When the infinite time averages above are all zero the invariant measure should exist for a suitable restricted class of initial conditions.

D. Archetypal example with some illustrations

Having discussed the properties of the surfaces C_t and H_t we now illustrate what is perhaps the archetypal case with $S_0(x_0,y_0)=x_0^2y_0/2$ and zero potentials.

Figure 2 illustrates the critical case $\mathcal{A}=0$ where the precaustic is a parabola and the prelevel surface consists of an ellipse and a line pair. The zero prelevel surface has equation

$$x_0^2\left(\frac{\left(y_0+\frac{1}{2t}\right)^2}{\left(\frac{1}{2t}\right)^2} + \frac{x_0^2}{\left(\frac{1}{t}\right)^2} - 1\right) = 0,$$

and the precaustic has equation

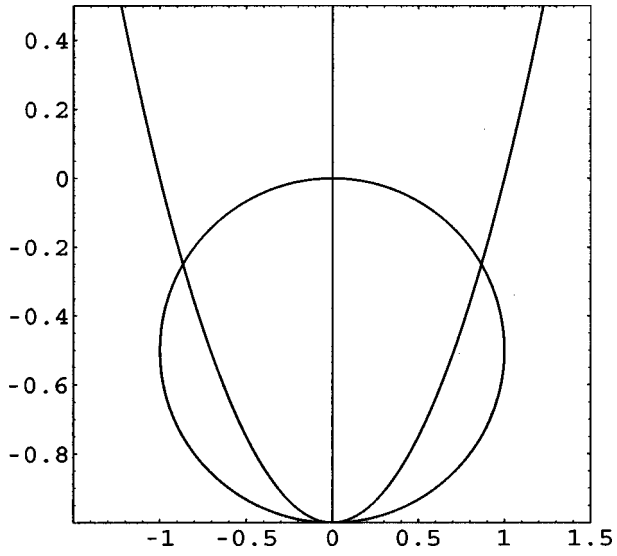

FIG. 2. Precaustic and prelevel surface.

$$1 + ty_0 = t^2 x_0^2.$$

We now map $(x,y)=\Phi_t(x_0,y_0)$ to obtain the hypocycloid tricorn

$$x = \frac{\cos\,\theta(1+\sin\,\theta)}{2t}, \quad y = \frac{\sin\,\theta(1-\sin\,\theta)}{2t}, \tag{4.53}$$

for $0 \leqslant \theta < 2\pi$, as the zero level surface at time t for the heat equation and semicubical parabolic cusp

$$8(yt+1)^3 = 27t^2x^2, \tag{4.54}$$

as the caustic at time t for the corresponding Burgers velocity field. Figure 3 illustrates the level surface H_t and the caustic C_t. The number of solutions $x_0(x,t)$ is also indicated for the three different regions (within, on and outwith the semicubical parabola). In this case $x_0(x,t)$ is the point $(a, y-ta^2/2)$ where $a \in \mathbb{R}$ satisfies the cubic $t^2a^3/2 - a(1+ty) + x = 0$ and $\tilde{x}_0(x,t)$ corresponds to the value of a minimizing $a^2(t^3a^4/8 - ta^3(1+4ty)/8 + y(1+ty)/2)$. We note that the vanishing of the

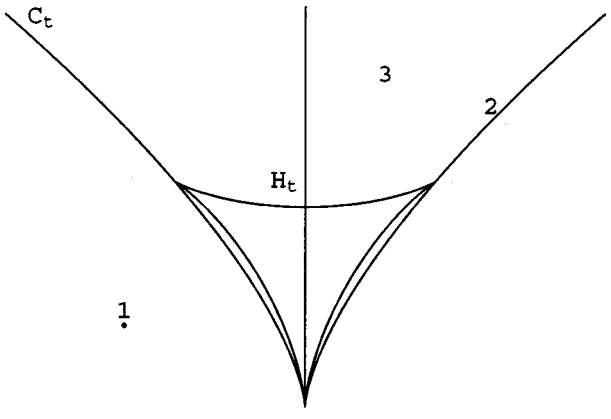

FIG. 3. Cusp and tricorn.

discriminant of the cubic for a defines the cusp caustic and that it can be shown that $\tilde{x}_0(x,t)$ jumps on crossing this caustic and nowhere else.

We now consider the stochastic case at $t=1$ where $\epsilon=\frac{1}{10}$ and $k(x,y,t)=x$. Figures 4 and 5 illustrate the case where we have $\mathcal{A}=0$.

Figures 6 and 7 illustrate the case of $\mathcal{A}=-\frac{1}{64}$.

We refrain from presenting a gallery of two- and three-dimensional images herein but such can be found in the recent doctoral theses of Reynolds and Reynolds.[31,32]

V. SINGULARITIES AND INTERMITTENCE OF TURBULENCE

We have analyzed the stochastic Burgers equation for small noise and shown how for our initial conditions resonance between the almost periodic noise and the underlying deterministic problem destroys any possibility of the existence of an invariant measure. We have also seen how for small noise the ensemble average and the distribution of the Burgers velocity inherit the singularity structure of the underlying Hamiltonian system, in particular the way that the caustics and shockwaves are still relevant.This is the main object lesson of the present work. These results rely heavily on our exact analysis of the harmonic oscillator and free cases.

Previously we detailed the caustic wavefront interaction in both the classical and stochastic case by appealing to geometrical properties of the Hamiltonian system. Now we have detailed information about these stochastic caustic wavefront structures in terms of the classical structures, at least in the case of small ϵ.

We now emphasize that new features emerge if one tries to use the above ideas to analyze the "intermittence" of stochastic turbulence as opposed to deterministic turbulence. The reason for the sharp contrast between stochastic and deterministic turbulence can already be seen here if we associate turbulent behavior with (an infinitely rapid) change in the number of cusped curves on the minimizing level surface of the Hamilton–Jacobi function. The times t when this occurs are just the times when the prelevel surfaces *touch* the precaustic. The times t when this number of curves changes in the deterministic case are simply the zeros of a deterministic function ζ, usually isolated zeros.

In the stochastic case ζ is a stochastic process whose zeros usually form a perfect set, i.e., an infinite set containing no isolated points. At these times the number of cusped curves changes with infinite frequency because of the infinitely rapid oscillation of the stochastic process ζ. This is in line with what one would expect for turbulent behavior. When the stochastic process ζ is *recurrent* this turbulent behavior is "intermittent" so that the scale of turbulent fluctuations varies in a random periodic way.

For example, in the two-dimensional case of $c\equiv 0$, $k_t(x,y)\equiv x$ and $S_0(x_0,y_0)=f(x_0)+g(x_0)y_0$, where f,g,f', and g' are zero at $x_0=a$, $g''(a)\neq 0$, the turbulent times t at which $n_c(t)$, the number of cusps on the zero prelevel surface of the Hamilton–Jacobi function changes are the zeros of the stochastic turbulence process ζ,

$$\zeta(t) = -a\epsilon W_t + \epsilon^2 W_t \int_0^t W_s \mathrm{d}s - \frac{\epsilon^2}{2}\int_0^t W_s^2 \mathrm{d}s.$$

The turbulence appears at the point $\Phi_t(a,-[(1+tf''(a))/tg''(a)]$ where $(a,-[(1+tf''(a))/tg''(a)]$ is a point on the precaustic with equation

$$y_0 = \frac{-1+t^2(g'(x_0))^2 - tf''(x_0)}{tg''(x_0)}.$$

Now $\{t:\zeta(t)=0\}$ is a perfect set and $\zeta(t)$ is recurrent to 0, while $\zeta_c(t)=\zeta(t)-c$ has exactly the same properties. Zeros of $\zeta_c(t)$ are times at which the number of cusps on the c prelevel surface of the Hamilton–Jacobi function changes (see Reynolds, Truman, and Williams[33]).

We may also introduce a singularity periodic in the (x_0,y_0) coordinates.

Lemma 5.1: Consider the initial function $S_0(x_0,y_0)=f(x_0)+g(x_0)\gamma(y_0)$. If f,f',g,g' are zero at

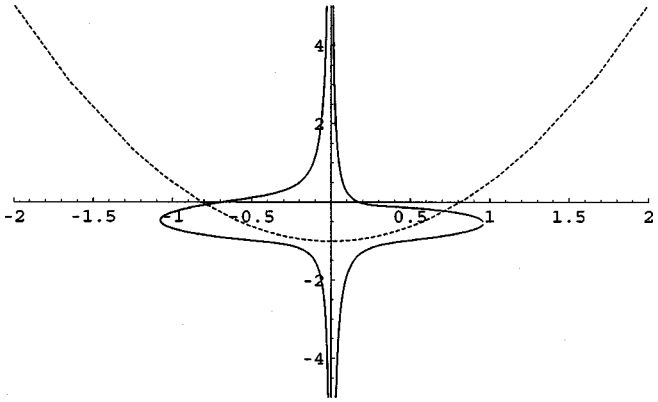

FIG. 4. Stochastic precaustic and prelevel surface.

α_i for $i=1,2,\ldots,n$ and $g''(\alpha_i)\neq 0$ then the zero precurves will touch at

$$\left(\alpha_i, \gamma^{-1}\left(\frac{-1-tf''(\alpha_i)}{tg''(\alpha_i)}\right)\right),$$

for $i=1,2,\ldots,n$ if γ is invertible.

Proof: The precurves meet at solutions x_0 of $F_0(x_0,t)=0$ where

$$F_0(x_0,t)=\frac{t}{2}(f'+g'\gamma(y_0(x_0)))^2+\frac{t}{2}g^2\gamma'(y_0(x_0))^2+f+g\gamma(y_0(x_0)),$$

and $y_0(x_0)$ is the precaustic. Now

$$\frac{\partial F_0}{\partial x_0}(x_0,t)=t(f'+g'\gamma(y_0(x_0)))\frac{\partial}{\partial x_0}(f'+g'\gamma(y_0(x_0)))+tgg'\gamma'(y_0(x_0))^2$$
$$+tg^2\gamma'(y_0(x_0))\gamma''(y_0(x_0))y_0'(x_0)+f'+g'\gamma(y_0(x_0))+g\gamma'(y_0(x_0))y_0'(x_0),$$

so that clearly $F_0(\alpha_i,t)=0$ and $\partial F_0/\partial x_0|_{x_0=\alpha_i}=0$. Hence the precurves will touch at $(\alpha_i,y_0(\alpha_i))$ where $y_0(x_0)$ is the precaustic. However in this case the precaustic is given by

$$(1+t(f''+g''\gamma(y_0)))(1+tg\gamma''(y_0))-t^2g'^2\gamma'(y_0)^2=0,$$

so that at $x_0=\alpha_i$

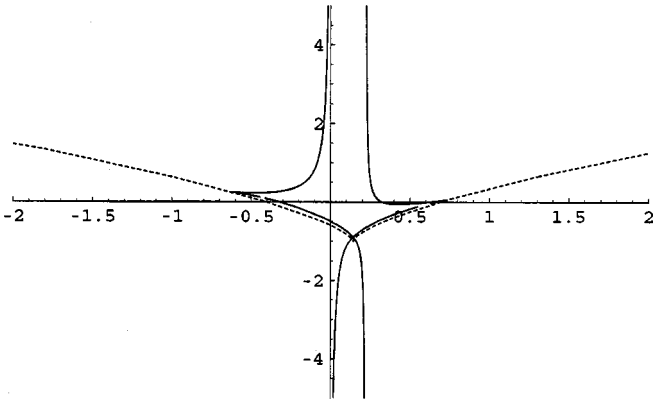

FIG. 5. Stochastic caustic and level surface.

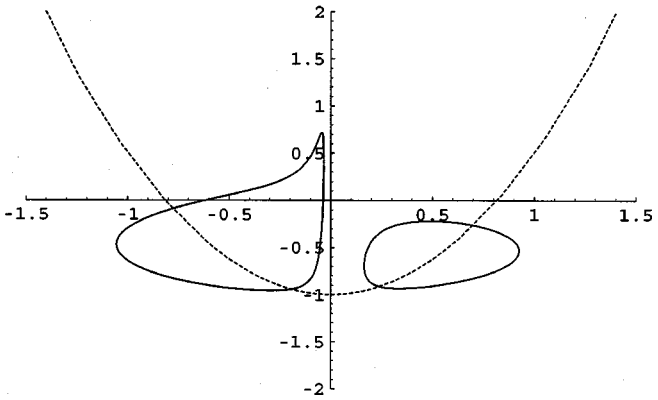

FIG. 6. Stochastic precaustic and prelevel surface.

$$\gamma(y_0) = \frac{-1 - tf''(\alpha_i)}{tg''(\alpha_i)}.$$

Hence

$$y_0(\alpha_i) = \gamma^{-1}\left(\frac{-1 - tf''(\alpha_i)}{tg''(\alpha_i)}\right).$$

■

Corollary 5.2: If $S_0(x_0,y_0) = f(x_0) + g(x_0)\gamma(y_0)$ *where* γ *is a periodic function with period* b *and* f, g, f', g' *are zero at* α_i *for* $i = 1,2,\ldots,n$ *while* $g''(\alpha_i) \neq 0$ *then the precurves will touch at*

$$(x_0,y_0) = \left(\alpha_i, \gamma^{-1}\left(\frac{-1 - tf''(\alpha_i)}{tg''(\alpha_i)}\right) + lb\right),$$

for $l \in \mathbb{Z}$ *and* $i = 1,2,\ldots,n$.

In order to obtain a periodic cusp singularity we set $\gamma(\cdot) := (b/2\pi)\sin(2\pi/b\cdot)$, where $b > 0$, so that γ has period b and $\gamma(y) \sim y$ for $y \sim 0$. Clearly if we take $f \equiv 0$ and $g(x_0) := (a^2/2\pi^2)\sin^2(\pi x_0/a)$ then f, g, f', and g' are zero at $x_0 = ka$ $(k \in \mathbb{Z})$ and $g''(ka) = 1$. Moreover

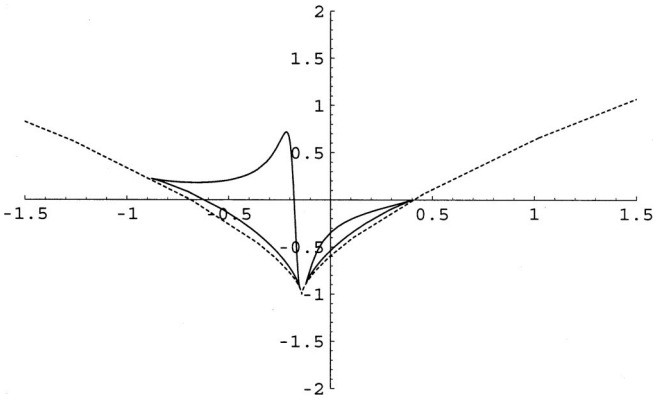

FIG. 7. Stochastic caustic and level surface.

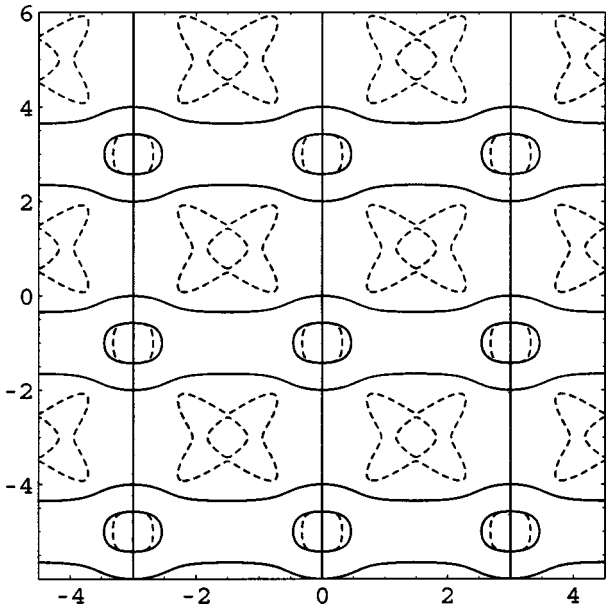

FIG. 8. Periodic zero prelevel surface and precaustic.

$$\gamma^{-1}\left(\frac{-1-tf''(ka)}{tg''(ka)}\right)=\gamma^{-1}\left(-\frac{1}{t}\right)=\frac{b}{2\pi}\arcsin\left(-\frac{2\pi}{bt}\right),$$

which exists if $b\geqslant 2\pi/t$. Since the conditions of Corollary 5.2 are satisfied we obtain the following proposition.

Proposition 5.3: Consider the initial function $S_0(x_0,y_0)=(a^2b/4\pi^3)\sin^2(\pi x_0/a)\sin(2\pi y_0/b)$. *If* $b\geqslant 2\pi/t$ *then the precurves will touch at*

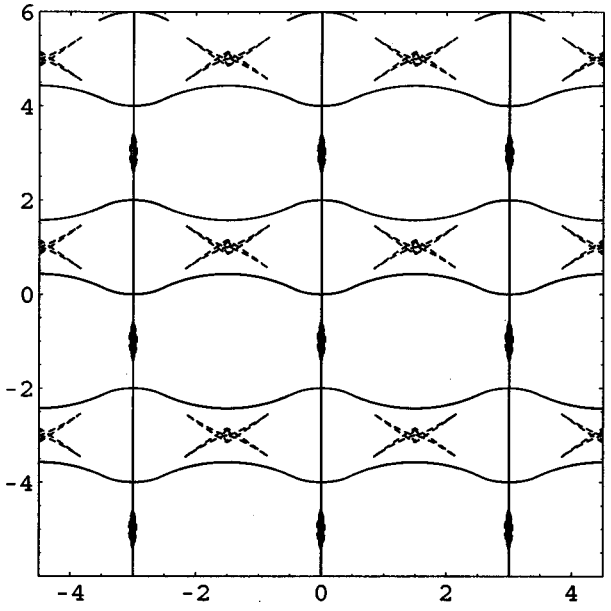

FIG. 9. Periodic zero level surface and caustic.

$$(x_0,y_0) = \left(ka, \frac{b}{2\pi} \arcsin\left(-\frac{2\pi}{bt} \right) + lb \right),$$

for $k,l \in \mathbb{Z}$.

In Figs. 8 and 9 we have shown the precurves and image curves, respectively, where $a=3$, $b=4$, and $t=2$ so that $b \geqslant 2\pi/t$.

We shall not pursue the notion of periodic singularities any further, but suffice to say many examples may be easily created.

Hence, the second object lesson of the present study is that the number of cusped curves on the wavefront will change infinitely rapidly in the stochastic case when the presurfaces touch and that this behavior will recur in a random periodic way if the stochastic process ζ is recurrent. This is the "intermittence" of stochastic turbulence in our model. There is no analog of this for the deterministic Burgers equation.

We hope to investigate these phenomena in more detail in a future paper.

ACKNOWLEDGMENTS

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On the asymptotics of some large Hankel determinants generated by Fisher–Hartwig symbols defined on the real line

T. M. Garoni[a)]
Institute for Mathematics and its Applications, University of Minnesota, Minneapolis, Minnesota 55455-0436

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We investigate the asymptotics of Hankel determinants of the form $\det_{j,k=0}^{N-1}[\int_\Omega dx\ \omega_N(x)\Pi_{i=1}^m|\mu_i-x|^{2q_i}x^{j+k}]$ as $N\to\infty$ with q and μ fixed, where Ω is an infinite subinterval of $\mathbb{R}$ and $\omega_N(x)$ is a positive weight on Ω. Such objects are natural analogs of Toeplitz determinants generated by Fisher–Hartwig symbols, and arise in random matrix theory in the investigation of certain expectations involving random characteristic polynomials. The reduced density matrices of certain one-dimensional systems of trapped impenetrable bosons can also be expressed in terms of Hankel determinants of this form. We focus on the specific cases of scaled Hermite and Laguerre weights. We compute the asymptotics by using a duality formula expressing the $N\times N$ Hankel determinant as a $2(q_1+\cdots+q_m)$-fold integral, which is valid when each q_i is natural. We thus verify, for such q, a recent conjecture of Forrester and Frankel derived using a log-gas argument. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1867981]

I. INTRODUCTION

Consider the multiple integral

$$H_{M,N,m,q}(\mu):=\int_\Omega \omega_N(z_1)dz_1\cdots\int_\Omega \omega_N(z_M)dz_M|\Delta_M(z)|^2\prod_{l=1}^{M}\prod_{i=1}^{m}|\mu_i-z_l|^{2q_i}, \tag{1}$$

where

$$q:=(q_1,\ldots,q_m),\quad \mu:=(\mu_1,\ldots,\mu_m), \tag{2}$$

$\omega_N(z)$ is a nonzero and continuous weight function, possibly depending on a parameter N, and

$$\Delta_M(z):=\det_{j,k=1}^{M}(z_k^{j-1})=\prod_{1\leqslant j<k\leqslant M}(z_k-z_j) \tag{3}$$

is the Vandermonde determinant. As a notational convenience we also define

$$H_{M,N}:=H_{M,N,0,}(\cdot) \tag{4}$$

$$=\int_\Omega \omega_N(z_1)dz_1\cdots\int_\Omega \omega_N(z_M)dz_M|\Delta_M(z)|^2. \tag{5}$$

a)Electronic mail: garoni@ima.umn.edu; URL: http://www.ima.umn.edu/~garoni

It is known that M-fold integrals of the form (1) can be identified with the determinant of an $M \times M$ matrix. Expanding the Vandermonde determinants in terms of sums over permutations, and simplifying appropriately, we find

$$H_{M,N,m,q}(\mu) = M! \det_{j,k=0}^{M-1} \left[\int_\Omega \mathrm{d}z \, a(z) z^j (z^*)^k \right], \tag{6}$$

where z^* denotes the complex conjugate of z, and

$$a(z) := \omega_N(z) \prod_{i=1}^{m} |\mu_i - z|^{2q_i}. \tag{7}$$

When $\Omega \subseteq \mathbb{R}$, Eq. (6) becomes

$$H_{M,N,m,q}(\mu) = M! \det_{j,k=0}^{M-1} [a_{j+k}], \tag{8}$$

where

$$a_n := \int_\Omega \mathrm{d}z \, a(z) z^n. \tag{9}$$

One says that the determinant (8) is *generated* by the function (7).

Since the entries in the determinant (8) are of the form a_{j+k}, we have thus identified the multiple integral (1), when $\Omega \subseteq \mathbb{R}$, with a Hankel determinant. Had we instead taken Ω to be $\mathbb{T}$, the unit circle in $\mathbb{C}$, then according to (6) the entries of the determinant would be a_{j-k}, and we would thus obtain a Toeplitz determinant. [It is conventional when discussing such Toeplitz determinants to set $z = e^{i\theta}$ and to define a_n as the integral of $a(z)z^n$ with respect to $\mathrm{d}\theta$ rather than $\mathrm{d}z$. This merely introduces the nonzero factor $ie^{i\theta}$ which is easily absorbed into the definition of $a(z)$, and so such technicalities are not relevant to our discussion here.]

When $z \in \mathbb{T}$, functions of the form (7) are known as *Fisher–Hartwig symbols*[1] (although we remark that they are not the most general examples of Fisher–Hartwig symbols). By extension, we can describe the Hankel determinant (8) as being generated by a Fisher–Hartwig symbol which is defined on the real line.

The asymptotic analysis of Toeplitz determinants generated by Fisher–Hartwig symbols is a fascinating and well studied subject (see, e.g., Ref. 1 and references therein), and rigorous results which describe the large M asymptotic behavior of Toeplitz determinants generated by symbols of the form (7) are known.[2] There are a number of important physical applications of such determinants (see, e.g., Refs. 3–5). It is often the case, as we discuss presently, that the quantity appearing in applications is actually the integral (1) rather than the determinant directly, and when $\Omega \subseteq \mathbb{R}$ we are naturally lead to Hankel determinants generated by the symbol (7). We discuss below a number of physical applications in which the asymptotics of such Hankel determinants is of interest. A rigorous treatment of these asymptotics is an open problem, however a conjectured form for the large M asymptotics has recently been reported by Forrester and Frankel in Ref. 5. Very recently, the $m=1$ case of this conjecture has been verified when $\Omega = \mathbb{R}$ and $\omega_N(x)$ is a Hermite weight, by using a Riemann–Hilbert approach.[6] In the present work we verify the conjecture of Forrester and Frankel when $\omega_N(z)$ is either a Hermite or Laguerre weight for any $m \in \mathbb{N}$, when each $q_i \in \mathbb{N}$.

A. Random matrix theory

The multiple integral (1) has a natural interpretation in random matrix theory. Let us consider the ensemble of random matrices with joint eigenvalue probability density function (pdf) given by

$$P_{M,N}(x) := \frac{1}{H_{M,N}} |\Delta_M(x)|^2 \prod_{l=1}^{M} \omega_N(x_l), \tag{10}$$

and whose eigenvalues lie in Ω. When $\Omega = \mathbb{R}$, concrete examples of such ensembles include the ubiquitous Gaussian unitary ensemble (GUE), corresponding to $\omega_N(x) = \exp(-2Nx^2)$, as well as more general unitary ensembles (UE), corresponding to $\omega_N(x) = \exp(-NV(x))$ with $V(x)$ an arbitrary polynomial of even degree with positive leading coefficient (see, e.g., Ref. 7). When $\Omega = (0, \infty)$ an important example is the Laguerre unitary ensemble (LUE), corresponding to $\omega_N(x) = x^\alpha \exp(-4Nx)$, which includes Wishart matrices and the Chiral GUE as special cases (the latter after a straightforward change of variables; see, e.g., Ref. 8). Setting $x = e^{i\theta}$ and $\omega_N(x) = 1$ in (10) we obtain the joint pdf for the eigenphases $\theta_l \in [0, 2\pi]$ of the ensemble of random unitary matrices with Haar measure, often called the circular unitary ensemble (CUE). For the purpose of computing expectations, the CUE is equivalent to (10) with $\Omega = \mathbb{T}$ and $\omega_N(z) = 1/iz$.

If we denote the characteristic polynomial of the $M \times M$ matrix X, with eigenvalues $x_1, \ldots, x_M$, by

$$\mathcal{Z}_M(\mu_i) := \det(\mu_i I - X) = \prod_{l=1}^{M} (\mu_i - x_l), \tag{11}$$

then (1) corresponds to the following expectation involving the absolute value of such characteristic polynomials:

$$\left\langle \prod_{i=1}^{m} |\mathcal{Z}_M(\mu_i)|^{2q_i} \right\rangle_{P_{M,N}} = \frac{H_{M,N,m,q}(\mu)}{H_{M,N}}, \tag{12}$$

where the expectation on the left-hand side of (12) is with respect to the joint eigenvalue pdf (10). The case $M = N$ is generally the case of interest.

From (6) we see that expectations of characteristic polynomials of the form appearing in (12) are characterized by a determinant generated by the symbol (7); when $\Omega \subseteq \mathbb{R}$, it is a Hankel determinant, and when $\Omega = \mathbb{T}$ it is a Toeplitz determinant.

A sizable literature on the correlations of products and ratios of characteristic polynomials of random matrices from various ensembles has emerged in recent years, see, e.g., Refs. 9–16, and significant progress has been made in the understanding of such objects. Such quantities have applications in diverse fields including number theory, quantum chaos, and many-body quantum mechanics. These works consider either exact algebraic relations that are valid for finite N, or the large N asymptotics in the usual universal microscopic scaling limits. We shall be interested not in scaling limits, but in the limit of large N with μ fixed. Investigations of objects of the form (12) in this limit have been reported in Refs. 5 and 17.

B. Impenetrable bosons

A compelling physical motivation for investigating multiple integrals of the form (1) arises from a consideration of certain one-dimensional many-body systems of impenetrable bosons. By impenetrability we simply mean that we require the wave function to vanish whenever two bosons occupy the same point in space. Such systems have been receiving renewed theoretical interest recently due to the possibility of their experimental realization in the near future using ultracold systems of atomic bosons confined in elongated traps; see, e.g., Refs. 18 and 19. Systems of impenetrable bosons with certain specific boundary conditions are known to have ground state wave functions of the form

$$\psi(x_1,\ldots,x_M) = \frac{1}{\sqrt{C_M}}\prod_{l=1}^{M}\sqrt{g_N(x_l)}\,|\Delta_M[f(x_1),\ldots,f(x_M)]|, \quad x_1,\ldots,x_M \in D \subseteq \mathbb{R}, \tag{13}$$

see, e.g., Refs. 20 and 21. Specifically, systems with periodic, Dirichlet, or Neumann boundary conditions have wave functions of this form, as do systems confined in an harmonic well. Of these, the harmonically confined system is perhaps the most relevant to current experiments.

It is worth emphasizing that the introduction of such zero-range infinite-strength interactions establishes a correspondence between impenetrable bosons and a corresponding system of free fermions, a fact first noted in Ref. 22, and this is one of the primary reasons for current experimental interest in such systems. Indeed, for the specific systems mentioned above, were it not for the absolute value surrounding the Vandermonde determinant, (13) would define the wave function for a system of free fermions. This fact implies that certain quantities such as the energy spectrum and the particle density are identical in the impenetrable boson system and its corresponding free fermion system. Quantities which depend on the phase of the wave function however will clearly differ significantly between these two systems.

One such quantity, of great significance, is the n-body density matrix, which for a system of $N+n$ particles is defined as

$$\rho_{N+n}^{(n)}(x_1,y_1,\ldots,x_n,y_n) := \binom{N+n}{n}\int_D \mathrm{d}\xi_1 \cdots \int_D \mathrm{d}\xi_N\, \psi(x_1,\ldots,x_n,\xi_1,\ldots,\xi_N)\psi^*(y_1,\ldots,y_n,\xi_1,\ldots,\xi_N). \tag{14}$$

A key observation is that wave functions of the form (13) admit the factorization

$$\begin{aligned}\psi(x_1,\ldots,x_n,\xi_1,\ldots,\xi_N) = {} & \sqrt{\frac{C_N}{C_{N+n}}}\prod_{l=1}^{n}\sqrt{g_N(x_l)}\,|\Delta_n[f(x_1),\ldots,f(x_n)]| \\ & \times \prod_{l=1}^{N}\prod_{i=1}^{n}|f(x_i)-f(\xi_l)|\cdot\psi(\xi_1,\ldots,\xi_N),\end{aligned} \tag{15}$$

and inserting (15) into (14) yields

$$\begin{aligned}\rho_{N+n}^{(n)}(x_1,y_1,\ldots,x_n,y_n) = {} & \binom{N+n}{N}\prod_{i=1}^{n}\sqrt{g_N(x_i)g_N(y_i)}\,|\Delta_n[f(x_1),\ldots,f(x_n)]\Delta_n[f(y_1),\ldots,f(y_n)]| \\ & \times \frac{1}{H_{N+n,N}}\,H_{N,N,2n,q}(f(x_1),\ldots,f(x_n),f(y_1),\ldots,f(y_n))|_{q=(1/2,\ldots,1/2)},\end{aligned} \tag{16}$$

where in the definition of $H_{N,N,2n,q}$ and $H_{N+n,N}$ we have $\Omega = f(D)$ and

$$\omega_N(z) = g_N(f^{-1}(z))\frac{\mathrm{d}f^{-1}}{\mathrm{d}z}(z). \tag{17}$$

For the four specific systems mentioned below (13), this $\omega_N(z)$ given in (17) is well defined, nonzero and continuous.

Hence, from (6) we see that $\rho_{N+n}^{(n)}$ is characterized by a determinant generated by the symbol (7). For systems subject to periodic boundary conditions this determinant will be a Toeplitz determinant,[23,24] whereas for systems confined by an harmonic well it will be a Hankel determinant.[24] Indeed, this link between density matrices for impenetrable bosons and Toeplitz determinants generated by Fisher–Hartwig symbols was originally one of the key motivations for investigating the asymptotics of such Toeplitz determinants.[3,4,23] In light of the possible future experimental realization of finite one-dimensional harmonically trapped systems of impenetrable bosons, an important theoretical question is the behavior of the corresponding density matrices

when N is large and $x_1, y_1, \ldots, x_n, y_n$ are fixed. This then provides a direct physical motivation for investigating the large N asymptotics of $N \times N$ Hankel determinants generated by symbols of the form (7).

Perhaps the most important quantity is the one-body density matrix. The asymptotics of the one-body density matrix for a system with periodic boundary conditions can be rigorously established from the asymptotics of the corresponding Toeplitz determinant. The leading order behavior of the one-body density matrix in the case of harmonic confinement was deduced in Ref. 24 using log-gas arguments, and has been recovered in Ref. 25 using a rather more direct, yet still nonrigorous, approach. The asymptotics of the one-body density matrix in the Dirichlet/Neumann case was deduced in Ref. 17, again by log-gas arguments, and has now been rigorously proved in Ref. 5, by making use of recent results in Refs. 26 and 27.

We conclude our discussion of impenetrable bosons by noting the correspondence between the joint eigenvalue pdf (10) and the wave function (13). The correspondence between the joint eigenvalue pdf (10) and the wave function for a system of free fermions is well known.[28] The correspondence between impenetrable bosons and random matrices was first noted by Sutherland,[29] between systems of impenetrable bosons with periodic boundary conditions and the CUE; see also Ref. 30. The correspondence between impenetrable bosons with Dirichlet or Neumann boundary conditions and the Jacobi unitary ensembles (JUE) was discussed in Refs. 17 and 20, and a similar interpretation for the LUE was noted in Ref. 5. Again, the most interesting case from an experimental perspective is the correspondence between the GUE and systems of impenetrable bosons confined in an harmonic well, and this particular system has been the focus of considerable recent theoretical study, see, e.g., Refs. 24, 25, and 31 and references therein.

C. Asymptotics of Hankel determinants

The asymptotics of large Toeplitz and Hankel determinants has been of long standing interest to mathematicians. For Toeplitz determinants generated by well behaved symbols, very precise asymptotic results are given by the Szegö limit theorems (see, e.g., Refs. 1 and 32). Toeplitz determinants generated by the symbol (7) are not amenable to the Szegö limit theorems however since (7) has zeros. Inspired in part by applications to impenetrable bosons Lenard[4,23] (see also Ref. 3) conjectured the asymptotics of Toeplitz determinants generated by symbols of the form (7), and this conjecture was subsequently proved by Widom.[2] The asymptotic behavior of Toeplitz determinants generated by (7), as well as more general Fisher–Hartwig symbols, is now well understood (see, e.g., Ref. 1). Analogously, the asymptotic behavior of large Hankel determinants generated by functions defined on $\Omega \subseteq \mathbb{R}$ has also been the subject of study. This problem was addressed by Szegö[33] and also Hirschman[34] with Ω a finite interval (see also Ref. 32). In the context of the UE and LUE of random matrix theory, as well as in the context of trapped systems of impenetrable bosons, we are interested in case where Ω is infinite, and recently Basor *et al.*[35] have considered the asymptotics of Hankel determinants generated by symbols defined on $\Omega = (0, \infty)$. However, a key restriction in these works is that the symbol be nowhere zero, and hence they do not apply to determinants generated by (7). Forrester and Frankel[5] have recently conjectured the asymptotic behavior of Hankel determinants generated by symbols of the form (7) defined on $\Omega \subseteq \mathbb{R}$. Complete and rigorous proofs of their conjectures remains an open problem. As mentioned above, a rigorous proof for the $m=1$ case when $\Omega = \mathbb{R}$ and $\omega_N(x)$ is a Hermite weight has very recently been reported in Ref. 6.

Specifically, Forrester and Frankel[5] consider the behavior of the ratio

$$\mathcal{H}_{N,m,q}(\mu) := \frac{H_{N,N,m,q}(\mu)}{H_{N+|q|,N}}, \tag{18}$$

where

$$|q| := q_1 + \cdots + q_m, \tag{19}$$

as $N \to \infty$ with μ and q fixed. Amongst other results, they consider the case $\omega_N(x) = e^{-NV(x)}$ with either $\Omega = \mathbb{R}$ or $\Omega = (0, \infty)$. For a particular choice of such $\omega_N(x)$ and Ω there corresponds the quantity $\rho(x)$, which, with $P_{N,N}$ defined as in (10), equals the limit of

$$\int_{\Omega^{N-1}} P_{N,N}(x, x_2, \ldots, x_N) \mathrm{d}x_2 \cdots \mathrm{d}x_N \tag{20}$$

as $N \to \infty$ with x held fixed; i.e., $\rho(x)$ is the limiting expected eigenvalue density of the ensemble of random matrices defined by $P_{N,N}$. We note that $\rho(x)$ is non-negative and has compact support. In what follows int(supp ρ) denotes the interior of the support of $\rho(x)$. For a detailed discussion of $\rho(x)$, and a number of other very interesting alternative characterizations of $\rho(x)$, the reader is referred to Ref. 7. The conjecture reported in Ref. 5 (in our notation) is the following.

Conjecture (Forrester–Frankel): *Let* $m, N \in \mathbb{N}$, $q \in (-1/2, \infty)^m$ *and* $\mu_1, \ldots, \mu_m \in \mathrm{int}(\mathrm{supp}\, \rho)$, *where* $\rho(x)$ *is defined as above. Furthermore, suppose either* $\Omega = \mathbb{R}$ *or* $\Omega = (0, \infty)$, *and take* $\omega_N(x) = e^{-NV(x)}$ *where* $V(x)$ *is a polynomial which is independent of* N *and which has positive leading coefficient and no zeros in* Ω. *Then*

$$\mathcal{H}_{N,m,q}(\mu) = N^{\sum_{i=1}^{m}(q_i^2 - q_i)} \prod_{i=1}^{m} [\omega_N(\mu_i)]^{-q_i} \prod_{i=1}^{m} \frac{G^2(q_i + 1)}{G(2q_i + 1)} (2\pi)^{q_i^2 - q_i}$$
$$\times \prod_{1 \leqslant j < k \leqslant m} |\mu_k - \mu_j|^{-2q_j q_k} \prod_{i=1}^{m} [\rho(\mu_i)]^{q_i^2} [1 + o(1)]. \tag{21}$$

Here and in the sequel G refers to Barnes' G-function.[36]

Despite first appearances, the structure of (21) is actually quite simple. Note that the only ensemble dependent quantities on the right-hand side are $\rho(x)$ and $\omega_N(x)$, and that the dependence of $\mathcal{H}_{M,m,q}(\mu)$ on these two quantities is universal. The other quantities on the right-hand side are truly universal. We note that the factor $G^2(q_i+1)/G(2q_i+1)$ occurs also in the asymptotics of Toeplitz determinants generated by Fisher–Hartwig symbols,[2] and has been discussed in the context of moments of random characteristic polynomials.[9,10] We should note that the actual conjecture reported in Ref. 5 is slightly more general than (21), but (21) is sufficient for our purposes.

As an aside, we remark that the ratio appearing in (16) is precisely of the form (18) and so the asymptotic behavior of all the n-body density matrices for a system of harmonically confined impenetrable bosons follows directly from (21).

The present paper focuses on two classical cases already mentioned, the case of the Hermite weight, corresponding to the GUE, and the case of the Laguerre weight, corresponding to the LUE. In the Hermite case

$$\omega_N(x) = e^{-2Nx^2}, \quad \Omega = \mathbb{R}, \quad \rho(\mu) = \frac{2}{\pi}\sqrt{1 - \mu^2}, \quad \mathrm{supp}(\rho) = [-1, 1], \tag{22}$$

and in the Laguerre case

$$\omega_N(x) = x^{\alpha} e^{-4Nx}, \quad \Omega = (0, \infty), \quad \rho(\mu) = \frac{2}{\pi}\sqrt{\frac{1}{\mu} - 1}, \quad \mathrm{supp}(\rho) = [0, 1]. \tag{23}$$

The conjecture reported in Ref. 5 was deduced by considering the specific examples of the Hermite and Laguerre cases, to find the general form in terms of $\rho(x)$ and $\omega_N(x)$. The asymptotics for these two cases was deduced by using the log-gas analogy to conjecture a factorization of (18), computing the asymptotics of each factor when the q_i were natural, and then conjecturing an analytic continuation to real q_i.

In this work we show how (21) can be proved rigorously for the Hermite and Laguerre cases, when each q_i is natural, by using a duality formula derived from a general result in Ref. 9. By a *duality* formula we mean an equation identifying the N-fold integral $\mathcal{H}_{N,m,q}(\mu)$ with a $2|q|$ - fold integral. Our results clarify the origin of the factors appearing in (21). A similar approach has been used in Ref. 25 to investigate a particular special case when the weight was of Hermite type, in the context of trapped impenetrable bosons.

Section II contains a discussion of the duality formula. Due to the similar nature of the Laguerre and Hermite cases, they can both be derived simultaneously. Section III then discusses the asymptotic analysis of the $2|q|$ - fold integral obtained from the duality formula by means of the saddle point method. We show how to deduce the general form of all terms and explicitly simplify the leading order term, and thus verify the conjecture (21) for the Hermite and Laguerre cases when each q_i is natural.

II. DUALITY FORMULA

Let us define

$$F_{K,N}(\lambda_1,\ldots,\lambda_K) := \frac{1}{\Delta_K(\lambda_1,\ldots,\lambda_K)} \det_{j,k=1}^{K} \pi_{N+j-1}^{(N)}(\lambda_k), \tag{24}$$

where $\{\pi_k^{(N)}\}_{k=0}^{\infty}$ are the monic orthogonal polynomials corresponding to $\omega_N(x)$ and Ω; i.e., they are uniquely defined by the following two conditions:

$$\int_\Omega \omega_N(x)\mathrm{d}x\ \pi_j^{(N)}(x)\pi_k^{(N)}(x) = 0, \quad j \neq k, \tag{25}$$

$$\pi_j^{(N)}(x) = x^j + O(x^{j-1}). \tag{26}$$

For the Hermite and Laguerre cases, the $\pi_{N+j-1}^{(N)}(x)$ can be expressed in terms of the standard Hermite and Laguerre polynomials found in Szegö's classic book[37] as follows:

$$\pi_{N+j-1}^{(N)}(x) = \begin{cases} 2^{-3(N+j-1)/2} N^{-(N+j-1)/2} H_{N+j-1}(\sqrt{2N}x), & \text{Hermite,} \\ (-1)^{N+j-1}(N+j-1)!(4N)^{-N-j+1} L_{N+j-1}^{(\alpha)}(4Nx), & \text{Laguerre.} \end{cases} \tag{27}$$

According to Brézin and Hikami,[9] we have the following very useful identity:

$$F_{K,N}(\lambda_1,\ldots,\lambda_K) = \frac{1}{H_{N,N}} \int_\Omega \omega_N(x_1)\mathrm{d}x_1 \cdots \int_\Omega \omega_N(x_N)\mathrm{d}x_N\, \Delta_N^2(x) \prod_{l=1}^{N}\prod_{i=1}^{K}(\lambda_i - x_l). \tag{28}$$

If we restrict ourselves to $q \in \mathbb{N}^m$ and set

$$K = 2q_1 + \cdots + 2q_m = 2|q|, \tag{29}$$

we can consider the confluent limit

$$\lim_{*} := \lim_{\lambda_{\pi(m)+2q_m}\to\mu_m} \cdots \lim_{\lambda_{\pi(m)+1}\to\mu_m} \cdots \lim_{\lambda_{2q_1+2q_2}\to\mu_2} \cdots \lim_{\lambda_{2q_1+1}\to\mu_2} \lim_{\lambda_{2q_1}\to\mu_1} \cdots \lim_{\lambda_1\to\mu_1}, \tag{30}$$

where

$$\pi(i) := \sum_{l=1}^{i-1} 2q_l. \tag{31}$$

Taking the limit (30) of both sides of (28), and using the elementary fact that $(\mu_i - x_l)^{2q_i} = |\mu_i - x_l|^{2q_i}$ when q_i is an integer and μ_i and x_l are real, we thus obtain

$$\lim_{*} F_{K,N}(\lambda_1,\ldots,\lambda_K) = \frac{H_{N,N,m,q}(\mu)}{H_{N,N}}, \tag{32}$$

and therefore

$$\mathcal{H}_{N,m,q}(\mu) = \frac{H_{N,N}}{H_{N+|q|,N}} \lim_{*} F_{K,N}(\lambda_1,\ldots,\lambda_K), \quad q \in \mathbb{N}^m. \tag{33}$$

This is the key relation we need to derive the duality formula for $\mathcal{H}_{N,m,q}(\mu)$, all that remains is to take the confluent limit of $F_{K,N}$.

For later convenience, we set

$$\pi^{(N)}_{N+j-1}(x) = \zeta_N(x) r_{N+j-1}(x). \tag{34}$$

If we insert (34) into (24) and take the limit (30), then by factoring the Vandermonde determinant we obtain

$$\begin{aligned}\lim_{*} F_{K,N}(\lambda_1,\ldots,\lambda_K) = \lim_{*} \prod_{1\leqslant j<k\leqslant m} \prod_{l_k=1}^{2q_k} \prod_{l_j=1}^{2q_j} (\lambda_{\tau(k)+l_k} - \lambda_{\tau(j)+l_j})^{-1} \prod_{j=1}^{K} \zeta_N(\lambda_j) \\ \times \lim_{*} \prod_{i=1}^{m} \Delta^{-1}_{2q_i}(\lambda_{\tau(i)+1},\ldots,\lambda_{\tau(i+1)}) \det_{j,k=1}^{K} r_{N+j-1}(\lambda_k)\end{aligned} \tag{35}$$

$$= \prod_{1\leqslant j<k\leqslant m} (\mu_k - \mu_j)^{-4q_k q_j} \prod_{i=1}^{m} \zeta_N^{2q_i}(\mu_i) \lim_{*} \prod_{i=1}^{m} \Delta^{-1}_{2q_i}(\lambda_{\tau(i)+1},\ldots,\lambda_{\tau(i+1)}) \det_{j,k=1}^{K} r_{N+j-1}(\lambda_k). \tag{36}$$

To compute the remaining limit in (36) we can use the following.

Lemma 1: Let $\mathbf{c}(\lambda)$ *denote a column vector with* $\tau(m+1)$ *entries, then for* $i=1,2,\ldots,m$

$$\begin{aligned}&\lim_{\lambda_{\tau(i)+2q_i}\to\mu_i} \cdots \lim_{\lambda_{\tau(i)+1}\to\mu_i} \frac{1}{\Delta_{2q_i}(\lambda_{\tau(i)+1},\ldots,\lambda_{\tau(i)+2q_i})} \\ &\quad \times G(2q_i+1)\det[\mathbf{c}(\lambda_1)\cdots\mathbf{c}(\lambda_{\tau(i)+1})\cdots\mathbf{c}(\lambda_{\tau(i)+2q_i})\cdots\mathbf{c}(\lambda_{\tau(m+1)})] \\ &= \det\left[\mathbf{c}(\lambda_1)\cdots\mathrm{c}(\lambda_{\tau(i)})\mathbf{c}(\mu_i)\frac{\mathrm{d}}{\mathrm{d}\mu_i}\mathbf{c}(\mu_i)\cdots\frac{\mathrm{d}^{2q_i-1}}{\mathrm{d}\mu_i^{2q_i-1}}\mathbf{c}(\mu_i)\mathbf{c}(\lambda_{\tau(i+1)+1})\cdots\mathbf{c}(\lambda_{\tau(m+1)})\right],\end{aligned} \tag{37}$$

where G is Barnes' G-function.

Proof: This is easily proven by induction using L'Hôpital's rule, and recalling the identity

$$\prod_{l=1}^{n} \Gamma(l) = G(n+2). \tag{38}$$

■

Applying Lemma 1 to (36) independently for each set $\{\lambda_{\tau(i)+1},\ldots,\lambda_{\tau(i)+2q_i}\}$ with $i=1,2,\ldots,m$, results in

$$\lim_{*} F_{K,N}(\lambda_1,\ldots,\lambda_K) = \prod_{1\leqslant j<k\leqslant m}(\mu_k-\mu_j)^{-4q_kq_j}\prod_{i=1}^{m}\frac{\zeta_N^{2q_i}(\mu_i)}{G(2q_i+1)}\det_{\substack{1\leqslant l_i\leqslant 2q_i\\ 1\leqslant i\leqslant m\\ 1\leqslant j\leqslant 2|q|}}\left[\frac{\mathrm{d}^{l_i-1}}{\mathrm{d}\mu_i^{l_i-1}}r_{N+j-1}(\mu_i)\right]. \tag{39}$$

In (39) the columns of the determinant are ordered such that one starts with $i=1$, writes out the $2q_1$ columns depending on l_1, and then moves to $i=2$, etc. We remark that we have now already obtained one of the two Barnes G-function factors that appear in (21).

The special property possessed by the Hermite and Laguerre polynomials that allows us to derive a duality formula for $\mathcal{H}_{N,m,q}(\mu)$ for the specific weights (22) and (23) is that they can be expressed in terms of contour integrals. Indeed, by suitably massaging the standard results in Szegö's book[37] we find

$$\pi_{N+j-1}^{(N)}(\mu_i) = \begin{cases} c_j(N)e^{2N\mu_i^2}\displaystyle\int_{\mathcal{C}}\mathrm{d}z\, e^{-2Nz\mu_i+Nz^2/2}z^{N+j-1}, & \text{Hermite},\\ c_j(N)\displaystyle\int_{\mathcal{C}}\mathrm{d}z\, e^{-2Nz\mu_i}\frac{(z+2)^{N+\alpha}}{z^{N+1}}\left(\frac{1}{z}+\frac{1}{2}\right)^{j-1}, & \text{Laguerre}, \end{cases} \tag{40}$$

$$c_j(N) = \begin{cases} \sqrt{\dfrac{2N}{\pi}}\dfrac{1}{i2^{N+j}}, & \text{Hermite},\\ (-1)^{N+j-1}\dfrac{(N+j-1)!}{N^{N+j-1}}\dfrac{1}{2^{2N+j+\alpha}\pi i}, & \text{Laguerre}, \end{cases} \tag{41}$$

where in the Hermite case the contour $\mathcal{C}$ lies along the imaginary axis and is oriented from $-i\infty$ to $+i\infty$, and in the Laguerre case $\mathcal{C}$ is a closed positively oriented contour which encircles the origin but does not contain the point $z=-2$.

It is now straightforward to compute the derivatives required in (39) from the contour integrals in (40). Defining

$$\zeta_N(\mu_i) = \begin{cases} e^{2N\mu_i^2}, & \text{Hermite},\\ 1, & \text{Laguerre}, \end{cases} \tag{42}$$

and recalling the definition (34) we obtain

$$\frac{\mathrm{d}^{l_i-1}}{\mathrm{d}\mu_i^{l_i-1}}r_{N+j-1}(\mu_i) = c_j(N)d_{l_i}(N)\int_{\mathcal{C}}\mathrm{d}z\, e^{-NS(z,\mu_i)}u(z)z^{l_i-1}[z^{\delta}+c]^{j-1}, \tag{43}$$

where

$$S(z,\mu_i) := \begin{cases} 2\mu_i z-\log(z)-\dfrac{z^2}{2}, & \text{Hermite},\\ 2\mu_i z+\log(z)-\log(z+2), & \text{Laguerre}, \end{cases} \tag{44}$$

$$u(z) := \begin{cases} 1, & \text{Hermite},\\ \dfrac{(z+2)^{\alpha}}{z}, & \text{Laguerre}, \end{cases} \tag{45}$$

$$d_{l_i}(N) := (-2N)^{l_i-1}, \tag{46}$$

and where $\delta=\pm 1$ and $c=0,1/2$ in the Hermite and Laguerre cases, respectively.

Our task now is to simplify the determinant appearing in (39) by using the contour integral (43). This is achieved by the following lemma.

Lemma 2: If $q \in \mathbb{N}^m$, *and* $\delta = \pm 1$, *and we define*

$$b_{\delta,q_i}(z) := \begin{cases} 1, & \delta = +1, \\ iz^{1-2q_i}, & \delta = -1, \end{cases} \tag{47}$$

then

$$\begin{aligned} &\det_{\substack{1\leqslant l_i\leqslant 2q_i \\ 1\leqslant i\leqslant m \\ 1\leqslant j\leqslant 2|q|}} \left[\int_{\mathcal{C}} \mathrm{d}z_{\tau(i)+l_i} e^{-NS(z_{\tau(i)+l_i},\mu_i)} u(z_{\tau(i)+l_i}) z_{\tau(i)+l_i}^{l_i-1} [z_{\tau(i)+l_i}^{\delta} + c]^{j-1} \right] \\ &\quad = \prod_{i=1}^{m} \frac{1}{\Gamma(2q_i+1)} \prod_{i=1}^{m} \prod_{l_i=\tau(i)+1}^{\tau(i+1)} \int_{\mathcal{C}} \mathrm{d}z_{l_i} e^{-NS(z_{l_i},\mu_i)} u(z_{l_i}) b_{\delta,q_i}(z_{l_i}) \prod_{i=1}^{m} \Delta_{2q_i}^2(z_{\tau(i)+1},\ldots,z_{\tau(i+1)}) \\ &\qquad \times \prod_{1\leqslant j<k\leqslant m} \prod_{l_k=\tau(k)+1}^{\tau(k+1)} \prod_{l_j=\tau(j)+1}^{\tau(j+1)} (z_{l_k}^{\delta} - z_{l_j}^{\delta}). \end{aligned} \tag{48}$$

Proof: We start with the identity

$$\begin{aligned} &\det_{\substack{1\leqslant l_i\leqslant 2q_i \\ 1\leqslant i\leqslant m \\ 1\leqslant j\leqslant 2|q|}} \left[\int \mathrm{d}z_{\tau(i)+l_i} g_{l_i}(z_{\tau(i)+l_i},\mu_i) [f(z_{\tau(i)+l_i})]^{j-1} \right] \\ &\quad = \prod_{i=1}^{m} \prod_{l_i=1}^{2q_i} \int \mathrm{d}z_{\tau(i)+l_i} g_{l_i}(z_{\tau(i)+l_i},\mu_i) \Delta_{2|q|}(f(z_1),\ldots,f(z_{2|q|})), \end{aligned} \tag{49}$$

which is valid for arbitrary integrable functions $f(z)$ and $g_{l_i}(z,\mu_i)$. If we apply (49) to the left-hand side (LHS) of (48) and use the elementary fact that

$$\Delta_n(z_1+c, z_2+c, \ldots, z_n+c) = \Delta_n(z_1, z_2, \ldots, z_n), \tag{50}$$

we obtain

$$\text{LHS of (48)} = \prod_{i=1}^{m} \prod_{l_i=1}^{2q_i} \int_{\mathcal{C}} \mathrm{d}z_{\tau(i)+l_i} z_{\tau(i)+l_i}^{l_i-1} \prod_{i=1}^{m} \prod_{l_i=\tau(i)+1}^{\tau(i+1)} e^{-NS(z_{l_i},\mu_i)} u(z_{l_i}) \cdot \Delta_{2|q|}(z_1^{\delta},\ldots,z_{2|q|}^{\delta}). \tag{51}$$

To proceed further we first note the following two useful identities.

Lemma 3: If $f(z_1,\ldots,z_{2|q|})$ *is a totally antisymmetric function of each set of variables* $\{z_{\tau(i)+1},\ldots,z_{\tau(i+1)}\}$, *for* $i = 1,2,\ldots,m$, *then*

$$\begin{aligned} &\prod_{i=1}^{m} \prod_{l_i=1}^{2q_i} \int \mathrm{d}z_{\tau(i)+l_i} z_{\tau(i)+l_i}^{l_i-1} f(z_1,\ldots,z_{2|q|}) \\ &\quad = \prod_{i=1}^{m} \frac{1}{\Gamma(2q_i+1)} \prod_{i=1}^{m} \left(\prod_{l_i=\tau(i)+1}^{\tau(i+1)} \int \mathrm{d}z_{l_i} \right) \Delta_{2q_i}(z_{\tau(i)+1},\ldots,z_{\tau(i+1)}) \cdot f(z_1,\ldots,z_{2|q|}). \end{aligned} \tag{52}$$

Proof: By expanding the Vandermonde determinant and then rearranging the order of integrations we see that

$$\prod_{i=1}^{m}\left(\prod_{l_i=\tau(i)+1}^{\tau(i+1)}\int \mathrm{d}z_{l_i}\right)\Delta_{2q_i}(z_{\tau(i)+1},\ldots,z_{\tau(i+1)})\cdot f(\ldots,z_{\tau(i)+1},\ldots,z_{\tau(i)+2q_i},\ldots)$$
$$=\prod_{i=1}^{m}\sum_{\sigma_i\in S_{2q_i}}\prod_{l_i=1}^{2q_i}\int \mathrm{d}z_{\tau(i)+\sigma_i(l_i)}z_{\tau(i)+\sigma_i(l_i)}^{l_i-1}(-1)^{\sigma_i}\cdot f(\ldots,z_{\tau(i)+1},\ldots,z_{\tau(i)+2q_i},\ldots), \tag{53}$$

and the antisymmetry of f then implies that the right-hand side of (53) equals

$$\prod_{i=1}^{m}\sum_{\sigma_i\in S_{2q_i}}\prod_{l_i=1}^{2q_i}\int \mathrm{d}z_{\tau(i)+\sigma_i(l_i)}\,z_{\tau(i)+\sigma_i(l_i)}^{l_i-1}\cdot f(\ldots,z_{\tau(i)+\sigma_i(1)},\ldots,z_{\tau(i)+\sigma_i(2q_i)},\ldots)$$
$$=\prod_{i=1}^{m}\sum_{\sigma_i\in S_{2q_i}}\prod_{l_i=1}^{2q_i}\int \mathrm{d}z_{\tau(i)+l_i}\,z_{\tau(i)+l_i}^{l_i-1}\cdot f(\ldots,z_{\tau(i)+1},\ldots,z_{\tau(i)+2q_i},\ldots), \tag{54}$$

where the last equality follows by simply relabeling integration variables. The stated result is now immediate. ■

Lemma 4: With q, δ and $b_{\delta,q_i}(z)$ as defined in Lemma 2 we have

$$\Delta_{2q_i}(z_1^{\delta},\ldots,z_{2q_i}^{\delta})\Delta_{2q_i}(z_1,\ldots,z_{2q_i})=\prod_{l=1}^{2q_i}b_{\delta,q_i}(z_l)\cdot\Delta_{2q_i}^2(z_1,\ldots,z_{2q_i}). \tag{55}$$

Proof: When $\delta=1$ there is nothing to prove, so take $\delta=-1$. Then

$$\Delta_{2q_i}(z_1^{\delta},\ldots,z_{2q_i}^{\delta})\Delta_{2q_i}(z_1,\ldots,z_{2q_i})=\prod_{1\leqslant j<k\leqslant 2q_i}\frac{(z_j-z_k)(z_k-z_j)}{z_jz_k} \tag{56}$$

$$=(-1)^{2q_i^2+q_i}\prod_{1\leqslant j<k\leqslant 2q_i}\frac{1}{z_jz_k}\cdot\Delta_{2q_i}^2(z_1,\ldots,z_{2q_i}) \tag{57}$$

$$=\prod_{l=1}^{2q_i}iz_l^{1-2q_i}\cdot\Delta_{2q_i}^2(z_1,\ldots,z_{2q_i}). \tag{58}$$

■

Armed with Lemmas 3 and 4 the proof of Lemma 2 follows at once. Applying Lemma 3 to (51) results in

$$\text{LHS of (48)}=\prod_{i=1}^{m}\frac{1}{\Gamma(2q_i+1)}\prod_{i=1}^{m}\left(\prod_{l_i=\tau(i)+1}^{\tau(i+1)}\int_{\mathcal{C}}\mathrm{d}z_{l_i}\right)\Delta_{2q_i}(z_{\tau(i)+1},\ldots,z_{\tau(i+1)})$$
$$\times\prod_{i=1}^{m}\prod_{l_i=\tau(i)+1}^{\tau(i+1)}e^{-NS(z_{l_i},\mu_i)}u(z_{l_i})\cdot\Delta_{2|q|}(z_1^{\delta},\ldots,z_{2|q|}^{\delta}) \tag{59}$$

$$=\prod_{i=1}^{m}\frac{1}{\Gamma(2q_i+1)}\prod_{i=1}^{m}\prod_{l_i=\tau(i)+1}^{\tau(i+1)}\int_{\mathcal{C}}\mathrm{d}z_{l_i}\,e^{-NS(z_{l_i},\mu_i)}u(z_{l_i})\prod_{i=1}^{m}\Delta_{2q_i}(z_{\tau(i)+1}^{\delta},\ldots,z_{\tau(i+1)}^{\delta})\Delta_{2q_i}(z_{\tau(i)+1},\ldots,z_{\tau(i+1)})$$
$$\times\prod_{1\leqslant j<k\leqslant m}\prod_{l_k=\tau(k)+1}^{\tau(k+1)}\prod_{l_j=\tau(j)+1}^{\tau(j+1)}(z_{l_k}^{\delta}-z_{l_j}^{\delta}). \tag{60}$$

Applying Lemma 4 to the right-hand side of (60) produces the stated result. ■

Now we substitute (43) into (39), factor out the constants $c_j(N)$ and $d_{l_i}(N)$ from the determinant, and apply Lemma 2 to finally obtain the following.

Proposition 1:

$$\mathcal{H}_{N,m,q}(\mu) = h_{N,m,q}\prod_{i=1}^{m}\frac{1}{G(2q_i+1)\Gamma(2q_i+1)}\prod_{i=1}^{m}\zeta_N^{2q_i}(\mu_i)\prod_{1\leqslant j<k\leqslant m}(\mu_k-\mu_j)^{-4q_jq_k}\cdot I_{N,m,q}(\mu), \tag{61}$$

where

$$\begin{aligned} I_{N,m,q}(\mu) \coloneqq & \prod_{i=1}^{m}\prod_{l_i=\tau(i)+1}^{\tau(i+1)}\int_{\mathcal{C}}\mathrm{d}z_{l_i}\, e^{-NS(z_{l_i},\mu_i)}\Delta_{2q_i}^2(z_{\tau(i)+1},\ldots,z_{\tau(i+1)}) \\ & \times\prod_{i=1}^{m}\prod_{l_i=\tau(i)+1}^{\tau(i+1)} g_{q_i}(z_{l_i})\prod_{1\leqslant j<k\leqslant m}\prod_{l_k=\tau(k)+1}^{\tau(k+1)}\prod_{l_j=\tau(j)+1}^{\tau(j+1)}(z_{l_k}^{\delta}-z_{l_j}^{\delta}), \end{aligned} \tag{62}$$

the function $g_{q_i}(z)$ *is*

$$g_{q_i}(z) \coloneqq u(z)b_{\delta,q_i}(z) \tag{63}$$

$$= \begin{cases} 1, & \text{Hermite}, \\ i\dfrac{(z+2)^{\alpha}}{z^{2q_i}}, & \text{Laguerre}, \end{cases} \tag{64}$$

and

$$h_{N,m,q} \coloneqq \prod_{j=1}^{\tau(m+1)} c_j(N)\prod_{i=1}^{m}\prod_{l_i=1}^{2q_i} d_{l_i}(N)\cdot\frac{H_{N,N}}{H_{N+|q|,N}}. \tag{65}$$

Proposition 1 is an exact duality formula when $q\in\mathbb{N}^m$, expressing the N-fold integral $\mathcal{H}_{N,m,q}(\mu)$ in terms of the $2|q|$-fold integral $I_{N,m,q}(\mu)$. This allows us to compute the large N asymptotics of $\mathcal{H}_{N,m,q}(\mu)$ by computing the large N asymptotics of $I_{N,m,q}(\mu)$, and the latter can be obtained by using the saddle point method. This is the subject of Sec. III.

The prefactor $h_{N,m,q}$ defined in (65) can be expressed in terms of the Barnes' G-function by using known results for the Selberg integral, see, e.g., Refs. 8 and 28, and the asymptotics can then be obtained from the known asymptotics of Barnes' G-function.[38] We obtain

$$h_{N,m,q} = \begin{cases} 2^{-|q|^2-3|q|/2+\sum_{i=1}^{m}2q_i^2}\pi^{-3|q|/2}N^{\sum_{i=1}^{m}2q_i^2+|q|^2/2+|q|N}\dfrac{G(N+2)}{G(N+|q|+2)}, & \text{Hermite}, \\ (-1)^{|q|}2^{-2|q|+\sum_{i=1}^{m}2q_i^2}\pi^{-2|q|}N^{(\alpha-|q|)|q|+\sum_{i=1}^{m}2q_i^2} & \\ \times\dfrac{G(N+2)}{G(N+1)}\dfrac{G(N+\alpha+1)}{G(N+\alpha+|q|+1)}\dfrac{G(N+2|q|+1)}{G(N+|q|+2)}, & \text{Laguerre}, \end{cases} \tag{66}$$

$$= \begin{cases} N^{\sum_{i=1}^{m}(2q_i^2-q_i)}e^{|q|N}2^{-|q|^2}\displaystyle\prod_{i=1}^{m}2^{2q_i^2-2q_i}\pi^{-2q_i}\left[1+O\left(\frac{1}{N}\right)\right], & \text{Hermite}, \\ N^{\sum_{i=1}^{m}(2q_i^2-q_i)}\displaystyle\prod_{i=1}^{m}(-1)^{q_i}2^{2q_i^2-2q_i}\pi^{-2q_i}\left[1+O\left(\frac{1}{N}\right)\right], & \text{Laguerre}. \end{cases} \tag{67}$$

It will be useful in Sec. III for us to introduce the notation

$$h_{N,m,q} = N^{\sum_{i=1}^{m}(2q_i^2-q_i)} h_0 \left[1 + O\left(\frac{1}{N}\right)\right], \tag{68}$$

where

$$h_0 := \begin{cases} e^{|q|N} 2^{-|q|^2} \prod_{i=1}^{m} 2^{2q_i^2-2q_i} \pi^{-2q_i}, & \text{Hermite}, \\ \prod_{i=1}^{m} (-1)^{q_i} 2^{2q_i^2-2q_i} \pi^{-2q_i}, & \text{Laguerre}. \end{cases} \tag{69}$$

III. ASYMPTOTICS

Now we begin the task of computing the large N asymptotics of the integral $I_{N,m,q}(\mu)$ for fixed μ and q. Since the only appearance that N makes in (62) is in the exponent of $e^{-NS(z,\mu_i)}$, this problem is a natural candidate for the saddle point method.

In both the Hermite and Laguerre cases, the function $S(z,\mu_i)$ has two saddle points, $z_{+,i}$ and its complex conjugate $z_{+,i}^*$. Explicitly

$$z_{+,i} = \begin{cases} \mu_i + i\sqrt{1-\mu_i^2}, & \text{Hermite}, \\ -1 + i\sqrt{\dfrac{1}{\mu_i} - 1}, & \text{Laguerre}. \end{cases} \tag{70}$$

It is worth noting that in both cases

$$\mathrm{Im}\{z_{+,i}\} = \frac{\pi}{2}\rho(\mu_i), \tag{71}$$

where $\rho(\mu_i)$ is as defined in (22) and (23), for the Hermite and Laguerre cases, respectively. Both saddle points are of equal importance, since

$$\mathrm{Re}\{S(z_{+,i},\mu_i)\} = \mathrm{Re}\{S(z_{+,i}^*,\mu_i)\}, \tag{72}$$

and we deform the contour $\mathcal{C}$ through both of them.

Let us denote the subset of the contour in neighborhoods of $z_{+,i}$ and $z_{+,i}^*$ by $\Omega_{+,i}$ and $\Omega_{-,i}$, respectively, and the complement of the union of these two neighborhoods in $\mathcal{C}$ by $\mathcal{C}_s$, so that

$$\mathcal{C} = \mathcal{C}_s \cup \Omega_{+,i} \cup \Omega_{-,i}. \tag{73}$$

By deforming $\mathcal{C}$ appropriately, the dominant contribution of each integral comes from $\Omega_{+,i}$ and $\Omega_{-,i}$, and the standard arguments of the saddle point method lead to

$$\begin{aligned} I_{N,m,q}(\mu) = {} & \prod_{i=1}^{m} \prod_{l_i=\tau(i)+1}^{\tau(i+1)} \left(\int_{\Omega_{+,i}} \mathrm{d}z_{l_i} + \int_{\Omega_{-,i}} \mathrm{d}z_{l_i} \right) e^{-NS(z_{l_i},\mu_i)} \cdot \Delta_{2q_i}^2(z_{\tau(i)+1},\ldots,z_{\tau(i+1)}) \\ & \times \prod_{i=1}^{m} \prod_{l_i=\tau(i)+1}^{\tau(i+1)} g_{q_i}(z_{l_i}) \prod_{1\le j<k\le m} \prod_{l_k=\tau(k)+1}^{\tau(k+1)} \prod_{l_j=\tau(j)+1}^{\tau(j+1)} (z_{l_k}^{\delta} - z_{l_j}^{\delta}) + \prod_{i=1}^{m} e^{-2q_i N \,\mathrm{Re}\{S_i\}} \cdot O(e^{-\varepsilon N}), \end{aligned} \tag{74}$$

for suitably small $\varepsilon > 0$, where we have defined

$$S_i := S(z_{+,i},\mu_i) = S(z_{+,i}^*,\mu_i)^*. \tag{75}$$

We would now like to expand out the $2|q|$-fold composition of the sum of the two integrals appearing in (74). To achieve this, we first note that the integrand in (74) is totally symmetric in each set of variables $\{z_{\tau(i)+1},\ldots,z_{\tau(i+1)}\}$, for $i=1,2,\ldots,m$. With this in mind we can then apply the following elementary result.

Lemma 5: If $f(z_1,\ldots,z_{\tau(i)+1},\ldots,z_{\tau(i+1)},\ldots,z_{\tau(m+1)})$ *is a totally symmetric function of the variables* $\{z_{\tau(i)+1},\ldots,z_{\tau(i+1)}\}$, *then*

$$\prod_{l_i=\tau(i)+1}^{\tau(i+1)}\left(\int_{\Omega_{+,i}}dz_{l_i}+\int_{\Omega_{-,i}}dz_{l_i}\right)f(z_1,\ldots,z_{\tau(i)+1},\ldots,z_{\tau(i+1)},\ldots,z_{\tau(m+1)})$$
$$=\sum_{n_i=0}^{2q_i}\binom{2q_i}{n_i}\prod_{l_i=\tau(i)+1}^{\tau(i)+n_i}\int_{\Omega_{+,i}}dz_{l_i}\prod_{l_i=\tau(i)+n_i+1}^{\tau(i+1)}\int_{\Omega_{-,i}}dz_{l_i}\,f(z_1,\ldots,z_{\tau(i)+1},\ldots,z_{\tau(i+1)},\ldots,z_{\tau(m+1)}). \quad (76)$$

Proof: All terms in the expansion with n_i integrals over $\Omega_{+,i}$ can be seen to be equal by swapping the order of the integrations, permuting the arguments of f in $\{z_{\tau(i)+1},\ldots,z_{\tau(i+1)}\}$, and then relabeling the integration variables appropriately. ■

Applying Lemma 5 to (74) results in

$$I_{N,m,q}(\mu)=\prod_{i=1}^{m}\sum_{n_i=0}^{2q_i}\binom{2q_i}{n_i}\prod_{l_i=\tau(i)+1}^{\tau(i)+n_i}\int_{\Omega_{+,i}}dz_{l_i}\prod_{l_i=\tau(i)+n_i+1}^{\tau(i+1)}\int_{\Omega_{-,i}}dz_{l_i}\prod_{i=1}^{m}\left(\prod_{l_i=\tau(i)+1}^{\tau(i+1)}e^{-NS(z_{l_i},\mu_i)}g_{q_i}(z_{l_i})\right)$$
$$\times\Delta_{2q_i}^2(z_{\tau(i)+1},\ldots,z_{\tau(i+1)})\cdot\prod_{1\leqslant j<k\leqslant m}\prod_{l_k=\tau(k)+1}^{\tau(k+1)}\prod_{l_j=\tau(j)+1}^{\tau(j+1)}(z_{l_k}^{\delta}-z_{l_j}^{\delta})+\prod_{i=1}^{m}e^{-2q_iN\,\mathrm{Re}\{S_i\}}\cdot O(e^{-\varepsilon N}). \quad (77)$$

Now let us parametrize the integration variables in (77) so that the paths $\Omega_{\pm,i}$ become line segments (of length 2η say), centered at $z_{+,i}$ and $z_{+,i}^*$, respectively, and lying along the direction of steepest descent

$$z_{l_i}=\begin{cases}z_{+,i}+e^{i\theta_i}t_{l_i}, & \tau(i)+1\leqslant l_i\leqslant\tau(i)+n_i,\\ z_{+,i}^*+e^{-i\theta_i}t_{l_i}, & \tau(i)+n_i+1\leqslant l_i\leqslant\tau(i)+2q_i.\end{cases} \quad (78)$$

The angles θ_i are chosen in the usual way so that with

$$a_i:=\frac{S''(z_{+,i},\mu_i)}{2}e^{2i\theta_i}=\frac{S''(z_{+,i}^*,\mu_i)}{2}e^{-2i\theta_i} \quad (79)$$

we have $a_i\in(0,\infty)$, and so

$$a_it_{l_i}^2=\frac{S''(z_{+,i},\mu_i)}{2}(z_{l_i}-z_{+,i})^2=\frac{S''(z_{+,i}^*,\mu_i)}{2}(z_{l_i}-z_{+,i}^*)^2, \quad (80)$$

with $t_{l_i}\in[-\eta,\eta]$. With this convention the integrals through $z_{+,i}$ are oriented in the negative direction, and we will compensate for this by introducing the explicit factor $(-1)^{n_i}$. Explicitly, since

$$\frac{S''(z_{+,i},\mu_i)}{2}=\begin{cases}\dfrac{\pi}{2}\rho(\mu_i)e^{i(\mathrm{Arcsin}(\mu_i)+\pi)}, & \text{Hermite},\\ \pi\mu_i^2\rho(\mu_i)e^{-i\pi/2}, & \text{Laguerre},\end{cases} \quad (81)$$

we obtain

$$\theta_i = \begin{cases} \dfrac{\pi - \operatorname{Arcsin}(\mu_i)}{2}, & \text{Hermite}, \\ \dfrac{\pi}{4}, & \text{Laguerre}, \end{cases} \tag{82}$$

$$a_i = \begin{cases} \dfrac{\pi}{2}\rho(\mu_i), & \text{Hermite}, \\ \pi\mu_i^2\rho(\mu_i), & \text{Laguerre}. \end{cases} \tag{83}$$

Note that $a_i > 0$ when $\mu_i \in \operatorname{int}(\operatorname{supp}\rho)$.

In making the change of variables (78) in (77), it is convenient to introduce the following definitions:

$$\phi_{N,i} := 4q_i\theta_i + 2N\,\mathrm{Im}\{S_i\}, \tag{84}$$

$$\varphi_i(t_{l_i}) := \sum_{k=1}^{\infty} \frac{2}{S''(z_{+,i},\mu_i)} \frac{S^{(k+2)}(z_{+,i},\mu_i)}{(k+2)!} (z_{l_i} - z_{+,i})^k|_{z_{l_i}=z_{+,i}+e^{i\theta_i}t_{l_i}}, \tag{85}$$

$$\Phi_n(t) := \prod_{i=1}^{m} \prod_{l_i=\tau(i)+1}^{\tau(i)+n_i} e^{-Na_it_{l_i}^2\varphi_i(t_{l_i})} \prod_{l_i=\tau(i)+n_i+1}^{\tau(i+1)} e^{-Na_it_{l_i}^2\varphi_i^*(t_{l_i})}, \tag{86}$$

$$G_n(t) := \prod_{i=1}^{m} \prod_{l_i=\tau(i)+1}^{\tau(i+1)} g_{q_i}(z_{l_i})|_{\bigstar}, \tag{87}$$

$$D_n(t) := \prod_{i=1}^{m} \prod_{k_i=\tau(i)+n_i+1}^{\tau(i+1)} \prod_{j_i=\tau(i)+1}^{\tau(i)+n_i} (z_{k_i} - z_{j_i})^2|_{\bigstar}, \tag{88}$$

$$H_n(t) := \prod_{1\le j<k\le m} \prod_{l_k=\tau(k)+1}^{\tau(k+1)} \prod_{l_j=\tau(j)+1}^{\tau(j+1)} (z_{l_k}^{\delta} - z_{l_j}^{\delta})|_{\bigstar}, \tag{89}$$

$$F_n(t) := G_n(t)D_n(t)H_n(t), \tag{90}$$

where $\bigstar$ on the right-hand sides of (87)–(89) refers to the change of variables (78), and $n := (n_1,\ldots,n_m)$. We also define the (unnormalized) integral operator

$$\mathbb{E}_{r,p}^{(i)} := \prod_{l_i=\tau(i)+r}^{\tau(i)+p} \int_{-\eta}^{\eta} \mathrm{d}t_{l_i}\, e^{-Na_it_{l_i}^2} \Delta_{p-r+1}^2(t_{\tau(i)+r},\ldots,t_{\tau(i)+p}). \tag{91}$$

Armed with these definitions, we see that since

$$\begin{aligned} &\Delta_{n_i}^2(z_{\tau(i)+1},\ldots,z_{\tau(i)+n_i})\Delta_{2q_i-n_i}^2(z_{\tau(i)+n_i+1},\ldots,z_{\tau(i)+2q_i}) \prod_{l_i=\tau(i)+1}^{\tau(i+1)} \mathrm{d}z_{l_i} \\ &= e^{i4q_i(q_i-n_i)\theta_i}\Delta_{n_i}^2(t_{\tau(i)+1},\ldots,t_{\tau(i)+n_i})\Delta_{2q_i-n_i}^2(t_{\tau(i)+n_i+1},\ldots,t_{\tau(i)+2q_i}) \prod_{l_i=\tau(i)+1}^{\tau(i+1)} \mathrm{d}t_{l_i}, \end{aligned} \tag{92}$$

and

$$\prod_{i=1}^{m}\prod_{l_i=\tau(i)+1}^{\tau(i+1)} e^{-NS(z_{l_i},\mu_i)} = \prod_{i=1}^{m} e^{-2q_iN\,\mathrm{Re}\{S_i\}}\prod_{i=1}^{m} e^{2i(q_i-n_i)N\,\mathrm{Im}\{S_i\}}\prod_{i=1}^{m}\prod_{l_i=\tau(i)+1}^{\tau(i+1)} e^{-Na_it_{l_i}^2}\Phi_n(t), \tag{93}$$

we arrive at the following more compact expression for $I_{N,m,q}(\mu)$:

$$I_{N,m,q}(\mu) = \prod_{i=1}^{m} e^{-2q_iN\,\mathrm{Re}\{S_i\}}\left[\prod_{i=1}^{m}\sum_{n_i=0}^{2q_i}\binom{2q_i}{n_i}(-1)^{n_i}e^{i(q_i-n_i)\phi_{N,i}}\mathbb{I}_{1,n_i}^{(i)}\mathbb{I}_{n_i+1,2q_i}^{(i)}\Phi_n(t)F_n(t)+O(e^{-\varepsilon N})\right]. \tag{94}$$

The factor $(-1)^{n_i}$ results from the fact that we traversed the line through $z_{+,i}$ in the negative direction, whereas the line through $z_{+,i}^*$ is traversed in the positive direction.

To obtain an asymptotic expansion of $I_{N,m,q}(\mu)$ from (94) we proceed in direct analogy with the one-dimensional saddle point method (see, e.g., Ref. 39) and introduce the following generalization of $\Phi_n(t)$:

$$\Phi_n(t,u) := \prod_{i=1}^{m}\prod_{l_i=\tau(i)+1}^{\tau(i)+n_i} e^{u_{l_i}\varphi_i(t_{l_i})}\prod_{l_i=\tau(i)+n_i+1}^{\tau(i+1)} e^{u_{l_i}\varphi_i^*(t_{l_i})}, \tag{95}$$

where $u\in\mathbb{R}^{2|q|}$. For convenience we also introduce the function

$$Q_n(t,u) := \Phi_n(t,u)F_n(t), \tag{96}$$

so that with

$$u_{l_i} = -Na_it_{l_i}^2 \quad \text{for each } 1\leqslant l_i\leqslant 2|q|, \tag{97}$$

we have

$$Q_n(t,\{-Na_it_{l_i}^2\}) = \Phi_n(t)F_n(t). \tag{98}$$

Let us suppose for the present that u is some arbitrary fixed parameter independent of t, and consider the kth degree Taylor polynomial of $Q_n(t,u)$ as a function of $t\in\mathbb{R}^{2|q|}$,

$$Q_n(t,u) = \sum_{0\leqslant|\alpha|\leqslant k}\frac{1}{\alpha!}\left[\frac{\partial^{\alpha_1}}{\partial t_1^{\alpha_1}}\cdots\frac{\partial^{\alpha_{2|q|}}}{\partial t_{2|q|}^{\alpha_{2|q|}}}Q_n(t,u)\right|_{t=0}\Bigg]t^{\alpha}+O(t^{\alpha})\big|_{|\alpha|=k+1}, \tag{99}$$

where $\alpha\in\mathbb{Z}_{\geqslant 0}^{2|q|}$ and we use the standard notations $\alpha!=\alpha_1!\cdots\alpha_{2|q|}!$ and $t^{\alpha}=t_1^{\alpha_1}\cdots t_{2|q|}^{\alpha_{2|q|}}$ and $|\alpha|=\alpha_1+\cdots+\alpha_{2|q|}$.

If in (99) we now choose u according to (97) we obtain

$$Q_n(t,\{-Na_it_{l_i}^2\}) = \sum_{0\leqslant|\alpha|\leqslant k}\frac{1}{\alpha!}\left[\frac{\partial^{\alpha_1}}{\partial t_1^{\alpha_1}}\cdots\frac{\partial^{\alpha_{2|q|}}}{\partial t_{2|q|}^{\alpha_{2|q|}}}\Phi_n(t,u)F_n(t)\right|_{t=0}\Bigg]\Bigg|_{\{u_{l_i}=-Na_it_{l_i}^2\}}t^{\alpha}+O(t^{\alpha})\big|_{|\alpha|=k+1}, \tag{100}$$

where we emphasize that the partial derivatives with respect to t on the right-hand side of (100) are performed with u fixed *before* making the substitution (97). The effect of constructing the Taylor series in this way is that when (100) is substituted into (94) and the integrations are performed, each term corresponding to a given value of $|\alpha|$ in (100) will have the same N dependence. To see this we need to consider the asymptotics of the integral operator (91) acting on a general monomial, which can be deduced simply by scaling N out of the integral. We thus deduce that

$$\prod_{i=1}^{m} \mathbb{E}^{(i)}_{1,n_i} \mathbb{E}^{(i)}_{n_i+1,2q_i} t^{\alpha} = O\left(N^{-\sum_{i=1}^{m} q_i^2 - \sum_{i=1}^{m} (n_i - q_i)^2 - |\alpha|/2}\right). \tag{101}$$

As a direct consequence of (101), we see that with $u_{l_i} = -a_i N t_{l_i}^2$ for each $1 \leqslant l_i \leqslant 2|q|$, we have

$$\prod_{i=1}^{m} \mathbb{E}^{(i)}_{1,n_i} \mathbb{E}^{(i)}_{n_i+1,2q_i} t^{\alpha} u^{\alpha'} = O\left(N^{-\sum_{i=1}^{m} q_i^2 - \sum_{i=1}^{m} (n_i - q_i)^2 - |\alpha|/2}\right) \tag{102}$$

for any $\alpha_1', \ldots, \alpha_{2|q|}' \in \mathbb{N}$; i.e., the left-hand sides of (101) and (102) have precisely the same asymptotic dependence on N. From (95) its clear that when computing the partial derivatives of $\Phi_n(t,u)F_n(t)$ for a given $|\alpha|$ various powers of u will appear, which after the substitution (97) will mean we need to calculate quantities of the form (102). However (101) and (102) tell us that all such quantities have the same N dependence. This would not be the case if we had just naively constructed the Taylor polynomial of $\Phi_n(t)F_n(t)$. We remark that since the symmetry of the integral operator (91) implies t^{α} is annihilated whenever $|\alpha|$ is odd, only integer powers of $1/N$ actually appear in the asymptotic expansion of $I_{N,m,q}(\mu)$, despite the appearance of $|\alpha|/2$ in the exponent in (102).

As a result of the expression (102) we can see that the dominant term in the asymptotic expansion of (94) occurs when both $n_i = q_i$ for all $i = 1, \ldots, m$, and $|\alpha| = 0$ in the Taylor expansion (100). In general, the coefficient of the term which is of order $1/N^k$ relative to the leading term is composed of all terms for which

$$\sum_{i=1}^{m} (n_i - q_i)^2 + \frac{|\alpha|}{2} = k. \tag{103}$$

If we are interested only in retaining the leading term the preceding arguments imply that

$$I_{N,m,q}(\mu) = \prod_{i=1}^{m} \frac{e^{-2q_i N \mathrm{Re}\{S_i\}}}{N^{q_i^2}} \cdot I_0 \left[1 + O\left(\frac{1}{N}\right)\right], \tag{104}$$

where the coefficient I_0 depends on μ and q but is independent of N. To obtain the explicit form of I_0 we first note that, since $\Phi_n(0) = 1$, we have

$$\mathbb{E}^{(i)}_{r+1,r+p} \Phi_n(0) F_n(0) = \frac{1}{N^{p^2/2}} F_n(0) Z_p(a_i) + O(e^{-\eta^2 a_i N}), \tag{105}$$

where

$$Z_p(a_i) := \int_{\mathbb{R}^p} \mathrm{d}^p x \, \Delta_p^2(x) \prod_{l=1}^{p} e^{-a_i x_l^2} \tag{106}$$

$$= \left(\frac{\pi}{2^{p-1}}\right)^{p/2} \frac{G(p+2)}{a_i^{p^2/2}}. \tag{107}$$

The quantity $Z_p(a_i)$ is the normalization of the joint eigenvalue pdf of the GUE and can be expressed in terms of the Selberg integral; see Refs. 8 and 28. If we substitute (100) into (94) and take the leading term, which corresponds to $\Sigma_{i=1}^{m} (n_i - q_i)^2 + |\alpha|/2 = 0$, then applying (105) we find that

$$I_0 = \prod_{i=1}^{m} \binom{2q_i}{q_i} (-1)^{q_i} Z_{q_i}^2(a_i) \cdot F_q(0). \tag{108}$$

The explicit form of $F_q(0)$ can be obtained from the following results:

$$D_q(0) = (-1)^{|q|}\pi^{\sum_{i=1}^m 2q_i^2}\prod_{i=1}^m \rho^{2q_i^2}(\mu_i), \tag{109}$$

$$G_q(0) = \begin{cases} 1, & \text{Hermite}, \\ \displaystyle\prod_{i=1}^m (-1)^{q_i}\mu_i^{2q_i^2}\mu_i^{-\alpha q_i}, & \text{Laguerre}, \end{cases} \tag{110}$$

$$H_q(0) = \prod_{1\leqslant j<k\leqslant m}(\mu_k-\mu_j)^{2q_jq_k} \times \begin{cases} 2^{|q|^{2-\sum_{i=1}^m q_i^2}}, & \text{Hermite}, \\ 1, & \text{Laguerre}. \end{cases} \tag{111}$$

Now let us put together what we have learned about the asymptotic behavior of $I_{N,m,q}(\mu)$ to describe the asymptotic behavior of $\mathcal{H}_{N,m,q}(\mu)$ when $q\in\mathbb{N}^m$. To this end, we substitute (109) into (108), then (108) into (104), and finally substitute (104) and (68) into (61), to obtain

$$\begin{aligned}\mathcal{H}_{N,m,q}(\mu) = {} & N^{\sum_{i=1}^m q_i(q_i-1)}\prod_{i=1}^m \frac{G^2(q_i+1)}{G(2q_i+1)}2^{-q_i^2+q_i}\pi^{2q_i^2+q_i}\rho^{2q_i^2}(\mu_i)\prod_{1\leqslant j<k\leqslant m}(\mu_k-\mu_j)^{-4q_jq_k} \\ & \times\prod_{i=1}^m e^{-2q_iN\,\mathrm{Re}\{S_i\}}\zeta_N^{2q_i}(\mu_i)a_i^{-q_i^2}\cdot G_q(0)H_q(0)\cdot h_0\left[1+O\left(\frac{1}{N}\right)\right].\end{aligned} \tag{112}$$

Using the explicit forms for $G_q(0)$ and $H_q(0)$, given by (110) and (111), respectively, one can easily verify that for both the Hermite and Laguerre cases we have the following identity:

$$\begin{aligned}\prod_{i=1}^m e^{-2q_iN\,\mathrm{Re}\{S_i\}}\zeta_N^{2q_i}(\mu_i)a_i^{-q_i^2}\cdot G_q(0)H_q(0)\cdot h_0 = {} & \prod_{i=1}^m \omega_N^{-q_i}(\mu_i)\rho^{-q_i^2}(\mu_i)2^{2q_i^2-2q_i}\pi^{-q_i^2-2q_i} \\ & \times\prod_{1\leqslant j<k\leqslant m}(\mu_k-\mu_j)^{2q_jq_k}.\end{aligned} \tag{113}$$

Inserting the identity (113) into (112) we finally obtain

$$\begin{aligned}\mathcal{H}_{N,m,q}(\mu) = {} & N^{\sum_{i=1}^m (q_i^2-q_i)}\prod_{i=1}^m [\omega_N(\mu_i)]^{-q_i}\prod_{i=1}^m \frac{G^2(q_i+1)}{G(2q_i+1)}(2\pi)^{q_i^2-q_i} \\ & \times\prod_{1\leqslant j<k\leqslant m}|\mu_k-\mu_j|^{-2q_jq_k}\prod_{l=1}^m [\rho(\mu_i)]^{q_i^2}\left[1+O\left(\frac{1}{N}\right)\right],\end{aligned} \tag{114}$$

which does indeed recover (21).

We emphasize that the derivation we have presented for (114) is entirely rigorous for $q\in\mathbb{N}^m$ for any $m\in\mathbb{N}$, thus verifying the legitimacy of the log-gas procedure used in Ref. 5 for the Hermite and Laguerre cases, for such q.

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Exact solutions of two complementary one-dimensional quantum many-body systems on the half-line

Martin Hallnäs and Edwin Langmann
Mathematical Physics, KTH Physics, AlbaNova, SE-106 91 Stockholm, Sweden

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We consider two particular one-dimensional quantum many-body systems with local interactions related to the root system C_N. Both models describe identical particles moving on the half-line with nontrivial boundary conditions at the origin, but in the first model the particles interact with the delta interaction while in the second via a particular momentum dependent interaction commonly known as delta-prime interaction. We show that the Bethe ansatz solution of the delta-interaction model is consistent even for the general case where the particles are distinguishable, whereas for the delta-prime interaction it only is consistent and nontrivial in the fermion case. We also establish a duality between the bosonic delta- and the fermionic delta-prime model, and we elaborate on the physical interpretations of these models. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1865320]

I. INTRODUCTION

Quantum mechanical models with interactions are, in general, very difficult to solve, but there exist a few important cases where exact solutions are available, allowing them to be understood completely. A prominent example is the delta interaction in one dimension which, in the simplest two-particle case, is defined by the Hamiltonian

$$H = -\partial_x^2 + c\,\delta(x), \tag{1}$$

where c is a real coupling constant and $x \in \mathbb{R}$ the relative coordinate of the two particles, $x = x_1 - x_2$. This latter model is popular because it allows for an explicit solution by simple means: since the delta interaction is restricted to $x=0$, it only manifests itself in the nontrivial boundary conditions for eigenfunctions $\psi(x)$ of H [we use the notation $\psi(\pm 0) \equiv \lim_{\varepsilon \downarrow 0} \psi(\pm\varepsilon)$, and similarly for the derivative ψ'],

$$\begin{aligned} \psi(+0) &= \psi(-0), \\ \psi'(+0) - \psi'(-0) &= c\,\psi(+0), \end{aligned} \tag{2}$$

and these can easily be accounted for. The natural generalization of this model to an arbitrary number N of identical particles defines a prominent exactly solvable quantum many-body system which, in the boson case, was solved by Lieb and Liniger[1] (see also Ref. 2) and, in the general case of distinguishable particles, by Yang[3] in a seminal paper where the Yang–Baxter relations first appeared.

Interactions localized at points have been studied extensively using the mathematical theory of defect indices; see Refs. 4–6 and references therein. From these studies it is well known that the delta interaction is only one of many possible local interactions, and that in general such interaction can be characterized by four real coupling parameters. One prominent example of such an interaction, often referred to as delta-prime interaction,[7,8] is defined by the following boundary conditions:

$$\psi'(+0) = \psi'(-0),$$
$$\psi(+0) - \psi(-0) = 4\lambda\psi'(+0), \tag{3}$$

with a real parameter λ. Recently it was shown that these latter boundary conditions arise also from the following formal Hamiltonian:

$$H = -\partial_x^2 + 4\lambda\partial_x\delta(x)\partial_x, \tag{4}$$

where the second term has a physical interpretation as a local interaction depending also on the momentum $\hat{p} = -i\partial_x$ (Ref. 9); see Sec. III A. This interpretation of the boundary conditions in Eq. (3) has the advantage that it does not require an infinite coupling constant renormalization as is the case with the usual one.[7,8] [Note that the coupling constant $\tilde{\lambda}$ in the formal Hamiltonian $-\partial_x^2 + \tilde{\lambda}\delta'(x)$ is dimensionless, whereas the parameter λ in Eq. (3) has the dimension of a length, consistent with Eq. (4). We feel that this former mismatch of physical dimensions is a strong argument in favor of our interpretation.] We will therefore refer to the boundary conditions in Eq. (3) as $\hat{p}\delta\hat{p}$ interaction (see Ref. 10 for yet another interpretation). The N-body generalization of this model is exactly solvable by the Bethe ansatz in the indistinguishable particle case when the particles are either bosons or fermions but, different from the delta-interaction case, not in the general case of distinguishable particles[9] (see also Refs. 5 and 11–13). Still, this model is complementary to the model with the delta interactions for at least three different reasons: first, for indistinguishable particles the delta-interaction model is known to be interesting only for bosons (since the delta interaction is trivial on fermion wave functions), whereas the $\hat{p}\delta\hat{p}$ interaction is trivial for bosons and nontrivial for fermions.[4] Second, while the delta-interaction model for bosons can be obtained as the nonrelativistic limit of the quantum sine Gordon model, the $\hat{p}\delta\hat{p}$-interaction model for fermions naturally arises as the nonrelativistic limit of the massive Thirring model.[9] Third, there exists an interesting weak coupling duality between the fermionic $\hat{p}\delta\hat{p}$-interaction model and the bosonic delta-interaction model.[12]

As is well-known, exactly solvable many-body systems of particles moving on the full real line are naturally associated with the root system A_{N-1}, and they often allow for extensions to other root systems such that the exact solubility is preserved.[14] An early example was given by Gaudin who solved the C_N root system variant of the delta-interaction model for bosons[15] (see also Ref. 16), while the general case of this model for arbitrary root systems and distinguishable particles was treated by Sutherland.[17] As pointed out by Cherednik,[18] models related to the root system C_N describe interacting particles on the half-line, and the exact solubility requires the so-called reflection equation to be added to the Yang–Baxter relations. The reflection equation has played a central role in many exactly solvable systems with a boundary; see, e.g., Refs. 19 and 20.

In this paper we consider the Bethe ansatz solution of the C_N versions of the models discussed above. Similarly as for the A_{N-1} case, we find that the delta-interaction model is exactly solvable in this way even for distinguishable particles, but for the model with momentum independent interactions we obtain its exact solution only for indistinguishable particles. We also elaborate on the physical interpretation of these models as describing particles on the half-line with nontrivial boundary conditions at the origin.

To be more specific, the models we discuss in the paper can be formally defined by the following Hamiltonians:

$$H = -\sum_{j=1}^{N}\partial_{x_j}^2 + 2c_1\sum_{j<k}[\delta(x_j - x_k) + \delta(x_j + x_k)] + c_2\sum_{j=1}^{N}\delta(x_j) \tag{5}$$

(delta interactions) and

$$H = -\sum_{j=1}^{N} \partial_{x_j}^2 + 2\lambda_1 \sum_{j<k} [(\partial_{x_j} - \partial_{x_k})\delta(x_j - x_k)(\partial_{x_j} - \partial_{x_k}) + (\partial_{x_j} + \partial_{x_k})\delta(x_j + x_k)(\partial_{x_j} + \partial_{x_k})]$$
$$+ 4\lambda_2 \sum_{j=1}^{N} \partial_{x_j}\delta(x_j)\partial_{x_j} \tag{6}$$

($\hat{p}\delta\hat{p}$ interactions). For simplicity we assume all coupling constants positive so that there are no bound states. Mathematically, the model in Eq. (5) is the C_N variant of the model solved by Yang,[3] and Eq. (6) defines the C_N variant of the model discussed in Ref. 9.

The plan of the rest of this paper is as follows. In Sec. II we consider the C_N delta-interaction model, starting by deriving the boundary conditions and thus turning the Schrödinger equation $H\psi = E\psi$ into a well-defined mathematical problem. We proceed to the Bethe ansatz solution of this model where the Yang–Baxter relations and the reflection equation play a central role. We conclude the section by elaborating on the physical interpretation of this model. In Sec. III we discuss the C_N variant of the $\hat{p}\delta\hat{p}$-interaction model, in large part paralleling our discussion for the delta interaction in Sec. II. We also present a duality relation between the fermionic $\hat{p}\delta\hat{p}$-interaction model and the bosonic delta-interaction model. Appendix A gives some details on the verification of the Yang–Baxter relations and the reflection equation. Appendix B contains a few mathematical facts about the Weyl group of the root system C_N, and Appendix C gives some details on the physical interpretation of these models.

II. DELTA INTERACTION

In this section we provide the exact solution of the C_N delta interaction in the case of distinguishable particles and elaborate on its physical interpretation.

A. Boundary conditions

The Hamiltonian (5) defining the C_N delta-interaction model is only formal, and to determine its eigenfunctions we must first convert it into a set of boundary conditions.

For completeness we start by discussing the Hamiltonian H in Eq. (1), which can be regarded also as the one-particle case of the Hamiltonian in Eq. (5), $N=1$. The first step in finding the eigenfunctions ψ of H is to note that the equation $H\psi = E\psi$ for all x is equivalent to $-\psi'' = E\psi$ for $x \neq 0$ together with the boundary conditions in Eq. (2). These boundary conditions are obtained by integrating the equation $H\psi = E\psi$, i.e., $-\psi''(x) + c\,\delta(x)\psi(0) = E\psi(x)$, twice, first from $x = -\varepsilon$ to $x > 0$ and then once more from $x = -\varepsilon$ to $x = \varepsilon$ yields the first condition in Eq. (2) in the limit $\varepsilon \downarrow 0$, and integrating from $x = -\varepsilon$ to $x = \varepsilon$ yields the second condition in Eq. (2) in the same limit. Thus in this case there are two regions free of interactions, $x < 0$ and $x > 0$, linked to each other by the boundary condition in Eq. (2) at $x = 0$.

For general N, the interaction terms of the Hamiltonian H in Eq. (5) are restricted to $x_j = \pm x_k$ and $x_j = 0$ for $1 \leqslant j < k \leqslant N$, and the eigenfunctions ψ of H therefore obey the equation

$$\left(\sum_{j=1}^{N} \partial_{x_j}^2 + E\right)\psi(x_1, \ldots, x_N) = 0 \quad \text{for } x_j \neq \pm x_k \text{ and } x_j \neq 0, \tag{7}$$

and for each of the boundaries of the interaction free regions one gets a pair of boundary conditions similarly to the ones for $N=1$,

$$\psi|_{x_j = \pm x_k + 0} = \psi|_{x_j = \pm x_k - 0},$$

$$(\partial_{x_j} - \partial_{x_k})\psi|_{x_j = \pm x_k + 0} - (\partial_{x_j} - \partial_{x_k})\psi|_{x_j = \pm x_k - 0} = 2c_1\, \psi|_{x_j = \pm x_k - 0}, \tag{8a}$$

$$\psi|_{x_j = +0} = \psi|_{x_j = -0},$$

$$\partial_{x_j}\psi|_{x_j=0} - \partial_{x_j}\psi|_{x_j=-0} = c_2\,\psi|_{x_j=+0} \tag{8b}$$

(these conditions are obtained by a straightforward generalization of the $N=1$ argument above, using $\partial_{x_j} \pm \partial_{x_k} = 2\partial_{x_j \pm x_k}$).

Obviously there are now many more regions free of interactions. One such region is $0 < x_1 < x_2 < \cdots < x_N$, and all others can be obtained from this one by permuting the particle labels, $j \to pj$ with $p \in S_N$ (=permutation group), and/or reflecting some of the coordinates, $x_j \to -x_j$. Thus all regions free of interactions can be characterized as follows:

$$0 < \sigma_1 x_{p1} < \sigma_2 x_{p2} < \cdots < \sigma_N x_{pN} < \infty, \tag{9}$$

where $\sigma_j = \pm 1$ and $p \in S_N$; we will refer to these regions as *wedges*. It is important to note that they can be labeled by elements Q in the group

$$W_N := (\mathbb{Z}/2\mathbb{Z})^N \rtimes S_N, \tag{10}$$

where the first factor corresponds to the reflections while the second factor corresponds to the permutations of the coordinates,

$$x_{Qj} = \sigma_j x_{pj} \quad \text{for } Q = (\sigma_1, \ldots, \sigma_N; p) \in W_N \text{ with } \sigma_j \in \{\pm 1\} \text{ and } p \in S_N. \tag{11}$$

In the sequel we will therefore use the following convenient notation for the wedges:

$$\Delta_Q, \quad 0 < x_{Q1} < x_{Q2} < \cdots < x_{QN} \tag{12}$$

with $Q \in W_N$. It is interesting to note that the group W_N is isomorphic to the Weyl group of the root system C_N; see, e.g., Ref. 21.

B. Bethe ansatz

Using the boundary conditions deduced in the preceding section we now proceed to determine all eigenfunctions of the C_N delta interaction, starting by recalling the physical motivation of the Bethe ansatz below. For that we first consider the Hamiltonian H in Eq. (1). In this case there are eigenfunctions $\psi(x) = \exp(ikx)$ for $x < 0$ which are equal to a particular linear combination of $\exp(ikx)$ and $\exp(-ikx)$ for $x > 0$. This can be interpreted as scattering by the delta interaction $\propto \delta(x)$ where a plane wave is partly transmitted and partly reflected. Regarding H in Eq. (1) as a two particle Hamiltonian with $x = x_1 - x_2$ the relative coordinate and $k = (k_1 - k_2)/2$ the relative momentum, we can interpret this very fact as scattering of a plane wave solution $\exp(ik_1x_1 + ik_2x_2)$ into a linear combination of this wave and another one where the particle momenta k_1 and k_2 are exchanged, $\exp(ik_2x_1 + ik_1x_2)$. This suggests that an eigenfunction ψ of the N-particle Hamiltonian in Eq. (5) which is equal to a plane wave $\exp(i\Sigma_{j=1}^N k_j x_j)$ in one wedge Δ_Q (12) will be transformed into a linear combination of plane waves $\exp(i\Sigma_{j=0}^N \tilde{k}_j x_j)$ in any other wedge where $\tilde{k}_j = \sigma_j k_{pj}$, with $\sigma_j = \pm 1$ resulting from the interactions $\propto \delta(x_j)$ which can invert momenta, $k_j \to -k_j$, and $p \in S_N$ resulting from the interactions $\propto \delta(x_j - x_\ell)$ which can interchange momenta, $k_j \leftrightarrow k_\ell$.

We thus see that the group in Eq. (10) naturally appears again, $\tilde{k}_j = k_{Pj}$ for some $P \in W_N$, and the discussion above suggests the following Bethe ansatz for the eigenfunctions of the Hamiltonian H in Eq. (5):

$$\psi(x) = \sum_{P \in W_N} A_P(Q) e^{ik_P \cdot x_Q} \quad \text{for } 0 < x_{Q1} < x_{Q2} < \cdots < x_{QN} \tag{13}$$

with $x = (x_1, \ldots, x_N)$ and $k_P \cdot x_Q \equiv \Sigma_{j=1}^N k_{Pj} x_{Qj}$, for all $Q \in W_N$. The corresponding eigenvalue is obviously $E = \Sigma_{j=1}^N k_j^2$.

One now has to take into account the boundary conditions in (8a) and (8b). For each $Q \in W_N$, the wedge Δ_Q (12) participates in N boundaries, $x_{Qi} = x_{Q(i+1)}$ for $i = 1, 2, \ldots (N-1)$ and $x_{Q1} = 0$, and for each of these boundaries we will get two conditions. More specifically, the boundary

at $x_{Qi}=x_{Q(i+1)}$ is between the wedges Δ_Q and Δ_{QT_i} where $T_i \in W_N$ is the transposition interchanging i and $(i+1)$, and the conditions implied by Eq. (8a) for $j=Qi$ and $k=Q(i+1)$ are

$$\begin{aligned} A_P(Q) + A_{PT_i}(Q) &= A_P(QT_i) + A_{PT_i}(QT_i) \\ i(k_{Pi} - k_{P(i+1)})[A_{PT_i}(QT_i) - A_P(QT_i) + A_{PT_i}(Q) - A_P(Q)] &= 2c_1[A_P(Q) + A_{PT_i}(Q)]. \end{aligned} \tag{14a}$$

The boundary at $x_{Q1}=0$ is between the wedges Δ_Q and Δ_{QR_1} with $R_1 \in W_N$ the reflection of the first argument, i.e., $x_{R_1 j}=x_j$ for $j\neq 1$ and $-x_j$ for $j=1$, and the conditions at $x_{Q1}=0$ implied by Eq. (8b) for $j=Q1$ are

$$\begin{aligned} A_P(Q) + A_{PR_1}(Q) &= A_P(QR_1) + A_{PR_1}(QR_1) \\ ik_{P1}[A_P(Q) - A_{PR_1}(Q) + A_P(QR_1) - A_{PR_1}(QR_1)] &= c_2[A_P(QR_1) + A_{PR_1}(QR_1)]. \end{aligned} \tag{14b}$$

We thus have $2N(2^N N!)^2$ linear, homogeneous equations for the $(2^N N!)^2$ coefficients $A_P(Q)$. The following beautiful argument due to Yang[3] shows that this system of equations has enough nontrivial solutions and, at the same time, gives a recipe to compute all the $A_P(Q)$.

For that it is important to note that W_N plays a third role, defining

$$(\hat{R})_{Q,Q'} = \delta_{Q',QR} \tag{15}$$

one can write

$$A_P(QR) = \sum_{Q' \in W_N} (\hat{R})_{Q,Q'} A_P(Q') = (\hat{R}A_P)(Q), \tag{16}$$

where the first equality is a trivial consequence of the definition, and in the second we interpret $(\hat{R})_{Q,Q'}$ as elements of an $n\times n$ matrix $\hat{R}$ with $n=2^N N!$ the rank of W_N. These matrices obviously define a representation $R\to\hat{R}$ of W_N acting on the coefficients $A_P(Q)$. It is worth noting that this is identical with the so-called (right) regular representation of W_N.

We can therefore insert $A_{PT_i}(QT_i)=(\hat{T}_i A_{PT_i})(Q)$ in Eq. (14a), and by a simple computation show that these latter equations are equivalent to

$$A_P = Y_i(k_{P(i+1)} - k_{Pi})A_{PT_i}, \tag{17}$$

where we have introduced the operator

$$Y_i(u) = \frac{iu\hat{T}_i + c_1\hat{I}}{iu - c_1} \tag{18}$$

and interpret A_P as a vector with $2^N N!$ elements $A_P(Q)$. In the same way we can rewrite the conditions in Eq. (14b) using $A_{PR_1}(QR_1)=(\hat{R}_1 A_{PR_1})(Q)$,

$$A_P = Z(2k_{P1})A_{PR_1} \tag{19}$$

with the operator

$$Z(u) = \frac{iu\hat{R}_1 + c_2\hat{I}}{iu - c_2}. \tag{20}$$

It is known that the group W_N is generated by the reflection R_1 and the transpositions T_i (see, e.g., p. 21 in Ref. 22). Thus one can use the identities in Eqs. (17), (19), and (16) to calculate recursively all coefficients $A_P(Q)$ from $A_I(I)$ using the operators Z and Y_i above. It is important to note that there is a possible inconsistency arising from the fact that the representation of an

element P in W_N as a product of the T_i's and R_1 is not unique. However, any two such representations can be converted into each other by using the defining relations of the group W_N,

$$T_iT_i = 1, \quad T_iT_j = T_jT_i \quad \text{for } |i-j| > 1,$$
$$T_iT_{i+1}T_i = T_{i+1}T_iT_{i+1}, \tag{21a}$$

$$R_1R_1 = 1, \quad R_1T_i = T_iR_1 \quad \text{for } i > 1,$$
$$R_1T_1R_1T_1 = T_1R_1T_1R_1. \tag{21b}$$

Thus no inconsistency can arise provided that

$$A_{PT_iT_i}(Q) = A_P(Q), \quad A_{PT_iT_j}(Q) = A_{PT_jT_i}(Q) \quad \text{for } |i-j| > 1,$$
$$A_{PT_iT_{i+1}T_i}(Q) = A_{PT_{i+1}T_iT_{i+1}}(Q), \tag{22a}$$

$$A_{PR_1R_1}(Q) = A_P(Q), \quad A_{PR_1T_i}(Q) = A_{PT_iR_1}(Q) \text{ for } i > 1,$$
$$A_{PR_1T_1R_1T_1}(Q) = A_{PT_1R_1T_1R_1}(Q) \tag{22b}$$

for all P, $Q \in W_N$. Using the recursion relations (17) and (19) one finds that these conditions hold true if and only if the following operator relations are fulfilled:

$$Y_i(-u)Y_i(u) = I, \quad Y_i(u)Y_j(v) = Y_j(v)Y_i(u) \quad \text{for } |i-j| > 1,$$
$$Y_i(v)Y_{i+1}(u+v)Y_i(u) = Y_{i+1}(u)Y_i(u+v)Y_{i+1}(v), \tag{23a}$$

$$Z(-u)Z(u) = I, \quad Z(u)Y_i(v) = Y_i(v)Z(u) \quad \text{for } i > 1,$$
$$Z(2v)Y_1(u+v)Z(2u)Y_1(u-v) = Y_1(u-v)Z(2u)Y_1(u+v)Z(2v) \tag{23b}$$

for all real u and v. The validity of this system of equations is necessary and sufficient in order for the Bethe ansatz above to be consistent and the model at hand to be exactly solvable. The first three relations are the so-called Yang–Baxter relations, and the last one is the reflection equation. The validity of these relations for arbitrary $\hat{T}_i$ and $\hat{R}_1$ can be checked by straightforward but somewhat tedious computations (of course, the validity of the Yang–Baxter relation in this case is known since a long time,[3] and this seems to be the case also for the reflection equation,[17,19] but for completeness we provide the essential steps in the verification in Appendix A 1).

Thus the Bethe ansatz (13) is consistent even in the general case of distinguishable particles, and we can calculate all coefficients A_P from A_I using the recursion relation

$$A_P = \mathcal{W}_P(k)A_I, \tag{24}$$

where $\mathcal{W}_P(k)$ is a product of the operators $Y_i(k_{P(i+1)} - k_{Pi})$ and $Z(2k_{P1})$ obtained by using repeatedly (17) and (19).

Interesting special cases of this solution are when the particles are indistinguishable, i.e., when the particles are fermions of bosons. In the former case $\hat{T}_i = -I$, and Eq. (18) implies $Y_i(u) = -I$ independent of the coupling constant c_1. This shows that the delta interaction is trivial for fermions. In the boson case we have $\hat{T}_i = +I$, and $Y_i(u)$ is a nontrivial phase. As discussed in more detail below, there are two different boson cases with different physical interpretations, namely $\hat{R}_1 = -I$ and $\hat{R}_1 = +I$.

C. Physical interpretation

As is well known, the C_N delta-interaction model describes interacting particles on the half-line with particular boundary conditions at the origin.[18] However, the general solution of the C_N delta-interaction model without any restrictions includes many more eigenfunctions than any model on the half-line, and the relation between these models is therefore not completely obvious. In this section we discuss the relation of these models in more detail. We also give a physical interpretation of the boundary conditions which occur as limits of particular external potentials restricting the particles to the half-line.

As discussed in Appendix B, in any irrep of the group W_N the reflections R_j of the particle coordinate x_j are represented either by $\hat{R}_j = +1$ or -1. For simplicity we now discuss in more detail the cases where all $\hat{R}_j$ are the same, either $+1$ or -1, which from a physical point of view are the most interesting ones. As discussed in Appendix B, these irreps of W_N can be rather easily understood since they are related in a simple way to irreps of S_N. Thus we can impose the following restriction on the eigenfunctions ψ of the Hamiltonian in Eq. (5),

$$(\hat{R}_j\psi)(x_1, \ldots, x_j, \ldots, x_N) \equiv \psi(x_1, \ldots, -x_j, \ldots, x_N) = \pm\, \psi(x_1, \ldots, x_j, \ldots, x_N). \tag{25}$$

With that assumption we can restrict ourselves to $x_j > 0$, and the boundary conditions in Eq. (8a) and Eq. (8b) reduce to

$$\begin{gathered} \psi|_{x_j=x_k+0} = \psi|_{x_j=x_k-0}, \\ (\partial_{x_j} - \partial_{x_k})\, \psi|_{x_j=x_k+0} - (\partial_{x_j} - \partial_{x_k})\, \psi|_{x_j=x_k-0} = 2c_1\, \psi|_{x_j=x_k+0}, \end{gathered} \tag{26a}$$

and

$$\begin{gathered} 2\partial_{x_j}\, \psi|_{x_j=+0} = c_2\, \psi|_{x_j=+0} \quad \text{for } \hat{R}_j = +1, \\ \psi|_{x_j=+0} = 0 \quad \text{for } \hat{R}_j = -1, \end{gathered} \tag{26b}$$

respectively. These are exactly the boundary conditions obtained from the Hamiltonian

$$H_0 = -\sum_{j=1}^{N} \partial_{x_j}^2 + 2c_1 \sum_{j<k} \delta(x_j - x_k) \tag{27}$$

describing particles on the half-line, $x_j > 0$, and the boundary conditions at the origin given in Eq. (26b).

It is also interesting to note that these later boundary conditions are obtained by allowing the particles to move on the full line, $x_j \in \mathbb{R}$, and adding a particular external potential $\Sigma_j V(x_j)$ to the Hamiltonian in Eq. (27) which effectively constrains the particles to the half-line $x_j > 0$. To be specific, these potentials are given by

$$V(x) = \begin{cases} V_0\Theta(-x) + (c_2/2 - \sqrt{V_0})\,\delta(x) & \text{if } \hat{R}_j = +1, \\ V_0\Theta(-x) & \text{if } \hat{R}_j = -1, \end{cases} \tag{28}$$

where $\Theta(-x)$ is the Heaviside function (equal to one for $x < 0$ and zero otherwise), and one must take the strong coupling limit $V_0 \to \infty$, as shown in Appendix C, in this latter limit the eigenfunctions of the Hamiltonian $H_0 + \Sigma_j V(x_j)$ on the full line, $x_j \in \mathbb{R}$, coincide with the ones of H_0 on the half-line, $x_j > 0$, and the boundary conditions in Eq. (26b).

As already mentioned, the most important cases in applications are the ones we have considered here, i.e., where all the $\hat{R}_j$ are the same. Nevertheless it would be of interest to consider the implications of allowing the $\hat{R}_j$ to take on different values, in effect dividing the particles into two groups distinguished by their interactions with the boundary.

III. LOCAL MOMENTUM-DEPENDENT INTERACTION

In this section we discuss the model with local momentum dependent interactions defined by the Hamiltonian in Eq. (6). While most of our discussion is in parallel with the one for the delta-interaction model in the preceding section, we find that the Bethe ansatz is consistent only in case of indistinguishable particles. We also present a duality relation between the fermionic variant of the model with local momentum dependent interactions and the bosonic delta-interaction model discussed in the preceding section.

A. Boundary conditions

Since this interaction is not as familiar as the delta interaction we give a somewhat more detailed discussion of how to turn the eigenvalue equation of the formal Hamiltonian in Eq. (6) into a well-defined mathematical problem in terms of boundary conditions. We stress that we give this argument only to substantiate our physical interpretation of the model we consider, and that one also could *define* the model in terms of the boundary conditions in Eqs. (30a) and (30b) below, as is often done for this type of models.[4,5] However, it seems that the results in Ref. 23 provide a framework making our formal computations mathematically precise.

To explain our method we start by considering the formal eigenvalue equation $H\psi=E\psi$ for the $N=1$ Hamiltonian in Eq. (4), i.e.,

$$-\psi''(x)+4\lambda\delta'(x)\psi'(0)=E\psi(x) \tag{29}$$

since $\partial_x\delta(x)\partial_x\psi(x)=\partial_x[\delta(x)\psi'(x)]$. It is important to note that the wave function $\psi(x)$ is not continuous at the singular point $x=0$, but we interpret $\psi'(0)$ as $\lim_{\varepsilon\downarrow 0}[\psi'(\varepsilon)+\psi'(-\varepsilon)]/2$ which is well defined. This amounts to a particular renormalization of this singular interaction; see Ref. 9 for a more detailed discussion on this. For $x\neq 0$ Eq. (29) again reduces to $-\psi''=E\psi$. To deduce the boundary conditions at $x=0$ we integrate Eq. (29) from $x=-\varepsilon$ to ε, and taking the limit $\varepsilon\downarrow 0$ we obtain the first condition in Eq. (3). Integrating Eq. (29) from $x=-\varepsilon$ to $x>0$ and then once more from $x=-\varepsilon$ to ε and taking the limit $\varepsilon\downarrow 0$ yields the second condition in Eq. (3).

It is straightforward to generalize this argument to the N-particle case: consider the formal eigenvalue equation $H\psi=E\psi$ for the Hamiltonian in Eq. (6) and treat each singular point $x_j=\pm x_k$ and $x_j=0$ separately, similarly as for the $N=1$ Hamiltonian above. For the singular points $x_j=0$ the argument is identical to the one for the $N=1$ case above. For any other singular point $x_j=\pm x_k$ we introduce new coordinates $y=x_j\mp x_k$ and $z=x_j\pm x_k$ in the vicinity of this point so that $H=-2(\partial_y^2+\partial_z^2+4\lambda_1\partial_y\delta(y)\partial_y+4\lambda_1\partial_z\delta(z)\partial_z)+\cdots$ where the dots represent terms which remain nonsingular as $y\to 0$, and then one can treat the singular point $y=0$ as explained in the $N=1$ case above.

Thus, we find that the eigenfunctions ψ of the Hamiltonian in Eq. (6) are determined by Eq. (7) together with the boundary conditions

$$\begin{aligned}
&(\partial_{x_j}-\partial_{x_k})\,\psi|_{x_j=\pm x_k+0}=(\partial_{x_j}-\partial_{x_k})\,\psi|_{x_j=\pm x_k-0},\\
&\psi|_{x_j=\pm x_k+0}-\psi|_{x_j=\pm x_k-0}=2\lambda_1(\partial_{x_j}-\partial_{x_k})\,\psi|_{x_j=\pm x_k-0},\\
&\partial_{x_j}\psi|_{x_j=+0}=\partial_{x_j}\psi|_{x_j=-0},
\end{aligned} \tag{30a}$$

$$\psi|_{x_j=+0} - \psi|_{x_j=-0} = 4\lambda_2 \partial_{x_j} \psi|_{x_j=+0}, \tag{30b}$$

where we used $2\partial_{x_j \mp x_k} = \partial_{x_j} \mp \partial_{x_k}$.

B. Bethe ansatz

We now discuss the Bethe ansatz for the eigenfunctions of the Hamiltonian H defined in Eq. (6). Obviously much of what we said for the delta-interaction case carries over straightforwardly to the present case. Due to the different boundary conditions in Eqs. (30a) and (30b), Eqs. (14a) and (14b) are changed to

$$\begin{aligned} &i(k_{Pi} - k_{P(i+1)})[A_{PT_i}(QT_i) - A_P(QT_i)] = i(k_{Pi} - k_{P(i+1)})[A_P(Q) - A_{PT_i}(Q)] \\ &A_P(QT_i) + A_{PT_i}(QT_i) - A_P(Q) - A_{PT_i}(Q) = 2\lambda_1 i(k_{Pi} - k_{P(i+1)})[A_P(Q) - A_{PT_i}(Q)], \end{aligned} \tag{31a}$$

$$\begin{aligned} &ik_{P1}[A_P(Q) - A_{PR_1}(Q)] = ik_{P1}[A_{PR_1}(QR_1) - A_P(QR_1)] \\ &A_P(Q) + A_{PR_1}(Q) - A_P(QR_1) - A_{PR_1}(QR_1) = 4\lambda_2 ik_{P1}[A_P(QR_1) - A_{PR_1}(QR_1)]. \end{aligned} \tag{31b}$$

We now also use Eq. (16) to convert these equations into the recursion relations

$$A_P = Y_i(k_{P_{i+1}} - k_{P_i}) A_{PT_i}, \tag{32}$$

and similarly

$$A_P = Z(2k_{P_1}) A_{PR_1}, \tag{33}$$

where now

$$Y_i(u) = \frac{iu\hat{I} - 1/\lambda_1 T_i}{iu - 1/\lambda_1} \tag{34}$$

and

$$Z(u) = \frac{iu\hat{I} - 1/\lambda_2 \hat{R}_1}{iu - 1/\lambda_2}. \tag{35}$$

As in the delta-interaction case these relations allow to recursively compute all coefficients A_P in terms of A_I, and the conditions for the absence of inconsistencies are identical to (22a) and (22b) of the delta-interaction case, leading to the Yang–Baxter relations (23a) and reflection equation (23b) but now with the operators (34) and (35). In contrast to the delta-interaction case, we find that these consistency relations are fulfilled only if $\hat{T}_i = \pm I$ for all i (see Appendix A 2 for details). We thus conclude that *the Bethe ansatz is consistent only if the particles are indistinguishable, i.e., A_I is chosen such that either $\hat{T}_i = I$ or $\hat{T}_i = -I$*, and in these two cases we can compute all coefficients A_P from A_I as

$$A_P = \mathcal{W}_P(k) A_I, \tag{36}$$

where $\mathcal{W}_P(k)$ is a product of operators $Y_i(k_{P_{i+1}} - k_{P_i})$ and $Z(2k_{P_1})$ in Eqs. (34) and (35) obtained by using repeatedly (32) and (33).

For $\hat{T}_i = +I$ we get from Eq. (34) that $Y_i(u) = I$ independent of λ_1, and we conclude that *the momentum-dependent interaction is trivial for bosons*. However, for $\hat{T}_i = -I$ (fermions) the $Y_i(u)$ are nontrivial phases. There are two different fermion cases, namely $\hat{R}_1 = \pm I$.

C. Duality

It is interesting to note that there exists a simple duality relation between the fermionic $\hat{p}\delta\hat{p}$-model and the bosonic C_N delta-interaction model discussed in Sec. II. Since the operators $Y_i(u)$ and $Z(u)$ for the latter model are identical with the ones of the fermionic $\hat{p}\delta\hat{p}$-model upon the substitution $\lambda_1 \to 1/c_1$ and $\lambda_2 \to 1/c_2$ [compare Eqs. (18) and (20) for $\hat{T}_i = \hat{R}_1 = +I$ and Eqs. (34) and (35) for $\hat{T}_i = \hat{R}_1 = -1$], Eqs. (24) and (36) imply that

$$A_P^{\delta}|_{\hat{T}_i=\hat{R}_1=+I} = A_P^{\hat{p}\delta\hat{p}}|_{\hat{T}_i=\hat{R}_1=-I,\lambda_1\to 1/c_1,\lambda_2\to 1/c_2}, \tag{37}$$

where A_P^{δ} are the coefficients of Sec. II B and $A_P^{\hat{p}\delta\hat{p}}$ the ones in Sec. III B. This implies that *the bosonic wave functions of the delta-model in Sec. II B and the fermionic wave functions of the $\hat{p}\delta\hat{p}$-model in Sec. III B are identical when restricted to the fundamental wedge*

$$\Delta_I, \quad 0 < x_1 < x_2 < \cdots < x_N, \tag{38}$$

provided that the coupling constants of these models are related as follows:

$$\lambda_1 = \frac{1}{c_1} \quad \textit{and } \lambda_2 = \frac{1}{c_2}. \tag{39}$$

This can be seen also more directly, assuming that the eigenfunction ψ of the Hamiltonian in Eq. (5) is bosonic, $\hat{T}_i = \hat{R}_1 = I$, it is enough to determine it in the fundamental wedge. Moreover, the continuity conditions in Eqs. (8a) and (8b) are fulfilled automatically for boson wave functions, whereas the conditions on the derivatives simplify to

$$\begin{gathered}(\partial_{x_j} - \partial_{x_{j+1}} - c_1)\ \psi|_{x_j=x_k+0} = 0, \\ (2\partial_{x_j} - c_2)\ \psi|_{x_j=+0} = 0\end{gathered} \tag{40}$$

for all x in the fundamental wedge. In a similar manner one finds that the fermionic eigenfunctions of the Hamiltonian in Eq. (6), $\hat{T}_i = \hat{R}_1 = -I$, are determined by the very same conditions in Eq. (40) with $c_{1,2}$ replaced by $1/\lambda_{1,2}$.

This generalizes the duality previously observed in the A_{N-1} case[9,12] to the C_N case.

D. Physical interpretation

As in the delta-interaction case, one can restrict the eigenfunctions ψ of the Hamiltonian in Eq. (6) by imposing the conditions in Eq. (25), reducing the boundary conditions in Eqs. (30a) and (30b) to

$$\begin{gathered}(\partial_{x_j} - \partial_{x_k})\ \psi|_{x_j=x_k+0} = (\partial_{x_j} - \partial_{x_k})\ \psi|_{x_j=x_k-0}, \\ \psi|_{x_j=x_k+0} - \psi|_{x_j=x_k-0} = 2\lambda_1(\partial_{x_j} - \partial_{x_k})\ \psi|_{x_j=x_k+0}\end{gathered} \tag{41a}$$

and

$$\begin{gathered}\partial_{x_j}\ \psi|_{x_j=+0} = 0 \quad \text{for } \hat{R}_j = +1, \\ \psi|_{x_j=+0} = 2\lambda_2\partial_{x_j}\ \psi|_{x_j=+0} \quad \text{for } \hat{R}_j = -1,\end{gathered} \tag{41b}$$

where $x_j > 0$. This shows that the eigenfunctions of the C_N Hamiltonian in Eq. (6) with the restriction in Eq. (25) are identical to the ones of the A_{N-1} Hamiltonian,

$$H_0 = -\sum_{j=1}^{N} \partial_{x_j}^2 + 2\lambda_1 \sum_{j<k} (\partial_{x_j} - \partial_{x_k}) \delta(x_j - x_k)(\partial_{x_j} - \partial_{x_k}), \tag{42}$$

restricted to the half-line, $x_j > 0$, and the boundary conditions at the origin given in Eq. (41b).

Moreover, as shown in Appendix C 2, the eigenfunctions ψ above restricted to $x_j > 0$ become identical to the ones of the Hamiltonian $H_0 + \Sigma_j V(x_j)$ on the full real line, $x_j \in \mathbb{R}$, with an external potential

$$V(x) = \begin{cases} V_0 \Theta(-x) + \sqrt{V_0} \partial_x \delta(x) \partial_x & \text{if } \hat{R}_j = +1, \\ V_0 \Theta(-x) + 2\lambda_2 \partial_x \delta(x) \partial_x & \text{if } \hat{R}_j = -1 \end{cases} \tag{43}$$

in the limit $V_0 \to \infty$.

IV. CONCLUDING REMARK

As discussed in the Introduction, there exists a four-parameter family of local interactions,[4] and the delta- and $\hat{p}\delta\hat{p}$ interactions only correspond to one-parameter subfamilies each. It is therefore natural to ask, what about the other local interactions? Are there other cases leading to exactly solvable models? It is thus interesting to note that there is a simple physical interpretation of the four-parameter family of local interactions which seems very natural to us but seems different from the one commonly used,[4,10] in the simplest case they correspond to the following generalization of the Hamiltonians in Eqs. (1) and (4):

$$H = -\partial_x^2 + c\,\delta(x) + 4\lambda \partial_x \delta(x) \partial_x + 2(\gamma + i\eta) \partial_x \delta(x) - 2(\gamma - i\eta) \delta(x) \partial_x, \tag{44}$$

which obviously is the most general hermitian Hamiltonian with interactions localized at $x = 0$ and containing only derivatives up to second order (higher derivatives than that do not lead to physically acceptable boundary conditions). This Hamiltonian is formally self-adjoint for arbitrary real parameters c, λ, γ, η, and it indeed corresponds to the well-known four-parameter family of local interactions mentioned above[24] (see also Ref. 23 and Sec. II.1 in Ref. 6). All these models have natural generalizations to the A_{N-1} many-body case, but only the following cases are exactly solvable by the coordinate Bethe ansatz even for distinguishable particles: $(c, 1/c, 0, 0)$ and $(c, 0, 0, \eta)$, for arbitrary real c and η (Ref. 24) (see also Refs. 5, 13, and 25). It is important to note that the many-body generalization of the Hamiltonian in Eq. (44) describes identical particles only if $\gamma = \eta = 0$, and the proof of this latter result therefore requires an extension of Yang's method of solution[3] to models of non-identical particles.[24] We conjecture that similar results hold true for the corresponding C_N models.

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APPENDIX A: VERIFICATION OF CONSISTENCY RELATIONS

In this appendix we sketch the verification of the consistency relations in Eqs. (23a) and (23b) (Yang–Baxter relations and the reflection equation).

1. Delta interaction

We start by writing the operators Y_i in the following way:

$$Y_i(u) = a(u)\hat{I} + b(u)\hat{T}_i, \tag{A1}$$

where

$$a(u) = \frac{c_1}{iu - c_1}, \quad b(u) = \frac{iu}{iu - c_1}. \tag{A2}$$

Inserting this expression into the equations in (23a) results in a number of relations between the coefficients $a(u)$ and $b(u)$, one for each equation and different permutation operator. Most of them are trivially fulfilled, but the following ones are nontrivial:

$$\begin{aligned} a(-u)a(u) + b(-u)b(u) &= 1, \\ a(-u)b(u) + b(-u)a(u) &= 0, \end{aligned} \tag{A3}$$

and

$$b(v)a(u+v)a(u) + a(v)a(u+v)b(u) = a(u)b(u+v)a(v). \tag{A4}$$

Inserting $a(u)$ and $b(u)$ from Eq. (A2) they can be verified by straightforward calculations. To verify Eq. (23b) we write the operator Z as

$$Z(u) = \tilde{a}(u)\hat{I} + \tilde{b}(u)\hat{R}_1, \tag{A5}$$

where

$$\tilde{a}(u) = \frac{c_2}{iu - c_2}, \quad \tilde{b}(u) = \frac{iu}{iu - c_2}. \tag{A6}$$

Substituting this and Eq. (A1) into the equations in (23b) leads to the following nontrivial relation:

$$\begin{aligned} &\tilde{b}(2v)b(u+v)\tilde{a}(2u)a(u-v) + \tilde{b}(2v)a(u+v)\tilde{a}(2u)b(u-v) + \tilde{a}(2v)a(u+v)\tilde{b}(2u)b(u-v) \\ &\quad = a(u-v)\tilde{b}(2u)b(u+v)\tilde{a}(2v) \end{aligned} \tag{A7}$$

in addition to

$$\begin{aligned} \tilde{a}(-u)\tilde{a}(u) + \tilde{b}(-u)\tilde{b}(u) &= 1, \\ \tilde{a}(-u)\tilde{b}(u) + \tilde{b}(-u)\tilde{a}(u) &= 0, \end{aligned} \tag{A8}$$

the validity of which follow from straightforward calculations.

We conclude that the Bethe ansatz is consistent even for distinguishable particles.

2. Local momentum-dependent interaction

In this case we get $Y_i(u)$ as in Eq. (A1) but with

$$a(u) = \frac{iu}{iu - 1/\lambda_1}, \quad b(u) = \frac{-1/\lambda_1}{iu - 1/\lambda_1}. \tag{A9}$$

With that the two equations in (A3) hold true but the equation in (A4) does not. We therefore conclude that *the Bethe ansatz is not consistent for distinguishable particles.*

For indistinguishable particles we have $\hat{T}_i = \pm I$ and the Yang–Baxter relations in Eq. (23a) are trivially fulfilled. Moreover, in this case it is also easy to check that the relations (23b) hold true for $\hat{R}_1 = \pm I$.

We conclude that the Bethe ansatz is consistent in the indistinguishable particle case but not in general.

APPENDIX B: REPRESENTATIONS OF THE GROUP W_N

In this appendix we discuss the irreducible representations of the group $W_N \equiv (\mathbb{Z}/2\mathbb{Z})^N \rtimes S_N$. In particular we will show the following.

Fact: There exists a set of irreducible representations of W_N isomorphic to the irreducible representations $\chi_\pm \otimes \rho$, where $\chi_\pm$ is a character (irreducible representation) of the (normal) abelian subgroup $(\mathbb{Z}/2\mathbb{Z})^N$ such that $\chi_\pm(R_j) = \pm 1$ for all $j = 1, 2, \ldots, N$ (same sign for all j) and ρ is an arbitrary irreducible representation of the permutation group S_N.

To show this we will use the notion of induced representations, following Sec. 8.2 of Ref. 26. We start by determining the group of characters $X = \mathrm{Hom}((\mathbb{Z}/2\mathbb{Z})^N, \mathbb{C})$ of the subgroup $(\mathbb{Z}/2\mathbb{Z})^N$. The fact that it is generated by the reflections R_j obeying the relations (see, e.g., p. 21 in Ref. 22)

$$R_j^2 = I, \quad j = 1, 2, \ldots, N \tag{B1}$$

implies that the characters $\chi \in X$ are functions such that

$$\chi(R_j) = e^{in_j\pi}, \quad n_j \in \mathbb{Z} \tag{B2}$$

for all $j = 1, 2, \ldots, N$. The group W_N acts on these characters by

$$(w\chi)(R) = \chi(w^{-1}Rw), \quad \forall\, w \in W_N, \chi \in X, R \in (\mathbb{Z}/2\mathbb{Z})^N. \tag{B3}$$

We now determine the orbits of the action of S_N in X, represented by a set χ_i where $i \in X/S_N$. Using the fact that the adjoint action of S_N permutes the reflections R_j, $T_{jk}R_jT_{jk} = R_k$ with T_{jk} the transposition interchanging j and k, we conclude that the orbits of S_N in X can be represented by the characters

$$\chi_k(R_j) = \begin{cases} 1, & j > k, \\ -1, & j \leqslant k, \end{cases} \tag{B4}$$

where $j, k = 1, 2, \ldots, N$. For each i let $(S_N)_i$ be that subgroup of S_N consisting of all $P \in S_N$ such that $P\chi_i = \chi_i$, and let further $\widetilde{W}_i = (\mathbb{Z}/2\mathbb{Z})^N \cdot (S_N)_i$. The structure of χ_i implies that $(S_N)_i = S_i \times S_{N-i}$. The character χ_i can be extended to all of $\widetilde{W}_i$ by setting

$$\chi_i(RP) = \chi(R), \quad R \in (\mathbb{Z}/2\mathbb{Z})^N,\ P \in (S_N)_i. \tag{B5}$$

Now let ρ_i be an irreducible representation of $(S_N)_i$ and combine it with the canonical projection $\widetilde{W}_i \to (S_N)_i$ to yield an irreducible representation $\widetilde{\rho}_i$ of $\widetilde{W}_i$. By taking the tensor product of χ_i and $\widetilde{\rho}_i$ we can now construct a set of irreducible representations $\chi_i \otimes \rho_i$ of $\widetilde{W}_i$. We denote the corresponding induced representation of the whole of W_N by θ_{i,ρ_i}. It follows from Proposition 25 in Ref. 26 that all irreducible representations of W_N are isomorphic to such a representation θ_{i,ρ_i}. In particular setting $i = 0$ and $i = N$ we arrive at the claim stated in the "Fact" at the beginning of the section.

APPENDIX C: PHYSICAL INTERPRETATION OF BOUNDARY CONDITIONS

In this appendix we substantiate the physical interpretations of the boundary conditions of the C_N models given in Secs. II and III in the main text.

1. Delta interaction

We first recall the eigenfunctions ψ of the one particle Hamiltonian in Eq. (1). Since this Hamiltonian is invariant under the reflection $x \to -x$ these eigenfunctions can be chosen such that $\psi(x) = \pm\psi(-x) \equiv \psi_\pm(x)$, and they can be computed using the ansatz

$$\psi_{\pm}(x) = \begin{cases} e^{-ikx} + A_{\pm}e^{ikx} & \text{for } x > 0, \\ \pm(e^{ikx} + A_{\pm}e^{-ikx}) & \text{for } x < 0, \end{cases} \tag{C1}$$

and the boundary conditions in Eq. (2) determine the constants $A_{\pm}$ as follows:

$$A_{+} = \frac{ik + c/2}{ik - c/2}, \quad A_{-} = -1 \tag{C2}$$

with A_{-} being independent of c corresponding to the fact that the delta interaction is trivial (i.e., invisible) for fermions. Obviously, these eigenfunctions obey

$$-\psi_{+}''(x) = k^2\psi_{+}(x) \quad \text{for } x > 0 \text{ and } \psi_{+}'(+0) = (c/2)\psi_{+}(+0) \tag{C3}$$

and

$$-\psi_{-}''(x) = k^2\psi_{-}(x) \quad \text{for } x > 0 \text{ and } \psi_{-}(+0) = 0, \tag{C4}$$

which is the simplest nontrivial case $N=1$ of the general relation between the C_N model and the A_{N-1} model discussed in Sec. II C.

We now show that these eigenfunctions $\psi_{\pm}(x)$ for $x>0$ are identical to the ones of the Hamiltonians,

$$H_{\pm} = -\partial_x^2 + V_0\Theta(-x) + g_{\pm}\delta(x), \tag{C5}$$

with

$$g_{+} = c/2 - \sqrt{V_0} \quad \text{and } g_{-} = 0 \tag{C6}$$

in the limit $V_0 \to \infty$. To show this we determine the eigenfunctions $\phi_{\pm}$ of $H_{\pm}$ with the ansatz

$$\phi_{\pm} = \begin{cases} e^{-ikx} + B_{\pm}e^{ikx} & \text{for } x > 0, \\ C_{\pm}e^{\omega x} & \text{for } x < 0, \end{cases} \tag{C7}$$

and by straightforward computations we find that

$$B_{\pm} = \frac{ik + (\omega + g_{\pm})}{ik - (\omega + g_{\pm})} \quad \text{and } \omega = \sqrt{V_0 - k^2} \tag{C8}$$

for $V_0 > k^2$. We thus see that

$$A_{\pm} = \lim_{V_0 \to \infty} B_{\pm} \tag{C9}$$

provided that $g_{\pm}$ are chosen as in Eq. (C6). This shows that the eigenfunctions ϕ_{+} of the Hamiltonian H_{+} on the full line in the limit $V_0 \to \infty$ become equal to $\psi_{+}(x)$ for $x>0$ (and zero otherwise), and similarly for ϕ_{-}, ψ_{-} and H_{-}.

This computation substantiates the physical interpretation of the C_N model in case $N=1$. However, since this interpretation only involves the boundary conditions at $x_j=0$ which are not affected by the interparticle interactions, this argument immediately generalizes to the $N>1$ particle case.

2. Local momentum dependent interaction

The discussion for the Hamiltonian in Eq. (4) is completely analogous to the one for the Hamiltonian in Eq. (1) given above, and we therefore only write down the formulas that change.

Equation (C1) determining the even and odd eigenfunctions $\psi_{\pm}$ remains the same but A_{+} and A_{-} are (essentially) interchanged,

$$A_+ = 1, \quad A_- = \frac{ik + 1/2\lambda}{ik - 1/2\lambda}, \tag{C10}$$

where now the boson eigenfunction is unaffected by the interaction. Moreover, these eigenfunctions solve the following problems on the half-axis:

$$-\psi_+''(x) = k^2\psi_+(x) \quad \text{for } x > 0 \text{ and } \psi_+'(+0) = 0 \tag{C11}$$

and

$$-\psi_-''(x) = k^2\psi_-(x) \quad \text{for } x > 0 \text{ and } \psi_-'(+0) = 2\lambda\psi_-(+0). \tag{C12}$$

The physical interpretation of these boundary conditions is provided by the following Hamiltonians with external fields:

$$H_\pm = -\partial_x^2 + V_0\Theta(-x) + \tilde{g}_\pm\partial_x\delta(x)\partial_x \tag{C13}$$

which has eigenfunctions as in Eq. (C7) but with

$$B_\pm = \frac{ik + \omega/(1 + \omega\tilde{g}_\pm)}{ik - \omega/(1 + \omega\tilde{g}_\pm)} \quad \text{and } \omega = \sqrt{V_0 - k^2}, \tag{C14}$$

which converge to $A_\pm$ for $V_0 \to \infty$ provided that, for example,

$$\tilde{g}_+ = \sqrt{V_0} \quad \text{and } \tilde{g}_- = 2\lambda. \tag{C15}$$

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Analytic controllability of time-dependent quantum control systems

Chunhua Lan[a] and Tzyh-Jong Tarn[b]
Department of Electrical and Systems Engineering, Washington University, St. Louis, Missouri 63130-4899

Quo-Shin Chi[c]
Department of Mathematics, Washington University, St. Louis, Missouri 63130-4899

John W. Clark[d]
Department of Physics, Washington University, St. Louis, Missouri 63130-4899

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The question of controllability is investigated for a quantum control system in which the Hamiltonian operator components carry explicit time dependence which is not under the control of an external agent. We consider the general situation in which the state moves in an infinite-dimensional Hilbert space, a drift term is present, and the operators driving the state evolution may be unbounded. However, considerations are restricted by the assumption that there exists an analytic domain, dense in the state space, on which solutions of the controlled Schrödinger equation may be expressed globally in exponential form. The issue of controllability then naturally focuses on the ability to steer the quantum state on a finite-dimensional submanifold of the unit sphere in Hilbert space—and thus on analytic controllability. A relatively straightforward strategy allows the extension of Lie-algebraic conditions for strong analytic controllability derived earlier for the simpler, time-independent system in which the drift Hamiltonian and the interaction Hamiltonian have no intrinsic time dependence. Enlarging the state space by one dimension corresponding to the time variable, we construct an augmented control system that can be treated as time independent. Methods developed by Kunita can then be implemented to establish controllability conditions for the one-dimension-reduced system defined by the original time-dependent Schrödinger control problem. The applicability of the resulting theorem is illustrated with selected examples. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1867979]

I. INTRODUCTION

Over the last two decades, quantum control has played an important part in theoretical and experimental progress toward the realization of laser control of chemical reactions and the development of quantum computers.[1–13] Essential to this contribution has been the integration of concepts and mathematical results from control engineering with the fundamental principles of quantum theory.

Geometric control, a treatment of differential equations rooted in differential geometry, unitary groups, and Lie algebras, provides a natural mathematical basis for quantum control theory. Explicitly or implicitly, its elements[14] pervade the manipulation of quantum states in both traditional and novel technologies. Indeed, the field of nuclear magnetic resonance (NMR) is largely

[a]Electronic mail: lancb@bc.edu; to whom correspondence should be addressed.
[b]Electronic mail: tarn@wuauto.wustl.edu
[c]Electronic mail: chi@math.wustl.edu
[d]Electronic mail: jwc@wuphys.wustl.edu

concerned with geometric control of collections of interacting nuclear spins.[12,15–17] Geometric control is also a key ingredient in the theory of quantum computation, figuring prominently in the works of Lloyd,[18] Deutsch, Barenco, and Ekert,[19] Akulin, Gershkovich, and Harel.[20]

In particular, Lloyd[18] was among the first to establish that almost all quantum logic gates are universal. More precisely, if one has available a gate that can operate on two qubits, plus a single-qubit operation, then an arbitrary unitary transformation on the variables of the system can be performed with arbitrary precision by implementing a finite sequence of local operations. Clark[21] and Ramakrishna *et al.*[22] and Ramakrishna and Rabitz[23] called attention to the close relationship between open-loop geometric quantum control methods and the application of quantum logic gates.[18,19]

Following Ref. 23, let us consider the differential system

$$\frac{\mathrm{d}X(t)}{\mathrm{d}t} = AX(t) + \sum_{i=1}^{m} B_i X(t) u_i(t), \quad X(0) = I, \tag{1}$$

which arises both in quantum computing and molecular control. Here, X is a $N \times N$ unitary matrix (I being the corresponding identity matrix), the matrices A and B_i, $i=1,\ldots,m$ are $N \times N$ skew-Hermitian, and the functions $u_i(t)$ are controls. This equation is the law of motion of the evolution operators which govern time development of the N-dimensional vector representing a pure state of the system in its N-dimensional Hilbert space. A necessary and sufficient condition for (1) to be controllable is that the set of all matrices generated by A, B_i, $i=1,\ldots,m$, and their commutators (i.e., the Lie algebra generated by A and B_i) equals the set of all $N \times N$ skew-Hermitian matrices. Additionally, when this condition is met, any X can be attained through some choice among the controls $u_i(t)$ restricted to piecewise-constant functions of time. In fact, the formulation adopted by Lloyd[18] in his universality proof corresponds to the special case $A=0$ and $m=2$ of system (1). Already in the 1970s, Sussmann and Jurdjevic[24,25] applied Lie-group theory to obtain rigorous results on controllability for finite-dimensional control problems corresponding to (1).

Quantum computation has mostly concerned itself with the manipulation of discrete systems with finite-dimensional state spaces. However, the fundamental quantum observables representing position and momentum, and functions thereof, are continuous in nature. In view of recent developments in quantum error correction[26–28] and quantum teleportation[29,30] of continuous variables, the potential of quantum computation over continuous variables warrants serious investigation, thus reopening issues of controllability on infinite-dimensional Hilbert spaces. Continuous quantum computers may in fact be able to perform some tasks more efficiently than their discrete counterparts.

As early as 1983, Huang, Tarn, and Clark (HTC)[5,31] proved a basic theorem on strong analytic controllability of quantum systems. This theorem explicitly embraces the case of quantum systems whose observables are continuous quantum variables acting on an infinite-dimensional state space, but the essential finite-dimensional results may be extracted as special cases. Because of the difficulties caused by infinite dimensionality and the unboundedness of operators, an analytic domain in the sense of Nelson[32] was introduced to deal with domain problems[5,31] and maintain key features of the application of Lie algebraic methods to finite-dimensional problems.

Infinite-dimensional control systems have been widely if not systematically studied outside the quantum context. Brockett[14] addressed the problem of realization of infinite-dimensional bilinear systems. Sakawa[33] introduced a method for design of finite-dimensional $\mathcal{H}_\infty$ controllers for diffusion systems with bounded input and output operators by using residual model filters. Keulen[34] designed infinite-dimensional $\mathcal{H}_\infty$ controllers for infinite-dimensional systems with bounded input and output operators by using the solutions to two kinds of Riccati equations in an infinite-dimensional space. Based on gap topology, Morris[35] constructed finite-dimensional $\mathcal{H}_\infty$ controllers for infinite-dimensional systems with bounded input and output operators. Morris[36] also showed that approximations of Galerkin type can be used to design controllers for an infinite-dimensional system. Costa and Kubrusly[37] derived necessary and sufficient conditions for existence of a state feedback controller that stabilizes a discrete-time infinite-dimensional stochastic

bilinear system and ensures that the influence of the additive disturbance on the output is smaller than some prescribed bound. In Ref. 38, optimizability and estimatability for infinite-dimensional linear systems are investigated; also, a theorem on the equivalence of input-output stability and exponential stability of well-posed infinite-dimensional linear systems is established. In Ref. 39, the Hilbert-space generalization of the circle criterion is used for finite-dimensional controller design of unstable infinite-dimensional systems. There is also literature on absolute stability problems and open-loop stability problems in infinite-dimensional systems.[40–44] In addition, the spectral factorization problem plays a central role in designing feedback control for the linear quadratic optimal control problem in infinite-dimensional state-space systems.[45–48] In contrast to this body of work, very little has been published on controllability for time-dependent infinite-dimensional quantum control systems.

In the microscopic world ruled by quantum mechanics, most interesting phenomena involve change, and all real-world quantum systems are influenced to a greater or lesser extent by interactions with their environments. The environment changes with time, so the Hamiltonians used to describe these open quantum systems are explicitly time dependent, as in Refs. 49 and 50. Tailored time-dependent perturbations are used to improve system performance[49] in high-resolution NMR spectroscopy, where versatile decoupling techniques are available to manipulate the overall spin Hamiltonian.[16] Colegrave and Abdalla studied quantum systems with a time-dependent mass to investigate the field intensities in a Fabry–Perot cavity.[51] They suggested possible applications to solid-state physics and quantum field theory.[52] Remaud and Hernandez[53] found that a time-dependent mass parameter offers a means of simulating input or removal of energy from the system. Implementation of controls on these time-dependent quantum systems requires guidance from mathematical studies of controllability for time-dependent Hamiltonian operators. Although the HTC theorem deals with controllability in infinite-dimensional Hilbert space, it is restricted to time-independent operators. This paper explores a more general case. We seek an extension of the HTC theorem that is applicable both to time-independent and time-dependent quantum systems, as well as to systems with discrete or continuous operators acting on finite- or infinite-dimensional state spaces.

Since this paper is aimed at an interdisciplinary readership that includes pure quantum theorists as well as control engineers, it is well to draw a clear distinction between time dependence of the system arising solely from influences that are directly under the control of an external, purposeful agent, and time dependence that is intrinsic to the physical system either in isolation or as embedded in a natural environment. In the accepted terminology of control theory, which we adopt, the former case defines a time-independent control system, and the latter, a time-dependent system. The issue of controllability has received considerable attention in the time-independent situation so identified (e.g., in Refs. 5, 8, 12, and 22); whereas relevant results for the time-dependent case are very limited.

The time-dependent quantum control problem that we shall address is stated formally in Sec. II. To cope with the unboundedness of operators involved in the Schrödinger equation, an analytic domain is introduced in Sec. III, such that solutions of the Schrödinger equation can be expressed globally in exponential form on this domain. In Sec. IV, we define an augmented system in a space enlarged by one dimension, enabling its description within the framework of time-independent control systems. Following the pattern of Kunita's proof[54] of strong controllability of a time-independent system, we then establish conditions for controllability of this kind for the one-dimension-reduced system defined by the original time-dependent Schrödinger equation. Three illustrative applications of the theorem are presented in Sec. V, and our findings are reviewed in Sec. VI.

II. PROBLEM FORMULATION

The following quantum control system is derived by applying the geometric quantization method[55] to a classical bilinear control system:[31,56]

$$i\hbar\frac{\partial}{\partial t}\psi(t) = \left[H_0'(t) + \sum_l u_l(t)H_l'(t)\right]\psi(t),$$
$$\psi(t_0) = \psi_0. \tag{2}$$

Here, $H_0'(t)$, and the $H_l'(t)$ with $l=1,2,\ldots,r$, are Hermitian operators on a unit sphere $S_{\mathcal{H}}$ of Hilbert space, the $u_l(t)$, $l=1,\ldots,r$ are restricted to piecewise-constant real functions of time, and $\psi(t)$ denotes a quantum state belonging to $S_{\mathcal{H}}$. In physical language, H_0' is the unperturbed or autonomous Hamiltonian, and the H_l' are interaction Hamiltonians. It is the coefficients $u_l(t)$ that are subject to purposeful control by an agent external to the system, within the specified class of functions. Setting $\hbar=1$ and dividing $H_0'(t)$ and the $H_l'(t)$ by i, we arrive at a more familiar control form,

$$\frac{\partial}{\partial t}\psi(t) = \left[H_0(t) + \sum_l u_l(t)H_l(t)\right]\psi(t),$$
$$\psi(t_0) = \psi_0 \in S_{\mathcal{H}}, \tag{3}$$

where the $H_i(t)$, $i=0,1,2,\ldots,r$, are skew-Hermitian operators on $S_{\mathcal{H}}$. From the standpoint of systems engineering, $H_0(t)$ is called the drift term in Eq. (3) because no control function directly modifies its action. Importantly, we depart from previous studies of quantum controllability in allowing the Hamiltonian operators $H_i(t)$ to their own carry explicit time dependence, which is assumed to be inherent in the physical structure of the system and therefore beyond the control of any external agent. The operators $H_i(t)$ are the counterparts of the structural matrices involved in standard formulations of linear control theory.

For the system (3), we know from arguments presented in Ref. 5 that the transitivity of states on $S_{\mathcal{H}}$ requires an infinite sequence of control manipulations within the control set $\{u_l(t)\}$ of piecewise-constant real functions. Clearly, such a process is strictly meaningless in practice, although under certain conditions it may be possible to find a finite series of control operations that approach the desired target state arbitrarily closely. Even so, we are naturally directed to consider the issue of controllability on a *finite-dimensional* submanifold of the unit sphere $S_{\mathcal{H}}$, for which in turn a finite-dimensional tangent space is generated by $H_0(t)\psi(t),\ldots,H_r(t)\psi(t)$.

Accordingly, our attention focuses on a finite-dimensional submanifold $M\subset S_{\mathcal{H}}$, on which the following dynamics prevail:

$$\frac{\partial}{\partial t}\psi(t) = \left[H_0(t) + \sum_l u_l(t)H_l(t)\right]\psi(t),$$
$$\psi(t_0) = \psi_0, \quad \psi(t) \in M, \quad \forall\, t \geqslant t_0. \tag{4}$$

Thus, instead of studying controllability on $S_{\mathcal{H}}$, we consider controllability on $M\subset S_{\mathcal{H}}$. On the submanifold M, the inherited topology of $S_{\mathcal{H}}$ still applies; hence it is paracompact and connected.

For system (4), we have available a set of vector fields $O(M)$ composed of skew-Hermitian operators on M with Lie algebra defined by $O(M)=\mathcal{L}\{H_0,\ldots,H_r\}$. Let V be a subset of $O(M)$. The Lie algebra generated by V is denoted by $\mathcal{L}(V)$. The restriction of $\mathcal{L}(V)$ to a point ψ on M, which is a tangent subspace of TM_ψ at ψ, is written as

$$\mathcal{L}(V)(\psi) = \{Y(\psi)\,|\,Y \in \mathcal{L}(V)\} \subset TM_\psi, \tag{5}$$

while

$$\tilde{\mathcal{L}}(V) = \{\mathcal{L}(V)(\psi) | \psi \in M\} \tag{6}$$

defines an involutive differential system. A vector field X is said to belong to $\tilde{\mathcal{L}}(V)$ if $X(\psi) \in \tilde{\mathcal{L}}(V)(\psi)$ holds for all $\psi \in M$.

III. SELECTING THE DOMAIN

Recognizing that operators in quantum mechanics are in general unbounded, we need to find a domain on which exponentiations of the operators entering the system (4) converge. To this end, we introduce the so-called analytic domain conceived by Nelson,[32] a dense domain invariant under the action of the operators in system (3). The solution of the Schrödinger equation can be expressed globally in exponential form on this domain, which is also invariant under the action of the exponentiations of the operators H_i.

Definition III.1: If H is an operator on the state space $\mathcal{H}$, we call an element ω of $\mathcal{H}$ an analytic vector for H in case the series expansion of $\exp(Ht)\omega$ *has a positive radius of absolute convergence, that is, provided*

$$\sum_{n=0}^{\infty} \frac{\|H^n \omega\|}{n!} s^n < \infty \tag{7}$$

for some $s > 0$.

If H is a bounded operator, then every vector in $\mathcal{H}$ is trivially an analytic vector for H.

The corresponding definition of analytic vectors for a Lie algebra of operators runs as follows.[32,57]

Definition III.2: A vector $\omega \in \mathcal{H}$ is said to be an analytic vector for the whole Lie algebra $\mathcal{L}$ if for some $s > 0$ and some linear basis $\{H_1, \ldots, H_d\}$ of the Lie algebra, the series

$$\sum_{n=0}^{\infty} \frac{1}{n!} \sum_{1 \leqslant i_1, \ldots, i_n \leqslant d} \|H_{i_1} \cdots H_{i_n} \omega\| s^n \tag{8}$$

is absolutely convergent.

The concept of analytic vectors is especially useful for our purposes, since for certain types of unbounded operators they form a dense set in the Hilbert space. In fact, the set of all analytic vectors for a Lie algebra $\mathcal{L}$ forms an analytic domain in the following sense.[32,57]

Definition III.3: Let $\mathcal{L}$ be the Lie algebra generated by the skew-Hermitian operators $H_0, \ldots, H_r$ on a unit sphere $S_{\mathcal{H}}$ of Hilbert space. An analytic domain $\mathcal{D}_A$ is said to exist for the H_i, $i = 0, 1, \ldots r$, if (i) there exists a common dense invariant subspace $\mathcal{D}_A \subset \mathcal{H}$ on which the corresponding unitary Lie group G can be expressed locally in exponential form with Lie algebra $\mathcal{L}$, (ii) $\mathcal{D}_A$ is invariant under G and *$\mathcal{L}$, and (iii) on $\mathcal{D}_A$, elements of G can be extended globally to all $t \in \mathbb{R}^+$.*

We now state Nelson's fundamental theorem, which provides conditions under which a Lie algebra $\mathcal{L}$ defined by a set of skew-Hermitian operators can be associated with a unitary group G having $\mathcal{L}$ as its Lie algebra.

Theorem III.1: (Nelson) Let $\mathcal{L}$ be a Lie algebra of skew-Hermitian operators in a Hilbert space $\mathcal{H}$ which have a common invariant dense domain $\mathcal{D}_A$. Let $X_1, \ldots, X_d$ be an operator basis for $\mathcal{L}$. If $T = X_1^2 + \cdots + X_d^2$ is essentially self-adjoint, then there is a unique unitary group G in $\mathcal{H}$ with Lie algebra $\mathcal{L}$. Let $\overline{T}$ denote the unique self-adjoint extension of T. Then the analytic vectors of $\overline{T}$ are analytic vectors for the whole Lie algebra $\mathcal{L}$ and form a set invariant under G and dense in $\mathcal{H}$.

Accordingly, on the analytic domain $\mathcal{D}_A$, the Lie algebra and its unitary Lie group are related through the familiar exponential formula. The Lie algebra is composed of skew-Hermitian operators which are vector fields defined on $\mathcal{D}_A \cap S_{\mathcal{H}}$. By property (iii) of the Definition III.3 of the analytic domain, these vector fields on $\mathcal{D}_A \cap S_{\mathcal{H}}$ are complete. Moreover, owing to the skew-

Hermiticity of the operators H_i of system (3), the corresponding transformation groups, taking a given state on $S_{\mathcal{H}}$ to another state on $S_{\mathcal{H}}$, are unitary. This feature guarantees preservation of the norm of quantum states, as required for the statistical interpretation of quantum mechanics.

In fact, Nelson's theorem only provides sufficient conditions for the important properties it yields. With this in mind, we shall assume an analytic domain $\mathcal{D}_A$ exists *without* explicitly imposing the conditions stated in this theorem, a stance also adopted in Ref. 5. This strategy clearly implies that the existence of such a domain must be established explicitly prior to application of the controllability results to be derived in the following sections.

We are now prepared to adapt the concept of controllability to problems involving unbounded operators.

Definition III.4: For system (3), if $\mathcal{D}_A$ exists for $\mathcal{L}$, and if for any ψ_0 and $\psi_f \in \mathcal{D}_A \cap S_{\mathcal{H}}$ there exist control functions $u_1(t), \ldots, u_r(t)$, and a time t_f (respectively, $\forall t_f$) such that the solution of control system (3) satisfies $\psi(t_0)=\psi_0$, $\psi(t_f)=\psi_f$, and $\psi(t) \in \mathcal{D}_A \cap S_{\mathcal{H}}$, where $t_0 \leqslant t \leqslant t_f$, then the system is called analytically controllable (*respectively strongly analytically controllable*) *on $S_{\mathcal{H}}$; moreover we then say that the corresponding unitary Lie group is analytically transitive on $S_{\mathcal{H}}$.*

As has been argued, the more pertinent concept is controllability on the submanifold M of $S_{\mathcal{H}}$. By assumption, $M \cap \mathcal{D}_A$ is dense in M, while $\dim(M \cap \mathcal{D}_A) = \dim M = m$. Denoting the tangent space of $M \cap \mathcal{D}_A$ at ψ by $TM_\psi = \mathcal{L}\{H_0, \ldots, H_r\}(\psi)$, the tangent bundle of the system (4) is given by $T(M \cap \mathcal{D}_A) = \cup_{\psi \in M \cap \mathcal{D}_A} TM_\psi$.

Let $R_t(\psi)$ denote the set of all points that are reachable from ψ at time t. The set $R(\psi) = \cup_{t>t_0} R_t(\psi)$ is then reachable from ψ at some time greater than t_0. We say that system (4) is analytically controllable on M if $R(\psi) = M \cap \mathcal{D}_A$, $\forall\, \psi \in M \cap \mathcal{D}_A$, and that the system is strongly analytically controllable on M if $R_t(\psi) = M \cap \mathcal{D}_A$, $\forall\, t > t_0$, $\forall\, \psi \in M \cap \mathcal{D}_A$.

IV. CONTROLLABILITY OF TIME-DEPENDENT QUANTUM CONTROL SYSTEMS

A. Reformulation as a time-independent augmented system

Most of the methods developed for determining controllability of time-independent bilinear or nonlinear systems[5,31,58–61] cannot be applied directly to the time-dependent bilinear control problem studied here, since these approaches rely upon the following property. Let $Y_t(\varphi)$ be an integral curve of the time-independent tangent vector Y starting from point φ and $t \in [t_0, t_0 + t_f]$, and let $cY_t(\varphi)$ be an integral curve of the tangent vector cY starting from φ and $t \in [t_0, t_0 + t_f/|c|]$; then the integral curves $Y_t(\varphi)$ and $cY_t(\varphi)$ coincide. This property holds for all time-independent tangent vectors, but it generally fails for time-dependent tangent vectors.

However, recognizing that this feature has been instrumental to controllability proofs for nonlinear systems, we recast the system (4) as a time-independent problem so that it can once again be exploited. Reformulation of the original problem is accomplished by regarding the time variable t as an additional parameter in the specification of the system state, supplementing the state vector ψ. Thus the state of the extended system is expressed as

$$\xi = \begin{pmatrix} t + t_0 \\ \psi \end{pmatrix}. \tag{9}$$

Making the corresponding extension of the manifold M, we form an augmented $(m+1)$-dimensional manifold defined by

$$N = \begin{Bmatrix} \mathbb{R} \\ M \cap \mathcal{D}_A \end{Bmatrix}, \tag{10}$$

where $\mathbb{R}$ is the real line. Next we define augmented vector fields W_l by

$$W_0(\xi) = \begin{bmatrix} 1 \\ H_0(t + t_0)\psi(t + t_0) \end{bmatrix},$$

$$W_l(\xi) = \begin{bmatrix} 0 \\ H_l(t+t_0)\psi(t+t_0) \end{bmatrix}, \tag{11}$$

with $l=1,2,\ldots,r$. Obviously, the W_l, with $l=0,1,\ldots,r$, depend on both t and ψ, i.e., the W_l now depend on the state ξ defined by Eq. (9).

The time-dependent control system (4) has thereby been reformulated as an augmented system of time-independent form. Explicitly,

$$\frac{\partial \xi(t)}{\partial t} = \left[W_0(\xi) + \sum_l u_l(t) W_l(\xi) \right],$$

$$\xi(0) = \eta = \begin{pmatrix} t_0 \\ \psi(t_0) \end{pmatrix} = \begin{pmatrix} t_0 \\ \psi_0 \end{pmatrix}, \tag{12}$$

$$\forall t \geqslant 0, \quad \psi_0 \in M \cap \mathcal{D}_A, \quad \xi \in N,$$

where N is the $n=(m+1)$-dimensional manifold constructed in Eq. (10) and M is now viewed as a one-dimension-reduced manifold of the augmented system. As always, the controls $u_l(t)$, with $l=1,\ldots,r$, are piecewise-constant real functions of time t.

It is convenient to employ $t+t_0$ instead of t in definitions (9) and (11), thereby setting the starting time at zero for the augmented system (12). Since the latter system is time-independent by construction, this can be done without affecting its trajectory. Thus, if the time for the augmented system is t, then the time for the original system (4) is $t+t_0$. Standard differential equation techniques can evidently be employed to analyze the behavior of the augmented system on the manifold N, and the results will reflect the behavior of the original system on manifold M.

We note peripherally that system (12) is in a decomposed form in the sense of Ref. 59, where several theorems were developed for decomposition of nonlinear control systems. However, these theorems do not specify reachable sets, so they cannot be applied here to obtain controllability results.

Reachable sets $\hat{R}_t(\eta)$ and $\hat{R}(\eta)$ are defined for the augmented system (12) in just the same manner as for system (4). From the work of Huang, Tarn, and Clark[5] based on the results of Chow,[62] Sussmann and Jurdjevic,[24] and Kunita,[54,58] it is to be expected that the issue of analytic controllability will hinge on the relationships among certain Lie algebras generated by the vector fields involved in the control system (4) or its augmented counterpart (12). For the latter problem, these Lie algebras are specified by $\hat{\mathcal{A}}=\mathcal{L}\{W_0,\ldots,W_r\}$, $\hat{\mathcal{B}}=\mathcal{L}\{W_1,\ldots,W_r\}$, and $\hat{\mathcal{C}}=\mathcal{L}\{\mathrm{ad}^m_{W_0}W_l, l=1,\ldots,r, m=0,\ldots,\infty\}$. By definition, $\mathrm{ad}^m_{W_0}W_l$ is built from repeated commutators of W_0, present in $\hat{\mathcal{A}}$ but not $\hat{\mathcal{B}}$, with any and all of the W_l present in $\hat{\mathcal{A}}$ or $\hat{\mathcal{B}}$; clearly,

$$\hat{\mathcal{B}} \subset \hat{\mathcal{C}} \subset \hat{\mathcal{A}}. \tag{13}$$

For future reference we note (in particular) that the restriction of $\hat{\mathcal{B}}$ to a point ψ on N, which is a tangent subspace of TN_ψ at ψ, is written as

$$\hat{\mathcal{B}}(\psi) = \{Y(\psi) | Y \in \hat{\mathcal{B}}\} \subset TN_\psi, \tag{14}$$

and in turn that

$$\widetilde{\hat{\mathcal{B}}} = \{\hat{\mathcal{B}}(\psi) | \psi \in N\} \tag{15}$$

is an involutive differential system.

B. Controllability of the augmented system

We must still face the situation that standard controllability results,[5,31,58–61] derived for time-independent systems, cannot be carried over directly to our problem as reformulated in the preceding section, since derivation of these results employs the vector-space property of the tangent space. Specifically, it is required that if Y is an acceptable tangent vector, then so is cY, where c is an arbitrary constant. But in our case, once the first component of a tangent vector of the augmented manifold is fixed at unity, it is not possible for both Y and cY, with $c \neq 1$, to be available tangent vectors. However, with the aid of a result of Kunita,[54] we may nevertheless establish one-dimension-reduced controllability of the augmented system; that is, we may prove strong analytic controllability of the original system since it is not necessary to control the time dimension.

First, let us identify certain properties of the reachable set $\hat{R}_t(\eta)$ that will be useful in proving strong analytic controllability.

Theorem IV.1: (References 24 and 25) *Assume that the Lie algebra $\hat{C}$ is locally finitely generated, and let $I(\eta)$ be the maximal connected integral manifold of $\hat{C}$ containing the point η. Then $\hat{R}_t(\eta) \subset \alpha_t^0(I(\eta))$, where α_t^0 is the integral curve whose vector field is W_0. Furthermore, the interior of $\hat{R}_t(\eta)$ with respect to the topology of $\alpha_t^0(I(\eta))$ is dense in $\hat{R}_t(\eta)$.*

In the rest of this section, we systematically develop the principal result of the paper, namely, under suitable conditions the reachable set of the augmented system (12) at time t, $\hat{R}_t(\eta)$, is equal to $\alpha_t^0(I(\eta))$. We begin by establishing a key relationship between the interior of the reachable set $\hat{R}_t(\eta)$ of the augmented system at time t and the interior of its closure, through the following lemma.

Lemma IV.2:

$$\text{int}(\text{cl}\,\hat{R}_t(\eta)) = \text{int}\,\hat{R}_t(\eta). \tag{16}$$

Proof: Let $\chi \in \text{int}(\text{cl}\,\hat{R}_t(\eta))$ and let $S_\epsilon(\chi)$ be the set of all χ' such that χ is reachable from χ' within time $\epsilon > 0$. Then $S_\epsilon(\chi)$ is the reachable set within time $\epsilon > 0$ for the dual control system

$$\frac{\partial v}{\partial t} = -\left[W_0(v) + \sum_l u_l(t) W_l(v) \right]. \tag{17}$$

Theorem IV.1 implies that $\text{int}\,S_\epsilon(\chi)$ is dense in $\text{cl}\,S_\epsilon(\chi)$, and $\text{int}\,\hat{R}_t(\eta)$ is dense in $\text{cl}\,\hat{R}_t(\eta)$. Since $\chi \in \text{cl}\,S_\epsilon(\chi)$, we know that

$$\text{cl}\,S_\epsilon(\chi) \cap \text{int}(\text{cl}\,\hat{R}_t(\eta)) \neq \varnothing \tag{18}$$

and hence that

$$\text{int}\,S_\epsilon(\chi) \cap \text{int}(\text{cl}\,\hat{R}_t(\eta)) \cap \hat{R}_t(\eta) \neq \varnothing\,. \tag{19}$$

If ζ belongs to the latter intersection, then ζ is reachable from η using time t, and χ is reachable from ζ in elapsed time less than or equal to ϵ. Therefore, χ is reachable from η in elapsed time between t and $t+\epsilon$. This argument holds for any $t > 0$ and any $\epsilon > 0$. Letting $\epsilon \to 0$, we conclude that χ is reachable from η in time t, so $\chi \in \hat{R}_t(\eta)$. Thus,

$$\text{int}(\text{cl}\,\hat{R}_t(\eta)) \subset \hat{R}_t(\eta) \Rightarrow \text{int}(\text{cl}\,\hat{R}_t(\eta)) \subset \text{int}\,\hat{R}_t(\eta).$$

But clearly $\text{int}\,\hat{R}_t(\eta) \subset \text{int}(\text{cl}\,\hat{R}_t(\eta))$ and the statement (18) follows.

From the control-theoretic perspective, the drift term is undesirable because no control is present to influence or remove its effect. It is therefore of strategic value to consider a suitably modified control system, called the auxiliary system, that will serve as a bridge to an effective controllability analysis of the augmented system. Let $e_0, e_1, \ldots, e_r$ be unit vectors in $\mathbb{R}^{r+1}$; in

particular, let $e_i=(0,\ldots,0,1,0,\ldots,0)$, in which only the $(i+1)$th element is unity and the others are zero. Denote by $\mathcal{U}_0$ the set of controls $u(t)=(u_0(t),\ldots,u_r(t))$ composed of piecewise-constant functions $u_i(t)$ taking the values $e_0,\pm e_1,\ldots,\pm e_r$ only. Consider then the control system expressed in the form

$$\frac{\partial \xi}{\partial t} = u_0(t)W_0(\xi) + \sum_l u_l(t)W_l(\xi), \quad \xi(t_0) = \eta, \tag{20}$$

where $u(t)\in\mathcal{U}_0$. The solution of this system may be written as

$$\alpha_t = \alpha_{t_k}^{i_k}\cdots\alpha_{t_j}^{i_j}\cdots\alpha_{t_1}^{i_1}, \tag{21}$$

where k is a positive integer and where $\alpha_{t_j}^{i_j}$ is the integral curve of W_{i_j} with $i_j=0,1,\ldots,r$, $j=1,\ldots,k$, and k a positive integer. The times t_j satisfy $t_j\geqslant 0$ if $i_j=0$, otherwise, $t_j\in\mathbb{R}$. We denote by $\hat{R}_t^0(\eta)$ the reachable set of the auxiliary system corresponding to the total time t since time zero, over which the control function $u_0(\cdot)$ is nonzero; the reachable set of the auxiliary system is then $\hat{R}^0(\eta)=\cup_{t>0}\hat{R}_t^0(\eta)$. Theorem IV.1 is valid for this control system.[24]

The following notations are convenient:

Exp $\hat{\mathcal{L}}$=the group of diffeomorphisms generated by the α_t^i, $t\in\mathbb{R}$, $i=0,\ldots,r$, where α_t^i is an integral curve of W_i,

$(\text{Exp}\,\hat{\mathcal{L}})_+$=the semigroup of diffeomorphisms generated by α_t^0, $t\geqslant 0$, and the α_t^l, with $t\in\mathbb{R}$ and $l=1,\ldots,r$,

$(\text{Exp}\,\hat{\mathcal{L}})_t$=the subset of $(\text{Exp}\,\hat{\mathcal{L}})_+$ generated by $\alpha_{t_k}^{i_k}\cdot\cdots\cdot\alpha_{t_1}^{i_1}$, with $\Sigma_{j=1}^k t_j\cdot 1_{\{i_j=0\}}=t$.

To clarify the meaning of the last line, we note that when the index j is such that $i_j=0$, we have $u_0=1$ (and all the other $u_i=0$), so W_0 is "turned on" and does play a role as an active vector field or tangent vector. Conversely, for indices j such that $i_j\neq 0$, the factor u_0 multiplying W_0 in system (20) vanishes, and W_0 plays no role. The sum appearing in the definition of $(\text{Exp}\,\hat{\mathcal{L}})_t$ gives the total time over which W_0 is active in the system dynamics.

From Chow's theorem,[24,62] it is known that the group Exp $\hat{\mathcal{L}}$ acts transitively on the manifold N when $\dim\hat{\mathcal{L}}\{W_0,W_1,\ldots,W_r\}=\dim N$, i.e., we know that $\{\alpha(\eta)\,|\,\alpha\in\text{Exp}\,\hat{\mathcal{L}}\}=N$ for any $\eta\in N$. On the other hand, the reachable set at time t for the auxiliary system (20) is $\hat{R}_t^0(\eta)=\{\alpha(\eta)\,|\,\alpha\in(\text{Exp}\,\hat{\mathcal{L}})_t\}$. (It is to be noted that in the present context t is the total time over which W_0 has been active since time zero, which is generally not equal to the actual elapsed time, since W_0 may be turned off over certain intervals.)

Lemma IV.3:

$$\text{cl}\,\hat{R}_t(\eta) = \text{cl}\,\hat{R}_t^0(\eta). \tag{22}$$

We may gain intuitive understanding of this lemma by analyzing a simple example.

Example: Let us compare the control system

$$\frac{d}{dt}\begin{pmatrix}x\\y\end{pmatrix} = \begin{pmatrix}1\\0\end{pmatrix} + u\begin{pmatrix}0\\1\end{pmatrix}, \tag{23}$$

wherein $u\in\mathbb{R}$, with the system

$$\frac{d}{dt}\begin{pmatrix}x\\y\end{pmatrix} = u_0\begin{pmatrix}1\\0\end{pmatrix} + u_1\begin{pmatrix}0\\1\end{pmatrix}, \tag{24}$$

wherein $(u_0,u_1)\in\{(0,\pm 1),(1,0)\}$. Clearly, the first of these corresponds to the augmented system, and the second to the auxiliary system. Let $\hat{R}_t(\eta)$ and $\hat{R}_t^0(\eta)$ denote, respectively, the reachable sets of systems (23) and (24), starting from the state η. While stopping short of rigorous argument,

explicit computation will be used to reveal the pertinent relationship between $\mathrm{cl}\,\hat{R}_t(\eta)$ and $\mathrm{cl}\,\hat{R}_t^0(\eta)$.

First consider the integral curve

$$\alpha_t(\eta) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{t_1} \cdot \begin{pmatrix} 0 \\ -1 \end{pmatrix}_{t_2} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{t} \in \hat{R}_t^0(\eta), \tag{25}$$

and for $n=1,2,3,\ldots$ form a series of integral curves $\beta_t^n(\eta) \in \hat{R}_t(\eta)$ defined by

$$\beta_t^n(\eta) = \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} + n\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right)_{t_1/n} \cdot \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} + n\begin{pmatrix} 0 \\ -1 \end{pmatrix}\right)_{t_2/n} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{t-(t_1/n)-(t_2/n)}. \tag{26}$$

As n goes to ∞, we find

$$\beta_t^n(\eta) \to \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{t_1} \cdot \begin{pmatrix} 0 \\ -1 \end{pmatrix}_{t_2} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{t}, \tag{27}$$

that is, $\beta_t^n(\eta) \to \alpha_t(\eta)$. Hence $\alpha_t(\eta) \in \mathrm{cl}\,\hat{R}_t(\eta)$.

On the other hand, consider

$$\beta_t(\eta) = \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} + m_1\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right)_{t_1} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{t_2} \cdot \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} + m_2\begin{pmatrix} 0 \\ -1 \end{pmatrix}\right)_{t_3} \in \hat{R}_t(\eta), \tag{28}$$

where m_1, $m_2 \in \mathbb{R}$ and $t=t_1+t_2+t_3$, and construct

$$\alpha_1^n = \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix}_{t_1/n} \cdot m_1\begin{pmatrix} 0 \\ 1 \end{pmatrix}_{t_1/n}\right]^n, \tag{29}$$

again for $n=1,2,3,\ldots$. Applying the Baker–Campbell–Hausdorff formula, it is straightforward to show that

$$\lim_{n\to\infty} \alpha_1^n = \lim_{n\to\infty}\left\{\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} + m_1\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right)_{t_1} + \frac{t_1^2}{2n} m_1\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right] + O\left(\frac{1}{n^2}\right)\right\} = \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} + m_1\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right)_{t_1}. \tag{30}$$

Similarly, let

$$\alpha_3^n = \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix}_{t_3/n} \cdot m_2\begin{pmatrix} 0 \\ -1 \end{pmatrix}_{t_3/n}\right]^n \tag{31}$$

and employ the Baker–Campbell–Hausdorff formula to obtain

$$\lim_{n\to\infty} \alpha_3^n = \lim_{n\to\infty}\left\{\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} + m_2\begin{pmatrix} 0 \\ -1 \end{pmatrix}\right)_{t_3} + \frac{t_3^2}{2n} m_2\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \end{pmatrix}\right] + O\left(\frac{1}{n^2}\right)\right\} = \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} + m_2\begin{pmatrix} 0 \\ -1 \end{pmatrix}\right)_{t_3}. \tag{32}$$

Obviously

$$\alpha_1^n \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{t_2} \cdot \alpha_3^n \in \hat{R}_t^0(\eta), \tag{33}$$

and we find that

$$\lim_{n\to\infty} \alpha_1^n\left(\begin{pmatrix}1\\0\end{pmatrix}_{t_2}\right)\alpha_3^n = \left(\left(\begin{pmatrix}1\\0\end{pmatrix} + m_1\begin{pmatrix}0\\1\end{pmatrix}\right)_{t_1} \cdot \begin{pmatrix}1\\0\end{pmatrix}_{t_2} \cdot \left(\begin{pmatrix}1\\0\end{pmatrix} + m_2\begin{pmatrix}0\\-1\end{pmatrix}\right)_{t_3} = \beta_t(\eta). \tag{34}$$

Therefore $\beta_t(\eta) \in \mathrm{cl}\,\hat{R}_t^0(\eta)$.

Now let us proceed with the proof of Lemma IV.3, showing first that $\mathrm{cl}\,\hat{R}_t^0(\eta) \subseteq \mathrm{cl}\,\hat{R}_t(\eta)$. Consider that $\alpha_t(\eta) \in \hat{R}_t^0(\eta)$ is expressible in the form of $\alpha_{t_k}^{i_k} \cdots \alpha_{t_1}^{i_1}(\eta)$, where $t = \Sigma_{j=1}^k t_j \cdot 1_{\{i_j=0\}}$. With the guidance of the example above, a sequence of controls $u^{(n)}(\cdot)$ associated with the diffeomorphism of this form is constructed as follows. For an arbitrary positive integer n such that $nt_m \geqslant \Sigma_{i_j\neq 0}|t_j|$, where m is the last subscript j such that $i_j = 0$, let

$$t_m^{(n)} = t_m - \frac{\sum_{i_j\neq 0}|t_j|}{n}. \tag{35}$$

Define real numbers $s_1^{(n)}, \ldots, s_k^{(n)}$, ordered so that $0 \leqslant s_1^{(n)} \leqslant s_2^{(n)} \leqslant \cdots \leqslant s_k^{(n)}$, by

$$\begin{aligned} s_1^{(n)} &= |t_1| \quad \text{if } i_1 = 0, \\ &= \frac{1}{n}|t_1| \quad \text{if } i_1 \neq 0, \\ s_{j\geqslant 2}^{(n)} &= s_{j-1}^{(n)} + |t_j^{(n)}| \quad \text{if last } j \text{ with } i_j = 0, \\ &= s_{j-1}^{(n)} + |t_j| \quad \text{if other } j \text{ with } i_j = 0, \\ &= s_{j-1}^{(n)} + \frac{1}{n}|t_j| \quad \text{if } i_j \neq 0. \end{aligned} \tag{36}$$

Further, let

$$\begin{aligned} u^{(n)}(\tau) &= n \cdot \mathrm{sgn}(t_j) e_{i_j} \quad \text{if } s_{j-1}^{(n)} \leqslant \tau \leqslant s_j^{(n)} \text{ and } i_j \neq 0, \\ &= 0 \quad \text{if } s_{j-1}^{(n)} \leqslant \tau \leqslant s_j^{(n)} \text{ and } i_j = 0, \\ &= 0 \quad \text{if } \tau \geqslant s_k^{(n)}, \end{aligned} \tag{37}$$

where $e_1, \ldots, e_r$ are unit vectors in $\mathbb{R}^r$. The solution $\beta_t^{(n)}$ of the system (12) associated with the control $u^{(n)}(\cdot)$ may be written

$$\beta_{s_k^{(n)}}^{(n)} = \beta_{|t_k|}^{n,i_k} \cdots \beta_{|t_1|}^{n,i_1} \in \hat{R}_t(\eta), \tag{38}$$

where $\beta_{|\tau|}^{n,i_j}$ is the integral curve of W_0 if $i_j = 0$, or the integral curve of $W_0 + n \cdot \mathrm{sgn}(\tau) W_{i_j}$ if $i_j \neq 0$, i.e.,

$$\begin{aligned} \beta_{|\tau|}^{n,i_j} &= (W_0)_\tau \quad \text{if } i_j = 0, \\ &= (W_0 + n \cdot \mathrm{sgn}(\tau) W_{i_j})_{|\tau|/n} \quad \text{if } i_j \neq 0. \end{aligned} \tag{39}$$

We note that $(W_0 + n \cdot \mathrm{sgn}(\tau) W_{i_j})_{|\tau|/n}$ and $[(1/n)W_0 + \mathrm{sgn}(\tau) W_{i_j}]_{|\tau|}$ describe the same integral curve on N, by virtue of the time-invariance property of system (12). Obviously, $\beta_{|t_p|}^{n,i_j} \to \alpha_{t_p}^{i_j}$ as $n \to \infty$. On the other hand,

$$s_k^{(n)} = \sum_j t_j \cdot 1_{\{i_j=0\}} - \frac{\sum_l |t_l| \cdot 1_{\{i_l \neq 0\}}}{n} + \frac{\sum_l |t_l| \cdot 1_{\{i_l \neq 0\}}}{n} = t. \tag{40}$$

Thus, as $n \to \infty$ we obtain

$$\beta^{(n)}_{s_k^{(n)}}(\eta) \to \alpha^{i_k}_{t_k} \cdots \alpha^{i_1}_{t_1}(\eta) = \alpha_t(\eta), \tag{41}$$

and hence $\alpha_t(\eta) \in \mathrm{cl}\, \hat{R}_t(\eta)$. Because $\alpha_t(\eta)$ is an arbitrary element in $\hat{R}^0_t(\eta)$, it follows that $\hat{R}^0_t(\eta) \subseteq \mathrm{cl}\, \hat{R}_t(\eta)$, and since $\mathrm{cl}\, \hat{R}_t(\eta)$ is closed, it follows in turn that $\mathrm{cl}\, \hat{R}^0_t(\eta) \subseteq \mathrm{cl}\, \hat{R}_t(\eta)$.

Next we show $\mathrm{cl}\, \hat{R}_t(\eta) \subseteq \mathrm{cl}\, \hat{R}^0_t(\eta)$. Consider $\beta(\eta) \in \hat{R}_t(\eta)$ of the form of $\beta^{c_k}_{u_k} \cdot \cdots \cdot \beta^{c_1}_{u_1}(\eta)$, with $\beta^{c_j}_{u_j} = \exp u_j(W_0 + c_j^1 W_1 + \cdots + c_j^r W_r)$ and $c_j = (c_j^1, \ldots, c_j^r)$. Here, c_j^l is the control applied to W_l during time period u_j, so c_j is the control set applied to $W_1, \ldots, W_r$ during the corresponding time interval u_j, with $u_j \in \mathbb{R}^+$ and $c_j^l \in \mathbb{R}$. For each $\beta^{c_j}_{u_j}$, $j = 1, \ldots, k$, take α_j^n in the form

$$\alpha_j^n = \left[\exp \frac{u_j}{n}(c_j^1 W_1) \cdots \exp \frac{u_j}{n}(c_j^r W_r) \exp \frac{u_j}{n} W_0 \right]^n. \tag{42}$$

Invoking the Baker–Campbell–Hausdorff formula,[63] we write

$$\begin{aligned} \lim_{n\to\infty} \alpha_j^n &= \lim_{n\to\infty} \left[\exp \frac{u_j}{n}(c_j^1 W_1) \cdots \exp \frac{u_j}{n}(c_j^r W_r) \cdot \exp \frac{u_j}{n} W_0 \right]^n \\ &= \lim_{n\to\infty} \exp \left[u_j(W_0 + c_j^1 W_1 + \cdots + c_j^r W_r) + \sum_{0 \leq p,q \leq r} \frac{u_j^2}{2n} c_j^p c_j^q [W_p, W_q] + O\left(\frac{1}{n^2}\right) \right] \\ &= \exp u_j(W_0 + c_j^1 W_1 + \cdots + c_j^r W_r) = \beta^{c_j}_{u_j}. \end{aligned} \tag{43}$$

Constructing $\alpha_1^n \cdots \alpha_k^n \in \hat{R}^0_t(\eta)$ we then obtain

$$\lim_{n\to\infty} \alpha_k^n \cdots \alpha_1^n(\eta) = \beta^{c_k}_{u_k} \cdots \beta^{c_1}_{r_1}(\eta) = \beta(\eta), \tag{44}$$

so that $\beta(\eta) \in \mathrm{cl}\, \hat{R}^0_t(\eta)$. Since $\beta(\eta)$ is an arbitrary element of $\hat{R}_t(\eta)$, we arrive at $\hat{R}_t(\eta) \subseteq \mathrm{cl}\, \hat{R}^0_t(\eta)$ and hence $\mathrm{cl}\, \hat{R}_t(\eta) \subseteq \mathrm{cl}\, \hat{R}^0_t(\eta)$. We conclude that $\mathrm{cl}\, \hat{R}_t(\eta) = \mathrm{cl}\, \hat{R}^0_t(\eta)$.

The time t labeling these reachable sets is to be interpreted as the time interval over which the control operation represented by W_0 is in effect, or "turned on." In fact, W_0 is necessarily *always* "on" in the augmented system, so the total time elapsing in the augmented system is the same as the time interval over which W_0 is turned on; hence the reachable sets $\hat{R}_t$ corresponding to these two times are identical. Of course, the same coincidence does not hold for the auxiliary system. However, this is immaterial, since the auxiliary system was only introduced to exploit the key relationship (22). Further, we may observe that the reachable set $\hat{R}^0_t(\eta)$ of system (20), with the control $u(t) = (u_0(t), \ldots, u_r(t))$ assuming values $(e_0, \pm e_1, \ldots, \pm e_r)$, is the same as the corresponding set for which the control $u(t)$ assumes the values $e_0, \pm c e_1, \ldots, \pm c e_r$, with $c \in \mathbb{R}^+$.

Since we can take advantage of the result (22) in this manner, it is clearly preferable to study the properties of $\hat{R}^0_t(\eta)$. The auxiliary system is easier to control, and the state at time t can be expressed as a composition of integral curves of W_i in the same style as Eq. (21). To do so, let the set of subscripts j with $i_j = 0$ be written as $\{p, \ldots, q, s\}$ in increasing order, of course with $t_p + \cdots + t_q + t_s = t$. Then we have

$$\alpha_t = (\alpha_{t_k}^{i_k} \cdots \alpha_{t_{s+1}}^{i_{s+1}}) \cdot (\alpha_{t_s}^0 \cdot \alpha_{t_{s-1}}^{i_{s-1}} \cdot \alpha_{-t_s}^0) \cdot (\alpha_{t_s}^0 \cdot \alpha_{t_{s-2}}^{i_{s-2}} \cdot \alpha_{-t_s}^0) \cdots (\alpha_{t_s+t_q}^0 \cdot \alpha_{t_{q-1}}^{i_{q-1}} \cdot \alpha_{-(t_s+t_q)}^0)$$
$$\cdot (\alpha_{t_s+t_q}^0 \cdot \alpha_{t_{q-2}}^{i_{q-2}} \cdot \alpha_{-(t_s+t_q)}^0) \cdots (\alpha_{t_s+t_q+\cdots+t_p}^0 \cdot \alpha_{t_{p-1}}^{i_{p-1}} \cdot \alpha_{-(t_s+t_q+\cdots+t_p)}^0) \cdots (\alpha_{t_s+t_q+\ldots+t_p}^0 \cdot \alpha_{t_1}^{i_1}$$
$$\cdot \alpha_{-(t_s+t_q+\ldots+t_p)}^0) \cdot \alpha_t^0 = \beta_0(\alpha_{t_k}^{i_k}) \cdots \beta_0(\alpha_{t_{s+1}}^{i_{s+1}}) \cdot \beta_{t_s}(\alpha_{t_{s-1}}^{i_{s-1}})$$
$$\cdot \beta_{t_s}(\alpha_{t_{s-2}}^{i_{s-2}}) \cdots \beta_{t_s+t_q}(\alpha_{t_{q-1}}^{i_{q-1}}) \cdot \beta_{t_s+t_q}(\alpha_{t_{q-2}}^{i_{q-2}}) \cdots \beta_t(\alpha_{t_{p-1}}^{i_{p-1}}) \cdots \beta_t(\alpha_{t_1}^{i_1}) \cdot \alpha_t^0, \tag{45}$$

where $\beta_t(\gamma) = \alpha_t^0 \cdot \gamma \cdot \alpha_{-t}^0$. This analysis stimulates us to define the following three sets of diffeomorphisms:

Exp $\hat{\mathcal{B}}$ = the group generated by α_t^l, $t \in \mathbb{R}$, $l = 1, \ldots, r$, where α_t^l is the integral curve whose vector field is W_l,

$$F_t = \cup_{k=1}^{\infty} \{\beta_{t_k}(\gamma_k) \cdot \cdots \cdot \beta_{t_1}(\gamma_1) \,|\, \gamma_j \in \text{Exp}\, \hat{\mathcal{B}}, 0 \leqslant t_k \leqslant \cdots \leqslant t_1 = t\},$$

$$G_t = \cup_{k=1}^{\infty} \{\beta_{t_k}(\gamma_k) \cdot \cdots \cdot \beta_{t_1}(\gamma_1) \,|\, \gamma_j \in \text{Exp}\, \hat{\mathcal{B}}, \min_j t_j \geqslant 0, \max_j t_j = t\}.$$

.

By construction,

$$\hat{R}_t^0(\eta) = F_t \alpha_t^0(\eta). \tag{46}$$

We observe that F_t is a semigroup of diffeomorphisms included in the group G_t, whose properties are established in the following lemma.

Lemma IV.4: First, the set G_t is a group. Furthermore, if $\dim \hat{\mathcal{C}}(\eta) = n - 1 = m$ *holds for all* $\eta \in N$, *then* $\{\alpha(\eta) \,|\, \alpha \in G_t\} = \alpha_t^0(I(\alpha_{-t}^0(\eta)))$ *is true for all* η, *where* $I(\nu)$ *is the maximal connected integral manifold containing* $\nu \in N$, *whose associated Lie algebra is* $\hat{\mathcal{C}}$.

Proof: For $\alpha_1, \alpha_2 \in G_t$, it is easily seen that $\alpha_1 \cdot \alpha_2 \in G_t$. Writing $\alpha \in G_t$ as $\alpha = \beta_{t_k}(\gamma_k) \cdot \cdots \cdot \beta_{t_1}(\gamma_1)$, we also see that $\alpha^{-1} = \beta_{t_1}(\gamma_1^{-1}) \cdot \cdots \cdot \beta_{t_k}(\gamma_k^{-1})$. Therefore G_t is a group.

Now, denote the set $\{\alpha(\eta) \,|\, \alpha \in G_t\}$ by $B_t(\eta)$. It is straightforward to show that (i) $B_t(\eta) = B_t(\xi)$ if $\xi \in B_t(\eta)$ and (ii) $B_t(\eta) \cap B_t(\xi) = \varnothing$ if $\xi \notin B_t(\eta)$.[54] We can demonstrate that (iii) $\eta \in \text{int}\, B_t(\eta)$ under the topology of $\alpha_t^0(I(\alpha_{-t}^0(\eta)))$ as follows. By definition, $\hat{R}_t^0(\eta)$ is the reachable set for the system (20). By the same reasoning that leads to Eq. (46), we have $\hat{R}_t^0(\alpha_{-t}^0(\eta)) \subset B_t(\eta)$ because $\hat{R}_t^0(\alpha_{-t}^0(\eta)) = F_t \cdot \alpha_t^0 \cdot \alpha_{-t}^0(\eta)$. Since $\hat{R}_t^0(\alpha_{-t}^0(\eta))$ has a nonempty interior with respect to the topology of $\alpha_t^0(I(\alpha_{-t}^0(\eta)))$ by Theorem IV.1, we see that $B_t(\eta)$ contains a non-null open set U. Given $\mu \in U$, choose $\alpha \in G_t$ such that $\alpha(\eta) = \mu$. Since α is a continuous map, $\alpha^{-1}(U)$ is an open set containing η.

In fact, $\alpha^{-1}(U)$ is included in $B_t(\eta)$. We know that G_t is a group, so $\alpha^{-1} \in G_t$ if $\alpha \in G_t$. Letting $\zeta \in \alpha^{-1}(U)$, we can find $\chi \in U$, such that $\chi = \alpha(\zeta) \in U \subset B_t(\eta)$ and also $\chi \in B_t(\zeta)$. By properties (i) and (ii), we obtain $\chi \in B_t(\zeta) \cap B_t(\eta) \neq \varnothing$. Hence $B_t(\zeta) = B_t(\eta)$ and $\zeta \in B_t(\eta)$. Accordingly, $\alpha^{-1}(U) \subset B_t(\eta)$ and $\eta \in \text{int}\, B_t(\eta)$ under the topology of $\alpha_t^0(I(\alpha_{-t}^0(\eta)))$.

The properties (i)–(iii) imply that $B_t(\eta)$ is maximally connected and open under the topology of $\alpha_t^0(I(\alpha_{-t}^0(\eta)))$. Thus we have $B_t(\eta) = \alpha_t^0(I(\alpha_{-t}^0(\eta)))$ for all $t > 0$ and $\eta \in N$. In addition, it is seen that $B_t(\eta) = \alpha_t^0(I(\alpha_{-t}^0(\eta))) = \left(\begin{smallmatrix} t_0 \\ M \cap \mathcal{D}_A \end{smallmatrix}\right)$. The proof of Lemma IV.4 is now complete.

Based on Lemmas IV.3 and IV.4, we could conclude that $\text{cl}\, \hat{R}_t(\alpha_{-t}^0(\eta)) = \alpha_t^0(I(\alpha_{-t}^0(\eta)))$ if we could establish that $F_t = G_t$. The following proof takes a slightly different path. Let Exp $\widetilde{\hat{\mathcal{B}}}$ denote the group of diffeomorphisms generated by all one parameter groups of transformations with respect to vector fields belonging to $\widetilde{\hat{\mathcal{B}}}$. The sets $\widetilde{F_t}$ and $\widetilde{G_t}$ are defined in the same way as F_t and G_t, i.e., via Eq. (17), but with Exp $\widetilde{\hat{\mathcal{B}}}$ entering in place of Exp $\hat{\mathcal{B}}$.

Obviously, $F_t \subset \widetilde{F_t}$ and $G_t \subset \widetilde{G_t}$ hold. We shall now establish that $\widetilde{F_t} = \widetilde{G_t}$.

Lemma IV.5: Let X be a complete vector field belonging to $\tilde{\tilde{\mathcal{B}}}$, *and let* γ_t *be the one-parameter group of transformations generated by X. Assume* $[\hat{\mathcal{B}},\hat{\mathcal{C}}](\eta)\subset\hat{\mathcal{B}}(\eta)$ *is satisfied for all* η. *Then* $\mathrm{d}\beta_s(\gamma_t)$ *is an isomorphism between* $\hat{\mathcal{B}}(\eta)$ *and* $\hat{\mathcal{B}}(\beta_s(\gamma_t)(\eta))$ *for each* η, *and* $\tilde{F}_t=\tilde{G}_t$ *is true for all* $t>0$.

Proof: Since $\beta_s(\gamma_{t_1})\cdot\beta_s(\gamma_{t_2})=\beta_s(\gamma_{t_1+t_2})$ holds, we have $\mathrm{d}\beta_s(\gamma_{t_1+t_2})=\mathrm{d}\beta_s(\gamma_{t_1})\cdot\mathrm{d}\beta_s(\gamma_{t_2})$. Hence it is enough to prove the lemma's assertion for sufficiently small $|t|$. Let $Y_{t,s}=\mathrm{d}\beta_s(\gamma_t)Z$, where $Z\in\tilde{\tilde{\mathcal{B}}}$. For each value of s, $\beta_s(\gamma_t)$ with $t\in R$ is the one parameter group of transformations generated by $\mathrm{d}\alpha_s^0 X$, while

$$\frac{\partial Y_{t,s}}{\partial t}=-\mathrm{d}\beta_s(\gamma_t)[\mathrm{d}\alpha_s^0 X,Z]=\mathrm{d}\beta_s(\gamma_t)[Z,\mathrm{d}\alpha_s^0 X]. \tag{47}$$

Therefore $[Z,\mathrm{d}\alpha_s^0 X]\in\tilde{\tilde{\mathcal{B}}}$ by assumption, because $\mathrm{d}\alpha_s^0 X$ belongs to $\tilde{\tilde{\mathcal{C}}}=\{\hat{\mathcal{C}}(\eta)\,|\,\eta\in N\}$.[64,65]

Now we fix a point η of N and a value of $s\in R$. Let $Z^1,\ldots,Z^n$ provide a basis of $\hat{\mathcal{B}}$ in an open neighborhood U of η. Then there exist C^∞ functions f_{ij} on U such that $[Z^i,\mathrm{d}\alpha_s^0 X]=\Sigma_{j=1}^n f_{ij}Z^j$ holds in U. Let ϵ be a positive number such that $\beta_s(\gamma_t)(\eta)\in U$ for $|t|<\epsilon$, noting that $\beta_s(\gamma_t)$ is a continuous map of t and $\beta_s(\gamma_0)(\eta)=\eta$. Then $\mathrm{d}\beta_s(\gamma_t)[Z^i,\mathrm{d}\alpha_s^0 X]=\Sigma_{j=1}^n f_{ij}\,\mathrm{d}\beta_s(\gamma_t)Z^j$ for $|t|<\epsilon$. Set $V^j(t)=\mathrm{d}\beta_s(\gamma_t)Z^j$. Then $V^j(t)$, with $|t|<\epsilon$, satisfies the linear differential equation

$$\frac{\mathrm{d}V^j(t)}{\mathrm{d}t}=\sum_{j=1}^n f_{jk}V^k(t)\quad j=1,\ldots,n. \tag{48}$$

The solution $V^j(t)$ can be written as $V^j(t)=\Sigma_{k=1}^n g_{jk}(t)V^k(0)$, where (g_{jk}) is a regular matrix. Also, we have $V^k(0)\in\hat{\mathcal{B}}(\eta)$ and $V^k(t)\in\hat{\mathcal{B}}(\beta_s(\gamma_t))(\eta)$. The map $\mathrm{d}\beta_s(\gamma_t):\hat{\mathcal{B}}(\eta)\to\hat{\mathcal{B}}(\beta_s(\gamma_t))(\eta)$ is bijective because (g_{jk}) is a regular matrix. Moreover, $\mathrm{d}\beta_s(\gamma_t)$ retains the structure of the Lie bracket with respect to $\mathrm{d}\alpha_s^0 X$. This establishes that $\mathrm{d}\beta_s(\gamma_t)$ is an isomorphism between $\hat{\mathcal{B}}(\eta)$ and $\hat{\mathcal{B}}(\beta_s(\gamma_t))(\eta)$ for $|t|<\epsilon$. Since $\gamma_t'\equiv\beta_s(\alpha)\cdot\gamma_t\cdot\beta_s(\alpha)^{-1}$ (with s fixed) is a one-parameter group of transformations generated by $\mathrm{d}\beta_s(\alpha)X$ and $\mathrm{d}\beta_s(\alpha)X$ belongs to $\tilde{\tilde{\mathcal{B}}}$, we know γ_t' (with $t\in R$) belongs to $\mathrm{Exp}\,\tilde{\tilde{\mathcal{B}}}$. But $\mathrm{Exp}\,\tilde{\tilde{\mathcal{B}}}$ is generated by all such γ_t, so we arrive at the relationship

$$\beta_t(\alpha)(\mathrm{Exp}\,\tilde{\tilde{\mathcal{B}}})\beta_t(\alpha)^{-1}\subset\mathrm{Exp}\,\tilde{\tilde{\mathcal{B}}}\quad\text{for }\alpha\in\tilde{\tilde{\mathcal{B}}}. \tag{49}$$

Let α be any element of $\tilde{G}_t$, written as

$$\alpha=\beta_{t_k}(\gamma_k)\cdot\cdots\cdot\beta_{t_1}(\gamma_1),\quad t_l\geqslant 0,\quad \max_l t_l=t. \tag{50}$$

By induction we can prove that there exist $\tilde{\gamma}_k,\ldots,\tilde{\gamma}_1$ of $\mathrm{Exp}\,\tilde{\tilde{\mathcal{B}}}$ and $0\leqslant s_k\leqslant\cdots\leqslant s_1=t$ such that

$$\beta_{t_k}(\gamma_k)\cdot\cdots\cdot\beta_{t_1}(\gamma_1)=\beta_{s_k}(\tilde{\gamma}_k)\cdot\cdots\cdot\beta_{s_1}(\tilde{\gamma}_1). \tag{51}$$

Here we only consider the case $k=2$. If $t_2\leqslant t_1$, there is no need for proof. Suppose $t_2>t_1$, and set $t_3=t_2-t_1$. Then we may write $\beta_{t_2}(\gamma_2)\cdot\beta_{t_1}(\gamma_1)=\beta_{t_1}(\beta_{t_3}(\gamma_2)\cdot\gamma_1)$. By relationship (49), there exists $\tilde{\gamma}_1$ of $\mathrm{Exp}\,\tilde{\tilde{\mathcal{B}}}$ such that $\beta_{t_3}(\gamma_2)\cdot\gamma_1\cdot\beta_{t_3}(\gamma_2)^{-1}=\tilde{\gamma}_1$, i.e., $\beta_{t_3}(\gamma_2)\cdot\gamma_1=\tilde{\gamma}_1\cdot\beta_{t_3}(\gamma_2)$. This implies

$$\beta_{t_2}(\gamma_2)\cdot\beta_{t_1}(\gamma_1)=\beta_{t_1}(\beta_{t_3}(\gamma_2)\cdot\gamma_1)=\beta_{t_1}(\tilde{\gamma}_1\cdot\beta_{t_3}(\gamma_2))=\beta_{t_1}(\tilde{\gamma}_1)\cdot\beta_{t_2}(\gamma_2). \tag{52}$$

More detailed proofs may be found in Refs. 54 and 66.

Theorem IV.6: *Suppose that* $\dim\hat{\mathcal{C}}(\eta)=n-1=m$ *holds for all* $\eta\in N$, *and suppose that* $[\hat{\mathcal{B}},\hat{\mathcal{C}}](\eta)\subset\hat{\mathcal{B}}(\eta)$ *holds for all* η. *Let* $I(\eta)$ *be the maximally connected integral manifold containing* η *whose corresponding Lie algebra is* $\hat{\mathcal{C}}$. *Then* $\alpha_t^0(I(\eta))=\hat{R}_t(\eta)$.

Proof: Clearly we have $\{\alpha\alpha_t^0(\eta)\,|\,\alpha\in F_t\}\subset\{\alpha\alpha_t^0(\eta)\,|\,\alpha\in\widetilde{F}_t\}$. In fact, the closures of these two sets coincide. Since $\widetilde{F}_t=\widetilde{G}_t\supset G_t$, it is seen that

$$\begin{aligned}\mathrm{cl}\,\hat{R}_t^0(\eta) &= \mathrm{cl}\{\alpha\alpha_t^0(\eta)|\alpha\in F_t\}\\ &= \mathrm{cl}\{\alpha\alpha_t^0(\eta)|\alpha\in\widetilde{F}_t\}\\ &= \mathrm{cl}\{\alpha\alpha_t^0(\eta)|\alpha\in\widetilde{G}_t\}\quad\text{(by Lemma IV.5)}\\ &= \mathrm{cl}\;\alpha_t^0(I(\alpha_{-t}^0(\alpha_t^0(\eta))))\quad\text{(by Lemma IV.4)}\\ &= \mathrm{cl}\;\alpha_t^0(I(\eta)).\end{aligned}\tag{53}$$

But Lemma IV.3 tells us that $\mathrm{cl}\,\hat{R}_t^0(\eta)=\mathrm{cl}\,\hat{R}_t(\eta)$, so we obtain $\mathrm{cl}\,\hat{R}_t(\eta)=\mathrm{cl}\;\alpha_t^0(I(\eta))$. From Lemma IV.2 we know that $\mathrm{int}\,\hat{R}_t(\eta)=\mathrm{int}(\mathrm{cl}\,\hat{R}_t(\eta))$, which implies $\mathrm{int}\hat{R}_t(\eta)=\alpha_t^0(I(\eta))$ under the topology of $\alpha_t^0(I(\eta))$. Finally, $\hat{R}_t(\eta)\subset\alpha_t^0(I(\eta))$ by Theorem IV.1, and we arrive at $\hat{R}_t(\eta)=\alpha_t^0(I(\eta))$.

C. Strong analytic controllability of the actual system

In Sec. IV B, we investigated the reachable set at time t of the time-independent augmented system formed by enlarging the state space to include an extra dimension corresponding to the variable t. Now we return to the original quantum control system (4) to discover conditions under which it is strongly analytically controllable.

Theorem IV.7: *For the control system defined by Eq. (4), let*

$$\begin{aligned}&\mathcal{B}(t)=\mathcal{L}\{H_1(t),\ldots,H_r(t)\},\\ &B_1(t)=-[H_0(t),\mathcal{B}(t)]+\frac{\partial}{\partial t}\mathcal{B}(t),\quad\ldots,\\ &B_n(t)=-[H_0(t),B_{n-1}(t)]+\frac{\partial}{\partial t}B_{n-1}(t),\quad\ldots,\\ &\mathcal{C}(t)=\mathcal{L}\{\mathcal{B}(t),B_1(t),\ldots,B_n(t),\ldots\}.\end{aligned}\tag{54}$$

Suppose $\dim\mathcal{C}(t)\psi(t)=m$ *holds for all* $\psi\in M\cap\mathcal{D}_A$, *and* $[\mathcal{B},\mathcal{C}](t)\subset\mathcal{B}(t)$ *is the case for all* t. *Then the time-dependent quantum control system (4) is strongly analytically controllable.*

Proof: We apply Theorem IV.6 to the augmented control system (12). To do so, we need to examine the Lie algebras $\hat{\mathcal{B}}$ and $\hat{\mathcal{C}}$ for this problem. For economy of expression, we sometimes omit the t argument in the following steps. For $\hat{\mathcal{B}}$ we readily find

$$\hat{\mathcal{B}}=\mathcal{L}\{W_1,\ldots,W_r\}=\mathcal{L}\left\{\begin{pmatrix}0\\H_1(t)\end{pmatrix},\ldots,\begin{pmatrix}0\\H_r(t)\end{pmatrix}\right\}\psi(t)=\begin{pmatrix}0\\\mathcal{L}\{H_1(t),\ldots,H_r(t)\}\end{pmatrix}\psi(t)=\begin{pmatrix}0\\\mathcal{B}(t)\psi(t)\end{pmatrix}.\tag{55}$$

Next let us construct $\hat{\mathcal{C}}$. For any

$$W(\eta)=W(t,\psi)=\begin{pmatrix}0\\H(t)\psi(t)\end{pmatrix}\in\hat{\mathcal{B}},\tag{56}$$

where $\eta\in N$, we have

$$\begin{aligned}\mathrm{ad}_{W_0} W &= [W_0, W] = \left[\begin{pmatrix} 1 \\ H_0(t)\psi(t) \end{pmatrix}, \begin{pmatrix} 0 \\ H(t)\psi(t) \end{pmatrix}\right] \\ &= \frac{\partial \begin{pmatrix} 0 \\ H(t)\psi(t) \end{pmatrix}}{\partial(t,\psi)} \begin{pmatrix} 1 \\ H_0(t)\psi(t) \end{pmatrix} - \frac{\partial \begin{pmatrix} 1 \\ H_0(t)\psi(t) \end{pmatrix}}{\partial(t,\psi)} \begin{pmatrix} 0 \\ H(t)\psi(t) \end{pmatrix} \\ &= \begin{Bmatrix} 0 \\ -[H_0, H] + \partial H/\partial t \end{Bmatrix} \psi(t). \end{aligned} \tag{57}$$

Similarly,

$$\mathrm{ad}_{W_0} \hat{\mathcal{B}} = \begin{pmatrix} 0 \\ -[H_0, \mathcal{B}] + \partial \mathcal{B}/\partial t \end{pmatrix} \psi(t). \tag{58}$$

Setting $B_1 = -[H_0, \mathcal{B}] + \partial \mathcal{B}/\partial t$, we may then derive

$$\mathrm{ad}^2_{W_0} \hat{\mathcal{B}} = \mathrm{ad}_{W_0} \mathrm{ad}_{W_0} \hat{\mathcal{B}} = \mathrm{ad}_{W_0} \begin{pmatrix} 0 \\ B_1\psi(t) \end{pmatrix} = \begin{pmatrix} 0 \\ -[H_0, B_1] + \partial B_1/\partial t \end{pmatrix} \psi(t). \tag{59}$$

Continuing in this fashion with

$$B_n = -[H_0, B_{n-1}] + \partial B_{n-1}/\partial t \tag{60}$$

for $n = 2, 3, \ldots$, we find

$$\mathrm{ad}^n_{W_0} \hat{\mathcal{B}} = \begin{pmatrix} 0 \\ -[H_0, B_{n-1}] + \dfrac{\partial B_{n-1}}{\partial t} \end{pmatrix} \psi(t) = \begin{pmatrix} 0 \\ B_n\psi(t) \end{pmatrix}. \tag{61}$$

Thus

$$\begin{aligned}\hat{\mathcal{C}} &= \mathcal{L}\{\hat{\mathcal{B}}, \mathrm{ad}_{W_0} \hat{\mathcal{B}}, \ldots, \mathrm{ad}^n_{W_0} \hat{\mathcal{B}}, \ldots\} \\ &= \mathcal{L}\left\{\begin{pmatrix} 0 \\ \mathcal{B}(t)\psi(t) \end{pmatrix}, \begin{pmatrix} 0 \\ B_1(t)\psi(t) \end{pmatrix}, \ldots, \begin{pmatrix} 0 \\ B_n(t)\psi(t) \end{pmatrix}, \ldots\right\} \\ &= \begin{pmatrix} 0 \\ \mathcal{L}\{\mathcal{B}(t), B_1(t), \ldots, B_n(t), \ldots\}\psi(t) \end{pmatrix} = \begin{pmatrix} 0 \\ \mathcal{C}(t)\psi(t) \end{pmatrix}. \end{aligned} \tag{62}$$

From the assumption that $[\mathcal{B}, \mathcal{C}](t) \subset \mathcal{B}(t)$, $\forall(t)$, we have

$$[\mathcal{B}, \mathcal{C}](t)\psi(t) \subset \mathcal{B}(t)\psi(t), \forall\,(t). \tag{63}$$

Hence

$$\left[\begin{pmatrix} 0 \\ \mathcal{B}\psi \end{pmatrix}, \begin{pmatrix} 0 \\ \mathcal{C}\psi \end{pmatrix}\right] \subset \begin{pmatrix} 0 \\ \mathcal{B}\psi \end{pmatrix}, \tag{64}$$

so that $[\hat{\mathcal{B}}, \hat{\mathcal{C}}](\eta) \subset \hat{\mathcal{B}}(\eta)$, $\forall\, \eta \in N$.

By assumption, $\dim \mathcal{C}(t)\psi(t) = m$, $\forall\, \psi \in M \cap \mathcal{D}_A$, which implies that $\dim \hat{\mathcal{C}}(\eta) = m = n - 1$ holds for all $\eta \in N$. According to Theorem IV.6, $\alpha^0_t(I(\eta)) = \hat{\mathcal{R}}_t(\eta)$, $\forall\, t > 0$, and since $\alpha^0_t(I(\alpha^0_{-t}(\eta))) = \begin{pmatrix} t_0 \\ M \cap \mathcal{D}_A \end{pmatrix}$, we obtain $\alpha^0_t(I(\eta)) = \begin{pmatrix} t+t_0 \\ M \cap \mathcal{D}_A \end{pmatrix}$.

Let $\pi: N \to M \cap \mathcal{D}_A$ be the projection map that in effect annihilates the time dimension of the augmented problem corresponding to the variable t, and brings us back to the original control

system. In fact, the extension and projection maps mediate a one-to-one correspondence between the states of the augmented system and those of the original system. The simplicity of this relationship stems from the fact that t is a strictly increasing variable.

To reiterate our strategy: We have dealt with the explicit time dependence of the original control problem by adding an extra dimension to its state space, such that, as viewed in the augmented space, the augmented control problem is time independent. After analyzing controllability within this extension, the results are projected to the original space by removing the extra time dimension, recovering the exact states of the original system.

Accordingly, $\pi(\alpha_t^0(I(\eta)))=M\cap\mathcal{D}_A$, while $\pi\hat{R}_t(\eta)=R_{t+t_0}(\psi)$, $\forall\,\psi\in M\cap\mathcal{D}_A$ and $\forall t>0$. Hence $R_t(\psi)=M\cap\mathcal{D}_A$, $\forall\,t>t_0$, and the system (4) is strongly analytically controllable on M.

We may note that upon introducing the Lie algebra $\mathcal{A}(t)=\mathcal{L}\{H_0(t),H_1(t),\ldots,H_r(t)\}$, it is readily established from property (13) that $\mathcal{B}\subset\mathcal{C}\subset\mathcal{A}$ for all t.

To complete the formal analysis, we state two corollaries that devolve immediately from Theorem IV.7.

Corollary IV.8: *From the operators H_i entering control system (4), form the Lie algebras $\mathcal{B}=\mathcal{L}\{H_1,\ldots,H_r\}$ and $\mathcal{C}=\mathcal{L}\{\mathcal{B},\mathrm{ad}_{H_0}\mathcal{B},\ldots,\mathrm{ad}_{H_0}^n\mathcal{B},\ldots\}$. Suppose that the H_i do not possess explicit dependence on the time t, that* $\dim\mathcal{C}\psi(t)=m$ *holds for all $\psi\in M\cap\mathcal{D}_A$, and that $[\mathcal{B},\mathcal{C}]\subset\mathcal{B}$ is satisfied. Then the time-invariant system (4) is strongly analytically controllable.*

Corollary IV.9: *For the control system (4), form the Lie algebra $\mathcal{B}(t)=\mathcal{L}(H_1(t),\ldots,H_r(t))$, and suppose that* $\dim\mathcal{B}(t)\psi(t)=m$ *holds for all $\psi\in M\cap\mathcal{D}_A$. Then system (4) is strongly analytically controllable.*

The latter corollary follows because $[\mathcal{B},\mathcal{C}](t)\subset\mathcal{B}(t)$ must hold, once $\dim\mathcal{B}(t)\psi(t)=m$.

V. EXAMPLES OF STRONG ANALYTIC CONTROLLABILITY

In this section, we present three examples that meet the criteria for analytic controllability enunciated in Theorem IV.7. The examples selected are relevant to problems of interest in mathematical physics or engineering applications of quantum mechanics.

Example 1: The strong analytic controllability theorem can be applied to the simple degenerate parametric oscillator, a problem of importance in physics and engineering. Introducing an appropriate effective Hamiltonian allows the corresponding control system to be written in the form[67]

$$i\frac{\partial}{\partial t}\psi=\left\{\omega(t)a^\dagger a+\frac{1}{2}\chi(t)[e^{-2i\omega t}(a^\dagger)^2+e^{2i\omega t}a^2]\right\}\psi. \tag{65}$$

Here $a^\dagger$ and a represent, in turn, the creation and annihilation operators of the pump mode of frequency $\omega(t)$, while $\chi(t)$ is the time-dependent coupling function related to the second-order nonlinear susceptibility of the pumped medium. We may consider $\omega(t)$ and $\chi(t)$ as control functions playing the role of the u_l in Eq. (4), since they are real and can be adjusted to piecewise-constant functions of time t, outside the system itself.

Following Refs. 68–71, we define the operators

$$K_+=\tfrac{1}{2}(a^\dagger)^2,\quad K_-=\tfrac{1}{2}a^2,\quad K_0=\tfrac{1}{2}(a^\dagger a+aa^\dagger), \tag{66}$$

which satisfy the commutation relations of SU (1, 1), thus

$$[K_0,K_\pm]=\pm K_\pm,\quad [K_+,K_-]=-2K_0. \tag{67}$$

Setting

$$H_0=-iK_0, \tag{68}$$

$$H_1=-\frac{i}{2}[e^{-2i\omega t}K_+ + e^{2i\omega t}K_-], \tag{69}$$

$$H_2 = \tfrac{1}{2}[e^{-2i\omega t}K_+ - e^{2i\omega t}K_-], \tag{70}$$

the control system (65) may be written in the more familiar form

$$\frac{\partial}{\partial t}\psi = [\omega(t)H_0 + \chi(t)H_1(t)]\psi. \tag{71}$$

The skew-Hermitian operators H_0, H_1, and H_2 satisfy the commutation relations

$$[H_0,H_1] = -H_2, \quad [H_0,H_2] = H_1, \quad [H_1,H_2] = H_0. \tag{72}$$

We observe that the system (71) does not have a drift term in the usual sense, because the factor $\omega(t)$ can be manipulated externally. We also see immediately that $\mathcal{A}=\mathcal{B}=\mathcal{C}=\mathcal{L}\{H_0,H_1,H_2\}$, and the second condition of Theorem IV.7 is obviated. In addition, H_0 has eigenvectors $|mk\rangle$, with $m=0,1,\ldots$ and $k=1/4,\ 3/4$, which span an analytic domain $\mathcal{D}_A$.[69,71] Consequently, we can choose a manifold M such that $\dim \mathcal{C}\psi = \dim M$, $\forall \psi \in \mathcal{D}_A \cap M$. All conditions of Theorem IV.7 being met, the system (65) is strongly analytically controllable on M.

Example 2: Defining $Q = i\partial_t + \partial_{x_1x_1} + \partial_{x_2x_2}$, the Schrödinger equation for a free particle moving in two spatial dimensions may be expressed simply as $Qu=0$. Determination of the maximal symmetry algebra of this equation leads to the following set of nine operators, which form the basis of a nine-dimensional complex Lie algebra:[72]

$$\begin{gathered} K_2 = -t^2\partial_t - t(x_1\partial_{x_1} + x_2\partial_{x_2}) - t + (i/4)(x_1^2 + x_2^2), \quad K_{-2} = \partial_t, \quad P_j = \partial_{x_j}, \\ B_j = -t\partial_{x_j} + ix_j/2, \quad J = x_1\partial_{x_2} - x_2\partial_{x_1}, \quad E = i, \quad D = x_1\partial_{x_1} + x_2\partial_{x_2} + 2t\partial_t + 1, \end{gathered} \tag{73}$$

with $j=1,2$. Of immediate concern is the real Lie algebra spanned by this basis, i.e., the Schrödinger algebra, which has, as alternative basis, the operators B_j, P_j, and E (yielding the five-dimensional Weyl algebra), plus the operator J and the three operators defined by $L_1=D$, $L_2=K_2+K_{-2}$, and $L_3=K_{-2}-K_2$. The pertinent nonvanishing commutators are specified by[72]

$$\begin{gathered} [L_1,L_2] = -2L_3, \quad [L_3,L_1] = 2L_2, \quad [L_2,L_3] = 2L_1, \quad [L_1,B_j] = B_j, \quad [L_1,P_j] = -P_j, \\ [P_j,J] = (-1)^{j+1}P_l, \quad [B_j,J] = (-1)^{j+1}B_l, \quad [L_2,B_j] = -P_j, \quad [L_3,B_j] = -P_j, \quad [L_2,P_j] = B_j, \\ [L_3,P_j] = -B_j, \quad [P_j,B_j] = E/2, \end{gathered} \tag{74}$$

where $j,\ l=1,\ 2,\ j\neq l$.

Now we consider the controllability of the system

$$\frac{\partial}{\partial t}\psi = [L_2 + u_1(t)L_1 + u_2(t)L_3 + u_3(t)P_1 + u_4(t)J]\psi. \tag{75}$$

In this case there is a time-dependent drift term in the vector field driving ψ. The relations (74) imply the equalities $\mathcal{B}=\mathcal{C}=\mathcal{L}\{L_1,L_2,L_3,P_1,P_2,B_1,B_2,J,E\}$, while the required analytic domain $\mathcal{D}_{\mathcal{A}}$ is furnished by the span of the eigenfunctions $\psi_{n,m}$ of L_3. These take the explicit, time-dependent form[72]

$$\begin{aligned} \psi_{n,m} &= (2^{m+n+1}\pi n!m!)^{-1/2}\exp[i\pi(m+n-1)/2] \\ &\quad \times \exp\left[\frac{(v_1^2+v_2^2)(1-iv_3)}{4}\right]\left(\frac{v_3+i}{v_3-i}\right)^{(m+n)/2} \times \frac{H_m(v_1/\sqrt{2})H_n(v_2/\sqrt{2})}{v_3-i}, \end{aligned} \tag{76}$$

where $x_1=v_1(1+v_3^2)^{1/2}$, $x_2=v_2(1+v_3^2)^{1/2}$, and $t=v_3$. It follows as before that the system (75) is strongly analytically controllable.

Example 3: A quantum control system with position-dependent effective mass $m=(2Ax)^{-1}$ has been described by the time-dependent Schrödinger equation[73]

$$i\frac{\partial}{\partial t}\psi=[iBI_0+u_1(t)A(t)I_0I_-+iu_2(t)C]\psi, \tag{77}$$

where B, $C\in\mathbb{R}$, and $A(t)$, is a real function of time t but in general not piecewise constant. The operators I_0 and $I_\pm$, which are independent of time, provide a basis for an SU(1, 1) algebra, and have the concrete realization

$$I_-=-\partial_x,\quad I_0=x\partial_x+1,\quad I_+=x^2\partial_x+2x, \tag{78}$$

which satisfies the commutative relations

$$[I_0,I_\pm]=\pm I_\pm,\quad [I_-,I_+]=-2I_0. \tag{79}$$

This effective-mass problem arises in the study of semiconductor heterostructures and, more generally, of inhomogeneous crystals.[74] In the semiconductor application, the effective mass of a carrier depends spatially on the graded composition of the semiconductor alloys used in the barrier and well regions of the microstructures.[75]

The wave functions of the stationary states of Eq. (77) can be written as

$$\begin{aligned}\psi_E(t,x)=&\frac{1}{\sqrt{2\pi}}\exp\left\{-iE\int_0^t B(\sigma)\mathrm{d}\sigma+\int_0^t\left[-C(\sigma)-\frac{1}{2}B(\sigma)\right]\mathrm{d}\sigma\right\}\\&\times\exp\{-a_1(t)(x\partial_{xx}+\partial_x)\}x^{-iE-1/2}=\frac{1}{\sqrt{2\pi}}\exp\left\{-iE\int_0^t B(\sigma)\mathrm{d}\sigma+\int_0^t\left[-C(\sigma)\right.\right.\\&\left.\left.-\frac{1}{2}B(\sigma)\right]\mathrm{d}\sigma\right\}\\&\times\sum_{n=0}^{\infty}\prod_{l=0}^{n}\left(iB(t)E+\frac{1}{2}+l\right)^2[-a_1(t)]^n\times\frac{x^{-iE-n-1/2}}{n!}.\end{aligned} \tag{80}$$

These eigenfunctions span the analytic domain relevant to Theorem IV.7.

Let us define

$$H_0=BI_0+u_2(t)C,\quad H_1=-iA(t)I_0I_-, \tag{81}$$

where we take $u_2(t)=-B/2C$. Equation (77) can be recast as the control system,

$$\frac{\partial}{\partial t}\psi=[H_0+u_1(t)H_1]\psi. \tag{82}$$

Here the drift term is time independent. Using the commutation relations (79), we obtain $[H_0,H_1]=-BH_1$. Obviously, $\mathcal{B}=\mathcal{C}\subset\mathcal{A}$, so $[\mathcal{B},\mathcal{C}]=\mathcal{B}$. Choosing a manifold M such that $\dim M=\dim \mathcal{C}\psi$ for all $\psi\in M$, we are assured that system (77) is strongly analytically controllable.

VI. CONCLUSIONS

In this paper, we have formulated the time-dependent quantum control problem and studied its controllability. Acknowledging the unbounded nature of operators commonly involved in quantum control systems, our analysis has been predicated on the existence of an analytic domain[32] on which exponentiations of such operators are guaranteed to converge. Within this framework, we have extended the established treatment of time-independent quantum control problems by introducing an augmented system described in a state space that is enlarged by one dimension, yet embodies the true dynamics of the original system. With the aid of techniques and results devel-

oped by Kunita,[54,58] we are able to explicate the one-dimension-reduced controllability of the augmented system. Projection onto the original state space then yields a proof of the analytic controllability of the original time-dependent quantum control system, under conditions similar to those required in the time-independent case. The theorem so established has been illustrated with examples drawn from mathematical physics and systems engineering.

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Control aspects of holonomic quantum computation

Dennis Lucarelli
The Johns Hopkins University, Applied Physics Laboratory, Laurel, Maryland 20723-6099

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A unifying framework for the control of quantum systems with non-Abelian holonomy is presented. It is shown that, from a control theoretic point of view, holonomic quantum computation can be treated as a control system evolving on a principal fiber bundle. An extension of methods developed for these classical systems may be applied to quantum holonomic systems to obtain insight into the control properties of such systems and to construct control algorithms for two established examples of the computing paradigm. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1888028]

I. INTRODUCTION

Geometric phases have long been a source of fascination and insight into classical and quantum physical theories.[1] In recent years, they have proven to be useful in describing the dynamics and control of certain nonholonomic mechanical systems with symmetry.[2] Inspired by the appearance of geometric phases in biology, engineers have sought to create motion in machines via cyclic variations in *shape space*. These endeavors[3–6] and the characterization of optimal trajectories[7–10] remain active areas of research.

Most recently, the quantum geometric phase has been realized as a way of constructing logic gates in a quantum computer.[11] Holonomic quantum computation (HQC) employs non-Abelian geometric phases (holonomies) for the purpose of quantum information processing. Here we present a unified framework for the control of quantum holonomic systems with applications to quantum computing by casting the model as a control system evolving on a principal bundle. The integration of control theoretic ideas into the HQC paradigm sharpens existing results for these systems and reveals computational techniques for solving two separate but related fundamental problems in quantum computing. First, the well known conditions for determining universal quantum computation must be translated to the holonomic framework. The determination of universality, however, is existential in nature and generally not constructive. Quantum logic gate synthesis or constructive controllability is the process of determining from the system dynamics the construction or concatenation from available transformations some desired dynamic transformation of the state. This latter task is required for executing quantum algorithms. Both of these issues have subtleties in the holonomic framework not encountered in the usual *dynamical* approach to quantum computing.

Since the introduction of this approach to quantum computing,[11] there has been considerable interest from the research community in proposing physical systems capable of performing HQC[12–19] and exploring its mathematical foundations.[20–30] This paper draws on much of this work to provide a characterization of the problem, introduce computational techniques, and present results for two classes of control architectures related to HQC. In particular, we state simple conditions for determining the holonomy group of a principal fiber bundle with connection. These conditions, well known and reported elsewhere,[8,5,27] circumvent the difficulties in directly applying the Ambrose–Singer theorem which was originally stated as the technique for determining universality of HQC. For quantum holonomy groups of dimension greater than 3, a direct application of Ambrose–Singer essentially neglects the contribution of nested Lie brackets of lifted vector fields, however these vector fields can provide new transformations available for manipulating quantum information. From the product bundle representing single qubit rotations and two

qubit interactions, conditions for universality can then be derived. Having established the decisive condition for determining universality, we explore the difficult inverse problem associated to constructing holonomies. Namely, given a desired holonomy what is the loop in parameter space that generates it? In principal, this information is sufficient for the experimentalist to construct particular holonomies in the laboratory. For the the $\mathbf{CP}^n$ model, holonomic logic gate synthesis has been successfully treated by a numerical optimization scheme in Refs. 29 and 28. Moreover, Ref. 28 refines the method to minimize the length of the loop in parameter space. Since the parameters must be driven sufficiently slowly for the adiabatic approximation to hold, minimizing length also minimizes the time to construct the logic gate. This criterion is perhaps relevant for combatting decoherence. Logic gate synthesis has also been treated analytically in Ref. 30, however these loops are characterized in the Grassmann manifold and not in parameter space. Characterizations of length minimizing loops can also be found in Refs. 8 and 9.

We apply the theory to two well studied models of HQC. We provide a complete analysis of the so-called *optical holonomic computer*.[21–26] We extend the results of Ref. 27 by carrying out the universality analysis and explicitly characterizing a parametric loop that can be employed to construct an arbitrary two-qubit logic gate. These results surmount a negative result reported for this model.[22] In a similar manner, we use the Cartan decomposition of the unitary group to solve the constructive controllability problem for holonomic systems involving a conditional Berry phase. To the best of our knowledge, aside from the $\mathbf{CP}^n$ model, the two control models treated here encompass all proposed holonomic computing schemes.

This paper is organized as follows: In Sec. II, following Ref. 22 the geometry of holonomic quantum computation is reviewed. Also in Sec. II, we introduce the product bundle describing single qubit holonomies and two qubit interaction holonomies and state conditions for universal holonomic quantum computation. In Sec. III, we introduce methods for solving the path ordered integral associated with logic gate synthesis in the holonomic framework. The main contributions of the paper are contained in Sec. IV, where we apply the theory of the preceding sections.

II. HOLONOMIC QUANTUM COMPUTATION

If a quantum state undergoes adiabatic evolution subject to a periodic Hamiltonian, it acquires a phase after one complete cycle. Berry's surprising discovery[31] was that, in addition to the well-known dynamical phase associated to the evolution, there is a phase of purely geometric origin. Berry's phase was then understood as the holonomy or geometric phase corresponding to a principal bundle with connection over a parameter space.[32] This phenomenon has been generalized in a variety of ways, most notably to nonadiabatic evolutions[33] and to degenerate systems possessing a non-Abelian phase factor.[34]

A. Preliminaries

We construct a family of degenerate Hamiltonians parametrized by elements of a parameter space M that govern the quantum dynamics. To allow for the possibility of a countably infinite dimensional Hilbert space, we consider universal classifying bundles. For further details see Refs. 22, 24, 35, and 36.

Let $\mathcal{H}$ be a separable (possibly infinite dimensional) Hilbert space, and define the manifolds

$$\mathrm{St}_k(\mathcal{H}) = \{V = (|v_1\rangle, \ldots, |v_k\rangle) \in \mathcal{H} \times \cdots \times \mathcal{H} | V^\dagger V = \mathbf{1}\}, \tag{1}$$

$$\mathrm{Gr}_k(\mathcal{H}) = \{X \in B(\mathcal{H}) | X^2 = X, X^\dagger = X, \mathrm{tr}\, X = n\}. \tag{2}$$

where $B(\mathcal{H})$ denotes the set of bounded linear operators on $\mathcal{H}$. These manifolds are known as the (universal) Stiefel and Grassmann manifolds, respectively. The space Gr_k is also known as a *classifying space* and can be defined as the union of Grassmann manifolds,[35]

$$\mathrm{Gr}_k(\mathcal{H}) \equiv \bigcup_{n=k}^{\infty} \mathrm{Gr}_{k,n}(\mathcal{H}). \tag{3}$$

Denote this $\mathrm{U}(k)$-bundle by P_k. Note that when $\mathcal{H} \cong \mathbb{C}^n$ and the system has a k-dimensional degeneracy, the bundle of interest is the more familiar $\mathrm{U}(k)$-bundle $\mathrm{St}_{k,n}(\mathbb{C}^n) \to \mathrm{Gr}_{k,n}(\mathbb{C}^n)$ which can be written in terms of homogeneous spaces as

$$\frac{\mathrm{U}(n)}{\mathrm{U}(n-k)} \to \frac{\mathrm{U}(n)}{\mathrm{U}(n-k) \times \mathrm{U}(k)}. \tag{4}$$

We continue with the infinite dimensional case with the understanding that the development specializes to this case when $\mathcal{H}$ is finite dimensional.

Let M be a finite dimensional parameter space and suppose the classifying map $\Pi_k: M \to \mathrm{Gr}_k$ (to be defined below) is given. Then form the pullback bundle $Q_k = \Pi_k^* P_k$,

$$\begin{array}{ccc} Q_k & \to & \mathrm{St}_k(\mathcal{H}) \\ \downarrow & & \downarrow \\ M & \overset{\Pi_k}{\to} & \mathrm{Gr}_k(\mathcal{H}). \end{array} \tag{5}$$

Let H_0 be a Hamilonian with a k-dimensional degeneracy spanned by the orthogonal basis $\{|v_j\rangle_{j=1}^k\}$. To simplify notation, let the degenerate eigenvalue be 0. In holonomic quantum computation, the degenerate subspaces of H_0 encode the quantum information. Suppose we have at our disposal a set of $\mathrm{U}(k)$ unitary transformations

$$\{W_1(x), W_2(x), \ldots, W_m(x)\} \tag{6}$$

parametrized by the base coordinate x. These are the (exponentiated) analogues of *control Hamiltonians*. Setting

$$\mathcal{U}_k(x) = \prod_j W_j(x), \tag{7}$$

we obtain the isospectral family of Hamiltonians given by

$$\mathcal{O}(H_0) \equiv \mathcal{U}_k(x) H_0 \mathcal{U}_k^\dagger(x). \tag{8}$$

In the adiabatic approximation, the adjoint orbit $\mathcal{O}(H_0)$ forms a family of Hamiltonians that govern the system since there are no energy level crossings. The classifying map is then defined as

$$\Pi_k(x) \equiv \mathcal{U}_k(x) \left(\sum_{j=1}^k |v_j\rangle\langle v_j| \right) \mathcal{U}_k^\dagger(x). \tag{9}$$

B. Control systems on principal fiber bundles

In general, let Q be a principal fiber bundle with structure group G over a base manifold M. Recall that a *connection* on Q defines a G-invariant distribution $\mathbb{H}$ such that $T_qQ = \mathbb{H}_q \oplus \mathbb{V}_q$, where $\mathbb{V}_q \equiv T_q(\mathcal{O}(q)) \cong \mathfrak{g}$ (the Lie algebra of G). Alternatively, a connection can be characterized by an Ad-equivariant $\mathfrak{g}$-valued one-form $\mathcal{A}$ on Q such that $\mathcal{A} \cdot \xi_q = \xi$, where ξ_q is the infinitesimal generator of the group action and $\xi \in \mathfrak{g}$. The horizontal subspace at a point $q \in Q$ is then defined as the kernel $\mathbb{H}_q = \{v_q | \mathcal{A} \cdot v_q = 0\}$. The local connection one-form, A, is defined with respect to a *local section* σ by $A \equiv \sigma^* \mathcal{A}$. Using Ad-equivariance and the fact that $\mathcal{A}$ is the identity on vertical vectors, we can obtain the local connection form in terms of the base variables only[35,37]

$$\mathcal{A} \cdot \dot{q} = \mathrm{Ad}_g(g^{-1}\dot{g} + A(x) \cdot \dot{x}). \tag{10}$$

We note that the term $g^{-1}\dot{g}$ is in the Lie algebra $\mathfrak{g}$, by interpreting $g^{-1}\dot{g}$ as the lifted action of g^{-1} on $\dot{g} \in T_g G$. Restricting the connection $\mathcal{A}$ to act on horizontal vectors yields an equation for the evolution of the group elements given by

$$g^{-1}\dot{g} = -A(x) \cdot \dot{x}. \tag{11}$$

Returning to the quantum setting, we note that the canonical connection on the bundle Q_k is given by $A_{wz} \equiv \mathcal{U}_k^{-1}\, \mathrm{d}\mathcal{U}_k$, The matrix elements of the connection form are given by

$$A^{\overline{vv}}_{x_\mu} \equiv \langle \overline{v} | \mathcal{U}_k^\dagger(x) \frac{\partial}{\partial x_\mu} \mathcal{U}_k(x) | v \rangle. \tag{12}$$

This is commonly known as the Wilczek–Zee connection.[34]

Assuming direct control over the base variables, we may interpret the quantum control system as a *control system evolving on a principal bundle* and write it locally as

$$g^{-1}\dot{g} = -A_{wz}(x) \cdot \dot{x},$$

$$\dot{x} = u, \tag{13}$$

where u is a vector of control inputs describing the controlled evolution in parameter space.

A formal solution to this system of equations corresponding to a particular path in parameter space is given by the *path ordered* integral

$$\mathbf{P} \exp \int_\gamma -A_{wz}\, \mathrm{d}x. \tag{14}$$

When γ is a closed curve in M, then $\mathbf{P} \exp \oint_\gamma -A_{wz}\, \mathrm{d}x$ lies in G and is known as the *holonomy* of γ. It is well known that the set of all such group elements taken over the set of closed curves in M is a subgroup of G and is known as the *holonomy group*. In *holonomic quantum computation*, quantum logic gates are implemented by holonomies acting on the degenerate subspaces.

C. Universality

A control system evolving on a principal fiber bundle is said to be *locally controllable* if any group element can be implemented on the state of the system. In the context of quantum computing, a system with this property is said to be (exactly) *universal*.[38] This property is a fundamental requirement for building a quantum processor. As is well known, in the usual dynamical approach to quantum computing (as opposed to the geometric approach addressed here), the Lie algebra generated by the system Hamiltonian and the control Hamiltonians determines the universality of the system. For an N qubit system, it is sufficient for this Lie algebra to span $\mathfrak{su}(2^n)$. We now show how these statements translate to the holonomic framework.

Let X^h denote the horizontal lift of a vector field X on M. This is the unique vector on TQ such that $T\pi(X^h) = X$ where π is the projection $\pi: Q \to M$. Then the *curvature* can be defined as a $\mathfrak{g}$-valued 2-form on Q given by

$$\mathcal{A}([X^h_{i_2}, X^h_{i_1}]) = -\mathcal{F}(X^h_{i_2}, X^h_{i_1}), \tag{15}$$

where $[\cdot,\cdot]$ denotes the Lie bracket on TQ. Thus evaluating the curvature determines the vertical component of the Lie bracket of horizontal vectors. Let $f: Q \to \mathfrak{g}$ be an Ad-equivariant function on Q, then

$$\mathcal{A}([X^h, f]) = -\mathrm{d}\mathcal{A}(X^h, f) + X^h(\mathcal{A}(f)) + f(\mathcal{A}(X^h)) \tag{16}$$

$$= X^h f, \tag{17}$$

since the function f is $\mathfrak{g}$-valued and $d\mathcal{A}(\cdot,\cdot)$ is zero if either argument is vertical.[35] Using the correspondence between covariant derivatives of the associated adjoint bundle and Lie derivatives of Ad-equivariant functions,[39] we obtain

$$\mathcal{A}([X^h, f]) = X^h f = D_{X^h} f. \tag{18}$$

Now, the curvature is an Ad-equivariant function on Q, so setting $\mathcal{F}=f$ and using the previous expression (18) to evaluate iterated Lie brackets of horizontally lifted vector fields, we can obtain the corollary to the well-known *Chow–Rashevski* theorem from control theory.[9]

Theorem 1: *(Ambrose–Singer–Chow–Rashevski) The system (13) is locally controllable at* $q \in Q$ *if the curvature* $F(X_{i_1}, X_{i_2})$ *and all of its covariant derivatives* $D_{X_{i_k}} \cdots D_{X_{i_3}} F(X_{i_1}, X_{i_2})$ *evaluated at the point* $x = \pi(q)$ *span the entire Lie algebra of* G.

Some remarks are in order. Following Ref. 9, we refer to the theorem as *Ambrose–Singer–Chow–Rashevski* since it can be considered to be a corollary to the *Ambrose–Singer*[39] theorem from the theory of holonomy. We note also that we have stated the theorem in terms of base vector fields and the local curvature. All the necessary ingredients of the theorem, although not explicitly stated, can be found in Ref. 39. In fact, the *infinitesimal holonomy algebra* is spanned by elements of the form

$$X^h_{i_k} \cdot X^h_{i_{k-1}} \cdots X^h_{i_3} \cdot \mathcal{F}(X^h_{i_1}, X^h_{i_2}). \tag{19}$$

We can then use the correspondence (18) to relate this to covariant derivatives of the associated adjoint bundle. This statement is used in our applications, since in some holonomic quantum computation problems the relevant holonomy algebra does not span the entire Lie algebra. However, it does contain *nonlocal* operations which together with holonomies corresponding to *local* operations do indeed span the entire Lie algebra. This is the usual local/nonlocal analysis often encountered in quantum information science.

For the purposes of building a quantum processor, the quantum information is stored in the $\mathbb{C}^2$ vector bundle associated to Q^2 and single qubit rotations are performed by SU (2) holonomies acting on the fiber $\mathbb{C}^2$. Interactions among qubits are modeled as SU (4) holonomies acting on the fibers of the vector bundle associated to Q^4.

Thus we may treat the control problems separately and form the product bundle (and its pullbacks)

$$\begin{array}{ccccccc} \cdots & \mathrm{St}_2(\mathcal{H}_i) & \times & \mathrm{St}_4(\cdots \otimes \mathcal{H}_i \otimes \mathcal{H}_j \otimes \cdots) & \times & \mathrm{St}_2(\mathcal{H}_j) & \cdots \\ & \downarrow & & \downarrow & & \downarrow & \\ \cdots & \mathrm{Gr}_2(\mathcal{H}_i) & \times & (\mathrm{Gr}_4)^{\mathrm{int}}(\cdots \otimes \mathcal{H}_i \otimes \mathcal{H}_j \otimes \cdots) & \times & \mathrm{Gr}_2(\mathcal{H}_j) & \cdots . \end{array} \tag{20}$$

To set notation, let

$$I_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad I_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad I_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathbf{1} = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}. \tag{21}$$

We define the *local algebra* generated by the elements

$$I_{k1} = I_k \otimes \mathbf{1}, \quad I_{k2} = \mathbf{1} \otimes I_k, \tag{22}$$

where $k \in \{x, y, z\}$ The local algebra is the Lie algebra corresponding to the *local group* SU(2) $\otimes$ SU(2).

To conclude exact universality (controllability) of the system, one should compute the *control Lie algebra* with the constituent holonomy algebras. For example, in the two-qubit system, compute the Lie algebra generated by $\mathfrak{su}(2) \otimes \mathbf{1}, \mathbf{1} \otimes \mathfrak{su}(2)$ and the interaction holonomy algebra $\mathfrak{hol}_{\mathrm{int}}$ associated with the bundle $\mathrm{St}_4(\mathcal{H}_i \otimes \mathcal{H}_j) \to (\mathrm{Gr}_4)^{\mathrm{int}}(\mathcal{H}_i \otimes \mathcal{H}_j)$. In the generic case, the control Lie

algebra will generate $\mathfrak{su}(4)$ provided that $\mathrm{Hol}_{\mathrm{int}}$ is not isomorphic to the local group or is trivial.

Theorem 2: *The two-qubit holonomic system is exactly universal if the Lie algebra generated by the local algebra and* $\mathfrak{hol}_{\mathrm{int}}$ *spans* $\mathfrak{su}(4)$.

III. CONSTUCTIVE CONTROLLABILITY

Having established conditions for determining universality in HQC, we now present various ways of solving or approximating the solution to the path ordered integral arising for the differential equation defining the group displacement

$$g^{-1}\dot{g} = -A(x)\cdot\dot{x}. \tag{23}$$

For control systems on principal bundles, this equation describes the group transformation obtained from a controlled cyclic variation of the parameters in the base manifold. Recall, that we assume direct access and complete controllability over the base variables. We endeavor to ascertain the desired group transformation resulting from a particular choice of loop in the base space. This is the notion of constructive controllability in the context of a control system on a principal bundle. In HQC these procedures provide explicit methods for logic gate synthesis. This requires dealing with the path ordered integral obtained from (23).

A. Path ordered integral

We define the path ordered integral as a product integral. Let γ be a curve in the base manifold M and let x^μ be local coordinates. We may express the local connection form A in terms of coordinates as

$$A(x) = A_\mu(x)\mathrm{d}x^\mu. \tag{24}$$

The curve γ is parametrized by an intrinsic parameter s, which is naturally considered to be time. In terms of s, A takes the form

$$A_\mu(x(s))\mathrm{d}x^\mu = A(s)\mathrm{d}s, \tag{25}$$

where

$$A(s) \equiv A_\mu(x(s))\frac{\mathrm{d}x^\mu(s)}{\mathrm{d}s}. \tag{26}$$

Let $[s_0, s_T]$ be a real interval over which the curve γ is defined. Consider a partition of the interval $P=\{s_0, s_1, \ldots, s_n\}$ such that $\Delta s_k = s_k - s_{k-1}$ and $s_n = s_T$. Then path ordering operator may be defined as

$$\mathbf{P}\exp\int_\gamma -A(s)\mathrm{d}s \equiv \lim_{n\to\infty}\prod_{s_0}^{s_n}\exp(-A(s_k)\Delta s_k). \tag{27}$$

This definition clearly shows the dependence on the ordering of the exponentials and the difficulties associated with its solution, given that we are naturally interested in the case where the relevant group is non-Abelian. When G is Abelian, then one can directly integrate the connection coefficients and apply the usual exponential operator.

B. Abelian substructures

A common technique in holonomic quantum computation for tackling the integral (27) is to restrict the class of loops and exploit Abelian substructures in the connection components.[12,21] The strategy is briefly described as follows. Choose a particular 2-manifold of M spanned by the

coordinates (σ,τ) such that the associated connection components commute, that is $[A_\sigma,A_\tau]=0$ but for which the local curvature form is not identically zero. For these restricted loops the path ordering in (27) can be avoided and the line integral

$$\oint_\gamma A(x)\mathrm{d}x = \oint_\gamma (A_\sigma\,\mathrm{d}\sigma + A_\tau\,\mathrm{d}\tau) \tag{28}$$

can be integrated directly and exponentiated.

Alternatively, one can use a non-Abelian Stokes theorem[40] for evaluating holonomies corresponding to curves lying in a 2-submanifold of parameter space.

C. Averaging

The exact results of the preceding section were accompanied by restrictions on the set of loops available to the controller or by exploiting Abelian substructures in the connection components. Here we review local approximations that can be used for any system evolving on a principal bundle.

In Ref. 41, Leonard and Krishnaprasad developed approximate control algorithms for left invariant control systems on Lie groups of the form

$$g^{-1}\dot{g} = \epsilon U(t) \tag{29}$$

where ϵ is a (small) parameter and $U(t)=T_\alpha u^\alpha(t)$ for a basis $\{T_\alpha\}$ of $\mathfrak{g}$. They employ a Magnus expansion for a representation of the solution

$$g(t) = g(0)\exp(\xi(t)) \tag{30}$$

given by

$$\xi(t) = \epsilon\int_0^t U(\tau)\mathrm{d}\tau + \frac{\epsilon^2}{2}\int_0^t [\tilde{U}(\tau),U(\tau)]\mathrm{d}\tau + \frac{\epsilon^3}{4}\int_0^t\left[\int_0^\tau [\tilde{U}(\sigma),U(\sigma)]\mathrm{d}\sigma,U(\tau)\right]\mathrm{d}\tau + \cdots, \tag{31}$$

where $\tilde{U}(t)$ is the effective input "averaged" over the time period.[41]

Radford and Burdick have generalized this expansion for systems evolving on principal bundles.[5] Let $\gamma:[0,T]\to M$ be a closed curve in the base space parametrized by $x\in M$, then it is shown in Ref. 5 that the holonomy associated to γ can be locally approximated by

$$g(T) = g(0)\exp(\xi(\gamma)), \tag{32}$$

where

$$\xi(\gamma) = -\frac{1}{2}F(X_i,X_j)\int_\gamma \mathrm{d}x_i\,\mathrm{d}x_j + \frac{1}{3}D_{X_i}(F(X_j,X_k))\int_\gamma \mathrm{d}x_i\,\mathrm{d}x_j\,\mathrm{d}x_k + \cdots. \tag{33}$$

Here $F(X_i,X_j)$ is the local curvature form evaluated on the base coordinate vectors $X_i=\partial/\partial_{x_i}$ evaluated at $\gamma(0)$, $D_{\partial/\partial_{x_i}}$ is the covariant derivative of the curvature along the base coordinate vector ∂/∂_{x_i} and the area integrals are defined by

$$\mathcal{I}_{x_ix_jx_k} = \int_\gamma \mathrm{d}x_i\,\mathrm{d}x_j\,\mathrm{d}x_k \equiv \int_0^T\int_0^{t_k}\int_0^{t_j}\dot{x}^i(t_i)\mathrm{d}t_i\,\dot{x}^j(t_j)\mathrm{d}t_j\,\dot{x}^k(t_k)\mathrm{d}t_k. \tag{34}$$

Higher order terms are given by higher order covariant derivatives of the curvature. This is plausible given expression (33) and the fact that iterated Lie brackets of horizontally lifted vector fields appear as covariant derivatives of the curvature.

IV. APPLICATIONS

In this section we apply the results of the preceding sections. We first review the $\mathbf{CP}^n$ model of quantum holonomy. This was the original system discovered by Wilczek and Zee[34] and subsequently proposed as a model for HQC. We then consider two very different models of quantum holonomic systems. Holonomic quantum computation with squeezed coherent states has a rich interaction holonomy group that can be exploited to obtain contructive controllability algorithms. On the other hand, quantum computation based on the conditional phase shift has become the dominant control strategy for a wide range of holonomic quantum computing schemes. We will see that the interaction holonomy for systems of this type is quite limited yet powerful enough for universal computation and constructive algorithms.

A. The $\mathbf{CP}^n$ model

The $\mathbf{CP}^n$ (Ref. 11) model gives a concrete example illustrating how non-Abelian holonomies can occur in highly degenerate systems. In this model, we assume that the Hilbert space $\mathcal{H}$ is finite dimensional from the outset. That is, we have the isomorphism $\mathcal{H}\cong\mathbb{C}^{n+1}=\{|\alpha\rangle\}_{\alpha=1}^{n+1}$. We further assume an n-dimensional degenerate subspace with eigenvalue 0. We may write the degenerate Hamiltonian H_0 as

$$H_0=\epsilon|n+1\rangle\langle n+1|=\begin{pmatrix}0 & 0 & \cdots & 0\\ 0 & \ddots & 0 & 0\\ \vdots & & \ddots & \\ 0 & 0 & 0 & \epsilon\end{pmatrix}. \tag{35}$$

Let $\{\mathcal{T}_{j,n+1}(x)\}_{j=1}^{l}$ denote a basis of $\mathfrak{u}(n)$ parametrized by $x\in M$ embedded in $\mathfrak{u}(n+1)$ and let $\mathcal{U}_n=\Pi_j^l\exp(\mathcal{T}_{j,n+1}(x))$. Given these control operations, it is perhaps not surprising that the holonomy group can be shown to be $\mathrm{U}(n)$ by considering the curvature coefficients only (and not its covariant derivatives).[34,11]. We have the isomorphism

$$\mathcal{O}(H_0)\cong\frac{\mathrm{U}(n+1)}{\mathrm{U}(n)\times\mathrm{U}(1)}\cong\frac{\mathrm{SU}(n+1)}{\mathrm{U}(n)}\cong\mathbf{CP}^n. \tag{36}$$

This system requires control over $2n=\dim_{\mathbb{R}}\mathbf{CP}^n$ real parameters to control an n-level system. For high dimensional systems, this may be an unrealistic requirement.

B. Squeezed coherent states

In this section we revisit the mathematical foundations of *holonomic quantum computation with squeezed coherent states*. There is considerable literature already on this model,[12,21–23,25,26] here we exploit the methods of geometric control. Originally, this model was proposed in the context of quantum optics[12] with displacers and squeezers operating on coherent laser beams in a nonlinear Kerr medium and thus known as the optical holonomic computer. However, other physical systems have quantum states that may be displaced and squeezed. As far as the control analysis is concerned, these systems are identical. Pachos has recently adapted the model to perform trapped ion quantum computation.[16] We, therefore, refer to this model generically as *holonomic quantum computation with squeezed coherent states*.

1. Harmonic oscillator

Recall that the commutation relations of the creation, annihilation, and number operator $N\equiv a^\dagger a$, are given by

$$[N,a^\dagger]=a^\dagger,\quad [N,a]=a,\quad [a,a^\dagger]=\mathbf{1}. \tag{37}$$

The underlying Hilbert space $\mathcal{H}$ is a Fock space and takes the form

$$\mathcal{H} = \{|n\rangle, \alpha \in \mathbf{N} \cup 0\}. \tag{38}$$

The creation and annihilation operators act on $\mathcal{H}$ according to

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \quad a|0\rangle = 0. \tag{39}$$

Thus a and $a^\dagger$ create and destroy quanta.

Since we are interested in the two-qubit system, we will use the subscript i to distinguish the creation and annihilation corresponding to the ith field of the harmonic oscillator. That is, we set $N_i = a_i^\dagger a_i$ and

$$a_1 = a \otimes \mathbf{1}, \quad a_1^\dagger = a^\dagger \otimes \mathbf{1}, \tag{40}$$

$$a_2 = \mathbf{1} \otimes a, \quad a_2^\dagger = \mathbf{1} \otimes a^\dagger. \tag{41}$$

To provide a concrete example, we will use the degenerate Hamiltonian

$$H^i = N_i(N_i - 1) \tag{42}$$

to encode the ith qubit in the degenerate subspace $\{|0_i\rangle, |1_i\rangle\}$ and

$$H^{12} = N_1(N_1 - 1) + N_2(N_2 - 1) \tag{43}$$

to obtain controlled interactions on the computation basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ where $|ij\rangle = |i\rangle \otimes |j\rangle$. In the optics context, this Hamiltonian corresponds (up to a constant) to placing lasers in a nonlinear Kerr medium.[12,21] However, the form of the degenerate Hamiltonian does not affect the control analysis. For our purposes, it is used only to encode the quantum information. With slight modification of some constants, the results in this section apply to the trapped ion model proposed in Ref. 16.

2. Single qubit

We consider first single qubit rotations. Consider the eigenvalue problem for a single creation operator. The state $|\alpha\rangle$ can be written in terms of the basis $\{|n\rangle\}$,

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n a^{\dagger n}}{n!} |0\rangle. \tag{44}$$

Which is equal to

$$|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} |0\rangle \tag{45}$$

and allows for the definition of the *displacement operator*

$$|\alpha\rangle = D(\alpha) = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} e^{-\alpha^* a} |0\rangle. \tag{46}$$

Note that the introduction of $e^{-\alpha^* a}$ does nothing since $a|0\rangle = |0\rangle$ By using the Campbell–Baker–Hausdorff formula and noting that $[\alpha a^\dagger, -\alpha^* a] = |\alpha|^2$, we may write

$$|\alpha\rangle = D(\alpha)|0\rangle = e^{\alpha a^\dagger - \alpha^* a}|0\rangle. \tag{47}$$

We see that the displacement operator creates a coherent state $|\alpha\rangle$ from the vacuum state $|0\rangle$. In HQC with squeezed coherent states, the displacement operator will be a control operator. The other transformation we have at our disposal is the *squeezing operator*, $S(\beta)$, defined by

$$S(\beta) = e^{\beta \Lambda_+ - \beta^* \Lambda_-}, \tag{48}$$

where

$$\Lambda_+ \equiv \tfrac{1}{2}a^{\dagger 2}, \quad \Lambda_- \equiv \tfrac{1}{2}a^2. \tag{49}$$

If we define,

$$\Lambda_3 \equiv \tfrac{1}{4}(aa^\dagger + a^\dagger a), \tag{50}$$

then we have the commutation relations,

$$[\Lambda_3, \Lambda_+] = \Lambda_+, \quad [\Lambda_3, \Lambda_-] = -\Lambda_-, \quad [\Lambda_+, \Lambda_-] = 2\Lambda_3. \tag{51}$$

These are the commutation relations for $\mathfrak{su}(1,1)$; thus we see that the squeeze operator is a representation of the noncompact group SU(1, 1). With these two unitary transformations, we form the product

$$\mathcal{U}_2(\alpha, \beta) = D(\alpha)S(\beta) \tag{52}$$

and the isospectral family of Hamiltonians

$$\mathcal{U}_2(\alpha, \beta)H^i\mathcal{U}_2^\dagger(\alpha, \beta). \tag{53}$$

The holonomy group for the single qubit system has been shown to be U(2).[12,21–23] Thus we have complete control over the single qubit.

3. Two qubit

To obtain universality over the entire quantum register it suffices to show nontrivial U(4) transformations on the computational basis and check the control Lie algebra. Analogously to the single qubit case, we employ displacement and squeeze operators as our control operations. Let

$$J_+ = a^\dagger{}_1 a_2, \quad J_- = a^\dagger{}_2 a_1, \quad J_3 = \tfrac{1}{2}(a^\dagger{}_1 a_1 - a^\dagger{}_2 a_2). \tag{54}$$

These generate SU(2) with the commutation relations,

$$[J_3, J_+] = J_+, \quad [J_3, J_-] = -J_-, \quad [J_+, J_-] = 2J_3. \tag{55}$$

The two-mode displacement operator is defined as

$$N(\xi) = \exp(\xi a_1^\dagger a_2 - \overline{\xi} a_1 a_2^\dagger). \tag{56}$$

Similarly, we may define the two-mode squeeze operator as a representation of SU(1, 1). Let

$$K_+ = a^\dagger{}_1 a^\dagger{}_2, \quad K_- = a_1 a_2, \quad K_3 = \tfrac{1}{2}(a^\dagger{}_1 a_1 + a^\dagger{}_2 a_2), \tag{57}$$

and

$$[K_3, K_+] = K_+, \quad [K_3, K_-] = -K_-, \quad [K_+, K_-] = -2K_3. \tag{58}$$

The two-mode squeeze operator is defined as

$$M(\zeta) = \exp(\zeta a_1^\dagger a_2^\dagger - \overline{\zeta} a_1 a_2), \tag{59}$$

where $\xi, \zeta \in \mathbf{C}$. Set

$$\mathcal{U}_4 = N(\xi)M(\zeta). \tag{60}$$

Setting $\zeta = r_2 e^{i\theta_2}$ and $\xi = r_3 e^{i\theta_3}$ and we obtain the two-qubit connection coefficients[21] listed in Appendix A. The interaction holonomy algebra spans $\mathfrak{su}(2) \times \mathfrak{su}(2) \times \mathfrak{u}(1)$ (Ref. 27) (also listed in Appendix B). Higher order covariant derivatives do not yield independent group directions. The matrices in $\mathfrak{hol}_{\text{int}}$ sit in $\mathfrak{u}(4)$ in a manner that allows for nonlocal U(4) transformations on the computational basis. By the reduction theorem for connections,[39] the connection is reducible to a

$\mathrm{su}(2)\times\mathrm{su}(2)\times\mathrm{u}(1)$-valued connection and we may reduce the total space to $\mathrm{St}_{2,4}(\mathcal{H}_1\otimes\mathcal{H}_2)$. To determine the reduced base manifold, we form the quotient

$$\frac{\mathrm{U}(4)}{\mathrm{SU}(2)\times\mathrm{SU}(2)\times\mathrm{U}(1)}\cong\frac{\mathrm{SU}(4)}{\mathrm{SU}(2)\times\mathrm{SU}(2)}\cong S\,\mathrm{Gr}_{2,4}\equiv(\mathrm{Gr}_{2,4})^{\mathrm{int}}. \tag{61}$$

In a similar manner, we can reduce the bundles $\mathrm{St}_2(\mathcal{H}_i)\mapsto\mathrm{Gr}_2(\mathcal{H}_i)$ corresponding to the single qubit rotations. The U(2) holonomies act in the product space $\mathcal{H}_1\otimes\mathcal{H}_2$ as $\mathrm{U}(2)\otimes\mathbf{1}$ and $\mathbf{1}\otimes\mathrm{U}(2)$. The bundles reduce to $\mathrm{St}_{2,4}(\mathcal{H}_1\otimes\mathcal{H}_2)\mapsto\mathrm{Gr}_{2,4}(\mathcal{H}_1\otimes\mathcal{H}_2)$. For the full two-qubit system, we have the reduced product bundle,

$$\begin{array}{ccccc}\mathrm{St}_{2,4}(\mathcal{H}_1\otimes\mathcal{H}_2) & \times & \mathrm{St}_{2,4}(\mathcal{H}_1\otimes\mathcal{H}_2) & \times & \mathrm{St}_{2,4}(\mathcal{H}_1\otimes\mathcal{H}_2)\\ \downarrow & & \downarrow & & \downarrow\\ \mathrm{Gr}_{2,4}(\mathcal{H}_1\otimes\mathcal{H}_2) & \times & (\mathrm{Gr}_{2,4})^{\mathrm{int}}(\mathcal{H}_1\otimes\mathcal{H}_2) & \times & \mathrm{Gr}_{2,4}(\mathcal{H}_1\otimes\mathcal{H}_2).\end{array} \tag{62}$$

4. Control algebra

To be complete, we will now demonstrate that all of SU(4) may be obtained from the single qubit rotations and the two-qubit transformations above. Of course, as we have mentioned earlier, this is generically true provided the two-qubit holonomy group is not isomorphic to the local group. Nonetheless, it is useful to go though the computations.

From the single qubit analysis, we know that we can perform local transformations of the form $\mathrm{SU}(2)\otimes\mathrm{SU}(2)$. To simplify matters further, we use linear combinations of the two-qubit curvature forms and covariant derivatives and consider only

$$\{F_{r_2r_3},F_{r_2\theta_3},F_{r_3\theta_3},D_{\partial/\partial\theta_2}F_{r_2\theta_2},\tilde{D}_{\partial/\partial r_2}F_{r_2\theta_2}\}, \tag{63}$$

where

$$\tilde{D}_{\partial/\partial r_2}F_{r_2\theta_2}=\begin{pmatrix}0&0&0&-e^{-i\theta_2}\\0&0&0&0\\0&0&0&0\\-e^{i\theta_2}&0&0&0\end{pmatrix}4i\sinh 2r_2. \tag{64}$$

From this set of matrices and the local algebra (22), we may build a set of holonomic transformations spanning $\mathfrak{su}(4)$. After taking iterated brackets from these sets, we find that one choice of spanning elements is given by

$$\mathfrak{su}(4)=\{\mathcal{C}_1\cup\mathcal{C}_2\cup\mathcal{C}_3\}, \tag{65}$$

where $\mathcal{C}_1=\{I_{x1},I_{y1},I_{z1},I_{x2},I_{y2},I_{z2}\}$ and

$$\mathcal{C}_2=\{F_{r_2r_3},F_{r_2r\theta_3},D_{\partial/\partial\theta_2}F_{r_2\theta_2},\tilde{D}_{\partial/\partial r_2}F_{r_2\theta_2}\},$$

$$\mathcal{C}_3=\{[I_{x1},F_{r_2r_3}],[I_{x1},F_{r_2\theta_3}],[I_{x2},F_{r_2r_3}],[I_{x2},F_{r_2\theta_3}],[[I_{x1},F_{r_2r_3}],I_{x2}]\}.$$

Please see Appendix C for the matrix representation of these elements.

5. An approximate holonomy in the Cartan subalgebra of $\mathfrak{su}(4)$

In the preceding section, we showed that it is indeed *possible* to create holonomic transformations spanning the full unitary group on two qubits. This was not a constructive procedure. In this section, we show that by using a combination of the methods in the preceding sections, we can solve the logic gate synthesis problem completely. We use the local expansion of the holonomy

procedure to construct an element in the Cartan subalgebra of $\mathfrak{su}(4)$ and use the Cartan decomposition of SU(4) to obtain the result.

The Cartan decomposition of the unitary groups is a powerful technique that has been used for constructing quantum control algorithms,[42,43] deriving time optimal control laws for quantum spin systems[44] and understanding the entanglement content of two-qubit unitaries,[45,46] Here we review the decomposition for the purposes of constructing control algorithms.

Let K denote a closed and compact subgroup of a Lie group G. Assume that $\mathfrak{g}$ admits a vector space decomposition,

$$\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}, \tag{66}$$

where $\mathfrak{k}$ is the Lie algebra of K and $\mathfrak{p}$ is vector space orthogonal to $\mathfrak{k}$ with respect to a biinvariant metric $\langle \cdot, \cdot \rangle$ on $\mathfrak{g}$. Further assume that $\mathfrak{k}$ and $\mathfrak{p}$ satisfy the following commutation relations:

$$[\mathfrak{k},\mathfrak{k}] \subset \mathfrak{k}, \quad [\mathfrak{p},\mathfrak{p}] \subset \mathfrak{k}, \quad [\mathfrak{p},\mathfrak{k}] \subset \mathfrak{p}. \tag{67}$$

We refer to a this decomposition as a Cartan decompostion of the Lie algebra $\mathfrak{g}$.

Let $\mathfrak{a}$ denote a maximal Abelian subalgebra contained in $\mathfrak{p}$. The algebra $\mathfrak{a}$ is often called the *Cartan subalgebra* of $\mathfrak{g}$. Then one can write G as

$$G = KAK, \tag{68}$$

where $A = \exp(\mathfrak{a})$.

In a two-qubit system, interactions among the qubits are modeled by the products

$$I_{kl} = 2I_k \otimes I_l, \tag{69}$$

where $k,l \in \{x,y,z\}$. For example,

$$I_{yy} = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}. \tag{70}$$

The Cartan decomposition of $\mathfrak{su}(4)$ is given by

$$\mathfrak{k} = i\{I_{x1}, I_{y1}, I_{z1}, I_{x2}, I_{y2}, I_{z2}\}, \tag{71}$$

$$\mathfrak{p} = i\{I_{xx}, I_{xy}, I_{xz}, I_{yx}, I_{yy}, I_{yz}, I_{zx}, I_{zy}, I_{zz}\}, \tag{72}$$

$$\mathfrak{a} = i\{I_{xx}, I_{yy}, I_{zz}\}. \tag{73}$$

Thus we can write any $g \in \mathrm{SU}(4)$ as

$$g = K_1 \exp(-i\phi_1 I_{xx} - i\phi_2 I_{yy} - i\phi_3 I_{zz}) K_2, \tag{74}$$

where ϕ_j is a real parameter and $K_j \in \mathrm{SU}(2) \otimes \mathrm{SU}(2)$.

By inspection of the two-qubit curvature forms and their covariant derivatives, it seems possible that I_{yy} can be obtained by linear combinations of the elements,

$$\{F_{r_2\theta_2}, F_{r_2\theta_3}, D_{\partial/\partial r_2} F_{r_2\theta_2}, D_{\partial/\partial r_2} F_{r_2\theta_3}\}. \tag{75}$$

Equivalently, I_{yy} is contained in the real span of

$$\left[\frac{\partial^h}{\partial x_k},\left[\frac{\partial^h}{\partial x_{k-1}},\cdots\left[\frac{\partial^h}{\partial x_2},\frac{\partial^h}{\partial x_1}\right]\right]\cdots\right], \tag{76}$$

where $x \in \{r_2, \theta_2, \theta_3\}$.

We therefore choose a candidate loop, γ^*, of the form

$$\theta_2(t) = \theta_2(0) + \Theta_2 \sin(t), \tag{77}$$

$$r_2(t) = r_2(0) + R_2 \cos(t) - R_2, \tag{78}$$

$$\theta_3(t) = \theta_3(0) + \Theta_3 \sin(nt), \quad n \neq 1, \tag{79}$$

$$r_3 = \text{const.}, \tag{80}$$

with the parameters $\{n, r_2(0), \theta_2(0), \theta_3(0), R_2; \Theta_2, \Theta_3\}$ to be determined. We compute the integrals appearing in the expansion (33), with the period $T=2\pi$ and choose some parameters to yield the expressions,

$$F_{r_2\theta_2} \cdot \mathcal{I}_{r_2\theta_2} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} 2i \sinh 2r_2(0) \cdot R_2\Theta_2\pi, \tag{81}$$

$$F_{r_2\theta_3}\big|_{\theta_3(0)=\pi} \cdot \mathcal{I}_{r_2\theta_3} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} i \sin 2r_3 \sinh 2r_2(0) \cdot \frac{R_2\Theta_3 \sin 2n\pi}{n^2-1}, \tag{82}$$

$$D_{\partial/\partial r_2} F_{\theta_3 r_2}\big|_{\theta_3(0)=\pi} \cdot \mathcal{I}_{r_2\theta_3 r_2} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} 2i \sin 2r_3 \cosh 2r_2(0) \cdot \frac{-6R_2^2\Theta_3 \sin 2n\pi}{n^4-5n^2+4}, \tag{83}$$

$$\begin{aligned} D_{\partial/\partial r_2} F_{r_2\theta_2}\big|_{\theta_2(0)=0} \cdot \mathcal{I}_{r_2 r_2 \theta_2} = & \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} 4i \sinh 2r_2(0) \cdot 2\Theta_2 R_2^2 \pi \\ & + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} 4i \cosh 2r_2(0) \cdot 2\Theta_2 R_2^2 \pi. \end{aligned} \tag{84}$$

We also have,

$$\mathcal{I}_{\theta_2 r_2 \theta_2} = 0, \tag{85}$$

$$F_{\theta_2\theta_3} = 0, \tag{86}$$

$$D_{\partial/\partial\theta_3} F_{r_2\theta_2} = 0, \tag{87}$$

$$D_{\partial/\partial\theta_3} F_{r_2\theta_3}|_{r_3(0)=\pi/4} = 0, \tag{88}$$

$$F_{r_2\theta_2} \cdot \mathcal{I}_{r_2\theta_2} = F_{\theta_2 r_2} \cdot \mathcal{I}_{\theta_2 r_2}, \tag{89}$$

$$F_{r_2\theta_3}|_{\theta_3(0)=\pi} \cdot \mathcal{I}_{r_2\theta_3} = F_{\theta_3 r_2}|_{\theta_3(0)=\pi} \cdot \mathcal{I}_{\theta_3 r_2}, \tag{90}$$

$$-2D_{\partial/\partial r_2} F_{r_2\theta_3}|_{\theta_3(0)=\pi} \cdot \mathcal{I}_{r_2 r_2\theta_3} = D_{\partial/\partial r_2} F_{\theta_3 r_2}|_{\theta_3(0)=\pi} \cdot \mathcal{I}_{r_2\theta_3 r_2}, \tag{91}$$

$$2D_{\partial/\partial r_2} F_{\theta_2 r_2}|_{\theta_2(0)=0} \cdot \mathcal{I}_{r_2\theta_2 r_2} = D_{\partial/\partial r_2} F_{r_2\theta_2}|_{\theta_2(0)=0} \cdot \mathcal{I}_{r_2 r_2\theta_2}. \tag{92}$$

The strategy now is to choose parameters so that the $F_{r_2\theta_2}$ terms kill the terms along the diagonal in the expressions $D_{\partial/\partial r_2} F_{r_2\theta_2}$ and $D_{\partial/\partial r_2} F_{\theta_2 r_2}$. Then, with those parameters chosen, we choose the rest of the parameters so that the remaining terms combine to yield $-i\theta I_{yy}$, where θ is a free parameter. Remembering to include the coefficients in the expansion, the first objective leads to the following equation:

$$r_2(0) = -\tfrac{1}{2} \operatorname{arctanh}(2R_2). \tag{93}$$

Setting $\Theta_2 = \Theta_3 = \theta$, and substituting the preceding equation defining $r_2(0)$ and R_2, the second objective yields

$$R_2 = -\frac{\sin 2n\pi}{4\pi(n^2 - 4)}. \tag{94}$$

If n is chosen so that (94) is nonzero and (93) is well defined, the loop γ^* determines the holonomy (up to third order)

$$\Gamma(\gamma^*) = \exp(-i\theta I_{yy}), \tag{95}$$

where θ is a free parameter.

Loops generating single qubit SU(2) holonomies can be characterized by *abelianizing* the dynamics.[21] Thus with this single two-qubit holonomy, we can construct any SU(4) transformation on the computational basis. To see this, recall that any SU(4) transformation may be written with the Cartan decomposition

$$g = K_1 \exp(-i\theta_1 I_{xx} - i\theta_2 I_{yy} - i\theta_3 I_{zz}) K_2, \tag{96}$$

where $K_j \in \mathrm{SU}(2) \otimes \mathrm{SU}(2)$.

We may obtain the transformations $\exp(-i\theta_1 I_{xx})$ and $\exp(-i\theta_1 I_{zz})$ by noting that

$$K_z^{-1}\left(\frac{\pi}{2}\right) \exp(-i\theta I_{yy}) K_z\left(\frac{\pi}{2}\right) = \exp(-i\theta I_{xx}), \tag{97}$$

$$K_x\left(\frac{\pi}{2}\right) \exp(-i\theta I_{yy}) K_x^{-1}\left(\frac{\pi}{2}\right) = \exp(-i\theta I_{zz}), \tag{98}$$

where

$$K_z(\theta) = \exp(-i\theta I_{z1}) \exp(-i\theta I_{z2}), \tag{99}$$

$$K_x(\theta) = \exp(-i\theta I_{x1})\exp(-i\theta I_{x2}). \tag{100}$$

Thus any $g \in \mathrm{SU}(4)$ can be approximated up to third order by

$$g = K_1 K_z^{-1}\left(\frac{\pi}{2}\right)\Gamma(\gamma^*)K_z\left(\frac{\pi}{2}\right)\Gamma(\gamma^*)K_x\left(\frac{\pi}{2}\right)\Gamma(\gamma^*)K_x^{-1}\left(\frac{\pi}{2}\right)K_2. \tag{101}$$

One can also use the *abelianization* procedure of the preceding section to construct a holonomy of the form[12,21]

$$\tilde{U} = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{2} & 0 & 0 & 0 \\ 0 & 1 & -i & 0 \\ 0 & -i & 1 & 0 \\ 0 & 0 & 0 & \sqrt{2} \end{pmatrix}. \tag{102}$$

One can then show that the Lie algebra element $\tilde{\xi}$ such that $\exp(\tilde{\xi}) = \tilde{U}$ along with the local algebra generates $\mathfrak{su}(4)$ under repeated bracketing. Thus $\tilde{U}$ is a so-called *universal logic gate*. However, this procedure does not give a prescription for building an arbitrary SU(4) transformation.

C. Conditional Berry phases

An interesting hybrid scheme to quantum computing involving *dynamical* SU(2) rotations and conditional Berry phases has been realized as a universal set of gates for several physical systems proposed for quantum computing. To date, there have been HQC implementations using this control paradigm with NMR,[13] trapped ions,[14] neutral atoms,[15] semiconductor nanostructures,[17] and Josephson junction networks.[18,19] We refer the reader to the literature for a description of the physical systems underlying these proposed quantum computing schemes.

Here we are interested in the control strategy of the experimentalist with the gates available in systems of this type. Namely, how does one build an arbitrary unitary transformation on two coupled qubits given only single qubit rotations and the conditional phase shift? It is perhaps surprising that indeed this is possible and one can entangle qubits with only the conditional phase shift as the nonlocal operation. We note that in these systems, the calculation of the geometric phase is trivial since one is able to exploit Abelian substructures in the case of the SU(2) phases and the Abelian Berry phase may be computed with the standard version of Stokes theorem.

Since the conditional phase gate is not an element of SU(4), we employ a Cartan decomposition of U(4). To this end, recall the notation of the preceding section and note that the real span of the sets

$$\mathfrak{k} = i\{I_{x1}, I_{y1}, I_{z1}, I_{x2}, I_{y2}, I_{z2}\}, \tag{103}$$

$$\mathfrak{p} = i\{\mathbf{1}_4, I_{xx}, I_{yy}, I_{zz}, I_{xy}, I_{xz}, I_{yx}, I_{yz}, I_{zx}, I_{zy}\} \tag{104}$$

form a basis of $\mathfrak{u}(4)$ in the tensor product representation. Moreover, one can check the commutation relations (67) to confirm that the set forms a Cartan decomposition of $\mathfrak{u}(4)$ where $\mathfrak{u}(4) = \mathfrak{k} \oplus \mathfrak{p}$. Since the maximal Abelian subalgebra $\mathfrak{a}$ contained in $\mathfrak{p}$ is just

$$\mathfrak{a} = i\{\mathbf{1}_4, I_{xx}, I_{yy}, I_{zz}\}, \tag{105}$$

we obtain the decomposition for any $G \in \mathrm{U}(4)$,

$$G = K_1 \exp(-i\phi_0 \mathbf{1}_4 - i\phi_1 I_{xx} - i\phi_2 I_{yy} - i\phi_3 I_{zz}) K_2, \tag{106}$$

where $\phi_i \in \mathbb{R}$ and $K_j \in K = \mathrm{SU}(2) \otimes \mathrm{SU}(2)$.

1. Control algorithms

Proceeding along the lines of Refs. 42, 44, and 43, we develop control algorithms with single qubit rotations and the conditional phase shift. The action of the conditional phase shift of the computational basis is as follows:

$$U_\phi|00\rangle = |00\rangle, \quad U_\phi|01\rangle = |01\rangle, \tag{107}$$

$$U_\phi|10\rangle = |10\rangle, \quad U_\phi|11\rangle = e^{-i\phi}|11\rangle. \tag{108}$$

Under the isomorphism $C^2 \otimes C^2 \cong C^4$, the conditional phase shift can be written as

$$U_\phi = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{-i\phi} \end{pmatrix}. \tag{109}$$

In terms of the basis (104) we can write

$$U_\phi = \exp\left(-i\frac{\phi}{2}(2\mathbf{1}_4 + I_{zz} - (I_{z1} + I_{z2}))\right). \tag{110}$$

Let

$$\tilde{K}_z = \exp\left(-i\frac{\phi}{4}(I_{z1} + I_{z2})\right), \tag{111}$$

since

$$[2\mathbf{1}_4, I_{zi}] = [I_{zz}, I_{zi}] = 0, \tag{112}$$

we have

$$\tilde{K}_z U_{\phi/2} = \exp\left(-i\frac{\phi}{4}(I_{z1} + I_{z2})\right) \cdot \exp\left(-i\frac{\phi}{4}(2\mathbf{1}_4 + I_{zz} - (I_{z1} + I_{z2}))\right) = \exp\left(-i\frac{\phi}{4}(2\mathbf{1}_4 + I_{zz})\right). \tag{113}$$

Let

$$K_j(\theta) = \exp(-i\theta I_{j1})\exp(-i\theta I_{j2}) \in K \tag{114}$$

for $j \in \{x, y\}$ and $\theta \in \mathbb{R}$ is a real parameter. We have the commutation relations,

$$[-i(I_{z1} + I_{z2}), -i(2\mathbf{1}_4 + I_{zz})] = [-i(I_{z1} + I_{z2}), -iI_{zz}] \tag{115}$$

and

$$[-iI_{zz}, [-i(I_{j1} + I_{j2}), -iI_{zz}]] = -i(I_{j1} + I_{j2}). \tag{116}$$

Thus by the Campbell–Baker–Hausdorff formula, we obtain

$$K_j(\theta)\tilde{K}_z U_{\phi/2} K_j^{-1}(\theta) = K_j(\theta)\exp\left(-i\frac{\phi}{4}(2\mathbf{1}_4 + I_{zz})\right)K_j^{-1}(\theta) \tag{117}$$

$$= \exp\left(- i\frac{\phi}{4}(2\mathbf{1}_4 + I_{zz}\cos(\theta) + [(-iI_{j1} - iI_{j2}), -iI_{zz}]\sin(\theta))\right). \tag{118}$$

We employ a π rotation to achieve the necessary decoupling. Using the preceding expression we get

$$K_j(\pi)\tilde{K}_z U_{\phi/2} K_j^{-1}(\pi) = K_j(\pi)\exp\left(- i\frac{\phi}{4}(2\mathbf{1}_4 + I_{zz})\right)K_j^{-1}(\pi) \tag{119}$$

$$= \exp\left(- i\frac{\phi}{4}(2\mathbf{1}_4 - I_{zz})\right). \tag{120}$$

So we obtain

$$\tilde{K}_z U_{\phi/2} \cdot K_j(\pi)\tilde{K}_z U_{\phi/2} K_j^{-1}(\pi) = \exp(-i\phi\mathbf{1}_4). \tag{121}$$

Similarly,

$$\tilde{K}'_z U_{\phi} \cdot K_j(\pi)\tilde{K}'_z U_{-\phi} K_j^{-1}(\pi) = \exp(-i\phi I_{zz}), \tag{122}$$

where $\tilde{K}'_z = \exp(-i(\phi/2)(I_{z1} + I_{z2}))$.

Finally, by noting that for

$$K_x(\theta) = \exp(-i\theta I_{x1})\exp(-i\theta I_{x2}) \tag{123}$$

$$K_y(\theta) = \exp(-i\theta I_{y1})\exp(-i\theta I_{y1}), \tag{124}$$

we have

$$K_y\left(\frac{\pi}{2}\right)\exp(-i\phi I_{zz})K_y^{-1}\left(\frac{\pi}{2}\right) = \exp(-i\phi I_{xx}), \tag{125}$$

$$K_x^{-1}\left(\frac{\pi}{2}\right)\exp(-i\phi I_{zz})K_x\left(\frac{\pi}{2}\right) = \exp(-i\phi I_{yy}). \tag{126}$$

Using (125) and (126), we can construct the desired decomposition for any $G \in \mathrm{U}(4)$,

$$G = K_1 \cdot \exp(-i\phi_0\mathbf{1}_4 - i\phi_1 I_{xx} - i\phi_2 I_{yy} - i\phi_3 I_{zz}) \cdot K_2 \tag{127}$$

$$= K_1 \cdot \exp(-i\phi_0\mathbf{1}_4) \cdot K_y\left(\frac{\pi}{2}\right)\exp(-i\phi_1 I_{zz})K_y^{-1}\left(\frac{\pi}{2}\right) \cdot$$

$$\times K_x^{-1}\left(\frac{\pi}{2}\right)\exp(-i\phi_2 I_{zz})K_x\left(\frac{\pi}{2}\right) \cdot \exp(-i\phi_3 I_{zz}) \cdot K_2. \tag{128}$$

This can now be written in terms of just elements of $\mathrm{SU}(2) \otimes \mathrm{SU}(2)$ and the conditional phase shift U_ϕ,

$$G = K_1 \cdot \tilde{K}_z U_{\phi_0/2} K_j(\pi)\tilde{K}_z U_{\phi_0/2} K_j^{-1}(\pi) \cdot K_y\left(\frac{\pi}{2}\right)\tilde{K}'_z U_{\phi_1} K_j(\pi)\tilde{K}'_z U_{-\phi_1} K_j^{-1}(\pi) K_y^{-1}\left(\frac{\pi}{2}\right) \cdot K_x^{-1}\left(\frac{\pi}{2}\right) \cdot \tilde{K}'_z$$

$$\times U_{\phi_2} K_j(\pi)\tilde{K}'_z U_{-\phi_2} K_j^{-1}(\pi) K_x\left(\frac{\pi}{2}\right)\tilde{K}'_z U_{\phi_3} K_j(\pi)\tilde{K}'_z U_{-\phi_3} K_j^{-1}(\pi) \cdot K_2. \tag{129}$$

Given the freedom of choosing j in K_j this sequence can be simplified somewhat. For example,

choose $j=y$ in the product $K_j^{-1}(\pi)\cdot K_y(\pi/2)$ to obtain $K_j^{-1}(\pi)\cdot K_y(\pi/2)=K_y(-\pi)\cdot K_y(\pi/2)=K_y(-\pi/2)$. Using this substitution and two others, the decomposition simplifies to

$$G = K_1\cdot\tilde{K}_z U_{\phi_0/2} K_j(\pi)\tilde{K}_z U_{\phi_0/2} K_y\left(-\frac{\pi}{2}\right)\tilde{K}_z' U_{\phi_1} K_j(\pi)\tilde{K}_z' U_{-\phi_1} K_y\left(-\frac{3\pi}{2}\right)K_x^{-1}\left(\frac{\pi}{2}\right)\tilde{K}_z' U_{\phi_2}$$

$$\times K_j(\pi)\tilde{K}_z' U_{-\phi_2}\cdot K_x\left(-\frac{\pi}{2}\right)\cdot\tilde{K}_z' U_{\phi_3} K_j(\pi)\tilde{K}_z' U_{-\phi_3} K_j^{-1}(\pi)\cdot K_2. \tag{130}$$

Finally, absorbing $\tilde{K}_z$ and $K_j^{-1}(\pi)$ into K_1 and K_2, respectively, we get

$$G = K_1 U_{\phi_0/2} K_j(\pi)\tilde{K}_z U_{\phi_0/2} K_y\left(\frac{\pi}{2}\right)\tilde{K}_z' U_{\phi_1} K_j(\pi)\tilde{K}_z' U_{-\phi_1} K_y\left(-\frac{3\pi}{2}\right)K_x^{-1}\left(\frac{\pi}{2}\right)\tilde{K}_z' U_{\phi_2} K_j(\pi)$$

$$\times\tilde{K}_z' U_{-\phi_2}\cdot K_x\left(-\frac{\pi}{2}\right)\tilde{K}_z' U_{\phi_3} K_j(\pi)\tilde{K}_z' U_{-\phi_3} K_2. \tag{131}$$

Some remarks are appropriate. This sequence of unitary transformations is exact and a precise prescription for building any U(4) logic gate with just local operations and the conditional phase shift. We make no claim that this decomposition is optimal with respect to number of elements nor time. In the holonomic framework, time optimality is constrained by the adiabatic requirement. In this case, one should then focus primarily on minimizing the number of loops necessary to build an arbitrary gate.

V. CONCLUSION

In this paper, we have considered holonomic quantum computation from a control theoretic point of view. A general framework for the control analysis is obtained by casting the relevant problems as control systems evolving on principal fiber bundles. We have applied this framework to two well established models of the computing scheme. To the best of our knowledge, all holonomic computing schemes proposed thus far fall into one of the two models considered here. From a control perspective, an interesting avenue for future work would be extending these ideas to the control of molecular systems in the Born–Oppenheimer approximation (as mentioned in Ref. 11). Holonomies can be realized in this regime[36] and it is reasonable to expect that a similar analysis can be carried out for these systems. However, a direct application of the methods proposed here will not suffice since the control parameters themselves are quantum degrees of freedom and therefore possess a nontrivial uncontrolled evolution of their own. In other words, the state equations analogous to those considered here (13) will be coupled quantum control problems.

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APPENDIX A

Two-qubit connection components,

$$A_{r_2} = \begin{pmatrix} 0 & 0 & 0 & -e^{-i\theta_2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ e^{i\theta_2} & 0 & 0 & 0 \end{pmatrix},$$

$$A_{r_3} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -e^{-i\theta_3} & 0 \\ 0 & e^{i\theta_3} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} (2\cosh^2 r_2 - 1),$$

$$A_{\theta_2} = \begin{pmatrix} 0 & 0 & 0 & e^{-i\theta_2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ e^{i\theta_2} & 0 & 0 & 0 \end{pmatrix} \frac{i}{2} \sinh 2r_2 + \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix} \frac{i}{2} (\cosh 2r_2 - 1),$$

$$A_{\theta_3} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & e^{-i\theta_3} & 0 \\ 0 & e^{i\theta 3} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \frac{i}{2} \cosh 2\, r_2 \sin 2r_3 + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} i \sin^2 r_3.$$

APPENDIX B

Interaction holonomy algebra,

$$F_{r_2 r_3} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -e^{-i\theta_3} & 0 \\ 0 & e^{i\theta_3} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} 2 \sinh 2r_2,$$

$$F_{r_2 \theta_2} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} 2i \sinh 2r_2,$$

$$F_{r_2 \theta_3} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & e^{-i\theta_3} & 0 \\ 0 & e^{i\theta_3} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} i \sin 2r_3 \sinh 2r_2,$$

$$F_{r_3 \theta_3} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} i \sin 2r_3 \sinh^2 2r_2,$$

$$D_{\partial/\partial\theta_2} F_{r_2 \theta_2} = \begin{pmatrix} 0 & 0 & 0 & -e^{-i\theta_2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ e^{i\theta_2} & 0 & 0 & 0 \end{pmatrix} 2 \sinh^2 2r_2,$$

$$D_{\partial/\partial r_2}F_{r_2\theta_2}=\begin{pmatrix}0&0&0&-e^{-i\theta_2}\\0&0&0&0\\0&0&0&0\\-e^{i\theta_2}&0&0&0\end{pmatrix}4i\sinh 2r_2+\begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&2\end{pmatrix}4i\cosh 2r_2,$$

$$D_{\partial/\partial\theta_2}D_{\partial/\partial\theta_2}F_{r_2\theta_2}=\begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&-1\end{pmatrix}2i\sinh^3 r_2+\begin{pmatrix}0&0&0&e^{-i\theta_2}\\0&0&0&0\\0&0&0&0\\e^{i\theta_2}&0&0&0\end{pmatrix}2i\sinh^2 2r_2\cosh 2r_2.$$

APPENDIX C

Higher order brackets,

$$[I_{x1},F_{r_2r_3}]=\begin{pmatrix}0&e^{i\theta_3}&0&0\\e^{-i\theta_3}&0&0&0\\0&0&0&-e^{i\theta_3}\\0&0&-e^{-i\theta_3}&0\end{pmatrix}i\sinh 2r_2,$$

$$[I_{x1},F_{r_2\theta_3}]=\begin{pmatrix}0&-e^{i\theta_3}&0&0\\e^{-i\theta_3}&0&0&0\\0&0&0&e^{i\theta_3}\\0&0&-e^{-i\theta_3}&0\end{pmatrix}\frac{1}{2}\sin 2r_2\sinh 2r_2,$$

$$[I_{x2},F_{r_2r_3}]=\begin{pmatrix}0&0&-e^{-i\theta_3}&0\\0&0&0&e^{-i\theta_3}\\-e^{i\theta_3}&0&0&0\\0&e^{i\theta_3}&0&\end{pmatrix}i\sinh 2r_2,$$

$$[I_{x2},F_{r_2\theta_3}]=\begin{pmatrix}0&0&-e^{-i\theta_3}&0\\0&0&0&e^{-i\theta_3}\\e^{i\theta_3}&0&0&0\\0&-e^{i\theta_3}&0&\end{pmatrix}\frac{1}{2}\sin 2r_2\sinh 2r_2,$$

$$[[I_{x1},F_{r_2r_3}],I_{x2}]=\begin{pmatrix}-1&0&0&\\0&1&0&0\\0&0&1&0\\0&0&0&-1\end{pmatrix}i\sin\theta_3\sinh 2r_2.$$

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Stability of three unit charges: Necessary conditions

D. K. Gridnev,[a] C. Greiner, and W. Greiner
Institut für Theoretische Physik, Robert-Mayer-Str. 8-10, D-60325 Frankfurt am Main, Germany

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We consider the stability of three Coulomb charges $\{+1,-1,-1\}$ with finite masses in the framework of nonrelativistic quantum mechanics. A simple physical condition on masses is derived to guarantee the absence of bound states below the dissociation thresholds. In particular this proves that certain negative muonic ions are unstable, thus extending the old result of Thirring to the actual values of all masses. The proof is done by reducing the initial problem to the question of binding of one particle in some effective potential. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1873039]

I. INTRODUCTION

The stability of three particles with pure Coulomb forces is an old and extensively studied problem, this is to explain why certain ions and molecules stay as a whole and some dissociate into a bound pair and a single particle. Under stability of the Hamiltonian H we shall understand the existence of a bound state with the energy strictly less than $\inf \sigma_{\mathrm{ess}}(H)$, i.e., a stationary state below all dissociation thresholds. As a quantum system three particles with Coulomb interactions demonstrate interesting behavior. It is known that three charges $\{1+\varepsilon,-1,-1\}$ for any $\varepsilon>0$ form the system, which is stable regardless of mass values. However at $\varepsilon=0$ the situation abruptly changes and due to the screening effect not all systems remain stable. The typical example is the unstable muonic hydrogen ion $p\mu^{-}e^{-}$, where the heavy muon is tightly bound to the proton and screens the positive charge for the electron. This interesting effect is well studied, in particular it has been proved[1] that for equal dissociation thresholds the system remains stable (Refs. 2 and 3 explain very well how stability depends on masses and charges).

Among the instability proofs for three unit charges the most appealing is that of Thirring,[4] which does not require any numerical calculations. Thirring considered a negative hydrogen ion with an infinitely heavy proton, and proved that such a negative ion is unstable when its second negatively charged particle is lighter than electron by a factor larger than π (π can be replaced[3,5] with a better constant 1.57). In his method Thirring exploited the fact that the ground state in the hydrogen atom is substantially separated from other states in its spectrum (the nondegenerate energy levels have $1/n^2$ dependence), and thus its role becomes emphasized. This suggests an idea to move the problem to the space spanned by the projector $P_0=|\phi_0\rangle\langle\phi_0|\otimes 1$, where ϕ_0 is the ground state of hydrogen. After estimating the part of the repulsion, which is present in this space, the problem reduces to checking the binding of one particle in some effective potential. The contribution from the attractive interaction term coming from additional particle is easy to treat because it commutes with P_0. Yet this is no longer true if one considers particles of finite mass or any system of four particles.

Thirring's bound was improved[2] and it was shown that the muonic ion $p\mu^{-}e^{-}$ is unstable for actual values of all masses. However this extension [Eq. (24) in Ref. 2] is weak in the sense that it fails when the second particle is heavy compared to other particles. (For a physical example, it does not prove that the ion $\mu^{-}pe^{+}$ is unstable, yet we shall prove it here.) This extension still uses

[a]Electronic mail: dima_gridnev@yahoo.com

Thirring's treatment of repulsion and it is unclear how one could extend it to four particles. Armour[6] with his method proved the instability of such systems as positron-hydrogen-atom e^-pe^+ and μ^-pe^+, but this method requires certain numerical assistance. It is also based on the separation of variables in the problem of two fixed centers, which makes it inapplicable to four particles because the variables do not separate even in the case of three fixed centers.

Here we follow the Thirring's idea but the nucleus does not have to be infinitely heavy. The derived physical condition restricts the ratio of Jacobi masses, which makes the system stable. It can be used in conjunction with Thirring's result and convexity properties of stability curve[2] for a reasonable determination of stability area free from any numerics. The present method has an important advantage in that it admits generalization to four particles. It should be mentioned that both Thirring's method and the new one share the same deficiency, namely, they are not applicable when the dissociation thresholds in the system are close or equal (e.g., when two like charges have equal masses). In particular, using such methods one cannot prove the "overheating" effect, when a system with charges $\{+1,-q,-q\}$ and equal masses loses its binding for some $q>1$. Nowadays various charged particles are produced in laboratories and it is, of course, of interest to know the principles behind formation of exotic atoms or molecules. All this motivates the present analysis.

II. FROM THREE PARTICLES TO ONE IN EFFECTIVE POTENTIAL

Let m_i, q_i, $\mathbf{r}_i \in \mathbb{R}^3$ denote masses, charges, and position vectors of particles $i=1,2,3$. We set $q_1=+1$ and $q_{2,3}=-1$, and the interactions between the particles are $V_{ik}=q_iq_k/|\mathbf{r}_i-\mathbf{r}_k|$. We enumerate the particles in such a way, that the particles (1,2) form the lowest dissociation threshold. The stability problem with Coulomb interactions is invariant with respect to scaling all masses,[2] so we can set $\hbar=1$. We separate the center of mass motion in the Jacobi frame[7] setting $\mathbf{x}=\mathbf{r}_1-\mathbf{r}_2$ and $\mathbf{y}=\mathbf{r}_3-\mathbf{r}_1+a\mathbf{x}$, where $a=m_2/(m_1+m_2)$ is the mass parameter invariant with respect to mass scaling. The reduced masses and Jacobi momenta are, respectively, $\mu_x=m_1m_2/(m_1+m_2)$, $\mu_y=m_3(m_1+m_2)/(m_1+m_2+m_3)$, and $p_{x,y}=-i\nabla_{x,y}$. It is convenient to scale all masses so that $\mu_x=2$. (In Sec. IV we shall rescale them back.) The Hamiltonian for the system on the tensor product space $L_2(\mathbb{R}^3)\otimes L_2(\mathbb{R}^3)$ is

$$H = h_{12}\otimes 1 + 1\otimes\frac{p_y^2}{2\mu_y} + W,$$

where

$$W = V_{13}+V_{23} = -\frac{1}{|a\mathbf{x}-\mathbf{y}|}+\frac{1}{|(1-a)\mathbf{x}+\mathbf{y}|} \tag{1}$$

and $h_{12}=p_x^2/4-1/x$ is the Hamiltonian of the pair of particles (1,2) (notation x is used instead of $|\mathbf{x}|$). The ground state wave function of h_{12} is $\phi_0=\sqrt{8/\pi}\exp(-2x)$ so that $h_{12}\phi_0=-\phi_0$. The Hamiltonian H is self-adjoint on $\mathcal{D}(H)=H^2(\mathbb{R}^6)$ (square integrable functions having partial derivatives up to the second order in the weak distributional sense) and by the HVZ theorem $\sigma_{\mathrm{ess}}(H)=[-1,\infty)$. We split positive and negative parts of W by introducing $W_-:=(|W|-W)/2$ and $W_+:=(-W)_-=(|W|+W)/2$ and we have $W=W_+-W_-$, where $W_\pm\geqslant 0$. Instead of H we shall consider the Hamiltonian

$$\tilde{H} = h_{12}\otimes 1 + 1\otimes\frac{p_y^2}{2\mu_y} - W_-. \tag{2}$$

Note that the part W_- can also be expressed as

$$W_- = -(V_{13}+V_{23}F(\mathbf{x},\mathbf{y})), \tag{3}$$

where $F=1$ when $|V_{13}|\geqslant|V_{23}|$ and $F=|V_{13}|/|V_{23}|$ when $|V_{13}|\leqslant|V_{23}|$, and we have $0\leqslant F\leqslant 1$. Because $\|V_{23}F\phi\|\leqslant\|V_{23}\phi\|$ we can directly apply Kato's theorem[8] on self-adjointness of atomic

Hamiltonians and find out that $\tilde{H}$ is self-adjoint on $\mathcal{D}(\tilde{H})=\mathcal{D}(H)$. We cannot though directly apply the HVZ theorem to locate $\inf \sigma_{\mathrm{ess}}(\tilde{H})$ but we observe that the following inequality holds $(H-V_{23})\leqslant\tilde{H}\leqslant H$. Here $(H-V_{23})$ is the original Hamiltonian without repulsion, which is bounded from below and by the HVZ theorem $\inf \sigma_{\mathrm{ess}}(H-V_{23})=-1$. Thus from the min–max principle[8] we get $\inf \sigma_{\mathrm{ess}}(\tilde{H})=-1$.

Now let us assume that H is stable, i.e., H has a bound state with the energy less than -1. Because $\tilde{H}\leqslant H$ from the variational principle we conclude that $\tilde{H}$ also has a bound state $\Psi\in\mathcal{D}(H)$ with the energy below $\inf \sigma_{\mathrm{ess}}(\tilde{H})=-1$ which means

$$\tilde{H}\Psi=-(-1-\delta)\Psi, \tag{4}$$

where $\delta>0$ is the extra binding energy. Let us introduce a projection operator $P_0=|\phi_0\rangle\langle\phi_0|\otimes 1$ $(P_0:\mathcal{D}(H)\to\mathcal{D}(H))$ and set $\eta:=P_0\Psi$ and $\xi:=(1-P_0)\Psi$, where obviously $\eta\perp\xi$ and $\Psi=\eta+\xi$ and $\eta,\ \xi\in\mathcal{D}(H)$. Taking the scalar product of each side of (4) with η and ξ we obtain

$$\left\langle \eta\left| 1\otimes\frac{p_y^2}{2\mu_y}-W_-\right|\eta\right\rangle-\langle\eta|W_-|\xi\rangle=-\delta\|\eta\|^2, \tag{5}$$

$$\langle\xi|h_{12}\otimes 1|\xi\rangle+\left\langle \xi\left| 1\otimes\frac{p_y^2}{2\mu_y}-W_-\right|\xi\right\rangle-\langle\xi|W_-|\eta\rangle=(-1-\delta)\|\xi\|^2, \tag{6}$$

where we have used $\langle\eta|1\otimes p_y^2|\xi\rangle=0$ because P_0 and $1\otimes p_y^2$ commute. We shall assume that $\|\eta\|$, $\|\xi\|\neq 0$ (we shall get rid of this assumption in Theorem 1), then we are free to choose such normalization of Ψ that $\|\xi\|=1$.

From the bound spectrum of h_{12} we have[4] $h_{12}\otimes 1\geqslant -P_0-1/4(1-P_0)$, hence for the first term in (6) we get the bound $\langle\xi|h_{12}\otimes 1|\xi\rangle\geqslant -1/4$. Introducing two non-negative constants $\alpha:=\sqrt{\langle\eta|W_-|\eta\rangle}$ and $\beta:=\sqrt{\langle\xi|W_-|\xi\rangle}$ we get by virtue of the Schwarz inequality $|\langle\xi|W_-|\eta\rangle|\leqslant\alpha\beta$. Now we can rewrite Eqs. (5) and (6) to obtain the main pair of inequalities,

$$\left\langle \eta\left| 1\otimes\frac{p_y^2}{2\mu_y}-W_-\right|\eta\right\rangle-\alpha\beta<0, \tag{7}$$

$$\left\langle \xi\left| 1\otimes\frac{p_y^2}{2\mu_y}-W_-\right|\xi\right\rangle-\alpha\beta<-\frac{3}{4}. \tag{8}$$

Using the second inequality we shall find $\max \beta/\alpha$ and by substituting this value into (7) we shall formulate the stability condition.

Lemma 1: Suppose that Eq. (8) holds and $\mu_y<3/2$, then the following inequality is true:

$$\beta<\left(\sqrt{\frac{3}{2\mu_y}}-1\right)^{-1}\alpha. \tag{9}$$

Proof: First, let us show that for $A\geqslant 0$,

$$\inf_{\substack{\chi\in\mathcal{D}(H)\\ \|\chi\|=1}}\left\langle \chi\left| 1\otimes\frac{p_y^2}{2\mu_y}-AW_-\right|\chi\right\rangle\geqslant-\frac{A^2\mu_y}{2}. \tag{10}$$

It suffices to prove this for $\chi\in C_0^\infty(\mathbb{R}^6)$. Using (3) from the variational principle we get

$$\left\langle \chi \left| 1 \otimes \frac{p_y^2}{2\mu_y} - AW_- \right| \chi \right\rangle \geqslant \int d\mathbf{x} \int d\mathbf{y}\, \chi^*(\mathbf{x},\mathbf{y}) \left(\frac{p_y^2}{2\mu_y} - \frac{A}{|a\mathbf{x}-y|} \right) \chi(\mathbf{x},\mathbf{y})$$

$$\geqslant -\frac{A^2\mu_y}{2} \int d\mathbf{x} \int d\mathbf{y} |\chi|^2(\mathbf{x}, a\mathbf{x}+\mathbf{y}) = -\frac{A^2\mu_y}{2} \|\chi\|^2 \tag{11}$$

from which (10) follows and where we have used the explicit expression for the ground state energy of the hydrogen atom. [Using an appropriate set of trial functions it is easy to show that there is an equality sign in (10), but we do not need this for our purposes]. Now using (10) we obtain the following chain of inequalities:

$$\inf_{\substack{\xi \in \mathcal{D}(H) \\ \|\xi\|=1 \\ \langle \xi | W_- | \xi \rangle = \beta^2}} \left\langle \xi \left| 1 \otimes \frac{p_y^2}{2\mu_y} - W_- \right| \xi \right\rangle = \max_{\lambda \geqslant -1} \inf_{\substack{\xi \in \mathcal{D}(H) \\ \|\xi\|=1 \\ \langle \xi | W_- | \xi \rangle = \beta^2}} \left(\left\langle \xi \left| 1 \otimes \frac{p_y^2}{2\mu_y} - (\lambda+1) W_- \right| \xi \right\rangle + \lambda\beta^2 \right)$$

$$\geqslant \max_{\lambda \geqslant -1} \inf_{\substack{\xi \in \mathcal{D}(H) \\ \|\xi\|=1}} \left(\left\langle \xi \left| 1 \otimes \frac{p_y^2}{2\mu_y} - (\lambda+1) W_- \right| \xi \right\rangle + \lambda\beta^2 \right)$$

$$\geqslant \max_{\lambda \geqslant -1} (\lambda\beta^2 - (\lambda+1)^2 \mu_y/2) = \frac{\beta^4}{2\mu_y} - \beta^2.$$

Substituting this result into (8) and setting $\alpha = s\beta$ we obtain

$$\frac{\beta^4}{2\mu_y} - (s+1)\beta^2 < -\frac{3}{4}. \tag{12}$$

Now simply minimizing the left-hand side of (12) over β^2 we obtain the lower bound on s, which gives us Eq. (9). ■

It is worth noting that the relation in the lemma is a version of the uncertainty principle, when β^2 grows, the kinetic energy term grows faster like β^4. Let us introduce an effective potential $V_{\text{eff}}(y) := \int d\mathbf{x} |\phi_0|^2 W_-$. We formulate the result as follows.

Theorem 1: *If the system of three charges is stable and* $\mu_y < 3/2$ *then the particle with mass* μ_y *must have a bound state in the potential* $-(1+(\sqrt{3/2\mu_y}-1)^{-1})V_{\text{eff}}$.

Proof: We have $\|\eta\|, \|\xi\| \neq 0$. The function η has the factorized form $\eta = \phi_0(\mathbf{x}) f(\mathbf{y})$, where $f \in H^2(\mathbb{R}^3)$, $\|f\| \neq 0$. By substituting (9) into (7) and using expressions for α^2 and η we get the necessary condition for stability

$$\left\langle f \left| \frac{p_y^2}{2\mu_y} - (1+(\sqrt{3/2\mu_y}-1)^{-1}) V_{\text{eff}} \right| f \right\rangle < 0. \tag{13}$$

In the next section we shall study $V_{\text{eff}}(y)$ and show that it is a continuous function decaying like $1/y^2$. Inequality (13) means that a particle having mass μ_y has a bound state in this potential.

Now let us complete the proof considering the case when either $\xi = 0$ or $\eta = 0$. If $\xi = 0$ we have $\beta = 0$ and substituting this into (7) we get a condition more stringent than Eq. (13). If $\eta = 0$ we have $\|\xi\| = 1$ and $\alpha = 0$, substituting this into (8) and using (10) for $\mu_y < 3/2$ results in the contradiction. ■

III. BINDING IN EFFECTIVE POTENTIAL

In this section we shall analyze the effective potential and find out at which values of the coupling constant λ the Hamiltonian $p_y^2 - \lambda V_{\text{eff}}$ may have bound states. It turns out that the effective potential in our case has a nonphysical term, which is a long-range attraction of the type $1/y^2$. This nonphysical behavior stems from cutting off the positive part of the potential and results in the infinite number of bound states at the point of binding (that is why it is meant nonphysical).

But as it is well known since the result of Hilbert and Courant,[9] even this long-range attraction does not guarantee binding, for $\lambda \max_y y^2 V_{\text{eff}}(y) \leqslant 1/4$ the inequality $p_y^2 - \lambda V_{\text{eff}} \geqslant 0$ holds, i.e., no binding occurs (see also the proof in Ref. 8, Vol. 2). Thus the nontrivial critical coupling constant exists, and we must determine it. On the other hand, in such potentials short-range repulsive terms do not play any role for binding.[10] It would be of interest to get rid of this nonphysical behavior in the future (pay attention that the Thirring's effective potential[4] behaves at infinity like $1/y^3$!).

To calculate V_{eff} we must cut off the positive part of W. From (1) $W \leqslant 0$ is equivalent to $\cos\theta \geqslant x/(\omega y)$, where $\omega = (a-1/2)^{-1}$ and $\cos\theta = \mathbf{x}\cdot\mathbf{y}/xy$. We shall consider separately two cases $a > 1/2$ and $a \leqslant 1/2$.

A. Case when $a > 1/2$

The integration is simpler in this case. After direct integration in spherical coordinates over the area where $\cos\theta \geqslant x/(\omega y)$ we obtain

$$V_{\text{eff}}(y) = 16y^2 \int_0^{\omega} \mathrm{d}s\, s e^{-4sy} \left(\frac{\sqrt{a(1-a)s^2+1}}{a(1-a)} - \frac{|as-1|}{a} - \frac{(1-a)s+1}{1-a} \right)$$
$$= \frac{16y^2}{a(1-a)} \int_0^{\omega} \mathrm{d}s\, s e^{-4sy} (\sqrt{a(1-a)s^2+1} - 1) + U, \tag{14}$$

where

$$U = 32y^2 \int_{1/a}^{\omega} \mathrm{d}s\, s e^{-4sy} (1/a - s) < 0. \tag{15}$$

Now we do not have to carry out integration in (15), it is enough to see that it is a short-range repulsion, which does not play a role in our case. To calculate the first term in (14) we use $\sqrt{a(1-a)s^2+1} \leqslant 1 + a(1-a)s^2/2$ to get

$$V_{\text{eff}} < 8y^2 \int_0^{\omega} \mathrm{d}s\, s^3 e^{-4sy} < \frac{3}{16y^2}, \tag{16}$$

where after the integration we have dropped the short-range negative terms. Finally, we have $p_y^2 - \lambda V_{\text{eff}} \geqslant p_y^2 - \lambda(3/16)y^{-2}$. The following inequality[8] holds $p_y^2 - (1/4)y^{-2} \geqslant 0$. Thus in the case of binding, i.e., when such f exists that $\langle f | p_y^2 - \lambda V_{\text{eff}} | f \rangle < 0$, we must have $\lambda > 4/3$. Comparing this with (13) we obtain that three charges form an unstable system if $\mu_y < 3/2$ and

$$2\mu_y (1 + (\sqrt{3/2\mu_y} - 1)^{-1}) < 4/3. \tag{17}$$

Solving this simple inequality tells us that the system is unstable when $\mu_y < 2(11 - 2\sqrt{10})/27 \simeq 0.3463$.

B. Case when $a \leqslant 1/2$

First let us take $a < 1/2$. We shall write $W(a)$ instead of W to point out the dependence on parameter a. We can alleviate the integration noting that $W(a) = -W(1-a)$, thus we have $W_-(a) = (-W(1-a))_- = W_+(1-a) = W(1-a) + W_-(1-a)$. From this we conclude $V_{\text{eff}}(a) = -\overline{W}(a) + V_{\text{eff}}(1-a)$. The additional integral $\overline{W}(a) := \int \mathrm{d}\mathbf{x} |\phi_0|^2 W$ is easy to calculate and $V_{\text{eff}}(1-a)$ for $a < 1/2$ we have already calculated. We obtain

$$-\overline{W}(a) = 16y^2 \int_0^\infty ds\, e^{-4sy} s\left(\left(\frac{1}{a} - \frac{1}{1-a}\right) + \left|s - \frac{1}{1-a}\right| - \left|s - \frac{1}{a}\right|\right)$$

$$= 32y^2 \int_{1/(1-a)}^{1/a} ds\, e^{-4sy}\left(s^2 - \frac{s}{1-a}\right) + 32y^2 \int_{1/a}^\infty ds\, e^{-4sy} s\left(\frac{1}{a} - \frac{1}{1-a}\right). \tag{18}$$

Using (14) and (15) and approximation for the square root $\sqrt{a(1-a)s^2+1} \leqslant 1 + a(1-a)s^2/2$ gives us

$$V_{\text{eff}}(1-a) \leqslant 8y^2 \int_0^{-\omega} ds\, s^3 e^{-4sy} + 32y^2 \int_{1/(1-a)}^{-\omega} ds\, e^{-4sy}\left(\frac{s}{1-a} - s^2\right). \tag{19}$$

Summing (18) and (19) and calculating the integrals explicitly gives us the following expression for $a < 1/2$:

$$V_{\text{eff}} < \frac{3}{16y^2} - e^{-4y/a}\left[\frac{8(1-a)y}{a^2} + 2\frac{2-a}{a} + \frac{1}{y}\right]$$

$$- e^{4\omega y}\left[-2y\omega(\omega+2)^2 + (3\omega/2+1)(\omega+2) - \frac{1}{y}(3\omega/4+1) + \frac{3}{16y^2}\right]. \tag{20}$$

For $a < 1/2$ we have $\omega < -2$, and it is easily seen that all terms in square brackets are positive (this leads again to short-range potentials), meaning that $V_{\text{eff}} < (3/16)y^{-2}$, which gives the same condition for stability as (17). We do not consider explicitly $a = 1/2$, it is done analogously and also results in (17).

IV. SUMMARY

We have initially scaled all masses $m_i \to 2m_i/\mu_x$, making $\mu_x = 2$. Now rescaling it back we get through (17) that the system of three charges is unstable if $\mu_y/\mu_x < (11 - 2\sqrt{10})/27 \simeq 0.1732$. In the case of infinitely heavy nucleus this is $m_3/m_2 < 0.1732$, which is worse than the refined[2,5] Thirring's estimate $m_3/m_2 < 1/1.57$. The accuracy is lost at the point of cutting the positive part of the potential, which induces a long-range attraction. However this is more than enough to prove that the muonic ions $p\mu^- e^-$ or $\mu^- p e^+$ are unstable for the actual values of all three masses. The case of four unit charges $\{+1, +1, -1, -1\}$ is treated similarly but the calculations are more involved[11] and results would be published elsewhere. Let us also stress that the obtained condition is physical. Both Jacobi masses determine Bohr radii for the particle orbits, the orbit within the pair of particles (1,2) and the orbit for the third particle in the field of this pair with respect to the pair's center of mass. If the orbit of one negative particle is outdistanced then the attraction from the positive charge is screened off by the other negative particle and the system becomes unbound.

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Strict deformation quantization for a particle in a magnetic field

Marius Măntoiu[a] and Radu Purice[b]
Institute of Mathematics "Simion Stoilow" of the Romanian Academy, P.O. Box 1-764, Bucarest, RO-014700, Romania

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Recently, we introduced a mathematical framework for the quantization of a particle in a variable magnetic field. It consists in a modified form of the Weyl pseudodifferential calculus and a C^*-algebraic setting, these two points of view being isomorphic in a suitable sense. In the present paper we leave Planck's constant vary, showing that one gets a strict deformation quantization in the sense of Rieffel. In the limit $\hbar \to 0$ one recovers a Poisson algebra induced by a symplectic form defined in terms of the magnetic field. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1887922]

I. INTRODUCTION

The present paper treats the semiclassical limit of the mathematical formalism describing a quantum, nonrelativistic particle without internal structure, placed in a variable magnetic field. The limit is considered in the precise sense of Rieffel's axioms (cf. Refs. 8,22,23), involving C^*-algebras. This setting is widely called *strict* quantization, to distinguish it from the version in terms of formal series (see Ref. 1, for example). It consists of several ingredients, which we outline here very briefly, referring to Sec. II for a detailed discussion.

(1) One needs first a natural family of classical observables. It is admitted that this should form a Poisson algebra $\mathfrak{A}$, which is roughly a real associative and commutative algebra endowed with a compatible Poisson bracket. This structure describes the classical physical system.

(2) For non-null values of Planck's constant $\hbar$, one must define C^*-algebras of quantum observables $\mathfrak{C}^\hbar$.

(3) It must be shown that for $\hbar \to 0$ "the quantum structure converges to the classical one." This is described precisely by Rieffel's system of axioms or some of its versions.

If a certain extra technical condition is verified, allowing to define on classical observables a family of "deformed products" indexed by $\hbar$, one speaks of *strict deformation quantization*.

In our case, a particle without spin moving in the N-dimensional configuration space $\mathbb{R}^N$ and placed under the influence of an external variable magnetic field, the natural Poisson algebra is well known. The observables are smooth functions defined on the phase space $\Xi := \mathbb{R}^{2N}$, the associative product is defined pointwise and the Poisson bracket is induced by the canonical symplectic form on Ξ, to which we add a magnetic contribution.[6,16] This is described in Sec. III.

Quite surprisingly, the algebras of quantum observables for this system were defined and developed only recently. One reason could be that the canonical variables in the magnetic case (the components of the position and those of the magnetic momentum) satisfy complicated commutation relations, that must be taken into account when defining more general observables as functions of these basic ones. The intensive use of *constant* magnetic fields and (or) special observables that are *quadratic* with respect to the momenta have also played a certain role. The setting which is correct (at least in our opinion) appeared in Refs. 6,7 and 13 (a pseudodifferential point

[a]Electronic mail: marius.mantoiu@imar.ro
[b]Electronic mail: radu.purice@imar.ro

of view) and in Refs. 12 and 14 (C^*-algebras). The right attitude can also be found in Ref. 11, but undeveloped and stated for a very particular case; it seems that it has been largely unnoticed. The critical point is *gauge invariance*: when several equivalent vector potentials corresponding to a given magnetic field are used in defining observables, the results should be connected by simple unitary equivalences. But to achieve this, one has to be very careful in defining the precise form of the observables as well as the composition laws to which they are submitted. We shall explain all these in Sec. IV.

In Sec. V we state our main theorem. It asserts that under certain hypothesis, to a magnetic field and to an Abelian algebra of "configurational observables" one can associate naturally a strict deformation quantization.

Sections VI–VIII are devoted to the proof of the main result. The three nontrivial axioms are verified separately. The Rieffel condition and the von Neumann condition follow from the results of Refs. 18 and 20 (Secs. VI and VII). Nevertheless, we also give a direct elementary proof for the von Neumann condition similar with that given for the Dirac condition (Secs. VII and VIII).

This paper is addressed also to people that do not have deformation quantization as their main skill. The system we treat has a certain physical interest (this is not always the case in this field). Thus we decided to avoid technical complications and to leave more general situations to subsequent works. In particular, we hope to be able to say something on strict deformation quantization by twisted groupoids (see Refs. 8–10 and 17, and references therein for the untwisted case), which should include the present work as a particular instance. A pure state quantization would also be an interesting topic.

Both in classical and in quantum theory one works with "real" observables. For any space $\mathcal{E}$ of complex functions we denote by $\mathcal{E}_{\mathbb{R}}$ the subspace of $\mathbb{R}$-valued elements in $\mathcal{E}$. For instance, $C^\infty(P)_{\mathbb{R}}$ will be the family of real C^∞ functions on the smooth manifold P. If $\mathfrak{C}$ is a C^*-algebra, we set $\mathfrak{C}_{\mathbb{R}}$ for the set of self-adjoint elements of $\mathfrak{C}$. Some other notations: If Y is a locally compact group we denote by $C(Y)$ the $*$-algebra of all continuous complex functions on Y. $BC(Y), BC_u(Y), C_0(Y)$ mean respectively "bounded and continuous," "bounded and uniformly continuous," and "continuous and small at infinity." If $\mathcal{H}$ is a Hilbert space, $K(\mathcal{H})$ will be the set of all compact operators in $\mathcal{H}$, forming an ideal in the C^*-algebra $B(\mathcal{H})$ of all the linear, bounded operators on $\mathcal{H}$. The unitary operators form the group $\mathcal{U}(\mathcal{H})$.

II. THE AXIOMS

We describe here Rieffel's framework for strict quantization. There are several versions of his axioms; we choose to work with the system of axioms which appears in Ref. 8, to which we also refer to for many other details. The starting point is a "classical algebra of observables" described by a Poisson algebra.

Definition 1.1: A Poisson algebra *is a triple* $(\mathfrak{A}, \circ, \{\cdot,\cdot\})$, *where* $\mathfrak{A}$ *is a real vector space,* $\circ, \{\cdot,\cdot\}$ *are bilinear maps* : $\mathfrak{A}\times\mathfrak{A}\to\mathfrak{A}$ *such that* $\circ$ *is associative and commutative,* $\{\cdot,\cdot\}$ *is antisymmetric and for each* $\varphi\in\mathfrak{A}$, $\{\varphi,\cdot\}$ *is a derivation both with respect to* $\circ$ *and to* $\{\cdot,\cdot\}$. *Thus, aside bilinearity, the two maps satisfy for all* $\varphi,\psi,\rho\in\mathfrak{A}$.

(i) $\psi\circ\varphi=\varphi\circ\psi$, $(\psi\circ\varphi)\circ\rho=\psi\circ(\varphi\circ\rho)$,
(ii) $\{\psi,\varphi\}=-\{\varphi,\psi\}$,
(iii) $\{\varphi,\psi\circ\rho\}=\psi\circ\{\varphi,\rho\}+\{\varphi,\psi\}\circ\rho$ (Leibnitz rule),
(iv) $\{\varphi,\{\psi,\rho\}\}=\{\{\varphi,\psi\},\rho\}+\{\psi,\{\varphi,\rho\}\}$ (Jacobi's identity).

The elements of $\mathfrak{A}$ are interpreted as observables of a classical description of a physical system. For each $\varphi\in\mathfrak{A}$ and each value $\hbar\neq 0$ of Planck's constant, one would like to have an object $\mathcal{Q}^\hbar(\varphi)$ representing the same observable in a quantum description of the system. One also hopes that the algebraic structure of the quantum observables should converge to the classical picture described by the Poisson algebra, in some suitable norm $\|\cdot\|_\hbar$ depending continuously of $\hbar$. This might be seen as a precise mathematical form of Bohr's correspondence principle.

A systematic justification of the next definitions may be found in Ref. 8. Note that usually in $\mathfrak{A}$ many classical observables are "unbounded;" the use of norms forces us to apply quantization only to certain subfamilies $\mathfrak{A}_0$ of $\mathfrak{A}$.

Definition 1.2: Let $\mathfrak{A}_0$ *be a Poisson algebra which is densely contained in the self-adjoint part* $\mathfrak{C}^0_{\mathbb{R}}$ *of an Abelian* C^**-algebra* $\mathfrak{C}^0$. A strict quantization of the Poisson algebra $(\mathfrak{A}_0, \circ, \{\cdot,\cdot\})$ *is a family of maps* $(\mathcal{Q}^\hbar : \mathfrak{A}_0 \to \mathfrak{C}^\hbar_{\mathbb{R}})_{\hbar \in I}$, *where we have the following:*

(i) *I is a subset of the real axis, for which the origin is an accumulation point contained in I.*

(ii) $\mathfrak{C}^\hbar$ *is a* C^**-algebra, with product and norm denoted, respectively, by* $\#^\hbar$ *and* $\|\cdot\|_\hbar$. *For* $\varphi^\hbar, \psi^\hbar \in \mathfrak{C}^\hbar_{\mathbb{R}}$ *(the self-adjoint part of* $\mathfrak{C}^\hbar$*) we set* $\varphi^\hbar \star^\hbar \psi^\hbar := \frac{1}{2}(\varphi^\hbar \#^\hbar \psi^\hbar + \psi^\hbar \#^\hbar \varphi^\hbar)$ (a Jordan product) *and* $\{\varphi^\hbar, \psi^\hbar\}_\hbar := (1/i\hbar)(\varphi^\hbar \#^\hbar \psi^\hbar - \psi^\hbar \#^\hbar \varphi^\hbar)$.

(iii) $\mathcal{Q}^\hbar : \mathfrak{A}_0 \to \mathfrak{C}^\hbar_{\mathbb{R}}$ *is* $\mathbb{R}$*-linear for each* $\hbar$ *and* $\mathcal{Q}^0$ *is just the inclusion map, and the following axioms are fulfilled:*

(a) *RIEFFEL'S CONDITION: For* $\varphi \in \mathfrak{A}_0$, *the map* $I \ni \hbar \to \|\mathcal{Q}^\hbar(\varphi)\|_\hbar \in \mathbb{R}_+$ *is continuous.*

(b) *VON NEUMANN CONDITION: For* $\varphi, \psi \in \mathfrak{A}_0$, $\|\mathcal{Q}^\hbar(\varphi) \star^\hbar \mathcal{Q}^\hbar(\psi) - \mathcal{Q}^\hbar(\varphi \circ \psi)\|_\hbar \to 0$ *when* $\hbar \to 0$.

(c) *DIRAC'S CONDITION: For* $\varphi, \psi \in \mathfrak{A}_0$, $\|\{\mathcal{Q}^\hbar(\varphi), \mathcal{Q}^\hbar(\psi)\}_\hbar - \mathcal{Q}^\hbar(\{\varphi, \psi\})\|_\hbar \to 0$ *when* $\hbar \to 0$.

(d) *COMPLETENESS:* $\mathcal{Q}^\hbar(\mathfrak{A}_0)$ *is dense in* $\mathfrak{C}^\hbar_{\mathbb{R}}$ *for all* $\hbar \in I$.

The word "strict" was coined by Rieffel in order to distinguish his framework from the (deformation) quantization defined in terms of formal series. Usually Poisson algebras are function spaces.

Definition 1.3: We call Poisson manifold *a smooth manifold M so that on* $C^\infty(M)_{\mathbb{R}}$ *a bracket* $\{\cdot,\cdot\}$ *is given such that, denoting by* $\circ$ *the pointwise multiplication, the triple* $(C^\infty(M)_{\mathbb{R}}, \circ, \{\cdot,\cdot\})$ *is a Poisson algebra.*

When M is not compact, $C^\infty(M)_{\mathbb{R}}$ is a very large, unnormed space. In quantization one deals with suitable families of smooth bounded observables.

Definition 1.4: A strict quantization of the Poisson manifold *M means the choice of a Poisson subalgebra* $\mathfrak{A}_0$ *of* $C^\infty(M)_{\mathbb{R}}$ *composed of bounded functions and a strict quantization of this Poisson subalgebra.*

One should be aware that the linear maps $\mathcal{Q}^\hbar$ tend to behave as morphisms only in the asymptotic limit $\hbar \to 0$. But under favorable circumstances (fulfilled rather often, but by no means always) they may serve to define modified products on $\mathfrak{C}^0$. In this case, one really is allowed to think in terms of "deformed products."

Definition 1.5: A strict quantization $(\mathcal{Q}^\hbar : \mathfrak{A}_0 \to \mathfrak{C}^\hbar_{\mathbb{R}})_{\hbar \in I}$ *is called* a strict deformation quantization *if for each* $\hbar$, $\mathcal{Q}^\hbar(\mathfrak{A}_0)$ *is a subalgebra of* $\mathfrak{C}^\hbar_{\mathbb{R}}$ *and* $\mathcal{Q}^\hbar$ *is injective.*

In such a case, for any $\hbar$, one defines $\#^\hbar : \mathfrak{A}_0 \times \mathfrak{A}_0 \to \mathfrak{A}_0$ such that $\mathcal{Q}^\hbar(\varphi \#^\hbar \psi) = \mathcal{Q}^\hbar(\varphi) \#^\hbar \mathcal{Q}^\hbar(\psi)$ for all $\varphi, \psi \in \mathfrak{A}_0$. The notational ambiguity is deliberate.

Remark: We shall briefly comment upon an alternative definition for *strict deformation quantization of a Poisson algebra* $\mathfrak{A}_0$, in the spirit of Rieffel's approach.[21–23] The maps $\mathcal{Q}^\hbar$ being injective (see Definition 1.5), we may identify all the algebras $\mathcal{Q}^\hbar[\mathfrak{A}_0]$ and consider the different C^*-algebras $\mathfrak{C}^\hbar$ as completions for different C^*-norms $\|.\|_\hbar$ of the same *-algebra $\mathbb{C} \otimes \mathfrak{A}_0$. We denote by $\overline{\mathbb{C} \otimes \mathfrak{A}_0}$ the completion taken with respect to the C^*-norm $|||.||| := \sup_{\hbar \in I} \|.\|_\hbar$. Then we may define a strict deformation quantization of the Poisson algebra $\mathfrak{A}_0$, as a family $\{\mathfrak{C}^\hbar\}_{\hbar \in I}$ of C^*-algebras (with products $\#^\hbar$ and C^*-norms $\|.\|_\hbar$) such that

(1) $\mathfrak{C}^0$ is Abelian;

(2) $\mathbb{C} \otimes \mathfrak{A}_0$ is dense in $\mathfrak{C}^\hbar$ for any $\hbar \in I$;

(3) the triple $(I, \{\mathfrak{C}^\hbar\}_{\hbar \in I}, \Gamma)$, with $\Gamma := C(I; \overline{\mathbb{C} \otimes \mathfrak{A}_0})$, defines a *a continuous field of* C^**-algebras*, cf. Ref. 5;

(4) (the Dirac condition) for any φ and ψ in $\mathfrak{A}_0$ we have

$$\lim_{\hbar\to 0}\left\|\frac{1}{i\hbar}(\varphi\#^{\hbar}\psi-\psi\#^{\hbar}\varphi)-\{\varphi,\psi\}\right\|_{\hbar}=0.$$

In fact our proof in this paper may be seen to give such a structure.

III. THE MAGNETIC POISSON ALGEBRA

For the convenience of the reader, we start by recalling briefly the way a symplectic manifold acquires a canonical Poisson structure. For a differentiable manifold M we denote by $C^\infty(M)$ the vector space of smooth real functions on M, by $\chi(M)$ the $C^\infty(M)$-module of vector fields on M and by $\Omega^k(M)$ the $C^\infty(M)$-module of k-forms on M (i.e., C^∞ sections of the fibre bundle of antisymetric k-linear forms $\Lambda^k_m M$ on $\mathbb{T}_m M$, the tangent space of M at $m\in M$). One has $\Omega^0(M)=C^\infty(M)$. We denote by $\mathrm{d}:\Omega^k(M)\to\Omega^{k+1}(M)$ the exterior differential. A symplectic form on M is just a closed nondegenerate 2-form $\Sigma\in\Omega^2(M)$.

It follows easily from the axioms that the bracket $\{\cdot,\cdot\}$ of any Poisson manifold M is given by *a Poisson bivector*. This means that one has $\{f,g\}=w(\mathrm{d}f,\mathrm{d}g)$ for all $f,\ g\in C^\infty(M)$, where $w:\Omega^1(M)\times\Omega^1(M)\to C^\infty(M)$ is bilinear, antisymmetric and satisfies an extra condition connected to the Jacobi identity (see Refs. 8 or 24 for details). The symplectic form will lead to such a Poisson bivector in a specific way. Being a nondegenerate bilinear form on each tangent space, Σ defines a $C^\infty(M)$-linear isomorphism $\beta:\Omega^1(M)\to\chi(M)$, $\theta(v):=\Sigma_m(\beta_m(\theta),v)$, $\forall(\theta,v)\in\mathbb{T}^*_m M\times\mathbb{T}_m M$. Then one defines

$$\{f,g\}_\Sigma:=\Sigma[\beta(\mathrm{d}f),\beta(\mathrm{d}g)], \tag{1}$$

so in this case the Poisson bivector is given by $w_\Sigma=\Sigma\circ(\beta\times\beta)$. One checks easily that, in this way, M becomes a Poisson manifold and we denote by $\mathcal{P}_0(M)$ the algebra $C^\infty(M)_{\mathbb{R}}$ endowed with the pointwise multiplication and the above canonical Poisson bracket.

We come back to our specific situation. The configuration space of our particle without internal structure is the space $X:=\mathbb{R}^N$, with elements q,x,y,z. The subsequent presence of a magnetic field demands $N\geqslant 2$. We denote by $X^\star$ the dual of the vector space X, with elements p,k,l and by $(x,p)\mapsto x\cdot p$ the duality between X and $X^\star$.

The phase-space of the system is the cotangent bundle $\mathbb{T}^*X$ of X, often denoted by Ξ and identified with the direct sum $X\times X^\star$ (by identifying all the fibers with $X^\star$, using the action through translations). Typical vectors in Ξ are $\xi=(q,p)$ or $\eta=(x,k)$. All the tangent spaces $\mathbb{T}_\xi(\Xi)$ will be identified with Ξ and all the cotangent spaces $\mathbb{T}^*_\xi(\Xi)$ will be viewed as $\Xi^\star$ and, furthermore, as $X^\star\times X$. On Ξ we have the canonical (constant) symplectic form defined by

$$\sigma:\Xi\times\Xi\to\mathbb{R},\quad \sigma[(x,k),(y,l)]:=y\cdot k-x\cdot l.$$

This structure is adequate for the description of the particle whith no magnetic field. When a magnetic field is present, this can be taken into account by a change in the symplectic structure, cf. Ref. 16.

We thus consider a special class of flat symplectic manifolds, representing perturbations of the above symplectic space and associated to a general (regular) magnetic field on X. In fact such *a magnetic field is described by a closed 2-form* $B\in\Omega^2(X)$. Starting with the canonical projection $\pi:\Xi\cong X\times X^\star\to X$, we define canonically an injection $\widetilde{\pi}_2:\Omega^2(X)\to\Omega^2(\Xi)$. Thus we get a new symplectic form σ_B on Ξ as the sum $\sigma_B:=\sigma+\widetilde{\pi}_2 B$, i.e.,

$$(\sigma_B)_{(q,p)}[(x,k),(y,l)]:=\sigma[(x,k),(y,l)]+(\widetilde{\pi}_2 B)_{(q,p)}[(x,k),(y,l)]=y\cdot k-x\cdot l+B_q(x,y).$$

Being the sum of two closed forms, this 2-form is closed. It is also nondegenerate, thus it is a symplectic form on Ξ. Then (1) gives

$$\{f,g\}_B \equiv \{f,g\}_{\sigma_B} = \sigma_B[\beta(\mathrm{d}f),\beta(\mathrm{d}g)],$$

so we badly need an explicit formula for β. Let us denote by $\langle\cdot,\cdot\rangle$ the duality between Ξ and $\Xi^\star$. The inverse $\beta_\xi^{-1}:\Xi\to\Xi^\star$ is defined, for $\xi=(q,p)$, $\eta=(x,k)$, $\zeta=(y,l)\in\Xi$, by

$$(\sigma_B)_{(q,p)}[(x,k),(y,l)] \equiv y\cdot k - x\cdot l + x\cdot \overline{B_q} y = \langle (x,k), \beta_{(q,p)}^{-1}(y,l)\rangle,$$

where $\overline{B_q}:X\to X^\star$ is the linear, antisymmetric operator defined by $B_q(x,y)=x\cdot\overline{B_q}y$, $\forall x,y\in X$. It follows easily that β^{-1} can be set in matrix form,

$$\beta_\xi^{-1} = \begin{pmatrix} \overline{B_q} & -1_{X^*} \\ 1_X & 0 \end{pmatrix} : X\times X^\star \to X^\star \times X,$$

which leads to the next matrix form of β_ξ,

$$\beta_\xi = \begin{pmatrix} 0 & 1_X \\ -1_{X^*} & \overline{B_q} \end{pmatrix} : X^\star \times X \to X\times X^\star.$$

Thus, writting $\mathrm{d}_\xi h = (\mathrm{d}_\xi^X h, \mathrm{d}_\xi^{X^\star} h)$, one gets

$$\{f,g\}_B(\xi) = \mathrm{d}_\xi^X f\cdot \mathrm{d}_\xi^{X^\star} g - \mathrm{d}_\xi^X g\cdot \mathrm{d}_\xi^{X^\star} f + B_q(\mathrm{d}_\xi^X f, \mathrm{d}_\xi^X g).$$

Using coordinates, one has $\mathrm{d}_\xi^X h = \Sigma_{j=1}^N (\partial_{p_j} h)(\xi)\mathrm{d}p_j$ and $\mathrm{d}_\xi^{X^\star} h = \Sigma_{j=1}^N (\partial_{q_j} h)(\xi)\mathrm{d}q_j$ [recall that $\mathrm{d}p_j \in (X^\star)^\star \equiv X$]. We get finally

$$\{f,g\}_B = \sum_{j=1}^N (\partial_{p_j} f\ \partial_{q_j} g - \partial_{q_j} f\ \partial_{p_j} g) + \sum_{j,k=1}^N B_{jk}(\cdot)\partial_{p_j} f\ \partial_{p_k} g. \tag{2}$$

We shall denote by $\mathcal{P}_B(\Xi)$ the Poisson algebra $C^\infty(\Xi)_\mathbb{R}$ endowed with the pointwise multiplication and the Poisson bracket $\{\cdot,\cdot\}_B$ given in (2). The different descriptions of the quantum observable algebras in the next section asks also for a partial Fourier transformed version of this Poisson algebra. This will be explained in Sec. V under favorable circumstances.

IV. THE QUANTUM MAGNETIC OBSERVABLES; THE C^*-ALGEBRAS FOR $\hbar\neq 0$

We are placed in the framework of the preceding section, but for most of the constructions the smoothness assumption on B will be useless. We assume for the moment only that B is continuous.

We present first a pseudodifferential approach to the magnetic quantum system, following Refs. 6,7, and 13. No C^*-algebras are in sight for the moment. We choose some vector potential A corresponding to the magnetic field B ($\mathrm{d}A=B$). It also can be chosen continuous; think of the transversal gauge for example. The vector potential is used to define a representation of some explicitely gauge invariant structure. Only this one will be used in the process of quantization.

Let us fix some value $\hbar\neq 0$ for the Planck constant. We would like to justify the construction of a correspondence $f\mapsto \mathfrak{Op}_A^\hbar(f)$ between (suitable) complex functions defined on the phase space Ξ and operators. To the function $(q,p)\mapsto q_j$ one wants to assign the operator Q_j of multiplication with q_j [i.e., $(Q_j u)(q) := q_j u(q)$] and to $(q,p)\mapsto p_j$ we associate the first-order differential operator $\Pi_{A,j}^\hbar := \hbar P_j - A_j(Q) = -i\hbar\partial_j - A_j$. The difficulty of defining a functional calculus $f\mapsto \mathfrak{Op}_A^\hbar(f) \equiv f(Q,\Pi_A^\hbar)$ for these $2N$ operators comes from their high degree of noncommutativity,

$$i[Q_j,Q_k]=0,\quad i[\Pi_{A,j}^\hbar, Q_k] = \hbar\delta_{j,k},\quad i[\Pi_{A,j}^\hbar,\Pi_{A,k}^\hbar] = \hbar B_{kj}(Q),\quad j,k=1,\ldots,N.$$

A convenient global form of these canonical commutation relations may be given in terms of *the magnetic Weyl system*. Recall the unitary group $(e^{iQ\cdot p})_{p\in X^\star}$ of the position as well as *the magnetic translations* $(U_A^\hbar(q) := e^{iq\cdot\Pi_A^\hbar})_{q\in X}$, given explicitly in the Hilbert space $\mathcal{H} := L^2(X)$ by

$$U_A^\hbar(q) = e^{-(i/\hbar)\Gamma_A([Q,Q+\hbar q])} e^{iq\cdot\hbar P}, \tag{3}$$

where $\Gamma_A([q',q'+\hbar q]) := \int_{[q',q'+\hbar q]} A$ is the circulation of the vector potential A along the segment

$$[q',q'+\hbar q] := \{q'+t\hbar q | t \in [0,1]\}.$$

The family $(U_A^\hbar(q))_{q\in X}$ satisfies

$$U_A^\hbar(q)U_A^\hbar(q') = \omega_B^\hbar(Q;q,q')U_A^\hbar(q+q'), \quad q,q' \in X,$$

where we set

$$\omega_B^\hbar(q_0;q,q') := e^{-(i/\hbar)\Gamma_B(\langle q_0,q_0+\hbar q,q_0+\hbar q+\hbar q'\rangle)}$$

and

$$\Gamma_B(\langle q_0,x,y\rangle) := \int_{\langle q_0,x,y\rangle} B$$

is the flux of B through the triangle $\langle q_0,x,y\rangle$ defined by the points q_0,x, and y. Now the magnetic Weyl system is the family $(W_A^\hbar(q,p))_{(q,p)\in\Xi}$ of unitary operators in $\mathcal{H}$ given by

$$W_A^\hbar(q,p) := e^{-i\sigma((q,p),(Q,\Pi_A^\hbar))} = e^{-i(Q+(\hbar/2)q)\cdot p} e^{-(i/\hbar)\Gamma_A([Q,Q+\hbar q])} e^{iq\cdot\hbar P}$$

and it satisfies for all (q,p), $(q',p') \in \Xi$,

$$W_A^\hbar(q,p)W_A^\hbar(q',p') = e^{(i/2)\sigma((q,p),(q',p'))}\omega_B^\hbar(Q;q,q')W_A^\hbar(q+q',p+p').$$

To construct $\mathfrak{Op}_A^\hbar(f) \equiv f(Q,\Pi_A^\hbar))$ one does not dispose of a spectral theorem. Having the functional calculus with a C_0 group in mind and having faith in the ability of the magnetic Weyl system to take into account the way $(Q_1,\dots,Q_N;\ \Pi_{A,1}^\hbar,\dots,\Pi_{A,N}^\hbar)$ fail to commute, one proposes

$$\mathfrak{Op}_A^\hbar(f) := \int_\Xi \mathrm{d}\xi (\mathfrak{F}_\Xi f)(\xi) W_A^\hbar(\xi),$$

where by $\mathfrak{F}_\Xi$ we denote the symplectic Fourier transform

$$(\mathfrak{F}_\Xi f)(\xi) := \int_\Xi \mathrm{d}\eta\, e^{-i\sigma(\xi,\eta)} f(\eta).$$

A suitable choice of the Haar measures on $X, X^\star$ and Ξ leads to the exact form of the formulas above, with no numerical factors in front of the integrals.

Some simple replacements lead to the following expression for the action of these operators on vectors $u \in L^2(X)$:

$$[\mathfrak{Op}_A^\hbar(f)u](x) = \hbar^{-N}\int_X\int_{X^\star} \mathrm{d}y\,\mathrm{d}k\, e^{(i/\hbar)(x-y)\cdot k} e^{-(i/\hbar)\Gamma_A([x,y])} f\left(\frac{x+y}{2},k\right) u(y). \tag{4}$$

To have $\mathfrak{Op}_A^\hbar(f)\mathfrak{Op}_A^\hbar(g) = \mathfrak{Op}_A^\hbar(f\circ^\hbar g)$ and $\mathfrak{Op}_A^\hbar(f)^* = \mathfrak{Op}_A^\hbar(f^{\circ^\hbar})$, one sets $f^{\circ^\hbar}(q,p) := \overline{f(q,p)}$ (independent of $\hbar$ or B) and

$$(f\circ^\hbar g)(\xi) := (2/\hbar)^{2N}\int_\Xi \mathrm{d}\eta \int_\Xi \mathrm{d}\zeta\, e^{-2(i/\hbar)\sigma(\xi-\eta,\xi-\zeta)} e^{-(i/\hbar)\Gamma_B(\langle q-y+x,x-q+y,y-x+q\rangle)} f(\eta)g(\zeta). \tag{5}$$

The composition law $\circ^\hbar \equiv \circ_B^\hbar$ depends only on the magnetic field and not on the choice of some vector potential.

Obviously, for $B=0$ and $A=0$ the above formulas reproduce the well-known formulas of the pseudodifferential calculus in Weyl form. In Ref. 13 they are studied in detail, their gauge-invariance is underlined and a rigorous meaning of them and of some of their extensions are outlined. See also Refs. 6,7 for other developments and for nice geometrical interpretations. We shall come back to this *magnetic Weyl calculus* after an excursion into twisted crossed product algebras.

The input for a crossed product is a locally compact group X acting on a C^*-algebra $\mathcal{A}$. One constructs a larger C^*-algebra $\mathcal{A}\rtimes X$ containing both $\mathcal{A}$ and a unitary representation of X, with a prescribed commutation rule between elements of these two sets. When a 2-cocycle of the group (with values in the unitary group of the algebra) is also given and when "unitary representation" is replaced by "projective representation" in some suitable generalized sense, then one gets a twisted crossed product. We shall be pragmatic and introduce only the object of strict interest for our situation in a somewhat ad hoc manner. In Ref. 12 and especially in Ref. 14 we give a more detailed description. The abstract theory of twisted crossed products was developed in Refs. 4,19,20.

So, let us start by remarking that $X=\mathbb{R}^N$ is indeed a locally compact second countable group. We shall call *admissible* C^*-algebra $\mathcal{A}$ composed of bounded, uniformly continuous complex functions on X which contains $C_0(X)$ and is invariant under translations, $a\in\mathcal{A}$, $x\in X$ imply $a(\cdot+x)\in\mathcal{A}$. Thus, for any $\hbar\neq 0$, one can define the continuous action of X by automorphisms of $\mathcal{A}$,

$$\theta^\hbar: X\to \mathrm{Aut}(\mathcal{A}),\quad [\theta^\hbar_x(a)](y) := a(y+\hbar x).$$

$\theta^\hbar$ is a group morphism and the maps $X\ni x\mapsto\theta^\hbar_x(a)\in\mathcal{A}$, $a\in\mathcal{A}$ are all continuous. Let us recall the function

$$(q,x,y)\mapsto \omega^\hbar_B(q;x,y) := e^{-(i/\hbar)\Gamma_B(\langle q,q+\hbar x,q+\hbar x+\hbar y\rangle)},$$

which governs the multiplication property of the magnetic translations. It can be interpreted as a map

$$\omega^\hbar_B: X\times X\to C(X;\mathbb{T}),\quad [\omega^\hbar_B(x,y)](q) := \omega^\hbar_B(q;x,y)$$

with values in the set of continuous functions on X taking values in the 1-torus $\mathbb{T}:=\{z\in\mathbb{C}\,|\,|z|=1\}$. It is easy to see that $\omega^\hbar_B$ satisfies *the 2-cocycle condition*

$$\omega^\hbar_B(x,y)\omega^\hbar_B(x+y,z)=\theta^\hbar_x[\omega^\hbar_B(y,z)]\omega^\hbar_B(x,y+z),\quad \forall\, x,y,z\in X,$$

easy to check with Stokes' theorem, since $\mathrm{d}B=0$. It is also *normalized*, i.e.,

$$\omega^\hbar_B(x,0)=1=\omega^\hbar_B(0,x),\quad \forall\, x\in X.$$

We have shown in Ref. 14 how to impose conditions on B in order to have a good connection between $\omega^\hbar_B$ and the admissible C^*-algebra $\mathcal{A}$. Let us denote by $S_\mathcal{A}$ the Gelfand spectrum of $\mathcal{A}$ (the space of characters with the pointwise convergence topology). Our assumptions on $\mathcal{A}$ imply that X can be identified with a dense subset of the locally compact space $S_\mathcal{A}$. We say that a continuous function on X is *of class* $\mathcal{A}$ if it extends to a continuous function on $S_\mathcal{A}$. The C^*-algebra $\mathcal{A}$ is unital iff $S_\mathcal{A}$ is compact (thus a compactification of X) and in this case "continuous" means also "bounded;" in the nonunital case many unbounded functions are allowed. If the components B_{jk} of the magnetic field are of class $\mathcal{A}$ the mapping $X\times X\ni(x,y)\mapsto\omega^\hbar_B(\cdot;x,y)\in C(S_\mathcal{A};\mathbb{T})$ is well defined and continuous with respect to the topology of uniform convergence on compact subsets of $S_\mathcal{A}$. [Note that $C(S_\mathcal{A};\mathbb{T})$ is exactly the unitary group $\mathcal{UM}(\mathcal{A})$ of the multiplier algebra of $\mathcal{A}$.] These are the needed conditions to call $(\theta^\hbar,\omega^\hbar_B)$ *a twisted action of* X *on* $\mathcal{A}$ and to make the quadruplet $(\mathcal{A},\theta^\hbar,\omega^\hbar_B,X)$ a particular case of *a twisted* C^**-dynamical system*. These are also conditions under which one can perform the construction of the twisted crossed product C^*-algebra that we now explain.

Consider first the Banach space $L^1(X;\mathcal{A})$ with the norm $\|\varphi\|_1 := \int_X \mathrm{d}x \|\varphi\|_{\mathcal{A}}$. As a rule, its elements will be considered as functions of two variables: $[\varphi(x)](q) \equiv \varphi(q;x)$, thus $\|\varphi\|_1 = \int_X \mathrm{d}x \sup_{q\in X}|\varphi(q;x)|$. We can introduce an involution by $\varphi^{\diamond}(q;x) := \varphi(q;-x)$ and a composition law

$$(\varphi \diamond^{\hbar} \psi)(q;x) := \int_X \mathrm{d}y\, \varphi\left(q - \frac{\hbar}{2}(x-y);y\right)\psi\left(q+\frac{\hbar}{2}y;x-y\right)e^{-(i/\hbar)\Gamma_B(\langle q-(\hbar/2)x,q-(\hbar/2)x+\hbar y,q+(\hbar/2)x\rangle)} \tag{6}$$

(we leave to the reader the task of suppressing the variable q and introducing the objects $\theta^{\hbar}$ and $\omega_B^{\hbar}$ in the right places to get a more abstract version of this formula). Endowed with this structure $L^1(X;\mathcal{A})$ is a Banach*-algebra.

Its enveloping C^*-algebra will be called *the twisted crossed product of* $\mathcal{A}$ *by the twisted action* $(\theta^{\hbar},\omega_B^{\hbar})$ *of* X. A comprehensive but awkward notation would be $\mathcal{A}\rtimes_{\theta^{\hbar}}^{\omega_B^{\hbar}}X$, which we abbreviate to $\mathfrak{C}_{\mathcal{A}}^{\hbar}$, insisting on its dependence on $\hbar$ and $\mathcal{A}$, the magnetic field B being fixed. We recall that $\mathfrak{C}_{\mathcal{A}}^{\hbar}$ is the completion of $L^1(X;\mathcal{A})$ under the C^*-norm,

$$\|\varphi\|_{\hbar} := \sup\{\|\pi(\varphi)\|_{B(\mathcal{H})} | \pi: L^1(X;\mathcal{A}) \to B(\mathcal{H}) \text{ representation}\}.$$

The main reason for $\mathfrak{C}_{\mathcal{A}}^{\hbar}$ to exist is the fact that its nondegenerate representations are in a one-to-one correspondence with *covariant representations* of the twisted C^*-dynamical system $(\mathcal{A},\theta^{\hbar},\omega_B^{\hbar},X)$, i.e., with triples $(\mathcal{H},r,U)$, where $\mathcal{H}$ is a Hilbert space, r is a nondegenerate representation of $\mathcal{A}$ and U is a strongly continuous map from X to the family of unitary operators on $\mathcal{H}$ satisfying for all x, $y\in X$ and $a\in\mathcal{A}$,

$$U(x)U(y) = r[\omega_B^{\hbar}(x,y)]U(x+y) \quad \text{and } U(x)r(a)U(x)^* = r[\theta_x^{\hbar}(a)]. \tag{7}$$

We shall use this for a single case, that of *the Schrödinger covariant representation* $(L^2(X),r,U_A^{\hbar})$ *associated to the vector potential* A (with $\mathrm{d}A=B$). Here $r:\mathcal{A}\to B[L^2(X)]$ is the usual representation of functions in $\mathcal{A}$ by multiplication operators [$r(a)\equiv a(Q)$ by a previous notation] and $U_B^{\hbar}$ has been introduced at (3). It is easy in this case to check (7) and to view it as another way to codify the commutation relations between positions and magnetic momenta. In fact this is the root of the close connection (see below) between $\mathfrak{C}_{\mathcal{A}}^{\hbar}$ and the magnetic pseudodifferential calculus sketched above. The representation of $\mathfrak{C}_{\mathcal{A}}^{\hbar}$ corresponding to $(L^2(X),r,U_A^{\hbar})$ is given (by abstract principles) by

$$\mathfrak{Rep}_A^{\hbar}(\varphi) := \int_X \mathrm{d}x\, r[\theta_{x/2}^{\hbar}(\varphi(x))]U_A^{\hbar}(x),$$

which gives for $\varphi\in L^1(X;\mathcal{A})$ and $u\in L^2(X)$,

$$[\mathfrak{Rep}_A^{\hbar}(\varphi)u](x) = \hbar^{-N}\int_X \mathrm{d}y\, e^{(i/\hbar)\Gamma_A([x,y])}\varphi\left(\frac{x+y}{2},\frac{y-x}{\hbar}\right)u(y). \tag{8}$$

By comparing (8) with (4) one sees that, at least formally, $\mathfrak{Rep}_A^{\hbar}$ and $\mathfrak{Op}_A^{\hbar}$ are connected to each other by a partial Fourier transformation, $\mathfrak{Op}_A^{\hbar}(f) = \mathfrak{Rep}_A^{\hbar}[\mathbb{F}(f)]$, with $\mathbb{F} := 1\otimes\mathcal{F}$ and $(\mathcal{F}b)(x) := \int_{X^*}\mathrm{d}k\, e^{-ix\cdot k}b(k)$ whenever it makes sense. It follows that the composition laws $\circ^{\hbar}$ and $\diamond^{\hbar}$ are intertwined by $\mathbb{F}$, i.e., $f\circ^{\hbar}g = \mathbb{F}^{-1}[(\mathbb{F}f)\diamond^{\hbar}(\mathbb{F}g)]$, as can also be checked by a direct calculation. We refer to Ref. 14 for details on the rigorous meaning of these connections in nontrivial cases. We do not need it here since actually all our verifications in Secs. VI–VIII are done in the setting of twisted crossed products. One defines the C^*-algebra $\mathfrak{B}_{\mathcal{A}}^{\hbar} := \mathbb{F}^{-1}\mathfrak{C}_{\mathcal{A}}^{\hbar}$. On suitable dense subsets of $\mathfrak{B}_{\mathcal{A}}^{\hbar}$ we are entitled to use (5) as it stands.

V. THE MAIN RESULT

In Sec. III, assuming that the components of our magnetic field B are C^∞ functions on $X=\mathbb{R}^N$, we endowed the space $C^\infty(\Xi)_\mathbb{R}$ of real smooth functions on the phase-space $\Xi=X\times X^\star$ with a B-dependent Poisson algebra structure, called $\mathcal{P}_B(\Xi)$. On the other hand, in Sec. IV we constructed for each $\hbar\in(0,1]$ a C^*-algebra $\mathfrak{B}_\mathcal{A}^\hbar$, which is the partial Fourier transform of the twisted crossed product C^*-algebra $\mathfrak{C}_\mathcal{A}^\hbar$ defined by the twisted action $(\theta^\hbar,\omega_B^\hbar)$ of X on the admissible C^*-algebra $\mathcal{A}$; we had to use the assumption that the components B_{jk} are functions of class $\mathcal{A}$.

In order to construct now a strict deformation quantization we must study the conditions to be imposed to the magnetic field in connection with the choice of the Poisson subalgebra $\mathfrak{A}_0$ of $\mathcal{P}_B(\Xi)$.

We recall that $\mathfrak{C}_\mathcal{A}^\hbar$ is a C^*-completion of the Banach*-algebra $L^1(X;\mathcal{A})$; the structure depends on $\hbar$ and B. Then for any subspace $\mathcal{A}_0$ of $\mathcal{A}$ and any subspace $\mathcal{S}$ of $L^1(X)$, the algebraic tensor product $\mathcal{A}_0\odot\mathcal{S}$ (finite combination of simple tensors) is a subspace of $L^1(X;\mathcal{A})$, thus also of $\mathfrak{C}_\mathcal{A}^\hbar$. The partial Fourier transformed version $\mathbb{F}^{-1}[\mathcal{A}_0\odot\mathcal{S}]=\mathcal{A}_0\odot\mathcal{F}^{-1}\mathcal{S}$ will be a subspace of $\mathbb{F}^{-1}[L^1(X;\mathcal{A})]$ and, therefore, a subspace of $\mathfrak{B}_\mathcal{A}^\hbar$. Note that $\mathcal{A}_0\odot\mathcal{F}^{-1}\mathcal{S}$ is also contained in $\mathcal{A}\odot C_0(X^\star)$, thus it is composed of complex functions defined on the phase space Ξ. If one also requires that $\mathcal{A}_0\subset C^\infty(X)$ and $\mathcal{F}^{-1}\mathcal{S}\subset C^\infty(X^\star)$, then $\mathcal{A}_0\odot\mathcal{F}^{-1}\mathcal{S}\subset C^\infty(\Xi)$ and both the classical and the quantum formalisms hold on $\mathcal{A}_0\odot\mathcal{F}^{-1}\mathcal{S}$. In fact several choices for $\mathcal{A}_0$ and $\mathcal{S}$ are available, their success hanging on the assumptions we impose on the magnetic field. With severe contraints on B one hopes to quantize larger classes of classical symbols. We shall study a simple, convenient situation; the reader could work out other cases for himself. We define $\mathcal{A}^\infty:=\{a\in\mathcal{A}\cap C^\infty(X)\,|\,\partial^\alpha a\in\mathcal{A},\forall\,\alpha\in\mathbb{N}^N\}$; it is a subspace of $\mathcal{A}\cap BC^\infty(X)$. Take $\mathcal{A}_0=\mathcal{A}^\infty$ and $\mathcal{S}=\mathcal{S}(X)$, the Schwartz space of functions on X which have rapidly decaying derivatives of any order. Then $\mathcal{F}^{-1}\mathcal{S}=\mathcal{S}(X^\star)$ is the Schwartz space defined on $X^\star$.

We also consider $\mathcal{S}(X^\star;\mathcal{A}^\infty)$, the space of functions $X^\star\ni p\mapsto f(p)\in\mathcal{A}^\infty$ such that for any l, $m\in\mathbb{N}$,

$$\|f\|_{l,m}:=\max\{\sup_{p\in X^\star}\|p^\alpha(\partial^\beta f)(p)\|_\mathcal{A}\;||\alpha|\leqslant l,|\beta|\leqslant m\}<\infty.$$

We remark that

$$\mathcal{S}(X^\star;\mathcal{A}^\infty)\subset C^\infty(\Xi)\cap\mathbb{F}^{-1}\{L^1(X;\mathcal{A})\}.$$

Then we have the following evident statement.

Proposition 4.1: Suppose that the components of the magnetic field B belong to $\mathcal{A}^\infty$. Then $\mathcal{S}(X^\star;\mathcal{A}^\infty)_\mathbb{R}$ is a Poisson subalgebra of $\mathcal{P}_B(\Xi)$ and a dense subset of the self-adjoint part of the Abelian C^*-algebra $\mathcal{A}\otimes C_0(X^\star)$.

We can now state the following.

Theorem 4.2: (Main result) *Assume that the components of the magnetic field B belong to $\mathcal{A}^\infty$. Then the family of injections $(\mathcal{S}(X^\star;\mathcal{A}^\infty)_\mathbb{R}\hookrightarrow\mathfrak{B}_\mathcal{A}^\hbar)_{\hbar\in[0,1]}$ is a strict deformation quantization (cf. Definitions 1.2 and 1.5).*

As seen in Sec. IV, one may say that $\mathfrak{B}_\mathcal{A}^\hbar$ is a C^*-algebra of (magnetic) pseudodifferential symbols and its represented versions $\mathfrak{Op}_A^\hbar(\mathfrak{B}_\mathcal{A}^\hbar)\subset B(L^2(X))$ are C^*-algebras of magnetic pseudodifferential operators. It will be more convenient to work in the other realization, that of twisted crossed products. There are two reasons.

(1) There exist results of Refs. 18 and 20 on continuous fields of twisted crossed products which lead almost immediately to Rieffel's condition.
(2) In the twisted crossed product formalism one disposes of the simple norm $\|\cdot\|_1$, which will be very convenient in checking the axioms of von Neumann and Dirac. Thus we state now a variant of Theorem 4.2; these two results are equivalent by the isomorphisms defined by the partial Fourier transformation. We need first to rewrite the magnetic Poisson structure. On $\mathcal{S}(X;\mathcal{A})$ (obvious definition) we set by transport of structure

$$\varphi \diamond^0 \psi := \mathbb{F}[(\mathbb{F}^{-1}\varphi)(\mathbb{F}^{-1}\psi)] \quad \text{and} \quad \{\varphi,\psi\}^B := \mathbb{F}[\{\mathbb{F}^{-1}\varphi,\mathbb{F}^{-1}\psi\}_B], \quad \varphi,\psi \in \mathcal{S}(X;\mathcal{A}).$$

A simple direct calculation gives

$$(\varphi \diamond^0 \psi)(q;x) = \int_X \mathrm{d}y\, \varphi(q;y)\psi(q;x-y); \tag{9}$$

$\diamond^0$ is pointwise multiplication in the first variable and convolution in the second. Slightly more effort is needed to prove that

$$\{\varphi,\psi\}^B = -i\sum_{j=1}^{N}[(Q_j^{(2)}\varphi)\diamond^0(\partial_j^{(1)}\psi) - (\partial_j^{(1)}\varphi)\diamond^0(Q_j^{(2)}\psi)] - \sum_{j,k=1}^{N} B_{jk}(\cdot)(Q_j^{(2)}\varphi)\diamond^0(Q_k^{(2)}\psi), \tag{10}$$

where $(Q_j^{(2)}\rho)(q;x) := x_j\rho(q;x)$ and $(\partial_j^{(1)}\rho)(q;x) = (\partial/\partial q_j)\rho(q;x)$.

Let us denote by $C^*(X)$ the group C^*-algebra of X; it is the enveloping C^*-algebra of $L^1(X)$, the convolution Banach*-algebra of X. It is isomorphic to $C_0(X^\star)$ by an extension of the Fourier transformation; thus the spectrum of $C^*(X)$ is homeomorphic to $X^\star$. Note that the twisted crossed product $\mathfrak{C}_{\mathcal{A}}^{\hbar} = \mathcal{A} \rtimes_{\theta^{\hbar}}^{\omega_{\hbar}^B} X$ collapses to $\mathcal{A}\otimes C^*(X)$ for $\hbar = 0$.

Proposition 4.3: Suppose that the components of the magnetic field B belong to $\mathcal{A}^\infty$; then the vector space $\mathcal{S}(X;\mathcal{A}^\infty)_{\mathbb{R}} = \mathbb{F}[\mathcal{S}(X^\star;\mathcal{A}^\infty)]_{\mathbb{R}}$ is a Poisson algebra for the composition laws (9) and (10). It is also dense in the self-adjoint part of the Abelian C^*-algebra $\mathcal{A}\otimes C^*(X)$.

The partial Fourier transformed version of our main result reads as follows.

Theorem 4.4: *Assume that the components of the magnetic field B belong to $\mathcal{A}^\infty$; then the family of injections $(\mathcal{S}(X;\mathcal{A}^\infty)_{\mathbb{R}} \hookrightarrow (\mathfrak{C}_{\mathcal{A}}^{\hbar})_{\mathbb{R}})_{\hbar\in[0,1]}$ is a strict deformation quantization (cf. Definitions 1.2 and 1.5).*

The completeness condition is obvious, $\mathcal{S}(X;\mathcal{A}^\infty)$ is dense in $(L^1(X;\mathcal{A}),\|\cdot\|_1)$, $L^1(X;\mathcal{A})$ is dense in $(\mathfrak{C}_{\mathcal{A}}^{\hbar},\|\cdot\|_{\hbar})$ and one has $\|\cdot\|_1 \leqslant \|\cdot\|_{\hbar}$. The conditions of Definition 1.5 are also clearly satisfied. We still must verify the conditions (a), (b), and (c) of Definition 1.2. This will be done in the next sections.

Remark: It would be in the spirit of many works in strict deformation quantization to consider only the case $\mathcal{A} = C_0(X)$. Since in this case $\mathfrak{C}_{C_0(X)}^{\hbar}$ is isomorphic to $K[L^2(X)]$, the C^*-algebra of all compact operators on $L^2(X)$ [cf. Ref. 14, Proposition 2.17 (b)], in fact one works with a field of C^*-algebras with two types of fibers: $C_0(\Xi)$ for $\hbar = 0$ and $K[L^2(X)]$ for $\hbar \neq 0$. We think that both the twisted crossed product $\mathfrak{C}_{\mathcal{A}}^{\hbar}$ and the pseudodifferential formalism are useful for arbitrary, admissible $\mathcal{A}$. In Ref. 15 it is shown how to calculate the essential spectrum and how to get localization results for generalized Schrödinger operators with anisotropic potentials and magnetic fields. The anisotropy is taken into account by the abelian algebra $\mathcal{A}$ and exploiting the structure of its spectrum is the key of the proofs.

Remark: Let us point out that if the spectrum of $\mathcal{A}$ is compact (and that is always the case in the applications to quantum Hamiltonians, where we expect $\mathcal{A}$ to have a unit), then the components of the magnetic field B being of type $\mathcal{A}$ evidently imply that they are bounded and uniformly continuous. Thus, in this case the requirement that the components of B are of class $\mathcal{A}^\infty$ [i.e., they are of class $C^\infty(X)$ and together with all their derivatives admit continuous extensions to the spectrum of $\mathcal{A}$] is rather optimal. If we allow the spectrum of $\mathcal{A}$ to be noncompact, then we can allow unbounded magnetic fields with components of class $\mathcal{A}$ but we must replace $\mathcal{A}^\infty$ with $\mathcal{A}_{\mathrm{c}}^\infty$ the subalgebra of elements of $\mathcal{A}^\infty$ that have compact support (with respect to the spectrum of $\mathcal{A}$).

An important technical ingredient in our proof relies on a result saying roughly that, under certain conditions, the twisted crossed product of a group with the sectional algebra of a C^*-bundle is the sectional algebra of a C^*-bundle of twisted crossed products. This can be found in Refs. 18 and 20; techniques of Refs. 3 and 21 are also relevant here. For us the most convenient reference is Ref. 18, from which we quote slightly reformulated the definition and the result below.

Definition 4.5: A continuous C^*-bundle *is a triple* $\mathbf{A}=(I,\{\mathcal{A}^\hbar\}_{\hbar\in I},\Gamma_0(\mathbf{A}))$, *where* I *is a Hausdorff, locally compact space,* $\mathcal{A}^\hbar$ *is a* C^**-algebra with norm* $\|\cdot\|_\hbar$ *and* $\Gamma_0(\mathbf{A})$ *a* C^**-algebra of sections such that*

(i) *for any* $\hbar\in I$, $\{F(\hbar)\,|\,F\in\Gamma_0(\mathbf{A})\}=\mathcal{A}^\hbar$,
(ii) *for any* $F\in\Gamma_0(\mathbf{A})$, *the map* $\hbar\mapsto\|F_\hbar\|_\hbar$ *belongs to* $C_0(I)$,
(iii) $\Gamma_0(\mathbf{A})$ *is a* $C_0(I)$*-module: if* $F\in\Gamma_0(\mathbf{A})$ *and* $\nu\in C_0(I)$, *then* νF *(defined pointwise) also belongs to* $\Gamma_0(\mathbf{A})$.

In fact the arguments in Ref. 20 show that the separability condition in their definition of the twisted crossed product is needed only in studying the structure of the group of cocycles. Thus, for our developments of the functional calculus with magnetic fields, we can consider a slightly general definition for twisted crossed products by eliminating the separability condition, and as the proof in Ref. 18 is still valid, we have in fact the theorem cited below.

Theorem 4.6: [Nielsen, 1996 (Ref. 18)] *Let* $\mathbf{A}$ *be a continuous* C^**-bundle*. . *Let* (Θ,Ω) *be a twisted action of an amenable, second countable locally compact group* X *on* $\Gamma_0(\mathbf{A})$ *by* $C_0(I)$*-automorphisms. Then there exists a continuous* C^**-bundle* $\mathbf{C}=(I,\{\mathcal{C}^\hbar\}_{\hbar\in I},\Gamma_0(\mathbf{C}))$ *such that*

(i) *for any* $\hbar\in I$, $\mathcal{C}^\hbar=\mathcal{A}^\hbar\rtimes^{w^\hbar}_{t^\hbar}X$, *where* $t^\hbar_x:X\to\mathrm{Aut}(\mathcal{A}^\hbar)$, $t^\hbar_x[F(\hbar)]:=[\Theta_x(F)](\hbar)$, $\forall x\in X$, $\forall F\in\Gamma_0(\mathbf{A})$ *and* $w^\hbar:X\times X\to\mathcal{UM}(\mathcal{A}^\hbar)$, $w^\hbar(x,y):=[\Omega(x,y)](\hbar)$, $\forall x,y\in X$,
(ii) *the map* $[(\chi\Phi)(\hbar)](x)=[\Phi(x)](\hbar)$, $\forall\hbar\in I$, $\forall x\in X$ *extends from* $C_c(X;\Gamma_0(A))$*to an isomorphism* $\chi:\Gamma_0(\mathbf{A})\rtimes^\Omega_\Theta X\to\Gamma_0(\mathbf{C})$ *such that for every* $\Phi\in L^1(X;\Gamma_0(\mathbf{A}))$ *one has* $(\chi\Phi)(\hbar)\in L^1(X;\mathcal{A}^\hbar)$.

VI. RIEFFEL'S CONDITION

We are placed in the framework of Sec. IV. We start by constructing a twisted action on a large C^*-algebra, consisting of functions depending both on the variables $\hbar\in[0,1]$ and $q\in X\equiv\mathbb{R}^N$. The same strategy has been used in Ref. 2 for the rotation algebras (which are also twisted crossed products) in order to explore the regularity of the spectrum of certain finite-difference operators, the parameter $\hbar$ being replaced there by the strength of a (discrete) magnetic field.

We consider first the C^*-bundle $\mathbf{A}=(I,\{\mathcal{A}^\hbar\}_{\hbar\in I},\Gamma_0(\mathbf{A}))$, where $I:=[0,1]$ is compact, $\mathcal{A}^\hbar:=\mathcal{A}$ (our admissible C^*-algebra) for all $\hbar$ and $\Gamma_0(\mathbf{A}):=C(I;\mathcal{A})$. One checks easily that $\mathbf{A}$ is indeed a continuous C^*-bundle. Note that the Gelfand spectrum of the C^*-algebra $C(I;\mathcal{A})$ is homeomorphic to $I\times S_\mathcal{A}$, where $S_\mathcal{A}$ is the spectrum of $\mathcal{A}$. Recalling the twisted actions $\{(\theta^\hbar,\omega^\hbar_B)\,|\,\hbar\in I\}$ of Sec. IV, one defines for all $\hbar\in I$, $q,x,y\in X$ and $F\in C(I;\mathcal{A})$,

$$\Theta:X\to\mathrm{Aut}[C(I;\mathcal{A})],\quad(\Theta_xF)(\hbar):=\theta^\hbar_x[F(\hbar)],\tag{11}$$

$$\Omega_B:X\times X\to C(I\times S_\mathcal{A};\mathbb{T}),\quad[\Omega_B(x,y)](\hbar,q):=\omega^\hbar_B(q;x,y).\tag{12}$$

By using notations as $[F(\hbar)](q)\equiv F(\hbar,q)$ [the elements of $C(I;\mathcal{A})\cong C(I\times S_\mathcal{A})$ may be seen as functions on $I\times X$], (11) can be rewritten $(\Theta_xF)(\hbar,q)=F(\hbar,q+\hbar x)$. The group $X=\mathbb{R}^N$, being Abelian, is amenable. Then it is easy to verify that $(C(I;\mathcal{A}),\Theta,\Omega_B,X)$ is a twisted C^*-dynamical system and that $\Theta_x(\nu F)=\nu\Theta_x(F)$ for all $x\in X$, $\nu\in C(I)$ and $F\in C(I;\mathcal{A})$, as required by Theorem 4.6.

To apply Theorem 4.6, one must compute first the twisted actions $\{(t^\hbar,w^\hbar)\,|\,\hbar\in I\}$ associated to (Θ,Ω_B). It easily comes out that $t^\hbar=\theta^\hbar$ and $w^\hbar=\omega^\hbar_B$; just use the explicit formulas. Thus the C^*-algebras $\mathcal{C}^\hbar$, the fibers of the continuous C^*-bundle $\mathbf{C}$, coincide (respectively) with the C^*-algebras $\mathfrak{C}^\hbar_\mathcal{A}$ defined in Sec. IV. To show that the map $\hbar\mapsto\|\varphi\|_\hbar$ is continuous for any $\varphi\in\mathcal{A}^\infty\odot\mathcal{S}(X)$, by the axiom (ii) of a continuous C^*-bundle, one has just to prove that any element $\varphi\in S(X;\mathcal{A}^\infty)$ defines a (constant) section belonging to $\Gamma_0(\mathbf{C})$. This is obvious even for $\varphi\in L^1(X;\mathcal{A})$, since the isomorphism χ just intertwines the variables $\hbar$ and x.

VII. THE VON NEUMANN CONDITION

We have to show that, for fixed $\varphi,\ \psi\in\mathcal{S}(X;\mathcal{A}^\infty)_{\mathbb{R}}$ we have

$$\lim_{\hbar\to 0}\|\tfrac{1}{2}(\varphi\diamondsuit^{\hbar}\psi+\psi\diamondsuit^{\hbar}\varphi)-\varphi\diamondsuit^{0}\psi\|_{\hbar}=0.$$

The operations $\diamondsuit^{\hbar}$ and $\diamondsuit^{0}$ are defined, respectively, at (6) and (9). Taking into account that $\|\cdot\|_{\hbar}\leqslant\|\cdot\|_1$ and by the triangle inequality, it is enough to prove

$$\lim_{\hbar\to 0}\|\varphi\diamondsuit^{\hbar}\psi-\varphi\diamondsuit^{0}\psi\|_1=0. \tag{13}$$

By standard arguments one can approach any function in $L^1(X;\Gamma_0(\mathbf{A}),$ in L^1-norm, with a continuous function with compact support, and show that (using the notations of Theorem 4.6)

$$\chi[L^1(X;\Gamma_0(\mathbf{A}))]=C(I;L^1(X,\mathcal{A})).$$

For any function $\varphi\in L^1(X;\mathcal{A})$ let us denote by $\varphi_\circ\in C(I;L^1(X;\mathcal{A})$ the constant function $\varphi_\circ(\hbar):=\varphi,\ \forall\hbar\in I$ and by $\widetilde{\varphi}\in L^1(X;C(I;\mathcal{A}))$ the function taking constant values $[\widetilde{\varphi}(x)](\hbar):=\varphi(x),\ \forall\hbar\in I$. Let us also remark that any constant function in $C(I;L^1(X;\mathcal{A}))$ is of the form $\varphi_\circ=\chi[\widetilde{\varphi}]$ for some $\varphi\in L^1(X;\mathcal{A})$. We denote by # the product in $\Gamma_0(\mathbf{A})\rtimes^{\Omega}_{\Theta}X$ and by $\diamondsuit$ the product in $\Gamma_0(\mathbf{C})$. Then for fixed $\varphi,\ \psi\in\mathcal{S}(X;\mathcal{A}^\infty)_{\mathbb{R}}\subset L^1(X;\mathcal{A})$, one has

$$[\varphi_\circ\diamondsuit\psi_\circ](\hbar)=\chi[\widetilde{\varphi}\#\widetilde{\psi}](\hbar)$$

and thus $\varphi_\circ\diamondsuit\psi_\circ\in C(I;L^1(X;\mathcal{A}))$. As a direct consequence, if we set $\mathbf{\Psi}(\varphi,\psi):=\varphi_\circ\diamondsuit\psi_\circ-(\varphi\diamondsuit^{0}\psi)_\circ\in C(I;L^1(X;\mathcal{A})$ we get

$$\lim_{\hbar\to 0}\|\mathbf{\Psi}(\varphi,\psi)(\hbar)-\mathbf{\Psi}(\varphi,\psi)(0)\|_1=0.$$

But

$$\mathbf{\Psi}(\varphi,\psi)(0)=(\varphi_\circ\diamondsuit\psi_\circ)(0)-(\varphi\diamondsuit^{0}\psi)_\circ(0)=\varphi\diamondsuit^{0}\psi-\varphi\diamondsuit^{0}\psi=0$$

so that

$$\|\varphi\diamondsuit^{\hbar}\psi-\varphi\diamondsuit^{0}\psi\|_{\hbar}=\|\mathbf{\Psi}(\varphi,\psi)(\hbar)\|_{\hbar}\leqslant\|\mathbf{\Psi}(\varphi,\psi)(\hbar)\|_1\underset{\hbar\to 0}{\longrightarrow}0$$

and thus we have got the von Neumann condition.

An alternative direct proof by elementary arguments can be given by studying the exponent of the cocycle appearing in the definition of $\diamondsuit^{\hbar}$,

$$-\frac{i}{\hbar}\Gamma_B\left(\left\langle q-\frac{\hbar}{2}x,q-\frac{\hbar}{2}x+\hbar y,q+\frac{\hbar}{2}x\right\rangle\right)=-\frac{i}{\hbar}\int_{\langle q-(\hbar/2)x,q-(\hbar/2)x+\hbar y,q+(\hbar/2)x\rangle}B.$$

Consider a parametrization for the triangle $\langle q-(\hbar/2)x,q-(\hbar/2)x+\hbar y,q+(\hbar/2)x\rangle$,

$$\left\langle q-\frac{\hbar}{2}x,q-\frac{\hbar}{2}x+\hbar y,q+\frac{\hbar}{2}x\right\rangle=\kappa_{q,(x,y)}[\Delta_2]$$

where $\Delta_2:=\{(t,s)\in\mathbb{R}^2\,|\,0\leqslant t\leqslant 1,0\leqslant s\leqslant t\}$ and

$$\kappa_{q,(x,y)}(t,s):=q-\frac{\hbar}{2}x+t\hbar y+s\hbar(x-y)=q+\left(s-\frac{1}{2}\right)\hbar x+(t-s)\hbar y.$$

Thus, by denoting e_t and e_s the tangent vectors corresponding to the two coordinate functions of $\mathbb{R}^2$, we have

$$\int_{\kappa[\Delta_2]} B = \int_{\Delta_2} \kappa^* B = \int_0^1 \mathrm{d}t \int_0^t \mathrm{d}s (\kappa^* B)(e_t, e_s).$$

An obvious calculation gives

$$(\kappa^* B)(e_t, e_s) = \sum_{j,k} B(\kappa_{q,(x,y)}(t,s)) \frac{\partial \kappa_j}{\partial t} \frac{\partial \kappa_k}{\partial s}$$

and thus we have

$$-\frac{i}{\hbar}\Gamma_B(\kappa_{q,(x,y)}[\Delta_2]) = -i\hbar \sum_{j,k} y_j (x-y)_k \int_0^1 \mathrm{d}t \int_0^t \mathrm{d}s\, B_{jk}\left[q + \left(s - \frac{1}{2}\right)\hbar x + (t-s)\hbar y\right]$$
$$=: -i\hbar \Omega_B(q,x,y;\hbar). \tag{14}$$

Now let us come back to (13) and estimate

$$\|\varphi \diamondsuit^{\hbar} \psi - \varphi \diamondsuit^{0} \psi\|_1 \leqslant \int_X \mathrm{d}x \int_X \mathrm{d}y \sup_{q \in X} \left| \varphi\left(q - \frac{\hbar}{2}(x-y); y\right) \psi\left(q + \frac{\hbar}{2} y; x - y\right) e^{-i\hbar \Omega_B(q,x,y;\hbar)} \right.$$
$$\left. - \varphi(q;y)\psi(q;x-y) \right|. \tag{15}$$

It is easy to see that the integral is bounded by the expression

$$2\left(\sup_{q \in X} \sup_{y \in X} \langle y \rangle^m \varphi(q;y)\right)\left(\sup_{q \in X} \sup_{x \in X} \langle x \rangle^m \psi(q;x)\right)\left(\int_X \mathrm{d}x \langle x \rangle^{-m}\right)^2,$$

that is finite and not depending of $\hbar$ for any $m > N$. On the other hand, the integrand in (15) is convergent pointwise to zero when $\hbar$ goes to 0, as can be seen after writing the inequality

$$\sup_{q \in X} \left| \varphi\left(q - \frac{\hbar}{2}(x-y); y\right) \psi\left(q + \frac{\hbar}{2} y; x - y\right) e^{-i\hbar \Omega_B(q,x,y;\hbar)} - \varphi(q;y)\psi(q;x-y) \right| \leqslant \left(\sup_{q \in X} \left| \varphi\left(q - \frac{\hbar}{2}(x \right.\right.\right.$$
$$\left.\left.\left. - y); y\right) - \varphi(q;y) \right|\right)\left(\sup_{q \in X} \left| \psi\left(q + \frac{\hbar}{2} y; x - y\right) \right|\right) + \left(\sup_{q \in X} |\varphi(q;y)|\right)\left(\sup_{q \in X} \left| \psi\left(q + \frac{\hbar}{2} y; x - y\right) \right.\right.$$
$$\left.\left. - \psi(q;x-y) \right|\right) + \left(\sup_{q \in X} |\varphi(q;y)\psi(q;x-y)|\right)\left(\sup_{q \in X} |e^{-i\hbar \Omega_B(q,x,y;\hbar)} - 1|\right).$$

For the first two lines we use the fact that φ and ψ belong to $\mathcal{S}(X;\mathcal{A}^\infty) \subset BC^\infty(X \times X)$. For the third one, the hypothesis that the components of the magnetic field are in $\mathcal{A}^\infty \subset BC^\infty(X)$ implies that for any $(x,y) \in X^2$ we have $\sup_{q \in X} |\Omega_B(q,x,y;\hbar)| \leqslant C(x,y)$ uniformly in $\hbar$. Thus $\sup_{q \in X} |\exp\{-i\hbar\Omega(q,x,y;\hbar)\} - 1|$ converges to 0 for $\hbar \to 0$.

VIII. THE DIRAC CONDITION

We need only to prove that the following convergence holds:

$$\left\| \frac{1}{i\hbar}(\varphi \diamondsuit^{\hbar} \psi - \psi \diamondsuit^{\hbar} \varphi) - \{\varphi, \psi\}_B \right\|_{1^{\hbar \to 0}} \to 0. \tag{16}$$

For that we shall need the exact form of the first order term in $\hbar$ of $\varphi \diamondsuit^{\hbar} \psi - \psi \diamondsuit^{\hbar} \varphi$. We use Taylor developments

$$\varphi\left(q-\frac{\hbar}{2}(x-y);y\right)=\varphi(q;y)-\frac{\hbar}{2}\sum_{j=1}^{N}(x_j-y_j)\int_0^1 \mathrm{d}s(\partial_j^{(1)}\varphi)\left(q-s\frac{\hbar}{2}(x-y);y\right)$$

and

$$\psi\left(q+\frac{\hbar}{2}y;x-y\right)=\psi(q;x-y)+\frac{\hbar}{2}\sum_{j=1}^{N}y_j\int_0^1 \mathrm{d}s(\partial_j^{(1)}\psi)\left(q+s\frac{\hbar}{2}y;x-y\right).$$

For $\rho\in\mathcal{S}(X;\mathcal{A}^\infty)$, $z\in X$ and $(q,x)\in X^2$ we shall use the notation $\nabla^{(1)}\rho$ for the gradient with respect to the first variable in $X\times X$ and set

$$(\mathfrak{L}_z^{\pm}\rho)(q;x):=\frac{1}{2}z\cdot\int_0^1 \mathrm{d}s(\nabla^{(1)}\rho)\left(q\pm s\frac{\hbar}{2}z;x\right). \tag{17}$$

Note that we have

$$\lim_{\hbar\to 0}(\mathfrak{L}_z^{\pm}\varphi)(q;x)=\tfrac{1}{2}z\cdot(\nabla^{(1)}\varphi)(q;x). \tag{18}$$

Then the Taylor developments above read

$$\varphi\left(q-\frac{\hbar}{2}(x-y);y\right)=\varphi(q;y)-\hbar(\mathfrak{L}_{x-y}^{-}\varphi)(q;y)$$

and

$$\psi\left(q+\frac{\hbar}{2}y;x-y\right)=\psi(q;x-y)+\hbar(\mathfrak{L}_{y}^{+}\varphi)(q;x-y).$$

Moreover, the assumption that $B_{jk}\in\mathcal{A}^\infty\subset BC^\infty(X)$ implies that for any x, $y\in X$, the function $X\times[0,1]\ni(q,\hbar)\mapsto\Omega_B(q,x,y;\hbar)\in\mathbb{R}$ is bounded and uniformly continuous. Thus, if we denote

$$R_B(q,x,y;\hbar):=\frac{1}{\hbar}(e^{-i\hbar\Omega_B(q,x,y;\hbar)}-e^{-i\hbar\Omega_B(q,x,y,0)}), \tag{19}$$

we get $\lim_{\hbar\to 0}|R_B(q,x,y;\hbar)|=0$.

Setting everything together we obtain

$$\begin{aligned}(\varphi\diamondsuit^{\hbar}\psi-\psi\diamondsuit^{\hbar}\varphi)(q;x)=&\int_X \mathrm{d}y[(1-\hbar\mathfrak{L}_{x-y}^{-})\varphi](q;y)[(1+\hbar\mathfrak{L}_{y}^{+})\psi](q;x-y)[e^{-i\hbar\Omega_B(q,x,y;0)}\\&+\hbar R_B(q,x,y;\hbar)]-\int_X \mathrm{d}y[(1-\hbar\mathfrak{L}_{x-y}^{-})\psi](q;y)[(1+\hbar\mathfrak{L}_{y}^{+})\varphi](q;x-y)\\&\times[e^{-i\hbar\Omega_B(q,x,y;0)}+\hbar R_B(q,x,y;\hbar)]=\int_X \mathrm{d}y\ \varphi(q,y)\psi(q;x-y)[e^{-i\hbar\Omega_B(q,x,y;0)}\\&-e^{-i\hbar\Omega_B(q,x,x-y;0)}]+\hbar\int_X \mathrm{d}y\ \varphi(q;y)[(\mathfrak{L}_{y}^{+}+\mathfrak{L}_{y}^{-})\psi](q;x-y)\\&-\hbar\int_X \mathrm{d}y[(\mathfrak{L}_{x-y}^{+}+\mathfrak{L}_{x-y}^{-})\varphi](q;y)\psi(q;x-y)+o(\hbar),\end{aligned}$$

where for obtaining the second identity, we have changed an integration variable from y to $x-y$. By using (18) and some simple arguments we get

$$(\varphi \diamond^{\hbar} \psi - \psi \diamond^{\hbar} \varphi)(q;x) = -i\hbar \sum_{j,k} B_{jk}(q) \int_X \mathrm{d}y\, y_j \varphi(q;y)(x-y)_k \psi(q;x-y)$$
$$+ \hbar \int_X \mathrm{d}y [y\varphi(q;y) \cdot (\nabla^{(1)}\psi)(q;x-y) - (\nabla^{(1)}\varphi)(q;y) \cdot (x-y)\psi(q;x-y)]$$
$$+ o(\hbar).$$

The result is now straightforward by the explicit form of the bracket $\{\cdot, \cdot\}^B$ and of the composition law $\diamond^0$.

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Algebraic methods for diagonalization of a quaternion matrix in quaternionic quantum theory

Tongsong Jiang[a)]
Department of Mathematics, Linyi Teacher's University, Shandong 276005, China and Department of Computer Science and Technology, Shandong University, Jinan 250100, China

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By means of complex representation and real representation of a quaternion matrix, this paper studies the problem of diagonalization of a quaternion matrix, gives two algebraic methods for diagonalization of quaternion matrices in quaternionic quantum theory. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1896386]

I. INTRODUCTION

In the study of quaternionic quantum mechanics and quantum fields,[1–3] the theory of diagonalization of quaternion matrices plays an important role. In practical calculation and applications in quaternionic quantum theory, one meets a problem of finding a nonsingular quaternion matrix S and reducing a quaternion matrix A to a diagonal matrix by a transformation of the form $A \to S^{-1}AS$. Because of the noncommutation of quaternions and the standard complex mathematical methods of resolution break down, the problem is more difficults. In Refs. 4 and 5, the authors discussed the problem of diagonalization of quaternion matrices, and gave a practical rule for diagonalization of quaternion matrices. In Ref. 6, by means of complex representation and companion vector, we studied the problems the eigenvalues and eigenvectors for a quaternion matrix, and derived an algorithm for the eigenvalues and eigenvectors for a quaternion matrix in quaternionic quantum theory. In this paper, by means of complex representation and real representation of a quaternion matrix, we study the problem of diagonalization of a quaternion matrix in two ways, give two algebraic methods for diagonalization of quaternion matrices in quaternionic quantum theory.

Let $\mathbf{R}$ denote the real number field, $\mathbf{C}$ the complex number field, $\mathbf{Q}=\mathbf{R}\oplus\mathbf{R}i\oplus\mathbf{R}j\oplus\mathbf{R}k$ the quaternion field, where $i^2=j^2=k^2=-1$, $ij=-ji=k$. For any matrix A, A^T and $\overline{A}$ denote the transpose and conjugate of A, respectively. $\mathbf{F}^{m\times n}$ denotes the set of $m\times n$ matrices on a field $\mathbf{F}$. $A\sim B$ means that A is similar to B for $A,B\in\mathbf{C}^{n\times n}$.

II. COMPLEX REPRESENTATION OF A QUATERNION MATRIX

For any quaternion matrix $A=B_1+B_2i+B_3j+B_4k\in\mathbf{Q}^{m\times n}$, $i^2=j^2=k^2=-1$, $ij=-ji=k$, $B_l\in\mathbf{R}^{m\times n}(l=1,2,3,4)$, A can be uniquely expressed as $A=(B_1+B_2i)+(B_3+B_4i)j=A_1+A_2j$, $A_1,A_2\in\mathbf{C}^{m\times n}$. It is easy to verify that for any $A\in\mathbf{C}^{m\times n}$, we have $Aj=j\overline{A}$, and $jAj=-A$. Define

$$A^f=\begin{bmatrix} A_1 & A_2 \\ -\overline{A_2} & \overline{A_1} \end{bmatrix}\in\mathbf{C}^{2m\times 2n}, \tag{2.1}$$

the complex matrix A^f is known as complex representation of the matrix A.

Let A, $B\in\mathbf{Q}^{m\times n}$, $C\in\mathbf{Q}^{n\times s}$, $a\in\mathbf{R}$, $P_t=\begin{pmatrix} I_t & 0 \\ 0 & -I_t \end{pmatrix}$, $Q_t=\begin{pmatrix} 0 & -I_t \\ I_t & 0 \end{pmatrix}$, I_t be $t\times t$ identity matrix. Then $P_t^2=I_{2t}$, $Q_tQ_t^T=I_{2t}$. By the definition of complex representation we easily get the following results:

a)Electronic mail: tsjemail@163.com

$$(A+B)^f = A^f + B^f, \quad (aA)^f = aA^f, \tag{2.2}$$

$$(AC)^f = A^f C^f, \tag{2.3}$$

$$\overline{A^f} = Q_m^T A^f Q_n. \tag{2.4}$$

For $A \in \mathbf{Q}^{n\times n}$, clearly by (2.3) the quaternion matrix A is nonsingular if and only if the complex representation A^f is nonsingular, and $(A^{-1})^f = (A^f)^{-1}$.

For $A \in \mathbf{Q}^{n\times n}$ and $\mathbf{x} \in \mathbf{C}^{2n\times 1}$, if $A^f\mathbf{x} = \lambda\mathbf{x}$, then by (2.4),

$$\overline{A^f}\overline{\mathbf{x}} = \overline{\lambda}\overline{\mathbf{x}} \Leftrightarrow A^f(Q_n^T\overline{\mathbf{x}}) = \overline{\lambda}(Q_n^T\overline{\mathbf{x}}), \tag{2.5}$$

clearly two vectors $\mathbf{x}$ and $Q_n^T\overline{\mathbf{x}}$ are linearly independent. Therefore the following result comes immediately from (2.5).

Proposition 2.1: Let $A \in \mathbf{Q}^{n\times n}$. Then the complex eigenvalues of complex representation A^f appear in conjugate pairs.

III. COMPLEX REPRESENTATION METHOD

In this section, we derive a technique for diagonalization of a quaternion matrix by means of complex representation in quaternionic quantum theory.

Let $A \in \mathbf{Q}^{n\times n}$, and A^f be the complex representation of quaternion matrix A.

If A is a diagonalizable matrix, then there exists a nonsingular quaternion matrix S such that $AS = SJ$, $J = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$, in which λ_t is an eigenvalue of quaternion matrix A. By Ref. 6, Lemma 3.1 let $\lambda_t = a_t + b_t i$ with real number a_t, b_t and $\mathrm{Im}\,\lambda_t \geqslant 0$, we have

$$A^f S^f = S^f J^f = S^f \begin{bmatrix} J & 0 \\ 0 & \overline{J} \end{bmatrix}, \tag{3.1}$$

therefore the complex representation A^f is diagonalizable.

Conversely, if complex representation A^f is diagonalizable, by Proposition 2.1 let all eigenvalues of A^f be $\lambda_1, \overline{\lambda_1}, \lambda_2, \overline{\lambda_2}, \ldots, \lambda_n, \overline{\lambda_n}$,in which $\mathrm{Im}\,\lambda_t \geqslant 0$, $t = 1, 2, \ldots, n$, and T be a nonsingular complex matrix such that

$$T^{-1}A^f T = \begin{bmatrix} J & 0 \\ 0 & \overline{J} \end{bmatrix} = J^f \Leftrightarrow A^f T = TJ^f, \tag{3.2}$$

where $J = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. By (2.4), the equation (3.2) is equivalent to

$$\overline{A^f}\overline{T} = \overline{TJ^f} \Leftrightarrow A^f(Q_n^T\overline{T}Q_n) = (Q_n^T\overline{T}Q_n)J^f. \tag{3.3}$$

Combine (3.2) and (3.3) there exists a nonzero matrix $\hat{T}$ such that

$$A^f\hat{T} = \hat{T}J^f, \tag{3.4}$$

where $\hat{T} = \frac{1}{2}(T + Q_n^T\overline{T}Q_n)$. Let

$$T = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix}, \tag{3.5}$$

where $T_{kl} \in \mathbf{C}^{n\times n}$. It is easy to get by direct calculation

$$\hat{T} = \begin{bmatrix} \hat{T}_1 & \hat{T}_2 \\ -\overline{\hat{T}}_2 & \overline{\hat{T}}_1 \end{bmatrix}, \tag{3.6}$$

where

$$\hat{T}_1 = \tfrac{1}{2}(T_{11} + \overline{T}_{22}), \quad \hat{T}_2 = \tfrac{1}{2}(T_{12} - \overline{T}_{21}). \tag{3.7}$$

From (3.6) construct a quaternion matrix

$$S = \hat{T}_1 + \hat{T}_2 j = \frac{1}{2}(I_n, -jI_n)\hat{T}\begin{bmatrix} I_n \\ jI_n \end{bmatrix}. \tag{3.8}$$

Clearly $S^f = \hat{T}$. Therefore (3.4) is equivalent to

$$A^f S^f = S^f J^f \Leftrightarrow AS = SJ. \tag{3.9}$$

Finally for any two complex numbers k_1, k_2, since

$$\begin{bmatrix} \hat{T}_1 & \hat{T}_2 \\ -\overline{\hat{T}}_2 & \overline{\hat{T}}_1 \end{bmatrix}\begin{bmatrix} k_1 \\ k_2 \end{bmatrix} = 0 \Leftrightarrow \begin{bmatrix} k_1 & k_2 \\ \overline{k}_2 & -\overline{k}_1 \end{bmatrix}\begin{bmatrix} \hat{T}_1 \\ \hat{T}_2 \end{bmatrix} = 0. \tag{3.10}$$

Clearly if $(k_1, k_2) \neq (0,0)$, then the equation (3.10) has only zero solution, $\hat{T}_1 = 0$, $\hat{T}_2 = 0$, i.e., $\hat{T} = 0$, a contradiction. Therefore nonzero $\hat{T}$ is nonsingular complex matrix, and from $S^f = \hat{T}$ we know that S is nonsingular quaternion matrix.

From the statement above we get the following result.

Theorem 3.1: Let $A \in \mathbf{Q}^{n\times n}$. Then A is a diagonalizable quaternion matrix if and only if A^f is a diagonalizable complex matrix, in which case, if A^f is a diagonalizable matrix and let all eigenvalues of A^f be $\lambda_1, \overline{\lambda}_1, \lambda_2, \overline{\lambda}_2, \ldots, \lambda_n, \overline{\lambda}_n$, in which $\mathrm{Im}\,\lambda_t \geqslant 0$, $t = 1, 2, \ldots, n$, and T be a nonsingular matrix such that

$$T^{-1}A^f T = \begin{bmatrix} J & 0 \\ 0 & \overline{J} \end{bmatrix} = J^f \Leftrightarrow A^f T = TJ^f,$$

where $J = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. Let

$$S = \frac{1}{4}(I_n, -jI_n)(T + Q_n^{-1}\overline{T}Q_n)\begin{bmatrix} I_n \\ jI_n \end{bmatrix}. \tag{3.11}$$

Then S is a nonsingular quaternion matrix and $S^{-1}AS = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$.

The proof of Theorem 3.1 is constructive. Theorem 3.1 turns the problem of diagonalization of a quaternion matrix into that of corresponding complex representation matrix by means of complex representation of a quaternion matrix. When a quaternion matrix is a diagonalizable matrix, it gives a formula algorithm for the diagonalization of the quaternion matrix by the formula (3.11).

Example: Let

$$A = \begin{bmatrix} 2i & -2j & j+k \\ -k & 2 & -1 \\ -j & 1-i & 1 \end{bmatrix}.$$

Is quaternion matrix A a diagonalizable matrix? If A is a diagonalizable matrix, then find a nonsingular quaternion matrix S such that $S^{-1}AS$ is a diagonal matrix.

Solution: It is easy to get by (2.1) that the complex representation A^f of quaternion matrix A is

$$A^f = \begin{bmatrix} 2i & 0 & 0 & 0 & -2 & 1+i \\ 0 & 2 & -1 & -i & 0 & 0 \\ 0 & 1-i & 1 & -1 & 0 & 0 \\ 0 & 2 & -1+i & -2i & 0 & 0 \\ -i & 0 & 0 & 0 & 2 & -1 \\ 1 & 0 & 0 & 0 & 1+i & 1 \end{bmatrix},$$

and $|xI_{2n}-A^f|=(x-1)^2(x-1-i)^2(x-1+i)^2$. Therefore the eigenvalues λ of A^f are 1, 1, $1+i$, $1+i$, $1-i$, $1-i$.

For $\lambda=1$, find two corresponding linearly independent eigenvectors by solving equation $(\lambda I_6-A^f)\mathbf{x}=0$, $\alpha_1=(1+i,0,0,0,-1,-i)^T$, $\alpha_2=(0,1,-i,1-i,0,0)^T$; for $\lambda=1+i$, find two corresponding linearly independent eigenvectors $\alpha_3=(i,0,0,0,-1,i)^T$, $\alpha_4=(i,0,0,0,0,1)^T$; and for $\lambda=1-i$, $\alpha_5=(0,1,i,-i,0,0)^T$, $\alpha_6=(0,0,-1,-i,0,0)^T$ are corresponding linearly independent eigenvectors.

Let $T=(\alpha_1,\alpha_3,\alpha_4,\alpha_2,\alpha_5,\alpha_6)$. Then T is a nonsingular matrix and

$$T^{-1}A^fT=\operatorname{diag}(J,\overline{J})=J^f,$$

where $J=\operatorname{diag}(1,1+i,1+i)$. Therefore A^f is diagonalizable, and then by Theorem 3.1 A is diagonalizable. Construct a quaternion matrix S by (3.11),

$$S=\frac{1}{4}(I_3,-jI_3)(T+Q_3^T\overline{T}Q_3)\begin{bmatrix} I_3 \\ jI_3 \end{bmatrix}=\begin{bmatrix} 1+i & i & i \\ j & j & 0 \\ -k & k & -j \end{bmatrix},$$

then S is a nonsingular quaternion matrix and such that

$$S^{-1}AS=\operatorname{diag}(1,1+i,1+i).$$

IV. REAL REPRESENTATION OF A QUATERNION MATRIX

For any quaternion matrix $A=A_1+A_2i+A_3j+A_4k\in\mathbf{Q}^{m\times n}$, $A_l\in\mathbf{R}^{m\times n}(l=1,2,3,4)$, define

$$A^f=\begin{bmatrix} A_1 & -A_2 & -A_3 & -A_4 \\ A_2 & A_1 & -A_4 & A_3 \\ A_3 & A_4 & A_1 & -A_2 \\ A_4 & -A_3 & A_2 & A_1 \end{bmatrix}\in\mathbf{R}^{4m\times 4n}, \tag{4.1}$$

the real matrix A^f is known as real representation of the quaternion matrix A.

Let

$$P_t=\begin{bmatrix} I_t & 0 & 0 & 0 \\ 0 & -I_t & 0 & 0 \\ 0 & 0 & I_t & 0 \\ 0 & 0 & 0 & -I_t \end{bmatrix},\quad Q_t=\begin{bmatrix} 0 & -I_t & 0 & 0 \\ I_t & 0 & 0 & 0 \\ 0 & 0 & 0 & I_t \\ 0 & 0 & -I_t & 0 \end{bmatrix},$$

$$R_t=\begin{bmatrix} 0 & 0 & 0 & -I_t \\ 0 & 0 & I_t & 0 \\ 0 & -I_t & 0 & 0 \\ I_t & 0 & 0 & 0 \end{bmatrix},\quad S_t=\begin{bmatrix} 0 & 0 & -I_t & 0 \\ 0 & 0 & 0 & -I_t \\ I_t & 0 & 0 & 0 \\ 0 & I_t & 0 & 0 \end{bmatrix}.$$

Then P_t,Q_t,R_t,S_t are unitary matrices, and

$$Q_t^2 = R_t^2 = S_t^2 = Q_t R_t S_t = -1. \tag{4.2}$$

Let $A, B \in \mathbf{Q}^{m\times n}$, $C \in \mathbf{Q}^{n\times s}$, $a \in \mathbf{R}$. By the definition of real representation we easily get the following results:

$$(A+B)^f = A^f + B^f, (aA)^f = aA^f, \tag{4.3}$$

$$(AC)^f = A^f C^f, \tag{4.4}$$

$$Q_m^T A^f Q_n = A^f, \tag{4.5}$$

$$R_m^T A^f R_n = A^f, \tag{4.6}$$

$$S_m^T A^f S_n = A^f. \tag{4.7}$$

Clearly, from (4.4) we know that the quaternion matrix A is nonsingular if and only if real representation matrix A^f is nonsingular, and $(A^{-1})^f = (A^f)^{-1}$.

For $A \in \mathbf{Q}^{n\times n}$ and $\mathbf{x} \in \mathbf{C}^{4n\times 1}$, if $A^f\mathbf{x} = \lambda\mathbf{x}$, then by (4.5)–(4.7) we have

$$A^f(Q_n^T\mathbf{x}) = \lambda(Q_n^T\mathbf{x}), \quad A^f(R_n^T\mathbf{x}) = \lambda(R_n^T\mathbf{x}), \quad A^f(S_n^T\mathbf{x}) = \lambda(S_n^T\mathbf{x}). \tag{4.8}$$

On the one hand, let λ be a real number, we may choose $\mathbf{x} \in \mathbf{R}^{4n\times 1}$, and from (4.8) we easily verify that $\mathbf{x}, Q_n^T\mathbf{x}, R_n^T\mathbf{x}, S_n^T\mathbf{x}$ are linearly independent. This means that real eigenvalues of A^f appear in fours. On the other hand, let λ be an imaginary number. If there exist three complex numbers k_1, k_2, k_3 such that $\mathbf{x} = k_1 Q_n^T\mathbf{x} = k_2 R_n^T\mathbf{x} = k_3 S_n^T\mathbf{x}$, then by (4.2) we easily know that $k_1^2 = k_2^2 = k_3^2 = k_1 k_2 k_3 = -1$, this is a contradiction. Without loss generality suppose that $\mathbf{x}, Q_n^T\mathbf{x}$ are linearly independent, and clearly $\mathbf{x}, Q_n^T\overline{\mathbf{x}}$ are also linearly independent, by (4.5) we have

$$A^f\mathbf{x} = \lambda\mathbf{x}, \quad A^f(Q_n^T\mathbf{x}) = \lambda(Q_n^T\mathbf{x}), \tag{4.9}$$

$$A^f\mathbf{x} = \lambda\mathbf{x}, \quad A^f(Q_n^T\overline{\mathbf{x}}) = \overline{\lambda}(Q_n^T\overline{\mathbf{x}}). \tag{4.10}$$

Therefore (4.9) and (4.10) mean that the imaginary eigenvalues of real representation A^f appear in pairs and in conjugate pairs.

Form the statement above we obtain the following result.

Proposition 4.1: Let $A \in \mathbf{Q}^{n\times n}$. Then the real eigenvalues of real representation A^f appear in fours; the imaginary eigenvalues of real representation A^f appear in pairs and in conjugate pairs. In other words, the complex eigenvalues of real representation A^f appear in double conjugate pairs, i.e., the complex eigenvalues of the $4n\times 4n$ real matrix A^f appear in the form

$$\lambda_1, \lambda_1, \lambda_2, \lambda_2, \ldots, \lambda_n, \lambda_n,$$

$$\overline{\lambda_1}, \overline{\lambda_1}, \overline{\lambda_2}, \overline{\lambda_2}, \ldots, \overline{\lambda_n}, \overline{\lambda_n}.$$

V. REAL REPRESENTATION METHOD

In this section, we discuss an analogue of technique for diagonalization of a quaternion matrix by means of real representation in quaternionic quantum theory.

For $A \in \mathbf{Q}^{n\times n}$, if A is a diagonalizable matrix, there exists a nonsingular quaternion matrix S such that

$$S^{-1}AS = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n), \tag{5.1}$$

in which λ_t is an eigenvalue of quaternion matrix A, $t=1,2,\ldots,n$. By Ref. 6, Lemma 3.1 we may let $\lambda_t = a_t + b_t i$ with $\mathrm{Im}\,\lambda_t \geqslant 0$. Let $J=\mathrm{diag}(\lambda_1,\lambda_2,\ldots,\lambda_n)=J_1+J_2 i$, in which $J_1=\mathrm{diag}(a_1,a_2,\ldots,a_n)$ and $J_2=\mathrm{diag}(b_1,b_2,\ldots,b_n)$. Then

$$(S^f)^{-1}A^f S^f = J^f = \begin{bmatrix} J_1 & -J_2 & 0 & 0 \\ J_2 & J_1 & 0 & 0 \\ 0 & 0 & J_1 & -J_2 \\ 0 & 0 & J_2 & J_1 \end{bmatrix}. \tag{5.2}$$

Therefore by the fact that

$$\begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix}^{-1} \begin{bmatrix} a_t & -b_t \\ b_t & a_t \end{bmatrix} \begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix} = \begin{bmatrix} a_t + b_t i & 0 \\ 0 & a_t - b_t i \end{bmatrix}$$

we have

$$A^f \sim J^f \sim \begin{bmatrix} a_1 & -b_1 & & & 0 \\ b_1 & a_1 & & & \\ & & \ddots & & \\ & & & a_n & -b_n \\ 0 & & & b_n & a_n \end{bmatrix} \oplus \begin{bmatrix} a_1 & -b_1 & & & 0 \\ b_1 & a_1 & & & \\ & & \ddots & & \\ & & & a_n & -b_n \\ 0 & & & b_n & a_n \end{bmatrix} \sim \begin{bmatrix} \lambda_1 & 0 & & & 0 \\ 0 & \overline{\lambda_1} & & & \\ & & \ddots & & \\ & & & \lambda_n & 0 \\ 0 & & & 0 & \overline{\lambda_n} \end{bmatrix}$$
$$\oplus \begin{bmatrix} \lambda_1 & 0 & & & 0 \\ 0 & \overline{\lambda_1} & & & \\ & & \ddots & & \\ & & & \lambda_n & 0 \\ 0 & & & 0 & \overline{\lambda_n} \end{bmatrix}. \tag{5.3}$$

That is the real representation A^f is diagonalizable.

Conversely, if real representation A^f is diagonalizable, by Proposition 4.1, (5.2) and (5.3) there exists a nonsingular complex matrix T such that

$$T^{-1}A^f T = J^f \Leftrightarrow A^f T = TJ^f, \tag{5.4}$$

where $J=\mathrm{diag}(\lambda_1,\lambda_2,\ldots,\lambda_n)$, and $\lambda_t = a_t + b_t i$ with $\mathrm{Im}\,\lambda_t \geqslant 0$, $t=1,2,\ldots,n$.

Let

$$T = \begin{bmatrix} T_{11} & T_{12} & T_{13} & T_{14} \\ T_{21} & T_{22} & T_{23} & T_{24} \\ T_{31} & T_{32} & T_{33} & T_{34} \\ T_{41} & T_{42} & T_{43} & T_{44} \end{bmatrix}, \tag{5.5}$$

where $T_{kl} \in \mathbf{C}^{n\times n}$. By (4.5)–(4.7) and (5.4) we have

$$A^f \overline{T} = \overline{T} J^f,$$

$$A^f (Q_n^T \overline{T} Q_n) = (Q_n^T \overline{T} Q_n) J^f,$$

$$A^f (R_n^T \overline{T} R_n) = (R_n^T \overline{T} R_n) J^f,$$

$$A^f(S_n^T\overline{T}S_n) = (S_n^T\overline{T}S_n)J^f, \tag{5.6}$$

let $\hat{T}=\frac{1}{4}(\overline{T}+Q_n^T\overline{T}Q_n+R_n^T\overline{T}R_n+S_n^T\overline{T}S_n)$, then clearly $\hat{T}$ is nonzero complex matrix and with

$$A^f\hat{T} = \hat{T}J^f. \tag{5.7}$$

It is easy to get by direct calculation

$$\hat{T} = \begin{bmatrix} \hat{T}_1 & -\hat{T}_2 & -\hat{T}_3 & -\hat{T}_4 \\ \hat{T}_2 & \hat{T}_1 & -\hat{T}_4 & \hat{T}_3 \\ \hat{T}_3 & \hat{T}_4 & \hat{T}_1 & -\hat{T}_2 \\ \hat{T}_4 & -\hat{T}_3 & \hat{T}_2 & \hat{T}_1 \end{bmatrix}, \tag{5.8}$$

where

$$\hat{T}_1 = \tfrac{1}{4}(\overline{T}_{11} + \overline{T}_{22} + \overline{T}_{44} + \overline{T}_{33}), \quad \hat{T}_2 = \tfrac{1}{4}(\overline{T}_{21} - \overline{T}_{12} - \overline{T}_{34} + \overline{T}_{43}),$$

$$\hat{T}_3 = \tfrac{1}{4}(\overline{T}_{31} - \overline{T}_{42} + \overline{T}_{24} - \overline{T}_{13}), \quad \hat{T}_4 = \tfrac{1}{4}(\overline{T}_{41} + \overline{T}_{32} - \overline{T}_{14} - \overline{T}_{23}).$$

From (5.8) construct a quaternion matrix,

$$S = \hat{T}_1 + \hat{T}_2 i + \hat{T}_3 j + \hat{T}_4 k = \frac{1}{4}(I_n, iI_n, jI_n, kI_n)\hat{T}\begin{bmatrix} I_n \\ -iI_n \\ -jI_n \\ -kI_n \end{bmatrix}. \tag{5.9}$$

Clearly $S^f=\hat{T}$, and by (4.4) and (5.7) we have $AS=SJ$. Similarly in Sec. III, we can also prove that S is nonsingular quaternion matrix, therefore A is a diagonalizable matrix.

The following result comes immediately from the statement above.

Theorem 5.1: Let $A \in \mathbf{Q}^{n\times n}$. Then A is a diagonalizable quaternion matrix if and only if real representation A^f is a diagonalizable real matrix, in which case, if A^f is a diagonalizable matrix and let complex eigenvalues of the $4n\times 4n$ real matrix A^f are in the form

$$\lambda_1, \lambda_1, \lambda_2, \lambda_2, \ldots, \lambda_n, \lambda_n,$$

$$\overline{\lambda_1}, \overline{\lambda_1}, \overline{\lambda_2}, \overline{\lambda_2}, \ldots, \overline{\lambda_n}, \overline{\lambda_n},$$

where $\operatorname{Im}\lambda_t \geqslant 0$, $t=1,2,\ldots,n$. Then

$$A^f \sim \begin{bmatrix} \lambda_1 & 0 & & & 0 \\ 0 & \overline{\lambda_1} & & & \\ & & \ddots & & \\ & & & \lambda_n & 0 \\ 0 & & & 0 & \overline{\lambda_n} \end{bmatrix} \oplus \begin{bmatrix} \lambda_1 & 0 & & & 0 \\ 0 & \overline{\lambda_1} & & & \\ & & \ddots & & \\ & & & \lambda_n & 0 \\ 0 & & & 0 & \overline{\lambda_n} \end{bmatrix} \sim J^f,$$

where $J=\operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. Let T be a nonsingular complex matrix such that

$$T^{-1}A^fT = J^f \Leftrightarrow A^fT = TJ^f.$$

Construct a quaternion matrix

$$S = \frac{1}{16}(I_n, iI_n, jI_n, kI_n)(\overline{T} + Q_n^T \overline{T} Q_n + R_n^T \overline{T} R_n + S_n^T \overline{T} S_n) \begin{bmatrix} I_n \\ -iI_n \\ -jI_n \\ -kI_n \end{bmatrix}. \tag{5.10}$$

Then S is nonsingular and $S^{-1}AS = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$.

The proof of Theorem 5.2 is also constructive. Theorem 5.2 turns the problem of diagonalization of a quaternion matrix into that of corresponding real representation matrix by means of real representation of a quaternion matrix. When a quaternion matrix is a diagonalizable matrix, it gives a formula algorithm for the diagonalization of the quaternion matrix by the formula (5.10).

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Symmetric informationally complete–positive operator valued measures and the extended Clifford group

D. M. Appleby[a)]
Department of Physics, Queen Mary University of London, London E1 4NS, United Kingdom

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We describe the structure of the extended Clifford group [defined to be the group consisting of all operators, unitary and antiunitary, which normalize the generalized Pauli group (or Weyl–Heisenberg group as it is often called)]. We also obtain a number of results concerning the structure of the Clifford group proper (i.e., the group consisting just of the unitary operators which normalize the generalized Pauli group). We then investigate the action of the extended Clifford group operators on symmetric informationally complete–positive operator valued measures (or SIC–POVMs) covariant relative to the action of the generalized Pauli group. We show that each of the fiducial vectors which has been constructed so far (including all the vectors constructed numerically by Renes *et al.*) is an eigenvector of one of a special class of order 3 Clifford unitaries. This suggests a strengthening of a conjecture of Zauner's. We give a complete characterization of the orbits and stability groups in dimensions 2–7. Finally, we show that the problem of constructing fiducial vectors may be expected to simplify in the infinite sequence of dimensions 7,13,19,21,31,… . We illustrate this point by constructing exact expressions for fiducial vectors in dimensions 7 and 19. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1896384]

I. INTRODUCTION

The statistics of an arbitrary quantum measurement are described by a positive operator valued measure, or POVM (Davies,[1] Busch *et al.*,[2] Peres,[3] Nielsen and Chuang[4] and references cited therein). Suppose the measurement has only a finite number of distinct outcomes. Then the corresponding POVM assigns to each outcome i the positive operator $\hat{E}_i$ with the property that $\mathrm{Tr}(\hat{E}_i\hat{\rho})$ is the probability of obtaining outcome i (where $\hat{\rho}$ is the density operator). Since $\Sigma_i \mathrm{Tr}(\hat{E}_i\hat{\rho})=1$ for all $\hat{\rho}$ we must have $\Sigma_i \hat{E}_i=1$.

A POVM is said to be *informationally complete* if the probabilities $\mathrm{Tr}(\hat{E}_i\hat{\rho})$ uniquely determine the density operator $\hat{\rho}$. The concept of informational completeness is originally due to Prugovečki[5] (also see Busch,[6] Busch *et al.*,[2] d'Ariano *et al.*,[7] Flammia *et al.*,[8] Finkelstein,[9] and references cited therein). It has an obvious relevance to the problem of quantum state determination. It also plays an important role in the Caves *et al.*[10–13] Bayesian approach to the interpretation of quantum mechanics, and in Hardy's[14,15] proposed axiomatization.

Suppose the Hilbert space has finite dimension d. Then it is easily seen that an informationally complete POVM must contain at least d^2 distinct operators $\hat{E}_i$. An informationally complete POVM is said to be *symmetric informationally complete* (or SIC) if it contains exactly this minimal number of distinct operators and if, in addition,

(1) $\lambda\hat{E}_i$ is a one-dimensional projector for all i and some fixed constant λ,

a)Electronic mail: d.m.appleby@qmul.ac.uk

(2) the overlap $\mathrm{Tr}(\hat{E}_i\hat{E}_j)$ is the same for every pair of distinct labels i,j.

It is straightforward to show that this is equivalent to the requirement that, for each i,

$$\hat{E}_i = \frac{1}{d}|\psi_i\rangle\langle\psi_i|, \tag{1}$$

where the d^2 vectors $|\psi_i\rangle$ satisfy

$$|\langle\psi_i|\psi_j\rangle| = \begin{cases} 1, & i = j, \\ \dfrac{1}{\sqrt{d+1}}, & i \neq j. \end{cases} \tag{2}$$

SIC–POVMs were introduced in a dissertation by Zauner,[16] and in Renes *et al.*[17] Wootters,[18] Bengtsson and Ericsson,[19,20] and Grassl[21] have made further contributions. There appear to be some intimate connections with the theory of mutually unbiased bases,[18,22,23] finite affine planes,[18–20] and polytopes.[19,20]

If SIC–POVMs existed in every finite dimension (or, failing that, in a sufficiently large set of finite dimensions) they would constitute a naturally distinguished class of POVMs which might be expected to have many interesting applications to quantum tomography, cryptography, and information theory generally. They would also be obvious candidates for the "fiducial" or "standard" POVMs featuring in the work of Fuchs[13] and Hardy.[14,15]

The question consequently arises, is it in fact true that SIC–POVMs exist in every finite dimension? The answer to this question is still unknown. Analytic solutions to Eqs. (2) have been constructed in dimensions 2, 3, 4, 5, 6, and 8. Moreover Renes *et al.*[17] have constructed numerical solutions in dimensions 5 to 45 (the actual vectors can be downloaded from their website[24]). So one may plausibly speculate that SIC–POVMs exist in every finite dimension. But it has not been proved.

With one exception, the SIC–POVMs which have so far been explicitly described in the literature are all covariant under the action of the generalized Pauli group (or Weyl–Heisenberg group, as it is often called). (The exception being the solution in dimension 8 described in Zauner's thesis.[16] Renes *et al.*[17] also mention that they have constructed numerical solutions which are covariant under the action of other groups, but they do not give any details.) It is therefore natural to investigate their behavior under the action of the extended Clifford group. The Clifford group proper is defined to be the normalizer of the generalized Pauli group, considered as a subgroup of $\mathrm{U}(d)$ (the group consisting of all unitary operators in dimension d). It is relevant to a number of areas of quantum information theory, and it has been extensively discussed in the literature.[25–31] Its relevance to the SIC–POVM problem has been stressed by Grassl.[21] As Grassl notes, it is related to the Jacobi group,[32] which has attracted some notice in the pure mathematical literature. We define the extended Clifford group to be the group which results when the Clifford group is enlarged, so as to include all *anti*unitary operators which normalize the generalized Pauli group. As we will see, this enlargement is essential if one wants to achieve a full understanding of the SIC–POVM problem.

In Secs. II–IV we give a self-contained account of the structure of the extended Clifford group. In the course of this discussion we obtain a number of results concerning the structure of the Clifford group proper which, to the best of our knowledge, have not previously appeared in the literature and which may be of some independent interest.

In Sec. V we define and establish some of the properties of a function we call the Clifford trace. We also identify a distinguished class of order 3 Clifford unitaries for which the Clifford trace$=-1$. We refer to these as *canonical* order 3 unitaries.

In Sec. VI we analyze the vectors constructed numerically by Renes *et al.*[17] (RBSC in the sequel) in dimension 5–45. We show that each of them is an eigenvector of a canonical order 3 Clifford unitary. This suggests the conjecture, that *every* GP fiducial vector is an eigenvector of a canonical order 3 unitary. We also show that, with one exception, the stability group of each RBSC

vector is order 3 (the exception being dimension 7, where the stability group is order 6).

In Sec. VII we show that RBSC's results also support a strengthened version of a conjecture of Zauner's[16] (also see Grassl[21]).

In Sec. VIII we use RBSC's numerical data, regarding the total number of fiducial vectors in dimensions 2–7, to give a complete characterization of the orbits and stability groups in dimensions 2–7. Our results show that in each of these dimensions *every* fiducial vector covariant under the action of the generalized Pauli group is an eigenvector of a canonical order 3 Clifford unitary. We also identify the total number of distinct orbits. It was already known[16,17,21] that there are infinitely many orbits in dimension 3, and one orbit in dimensions 2 and 6. We show that there is, likewise, only one orbit in dimensions 4 and 5, but two distinct orbits in dimension 7. We also construct exact expressions for two fiducial vectors in dimension 7 (one on each of the two distinct orbits).

RBSC's numerical data may suggest that, after dimension 7, the stability group of every fiducial vector has order 3. In Sec. IX we show that there is at least one exception to that putative rule by constructing an exact expression for a fiducial vector in dimension 19 for which the stability group has order $\geqslant 18$.

Our construction of exact solutions in dimensions 7 and 19 was facilitated by the fact that in these dimensions there exist canonical order 3 unitaries having a particularly simple form. In Sec. X we show that a similar simplification occurs in every dimension d for which (a) d has at least one prime factor $=1 \pmod 3$, (b) d has no prime factors $=2 \pmod 3$, and (c) d is not divisible by 9. In other words, it happens when $d=7,13,19,21,31,\ldots$.

II. FIDUCIAL VECTORS FOR THE GENERALIZED PAULI GROUP

The SIC–POVMs which have been constructed to date all have a certain group covariance property. Let G be a finite group having d^2 elements, and suppose we have an injective map $g \rightarrow \hat{U}_g$ which associates to each $g \in G$ a unitary operator $\hat{U}_g$ acting on d-dimensional Hilbert space. Suppose that for all g, g',

$$\hat{U}_g \hat{U}_{g'} = e^{i\xi_{gg'}} \hat{U}_{gg'}, \tag{3}$$

where $e^{i\xi_{gg'}}$ is a phase [so the map defines a group homomorphism of G into the quotient group $\mathrm{U}(d)/\mathrm{U}_c(d)$, where $\mathrm{U}_c(d)$ is the center of $\mathrm{U}(d)$]. (In other words it defines a projective representation of the group G. Such representations also play an important role in the theory of "nice" error bases.[33–35]) Finally (and this, of course, is the difficult part) suppose we can find a vector $|\psi\rangle \in \mathbb{C}^d$ such that $\langle\psi|\psi\rangle = 1$ and

$$|\langle\psi|\hat{U}_g|\psi\rangle| = \frac{1}{\sqrt{d+1}} \tag{4}$$

for all $g \neq e$ (e being the identity of G). Then the assignment

$$\hat{E}_g = \frac{1}{d}\hat{U}_g|\psi\rangle\langle\psi|\hat{U}_g^\dagger \tag{5}$$

defines a SIC–POVM on $\mathbb{C}^d$. The vector $|\psi\rangle$ is said to be a *fiducial vector*.

To date attention has been largely focussed on the case $G=(\mathbb{Z}_d)^2$, where $\mathbb{Z}_d$ is the set of integers 0,1, …, $d-1$ under addition *modulo d* (although there is numerical evidence that fiducial vectors exist for other choices of group[17]). That is also the case on which we will focus here.

To construct a suitable map $(\mathbb{Z}_d)^2 \rightarrow \mathrm{U}(d)$, let $|e_0\rangle, |e_1\rangle, \ldots |e_{d-1}\rangle$ be an orthonormal basis for $\mathbb{C}^d$, and let $\hat{T}$ be the operator defined by

$$\hat{T}|e_r\rangle = \omega^r|e_r\rangle, \tag{6}$$

where $\omega = e^{2\pi i/d}$. Let $\hat{S}$ be the shift operator

$$\hat{S}|e_r\rangle = \begin{cases} |e_{r+1}\rangle & r = 0,1,\ldots,d-2, \\ |e_0\rangle & r = d-1. \end{cases} \tag{7}$$

Then define, for each pair of integers $\mathbf{p}=(p_1,p_2)\in\mathbb{Z}^2$,

$$\hat{D}_{\mathbf{p}} = \tau^{p_1 p_2}\hat{S}^{p_1}\hat{T}^{p_2}, \tag{8}$$

where $\tau=-e^{\pi i/d}$ (the minus sign means that $\tau^{d^2}=1$ for all d, thereby simplifying some of the formulas needed in the sequel). We have, for all $\mathbf{p},\mathbf{q}\in\mathbb{Z}^2$,

$$\hat{D}_{\mathbf{p}}^{\dagger} = \hat{D}_{-\mathbf{p}}, \tag{9}$$

$$\hat{D}_{\mathbf{p}}\hat{D}_{\mathbf{q}} = \tau^{\langle \mathbf{p},\mathbf{q}\rangle}\hat{D}_{\mathbf{p}+\mathbf{q}}, \tag{10}$$

and

$$\hat{D}_{\mathbf{p}+\mathrm{d}\mathbf{q}} = \begin{cases} \hat{D}_{\mathbf{p}} & \text{if } d \text{ is odd}, \\ (-1)^{\langle \mathbf{p},\mathbf{q}\rangle}\hat{D}_{\mathbf{p}} & \text{if } d \text{ is even}, \end{cases} \tag{11}$$

where $\langle \mathbf{p},\mathbf{q}\rangle$ is the symplectic form

$$\langle \mathbf{p},\mathbf{q}\rangle = p_2 q_1 - p_1 q_2. \tag{12}$$

Consequently the map $\mathbf{p}\in(\mathbb{Z}_d)^2\to\hat{D}_{\mathbf{p}}\in \mathrm{U}(d)$ has all the required properties. The operators $\hat{D}_{\mathbf{p}}$ are sometimes called generalized Pauli matrices. So we will say that a vector $|\psi\rangle\in\mathbb{C}^d$ is a generalized Pauli fiducial vector, or *GP fiducial vector* for short, if it is a fiducial vector relative to the action of these operators, i.e., if $\langle\psi|\psi\rangle=1$ and

$$|\langle\psi|\hat{D}_{\mathbf{p}}|\psi\rangle| = \frac{1}{\sqrt{d+1}} \tag{13}$$

for every $\mathbf{p}\in\mathbb{Z}^2\neq\mathbf{0}(\mathrm{mod}\ d)$.

The set of operators $\hat{D}_{\mathbf{p}}$ is not a group. However, it becomes a group if we allow each $\hat{D}_{\mathbf{p}}$ to be multiplied by an arbitrary phase. We will refer to the group $\mathrm{GP}(d)=\{e^{i\xi}\hat{D}_{\mathbf{p}}:\xi\in\mathbb{R},\mathbf{p}\in\mathbb{Z}^2\}$ so obtained as the generalized Pauli group. **(**Also known as the Weyl–Heisenberg group. Our definition is, perhaps, slightly unconventional. It would be more usual to define $\mathrm{GP}(d)=\{\tau^n\hat{D}_{\mathbf{p}}:n\in\mathbb{Z},\mathbf{p}\in\mathbb{Z}^2\}$—i.e., the subgroup generated by the operators $\hat{D}_{\mathbf{p}}$. It appears to us that our definition, and our corresponding definition of the group $\mathrm{C}(d)$ (see below), make the analysis (slightly) simpler. It will be observed that on our definitions $\mathrm{GP}(d)$ and $\mathrm{C}(d)$ are both infinite. For some purposes this might be considered a disadvantage. However, in this paper we are really only interested in the groups which result when the phases are factored out. Consequently, it makes no important difference whether one adopts our definitions [on which $\mathrm{GP}(d)$ and $\mathrm{C}(d)$ are infinite] or the more conventional definitions (on which they are finite).**)**

We now want to investigate the normalizer of $\mathrm{GP}(d)$, i.e., the group $\mathrm{C}(d)$ consisting of all unitary operators $\hat{U}\in\mathrm{U}(d)$ with the property

$$\hat{U}\,\mathrm{GP}(d)\hat{U}^{\dagger} = \mathrm{GP}(d). \tag{14}$$

The significance of this group for us is that it generates automorphisms of $\mathrm{GP}(d)$ according to the prescription

$$\hat{P}\to\hat{U}\hat{P}\hat{U}^{\dagger}. \tag{15}$$

Consequently, if $|\psi\rangle$ is a GP fiducial vector, then so is $\hat{U}|\psi\rangle$ for every $\hat{U}\in\mathrm{C}(d)$.

The group $\mathrm{C}(d)$ is known as the Clifford group, and has been extensively discussed in the literature.[25–31] Its relevance to the SIC–POVM problem has been stressed by Grassl.[21] However, none of these accounts derive all the results needed for our analysis of the RBSC vectors. In the interests of readability we give a unified treatment in the next section.

III. THE CLIFFORD GROUP: STRUCTURE, AND CALCULATION OF THE UNITARIES

We begin with some definitions. Let

$$\overline{d} = \begin{cases} d & \text{if } d \text{ is odd,} \\ 2d & \text{if } d \text{ is even.} \end{cases} \tag{16}$$

Let $\mathrm{SL}(2,\mathbb{Z}_{\overline{d}})$ be the group consisting of all 2×2 matrices,

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}, \tag{17}$$

such that $\alpha,\beta,\gamma,\delta \in \mathbb{Z}_{\overline{d}}$ and $\alpha\delta-\beta\gamma=1 \pmod{\overline{d}}$. Note that inverses exist in this group because the condition $\alpha\delta-\beta\gamma=1 \pmod{\overline{d}}$ implies

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}\begin{pmatrix} \delta & -\beta \\ -\gamma & \alpha \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{18}$$

in arithmetic *modulo* $\overline{d}$.

We then have the following.

Lemma 1: For each unitary operator $\hat{U} \in \mathrm{C}(d)$ *there exists a matrix* $F \in \mathrm{SL}(2,\mathbb{Z}_{\overline{d}})$ *and a vector* $\boldsymbol{\chi} \in (\mathbb{Z}_d)^2$ *such that*

$$\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^{\dagger} = \omega^{\langle \boldsymbol{\chi}, F\mathbf{p}\rangle}\hat{D}_{F\mathbf{p}} \tag{19}$$

for all $\mathbf{p} \in \mathbb{Z}^2$ *(where* $\omega=\tau^2=e^{2\pi i/d}$*, as before).*

Proof: If $\hat{U} \in \mathrm{C}(d)$ it is immediate that there exist functions f and g such that

$$\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^{\dagger} = e^{ig(\mathbf{p})}\hat{D}_{f(\mathbf{p})} \tag{20}$$

for all $\mathbf{p} \in \mathbb{Z}^2$. It follows from Eq. (10) that

$$(e^{ig(\mathbf{p})}\hat{D}_{f(\mathbf{p})})(e^{ig(\mathbf{q})}\hat{D}_{f(\mathbf{q})}) = \tau^{\langle \mathbf{p},\mathbf{q}\rangle}(e^{ig(\mathbf{p}+\mathbf{q})}\hat{D}_{f(\mathbf{p}+\mathbf{q})}) \tag{21}$$

for all $\mathbf{p},\mathbf{q} \in \mathbb{Z}^2$. Consequently

$$e^{i(g(\mathbf{p})+g(\mathbf{q}))}\tau^{\langle f(\mathbf{p}),f(\mathbf{q})\rangle}\hat{D}_{f(\mathbf{p})+f(\mathbf{q})} = e^{ig(\mathbf{p}+\mathbf{q})}\tau^{\langle \mathbf{p},\mathbf{q}\rangle}\hat{D}_{f(\mathbf{p}+\mathbf{q})} \tag{22}$$

which implies $f(\mathbf{p}+\mathbf{q})=f(\mathbf{p})+f(\mathbf{q})(\mathrm{mod}\, d)$. We may therefore write

$$f(\mathbf{p}) = F'\mathbf{p} + \mathrm{d}h(\mathbf{p}) \tag{23}$$

for some matrix F' and function h. Inserting this expression in Eq. (20) gives, in view of Eq. (11),

$$\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^{\dagger} = e^{ig(\mathbf{p})}\hat{D}_{F'\mathbf{p}+\mathrm{d}h(\mathbf{p})} = \begin{cases} e^{ig(\mathbf{p})}\hat{D}_{F'\mathbf{p}}, & d \text{ odd} \\ e^{ig(\mathbf{p})}(-1)^{\langle \mathbf{p},h(\mathbf{p})\rangle}\hat{D}_{F'\mathbf{p}}, & d \text{ even.} \end{cases} \tag{24}$$

With the appropriate definition of g' this means

$$\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^{\dagger} = e^{ig'(\mathbf{p})}\hat{D}_{F'\mathbf{p}} \tag{25}$$

for all $\mathbf{p}$. Repeating the argument which led to Eq. (22) we find

$$e^{ig'(\mathbf{p}+\mathbf{q})-g'(\mathbf{p})-g'(\mathbf{q})}\tau^{\langle \mathbf{p},\mathbf{q}\rangle-\langle F'\mathbf{p},F'\mathbf{q}\rangle} = 1. \tag{26}$$

Interchanging $\mathbf{p}$ and $\mathbf{q}$ gives

$$e^{ig'(\mathbf{p}+\mathbf{q})-g'(\mathbf{p})-g'(\mathbf{q})}\tau^{-\langle \mathbf{p},\mathbf{q}\rangle+\langle F'\mathbf{p},F'\mathbf{q}\rangle} = 1, \tag{27}$$

We consequently require

$$\omega^{\langle \mathbf{p},\mathbf{q}\rangle-\langle F'\mathbf{p},F'\mathbf{q}\rangle} = \tau^{2(\langle \mathbf{p},\mathbf{q}\rangle-\langle F'\mathbf{p},F'\mathbf{q}\rangle)} = 1 \tag{28}$$

for all $\mathbf{p},\mathbf{q}$. It is readily verified that $\langle F'\mathbf{p},F'\mathbf{q}\rangle = (\mathrm{Det}\, F')\langle \mathbf{p},\mathbf{q}\rangle$. We must therefore have

$$\mathrm{Det}\, F' = 1 (\mathrm{mod}\, d). \tag{29}$$

If d is odd, or if d is even and $\mathrm{Det}\, F' = 1 (\mathrm{mod}\, \overline{d})$, we can find a matrix $F \in \mathrm{SL}(2,\mathbb{Z}_{\overline{d}})$ such that $F = F' (\mathrm{mod}\, \overline{d})$. It then follows from Eq. (11) that $\hat{D}_{F\mathbf{p}} = \hat{D}_{F'\mathbf{p}}$ for all $\mathbf{p}$.

Suppose, on the other hand, d is even and $\mathrm{Det}\, F' \neq 1 (\mathrm{mod}\, \overline{d})$. Then $\mathrm{Det}\, F' = d+1 (\mathrm{mod}\, \overline{d})$. Write

$$F' = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}. \tag{30}$$

We know $\alpha\delta - \beta\gamma = \mathrm{Det}\, F'$ is odd. So either α, δ are both odd, or else β, γ are both odd. If α, δ are both odd let

$$\Delta = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{31}$$

while if β, γ are both odd let

$$\Delta = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \tag{32}$$

Then $\mathrm{Det}(F' + \mathrm{d}\Delta) = 1 (\mathrm{mod}\, \overline{d})$. We can therefore choose a matrix $F \in \mathrm{SL}(2,\mathbb{Z}_{\overline{d}})$ such that $F = F' + \mathrm{d}\Delta (\mathrm{mod}\, \overline{d})$. Inserting this expression in Eq. (25) we have, in view of Eq. (11),

$$\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^{\dagger} = e^{ig'(\mathbf{p})}\hat{D}_{(F-\mathrm{d}\Delta)\mathbf{p}} = e^{ig'(\mathbf{p})}(-1)^{\langle F\mathbf{p},\Delta\mathbf{p}\rangle}\hat{D}_{F\mathbf{p}}. \tag{33}$$

We conclude that there is, in every case, a function g'' and a matrix $F \in \mathrm{SL}(2,\mathbb{Z}_{\overline{d}})$ such that

$$\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^{\dagger} = e^{ig''(\mathbf{p})}\hat{D}_{F\mathbf{p}} \tag{34}$$

for all $\mathbf{p}$.

It remains to establish the form of the function g''. We note, first of all, that it follows from Eqs. (8) and (10) that

$$(\hat{D}_{\mathbf{p}})^d = \hat{D}_{\mathrm{d}\mathbf{p}} = \tau^{d^2 p_1 p_2}\hat{S}^{\mathrm{d}p_1}\hat{T}^{\mathrm{d}p_2} = 1 \tag{35}$$

for all $\mathbf{p}$ (because $\hat{S}^d = \hat{T}^d = \tau^{d^2} = 1$). Consequently,

$$1 = \hat{U}(\hat{D}_{\mathbf{p}})^d\hat{U}^\dagger = (\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^\dagger)^d = e^{i\,dg''(\mathbf{p})}(\hat{D}_{F\mathbf{p}})^d = e^{i\,dg''(\mathbf{p})} \tag{36}$$

for all $\mathbf{p}$. We must therefore have $e^{ig''(\mathbf{p})} = \omega^{\tilde{g}(\mathbf{p})}$ for some function $\tilde{g}$ taking values in $\mathbb{Z}_d$. Repeating the argument which led to Eq. (26) we find

$$\omega^{\tilde{g}(\mathbf{p}+\mathbf{q})-\tilde{g}(\mathbf{p})-\tilde{g}(\mathbf{q})}\tau^{\langle\mathbf{p},\mathbf{q}\rangle-\langle F\mathbf{p},F\mathbf{q}\rangle} = 1. \tag{37}$$

We have $\langle\mathbf{p},\mathbf{q}\rangle - \langle F\mathbf{p},F\mathbf{q}\rangle = (1-\mathrm{Det}\,F)\langle\mathbf{p},\mathbf{q}\rangle = 0 \pmod{\overline{d}}$. Consequently, $\tau^{\langle\mathbf{p},\mathbf{q}\rangle-\langle F\mathbf{p},F\mathbf{q}\rangle'} = 1$ (because $\tau^{\overline{d}} = 1$) and so

$$\tilde{g}(\mathbf{p}+\mathbf{q}) = \tilde{g}(\mathbf{p}) + \tilde{g}(\mathbf{q}) (\mathrm{mod}\, d) \tag{38}$$

for all $\mathbf{p},\mathbf{q}$. This implies $\tilde{g}(\mathbf{p}) = \langle\boldsymbol{\chi}',\mathbf{p}\rangle \pmod d$ for all $\mathbf{p}$ some fixed $\boldsymbol{\chi}' \in (\mathbb{Z}_d)^2$. Setting $\boldsymbol{\chi} = F\boldsymbol{\chi}'$, and using the fact that $\langle F^{-1}\boldsymbol{\chi},\mathbf{p}\rangle = \langle\boldsymbol{\chi},F\mathbf{p}\rangle \pmod d$ we conclude

$$\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^\dagger = \omega^{\langle\boldsymbol{\chi},F\mathbf{p}\rangle}\hat{D}_{F\mathbf{p}} \tag{39}$$

for all $\mathbf{p}$. □

We now want to prove the converse of Lemma 1. That is, we want to prove that, for each pair $F \in \mathrm{SL}(2,\mathbb{Z}_{\overline{d}})$ and $\boldsymbol{\chi} \in (\mathbb{Z}_d)^2$ there is a corresponding operator $\hat{U} \in \mathrm{C}(d)$. We also want to derive an explicit expression for the operator $\hat{U}$ (this has, in effect, already been done by Hostens *et al.*;[29] however, the formulas we derive are different, and better adapted to the questions addressed in this paper).

We begin by focussing on a special class of matrices F. Let $[n_1,n_2,\ldots,n_r]$ denote the GCD (greatest common divisor) of the integers $n_1,n_2,\ldots,n_r$. We define the class of *prime matrices* to be the set of all matrices

$$F = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \tag{40}$$

$\in \mathrm{SL}(2,\mathbb{Z}_{\overline{d}})$ such that $[\beta,\overline{d}] = 1$ (so that β has a multiplicative inverse in $\mathbb{Z}_{\overline{d}}$). We then have the following.

Lemma 2: Let

$$F = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \tag{41}$$

be a prime matrix $\in \mathrm{SL}(2,\mathbb{Z}_{\overline{d}})$. *Let*

$$\hat{V}_F = \frac{1}{\sqrt{d}}\sum_{r,s=0}^{d-1}\tau^{\beta^{-1}(\alpha s^2-2rs+\delta r^2)}|e_r\rangle\langle e_s| \tag{42}$$

[where $\beta^{-1} \in \mathbb{Z}_{\overline{d}}$ *is such that* $\beta^{-1}\beta = 1 \pmod{\overline{d}}$*]. Then* $\hat{V}_F$ *is a unitary operator* $\in \mathrm{C}(d)$ *such that*

$$\hat{V}_F\hat{D}_{\mathbf{p}}\hat{V}_F^\dagger = \hat{D}_{F\mathbf{p}} \tag{43}$$

for all $\mathbf{p}$.

Proof: Let

$$\hat{S}' = \hat{D}_{(\alpha,\gamma)} \quad \text{and } \hat{T}' = \hat{D}_{(\beta,\delta)}. \tag{44}$$

We proceed by constructing a complete set of eigenvectors for $\hat{T}'$. It turns out that $\hat{S}'$ is the shift operator for these eigenvectors. It is then straightforward to verify that $\hat{V}_F$ has the stated property.

Define

$$|f_0\rangle = \frac{1}{\sqrt{d}} \sum_{r=0}^{d-1} (\hat{T}')^r |e_0\rangle. \tag{45}$$

It follows from Eq. (35) that $(\hat{T}')^d = 1$. Consequently

$$\hat{T}'|f_0\rangle = |f_0\rangle. \tag{46}$$

It follows from Eq. (10) that $\hat{T}'\hat{S}' = \omega \hat{S}'\hat{T}'$. So we can obtain a complete set of eigenvectors by laddering. Specifically, let

$$|f_r\rangle = (\hat{S}')^r |f_0\rangle \tag{47}$$

for $r = 1, \ldots, d-1$. Then

$$\hat{T}'|f_r\rangle = \omega^r |f_r\rangle \tag{48}$$

for all r. Since $(\hat{S}')^d = 1$ [as follows from Eq. (35)] we also have

$$\hat{S}'|f_r\rangle = |f_{r \oplus_d 1}\rangle \tag{49}$$

for all r (where $\oplus_d$ signifies addition *modulo d*).

We next show that the vectors $|f_r\rangle$ are orthonormal. It follows from Eqs. (6)–(8) and (10) that

$$(\hat{T}')^r |e_0\rangle = \hat{D}_{(r\beta, r\delta)} |e_0\rangle = \tau^{\beta\delta r^2} \hat{S}^{\beta r} |e_0\rangle \tag{50}$$

and consequently

$$|f_0\rangle = \left(\frac{1}{\sqrt{d}} \sum_{r=0}^{d-1} \tau^{\beta\delta r^2} \hat{S}^{\beta r} \right) |e_0\rangle = \left(\frac{1}{\sqrt{d}} \sum_{r=0}^{d-1} \tau^{\beta^{-1}\delta(\beta r)^2} \hat{S}^{\beta r} \right) |e_0\rangle \tag{51}$$

(where we have used the fact that $\tau^{\overline{d}} = 1$). We need to be careful at this point, due to the fact that congruence *modulo d* need not imply congruence *modulo* $\overline{d}$. Let q_r be the quotient of βr on division by d, and let t_r be the remainder. So $\beta r = q_r d + t_r$ and

$$|f_0\rangle = \left(\frac{1}{\sqrt{d}} \sum_{r=0}^{d-1} \tau^{\beta^{-1}\delta(q_r d + t_r)^2} \hat{S}^{q_r d + t_r} \right) |e_0\rangle. \tag{52}$$

We have

$$\hat{S}^{q_r d + t_r} = \hat{S}^{t_r} \tag{53}$$

and

$$\tau^{\beta^{-1}\delta(q_r d + t_r)^2} = \tau^{\beta^{-1}\delta(t_r^2 + 2d q_r t_r + d^2 t_r^2)} = \tau^{\beta^{-1}\delta t_r^2} \tag{54}$$

(because $\tau^{2d} = \tau^{d^2} = 1$). Consequently

$$|f_0\rangle = \left(\frac{1}{\sqrt{d}} \sum_{r=0}^{d-1} \tau^{\beta^{-1}\delta t_r^2} \hat{S}^{t_r} \right) |e_0\rangle = \frac{1}{\sqrt{d}} \sum_{r=0}^{d-1} \tau^{\beta^{-1}\delta t_r^2} |e_{t_r}\rangle. \tag{55}$$

The fact that $[\beta, \overline{d}] = 1$ implies that $[\beta, d] = 1$. It follows that, as r runs over the integers $0, 1, \ldots, d-1$, so does t_r (though not necessarily in the same order). Consequently

$$|f_0\rangle = \frac{1}{\sqrt{d}} \sum_{t=0}^{d-1} \tau^{\beta^{-1}\delta t^2} |e_t\rangle. \tag{56}$$

It follows that

$$\langle f_r | f_r \rangle = \langle f_0 | (\hat{S}')^{-r} (\hat{S}')^r | f_0 \rangle = \langle f_0 | f_0 \rangle = 1. \tag{57}$$

The fact that $\langle f_r | f_s \rangle = 0$ when $r \neq s$ is an immediate consequence of the fact that $|f_r\rangle, |f_s\rangle$ are eigenvectors of $\hat{T}'$ corresponding to different eigenvalues. We conclude that

$$\langle f_r | f_s \rangle = \delta_{rs} \tag{58}$$

as claimed.

We now want to calculate an explicit formula for $|f_r\rangle$ when $r > 0$. It follows from previous results that

$$|f_r\rangle = \hat{D}_{r\alpha, r\gamma} |f_0\rangle = \frac{1}{\sqrt{d}} \sum_{t=0}^{d-1} \tau^{\beta^{-1}\delta t^2 + \alpha\gamma r^2 + 2\gamma r t} (\hat{S})^{r\alpha} |e_t\rangle. \tag{59}$$

By an argument similar to the one leading to Eq. (56) we deduce

$$|f_r\rangle = \frac{1}{\sqrt{d}} \sum_{t=0}^{d-1} \tau^{\beta^{-1}\delta(t-\alpha r)^2 + \alpha\gamma r^2 + 2\gamma r(t-\alpha r)} |e_t\rangle \tag{60}$$

$$= \frac{1}{\sqrt{d}} \sum_{t=0}^{d-1} \tau^{\beta^{-1}(\delta t^2 - 2rt + \alpha r^2)} |e_t\rangle \tag{61}$$

[since $\alpha\delta - \beta\gamma = 1 \pmod{\overline{d}}$]. Comparing with Eq. (42) we see that

$$\hat{V}_F = \sum_{r=0}^{d-1} |f_r\rangle\langle e_r| \tag{62}$$

which shows that $\hat{V}_F$ is unitary. Moreover,

$$\hat{V}_F \hat{T} \hat{V}_F^\dagger |f_r\rangle = \hat{V}_F \hat{T} |e_r\rangle = \omega^r |f_r\rangle \tag{63}$$

for all r. Comparing with Eq. (48) we deduce $\hat{V}_F \hat{T} \hat{V}_F^\dagger = \hat{T}'$. Similarly $\hat{V}_F \hat{S} \hat{V}_F^\dagger = \hat{S}'$. Hence

$$\hat{V}_F \hat{D}_{\mathbf{p}} \hat{V}_F^\dagger = \tau^{p_1 p_2} \hat{V}_F \hat{S}^{p_1} \hat{T}^{p_2} \hat{V}_F^\dagger \tag{64}$$

$$= \tau^{p_1 p_2} \hat{D}_{\alpha p_1, \gamma p_1} \hat{D}_{\beta p_2, \delta p_2} \tag{65}$$

$$= \tau^{(1-\beta\gamma+\alpha\delta) p_1 p_2} \hat{D}_{F\mathbf{p}} \tag{66}$$

$$= \hat{D}_{F\mathbf{p}} \tag{67}$$

for all $\mathbf{p}$. □

To extend this result to the case of an arbitary matrix $\in \mathrm{SL}(2, \mathbb{Z}_{\overline{d}})$ we need the following decomposition lemma, which states that every nonprime matrix can be written as the product of two prime matrices.

Lemma 3: Let

$$F = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \tag{68}$$

be a nonprime matrix $\in \mathrm{SL}(2, \mathbb{Z}_{\overline{d}})$. *Then there exists an integer x such that* $\delta + x\beta$ *is nonzero and* $[\delta + x\beta, \overline{d}] = 1$. *Let x be any integer having that property, and let*

$$F_1 = \begin{pmatrix} 0 & -1 \\ 1 & x \end{pmatrix}, \tag{69}$$

$$F_2 = \begin{pmatrix} \gamma + x\alpha & \delta + x\beta \\ -\alpha & -\beta \end{pmatrix}. \tag{70}$$

Then F_1, F_2 *are prime matrices* $\in \mathrm{SL}(2, \mathbb{Z}_{\overline{d}})$ *such that*

$$F = F_1 F_2. \tag{71}$$

Proof: Suppose, to begin with, that β, δ are both nonzero. Let $k = [\beta, \delta]$. We then have

$$\beta = k\beta_0, \tag{72}$$

$$\delta = k\delta_0, \tag{73}$$

where $[\beta_0, \delta_0] = 1$. We also have $[k, \overline{d}] = 1$ [because $\alpha\delta - \beta\gamma = 1 (\mathrm{mod}\, \overline{d})$]. The fact that β_0, δ_0 are relatively prime means we can use Dirichlet's theorem (see, for example, Nathanson[36] or Rose[37]) to deduce that the sequence

$$\delta_0,\ (\delta_0 + \beta_0),\ (\delta_0 + 2\beta_0),\ \ldots \tag{74}$$

contains infinitely many primes. Consequently, there exists an integer x such that $\delta_0 + x\beta_0 \neq 0$ and $[\delta_0 + x\beta_0, \overline{d}] = 1$. The fact that $k \neq 0$ and $[k, \overline{d}] = 1$ then implies that $\delta + x\beta \neq 0$ and $[\delta + x\beta, \overline{d}] = 1$. The claim is now immediate.

It remains to consider the case when β, δ are not both nonzero. If $\delta = 0$ the fact that $\det F = 1 (\mathrm{mod}\, \overline{d})$ would imply that $\beta \neq 0$ and $[\beta, \overline{d}] = 1$—contrary to the assumption that the matrix F is nonprime. Suppose, on the other hand, that $\beta = 0$. Then the fact that $\det F = 1 (\mathrm{mod}\, \overline{d})$ implies that $\delta \neq 0$ and $[\delta, \overline{d}] = 1$. So the claim is true for every choice of x. □

We can now deduce the following converse of Lemma 1.

Lemma 4: Let $(F, \boldsymbol{\chi})$ *be any pair* $\in \mathrm{SL}(2, \mathbb{Z}_{\overline{d}}) \times (\mathbb{Z}_d)^2$. *If F is a prime matrix define*

$$\hat{U} = \hat{D}_{\boldsymbol{\chi}} \hat{V}_F \tag{75}$$

[where $\hat{V}_F$ *is the operator defined by Eq. (42)]. If F is nonprime choose two prime matrices* F_1, F_2 *such that* $F = F_1 F_2$ *(the existence of such matrices being guaranteed by Lemma 3), and define*

$$\hat{U} = \hat{D}_{\boldsymbol{\chi}} \hat{V}_{F_1} \hat{V}_{F_2} \tag{76}$$

[where $\hat{V}_{F_1}, \hat{V}_{F_2}$ *are the operators defined by Eq. (42)]. Then*

$$\hat{U} \hat{D}_{\mathbf{p}} \hat{U}^\dagger = \omega^{\langle \boldsymbol{\chi}, F\mathbf{p} \rangle} \hat{D}_{F\mathbf{p}} \tag{77}$$

for all $\mathbf{p} \in \mathbb{Z}^2$.

Proof: The claim is an immediate consequence of Eqs. (9) and (10) and Lemma 2. □

If $\hat{U}, \hat{U}'$ differ by a phase, so that $\hat{U}' = e^{i\theta} \hat{U}$, they have the same action on the generalized Pauli group,

$$\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^{\dagger} = \hat{U}'\hat{D}_{\mathbf{p}}\hat{U}'^{\dagger} \tag{78}$$

for all $\mathbf{p}$. So the object of real interest is not the Clifford group itself, but the group $\mathrm{C}(d)/\mathrm{I}(d)$ which results when the phases are factored out. Here $\mathrm{I}(d)$ is the subgroup consisting of all operators of the form $e^{i\theta}\hat{I}$, where $\hat{I}$ is the identity operator and $\theta \in \mathbb{R}$. The elements of $\mathrm{C}(d)/\mathrm{I}(d)$ are often called *Clifford operations.*

Let $\mathrm{SL}(2,\mathbb{Z}_d) \ltimes (\mathbb{Z}_d)^2$ be the canonical semidirect product of $\mathrm{SL}(2,\mathbb{Z}_d)$ and $(\mathbb{Z}_d)^2$, i.e., the group which results when the set $\mathrm{SL}(2,\mathbb{Z}_d) \times (\mathbb{Z}_d)^2$ is equipped with the composition rule

$$(F_1, \boldsymbol{\chi}_1) \circ (F_2, \boldsymbol{\chi}_2) = (F_1 F_2, \boldsymbol{\chi}_1 + F_1 \boldsymbol{\chi}_2). \tag{79}$$

Then we have the following structure theorem, which states that $\mathrm{C}(d)/\mathrm{I}(d)$ is naturally isomorphic to $\mathrm{SL}(2,\mathbb{Z}_d) \ltimes (\mathbb{Z}_d)^2$ when d is odd, and naturally isomorphic to a quotient group of $\mathrm{SL}(2,\mathbb{Z}_d) \ltimes (\mathbb{Z}_d)^2$ when d is even.

Theorem 1: *There exists a unique surjective homomorphism,*

$$f{:}\mathrm{SL}(2,\mathbb{Z}_d) \ltimes (\mathbb{Z}_d)^2 \to \mathrm{C}(d)/\mathrm{I}(d) \tag{80}$$

with the property $\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^{\dagger} = \omega^{\langle \boldsymbol{\chi}, F\mathbf{p}\rangle}\hat{D}_{F\mathbf{p}}$ *for each* $\hat{U} \in f(F, \boldsymbol{\chi})$ *and all* $\mathbf{p} \in \mathbb{Z}^2$.

If d is odd f is an isomorphism. If d is even the kernel of f is the subgroup $K_f \subseteq \mathrm{SL}(2,\mathbb{Z}_d) \ltimes (\mathbb{Z}_d)^2$ *consisting of the* 8 *elements of the form*

$$\left(\begin{pmatrix} 1+rd & sd \\ td & 1+rd \end{pmatrix}, \begin{pmatrix} sd/2 \\ td/2 \end{pmatrix} \right), \tag{81}$$

where $r, s, t = 0$ *or* 1.

Proof: An operator $\hat{U} \in \mathrm{C}(d)$ has the property

$$\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^{\dagger} = \hat{D}_{\mathbf{p}} \tag{82}$$

for all $\mathbf{p}$ if and only if it is a multiple of the identity (due to the irreducibility of the projective representation $\mathbf{p} \to \hat{D}_{\mathbf{p}}$, and Schur's lemma). So it follows from results already proved that there is exactly one surjective map,

$$f{:}\mathrm{SL}(2,\mathbb{Z}_d) \ltimes (\mathbb{Z}_d)^2 \to \mathrm{C}(d)/\mathrm{I}(d) \tag{83}$$

such that $\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^{\dagger} = \omega^{\langle \boldsymbol{\chi}, F\mathbf{p}\rangle}\hat{D}_{F\mathbf{p}}$ for each $\hat{U} \in f(F, \boldsymbol{\chi})$ and all $\mathbf{p} \in \mathbb{Z}^2$. The fact that f is actually a homomorphism is then an immediate consequence of the definitions.

Let K_f be the kernel of f. Then $(F, \boldsymbol{\chi}) \in K_f$ if and only if

$$\omega^{\langle \boldsymbol{\chi}, F\mathbf{p}\rangle}\hat{D}_{F\mathbf{p}} = \hat{D}_{\mathbf{p}} \tag{84}$$

for all $\mathbf{p}$. For that to be true we must have $F = 1 (\mathrm{mod}\, d)$. If d is odd this implies $\hat{D}_{F\mathbf{p}} = \hat{D}_{\mathbf{p}}$ for all $\mathbf{p}$. Equation (84) then becomes $\omega^{\langle \boldsymbol{\chi}, \mathbf{p}\rangle} = 1$ for all $\mathbf{p}$, implying $\boldsymbol{\chi} = (0\ 0)$. So the kernel is trivial, and f is an isomorphism as claimed.

Suppose, on the other hand, that d is even. The condition $F = 1 (\mathrm{mod}\, d)$ then implies that $F = 1 + \mathrm{d}\Delta$, where Δ is a matrix of the form

$$\Delta = \begin{pmatrix} r_1 & s \\ t & r_2 \end{pmatrix} \tag{85}$$

with $r_1, r_2, s, t = 0$ or 1. Inserting this expression in Eq. (84) we find, in view of Eqs. (9)–(11), that $(F, \boldsymbol{\chi}) \in K_f$ if and only if

$$1 = \omega^{\langle \boldsymbol{\chi}, F\mathbf{p}\rangle}\hat{D}_{F\mathbf{p}}\hat{D}_{-\mathbf{p}} = \omega^{\langle \boldsymbol{\chi},\mathbf{p}\rangle}\tau^{d\langle \mathbf{p},\Delta\mathbf{p}\rangle} \tag{86}$$

for all $\mathbf{p}$. After rearranging the condition

$$\omega^{\chi_2 p_1 - \chi_1 p_2} = (-1)^{(r_1-r_2)p_1p_2 - tp_1^2 + sp_2^2} = (-1)^{(r_1-r_2)p_1p_2 + tp_1 - sp_2} \tag{87}$$

for all $\mathbf{p}$. This is true if and only if $r_1 = r_2$, $\chi_1 = sd/2$, and $\chi_2 = td/2$. □

We conclude with a result concerning the order of the group $\mathrm{C}(d)/\mathrm{I}(d)$ which will be needed later on. Let $\nu(n,d)$ be the number of distinct ordered pairs $(x,y) \in (\mathbb{Z}_d)^2$ such that $xy = n \pmod d$. We then have the following.

Lemma 5: The order of the group $\mathrm{C}(d)/\mathrm{I}(d)$ *is*

$$|\mathrm{C}(d)/\mathrm{I}(d)| = d^2\left(\sum_{n=0}^{d-1} \nu(n,d)\,\nu(n+1,d)\right). \tag{88}$$

If d is a prime number this reduces to

$$|\mathrm{C}(d)/\mathrm{I}(d)| = d^3(d^2-1). \tag{89}$$

Proof: We begin by showing that $\mathrm{C}(d)/\mathrm{I}(d)$ and $\mathrm{SL}(2,\mathbb{Z}_d) \ltimes (\mathbb{Z}_d)^2$ have the same cardinality when considered as *sets*. This is true for all d, notwithstanding the fact that when d is even $\mathrm{C}(d)/\mathrm{I}(d)$ and $\mathrm{SL}(2,\mathbb{Z}_d) \ltimes (\mathbb{Z}_d)^2$ are not naturally isomorphic as *groups*.

The statement is immediate when d is odd. Suppose, on the other hand, that d is even. Let $g:\mathrm{SL}(2,\mathbb{Z}_{2d}) \to \mathrm{SL}(2,\mathbb{Z}_d)$ be the natural homomorphism defined by

$$g:\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \mapsto \begin{pmatrix} [\alpha]_d & [\beta]_d \\ [\gamma]_d & [\delta]_d \end{pmatrix}, \tag{90}$$

where $[x]_d$ denotes the residue class of x *modulo* d. It is easily seen that d is surjective. In fact, consider arbitrary

$$F = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \in \mathrm{SL}(2,\mathbb{Z}_d). \tag{91}$$

Then $\alpha\delta - \beta\gamma = 1 + nd$ for some integer n. If n is even then $F \in \mathrm{SL}(2,\mathbb{Z}_{\bar{d}})$ and $F = g(F)$. Suppose, on the other hand, that n is odd. Then either α or β is odd. If α is odd $F = g(F')$ where

$$F' = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta + d \end{pmatrix} \in \mathrm{SL}(2,\mathbb{Z}_{\bar{d}}) \tag{92}$$

while if β is odd $F = g(F'')$ where

$$F'' = \begin{pmatrix} \alpha & \beta \\ \gamma + d & \delta \end{pmatrix} \in \mathrm{SL}(2,\mathbb{Z}_{\bar{d}}). \tag{93}$$

Now let K_g be the kernel of g. A matrix $F \in K_g$ if and only if

$$F = \begin{pmatrix} 1 + r_1 d & sd \\ td & 1 + r_2 d \end{pmatrix}, \tag{94}$$

where $r_1, r_2, s, t = 0$ or 1 and $(1+r_1d)(1+r_2d) - std^2 = 1 \pmod{2d}$. We have

$$(1 + r_1 d)(1 + r_2 d) - std^2 = 1 + (r_1 + r_2)d \pmod{2d} \tag{95}$$

[bearing in mind that d is even, so $d^2 = 0 \pmod{2d}$]. We therefore require $r_1 = r_2$. It follows that K_g consists of the eight matrices of the form

$$\begin{pmatrix} 1+rd & sd \\ td & 1+rd \end{pmatrix}, \tag{96}$$

where $r,s,t=0$ or 1. The fact that g is surjective and $|K_g|=8$ implies $|\mathrm{SL}(2,\mathbb{Z}_{2d})|=8|\mathrm{SL}(2,\mathbb{Z}_d)|$. In view of Theorem 1 this means

$$|\mathrm{C}(d)/\mathrm{I}(d)| = \tfrac{1}{8}|\mathrm{SL}(2,\mathbb{Z}_{2d})||(\mathbb{Z}_d)^2| = |\mathrm{SL}(2,\mathbb{Z}_d)||(\mathbb{Z}_d)^2| = |\mathrm{SL}(2,\mathbb{Z}_d) \ltimes (\mathbb{Z}_d)^2| \tag{97}$$

as claimed.

We have shown that $|\mathrm{C}(d)/\mathrm{I}(d)|=|\mathrm{SL}(2,\mathbb{Z}_d)\ltimes(\mathbb{Z}_d)^2|=d^2|\mathrm{SL}(2,\mathbb{Z}_d)|$ for all d, odd or even. It remains to calculate $|\mathrm{SL}(2,\mathbb{Z}_d)|$. For each $n\in\mathbb{Z}_d$ let $M_n\subseteq\mathrm{SL}(2,\mathbb{Z}_d)$ be the set of matrices

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \tag{98}$$

for which $\alpha\delta=n+1(\mathrm{mod}\,d)$ and $\beta\gamma=n(\mathrm{mod}\,d)$. The sets M_n are disjoint. Moreover, $\mathrm{SL}(2,\mathbb{Z}_d)=\cup_{n=0}^{d-1}M_n$ and $|M_n|=\nu(n,d)\nu(n+1,d)$. It follows that

$$|\mathrm{SL}(2,\mathbb{Z}_d)| = \sum_{n=0}^{d-1} \nu(n,d)\nu(n+1,d). \tag{99}$$

Equation (88) is now immediate.

If d is a prime number

$$\nu(n,d) = \begin{cases} 2d-1 & \text{if } n=0 \ (\mathrm{mod}\,d), \\ d-1 & \text{otherwise} \end{cases} \tag{100}$$

implying

$$\sum_{n=0}^{d-1} \nu(n,d)\nu(n+1,d) = d(d^2-1). \tag{101}$$

Equation (89) is now immediate. □

IV. THE EXTENDED CLIFFORD GROUP

It can be seen from Eqs. (6)–(8) and (13) that, if $|\psi\rangle=\Sigma_{r=0}^{d-1}\psi_r|e_r\rangle$ is a GP fiducial vector, then so is the vector $|\psi^*\rangle=\Sigma_{r=0}^{d-1}\psi_r^*|e_r\rangle$ obtained by complex conjugation. So to make the analysis complete we need to consider automorphisms of GP(d) which are generated by antiunitary operators.

An antilinear operator is a map $\hat{L}:\mathbb{C}^d\to\mathbb{C}^d$ with the property

$$\hat{L}(\alpha|\phi\rangle+\beta|\psi\rangle) = \alpha^*\hat{L}|\phi\rangle + \beta^*\hat{L}|\psi\rangle \tag{102}$$

for all $|\phi\rangle,|\psi\rangle\in\mathbb{C}^d$ and all $\alpha,\beta\in\mathbb{C}$. The adjoint $\hat{L}^\dagger$ is defined to be the unique antilinear operator with the property

$$\langle\phi|\hat{L}^\dagger|\psi\rangle = \langle\psi|\hat{L}|\phi\rangle \tag{103}$$

for all $|\phi\rangle,|\psi\rangle\in\mathbb{C}^d$. [The existence and uniqueness of $\hat{L}^\dagger$ can be established by a variant of the argument which establishes the existence and uniqueness of the adjoint of a linear operator (see, for example, Greub[38]). Alternatively, one can exploit the operator $\hat{J}$ defined in Eq. (106). If $\hat{L}$ is antilinear then $\hat{L}\hat{J}$ is linear. So there exists a unique operator $(\hat{L}\hat{J})^\dagger$ with the property $\langle\phi|(\hat{L}\hat{J})^\dagger|\psi\rangle=(\langle\psi|(\hat{L}\hat{J})|\phi\rangle)^*$ for all $|\phi\rangle,|\psi\rangle$. It follows from the definition of $\hat{J}$ that $\langle\phi|\hat{J}|\psi\rangle=\langle\psi|\hat{J}|\phi\rangle$ for all $|\phi\rangle,|\psi\rangle$. It is now straightforward to confirm that, if one defines $\hat{L}^\dagger=\hat{J}(\hat{L}\hat{J})^\dagger$, then $\hat{L}^\dagger$ satisfies Eq. (103) for all $|\phi\rangle,|\psi\rangle$, and, furthermore, that there is no other operator with that

property.] An operator $\hat{U}$ is said to be antiunitary if it is antilinear and $\hat{U}^\dagger\hat{U}=1$ (or, equivalently, $\hat{U}\hat{U}^\dagger=1$).

We now define the *extended Clifford Group* to be the group $\mathrm{EC}(d)$ consisting of all unitary or antiunitary operators $\hat{U}$ having the property

$$\hat{U}\,\mathrm{GP}(d)\hat{U}^\dagger=\mathrm{GP}(d). \tag{104}$$

Let us also define $\mathrm{ESL}(2,\mathbb{Z}_{\bar{d}})$ to be the group consisting of all 2×2 matrices

$$\begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix} \tag{105}$$

such that $\alpha,\beta,\gamma,\delta\in\mathbb{Z}_{\bar{d}}$ and $\alpha\delta-\beta\gamma=\pm 1(\mathrm{mod}\,\bar{d})$. In the last section we showed that there is a natural homomorphism $f:\mathrm{SL}(2,\mathbb{Z}_{\bar{d}})\ltimes(\mathbb{Z}_d)^2\to\mathrm{C}(d)/\mathrm{I}(d)$. We are going to show that this extends to a natural homomorphism $f_E:\mathrm{ESL}(2,\mathbb{Z}_{\bar{d}})\ltimes(\mathbb{Z}_d)^2\to\mathrm{EC}(d)/\mathrm{I}(d)$.

Let $\hat{J}$ be the antilinear operator which replaces components in the standard basis with their complex conjugates,

$$\hat{J}:\sum_{r=0}^{d-1}\psi_r|e_r\rangle\mapsto\sum_{r=0}^{d-1}\psi_r^*|e_r\rangle. \tag{106}$$

Clearly $\hat{J}^\dagger=\hat{J}$ and $\hat{J}^\dagger\hat{J}=\hat{J}^2=1$. So $\hat{J}$ is an antiunitary operator. Furthermore, it follows from Eqs. (6)–(8) that

$$\hat{J}\hat{D}_{\mathbf{p}}\hat{J}^\dagger=\hat{D}_{\tilde{J}\mathbf{p}} \tag{107}$$

for all $\mathbf{p}$, where

$$\tilde{J}=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{108}$$

So $\hat{J}\in\mathrm{EC}(d)$. Note that $\mathrm{Det}\,\tilde{J}=-1(\mathrm{mod}\,\bar{d})$, so $\tilde{J}\in\mathrm{ESL}(2,\mathbb{Z}_{\bar{d}})$.

Now let $\mathrm{C}^*(d)$ be the set of antiunitary operators $\in\mathrm{EC}(d)$ [so $\mathrm{EC}(d)$ is the disjoint union $\mathrm{EC}(d)=\mathrm{C}(d)\cup\mathrm{C}^*(d)$]. The mapping $\hat{U}\mapsto\hat{J}\hat{U}$ defines a bijective correspondence between $\mathrm{C}^*(d)$ and $\mathrm{C}(d)$. We can use this to prove the following extension of Theorem 1.

Theorem 2: *There is a unique surjective homomorphism,*

$$f_E:\mathrm{ESL}(2,\mathbb{Z}_{\bar{d}})\ltimes(\mathbb{Z}_d)^2\to\mathrm{EC}(d)/\mathrm{I}(d) \tag{109}$$

such that, for each $(F,\boldsymbol{\chi})\in\mathrm{ESL}(2,\mathbb{Z}_{\bar{d}})\ltimes(\mathbb{Z}_d)^2$ *and* $\hat{U}\in f_E(F,\boldsymbol{\chi})$,

$$\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^\dagger=\omega^{\langle\boldsymbol{\chi},F\mathbf{p}\rangle}\hat{D}_{F\mathbf{p}} \tag{110}$$

for all $\mathbf{p}$. $\hat{U}$ *is unitary if* $\mathrm{Det}\,F=1(\mathit{mod}\,\bar{d})$ *and antiunitary if* $\mathrm{Det}\,F=-1(\mathit{mod}\,\bar{d})$. f_E *extends the homomorphism* f *defined in Theorem 1, and has the same kernel. So* f_E *is an isomorphism if* d *is odd, while if* d *is even its kernel is the subgroup* K_f *defined in Theorem 1.*

Proof: Let $\hat{U}$ be an arbitrary antiunitary operator $\in\mathrm{C}^*(d)$. The fact that $\hat{J},\hat{U}$ are both antiunitary means that $\hat{J}\hat{U}$ is unitary. So $\hat{J}\hat{U}\in\mathrm{C}(d)$. It then follows from Theorem 1 that there exists $(F',\boldsymbol{\chi}')\in\mathrm{SL}(2,\mathbb{Z}_{\bar{d}})\ltimes(\mathbb{Z}_d)^2$ such that

$$(\hat{J}\hat{U})\hat{D}_{\mathbf{p}}(\hat{J}\hat{U})^\dagger=\omega^{\langle\boldsymbol{\chi}',F'\mathbf{p}\rangle}\hat{D}_{F'\mathbf{p}} \tag{111}$$

for all $\mathbf{p}$. Define $F=\tilde{J}F'$ and $\boldsymbol{\chi}=\tilde{J}\boldsymbol{\chi}'$. In view of Eq. (107), and the fact that $\hat{J}^2=1$, we deduce

$$\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^{\dagger} = \hat{J}(\hat{J}\hat{U})\hat{D}_{\mathbf{p}}(\hat{J}\hat{U})^{\dagger}\hat{J}^{\dagger} = \omega^{-\langle \boldsymbol{\chi}', F'\mathbf{p}\rangle}\hat{D}_{\tilde{J}F'\mathbf{p}} = \omega^{\langle \boldsymbol{\chi}, F\mathbf{p}\rangle}\hat{D}_{F\mathbf{p}} \tag{112}$$

for all $\mathbf{p}$ (where we have used the fact that $\langle \boldsymbol{\xi}, \boldsymbol{\eta}\rangle = -\langle \tilde{J}\boldsymbol{\xi}, \tilde{J}\boldsymbol{\eta}\rangle$ for all $\boldsymbol{\xi}, \boldsymbol{\eta}$). We have $\mathrm{Det}(F) = (\mathrm{Det}\, J)(\mathrm{Det}\, F') = -1$, so $(F, \boldsymbol{\chi}) \in \mathrm{ESL}(2, \mathbb{Z}_{\bar{d}}) \ltimes (\mathbb{Z}_d)^2$.

Reversing the argument we deduce the converse proposition, for each $(F, \boldsymbol{\chi}) \in \mathrm{ESL}(2, \mathbb{Z}_{\bar{d}}) \ltimes (\mathbb{Z}_d)^2$, there exists $\hat{U} \in \mathrm{EC}(d)$ such that $\hat{U}\hat{D}_{\mathbf{p}}\hat{U}^{\dagger} = \omega^{\langle \boldsymbol{\chi}, F\mathbf{p}\rangle}\hat{D}_{F\mathbf{p}}$ for all $\mathbf{p}$. The fact that an operator commutes with $\hat{D}_{\mathbf{p}}$ for all $\mathbf{p}$ if and only if it is a multiple of the identity means that $\hat{U}$ is unique up to a phase.

This establishes the existence and uniqueness of the homomorphism f_E. The proof of the remaining statements is straightforward, and is left to the reader. □

Finally, we have the following result which, together with Lemma 5, enables us to calculate the order of $\mathrm{EC}(d)/\mathrm{I}(d)$.

Lemma 6:

$$\left|\mathrm{EC}(d)/\mathrm{I}(d)\right| = 2\left|\mathrm{C}(d)/\mathrm{I}(d)\right| \tag{113}$$

for all d.

Proof: The map

$$\hat{U}\mathrm{I}(d) \mapsto \hat{J}\hat{U}\mathrm{I}(d) \tag{114}$$

defines a bijective correspondence between $\mathrm{C}^*(d)/\mathrm{I}(d)$ and $\mathrm{C}(d)/\mathrm{I}(d)$. So the set $\mathrm{C}^*(d)/\mathrm{I}(d)$ contains the same number of elements as $\mathrm{C}(d)/\mathrm{I}(d)$. The statement is now immediate. □

V. THE CLIFFORD TRACE

We now define the Clifford trace. The significance of this function for us is that every GP fiducial vector which has been constructed to date is an eigenvector of a Clifford unitary having Clifford trace $=-1$.

Let $[F, \boldsymbol{\chi}] \in \mathrm{EC}(d)/\mathrm{I}(d)$ be the image of $(F, \boldsymbol{\chi})$ under the homomorphism f_E defined in Theorem 2. We refer to $[F, \boldsymbol{\chi}]$ as an extended Clifford operation [or Clifford operation if it $\in \mathrm{C}(d)/\mathrm{I}(d)$]. The operators $\in [F, \boldsymbol{\chi}]$ only differ by a phase. It is therefore convenient to adopt a terminology which blurs the distinction between the operation $[F, \boldsymbol{\chi}]$ and the operators $\hat{U} \in [F, \boldsymbol{\chi}]$. In particular, we will adopt the convention that properties which hold for each $\hat{U} \in [F, \boldsymbol{\chi}]$ may also be attributed to $[F, \boldsymbol{\chi}]$. Thus, we will say that $[F, \boldsymbol{\chi}]$ is unitary (respectively antiunitary) if the operators $\hat{U} \in [F, \boldsymbol{\chi}]$ are unitary (respectively, antiunitary). Similarly, we will say that $|\psi\rangle \in \mathbb{C}^d$ is an eigenvector of $[F, \boldsymbol{\chi}]$ if it is an eigenvector of the operators $\hat{U} \in [F, \boldsymbol{\chi}]$.

It is easily verified that $\mathrm{Tr}(F_1) = \mathrm{Tr}(F_2) \pmod{d}$ whenever $[F_1, \boldsymbol{\chi}_1] = [F_2, \boldsymbol{\chi}_2]$ [note that it is not necessarily true that $\mathrm{Tr}(F_1) = \mathrm{Tr}(F_2) \pmod{\bar{d}}$ if d is even]. We therefore obtain a well-defined function $\mathrm{EC}(d)/\mathrm{I}(d) \to \mathbb{Z}_d$ if we assign to each operation $[F, \boldsymbol{\chi}]$ the value $\mathrm{Tr}(F) \pmod{d}$. We obtain a function $\mathrm{EC}(d) \to \mathbb{Z}_d$ by assigning to each $\hat{U} \in [F, \boldsymbol{\chi}]$ the value $\mathrm{Tr}(F) \pmod{d}$. We use the term "Clifford trace" to refer to either of these functions. (The Clifford trace is a modular character in the case when d is prime. For the theory of modular representations see, for example, Serre.[39])

We now prove the main result of this section, which states that there is a connection between the order of a Clifford operation and its Clifford trace.

Lemma 7: Let $[F, \boldsymbol{\chi}] \in \mathrm{C}(d)/\mathrm{I}(d)$, *where d is any* dimension $\neq 3$. *Then* $[F, \boldsymbol{\chi}]$ *is of order* 3 *if* $\mathrm{Tr}(F) = -1 \ (mod\ d)$.

Let $[F, \boldsymbol{\chi}] \in \mathrm{C}(d)/\mathrm{I}(d)$, *where d is any* prime dimension $\neq 3$. *Then the stronger statement is true,* $[F, \boldsymbol{\chi}]$ *is of order* 3 *if and only if* $\mathrm{Tr}(F) = -1 \ (mod\ d)$.

Remark: The restriction to operations $\in \mathrm{C}(d)/\mathrm{I}(d)$ is essential (because if $[F, \boldsymbol{\chi}]$ is antiunitary its order must be even).

Proof: Let $[F, \boldsymbol{\chi}] \in \mathrm{C}(d)/\mathrm{I}(d)$, and let $\kappa = \mathrm{Tr}(F)$. Then, taking into account the fact that $\mathrm{Det}(F) = 1 \pmod{\bar{d}}$, it is straightforward to show

$$F^2 = \kappa F - 1 \pmod{\overline{d}} \tag{115}$$

implying

$$F^3 = (\kappa^2 - 1)F - \kappa \pmod{\overline{d}}, \tag{116}$$

$$1 + F + F^2 = (\kappa + 1)F \pmod{\overline{d}}. \tag{117}$$

Now suppose that $\kappa = -1 \pmod{d}$. Then there are three possibilities, (a) d is odd; (b) d is even and $\kappa = -1 \pmod{\overline{d}}$; (c) d is even and $\kappa = -1 + d \pmod{\overline{d}}$. In case (a) or (b) we have

$$F^3 = 1 \pmod{\overline{d}}, \tag{118}$$

$$1 + F + F^2 = 0 \pmod{\overline{d}}, \tag{119}$$

while in case (c) we have $\kappa^2 - 1 = d^2 - 2d = 0 \pmod{\overline{d}}$, and consequently

$$F^3 = \begin{pmatrix} 1+d & 0 \\ 0 & 1+d \end{pmatrix} \pmod{\overline{d}}, \tag{120}$$

$$1 + F + F^2 = 0 \pmod{d}. \tag{121}$$

Referring to the definition of K_f (see Theorem 1) we deduce that, in every case,

$$(F, \boldsymbol{\chi})^3 = (F^3, (1 + F + F^2)\boldsymbol{\chi}) \in K_f \tag{122}$$

implying that $[F, \boldsymbol{\chi}]^3 = [1, \mathbf{0}]$. It remains to show that neither $[F, \boldsymbol{\chi}]$ nor $[F, \boldsymbol{\chi}]^2 = [1, \mathbf{0}]$. To see that $[F, \boldsymbol{\chi}] \neq [1, \mathbf{0}]$ observe that the contrary would imply $-1 = \kappa = \mathrm{Tr}(1) = 2 \pmod{d}$, which is not possible given that $d \neq 3$. Similarly, if $[F, \boldsymbol{\chi}]^2 = [1, \mathbf{0}]$ it would follow [taking the trace on both sides of Eq. (115)] that $2 = \kappa^2 - 2 = -1 \pmod{d}$, contrary to the assumption that $d \neq 3$. We conclude that $[F, \boldsymbol{\chi}]$ is of order 3, as claimed.

To prove the second part of the lemma suppose that d is a prime number $\neq 3$ and $[F, \boldsymbol{\chi}]$ is of order 3. Then $(F^3, (1 + F + F^2)\boldsymbol{\chi}) \in K_f$, implying $F^3 = 1 \pmod{d}$. In view of Eq. (116) this means

$$(\kappa + 1)((\kappa - 1)F - 1) = 0 \pmod{d}. \tag{123}$$

We now proceed by *reductio ad absurdum*. Suppose that $\kappa \neq -1 \pmod{d}$. Then Eq. (123) and the fact that d is prime implies

$$(\kappa - 1)F = 1 \pmod{d}. \tag{124}$$

Taking the trace on both sides gives $(\kappa + 1)(\kappa - 2) = 0 \pmod{d}$ implying $\kappa = 2 \pmod{d}$. Substituting this value into Eq. (124) we deduce $F = 1 \pmod{d}$, implying $F^2 = 1 \pmod{\overline{d}}$ and $F^3 = F \pmod{\overline{d}}$. So

$$(F, 3\boldsymbol{\chi}) = (F, \boldsymbol{\chi})^3 \in K_f \tag{125}$$

implying $(F, \boldsymbol{\chi}) \in K_f$. But that would mean $[F, \boldsymbol{\chi}]$ is of order 1, contrary to assumption. We conclude that $\kappa = -1 \pmod{d}$, as claimed. □

The result does not hold when $d = 3$ because then the identity has Clifford trace $= -1$. It is, however, easily verified that in dimension 3 (as in every other prime dimension) every order 3 Clifford operation has Clifford trace $= -1$.

If d is not a prime number there may exist order 3 Clifford operations for which the Clifford trace $\neq -1$. Consider, for example,

$$[F,\boldsymbol{\chi}]=\left[\begin{pmatrix}5 & 4\\ 2 & -3\end{pmatrix},\begin{pmatrix}-4\\ 5\end{pmatrix}\right]\in \mathrm{C}(6)/\mathrm{I}(6). \tag{126}$$

Then $[F,\boldsymbol{\chi}]$ is of order 3 yet $\mathrm{Tr}(F)=2 \pmod 6$.

Because these results will play an important role in the following it is convenient to introduce some terminology. We will say that an operation $[F,\boldsymbol{\chi}]\in \mathrm{C}(d)/\mathrm{I}(d)$ is a *canonical* order 3 unitary if

(a) $\mathrm{Tr}(F)=-1 \pmod d$,
(b) F is not the identity matrix.

Note that the second stipulation is only needed because of the possibility that $d=3$. If $d\neq 3$ an operation $[F,\boldsymbol{\chi}]\in \mathrm{C}(d)/\mathrm{I}(d)$ is a canonical order 3 unitary if and only if $\mathrm{Tr}(F)=-1 \pmod d$.

VI. THE RBSC VECTORS

For $5\leqslant d\leqslant 45$ RBSC[17,24] have constructed GP fiducial vectors numerically. In this section we examine the behavior of these vectors under the action of the extended Clifford group. In particular we show that each of them is an eigenvector of a canonical order 3 Clifford unitary. This suggests the following.

Conjecture A: GP fiducial vectors exist in every finite dimension. Furthermore, every such vector is an eigenvector of a canonical order 3 unitary.

Conjecture A is related to a conjecture of Zauner's. Let

$$[Z,\mathbf{0}]=\left[\begin{pmatrix}0 & -1\\ 1 & -1\end{pmatrix},\begin{pmatrix}0\\ 0\end{pmatrix}\right]. \tag{127}$$

It will be observed that $[Z,\mathbf{0}]$ is defined, and $\in \mathrm{C}(d)/\mathrm{I}(d)$, for every dimension d, and that it is canonical order 3. Zauner[16] has conjectured the following.

Conjecture B: In each dimension d there exists a GP fiducial vector which is an eigenvector of $[Z,\mathbf{0}]$.

In Sec. VII we will see that RBSC's numerical data also provides further support for Conjecture B.

Let $|\psi_d\rangle$ be the RBSC vector in dimension d. In Table I we list, for each value of d, a unitary Clifford operation $[F_d,\boldsymbol{\chi}_d]$ having $|\psi_d\rangle$ as one of its eigenvectors (to the precision that RBSC's numerical data permits). It will be seen that, in every case, $\mathrm{Tr}(F_d)=-1 \pmod d$, implying that $[F_d,\boldsymbol{\chi}_d]$ is canonical order 3. Clearly, $|\psi_d\rangle$ is also an eigenvector of $[F_d,\boldsymbol{\chi}_d]^2$. Moreover, $[F_d,\boldsymbol{\chi}_d]^2$ also has Clifford trace$=-1$. $[F_d,\boldsymbol{\chi}_d]$ and $[F_d,\boldsymbol{\chi}_d]^2$ are, however, the only trace -1 unitary Clifford operations of which $|\psi_d\rangle$ is an eigenvector (to the stated degree of precision).

In Table I we also list (n_{d1},n_{d2},n_{d3}), the dimensions of the three eigenspaces of $[F_d,\boldsymbol{\chi}_d]$, and n_d, the dimension of the particular eigenspace to which $|\psi_d\rangle$ belongs. It will be seen that, with one exception, $|\psi_d\rangle$ always belongs to an eigenspace of highest dimension (the exception being $d=17$, where $|\psi_d\rangle$ belongs to the eigenspace of *lowest* dimension).

We used a computer algebra package (*Mathematica*) to construct the table. To illustrate the method employed we give a detailed description for the case $d=5$. We begin with the observation that, if $|\psi_5\rangle$ is an eigenvector of $[F,\boldsymbol{\chi}]$, then

$$\langle\psi_5|\hat{D}_{\mathbf{p}}|\psi_5\rangle=e^{(2\pi i/5)\langle\boldsymbol{\chi},F\mathbf{p}\rangle}\langle\psi_5|\hat{D}_{F\mathbf{p}}|\psi_5\rangle \tag{128}$$

for all $\mathbf{p}$. So, using the value of $|\psi_5\rangle$ which is available on RBSC's website,[24] we look for values of $\mathbf{p},\mathbf{q}$ such that

TABLE I. For each d the RBSC vector $|\psi_d\rangle$ is an eigenvector of the unitary operation $[F_d, \boldsymbol{\chi}_d]$. Note that in every case $\mathrm{Tr}\, F_d = -1$, implying that $[F_d, \boldsymbol{\chi}_d]$ is canonical order 3. (n_{d1}, n_{d2}, n_{d3}) are the dimensions of the three eigenspaces of $[F_d, \boldsymbol{\chi}_d]$, and n_d is the dimension of the eigenspace to which $|\psi_d\rangle$ belongs. Note that $n_d = \max(n_{d1}, n_{d2}, n_{d3})$, with the single exception of $d=17$.

d	F_d	$\boldsymbol{\chi}_d$	(n_{d1}, n_{d2}, n_{d3})	n_d	d	F_d	χ_d	(n_{d1}, n_{d2}, n_{d3})	n_d
5	$\begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 2 \\ 2 \end{pmatrix}$	(1,2,2)	2	26	$\begin{pmatrix} -7 & -9 \\ -1 & 6 \end{pmatrix}$	$\begin{pmatrix} -11 \\ 11 \end{pmatrix}$	(8,9,9)	9
6	$\begin{pmatrix} -2 & 3 \\ -1 & 1 \end{pmatrix}$	$\begin{pmatrix} 3 \\ 0 \end{pmatrix}$	(1,2,3)	3	27	$\begin{pmatrix} -10 & 1 \\ -10 & 9 \end{pmatrix}$	$\begin{pmatrix} -3 \\ -12 \end{pmatrix}$	(8,9,10)	10
7	$\begin{pmatrix} -2 & -2 \\ -2 & 1 \end{pmatrix}$	$\begin{pmatrix} 2 \\ 0 \end{pmatrix}$	(2,2,3)	3	28	$\begin{pmatrix} -3 & 21 \\ 5 & 2 \end{pmatrix}$	$\begin{pmatrix} -10 \\ -6 \end{pmatrix}$	(9,9,10)	10
8	$\begin{pmatrix} -4 & 3 \\ 1 & 3 \end{pmatrix}$	$\begin{pmatrix} 3 \\ -1 \end{pmatrix}$	(2,3,3)	3	29	$\begin{pmatrix} -13 & -6 \\ 2 & 12 \end{pmatrix}$	$\begin{pmatrix} -10 \\ 12 \end{pmatrix}$	(9,10,10)	10
9	$\begin{pmatrix} -3 & 2 \\ 1 & 2 \end{pmatrix}$	$\begin{pmatrix} 2 \\ 1 \end{pmatrix}$	(2,3,4)	4	30	$\begin{pmatrix} -8 & -7 \\ -9 & 7 \end{pmatrix}$	$\begin{pmatrix} 11 \\ -3 \end{pmatrix}$	(9,10,11)	11
10	$\begin{pmatrix} -4 & -7 \\ -1 & 3 \end{pmatrix}$	$\begin{pmatrix} -2 \\ 0 \end{pmatrix}$	(3,3,4)	4	31	$\begin{pmatrix} -9 & -10 \\ -2 & 8 \end{pmatrix}$	$\begin{pmatrix} -14 \\ 6 \end{pmatrix}$	(10,10,11)	11
11	$\begin{pmatrix} -5 & 4 \\ 3 & 4 \end{pmatrix}$	$\begin{pmatrix} -5 \\ 0 \end{pmatrix}$	(3,4,4)	4	32	$\begin{pmatrix} -11 & -31 \\ -15 & 10 \end{pmatrix}$	$\begin{pmatrix} 11 \\ -7 \end{pmatrix}$	(10,11,11)	11
12	$\begin{pmatrix} -4 & 11 \\ 1 & 3 \end{pmatrix}$	$\begin{pmatrix} 4 \\ -5 \end{pmatrix}$	(3,4,5)	5	33	$\begin{pmatrix} -7 & -5 \\ 2 & 6 \end{pmatrix}$	$\begin{pmatrix} 8 \\ -5 \end{pmatrix}$	(10,11,12)	12
13	$\begin{pmatrix} -2 & -2 \\ -5 & 1 \end{pmatrix}$	$\begin{pmatrix} 6 \\ 0 \end{pmatrix}$	(4,4,5)	5	34	$\begin{pmatrix} -12 & 3 \\ 1 & 11 \end{pmatrix}$	$\begin{pmatrix} -1 \\ -16 \end{pmatrix}$	(11,11,12)	12
14	$\begin{pmatrix} -2 & -3 \\ 1 & 1 \end{pmatrix}$	$\begin{pmatrix} -5 \\ 1 \end{pmatrix}$	(4,5,5)	5	35	$\begin{pmatrix} -13 & -12 \\ 16 & 12 \end{pmatrix}$	$\begin{pmatrix} 11 \\ -12 \end{pmatrix}$	(11,12,12)	12
15	$\begin{pmatrix} -5 & 1 \\ -6 & 4 \end{pmatrix}$	$\begin{pmatrix} -7 \\ -6 \end{pmatrix}$	(4,5,6)	6	36	$\begin{pmatrix} -8 & 21 \\ -13 & 7 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 7 \end{pmatrix}$	(11,12,13)	13
16	$\begin{pmatrix} -8 & 13 \\ 3 & 7 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	(5,5,6)	6	37	$\begin{pmatrix} -16 & 1 \\ 18 & 15 \end{pmatrix}$	$\begin{pmatrix} -4 \\ 3 \end{pmatrix}$	(12,12,13)	13
17	$\begin{pmatrix} -5 & -7 \\ 3 & 4 \end{pmatrix}$	$\begin{pmatrix} 6 \\ 7 \end{pmatrix}$	(5,6,6)	5	38	$\begin{pmatrix} -6 & -31 \\ 1 & 5 \end{pmatrix}$	$\begin{pmatrix} 12 \\ -10 \end{pmatrix}$	(12,13,13)	13
18	$\begin{pmatrix} -5 & 5 \\ 3 & 4 \end{pmatrix}$	$\begin{pmatrix} 9 \\ 0 \end{pmatrix}$	(5,6,7)	7	39	$\begin{pmatrix} -17 & -11 \\ 0 & 16 \end{pmatrix}$	$\begin{pmatrix} 8 \\ 15 \end{pmatrix}$	(12,13,14)	14
19	$\begin{pmatrix} -2 & 4 \\ 4 & 1 \end{pmatrix}$	$\begin{pmatrix} -7 \\ -4 \end{pmatrix}$	(6,6,7)	7	40	$\begin{pmatrix} -3 & 19 \\ -13 & 2 \end{pmatrix}$	$\begin{pmatrix} -12 \\ -19 \end{pmatrix}$	(13,13,14)	14
20	$\begin{pmatrix} -2 & -3 \\ 1 & 1 \end{pmatrix}$	$\begin{pmatrix} -9 \\ -6 \end{pmatrix}$	(6,7,7)	7	41	$\begin{pmatrix} -2 & -10 \\ -12 & 1 \end{pmatrix}$	$\begin{pmatrix} 19 \\ 13 \end{pmatrix}$	(13,14,14)	14
21	$\begin{pmatrix} -5 & -6 \\ -7 & 4 \end{pmatrix}$	$\begin{pmatrix} -6 \\ 1 \end{pmatrix}$	(6,7,8)	8	42	$\begin{pmatrix} -15 & 11 \\ 19 & 14 \end{pmatrix}$	$\begin{pmatrix} 0 \\ -15 \end{pmatrix}$	(13,14,15)	15
22	$\begin{pmatrix} -2 & -1 \\ 3 & 1 \end{pmatrix}$	$\begin{pmatrix} 8 \\ 2 \end{pmatrix}$	(7,7,8)	8	43	$\begin{pmatrix} -11 & 1 \\ 18 & 10 \end{pmatrix}$	$\begin{pmatrix} -1 \\ 21 \end{pmatrix}$	(14,14,15)	15
23	$\begin{pmatrix} -11 & -10 \\ -5 & 10 \end{pmatrix}$	$\begin{pmatrix} 0 \\ -3 \end{pmatrix}$	(7,8,8)	8	44	$\begin{pmatrix} -8 & -29 \\ 5 & 7 \end{pmatrix}$	$\begin{pmatrix} 16 \\ -5 \end{pmatrix}$	(14,15,15)	15

TABLE I. (*Continued.*)

d	F_d	$\boldsymbol{\chi}_d$	(n_{d1},n_{d2},n_{d3})	n_d	d	F_d	χ_d	(n_{d1},n_{d2},n_{d3})	n_d
24	$\begin{pmatrix}-2 & -3\\ 1 & 1\end{pmatrix}$	$\begin{pmatrix}0\\ -3\end{pmatrix}$	(7,8,9)	9	45	$\begin{pmatrix}-20 & -1\\ 21 & 19\end{pmatrix}$	$\begin{pmatrix}-8\\ 6\end{pmatrix}$	(14,15,16)	16
25	$\begin{pmatrix}-6 & -1\\ 6 & 5\end{pmatrix}$	$\begin{pmatrix}-7\\ 12\end{pmatrix}$	(8,8,9)	9					

$$\frac{5}{2\pi}(\arg(\langle\psi_5|\hat{D}_{\mathbf{p}}|\psi_5\rangle) - \arg(\langle\psi_5|\hat{D}_{\mathbf{q}}|\psi_5\rangle)) \tag{129}$$

is an (approximate) integer. We find that if $\mathbf{p}=(1,0)$ this is only true when $\mathbf{q}=(1,0)$, $(-1,1)$ or $(0,-1)$ (mod 5), and that if $\mathbf{p}=(0,1)$ it is only true when $\mathbf{q}=(0,1)$, $(-1,0)$ or $(1,-1)$ (mod 5). Taking account of the requirement $\mathrm{Det}(F)=1$ (mod 5) we deduce that the only candidates are (apart from the identity)

$$[F_5,\boldsymbol{\chi}_5] = \left[\begin{pmatrix}-1 & -1\\ 1 & 0\end{pmatrix},\begin{pmatrix}2\\ 2\end{pmatrix}\right] \tag{130}$$

and its square, $[F_5,\boldsymbol{\chi}_5]^2$. To check that $|\psi_5\rangle$ actually is an eigenvector of $[F_5,\boldsymbol{\chi}_5]$ we observe that F_5 is a prime matrix. So in view of Lemma 4 we have the following explicit formula for the $\hat{U}\in[F_5,\boldsymbol{\chi}_5]$:

$$\hat{U} = \frac{1}{\sqrt{5}}e^{i\theta}\hat{D}_{(2,2)}\left(\sum_{r,s=0}^{4} e^{-(4\pi i/5)s(s+2r)}|e_r\rangle\langle e_s|\right) \tag{131}$$

$e^{i\theta}$ being an arbitrary phase. Suppose we choose $\theta=7\pi/15$. Then we find $\hat{U}^3=1$ and

$$\|(\hat{U}-1)|\psi_5\rangle\|^2 = 0 \tag{132}$$

to machine precision. This confirms that $|\psi_5\rangle$ is indeed an eigenvector of $[F_5,\boldsymbol{\chi}_5]$. To calculate the dimensions of the eigenspaces define, for $r=0,\pm1$ (and with the same choice of θ),

$$\hat{P}_r = \tfrac{1}{3}(1 + e^{-2r\pi i/3}\hat{U} + e^{2r\pi i/3}\hat{U}^2). \tag{133}$$

Then $\hat{P}_r$ projects onto the eigenspace of $\hat{U}$ with eigenvalue $e^{2r\pi i/3}$. We find

$$\mathrm{Tr}(\hat{P}_r) = \begin{cases}1, & r=1,\\ 2, & r=-1 \text{ or } 0,\end{cases} \tag{134}$$

implying that the dimensions of the eigenspaces are 1,2,2, and that $|\psi_5\rangle$ is in one of the eigenspaces with dimension 2.

In dimensions 6–45 the calculation goes through in essentially the same way. The calculation is, however, slightly more complicated when d is even, due to the fact that we must then require $\mathrm{Det}\,F_d=1$ (mod $2d$). Note, also, that when $d=6$, 21, 24, 28 or 36 the matrix F_d is nonprime, so we must use the decomposition of Lemma 3.

This method also enables us to establish (to the precision that RBSC's numerical data permits) the full stability group of $|\psi_d\rangle$, i.e., the set of all operations (unitary or antiunitary) $\in \mathrm{EC}(d)/I(d)$ of which $|\psi_d\rangle$ is an eigenvector. It turns out that, with one exception, the stability group is the order 3 cyclic subgroup generated by $[F_d,\boldsymbol{\chi}_d]$. The exception is dimension 7, where the stability group is the order 6 cyclic subgroup generated by the antiunitary operation

TABLE II.

d	L_d	η_d	d	L_d	η_d	d	L_d	η_d
5	$\begin{pmatrix}1&0\\1&1\end{pmatrix}$	$\begin{pmatrix}0\\-2\end{pmatrix}$	19	$\begin{pmatrix}2&1\\0&-9\end{pmatrix}$	$\begin{pmatrix}5\\-6\end{pmatrix}$	33	$\begin{pmatrix}6&2\\5&-15\end{pmatrix}$	$\begin{pmatrix}13\\15\end{pmatrix}$
6	$\begin{pmatrix}0&1\\1&-1\end{pmatrix}$	$\begin{pmatrix}1\\-1\end{pmatrix}$	20	$\begin{pmatrix}0&1\\-1&-1\end{pmatrix}$	$\begin{pmatrix}9\\-3\end{pmatrix}$	34	$\begin{pmatrix}0&1\\-1&-11\end{pmatrix}$	$\begin{pmatrix}13\\3\end{pmatrix}$
7	$\begin{pmatrix}2&0\\-3&-3\end{pmatrix}$	$\begin{pmatrix}0\\3\end{pmatrix}$	21	$\begin{pmatrix}2&1\\-4&8\end{pmatrix}$	$\begin{pmatrix}-3\\-7\end{pmatrix}$	35	$\begin{pmatrix}14&2\\10&4\end{pmatrix}$	$\begin{pmatrix}4\\6\end{pmatrix}$
8	$\begin{pmatrix}0&1\\-1&-3\end{pmatrix}$	$\begin{pmatrix}-2\\3\end{pmatrix}$	22	$\begin{pmatrix}1&0\\2&1\end{pmatrix}$	$\begin{pmatrix}8\\6\end{pmatrix}$	36	$\begin{pmatrix}17&1\\5&-4\end{pmatrix}$	$\begin{pmatrix}-2\\-5\end{pmatrix}$
9	$\begin{pmatrix}2&0\\-3&-4\end{pmatrix}$	$\begin{pmatrix}0\\-4\end{pmatrix}$	23	$\begin{pmatrix}0&3\\-8&-7\end{pmatrix}$	$\begin{pmatrix}-10\\-4\end{pmatrix}$	37	$\begin{pmatrix}6&0\\-15&-6\end{pmatrix}$	$\begin{pmatrix}-7\\-6\end{pmatrix}$
10	$\begin{pmatrix}3&1\\-7&-2\end{pmatrix}$	$\begin{pmatrix}2\\4\end{pmatrix}$	24	$\begin{pmatrix}0&1\\-1&-1\end{pmatrix}$	$\begin{pmatrix}3\\0\end{pmatrix}$	38	$\begin{pmatrix}0&1\\-1&-5\end{pmatrix}$	$\begin{pmatrix}-6\\16\end{pmatrix}$
11	$\begin{pmatrix}1&1\\2&3\end{pmatrix}$	$\begin{pmatrix}0\\5\end{pmatrix}$	25	$\begin{pmatrix}1&0\\6&1\end{pmatrix}$	$\begin{pmatrix}3\\4\end{pmatrix}$	39	$\begin{pmatrix}7&2\\2&6\end{pmatrix}$	$\begin{pmatrix}17\\14\end{pmatrix}$
12	$\begin{pmatrix}0&1\\-1&-3\end{pmatrix}$	$\begin{pmatrix}3\\2\end{pmatrix}$	26	$\begin{pmatrix}9&0\\11&-23\end{pmatrix}$	$\begin{pmatrix}2\\-7\end{pmatrix}$	40	$\begin{pmatrix}27&1\\14&-35\end{pmatrix}$	$\begin{pmatrix}-19\\2\end{pmatrix}$
13	$\begin{pmatrix}4&2\\5&6\end{pmatrix}$	$\begin{pmatrix}-6\\-5\end{pmatrix}$	27	$\begin{pmatrix}1&0\\10&-1\end{pmatrix}$	$\begin{pmatrix}-4\\7\end{pmatrix}$	41	$\begin{pmatrix}18&0\\-5&16\end{pmatrix}$	$\begin{pmatrix}1\\-15\end{pmatrix}$
14	$\begin{pmatrix}0&1\\-1&-1\end{pmatrix}$	$\begin{pmatrix}-4\\3\end{pmatrix}$	28	$\begin{pmatrix}12&1\\-25&26\end{pmatrix}$	$\begin{pmatrix}-6\\-8\end{pmatrix}$	42	$\begin{pmatrix}2&1\\11&-36\end{pmatrix}$	$\begin{pmatrix}8\\7\end{pmatrix}$
15	$\begin{pmatrix}1&0\\5&-1\end{pmatrix}$	$\begin{pmatrix}0\\7\end{pmatrix}$	29	$\begin{pmatrix}11&0\\-2&8\end{pmatrix}$	$\begin{pmatrix}-4\\-2\end{pmatrix}$	43	$\begin{pmatrix}8&1\\-16&-18\end{pmatrix}$	$\begin{pmatrix}14\\16\end{pmatrix}$
16	$\begin{pmatrix}3&1\\-11&-14\end{pmatrix}$	$\begin{pmatrix}5\\8\end{pmatrix}$	30	$\begin{pmatrix}10&1\\29&3\end{pmatrix}$	$\begin{pmatrix}12\\1\end{pmatrix}$	44	$\begin{pmatrix}7&1\\-37&20\end{pmatrix}$	$\begin{pmatrix}6\\19\end{pmatrix}$
17	$\begin{pmatrix}1&1\\2&3\end{pmatrix}$	$\begin{pmatrix}8\\-4\end{pmatrix}$	31	$\begin{pmatrix}11&0\\6&-14\end{pmatrix}$	$\begin{pmatrix}-5\\4\end{pmatrix}$	45	$\begin{pmatrix}1&0\\20&1\end{pmatrix}$	$\begin{pmatrix}14\\-6\end{pmatrix}$
18	$\begin{pmatrix}2&1\\7&-14\end{pmatrix}$	$\begin{pmatrix}-3\\3\end{pmatrix}$	32	$\begin{pmatrix}27&1\\-8&-5\end{pmatrix}$	$\begin{pmatrix}13\\-15\end{pmatrix}$			

$$[A_7,\boldsymbol{\xi}_7]=\left[\begin{pmatrix}2&-1\\-1&0\end{pmatrix},\begin{pmatrix}1\\1\end{pmatrix}\right]. \tag{135}$$

Note that $[A_7,\boldsymbol{\xi}_7]^2=[F_7,\boldsymbol{\chi}_7]$.

VII. ZAUNER'S CONJECTURE

In the preceding section we saw that RBSC's numerical results support Conjecture A. Their results also support Conjecture B, i.e., Zauner's conjecture, that in each dimension d there exists a GP fiducial vector which is an eigenvector of $[Z,\mathbf{0}]$.

In fact, for each $5\leqslant d\leqslant 45$ let $[L_d,\boldsymbol{\eta}_d]$ be the operation specified in Table II. It is easily verified that

TABLE III. Stability groups in dimensions 2–7. In every case the stability group includes an order 3 cyclic subgroup generated by a unitary operation having Clifford trace $=-1$.

	Stability group		
Dimension	Type	Order	Number of orbits
2	Non-Abelian	6	1
3	Non-Abelian	6	∞
	Non-Abelian	12	1
	Non-Abelian	48	1
4	Cyclic	6	1
5	Cyclic	3	1
6	Cyclic	3	1
7	Cyclic	3	1
	Cyclic	6	1

$$[L_d, \boldsymbol{\eta}_d][F_d, \boldsymbol{\chi}_d][L_d, \boldsymbol{\eta}_d]^{-1} = [Z, \mathbf{0}]. \tag{136}$$

This means that if $\hat{U} \in [L_d, \boldsymbol{\eta}_d]$, and if $|\psi_d\rangle$ is the RBSC vector in dimension d, then $\hat{U}|\psi_d\rangle$ is a GP fiducial vector which is an eigenvector of $[Z, \mathbf{0}]$. Conjecture B is thus confirmed numerically for every dimension $\leqslant 45$. This suggests the following.

Conjecture C: GP fiducial vectors exist in every finite dimension. Furthermore, every such vector is an eigenvector of a canonical order 3 unitary which is conjugate to $[Z, \mathbf{0}]$.

Conjecture C is clearly stronger than Conjecture B. It also implies Conjecture A.

An operation conjugate to $[Z, \mathbf{0}]$ is automatically a canonical order 3 unitary. It would be interesting to know whether the converse is also true, i.e., whether every canonical order 3 unitary is conjugate to $[Z, \mathbf{0}]$. If that were not the case Conjecture C would be strictly stronger than Conjecture A.

VIII. DIMENSIONS 2–7: VECTORS, ORBITS, AND STABILITY GROUPS

In dimensions 2–7 RBSC made a numerical search, in an attempt to find the total number of GP fiducial vectors. On the assumption that their search was exhaustive we use their data to calculate, for dimensions 2–7, the number of distinct orbits under the action of the extended Clifford group. We also calculate the order of the stability group corresponding to each orbit. Our results are tabulated in Table III. They confirm that in dimensions 2–7 *every* GP fiducial vector is an eigenvector of a canonical order 3 Clifford unitary (in agreement with Conjecture A). We incidentally give exact expressions for two of the GP fiducial vectors in dimension 7 (one on each of the two distinct orbits).

The calculations on which these statements are based are somewhat lengthy, and there is not the space to reproduce them here. We therefore confine ourselves to summarizing the end results, which it is straightforward (albeit tedious) to confirm with the help of (for example) *Mathematica*.

Dimension 2: Exact solutions in dimension 2 have been obtained by Zauner[16] and RBSC.[17] In dimension 2 the GP fiducial vectors all lie on a single orbit of the extended Clifford group. Consider the GP fiducial vector

$$|\psi_2\rangle = \sqrt{(3+\sqrt{3})/6}|e_0\rangle + e^{i\pi/4}\sqrt{(3-\sqrt{3})/6}|e_1\rangle. \tag{137}$$

The stability group of $|\psi_2\rangle$ is the order 6, non-Abelian subgroup of $\mathrm{EC}(2)/\mathrm{I}(2)$ generated by the unitary operation

$$[F_2,\mathbf{0}]=\left[\begin{pmatrix}0 & 1\\ -1 & -1\end{pmatrix},\begin{pmatrix}0\\0\end{pmatrix}\right] \tag{138}$$

and the antiunitary operation

$$[A_2,\mathbf{0}]=\left[\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\begin{pmatrix}0\\0\end{pmatrix}\right]. \tag{139}$$

Note that $[F_2,\mathbf{0}]$ is canonical order 3. It follows from Lemmas 5 and 6 that $|\mathrm{EC}(2)/\mathrm{I}(2)|=48$. So the orbit consists of $48/6=8$ fiducial vectors (identifying vectors which only differ by a phase), constituting two distinct SIC–POVM's (as described by RBSC).

Dimension 3: Exact solutions in dimension 3 have been obtained by Zauner[16] and RBSC.[17] We saw in Sec. V that dimension 3 is unusual in that it is the only dimension for which the identity operator has Clifford trace $=-1$. It seems to be unusual in another respect also, for it is the only case presently known where the GP fiducial vectors constitute infinitely many distinct orbits of the extended Clifford group.

Consider the one parameter family of GP fiducial vectors

$$|\psi_3(t)\rangle=\frac{1}{\sqrt{2}}(e^{-it}|e_1\rangle-e^{it}|e_2\rangle). \tag{140}$$

The complete set of GP fiducial vectors is obtained by acting on the vectors $|\psi_3(t)\rangle$ with elements of EC(3).

Let $\hat{T}$ and $\hat{J}$ be the operators defined by Eqs. (6) and (106), respectively. Then

$$\hat{T}|\psi_3(t)\rangle=-\left|\psi_3\left(t+\frac{\pi}{3}\right)\right\rangle \quad \text{and} \quad \hat{J}|\psi_3(t)\rangle=|\psi_3(-t)\rangle. \tag{141}$$

So $|\psi_3(t)\rangle$ and $|\psi_3(t')\rangle$ are on the same orbit if $t'=(n\pi/3)\pm t$ for some integer n. At the cost of rather more computational effort one can show that this condition is not only sufficient but also necessary for $|\psi_3(t)\rangle$ and $|\psi_3(t')\rangle$ to be on the same orbit. So for each distinct orbit there is exactly one value of $t\in[0,\pi/6]$ such that $|\psi_3(t)\rangle$ is on the orbit.

As Zauner[16] has previously shown, there are three kinds of orbit, a set of infinitely many generic orbits corresponding to values of t in the interior of the interval $[0,\pi/6]$, and two exceptional orbits corresponding to the two endpoints $t=0$ and $\pi/6$.

The stability group of the exceptional vector $|\psi_3(0)\rangle$ consists of all 48 operations of the form $[F,\mathbf{0}]$, where F is any element of $\mathrm{ESL}(2,\mathbf{Z}_3)$. The orbit thus consists of $432/48=9$ fiducial vectors, constituting a single SIC–POVM.

The stability group of the exceptional vector $|\psi_3(\pi/6)\rangle$ is the order 12 non-Abelian subgroup of $\mathrm{EC}(3)/\mathrm{I}(3)$ generated by the unitary operation

$$[F_3,\boldsymbol{\chi}_3]=\left[\begin{pmatrix}-1 & 0\\ -1 & -1\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix}\right] \tag{142}$$

and the antiunitary operation

$$[A_3,\boldsymbol{\chi}_3]=\left[\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix}\right]. \tag{143}$$

Note that

$$[F_3,\boldsymbol{\chi}_3]^2=\left[\begin{pmatrix}1 & 0\\ -1 & 1\end{pmatrix},\begin{pmatrix}0\\0\end{pmatrix}\right] \tag{144}$$

is canonical order 3. The orbit thus consists of $432/12=36$ fiducial vectors, constituting four distinct SIC–POVMs.

The stability group of a generic vector $|\psi_3(t)\rangle$ with $0<t<\pi/6$ is the order 6 non-Abelian subgroup generated by the unitary operation

$$[F_3,\boldsymbol{\chi}_3]^2=\left[\begin{pmatrix}1&0\\-1&1\end{pmatrix},\begin{pmatrix}0\\0\end{pmatrix}\right] \tag{145}$$

and the antiunitary operation

$$[F_3,\boldsymbol{\chi}_3]\circ[A_3,\boldsymbol{\chi}_3]=\left[\begin{pmatrix}-1&0\\-1&1\end{pmatrix},\begin{pmatrix}0\\0\end{pmatrix}\right]. \tag{146}$$

The orbit thus consists of $432/6=72$ fiducial vectors, constituting eight distinct SIC–POVMs.

Dimension 4: The vector

$$|\psi_4\rangle=\sqrt{\frac{5-\sqrt{5}}{40}}\Bigg(2\cos\frac{\pi}{8}|e_0\rangle+i(e^{-i\pi/8}+(2+\sqrt{5})^{1/2}e^{i\pi/8})|e_1\rangle+2i\sin\frac{\pi}{8}|e_2\rangle$$
$$+i(e^{-i\pi/8}-(2+\sqrt{5})^{1/2}e^{i\pi/8})|e_3\rangle\Bigg) \tag{147}$$

is a GP fiducial vector in dimension 4, as discovered by Zauner[16] and RBSC.[17]

In Zauner's notation $|\psi_4\rangle$ is the vector

$$e^{-i\pi/8}(X\psi_{1a}+\rho^3Y\psi_{1b}). \tag{148}$$

In RBSC's notation it is the vector

$$r_0|e_0\rangle+r_+e^{i\theta_+}|e_1\rangle+r_1e^{i\theta_1}|e_2\rangle+r_-e^{i\theta_-}|e_3\rangle \tag{149}$$

for the case $n=j=m=1$ and $k=0$ [note, however, that there is a typographical error in RBSC,[17] their expression for r_0 should read $r_0=\sqrt{(1-1/\sqrt{5})/(2\sqrt{2-\sqrt{2}})}$].

The stability group of $|\psi_4\rangle$ is the order 6 cyclic subgroup of EC(4)/I(4) generated by the antiunitary operation

$$[A_4,\boldsymbol{\chi}_4]=\left[\begin{pmatrix}-1&1\\-1&2\end{pmatrix},\begin{pmatrix}2\\0\end{pmatrix}\right]. \tag{150}$$

Note that

$$[A_4,\boldsymbol{\chi}_4]^2=\left[\begin{pmatrix}0&1\\-1&3\end{pmatrix},\begin{pmatrix}0\\2\end{pmatrix}\right]=\left[\begin{pmatrix}0&1\\-1&-1\end{pmatrix},\begin{pmatrix}0\\0\end{pmatrix}\right] \tag{151}$$

is canonical order 3 [where we used Eq. (81) to obtain the last expression on the right-hand side].

It follows from Lemmas 5 and 6 that the group EC(4)/I(4) is of order 1536. So the orbit generated by $|\psi_4\rangle$ contains $1536/6=256$ fiducial vectors, constituting $256/16=16$ SIC–POVMs. RBSC's numerical search found a total of 16 SIC–POVMs in dimension 4. If their search was exhaustive, it would follow that the fiducial vectors all lie on a single orbit of the extended Clifford group.

Dimension 5: Let $|\psi_5\rangle$ be RBSC's numerical vector in dimension 5. We noted in the preceding section that the stability group of $|\psi_5\rangle$ is of order 3. It follows from Lemmas 5 and 6 that the group EC(5)/I(5) is of order 6000. So the orbit generated by $|\psi_5\rangle$ contains $6000/3=2000$ fiducial vectors, constituting $2000/25=80$ SIC–POVMs. RBSC found a total of 80 SIC–POVMs in dimension 5. If their search was exhaustive, it would follow that the fiducial vectors all lie on a single orbit of the extended Clifford group.

Note that Zauner's analytic solution in dimension 5 (on p. 63 of his thesis[16]) can be used to give exact expressions for each of the vectors on the orbit.

Dimension 6: Let $|\psi_6\rangle$ be RBSC's numerical vector in dimension 6. We noted in the preceding

section that the stability group of $|\psi_6\rangle$ is of order 3. It follows from Lemmas 5 and 6 that the group EC(6)/I(6) is of order 10 368. So the orbit generated by $|\psi_6\rangle$ contains $10\,368/3=3456$ fiducial vectors, constituting $3456/36=96$ SIC–POVMs. RBSC found a total of 96 SIC–POVMs in dimension 5. If their search was exhaustive, it would follow that the fiducial vectors all lie on a single orbit of the extended Clifford group (in agreement with Grassl's[21] analysis, based on his exact solution in dimension 6).

Note that Grassl's[21] analytic solution can be used to give exact expressions for each of the vectors on the orbit.

Dimension 7: Let $|\psi_7\rangle$ be RBSC's numerical vector in dimension 7. We noted in the last section that the stability group of $|\psi_7\rangle$ is of order 6. It follows from Lemmas 5 and 6 that the group EC(6)/I(6) is of order 32 928. So the orbit generated by $|\psi_7\rangle$ contains $32\,928/6=5488$ fiducial vectors, constituting $5488/49=112$ SIC–POVMs. However, RBSC found 336 SIC–POVMs in dimension 7. This indicates the existence of at least one other orbit.

The search for the additional orbit or orbits is facilitated by the fact that in dimension 7 there exists a canonical order 3 Clifford unitary for which the F matrix is diagonal, namely

$$[F_7',\mathbf{0}]=\left[\begin{pmatrix}-3 & 0\\ 0 & 2\end{pmatrix},\begin{pmatrix}0\\0\end{pmatrix}\right]. \tag{152}$$

The fact that F_7' is diagonal means that the $\hat{U}\in[F_7',\mathbf{0}]$ are permutation matrices. Specifically

$$\hat{U}=e^{i\theta}\sum_{r=0}^{6}|e_{4r}\rangle\langle e_r| \tag{153}$$

for every $\hat{U}\in[F_7',\mathbf{0}]$ (where $e^{i\theta}$ is an arbitrary phase, and where we have used the decomposition described in Lemma 3). This considerably simplifies the calculations. We will also have occasion to consider the antiunitary operation

$$[A_7',\mathbf{0}]=\left[\begin{pmatrix}-2 & 0\\ 0 & -3\end{pmatrix},\begin{pmatrix}0\\0\end{pmatrix}\right] \tag{154}$$

which is a square root of $[F_7',\mathbf{0}]$.

We look for eigenvectors of $[F_7',\mathbf{0}]$. Let

$$l_r=\begin{cases}1 & \text{if } r=1,\,2 \text{ or } 4,\\ -1 & \text{if } r=3,\,5 \text{ or } 6.\end{cases} \tag{155}$$

Also let

$$a_0=\frac{1}{2}\left(\sqrt{\frac{1}{4-\sqrt{2}}}+i\sqrt{\frac{4-\sqrt{2}}{2}}\right),\quad a_1=\frac{1}{4}\sqrt{\frac{8-5\sqrt{2}}{7}},\quad a_2=2^{-7/4} \tag{156}$$

and

$$b_0=\sqrt{\frac{2+3\sqrt{2}}{14}},\quad b_1=\sqrt{\frac{4-\sqrt{2}}{28}},\quad \theta=\cos^{-1}\left(-\frac{\sqrt{\sqrt{2}+1}}{2}\right). \tag{157}$$

Then define

$$|\psi_7'\rangle=a_0|e_0\rangle-\sum_{r=1}^{6}(a_1+l_r a_2)|e_r\rangle, \tag{158}$$

$$|\psi_7''\rangle = b_0|e_0\rangle + \sum_{r=1}^{6} b_1 e^{il_r\theta}|e_r\rangle. \tag{159}$$

It is readily confirmed that $|\psi_7'\rangle$ and $|\psi_7''\rangle$ are both GP fiducial vectors. The stability group of $|\psi_7'\rangle$ is the order 3 subgroup generated by $[F_7', \mathbf{0}]$, while the stability group of $|\psi_7''\rangle$ is the order 6 subgroup generated by $[A_7', \mathbf{0}]$. Since the stability groups are nonisomorphic the orbits generated by $|\psi_7'\rangle$ and $|\psi_7''\rangle$ are disjoint. The orbit generated by $|\psi_7'\rangle$ contains $32\,928/3 = 10\,976$ fiducial vectors, constituting $10\,976/49 = 224$ SIC–POVMs. The orbit generated by $|\psi_7''\rangle$ contains 5488 fiducial vectors, constituting a further 112 SIC–POVMs. This accounts for all 336 of the SIC–POVMs identified by RBSC. If we assume that RBSC's search was exhaustive it would follow that there are no other orbits, apart from these two.

For the sake of completeness let us note that

$$|\psi_7\rangle = \hat{U}|\psi_7''\rangle, \tag{160}$$

where $|\psi_7\rangle$ is RBSC's numerical vector and $\hat{U}$ is a unitary operator

$$\hat{U} \in \left[\begin{pmatrix} 1 & 1 \\ -3 & -2 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right]. \tag{161}$$

Finally, let us remark that l_r is the Legendre symbol (see, e.g., Nathanson[36] or Rose[37])

$$l_r = \left(\frac{r}{7} \right). \tag{162}$$

It has the important property that $l_{rs} = l_r l_s$ for all $r, s \in \mathbb{Z}$.

IX. A FIDUCIAL VECTOR IN DIMENSION 19

In Sec. VI we saw that, apart from the solution in dimension 7, RBSC's numerical solutions in dimensions 5–45 all have stability group of order 3. This might encourage one to speculate that when $d > 7$ the stability group is *always* of order 3. In this section we show that there is at least one exception to that putative rule, by constructing a GP fiducial vector in dimension 19 for which the stability group has order $\geqslant 18$.

The vector we construct is an eigenvector of the order 18 antiunitary operation

$$[A_{19}', \mathbf{0}] = \left[\begin{pmatrix} -9 & 0 \\ 0 & -2 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right] \in \mathrm{EC}(19)/\mathrm{I}(19). \tag{163}$$

Note that

$$[F_{19}', \mathbf{0}] = [A_{19}', \mathbf{0}]^6 = \left[\begin{pmatrix} -8 & 0 \\ 0 & 7 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right] \tag{164}$$

is canonical order 3.

The construction is similar to our construction of the vector $|\psi_7''\rangle$ in the last section. Let l_r' be the Legendre symbol

$$l_r' = \left(\frac{r}{19} \right) = \begin{cases} 1 & \text{if } r = 1, 4, 5, 6, 7, 9, 11, 16 \text{ or } 17, \\ -1 & \text{if } r = 2, 3, 8, 10, 12, 13, 14, 15 \text{ or } 18, \end{cases} \tag{165}$$

and let

$$b_0' = \sqrt{\frac{5+9\sqrt{5}}{95}}, \quad b_1' = \sqrt{\frac{10-\sqrt{5}}{190}}, \quad \theta' = \cos^{-1}\left(\sqrt{\frac{\sqrt{5}-1}{8}}\right). \tag{166}$$

Then define

$$|\psi_{19}'\rangle = b_0'|e_0\rangle + \sum_{r=1}^{18} b_1' e^{il_r'\theta'}|e_r\rangle. \tag{167}$$

It is readily confirmed that $|\psi_{19}'\rangle$ is a GP fiducial vector, and an eigenvector of $[A_{19}', \mathbf{0}]$.

Observe that the orbit generated by $|\psi_{19}'\rangle$ is disjoint from the orbit generated by RBSC's numerical vector $|\psi_{19}\rangle$ (because the stability groups are nonisomorphic). It follows that there are at least two distinct orbits in dimension 19.

X. DIAGONALIZING THE *F* MATRIX

Our construction of the exact solutions $|\psi_7'\rangle$, $|\psi_7''\rangle$, and $|\psi_{19}'\rangle$ in Eqs. (158), (159), and (167) was facilitated by the fact that in dimensions 7 and 19 there exist canonical order 3 unitaries for which the corresponding F matrix is diagonal. It is natural to ask in what other dimensions that is true. The theorem proved below answers that question.

We will need the following lemma.

Lemma 8: Let p be a prime number $=1 \pmod 3$, *and let n be any* integer $\geqslant 1$. *Then there exists an integer* α *such that*

$$\alpha^2 + \alpha + 1 = 0 \pmod{p^n}. \tag{168}$$

Proof: The proof relies heavily on the theory of primitive roots, as described in (for example) Chap. 3 of Nathanson[36] or Chap. 5 of Rose.[37] Let ϕ be Euler's phi, or totient function [so for every integer $x \geqslant 1$, $\phi(x)$ is the number of integers y in the range $1 \leqslant y < x$ which are relatively prime to x]. Then there exists a single positive integer g such that for every integer $m \geqslant 1$ the multiplicative order of g, considered as an element of $\mathbb{Z}_{p^m}$, is $\phi(p^m) = (p-1)p^{m-1}$ (see, for example, Nathanson,[36] p. 93, or Rose,[37] p. 91). The fact that $p = 1 \pmod 3$ means $p = 3k+1$ for some integer $k \geqslant 1$. Define

$$\alpha = g^{kp^{n-1}}. \tag{169}$$

It is then immediate that

$$\alpha^3 = g^{\phi(p^n)} = 1 \pmod{p^n}. \tag{170}$$

It is also true that $\alpha - 1$ is relatively prime to p. Suppose that were not the case. It would then follow from the definition of α, and the fact that g is a primitive root *modulo p*, that

$$kp^{n-1} = l(p-1) - 3kl \tag{171}$$

for some integer $l \geqslant 1$. That, however, is impossible since p is not a multiple of 3.

The fact that $\alpha - 1$ is relatively prime to p means that there exists an integer β such that

$$\beta(\alpha - 1) = 1 \pmod{p^n}. \tag{172}$$

It now follows from Eqs. (170) and (172) that

$$\alpha^2 + \alpha + 1 = \beta(\alpha^3 - 1) = 0 \pmod{p^n}. \tag{173}$$

□

We are now in a position to prove our main result.

Theorem 3: *There exists a canonical order 3 unitary* $[F, \boldsymbol{\chi}] \in \mathrm{C}(d)/\mathrm{I}(d)$ *for which the matrix F is diagonal if and only if each of the following is true:*

(1) *d has at least one* prime divisor $= 1$ (*mod* 3).

(2) *d has no* prime divisors $=2$ (*mod* 3).
(3) *d is not divisible by* 9.

Remark: So there exist canonical order 3 unitaries $[F,\boldsymbol{\chi}]$ for which F is diagonal in dimension 7,13,19,21,31,37,39,43,49, … .

Proof: We begin by proving sufficiency. Suppose that conditions (1), (2), and (3) are all true. Then we have, for some $t \geqslant 1$,

$$d = 3^{n_0} p_1^{n_1} \cdots p_t^{n_t}, \tag{174}$$

where the p_i are distinct prime numbers $=1 \pmod 3$, where the integer $n_0 = 0$ or 1, and where the integers $n_1, \ldots, n_t$ are all $\geqslant 1$. It follows from Lemma 8 that there exist integers $\alpha_1, \ldots, \alpha_t$ such that

$$\alpha_i^2 + \alpha_i + 1 = 0 \pmod{p_i^{n_i}} \tag{175}$$

for $i = 1, \ldots, t$. We now use the Chinese remainder theorem (see, for example, Nathanson[36] or Rose[37]) to deduce that there exists a single integer α such that

$$\alpha = 1 \pmod 3 \tag{176}$$

and

$$\alpha = \alpha_i \pmod{p_i^{n_i}} \tag{177}$$

for $i = 1, \ldots, t$. We then have

$$\alpha^2 + \alpha + 1 = 0 \pmod d \tag{178}$$

implying that the matrix

$$F = \begin{pmatrix} \alpha & 0 \\ 0 & -\alpha - 1 \end{pmatrix} \tag{179}$$

$\in \mathrm{SL}(2, \mathbb{Z}_d)$ (bearing in mind that d is odd). Moreover, $\mathrm{Tr}(F) = -1 \pmod d$. Since $d \neq 3$ we conclude that $[F,\boldsymbol{\chi}]$ is a canonical order 3 unitary for all $\boldsymbol{\chi} \in (\mathbb{Z}_d)^2$. This proves sufficiency.

To prove necessity suppose

$$F = \begin{pmatrix} \alpha & 0 \\ 0 & \delta \end{pmatrix} \in \mathrm{SL}(2, \mathbb{Z}_d) \tag{180}$$

is such that $[F,\boldsymbol{\chi}]$ is canonical order 3 for some $\boldsymbol{\chi} \in (\mathbb{Z}_d)^2$. Then $\alpha + \delta = -1 \pmod d$, implying

$$\alpha^2 + \alpha + 1 = 0 \pmod d, \tag{181}$$

$$\alpha^3 = 1 \pmod d \tag{182}$$

[in view of the fact that $\alpha\delta = 1 \pmod d$].

To show that d has no prime divisors $=2 \pmod 3$ assume the contrary. It would then follow from Eqs. (181) and (182) that

$$\alpha^2 + \alpha + 1 = 0 \pmod p, \tag{183}$$

$$\alpha^3 = 1 \pmod p \tag{184}$$

for some prime number $p = 2 \pmod 3$. Let r be a primitive root of p and let $k \in \mathbb{Z}$ be such that $0 \leqslant k < p-1$ and $\alpha = r^k \pmod p$ (see, for example, Nathanson[36] or Rose[37]). Then Eq. (184) implies $r^{3k} = 1 \pmod p$ which, in view of the fact that r is a primitive root, means $3k = l(p-1)$ for some $l \in \mathbb{Z}$. The fact that $0 \leqslant k < p-1$ implies $0 \leqslant l < 3$. Taking into account the fact that $p-1$ is not

divisible by 3 [because $p=2 \pmod 3$] we deduce that $l=0$. But then $k=0$, implying $\alpha = 1 \pmod p$. In view of Eq. (183) this means $3=0 \pmod p$, which is a contradiction.

To prove that d is not divisible by 9 we again proceed by *reductio ad absurdum*. Suppose that d were divisible by 9. It would then follow from Eq. (181) that

$$\alpha^2 + \alpha + 1 = 0 \pmod 9. \tag{185}$$

However, it is easily verified (by explicit enumeration) that this equation has no solutions.

Finally, suppose that d had no prime divisors $=1 \pmod 3$. In view of the results just proved it would follow that $d=3$. But if $d=3$, Eq. (181) implies $\alpha=1 \pmod 3$. Taking into account the requirement $\alpha\delta=\det F=1 \pmod 3$ this means $\delta=1 \pmod 3$. But then F is the identity matrix, which contradicts the assumption that $[F,\boldsymbol{\chi}]$ is a canonical order 3 unitary. We conclude that d must have at least one prime divisor $=1 \pmod 3$. □

XI. CONCLUSION

RBSC conclude their paper by saying "a rigorous proof of existence of SIC–POVMs in all finite dimensions seems tantalizingly close, yet remains somehow distant." That well expresses our own perception of the matter. While working on this problem we have several times had the sense that the crucial discovery lay just round the corner, only to find that our hopes were illusory. We make our results public in the hope that they may, nevertheless, contain a few clues, which will help to take us further forward.

In particular it seems to us that significant progress would be made if it could be established whether it is in fact true that every GP fiducial vector is an eigenvector of a canonical order 3 unitary. Also, if that is the case, one would like to know exactly *why* it is the case.

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Mathematical analysis of the Mandelstam–Tamm time-energy uncertainty principle

John E. Gray[a)]
Code B10 (Quantum Processing Group), Naval Surface Warfare Center Dahlgren Division, Dahlgren, Virginia 22485

Andrew Vogt[b)]
Department of Mathematics, Georgetown University, Washington, DC 20057-1233

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In the Mandelstam–Tamm version of the time-energy uncertainty principle Δt denotes the infimum of time intervals that elapse before the change in the mean of any observable has the same magnitude as its standard deviation. We clarify this interpretation, and show that the infimum is achieved for certain observables and thus that this famous inequality is actually an equality. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1897164]

I. INTRODUCTION

The time-energy uncertainty principle (TEUP) has many versions.[1–8] In one of its standard forms, due to Mandelstam and Tamm[9] [we follow the formulation in Messiah's book (Ref. 1, pp. 319–320)], Δt represents the infimum of times that must pass for the change in the mean of some observable to be comparable in size to the standard deviation of that observable at the initial time. TEUP asserts that this time is greater than or equal to Planck's constant $\hbar$ divided by twice the standard deviation of the energy observable at the initial time.

In this note we clarify the meaning of the symbol Δt. We strive for exactness and introduce notions of *dynamic uncertainty per unit time* and *static uncertainty* to aid our discussion. Indeed, as we shall explain, Δt is only in a crude sense a lower bound for the time needed for significant change to occur, and is more accurately regarded as the infimum of the absolute ratio of static uncertainty to dynamic uncertainty per unit time among observables satisfying technical conditions which ensure that this ratio is properly defined. Moreover, there are observables (corresponding even to bounded operators) for which this infimum is actually achieved, and thus the Mandelstam–Tamm inequality is an equality. Defined for a given Hamiltonian and a given initial state, Δt is a characteristic time for measurable change to occur in a system. The observables used to observe such change, as one might expect, are ones that measure the component of the time derivative of the state perpendicular to the initial state.

An alternative view of the TEUP, taken in quantum estimation theory, is that Δt is the standard error of an estimate for the time at which some quantum event occurs, and the Mandelstam–Tamm inequality is a special case of a quantum Cramer–Rao inequality.[10–12] The time in quantum mechanics thus appears to be interpreted not as a variable but as a fixed parameter to be estimated as parameters are estimated in classical statistics. In our discussion here we adopt instead the traditional Newtonian view of time.

II. PRELIMINARIES

As is customary, we identify an observable with a self-adjoint operator A on the Hilbert space containing the state vectors ψ. For convenience neither positive operator valued measures nor

a)Electronic mail: john.e.gray@navy.mil
b)Author to whom correspondence should be addressed. Electronic mail: vogt@math.georgetown.edu

density matrices are considered. The inner product $\langle,\rangle$ in the Hilbert space is assumed to be linear in the first variable, conjugate linear in the second. We will be careful to point out domain restrictions in our discussion.

The mean, or the expected value, of an observable A for the state ψ is given by

$$\mu_\psi(A) = \langle A(\psi), \psi\rangle, \tag{1}$$

while the standard deviation of the observable A is

$$\Delta_\psi A = \|(A - \mu_\psi(A)I)(\psi)\|. \tag{2}$$

The mean and standard deviation are defined if and only if ψ is in the domain of the operator A, denoted by $D(A)$. Furthermore, a state ψ is an eigenstate of the operator A iff ψ is in $D(A)$ and $\Delta_\psi A = 0$.

Although the mean of an observable may appear to be a specialized notion of limited value, it actually includes the full range of quantum-mechanical probability considerations. If $P_A(\ )$ is the projection-valued measure associated with the self-adjoint operator A, then for any Borel subset I of the real numbers $P_A(I)$ is a bounded observable (in fact an orthogonal projection onto a closed subspace) and $\mu_\psi(P_A(I))$ is the probability that a measurement of the observable A when the state is ψ yields a value in the set I. As we vary I, we obtain the probability distribution for the observable A. Thus, means incorporate all of the probability theory, and no domain questions arise since ψ is always in $D(P_A(I))$.

The Cauchy–Schwarz inequality, applied to (2) for observables A and B, takes the form

$$\begin{aligned}\Delta_\psi A \Delta_\psi B &\geqslant \tfrac{1}{2}|\langle (A - \mu_\psi(A)I)(\psi), (B - \mu_\psi(B)I)(\psi)\rangle - \langle (B - \mu_\psi(B)I)(\psi), (A - \mu_\psi(A)I)(\psi)\rangle| \\ &= \tfrac{1}{2}|\langle A(\psi), B(\psi)\rangle - \langle B(\psi), A(\psi)\rangle) = |\mathrm{Im}(\langle A(\psi), B(\psi)\rangle|,\end{aligned} \tag{3}$$

where ψ is in $D(A) \cap D(B)$. If ψ is in the set $D = \{\psi: \psi$ is in $D(A) \cap D(B), A(\psi)$ is in $D(B)$, and $B(\psi)$ is in $D(A)\}$, then (3) can be rewritten as

$$\Delta_\psi A \Delta_\psi B \geqslant \tfrac{1}{2}|\langle i(AB - BA)(\psi), \psi\rangle| = \tfrac{1}{2}|\mu_\psi([A,B])|, \tag{4}$$

where in general $[A,B] = i(AB - BA)$ defines a unique self-adjoint operator, the commutator of A and B, whose domain $D([A,B])$ contains the subspace D.

III. THE MANDELSTAM–TAMM TEUP

Fundamental to quantum mechanics is an evolution of the state between measurements described by the Schrödinger equation

$$i\hbar \frac{\mathrm{d}\psi}{\mathrm{d}t} = H(\psi), \tag{5}$$

where H is the energy observable of the system, called its *Hamiltonian*. For simplicity we assume H is time independent. The state at time t is given by $\psi(t) = \exp(-it/\hbar)H(\psi)$ where $\psi(0) = \psi$ is the state at time 0, and $\{\exp(-it/\hbar)H: t \in \mathcal{R}\}$ is a one-parameter group of unitary operators generated by H. Since the statistics are contained in ψ, the statistics also must evolve.

Although the wave function $\psi(t)$ is defined for all t, the existence of derivatives depends upon whether ψ is in the (dense) domain of the energy operator H, and, if we are taking the derivative of the mean of some observable, in the domain of the associated operator A. The time derivative of the mean of an observable A at time $t = 0$ is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mu_\psi(A)) = \frac{\mathrm{d}}{\mathrm{d}t}(\langle A(\psi(t)), \psi(t)\rangle)$$

$$= \lim_{t\to 0} \frac{1}{t}(\langle A(\psi(t)), \psi(t)\rangle - \langle A(\psi), \psi\rangle)$$

$$= \lim_{t\to 0}\left(\left\langle \frac{\psi(t)-\psi}{t}, A(\psi(t)-\psi)\right\rangle + \left\langle \frac{\psi(t)-\psi}{t}, A(\psi)\right\rangle + \left\langle A(\psi), \frac{\psi(t)-\psi}{t}\right\rangle\right)$$

$$= 0 + \frac{-i}{\hbar}(\langle H(\psi), A(\psi)\rangle - \langle A(\psi), H(\psi)\rangle) = \frac{2}{\hbar}\,\mathrm{Im}(\langle H(\psi), A(\psi)\rangle). \tag{6}$$

For these equations to be valid we assume that

$$\psi \text{ is in } D(H), \tag{7a}$$

$$\psi(t) \text{ is in } D(A) \text{ for } t \text{ near } 0, \text{ and} \tag{7b}$$

$$\langle \psi(t)-\psi, A(\psi(t)-\psi)\rangle = o(t). \tag{7c}$$

Conditions (7a) and (7b) are plausible requirements, but (7c) is less so. The notation $o(t^\delta)$ describes any scalar quantity $q(t)$ such that $\lim_{t\to 0} q(t)/t^\delta = 0$. If (7a) holds, then $\|\psi(t)-\psi\| = o(t^{1-\epsilon})$ for any $\epsilon > 0$, but since A may be unbounded, (7c) is not guaranteed[1].

Proposition: Suppose (7a) holds. It follows that

(i) if A is bounded, then (7b) and (7c) hold;
(ii) if (7b) holds, A is semibounded, and $(\mathrm{d}/\mathrm{d}t)(\mu_\psi(A))$ exists as a two-sided derivative, then (7c) holds; and
(iii) if (7b) holds and $\{A(\psi(t)) : |t| < \epsilon\}$ is a bounded set for some $\epsilon > 0$, then (7c) holds.

Proof: If A is bounded, $D(A)$ is the whole Hilbert space and the expression in (7c) is $o(t^{2(1-\epsilon)})$ for small ϵ and *a fortiori* $o(t)$, which establishes (i).

In (ii), since $(\mathrm{d}/\mathrm{d}t)(\mu_\psi(A))$ exists, $\lim_{t\to 0}(1/t)\langle \psi(t)-\psi, A(\psi(t)-\psi)\rangle = p$ for some scalar p. Since A is semibounded, $\langle \theta, A(\theta) - c\theta\rangle \geq 0$ for some real number c and all vectors θ in $D(A)$ (or else $-A$ satisfies such an inequality and the same argument can be applied to $-A$). Since $\lim_{t\to 0}(1/t)\langle \psi(t)-\psi, c(\psi(t)-\psi)\rangle = 0$, it follows that for t converging to 0^+, $p \geq 0$; while for t converging to 0^-, $p \leq 0$; and so $p = 0$.

To establish (iii), let $M = \sup\{\|A(\psi(t))\| : |t| < \epsilon\}$. Given $\epsilon_1 > 0$, choose $\delta_1 > 0$ in $(0, \epsilon)$ so that if $|t| < \delta_1$ then $\|\{[\psi(t)-\psi]/t\} + (i/\hbar)H(\psi)\| < \epsilon_1/6M$. Choose θ in the dense domain $D(A)$ so that $\|\theta + (i/\hbar)H(\psi)\| < \epsilon_1/6M$, and choose $\delta_2 \leq \delta_1$ so that for $|t| < \delta_2$, $\|\psi(t)-\psi\| < \epsilon_1/(3(\|A(\theta)\|+1))$. Then for $|t| < \delta_2$,

$$\left|\frac{\langle \psi(t)-\psi, A(\psi(t)-\psi)\rangle}{t}\right| \leq \left|\left\langle \frac{\psi(t)-\psi}{t} + \frac{i}{\hbar}H(\psi), A(\psi(t)-\psi)\right\rangle\right| + \left|\left\langle \frac{i}{\hbar}H(\psi) + \theta, A(\psi(t)-\psi)\right\rangle\right|$$

$$+ |\langle \theta, A(\psi(t)-\psi)\rangle| < \frac{\epsilon_1}{6M}\cdot 2M + \frac{\epsilon_1}{6M}\cdot 2M + \frac{\epsilon_1}{3} = \epsilon_1.$$

This establishes (7c). ■

[1]We have not found examples of self-adjoint operators H, A and a state ψ for which (7a) and (7b) hold but not (7c). The following may perhaps suggest an example. In the Hilbert space $l_2(\mathcal{N})$, define a sequence of vectors $\{a_k : k \geq 1\}$ by $a_k(n) = 1/(kn^{3/4})$ for $n \leq k^2$, $a_k(n) = 0$ else, and let A be the number operator satisfying $A(a_k)(n) = na_k(n)$ for $k, n \geq 1$. Then $\{a_k\}$ is analogous to $\{\psi(t)-\psi\}$, with t replaced by $1/k$. Moreover $\lim_{k\to\infty} ka_k = c$ where $c(n) = 1/n^{3/4}$ for $n \geq 1$, and $\lim_{k\to\infty}\langle ka_k, A(a_k)\rangle = 2$.

If in addition to (7), we assume that $A(\psi)$ is in $D(H)$, $H(\psi)$ is in $D(A)$, and $[H,A]$ exists, then we can rewrite (6) as $(\mathrm{d}/\mathrm{d}t)\mu_\psi(A)=(1/\hbar)\mu_\psi([H,A])$.

If ψ is an eigenvector of the energy operator, then $H(\psi)=c\psi$ for some real number c. For any time interval $[0,t]$ during which Schrödinger evolution occurs, $\psi(t)=[\exp(-ict/\hbar)](\psi)$ and the state remains unchanged since wave functions that differ by a scalar multiple represent the same state. If $A(\psi)$ is defined, then so is $A(\psi(t))$ in this case, and

$$\langle H(\psi(t)),A(\psi(t))\rangle = c\langle \psi(t),A(\psi(t))\rangle = c\mu_{\psi(t)}(A) \tag{8}$$

has imaginary part equal to zero. Thus, by (6), $\langle A(\psi(t)),\psi(t)\rangle$ stays constant. This follows directly because

$$\langle A(\psi(t)),\psi(t)\rangle = \left\langle A\left(\exp\frac{-ict}{\hbar}\right)(\psi),\left(\exp\frac{-ict}{\hbar}\right)(\psi)\right\rangle \equiv \langle A(\psi),\psi\rangle. \tag{9}$$

Since all bounded observables, including orthogonal projections, have constant means, the statistics associated with every observable remain constant in time. This is a familiar property of the evolution of energy eigenstates.

In any case we can combine (3) and (6), with $B=H$, to obtain

$$\Delta_\psi A\Delta_\psi H \geqslant \frac{\hbar}{2}\left|\frac{\mathrm{d}}{\mathrm{d}t}\mu_\psi(A)\right|. \tag{10}$$

Instead of regarding $\Delta_\psi A$ as the standard deviation, we choose to call it the *static uncertainty* of the observable A when the state is ψ. This label emphasizes that $\Delta_\psi A$ is a measure of the variability of A at a given time. The quantity $(\mathrm{d}/\mathrm{d}t)\mu_\psi(A)$ is the *dynamic uncertainty per unit time*: it measures the variability of the central value of A per unit time. Typically in one unit of time the value of $\mu_\psi(A)$ changes by approximately $(\mathrm{d}/\mathrm{d}t)\mu_\psi(A)\cdot 1$. Thus it is quite natural (after Messiah) to make the following definition when ψ is a unit vector in $D(H)$ that is not an eigenvector of H,

$$\Delta_\psi t \overset{\text{def}}{=} \inf_A\left\{\frac{\Delta_\psi A}{\left|\frac{\mathrm{d}}{\mathrm{d}t}\mu_\psi(A)\right|}: A \text{ self-adjoint}, A \text{ satisfies (7)}, \text{and} \frac{\mathrm{d}}{\mathrm{d}t}\mu_\psi(A)\neq 0\right\}. \tag{11}$$

If ψ is an eigenvector of H, then the denominator in (11) is always zero, thus no observable varies in time. Thinking of $\Delta_\psi t$ as infinity in this case makes sense.

The quantity $\Delta_\psi t$ is, roughly speaking, the minimum time required for the dynamic uncertainty in some observable to achieve the same magnitude as its static uncertainty, the minimum time interval until the evolution of the state introduces variation large enough to match the intrinsic variability at the initial time.

This description is only approximate for multiple reasons. The conditions in (7) may not be fulfilled. In addition, the dynamics are described by a linear approximation to $\mu_{\psi(t)}(A)$, namely, $\mu_{\psi(0)}(A)+(\mathrm{d}/\mathrm{d}t)(\mu_{\psi(t)}(A))|_{t=0}(t-0)$. Observables A for which $(\mathrm{d}/\mathrm{d}t)(\mu_{\psi(t)}(A))|_{t=0}$ equals zero and a second or higher order approximation might be relevant are excluded from consideration. This happens whenever ψ is an eigenvector of A, for then $\Delta_\psi A=0$ and by (10) $(\mathrm{d}/\mathrm{d}t)\mu_\psi(A)=0$. Also ignored is the possibility that linear approximation is not accurate over the time interval of interest, short as it may be, because, say, the first derivative changes very rapidly. Finally, although changes in the mean of a variable are important, we cannot argue that they are the only significant measures of change as time passes or that any change smaller than one standard deviation is truly negligible. In fact, if the observable is taken to be $P_A(I)$, the mean $\langle P_A(I)\psi,\psi\rangle=p$ is the probability that A lies in the Borel set I, and the standard deviation or static uncertainty is $\sqrt{p-p^2}$, a number that is larger than p for $p<\frac{1}{2}$. Messiah (Ref. 1, pp. 319–320) calls $\Delta_\psi t$ "the characteristic time of evolution." This formulation recommends itself since it does not promise too much. The precise meaning of $\Delta_\psi t$ is given by (11).

The existence of observables A satisfying the conditions in (11) is established below, so that the definition is not vacuous.

Assuming such observables exist, by combining (11) with inequality (10), we obtain

$$\Delta_\psi t \Delta_\psi H \geqslant \frac{\hbar}{2} \tag{12}$$

for all unit vectors ψ in $D(H)$ that are not eigenvectors of H. This is the TEUP (Ref. 1, pp. 319–320).

The quantity $\Delta_\psi t$ depends not only on the state ψ but also on the time evolution of ψ, that is, on the particular Hamiltonian H that governs the evolution of the state. Furthermore, (11) and (6) imply that

$$\begin{aligned}\Delta_\psi t &\geqslant \inf_A \left\{ \frac{\hbar \Delta_\psi A}{2|\mathrm{Im}(\langle H(\psi), A(\psi)\rangle)|} : A \text{ self-adjoint}, \psi \in D(A), \mathrm{Im}(\langle H(\psi), A(\psi)\rangle) \neq 0 \right\} \\ &\geqslant \inf_\theta \left\{ \frac{\hbar \| \theta - \langle \theta, \psi\rangle \psi \|}{2|\mathrm{Im}(\langle H(\psi), \theta\rangle)|} : \theta \text{ a vector}, \mathrm{Im}(\langle \psi, \theta\rangle) = 0 \neq \mathrm{Im}(\langle H(\psi), \theta\rangle) \right\}. \end{aligned} \tag{13}$$

To obtain (13), we have replaced the time derivative of the mean in (11) by its value in (6), and then replaced $A(\psi)$ by a vector θ. Since the infimum in (11) and those in (13) are effectively over progressively larger sets, the inequalities are as indicated. The theorem below establishes that these inequalities are in fact equalities.

Theorem: Let ψ be a unit vector in $D(H)$ that is not an eigenvector of H. Then

$$\Delta_\psi t \Delta_\psi H = \frac{\hbar}{2}. \tag{14}$$

Furthermore, the infimum $\Delta_\psi t$ is achieved precisely for self-adjoint operators A satisfying (7) and taking ψ to $\alpha\psi + i\beta PH(\psi)$ where P is the orthogonal projection of the Hilbert space to the subspace $(\mathrm{span}\{\psi\})^\perp$, and α and β are real numbers with β nonzero.

Remarks: The theorem tells us that $\Delta_\psi t = \hbar/2\Delta_\psi H$. It also tells us that there are three kinds of observables A, (i) those for which the absolute ratio of static uncertainty to dynamic uncertainty per unit time is undefined [i.e., (7) fails or $\mathrm{d}/\mathrm{d}t\mu_\psi(A) = 0$], (ii) those for which this ratio is larger than $\Delta_\psi t$, and (iii) those for which the ratio equals $\Delta_\psi t$. The theorem also characterizes the third kind of observable.

Before proceeding to the proof, we establish the existence of observables for which the absolute ratio is defined. If θ is any vector such that $\langle \psi, \theta\rangle$ is real, then there always exist self-adjoint operators A that take the unit vector ψ to θ. Indeed, for an arbitrary Hilbert space vector ψ', A may always be defined by $A(\psi') =^{\mathrm{def}} \langle \psi', P(\theta)\rangle \psi + \langle \psi', \psi\rangle \theta + BP(\psi')$, where B is a self-adjoint operator defined on the Hilbert subspace $(\mathrm{span}\{\psi\})^\perp$. It is straightforward to verify that A is self-adjoint if and only if B is, and A is bounded if and only if B is.

Now take θ to satisfy $\mathrm{Im}(\langle H(\psi), \theta\rangle) \neq 0$. Then corresponding operators A exist with $A(\psi) = \theta$. So the two infima on the right-hand side of (13) are over the same set and hence are equal. If B is taken to be a bounded operator on $(\mathrm{span}\{\psi\})^\perp$, then A is bounded. This implies that A satisfies (7). Hence $\Delta_\psi t$ is well defined.

If θ is chosen as in the theorem [i.e., $\theta = \alpha\psi + i\beta PH(\psi)$, with α and β real and β nonzero], then $\langle \theta, \psi\rangle = \alpha$ is real and $\langle H(\psi), \theta\rangle = \alpha\langle H(\psi), \psi\rangle - i\beta\langle H(\psi), PH(\psi)\rangle$, so that $\mathrm{Im}(\langle H(\psi), \theta\rangle) = -\beta\|PH(\psi)\|^2 \neq 0$ since ψ is not an eigenvector of H. A self-adjoint operator A taking ψ to θ exists, constructed as in the preceding paragraphs, and if B is taken to be bounded, A satisfies (7). Thus operators A fitting the description in the theorem exist. In particular, a simple example of such an operator A is obtained by setting $B = 0$, $\alpha = 0$, and $\beta = 1/\|PH(\psi)\|$. Then

$$A(\psi') = \langle \psi', e^+ \rangle e^+ - \langle \psi', e^- \rangle e^-, \tag{15}$$

where

$$e^{\pm} = \frac{1}{\sqrt{2}} \left(i \frac{PH(\psi)}{\|PH(\psi)\|} \pm \psi \right). \tag{16}$$

This choice of A is bounded and has the discrete spectrum $\sigma(A) = \{1, -1, 0\}$ and corresponding eigenspaces span$\{e^+\}$, span$\{e^-\}$, and (span$\{e^+, e^-\}$)$^\perp$. In fact $\psi(t) = \exp(-it/\hbar)H(\psi)$ is in the range space of A, i.e., span$\{e^+, e^-\}$, to first order in t.

Proof: We establish that the infimum in the last expression in (13) is a minimum. Then the remarks above show that the previous expressions in (13) are also infimized since θ gives rise to a self-adjoint operator A such that $A(\psi) = \theta$ and A even can be chosen to satisfy (7) (for example, take A to be globally defined and thus bounded).

Write θ in (13) in the form $\theta = \alpha\psi + \gamma PH(\psi) + \psi'$, where ψ' is taken to be orthogonal to ψ and $PH(\psi)$, and α and γ are unknown scalars. Since we require in (13) that $\mathrm{Im}(\langle \psi, \theta \rangle) = 0 \neq \mathrm{Im}(\langle H(\psi), \theta \rangle)$, then α must be real and

$$\begin{aligned} \mathrm{Im}(\langle H(\psi), \theta \rangle) &= \mathrm{Im}(\langle H(\psi), \gamma PH(\psi) \rangle) \\ &= \mathrm{Im}(\overline{\gamma})(\|PH(\psi)\|^2) = \mathrm{Im}(\overline{\gamma})(\|H(\psi) - \langle H(\psi), \psi \rangle \psi\|^2) = \mathrm{Im}(\overline{\gamma})(\Delta_\psi H)^2. \end{aligned} \tag{17}$$

So γ cannot be real.

The ratio inside the final set of braces in (13) (with $\hbar/2$ omitted) is

$$\frac{\|\theta - \langle \theta, \psi \rangle \psi\|}{|\mathrm{Im}(\langle H(\psi), \theta \rangle)|} = \frac{\sqrt{|\gamma|^2 (\Delta_\psi H)^2 + \|\psi'\|^2}}{|\mathrm{Im}(\overline{\gamma})| (\Delta_\psi H)^2} \geqslant \frac{1}{\Delta_\psi H} \tag{18}$$

and equality holds if and only if ψ' is the zero vector and γ is a nonzero pure imaginary number $i\beta$. ■

The above proof establishes the TEUP, and even transforms it into an equality. The quantity $\Delta_\psi t = \hbar/2\Delta_\psi H$ depends on both ψ and H, and can be thought of as a kind of fundamental unit of time for the given state and evolutionary law. In any shorter time interval, with the caveats noted earlier, there is no appreciable distinction between dynamics and statics. Since $\hbar$ is small, this unit is usually small, but in some cases (states that are approximate eigenvectors of the energy observable) it can be large and the system is in a metastable state.

Certain observables allow one to achieve the infimum $\Delta_\psi t$, and allow us, so to speak, to detect the temporal change in statistics. These observables take ψ to $\alpha\psi + i\beta PH(\psi)$, and the significant part of this (set $\beta = -1/\hbar$ and $\alpha = 0$) is merely $(-i/\hbar)PH(\psi) = P(\mathrm{d}\psi/\mathrm{d}t)$, the projection of the time derivative of ψ perpendicular to ψ. From this perspective the TEUP, despite its assured perennial interest, appears almost trivial, the time required to detect change is the time τ required for the dynamic uncertainty of such an observable A to achieve the same magnitude as its static uncertainty. A moment's computation shows that the static uncertainty is

$$\begin{aligned} \Delta_\psi A = \|A(\psi) - \langle A(\psi), \psi \rangle \psi\| &= \left\| P\left(\frac{\mathrm{d}}{\mathrm{d}t}\psi\right) - \left\langle P\left(\frac{\mathrm{d}}{\mathrm{d}t}\psi\right), \psi \right\rangle \psi \right\| \\ &= \left\| P\left(\frac{\mathrm{d}}{\mathrm{d}t}\psi\right) \right\| = \frac{1}{\hbar}\|PH(\psi)\| = \frac{1}{\hbar}\|H(\psi) - \langle H(\psi), \psi \rangle \psi\| = \frac{1}{\hbar}\Delta_\psi H \end{aligned}$$

and by (6)

$$\frac{\mathrm{d}}{\mathrm{d}t}\mu_\psi(A) = \frac{2}{\hbar}\,\mathrm{Im}(\langle H(\psi), A(\psi)\rangle) = \frac{2}{\hbar}\,\mathrm{Im}\left(\left\langle H(\psi), P\left(\frac{\mathrm{d}}{\mathrm{d}t}\psi\right)\right\rangle\right)$$

$$= \frac{2}{\hbar}\,\mathrm{Im}\left(\frac{-i}{\hbar}\langle H(\psi), PH(\psi)\rangle\right) = \frac{2}{\hbar^2}\|PH(\psi)\|^2 = \frac{2}{\hbar^2}(\Delta_\psi H)^2.$$

Since $\tau\times(2/\hbar^2)(\Delta_\psi H)^2 = |(1/\hbar)\Delta_\psi H|$, we find that $\tau = \hbar/2\Delta_\psi H$.

IV. AFTERWORD

An alternative to the TEUP discussed here is the *half-life* version, in which Δt is an estimate of the time that must elapse before there is a 50% probability that the state is orthogonal to the original state. Pfeifer and Fröhlich[8] propose six different variants of the half-life TEUP. Allcock[2–4] and Wigner[5] have also proposed versions of the TEUP. Their treatments are somewhat obscure since they do not establish square integrability of the wave function with respect to time. Quantum estimation theory, as already mentioned, yields a quantum Cramer–Rao inequality which has the form of a general TEUP.

Busch[13] proposes three useful notions of time: (1)laboratory or clock or external time, (2) dynamic or internal time, and (3) observable or event time. TEUPs can be formulated in terms of each.

Indeed, multiple versions and interpretations of the TEUP should be accepted as a fact of life. The product of time and energy has the same units as Planck's celebrated constant, and it should not be surprising to find that significant time intervals and energy intervals derived from a variety of physical scenarios can be related to $\hbar$.

The status of Δt in the Mandelstam–Tamm TEUP and most other TEUPs is quite different from that of Δx in Heisenberg's uncertainty principle. An important part of the program of relativistic quantum mechanics is to establish the comparability and equal footing of space and time. However, the Mandelstam–Tamm and half-life version of the TEUP, and the equality established in this paper, are actually obstacles to achieving this objective. Time here is clock time and is the parameter of the unitary group of state evolution generated by the Hamiltonian. The quantity $\Delta_\psi t$ is not the standard deviation of an observable, but is the infimum of the ratio of static uncertainty to dynamic uncertainty per unit time, with the caveats noted above.

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Saturated Kochen–Specker-type configuration of 120 projective lines in eight-dimensional space and its group of symmetry

Artur E. Ruuge
Department of Quantum Statistics and Field Theory, Faculty of Physics, Moscow State University , Vorobyovy Gory, 119899 Moscow, Russia and Department of Mathematics and Computer Science, University of Antwerp, Middelheim Campus, Building G, Meddelheimlaan 1, B-2020 Antwerp, Belgium

Freddy van Oystaeyen
Department of Mathematics and Computer Science, University of Antwerp, Middelheim Campus, Building G, Meddelheimlaan 1, B-2020 Antwerp, Belgium

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There exists an example of a set of 40 projective lines in eight-dimensional Hilbert space producing a Kochen–Specker-type contradiction. This set corresponds to a known no-hidden variables argument due to Mermin. In the present paper it is proved that this set admits a finite saturation, i.e., an extension up to a finite set with the following property: every subset of pairwise orthogonal projective lines has a completion, i.e., is contained in at least one subset of eight pairwise orthogonal projective lines. An explicit description of such an extension consisting of 120 projective lines is given. The idea to saturate the set of projective lines related to Mermin's example together with the possibility to have a finite saturation allow to find the corresponding group of symmetry. This group is described explicitely and is shown to be generated by reflections. The natural action of the mentioned group on the set of all subsets of pairwise orthogonal projective lines of the mentioned extension is investigated. In particular, the restriction of this action to complete subsets is shown to have only four orbits, which have a natural characterization in terms of the construction of the saturation. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1887923]

I. INTRODUCTION

The analysis of the foundations of quantum theory has two important results, (1) Bell's inequalities; (2) Kochen–Specker theorem. Both of them show that in quantum mechanics a statistical model of a physical experiment may not admit a realization by way of a probability space $(\Omega,\mathcal{F},P)$. The first result shows, that even if one assumes the existence of a measurable space $(\Omega,\mathcal{F})$, one might not be able to consruct a probability measure P. The second result shows that the assumption about the existence of $(\Omega,\mathcal{F})$ may itself be contradictory.

The Bell–Kochen–Specker theory[2,5] restricts itself to considering the measuring devices with only two possible indications. In this case the problem cocerning the existence of $(\Omega,\mathcal{F})$ reduces to a problem about coloring projective lines in a finite dimensional Hilbert space. It is possible to reformulate this problem as follows.[8] Let $\mathcal{H}$ be a Hilbert space over $\mathbb{C}$ of finite dimension $n := \dim_{\mathbb{C}} \mathcal{H}$. Suppose one is given a family of $m \in \mathbb{N}$ orthonormal bases in $\mathcal{H}$: $\{e_i^{(\alpha)}\}_{i=1}^{n}$, $\alpha=\overline{1,m}$. Choose from each basis an element $e_{i_\alpha}^{(\alpha)}$, $\alpha=\overline{1,m}$, and look at the inner products $(e_{i_\alpha}^{(\alpha)}, e_{i_\beta}^{(\beta)})$, $\alpha,\beta=\overline{1,m}$. Is it always possible to make this choice in such a way, that for all α and β the inner product of $e_{i_\alpha}^{(\alpha)}$ and $e_{i_\beta}^{(\beta)}$ does not vanish, i.e., the (projective) lines $\mathbb{C}e_{i_\alpha}^{(\alpha)}$ and $\mathbb{C}e_{i_\beta}^{(\beta)}$ are *not* orthogonal?

One says that a collection of projective lines $\{\mathbb{C}e_i^{(\alpha)}\}_{i,\alpha}$ produces a *Kochen–Specker-type con-*

tradiction if the answer to the formulated question is "No." The original construction by Kochen and Specker in the proof of their theorem generates the first example of this contradiction. Since then several other examples of this type have been found, in particular Refs. 7, 6, 9, 4, and 1. In the present paper we analyze one of them—the example coming from the proof of a no-hidden-variables theorem given by Mermin.[6] Note, that the latter example can be related to the discussion of Einstein–Podolsky–Rosen paradox and Bell's theorem in Ref. 3.

The original construction of Kochen and Specker is quite sophisticated. This is determined by the fact that the authors work in a three-dimensional space. The construction of Mermin and the corresponding proof are much more simple, but the space is eight-dimensional. To be exact, the original paper of Mermin is written in terms of operators on a Hilbert space and the reformulation in terms of projective lines is due to Kernaghan and Peres.[4] In general, the latter consists in the following. One defines a set of 40 projective lines in $\mathbb{C}^8$. The corresponding description is explicit and quite simple. If one views the elements of $\mathbb{C}^8$ as columns of eight complex numbers, then it is possible to represent each of the 40 projective lines by a column with entries 0, 1 or −1. Thus in fact the projective lines can even be viewed as real. The corresponding Kochen–Specker contradiction is then established by some simple arithmetic argument. The link with the Mermin's formulation is as follows. The described set splits into five distinct tuples, each containing eight pairwise orthogonal projective lines. Identifying $\mathbb{C}^8$ with $(\mathbb{C}^2)^{\otimes 3}$ and interpreting each of the five tuples as coming from an orthonormal basis corresponding to some complete set of pairwise commuting orthogonal projectors, one arrives at five complete sets playing a key role in Ref. 6.

There is another well-known example—the "Penrose dodecahedron"—studied in detail by Zimba and Penrose in Ref. 9. In this case one again makes use of 40 projective lines, but this time in $\mathbb{C}^4$. In the corresponding construction one considers a dodecahedron and associates in a certain way to each of its 20 vertices two projective lines in $\mathbb{C}^4$. The whole construction has the symmetry group of a dodecahedron, which naturally acts on the resulting set of 40 projective lines. Comparing the examples of Penrose and of Mermin, it is natural to ask, what can one say about the symmetry of Mermin's example? An additional motivation for this is given by the two examples described in Ref. 1 which also have a high degree of symmetry. One of them is associated to a 120 cell (a four-dimensional analog of dodecahedron), and the other to a 600 cell (a four-dimensional analog of icosahedron). It turns out, that despite of the fact that the projective lines in Mermin's case look quite simple, an answer to this question, as was mentioned in Ref. 4, presents a problem. Its possible solution constitutes the subject of the present paper.

II. SATURATED KOCHEN–SPECKER

Let A denote a set of projective lines in Hilbert space $\mathcal{H}$, $\dim_{\mathbb{C}} \mathcal{H}=n<\infty$. The set A is called *saturated* with respect to orthogonality relation $\perp$ if any of its subsets $B\subset A$ of pairwise orthogonal projective lines can be embedded into a subset $C\subset A$ of n pairwise orthogonal projective lines. Denote $\mathcal{P}_{\perp}(A):=\{B\subset A \,|\, \forall x,y\in B: x\neq y \Rightarrow x\perp y\}$. Denote $C(A):=\{B\in\mathcal{P}_{\perp}(A)\,|\,\#B=n\}$. The elements of $C(A)$ will be called *complete* subsets of A. Note that $\mathcal{P}_{\perp}(A)$ contains an empty set and all subsets of cardinality 1. Note that if A produces a Kochen–Specker contradiction, then $C(A)$ is not empty.

If one looks at the mentioned example of Mermin, one observes that the corresponding set is *not* saturated with respect to $\perp$. Intuitively, a saturated set should have a higher degree of symmetry than an unsaturated part of it [an example of a saturated set is the set $\mathbb{P}(\mathcal{H})$ of *all* projective lines in $\mathcal{H}$]. This leads to the idea of how to investigate the symmetry of Mermin's example. One may try to add projective lines to the given set so that to get a saturated set. After that it makes sense to proceed with the symmetry. Naively, such an attempt should look as follows. One takes a subset of pairwise orthogonal lines, tries to find a complete set containing it, and in case there is no such one, invents several other pairwise orthogonal projective lines to make it complete. These new projective lines are added to the initial set, and the whole process is repeated until one reaches a saturation. At each step one solves the problem for the chosen subset, but at the same time one may create other subsets of pairwise orthogonal elements which require a completion. It means, that *a priori* the described algorythm is not even finite.

In the next section we are going to describe a *finite* set A of projective lines in $\mathcal{H}$, $\dim_{\mathbb{C}} \mathcal{H} = 8$, with the following properties: (1) A is saturated with respect to $\perp$; (2) A contains a set of Mermin–Kernaghan–Peres projective lines and due to this, in particular, produces a Kochen–Specker-type contradiction; (3) *every* element of A can be represented by a column with each of the eight entries being 0, 1 or -1.

After that we proceed with the study of the symmetry of the set A. One looks at $Bij(A)$—a group of all bijections of A, and denotes by $Bij_{\perp}(A)$ its subgroup consisting of all bijections which respect the orthogonality relation $\perp$. The set $C(A)$ naturally splits into four disjoint subsets denoted as $C_k(A)$, $k=1,2,4,8$, as will be explained below. We describe a subgroup $\mathcal{G}$ in $Bij_{\perp}(A)$ by giving explicit formulas for a set of its generators and prove, that this group has an action on $C(A)$ such that $C_k(A)$'s conicide with its orbits. It means that one can take any element of $C_k(A)$ and then generate all the other complete subsets belonging $C_k(A)$ by applying the elements of this group. This allows to describe the symmetry of Mermin's example.

III. 120 PROJECTIVE LINES

We shall now describe a set A which will later be proved to be a saturated extension of Mermin's example. Set $\mathcal{H} := \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$. Recall that one has denoted the set of all projective lines in $\mathcal{H}$ by $\mathbb{P}(\mathcal{H})$. Let V denote a set of four symbols, $V=\{e,f,g,h\}$. We are going to describe a map

$$\xi: \mathcal{P}(V)^{\times} := \mathcal{P}(V) \setminus \{\varnothing\} \to C(\mathbb{P}(\mathcal{H})),$$

such that $\forall U, U' \in \mathcal{P}(V)^{\times}: U \neq U' \Rightarrow \xi(U) \cap \xi(U') = \varnothing$. Note that the latter in particular implies that ξ is injective. Since $\#\mathcal{P}(V)^{\times} = 15$ and $\dim_{\mathbb{C}}(\mathcal{H}) = 8$, the union of all the sets from the image of ξ must yield 120 projective lines. This will produce the set A.

The set $\mathcal{P}(V)^{\times}$ may be visualized as a tetrahedron with vertices labeled as e, f, g, and h. Considering the subsets of V, one identifies the vertices with the subsets of cardinality 1, the edges with subsets of cardinality 2, faces with subsets of cardinality 3, and the body of the tetrahedron with V. Assign to the edges of this graph labels of the form $\overset{\omega}{\varphi}$ or $\overset{\omega}{\psi}$ where φ and ψ are two symbols and ω is a number 1, 2 or 3. Require, that the edges associated to the same vertex have different numbers ω. This defines the labelling of the edges of the graph up to a permutation of labels of vertices. Without loss of generality, one may choose and fix the labeling as shown in

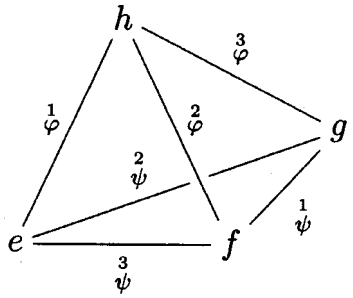

(1)

Note that this tetrahedron appears in Ref. 8.

Choose an arbitrary orthonormal basis $\{\varphi_\alpha\}_{\alpha=0,1}$ in $\mathbb{C}^2$. It will be convenient to view the possible values 0 and 1 of the index α as elements of the group $\mathbb{Z}_2$ with the group operation written additively (addition modulo 2). Consider a matrix $u := \|u(\alpha,\beta)\|_{\alpha,\beta\in\mathbb{Z}_2}$ with entries $u(\alpha,\beta) = -1$ if $(\alpha,\beta) = (1,1)$ and $u(\alpha,\beta) = 1$ otherwise. Note that it can be viewed as a character matrix of $\mathbb{Z}_2$. There exist the following properties:

$$(1) \quad u(\alpha,\beta) = u(\beta,\alpha) \in \mathbb{R},$$

$$(2)\quad \sum_{\beta} u(\alpha,\beta)u(\beta,\gamma) = 2\delta_{\alpha,\gamma},$$

$$(3)\quad u(\alpha,1+\alpha) = 1, \tag{2}$$

$$(4)\quad u(\alpha,\beta+\gamma) = u(\alpha,\beta)u(\alpha,\gamma),$$

where α, β, γ run over $\mathbb{Z}_2$. Denote $u^{\beta}_{\alpha} := u(\alpha,\beta)/\sqrt{2}$ and define another orthonormal basis $\{\psi_\alpha\}_\alpha$ in $\mathbb{C}^2$: $\psi_\alpha := \Sigma_\beta u^{\beta}_{\alpha}\varphi_\beta$.

We shall associate to the mentioned graph and a fixed choice of an orthonormal basis $\{\varphi_\alpha\}_\alpha$ a set A of 120 projective lines in $\mathcal{H}$ expressed via the functions φ_α and the matrix u. It means that there will be a complete set associated to every vertex of the graph (this gives four complete sets), to every edge (this gives six more complete sets), to every face (this gives four complete sets) and to the whole tetrahedron (this gives one complete set). In what follows we use the notation: write $\hat{e}$ instead of $\{e\}$ to refer to a vertex, write ef instead of $\{e,f\}$ to denote an edge, write efg or $\overline{h}$ to denote the face $\{e,f,g\}$, and write $efgh$ instead of $\{e,f,g,h\}$.

Let us start with the description of the complete sets corresponding to vertices. Denote a set of all edges having a common vertex $v \in V$ by E_v, and consider a set

$$S_{\hat{v}} := \mathrm{Maps}(E_v \to \mathbb{Z}_2), \quad v \in V.$$

This set is not empty and contains eight elements. Take any v, say $v=e$, and take any $\sigma \in S_{\hat{e}}$. The labels of the edges eh, eg, and ef from E_e are of the form φ^1, ψ^2, and ψ^3, respectively. Associate to this fact a vector $\Psi^{(e)}_{\sigma} := \varphi_{\sigma(eh)} \otimes \psi_{\sigma(eg)} \otimes \psi_{\sigma(ef)}$. The vectors $\Psi^{(v)}_{\sigma}$ for other $v \in V$ are defined in a similar way. As a result one gets for every vertex v an orthonormal basis $\{\Psi^{(v)}_{\sigma}\}_{\sigma\in S_{\hat{v}}}$. Denote $\Psi^{v}_{\sigma} := \mathbb{C}\Psi^{(v)}_{\sigma}$. It follows, that one has four complete sets of projective lines associated to each vertex. One defines $\xi(\hat{v}) := \{\Psi^{v}_{\sigma}\}_{\sigma\in S_{\hat{v}}}$, $v \in V$.

The complete sets associated to edges make use of a slightly more sophisticated indexing. We denote by $E := \{ef, eg, eh, fg, fh, gh\}$ the set of all edges. To define a complete set of projective lines corresponding to an edge, one first takes an arbitrary *ordered* pair of two distinct vertices (v,w). Let z and t denote the remaining two vertices of the graph. Consider a disjoint union of a one-element set $\{vw\}$ and a two-element set $\{z,t\}$ and denote

$$K_{vw} := \mathrm{Maps}(\{vw\} \sqcup \{z,t\} \to \mathbb{Z}_2).$$

Note, that $\#K_{vw}=8$. The complete set of projective lines corresponding to the edge vw will be indexed by the elements of K_{vw}. Take $v=e$, $w=f$ and take arbitrary $\varkappa \in K_{ef}$. Recall that the labels of the edges eh, eg, and ef from E_e are of the form φ^1, ψ^2, and ψ^3, respectively. Denote

$$X^{(e\to f)}_{\varkappa} := \sum_{\alpha,\mu\in\mathbb{Z}_2} u^{\mu}_{\alpha} u^{\varkappa(h)}_{\alpha} u^{\varkappa(g)}_{\mu} \varphi_\alpha \otimes \psi_\mu \otimes \psi_{\varkappa(ef)}.$$

One defines the vectors $X^{(v\to w)}_{\varkappa}$, $\varkappa \in K_{vw}$, corresponding to every ordered pair (v,w), $v \neq w$, in a similar way. Using the properties of the matrix u, one can prove that

(1) the vectors $X^{(v\to w)}_{\varkappa}$, $\varkappa \in K_{vw}$, are pairwise orthogonal,
(2) the projective lines $\mathbb{C}X^{(v\to w)}_{\varkappa}$ and $\mathbb{C}X^{(w\to v)}_{\varkappa}$ coincide.

The latter fact motivates the notation $X^{vw}_{\varkappa} := \mathbb{C}X^{(v\to w)}_{\varkappa}$. The first fact implies, that $\{X^{vw}_{\varkappa}\}_{\varkappa\in K_{vw}}$ is a complete set of projective lines. It follows, that one gets six complete sets of projective lines associated to each edge of the graph. One defines $\xi(\epsilon) := \{X^{\epsilon}_{\varkappa}\}_{\varkappa\in K_{\epsilon}}$, $\epsilon \in E$.

Let us construct the complete sets associated to faces of the tetrahedron. Actually, every face is determined by an opposite vertex of the tetrahedron, and in this sense the complete sets to be constructed can be viewed as associated to vertices. It is simply natural to view them as associated to faces since the role of complete sets associated to vertices is already occupied. Denote

$$R_{\overline{v}} := \mathrm{Maps}(E \setminus E_v \to \mathbb{Z}_2), \quad v \in V.$$

This set is not empty, contains eight elements, and moreover, there is a natural bijection $\nu_v : R_{\overline{v}} \xrightarrow{\sim} S_{\hat{v}}$ established by the formula $\nu_v(\rho)(vw) = \rho(zt)$, where z and t are the vertices complementing $\{v, w\}$ up to V. If there is no risk of confusion, we write ρ^* instead of $\nu_v(\rho)$, $\rho \in R_{\overline{v}}$, as well as σ^* instead of $\nu_v^{-1}(\sigma)$, $\sigma \in S_{\overline{v}}$. Now take $v = e$ and any $\rho \in R_{\overline{e}}$. Recall that the labels of the edges eh, eg, and ef from E_e are of the form φ^1, ψ^2, and ψ^3, respectively. Denote

$$\Phi_\rho^{(e \to f)} := \sum_{\alpha, \mu \in \mathbb{Z}_2} u_\alpha^{\rho^*(eh)+\rho^*(ef)} u_\mu^{\rho^*(eg)+\rho^*(ef)} \varphi_\alpha \otimes \psi_\mu \otimes \psi_{\Delta_\rho + \alpha + \mu},$$

where $\Delta_\rho := \Sigma_{\epsilon \in E \setminus E_e} \rho(\epsilon)$. The vectors $\Phi_\rho^{(v \to w)}$ corresponding to other choices of $v, w \in V, v \neq w$ are defined in a similar way. The properties of the matrix u imply that the vectors $\Phi_\rho^{(v \to w)}, \rho \in R_{\overline{v}}$, are pairwise orthogonal and that $\mathbb{C}\Phi_\rho^{(v \to w)}$ does not depend on the choice of w. Denote, $\Phi_\rho^v := \mathbb{C}\Phi_\rho^{(v \to w)}$. It follows, that to every face $\overline{v}$ one associates a complete set of projective lines $\{\Phi_\rho^v\}_{\rho \in R_{\overline{v}}}$. One defines $\xi(\overline{v}) := \{\Phi_\rho^v\}_{\rho \in R_{\overline{v}}}$, $v \in V$.

Let us finally associate a complete set of projective lines to the whole tetrahedron. Denote

$$\Lambda := \left\{ \pi : V \to \mathbb{Z}_2 \middle| \sum_{v \in V} \pi(v) = 1 \right\}.$$

Note, that $\#\Lambda = 8$. Take an *ordered* pair $(e, f) \in V \times V$. Recall that the labels of the edges eh, eg, and ef from E_e are of the form φ^1, ψ^2, and ψ^3, respectively,

$$F_\pi^{(e \to f)} := \sum_{\alpha, \mu \in \mathbb{Z}_2} u_{\pi(h)}^{\pi(g)+\mu} u_\alpha^{\pi(g)+\mu} \varphi_\alpha \otimes \psi_\mu \otimes \psi_{\pi(e)+\alpha+\mu}.$$

Note, that using the properties of the matrix u one can prove that the expression $u_a^{m+\mu} u_\alpha^{m+\mu}$ remains invariant under the transposition $(a, \alpha) \rightleftarrows (m, \mu)$. The vectors $F_\pi^{(u \to v)}$ corresponding to other ordered pairs are defined in a similar way. Using the properties of u, one can prove, that

(1) the vectors $F_\pi^{(v \to w)}$, $\pi \in \Lambda$, are pairwise orthogonal,
(2) the projective line $\mathbb{C}F_\pi^{(v \to w)}$ does not depend on the choice of the ordered pair (v, w).

The latter fact motivates the notation $F_\pi := \mathbb{C}F_\pi^{(v \to w)}$. The first fact implies, that $\{F_\pi\}_{\pi \in \Lambda}$ is a complete set of projective lines. One defines $\xi(efgh) := \{F_\pi\}_{\pi \in \Lambda}$. This completes the definition of ξ.

Note that the projective lines of the form Ψ_σ^v and F_π have been introduced in Ref. 8, but the set $\{F_\pi\}_\pi$ was not viewed as a complete set associated to the whole tetrahedron (1), since the projective lines of the form $X_\varkappa^{vw}$ and Φ_ρ^v did not exist. One can find the calculations illustrating the mentioned properties of F_π in Ref. 8. The definition of $X_\varkappa^{vw}$ and Φ_ρ^v is new.

Now we have a map $\xi : \mathcal{P}(V)^\times \to C(\mathbb{P}(\mathcal{H}))$. One verifies, that all the described projective lines are distinct. It means, that one gets 15 disjoint complete sets of projective lines in $\mathcal{H}$, for every vertex $v \in V$ a set $\{\Psi_\sigma^v\}_{\sigma \in S_{\hat{v}}}$; for every edge $\epsilon \in E$ a set $\{X_\varkappa^\epsilon\}_{\varkappa \in K_\epsilon}$; for every face $\overline{v}$, $v \in V$, a set $\{\Phi_\rho^v\}_{\rho \in R_{\overline{v}}}$; and for the whole tetrahedron a set $\{F_\pi\}_{\pi \in \Lambda}$. The set $A := \sqcup_{U \in Im(\xi)} U$ has a cardinality $\#A = 120$. We claim, that the set A is saturated with respect to the orthogonality relation $\perp$ and produces a Kochen–Specker-type contradiction.

IV. RELATIONS BETWEEN THE PROJECTIVE LINES

Let us describe the orthogonality relations between the elements of the set A. All these relations follow from the properties (2) of the matrix u. Recall that if $\rho \in R_{\overline{v}}$, then one denotes by ρ^* its image under the natural bijection $\nu_v : R_{\overline{v}} \xrightarrow{\sim} S_{\hat{v}}$. Simillarly, if $\sigma \in S_{\hat{v}}$, one writes σ^* instead of

$\nu_v^{-1}(\sigma) \in R_{\bar{v}}$. If $\sigma \in S_{\hat{v}}$, let $\nabla_\sigma := \Sigma_{\epsilon \in E_v} \sigma(\epsilon)$. If $\varkappa \in K_{\boldsymbol{\epsilon}}$, say $\boldsymbol{\epsilon} = ef$, then let $\tilde{\varkappa}$ denote an element of K_{ef} defined by $\tilde{\varkappa}(ef) = 1 + \varkappa(ef) + \varkappa(g) + \varkappa(h)$, $\tilde{\varkappa}(g) = \varkappa(h)$, $\tilde{\varkappa}(h) = \varkappa(g)$. For other $\boldsymbol{\epsilon}$ the notation $\tilde{\varkappa}$ for $\varkappa \in K_{\boldsymbol{\epsilon}}$ is defined in a similar way. Note that $\rho^{**} = \rho$, $\sigma^{**} = \sigma$, and $\tilde{\tilde{\varkappa}} = \varkappa$.

We explicitly describe part of the relations. The others are obtained by permutation of the symbols e, f, g, and h,

(1) $\Psi^e_\sigma \perp \Psi^e_{\sigma'}$ iff $\sigma(\cdot) \neq \sigma'(\cdot)$,
(2) $\Psi^e_\sigma \perp \Psi^f_{\sigma_1}$ iff $\sigma(ef) = 1 + \sigma_1(ef)$,
(3) $\Phi^e_\rho \perp \Phi^e_{\rho'}$ iff $\rho^*(\cdot) \neq \rho'^*(\cdot)$,
(4) $\Phi^e_\rho \perp \Phi^f_{\rho_1}$ iff $\rho^*(ef) = 1 + \rho_1^*(ef)$,
(5) $X^{ef}_\varkappa \perp X^{ef}_{\varkappa'}$ iff $\varkappa(\cdot) \neq \varkappa'(\cdot)$,
(6) $X^{ef}_\varkappa \perp X^{eg}_{\varkappa_1}$ iff $\varkappa(ef) + \varkappa(h) = 1 + \varkappa_1(eg) + \varkappa_1(h)$,
(7) $X^{ef}_\varkappa \perp X^{gh}_{\varkappa_1}$ iff $\varkappa(g) + \varkappa(h) = \varkappa_1(e) + \varkappa_1(f)$,
(8) $F_\pi \perp F_{\pi'}$ iff $\pi(\cdot) \neq \pi'(\cdot)$,
(9) $\Psi^e_\sigma \perp \Phi^e_\rho$ iff $\nabla_\sigma = 1 + \nabla_{\rho^*}$,
(10) $\Psi^e_\sigma \perp \Phi^f_\rho$ iff $\nabla_\sigma + \sigma(ef) = 1 + \nabla_{\rho^*} + \rho^*(ef)$,
(11) $\Psi^e_\sigma \perp X^{ef}_\varkappa$ iff $\sigma(ef) = 1 + \varkappa(ef)$,
(12) $\Psi^e_\sigma \perp X^{fg}_\varkappa$ iff $\sigma(ef) + \sigma(eg) = 1 + \tilde{\varkappa}(e)$,
(13) $\Phi^e_\rho \perp X^{ef}_\varkappa$ iff $\rho^*(ef) = 1 + \tilde{\varkappa}(ef)$,
(14) $\Phi^e_\rho \perp X^{fg}_\varkappa$ iff $\rho^*(ef) + \rho^*(eg) = 1 + \varkappa(e)$,
(15) $\Psi^e_\sigma \perp F_\pi$ iff $\nabla_\sigma = 1 + \pi(e)$,
(16) $\Phi^e_\rho \perp F_\pi$ iff $\nabla_{\rho^*} = 1 + \pi(e)$,
(17) $X^{ef}_\varkappa \perp F_\pi$ iff $\varkappa(g) + \varkappa(h) = 1 + \pi(g) + \pi(h)$.

Note, that there is no 1 in the formula (7). Note that these relations have a self-duality property. Namely, the condition for orthogonality in (5) is equivalent to $\tilde{\varkappa}(\cdot) \neq \tilde{\varkappa}'(\cdot)$, the condition in (6) is equivalent to $\tilde{\varkappa}(ef) + \tilde{\varkappa}(h) = 1 + \tilde{\varkappa_1}(eg) + \tilde{\varkappa_1}(h)$, the condition in (7) is equivalent to $\tilde{\varkappa}(g) + \tilde{\varkappa}(h) = \tilde{\varkappa_1}(e) + \tilde{\varkappa_1}(f)$, and the condition in (17) is equivalent to $\tilde{\varkappa}(g) + \tilde{\varkappa}(h) = 1 + \pi(g) + \pi(h)$. It follows, that if one has a set of pairwise orthogonal projective lines of the form $\{\Psi^{v_i}_{\sigma_i}\}_{i \in I} \cup \{X^{\epsilon_j}_{\varkappa_j}\}_{j \in J} \cup \{\Phi^{w_l}_{\rho_l}\}_{l \in L} \cup \{F_{\pi_m}\}_{m \in M}$, where I, J, L, M are some index sets, $v_i, w_l \in V$, $\boldsymbol{\epsilon}_j \in E$, then by replacing $\Psi^{v_i}_{\sigma_i}$ with $\Phi^{v_i}_{\sigma_i^*}$, $\Phi^{w_l}_{\rho_l}$ with $\Psi^{w_l}_{\rho_l^*}$ and $X^{\epsilon_j}_{\varkappa_j}$ with $X^{\bar{\epsilon}_j}_{\tilde{\varkappa}_j}$, one obtains a set of projective lines $\{\Phi^{v_i}_{\sigma_i^*}\}_{i \in I} \cup \{X^{\epsilon_j}_{\tilde{\varkappa}_j}\}_{j \in J} \cup \{\Psi^{w_l}_{\rho_l^*}\}_{l \in L} \cup \{F_{\pi_m}\}_{m \in M}$, which are still pairwise orthogonal. It follows, that one has a map $\delta: A \to A$, $\delta^2 = id$, which respects the orthogonality relation $\perp$. Call $\delta \in Bij_\perp(A)$ the *duality map*.

V. LINK TO MERMIN'S EXAMPLE

Let us prove that the set A produces a Kochen–Specker-type contradiction and establish the link with the example of Mermin. Denote

$$\Gamma(A) := \{\phi: C(A) \to A \,|\, \forall\, B \in C(A): \phi(B) \in B\},$$

$$\Delta(A) := \{\phi \in \Gamma(A) \,|\, \forall\, B, B' \in C(A): B \neq B' \Rightarrow \neg\, (\phi(B) \perp \phi(B'))\}.$$

One must show, that $\Delta(A) = \varnothing$. Suppose the contrary, $\Delta(A) \neq \varnothing$. Denote $B_v := \{\Psi^v_\sigma\}_{\sigma \in S_{\hat{v}}}$ ($v \in V$), $\hat{B} := \{F_\pi\}_{\pi \in \Lambda}$. Take $\phi \in \Delta(A)$. The definition of $\Gamma(A) \supset \Delta(A)$ implies, that for every $v \in V$ one has an element $\phi(B_v) \in B_v$, i.e., $\phi(B_v) = \Psi^v_{\sigma_v^\phi}$, where σ_v^ϕ is some element of $S_{\hat{v}}$. Simillarly, $\phi(\hat{B}) = F_{\pi^\phi}$, where π^ϕ is some element of Λ. The definition of $\Delta(A)$ implies, that $\Psi^v_{\sigma_v^\phi}$ is not orthogonal to $\Psi^w_{\sigma_w^\phi}$ (for any $v \neq w$). Using the orthogonality relations one concludes, that $\sigma_v^\phi(vw) = \sigma_w^\phi(vw)$. It means, that a set of functions $\{\sigma_v^\phi\}_{v \in V}$ induces a function $\tau^\phi: E \to \mathbb{Z}_2$ by the formula $\tau^\phi(vw) := \sigma_v^\phi(vw) = \sigma_w^\phi(vw)$ (for any $vw \in E$). Now invoke the fact, that the definition of

$\Delta(A)$ also implies, that for every $v \in V$ the line $\phi(\hat{B})$ should not be orthogonal to $\phi(B_v)$, i.e., $\neg(F_{\pi^\phi} \perp \Psi_{\sigma_v^\phi})$. It follows, that $\forall v \in V: \nabla_{\sigma_v^\phi} = \pi^\phi(v)$. Taking the sum over all $v \in V$ and invoking the definition of Λ, one gets $\Sigma_{v \in V} \nabla_{\sigma_v^\phi} = \Sigma_{v \in V} \pi^\phi(v) = 1$. On the other hand,

$$\sum_{v \in V} \nabla_{\sigma_v^\phi} = \sum_{v \in V} \sum_{\epsilon \in E_v} \sigma_v^\phi(\epsilon) = \sum_{\epsilon \in E} (\tau^\phi(\epsilon) + \tau^\phi(\epsilon)) = 0.$$

Thus one arrives to a contradiction $0=1$. It means that $\nexists \phi \in \Delta(A)$, i.e., $\Delta(A) = \varnothing$.

The link with Mermin's example is established as follows. Let the standard basis in $\mathbb{C}^2$ play the role of the basis $\{\varphi_\alpha\}_{\alpha \in \mathbb{Z}_2}$ involved in the construction of A. Note, that in the proof of $\Delta(A) = \varnothing$ we have used only five complete subsets, B_v $(v = e, f, g, h)$ and $\hat{B}$. The proof of no-hidden-variables theorem by Mermin is given in terms of operators in $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$. There are five complete sets of pairwise commuting orthogonal projectors present in that proof. If one looks at the one-dimensional eigenspaces (i.e., the projective lines) associated to each of these sets, one obtains $B_e \sqcup B_f \sqcup B_g \sqcup B_h \sqcup \hat{B}$.

VI. SATURATION PROPERTY, PART 1

The proof that the set A is saturated with respect to $\perp$ is more bulky. Recall that we have an injective map $\xi: \mathcal{P}(V)^\times \rightarrowtail C(\mathbb{P}(\mathcal{H}))$, where V is a set of 4 symbols $V = \{e, f, g, h\}$. This map has a property $\forall U, U' \in \mathcal{P}(V)^\times, U \neq U': \xi(U) \cap \xi(U') = \varnothing$. It follows, that one can define a map $\eta: A \rightarrow \mathcal{P}(V)$ as follows: one chooses $U \in \mathcal{P}(V)^\times$ to be the value $\eta(l)$ of the map η on a projective line $l \in A$ whenever $l \in \xi(U)$, i.e., η is defined from the requirement $\forall U \in \mathcal{P}(V)^\times: l \in \xi(U) \Leftrightarrow \eta(l) = U$. Note, that η induces a surjection onto $\mathcal{P}(V)^\times$.

The projective lines constituting A may be classified as follows. Call $\#\eta(l)$ the *type* of the projective line $l \in A$. There are four types of projective lines. The image $\eta(l)$ is termed the *kind* of the line l. There are 4 kinds in type 1, 6 kinds in type 2, 4 kinds in type 3, and 1 kind in type 4. We shall also refer to projective lines of the types 1, 2, 3, 4, as being projective lines of Ψ type, X type, Φ type, and F type, respectively. In a similar way, if $\eta(l) = \hat{e}$, the line l is said to be of Ψ^e kind, if $\eta(l) = ef$, the line l is said to be of X^{ef} kind, etc.

Naively, in order to prove the saturation property for A one may think of having to do the following: one must take every subset B of A and test if its elements are pairwise orthogonal; if it happens to be so, one must find a complete subset in A containing B. All this appears to be a very boring problem since $\#\mathcal{P}(A) = 2^{120}$. There is of course a group of permutations S_4 acting on $\mathcal{P}_\perp(A)$ and an observation about the existence of the duality map δ, but the $\#S_4$ is just $4! = 24$ and the order of δ as an element of $Bij_\perp(A)$ is just 2, i.e., $\delta^2 = id$. It means, that one must find a more sophisticated approach to prove the saturation.

We have a map $\eta: A \rightarrow \mathcal{P}(V)$. It induces a map $\mathcal{P}(\eta): \mathcal{P}(A) \rightarrow L := \mathcal{P}(\mathcal{P}(V))$. How to describe an image of the composition $\mathcal{P}_\perp(A) \rightarrowtail \mathcal{P}(A) \rightarrow L$, where the first arrow is the canonical injection?

There exists a natural monomorphism of groups m: $Bij(V) \rightarrowtail Bij(\mathcal{P}(V))$, $\beta \mapsto \mathcal{P}(\beta)$. There also exists a natural monomorphism μ: $Bij(V) \rightarrowtail Bij(A)$, such that for every $\beta \in Bij(V)$ there is a commutative diagram

$$\begin{array}{ccc} A & \xrightarrow{\mu(\beta)} & A \\ \eta \downarrow & & \downarrow \eta \\ \mathcal{P}(V) & \xrightarrow[m(\beta)]{} & \mathcal{P}(V) \end{array} .$$

The monomorphism μ is defined as follows. Take any $\beta \in \mathcal{P}(V)$ and describe explicitly the values of $\mu(\beta)(\cdot)$ on the elements of the form Ψ_σ^v, $X_\varkappa^\epsilon$, Φ_ρ^v, and F_π, where $v \in V$, $\epsilon \in E$, $\sigma \in S_{\hat{v}}$, $\varkappa \in K_\epsilon$, $\rho \in R_{\bar{v}}$, and $\pi \in \Lambda$. Let $\mu(\beta)(\Psi_\sigma^v) := \Psi_{\sigma'}^{v'}$, where $v' = \beta(v)$ and $\forall \epsilon_1 \in E_{v'}: \sigma'(\epsilon_1) = \sigma(\mathcal{P}(\beta^{-1})(\epsilon_1))$;

$\mu(\beta)(X^{\epsilon}_{\varkappa}) := X^{\epsilon'}_{\varkappa'}$, where $\epsilon' = \mathcal{P}(\beta)(\epsilon)$ and $\varkappa'(\epsilon') = \varkappa(\epsilon)$, $\forall v_1 \in V \setminus \epsilon' : \varkappa'(v_1) = \varkappa(\beta^{-1}(v_1))$; $\mu(\beta)(\Phi^{v}_{\rho})$ $:= \Phi^{v'}_{\rho'}$, where $v' = \beta(v)$ and $\forall \epsilon_1 \in E_{v'} : \rho'^{*}(\epsilon_1) = \rho^{*}(\mathcal{P}(\beta^{-1})(\epsilon_1))$; finally $\mu(\beta)(F_{\pi}) := F_{\pi'}$, where $\forall v_1 \in V : \pi'(v_1) = \pi(\beta^{-1}(v_1))$. Note, that for every $\beta \in Bij(V)$ the map $\mu(\beta)$ respects the orthogonality relation $\perp$ on A, and the fact that this relation has a symmetry with respect to the group of permutations of e, f, g, and h can be expressed as

$$\forall \beta \in Bij(V)\ \forall\, l, l' \in A : l \perp l' \Rightarrow \mu(\beta)(l) \perp \mu(\beta)(l').$$

It follows, that whenever an element $Q \in L$ stems from some element $B \in \mathcal{P}_{\perp}(A)$, the element of the form $\mathcal{P}(m(\beta))(Q)$, $\beta \in Bij(V)$, also stems from an element of $\mathcal{P}_{\perp}(A)$, namely from $\mathcal{P}(\mu(\beta))(B)$. Factorize L with respect to the equivalence relation $\sim$ induced by permutations,

$$Q \sim Q' :\Leftrightarrow \exists\, \beta \in Bij(V) : \mathcal{P}(m(\beta))(Q) = Q'.$$

Denote $\Gamma := L/\sim$. The problem of the description of the image of $\mathcal{P}_{\perp}(A)$ in L is then reduced to describing the image of the composition

$$\mathcal{P}_{\perp}(A) \rightarrowtail \mathcal{P}(A) \xrightarrow{\mathcal{P}(\eta)} L \twoheadrightarrow \Gamma,$$

where the first arrow is the canonical injection and the last arrow is the canonical surjection.

It is convenient to introduce graphical notation for the elements of L and Γ. Consider an example. Let $Q = \{\hat{e}, \hat{f}, \overline{e}, eg, efgh\} \in L$. It is represented by a graph,

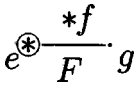

The general principle is the following. A graph may have up to four vertices labeled by the symbols e, f, g or h. If Q contains $\hat{v}$, introduce a vertex labeled by the symbol v and mark it with *; if Q contains $\overline{v}$, introduce a vertex v and draw a circle around it; if there is $vw \in Q$, introduce two vertices v and w and connect them by an edge; finally if Q contains $efgh$, set a letter F near the corresponding figure. Thus to each $Q \in L$ a graph is associated. Note, that if an element Q $\in L$ stems from some element $B \in \mathcal{P}(A)$, i.e., $\mathcal{P}(\eta)(B) = Q$, then by looking at a graph that represents Q one cannot tell everything about B, but the kinds of projective lines that are present in B can be understood.

The graphs representing the elements of Γ are similar to the graphs representing the elements of L. They are obtained by omitting the labels e, f, g, and h of the vertices. For instance, if Q $\in L$ is as in the example given above, and $[Q] \in \Gamma$ is its image under the natural surjection $L \twoheadrightarrow \Gamma$, then $[Q]$ is represented by the graph

Whenever one has an element of Γ of the form $[\mathcal{P}(\eta)(B)]$, where B is some subset of A, the graph that represents this element is called a *shadow* of B.

Let us introduce more terminology. A graph representing an element of Γ is called *admissible* iff by definition it represents an element of the image of $\mathcal{P}_{\perp}(A) \rightarrow \Gamma$; otherwise it is called *non-admissible*. One would like to describe all the admissible graphs. Whenever a graph represents an image of some $Q \in L$ under the canonical surjection $L \twoheadrightarrow \Gamma$, the cardinality $\#Q$ is called the *degree* of this graph. Whenever a graph represents an image of some $B \in \mathcal{P}_{\perp}(A)$ under $\mathcal{P}_{\perp}(A) \rightarrow \Gamma$, one says that B *hangs over* this graph. Any $B' \in P_{\perp}(A)$ containing B is called an *extension* of B. It is called a *pure* extension, iff by definition B' and B hang over the same graph. An extension satisfying $B' = B$ is called *trivial*. An extension B' of B is called *complete* iff by definition $\#B' = 8$ [recall that $8 = \dim_{\mathbb{C}}(\mathcal{H})$, $A \subset \mathbb{P}(\mathcal{H})$].

Proposition 1: (1) *The graph* $*$ *is admissible and any element of* $\mathcal{P}_\perp(A)$ *hanging over this graph admits a pure complete extension.*

(2) *The graph* $**$ *is admissible and any element of* $\mathcal{P}_\perp(A)$ *hanging over this graph admits a pure complete extension.*

(3) *The graph* $\triangle$ *is not admissible.*

(4) *The graph* $***$ *is admissible and any element of* $\mathcal{P}_\perp(A)$ *hanging over this graph admits a pure extension up to a set of cardinality 6. Any element of* $\mathcal{P}_\perp(A)$ *of cardinality 6, which hangs over this graph, has a complete extension hanging over* $***\odot$.

(5) *The graph* $***\odot$ *is admissible and any element of* $\mathcal{P}_\perp(A)$ *hanging over this graph admits a pure complete extension.*

(6) *The graph* $****$ *is admissible and any element of* $\mathcal{P}_\perp(A)$ *hanging over this graph does not have nontrivial pure extensions. Any element of* $\mathcal{P}_\perp(A)$ *hanging over this graph has a complete extension hanging over* $\circledast\circledast\circledast\circledast$.

(7) *The graph* $****F$ *is not admissible.*

Proof: (1) A set consisting of one projective line Ψ^e_σ, where σ is some element of $S_{\hat{e}}$, gives an example of a set hanging over $*$. Every set hanging over this graph is of the form $B=\{\Psi^v_\sigma\}_{\sigma\in S}$, where v is some element of V and S is some nonempty subset of $S_{\hat{v}}$. This subset B is always a subset of a complete set $\{\Psi^v_\sigma\}_{\sigma\in S_{\hat{v}}}$.

(2) Take any $a\in\mathbb{Z}_2$ and choose any $\sigma\in S_{\hat{e}}$ such that $\sigma(ef)=a$, and any $\sigma_1\in S_{\hat{f}}$ such that $\sigma_1(ef)=1+a$. Then the projective lines Ψ^e_σ and $\Psi^f_{\sigma_1}$ are orthogonal and one can take them two as a set which hangs over the graph $**$. An arbitrary set B hanging over this graph is always of the form $B=\{\Psi^v_\sigma\}_{\sigma\in S}\cup\{\Psi^w_{\sigma_1}\}_{\sigma_1\in S_1}$, where S and S_1 are some nonempty subsets of $S_{\hat{v}}$ and $S_{\hat{w}}$, respectively, v, $w\in V$, $v\neq w$. One associates to B a parameter $a:=\sigma(vw)=1+\sigma_1(vw)$, where σ is any element of S and σ_1 is any element of S_1. Denote $S':=\{\sigma\in S_{\hat{v}}|\,\sigma(vw)=a\}$ and $S'_1:=\{\sigma_1\in S_{\hat{w}}|\,\sigma_1(vw)=1+a\}$. Since $\#S'=\#S'_1=4$, the set $B':=\{\Psi^v_\sigma\}_{\sigma\in S'}\cup\{\Psi^w_{\sigma_1}\}_{\sigma_1\in S'_1}$ gives the required pure complete extension of B.

(3) If the graph $\triangle$ is admissible, then there should exist three pairwise orthogonal projective lines of the form $X^{ef}_\varkappa$, $X^{eg}_{\varkappa_1}$ and $X^{fg}_{\varkappa_3}$, where $\varkappa$, $\varkappa_1$, and $\varkappa_2$ are some elements of K_{ef}, K_{eg}, and K_{fg}, respectively. The orthogonality relations yield three equations,

$$X^{ef}_\varkappa \perp X^{eg}_{\varkappa_1} \Leftrightarrow \varkappa(ef)+\varkappa(h)=1+\varkappa_1(eg)+\varkappa_1(h),$$

$$X^{ef}_\varkappa \perp X^{fg}_{\varkappa_2} \Leftrightarrow \varkappa(ef)+\varkappa(h)=1+\varkappa_2(fg)+\varkappa_2(h),$$

$$X^{eg}_{\varkappa_1} \perp X^{fg}_{\varkappa_2} \Leftrightarrow \varkappa_1(eg)+\varkappa_1(h)=1+\varkappa_2(fg)+\varkappa_2(h).$$

Taking the sum of these three equations one arrives to a contradiction $0=1$. This means, that the mentioned triangle is not admissible.

(4) One can construct an example of three pairwise orthogonal lines of the form Ψ^e_σ, $\Psi^f_{\sigma_1}$, $\Psi^g_{\sigma_2}$ as follows: take any $a,b,c\in\mathbb{Z}_2$ and choose $\sigma\in S_{\hat{e}}$ such that $\sigma(ef)=a$, $\sigma(eg)=b$, any $\sigma_1\in S_{\hat{f}}$ such that $\sigma_1(ef)=1+a$, $\sigma_1(fg)=c$, and $\sigma_2\in S_{\hat{g}}$ such that $\sigma_2(eg)=1+b$, $\sigma_2(fg)=1+c$. Then the orthogonality relations between the mentioned three lines are fulfilled and the set consisting of these three hangs over the graph $***$. An arbitrary set hanging over this graph is of the form $B=\{\Psi^v_\sigma\}_{\sigma\in S}\cup\{\Psi^w_\sigma\}_{\sigma_1\in S_1}\cup\{\Psi^z_\sigma\}_{\sigma_2\in S_2}$, where S, S_1, and S_2 are some nonempty subsets of $S_{\hat{v}}$, $S_{\hat{w}}$, and $S_{\hat{z}}$, respectively, $v,w,z\in V$, $v\neq w$, $v\neq z$, $w\neq z$. Without loss of generality one may specialize v, w and z to e, f, and g, respectively. Associate to B three parameters $a,b,c\in\mathbb{Z}_2$: $a:=\sigma(ef)=1+\sigma_1(ef)$, $b:=\sigma(eg)=1+\sigma_2(eg)$, $c:=\sigma_1(fg)=1+\sigma_2(fg)$, where σ, σ_1 and σ_2 are elements of S, S_1, and S_2, respectively. Denote $S':=\{\sigma\in S_{\hat{e}}|\,\sigma(ef)=a\&\sigma(eg)=b\}$, $S'_1:=\{\sigma_1\in S_{\hat{f}}|\,\sigma_1(ef)=1+a\&\sigma_1(fg)=c\}$, and $S'_2:=\{\sigma_2\in S_{\hat{g}}|\,\sigma_2(eg)=1+b\&\sigma_2(fg)=1+c\}$. Since $\#S'=\#S'_1=\#S'_2=2$, the set

$B' := \{\Psi^v_\sigma\}_{\sigma\in S'} \cup \{\Psi^w_\sigma\}_{\sigma_1\in S'_1} \cup \{\Psi^z_\sigma\}_{\sigma_2\in S'_2}$ is a pure extension of B up to a set of cardinality 6. Now look for a projective line Φ^h_ρ, $\rho \in R_{\bar{h}}$, which is orthogonal to every element of B'. This yields the following equations:

$$\forall \sigma \in S' : \nabla_\sigma + \sigma(eh) = 1 + \nabla_{\rho^*} + \rho^*(eh),$$

$$\forall \sigma_1 \in S'_1 : \nabla_{\sigma_1} + \sigma_1(fh) = 1 + \nabla_{\rho^*} + \rho^*(fh),$$

$$\forall \sigma_2 \in S'_2 : \nabla_{\sigma_2} + \sigma_2(gh) = 1 + \nabla_{\rho^*} + \rho^*(gh).$$

Observe that the left-hand sides of these equations may be expressed in terms of parameters a, b, and c as $\nabla_\sigma + \sigma(eh) = \sigma(ef) + \sigma(eg) = a + b$, $\nabla_{\sigma_1} + \sigma_1(fh) = \sigma_1(ef) + \sigma_1(fg) = (1+a) + c$, and $\nabla_{\sigma_2} + \sigma_2(gh) = \sigma_1(eg) + \sigma_1(fg) = (1+b) + (1+c)$. Reduce the equations for ρ to $\rho^*(fh) + \rho^*(gh) = 1 + a + b$, $\rho^*(eh) + \rho^*(gh) = a + c$ and $\rho^*(eh) + \rho^*(fh) = 1 + b + c$. The latter equation is nothing but a sum of the first two and may be dropped. Denote $R' := \{\rho \in R_{\bar{h}} \mid \rho^*(fh) + \rho^*(gh) = 1 + a + b \,\&\, \rho^*(eh) + \rho^*(gh) = a + c\}$. Taking into account that $\#R = 2$, one obtains a set $B'' := B' \cup \{\Phi^h_\rho\}_{\rho\in R'}$, which is a complete extension of B' and hangs over $***\odot$.

(5) The admissibility of $***\odot$ follows from (4). Consider any $B \in \mathcal{P}_\perp(A)$ hanging over this graph. Without loss of generality, one may assume, that $B = \{\Psi^e_\sigma\}_{\sigma\in S} \cup \{\Psi^f_\sigma\}_{\sigma_1\in S_1} \cup \{\Psi^g_\sigma\}_{\sigma_2\in S_2} \cup \{\Phi^h_\rho\}_{\rho\in R}$, where S, S_1, S_2, and R are some nonempty subsets of $S_{\hat{e}}$, $S_{\hat{f}}$, $S_{\hat{g}}$, and $R_{\bar{h}}$, respectively. Consider a subset of B consisting of all projective lines of Ψ type and associate to it the parameters $a, b, c \in \mathbb{Z}_2$ in a way as described in the proof of (4). Let S', S'_1, S'_2, and R' be defined as in the proof of (4). Then the set $\tilde{B} := \{\Psi^e_\sigma\}_{\sigma\in S'} \cup \{\Psi^f_\sigma\}_{\sigma_1\in S'_1} \cup \{\Psi^g_\sigma\}_{\sigma_2\in S'_2} \cup \{\Phi^h_\rho\}_{\rho\in R'}$ is the required pure complete extension of B.

(6) A set of pairwise orthogonal projective lines Ψ^e_σ, $\Psi^f_{\sigma_1}$, $\Psi^g_{\sigma_2}$, and $\Psi^h_{\sigma_3}$, which is required to establish the admissibility of the graph $****$, can be constructed as follows. Take any $\mathbb{Z}_2$-valued function φ on $E := \{ef, eg, eh, fg, fh, gh\}$. Denote $a := \varphi(ef)$, $b := \varphi(eg)$, $c := \varphi(fg)$, $p := \varphi(eh)$, $q := \varphi(fh)$, $r := \varphi(gh)$. Take the following σ, σ_1, σ_2, and σ_3: $\sigma(ef) = a$, $\sigma(eg) = b$, $\sigma(eh) = p$; $\sigma_1(ef) = 1 + a$, $\sigma_1(fg) = c$, $\sigma_1(fh) = q$; $\sigma_2(eg) = 1 + b$, $\sigma_2(fg) = 1 + c$, $\sigma_2(gh) = r$; $\sigma_3(eh) = 1 + p$, $\sigma_3(fh) = 1 + q$, $\sigma_3(gh) = 1 + r$. Then the projective lines Ψ^e_σ, $\Psi^f_{\sigma_1}$, $\Psi^g_{\sigma_2}$, and $\Psi^h_{\sigma_3}$ constitute a set as required. An arbitrary set B hanging over the mentioned graph is of the form $B = \{\Psi^e_\sigma\}_{\sigma\in S} \cup \{\Psi^f_{\sigma_1}\}_{\sigma_1\in S_1} \cup \{\Psi^g_{\sigma_2}\}_{\sigma_2\in S_2} \cup \{\Psi^h_{\sigma_3}\}_{\sigma_3\in S_3}$, where S, S_1, S_2, and S_3 are some nonempty subsets of $S_{\hat{e}}$, $S_{\hat{f}}$, $S_{\hat{g}}$, and $S_{\hat{h}}$ respectively. To every such B associate φ: $E \to \mathbb{Z}_2$ by setting $\varphi(ef) = \sigma(ef)$, $\varphi(eg) = \sigma(eg)$, $\varphi(eh) = \sigma(eh)$, $\varphi(fg) = \sigma_1(fg)$, $\varphi(fh) = \sigma_1(fh)$, $\varphi(gh) = \sigma_2(gh)$, where σ, σ_1, and σ_2 can be taken to be any elements of S, S_1, and S_2, respectively. The set S is a nonempty subset of $S' := \{\sigma \in S_{\hat{e}} \mid \sigma(ef) = \varphi(ef) \,\&\, \sigma(eg) = \varphi(eg) \,\&\, \sigma(eh) = \varphi(eh)\}$. Since $\#S' = 1$, we see that $\#S = 1$. Similarly, $\#S_1 = \#S_2 = \#S_3 = 1$. In the latter case $S_3 \subset S'_3 := \{\sigma_3 \in S_{\hat{h}} \mid \sigma_3(eh) = 1 + \varphi(eh) \,\&\, \sigma_3(fh) = 1 + \varphi(fh) \,\&\, \sigma_3(gh) = 1 + \varphi(gh)\}$. This means that a set hanging over $****$ cannot have nontrivial pure extensions.

Let us now construct a complete extension of a set B, where B hangs over $****$. Let φ denote the function associated to $B = \{\Psi^e_\sigma, \Psi^f_{\sigma_1}, \Psi^g_{\sigma_2}, \Psi^h_{\sigma_3}\} \in \mathcal{P}_\perp(A)$ as described above, and let a, b, c, p, q, and r be its values on the edges ef, eg, fg, eh, fh, and gh, respectively. Looking for an extension which hangs over $\circledast\circledast\circledast\circledast$, we need to construct projective lines of the form Φ^e_ρ, $\Phi^f_{\rho_1}$, $\Phi^g_{\rho_2}$, and $\Phi^h_{\rho_3}$. Define ρ, ρ_1, ρ_2, and ρ_3 by the formulas $\rho^*(ef) = a + b + c + p + q$, $\rho^*(eg) = 1 + a + b + c + p + r$, $\rho^*(eh) = a + b + p + q + r$; $\rho^*_1(ef) = 1 + a + b + c + p + q$, $\rho^*_1(fg) = a + b + c + q + r$, $\rho^*_1(fh) = 1 + a + c + p + q + r$; $\rho^*_2(eg) = a + b + c + p + r$, $\rho^*_2(fg) = 1 + a + b + c + q + r$, $\rho^*_2(gh) = b + c + p + q + r$; $\rho^*_3(eh) = 1 + a + b + p + q + r$, $\rho^*_3(fh) = a + c + p + q + r$, $\rho^*_3(gh) = 1 + b + c + p + q + r$. Straightforward computation establishes that $B' := B \cup \{\Phi^e_\rho, \Phi^f_{\rho_1}, \Phi^g_{\rho_2}, \Phi^h_{\rho_3}\}$ is a complete extension of B.

(7) It is necessary to show that five projective lines of the form Ψ^e_σ, $\Psi^f_{\sigma_1}$, $\Psi^g_{\sigma_2}$, $\Psi^h_{\sigma_3}$, and F_π cannot be pairwise *orthogonal*. Recall that we already know that they cannot be pairwise *nonorthogonal*. The conditions of orthogonality between the projective lines of Ψ type yield a system of

equations, $\sigma(ef)+\sigma_1(ef)=1$, $\sigma(eg)+\sigma_2(eg)=1$, $\sigma(eh)+\sigma_3(eh)=1$, $\sigma_1(fg)+\sigma_2(fg)=1$, $\sigma_1(fh)+\sigma_3(fh)=1$, and $\sigma_2(gh)+\sigma_3(gh)=1$. By summation, one obtains $\nabla_\sigma+\nabla_{\sigma_1}+\nabla_{\sigma_2}+\nabla_{\sigma_3}=0$. On the other hand, the orthogonality conditions with F_π yield the equations, $\pi(e)=1+\nabla_\sigma$, $\pi(f)=1+\nabla_{\sigma_1}$, $\pi(g)=1+\nabla_{\sigma_2}$, and $\pi(h)=1+\nabla_{\sigma_3}$. Recalling that $\Sigma_{v\in V}\pi(v)=1$, and summing the foregoing equations yields $1=\nabla_\sigma+\nabla_{\sigma_1}+\nabla_{\sigma_2}+\nabla_{\sigma_3}$. Hence, the requirement that all five projective lines are pairwise orthogonal leads to a contradiction $1=0$. □

Proposition 2: Let $B\in\mathcal{P}_\perp(A)$ be a set hanging over ∗∗∗∗.

(1) *For every $v\in V$ there exists a unique projective line of Φ^v-kind which is orthogonal to every projective line belonging to B.*

(2) *There exist no extensions of B which contain a projective line of X type or of F type.*

(3) *The complete extension of B is unique and hangs over ⊛⊛⊛⊛.*

Proof: (1) It is sufficient to consider $v=e$. If Ψ^e_σ, $\Psi^f_{\sigma_1}$, $\Psi^g_{\sigma_2}$, and $\Psi^h_{\sigma_3}$ are four pairwise orthogonal projective lines, then the requirement that Φ^e_ρ is orthogonal to each of them yields four equations, $\nabla_{\rho^*}=1+\nabla_\sigma$, $\nabla_{\rho^*}+\rho^*(ef)=1+\nabla_{\sigma_1}+\sigma_1(ef)$, $\nabla_{\rho^*}+\rho^*(eg)=1+\nabla_{\sigma_2}+\sigma_2(eg)$, and $\nabla_{\rho^*}+\rho^*(eh)=1+\nabla_{\sigma_3}+\sigma_3(eh)$. Expressing ∇_{ρ^*} from the first equation and substituting it into the other three, one finds the expressions for the values of ρ^* via σ, σ_1, σ_2, and σ_3.

(2) The fact that B cannot have an extension containing a projective line of F type follows from the nonadmissibility of the graph $\ast\ast\ast\ast F$. Let us show that the graph $\ast$—$\ast$ is nonadmissible. This will imply that an extension of B cannot contain an element of X type. Consider three projective lines of the form Ψ^e_σ, $\Psi^f_{\sigma_1}$, and $X^{ef}_\varkappa$, and impose the condition that they are pairwise orthogonal. This yields the equations, $\sigma(ef)=1+\sigma_1(ef)$, $\sigma(ef)=1+\varkappa(ef)$, and $\sigma_1(ef)=1+\varkappa(ef)$. The sum of the second and the third equations yields $\sigma(ef)+\sigma_1(ef)=0$, contradicting the first equation. It means that the mentioned graph is not admissible.

(3) The existence of the extension of B hanging over ⊛⊛⊛⊛ has been proved in the previous proposition. Since an extension of B cannot contain elements of X or F type, it should hang over a graph which may contain only stars and circles. According to the previous proposition, a set hanging over a graph ∗∗∗∗ cannot have nontrivial pure extensions. It follows, that a complete extension of B contains projective lines of the form Φ^v_ρ. Every such projective line is uniquely defined according to (1). It follows that a complete extension of B hangs over ⊛⊛⊛⊛ and is unique. □

VII. GROUP OF SYMMETRY

We have given an *explicit* description of every element of the finite set A and by that we have an opportunity to *construct* the maps φ: $A\to A$ by simply saying for each $l\in A$ which $l'\in A$ corresponds to it under φ. One would like to have a similar opportunity for the set $\mathcal{P}_\perp(A)$, i.e., one needs to *characterize* the elements of $\mathcal{P}_\perp(A)$. In particular, for the set of all complete sets $C(A)\subset\mathcal{P}_\perp(A)$ it would be nice to have some group transitively acting on $C(A)$, so that having found just one complete set, one could automatically generate all the others.

Recall that there is a map η: $A\to\mathcal{P}(V)$, where V is a set of four symbols $V=\{e,f,g,h\}$. We shall describe a group G which acts on the set $L=\mathcal{P}(\mathcal{P}(V))$ and then describe a group $\mathcal{G}$ which acts on $\mathcal{P}_\perp(A)$.

We start with the definition of the group G. Consider the group $Bij(\mathcal{P}(V))$ of all bijections of the power set of V. One has $\#V=4$, $\#\mathcal{P}(V)=16$, $\#Bij(\mathcal{P}(V))=16!$. Associate to each $S\in\mathcal{P}(V)$ a map T_S: $\mathcal{P}(V)\to\mathcal{P}(V)$ defined by the formula

$$T_S(U) := \begin{cases} U, & \text{if } \#(S\cap U) \text{ is even},\\ \overline{U\Delta S}, & \text{if } \#(S\cap U) \text{ is odd}, \end{cases} \tag{3}$$

where U varies over $\mathcal{P}(V)$, the bar denotes the completion of a set in V and Δ denotes the symmetric difference of two subsets. For any S one has $T_S^2=id$. In particular, T_S is a bijection, $T_S\in Bij(\mathcal{P}(V))$. Define G to be a subgroup in $Bij(\mathcal{P}(V))$ generated by reflections T_S, $S\in\mathcal{P}(V)$:

$$G := \langle\{T_S | S\in\mathcal{P}(V)\}\rangle\subset Bij(\mathcal{P}(V)).$$

Note, that $T_{\varnothing}=T_{efgh}=id$. Note for any S, that $T_S(\varnothing)=\varnothing$.

For a given $S\in\mathcal{P}(V)$, write $U_1\leftrightarrow U_2$ to express that $T_S(U_1)=U_2\&T_S(U_2)=U_1$, and $U=inv$ to express $T_S(U)=U$. Then, for example, $T_{\hat{e}}$, T_{ef}, and $T_{\overline{e}}$ are explicitly described as follows. $T_{\hat{e}}$ corresponds to

$$\hat{e}\leftrightarrow efgh,\quad \overline{f}\leftrightarrow ef,\quad \overline{g}\leftrightarrow eg,\quad \overline{h}\leftrightarrow eh,$$

$$\varnothing,\overline{e},\hat{f},\hat{g},\hat{h},fg,fh,gh=inv;$$

T_{ef} corresponds to

$$e\leftrightarrow\overline{f},\quad f\leftrightarrow\overline{e},\quad eg\leftrightarrow eh,\quad fg\leftrightarrow fh,$$

$$\varnothing,g,h,\overline{g},\overline{h},ef,gh,efgh=inv;$$

and $T_{\overline{e}}$ corresponds to

$$\overline{e}\leftrightarrow efgh,\quad \hat{f}\leftrightarrow ef,\quad \hat{g}\leftrightarrow eg,\quad \hat{h}\leftrightarrow eh,$$

$$\varnothing,\hat{e},\overline{f},\overline{g},\overline{h},fg,fh,gh=inv.$$

Explicit descriptions of the other $T_{\hat{v}}$, T_{vw}, and $T_{\overline{v}}$ are obtatined via permutations of symbols e, f, g, and h. Note that for every $S\in\mathcal{P}(V)$,

$$T_{m(\beta)(S)}=m(\beta)T_S m(\beta^{-1}),\quad \beta\in Bij(V),$$

where m is the natural monomorphism of groups, m: $Bij(V)\rightarrowtail Bij(\mathcal{P}(V))$, $\beta\mapsto\mathcal{P}(\beta)$.

Recall that there also exists a natural monomorphism μ: $Bij(V)\rightarrowtail Bij(A)$ described in the previous section.

Every element $g\in G$ is a map $g:\mathcal{P}(V)\tilde{\to}\mathcal{P}(V)$. It induces a map $\mathcal{P}(g):L\tilde{\to}L$, $L=\mathcal{P}(\mathcal{P}(V))$. It means that there is a natural action of G on L. Recall that we have a map $\eta:A\to\mathcal{P}(V)$. It turns out that the maps T_S, $S\in\mathcal{P}(V)$, can be lifted up to maps $\theta_S:A\tilde{\to}A$ in such a way that the subgroup of $Bij(A)$ generated by $\{\theta_S\}_S$ has a natural action on the set $\mathcal{P}_{\perp}(A)$.

Proposition 3: For every $S\in\mathcal{P}(V)$ there exists a map $\theta_S:A\to A$ such that

(1) $\forall l,l'\in A: l\perp l'\Rightarrow\theta_S(l)\perp\theta_S(l')$;

(2) *The map θ_S renders the following diagram commutative:*

$$\begin{array}{ccc} A & \xrightarrow{\theta_S} & A \\ {\scriptstyle\eta}\downarrow & & \downarrow{\scriptstyle\eta} \\ \mathcal{P}(V) & \xrightarrow[T_S]{} & \mathcal{P}(V) \end{array} \tag{4}$$

(3) $\theta_S^2=id$.

Proof: If $S=\varnothing$ or $S=V$, then the corresponding $T_S=id$ and one may take $\theta_S=id$. It means that essentially one must to consider the cases of nonempty proper subsets $S\subset V$. We describe explicit formulas for $\theta_{\hat{e}}$, θ_{ef}, and $\theta_{\overline{e}}$. The other maps are defined by permutations of e, f, g, and h.

We start with $\theta_{\hat{e}}$. Invoking the explicit description for $T_{\hat{e}}$ given above, one has, for example, $\hat{e}\leftrightarrow efgh$. Thus, a projective line of the form Ψ^e_{σ}, $\sigma\in S_{\hat{e}}$, should map under the action of $\theta_{\hat{e}}$ to a projective line of the form $F_{\pi'}$, where π' is some element of Λ. Denote this by $\Psi^e_{\sigma}\overset{\theta_{\hat{e}}}{\rightsquigarrow}F_{\pi'}$. A complete description of $\theta_{\hat{e}}$ consists in the description of its actions on the elements of the form

$$\Psi^e_{\sigma},\quad \Psi^f_{\sigma_1},\quad \Psi^g_{\sigma_2},\quad \Psi^h_{\sigma_3},$$

$$\Phi^e_\rho, \quad \Phi^f_{\rho_1}, \quad \Phi^g_{\rho_2}, \quad \Phi^h_{\rho_3},$$

$$X^{ef}_\varkappa, \quad X^{eg}_{\varkappa_1}, \quad X^{eh}_{\varkappa_2}, \quad X^{fg}_{\varkappa_3}, \quad X^{fh}_{\varkappa_4}, \quad X^{gh}_{\varkappa_5}, \quad F_\pi.$$

Define $\theta_{\hat{e}}$ as follows:

$$\Psi^e_\sigma \overset{\theta_{\hat{e}}}{\rightsquigarrow} F_{\pi'}: \qquad F_\pi \overset{\theta_{\hat{e}}}{\rightsquigarrow} \Psi^e_{\sigma'}:$$
$$\pi'(e) := 1 + \nabla_\sigma, \quad \sigma'(ef) := \pi(f),$$
$$\pi'(f) := \sigma(ef), \quad \sigma'(eg) := \pi(g),$$
$$\pi'(g) := \sigma(eg), \quad \sigma'(eh) := \pi(h).$$
$$\pi'(h) := \sigma(eh).$$

$$\Phi^f_{\rho_1} \overset{\theta_{\hat{e}}}{\rightsquigarrow} X^{ef}_{\varkappa'}: \qquad X^{ef}_\varkappa \overset{\theta_{\hat{e}}}{\rightsquigarrow} \Phi^f_{\rho_1'}:$$
$$\varkappa'(ef) := \nabla_{\rho_1^*}, \qquad \rho_1'^*(ef) := \varkappa(ef) + \varkappa(g) + \varkappa(h),$$
$$\varkappa'(g) := \rho_1^*(ef) + \rho_1^*(fg), \qquad \rho_1'^*(fg) := \varkappa(ef) + \varkappa(h),$$
$$\varkappa'(h) := \rho_1^*(ef) + \rho_1^*(fh). \qquad \rho_1'^*(fh) := \varkappa(ef) + \varkappa(g).$$

$$\Phi^g_{\rho_2} \overset{\theta_{\hat{e}}}{\rightsquigarrow} X^{eg}_{\varkappa_1'}: \qquad X^{eg}_{\varkappa_1} \overset{\theta_{\hat{e}}}{\rightsquigarrow} \Phi^g_{\rho_2'}:$$
$$\varkappa_1'(eg) := \nabla_{\rho_2^*}, \qquad \rho_2'^*(eg) := \varkappa_1(eg) + \varkappa_1(f) + \varkappa_1(h),$$
$$\varkappa_1'(f) := \rho_2^*(eg) + \rho_2^*(fg), \qquad \rho_2'^*(fg) := \varkappa_1(eg) + \varkappa_1(h),$$
$$\varkappa_1'(h) := \rho_2^*(eg) + \rho_2^*(gh). \qquad \rho_2'^*(gh) := \varkappa_1(eg) + \varkappa_1(f).$$

$$\Phi^h_{\rho_3} \overset{\theta_{\hat{e}}}{\rightsquigarrow} X^{eh}_{\varkappa_2'}: \qquad X^{eh}_{\varkappa_2} \overset{\theta_{\hat{e}}}{\rightsquigarrow} \Phi^h_{\rho_3'}:$$
$$\varkappa_2'(eh) := \nabla_{\rho_3^*}, \qquad \rho_3'^*(eh) := \varkappa_2(eh) + \varkappa_2(f) + \varkappa_2(g),$$
$$\varkappa_2'(f) := \rho_3^*(eh) + \rho_3^*(fh), \qquad \rho_3'^*(fh) := \varkappa_2(eh) + \varkappa_2(g),$$
$$\varkappa_2'(g) := \rho_3^*(eh) + \rho_3^*(gh). \qquad \rho_3'^*(gh) := \varkappa_2(eh) + \varkappa_2(f).$$

$$\Psi^f_{\sigma_1} \overset{\theta_{\hat{e}}}{\rightsquigarrow} \Psi^f_{\sigma_1'}: \qquad X^{gh}_{\varkappa_5} \overset{\theta_{\hat{e}}}{\rightsquigarrow} X^{gh}_{\varkappa_5'}:$$
$$\sigma_1'(ef) := \nabla_{\sigma_1}, \qquad \varkappa_5'(gh) := \varkappa_5(gh),$$
$$\sigma_1'(fg) := \sigma_1(fg), \qquad \varkappa_5'(e) := \varkappa_5(e),$$
$$\sigma_1'(fh) := \sigma_1(fh). \qquad \varkappa_5'(f) := 1 + \varkappa_5(e) + \varkappa_5(f).$$

$$\Psi^g_{\sigma_2} \overset{\theta_{\hat{e}}}{\rightsquigarrow} \Psi^g_{\sigma_2'}: \qquad X^{fh}_{\varkappa_4} \overset{\theta_{\hat{e}}}{\rightsquigarrow} X^{fh}_{\varkappa_4'}:$$
$$\sigma_2'(eg) := \nabla_{\sigma_2}, \qquad \varkappa_4'(fh) := \varkappa_4(fh),$$
$$\sigma_2'(fg) := \sigma_2(fg), \qquad \varkappa_4'(e) := \varkappa_4(e),$$
$$\sigma_2'(gh) := \sigma_2(gh). \qquad \varkappa_4'(g) := 1 + \varkappa_4(e) + \varkappa_4(g).$$

$$\Psi^{h}_{\sigma_3} \overset{\theta_{\hat{e}}}{\rightsquigarrow} \Psi^{h}_{\sigma'_3}: \qquad X^{fg}_{\varkappa_3} \overset{\theta_{\hat{e}}}{\rightsquigarrow} X^{fg}_{\varkappa'_3}:$$

$$\sigma'_3(eh) := \nabla_{\sigma_3}, \qquad \sigma'_3(fg) := \varkappa_3(fg),$$

$$\sigma'_3(fh) := \sigma_3(fh), \qquad \varkappa'_3(e) := \varkappa_3(e),$$

$$\sigma'_3(gh) := \sigma_3(gh). \qquad \varkappa'_3(h) := 1 + \varkappa_3(e) + \varkappa_3(h).$$

$$\Phi^{e}_{\rho} \overset{\theta_{\hat{e}}}{\rightsquigarrow} \Phi^{e}_{\rho'}:$$

$$\rho'^{*}(ef) := 1 + \rho^{*}(ef),$$

$$\rho'^{*}(eg) := 1 + \rho^{*}(eg),$$

$$\rho'^{*}(eh) := 1 + \rho^{*}(eh).$$

Note, that the formulas defining $\theta_{\hat{e}}$ have a symmetry with respect to the permutations of symbols f, g, h. It is a straightforward calculation to show that $\theta_{\hat{e}}$ respects the orthogonality relation $\perp$ on A. The commutativity of the mentioned diagram follows directly from the construction of $\theta_{\hat{e}}$. The verification that $\theta_{\hat{e}}$ is indeed a reflection is also straightforward.

Now define θ_{ef},

$$\Psi^{e}_{\sigma} \overset{\theta_{ef}}{\rightsquigarrow} \Phi^{f}_{\rho'_1}: \qquad \Phi^{f}_{\rho_1} \overset{\theta_{ef}}{\rightsquigarrow} \Psi^{e}_{\sigma'}:$$

$$\rho'^{*}_1(ef) := \sigma(ef), \qquad \sigma'(ef) := \rho^{*}_1(ef),$$

$$\rho'^{*}_1(fg) := \sigma(ef) + \sigma(eh), \qquad \sigma'(eg) := \rho^{*}_1(ef) + \rho^{*}_1(fh),$$

$$\rho'^{*}_1(fh) := \sigma(ef) + \sigma(eg). \qquad \sigma'(eh) := \rho^{*}_1(ef) + \rho^{*}_1(fg).$$

$$\Psi^{f}_{\sigma_1} \overset{\theta_{ef}}{\rightsquigarrow} \Phi^{e}_{\rho'}: \qquad \Phi^{e}_{\rho} \overset{\theta_{ef}}{\rightsquigarrow} \Psi^{f}_{\sigma'_1}:$$

$$\rho'^{*}(ef) := \sigma_1(ef), \qquad \sigma'_1(ef) := \rho^{*}(ef),$$

$$\rho'^{*}(eg) := \sigma_1(ef) + \sigma_1(fh), \qquad \sigma'_1(fg) := \rho^{*}(ef) + \rho^{*}(eh),$$

$$\rho'^{*}(eh) := \sigma_1(ef) + \sigma_1(fg). \qquad \sigma'_1(fh) := \rho^{*}(ef) + \rho^{*}(eg).$$

$$X^{eg}_{\varkappa_1} \overset{\theta_{ef}}{\rightsquigarrow} X^{eh}_{\varkappa'_2}: \qquad X^{eh}_{\varkappa_2} \overset{\theta_{ef}}{\rightsquigarrow} X^{eg}_{\varkappa'_1}:$$

$$\varkappa'_2(eh) := \varkappa_1(f), \qquad \varkappa'_1(eg) := \varkappa_2(f),$$

$$\varkappa'_2(f) := \varkappa_1(eg), \qquad \varkappa'_1(f) := \varkappa_2(eh),$$

$$\varkappa'_2(g) := 1 + \varkappa_1(eg) + \varkappa_1(f) + \varkappa_1(h). \qquad \varkappa'_1(h) := 1 + \varkappa_2(eh) + \varkappa_2(f) + \varkappa_2(g).$$

$$X^{fg}_{\varkappa_3} \overset{\theta_{ef}}{\rightsquigarrow} X^{fh}_{\varkappa'_4}: \qquad X^{fh}_{\varkappa_4} \overset{\theta_{ef}}{\rightsquigarrow} X^{fg}_{\varkappa'_3}:$$

$$\varkappa'_4(fh) := \varkappa_3(e), \qquad \varkappa'_3(fg) := \varkappa_4(e),$$

$$\varkappa'_4(e) := \varkappa_3(fg), \qquad \varkappa'_3(e) := \varkappa_4(fh),$$

$$\varkappa'_4(g) := 1 + \varkappa_3(fg) + \varkappa_3(e) + \varkappa_3(h). \qquad \varkappa'_3(h) := 1 + \varkappa_4(fh) + \varkappa_4(e) + \varkappa_4(g).$$

$$\Psi^{g}_{\sigma_2} \overset{\theta_{ef}}{\rightsquigarrow} \Psi^{g}_{\sigma_2'}: \qquad \Phi^{g}_{\rho_2} \overset{\theta_{ef}}{\rightsquigarrow} \Phi^{g}_{\rho_2'}:$$

$$\sigma_2'(eg) := \sigma_2(eg) + \sigma_2'(gh), \quad \rho_2'^{*}(eg) := \rho_2^{*}(eg) + \rho_2^{*}(gh),$$
$$\sigma_2'(fg) := \sigma_2'(fg) + \sigma_2'(gh), \quad \rho_2'^{*}(fg) := \rho_2^{*}(fg) + \rho_2^{*}(gh),$$
$$\sigma_2'(gh) := \sigma_2'(gh). \qquad \rho_2'^{*}(gh) := \rho_2^{*}(gh).$$

$$\Psi^{h}_{\sigma_3} \overset{\theta_{ef}}{\rightsquigarrow} \Psi^{h}_{\sigma_3'}: \qquad \Phi^{h}_{\rho_3} \overset{\theta_{ef}}{\rightsquigarrow} \Phi^{h}_{\rho_3'}:$$

$$\sigma_3'(eh) := \sigma_3(eh) + \sigma_3(gh), \quad \rho_3'^{*}(eh) := \rho_3^{*}(eh) + \rho_3^{*}(gh),$$
$$\sigma_3'(fh) := \sigma_3(fh) + \sigma_3(gh), \quad \rho_3'^{*}(fh) := \rho_3^{*}(fh) + \rho_3^{*}(gh),$$
$$\sigma_3'(gh) := \sigma_3(gh). \qquad \rho_3'^{*}(gh) := \rho_3^{*}(gh).$$

$$X^{ef}_{\varkappa} \overset{\theta_{ef}}{\rightsquigarrow} X^{ef}_{\varkappa'}: \qquad X^{gh}_{\varkappa_5} \overset{\theta_{ef}}{\rightsquigarrow} X^{gh}_{\varkappa_5'}:$$

$$\varkappa'(ef) := 1 + \varkappa(ef) + \varkappa(g) + \varkappa(h), \quad \varkappa_5'(gh) := \varkappa_5(gh),$$
$$\varkappa'(g) := \varkappa(g), \qquad \varkappa_5'(e) := \varkappa_5(e),$$
$$\varkappa'(h) := \varkappa(h). \qquad \varkappa_5'(f) := \varkappa_5(f).$$

$$F_{\pi} \overset{\theta_{ef}}{\rightsquigarrow} F_{\pi'}:$$

$$\pi'(e) := \pi(f), \quad \pi'(f) := \pi(e),$$
$$\pi'(g) := \pi(g), \quad \pi'(h) := \pi(h).$$

The verification that θ_{ef} satisfies all the conditions of the proposition is straightforward just as in the case with $\theta_{\hat{e}}$. Note, that the formulas for θ_{ef} are invariant under the transposition of symbols e and f and under the transposition of symbols g and h.

Now define $\theta_{\overline{e}}$,

$$\Phi^{e}_{\rho} \overset{\theta_{\overline{e}}}{\rightsquigarrow} F_{\pi'}: \qquad F_{\pi} \overset{\theta_{\overline{e}}}{\rightsquigarrow} \Phi^{e}_{\rho'}:$$

$$\pi'(e) := 1 + \nabla_{\rho^*}, \quad \rho'^{*}(ef) := \pi(f),$$
$$\pi'(f) := \rho^{*}(ef), \quad \rho'^{*}(eg) := \pi(g),$$
$$\pi'(g) := \rho^{*}(eg), \quad \rho'^{*}(eh) := \pi(h).$$
$$\pi'(h) := \rho^{*}(eh).$$

$$\Psi^{f}_{\sigma_1} \overset{\theta_{\overline{e}}}{\rightsquigarrow} X^{ef}_{\varkappa'}: \qquad X^{ef}_{\varkappa} \overset{\theta_{\overline{e}}}{\rightsquigarrow} \Psi^{f}_{\sigma_1'}:$$

$$\varkappa'(ef) := 1 + \sigma_1(ef), \qquad \sigma_1'(ef) := 1 + \varkappa(ef),$$
$$\varkappa'(g) := \sigma_1(ef) + \sigma_1(fh), \quad \sigma_1'(fg) := 1 + \varkappa(ef) + \varkappa(h),$$
$$\varkappa'(h) := \sigma_1(ef) + \sigma_1(fg). \quad \sigma_1'(fh) := 1 + \varkappa(ef) + \varkappa(g).$$

$$\Psi^{g}_{\sigma_2} \overset{\theta_{\overline{e}}}{\rightsquigarrow} X^{eg}_{\varkappa_1'}: \qquad X^{eg}_{\varkappa_1} \overset{\theta_{\overline{e}}}{\rightsquigarrow} \Psi^{g}_{\sigma_2'}:$$

$$\varkappa_1'(eg) := 1 + \sigma_2(eg), \qquad \sigma_2'(eg) := 1 + \varkappa_1(eg),$$
$$\varkappa_1'(f) := \sigma_2'(eg) + \sigma_2(gh), \quad \sigma_2'(fg) := 1 + \varkappa_1(eg) + \varkappa_1(h),$$
$$\varkappa_1'(h) := \sigma_2(eg) + \sigma_2(fg). \quad \sigma_2'(gh) := 1 + \varkappa_1(eg) + \varkappa_1(f).$$

$$\Psi^{h}_{\sigma_3} \overset{\theta_{\bar{e}}}{\rightsquigarrow} X^{eh}_{\varkappa'_2}: \qquad X^{eh}_{\varkappa_2} \overset{\theta_{\bar{e}}}{\rightsquigarrow} \Psi^{h}_{\sigma'_3}:$$

$$\varkappa'_2(eh) := 1 + \sigma_3(eh), \qquad \sigma'_3(eh) := 1 + \varkappa_2(eh),$$
$$\varkappa'_2(f) := \sigma_3(eh) + \sigma_3(gh), \qquad \sigma'_3(fh) := 1 + \varkappa_2(eh) + \varkappa_2(g),$$
$$\varkappa'_2(g) := \sigma_3(eh) + \sigma_3(fh). \qquad \sigma'_3(gh) := 1 + \varkappa_2(eh) + \varkappa_2(f).$$

$$\Phi^{f}_{\rho_1} \overset{\theta_{\bar{e}}}{\rightsquigarrow} \Phi^{f}_{\rho'_1}: \qquad X^{gh}_{\varkappa_5} \overset{\theta_{\bar{e}}}{\rightsquigarrow} X^{gh}_{\varkappa'_5}:$$

$$\rho'^{*}_1(ef) := \nabla_{\rho^{*}_1}, \qquad \varkappa'_5(gh) := 1 + \varkappa_5(gh) + \varkappa_5(f),$$
$$\rho'^{*}_1(fg) := \rho^{*}_1(fg), \qquad \varkappa'_5(e) := 1 + \varkappa_5(e) + \varkappa_5(f),$$
$$\rho'^{*}_1(fh) := \rho^{*}_1(fh). \qquad \varkappa'_5(f) := \varkappa_5(f).$$

$$\Phi^{g}_{\rho_2} \overset{\theta_{\bar{e}}}{\rightsquigarrow} \Phi^{g}_{\rho'_2}: \qquad X^{fh}_{\varkappa_4} \overset{\theta_{\bar{e}}}{\rightsquigarrow} X^{fh}_{\varkappa'_4}:$$

$$\rho'^{*}_2(eg) := \nabla_{\rho^{*}_2}, \qquad \varkappa'_4(fh) := 1 + \varkappa_4(fh) + \varkappa_4(g),$$
$$\rho'^{*}_2(fg) := \rho^{*}_2(fg), \qquad \varkappa'_4(e) := 1 + \varkappa_4(e) + \varkappa_4(g),$$
$$\rho'^{*}_2(gh) := \rho^{*}_2(gh). \qquad \varkappa'_4(g) := \varkappa_4(g).$$

$$\Phi^{h}_{\rho_3} \overset{\theta_{\bar{e}}}{\rightsquigarrow} \Phi^{h}_{\rho'_3}: \qquad X^{fg}_{\varkappa_3} \overset{\theta_{\bar{e}}}{\rightsquigarrow} X^{fg}_{\varkappa'_3}:$$

$$\rho'^{*}_3(eh) := \nabla_{\rho^{*}_3}, \qquad \varkappa'_3(fg) := 1 + \varkappa_3(fg) + \varkappa_3(h),$$
$$\rho'^{*}_3(fh) := \rho^{*}_3(fh), \qquad \varkappa'_3(e) := 1 + \varkappa_3(e) + \varkappa_3(h),$$
$$\rho'^{*}_3(gh) := \rho^{*}_3(gh). \qquad \varkappa'_3(h) := \varkappa_3(h).$$

$$\Psi^{e}_{\sigma} \overset{\theta_{\bar{e}}}{\rightsquigarrow} \Psi^{e}_{\sigma'}:$$

$$\sigma'(ef) := 1 + \sigma(ef),$$
$$\sigma'(eg) := 1 + \sigma(eg),$$
$$\sigma'(eh) := 1 + \sigma(eh).$$

In order to obtain formulas for $\theta_{\bar{e}}$ one may take the formulas defining $\theta_{\hat{e}}$ and perform the replacements of the symbols $\sigma \leftrightarrow \rho^{*}$, $\varkappa \to \tilde{\varkappa}$, $\pi \equiv \pi$, and similar for $(\cdot)'$ symbols. The verification that $\theta_{\bar{e}}$ satisfies the three conditions of the proposition is again straightforward.

The other $\theta_{\hat{v}}$, θ_{vw}, and $\theta_{\bar{v}}$ $(v, w \in V, v \neq w)$ are defined from $\theta_{\hat{e}}$, θ_{ef}, and $\theta_{\bar{e}}$ via the permutations of symbols e, f, g, and h, i.e., in such a way that for every $S \in \mathcal{P}(V)$,

$$\theta_{m(\beta)(S)} = \mu(\beta)\theta_S\mu(\beta^{-1}), \quad \beta \in Bij(V),$$

where μ is the natural monomorphism, μ: $Bij(V) \rightarrowtail Bij(A)$. □

Denote by $Bij_{\perp}(A)$ the subgroup of $Bij(A)$ consisting of all bijections of A which respect the orthogonality relation $\perp$ on A. We have constructed a family of reflections $\theta_S \in Bij_{\perp}(A)$, $S \in \mathcal{P}(V)$. Denote by $\mathcal{G}$ the subgroup of $Bij_{\perp}(A)$ generated by these reflections,

$$\mathcal{G} := \langle \{\theta_S | S \in \mathcal{P}(V)\} \rangle \subset Bij_{\perp}(A).$$

Note that the correspondence $T_S \mapsto \theta_S$ *does not* define a homomorphism from G to $\mathcal{G}$, since, for example, the order of an element $T_{\bar{f}}T_{\hat{e}} \in G$ is 2, and the order of $\theta_{\bar{f}}\theta_{\hat{e}} \in G$ is 4.

Let us mention some properties of the groups G and $\mathcal{G}$. First of all, recall that we have natural monomorphisms, m: $Bij(V)\rightarrowtail Bij(\mathcal{P}(V))$, μ: $Bij(V)\rightarrowtail Bij(A)$. It turns out, that the images of these monomorfisms are in fact contained in G and $\mathcal{G}$, respectively, i.e., each of the two groups contains a copy of S_4. Denote by t_{ef} the bijection $V\tilde{\rightarrow}V$ which interchanges the symbols e and f, i.e., $t_{ef}: e\mapsto f, f\mapsto e, g\mapsto g, h\mapsto h$. Let us write (ef) instead of $m(t_{ef})$ and $(\tilde{ef})$ instead of $\mu(t_{ef})$. One defines in a similar way the transformations (vw) and $(v\tilde{w})$ for all $v,w\in V, v\neq w$.

Proposition 4: For all $v,w,z\in V$, $v\neq w$, $v\neq z$, $w\neq z$,

$$T_{vw}T_{uz}T_{uw}=(wz),$$

$$\theta_{vw}\theta_{vz}\theta_{vw}=(\tilde{w}z). \tag{5}$$

Proof: It is sufficient to verify that $T_{ef}T_{eg}T_{ef}=(fg)$ and that $\theta_{ef}\theta_{eg}\theta_{ef}=(\tilde{fg})$. The latter is established by a straightforward computation. □

Consider a product $D:=(ef)(gh)T_{ef}T_{gh}$. For every $U\in\mathcal{P}(V)$, $D(U)=\overline{U}$ if $\#U$ is odd, and $D(U)=U$ if $\#U$ is even. Hence the map D is obtained by

$$\hat{e}\leftrightarrow\overline{e},\quad \hat{f}\leftrightarrow\overline{f},\quad \hat{g}\leftrightarrow\overline{g},\quad \hat{g}\leftrightarrow\overline{h},$$

$$\varnothing,ef,eg,eh,fg,fh,gh,efgh=inv.$$

Note, that for any $\epsilon\in E$, $D=(\epsilon)(\overline{\epsilon})T_{\epsilon}T_{\overline{\epsilon}}$. Consider an analog of D in $\mathcal{G}$, the product $\delta:=(\tilde{ef})(\tilde{gh})\theta_{ef}\theta_{gh}$. Observe that δ is just the duality transformation mentioned in the section describing the orthogonality relation on A, $\delta(\Psi^{v}_{\sigma})=\Phi^{v}_{\sigma^*}$, $\delta(X^{\epsilon}_{\varkappa})=X^{\epsilon}_{\tilde{\varkappa}}$, $\delta(\Phi^{v}_{\rho})=\Psi^{v}_{\rho^*}$, and $\delta(F_{\pi})=F_{\pi}$ (notation σ^*, ρ^*, and $\tilde{\varkappa}$ as in that section). More generally, for any $\epsilon\in E$ one has $\delta=(\tilde{\epsilon})(\tilde{\overline{\epsilon}})\theta_{\epsilon}\theta_{\overline{\epsilon}}$. The transformations $D\in G$ and $\delta\in\mathcal{G}$ allow to obtain $T_{\overline{v}}$ and $\theta_{\overline{v}}$ $(v\in V)$ from $T_{\hat{v}}$ and $\theta_{\hat{v}}$ according to $T_{\overline{v}}=DT_{\hat{v}}D$ and $\theta_{\overline{v}}=\delta\theta_{\hat{v}}\delta$. Any transformation T_{ϵ} $(\epsilon\in E)$ commutes with D, $DT_{\epsilon}=T_{\epsilon}D$, and any transformation θ_{ϵ} $(\epsilon\in E)$ commutes with δ, $\delta\theta_{\epsilon}=\theta_{\epsilon}\delta$.

Note that $(ev)T_{\hat{e}}(ev)=T_{\hat{v}}$, $v\in V$, $v\neq e$. Since every transformation of the form (vw) and the transformation D belong to a subgroup G_2 of G generated by $\{T_{\epsilon}\}_{\epsilon\in E}$, any set generating G_2 appended with an element $T_{\hat{e}}$, generates the whole group G. Similarly, if one denotes by $\mathcal{G}_2$ the subgroup of $\mathcal{G}$ generated by $\{\theta_{\epsilon}\}_{\epsilon\in E}$, then any set of generators of $\mathcal{G}_2$ appended with an element $\theta_{\hat{e}}$ generates the whole group $\mathcal{G}$.

The groups G_2 and $\mathcal{G}_2$ should be investigated in more detail. We start with the group G_2. It is convenient to consider $W_{vw}:=(vw)T_{vw}$ $(v,w\in V, v\neq w)$. Denote by G_2' the subgroup of G_2 generated by (vw)'s, and by G_2'' a subgroup of G_2 generated by W_{vw}'s. Together G_2' and G_2'' generate the whole G. The explicit description of W_{ef} is

$$\hat{e}\leftrightarrow\overline{e},\quad \hat{f}\leftrightarrow\overline{f},\quad eg\leftrightarrow fh,\quad eh\leftrightarrow fg,$$

$$\varnothing,\hat{g},\hat{h},\overline{g},\overline{h},ef,gh,efgh=inv.$$

and the explicit descriptions of the other W_{vw} are similar. One verifies that $W_{ef}W_{fg}=W_{eg}$. More generally, for any v, w, $z\in V$, $v\neq w$, $v\neq z$, $w\neq z$,

$$W_{vw}W_{wz}=W_{vz}.$$

It follows, that G_2'' consists of all elements of the form W_{ϵ}, $\epsilon\in E$, an element $D=W_{ef}W_{gh}$ and a unit element of G. Since every element $b\in G_2'$ preserves the cardinality [i.e., $\#b(U)=\#U$, $U\in\mathcal{P}(V)$], and no element $w\in G_2''$ except the unit preseves the cardinality, it follows that the intersection of G_2' and G_2'' is trivial. Moreover, the group G_2'' is normal in G_2 since $(ef)W_{ef}(ef)=W_{ef}$, $(eg)W_{ef}(eg)=W_{fg}$, and $(gh)W_{ef}(gh)=W_{ef}$, and there exists a natural action of G_2' on G_2'' defined as follows. From the explicit description of W_{vw} one observes that G_2'' is isomorphic to a group Λ_0 of

$\mathbb{Z}_2$-valued functions ϕ on V satisfying a condition $\Sigma_{v\in V}\phi(v)=0$, i.e., it is a sample of $(\mathbb{Z}_2)^3$. An element $\beta\in Bij(V)$ acts on Λ_0 by the formula $\phi\mapsto\phi\circ\beta^{-1}$. This induces an action of $G_2'\simeq Bij(V)$ on $G_2''\simeq\Lambda_0$. Since $Bij(V)\simeq S_4$ and $\Lambda_0\simeq(\mathbb{Z}_2)^3$, it follows that one may view the group G_2 as a semidirect product $(\mathbb{Z}_2)^3\rtimes S_4$.

The considerations about the group $\mathcal{G}_2$ are similar to the considerations about G_2. In particular, the elements $\omega_{vw}:=(v\tilde{w})\theta_{vw}$ have the properties similar to the properties of W_{vw}. As a result, one gets that $\mathcal{G}_2\simeq(\mathbb{Z}_2)^3\rtimes S_4$ as well.

G is a group generated by the following five elements: (ef), (fg), (gh), $T_{\hat{e}}$, and W_{ef}. The corresponding Coxeter matrix is defined by

$$\mathrm{ord}((ef)T_{\hat{e}})=3,\quad \mathrm{ord}((fg)T_{\hat{e}})=2,\quad \mathrm{ord}((gh)T_{\hat{e}})=2,$$

$$\mathrm{ord}((ef)W_{ef})=2,\quad \mathrm{ord}((fg)W_{ef})=4,\quad \mathrm{ord}((gh)W_{ef})=2,$$

$$\mathrm{ord}((ef)(fg))=3,\quad \mathrm{ord}((ef)(gh))=2,\quad \mathrm{ord}((fg)(gh))=3,$$

$$\mathrm{ord}(W_{ef}T_{\hat{e}})=3,$$

where $\mathrm{ord}(\cdot)$ denotes the order of a group element. One verifies that the Coxeter matrix associated to the original set of generators $\{T_S\}_S$, $S\in\mathcal{P}(V)$, is defined by the formula

$$\mathrm{ord}(T_{S_2}T_{S_1})=\begin{cases}2, & \text{if } \#(S_1\setminus S_2) \text{ is even and } \#(S_2\setminus S_1) \text{ is even},\\ 3, & \text{if } \#(S_1\setminus S_2) \text{ is odd and } \#(S_2\setminus S_1) \text{ is odd},\\ 4, & \text{otherwise}.\end{cases}$$

Note, that the group G contains other reflections besides the ones already mentioned. In particular, there exist reflections which interchange $ef\leftrightarrow efgh$, for example, $T_{\hat{f}}W_{ef}T_{\hat{e}}W_{ef}$. At least some of the reflections can be generated starting from $\{T_S\}_S$ by using the following facts: whenever R_1 and R_2 are two reflections, $R_2R_1R_2$ is again a reflection; if R_1 and R_2 commute, then their product R_2R_1 is again a reflection.

Note that there is another way of expressing (vw) and D in G. Verify that additioned to (5) there is also a formula $T_{\hat{e}}T_{\hat{f}}T_{\hat{e}}=(ef)$ and $T_{\hat{e}}T_{\bar{e}}T_{\hat{e}}=D$. After replacing the left-hand and right-hand sides of these equalities by their analoges in $\mathcal{G}$, one observes, that $\theta_{\hat{e}}\theta_{\bar{e}}\theta_{\hat{e}}=\delta$, but $\theta_{\hat{e}}\theta_{\hat{f}}\theta_{\hat{e}}\neq(\widetilde{ef})$. What is the deviation of the value of $(\widetilde{ef})\theta_{\hat{e}}\theta_{\hat{f}}\theta_{\hat{e}}$ from identity? We need more notation to express that. Consider an Abelian group $\mathcal{F}$ of all $\mathbb{Z}_2$-valued functions on the set of all edges $E=\{\epsilon\subset V|\,\#\epsilon=2\}$. We shall associate to every $\varphi\in\mathcal{F}$ a transformation $I_\varphi\in Bij(A)$ and then show that in fact I_φ falls into the group $\mathcal{G}$. The product $(v\tilde{w})\theta_{\hat{v}}\theta_{\hat{w}}\theta_{\hat{v}}$ will be equal to I_φ where φ is some element of $\mathcal{F}$.

Take any $\varphi\in\mathcal{F}$. Denote $a:=\varphi(ef)$, $b:=\varphi(eg)$, $c:=\varphi(fg)$, $p:=\varphi(eh)$, $q:=\varphi(fh)$, $r:=\varphi(gh)$. The transformation I_φ will not change the kind of a projective line and we will describe its action on Ψ^e_σ, $X^{ef}_\varkappa$, Φ^e_ρ, and F_π. The other cases are obtained by permutation of the symbols e, f, g, h. A projective line Ψ^e_σ is mapped by I_φ to $\Psi^e_{\sigma'}$ with $\sigma'(ef)=\sigma(ef)+a$, $\sigma'(eg)=\sigma(eg)+b$, $\sigma'(eh)=\sigma(eh)+p$. A projective line $X^\epsilon_\varkappa$ maps to $X^\epsilon_{\varkappa'}$ with $\varkappa'(ef)=\varkappa(ef)+a$, $\varkappa'(g)=\varkappa(g)+p+q$, $\varkappa'(h)=\varkappa(h)+b+c$. A projective line Φ^e_ρ maps to $\Phi^e_{\rho'}$ with $\rho'(\cdot)$ defined by $\rho'^*(ef)=\rho^*(ef)+b+c+p+q+r$, $\rho'^*(eg)=\rho^*(eg)+a+c+p+q+r$, $\rho'^*(eh)=\rho^*(eh)+a+b+c+q+r$. Finally, the projective line F_π is mapped by I_φ to $F_{\pi'}$, where $\pi'(\cdot)$ is defined as $\pi'(e)=\pi(e)+a+b+p$, $\pi'(f)=\pi(f)+a+c+q$, $\pi'(g)=\pi(g)+b+c+r$, $\pi'(h)=\pi(h)+p+q+r$. Note, that since $\Sigma_{v\in V}\pi(v)=1$, one gets $\Sigma_{v\in V}\pi'(v)=1$. The difference $\pi'-\pi$ satisfies $\Sigma_{v\in V}(\pi'-\pi)(v)=0$.

We have defined a collection $\{I_\varphi\}_{\varphi\in\mathcal{F}}$ of maps $A\to A$, such that $I_\varphi^2=id$. This implies, in particular, that I_φ is a bijection, and one may consider the subgroup in $Bij(A)$ generated by

$\{I_\varphi\}_{\varphi\in\mathcal{F}}$. Since for every $\varphi_1, \varphi_2 \in \mathcal{F}$ we have $I_{\varphi_1} I_{\varphi_2} = I_{\varphi_1+\varphi_2}$, this subgroup is Abelian. Denote by χ_ϵ ($\epsilon \in E$) the element of $\mathcal{F}$ which has a value 1 on the edge ϵ and a value 0 on all other edges. Straightforward computation establishes that

$$(v\tilde{w})\,\theta_{\hat{v}}\theta_{\hat{w}}\theta_{\hat{v}} = I_{\chi_{vw}} \tag{6}$$

(for every $v, w \in V$, $v \neq w$). Since every map I_φ, $\varphi \in \mathcal{F}$, may be represented as a composition of maps of the form I_{χ_ϵ}, $\epsilon \in E$, it follows from (6) that every map I_φ is in $\mathcal{G}$. It follows that the set $\{I_\varphi\}_{\varphi\in\mathcal{F}}$ generates some Abelian subgroup $\mathcal{N}$ in $\mathcal{G}$.

Proposition 5: The group $\mathcal{N}$ generated by $\{I_\varphi\}_{\varphi\in\mathcal{F}}$ is a normal subgroup of $\mathcal{G}$.

Proof: We define for $S \in \mathcal{P}(V)$ a morphism τ_S, $\mathcal{F}\to\mathcal{F}$, such that $\forall\varphi\in\mathcal{F}$: $\theta_S I_\varphi = I_{\tau_S(\varphi)}\theta_S$. Since $\theta_\varnothing = \theta_V = id$, set $\tau_\varnothing := id$ and $\tau_V := id$. The set of formulas for the other cases of S will have a symmetry with respect to the permutations of e, f, g, and h, and in fact the nontrivial part of the proof will consist in providing the definitions of $\tau_{\hat{e}}$, τ_{ef}, and $\tau_{\bar{e}}$.

There exists a natural monomorphism ν: $Bij(V) \rightarrowtail End(\mathcal{F})$ defined as follows: for every $\beta \in Bij(V)$ the morphism $\nu(\beta)$: $\mathcal{F}\to\mathcal{F}$ is defined by $\varphi \mapsto \varphi'$, $\varphi'(\epsilon) := \varphi(m(\beta^{-1})(\epsilon))$ for all $\epsilon \in E$, where m is the natural monomorphism $Bij(V) \rightarrowtail Bij(\mathcal{P}(V))$. Recall that there also exists a natural monomorphism μ: $Bij(V) \rightarrowtail Bij(A)$.

The I_φ are defined in such a way, that $\forall\beta \in Bij(V): \mu(\beta) I_\varphi \mu(\beta^{-1}) = I_{\nu(\beta)(\varphi)}$. Recall that for every $\beta \in Bij(V)$ and every $S \in \mathcal{P}(V)$, $\mu(\beta)\theta_S\mu(\beta^{-1}) = \theta_{m(\beta)(S)}$. Hence,

$$\begin{aligned} I_{\tau_{m(\beta)(S)}(\varphi)} &= \theta_{m(\beta)(S)} I_\varphi \theta^{-1}_{m(\beta)(S)} = \mu(\beta)\theta_S\mu(\beta^{-1}) I_\varphi [\mu(\beta)\theta_S\mu(\beta^{-1})]^{-1} = \mu(\beta)\theta_S I_{\nu(\beta^{-1})(\varphi)}\theta_S^{-1}\mu(\beta^{-1}) \\ &= \mu(\beta) I_{(\tau_S\nu(\beta^{-1}))(\varphi)}\mu(\beta^{-1}) = I_{(\nu(\beta)\tau_S\nu(\beta^{-1}))(\varphi)}, \end{aligned}$$

where $\varphi \in \mathcal{F}$. It follows, that the collection $\{\tau_S\}_{S\in\mathcal{P}(V)}$ should satisfy $\nu(\beta)\tau_S\nu(\beta^{-1}) = \tau_{m(\beta)(S)}$, $\beta \in Bij(V)$. Hence it is necessary to describe just three morphisms $\tau_{\hat{e}}, \tau_{ef}, \tau_{\bar{e}}: \mathcal{F}\to\mathcal{F}$.

It is convenient to represent an element of $\mathcal{F}$ by a graph, which is a tetrahedron with vertices e, f, g, h, and equip its edges with the values of the considered element of $\mathcal{F}$ on the corresponding edge. Take any $\varphi \in \mathcal{F}$ and denote by a, b, c, p, q, and r the values of φ on the edges ef, eg, fg, eh, fh, and gh, respectively. Define $\tau_{\hat{e}}$, τ_{ef}, and $\tau_{\bar{e}}$ as follows:

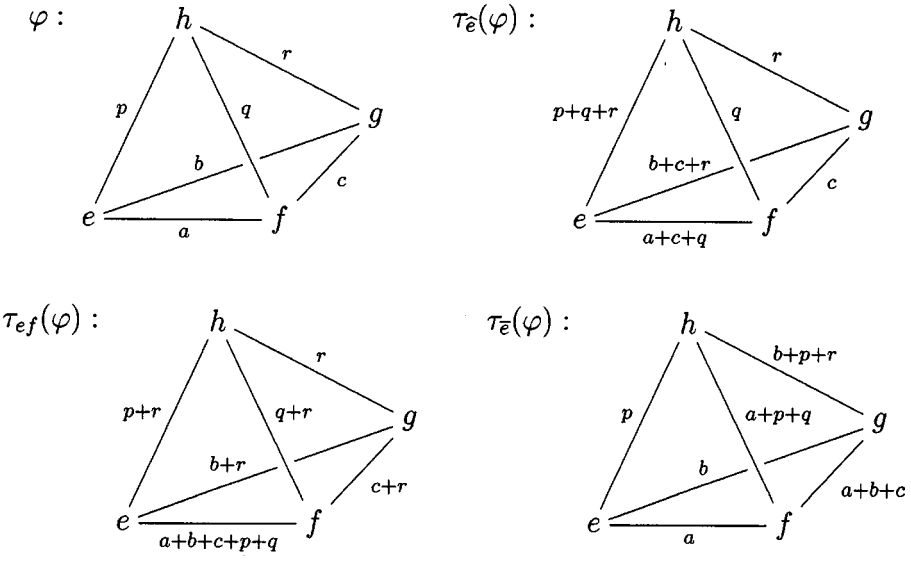

(7)

The explicit descriptions of the other τ_S are induced by permutations of labels of vertices e, f, g,

and h. Recall that $\tau_{\varnothing}=\tau_V=id$. Straightforward computation establishes that $\theta_{\hat{e}}I_{\varphi}=I_{\tau_{\hat{e}}(\varphi)}\theta_{\hat{e}}$, $\theta_{ef}I_{\varphi}=I_{\tau_{ef}(\varphi)}\theta_{ef}$, and $\theta_{\bar{e}}I_{\varphi}=I_{\tau_{\bar{e}}(\varphi)}\theta_{\bar{e}}$. This completes the proof that the group $\mathcal{N}$ is a normal subgroup of the group $\mathcal{G}$. □

Note that now one has three types of transformations indexed by $S\in\mathcal{P}(V)$, a bijection $T_S\in Bij(\mathcal{P}(V))$ [refer to (3)], a bijection $\theta_S\in Bij_{\perp}(A)$ [refer to (4)], and an automorphism $\tau_S\in Aut(\mathcal{F})$ [refer to (7)].

The groups G and $\mathcal{G}$ will play a key role in the proof of the saturation property of A. In particular, it will be shown below that the image of the composition of maps $\mathcal{P}_{\perp}(A)\rightarrowtail\mathcal{P}(A)\xrightarrow{\mathcal{P}(\eta)}L$, where the first arrow is a canonical injection, is invariant under the G action. It will be shown, that an image of a complete set under this composition can have a cardinality only 1, 2, 4 or 8. This induces a partition of $C(A)$ into four subsets. The $\mathcal{G}$ action will fix each of these subsets and it will turn out that $\mathcal{G}$ acts transitively on each one of them.

VIII. SATURATION PROPERTY, PART 2

We have constructed a group G and an action of G on L. Let H be a subgroup of G. Two graphs corresponding to some elements of Γ are called *H-equivalent* iff they can be represented in L by elements of the same H orbit.

In the group G there is an element D. Its action on L induces a map $\partial:\Gamma\rightarrow\Gamma$, which in terms of graphs replaces a star $*$ by a circle $\odot$ around the same vertex and a circle $\odot$ by a star $*$ at the same vertex; the edges $\cdot$—$\cdot$ and the symbol F remain untouched. It means that if one is given a graph, then by applying if necessary the transformation ∂, it is possible to produce a graph with the number of stars $*$ greater or equal to the number of circles $\odot$. We shall call a graph satisfying this condition, *primary*, and a graph not satisfying this condition, *secondary*. For example, a graph $F*\circledast$—$\cdot$ is primary, and a graph $F\odot\circledast$—$\cdot$ is secondary. If the graphs represent the elements of Γ related to one another by the transformation ∂, one calls these graphs mutually *dual*. If a graph coincides with its dual, it is called *self-dual*. For example, the graph $*$—$\odot$ is self-dual.

Note, that any G-equivalence class is invariant under the transformation induced by ∂. The set of elements constituting a G-equivalence class, is completely determined by a list of all primary elements belonging to it; the other elements are obtained by duality.

Proposition 6: (1) The complete list of primary graphs from the G-equivalence class of the graph $\triangle$ *is of the form*

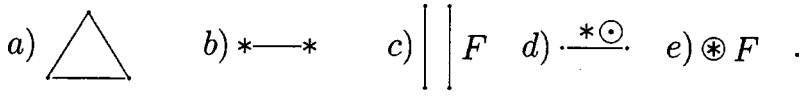

(2) The complete list of primary graphs from the G-equivalence class of the graph $***\odot$ *is of the form:*

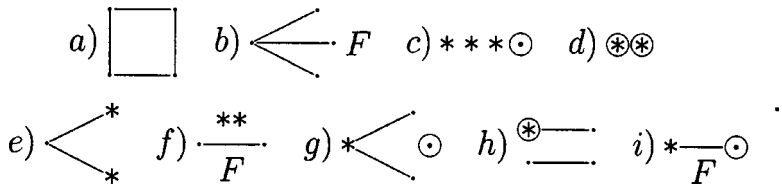

(3) The complete list of primary graphs from the G-equivalence class of the graph $****F$ *is of the form:*

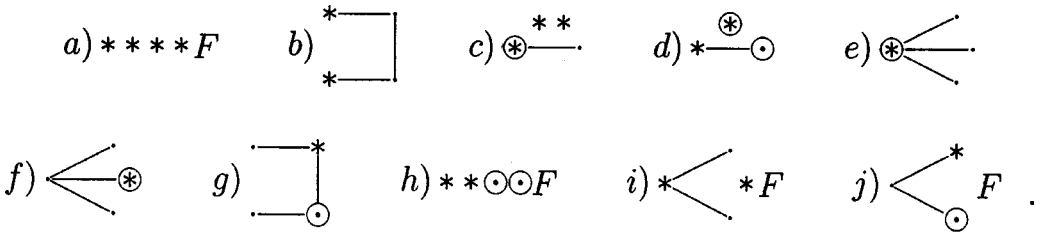

(4) The complete list of primary elements of the G-equivalence class of the graph ⊛⊛⊛⊛ is of the form

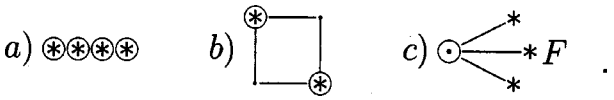

Proof: The proof is straightforward. Let us consider the proof of (1) in more detail. Note that all the graphs listed in (1) except the graph (b) are self-dual. Denote a graph obtained by duality from (b) as (b'); it is of the form $\odot$—$\odot$. Denote the set of graphs (1) appended with (b') as N_3 (N stands for nonadmissible and 3 stands for the degree).

That the G-equivalence class of the triangle indeed coincides with N_3, follows from two facts: (i) the list N_3 is complete, i.e., there is no other graph not present in the list, which is G-equivalent to some member of the list; (ii) any two members of the list N_3 are G-equivalent. In order to establish (i), let us choose and fix some representative in L for each element of N_3. This is equivalent to assigning some labels to the vertices of the graphs and can be done, for example, as follows:

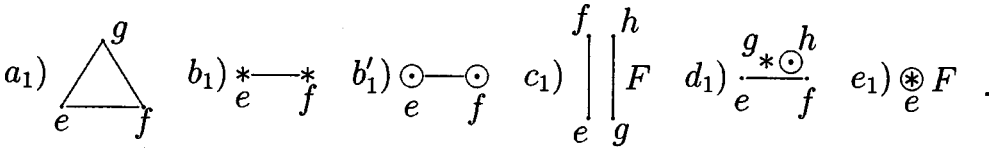

Now for each of these labeled graphs calculate the result of the action on them of the transformations induced by $T_{\hat{v}}$ and T_{vw} $(v,w \in V, v \neq w)$, and after that delete the labels e, f, g, h. For example, if one takes the graph (a_1), then the transformation associated to $T_{\hat{e}}$ followed by the deletion of symbols e, f, g, and h, generates a graph $\odot$—$\odot$. If instead of $T_{\hat{e}}$ one takes $T_{\hat{h}}$, then the result will be the unlabeled triangle. Performing similar calculations, in each case one obtains an element of N_3, i.e., N_3 is complete.

Now let us establish (ii), i.e., the fact that N_3 is just one G-equivalence class. It is convenient to do this in several steps by taking bigger and bigger subgroups H of G and splitting N_3 into H-equivalence classes. Denote by G_1 the subgroup of G generated by $\{T_{\hat{v}}\}_{v \in V}$. Then N_3 splits into three G_1-equivalence classes: the first class consists of (a) and (b'); the second class consists of (b) and (e); and the third class consists of (c) and (d). Denote by $G_{1,3}$ the subgroup of G generated by $T_{\hat{v}}$ and $T_{\bar{v}}$, $v \in V$. Recall that $T_{\bar{v}} = DT_{\hat{v}}D$ where $D = T_{ef}T_{gh}$. Hence, $G_{1,3}$ is generated by the $\{T_{\hat{v}}\}_{v \in V}$ and D. The list N_3 splits into two $G_{1,3}$-equivalence classes, the first class contains the graphs (a), (b), (b'), and (e); and the other (c) and (d). Finally, the action associated to T_{eg} on the graph e^*—$^*f$ gives a graph, e—$h^*f \odot g$. Hence, one obtains a transition from (b) to (d), i.e., a

link between the two mentioned $G_{1,3}$-equivalence classes. It follows, that any two elements of N_3 are G-equivalent and this completes the proof of the first part of the proposition.

The proof of (2), (3), and (4) is similar. □

We have calculated some of the G-equivalence classes of some examples of graphs representing the elements of Γ. It will be interesting to describe for every given degree the sets of G-equivalence classes of admissible graphs.

Proposition 7: If γ_1 is an admissible graph and γ_2 is a graph G-equivalent to γ_1, then it is also admissible. Moreover, if B_1 hangs over γ_1, then there exists a set B_2 which hangs over γ_2 and has the same cardinality as B_1.

Proof: Choose a representative Q_1 for γ_1 in L and a representative Q_2 for γ_2 in L. Hence γ_1 is associated to $[Q_1]\in\Gamma$ and γ_2 is associated to $[Q_2]\in\Gamma$. The assumption that γ_1 and γ_2 are G-equivalent implies that Q_1 and Q_2 are related as $Q_2=\hat{T}(Q_1)$, where $\hat{T}:=T_{S_1}T_{S_2}\cdots T_{S_m}\in G$, m is some natural number and $S_1,S_2,\ldots,S_m$ are some nonempty proper subsets of $V=\{e,f,g,h\}$. Since Q_1 is admissible, choose a set $B_1\in\mathcal{P}_\perp(A)\subset\mathcal{P}(A)$, such that $\mathcal{P}(\eta)(B_1)=Q_1$, where $\eta:A\to\mathcal{P}(V)$ is the natural map. For every $l\in B_1$ look at $l':=\hat{\theta}(l)$, where $\hat{\theta}:=\theta_{S_1}\theta_{S_2}\ldots\theta_{S_m}\in\mathcal{G}$. As l runs over the whole B_1, l' sweeps up some set $B_2\subset A$. Note, that since every θ_S is a bijection, $\hat{\theta}$ is a bijection as well, and the sets B_1 and B_2 have the same cardinality. Using the commutative diagram relating T_S and θ_S, $S\in\mathcal{P}(V)$, and the fact that every θ_S respects $\perp$, one concludes that $B_2\in\mathcal{P}_\perp(A)$ and that $\mathcal{P}(\eta)(B_2)=Q_2$. In particular, B_2 hangs over γ_2, and by that provides a realization of the admissiblity of γ_2. □

The graph * is an admissible graph of degree 1. The complete list of all primary elements from its G-equivalence class is of the form

It means, that the G-equivalence class of the graph $*$ coincides with the set of all graphs of degree 1.

Similarly, one has an admissible graph $**$ of degree 2. The complete list of all primary elements from its G-equivalence class is of the form

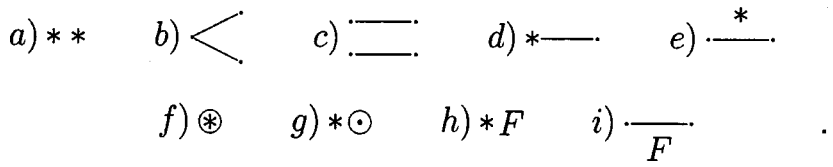

This G-equivalence class coincides with the set of all graphs of degree 2.

In degree 3 there exist admissible, as well as nonadmissible graphs.

Proposition 8: The set of all admissible graphs of degree 3 coincides with the G-equivalence class of the graph $***$.

Proof: Let us generate a list of all primary graphs of degree 3. It is convenient to present it in a systematic way. Denote by Γ_{k_1,k_2,k_3,k_4} a subset of Γ consisting of all the elements which are associated to the graphs which have k_1 stars, k_2 edges, k_3 circles, and k_4 instances of the symbol F. Look at all decompositions of 3 into a sum of four non-negative integers, $3=3+0+0+0=2+1+0+0=1+1+1+0$. Each of the mentioned three variants corresponds to some Γ_{k_1,k_2,k_3,k_4} with $k_1\geqslant k_2\geqslant k_3\geqslant k_4$, one gets $\Gamma_{3,0,0,0}$, $\Gamma_{2,1,0,0}$, and $\Gamma_{1,1,1,0}$. After that one generates the other Γ_{k_1,k_2,k_3,k_4} by permuting the arguments k_1, k_2, k_3, k_4 in the obtained three variants. Finally, one deletes from the list all the entries which do not satisfy $k_1\geqslant k_3$ and $k_4\leqslant 1$. Inside each of the sets Γ_{k_1,k_2,k_3,k_4} one

generates the corresponding graphs by exploring the different variants. After excluding the known nonadmissible graphs of degree 3, i.e., the graphs which are G-equivalent to a triangle, the list becomes

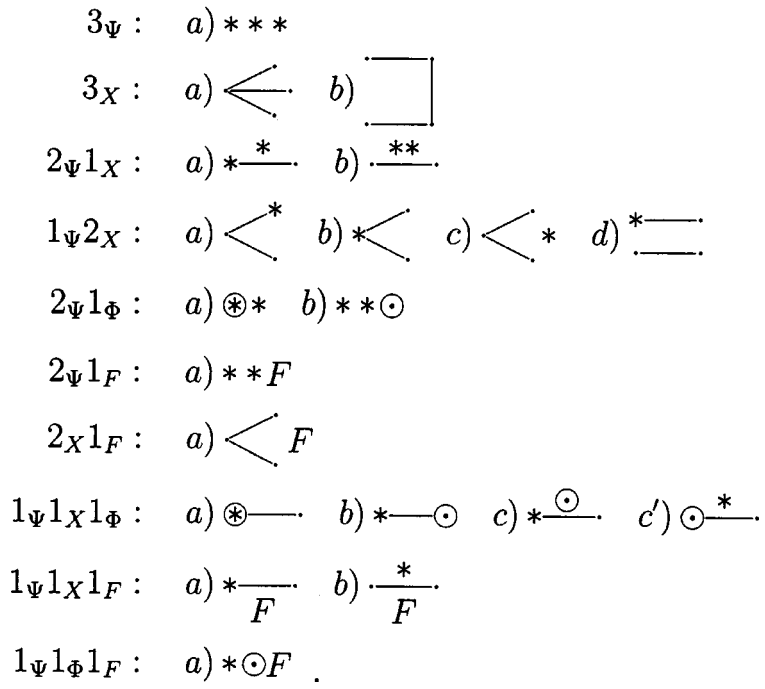

Here we use the labels of the form $1_\Psi 2_X$, $1_\Psi 1_X 1_F$, etc., to classify the graphs. The label $1_\Psi 2_X$ is associated to admissible graphs from $\Gamma_{1,2,0,0}$, $1_\Psi 1_X 1_F$ is associated to admissible graphs from $\Gamma_{1,1,0,1}$, etc. In a way, similar to the proof of the previous proposition, check that all the presented graphs are in fact a set of all primary graphs of a G-equivalence class of $***$. □

Now let us look at the graphs of degree 4. Note, that any admissible graph of degree 4 should satisfy a *necessary* condition, it does not contain a nonadmissible graph of degree 3. More precisely, one says that a graph γ_1 is *contained* in the graph γ_2 by definition iff these two graphs can be represented in L by Q_1 and Q_2, respectively, in such a way that $Q_1 \subset Q_2$.

Proposition 9: (1) A graph of degree 4 is admissible iff it does not contain a nonadmissible graph of degree 3.

(2) The set of all admissible graphs of degree 4 splits into two G-equivalence classes, one of the graph $***\odot$ *and the other of the graph* $****$.

Proof: Consider the set of *all* graphs of degree 4, which do not contain a nonadmissible graph of degree 3. The set of all *admissible* graphs of degree 4 is a subset of this set. One generates the required list in analogy with the case of degree 3. There are five ways to decompose 4 into a sum of four non-negative integers, $4=4+0+0+0=3+1+0+0=2+2+0+0=2+1+1+0=1+1+1+1$. It means, in particular, that one must have a series of graphs marked by labels 4_Ψ, $3_\Psi 1_X$, $2_\Psi 2_X$, $2_\Psi 1_X 1_\Phi$, and $1_\Psi 1_X 1_\Phi 1_F$. The label 4_Ψ generates 4_X, 4_Φ, and 4_F. Since a graph cannot contain more than one symbol F, delete 4_F. Since it suffices to consider only primary graphs, exclude the case 4_Φ. Treating the other labels in a similar fashion, one arrives at the following: $3_\Psi 1_X$ generates $3_\Psi 1_\Phi$, $3_\Psi 1_F$, $1_\Psi 3_X$, and $3_X 1_F$; $2_\Psi 2_X$ generates $2_\Psi 2_\Phi$; $2_\Psi 1_X 1_\Phi$ generates $2_\Psi 1_X 1_F$, $2_\Psi 1_\Phi 1_F$, $1_\Psi 2_X 1_\Phi$, and $1_\Psi 2_X 1_F$; finally, $1_\Psi 1_X 1_\Phi 1_F$ does not generate more labels. Having a set of all possible labels classifying the mentioned graphs, one generates a set of graphs present under each label by exploring different variants. The resulting complete list of primary graphs is given below,

4_Ψ : $a)\ ****$

4_X : $a)$ 

$3_\Psi 1_X$: $a)$ 

$3_\Psi 1_\Phi$: $a)\ \circledast **$ $b)\ ***\odot$

$3_\Psi 1_F$: $a)\ ***F$

$1_\Psi 3_X$: $a)$  $b)$ 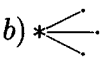 $c)$  $d)$ 

$3_X 1_F$: $a)$ 

$2_\Psi 2_X$: $a)$  $b)$ 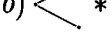 $c)$  $d)$ 

$2_\Psi 2_\Phi$: $a)\ \circledast\circledast$ $b)\ \circledast *\odot$ $c)\ **\odot\odot$

$2_\Psi 1_X 1_\Phi$: $a)$  $b)$ 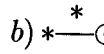 $c)$  $d)$ 

$2_\Psi 1_X 1_F$: $a)$  $b)$ 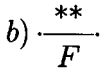

$2_\Psi 1_\Phi 1_F$: $a)\ **\odot F$

$1_\Psi 2_X 1_\Phi$: $a)$  $b)$ 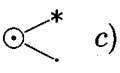 $c)$  $d)$  $e)$

$f)$  $g)$  $h)$  $i)$  $j)$ 

$1_\Psi 2_X 1_F$: $a)$  $b)$ 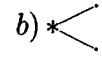 $c)$ 

$1_\Psi 1_X 1_\Phi 1_F$: $a)$  $b)$ 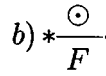 $c)$ 

Note, that the existence of nonadmissible graphs of degree 3 excludes many variants of the graphs of degree 4. Now exclude all the graphs G-equivalent to $***\odot$. It is easily verified, that all the remaining graphs constitute in fact the set of all primary graphs from the G-equivalence class of $****$. □

We have shown, that the set of all admissible graphs of degree 4 splits into two G-equivalence classes, one containing the graph $****$ and the second, the graph $***\odot$. The elements from the first class will be referred to as *singlets* and the elements of the second class as *doublets*.

Now consider the case of the graphs of degree 5. Recall that one knows at least some of the nonadmissible graphs of this degree, these are the graphs from the G-equivalence class of the graph $****F$.

Proposition 10: (1) A graph of degree 5 is admissible iff it does not contain a nonadmissible graph of degree 3 and does not belong to the G-equivalence class of the graph $****F$;

(2) *Every admissible graph of degree 5 is G-equivalent to the graph* $\circledast***$.

Proof: Let us generate the list of all graphs of degree 5 which do not contain a non-admissible subgraph of degree 3. There exist six ways to decompose 5 into a sum of four non-negative integers, $5=5+0+0+0=4+1+0+0=3+2+0+0=3+1+1+0=2+2+1+0=2+1+1+1$. This gives six labels, 5_Ψ, $4_\Psi 1_X$, $3_\Psi 2_X$, $3_\Psi 1_X 1_\Phi$, $2_\Psi 2_X 1_\Phi$, $2_\Psi 1_X 1_\Phi 1_F$. By permuting the symbols Ψ, X, Φ, and F, one generates the other labels. Excluding from the resulting set of labels the ones, which do not satisfy the conditions $k_3 \leqslant k_1 \leqslant 4$ and $k_4 \leqslant 1$, where k_1, k_3, and k_4 are the numbers in a label associated to the symbols Ψ, Φ, and F, respectively, one arrives at the following: 5_Ψ generates 5_X, but itself is deleted from the list; $4_\Psi 1_X$ generates $4_\Psi 1_\Phi$, $4_\Psi 1_F$, $4_X 1_F$, and $1_\Psi 4_X$; $3_\Psi 2_X$ generates

$3_\Psi 2_\Phi$, $2_\Psi 3_X$; $3_\Psi 1_X 1_\Phi$ generates $3_\Psi 1_X 1_F$, $3_\Psi 1_\Phi 1_F$, $1_\Psi 3_X 1_\Phi$, and $1_\Psi 3_X 1_F$; $2_\Psi 2_X 1_\Phi$ generates $2_\Psi 2_X 1_F$, $2_\Psi 2_\Phi 1_F$, and $2_\Psi 1_X 2_\Phi$; finally, $2_\Psi 1_X 1_\Phi 1_F$ generates $1_\Psi 2_X 1_\Phi 1_F$. This yields 20 labels in total. Inside each label the corresponding graphs are generated by exploring all the possible variants. Note, that in some of the cases one inevitably obtains a graph containing a nonadmissible part of degree 3, a graph under the label 5_X should contain a triangle since there are maximum four vertices on a graph; a graph under the label $4_\Psi 1_X$ always contains $*$—$*$; and a graph under the label $4_X 1_F$ contains either a triangle or a graph $\|F$. It means that the labels 5_X, $4_\Psi 1_X$, and $4_X 1_F$ can be omitted. After deleting from the list the known nonadmissible graphs of degree 5, i.e., the graphs which are G-equivalent to the graph $****F$, the following list is obtained:

$4_\Psi 1_\Phi$: $a)\ \circledast***$

$4_\Psi 1_F$: $\emptyset$

$1_\Psi 4_X$: $a)$ 

$3_\Psi 2_X$: $a)$ 

$3_\Psi 2_\Phi$: $a)\ \circledast\circledast*$ $b)\ \circledast**\odot$

$2_\Psi 3_X$: $a)$  $b)$ 

$3_\Psi 1_X 1_\Phi$: $a)$ 

$3_\Psi 1_X 1_F$: $a)$ 

$3_\Psi 1_\Phi 1_F$: $a)\ ***\odot F$

$1_\Psi 3_X 1_\Phi$: $a)$  $b)$ $c)$  $d)$ 

$1_\Psi 3_X 1_F$: $a)$  F $b)$ F

$2_\Psi 2_X 1_\Phi$: $a)$  $b)$ $c)$ $d)$

$e)$  $f)$

$2_\Psi 2_X 1_F$: $a)$  F $b)$ $*F$

$2_\Psi 2_\Phi 1_F$: $\emptyset$

$2_\Psi 1_X 2_\Phi$: $a)$

$2_\Psi 1_X 1_\Phi 1_F$: $a)$  $b)$

$1_\Psi 2_X 1_\Phi 1_F$: $a)$  F $b)$ F .

One verifies, that this list coincides with the set of all primary graphs belonging to the G-equivalence class of the graph $***\circledast$. Since the latter graph is known to be admissible, all these graphs are admissible. □

One could proceed in a similar way and investigate the cases of the graphs of degree 6, 7, and

8, but it turns out that one does not have to do it. Recall that the aim is to prove that the set of projective lines A is saturated with respect to the orthogonality relation $\perp$.

Theorem 1: *The set A is saturated with respect to* $\perp$. *Moreover, for every* $B \in \mathcal{P}_{\perp}(A)$, *one has the following*:

(1) *If B has a shadow of degree* 1 *or* 2, *then it admits a pure complete extension.*
(2) *If B has a shadow of degree 3, then it admits a complete extension hanging over a doublet.*
(3) *If the shadow of B is a doublet, then B has a unique pure complete extension.*
(4) *If the shadow of B is a singlet, then B has a unique complete extension; this extension has a shadow of degree 8.*
(5) *If the degree of the shadow of B is* $\geqslant 5$, *then B has a unique complete extension; this extension has a shadow of degree 8.*

Proof: Take any $B \in \mathcal{P}_{\perp}(A)$ and denote $Q := \mathcal{P}(\eta)(B) \in L$. Let γ denote the shadow of B, i.e., the graph associated to $[Q] \in \Gamma$, and d denote the degree of γ.

(1) Suppose that $d=1$ or $d=2$. Then γ is G-equiavalent to $*$, or respectively, $**$. Represent the corresponding latter graph by some $Q' \in L$. There exists $\hat{T} := T_{S_1} T_{S_2} \ldots T_{S_m}$, where $S_1, S_2, \ldots, S_m$ are some nonempty proper subsets of V (m is some natural number), such that $Q' = \hat{T}(Q)$. Denote $B' := \hat{\theta}(B)$, where $\hat{\theta} := \theta_{S_1} \theta_{S_2} \cdots \theta_{S_m}$. Choose a complete set B'' containing B' such that $\mathcal{P}(\eta)(B'') = \mathcal{P}(\eta)(B')$. The set $\hat{B} := \hat{\theta}^{-1}(B)$ yields the required pure complete extension of B.

(2) The case of $d=3$ is similar and the difference is that γ is now G-equivalent to $***$. Let one choose Q' and construct $\hat{T}$, $\hat{\theta}$ and B' by analogy with the previous case. The complete set $B'' \supset B'$ cannot be chosen now to have the same shadow as B', but it can have a shadow $***\odot$. Denote $Q'' := \mathcal{P}(\eta)(B'')$. The set $\hat{B} := \hat{\theta}^{-1}(B'')$ gives the required extension of B. This extension hangs over a graph associated to $[\hat{Q}]$, where $\hat{Q} := \hat{T}^{-1}(Q'')$, which is G-equivalent to $***\odot$ and by that is a doublet.

(3) Suppose that $d=4$ and γ is a doublet. Then it is G-equivalent to $***\odot$. Choose Q' and define $\hat{T}$, $\hat{\theta}$, and B' in analogy with the two previous cases. There exists a unique pure extension B'' of B'. The required unique pure complete extension $\hat{B}$ of B will be of the form $\hat{B} := \hat{\theta}^{-1}(B'')$. Note that not all the complete extensions of a set B have to be pure.

(4) Suppose that $d=4$ and γ is a singlet. Then γ is G-equivalent to $****$. Choose Q' and construct $\hat{T}$, $\hat{\theta}$, and B' in analogy with the three previous cases, i.e., we have $Q' = \hat{T}(Q)$, $B' = \hat{\theta}(B)$, $\eta \circ \hat{\theta} = \hat{T} \circ \eta$. The set B' has a unique complete extension B'' and this extension hangs over $\circledast\circledast\circledast\circledast$. The set $\hat{B} := \hat{\theta}^{-1}(B'')$ is the unique complete extension of the original set B. The shadow of $\hat{B}$ is of degree 8 and is given by the graph associated to $[\hat{T}^{-1}(Q'')]$, where $Q'' := \mathcal{P}(\eta)(B'')$.

(5) Suppose that $d \geqslant 5$. Recall that the set of all admissible graphs of degree 5 is the G-equivalence class of the graph $***\circledast$. This graph contains a singlet $****$. It follows, that every admissible graph of degree 5 contains a singlet, since a singlet can be G-equivalent only to a singlet. Whenever a set B_0 hangs over a singlet $****$, the corresponding complete extension exists and is unique. At the same time, for every $v \in V$ there exists a unique projective line of the form Φ^v_ρ, $\rho \in R_{\overline{v}}$, which is orthogonal to every element of B_0; there exist no projective lines of X or F type, which are orthogonal to every element of B_0. Thus the construction of the complete extension of B_0 may be viewed as a step-by-step appending of the mentioned unique Φ^v_ρ to the set B_0 as v runs over V. One concludes, that whenever one has some sets B_1, B_2, B_3, and B_4 hanging over the graphs $***\circledast$, $**\circledast\circledast$, $*$, and $\circledast\circledast\circledast\circledast$, respectively, one may extract from each of them a part $B_i^0 \subset B_i$ ($i=1,2,3,4$) hanging over $****$; the unique complete extension $\hat{B}_i^0$ of B_i^0 at the same time plays a role of a unique complete extension of B_i and one has $B_i^0 \subset B_i \subset \hat{B}_i^0$, $i=1,2,3,4$.

Now let $B \in \mathcal{P}_{\perp}(A)$ have an arbitrary shadow γ of degree $d \geqslant 5$. Every such γ should contain an admissible graph $\overline{\gamma}$ of degree 5 and it is possible to choose in B a subset $\overline{B}$ hanging over $\overline{\gamma}$. Using the lists of graphs from the proofs of the two previous propositions, one verifies in a straightforward way that every admissible graph of degree 5 contains a singlet. It means, that one

can always find in $\overline{\gamma}$ some singlet γ_0 and choose $B_0 \subset \overline{B}$ which hangs over this singlet. The graph γ_0, as any other singlet, is G-equivalent to $****$. Denote $Q_0 := \eta(B_0)$ and choose any $Q_0' \in L$ representing the $****$. There exists a collection of nonempty proper subsets $S_i \subset V$, $i = 1, 2, \ldots, m$ (m is some integer), such that $Q_0' = \hat{T}(Q_0)$, where $\hat{T} := T_{S_1} T_{S_2} \cdots T_{S_m} \in G$. Denote $\hat{\theta} := \theta_{S_1} \theta_{S_2} \cdots \theta_{S_m}$. The set $\hat{\theta}(B_0)$ has a shadow $****$, the set $\hat{\theta}(\overline{B})$ has a shadow $\circledast***$ and the set $\hat{\theta}(B)$ has a shadow consisting of four stars $*$ and $d-4$ circles $\odot$. A unique complete extension $\tilde{B}$ of $\hat{\theta}(B_0)$ is at the same time a unique complete extension for $\hat{\theta}(\overline{B})$ and $\hat{\theta}(B)$. The shadow of $\tilde{B}$ has a degree 8 and is of the form $\circledast\circledast\circledast\circledast$. The set $\hat{B} := \hat{\theta}^{-1}(\tilde{B})$ has a shadow of degree 8 as well and provides the required unique complete extension of the set B. □

IX. TRANSITIVE ACTION

We have the set A of 120 projective lines in $\mathcal{H} \simeq \mathbb{C}^8$ which produces a Kochen–Specker-type contradiction and is saturated with respect to the orthogonality relation $\perp$. Note, that if one extracts a subset A_0 from A consisting of all projective lines of Ψ and Φ type, one can still prove that A_0 is saturated with respect to $\perp$, but A_0 will not produce a Kochen–Specker-type contradiction. Consider the set $C(A)$ of all complete subsets of A and denote by $C_d(A)$ the subset of $C(A)$ consisting of all the elements which have a shadow of degree $d \in \mathbb{N}$.

Theorem 2: (1) *The set* $C_d(A) \neq \emptyset$ *iff* d *is equal to* 1, 2, 4 *or* 8;
(2) *The group* $\mathcal{G}$ *acts transitively on each of the* $C_d(A)$, $d = 1, 2, 4, 8$.

Proof: (1) The statement that d cannot be other than 1, 2, 4 or 8 whenever $C_d(A) \neq \emptyset$ follows from the fact that a set hanging over a graph of degree 3 cannot have pure complete extensions and the fact that if a set hangs over a graph of degree $\geqslant 5$, then its complete extension always has a shadow of degree 8. The examples of realizations of all four mentioned possibilities have been given in the proof of Proposition 1.

(2) Recall that $\mathcal{G}$ is a subgroup of $Bij(A)$ and the action of $\theta \in \mathcal{G}$ on $B \in C(A)$ is given by $\mathcal{P}(\theta)(B)$. Let us start with the component $C_8(A)$. Every element $B \in C_8(A)$ can be viewed as $B = \mathcal{P}(\theta)(B_0)$, where B_0 is some element of $C_8(A)$ with a shadow $\circledast\circledast\circledast\circledast$ and θ is some element of $\mathcal{G}$. Denote by $C_8^0(A) \subset C_8(A)$ the set of all complete subsets with the specified shadow. It follows, that the problem is reduced to the following: for every two $B, B' \in C_8^0(A)$ show that there exists $\theta \in \mathcal{G}$ such that $\mathcal{P}(\theta)(B) = B'$. Every element of $C_8^0(A)$ is determined by its part which hangs over a singlet $****$. There are as many elements in $C_8^0(A)$ as the sets hanging over this singlet. Take any $B, B' \in C_8^0(A)$ and denote by $B_1 \subset B$ and by $B_1' \subset B'$ their parts hanging over $****$. One associates in the way described in part (6) of the proof of Proposition 1 to B_1 and B_1' some functions φ and φ', respectively, $\varphi, \varphi' : E \to \mathbb{Z}_2$, where E is the set of all edges of the tetrahedron representing $\mathcal{P}(V)^{\times}$. One verifies, that $B_1' = \mathcal{P}(I_{\varphi+\varphi'})(B_1)$. This implies that the action of $\mathcal{G}$ on $C_8(A)$ is transitive.

Now consider the case of $C_4(A)$. This set consists of all those complete subsets of A hanging over a doublet. Denote by $C_4^0(A) \subset C_4(A)$ the set of all complete subsets with shadow $***\odot$. In analogy to the case of $C_8(A)$, the original problem reduces to the problem to show that for every $B, B' \in C_4^0(A)$ such that $\mathcal{P}(\eta)(B) = \mathcal{P}(\eta)(B')$ [recall that $\eta : A \to \mathcal{P}(V)$ denotes the natural map], there exists $\theta \in \mathcal{G}$ such that $\mathcal{P}(\theta)(B) = B'$. Take any of the mentioned B and B' and assume without loss of generality that $\mathcal{P}(\eta)(B) \in L$ is visualized by a graph ${}_e*{}_f*{}_g\odot_h$. One associates in the way as pointed out in part (5) of the proof of Proposition 1 to B a triple of parameters a, b, and c. Let $\psi : \{ef, eg, fg\} \to \mathbb{Z}_2$ denote the function, which has values on the edges ef, eg, and fg given by a, b, and c, respectively. In a similar way a function $\psi' : \{ef, eg, fg\} \to \mathbb{Z}_2$ is associated to the set B'. Choose any $\varphi, \varphi' : E \to \mathbb{Z}_2$ such that their restrictions to $\{ef, eg, fg\}$ coincide with ψ and ψ', respectively. It is clear that $B' = \mathcal{P}(I_{\varphi+\varphi'})(B)$. This completes the proof for the case $C_4(A)$.

The investigation of the case $C_2(A)$ is similar and contains a graph $**$ and a pair of $\mathbb{Z}_2$-valued functions on just one edge. The case $C_1(A)$ involves a graph $*$ and does not require a similar construction of $\mathbb{Z}_2$-valued functions. □

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Some useful combinatorial formulas for bosonic operators

P. Blasiak[a)]
Université Pierre et Marie Curie, Laboratoire de Physique Théorique de la Matière Condensée, CNRS UMR 7600, Tour 24, 2ième étage, 4 Place Jussieu, F 75252 Paris Cedex 05, France and H. Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences, ul. Radzikowskiego 152, PL 31342 Kraków, Poland

K. A. Penson[b)]
Université Pierre et Marie Curie, Laboratoire de Physique Théorique de la Matière Condensée, CNRS UMR 7600, Tour 24, 2ième étage, 4 Place Jussieu, F 75252 Paris Cedex 05, France

A. I. Solomon[c)]
Université Pierre et Marie Curie, Laboratoire de Physique Théorique de la Matière Condensée, CNRS UMR 7600, Tour 24, 2ième étage, 4 Place Jussieu, F 75252 Paris Cedex 05, France and The Open University, Physics and Astronomy Department, Milton Keynes MK7 6AA, United Kingdom

A. Horzela[d)]
H. Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences, ul. Radzikowskiego 152, PL 31342 Kraków, Poland

G. H. E. Duchamp[e)]
Institut Galilée, LIPN, CNRS UMR 7030, 99 Av. J.-B. Clément, F 93430 Villetaneuse, France

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We give a general expression for the normally ordered form of a function $F[\hat{w}(a,a^\dagger)]$ where $\hat{w}$ is a function of boson creation and annihilation operators satisfying $[a,a^\dagger]=1$. The expectation value of this expression in a coherent state becomes an exact generating function of Feynman-type graphs associated with the zero-dimensional quantum field theory defined by $F(\hat{w})$. This enables one to enumerate explicitly the graphs of given order in the realm of combinatorially defined sequences. We give several examples of the use of this technique, including the applications to Kerr-type and superfluidity-type Hamiltonians. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1904161]

In the normally ordered form of a function $F(a,a^\dagger)$ of boson creation and annihilation operators all the annihilation operators are moved to the right using the commutation relation $[a,a^\dagger]=1$. The importance of the normal form, denoted by $\mathcal{N}[F(a,a^\dagger)]$ and satisfying $F(a,a^\dagger)=\mathcal{N}[F(a,a^\dagger)]$, is evident, as with it the expectation values of $F(a,a^\dagger)$ can be easily evaluated in such canonical states as the vacuum $|0\rangle$ and coherent states $|z\rangle=e^{-|z|^2/2}\Sigma_{n=0}^{\infty}z^n/\sqrt{n!}|n\rangle$, ($z$ complex and $a^\dagger a|n\rangle=n|n\rangle$). The role of the normal form in quantum field theory (QFT) is pre-eminent.[1,2]

In this work we consider functions $F(\hat{w})$ that involve operators $\hat{w}(a,a^\dagger)$ in the form of a product of positive powers of $a^\dagger$ and a, and powers of $(a+a^\dagger)$, although the formulas derived below are valid for more general $\hat{w}$'s. Our considerations are based on the following operational

[a)]Electronic mail: blasiak@lptl.jussleu.fr
[b)]Electronic mail: penson@lptl.jussieu.fr
[c)]Electronic mail: a.i.solomon@open.ac.uk
[d)]Electronic mail: andrzej.horzela@ifj.edu.pl
[e)]Electronic mail: ghed@lipn-univ.paris13.fr

property of formal power series. Let $f(x)=\Sigma_{n=0}^{\infty}f_n x^n/n!$ and $g(x)=\Sigma_{n=0}^{\infty}g_n x^n/n!$ be two formal power series, also called the exponential generating functions (egf) of sequences $\{f_n\}_{n=0}^{\infty}$ and $\{g_n\}_{n=0}^{\infty}$, respectively. Then it can be verified that

$$f\left(\lambda\frac{d}{dx}\right)g(x)\bigg|_{x=0}=g\left(\lambda\frac{d}{dx}\right)f(x)\bigg|_{x=0}=\sum_{n=0}^{\infty}f_n\cdot g_n\frac{\lambda^n}{n!},$$

which we shall call the product formula (PF). This implies the following property satisfied by $F(\lambda\hat{w})$ with indeterminate λ:

$$F(\lambda\hat{w})=F\left(\lambda\frac{d}{dx}\right)e^{x\hat{w}}\bigg|_{x=0}, \tag{1}$$

which by taking the normal form of both sides becomes

$$\mathcal{N}[F(\lambda\hat{w})]=F\left(\lambda\frac{d}{dx}\right)\mathcal{N}(e^{x\hat{w}})\bigg|_{x=0}. \tag{2}$$

Note that in Eq. (2) a separation has been achieved between the functional aspect (defined by F) and the operator aspect (defined by $\hat{w}$) of the normal ordering. Conventionally we implement $\mathcal{N}(e^{x\hat{w}})$ by using the auxiliary symbol $::$ with $\mathcal{N}(e^{x\hat{w}})\equiv :G_{\hat{w}}(x,a,a^{\dagger}):$, where under the symbol $::$ the function $G_{\hat{w}}(x,a,a^{\dagger})$ is normally ordered assuming that $a^{\dagger}$ and a *commute*.[3,4] Then Eq. (2) becomes

$$\mathcal{N}[F(\lambda\hat{w})]=F\left(\lambda\frac{d}{dx}\right):G_{\hat{w}}(x,a,a^{\dagger}):\bigg|_{x=0}. \tag{3}$$

Note that the expression of Eq. (3) arises in the evaluation of the partition function Z_{β} for the system defined by the Hamiltonian $\mathcal{H}(\hat{w})$,

$$Z_{\beta}=\mathrm{Tr}\,e^{-\beta\mathcal{H}(\hat{w})}=\frac{1}{\pi}\int d^2z[\,e^{-\beta\mathcal{H}(d/dx)}G_{\hat{w}}(x,z,z^{*})|_{x=0}],$$

taking the trace over the coherent state representation, $\beta=(k_BT)^{-1}$.[5] The problem of finding $\mathcal{N}[F(\lambda\hat{w})]$ reduces to that of finding $\mathcal{N}(e^{x\hat{w}})$, still however a nontrivial task, *vide* the classical references.[3,4,6] We have recently found expressions for $G_{\hat{w}}(x,a,a^{\dagger})$ for several types of operators $\hat{w}$ of the form $\hat{w}_{(r,s)}=(a^{\dagger})^r a^s$ (Ref. 7) as well as for $\hat{w}_{(\vec{r},\vec{s})}=\Pi_{k=1}^{M}\hat{w}_{(r_k,s_k)}$ with r, s, r_k, s_k positive integers.[8]

At this point it is already possible to relate Eq. (3) to enumerative formulas for Feynman-type graphs in QFT.[9] Assume that our formal power series $F(x)$ can be written in the form $F(x)=\exp[\Sigma_{m=1}^{\infty}L_m(x^m/m!)]$, and we similarly assume that we may define operators $V_n^{(\hat{w})}(a,a^{\dagger})$ by

$$:G_{\hat{w}}(x,a,a^{\dagger}):=:\exp\left(\sum_{n=1}^{\infty}V_n^{(\hat{w})}(a,a^{\dagger})\frac{x^n}{n!}\right):. \tag{4}$$

Explicit examples[7] from which the operators $V_n^{(\hat{w})}(a,a^{\dagger})$ may be read off include

$$\hat{w}=a^{\dagger}a,\quad \mathcal{N}[\exp(xa^{\dagger}a)]=:\exp[a^{\dagger}a(e^x-1)]:, \tag{5}$$

$$\hat{w} = (a^\dagger)^r a, \quad \mathcal{N}[\exp(x(a^\dagger)^r a)] = :\exp\left[a^\dagger a \sum_{n=1}^{\infty} (a^\dagger)^{(r-1)n} (r-1)^n \frac{\Gamma\left(n + \frac{1}{r-1}\right)}{\Gamma\left(\frac{1}{r-1}\right)} \frac{x^n}{n!} \right]: , \tag{6}$$

with $r=2,3,\ldots,$ as well as more involved expressions for other $\hat{w}(a,a^\dagger)$. Thus, Eq. (3) may be written as

$$\mathcal{N}[F(\lambda\hat{w})] = \exp\left(\sum_{m=1}^{\infty} \frac{L_m}{m!} \lambda^m \frac{d^m}{dx^m} \right) \cdot :\exp\left(\sum_{n=1}^{\infty} V_n^{(\hat{w})}(a,a^\dagger) \frac{x^n}{n!} \right): \Bigg|_{x=0} . \tag{7}$$

We eliminate the operators a and $a^\dagger$ by taking the matrix element of Eq. (7) in the coherent state $|z\rangle$ and using $a|z\rangle = z|z\rangle$. This yields

$$\langle z|\mathcal{N}[F(\lambda\hat{w})]|z\rangle = \exp\left(\sum_{m=1}^{\infty} \frac{L_m}{m!} \lambda^m \frac{d^m}{dx^m} \right) \cdot \exp\left(\sum_{n=1}^{\infty} V_n^{(\hat{w})}(z,z^*) \frac{x^n}{n!} \right) \Bigg|_{x=0} . \tag{8}$$

By specifying $z=1$ in Eq. (8), defining $V_n^{(\hat{w})}(1,1) = V_n^{(\hat{w})}$, $\mathbf{V} = \{V_n^{(\hat{w})}\}_{n=1}^{\infty}$, and $\mathbf{L} = \{L_m\}_{m=1}^{\infty}$ we obtain

$$Z(\mathbf{L},\mathbf{V},\lambda) \equiv \langle 1|\mathcal{N}[F(\lambda\hat{w})]|1\rangle = \exp\left(\sum_{m=1}^{\infty} \frac{L_m}{m!} \lambda^m \frac{d^m}{dx^m} \right) \cdot \exp\left(\sum_{n=1}^{\infty} V_n^{(\hat{w})} \frac{x^n}{n!} \right) \Bigg|_{x=0} \tag{9}$$

which is essentially the counting formula cited by Bender *et al.*[9] Due to the symmetry of the PF, we have $Z(\mathbf{L},\mathbf{V},\lambda) = Z(\mathbf{V},\mathbf{L},\lambda)$, which may facilitate the calculations. Furthermore it can be demonstrated that for all the forms of $\hat{w}$ used here the sequence $\mathbf{V}$ consists of positive integers. The formula Eq. (9) was employed in Ref. 9 as an enumerative tool for counting the Feynman-type graphs in zero-dimensional QFT models, where the values of all Feynman integrals are equal to 1. Our derivation sheds light on its quantum origin by tracing back its sources to the boson normal ordering problem. By specifying the sets $\mathbf{L}$ and $\mathbf{V}$ one can attempt to produce a (in general divergent) power series expansion in λ,

$$Z(\mathbf{L},\mathbf{V},\lambda) = \sum_{n=0}^{\infty} A_n(\mathbf{L},\mathbf{V}) \frac{\lambda^n}{n!} \tag{10}$$

in which $A_n(\mathbf{L},\mathbf{V})$ can be related to known objects. To see that, recall the definition of the multivariate Bell polynomials $\mathbb{B}(\mathbf{h},u)$ related to a function $h(x) = \Sigma_{n=1}^{\infty} h_n x^n/n!$ through ($\mathbf{h} = \{h_n\}_{n=1}^{\infty}$)

$$e^{uh(x)} = \sum_{n=0}^{\infty} \frac{x^n}{n!} \sum_{k=1}^{n} u^k \mathbb{B}_{nk}(\mathbf{h}) = \sum_{n=0}^{\infty} \frac{x^n}{n!} \mathbb{B}_n(\mathbf{h},u), \tag{11}$$

where the coefficients of the expansion $\mathbb{B}_n(\mathbf{h},u) = \Sigma_{k=1}^{n} u^k \mathbb{B}_{nk}(\mathbf{h})$ depend only on $h_1,\ldots,h_n$. We refer to Refs. 10 and 11 for further properties of $\mathbb{B}_n(\mathbf{h},u)$.

With $\mathbb{B}_n(\mathbf{f}) = \mathbb{B}_n(\mathbf{f},1)$ we see that the coefficients $A_n = A_n(\mathbf{L},\mathbf{V})$ factorize

$$A_n = \mathbb{B}_n(\mathbf{L}) \cdot \mathbb{B}_n(\mathbf{V}) \tag{12}$$

which for given $\mathbf{L}$ and $\mathbf{V}$ can be worked out (see below).

The utility of Eqs. (9) and (12) goes beyond the specific definition of initial $\hat{w}$, and this is the philosophy of Ref. 9 where it was suggested that $\mathbf{L}$ and $\mathbf{V}$ could be treated as initial *input* for QFT models. From this perspective Eqs. (9) and (12) provide the starting point for a Feynman-type graph representation of the coefficients A_n in Eq. (10), where A_n counts the number of graphs with n labeled lines. The graph construction rules are as follows: a line starts from a white dot, the *origin*, and ends at a black dot, the *vertex*. We further associate strengths V_k with each vertex

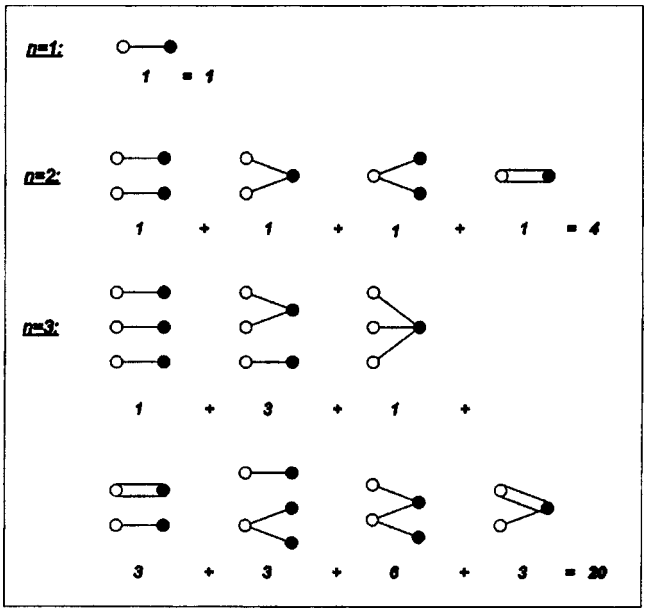

FIG. 1. Lowest order Feynman-type graphs for Example 1 with $n=1,2,3$ lines. The number below each graph is its multiplicity.

receiving k lines and multipliers L_m with a white dot which is the origin of m lines. Counting such graphs consists in calculating their multiplicity due to the labelling of lines and the factors L_m and V_k.

We now specify **L** and **V** and give some examples of the explicit evaluation of A_n along with the explicit graph representation.

Example 1: $L_1=1$, $L_M=1$ $(M>1)$, and $L_m=0$ otherwise, giving the function $F(x)=\exp(x+x^M/M!)$; $V_n^{(\hat{w})}=1$ for $n=1,2\ldots$, which arises from the string $\hat{w}=a^\dagger a$, see Eq. (5). This corresponds to the normal ordering problem $\mathcal{N}[\exp(\lambda a^\dagger a+(\lambda^M/M!)(a^\dagger a)^M)]$. Note that the case $M=2$ describes the normal ordering of the exponential of the Kerr-type Hamiltonian[12] $\mathcal{H}=\lambda a^\dagger a(1+(\lambda/2)a^\dagger a)$. Using the definition of the two variable Hermite–Kampé de Fériet polynomials $H_n^{(M)}(x,y)$ (see Ref. 13 and references therein)

$$\sum_{n=0}^{\infty} H_n^{(M)}(x,y)\frac{t^n}{n!}=e^{xt+yt^M}, \tag{13}$$

where $H_n^{(M)}(x,y)=n!\Sigma_{r=0}^{[n/M]}[(x^{n-Mr}y^r)/(n-Mr)!r!]$, $F(x)$ can be expanded as

$$F(x)=e^{x+(x^M/M!)}=\sum_{n=0}^{\infty} H_n^{(M)}\left(1,\frac{1}{M!}\right)\frac{x^n}{n!}. \tag{14}$$

Equation (10) yields $A_n=H_n^{(M)}(1,1/M!)\cdot B_n$, where the *Bell* numbers B_n are defined through their egf, $\exp(e^x-1)=\Sigma_{n=0}^{\infty}B_nx^n/n!$.[9–11] Observe that for $M=2$, $H_n^{(2)}(1,\frac{1}{2})=(i/\sqrt{2})^nH_n(-i/\sqrt{2})=1,2,4,10,26,76,232,\ldots$ are the *involution* numbers[10] expressible using Hermite polynomials $H_n(x)$. The initial terms of A_n for $M=2$ are 1,4,20,150,1352,15 428,…, see Fig. 1, and for $M=3$, are $1,2,10,75,527,6293,\ldots$, etc. Note that whereas B_n counts all the partitions of an n-set, $H_n^{(M)}(1,1/M!)$ counts partitions of an n-set into singletons and M-tons.

Example 2: $L_m=m$ for $m=1,2,\ldots$, giving rise to $F(x)=\exp[\Sigma_{m=1}^{\infty}m(x^m/m!)]=\exp(xe^x)=\Sigma_{n=0}^{\infty}I_nx^n/n!$, where $I_n=\Sigma_{k=0}^{\infty}\binom{n}{k}k^{n-k}$ are *idempotent* numbers.[10] Again choosing $V_n^{(\hat{w})}=1$, n

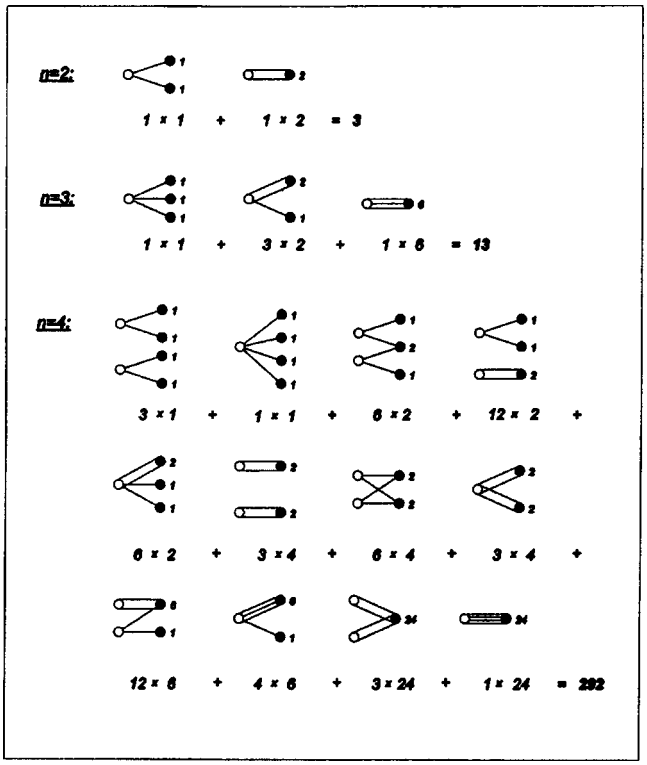

FIG. 2. Lowest order Feynman-type graphs for Example 3 with $n=2,3,4$ lines. The number below each graph is (*multiplicity*) $\times \Pi_k$(*vertex factor* $V_k=k!$). Numbers at black dots (vertices) are vertex factors.

$=1,2,\ldots$, with $\hat{w}=a^\dagger a$, gives $A_n=I_n$. $B_n=1,6,50,615,10\,192,214\,571,\ldots$. This corresponds to normally ordering $\mathcal{N}[\exp(\lambda(a^\dagger a)e^{\lambda(a^\dagger a)})]$.

Example 3: $L_1=0$, $L_m=1$ for $m=2,3,\ldots$, leading to $F(x)=\exp(e^x-1-x)=\Sigma_{n=0}^{\infty}B_n^{(1)}x^n/n!$, where $B_n^{(1)}$ are *restricted Bell* numbers which are defined as counting partitions without singletons. **(**Note that $B_n^{(1)}=(1/e)\Sigma_{k=0}^{\infty}[(k-1)^n/k!]$**)**. Here we choose $V_n^{(\hat{w})}=n!$, $n=1,2,\ldots$, derived from the string $\hat{w}=(a^\dagger)^2a$, and producing via $\exp[x/(1-x)]=\Sigma_{n=0}^{\infty}B_n^{(2,1)}x^n/n!$ [see Eq. (37) of Ref. 7], $A_n=B_n^{(1)}\cdot B_n^{(2,1)}=0,3,13,292,5511,166\,091,\ldots$, see Fig. 2. This corresponds to the normal ordering of $\exp(e^{\lambda(a^\dagger)^2a}-1-\lambda(a^\dagger)^2a)$.

Example 4: $L_{2m}=2m$, $L_{2m+1}=0$ for $m=0,1,2,\ldots$, giving $F(x)=\exp(x\sinh(x))$. If, as in Examples 1 and 2, $V_n^{(\hat{w})}=1$, $n=1,2,\ldots$, $\hat{w}=a^\dagger a$, then by defining the *indempotent* polynomials $I_n(t)=\Sigma_{k=0}^{n}\binom{n}{k}k^{n-k}t^k$ we obtain $A_n=I_n^{(2)}.B_n=0,4,0,240,0,49\,938,0,24\,608\,160,0,\ldots$, where $I_n^{(2)}=\Sigma_{k=0}^{n}\binom{n}{k}(-1)^kI_k(-\frac{1}{2})I_{n-k}(\frac{1}{2})$, yielding $\mathcal{N}[\exp(\lambda a^\dagger a\,\sinh(\lambda a^\dagger a))]$.

Example 5: In the last example we shall treat the function $\hat{w}=a+a^\dagger$, using $F(x)=e^{x^M/M!}$, $M=1,2,3,\ldots$. First observe that $\mathcal{N}(e^{x\hat{w}})=:G_{\hat{w}}(x,a,a^\dagger):=:e^{x^2/2}e^{x(a+a^\dagger)}:$ which is a consequence of the Heisenberg algebra. It follows that $V_1^{(\hat{w})}(a,a^\dagger)=a+a^\dagger$, $V_2^{(\hat{w})}(a,a^\dagger)=1$ and $V_n^{(\hat{w})}(a,a^\dagger)=0$ for $n>2$, see Eq. (4), giving $\mathbf{V}=\{2,1,0,0,\ldots\}$ and $\mathbf{L}=\{\delta_{m,M}\}_{m=1}^{\infty}$. Let us define the modified Hermite polynomials $h_n(x)=(-i/\sqrt{2})^nH_n(ix/\sqrt{2})$ and then $\exp(2x+x^2/2)=\Sigma_{n=0}^{\infty}[h_n(2)/n!]x^n$. Using Eqs. (10) and (12) we get

$$Z_M(\mathbf{L},\mathbf{V},\lambda)=\exp\left(\frac{\lambda^M}{M!}\frac{d^M}{dx^M}\right)\cdot\exp\left(2x+\frac{x^2}{2}\right)\Bigg|_{x=0}=\sum_{n=0}^{\infty}\frac{h_{Mn}(2)}{n!}\left(\frac{\lambda^M}{M!}\right)^n. \tag{15}$$

Starting with the simplest case $M=1$, the function $Z_1(\mathbf{L},\mathbf{V},\lambda)=\exp(2\lambda+\lambda^2/2)$ gives $A_n=h_n(2)=1,2,5,14,43,142,499,1850,\ldots$, $n=0,1,2,\ldots$, The series of Eq. (15) can also be written down

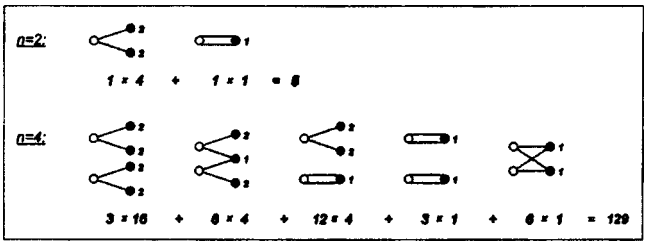

FIG. 3. Lowest order Feynman-type graphs for Example 5 with $n=2,4$ lines. The number below each graph is $(multiplicity)\times\Pi_k(vertex\ factor\ V_k=2\delta_{k,1}+\delta_{k,2})$.

in closed form for $M=2$, corresponding to a single mode superfluidity-type Hamiltonian $\mathcal{H}\sim(a+a^\dagger)^2$,[14] and for $M=3$,[15]

$$Z_2(\mathbf{L},\mathbf{V},\lambda)=\sum_{n=0}^{\infty}\frac{h_{2n}(2)}{n!}\left(\frac{\lambda^2}{2!}\right)^n=\frac{1}{(1-\lambda^2)^{1/2}}\exp\left(\frac{2\lambda^2}{1-\lambda^2}\right), \tag{16}$$

$$Z_3(\mathbf{L},\mathbf{V},\lambda)=\sum_{n=0}^{\infty}\frac{h_{3n}(2)}{n!}\left(\frac{\lambda^3}{3!}\right)^n=\frac{\exp\left(\phi^3\frac{\lambda^3}{6}-\phi^4\frac{\lambda^6}{8}\right)}{(1-\phi\lambda^3)^{1/2}}{}_2F_0\left(\frac{1}{6},\frac{5}{6};-;\frac{3\lambda^6}{2(1-\phi\lambda^3)^3}\right), \tag{17}$$

where $\phi(\lambda)=(1-\sqrt{1-4\lambda^3})/\lambda^3$ and ${}_2F_0$ is the hypergeometric function. In these examples Z_1 and Z_2 are convergent series in λ while Z_3 is formal power series. From Eq. (15) we can read off the values of A_n: $A_{Mn}=[(Mn)!/(M!)^n n!]h_{Mn}(2)$ and zero otherwise, giving for $M=2$, $A_{2n}=1,5,129,7485,755\,265,116\,338\,005,\ldots$, see Fig. 3. Note, that whenever Z is known in closed form the equation$Z(\lambda)=\exp[\lambda(d/dx)]Z(x)|_{x=0}$ leads immediately to a set of graphs for which $L_m=\delta_{m,1}$. Thus for $M=2$, with Eq. (16) we have the following alternative descriptions: (a) $L_m=\delta_{m,2}$; $V_1=2$, $V_2=1$, $V_{n>2}=0$ and (b) $L_m=\delta_{m,1}$; $V_{2n}=(4n+1)(2n-1)!$. However even if Z is not known explicitly method (a) leads to a simple, alternative, graphical description using Eq. (15).

In conclusion we see that the technique described herein and hinging on Eq. (9) leads to a combinatorial and graphical description of many physical systems.

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Vortices set and the applied magnetic field for superconductivity in dimension three

Zuhan Liu[a)]
Department of Mathematics, Xuzhou Normal University, Xuzhou 221116, China

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In this paper, the structure of vortices set of the Ginzburg–Landau system of the superconductivity in dimension three was studied when applied magnetic field $|h_{\mathrm{ex}}|=O(|\ln \varepsilon|)$. This singularities set is one-dimensional rectifiable. Its generalized mean curvature was given. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Consider the following Ginzburg–Landau equations, referred to as GL:

$$\mathrm{GL}\begin{cases} -(\nabla - iA)^2 u = \dfrac{u}{\varepsilon^2}(1-|u|^2) & \text{in} \quad \Omega \\ -\operatorname{curl} h = (iu, \nabla_A u) & \text{in} \quad \Omega \\ h \times \nu = h_{\mathrm{ex}} \times \nu & \text{on} \quad \partial\Omega \\ (\nabla u - iAu)\cdot \nu = 0 & \text{on} \quad \partial\Omega. \end{cases}$$

The solutions of this system are the critical points of the following Ginzburg–Landau energy:

$$J(u,A) = \frac{1}{2}\int_{\Omega}\left[|\nabla_A u|^2 + \frac{1}{2\varepsilon^2}(1-|u|^2)^2 + |h-h_{\mathrm{ex}}|^2\right]. \tag{1.1}$$

This energy-functional was introduced by the physicists Ginzburg and Landau in the 1950s as a model for superconductivity. Ω is a bounded smooth domain in $\mathbb{R}^3$. $\kappa = 1/\varepsilon$ is a dimensionless constant (the Ginzburg–Landau parameter). h_{ex} is the applied magnetic field, $A:\Omega \mapsto \mathbb{R}^3$ is the vector potential, and the induced magnetic field in the material is $h = \operatorname{curl} A$. $\nabla_A = \nabla - iA$. The complex order parameter u indicates the local state of the material. $|u|$ represents the density of superconducting electron pairs, so that $|u| \simeq 1$ corresponds to the superconducting state, $|u| \simeq 0$ corresponds to the normal state.

We know that a superconductor placed in an applied magnetic field may change its phases when the field varies. When the lower critical value H_{c_1} of applied magnetic field is reached, there is a phase transition from the superconducting state to the "mixed state," where vortices appear (zero-set of u). The motion of vortices generates an electric field and leads to current dissipation. On the other hand, energy concentrates and blows up like the order $|\ln \varepsilon|$ on vortices set, hence singularities happen. So, to understand the vortices structure is of great importance not only in mathematical theory but also in application. The Ginzburg–Landau equations and functional are invariant under $U(1)$ gauge transformations of the type: $u \mapsto ue^{i\Phi}$, $A \mapsto A + \nabla\Phi$. We choose the Coulomb gauge

[a)]Electronic mail: zuhanl@yahoo.com

$$\operatorname{div} A = 0 \text{ in } \Omega, \quad A \cdot \nu = 0 \text{ on } \partial\Omega. \tag{1.2}$$

In the case $\Omega \subset \mathbb{R}^2$, Sandier and Serfaty[13–15] already studied global minimizers of energy-functional (1.1) and describe their vortices structure as $\varepsilon \to 0$. In Refs. 16–18, Serfaty studied vortices structure of local minimizer of (1.1), as $\varepsilon \to 0$, under assumption $\mathcal{E}_\varepsilon(u) = \frac{1}{2}\int_\Omega [|\nabla u|^2 + (1/2\varepsilon^2)(1-|u|^2)^2] \leqslant M_0 |\ln \varepsilon|$.

In the case $\Omega \subset \mathbb{R}^3$, experiments have indicated the possibility of quite complicated vortices configurations and it remains a challenge to capture these codimension two singularities in a rigorous mathematical way. In this paper, we are interested in the asymptotic behavior of vortices set (concentrating measures) associated with solutions to GL and concentrate our attention on singularities of codimension two, then it is natural to assume that the energy of u_ε blows up like $|\ln \varepsilon|$:

$$\mathcal{E}_\varepsilon(u_\varepsilon) = \frac{1}{2}\int_\Omega \left[|\nabla u_\varepsilon|^2 + \frac{1}{2\varepsilon^2}(1-|u_\varepsilon|^2)^2 \right] \mathrm{d}x \leqslant M_0 |\ln \varepsilon|, \tag{1.3}$$

where M_0 is a fixed constant. This condition implies that the length of the vortices set is finite. Such an assumption is automatically satisfied if $(u_\varepsilon, A_\varepsilon)$ is a minimizer of $J(u,A)$ with Dirichlet boundary condition (see Ref. 11).

In order to state our main result, it is convenient to introduce the following measures and Jacobian:[2,9,12]

$$\mu_\varepsilon := \frac{e_\varepsilon(u_\varepsilon)}{|\ln \varepsilon|}\mathrm{d}x, \quad Ju_\varepsilon = \Sigma_{i<j}(\partial_i u_\varepsilon \times \partial_j u_\varepsilon)\mathrm{d}x_i \wedge \mathrm{d}x_j,$$

where

$$e_\varepsilon(u_\varepsilon) = \frac{1}{2}\left[|\nabla u_\varepsilon|^2 + \frac{1}{2\varepsilon^2}(b_\varepsilon - |u_\varepsilon|^2)^2 \right], \; b_\varepsilon = 1 + \varepsilon^2 |A_\varepsilon|^2.$$

In view of assumption (1.3), μ_ε is bounded. Therefore, up to a subsequence we may assume

$$\mu_\varepsilon \rightharpoonup \mu_* \text{ as measures}. \tag{1.4}$$

By (1.3), Ju_ε is bounded in $[C^{0,\alpha}(K)]^*$ for any compact $K \subset \Omega$ any $0 < \alpha < 1$ (see Ref. 8). Going to a subsequence, we have

$$Ju_\varepsilon \to J_* \text{ in } [C^{0,\alpha}(K, \Lambda_2 \mathbb{R}^3)]^*, \tag{1.5}$$

for any compact $K \subset \Omega$. Recall that, for a radon measure $\nu \in \mathcal{M}(\Omega)$ and $m > 0$, the m dimensional density of ν at $x \in \Omega$ is defined by

$$\Theta_m(\nu, x) := \liminf_{r \to 0} \frac{\nu(B(x,r))}{r^m}.$$

Set

$$\Sigma_\mu = \{x \in \Omega : \Theta_1(\mu_*, x) > 0\}. \tag{1.6}$$

Then we have the following main theorem.

Theorem 1.1: *Let $(u_\varepsilon, A_\varepsilon)$ be the solutions to GL with (1.3). Assume h_{ex} is a given constant vector satisfying $|h_{\text{ex}}| \leqslant C|\ln \varepsilon|$. The following properties hold.*

i) The set Σ_μ is closed in Ω and 1-rectifiable. There exists a constant $\eta_0 > 0$ such that for each $x_0 \in \Sigma_\mu$,

$$\Theta_*(x_0) := \Theta_1(\mu_*, x_0) \geqslant \eta_0. \tag{1.7}$$

Moreover, for every compact set $K \subset \Omega \setminus \Sigma_\mu$,

$$|u_\varepsilon(x)| \to 1 \text{ uniformly on } K \text{ as } \varepsilon \to 0. \tag{1.8}$$

ii) The measure μ_* *can be decomposed as*

$$\mu_* = |\nabla h(x)|^2 \cdot \mathcal{H}^3 + \Theta_*(x) \cdot \mathcal{H}^1 \lfloor \Sigma_\mu , \tag{1.9}$$

where h is some harmonic function.

iii) The varifold $V := V(\Sigma_\mu, \Theta_*)$ *satisfies*

$$\vec{H}(x) = * \left(\vec{a} \wedge * \frac{dJ_*}{d\mu_*} \right) \text{ for } \mu_* - \text{a.e. } x \text{ in } \Sigma_\mu, \tag{1.10}$$

where $\vec{H}(x)$ *denotes the generalized mean curvature of V at x and is defined by*

$$\int_\Omega \operatorname{div}_{\Sigma_\mu} \vec{X} = - \int_\Omega \vec{H} \cdot \vec{X} \text{ for all } \vec{X} \in C_0^\infty(\Omega, \mathbb{R}^3),$$

$*$ *refers to the Hodge duality, and* $dJ_*/d\mu_*$ *is the Radon-Nikodym derivative of* J_* *with respect to* μ_*, $\vec{a} = \lim_{\varepsilon \to 0}(A_\varepsilon | / \ln \varepsilon |)$.

Remark 1.1: From the proof of Lemma 2.2, we have, for $h_{\text{ex}} = o(|\ln \varepsilon|)$, *that*

$$\vec{H}(x) = 0 \text{ for } \mu_* - \text{a.e. } x \text{ in } \Sigma_\mu.$$

This means that V is a stationary varifold. The limiting vortex set Σ_μ *consists of line segments. But, when* $h_{\text{ex}} = O(|\ln \varepsilon|)$, *for the solutions with the bound (1.3), vortices will be curved according to the equation* $\vec{\kappa} = \vec{a} \times \vec{\tau}$ *provided*

$$\frac{d\|J_*\|}{d\mu_*} = 1.$$

$\vec{\tau}$ *is the unit tangent vector to V and* $\vec{\kappa}$ *its curvature vector.*

Remark 1.2: The main motivation of assumption (1.3) come from Refs. 16, 17, and 3. Theorem 1.1 extend the results in Refs. 16 and 17 from two dimensions to three dimensions. We would like to mention that the method here is completely different than that in Refs. 16 and 17. Our proofs borrow many ingredients from Refs. 3–5 and 10, in particular, borrowing ideas from the proof of Theorem 3 of Ref. 5. The first important tool in our proof is monotonicity formula. In order to establish the monotonicity formula, we need to obtain the uniform estimate on A_ε *and refined estimates on Jacobian integrals, which is a conjecture by Bourgain, Brezis, and Mironescu (Ref. 7), were just proven by Bethuel, Orlandi, and Smets (Ref. 6). This step is different than that in Theorem 3 of Ref. 5. The second important ingredient is the* η*-compactness theorem.*

Remark 1.3: In Ref. 11, Rivière studied the global minimizer of the three-dimensional Higgs model. Theorem 1.1 can be extended to the critical points of that model which satisfy (1.3).

We organize the paper as follows: In Sec. II, we derive the monotonicity formula and η-compactness theorem. In Sec. III, we prove the main Theorem 1.1.

II. THE MONOTONICITY FORMULA AND η-COMPACTNESS THEOREM

In this section, we will derive the monotonicity formula of the energy. First of all, we establish some basic estimates on A_ε. By maximum principles, we have the following lemmas (see Ref. 11).

Lemma 2.1: Let $(u_\varepsilon, A_\varepsilon)$ *be the solutions to GL. We have*

$$\|u_\varepsilon\|_{L^\infty(\Omega)} \leqslant 1, \quad \|\nabla_A u\|_{L^\infty(\Omega)} \leqslant \frac{C}{\varepsilon}. \tag{2.1}$$

Now we establish an estimate of A_ε.

Lemma 2.2: Let $(u_\varepsilon, A_\varepsilon)$ *be the solutions to GL with assumption (1.3). We have*

$$\|A_\varepsilon\|_{w^{1,6}(\Omega)} \leqslant C_0|\ln \varepsilon|. \tag{2.2}$$

In particular,

$$\|A_\varepsilon\|_{C^\alpha(\bar{\Omega})} \leqslant C_0|\ln\ \varepsilon| \tag{2.3}$$

where $0<\alpha<1$ *and* C_0 *is independent of* ε.

Proof: It is well known that for the given h_{ex}, there exists a unique smooth vector field F on Ω such that

$$\operatorname{curl} F = h_{\text{ex}}, \quad \operatorname{div} F = 0 \text{ in } \Omega, \quad F\cdot\nu = 0 \text{ on } \partial\Omega. \tag{2.4}$$

From GL, we have

$$\operatorname{curl}^2(A-F) + |u|^2A = (iu, \nabla u) \text{ in } \Omega, \tag{2.5}$$

$$\operatorname{curl}(A-F)\times\nu = 0 \text{ on } \partial\Omega. \tag{2.6}$$

We see that $\|\operatorname{curl}A\|_{L^2(\Omega)}$ is an equivalent norm of space

$$H(\Omega,\operatorname{div}) = \{A\in H^1(\Omega,\mathbb{R}^2):\operatorname{div}A = 0 \text{ in } \Omega, A\cdot\nu = 0 \text{ on } \partial\Omega\}.$$

Multiplying (2.5) by $A-F$, integrating by parts, then using Lemma 2.1, (1.3), and Young's inequality, we obtain

$$\|A-F\|^2_{H^1(\Omega)} \leqslant C|\ln\varepsilon| + \|F\|^2_{L^2(\Omega)}. \tag{2.7}$$

So,

$$\|A\|^2_{H^1(\Omega)} \leqslant C|\ln\varepsilon| + \|F\|^2_{H^1(\Omega)} \leqslant C|\ln\varepsilon| + C\|\operatorname{curl}F\|^2_{L^2(\Omega)} \leqslant C|\ln\varepsilon|^2. \tag{2.8}$$

Since $\operatorname{div}A=0$ in Ω, we have, from GL, that

$$-\Delta A + |u|^2A = (iu, \nabla u) \text{ in } \Omega. \tag{2.9}$$

By elliptic estimate, we have the following interior estimate:

$$\|A\|^2_{H^2(K)} \leqslant C(K)(|\ln\varepsilon| + \|A\|^2_{H^1(\Omega)}) \leqslant C(K)|\ln\varepsilon|^2, \ \forall\, K\subset\subset\Omega. \tag{2.10}$$

To derive the boundary estimates, we shall straighten a portion of boundary and study the equation in the half ball B_R^+. Now, we fix a point x^0 on $\partial\Omega$. If there exists an R_0 such that $\Omega\cap B_{R_0}(x_0)\subset\{(x_1,x_2,x_3):x_3>0\}$, $\Gamma_{R_0}=\partial\Omega\cap B_{R_0}(x_0)\subset\{(x_1,x_2,0)\}$, then we have the boundary conditions

$$\partial_3A_1 = h^2_{\text{ex}}, \quad \partial_3A_2 = -h^1_{\text{ex}}, \quad A_3 = 0 \text{ on } \Gamma_{R_0}.$$

Combining this relation with (2.9), by the elliptic estimates, we have the following boundary estimate:

$$\|A\|_{H^2(B^+_{R_0/2})} \leqslant C[\|\nabla_A u\|_{L^2(\Omega)} + \|A\|_{H^1(\Omega)} + \|h_{\text{ex}}\|_{H^1(\Gamma_{R_0})}] \leqslant C|\ln\varepsilon|.$$

In general case, we will straighten a portion of $\partial\Omega$ around x_0. For simplicity, assume that $x^0=0$ and express a portion of $\partial\Omega$ around 0 by $r=r(y_1,y_2)$, $r(0,0)=0$. Let ∂_j denote ∂_{y_j}. Denote $r_i=\partial_i r$, $n=r_1\times r_2/|r_1\times r_2|$ and $g_{ij}=r_i\cdot r_j$. Choosing (y_1,y_2) as the normal coordinates of the portion of surface and ν to be the inward normal vector to $\partial\Omega$, we have $g_{ij}(0,0)=\delta_{ij}$. Denote $e_1=r_1$, $e_2=r_2$, and $e_3=n$. We will choose the isothermal coordinates (y_1,y_2). Denote k_1 and k_2 the principle curvature. Now, define a map

$$x = \mathcal{F}(y) = r(y_1, y_2) + y_3 n(y_1, y_2), \tag{2.11}$$

which is defined on some B_R^+ and straightens a portion of $\partial\Omega$ around x^0. We compute $\partial_j \mathcal{F}$ and $G_{ij} = \partial_i \mathcal{F} \cdot \partial_j \mathcal{F}$:

$$\partial_1 \mathcal{F} = [1 - k_1 y_3] r_1, \quad \partial_2 \mathcal{F} = [1 - k_2 y_3] r_2, \quad \partial_3 \mathcal{F} = n,$$

$$G_{11} = g_{11}[1 - k_1 y_3]^2,$$

$$G_{22} = g_{22}[1 - k_2 y_3]^2,$$

$$G_{33} = 1,$$

$$G_{12} = G_{13} = G_{23} = 0.$$

Let G^{ij} denote the element of the inverse of the matrix (G_{ij}). Then

$$G^{11} = 1/G_{11}, \quad G^{22} = 1/G_{22}, \quad G^{33} = 1, \quad G^{12} = G^{13} = G^{23} = 0.$$

Given a function u and a vector A, we write them in the new variables as follows:

$$\tilde{u}(y) = u(\mathcal{F}(y)), \tag{2.12}$$

$$\tilde{A}(y) = A(\mathcal{F}(y)) = \sum_{j=1}^{3} G^{jj} a_j \partial_j \mathcal{F}(y), \tag{2.13}$$

where

$$a_j = A(\mathcal{F}(y)) \cdot \partial_j \mathcal{F}(y).$$

Now, let $g_1 = 1 - y_3 k_1$, $g_2 = 1 - y_3 k_2$, then the differential operator in the new coordinates can be defined as

$$D_{\tilde{A}} W = (D_{\tilde{A}_1} W, D_{\tilde{A}_2} W, D_{\tilde{A}_3} W), \tag{2.14}$$

where $D_{\tilde{A}_1} W = (1/g_1)(\partial_1 - i\tilde{A}_1) W$, $D_{\tilde{A}_2} W = (1/g_2)(\partial_2 - i\tilde{A}_2) W$ and $D_{\tilde{A}_3} W = (\partial_3 - i\tilde{A}_3) w$. Then we have the following equations for $\tilde{A}$:

$$\frac{1}{G_{11}}(\partial_1^2 \tilde{A}) + \frac{1}{G_{22}}(\partial_2^2 \tilde{A}) + \partial_3^2 \tilde{A} = Y(\tilde{A}, \partial_1 \tilde{A}, \partial_2 \tilde{A}, \partial_3 \tilde{A}) + (i\tilde{u}, D_{\tilde{A}} \tilde{u}) \text{ in } B_R^+, \tag{2.15}$$

$$\partial_3 \tilde{A}_1 = h_{\text{ex}} g_{22}^{-1} e_2, \quad \partial_3 \tilde{A}_2 = -h_{\text{ex}} g_{11}^{-1} e_1, \quad \tilde{A}_3 = 0 \text{ on } \Gamma_R, \tag{2.16}$$

where $\Gamma_R = \{(y_1, y_2, 0) : |y_1|^2 + |y_2|^2 \leqslant R^2\}$, $Y(\tilde{A}, \partial_1 \tilde{A}, \partial_2 \tilde{A}, \partial_3 \tilde{A})$ denotes linear combination of these factors.

From the elliptic estimate to (2.15), (2.16), and (2.8), we have

$$\|\tilde{A}\|_{H^2(B_{R/2}^+)} \leqslant C(|\ln \varepsilon| + \|h_{\text{ex}} g_{11}^{-1} e_1\|_{H^1(\Gamma_R)} + \|h_{\text{ex}} g_{22}^{-1} e_2\|_{H^1(\Gamma_R)}) \leqslant C|\ln\ \varepsilon|. \tag{2.17}$$

From (2.10) and (2.17), we have

$$\|A\|_{H^2(\Omega)} \leqslant C|\ln \varepsilon|. \tag{2.18}$$

By Sobolev embedding, we have

$$\|A\|_{W^{1,6}(\Omega)} \leqslant C|\ln \varepsilon|, \quad \|A\|_{C^{\alpha}(\bar{\Omega})} \leqslant C|\ln \varepsilon|, \tag{2.19}$$

where $0<\alpha<1$. The proof of Lemma 2.2 is completed. □

For $x_0 \in \Omega$ and $r>0$ such that $B_r(x_0) \subset \Omega$, define

$$\widetilde{E}_{\varepsilon}(u_{\varepsilon},x_0,r) := \frac{1}{r}E_{\varepsilon}(u_{\varepsilon},x_0,r) \equiv \frac{1}{r}\int_{B_r(x_0)}\left[\frac{1}{2}|\nabla u_{\varepsilon}|^2 + \frac{(b_{\varepsilon}(x)-|u_{\varepsilon}|^2)^2}{4\varepsilon}\right]. \tag{2.20}$$

When this will not lead to a confusion, we will also denote it $\widetilde{E}_{\varepsilon}(x_0,r)$ or even $\widetilde{E}_{\varepsilon}(r)$. A computation directly gives the following (see Refs. 3 and 5).

Lemma 2.3: Let $(u_{\varepsilon},A_{\varepsilon})$ satisfy GL and $B_R(x_0)\subset\Omega$, then for $0<r<R$,

$$\frac{\mathrm{d}}{\mathrm{d}r}(\widetilde{E}_{\varepsilon}(x_0,r)) = \frac{1}{r}\int_{\partial B_r(x_0)}\left|\frac{\partial u_{\varepsilon}}{\partial n}\right|^2 + \frac{1}{r^2}\int_{B_r(x_0)}\frac{(b_{\varepsilon}(x)-|u_{\varepsilon}|^2)}{2\varepsilon^2} - \frac{2}{r^2}\int_{B_r(x_0)}\langle Ju_{\varepsilon},A_{\varepsilon i}\xi_i(x-x_0)\rangle$$
$$-\frac{1}{2r^2}\int_{B_r(x_0)}((x-x_0)\cdot\nabla|A_{\varepsilon}|^2)(b_{\varepsilon}-|u_{\varepsilon}|^2), \tag{2.21}$$

where $\xi_j(x)=\Sigma_{i\neq j}x_i\mathrm{d}x_j\wedge\mathrm{d}x_i$, for $j=1,2,3$.

Lemma 2.4: There exists $C>0$ which is independent of ε such that for $B_R(x_0)\subset\Omega$,

$$\Lambda = C(C_0+1)|\ln\varepsilon| \tag{2.22}$$

and for any $(u_{\varepsilon},A_{\varepsilon})$ satisfying GL with (1.3), we have

$$\frac{\mathrm{d}}{\mathrm{d}r}(\exp(\Lambda r)(\widetilde{E}_{\varepsilon}(x_0,r)+CC_0\varepsilon^2|\ln\varepsilon|^3)) \geqslant \frac{1}{r}\int_{\partial B_r}\left|\frac{\partial u_{\varepsilon}}{\partial n}\right|^2 + \frac{1}{r^2}\int_{B_r}\frac{(b_{\varepsilon}(x)-|u_{\varepsilon}|^2)^2}{4\varepsilon^2} \geqslant 0 \tag{2.23}$$

for $0<r<R$. In particular, $\exp(\Lambda r)(\widetilde{E}_{\varepsilon}(x_0,r)+C\varepsilon^2|\ln\varepsilon|^3)$ is increasing.

Proof: From Lemma 2.3, we need to estimate the last two terms in (2.21). The conclusion follows by using Lemma 2.2 immediately. □

In order to establish the monotonicity formula on larger balls, refined estimates on Jacobian integrals are needed because we only have C^{α} estimate on A_{ε}.

Lemma 2.5: (Refs. 6 and 7) Let $w\in H^1_{\mathrm{loc}}(\Omega,\mathbb{C})$, $\varphi\in C_0^{\infty}(\Omega,\Lambda^1\mathbb{R}^3)$ and $K:=\mathrm{supp}\,\varphi$. Moreover, assume that there exists $q>6$ such that w verifies

$$\|w\|_{L^q(\Omega)} \leqslant C_q. \tag{2.24}$$

Then,

$$\left|\int_{\Omega}\langle Jw,\varphi\rangle\right| \leqslant C\left(\frac{\int_K e_{\varepsilon}(w)}{|\ln\varepsilon|} + \varepsilon^{\alpha_0}\left(\int_K e_{\varepsilon}(w)\right)^{\alpha_1}\right)\|\varphi\|_{\dot{W}^{1,3}(\Omega)}, \tag{2.25}$$

for some constants $C>0$ and $0<\alpha_0<1, 0<\alpha_1<1$, depending only on q, C_q.

Now we prove the following monotonicity formula.

Proposition 2.1: There exist $C>0$ and $\beta>0$ depending not on ε such that for $B_R(x_0)\subset\Omega$ and for any $(u_{\varepsilon},A_{\varepsilon})$ satisfying GL with (1.3), we have

$$\widetilde{E}_{\varepsilon}(x_0,\theta r) \leqslant C(\widetilde{E}_{\varepsilon}(x_0,r)+\varepsilon^{\beta}) \tag{2.26}$$

for $0<\theta<1/2$ and $0<r<\min(R,2/(C_0+1))$.

Proof: We follow closely the lines of Lemma A.6 in Ref. 5 and drop off the subscript ε for simplicity.

Step 1: We define a smooth cut-off function f by

$$f(r,a)=\begin{cases}1 & \text{if a} \leqslant \text{r}\\ 2-a/r & \text{if r} \leqslant \text{a} \leqslant \text{2r}\\ 0 & \text{if } a \geqslant 2r,\end{cases} \tag{2.27}$$

where $r>0$. For $x_0 \in \Omega$ and $r>0$ such that $B_{2r}(x_0) \subset \Omega$, set

$$\overline{E_\varepsilon}(x_0,r) := \frac{1}{r}\int_{B_{2r}(x_0)} e_\varepsilon(u) f(r,|x-x_0|)\mathrm{d}x, \tag{2.28}$$

then for $0<r<R/2$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}r}(\overline{E_\varepsilon}(x_0,r)) = {}& \frac{1}{r}\int_1^2 t\int_{\partial B_{tr}(x_0)}\left|\frac{\partial u}{\partial n}\right|^2 + \frac{1}{r^2}\int_{B_{2r}(x_0)}\frac{(b_\varepsilon-|u|^2)^2}{2\varepsilon^2} f(r,|x-x_0|)\\ & -\frac{1}{r^2}\int_{B_{2r}(x_0)}\left\langle Ju, 2\sum_i A_i(x)\xi_i(x-x_0) f(r,|x-x_0|)\right\rangle - \frac{1}{2r^2}\int_{B_{2r}(x_0)}((x-x_0)\cdot\nabla|A|^2)\\ & \times(b_\varepsilon(x)-|u|^2) f(r,|x-x_0|).\end{aligned} \tag{2.29}$$

Step 2: There exists a constant $C>0$ such that for $B_{2r}(x_0)\subset\Omega$,

$$\overline{E_\varepsilon}(x_0,\theta r) \leqslant CC_0\exp(CC_0 r)\left(\overline{E_\varepsilon}(x_0,r)+\frac{\varepsilon^{\alpha_0}|\ln\varepsilon|^{\alpha_1+1}}{\theta r}+\varepsilon^2|\ln\varepsilon|^4\right) \tag{2.30}$$

for $0<\theta\leqslant 1$. In fact, we need to estimate the last two terms in (2.29). We may assume $x_0=0$. The second one is treated as before,

$$\left|\frac{1}{2r^2}\int_{B_{2r}(x_0)}((x-x_0)\cdot\nabla|A|^2)(b_\varepsilon(x)-|u|^2) f(r,|x-x_0|)\right| \leqslant \overline{E_\varepsilon}(2r)+CC_0\varepsilon^2|\ln\varepsilon|^4. \tag{2.31}$$

For the first term, note that the two-form

$$\varphi(x) := \sum_i 2A_i(x)\xi_i(x) f(r,|x|) \tag{2.32}$$

satisfies the estimates, using Lemma 2.2,

$$\|\varphi\|_{\dot{W}^{1,3}(B_{2r})} \leqslant CC_0|\ln\varepsilon| r. \tag{2.33}$$

Hence, using Lemma 2.5, we have

$$\frac{1}{r^2}\int_{B_{2r}(x_0)}\left\langle Ju, 2\sum_i A_i(x)\xi_i(x-x_0) f(r,|x-x_0|)\right\rangle \leqslant CC_0\overline{E_\varepsilon}(2r)+\frac{CC_0}{r}\varepsilon^{\alpha_0}|\ln\varepsilon|^{\alpha_1+1}. \tag{2.34}$$

Combining (2.31), (2.34), and (2.29), we have

$$\frac{\mathrm{d}}{\mathrm{d}r}(\overline{E_\varepsilon}(x_0,r)) \geqslant -CC_0\overline{E_\varepsilon}(2r)-CC_0\left(\varepsilon^2|\ln\varepsilon|^4+\frac{1}{r}\varepsilon^{\alpha_0}|\ln\varepsilon|^{\alpha_1+1}\right). \tag{2.35}$$

(2.30) then follows from a version of Gronwall's lemma given in Lemma A.7, Ref. 5.

Step 3: First, consider the case

$$\theta r < p := (|\ln\varepsilon|(C_0+1))^{-1} < r/2. \tag{2.36}$$

Using Lemma 2.4, we obtain that

$$\tilde{E}_\varepsilon(\theta r) \leqslant C(\tilde{E}_\varepsilon(\rho) + \varepsilon^2|\ln \varepsilon|^3). \tag{2.37}$$

Next, using (2.30) and the definition of ρ,

$$\tilde{E}_\varepsilon(\rho) \leqslant \overline{E}_\varepsilon(\rho) \leqslant C\left(\overline{E}_\varepsilon(r/2) + \frac{\varepsilon^{\alpha_0}|\ln \varepsilon|^{\alpha_1+1}}{\rho} + |\ln \varepsilon|^4\varepsilon^2\right) \leqslant C(\tilde{E}_\varepsilon(r) + \varepsilon^{\alpha_0}|\ln \varepsilon|^{\alpha_1+2} + \varepsilon^2|\ln \varepsilon|^4). \tag{2.38}$$

Letting $\beta = \alpha_0/2$ and combining (2.37) and (2.38), we get the desired (2.26). In the case $\theta r \geqslant \rho$ (respectively, $r \leqslant \rho$), it suffices to use (2.30) (respectively, Lemma 2.4) to obtain (2.26) directly. This completes the proof of Proposition 2.1. □

Using Lemma 2.2 and Proposition 2.1, the same argument of Theorem 2 in Ref. 5 gives the following η-compactness theorem, which bounds $|u_\varepsilon|$ away from zero as soon as the local energy is bounded by $\eta|\ln \varepsilon|$ with η small.

Theorem 2.6: *(η-compactness theorem) Let $(u_\varepsilon, A_\varepsilon)$ be a solution of GL with (1.3) and $\sigma > 0$ be given. Then, there exist $\eta > 0$ and $\varepsilon_0 > 0$, depending only on $\sigma > 0$, C_0 such that if $x_0 \in \Omega$, $\varepsilon \leqslant \varepsilon_0$, $\sqrt{\varepsilon} \leqslant r \leqslant 1/(1+C_0)$, $B_{2r}(x_0) \subset \Omega$, and*

$$\tilde{E}_\varepsilon(x_0, r) \leqslant \eta|\ln \varepsilon|, \tag{2.39}$$

then

$$|u_\varepsilon(x_0)| \geqslant 1 - \sigma. \tag{2.40}$$

Corollary 2.7: Under the assumption of Theorem 2.6. Let $0 < \sigma < 1$, $\eta > 0$, and $\varepsilon_0 > 0$ be given by Theorem 2.6. Let $x_0 \in \Omega$ and $r > 0$ such that $B(x_0, 2r) \subset \Omega$ and $4\sqrt{\varepsilon} < r < 4/(1+C_0)$. Then, for $\varepsilon < \varepsilon_0$, if

$$\tilde{E}_\varepsilon(x_0, r) \leqslant \tfrac{1}{4}\eta|\ln \varepsilon| \tag{2.41}$$

we have

$$|1 - |u(x)|| \leqslant \sigma \quad \forall\, x \in B(x_0, 3r/4). \tag{2.42}$$

III. PROOF OF THEOREM 1.1

In this section we will prove Theorem 1.1. Recall that, by Lemma 2.2 and assumption (1.3),

$$E_\varepsilon(u_\varepsilon) = \int_\Omega e_\varepsilon(u_\varepsilon) \leqslant (2M_0 + 1)|\ln \varepsilon|, \tag{3.1}$$

where $e_\varepsilon(u_\varepsilon) = (1/2)[|\nabla u_\varepsilon|^2 + (1/2\varepsilon^2)(b_\varepsilon - |u_\varepsilon|^2)^2]$. By (3.1), we have

$$\mu_\varepsilon := \frac{e_\varepsilon(u_\varepsilon)}{|\ln \varepsilon|}\mathrm{d}x$$

is bounded. Therefore, up to a subsequence we may assume that

$$\mu_\varepsilon \rightharpoonup \mu_* \text{ as measures.} \tag{3.2}$$

We set

$$\Sigma_\mu = \{x \in \Omega : \Theta_1(\mu_*, x) > 0\}, \tag{3.3}$$

where

$$\Theta_1(\mu_*,x) := \liminf_{r\to 0} \frac{\mu_*(B(x,r))}{r}.$$

Lemma 3.1: Let $\Theta_*(x_0) := \Theta_1(\mu_*,x_0)$. *Then, there exists a constant* $\eta_0>0$ *such that if* $x_0 \in \Sigma_\mu$, *we have*

$$\Theta_*(x_0) \geqslant \eta_0.$$

Proof: Let $\eta_0=\frac{1}{4}\eta$, where $\eta>0$ and $\varepsilon_0>0$ are given by Theorem 2.6. The conclusion follows by using contradiction argument as in the proof of Lemma B.11 in Ref. 5. □

By the upper-semicontinuity of Θ_*, we have the following lemma.

Lemma 3.2: Σ_μ *is closed in* Ω.

From Lemma 3.1 and Corollary 2.7 we have the following uniformly convergence result away from Σ_μ.

Lemma 3.3: Let $K\subset\Omega\backslash\Sigma_\mu$ *be any compact subset. For any* $\sigma>0$, *there exists a constant* $\varepsilon_2>0$ *depending on K,* σ *such that, for* $\varepsilon<\varepsilon_2$,

$$|1-|u|| \leqslant \sigma \text{ on } K. \tag{3.4}$$

Lemma 3.4: We have

$$\mu_* = g(x)\mathcal{H}^3 + h(x)\mathcal{H}^1\lfloor\Sigma_\mu\,,$$

where $g,h\in L^\infty_{\mathrm{loc}}(\Omega)$ *and*

$$\eta_0 \leqslant \Theta_*(x) \leqslant h(x) \leqslant \Theta^*(x) := \limsup_{r\to 0} \frac{\mu_*(B(x,r))}{r} \leqslant CM_0.$$

Proof: Since Σ_μ is closed in Ω, hence Σ_μ is measurable. We have

$$\mu_* = \mu_*\lfloor\Sigma_\mu + \mu_*\lfloor(\Omega\backslash\Sigma_\mu)\,.$$

By Corollary 2.7, the same argument of Theorem VIII.1 in Ref. 3 yields

$$\mathcal{H}^1(\Sigma_\mu) \leqslant CM_0.$$

By the monotonicity formula of Proposition 2.1, we have that for any $x\in\Omega$,

$$\Theta^*(x) := \limsup_{r\to 0} \frac{\mu_*(B(x,r))}{r} \leqslant CM_0.$$

According to the Radon–Nikodym theorem, we obtain

$$\mu_*\lfloor\Sigma_\mu = h(x)\ \mathcal{H}^1\lfloor\mu_* \tag{3.5}$$

for $\Theta_*\leqslant h(x)\leqslant\Theta^*$. Let $x_0\in\Omega\backslash\Sigma_\mu$, $r>0$ such that $\overline{B}(x_0,2r)\subset\Omega\backslash\Sigma_\mu$. By Lemma 3.3, we obtain

$$\sigma := \|1-|u|\|_{L^\infty(\overline{B}(x_0,2r))} = o(1) \text{ as } \varepsilon\to 0.$$

It is easy to show that

$$E_\varepsilon\left(x_0,\tfrac{3}{4}r\delta\right) \leqslant C(\delta^3+\sigma+C_0\varepsilon^2|\ln\varepsilon|+\varepsilon)E_\varepsilon(x_0,r) + CC_0\varepsilon|\ln\varepsilon|^2. \tag{3.6}$$

Note that $\sigma=\sigma(\varepsilon)=o(1)$. Dividing both sides of (3.6) by $|\ln\varepsilon|$ and sending $\varepsilon\to 0$ we obtain

$$\mu_*\left(B\left(x_0,\tfrac{3}{4}r\delta\right)\right) \leqslant C\delta^3\mu_*(B(x_0,r)),$$

which implies that $\mu_*\lfloor(\Omega\backslash\Sigma_\mu)$ is absolutely continuous with respect to the Lebesgue measure, and by the Radon–Nikodym theorem again we obtain

$$\mu_* = g(x)\mathcal{H}^3 + h(x)\mathcal{H}^1\lfloor\Sigma_\mu \tag{3.7}$$

for some locally bounded function g. The proof of Lemma 3.4 is completed. □

The same proof of Theorem A.(iv) in Ref. 4 gives

Lemma 3.5: We have

$$g(x) = |\nabla h_*(x)|^2 \text{a.e. in } \Omega,$$

where h_* is some harmonic function.

Lemma 3.6: Σ_μ is rectifiable,

$$\vec{H}(x) = *\left(\vec{a} \wedge *\frac{\mathrm{d}J_*}{\mathrm{d}\mu_*}\right)$$

for μ_*-a.e. x in Σ_μ.

Proof: Let $\vec{X} \in \mathcal{D}(\Omega, \mathbb{R}^3)$ be a smooth vector field. Then,

$$\frac{1}{|\ln\varepsilon|}\int_\Omega \left(e_\varepsilon(u)\delta_{ij} - \frac{\partial u}{\partial x_i}\frac{\partial u}{\partial x_j}\right)\frac{\partial X^i}{\partial x_j} = -\int_\Omega \left\langle *\left(\frac{2A_\varepsilon}{|\ln\varepsilon|} \wedge *Ju\right), \vec{X}\right\rangle + \frac{1}{2|\ln\varepsilon|}\int_\Omega (b_\varepsilon - |u|^2)\vec{X}\cdot\nabla|A_\varepsilon|^2, \tag{3.8}$$

where $*$ refers to the Hodge duality. Let

$$\alpha_\varepsilon^{ij} := \frac{1}{|\ln\varepsilon|}\left(e_\varepsilon(u)\delta_{ij} - \frac{\partial u}{\partial x_i}\frac{\partial u}{\partial x_j}\right).$$

$(\alpha_\varepsilon^{ij})$ is a symmetric matrix with trace larger than μ_ε. Hence, its eigenvalues are less or equal to μ_ε. Note that

$$|\alpha_\varepsilon^{ij}| \leqslant 3\mu_\varepsilon. \tag{3.9}$$

Passing to a subsequent, we may assume that

$$\alpha_\varepsilon^{ij} \to \alpha_*^{ij} \text{ in the sense of measures.}$$

By (3.9), we obtain $|\alpha_*^{ij}| \leqslant 3\mu_*$. Therefore,

$$\alpha_*^{ij}(x) = A^{ij}(x)\mu_* \text{ for } \mu_* - \text{a.e. } x \in \Omega,$$

where the matrix $A^{ij}(x)$ is symmetric and its trace equal to 1 and eigenvalues less or equal to 1. From (3.9), we also have

$$A^{ij} \geqslant -3\delta^{ij} \text{ for } \mu_* - a\,.\,e\,.\ x \in \Omega. \tag{3.10}$$

Now we deal with the last term of the right-hand side of (3.8). By Lemma 2.2, we have

$$\left|\frac{1}{2}\int_\Omega (b_\varepsilon - |u|^2)\frac{\vec{X}\cdot\nabla|A|^2}{|\ln\varepsilon|}\right| \leqslant C\varepsilon\|A\|_{L^\infty}\left(\int_\Omega |\nabla A|^2\right)^{1/2}\frac{1}{|\ln\varepsilon|}\left(\int_\Omega \frac{b_\varepsilon - |u|^2}{\varepsilon^2}\right)^{1/2}$$
$$\leqslant C\varepsilon|\ln\varepsilon| \to 0 \text{ as } \varepsilon \to 0. \tag{3.11}$$

On the other hand, from Lemma 2.2, passing to a subsequence, there exists an $\vec{a}$ such that

$$\frac{A_\varepsilon}{|\ln\varepsilon|} \to \vec{a} \text{ in } C^\alpha(\overline{\Omega}) \text{ as } \varepsilon \to 0. \tag{3.12}$$

Therefore, passing to the limit in (3.8), we have

$$\int_\Omega A^{ij}(x)\frac{\partial X^i}{\partial x_j}\mathrm{d}\mu_*(x) = -\int_\Omega \left\langle *\left(\vec{a}\wedge *\frac{dJ_*}{d\mu_*}\right),\vec{X}\right\rangle \mathrm{d}\mu_*. \tag{3.13}$$

We decompose the right-hand side of (3.13) as

$$\int_\Omega A^{ij}(x)\frac{\partial X^i}{\partial x_j}\mathrm{d}\mu_*(x) = \int_\Omega A^{ij}(x)\frac{\partial X^i}{\partial x_j}\mathrm{d}\mu_*(x)\lfloor\Sigma_\mu + \int_\Omega \left(\frac{|\nabla h_*|^2}{2}\delta_{ij} - \frac{\partial h_*}{\partial x_i}\frac{\partial h_*}{\partial x_j}\right)\frac{\partial X^i}{\partial x_j}\mathrm{d}x. \tag{3.14}$$

Since $\Delta h_* = 0$, we have

$$\int_\Omega \left(\frac{|\nabla h_*|^2}{2}\delta_{ij} - \frac{\partial h_*}{\partial x_i}\frac{\partial h_*}{\partial x_j}\right)\frac{\partial X^i}{\partial x_j}\mathrm{d}x = 0. \tag{3.15}$$

From (3.13) and (3.15), we obtain

$$\int_\Omega A^{ij}(x)\frac{\partial X^i}{\partial x_j}\mathrm{d}\mu_*(x)\lfloor\Sigma_\mu = -\int_\Omega \left\langle *\left(\vec{a}\wedge *\frac{dJ_*}{d\mu_*}\right),\vec{X}\right\rangle \mathrm{d}\mu_*\lfloor\Sigma_\mu . \tag{3.16}$$

Since $\vec{X}$ was arbitrary, (3.16) implies that the generalized 1-varifold (defined in Ref. 1) $\tilde{V} := \delta_{A^{ij}(x)}\mu_*\lfloor\Sigma_\mu$ has a first variation. By Theorem 3.8(c) in Ref. 1 we obtain that $\tilde{V}$ is a real rectifiable 1-varifold. In particular, Σ_μ is rectifiable which implies

$$\Theta_*(x) = \Theta^*(x)\ \ \mu_* - a.e.\ \ x\in\Sigma_\mu,$$

thus,

$$\mu_* = g(x)\mathcal{H}^3 + \Theta_*(x)\mathcal{H}^1\lfloor\Sigma_\mu, \quad \tilde{V} = V(\Sigma_\mu,\Theta_*). \tag{3.17}$$

By (3.16), we also have

$$\vec{H} = *\left(\vec{a}\wedge *\frac{\mathrm{d}J_*}{\mathrm{d}\mu_*}\right) \text{ for } \mu_* - a.e.\ \ x\in\Sigma_\mu.$$

The proof of Theorem 1.1 is now completed. □

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Strong-electric-field eigenvalue asymptotics for the Iwatsuka model

Shin-ichi Shirai[a)]
Research Institute for Mathematical Sciences, Kyoto University, Sakyo, Kyoto 606-8502, Japan

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We consider the two-dimensional Schrödinger operator, $H_g(b)=-\partial^2/\partial x^2+[(1/\sqrt{-1})(\partial/\partial y)-b(x)]^2-gV(x,y)$, where V is a non-negative scalar potential decaying at infinity like $(1+|x|+|y|)^{-m}$, and $(0,b(x))$ is a magnetic vector potential. Here, b is of the form $b(x)=\int_0^x B(t)\mathrm{d}t$ and the magnetic field B is assumed to be positive, bounded, and monotonically increasing on $\mathbf{R}$ (the Iwatsuka model). Following the argument as in Refs. 15, 16, and 17 [Raikov, G. D., Lett. Math. Phys., **21**, 41–49 (1991); Raikov, G. D, Commun. Math. Phys., **155**, 415–428 (1993); Raikov, G. D. Asymptotic Anal., **16**, 87–89 (1998)], we obtain the asymptotics of the number of discrete spectra of $H_g(b)$ crossing a real number λ in the gap of the essential spectrum as the coupling constant g tends to $\pm\infty$, respectively. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1897844]

I. INTRODUCTION

We consider the two-dimensional Schrödinger operator with electromagnetic field

$$H_g(b)=-\frac{\partial^2}{\partial x^2}+\left(\frac{1}{\sqrt{-1}}\frac{\partial}{\partial y}-b(x)\right)^2-gV(x,y).$$

Here, $V(x,y)$ is a scalar potential decaying at infinity and $(0,b(x))$ is a magnetic vector potential given by the form $b(x)=\int_0^x B(t)\mathrm{d}t$ for a positive magnetic field B, which depends only on the variable x of $(x,y)\in\mathbf{R}^2$.

The purpose of this paper is to investigate the number of discrete spectra of $H_g(b)$ crossing a real number λ in the gap of the essential spectrum as the coupling constant g tends to $\pm\infty$, respectively (the precise formulation is given below).

We fix some notations. We denote the set of all integers by $\mathbf{Z}$ and denote the set of *non-negative* integers by $\mathbf{N}$. We denote the cardinal number of set A by $\sharp A$. We denote both $\partial/\partial x$ and $\mathrm{d}/\mathrm{d}x$ by ∂_x, etc. We denote by $C^k(\Omega,\Omega')$ the set of all Ω'-valued, C^k-functions on Ω, and by $C_0^\infty(\Omega)$ the set of all compactly supported, smooth functions on Ω. We use $|\cdot|$ to denote the Euclidean norms and use the notations $\langle z\rangle=(1+|z|^2)^{1/2}$ for any $z\in\mathbf{R}^n$ and $\langle x;y\rangle=(1+|x|^2+|y|^2)^{1/2}$ for any $(x,y)\in\mathbf{R}^n\times\mathbf{R}^m$. We denote by $Q(z,r)$ the open cube of radius r, centered at z, with sides parallel to the coordinate axes. We denote by $\mathrm{Spec}(A)$ the spectrum of any self-adjoint operator A, and by $N(\alpha<A<\beta)$ the dimension of the range of the spectral projection for A on the interval (α,β). The notations $N(A>\alpha)$, $N(A<\beta)$, etc., are defined similarly.

To formulate our results we make the following assumptions for the magnetic field B and the electric potential V.

(B.1) The magnetic field B is a real-valued, smooth and monotonically increasing function on $\mathbf{R}$. Moreover, there exist positive numbers $B_\pm$ such that $B_-<B_+$, and $\lim_{x\to\pm\infty}B(x)=B_\pm$ hold, respectively.

[a)]Electronic mail: qzy05360@nifty.ne.jp

(B.2) In addition to (*B*.1), there exists a positive number M such that, for any multi-index α, the estimate $|\partial_x^\alpha(B(x)-B_\pm)| \leqslant C_\alpha \langle x\rangle^{-M}$ holds for $\pm x \geqslant 0$, respectively. Here, the constant C_α is independent of x, and $B_\pm$ are as in (B.1).

(V.1) The scalar potential V is a non-negative smooth function on $\mathbf{R}^2$. Moreover, there exists a positive number m such that, for any multi-index α, the estimate $|\partial_z^\alpha V(z)| \leqslant C_\alpha \langle z\rangle^{-m-|\alpha|}$ holds for all $z \in \mathbf{R}^2$. Here, the constant C_α is independent of z.

(V.2) There exists a positive number C such that the estimate $V(z) \geqslant C\langle z\rangle^{-m}$ holds for all $z \in \mathbf{R}^2$.

(V.3) Let $(r,\omega) \in [0,\infty)\times S^1$ be the polar coordinates of $z \in \mathbf{R}^2$, i.e., $r=|z|$ and $\omega = z/|z|$. There exists a measurable, bounded and positive function v on the unit circle S^1 such that $\lim_{r\to\infty} r^m V(z) = v(\omega)$ holds for any $\omega = z/|z| \in S^1$.

(V.4) In addition to (*V*.1), we have the limit

$$\lim_{\varepsilon\downarrow 0} \limsup_{\mu\downarrow 0} \mu^{2/m} \operatorname{Vol}\{z \in \mathbf{R}^2 | (1-\varepsilon)\mu < V(z) < (1+\varepsilon)\mu\} = 0.$$

Here, "Vol" stands for the Euclidean volume, and m is as in (*V*.1).

Under the assumptions (*B*.1) and (*V*.1), the operator $H_g(b)$ is essentially self-adjoint on $C_0^\infty(\mathbf{R}^2)$ for any $g \in \mathbf{R}$ [see Avron, Herbst, and Simon (1978)]. In what follows we identify any closable operator with its operator closure if there is no fear of confusion. Iwatsuka (1985) investigated the spectral properties of the unperturbed operator $H_0(b)$, which is called *the Iwatsuka model* by some authors [Mantoiu and Purice (1997), Exner and Kovařik (1999), and Shirai (2003)]. Iwatsuka's result says that, under (*B*.1), the spectrum of $H_0(b)$ is absolutely continuous and $\operatorname{Spec}(H_0(b)) = \cup_{n=0}^\infty [\Lambda_n^-, \Lambda_n^+]$ holds, where we set $\Lambda_n^\pm = (2n+1)B_\pm$ for any $n \in \mathbf{N}$, respectively, and for notational convenience, we set $\Lambda_{-1}^+ = \Lambda_{-1}^- = 0$.

Under (*B*.1) and (*V*.1), the multiplication operator V is relatively compact with respect to $H_0(b)$, so the essential spectrum of $H_g(b)$ coincides with that of $H_0(b)$ for any g [see, e.g., Reed and Simon (1978, Sec. XIII.4)]. In particular, the operator $H_g(b)$ may have discrete spectra (i.e., discrete eigenvalues of finite multiplicity) in the gaps of the essential spectrum.

We make some additional notations. Let v be as in (*V*.3). Set $S_\pm^1 = \{z=(x,y) \in \mathbf{R}^2 \,|\, |z|=1, \pm x \geqslant 0\}$ and set $\hat{v}_\pm = \int_{S_\pm^1} v(\omega)^{2/m}\, d\omega$, respectively. For any $\lambda \in \mathbf{R}\backslash \operatorname{Spec}(H_0(b))$ and for any $l \in \mathbf{N}$, set

$$\nu_l(\lambda) = \frac{1}{4\pi}(B_+\hat{v}_+|\Lambda_l^+ - \lambda|^{-2/m} + B_-\hat{v}_-|\Lambda_l^- - \lambda|^{-2/m}).$$

For any interval $[\lambda,\mu] \subset \mathbf{R}\backslash \operatorname{Spec}(H_0(b))$ and for any $l \in \mathbf{N}$, set

$$\nu_l([\lambda,\mu]) = \frac{1}{2\pi m}\left(B_+\hat{v}_+ \int_\lambda^\mu |\Lambda_l^+ - t|^{-2/m-1}\, dt + B_-\hat{v}_- \int_\lambda^\mu |\Lambda_l^- - t|^{-2/m-1}\, dt\right).$$

If we assume that $0 < \Lambda_n^+ < \lambda < \mu < \Lambda_{n+1}^-$ for some $n \in \mathbf{N}$, the sums $\Sigma_{l\in\mathbf{N}}\nu_l(\lambda)$ and $\Sigma_{l\in\mathbf{N}}\nu_l([\lambda,\mu])$ converge when $0<m<2$, and the relation $\nu_l([\lambda,\mu]) = \nu_l(\mu) - \nu_l(\lambda)$ holds when $l \geqslant n+1$.

We denote by $N_g^\pm(\lambda)$ the number of eigenvalues of $H_{\pm g'}(b)$ crossing λ as g' increases from zero to g, i.e., $N_g^\pm(\lambda) = \Sigma_{0<g'<g} \dim \operatorname{Ker}(H_{\pm g'}(b) - \lambda)$, respectively. Note that the sum above is meaningful under the assumptions (*B*.1) and (*V*.2), since the standard perturbation theory shows that for every fixed $g>0$ the set of values of $g' \in (0,g)$ for which $\dim \operatorname{Ker}(H_{\pm g'}(b) - \lambda)$ is not equal to zero is finite [see, e.g, Reed and Simon (1978)].

The main results in this paper are the following.

Theorem 1.1: *Let $\Lambda_{n-1}^+ < \lambda < \Lambda_n^-$ for some $n \in \mathbf{N}$. Assume that (B.1), (B.2), (V.1)–(V.4) hold. Moreover, assume that the constant m in (V.1) satisfies $0<m<2$. Then we have*

$$\lim_{g\to\infty} g^{-2/m} N_g^+(\lambda) = \sum_{l\geqslant n} \nu_l(\lambda). \tag{1.1}$$

Remark 1.2: In fact, the conclusion of Theorem 1.1 is still valid under weaker conditions on

B and V in the case of $\lambda<\Lambda_0^-$. *See Lemma 3.8 in Sec.* III *below*.

Corollary 1.3: Let $\Lambda_{n-1}^+<\lambda<\mu<\Lambda_n^-$ *for some* $n\in\mathbf{N}$. *Under the same assumption as in Theorem 1.1, we have* $\lim_{g\to\infty} g^{-2/m}N(\lambda\leqslant H_g(b)<\mu)=\Sigma_{l\geqslant n}\nu_l([\lambda,\nu])$.

Theorem 1.4: *Let* $\Lambda_n^+<\lambda<\Lambda_{n+1}^-$ *for some* $n\in\mathbf{N}$. *Assume that (B.1), (B.2), (V.1)–(V.4) hold. Then we have* $\lim_{g\to\infty} g^{-2/m}N_g^-(\lambda)=\Sigma_{0\leqslant l\leqslant n}\nu_l(\lambda)$.

Theorem 1.5: *Let* $\Lambda_{n-1}^+<\lambda<\mu<\Lambda_n^-$ *for some* $n\in\mathbf{N}$. *Assume that (B.1), (B.2), (V.1)–(V.4) hold. Moreover, assume that the constant m in (V.1) satisfies* $m>2$. *Then we have* $\liminf_{g\to\infty} g^{-2/m}N(\lambda\leqslant H_g(b)<\mu)\geqslant\Sigma_{l\geqslant n}\nu_l([\lambda,\mu])$.

At present, the author has not obtained the upper estimate for $N(\lambda\leqslant H_g(b)<\mu)$ in the case of $m>2$, nor the results for the case of $m=2$.

Remark 1.6:

(1) *The study of eigenvalues in the spectral gaps of the Schrödinger operators has a long history [see, e.g., Birman (1991), Alama, Deift, and Hempel (1989), Hempel and Levendorskiĭ (1998) and references therein]. In the case of constant magnetic fields (i.e., the case of* $B_+=B_-$ *in our notation), Raikov (1991, 1993) has obtained the strong-electric-field asymptotics as in Theorem 1.1 and Corollary 1.3 above when the scalar potential decays slowly at infinity (i.e., the case of* $0<m\leqslant 2$ *in our situation). Moreover, for a class of nonconstant magnetic fields which includes the Iwatsuka model, Raikov (1998, 1993) shows that the asymptotics of* $N_g^+(\lambda)$ *are Weylian, i.e., the asymptotic relation* $\lim_{g\to\infty} g^{-1}N_g^+(\lambda)=(1/4\pi)\int_{\mathbf{R}^2}V(x,y)\mathrm{d}x\,\mathrm{d}y$ *holds when the scalar potential decays rapidly (the case of* $m>2$ *in our situation).*

(2) *Hempel and Levendorskiĭ (1998) [see also Levendorskiĭ (1995, 1996)] study the asymptotics of* $N_g^\pm(\lambda)$ *for the magnetic Schrödinger operators* $H-gV=(-\sqrt{-1}\nabla-\mathbf{a})^2+W-gV$ *on* $L^2(\mathbf{R}^n)$ *under rather general conditions on* $\mathbf{a}$, W, *and* V. *Especially,* V *is not assumed to have a definite sign. They assume, however, the existence of the density of states* $\rho(\lambda,H)=\lim_{R\to\infty} N(H|_{Q_R}<\lambda)/\mathrm{Vol}(Q_R)$ *for the unperturbed operator* H, *for which the asymptotic coefficient as in Theorem 1.1 is expressed as*

$$\lim_{g\to\infty} g^{-n/m}N_g^+(\lambda)=\int_{\mathbf{R}^n}\mathrm{d}z\int_\lambda^{\lambda+v(\omega)r^{-m}}\mathrm{d}\rho(t,H)$$

when $V(z)=v(\omega)r^{-m}$ *at infinity and* $0<m<2$, *for example. Here,* Q_R *is a cube of side length R and we denote by* $H|_{Q_R}$ *the Dirichlét realization of H on* Q_R. *On the contrary, the Iwatsuka model has no canonical density of states because of lack of spacial symmetry of the magnetic field B. Thus, at least, we need modify their argument. Indeed, although the isotropic density of states* $\rho(\lambda,H_0(b))=(B_+/4\pi)\sharp\{l\in\mathbf{N}\,|\,\Lambda_l^+<\lambda\}+(B_-/4\pi)\sharp\{l\in\mathbf{N}\,|\,\Lambda_l^-<\lambda\}$ *for the Iwatsuka model do exist under the assumption in Theorem 1.1, the quantity*

$$\int_{\mathbf{R}^2}\mathrm{d}x\,\mathrm{d}y\int_\lambda^{\lambda+v(\omega)r^{-m}}\mathrm{d}\rho(t,H_0(b))=\frac{B_+}{4\pi}\frac{\hat{v}}{2}\sum_{l\geqslant n+1}|\Lambda_l^+-\lambda|^{-2/m}+\frac{B_-}{4\pi}\frac{\hat{v}}{2}\sum_{l\geqslant n+1}|\Lambda_l^--\lambda|^{-2/m},$$

where $\hat{v}=\int_{S^1}v(\omega)^{2/m}\,\mathrm{d}\omega$, *does not give the correct asymptotic coefficient* (1.1), *which can be expressed as*

$$\int_{\{x\geqslant 0\}}\mathrm{d}x\,\mathrm{d}y\int_\lambda^{\lambda+v(\omega)r^{-m}}\mathrm{d}\rho_+(t,H_0(b))+\int_{\{x\leqslant 0\}}\mathrm{d}x\,\mathrm{d}y\int_\lambda^{\lambda+v(\omega)r^{-m}}\mathrm{d}\rho_-(t,H_0(b)),$$

where $\rho_\pm(t,H_0(b))=(B_\pm/4\pi)\sharp\{l\in\mathbf{N}\,|\,\Lambda_l^\pm<t\}$, *respectively.*

The organization of this paper is as follows: Sec. II contains some preliminary results from functional analysis and the theory of pseudodifferential operators. In Sec. III, we give a proof of Theorem 1.1 in the case where the control point λ is fixed below the infimum of the essential spectrum of $H_g(b)$. In Sec. IV, we recall the spectral properties of the Iwatsuka model $H_0(b)$ and

derive some decay estimates for the band functions and the corresponding (generalized) eigenfunctions of $H_0(b)$. Proofs of Theorem 1.1 for λ in general gaps, Theorem 1.4 and Theorem 1.5 are given in Sec. V.

II. PRELIMINARIES

A. Variational principle

In this section we recall some results concerning the variational principle used mainly in Sec. III. All the results are well known, so we omit proofs.

For any sesquilinear form, which is referred to as *form* in the sequel, q on a Hilbert space, we denote its form domain by $D(q)$. For any semibounded, closable form q, there exists a unique self-adjoint operator A_q such that the operator domain $D(A_q)$ is a form core for the form closure $\overline{q}$ and the relation $q[u]=(A_q u,u)$ holds for any $u \in D(A_q)$. Throughout the paper, we identify such a form q with the corresponding self-adjoint operator A_q, and we denote the counting function $N(A_q<\lambda)$ simply by $N(q<\lambda)$ for any real number λ.

The following result is a consequence of the min–max principle [see, e.g., Reed and Simon (1978, Vol. IV), Colin de Verdiere (1986, Lemma 5.1)].

Lemma 2.1: Let $(\mathcal{H}_j,q_j,D(q_j))$ be a triplet of a Hilbert space $\mathcal{H}_j$, a semibounded, closable form q_j and the form domain $D(q_j)$ for $j=1,2$ and let J be an isometry from $D(q_1)$ to $D(q_2)$ with respect to norms of $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. Suppose that there exist positive constants C_1 and C_2 such that $q_1[u] \geqslant C_1 q_2[Ju]-C_2\|u\|^2_{\mathcal{H}_1}$ holds for all $u \in D(q_1)$. Then we have $N(q_1<\lambda) \leqslant N(q_2<(\lambda+C_2)/C_1)$ for any $\lambda \in \mathbf{R}$.

For any $\tilde{b} \in C^1(\mathbf{R}^2,\mathbf{R})$, we define

$$H_g(\tilde{b}) = -\frac{\partial^2}{\partial x^2} + \left(\frac{1}{\sqrt{-1}}\frac{\partial}{\partial y} - \tilde{b}(x,y)\right)^2 - gV(x,y). \tag{2.1}$$

In what follows, for any open subset Ω in $\mathbf{R}^2$, we denote by $H_g(\tilde{b})|_\Omega$ the minimal self-adjoint realization of $H_g(\tilde{b})$ starting from $C_0^\infty(\Omega)$, i.e., the Dirichlét realization of $H_g(\tilde{b})$ on Ω.

Proposition 2.2: [Colin de Verdiere (1986, Theorem 1.3)] Let r be a positive number and let Λ be a real number. Then we have the upper bound

$$N((-\infty,\Lambda)|H_0(B_0x)|_{Q(0,r)}) \leqslant \frac{B_0}{2\pi}r^2 \sharp\{l \in \mathbf{N}|(2l+1)B_0<\Lambda\},$$

where $H_0(B_0x)$ is the operator of the form (2.1) *with $\tilde{b}(x,y)=B_0x$ and $g=0$, and the lower bound*

$$N((-\infty,\Lambda)|H_0(B_0x)|_{Q(0,r)}) \geqslant \frac{B_0}{2\pi}(r-r_1)^2 \sharp\{l \in \mathbf{N}|(2l+1)B_0<\Lambda-Cr_1^{-2}\}.$$

Here, the constant C is independent of Λ, r and r_1 with $0<r_1<r$.

The following result is the so-called IMS (Ismagilov, Morgan, Sigal, Simon) localization formula for the magnetic Schrödinger operators [see Cycon *et al.*].

Lemma 2.3: Let $\tilde{\Omega}$ be an open subset of $\mathbf{R}^2$ and let $\{\Omega_j\}_{j\in J}$ be a locally finite open covering of $\tilde{\Omega}$. Let $\{\chi_j\}_{j\in J}$ be a partition of unity subject to the covering $\{\Omega_j\}$ satisfying the conditions $\mathrm{supp}(\chi_j) \subset \Omega_j, 0 \leqslant \chi_j \leqslant 1$ *and $\chi_j \in C^1(\Omega_j)$ for any $j \in J$. Moreover, $\Sigma_{j\in J}\chi_j^2=1$ on $\tilde{\Omega}$. Assume that $\tilde{b} \in C^\infty(\tilde{\Omega},\mathbf{R})$. Then we have $(H_g(\tilde{b})u,u)=\Sigma_{j\in J}(H_g(\tilde{b})\chi_j u,\chi_j u)-(\Sigma_{l\in J}|\nabla\chi l|^2 u,u)$ for any $u \in C_0^\infty(\tilde{\Omega})$.*

The next result follows from an elementary inequality $2XY \leqslant \varepsilon X^2+Y^2/\varepsilon$.

Lemma 2.4: Assume that $\tilde{b} \in C^1(\mathbf{R}^2,\mathbf{R})$ and $0<\varepsilon<1$. Then we have

$$(1-\varepsilon)(H_0(\tilde{b})u,u) - g(Vu,u) - (1+1/\varepsilon)\|(b-\tilde{b})u\|^2 \leqslant (H_g(b)u,u)$$
$$\leqslant (1+\varepsilon)(H_0(\tilde{b})u,u) - g(Vu,u) + (1+1/\varepsilon)\|(b-\tilde{b})u\|^2$$

for any $u \in C_0^\infty(\mathbf{R}^2)$.

B. Pseudodifferential operators

In this section we introduce a class of pseudodifferential operators (ΨDOs) and recall some basic results. All the results are well known in the theory of ΨDOs, so we omit proofs.

For any $m \in \mathbf{R}$ and $a \in C^\infty(\mathbf{R}^2)$, we say that *a belongs to the class of symbols* S^m if the quantity

$$\eta_{\alpha\beta}^{(m)}(a) = \sup_{(x,\xi)\in\mathbf{R}^2} \langle x;\xi\rangle^{-m+\alpha} |\partial_x^\beta \partial_\xi^\alpha a(x,\xi)| \tag{2.2}$$

is finite for each $\alpha,\beta \in \mathbf{N}$. The seminorms $\{\eta_{\alpha\beta}^{(m)}\}_{\alpha,\beta}$ gives a Fréchet space topology on the space S^m. We set $S^{-\infty} = \cap_{m\in\mathbf{R}} S^m$, which coincides with $S(\mathbf{R})$.

The symbol class S^m is an example of the class introduced by Beals (1975) [$\Phi(x,\xi) = \langle x;\xi\rangle, \varphi\langle x,\xi\rangle = 1, \lambda = \log(\langle x;\xi\rangle^m)$ and $S^\lambda_{\Phi,\varphi} = S^m$ in his convention], or by Robert (1978), Dauge and Robert (1987) [$m = \langle x;\xi\rangle^m, \phi = \langle x;\xi\rangle, \varphi = 1, S(m;\phi,\varphi) = S^m$ in their convention]. Hence, by the standard argument as in Beals (1975) or in Hörmander (1979) [$g_{x,\xi}(y,\eta) = |y|^2 + |\eta|^2/\langle x;\xi\rangle^2$ in his convention], one can find that, for any $a \in S^m$, the associated ΨDO,

$$Op(a)u(x) = \int\int_{\mathbf{R}^2} e^{\sqrt{-1}(x-y)\xi} a\left(\frac{x+y}{2},\xi\right) u(y)\mathrm{d}y\,\mathrm{d}\xi$$

is a well-defined oscillatory integral for any $u \in S(\mathbf{R})$. Here, we set $\mathrm{d}\xi = \mathrm{d}\xi/(2\pi)$. Moreover, $Op(a)$ maps $\mathcal{S}(\mathbf{R})$ to itself continuously [so, extends to a continuous map from $\mathcal{S}'(\mathbf{R})$ to itself by duality based on L^2-norm]. For an operator A from $\mathcal{S}'(\mathbf{R})$ to $\mathcal{S}'(\mathbf{R})$, we say $A \in OpS^m$ if A is expressed as $Op(a)$ for some $a \in S^m$.

Note that the original results in Beals (1975) are formulated in terms of the standard quantization $\int\int_{\mathbf{R}^2} e^{\sqrt{-1}(x-y)\xi} a(x,\xi)u(y)\mathrm{d}y\,\mathrm{d}\xi$. However, all the corresponding results below are still valid for the Weyl quantization; to see this, it suffices to chase the proofs in Beals (1975) carefully, or use the relation between the standard and the Weyl quantizations as in Theorem 4.5 in Hörmander (1979). For omitted proofs, we refer to Proposition 6.17, Theorems 6.1, 7.2, and 7.7 in Beals (1975), and for Lemma 2.7 below we refer to Proposition 26.2 in Shubin (1987). Although the class of symbols considered in Shubin's book is slightly defferent from the class S^m above, the proof of Proposition 26.2 in his book is valid also for symbols in S^m with obvious modifications.

Lemma 2.5: Let $m, m' \in \mathbf{R}$. *We have the following assertions.*

(1) *If* $A \in OpS^m$ *and* $B \in OpS^{m'}$, *then* $AB \in OpS^{m+m'}$ *and the symbol of* AB *has an asymptotic expansion as usual.*
(2) *If* $A \in OpS^m$, *then* $A^* \in OpS^m$ *and the symbol of* A^* *is expressed as usual.*
(3) *If* $A \in OpS^0$, *then* A *defines a bounded operator on* $L^2(\mathbf{R})$. *Moreover, if* $A \in OpS^m$ *for some negative* m, *then* A *defines a compact operator on* $L^2(\mathbf{R})$.
(4) *If* $m > 0$ *and* $a \in S^{-m}$, *then there exists* $l \in \mathbf{N}$ *such that* $\|Op(a)\|_{\mathbf{B}(L^2(\mathbf{R}))} \leqslant C\Sigma_{\alpha+\beta\leqslant l}\eta_{\alpha\beta}^{(-m)}(a)$ *holds for some constant* $C > 0$, *independent of* a.
(5) *If* $A \in OpS^{-\infty}$, *then* A *maps* $\mathcal{S}'(\mathbf{R})$ *to* $\mathcal{S}(\mathbf{R})$ *continuously.*

We introduce the weighted Sobolev space H^m as the (finite) linear hull of the set $\{Au \,|\, u \in L^2(\mathbf{R}), A \in OpS^{-m}\}$ equipped with the weakest topology which makes the map $(A: L^2(\mathbf{R}) \to H^m)$ continuous for all $A \in OpS^{-m}$. The basic properties of H^m are summarized as follows.

Lemma 2.6:

(1) *The space* H^0 *coincides with* $L^2(\mathbf{R})$ *topologically.*
(2) *The embeddings* $\mathcal{S}(\mathbf{R}) \subset H^m \subset \mathcal{S}'(\mathbf{R})$ *are densely and continuously for any* m.

(3) *$H^m \subset H^{m'}$ holds if $m' < m$, and $(H^m)' = H^{-m}$ topologically for any m.*
(4) *If $A \in OpS^m$, then A maps $H^{m+m'}$ to $H^{m'}$ continuously for all m, m'.*
(5) *For any m, m', there exists $A \in OpS^m$ which gives a topologically isomorphism from $H^{m+m'}$ onto $H^{m'}$. In particular, H^m has the topology of a Hilbert space for any m.*

Lemma 2.7: Let D_0 be a dense subspace of $\mathcal{S}(\mathbf{R})$. Let $m > 0$ and $a \in S^m$. Assume that $Op(a)$ is symmetric on D_0 and $|a(x,\xi)| \geqslant C\langle x;\xi\rangle^m$ holds for some $C > 0$. Then

(1) *The operator $Op(a)|_{D_0}$ [the restriction of $Op(a)$ on D_0] is essentially self-adjoint, and $D(\overline{Op(a)|_{D_0}})$ coincides with $\{u \in L^2(\mathbf{R}) \,|\, Op(a)u \in L^2(\mathbf{R})\}$.*
(2) *The space $D(\overline{Op(a)|_{D_0}})$ equipped with graph norm coincides with H^m topologically.*

The following result concerning the eigenvalue asymptotics of ΨDOs of negative order plays an important role in Sec. V.

Proposition 2.8: [Dauge and Robert (1987, Theorem 1.3)] Let $m > 0$ and let $a \in S^{-m}$ and a be real valued. Assume that the following two estimates,

$$\lim_{\varepsilon \downarrow 0} \limsup_{\mu \downarrow 0} \mu^{2/m} \mathrm{Vol}\{(x,\xi) \in \mathbf{R}^2 | (1-\varepsilon)\mu < \pm a(x,\xi) < (1+\varepsilon)\mu\} = 0, \tag{2.3}$$

are satisfied. Then we have $N(\pm Op(a) > \mu) = (1/2\pi)\mathrm{Vol}\{(z,\xi) \in \mathbf{R}^2 \,|\, \pm a(x,\xi) > \mu\} + o(\mu^{-2/m})$ as $\mu \downarrow 0$, respectively.

Note that the conditions (2.3) imply the condition (T) in Dauge and Robert (1987) for the volume functions $\mathrm{Vol}\{z \,|\, \pm a(z) > \mu\}$. As an immediate consequence of Proposition 2.8, for any $m > 0$ and any $a \in S^{-m}$, the following rough estimate,

$$N(\pm Op(a) > \mu) = O(\mu^{-2/m}), \tag{2.4}$$

holds as $\mu \downarrow 0$.

III. PROOF OF THEOREM 1.1 IN THE CASE OF $\lambda < B_-$

A. Upper bound for $N(H_g(b) < \lambda)$

1. Partition of $\mathbf{R}^2$ and sesquilinear forms

In this section, we give a proof of Theorem 1.1 in the case of $\lambda < \Lambda_0^-(=B_-)$. For general $\lambda > \Lambda_0^+$ the proof of Theorem 1.1 given in Sec. V needs this special case, as in Raikov (1993).

We introduce a partition of $\mathbf{R}^2$ and a corresponding partition of unity. Let $K = \{0, 1, +, -\}$. Take and fix positive numbers α, β, and σ so that

$$0 < \sigma < \min\left\{\frac{1}{4m}, \frac{1}{2-m}, \frac{M}{m(1+M)}, \frac{1}{2m(m+1)}\right\}, \quad \alpha = \frac{1}{m} - 2\sigma, \quad \beta = \frac{1}{m} + \sigma.$$

Note that $0 < \sigma < \alpha < 1/m < \beta$. For any $g > 0$, we set $\Omega_0 = \{(x,y) \in \mathbf{R}^2 \,|\, |x| \leqslant g^\alpha, |y| \leqslant g^\beta\}$, $\Omega_\pm = \{(x,y) \in \mathbf{R}^2 \,|\, g^\alpha \leqslant \pm x \leqslant g^\beta, |y| \leqslant g^\beta\}$, respectively, $\Omega_1 = \mathbf{R}^2 \setminus (\Omega_0 \cup \Omega_+ \cup \Omega_-)$ and $\tilde{\Omega}_k = \{z \in \mathbf{R}^2 \,|\, \mathrm{dist}(z, \Omega_k) < g^\sigma\}$ for any $k \in K$. Let $\{\varphi_k\}_{k \in K}$ be a partition of unity subject to the open covering $\{\tilde{\Omega}_k\}_{k \in K}$ of $\mathbf{R}^2$ satisfying the following:

$(P.1)$ $\varphi_k \in C^\infty(\tilde{\Omega}_k)$, $\mathrm{supp}(\varphi_k) \subset \tilde{\Omega}_k$ and $0 \leqslant \varphi_k \leqslant 1$ hold, and for each multi-index γ, there exists $C_\gamma > 0$ such that $\sup_{z \in \mathbf{R}^2} |\varphi_k(z)| \leqslant C_\gamma g^{-|\gamma|\sigma}$ holds for any $k \in K$. Moreover, $\Sigma_{k \in K} \varphi_k^2 = 1$ holds on $\mathbf{R}^2$.

For each $k \in K$, we define a form q_k by $q_k[u] = (H_g(b)u, u) - (\Sigma_{l \in K} |\nabla_{\varphi l}|^2 u, u)$ with form domain $C_0^\infty(\tilde{\Omega}_k)$. Then it follows from Lemma 2.3 that $(H_g(b)u, u) = \Sigma_{k \in K} q_k[\varphi_k u]$ holds for any $u \in C_0^\infty(\mathbf{R}^2)$. Considering the isometry J from $L^2(\mathbf{R}^2)$ to $\oplus_{k \in K} L^2(\tilde{\Omega}_k)$ defined by $J(u) = \oplus_{k \in K}(\varphi_k u)$, by Lemma 2.1, we find that $N(H_g(b) < \lambda) \leqslant \Sigma_{k \in K} N(q_k < \lambda)$ holds for any $g > 0$.

2. Estimates of $N(q_0<\lambda)$ and $N(q_1<\lambda)$

In what follows we use the symbols c and C (possibly with superscripts or subscripts) to denote various positive constants in estimates, which may vary from line to line.

Let $0<\eta<1$ and let $J=\{j\in\mathbf{Z}^2\,|\,\tilde{\Omega}_0\cap Q(j,1)\neq\emptyset\}$. Let $\{\chi_j\}_{j\in J}$ be a partition of unity subject to the open covering $\{Q(j,1+\eta)\}_{j\in J}$ of $\tilde{\Omega}_0$ satisfying the following:

(*P*.2) $\chi_j\in C_0^\infty(Q(j,1+\eta))$, and $0\leqslant\chi_j\leqslant 1$ hold, and for each multi-index γ, there exists $C_\gamma>0$, independent of j,η, such that $\sup_{z\in\mathbf{R}^2}|\chi_j(z)|\leqslant C_\gamma\eta^{-|\gamma|}$ holds for any $j\in J$. Moreover, $\Sigma_{j\in J}\chi_j^2=1$ holds on $\tilde{\Omega}_0$.

For each $j=(j_1,j_2)\in J$, we introduce the auxiliary magnetic potential $b_j(x)=\int_0^{j_1}B(t)\mathrm{d}t+B(j_1)\times(x-j_1)$, which gives the constant magnetic field $B(j_1)$.

Lemma 3.1: Let q_0 and λ be as above. We have $N(q_0<\lambda)=o(g^{2/m})$ as $g\to\infty$.

Proof: By Lemmata 2.3, 2.1, 2.4 and Proposition 2.2, we have the estimate

$$\begin{aligned}N(q_0<\lambda)&\leqslant\sum_{j\in J}N((1-\varepsilon)H_0(b_j)-Cg\langle j\rangle^{-m}-C_{\eta\varepsilon}<\lambda)\\&\leqslant\sum_{j=(j_1,j_2)\in J}\frac{B(j_1)}{2\pi}(1+\eta)^2\,\sharp\,\{l\in\mathbf{N}\,|\,(1-\varepsilon)(2l+1)B(j_1)<\lambda+Cg\langle j\rangle^{-m}+C_{\eta\varepsilon}\}\\&\leqslant C_{\eta\varepsilon\lambda}(\sharp J)+C_{\eta\varepsilon\lambda}g\sum_{j\in J}\langle j\rangle^{-m}\end{aligned}\tag{3.1}$$

for any small $\varepsilon>0$, where we used (*P*.2) and the fact that the estimates $|V(z)|\leqslant C\langle j\rangle^{-m}$ and $|b(x)-b_j(x)|\leqslant|\int_{j_1}^x(B(t)-B(j_1))\mathrm{d}t|\leqslant 2(1+\eta)B_+$ hold on $Q(j,1+\eta)$ in the first inequality. By the definition of J, there exists $C>0$, independent of g, such that $\sharp(J)\leqslant C\mathrm{Vol}(\tilde{\Omega}_0)\leqslant Cg^{\alpha+\beta}=o(g^{2/m})$ as $g\to\infty$, since $\alpha+\beta=2/m-\sigma$. The second term on the right-hand side (rhs) of (3.1) is less than or equal to

$$Cg\int_{\tilde{\Omega}_0}\langle z\rangle^{-m}\,\mathrm{d}z\leqslant 4Cg\int_0^{g^\alpha+g^\sigma}\mathrm{d}x\int_0^{g^\beta+g^\sigma}\mathrm{d}y\langle x;y\rangle^{-m}.\tag{3.2}$$

To estimate the above integral, we use the following elementary estimate: If $m>0$ and $1<A<B$, then there exists $C_m>0$, independent of A,B, such that

$$\int_0^A\mathrm{d}x\int_0^B\mathrm{d}y\langle x;y\rangle^{-m}\leqslant\begin{cases}C_mAB^{1-m} & \text{if } 0<m<1,\\ C_1A\log B & \text{if } m=1,\\ C_m(AB^{1-m}+1) & \text{if } m>1.\end{cases}$$

Then, if $0<m<1$, the rhs of (3.2) is estimated from above by $C_mg(g^\alpha+g^\sigma)(g^\beta+g^\sigma)^{1-m}=o(g^{1+\alpha+\beta(1-m)})=o(g^{2/m})$ as $g\to\infty$. Similarly, if $m=1$, the rhs of (3.2) is estimated from above by $C_1g(g^\alpha+g^\sigma)\log(g^\beta+g^\sigma)=o(g^{1+\alpha}\log g)=o(g^{2/m})$ as $g\to\infty$, and if $1<m<2$, the rhs of (3.2) is estimated from above by $C_mg((g^\alpha+g^\sigma)(g^\beta+g^\sigma)^{1-m}+1)=o(g^{1+\alpha-\beta(m-1)})=o(g^{2/m})$ as $g\to\infty$. This completes the proof. ■

Lemma 3.2: Let q_1 and λ be as above. We have $N(q_1<\lambda)=0$ for large $g>0$.

Proof: For any $u\in C_0^\infty(\tilde{\Omega}_1)$, we have $q_1[u]=(H_g(b)u,u)-g(Vu,u)-(\Sigma_{l\in K}|\nabla\varphi_l|^2u,u)\geqslant(H_g(b)u,u)-C(g^{1-m\beta}+g^{-2\sigma})\|u\|^2=(H_g(b)u,u)-o(1)\|u\|^2$ as $g\to\infty$, where we used (*V*.1), (*P*.1) and the fact that $1-m\beta=1-m(1/m+\sigma)=-m\sigma<0$. Then the min–max argument yields that $N(q_1<\lambda)\leqslant N(H_0(b)|_{\tilde{\Omega}_1}<\lambda+o(1))$ holds as $g\to\infty$. Hence we conclude that $N(H_0(b)|_{\tilde{\Omega}_1}<\lambda+o(1))=0$ for large g since $\inf\mathrm{Spec}(H_0(b)|_{\tilde{\Omega}_1})=\inf_{u\in C_0^\infty(\tilde{\Omega}_1),\|u\|=1}(H_0(b)u,u)\geqslant\inf\mathrm{Spec}(H_0(b))(=B_-)>\lambda)$ holds as $g\to\infty$ again by the min–max argument. ■

3. Estimate of $N(q_\pm<\lambda)$

Let $0<\eta<1$. For any $j=(j_1,j_1)\in\mathbf{Z}^2$, we set

$$Q_j=\{(x,y)\in\mathbf{R}^2|j_1<g^{-\sigma}x<j_1+1,j_2<g^{-\sigma}y<j_2+1\},\tag{3.3}$$

$$Q_{j\eta}=\{z\in\mathbf{R}^2|\mathrm{dist}(z,Q_j)<\eta g^{\sigma}\}\tag{3.4}$$

and $J_\pm=\{j\in\mathbf{Z}^2|Q_j\cap\tilde{\Omega}_\pm\neq\emptyset\}$. Let $\{\chi_j\}_{j\in J_\pm}$ be a partition of unity subject to the covering $\{Q_{j\eta}\}_{j\in J_\pm}$ of $\tilde{\Omega}_\pm$ satisfying the following conditions (respectively, for $\pm$):

$(P.3)$ ${}_\pm\chi_j\in C_0^\infty(Q_{j\eta}),0\leqslant\chi_j\leqslant1$, and for each multi-index γ, there exists $C_\gamma>0$, independent of g,η,j, such that $\sup_{z\in\mathbf{R}^2}|\partial^\gamma\chi_j(z)|\leqslant C_\gamma(\eta g^\sigma)^{-|\gamma|}$ holds for any $j\in J_\pm$. Moreover, $\Sigma_{j\in J_\pm}\chi_j^2=1$ holds on $\tilde{\Omega}_\pm$.

In what follows, for simplicity, we omit the phrase "respectively (for $\pm$)" if there is no fear of confusion.

Let $z_j=(x_j,y_j)$ be the center of Q_j and we introduce the auxiliary magnetic potentials,

$$b_{j,\pm}(x)=\int_0^{x_j}B(t)\mathrm{d}t+B_\pm(x-x_j),\tag{3.5}$$

which gives the constant magnetic field $B_\pm$.

Lemma 3.3: Let $j\in J_\pm$. There exists $C>0$, independent of j,g, and η, such that $\|(b-b_{j,\pm})u\|\leqslant Cg^{\sigma-M\alpha}\|u\|$ holds for any $u\in C_0^\infty(Q_{j\eta})$, and for any $g\geqslant1$.

Proof: On $Q_{j\eta}$, we have $|b(x)-b_{j,\pm}(x)|\leqslant|\int_{x_j}^x(B(t)-B_\pm)\mathrm{d}t|\leqslant C\langle g^\alpha-g^\sigma-\eta g^\sigma\rangle^{-M}|x-x_j|\leqslant Cg^{-M\alpha+\sigma}$ as $g\to\infty$, where we used (B.2) in the second inequality. ■

Lemma 3.4: Let $j\in J_\pm$. There exists $C>0$, independent of j,g, and η such that $(1-Cg^{-(\alpha-2\sigma)})V(z)\leqslant V(z')\leqslant(1+Cg^{-(\alpha-2\sigma)})V(z)$ holds for any $z,z'\in Q_{j\eta}$. Here, $\overline{Q}$ stands for the closure of Q.

Proof: Let $z,z'\in\overline{Q_{j\eta}}$. If we write $z=(x,y)$, then

$$|z|\geqslant|x|\geqslant g^\alpha-g^\sigma-(1+\eta)g^\sigma\geqslant g^\alpha/2\tag{3.6}$$

and $|z|\leqslant|z'|+|z-z'|\leqslant|z'|+\sqrt{2}(1+\eta)g^\sigma\leqslant|z'|+Cg^{-(\alpha-\sigma)}|z|$ hold for large $g>0$, so there exists $C>0$, independent of j,g,z,z', such that

$$C^{-1}\langle z\rangle\leqslant\langle z'\rangle\leqslant C\langle z\rangle\tag{3.7}$$

holds. The first order Taylor expansion yields $|V(z)-V(z')|\leqslant|z-z'|\sup_{w\in Q_{j\eta}}|\nabla V(w)|\leqslant C(1+\eta)^2g^{2\sigma}\sup_{w\in Q_{j\eta}}\langle w\rangle^{-m-1}\leqslant C(1+\eta)^2g^{-(\alpha-2\sigma)}\sup_{w\in Q_{j\eta}}\langle w\rangle^{-m}\leqslant Cg^{-(\alpha-2\sigma)}V(z)$ for large g, where we used (3.6) in the third inequality, $(V.1)$, $(V.2)$ in the second and the fourth inequalities, (3.7) in the last inequality. Here, the constant C is independent of j,η,g,z, and z'. This proves the lemma. ■

Lemma 3.5: For any ε satisfying $0<\varepsilon<1$, we have

$$N(q_\pm<\lambda)\leqslant(1+\varepsilon)^2\frac{B_\pm}{2\pi}\sum_{l\in N}\mathrm{Vol}(\Omega_\pm^{(+)}(\varepsilon,l)),\tag{3.8}$$

where we set $\Omega_\pm^{(+)}(\varepsilon,l)=\{z\in\mathbf{R}^2|\pm x\geqslant0,(1-2\varepsilon)\Lambda_l^\pm<\lambda+g(1+\varepsilon)V(z)\}$. In fact, the sum on the rhs of (3.8) *terminates for each ε and g.*

Proof: By Lemma 2.1 and $(P.3)$, there exists $C>0$, independent of j,g,η, such that

$$q_{\pm}[u] \geqslant \sum_{j\in J_{\pm}} ((1-\varepsilon)(H_0(b_{j,\pm})\chi_j u,\chi_j u) - g(V\chi_j u,\chi_j u) - (1+1/\varepsilon)\|(b-b_{j,\pm})\chi_j u\|^2 - C(\eta g^{\sigma})^{-2}\|\chi_j u\|^2$$
$$- Cg^{-2\sigma}\|\chi_j u\|^2) \geqslant \sum_{j\in J_{\pm}} \left((1-\varepsilon)(H_0(b_{j,\pm})\chi_j u,\chi_j u) - g\sup_{Q_{j\eta}}|V|(\chi_j u,\chi_j u) - o(1)\|\chi_j u\|^2\right)$$

holds for any $u \in C_0^{\infty}(\tilde{\Omega}_{\pm})$, where we write $\sup_Q|V|$ for $\sup_{z\in Q}|V(z)|$ for short. Then the min–max theorem yields that

$$N(q_{\pm}<\lambda) \leqslant \sum_{j\in J_{\pm}} N((1-2\varepsilon)H_0(b_{j,\pm}) < \lambda + g\sup_{Q_{j\eta}}|V|)$$
$$\leqslant (1+\eta)^2 g^{2\sigma}\frac{B_{\pm}}{2\pi}\sum_{j\in J_{\pm}} \sharp\{l\in\mathbf{N}|(1-2\varepsilon)\Lambda_l^{\pm} < \lambda + g\sup_{Q_{j\eta}}|V|\}$$
$$= (1+\eta)^2 g^{2\sigma}\frac{B_{\pm}}{2\pi}\sum_{l\in N}\sum_{j\in J_{\pm}} F((1-2\varepsilon)\Lambda_l^{\pm} < \lambda + g\sup_{Q_{j\eta}}|V|) \tag{3.9}$$

holds for large g, where we used Proposition 2.2 in the second inequality. Here, $F(P)=0$ if P is true and $F(P)=1$ if P is false.

Set $\tilde{J}_{\pm}=\{j\in J_{\pm}|\,Q_j\subset\Omega_{\pm}^{(+)}(\varepsilon,l)\}$. We claim that, if $j\in J_{\pm}\backslash\tilde{J}_{\pm}$, then $F((1-2\varepsilon)\Lambda_l^{\pm}<\lambda+g\sup_{Q_{j\eta}}|V|)=0$ holds for large $g>0$ uniformly in j,l. Indeed, for such j, there exists $\overline{z}\in Q_j$ such that $\overline{z}\notin\Omega_{\pm}^{(+)}(\varepsilon,l)$, i.e.,

$$(1-2\varepsilon)\Lambda_l^{\pm} \geqslant \lambda + g(1+\varepsilon)V(\overline{z}). \tag{3.10}$$

Note that if we write $\overline{z}=(\overline{x},\overline{y})\in Q_j$, then $\pm\overline{x}\geqslant 0$ since $0<\sigma<\alpha$. Then we find that, for any $\varepsilon>0$ fixed, $(1-2\varepsilon)\Lambda_l^{\pm}-\lambda-g\sup_{Q_{j\eta}}|V|=(1-2\varepsilon)\Lambda_l^{\pm}-\lambda-g(1+\varepsilon)V(\overline{z})+g((1+\varepsilon)V(\overline{z})-\sup_{Q_{j\eta}}|V|)\geqslant g((1+\varepsilon)V(\overline{z})-\sup_{Q_{j\eta}}|V|)\geqslant g((1+\varepsilon)V(\overline{z})-(1+Cg^{-(\alpha-2\sigma)})V(\overline{z}))=g(\varepsilon-Cg^{-(\alpha-2\alpha)})V(\overline{z})\geqslant 0$ holds for large g (uniformly in j,l), where we used (3.10) in the first inequality, Lemma 3.4 in the second inequality and (V.2) in the last. This shows the claim.

Hence, it follows that, for large g, the rhs of (3.9) is less than or equal to $(1+\eta)^2(B_{\pm}/2\pi)\Sigma_{l\in N}\Sigma_{j\in J_{\pm}}\mathrm{Vol}(Q_j)\leqslant(1+\eta)^2(B\pm/2\pi)\Sigma_{l\in N}\mathrm{Vol}(\Omega_{\pm}^{(+)}(\varepsilon,l))$. Then the lemma follows since the set $\Omega_{\pm}^{(+)}$ is empty if l is so large that $(1-2\varepsilon)\Lambda_l^{\pm}\geqslant\lambda+Cg\sup_{\mathbf{R}^2}|V|$. ■

Lemma 3.6: Assume that $\lambda<B_-$. *Then we have* $\limsup_{g\to\infty} g^{-2/m}N_g^+(\lambda)\leqslant\Sigma_{l\in\mathbf{N}}\nu_l(\lambda)$.

Proof: Let $\Omega_{\pm}^{(+)}(\varepsilon,l)$ be as in the previous lemma. Set $I_0=\mathrm{Vol}\{z\in\Omega_{\pm}^{(+)}(\varepsilon,l)\,|\,|z|\leqslant R\}$ and $I_{\infty}^{\pm}=\{z=(x,y)\in\Omega_{\pm}^{(+)}(\varepsilon,l)\,|\,\pm x\geqslant 0,|z|\geqslant R\}$. Then $\mathrm{Vol}(\Omega_{\pm}^{(+)}(\varepsilon,l))=I_0+I_{\infty}^{+}+I_{\infty}^{-}$. We observe that $I_0\leqslant\pi R^2$, and $I_{\infty}^{\pm}\leqslant\frac{1}{2}g^{2/m}(\Lambda_l^{\pm}-\lambda)^{-2/m}\int_{S^1}v(\omega)^{2/m}\,\mathrm{d}\omega+O(1)$ as $\varepsilon\downarrow 0$ (the remainder term is uniformly bounded in g), since by (V.3), for any small $\varepsilon>0$, there exists $R>0$ such that $|r^mV(z)-v(\omega)|<\varepsilon$ if $r=|z|\geqslant R$. Then, taking a limit $\varepsilon\downarrow 0$ in (3.8), we derive from Lemmas 3.2, 3.1, and 3.5 that $\limsup_{g\to\infty}g^{-2/m}N(H_g(b)<\lambda)\leqslant\Sigma_{l\in N}\nu_l(\lambda)$, by Lebesgue's dominated convergence theorem. The lemma follows since $N(H_g(b)<\lambda)=N_g^+(\lambda)$ holds if $\lambda<B_-$ because of the non-negativity of V. ■

B. Lower bound for $N(H_g(b)<\lambda)$

Let K and $\{\Omega_k\}_{k\in K}$ be as in the beginning of this section. Applying Lemma 2.1 to the pair of triplets $(\Sigma_{k\in K}\oplus L^2(\Omega_k),t_1,\oplus_{k\in K}C_0^{\infty}(\Omega_k))$ and $(L^2(\mathbf{R}^2),t_2,C_0^{\infty}(\mathbf{R}^2))$, where we set $t_1[\oplus_{k\in K}v_k]=\Sigma_{k\in K}(H_g(b)|_{\Omega_k}v_k,v_k)$ for $\oplus_{k\in K}(v_k)\in\oplus_{k\in K}C_0^{\infty}(\Omega_k)$, $t_2[u]=(H_g(b)u,u)$ for $u\in C_0^{\infty}(\mathbf{R}^2)$ and $J:\oplus_{k\in K}C_0^{\infty}(\Omega_k)\ni\oplus_{k\in K}(v_k)\mapsto\Sigma_{k\in K}v_k\in C_0^{\infty}(\mathbf{R}^2)$, we have

$$N(H_g(b)<\lambda) \geqslant \sum_{k\in K} N(H_g(b)|_{\Omega_k}<\lambda). \tag{3.11}$$

As in the proof of Lemma 3.1, we can show that

$$N\big(H_g(b)\big|_{\Omega_0} < \lambda\big) = o(g^{2/m}) \tag{3.12}$$

as $g \to \infty$, using the upper estimate in Lemma 2.4. Also, as in the proof of Lemma 3.2, we can show that

$$N\big(H_g(b)\big|_{\Omega_1} < \lambda\big) \leqslant N\big(H_0(b)\big|_{\Omega_1} < \lambda + o(1)\big) = 0 \tag{3.13}$$

holds for large $g > 0$.

Lemma 3.7: For any $l \in \mathbf{N}$ and any ε satisfying $0 < \varepsilon < 1$, set

$$\Omega_{\pm}^{(-)}(\varepsilon, l) = \{z \in \mathbf{R}^2 \,|\, \pm x \geqslant 0, (1+2\varepsilon)\Lambda_l^{\pm} < \lambda + (1-\varepsilon)gV(z)\},$$

respectively. Then for any ε satisfying $0 < \varepsilon < 1$, we have

$$N(H_g(b)|_{\Omega_{\pm}} < \lambda) \geqslant (1-\varepsilon)^2 \frac{B_{\pm}}{2\pi} \sum_{l \in \mathrm{N}} \mathrm{Vol}(\Omega_{\pm}^{(-)}(\varepsilon, l)) + o(g^{2/m})$$

as $g \to \infty$, respectively.

Proof: Let $0 < \eta < 1$ and $j \in \mathbf{Z}^2$. Let Q_j and $Q_{j\eta}$ be the cubes defined by (3.3) and (3.4), respectively. Set $J'_{\pm} = \{j \in \mathbf{Z}^2 \,|\, Q_j \subset \tilde{\Omega}_{\pm}, Q_j \cap \Omega_{\pm}^{(-)}(\varepsilon, l) \neq \emptyset\}$, respectively. Let $b_{j,\pm}$ be as in (3.5). Then, as in the proof of Lemma 3.5, it follows from Lemma 2.4, Lemma 2.1, and Lemma 2.3 that, for any ε satisfying $0 < \varepsilon < 1$,

$$\begin{aligned} N(H_g(b)|_{\Omega_{\pm}} < \lambda) &\geqslant \sum_{j \in J'_{\pm}} N((1+2\varepsilon)H_0(b)|Q_j < \lambda + g \sup_{Q_{j\eta}} |V|) \\ &\geqslant (1-\varepsilon)^2 \frac{B_{\pm}}{2\pi} \sum_{j \in J'_{\pm}} \mathrm{Vol}(Q_j) \sharp \{l \in \mathbf{N} | (1+2\varepsilon)\Lambda_l^{\pm} < \lambda + g \sup_{Q_{j\eta}} |V|\} \\ &\geqslant (1-\varepsilon)^2 \frac{B_{\pm}}{2\pi} \sum_{l \in \mathrm{N}} \sum_{j \in J'_{\pm}} \mathrm{Vol}(Q_j) F((1+2\varepsilon)\Lambda_l^{\pm} < \lambda + g \sup_{Q_{j\eta}} |V|), \end{aligned} \tag{3.14}$$

where we used Proposition 2.2 with $r_1 = \varepsilon$ in the third inequality.

We claim that, if $j \in J'_{\pm}$, then $F((1+2\varepsilon)\Lambda_l^{\pm} < \lambda + g \sup_{Q_{j\eta}} |V|) = 1$ holds for large $g > 0$ uniformly in j, l. Indeed, if $j \in J'_{\pm}$, there exists $\overline{z} \in Q_j \cap \Omega_{\pm}^{(-)}(\varepsilon, l)$, i.e., $\overline{z} \in Q_j$ and $(1+2\varepsilon)\Lambda_l^{\pm} < \lambda + g(1-\varepsilon)V(\overline{z})$ hold. Then, by Lemma 3.4 and $(V.2)$, we have $\lambda + g \sup_{Q_{j\eta}} |V| - (1+2\varepsilon)\Lambda_l^{\pm} \geqslant g(\sup_{Q_{j\eta}} |V| - (1-\varepsilon)V(\overline{z})) \geqslant g(\varepsilon - Cg^{-(\alpha-2\sigma)})V(\overline{z}) > 0$ for large $g > 0$. This shows the claim. So, for large $g > 0$, the rhs of (3.14) is bounded from below by

$$\begin{aligned} &(1-\varepsilon)^2 \frac{B_{\pm}}{2\pi} \sum_{l \in \mathbf{N}} \sum_{j \in J'_{\pm}} \mathrm{Vol}(Q_j) \\ &\geqslant (1-\varepsilon)^2 \frac{B_{\pm}}{2\pi} \sum_{l \in N} \mathrm{Vol}((\Omega_{\pm} \cap \Omega_{\pm}^{(-)}(\varepsilon, l)) \setminus \{z \in \Omega_{\pm} \cap \Omega_{\pm}^{(-)}(\varepsilon, l) | \mathrm{dist}(z, \partial\Omega_{\pm}) \leqslant g^{\sigma}\}) \\ &\geqslant (1-\varepsilon)^2 \frac{B_{\pm}}{2\pi} \sum_{l \in \mathbf{N}} \mathrm{Vol}(\Omega_{\pm} \cap \Omega_{\pm}^{(-)}(\varepsilon, l)) - (1-\varepsilon)^2 \frac{B_{\pm}}{2\pi} \sum_{l=0}^{C_g 1-m\alpha} \mathrm{Vol}\{z \in \Omega_{\pm} \cap \Omega_{\pm}^{(-)}(\varepsilon, l) | \mathrm{dist}(z, \partial\Omega_{\pm}) \\ &\leqslant g^{\sigma}\}, \end{aligned} \tag{3.15}$$

where we used the fact that $(\Omega_{\pm} \cap \Omega_{\pm}^{(-)}(\varepsilon, l)) \setminus \{z \in \Omega_{\pm} \cap \Omega_{\pm}^{(-)}(\varepsilon, l) \,|\, \mathrm{dist}(z, \partial\Omega_{\pm}) \leqslant g^{\sigma}\} \subset \cup_{j \in J'_{\pm}} Q_j$, where the rhs is a disjoint union, in the first inequality and used, in the last inequality, the fact that the set $\Omega_{\pm} \cap \Omega_{\pm}^{(-)}(\varepsilon, l) = \{z \in \Omega_{\pm} | (1+2\varepsilon)\Lambda_l^{\pm} < \lambda + (1-\varepsilon)gV(z)\}$ is empty for all l satisfying $(1+2\varepsilon)\Lambda_l^{\pm} \geqslant \lambda + Cg^{1-m\alpha}$ since $\sup_{\Omega_{\pm}} |V| \leqslant C\langle g^{\alpha} - g^{\sigma}\rangle^{-m} \leqslant Cg^{-m\alpha}$ holds for large g.

From geometry, we have $\mathrm{Vol}(\Omega_0 \cap \Omega_{\pm}^{(-)}(\varepsilon,l)) \leqslant \mathrm{Vol}\,\Omega_0 \leqslant Cg^{\alpha+\beta} = o(g^{2/m})$ and $\mathrm{Vol}(\Omega_{\mp} \cap \Omega_{\pm}^{(-)}(\varepsilon,l)) = \mathrm{Vol}(\Omega_1 \cap \Omega_{\pm}^{(-)}(\varepsilon,l)) = 0$ as $g \to \infty$, where we used the fact that $\Omega_1 \subset \{z \in \mathbf{R}^2 \,|\, |z| \geqslant g^{\beta}\} \subset \{z \in \mathbf{R}^2 \,|\, |z| \geqslant 2Cg^{1/m}\}$ and $\Omega_{\pm}^{(-)} \subset \{z \in \mathbf{R}^2 \,|\, B_- < \lambda + Cg\langle z\rangle^{-m}\} \subset \{z \in \mathbf{R}^2 \,|\, |z| \leqslant Cg^{1/m}\}$ for some $C > 0$. Hence, we have

$$\mathrm{Vol}\big(\Omega_{\pm} \cap \Omega_{\pm}^{(-)}(\varepsilon,l)\big) = \mathrm{Vol}\big(\Omega_{\pm}^{(-)}(\varepsilon,l)\big) + o(g^{2/m}) \tag{3.16}$$

as $g \to \infty$, and we observe that

$$\sum_{l=0}^{Cg^{1-m\alpha}} \mathrm{Vol}\{z \in \Omega_{\pm} \cap \Omega_{\pm}^{(-)}(\varepsilon,l) \,|\, \mathrm{dist}(z, \partial\Omega_{\pm}) \leqslant g^{\sigma}\} \leqslant Cg^{1-m\alpha} g^{\beta+\sigma} = o(g^{2/m}) \tag{3.17}$$

as $g \to \infty$, since $\Omega_{\pm} \cap \Omega_{\pm}^{(-)}(\varepsilon,l) \subset \Omega_{\pm}$ and $1 - m\alpha + \beta + \sigma = 2/m - (1/m - 2(m+1)\sigma) < 2/m$. Then the lemma follows from (3.14)–(3.17). ■

Lemma 3.8: Let $\lambda < B_-$. Under the same assumption on B and V as in Theorem 1.1, we have $\lim_{g\to\infty} g^{-2/m} N_g^+(\lambda) = \Sigma_{l\in\mathbf{N}} \nu_l(\lambda)$.

Proof: We can deduce from (3.11) and (3.12) and Lemma 3.7 that $\liminf_{g\to\infty} g^{-2/m} N_g^+(\lambda) \geqslant \Sigma_{l\in\mathbf{N}} \nu_l(\lambda)$ in the same way as in the proof of Lemma 3.6. Then, combining this and Lemma 3.6, we have the result. ■

Remark 3.9: Our proof shows that we can replace the assumptions on B and V in Lemma 3.8 by the following weaker assumptions.

$(B)'$ In addition to (B.1), there exist $M > 0$ and $C > 0$ such that $|B(x) - B_{\pm}| \leqslant C\langle x\rangle^{-M}$ hold as $x \to \pm\infty$, respectively.

$(V)'$ The non-negative scalar potential V belongs to $C^1(\mathbf{R})$, and there exist $m > 0$ and $C > 0$ such that $0 < m < 2$ and $|\partial^{\alpha} V(z)| \leqslant C\langle z\rangle^{-m-|\alpha|}$ holds for all $z \in \mathbf{R}^2$ and for any multi-index α satisfying $|\alpha| \leqslant 1$. Moreover, the conditions (V.2) and (V.3) hold.

IV. SPECTRAL PROPERTIES OF THE IWATSUKA MODEL

A. Direct decomposition

In this section we recall from Iwatsuka (1985) the spectral representation of the Iwatsuka $H_0(b)$. We introduce the partial Fourier transform $(\mathcal{F}u)(x,\eta) = (2\pi)^{-1/2} \int_{\mathbf{R}} e^{-\sqrt{-1}y\eta} u(x,y)\mathrm{d}y$, which defines a unitary operator on $L^2(\mathbf{R}^2)$. We write L_0 for $\mathcal{F}H_0(b)\mathcal{F}^{-1}$. Then L_0 has the direct integral decomposition $L_0 = \int_{\mathbf{R}}^{\oplus} L(\eta)\mathrm{d}\eta$ acting on the Hilbert space $\int_{\mathbf{R}}^{\oplus} L^2(\mathbf{R})\mathrm{d}\eta$. Here, for each $\eta \in \mathbf{R}$, the fiber $L(\eta)$ of L_0 is given by

$$L(\eta) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + (\eta - b(x))^2, \tag{4.1}$$

acting on the fiber $L^2(\mathbf{R})$ of $\int_{\mathbf{R}}^{\oplus} L^2(\mathbf{R})\mathrm{d}\eta$.

The spectral properties of $L(\eta)$ are summarized as follows.

Lemma 4.1: [Iwatsuka[11], Lemmas 2.3 and 3.5)] Assume that (B.1) holds. For each $\eta \in \mathbf{R}$, the operator $L(\eta)$ is essentially self-adjoint on $C_0^{\infty}(\mathbf{R})$ and has a complete orthonormal system of eigenfunctions $\{\varphi_n(\cdot,\eta)\}_{n\in\mathbf{N}}$ and the corresponding eigenvalues $\{\lambda_n(\eta)\}_{n\in\mathbf{N}}$ so that $L(\eta)\varphi_n(\cdot,\eta) = \lambda_n(\eta)\varphi_n(\cdot,\eta)$ and $0 < \lambda_0(\eta) < \lambda_1(\eta) < \lambda_2(\eta) < \cdots \to \infty$ hold for each $n \in \mathbf{N}$.

Moreover, the following properties (1)–(5) hold for each $n \in \mathbf{N}$.

(1) *$\lambda_n(\eta)$ is nondegenerate and depends analytically on η.*
(2) *$\lambda_n(\eta)$ is monotonically increasing in η, and $\lim_{\eta\to\pm\infty} \lambda_n(\eta) = \Lambda_n^{\pm}$ hold, respectively.*
(3) *$\varphi_n(\cdot,\eta)$ belongs to $D(L(0))$ and depends analytically on η with respect to the graph norm $(\|u\|^2 + \|L(0)u\|^2)^{1/2}$.*
(4) *$\varphi_n(x,\eta)$ is a real-valued continuous function of x and η, and moreover, $\varphi_n(x,\eta)$ is infinitely differentiable in x for each η and is analytic in η for each x.*
(5) *The estimate $|\varphi_n(x,\eta)| \leqslant \Phi_n(x - b^{-1}(\eta))$ holds for a function Φ_n satisfying $0 < \Phi_0(x) < \cdots$*

$<\Phi_n(x)<\cdots$ *and*

$$\Phi_n(x) \leqslant \begin{cases} \sqrt{2}(\Lambda_n^+)^{1/4} & \text{if } |x| \leqslant \sqrt{\Lambda_n^+}/B_-, \\ \sqrt{2}(\Lambda_n^+)^{1/4} \exp\{-B_-(|x|-L_n)^2/2\} & \text{if } |x| \geqslant \sqrt{\Lambda_n^+}/B_-. \end{cases}$$

The next result follows easily from (*B*.1) and the definition of b.

Lemma 4.2: Under the assumption (B.1), the function b has the inverse b^{-1} *and moreover, for any* x,y,η, *we have* $B_-|x-b^{-1}(\eta)| \leqslant |b(x)-\eta| \leqslant B_+|x-b^{-1}(\eta)|$ *and* $B_-|x-y| \leqslant |b(x)-b(y)| \leqslant B_+|x-y|$.

For any $k \in \mathbf{N}$, we introduce the Banach space $B^k=\{u \in \mathcal{S}'(\mathbf{R}) \,|\, x^\alpha \partial_x^\beta u \in L^2(\mathbf{R})$ if $\alpha+\beta \leqslant k\}$ with norm $\|u\|_{B^k}=(\Sigma_{\alpha+\beta\leqslant k}\|x^\alpha\partial_x^\beta u\|^2)^{1/2}$.

Lemma 4.3: Let D_0 *denote either* $C_0^\infty(\mathbf{R})$ *or* $\mathcal{S}(\mathbf{R})$. *We have the following assertions.*

(1) *For any* $k \in \mathbf{N}$, *the operator* $L(\eta)^k|_{D_0}$ *is essentially self-adjoint and* $\overline{L(\eta)^k|_{D_0}}=(\overline{L(\eta)|_{D_0}})^k$. *Moreover,* $D(\overline{L(\eta)^k|_{D_0}})=\{u \in L^2(\mathbf{R}) \,|\, L(\eta)^k_{\mathrm{dist}} u \in L^2(\mathbf{R})\}$. *Here,* L_{dist} *stands for the differential operator L with domain* $\mathcal{S}'(\mathbf{R})$.

(2) *The Banach space* $D(\overline{L(\eta)^k|_{D_0}})$ *equipped with the graph norm* $\overline{L(\eta)^k|_{D_0}}$ *coincides with the Banach space* $D(\overline{L(0)^k|_{D_0}})$ *equipped with (equivalent) norm by* $\overline{L(0)^k|_{D_0}}$.

(3) *If we denote by* $\widetilde{B}^k$ *the space as in the assertion (2) above, then* $\widetilde{B}^k$ *coincides with* B^k *as a Banach space. In particular, the space* $\cap_{k\in\mathbf{N}}\widetilde{B}^k$ *coincides with* $\mathcal{S}(\mathbf{R})$ *as a Fréchet space.*

Proof: We note that $L(\eta) \in OpS^2$, so $L(\eta)^k \in OpS^{2k}$ for any η. It is easy to see that the symbol of $L(\eta)^k$ satisfies the ellipticity condition as in Lemma 2.7 and $L(\eta)$ is symmetric on D_0. Then, by Lemma 2.7, the operator $L(\eta)^k|_{D_0}$ is essentially self-adjoint and $D(\overline{L(\eta)^k|_{D_0}})=\{u \in L^2(\mathbf{R}) \,|\, L(\eta)^k_{\mathrm{dist}} u \in L^2(\mathbf{R})\}$. Also, we find that $L(\eta)^k|_{D_0}=(\overline{L(\eta)|_{D_0}})^k|_{D_0}$ since $L(\eta)$ leaves D_0 invariant. This implies that $\overline{L(\eta)^k|_{D_0}} \subset (\overline{L(\eta)|_{D_0}})^k$, which are both self-adjoint, so coincide. This shows the assertion (1).

The assertion (2) follows from Lemma 2.7 with $Op(a)=L(\eta)^k$ and with $Op(a)=L(0)^k$ since the topology of the weighted Sobolev spaces H^m is independent of specific $Op(a)$ by the (original) definition. As a byproduct, we find that $D(\overline{L(\eta)^k|_{D_0}})$ coincides with H^{2k}.

Finally we show the assertion (3). It is enough to show in the case of $\eta=0$. Note that $B_-|x| \leqslant |b(x)| \leqslant B_+|x|$ holds for all $x \in \mathbf{R}$ by Lemma 4.2, and each derivative of b is bounded. Then there exists $C_k>0$ such that

$$\|L(0)^k u\|^2 + \|u\|^2 \leqslant C_k \|u\|^2_{B^{2k}} \tag{4.2}$$

holds for any $u \in D_0$. Conversely, by the assertion (4) in Lemma 2.6, the operator $x^\beta\partial_x^\alpha$ maps H^{2k}, which coincides with $D(\overline{L(\eta)^k|_{D_0}})$ as stated above, to $L^2(\mathbf{R})$ continuously provided $\alpha+\beta \leqslant 2k$. This means the inequality $\|x^\beta\partial_x^\alpha u\| \leqslant C(\|L(0)^k u\|+\|u\|)$ for any $u \in D_0$. The density of D_0 completes the proof. ■

B. Exponential decay of φ_n

In this section, using the so-called Agmon estimate, we derive an exponential decay estimates of the eigenfunction φ_n and obtain the estimates for the band function λ_n. To the end of this section, we set $g(x,\eta)=(x-b^{-1}(\eta))^2$ for any $x,\eta \in \mathbf{R}$.

Lemma 4.4: Let $\eta \in \mathbf{R}$ *and let* $L(\eta)$ *be as in* (4.1). *Assume that* $f \in L^2(\mathbf{R})$ *and there exists* $\kappa>0$ *such that* $\|e^{\kappa g(\cdot,\eta)} f\|$ *is finite. Assume that* ψ *in* $D(L(\eta))$ *satisfies the equation* $(L(\eta)-\lambda_n(\eta))\psi=f$. *Then there exists* $C_n=C_n(\kappa,B_-)>0$, *independent of* η, *such that*

$$\|e^{\alpha g(\cdot,\eta)}\psi\| \leqslant C_n(\|e^{\kappa g(\cdot,\eta)} f\| + \|\psi\|)$$

holds if $0<\alpha<\min\{\kappa, B_-^2/\sqrt{8}\}$.

Proof: This is an easy consequence of the method of Agmon estimates. However, we give a

proof for the sake of completeness. Let $\chi \in C^\infty([0,\infty))$ such that $\chi(t)=t$ if $0\leqslant t\leqslant 1/2$, $\chi(t)=1$ if $t\geqslant 2$, $\sup_{t\geqslant 0}|\chi'(t)|\leqslant 1$ and χ is monotonically increasing. For any large $R>0$, we set $g_R(x,\eta)=R^2\chi(g(x,\eta)/R^2)$. We can find that

$$|g_R(x,\eta)|\leqslant \min\{R^2, g(x,\eta)\}, \quad |\partial_x g_R(x,\eta)|\leqslant 2|x-b^{-1}(\eta)| \tag{4.3}$$

and $\lim_{R\to\infty} g_R(x,\eta)=g(x,\eta)$ for any (x,η).

We may assume that ψ is not identically zero. The standard Agmon-type argument shows that $\mathrm{Re}(e^{\alpha g_R}(L(\eta)-\lambda_n(\eta))e^{\alpha g_R})\geqslant (b-\eta)^2-\alpha^2|\partial_x g_R|^2-\lambda_n\geqslant (B_-^2-4\alpha^2)|x-b^{-1}(\eta)|^2-\Lambda_n^+$ holds for any $\alpha \in \mathbf{R}$, where we used Lemma 4.2 in the first inequality and "Re" stands for the real part. Then it follows that

$$\|e^{\alpha g_R}\psi\|\|e^{\alpha g_R}f\|\geqslant |\mathrm{Re}(e^{2\alpha g_R}\psi, f)|\geqslant (e^{\alpha g_R}\psi, ((B_-^2-4\alpha^2)|x-b^{-1}|^2-\Lambda_n^+)e^{\alpha g_R}f). \tag{4.4}$$

Take $\phi\in C_0^\infty([0,\infty))$ so that $\phi(t)=1$ if $0\leqslant t\leqslant 1$, $\phi(t)=0$ if $t\geqslant 2$ and ϕ is monotonically decreasing. Set $\phi_\eta(x)=\phi(B_-^2 g(x,\eta)/(2\Lambda_n^+))$. Then we find that

$$(B_-^2-4\alpha^2)|x-b^{-1}|^2-\Lambda_n^+\geqslant (1-8\alpha^2/B_-^2)\Lambda_n^+-6\Lambda_n^+\phi_\eta \tag{4.5}$$

using the fact that $g(x,\eta)\leqslant 4\Lambda_n^+/B_-^2$ holds on supp ϕ_η and $g(x,\eta)\geqslant 2\Lambda_n^+/B_-^2$ holds on supp $(1-\phi_\eta)$, and we find from (4.4) and (4.5) that $(1-8\alpha^2/B_-^2)\Lambda_n^+\|e^{\alpha g_R}\psi\|\leqslant \|e^{\alpha g_R}f\|+6\Lambda_n^+ e^{4\alpha\Lambda_n^+/B_-^2}\|\psi\|$, since $g_R(x,\eta)\leqslant g(x,\eta)\leqslant 4\Lambda_n^+/B_-^2$ holds on supp ϕ_η. Taking a limit $R\to\infty$, we have the conclusion. ■

Lemma 4.5: Let $\alpha\in\mathbf{N}$. There exists $\kappa=\kappa_{\alpha,n}>0$ such that

$$\sup_{\eta\in\mathbf{R}}\|e^{\kappa g}\partial_\eta^{\alpha'}\varphi_n(\eta)\|<\infty \quad \text{and} \quad \sup_{\eta\in\mathbf{R}}|\partial_\eta^{\alpha'+1}\lambda_n(\eta)|<\infty \tag{4.6}$$

hold if $0\leqslant\alpha'\leqslant\alpha$.

Proof: We show this by induction on α. We abbreviate the assertion to $P(\alpha)$. When $\alpha=0$, the first estimate in (4.6) follows from Lemma 4.1 (v). The Feynman–Hellman formula yields that

$$\partial_\eta\lambda_n(\eta)=(\varphi_n,(\partial_\eta L(\eta))\varphi_n)=2(\varphi_n,(\eta-b)\varphi_n). \tag{4.7}$$

Then the second estimate in (4.6) follows from the exponential decay of φ_n with respect to $\eta-b$. This shows that $P(0)$ is true.

We assume that $P(\alpha)$ is true. First, under this assumption, we show the estimate

$$\sup_{\eta\in\mathbf{R}}\|\partial_\eta^{\alpha+1}\varphi_n(\eta)\|<\infty. \tag{4.8}$$

Differentiating the equation $(L(\eta)-\lambda_n(\eta))\varphi_n(\eta)=0$ with respect to η in $(\alpha+1)$ times, we obtain

$$(L(\eta)-\lambda_n(\eta))\partial_\eta^{\alpha+1}\varphi_n(\eta)=-\sum_{0\leqslant\alpha'\leqslant\alpha} C_{\alpha+1,\alpha'}\partial_\eta^{\alpha+1-\alpha'}((b-\eta)^2-\lambda_n(\eta))\partial_\eta^{\alpha'}\varphi_n(\eta). \tag{4.9}$$

In the case of $j\neq n$, taking an inner product with φ_j, we obtain

$$(\lambda_j(\eta)-\lambda_n(\eta))(\partial_\eta^{\alpha+1}\varphi_n,\varphi_j)=-\sum_{0\leqslant\alpha'\leqslant\alpha} C_{\alpha+1,\alpha'}(\partial_\eta^{\alpha+1-\alpha'}((b-\eta)^2-\lambda_n(\eta))\partial_\eta^{\alpha'}\varphi_n,\varphi_j).$$

Then the Schwarz inequality yields that

$$|(\partial_\eta^{\alpha+1}\varphi_n,\varphi_j)|^2 \leqslant \left(C_\alpha\delta_n^{-1}\sum_{0\leqslant\alpha'\leqslant\alpha}|(\partial_\eta^{\alpha+1-\alpha'}((b-\eta)^2-\lambda_n(\eta))\partial_\eta^{\alpha'}\varphi_n,\varphi_j)|\right)^2$$
$$\leqslant C'_\alpha\delta_n^{-2}\sum_{0\leqslant\alpha'\leqslant\alpha}|(\partial_\eta^{\alpha+1-\alpha'}((b-\eta)^2-\lambda_n(\eta))\partial_\eta^{\alpha'}\varphi_n,\varphi_j)|^2 \tag{4.10}$$

for some $C_\alpha, C'_\alpha>0$ independent of η. Here, we introduced a positive number δ_n as

$$\delta_n=\begin{cases}\min\{\inf_{\eta\in\mathbf{R}}(\lambda_{n+1}(\eta)-\lambda_n(\eta)),\inf_{\eta\in\mathbf{R}}(\lambda_n(\eta)-\lambda_{n-1}(\eta))\} & \text{if } n\geqslant 2,\\ \inf_{\eta\in\mathbf{R}}(\lambda_2(\eta)-\lambda_1(\eta)) & \text{if } n=1.\end{cases}$$

In the case of $j=n$, differentiating the relation $(\varphi_n,\varphi_n)=1$ with respect to η in $(\alpha+1)$ times, we find that $2(\partial_\eta^{\alpha+1}\varphi_n,\varphi_n)=-\Sigma_{1\leqslant\alpha'\leqslant\alpha}C_{\alpha+1,\alpha'}(\partial_\eta^{\alpha+1-\alpha'}\varphi_n,\partial_\eta^{\alpha'}\varphi_n)$, where we used the reality of φ_n. Then we have

$$|(\partial_\eta^{\alpha+1}\varphi_n,\varphi_n)|\leqslant C_\alpha\sum_{1\leqslant\alpha'\leqslant\alpha}\|\partial_\eta^{\alpha+1-\alpha'}\varphi_n\|\|\partial_\eta^{\alpha'}\varphi_n\| \tag{4.11}$$

for some $C_\alpha>0$ independent of η. Hence it follows from (4.10) and (4.11) that

$$\|\partial_\eta^{\alpha+1}\varphi_n\|^2=\sum_{j\in N}|(\partial_\eta^{\alpha+1}\varphi_n,\varphi_j)|^2\leqslant C'_\alpha\delta_n^{-2}\sum_{0\leqslant\alpha'\leqslant\alpha}\|(\partial_\eta^{\alpha+1-\alpha'}((b-\eta)^2-\lambda_n(\eta)))\partial_\eta^{\alpha'}\varphi_n\|^2$$
$$+\left(C_\alpha\sum_{1\leqslant\alpha'\leqslant\alpha}\|\partial_\eta^{\alpha+1-\alpha'}\varphi_n\|\|\partial_\eta^{\alpha'}\varphi_n\|\right)^2, \tag{4.12}$$

where we used the fact that $\{\varphi_j(\cdot,\eta)\}_{j\in\mathbf{N}}$ is an ONB in $L^2(\mathbf{R})$. By the assumption $P(\alpha)$, all terms on the rhs of (4.12) are bounded uniformly in η. Thus we have proved (4.8) under $P(\alpha)$.

Next, we apply Lemma 4.4 to (4.9) with $\psi=\partial_\eta^{\alpha+1}\varphi_n, f=f_\alpha$=the rhs of (4.9). We may assume that the constant α in the exponent in Lemma 4.4 is equal to κ since we can take κ small enough. Then it follows that there exists $C_n>0$ such that the estimate $\|e^{\kappa g}\partial_\eta^{\alpha+1}\varphi_n\|\leqslant C_n(\|e^{\kappa g}f_\alpha\|+\|\partial_\eta^{\alpha+1}\varphi_n\|)$. The first term on the rhs is bounded uniformly in η under $P(\alpha)$, since the maximal order of derivatives of φ_n is less than or equal to α and the maximal order of derivatives of λ_n is less than or equal to $\alpha+1$ in the expression of f_α. The second term on the rhs is also uniformly bounded because of (4.8) we have already proved. Hence, we have proved the first estimate in (4.6) for $P(\alpha+1)$, assuming $P(\alpha)$.

Finally, we show the second estimate in (4.6) for $P(\alpha+1)$, assuming $P(\alpha)$. Differentiating (4.7) with respect to η in $(\alpha+1)$ times, we obtain

$$\partial_\eta^{\alpha+2}\lambda_n(\eta)=2\partial_\eta^{\alpha+1}(\varphi_n,(\eta-b)\varphi_n)=2\sum_{0\leqslant\alpha'\leqslant\alpha+1}C_{\alpha+1,\alpha'}(\partial_\eta^{\alpha+1-\alpha'}\varphi_n,\partial_\eta^{\alpha'}((\eta-b)\varphi_n)). \tag{4.13}$$

Since the maximal order of derivatives of φ_n on the rhs of (4.13) is less than or equal to $\alpha+1$, the uniform boundedness of the rhs of (4.13) with respect to η follows from the first estimate in (4.6) for $P(\alpha)$ and the exponential decay property of $\partial_\eta^{\alpha+1}\varphi_n$ we have proved above. Thus we have proved all the assertion of $P(\alpha+1)$, assuming $P(\alpha)$. This completes the induction. ■

Lemma 4.6: Let $\beta\in\mathbf{N}$. *For any* $\alpha\in\mathbf{N}$, *there exists* $\kappa=\kappa(\alpha,\beta,n)>0$ *such that* $\sup_{\eta\in\mathbf{R}}\|e^{\kappa g}\partial_x^\beta\partial_\eta^\alpha\varphi_n(\eta)\|<\infty$.

Proof: We show this by induction on β. We abbreviate the assertion to $P(\beta)$. The assertion $P(0)$ is true by Lemma 4.5.

We assume that $P(\beta)$ is true. Then, for any α, we have

$$\|e^{\kappa g}\partial_x^{\beta+1}\partial_\eta^\alpha\varphi_n(\eta)\|^2=-(e^{2\kappa g}\partial_x^\beta\partial_\eta^\alpha\partial_x^2\varphi_n,\partial_x^\beta\partial_\eta^\alpha\varphi_n)-4\kappa((x-b^{-1}(\eta))e^{2\kappa g}\partial_x^{\beta+1}\partial_\eta^\alpha\varphi_n,\partial_x^\beta\partial_\eta^\alpha\varphi_n)$$
$$=(e^{2\kappa g}\partial_x^\beta\partial_\eta^\alpha(\lambda_n(\eta)-(b-\eta)^2)\varphi_n,\partial_x^\beta\partial_\eta^\alpha\varphi_n)$$
$$-4\kappa(\partial_x^{\beta+1}\partial_\eta^\alpha\varphi_n,(x-b^{-1}(\eta))e^{2\kappa g}\partial_x^\beta\partial_\eta^\alpha\varphi_n), \tag{4.14}$$

where we used the equation $(L-\lambda_n)\varphi_n=0$ in the third equality. The first term on the rhs of (4.14) is bounded uniformly in η by the assumption $P(\beta)$ and the second estimate in (4.6) if we choose $\kappa>0$ sufficiently small (the choice is independent of η). The second term on the rhs of (4.14) is bounded from above by $4\kappa\|e^{\kappa g}\partial_x^{\beta+1}\partial_\eta^\alpha\varphi_n\|\|(x-b^{-1}(\eta))e^{\kappa g}\partial_x^\beta\partial_\eta^\alpha\varphi_n\|\leq 2\kappa\|e^{\kappa g}\partial_x^{\beta+1}\partial_\eta^\alpha\varphi_n\|^2+2\kappa\|(x-b^{-1})e^{\kappa g}\partial_\beta\partial_\eta^\alpha\varphi_n\|^2$, which is uniformly bounded since $P(\beta)$ is assumed to be true. ■

Lemma 4.7: For any $n,\alpha,\beta\in\mathbf{N}$, there exists a positive constant $\kappa=\kappa(\alpha,\beta,n)$ such that $\sup_{(x,\eta)\in\mathbf{R}^2}|e^{\kappa g}\partial_x^\beta\partial_\eta^\alpha\varphi_n(x,\eta)|<\infty$ holds.

Proof: For any $\gamma\in\mathbf{N}$, we have $\partial_x^\gamma(e^{\kappa g}\partial_x^\beta\partial_\eta^\alpha\varphi_n)=\Sigma_{0\leq\gamma'\leq\gamma}C_{\gamma,\gamma'}(\partial_x^{\gamma-\gamma'}e^{\kappa g})(\partial_x^{\beta+\gamma'}\partial_\eta^\alpha\varphi_n)$. Since each of the functions $\partial_x^{\gamma-\gamma'}e^{\kappa g}$ is of the form "a polynomial of $(x-b^{-1}(\eta))$ times $e^{\kappa g}$," we obtain the estimate

$$\|\partial_x^\gamma(e^{\kappa g}\partial_x^\beta\partial_\eta^\alpha\varphi_n)\|\leq\sum_{0\leq\gamma'\leq\gamma}C_{\gamma,\gamma'}\|e^{\kappa' g}\partial_x^{\beta+\gamma'}\partial_\eta^\alpha\varphi_n\| \tag{4.15}$$

for some $\kappa'>0$ satisfying $0<\kappa'<\kappa$ uniformly in η. The rhs of (4.15) is bounded uniformly in η by Lemma 4.6 for an appropriate choice of κ,κ'. This means that the γth Sobolev norm of $e^{\kappa g}\partial_x^\beta\partial_\eta^\alpha\varphi_n$ is bounded uniformly in η for each γ. Hence, Sobolev's embedding theorem yields that

$$\sup_{x\in\mathbf{R}}|e^{\kappa g}\partial_x^\beta\partial_\eta^\alpha\varphi_n|\leq C(\|e^{\kappa g}\partial_x^\beta\partial_\eta^\alpha\varphi_n\|+\|\partial_x(e^{\kappa g}\partial_x^\beta\partial_\eta^\alpha\varphi_n)\|) \tag{4.16}$$

for some $C>0$. The above observation shows that the rhs of (4.16) is uniformly bounded in η if we choose κ small enough. This shows the lemma. ■

C. Decay estimate of λ_n

In this section, we derive the following decay estimate of the band function λ_n at infinity.

Lemma 4.8: Assume that $(B.2)_+$ holds. Then, for any $n\in\mathbf{N}$, there exists $C_n>0$ such that $|\Lambda_n^+-\lambda_n(b(x))|\leq C_n\langle x\rangle^{-M}$ holds if $x\geq 0$. Similarly, if we assume $(B.2)_-$ then the same estimate replaced Λ_n^+ by Λ_n^- holds if $x\leq 0$.

Proof: We mimic the proof of Lemma 4.1 in Iwatsuka (1985). We first consider the case of $x\geq 0$. Let n be fixed and $j,k\leq n$. Set $L_c(s)=-\partial_x^2+B_+^2(x-s)^2$ in $L^2(\mathbf{R})$ and $\alpha_{jk}(s)=(L_c(s)\varphi_j(\cdot,b(s)),\varphi_k(\cdot,b(s)))$. Then, using the equation $(L(b(s))\varphi_j(\cdot,b(s)),\varphi_k(\cdot,b(s)))=\lambda_j(b(s))\delta_{jk}$, we find that

$$\begin{aligned}
|\alpha_{jk}(s)-\lambda_j(b(s))\delta_{jk}| &\leq \int_{\mathbf{R}}|B_+^2(x-s)^2-(b(x)-b(s))^2|\varphi_j(x,b(s))\|\varphi_k(x,b(s))|\mathrm{d}x\\
&\leq 2B_+\int_{\mathbf{R}}\left\{|x-s|\left|\int_s^x(B_+-B(t))\mathrm{d}t\right|\Phi_n(x-s)^2\right\}\mathrm{d}x\\
&=2B_+\int_{-\infty}^{-s/2}\left\{|y|\left|\int_s^{y+s}(B_+-B(t))\mathrm{d}t\right|\Phi_n(y)^2\right\}\mathrm{d}y\\
&\quad+2B_+\int_{-s/2}^{\infty}\left\{|y|\left|\int_s^{y+s}(B_+-B(t))\mathrm{d}t\right|\Phi_n(y)^2\right\}\mathrm{d}y,
\end{aligned} \tag{4.17}$$

where we used the facts that $|B_+^2(x-s)^2-(b(x)-b(s))^2|=|\int_s^x(B_++B(t))\mathrm{d}t\|\int_s^x(B_+-B(t))\mathrm{d}t|\leq 2B_+|x-s\|\int_s^x(B_+-B(t))\mathrm{d}t|$ holds and that $|\varphi_j(x,b(s))|\leq\Phi_n(x-s)$ hold if $j\leq n$ by Lemma 4.1. For any large $N\in\mathbf{N}$ and any large $s>0$, the first term on the rhs of (4.17) is bounded from above by

$$(2B_+)^2\int_{-\infty}^{-s/2}|y|^2\Phi_n(y)^2\,dy \leqslant 4B_+^2\int_{-\infty}^{-s/2}C_{N,n}\langle y\rangle^{-2N}\,dy \leqslant C'_{N,n}\langle s\rangle^N \tag{4.18}$$

for some constant $C'_{N,n}$, where we used Lemma 4.1. Since $(B.2)_+$ implies that there exists $s_0>0$ and $C_n>0$ such that $\sup_{t\geqslant s/2}|B_+-B(t)|\leqslant C_n\langle s\rangle^{-N}$ holds if $s>s_0$, it follows that the second term on the rhs of (4.17) is bounded from above by

$$2B_+C_n\langle s\rangle^{-M}\int_{-s/2}^{\infty}|y|^2\Phi_n(y)^2\,dy \leqslant C'_nB_+\langle s\rangle^{-M} \tag{4.19}$$

if $s>s_0$. Hence it follows from (4.17)–(4.19) that

$$\sup_{s>s_0}s^M|\alpha_{jk}(s)-\lambda_j(b(s))\delta_{jk}|\leqslant C_n \tag{4.20}$$

holds for some $C_n>0$, if we choose s_0 sufficiently large.

If we denote by $V_n(s)$ the linear subspace of $L^2(\mathbf{R})$ spanned by $\{\varphi_j(\cdot,b(s))\}_{j\leqslant n}$, then $(\alpha_{jk}(s))_{j,k\leqslant n}$ is the Hermitian symmetric matrix of $L_c(s)|_{V_n(s)}$ with respect to the basis $\{\varphi_j(\cdot,b(s))\}_{j\leqslant n}$. Let $\mu_0(s)\leqslant\cdots\leqslant\mu_n(s)$ be the eigenvalues of $(\alpha_{jk}(s))_{j,k\leqslant n}$. Let (a_{ij}) and (b_{ij}) be $n\times n$ Hermitian matrices and let $\alpha_1\leqslant\cdots\leqslant\alpha_n$ and $\beta_1\leqslant\cdots\leqslant\beta_n$ be their eigenvalues, respectively. Then it is easy to see that $|\alpha_k-\beta_k|^2\leqslant\Sigma_{i,j}|a_{ij}-b_{ij}|^2$ holds for any k. Hence it follows from (4.20) that

$$\sup_{s>s_0}s^M|\mu_j(s)-\lambda_j(b(s))|\leqslant C'_n. \tag{4.21}$$

Then, by the variational principle [Reed and Simon (1978, Vol. IV, Theorem XIII.3)], we have $\Lambda_j^+\leqslant\mu_j(s)$ for any $j\leqslant n$. Since Λ_j^+ is the jth eigenvalue of $L_c(s)$ and $\lambda_j(b(s))\leqslant\Lambda_j^+$, we can deduce from (4.21) that

$$\sup_{s>s_0}s^M|\Lambda_j^+-\lambda_j(b(s))|\leqslant C''_n \tag{4.22}$$

holds if $j\leqslant n$. This shows the first assertion of the lemma.

In the case of $s\to-\infty$, we have the conclusion in a similar way, replacing the objects $\alpha_{jk},L_c(s),L(b(s))$ and $\mu_j(s)$'s by $(L(b(s))\psi_j(\cdot,s),\psi_k(\cdot,s)),L(b(s)),-\partial_x^2+B_-^2(x-s)^2$ and the eigenvalues of the matrix $((L(b(s))\psi_j(\cdot,s),\psi_k(\cdot,s)))_{j,k\leqslant n}$, respectively. Here, $\psi_k(\cdot,s)$ is the eigenfunction of $-\partial_x^2+B_-^2(x-s)^2$ corresponding to the kth eigenvalue Λ_k^-. ■

V. PROOF OF THEOREMS

A. Operators on the direct sum

To the end of this paper, we always assume $(B.1)$, $(B.2)$, $(V.1)$–$(V.4)$.

Let $\{\varphi_n\}_{n\in\mathbf{N}}$ be the eigenfunctions given in Lemma 4.1. Because of Lemma 4.1, for any $l\in\mathbf{N}$, we can define a partial isometry T_l from $L^2(\mathbf{R})$ into $L^2(\mathbf{R}^2)$ by $(T_lf)(x,\eta)=\varphi_l(x,\eta)f(\eta)$ for any $f\in L^2(\mathbf{R})$. The adjoint operator T_l^* from $L^2(\mathbf{R}^2)$ onto $L^2(\mathbf{R})$ is given by $(T_l^*F)(\eta)=\int_{\mathbf{R}}\varphi_l(x,\eta)F(x,\eta)dx$ for any $F\in L^2(\mathbf{R}^2)$. We now extend T_ls to an operator on the direct sum of Hilbert spaces $\Sigma_{l\in\mathbf{N}}\oplus L^2(\mathbf{R})$, more precisely, we define a partial isometry T from $\Sigma_{l\in\mathbf{N}}\oplus L^2(\mathbf{R})$ into $L^2(\mathbf{R}^2)$ by $T(\oplus_{l\in\mathbf{N}}(f_l))=\Sigma_{l\in\mathbf{N}}T_lf_l$ for any $\oplus_{l\in\mathbf{N}}(f_l)\in\Sigma_{l\in\mathbf{N}}\oplus L^2(\mathbf{R})$. The unitarity of T follows from the L^2-orthogonality of φ_l's with respect to the first variable. The adjoint operator T^* from $L^2(\mathbf{R}^2)$ onto $\Sigma_{l\in\mathbf{N}}\oplus L^2(\mathbf{R})$ is given by $T^*F=\oplus_{l\in\mathbf{N}}T_l^*F$ for any $F\in L^2(\mathbf{R}^2)$. We set

$$\mathcal{W}=T^*\mathcal{F}W\mathcal{F}^*T \tag{5.1}$$

for any multiplication operator W on $L^2(\mathbf{R}^2)$ and set $\mathcal{H}_g=T^*\mathcal{F}H_g(b)\mathcal{F}^*T(=\mathcal{H}_0-g\mathcal{V})$, both acting on the Hilbert space $\Sigma_{l\in\mathbf{N}}\oplus L^2(\mathbf{R})$, where $\mathcal{F}$ is the partial Fourier transform as in the preceding section and $\mathcal{V}$ is the operator (5.1) with $W=V$.

For an operator A acting on the space $\Sigma_{l\in\mathbf{N}}\oplus L^2(\mathbf{R})$, we say *$A$ belongs to OpS^m* if all the matrix elements $A_{jk}(j,k\in\mathbf{N})$ of A (with respect to the direct sum decomposition) belong to the class OpS^m. When all the matrix-valued ΨDOs under consideration have finitely many nonzero components, the standard ΨDO calculus as in Sec. II B is applicable also for the matrix-valued ΨDOs. In particular, Proposition 2.8 remains valid for the matrix-valued ΨDO with obvious modifications (e.g., we regard the product of symbols as the usual matrix product, etc.).

In the rest of this section we are concerned with the matrix-valued ΨDO $\mathcal{V}=T^*\mathcal{F}V\mathcal{F}^*T$.

Lemma 5.1: Let $m>0$ be as in (V.1). We have the following assertions.

(1) *The operator $T_n^*\mathcal{F}V\mathcal{F}^*T_n$ on $L^2(\mathbf{R})$ belongs to OpS^{-m} for any $n\in\mathbf{N}$, and moreover, for any $\alpha,\beta\in\mathbf{N}$, there exists $C_{\alpha\beta}>0$ such that the Weyl symbol p_V of $T_n^*\mathcal{F}V\mathcal{F}^*T_n$ on $L^2(\mathbf{R})$ satisfies the estimate*

$$\eta_{\alpha\beta}^{(-m)}(p_V)\leqslant C_{\alpha\beta}\eta_{\alpha\beta}^{(-m)}(V). \tag{5.2}$$

Here, $\eta_{\alpha\beta}^{(m)}$ is the seminorm as in (2.2).

(2) *A principal symbol q_V of $T_n^*\mathcal{F}V\mathcal{F}^*T_n$ is given by $q_V(\eta,\eta^*)=V(b^{-1}(\eta),-\eta^*)$, and moreover, for any $\alpha,\beta\in\mathbf{N}$, there exists $C_{\alpha\beta}>0$ such that the remainder estimates*

$$\eta_{\alpha\beta}^{(-m-1)}(p_V-q_V)\leqslant C_{\alpha\beta}\eta_{\alpha\beta}^{(-m-1)}(\nabla V) \tag{5.3}$$

holds. Here, we denote by ∇V the first order derivatives of V.

(3) *The operator $T_i^*\mathcal{F}V\mathcal{F}^*T_j$ on $L^2(\mathbf{R})$ belongs to OpS^{-m-1} for any $i,j\in\mathbf{N}$ satisfying $i\neq j$, and moreover, for any $\alpha,\beta\in\mathbf{N}$, there exists $C_{\alpha\beta}>0$ such that the Weyl symbol r_V of $T_i^*\mathcal{F}V\mathcal{F}^*T_j$ on $L^2(\mathbf{R})$ satisfies the estimate*

$$\eta_{\alpha\beta}^{(-m-1)}(r_V)\leqslant C_{\alpha\beta}\eta_{\alpha\beta}^{(-m-1)}(\nabla V). \tag{5.4}$$

Proof: First, assuming further that $V\in\mathcal{S}(\mathbf{R}^2)$, we show the assertions (1)–(3). For any $i,j\in\mathbf{N}$, we find that the operator $T_i^*\mathcal{F}V\mathcal{F}^*T_j$ has the integral kernel $K(\eta,\eta')=\int\int_{\mathbf{R}^2}\varphi_i(x,\eta)\varphi_j(x,\eta')V(x,y)e^{-\sqrt{-1}y(\eta-\eta')}\,dx\bar{d}y$, which converges absolutely for each η,η', and so the Weyl symbol p_V is given by

$$\begin{aligned}p_V(\eta,\eta^*)&=\int_{\mathbf{R}}e^{-\sqrt{-1}w\eta^*}K(\eta+w/2,\eta-w/2)dw\\&=\int\int\int_{\mathrm{R}^3}dx\,\bar{d}w\,dz\,e^{-\sqrt{-1}wz}\varphi_i(x,\eta+w/2)\varphi_j(x,\eta-w/2)V(x,z-\eta^*),\end{aligned} \tag{5.5}$$

where we changed the variable $z=y+\eta^*$ in the last line. An integration by parts yields that the rhs of (5.5) is equal to

$$\int\int\int_{\mathbf{R}^3}\dot{d}x\,\bar{d}w\,dz\langle z\rangle^{-2N}e^{-\sqrt{-1}wz}\langle D_w\rangle^{2N}(\varphi_n(x,\eta+w/2)\varphi_n(x,\eta-w/2))V(x,z-\eta^*) \tag{5.6}$$

for any $N\in\mathbf{N}$. Using the estimate $\langle\eta;\eta^*\rangle\leqslant C\langle x;z-\eta^*\rangle\langle\eta-b(x)\rangle\langle z\rangle$, we find that, for any α,β,

$$\begin{aligned}&\langle\eta;\eta^*\rangle^{m+\alpha}|\partial_\eta^\beta\partial_{\eta^*}^\alpha p_V(\eta,\eta^*)|\\&\leqslant C\int\int\int_{\mathbf{R}^3}dx\,\bar{d}w\,dz\langle z\rangle^{-2N+m+\alpha}\langle\eta-b(x)\rangle^{m+\alpha}\\&\times|\partial_\eta^\beta\langle D_w\rangle^{2N}(\varphi_i(x,\eta+w/2)\varphi_j(x,\eta-w/2))|\langle x;z-\eta^*\rangle^{m+\alpha}\\&|\partial_{\eta^*}^\alpha V(x,z-\eta^*)|\end{aligned}$$

$$\leqslant C'\,\eta_{\alpha 0}^{(-m)}(V)\int\int_{\mathbf{R}^2}\mathrm{d}x\,\bar{d}w\langle\eta-b(x)\rangle^{m+\alpha}|\partial_\eta^\beta\langle D_w\rangle^{2N}(\varphi_i(x,\eta+w/2)\varphi_j(x,\eta-w/2))| \tag{5.7}$$

if we take N so that $2N-m-\alpha>1$. By Lemma 4.7, we have

$$\begin{aligned}
&|\partial_\eta^\beta\langle D_w\rangle^{2l}(\varphi_i(x,\eta+w/2)\varphi_j(x,\eta-w/2))|\\
&\quad\leqslant C_{\beta N}\sum_{0\leqslant\beta'\leqslant\beta}\sum_{0\leqslant N'\leqslant 2N}\left|\partial_\eta^{\beta-\beta'+2N-N'}\varphi_i(x,\eta+w/2)\partial_\eta^{\beta'+N'}\varphi_j(x,\eta-w/2)\right|\\
&\quad\leqslant C'_{\beta N}\exp(-c((b(x)-\eta-w/2)^2-(b(x)-\eta+w/2)^2))=C'_{\beta N}\exp(-2c(b(x)-\eta)^2-cw^2/2)
\end{aligned}$$

Hence, the integral on the rhs of (5.7) converges absolutely, because of Lemma 4.2. Especially, when $i=j=n$, this proves the assertion (1) under the temporal assumption on V.

We show the assertions (2) and (3). The first order Taylor expansion yields that

$$\begin{aligned}
V(x,z-\eta^*)&=V(b^{-1}(\eta),-\eta^*)+(x-b^{-1}(\eta))\int_0^1(\partial_1V)(\theta x+(1-\theta)b^{-1}(\eta),\theta(z-\eta^*)-(1-\theta)\eta^*)\mathrm{d}\theta\\
&\quad+z\int_0^1(\partial_2V)(\theta x+(1-\theta)b^{-1}(\eta),\theta(z-\eta^*)-(1-\theta)\eta^*)\mathrm{d}\theta,
\end{aligned}\tag{5.8}$$

where ∂_jV denotes the derivative of V with respect to the jth variable. In (5.5), the symbol corresponding to the first term on the rhs of (5.8) is given by

$$\begin{aligned}
&\int\int\int_{\mathbf{R}^3}\mathrm{d}x\,\bar{d}w\,\mathrm{d}z\,e^{-\sqrt{-1}wz}\varphi_i(x,\eta+w/2)\varphi_j(x,\eta-w/2)V(b^{-1}(\eta),-\eta^*)\\
&\quad=\int_{\mathbf{R}}\varphi_i(x,\eta)\varphi_j(x,\eta)\mathrm{d}x\,V(b^{-1}(\eta),-\eta^*)=V(b^{-1}(\eta),-\eta^*)\delta_{ij},
\end{aligned}$$

where we used the Fourier inversion formula. We can derive the estimate (5.3) for the symbols corresponding to the second and the third terms on the rhs of (5.8) in the same way as in the proof of (5.2), using the facts that $|\partial_\eta^\alpha(x-b^{-1}(\eta))|\leqslant C_\alpha\langle x-b^{-1}(\eta)\rangle$, which follows from (*B*.2), and that $\langle\eta;\eta^*\rangle\leqslant C\langle b^{-1}(\eta);-\eta^*\rangle\leqslant C'\langle\theta x+(1-\theta)b^{-1}(\eta);\theta(z-\eta^*)-(1-\theta)\eta^*\rangle\langle x-b^{-1}(\eta)\rangle\langle z\rangle$. Then we have the assertions (2) and (3) when $V\in\mathcal{S}(\mathbf{R}^2)$.

Finally, we give a proof for general Vs. We consider only the case of $i=j=n$, since the case of $i\neq j$ is similar. Since the space $\mathcal{S}(\mathbf{R})$ is dense in S^{-k} for any $k>0$, we can approximate V by an appropriate sequence$\{V_l\}_{l=1}^\infty(\subset\mathcal{S}(\mathbf{R}^2))$ in S^{-k} for any $k>0$. We consider the equality

$$T_n^*\mathcal{F}V_l\mathcal{F}^*T_n=Op(q_{V_1})+R(\nabla V_l), \tag{5.9}$$

where $R(\nabla V_l)$ stands for the remainder term. Then it follows from Lemma 2.5, (5.2) and (5.3) that the rhs of (5.9) converges to $Op(q_V)+R(\nabla V)$ as $l\to\infty$ in the norm operator topology. On the other hand, the left-hand side (lhs) of (5.9) converges to $T_n^*\mathcal{F}V\mathcal{F}^*T_n$ as $l\to\infty$ in the weak operator topology by definition. Thus, the lemma is true for general V's. ■

The next lemma follows immediately from Lemma 5.1 if we replace V by V^α.

Lemma 5.2: Let $\mathcal{V}$ *be the operator* (5.1) *with* $W=V$. *Let* $\alpha>0$. *Set* $\mathcal{V}_{ij}^\alpha=T_i\mathcal{F}V^\alpha\mathcal{F}^*T_j$ *for any* $i,j\in\mathbf{N}$. *If we regard* $\mathcal{V}_{ij}^\alpha$ *as an operator from the* jth *component to the* ith *component of* $\Sigma_{l\in\mathbf{N}}\oplus L^2(\mathbf{R})$, *then* $\mathcal{V}_{ij}^\alpha$ *is a*Ψ DO *whose symbol is given by the form* $V(b^{-1}(\eta),-\eta^*)\delta_{ij}+OpS^{-m\alpha-1}$.

We need the following result in the place where we use Proposition 2.8.

Lemma 5.3: Let $\lambda\in\mathbf{R}\backslash\mathrm{Spec}(H_0(b))$ *and let*ν_l *be as in* Sec. I. *For any* $l\in\mathbf{N}$, *we have* $\lim_{g\to\infty}g^{-2/m}\,\mathrm{Vol}\{(x,\xi)\in\mathbf{R}^2\,|\,V(b^{-1}(x),-\xi)>g^{-1}|\lambda_l(x)-\lambda|\}=\nu_l(\lambda)$.

Proof: Note that $|\lambda_l(b(x))-\lambda|\geqslant C_\lambda>0$ holds for some C_λ, independent of l,x. For simplicity,

we set $F_l=\{(x,\xi)\in\mathbf{R}^2\,|\,V(b^{-1}(x),-\xi)>g^{-1}|\lambda_l(x)-\lambda|\}$, $F_l'=\{(x,\xi)\in\mathbf{R}^2\,|\,V(x,\xi)>g^{-1}|\lambda_l(b(x))-\lambda|\}$ for any $l\in\mathbf{N}$. By changing the variables $(x,\xi)\to(b(x),-\xi)$, we find that $(1/2\pi)\mathrm{Vol}(F_l)=\int\int_{F_l'}B(x)\mathrm{d}x\,\mathrm{d}\xi=J_0+J_++J_-$, where we set

$$J_0=\int\int_{F_l'\cap\{|x|\leqslant g^{1/2m}\}}B(x)\mathrm{d}x\,\mathrm{d}\xi,\quad J_\pm=\int\int_{F_l'\cap\{\pm x\geqslant g^{1/2m}\}}B(x)\mathrm{d}x\,\mathrm{d}\xi,$$

respectively. We first consider the integral J_0. By $(B.1)$, $(V.1)$, there exists $C>0$ such that $J_0\leqslant B_+\,\mathrm{Vol}\{(x,\xi)\in\mathbf{R}^2\,|\,C\langle x,\xi\rangle^{-m}>C_\lambda g^{-1},|x|\leqslant g^{1/2m}\}=o(g^{2/m})$ holds as $g\to\infty$. Next, we consider the integral J_+. We divide $J_+=J_{+,1}+J_{+,2}$ with

$$J_{+,1}=\int\int_{F_l'\cap\{x\geqslant g^{1/2m}\}}(B(x)-B_+)\mathrm{d}x\,\mathrm{d}\xi,$$

$$J_{+,2}=\frac{B_+}{2\pi}\mathrm{Vol}\{(x,\xi)\in\mathbf{R}^2|V(x,\xi)>g^{-1}|\lambda_l(b(x))-\lambda|,x\geqslant g^{1/2m}\}.$$

Using $(B.2)$ we find that $|J_{+,1}|$ is bounded from above by

$$C\int\int_{F_l'\cap\{x\geqslant g^{1/2m}\}}\langle x\rangle^{-M}\,\mathrm{d}x\mathrm{d}\xi\leqslant Cg^{-M/2m}\,\mathrm{Vol}\{(x,\xi)\in\mathbf{R}^2|\langle x;\xi\rangle^{-m}>C_\lambda g^{-1},x\geqslant g^{1/2m}\},$$

which is of order $o(g^2/m)$ as $g\to\infty$. If $x\leqslant g^{1/2m}$, then $|\lambda_l(b(x))-\lambda|\geqslant|\Lambda_l^+-\lambda|-|\lambda_l(b(x))-\Lambda_l^+|\geqslant|\Lambda_l^+-\lambda|-C\langle x\rangle^{-M}\geqslant|\Lambda_l^+-\lambda|-Cg^{-M/2m}$ holds because of Lemma 4.8. Then we find that $J_{+,2}=(B_+/4\pi)|\Lambda_l^+-\lambda|^{-2/m}\hat{v}+g^{2/m}+o(g^{2/m})$ as $g\to\infty$ in the same way as in the proof of Lemma 3.6. We can estimate the integral J_- similarly. ■

B. Preliminary estimates

The proofs of Theorems 1.1, 1.4, and 1.5 given below are essentially the same as those of Theorems 1.2, 1.1 in Raikov (1993) and that of Theorem 2.2 in Raikov (1998), respectively. However, we reproduce the proofs of Theorems 1.1–1.5 for the sake of completeness.

Let $\Lambda_{n-1}^+<\lambda<\Lambda_n^-$. Take an integer N_0 greater than n and set $I_-=\{-1,0,\ldots,n-1\}$, $I_+=\{n,n+1,\ldots,N_0\}$. Define the orthogonal projections P_+,P_-,P_∞, and P_-^c on the space $\Sigma_{l\in\mathbf{N}}\oplus L^2(\mathbf{R})$ by $P_\pm=\Sigma_{l\in I_\pm}\oplus\mathrm{id}L^2(\mathbf{R})$, respectively, $P_\infty=\mathrm{id}-P_--P_+$ and $P_-^c=P_++P_\infty=\mathrm{id}-P_-$. Here, "id" stands for the identity operator. These projections $P_\pm,P_\infty$ commute with each other and with the operator $\mathcal{H}_0$.

Lemma 5.4: We have the asymptotic relations

$$\lim_{g\to\infty}g^{-2/m}N(g^{-1}<\mathcal{V}^{1/2}P_\pm|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2})=\sum_{l\in I_\pm}\nu_l(\lambda),\tag{5.10}$$

$$\lim_{g\to\infty}g^{-2/m}N(g^{-1}<P_\pm\mathcal{V}^{1/2}P_\pm|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}P_\pm)=\sum_{l\in I_\pm}\nu_l(\lambda),\tag{5.11}$$

respectively. Here, the operators $\mathcal{H}_0$ and $\mathcal{V}$ are as in Sec. V A.

Proof: It follows from $\mathrm{Spec}(A^*A)\backslash\{0\}=\mathrm{Spec}(AA^*)\backslash\{0\}$ that

$$N(g^{-1}<\mathcal{V}^{1/2}P_\pm|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2})=N(g^{-1}<|\mathcal{H}_0-\lambda|^{-1/2}P_\pm\mathcal{V}P_\pm|\mathcal{H}_0-\lambda|^{-1/2}).$$

The operators $|\mathcal{H}_0-\lambda|^{-1}P_\pm$ are matrix-valued ΨDOs on $\Sigma_{l\in I_\pm}\oplus L^2(\mathbf{R})$ and have the symbol $(|\lambda_l(\eta)-\lambda|^{-1}\delta_{ij})_{i,j\in I_\pm}$, which belong to the class OpS^0 by Lemma 4.5, and the operators $|\mathcal{H}_0-\lambda|^{-1/2}P_\pm\mathcal{V}P_\pm|\mathcal{H}_0-\lambda|^{-1/2}$ are matrix-valued ΨDOs whose principal symbols are given by $(|\lambda_l(\eta)$

$-\lambda|^{-1}V(b^{-1}(\eta),\eta^*)\delta_{ij})_{i,j\in I_\pm}$, respectively, because of Lemma 5.2. Then (5.10) follows from a matrix-valued ΨDO version of Proposition 2.8. The proof of (5.11) is similar. ■

Lemma 5.5: We have the asymptotic relations

$$\lim_{\mu\downarrow 0}\mu^{2/m}N(\mu<P_-^c\mathcal{V}^{1/2}P_-|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}P_-^c)=0, \tag{5.12}$$

$$\lim_{\mu\downarrow 0}\mu^{2/m}N(\mu<P_-\mathcal{V}^{1/2}P_+|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}P_-)=0, \tag{5.13}$$

$$\lim_{N_0\to\infty}\limsup_{\mu\downarrow 0}\mu^{2/m}N(\mu<P_-\mathcal{V}^{1/2}P_\infty|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}P_-)=0. \tag{5.14}$$

Proof: Since $P_-\mathcal{V}^{1/2}P_-^c\mathcal{V}^{1/2}P_-=P_-\mathcal{V}^{1/2}(\mathrm{id}-P_-)\mathcal{V}^{1/2}P_-=P_-\mathcal{V}P_--(P_-\mathcal{V}^{1/2}P_-)^2$, we can deduce from Lemma 5.2 that $P_-\mathcal{V}^{1/2}P_-^c\mathcal{V}^{1/2}P_-$ belongs to OpS^{-m-1}. Then it follows from (2.4) that $N(\mu<|\mathcal{H}_0-\lambda|^{-1/2}P_-\mathcal{V}^{1/2}P_-^c\mathcal{V}^{1/2}P_-|\mathcal{H}_0-\lambda|^{-1/2})=O(\mu^{-2/(m+1)})=o(\mu^{-2/(m+1)})$ as $\mu\downarrow 0$. This proves (5.12) since $\mathrm{Spec}(A^*A)\backslash\{0\}=\mathrm{Spec}(AA^*)\backslash\{0\}$.

The operator $P_-\mathcal{V}^{1/2}P_+$ belongs to $OpS^{-m/2-1}$ by Lemma 5.2 since $\Sigma_{l\in I_-}\oplus L^2(\mathbf{R})$ and $\Sigma_{l\in I_+}\oplus L^2(\mathbf{R})$ are orthogonal, and $P_+\mathcal{V}^{1/2}P_-\mathcal{V}^{1/2}P_+=(P_-\mathcal{V}^{1/2}P_+)^*(P_-\mathcal{V}^{1/2}P_+)$ belongs to OpS^{-m-2}. Then (2.4) proves (5.13).

By the definition of P_∞ and the min–max argument, we have

$$N(\mu<P_-\mathcal{V}^{1/2}P_\infty|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}P_-)\leqslant N((\Lambda^-_{N_0+1}-\lambda)_\mu<P_-\mathcal{V}P_-)\leqslant C(\Lambda^-_{N_0+1}-\lambda)^{-2/m}\mu^{-2/m},$$

where we used the fact that $P_-\mathcal{V}P_-\in OpS^{-m}$ and (2.4) in the last inequality. Since $\Lambda^-_{N_{0+1}}$ tends to infinity as $N_0\to\infty$, we have the conclusion. ■

Lemma 5.6: We have $\lim_{N_0\to\infty}\limsup_{\mu\downarrow 0}\mu^{2/m}N(\mu<\mathcal{V}^{1/2}P_\infty|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2})=0$.

Proof: If we choose $N_0>0$ so large that $\lambda\leqslant\Lambda^-_{N_0+1}/2$ holds, then $\Lambda_j(\eta)-\lambda\geqslant\lambda_j(\eta)-\Lambda^-_{N_0+1}/2\geqslant(\lambda_j(\eta)+\Lambda^-_{N_0+1})/4$ holds for any $j\geqslant N_0+1$ and for any $\eta\in\mathbf{R}$, from which we have $P_\infty|\mathcal{H}_0-\lambda|^{-1}\leqslant 4(\mathcal{H}_0+\Lambda^-_{N_0+1})^{-1}$. Then the variational principle yields the estimate $N(\mu<\mathcal{V}^{1/2}P_\infty|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2})\leqslant N(\mu<4\mathcal{V}^{1/2}(\mathcal{H}_0+\Lambda^-_{N_0+1})^{-1}\mathcal{V}^{1/2})=N(H_{4/\mu}(b)<-\Lambda_{N_0+1})=\Sigma_{l\in\mathbf{N}}\nu_l(-\Lambda^-_{N_0+1})(4/\mu)^{2/m}(1+o(1))$ as $\mu\downarrow 0$, where we used Theorem 1.1 proved in Sec. III in the last inequality. Finally, the lemma follows from the asymptotic relation $\lim_{N_0\to\infty}\Sigma_{l\in\mathbf{N}}\nu_l(-\Lambda^-_{N_0+1})=0$. ■

C. Proof of Theorem 1.1

Using the inequality $\mathcal{V}^{1/2}(\mathcal{H}_0-\lambda)^{-1}\mathcal{V}^{1/2}\leqslant\mathcal{V}^{1/2}P_-^c|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}$, we have, for any small $\varepsilon>0$,

$$\begin{aligned}N_g^+(\lambda)&\leqslant N(g^{-1}<\mathcal{V}^{1/2}P_-^c|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2})\leqslant N((1-\varepsilon)g^{-1}<\mathcal{V}^{1/2}P_+|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2})\\&\quad+N(\varepsilon g^{-1}<\mathcal{V}^{1/2}P_\infty|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}),\end{aligned}$$

where we used the (generalized) Birman–Schwinger principle [see, e.g., Alama, Deift, and Hempel (1989), Birman (1991)] and the Weyl–KyFan inequality. Then by Lemma 5.4 and Lemma 5.6, we obtain the upper bound $\limsup_{g\to\infty}g^{-2/m}N_g^+(\lambda)\leqslant\Sigma_{l\in I_+}\nu_l(\lambda)$, taking a limit $\varepsilon\downarrow 0$ and $N_0\to\infty$. Next, we obtain the lower bound. For any small $\varepsilon>0$, we have

$$\begin{aligned}P_-^c\mathcal{V}^{1/2}(\mathcal{H}_0-\lambda)^{-1}\mathcal{V}^{1/2}P_-^c&=P_-^c\mathcal{V}^{1/2}P_-(\mathcal{H}_0-\lambda)^{-1}\mathcal{V}^{1/2}P_-^c+P_-^c\mathcal{V}^{1/2}P_-^c(\mathcal{H}_0-\lambda)^{-1}\mathcal{V}^{1/2}P_-^c\\&\geqslant P_-^c\mathcal{V}^{1/2}P_-(\mathcal{H}_0-\lambda)^{-1}\mathcal{V}^{1/2}P_-^c+\mathcal{V}^{1/2}P_-^c(\mathcal{H}_0-\lambda)^{-1}\mathcal{V}^{1/2}\\&\quad-2\,\mathrm{Re}(P_-\mathcal{V}^{1/2}P_-^c(\mathcal{H}_0-\lambda)^{-1}\mathcal{V}^{1/2})\geqslant(1-\varepsilon)\mathcal{V}^{1/2}P_-^c|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}\\&\quad-P_-^c\mathcal{V}^{1/2}P_-|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}P_-^c-\varepsilon^{-1}P_-\mathcal{V}^{1/2}P_-^c|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}P_-,\end{aligned}$$

where we used the inequality $P_-\mathcal{V}^{1/2}P_-^c(\mathcal{H}_0-\lambda)^{-1}\mathcal{V}^{1/2}P_-\geqslant 0$ in the first inequality and used the estimate $2|(u,\mathcal{V}^{1/2}P_-^c(\mathcal{H}_0-\lambda)^{-1}\mathcal{V}^{1/2}P_-u)|\leqslant\varepsilon\||\mathcal{H}_0-\lambda|^{-1/2}P_-^c\mathcal{V}^{1/2}u\|^2+\varepsilon^{-1}\|P_-^c|\mathcal{H}_0-\lambda|^{-1/2}\mathcal{V}^{1/2}P_-u\|^2$ in

the second inequality. Then, by a variational argument similar to that used in the case of the upper bound, we can derive the lower bound $\liminf_{g\to\infty} g^{-2/m}N_g^+(\lambda)\geqslant\Sigma_{l\in I_+}\nu_l(\lambda)$, using Lemma 5.4 and Lemma 5.5. This completes the proof of Theorem 1.1.

D. Proof of Theorem 1.4

By the Birman–Schwinger principle, we have the upper bound

$$N_g^-(\lambda)=N(g^{-1}<-\mathcal{V}^{1/2}(\mathcal{H}_0-\lambda)^{-1}\mathcal{V}^{1/2})\leqslant N(g^{-1}<\mathcal{V}^{1/2}P_-|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2})$$
$$\leqslant\sum_{l\in I_-}\nu_l(\lambda)g^{-2/m}(1+o(1))$$

as $g\to\infty$, where we used the inequality $-\mathcal{V}^{1/2}(\mathcal{H}_0-\lambda)^{-1}\mathcal{V}^{1/2}=\mathcal{V}^{1/2}P_-|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}-\mathcal{V}^{1/2}P_-^c|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}\leqslant\mathcal{V}^{1/2}P_-|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}$ in the first inequality and used (5.10) in the last inequality. Next, for any small $\varepsilon>0$, there exists $C_\varepsilon>0$, independent of g,N_0, such that

$$\begin{aligned}N_g^-(\lambda)&\geqslant N(g^{-1}<-P_-\mathcal{V}^{1/2}(\mathcal{H}_0-\lambda)^{-1}\mathcal{V}^{1/2}P_-)\geqslant N((1+\varepsilon)g^{-1}<P_-\mathcal{V}^{1/2}P_-|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}P_-)\\&\quad-N(C_\varepsilon g^{-1}<P_-\mathcal{V}^{1/2}P_-^c|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}P_-)\geqslant N((1+\varepsilon)g^{-1}<P_-\mathcal{V}^{1/2}P_-|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}P_-)\\&\quad-N(C'_\varepsilon g^{-1}<P_-\mathcal{V}^{1/2}P_+|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}P_-)-N(C'_\varepsilon g^{-1}<P_-\mathcal{V}^{1/2}P_\infty|\mathcal{H}_0-\lambda|^{-1}\mathcal{V}^{1/2}P_-)\\&\geqslant\sum_{l\in I_-}\nu_l(\lambda)(g/(1+\varepsilon))^{2/m}(1+o(1))\end{aligned}$$

as $g,N_0\to\infty$, where we used the Weyl–KyFan inequality in the second and the third inequalities and Lemma 5.4 in the last line. This gives the lower bound and we complete the proof.

E. Proof of Theorem 1.5

Let $\Lambda_{n-1}^+<\lambda<\mu<\Lambda_n^-$. Set $\gamma=(\mu+\lambda)/2,\tau=(\mu-\lambda)/2$ and set $P_+^c=P_-+P_\infty$. Since $P_+(\mathcal{H}_g-\gamma)^2P_+=(P_+(\mathcal{H}_g-\gamma)P_+)^2-g^2P_+\mathcal{V}P_+^c\mathcal{V}P_+$, we have, for small $\varepsilon>0$, $N(\lambda\leqslant H_g(b)<\mu)\geqslant N((\mathcal{H}_g-\gamma)^2<\tau^2)\geqslant N(P_+(\mathcal{H}_g-\gamma)^2P_+<\tau^2)\geqslant N((P_+(\mathcal{H}_g-\gamma)P_+)^2<\tau^2-\varepsilon)-N(C_\varepsilon<g^2P_+\mathcal{V}P_+^c\mathcal{V}P_+)=N((P_+(\mathcal{H}_g-\gamma)P_+)^2<\tau^2-\varepsilon)+o(g^{2/m})$ as $g\to\infty$. Here, we used the fact that the operator $P_+\mathcal{V}P_+^c\mathcal{V}P_+=P_+\mathcal{V}^2P_+-(\underline{P_+\mathcal{V}P_+})^2$ is a matrix-valued ΨDO of the class OpS^{-2m-1}. Setting $\lambda_1=\gamma-\sqrt{\tau^2-\varepsilon}$ and $\mu_1=\gamma+\sqrt{\tau^2-\varepsilon}$, we have $N(\lambda_1<P_+\mathcal{H}_gP_+<\mu_1)\geqslant N(g^{-1}<\mathcal{V}^{1/2}P_+(\mathcal{H}_0-\mu_1)^{-1}P_+\mathcal{V}^{1/2})-N(g^{-1}<\mathcal{V}^{1/2}P_+(\mathcal{H}_0-\lambda_1)^{-1}P_+\mathcal{V}^{1/2})=\Sigma_{l\in I_+}\nu_l([\lambda_1,\mu_1])g^{2/m}(1+o(1))$ as $g\to\infty$, where we used the Birman–Schwinger principle and Theorem 1.1. Finally, we have Theorem 1.5 from these, letting $\varepsilon\downarrow 0$ and $N_0\to\infty$.

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Phase space properties and the short distance structure in quantum field theory

Henning Bostelmann[a)]
Universität Göttingen, Institut für Theoretische Physik, 37077 Göttingen, Germany

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The paper investigates relations between the phase space structure of a quantum field theory ("nuclearity") and the concept of pointlike localized fields. Given a net of local observable algebras, a phase space condition is introduced that allows a very detailed description of the theory's field content. An appendix discusses non-interacting models as examples. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Quantum fields are a basic ingredient of relativistic quantum physics. It is common to express almost all aspects of a theory, including the dynamics, in terms of these pointlike localized fields and related concepts (Lagrangians, field equations, path integrals). While this *ansatz* has proved to be very fruitful for the construction of models and in perturbation theory, it contains technical pitfalls which make its consistent handling rather difficult.

The main problem arises from Heisenberg's uncertainty relation, which says that measurements with sharp localization in configuration space are completely delocalized in momentum space, i.e., they show a singular high energy behavior. This is reflected in peculiar mathematical properties of quantum fields: They cannot be defined as operators, their products do not exist, and nonlinear field equations require subtle limiting processes which are difficult to control.

Thus, the concept of pointlike localized fields may be regarded as an over-idealization. Since it is well known that physical operations in finite space–time regions (rather than at points) do not show the singular behavior mentioned above, it seems worth while to study how pointlike fields emerge from such a physically more meaningful setting, and in that way to gain more information about the fields' properties.

A framework for such an investigation is provided by algebraic field theory,[1] where operations localized in an open space–time region $\mathcal{O}$ form an algebra $\mathfrak{A}(\mathcal{O})$ of bounded operators. It is possible to encode all physically relevant properties (locality, covariance, positivity of energy) in terms of these algebras and their transformation behavior under the Poincaré group, without reference to pointlike structures.

While it has extensively been discussed in the literature how to pass to the local algebras from a given field-theoretic model,[2] the reverse step is less well understood. Heuristically, pointlike fields $\phi(x)$ should be derived as limits of operations localized in regions shrinking to the point x.[3,4] However, the details of this limit depend on the high energy behavior of the fields. Following Fredenhagen and Hertel,[3] we will focus on fields satisfying *polynomial H-bounds*, i.e., fulfilling for some $\ell > 0$,

$$\|R^\ell \phi(x) R^\ell\| < \infty, \quad \text{where } R = (1+H)^{-1}; \tag{1.1}$$

H denotes the (positive) Hamiltonian. These H-bounds are satisfied in all models constructed so far, more generally in theories which satisfy a sharpened version of the Osterwalder–Schrader

a)Electronic mail: bostelm@theorie.physik.uni-goettingen.de

axioms.[5] It has been shown in Ref. 3 that fields of this kind can be recovered from the local algebras by means of the formula

$$R^\ell \phi(x) R^\ell \in \bigcap_{\mathcal{O} \ni x} \overline{R^\ell \mathfrak{A}(\mathcal{O}) R^\ell}^w, \tag{1.2}$$

where $\overline{}^w$ denotes the weak closure.[6] So one can calculate the field content of an algebraic theory; however, many details about the fields' properties remained unclear, e.g., the question whether the fields possess finite spin, or the existence of product expansions.

To gain more insight in this respect, we will make use of an additional property of quantum field theories, known as *phase space conditions*. These reflect the heuristic expectation that the number of local degrees of freedom of a physical system is limited: A system restricted both in momentum and configuration space, thus being localized in a finite phase space volume, will possess only a finite number of independent physical states. (This is easily understood by appealing to a semiclassical picture, such as Bohr–Sommerfeld quantization.) Clearly, the notion of a "finite phase space volume" must be handled with care; however, such properties can be formulated in a mathematically precise way in terms of *compactness* or *nuclearity* conditions,[7–9] which lead to interesting structural results on the system's physical behavior.[10] For the sake of concreteness, consider the following compactness condition:[11] Let $\mathcal{H}$ be the theory's underlying Hilbert space, Σ the set of weak-$*$-continuous functionals on $\mathfrak{B}(\mathcal{H})$ ("state space"), $P_H(E)$ the spectral projectors of H, and $\mathcal{O}_r$ the standard double cone of radius r centered at the origin. We require that for any E, $r>0$, the map

$$\Xi_{E,r}\colon P_H(E)\Sigma P_H(E) \to \mathfrak{A}(\mathcal{O}_r)_*, \tag{1.3}$$

$$\sigma \mapsto \sigma\restriction \mathfrak{A}(\mathcal{O}_r)$$

is compact, i.e., can be expanded into a series of rank-1 operators in the norm topology. This condition was verified explicitly in noninteracting models.[9]

The connection of these properties with the point field structure was first realized by Haag and Ojima:[12,13] Following the compactness condition mentioned above, the image of the map $\Xi_{E,r}$ is "almost finite-dimensional" (up to some degree of precision). If we assume that this finite-dimensional space does not change in the limit $r \to 0$ (which may be expected in theories that are dilation invariant in their short distance limit), then we have found finitely many independent states that represent the short distance structure of the theory, and one may hope to interpret a corresponding dual basis as pointlike localized quantum fields located at $x=0$.

The present paper aims at putting these heuristic ideas into a precise mathematical form. We introduce a phase space condition, specifically sensitive in the short distance limit, that selects a relevant class of models with "regular" short distance behavior. Its implications can be summarized as follows.

(1) The field content of these theories can be determined, with detailed results on the singular properties of the fields and their connection to the theory in finite regions. All fields can be shown to comply with the Wightman axioms; moreover, they transform covariantly both under unbroken and spontaneously broken symmetries.
(2) Operator product expansions[14] can be established rigorously with specific convergence properties, and allow for a model-independent, nonperturbative definition of normal products in the sense of Zimmermann.[15,16] The field content includes all composite fields.

In this paper, we shall restrict ourselves to the first named aspect; the latter point will be treated in another publication.[17] Section II introduces the phase space condition which lies at the root of our analysis. Using this condition, we construct the field content of the algebraic theory in Sec. III, while symmetry aspects and the proof of Wightman's axioms are discussed in Sec. IV. We end with a brief outlook on generalizations in Sec. V. In the Appendix, we show that the phase space condition is fulfilled in models from free field theory.

The present paper is based on the author's thesis.[18] It presents an abbreviated and somewhat simplified version of material developed there; for further details and additional technical and mathematical aspects, the reader is referred to the original work.

II. A PHASE SPACE CONDITION

This section will introduce the specific phase space condition which characterizes the short distance structure of a quantum field theory. First of all, we shall briefly define our mathematical setting.

We use the framework of local quantum physics.[1] Our field-theoretic model is given by means of a net $\mathcal{O}\mapsto\mathfrak{A}(\mathcal{O})$, which associates with any open space–time region $\mathcal{O}\subset\mathbb{R}^{s+1}$ a von Neumann algebra $\mathfrak{A}(\mathcal{O})\subset\mathfrak{B}(\mathcal{H})$, where $\mathcal{H}$ is some fixed Hilbert space. We assume isotony and locality. In most cases, it will suffice to consider the algebras $\mathfrak{A}(r):=\mathfrak{A}(\mathcal{O}_r)$ associated with standard double cones $\mathcal{O}_r$ of radius r centered at the origin. We will restrict our attention to the vacuum sector; i.e., we assume a strongly continuous unitary representation $U(x,\Lambda)$ of the connected Poincaré group on $\mathcal{H}$ that has a geometric action on the net $\mathfrak{A}$ (*covariance*), and a vector $\Omega\in\mathcal{H}$ (the *vacuum*), unique up to a phase, which is invariant under all $U(x,\Lambda)$. For the translation part of this representation, $U(x)=\exp(iP_\mu x^\mu)$, we will assume the *spectrum condition*, i.e., the joint spectrum of its generators P_μ falls into the closed forward light cone $\overline{\mathcal{V}_+}$; here $H=P_0\geqslant 0$ is the Hamiltonian. We also require the net $\mathfrak{A}$ to act *irreducibly* on $\mathcal{H}$, in the sense that $\cup_{\mathcal{O}}\mathfrak{A}(\mathcal{O})\Omega$ is dense in $\mathcal{H}$, where the union runs over bounded regions $\mathcal{O}$ only. $\Sigma:=\mathfrak{B}(\mathcal{H})_*$ is the set of weak-$*$-continuous functionals on $\mathfrak{B}(\mathcal{H})$, the positive normed elements of which represent the physical states. Both $\mathfrak{B}(\mathcal{H})$ and Σ will be considered with their norm topology unless otherwise noted.

In analogy to Ref. 3, we will often use the space of polynomially energy-damped functionals,

$$\mathcal{C}^\infty(\Sigma):=\bigcap_{\ell>0}R^\ell\Sigma R^\ell\subset\Sigma, \tag{2.1}$$

where $R=(1+H)^{-1}$ as before. On this space, we define the norms $\|\sigma\|^{(\ell)}:=\|R^{-\ell}\sigma R^{-\ell}\|$ $(\ell>0)$, and equip $\mathcal{C}^\infty(\Sigma)$ with the locally convex (metrizable) topology of simultaneous convergence with respect to all these norms. As is easily seen, a linear map φ from $\mathcal{C}^\infty(\Sigma)$ to some Banach space $(\mathcal{E},\|\cdot\|_{\mathcal{E}})$ is continuous with respect to this topology if and only if

$$\|\varphi\|^{(\ell)}:=\sup_\sigma\frac{\|\varphi(\sigma)\|_\mathcal{E}}{\|\sigma\|^{(\ell)}}<\infty\quad\text{for some }\ell>0. \tag{2.2}$$

We set $\Psi:=\mathcal{L}(\mathcal{C}^\infty(\Sigma),\Sigma)$, the space of continuous linear maps between these spaces. A prominent element of Ψ is the inclusion

$$\Xi:\mathcal{C}^\infty(\Sigma)\to\Sigma,$$

$$\sigma\mapsto\sigma, \tag{2.3}$$

which bears some analogy with (1.3). A map $\psi\in\Psi$ of finite rank has the form

$$\psi=\sum_{j=1}^{J}\sigma_j\phi_j\quad\text{with }\sigma_j\in\Sigma\quad\text{and }\phi_j\in\mathcal{C}^\infty(\Sigma)^*. \tag{2.4}$$

(This means that the ϕ_j are linear forms with $\|\phi_j\|^{(\ell)}=\|R^\ell\phi_jR^\ell\|<\infty$ for large ℓ.)

For our purposes, it will be critical to control the behavior of the objects mentioned above in the short distance limit. To achieve this, we introduce some additional structure. For $\sigma\in\Sigma$, we define

$$\|\sigma\|_r:=\|\sigma\lceil\mathfrak{A}(r)\|\quad(r>0). \tag{2.5}$$

Likewise, for $\psi\in\Psi$ we consider

$$\|\psi\|_r^{(\ell)} := \|\psi(\cdot)\lceil\mathfrak{A}(r)\|^{(\ell)} = \sup_{\sigma\in\Sigma}\sup_{A\in\mathfrak{A}(r)}\frac{|\psi(R^\ell\sigma R^\ell)(A)|}{\|\sigma\|\,\|A\|}, \tag{2.6}$$

which is finite for sufficiently large ℓ. We devote special attention to the question how fast such a seminorm $\|\cdot\|_r^{(\ell)}$ vanishes in the limit $r\to 0$, and therefore define for $\gamma\geqslant 0$,

$$\delta_\gamma(\psi) := \begin{cases} 0 & \text{if } r^{-\gamma}\|\psi\|_r^{(\ell)} \xrightarrow[r\to 0]{} 0 \quad \text{for some } \ell > 0, \\ 1 & \text{otherwise.} \end{cases} \tag{2.7}$$

Each δ_γ induces a pseudometric on Ψ. Equipping Ψ with the pseudometric

$$\hat{\delta}(\psi,\psi') := \int_0^\infty e^{-\gamma}\delta_\gamma(\psi-\psi')\mathrm{d}\gamma, \tag{2.8}$$

we have found a topology on Ψ which describes short-distance convergence "to all polynomial orders."

[Note that Ψ is a presheaf over $\mathbb{R}^{s+1}$ with respect to $\Psi(\mathcal{O}) := \Psi\lceil\mathfrak{A}(\mathcal{O})$, and that the δ_γ are not so much functions on Ψ, but rather on the stalk of Ψ at $x=0$; so we have defined a topology on the stalk. However, we shall not consider these sheaf-theoretic aspects any further.]

We can now turn to formulating the approximation of Ξ with operators of finite rank. We start with a net $\mathcal{O}\mapsto\mathfrak{A}(\mathcal{O})$ that meets the standard requirements listed at the beginning of this section. We can analyze the short distance behavior of the theory with the help of the concepts introduced above by considering the numbers

$$N_\gamma := \min\{n \mid \exists\, \psi\in\Psi\text{: rank } \psi = n,\ \delta_\gamma(\Xi-\psi)=0\}, \tag{2.9}$$

setting $N_\gamma=\infty$ if the set on the right-hand side is empty. It is obvious that $N_\gamma\geqslant N_{\gamma'}$ for $\gamma\geqslant\gamma'$. Thus, our theory falls into one out of the following three classes:

(1) $N_\gamma\to\infty$ for $\gamma\to\infty$, but $N_\gamma<\infty$ for all $\gamma\geqslant 0$. We shall show in the subsequent sections that the theory then has a nontrivial field content of Wightman fields. As will be discussed in the Appendix, a large variety of free field theories falls into this class; one may expect that physically relevant interacting models exhibit the same behavior.

(2) $N_\gamma\leqslant N$ for some fixed $N<\infty$ and all $\gamma\geqslant 0$. In this case, only very few observables "survive" in the short distance limit. In fact, we shall see that in this case necessarily $N_\gamma=1$ for all γ, and that the theory's field content is trivial. An example for this behavior was discussed by Lutz;[19] cf. also the Appendix. More generally, one expects that models of this kind are *not* generated by pointlike fields, but possibly by other, nonpointlike objects, such as Mandelstam strings or Wilson loops.

(3) $N_\gamma=\infty$ for some finite $\gamma\geqslant 0$. Such theories have a peculiar complex short distance behavior which does not allow Ξ to be approximated by maps of finite rank in the specified sense. Examples are free theories with infinitely many species of particles. One also expects that theories in $1+1$ dimensions, where the fields as well as their Wick products have a "scaling dimension" of 0, are members of this class.

In what follows, we will disregard the latter case and assume that N_γ is finite for all γ. We may encode this into a phase space criterion which selects theories of a sufficiently regular short distance behavior.

Definition 2.1: A net $\mathcal{O}\mapsto\mathfrak{A}(\mathcal{O})$ is said to satisfy the microscopic phase space condition *if for every $\gamma\geqslant 0$, there exists a map $\psi\in\Psi$ of finite rank such that*

$$\delta_\gamma(\Xi-\psi)=0,$$

or, equivalently,

$$r^{-\gamma}\|\Xi - \psi\|_r^{(\ell)} \to 0 \quad \textit{for sufficiently large } \ell > 0.$$

This condition shows a formal analogy with the well-known compactness and nuclearity conditions in finite regions:[8,9] It demands that the map Ξ can be expanded into a series of rank-1 operators, where the series is meant to converge in the pseudometric $\hat{\delta}$ introduced in Eq. (2.8).

Our task will be to analyze the consequences of the microscopic phase space condition, especially regarding the theory's point field structure. We will show that the size of the field content is determined by the "approximation numbers" N_γ, and prove that these fields fulfill certain regularity properties.

III. DETERMINING THE FIELD CONTENT

We will now set out from a net $\mathcal{O} \mapsto \mathfrak{A}(\mathcal{O})$ that satisfies the microscopic phase space condition. Our task is to analyze the point field content of this net. Our line of analysis can be sketched as follows.

Given $\gamma \geqslant 0$, let $\psi \in \Psi$ be a map of finite rank that approximates Ξ in the short distance limit: $\delta_\gamma(\Xi - \psi) = 0$. Provided that rank ψ is minimal with this property (i.e., ψ does not contain redundant terms that do not contribute to the approximation), one will expect that the image of the dual map $\psi^* : \mathfrak{B}(\mathcal{H}) \to \mathcal{C}^\infty(\Sigma)^*$ consists of pointlike fields. [Note that img ψ^* is spanned by the linear forms ϕ_j in Eq. (2.4).] In fact, we will show that $\Phi_\gamma := \text{img } \psi^*$ depends on γ only, and that its elements are indeed localized fields. Furthermore, we will prove that the union of the spaces Φ_γ exhausts the field content as defined by Fredenhagen and Hertel.[3]

Let $\gamma \geqslant 0$ be fixed in the following. We begin our analysis of the map ψ with the following lemma.

Lemma 3.1: Let $\psi \in \Psi$ *such that* rank $\psi = N_\gamma$ *and* $\delta_\gamma(\Xi - \psi) = 0$. *Then it holds for all* $\sigma \in \text{img } \psi \backslash \{0\}$ *that*

$$r^{-\gamma}\|\sigma\|_r \not\to 0 \quad (r \to 0).$$

Proof: Assume that the proposition is violated for some $\sigma \in \text{img } \psi \backslash \{0\}$. We choose a decomposition $\psi = \psi' \oplus \sigma\phi$, where $\phi \in \mathcal{C}^\infty(\Sigma)^*$, $\psi' \in \Psi$, and rank $\psi' = N_\gamma - 1$. Since $r^{-\gamma}\|\sigma\|_r \to 0$ and $\|\phi\|^{(\ell)} < \infty$ for large ℓ, we obviously have $\delta_\gamma(\sigma\phi) = 0$ and thus $\delta_\gamma(\Xi - \psi') = 0$, in contradiction to the minimality property of N_γ [cf. Eq. (2.9)]. □

Certainly, ψ is not fixed uniquely by the conditions of Lemma 3.1. However, we shall show that these conditions fix img ψ^*. To this end, we prove the following.

Lemma 3.2: Let ψ *be as in Lemma 3.1. For arbitrary* $\sigma \in \mathcal{C}^\infty(\Sigma)$, *the following equivalences hold*:

$$\sigma[\text{img } \psi^* = 0 \;\Leftrightarrow\; \psi(\sigma) = 0 \;\Leftrightarrow\; r^{-\gamma}\|\sigma\|_r \to 0.$$

Proof: The first equivalence is obvious. Moreover, for $\sigma \neq 0$, the approximation property $\delta_\gamma(\Xi - \psi) = 0$ gives $r^{-\gamma}\|(\Xi - \psi)(\sigma)\|_r = r^{-\gamma}\|\sigma - \psi(\sigma)\|_r \to 0$. So $\psi(\sigma) = 0$ implies $r^{-\gamma}\|\sigma\|_r \to 0$. Conversely, if $r^{-\gamma}\|\sigma\|_r \to 0$, we conclude $r^{-\gamma}\|\psi(\sigma)\|_r \to 0$, and thus $\psi(\sigma) = 0$ according to Lemma 3.1.□

Since the right-hand side of the equivalence in Lemma 3.2 does not refer to ψ, the space img ψ^* is independent of ψ as well. Thus, we have established the following.

Theorem 3.3: *Let the net* $\mathfrak{A}$ *fulfill the microscopic phase space condition. For each* $\gamma \geqslant 0$, *there is a unique subspace* $\Phi_\gamma \subset \mathcal{C}^\infty(\Sigma)^*$ *of dimension* N_γ *with the following property: If* $\psi \in \Psi$, rank $\psi = N_\gamma$, *and* $\delta_\gamma(\Xi - \psi) = 0$, *then* img $\psi^* = \Phi_\gamma$.

Note that the microscopic phase space condition guarantees such a ψ to exist for every γ. The theorem requires the rank of ψ to be "minimized" (rank $\psi = N_\gamma$). If rank $\psi > N_\gamma$, we can still find a representation

$$\psi = \psi_{\text{I}} \oplus \psi_{\text{II}},$$

$$\text{where} \quad \operatorname{img} \psi_{\mathrm{I}}^{*} = \Phi_{\gamma}, \quad r^{-\gamma}\|\sigma\|_r \to 0 \;\forall\; \sigma \in \operatorname{img} \psi_{\mathrm{II}}. \tag{3.1}$$

[To see this, choose a map ψ_{I} of rank N_γ such that $\delta_\gamma(\Xi - \psi_{\mathrm{I}}) = 0$, and set $\psi_{\mathrm{II}} := \psi - \psi_{\mathrm{I}}$. It follows that $\delta_\gamma(\psi_{\mathrm{II}}) = 0$, so $r^{-\gamma}\|\sigma\|_r \to 0$ for all $\sigma \in \operatorname{img} \psi_{\mathrm{II}}$. Since Lemma 3.1 applies to ψ_{I}, the intersection of img ψ_{I} with img ψ_{II} is trivial; thus $\psi = \psi_{\mathrm{I}} + \psi_{\mathrm{II}}$ is a direct sum.] As a consequence hereof, and since $\delta_\gamma(\cdot) \leqslant \delta_{\gamma'}(\cdot)$ for $\gamma \leqslant \gamma'$, we obviously have $\Phi_\gamma \subset \Phi_{\gamma'}$—the Φ_γ form an increasing sequence of vector spaces.

We will show now that the elements of Φ_γ are Wightman fields. To this end, we will approximate $\phi \in \Phi_\gamma$ with a sequence of bounded operators localized in smaller and smaller regions. Our aim is the following proposition.

Proposition 3.4: Let $\phi \in \Phi_\gamma$. One can find a sequence of operators $A_r \in \mathfrak{A}(r)$ $(r > 0)$ such that

$$\|\phi - A_r\|^{(\ell)} \to 0 \quad \textit{for some } \ell > 0$$

(*more precisely* $\|\phi - \Xi^* A_r\|^{(\ell)} \to 0$).

We will carry out—or rather sketch—the proof in four steps. We choose $\psi \in \Psi$ of rank N_γ such that $\delta_\gamma(\Xi - \Psi) = 0$ and set $S := \operatorname{img} \psi$.

(a) First, consider the case of a rank-1 operator $\psi = \sigma\phi$. According to Lemma 3.1, we may choose a null sequence ρ such that $\|\sigma\|_r \geqslant c \cdot r^\gamma$ for some $c > 0$, where $r \in \rho$. For $r \in \rho$, we define A_r as a linear form on the one-dimensional subspace of $\mathfrak{A}(r)_*$ spanned by $\sigma\lceil\mathfrak{A}(r)$, namely by setting $\sigma(A_r) = 1$. We can then apply the Hahn–Banach theorem to continue this form to an operator $A_r \in \mathfrak{A}(r) = (\mathfrak{A}(r)_*)^*$; its norm is bounded by $\|A_r\| \leqslant (\|\sigma\|_r)^{-1} \leqslant c^{-1} r^{-\gamma}$. We must show that $\|\phi - \Xi^* A_r\|^{(\ell)} \to 0$: This follows from

$$\|\phi - \Xi^* A_r\|^{(\ell)} = \|\psi^* A_r - \Xi^* A_r\|^{(\ell)} \leqslant \|\psi - \Xi\|_r^{(\ell)} \|A_r\| \leqslant c^{-1} r^{-\gamma} \|\psi - \Xi\|_r^{(\ell)} \to 0 \tag{3.2}$$

for large ℓ and for $r \in \rho$. Thus $A_r \to \phi$ on ρ, and we may easily find suitable A_r for any $r > 0$ by choosing A_r to be "piecewise constant."

(b) Now let $\dim S > 1$, but let all $\sigma \in S$ have "the same short distance behavior," i.e., we assume that a function $\eta : \mathbb{R}^+ \to \mathbb{R}^+$ exists such that

$$c_1(\sigma)\,\eta(r) \geqslant \|\sigma\|_r \geqslant c_2(\sigma)\,\eta(r) \quad \text{for all } r \in \rho, \sigma \in S, \tag{3.3}$$

where ρ is some fixed null sequence, and c_1, c_2 are positive constants depending on σ. We also assume $\eta(r) \geqslant r^\gamma$ for $r \in \rho$. It is easily seen that c_1, c_2 can be chosen to be locally uniform in S, and thus we can choose them uniformly on the unit sphere of S (with respect to some fixed norm $\|\cdot\|_S$, independent of r). We can find constants $c_1', c_2' > 0$ such that

$$c_1'\,\eta(r)\|\sigma\|_S \geqslant \|\sigma\|_r \geqslant c_2'\,\eta(r)\|\sigma\|_S \quad \text{for all } r \in \rho, \sigma \in S. \tag{3.4}$$

Now let $\phi \in \Phi_\gamma$, and write $\psi = \sigma_0\phi \oplus \psi'$ with some fixed $\sigma_0 \in S$ and rank $\psi' = N_\gamma - 1$. Again, we define A_r $(r \in \rho)$ as a linear form on $S\lceil\mathfrak{A}(r)$ by

$$\sigma_0(A_r) = 1, \quad A_r\lceil\operatorname{img} \psi' = 0, \tag{3.5}$$

thus achieving $\psi^* A_r = \phi$. The norm of A_r can be estimated as

$$\|A_r\lceil S\| = \sup_{\sigma \in S} \frac{|\sigma(A_r)|}{\|\sigma\|_r} \leqslant \frac{\|A_r\|_S}{c_2'\,\eta(r)} \leqslant \frac{c_3}{\eta(r)} \quad (r \in \rho) \tag{3.6}$$

with some constant $c_3 > 0$. We may now extend A_r to an element of $\mathfrak{A}(r)$ and establish convergence using the methods outlined in (a).

(c) More generally, let us assume that S has the structure

$$S = S_1 \oplus \cdots \oplus S_k \tag{3.7}$$

with finite-dimensional spaces S_j which fulfill conditions of the type (3.3) with respect to functions $\eta_j(r)$ and a common null sequence ρ; moreover, we require $\eta_{j+1}(r)/\eta_j(r) \to 0$ and $\eta_k(r) \geqslant r^\gamma$ on ρ.

[For example, this is the situation met in free field theory, where the functions $\eta_j(r)$ are powers of r, and ρ is arbitrary.] We write $\psi=\psi_1\oplus\cdots\oplus\psi_k$ with respect to the direct sum (3.7), and prove the proposition for $\phi\in\mathrm{img}\,\psi_j^*$ by induction on j. Let the statement be true for all $j'<j$ in place of j (we include the case $j=1$ here). For $\phi\in\mathrm{img}\,\psi_j^*$, define A_r $(r\in\rho)$ as a linear form on S_j by $\psi_j^*A_r=\phi$; as in (b), we have $\|A_r\lceil S_j\|\leqslant c/\eta_j(r)$ with some constant $c>0$, and thus we can extend A_r to an element of $\mathfrak{A}(r)$ with the same bounds on its norm. Now observe that for ℓ sufficiently large,

$$\|\phi-\Xi^*A_r+\sum_{m=1}^{j-1}\psi_m^*A_r\|^{(\ell)}\leqslant\|\psi^*A_r-\Xi^*A_r\|^{(\ell)}+\sum_{m=j+1}^{k}\|\psi_m^*A_r\|^{(\ell)}\leqslant\|\psi-\Xi\|_r^{(\ell)}\|A_r\|+\sum_{m=j+1}^{k}\|\psi_m\|_r^{(\ell)}\|A_r\|$$

$$\leqslant\|\psi-\Xi\|_r^{(\ell)}\frac{c}{\eta_j(r)}+\sum_{m=j+1}^{k}\frac{\eta_m(r)}{\eta_j(r)}\cdot\mathrm{const}\to 0\quad(r\in\rho).\tag{3.8}$$

Thus we conclude by induction,

$$\phi\in\overline{\mathfrak{A}(r)+\bigoplus_{m=1}^{j-1}\mathrm{img}\,\psi_m^*}\subset\overline{\mathfrak{A}(r)+\mathfrak{A}(r)}=\overline{\mathfrak{A}(r)}\quad\text{for any } r>0,\tag{3.9}$$

where the bar denotes closure with respect to $\|\cdot\|^{(\ell)}$.

(d) In the general case, the short distance behavior within S may be more complicated than assumed above, and possibly depend crucially on the choice of ρ. Let ρ be any fixed null sequence. Instead of considering $\delta_\gamma(\cdot)$, we introduce a weaker pseudometric $\delta_\gamma^\rho(\cdot)$ defined as in Eq. (2.7), but restricting convergence to $r\in\rho$. The results established so far for $\delta_\gamma(\cdot)$ and Φ_γ hold in an analogous way for $\delta_\gamma^\rho(\cdot)$ and corresponding spaces $\Phi_\gamma^\rho\subset\Phi_\gamma$. If $\rho'\subset\rho$ is a subsequence, then $\Phi_\gamma^{\rho'}\subset\Phi_\gamma^\rho$; in case equality holds here for all subsequences ρ', we will call ρ a *stable* sequence. Let ρ fulfill this condition, and choose rank ψ' minimal such that $\delta_\gamma^\rho(\Xi-\psi')=0$. By passing to subsequences of ρ, we can step by step enforce an "ordering" in the short distance behavior of the elements of $\mathrm{img}\,\psi'$, and arrive at a situation as outlined in (c). Since ρ is stable, passing to subsequences does not affect the approximation property of ψ'; so we can use the methods developed in (c) to establish the proposition for $\phi\in\mathrm{img}\,\psi'^*=\Phi_\gamma^\rho$.

It remains to verify that $\cup_\rho\Phi_\gamma^\rho$ spans all of Φ_γ, where the union runs over all stable sequences ρ. To accomplish this, assume that $\Phi_{\mathrm{st}}:=\mathrm{span}(\cup_\rho\Phi_\gamma^\rho)$ is a proper subspace of Φ_γ. Choose $\phi\in\Phi_\gamma\backslash\Phi_{\mathrm{st}}$ and appropriate $\sigma_0\in\Sigma$, $\psi_{\mathrm{st}}\in\Psi$ such that

$$\psi=\psi_{\mathrm{st}}\oplus\sigma_0\phi,\quad\mathrm{img}\,\psi_{\mathrm{st}}^*\supset\Phi_{\mathrm{st}}.\tag{3.10}$$

According to Lemma 3.1, we may choose ρ such that $\|\sigma_0\|_r\geqslant r^\gamma\cdot\mathrm{const}$ for $r\in\rho$, where we may take ρ to be stable, possibly replacing it by a subsequence. In analogy with (3.1), we split up ψ as

$$\psi=\psi_{\mathrm{I}}\oplus\psi_{\mathrm{II}},$$

$$\text{where } \mathrm{img}\,\psi_{\mathrm{I}}^*=\Phi_\gamma^\rho,\quad r^{-\gamma}\|\sigma\|_r\underset{\rho}{\to}0\ \forall\,\sigma\in\mathrm{img}\,\psi_{\mathrm{II}}.\tag{3.11}$$

But since $\Phi_\gamma^\rho\subset\Phi_{\mathrm{st}}$, it follows from Eqs. (3.10) and (3.11) that $\sigma_0\in\mathrm{img}\,\psi_{\mathrm{II}}$; thus $r^{-\gamma}\|\sigma_0\|_r\to 0$ on ρ, which gives us a contradiction. This completes the proof. □

Having verified Proposition 3.4, we may now apply the results of Fredenhagen and Hertel,[3] who considered (when expressed in our notation) the following set of linear forms:

$$\Phi_{\mathrm{FH}}:=\{\phi\in\mathcal{C}^\infty(\Sigma)^*\,|\,R^\ell\phi R^\ell\in\bigcap_{r>0}\overline{R^\ell\mathfrak{A}(r)R^\ell}^w\ \text{for some } \ell>0\},\tag{3.12}$$

where $-^w$ denotes the weak closure. Φ_{FH} can be interpreted as the theory's field content. The authors showed that any $\phi\in\Phi_{\mathrm{FH}}$ is a local field associated with the net $\mathfrak{A}$; more precisely,

$$f \mapsto \phi(f) = \int f(x) U(x) \phi U(x)^* d^{s+1}x \tag{3.13}$$

can be extended to an operator valued tempered distribution on the domain $\mathcal{C}^\infty(\mathcal{H}) = \cap_{\ell>0} R^\ell \mathcal{H}$, which is local and relatively local; $\phi(f)$ is closable, and its closure $\phi(f)^-$ is affiliated with the local algebras,

$$\phi(f)^- \eta \mathfrak{A}(\mathcal{O}) \quad \text{if supp } f \subset \mathcal{O}. \tag{3.14}$$

In particular, these statements apply to the fields constructed here, since Proposition 3.4 shows that $\Phi_\gamma \subset \Phi_{\mathrm{FH}}$ for any $\gamma \geqslant 0$. In fact, we will show that our spaces Φ_γ exhaust Φ_{FH}. To this end, we first derive improved approximation properties for the fields $\phi \in \Phi_{\mathrm{FH}}$.

Lemma 3.5: Let $\phi \in \Phi_{\mathrm{FH}}$. One can find constants $\ell > 0$, $k > 0$ and operators $A_r \in \mathfrak{A}(r)$ for each $r > 0$ such that

$$\|A_r - \phi\|^{(\ell)} = O(r), \quad \|A_r\| = O(r^{-k}).$$

Proof: We choose a test function $f \in \mathcal{S}(\mathbb{R}^{s+1})$ with $f \geqslant 0$, $\int f(x) d^{s+1}x = 1$, supp $f \subset \mathcal{O}_{r=1}$, and set $f_r := r^{-(s+1)} f(r^{-1}x)$. Now let r be fixed, and let $\phi(f_r)^- = V_r D_r$ be the polar decomposition of this operator, where V_r is a partial isometry, and D_r is self-adjoint. Since $\phi(f_r)^- \eta \mathfrak{A}(r)$, both V_r and all bounded functions of D_r belong to $\mathfrak{A}(r)$.[20] Let ℓ be sufficiently large such that $\|\phi\|^{(\ell)} < \infty$; for $\epsilon > 0$, set

$$A_{r,\epsilon} := \epsilon^{-1} V_r \sin(\epsilon D_r) \in \mathfrak{A}(r). \tag{3.15}$$

Using the inequality

$$(x - \epsilon^{-1} \sin \epsilon x)^2 \leqslant \epsilon^2 x^4 \quad \forall\, x \geqslant 0,\ \epsilon > 0, \tag{3.16}$$

we can establish the estimate

$$\|(A_{r,\epsilon} - \phi(f_r)) R^{4\ell}\|^2 \leqslant \|(\epsilon^{-1} \sin(\epsilon D_r) - D_r) R^{4\ell}\|^2 \leqslant \epsilon^2 \|D_r^2 R^{4\ell}\|^2 = \epsilon^2 \|\phi(f_r)^* \phi(f_r) R^{4\ell}\|^2. \tag{3.17}$$

By repeated use of the relation

$$[R, \phi(f_r)] = -iR\phi(\partial_0 f_r)R \tag{3.18}$$

[compare Eq. (2.4) in Ref. 3] and of the bound $\|\phi(g)\|^{(\ell)} \leqslant \int |g(x)| d^{s+1}x \cdot \text{const}$, we can establish

$$\|\phi(f_r)^* \phi(f_r) R^{4\ell}\| \leqslant r^{-4\ell} c \tag{3.19}$$

with some constant $c > 0$ independent of r. Applying Eq. (3.17), that yields

$$\|A_{r,\epsilon} - \phi(f_r)\|^{(4\ell)} \leqslant \epsilon r^{-4\ell} c. \tag{3.20}$$

Using the integral representation of $\phi(f_r)$ and the spectral properties of the translation operators, one also verifies that

$$\|\phi(f_r) - \phi\|^{(\ell+1)} = O(r). \tag{3.21}$$

Choosing now $A_r := A_{r,\epsilon}$ with $\epsilon = r^{4\ell+1}$, we can combine (3.20) and (3.21) to show

$$\|\phi - A_r\|^{(4\ell+1)} = O(r), \tag{3.22}$$

which proves the lemma, since the required bounds on $\|A_r\|$ are obvious. □

Remarks: Certainly, ℓ and k can be chosen uniformly on any finite-dimensional subspace of Φ_{FH}. Furthermore, by again smearing $A_{r,\epsilon}$ with f_r and rescaling, we may assume that A_r is of the form $\hat{A}_r(f_r)$.

We are now in the position to prove that the Φ_γ exhaust Φ_{FH}. To this end, let $\phi \in \Phi_{\mathrm{FH}}$. Choose a sequence A_r as in Lemma 3.5, and fix γ such that $\|A_r\| = O(r^{-\gamma})$. We will show that $\phi \in \Phi_\gamma$: Choosing $\psi \in \Psi$, $\ell > 0$ such that img $\psi^* = \Phi_\gamma$ and $r^{-\gamma}\|\Xi - \psi\|_r^{(\ell)} \to 0$, we can achieve

$$\|\Xi^* A_r - \psi^* A_r\|^{(\ell)} \to 0. \tag{3.23}$$

Since $\|\Xi^* A_r - \phi\|^{(\ell)} \to 0$ by construction (if ℓ is sufficiently large), this means

$$\psi^* A_r \underset{r\to 0}{\to} \phi \quad \text{with respect to } \|\cdot\|^{(\ell)}. \tag{3.24}$$

Note that the left-hand side of Eq. (3.24) does not leave the finite-dimensional space Φ_γ, which is closed; thus $\phi \in \Phi_\gamma$. We have shown the following.

Theorem 3.6: *If the net* $\mathfrak{A}$ *satisfies the microscopic phase space condition, then*

$$\Phi_{\mathrm{FH}} = \bigcup_{\gamma \geqslant 0} \Phi_\gamma.$$

According to the results in Ref. 3, this means that our construction describes all local fields affiliated with the net and satisfying polynomial *H*-bounds.

IV. SYMMETRY ASPECTS

In this section, we will investigate the action of symmetry transformations on the pointlike fields we have constructed, and eventually show that these fields satisfy the Wightman axioms.

First, we will revisit the structure connected with the spaces Φ_γ of local fields. Given $\gamma \geqslant 0$, we choose a map $\psi \in \Psi$ of rank N_γ such that $\delta_\gamma(\Xi - \psi) = 0$; then img $\psi^* = \Phi_\gamma$. We can define the finite-dimensional space

$$\Sigma_\gamma := \mathcal{C}^\infty(\Sigma)/\ker \psi; \tag{4.1}$$

by virtue of Lemma 3.2, this definition is independent of ψ. In a natural way, we have $\Sigma_\gamma^* = \Phi_\gamma$, and denoting the canonical projection onto Σ_γ by p_γ, its dual map p_γ^* is just the inclusion $\Phi_\gamma \hookrightarrow \mathcal{C}^\infty(\Sigma)^*$. In summary, we get the following diagram, where dashed lines connect pairs of dual spaces:

$$\begin{array}{ccc} \mathcal{C}^\infty(\Sigma) & \xrightarrow{\;p_\gamma\;} & \Sigma_\gamma \\ \vdots & & \vdots \\ \mathcal{C}^\infty(\Sigma)^* & \xleftarrow[\;p_\gamma^*\;]{} & \Phi_\gamma \end{array} \tag{4.2}$$

The elements of Σ_γ correspond to "germs of states" as described by Haag and Ojima.[13]

The phase space approximation "$\Xi \approx \psi$" can be introduced into this scheme in a simple way: Let $p: \mathcal{C}^\infty(\Sigma)^* \to \mathcal{C}^\infty(\Sigma)^*$ be an arbitrary projection onto Φ_γ, continuous with respect to the weak topology on $\mathcal{C}^\infty(\Sigma)^*$. Then the predual map p_* exists, and since Φ_γ is finite dimensional, we have

$$\|p_*\|^{(\ell)} = \sup_{\sigma \in \mathcal{C}^\infty(\Sigma)} \frac{\|p_*\sigma\|^{(\ell)}}{\|\sigma\|^{(\ell)}} < \infty \tag{4.3}$$

for large ℓ. This implies

$$\|\Xi p_* - \Xi\|_r^{(\ell)} \leqslant \|(\Xi - \psi)p_*\|_r^{(\ell)} + \|\Xi - \psi p_*\|_r^{(\ell)} \leqslant \|\Xi - \psi\|_r^{(\ell)} \|p_*\|^{(\ell)} + \|\Xi - \psi\|_r^{(\ell)} = o(r^\gamma), \tag{4.4}$$

so we can express the approximation by $\delta_\gamma(\Xi p_* - \Xi) = 0$, without referring to a specific map ψ.

Now we will turn to the investigation of symmetry operations. The action of such symmetries (e.g., Lorentz transformations) is usually given on $\mathfrak{B}(\mathcal{H})$, and by virtue of diagram (4.2) we will transfer this action to the spaces Φ_γ. First of all, let us define the class of "admissible transformations" that we will consider.

Definition 4.1: Let $U \in \mathfrak{B}(\mathcal{H})$ be a unitary. The transformation $\alpha = \mathrm{ad}\, U : \mathfrak{B}(\mathcal{H}) \to \mathfrak{B}(\mathcal{H})$ is called a microscopic symmetry *if the following two conditions hold:*

(1) *For every $\ell > 0$, there is an $\ell' > 0$ such that $\|R^{-\ell} U R^{\ell'}\| < \infty$.*
(2) *There are constants $c, R > 0$ such that $\alpha\mathfrak{A}(r) \subset \mathfrak{A}(c \cdot r)\ \forall\, r \in (0, R)$.*

Condition (1) allows us to extend α to a map $\alpha : \mathcal{C}^\infty(\Sigma)^* \to \mathcal{C}^\infty(\Sigma)^*$. Regarding this extension, we prove the following.

Proposition 4.2: Let α be a microscopic symmetry. Then

$$\alpha\Phi_\gamma \subset \Phi_\gamma \quad \forall\ \gamma \geqslant 0.$$

Proof: Using condition (1) in Definition 4.1, we can define the predual map $\alpha_* : \mathcal{C}^\infty(\Sigma) \to \mathcal{C}^\infty(\Sigma)$. Let $\gamma \geqslant 0$ be fixed. Lemma 3.2 shows us that in diagram (4.2),

$$\ker p_\gamma = \{\sigma \in \mathcal{C}^\infty(\Sigma) \mid r^{-\gamma} \|\sigma\|_r \to 0\}. \tag{4.5}$$

Together with condition (2) in Definition 4.1, this yields $\alpha_* \ker p_\gamma \subset \ker p_\gamma$; thus α has a well-defined action on the quotient space Σ_γ and on its dual Φ_γ. By construction, this action is compatible with the inclusion $p_\gamma^* : \Phi_\gamma \hookrightarrow \mathcal{C}^\infty(\Sigma)^*$, which proves the proposition. □

Microscopic symmetries α thus leave the spaces Φ_γ of pointlike fields stable. In the case of a group representation $g \mapsto \alpha(g)$, we get corresponding finite-dimensional representations on every field space Φ_γ. An example for this case are Lorentz transformations: Each Φ_γ carries a finite-dimensional representation of the Lorentz group. Another example for microscopic symmetries are dilations, provided they exist as a symmetry of the net. Furthermore, our analysis allows us to handle inner symmetries, both broken and unbroken. In the case of a spontaneously broken symmetry, one expects that $\alpha = \mathrm{ad}\, U$ preserves localization only in regions of some limited size—this corresponds to the case $R < \infty$ in Definition 4.1. [Compare Ref. 21. To include the situation considered there in our context, it is necessary to extend our framework from the observable algebras $\mathfrak{A}(\mathcal{O})$ to the field algebras $\mathfrak{F}(\mathcal{O})$, including also nonobservable fields, which should however be straightforward.]

In extension of our methods introduced above, one observes that the antilinear involution $A \mapsto A^*$ can be treated in a similar manner, showing that the field spaces Φ_γ are invariant under Hermitean conjugation $\phi \mapsto \phi^*$. Defining the translated fields as $\phi(x) := U(x)\phi U(x)^*$, or passing over to the "smeared" fields $\phi(f)$, we may also derive symmetry properties under the (connected part of the) full Poincaré group.

The only remaining part in establishing the Wightman axioms then is irreducibility, i.e., the question whether the vacuum vector Ω is cyclic for the fields. As will be discussed below, we cannot expect this in the general case. However, for each γ we may consider a "reduced" Hilbert space,

$$\mathcal{H}_\gamma := \overline{\mathcal{P}_\gamma(\mathcal{O})\Omega} \subset \mathcal{H}, \tag{4.6}$$

where $\mathcal{O}$ is some open subset of $\mathbb{R}^{s+1}$, and $\mathcal{P}_\gamma(\mathcal{O})$ is the polynomial algebra generated by the fields $\phi(f)$ with $\phi \in \Phi_\gamma$ and $\mathrm{supp}\, f \subset \mathcal{O}$. (Due to the Reeh–Schlieder theorem, the space $\mathcal{H}_\gamma$ does not depend on $\mathcal{O}$.) Considered on $\mathcal{H}_\gamma$, the set Φ_γ is certainly irreducible. Thus, we have established the following.

Theorem 4.3: *Let $\mathcal{O} \mapsto \mathfrak{A}(\mathcal{O})$ satisfy the microscopic phase space condition. For every $\gamma \geqslant 0$, there exists a basis $\{\phi_1, \ldots, \phi_{N_\gamma}\}$ of Φ_γ and a Hilbert space $\mathcal{H}_\gamma \subset \mathcal{H}$ such that $\{f \mapsto \phi_j(f)\}$ is a set of quantum fields on $\mathcal{H}_\gamma$ in the sense of the Wightman axioms.*

Here we refer to the Wightman axioms as put forward in Ref. 22. Note that in our case, the fields always have finite spin. In the more general framework of Ref. 3, this is not guaranteed. Also note that we need to allow $\mathcal{H}_\gamma$ to grow with γ: While at any fixed γ, we are sure to find only a finite number of fields, more and more independent fields may occur in the phase space approximation as we increase the energy dimension.

Let us briefly return to the question whether, or on which Hilbert space, the entire field content Φ_{FH} is irreducible. In general, we cannot expect Φ_{FH} to be an irreducible set on $\mathcal{H}$, since there exist nontrivial theories which fulfill the microscopic phase space condition, but have a trivial field content, i.e., $\Phi_{\mathrm{FH}}=\mathbb{C}\mathrm{l}$ (cf. the Appendix). These theories might always occur as a tensor factor of $\mathfrak{A}$. To exclude such nonpointlike components from the theory, we can define the following subnet $\mathfrak{A}_F$ of $\mathfrak{A}$ using the methods exposed in Ref. 23:

$$\mathfrak{A}_F(\mathcal{O}) := \mathcal{P}(\mathcal{O})'', \tag{4.7}$$

where $\mathcal{P}(\mathcal{O})$ is the polynomial algebra generated by Φ_{FH}, and $(\cdots)'$ denotes the weak commutant. If $\mathfrak{A}$ fulfills the microscopic phase space condition, then so does $\mathfrak{A}_F$, leading to the same field content as $\mathfrak{A}$; thus we may call $\mathfrak{A}_F$ the point field part of the theory. It is $\mathcal{H}_F := \overline{\mathcal{P}(\mathcal{O})\Omega}$ which we should consider as the natural Hilbert space for the Wightman fields. In fact, using the techniques of Bisognano and Wichmann,[24] it should be possible to show that

$$\mathcal{H}_F = \mathcal{H} \;\Leftrightarrow\; \mathfrak{A}_F = \mathfrak{A}, \tag{4.8}$$

meaning that Φ_{FH} is irreducible on $\mathcal{H}$ if, and only if, the theory is completely determined by pointlike observables.

We can incorporate derivatives of fields into our context as well. It is easy to see that together with ϕ, its derivatives

$$\partial_\mu \phi := \frac{\partial}{\partial x^\mu}\, U(x)\phi U(x)^*\big|_{x=0} = i[P_\mu, \phi] \tag{4.9}$$

are contained in Φ_{FH}; so we can take ∂_μ to be a linear operator from Φ_γ into some $\Phi_{\gamma'}$. Usually, we must choose $\gamma' > \gamma$ here, since the "energy dimension" of fields increases when applying time derivatives: If $\|\partial_0^n \phi\|^{(\ell)} < \infty$ for some fixed ℓ and *any* $n \in \mathbb{N}$, then it follows that $\|\phi\Omega\| < \infty$; however, this is only possible if ϕ is a multiple of the identity.[25] In particular, the case of a finite-dimensional Φ_{FH} automatically leads to $\Phi_{\mathrm{FH}}=\mathbb{C}\mathrm{l}$.

V. CONCLUSIONS AND OUTLOOK

Starting from a relativistic quantum theory in the algebraic framework, i.e., expressed in terms of observables localized at finite distances, we have shown that its field content can be characterized by its phase space structure in the short distance limit. We have introduced a physically motivated phase space criterion that distinguishes a class of models with "regular" short distance behavior. Assuming that this criterion is fulfilled, we have established very detailed results on the approximation of pointlike fields by bounded local observables. The field content is exhausted by an increasing sequence of finite-dimensional spaces Φ_γ, each of which is invariant under Lorentz transformations, Hermitian conjugation and other symmetries. Their dimension $N_\gamma = \dim \Phi_\gamma$ can be read off directly from the phase space behavior. The label γ may be interpreted as a "short distance dimension" of the fields.

In mathematical terms, we have developed a method of classifying the short distance behavior of a net of algebras $\mathcal{O} \mapsto \mathfrak{A}(\mathcal{O})$; the field space dimensions N_γ are "invariants" of the net. Such a classification should depend on local properties at small distances only. Strictly speaking, this goal is not completely reached in our analysis: We incorporate the energy operator H as a global property. However, H enters the construction not as the generator of a global symmetry, but only through the more qualitative feature of energy damping, and via its role as a generator of the unitary group used for "smearing" the fields. One should therefore be able to replace the Hamil-

tonian with the local symmetry generators established by Buchholz, D'Antoni, and Longo[26] through the use of a "universal localizing map." It is also worth noting that with respect to certain phase space properties, H may be replaced[27] with a suitable modular operator Δ. This might point to an extension of our results even to situations without any space–time symmetries. Since $-\log \Delta$ corresponds to energy-momentum *transfer* rather than to total energy, though, it is unclear how the concept of polynomial bounds can be substituted.

Besides a characterization of the short distance limit, our results provide a sufficient technical basis for a rigorous proof of the existence of operator product expansions; this will be discussed in a forthcoming paper.[17]

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APPENDIX: SOME SIMPLE MODELS

The claim that our phase space condition should hold in physically relevant theories may be supported by the fact that it is fulfilled at least in some simple situations. In this appendix, we will therefore investigate the structures introduced in the main text in specific noninteracting models.

We will first consider a real scalar free field and argue that this theory fulfills the microscopic phase space condition in $s \geqslant 3$ spatial dimensions. Then we discuss extensions of this result to more general (still noninteracting) situations.

The real scalar free field

Most of the relevant techniques that allow us to discuss the short distance structure of free fields are already visible in the case of a single real scalar field. For this theory, the following theorem holds.

Theorem A.1: *The theory of a real scalar free field of mass $m \geqslant 0$ in $s+1$ space–time dimensionsl, $s \geqslant 3$, satisfies the microscopic phase space condition.*

This result was proved in Chap. 7 of Ref. 18 for a slightly modified version of the phase space condition. The proof carries over to our situation; however, the construction is quite involved, and it would go beyond the scope of the current paper to reproduce the complete discussion. Instead, we shall confine ourselves to a rough and somewhat heuristic sketch of the arguments; the reader is referred to Ref. 18 for details.

In order to fix our notation, we shall briefly recall the definition of a real scalar free field. Our Hilbert space $\mathcal{H}$ is the symmetric Fock space over the single particle space $\mathcal{K} = \mathcal{L}^2(\mathbb{R}^s, d^s p)$ ("wave functions in momentum space"). The scalar product on $\mathcal{K}$ will be denoted as $\langle \cdot | \cdot \rangle$, as opposed to the scalar product $(\cdot|\cdot)$ on $\mathcal{H}$. On $\mathcal{K}$, we have the generator of time translations $\omega = \sqrt{\mathbf{p}^2 + m^2}$, which fixes the Hamiltonian H on Fock space by means of "second quantization." The spectral projectors of ω will be denoted as $P_\omega(E)$, those of H as $P_H(E)$.

The local algebras $\mathfrak{A}(r)$ are then generated by Weyl operators $W(f) = \exp i(a(f) + a^*(f))$ with $f = f^+ + if^-$, where $f^\pm \in \mathcal{K}$ are localized functions in configuration space, in the sense that the Fourier transforms of $\omega^{\pm 1/2} f^\pm$ are real-valued and smooth and have their support within the ball $|\mathbf{x}| < r$.

In order to prove Theorem A.1, we must find a series expansion of the kind

$$\Xi = \sum_j \sigma_j \phi_j. \tag{A1}$$

with linear forms $\phi_j \in \mathcal{C}^\infty(\Sigma)^*$ and functionals $\sigma_j \in \Sigma$, valid for localized arguments of σ_j and energy-damped expectation values of ϕ_j. We will establish this expansion in four steps.

Step 1: Single particle space. For a start, we will derive a series expansion of the single–particle scalar product

$$\langle f^\pm | k \rangle = \langle \omega^{\pm 1/2} f^\pm | \omega^{\mp 1/2} k \rangle, \tag{A2}$$

where $f^\pm$ is localized with radius r (as above), and k is an energy-bounded function, i.e., $k \in P_\omega(E)\mathcal{K}$ for some E. Since $\omega^{\mp 1/2}k$ is also energy bounded, its Fourier transform $\mathcal{F}[\omega^{\mp 1/2}k]$ is analytic, and thus we can replace it with its Taylor series,

$$\mathcal{F}[\omega^{\mp 1/2}k](\mathbf{x}) = \sum_\kappa \frac{1}{\kappa!} \frac{\partial^\kappa}{\partial x^\kappa} \mathcal{F}[\omega^{\mp 1/2}k]|_{\mathbf{x}=0} x^\kappa \tag{A3}$$

—the sum runs over multi-indices κ here. Inserting this expansion into Eq. (A2), and rewriting the spatial derivatives as integrals in momentum space, we arrive at

$$\langle f^\pm | k \rangle = \sum_\kappa \langle f^\pm | \underbrace{\frac{\sqrt{2}}{\kappa!} \omega^{\pm 1/2} \mathcal{F}^{-1}[x^\kappa]}_{=: h_\kappa^\pm} \rangle \langle \underbrace{\frac{i^{-|\kappa|}}{\sqrt{2}(2\pi)^{s/2}} \omega^{\mp 1/2} p^\kappa}_{=: g_\kappa^\pm} | k \rangle = \sum_\kappa \langle f^\pm | h_\kappa^\pm \rangle \langle g_\kappa^\pm | k \rangle. \tag{A4}$$

The scalar products with the "improper vectors" $g_\kappa^\pm$ and $h_\kappa^\pm$ can be justified due to the given localization properties of $f^\pm$ and k. Note that $g_\kappa^\pm$ and $h_\kappa^\pm$ are independent not only of $f^\pm$ and k, but also of E and r. Using that the coefficients $\langle f^\pm | h_\kappa^\pm \rangle$ are real, we can thus write

$$f^\pm = \sum_\kappa \langle f^\pm | h_\kappa^\pm \rangle g_\kappa, \tag{A5}$$

where the sum is to be read "under energy restriction."

We note that regarding the short-distance or high-energy behavior of the functions introduced above, one has

$$\| P_\omega(E) g_\kappa^\pm \| \sim E^{|\kappa| + (s \mp 1)/2}, \quad |\langle f^\pm | h_\kappa^\pm \rangle| \sim r^{|\kappa| + (s \mp 1)/2}; \tag{A6}$$

in particular, there are only finitely many terms in the sum (A4) which correspond to a given "scaling dimension."

Step 2: Expansion of Weyl operators. In order to transfer our results in single-particle space to the theory in Fock space, we will next aim at a series expansion of local Weyl operators $W(f)$, where $f = f^+ + if^-$ as before. We can certainly expand them as

$$W(f) = e^{-\|f\|^2/2} e^{ia^*(f)} e^{ia(f)} = e^{-\|f\|^2/2} \sum_{m^\pm, n^\pm \in \mathbb{N} \cup \{0\}} \frac{i^{m^+ + n^+ + 2m^-}}{m^+! m^-! n^+! n^-!} a^*(f^+)^{m^+} a^*(f^-)^{m^-} a(f^+)^{n^+} a(f^-)^{n^-}. \tag{A7}$$

If this sum is evaluated in energy-restricted states, we can insert our result (A5) here, writing, for example,

$$a^*(f^+) = \sum_\kappa \langle f^+ | h_\kappa^+ \rangle a^*(g_\kappa^+). \tag{A8}$$

However, this leaves us with additional $m^+ + m^- + n^+ + n^-$ summation (multi-)indices in each summand of (A7). In order to simplify the notation, we will reorganize this multiple sum by the following:

(i) relabeling the functions $g_\kappa^\pm$ and $h_\kappa^\pm$ with natural numbers j instead of multi-indices κ,

(ii) grouping terms with equal powers of $\langle f^+|h_j^+\rangle$ and $\langle f^-|h_j^-\rangle$ into one, and
(iii) labeling these terms with two multi-indices $\mu^\pm=(\mu_1^\pm,\ldots)$, where μ_1^+ counts the power of $\langle f^+|h_1^+\rangle$, etc. Additionally, we will combine μ^+ and μ^- into a single multi-index $\mu=(\mu^+,\mu^-)$.

This leads us to an expression

$$W(f)=\sum_\kappa e^{-\|f\|^2/2}\prod_j \langle f^+|h_j^+\rangle^{\mu_j^+}\langle f^-|h_j^-\rangle^{\mu_j^-}\cdot\phi_\mu, \tag{A9}$$

where ϕ_μ are quadratic forms of the sort

$$\phi_\mu=\sum \frac{i^{m^++n^++2m^-}}{m^+!m^-!n^+!n^-!}a^*(g_?)\cdots a(g_?)\cdots\ . \tag{A10}$$

Here $a^*(g_?)\cdots a(g_?)\cdots$ are certain products of annihilation and creation operators of $g_j^\pm$, with their multiplicity given by $\mu^\pm$. The ϕ_μ can be shown to be elements of $\mathcal{C}^\infty(\Sigma)^*$. Their detailed structure is not relevant for our purposes—see, however, the end of this section for some examples. Regarding the scaling properties of the expansion terms, we find

$$\|P_H(E)\phi_\mu P_H(E)\|\sim E^{\vartheta(\mu)},\quad \prod_j \langle f^+|h_j^+\rangle^{\mu_j^+}\langle f^-|h_j^-\rangle^{\mu_j^-}\sim r^{\vartheta(\mu)}. \tag{A11}$$

The exponent $\vartheta(\mu)$ results from Eq. (A6), and its detailed form is not of much importance; the crucial point is that for every $\gamma\geqslant 0$, the set $\{\mu|\,\vartheta(\mu)\leqslant\gamma\}$ is finite, given that $s\geqslant 2$.

Step 3: Linear extension. Our next step is to generalize the expansion (A9) to arbitrary $A\in\mathfrak{A}(r)$ in place of the generating $W(f)$. To that end, we need to replace the numerical factors involving $f^\pm$ with an expression that is linear in $W(f)$; i.e., we need to find linear functionals σ_μ such that

$$\sigma_\mu(W(f))=e^{-\|f\|^2/2}\prod_j \langle f^+|h_j^+\rangle^{\mu_j^+}\langle f^-|h_j^-\rangle^{\mu_j^-}. \tag{A12}$$

In fact, we note that functionals of the type

$$\sigma(\cdot)=(\Omega|[a(b),[a^*(b'),\cdot\,]]\Omega)\quad \text{with } b,b'\in\mathcal{K} \tag{A13}$$

evaluate on Weyl operators to

$$\sigma(W(f))=e^{-\|f\|^2/2}\langle b|if\rangle\langle if|b'\rangle. \tag{A14}$$

For a given multi-index $\mu=(\mu^+,\mu^-)$, we can construct a functional τ_μ in a similar way such that for given b_j, $b_j'\in\mathcal{K}$,

$$\tau_\mu(W(f))=e^{-\|f\|^2/2}\prod_j \langle b_j|if\rangle^{\mu_j^+}\langle if|b_j'\rangle^{\mu_j^-}. \tag{A15}$$

This is not exactly the form (A12) we need. However, inserting $f=f^++if^-$, we may build certain linear combinations of the τ_μ in order to form the σ_μ we require; this combinatorial problem can be solved by means of a generating function technique, which we shall not present in detail here.

After establishing the functionals σ_μ, we can rewrite (A9) as

$$\Xi=\sum_\mu \sigma_\mu\phi_\mu, \tag{A16}$$

where, at this time, the series is meaningful on a sufficiently restricted domain.

Step 4: Convergence. In order to establish the phase space condition, our objective is to show that the series expansion of Ξ in Eq. (A16) holds with respect to the pseudometric $\hat{\delta}$ defined in Eq.

(2.8). Loosely speaking, we have dealt with the algebraic aspects of this expansion up to now, while we still must handle the topological problems, i.e., establish convergence. Roughly, this includes the following tasks.

First, we need to establish precise estimates for the norms of ϕ_μ and σ_μ, depending on the energy and configuration space localization E and r. This involves all parts of the calculation in steps 1–3 above. The goal is to establish an estimate of the form

$$\|\sigma_\mu[\mathfrak{A}(r)\| \cdot \|P_H(E)\phi_\mu P_H(E)\| \leqslant c_\mu (Er)^{\vartheta(\mu)}, \tag{A17}$$

where the constants c_μ do not increase too fast when varying μ.

Second, we need to sum the terms in Eq. (A17) in order to establish norm convergence of the series (A16) at fixed E and r. Unfortunately, it turns out that the estimates which we can establish in Eq. (A17) are not strict enough: We encounter convergence problems at "high particle numbers," i.e., at high values of $|\mu|$. This problem is solved by handling the terms for high $|\mu|$ according to a different expansion with better convergence properties, using the techniques developed by Buchholz and Porrmann.[9] Their methods, however, result in expansion terms that are explicitly dependent of E and r, so that they are useful for discussing the convergence issues in question, but cannot be used in our main expansion. In this part of the construction, the condition $s \geqslant 3$ is needed.

Third, once that the series is established at fixed E and r, we need to apply the results to the pseudometrics δ_γ, which means in particular to pass from the sharp energy bounds to the polynomial bounds used in the main text, and to consider the limit $r \to 0$. As a result of this calculation, we can show that for each $\gamma \geqslant 0$,

$$\delta_\gamma\left(\Xi - \sum_{\vartheta(\mu)\leqslant\gamma} \sigma_\mu \phi_\mu\right) = 0. \tag{A18}$$

This relation finally proves Theorem A.1.

It is instructive to see how the approximation terms $\sigma_\mu\phi_\mu$ are formed explicitly. When working out the details of the construction, one easily sees that the first term of the expansion, corresponding to $\mu=(0,0,0,\ldots)$, leads to $\phi_\mu=\mathbb{1}$ and $\sigma_\mu=(\Omega|\cdot|\Omega)$. In the next term [with the next lowest value of $\vartheta(\mu)$] the form ϕ_μ is the usual scalar field $\phi(0)$. Higher-order terms involve derivatives of the field and Wick products. For $s=3$, the beginning of the expansion reads

$$\begin{aligned}
\Xi = {} & (\Omega|\cdot|\Omega) && \cdot \mathbb{1} && \Big\} \vartheta(\mu)=0 \\
& + \frac{1}{2}((h|\cdot|\Omega) + (\Omega|\cdot|h)) && \cdot \phi(0) && \Big\} \vartheta(\mu)=1 \\
& + \frac{1}{2}\sum_{j=1}^{3} ((\hat{x}_j h|\cdot|\Omega) + (\Omega|\cdot|\hat{x}_j h)) && \cdot \partial_j\phi(0) && \Big\} \vartheta(\mu)=2 \\
& + \frac{1}{2i}((\omega^{-1}h|\cdot|\Omega) - (\Omega|\cdot|\omega^{-1}h)) && \cdot \partial_0\phi(0) && \\
& + \sigma_Q(\cdot) && \cdot :\phi^2:(0) && \\
& + \cdots . && &&
\end{aligned} \tag{A19}$$

Here $h=h_{\kappa=0}$ is the function introduced in (A4), the operator $\hat{x}_j$ stands for $\omega^{1/2}\mathcal{F}^{-1}x_j\mathcal{F}\omega^{-1/2}$, with $\mathcal{F}$ being the operator of Fourier transformation, and σ_Q denotes the following functional:

$$\sigma_Q(\cdot) = \frac{1}{4\sqrt{2}}((h \otimes h| \cdot |\Omega) + (\Omega| \cdot |h \otimes h)) + \frac{1}{4}(h| \cdot |h) - \frac{\|h\|^2}{4}(\Omega| \cdot |\Omega). \tag{A20}$$

We have $N_0=1$, $N_1=2$, $N_2=7$, and $N_3=21$ [the latter not being shown in Eq. (A19)]. The corresponding spaces Φ_γ have the following form:

$$\Phi_0 = \mathrm{span}\{\mathbb{1}\},$$

$$\Phi_1 = \mathrm{span}\{\mathbb{1}, \phi\},$$

$$\Phi_2 = \mathrm{span}\{\mathbb{1}, \phi, \partial_j\phi, \partial_0\phi, :\phi^2:\},$$

$$\Phi_3 = \mathrm{span}\{\mathbb{1},\ \phi,\ \partial_j\phi,\ \partial_0\phi,\ :\phi^2:,\ \partial_j^2\phi,\ \partial_j\partial_k\phi,\ \partial_0\partial_j\phi,\ :\phi\partial_j\phi:,\ :\phi\partial_0\phi:,\ :\phi^3:\}, \tag{A21}$$

where $j,k=1\ldots3, j>k$, and the argument of the field has been omitted. Note that the second-order time derivative $\partial_0^2\phi$ lies in Φ_3, but is a linear combination of the basis elements listed above—this reflects the field equation of the model.

More applications

The methods we have sketched above are not restricted to the simple case of a real scalar field. Similar results can be derived in a large class of free theories, including

(i) charged fields and fields of higher spin,
(ii) theories with more than one field (but finitely many), massive or massless, in $s \geqslant 3$ dimensions,
(iii) massive theories in $s=2$,

where on the technical side, only the single particle space expansions must be adapted appropriately.

It has not yet been possible to establish the criterion in the $(2+1)$-dimensional massless case. This results from the model's peculiar infrared structure that causes certain nuclearity conditions to be violated (cf. Ref. 9), leading to convergence problems at high particle numbers. Also, there is no result for the $(1+1)$-dimensional case (irrespective of m); here the Wick powers $:\phi^n:$ have the same energy dimension as the field itself, thus one would not expect finite-dimensional field spaces Φ_γ to exist.

The criterion is explicitly violated in theories with infinitely many free fields (see Sec. 8.1 of Ref. 18). In this case, we find $N_\gamma=\infty$ for all $\gamma \geqslant 1$.

In conclusion, we briefly sketch a model discussed by Lutz,[19] which is interesting in this context since its field content is trivial. We proceed from a free massless theory in $(s+1)+1$ space–time dimensions, with the local algebras generated by Weyl operators $W(f)$ as before, but with test functions f of the type

$$f(\mathbf{p}) = (p_{s+1})^{2n(r)} f_0(\mathbf{p}), \tag{A22}$$

where $n(r)$ is an integer function tending to infinity as $r \to 0$, and x_{s+1} is the "additional" spatial coordinate. When restricting the net to $s+1$ space–time dimensions, we can apply the above arguments to show that the theory fulfills the microscopic phase space condition. Indeed, we see from (A4) that every fixed expansion term h_κ in the single particle space simply drops out if $n(r)$ is sufficiently large, i.e., if r is sufficiently small. This leads to the result

$$\delta_\gamma(\Xi - (\Omega| \cdot |\Omega)\mathbb{1}) = 0 \quad \forall\ \gamma \geqslant 0, \tag{A23}$$

which implies $\Phi_\gamma = \mathbb{C}\mathbb{1}$ for all γ.

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Wilson polynomials and the Lorentz transformation properties of the parity operator

Carl M. Bender, Peter N. Meisinger, and Qinghai Wang
Department of Physics, Washington University, St. Louis, Missouri 63130

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The parity operator for a parity-symmetric quantum field theory transforms as an infinite sum of irreducible representations of the homogeneous Lorentz group. These representations are connected with Wilson polynomials. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1870733]

I. INTRODUCTION

The objective of this paper is to determine the Lorentz transformation properties of the parity operator $\mathcal{P}$. The operator $\mathcal{P}$ for a quantum field theory has the effect

$$\mathcal{P}\varphi(\mathbf{x},t)\mathcal{P} = \varphi(-\mathbf{x},t) \quad \text{(scalar field)},$$

$$\mathcal{P}\varphi(\mathbf{x},t)\mathcal{P} = -\varphi(-\mathbf{x},t) \quad \text{(pseudoscalar field)}.$$

For purposes of comparison, we can also define an *intrinsic* parity operator $\mathcal{P}_I$. This operator has the same effect as $\mathcal{P}$ except that it does not reverse the sign of the spatial argument of the quantum field,[1]

$$\mathcal{P}_I\varphi(\mathbf{x},t)\mathcal{P}_I = \varphi(\mathbf{x},t) \quad \text{(scalar field)},$$

$$\mathcal{P}_I\varphi(\mathbf{x},t)\mathcal{P}_I = -\varphi(\mathbf{x},t) \quad \text{(pseudoscalar field)}.$$

To determine the Lorentz transformation properties of any operator in a quantum field theory one must calculate the commutator of this operator with the generators of the Lorentz group $J^{\mu\nu}$. If this operator, like the parity operator $\mathcal{P}$, does not depend on the space–time coordinates $(\mathbf{x},t)$ and it commutes with $J^{\mu\nu}$, then it is a scalar under Lorentz transformations.

In this paper we will assume that the Hamiltonian H of our quantum field theory has parity symmetry; that is, $[\mathcal{P},H]=0$. An example of such a theory is the free scalar quantum field theory whose Hamiltonian is

$$H = \int d\mathbf{x}\left\{\tfrac{1}{2}\pi^2(\mathbf{x},t) + \tfrac{1}{2}[\nabla\varphi(\mathbf{x},t)]^2 + \tfrac{1}{2}\mu^2\varphi^2(\mathbf{x},t)\right\}.$$

For such a theory it is easy to see that the intrinsic parity operator is not only a rotational scalar but also a Lorentz scalar because it commutes with all six generators of the homogeneous Lorentz group,

$$[\mathcal{P}_I, J^{\mu\nu}] = 0.$$

Like the intrinsic parity operator $\mathcal{P}_I$, the conventional parity operator $\mathcal{P}$ is a rotational scalar because it commutes with the three generators of spatial rotations,

$$[\mathcal{P}, J^{ij}] = 0.$$

However, in contrast with $\mathcal{P}_I$, $\mathcal{P}$ does *not* commute with the Lorentz-boost generators. Either by

direct calculation or by using the fact that J^{0i} is a vector (like the electric field vector) under spatial reflection, we can show that

$$[\mathcal{P}, J^{0i}] = -2J^{0i}\mathcal{P}. \tag{1}$$

Therefore, the parity operator $\mathcal{P}$ is not a Lorentz scalar. Furthermore, as we will see, $\mathcal{P}$ is not the spin-0 component of a vector, a tensor, or indeed any finite-dimensional representation of the Lorentz group.

This observation raises a fundamental question: How does $\mathcal{P}$ transform under the Lorentz group? In this paper we provide a partial answer to this question. We argue that $\mathcal{P}$ transforms as an infinite direct sum of finite-dimensional tensorial representations of the Lorentz group.

This paper is organized as follows: In Sec. II we review the general theory of the irreducible representations of the Lorentz group. Then in Sec. III we show that $\mathcal{P}$ transforms as a direct sum of irreducible representations of the Lorentz group, and that to identify each of these irreducible representations one must solve a difference-equation eigenvalue problem. In Secs. IV and V we perform an analysis of special cases of this difference equation and show that the eigenfunctions are closely associated with the Wilson polynomials. Finally, in Sec. VI we make some concluding remarks about the structure of the solutions to the general difference-equation eigenvalue problem that is derived in Sec. III. The properties of the Wilson polynomials are summarized in the Appendixes.

II. IRREDUCIBLE REPRESENTATIONS OF THE LORENTZ GROUP

In this section we review briefly the classification of irreducible representations of the Lorentz group. Following the exposition of the irreducible representations of the Lorentz group by Gel'fand, Minlos, and Shapiro,[2] Bender and Griffiths,[3] and Griffiths,[4] we note that all irreducible representations of the Lorentz group are characterized and labeled by a pair of numbers (ℓ_0, ℓ_1). The first number, ℓ_0, is a non-negative integer and the second number, ℓ_1, is in general complex. Any irreducible representation of the Lorentz group is a direct sum of irreducible representations of the rotation subgroup SO(3) and ℓ_0 is the lowest-spin of the representations contained in this sum.

If $\ell_1 - \ell_0 = 0$ or noninteger, then the representation belongs to the *nonsingular class* of infinite-dimensional representations. Such a representation contains an infinite tower of spins beginning with ℓ_0; the spins ℓ in this representation are $\ell = \ell_0, \ell_0+1, \ell_0+2, \ldots$. Each spin in this sequence occurs once and only once.

If $\ell_1 - \ell_0$ is a nonzero integer, then the representation belongs to the *singular class*. For this case if $|\ell_1| > \ell_0$, the representation is finite dimensional; it contains all spins ℓ with $\ell_0 \leqslant \ell \leqslant |\ell_1| - 1$ and each spin occurs exactly once. If $|\ell_1| < \ell_0$, the representation is infinite dimensional; it contains all spins, ℓ, $\ell_0 \leqslant \ell < \infty$ and again each spin occurs exactly once.

Since the Lorentz group is noncompact, it also has indecomposable representations. However, this situation does not arise in this paper.

To describe the Lorentz transformation properties of a space–time-dependent quantity, such as a quantum field, we must specify all of the spin components of the field $(Q_{\ell_0}, Q_{\ell_0+1}, Q_{\ell_0+2}, \ldots)$. Let us suppose first that this field transforms irreducibly under the Lorentz group and let us also suppose that the lowest-spin component has spin 0. Then, an infinitesimal Lorentz transformation of the spin-0 component $Q_0(\mathbf{x}, t)$ has an orbital and a spin part. Specifically,

$$-i[Q_0, J^{0i}] = t\partial^i Q_0 - x^i \partial^0 Q_0 + Q_1^i, \tag{2}$$

where Q_1^i is the spin-1 component of the irreducible representation. Under an infinitesimal Lorentz transformation, this spin-1 component then transforms like

$$-i[Q_1^j, J^{0i}] = t\partial^i Q_1^j - x^i \partial^0 Q_1^j + Q_2^{ij} + \alpha \delta^{ij} Q_0, \tag{3}$$

where Q_2^{ij} is the spin-2 component of the representation. Note that Q_2^{ij} is a *pure* spin-2 object and

is therefore symmetric and traceless, $Q_2^{ii}=0$. (Repeated indices indicate summation.) The number α in (3) is directly related to the parameter ℓ_1 for the irreducible representation by the formula[3]

$$\alpha = \tfrac{1}{3}(\ell_1^2 - 1). \tag{4}$$

This process of evaluating commutators can be used iteratively to calculate all of the spin components of the irreducible representation.

Now suppose that Q_0 is the spin-0 component of a representation of the Lorentz group, but that this representation is not irreducible. This means that there may be more than one component of each spin. Thus, under an infinitesimal transformation we have

$$-i[Q_0, J^{0i}] = t\partial^i Q_0 - x^i \partial^0 Q_0 + N_1^i(Q_0), \tag{5}$$

where N_1^i is one of the spin-1 components of the representation. An infinitesimal Lorentz transformation of this spin-1 component produces a spin-2 component $N_2^{ij}(Q_0)$, for which $N_2^{ii}(Q_0)=0$, and a new spin-0 component $N_0(Q_0)$,

$$-i[N_1^j(Q_0), J^{0i}] = t\partial^i N_1^j(Q_0) - x^i \partial^0 N_1^j(Q_0) + N_2^{ij}(Q_0) + \delta^{ij} N_0(Q_0). \tag{6}$$

Since this representation is not irreducible, $N_0(Q_0)$ is not a multiple of Q_0.

This process of calculating commutators can again be used to generate all of the spin components of the representation. For example, commuting $N_2^{ij}(Q_0)$ with the Lorentz boost will define a spin-3 component $N_3^{ijk}(Q_0)$. However, the procedure is significantly more complicated than that for an irreducible representation because there may be many components for each spin. Indeed, it may be that there are an infinite number of spin-0 components, Q_0, $N_0(Q_0)$, $N_0'(Q_0)$, and so on, and we will see that this is the case with the parity operator $\mathcal{P}$.

III. INFINITESIMAL LORENTZ TRANSFORMATION OF THE $\mathcal{P}$ OPERATOR

Like the generators of space–time translations P^μ, the parity operator $\mathcal{P}$ is a global symmetry operator and is not an explicit function of the space–time coordinates x^μ; that is, $\partial^\mu \mathcal{P}=0$. As a consequence, the orbital terms in (5) vanish and we get [see (1)]

$$N_1^i(\mathcal{P}) \equiv -i[\mathcal{P}, J^{0i}] = 2iJ^{0i}\mathcal{P}. \tag{7}$$

This identifies the spin-1 term that arises after commuting with the generator of a Lorentz boost.

A second commutation with the Lorentz boost gives a spin-2 component and a new spin-0 component,

$$-i[N_1^j(\mathcal{P}), J^{0i}] = N_2^{ij}(\mathcal{P}) + \delta^{ij} N_0(\mathcal{P}), \tag{8}$$

where the new spin-0 component is

$$N_0(\mathcal{P}) = -\tfrac{4}{3} J^{0i} J^{0i} \mathcal{P}. \tag{9}$$

Since $N_0(\mathcal{P})$ is not a constant multiple of $\mathcal{P}$, we conclude immediately that $\mathcal{P}$ does not belong to an irreducible representation of the Lorentz group.

To analyze the Lorentz transformation properties of the parity operator it is convenient to introduce the following notation. First, we define two 3-vectors:

$$K^i \equiv J^{0i}, \qquad L^i \equiv \tfrac{1}{2}\epsilon^{ijk} J^{jk}. \tag{10}$$

These operator quantities satisfy the following commutation relations:

$$[L^i, L^j] = i\epsilon^{ijk} L^k,$$

$$[K^i,L^j] = i\epsilon^{ijk}K^k,$$

$$[K^i,K^j] = -i\epsilon^{ijk}L^k. \tag{11}$$

Next, we define three operator products,

$$W \equiv K^iK^i,$$

$$A \equiv L^iL^i, \tag{12}$$

$$m \equiv K^iL^i = L^iK^i.$$

These three operators are mutually commuting,

$$[W,A] = [A,m] = [m,W] = 0. \tag{13}$$

The W, A, and m operators have the following commutation relations with the generators of the Lorentz group:

$$\begin{aligned} [W,K^i] = [A,K^i] &= -2i\epsilon^{ijk}L^jK^k - 2K^i, \\ [W,L^i] = [A,L^i] = [m,K^i] &= [m,L^i] = 0. \end{aligned} \tag{14}$$

Next, we define the operator B,

$$B \equiv A - W. \tag{15}$$

Observe that from (14) the operator B commutes with the generators of the Lorentz group,

$$[B,K^i] = [B,L^i] = 0. \tag{16}$$

Since B commutes with L^i, it is a rotational scalar, and since it also commutes with K^i, it is either a Lorentz scalar or a Lorentz pseudoscalar. However, B also commutes with the parity operator $\mathcal{P}$,

$$[B,\mathcal{P}] = 0. \tag{17}$$

Thus, B transforms as a Lorentz scalar. The operator m also commutes with the generators of the Lorentz group but m is a pseudoscalar because

$$\mathcal{P}m\mathcal{P} = -m. \tag{18}$$

Finally, we define the scalar operator M by

$$M \equiv m^2. \tag{19}$$

The four operators B, M, W, and parity $\mathcal{P}$ are a mutually commuting set

$$[B,M] = [B,W] = [M,W] = [B,\mathcal{P}] = [M,\mathcal{P}] = [W,\mathcal{P}] = 0. \tag{20}$$

We know that the parity operator does not transform irreducibly under the Lorentz group. We will assume that it transforms as a direct sum of operators that *do* transform irreducibly. From the commutation properties of the operators defined above we know that the most general form of the spin-0 component of any operator that could be produced by repeated commutation of $\mathcal{P}$ with the generators of the Lorentz group has the form $f(B,M,W)\mathcal{P}$, where $f(B,M,W)$ is an as yet unknown function of the operators B, M, and W. Let us assume that the function $f(B,M,W)$ has a general power series representation of the form

$$f(B,M,W)=\sum_{l,m,n} a_{lmn}B^l M^m W^n. \tag{21}$$

Using these series as a starting *ansatz*, we use mathematical induction to calculate the double commutator of $f(B,M,W)\mathcal{P}$ with the generators of the Lorentz group, and obtain the new spin-0 component,

$$\begin{aligned}N_0[f(B,M,W)\mathcal{P}] = &-\frac{2}{3}\left(W+\frac{M}{B+W}\right)f(B,M,W)\mathcal{P}-\frac{1}{3\sqrt{1+4B+4W}}\\ &\times\left\{\left[2B+4W+\left(W-\frac{M}{B+W}\right)(\sqrt{1+4B+4W}-1)\right]\right.\\ &\times f(B,M,W+1+\sqrt{1+4B+4W})\\ &+\left[-2B-4W+\left(W-\frac{M}{B+W}\right)(\sqrt{1+4B+4W}+1)\right]\\ &\left.\times f(B,M,W+1-\sqrt{1+4B+4W})\right\}\mathcal{P}.\end{aligned} \tag{22}$$

Let us now suppose that $f(B,M,W)\mathcal{P}$ transforms as the irreducible $(0,\ell_1)$ representation of Lorentz group. Then, from (4) we have[5]

$$N_0[f(B,M,W)\mathcal{P}]=\tfrac{1}{3}(\ell_1^2-1)f(B,M,W)\mathcal{P}. \tag{23}$$

Combining (22) and (23), we conclude that $f(B,M,W)$ satisfies the functional relation

$$\begin{aligned}&2\left(W+\frac{M}{B+W}\right)f(B,M,W)+\frac{1}{\sqrt{1+4B+4W}}\\ &\quad\times\left\{\left[2B+4W+\left(W-\frac{M}{B+W}\right)(\sqrt{1+4B+4W}-1)\right]f(B,M,W+1+\sqrt{1+4B+4W})\right.\\ &\quad\left.+\left[-2B-4W+\left(W-\frac{M}{B+W}\right)(\sqrt{1+4B+4W}+1)\right]f(B,M,W+1-\sqrt{1+4B+4W})\right\}\\ &=(1-\ell_1^2)f(B,M,W).\end{aligned} \tag{24}$$

This functional equation is a *difference-equation eigenvalue problem* in which the eigenvalue $(1-\ell_1^2)$ determines the representation of the Lorentz group under which the operator $f(B,M,W)\mathcal{P}$ transforms. We do not yet know how to find the general analytical solution to this equation. However, in the next two sections we show how to solve analytically this master equation for two important special cases.

IV. SPECIAL CASE I: $B=0$ AND $M=0$

In this section we solve a special case of the difference-equation eigenvalue problem (24). This special case serves as a useful toy model that will teach us how to approach the difficult equation (24). Let us set $B=0$ and $M=0$. Then, (24) simplifies to

$$\begin{aligned}&2Wf(W)+\frac{(3+\sqrt{1+4W})W}{\sqrt{1+4W}}f(W+1+\sqrt{1+4W})-\frac{(3-\sqrt{1+4W})W}{\sqrt{1+4W}}f(W+1-\sqrt{1+4W})\\ &=(1-\ell_1^2)f(W).\end{aligned} \tag{25}$$

To solve this equation we make the change of independent variable

$$z = \sqrt{W + \tfrac{1}{4}}. \tag{26}$$

In terms of this new variable $f(W) = f\left(z^2 - \frac{1}{4}\right)$. Next, we introduce the dependent variable $g(z)$ by

$$g(z) = e^{-i\pi z} \frac{f\left(z^2 - \frac{1}{4}\right)}{z^2 - \frac{1}{4}}. \tag{27}$$

The functional equation satisfied by $g(z)$ is

$$(2z+1)(2z+3)^2 g(z+1) - 4z(2z-1)(2z+1)g(z) + (2z-1)(2z-3)^2 g(z-1) = 8z(\ell_1^2 - 1)g(z). \tag{28}$$

In order to determine the eigenvalues $(\ell_1^2 - 1)$ we must impose an eigenvalue condition, to wit, we will assume that $f(W)$ is an *entire* function of W. This condition is difficult to justify at a physical level but it is a natural mathematical choice because it eliminates the possibility that the irreducible representation of the Lorentz group in (23) could be a nonsmooth function of the physical parameters B, M, and W. The condition that we use here leads us to make a polynomial truncation in the same way that the eigenfunctions of the quantum harmonic oscillator truncate into Hermite polynomials. (A similar eigenvalue condition based on the entirety of a solution to a difference equation may be found in Ref. 6.)

Imposing this constraint gives an infinite sequence of allowed values for ℓ_1,

$$\ell_1(n) = 2n + 1 \quad (n = 0, 1, 2, 3, \ldots). \tag{29}$$

Note that the eigenvalues involve the square of ℓ_1 but we may assume that ℓ_1 is positive.[7] The irreducible representations of the Lorentz group corresponding to these values of $\ell_1(n)$ are traceless, totally symmetric tensors of rank $2n$: T, $T^{\mu\nu}$, $T^{\mu\nu\lambda\sigma}$, and so on. Thus, we see that the parity operator transforms as a direct sum of the spin-0 components of these tensors [see (47)].

The eigenfunctions corresponding to the above eigenvalues are all polynomials in z^2 except for the eigenfunction corresponding to the lowest eigenvalue for which the eigenfunction is a rational function,

$$\begin{aligned}
g_0(z) &= \frac{1}{z^2 - \frac{1}{4}}, \\
g_1(z) &= 1, \\
g_2(z) &= z^2 + \tfrac{3}{4}, \\
g_3(z) &= z^4 + \tfrac{7}{2}z^2 + \tfrac{117}{80}, \\
g_4(z) &= z^6 + \tfrac{37}{4}z^4 + \tfrac{1957}{112}z^2 + \tfrac{2385}{448}, \\
g_5(z) &= z^8 + 19z^6 + \tfrac{747}{8}z^4 + \tfrac{2011}{16}z^2 + \tfrac{55575}{1792},
\end{aligned} \tag{30}$$

and so on. We have normalized the eigenfunctions so that each of the polynomials is *monic*; that is, the coefficient of the highest power of z^2 is unity.

The polynomial eigenfunctions in (30) are *Wilson* polynomials $W_n(x^2; a, b, c, d)$, where the parameters are given by $a = b = 1/2$ and $c = d = 3/2$ (see Appendix A),

$$g_n(z) = \frac{(n+1)!}{(2n)!} W_{n-1}\left(-z^2; \frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{3}{2}\right). \tag{31}$$

These polynomials can be expressed as generalized hypergeometric functions,

$$g_n(z) = \frac{(n-1)!(n!)^2(n+1)!}{(2n)!} {}_4F_3\left(1-n, n+2, \frac{1}{2}-z, \frac{1}{2}+z; 1, 2, 2; 1\right). \tag{32}$$

From the solutions $g_0(z)$ in (30) and $g_n(z)$ in (32) we can construct the eigenfunction solutions to (25),

$$f_n(W) = \begin{cases} e^{i\pi\sqrt{W+1/4}} \quad (n=0), \\ e^{i\pi\sqrt{W+1/4}} \dfrac{(n-1)!(n!)^2(n+1)!}{(2n)!} W \\ \times {}_4F_3\left(1-n, n+2, \dfrac{1}{2}-\sqrt{W+\dfrac{1}{4}}, \dfrac{1}{2}+\sqrt{W+\dfrac{1}{4}}; 1, 2, 2; 1\right) \quad (n>0). \end{cases} \tag{33}$$

Here are the first six solutions,

$$\begin{aligned} f_0(W) &= e^{i\pi\sqrt{W+1/4}}, \\ f_1(W) &= e^{i\pi\sqrt{W+1/4}} W, \\ f_2(W) &= e^{i\pi\sqrt{W+1/4}} W(W+1), \\ f_3(W) &= e^{i\pi\sqrt{W+1/4}} W\left(W^2 + 4W + \tfrac{12}{5}\right), \\ f_4(W) &= e^{i\pi\sqrt{W+1/4}} W\left(W^3 + 10W^2 + \tfrac{156}{7} W + \tfrac{72}{7}\right), \\ f_5(W) &= e^{i\pi\sqrt{W+1/4}} W\left(W^4 + 20W^3 + 108W^2 + 176W + \tfrac{480}{7}\right). \end{aligned} \tag{34}$$

The difference equation (28) is second order and linear, and this means that for each eigenvalue there are two linearly independent solutions. It is straightforward to use the method of reduction of order (which is ordinarily used for linear differential equations) to calculate the second solution. We seek a second solution of the general form

$$h_n(z) = g_n(z) u_n(z), \tag{35}$$

where $u_n(z)$ is an unknown function to be determined. The function $u_n(z)$ is easy to find because it satisfies a first-order difference equation,

$$\frac{u_n(z+1) - u_n(z)}{u_n(z) - u_n(z-1)} = \frac{(2z-1)(2z-3)^2 g_n(z-1)}{(2z+1)(2z+3)^2 g_n(z+1)}. \tag{36}$$

From this equation we find that apart from a multiplicative constant, we have

$$u_n(z) - u_n(z-1) = \frac{1}{(2z-3)^2(2z-1)^3(2z+1)^2 g_n(z-1) g_n(z)}. \tag{37}$$

Summing both sides of this equation, we get $u_n(z)$ (apart from an additive constant),

$$u_n(z) = \sum_{x=z_0}^{z} \frac{1}{(2x-3)^2(2x-1)^3(2x+1)^2 g_n(x-1)g_n(x)}, \tag{38}$$

where z_0 is arbitrary.

This sum can be evaluated analytically for the case $n=0$ and we obtain

$$h_0(z) = \frac{1}{\left(z^2-\frac{1}{4}\right)^2}. \tag{39}$$

When $n>0$ we must leave the second solution in the form of a sum,

$$h_n(z) = g_n(z)\sum_{x=z_0}^{z} \frac{1}{(2x-3)^2(2x-1)^3(2x+1)^2 g_n(x-1)g_n(x)}. \tag{40}$$

The general solution to (28) is a linear combination of $g_n(z)$ and $h_n(z)$. However, as a quantization condition, if we demand that the solution to (25) be entire, then the coefficient of $h_n(z)$ must vanish.

Our objective now is to reconstruct the parity operator as a direct sum over the irreducible representations constructed by multiplying $f_n(W)$ in (33) by the parity operator $\mathcal{P}$,

$$\mathcal{P} = \sum_{n=0}^{\infty} c_n f_n(W)\mathcal{P}, \tag{41}$$

where $\{c_n\}$ are coefficients that must be determined from the equation

$$1 = \sum_{n=0}^{\infty} c_n f_n(W) = e^{i\pi z}\left[c_0 + \left(z^2-\frac{1}{4}\right)\sum_{n=1}^{\infty} c_n g_n(z)\right], \tag{42}$$

which is obtained from (41) by multiplying by $\mathcal{P}$.

Equation (42) must hold for every value of z. Thus, if we let $z=\frac{1}{2}$, we obtain

$$c_0 = -i. \tag{43}$$

For $n\geqslant 1$, the coefficients c_n satisfy

$$\frac{e^{-i\pi z}+i}{z^2-\frac{1}{4}} = \sum_{n=1}^{\infty} c_n g_n(z) = \sum_{n=0}^{\infty} (-1)^n c_{n+1} P_n(-z^2), \tag{44}$$

where $P_n(x^2)$ is defined in (A1). We solve this formal functional equation by continuing it analytically into the complex z-plane and then making the change of variable $x=iz$. Equation (44) then becomes

$$-\frac{4(e^{-x\pi}+i)}{1+4x^2} = \sum_{n=0}^{\infty} (-1)^n c_{n+1} P_n(x^2). \tag{45}$$

We then multiply both sides of this equation by $\frac{1}{4}\pi^2 x(1+4x^2)^2 \sinh(x\pi)P_m(x^2)/\cosh^3(x\pi)$ and integrate over x from 0 to ∞. Using the orthogonality property of the Wilson polynomials in (A2), we obtain the following quadrature formula for c_n for $n\geqslant 1$:

$$c_n = \pi^2 \frac{(-1)^n[(2n)!]^2(2n+1)!}{[(n-1)!]^2(n!)^4[(n+1)!]^4}\int_0^{\infty} dx\, x(1+4x^2)\frac{(e^{-x\pi}+i)\sinh(x\pi)}{\cosh^3(x\pi)}P_{n-1}(x^2). \tag{46}$$

Note that this analytic continuation is an extremely delicate process because the series in (41) has only a formal existence. Indeed, while the Wilson polynomials (A1) are complete and orthogo-

nal, the polynomials obtained by replacing x^2 by $-z^2$ [see (44)] are not orthogonal with a positive weight function and not complete in the usual sense. Thus, the analytic continuation above is a procedure that converts a purely formal series identity into a series that actually converges with coefficients that can be determined.

If we substitute the expression for c_n ($n \geqslant 1$) in (46) and also the value of c_0 in (43) into (41), then (41) becomes an identity. This implies that we have decomposed the representation under which $\mathcal{P}$ transforms into a direct sum of finite-dimensional irreducible representations

$$(0,1) \oplus (0,3) \oplus (0,5) \oplus (0,7) \oplus \cdots . \tag{47}$$

That is, we have shown that $\mathcal{P}$ transforms as a scalar plus the spin-0 component of a two-index symmetric traceless tensor plus the spin-0 component of a four-index symmetric traceless tensor plus the spin-0 component of a six-index symmetric traceless tensor, and so on. This is the central result of our analysis.

We conclude this section with the remark that the first term in the direct sum above is a scalar; that is, the term $f_0(W)\mathcal{P}$ transforms like a Lorentz scalar. Thus, $\mathcal{P}$ transforms like the elementary structure $e^{-i\pi\sqrt{W+1/4}}$.

V. SPECIAL CASE II: $M=0$

In this section we solve an eigenvalue equation that is much more general than that solved in Sec. IV. We consider here the case $M=0$ but we allow B and W to be arbitrary. Now, (24) simplifies to

$$2Wf(B,W) + \frac{1}{\sqrt{1+4B+4W}}\left[(2B+3W+W\sqrt{1+4B+4W})f(B,W+1+\sqrt{1+4B+4W})\right.$$
$$\left. -(2B+3W-W\sqrt{1+4B+4W})f(B,W+1-\sqrt{1+4B+4W})\right] = (1-\ell_1^2)f(B,W). \tag{48}$$

To analyze this equation we generalize the substitution that we made in (26) and make the change of independent variable

$$z = \sqrt{W+B+\tfrac{1}{4}}. \tag{49}$$

In terms of this new variable we have $f(B,W) = f\left(B, z^2 - B - \frac{1}{4}\right)$. Next, we introduce the new dependent variable by the substitution

$$g(B,z) = e^{-i\pi z} f\left(B, z^2 - B - \tfrac{1}{4}\right), \tag{50}$$

which is a generalization of (27). We obtain the following functional equation satisfied by $g(B,z)$:

$$2\left(z^2 - B - \frac{1}{4}\right)g(B,z) - \frac{1}{2z}\left[3z^2 - B - \frac{3}{4} + 2z\left(z^2 - B - \frac{1}{4}\right)\right]g(B,z+1)$$
$$+ \frac{1}{2z}\left[3z^2 - B - \frac{3}{4} - 2z\left(z^2 - B - \frac{1}{4}\right)\right]g(B,z-1) = (1-\ell_1^2)g(B,z). \tag{51}$$

The solutions to this difference equation are Wilson polynomials $W_n(x^2;a,b,c,d)$ with parameters $a=b=\frac{1}{2}$, $c=\frac{1}{2}-\sqrt{B+1}$, $d=\frac{1}{2}+\sqrt{B+1}$ (see Appendix B). Thus,

$$g_n(B,z) = \frac{n!}{(2n)!} W_n\left(-z^2; \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - \sqrt{B+1}, \frac{1}{2} + \sqrt{B+1}\right)$$
$$= \frac{(n!)^2 \Gamma(n+1-\sqrt{B+1})\Gamma(n+1+\sqrt{B+1})}{(2n)!\Gamma(1-\sqrt{B+1})\Gamma(1+\sqrt{B+1})}$$
$$\times {}_4F_3\left(-n, n+1, \frac{1}{2} - z, \frac{1}{2} + z; 1, 1-\sqrt{B+1}, 1+\sqrt{B+1}; 1\right). \tag{52}$$

The first four of these polynomials are

$$\begin{aligned} g_0(B,z) &= 1, \\ g_1(B,z) &= z^2 - \tfrac{1}{2}B - \tfrac{1}{4}, \\ g_2(B,z) &= z^4 - \left(B - \tfrac{1}{2}\right)z^2 + \tfrac{1}{6}B^2 - \tfrac{1}{4}B - \tfrac{3}{16}, \\ g_3(B,z) &= z^6 - \left(\tfrac{3}{2}B - \tfrac{13}{4}\right)z^4 + \left(\tfrac{3}{5}B^2 - \tfrac{57}{20}B + \tfrac{47}{80}\right)z^2 - \tfrac{1}{20}B^3 + \tfrac{2}{5}B^2 - \tfrac{63}{160}B - \tfrac{117}{320}. \end{aligned} \tag{53}$$

Correspondingly, the solutions of (48) are

$$f_n(B,W) = e^{i\pi\sqrt{W+B+1/4}} \frac{(n!)^2 \Gamma(n+1-\sqrt{B+1})\Gamma(n+1+\sqrt{B+1})}{(2n)!\Gamma(1-\sqrt{B+1})\Gamma(1+\sqrt{B+1})} {}_4F_3\left(-n, n+1, \frac{1}{2} - \sqrt{W+B+\frac{1}{4}}, \frac{1}{2}\right.$$
$$\left. + \sqrt{W+B+\frac{1}{4}}; 1, 1-\sqrt{B+1}, 1+\sqrt{B+1}; 1\right) \tag{54}$$

and the first four of these solutions are

$$\begin{aligned} f_0(B,W) &= e^{i\pi\sqrt{B+W+1/4}}, \\ f_1(B,W) &= e^{i\pi\sqrt{B+W+1/4}}\left(\tfrac{1}{2}B + W\right), \\ f_2(B,W) &= e^{i\pi\sqrt{B+W+1/4}}\left[\tfrac{1}{6}B^2 + B\left(W + \tfrac{1}{2}\right) + W(W+1)\right], \\ f_3(B,W) &= e^{i\pi\sqrt{B+W+1/4}}\left[\tfrac{1}{20}B^3 + B^2\left(\tfrac{3}{5}W + \tfrac{19}{20}\right) + B\left(\tfrac{3}{2}W^2 + \tfrac{22}{5}W + \tfrac{6}{5}\right) + W\left(W^2 + 4W + \tfrac{12}{5}\right)\right]. \end{aligned} \tag{55}$$

It is interesting that while we are now treating B as an arbitrary parameter, the eigenvalues are independent of B and thus are the same as in the case considered in Sec. IV [see (29)]. Note that in the limit $B \to 0$ the eigenfunctions in (55) smoothly reduce to the simpler simpler eigenfunctions in (34).

To find the Lorentz transformation properties of the parity operator we need to reconstruct the parity operator in terms of these solutions $f_n(B,W)$,

$$\mathcal{P} = \sum_{n=0}^{\infty} c_n f_n(B,W)\mathcal{P}. \tag{56}$$

This requires that we find the coefficients c_n in the identity

$$1 = \sum_{n=0}^{\infty} c_n f_n(B,W) = e^{i\pi z} \sum_{n=0}^{\infty} c_n g_n(B,z). \tag{57}$$

To analyze this identity we multiply it by $e^{-i\pi z}$ and obtain

$$e^{-i\pi z} = \sum_{n=0}^{\infty} c_n g_n(B,z). \tag{58}$$

Next, we continue analytically this formal functional equation to the complex z-plane and let $x = iz$. Equation (58) now becomes

$$e^{-x\pi} = \sum_{n=0}^{\infty} (-1)^n c_n P_n(x^2), \tag{59}$$

where $P_n(x^2)$ is defined in (B1). Next, we multiply both sides of (59) by

$$\frac{4\pi^2(2n)!(2n+1)!x\tanh(x\pi)}{(n!)^4\Gamma^2(n+1-\sqrt{B+1})\Gamma^2(n+1+\sqrt{B+1})[\cos(2\pi\sqrt{B+1})+\cosh(2x\pi)]}P_m(x^2)$$

and then integrate over x from 0 to ∞. Using the orthogonality property of Wilson polynomials in (B2), we get the formula for c_n,

$$c_n = \frac{4(-1)^n\pi^2(2n)!(2n+1)!}{(n!)^4\Gamma^2(n+1-\sqrt{B+1})\Gamma^2(n+1+\sqrt{B+1})}\int_0^{\infty} dx \frac{xe^{-x\pi}\tanh(x\pi)}{\cos(2\pi\sqrt{B+1})+\cosh(2x\pi)}P_n(x^2). \tag{60}$$

We conclude that we have decomposed the representation under which $\mathcal{P}$ transforms into a direct sum of finite-dimensional irreducible representations. Even though the operator B is taken to be nonzero, the eigenvalues in the difference-equation eigenvalue problem (48) remain unchanged. Thus, the conclusion of Sec. IV that the parity operator $\mathcal{P}$ transforms as the direct sum of the spin-0 components of the finite-dimensional tensor representations $(0,1)\oplus(0,3)\oplus(0,5)\oplus(0,7)\oplus\cdots$ remains unchanged.

Finally, as we observed at the end of Sec. IV, we point out that the first irreducible representation $f_0(B,W)\mathcal{P}$ in the direct sum (56) is a scalar. Thus, we may conclude that under a Lorentz transformation the parity operator $\mathcal{P}$ transforms as the operator $e^{-i\pi\sqrt{B+W+1/4}}$.

VI. FINAL REMARKS

The general case for (24) is obtained when all three parameters, B, M, and W, are nonzero. For this case we cannot solve (24) in terms of polynomials but we conjecture that the eigenvalues in (29) remain unchanged.[8] Assuming that this is indeed the case, we may conclude that the Lorentz transformation properties of the parity operator are unchanged from what we found in Secs. IV and V; namely, the parity operator transforms like the direct sum of irreducible representations in (47).

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APPENDIX A: PROPERTIES OF WILSON POLYNOMIALS

In this appendix, we list the properties of the Wilson polynomials $W_n(x^2;a,b,c,d)$ with parameters $a=b=\frac{1}{2}$, $c=d=\frac{3}{2}$.[9–11] For simplicity, we define the associated *monic* Wilson polynomials

$$P_n(x^2) \equiv \frac{(-1)^n(n+2)!}{(2n+2)!}W_n\left(x^2;\frac{1}{2},\frac{1}{2},\frac{3}{2},\frac{3}{2}\right). \tag{A1}$$

(The coefficient of the highest power in a *Monic* polynomial is unity.) These polynomials are used in Sec. IV.

The orthogonality condition is[11]

$$\frac{\pi^2}{4}\int_0^\infty dx\, x(1+4x^2)^2\frac{\sinh(x\pi)}{\cosh^3(x\pi)}P_n(x^2)P_m(x^2)=\frac{(n!)^2[(n+1)!]^4[(n+2)!]^4}{[(2n+2)!]^2(2n+3)!}\delta_{nm}. \tag{A2}$$

The polynomials $P_n(x^2)$ satisfy a three-term recurrence relation,

$$P_n(x^2)=\left[x^2-\frac{1}{2}n(n+1)\right]P_{n-1}(x^2)+\frac{(n-1)^2n^2(n+1)^2}{4(2n-1)(2n+1)}P_{n-2}(x^2), \tag{A3}$$

where the first two polynomials are $P_0(x^2)=1$ and $P_1(x^2)=x^2-\frac{3}{4}$.

Some generating functions for these polynomials are

$$\sum_{n=0}^\infty\frac{2(2n+2)!P_n(x^2)t^n}{(n!)^2[(n+2)!]^2}={}_2F_1\left(\frac{1}{2}+ix,\frac{1}{2}+ix;1;-t\right){}_2F_1\left(\frac{3}{2}-ix,\frac{3}{2}-ix;1;-t\right),$$

$$\sum_{n=0}^\infty\frac{(2n+2)!P_n(x^2)t^n}{n![(n+1)!]^2(n+2)!}={}_2F_1\left(\frac{1}{2}+ix,\frac{3}{2}+ix;2;-t\right){}_2F_1\left(\frac{1}{2}-ix,\frac{3}{2}-ix;2;-t\right), \tag{A4}$$

$$\sum_{n=0}^\infty\frac{(2n+2)!P_n(x^2)t^n}{(n!)^2[(n+1)!]^2}=\frac{1}{(1+t)^3}{}_4F_3\left[\frac{3}{2},2,\frac{1}{2}+ix,\frac{1}{2}-ix;1,2,2;\frac{4t}{(1+t)^2}\right].$$

APPENDIX B: FURTHER PROPERTIES OF WILSON POLYNOMIALS

In this appendix, we list the properties of the Wilson polynomials $W_n(x^2;a,b,c,d)$ with parameters $a=b=\frac{1}{2}$, $c=\frac{1}{2}-\sqrt{B+1}$, $d=\frac{1}{2}+\sqrt{B+1}$.[9–11] We define the associated monic polynomials,

$$P_n(x^2)\equiv\frac{(-1)^n n!}{(2n)!}W_n\left(x^2;\frac{1}{2},\frac{1}{2},\frac{1}{2}-\sqrt{B+1},\frac{1}{2}+\sqrt{B+1}\right). \tag{B1}$$

These polynomials are used in Sec. V.

Orthogonality,[11]

$$4\pi^2\int_0^\infty dx\, x\frac{\tanh(x\pi)}{\cos(2\pi\sqrt{B+1})+\cosh(2x\pi)}P_n(x^2)P_m(x^2)$$
$$=\frac{(n!)^4\Gamma^2(n+1-\sqrt{B+1})\Gamma^2(n+1+\sqrt{B+1})}{(2n)!(2n+1)!}\delta_{nm}. \tag{B2}$$

Recurrence relation,

$$P_n(x^2)=\left[x^2-\frac{B}{2}-\frac{1}{4}+\frac{n(n+1)}{2}\right]P_{n-1}(x^2)+\frac{n^2[B-(n-1)(n+1)]^2}{4(2n-1)(2n+1)}P_{n-2}(x^2), \tag{B3}$$

with $P_0(x^2)=1$ and $P_1(x^2)=x^2+\frac{1}{2}B+\frac{1}{4}$.

Generating functions,

$$\sum_{n=0}^{\infty} \frac{(2n)!P_n(x^2)t^n}{(n!)^4} = {}_2F_1\left(\frac{1}{2}+ix,\frac{1}{2}+ix;1;-t\right)\,{}_2F_1\left(\frac{1}{2}-\sqrt{B+1}-ix,\frac{1}{2}+\sqrt{B+1}-ix;1;-t\right) \tag{B4}$$

and

$$\begin{aligned}\sum_{n=0}^{\infty} &\frac{(2n)!P_n(x^2)t^n}{(n!)^2\Gamma(n+1-\sqrt{B+1})\Gamma(n+1+\sqrt{B+1})}\\ &= \frac{\sin(\pi\sqrt{B+1})}{\pi\sqrt{B+1}}\,{}_2F_1\left(\frac{1}{2}+ix,\frac{1}{2}-\sqrt{B+1}+ix;1-\sqrt{B+1};-t\right)\\ &\quad\times {}_2F_1\left(\frac{1}{2}-ix,\frac{1}{2}+\sqrt{B+1}-ix;1+\sqrt{B+1};-t\right)\\ &= \frac{\sin(\pi\sqrt{B+1})}{\pi(1+t)\sqrt{B+1}}\,{}_4F_3\left(\frac{1}{2},1,\frac{1}{2}+ix,\frac{1}{2}-ix;1,1-\sqrt{B+1},1+\sqrt{B+1};\frac{4t}{(1+t)^2}\right).\end{aligned} \tag{B5}$$

[1] Note that both $\mathcal{P}$ and $\mathcal{P}_I$ are reflection operators in the sense that their squares are the unity operator, $\mathcal{P}^2=\mathcal{P}_I^2=\mathbb{1}$.

[2] I. M. Gel'fand, R. A. Minlos, and Z. Ya. Shapiro, *Representations of the Rotation and Lorentz Groups and Their Applications* (MacMillan, New York, 1963).

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[5] Note that this equation makes use of a specified function $f(B,M,W)$ in (21), where the series coefficients are determined by (22) and (23). These equations are equivalent to (24), which is the statement that $f(B,M,W)\mathcal{P}$ is the spin-0 component of the irreducible $(0,\ell_1)$ representation.

[6] C. M. Bender and S. A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers* (Springer, New York, 1999), pp. 231–233.

[7] For the irreducible representations of the Lorentz group if the parameter $\ell_0=0$, then $(0,\ell_1)$ and $(0,-\ell_1)$ label exactly the same representation. Thus, we may assume without loss of generality that ℓ_1 is a positive number. See Ref. 2.

[8] Verifying this claim is difficult and requires heavy numerical analysis. We believe that the situation is similar to that for the eigenfunctions for the quantum harmonic and anharmonic oscillators. In the former case, after the Gaussian is divided off, the eigenfunctions satisfy the boundary conditions in a simple way; namely, by truncating in the form of Hermite polynomials. In the latter case, after the Gaussian is removed, the eigenfunctions do not truncate, but they still satisfy the boundary conditions as one can verify numerically.

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Cauchy problems of the gauged sigma model

Hyungjin Huh[a)]
School of Mathematical Sciences, Seoul National University, Seoul 151-747, Korea

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We study the gauged sigma model. In $\mathbb{R}^{1+1}$ the existence of the global smooth solution will be proved. Furthermore we show that the global weak solutions exist in $\mathbb{R}^{n+1}$ $(n=2,3)$. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The O (3) sigma model is a popular one in theoretical physics. From the point of view of a particle physicist, however, the model has one important drawback, it is scale invariant and as a result its soliton solutions have arbitrary size, making them unsuitable as models for particles. In Ref. 13, the new possibility of breaking the scale invariance of the sigma model was proposed by introducing a U (1) gauge field whose dynamics is governed by Maxwell terms. Adding also a suitable potential one obtains a field theory of Bogomol'nyi type with topological solitons. Some analysis of the self-dual equations can be found in Refs. 3 and 21.

We will study time-dependent problems. In the usual sigma model (called wave map), evolution problems have been studied extensively (see Refs. 16 and 18). Let us review briefly the results for global existence in time. Wave map in $(1+1)$ dimension extends smoothly all the time.[6,15] In $(3+1)$ dimension, development of singularities from smooth initial data was showed in Ref. 15 by using the self-similar structure of the sigma model. Also Shatah proved that there exists global weak solution to wave map which has a S^n target manifold. Space two-dimensional case is critical. Recently Tatatu[19] and Tao[20] proved global regularity of wave maps in $(2+1)$-dimension under the assumption of small Besov norm, respectively, small energy. Also we refer to the subsequent works by Klainerman-Rodnianski,[9] Nahmod–Stefanov–Uhlenbeck,[12] Shatah-Struwe,[17] as well as Krieger.[10]

We shall pursue the similar results for the gauged sigma model. In Sec. II the equations and basic facts will be presented. In Sec. III the global existence of a smooth solution in $(1+1)$ will be proved, while the global weak solution in $n+1$ $(n=2,3)$ will be treated in Sec. IV.

II. EQUATIONS AND BASIC FACTS

A point in the $(n+1)$-dimensional Minkowski space will be denoted by $(t,x)=(x_\alpha)_{0\le\alpha\le n}$. The space–time derivatives of a function $f:=\mathbb{R}\times\mathbb{R}^n\to\mathbb{R}$ are denoted by $\partial f=(\partial_t f,\nabla f)=(\partial_t f,\partial_1 f,\ldots,\partial_n f)$. We raise and lower indices with the Minkowski metric $\eta=(\eta_{\alpha\beta})=\eta^{-1}=(\eta^{\alpha\beta})=\mathrm{diag}(-1,1,\ldots,1)$. We also use the summation convention where we sum over repeated indices. Therefore, the wave operator is denoted by $\Box=\partial_\alpha\partial^\alpha$. Greek indices are used for denoting $0,\ldots,n$ while italic for $1,\ldots,n$.

The target manifold of ϕ is S^2, i.e., $\phi=(\phi_1,\phi_2,\phi_3)$ such that $\phi_1^2+\phi_2^2+\phi_3^2=1$. Introduce the Maxwell field $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$. The Lagrangian of the gauged O (3) model is

$$\mathcal{L}(\phi,A)=\frac{1}{2}\int\langle D^\mu\phi,D_\mu\phi\rangle+(1-n\cdot\phi)^2+\frac{1}{2}F^{\mu\nu}F_{\mu\nu},\tag{1}$$

where $\langle .,.\rangle$ is usual inner product in $\mathbb{R}^3$ and the gauge-covariant derivatives on ϕ are defined by

[a)]Electronic mail: hjhuh3@math.snu.ac.kr

$$D_\mu\phi = \partial_\mu\phi + A_\mu(n\times\phi) \quad [n=(0,0,1)].$$

The Euler–Lagrange equations are

$$D_\mu D^\mu\phi + (0,0,1-\phi_3) + \phi(\langle D^\mu\phi, D_\mu\phi\rangle + \phi_3(\phi_3-1)) = 0, \tag{2}$$

$$\partial_\mu F^{\mu\nu} = \langle D^\nu\phi, n\times\phi\rangle. \tag{3}$$

The Lagrangian action is invariant under the following gauge transformations:

$$\phi=(z,\phi_3)\to(ze^{i\chi},\phi_3), \quad A_\mu\to A_\mu-\partial_\mu\chi,$$

where $\chi:\mathbb{R}^{n+1}\to\mathbb{R}$ is a smooth function and we use the notation $(\phi_1,\phi_2)=z_1+iz_2=z$. A suitable gauge condition will be chosen according to the problem.

The constraint $|\phi|=1$ will be preserved as follows. If the equations (2) are satisfied in the $[0,T]\times\mathbb{R}^n$ then $\rho=|\phi|^2-1$ is the solution of the following equation:

$$[\partial_\mu\partial^\mu + 2\langle D_\mu\phi, D^\mu\phi\rangle + 2\phi_3(\phi_3-1)](|\phi|^2-1)=0.$$

This is a linear Klein–Gordon equation for the function ρ with external potential $2\langle D_\mu, D^\mu\rangle + 2\phi_3(\phi_3-1)$. Together with the initial conditions $\rho(0)=|\phi(0,\cdot)|^2-1$ and $\partial_t\rho(0)=\langle\phi(0,\cdot),\partial_t\phi(0,\cdot)\rangle=0$, it implies that $\rho=0$ in $[0,T]\times\mathbb{R}^n$.

The conserved energy $\mathcal{E}(t)$ for gauged O (3) model is

$$\mathcal{E}(t)=\int_{\Sigma_t}\langle D_\mu\phi, D_\mu\phi\rangle + (1-n\cdot\phi)^2 + \frac{1}{2}F_{\mu\nu}F_{\mu\nu} = \mathcal{E}(0), \tag{4}$$

where $\Sigma_\tau=\{(t,x)\in\mathbb{R}^{n+1}\,|\,t=\tau\}$. $H^s(\mathbb{R}^n)$ denotes the usual Sobolev space $W^{s,2}(\mathbb{R}^n)$ and $\dot{H}^s(\mathbb{R}^n)$ homogeneous Sobolev space $\dot{W}^{s,2}(\mathbb{R}^n)$.

III. EXISTENCE OF A SMOOTH SOLUTION IN $\mathbb{R}^{1+1}$

Here Lorentz gauge will be considered. Equations (2) and (3) with the condition $\partial_\mu A^\mu=0$ can be rewritten as

$$D_\mu D^\mu\phi + (0,0,1-\phi_3) + \phi(\langle D^\mu\phi, D_\mu\phi\rangle + \phi_3(\phi_3-1)) = 0, \tag{5}$$

$$\partial_\mu\partial^\mu A^\nu = \langle D^\nu\phi, n\times\phi\rangle, \tag{6}$$

$$\partial_\mu A^\mu = 0. \tag{7}$$

With the finite energy smooth initial data $(\phi(0,\cdot),\partial_t\phi(0,\cdot),A_\mu(0,\cdot),\partial_t A_\mu(0,\cdot))$ such that $|\phi(0,\cdot)|=1, \langle\phi(0,\cdot),\partial_t\phi(0,\cdot)\rangle=0$ and $\partial_\mu A^\mu=0$ the Cauchy problem will be considered. Note that the equation (7) is automatically satisfied as long as the solutions of the equations (5) and (6) exist if the initial data satisfy $\partial_\mu A^\mu(0,\cdot)=0$.

The short time existence of smooth solution is classical. We introduce the pseudoenergy of the equations

$$E^{(1)}(t)=\sum_{|I|\le 1}\|\partial^I A_\alpha(t,\cdot)\|_{L^2(\mathrm{R})} + \|(1-n\cdot\phi)(t,\cdot)\|_{L^2(\mathrm{R})} + \sum_{\alpha=0,1}\|\partial_\alpha\phi(t,\cdot)\|_{L^2(\mathrm{R})}.$$

It is seen that

$$E^{(1)}(t)\le C(1+t^2)\mathcal{E}^{1/2}(0).$$

Especially $\|A_\alpha\|_{L^2(R)}$ may be estimated in the following way:

$$\partial_t \|A_\alpha(t)\|_{L^2(\mathrm{R})} \leqslant \|\partial_t A_\alpha(t)\|_{L^2(\mathrm{R})} \leqslant \int_0^t \|\langle D_\alpha \phi, n \times \phi\rangle\|_{L^2(\mathrm{R})}\, \mathrm{d}s \leqslant t\mathcal{E}^{1/2}(0).$$

Our main purpose is to *a priori* estimate the L^2 norm of the second derivative of (A, ϕ),

$$E^{(2)}(t) = \sum_{|I|\leqslant 2} \|\partial^I A_\alpha(t,\cdot)\|_{L^2(\mathrm{R})} + \|(1 - n\cdot\phi)(t,\cdot)\|_{L^2(\mathrm{R})} + \sum_{1\leqslant|I|\leqslant 2} \|\partial^I \phi(t,\cdot)\|_{L^2(\mathrm{R})}.$$

If we can control $\|D_\mu D_\nu \phi(t,\cdot)\|_{L^2(\mathrm{R})}$, then $\|\partial^2 A(t,\cdot)\|_{L^2(R)}$ is bounded by an energy estimate applied to (6). *A priori* bound for $E^{(2)}(t)$ will be obtained by Gronwall's inequality. Considering the fact $|\phi|=1$ in $[0,T]\times\mathbb{R}^n$ and the definition of D_μ, we know

$$\partial_\mu\langle\phi,\psi\rangle = \langle D_\mu\phi,\psi\rangle + \langle\phi, D_\mu\psi\rangle, \tag{8}$$

$$0 = \langle D_\mu\phi, D_\nu\phi\rangle + \langle\phi, D_\mu D_\nu\phi\rangle, \tag{9}$$

$$D_\mu D_\nu\phi - D_\nu D_\mu\phi = F_{\mu\nu}(n\times\phi), \tag{10}$$

which are used in next inequality.

$$\frac{1}{2}\frac{d}{dt}\int_{\mathrm{R}} \langle D_\mu D_\nu\phi, D_\mu D_\nu\phi\rangle \leqslant \int_{\mathrm{R}} \langle (D_0D_0 - D_1D_1)(D_\nu\phi), D_0D_\nu\phi\rangle + F_{01}\langle n\times D_\nu\phi, D_1D_\nu\phi\rangle. \tag{11}$$

Operating D_ν on the equation (5) and using the fact that

$$\langle\phi\langle DD\phi, D\phi\rangle, D_\mu D_\nu\phi\rangle = -\langle DD\phi, D\phi\rangle\langle D_\mu\phi, D_\nu\phi\rangle,$$

we obtain the following inequality:

$$\frac{1}{2}\frac{d}{dt}\int_{\mathrm{R}} \langle D_\mu D_\nu\phi, D_\mu D_\nu\phi\rangle \leqslant C\int_{\mathrm{R}} |DD\phi||\partial F| + |F||D\phi| + |DD\phi||D\phi| + C\int_{\mathrm{R}} |DD\phi||D\phi|^3 + |F||DD\phi||D\phi|, \tag{12}$$

where $D\phi$ and F are used schematically. At first ∂F consist of $\partial_0 F_{01}$ and $\partial_1 F_{01}$. Lorentz gauge shows that

$$|\partial_0 F_{01}| = |\partial_0\partial_0 A_1 - \partial_1\partial_1 A_1| = |\langle D_1\phi, n\times\phi\rangle| \leqslant |D_1\phi|,$$

$$|\partial_1 F_{01}| = |\partial_0\partial_0 A_0 - \partial_1\partial_1 A_0| = |\langle D_0\phi, n\times\phi\rangle| \leqslant |D_0\phi|.$$

Therefore the term $|\partial F|$ may be bounded by $|D\phi|$. The most difficult terms which we must treat are the integrand of the second line of (12). The formulation of the following covariant Sobolev inequalities is essentially the same as Proposition A.1. of Ref. 5.

Proposition 3.1: Let $n\geqslant 1, 1\leqslant q\leqslant\infty, 1\leqslant r\leqslant\infty$, *and let* σ *and* p *satisfy* $0\leqslant\sigma\leqslant 1, 1\leqslant p\leqslant\infty$, *and* $1/p=[(1-\sigma)/r]+\sigma[(1/q)-(1/n)]$. *Assume in addition that if* $p=\infty$, *then* $r<\infty$ *and* $\sigma<1$. *Then there exists a constant C, depending only on* n,p,q,r *such that the following inequality holds:*

$$\|\|\phi\|\|_{L^p} \leqslant C\|\|\phi\|\|_{L^r}^{1-\sigma}\left\{\sum_{1\leqslant j\leqslant n} \|\|D_j\phi\|\|_{L^q}\right\}^{\sigma},$$

provided in the case $r=\infty$ *and* $q<n$, *we assume in addition that either* ϕ *tends to zero at infinity or* $\phi\in L^{r_0}$ *for some finite* $r_0>0$.

Using the covariant Sobolev inequality, we know

$$\int_{\mathrm{R}} |DD\phi||D\phi|^3 \leqslant \|D\phi\|^3_{L^6(\mathrm{R})}\|DD\phi\|_{L^2(\mathrm{R})} \leqslant C\|D\phi\|^2_{L^2(\mathrm{R})}\|DD\phi\|^2_{L^2(\mathrm{R})}$$

and

$$\begin{aligned}\int_{\mathrm{R}} |DD\phi||D\phi||F| &\leqslant C\|DD\phi\|_{L^2(\mathrm{R})}\|D\phi\|_{L^4(\mathrm{R})}\|F\|_{L^4(\mathrm{R})} \leqslant C\|DD\phi\|^{5/4}_{L^2}\|D\phi\|^{3/4}_{L^2}\|F\|^{3/4}_{L^2}\|\partial F\|^{1/4}_{L^2}\\ &\leqslant C\|DD\phi\|^{5/4}_{L^2}\|D\phi\|_{L^2}\|\partial A\|^{3/4}_{L^2} \leqslant C\|DD\phi\|^{5/4}_{L^2}\mathcal{E}^{1/2}(0)\left(1+\int_0^t \|\langle D\phi, n\times\phi\rangle\|_{L^2}\right)^{3/4}\\ &\leqslant C\mathcal{E}^{1/2}(0)(1+t\mathcal{E}^{1/2}(0))^{3/4}\|DD\phi\|^{5/4}_{L^2(\mathrm{R})},\end{aligned}$$

where the usual Gagliardo–Nirenberg inequality $\|F\|_{L^4(\mathrm{R})} \leqslant C\|F\|^{3/4}_{L^2(\mathrm{R})}\|\nabla F\|^{1/4}_{L^2(\mathrm{R})}$ is used. Therefore, we conclude that

$$\frac{d}{dt}\|D_\mu D_\nu\phi\|^2_{L^2(\mathrm{R})} \leqslant C(\mathcal{E}(0)+1)\|D_\mu D_\nu\phi\|^2_{L^2(\mathrm{R})} + C(1+t\mathcal{E}^{7/6}(0))^{3/4}\|D_\mu D_\nu\phi\|^{5/4}_{L^2(\mathrm{R})}.$$

It is sufficient to conclude that $E^{(2)}$ is bounded. We can proceed to get the higher regularities by a boostrap argument, hence (ϕ, A) extends as smooth solution.

IV. EXISTENCE OF THE WEAK SOLUTION

First we shall prove the existence of weak solutions to the gauged O(3) sigma model in the three-dimensional spatial case. Here the Coulomb gauge $\nabla_i A^i = 0$ will be considered. Equations (2) and (3) under the Coulomb gauge condition can be rewritten as

$$D_\mu D^\mu\phi + (0,0,1-\phi_3) + \phi(\langle D^\mu\phi, D_\mu\phi\rangle + \phi_3(\phi_3-1)) = 0, \tag{13}$$

$$\partial_\mu\partial^\mu A_i = \langle D_i\phi, n\times\phi\rangle + \partial_i\partial^0 A_0, \tag{14}$$

$$\Delta A_0 = \langle D_0\phi, n\times\phi\rangle, \tag{15}$$

$$\nabla_i A^i = 0. \tag{16}$$

Following the idea of Ref. 8, we take the divergence-free projection operator $\mathcal{P}$ on (14), i.e., for any vector field A,

$$\mathcal{P}A = \Delta^{-1}(\nabla\times(\nabla\times A)).$$

If $\nabla_i A^i = 0$ then $\mathcal{P}A = A$. In view of this, the equation (14) implies

$$\partial_\mu\partial^\mu A_i = \mathcal{P}\langle D_i\phi, n\times\phi\rangle.$$

Note that the equation (16) is automatically satisfied as long as (14) are satisfied if the initial data are taken as $\nabla_i A^i(0) = 0$. Therefore our initial value problem reduces to the following one:

$$D_\mu D^\mu\phi + (0,0,1-\phi_3) + \phi(\langle D^\mu\phi, D_\mu\phi\rangle + \phi_3(\phi_3-1)) = 0, \tag{17}$$

$$\partial_\mu\partial^\mu A_i = \mathcal{P}\langle D_i\phi, n\times\phi\rangle, \tag{18}$$

$$\Delta A_0 = \langle D_0\phi, n \times \phi\rangle, \tag{19}$$

with the initial data $(\phi_0(0,\cdot)-n, \phi_1(0,\cdot), A_i(0,\cdot), \partial A_i(0,\cdot))$ in $(H^1(\mathbb{R}^3)\times L^2(\mathbb{R}^3)\times \dot{H}^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3))$ satisfying

$$|\phi(0,\cdot)| = 1, \quad \langle \phi(0,\cdot), \phi_1(0,\cdot)\rangle = 0,$$

$$\nabla^i A_i(0,\cdot) = 0, \quad \Delta A_0(0,\cdot) = \langle D_0\phi(0,\cdot), n \times \phi(0,\cdot)\rangle.$$

We consider the following approximation equations:

$$D_\mu D^\mu \phi^l + (0,0,1-\phi_3^l) + l(|\phi^l|^2 - 1)\phi^l = 0, \tag{20}$$

$$\Box A_i^l = \mathcal{P}\langle D_i\phi^l, n \times \phi^l\rangle, \tag{21}$$

$$\Delta A_0^l = \langle D_0\phi^l, n \times \phi^l\rangle \tag{22}$$

with the same data $(\phi_0(0,\cdot)-n, \phi_1(0,\cdot), A_i(0,\cdot), \partial A_i(0,\cdot))$. The main part of equations (20)–(22) look like Maxwell–Klein–Gordon with potential under Coulomb gauge. The global existence of finite energy solutions is shown in the Appendix. We will use the fact that (20)–(22) admit global finite energy solution for all l. Then the solution (A^l, ϕ^l) satisfy the energy inequality

$$\begin{aligned} E_l(t) &= \int_{\Sigma_t} \langle D_\mu\phi^l, D_\mu\phi^l\rangle + (1 - n\cdot\phi^l)^2 + \frac{1}{2}|F_{\mu\nu}^l|^2 + \frac{l}{4}\int_{\Sigma_t}(|\phi^l|^2-1)^2 \leqslant E_l(0) = E(0) \\ &= \int_{\Sigma_0} \langle D_\mu\phi, D_\mu\phi\rangle + (1-n\cdot\phi)^2 + \frac{1}{2}|F_{\mu\nu}|^2 \end{aligned} \tag{23}$$

uniformly in t for all l. Note that the initial condition $|\phi(0,\cdot)|=1$ is used at the last equality in (23).

The Coulomb gauge condition implies $\Delta A_j^l = \partial^i F_{ij}^l, \Delta A_0^l = \partial^i F_{i0}^l$. Thus given $F_{\alpha\beta}^l \in L^2(\mathbb{R}^3)$ there exists a unique A_μ^l which belongs to the homogeneous Sobolev space $\dot{H}^1(\mathbb{R}^3)$. Furthermore, we have

$$\|\nabla A_\mu^l\|_{L^2(\mathbb{R}^3)} \leqslant C\|F^l\|_{L^2(\mathbb{R}^3)} \leqslant CE(0)^{1/2}, \tag{24}$$

and

$$\|\partial_\mu\phi^l\|_{L^2(\mathbb{R}^3)} \leqslant \|D_\mu\phi^l\|_{L^2(\mathbb{R}^3)} + \|A_\mu^l\|_{L^6(\mathbb{R}^3)}\|n\times\phi^l\|_{L^3(\mathbb{R}^3)} \leqslant \|D_\mu\phi^l\|_{L^2(\mathbb{R}^3)} + C\|\nabla A_\mu^l\|_{L^2(\mathbb{R}^3)}\|n\times\phi^l\|_{L^3(\mathbb{R}^3)}, \tag{25}$$

where we used $\|A^l\|_{L^6(\mathbb{R}^3)} \leqslant C\|\nabla A^l\|_{L^2(\mathbb{R}^3)}$ for $A^l \in \dot{H}^1(\mathbb{R}^3)$. To estimate $\|n\times\phi^l\|_{L^3(\mathbb{R}^3)}^2$ the two facts will be used.

(i) $$\begin{aligned} \frac{\partial}{\partial t}\int_{\mathbb{R}^3}|n\times\phi^l|^2\,dx &= \frac{\partial}{\partial t}\int_{\mathbb{R}^3}|(\phi_1^l,\phi_2^l,0)|^2\,dx = \int_{\mathbb{R}^3} 2\langle(\phi_1^l,\phi_2^l,0), D_t(\phi_1^l,\phi_2^l,0)\rangle \\ &\leqslant 2\|(\phi_1^l,\phi_2^l,0)\|_{L^2(\mathbb{R}^3)}\|D_t\phi^l\|_{L^2(\mathbb{R}^3)}. \end{aligned}$$

Therefore we have

$$\|(n\times\phi^l)(t,\cdot)\|_{L^2(\mathbb{R}^3)} \leqslant C(1+t),$$

where C depends only on the initial data.

(ii) The algebraic inequality $x^4 \leqslant 10(y-1)^2+10(x^2+y^2-1)^2$ implies that $\|(n\times\phi^l)\|^4_{L^4(\mathbb{R}^3)} \leqslant 10\|1-n\cdot\phi^l\|^2_{L^2(\mathbb{R}^3)}+10\||\phi^l|^2-1\|^2_{L^2(\mathbb{R}^3)} \leqslant CE(t) \leqslant CE(0)$. Note that (i), (ii) do not depend on the dimension of space. With (i), (ii) the interpolation inequality shows that

$$\|(n\times\phi^l)(t,\cdot)\|_{L^3(\mathbb{R}^3)} \leqslant C(1+t),$$

which implies $\|\partial_\mu\phi^l\|_{L^2(\mathbb{R}^3)} \leqslant C(1+t)$.

To estimate $\partial_t A^l_0$ the following lemma will be used.

Lemma 4.1: Let f be a compactly supported integrable function and u the unique solution of the Poisson equation $\Delta u = f$ in $\mathbb{R}^n$, sufficiently small at $|x|\to\infty$. Then for $f\in L^p(\mathbb{R}^n)(1<p<n), 1/q=(1/p)-(1/n)$,

$$\nabla u \in L^q(\mathbb{R}^n) \quad \textit{and} \quad \|\nabla u\|_{L^q(\mathbb{R}^n)} \leqslant C\|f\|_{L^p(\mathbb{R}^n)}.$$

We should mention that the equation (20) implies

$$\partial^\alpha\langle D_\alpha\phi^l, n\times\phi^l\rangle = 0. \tag{26}$$

In fact,

$$\begin{aligned}\partial^\alpha\langle D_\alpha\phi^l, n\times\phi^l\rangle = \langle D_\alpha D^\alpha\phi^l, n\times\phi^l\rangle + \langle D_\alpha\phi^l, D^\alpha(n\times\phi^l)\rangle = -l(|\phi^l|^2-1)\langle\phi^l, n\times\phi^l\rangle + \langle\partial_\alpha\phi^l, \partial^\alpha(n\\ \times\phi^l)\rangle + A^{l\alpha}A^l_\alpha\langle n\times\phi^l, n\times n\times\phi^l\rangle + A^l_\alpha\langle\partial^\alpha\phi^l, n\times n\times\phi^l\rangle + A^l_\alpha\langle n\times\phi^l, \partial^\alpha(n\\ \times\phi^l)\rangle = 0.\end{aligned}$$

We differentiate equation (22) with respect to t and derive, with the help of (26), $\Delta\partial_t A^l_0 = \partial_i\langle D_i\phi^l, n\times\phi^l\rangle$. By Lemma 4.1 we show

$$\|\partial_t A^l_0\|_{L^2(\mathbb{R}^3)} \leqslant \|\Delta^{-1/2}\partial_i\langle D_i\phi^l, n\times\phi^l\rangle\|_{L^{6/5}(\mathbb{R}^3)} \leqslant \|D_i\phi^l\|_{L^2(\mathbb{R}^3)}\|n\times\phi^l\|_{L^3(\mathbb{R}^3)} \leqslant C(1+t).$$

Therefore for a given T, we can select a subsequence of $\{\phi^l, A^l\}$ which converges to a limit ϕ, A in the sense that as $l\to\infty$,

$$\partial_\mu\phi^l \to \partial_\mu\phi \text{ weakly}\star \text{ in } L^\infty([0,T];L^2(\mathbb{R}^3)), \tag{27}$$

$$\phi^l \to \phi \text{ locally in } L^2_{\text{loc}}([0,T]\times\mathbb{R}^3), \tag{28}$$

$$\partial A^l \to \partial A \text{ weakly}\star \text{ in } L^\infty([0,T];L^2(\mathbb{R}^3)). \tag{29}$$

Moreover, $\phi^l(t)\to\phi(t)$ in $L^2_{\text{loc}}(\mathbb{R}^3)$ locally uniformly in $t\in[0,T]$. Hence for any $t\in[0,T]$, by Fatou's lemma

$$\int_{\mathbb{R}^3}(|\phi|^2-1)^2 \leqslant \liminf\int_{\mathbb{R}^3}(|\phi^l|^2-1)^2 = 0.$$

So we conclude that $\phi:\mathbb{R}^{3+1}\to S^2$. Passing to the limit in (20), we just follow the idea of Ref. 15. We consider equivalent equations to (17)–(19), i.e.,

$$D_\mu(D^\mu\phi\wedge\phi) + (0,0,1-\phi_3)\wedge\phi = 0, \tag{30}$$

$$\partial_\mu\partial^\mu A_i = \mathcal{P}\langle D_i\phi, n\times\phi\rangle, \tag{31}$$

$$\Delta A_0 = \langle D_0\phi, n\times\phi\rangle. \tag{32}$$

Proposition 4.2: Assume (ϕ, A) satisfy the properties (27)–(29) *then (ϕ, A) is a weak solution*

of (17)–(19) *if and only if* (ϕ,A) *is a weak solution of* (30)–(32).

Proof: There is just one nontrivial relation between (17) and (30) which we must verify. We take the wedge product of (17) with ϕ to obtain

$$D^\mu D_\mu \phi \wedge \phi + (0,0,1-\phi_3)\wedge\phi = D^\mu(D_\mu\phi\wedge\phi) - D^\mu\phi\wedge D_\mu\phi + (0,0,1-\phi_3)\wedge\phi = 0,$$

i.e., $D^\mu(D_\mu\phi\wedge\phi)+(0,0,1-\phi_3)\wedge\phi=0$ in the sense of distribution.

Conversely, if $D^\mu(D_\mu\phi\wedge\phi)+(0,0,1-\phi_3)\wedge\phi=0$ then $D^\mu D_\mu\phi\wedge\phi+(0,0,1-\phi_3)\wedge\phi=0$ which implies

$$D^\mu D_\mu \phi + (0,0,1-\phi_3) + \lambda\phi = 0. \tag{33}$$

Multiplying equation (33) by ϕ and considering $|\phi|=1$, almost everywhere, we obtain

$$\lambda = \langle D_\mu\phi, D^\mu\phi\rangle + \phi_3(\phi_3-1).$$

Taking the exterior product of (20) with ϕ^l and using the fact that the nonlinear term always points in the direction of ϕ^l, we obtain

$$D_\mu(D^\mu\phi^l\wedge\phi^l) + (0,0,1-\phi_3^l)\wedge\phi^l = 0 \tag{34}$$

for all l. In the limit $l\to\infty$, the equation (34) is valid in the sense of distributions implying that (A,ϕ) weakly solve (17). Since $\phi^l-n\in L^2([0,T]\times\mathbb{R}^3)$ with $\partial\phi^l\in L^\infty([0,T];L^2(\mathbb{R}^3))$ we have $\phi^l\to\phi$ in $C([0,T];L^2(\mathbb{R}^3))$. Moreover testing (30) and (34) by a vector $\psi\in C_0^\infty(\mathbb{R}\times\mathbb{R}^3)$ over $\mathbb{R}^{3+1}$ and integrating by parts we get

$$\int_{\{0\}\times\mathrm{R}^3}\langle D_0\phi\wedge\phi - D_0\phi^l\wedge\phi^l,\psi\rangle \mathrm{d}x = \int_0^\infty\int_{\mathrm{R}^3}\langle (D_\alpha\phi^l\wedge\phi^l) - D_\alpha\phi\wedge\phi), D^\alpha\psi\rangle \mathrm{d}x\,\mathrm{d}t$$
$$+\int_0^\infty\int_{\mathrm{R}^3}\langle (0,0,1-\phi_3)\wedge\phi - (0,0,1-\phi_3^l)\wedge\phi^l,\psi\rangle \mathrm{d}x\,\mathrm{d}t.$$

In the limit $l\to\infty$, we can conclude that

$$D_0\phi(0,\cdot)\wedge\phi(0,\cdot) - D_0\phi^l(0,\cdot)\wedge\phi^l(0,\cdot) = (\partial_t\phi(0,\cdot)-\phi_1)\wedge\phi_0 = 0,$$

i.e., $\partial_t\phi(0,\cdot)=\phi_1$ in the sense of traces. Here we used the fact that both $\partial_t\phi(0,\cdot)$ and ϕ_1 are tangent to S^2 along ϕ_0.

From now on, we are concerned about the two-dimensional spatial case. The approximate equations can be obtained through the similar reduction procedure but we do not know if there is a result which states that Maxwell–Higgs equations in $\mathbb{R}^{2+1}$ under the condition of Coulomb gauge exist global in time with the initial data $(\phi-n,\partial\phi,A,\partial A)\in H^1(\mathbb{R}^2)\times L^2(\mathbb{R}^2)\times\dot{H}^1(\mathbb{R}^2)\times L^2(\mathbb{R}^2)$. Here we assume that the initial data $(\phi-n,\partial\phi,A,\partial A)$ can be approximated by the smooth function sequences $(\phi^k-n,\partial\phi^k,A^k,\partial A^k)$ with the constraint $|\phi^k(0,\cdot)|=1$. In fact we should note the following.

Remark: Let Σ be a smooth compact Riemannian surface and N be compact k-manifold. Then by a result of Ref. 13 the space $C^\infty(\Sigma;N)$ of smooth maps $u:\Sigma\to N\subset\mathbb{R}^m$ is dense in $H^1(\Sigma;N)$. But we do not know what happens if Σ is unbounded surface. Moreover is it possible that (ϕ_0-n,ϕ_1) satisfying $|\phi_0|=1$, $\langle\phi_0,\phi_1\rangle$ can be approximated in the $H^1(\mathbb{R}^2)\times L^2(\mathbb{R}^2)$ norm by the smooth function sequences $(\phi^k(0,\cdot)-n,\partial_t\phi^k(0,\cdot))$ with the constraint $|\phi^k(0,\cdot)|=1$, $\langle\phi^k(0,\cdot),\partial_t\phi^k(0,\cdot)\rangle=0$? Therefore our results below are conditional.

Remark: For a domain manifold M of dimension $m>2$ a result of Ref. 1 shows that the space $C^\infty(M;N)$ is dense in $H^1(M;N)$ if and only if $\pi_2(N)=0$ [where $\pi_2(N)$ is a second fundamental group of N]. Therefore in the three-dimensional spatial case we cannot assume approximation sequence ϕ^k generally.

We will use the fact that equations (20)–(22) with initial data $[\phi^k(0)-n, \partial\phi^k(0), A^k(0), \partial A^k(0)]$ admit global smooth solution for all k. In fact Maxwell–Higgs equations have the global smooth solution under the Lorentz gauge $\partial_\mu \tilde{A}^\mu = 0$ (see Ref. 2). Then by the suitable gauge transform the equations are changed into one with Coulomb gauge $\partial_i \tilde{A}^i = 0 (A_\mu = \tilde{A}_\mu + \partial_\mu \chi)$. The solutions (A^k, ϕ^k) satisfy the energy inequality

$$E_k(\phi^k, A^k)(t) = \int_{\Sigma_t} \langle D_\mu \phi^k, D_\mu \phi^k \rangle + (1 - n \cdot \phi^k)^2 + \frac{1}{2}|F^k_{\mu\nu}|^2 + \frac{l}{4}\int_{\Sigma_t} (|\phi^k|^2 - 1)^2 \leqslant E(\phi^k, A^k)(0)$$

$$= E(\phi, A)(0) + \frac{1}{2^k}. \tag{35}$$

The inequality (24) can be also obtained,

$$\| \nabla A^k_\mu \|_{L^2(R^2)} \leqslant C \| F^k_\mu \|_{L^2(R^2)} \leqslant C E(0)^{1/2},$$

and

$$\| \partial_\mu \phi^k \|_{L^2(R^2)} \leqslant \| D_\mu \phi^k \|_{L^2(R^2)} + \| A^k_\mu \|_{L^4(R^2)} \| n \times \phi^k \|_{L^4(R^2)}.$$

To estimate $\|A^k_\mu\|_{L^4(\mathrm{R}^2)}$ the two facts will be used. Note that $\dot{H}^1(\mathbb{R}^2)$ does not embed into $L^4(\mathbb{R}^2)$.

(a) To estimate L^2 norm of the solution itself A_i, use will be made of the following lemma. The proof is in Ref. 11.

Lemma 4.3: If u solves the Cauchy problem,

$$\Box u = \sum_{\alpha=0}^{2} \partial_\alpha G_\alpha, \quad u(0, \cdot) = f, \quad \partial_t u(0, \cdot) = g,$$

then

$$\| u(t, \cdot) \|_{L^2(R^2)} \leqslant \sum_{\alpha=0}^{2} \int \| G_\alpha(s, \cdot) \|_{L^2(R^2)} \, ds + C(f, g, G_0(0, \cdot)) \log(2 + t),$$

where $C(f, g, G_0(0, \cdot))$ is some constant depending on some weighted Sobolev norm of initial data f and g.

Applying Lemma 4.3 to $\Box A^k_j = \partial^\mu F^k_{\mu j} + \partial^0 \partial_j A^k_0$ we have

$$\| A^k_j(t) \|_{L^2(R^2)} \leqslant C \log(2 + t) + \int_0^t \| F^k(s) \|_{L^2(R^2)} \, ds \leqslant C(1 + tE(0)^{1/2}).$$

Therefore given $t \in [0, T]$, $A^k_j(t) \in H^1(\mathbb{R}^2)$ which implies

$$\| A^k_j(t) \|^2_{L^4(R^2)} \leqslant \| A^k_j(t) \|_{L^2(R^2)} \| \nabla A^k_j(t) \|_{L^2(R^2)} \leqslant C(1 + tE(0)^{1/2}).$$

(b) To estimate $\|A^k_0(t)\|_{L^4(\mathrm{R}^2)}$ we are going to estimate $\partial_t A^k_0$. We differentiate Eq. (22) with respect to t and derive, with the help of (26), $\Delta \partial_t A^k_0 = \partial_i \langle D_i \phi^k, n \times \phi^k \rangle$. By Lemma 4.1 we show

$$\| \partial_t A^k_0(t) \|_{L^4(R^2)} \leqslant \| \Delta^{-1/2} \partial_i \langle D_i \phi^k, n \times \phi^k \rangle \|_{L^{4/3}(R^2)} \leqslant \| D_i \phi^k \|_{L^2(R^2)} \| n \times \phi^k \|_{L^4(R^2)} \leqslant C E(0)^{1/4}. \tag{36}$$

Now using the inequality

$$4\|A_0^k\|_{L^4(R^2)}^3 \partial_t \|A_0^k\|_{L^4(R^2)} = \partial_t \int_{R^2} (A_0^k)^4 \, dx \leqslant 4\|A_0^k\|_{L^4(R^2)}^3 \|\partial_t A_0^k\|_{L^4(R^2)},$$

we derive

$$\|A_0^k(t)\|_{L^4(R^2)} \leqslant \|A_0^k(0)\|_{L^4(R^2)} + \int_0^t \|\partial_t A_0^k(s)\|_{L^4(R^2)} \, ds \leqslant C(1 + tE(0)^{1/4}).$$

By the observation (a), (b) we have

$$\|\partial_\mu \phi^k\|_{L^2(R^2)} \leqslant C(1 + t).$$

The remaining argument is the same as the previous one given in the case of three dimensions.

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APPENDIX

Here we show that the system (20)–(22) admits a global finite energy solution. The fine structure was used to prove the global finite energy solution of Maxwell–Klein–Gordon (MKG) equation in Ref. 8. Following the line of Ref. 8 we check the nontrivial points. To compare with Maxwell–Klein–Gordon equation in Ref. 8 we rewrite (20)–(22) with the notation $u = \phi_1 + \sqrt{-1}\phi_2$, $v = \phi_3 - 1$, and $D_\mu u = \partial_\mu u + \sqrt{-1}A_\mu u$,

$$D_\mu D^\mu u + \underbrace{l(|u|^2 + v^2 + 2v)u} = 0, \tag{A1}$$

$$\partial_\mu \partial^\mu v - v + l(|u|^2 + v^2 + 2v)(v + 1) = 0, \tag{A2}$$

$$\partial_\mu \partial^\mu A_i = -\mathcal{P}\,\mathrm{Im}(u\overline{D_i u}), \tag{A3}$$

$$\Delta A_0 = -\mathrm{Im}(u\overline{D_0 u}). \tag{A4}$$

Note that (A1)–(A4) are the same as equations in Ref. 8 except the braced part of (A1) and (A2). Let $A = (A_1, A_2, A_3)$ and define pseudoenergy,

$$\mathcal{Q}(A,u,v)(t) = \|\partial A(t,\cdot)\|_{L^2} + \|u(t,\cdot)\|_{L^2} + \|\partial u(t,\cdot)\|_{L^2} + \|v(t,\cdot)\|_{L^2} + \|\partial v(t,\cdot)\|_{L^2}.$$

The main theorem is as follows.

Theorem 5.1: *Consider initial data satisfying* $\nabla_i A^i(0,\cdot) = 0$ *such that* $\mathcal{Q}(0)$ *is finite. Under this hypothesis there exists a unique global generalized solution to the equation (A1)–(A4) verifying the energy inequality*

$$E_l(t) \leqslant C\mathcal{Q}^2(0)$$

as well as

$$(i) \quad \mathcal{Q}(t) \leqslant C(1 + t)\mathcal{Q}(0).$$

And on any finite interval $[0, T]$,

$$(ii) \quad \int_0^T (\|\Box A(t,\cdot)\|_{L^2} + \|\Box u(t,\cdot)\|_{L^2} + \|\Box v(t,\cdot)\|_{L^2}) dt \leqslant \infty.$$

The first nontrivial check point is the pp. 31–35 of Ref. 8. To estimate $\partial_t A_0$, the precise form of MKG equation was used. It is possible to construct the corresponding parts despite of the different form of potential. With the help of the relation (26) we have

$$\Delta \partial_t A_0 = \partial_t \langle D_0 \phi, n \times \phi \rangle = \partial_i \langle D_i \phi, n \times \phi \rangle.$$

So we may obtain the corresponding one of Proposition 3.2 in Ref. 8.

The second part is the pp. 35–39 in Ref. 8. Following the idea of Ref. 8 we will show the estimate

$$X(T) \leqslant CT^{1/2}(1 + \mathcal{Q}(0) + X(T))^4, \tag{A5}$$

where $X(T) = \int_0^T (\|\Box A(t,\cdot)\|_{L^2} + \|\Box u(t,\cdot)\|_{L^2} + \|\Box v(t,\cdot)\|_{L^2}) \mathrm{d}t$ and $0 < T < T^*$ is small, C is independent on both T^* and $\mathcal{Q}(0)$. With the standard form of the energy estimate applied to u, v, and A we have

$$\mathcal{Q}(t) \leqslant (\mathcal{Q}(0) + X(t)).$$

In view of the equation (A1)–(A3) we have

$$\begin{aligned} X(T) \leqslant & \int_0^T \|\mathcal{P}\,\mathrm{Im}(u\overline{Du})\|_{L^2} + 2\|u\partial_t A_0\|_{L^2} + 2\|A_0 \partial_t u\|_{L^2} + \int_0^T \|A \cdot \nabla u\|_{L^2} + \||A_0|^2 u\|_{L^2} + \||A|^2 u\|_{L^2} \\ & + \int_0^T l\|(|u|^2 + v^2 + 2v)u\|_{L^2} + l\|(|u|^2 + v^2 + 2v)(v+1)\|_{L^2}. \end{aligned} \tag{A6}$$

The first and second line of (A6) can be estimated in the same way as Ref. 8 using Sobolev inequalities, Strichartz and null form estimates. The third line can be estimated in a easier way,

$$\int_0^T \|uv^2\|_{L^2} \leqslant \int_0^T \|u\|_{L^6} \|v\|_{L^6}^2 \leqslant C \int_0^T \|\nabla u\|_{L^2} \|\nabla v\|_{L^2}^2 \leqslant C(\mathcal{Q}(0) + X(T))^3.$$

We show the inequality (A5) then the rest is straightforward as in Ref. 8.

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The symmetries of the Dirac–Pauli equation in two and three dimensions

C. Adam[a] and J. Sánchez-Guillén[b]
Departamento de Física de Partículas, Facultad de Física, Universidad de Santiago, E-15706 Santiago de Compostela, Spain and Instituto Galego de Fisica de Altas Enerxias, E-15706 Santiago de Compostela, Spain

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We calculate all symmetries of the Dirac–Pauli equation in two-dimensional and three-dimensional Euclidean space. Further, we use our results for an investigation of the issue of zero mode degeneracy. We construct explicitly a class of multiple zero modes with their gauge potentials. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1884885]

I. INTRODUCTION

The abelian Dirac equation in Euclidean space in two and three dimensions is

$$\mathcal{D}\Psi \equiv \sigma^k(-i\partial_k - G^k(\mathbf{r}))\Psi(\mathbf{r}) = 0, \tag{1}$$

where, in three dimensions, $\mathbf{r}=(x,y,z)^t$, $k=x,y,z$, σ^k are the Pauli matrices, and $G^k \equiv (G^x,G^y,G^z)$ is the gauge potential (we use superscripts for the components because subscripts will be exclusively reserved to describe partial derivatives). In two dimensions all z components are absent. Further, $\Psi=(\Phi,\chi)^t$ is a two-component spinor.

The Pauli equation is obtained from the Dirac equation by simply squaring the Dirac operator $\mathcal{D}$ acting on Ψ,

$$((-i\partial_k - G^k)^2 - \sigma^l H^l)\Psi = 0, \tag{2}$$

where $\vec{H}$ is the magnetic field, $\vec{H}=\nabla\times\vec{G}$. Solutions of the Dirac equation (1) are, at the same time, solutions of the Pauli equation, therefore we shall treat them on an equal footing.

Solutions to the Pauli or Dirac equation are relevant in several instances. They describe the behavior of nonrelativistic electrons in the presence of magnetic fields, and their existence, among other issues, influences the stability of nonrelativistic matter.[1,2] On the other hand, they influence the behavior of the fermion determinant $\det \mathcal{D}$ for relativistic electrons and are, therefore, relevant for the strong field behavior of relativistic electrons,[3–5] and for a proper path-integral quantization of quantum electrodynamics (QED) in two[6–8] and three dimensions.

For the Dirac equation in two dimensions the most important information on solutions is provided by the Aharanov–Casher theorem,[9] which states that there are n square-integrable solutions when the magnetic flux divided by 2π is between n and $n+1$, i.e., $n<(\text{flux}/2\pi)\leqslant n+1$. For the Dirac equation in three dimensions the available information is much scarcer. The first examples of solutions have been given in 1986, see Ref. 2. Further examples have been provided in Refs. 10–12, and the existence of multiple solutions (zero mode degeneracy) has been first demonstrated in Refs. 13–15. Further results on zero-mode supporting gauge potentials may be found in Refs. 16–18. A general classification of zero-mode supporting gauge fields is still missing.

[a]Electronic mail: adam@radon.mat.univie.ac.at
[b]Electronic mail: joaquin@fpaxp1.usc.es

In this paper we study the symmetries of the Dirac equation (1) both in two and three dimensions, in order to gain some further insight into the solution space of these equations. In Sec. II we calculate the symmetries of the Dirac equation in two dimensions and briefly apply our results to the issue of multiple zero modes. In Sec. III we calculate the symmetries of the Dirac equation in three dimensions. We use the method of prolongations for all our symmetry calculations, which is described in detail in Ref. 19. In Sec. IV, we use our results on symmetries of the three-dimensional Dirac equation for a discussion of the issue of zero mode degeneracy (i.e., multiple solutions) in three dimensions. In Sec. IV A, we discuss how our results on symmetries can be used to construct multiple zero modes in principle. In Sec. IV B, we apply the results of Sec. IV A for the explicit construction of a class of multiple zero modes together with their corresponding gauge potentials.

II. SYMMETRIES OF THE DIRAC EQUATION IN TWO DIMENSIONS

For the Dirac equation in two dimensions it is known from the Aharanov–Casher theorem that all zero modes (i.e., square-integrable solutions) are either left handed (i.e., the lower component of Ψ is zero) or right handed (the upper component of Ψ is zero). Further, a solution of the first type (left handed) may be mapped into a solution of the second type by the simple replacement $G^k \rightarrow -G^k$, therefore we may restrict, e.g., to the left-handed case

$$(-i\partial_x - G^x + \partial_y - iG^y)\Phi = 0. \tag{3}$$

By introducing the modulus and phase of Φ via $\ln \Phi = \rho + i\lambda$ we may rewrite Eq. (3) in terms of two real first order equations as

$$\Delta_1 \equiv \rho_y + \lambda_x - G^x = 0, \tag{4}$$

$$\Delta_2 \equiv \rho_x - \lambda_y + G^y = 0, \tag{5}$$

where from now on subscripts denote partial derivatives, i.e., $\rho_x \equiv \partial_x \rho$, etc.

The vector field generating generic transformations on the independent and dependent variables is

$$v = X\partial_x + Y\partial_y + R\partial_\rho + L\partial_\lambda + F^x\partial_{G^x} + F^y\partial_{G^y}, \tag{6}$$

where X, Y, R, L, F^x, F^y may depend on all independent and dependent variables. The equations (4) and (5) contain first derivatives of the variables λ and ρ, therefore we need the first prolongation of v with respect to these variables,

$$\mathrm{pr}\, v = v + R^x\partial_{\rho_x} + R^y\partial_{\rho_y} + L^x\partial_{\lambda_x} + L^y\partial_{\lambda_y}, \tag{7}$$

where, e.g.,

$$R^x = D_x R - \rho_x D_x X - \rho_y D_x Y. \tag{8}$$

Here D_x is a total derivative, and we give the explicit (rather lengthy) expressions in Appendix A.

Now, a symmetry of a partial differential equation (PDE) $F(\rho, \rho_j, \ldots) = 0$ (of nth order, say) is a solution of the equation $\mathrm{pr}^{(n)} v(F) = 0$ which holds on-shell, i.e., when the original PDE is used together with its prolongations (PDEs that follow from $F = 0$ by applying total derivatives). As said, for the details of the used formalism we refer to Ref. 19.

Concretely, the determination of the symmetry transformation proceeds as follows. We require that $\mathrm{pr}\, v(\Delta_1) = 0 = \mathrm{pr}\, v(\Delta_2)$ whenever the equations (4) and (5) hold. Explicitly this means that

$$R^y + L^x - F^x = 0, \tag{9}$$

$$R^x - L^y + F^y = 0, \tag{10}$$

whenever the equations (4) and (5) hold. Equations (9) and (10) contain a number of algebraically independent functions (like ρ_x, $\rho_x G^y_x$, etc.) multiplying the coefficients (like R_x, R_ρ, etc.) which we want to determine. We may use the equations (4) and (5) to eliminate, e.g., λ_x and λ_y from the equations (9) and (10). Then we demand that the coefficient of each algebraically independent function (like ρ_x, $\rho_x G^y_x$, etc.) vanishes separately. This leads to more than 30 conditions for each of the two equations (9) and (10). Fortunately, most of these conditions are quite trivial, like, e.g., $X_\lambda = 0 = X_{A^x}$, etc. The final result is that Eq. (9) leads to the conditions

$$X = X(x,y), \quad Y = Y(x,y), \tag{11}$$

$$R = R(\rho,\lambda,x,y), \quad L = L(\rho,\lambda,x,y), \tag{12}$$

$$R_\rho - L_\lambda = Y_y - X_x, \tag{13}$$

$$L_\rho + R_\lambda = X_y + Y_x, \tag{14}$$

and

$$F^x = L_x + R_y + (L_\lambda - X_x)G^x + (R_\lambda - Y_x)G^y, \tag{15}$$

whereas Eq. (10) leads to the conditions

$$X = X(x,y), \quad Y = Y(x,y), \tag{16}$$

$$R = R(\rho,\lambda,x,y), \quad L = L(\rho,\lambda,x,y), \tag{17}$$

$$R_\rho - L_\lambda = -Y_y + X_x, \tag{18}$$

$$L_\rho + R_\lambda = -X_y - Y_x, \tag{19}$$

and

$$F^y = L_y - R_x - (R_\lambda + X_y)G^x + (L_\lambda - Y_y)G^y. \tag{20}$$

For later convenience we introduce the complex notation

$$z \equiv x + iy, \quad Z \equiv X + iY, \quad \sigma \equiv \rho + i\lambda, \quad \Sigma \equiv R + iL \tag{21}$$

and

$$G \equiv \tfrac{1}{2}(G^x + iG^y), \quad F \equiv \tfrac{1}{2}(F^x + iF^y) \tag{22}$$

which implies

$$\partial_\sigma \equiv \tfrac{1}{2}(\partial_\rho - i\partial_\lambda), \tag{23}$$

etc. Compatibility between the two sets of equations requires

$$X_x = Y_y, \quad X_y = -Y_x \tag{24}$$

which are just the Cauchy–Riemann equations, and

$$L_\rho = L_\lambda, \quad R_\lambda = -L_\rho, \tag{25}$$

which are the Cauchy–Riemann equations with respect to the target space variable $\sigma=\rho+i\lambda$. Therefore, X and Y are the real and imaginary part of a holomorphic function,

$$X + iY = Z(z), \quad z = x + iy, \tag{26}$$

whereas L and R are the real and imaginary part of a holomorphic function in the variable σ,

$$R + iL = \Sigma(\sigma, z, \bar{z}), \tag{27}$$

where Σ may still depend on $z, \bar{z}$. Finally, for F we find

$$F \equiv \tfrac{1}{2}(F^x + iF^y) = -i\Sigma_{\bar{z}} - G\bar{Z}_{\bar{z}} + G\Sigma_\sigma. \tag{28}$$

The most general symmetry generator

$$v = Z\partial_z + \bar{Z}\partial_{\bar{z}} + \Sigma\partial_\sigma + \bar{\Sigma}\partial_{\bar{\sigma}} + F\partial_G + \bar{F}\partial_{\bar{G}} \tag{29}$$

may be expressed as the semidirect sum of a symmetry generator v_Z with respect to the holomorphic function $Z(z)$ and a generator v_Σ with respect to the function $\Sigma(\sigma, z, \bar{z})$, where

$$v_Z = Z\partial_z + \bar{Z}\partial_{\bar{z}} - G\bar{Z}_{\bar{z}}\partial_G - \bar{G}Z_z\partial_{\bar{G}} \tag{30}$$

and

$$v_\Sigma = \Sigma\partial_\sigma + \bar{\Sigma}\partial_{\bar{\sigma}} + (-i\Sigma_{\bar{z}} + G\Sigma_\sigma)\partial_G + (i\bar{\Sigma}_z + \overline{G\Sigma_\sigma})\partial_{\bar{G}}. \tag{31}$$

Further, they obey the infinite-dimensional Lie algebra,

$$[v_{Z_1}, v_{Z_2}] = v_{Z_3}, \quad Z_3 = Z_1 Z_2' - Z_2 Z_1', \tag{32}$$

$$[v_{\Sigma_1}, v_{\Sigma_2}] = v_{\Sigma_3}, \quad \Sigma_3 = \Sigma_1 \Sigma_{2,\sigma} - \Sigma_2 \Sigma_{1,\sigma}, \tag{33}$$

which are just two copies of the Virasoro algebra in coordinate and target space, and

$$[v_Z, v_\Sigma] = v_{\tilde{\Sigma}}, \quad \tilde{\Sigma} = \Sigma_z Z + \Sigma_{\bar{z}}\bar{Z}. \tag{34}$$

It is quite interesting that the symmetry turns out to be so large, the semidirect product of two conformal groups in two dimensions.

[*Remark:* the symmetry transformations we found cover the whole solution space in the sense that any solution Φ of the Dirac equation (3) for any gauge potential G can be found by applying a symmetry transformation to the trivial solution $\Phi=1$, $G=0$. In fact, a target space transformation Σ of the type $\Sigma=f(z,\bar{z})$ is sufficient. For this subclass of transformations the above Lie algebra is abelian, therefore the exponentiation for finite Σ is trivial.]

As an application let us briefly discuss the issue of degeneracy of zero modes (i.e., multiple solutions of the Dirac equation for one gauge field G). The condition that the gauge field does not change is, of course, that the F in Eq. (28) is zero, which leads to the conditions $\Sigma_\sigma=\Sigma_{\bar{z}}=0$, that is $\Sigma=g(z)$ is a function in the variable z only. As said, the exponentiation of such Σ is trivial, therefore a

$$\Phi' = e^{g(z)}\Phi \tag{35}$$

is a local zero mode for the same gauge potential as Φ. Single valuedness of Φ' on the whole Euclidean plane restricts the allowed g [$\exp g(z)$ should be single valued] and the condition of square integrability further restricts the allowed $g(z)$. The fact that further zero modes of the same

Dirac operator may be produced by multiplying the given one with analytic functions of z is, of course, well known.

III. SYMMETRIES OF THE DIRAC EQUATION IN THREE DIMENSIONS

Introducing the real and imaginary part of the spinor components via $\Phi=\alpha+i\beta$, $\chi=\gamma+i\delta$, the Dirac equation (1) in three dimensions is equivalent to the four real equations,

$$\begin{aligned} \mathrm{I} &\equiv \beta_z + \delta_x - \gamma_y - G^z\alpha - G^x\gamma - G^y\delta = 0, \\ \mathrm{II} &\equiv \alpha_z + \gamma_x + \delta_y + G^z\beta + G^x\delta - G^y\gamma = 0, \\ \mathrm{III} &\equiv \beta_x + \alpha_y - \delta_z - G^x\alpha + G^y\beta + G^z\gamma = 0, \\ \mathrm{IV} &\equiv \alpha_x - \beta_y - \gamma_z + G^x\beta + G^y\alpha - G^z\delta = 0. \end{aligned} \tag{36}$$

If viewed as a system of algebraic equations for the three real unknowns (G^x, G^y, G^z), these four equations must be algebraically dependent. The dependence is given by the condition

$$V \equiv \nabla \cdot \vec{\Sigma} = 2(\alpha\gamma+\beta\delta)_x + 2(\alpha\delta-\beta\gamma)_y + (\alpha^2+\beta^2-\gamma^2-\delta^2)_z = 0, \tag{37}$$

where

$$\vec{\Sigma} \equiv \Psi^\dagger \vec{\sigma} \Psi = \begin{pmatrix} 2(\alpha\gamma+\beta\delta) \\ 2(\alpha\delta-\beta\gamma) \\ \alpha^2+\beta^2-\gamma^2-\delta^2 \end{pmatrix} \tag{38}$$

is the spin density of the spinor Ψ.

Again, we want to study the symmetries of the above equations (36) using the method of prolongations. The symmetry generating vector field is

$$v = X\partial_x + Y\partial_y + Z\partial_z + A\partial_\alpha + B\partial_\beta + C\partial_\gamma + D\partial_\delta + F^x\partial_{G^x} + F^y\partial_{G^y} + F^z\partial_{G^z} \tag{39}$$

and its prolongation to the needed order is

$$\begin{aligned} \mathrm{pr}\, v = v &+ A^x\partial_{\alpha_x} + A^y\partial_{\alpha_y} + A^z\partial_{\alpha_z} + B^x\partial_{\beta_x} + B^y\partial_{\beta_y} + B^z\partial_{\beta_z} + C^x\partial_{\gamma_x} + C^y\partial_{\gamma_y} + C^z\partial_{\gamma_z} + D^x\partial_{\delta_x} + D^y\partial_{\delta_y} \\ &+ D^z\partial_{\delta_z}, \end{aligned} \tag{40}$$

where, e.g., A^x is given by

$$A^x = A_x + A_\alpha\alpha_x + A_\beta\beta_x + A_\gamma\gamma_x + A_\delta\delta_x - \alpha_x X_x - \alpha_y Y_x - \alpha_z Z_x. \tag{41}$$

Here, we have already used some first results of the calculation below, namely that (analogously to the case in two dimensions) no coefficient depends on the gauge potential, and that the coefficients X, Y, Z of the translations in base space only depend on the base space coordinates x, y, z [otherwise the resulting expression (41) would be more complicated, analogously to the R^x of the two-dimensional case, which is given in Appendix A].

Acting with the prolonged vector field on the four equations (36) [$\mathrm{pr}\, v(I)=0$, etc.] leads to the following set of four equations:

$$G^x C + G^y D + G^z A + F^x \gamma + F^y \delta + F^z \alpha - D^x + C^y - B^z = 0,$$

$$G^x D - G^y C + G^z B + F^x \delta - F^y \gamma + F^z \beta + C^x + D^y + A^z = 0,$$

$$- G^x A + G^y B + G^z C - F^x \alpha + F^y \beta + F^z \gamma + B^x + A^y - D^z = 0, \tag{42}$$

$$G^x B + G^y A - G^z D + F^x \beta + F^y \alpha - F^z \delta + A^x - B^y - C^z = 0.$$

Next we must insert the explicit expressions for A^x, etc. We obtain algebraic expressions in terms of the target space variables and their partial derivatives, where we may eliminate four derivative terms with the help of the Dirac equations (36). (Explicitly, we eliminated δ_x, δ_y, δ_z, and γ_z.) For the resulting expressions one must require that the coefficient multiplying each partial derivative of the target space variables (like α_x or G^x_x) or product of partial derivatives vanishes separately. Doing this one realizes quickly that nothing may depend on the gauge potential and that the coefficients X, Y, Z may only depend on x, y, z.

The remaining coefficients which are multiplied by at least one partial derivative of a target space variable serve to determine the coefficients X, Y, Z and A, B, C, D. They are of two types. The first type consists of pairs of equations like

$$A_\delta + D_\alpha = Y_z + Z_y, \quad A_\delta + D_\alpha = - Y_z - Z_y \Rightarrow A_\delta + D_\alpha = 0, \quad Y_z + Z_y = 0$$

which lead to equations for the X, Y, Z and A, B, C, D independently. The equations for X, Y, Z are

$$X_x = Y_y = Z_z,$$

$$X_y + Y_x = 0, \quad X_z + Z_x = 0, \quad Y_z + Z_y = 0 \tag{43}$$

and have the conformal transformations in three-dimensional space as general solutions,

$$X = \frac{\theta^1}{2}(x^2 - y^2 - z^2) + \theta^2 xy + \theta^3 xz - l^3 y + l^2 z + \sigma x + x^0,$$

$$Y = \frac{\theta^2}{2}(y^2 - x^2 - z^2) + \theta^1 xy + \theta^3 yz + l^3 x - l^1 z + \sigma y + y^0, \tag{44}$$

$$Z = \frac{\theta^3}{2}(z^2 - x^2 - y^2) + \theta^1 xz + \theta^2 yz - l^2 x + l^1 y + \sigma z + z^0.$$

Here θ^i, l^i, σ, and $\vec{r}^0$ are constant parameters which parametrize the infinitesimal conformal transformations.

The equations for A, B, C, D are

$$A_\alpha = B_\beta = C_\gamma = D_\delta,$$

$$A_\beta + B_\alpha = 0, \quad A_\gamma + C_\alpha = 0, \quad A_\delta + D_\alpha = 0, \tag{45}$$

$$B_\gamma + C_\beta = 0, \quad B_\delta + D_\beta = 0, \quad C_\delta + D_\gamma = 0,$$

and have the conformal transformations in the four-dimensional target space as solutions,

$$A = \frac{\zeta^1}{2}(\alpha^2 - \beta^2 - \gamma^2 - \delta^2) + \zeta^2\alpha\beta + \zeta^3\alpha\gamma + \zeta^4\alpha\delta + \lambda\alpha - v^3\beta + v^2\gamma - v^1\delta + \alpha^0,$$

$$B = \frac{\zeta^2}{2}(\beta^2 - \alpha^2 - \gamma^2 - \delta^2) + \zeta^1\alpha\beta + \zeta^3\beta\gamma + \zeta^4\beta\delta + \lambda\beta + v^3\alpha - u^1\gamma - u^2\delta + \beta^0,$$

$$C = \frac{\zeta^3}{2}(\gamma^2 - \alpha^2 - \beta^2 - \delta^2) + \zeta^1\alpha\gamma + \zeta^2\beta\gamma + \zeta^4\gamma\delta + \lambda\gamma - v^2\alpha + u^1\beta - u^3\delta + \gamma^0, \tag{46}$$

$$D = \frac{\zeta^4}{2}(\delta^2 - \alpha^2 = \beta^2 - \gamma^2) + \zeta^1\alpha\delta + \zeta^2\beta\delta + \zeta^3\gamma\delta + \lambda\delta + v^1\alpha + u^2\beta + u^3\gamma + \delta^0.$$

Here the parameters ζ^j, u^i, v^i, λ and α^0, β^0, γ^0, δ^0 may still depend on the base space coordinates (x,y,z).

The second type of equations consists of equations like $C_\delta - A_\beta = X_y$ and establishes relations between the A, B, C, D and the X, Y, Z, thereby further restricting the possible A, B, C, D. The result is that the proper conformal transformation on target space must be absent, $\zeta^j \equiv 0$, and that the six target space rotation parameters are no longer independent,

$$u^1 - v^1 = l^1 + \theta^2 z - \theta^3 y \equiv L^1,$$

$$u^2 - v^2 = l^2 + \theta^3 x - \theta^1 z \equiv L^2, \tag{47}$$

$$u^3 - v^3 = l^3 + \theta^1 y - \theta^2 x \equiv L^3$$

leading to

$$A = \lambda\alpha - v^3\beta + v^2\gamma - v^1\delta + \alpha^0,$$

$$B = \lambda\beta + v^3\alpha - (v^1 + L^1)\gamma - (v^2 + L^2)\delta + \beta^0,$$

$$C = \lambda\gamma - v^2\alpha + (v^1 + L^1)\beta - (v^3 + L^3)\delta + \gamma^0, \tag{48}$$

$$D = \lambda\delta + v^1\alpha + (v^2 + L^2)\beta + (v^3 + L^3)\gamma + \delta^0,$$

where λ, v^i, and $\alpha^0, \cdots$ may still depend on (x,y,z). By shifting $v^i \to v^i - (L^i/2)$ the L^i are distributed more symmetrically,

$$
\begin{aligned}
A &= \lambda\alpha - \left(v^3 - \frac{L^3}{2}\right)\beta + \left(v^2 - \frac{L^2}{2}\right)\gamma - \left(v^1 - \frac{L^1}{2}\right)\delta + \alpha^0, \\
B &= \lambda\beta + \left(v^3 - \frac{L^3}{2}\right)\alpha - \left(v^1 + \frac{L^1}{2}\right)\gamma - \left(v^2 + \frac{L^2}{2}\right)\delta + \beta^0, \\
C &= \lambda\gamma - \left(v^2 - \frac{L^2}{2}\right)\alpha + \left(v^1 + \frac{L^1}{2}\right)\beta - \left(v^3 + \frac{L^3}{2}\right)\delta + \gamma^0, \\
D &= \lambda\delta + \left(v^1 - \frac{L^1}{2}\right)\alpha + \left(v^2 + \frac{L^2}{2}\right)\beta + \left(v^3 + \frac{L^3}{2}\right)\gamma + \delta^0,
\end{aligned}
\tag{49}
$$

and we find the half-integer valued representation of the base space rotations (with parameters l^i) acting on the (spinor) target space variables. It is interesting to note that the half-integer values appear also for the parameters of the proper conformal transformations on base space (remember $L^i \equiv l^i + \epsilon^{ijk}\theta^j r^k$).

[*Remark:* for a Dirac equation without the additional condition $\nabla\cdot\vec{\Sigma}=0$, see Eq. (37), the above expressions would be the final result. This is the case, for instance, for the Dirac equation for a Weyl (i.e., two component) spinor in Euclidean space in four dimensions, for which expressions analogous to (49) would constitute the final result (with the conformal base space transformations in four instead of three dimensions, of course).]

We have used all information from the coefficients of Eqs. (42) which contain at least one partial derivative of a target space variable. It remains to evaluate the parts without a partial derivative (i.e., the coefficients of the identity). These contain the coefficients F^x, F^y, F^z linearly and are therefore just the determining linear equations for these coefficients. However, they give four equations for three unknowns, therefore they must be linearly dependent, which leads to one further constraint equation. An easier way to calculate this constraint is to calculate the action of the prolonged vector field (40) on the original constraint (37),

$$\mathrm{pr}\, v(V) = 0 \tag{50}$$

or explicitly

$$
\begin{aligned}
&A^x\gamma + \alpha_x C + A\gamma_x + \alpha C^x + B^x\delta + \beta_x D + B\delta_x + \beta D^x + A^y\delta + \alpha_y D + A\delta_y + \alpha D^y - B^y\gamma - \beta_y C - B\gamma_y \\
&\quad - \beta C^y + A^z\alpha + \alpha_z A + B^z\beta + \beta_z B - C^z\gamma - \gamma_z C - D^z\delta - \delta_z D = 0.
\end{aligned}
\tag{51}
$$

Inserting the explicit expressions for A^x, etc., leads to an expression containing both coefficients multiplying partial derivatives of the target space variables (like α_x) and a coefficient of the identity 1. After eliminating four partial derivatives (e.g., δ_x, δ_y, δ_z, and γ_z) with the help of the equations of motion, one realizes that the coefficients of the remaining partial derivatives vanish identically. It remains to evaluate the coefficient of the identity. This leads in fact to four conditions, because the use of the equations of motion has reintroduced the gauge potential functions G^x, G^y, G^z into the above expression. As none of the coefficients (A, etc.) may depend on the gauge potential, the total coefficient multiplying each gauge potential function must vanish separately, as well as the remainder. The conditions that the coefficients multiplying G^x, G^y, G^z vanish leads to

$$\alpha^0 = \beta^0 = \gamma^0 = \delta^0 = 0, \quad v^1 = v^2 = 0, \tag{52}$$

and the condition that the remainder vanishes leads to

$$(\nabla\lambda + \vec{\theta})\cdot\vec{\Sigma} = 0. \tag{53}$$

With the shift

$$\lambda \to \lambda - \Theta, \quad \Theta \equiv \vec{\theta} \cdot \vec{r} \equiv \theta^1 x + \theta^2 y + \theta^3 z \tag{54}$$

and the definition

$$\phi \equiv - v^3 \tag{55}$$

we therefore arrive at

$$\begin{aligned} A &= \lambda\alpha + \phi\beta - \Theta\alpha + \frac{L^3}{2}\beta - \frac{L^2}{2}\gamma + \frac{L^1}{2}\delta, \\ B &= \lambda\beta - \phi\alpha - \Theta\beta - \frac{L^3}{2}\alpha - \frac{L^1}{2}\gamma - \frac{L^2}{2}\delta, \\ C &= \lambda\gamma + \phi\delta - \Theta\gamma + \frac{L^2}{2}\alpha + \frac{L^1}{2}\beta - \frac{L^3}{2}\delta, \\ D &= \lambda\delta - \phi\gamma - \Theta\delta - \frac{L^1}{2}\alpha + \frac{L^2}{2}\beta + \frac{L^3}{2}\gamma, \end{aligned} \tag{56}$$

with

$$(\nabla\lambda) \cdot \vec{\Sigma} = 0. \tag{57}$$

Here λ and ϕ are scale and gauge transformations on (spinor) target space, whereas the remainder is the representation on spinor space of the infinitesimal base space symmetries.

However, there is a problem with the constraint (57). The constrained function λ is still algebraically independent of $\vec{\Sigma}$ (i.e., of the α, β, etc.), therefore the constraint does not contradict our basic assumptions. The problem is that the Lie algebra of all infinitesimal transformations does not close on the constraint (57). For example, the commutator of a target space scale transformation and a base space rotation about the z axis leads to another target space scale transformation which no longer obeys the constraint (57),

$$[v_\lambda, v_{l^3}] = v_{\tilde{\lambda}}, \quad (\nabla\tilde{\lambda}) \cdot \vec{\Sigma} \neq 0. \tag{58}$$

This is, in fact, not a surprise, because the gradient of the rotated scale function $\tilde{\lambda}$ must be perpendicular to the rotated vector $\vec{\tilde{\Sigma}}$, $(\nabla\tilde{\lambda}) \cdot \vec{\tilde{\Sigma}} = 0$, and analogously for other base space transformations.

Therefore, in order to have a closing Lie algebra of base space and target space transformations, we must restrict to constant target space scale transformations, $\lambda = \text{const}$.

However, as transformations with nonconstant λ obeying the constraint (57) map solutions of the Dirac equation to new solutions and are of some interest as such, one may instead choose another restriction by restricting to the target space transformations parametrized by λ and ϕ (i.e., by setting all base space transformation parameters equal to zero). The resulting Lie algebra is abelian and closes therefore trivially.

We still must calculate the coefficients F^x, F^y, F^z from the coefficients of the identity of Eqs. (42). After a lengthy calculation one obtains the simple result

$$\vec{F} = - (\Theta + \sigma)\vec{G} + \vec{L} \times \vec{G} - \nabla\phi - \frac{1}{|\vec{\Sigma}|}\vec{\Sigma} \times \nabla\lambda. \tag{59}$$

IV. MULTIPLE ZERO MODES

In this section, we would like to apply the results on symmetries of Sec. III to the issue of zero mode degeneracy (i.e., multiple solutions for a Dirac equation with the same gauge potential). We shall give a more general discussion in Sec. IV A, whereas we will provide some explicit, new examples of multiple zero modes in Sec. IV B.

A. General discussion

The condition that a target space symmetry transformation of a spinor does not change the gauge field is $\vec{F}=0$, see Eq. (59), or

$$\nabla\phi = -\frac{1}{|\vec{\Sigma}|}\vec{\Sigma}\times\nabla\lambda \tag{60}$$

which, together with condition (57), implies that $\vec{\Sigma}$, $\nabla\phi$, and $\nabla\lambda$ are mutually perpendicular. Further, Darboux's theorem tells us that (at least locally) we may express $\vec{\Sigma}$ like

$$\vec{\Sigma} = \nabla\xi^1\times\nabla\xi^2, \tag{61}$$

where $\xi^a=\xi^a(\mathbf{r})$, $a=1,2$. If we now assume that ϕ and λ are functions of ξ^a only, then their gradients are automatically perpendicular to $\vec{\Sigma}$, and it remains to solve

$$|\nabla\phi| = |\nabla\lambda|, \quad \nabla\phi\cdot\nabla\lambda = 0. \tag{62}$$

This problem can be solved relatively easily for a subclass of functions ξ^a which fulfill one additional requirement, namely that the scalar products of the gradients of the ξ^a can be expressed in terms of the ξ^a again, up to a *common* factor, that is

$$\nabla\xi^a\cdot\nabla\xi^b = h(\mathbf{r})g^{ab}(\xi^c). \tag{63}$$

Here g^{ab} plays the role of a metric in some two-dimensional space parametrized by the coordinates ξ^a. If Eq. (63) holds, then Eq. (60) simplifies to

$$\phi_a\tilde{\epsilon}^{ac} = g^{cb}\lambda_b, \tag{64}$$

where $\phi_a\equiv\partial_{\xi^a}\phi$, etc., and

$$\tilde{\epsilon}^{ab} = g^{1/2}\epsilon^{ab}, \quad g\equiv\det(g_{ab}) = g_{11}g_{22}-g_{12}g_{21}, \tag{65}$$

and ϵ^{ab} is the usual antisymmetric symbol in two dimensions. Equations (64) can be solved by observing that they just provide a generalization of the Cauchy–Riemann equations to the case of a general surface. We must only find the coordinate transformation from ξ'^a to some new coordinates ξ'^a such that the metric g'^{ab} with respect to the new coordinates is conformally equivalent to the flat metric δ^{ab}, that is

$$g'^{ab} \equiv \frac{\partial\xi'^a}{\partial\xi^c}\frac{\partial\xi'^b}{\partial\xi^d}g^{cd} = h(\xi')\delta^{cd}. \tag{66}$$

This problem always has a solution in two dimensions.[20] In terms of the coordinates ξ'^a, Eq. (64) reads

$$\phi_a\epsilon^{ac} = \delta^{cb}\lambda_b \tag{67}$$

which is just the Cauchy–Riemann equation. Therefore, our problem is solved by an arbitrary complex function u of the complex variable ζ', where

$$u(\zeta') = \exp(\lambda + i\phi), \quad \zeta' = \xi'^1 + i\xi'^2. \tag{68}$$

Here "solution" means that if a spinor Ψ with $\Psi^\dagger \vec{\sigma} \Psi \equiv \vec{\Sigma}$ solves a certain Dirac equation, then $u\Psi$ locally solves the same Dirac equation,

$$\mathcal{D}\Psi = 0 \Rightarrow \mathcal{D}u\Psi = 0. \tag{69}$$

Regularity requirements further restrict the allowed u. For instance, the functions ξ^a need not be well defined in all $\mathbb{R}^3$ (they usually are not), but u certainly must be well-defined (which may not be possible, in which case the problem has no acceptable solution). The condition that $u\Psi$ is square-integrable restricts to a finite number (which, again, may be zero) of linearly independent functions u. It should be emphasized that *all* known examples of multiple zero modes are of the above type (69), see Refs. 13–15. It is an interesting open question whether there exist other types, as well.

Finally, let us point out that the procedure described above can certainly be reversed. That is to say, choose a pair of functions ξ^a which obey Eq. (63) and calculate the corresponding ξ'^a via Eq. (66). Then $u\Psi$ with u given by Eq. (68) will provide additional local zero modes for a whole class of spinors Ψ with spin densities given by $\vec{\Sigma} = F(\xi^a)\nabla\xi^1 \times \nabla\xi^2$ for (almost) arbitrary real functions $F(\xi^a)$ (of course, F should be well defined in all $\mathbb{R}^3$). It is not difficult to reconstruct the spinor Ψ from the spin density $\vec{\Sigma}$ and the gauge potential $\vec{G}$ from the spinor Ψ (see, e.g., Ref. 2). We shall explicitly demonstrate how this works by constructing a class of multiple zero modes in the next section.

[*Remark:* Equations (62) can be expressed in terms of the complex variable $u = \exp(\lambda + i\phi)$ like

$$(\nabla u)^2 = 0 \tag{70}$$

which is the complex static eikonal equation. Further, condition (63) is equivalent to the condition that u—when interpreted as a map from one-point compactified $\mathbb{R}^3_0$ to one-point compactified $\mathbb{C}_0$—is a Riemannian submersion up to Weyl transformations (local conformal rescalings of the metric). That is to say, u is a composition of maps

$$u: \mathbb{R}^3_0 \overset{\text{W}}{\rightarrow} \mathcal{M}^3 \overset{\text{RS}}{\longrightarrow} \mathcal{N}^2 \overset{\text{W}}{\rightarrow} \mathbb{C}_0, \tag{71}$$

where W is a Weyl transformation, RS is a Riemannian submersion, and $\mathcal{M}^3$ and $\mathcal{N}^2$ are compact manifolds in three and two dimensions, respectively. A detailed discussion of these issues can be found in Ref. 21. In Ref. 15, Riemannian submersions were used to construct multiple zero modes within a more geometrical context.]

B. A class of multiple zero modes

Here we want to construct explicitly a class of multiple zero modes by starting with a pair of functions ξ^a which obey Eq. (63), as explained in the preceding section. In particular, we want to make use of the results of Ref. 21, where a class of Hopf maps obeying the eikonal equation (70) were found, and where the geometric explanation for their existence was provided. In concordance with these results, we therefore choose the functions

$$\xi^1 = \ln \sinh \eta \equiv \tfrac{1}{2} \ln T, \quad \xi^2 = m\vartheta + n\varphi, \tag{72}$$

where we introduced toroidal coordinates $(\eta, \vartheta, \varphi)$ (and, for later convenience, the variable $T \equiv \sinh^2 \eta$) related to the Cartesian coordinates (x, y, z) via

$$T \equiv \sinh^2 \eta = \frac{4(x^2+y^2)}{4z^2+(r^2-1)^2}, \quad \vartheta = \arctan \frac{2z}{r^2-1}, \quad \varphi = \arctan \frac{y}{x}. \tag{73}$$

Further, m and n are nonzero integers such that $\exp(2\pi i l \xi^2)$ is a single-valued function for integer l [the geometric significance of the integers m and n is that they provide the complex function (Hopf map) $f=\exp(\xi^1+i\xi^2)$ with the Hopf index $H=mn$].

Following the results of Ref. 21, it can be shown that the pair ξ^1, ξ^2 obeys Eq. (63), and that a new pair ξ'^1, ξ'^2 obeying Eq. (66) can be found without difficulty. Indeed, one finds easily that ξ^a obey Eq. (63) with

$$h(\mathbf{r}) = \frac{(\cosh \eta - \cos \vartheta)^2 \cosh^2 \eta}{\sinh^2 \eta}, \tag{74}$$

$$g^{11}=1, \quad g^{12}=g^{21}=0, \quad g^{22}=\frac{m^2 \sinh^2 \eta + n^2}{\cosh^2 \eta}. \tag{75}$$

Hence, the induced metric g^{ab} is already diagonal but not yet conformally flat. However, as g^{22} only depends on ξ^1 (i.e., on η), a coordinate transformation involving only ξ^1 is sufficient, $\xi^1 \rightarrow \xi'^1(\xi^1)$, $\xi'^2 \equiv \xi^2$, such that $g^{11} \rightarrow g'^{11}=g^{22} \equiv g'^{22}$. Explicitly, the transformation reads

$$\xi'^1 = \ln\left(\sinh^{|n|} \eta \, \frac{(|m|\cosh \eta + \sqrt{n^2+m^2 \sinh^2 \eta})^{|m|}}{(|n|\cosh \eta + \sqrt{n^2+m^2 \sinh^2 \eta})^{|n|}} \right), \tag{76}$$

see Ref. 21. The function $\zeta' = \xi'^1 + i\xi'^2$ itself is not single valued, but the function

$$\zeta \equiv \exp \zeta' = \exp(\xi'^1 + i\xi'^2) \tag{77}$$

is. It follows that for each spinor Ψ with spin density $\vec{\Sigma} \equiv \Psi^\dagger \vec{\sigma} \Psi = F(\xi^a) \nabla \xi^1 \times \nabla \xi^2$ (which is a formal zero mode for some gauge potential, because $\vec{\Sigma}$ obeys $\nabla \cdot \vec{\Sigma}=0$), $u(\zeta)\Psi$ are further formal zero modes for the same gauge potential, where u is a rational function of its argument. A customary basis for the functions u is $u=\zeta^l$ for integer l.

The formal zero modes described so far (implicitly via their spin density) are single-valued functions on all $\mathbb{R}^3$, but we have not yet taken into account the condition of square integrability. Before doing so, we want to make some simplifying assumptions on the type of spin density we want to discuss. First, we assume that the function F depends on ξ^1 (i.e., on η or T) only. Second, we reexpress F like $F=e^M[4T/(1+T)^2]$, where the function of $M(T)$ will be specified below, that is, we write for a general spin density

$$\vec{\Sigma}^{(M)} = e^{M(T)} \vec{\Sigma}^{(0)}, \quad \vec{\Sigma}^{(0)} = \frac{4T}{(1+T)^2} \nabla \xi^1 \times \nabla \xi^2. \tag{78}$$

The reason for this is that $\vec{\Sigma}^{(0)}$ is a well behaved and integrable spin density, whereas $\nabla \xi^1 \times \nabla \xi^2$ is not (clearly, integrability of the spin density $\int d^3\mathbf{r} |\vec{\Sigma}| < \infty$ is the same as square integrability of the corresponding spinor). Another reason for the choice of $\vec{\Sigma}^{(0)}$, which does not concern us much here, is the fact that $\vec{\Sigma}^{(0)}$ is the Hopf curvature for the Hopf map $\exp(\xi^1+i\xi^2)$. In Cartesian coordinates, $\vec{\Sigma}^{(0)}$ reads

$$\vec{\Sigma}^{(0)} = \frac{16}{(1+r^2)^3} \begin{pmatrix} 2nxz - 2my \\ 2nyz + 2mx \\ n(1-r^2+2z^2) \end{pmatrix} \tag{79}$$

and its spinor $\Psi^{(0)}$ with $\vec{\Sigma}^{(0)} = \Psi^{(0)\dagger} \vec{\sigma} \Psi^{(0)}$ is

$$\Psi^{(0)} = \frac{2\sqrt{2}}{(1+r^2)^{3/2}\sqrt{(1+r^2)\Gamma + n(2z^2+1-r^2)}} \tag{80}$$

$$\times \begin{pmatrix} n(2z^2+1-r^2) + (1+r^2)\Gamma \\ 2(x+iy)(nz+im) \end{pmatrix}, \tag{81}$$

where

$$\Gamma := \left(\frac{n^2 + m^2 T}{1+T}\right)^{1/2} = \left(\frac{n^2 + m^2 \sinh^2 \eta}{\cosh^2 \eta}\right)^{1/2} \tag{82}$$

and we choose the gauge such that the upper component is real. The calculation of the spinor $\Psi^{(0)}$ from the spin density $\vec{\Sigma}^{(0)}$ is explained in Appendix B. The spinor (81) is regular everywhere. Further, it is a zero mode for some gauge potential $\vec{G}^{(0)}$, by construction (this gauge potential is well behaving and leads to a square-integrable magnetic field $\vec{H}^{(0)} = \nabla \times G^{(0)}$; its explicit expression, which is quite lengthy, is displayed in Appendix B, together with an explanation of its calculation). Additional formal zero modes $\zeta^l \Psi^{(0)}$ for the same gauge potential are not square integrable, i.e., the corresponding spin density $|\zeta^* \zeta|^l \vec{\Sigma}^{(0)}$ is not integrable (for either positive or negative integer l), as may be inferred easily from the explicit expression for $\vec{\Sigma}^{(0)}$ and from the limiting behavior,

$$\lim_{T\to 0} |\zeta^* \zeta| \sim T^{|n|}, \quad \lim_{T\to\infty} |\zeta^* \zeta| \sim T^{|m|}. \tag{83}$$

But with an appropriate choice of M, it is easy to find spin densities $\vec{\Sigma}^{(M)}$ such that $|\zeta^* \zeta|^l \vec{\Sigma}^{(M)}$ remains integrable for some nonzero values of l.

Concretely, we assume that $M(T)$ and $M'(T)$ are finite for all finite values of T, i.e.,

$$|M(T)| < \infty \ \wedge \ |M'(T)| < \infty \quad \text{for } T < \infty, \tag{84}$$

and that M behaves for large T like

$$\lim_{T\to\infty} M(T) \sim -mk \ln T + \overline{M}(T), \tag{85}$$

where k is a postive integer and the remainder $\overline{M}$ must obey

$$\lim_{T\to\infty} |T\overline{M}(T)| < \infty. \tag{86}$$

Here the conditions (84) and (86) are chosen in order to avoid both spurious (i.e., pure gauge) and physical singularities for the corresponding gauge potential, and condition (85) is chosen in order to have a nontrivial result (i.e., multiple square-integrable zero modes). Condition (85) induces a spurious (gauge) singularity in the corresponding gauge potential at $T=\infty$ which must be cured by an appropriate gauge fixing. Consequently, the spinor $\Psi^{(M)}$ for the spin density $\vec{\Sigma}^{(M)}$ with the appropriate gauge fixing is

$$\Psi^{(M)} := e^{M/2} e^{ikm\vartheta} \Psi^{(0)}, \tag{87}$$

where the additional factor $\exp(ikm\vartheta)$ provides the gauge fixing, see below. Under the above assumptions the spinors

$$\Psi_l^{(M)} = \zeta^l \Psi^{(M)}, \quad l = 0, \ldots, k \tag{88}$$

are all square-integrable zero modes for the same gauge potential $\vec{G}^{(M)}$.

It remains to determine $\vec{G}^{(M)}$ explicitly, which will be obtained with Eq. (59) of Sec. III. In fact, using Eq. (59) [where $M/2 \sim \lambda$ and $km\vartheta \sim \phi$; remember that Eq. (59) also holds for finite λ and ϕ because of the abelian nature of the target space symmetry transformations] one easily calculates

$$\vec{G}^{(M)} = \vec{G}^{(0)} - \frac{M'T}{\Gamma}(m\nabla\vartheta + n\nabla\varphi) - mk\nabla\vartheta \tag{89}$$

(as said, the expression for $\vec{G}^{(0)}$ is provided in Appendix B). Here the additional pure gauge term precisely cancels a pure gauge singularity at $T=\infty$, as may be checked easily. Further, we may see how it works that multiplication of the spinor $\Psi^{(M)}$ by ζ does not change the gauge potential. The crucial point is that multiplication by ζ corresponds to choosing $M=|\zeta^*\zeta|$, and for this M it holds that $M'T/\Gamma=-1$, so that the M dependent term in (89) is, in fact, pure gauge and is cancelled by the contribution $\nabla \arg\zeta = \nabla\xi^2$, see (72). This just shows explicitly that $M/2 \equiv \xi'^1 \sim \lambda$ and $\xi^2 \sim \phi$ fulfill Eq. (60) which, of course, must be true by construction.

Therefore, we have succeeded in constructing explicitly a class of multiple zero modes together with their gauge potentials starting from the functions (72) (or, equivalently, starting from the higher toroidal Hopf maps of Ref. 21). For the simplest Hopf map (i.e., for $m=n=1$) these zero modes have already been obtained in Refs. 13–15, whereas for the higher toroidal Hopf maps they are new.

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APPENDIX A

The coefficients for the prolongation $\mathrm{pr}\, v$ of the vector field v in Sec. II are

$$R^x = D_x R - \rho_x D_x X - \rho_y D_x Y, \tag{A1}$$

$$R^y = D_y R - \rho_x D_y X - \rho_y D_y Y, \tag{A2}$$

$$L^x = D_x L - \lambda_x D_x X - \lambda_y D_x Y, \tag{A3}$$

$$L^y = D_y L - \lambda_x D_y X - \lambda_y D_y Y, \tag{A4}$$

where D_x and D_y are total derivatives with respect to x and y, respectively. Explicitly, R^x reads

$$\begin{aligned} R^x = {} & R_x + R_\rho\rho_x + R_\lambda\lambda_x + R_{G^x}G^x_x + R_{G^y}G^y_x - \rho_x(X_x + X_\rho\rho_x + X_\lambda\lambda_x + X_{G^x}G^x_x + X_{G^y}G^y_x) \\ & - \rho_y(Y_x + Y_\rho\rho_x + Y_\lambda\lambda_x + Y_{G^x}G^x_x + Y_{G^y}G^y_x) \end{aligned} \tag{A5}$$

and analogously for the other coefficients.

APPENDIX B

The calculation of the spinor $\Psi^{(0)}$ from the spin density $\vec{\Sigma}^{(0)}$ proceeds as follows. For a gauge such that the upper component of the spinor is real, a spinor Ψ may be obtained from its spin density $\vec{\Sigma}$ formally by the algebraic relation, see Ref. 2,

$$\Psi = \frac{1}{\sqrt{2(|\vec{\Sigma}| + \Sigma^3)}} \begin{pmatrix} |\vec{\Sigma}| + \Sigma^3 \\ \Sigma^1 + i\Sigma^2 \end{pmatrix}. \tag{B1}$$

This gauge is globally admissible provided that the third component of $\vec{\Sigma}$ is positive whenever its first and second component are zero, i.e.,

$$\Sigma^1 = 0 \ \wedge \ \Sigma^2 = 0 \ \Rightarrow \ \Sigma^3 > 0 \tag{B2}$$

which holds for the spin density $\vec{\Sigma}^{(0)}$ of Eq. (79). Therefore, the spinor $\Psi^{(0)}$ of Eq. (80) may be computed with the help of the above expression.

The calculation of the gauge potential $\vec{G}^{(0)}$ for the spinor (zero mode) $\Psi^{(0)}$ proceeds as follows. Remember that once a zero mode Ψ is given, the Dirac equation may be viewed as an overconstrained system of linear, algebraic equations for the three components of the gauge potential. If the constraint is fulfilled, this system can be solved explicitly and results in the following expression for the corresponding gauge potential $\vec{G}$, see Ref. 2:

$$\vec{G} = \frac{1}{2|\vec{\Sigma}|}(\nabla \times \vec{\Sigma} + 2\,\mathrm{Im}(\Psi^\dagger \nabla \Psi)). \tag{B3}$$

Inserting the explicit expression for $\Psi^{(0)}$ into the above formula leads to the following rather lengthy expression for $\vec{G}^{(0)}$:

$$\vec{G}^{(0)} = \frac{1}{\Gamma(1+r^2)^2} \begin{pmatrix} -n(5-r^2)y + 6mxz \\ n(5-r^2)x + 6myz \\ m(6z^2 + 2 - 4r^2) \end{pmatrix} + \frac{2}{\Gamma(1+r^2)[\Gamma(1+r^2) + n(2z^2 + 1 - r^2)]} \begin{pmatrix} -(n^2z^2 + m^2)y \\ (n^2z^2 + m^2)x \\ mn(r^2 - z^2) \end{pmatrix} \tag{B4}$$

[for a direct comparison with the results of Refs. 13 and 14 for the case $m=n=1$, one must take into account the fact that the gauge chosen in Refs. 13 and 14 differs from the one chosen here by the gauge function $\phi = \arctan(z)$]. Further, Eq. (B3) shows that $\vec{G}$ is singular whenever $|\vec{\Sigma}|$ is zero. This singularity may be a spurious (gauge) singularity, in which case it can be cured by an appropriate gauge fixing as in Eq. (89), or it may be physical, in which case the corresponding zero mode is not admissible (of course, all the zero modes given in Sec. IV B are admissible).

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The Kähler potential of Abelian Higgs vortices

Heng-Yu Chen[a] and N. S. Manton[b]
Department of Applied Mathematics and Theoretical Physics, University of Cambridge,, Wilberforce Road, Cambridge CB3 0WA, United Kingdom

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We calculate the Kähler potential for the Samols metric on the moduli space of Abelian Higgs vortices on $\mathbb{R}_2$, in two different ways. The first uses a scaling argument. The second depends on a variant of the relationship between accessory parameters and the regularized action in Liouville field theory. The Kähler potential on the moduli space of vortices on $\mathbb{H}_2$ is also derived, and we are led to a geometrical reinterpretation of these vortices. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1874334]

I. INTRODUCTION

The $(2+1)$-dimensional Abelian Higgs model, with Lagrangian density

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \frac{1}{2}\overline{D_\mu\Phi}D^\mu\Phi - \frac{\lambda}{8}(|\Phi|^2-1)^2, \tag{1.1}$$

is known to have static and moving vortex solutions.[1,2] The static solutions are the field configurations minimizing the potential energy functional. When the coupling constant λ takes the critical value of 1, there are no net forces between the vortices, and they satisfy first-order Bogomolny equations [see (2.3) and (2.4)). Static N-vortex solutions in $\mathbb{R}^2$ or equivalently the complex plane $\mathcal{C}$ are uniquely characterized by the N unordered, and not necessarily distinct points $\{Z_1,\ldots,Z_N\}$ in $\mathcal{C}$ where the Higgs field Φ vanishes. As a manifold, the moduli space $\mathcal{M}_N$ of solutions is therefore $\mathcal{C}^N$, with the fundamental symmetrized polynomials in $\{Z_1,\ldots,Z_N\}$ as coordinates. In practice, these are awkward to deal with, and it is more convenient to treat the vortex positions $\{Z_1,\ldots,Z_N\}$ as local coordinates on moduli space, which is justified when they are distinct. This is what we shall do in this paper. Vortex coalescence may be investigated by a limiting procedure.

The so-called "moduli space approximation" is a powerful approach for studying the low-energy dynamics of N solitonic objects in field theories with Bogomolny equations.[3] The idea is that, in the low-energy limit, most of the field degrees of freedom are effectively frozen, and the field approximately follows a trajectory in moduli space. The field is at each instant a static solution of the Bogomolny equations, but with moduli that are time dependent. The kinetic terms in the field theory Lagrangian restrict to a kinetic energy expression for trajectories in moduli space. For N vortices, the resulting quadratic form on tangent vectors to $\mathcal{M}_N$ defines the Samols metric on $\mathcal{M}_N$.[4] The field potential energy in the N-vortex sector takes its minimal, constant value on $\mathcal{M}_N$, and can be neglected, so the dynamical trajectories are the geodesics on $\mathcal{M}_N$. These accurately model the scattering of vortices.[5]

Samols found a general, but not explicit, formula for the metric on $\mathcal{M}_N$, and using this, showed that the metric is Kähler.[4] The metric is smooth and complete, but not flat. The most interesting geodesic describes a head-on collision, where two vortices scatter through a right angle. Recently, an explicit formula in terms of modified Bessel functions was given for N

[a]Electronic mail: H.Y.Chen@damtp.cam.ac.uk
[b]Electronic mail: N.S.Manton@damtp.cam.ac.uk

well-separated vortices, and a formula for the Kähler potential was also found.[6] Our main purpose in this paper is to construct a Kähler potential $\mathcal{K}$ for the Samols metric with vortices at arbitrary separation.

We present two different approaches to calculating $\mathcal{K}$. The first is to explicitly construct it from the quantities in Samols' metric. This reduces to a $\overline{\partial}$ problem, which can be solved here by a scaling argument. The second approach is inspired by the relationship between the so-called "accessory parameters" in the context of uniformization of Riemann surfaces, and a regularized Liouville action. This relationship was first conjectured by Polyakov and later proved by Takhtajan and Zograf,[7] and an accessible recent account with a simplified proof can be found in Ref. 8. Similar results on Riemann surfaces with a range of singularities have also been investigated in Refs. 9 and 10. It turns out that in the vortex situation, there are analogous quantities to the accessory parameters, and we can construct a modification of the regularized Liouville action as their generating function. This regularized action is the interacting part of the Kähler potential on $\mathcal{M}_N$.

Also interesting is the Abelian Higgs model for vortices defined on the hyperbolic plane $\mathbb{H}^2$ with Ricci scalar -1. Such vortices were shown to be integrable by Witten,[11] as the Bogomolny equations in this case reduce to the Liouville equation. The metric on the moduli space of N hyperbolic vortices was first derived and shown to be Kähler by Strachan.[12] We construct the Kähler potential and also uncover a new geometrical interpretation of the Higgs field.

This paper is organized as follows: In Sec. II, we briefly review Abelian Higgs vortices in $\mathbb{R}^2$, and the Samols metric on $\mathcal{M}_N$. In Sec. III, a general formula for the Kähler potential on $\mathcal{M}_N$ is derived using the scaling argument. In Sec. IV, we review the regularized action of Liouville field theory and the results of Takhtajan and Zograf, and show how the interacting part of the Kähler potential on $\mathcal{M}_N$ can be constructed from an analogous action. In Sec. V, we discuss vortices in the hyperbolic plane, present the geometrical interpretation of the Higgs field, and show that in this case the regularized Liouville action is the entire Kähler potential. In Sec. VI we summarize our results.

II. ABELIAN HIGGS VORTICES

At critical coupling, $\lambda=1$, the field potential energy in the Abelian Higgs model is

$$E=\frac{1}{2}\int d^2x\left\{F_{12}^2+\overline{D_i\Phi}D_i\Phi+\frac{1}{4}(|\Phi|^2-1)^2\right\}, \tag{2.1}$$

where $F_{12}=\partial_1A_2-\partial_2A_1=B$ is the magnetic field in the plane and $D_j\Phi=\partial_j\Phi-iA_j\Phi$, $j=1,2$, is the covariant derivative of the complex Higgs field Φ. The boundary conditions are that $|\Phi|\to 1$ as $|\mathbf{x}|\to\infty$, so Φ becomes pure phase, and the gauge field becomes pure gauge at spatial infinity, such that F_{12} and $D_j\Phi$ vanish. The winding number of Φ at infinity is denoted by N, and is assumed to be a positive integer.

We can rearrange E into the Bogomolny form by completing the square

$$E=\frac{1}{2}\int d^2x\left\{\left(F_{12}+\frac{1}{2}(|\Phi|^2-1)\right)^2+(\overline{D_1\Phi}-i\overline{D_2\Phi})(D_1\Phi+iD_2\Phi)+F_{12}\right\}, \tag{2.2}$$

and discarding boundary terms that vanish at spatial infinity. As the first two terms in (2.2) are both non-negative, the minimal value of E is obtained when A_i and Φ satisfy the Bogomolny equations

$$F_{12}+\frac{1}{2}(|\Phi|^2-1)=0, \tag{2.3}$$

$$D_1\Phi+iD_2\Phi=0. \tag{2.4}$$

E is then related to the winding number through Stokes' theorem,

$$E = \frac{1}{2}\int d^2x\, F_{12} = N\pi, \tag{2.5}$$

and it can be interpreted as the energy of N vortices with no static interactions.

Let us rewrite (2.3) and (2.4) in terms of the complex coordinate $z = x^1 + ix^2$,

$$iF_{z\bar{z}} = \frac{1}{4}(|\Phi|^2 - 1), \tag{2.6}$$

$$D_{\bar{z}}\Phi = \partial_{\bar{z}}\Phi - iA_{\bar{z}}\Phi = 0. \tag{2.7}$$

Equation (2.7) is solved by $A_{\bar{z}} = -i\partial_{\bar{z}}\log\Phi$. Next express Φ in terms of a gauge-invariant quantity h and a phase factor χ as $\Phi = e^{(1/2)h+i\chi}$, where $h \to 0$ as $|\mathbf{x}| \to \infty$. Substituting these into (2.6), we obtain the gauge-invariant, Taubes equation for the vortices[1]

$$4\partial_z\partial_{\bar{z}}h - e^h + 1 = 4\pi\sum_{r=1}^{N}\delta(z - Z_r), \tag{2.8}$$

where $\{Z_1, \ldots, Z_N\}$ are the vortex positions in $\mathcal{C}$. Here, these positions are taken as distinct, simple zeros of Φ, which fixes the strength of the δ functions, although the zeros can coalesce. There is a unique solution for any choice of positions, as proved by Jaffe and Taubes.[1] Therefore, on a large stratum of the moduli space $\mathcal{M}_N$ of N-vortex solutions, $\{Z_1, \ldots, Z_N\}$ are good local coordinates. Notice that (2.8) has a form very similar to the Liouville equation on a punctured Riemann surface. However, the constant 1 in (2.8), the Higgs vacuum expectation value, sets the scale for the system, and breaks conformal invariance.

Close to the rth vortex position Z_r, h has the following expansion:

$$h = \log|z - Z_r|^2 + a_r + \frac{1}{2}\bar{b}_r(z - Z_r) + \frac{1}{2}b_r(\bar{z} - \bar{Z}_r) + \bar{c}_r(z - Z_r)^2 - \frac{1}{4}|z - Z_r|^2 + c_r(\bar{z} - \bar{Z}_r)^2 + \cdots. \tag{2.9}$$

The expansion coefficients a_r, b_r, $\bar{b}_r$, c_r, and $\bar{c}_r$ are functions of the separations between Z_r and all other vortex positions Z_s, $s \neq r$. The coefficient a_r plays the role of a local scaling factor. b_r and $\bar{b}_r$ measure the deviation from circular symmetry of h around Z_r due to the overlap with the other vortices.

Starting from the field kinetic energy in the Abelian Higgs model, Samols showed that b_r and $\bar{b}_r$ determine the metric G on the moduli space, the formula being[4]

$$G = \sum_{r,s=1}^{N}\left(\delta_{rs} + 2\frac{\partial b_s}{\partial Z_r}\right)dZ_r\, d\bar{Z}_s. \tag{2.10}$$

The δ_{rs} term gives a flat, noninteracting metric, and the remaining term, which decays exponentially as the vortices separate, leads to dynamical vortex interactions in the moduli space approximation. Although the coefficients of G become singular as the vortices coalesce, these singularities can be removed by a change of coordinates, and the metric is smooth and complete. The reality of the field kinetic energy implies that the metric is Hermitian, so

$$\frac{\partial b_s}{\partial Z_r} = \frac{\partial \bar{b}_r}{\partial \bar{Z}_s}. \tag{2.11}$$

From this it follows that the metric is Kähler, and there is therefore a Kähler potential $\mathcal{K}$ related to the metric coefficients by

$$\frac{\partial^2 \mathcal{K}}{\partial Z_r \, \partial \overline{Z}_s} = \delta_{rs} + 2\frac{\partial b_s}{\partial Z_r}. \tag{2.12}$$

In addition, b_r has been shown to obey a symmetric identitity,[13]

$$\frac{\partial b_r}{\partial \overline{Z}_s} = \frac{\partial b_s}{\partial \overline{Z}_r}. \tag{2.13}$$

Both (2.11) and (2.13) have recently been proved directly, as symmetry properties of the Green's function of the linearized Taubes equation (see Ref. 2 p. 209). The Kähler property and translational invariance imply that $\Sigma_{r=1}^N b_r = \Sigma_{r=1}^N \overline{b}_r = 0$, and rotational invariance implies that $\Sigma_{r=1}^N Z_r \overline{b}_r$ is real.[14]

III. THE VORTEX KÄHLER POTENTIAL AND THE SCALING INTEGRAL

We seek a real function $\widetilde{\mathcal{K}}$ of the coordinates $\{Z_1, \ldots, Z_N; \overline{Z}_1, \ldots, \overline{Z}_N\}$ such that

$$\frac{\partial \widetilde{\mathcal{K}}}{\partial \overline{Z}_r} = 2b_r, \quad \frac{\partial \widetilde{\mathcal{K}}}{\partial Z_r} = 2\overline{b}_r. \tag{3.1}$$

Given $\widetilde{\mathcal{K}}$, the identities (2.11) and (2.13) trivially follow. $\widetilde{\mathcal{K}}$ is a Kähler potential for the interacting part of the metric. The first of Eqs. (3.1) is a $\overline{\partial}$ problem, and the second its conjugate. We do not solve these equations separately, but consider the following linear combination:

$$\sum_{r=1}^N \left\{ Z_r \frac{\partial}{\partial Z_r} + \overline{Z}_r \frac{\partial}{\partial \overline{Z}_r} \right\} \widetilde{\mathcal{K}} = 2 \sum_{r=1}^N \{ Z_r \overline{b}_r + \overline{Z}_r b_r \}. \tag{3.2}$$

On the left-hand side we have the overall scaling operator on the vortex moduli space acting on $\widetilde{\mathcal{K}}$.

We make the ansatz that all Z_r are parametrized by a single scale variable τ, i.e., $Z_r(\tau) = Z_r \tau$. We can then express the overall scaling operator in terms of τ,

$$\tau \frac{d}{d\tau} \widetilde{\mathcal{K}} = \sum_{r=1}^N \left\{ Z_r(\tau) \frac{\partial}{\partial Z_r(\tau)} + \overline{Z}_r(\tau) \frac{\partial}{\partial \overline{Z}_r(\tau)} \right\} \widetilde{\mathcal{K}}. \tag{3.3}$$

Combining this with (3.2), and integrating, we find

$$\widetilde{K} = 2 \int_\infty^1 \frac{d\tau}{\tau} \sum_{r=1}^N \left(Z_r(\tau) \overline{b}_r(\tau) + \overline{Z}_r(\tau) b_r(\tau) \right). \tag{3.4}$$

$b_r(\tau)$ are the expansion parameters b_r in (2.9) when the vortices are at $Z_r(\tau)$.

In an analysis of a model of first-order vortex dynamics,[15] it was shown that some conserved quantities can be expressed in terms of integrals involving h and its derivatives. The integral of h itself, which remains finite despite the logarithmic divergences of h, was also computed by using a Pohozaev hozaev identity. For N noncoincident vortices

$$\int_{\mathcal{C}} d^2x \, h = -\pi \sum_{r=1}^N (Z_r \overline{b}_r + \overline{Z}_r b_r + 6). \tag{3.5}$$

This result combined with (3.4) gives the rather interesting expression

$$\tilde{\mathcal{K}} = -2\int_{\infty}^{1}\frac{d\tau}{\tau}\left\{\frac{1}{\pi}\int d^2x\, h(\mathbf{x};\tau) + 6N\right\}. \tag{3.6}$$

Here, $h(\mathbf{x};\tau)$ denotes $h(\mathbf{x})$ with the vortices at $Z_r(\tau)$. The entire Kähler potential by this scaling argument is therefore

$$\mathcal{K} = \sum_{r=1}^{N} Z_r\overline{Z_r} - 2\int_{\infty}^{1}\frac{d\tau}{\tau}\left\{\frac{1}{\pi}\int d^2x\, h(\mathbf{x};\tau) + 6N\right\}, \tag{3.7}$$

where the first term gives the δ_{rs} in Samols' metric (2.10). With a suitable change of coordinates, this reduces to the expression given in Ref. 16 for the case of $N=2$.

As a simple test, we consider two well-separated vortices. We work in the center of mass frame, and use the asymptotic b_r values as calculated in Ref. 6. Using the notation $Z_1=\sigma e^{i\theta}=-Z_2$ and $b_1=b(\sigma)e^{i\theta}=-b_2$, where σ is the separation from the origin, we have $\Sigma_{r=1}^{2}\{Z_r\overline{b_r}+\overline{Z_r}b_r\}=4\sigma b(\sigma)$. $b(\sigma)$ equals $\sqrt{32}K_1(2\sigma)$ for large σ, where the prefactor derives from a string duality argument of Tong.[17] Calculating the integral (3.4), and adding the flat term, gives the asymptotic Kähler potential,

$$\mathcal{K} = 2\sigma^2 - 8\sqrt{8}K_0(2\sigma), \tag{3.8}$$

which coincides with the formula in Ref. 6 (after a change in normalization convention). K_0, K_1 are the modified Bessel functions of the second kind, and we have used Bessel function identities in deriving (3.8).

IV. REGULARIZED LIOUVILLE ACTION AND VORTEX KÄHLER POTENTIAL

In this section we present a different approach to solving the equations (3.1). We show that $\tilde{\mathcal{K}}$ is a suitably regularized modified Liouville action, whose variational equation is the Taubes equation (2.8). Our motivation came from the striking similarity of $\overline{b_r}$ to the accessory parameters in the Liouville field theory. We first review the relevant aspects of Liouville theory, following Ref. 8.

Consider a Liouville field ϕ, satisfying

$$\partial_z\partial_{\bar{z}}\phi = \frac{1}{2}e^{\phi}, \tag{4.1}$$

and defined over an n-punctured Riemann sphere, $\Sigma\cong\hat{\mathcal{C}}/\{z_1,z_2,\ldots,z_n\}$, $\hat{\mathcal{C}}=\mathcal{C}\cup\{\infty\}$, where $z_{n-2}=0$, $z_{n-1}=1$, $z_n=\infty$ and $n\geqslant 3$. Assume the punctures are parabolic singularities, where ϕ has asymptotic behavior,

$$\phi = \begin{cases} -2\log|z-z_r| - 2\log|\log|z-z_r|| + O(1), & \text{as } z\to z_r, \quad r\neq n, \\ -2\log|z| - 2\log\log|z| + O(1), & \text{as } z\to z_n=\infty. \end{cases} \tag{4.2}$$

The Liouville equation (4.1) implies that the Poincaré metric $ds^2=e^{\phi}\,dz\,d\bar{z}$ on Σ has constant Ricci scalar $R_\Sigma=-2$. (The Gaussian curvature is half this.)

The zz component of the energy–momentum tensor for ϕ is defined by

$$T_\phi(z) = \partial_z\partial_z\phi - \frac{1}{2}(\partial_z\phi)^2, \tag{4.3}$$

and the Liouville equation implies that $T_\phi(z)$ is a meromorphic function, $\partial_{\bar{z}}T_\phi(z)=0$. For the punctured sphere with parabolic singularities, $T_\phi(z)$ is given by the finite sum

$$T_\phi(z) = \sum_{r=1}^{n-1} \left\{ \frac{1}{2(z-z_r)^2} + \frac{c_r}{(z-z_r)} \right\}, \tag{4.4}$$

and has the expansion around $z=\infty$,

$$T_\phi(z) \sim \frac{1}{2z^2} + \frac{c_n}{z^3} + O\left(\frac{1}{z^4}\right). \tag{4.5}$$

The coefficient of each term $1/(z-z_r)^2$, $r=1,\ldots,n-1$ and also of $1/z^2$ for $z_n=\infty$, is half the conformal weight, so each parabolic singularity z_r has conformal weight 1. The complex constants c_r, $r=1,\ldots,n$, are the accessory parameters. They are uniquely determined by the positions of the punctures $z_1,\ldots,z_n$. Matching the first expression with the second expression for $T_\phi(z)$ as $z\to\infty$, gives the constraints

$$\sum_{r=1}^{n-1} c_r = 0, \quad \sum_{r=1}^{n-1} c_r z_r = 1 - \frac{n}{2}, \quad \sum_{r=1}^{n-1} (z_r + c_r z_r^2) = c_n. \tag{4.6}$$

Polyakov conjectured, and Takhtajan and Zograf then proved,[7,8] that for a Riemann sphere with n punctures, a suitably regularized Liouville action evaluated at the classical solution is the generating function for c_r, i.e.,

$$c_r = -\frac{1}{2\pi}\frac{\partial S_{\rm cl}}{\partial z_r}, \quad r=1,\ldots,n-3. \tag{4.7}$$

The regularized Liouville action is

$$S_{\rm cl} = \lim_{\epsilon\to 0}\left\{ \frac{i}{2}\int_{\Sigma_\epsilon} dz\wedge d\bar{z}(\partial_z\phi\,\partial_{\bar z}\phi + e^\phi) + 2\pi(n\log\epsilon + 2(n-2)\log|\log\epsilon|) \right\}, \tag{4.8}$$

where $(i/2)dz\wedge d\bar{z} = dx^1\wedge dx^2$, and the integration region is $\Sigma_\epsilon = \mathcal{C}/(\{\cup_{r=1}^{n-1}|z-z_r|<\epsilon\}\cup\{|z|>1/\epsilon\})$, whose boundaries are a circle near ∞ and infinitesimal circles around the punctures.

We now turn to the Taubes equation (2.8) for N vortices in $\mathcal{C}$. Define, by analogy with the Liouville field, $T_h = \partial_z\partial_z h - \frac{1}{2}(\partial_z h)^2$. Using the expansion of h around each vortex center (2.9), we have

$$T_h = T_h(z,\bar z) = \sum_{r=1}^{N}\left\{ -\frac{3}{2(z-Z_r)^2} - \frac{\bar{b_r}}{2(z-Z_r)} \right\} + O(1), \tag{4.9}$$

where the $O(1)$ terms are not all holomorphic. The conformal weight is -3 at each point Z_r, and we may identify $-\bar{b_r}/2$ as the accessory parameter at Z_r. Notice that the constraints $\Sigma_{r=1}^N \bar{b_r}=0$ and $\Sigma_{r=1}^N Z_r\bar{b_r}$ are real, and look remarkably similar to the first two constraints (4.6). If we consider the Poincaré-type metric $ds^2 = e^h\,dz\,d\bar z$, then each vortex corresponds to a conical singularity of deficit angle -2π. For the Liouville equation on Σ, it would not be possible for the conformal weight at each singularity to be negative, but for the Taubes equation with our boundary conditions, it is.

We now show that the regularized action for h is the generating function for $\bar{b_r}$. The unregularized action for h, whose formal variation gives Taubes' equation, is

$$S_h = \frac{i}{2\pi}\int_{\tilde{\mathcal{C}}} dz\wedge d\bar z(2\,\partial_z h\,\partial_{\bar z}h + e^h - h - 1), \tag{4.10}$$

where the integration region $\tilde{\mathcal{C}}$ is $\mathcal{C}$ with N small disks of radius ϵ centered at the vortex locations $\{Z_1,\ldots,Z_N\}$ being punctured out, and the limit $\epsilon\to 0$ taken. As the integrals of h and e^h-1 are known to be finite as $\epsilon\to 0$, the only singular term in the integral comes from $\partial_z h\,\partial_{\bar z}h$, which gives a contribution of $-4N\log\epsilon + O(1)$. This $\log\epsilon$ term needs to be removed. We also require of a

regularized action that at a classical solution, i.e., h satisfying the Taubes equation (2.8), the action should be stationary against variations δh. Now, the variation of S_h only comes from boundary contributions, as other terms can be eliminated by using (2.8), so we have

$$\delta S_h = \frac{i}{2\pi}\int_{\tilde{C}} dz \wedge d\bar{z}\big(2\partial_z(\delta h\, \partial_{\bar{z}} h) + 2\partial_{\bar{z}}(\delta h\, \partial_z h)\big) = -\frac{i}{2\pi}\sum_{r=1}^{N}\left\{2\int_{\gamma_r} d\bar{z}\, \delta h\, \partial_{\bar{z}} h - 2\int_{\gamma_r} dz\, \delta h\, \partial_z h\right\}, \tag{4.11}$$

where γ_r is the small circle of radius ϵ centered at Z_r. We allow δh to be as general as possible, but keep the vortex centers $\{Z_1, \ldots, Z_N\}$ fixed, and restrict the leading-order behavior of h around Z_r to remain $h = \log|z - Z_r|^2$, because the Higgs field Φ would acquire a branch point at Z_r if the power dependence varied. So near Z_r,

$$\delta h = \delta a_r + \frac{1}{2}\delta\bar{b}_r(z - Z_r) + \frac{1}{2}\delta b_r(\bar{z} - \bar{Z}_r) + O(\epsilon^2). \tag{4.12}$$

Substituting (4.12) into (4.11), we find that $\delta S_h = -4\Sigma_{r=1}^{N}\, \delta a_r$ by a similar calculation to those in Ref. 15. This variation can be cancelled by adding a term $4\Sigma_{r=1}^{N} a_r$ to S_h. So combined with the additional $\log \epsilon$ term, we obtain the regularized action

$$S_h^{\text{reg.}} = \lim_{\epsilon\to 0}\left\{\frac{i}{2\pi}\int_{\tilde{C}} dz \wedge d\bar{z}(2\,\partial_z h\, \partial_{\bar{z}} h + e^h - h - 1) + 4\sum_{r=1}^{N} a_r + 4N\log\epsilon\right\}, \tag{4.13}$$

which is finite, and stationary for solutions of the Taubes equation.

From now on, only consider $S_h^{\text{reg.}}$ evaluated at the classical solutions, and hence a function of $\{Z_1, \ldots, Z_N; \bar{Z}_1, \ldots, \bar{Z}_N\}$. Then

$$\frac{\partial S_h^{\text{reg.}}}{\partial Z_s} = \frac{i}{2\pi}\int_{\tilde{C}} dz \wedge d\bar{z}\frac{\partial}{\partial Z_s}(2\,\partial_z h\, \partial_{\bar{z}} h + e^h - h - 1) + 4\sum_{r=1}^{N}\frac{\partial a_r}{\partial Z_s} - \frac{i}{2\pi}\int_{\gamma_s} d\bar{z}(2\,\partial_z h\, \partial_{\bar{z}} h + e^h - h - 1). \tag{4.14}$$

The contribution on the second line of (4.14) comes because a displacement of Z_s, the sth vortex position, induces a displacement of the small circle γ_s. One can use the field equation to derive the useful identity

$$dz \wedge d\bar{z}\frac{\partial}{\partial Z_s}(2\,\partial_z h\, \partial_{\bar{z}} h + e^h - h - 1) = d\{2\, d\bar{z}(\partial_{Z_s} h\, \partial_{\bar{z}} h) - 2\, dz(\partial_{Z_s} h\, \partial_z h)\}. \tag{4.15}$$

Using this, the terms on the first line of (4.14) become boundary integrals, hence

$$\frac{\partial S_h^{\text{reg.}}}{\partial Z_s} = -\frac{i}{2\pi}\sum_{r=1}^{N}\left\{2\int_{\gamma_r} d\bar{z}(\partial_{Z_s} h\, \partial_{\bar{z}} h) - 2\int_{\gamma_r} dz(\partial_{Z_s} h\, \partial_z h)\right\} + 4\sum_{r=1}^{N}\frac{\partial a_r}{\partial Z_s} - \frac{i}{2\pi}\int_{\gamma_s} d\bar{z}(2\,\partial_z h\, \partial_{\bar{z}} h + e^h - h - 1). \tag{4.16}$$

Evaluating these boundary integrals using the expansion (2.9), we find

$$\frac{\partial S_h^{\text{reg.}}}{\partial Z_s} = \left(\bar{b}_s - 2\sum_{r=1}^{N}\frac{\partial a_r}{\partial Z_s}\right) + \left(2\bar{b}_s - 2\sum_{r=1}^{N}\frac{\partial a_r}{\partial Z_s}\right) + 4\sum_{r=1}^{N}\frac{\partial a_r}{\partial Z_s} - \bar{b}_s = 2\bar{b}_s, \tag{4.17}$$

which is our main result. As $S_h^{\text{reg.}}$ is manifestly real, we also have $\partial S_h^{\text{reg.}}/\partial \bar{Z}_s = 2b_s$. $S_h^{\text{reg.}}$ is therefore the generating function of b_s and $\bar{b}_s$, and hence by the remark following (3.1), $S_h^{\text{reg.}}$ is the inter-

acting part $\tilde{\mathcal{K}}$ of the Kähler potential for the Samols metric on $\mathcal{M}_N$. The entire Kähler potential on $\mathcal{M}_N$ is

$$\mathcal{K} = \sum_{r=1}^{N} Z_r \overline{Z_r} + S_h^{\text{reg.}}. \tag{4.18}$$

$S_h^{\text{reg.}}$ has the symmetries of the N-vortex system, namely the translational invariance,

$$\sum_{r=1}^{N} \frac{\partial S_h^{\text{reg.}}}{\partial Z_r} = 0, \tag{4.19}$$

and rotational invariance

$$\sum_{r=1}^{N} \left\{ Z_r \frac{\partial}{\partial Z_r} - \overline{Z}_r \frac{\partial}{\partial \overline{Z}_r} \right\} S_h^{\text{reg.}} = 0, \tag{4.20}$$

which translate into $\Sigma_{r=1}^{N} \overline{b_r} = 0$ and $\Sigma_{r=1}^{N} Z_r \overline{b_r} = \Sigma_{r=1}^{N} \overline{Z_r} b_r$, respectively. Notice that these symmetries restrict the forms of additional holomorphic or antiholomorphic functions we could add to our Kähler potential.

One final remark about $S_h^{\text{reg.}}$ is that it can be simplified, because $1 - e^h$ is twice the magnetic field, whose integral over the plane is a constant in the N-vortex sector. The term proportional to $1 - e^h$ in the integrand of (4.13) can therefore be dropped. However, this simplification only applies to $S_h^{\text{reg.}}$ evaluated on the classical solutions.

V. THE KÄHLER POTENTIAL FOR HYPERBOLIC VORTICES

Abelian Higgs vortices on the hyperbolic plane $\mathbb{H}^2$ with Ricci scalar -1 were first considered by Witten,[11] and an expression for the Kähler metric on the moduli space was derived by Strachan.[12] A feature of the hyperbolic case is that the N-vortex system can be described by a Liouville field ψ with sources, as an alternative to h.

On a general curved surface, we can always choose coordinates such that the metric is $g = e^{\sigma(z,\overline{z})}\, dz\, d\overline{z}$. The gauge-invariant field equation for N vortices becomes

$$4\partial_z \partial_{\overline{z}} h - e^{\sigma(z,\overline{z})}(e^h - 1) = 4\pi \sum_{r=1}^{N} \delta(z - Z_r), \tag{5.1}$$

with the boundary condition $h \to 0$. Solutions exist as before, with arbitrary locations Z_r,[18] and the generalized Samols metric on the N-vortex moduli space, again derived from the kinetic terms of the Lagrangian, is[19]

$$G = \sum_{r,s=1}^{N} \left\{ e^{\sigma(Z_r,\overline{Z}_r)} \delta_{rs} + 2\frac{\partial b_s}{\partial Z_r} \right\} dZ_r\, d\overline{Z}_s. \tag{5.2}$$

The quantities b_r are defined as earlier, through the expansion (2.9) of h near the vortex centers; the only difference being that in the middle quadratic term of (2.9), the coefficient $\frac{1}{4}$ is replaced by $\frac{1}{4} e^{\sigma(Z_r,Z_r)}$.

For vortices on the hyperbolic plane $\mathbb{H}^2$ in the standard disk model, with Ricci scalar $R = -1$, the conformal factor is

$$e^{\sigma} = \frac{8}{(1 - z\overline{z})^2}, \quad |z| < 1, \tag{5.3}$$

and σ satisfies the Liouville equation $\partial_z \partial_{\overline{z}} \sigma = \frac{1}{4} e^{\sigma}$. Now consider the conformal transformation on the hyperbolic plane, $g \to \hat{g} = e^h g = e^{h+\sigma}\, dz\, d\overline{z}$. The Ricci scalar transforms to

$$\hat{R} = e^{-h}(R - 4e^{-\sigma}\partial_z \partial_{\bar{z}} h) = e^{-h}(-1 - 4e^{-\sigma}\partial_z \partial_{\bar{z}} h). \tag{5.4}$$

We see that if h satisfies (5.1), then, away from the singularities, $\hat{R}=-1$. Moreover, the field $\psi = \sigma + h$ also satisfies the Liouville equation $\partial_z \partial_{\bar{z}} \psi = \frac{1}{4} e^{\psi}$.

The squared magnitude of the Higgs field $|\Phi|^2 = e^h$ of hyperbolic vortices therefore has a geometrical interpretation; it plays the role of a conformal factor changing the hyperbolic plane into a hyperbolic plane $\hat{\mathbb{H}}^2$ of the same curvature, however, with conical singularities at $\{Z_1, \ldots, Z_N\}$.

Since ψ is a Liouville field, e^{ψ} can be expressed in terms of some rational function $f(z)$. f needs to satisfy the condition $|f|<1$ for $|z|<1$, to map disk into disk, and also the boundary condition $|f| \to 1$ as $|z| \to 1$. The metric $\hat{g}$ is

$$\hat{g} = e^{\psi}\, dz\, d\bar{z} = \frac{8\left|\frac{df}{dz}\right|^2 dz\, d\bar{z}}{(1 - f\bar{f})^2} = \frac{8\, df\, d\bar{f}}{(1 - f\bar{f})^2}. \tag{5.5}$$

$f(z)$ is a map from $\hat{\mathbb{H}}^2$ to $\mathbb{H}^2$, and the metric $\hat{g}$ is the pull-back of the standard hyperbolic metric on $\mathbb{H}^2$. Conical singularities occur on $\hat{\mathbb{H}}^2$, because the inverse of f is multivalued in general. Using (5.3), we see that

$$|\Phi|^2 = e^h = \left|\frac{df}{dz}\right|^2 \frac{(1 - z\bar{z})^2}{(1 - f\bar{f})^2}, \tag{5.6}$$

and the phase of Φ can be chosen so that

$$\Phi = \left(\frac{df}{dz}\right)\frac{(1 - z\bar{z})}{(1 - f\bar{f})}. \tag{5.7}$$

For N distinct vortices, df/dz should vanish at N distinct points within the unit disk. The general form of f satisfying these requirements is given in Ref. 12.

Consider now the expansion of ψ around the rth vortex position Z_r,

$$\psi = \log|z - Z_r|^2 + A_r + \frac{1}{2}\bar{B}_r(z - Z_r) + \frac{1}{2}B_r(\bar{z} - \bar{Z}_r) + \bar{C}_r(z - Z_r)^2 + C_r(\bar{z} - \bar{Z}_r)^2 + \cdots. \tag{5.8}$$

Since $\psi = h + \sigma = h + \log(8/(1 - z\bar{z})^2)$, the expansion coefficients of ψ are related to those of h by

$$A_r = a_r + \log\left\{\frac{8}{(1 - Z_r\bar{Z}_r)^2}\right\},$$

$$\bar{B}_r = \bar{b}_r + \frac{4\bar{Z}_r}{(1 - Z_r\bar{Z}_r)}, \quad B_r = b_r + \frac{4Z_r}{(1 - Z_r\bar{Z}_r)},$$

$$\bar{C}_r = \bar{c}_r + \frac{\bar{Z}_r^2}{(1 - Z_r\bar{Z}_r)^2}, \quad C_r = c_r + \frac{Z_r^2}{(1 - Z_r\bar{Z}_r)^2}. \tag{5.9}$$

One can show by computing the zz component of the energy–momentum tensor for ψ, that at Z_r the conformal weight is -3 and the accessory parameter is $-\bar{B}_r/2$.

The regularized Liouville action for ψ is

$$S_\psi^{\text{reg.}} = \lim_{\epsilon\to 0}\left\{ \frac{i}{2\pi}\int_{\tilde{\mathbb{D}}} dz\wedge d\bar{z}(2\,\partial_z\psi\,\partial_{\bar{z}}\psi + e^{\psi}) + 4\sum_{r=1}^{N} A_r - \frac{8}{\epsilon} + (4N-8)\log\epsilon \right\}, \tag{5.10}$$

where $\tilde{\mathbb{D}}=\mathbb{D}/(\{\cup_{r=1}^{N}|z-Z_r|<\epsilon\}\cup\{|z|>1-\epsilon\})$ and $\mathbb{D}$ is the unit disk. As before, $S_\psi^{\text{reg.}}$ evaluated on an N-vortex solution becomes a function just of the vortex positions. By differentiating $S_\psi^{\text{reg.}}$, we obtain, by a calculation similar to that in Sec. IV.,

$$\frac{\partial S_\psi^{\text{reg.}}}{\partial Z_r} = 2\overline{B_r}, \quad \frac{\partial S_\psi^{\text{reg.}}}{\partial \overline{Z_r}} = 2B_r, \tag{5.11}$$

and therefore

$$\frac{\partial^2 S_\psi^{\text{reg.}}}{\partial Z_s\,\partial\overline{Z_r}} = 2\frac{\partial B_r}{\partial Z_s} = \left\{ \frac{8\delta_{rs}}{(1-Z_r\overline{Z_r})^2} + 2\frac{\partial b_r}{\partial Z_s} \right\}. \tag{5.12}$$

By comparing with (5.2), we see that (5.12) is the coefficient of $dZ_r d\overline{Z_s}$ in the Samols/Strachan metric on the N-vortex moduli space. This shows that $S_\psi^{\text{reg.}}$ is the entire Kähler potential for the hyperbolic vortices. Unlike vortices in $\mathbb{R}^2$, we do not have to add a further term.

VI. CONCLUSION

In this paper, we presented two expressions for the Kähler potential for N distinct Abelian Higgs vortices on $\mathbb{R}^2$, both involving integrals of the gauge invariant quantity $h=\log|\Phi|^2$.

Our first approach used a scaling argument and appears to be the easiest. The result agrees with the Kähler potential for two well-separated vortices given in Ref. 6. The second approach exploits the striking analogy between the expansion coefficients $\overline{b_r}$ of the field h, and the accessory parameters c_r in Liouville field theory. The regularized action for h evaluated on classical solutions was shown to be the interacting part of the Kähler potential. By adding the flat part $\Sigma_{r=1}^{N} Z_r\overline{Z_r}$, we obtained the full Kähler potential on the N-vortex moduli space.

We also investigated vortices on the hyperbolic plane $\mathbb{H}_2$ with Ricci scalar -1. It was convenient to describe hyperbolic vortices using the Liouville field ψ, instead of the related h. The expansion coefficients $\overline{b_r}$ in this case are directly related to the accessory parameters of the Liouville field. The regularized action for ψ was shown to be the entire Kähler potential on the N-vortex moduli space. It would be interesting to compare the N-vortex metric and the Weil–Petersson metric for the hyperbolic plane with N punctures.

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Spectral properties of a Dirac operator in the chiral quark soliton model

Asao Arai,[a] Kunimitsu Hayashi, and Itaru Sasaki
Department of Mathematics, Hokkaido University, Sapporo 060-0810, Japan

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We consider a Dirac operator H acting in the Hilbert space $L^2(\mathbb{R}^3;\mathbb{C}^4)\otimes\mathbb{C}^2$, which describes a Hamiltonian of the chiral quark soliton model in nuclear physics. The mass term of H is a matrix-valued function formed out of a function $F:\mathbb{R}^3\to\mathbb{R}$, called a profile function, and a vector field $\mathbf{n}$ on $\mathbb{R}^3$, which fixes pointwise a direction in the isospin space of the pion. We first show that, under suitable conditions, H may be regarded as a generator of a supersymmetry. In this case, the spectra of H are symmetric with respect to the origin of $\mathbb{R}$. We then identify the essential spectrum of H under some condition for F. For a class of profile functions F, we derive an upper bound for the number of discrete eigenvalues of H. Under suitable conditions, we show the existence of a positive energy ground state or a negative energy ground state for a family of scaled deformations of H. A symmetry reduction of H is also discussed. Finally a unitary transformation of H is given, which may have a physical interpretation. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1896388]

I. INTRODUCTION

Let $\sigma_j (j=1,2,3)$ be the Pauli matrices,

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.1}$$

and

$$\alpha_j := \begin{pmatrix} \sigma_j & 0_2 \\ 0_2 & -\sigma_j \end{pmatrix} \quad (j=1,2,3), \quad \beta := \begin{pmatrix} 0_2 & 1_2 \\ 1_2 & 0_2 \end{pmatrix}, \tag{1.2}$$

where 0_2 and 1_2 are the 2×2 zero matrix and the 2×2 identity matrix, respectively. The matrix

$$\gamma_5 := -i\alpha_1\alpha_2\alpha_3 \tag{1.3}$$

is Hermitian with $\gamma_5^2 = 1_4$ (the 4×4 identity matrix) satisfying the following relations:

$$[\alpha_j, \gamma_5] = 0 \ (j=1,2,3), \quad \{\beta, \gamma_5\} = 0, \tag{1.4}$$

where $[A,B] := AB - BA$ and $\{A,B\} := AB + BA$. We set

$$\boldsymbol{\sigma} := (\sigma_1, \sigma_2, \sigma_3), \quad \boldsymbol{\alpha} := (\alpha_1, \alpha_2, \alpha_3). \tag{1.5}$$

For objects $\mathbf{A} = (A_1, A_2, A_3)$ and $\mathbf{B} = (B_1, B_2, B_3)$ such that the products $A_j B_j$ $(j=1,2,3)$ and their sum are defined, we write $\mathbf{A}\cdot\mathbf{B} := \sum_{j=1}^3 A_j B_j$.

We consider a Dirac operator acting in the Hilbert space

[a]Author to whom correspondence should be addressed. Electronic mail: arai@math.sci.hokudai.ac.jp

$$\mathcal{H} := L^2(\mathbb{R}^3;\mathbb{C}^4) \otimes \mathbb{C}^2, \tag{1.6}$$

where $L^2(\mathbb{R}^3;\mathbb{C}^4)$ is the Hilbert space of $\mathbb{C}^4$-valued square integrable functions on $\mathbb{R}^3$. Let $\nabla := (D_1, D_2, D_3)$ with D_j the generalized partial differential operator in the variable x_j, the jth component of $\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$. Then the free Dirac operator with mass zero is defined by

$$H_0 := -i\boldsymbol{\alpha} \cdot \nabla \otimes 1_2 \tag{1.7}$$

acting in $\mathcal{H}$. To introduce a perturbation to H_0, let $F : \mathbb{R}^3 \to \mathbb{R}$ be Borel measurable and finite almost everywhere (a.e.) in $\mathbb{R}^3$ and set

$$U_F := \cos F + i\gamma_5 \otimes \boldsymbol{\tau} \cdot \mathbf{n} \sin F, \tag{1.8}$$

where $\boldsymbol{\tau} := (\tau_1, \tau_2, \tau_3)$ with $\tau_j := \sigma_j (j = 1, 2, 3)$, $\mathbf{n} := (n_1, n_2, n_3)$ with n_j a real-valued measurable function on $\mathbb{R}^3$ such that

$$|\mathbf{n}(\mathbf{x})|^2 = 1, \quad \text{a.e. } \mathbf{x} \in \mathbb{R}^3. \tag{1.9}$$

Let $M > 0$ be a constant. Then, by the second relation in (1.4), $M(\beta \otimes 1_2)U_F$ is a bounded self-adjoint operator on $\mathcal{H}$. Hence, by the Kato–Rellich theorem, the operator

$$H := H_0 + M(\beta \otimes 1_2)U_F \tag{1.10}$$

is self-adjoint with domain $D(H) = D(H_0)$. This is the Dirac operator we consider in this paper. The operator H appears as the Hamiltonian of the so-called the chiral quark soliton model in nuclear physics (e.g., Ref. 1 and references therein). In this context, M and

$$\Phi_F := \cos F + i \sin F \otimes \boldsymbol{\tau} \cdot \mathbf{n} \tag{1.11}$$

(U_F with γ_5 replaced by 1_4) denote the mass of a quark and the pion field, respectively, and F is called a profile function. The Dirac operator H is not only physically important, but also may have interests from purely mathematical points of view. As far as we know, no mathematically rigorous analysis has been made on the Dirac operator H (a study of a Dirac operator with a variable mass is given in Ref. 2, but, in that paper, the mass is a scalar function and the point there is to establish self-adjointness of such a Dirac opeartor in cases where the Kato–Rellich theorem is no longer applicable to it; in this sense Ref. 2 does not bear upon the topics of the present paper).

The present paper is organized as follows. In Sec. II, we show that the Dirac operator H can be regarded as a generator of a supersymmetry, and describe its implications on the spectra of H. In Sec. III we identify the essential spectrum of H. We also derive an upper bound for the number of discrete eigenvalues of H. In particular, for a class of F and $\mathbf{n}$, the absence of discrete eigenvalues of H is proven. Sections IV and V are concerned with existence of discrete eigenvalues of H. In Sec. IV we introduce a concept of a positive energy ground state and that of a negative energy ground state of H and show, under some condition for F, that a scaled deformation of H has a positive energy ground state or a negative ground state. In Sec. V we discuss a symmetry reduction of H to smaller mutually orthogonal closed subspaces which are indexed by triples $(\ell, s, t) \in \mathbb{Z} \times \{\pm 1\} \times \{\pm 1\}$, where ℓ denote an eigenvalue of the third component of the angular momentum operator, $s/2$ the spin of the quark and $t/2$ the isospin of the pion. We prove that, under suitable conditions, each reduced part of H or its scaled version has a discrete positive ground state or a discrete negative ground state. In the last section we present a unitary transformation which brings H to a Dirac operator with a magnetic moment.

II. SUPERSYMMETRIC ASPECTS

In this section we assume the following.

Hypothesis (I): Each $n_j (j = 1, 2, 3)$ is continuously differentiable on $\mathbb{R}^3$ and

$$(n_1(\mathbf{x}), n_2(\mathbf{x})) \neq (0, 0), \quad \mathbf{x} \in \mathbb{R}^3. \tag{2.1}$$

Let

$$\xi(\mathbf{x}) := \frac{(\tau_1 n_2(\mathbf{x}) - \tau_2 n_1(\mathbf{x}))}{\sqrt{n_1(\mathbf{x})^2 + n_2(\mathbf{x})^2}}, \quad \mathbf{x} \in \mathbb{R}^3. \tag{2.2}$$

Then $\xi(\mathbf{x})^2 = 1$, $\mathbf{x} \in \mathbb{R}^3$. For all $\mathbf{x} \in \mathbb{R}^3$, we can define a matrix tensor

$$\Gamma(\mathbf{x}) := \alpha_1\alpha_2\alpha_3\beta \otimes \xi(\mathbf{x}) \tag{2.3}$$

acting on $\mathbb{C}^4 \otimes \mathbb{C}^2$. It is easy to see that $\Gamma(\mathbf{x})$ is self-adjoint with $\Gamma(\mathbf{x})^2 = I$ (I denotes identity). By the natural identification $\mathcal{H} = L^2(\mathbb{R}^3; \mathbb{C}^4 \otimes \mathbb{C}^2)$, we denote the multiplication operator by the matrix-tensor valued function $\Gamma(\cdot)$ by the same symbol Γ. Then Γ is self-adjoint and unitary on $\mathcal{H}$.

Proposition 2.1: *Suppose that Hypothesis (I) holds and $\xi(\mathbf{x})$ is a constant matrix. Then, for all $\psi \in D(H)$, $\Gamma\psi \in D(H)$ and*

$$\{\Gamma, H\}\psi = 0, \quad \psi \in D(H). \tag{2.4}$$

Proof: By direct computations, we have

$$\{\alpha_1\alpha_2\alpha_3\beta, \alpha_j\} = 0 \quad (j = 1,2,3), \quad \{\xi(\mathbf{x}), \boldsymbol{\tau} \cdot \mathbf{n}(\mathbf{x})\} = 0. \tag{2.5}$$

Using these relations and the constancy of $\xi(\cdot)$, we see that, for all $\psi \in D(H) = D(H_0)$, $\Gamma\psi \in D(H_0)$ and $H_0\Gamma\psi = -\Gamma H_0\psi$. Similarly, using (2.5) and $[\alpha_1\alpha_2\alpha_3\beta, \beta\gamma_5] = 0$, we see that $\{M(\beta \otimes 1_2)U_F, \Gamma\}\psi = 0$. Thus (2.4) follows. ■

Proposition 2.1 shows that the Dirac operator H may be regarded as a generator of a supersymmetry, i.e., a supercharge with respect to Γ (e.g., p. 140 in Ref. 3).

For a self-adjoint operator T, we denote by $\sigma(T)$ [respectively, $\sigma_{\mathrm{p}}(T)$] the spectrum of T (respectively, the point spectrum of T). The discrete spectrum of T (the set of isolated eigenvalues of T with finite multiplicity) is denoted $\sigma_{\mathrm{d}}(T)$.

Theorem 2.2: *Suppose that Hypothesis (I) holds and $\xi(\mathbf{x})$ is a constant matrix. Then*

(i) *$\sigma(H)$ is symmetric with respect to the origin of $\mathbb{R}$, i.e., if $\lambda \in \sigma(H)$, then $-\lambda \in \sigma(H)$.*
(ii) *$\sigma_{\#}(H)(\#=\mathrm{p},\mathrm{d})$ is symmetric with respect to the origin of $\mathbb{R}$. The multiplicity $\lambda \in \sigma_{\#}(H)$ coincides with that of $-\lambda \in \sigma_{\#}(H)$.*

Proof: By Proposition 2.1 we have $\Gamma H \Gamma^{-1} = -H$ (the unitary equivalence of H and $-H$). This implies the desired results. ■

Remark 2.1: The properties stated in Theorem 2.2 may differ from spectral properties of the usual Dirac operator $H_0 + M\beta + V$, where V is a scalar potential.

III. THE ESSENTIAL SPECTRUM AND FINITENESS OF THE DISCRETE SPECTRUM OF *H*

A. Structure of the spectrum of *H*

For a self-adjoint operator T, we denote by $\sigma_{\mathrm{ess}}(T)$ the essential spectrum of T.

Theorem 3.1: *Suppose that*

$$\lim_{|\mathbf{x}| \to \infty} F(\mathbf{x}) = 0. \tag{3.1}$$

Then

$$\sigma_{\mathrm{ess}}(H) = (-\infty, -M] \cup [M, \infty), \tag{3.2}$$

$$\sigma_{\mathrm{d}}(H) \subset (-M, M). \tag{3.3}$$

Proof: We write $H = H_0 + M(\beta \otimes I_2) + V$ with $V := M(\beta \otimes I_2)(U_F - I)$. We have $\|V(x)\| \leqslant M(|1 - \cos F(x)| + |\sin F(x)|) \to 0 (|x| \to \infty)$. Hence we can apply Theorem 4.7, Remark 2 on p. 117 in Ref.

3 to H to obtain (3.2). This implies (3.3). ■

B. Bound for the number of discrete eigenvalues of *H*

Assume (3.1). Then, by Theorem 3.1, we can define the number of discrete eigenvalues of H counting multiplicities,

$$N_H := \dim \mathrm{Ran}\, E_H((-M,M)), \tag{3.4}$$

where E_H is the spectral measure of H and $\mathrm{Ran}\, E_H((-M,M))$ means the range of $E_H((-M,M))$. To estimate an upper bound for N_H, we introduce a hypothesis for F and $\mathbf{n}$.

Hypothesis (II):

(i) The functions F and n_j $(j=1,2,3)$ are continuously differentiable on $\mathbb{R}^3$.
(ii) The functions D_jF and D_jn_k $(j,k=1,2,3)$ are bounded on $\mathbb{R}^3$.

Under this assumption, we can define

$$V_F(\mathbf{x}) := \sqrt{|\nabla F(\mathbf{x})|^2 + \sum_{k=1}^{3} |\nabla n_k(\mathbf{x})|^2 \sin^2 F(\mathbf{x})}, \quad \mathbf{x} \in \mathbb{R}^3. \tag{3.5}$$

Theorem 3.2: *Assume (3.1) and Hypothesis (II). Suppose that*

$$C_F := \int_{\mathbb{R}^6} \frac{V_F(\mathbf{x})V_F(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2} d\mathbf{x}\, d\mathbf{y} < \infty. \tag{3.6}$$

Then N_H is finite with

$$N_H \leqslant \frac{M^2 C_F}{2\pi^2}. \tag{3.7}$$

To prove this theorem we present a general lemma. Let $\mathcal{K}$ be a complex Hilbert space and $\mathsf{B}(\mathcal{K})$ be the Banach space of bounded linear operators on $\mathcal{K}$. Let $V:\mathbb{R}^d \to \mathsf{B}(\mathcal{K})$ $(d \in \mathbb{N})$ be a measurable function. The function V defines a unique multiplication operator acting in the Hilbert space $L^2(\mathbb{R}^d;\mathcal{K})$ of $\mathcal{K}$-valued square integrable functions on $\mathbb{R}^d$. We denote it by the same symbol V. We assume the following (Δ is the d-dimensional generalized Laplacian):

(V.1) $D((-\Delta)^{1/2}) \subset D(|V|^{1/2}) \cap D(|V^*|^{1/2})$ and the form sum

$$L_0 := -\Delta \dotplus \begin{pmatrix} -|V| & 0 \\ 0 & -|V^*| \end{pmatrix}$$

acting in $\oplus^2 L^2(\mathbb{R}^d;\mathcal{K})$ with form domain $D((-\Delta)^{1/2})$ defines a unique self-adjoint operator bounded from below. Moreover, $\sigma_{\mathrm{ess}}(L_0) \subset [0,\infty)$.

(V.2) The operator

$$L := -\Delta + \begin{pmatrix} 0 & V^* \\ V & 0 \end{pmatrix}$$

acting in $\oplus^2 L^2(\mathbb{R}^d;\mathcal{K})$ is self-adjoint on $D(\Delta)$, bounded from below, and $\sigma_{\mathrm{ess}}(L) \subset [0,\infty)$.

For a self-adjoint operator A, we denote by $N_-(A)$ the number of negative eigenvalues of A counting multiplicities.

Lemma 3.3: *Assume (V.1) and (V.2). Then $N_-(L) \leqslant N_-(L_0)$.*

Proof: Let

$$Q := \begin{pmatrix} 0 & V^* \\ V & 0 \end{pmatrix}.$$

Then Q is self-adjoint and

$$Q^2 = \begin{pmatrix} |V|^2 & 0 \\ 0 & |V^*|^2 \end{pmatrix},$$

which implies that

$$|Q| = \begin{pmatrix} |V| & 0 \\ 0 & |V^*| \end{pmatrix}.$$

It is obvious that $Q \geqslant -|Q|$. Hence $L \geqslant L_0$. This inequality and the min–max principle (e.g., Theorem XIII.1, Problem 1 in Ref. 4) imply the inequality $N_-(L) \leqslant N_-(L_0)$. ■

Proof of Theorem 3.2: We note that H has the operator matrix representation

$$H = H_0 + M \begin{pmatrix} 0 & \Phi_F^* \\ \Phi_F & 0 \end{pmatrix}, \tag{3.8}$$

where Φ_F is defined by (1.11). Hence

$$H^2 = L(F) + M^2 \tag{3.9}$$

with

$$L(F) := -\Delta + M \begin{pmatrix} 0 & W_F^* \\ W_F & 0 \end{pmatrix}, \tag{3.10}$$

where $W_F := i\boldsymbol{\sigma} \cdot (\nabla \Phi_F)$. Note that, by Hypothesis (II) (ii), the second term on the right-hand side of (3.10) is a bounded self-adjoint operator and hence $L(F)$ is self-adjoint with $D(L(F)) = D(\Delta)$. By direct computations, we have

$$W_F(\mathbf{x})^* W_F(\mathbf{x}) = W_F(\mathbf{x}) W_F(\mathbf{x})^* = |\nabla F(\mathbf{x})|^2 + \sum_{j=1}^{3} |\nabla n_j(\mathbf{x})|^2 \sin^2 F(\mathbf{x}),$$

where we have used (1.9). Hence $|W_F| = |W_F^*| = V_F$. Let $L_0(F) := -\Delta - MV_F$. By Theorem 3.1, $\sigma_{\mathrm{ess}}(L(F)) = [0, \infty)$. Condition (3.6) implies that V_F is a potential in the Rollnik class (p. 170 in Ref. 5). Hence it follows from Example 7, p. 118 in Ref. 4 and Weyl's essential spectrum theorem (Theorem XIII.14, p. 112 in Ref. 4) that $\sigma_{\mathrm{ess}}(L_0(F)) = \sigma_{\mathrm{ess}}(-\Delta) = [0, \infty)$. Therefore the assumption of Lemma 3.3 with $L = L(F)$ and $L_0 = L_0(F)$ is satisfied. Hence $N_-(L(F)) \leqslant N_-(L_0(F))$. It is well known that $N_-(L_0(F)) \leqslant 8M^2 C_F / (4\pi)^2$ (Theorem XIII.10 in Ref. 4), where the factor $8 = \dim \mathbb{C}^4 \otimes \mathbb{C}^2$. On the other hand, by the spectral theorem, $N_H \leqslant N_-(L_F)$. Thus (3.7) follows. ■

Theorem 3.2 implies the absence of discrete eigenvalues of H for F's such that the Rollnik norm of MV_F is sufficiently small.

Corollary 3.4: *Assume (3.1) and Hypothesis (II). Let* $M^2 C_F < 2\pi^2$. *Then* $\sigma_{\mathrm{d}}(H) = \emptyset$.

IV. EXISTENCE OF DISCRETE GROUND STATES

For a self-adjoint operator A bounded from below, we set

$$E_0(A) := \inf \sigma(A).$$

If $E_0(A) \in \sigma_{\mathrm{p}}(A)$, then we say that A has a ground state and we call a nonzero vector in $\ker(A - E_0(A))$ a ground state of A. If $E_0(A) \in \sigma_{\mathrm{d}}(A)$, then we say that A has a discrete ground state.

Definition 4.1: Let

$$E_0^+(H) := \inf(\sigma(H) \cap [0,\infty)), \quad E_0^-(H) := \sup(\sigma(H) \cap (-\infty,0]). \tag{4.1}$$

If $E_0^+(H)$ [respectively, $E_0^-(H)$] is an eigenvalue of H, then we say that H has a positive (respectively, negative) energy ground state and we call a nonzero vector in $\ker(H-E_0^+(H))$ [respectively, $\ker(H-E_0^-(H))$] a positive (respectively, negative) energy ground state of H. If $E_0^+(H)$ [respectively, $E_0^-(H)$] is a discrete eigenvalue of H, then we say that H has a discrete positive (respectively, negative) energy ground state.

Remark 4.1: If the spectrum of H is symmetric with respect to the origin of $\mathbb{R}$ as in Theorem 2.2, then $E_0^+(H) = -E_0^-(H)$, and H has a positive energy ground state if and only if it has a negative energy ground state.

We assume Hypothesis (II). Then the operators

$$S_\pm(F) := -\Delta \pm M(D_3 \cos F) = -\Delta \mp M(D_3 F)\sin F \tag{4.2}$$

are self-adjoint with $D(S_\pm(F)) = D(\Delta)$ and bounded from below.

Theorem 4.2: *Assume Hypothesis (II) and (3.1). Suppose that $E_0(S_+(F)) < 0$ or $E_0(S_-(F)) < 0$. Then H has a discrete positive energy ground state or a discrete negative ground state.*

Proof: For each $f \in D(\Delta)$ and $u \in \mathbb{C}^2$ with $\|u\| = 1$, we define

$$\psi_f^+ := (f \otimes u, 0, if \otimes u, 0) \in \mathcal{H}, \quad \psi_f^- := (0, f \otimes u, 0, if \otimes u) \in \mathcal{H}.$$

Then we have

$$\langle \psi_f^\pm, L(F)\psi_f^\pm \rangle = 2\langle f, S_\pm(F) f \rangle.$$

In the case where $E_0(S_+(F)) < 0$, there exists a unit vector $f \in D(\Delta)$ such that $\langle f, S_+(F) f \rangle < 0$. Hence $\langle \psi_f^+, L(F)\psi_f^+ \rangle < 0$. By Theorem 3.1 and the spectral theorem, we have

$$\sigma_{\mathrm{ess}}(L(F)) = [0,\infty). \tag{4.3}$$

Thus, by the min–max principle, $L(F)$ has a discrete ground state. Similarly, in the case where $E_0(S_-(F)) < 0$ too, $L(F)$ has a discrete ground state. This implies that H has a discrete positive energy ground state or a discrete negative ground state. ■

To construct examples of F satisfying the conditions as stated in Theorem 4.2, we consider a scaling. For a constant $\varepsilon > 0$ and a function f on $\mathbb{R}^d$, we define a function f_ε on $\mathbb{R}^d$ by

$$f_\varepsilon(x) := f(\varepsilon x), \quad x \in \mathbb{R}^d.$$

Lemma 4.3: *Let $V: \mathbb{R}^d \to \mathbb{R}$ be in $L^2_{\mathrm{loc}}(\mathbb{R}^d)$ and, for a constant $\varepsilon > 0$,*

$$S_\varepsilon := -\Delta + V_\varepsilon.$$

Suppose that the following conditions are satisfied:

(i) *For all $\varepsilon > 0$, S_ε is self-adjoint and bounded from below and $\sigma_{\mathrm{ess}}(S_\varepsilon) \subset [0,\infty)$.*
(ii) *There exists a nonempty open set $\Omega \subset \{x \in \mathbb{R}^d \mid V(x) < 0\}$.*

Then there exists a constant $\varepsilon_0 > 0$ such that, for all $\varepsilon \in (0,\varepsilon_0)$, S_ε has a discrete ground state.

Proof: By condition (ii), we can take a nonzero vector $f \in C_0^\infty(\Omega)$ (the set of infinitely differentiable functions on $\mathbb{R}^d$ with compact support in Ω). Then it is easy to see that $\langle f_\varepsilon, S_\varepsilon f_\varepsilon \rangle = \varepsilon^{-d}(a_f \varepsilon^2 - |b_f|)$, where $a_f := \|\nabla f\|^2$, $b_f = \langle f, Vf \rangle < 0$. Hence, taking $\varepsilon_0 := \sqrt{|b_f|/a_f}$ (note that $a_f \neq 0$), we have $\langle f_\varepsilon, S_\varepsilon f_\varepsilon \rangle < 0$ for all $\varepsilon \in (0,\varepsilon_0)$. Hence, by the min–max principle and condition (i), $E_0(S_\varepsilon) \in \sigma_{\mathrm{d}}(S_\varepsilon)$. ■

Lemma 4.4: *Let $V: \mathbb{R}^d \to \mathbb{R}$ be continuous on $\mathbb{R}^d$ with $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = 0$. Suppose that $\Omega_- := \{x \in \mathbb{R}^d \mid V(x) < 0\} \neq \emptyset$. Then the following hold:*

(i) *$-\Delta + V$ acting in $L^2(\mathbb{R}^d)$ is self-adjoint and bounded from below.*
(ii) *$\sigma_{\mathrm{ess}}(-\Delta + V) = [0,\infty)$.*

(iii) *S_ε has a discrete ground state for all $\varepsilon\in(0,\varepsilon_0)$ with some $\varepsilon_0>0$.*

Proof: Part (i) follows from the Kato–Rellich theorem. Part (ii) is proven by a simple application of Theorem XIII.15-(b) in Ref. 4.

Since V is continuous, the set Ω_- is open. Hence Lemma 4.3 implies the existence of a ground state of S_ε for all $\varepsilon\in(0,\varepsilon_0)$ with some $\varepsilon_0>0$. ■

We consider a one-parameter family of Dirac operators,

$$H_\varepsilon := H_0 + \frac{1}{\varepsilon} M(\beta\otimes 1_2)U_{F_\varepsilon}, \tag{4.4}$$

which is a scaled deformation of H.

Theorem 4.5: *Assume Hypothesis (II) and (3.1). Suppose that $D_3\cos F$ is not identically zero. Then there exists a constant $\varepsilon_0>0$ such that, for all $\varepsilon\in(0,\varepsilon_0)$, H_ε has a discrete positive energy ground state or a discrete negative ground state.*

Proof: We write $S_\pm(F,M):=S_\pm(F)$ to make explicit the dependence of $S_\pm(F)$ on M. At least one of the sets $\{\mathbf{x}\in\mathbb{R}^3|(D_3\cos F)(\mathbf{x})>0\}$ and $\{\mathbf{x}\in\mathbb{R}^3(D_3\cos F)(\mathbf{x})<0\}$ is not empty. The function $D_3\cos F=-(D_3F)\sin F$ is bounded and continuous satisfying $\lim_{|\mathbf{x}|\to\infty}(D_3F)(\mathbf{x})=0$. Hence we can apply Lemma 4.4 to conclude that $S_+(F_\varepsilon,\varepsilon^{-1}M)$ or $S_-(F_\varepsilon,\varepsilon^{-1}M)$ has a discrete ground state for all $\varepsilon\in(0,\varepsilon_0)$ with some $\varepsilon_0>0$. This fact and Theorem 4.2 yield the desired result. ■

V. SYMMETRY REDUCTION OF *H*

In this section, we show that, if F is invariant under the rotations around the x_3 axis, then there exist infinitely many mutually orthogonal closed subspaces of $\mathcal{H}$ that reduce H_ε for all $\varepsilon>0$ and each reduced part of H_ε may have a positive energy ground state or a negative energy ground state. We use the cylindrical coordinates for points $\mathbf{x}=(x_1,x_2,x_3)\in\mathbb{R}^3$,

$$x_1 = r\cos\theta, \quad x_2 = r\sin\theta, \quad x_3 = z,$$

where $\theta\in[0,2\pi)$, $r>0$. We assume the following.

Hypothesis (III): There exists a continuously differentiable function $G:(0,\infty)\times\mathbb{R}\to\mathbb{R}$ such that (i) $F(\mathbf{x})=G(r,z)$, $\mathbf{x}\in\mathbb{R}^3\backslash\{0\}$; (ii) $\lim_{r+|z|\to\infty}G(r,z)=0$; (iii) $\sup_{r>0,z\in\mathbb{R}}(|\partial G(r,z)/\partial r|+|\partial G(r,z)/\partial z|)<\infty$.

We take the vector field $\mathbf{n}$ to be of the form

$$\mathbf{n}(\mathbf{x}) := (\sin\Theta(r,z)\cos(m\theta), \sin\Theta(r,z)\sin(m\theta), \cos\Theta(r,z)), \tag{5.1}$$

where $\Theta:(0,\infty)\times\mathbb{R}\to\mathbb{R}$ is continuous and m is a real constant.

Let $L_3 := -ix_1D_2+ix_2D_1$, the third component of the angular momentum. It is well known that L_3 is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. We denote its closure by the same symbol L_3. We set

$$\Sigma_3 := \sigma_3\oplus\sigma_3$$

acting on $\mathbb{C}^4$ and define

$$K_3 := L_3\otimes 1_2 + \frac{1}{2}\Sigma_3\otimes 1_2 + \frac{m}{2}I\otimes\tau_3, \tag{5.2}$$

which is a self-adjoint operator acting in $\mathcal{H}$.

We denote by T_ε ($\varepsilon>0$) the unitary dilation on $L^2(\mathbb{R}^3)$ with power ε,

$$(T_\varepsilon f)(\mathbf{x}) := \varepsilon^{3/2} f(\varepsilon\mathbf{x}), \quad f\in L^2(\mathbb{R}^3), \text{ a.e. } \mathbf{x}. \tag{5.3}$$

Lemma 5.1: *For all $\varepsilon>0$, $T_\varepsilon L_3 T_\varepsilon^{-1}=L_3$. Hence $(T_\varepsilon\otimes 1_2)K_3(T_\varepsilon\otimes 1_2)^{-1}=K_3$ for all $\varepsilon>0$.*

Proof: It is straightforward to see that, for all $f\in C_0^\infty(\mathbb{R}^3)$, $T_\varepsilon L_3 f=L_3T_\varepsilon f$. Since $C_0^\infty(\mathbb{R}^3)$ is a core of L_3, this equality extends to all $f\in D(L_3)$ showing that $L_3\subset T_\varepsilon^{-1}L_3T_\varepsilon$. The both sides are

self-adjoint. Hence they coincide. ■

Lemma 5.2: *Assume that*

$$\Theta(\varepsilon r, \varepsilon z) = \Theta(r,z), \quad (r,z) \in (0,\infty) \times \mathbb{R}, \quad \varepsilon > 0. \tag{5.4}$$

Then, for all $t \in \mathbb{R}$ *and* $\varepsilon > 0$, *the operator equality*

$$e^{itK_3} H_\varepsilon e^{-itK_3} = H_\varepsilon \tag{5.5}$$

holds.

Proof: We first prove (5.5) with $\varepsilon = 1$. We have for all $t \in \mathbb{R}$,

$$e^{itK_3} = e^{itL_3} e^{it\Sigma_3/2} \otimes e^{itm\tau_3/2}.$$

For all $f \in C_0^\infty(\mathbb{R}^3)$, we have

$$(e^{itL_3} f)(\mathbf{x}) = f(x_1 \cos t - x_2 \sin t, x_1 \sin t + x_2 \cos t, z), \quad \mathbf{x} \in \mathbb{R}^3.$$

Hence e^{itL_3} leaves $C_0^\infty(\mathbb{R}^3)$ invariant. It follows that, for all $f \in C_0^\infty(\mathbb{R}^3; \mathbb{C}^4) \otimes \mathbb{C}^2$, $e^{itK_3} f \in D(H_0) = D(H)$ and

$$H_0 e^{itL_3} f = e^{itL_3}\{(-i\alpha_1 \cos t + i\alpha_2 \sin t) D_1 f + (-i\alpha_1 \sin t - i\alpha_2 \cos t) D_2 f - i\alpha_3 D_3 f\}. \tag{5.6}$$

Using the matrix representation of α_j, one can check that

$$\alpha_j e^{it\Sigma_3/2} = e^{-it\Sigma_3/2} \alpha_j \quad (j = 1,2), \quad [\alpha_3, e^{it\Sigma_3}] = 0.$$

It follows from these relations and (5.6),

$$H_0 e^{itK_3} f = e^{itK_3} H_0 f. \tag{5.7}$$

We have

$$\tau_j e^{itm\tau_3/2} = e^{itm\tau_3/2} \tau_j e^{itm\tau_3} \quad (j = 1,2), \quad \tau_3 e^{itm\tau_3/2} = e^{itm\tau_3/2} \tau_3$$

and

$$e^{-itL_3} \mathbf{n}(\mathbf{x}) e^{itL_3} = (\sin\Theta(r,z)\cos m(\theta - t), \sin\Theta(r,z)\sin m(\theta - t), \cos\Theta(r,z)).$$

It follows from these relations that

$$\beta \otimes 1_2 U_F e^{itK_3} f = e^{itK_3} (\beta \otimes 1_2) U_F f. \tag{5.8}$$

Combining (5.7) together with (5.8), we obtain $He^{itK_3} f = e^{itK_3} Hf$. Since $C_0^\infty(\mathbb{R}^3; \mathbb{C}^4) \otimes \mathbb{C}^2$ is a core of H, this equality extends to all $f \in D(H) = D(H_0)$ showing $H \subset e^{-itK_3} H e^{itK_3}$. The both sides are self-adjoint. Thus (5.5) follows.

We next consider the case where $\varepsilon \neq 1$. We write $U_F = U(F, \mathbf{n})$. By Lemma 5.1, (5.8) and the fact that T_ε is a bijection from $C_0^\infty(\mathbb{R}^3)$ onto itself, we have $\beta \otimes 1_2 U(F_\varepsilon, \mathbf{n}_\varepsilon) e^{itK_3} f = e^{itK_3} (\beta \otimes 1_2) U(F_\varepsilon, \mathbf{n}_\varepsilon) f$. By condition (5.4), $\mathbf{n}_\varepsilon = \mathbf{n}$. Hence $\beta \otimes 1_2 U(F_\varepsilon, \mathbf{n}_\varepsilon) e^{itK_3} f = e^{itK_3} (\beta \otimes 1_2) U(F_\varepsilon, \mathbf{n}) f$. Therefore (5.8) holds with F replaced by F_ε. Thus, in the same way as in the preceding paragraph, one can prove (5.5). ■

We say that two self-adjoint operators on a Hilbert space strongly commute if their spectral measures commute.

Lemma 5.3: *Assume (5.4). Then, for all* $\varepsilon > 0$, H_ε *and* K_3 *strongly commute.*

Proof: It follows from Lemma 5.2 and the functional calculus for self-adjoint operators that $e^{itK_3} e^{isH_\varepsilon} = e^{isH_\varepsilon} e^{itK_3}$ for all s, $t \in \mathbb{R}$ and all $\varepsilon > 0$. This implies the strong commutativity of H_ε and K_3 (see Theorem VIII.13 in Ref. 6 for general criteria of the strong commutativity of self-adjoint operators). ■

Let

$$E := (0,\infty) \times [0,2\pi) \times \mathbb{R} = \{(r,\theta,z) | r > 0, \theta \in [0,2\pi), z \in \mathbb{R}\}$$

and $\mathrm{d}\mu := r\,\mathrm{d}r \otimes \mathrm{d}\theta \otimes \mathrm{d}z$, a measure on E. Then one can define a unitary operator $Y: L^2(\mathbb{R}^3) \to L^2(E, \mathrm{d}\mu)$ by

$$(Yf)(r,\theta,z) := f(r\cos\theta, r\sin\theta, z), \quad f \in L^2(\mathbb{R}^3).$$

For each $\ell \in \mathbb{Z}$, we define $\phi_\ell : [0,2\pi) \to \mathbb{C}$ by

$$\phi_\ell(\theta) := \frac{1}{\sqrt{2\pi}} e^{i\ell\theta}, \quad \theta \in [0,2\pi). \tag{5.9}$$

It is well known that $\{\phi_\ell\}_{\ell\in\mathbb{Z}}$ is a complete orthonormal system of $L^2([0,2\pi))$. For each $f \in L^2(E, \mathrm{d}\mu)$, we define $\hat{f} : (0,\infty) \times \mathbb{Z} \times \mathbb{R}$ by

$$\hat{f}(r, \ell, z) := \int_0^{2\pi} \phi_\ell(\theta)^* f(r,\theta,z)\mathrm{d}\theta.$$

We define an operator D_θ on $L^2(E, \mathrm{d}\mu)$ as follows:

$$D(D_\theta) := \left\{ f \in L^2(E,\mathrm{d}\mu) \middle| \sum_{\ell=-\infty}^{\infty} \ell^2 \int_0^\infty \mathrm{d}r\, r \int_{\mathbb{R}} \mathrm{d}z |\hat{f}(r, \ell, z)|^2 < \infty \right\},$$

$$(\widehat{D_\theta f})(r, \ell, \theta) = i\,\ell\,\hat{f}(r, \ell, \theta), \quad f \in D(D_\theta).$$

Then $-iD_\theta$ is self-adjoint with

$$\sigma(-iD_\theta) = \sigma_{\mathrm{p}}(-iD_\theta) = \{\ell\}_{\ell\in\mathbb{Z}} = \mathbb{Z}, \tag{5.10}$$

$$\ker(-iD_\theta - \ell) = \left\{ g\phi_\ell \middle| g: (0,\infty) \times \mathbb{R} \to \mathbb{C}, \int_0^\infty \mathrm{d}r\, r \int_{\mathbb{R}} \mathrm{d}z |g(r,z)|^2 < \infty \right\}. \tag{5.11}$$

It is not so hard to see that

$$YL_3Y^{-1} = -iD_\theta. \tag{5.12}$$

Hence

$$\sigma(L_3) = \sigma_{\mathrm{p}}(L_3) = \mathbb{Z}. \tag{5.13}$$

Let

$$\mathcal{M}_\ell := \ker(L_3 - \ell) = Y^{-1} \ker(-iD_\theta - \ell). \tag{5.14}$$

Then we have the orthogonal decomposition

$$L^2(\mathbb{R}^3) = \oplus_{\ell=-\infty}^{\infty} \mathcal{M}_\ell, \quad L^2(E,\mathrm{d}\mu) = \oplus_{\ell=-\infty}^{\infty} Y\mathcal{M}_\ell. \tag{5.15}$$

By (5.13), we have

$$\sigma(K_3) = \sigma_{\mathrm{p}}(K_3) = \left\{ \ell + \frac{s}{2} + \frac{mt}{2} \middle| \ell \in \mathbb{Z}, s = \pm 1, t = \pm 1 \right\}. \tag{5.16}$$

The eigenspace of K_3 with eigenvalue $\ell + (s/2) + (mt/2)$ is given by

$$\mathcal{M}_{\ell,s,t} := \mathcal{M}_\ell \otimes \mathcal{C}_s \otimes \mathcal{T}_t \tag{5.17}$$

under the natural identificaion $\mathcal{H}=L^2(\mathbb{R}^3)\otimes\mathbb{C}^4\otimes\mathbb{C}^2$, where $\mathcal{C}_s := \ker(\Sigma_3 - s)$ and $\mathcal{T}_t := \ker(\tau_3 - t)$. Then $\mathcal{H}$ has the orthogonal decomposition

$$\mathcal{H} = \oplus_{\ell\in\mathbb{Z},s,t\in\{\pm1\}}\mathcal{M}_{\ell,s,t}. \tag{5.18}$$

Lemma 5.3 implies the following fact.

Lemma 5.4: *Assume (5.4). Then, for all $\varepsilon>0$, H_ε is reduced by each $\mathcal{M}_{\ell,s,t}$.*

We denote by $H_\varepsilon(\ell,s,t)$ by the reduced part of H_ε to $\mathcal{M}_{\ell,s,t}$ and set

$$H(\ell,s,t) := H_1(\ell,s,t), \tag{5.19}$$

the reduced part of H to $\mathcal{M}_{\ell,s,t}$.

For $s=\pm1$ and $\ell\in\mathbb{Z}$, we define

$$S_s(G,\ell) := -\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \frac{\ell^2}{r^2} + \frac{\partial^2}{\partial z^2} + sM\frac{\partial \cos G}{\partial z} \tag{5.20}$$

acting in $L^2((0,\infty)\times\mathbb{R}, r\,\mathrm{d}r\,\mathrm{d}z)$ with domain $D(S_s(G,\ell)) := C_0^\infty((0,\infty)\times\mathbb{R})$ and set

$$\mathcal{E}_0(S_s(G,\ell)) := \inf_{f\in C_0^\infty((0,\infty)\times\mathbb{R}),\|f\|_{L^2((0,\infty)\times\mathbb{R},r\,\mathrm{d}r\,\mathrm{d}z)}=1} \langle f, S_s(G,\ell) f\rangle.$$

Theorem 5.5: *Assume Hypothesis (III). Fix an $\ell\in\mathbb{Z}$ arbitrarily and $s=\pm1$. Suppose that $\mathcal{E}_0(S_s(G,\ell))<0$. Then, for each $t=\pm1$, $H(\ell,s,t)$ has a discrete positive energy ground state or a discrete negative ground state.*

Proof: Let

$$c_\ell := \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{-i\ell\theta}\cos(m\theta), \quad \mathrm{d}_\ell := \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{-i\ell\theta}\sin(m\theta),$$

$$n_{j,\ell}(r,z) := (\sin\Theta(r,z)c_\ell, \sin\Theta(r,z)d_\ell, \cos\Theta(r,z)),$$

$$\Phi_{G,\ell,t} := \cos G + i\sum_{j=1} n_{j,\ell}\sin G\otimes\tau_j + itn_{3,\ell}\sin G,$$

$$D_{1,\ell} := c_\ell\frac{\partial}{\partial r} - \frac{d_\ell}{r}\frac{\partial}{\partial\theta}, \quad D_{2,\ell} := d_\ell\frac{\partial}{\partial r} + \frac{c_\ell}{r}\frac{\partial}{\partial\theta}$$

and

$$W_{G_\varepsilon,\ell,s,t} := i\sum_{j=1}^{2}\sigma_j D_{j,\ell}\Phi_{G_\varepsilon,\ell,t} + isD_z\Phi_{G_\varepsilon,\ell,t}, \quad \varepsilon>0.$$

Then we have

$$(Y\otimes 1_2)H_\varepsilon(\ell,s,t)^2(Y\otimes 1_2)^{-1} = -\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \frac{\ell^2}{r^2} + \frac{\partial^2}{\partial z^2} + \varepsilon^{-1}M\begin{pmatrix} 0 & W^*_{G_\varepsilon,\ell,s,t} \\ W_{G_\varepsilon,\ell,s,t} & \end{pmatrix} + M^2$$
$$=: L_\varepsilon(\ell,s,t) + M^2$$

on $C_0^\infty((0,\infty)\times\mathbb{R})$.

For each $f\in C_0^\infty((0,\infty)\times\mathbb{R})$ and $u_t\in\mathbb{C}^2$ satisfying $\|f\|=1$, $\|u_t\|=1$, and $\tau_3 u_t = tu_t (t=\pm1)$, we define

$$\psi_f^{(1)} := (f \otimes u_t, 0, if \otimes u_t, 0) \in \mathcal{M}(\ell, 1, t),$$

$$\psi_f^{(-1)} := (0, f \otimes u_t, 0, if \otimes u_t) \in \mathcal{M}(\ell, -1, t).$$

Then we have

$$\langle \psi_f^{(s)}, YL_1(\ell, s, t) Y^{-1} \psi_f^{(s)} \rangle = 2\langle f, S_s(F, \ell) f \rangle.$$

By the present assumption, there exists a unit vector $f \in C_0^\infty((0,\infty) \times \mathbb{R})$ such that $\langle f, S_s(F, \ell) f \rangle < 0$. Note that $\sigma_{\mathrm{ess}}(L_1(\ell, s, t)) \subset [0, \infty)$. Hence, by the min–max principle, $L_1(\ell, s, t)$ has a discrete ground state. This implies that $H(\ell, s, t)$ has a discrete positive energy ground state or a discrete negative ground state. ■

Theorem 5.6: *Assume Hypothesis (III) and (5.4). Suppose that* $\partial \cos G / \partial z$ *is not identically zero. Then, for each* $\ell \in \mathbb{Z}$, *there exists a constant* $\varepsilon_\ell > 0$ *such that, for all* $\varepsilon \in (0, \varepsilon_\ell)$, *each* $H_\varepsilon(\ell, s, t)$ *has a discrete positive energy ground state or a discrete negative ground state.*

Proof: We write $S_{s,M}(F, \ell) := S_s(F, \ell)$ to make explicit the dependence of $S_s(F, \ell)$ on M. In the same way as in the proof of Theorem 4.5, one can take a vector $f_\varepsilon \in C_0^\infty((0,\infty) \times \mathbb{R})$ such that $\langle f_\varepsilon, S_{s,\varepsilon^{-1}M}(F_\varepsilon(\ell)) f_\varepsilon \rangle < 0$ for all sufficiently small $\varepsilon > 0$, where the smallness depends on ℓ. It follows from the proof of the preceding theorem that $L_\varepsilon(\ell, s, t)$ has a discrete ground state. ■

Corollary 5.7: *Assume Hypothesis (III) and (5.4). Suppose that* $\partial \cos G / \partial z$ *is not identically zero. Let* ε_ℓ *be as in Theorem 5.6 and, for each* $N \in \mathbb{N}$ *and* $k > n$ $(k, n \in \mathbb{Z})$, $\nu_{k,n} := \min_{n+1 \leqslant \ell \leqslant k} \varepsilon_\ell$. *Then, for each* $\varepsilon \in (0, \nu_{k,n})$, H_ε *has at least* $(k-n)$ *discrete eigenvalues counting multiplicities.*

Proof: We have $\sigma_{\mathrm{p}}(H_\varepsilon) = \cup_{\ell \in \mathbb{Z}, s, t = \pm 1} \sigma_{\mathrm{p}}(H_\varepsilon(\ell, s, t))$. By the preceding theorem, for each $\ell = n+1, \ldots, k$, $H_\varepsilon(\ell, s, t)$ has a discrete eigenvalue. Thus the desired result follows. ■

Remark 5.1: This result is consistent with Theorem 3.2, because it reads in the present case

$$N_{H_\varepsilon} \leqslant \frac{1}{\varepsilon^4} \frac{M^2 C_F}{2\pi^2}$$

and the right-hand side diverges as $\varepsilon \to 0$.

VI. A UNITARY TRANSFORMATION

In this section we show that, under Hypothesis (II), the Hamiltonian H with $\mathbf{n}$ constant is unitarily equivalent to an operator which resembles a Dirac operator with a magnetic moment.

It is easy to see that the operator

$$X_F := \begin{pmatrix} e^{iF \otimes \boldsymbol{\tau} \cdot \mathbf{n}/2} & 0 \\ 0 & e^{-iF \otimes \boldsymbol{\tau} \cdot \mathbf{n}/2} \end{pmatrix} \tag{6.1}$$

is unitary. Under Hypothesis (II), we can define the following functions:

$$B_j(\mathbf{x}) := \tfrac{1}{2} D_j(F(\mathbf{x}) \otimes \boldsymbol{\tau} \cdot \mathbf{n}(\mathbf{x})), \quad \mathbf{x} \in \mathbb{R}^3, \ j = 1,2,3. \tag{6.2}$$

We set

$$\mathbf{B} := (B_1, B_2, B_3) \tag{6.3}$$

and introduce

$$H(\mathbf{B}) := H_0 + M\beta - \boldsymbol{\sigma} \cdot \mathbf{B} \tag{6.4}$$

acting in $\mathcal{H}$. Note that, under Hypothesis (II), the operator $-\boldsymbol{\sigma} \cdot \mathbf{B}$ is a bounded self-adjoint operator. Hence, by a simple application of the Kato–Rellich theorem, $H(\mathbf{B})$ is self-adjoint with $D(H(\mathbf{B})) = D(H_0)$.

Proposition 6.1: *Assume Hypothesis (II) and that* $\mathbf{n}$ *is constant. Then*

$$X_F H X_F^{-1} = H(\mathbf{B}). \tag{6.5}$$

Proof: Noting the fact that $(\boldsymbol{\tau}\cdot\mathbf{n})^2 = 1_2$, we have

$$\Phi_F = e^{iF\otimes\boldsymbol{\tau}\cdot\mathbf{n}}.$$

It follows from this fact and (3.8) that $X_F H X_F^{-1}\psi = H(\mathbf{B})\psi$ for all $\psi \in [\oplus^4 C_0^\infty(\mathbb{R}^3)]\otimes\mathbb{C}^2$. Since $[\oplus^4 C_0^\infty(\mathbb{R}^3)]\otimes\mathbb{C}^2$ is a core of $H(\mathbf{B})$, the operator equality (6.5) follows. ■

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The large-Z Behavior of pseudorelativistic atoms

Thomas Østergaard Sørensen[a)]
Mathematisches Institut, Universität München, Theresienstrasse 39, D-80333 Munich, Germany

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In this paper we study the large-Z behavior of the ground state energy of atoms with electrons having relativistic kinetic energy $\sqrt{p^2c^2+m^2c^4}-mc^2$. We prove that to leading order in Z the energy is the same as in the nonrelativistic case, given by (nonrelativistic) Thomas–Fermi theory. For the problem to make sense, we keep the product $Z\alpha$ fixed (here α is Sommerfeld's fine structure constant), and smaller than, or equal to, $2/\pi$, which means that as Z tends to infinity, α tends to zero. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1897645]

I. INTRODUCTION AND RESULTS

As a model for a relativistic atom with nuclear charge Z and N electrons, we consider the operator

$$H_{\mathrm{rel}}=\sum_{i=1}^{N}\left\{\sqrt{-\alpha^{-2}\Delta_i+\alpha^{-4}}-\alpha^{-2}-\frac{Z}{|x_i|}\right\}+\sum_{1\leqslant i<j\leqslant N}\frac{1}{|x_i-x_j|}.$$

Here, $x_i\in\mathbb{R}^3$ is the coordinate of the ith electron, Δ_i is the Laplacian with respect to x_i, and α is Sommerfeld's fine structure constant (the physical value of α is approximately $1/137.037$). This is the expression one obtains using $\sqrt{p^2c^2+m^2c^4}-mc^2$ for the kinetic energy of the electrons (and making the substitution $p\to-i\hbar\nabla$), measuring energies (H_{rel}) in units of Rydberg, and lengths (the x_i's) in units of the Bohr radius.

This model has been much studied over the past 30 years. Stability in the case $N=1$ was proved independently by Herbst[9] and Weder.[22] The stability of matter for the model was first proved by Conlon,[2] later by Fefferman and de la Llave,[7] and also by Lieb and Yau;[17] see the latter for an overview. A nonexhaustive list of other works on this model is Refs. 10, 21, 20, 19, and 1.

It is well known that the operator H_{rel} is bounded from below on $C_0^\infty(\mathbb{R}^{3N})$ if, and only if, $Z\alpha\leqslant 2/\pi$. Only in this case is the atom stable; and we define the operator H_{rel} as a self-adjoint, unbounded operator by Friedrichs extending this semibounded operator. To study the energy of large atoms, one would normally then consider the limit as $Z\to\infty$ of the infimum of the spectrum of this operator. However, due to the upper bound on Z resulting from the restriction $Z\alpha\leqslant 2/\pi$, this is not possible here. To overcome this problem, we consider

$$H_{\mathrm{rel}}=\alpha^{-1}\left\{\sum_{i=1}^{N}\left\{\sqrt{-\Delta_i+\alpha^{-2}}-\alpha^{-1}-\frac{\delta}{|x_i|}\right\}+\sum_{1\leqslant i<j\leqslant N}\frac{\alpha}{|x_i-x_j|}\right\},$$

where $\delta=Z\alpha$ is held *fixed*. This ensures that as $Z\to\infty$, and therefore $\alpha\to 0$, the operator H_{rel} remains well defined—as long as $0\leqslant\delta\leqslant 2/\pi$. Also, we shall keep $\lambda\equiv N/Z$ fixed. The energy of the atom is then defined as

[a)]On leave from Department of Mathematical Sciences, Aalborg University, Fredrik Bajers Vej 7G, DK-9220 Aalborg East, Denmark. Electronic mail: sorensen@mathematik.uni-muenchen.de

$$E_N(Z,\delta) := \inf \sigma_{\mathcal{H}_F}(H_{\mathrm{rel}}),$$

where the spectrum of H_{rel} is calculated on $\mathcal{H}_F = \wedge^N L^2(\mathbb{R}^3, \mathbb{C}^q)$, the Fermionic Hilbert space, describing N Fermions, each with q possible spin states. We will take $q=2$ from now on (but this is no restriction). We note that since (the extension of) H_{rel} is self-adjoint and bounded from below, we have the Rayleigh–Ritz principle. If $\mathcal{C}$ is a form core for the corresponding quadratic form, then

$$\inf \sigma_{\mathcal{H}_F}(H_{\mathrm{rel}}) = \inf_{\{\psi \in \mathcal{C} \| \|\psi\|=1\}} \langle \psi, H_{\mathrm{rel}} \psi \rangle.$$

Our main result is the following.

Theorem 1.1: *Let $\delta \in (0, 2/\pi]$ and $\lambda > 0$ be fixed and let H_{rel} and $E_{N=\lambda Z}(Z,\delta)$ be as above. Then*

$$E_{\lambda Z}(Z,\delta) = -C_{\mathrm{TF}}(\lambda) Z^{7/3} + o(Z^{7/3}), \quad Z \to \infty, \tag{1.1}$$

where $-C_{\mathrm{TF}}(\lambda) Z^{7/3}$ is the (nonrelativistic) Thomas–Fermi energy of the atom.

This shows that, to leading order, the ground-state energy of a relativistic atom is given by the (nonrelativistic) semiclassical Thomas–Fermi energy approximation, as it is for the nonrelativistic atom (note that the case $\delta = 2/\pi$ is included). (In the nonrelativistic case this was first proved by Lieb and Simon;[14] see also Lieb.[11]) This expresses the fact that for large atoms the majority of the electrons are nonrelativistic.

The second term in the expansion (1.1) will be studied in a forthcoming paper.[18]

The proof of Theorem 1.1 will be by finding upper and lower bounds on $E_{\lambda Z}(Z,\delta)$. Note that the relativistic kinetic energy is always lower than the nonrelativistic one,

$$\sqrt{\alpha^{-2} q^2 + \alpha^{-4}} - \alpha^{-2} = \alpha^{-2}\left(\sqrt{1 + (\alpha q)^2} - 1\right) \leqslant \frac{q^2}{2}. \tag{1.2}$$

(Note, since we will later make Taylor expansions of the square root in the relativistic kinetic energy, we will have to insist on the nonrelativistic kinetic energy being $-\Delta/2$.) This means that all upper bounds derived earlier[14,11] for the nonrelativistic operator

$$H_{\mathrm{cl}} = \sum_{i=1}^{N} \left\{ \frac{p_i^2}{2} - \frac{Z}{|x_i|} \right\} + \sum_{1 \leqslant i < j \leqslant N} \frac{1}{|x_i - y_i|}$$

will also be upper bounds for H_{rel}; in particular, to prove Theorem 1.1, we need only derive a lower bound.

II. ORGANIZATION OF THE PAPER

We start in Sec. III by reducing the N-body operator H_{rel} to a one-particle one; having done that, we only need to consider wave functions given as Slater determinants when trying to minimize the energy. To proceed, we need to localize the kinetic energy. To do so, we use (in Sec. IV) an analogue of the IMS localization formula for the Schrödinger operator, see Ref. 3, p.27. This formula has already been developed by Lieb and Yau in Ref. 17 for both the operator $\sqrt{-\Delta + \alpha^{-2}} - \alpha^{-1}$ and the hyperrelativistic kinetic energy $|p|$. This is essentially done by finding the integral kernels of these operators. For $\sqrt{-\Delta + \alpha^{-2}} - \alpha^{-1}$, this involves the modified Bessel function K_2, and the derivation of the formula and of needed properties of K_2 are carried out in Appendix A. The localization error, given by a bounded operator $L^{(\alpha)}$ expressed as an integral operator involving K_2, is then estimated (in Sec. V). Estimating the error is rather technical (calculative) and involves localization of the operator and the above-mentioned properties of K_2. Some of the localized terms are estimated with the localized energy itself (Secs. VI and VII).

Coming to the localized energy, we must estimate the kinetic energy close to the nucleus. Since this is the high-energy region, this is where the electrons are relativistic, and so this term should be of lower order, since, to leading order, there should be no relativistic contribution to the

energy. As the relativistic kinetic energy is asymptotically linear in p in the high-energy region—as opposed to the classical one which is quadratic—the singularity in the potential causes substantially more trouble. This problem is solved (in Sec. VI) by a clever choice of parameters in an estimate by Lieb and Yau in Ref. 17 on the sum of the eigenvalues of the energy in a ball around the nucleus. This also determines the scale on which one can localize close to the nucleus. A part of two of the localized terms of the operator $L^{(\alpha)}$ is estimated along with this term.

In the outer region, one uses (in Sec. VIII) essentially the same idea as Lieb did in the classical case, see Ref. 12, to refind the desired phase space integral, which is to give the semiclassical Thomas–Fermi energy. This involves introducing coherent states and estimating the error by doing so. The formulas for the relativistic case were developed in Ref. 16, but the error obtained there is too rough for our purposes. We therefore develop (in Appendix B) a better estimate by a more careful analysis. In order to make all this work, one needs the coherent state to be supported further out than the initial cutoff around the nucleus. To get this, an intermediary zone is introduced (also in Sec. IV) by an additional cutoff. The energy in this shell is estimated (in Sec. VII) by a generalized version of the Lieb–Thirring inequality, proved by Daubechies in Ref. 4. Also the other part of the previously mentioned two terms of the localized operator $L^{(\alpha)}$ is estimated in this way. (For another work which uses coherent states in a relativistic setup, see Ref. 6.)

Finally we relate (in Sec. VIII) the energy in the outer region to the Thomas–Fermi energy from the classical (that is, the Schrödinger) case. In this region, the kinetic energy is small, and using the specific scaling property of Thomas–Fermi theory allows one to make the change from the relativistic energy $\sqrt{-\alpha^{-2}\Delta+\alpha^{-4}}-\alpha^{-2}$ to the nonrelativistic one, $-\Delta/2$, getting errors of the desired order.

III. REDUCTION TO A ONE-PARTICLE PROBLEM

We will use the notation

$$H=\alpha H_{\mathrm{rel}}=\sum_{i=1}^{N}\left\{\sqrt{-\Delta_i+\alpha^{-2}}-\alpha^{-1}-\frac{\delta}{|x_i|}\right\}+\sum_{1\leqslant i<j\leqslant N}\frac{\alpha}{|x_i-x_j|}. \tag{3.1}$$

Recall that $\delta=Z\alpha$ is *fixed* and that the ground state energy of H_{rel} is to be proven to be of leading order $Z^{7/3}$. Since we wish to consider α as the free parameter, the relevant order of all error terms will be $o(\alpha^{-4/3})$. Also, we will denote the operator $\sqrt{-\Delta+\alpha^{-2}}$ by $\sqrt{p^2+\alpha^{-2}}$, and so $T(p)=\sqrt{p^2+\alpha^{-2}}-\alpha^{-1}$ will be the kinetic energy.

We start by reducing the problem from an N-particle problem to a one-particle one. This is done by using an inequality on the electron–electron interaction $\Sigma_{i<j}|x_i-x_j|^{-1}$, which will reduce this to a one-particle potential.

Choose a spherically symmetric function $g\in C_0^\infty(\mathbb{R}^3)$, non-negative, supported in the unit ball $B(0,1)$ of $\mathbb{R}^3$, and such that $\int g(x)^2d^3x=1$. Let $\phi(x)=g(x)^2$ and let for $a>0$ (a to be chosen later), $\phi_a(x)=a^{-3}\phi(x/a)$, so that $\int\phi_a(x)d^3x=1$. Then for all $\rho:\mathbb{R}^3\to\mathbb{R}$ we have

$$\begin{aligned}\sum_{1\leqslant i<j\leqslant N}\frac{1}{|x_i-x_j|}&\geqslant\sum_{1\leqslant i<j\leqslant N}\int\int\frac{\phi_a(x-x_i)\phi_a(y-x_j)}{|x-y|}d^3x\,d^3y\\&=\frac{1}{2}\sum_{i,j=1}^{N}\int\int\frac{\phi_a(x-x_i)\phi_a(y-x_j)}{|x-y|}d^3x\,d^3y-\frac{1}{2}N\int\int\frac{\phi_a(x)\phi_a(y)}{|x-y|}d^3x\,d^3y\\&=\sum_{i=1}^{N}\int\int\frac{\rho(y)\phi_a(x-x_i)}{|x-y|}d^3x\,d^3y-\frac{1}{2}\int\int\frac{\rho(x)\rho(y)}{|x-y|}d^3x\,d^3y-c(\phi)Na^{-1}\\&\quad+\frac{1}{2}\int\int\frac{\left(\sum_i\phi_a(x-x_i)-\rho(x)\right)\left(\sum_j\phi_a(y-x_j)-\rho(y)\right)}{|x-y|}d^3x\,d^3y\end{aligned}$$

$$\geqslant \sum_{i=1}^{N} \int\int \frac{\rho(y)\phi_a(x-x_i)}{|x-y|} d^3x\, d^3y - \frac{1}{2}\int\int \frac{\rho(x)\rho(y)}{|x-y|} d^3x\, d^3y - c(\phi)Na^{-1}.$$

In the last inequality we used that $|x-y|^{-1}$ is of positive type (a positive kernel) since

$$\int\int \frac{\overline{f(x)}f(y)}{|x-y|} d^3x\, d^3y = 4\pi \int \frac{|\hat{f}(p)|^2}{|p|^2} d^3p.$$

The constant $c(\phi)$ is independent of a,

$$c(\phi) = \frac{1}{2}\int\int \frac{\phi(x)\phi(y)}{|x-y|} d^3x\, d^3y = 2\pi \int \frac{|\hat{\phi}(p)|^2}{|p|^2} d^3p.$$

Noting that (using the spherical symmetry of ϕ_a)

$$\int\int \frac{\rho(y)\phi_a(x-x_i)}{|x-y|} d^3x\, d^3y = \int\int \frac{\rho(y)\phi_a(z)}{|z-(x_i-y)|} d^3z\, d^3y$$

$$= \int \rho(y)(\phi_a * |\cdot|^{-1})(x_i-y) d^3y = (\rho * \phi_a * |\cdot|^{-1})(x_i) \equiv \rho * \phi_a * |x_i|^{-1},$$

we get the operator inequality [see (3.1) for H],

$$H \geqslant \sum_{i=1}^{N} \left\{ \sqrt{p_i^2 + \alpha^{-2}} - \alpha^{-1} - \frac{\delta}{|x_i|} + \alpha\rho * \phi_a * |x_i|^{-1} \right\} - \frac{\alpha}{2}\int\int \frac{\rho(x)\rho(y)}{|x-y|} d^3x\, d^3y - \alpha c(\phi)Na^{-1}. \tag{3.2}$$

Having reduced the N-body operator H to a one-body operator, we only need to consider Slater determinants when trying to minimize the energy. That is, when considering $\langle \psi, H\psi \rangle$ we need only consider those $\psi \in \mathcal{H}_F$ which are given by

$$\psi(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \det(m_i(x_j)),$$

where $m_i \in L^2(\mathbb{R}^3)$, $i = 1, \ldots, N$, are orthonormal. Note also that since $C_0^\infty(\mathbb{R}^3)$ is a core for the operator $\sqrt{p^2+\alpha^{-2}} - \alpha^{-1} - \delta/|x|$, $\delta \in [0, 2/\pi]$ (see Herbst[9]), we need only consider m_i's in this space. Then, as soon as h is a one-particle operator acting on $L^2(\mathbb{R}^3)$, we have that

$$\left\langle \psi, \sum_{i=1}^{N} h_i \psi \right\rangle = \sum_{i=1}^{N} (m_i, h m_i).$$

Here, $\langle , \rangle$ and $(,)$ denote inner products in $L^2(\mathbb{R}^{3N})$, respectively, $L^2(\mathbb{R}^3)$, both linear in the second variable, and h_i is h acting on the variable x_i of ψ. Also, we will use $\|\cdot\|_p$ for the norm in $L^p(\mathbb{R}^3)$.

IV. LOCALIZATION OF THE KINETIC ENERGY

In order to treat the one-body operator in (3.2) and in particular the singularity in the Coulomb potential—which causes considerably more trouble than in the nonrelativistic case—we introduce, following Lieb and Yau,[17] a partition of unity (see also Cycon *et al.*, Ref. 3, Definition 3.1), For some $\beta \in (0, \frac{1}{2})$, let θ_1 and θ_2 be monotone positive smooth functions on $\mathbb{R}_+$, $0 \leqslant \theta_i \leqslant 1$, such that

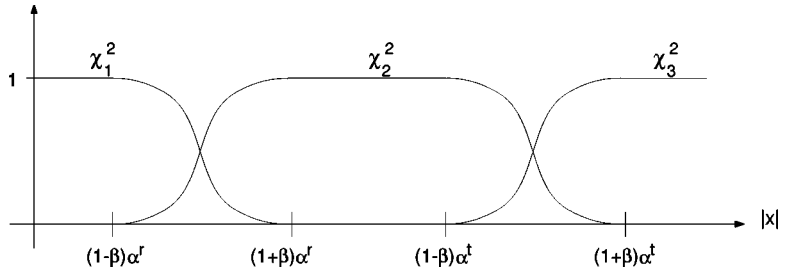

FIG. 1. The partition of unity.

$$\theta_1(\xi) = \begin{cases} 1 & \text{if } \xi < 1-\beta, \\ 0 & \text{if } \xi > 1+\beta, \end{cases} \qquad \theta_2(\xi) = \begin{cases} 0 & \text{if } \xi < 1-\beta, \\ 1 & \text{if } \xi > 1+\beta, \end{cases}$$

and such that $\theta_1(\xi)^2+\theta_2(\xi)^2=1$ for all $\xi \in \mathbb{R}_+$. Now define, with $8/9<r<1$ and $1/3<t<2/3$ (these choices of parameters are governed by the later analysis), the following three functions, which (for α sufficiently small) is a partition of unity in $\mathbb{R}^3$:

$$\chi_1(x) = \theta_1\left(\frac{|x|}{\alpha^r}\right), \quad \chi_2(x) = \theta_1\left(\frac{|x|}{\alpha^t}\right)\theta_2\left(\frac{|x|}{\alpha^r}\right), \quad \chi_3(x) = \theta_2\left(\frac{|x|}{\alpha^t}\right). \tag{4.1}$$

Then, at least for α sufficiently small, we have the picture in Fig. 1.

According to Lieb and Yau (Ref. 17, Theorem 9; α^{-1} corresponds to m) we have for $f \in C_0^\infty(\mathbb{R}^3)$ that

$$(f, \sqrt{p^2+\alpha^{-2}}f) = \sum_{j=1}^{3} (f, \chi_j\sqrt{p^2+\alpha^{-2}}\chi_j f) - (f, L^{(\alpha)}f), \tag{4.2}$$

where $L^{(\alpha)}$ is a bounded operator on $L^2(\mathbb{R}^3)$, given by the kernel

$$L^{(\alpha)}(x,y) = \frac{\alpha^{-2}}{4\pi^2}\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}\sum_{j=1}^{3}(\chi_j(x)-\chi_j(y))^2.$$

Here K_2 is a modified Bessel function, defined on $(0,\infty)$ by

$$K_2(t) = \frac{1}{2}\int_0^\infty x e^{-(1/2)t(x+x^{-1})}\,dx.$$

For completeness, we derive this in Appendix A.

Using this we find, with $T(p)=\sqrt{p^2+\alpha^{-2}}-\alpha^{-1}$, $V(x)=\delta/|x|$ and ψ a Slater determinant as mentioned in the preceding section, that

$$\begin{aligned}\left\langle \psi, \sum_{i=1}^{N}\{T(p_i)-V(x_i)+\alpha\rho * \phi_a * |x_i|^{-1}\}\psi \right\rangle &= \sum_{i=1}^{N}(m_i, \{T(p)-V(x)+\alpha\rho * \phi_a * |x|^{-1}\}m_i) \\ &= \sum_{j=1}^{3}\sum_{i=1}^{N}(m_i, \chi_j\{T(p)-V(x)+\alpha\rho * \phi_a * |x|^{-1}\}\chi_j m_i) \\ &\quad - \sum_{i=1}^{N}(m_i, L^{(\alpha)}m_i),\end{aligned} \tag{4.3}$$

since $\Sigma_{j=1}^3 \chi_j(x)^2=1$ for all $x \in \mathbb{R}^3$ (and α sufficiently small).

V. THE LOCALIZATION ERROR

We now estimate the error introduced by the localization of the kinetic energy carried out in the last section. This error is given by a bounded operator $L^{(\alpha)}$,

$$L^{(\alpha)}(x,y) = \sum_{j=1}^{3} L_j^{(\alpha)}(x,y), \quad L_j^{(\alpha)}(x,y) = \frac{\alpha^{-2}}{4\pi^2} \frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2} (\chi_j(x) - \chi_j(y))^2.$$

As noted above, this expression is derived in Appendix A. We shall start by localizing this operator, thereby splitting it into 12 terms which we will then treat individually. These terms are going to fall into groups though, and the terms in each of these will be estimated together by different means. Two of the terms will be estimated in later sections, together with the energies near the nucleus and in the intermediary zone, related to, respectively, χ_1 and χ_2.

In this section, the scale of the inner cutoff will be called l, that is, $l=\alpha^r$, $8/9<\mathrm{r}<1$. Let χ_- be the characteristic function of the ball $B(0,2l)$ in $\mathbb{R}^3$ and χ_+ that for the complement of this ball. Then each $L_j^{(\alpha)}$, $j=1$, 2, 3, splits into four terms,

$$L_j^{(\alpha)}(x,y) = \chi_+(x)L_j^{(\alpha)}(x,y)\chi_+(y) + \chi_+(x)L_j^{(\alpha)}(x,y)\chi_-(y) + \chi_-(x)L_j^{(\alpha)}(x,y)\chi_+(y) + \chi_-(x)L_j^{(\alpha)}(x,y)\chi_-(y).$$

The following lemma will eventually take care of six of these 12 terms.

Lemma 5.1: *Let* $l=\alpha^r$, $8/9<r<1$ *and assume that, with* $\gamma \equiv 1-(b/a)>0$,

$$|x| > al \quad \text{and } |y| < bl \text{ on supp } \chi_+(x)L_j^{(\alpha)}(x,y)\chi_-(y).$$

Then, for $f \in L^2(\mathbb{R}^3)$,

$$|(f,\chi_+L_j^{(\alpha)}\chi_-f)| \leq \rho(\alpha)\|f\|_2^2,$$

where $\rho(\alpha)=o(e^{-2\epsilon\alpha^{r-1}})$ *as* $\alpha\to 0$ *for all* ϵ *such that* $0<\epsilon<\gamma$. *In particular,* $\rho(\alpha)=o(\alpha^n)$ *as* $\alpha \to 0$ *for all* $n \in \mathbb{N}$.

Remark 5.2: Note that the result with x and y interchanged also holds.

Proof: By assumption we have that

$$|x-y| > \gamma|x| \quad \text{on supp } \chi_+L_j^{(\alpha)}\chi_-.$$

Since both $|x|^{-2}$ and $K_2(\alpha^{-1}|x|)$ are decreasing in $|x|$ (the last is obvious from the definition of K_2), and since $(\chi_j(x)-\chi_j(y))^2 \leq 1$, we get that pointwise,

$$\chi_+(x)L_j^{(\alpha)}(x,y)\chi_-(y) \leq \chi_+(x)\frac{\alpha^{-2}}{4\pi^2}\frac{K_2(\alpha^{-1}\gamma|x|)}{(\gamma|x|)^2}\chi_-(y)$$

on supp $\chi_+L_j^{(\alpha)}\chi_-$. Therefore

$$|(f,\chi_+L_j^{(\alpha)}\chi_-f)| \leq \left(\int |f(y)|\chi_-(y)d^3y\right)\left(\frac{(\alpha\gamma)^{-2}}{4\pi^2}\int |f(x)|\chi_+(x)\frac{K_2(\alpha^{-1}\gamma|x|)}{|x|^2}d^3x\right). \tag{5.1}$$

We estimate both of these terms using the Cauchy–Schwartz inequality. For the first we get

$$\int |f(y)|\chi_-(y)d^3y \leq \|f\|_2\|\chi_-\|_2 = Cl^{3/2}\|f\|_2, \tag{5.2}$$

and for the second

$$\int |f(x)|\chi_+(x)\frac{K_2(\alpha^{-1}\gamma|x|)}{|x|^2}d^3x \leq \|f\|_2\left(\int \left(\chi_+(x)\frac{K_2(\alpha^{-1}\gamma|x|)}{|x|^2}\right)^2 d^3x\right)^{1/2}. \tag{5.3}$$

Using the estimate (A7) in Appendix A on K_2, we get the estimate

$$\int \left(\chi_+(x)\frac{K_2(\alpha^{-1}\gamma|x|)}{|x|^2}\right)^2 d^3x \leqslant 4\pi\int_{2l}^{\infty}\frac{16}{|x|^4}\frac{\pi e^{-2\alpha^{-1}\gamma|x|}}{2\alpha^{-1}\gamma|x|}(1+(2\alpha^{-1}\gamma|x|)^{-1}+(2\alpha^{-1}\gamma|x|)^{-2})^2|x|^2\mathrm{d}|x|$$

$$= 128\pi^2\alpha^{-1}\gamma\int_{4\gamma l\alpha^{-1}}^{\infty} t^{-3}e^{-t}\left(1+\frac{1}{t}+\frac{1}{t^2}\right)^2 \mathrm{d}t,$$

where the last equality follows by the change of variables $t=2\gamma\alpha^{-1}|x|$. Dominating e^{-t} in the integrand by $e^{-4\gamma l\alpha^{-1}}$ and working out the resulting integral, we arrive at [using (5.1)–(5.3); recall that $l=\alpha^r$]

$$|(f,\chi_+L_j^{(\alpha)}\chi_-f)| \leqslant C\|f\|_2^2\alpha^{(3r-5)/2}e^{-2\gamma\alpha^{r-1}}\{\cdots\}^{1/2},$$

where

$$\{\cdots\}^{1/2}=\left\{\tfrac{1}{4}(4\gamma)^{-4}\alpha^{4(1-r)}+\tfrac{2}{5}(4\gamma)^{-5}\alpha^{5(1-r)}+\tfrac{1}{2}(4\gamma)^{-6}\alpha^{6(1-r)}+\tfrac{2}{7}(4\gamma)^{-7}\alpha^{7(1-r)}+\tfrac{1}{8}(4\gamma)^{-8}\alpha^{8(1-r)}\right\}^{1/2}.$$

Now, since $8/9<r<1$, this term tends to zero as α tends to zero. Also

$$\alpha^{(3r-5)/2}e^{-2\gamma\alpha^{r-1}}=o(e^{-2\epsilon\alpha^{r-1}}),\quad \alpha\to 0,$$

for all ϵ satisfying $0<\epsilon<\gamma$. This proves the lemma. □

We now return to investigating the above-mentioned 12 terms. First, note that two of these terms are actually zero,

$$\chi_+(x)L_1^{(\alpha)}(x,y)\chi_+(y)\equiv 0,$$

$$\chi_-(x)L_3^{(\alpha)}(x,y)\chi_-(y)\equiv 0,$$

as is easily seen by looking at the supports of χ_+, χ_-, χ_1, and χ_3. Next, we note that the following three terms fulfill the conditions in Lemma 5.1 and therefore are $o(\alpha^n)$, $\alpha\to 0$, for all $n\in\mathbb{N}$:

$$\chi_+(x)L_1^{(\alpha)}(x,y)\chi_-(y)\neq 0 \quad \text{for} \quad |x|>2l \quad \text{and} \quad |y|<(1+\beta)l,$$

$$\chi_+(x)L_3^{(\alpha)}(x,y)\chi_-(y)\neq 0 \quad \text{for} \quad |x|>(1-\beta)\alpha^t \quad \text{and} \quad |y|<2l,$$

$$\chi_+(x)L_2^{(\alpha)}(x,y)\chi_-(y)\neq 0 \quad \text{for} \quad |x|>(1-\beta)\alpha^t \quad \text{and} \quad |y|<2l,$$

$$\text{and for } |x|\in[2l,(1-\beta)\alpha^t] \quad \text{and} \quad |y|<(1+\beta)l.$$

This is due to the fact that for α small enough, $\alpha^t>\alpha^r$, since $t<2/3<8/9<r$. The above is symmetric in x and y, which gives another three terms.

We are then left with four terms. For these we will use that, by the mean value theorem, $(\chi_j(x)-\chi_j(y))^2\leqslant\|\nabla\chi_j\|_\infty^2|x-y|^2$. Note that for the four remaining terms,

$$\chi_+L_2^{(\alpha)}\chi_+,\quad \chi_-L_1^{(\alpha)}\chi_-,\quad \chi_+L_3^{(\alpha)}\chi_+,\quad \chi_-L_2^{(\alpha)}\chi_-, \tag{5.4}$$

we only need to take the supremum of $|\nabla\chi_j(\xi)|$ over the ξ's between x and y in the support of the relevant term. In this way we get

$$|(f,\chi_\pm L_j^{(\alpha)}\chi_\pm f)| \leqslant \int\int |f(x)|\chi_\pm(x)|f(y)|\chi_\pm(y)L_j^{(\alpha)}(x,y)d^3x\,d^3y$$
$$\leqslant \frac{c_j^\pm(\alpha)\alpha^{-2}}{4\pi^2}\int |f(x)|\chi_\pm(x)((|f|\chi_\pm)*G_\alpha)(x)d^3x,$$

where $G_\alpha(x)=K_2(\alpha^{-1}|x|)$ and $c_j^\pm(\alpha)=\sup_{|x|\gtrless 2l}|\nabla\chi_j(x)|^2$. By first using the Cauchy–Schwartz inequality, then Young's inequality, we get

$$|(f,\chi_\pm L_j^{(\alpha)}\chi_\pm f)| \leqslant \frac{c_j^\pm(\alpha)\alpha^{-2}}{4\pi^2}\|f\chi_\pm\|_2\|(|f|\chi_\pm)*G_\alpha\|_2 \leqslant \frac{c_j^\pm(\alpha)}{4\pi^2\alpha^2}\|f\chi_\pm\|_2^2\|G_\alpha\|_1.$$

Since

$$\|G_\alpha\|_1 = \int K_2(\alpha^{-1}|x|)d^3x = 4\pi\int_0^\infty \alpha^2t^2K_2(t)\alpha\,\mathrm{d}t = 6\pi^2\alpha^3$$

[see (A6) in Appendix A for $\int_0^\infty t^2K_2(t)\mathrm{d}t$] we get the following inequality:

$$|(f,\chi_\pm L_j^{(\alpha)}\chi_\pm f)| \leqslant \frac{3c_j^\pm(\alpha)\alpha}{2}\|f\chi_\pm\|_2^2. \tag{5.5}$$

For two of the terms in (5.4), $\chi_+L_2^{(\alpha)}\chi_+$ and $\chi_+L_3^{(\alpha)}\chi_+$, this is sufficient, since [see (4.1); recall that $l=\alpha^r$]

$$c_j^+(\alpha) = \sup_{|x|>2l}|\nabla\chi_j|^2 = c_j^+\alpha^{-2t}, \quad j=2,3,$$

and since $t<2/3$ we get, using (5.5), that

$$\sum_{i=1}^N (m_i,\chi_+L_3^{(\alpha)}\chi_+m_i) \leqslant N\frac{3}{2}c_j^+\alpha^{1-2t} = o(\alpha^{-4/3}), \quad \alpha\to 0,$$

as $N=\lambda Z=\lambda\delta\alpha^{-1}$ (λ and δ fixed) and $\|m_i\|_2=1$. Similarly for $\chi_+L_2^{(\alpha)}\chi_+$.

For the other two terms in (5.4), note that

$$\|f\chi_-\|_2^2 = \int |f(x)|^2|\chi_-(x)|^2\,d^3x$$
$$= \int |f(x)|^2\chi_-(x)d^3x = (f,\chi_-f) = (f,\chi_-(\chi_1^2+\chi_2^2)f) = (\chi_1f,\chi_-\chi_1f) + (\chi_2f,\chi_-\chi_2f),$$

since $\chi_-^2=\chi_-$ and $\chi_1^2+\chi_2^2=1$ on supp χ_-. Using this and (5.5), we obtain (since $\chi_-\chi_1=\chi_1$):

$$\sum_{i=1}^N (m_i,\chi_-(L_1^{(\alpha)}+L_2^{(\alpha)})\chi_-m_i) \leqslant C\alpha^{1-2r}\left(\sum_{i=1}^N(\chi_1m_i,\chi_1m_i) + \sum_{i=1}^N(\chi_2m_i,\chi_-\chi_2m_i)\right), \tag{5.6}$$

where

$$C=\tfrac{3}{2}(c_1+c_2), \quad c_j\alpha^{-2r} = \sup_{|x|<2l}|\nabla\chi_j(x)|^2, \quad j=1,2.$$

The two terms in (5.6) will be estimated in the following two sections, the first one along with the energy at the nucleus, the second one with the energy in the intermediary zone.

VI. THE ENERGY NEAR THE NUCLEUS

In this section we estimate the energy at the nucleus, that is [see (4.3)], the term

$$\sum_{i=1}^{N} (m_i, \chi_1\{T(p) - V(x) + \alpha\rho * \phi_a * |x|^{-1}\}\chi_1 m_i). \tag{6.1}$$

Also, half of the remaining term (5.6) of the localization error, treated in the preceding section, will be estimated here. We start by noting that $\rho * \phi_a * |x|^{-1}$ is positive, so that we get a lower bound to (6.1) by dropping this term. The remaining expression will be treated by using the following result by Lieb and Yau (Ref. 17, Theorem 11) on the hyperrelativistic operator $|p|$.

Theorem 6.1: *Let* $C_0 > 0$ *and* $R > 0$ *and let*

$$H_{C_0R} = |p| - \frac{2}{\pi}|x|^{-1} - C_0/R$$

be defined on $L^2(\mathbb{R}^3)$ *as a quadratic form. Let* $0 \leqslant \gamma \leqslant q$ *be a density matrix [that is, any bounded operator on* $L^2(\mathbb{R}^3)$ *which satisfies the operator inequality* $0 \leqslant \gamma \leqslant q$ *and for which* $\mathrm{Tr}(\gamma) < \infty$*] and let* χ *be any function with support in* $B_R = \{x \,|\, |x| \leqslant R\}$. *Then*

$$\mathrm{Tr}(\overline{\chi}\gamma\chi H_{C_0R}) \geqslant -4.4827\ C_0^4 R^{-1} q\{(3/4\pi R^3) \int |\chi(x)|^2\, d^3x\}. \tag{6.2}$$

Note, that when $\chi \equiv 1$ *in* B_R, *then the factor in braces* { } *in* (6.2) *is 1*.

Here, $\mathrm{Tr}(\gamma h)$ is shorthand for $\Sigma_k (f_k, hf_k)\gamma_k$, where (f_k, γ_k) are the eigenfunctions and eigenvalues of γ. For more details, see Lieb.[13] In our situation, $q = 2$. For our purpose, let Π be the projection on $\mathrm{span}\{m_i \,|\, i = 1, \ldots, N\}$, then Π is a density matrix as above, and

$$\mathrm{Tr}(\chi_1 \Pi \chi_1 H_{C_0R}) = \sum_{i=1}^{N} (m_i, \chi_1 H_{C_0R} \chi_1 m_i).$$

Since $\mathrm{supp}\, \chi_1 \subseteq B(0, (1+\beta)\alpha^r)$ with $8/9 < r < 1$, set $R = (1+\beta)\alpha^r$ and $C_0 = 2(1+\beta)\alpha^{r-1}$. Then

$$T(p) - V(x) = \sqrt{p^2 + \alpha^{-2}} - \alpha^{-1} - \frac{\delta}{|x|} \geqslant |p| - \alpha^{-1} - \frac{2}{\pi}|x|^{-1} = H_{C_0R} + \alpha^{-1},$$

since $\sqrt{p^2 + \alpha^{-2}} - \alpha^{-1} \geqslant |p| - \alpha^{-1}$ and $\delta \leqslant 2/\pi$. Including the first term in (5.6) we now have, applying (6.2),

$$\begin{aligned} &\sum_{i=1}^{N} (m_i, \chi_1\{T(p) - V(x)\}\chi_1 m_i) - C\alpha^{1-2r} \sum_{i=1}^{N} (m_i, \chi_1\chi_1 m_i) \\ &\quad \geqslant \sum_{i=1}^{N} (m_i, \chi_1\{H_{C_0R} + \alpha^{-1} - C\alpha^{1-2r}\}\chi_1 m_i) \\ &\quad \geqslant \sum_{i=1}^{N} (m_i, \chi_1 H_{C_0R}\chi_1 m_i) = \mathrm{Tr}(\overline{\chi_1}\Pi\chi_1 H_{C_0R}) \geqslant -C\alpha^{3r-4}. \end{aligned} \tag{6.3}$$

The second inequality is valid for α small enough, since $r < 1$, so that $\alpha^{2(1-r)} \to 0$ for $\alpha \to 0$. Since $3r - 4 > -4/3$ (as $8/9 < r$), the right-hand side (RHS) of (6.3) is $o(\alpha^{-4/3})$, $\alpha \to 0$, which is the desired order. Note that the above procedure is what decides the scale α^r, $8/9 < r < 1$, on which one can localize near the nucleus.

VII. THE INTERMEDIARY ZONE

The energy in this area is given by the term [see (4.3)]

$$\sum_{i=1}^{N} (m_i, \chi_2\{T(p) - V(x) + \alpha\rho * \phi_a * |x_i|^{-1}\}\chi_2 m_i). \tag{7.1}$$

The zone defined by the χ_2 was introduced to separate the outer zone defined by χ_3 and the support of the coherent states to be introduced later. As in the preceding section we note that by dropping the term involving $\rho * \phi_a * |x|^{-1}$, we get a lower bound of the energy in (7.1). The remaining expression will be estimated by a generalization of the Lieb–Thirring inequality (see Lieb and Thirring[15]), proved by Daubechies in Ref. 4, p. 518. See also p. 516, Ref. 4, for the conditions on the function $T(p)$.

Proposition 7.1: *Let* $F(s) = \int_0^s \mathrm{d}t[T^{-1}(t)]^3$, *where* $T(p) = T(|p|) = \sqrt{|p|^2 + \alpha^{-2}} - \alpha^{-1}$ *as a function. Then*

$$\left\langle \psi, \sum_{i=1}^{N} \{T(p_i) - V(x_i)\}\psi \right\rangle \geqslant -q\tilde{C} \int F(|V(x)|) d^3x,$$

where $\tilde{C} \leqslant 0.163$.

Note that this in particular means that the negative part of the spectrum of the operator $T(p) - V(x)$ is discrete and that the sum of the negative eigenvalues of this operator is bounded from below by the quantity $-q\tilde{C}\int F(|V(x)|)d^3x$. To see this, let $\{e_j\}_{j=0}^{\infty}$ be these negative eigenvalues, $e_0 \leqslant e_1 \leqslant \cdots$, and $\{g_j\}_{j=0}^{\infty}$ corresponding orthonormal eigenfunctions, and let ψ be the Slater determinant of the first N of the g_j's. Then, by the above proposition,

$$-q\tilde{C} \int F(|V(x)|) d^3x \leqslant \left\langle \psi, \sum_{i=1}^{N} \{T(p_i) - V(x_i)\}\psi \right\rangle = \sum_{j=1}^{N} (g_j, \{T(p) - V(x)\}g_j) = \sum_{j=1}^{N} e_j. \tag{7.2}$$

Since the left-hand-side is independent of N, we get the statement by taking the limit $N \to \infty$. This will, as mentioned above, be used on the energy related to the cutoff χ_2, but also on the remaining half of the term $\chi_-(L_1^{(\alpha)} + L_2^{(\alpha)})\chi_-$ discussed in Sec. V, see (5.6). First, let us calculate F,

$$T(p) = T(|p|) = \sqrt{|p|^2 + \alpha^{-2}} - \alpha^{-1} \Rightarrow T^{-1}(t) = \sqrt{t^2 + 2\alpha^{-1}t}.$$

Then

$$F(s) = \int_0^s (t^2 + 2\alpha^{-1}t)^{3/2}\, \mathrm{d}t = \int_0^s \left(\frac{2t}{\alpha}\right)^{3/2} \left(1 + \frac{\alpha t}{2}\right)^{3/2} \mathrm{d}t.$$

Now, by a Taylor expansion of the second term in the integral, we get

$$(1 + (\alpha t)/2)^{3/2} \leqslant 1 + \frac{3\alpha}{4}t + \frac{3\alpha^2}{32}t^2. \tag{7.3}$$

That is, for $s \geqslant 0$,

$$F(s) \leqslant \left(\frac{2}{\alpha}\right)^{3/2} \left\{ \frac{2}{5}s^{5/2} + \frac{3\alpha}{14}s^{7/2} + \frac{\alpha^2}{48}s^{9/2} \right\}. \tag{7.4}$$

The two terms we wish to estimate in this section are, as mentioned above,

$$\sum_{i=1}^{N} (m_i, \chi_2\{T(p) - V(x)\}\chi_2 m_i) \quad \text{and } C\alpha^{1-2r} \sum_{i=1}^{N} (\chi_2 m_i, \chi_- \chi_2 m_i).$$

In order to do so, note that on $\operatorname{supp} \chi_-\chi_2$ we have [χ_- being the characteristic function of $B(0, 2\alpha^r)$]

$$V(x) = \frac{\delta}{|x|} \geqslant \frac{\delta}{2\alpha^r} \geqslant C\alpha^{1-2r}$$

for α small enough, since $r<1$, so that $\alpha^{1-r}\to 0$ as $\alpha\to 0$. Therefore, by the estimate (7.4) on $F(s)$, and still for α small enough, we have

$$\sum_{i=1}^{N}(m_i,\chi_2\{T(p)-V(x)\}\chi_2 m_i) - C\alpha^{1-2r}\sum_{i=1}^{N}(m_i,\chi_2\chi_-\chi_2 m_i) \geqslant \sum_{i=1}^{N}(m_i,\chi_2\{T(p)-2\hat{V}(x)\}\chi_2 m_i) \tag{7.5}$$

with $\hat{V}(x)=\chi_2(x)V(x)$. Letting (e_j,g_j) be the negative eigenvalues and corresponding orthonormal eigenvectors for the operator $T(p)-2\hat{V}(x)$ as before, we then have

$$\begin{aligned}\sum_{i=1}^{N}(m_i,\chi_2\{T(p)-2\hat{V}(x)\}\chi_2 m_i) &\geqslant \sum_{i=1}^{N}\left(\chi_2 m_i,\left\{\sum_j e_j(g_j,\cdot)g_j\right\}\chi_2 m_i\right) = \sum_j\sum_{i=1}^{N} e_j|(\chi_2 m_i,g_j)|^2\\ &= \sum_j\sum_{i=1}^{N} e_j|(m_i,\chi_2 g_j)|^2 \geqslant \sum_j e_j\|\chi_2 g_j\|^2 \geqslant \sum_j e_j.\end{aligned} \tag{7.6}$$

Here we used Bessel's inequality (remember that the m_i's are orthonormal), that $e_j<0$ and that $0\leqslant\chi_2\leqslant 1$. Using (7.2) on $T(p)-2\hat{V}(x)$, in the limit $N\to\infty$, we now reach [using (7.4)–(7.6)]

$$\begin{aligned}&\sum_{i=1}^{N}(m_i,\chi_2\{T(p)-V(x)\}\chi_2 m_i) - C\alpha^{1-2r}\sum_{i=1}^{N}(m_i,\chi_2\chi_-\chi_2 m_i) \geqslant -2\tilde{C}\int_{\operatorname{supp}\chi_2} F(2|V(x)|)d^3x\\ &\geqslant -C\int_{\operatorname{supp}\chi_2}\left(\frac{2}{\alpha}\right)^{3/2}\left\{\frac{2}{5}(2|V(x)|)^{5/2}+\frac{3\alpha}{14}(2|V(x)|)^{7/2}+\frac{\alpha^2}{48}(2|V(x)|)^{9/2}\right\}d^3x\\ &= -C4\pi\int_{\alpha^r}^{\alpha^t}\left(\frac{2}{\alpha}\right)^{3/2}\left\{\frac{2}{5}\left(\frac{2\delta}{|x|}\right)^{5/2}+\frac{3\alpha}{14}\left(\frac{2\delta}{|x|}\right)^{7/2}+\frac{\alpha^2}{48}\left(\frac{2\delta}{|x|}\right)^{9/2}\right\}|x|^2\mathrm{d}|x|\\ &= -C\left[\frac{4}{5}(\alpha^{(t-3)/2}-\alpha^{(r-3)/2})+\frac{6\delta}{7}(\alpha^{[-(r+1)]/2}-\alpha^{[-(t+1)]/2})+\frac{4\delta^2}{72}(\alpha^{(1-3r)/2}-\alpha^{(1-3t)/2})\right].\end{aligned}$$

Since $8/9<r<1$ and $1/3<t<2/3$, all of these terms are $o(\alpha^{-4/3})$, which is the desired order. We note that it is this analysis that decides the scale α^t of the outer cutoff χ_3.

VIII. THE OUTER ZONE AND THOMAS–FERMI TEORY

Up to order $o(\alpha^{-4/3})$ we are now left with

$$\sum_{i=1}^{N}(m_i,\chi_3\{T(p)-V(x)+\alpha\rho*\phi_a*|x|^{-1}\}\chi_3 m_i) - \frac{\alpha}{2}\int\int\frac{\rho(x)\rho(y)}{|x-y|}d^3x\,d^3y - \alpha\, c(\phi)Na^{-1}.$$

This expression will now be related to the semiclassical Thomas–Fermi energy. This is done by introducing coherent states, following Lieb and Yau in Ref. 16, proof of Lemma B.3. Let g be the function chosen in Sec. III, that is, $g\in C_0^\infty(\mathbb{R}^3)$, spherically symmetric, non-negative, supported in the unit ball $B(0,1)$ of $\mathbb{R}^3$ and such that $\int g(x)^2d^3x=1$. Let $g_\alpha(x)=\alpha^{-3s/2}g(x/\alpha^s)$, $1/3<t<s<2/3$, that is, $\phi_a(x)=g_\alpha(x)^2$ with $a=\alpha^s$. In this way, since $N=\lambda Z=\lambda\delta\alpha^{-1}$,

$$\alpha\, c(\phi)Na^{-1} = \lambda\delta\, c(\phi)\alpha^{-s} = o(\alpha^{-2/3}),$$

which is also $o(\alpha^{-4/3})$, $\alpha\to 0$. Define now the coherent states $g_\alpha^{p,q}, p, q\in\mathbb{R}^3$ by

$$g_\alpha^{p,q}(x) = g_\alpha(x-q)e^{ipx}.$$

With $\tilde{T}(p)$ the function $\sqrt{p^2+\alpha^{-2}}-\alpha^{-1}$, we then have the formulas

$$(f,f) = \frac{1}{(2\pi)^3}\int\int d^3p\, d^3q (f,g_\alpha^{p,q})(g_\alpha^{p,q},f),$$

$$(f,(V*g_\alpha^2)f) = \frac{1}{(2\pi)^3}\int\int d^3p\, d^3q V(q)(f,g_\alpha^{p,q})(g_\alpha^{p,q},f),$$

$$(f,T(p)f) \geqslant \frac{1}{(2\pi)^3}\int\int d^3p\, d^3q \tilde{T}(p)(f,g_\alpha^{p,q})(g_\alpha^{p,q},f) - o(\alpha^{-1/3}). \tag{8.1}$$

The proof of these formulas is carried out in Appendix B. In this way, letting $\tilde{V}(x)=\delta/|x| - \alpha\rho * |x|^{-1}$ (remember that $\phi_{\alpha^s}=g_\alpha^2$),

$$\begin{aligned}
&\sum_{i=1}^N (m_i,\chi_3\{T(p)-V(x)+\alpha\rho*\phi_a*|x|^{-1}\}\chi_3 m_i)\\
&\quad=\sum_{i=1}^N\left(m_i,\chi_3\left\{T(p)-\tilde{V}(x)*\phi_{\alpha^s}+\frac{\delta}{|x|}*\phi_{\alpha^s}-\frac{\delta}{|x|}\right\}\chi_3 m_i\right)\\
&\quad=\sum_{i=1}^N (m_i,\chi_3\{T(p)-\tilde{V}(x)*\phi_{\alpha^s}\}\chi_3 m_i)\\
&\quad=\frac{1}{(2\pi)^3}\int\int d^3p\, d^3q(\tilde{T}(p)-\tilde{V}(q))\left(\sum_{i=1}^N |(m_i\chi_3,g_\alpha^{p,q})|^2\right) - No(\alpha^{-1/3}).
\end{aligned}$$

The second equality follows from Newton's theorem (since ϕ_{α^s} is spherically symmetric), $|x|^{-1} - |x|^{-1}*\phi_{\alpha^s}\equiv 0$ outside supp ϕ_{α^s}, and since supp $\chi_3\cap$ supp $\phi_{\alpha^s}=\varnothing$ for α sufficiently small (as $s>t$),

$$\sum_{i=1}^N\left(m_i,\chi_3\left\{\frac{\delta}{|x_i|}*\phi_{\alpha^s}-\frac{\delta}{|x_i|}\right\}\chi_3 m_i\right)=0.$$

This is one of the reasons for introducing the intermediary zone by the function χ_2. Note also that $No(\alpha^{-1/3})=o(\alpha^{-4/3})$. Now, for α small enough, $\alpha^{s-t}<1/4$, since $s>t$, so that if $|q|<\frac{1}{4}\alpha^t$, then

$$|x-q|<\alpha^s \Rightarrow |x|<\tfrac{1}{2}\alpha^t,$$

and so $(m_i\chi_3,g_\alpha^{p,q})=0$, since supp $g_\alpha\subset B(0,\alpha^s)$ and supp $\chi_3\subset\mathbb{R}^3\setminus B(0,\frac{1}{2}\alpha^t)$. That is, for α small enough

$$\text{supp}_q|(m_i\chi_3,g_\alpha^{p,q})|^2\subseteq\mathbb{R}^3\setminus B\left(0,\tfrac{1}{4}\alpha^t\right),$$

so that for any $\mu\geqslant 0$ we have, with $M(p,q)=\Sigma_{i=1}^N|(m_i\chi_3,g_\alpha^{p,q})|^2$ and $[f]_\pm=\max\{\pm f,0\}$,

$$\frac{1}{(2\pi)^3}\int\int d^3p\, d^3q(\tilde{T}(p)-\tilde{V}(q))\left(\sum_{i=1}^{N}|(m_i\chi_3,g_\alpha^{p,q})|^2\right)$$

$$=\frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t} d^3p\, d^3q(\tilde{T}(p)-(\tilde{V}(q)-\alpha\mu))M(p,q)-\alpha\mu\sum_{i=1}^{N}(\chi_3 m_i,\chi_3 m_i)$$

$$\geqslant -\frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t} d^3p\, d^3q[\tilde{T}(p)-(\tilde{V}(q)-\alpha\mu)]_- -\alpha\mu N,$$

since $0\leqslant M(p,q)\leqslant 1$ and $(\chi_3 m_i,\chi_3 m_i)\leqslant\|m_i\|_2^2=1$. The first is seen by Bessel's inequality, since the m_i's are orthonormal and $\|\chi_3 g_\alpha^{p,q}\|_2\leqslant\|g_\alpha^{p,q}\|_2=1$. In this way we have shown that for $\mu\leqslant 0$, $\rho:\mathbb{R}^3\to\mathbb{R}$ and $\psi\in\mathcal{H}_F=\wedge^N L^2(\mathbb{R}^3,\mathbb{C}^2)$,

$$\langle\psi,H\psi\rangle\geqslant -\frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t} d^3p\, d^3q[\tilde{T}(p)-(\tilde{V}(q)-\alpha\mu)]_- -\frac{\alpha}{2}\int\int\frac{\rho(x)\rho(y)}{|x-y|}d^3x\, d^3y-\alpha\mu N$$
$$-o(\alpha^{-4/3}). \tag{8.2}$$

Choose now ρ to be the Thomas–Fermi density $\rho_{\mathrm{TF}}^{N,Z}$, that is, the function that minimizes the Thomas–Fermi functional [here, $\gamma=(3\pi^2)^{2/3}$],

$$\mathcal{E}_{\mathrm{TF}}(\rho)=\frac{3}{5}\gamma\int\rho(x)^{5/3}\,d^3x-\int\rho(x)\frac{Z}{|x|}d^3x+\frac{1}{2}\int\int\frac{\rho(x)\rho(y)}{|x-y|}d^3x\, d^3y \tag{8.3}$$

over the set

$$\left\{\rho\in L^{5/3}(\mathbb{R}^3)\cap L^1(\mathbb{R}^3)\,|\,\rho\geqslant 0,\int\rho(x)d^3x\leqslant N\right\}.$$

(For the Thomas–Fermi theory, see Lieb and Simon[14] and Lieb.[11]) Then $\rho_{\mathrm{TF}}^{N,Z}$ satisfies the Thomas–Fermi equation,

$$\gamma\rho(x)^{2/3}=\left[\frac{Z}{|x|}-\rho*|x|^{-1}-\mu\right]_+ \tag{8.4}$$

for some unique $\mu=\mu(N)$. Furthermore,

$$\text{for } N\leqslant Z,\quad \int\rho_{\mathrm{TF}}^{N,Z}(x)d^3x=N\quad\text{and}\quad\mu(N)>0,$$

$$\text{for } N>Z,\quad \int\rho_{\mathrm{TF}}^{N,Z}(x)d^3x=Z\quad\text{and}\quad\mu(N)=0$$

[see Lieb and Simon (Ref. 14, Theorems II.17, 18, and 20)]. In this way, $\int\rho_{\mathrm{TF}}^{N,Z}(x)d^3x<N$ implies $N>Z$, and therefore $\mu(N)=0$, so that we always have

$$\mu(N)\int\rho_{\mathrm{TF}}^{N,Z}(x)d^3x=\mu(N)N. \tag{8.5}$$

Let $\mathcal{E}_{\mathrm{TF}}(N,Z)\equiv\mathcal{E}_{\mathrm{TF}}(\rho_{\mathrm{TF}}^{N,Z})$ and define the Thomas–Fermi potential by

$$V_{\mathrm{TF}}^{N,Z}(x)\equiv Z/|x|-\rho_{\mathrm{TF}}^{N,Z}*|x|^{-1}-\mu(N),$$

then we have the following scaling [Ref. 14, (2.24) p. 608] (remember, that $\lambda=N/Z$ is fixed):

$$\mathcal{E}_{\mathrm{TF}}(N,Z) = Z^{7/3}\mathcal{E}_{\mathrm{TF}}(\lambda,1) \equiv -C_{\mathrm{TF}}(\lambda)Z^{7/3}, \tag{8.6}$$

$$V_{\mathrm{TF}}^{N,Z}(x) = Z^{4/3}V_{\mathrm{TF}}^{\lambda,1}(Z^{1/3}x) \equiv Z^{4/3}V_{\mathrm{TF}}(Z^{1/3}x). \tag{8.7}$$

The idea is now to estimate the difference between the integral in (8.2) [with $\rho=\rho_{\mathrm{TF}}^{N,Z}$ and $\mu = \mu(N)$] and

$$-\frac{\alpha}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t} d^3p\, d^3q\left[\frac{p^2}{2} - \left(\frac{Z}{|q|} - \rho_{\mathrm{TF}}^{N,Z} * |q|^{-1} - \mu(N)\right)\right]_-.$$

This is done in two step, first, we change the domain of the integration, then we change the integrand, each time estimating the error.

First,

$$\begin{aligned}
&-\frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t} d^3p\, d^3q[\tilde{T}(p) - \alpha V_{\mathrm{TF}}^{N,Z}(q)]_- \\
&\quad= \frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t;\tilde{T}(p)<\alpha V_{\mathrm{TF}}^{N,Z}(q)} d^3p\, d^3q(\tilde{T}(p) - \alpha V_{\mathrm{TF}}^{N,Z}(q)) \\
&\quad= \frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t;\alpha(p^2/2)<\alpha V_{\mathrm{TF}}^{N,Z}(q)} d^3p\, d^3q(\tilde{T}(p) - \alpha V_{\mathrm{TF}}^{N,Z}(q)) \\
&\quad+ \frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t;\tilde{T}(p)<\alpha V_{\mathrm{TF}}^{N,Z}(q)<\alpha(p^2/2)} d^3p\, d^3q(\tilde{T}(p) - \alpha V_{\mathrm{TF}}^{N,Z}(q)).
\end{aligned}$$

Since $\tilde{T}(p) \geqslant 0$, we get

$$\begin{aligned}
&\int\int_{|q|>\frac{1}{4}\alpha^t;\tilde{T}(p)<\alpha V_{\mathrm{TF}}^{N,Z}(q)<\alpha(p^2/2)} d^3p\, d^3q(\alpha V_{\mathrm{TF}}^{N,Z}(q) - \tilde{T}(p)) \\
&\quad\leqslant \alpha\int\int_{|q|>\frac{1}{4}\alpha^t;\tilde{T}(p)<\alpha V_{\mathrm{TF}}^{N,Z}(q)<\alpha(p^2/2)} d^3p\, d^3q V_{\mathrm{TF}}^{N,Z}(q).
\end{aligned}$$

Using the scaling (8.7) and the change of variables $\omega = \delta^{1/3}\alpha^{-1/3}q$, the above is equal to

$$\delta^{1/3}\alpha^{2/3}\int\int_{|\omega|>\frac{1}{4}\delta^{1/3}\alpha^{t-1/3}\tilde{T}(p)<\delta^{4/3}\alpha^{-1/3}V_{\mathrm{TF}}(\omega)<\alpha(p^2/2)} d^3p\, d^3\omega\, V_{\mathrm{TF}}(\omega). \tag{8.8}$$

The limits in the integral means that

$$2\delta^{4/3}\alpha^{-4/3}V_{\mathrm{TF}}(\omega) \leqslant p^2 \leqslant 2\delta^{4/3}\alpha^{-4/3}V_{\mathrm{TF}}(\omega)\left(1 + \tfrac{1}{2}\delta^{4/3}\alpha^{2/3}V_{\mathrm{TF}}(\omega)\right)$$

so that with

$$X = 2\delta^{4/3}\alpha^{-4/3}V_{\mathrm{TF}}(\omega), \quad Y = \tfrac{1}{2}\delta^{4/3}\alpha^{2/3}V_{\mathrm{TF}}(\omega), \quad Z = |p|^2, \quad W = \tfrac{1}{4}\delta^{1/3}\alpha^{t-1/3},$$

we have

$$(8.8) = (4\pi)^2\delta^{1/3}\alpha^{2/3}\int_W^\infty \mathrm{d}|\omega||\omega|^2 V_{\mathrm{TF}}(\omega)\left(\int_X^{X(1+Y)}\frac{\sqrt{Z}}{2}\mathrm{d}Z\right)$$
$$= (4\pi)^2\delta^{1/3}\alpha^{2/3}\int_W^\infty \mathrm{d}|\omega||\omega|^2 V_{\mathrm{TF}}(\omega)\frac{X^{3/2}}{3}((1+Y)^{3/2}-1).$$

By the Taylor expansion (7.3), we have $(1+Y)^{3/2}\leqslant 1+\frac{3}{2}Y+\frac{3}{8}Y^2$, and so

$$(8.8) \leqslant C\delta^{7/3}\alpha^{-4/3}\int_W^\infty |\omega|^2 V_{\mathrm{TF}}(\omega)^{5/2}\left(\frac{3}{4}\delta^{4/3}\alpha^{2/3}V_{\mathrm{TF}}(\omega)+\frac{3}{32}\delta^{8/3}\alpha^{4/3}V_{\mathrm{TF}}(\omega)^2\right)\mathrm{d}|\omega|.$$

Using that $V_{\mathrm{TF}}^{N,Z}(x)\leqslant Z/|x|$, since $\mu(N)\geqslant 0$ and $\rho_{\mathrm{TF}}^{N,Z}\geqslant 0$ (remember that $V_{\mathrm{TF}}\equiv V_{\mathrm{TF}}^{\lambda,1}$), we arrive at

$$(8.8) \leqslant C\delta^{11/3}\alpha^{-2/3}\int_W^\infty \mathrm{d}|\omega||\omega|^{-3/2}+\sqrt{2}\pi^2\delta^5\int_W^\infty \mathrm{d}|\omega||\omega|^{-5/2}$$
$$\sim \alpha^{-2/3}W^{-1/2}+W^{-3/2}\sim \alpha^{-2/3}\alpha^{1/6-t/2}+\alpha^{(1-3t)/2}=o(\alpha^{-5/6})+o(\alpha^{-1/2}),$$

since $t<2/3$. This means, that

$$-\frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t} d^3p\,d^3q[\tilde{T}(p)-\alpha V_{\mathrm{TF}}^{N,Z}(q)]_-$$
$$\geqslant \frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t;\alpha(p^2/2)<\alpha V_{\mathrm{TF}}^{N,Z}(q)} d^3p\,d^3q(\tilde{T}(p)-\alpha V_{\mathrm{TF}}^{N,Z}(q))-o(\alpha^{-4/3}).$$

Next note that since $|q|>\frac{1}{4}\alpha^t$ and $\alpha V_{\mathrm{TF}}^{N,Z}(q)\leqslant \delta/|q|$ in the area of integration, we have that

$$\tilde{T}(p)=\sqrt{p^2+\alpha^{-2}}-\alpha^{-1}\geqslant \alpha\frac{p^2}{2}-\alpha^3\frac{p^4}{8}.$$

In this way, we get

$$\frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t;\alpha(p^2/2)<\alpha V_{\mathrm{TF}}^{N,Z}(q)} d^3p\,d^3q(\tilde{T}(p)-\alpha V_{\mathrm{TF}}^{N,Z}(q))$$
$$\geqslant \frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t;\alpha(p^2/2)<\alpha V_{\mathrm{TF}}^{N,Z}(q)} d^3p\,d^3q\left(\alpha\frac{p^2}{2}-\alpha^3\frac{p^4}{8}-\alpha V_{\mathrm{TF}}^{N,Z}(q)\right)$$
$$=\frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t;\alpha(p^2/2)<\alpha V_{\mathrm{TF}}^{N,Z}(q)} d^3p\,d^3q\left(a\frac{p^2}{2}-\alpha V_{\mathrm{TF}}^{N,Z}(q)\right)$$
$$-\alpha^3\frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t;\alpha(p^2/2)<\alpha V_{\mathrm{TF}}^{N,Z}(q)}\frac{p^4}{8}d^3p\,d^3q. \tag{8.9}$$

Note that

$$\frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t;\alpha(p^2/2)<\alpha V_{\mathrm{TF}}^{N,Z}(q)} d^3p\,d^3q\left(\alpha\frac{p^2}{2}-\alpha V_{\mathrm{TF}}^{N,Z}(q)\right)$$
$$=-\frac{\alpha}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t} d^3p\,d^3q\left[\frac{p^2}{2}-\left(\frac{Z}{|q|}-\rho_{\mathrm{TF}}^{N,Z}*|q|^{-1}-\mu(N)\right)\right]_-$$
$$\geqslant-\frac{\alpha}{(2\pi)^3}\int\int d^3p\,d^3q\left[\frac{p^2}{2}-\left(\frac{Z}{|q|}-\rho_{\mathrm{TF}}^{N,Z}*|q|^{-1}-\mu(N)\right)\right]_-.$$

Let us now look at the last term in (8.9). Again using that $V_{\mathrm{TF}}^{N,Z}(x)\leqslant Z/|x|$, we have that

$$\int\int_{|q|>\frac{1}{4}\alpha^t;\alpha(p^2/2)<\alpha V_{\mathrm{TF}}^{N,Z}(q)}\frac{p^4}{8}d^3p\,d^3q$$
$$\leqslant\int\int_{|q|>\frac{1}{4}\alpha^t;\alpha(p^2/2)<\delta/|q|}\frac{p^4}{8}d^3p\,d^3q$$
$$=(4\pi)^2\int_{\frac{1}{4}\alpha^t}^{\infty}\mathrm{d}|q|\left(|q|^2\int_0^{\sqrt{2Z/|q|}}\frac{|p|^4}{8}|p|^2\mathrm{d}|p|\right)$$
$$=2\pi^2\int_{\frac{1}{4}\alpha^t}^{\infty}\mathrm{d}|q|\left(|q|^2[t^7/7]_0^{\sqrt{2Z/|q|}}\right)=\frac{2\pi^2(2Z)^{7/2}}{7}\int_{\frac{1}{4}\alpha^t}^{\infty}|q|^{-3/2}\mathrm{d}|q|=\frac{8\pi^2(2Z)^{7/2}}{7}\alpha^{-t/2}.$$

Using this, we then get the following:

$$\frac{1}{(2\pi)^3}\int\int_{|q|>\frac{1}{4}\alpha^t;\alpha(p^2/2)<\alpha V_{\mathrm{TF}}^{N,Z}(q)} d^3p\,d^3q(\tilde{T}(p)-\alpha V_{\mathrm{TF}}^{N,Z}(q))$$
$$\geqslant-\frac{\alpha}{(2\pi)^3}\int\int d^3p\,d^3q\left[\frac{p^2}{2}-\left(\frac{Z}{|q|}-\rho_{\mathrm{TF}}^{N,Z}*|q|^{-1}-\mu(N)\right)\right]_--\alpha^{(6-t)/2}\frac{(2Z)^{7/2}}{7\pi}.$$

Hence, since $\delta=Z\alpha$ is fixed and $t<2/3$, we have

$$\alpha^{(6-t)/2}\frac{(2Z)^{7/2}}{7\pi}=\frac{8\sqrt{2}}{7\pi}\alpha^{-(1+t)/2}\delta^{7/2}=o(\alpha^{-4/3}),\quad \alpha\to 0.$$

Summing up, we have now proved that for $\psi\in\mathcal{H}_F=\wedge^N L^2(\mathbb{R}^3,\mathbb{C}^2)$,

$$\langle\psi,H\psi\rangle\geqslant-\frac{\alpha}{(2\pi)^3}\int\int d^3p\,d^3q\left[\frac{p^3}{2}-\left(\frac{Z}{|q|}-\rho_{\mathrm{TF}}^{N,Z}*|q|^{-1}-\mu(N)\right)\right]_-$$
$$-\frac{\alpha}{2}\int\int\frac{\rho_{\mathrm{TF}}^{N,Z}(x)\rho_{\mathrm{TF}}^{N,Z}(y)}{|x-y|}d^3x\,d^3y-\alpha\mu(N)N-o(\alpha^{-4/3}).\tag{8.10}$$

Integrating first in p in the first integral in (8.10), we get, for each q fixed,

$$\int d^3p\left[\frac{p^2}{2}-\left(\frac{Z}{|q|}-\rho_{\mathrm{TF}}^{N,Z}*|q|^{-1}-\mu(N)\right)\right]_-$$
$$=\int_{(p^2/2)<V_{\mathrm{TF}}^{N,Z}}\left(\frac{p^2}{2}-\left(\frac{Z}{|q|}-\rho_{\mathrm{TF}}^{N,Z}*|q|^{-1}-\mu(N)\right)\right)d^3p$$
$$=-\frac{16\sqrt{2}\pi}{15}\left[V_{\mathrm{TF}}^{N,Z}(q)\right]_+^{5/2}.\tag{8.11}$$

The $[\cdots]_+$, since, if the term in brackets is negative, the integrand in (8.11) will be zero.

Now, because $\rho_{\mathrm{TF}}^{N,Z}$ satifies the equation (8.4), we get, that

$$\left[\frac{Z}{|q|}-\rho_{\mathrm{TF}}^{N,Z}*|q|^{-1}-\mu(N)\right]_+^{5/2}=\gamma^{5/2}\rho_{\mathrm{TF}}^{N,Z}(q)^{5/3}=\gamma^{3/2}\rho_{\mathrm{TF}}^{N,Z}(q)\left[\frac{Z}{|q|}-\rho_{\mathrm{TF}}^{N,Z}*|q|^{-1}-\mu(N)\right].$$

In the last equation, no $[\cdots]_+$ is needed, since, if the last term is negative, $\rho_{\mathrm{TF}}^{N,Z}$ is zero, because of (8.4). In this way, by the above and by (8.5),

$$\begin{aligned}
&-\frac{\alpha}{(2\pi)^3}\int\int d^3p\,d^3q\left[\frac{p^2}{2}-\left(\frac{Z}{|q|}-\rho_{\mathrm{TF}}^{N,Z}*|q|^{-1}-\mu(N)\right)\right]_- -\frac{\alpha}{2}\int\int\frac{\rho_{\mathrm{TF}}^{N,Z}(x)\rho_{\mathrm{TF}}^{N,Z}(y)}{|x-y|}d^3x\,d^3y\\
&\quad-\alpha\mu(N)N=\alpha\frac{3}{5}\gamma\int\rho_{\mathrm{TF}}^{N,Z}(q)^{5/3}\,d^3q-\alpha\int\rho_{\mathrm{TF}}^{N,Z}(q)\frac{Z}{|q|}d^3q+\alpha\int\rho_{\mathrm{TF}}^{N}(q)\rho_{\mathrm{TF}}^{N,Z}*|q|^{-1}\,d^3q\\
&\quad+\alpha\mu(N)\int\rho_{\mathrm{TF}}^{N,Z}(q)d^3q-\frac{\alpha}{2}\int\int\frac{\rho_{\mathrm{TF}}^{N,Z}(x)\rho_{\mathrm{TF}}^{N,Z}(y)}{|x-y|}d^3x\,d^3y-\alpha\mu(N)N\\
&=\alpha\left(\frac{3}{5}\gamma\int\rho_{\mathrm{TF}}^{N,Z}(x)^{5/3}\,d^3x-\int\rho_{\mathrm{TF}}^{N,Z}(x)\frac{Z}{|x|}d^3x+\frac{1}{2}\int\int\frac{\rho_{\mathrm{TF}}^{N,Z}(x)\rho_{\mathrm{TF}}^{N,Z}(y)}{|x-y|}d^3x\,d^3y\right)=\alpha\mathcal{E}_{\mathrm{TF}}(N,Z).
\end{aligned}$$

Since $H_{\mathrm{rel}}=\alpha^{-1}H$, and $Z=\delta\alpha^{-1}$, with δ fixed, $0\leqslant\delta\leqslant 2/\pi$, this shows, that for all $\psi\in\mathcal{H}_F=\wedge^N L^2(\mathbb{R}^3,\mathbb{C}^2)$,

$$\langle\psi,H_{\mathrm{rel}}\psi\rangle\geqslant -C_{\mathrm{TF}}Z^{7/3}-o(Z^{7/3}),\quad Z\to\infty,$$

because of the scaling (8.6). This ends the proof of Theorem 1.1. □

APPENDIX A: A FORMULA FOR THE KINETIC ENERGY

In this appendix we shall prove the localization-formula (4.2) for the operator $\sqrt{p^2+\alpha^{-2}}$ [which is the equivalent of the IMS Localization Formula for the Laplace operator $-\Delta$, see Cycon *et al.* (Ref. 3, Theorem 3.2)]. Let first K_2 be a modified Bessel function of second order, defined on $(0,\infty)$ by

$$K_2(t)=\frac{1}{2}\int_0^\infty xe^{-\frac{1}{2}t(x+x^{-1})}\,\mathrm{d}x.$$

It is easily seen that K_2 is well-defined, decreasing and differentiable. Other properties of K_2 will be derived later. Let then χ_j, $j=1,\ldots,k$ be smooth positive functions on $\mathbb{R}^3$, such that $\Sigma_j\chi_j^2(x)=1$ for all x in $\mathbb{R}^3$ and define on $L^2(\mathbb{R}^3)$ the bounded operator $L^{(\alpha)}$ by the kernel

$$L^{(\alpha)}(x,y)=\frac{\alpha^{-2}}{(2\pi)^2}\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}\sum_{j=1}^k(\chi_j(x)-\chi_j(y))^2.$$

Then for $f\in\mathcal{S}(\mathbb{R}^3)$ one has the formula

$$(f,\sqrt{p^2+\alpha^{-2}}f)=\sum_{j=1}^k(f,\chi_j\sqrt{p^2+\alpha^{-2}}\chi_j f)-(f,L^{(\alpha)}f).\tag{A1}$$

The proof of the localization formula (A1) will be a consequence of the following formula.

Lemma A.1: For $f\in\mathcal{S}(\mathbb{R}^3)$,

$$(f,(\sqrt{p^2+\alpha^{-2}}-\alpha^{-1})f)=\frac{\alpha^{-2}}{(2\pi)^2}\int\int|f(x)-f(y)|^2\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}d^3x\,d^3y.\tag{A2}$$

Proof: Let $\hat{f}$ be the Fourier transform of f. Note that by dominated convergence in momentum space, we have

$$(f,\sqrt{p^2+\alpha^{-2}}f)=\lim_{t\searrow 0}\frac{1}{t}\{(f,f)-(f,e^{-t\sqrt{p^2+\alpha^{-2}}}f)\}.$$

To calculate the integral kernel $\exp[-t\sqrt{p^2+\alpha^{-2}}](x,y)$, expand the Fourier transforms:

$$(f,e^{-t\sqrt{p^2+\alpha^{-2}}}f)=\int|\hat{f}(p)|^2e^{-t\sqrt{p^2+\alpha^{-2}}}d^3p=\frac{1}{(2\pi)^3}\int\int\overline{f(x)}f(y)\left(\int e^{-t\sqrt{p^2+\alpha^{-2}}}e^{i(x-y)\cdot p}\,d^3p\right)d^3x\,d^3y.$$

This is justified by the fact that $f\in\mathcal{S}(\mathbb{R}^3)$. Now, for x,y fixed, choose polar coordinates $(|p|,\theta,\phi)$, for p such that $(x-y)\cdot p=-|p||x-y|\cos\theta$. Then

$$\int e^{-t\sqrt{p^2+\alpha^{-2}}}e^{i(x-y)\cdot p}\,d^3p=\int_0^\infty\int_0^{2\pi}\int_0^{\pi}e^{-t\sqrt{p^2+\alpha^{-2}}}e^{-i|p||x-y|\cos\theta}\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi|p|^2\mathrm{d}|p|$$

$$=2\pi\int_0^\infty|p|^2e^{-t\sqrt{p^2+\alpha^{-2}}}\left(\int_{-1}^{1}e^{i|p||x-y|u}\,\mathrm{d}u\right)\mathrm{d}|p|,\ u=-\cos\theta$$

$$=\frac{4\pi}{|x-y|}\int_0^\infty|p|e^{-t\sqrt{p^2+\alpha^{-2}}}\sin(|p||x-y|)\mathrm{d}|p|$$

$$=\frac{4\pi}{|x-y|}t\alpha^{-2}|x-y|(|x-y|^2+t^2)^{-1}K_2[\alpha^{-1}(|x-y|^2+t^2)^{1/2}],$$

where the last equality is given in Erdelyi *et al.* [Ref. 5, p. 75, 2.4 (35)]. In this way,

$$(f,e^{-t\sqrt{p^2+\alpha^{-2}}}f)=\frac{t\alpha^{-2}}{2\pi 2}\int\int\overline{f(x)}f(y)\frac{K_2[\alpha^{-1}(|x-y|^2+t^2)^{1/2}]}{|x-y|^2+t^2}d^3x\,d^3y. \tag{A3}$$

Now, letting $F_t(p)=e^{-t\sqrt{p^2+\alpha^{-2}}}$, the above shows that

$$\check{F}_t(x)=\frac{1}{(2\pi)^{3/2}}\int F_t(p)e^{ix\cdot p}\,d^3p=\sqrt{\frac{2}{\pi}}t\alpha^{-2}\frac{K_2[\alpha^{-1}(|x|^2+t^2)^{1/2}]}{|x|^2+t^2},$$

and therefore, for all $y\in\mathbb{R}^3$:

$$\frac{t\alpha^{-2}}{2\pi 2}\int\frac{K_2[\alpha^{-1}(|x-y|^2+t^2)^{1/2}]}{|x-y|^2+t^2}d^3x=F_t(0)=e^{-t\alpha^{-1}}. \tag{A4}$$

Hence we get, using (A3) and (A4), which are both symmetric in x and y, that

$$\begin{aligned}\frac{1}{t}\{(f,f)-(f,e^{-t\sqrt{p^2+\alpha^{-2}}}f)\}&=\frac{1}{t}\{(f,f)-(f,e^{-t\alpha^{-1}}f)\}+\frac{1}{t}\{(f,e^{-t\alpha^{-1}}f)-(f,e^{-t\sqrt{p^2+\alpha^{-2}}}f)\}\\&=-\frac{e^{-t\alpha^{-1}}-e^{-0\cdot\alpha^{-1}}}{t-0}(f,f)+\frac{1}{t}\left\{\int\frac{1}{2}((|f(x)|^2+|f(y)|^2)-\overline{f(x)}f(y)-\overline{f(y)}f(x))\right.\\&\quad\left.\times\frac{t\alpha^{-2}}{2\pi^2}\frac{K_2[\alpha^{-1}(|x-y|^2+t^2)^{1/2}]}{|x-y|^2+t^2}d^3x\,d^3y\right\}.\end{aligned}$$

Cancelling t and noting that

$$\lim_{t\searrow 0}\frac{e^{-t\alpha^{-1}}-e^{-0\cdot\alpha^{-1}}}{t-0}=\left.\frac{d}{dt}(e^{-t\alpha^{-1}})\right|_{t=0}=-\alpha^{-1},$$

we get that

$$\lim_{t\searrow 0}\frac{1}{t}\{(f,f)-(f,e^{-t\sqrt{p^2+\alpha^{-2}}}f)\}=\alpha^{-1}+\frac{\alpha^{-2}}{(2\pi)^2}\int\int|f(x)-f(y)|^2\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}d^3x\,d^3y.$$

This proves the lemma. □

Now, to prove the formula (A1), we simply use the fact that $\Sigma_j\chi_j^2(x)=1$ for all x in $\mathbb{R}^3$:

$$\sum_{j=1}^{k}|\chi_j(x)f(x)-\chi_j(y)f(y)|^2=|f(x)|^2+|f(y)|^2-\sum_{j=1}^{k}\chi_j(x)\chi_j(y)(\overline{f(y)}f(x)+\overline{f(x)}f(y))$$

$$=|f(x)-f(y)|^2+\sum_{j=1}^{k}\chi_j(x)(\overline{f(y)}f(x)+\overline{f(x)}f(y))(\chi_j(x)-\chi_j(y)).$$

Note that $\chi_j f\in\mathcal{S}(\mathbb{R}^3)$, since χ_j is smooth and bounded, so that using the formula (A2),

$$\sum_{j=1}^{k}(f,\chi_j(\sqrt{p^2+\alpha^{-2}}-\alpha^{-1})\chi_j f)=\sum_{j=1}^{k}(\chi_j f,(\sqrt{p^2+\alpha^{-2}}-\alpha^{-1})\chi_j f)$$

$$=\frac{\alpha^{-2}}{(2\pi)^2}\int\int\sum_{j=1}^{k}|\chi_j(x)f(x)-\chi_j(y)f(y)|^2\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}d^3x\,d^3y$$

$$=\frac{\alpha^{-2}}{(2\pi)^2}\int\int\left\{|f(x)-f(y)|^2+\sum_{j=1}^{k}\chi_j(x)(\overline{f(y)}f(x)\right.$$

$$\left.+\overline{f(x)}f(y))(\chi_j(x)-\chi_j(y))\right\}\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}d^3x\,d^3y. \tag{A5}$$

Using now that

$$\int\int\chi_j(x)\overline{f(y)}f(x)(\chi_j(x)-\chi_j(y))\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}d^3x\,d^3y$$

$$=-\int\int\chi_j(y)\overline{f(x)}f(y)(\chi_j(x)-\chi_j(y))\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}d^3x\,d^3y$$

simply by interchanging x and y, we finally get from (A5) that

$$\sum_{j=1}^{k}(f,\chi_j\sqrt{p^2+\alpha^{-2}}\chi_j f)=\frac{\alpha^{-2}}{(2\pi)^2}\int\int|f(x)-f(y)|^2\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}d^3x\,d^3y$$

$$+\frac{\alpha^{-2}}{(2\pi)^2}\int\int\overline{f(x)}f(y)\sum_{j=1}^{k}(\chi_j(x)-\chi_j(y))^2\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}d^3x\,d^3y$$

which, using (A2), proves the formula (A1). □

We now derive two facts about the function K_2,

$$\int_0^\infty t^2K_2(t)\mathrm{d}t=\frac{3\pi}{2}, \tag{A6}$$

$$K_2(t) \leqslant 4\sqrt{\frac{\pi}{2t}}e^{-t}\left(1+\frac{1}{2t}+\frac{1}{(2t)^2}\right) \quad \text{for all } t \in \mathbb{R}_+. \tag{A7}$$

The proof of (A6) is straightforward by using the definition of K_2,

$$\int_0^\infty t^2 K_2(t)\mathrm{d}t = \int_0^\infty t^2\left(\frac{1}{2}\int_0^\infty x e^{-\frac{1}{2}(x+x^{-1})}\,\mathrm{d}x\right)\mathrm{d}t = \frac{1}{2}\int_0^\infty x\left(\int_0^\infty t^2 e^{-\frac{1}{2}(x+x^{-1})}\,\mathrm{d}t\right)\mathrm{d}x$$

where the interchanging of the order of integration is allowed by Tonelli's theorem. By applying partial integration three times,

$$\int_0^\infty t^2 e^{-\frac{1}{2}(x+x^{-1})}\,\mathrm{d}t = \frac{16}{(x+x^{-1})},$$

and so

$$\int_0^\infty t^2 K_2(t)\mathrm{d}t = \frac{1}{2}\int_0^\infty \frac{16x}{(x+x^{-1})}\mathrm{d}x = 4\int_{-\infty}^\infty \frac{x^4}{(x^2+1)^3}\mathrm{d}x = 4\cdot 2\pi i\,\mathrm{Res}\left(\frac{z^4}{(z^2+1)^3}, i\right) = 8\pi i\frac{6}{32i} = \frac{3\pi}{2}.$$

For the estimate (A7), we need to rewrite K_2. This is done following Gray and Mathews (Ref. 18, pp. 50).

Observation A.2:

$$K_2(t) = \sqrt{\frac{\pi}{2t}}\frac{1}{\Gamma\left(\frac{5}{2}\right)}e^{-t}\int_0^\infty e^{-\xi}\xi^{3/2}\left(1+\frac{\xi}{2t}\right)^{3/2}\mathrm{d}\xi. \tag{A8}$$

To prove the observation, we start on the right-hand side of (A8). Setting $t+\xi=\sqrt{t^2+\eta}$, one gets, since then $\eta=\xi^2+2t\xi$, that

$$\mathrm{RHS(A8)} = \sqrt{\frac{\pi}{2t}}\frac{1}{\Gamma\left(\frac{5}{2}\right)}\int_0^\infty e^{-\sqrt{t^2+\eta}}\left(\frac{\eta}{2t}\right)^{3/2}\frac{\mathrm{d}\eta}{2\sqrt{t^2+\eta}}.$$

Using the formula

$$\int_0^\infty e^{-(a^2\xi^2+b^2/\xi^2)}\,\mathrm{d}\xi = \frac{\sqrt{\pi}}{2a}e^{-2ab}$$

[which holds since both sides satisfy the differential equation $\mathrm{d}f/\mathrm{d}b=-2af$, $f(b=0)=\sqrt{\pi}/2a$] with $a=\sqrt{t^2+\eta}$, $b=1/2$, we arrive at

$$\begin{aligned}\mathrm{RHS(A8)} &= \frac{1}{\Gamma\left(\frac{5}{2}\right)(2t)^2}\int_0^\infty \eta^{3/2}\left(\int_0^\infty e^{-((t^2+\eta)\xi^2+1/(2\xi)^2)}\,\mathrm{d}\xi\right)\mathrm{d}\eta \\ &= \frac{1}{\Gamma\left(\frac{5}{2}\right)(2t)^2}\int_0^\infty e^{-(t^2\xi^2+1/(2\xi)^2)}\left(\int_0^\infty e^{-\eta\xi^2}\eta^{3/2}\,\mathrm{d}\eta\right)\mathrm{d}\xi \\ &= \frac{1}{(2t)^2}\int_0^\infty e^{-(t^2\xi^2+1/(2\xi)^2)}\xi^{-5}\,\mathrm{d}\xi\end{aligned}$$

since one has the formula

$$\int_0^\infty e^{-\eta\xi^2}\eta^{3/2}\,\mathrm{d}\eta = \xi^{-5}\Gamma\left(\frac{5}{2}\right).$$

Making the change of variables $x=1/2t\xi^2$, we finally get

$$\mathrm{RHS(A8)} = \frac{1}{2}\int_0^\infty x e^{-(1/2)t(x+x^{-1})}\,\mathrm{d}x = K_2(t).$$

Now, to prove the estimate (A7), use the Tayloer expansion (7.3) on the integrand in (A8), to get

$$\begin{aligned}
K_2(t) &\leqslant \sqrt{\frac{\pi}{2t}}\frac{1}{\Gamma\left(\frac{5}{2}\right)}e^{-t}\int_0^\infty e^{-\xi}\xi^{3/2}\left(1+\frac{3}{4t}\xi+\frac{3}{32t^2}\xi^2\right)\mathrm{d}\xi \\
&= \sqrt{\frac{\pi}{2t}}\frac{1}{\Gamma\left(\frac{5}{2}\right)}e^{-t}\left(\int_0^\infty e^{-\xi}\xi^{3/2}\,\mathrm{d}\xi+\frac{3}{4t}\int_0^\infty e^{-\xi}\xi^{5/2}\,\mathrm{d}\xi+\frac{3}{32t^2}\int_0^\infty e^{-\xi}\xi^{7/2}\,\mathrm{d}\xi\right) \\
&= \sqrt{\frac{\pi}{2t}}\frac{1}{\Gamma\left(\frac{5}{2}\right)}e^{-t}\left(\Gamma\left(\tfrac{5}{2}\right)+\frac{3}{4t}\Gamma\left(\tfrac{7}{2}\right)+\frac{3}{32t^2}\Gamma\left(\tfrac{9}{2}\right)\right) \\
&= \sqrt{\frac{\pi}{2t}}e^{-t}\left(1+\frac{15}{8t}+\frac{105}{128t^2}\right) \leqslant 4\sqrt{\frac{\pi}{2t}}e^{-t}\left(1+\frac{1}{2t}+\frac{1}{(2t)^2}\right).
\end{aligned}$$

APPENDIX B: INTRODUCING COHERENT STATES

In this section we will introduce coherent states and prove the formulas in Sec. VIII. The error introduced by using coherent states will also be estimated here.

Lemma B.1: Let $g \in C_0^\infty(\mathbb{R}^3)$ be spherically symmetric, non-negative, supported in the unit ball and such that $\|g\|_2=1$, and let $g^{p,q}(x)=g(x-q)e^{ipx}$. Then

$$(f,f) = \frac{1}{(2\pi)^3}\int\int d^3p\, d^3q (f,g^{p,q})(g^{p,q},f),$$

$$(f,(V*|g|^2)f) = \frac{1}{(2\pi)^3}\int\int d^3p\, d^3q\, V(q)(f,g^{p,q})(g^{p,q},f),$$

$$(f,\sqrt{p^2+\alpha^{-2}}f) \geqslant \frac{1}{(2\pi)^3}\int\int d^3p\, d^3q \sqrt{p^2+\alpha^{-2}}(f,g^{p,q})(g^{p,q},f) - 3\alpha\|\nabla g\|_\infty^2 \mathrm{Vol}(\mathrm{supp}\, g)\|f\|_2^2. \tag{B1}$$

Proof: The idea of the above formulas is to write the identity and other operators on $L^2(\mathbb{R}^3)$ as superpositions of the one-rank operators $\pi_{pq}=(\ ,g^{p,q})g^{p,q}$. To prove the above formulas, start with the right-hand side of the second formula (the proof of the first formula is similar, just more simple):

$$\begin{aligned}
\frac{1}{(2\pi)^3}\int\int d^3p\, d^3q V(q)(f,g^{p,q})(g^{p,q},f) &= \frac{1}{(2\pi)^3}\int\int d^3p\, d^3q\, V(q)\left[\overline{\int f(y)\overline{g(y-q)}e^{-ipy}\,d^3y}\right] \\
&\quad\times\left[\int f(x)\overline{g(x-q)}e^{-ipx}\,d^3x\right].
\end{aligned} \tag{B2}$$

Notice, that the function in the last brackets is $(2\pi)^{3/2}$ times the Fourier transform of the function $F_q(x)=f(x)\overline{g(x-q)}$. In this way we get, by Parseval's formula,

$$\begin{aligned}(\mathrm{B2}) &= \int\int d^3p\, d^3q\, V(q)|\hat{F}_q(p)|^2 = \int d^3q\, V(q)\|\hat{F}_q\|_2^2 = \int d^3q\, V(q)\|F_q\|_2^2 \\ &= \int d^3q\, V(q)\left(\int |f(x)|^2|g(x-q)|^2\, d^3x\right) = \int d^3x|f(x)|^2\left(\int V(q)|g(x-q)|^2\, d^3q\right) \\ &= (f,(V*|g|^2)f).\end{aligned}$$

This proves the second (and the first) formula.

To prove the formula for the operator $\sqrt{p^2+\alpha^{-2}}$, note that

$$\int g(x-q)^2\, d^3q = 1 \text{ for all } x \text{ in } \mathbb{R}^3,$$

so that, by the symmetry of the operator $\sqrt{p^2+\alpha^{-2}}$,

$$\begin{aligned}(f,\sqrt{p^2+\alpha^{-2}}f) &= \frac{1}{2}\int\int \overline{f(x)}g(x-q)^2(\sqrt{p^2+\alpha^{-2}}f)(x)d^3q\, d^3x \\ &\quad + \frac{1}{2}\int\int \overline{(\sqrt{p^2+\alpha^{-2}}f)(x)}g(x-q)^2 f(x)d^3q\, d^3x \\ &= \frac{1}{2}\int\int \overline{f(x)}g_q(x)^2(\sqrt{p^2+\alpha^{-2}}f)(x)d^3q\, d^3x \\ &\quad + \frac{1}{2}\int\int \overline{f(x)}(\sqrt{p^2+\alpha^{-2}}(g_q^2 f))(x)d^3q\, d^3x. \qquad (\mathrm{B3})\end{aligned}$$

Here, $g_q(x)=g(x-q)$. Remembering that $g_q(x)^2$ is real and letting g_q^2 denote the multiplication operator defined by this function, we have

$$\begin{aligned}(\mathrm{B3}) &= \int\int \overline{(g_q f)(x)}[\sqrt{p^2+\alpha^{-2}}(g_q f)](x)d^3q\, d^3x + \frac{1}{2}\int\int \overline{f(x)}[({g_q}^2\sqrt{p^2+\alpha^{-2}} + \sqrt{p^2+\alpha^{-2}}{g_q}^2 \\ &\quad - 2g_q\sqrt{p^2+\alpha^{-2}}g_q)f](x)d^3q\, d^3x = \frac{1}{2}\int\int \overline{f(x)}(L_q f)(x)d^3q\, d^3x \\ &\quad + \int\int\left(\int \sqrt{p^2+\alpha^{-2}}\left(\int e^{-ipy}g_q(y)f(y)d^3y\right)e^{ipx}\, d^3p\right)g_q(x)\overline{f(x)}d^3q\, d^3x, \qquad (\mathrm{B4})\end{aligned}$$

where

$$(L_q f)(x) = \int\left\{\int [g_q(y)^2 + g_q(x)^2 - 2g_q(x)g_q(y)]\sqrt{p^2+\alpha^{-2}}e^{ip(x-y)}\, d^3p\right\}f(y)d^3y. \qquad (\mathrm{B5})$$

The second term in (B4) is equal to

$$\begin{aligned}&\int\int d^3p\, d^3q\sqrt{p^2+\alpha^{-2}}\left(\int \overline{f(x)}g_q(x)e^{ipx}d^3x\right)\left(\int f(y)g_q(y)e^{-ipy}\, d^3y\right) \\ &\quad = \int\int d^3p\, d^3q\sqrt{p^2+\alpha^{-2}}(f,g^{p,q})(g^{p,q},f).\end{aligned}$$

The first term in (B4) is the error, which will now be estimated. Keeping x and y fixed, we have, as showed in the proof of (A2),

$$L_q(x,y) = \int [g_q(y)^2 + g_q(x)^2 - 2g_q(x)g_q(y)]\sqrt{p^2+\alpha^{-2}}e^{ip(x-y)}\,d^3p$$
$$= [g_q(x) - g_q(y)]^2 \frac{\alpha^{-2}}{4\pi^2}\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}.$$

In this way, using the same ideas as in Sec. V, we reach the estimate

$$L_q(x,y) \leqslant \|\nabla g_q\|_\infty^2 \frac{\alpha^{-2}}{4\pi^2} K_2(\alpha^{-1}|x-y|)(\chi_{\text{supp } g_q}(x) + \chi_{\text{supp } g_q}(y)),$$

where $\chi_{\text{supp } g_q}$ is the characteristic function of supp g_q. This gives us that

$$\int L_q(x,y)d^3q \leqslant \int \|\nabla g_q\|_\infty^2 \frac{\alpha^{-2}}{4\pi^2} K_2(\alpha^{-1}|x-y|)(\chi_{\text{supp } g_q}(x) + \chi \text{ supp } g_q(y))d^3q$$
$$= 2\|\nabla g\|_\infty^2 \frac{\alpha^{-2}}{4\pi^2} K_2(\alpha^{-1}|x-y|)\text{Vol}(\text{supp } g).$$

By this we finally get, by using first the Cauchy–Schwartz, then Young's inequality, that

$$\left|\int\int \overline{f(x)} \int L_q(x,y)d^3q\, f(y)d^3x\, d^3y\right| \leqslant \int\int |f(x)|\left(2\|\nabla g\|_\infty^2 \frac{\alpha^{-2}}{4\pi^2} K_2(\alpha^{-1}|x-y|)\text{Vol}(\text{supp } g)\right)$$
$$\times |f(y)|d^3x\, d^3y$$
$$\leqslant 2\|\nabla g\|_\infty^2 \frac{\alpha^{-2}}{4\pi^2}\|f\|_2 \||f| * G_\alpha\|_2 \text{Vol}(\text{supp } g),$$
$$G_\alpha(x) = K_2(\alpha^{-1}|x|) \leqslant \|\nabla_g\|_\infty^2 \frac{\alpha^{-2}}{2\pi^2}\|f\|_2^2 \|G_\alpha\|_1 \text{Vol}(\text{supp } g)$$
$$= \|\nabla g\|_\infty^2 \frac{\alpha^{-2}}{2\pi^2} 6\pi^2\alpha^3 \|f\|_2^2 \text{Vol}(\text{supp } g) \quad [\text{see (A6) for } \|G_\alpha\|_1]$$
$$= 3\alpha\|\nabla g\|_\infty^2 \text{Vol}(\text{supp } g)\|f\|_2^2.$$

□

For the case (8.1) in Sec. VIII, let the coherent state $g^{p,q}$ be defined from the scaled version of the function g chosen there—that is, $g \in C_0^\infty(\mathbb{R}^3)$, spherically symmetric, non-negative and with support in the unit ball $B(0,1)$ of $\mathbb{R}^3$. Then the coherent states are

$$g_\alpha^{p,q}(x) = g_\alpha(x-q)e^{ipx} = \alpha^{-3s/2} g\left(\frac{x-q}{\alpha^s}\right)e^{ipx}.$$

In this way, $\|\nabla g_\alpha\|_\infty^2 = \alpha^{-5s}\|\nabla g\|_\infty^2$ and $\text{Vol}(\text{supp } g_\alpha) = (4\pi/3)\alpha^{3s}$, and therefore

$$(f, \sqrt{p^2+\alpha^{-2}}f) \geqslant \frac{1}{(2\pi)^3}\int\int d^3p\, d^3q \sqrt{p^2+\alpha^{-2}}(f, g_\alpha^{p,q})(g_\alpha^{p,q}, f) - o(\alpha^{-1/3}),$$

since, as $s < 2/3$,

$$3\alpha\alpha^{-5s}\|\nabla g\|_\infty^2 \frac{4\pi}{3}\alpha^{3s}\|f\|_2^2 = C\alpha^{1-2s} = o(\alpha^{-1/3}), \quad \alpha \to 0.$$

This proves the formula (8.1), since

$$(f,f) = \frac{1}{(2\pi)^3} \int \int d^3p\, d^3q (f, g_\alpha^{p,q})(g_\alpha^{p,q}, f)$$

and $T(p) = \sqrt{p^2 + \alpha^{-2}} - \alpha^{-1}$.

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Local existence of quasispherical space–time initial data

Jason Sharples[a)]
School of Mathematics and Statistics, University of Canberra, A.C.T. 2601, Australia

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We consider the system of Einstein constraint equations in the special case when the spacelike 3-manifold is assumed to satisfy the quasispherical ansatz of Bartnik. We introduce two different time slicing conditions, under each of which we may view the resulting constraint equations as a parabolic/elliptic/ODE system of partial differential equations. We combine recent existence results for parabolic equations in Sobolev space with an iterative method to prove local existence results for the quasispherical Einstein constraint equations under the two different time slicing conditions. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1864250]

I. INTRODUCTION

In general relativity, the Einstein field equations allow us to study the evolution of a spacelike 3-manifold, provided that its metric and extrinsic curvature satisfy a system of geometric constraint equations. The Einstein constraint equations, arise as a consequence of the fact that the 3-manifold in question is necessarily a submanifold of the spacetime its evolution defines. The constraint equations on a 3-manifold Σ with metric h and second fundamental form K are

$$\mathcal{R}_h + (\mathrm{tr}_h K)^2 - \|K\|^2 = 16\pi T_{00}, \tag{1.1}$$

$$D^j K_{ij} - D_i(\mathrm{tr}_h K) = 8\pi T_{0i}, \quad i = 1,2,3. \tag{1.2}$$

Here T is the stress-energy tensor and $\mathcal{R}_h$ and D denote the scalar curvature and Levi–Civita connection of the metric h.

Traditionally, solutions of the constraint equations are constructed using the method of Lichnerowicz,[12] which is based on the conformal class of h. This method has been studied extensively, for example in Refs. 7–10. Accordingly, the data set

$$h = \phi^4 \hat{h},$$

$$K = \phi^{-2}\hat{A} + \phi^{-2} l_{\hat{h}}(W) + \tfrac{1}{3}\tau\phi^4\hat{h},$$

satisfies the initial data constraints (1.1) and (1.2) if ϕ and W satisfy the semilinear elliptic system

$$8\Delta_{\hat{h}}\phi = \phi\mathcal{R}_{\hat{h}} - \|\hat{A} + l_{\hat{h}}(W)\|^2\phi^{-7} + \tfrac{2}{3}\tau^2\phi^5 - 16\pi\hat{T}_{00}, \tag{1.3}$$

$$\hat{D}_j[l_{\hat{h}}(W)]^{ij} = \tfrac{2}{3}\phi^6\hat{D}^i\tau + 8\pi\hat{T}^{0i}, \tag{1.4}$$

where l_h is the conformal Killing operator; $l_h(W) = \mathcal{L}_W h - \frac{1}{3}h\,\mathrm{tr}_h(\mathcal{L}_W h)$.

This conformal method has both advantages and disadvantages; on the one hand, every solution of (1.1) and (1.2) may be obtained in this manner from suitable $\hat{h}$, τ, $\hat{A}$, while on the other

[a)]Present address: Centre for Resource and Environmental Studies, Australian National University, Canberra, Australia, 0200. Electronic mail: jasons@cres.anu.edu.au

hand, the elliptic system (1.3) and (1.4) does not always admit solutions, it is difficult to solve numerically in general, and distinct data can give rise to diffeomorphically equivalent solutions of the constraint equations.[5]

More particularly, the conformal method has been shown to be inadequate for the solution of a problem encountered when considering the notion of quasilocal mass in general relativity.[3] In Ref. 2 one is confronted with the following extension problem:

Given a bounded data set (Σ_0, h_0, K_0), find an asymptotically flat data set (Σ, h, K) with boundary $\Gamma = \partial\Sigma \simeq \partial\Sigma_0$ such that the complete manifold $\Sigma \cup_\Gamma \Sigma_0$, obtained by gluing Σ and Σ_0 along Γ, forms an initial data set.

Requiring that (Σ, h) have bounded curvature across Γ implies the boundary conditions for the metric h and mean curvature $H_\Gamma = \mathrm{tr}_\Gamma K$,

$$h|_{T\Gamma} = h_0|_{T\partial\Sigma_0}, \quad H_\Gamma = H_{\partial\Sigma_0}. \tag{1.5}$$

Given a metric $\hat{h}$ on $\Sigma \setminus \Sigma_0$, for the conformal method, we must solve the semilinear elliptic equation,[3]

$$\left(\Delta_{\hat{h}} - \tfrac{1}{8}\mathcal{R}_{\hat{h}}\right)\phi = -\tfrac{1}{8}\phi^5 \mathcal{R}_h,$$

where $h = \phi^4 \hat{h}$ is the required 3-metric. The boundary conditions (1.5) imply that $\hat{h}|_{T\Gamma} = h_0|_{T\partial\Sigma}$ without loss of generality.

Under conformal change of the metric the mean curvature of Γ transforms as

$$H_{\Gamma,h} = 8\phi^{-3}\partial_{\hat{n}}\phi + \phi^{-2} H_{\Gamma,\hat{h}}, \tag{1.6}$$

where $\partial_{\hat{n}}$ is the outward $\hat{h}$-unit normal derivative.

Equation (1.6) implies that the boundary conditions (1.5) are equivalent to the boundary conditions for ϕ on Γ

$$\phi = 1, \quad \partial_n \phi = H_{\Gamma,\hat{h}} - H_{\partial\Sigma_0,h_0},$$

where $H_{\Gamma,\hat{h}}$ and $H_{\partial\Sigma_0,h_0}$ are the given mean curvatures. Clearly these boundary conditions are ill-posed.

In this paper we outline an alternative method for constructing solutions to the constraint equations based on the quasispherical (QS) ansatz of Bartnik.[4] Moreover, we establish local existence results for the constraint equations for a spacelike hypersurface in the QS gauge (Theorems 5.25 and 5.20). We make no mention of the generality of this gauge; the extent to which the QS ansatz applies remains an open problem.

After briefly describing and imposing the quasispherical gauge in Sec. II, we provide an argument to show that the resulting system of constraint equations may be viewed as a coupled system of partial differential equations consisting of a parabolic equation, a first-order elliptic system and (essentially) a system of ordinary differential equations. This system admits several Cauchy problem formulations, depending on which fields are considered as prescribed. In Sec. III we describe two such formulations that arise naturally through geometric considerations. In Sec. IV we reformulate the systems via a complexification of the sphere and introduce an additional constraint equation that allows us to write the systems in a more tractable form. In Sec. V we use a contraction mapping argument, based on an iterative system of partial differential equations, to prove local existence results for the two Einstein constraint systems that were formulated in the preceding sections of the paper.

II. THE QUASISPHERICAL METHOD

We assume that the 3-manifold, Σ, can be foliated by surfaces of constant positive Gauss curvature (i.e., rescaled 2-spheres), such that the area function $4\pi r^2 \in C^\infty(\Sigma)$ can be used as a

global coordinate. Using standard polar coordinates (ϑ,φ) on the 2-spheres, the most general metric compatible with these assumptions may be written as (Ref. 4, Lemma 2.1)

$$ds^2 = u^2\,dr^2 + (\beta^1\,dr + r\,d\vartheta)^2 + (\beta^2\,dr + r\sin\vartheta\,d\varphi)^2, \tag{2.1}$$

for functions $u(r,\vartheta,\varphi)>0$, $\beta^A(r,\vartheta,\varphi)$, $A=1,2$. We call the metric in these coordinates *quasispherical*, since this naturally generalizes the class of spherically symmetric metrics.

Computing the scalar curvature $\mathcal{R}$ of (2.1) we find that[4]

$$2r\partial_r u - 2\beta_A\nabla_A u = \gamma u^2\Delta u + (1+\gamma B)u - \gamma\left(1-\tfrac{1}{2}\mathcal{R}r^2\right)u^3, \tag{2.2}$$

where

$$B = \tfrac{1}{2}|\mathrm{div}\,\beta|^2 + \tfrac{1}{2}\left|\nabla_{(A}\beta_{B)}\right|^2 - r\partial_r(\mathrm{div}\,\beta) + \beta_A\nabla_A(\mathrm{div}\,\beta) - \tfrac{3}{2}\mathrm{div}\,\beta,$$

and

$$\gamma = \left(1-\tfrac{1}{2}\mathrm{div}\,\beta\right)^{-1}, \quad \mathrm{div}\,\beta = \nabla^A\beta_A.$$

Equation (2.2) is a semilinear parabolic equation on S^2 for u, with β^A and $\mathcal{R}$ regarded as prescribed fields. General global existence theorems for solutions of (2.2) have been proven in Ref. 4, under suitable regularity and boundedness assumptions about the prescribed fields. In particular, to ensure that (2.2) is parabolic evolution in the direction of increasing r, β is required to satisfy

$$2 - \mathrm{div}\,\beta > 0. \tag{2.3}$$

The parabolic equation (2.2) provides a method of solving the Hamiltonian constraint. Using the Hamiltonian constraint (1.1) to *define* the scalar curvature $\mathcal{R}$ in terms of $T_{00}, \|K\|^2$ and $\mathrm{tr}_h K$, specifying β appropriately and solving (2.2) for u yields a quasispherical metric satisfying the Hamiltonian constraint. It is of interest to point out in passing that the quasispherical form of the metric fares much better with the extension problem than the conformal method. If S_r^2 denotes a leaf of the quasispherical foliation, defined by

$$S_r^2 = \{p\in\Sigma : r(p) = r\}$$

then the mean curvature of S_r^2 is

$$H_r = H_{S_r^2} = \frac{1}{ru}(2 - \mathrm{div}\,\beta).$$

Therefore if β is given and satisfies (2.3), then prescribing $H_{r_0}>0$ amounts to specifying $u(r_0)$ which may then be taken as initial data for (2.2). Solution of (2.2), with initial data so defined, then yields an extension metric, at least in the case when the mean curvature is prescribed on a standard S^2. This idea has also been exploited in recent works concerning the connectedness of the space of initial data sets for the Einstein equations[17] and in connection with the positive mass theorem and boundary behaviour of compact manifolds.[16]

To solve the momentum constraints (1.2) it is convenient to reparametrize K. We define the quasispherical orthonormal coframe

$$\theta^1 = \beta^1\,dr + r\,d\vartheta,$$

$$\theta^2 = \beta^2\,dr + r\sin\vartheta\,d\varphi,$$

$$\theta^3 = u\,dr$$

and write

$$K_{ij}\theta^i\theta^j = \left(\eta_{AB} + \tfrac{1}{2}\mu\delta_{AB}\right)\theta^A\theta^B + \kappa_A(\theta^A\theta^3 + \theta^3\theta^A) + (H-\mu)\theta^3\theta^3, \tag{2.4}$$

where η_{AB} is a symmetric, traceless, 2-tensor on S^2. The momentum constraints (1.2) may then be written in terms of this quasispherical parametrization as

$$8\pi T_{03} ru = -(r\partial_r\mu - \beta^A\nabla_A\mu + (3 - \operatorname{div}\beta)\mu) + u \operatorname{div}\kappa + \kappa^A\nabla_A u + \eta^{AB}\nabla_{(B}\beta_{A)} + (2 - \operatorname{div}\beta)H, \tag{2.5}$$

$$8\pi T_{0\hat{A}} ru = \nabla^B(u\eta_{AB}) + \mu\nabla_A u + \nabla_A\left(u\left(\tfrac{1}{2}\mu - H\right)\right) + r\partial_r\kappa_A - \beta^B\nabla_B\kappa_A + ((3 - \operatorname{div}\beta)\delta_{AB} - \nabla_{(A}\beta_{B)})\kappa^B. \tag{2.6}$$

Hence if we consider the scalar curvature $\mathcal{R}$ as given in terms of μ, η, κ, and H via (1.1) and (2.4); that is,

$$\mathcal{R} = 16\pi T_{00} + \|\eta\|^2 + 2\|\kappa\|^2 + \tfrac{3}{2}\mu^2 - 2\mu H,$$

then the system of equations (2.2), (2.5), and (2.6) comprise the spacetime intial data constraints in the quasispherical gauge, and so will be referred to as the *quasispherical Einstein constraint system* (QSECS).

As mentioned already, for Eq. (2.2) to be considered parabolic it is required that β satisfy the condition (2.3). To ensure that this condition is met we *prescribe* β as any element of the set $\{f \in \Gamma^\infty(TS^2 \times [0,\infty)) : 2 - \operatorname{div} f > 0.\}$. This leaves u as the only remaining metric parameter. We therefore cannot prescribe u; it must be found by solving the QSECS subject to appropriate boundary conditions.

Now that we have established that u cannot be prescribed, we must consider the remaining fields μ, η_{11}, η_{12}, κ_1, κ_2, and H. Since we have only four equations in the QSECS, it is obvious that we need to prescribe at least three of these fields and consider the other three as to be determined by the QSECS, subject to suitable boundary conditions. The following question remains: Which of the fields μ, η_{11}, η_{12}, κ_1, κ_2, and H should we consider as prescribed? As we will see in a moment, prescribing either H or μ allows us to gain a certain control over the geometrical nature of the initial data. We will thus consider μ *or* H as prescribed, never both. This leaves us with two remaining fields to prescribe. The only choices are the components of η or the components of κ (it seems implausible to prescribe one component of each). Seeing that κ appears more frequently in the QSECS than does η, we choose to prescribe κ. As we might have hoped, we will see that this choice simplifies the structure of the QSECS, for only a minor cost. We make the comment, in passing, that the case for prescribing η is potentially interesting as well. This case will not be treated here, however.

III. TIME SLICING CONDITIONS

In the conformal method approach to constructing spacetime initial data, prescribing the mean curvature has been made standard practice. This has many advantages both geometrically and physically. Indeed the so-called maximal gauge or maximal time slicing, which amounts to the assumption that the mean curvature is zero, is quite often employed since it greatly simplifies the analysis and may be assumed, without loss of generality, for any asymptotically flat spacetime satisfying an interior condition.[1] These considerations suggest the following boundary value problem.

Problem 1a: QSECS with prescribed mean curvature. Given the prescribed fields $T_{0\alpha}$, β, κ, and H, do there exist solutions u, μ, and η of (2.2), (2.5), and (2.6) satisfying the boundary conditions $(u,\mu)|_{S^2_1} = (u_0,\mu_0)$? Note that $S^2_1 = \{p \in \Sigma : r(p) = 1\}$ is the unit sphere. It may be possible to assign boundary values on a more general 2-surface but in this work we will only treat the case where boundary values are assigned on the unit sphere.

Another less familiar but potentially interesting time slicing condition is given by prescribing μ. In general μ is defined as

$$\mu = g^{AB}K_{AB},$$

where g^{AB}, $A, B=1, 2$ refers to the components of the inverse of the induced (spherical) metric.

To illustrate the geometric meaning of prescribing μ we consider the case of spherically symmetric spacetimes with metric given by

$$ds^2 = -X^2\,dt^2 + 2Y\,dr\,dt + Z^2\,dr^2 + r^2\,d\sigma^2. \tag{3.1}$$

Calculating μ for the surfaces defined by constant t in this metric, we easily obtain

$$r\mu = 2X^{-1}Y.$$

If it were the case that the metric were written in polar coordinates (for which $Y=0$), we would find that $\mu=0$. For this reason we will refer to the slicing defined by $\mu=0$ as the *polar gauge* and we will call the quantity μ the *polar curvature*.

Next consider a surface defined by $t=f(r)$ in the metric (3.1). The tangent to this surface is given by $\dot{x}=\partial_r+f'\partial_t$. The normal to the surface is given by $n=a\partial_r+b\partial_t$, where a and b are determined by the conditions $g(\dot{x},n)=0$ and $g(n,n)=-1$, which lead to

$$a = \frac{X^2f' - Y}{Z^2 + Yf'}b,$$

$$b^{-2} = X^2 - \frac{2Y(X^2f' - Y)}{Z^2 + Yf'} - \frac{(X^2f' - Y)^2}{(Z^2 + Yf')^2}.$$

The polar curvature is given by

$$r\mu = 2a.$$

The polar gauge ($\mu=0$) then implies that $f'=YX^{-2}$ and so the tangent to the surface is given by

$$\dot{x} = \partial_r + YX^{-2}\partial_t,$$

while its normal is

$$n = X^{-1}\partial_t.$$

Calculating the gradient of r, we have

$$\nabla r = g^{\alpha\beta}\partial_\alpha r\partial_\beta = \frac{X^2}{X^2Z^2 + Y^2}(\partial_r + YX^{-2}\partial_t).$$

Hence, at least in the case of spherically symmetric spacetimes, the $\mu=0$ surfaces are those which have ∇r, the gradient of r, as their tangent vector.

Furthermore, the polar curvature arises naturally upon consideration of the trapped surface condition. If we condsider a spacelike 2-surface S, with normal N and second fundamental form $\mathbb{II}$, embedded in a spacelike 3-manifold with normal T and second fundamental form K, the expansion of the null congruences associated with $T\pm N$ are given by

$$\theta_\pm = \mathrm{tr}_S\langle\nabla_{e_A}e_B, T \pm N\rangle, = \mathrm{tr}_S(K_{AB} \pm \mathbb{II}_{AB}) = \mu \pm \mathrm{tr}_S\,\mathbb{II}.$$

Thus the trapped surface condition is $\mu = \pm\mathrm{tr}_S\mathbb{II}$.

The role the polar curvature plays in more general spacetimes is potentially very interesting but has not as yet been investigated in any detail. However, in anticipation of this investigation we will consider the QSECS with μ a prescribed field. This gives us a second formulation of the QSECS as a boundary value problem.

Problem 2a: QSECS with prescribed polar curvature. Given the prescribed fields $T_{0\alpha}$, β, κ and μ, do there exist solutions u, H, and η of (2.2), (2.5), and (2.6) satisfying the boundary conditions $u|_{S_1^2}=u_0$?

IV. REWRITING THE EQUATIONS

In this section we introduce a complex notation and a coordinate transformation that enables us to write the QSECS in a more tractable form. We define the following complex fields:

$$\beta = \frac{1}{\sqrt{2}}(\beta^1 - i\beta^2),$$

$$\kappa = \frac{1}{\sqrt{2}}(\kappa^1 - i\kappa^2),$$

$$\eta = \eta_{11} - i\eta_{12},$$

$$T_0 = \frac{1}{\sqrt{2}}(T_{01} - iT_{02}),$$

and the subsidiary field

$$\rho = 2 - \operatorname{div}\beta = \gamma^{-1}.$$

We may consider β and κ as S^2 vector fields or as spin-1 sections of the complex line bundle over S^2.[6,13] Similarly we may consider η as a symmetric, traceless 2-tensor over S^2 or as a spin-2 section of the complex line bundle over S^2. The context in which these fields are used should make it clear which representation is being employed.

The complex notation suggests encoding the angular derivatives in terms of the differential operator ð (a phonetic symbol pronounced "eth"[13]) defined on a spin-s field ψ by

$$ð\psi = \frac{1}{\sqrt{2}}\sin^s\vartheta(\partial_\vartheta - i\csc\vartheta\,\partial_\varphi)(\psi\sin^{-s}\vartheta).$$

All the standard differential operators on S^2 may be expressed in terms of ð, for example,

$$\operatorname{div}\beta = ð\bar{\beta} + \bar{ð}\beta,$$

$$\operatorname{curl}\beta = i(\bar{ð}\beta - ð\bar{\beta},$$

$$\Delta\psi = (ðð + \bar{ð}ð)\psi.$$

The spin-weighted spherical harmonics Y^s_{lm} are then the eigenfields of the Laplacian, satisfying

$$\Delta Y^s_{lm} = (s^2 - l(l+1))Y^s_{lm},$$

with $|s|\leqslant l$. The eigenfields Y^s_{lm} may be taken proportional to $ð^sY_{lm}$ for $s\geqslant 0$ and $\bar{ð}^{-s}Y_{lm}$ for $s<0$, where Y_{lm} are the usual spherical harmonics.[14]

An important result concerning $\bar{ð}$ which will have bearing on our consideration of the QSECS is as follows.[13,14]

Lemma 4.1: Suppose $s \geqslant 0$ *and let* $\mathcal{L}^s$ *denote the space of spin-s sections. The mapping* $\bar{\eth}: \mathcal{L}^{s+1} \to \mathcal{L}^s$ *has cokernel* $\mathcal{C} = \mathrm{span}\{Y^s_{sm}\}$.

We have the obvious corollary.

Corollary 4.2: Suppose $s \geqslant 0$. *The mapping* $\bar{\eth}: \mathcal{L}^{s+1} \to \mathrm{span}\{Y^s_{lm}: l \geqslant s+1\}$ *is a surjection.*

Due to the repeated appearance of the operator $r\partial_r - \nabla_\beta$ we will find it convenient to make a change of coordinates that will simplify the structure. We introduce the diffeomorphism of $S^2 \times \mathbb{R}$

$$\Phi: (t, \xi^A) \mapsto (e^t, \Theta^A(t,\xi)) = (r, \zeta^A), \tag{4.1}$$

where $\zeta = (\vartheta, \varphi)$ and $\Theta(t,\xi)$ is defined to be the solution of

$$\frac{\partial}{\partial t}\Theta(t,\xi) = -\beta(e^t, \Theta(t,\xi)), \tag{4.2}$$

subject to suitable boundary conditions, $\beta|_{t=0} = \beta_0$.

Hence, defining $\tilde{f}(t,\xi) = f(e^t, \Theta(t,\xi))$, we then have

$$\partial_t \tilde{f}(t,\xi) = \left. e^t \frac{\partial f}{\partial r} + \frac{\partial f}{\partial \zeta^A}\frac{\partial \Theta^A}{\partial t}\right|_{(r,\zeta)=(e^t,\Theta(t,\xi))} = \left(r\frac{\partial}{\partial r} - \beta^A \frac{\partial}{\partial \zeta^A}\right) f(e^t, \Theta(t,\xi)) = (r\partial_r - \nabla_\beta) f(e^t, \Theta(t,\xi)).$$

We may then write (2.2), (2.5), and (2.6) in terms of (t,ξ) as

$$2\tilde{\rho}\partial_t \tilde{u} = \tilde{u}^2 \tilde{\Delta}\tilde{u} + \tilde{\rho}(1 + \tilde{\gamma}\tilde{B})\tilde{u} - \left(1 - \tfrac{1}{2}\tilde{\mathcal{R}}e^{2t}\right)\tilde{u}^3,$$

$$8\pi \tilde{T}_{03}\tilde{u}e^t = -(\partial_t \tilde{\mu} + (1+\tilde{\rho})\tilde{\mu}) + \tilde{u}(\widetilde{\mathrm{div}\,\kappa}) + (\widetilde{\kappa^A \nabla_A u}) + (\widetilde{\eta^{AB}\nabla_{(B}\beta_{A)}}) + \tilde{\rho}\tilde{H},$$

$$8\pi \tilde{T}_0 \tilde{u}e^t = \partial_t \tilde{\kappa} + \left(\bar{\eth}(u\eta) + \mu \eth u + \tfrac{1}{2}\eth(u\mu) - \eth(uH) + (1+\rho)\kappa + \bar{\kappa}\eth\beta + \kappa\eth\bar{\beta}\right).$$

We note that since we have employed the coordinate transformation given by Φ, the Laplacian $\tilde{\Delta}$ appearing in the first of the above equations is with respect to the pulled back metric $\tilde{h} = \Phi^* h$.

As we can see, implementing the coordinate transformation Φ, simplifies the structure of the system in question. It does, however, leave us with a technical hitch. Since the natural angular derivatives will now be in terms of the ξ^A-coordinates, when we come to differentiate the equations, terms involving derivatives of β will arise via (4.2). This is not a problem, as we will assume throughout that β is a smooth, prescribed field and so the terms that arise will be bounded by uniform constants. Moreover, since we assume that β is smooth, the standard regularity theory for ordinary differential equations dependent upon a parameter implies that Φ is a smooth diffeomorphism.

With this observation in mind we may supress the tilde's. Introducing the notation $\dot{f} = \partial_t f$ and defining the auxiliary field $\hat{\eta} = u\eta$ we then write the QSECS as

$$2\rho\dot{u} = u^2 \Delta u + \rho(1+\gamma B)u - \left(1 - \tfrac{1}{2}\mathcal{R}\mathrm{e}^{2t}\right)u^3, \tag{4.3}$$

$$8\pi T_{03} u e^t = -(\dot{\mu} + (1+\rho)\mu) + u\,\mathrm{div}\,\kappa + \kappa^A \nabla_A u + \eta^{AB}\nabla_{(B}\beta_{A)} + \rho H, \tag{4.4}$$

$$8\pi T_0 u e^t = \bar{\eth}(\hat{\eta}) + \mu\eth u + \tfrac{1}{2}\eth(u\mu) - \eth(uH) + \dot{\kappa} + (1+\rho)\kappa + \bar{\kappa}\eth\beta + \kappa\eth\bar{\beta}. \tag{4.5}$$

To simplify the discussion and to be in keeping with the usual notions accompanying parabolic equations, we will call $t = \ln r$ "time" and refer to the values of the various fields on the unit sphere as initial values.

Unfortunately a problem arises if we consider (4.5) as giving an equation for $\hat{\eta}$. In making such a consideration we find that (4.5) is of the form $\bar{\eth} f = g$ with $f \in \mathcal{L}^2$. Observing Lemma 4.1, an equation of this form is only solvable if $g \in \text{span}\{Y^1_{lm} : l \geqslant 2\}$, that is to say if g is devoid of $l=1$ spherical harmonic components. Hence if we consider (4.5) as giving an equation for $\hat{\eta}$, then we do not have the freedom to prescribe all the fields we have thus far considered prescribed.

Typically the stress-energy tensor will be determined by the matter occupying the spacetime, and we would like to freely specify H or μ for geometric reasons. It is also best to completely specify the metric parameter β so that there is no chance of (2.3) being violated. That leaves us with κ, and we conclude that it is not possible to consider (4.5) as giving an equation for $\hat{\eta}$ and at the same time treat κ as freely specifiable.

We thus look to constrain κ in such a way that (4.5) is solvable. This will produce another equation (the κ constraint) which must then be included as part of the QSECS.

To obtain the required equation we spectrally decompose κ as follows:

$$\kappa = \sum_{m=-1}^{1} k^m Y^1_{1m} + \sum_{l=2}^{\infty} \sum_{m=-l}^{l} \kappa^{lm} Y^1_{lm} = k + \sigma,$$

where $\sigma = \Sigma_{l \geqslant 2} \Sigma_{|m| \leqslant l} \kappa^{lm} Y^1_{lm}$ is devoid of $l=1$ components.

Let $\mathcal{P}_1$ denote the projection onto the subspace spanned by $\{Y^1_{1m} : m = -1, 0, 1\}$. It is easy to check that if k satisfies

$$-\dot{k} = \mathcal{P}_1 \left\{ \mu \eth u + \tfrac{1}{2} \eth (u\mu) - \eth (uH) + (1+\rho)\kappa + \bar{\kappa} \eth \beta + \kappa \eth \bar{\beta} + 8\pi T_0 u e^t \right\} \tag{4.6}$$

then (4.5) reduces to

$$-\bar{\eth} \hat{\eta} = \dot{\sigma} + (1 - \mathcal{P}_1) \left\{ \mu \eth u + \tfrac{1}{2} \eth (u\mu) - \eth (uH) + (1+\rho)\kappa + \bar{\kappa} \eth \beta + \kappa \eth \bar{\beta} + 8\pi T_0 u e^t \right\}. \tag{4.7}$$

This equation is of the form $\bar{\eth} f = g$ with $g \in \text{span}\{Y^1_{lm} : l \geqslant 2\}$, and so is uniquely solvable by Corollary 4.2.

Replacing (4.5) with (4.6) and (4.7), the constraint system may now be written as

$$2\rho \dot{u} = u^2 \Delta u - u^3 \left(1 - \tfrac{1}{2} e^{2t} \left(16\pi T_{00} + 2\|\kappa\|^2 + \tfrac{3}{2}\mu^2 - 2\mu H \right) \right) + \rho \left(1 + \tfrac{1}{2} \gamma e^{2t} \|\hat{\eta}\|^2 + \gamma B \right) u, \tag{4.8}$$

$$\dot{\mu} = \text{div}(u\kappa) - (1+\rho)\mu + u^{-1} \hat{\eta}^{AB} \nabla_{(B} \beta_{A)} + \rho H - 8\pi T_{03} u e^t, \tag{4.9}$$

$$-\dot{k} = \mathcal{P}_1 \left\{ \mu \eth u + \tfrac{1}{2} \eth (u\mu) - \eth (uH) + (1+\rho)\kappa + \bar{\kappa} \eth \beta + \kappa \eth \bar{\beta} + 8\pi T_0 u e^t \right\}, \tag{4.10}$$

$$-\bar{\eth} \hat{\eta} = \dot{\sigma} + (1 - \mathcal{P}_1) \left\{ \mu \eth u + \tfrac{1}{2} \eth (u\mu) - \eth (uH) + (1+\rho)\kappa + \bar{\kappa} \eth \beta + \kappa \eth \bar{\beta} + 8\pi T_0 u e^t \right\}. \tag{4.11}$$

The problems 1a and 1b may now be stated more correctly as follows.

Problem 1b: QSECS with prescribed mean curvature. Given the prescribed fields $T_{0\alpha}$, β, σ, and H, do there exist solutions u, μ, $\hat{\eta}$, and k of (4.8)–(4.11) satisfying the initial conditions $(u, \mu, k)|_{S^2 \times \{0\}} = (u_0, \mu_0, k_0)$?

Problem 2b: QSECS with prescribed polar curvature. Given the prescribed fields $T_{0\alpha}$, β, σ, and μ, do there exist solutions u, H, $\hat{\eta}$, and k of (4.8)–(4.11) satisfying the initial conditions $(u, k)|_{S^2 \times \{0\}} = (u_0, k_0)$?

We have not yet made mention about which function spaces we will be posing Problems 1b and 2b in. Which spaces are to be used will be made clear in the next section after we discuss an iterative, linear system of partial differential equations based on the QSECS. In fact, the existence of solutions to the QSECS will follow from the convergence of the iterative system to a fixed point.

We will begin by considering Problem 1b.

V. LOCAL EXISTENCE

In Ref. 4 the author gives a detailed proof of the global existence and uniqueness of solutions of (2.2) with β and $\mathcal{R}$ prescribed, and satisfying certain conditions. When considering the QSECS with prescribed mean curvature, however, we may not consider $\mathcal{R}$ as completely prescribed, but as determined by the additional fields μ, $\hat{\eta}$, and k, each of which is constrained so as to satisfy (2.5) and (2.6).

To prove the local existence and uniqueness of solutions to the QSECS with prescribed mean curvature, we will not borrow from Bartnik's treatment. Instead we will define a linear system of partial differential equations and produce a sequence of iterates that converge to a solution of the QSECS. In defining the iterative scheme we will see that it is imperative that we have a theory dealing with linear parabolic equations in which the regularity of the coefficients is comparable to that of the solution. Such results were obtained in Ref. 15 where the following general second order parabolic equation was considered:

$$\partial_t u + A_t u = g \quad \text{on } S^2 \times [0,T],$$

$$u = u_0 \quad \text{on } S^2 \times \{0\}. \tag{5.1}$$

Here A_t is a linear differentiable operator of second order on S^2, which is expressible in divergence form. That is, for a twice differentiable function $u: S^2 \times [0,T] \to \mathbb{R}$, we may write $A_t u$ in local coordinates as

$$A_t u(x,t) = -\nabla_j (a^{ij}(x,t)\nabla_i u(x,t)) + b^i(x,t)\nabla_i u(x,t) + c(x,t)u(x,t), \tag{5.2}$$

where ∇ denotes the S^2 covariant derivative.

To ensure that (5.1) is a parabolic equation we assume that the operator A_t is an elliptic operator for each value of t, in the sense that for each $\xi \in TS^2$, and each fixed $t \in [0,T]$ we have

$$a^{ij}(x,t)\xi_i\xi_j \geqslant \theta \bar{g}^{ij}\xi_i\xi_j,$$

for a.e. $x \in S^2$, where $\theta > 0$ is a constant and where $\bar{g}$ is the standard S^2-metric.

Before stating the existence result for (5.1) we define the parabolic Sobolev spaces in which the solutions reside. Let $f, g: S^2 \times [0,T] \to \mathbb{R}$ be smooth functions and let

$$\langle f, g \rangle_{LH^s_{\nu,T}} = \int_0^T e^{-2\nu t} \langle f(\cdot,t), g(\cdot,t) \rangle_{H^s(S^2)} \, \mathrm{d}t.$$

We define LH^s_ν to be the Hilbert space formed by completion of $C^\infty(S^2 \times [0,T])$ in the corresponding norm. The parabolic Sobolev spaces we require may then be defined as

$$P^m_{\nu,T} = \left\{ f: S^2 \times [0,T] \to \mathbb{R} : \|\partial_t^i f\|_{LH^{2(m-i)}_{\nu,T}} < \infty, \ \forall\, i \leqslant m \right\}$$

and its associated inner product

$$\langle f, g \rangle_{P^m_{\nu,T}} = \sum_{i \leqslant m} \langle \partial_t^i f, \partial_t^i g \rangle_{LH^{2(m-i)}_{\nu,T}}.$$

Roughly speaking, a parabolic equation tells us that one time derivative is equivalent to two space derivatives. Hence, in a sense, the Hilbert space $P^m_{\nu,T}$ describes the set of functions that are in total $2m$ times differentiable. We also make the following definition in order to classify functions that have odd total derivative:

$$P^{m+1/2}_{\nu,T} = \left\{ f{:}S^2 \times [0,T] \to \mathbb{R}{:} \|\partial_t^i f\|_{LH^{2(m-i)+1}_{\nu,T}} < \infty,\ \forall\ i \leqslant m \right\}$$

and its associated inner product,

$$\langle f,g\rangle_{P^{m+1/2}_{\nu,T}} = \sum_{i\leqslant m} \langle \partial_t^i f, \partial_t^i g\rangle_{LH^{2(m-i)+1}_{\nu,T}}.$$

We note that $P^0_{\nu,T}=LH^0_{\nu,T}$ and $P^{1/2}_{\nu,T}=LH^1_{\nu,T}$. The required existence theorem may now be stated as Ref. 15.

Theorem 5.1: *Suppose* $m \geqslant m_0 = 4\frac{1}{2}$, $u_0 \in H^{2m}(S^2)$ *and* $g \in P^{m-1/2}_{\nu,T}$. *There is a unique solution* u of *(5.1) belonging to the class* $P^{m+1/2}_{\nu,T}$ *and satisfying the estimate*

$$\|u\|^2_{P^{m+1/2}_{\nu,T}} \leqslant \mathcal{Q}\left(\|u_0\|^2_{H^{2m}(S^2)} + \|g\|^2_{P^{m-1/2}_{\nu,T}} \right). \tag{5.3}$$

The constant $\mathcal{Q}$ *depends only on* m *and the norms* $\|a\|_{P^m_{\nu,T}}$, $\|b\|_{P^{m-1/2}_{\nu,T}}$ *and* $\|c\|_{P^{m-1/2}_{\nu,T}}$.

In addition to the already mentioned linear parabolic theory, we will need to employ results from linear elliptic equations and linear ordinary differential equations. These will be derived as they are needed.

We begin by proposing an iterative system of partial differential equations before going on to prove that it is well defined.

A. The iteration scheme

Keeping in mind that we are dealing with the QSECS with prescribed mean curvature, we may consider H as some given field. We therefore define the following iterative system for generating the sequence $\{(u_n,\mu_n,\hat{\eta}_n,k_n)\}_{n=0}^{\infty}$:

$$\dot{u}_{n+1} = \hat{\gamma} u_n^2 \Delta u_{n+1} - \hat{\gamma} u_n^3 \left(1 - \tfrac{1}{2} e^{2t}\left(16\pi T_{00} + 2\|\kappa_n\|^2 + \tfrac{3}{2}\mu_n^2 - 2\mu_n H\right)\right) + \tfrac{1}{2}\left(1 + \tfrac{1}{2}\gamma e^{2t}\|\hat{\eta}_n\|^2 + \gamma B\right) u_n, \tag{5.4}$$

$$\dot{\mu}_{n+1} = \mathrm{div}(u_{n+1}\kappa_{n+1}) - (1+\rho)\mu_{n+1} + u_n^{-1}\hat{\eta}_n^{AB}\nabla_{(B}\beta_{A)} + \rho H - 8\pi T_{03} u_{n+1} e^t, \tag{5.5}$$

$$\dot{k}_{n+1} = -\mathcal{P}_1\left\{ \mu_{n+1}\eth u_{n+1} + \tfrac{1}{2}\eth(u_{n+1}\mu_n) - \eth(u_{n+1}H) + (1+\rho)\kappa_n + \overline{\kappa}_n\eth\beta + \kappa_n\eth\overline{\beta} + 8\pi e^t u_{n+1} T_0 \right\}, \tag{5.6}$$

$$\begin{aligned} -\overline{\eth}\,\hat{\eta}_{n+1} = \dot{\sigma} + (1-\mathcal{P}_1)\Big\{ & \mu_{n+1}\eth u_{n+1} + \tfrac{1}{2}\eth(u_{n+1}\mu_{n+1}) - \eth(u_{n+1}H) + (1+\rho)\kappa_{n+1} + \overline{\kappa}_{n+1}\eth\beta + \kappa_{n+1}\eth\overline{\beta} \\ & + 8\pi e^t u_{n+1} T_0 \Big\}. \end{aligned} \tag{5.7}$$

We have set $\hat{\gamma}=\frac{1}{2}\gamma$ and $\hat{\rho}=\frac{1}{2}\rho$ for convenience. $\hat{\gamma}$ and $\hat{\rho}$ are still just smooth fields depending on β. From here on, unless otherwise stated, we assume that all of the prescribable fields are elements of $C^\infty(S^2\times[0,\infty))$. Note also that $\kappa_n = k_n + \sigma$.

The proposed iteration scheme is comprised of a hierarchical system of partial differential equations. The basic idea behind using (5.4)–(5.7) to generate a sequence of iterates may be stated informally as follows. Define the zeroth iterate $(u,\mu,k,\hat{\eta})_{\tilde{0}}$, by making an identification between the initial values u_0, μ_0, and k_0, and the zeroth iterates $u_{\tilde{0}}$, $\mu_{\tilde{0}}$, and $k_{\tilde{0}}$. The zeroth $\hat{\eta}$ iterate, $\hat{\eta}_{\tilde{0}}$, is then defined as the solution of (5.7), with $n=-1$.

Equation (5.4) is a linear parabolic equation, and so given appropriate initial data u_0, we may define its solution u_{n+1}, a function of prescribed regularity, provided that u_n, μ_n, k_n, and $\hat{\eta}_n$ are known functions of suitable regularity. Equations (5.5) and (5.6) form a coupled system of ordinary differential equations for (μ_{n+1}, k_{n+1}). Hence if we are given appropriate initial data (μ_0, k_0), we may define (μ_{n+1}, k_{n+1}) as the (prescribed regularity) solution of (5.5) and (5.6) provided that u_{n+1}, as given by (5.4), and u_n, μ_n, k_n, and $\hat{\eta}_n$ are functions of suitable regularity.

The last equation (5.7), is a first order elliptic system which, by construction, may be uniquely solved for $\hat{\eta}_{n+1}$ provided that u_{n+1}, μ_{n+1}, and k_{n+1}, as given by (5.4)–(5.6), are suitably regular.

The claim is that by iterating the procedure described above, we can construct a sequence of iterates $(u,\mu,k,\hat{\eta})_n$. We will now make these ideas more precise by showing that the above iteration scheme is consistently defined.

B. Consistency of the iteration scheme

As suggested by the preceding remarks about the iteration scheme, we begin by considering Eq. (5.4). Let us suppose that u_n, μ_n, k_n, $\hat{\eta}_n \in P^m_{0,T}$, $u_n(\xi,t) \geqslant \delta_1 > 0$, for all $(\xi,t) \in S^2 \times [0,T]$ and that $u_0 \in H^{2m}(S^2)$ with $u_0(\xi) \geqslant \delta_2 > 0$, for all $\xi \in S^2$. Note here that the u_0 we have referred to is the initial value, not the zeroth iterate $\tilde{u_0}$ which is defined as the time constant extension of $u_0 \in H^{2m}(S^2)$ to $S^2 \times [0,\infty)$, that is

$$\tilde{u_0}(\xi,t) = u_0(\xi).$$

Equation (5.4) is a linear parabolic equation for u_{n+1} subject to the initial condition $u_{n+1}|_{S^2\times\{0\}} = u_0$, which is seen to be of the form

$$\dot{u}_{n+1} = \mathcal{A}^n_t u_{n+1} + F_n, \qquad u_{n+1}|_{t=0} = u_0,$$

where the operator $\mathcal{A}^n_t$ is given as

$$\mathcal{A}^n_t = \hat{\gamma} u_n^2 \Delta.$$

The operator $\mathcal{A}^n_t$ may be written in divergence form (5.2), with

$$a^{ij} = \hat{\gamma} u_n^2 \bar{g}^{ij},$$

$$b^i = -(u_n^2 \nabla_k \hat{\gamma} \bar{g}^{ik} + 2\hat{\gamma} u_n \nabla_k u_n \bar{g}^{ik}),$$

$$c = 0. \tag{5.8}$$

The source field F_n is defined as

$$F_n = \tfrac{1}{2}\left(1 + \tfrac{1}{2}\gamma e^{2t}\|\hat{\eta}_n\|^2 + \gamma B\right)u_n - \hat{\gamma}\left(1 - \tfrac{1}{2}e^{2t}\left(16\pi T_{00} + 2\|\kappa_n\|^2 + \tfrac{3}{2}\mu_n^2 - 2\mu_n H\right)\right)u_n^3.$$

Recalling Theorem 5.1 we find that if $m \geqslant m_0$, u_n, $\hat{\eta}_n$, $k_n \in P^m_{0,T}$ and the prescribable fields are smooth then u_{n+1} is uniquely defined as an element of $P^{m+1/2}_{0,T}$.

It is important to note that for Theorem 5.1 to apply it is imperative that $\hat{\gamma} u_n^2 \Delta$ be an elliptic operator. The ellipticity of this operator is solely dependent upon u_n's capacity to stay above zero. Although we have assumed that $u_n(\xi,t) \geqslant \delta_1 > 0$ for all $(\xi,t) \in S^2 \times [0,T]$, it could happen that u_{n+1} falls below δ_1 after some time $T_* < T$. This possibility means that successive iterates might only be defined as elements of $P^{m+1/2}_{0,T_n}$, with $\{T_n\}$ a decreasing sequence of times. We will say more about this point later on.

Given that u_{n+1} exists and belongs to the class $P^{m+1/2}_{0,T}$ we move on to consider the coupled ordinary differential equation system (5.5) and (5.6).

We note first that, given $t \in [0,\infty)$, $k(\cdot,t)$ is an element of $\mathrm{Span}\{Y^1_{1m} : m = -1,0,1\}$ and as such we may equivalently consider $k(\cdot,t)$ simply as an element of $\mathbb{C}^3$. Indeed, we may write

$$k(\xi,t) = k^m(t) Y^1_{1m}(\xi), \quad m = -1,0,1,$$

and since the Y^1_{1m}'s are given, we may think of k as mapping $[0,\infty)$ into $\mathbb{C}^3$ as follows:

$$k:[0,\infty) \to \mathbb{C}^3 t \mapsto (k^{-1}(t), k^0(t), k^1(t)).$$

For simplicity, we will refer to $k(\cdot,t)$ simply as $k(t)$. Note that there will now be an ambiguity surrounding our use of the symbol $k(t)$ since we will use it to denote both a field over S^2, and the components of that field over $\mathbb{C}^3$. When we say "$k \in P^m_{0,T}$" we mean $k(t) \in \mathrm{Span}\{Y^1_{1m} : m = -1, 0, 1\}$. Drawing the distinction between this representation and k's representation over $\mathbb{C}^3$, we have that

$$k = (k^{-1}, k^0, k^1) \in H^m([0,T];\mathbb{C}^3) \quad \text{if and only if } k = k^m Y^1_{1m} \in P^m_{0,T},$$

where $H^m([0,T];\mathbb{C}^3)$ is the Sobolev space with norm given by

$$\|f\|^2_{H^m([0,T];\mathbb{C}^3)} = \sum_{i=1}^{m} \int_0^T \|\partial_t^i f(s)\|^2_{\mathbb{C}^3} \, \mathrm{d}s.$$

The context in which the symbol k (or k_n) is used should make it clear which representation we are employing.

Furthermore, for any fixed value of t we have $(\mu(t), k(t)) \in \mathcal{F}(S^2) \times \mathbb{C}^3$, where $\mathcal{F}(S^2)$ is some appropriate function space; we will see that the Sobolev spaces $H^{2j}(S^2)$, with $j \geqslant m_0$, will suit our needs. Hence we can view the equations (5.5) and (5.6) as a coupled system of ordinary differential equations on $E^j := H^{2j}(S^2) \times \mathbb{C}^3$, and so writing

$$\mathcal{M}(t) := (\mu(t), k(t)),$$

we have

$$\dot{\mathcal{M}}_{n+1} = A_n \mathcal{M}_{n+1} + B_n, \tag{5.9}$$

where

$$A_n \mathcal{M} = (k^m[\eth(u_{n+1}\bar{\eth}Y_{1m}) + \bar{\eth}(u_{n+1}\eth Y_{1m})] - (1+\rho)\mu - \mathcal{P}_1[\mu \eth u_{n+1}]), \tag{5.10}$$

and

$$B_n = \Big(\mathrm{div}(u_{n+1}\sigma) + u_n^{-1}\hat{\eta}_n^{AB}\nabla_{(B}\beta_{A)} + \rho H - 8\pi T_{03}u_{n+1}e^t - \mathcal{P}_1\Big[\tfrac{1}{2}\eth(u_{n+1}\mu_n) - \eth(u_{n+1}H) + (1+\rho)\kappa_n + \bar{\kappa}_n\eth\beta + \kappa_n\eth\bar{\beta} - 8\pi T_0 u_{n+1}e^t\Big]\Big). \tag{5.11}$$

We then have the following result, which asserts that the operator A_n is bounded, provided u_{n+1} satisfies certain conditions. We note also, in passing, that the operator A_n is linear.

Lemma 5.2: Let $u_{n+1}(t) \in H^{2j+1}(S^2)$ *for all* $t \in [0,T]$, and $\beta \in \Gamma^\infty(TS^2 \times [0,\infty))$. *The operator defined above by (5.10) satisfies*

$$A_n(t): H^{2j}(S^2) \times \mathbb{C}^3 \to H^{2j}(S^2) \times \mathbb{C}^3$$

and

$$\|A_n \mathcal{M}(t)\|_{H^{2j}(S^2)\times\mathbb{C}^3} \leqslant C(1 + \|u_{n+1}(t)\|_{H^{2j+1}(S^2)})\|\mathcal{M}(t)\|_{H^{2j}(S^2)\times\mathbb{C}^3},$$

for each $t \in [0,T]$ *and some constant* C *depending only on the smooth field* β. *That is to say that* $A_n(t)$ *is a uniformly bounded operator for each* n, *with norm given by*

$$\|A_n(t)\|_j = C(1 + \|u_{n+1}(t)\|_{H^{2j+1}(S^2)}).$$

Proof: Let $E^j := H^{2j}(S^2) \times \mathbb{C}^3$ and note that

$$\|A_n\mathcal{M}\|_{E^j}^2 = \|k^m[\eth(u_{n+1}\bar{\eth}Y_{1m}) + \bar{\eth}(u_{n+1}\eth Y_{1m})] - (1+\rho)\mu\|_{H^{2j}(S^2)}^2 + \|\mathcal{P}_1(\mu\eth u_{n+1})\|_{\mathbb{C}^3}^2$$
$$\leqslant 2\|k^m[\eth(u_{n+1}\bar{\eth}Y_{1m}) + \bar{\eth}(u_{n+1}\eth Y_{1m})]\|_{H^{2j}(S^2)}^2 + 2\|(1+\rho)\mu\|_{H^{2j}(S^2)}^2 + \|\mathcal{P}_1(\mu\eth u_{n+1})\|_{\mathbb{C}^3}^2.$$

Estimating the first term on the right-hand side we have

$$\|k^m[\eth(u_{n+1}\bar{\eth}Y_{1m}) + \bar{\eth}(u_{n+1}\eth Y_{1m})]\|_{H^{2j}(S^2)} \leqslant \|k^m\eth u_{n+1}\bar{\eth}Y_{1m}\|_{H^{2j}(S^2)} + \|k^m\bar{\eth}u_{n+1}\eth Y_{1m}\|_{H^{2j}(S^2)}$$
$$+ \|k^m u_{n+1}\Delta Y_{1m}\|_{H^{2j}(S^2)} \leqslant C\|u_{n+1}\|_{H^{2j+1}(S^2)}\|k\|_{\mathbb{C}^3}, \tag{5.12}$$

while for the second term we have

$$\|(1+\rho)\mu\|_{H^{2j}(S^2)} \leqslant C\|\mu\|_{H^{2j}(S^2)}. \tag{5.13}$$

The remaining term is estimated as follows:

$$\|\mathcal{P}_1(\mu\eth u_n)\|_{\mathbb{C}^3}^2 = \sum_{m=-1}^{1}\left|\oint \mu\eth u_{n+1}Y_{1m}^1\,\mathrm{d}\Omega^2\right|^2 \leqslant C\sum_{m=-1}^{1}\left(\oint|\mu\eth u_{n+1}|\,\mathrm{d}\Omega^2\right)^2 \leqslant C\|\mu\|_{L^2(S^2)}^2\|\eth u_{n+1}\|_{L^2(S^2)}^2 \tag{5.14}$$

for any $j \geqslant 0$.

Adding (5.12), (5.13), and (5.14) we obtain

$$\|A_n\mathcal{M}\|_{E^j} \leqslant C(1+\|u_{n+1}\|_{H^{2j+1}(S^2)})(\|\mu\|_{H^{2j}(S^2)} + \|k\|_{\mathbb{C}^3}),$$

as required. ■

The boundedness of a linear operator A_n, such as that just established in Lemma 5.2, is the standard property required to infer the existence of solutions of (5.9). The following result is a special case of the standard local existence result for ordinary differential equations in Banach space. See Ref. 11, for example.

Lemma 5.3: Let $E^j = H^{2j}(S^2)\times\mathbb{C}^3$, and suppose $A(t): E^j \to E^j$ is a uniformly bounded linear operator for each $t\in[0,T]$, with norm $\|A(t)\|_j$. Further suppose that $\mathcal{M}_0 \in E^j$ and $B\in L^1([0,T];E^j)$. Then there exists a unique $\mathcal{M}\in C^1([0,T];E^j)$ satisfying

$$\dot{\mathcal{M}} = A\mathcal{M} + B,$$

$$\mathcal{M}(0) = \mathcal{M}_0.$$

The boundedness of the operator A_n is also the foundation for *a priori* estimates for solutions of (5.9). The basic result is as follows.

Lemma 5.4: Let A and B satisfy the hypotheses of Lemma 5.3 and let $\mathcal{M}$ be a solution of

$$\dot{\mathcal{M}} = A\mathcal{M} + B,$$

with initial value $\mathcal{M}_0$. For all $t\in[0,T]$, we have the estimate

$$\|\mathcal{M}(t)\|_{E^j}e^{-t\|A\|_j} \leqslant \|\mathcal{M}_0\|_{E^j} + \int_0^t \|B(s)\|_{E^j}\,\mathrm{d}s.$$

Proof: We note first that $E^j = H^{2m}(S^2)\times\mathbb{C}^3$ is in fact a Hilbert space and so, fixing $t\in[0,T]$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\mathcal{M}(t)\|_{E^j}^2 = 2\langle\mathcal{M}(t),\dot{\mathcal{M}}(t)\rangle_{E^j} \leqslant 2\|\mathcal{M}(t)\|_{E^j}\|\dot{\mathcal{M}}(t)\|_{E^j}.$$

Hence we must have

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\mathcal{M}(t)\|_{Ej} \leqslant \|\dot{\mathcal{M}}(t)\|_{Ej} \leqslant \|A\mathcal{M}(t)\|_{Ej} + \|B(t)\|_{Ej} \leqslant C\|\mathcal{M}(t)\|_{Ej} + \|B(t)\|_{Ej},$$

where it is clear that the smallest such C for which this inequality holds is the norm $\|A\|_j$ of the operator A.

Gronwall's inequality then gives

$$\|\mathcal{M}(t)\|_{Ej} \leqslant e^{Ct}\left(\|\mathcal{M}_0\|_{Ej} + \int_0^t \|B(s)\|_{Ej}\,\mathrm{d}s\right)$$

as required. ■

Applying Lemmas 5.3 and 5.4 to (5.9), noting Lemma 5.2, we have the following result.

Corollary 5.5: *Suppose that* u_n, μ_n, k_n, $\hat{\eta}_n \in P^m_{0,T}$ *and* $u_{n+1} \in P^{m+1//2}_{0,T}$ *is the solution of (5.4), subject to the initial condition* $u_0 \in H^{2m}(S^2)$. *Equation (5.9), subject to the initial condition* $\mathcal{M}_{n+1}|_{t=0} = \mathcal{M}_0 \in E^m$, *defines* $\mathcal{M}_{n+1} \in C^1([0,T];E^m)$, *which satisfies*

$$\|\mathcal{M}_{n+1}(t)\|_{E^m} e^{-t\|A_n\|_m} \leqslant \|\mathcal{M}_0\|_{E^m} + \int_0^t \|B_n(s)\|_{E^m}\,\mathrm{d}s, \tag{5.15}$$

for all $t \in [0,T]$.

Proof: Since we have already assumed that $m \geqslant m_0$ we have no problem meeting the conditions $u_{n+1}(t) \in H^{2j+1}(S^2)$ and $B_n \in L^1([0,T];E^m)$. Lemma 5.3 applies and so $\mathcal{M}_{n+1}$ is uniquely defined as the solution of (5.9) with $\mathcal{M}|_{t=0} = \mathcal{M}_0$. Lemma 5.4 also applies and gives (5.15). ■

To establish the higher temporal regularity of solutions of (5.9) we will consider the following Banach spaces:

$$\mathcal{O}^m_{0,T} := P^m_{0,T} \times H^m([0,T];\mathbb{C}^3),$$

and their respective norms,

$$\|\mathcal{M}\|^2_{\mathcal{O}^m_{0,T}} = \sum_{l=0}^{m} \int_0^T \|\partial_t^l \mathcal{M}(s)\|^2_{E^{m-l}}\,\mathrm{d}s.$$

We note that upon inspection of (5.5) and (5.6), $\mathcal{O}^m_{0,T}$ is the natural space in which to look for solutions of (5.9) given $u_{n+1} \in P^{m+1/2}_{0,T}$.

To obtain the desired estimate, from which the higher regularity of solutions of (5.9) will follow, we will first need to establish some (essentially trace-type) results concerning the properties of the $P^m_{0,T}$ spaces.

Lemma 5.6: *Suppose that* $T \geqslant \epsilon > 0$. *Let* u *be a function belonging to the class* $P^{k+1/2}_{0,T}$ *with* $k \geqslant 1$. *Then*

$$\|u(\cdot,t)\|_{H^{2k}(S^2)} \leqslant C\|u\|_{P^{k+1/2}_{0,T}},$$

for any $t \in [0,T]$. *The constant depends only on* ϵ.

Proof: We first suppose that $u \in C^\infty(S^2 \times [0,T])$. We have that $u(\cdot,t) \in L^2(S^2)$, for each $t \in \mathbb{R}^+$, we may write u spectrally as follows:

$$u(x,t) = \sum_j c_j(t)\phi_j(x),$$

where the ϕ_j's form an orthonormal basis for $L^2(S^2)$ satisfying $\Delta\phi_j = -\lambda_j^2\phi_j$.

We define the function $\tilde{u}(\cdot,t) = u(\cdot,t_0+t)\chi(t)$, where χ is a smooth function satisfying

$$\chi(s) = \begin{cases} 1, & s < \dfrac{T}{4}, \\ 0, & s > \dfrac{3T}{4}, \end{cases}$$

so that $\tilde{u}(\cdot,T)=0$ and $\tilde{u}(\cdot,0)=u(\cdot,t_0)$. Then given that $k\geqslant 1$, we have

$$\begin{aligned} \|u(\cdot,t_0)\|^2_{H^{2k}(S^2)} &= \sum_j |c_j(t_0)|^2 |\lambda_j|^{2k} \\ &= \sum_j |\tilde{c}_j(0)|^2 |\lambda_j|^{2k} \\ &= \sum_j |\lambda_j|^{2k} \int_0^T \frac{\mathrm{d}}{\mathrm{d}s} |\tilde{c}_j(s)|^2 \,\mathrm{d}s \\ &\leqslant \sum_j \int_0^T |\tilde{c}_j(s)|^2 |\lambda_j|^{2k+1} + |\dot{\tilde{c}}_j(s)|^2 |\lambda_j|^{2k-1} \,\mathrm{d}s \leqslant \|\tilde{u}\|^2_{P^{k+1/2}_{0,T}} \leqslant C\|u\|^2_{P^{k+1/2}_{0,T}}. \end{aligned}$$

Note that the constant depends only on the cutoff function χ. With the result now established for smooth functions it is an easy matter to get the result for $u\in P^{k+1/2}_{0,T}$; it follows, after mollifying u, by a standard approximation argument. ■

Corollary 5.7: *Suppose that* $T\geqslant\epsilon>0$. *Let u belong to the class* $P^{m+1/2}_{0,T}$, *then*

$$\|\partial_t^j u(\cdot,t)\|_{H^{2(m-j)}(S^2)} \leqslant C\|u\|_{P^{m+1/2}_{0,T}},$$

for all $j\leqslant m$ *and* $t\in[0,T]$. *The constant depends only on* ϵ.

Proof: We note that $u\in P^{m+1/2}_{0,T}$ means that $\partial_t^j u\in P^{m-j+1/2}_{0,T}$ and so applying Lemma 5.6 with $k=m-j$ we have the result. ■

In the above trace-type results we saw that we may control the spatial norms of time derivatives of functions, by a constant multiple of the $P^{m+1/2}_{0,T}$-norm. Unfortunately the constant's dependence upon ϵ means that we lose that control as ϵ approaches zero. The following result shows how, with the loss of one time derivative of regularity, we may control the spatial norms of time derivatives by a constant which approaches zero as we consider smaller and smaller time intervals.

Lemma 5.8: *Let* $u\in P^{k+1}_{0,T}$, *with* $k\geqslant 0$, *then*

$$\|u(t)\|^2_{H^{2k}(S^2)} \leqslant \|u_0\|^2_{H^{2k}(S^2)} + CT\|u\|^2_{P^{k+1}_{0,T}},$$

for any $t\in[0,T]$. *The constant C depends only on k*.

Proof: Fixing $\xi\in S^2$, we have

$$u(\xi,t) = u(\xi,0) + \int_0^t \partial_t u(\xi,s)\mathrm{d}s.$$

It follows, using the Hölder inequality, that

$$|\nabla^{2j}(u(\xi,t)-u_0(\xi))| \leqslant \sqrt{T}\left(\int_0^T |\partial_t \nabla^{2j} u(\xi,s)|^2 \,\mathrm{d}s\right)^{1/2}$$

for any $0\leqslant j\leqslant m$ and $t\in[0,T]$. Integrating this result gives

$$\|u(\cdot,t)-u_0\|^2_{H^{2k}(S^2)} \leqslant C\oint |\nabla^{2k}(u-u_0)|^2+|u-u_0|^2\,\mathrm{d}\mu_g$$
$$\leqslant \oint T\int_0^T |\partial_t u|^2+|\partial_t\nabla^{2k}u|^2\,\mathrm{d}t\,\mathrm{d}\mu_g \leqslant T\|u\|^2_{P^{k+1}_{0,T}}.$$

The result follows after observing the elementary inequality $\|x\|-\|y\|\leqslant\|x-y\|$. ■

Remark: Applying Lemma 5.8 to $\partial_t^l u$ gives

$$\|\partial_t^l u(t)\|^2_{H^{2(k-l)}(S^2)} \leqslant \|\partial_t^l u(0)\|^2_{H^{2(k-l)}(S^2)} + CT\|u\|^2_{P^{k+1}_{0,T}}.$$

If it happened that u was also the solution of say a parabolic equation, then we could reduce the above estimate to

$$\|\partial_t^l u(t)\|^2_{H^{2(k-l)}(S^2)} \leqslant C\Big(\|u_0\|^2_{H^{2k}(S^2)} + T\|u\|^2_{P^{k+1}_{0,T}}\Big),$$

where the constant C now depends on the coefficients and source functions appearing in the parabolic equation.

We now proceed to derive the basic $\mathcal{O}^m_{0,T}$ *a priori* estimates for $\mathcal{M}_{n+1}$, the solutions of (5.9).

Proposition 5.9: Suppose $u_{n+1}\in P^{m+1/2}_{0,T}$ *and let* $\mathcal{M}_{n+1}$ *be the solution of* (5.9). *Then* $\mathcal{M}_{n+1}$ *satisfies the inequality*,

$$\|\mathcal{M}_{n+1}\|^2_{\mathcal{O}^m_{0,T}} \leqslant TC\Big\{1+\|B_n\|^2_{\mathcal{O}^m_{0,T}}\Big\}. \tag{5.16}$$

The constant C depends on $\|u_{n+1}\|_{P^{m+1/2}_{0,T}}$, $\|u_0\|_{H^{2m}(S^2)}$ *and* $\|\mathcal{M}_0\|_{E^m}$.

Proof: We begin by noting that if we square, then integrate (5.15), we obtain

$$\int_0^T \|\mathcal{M}_{n+1}(t)\|^2_{E^m}\,\mathrm{d}t \leqslant 2Te^{TC}\Big(\|\mathcal{M}_0\|^2_{E^m}+\|B_n\|^2_{\mathcal{O}^m_{0,T}}\Big), \tag{5.17}$$

where the constant C depends on $\|u_{n+1}\|_{P^{m+1/2}_{0,T}}$. This gives us a bound for the first term in the sum

$$\|\mathcal{M}_{n+1}\|^2_{\mathcal{O}^m_{0,T}} = \sum_{l=0}^m \int_0^T \|\partial_t^l\mathcal{M}_{n+1}\|^2_{E^{m-l}}\,\mathrm{d}t. \tag{5.18}$$

Considering the $(j+1)^{\text{th}}$ term in (5.18) we have, upon differentiating (5.24),

$$\int_0^T \|\partial_t^j\mathcal{M}_{n+1}\|^2_{E^{m-j}}\,\mathrm{d}t \leqslant \int_0^T C_j\sum_{l=0}^{j-1}\|\partial_t^l A_n\partial_t^{j-l-1}\mathcal{M}_{n+1}\|^2_{E^{m-j}}+\|\partial_t^{j-1}B_n\|^2_{E^{m-j}}\,\mathrm{d}t, \tag{5.19}$$

where C_j is a constant dependent upon j. The expression $\partial_t^l A_n\partial_t^{j-l-1}\mathcal{M}_{n+1}$ represents the outcome of the operator $\partial_t^l A_n$, given by (5.10) with u_{n+1} replaced by $\partial_t^l u_{n+1}$, acting on $\partial_t^{j-l-1}\mathcal{M}_{n+1}$. It is obvious that results analagous to Lemma 5.2 exist for $\partial_t^l A_n$ as well. Hence

$$\|\partial_t^l A_n\partial_t^{j-l-1}\mathcal{M}_{n+1}\|^2_{E^{m-j}} \leqslant C_l\|\partial_t^{j-l-1}\mathcal{M}_{n+1}\|^2_{E^{m-j}},$$

where, by virtue of Lemma 5.8, we see that

$$C_l \leqslant C\Big(\|u_0\|^2_{H^{2m}(S^2)}+T\|u_{n+1}\|^2_{P^{m+1/2}_{0,T}}\Big),$$

where we have used the fact that u_{n+1} is the solution of (4.8) to control the initial values of the time derivatives of u_{n+1}.

Observing that Lemma 5.8 may easily be extended to apply to the E^{m-j} and $\mathcal{O}^m_{0,T}$ spaces, the second term on the right-hand side of (5.19) satisfies

$$\|\partial_t^{j-1}B_n(\cdot,s)\|^2_{E^{m-j}} \leqslant \mathcal{C}\Big(1+T\|B_n\|^2_{\mathcal{O}^m_{0,T}}\Big),$$

for all $s\leqslant T$. The constant $\mathcal{C}$ depends on $\|\partial_t^{j-1}B_n(\cdot,0)\|_{E^{m-j}}$. This quantity can be expressed in terms of E^{m-j}-norms of the $(j-1)$th time derivatives of u_{n+1}, μ_n, k_n, and $\hat{\eta}_n$ evaluated at $t=0$. Since these functions are themselves solutions of their respective equations, we may in turn express time derivatives of u_{n+1}, μ_n, k_n, and $\hat{\eta}_n$, evaluated at $t=0$, in terms of the initial values u_0, μ_0, and k_0. We therefore have

$$\begin{aligned}\int_0^T \|\partial_t^j\mathcal{M}_{n+1}\|^2_{E^{m-j}}\,\mathrm{d}t &\leqslant C\sum_{l=0}^{j-1}\int_0^T \|\partial_t^{j-l-1}\mathcal{M}_{n+1}\|^2_{E^{m-j}} + T\|B_n\|^2_{\mathcal{O}^m_{0,T}} + 1\,\mathrm{d}t\\ &\leqslant CT\Big(1+T\|B_n\|^2_{\mathcal{O}^m_{0,T}}\Big) + C\sum_{l=0}^{j-1}\int_0^T \|\partial_t^{j-l-1}\mathcal{M}_{n+1}\|^2_{E^{m-j}}\,\mathrm{d}t, \qquad (5.20)\end{aligned}$$

where C depends on $\|u_{n+1}\|_{P^{m+1/2}_{0,T}}$, $\|u_0\|_{H^{2m-1}(S^2)}$, $\|\mu_0\|_{H^{2(m-1)}(S^2)}$, and $\|k_0\|_{\mathbb{C}^3}$.

The estimate (5.16) is then obtained by using (5.20) to iterate from $j=1$ to m starting from (5.17). ■

Thus in light of Lemma 5.3 and Proposition 5.9, we find that if $u_0\in H^{2m}(S^2)$, $\mathcal{M}_0\in E^m$, $u_n\in P^{m+1/2}_{0,T}$, $u_{n+1}\in P^{m+1/2}_{0,T}$, and $\mathcal{M}_n\in\mathcal{O}^m_{0,T}$ then $\mathcal{M}_{n+1}$ exists and belongs to $\mathcal{O}^m_{0,T}$.

Moving now to the final equation in the iteration scheme, the elliptic system for $\hat{\eta}_{n+1}$. We note again that by construction (5.7) is guaranteed to have a solution. Hence $\hat{\eta}_{n+1}$ exists and the following results establish that $\hat{\eta}_{n+1}\in P^m_{0,T}$ provided $(u_{n+1},\mathcal{M}_{n+1})\in P^{m+1/2}_{0,T}\times\mathcal{O}^m_{0,T}$.

Lemma 5.10: Suppose $g\in L^2(\mathrm{span}\{Y^1_{lm}: l\geqslant 2\})$ *and let* $\hat{\eta}$ *be the solution of*

$$\bar{\eth}\,\hat{\eta} = g. \qquad (5.21)$$

We have the estimate

$$\|\hat{\eta}\|^2_{H^1(S^2)} \leqslant C\|g\|^2_{L^2(S^2)},$$

where C is a constant.

Proof: The result follows easily from the observation that since $\bar{\eth}\,\hat{\eta}$ is devoid of $l=1$ spherical harmonics, we may solve (5.21). Moreover, we are able to write $\hat{\eta}$ explicitly, using spectral decomposition as

$$\hat{\eta} = \sum_{l=2}^{\infty}\sum_{m=-l}^{l}\hat{\eta}_{lm}Y^2_{lm}.$$

It follows that we may write

$$\bar{\eth}\,\hat{\eta} = \sum_{l=2}^{\infty}\sum_{m=-l}^{l}C_l\hat{\eta}_{lm}Y^1_{lm},$$

where C_l, $l=0,2,3,\ldots$ are constants. Checking the norms in question we then find

$$\|\bar{\eth}\,\hat{\eta}\|^2_{L^2(S^2)} = \oint\left|\sum_{l,m}C_l\hat{\eta}_{lm}Y^1_{lm}\right|^2\mathrm{d}\Omega^2 \geqslant \sum_{l,m}C_l^2\hat{\eta}^2_{lm},$$

and

$$\|\hat{\eta}\|^2_{H^1(S^2)} = \oint|\nabla\hat{\eta}|^2 + |\hat{\eta}|^2\,\mathrm{d}\Omega^2 \leqslant \oint 2|\bar{\eth}\,\hat{\eta}|^2 + |\hat{\eta}|^2\,\mathrm{d}\Omega^2 \leqslant C\sum_{l,m}C_l^2\hat{\eta}^2_{lm}.$$

Thus we have

$$\|\hat{\eta}\|^2_{H^1(S^2)} \leqslant C\sum_{l,m} C_l^2 \hat{\eta}^2_{lm} \leqslant C\|\bar{\eth}\hat{\eta}\|^2_{L^2(S^2)},$$

and the result follows from Eq. (5.21). ■

Lemma 5.11: Suppose $\hat{\eta}$ is a solution of (5.21), where now $g \in H^k(\mathrm{span}\{Y^1_{lm} : l \geqslant 2\})$. We have the estimate

$$\|\hat{\eta}\|^2_{H^{k+1}(S^2)} \leqslant C_k \|g\|^2_{H^k(S^2)}, \tag{5.22}$$

where C_k is a constant depending only on k.

Proof: Estimating the right-hand side of (5.22) we have

$$\begin{aligned}
\|\hat{\eta}\|^2_{H^{k+1}(S^2)} &= \|\nabla^{k+1}\eta\|^2_{L^2(S^2)} + \|\hat{\eta}\|^2_{H^k(S^2)} \\
&\leqslant \|\nabla^k \hat{\eta}\|^2_{H^1(S^2)} + C_k\|\bar{\eth}\hat{\eta}\|^2_{H^{k-1}(S^2)} \\
&\leqslant C\|\bar{\eth}\nabla^k\eta\|^2_{L^2(S^2)} + C_k\|\bar{\eth}\hat{\eta}\|^2_{H^k(S^2)} \\
&= C\|\nabla^k\bar{\eth}\hat{\eta}\|^2_{L^2(S^2)} + C'_k\|\bar{\eth}\hat{\eta}\|^2_{H^k(S^2)} \leqslant C\|\bar{\eth}\hat{\eta}\|^2_{H^k(S^2)} + C'_k\|\bar{\eth}\hat{\eta}\|^2_{H^k(S^2)} \leqslant C''_k\|\bar{\eth}\hat{\eta}\|^2_{H^k(S^2)}.
\end{aligned}$$

The result follows from Eq. (5.21). ■

The following result is now immediate from the definition of $P^k_{0,T}$.

Corollary 5.12: Let g, belonging to the class $P^k_{0,T}$, be devoid of $l=1$ spherical harmonic components so that $\hat{\eta}$ exists as a solution of (5.21). Then

$$\|\hat{\eta}\|_{P^{k+1/2}_{0,T}} \leqslant C_k\|g\|_{P^k_{0,T}}.$$

C_k is a constant depending only on k.

The foregoing results have shown that if,

$$(u_n, \mu_n, k_n, \hat{\eta}_n) \in P^{m+1/2}_{0,T} \times \mathcal{O}^m_{0,T} \times P^m_{0,T}$$

and

$$(u_0, \mu_0, k_0) \in H^{2m+1}(S^2) \times E^{m+1/2}$$

then

$$(u_{n+1}, \mu_{n+1}, k_{n+1}, \hat{\eta}_{n+1}) \in P^{m+1/2}_{0,T} \times \mathcal{O}^m_{0,T} \times P^m_{0,T}$$

also.

For the sake of brevity we consider the four iterates as a single entity residing in the appropriate Banach space. In particular we define the four-tuple,

$$\mathbf{U}_n := (u_n, \mu_n, k_n, \hat{\eta}_n),$$

residing in the Banach space,

$$\Psi^m_{0,T} := P^{m+1/2}_{0,T} \times P^m_{0,T} \times H^m([0,T];\mathbb{C}^3) \times P^m_{0,T}.$$

To summarize, we have proven the following result.

Theorem 5.13: *Let $m \geqslant m_0$ and let $u_0 \in H^{2m+1}(S^2)$, $\mu_0 \in H^{2m}(S^2)$, and $k_0 \in \mathbb{C}^3$. There exists a nonincreasing, but possibly decreasing sequence $\{T_n\}_{n=1}^{\infty}$ with $T_n > 0$, and a sequence of iterates $\mathbf{U}_n \in \Psi^m_{0,T_n}$ which satisfy (5.4)–(5.7).*

Theorem 5.13 is not ideal. It tells us that the iterates exist as elements of Ψ^m_{0,T_n}, with the possibilty of $T_n \to 0$. To be able to prove local existence for the QSECS however, we will need the

iterates to be defined over some nonzero time interval. This means that we will need to show that there exists an $\epsilon > 0$ such that $T_n \geqslant \epsilon$, for all n. This fact will follow from the uniform estimates we derive for the iterates in the next section.

C. Uniform estimates for the iterates

In this section we will show that all of the iterates satisfy uniform bounds, at least locally in time. We consider the iteration scheme proposed by (5.4)–(5.7), which we may write more simply as

$$\dot{u}_{n+1} = \hat{\gamma} u_n^2 \Delta u_{n+1} + F_n, \tag{5.23}$$

$$\dot{\mathcal{M}}_{n+1} = A_n \mathcal{M}_{n+1} + B_n, \tag{5.24}$$

$$\bar{\eth}\,\hat{\eta}_{n+1} = \mathcal{L}(u_{n+1}, \mathcal{M}_{n+1}) - \dot{\sigma}, \tag{5.25}$$

where A_n and B_n are defined by (5.10) and (5.11), respectively, and where

$$F_n = \tfrac{1}{2}\Big(1 + \tfrac{1}{2}\gamma e^{2t}\|\hat{\eta}_n\|^2 + \gamma B\Big)u_n - \hat{\gamma}\Big(1 - \tfrac{1}{2}e^{2t}\Big(16\pi T_{00} + 2\|\kappa_n\|^2 + \tfrac{3}{2}\mu_n^2 - 2\mu_n H\Big)\Big)u_n^3 \tag{5.26}$$

and

$$\mathcal{L}(u, \mathcal{M}) = (1 - \mathcal{P}_1)\Big\{\mu \eth u + \tfrac{1}{2}\eth(u\mu) - \eth(uH) + (1 + \rho)\kappa + \bar{\kappa}\eth\beta + \kappa\eth\bar{\beta} + 8\pi T_0 u e^t\Big\}. \tag{5.27}$$

The key result needed to prove that the iterates satisfy uniform bounds is the following simple inequality.

Lemma 5.14: Suppose u belongs to the localized parabolic space $P^1_{0,T}$. Then

$$\|u\|^2_{P^0_{0,T}} \leqslant 2T\Big(\|u_0\|^2_{L^2(S^2)} + \|u\|^2_{P^1_{0,T}}\Big).$$

Proof: From the definition of $P^0_{0,T}$ we have

$$\|u - u_0\|^2_{P^0_{0,T}} \leqslant \int_0^T \oint \int_0^t |\partial_t u(\xi, s)|^2 \, \mathrm{d}s \, \mathrm{d}\mu_{\bar{g}} \mathrm{d}t \leqslant \int_0^T (T - s) \oint |\partial_t u(\xi, s)|^2 \, \mathrm{d}\mu_{\bar{g}} \mathrm{d}s \leqslant T\|\partial_t u\|^2_{P^0_{0,T}}.$$

The result then follows since $\|u_0\|^2_{P^0_{0,T}} = T\|u_0\|^2_{L^2(S^2)}$.

Corollary 5.15: Any $u \in P^{m+1}_{0,T}$ satisfies the estimate

$$\|u\|^2_{P^m_{0,T}} \leqslant CT\Big(1 + \|u\|^2_{P^{m+1}_{0,T}}\Big). \tag{5.28}$$

The constant C depends on m and $\|\partial_t^j u(\cdot, 0)\|_{H^{2(m-j)}(S^2)}$, $j = 0, \ldots, m$.

Proof: We need only check terms of the form $\int_0^T \|\partial_t^j u\|^2_{H^{2(m-j)}(S^2)} \, \mathrm{d}t$. We have

$$\int_0^T \|\partial_t^j u\|^2_{H^{2(m-j)}(S^2)} \, \mathrm{d}t \leqslant C \int_0^T \|\partial_t^j \nabla^{2(m-j)} u\|^2_{L^2(S^2)} + \|\partial_t^j u\|^2_{L^2(S^2)} \, \mathrm{d}t$$

$$= C\Big(\|\partial_t^j \nabla^{2(m-j)} u\|^2_{P^0_{0,T}} + \|\partial_t^j u\|^2_{P^0_{0,T}}\Big) \leqslant 4CT\Big(\|\partial_t^j u(\cdot, 0)\|_{H^{2(m-j)}(S^2)} + \|u\|^2_{P^{m+1}_{0,T}}\Big).$$

The estimate (5.28) is then obtained by summing the terms above from $j = 0$ to m. ■

Remark: If we also know that u is a solution of a parabolic equation we may express the constant C in terms of the initial values of u, the coefficients and source function. In particular, if u_n is the solution of (5.4) we have

$$\|u_n\|^2_{P^m_{0,T}} \leqslant T\mathcal{C}\left(1+\|u_n\|^2_{P^{m+1}_{0,T}}\right), \tag{5.29}$$

where the constant $\mathcal{C}$ depends on m, $\|u_0\|_{H^{2m}(S^2)}$, $\|\mu_0\|_{H^{2m}(S^2)}$, and $\|k_0\|_{\mathbb{C}^3}$.

We now prove that given suitable bounds on the initial data (which constitute $\mathbf{U}_0$), all the iterates $\{\mathbf{U}_n\}_{n=0}^{\infty}$ may be confined within a ball in $\Psi^m_{0,T}$, for some $T>0$.

Proposition 5.16: Let $m\geqslant m_0$ and suppose $u_0\in H^{2m+1}(S^2)$, $\mu_0\in H^{2m}(S^2)$, and $k_0\in\mathbb{C}^3$. There exists $T^*>0$ and $N>0$, depending only on m, the initial data and the prescribable fields, such that

$$\|\mathbf{U}_n\|_{\Psi^m_{0,T^*}} \leqslant N$$

for all $n\in\mathbb{N}$.

Proof: Since $u_0\in H^{2m+1}(S^2)$, $\mu_0\in H^{2m}(S^2)$, and $k_0\in\mathbb{C}^3$, there exist numbers N_1, N_2, N_3, and N_4 such that

$$\|u_0\|_{H^{2m+1}(S^2)} \leqslant N_1, \quad \|\mu_0\|_{H^{2m}(S^2)} \leqslant N_2, \quad \|k_0\|_{\mathbb{C}^3} \leqslant N_3, \quad \|\hat{\eta}_0\|_{H^{2m}(S^2)} \leqslant N_4. \tag{5.30}$$

Defining the zeroth iterates as the time constant extensions of these initial values and assuming, without loss of generality, that $T\leqslant 1$ we find that (5.30) implies

$$\|u_{\tilde{0}}\|_{P^{m+1/2}_{0,T}} \leqslant N_1, \quad \|\mu_{\tilde{0}}\|_{P^m_{0,T}} \leqslant N_2, \quad \|k_{\tilde{0}}\|_{H^m([0,T];\mathbb{C}^3)} \leqslant N_3, \quad \|\hat{\eta}_{\tilde{0}}\|_{P^m_{0,T}} \leqslant N_4,$$

where we have used the subscript $\tilde{0}$ to distinguish the zeroth iterates $u_{\tilde{0}}$, $\mu_{\tilde{0}}$, $k_{\tilde{0}}$, and $\hat{\eta}_{\tilde{0}}$ from the intial values u_0, μ_0, k_0, and $\hat{\eta}_0$. Hence Proposition 5.16 holds for $n=\tilde{0}$, with $N=\Sigma_{i=1}^4 N_i$.

Hypothesizing then, that

$$\|u_j\|_{P^{m+1/2}_{0,T}} \leqslant N_1, \quad \|\mu_j\|_{P^m_{0,T}} \leqslant N_2, \quad \|k_j\|_{H^m([0,T];\mathbb{C}^3)} \leqslant N_3, \quad \|\hat{\eta}_j\|_{P^m_{0,T}} \leqslant N_4,$$

for all $j\in[0,n]_{\mathbb{N}}$ and some $T>0$, we aim to show the same is true for the $(n+1)$th iterates.

We consider (5.23), which is a linear parabolic equation for u_{n+1}. Since $m\geqslant m_0$, (5.3) gives

$$\|u_{n+1}\|^2_{P^{m+1/2}_{0,T_1}} \leqslant \mathcal{Q}\left(\|u_0\|^2_{H^{2m}(S^2)}+\|F_n\|^2_{P^{m-1/2}_{0,T_1}}\right).$$

We note that the constant $\mathcal{Q}$ depends on the P^m_{0,T_1} norm of the coefficients, which in this case, observing (5.8), amount to u_n. Hence

$$\mathcal{Q}=\mathcal{Q}(\|u_n\|_{P^m_{0,T_1}}).$$

However, since u_n is itself the solution of a linear parabolic equation, (5.29) applies and we have

$$\|u_n\|^2_{P^m_{0,T_1}} \leqslant T_1\mathcal{C}\left(1+\|u_n\|^2_{P^{m+1}_{0,T_1}}\right). \tag{5.31}$$

Moreover, by inspection of the proof of (Ref. 15, Theorem 4.6, p. 132), it can be seen that the constant $\mathcal{Q}$ depends on $\|u_n\|_{P^m_{0,T_1}}$ in such a way that, if $\|u_n\|_{P^m_{0,T_1}}$ is bounded as in (5.31), then $\mathcal{Q}(\|u_n\|_{P^m_{0,T_1}})$ is also bounded and satisfies the inequality

$$\mathcal{Q}(\|u_n\|_{P^m_{0,T_1}}) \leqslant T_1\tilde{\mathcal{Q}}, \tag{5.32}$$

where the constant $\tilde{\mathcal{Q}}$ depends on $\|u_n\|_{P^{m+1}_{0,T_1}}$.

The P^{m+1}_{0,T_1} norm of u_n can also be estimated using (5.3),

$$\|u_n\|^2_{P^{m+1}_{0,T_1}} \leqslant \mathcal{Q}^*\left(\|u_0\|^2_{H^{2m+1}(S^2)} + \|F_n\|^2_{P^m_{0,T_1}}\right). \tag{5.33}$$

The constant $\mathcal{Q}^*$ depends only on $\|u_{n-1}\|_{P^{m+1/2}_{0,T_1}}$ which by hypothesis is less than N_1. Similarly, $\|F_n\|^2_{P^m_{0,T_1}}$ can be controlled by a constant depending on N_1, N_2, N_3, N_4 and the prescribable fields. Hence $\|u_n\|_{P^{m+1}_{0,T_1}}$ is bounded by a constant that depends only on N_1, N_2, N_3, N_4 and the prescribable fields also. This in turn implies that the constant $\tilde{\mathcal{Q}}$ is also bounded by a term involving only N_1, N_2, N_3, N_4 and the norms of the prescribable fields.

The above argument implies that, given the induction hypotheses, if we take $T_1 \leqslant T$ then

$$\|u_{n+1}\|^2_{P^{m+1/2}_{0,T_1}} \leqslant T_1 C_1, \tag{5.34}$$

where C_1 is a constant depending on the prescribable fields, N_1, N_2, N_3, and N_4. Thus provided that

$$T_1 \leqslant \min\left\{T, \frac{N_1^2}{C_1}\right\}$$

we have

$$\|u_{n+1}\|_{P^{m+1/2}_{0,T_1}} \leqslant N_1. \tag{5.35}$$

Turning our attention now to (5.24), Proposition 5.9 gives

$$\|\mathcal{M}_{n+1}\|^2_{\mathcal{O}^m_{0,T_2}} \leqslant C T_2\left(1 + \|B_n\|^2_{\mathcal{O}^m_{0,t_2}}\right)$$

provided that $T_2 \leqslant T_1$. By hypothesis again, we can control the $\mathcal{O}^m_{0,T_2}$ norm of B_n by a constant depending on N_1, N_2, N_3, and N_4. That is,

$$\|\mathcal{M}_{n+1}\|^2_{\mathcal{O}^m_{0,T_2}} \leqslant T_2 C_2. \tag{5.36}$$

Therefore, so long as

$$T_2 \leqslant \min\left\{T_1, \frac{N_2^2}{C_2}, \frac{N_3^2}{C_2}\right\},$$

we have

$$\|\mu_{n+1}\|_{P^m_{0,T_2}} \leqslant N_2, \quad \text{and } \|k_{n+1}\|_{H^m([0,T_2];\mathbb{C}^3)} \leqslant N_3. \tag{5.37}$$

Finally, from Corollary 5.12, we have

$$\|\hat{\eta}_{n+1}\|_{P^m_{0,T_3}} \leqslant C_m \|\bar{\eth}\hat{\eta}_{n+1}\|_{P^{m-1/2}_{0,T_3}} \leqslant C_m \|\mathcal{L}(u_{n+1}, \mathcal{M}_{n+1}) - \dot{\sigma}\|_{P^{m-1/2}_{0,T_3}}.$$

Observing (5.27), we thus find that

$$\|\hat{\eta}_{n+1}\|^2_{P^m_{0,t_3}} \leqslant C\left(\|u_{n+1}\|^2_{P^m_{0,T_3}} + \|\mu_{n+1}\|^2_{P^m_{0,T_3}} + \|k_{n+1}\|^2_{H^m([0,T_3];\mathbb{C}^3)} + \|\sigma\|^2_{P^{m+1/2}_{0,T_3}}\right) \leqslant T_3 C_3 + C_4 \|\sigma\|^2_{P^{m+1/2}_{0,T}},$$

provided that $T_3 \leqslant T_2$, so that our use of (5.34) and (5.36) is justified. The constant C_3 depends only on the prescribable fields, N_1, N_2, and N_3 and the constant C_4 depends only on the prescribable fields.

Hence, given that

$$T_3 \leqslant \min\left\{ T_2, \frac{N_4^2 - C_4\|\sigma\|^2_{P^{m+1/2}_{0,T}}}{C_3} \right\},$$

we find that

$$\|\hat{\eta}_{n+1}\|_{P^m_{0,T_3}} \leqslant N_4. \tag{5.38}$$

Note that we require $N_4^2 > C_4\|\sigma\|^2_{P^{m+1/2}_{0,T}}$, but this is easily arranged.

Hence, setting $T^* = T_3$, (5.35), (5.37), and (5.38) imply $\|u_{n+1}\|_{P^{m+1/2}_{0,T^*}} \leqslant N_1$, $\|\mu_{n+1}\|_{P^m_{0,T^*}} \leqslant N_2$, $\|k_{n+1}\|_{H^m([0,T^*];\mathbb{C}^3)} \leqslant N_3$, and $\|\hat{\eta}_{n+1}\|_{P^m_{0,T^*}} \leqslant N_4$. The result follows by induction with $N = \Sigma_{i=1}^4 N_i$. ■

This last result has bearing on the problem encountered in Theorem 5.13. There we found that, due to the possibility that u_n might become negative after some ever decreasing interval of time, the iterates were possibly only defined on the interval $[0, T_n]$ with $T_n \to 0$. Now that we have uniform bounds for all of the iterates in a Sobolev space of high enough order, however, we may conclude that the supremum of $|\partial_t u_n|$ over $S^2 \times [0, T^*]$ is no greater than N_1. This leads to the following result.

Theorem 5.17: *Let $m \geqslant m_0$ and let $u_0 \in H^{2m+1}(S^2)$ satisfy $\inf_{S^2} u_0 \geqslant 2\delta > 0$. Also suppose $\mu_0 \in H^{2m}(S^2)$ and $k_0 \in \mathbb{C}^3$. There exists a $T > 0$, depending on the initial values and prescribable fields, such that u_n, as defined by (5.4), satisfies*

$$\inf_{S^2 \times [0,T]} u_n \geqslant \delta.$$

Hence there exists a sequence of iterates $\{\mathbf{U}_n\}_{n=0}^{\infty} \subset \Psi^m_{0,T}$ which satisfy (5.4)–(5.7) and $\|\mathbf{U}_n\|_{\Psi^m_{0,T}} \leqslant N$.

Proof: We already mentioned above that $\sup_{S^2 \times [0,T]} |\partial_t u_n| \leqslant N_1$. This fact implies that $\inf_{S^2 \times [0, \delta/N_1]} u_n \geqslant \delta$, since

$$u_n(\xi, t) = u_n(\xi, 0) + \int_0^t \partial_t u_n(\xi, s)\mathrm{d}s \geqslant 2\delta - T \sup_{S^2 \times [0,T]} |\partial_t u_n| \geqslant 2\delta - TN_1 \geqslant \delta$$

if $T \leqslant \delta / N_1$. ■

D. Convergence of the iteration scheme

The uniform bounds obtained in Proposition 5.16 will now be used to prove that $\{\mathbf{U}_n\}_{n=0}^{\infty}$ is a Cauchy sequence in an appropriate Banach space. The Banach space we will aim to show convergence in $\Psi^1_{0,T}$, for some appropriate $T > 0$. This will be enough to infer the existence of strong local solutions to the quasispherical constraint system; the higher regularity of these solutions will follow from Proposition 5.16. In what follows we will use the shorthand notation $f(t) = f(\cdot, t)$.

If we define

$$w_{n+1} = u_{n+1} - u_n,$$

then w_{n+1} satisfies the following equation:

$$\dot{w}_{n+1} = \gamma u_n^2 \Delta w_{n+1} + \gamma w_n \overline{w}_n \Delta u_n + F_n - F_{n-1}, \tag{5.39}$$

where $\overline{w}_n = u_n + u_{n-1}$ and where F_n is given by (5.26).

Estimating the $H^3(S^2)$-norm of w_{n+1} we have

$$\tfrac{1}{2}\partial_t\|\nabla^3 w_{n+1}\|^2_{L^2(S^2)} = \oint \nabla^3 w_{n+1}\nabla^3\dot{w}_{n+1}\,\mathrm{d}\Omega^2 = \oint \nabla^3 w_{n+1}\nabla^3(\gamma u_n^2\Delta w_{n+1} + \gamma w_n\overline{w}_n\Delta u_n + F_n - F_{n-1})\mathrm{d}\Omega^2.$$

It is apparent upon inspection of this expression, that the highest order derivatives are fourth order (integrating by parts wherever necessary). Using the parabolic Sobolev imbedding (Ref. 14, Lemma 3.3.5), Proposition 5.16 gives us pointwise bounds for all such derivatives, and it is an easy matter to obtain an expression of the form

$$\partial_t\|\nabla^3 w_{n+1}(t)\|^2_{L^2(S^2)} \leqslant C_1\|w_{n+1}(t)\|^2_{H^3(S^2)} + C_2\|w_n(t)\|^2_{H^3(S^2)}.$$

This expression should only be considered true if $t\in[0,T^*]$. The constants C_1 and C_2 depend on the prescribable fields and N.

Estimating $\partial_t\|\nabla^2 w_{n+1}(t)\|^2_{L^2(S^2)}$, $\partial_t\|\nabla w_{n+1}(t)\|^2_{L^2(S^2)}$, and $\partial_t\|w_{n+1}(t)\|^2_{L^2(S^2)}$ in the same way, we find

$$\partial_t\|w_{n+1}(t)\|^2_{H^3(S^2)} \leqslant C_1'\Big(\|w_{n+1}(t)\|^2_{H^3(S^2)} + \|w_n(t)\|^2_{H^3(S^2)}\Big), \tag{5.40}$$

for all $t\in[0,T^*]$.

To obtain a similar sort of control over the other fields let us also define the following differences:

$$\upsilon_{n+1} = \mu_{n+1} - \mu_n,$$

$$q_{n+1} = k_{n+1} - k_n,$$

$$\chi_{n+1} = \hat{\eta}_{n+1} - \hat{\eta}_n.$$

Then since the iterative system defining these quantities is linear it is a simple matter to show that υ_{n+1}, q_{n+1}, and χ_{n+1} satisfy the following equations:

$$\dot{\upsilon}_{n+1} = \mathrm{div}(u_{n+1}q_{n+1}) + \mathrm{div}(w_{n+1}k_n) + \mathrm{div}(w_{n+1}\sigma) - (1+\rho)\upsilon_{n+1} - w_n u_n^{-1}u_{n-1}^{-1}\hat{\eta}_n^{AB}\nabla_{(B}\beta_{A)} + u_n^{-1}\chi_n\nabla_{(B}\beta_{A)} - 8\pi T_{03}\mathrm{e}^t w_{n+1}, \tag{5.41}$$

$$\dot{q}_{n+1} = -\mathcal{P}_1\big\{\mu_{n+1}\eth w_{n+1} + \upsilon_{n+1}\eth u_n + \tfrac{1}{2}\eth(u_{n+1}\upsilon_n) + \tfrac{1}{2}\eth(w_{n+1}\mu_{n-1}) - \eth(w_{n+1}H) + (1+\rho)q_n + \overline{q}_n\eth\beta + q_n\eth\overline{\beta} + 8\pi T_0 e^t w_{n+1}\big\}, \tag{5.42}$$

$$\overline{\eth}\chi_{n+1} = (1-\mathcal{P}_1)\big\{\upsilon_{n+1}\eth u_{n+1} + \mu_n\eth w_{n+1} + \tfrac{1}{2}\eth(u_{n+1}\upsilon_{n+1}) + \tfrac{1}{2}\eth(u_n\upsilon_{n+1}) - \eth(w_{n+1}H) + (1+\rho)q_{n+1} + \overline{q}_{n+1}\eth\beta + q_{n+1}\eth\overline{\beta} + 8\pi T_0\mathrm{e}^t w_{n+1}\big\}. \tag{5.43}$$

Focusing on (5.41), we may again use Proposition 5.16 to infer pointwise control over spatial derivatives of up to third order. Estimating the $H^2(S^2)$-norm of $\upsilon_{n+1}(t)$, we then have

$$\begin{aligned}\partial_t\|\nabla^2\upsilon_{n+1}(t)\|^2_{L^2(S^2)} &= 2\oint \nabla^2\upsilon_{n+1}(t)\nabla^2\dot{\upsilon}_{n+1}(t)\mathrm{d}\Omega^2\\ &\leqslant C_1\|\upsilon_{n+1}(t)\|^2_{H^2(S^2)} + C_2\|w_{n+1}(t)\|^2_{H^3(S^2)}\\ &\quad + C_3\|q_{n+1}(t)\|^2_{\mathbb{C}^3} + C_4\|\chi_n(t)\|^2_{H^2(S^2)} + C_5\|w_n(t)\|^2_{H^3(S^2)},\end{aligned}$$

for all $t\in[0,T^*]$. The constants $C_1,\ldots,C_5$ depend only on the prescribable fields and N. Similar estimates for $\partial_t\|\nabla\upsilon_{n+1}(t)\|^2_{L^2(S^2)}$ and $\partial_t\|\upsilon_{n+1}(t)\|^2_{L^2(S^2)}$ combine to give

$$\partial_t \|v_{n+1}(t)\|^2_{H^2(S^2)} \leqslant C_2'\Big(\|v_{n+1}(t)\|^2_{H^2(S^2)} + \|w_{n+1}(t)\|^2_{H^3(S^2)} + \|q_{n+1}(t)\|^2_{\mathbb{C}^3} + \|\chi_n(t)\|^2_{H^2(S^2)} + \|w_n(t)\|^2_{H^3(S^2)}\Big), \tag{5.44}$$

for all $t\in[0,T^*]$. In a similar fashion we may obtain

$$\partial_t \|q_{n+1}(t)\|^2_{\mathbb{C}^3} \leqslant C_3'(\|q_{n+1}(t)\|^2_{\mathbb{C}^3} + \|v_{n+1}(t)\|^2_{H^2(S^2)} + \|w_{n+1}(t)\|^2_{H^3(S^2)} + \|q_n(t)\|^2_{\mathbb{C}^3} + \|v_n(t)\|^2_{H^2(S^2)}), \tag{5.45}$$

for all $t\in[0,T^*]$, from (5.42).

Adding (5.40), (5.44), and (5.45) and integrating via Gronwall's inequality, we find

$$\|w_{n+1}(t)\|^2_{H^3(S^2)} + \|v_{n+1}(t)\|^2_{H^2(S^2)} + \|q_{n+1}(t)\|^2_{\mathbb{C}^3} \leqslant C\int_0^t \|w_n(s)\|^2_{H^3(S^2)} + \|v_n(s)\|^2_{H^2(S^2)} + \|q_n(s)\|^2_{\mathbb{C}^3} + \|\chi_n(s)\|^2_{H^2(S^2)}\,\mathrm{d}s, \tag{5.46}$$

for all $t<T^*$.

Finally from the elliptic estimate (5.22) and (5.43) we have

$$\|\chi_{n+1}\|^2_{H^2(S^2)} \leqslant C_4\Big(\|w_{n+1}\|^2_{H^3(S^2)} + \|v_{n+1}\|^2_{H^2(S^2)} + \|q_{n+1}\|^2_{\mathbb{C}^3}\Big). \tag{5.47}$$

For convenience we define

$$\mathcal{H}^j := H^{j+1}(S^2)\times H^j(S^2)\times\mathbb{C}^3\times H^j(S^2),$$

so that upon combining (5.46) and (5.47) and integrating from 0 to $T<T^*$, we have

$$\int_0^T \|(w_{n+1},v_{n+1},q_{n+1},\chi_{n+1})\|^2_{\mathcal{H}^2}\,\mathrm{d}t \leqslant CT\int_0^T \|(w_n,v_n,q_n,\chi_n)\|^2_{\mathcal{H}^2}\,\mathrm{d}t. \tag{5.48}$$

The constant C depends on the prescribable fields and the number N encountered in Proposition 5.16.

Returning to Eqs. (5.39) and (5.41)–(5.43) we may use (5.48) to obtain

$$\int_0^T \|(\dot{w}_{n+1},\dot{v}_{n+1},\dot{q}_{n+1},\dot{\chi}_{n+1})\|^2_{\mathcal{H}^0}\,\mathrm{d}t \leqslant CT\int_0^T \|(w_n,v_n,q_n,\chi_n)\|^2_{\mathcal{H}^2}\,\mathrm{d}t,$$

with the constant C depending on the same quantities as the constant in (5.48).

Let $\delta\mathbf{U}_{n+1}=\mathbf{U}_{n+1}-\mathbf{U}_n$ denote the difference between two successive iterates, then choosing $T<1/C$ we have proven the following result.

Proposition 5.18: Let the initial data satisfy the hypotheses of Proposition 5.16. There exists a $T_*>0$, depending on the prescribable fields and the initial data, such that

$$\|\delta\mathbf{U}_{n+1}\|_{\Psi^1_{0,T_*}} \leqslant \alpha\|\delta\mathbf{U}_n\|_{\Psi^1_{0,T_*}},$$

with $\alpha<1$.

Proposition 5.18 asserts that the iteration scheme defined by (5.4)–(5.7), when considered over $S^2\times[0,T_*]$, defines a mapping $\Gamma:\mathbf{U}_n\mapsto\mathbf{U}_{n+1}$ which is a contraction with respect to the Ψ^1_{0,T_*} norm. This fact gives us the following corollary.

Corollary 5.19: Let the initial data satisfy the hypotheses of Proposition 5.16. There exists a $T_*>0$, depending on the prescribable fields and the initial data, such that the sequence $\{\mathbf{U}_n\}_{n=0}^{\infty}$ is a Cauchy sequence with respect to the Ψ^1_{0,T_*} norm.

Proof: From Proposition 5.18 it is clear, upon iterating the result, that

$$\|\delta\mathbf{U}_{n+1}\|_{\Psi^1_{0,T_*}} \leqslant \alpha^n \|\delta\mathbf{U}_1\|_{\Psi^1_{0,T_*}}.$$

Since $\alpha<1$ it is obvious that $\|\delta\mathbf{U}_{n+1}\|_{\Psi^1_{0,T_*}} \to 0$ as $n\to\infty$. Clearly this means that $\{\mathbf{U}_n\}_{n=0}^{\infty}$ is a Cauchy sequence in Ψ^1_{0,T_*}. ■

Theorem 5.20: *Let the prescribable fields β, H, $T_{0\alpha}$, $\sigma\in C^\infty(S^2\times\mathbb{R}^+)$ and let the initial data satisfy $u_0\in H^{2m+1}(S^2)$, $\mu_0\in H^{2m}(S^2)$, and $k_0\in\mathbb{C}^3$, with $m>m_0$. There exists a $T>0$ depending on the prescribable fields and the initial data such that the system of equations (4.8)–(4.11) with the above data, has a unique solution*

$$\mathbf{U} = (u, \mu, k, \hat{\eth}) \in \Psi^m_{0,T}.$$

Proof: Given the hypotheses of the theorem, Corollary 5.19 applies and so there exists a $T>0$ such that the sequence $\{\mathbf{U}_n\}_{n=0}^{\infty}$ is Cauchy in $\Psi^1_{0,T}$. Now $\Psi^1_{0,T}$ is a complete space, and so $\mathbf{U}_n$ converges to $\mathbf{U}\in\Psi^1_{0,T}$. The limit $\mathbf{U}$ is the unique fixed point of the iteration and so clearly uniquely satisfies the system (4.8)–(4.11), with the given data. We note that since $\mathbf{U}\in\Psi^1_{0,T}$, $\mathbf{U}$ is regular enough to satisfy the system in the strong sense. Moreover, Proposition 5.16 states that $\|\mathbf{U}_n\|_{\Psi^m_{0,T}}\leqslant N$ and so there is a subsequence $\{\mathbf{U}_{n_j}\}_{j=0}^{\infty}\subset\{\mathbf{U}_n\}_{n=0}^{\infty}$ and $\mathbf{V}\in\Psi^m_{0,T}$ such that $\mathbf{U}_{n_j}\rightharpoonup\mathbf{V}$ in $\Psi^m_{0,T}$. However, since the fixed point $\mathbf{U}$ is unique, we conclude that $\mathbf{U}=\mathbf{V}\in\Psi^m_{0,T}$. ■

This last result gives us a partial solution to Problem 1b. It says that the QSECS with prescribed mean curvature is uniquely solvable at least on some finite interval of time. We will now derive a similar result concerning Problem 2b, the QSECS with prescribed polar curvature.

E. Prescribing the polar curvature

In Sec. III we saw that we could ascribe a potentially interesting geometric nature to our space–time initial data if we were to allow for the possibility of prescribing the polar curvature. Our aim in this section then, is to prove a theorem analagous to Theorem 5.20, where now μ is taken as prescribed instead of H. Our method will again be to look at an associated linear iterative system of partial differential equations, and infer the convergence of this system to a unique fixed point. To this end we will consider the following iterative system of equations:

$$\dot{u}_{n+1} = \hat{\gamma}u_n^2\Delta u_{n+1} - \hat{\gamma}u_n^3\left(1-\tfrac{1}{2}e^{2t}\left(16\pi T_{00}+2\|\kappa_n\|^2+\tfrac{3}{2}\mu^2-2\mu H_n\right)\right)+\tfrac{1}{2}(1+\hat{\gamma}e^{2t}\|\hat{\eta}_n\|^2+\gamma B)u_n, \tag{5.49}$$

$$\dot{k}_{n+1} = -\mathcal{P}_1\left\{\mu\eth u_{n+1}+\tfrac{1}{2}\eth(\mu u_{n+1})-\eth(u_{n+1}H_n)+(1+\rho)\kappa_{n+1}+\overline{\kappa}_n\eth\beta+\kappa_n\eth\overline{\beta}+8\pi e^t u_{n+1}T_0\right\}, \tag{5.50}$$

$$\begin{aligned}-\overline{\eth}\hat{\eta}_{n+1} = \dot{\sigma}+(1-\mathcal{P}_1)\Big\{&\mu\eth u_{n+1}+\tfrac{1}{2}\eth(\mu u_{n+1})-\eth(u_{n+1}H_n)+(1+\rho)\kappa_{n+1}+\overline{\kappa}_{n+1}\eth\beta+\kappa_{n+1}\eth\overline{\beta}\\&+8\pi e^t u_{n+1}T_0\Big\},\end{aligned} \tag{5.51}$$

$$\rho H_{n+1} = \dot{\mu}-\operatorname{div}(u_{n+1}\kappa_{n+1})+(1+\rho)\mu+u_{n+1}^{-1}\hat{\eta}^{AB}_{n+1}\nabla_{(B}\beta_{A)}+8\pi T_{03}u_{n+1}e^t. \tag{5.52}$$

Informally, we implement the scheme as follows.

Define the zeroth iterate $(u,\hat{\eta},k,H)_0^{\sim}$ by first defining $u_0^{\sim}$ and $k_0^{\sim}$ as the time constant extensions of the initial data u_0 and k_0, respectively. We may then use Eq. (5.50) with $n=-1$, to define H_{-1}. Note that this is possible since (5.50) may be considered as an algebraic equation for H_n since $\mathcal{P}_1\eth$ is just a multiplier. This is the only time we will consider (5.50) as an equation for H_n; from now on we will consider it as an equation for k_n. Moreover, we may dispense with H_{-1} after we substitute it into (5.51) with $n=-1$, and we define $\hat{\eta}_0^{\sim}$ as the solution of the resulting equation. With $u_0^{\sim}, k_0^{\sim}$, and $\hat{\eta}_0^{\sim}$ all defined, we may take $n=-1$ and define $H_0^{\sim}$ as the solution of the algebraic equation (5.52).

If we take $u_0 \in H^{2m+1}(S^2)$ and $k_0 \in \mathbb{C}^3$ then it is clear that $(u, \hat{\eta}, k, H)_0^{\sim} \in \Psi_{0,T}^m$.

Using Theorem 5.1, it is an easy matter to see that if $(u, \hat{\eta}, k, H)_n \in \Psi_{0,T}^m$ then $u_{n+1} \in P_{0,T}^{m+1/2}$ exists as the solution to (5.49) with data u_0, for any $T \in [0, \infty)$.

Moving on to (5.50), we may pose this equation equivalently as the following ordinary differential equation over $\mathbb{C}^3$:

$$\dot{k}_{n+1} = Ak_{n+1} + B_n, \tag{5.53}$$

where now

$$Ak = -\mathcal{P}_1\{(1+\rho)k\} \tag{5.54}$$

and

$$B_n = -\mathcal{P}_1\Big\{\mu \eth u_{n+1} + \tfrac{1}{2}\eth(\mu u_{n+1}) - \eth(u_{n+1}H_n) + (1+\rho)\sigma + \overline{\kappa}_n \eth\beta + \kappa_n \eth\overline{\beta} + 8\pi e^t u_{n+1} T_0\Big\}.$$

The following result, which is analogous to Lemma 5.2, is a simple consequence of the definition (5.54)

Lemma 5.21: Let $\beta \in \Gamma^\infty(TS^2 \times [0,\infty))$. The operator $A: \mathbb{C}^3 \to \mathbb{C}^3$ defined by (5.54) is a bounded linear operator.

Proof: Linearity is obvious from the definition as is the fact that

$$\|Ak\|_{\mathbb{C}^3}^2 \leqslant C_\rho \|k\|_{\mathbb{C}^3}^2.$$

■

We may use Lemma 5.3, substituting $\mathbb{C}^3$ for E^j, to infer the unique existence of $k_{n+1} \in C^1([0,T]; \mathbb{C}^3)$, the solution of (5.53) subject to the initial value $k_0 \in \mathbb{C}^3$, provided that $u_{n+1} \in P_{0,T}^{m+1/2}$, $k_n \in H^m([0,T]; \mathbb{C}^3)$, and $H_n \in P_{0,T}^m$. Similarly we may use Lemma 5.4 to obtain the estimate

$$\|k_{n+1}(t)\|_{\mathbb{C}^3} e^{-C_\rho t} \leqslant \|k_0\|_{\mathbb{C}^3} + \int_0^t \|B_n(s)\|_{\mathbb{C}^3}\, \mathrm{d}s,$$

for all $t \in [0,T]$.

It is an easy matter to amend the proof of Proposition 5.9 to give the following result which establishes the higher regularity of solutions to (5.53).

Lemma 5.22: Let $k_0 \in \mathbb{C}^3$ and suppose $u_{n+1} \in P_{0,T}^{m+1/2}$ and $(H_n, k_n) \in \mathcal{O}_{0,T}^m$. Then k_{n+1}, the solution of (5.53) satisfies

$$\|k_{n+1}\|_{H^m([0,T];\mathbb{C}^3)}^2 \leqslant TC\Big(1 + \|B_n\|_{H^m([0,T];\mathbb{C}^3)}^2\Big).$$

The constant C depends on β, $\|u_0\|_{H^{2m}(S^2)}$ and $\|k_0\|_{\mathbb{C}^3}$.

Proof: The result is just Proposition 5.9 with k_{n+1} replacing $\mathcal{M}_{n+1}$ and the much simpler equation (5.53) replacing (5.9). Note in particular that there is no dependence of the constant on u_n, only β. Other than these minor details, the proof is identical. ■

In light of this last result we see that if $u_0 \in H^{2m}(S^2)$, $k_0 \in \mathbb{C}^3$, $u_{n+1} \in P_{0,T}^{m+1/2}$, and $(H_n, k_n) \in \mathcal{O}_{0,T}^m$ then k_{n+1} exists and belongs to $H^m([0,T]; \mathbb{C}^3)$.

As was the case with (5.7), (5.51) is solvable by construction, with the higher regularity of solutions being governed by Corollary 5.12. The equation for H_{n+1}, (5.52), is algebraic and so it is easy to see that $\hat{\eta}_{n+1}$, $H_{n+1} \in P_{0,T}^m$ provided that $u_{n+1} \in P_{0,T}^{m+1/2}$ and $k_{n+1} \in H^m([0,T]; \mathbb{C}^3)$.

For brevity we introduce the following notation:

$$\tilde{\mathbf{U}}_n = (u, \hat{\eta}, k, H)_n.$$

Despite being rather heuristic in nature, the foregoing discussion shows how the results proven in the preceding section can be amended to give analogous results concerning the iteration scheme

presently under consideration. In particular, we have the following analog of Theorem 5.13.

Theorem 5.23: *Let* $m \geqslant m_0$ *and let* $u_0 \in H^{2m+1}(S^2)$ *and* $k_0 \in \mathbb{C}^3$. *There exists a nonincreasing, but possibly decreasing sequence* $\{T_n\}_{n=1}^{\infty}$ *with* $T_n \geqslant 0$, *and a sequence of iterates* $\tilde{\mathbf{U}}_n \in \Psi^m_{0,T_n}$ *which satisfy (5.4)–(5.7).*

Proposition 5.16 also has an analogous result concerning the iteration scheme presently under consideration. In fact, using the same ideas as those found in the proof of Proposition 5.16 it is a fairly simple matter to obtain.

Proposition 5.24: Let $m \geqslant m_0$ *and suppose* $u_0 \in H^{2m+1}(S^2)$ *and* $k_0 \in \mathbb{C}^3$. *There exists* $T^* > 0$ *and* $\tilde{N} > 0$, *depending only on m, the initial data and the prescribable fields, such that*

$$\|\tilde{\mathbf{U}}_n\|_{\tilde{\Psi}^m_{0,T^*}} \leqslant \tilde{N}$$

for all $n \in \mathbb{N}$.

As in Theorem 5.17, we can use Proposition 5.24 to deduce that the proposed iteration scheme (5.49)–(5.52) is consistently defined and produces a sequence of iterates $\{\tilde{\mathbf{U}}_n\}_{n=0}^{\infty} \subset \Psi^m_{0,T^*}$. Moreover, results analogous to Proposition 5.18 and Corollary 5.19 are obtained with practically identical proofs and the counterpart to Theorem 5.20 follows easily.

Theorem 5.25: *Let the prescribable fields* β, μ, $T_{0\alpha}$, $\sigma \in C^{\infty}(S^2 \times \mathbb{R}^+)$ *and let the initial data satisfy* $u_0 \in H^{2m+1}(S^2)$ *and* $k_0 \in \mathbb{C}^3$, *with* $m \geqslant m_0$. *There exists a* $T > 0$ *depending on the prescribable fields and the initial data such that the system of equations (4.8)–(4.11), with the above data, has a unique solution*

$$\tilde{\mathbf{U}} = (u, \hat{\eta}, k, H) \in \Psi^m_{0,T}.$$

This gives us the sought after result concerning Problem 2b.

It is clear that by construction we may transform the solutions given by Theorems 5.20 and 5.25 under the inverse of (4.1) and thereby construct quasispherical initial data which locally satisfies the Einstein constraint equations.[7–10]

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The two NUT-like solutions of Ernst equation

Yabo Wu,[a] Peng Dong, Xuemei Deng, and Guoming Zhao
Department of Physics, Liaoning Normal University, Dalian (116029), People's Republic of China

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By applying Ehlers transformation to Schwarzschild and Kerr solutions of Ernst equation and choosing the suitable coordinate transformations, the two NUT-like solutions, i.e., the so called NUT–Taub-like and the Kerr–NUT-like solutions are obtained which not only can, respectively, reduce to Schwarzschild and Kerr solutions when the parameter $\ell' = 0$, but also can also reduce to the NUT–Taub metric and Kerr–NUT metric, respectively, when ℓ' satisfies the some approximation. Meanwhile it is shown that in the NUT–Taub and Kerr–NUT solutions the range of value for the parameter ℓ interpreted as the gravomagnetic monopole cannot be arbitrary and should be confined by mass of the source to $|\ell| \ll m$. Furthermore, the differences in the geometrical structure between the NUT–Taub-like and NUT–Taub solutions are discussed and the physical properties of the horizons on the Kerr–NUT-like space–time are analyzed. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1895825]

I. INTRODUCTION

The Ernst equation[1] is the basic equation for finding stationary axisymmetric vacuum solutions of Einstein's equations. The symmetric groups and generation of new solutions of Ernst equation have been extensively studied.[2–9] Especially, Reina and Treves[10] obtained NUT–Taub(NT) and Kerr–NUT(KN) solutions[11,12] by using an unitary transformation on Schwarzschild solution ξ_S and Kerr solution ξ_K, respectively. In this paper, by applying Ehlers transformation[13] to ξ_S and ξ_K we find two solutions, one with three parameters and the other with four parameters. Furthermore, by means of the mappings and coordinates transformations given by us, we obtain two NUT-like solutions, i.e., the so-called NUT–Taub-like (NT-like) and Kerr–NUT-like (KN-like) solutions, which can be reduced to NT metric and KN metric, respectively, when we consider some special case. In Sec. II, some brief recalls of the Ernst equation and its solutions, especially the general process of the resolution are given. In Sec. III the NUT–Taub-like metric is obtained and the differences in the geometrical structure between the NUT–Taub-like and NUT–Taub solutions are discussed according to the curvature tensors of the NUT–Taub-like metric given by us. The Kerr–NUT-like metric is obtained successively and the properties of the horizons on the Kerr–NUT-like space–time are analyzed in Sec. IV. Finally, Sec. V is devoted to the conclusions. Appendixes A and B follow.

II. BRIEF RECALL ON THE RESOLUTION OF THE ERNST EQUATION

The line element of a stationary axisymmetric Einstein vacuum field called the Papapetrou form in the cylindrical coordinates (ρ, z, ϕ) reads

$$ds^2 = f(dt - \omega\, d\phi)^2 - f^{-1}[e^{2\gamma}(d\rho^2 + dz^2) + \rho^2\, d\phi^2], \tag{1}$$

where the gravitational potentials f, ω, and γ are real functions of ρ and z only. It is known that γ is determined by f and ω. The Ernst equation[1] is

[a]Electronic mail: zwyb@mail.dlptt.ln.cn

$$(\xi\bar{\xi}-1)\nabla^2\xi = 2\bar{\xi}\nabla\,\xi\cdot\nabla\,\xi, \tag{2}$$

where $\nabla\equiv(\partial_\rho,\partial_z)$ and $\nabla^2\equiv\partial_\rho^2+\rho^{-1}\partial_\rho+\partial_z^2$ denote the three-dimensional divergence and Laplacian operators, respectively, $\bar{\xi}$ is the conjugated complex potential of ξ.

The canonical coordinates of Weyl, ρ and z, can be given in terms of prolate spheroidal coordinates, x and y, by the relations

$$\rho = k(x^2-1)^{1/2}(1-y^2)^{1/2} \quad \text{and } z = kxy, \tag{3}$$

with

$$x \geqslant 1, \quad -1 \leqslant y \leqslant 1, \quad k = \text{constant}. \tag{4}$$

In these coordinates, the line element (1) assumes the form

$$\mathrm{d}s^2 = f(\mathrm{d}t-\omega\,\mathrm{d}\phi)^2 - k^2f^{-1}\left[e^{2\gamma}(x^2-y^2)\left(\frac{\mathrm{d}x^2}{x^2-1}+\frac{\mathrm{d}y^2}{1-y^2}\right)+(x^2-1)(1-y^2)\mathrm{d}\phi^2\right]. \tag{5}$$

To determine the potentials f,ω, and γ of the metric (5), the method often to be used is the following relation between f, the twist potential Φ and ξ:

$$f+i\Phi = \frac{\xi-1}{\xi+1}, \tag{6}$$

where Φ is the twist potential defined up to a constant and related to the dragging ω by the following differential equations:[14]

$$\frac{\partial\omega}{\partial x} = \frac{k(1-y^2)}{f^2}\frac{\partial\Phi}{\partial y} \quad \text{and} \quad \frac{\partial\omega}{\partial y} = -\frac{k(x^2-1)}{f^2}\frac{\partial\Phi}{\partial x}, \tag{7}$$

and γ is determined by the following equation:

$$e^{2\gamma} = C\frac{A}{(x^2-y^2)^\delta}, \tag{8}$$

where C is integral constant, and C and δ is determined by the boundary condition,

$$e^{2\gamma}\to 1 \quad \text{when } x\to\infty. \tag{9}$$

It is well known that there are two classical solutions of the Ernst equation, one is Schwarzschild solution,

$$\xi_S = x, \tag{10}$$

the other is Kerr solution,

$$\xi_K = px+iqy, \tag{11}$$

where p and q are real constants satisfying

$$p^2+q^2 = 1. \tag{12}$$

Reina and Treves performed a unitary transformation on ξ_S and ξ_K and obtained NUT–Taub (NT) and Kerr–NUT (KN) solutions[10] as follows:

$$ds^2=\left(1-2\frac{mr+\ell^2}{r^2+\ell^2}\right)(dt-2\ell\cos\theta\,d\phi)^2-\left(1-2\frac{mr+\ell^2}{r^2+\ell^2}\right)^{-1}dr^2-(r^2+\ell^2)(d\theta^2+\sin^2\theta\,d\phi^2) \tag{13}$$

and

$$\begin{aligned}ds^2=&\left(1-2\frac{mr-a\ell\cos\theta+\ell^2}{r^2+a^2\cos^2\theta+\ell^2-2a\ell\cos\theta}\right)\left[dt-\left(2a\sin^2\theta\frac{mr-a\ell\cos\theta+\ell^2}{r^2-2mr+a^2\cos^2\theta-\ell^2}\right.\right.\\&\left.\left.-2\ell\cos\theta\right)d\phi\right]^2-(r^2+a^2\cos^2\theta+\ell^2-2a\ell\cos\theta)\left(\frac{dr^2}{r^2-2mr+a^2-\ell^2}+d\theta^2\right)\\&-\frac{(r^2+a^2\cos^2\theta+\ell^2-2a\ell\cos\theta)(r^2-2mr+a^2-\ell^2)}{r^2-2mr+a^2\cos^2\theta-\ell^2}\sin^2\theta\,d\phi^2.\end{aligned} \tag{14}$$

III. THE NUT–TAUB-LIKE METRIC

Let ξ_0 and ξ be any two solutions of Ernst equation (2), which can be related by Ehlers transformation,

$$T:\xi_0\to\xi,\quad \text{i.e., } \xi=\frac{a\xi_0+\overline{b}}{b\xi_0+\overline{a}}, \tag{15}$$

where a and b are complex numbers and $\overline{a},\overline{b}$ are their complex conjugate, respectively, which satisfy

$$\begin{pmatrix}a & \overline{b}\\ b & \overline{a}\end{pmatrix}\in \mathrm{SU}(1,1),\quad a\overline{a}-b\overline{b}=1. \tag{16}$$

Now taking $\xi_0=\xi_S$, then we can find the potentials corresponding to the solution ξ of the Ernst equation,

$$f=\frac{x^2-1}{(\beta_1^2+\beta_2^2)x^2+2(\beta_1^2-\beta_2^2)x+\beta_1^2+\beta_2^2}, \tag{17}$$

$$\Phi=\frac{(\alpha_2\beta_1-\alpha_1\beta_2)(x^2-1)+2(\alpha_2\beta_1-\alpha_1\beta_2)}{(\beta_1^2+\beta_2^2)x^2+2(\beta_1^2-\beta_2^2)x+\beta_1^2+\beta_2^2}, \tag{18}$$

$$\omega=-4k\beta_1\beta_2 y, \tag{19}$$

$$e^{2\gamma}=\frac{x^2-1}{x^2-y^2}, \tag{20}$$

where α and β are introduced by $\alpha=a-b$, $\beta=a+b$, and can be decomposed as $\alpha=\alpha_1+i\alpha_2$, $\beta=\beta_1+i\beta_2$, where $\alpha_1,\alpha_2,\beta_1$, and β_2 satisfy

$$\alpha_1\beta_1+\alpha_2\beta_2=1. \tag{21}$$

We see from Eqs. (17)–(21) that the solution has three free parameters.

If we let

$$\alpha_1 = \beta_1 \quad \text{and } \alpha_2 = \beta_2, \tag{22}$$

then we can get the known NUT–Taub (KN) solution.

If taking

$$\alpha_1 = \beta_1 \quad \text{and } \alpha_2 = -\beta_2, \tag{23}$$

Eq. (21) turns into

$$\beta_1^2 - \beta_2^2 = 1. \tag{24}$$

Now we introduce the hyperbolic function

$$\beta_1 = \coth \varphi \quad \text{and } \beta_2 = \sinh \varphi, \tag{25}$$

which satisfy the relation (24) obviously. In order to write this metric in Boyer–Lindquist-type coordinates[4] the following mappings are introduced:

$$\begin{gathered} x \to \frac{r-m}{k}, \quad y \to \cos\theta, \\ \coth 2\varphi \to \frac{m}{\sqrt{m^2 - \ell'^2}}, \quad \sinh 2\varphi \to \frac{-\ell'}{\sqrt{m^2 - \ell'^2}}, \end{gathered} \tag{26}$$

with

$$k \to \frac{m^2}{\sqrt{m^2 - \ell'^2}}. \tag{27}$$

We see from above that the value of parameter ℓ' has a range of

$$-m < \ell' < m, \ \ell' \neq \pm m. \tag{28}$$

By the complicated calculation, we can finally find the following metric:

$$\begin{aligned} ds^2 = {} & \sqrt{\frac{m^2 - \ell'^2}{m^2}}\left(1 - 2\frac{mr + \frac{m^2}{m^2-\ell'^2}\ell'^2}{r^2 + \frac{m^2}{m^2-\ell'^2}\ell'^2}\right)\left(dt - 2\frac{m^2}{m^2 - \ell'^2}\ell' \cos\theta\, d\phi\right)^2 - \sqrt{\frac{m^2}{m^2 - \ell'^2}}\Bigg(1 \\ & - 2\frac{mr + \frac{m^2}{m^2-\ell'^2}\ell'^2}{r^2 + \frac{m^2}{m^2-\ell'^2}\ell'^2}\Bigg)^{-1} dr^2 - \sqrt{\frac{m^2}{m^2 - \ell'^2}}\left(r^2 + \frac{m^2}{m^2 - \ell'^2}\ell'^2\right)(d\theta^2 + \sin^2\theta\, d\phi^2), \end{aligned} \tag{29}$$

where r and θ are spherical coordinates. When $\ell' = 0$, this metric becomes the Schwarzschild solution, which indicates that the parameter m is mass of the source and ℓ' is a parameter with mass dimension obviously. It is more worthy of note that if we assume the following approximation,

$$1 - \left(\frac{\ell'}{m}\right)^2 \approx 1 \quad \text{when } |\ell'| \ll m, \tag{30}$$

then this metric becomes

$$ds^2 = \left(1 - 2\frac{mr + \ell'^2}{r^2 + \ell'^2}\right)(dt + 2\ell' \cos\theta\, d\phi)^2 - \left(1 - 2\frac{mr + \ell'^2}{r^2 + \ell'^2}\right)^{-1} dr^2 - (r^2 + \ell'^2)(d\theta^2 + \sin^2\theta\, d\phi^2). \tag{31}$$

It is just the NT solution (13) when $\ell' = \ell$. Thus here we call this solution (29) the NT-like metric and give the following comments.

(1) The value of the parameter ℓ interpreted as the gravomagnetic monopole[5,12] in the NT solution (13) is limited by the mass of source, i.e., $|\ell| \ll m$. But in the NT-like solution (29), the parameter satisfies $-m < \ell' < m$.

(2) According to the curvature tensors $R_{\mu\nu\lambda\rho}$ (see the Appendixes) corresponding to the NT and NT-like metrics we can see the space–time structure of the NT-like solution is different from the one for the NT solution. And the case of $\ell' = \pm m$ leads the curvature of NUT-like space–time to diverge, this implies that the solution is "everywhere" singular and therefore meaningless when $\ell' = \pm m$. But in the case of $|\ell'| \ll m$, the geometrical properties of both are the same owing to having the same curvature tensors.

IV. THE KERR–NUT-LIKE METRIC

If we take $\xi_0 = \xi_K$ (Kerr solution) in Ehlers transformation (15), we get

$$\xi' = \frac{a\xi_K + \overline{b}}{b\xi_K + \overline{a}}, \tag{32}$$

By applying the same method as Sec. III and making the complicated calculation, we can find the potentials corresponding to the solution ξ' of the Ernst equation,

$$f = \frac{p^2x^2 + q^2y^2 - 1}{(\beta_1^2 + \beta_2^2)(p^2x^2 + q^2y^2) + 2(\beta_1^2 - \beta_2^2)px - 4\beta_1\beta_2 qy + \beta_1^2 + \beta_2^2}, \tag{33}$$

$$\Phi = \frac{(\alpha_2\beta_1 - \alpha_1\beta_2)(p^2x^2 + q^2y^2 + 2qy + 1) - 2(\alpha_2\beta_1 + \alpha_1\beta_2)px}{(\beta_1^2 + \beta_2^2)(p^2x^2 + q^2y^2) + 2(\beta_1^2 - \beta_2^2)px - 4\beta_1\beta_2 qy + \beta_1^2 + \beta_2^2}, \tag{34}$$

$$\omega = -\frac{2kq}{p}\frac{1 - y^2}{p^2x^2 + q^2y^2 - 1}(2\beta_1\beta_2 qy - px - \beta_1^2 - \beta_2^2) - \frac{4\beta_1\beta_2 ky}{p}, \tag{35}$$

$$e^{2\gamma} = \frac{p^2x^2 + q^2y^2 - 1}{p^2(x^2 - y^2)}, \tag{36}$$

where $\alpha_1, \alpha_2, \beta_1$, and β_2 still satisfy Eq. (21). We easily see from Eqs. (33)–(36) the above solution contains four free parameters, and Kerr–NUT (KN) solution is contained as a special case which satisfies the relation (22). On the other hand, if we consider Eqs. (23)–(25), and introduce the following crucial mappings in Boyer–Lindquist-type coordinates:

$$x \to \frac{r - m}{k}, \quad y \to \cos\theta,$$

$$\coth 2\varphi \to \frac{m}{\sqrt{m^2 - \ell'^2}}, \quad \sinh 2\varphi \to \frac{\ell'}{\sqrt{m^2 - \ell'^2}},$$

$$p \to \frac{\sqrt{m^2 - a^2}}{m}, \quad q \to \frac{a}{m}, \tag{37}$$

with

$$k \to m\sqrt{\frac{m^2 - a^2}{m^2 - \ell'^2}},$$

then we see from Eq. (37) that the value of parameter ℓ' has the same range as (28). And under the above mappings we can finally get the metric

$$\begin{aligned} ds^2 = & \sqrt{\frac{m^2 - \ell'^2}{m^2}}\left(1 - 2\frac{\frac{m^2-\ell'^2}{m^2}mr - a\ell' \cos\theta + \ell'^2}{\frac{m^2-\ell'^2}{m^2}r^2 + a^2\cos^2\theta - 2a\ell' \cos\theta + \ell'^2}\right)\Bigg[dt \\ & - \left(2a\sin^2\theta \frac{mr - \frac{m^2}{m^2-\ell'^2}(a\ell' \cos\theta - \ell'^2)}{\frac{m^2-\ell'^2}{m^2}(r^2 - 2mr) + a^2\cos^2\theta - \ell'^2} - 2\frac{m^2}{m^2 - \ell'^2}\ell' \cos\theta\right)d\phi\Bigg]^2 \\ & - \sqrt{\frac{m^2}{m^2 - \ell'^2}}\left(\frac{m^2 - \ell'^2}{m^2}r^2 + a^2\cos^2\theta - 2a\ell' \cos\theta + \ell'^2\right)\left(\frac{dr^2}{\frac{m^2-\ell'^2}{m^2}(r^2 - 2mr) + a^2 - \ell'^2}\right. \\ & \left. + \frac{m^2}{m^2 - \ell'^2}d\theta^2\right) - \sqrt{\frac{m^2}{m^2 - \ell'^2}}\left(1 - 2\frac{\frac{m^2-\ell'^2}{m^2}mr - a\ell' \cos\theta + \ell'^2}{\frac{m^2-\ell'^2}{m^2}r^2 + a^2\cos^2\theta - 2a\ell' \cos\theta + \ell'^2}\right)^{-1}\Bigg[r^2 - 2mr \\ & + \frac{m^2}{m^2 - \ell'^2}(a^2 - \ell'^2)\Bigg]\sin^2\theta\, d\phi^2, \end{aligned} \tag{38}$$

where r and θ are spherical coordinates. When $\ell' = 0$, this metric becomes the Kerr metric which indicates that the parameters m and a are the mass and the angular momentum per unit mass of the source, respectively, and ℓ' is a parameter with mass dimension obviously. It is noted that for the parameter ℓ' its range of the value and the physical explanation are the same as those in NT-like metric. On the other hand, this metric can be reduced to NT-like metric, when $a = 0$. It is worthy of emphasizing that if we take the approximation (28), i.e., $1 - (\ell'/m)^2 \approx 1$ when $|\ell'| \ll m$, then we find that the metric (38) can be reduced to KN metric (14). It follows that this metric contains KN metric as a special case. Hence here we call it the KN-like metric. Furthermore, we find the KN-like solution has the different physical properties from the KN solution. As an example, below we will discuss the horizons on the KN-like space–time in order to show the differences between both.

Generally, the horizon function $f(x^\mu)$ (exactly null-hypersurface) satisfies[13]

$$n_\mu n^\mu = g^{\mu\nu}\frac{\partial f}{\partial x^\mu}\frac{\partial f}{\partial x^\nu} = 0, \tag{39}$$

where $n_\mu \equiv \partial f/\partial x^\mu$ is the normal vector of the null hypersurface. For a stationary axisymmetric space–time, Eq. (39) can be written as

$$\hat{g}_{00}\left[g^{11}\left(\frac{\partial f}{\partial r}\right)^2 + g^{22}\left(\frac{\partial f}{\partial \theta}\right)^2\right] = 0, \tag{40}$$

where

$$\hat{g}_{00} \equiv g_{00} - \frac{g_{03}^2}{g_{33}}. \tag{41}$$

Thus we get the following two equations:

$$g^{11}\left(\frac{\partial f}{\partial r}\right)^2 + g^{22}\left(\frac{\partial f}{\partial \theta}\right)^2 = 0 \quad \text{or } \hat{g}_{00} = 0, \tag{42}$$

it is easy to identify that the two equations in (42) give the same equation as follows according to the KN-like metric (38):

$$\frac{m^2 - \ell'^2}{m^2}(r^2 - 2mr) + a^2 - \ell'^2 = 0. \tag{43}$$

The solutions of the above equation are

$$r_{\pm}^h = m\left(1 \pm \sqrt{\frac{m^2 - a^2}{m^2 - \ell'^2}}\right). \tag{44}$$

These horizons split into the Cauchy horizon, with radius $r_{ch}=m(1-\sqrt{(m^2-a^2)/(m^2-\ell'^2)})$, and the event horizon, with radius $r_{eh}=m(1+\sqrt{(m^2-a^2)/(m^2-\ell'^2)})$. Obviously by comparing with the horizons of the KN metric, $r_{\pm}^h(\mathrm{KN})=m(1\pm\sqrt{(m^2-a^2+\ell^2)/m^2})$, we can see there is the difference between the radial location of the horizons of the KN-like and KN solutions due to the property of the latter to hold if $|\ell| \ll m$, i.e., $r_{\pm}^h(\mathrm{KN})$ can be deduced from $r_{\pm}^h$ in (44) as follows:

$$\begin{aligned} r_{\pm}^h &= m\left(1 \pm \sqrt{\frac{1-\frac{a^2}{m^2}}{1-\frac{\ell'^2}{m^2}}}\right) \doteq m\left(1 \pm \sqrt{1 - \frac{a^2}{m^2} + \frac{\ell'^2}{m^2} - \frac{a^2\ell'^2}{m^4}}\right) = m\left(1 \pm \sqrt{\frac{m^2 - a^2 + \ell'^2 - \frac{a^2\ell'^2}{m^2}}{m^2}}\right) \\ &\doteq m\left(1 \pm \sqrt{\frac{m^2 - a^2 + \ell^2}{m^2}}\right) = r_{\pm}^h(\mathrm{KN}), \end{aligned} \tag{45}$$

where $\ell' = \ell$ when $|\ell'| \ll m$. And this justifies neglecting the term $a^2\ell'^2/m^2$ with respect to a^2 in (45). Especially, it should be noted that the extreme black hole of the KN-like solution satisfies the condition $a=m$ which is the same as the Kerr metric's case, but differs from the condition corresponding to the extreme black hole of the Kerr–NUT metric, which is $a=\sqrt{m^2+\ell^2}$.

V. CONCLUSIONS

So far we have obtained the NUT–Taub-like metric and the Kerr–NUT-like metric by applying Ehlers transformation to Schwarzschild and Kerr solutions of Ernst equation and choosing the suitable mappings in Boyer–Lindquist-like coordinates. When $\ell'=0$ the two solutions can, respectively, reduce to Schwarzschild and Kerr solutions; and when ℓ' satisfies the approximation (30) they can also reduce to the NUT–Taub metric and Kerr–NUT metric, respectively. In this sense, we believe that in the NUT–Taub and Kerr–NUT metrics the value of the NUT parameter ℓ interpreted as the gravomagnetic monopole[10,14] cannot be arbitrary and should be confined to $|\ell| \ll m$. Whether the limit of the parameter ℓ may influence on the prediction of observable effects[10,14] for the parameter ℓ is worthy of taking a further investigation. In addition, as concrete examples we not only calculated the curvature tensors of the NT-like solution and pointed out there are the differences in the geometrical structure between the NUT–Taub-like and NUT–Taub solutions, but also gave the horizons on the Kerr–NUT-like space–time and discussed the difference of the extreme black hole between the Kerr–NUT-like metric and the Kerr–NUT metric. For other physical properties of the two solutions such as ergospheres, singularities, geodesics, and so on we will investigate in our forthcoming paper. The relation among the above solutions can be

figured as follows:

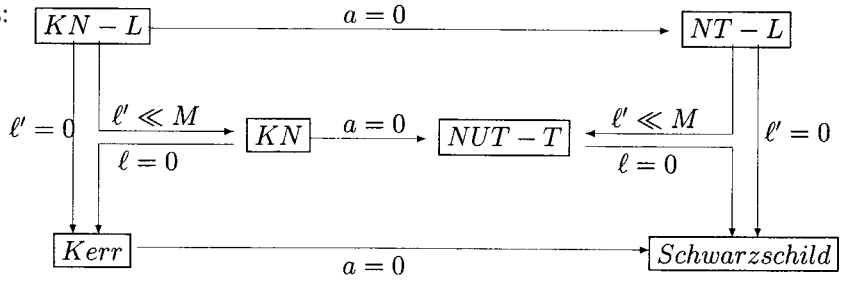

where KN and NUT–T denote Kerr–NUT and NUT–Taub solutions, while KN-L and NT-L denote, respectively, Kerr–NUT-like and NUT–Taub-like solutions.

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APPENDIX A: THE NONZERO CURVATURE TENSORS OF THE NUT–TAUB (NT) METRIC

The NUT–Taub metric in spheroidal coordinates are

$$g_{\mu\nu}=\begin{pmatrix} \frac{\mathcal{H}}{\mathcal{U}} & 0 & 0 & -2\ell\cos\theta\left(\frac{\mathcal{H}}{\mathcal{U}}\right) \\ 0 & -\left(\frac{\mathcal{U}}{\mathcal{H}}\right) & 0 & 0 \\ 0 & 0 & -\mathcal{U} & 0 \\ -2\ell\cos\theta\left(\frac{\mathcal{H}}{\mathcal{U}}\right) & 0 & 0 & 4\ell^2\cos^2\theta\left(\frac{\mathcal{H}}{\mathcal{U}}\right)-\mathcal{U}\sin^2\theta \end{pmatrix} \tag{A1}$$

and its inverse

$$g^{\mu\nu}=\begin{pmatrix} \frac{(r^2+\ell^2)}{(r^2-2mr-\ell^2)}-\frac{4\ell^2\cos^2\theta}{(r^2+\ell^2)\sin^2\theta} & 0 & 0 & \frac{-2\ell\cos\theta}{(r^2+\ell^2)\sin^2\theta} \\ 0 & -\left(\frac{r^2-2mr-\ell^2}{r^2+\ell^2}\right) & 0 & 0 \\ 0 & 0 & -\frac{1}{r^2+\ell^2} & 0 \\ \frac{-2\ell\cos\theta}{(r^2+\ell^2)\sin^2\theta} & 0 & 0 & -\frac{1}{(r^2+\ell^2)\sin^2\theta} \end{pmatrix}, \tag{A2}$$

where

$$\mathcal{U}=r^2+\ell^2, \quad \mathcal{H}=r^2-2Mr-\ell^2.$$

The nonzero curvature tensors of the NUT–Taub metric are

$$R_{1212}=\frac{\mathcal{N}}{\mathcal{H}\mathcal{U}}, \quad R_{0101}=2\frac{\mathcal{N}}{\mathcal{U}^3}, \quad R_{1301}=4\frac{\mathcal{N}}{\mathcal{U}^3}\ell\cos\theta, \quad R_{2301}=-2\frac{\mathcal{K}}{\mathcal{U}^2}\ell\sin\theta,$$

$$R_{1302}=-\frac{\mathcal{K}}{\mathcal{U}^2}\ell\sin\theta, \quad R_{2302}=-2\frac{\mathcal{N}\mathcal{H}}{\mathcal{U}^3}\ell\cos\theta, \quad R_{1203}=\frac{\mathcal{K}}{\mathcal{U}^2}\ell\sin\theta,$$

$$R_{0303}=-\frac{\mathcal{N}\mathcal{H}}{\mathcal{U}^3}\sin^2\theta, \quad R_{2313}=-6\frac{\mathcal{K}}{\mathcal{R}^2}\ell^2\cos\theta\sin\theta, \quad R_{2002}=\frac{\mathcal{N}\mathcal{H}}{\mathcal{U}^3},$$

$$R_{1313}=\frac{\mathcal{N}}{\mathcal{HR}}\left(8\frac{\mathcal{H}}{\mathcal{U}^2}\ell^2\cos^2\theta+\sin^2\theta\right),\quad R_{2323}=-2\frac{\mathcal{N}}{\mathcal{U}}\left(2\frac{\mathcal{H}}{\mathcal{U}^2}\ell^2\cos^2\theta+\sin^2\theta\right),\tag{A3}$$

where

$$\mathcal{N}=mr^3+3\ell^2r^2-3m\ell^2r-\ell^4,\quad \mathcal{K}=r^3-3mr^2-3\ell^2r+m\ell^2.$$

APPENDIX B: THE NONZERO CURVATURE TENSORS OF THE NUT–TAUB-LIKE (NT-LIKE) METRIC

The NUT–Taub-like metric is

$$g_{\mu\nu}=\begin{pmatrix}\Delta\frac{G}{H} & 0 & 0 & -2\frac{G}{H}S\cos\theta\\ 0 & -\Delta^{-1}\frac{H}{G} & 0 & 0\\ 0 & 0 & -\Delta^{-1}H & 0\\ -2\frac{G}{H}S\cos\theta & 0 & 0 & \Delta^{-1}\left(4\frac{G}{H}S^2\cos^2\theta-H\sin^2\theta\right)\end{pmatrix}\tag{B1}$$

and its inverse is

$$g^{\mu\nu}=\begin{pmatrix}\Delta^{-1}\left[\frac{H}{G}-\frac{4S\cos^2\theta}{H\sin^2\theta}\right] & 0 & 0 & -\frac{2S\cos\theta}{H\sin^2\theta}\\ 0 & -\Delta\left(\frac{G}{H}\right) & 0 & 0\\ 0 & 0 & -\frac{\Delta}{H} & 0\\ -\frac{2S\cos\theta}{H\sin^2\theta} & 0 & 0 & -\frac{\Delta}{H\sin^2\theta}\end{pmatrix},\tag{B2}$$

where

$$\Delta=\sqrt{\frac{m^2-\ell'^2}{m^2}},\quad G=r^2-2mr-S^2,\quad H=r^2+S^2,\quad \mathrm{S}=\ell'\sqrt{\frac{m^2}{m^2-\ell'^2}}.$$

The nonzero curvature tensors of the NUT–Taub-like metric are

$$R_{1212}=\Delta^{-1}\frac{N}{HG},\quad R_{0101}=2\Delta\frac{N}{H^3},\quad R_{1301}=4\frac{N}{H^3}S\cos\theta,$$

$$R_{2301}=-2\frac{K}{H^2}S\sin\theta,\quad R_{1302}=-\frac{K}{H^2}S\sin\theta,\quad R_{2302}=-2\frac{NG}{H^3}S\cos\theta,$$

$$R_{1203}=H^2S\sin\theta,\quad R_{0303}=-\Delta\frac{NG}{H^3}\sin^2\theta,\quad R_{2313}=-6\Delta^{-1}\frac{K}{H^2}S^2\cos\theta\sin\theta,$$

$$R_{2002}=\Delta\frac{NG}{H^3},\quad R_{1313}=\Delta^{-1}\frac{N}{HG}\left(8\frac{G}{H^2}S^2\cos^2\theta+\sin^2\theta\right),$$

$$R_{2323}=-2\Delta^{-1}\frac{N}{H}\left(2\frac{G}{H^2}S^2\cos^2\theta+\sin^2\theta\right),\tag{B3}$$

where

$$N=mr^3+3S^2r^2-3mS^2r-S^4,\quad K=r^3-3mr^2-3S^2r+mS^2.$$

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Charging a double Kerr solution in five-dimensional Einstein–Maxwell–Kalb–Ramond theory

Ricardo Becerril[a)]
Instituto de Física y Matemáticas, Universidad Michoacana de San Nicolás de Hidalgo, Edificio C-3, Ciudad Universitaria, Morelia, Michoacan, CP 58040 Mexico

Alfredo Herrera-Aguilar[b)]
Instituto de Física y Matemáticas, Universidad Michoacana de San Nicolás de Hidalgo, Edificio C-3, Ciudad Universitaria, Morelia, Michoacan, CP 58040 Mexico and Theoretical Physics Department, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

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We consider the low-energy effective action of the five-dimensional (5D) Einstein–Maxwell–Kalb–Ramond theory. After compactifying this truncated model on a two-torus and switching off the U(1) vector fields of this theory, we recall a formulation of the resulting three-dimensional action as a double Ernst system coupled to gravity. Further, by applying the so-called normalized Harrison transformation on a generic solution of this double Ernst system we recover the U(1) vector field sector of the theory. Afterward, we compute the field content of the generated charged configuration for the special case when the starting Ernst potentials correspond to a pair of interacting Kerr black holes, obtaining in this way an exact field configuration of the 5D Einstein–Maxwell–Kalb–Ramond theory endowed with effective Coulomb and dipole terms with momenta. Some physical properties of this object are analyzed as well as the effect of the normalized Harrison transformation on the double Kerr seed solution. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1897843]

I. INTRODUCTION

Recently some natural interest has been shown to the study of field configurations that describe interacting black holes coupled to some matter fields, both in the framework of general relativity[1,2] and string theory.[3–5] One of the reasons for such an interest is the development reached in the statistical approach to physics of single black holes (for a review, see for instance, Refs. 6 and 7) and its possible generalization to more complicated systems of interacting black holes coupled to matter.

In this paper we construct a charged field configuration that consists of a pair of interacting sources of black hole type coupled to an antisymmetric Kalb–Ramond tensor field and a set of Abelian gauge fields in the framework of the truncated five-dimensional Einstein–Maxwell–Kalb–Ramond (EMKR) theory. The construction is carried out by applying the normalized Harrison charging symmetry, which acts on the target space of the effective three-dimensional heterotic string theory and preserves the asymptotic properties of the starting field configurations, on a seed solution that corresponds to a double Ernst system in the framework of the toroidally reduced five-dimensional Einstein–Kalb–Ramond (EKR) theory. Several interesting results have been achieved regarding the physical properties of five-dimensional black objects;[8] it turns out that the Bogomolnyi-Prasad-Sommerfield (BPS) bound of rotating black holes is saturated precisely in five or more dimensions.

[a)]Electronic mail: becerril@ifm.umich.mx
[b)]Electronic mail: aherrera@auth.gr

The paper is organized as follows: in Sec. II we briefly review the matrix Ernst potential (MEP) formalism for the effective field theory of the heterotic string (for an arbitrary number of dimensions) and its formal analogy to the stationary Einstein–Maxwell (EM) system. It turns out that after setting to zero the dilaton and all U(1) vector fields, and considering the compactification of this theory on a two-torus, the resulting three-dimensional subsystem admits a Kähler representation which is defined by two vacuum Ernst potentials.

In Sec. III the parametrization which gives rise to this double Ernst system is pointed out and a discrete transformation between the metric and Kalb–Ramond degrees of freedom is established. In Sec. IV we recall the normalized Harrison transformation (NHT) and apply it on a generic seed solution of the EKR theory which corresponds to two complex Ernst potentials in order to get a charged field configuration and recover, in this way, the U(1) vector field sector of the EMKR theory.

Further, in Sec. V we reduce the system to two effective dimensions (dependence of just two dynamical coordinates) in order to be able to consider as seed solution a pair of Ernst potentials which correspond to interacting Kerr black holes. In this case, the five-dimensional line element explicitly depends on the Ernst potentials and the resulting field configuration contains a Kalb–Ramond dipole hidden inside a horizon. In Sec. VI we explicitly compute the generated charged solution, study its asymptotical behavior and give an interpretation of the field configuration. Finally, we sketch our conclusions and discuss on the further development of the present work.

II. MATRIX ERNST POTENTIAL FORMALISM

In this section we review the MEP formalism for the D-dimensional effective field theory of the heterotic string and indicate an algorithm for generating a charged solution of the double Ernst system starting from a neutral one by making use of a matrix Lie–Bäcklund transformation of Harrison type.

We consider the effective action of the heterotic string theory at tree level,

$$S^{(D)}=\int d^{(D)}x|G^{(D)}|^{1/2}e^{-\phi^{(D)}}\left(R^{(D)}+\phi^{(D)}_{;M}\phi^{(D);M}-\tfrac{1}{12}H^{(D)}_{MNP}H^{(D)MNP}-\tfrac{1}{4}F^{(D)I}_{MN}F^{(D)IMN}\right), \tag{1}$$

where

$$F^{(D)I}_{MN}=\partial_M A^{(D)I}_N-\partial_N A^{(D)I}_M, \quad H^{(D)}_{MNP}=\partial_M B^{(D)}_{NP}-\tfrac{1}{2}A^{(D)I}_M F^{(D)I}_{NP}+\text{cycl perms of } M,N,P.$$

Here $G^{(D)}_{MN}$ is the metric, $B^{(D)}_{MN}$ is the antisymmetric Kalb–Ramond field, $\phi^{(D)}$ is the dilaton, $A^{(D)I}_M$ is a set of U(1) vector fields ($I=1,2,\ldots,n$), D is the original number of space–time dimensions; capital letters $M,N,\ldots,P$ are related to the whole set of space–time coordinates, lower case letters m,n label the extra dimensions, whereas Greek letters μ,ν stand for the noncompactified coordinates. In the consistent critical case $D=10$ and $n=16$, but we shall leave these parameters arbitrary for the time being and will fix them later in Sec. III. In Refs. 9 and 10 it was shown that after the compactification of this model on a $D-3=d$-torus, the resulting three-dimensional theory possesses the SO $(d+1,d+n+1)$ symmetry group that later was identified as U-duality[11] and describes gravity through the metric tensor

$$g_{\mu\nu}=e^{-2\phi}(G^{(D)}_{\mu\nu}-G^{(D)}_{m+3,\mu}G^{(D)}_{n+3,\nu}G^{mn}),$$

coupled to the following set of three-dimensional fields:

(a) scalar fields,

$$G\equiv G_{mn}=G^{(D)}_{m+3,n+3}, \quad B\equiv B_{mn}=B^{(D)}_{m+3,n+3}, \quad A\equiv A^I_m=A^{(D)I}_{m+3}, \quad \phi=\phi^{(D)}-\tfrac{1}{2}\ln|\det G|, \tag{2}$$

(b) tensor field,

$$B_{\mu\nu} = B^{(D)}_{\mu\nu} - 4B_{mn}A^m_\mu A^n_\nu - 2(A^m_\mu A^{m+d}_\nu - A^m_\nu A^{m+d}_\mu), \tag{3}$$

(c) vector fields $A^{(a)}_\mu = ((A_1)^m_\mu, (A_2)^{m+d}_\mu, (A_3)^{2d+I}_\mu)$,

$$(A_1)^m_\mu = \tfrac{1}{2}G^{mn}G^{(D)}_{n+3,\mu}, \quad (A_3)^{I+2d}_\mu = -\tfrac{1}{2}A^{(D)I}_\mu + A^I_n A^n_\mu, \quad (A_2)^{m+d}_\mu = \tfrac{1}{2}B^{(D)}_{m+3,\mu} - B_{mn}A^n_\mu + \tfrac{1}{2}A^I_m A^{I+2d}_\mu, \tag{4}$$

where the subscripts $m,n=1,2,\ldots,d$; and $a=1,\ldots,2d+n$. In this paper we set $B_{\mu\nu}=0$ since an antisymmetric tensor has no dynamical degrees of freedom in three dimensions; this is equivalent to removing the effective cosmological constant which, in general, is included in the spectrum of the three-dimensional effective theory.

We dualize all vector fields on-shell with the aid of the pseudoscalar fields u, v, and s as follows:

$$\nabla \times \vec{A}_1 = \tfrac{1}{2}e^{2\phi}G^{-1}\left(\nabla u + \left(B + \tfrac{1}{2}AA^T\right)\nabla v + A\nabla s\right),$$

$$\nabla \times \vec{A}_3 = \tfrac{1}{2}e^{2\phi}(\nabla s + A^T\nabla v) + A^T\nabla \times \vec{A}_1, \tag{5}$$

$$\nabla \times \vec{A}_2 = \tfrac{1}{2}e^{2\phi}G\nabla v - \left(B + \tfrac{1}{2}AA^T\right)\nabla \times \vec{A}_1 + A\nabla \times \vec{A}_3.$$

Thus, the effective three-dimensional theory describes gravity $g_{\mu\nu}$ coupled to the scalars G, B, A, ϕ and pseudoscalars u, v, s. In Ref. 12 it was shown that all these matter fields can be arranged in the following pair of MEP:

$$\mathcal{X} = \begin{pmatrix} -e^{-2\phi} + v^TXv + v^TAs + \frac{1}{2}s^Ts & v^TX - u^T \\ Xv + u + As & X \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} s^T + v^TA \\ A \end{pmatrix}, \tag{6}$$

where $X=G+B+\frac{1}{2}AA^T$, in such a way that they reproduce the field equations of the three-dimensional theory. These matrices have dimensions $(d+1)\times(d+1)$ and $(d+1)\times n$, respectively.

In terms of the MEP the effective three-dimensional theory adopts the form

$${}^3S = \int d^3x|g|^{1/2}\left\{-R + \mathrm{Tr}\left[\tfrac{1}{4}(\nabla\mathcal{X} - \nabla\mathcal{A}\mathcal{A}^T)\mathcal{G}^{-1}(\nabla\mathcal{X}^T - \mathcal{A}\nabla\mathcal{A}^T)\mathcal{G}^{-1} + \tfrac{1}{2}\nabla\mathcal{A}^T\mathcal{G}^{-1}\nabla\mathcal{A}\right]\right\}, \tag{7}$$

where $\mathcal{X}=\mathcal{G}+\mathcal{B}+\frac{1}{2}\mathcal{A}\mathcal{A}^T$, then $\mathcal{G}=\frac{1}{2}(\mathcal{X}+\mathcal{X}^T-\mathcal{A}\mathcal{A}^T)$ and

$$\mathcal{G} = \begin{pmatrix} -e^{-2\phi} + v^TGv & v^TG \\ Gv & G \end{pmatrix}, \quad \mathcal{B} = \begin{pmatrix} 0 & v^TB - u^T \\ Bv + u & B \end{pmatrix}. \tag{8}$$

In Ref. 12 it also was shown that there exists a map between the stationary actions of the heterotic string and EM theories. The map reads

$$\mathcal{X} \leftrightarrow -E, \quad \mathcal{A} \leftrightarrow F,$$
$$\text{matrix transposition} \leftrightarrow \text{complex conjugation}, \tag{9}$$

where E and F are the conventional complex Ernst potentials of the stationary EM theory.[13] This map allows us to extrapolate the results obtained in the EM theory to the heterotic string realm using the MEP formulation.

The normalized Harrison transformation

In the language of the MEP the three-dimensional action (7) possesses a set of symmetries which has been classified according to their charging properties in Ref. 14. Among them one finds

the matrix Ehlers and Harrison transformations,[15] which are symmetries that change the properties of the space–time in a nontrivial way; they represent the matrix counterpart of the Bäcklund transformation of the sine-Gordon equation in the realm of the stationary heterotic string theory. For instance, the so-called normalized Harrison transformation allows us to construct charged string vacua from neutral ones preserving the asymptotical values of the three-dimensional seed fields. Namely, the matrix transformation

$$\begin{aligned}\mathcal{A} &\to \left(1+\tfrac{1}{2}\Sigma\lambda\lambda^T\right)\left(1-\mathcal{A}_0\lambda^T+\tfrac{1}{2}\mathcal{X}_0\lambda\lambda^T\right)^{-1}(A_0-\mathcal{X}_0\lambda)+\Sigma\lambda,\\ \mathcal{X} &\to \left(1+\tfrac{1}{2}\Sigma\lambda\lambda^T\right)\left(1-\mathcal{A}_0\lambda^T+\tfrac{1}{2}\mathcal{X}_0\lambda\lambda^T\right)^{-1}\left[\mathcal{X}_0+\left(\mathcal{A}_0-\tfrac{1}{2}\mathcal{X}_0\lambda\right)\lambda^T\Sigma\right]+\tfrac{1}{2}\Sigma\lambda\lambda^T\Sigma,\end{aligned} \tag{10}$$

where $\Sigma=\mathrm{diag}(-1,-1,1,\ldots,1)$ stands for the signature that the MEP $\mathcal{X}$ adopts at spatial infinity and λ is an arbitrary constant $(d+1)\times n$-matrix, generates charged string solutions (with nonzero potential $\mathcal{A}$) from neutral ones if we start from the seed potentials

$$\mathcal{X}_0 \neq 0, \quad \mathcal{A}_0 = 0.$$

The parameters that enter the matrix λ can be interpreted as electromagnetic charges that couple to the original seed object. It is precisely with the aid of this Bäcklund transformation that we shall charge the double 5D Ernst system in the next section.

III. 5D EINSTEIN–KALB–RAMOND VS DOUBLE ERNST SYSTEM

In this section we present a formulation of the resulting three-dimensional model, upon toroidal compactification of the 5D EKR theory, as a double Ernst system by means of a complete parametrization of the matrices $\mathcal{G}$ and $\mathcal{B}$ in terms of the real and imaginary parts of a pair of complex Ernst potentials.

Let us begin by setting to zero all the U(1) gauge fields which correspond to the winding modes of the three-dimensional theory [this is equivalent to dropping the matrix $\mathcal{A}$ in (7)]. Thus, we obtain the following action in terms of the MEP $\mathcal{X}$:

$${}^3S=\int d^3x|g|^{1/2}\left\{-R+\frac{1}{4}\mathrm{Tr}[\nabla\mathcal{X}\mathcal{G}^{-1}\nabla\mathcal{X}^T\mathcal{G}^{-1}]\right\}=\int d^3x|g|^{1/2}\left\{-R+\frac{1}{4}\mathrm{Tr}(J^{\mathcal{X}}J^{\mathcal{X}^T})\right\}, \tag{11}$$

where now $\mathcal{X}=\mathcal{G}+\mathcal{B}$, $\mathcal{G}=\frac{1}{2}(\mathcal{X}+\mathcal{X}^T)$, and $J^{\mathcal{X}}=\nabla\mathcal{X}\mathcal{G}^{-1}$.

There are two physically different effective theories that can be expressed by the action (11), and hence admit a double Ernst formulation. On the one hand, we have the $D=5$ EKR model, where the dilaton field is set to zero as well.[3] On the other hand, we have the $D=4$ bosonic string theory, for which a charged pair of rotating interacting black holes coupled to dilaton and Kalb–Ramond fields was constructed in Ref. 5 and its charged dual string vacua were studied in Ref. 16. Here we will consider again the 5D EKR theory in order to apply the NHT on a neutral family of field configurations that correspond to the double Ernst system.

Thus, we start with the five-dimensional truncated action

$${}^5S=\int d^5x|{}^5G|^{1/2}\left({}^5R-\frac{1}{12}{}^5H^2\right), \tag{12}$$

where ${}^5R$ is the Ricci scalar constructed on the five-dimensional metric ${}^5G_{MN}$ and

$${}^5H_{MNP}=\partial_M{}^5B_{NP}+\text{cycl perms of } M,N,P. \tag{13}$$

It is worth noticing that we are considering a truncation which imposes the following condition on the Kaluza–Klein and Kalb–Ramond vector fields:

$$^5G_{\mu,n+2} = {}^5B_{\mu,n+2} = 0; \tag{14}$$

this implies that the vector fields A_1 and A_2 must vanish identically, and hence, the pseudoscalar fields u and v also vanish [see (5)]. Such a restriction does not provide any constraint on the remaining dynamical variables and can be considered as a consistent nontrivial ansatz for the EKR theory.

After the Kaluza–Klein reduction on T^2 we get the stationary effective action (11) (see, for instance, Refs. 3 and 10) with the matter field spectrum of the theory encoded in the (2×2)-matrices $\mathcal{G}\equiv G$ and $\mathcal{B}\equiv B$ which can be parametrized in the following form:

$$\mathcal{G} = \frac{p_1}{p_2}\begin{pmatrix} 1 & q_2 \\ q_2 & p_2^2+q_2^2 \end{pmatrix}, \quad \mathcal{B} = q_1\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = q_1\sigma_2, \tag{15}$$

where σ_2 is the Pauli matrix. Under such assumptions, the five-dimensional interval reads

$$\mathrm{d}s_5^2 = g_{\mu\nu}\,\mathrm{d}x^\mu\,\mathrm{d}x^\nu + \mathcal{G}_{mn}\,\mathrm{d}x^m\,\mathrm{d}x^n. \tag{16}$$

By substituting (15) into (11) the action of the "matter fields" adopts the form

$$^3S_m = \frac{1}{2}\int d^3x|g|^{1/2}\{p_1^{-2}[(\nabla p_1)^2+(\nabla q_1)^2]+p_2^{-2}[(\nabla p_2)^2+(\nabla q_2)^2]\}, \tag{17}$$

which allows us to introduce two independent Ernst potentials,

$$\epsilon_1 = p_1 + iq_1, \quad \epsilon_2 = p_2 + iq_2. \tag{18}$$

In terms of these field variables, the action of the system can be rewritten as a double Ernst system in the Kähler form,[17]

$$^3S = \int d^3x|g|^{1/2}\{-\,{}^3R + 2(J^{\epsilon_1}J^{\bar{\epsilon_1}} + J^{\epsilon_2}J^{\bar{\epsilon_2}})\}, \tag{19}$$

where $J^{\epsilon_1} = \nabla\epsilon_1(\epsilon_1+\bar{\epsilon_1})^{-1}$ and $J^{\epsilon_2} = \nabla\epsilon_2(\epsilon_2+\bar{\epsilon_2})^{-1}$.

A mathematically equivalent, but physically different 2×2-matrix representation arises from (12) by making use of the discrete symmetry $p_1\leftrightarrow p_2$, $q_1\leftrightarrow q_2$. This fact allows us to define new matrices

$$\mathcal{G}' = \frac{p_2}{p_1}\begin{pmatrix} 1 & q_1 \\ q_1 & p_1^2+q_1^2 \end{pmatrix}, \quad \mathcal{B}' = q_2\sigma_2 \tag{20}$$

and, hence, $\mathcal{X}' = \mathcal{G}' + \mathcal{B}'$ and to write down the action that corresponds to these magnitudes,

$$^3S = \int d^3x|g|^{1/2}\left\{-R + \frac{1}{4}\mathrm{Tr}(J^{\mathcal{X}'}J^{\mathcal{X}'^T})\right\} = \int d^3x|g|^{1/2}\{-R + 2(J^{\epsilon_1'}J^{\bar{\epsilon_1'}} + J^{\epsilon_2'}J^{\bar{\epsilon_2'}})\}, \tag{21}$$

where similarly $J^{\mathcal{X}'} = \nabla\mathcal{X}'\mathcal{G}'^{-1}$, $J^{\epsilon_1'} = \nabla\epsilon_1'(\epsilon_1'+\bar{\epsilon_1'})^{-1}$, $J^{\epsilon_2'} = \nabla\epsilon_2'(\epsilon_2'+\bar{\epsilon_2'})^{-1}$, $\epsilon_1' = p_2 + iq_2$, and $\epsilon_2' = p_1 + iq_1$.

In terms of the MEP the above-mentioned discrete transformation reads

$$\mathcal{X}\leftrightarrow\mathcal{X}'; \tag{22}$$

thus, the matrices $\mathcal{G}'$ and $\mathcal{B}'$ must be interpreted as new Kaluza–Klein and Kalb–Ramond fields, respectively. This symmetry mixes the gravitational and matter degrees of freedom of the theory. It recalls the Bonnor transformation of the EM theory,[18] but in the bosonic string realm. It can be used to generate new solutions starting, for instance, from pure Kaluza–Klein string vacua (see Ref. 16 as well).

IV. APPLYING THE NHT ON THE DOUBLE ERNST SYSTEM

Let us now proceed to apply the NHT on the neutral double Ernst system. This will generate a nonzero electromagnetic potential $\mathcal{A}$ which accounts for nontrivial Abelian U(1) gauge fields. In order to achieve this aim, we must consider the following seed MEP:

$$\mathcal{X}_0 = \begin{pmatrix} \frac{p_1}{p_2} & \frac{p_1q_2 - q_1p_2}{p_2} \\ \frac{p_1q_2 + q_1p_2}{p_2} & \frac{p_1}{p_2}(p_2^2 + q_2^2) \end{pmatrix}, \quad \mathcal{A}_0 = 0. \tag{23}$$

In this case, the charge matrix λ that parametrizes the NHT has the form

$$\lambda = \begin{pmatrix} \lambda_{11} & \lambda_{12} & \cdots & \lambda_{1n} \\ \lambda_{21} & \lambda_{22} & \cdots & \lambda_{2n} \end{pmatrix}, \tag{24}$$

where $n \geqslant 2$ for consistency. Thus after applying the NHT on this double Ernst seed solution, the transformed MEP read

$$\mathcal{X}_{11} = \frac{1}{\Xi}[(4 + \Lambda^2|\epsilon_2|^2)\mathrm{Re}\,\epsilon_1 + 2(\lambda_{1j}^2 + \lambda_{2j}^2|\epsilon_1|^2)\mathrm{Re}\,\epsilon_2 + 4\lambda_{1j}\lambda_{2j}\,\mathrm{Re}\,\epsilon_2\,\mathrm{Im}\,\epsilon_1], \tag{25}$$

$$\mathcal{X}_{12} = \frac{1}{\Xi}\{\Gamma_+(\mathrm{Re}\,\epsilon_1\,\mathrm{Im}\,\epsilon_2 - \mathrm{Re}\,\epsilon_2\,\mathrm{Im}\,\epsilon_1) + 2\lambda_{1j}\lambda_{2j}[(1 - |\epsilon_1|^2)\mathrm{Re}\,\epsilon_2 - (1 - |\epsilon_2|^2)\mathrm{Re}\,\epsilon_1]\}, \tag{26}$$

$$\mathcal{X}_{21} = \frac{1}{\Xi}\{\Gamma_-(\mathrm{Re}\,\epsilon_1\,\mathrm{Im}\,\epsilon_2 + \mathrm{Re}\,\epsilon_2\,\mathrm{Im}\,\epsilon_1) + 2\lambda_{1j}\lambda_{2j}[(1 - |\epsilon_2|^2)\mathrm{Re}\,\epsilon_1 + (1 - |\epsilon_1|^2)\mathrm{Re}\,\epsilon_2]\}, \tag{27}$$

$$\mathcal{X}_{22} = \frac{1}{\Xi}[(\Lambda^2 + 4|\epsilon_2|^2)\mathrm{Re}\,\epsilon_1 + 2(\lambda_{2j}^2 + \lambda_{1j}^2|\epsilon_1|^2)\mathrm{Re}\,\epsilon_2 - 4\lambda_{1j}\lambda_{2j}\,\mathrm{Re}\,\epsilon_2\,\mathrm{Im}\,\epsilon_1], \tag{28}$$

$$\mathcal{A}_{1j} = \frac{2}{\Xi}\{[(2 - \lambda_{2j}^2|\epsilon_1|^2)\mathrm{Re}\,\epsilon_2 - (2 - \lambda_{2j}^2|\epsilon_2|^2)\mathrm{Re}\,\epsilon_1 + \lambda_{1j}\lambda_{2j}(\mathrm{Re}\,\epsilon_1\,\mathrm{Im}\,\epsilon_2 - \mathrm{Re}\,\epsilon_2\,\mathrm{Im}\,\epsilon_1)]\lambda_{1j} - [(2 + \lambda_{1j}^2)(\mathrm{Re}\,\epsilon_1\,\mathrm{Im}\,\epsilon_2 - \mathrm{Re}\,\epsilon_2\,\mathrm{Im}\,\epsilon_1) + \lambda_{1j}\lambda_{2j}(|\epsilon_2|^2\,\mathrm{Re}\,\epsilon_1 - |\epsilon_1|^2\,\mathrm{Re}\,\epsilon_2)]\lambda_{2j}\}, \tag{29}$$

$$\mathcal{A}_{2j} = \frac{-2}{\Xi}\{[(2 + \lambda_{2j}^2)(\mathrm{Re}\,\epsilon_1\,\mathrm{Im}\,\epsilon_2 + \mathrm{Re}\,\epsilon_2\,\mathrm{Im}\,\epsilon_1) + \lambda_{1j}\lambda_{2j}(\mathrm{Re}\,\epsilon_1 - |\epsilon_1|^2\,\mathrm{Re}\,\epsilon_2)]\lambda_{1j} - [(\lambda_{1j}^2 - 2|\epsilon_2|^2)\mathrm{Re}\,\epsilon_1 + (2 - \lambda_{1j}^2|\epsilon_1|^2)\mathrm{Re}\,\epsilon_2 + \lambda_{1j}\lambda_{2j}(\mathrm{Re}\,\epsilon_1\,\mathrm{Im}\,\epsilon_2 + \mathrm{Re}\,\epsilon_2\,\mathrm{Im}\,\epsilon_1)]\lambda_{2j}\}, \tag{30}$$

$$\Xi = 2(\lambda_{1j}^2 + \lambda_{2j}^2|\epsilon_2|^2)\mathrm{Re}\,\epsilon_1 + (4 + \Lambda^2|\epsilon_1|^2)\mathrm{Re}\,\epsilon_2 + 4\lambda_{1j}\lambda_{2j}\,\mathrm{Re}\,\epsilon_1\,\mathrm{Im}\,\epsilon_2, \tag{31}$$

where $\Lambda^2 = \lambda_{1j}^2\lambda_{2j}^2 - (\lambda_{1j}\lambda_{2j})^2$, $\Gamma_+ = 4 + 2\lambda_{1j}^2 - 2\lambda_{2j}^2 - \Lambda^2$, $\Gamma_- = 4 - 2\lambda_{1j}^2 + 2\lambda_{2j}^2 - \Lambda^2$, and the nontrivial character of the matrix $\mathcal{A}$ is evident. The fields configurations corresponding to these potentials live now in the 5D EMKR theory since we have recovered the U(1) vector fields of the system.

V. DOUBLE KERR SEED SOLUTION

In this section, following Ref. 3 we impose one more symmetry on the fields of the three-dimensional effective theory under consideration in order to use as seed solution a pair of Kerr black holes. Thus, we can write the line element in the Lewis–Papapetrou form making use of the Weyl coordinates as follows:

$$^{5}ds^2 = \mathcal{G}_{mn}\, dx^m\, dx^n + e^{2\gamma}(d\rho^2 + dz^2) - \rho^2\, d\tau^2, \tag{32}$$

where $\mathcal{G}_{mn}$ and γ are τ-independent. Thus, a solution of our system can be constructed using the solutions of the double vacuum Einstein equations written in the Ernst form in terms of ϵ_k and γ^{ϵ_k} $(k=1,2)$,

$$\nabla(\rho J^{\epsilon_k}) = \rho J^{\epsilon_k}(J^{\epsilon_k} - J^{\overline{\epsilon_k}}),$$

$$\partial_z \gamma^{\epsilon_k} = \rho[(J^{\epsilon_k})_z (J^{\overline{\epsilon_k}})_\rho + (J^{\overline{\epsilon_k}})_z (J^{\epsilon_k})_\rho], \tag{33}$$

$$\partial_\rho \gamma^{\epsilon_k} = \rho[|(J^{\epsilon_k})_\rho|^2 - |(J^{\epsilon_k})_z|^2],$$

if one identifies the function γ that accounts for the general relativistic interaction between the black holes, in the following way: $\gamma \equiv \gamma^{\epsilon_1} + \gamma^{\epsilon_2}$.

For instance, we can take as seed solution a double Kerr system consisting of a pair of rotating interacting black holes. In the framework of general relativity, the Ernst potentials corresponding to two Kerr solutions with sources in different points of the symmetry axis read

$$\epsilon_k = 1 - \frac{2m_k}{r_k + i\alpha_k \cos\theta_k}, \tag{34}$$

where m_k and α_k are constant parameters which define the masses and rotations of the sources of the Kerr field configurations. Weyl and Boyer–Lindquist coordinates are related through

$$\rho = [(r_k - m_k)^2 - \zeta_k^2]^{1/2} \sin\theta_k, \quad z = z_k + (r_k - m_k)\cos\theta_k, \tag{35}$$

where the sources are located at z_k and $\zeta_k^2 = m_k^2 - a_k^2$. Thus, for the function γ_k we have

$$e^{2\gamma_k} = \frac{P_k}{Q_k}, \tag{36}$$

where $P_k = \Delta_k - \alpha_k^2 \sin^2\theta_k$, $Q_k = \Delta_k + \zeta_k^2 \sin^2\theta_k$, and $\Delta_k = r_k^2 - 2m_k r_k + \alpha_k^2$.

We would like to make a remark at this point. When parametrizing the 5D interval (32) in the Lewis–Papapetrou form, one could choose a completely spatial (Euclidean) three-dimensional interval and require that the signature of the matrix $\mathcal{G}$ to be negative definite, i.e., $\mathcal{G}|_\infty = -I_2$ (the same signature holds for the matrix $\mathcal{X}|_\infty$). Thus, the five-dimensional metric would possess a signature with two timelike coordinates. Such kind of models have been studied in Ref. 19 and represent another line of investigation within this approach. It is clear that in order to fulfill this condition either ϵ_1 or ϵ_2 must adopt the asymptotic value -1, since when both potentials have the same asymptotic behavior (with the same sign) the signature of the matrix $\mathcal{G}$ is positive definite.

Thus, in the language of the complex Ernst potentials the field configuration adopt the form

$$ds_5^2 = e^{2\gamma}(d\rho^2 + dz^2) - \rho^2\, d\tau^2 + \frac{\epsilon_1 + \overline{\epsilon_1}}{\epsilon_2 + \overline{\epsilon_2}} |du + i\overline{\epsilon_2}\, dv|^2, \tag{37}$$

$$\mathcal{B} = \frac{\epsilon_1 - \overline{\epsilon_1}}{2i}\sigma_2, \tag{38}$$

where $u = x^4$, $v = x^5$, and $\gamma = \gamma^{\epsilon_1} + \gamma^{\epsilon_2}$ as it was pointed out above.

In the case when the Ernst potentials correspond to two interacting Kerr black holes, the symmetric matrix $\mathcal{G}$ is determined by the follow

$$\mathcal{G}_{uu}=\frac{(r_1^2-2m_1r_1+\alpha_1^2\cos^2\theta_1)(r_2^2+\alpha_2^2\cos^2\theta_2)}{(r_2^2-2m_2r_2+\alpha_2^2\cos^2\theta_2)(r_1^2+\alpha_1^2\cos^2\theta_1)},$$

$$\mathcal{G}_{uv}=\frac{2m_2\alpha_2\cos\theta_2(r_1^2-2m_1r_1+\alpha_1^2\cos^2\theta_1)}{(r_2^2-2m_2r_2+\alpha_2^2\cos^2\theta_2)(r_1^2+\alpha_1^2\cos^2\theta_1)}, \tag{39}$$

$$\mathcal{G}_{vv}=\frac{(r_1^2-2m_1r_1+\alpha_1^2\cos^2\theta_1)(r_2^2-4m_2r_2+4m_2^2+\alpha_2^2\cos^2\theta_2)}{(r_2^2-2m_2r_2+\alpha_2^2\cos^2\theta_2)(r_1^2+\alpha_1^2\cos^2\theta_1)},$$

ing relations:the factor $e^{2\gamma}$ reads

$$e^{2\gamma}=\frac{(r_1^2-2m_1r_1+\alpha_1^2\cos^2\theta_1)(r_2^2-2m_2r_2+\alpha_2^2\cos^2\theta_2)}{(r_1^2-2m_1r_1+\alpha_1^2\cos^2\theta_1+m_1^2\sin^2\theta_2)(r_2^2-2m_2r_2+\alpha_2^2\cos^2\theta_2+m_2^2\sin^2\theta_2)}, \tag{40}$$

and the Kalb–Ramond matrix $\mathcal{B}$ is defined as

$$\mathcal{B}=\frac{2m_1\alpha_1\cos\theta_1}{r_1^2+\alpha_1^2\cos^2\theta_1}\sigma_2 \tag{41}$$

and can be interpreted as a matrix Kalb–Ramond dipole configuration with momentum $m_1\alpha_1$ located at z_1 and hidden inside the horizon $r_1=m_1+\sqrt{m_1^2-\alpha_1^2}$ of the metric (37). Simultaneously, the $\mathcal{G}_{uv}$ metric component also constitutes a dipole configuration but possesses momentum $m_2\alpha_2$ and is located at z_2, hidden inside the horizon $r_2=m_2+\sqrt{m_2^2-\alpha_2^2}$.

VI. CHARGED FIELD CONFIGURATIONS IN 5D EMKR THEORY

After applying the NHT on the double Ernst seed solution we get the following field configurations:

$$\mathcal{G}_{uu}=\mathcal{X}_{11}-\tfrac{1}{2}\mathcal{A}_{1j}^2,\quad \mathcal{G}_{uv}=\tfrac{1}{2}(\mathcal{X}_{12}+\mathcal{X}_{21}-\mathcal{A}_{1j}\mathcal{A}_{2j}),\quad \mathcal{G}_{vv}=\mathcal{X}_{22}-\tfrac{1}{2}\mathcal{A}_{2j}^2, \tag{42}$$

$$\mathcal{B}=\tfrac{1}{2}(\mathcal{X}_{21}-\mathcal{X}_{12})\sigma_2,\quad \mathcal{A}\equiv A=\begin{pmatrix}\mathcal{A}_{1j}\\ \mathcal{A}_{2j}\end{pmatrix}, \tag{43}$$

where the appearance of the electromagnetic potential is obvious. By substituting the Ernst potentials ϵ_k by the corresponding double Kerr black hole system we obtain the following charged field configuration:

$$\mathcal{G}_{uu}=\frac{DQ\Delta_1\Delta_2+4m_1(L^2r_1+2m_1\lambda_{2j}^2+2\lambda_{1j}\lambda_{2j}\alpha_1\cos\theta_1)\Delta_2+2m_2[(4-\Lambda^2)r_2+2\Lambda^2m_2]\Delta_1}{DQ\Delta_1\Delta_2+4m_2(L^2r_2+2m_2\lambda_{2j}^2+2\lambda_{1j}\lambda_{2j}\alpha_2\cos\theta_2)\Delta_1+2m_1[(4-\Lambda^2)r_1+2\Lambda^2m_1]\Delta_2}$$
$$-\frac{8(h_1\lambda_{1j}-h_2\lambda_{2j})^2+2\Lambda^2(h_2\lambda_{1j}-h_3\lambda_{2j})^2-8\Lambda^2(h_1h_3-h_2^2)}{[DQ\Delta_1\Delta_2+4m_2(L^2r_2+2m_2\lambda_{2j}^2+2\lambda_{1j}\lambda_{2j}\alpha_2\cos\theta_2)\Delta_1+2m_1[(4-\Lambda^2)r_1+2\Lambda^2m_1]\Delta_2]^2}, \tag{44}$$

$$\mathcal{G}_{uv}=\frac{4m_1[2\lambda_{1j}\lambda_{2j}(r_1-m_1)-L^2\alpha_1\cos\theta_1]\Delta_2+2(4-\Lambda^2)m_2\alpha_2\cos\theta_2\Delta_1}{DQ\Delta_1\Delta_2+4m_2(L^2r_2+2m_2\lambda_{2j}^2+2\lambda_{1j}\lambda_{2j}\alpha_2\cos\theta_2)\Delta_1+2m_1[(4-\Lambda^2)r_1+2\Lambda^2m_1]\Delta_2}$$
$$+\frac{4(l_1^2h_1h_4+l_2^2h_2h_6)+2\Lambda^2[(2+\lambda_{1j}^2)h_2h_5-(2+\lambda_{2j}^2)h_3h_4]-2\lambda_{1j}\lambda_{2j}[4h_1h_6+\Lambda^2h_3h_5+(4-\Lambda^2)h_2h_4]}{[DQ\Delta_1\Delta_2+4m_2(L^2r_2+2m_2\lambda_{2j}^2+2\lambda_{1j}\lambda_{2j}\alpha_2\cos\theta_2)\Delta_1+2m_1[(4-\Lambda^2)r_1+2\Lambda^2m_1]\Delta_2]^2}, \tag{45}$$

$$\mathcal{G}_{vv} = \frac{DQ\Delta_1\Delta_2 - 2m_2[(4-\Lambda^2)r_2 - 8m_2]\Delta_1 - 4m_1(L^2 r_1 - 2m_1\lambda_{1j}^2 + 2\lambda_{1j}\lambda_{2j}\alpha_1\cos\theta_1)\Delta_2}{DQ\Delta_1\Delta_2 + 4m_2(L^2 r_2 + 2m_2\lambda_{2j}^2 + 2\lambda_{1j}\lambda_{2j}\alpha_2\cos\theta_2)\Delta_1 + 2m_1[(4-\Lambda^2)r_1 + 2\Lambda^2 m_1]\Delta_2}$$
$$- \frac{8(h_4h_{1j} - h_6\lambda_{2j})^2 + 2\Lambda^2(h_5\lambda_{1j} + h_4\lambda_{2j})^2 + 8\Lambda^2(h_5h_6 + h_4^2)}{[DQ\Delta_1\Delta_2 + 4m_2(L^2 r_2 + 2m_2\lambda_{2j}^2 + 2\lambda_{1j}\lambda_{2j}\alpha_2\cos\theta_2)\Delta_1 + 2m_1[(4-\Lambda^2)r_1 + 2\Lambda^2 m_1]\Delta_2]^2}, \tag{46}$$

$$\mathcal{B}_{uv} = \frac{2(4-\Lambda^2)m_1\alpha_1\cos\theta_1\Delta_2 + 4m_2[2\lambda_{1j}\lambda_{2j}(r_2 - m_2) - L^2\alpha_2\cos\theta_2]\Delta_1}{DQ\Delta_1\Delta_2 + 4m_2(L^2 r_2 + 2m_2\lambda_{2j}^2 + 2\lambda_{1j}\lambda_{2j}\alpha_2\cos\theta_2)\Delta_1 + 2m_1[(4-\Lambda^2)r_1 + 2\Lambda^2 m_1]\Delta_2}, \tag{47}$$

$$\mathcal{A}_{1j} = \frac{2[2h_1 - \lambda_{2i}^2 h_3 + \lambda_{1i}\lambda_{2i}h_2]\lambda_{1j} + 2[\lambda_{1i}\lambda_{2i}h_3 - (2+\lambda_{1i}^2)h_2]\lambda_{2j}}{DQ\Delta_1\Delta_2 + 4m_2(L^2 r_2 + 2m_2\lambda_{2j}^2 + 2\lambda_{1j}\lambda_{2j}\alpha_2\cos\theta_2)\Delta_1 + 2m_1[(4-\Lambda^2)r_1 + 2\Lambda^2 m_1]\Delta_2}, \tag{48}$$

$$\mathcal{A}_{2j} = \frac{-2[(2+\lambda_{2i}^2)h_4 + \lambda_{1i}\lambda_{2i}h_5]\lambda_{1j} + 2[\lambda_{1i}^2 h_5 + \lambda_{1i}\lambda_{2i}h_4 + 2h_6]\lambda_{2j}}{DQ\Delta_1\Delta_2 + 4m_2(L^2 r_2 + 2m_2\lambda_{2j}^2 + 2\lambda_{1j}\lambda_{2j}\alpha_2\cos\theta_2)\Delta_1 + 2m_1[(4-\Lambda^2)r_1 + 2\Lambda^2 m_1]\Delta_2}, \tag{49}$$

where

$$h_1 = 2(m_1 r_1\Delta_2 - m_2 r_2\Delta_1), \quad h_2 = 2(m_2\alpha_2\cos\theta_2\Delta_1 - m_1\alpha_1\cos\theta_1\Delta_2),$$

$$h_3 = 4(m_1^2\Delta_2 - m_2^2\Delta_1) - h_1, \quad h_4 = 2(m_1\alpha_1\cos\theta_1\Delta_2 + m_2\alpha_2\cos\theta_2\Delta_1),$$

$$h_5 = 2[m_1(r_1 - 2m_1)\Delta_2 + m_2 r_2\Delta_1], \quad h_6 = 2[m_1 r_1\Delta_2 + m_2(r_2 - 2m_2)\Delta_1], \tag{50}$$

$L^2 = \lambda_{1j}^2 - \lambda_{2j}^2$, $l_k^2 = 2\lambda_{kj}^2 + \Lambda^2$, $\Delta_k = r_k^2 - 2m_k r_k + \alpha_k^2\cos^2\theta_k$ $(k=1,2)$ and, finally, $DQ = 4 + 2\lambda_{1j}^2 + 2\lambda_{2j}^2 + \Lambda^2$.

A consistency checking of the generated solution consists of setting the parameters λ_{1j} and λ_{2j} to zero in order to recover the starting field configuration (39)–(41). It is straightforward to verify that this is indeed the case.

The asymptotical behavior of the generated three-dimensional field configurations read

$$\mathcal{G}_{uu}|_\infty \sim 1 - \frac{2\Gamma_-(m_1 - m_2)}{DQr} + \frac{8\lambda_{1j}\lambda_{2j}(m_1\alpha_1\cos\theta_1 - m_2\alpha_2\cos\theta_2)}{DQr^2} + \mathcal{O}(r^{-2}), \tag{51}$$

$$\mathcal{G}_{uv}|_\infty \sim \frac{8\lambda_{1j}\lambda_{2j}m_1}{DQr} - \frac{4L^2 m_1\alpha_1\cos\theta_1 - 2(4-\Lambda^2)m_2\alpha_2\cos\theta_2}{DQr^2} + \mathcal{O}(r^{-2}), \tag{52}$$

$$\mathcal{G}_{vv}|_\infty \sim 1 - \frac{2\Lambda_+(m_1 + m_2)}{DQr} - \frac{8\lambda_{1j}\lambda_{2j}(m_1\alpha_1\cos\theta_1 + m_2\alpha_2\cos\theta_2)}{DQr^2} + \mathcal{O}(r^{-2}), \tag{53}$$

$$\mathcal{B}_{uv}|_\infty \sim \frac{8\lambda_{1j}\lambda_{2j}m_2}{DQr} + \frac{2(4-\Lambda^2)m_1\alpha_1\cos\theta_1 - 4L^2 m_2\alpha_2\cos\theta_2}{DQr^2} + \mathcal{O}(r^{-2}), \tag{54}$$

$$\mathcal{A}_{1j}|_{\infty} \sim \frac{4[(2+\lambda_{2i}^2)\lambda_{1j}-\lambda_{1i}\lambda_{2i}\lambda_{2j}](m_1-m_2)}{DQr} - \frac{4[\lambda_{1i}\lambda_{2i}\lambda_{1j}-(2+\lambda_{1i}^2)\lambda_{2j}](m_1\alpha_1\cos\theta_1-m_2\alpha_2\cos\theta_2)}{DQr^2}+\mathcal{O}(r^{-2}), \tag{55}$$

$$\mathcal{A}_{2j}|_{\infty} \sim \frac{-4[\lambda_{1i}\lambda_{2i}\lambda_{1j}-(2+\lambda_{1i}^2)\lambda_{2j}](m_1+m_2)}{DQr} + \frac{4[(2+\lambda_{2i}^2)\lambda_{1j}-\lambda_{1i}\lambda_{2i}\lambda_{2j}](m_1\alpha_1\cos\theta_1+m_2\alpha_2\cos\theta_2)}{DQr^2}+\mathcal{O}(r^{-2}). \tag{56}$$

From this analysis it is clear that under the NHT, all the generated fields (gravitational, Kalb–Ramond, and electromagnetic) effectively develop both Coulomb and dipole terms. Thus, from one side, the $\mathcal{G}_{uu}$ component of the constructed metric possesses mass terms defined by $M_{uu_1}=\Gamma_- m_1/DQ$ at z_1 and $M_{uu_2}=\Gamma_- m_2/DQ$ at z_2, and from the other side, it acquires dipole sources with masses $\tilde{M}_{uu_1}=8\lambda_{1j}\lambda_{2j}m_1/DQ$, $\tilde{M}_{uu_2}=-8\lambda_{1j}\lambda_{2j}m_2/DQ$, and their corresponding momenta $\tilde{M}_{uu_1}\alpha_1$, $\tilde{M}_{uu_2}\alpha_2$, located at z_1 and z_2, respectively. In a similar way the $\mathcal{G}_{vv}$ component of the metric has masses $M_{vv_1}=\Gamma_+ m_1/DQ$ at z_1 and $M_{vv_2}=\Gamma_+ m_2/DQ$ at z_2; indeed, it possesses as well the massive dipole terms defined by $\tilde{M}_{vv_1}=-8\lambda_{1j}\lambda_{2j}m_1/DQ$ at z_1 and $\tilde{M}_{uu_2}=-8\lambda_{1j}\lambda_{2j}m_2/DQ$ at z_2 with the momenta $\tilde{M}_{vv_1}\alpha_1$ and $\tilde{M}_{vv_2}\alpha_2$, respectively.

The transformed Kalb–Ramond tensor field also acquires a Coulomb term determined by the charge $M_B=8\lambda_{1j}\lambda_{2j}m_2/DQ$ located at z_2 and now possesses two dipole sources with masses $M_{B_1}=(4-\Lambda^2)m_1/DQ$, $M_{B_2}=-4L^2m_2/DQ$ and momenta $M_{B_1}\alpha_1$, $M_{B_2}\alpha_2$, located at z_1 and z_2, respectively. The same situation exactly takes place for the $\mathcal{G}_{uv}$ component of the metric, which usually corresponds to the rotation of the gravitational field. Thus, the generated gravitational potential $\mathcal{G}_{uv}$ has a Coulomb source with mass $M_{uv}=8\lambda_{1j}\lambda_{2j}m_1/DQ$ located at z_1 and dipole sources with masses $\tilde{M}_{uv_1}=-2L^2m_1/DQ$, $\tilde{M}_{uv_2}=(4-\Lambda^2)m_2/DQ$ and momenta $\tilde{M}_{uv_1}\alpha_1$, $\tilde{M}_{uv_2}\alpha_2$, located at z_1 and z_2, respectively.

At this point we would like to point out that the discrete symmetry (22) which relates gravitational and Kalb–Ramond degrees of freedom is still present asymptotically and is quite evident in the language of the masses and charges of the components $\mathcal{G}_{uv}$ and $\mathcal{B}_{uv}$, since one can clearly see that these components transform into each other under the interchange of the respective masses and charges, even after the implementation of the nonlinear NHT.

Finally, the generated field configuration possesses an evidently nontrivial electromagnetic sector and its asymptotic structure reveals its usual Coulomb form, defining in this way the effective electromagnetic charges of the system. These fields also have effective dipole sources. Thus, the electromagnetic fields $\mathcal{A}_{1j}$ possess momenta defined by the expressions $4[\lambda_{1i}\lambda_{2i}\lambda_{1j}-(2+\lambda_{1i}^2)\lambda_{2j}]m_1\alpha_1/DQ$ and $-4[\lambda_{1i}\lambda_{2i}\lambda_{1j}-(2+\lambda_{1i}^2)\lambda_{2j}]m_2\alpha_2/DQ$, whereas the respective momenta for the electromagnetic fields $\mathcal{A}_{2j}$ read $4[(2+\lambda_{2i}^2)\lambda_{1j}-\lambda_{1i}\lambda_{2i}\lambda_{2j}]m_1\alpha_1/DQ$ and $4[(2+\lambda_{2i}^2)\lambda_{1j}-\lambda_{1i}\lambda_{2i}\lambda_{2j}]m_2\alpha_2/DQ$.

Thus, under the NHT, the double Kerr seed solution does not acquire just the electromagnetic charges, but it develops as well effective Coulomb and dipole terms for all the fields of the field configuration, gravitational, Kalb–Ramond, and electromagnetic fields.

VII. CONCLUSION AND DISCUSSION

In this paper we have obtained a charged field configuration of the five-dimensional EMKR theory starting from a neutral one that corresponds to a double Ernst (double Kerr, in particular) system. The generation of the new charged solution was carried out via a matrix Lie–Bäcklund transformation of Harrison type that preserves the asymptotical values of the seed fields.

An interesting feature of the generated exact solution is that all the fields of the field configuration develop effective Coulomb and dipole terms asymptotically. Thus, after applying the NHT, the 5D double Kerr seed solution acquires effective Coulomb terms and dipole sources with momenta. This is in contrast with the effect that the NHT produces on a neutral seed solution in the framework of the general theory of relativity where it just endows the initial field configuration with a set of electromagnetic charges.

The statistical analysis of such a configuration is an appealing direction to conduct the present research. The equilibrium properties of the generated solution is of interest as well and would generalize to the 5D case some previous results obtained in the framework of the four-dimensional general relativity.[2,20,21] These issues are under current investigation.

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Commuting flows and conservation laws for noncommutative Lax hierarchies

Masashi Hamanaka[a)]
Graduate School of Mathematics, Nagoya University, Chikusa-ku, Nagoya, 464-8602, Japan

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We discuss commuting flows and conservation laws for Lax hierarchies on noncommutative spaces in the framework of the Sato theory. On commutative spaces, the Sato theory has revealed essential aspects of the integrability for wide class of soliton equations which are derived from the Lax hierarchies in terms of pseudo-differential operators. Noncommutative extension of the Sato theory has been already studied by the author and Toda, and the existence of various noncommutative Lax hierarchies are guaranteed. In this paper, we present conservation laws for the noncommutative Lax hierarchies with both space–space and space–time noncommutativities and prove the existence of infinite number of conserved densities. We also give the explicit representations of them in terms of Lax operators. Our results include noncommutative versions of KP, KdV, Boussinesq, coupled KdV, Sawada-Kotera, modified KdV equation and so on. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1865321]

I. INTRODUCTION

Noncommutative (NC) extension of field theories has been studied intensively for the last several years.[1] NC gauge theories are equivalent to ordinary gauge theories in the presence of background magnetic fields and succeeded in revealing various aspects of them.[2] NC solitons especially play important roles in the study of D-brane dynamics, such as the confirmation of Sen's conjecture on tachyon condensation.[3] One of the distinguished features of NC theories is resolution of singularities. This gives rise to various new physical objects such as U(1) instantons and makes it possible to analyze singular configurations as usual.

NC extension of integrable equations such as the Korteweg–de Vries (KdV) equation[4] is also one of the hot topics.[5–37] These equations imply no gauge field and NC extension of them perhaps might have no physical picture or no good property on integrabilities. To make matters worse, the NC extension of $(1+1)$-dimensional equations introduces infinite number of time derivatives, which makes it hard to discuss or define the integrability. However, some of them actually possess integrable properties, such as the existence of infinite number of conserved quantities[7–9,20] and the linearizability[30,31] which are widely accepted as definition of complete integrability of equations. Furthermore, a few of them can be derived from NC (anti-)self-dual Yang–Mills (YM) equations by suitable reductions.[14,30,33] This fact may give some physical meanings and good properties to the lower-dimensional NC field equations and makes us expect that the Ward conjecture[38] still holds on NC spaces.[27] So far, however, those equations have been examined one by one. Now it is very natural to discuss their integrabilities in more general framework.

The author and Toda have studied systematic NC extension of integrable systems.[27,30,36] In the previous paper,[36] we have obtained wide class of NC Lax hierarchies which include various NC versions of soliton equations in the framework of the Sato theory.[39] On commutative spaces, the Sato theory is known to be one of the most beautiful theories of solitons and reveals essential

a)Electronic mail: hamanaka@math.nagoya-u.ac.jp

aspects of the integrability, such as, the construction of exact multisoliton solutions, the structure of the solution space, the existence of infinite conserved quantities, and the hidden symmetry of them. In the Sato theory, the soliton equations are described by Lax hierarchies in terms of pseudodifferential operators.

In the present paper, we prove the existence of infinite conserved quantities for Lax hierarchies on NC spaces in the framework of the Sato theory. We show the conservation laws for them and give the explicit representations with both space–space and space–time noncommutativities. This suggests that the NC soliton equations are also completely integrable and infinite-dimensional symmetries would be hidden. Our results include wide class of NC soliton equations, such as, NC versions of Kadomtsev–Petviashvili (KP),[40] KdV, Boussinesq,[41] coupled KdV,[42] Sawada–Kotera,[43] modified KdV (mKdV) equations and so on.

II. COMMENTS ON NONCOMMUTATIVE FIELD THEORIES

NC spaces are defined by noncommutativity of the coordinates,

$$[x^i,x^j]=i\theta^{ij}, \tag{2.1}$$

where θ^{ij} are real constants and called the *NC parameters*.

NC field theories are obtained from given commutative field theories by exchange of ordinary products in the commutative field theories for *star-products*. The star-product is defined for ordinary fields on commutative spaces. On Euclidean spaces, it is explicitly given by

$$f(x)\star g(x):=f(x)\exp\left(\frac{i}{2}\overleftarrow{\partial}_i\theta^{ij}\overrightarrow{\partial}_j\right)g(x)=f(x)g(x)+\frac{i}{2}\theta^{ij}\partial_i f(x)\partial_j g(x)+\mathcal{O}(\theta^2), \tag{2.2}$$

where $\partial_i:=\partial/\partial x^i$. This explicit representation is known as the *Moyal product*.[44]

The star-product possesses associativity, $f\star(g\star h)=(f\star g)\star h$, and returns back to the ordinary product in the commutative limit, $\theta^{ij}\to 0$. The modification of the product makes the ordinary spatial coordinates "noncommutative," that is, $[x^i,x^j]_\star:=x^i\star x^j-x^j\star x^i=i\theta^{ij}$.

We note that the fields themselves take c-numbers values and the differentiation and the integration for them are well-defined as usual. NC field theories should be interpreted as deformed theories from commutative ones. One of the nontrivial points in the NC extension is the order of nonlinear terms. The difference between commutative equations and the NC equations arises as commutators of fields which sometimes become serious obstructions.

Here we point out a special property of the NC commutators of fields. It is convenient to introduce the following symbol:

$$P:=\tfrac{1}{2}\overleftarrow{\partial}_i\theta^{ij}\overrightarrow{\partial}_j, \tag{2.3}$$

and the *Strachan product*[45]

$$f(x)\ \diamondsuit\ g(x):=f(x)\left(\sum_{s=0}^{\infty}\frac{(-1)^s}{(2s+1)!}P^{2s}\right)g(x). \tag{2.4}$$

A commutator of fields is straightforwardly calculated as follows:

$$\begin{aligned}[f(x),g(x)]_\star &= f(x)(e^{iP}-e^{-iP})g(x)=:2if(x)(\sin P)g(x)\\ &=-\theta^{ij}\partial_i f(x)\ \diamondsuit\ \partial_j g(x)=-\theta^{ij}\partial_i(f(x)\ \diamondsuit\ \partial_j g(x)).\end{aligned} \tag{2.5}$$

In the second line, we use the fact that $\sin P$ is the composite of P and "$P^{-1}\sin P$" and the Strachan product "$\diamondsuit$" corresponds to the latter. This derivation was first presented by Dimakis and Müller-Hoissen in order to generate infinite number of conserved densities of the NC nonlinear Schrödinger (NLS) equation,[7] the NC KdV equation,[8] and the NC extended matrix-NLS equation.[9] Here more widely, we would like to stress that *commutators of fields on NC spaces*

always appear as total derivatives in the NC directions. This will be crucial in the derivation of conservation laws in Sec. V.

As a consequence, we can prove

$$\int \mathrm{d}^D x\, f(x) \star g(x) = \int d^D x\, f(x) g(x), \tag{2.6}$$

where the integration is taken in all NC directions.

III. NONCOMMUTATIVE LAX HIERARCHIES IN SATO'S FRAMEWORK

In this section, we derive various NC Lax equations in terms of pseudodifferential operators which include negative powers of differential operators. We note that the present discussion in this section can be applied to more general cases where the products are not necessarily the star-products but noncommutative associative products with differentiations, which has already been discussed in, e.g., Ref. 46. However, we believe that some explicit examples here are new equations and would be useful for further studies.

An Nth order (monic) pseudodifferential operator A is represented as follows:

$$A = \partial_x^N + a_{N-1}\partial_x^{N-1} + \cdots + a_0 + a_{-1}\partial_x^{-1} + a_{-2}\partial_x^{-2} + \cdots . \tag{3.1}$$

Here we introduce useful symbols,

$$A_{\geqslant r} := \partial_x^N + a_{N-1}\partial_x^{N-1} + \cdots + a_r \partial_x^r, \tag{3.2}$$

$$A_{\leqslant r} := A - A_{\geqslant r+1} = a_r \partial_x^r + a_{r-1}\partial_x^{r-1} + \cdots , \tag{3.3}$$

$$\mathrm{res}_r A := a_r. \tag{3.4}$$

The symbol $\mathrm{res}_{-1} A$ is especially called the *residue* of A.

The action of a differential operator ∂_x^n on a multiplicity operator f is formally defined as the following generalized Leibniz rule:

$$\partial_x^n \cdot f := \sum_{i \geqslant 0} \binom{n}{i} (\partial_x^i f) \partial^{n-i}, \tag{3.5}$$

where the binomial coefficient is given by

$$\binom{n}{i} := \frac{n(n-1)\cdots(n-i+1)}{i(i-1)\cdots 1}. \tag{3.6}$$

We note that the definition of the binomial coefficient (3.6) is applicable to the case for negative n, which just defines the action of negative power of differential operators. The examples are

$$\begin{aligned} \partial_x^{-1} \cdot f &= f\partial_x^{-1} - f'\partial_x^{-2} + f''\partial_x^{-3} - \cdots , \\ \partial_x^{-2} \cdot f &= f\partial_x^{-2} - 2f'\partial_x^{-3} + 3f''\partial_x^{-4} - \cdots , \\ \partial_x^{-3} \cdot f &= f\partial_x^{-3} - 3f'\partial_x^{-4} + 6f''\partial_x^{-5} - \cdots , \end{aligned} \tag{3.7}$$

where $f' := \partial f/\partial x$, $f'' := \partial^2 f/\partial x^2$ and so on, and ∂_x^{-1} in the RHS acts as an integration operator $\int^x \mathrm{d}x$.

The composition of pseudodifferential operators is also well-defined and the total set of pseudodifferential operators forms an operator algebra. For more on pseudodifferential operators and the Sato theory, see, e.g., Refs. 47–49.

Let us introduce a Lax operator as the following first-order pseudodifferential operator:

$$L = \partial_x + u_1 + u_2\partial_x^{-1} + u_3\partial_x^{-2} + u_4\partial_x^{-3} + \cdots, \tag{3.8}$$

where the coefficients $u_k(k=1,2,\ldots)$ are functions of infinite variables $(x^1,x^2,\ldots)$ with $x^1 \equiv x$,

$$u_k = u_k(x^1,x^2,\ldots). \tag{3.9}$$

The noncommutativity is arbitrarily introduced for the variables $(x^1,x^2,\ldots)$ as Eq. (2.1) here.

The Lax hierarchy is defined in Sato's framework as

$$\partial_m L = [B_m, L]_\star, \quad m = 1,2,\ldots, \tag{3.10}$$

where the action of ∂_m on the pseudodifferential operator L should be interpreted to be coefficient-wise, that is, $\partial_m L := [\partial_m, L]$ or $\partial_m \partial_x^k = 0$. The operator B_m is given by

$$B_m := \underbrace{(L\star\cdots\star L)}_{m \text{ times}}{}_{\geqslant r} =: (L^m)_{\geqslant r}, \tag{3.11}$$

where r is 0 for $u_1=0$ and 1 for $u_1 \neq 0$ as commutative cases.[50,51] The Lax hierarchy gives rise to a set of infinite differential equations with respect to infinite kinds of fields from the coefficients in Eq. (3.10) for a fixed m. Hence it contains huge amount of differential (evolution) equations for all m. The left-hand side (LHS) of Eq. (3.10) becomes $\partial_m u_k$ which shows a flow in the x^m direction.

If we set the constraint $L^l = B_l$ on the Lax hierarchy (3.10), we get an infinite set of NC (reduced) Lax hierarchies. We can easily show

$$\frac{\partial u_k}{\partial x^{Nl}} = 0, \tag{3.12}$$

for all N, k because

$$\frac{\mathrm{d}L^l}{\mathrm{d}x^{Nl}} = [B_{Nl}, L^l]_\star = [(L^l)^N, L^l]_\star = 0, \tag{3.13}$$

which implies Eq. (3.12). The reduced NC hierarchy is called the *l-reduction* of the NC KP hierarchy. This time, the constraint $L^l = B_l$ gives simple relationships which make it possible to represent infinite kind of fields $u_{l-r+1}, u_{l-r+2}, u_{l-r+3}, \ldots$ in terms of $(l-1)$ kind of fields $u_{2-r}, u_{3-r}, \ldots, u_{l-r}$ (cf. Appendix).

From now on, let us see that those equations in the Lax hierarchy contain various soliton equations with some constraints. We discuss it separately in the following two cases: $u_1=0 (r=0)$ case and $u_1 \neq 0 (r=1)$ case. Some of them are already discussed in Ref. 36. For commutative discussions, see also Ref. 52.

For $u_1 = 0$ $(r=0)$: In this case, the Lax hierarchy (3.10) is just the NC KP hierarchy which includes the NC KP equation.[16,46] Let us see it explicitly.

(i) NC KP hierarchy. The coefficients of each powers of (pseudo) differential operators in the Lax hierarchy (3.10) yield a series of infinite NC "evolution equations," that is, for $m=1$,

$$\partial_x^{1-k} \quad \partial_1 u_k = u_k', \quad k = 2,3,\ldots \Rightarrow x^1 \equiv x, \tag{3.14}$$

for $m=2$,

$$\begin{aligned} &\partial_x^{-1} \quad \partial_2 u_2 = u_2'' + 2u_3', \\ &\partial_x^{-2} \quad \partial_2 u_3 = u_3'' + 2u_4' + 2u_2 \star u_2' + 2[u_2, u_3]_\star, \\ &\partial_x^{-3} \quad \partial_2 u_4 = u_4'' + 2u_5' + 4u_3 \star u_2' - 2u_2 \star u_2'' + 2[u_2, u_4]_\star, \end{aligned} \tag{3.15}$$

$$\partial_x^{-4} \quad \partial_2 u_5 = \cdots,$$

and for $m=3$,

$$\partial_x^{-1} \quad \partial_3 u_2 = u_2''' + 3u_3'' + 3u_4' + 3u_2' \star u_2 + 3u_2 \star u_2',$$

$$\partial_x^{-2} \quad \partial_3 u_3 = u_3''' + 3u_4'' + 3u_5' + 6u_2 \star u_3' + 3u_2' \star u_3 + 3u_3 \star u_2' + 3[u_2, u_4]_\star,$$

$$\partial_x^{-3} \quad \partial_3 u_4 = u_4''' + 3u_5'' + 3u_6' + 3u_2' \star u_4 + 3u_2 \star u_4' + 6u_4 \star u_2' - 3u_2 \star u_3'' - 3u_3 \star u_2'' + 6u_3 \star u_3' + 3[u_2, u_5]_\star + 3[u_3, u_4]_\star,$$

$$\partial_x^{-4} \quad \partial_3 u_5 = \cdots. \tag{3.16}$$

These just imply the $(2+1)$-dimensional NC KP equation[16,46] with $2u_2 \equiv u, x^2 \equiv y, x^3 \equiv t$,

$$\frac{\partial u}{\partial t} = \frac{1}{4}\frac{\partial^3 u}{\partial x^3} + \frac{3}{4}\frac{\partial (u \star u)}{\partial x} + \frac{3}{4}\int^x dx' \frac{\partial^2 u(x')}{\partial y^2} - \frac{3}{4}\left[u, \int^x dx' \frac{\partial u(x')}{\partial y} \right]_\star. \tag{3.17}$$

The important point is that infinite kinds of fields $u_3, u_4, u_5, \ldots$ are represented in terms of one kind of field $2u_2 \equiv u$ as is seen in Eq. (3.15). This guarantees the existence of the NC KP hierarchy which implies the existence of reductions of the NC KP hierarchy. The order of nonlinear terms are determined in this way.

(ii) NC KdV hierarchy (2-reduction of the NC KP hierarchy). Taking the constraint $L^2 = B_2 =: \partial_x^2 + u$ for the NC KP hierarchy, we get the NC KdV hierarchy. This time, the following NC Lax hierarchy,

$$\frac{\partial u}{\partial x^m} = [B_m, L^2]_\star, \tag{3.18}$$

include neither positive nor negative power of (pseudo) differential operators for the same reason as the commutative case (see, e.g., Ref. 53) and gives rise to the mth KdV equation for each m. For example, the NC KdV hierarchy (3.18) becomes the $(1+1)$-dimensional NC KdV equation[8] for $m=3$ with $x^3 \equiv t$,

$$\dot{u} = \tfrac{1}{4} u''' + \tfrac{3}{4}(u \star u)', \tag{3.19}$$

and the $(1+1)$-dimensional fifth NC KdV equation[23] for $m=5$ with $x^5 \equiv t$,

$$\dot{u} = \tfrac{1}{16} u'''''' + \tfrac{5}{16}(u \star u'''' + u'''' \star u) + \tfrac{5}{8}(u' \star u' + u \star u \star u)', \tag{3.20}$$

where $\dot{u} =: \partial u / \partial t$.

(iii) NC Boussinesq hierarchy (3-reduction of the NC KP hierarchy). The 3-reduction $L^3 = B_3$ yields the NC Boussinesq hierarchy which includes the $(1+1)$-dimensional NC Boussinesq equation[23] with $t \equiv x^2$,

$$\ddot{u} = \tfrac{1}{3} u'''' + (u \star u)'' + ([u, \partial_x^{-1} \dot{u}]_\star)', \tag{3.21}$$

where $\ddot{u} =: \partial^2 u / \partial t^2$ and $\partial_x^{-1} = \int^x dx$.

(iv) NC coupled KdV hierarchy (4-reduction of the NC KP hierarchy). The hierarchy includes the $(1+1)$-dimensional NC coupled KdV equation $t \equiv x^3$,

$$\dot{u} = \tfrac{1}{4} u''' + \tfrac{3}{4}(u \star u)' + \tfrac{3}{4}(\omega - \phi^2)' - \tfrac{3}{4}[u, \phi']_\star, \tag{3.22}$$

and the other two equations with respect to three kinds of fields u, ω, and ϕ, which are determined by Eqs. (3.15) and (3.16). The x^2-dependence of the fields is absorbed by the fields ω, ϕ. In this way, we can generate infinite set of the l-reduced NC hierarchies. If we take other set-up, we can get many other hierarchies.

(v) NC Sawada–Kotera hierarchy (3-reduction of the NC BKP hierarchy). The NC version of BKP hierarchy[54] is obtained from the NC KP hierarchy by the constraint that the constant terms of B_m for $m=1,3,5,\ldots$ should vanish. The 3-reduction of the NC BKP hierarchy includes the $(1+1)$-dimensional NC Sawada–Kotera equation with $t\equiv x^5$, $u\equiv 3u_2$,

$$\dot{u}+\tfrac{1}{9}u''''+\tfrac{5}{9}u'''\star u+\tfrac{5}{9}u''\star u'+\tfrac{5}{9}u\star u'\star u=0, \tag{3.23}$$

which is new.

For $u_1\neq 0(r=1)$: On commutative spaces, this situation generates modified KP (mKP) hierarchy and its reductions. On NC spaces, however, the existence of them is not always guaranteed. For the NC KP hierarchy, infinite kinds of fields are described by one kind of x^2-flow equations (3.15). However, this time the flow equation becomes

$$\begin{aligned}
&\partial_x^0 \quad \partial_2 u_1 = u_1''+2u_2'+2u_1\star u_1'+2[u_1,u_2]_\star,\\
&\partial_x^{-1} \quad \partial_2 u_2 = u_2''+2u_3'+2u_1\star u_2'+2[u_1,u_3]_\star,\\
&\partial_x^{-2} \quad \partial_2 u_3 = \cdots .
\end{aligned} \tag{3.24}$$

Hence due to the commutator $[u_1,u_k]$, it is very hard to represent the field u_k in terms of $u_1,u_2,\ldots,u_{k-1}$. The same is true of other flows. That is why the existence of NC modified KP hierarchy is nontrivial.

Some reduced hierarchies are obtained from constraint conditions.

(i) NC mKdV hierarchy (2-reduction of the "NC mKP hierarchy"). This time, the 2-reduction constraint $L^2=B_2$ makes it possible to represent infinite kinds of fields $u_2,u_3,\ldots$ in terms of one kind of field $2u_1\equiv v$. The NC mKdV hierarchy includes the $(1+1)$-dimensional NC mKdV equation for $m=3$ with $t_3\equiv t$,

$$\dot{v}=\tfrac{1}{4}v'''-\tfrac{3}{8}v\star v'\star v+\tfrac{3}{8}[v,v'']_\star. \tag{3.25}$$

(ii) NC Burgers hierarchy.[30] This is obtained by an irregular reduction. Setting the constraint $L_{\leqslant -1}=0$ or $L=:\partial_x+v$, the Lax hierarchy (3.10) yields the NC Burgers hierarchy which includes neither positive nor negative power of differential operator. For $m=2$, the hierarchy becomes the $(1+1)$-dimensional NC Burgers equation with $t\equiv x^2$,

$$\dot{v}=[B_2,L]_\star=[\partial_x^2+2v\partial_x,\partial_x+v]_\star=v''+2v\star v'. \tag{3.26}$$

The NC Burgers equation is linearizable and easily solved via NC Cole–Hopf transformation.[30,31] In the linearization, the order of the nonlinear term plays crucial roles. This order is automatically realized from Sato's framework.

The present discussion is applicable to the matrix Sato theory where the fields $u_k(k=1,2,\ldots)$ are $N\times N$ matrices. For $N=2$, the Lax hierarchy includes the Ablowitz–Kaup–Newell–Segur (AKNS) system,[55] the Davey–Stewarson equation, the NLS equation and so on. (For commutative discussion, see, e.g., Ref. 48.)

NC version[23] of the Bogoyavlenskii–Calogero–Schiff (BCS) equation[56] is also derived from this framework because the Sato theory works well on the commutative BCS equation.

IV. COMMUTING FLOWS FOR NC LAX HIERARCHIES

First let us show all flows are commuting,

$$\partial_m \partial_n u_k = \partial_n \partial_m u_k \tag{4.1}$$

for any m, n, k. The derivation in this section is straightforward as the commutative case[57,53] and already discussed in a more general situation where the products are noncommutative associative products with differentiations. (See, e.g., Refs. 46, 58, and 59.)

From NC Lax equation (3.10), we get

$$\partial_m \partial_n L = [\partial_m B_n, L]_\star + [B_n, \partial_m L]_\star = [\partial_m B_n, L]_\star + [B_n, [B_m, L]_\star]_\star. \tag{4.2}$$

Hence

$$[\partial_m, \partial_n] L = [F_{mn}, L]_\star, \tag{4.3}$$

where

$$F_{mn} := \partial_m B_n - \partial_n B_m - [B_m, B_n]_\star. \tag{4.4}$$

Now we show the "zero-curvature equation" $F_{mn}=0$. We note that

$$\partial_m B_n = \partial_m (L^n)_{\geqslant r} = (\partial_m L^n)_{\geqslant r} = [B_m, L^n]_{\star \geqslant r} = -[B_m^c, L^n]_{\star \geqslant r} = -[B_m^c, B_n]_{\star \geqslant r}, \tag{4.5}$$

where the operator B_m^c is the compliment of B_m and defined by

$$B_m^c := L^m - B_m, \tag{4.6}$$

and the suffix r is equal to 0 for $u_1=0$ and 1 for $u_1 \neq 0$. Therefore we get

$$\begin{aligned} F_{mn} &= -[B_m^c, B_n]_{\star \geqslant r} + [B_n^c, B_m]_{\star \geqslant r} - [B_m, B_n]_\star = -[B_m^c, L^n - B_n^c]_{\star \geqslant r} + [L^n - B_n, B_m]_{\star \geqslant r} - [B_m, B_n]_{\star \geqslant r} \\ &= [B_m^c, B_n^c]_{\star \geqslant r} = 0, \end{aligned} \tag{4.7}$$

which implies

$$\partial_m \partial_n L = \partial_n \partial_m L. \tag{4.8}$$

Hence Eq. (4.1) is proved.

We note that the present discussion works well for arbitrary noncommutativity. Here we call the Eq. (4.7) the *NC Zakharov–Shabat equation* because reduces to the usual Zakharov–Shabat equation in the commutative limit,

$$\partial_m B_n - \partial_n B_m - [B_m, B_n]_\star = 0. \tag{4.9}$$

Of course, we can get the conjugate of the NC Zakharov–Shabat equation in terms of B_n^c,

$$\partial_m B_n^c - \partial_n B_m^c + [B_m^c, B_n^c]_\star = 0. \tag{4.10}$$

V. CONSERVATION LAWS FOR NC LAX HIERARCHIES

Here let us prove the conservation laws for NC Lax equations, which are the main results in the present paper.

First we would like to comment on conservation laws of NC field equations.[30] The discussion is basically the same as the commutative case because both the differentiation and the integration are the same as the commutative ones in the Moyal representation.

Let us suppose the conservation law,

$$\frac{\partial \sigma(t, x^i)}{\partial t} = \partial_i J^i(t, x^i), \tag{5.1}$$

where $\sigma(t, x^i)$ and $J^i(t, x^i)$ are called the *conserved density* and the *associated flux*, respectively. The conserved quantity is given by spatial integral of the conserved density,

$$Q(t) = \int_{\text{space}} \mathrm{d}^D x\, \sigma(t,x^i), \tag{5.2}$$

where the integral $\int_{\text{space}} \mathrm{d}x^D$ is taken for spatial coordinates. The proof is straightforward,

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = \frac{\partial}{\partial t}\int_{\text{space}} \mathrm{d}^D x\, \sigma(t,x^i) = \int_{\text{space}} \mathrm{d}^D x\, \partial_i J_i(t,x^i) = \int_{\substack{\text{spatial}\\ \text{infinity}}} \mathrm{d}S^i\, J_i(t,x^i) = 0, \tag{5.3}$$

unless the surface term of the integrand $J_i(t,x^i)$ vanishes. The convergence of the integral is also expected because the star-product naively reduces to the ordinary product at spatial infinity due to $\partial_i \sim \mathcal{O}(r^{-1})$ where $r := |x|$.

For commutative field equations, the existence of infinite number of conserved quantities is expected to lead to infinite-dimensional hidden symmetry from Noether's theorem. For NC field equations, this would also be true and the existence of infinite number of conserved quantities would be special and meaningful, and suggest an infinite-dimensional hidden symmetry deformed from the commutative one.

In order to discuss conservation laws for the NC Lax hierarchies, let us first calculate the differential of the residue of L^n following Wilson's approach:[57]

$$\partial_m \operatorname{res}_{-1} L^n = \operatorname{res}_{-1}(\partial_m L^n) = \operatorname{res}_{-1}[B_m, L^n]_\star. \tag{5.4}$$

Here we note that

$$\begin{aligned}\operatorname{res}_{-1}[f\partial_x^p, g\partial_x^q]_\star &= \binom{p}{p+q+1}(f\star g^{(p+q+1)} - (-1)^{p+q+1} g\star f^{(p+q+1)}) \\ &= \binom{p}{p+q+1}\left\{\left(\sum_{k=0}^{p+q}(-1)^k f^{(k)}\star g^{(p+q-k)}\right)' + (-1)^{p+q}[g, f^{(p+q+1)}]_\star\right\},\end{aligned} \tag{5.5}$$

where $f^{(N)} := \partial^N f/\partial x^N$. Hence we can see that on NC spaces, there is an additional term as a commutator in Eq. (5.5) which vanishes in the commutative limit. However as we saw in Sec. II, commutators of fields can be represented as total derivatives, which is very important here.

Let us describe the explicit representations of the conservation laws. From the explicit forms of the Lax pair,

$$\begin{aligned} L^n &= \partial_x^n + \sum_{l=1}^{\infty} a_{n-l}\partial_x^{n-l}, \\ B_m &= \partial_x^m + \sum_{k=1}^{m} b_{m-k}\partial_x^{m-k}, \end{aligned} \tag{5.6}$$

we can evaluate Eq. (5.4) as

$$\begin{aligned}\partial_m \operatorname{res}_{-1} L^n &= \operatorname{res}_{-1}\left[\partial_x^m + \sum_{k=1}^{m} b_{m-k}\partial_x^{m-k}, \partial_x^n + \sum_{l=1}^{\infty} a_{n-l}\partial_x^{n-l}\right]_\star \\ &= \sum_{l=n+1}^{m+n}\binom{m}{l-n-1} a_{n-l}^{(m+n-l+1)} + \sum_{k=1}^{m}\sum_{l=n+1}^{n+1+m-k}\binom{m-k}{l-n-1} \\ &\quad\times\left\{\left(\sum_{N=0}^{m+n-k-l}(-1)^N b_{m-k}^{(N)}\star a_{n-l}^{(m+n-k-l-N)}\right)' + (-1)^{m+n-k-l}[a_{n-l}, b_{m-k}^{(m+n-k-l+1)}]_\star\right\}\end{aligned}$$

$$= \left\{ \sum_{l=n+1}^{m+n} \binom{m}{l-n-1} a_{n-l}^{(m+n-l)} + \sum_{k=1}^{m} \sum_{l=n+1}^{n+1+m-k} \binom{m-k}{l-n-1} \right.$$
$$\left. \times \sum_{N=0}^{m+n-k-l} (-1)^N b_{m-k}^{(N)} \star a_{n-l}^{(m+n-k-l-N)} \right\}' - \sum_{k=1}^{m} \sum_{l=n+1}^{n+1+m-k} \binom{m-k}{l-n-1}$$
$$\times (-1)^{m+n-k-l} \theta^{ij} \partial_i \left(a_{n-l} \diamondsuit \partial_j b_{m-k}^{(m+n-k-l+1)} \right).$$

This is the generalized conservation laws for the NC Lax hierarchies. The right-hand side (RHS) contains derivatives in all NC directions. When we interpret this as conservation laws, we must specify what coordinates correspond to time and space and introduce the noncommutativities in the space–time directions only.

If we identify the coordinate x^m with time t, we get the conserved density as follows:

$$\sigma = \mathrm{res}_{-1} L^n + \theta^{im} \sum_{k=0}^{m-1} \sum_{l=0}^{k} (-1)^{k-l} \binom{k}{l} \mathrm{res}_{-(l+1)} L^n \diamondsuit \partial_i \partial_x^{k-l} \mathrm{res}_k L^m, \tag{5.7}$$

for $n=1,2,\ldots$, where the suffices i must run in the space–time directions only. We can easily see that deformation terms appear in the second term of Eq. (5.7) in the case of space-time noncommutativity. On the other hand, in the case of space–space noncommutativity, the conserved density is given by the residue of L^n as the commutative case.

Let us show more explicit representations as follows.

(i) In the case that the space–time coordinates are $(x,y,t) \equiv (x^1,x^2,x^3)$. The conserved density is given by

$$\sigma = \mathrm{res}_{-1} L^n + \theta^{i3} \sum_{k=0}^{2} \sum_{l=0}^{k} (-1)^{k-l} \binom{k}{l} \mathrm{res}_{-(l+1)} L^n \diamondsuit \partial_i \partial_x^{k-l} \mathrm{res}_k L^3, \tag{5.8}$$

more explicitly, for $u_1=0$ and $[t,x]=i\theta$, which includes the NC KP equation with space–time noncommutativity, the NC KdV equation and so on,

$$\sigma = \mathrm{res}_{-1} L^n - 3\theta((\mathrm{res}_{-1} L^n) \diamondsuit u_3' + (\mathrm{res}_{-2} L^n) \diamondsuit u_2'), \tag{5.9}$$

and for $u_1 \neq 0$ and $[t,x]=i\theta$, which includes the NC modified KdV equation and so on,

$$\sigma = \mathrm{res}_{-1} L^n + 3\theta((\mathrm{res}_{-1} L^n) \diamondsuit (u_2 + u_1^2)'' - (\mathrm{res}_{-2} L^n) \diamondsuit (u_2 - u_1' - u_1^2)' - (\mathrm{res}_{-3} L^n) \diamondsuit u_1'). \tag{5.10}$$

(ii) In the case that the space–time coordinates are $(x,t) \equiv (x^1,x^2)$ with $[t,x]=i\theta$. The conserved density is given by

$$\sigma = \mathrm{res}_{-1} L^n - \theta \sum_{k=0}^{1} \sum_{l=0}^{k} (-1)^{k-l} \binom{k}{l} \mathrm{res}_{-(l+1)} L^n \diamondsuit \partial_i \partial_x^{k-l} \mathrm{res}_k L^2, \tag{5.11}$$

more explicitly, for $u_1=0$, which includes the NC Boussinesq equation and so on,

$$\sigma = \mathrm{res}_{-1} L^n + 2\theta(\mathrm{res}_{-1} L^n) \diamondsuit u_2', \tag{5.12}$$

and for $u_1 \neq 0$:

$$\sigma = \mathrm{res}_{-1} L^n + 2\theta((\mathrm{res}_{-1} L^n) \diamondsuit u_1'' - (\mathrm{res}_{-2} L^n) \diamondsuit u_1'). \tag{5.13}$$

We note that for space–space noncommutativity, conserved quantities (not densities) are all the same as commutative ones because of Eq. (2.6). This is consistent with the present results, of course. Furthermore, for l-reduced hierarchies, the conserved densities (5.7) become trivial for

$n=Nl$ $(N=1,2,\ldots)$. The NC Burgers hierarchy is obtained by a "1-reduction" and contains no negative power of differential operators. Hence we cannot generate any conserved density for the NC Burgers equation in the present approach. This is considered to suggest that the NC Burgers equation is not a conservative system but a dispersive system as a commutative case.

We have one comment on conserved densities for the one-soliton configuration. One soliton solutions can always reduce to the commutative ones because $f(t-x)\star g(t-x)=f(t-x)g(t-x)$.[8,30] Hence the conserved densities are not deformed in the NC extension.

The present discussion is applicable to the NC matrix Sato theory, including the NC AKNS system, the NC Davey–Stewarson equation, the NC NLS equation, and the NC BCS equation.

VI. CONCLUSION AND DISCUSSION

In the present paper, we showed that the existence of an infinite number of conserved densities for a wide class of NC Lax hierarchies and obtained the explicit representations of them for both space–space and space–time noncommutativities. This suggests that NC soliton equations are completely integrable and infinite-dimensional symmetries would be hidden, which would be considered as some deformed affine Lie algebras.

In order to reveal what the hidden symmetry is, we must first study NC extension of Hirota's bilinearization.[60] This could be realized as a simple generalization of the Cole–Hope transformation whose extension to NC spaces are already successful in Refs. 30 and 31. Hirota's bilinearization leads to the theory of tau-functions which is essential in the discussion of the Lie algebraic structure of symmetry of the solution space.[47,54,61,62] After submission of the present paper, progress has been reported in, e.g., Refs. 63–65.

Our results guarantee that NC extension of soliton theories would be actually fruitful and worth studying. There are many further directions, such as, the study of relation to q-deformations of integrable systems, NC extension of the r-matrix formalism,[48,66] the inverse scattering method and the Bäcklund transformation, and so on. NC extension of the Ward conjecture[38] (see also Ref. 67) would be also very interesting.[27] Some NC equations are actually derived from NC (anti-)self-dual YM equations by reduction[14,30,33] and embedded[15,17,68] in $N=2$ string theories.[69] This guarantees that NC soliton equations would have physical meanings and might be helpful to understand new aspects of the corresponding string theory.

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APPENDIX: MISCELLANEOUS FORMULAS

We present explicit calculations of L^n for $n=1$, 2, 3, 4, 5 up to some order of the pseudodifferential operator ∂_x. We can read reduction conditions, e.g., $L^l=B_l$, and the explicit representations of $\mathrm{res}_r L^n$ and B_m.

For $u_1=0(r=0)$:

$$L=\partial_x+u_2\partial_x^{-1}+u_3\partial_x^{-2}+u_4\partial_x^{-3}+u_5\partial_x^{-4}+u_6\partial_x^{-5}+\cdots,$$

$$\begin{aligned}L^2=\partial_x^2+2u_2+(2u_3+u_2')\partial_x^{-1}+(2u_4+u_3'+u_2\star u_2)\partial_x^{-2}+(2u_5+u_4'+u_2\star u_3+u_3\star u_2-u_2\star u_2')\partial_x^{-3}\\+(2u_6+u_5'+u_2\star u_4+u_4\star u_2+u_3\star u_3-u_2\star u_3'-2u_3\star u_2'+u_2\star u_2'')\partial_x^{-4}+\cdots,\end{aligned}$$

$$L^3=\partial_x^3+3u_2\partial_x+3(u_3+u_2')+(3u_4+3u_3'+u_2''+3u_2\star u_2)\partial_x^{-1}+(3u_5+3u_4'+u_3''+3u_2\star u_3+3u_3\star u_2+u_2'\star u_2-u_2\star u_2')\partial_x^{-2}+(3u_6+3u_5'+u_4''+3u_2\star u_4+3u_4\star u_2+3u_3\star u_3+u_2\star u_2\star u_2+u_2'\star u_3-u_2\star u_3'+u_3'\star u_2-4u_3\star u_2'-u_2'\star u_2'+u_2\star u_2'')\partial_x^{-3}+\cdots,$$

$$L^4=\partial_x^4+4u_2\partial_x^2+(4u_3+6u_2')\partial_x+(4u_4+6u_3'+4u_2''+6u_2\star u_2)+(4u_5+6u_4'+4u_3''+u_2'''+6u_2\star u_3+6u_3\star u_2+4u_2'\star u_2+2u_2\star u_2')\partial_x^{-1}+(4u_6+6u_5'+4u_4''+u_3'''+6u_2\star u_4+6u_4\star u_2+6u_3\star u_3+4u_2\star u_2\star u_2+4u_2'\star u_3+2u_2\star u_3'+4u_3'\star u_2-4u_3\star u_2'-u_2'\star u_2'+u_2''\star u_2+u_2\star u_2'')\partial_x^{-2}+\cdots,$$

$$L^5=\partial_x^5+5u_2\partial_x^3+5(u_3+2u_2')\partial_x^2+5(u_4+2u_3'+2u_2''+2u_2\star u_2)\partial_x+5(u_5+2u_4'+2u_3''+u_2'''+2u_2\star u_3+2u_3\star u_2+2u_2'\star u_2+2u_2\star u_2')+(5u_6+10u_5'+10u_4''+5u_3'''+u_2''''+10u_2\star u_4+10u_4\star u_2+10u_3\star u_3+10u_2\star u_2\star u_2+10u_2'\star u_3+10u_2\star u_3'+10u_3'\star u_2+5u_2'\star u_2'+5u_2''\star u_2+5u_2\star u_2'')\partial_x^{-1}+\cdots.$$

For $u_1\neq 0 (r=1)$:

$$L=\partial_x+u_1+u_2\partial_x^{-1}+u_3\partial_x^{-2}+u_4\partial_x^{-3}+u_5\partial_x^{-4}+u_6\partial_x^{-5}+\cdots,$$

$$L^2=\partial_x^2+2u_1\partial_x+(2u_2+u_1'+u_1^2)+(2u_3+u_2'+u_1\star u_2+u_2\star u_1)\partial_x^{-1}+(2u_4+u_3'+u_1\star u_3+u_3\star u_1+u_2\star u_2-u_2\star u_1')\partial_x^{-2}+(2u_5+u_4'+u_1\star u_4+u_4\star u_1+u_2\star u_3+u_3\star u_2-2u_3\star u_1'-u_2\star u_2'+u_2\star u_1'')\partial_x^{-3}+\cdots,$$

$$L^3=\partial_x^3+3u_1\partial_x^2+3(u_2+u_1'+u_1\star u_1)\partial_x+(3u_3+3u_2'+3u_1''+3u_1\star u_2+3u_2\star u_1+u_1'\star u_1+2u_1\star u_1'+u_1\star u_1\star u_1)+(3u_4+3u_3'+u_2''+3u_1\star u_3+3u_3\star u_1+3u_2\star u_2+u_1'\star u_2+2u_1\star u_2'+u_2'\star u_1-2u_2\star u_1'+u_1\star u_1\star u_2+u_1\star u_2\star u_1+u_2\star u_1\star u_1)\partial_x^{-1}+\cdots,$$

$$L^4=\partial_x^4+4u_1\partial_x^3+(4u_2+6u_1'+6u_1\star u_1)\partial_x^2+(4u_3+6u_2'+4u_1''+6u_1\star u_2+6u_2\star u_1+4u_1'\star u_1+8u_1\star u_1'+4u_1\star u_1\star u_1)\partial_x+(4u_4+6u_3'+4u_2''+u_1'''+6u_1\star u_3+6u_3\star u_1+6u_2\star u_2+4u_1'\star u_2+6u_1\star u_2'+4u_2'\star u_1-2u_2\star u_1'+2u_1''\star u_1+2u_1\star u_1''+3u_1'\star u_1'+4u_1\star u_1\star u_2+4u_1\star u_2\star u_1+4u_2\star u_1\star u_1+u_1'\star u_1\star u_1+2u_1\star u_1'\star u_1+3u_1\star u_1\star u_1'+u_1\star u_1\star u_1\star u_1)+\cdots,$$

$$L^5=\partial_x^5+5u_1\partial_x^4+5(u_2+2u_1'+2u_1\star u_1)\partial_x^3+5(u_3+2u_2'+2u_1''+2u_1\star u_2+2u_2\star u_1+2u_1'\star u_1+4u_1\star u_1'+2u_1\star u_1\star u_1)\partial_x^2+(5u_4+10u_3'+10u_2''+5u_1'''+10u_1\star u_3+10u_3\star u_1+10u_2\star u_2+10u_1'\star u_2+20u_1\star u_2'+10u_2'\star u_1+4u_2\star u_1'+6u_1''\star u_1+15u_1'\star u_1'+11u_1\star u_1''+10u_1\star u_1\star u_2+10u_1\star u_2\star u_1+10u_2\star u_1\star u_1+5u_1'\star u_1\star u_1+10u_1\star u_1'\star u_1+15u_1\star u_1\star u_1'+5u_1\star u_1\star u_1\star u_1)\partial_x+\cdots.$$

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Central potentials on spaces of constant curvature: The Kepler problem on the two-dimensional sphere S^2 and the hyperbolic plane H^2

José F. Cariñena[a] and Manuel F. Rañada[b]
Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, 50009 Zaragoza, Spain

Mariano Santander[c]
Departamento de Física Teórica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid, Spain

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The Kepler problem is a dynamical system that is well defined not only on the Euclidean plane but also on the sphere and on the hyperbolic plane. First, the theory of central potentials on spaces of constant curvature is studied. All the mathematical expressions are presented using the curvature κ as a parameter, in such a way that they reduce to the appropriate property for the system on the sphere S^2, or on the hyperbolic plane H^2, when particularized for $\kappa>0$, or $\kappa<0$, respectively; in addition, the Euclidean case arises as the particular case $\kappa=0$. In the second part we study the main properties of the Kepler problem on spaces with curvature, we solve the equations and we obtain the explicit expressions of the orbits by using two different methods, first by direct integration and second by obtaining the κ-dependent version of the Binet's equation. The final part of the paper, that has a more geometric character, is devoted to the study of the theory of conics on spaces of constant curvature. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1893214]

I. INTRODUCTION

The hydrogen atom in a spherical geometry S^3 was first studied by Schrödinger[1] in 1940 and analyzed by Infeld[2] and Stevenson[3] at the next year; some five years later Infeld and Schild[4] obtained the spectrum of this system in an "open universe of constant negative curvature" (hyperbolic space H^3). Later on, Higgs[5] and Leemon[6] analyzed the characteristics of the two fundamental central potentials, Kepler problem and harmonic oscillator, on the N-dimensional sphere and Kalnins *et al.*, in a study of the dynamical $O(4)$ symmetry of the hydrogen atom,[7] considered the separation of variables of the Schrödinger equation with a Coulomb potential on the sphere S^3 using a classification of coordinate systems separating the Laplace equation in the Riemannian spaces of constant curvature previously obtained by Olevskii.[8] Since then, a certain number of authors have studied this question from both the classical (Kepler problem) and the quantum (hydrogen atom) points of view.[9–24] The Kepler problem and the harmonic oscillator are the two most important superseparable systems and, because of this, their spherical and hyperbolic versions have been occasionally obtained, in some of the quoted references, as particular cases in the study of superintegrable systems on non-Euclidean configuration spaces.

The Euclidean superintegrable systems in the plane were studied by Fris *et al.*[25] and in the three-dimensional space by Evans;[26] later on different authors have considered this question[27–39]

[a]Electronic mail: jfc@unizar.es
[b]Electronic mail: mfran@unizar.es
[c]Electronic mail: santander@fta.uva.es

from different points of view. In Ref. 16 we studied the existence of the spherical and hyperbolic versions of these superintegrable systems taking the space curvature as a parameter; next the properties of the isotropic and nonisotropic harmonic oscillator and of those superintegrable systems related with the harmonic oscillator were analyzed.[19,20,23,24] Now, our objective is the study of the Kepler problem on the sphere S^2 and the hyperbolic plane H^2, both coming naturally from reduction from the true Kepler problem in a three-dimensional curved space S^3 or H^3.

In differential geometric terms, the Euclidean plane $\mathbb{E}^2$ is in fact a very particular limiting case of the constant curvature spaces; accordingly, in dynamical terms, certain classical and well-known potentials (Kepler problem, harmonic oscillator, and systems related with them) can also be considered as very particular limiting cases of more general curved systems. If the curvature κ is introduced as a parameter then the question is the analysis of certain potentials in the space with constant curvature κ (we may term these as κ-dependent potentials) with appropriate flat limit. As many different κ-dependent functions may have the same limit when $\kappa \to 0$ we must require that certain fundamental properties of the Euclidean system continue to hold for the curved system. By fundamental properties we mean those related with separability (superseparability) and integrability (superintegrability). The important point is that the spherical and hyperbolic Kepler potential, to be studied in this paper, can be characterized as a very specific κ deformation of the well-known Euclidean system, and conversely, the Euclidean Kepler potential arises as the particular $\kappa=0$ case of the κ-dependent curved system.

The main purpose of this paper is to study and solve the Kepler problem in the space of constant curvature κ. As we will see, one of the advantages of this κ-dependent formalism is that the study runs parallel to that of the Euclidean case. So the structure of this paper is very similar to that of the corresponding chapter (or sections) devoted to central potentials and Kepler problem in some classical books of theoretical mechanics.[40,41] In fact this is the idea of using the deformation as an approach, the curvature κ will modify many things but will preserve the fundamental structure; this is so because the deep properties ensuring the possibility of exact solution for the Euclidean Kepler problem are preserved when a constant curvature is ascribed to the space. Of course, there are significant differences; one of them will be the geometric interpretation of the solutions that, although rather simple in the Euclidean plane, will pose some interesting geometric questions in spaces of constant curvature.

In more detail, the plan of this paper is as follows: In Sec. II we analyze the free geodesic motion on the spaces S^2, $\mathbb{E}^2$, and H^2, as well as the existence of κ-dependent Noether symmetries. In Sec. III we study some general questions concerning the central potentials on spaces of constant curvature. Section IV, that can be considered as the central part of the paper, is devoted to the study of the κ-dependent Kepler problem on the spaces $(S^2, \mathbb{E}^2, H^2)$. We have divided this section into three sections. In the first part we consider the equivalent one-dimensional problem and we draw a rough classification of the orbits without requiring explicit solutions; in the second part we solve explicitly the problem and we obtain the expressions of the orbits; we arrive at the results by using two different methods. First by direct integration and second by obtaining the κ-dependent version of the Binet's equation. The third section is devoted to the analysis and classification of the κ-dependent orbits; first on the sphere S^2 $(\kappa>0)$, and then in the hyperbolic plane H^2 $(\kappa<0)$. This third section poses the difficult problem of interpreting the κ-dependent equations as conics in curved spaces; of course all the obtained results reduce to well-known Euclidean trajectories when we consider the particular value $\kappa=0$. Section V, that has a geometric character, is devoted to the study of (non-Euclidean) conics on the sphere S^2 and on the hyperbolic plane H^2, which leads to the identification of the orbits of the Kepler problem with conics for any value of the curvature. Finally, in Sec. VI we discuss the results and make some final comments.

II. GEODESIC MOTION, NOETHER SYMMETRIES AND CONSTANTS OF MOTION ON $(S^2, \mathbb{E}^2, H^2)$

In the following we will make use of the same notation and techniques introduced for the oscillator in the above-mentioned previous articles. That is, from now on all the mathematical expressions will depend on the curvature κ as a parameter, in such a way that when assuming

$\kappa>0$, $\kappa=0$, or $\kappa<0$, we will obtain the corresponding property particularized on the sphere, on the Euclidean plane, or on the hyperbolic plane. In order to present these expressions in a form which holds simultaneously for any value of κ, we will use the following "tagged" trigonometric functions:

$$C_\kappa(x)=\begin{cases}\cos\sqrt{\kappa}x & \text{if } \kappa>0,\\ 1 & \text{if } \kappa=0,\\ \cosh\sqrt{-\kappa}x & \text{if } \kappa<0,\end{cases}\qquad S_\kappa(x)=\begin{cases}\dfrac{1}{\sqrt{\kappa}}\sin\sqrt{\kappa}x & \text{if } \kappa>0,\\ x & \text{if } \kappa=0,\\ \dfrac{1}{\sqrt{-\kappa}}\sinh\sqrt{-\kappa}x & \text{if } \kappa<0,\end{cases}\tag{1}$$

and the κ-dependent tangent function $T_\kappa(x)$ defined in the natural way, $T_\kappa(x)=S_\kappa(x)/C_\kappa(x)$. The fundamental properties of these curvature-dependent trigonometric functions are

$$C_\kappa^2(x)+\kappa S_\kappa^2(x)=1,$$

and

$$C_\kappa(2x)=C_\kappa^2(x)-\kappa S_\kappa^2(x),\quad \frac{\mathrm{d}}{\mathrm{d}x}S_\kappa(x)=C_\kappa(x),$$

$$S_\kappa(2x)=2S_\kappa(x)C_\kappa(x),\quad \frac{\mathrm{d}}{\mathrm{d}x}C_\kappa(x)=-\kappa S_\kappa(x).\tag{2}$$

It is well known that the appropriate coordinates for the study of central potentials are polar (r,ϕ) coordinates (see the Appendix); according to the intrinsic viewpoint, the coordinate r in any space of constant curvature κ is the actual distance measured along the geodesics emanating from an arbitrarily chosen origin point O, while ϕ has the same meaning as in E^2, the angle between this geodesic and a reference geodesic through O.[42] The range of r depends on κ; specifically $r\in[0,\pi/2\sqrt{\kappa}]$ for $\kappa>0$ and $r\in[0,\infty]$ for $\kappa\leqslant 0$. The range of ϕ is the interval $[0,2\pi]$. So we start with the following κ-dependent expression:

$$\mathrm{d}s^2=\mathrm{d}r^2+S_\kappa^2(r)\mathrm{d}\phi^2,$$

that represents the differential line element on the spaces $(S^2,\mathbb{E}^2,H^2)$ with constant curvature κ. This metric reduces to

$$\mathrm{d}s_1^2=\mathrm{d}r^2+(\sin^2 r)\mathrm{d}\phi^2,\quad \mathrm{d}s_0^2=\mathrm{d}r^2+r^2\,\mathrm{d}\phi^2,\quad \mathrm{d}s_{-1}^2=\mathrm{d}r^2+(\sinh^2 r)\mathrm{d}\phi^2,$$

in the three particular cases of the unit sphere $\kappa=1$, Euclidean plane $\kappa=0$, and unit Lobachewski plane $\kappa=-1$.

The three κ-dependent vector fields Y_1, Y_2, Y_J, with coordinate expressions given by

$$Y_1(\kappa)=(\cos\phi)\frac{\partial}{\partial r}-\left(\frac{C_\kappa(r)}{S_\kappa(r)}\sin\phi\right)\frac{\partial}{\partial\phi},$$

$$Y_2(\kappa)=(\sin\phi)\frac{\partial}{\partial r}+\left(\frac{C_\kappa(r)}{S_\kappa(r)}\cos\phi\right)\frac{\partial}{\partial\phi},$$

$$Y_J = \frac{\partial}{\partial \phi},$$

are generators of three different one-parameter groups of diffeomorphisms preserving the metric ds^2 (isometries of the Riemannian manifold).[24] In fact, the commutators of these vector fields are given by

$$[Y_1(\kappa), Y_2(\kappa)] = -\kappa Y_J, \quad [Y_1(\kappa), Y_J] = -Y_2(\kappa), \quad [Y_2(\kappa), Y_J] = Y_1(\kappa),$$

so that they close the Lie algebra of the group of isometries of the spherical (Euclidean, hyperbolic) space. Notice that only when $\kappa=0$ (Euclidean plane) Y_1 and Y_2 will commute. Moreover, the Lagrangian for the geodesic (free) motion is given by the kinetic term arising from the Riemannian metric; that is

$$L_0(r, \phi, v_r, v_\phi; \kappa) = T(\kappa) = \left(\tfrac{1}{2}\right)(v_r^2 + S_\kappa^2(r) v_\phi^2),$$

and is invariant under the actions of $Y_1(\kappa)$, $Y_2(\kappa)$, and $Y_J(\kappa)$.

A general standard Lagrangian (κ-dependent kinetic term minus a potential) has the following form:

$$L(r, \phi, v_r, v_\phi; \kappa) = \left(\tfrac{1}{2}\right)(v_r^2 + S_\kappa^2(r) v_\phi^2) - U(r, \phi; \kappa),$$

in such a way that for $\kappa=0$ we recover a standard Euclidean system

$$\lim_{\kappa \to 0} L = \left(\tfrac{1}{2}\right)(v_r^2 + r^2 v_\phi^2) - V(r, \phi), \quad V(r, \phi) = U(r, \phi; 0).$$

In some particular cases this Lagrangian system possesses the vector fields Y_1, Y_2, or Y_J, as exact Noether symmetries. If we denote by Y_s^t, $s=1,2,J$, the natural lift to the tangent bundle (phase space) of the vector field Y_s and by θ_L the Cartan semibasic one-form[43]

$$\theta_L = \frac{\partial L}{\partial v_r} \mathrm{d}r + \frac{\partial L}{\partial v_\phi} \mathrm{d}\phi = v_r \, \mathrm{d}r + S_\kappa^2(r) v_\phi \, \mathrm{d}\phi,$$

then the cases with exact Noether symmetries are the following:

(1) If the potential U is of the form $U=U(z_2)$, with $z_2=S_\kappa(r)\sin\phi$, then

$$P_1(\kappa) = i(Y_1^t(\kappa))\theta_L = (\cos\phi) v_r - (C_\kappa(r) S_\kappa(r) \sin\phi) v_\phi$$

is a constant of motion.

(2) If the potential U is of the form $U=U(z_1)$, $z_1=S_\kappa(r)\cos\phi$, then

$$P_2(\kappa) = i(Y_2^t(\kappa))\theta_L = (\sin\phi) v_r + (C_\kappa(r) S_\kappa(r) \cos\phi) v_\phi$$

is a constant of motion.

(3) If the potential U depends only on the coordinate r (central potential), then

$$J(\kappa) = i(Y_J^t)\theta_L = S_\kappa^2(r) v_\phi$$

is a constant of motion.

We remark that the dependence on the curvature κ is only explicit in the radial dependence of these functions; the angular dependence, contained in $\cos\phi$ or $\sin\phi$, is κ independent. As an example, the vector field Y_J is κ independent but the integral of motion $J(\kappa)$ is κ dependent. These quantities P_1, P_2, J, are the κ-dependent versions of the two components of the linear momentum and the angular momentum.

III. CENTRAL POTENTIALS ON ($S^2, \mathbb{E}^2, H^2$)

Making use of the three κ-dependent functions, P_1, P_2, and J, the kinetic energy $T(\kappa)$ can be rewritten as follows:

$$T(\kappa) = \left(\tfrac{1}{2}\right)(P_1^2(\kappa) + P_2^2(\kappa) + \kappa J^2(\kappa)),$$

so that the total energy becomes

$$E(\kappa) = \left(\tfrac{1}{2}\right)(P_1^2(\kappa) + P_2^2(\kappa) + \kappa J^2(\kappa)) + U(r, \phi; \kappa),$$

showing that, on spaces of (constant) nonzero curvature, the angular momentum has a contribution to the total energy of the system, proportional to the curvature κ.

A κ-dependent potential U whose expression in polar coordinates (r, ϕ) has the structure

$$U = F(r) + \frac{G(\phi)}{S_\kappa^2(r)},$$

is Hamilton–Jacobi separable.[24] It is, therefore, integrable and has the following two quadratic integrals of motion:

$$I_1(\kappa) = P_1^2(\kappa) + P_2^2(\kappa) + 2F(r) + \frac{2G(\phi)}{T_\kappa^2(r)},$$

$$I_2(\kappa) = J^2(\kappa) + 2G(\phi).$$

Then, in this separable case, the total energy splits as a sum of two independent constants of motion

$$E(\kappa) = \left(\tfrac{1}{2}\right)I_1(\kappa) + \left(\tfrac{1}{2}\right)\kappa I_2(\kappa).$$

Of course, if $G=0$ then $U=F(r)$ is a central potential and the function $I_2(\kappa)$ just reduces to $I_2 = J^2(\kappa)$.

The Lagrangian of a κ-dependent central potential is given by

$$L(\kappa) = \left(\tfrac{1}{2}\right)(v_r^2 + S_\kappa^2(r)v_\phi^2) - U(r; \kappa),$$

so that the dynamics is represented by the vector field

$$X_L = v_r\frac{\partial}{\partial r} + v_\phi\frac{\partial}{\partial \phi} + f_r\frac{\partial}{\partial v_r} + f_\phi\frac{\partial}{\partial v_\phi}$$

with the functions f_r and f_ϕ given by

$$f_r = S_\kappa(r)C_\kappa(r)v_\phi^2 - U_r',$$

$$f_\phi = -2\left(\frac{C_\kappa(r)}{S_\kappa(r)}\right)v_r v_\phi.$$

The associated two equations are

$$\frac{\mathrm{d}}{\mathrm{d}t}v_r = S_\kappa(r)C_\kappa(r)v_\phi^2 - U_r', \quad U_r' = \frac{\mathrm{d}U}{\mathrm{d}r},$$

$$\frac{\mathrm{d}}{\mathrm{d}t}J(\kappa)=0, \quad J(\kappa)=S_\kappa^2(r)v_\phi,$$

where the time derivative $\mathrm{d}/\mathrm{d}t$ can be interpreted, in geometric terms, as the Lie derivative along X_L. The ϕ equation just gives the conservation law of the κ-dependent angular momentum (or the law of areas); concerning the radial equation it can be rewritten as follows:

$$\dot{v}_r=\ddot{r}=-\frac{\mathrm{d}}{\mathrm{d}t}\left[\left(\frac{1}{2}\right)\frac{J^2}{S_\kappa^2(r)}+U(r;\kappa)\right],$$

so that, after multiplying by $v_r=\dot{r}$, it leads to

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\left(\frac{1}{2}\right)v_r^2+\left(\frac{1}{2}\right)\frac{J^2}{S_\kappa^2(r)}+U(r;\kappa)\right]=0,$$

that represents the conservation law of the energy

$$\left(\frac{1}{2}\right)v_r^2+\left(\frac{1}{2}\right)\frac{J^2}{S_\kappa^2(r)}+U(r;\kappa)=E, \quad \frac{\mathrm{d}}{\mathrm{d}t}E=0.$$

Solving for $\dot{r}$, we obtain

$$\frac{\mathrm{d}r}{\mathrm{d}t}=\sqrt{2\left(E-U(r;\kappa)-\left(\frac{1}{2}\right)\frac{J^2}{S_\kappa^2(r)}\right)},$$

that can be solved for $\mathrm{d}t$ and integrated

$$t=\int\frac{\mathrm{d}r}{\sqrt{2\left[E-U(r;\kappa)-\left(\frac{1}{2}\right)(J^2/S_\kappa^2(r))\right]}},$$

so that in the particular $\kappa=0$ case we recover the integral of the Euclidean case appearing in the books of theoretical mechanics

$$t=\int\frac{\mathrm{d}r}{\sqrt{2\left[E-V(r)-\left(\frac{1}{2}\right)(J^2/r^2)\right]}}.$$

Coming back to the general $\kappa\neq 0$ case, if we consider a change of variable from r to a new variable $u_\kappa=C_\kappa(r)/S_\kappa(r)$, by using (2) we get

$$\mathrm{d}r=-\frac{\mathrm{d}u_\kappa}{u_\kappa^2+\kappa},$$

and by considering the potential $U=U(r;\kappa)$ as a function of the new radial variable, $U=U(u_\kappa;\kappa)$, the above integral for t becomes

$$t=\int\frac{\mathrm{d}u_\kappa}{(u_\kappa^2+\kappa)\sqrt{2\left[E_P-U(u_\kappa;\kappa)-\left(\frac{1}{2}\right)J^2u_\kappa^2\right]}},$$

where E_P denotes a constant of motion which plays an important role,

$$E_P=E-\left(\frac{1}{2}\right)\kappa J^2.$$

(Notice the true energy for curvature κ is E and not E_P; however E_P can be seen as a kind of κ deformation of the Euclidean energy because $E_P=E$ for $\kappa=0$.) This integral gives the value of t as a function of u_κ and consequently also of r; it can be inverted, at least formally, and we can obtain

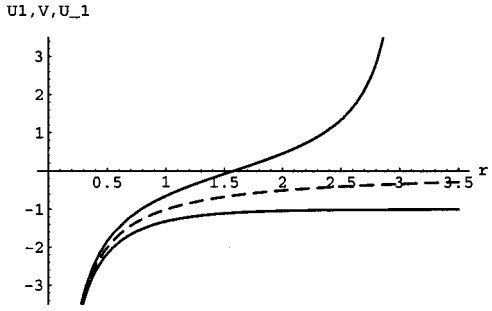

FIG. 1. Plot of the Kepler potential as a function of r, for the unit sphere $\kappa=1$ (upper curve), Euclidean plane $\kappa=0$ (dashed line), and unit Lobachewski plane $\kappa=-1$ (lower curve). The three functions are singular at $r=0$ but the Euclidean function $U_0=V$ appears in this formalism as making a separation between two different behaviors. In fact $U_0=V$ is the only potential that vanishes at long distances.

u_κ (or r) as a function of t and the two constants E_P and J. The expression of ϕ as a function of t is just given by

$$\phi = J \int (u_\kappa^2 + \kappa)\mathrm{d}t + \phi_0.$$

We close this section by calling attention to the factor $(u_\kappa^2+\kappa)$ in the above integral for t that clearly resembles the factor appearing in the elliptic integrals of the third kind.

IV. THE KEPLER PROBLEM ON $(S^2, \mathbb{E}^2, H^2)$

The following spherical (hyperbolic) Lagrangian with curvature κ,

$$L_K(\kappa)\left(\tfrac{1}{2}\right) = (v_r^2 + S_\kappa^2(r)v_\phi^2) - U_K(r;\kappa), \quad U_K = -\frac{k}{T_\kappa(r)},$$

represents the κ-dependent version of the Euclidean Kepler problem; the potential U_K reduces to

$$U_1(r) = -\frac{k}{\tan r}, \quad U_0(r) = V(r) = -\frac{k}{r}, \quad U_{-1}(r) = -\frac{k}{\tanh r},$$

in the three particular cases of the unit sphere $(\kappa=1)$, Euclidean plane $(\kappa=0)$, and unit Lobachewski plane $(\kappa=-1)$; the Euclidean function $V(r)$ appears in this formalism as making separation between two different behaviors (see Fig. 1). The global sign has been chosen so that $k>0$ corresponds to an attractive potential.

This potential is actually worthy of the name Kepler in curvature κ due to two reasons. First, this potential is the spherically symmetric potential satisfying Gauss law in a *three-dimensional space of constant curvature* κ, where the area of a sphere of radius r is $4\pi S_\kappa^2(r)$, where the flux of the corresponding radial force field across a sphere of radius r, which clearly equals $4\pi S_\kappa^2(r) \times(\mathrm{d}U_K/\mathrm{d}r)$ should be a constant independent of r; this condition leads directly to the potential U_K. [As in the Euclidean case, the potential $-(k/T_\kappa(r))$ does not satisfy the Gauss law in two dimensions.] The second reason is based on superintegrability; what singularizes U_K among other central potentials with the correct $-k/r$ Euclidean limit is the property of being a superintegrable system for all the values of the curvature κ.[16] In fact, U_K is endowed with the following two additional integrals of motion:

$$I_3(\kappa) = P_2(\kappa)J(\kappa) - k\cos\phi,$$

$$I_4(\kappa) = P_1(\kappa)J(\kappa) + k \sin \phi,$$

that represent the two-dimensional curvature versions of the Runge–Lenz constant of motion, whose existence is a consequence of the additional separability of $U_K(r;\kappa)$ in two different systems of κ-dependent parabolic coordinates (this superseparability is not studied in this paper). Of course only three of the four integrals are functionally independent; so we have several possibilities for the choice of a fundamental set of κ-dependent integrals of motion as, for example, $\{E(\kappa), J(\kappa), I_3(\kappa)\}$, $\{E(\kappa), J(\kappa), I_4(\kappa)\}$, or $\{E(\kappa), I_3(\kappa), I_4(\kappa)\}$.

A. The classification of orbits and the equivalent one-dimensional problem

Let us start for an arbitrary central potential $U(r)$. We have previously obtained

$$\left(\frac{1}{2}\right)v_r^2 + U(r;\kappa) + \left(\frac{1}{2}\right)\frac{J^2}{S_\kappa^2(r)} = E,$$

so, if we introduce the effective one-dimensional equivalent κ-dependent potential W defined as

$$W_\kappa(r) = U(r;\kappa) + \frac{J^2}{2S_\kappa^2(r)},$$

where the term $J^2/(2S_\kappa^2(r))$ plays clearly the role of the centrifugal barrier potential, then the above property reduces to conservation of the energy for the fictitious κ-dependent one-dimensional problem arising from the potential W_κ,

$$\left(\tfrac{1}{2}\right)v_r^2 + W_\kappa(r) = E,$$

so that we can use, also in this κ-dependent case, the method of the classification of the orbits by analyzing the behavior of W_κ.

Next we will study the main characteristics of the orbits for the Kepler potential in curvature κ where W_κ is given by

$$W_\kappa(r) = -\frac{k}{T_\kappa(r)} + \frac{J^2}{2S_\kappa^2(r)},$$

so it reduces to

$$W_1 = -\frac{k}{\tan r} + \frac{J^2}{2\sin^2 r},$$

$$W_0 = -\frac{k}{r} + \frac{J^2}{2r^2},$$

$$W_{-1} = -\frac{k}{\tanh r} + \frac{J^2}{2\sinh^2 r},$$

in the three particular one-dimensional problems associated to the unit sphere ($\kappa=1$), Euclidean plane ($\kappa=0$), and unit Lobachewski plane ($\kappa=-1$).

(1) Analysis of the potentials W_1 and W_c ($c=\sqrt{\kappa}>0$).

The function W_1 satisfies the following limits in the boundaries:

$$\lim_{r\to 0} W_1(r) = +\infty, \quad \lim_{r\to \pi} W_1(r) = +\infty,$$

it cuts the r axis at the points $r_{1,2}$ solutions of the equation $\sin(2r_{1,2}) = J^2/k$, and it has a minimum at the point r_m^s given by $r_m^s = \mathrm{tg}^{-1}(J^2/k)$. It represents, therefore, a potential well with barriers of

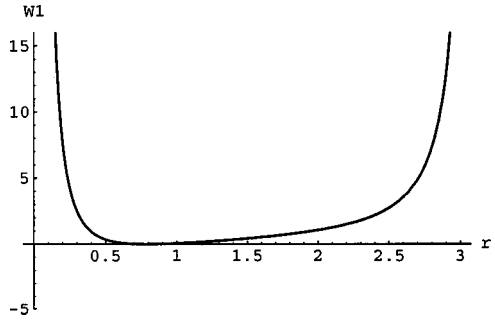

FIG. 2. Plot of W_c as a function of r, for $\kappa=1$ with k and J given by $(k=1, J=1)$.

infinite height at both extremes, $r=0$ and $r=\pi$, and one single minimum placed inside the left half-interval ($r_m^s<\pi/2$) with a value $W_m^s=(1/2)(J^2-k^2/J^2)$ (Fig. 2). Thus, all the trajectories are bounded and all of them describe nonlinear one-dimensional oscillations between the two turning points.

In the general case of the function W_c, the points $r_{1,2}$ are given by the two roots of $\sin(2cr_{1,2})=c(J^2/k)$ and the minimum is placed in the point $r_m^s=(1/c)\mathrm{tg}^{-1}(cJ^2/k)$ with a value given by $W_m^s=(1/2)(c^2J^2-k^2/J^2)$. All these expressions are c dependent and have the correct limits for W_0,

$$\lim_{c\to 0} r_1=\frac{J^2}{2k},\quad \lim_{c\to 0} r_2=+\infty,\quad \lim_{c\to 0} r_m^s=\frac{J^2}{k},\quad \lim_{c\to 0} W_m^s=-\frac{k^2}{2J^2}$$

(see Fig. 3).

(2) Analysis of the potentials W_{-1} and W_{-c} ($c=\sqrt{-\kappa}>0$).

The function W_{-1} satisfies the two following limits:

$$\lim_{r\to 0} W_{-1}(r)=+\infty,\quad \lim_{r\to\infty} W_{-1}(r)=-k,$$

it cuts the r axis in the point r_1 unique solution of the equation $\sinh(2r_1)=J^2/k$ and, in the case that k and J satisfy the condition $J^2/k<1$, then it has a unique minimum in the point r_m^h given by $r_m^h=\tanh^{-1}(J^2/k)$ with the value $W_m^h=-(1/2)(J^2+k^2/J^2)$. There exist therefore two possible situations, as follows:

(1) If $J^2/k<1$ the motion is bounded (periodic) for small energies $W_m^h\leqslant E<-k$, and unbounded for higher energies $E\geqslant -k$.

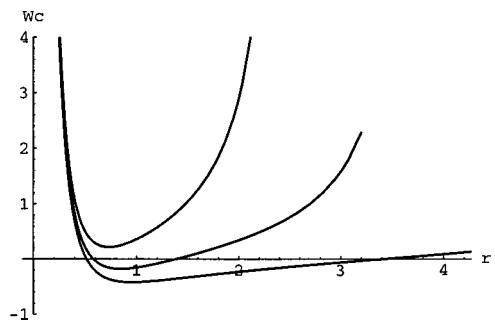

FIG. 3. Plot of W_c as a function of r, for $(k=1, J=1)$ and three different values of the curvature $c=\sqrt{\kappa}$, $c=1.2$ (upper curve), $c=0.8$ (middle curve), and $c=0.4$ (lower curve).

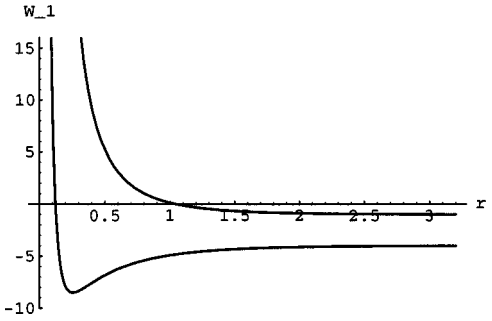

FIG. 4. Plot of W_{-c} as a function of r, for $c=1$ ($\kappa=-1$). The upper curve corresponds to ($k=1, J=2$) and lower curve corresponds to ($k=4, J=1$).

(2) If $J^2/k \geqslant 1$ the function W_{-1} will take the form of a potential barrier with infinite height at the the origin $r=0$; only energies satisfying $E \geqslant -k$ will be allowed and all the trajectories will be unbounded (scattering) open curves.

These two possible behaviors are represented in Fig. 4.
The general hyperbolic function W_{-c} satisfies

$$\lim_{r\to 0} W_{-c}(r) = +\infty, \quad \lim_{r\to\infty} W_{-c}(r) = -ck,$$

it cuts the r axis in the point r_1 solution of $\sinh(2cr_1)=c(J^2/k)$ and, if the condition $c(J^2/k)<1$ is satisfied, then it has a unique minimum in the point $r_m^h=(1/c)\tanh^{-1} c(J^2/k)$ with a value W_m^h given by $W_m^h=-(1/2)(c^2J^2+k^2/J^2)$. It is clear that the smaller the value of c is, the easier of satisfying is the condition for the existence of a well, so that the behavior (1) is becoming more and more dominant. Finally, the Euclidean limit is given by

$$\lim_{c\to 0} r_1 = \frac{J^2}{2k}, \quad \lim_{c\to 0} r_m^h = \frac{J^2}{k}, \quad \lim_{c\to 0} W_m^h = -\frac{k^2}{2J^2}.$$

The convergence of W_{-c} into W_0 is represented in Fig. 5.

B. Determination of the orbits of the κ-dependent Kepler problem

1. Method I: Direct integration

We have previously obtained, making use of the conservation of the total energy E and the angular momentum J, two expressions for $\dot{r}$ and $\dot{\phi}$, which can be written as

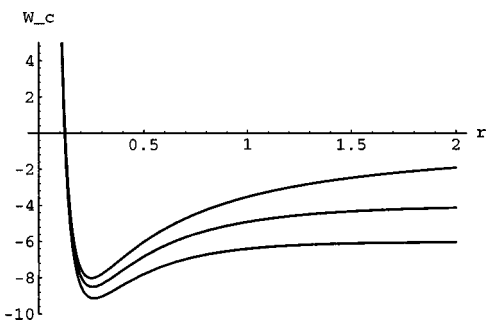

FIG. 5. Plot of W_{-c} as a function of r, for ($k=4, J=1$) and three different values of the curvature $c=\sqrt{-\kappa}$, $c=1.5$ (lower curve), $c=1$ (middle curve), and $c=0.5$ (upper curve).

$$\mathrm{d}t = \frac{\mathrm{d}r}{\sqrt{2[E - U - (1/2)(J^2/S_\kappa^2(r))]}}, \quad \mathrm{d}t = \left(\frac{S_\kappa^2(r)}{J}\right)\mathrm{d}\phi.$$

Eliminating t between both equations we have

$$\mathrm{d}\phi = \frac{J\,\mathrm{d}r}{S_\kappa^2(r)\sqrt{2[E - U - (1/2)(J^2/S_\kappa^2(r))]}},$$

that after the change of variable $r \to u_\kappa$ with $u_\kappa = 1/T_\kappa(r)$, $\mathrm{d}r = -S_\kappa^2(r)\mathrm{d}u_\kappa$, becomes

$$\mathrm{d}\phi = -\frac{\mathrm{d}u_\kappa}{\sqrt{R(u_\kappa)}},$$

where $R(u_k)$ denotes the following function:

$$R(u_k) = \frac{2E}{J^2} - \frac{2U}{J^2} - (u_\kappa^2 + r_\kappa^2) = \frac{2E_P}{J^2} - \frac{2U}{J^2} - u_\kappa^2.$$

All this is valid for a general potential. Next we particularize for the κ-Kepler problem, $U_K(r;\kappa) = -k/T_\kappa(r)$, and then we obtain

$$\phi = \phi_0 - \frac{\mathrm{d}u_\kappa}{\sqrt{R(u_\kappa)}}, \quad R(u_k) = \alpha + \beta u_\kappa + \gamma u_\kappa^2,$$

with coefficients α, β, and γ given by

$$\alpha = \frac{2E_P}{J^2}, \quad \beta = \frac{2k}{J^2}, \quad \gamma = -1.$$

In this particular case the integration is elementary and we arrive at

$$\phi = \phi_0 - \cos^{-1}\left(\frac{u_\kappa - (k/J^2)}{(k/J^2)\sqrt{1 + z_\kappa}}\right), \quad z_\kappa = \left(\frac{2J^2}{k^2}\right)E_P,$$

leading to

$$u_\kappa(\phi) = \left(\frac{k}{J^2}\right)[1 + e_\kappa \cos(\phi - \phi_0)], \quad e_\kappa = \sqrt{1 + z_\kappa}. \tag{3}$$

This is the polar equation of the orbit in either space $(S_\kappa^2, \mathbb{E}^2, H_\kappa^2)$, for any value of the curvature κ. It reduces to

$$\frac{1}{\tan r} = \left(\frac{k}{J^2}\right)[1 + e_1 \cos(\phi - \phi_0)],$$

$$\frac{1}{r} = \left(\frac{k}{J^2}\right)[1 + e_0 \cos(\phi - \phi_0)],$$

$$\frac{1}{\tanh r} = \left(\frac{k}{J^2}\right)[1 + e_{-1} \cos(\phi - \phi_0)],$$

in the three particular cases of the unit sphere ($\kappa = 1$), Euclidean plane ($\kappa = 0$), and unit Lobachewski plane ($\kappa = -1$), respectively.

We recall that, as only three of the several integrals of motion can be functionally independent, there must exist some relations between them. Concerning the couple $I_3(\kappa)$, $I_4(\kappa)$, that, as stated above, represent the κ-dependent version of the Euclidean Runge–Lenz constants of motion, they are related with E_P and J by

$$I_3^2 + I_4^2 = 2E_P J^2 + k^2$$

so that we arrive to

$$e_\kappa = \frac{1}{k}\sqrt{I_3^2 + I_4^2}$$

that represents the natural extension to the curvature-dependent case of a well-known property of the Euclidean case.

Let us close this direct integration approach with three observations. First, it turns out that in any of the three manifolds $(S_\kappa^2, \mathbb{E}^2, H_\kappa^2)$, and for any value of κ, this curve is a *conic with a focus at the origin*, where conic must be taken in a metric sense, relative to the intrinsic metric in each space. This follows from the geometrical study to be presented in Sec. V. Second, notice that the quantity e_κ is related to the partial energy E_P exactly as the Euclidean eccentricity of the conic is related to the total energy, yet only in the Euclidean case $(\kappa=0)$ this function E_P coincides with E. In the general case $(\kappa\neq 0)$ the characteristics of the orbit will be more easily associated to the values of the e_κ and/or E_P than to the total energy E. Third, both the method and the results obtained show a close similarity with the Euclidean ones. In fact, the important point is that the classical and well known change of variable $r\to u=1/r$ admits as a generalization the κ-dependent change $r\to u_\kappa=1/T_\kappa(r)$ which affords a significant simplification for all values of κ; conversely, this κ-dependent change reduces to the Euclidean change $r\to u_0=1/r$ for $\kappa=0$.

2. Method II: Equation of Binet

The definition of the angular momentum J determines a κ-dependent relation between the differentials of the time t and the angle ϕ.

$$J\,\mathrm{d}t = S_\kappa^2(r)\mathrm{d}\phi.$$

The corresponding relation between the derivatives with respect to t and ϕ is

$$\frac{\mathrm{d}}{\mathrm{d}t} = \left(\frac{J}{S_\kappa^2(r)}\right)\frac{\mathrm{d}}{\mathrm{d}\phi},$$

so that the second derivative with respect to t is given by

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} = \left(\frac{J}{S_\kappa^2(r)}\right)\frac{\mathrm{d}}{\mathrm{d}\phi}\left[\left(\frac{J}{S_\kappa^2(r)}\right)\frac{\mathrm{d}}{\mathrm{d}\phi}\right].$$

Introducing this notation in the radial equation, it becomes

$$\left(\frac{J}{S_\kappa^2(r)}\right)\frac{\mathrm{d}}{\mathrm{d}\phi}\left[\left(\frac{J}{S_\kappa^2(r)}\right)\frac{\mathrm{d}r}{\mathrm{d}\phi}\right] - \left(\frac{C_\kappa(r)}{S_\kappa^3(r)}\right)J^2 = -U_r'.$$

This equation can be simplified in two steps, first, the left-hand side can be rewritten by making use of

$$\frac{\mathrm{d}}{\mathrm{d}\phi}\left(\frac{C_\kappa(r)}{S_\kappa(r)}\right) = -\left(\frac{1}{S_\kappa^2(r)}\right)\frac{\mathrm{d}r}{\mathrm{d}\phi};$$

second, we introduce the change $r\to u_\kappa$ in such a way that the potential $U=U(r;\kappa)$ be considered as a function of u_κ; then we have

$$U_r' = -\left(\frac{1}{S_\kappa^2(r)}\right)U_u', \quad U_u' = \frac{\mathrm{d}U}{\mathrm{d}u_\kappa}.$$

In this way we arrive at the differential equation of the orbit

$$\frac{\mathrm{d}^2 u_\kappa}{\mathrm{d}\phi^2} + u_\kappa = -\left(\frac{1}{J^2}\right)U_u',$$

that permits us to obtain ϕ as a function of u_κ for the given potential $U(r;\kappa)$ when considered as a function of u_κ,

$$\phi = \int \left\{c - \left(\frac{2}{J^2}\right)U - u_\kappa^2\right\}^{-(1/2)} \mathrm{d}u_\kappa.$$

Let us now particularize for the Kepler problem. In this case the potential U_K is given by $U_K = -ku_\kappa$, and the equation reduces to a linear equation with constant coefficients,

$$\frac{\mathrm{d}^2 u_\kappa}{\mathrm{d}\phi^2} + u_\kappa = \frac{k}{J^2},$$

which has the general solution

$$u_\kappa = A\cos(\phi - \phi_0) + \frac{k}{J^2} = \left(\frac{k}{J^2}\right)[1 + e\cos(\phi - \phi_0)], \tag{4}$$

where A [or $e = A(J^2/k)$] and ϕ_0 are the two constants of integration.

Remark that the differential equation of the orbit, usually known as the Binet's equation, is preserved by the κ deformation. That is, u_0 deforms to u_κ but the the equation by itself remains invariant.

C. Analysis of the orbits

From the geometrical viewpoint, one of the integration constants in (3) or (4) can be made to disappear by simply choosing ϕ to be measured from the orbit position closest to the focus. Thus the orbit is

$$T_\kappa(r) = \frac{D}{1 + e\cos\phi} \tag{5}$$

which depends on two geometric parameters, the constants D and e. Comparing with (3) or (4), these two geometric parameters are related to the angular momentum J and the total energy E by means of the expressions

$$D = \frac{J^2}{k}, \quad e_\kappa = \sqrt{1 + \frac{2J^2}{k^2}\left(E - \kappa\frac{J^2}{2}\right)}, \tag{6}$$

remaining valid for any value of the curvature κ and reducing to the known expressions for the Euclidean case, $\kappa = 0$. Thus, as advanced before, the relation between the geometric constants D, e, and the physical constants J, $E - (1/2)\kappa J^2 = E_P$, is the same for all values of curvature; here we see again the quantity E_P plays a role; it can be considered as a kind of translational part of the energy, not taking into account the contribution to the energy of the angular momentum.

The nature of the orbit depends on the values of these constants. We discuss separately the cases with positive and negative κ.

(i) Spherical space, $\kappa > 0$. The polar equation of the orbits is

$$\frac{1}{T_\kappa(r)} = \frac{\sqrt{\kappa}}{\tan\sqrt{\kappa}r} = \left(\frac{k}{J^2}\right)[1 + e_\kappa \cos(\phi - \phi_0)].$$

The orbit is always a closed curve and for any value of e_κ this curve is a spherical ellipse with a focus at the origin. For a fixed J the minimal value of the total energy corresponds to orbits with $e_\kappa = 0$, which are circles with radius $r = J^2/k$ and total energy $E_{\text{cir}} = (1/2)(-k^2/J^2 + \kappa J^2)$ (which may be either negative or positive). The possible energies for given J fill the interval $[E_{\text{cir}}, \infty]$ and correspond to the parameter e_κ in the interval $[0, \infty]$ and to E_P in the interval $[-(1/2)(k^2/J^2), \infty]$. In the following description the focus will be conventionally placed at the North pole, and upper and lower half-spheres refer to the North and South hemispheres. This orbit has always a vertex closest to the focus given by the unique solution of the equation $1/T_\kappa(r) = (k/J^2)(1 + e_\kappa)$, and depending on the value of e_κ we may however distinguish three possible behaviors for the second vertex.

(a) When $e_\kappa < 1$ the orbit is completely contained in the upper half-sphere centered at the focus, and the values of r always remain less than the length $\pi/(2\sqrt{\kappa})$ of a quadrant on the sphere of curvature κ. In some respects this reminds the case of Euclidean ellipses.

(b) If $e_\kappa = 1$, the ellipse has the second vertex at $r = \pi/(2\sqrt{\kappa})$ (reducing to $r = \pi/2$ when $\kappa = 1$), and is a curve touching tangentially the equator associated to the focus at the origin. When $\kappa \to 0$, the limit of the distance $r = \pi/(2\sqrt{\kappa})$ between the origin and the equator on a sphere S^2_κ is $r = \infty$ and thus this curve is analogous to a Euclidean parabola, touching the spatial infinity at a point.

(c) When $e_\kappa > 1$, the orbit has the second vertex at $r > \pi/(2\sqrt{\kappa})$; it is a big spherical ellipse crossing the equator of the focus and entering into the lower half-sphere. This is somehow analogous to an Euclidean hyperbola.

(ii) Hyperbolic space $\kappa < 0$. Let us consider the general case of arbitrary negative curvature. The orbit equation is now

$$\frac{1}{T_\kappa(r)} = \frac{\sqrt{-\kappa}}{\tanh\sqrt{-\kappa}r} = \left(\frac{k}{J^2}\right)[1 + e_\kappa \cos(\phi - \phi_0)], \quad \kappa < 0,$$

and the relations (6) also apply but now with $\kappa < 0$. For a fixed value of J, the diagram of the effective equivalent potential reveals two essentially different situations for the behavior of $W(r)$, corresponding to values of J smaller or larger than the particular value J_∞ of J,

$$J^2_\infty = \frac{k}{\sqrt{-\kappa}}.$$

When $J < J_\infty$ ($J^2/k < 1/\sqrt{-\kappa}$), the equivalent potential is qualitatively as its Euclidean counterpart; it has a minimum at $r = r_{\text{cir}}$ determined by $T_\kappa(r_{\text{cir}}) = J^2/k$, with a *negative* value for $W(r_{\text{cir}}) = E_{\text{cir}} = -k^2/2J^2 + \kappa J^2/2$ and when r increases from r_{cir} to $r \to \infty$, the effective potential tends from below to a *negative* constant value $-k\sqrt{-\kappa}$. When $J = J_\infty$ then the minimum occurs at $r = \infty$. When $J > J_\infty$ there is no longer a minimum in the equivalent potential, which is a monotone function of r, tending when $r \to \infty$ to the value $-k\sqrt{-\kappa}$ from above. This discussion alone suffices to establish two landmark values for the energies (at a fixed value of J) as follows:

(a) $E = E_{\text{cir}} = (1/2)(-k^2/J^2 + \kappa J^2)$, with $J^2/k < 1/\sqrt{-\kappa}$, corresponding to the circular orbits with $E_{P_{\text{cir}}} = -(1/2)(k^2/J^2)$;

(b) $E = E_\infty = -k\sqrt{-\kappa}$, with $E_{P\infty} = -k\sqrt{-\kappa} - (1/2)\kappa J^2_\infty = -(1/2)k\sqrt{-\kappa}$ for orbits where the particle barely reaches spatial infinity with velocity 0.

To go further in any analysis about the exact nature of the orbits is easier starting from some

geometric knowledge of the properties of conics, to be sketched in the next section. However, at this point we can provide a first classification into closed and open orbits, and we may discuss its main characteristics.

When the energy is in the interval $[E_{\mathrm{cir}}, E_\infty)$, the motion is bounded and periodic, while for E in the interval $(E_\infty, \infty]$, the motion is not periodic and the orbit goes to the infinity; notice that $E=0$ is contained *within* this second interval, and thus is *not* the separating value between bounded and unbounded orbits. The angular momentum provides a second constant of motion, which may have values in the two subintervals $J^2/k \in [T_\kappa(r_{\mathrm{cir}}), 1/\sqrt{-\kappa}]$ or $J^2/k \in [1/\sqrt{-\kappa}, \infty]$; it is pertinent to discuss these two possibilities successively.

Let us first discuss the subcase $J < J_\infty$, where the equivalent potential has a minimum.

(1) If the parameter $e_\kappa = 0$ then the solution is clearly a circular orbit (circle in the hyperbolic plane) of radius r_{cir} such that $T_\kappa(r_{\mathrm{cir}}) = J^2/k$ which happens precisely at the minimum for the equivalent potential. The total energy for a circular orbit is given by $E_{\mathrm{cir}} = -(1/2)(k^2/J^2 - \kappa J^2)$ that corresponds to $E_{P_{\mathrm{cir}}} = -(1/2)(k^2/J^2)$. This is, the angular momentum of any circular orbit should remain lower than the limit value J_∞ which is approached for the circular orbit with $r \to \infty$. In the Euclidean case the value of J is not bounded for circular orbits (J_∞ tends to infinity for $\kappa \to 0$).

(2) If e_κ is greater than 0 but in the interval $0 < e_\kappa < 1 - \sqrt{-\kappa}(J^2/k)$ then the orbit will be a closed curve not reaching the spatial infinity. As we will check in Sec. V, this curve is indeed a hyperbolic *ellipse*, with a focus at the potential origin. The interval of allowed values for the total energy E turns out to be

$$-\frac{k^2}{2J^2} + \frac{1}{2}\kappa J^2 < E < -k\sqrt{-\kappa},$$

or equivalently, if we consider the "translational" part of the energy,

$$-\frac{k^2}{2J^2} < E_P < \frac{1}{2}\kappa J^2 - k\sqrt{-\kappa}.$$

(3) If e_κ is in the remaining interval, $1 - \sqrt{-\kappa}(J^2/k) < e_\kappa$, corresponding to the values $-\sqrt{-\kappa}k < E < \infty$ of the energy E, then the motion is nonperiodic and the orbits are unbounded open curves. The border value for e between these closed periodic and open not periodic types of orbits is the value $e_\kappa = 1 - \sqrt{-\kappa}(J^2/k)$, which should be thought of as corresponding to the last ellipse, or *horoellipse*. It is not immediately clear whether the orbits with e above this value are *parabolas* or *hyperbolas* in the hyperbolic plane. However, it is natural to expect some special status for the orbits with $E=0$, $e_\kappa = \sqrt{1 - \kappa(J^4/k^2)} > 1$, which we might expect to be *parabolas* in the hyperbolic plane. This would imply that at least all orbits in a finite interval of values of the e_κ parameter, whose lower bound is $1 - \sqrt{-\kappa}(J^2/k)$ and which contains $e_\kappa = \sqrt{1 - \kappa(J^4/k^2)}$ are parabolas; notice that this interval should reduce to the single value $e_\kappa = 1$ in the Euclidean limit $\kappa \to 0$, so the existence of many different parabolic orbits does not spoil the known fact that there is only a parabolic orbit in E^2. All these conjectural properties are indeed true, as we will confirm in Sec. V.

We can summarize these three points as follows: the different types of trajectories in H^2_κ, $\kappa < 0$ as a function of the parameter e_κ are the following:

$$\text{hyperbolic circle,} \quad 0 = e_\kappa,$$

$$\text{hyperbolic ellipses,} \quad 0 < e_\kappa < 1 - \sqrt{-\kappa}(J^2/k),$$

$$\text{hyperbolic horoellipse,} \quad 1 - \sqrt{-\kappa}(J^2/k) = e_\kappa,$$

$$\text{hyperbolic open conics,} \quad 1-\sqrt{-\kappa}(J^2/k) < e_\kappa < \infty.$$

Alternatively, the landmark values can also be given for the classification as a function of the total energy E,

$$\text{hyperbolic circle,} \quad E = -(1/2)(k^2/J^2 - \kappa J^2),$$

$$\text{hyperbolic ellipses,} \quad -(1/2)(k^2/J^2 - \kappa J^2) < E < -k\sqrt{-\kappa},$$

$$\text{hyperbolic horoellipse,} \quad E = -k\sqrt{-\kappa},$$

$$\text{hyperbolic open conics,} \quad -k\sqrt{-\kappa} < E < \infty.$$

Thus the behavior of the hyperbolic dynamics shows some important differences with respect to the Euclidean case. We postpone until the next section the establishment of the particular value of e_κ, or E, separating the open conics into parabolic and hyperbolic regimes, and we simply state that $e_\kappa = \sqrt{1-\kappa(L^4/k^2)}$, corresponding to $E=0$, gives an orbit which is a parabola in H^2. The value of e_κ, or the corresponding energy E, separating from parabolic to hyperbolic trajectories is a κ-dependent positive value to be determined; this will be done in the next section. When the parameter e_κ is greater than the upper value for parabolic orbits, then we will have hyperbolas in H^2 as orbits.

The remaining cases happen when $J > J_\infty$. For these values of J the equivalent potential is a decreasing function of r with no minimum at all, and hence the possible motions should have energies above E_∞; these would be always nonperiodic motions and open orbits. We will classify them into parabolas and hyperbolas in the next section.

V. CONICS ON SPACES OF CONSTANT CURVATURE

In this section we give a geometric description of conics in the three $\kappa > 0$, $\kappa = 0$, $\kappa < 0$, constant curvature spaces S^2_κ, E^2, H^2_κ, emphasizing those aspects relevant in relation with Kepler motion in these spaces. To stay within a reasonable extension limits we restrict to a mainly statement of facts presentation, which should either confirm the conjectures advanced in the dynamical part, or serve as a geometric foundation for them. The important thing is the perfect matching between the dynamical approach in Sec. IV and the results here.

As customary in this context, *lines* will mean the *geodesics* of the constant curvature space. The metric intrinsic *geometric* definition of conics, that can be applied to any two-dimensional (2D) space of constant curvature κ involves *focal elements*, i.e., either oriented points or cooriented lines. In any such space, and by definition.

An *ellipse/hyperbola* will be the set of points with a constant sum/difference $2a$ of distances r_1, r_2, to two fixed points F_1, F_2, called *foci* and separated a distance $2f$.

A *parabola* will be the set of points with a constant sum/difference 2α of distances r_1, $\tilde{r}_2$, to a fixed point F_1, called *focus*, and to a fixed cooriented line f_2, called *focal line*; the *oriented* distance 2φ between F_1 and f_2 plays here the role of focal separation.

An *ultraellipse/ultrahyperbola* will be the set of points with a constant sum/difference $2a$ of oriented distances $\tilde{r}_1$, $\tilde{r}_2$, to two fixed intersecting lines f_1, f_2, separated by an angle $2F$ and called *focal lines*.

In the generic case of constant curvature $\kappa \neq 0$ these three pairs of curves, each pair sharing the same focal elements, are the *generic* conics; Euclidean plane is *not generic* among the family of constant curvature spaces, thus some Euclidean properties of conics are very special and do not provide a good starting viewpoint to discuss the $\kappa \neq 0$ properties.

Further to generic conics, *particular distinguished conics* appear for instance when the focal separation vanishes ($f=0, \varphi=0, F=0$) and *limiting conics* when some focal elements go to infinity

(if possible at all); both particular and limiting conics can be obtained as suitable limits from the generic ones.

We first list some particular conics. When the focal separation vanishes $f=0$, the ellipse is a *circle* and the hyperbola is a pair of intersecting *lines*. No useful intuition about parabolas can be drawn from the nongeneric Euclidean case; a parabola with vanishing focal separation $\varphi=0$ is only a particular instance of parabola, to be named here *equiparabola*, but when $\kappa\neq 0$ there are other parabolas, with any positive or negative $\varphi\neq 0$, which are not equiparabolas. The main point is that general parabolas are *not* to be considered here as limiting conics, as usually done in E^2. An ultraellipse with focal angle $F=0$ is a *ultracircle* (an equidistant curve, the set of points equidistant from a fixed line), while an ultrahyperbola with $F=0$ is a pair of *lines*.

The three *generic types* of conics, as well as these *particular* conics with zero focal separation do exist in any space of constant curvature κ. Further to that, when the curvature is *negative*, there are new types of *limiting conics*, where either the foci or the focal lines may go to infinity.

A. Conics in geodesic polar coordinates in a space of curvature κ

Now let us describe conics in the three essentially different spaces S^2_κ, E^2, H^2_κ.

In the sphere S^2_κ, with $\kappa>0$ the situation is rather simple. First, as there are neither points nor lines at the infinity, there are no limiting cases in the sense they will appear in H^2_κ. Second, as there is a one-to-one correspondence (the usual polarity) between oriented points and co-oriented lines (North Pole versus Equator), with a constant distance $\pi/2\sqrt{\kappa}$ separating them, it follows that any focal element (either point or line) implies the existence of a polar focal element (line or point); thus any conic of one of the three given type pairs may be considered as a conic of any other prescribed type pair. And further, as the distance between two antipodal points is constant $\pi/\sqrt{\kappa}$, by changing a focus F_2 to its antipodal point $\overline{F_2}$ (which according to the definition is again a focus of the conic), an hyperbola with focus F_1, F_2, will be as well an ellipse with focus F_1, $\overline{F_2}$. A similar possibility exists for focal lines which may be changed to their antipodal lines, with coorientation changed. Thus all spherical conics can be seen as *spherical ellipses*, including the two particular zero focal separation cases, i.e., circles (spherical parallel circles) and pairs of lines (a pair of intersecting large circles in the sphere). For the purposes of getting a common view we may still think in three generic types, keeping in mind that all three coincide and there is complete freedom in understanding a given spherical conic as either an ellipse, or a parabola or a hyperbola (just as a geodesic circle can be seen at the same time as a geodesic circle, with center at O or as an equidistant curve to the polar of O); more on this will be said later.

In the Euclidean plane E^2 ultraellipses and ultrahyperbolas (with any focal angle F) are just pairs of parallel lines, in directions parallel to the two bisectors of the focal angle; in the standard algebraic classification of Euclidean conics these appear as degenerate conics. But when compared to S^2_κ or H^2_κ, another more important degeneracy happens in E^2: two families of parabolas with the same focus and any two parallel focal lines will coincide (because a pair of parallel lines are equidistant in E^2). This means that the *parabolic focal separation* between the focus and the focal line can be chosen arbitrarily for a fixed Euclidean parabola, which only determines its focus and the direction of the focal line. As a consequence parabolas are no longer generic conics in E^2. While parabolas have always some intermediate status between ellipses and hyperbolas, in the Euclidean case parabolas appear exclusively as limiting cases between ellipses and hyperbolas, and not as the full fledged species of conics they are in the generic $\kappa\neq 0$ case.

The hyperbolic case H^2_κ with *negative* constant curvature is richer. The limiting conics obtained from an ellipse/hyperbola through a point P when a focus stays fixed and the other goes to infinity are called *horoellipse/horohyperbola*. The limiting conics obtained from an ultraellipse/ultrahyperbola through a point P when a focal line stays fixed and the other goes to infinity are called *horoultraellipse/horoultrahyperbola*. These four types of conics are also limiting forms of parabolas, with either focus fixed and focal line going to infinity, or focal line fixed and focus going to infinity. In E^2 all these limiting conics collapse precisely to either Euclidean parabolas or pairs of lines.

There are more limiting conics in H^2_κ: the *horocycle*, obtained either from a circle through P

when its center goes to infinity, or from an ultracircle through P when the baseline goes to infinity, and the *osculating parabola*, the limit of a parabola when the focus goes to infinity along the fixed focal line.

In order to make contact with the results in the dynamical part, let us draw our attention precisely on the conics with a proper focus. From now on we completely disregard ultraellipses and ultrahyperbolas, which have two focal lines, and osculating parabolas, which have not a proper focus. We consider exclusively ellipses/hyperbolas and parabolas, as well as their limiting cases—horoellipses and horohyperbolas—and particular cases—circles, lines and equiparabolas corresponding to vanishing focal separations. All these conics have a proper focus, which we may place at the origin point, as well as another focal element, which may be another focus or a focal line. In either case the conics have as a symmetry axis the line joining the two foci or going through the focus and orthogonal to the focal line. To match with the familiar Euclidean expressions, we introduce polar coordinates in S^2_κ, E^2, H^2_κ, taking the origin at the fixed focus and the symmetry axis of the conic as the half-line $\phi=0$. With this choice, the common equation of the whole family of conics described above may be written in the form

$$T_\kappa(r) = \frac{D}{1 + e\cos\phi} \tag{7}$$

with D and e non-negative. This can be derived by trigonometric considerations from the definition of the conic in the space of constant curvature κ using the relations given in Ref. 44 and will be discussed elsewhere. This relation justifies the claim made in Sec. V: the orbits of the Kepler problem in either S^2_κ, E^2, H^2_κ, are conics with a focus at the origin of the potential. The dependence on the polar angle ϕ is exactly the same as in the Euclidean case and this may suggest to consider e as the non-Euclidean analog of the *eccentricity of the conic*, though when $\kappa\neq 0$ the link between the values of e and the *type* of the conic is not so direct as in E^2. We should mention that there are at least two other quantities keeping different properties of the Euclidean eccentricity, and no single quantity keeps all properties; in this paper we will only be concerned with e, and for brevity we shall refer to it as eccentricity.

For an ellipse/hyperbola with focal distance $2f$ and $2a$ as the sum/difference of distances to the focus, and for a parabola with focal separation 2φ and 2α as sum/difference of distances to focus and focal line, the eccentricities turn out to be

$$e_{\text{ell/hyp}} = \frac{S_\kappa(2f)}{S_\kappa(2a)}, \quad e_{\text{par}} = \frac{C_\kappa(2\varphi)}{C_\kappa(2\alpha)}$$

reducing in the Euclidean $\kappa=0$ case to the well known f/a for ellipses/hyperbolas and 1 for parabolas.

In the polar coordinate system (r,ϕ), when $\kappa>0$ or $\kappa=0$, the range of values of $T_\kappa(r)$ is the whole real line (completed with ∞), but when $\kappa<0$, the values of $T_\kappa(r)$ are confined to the interval $[0, 1/\sqrt{-\kappa}]$, or to $[-1/\sqrt{-\kappa}, 1/\sqrt{-\kappa}]$ if negative values for r are allowed along the opposite semiaxis according to the usual practice.

Now, for the conic (7) the minimum value for r happens when $\phi=0$. This means that D and e are independent constants when $\kappa\geqslant 0$ but must fulfill the inequality $0\leqslant D/(1+e)<1/\sqrt{-\kappa}$ when $\kappa<0$.

Notice that in (7) the periastron of the orbit is placed on the semiaxis $\phi=0$ at $r=r_{\text{per}}$, and thus r_{per} is related to D and e by

$$T_\kappa(r_{\text{per}}) = \frac{D}{1+e}$$

which for any value of κ has always a unique root for r_{per}. Next, let us look for the intersection of the conic with the line orthogonal to the conic symmetry axis through the focus, which corresponds to $\phi=\pi/2$. The distance between this intersection point and the focus is traditionally called

semilatus rectum of the conic (in the Euclidean case) and will be denoted by p. For $\kappa=0$ all Euclidean conics (except the limiting double straight line with $p=\infty$) intersect this semilatus line. For any $\kappa\neq 0$, p would satisfy

$$T_\kappa(p) = D,$$

but there is a difference between the cases with $\kappa\geqslant 0$ or $\kappa\leqslant 0$. While for $\kappa>0$, any D will determine a unique p, when $\kappa<0$ this equation will define a real semilatus rectum only when $D<1/\sqrt{-\kappa}$, the semilatus rectum will be formally infinite when $D=1/\sqrt{-\kappa}$ and will not exist at all when $D>1/\sqrt{-\kappa}$. This means that in the case of the hyperbolic plane H^2_κ the family of conics we are considering includes conics intersecting the semilatus line at a proper point, only at infinity or not intersecting at all. We have arrived at the following situation: all conics with given fixed focus and symmetry axis intersect this line in S^2_κ, exactly one does not intersect in E^2, and an infinite number of them do not intersect in H^2_κ.

Thus, when $\kappa\geqslant 0$ the equation of the complete family of conics we are considering is

$$T_\kappa(r) = \frac{T_\kappa(p)}{1 + e\cos\phi} \tag{8}$$

but in the negative curvature case $\kappa<0$, there will be some conics—precisely those with $D>1/\sqrt{-\kappa}$—not described under (8). To cater for these cases it will prove useful to introduce another real distance $\tilde{p}$, complementary to the ideal semilatus rectum, related to D by

$$\frac{1}{(-\kappa)T_\kappa(\tilde{p})} = D$$

and in terms of this choice, when $\kappa<0$ the equation of the complete family of conics we are considering is given by one of the two mutually exclusive possibilities,

$$T_\kappa(r) = \frac{T_\kappa(p)}{1 + e\cos\phi}, \quad T_\kappa(r) = \frac{1}{(-\kappa)T_\kappa(\tilde{p})(1 + e\cos\phi)}, \tag{9}$$

where the ranges are $0\leqslant p<\infty$ and $\infty>\tilde{p}\geqslant 0$, respectively. The conic

$$T_\kappa(r) = \frac{1}{\sqrt{-\kappa}(1 + e\cos\phi)} \tag{10}$$

is the common limit $p\to\infty$ and $\tilde{p}\to\infty$ of (9). Notice the two expressions (9) can be used as well when $\kappa>0$ but then each of the two alternatives covers actually all cases, and are then redundant. Only the first possibility in (9) has a sensible Euclidean limit because the $\kappa\to 0$ limit of the $\tilde{p}$ family gives a straight line at the infinity of the Euclidean plane; thus the family $\tilde{p}$ as a set of conics different from the p family is specific to the hyperbolic plane.

Now the only remaining problem is to link the values of the two parameters D and e to the type the conic belongs. When is such a conic an ellipse, a parabola or a hyperbola according to their definitions in the space of curvature κ? When is it a particular conic, either a circle, a equiparabola or a line? And finally, only for the hyperbolic plane H^2_κ, when is it a limiting horoellipse or horohyperbola?

In the Euclidean plane the answer is well known and easy, the conic type depends *only* on e, and not on p. This is *not so* when $\kappa\neq 0$.

B. Conics on the sphere S^2_κ

A given conic in S^2_κ will have a unique and well defined parameter e in (8). But labelling it as an ellipse, or parabola or hyperbola, requires to choose a particular set of two focal elements, and a $\pm$ sign to decide between the sum or difference in the definitions. Unlike on H^2_κ where these choices are unique, for the sphere they may be made in several ways. By means of suitable

choices, *any spherical conic with any* $0 \leqslant e \leqslant \infty$ may be considered as an ellipse, as a parabola or as a hyperbola. This is an unavoidable consequence of the definitions, which are clearly natural ones for nonzero curvature.

If we want to classify conics in S^2 into three *disjoint* species, this would require adopting an additional convention (somehow bypassing the definition), which may be chosen in several reasonable ways, but which nevertheless remains as a convention.

A possibility would be to class spherical ellipses with $0<e<1$ as ellipses, those with $e=1$ as parabolas, and those with $e>1$ as hyperbolas. This is the convention adopted by Higgs[5] who formulated it according to the property of not crossing, touching or crossing the equator, which can be easily shown to be equivalent to the requirement $e<1$, $e=1$, or $e>1$, respectively. Another different convention follows from the fact that any ellipse/hyperbola with focus F_1, F_2 (and focal separation $2f$) can also be considered as a hyperbola/ellipse with focus $F_1, \overline{F_2}$ [and focal separation $2\tilde{f}=2(\pi/2\sqrt{\kappa}-f)$]. The sum of the two focal half-separations f and $\tilde{f}$ is $\pi/2\sqrt{\kappa}$, this is, the length of a quadrant on the sphere. Thus, we may consider as ellipses exclusively those spherical ellipses with a value of the focal separation $2f$ less than a quadrant, that is, $2f<\pi/2\sqrt{\kappa}$, and as hyperbolas exclusively those spherical ellipses with a value of $2f$ greater than a quadrant, that is, $2f>\pi/2\sqrt{\kappa}$. Within this convention, and if we want artificially to enforce nonredundancy, the name parabolas will only be left for the spherical ellipses with precisely $2f=\pi/2\sqrt{\kappa}$, which in our previous nomenclature were called equiparabola (as $2f=\pi/2\sqrt{\kappa}$ between two focus means that one focus will be incident with the polar of the other focus, which is the focal line). In this view ellipses are completely contained in the half-sphere with center at the ellipse center, while hyperbolas will go through the boundary of the half-sphere centered at the hyperbola center.

C. Conics on the hyperbolic plane H^2_κ

The case of the hyperbolic plane H^2_κ is different and there is no conventionality in it. In the following paragraphs we are implicitly assuming $\kappa<0$.

When is the conic (9) an *ellipse*? In addition to the actual vertex at the point of closest approach to the focus, placed on the $\phi=0$ axis, ellipses will have another vertex, placed on the $\phi=\pi$ semiaxis with a *positive* value for $T_\kappa(r_{\text{apo}})$ which anyhow should belong to the interval $[T_\kappa(r_{\text{per}}), 1/\sqrt{-\kappa}]$. The lower bound in this interval corresponds to circular orbits while the upper places the apoastron at the infinity, and the ellipse will go to a *horoellipse*. It is easy to conclude that the positivity condition requires e to be in the interval $[0, 1]$ and then $T_\kappa(r_{\text{apo}}) \in [T_\kappa(r_{\text{peri}}), 1/\sqrt{-\kappa}]$ only happens within the first alternative in (9), provided that the eccentricities lie in the interval

$$0 < e_{\text{ell}} < 1 - \sqrt{-\kappa}\,T_\kappa(p).$$

Notice this interval *depends on p* and for any $p \neq 0$ is strictly smaller than the Euclidean one, which is recovered of course, when $\kappa \to 0$. The lower bound for e corresponds to circular orbits, while the upper bound is the limiting value corresponding to *horoellipses*,

$$e_{\text{cir}} = 0, \quad e_{\text{horoell}} = 1 - \sqrt{-\kappa}\,T_\kappa(p).$$

When will the conic (9) be a *hyperbola*? In this case, in addition to the vertex at the periastron, the conic will have another vertex point (on the other hyperbola branch, thus not actually on the physical orbit) on the $\phi=0$ semiaxis, which will appear on the equation as a *negative* value for $T_\kappa(r_{\text{apo}})$ on the $\phi=\pi$ semiaxis. Hence, the values of $T_\kappa(r)$ for $\phi=\pi$ must belong to the interval $[-1/\sqrt{-\kappa}, -T_\kappa(r_{\text{per}})]$, with the lower value corresponding to *horohyperbolas*, and the upper value to lines. By using the same strategy, it is easy to conclude that the negativity condition requires $e \in [1, \infty]$, and then $T_\kappa(r_{\text{apo}})$ may lie in the required interval in either of the two alternatives (9), with e parameters, respectively, in the intervals

$$1+\sqrt{-\kappa}T_\kappa(p)<e_{\text{hyp}},\quad 1+\frac{1}{\sqrt{-\kappa}T_k(\tilde{p})}<e_{\text{hyp}}.$$

Notice both conditions lead to a common limit when $p,\tilde{p}\to\infty$, namely, $2<e_{\text{hyperbolas}}$ for the conics (10). Here particular and limiting conics correspond to

$$e_{\text{horohyp}}=1+\sqrt{-\kappa}T_\kappa(p),\quad e_{\text{horohyp}}=1+\frac{1}{\sqrt{-\kappa}T_\kappa(\tilde{p})},\quad e_{\text{lines}}=\infty.$$

Once we have characterized the intervals of eccentricity for ellipses and hyperbolas, the remaining gap correspond to parabolas. Thus, within the first family,

$$1-\sqrt{-\kappa}T_\kappa(p)<e_{\text{par}}<1+\sqrt{-\kappa}T_\kappa(p),$$

and within the second,

$$1-\frac{1}{\sqrt{-\kappa}T_\kappa(\tilde{p})}<e_{\text{par}}.$$

The particular parabolas with zero focal separation, this is, the equiparabolas, corresponds to the values,

$$e_{\text{equipar}}=1/C_k(p)=\sqrt{1+\kappa T_\kappa^2(p)},\quad e_{\text{equipar}}=C_k(\tilde{p})=1/\sqrt{1+\kappa T_\kappa^2(\tilde{p})},$$

and are different from the parabolas with $e=1$.

This way we get the following result. Conics (9) in the hyperbolic plane H^2, with a fixed value of p may be either ellipses, parabolas or hyperbolas, according to the value of their eccentricity as follows:

$$\text{circle},\quad e_{\text{cir}}=0,$$

$$\text{ellipses},\quad 0<e_{\text{ell}}<1-\sqrt{-\kappa}T_\kappa(p),$$

$$\text{horoellipse},\quad e_{\text{horoell}}=1-\sqrt{-\kappa}T_\kappa(p),$$

$$\text{parabolas},\quad 1-\sqrt{-\kappa}T_\kappa(p)<e_{\text{par}}<1+\sqrt{-\kappa}T_\kappa(p),$$

$$\text{horohyperbolas},\quad e_{\text{horohyp}}=1+\sqrt{-\kappa}T_\kappa(p),$$

$$\text{hyperbolas},\quad 1+\sqrt{-\kappa}T_\kappa(p)<e_{\text{hyp}}<\infty,$$

and conics (9) with a fixed $\tilde{p}$ may be only parabolas or hyperbolas,

$$1-\frac{1}{\sqrt{-\kappa}T_\kappa(\tilde{p})}<e_{\text{par}}<1+\frac{1}{\sqrt{-\kappa}T_\kappa(\tilde{p})}<e_{\text{hyp}}<\infty.$$

The most remarkable property is the existence, for a fixed value of the semilatus rectum p, of a full interval of values for eccentricity corresponding to parabolas, including always two special values, $e=1/C_k(p)$ and $e=1$; in the Euclidean limit $\kappa\to 0$ this interval collapses to the single value $e_{\text{par}}=1$, and there is a single Euclidean parabola for a given p.

Now let us consider the complete family of conics corresponding to trajectories with a given *periastron* distance, say r_{per}; these would correspond to the trajectories of a particle launched orthogonally to the radial direction from a point at distance r_{per} from the potential origin and with a given velocity. The corresponding pattern for the Kepler problem in the Euclidean case is well

known, a circle, a family of ellipses of increasing eccentricity $0<e<1$, a separating parabola, a family of hyperbolas of increasing eccentricity $1<e<\infty$ and finally a limiting straight line corresponding to infinite velocity. How about the analog of this pattern in the nonzero curvature case?

First we require all conics will have a periastron at r_{per}. Within the two families the relation between p or $\tilde{p}$ with r_{per} is given by

$$T_\kappa(r_{\mathrm{per}})=\frac{T_\kappa(p)}{1+e},\quad T_\kappa(r_{\mathrm{per}})=\frac{1}{(-\kappa)T_\kappa(\tilde{p})(1+e)},$$

and, using these expressions in the classification stated above, we get the landmark values of p or $\tilde{p}$ corresponding to the different types of conic,

$$T_\kappa(r_{\mathrm{per}})<T_\kappa(p_{\mathrm{ell}})<\frac{2T_\kappa(r_{\mathrm{per}})}{1+\sqrt{-\kappa}T_\kappa(r_{\mathrm{per}})}<T_\kappa(p_{\mathrm{par}})<\frac{2T_\kappa(r_{\mathrm{per}})}{1-\sqrt{-\kappa}T_\kappa(r_{\mathrm{per}})}<T_\kappa(p_{\mathrm{hyp}}),$$

which in the Euclidean limit, with $\kappa=0$ and $T_0(x)=x$, reduces to the well known

$$r_{\mathrm{per}}<p_{\mathrm{ell}}<2r_{\mathrm{per}}=p_{\mathrm{par}}=2r_{\mathrm{per}}<p_{\mathrm{hyp}},\quad \text{when } \kappa=0.$$

For the hyperbolic $\tilde{p}$ family, which has no Euclidean limit, we have

$$T_\kappa(\tilde{p}_{\mathrm{hyp}})<\frac{1-\sqrt{-\kappa}T_\kappa(r_{\mathrm{per}})}{(-2\kappa)T_\kappa(r_{\mathrm{per}})}<T_\kappa(\tilde{p}_{\mathrm{par}}).$$

Figures 6(a) and 6(b) represent a set of Kepler orbits in the hyperbolic plane H^2.

VI. FINAL COMMENTS AND OUTLOOK

We have solved the Kepler problem on the three spaces of constant curvature. As we have stated in the introduction, one of the fundamental characteristic of this approach is the use of the curvature κ as a parameter. In this way, all the κ-dependent properties that we have obtained reduce to the appropriate property for the system on the sphere S^2, or on the hyperbolic plane H^2, when particularized for $\kappa>0$, or $\kappa<0$, respectively; in addition, the Euclidean case arises as the very particular (but important) case $\kappa=0$. So, we can summarize this situation pointing out two important facts.

(1) The Kepler problem is not a specific or special characteristic of the Euclidean space but it is well defined in all the three spaces of constant curvature.
(2) There are not three different Kepler problems but only one that is defined, at the same time, in three different manifolds.

Of course, since the three manifolds are geometrically different, many dynamical properties show differences according to the characteristics of the manifolds; nevertheless, the important point is that there is only one theory that is simultaneously valid for the three manifolds and for any value of the curvature. We illustrate this situation recalling the following two important results:

(1) the equation of Binet remains true in the three cases;
(2) the orbits are conics in the three cases.

It is well known that the classical Euclidean Kepler problem is one of the systems endowed with more interesting properties. Therefore, it would be interesting to study all of them, in the general non-Euclidean $\kappa\neq 0$ case; as an example, we have made use, in Sec. IV, of two constants of motion, $I_3(\kappa)$ and $I_4(\kappa)$, that represent the κ-dependent version of the Runge–Lenz vector. The Runge–Lenz vector plays a very important role in the Euclidean case, so it is natural to suppose that the same situation will be true for the case of the general curved system. In fact, we think that, as the Euclidean system is just a very particular case of a much more general system, all the

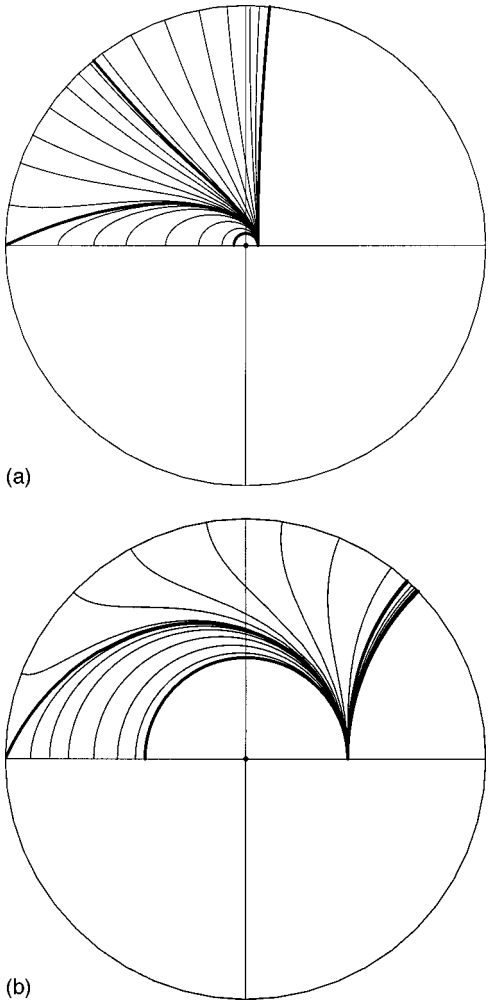

FIG. 6. (A) and (B) A set of Kepler orbits with a fixed periastron distance, depicted in the conformal Poincare disk model of hyperbolic plane, for small r_{per} (A) and large r_{per} (B). The potential center is at the origin, which is a focus of the conics. Thick lines represent particular and limiting conics, circle, horoellipse, horohyperbola, and straight line. A suitable selection (with the other focal elements chosen as to make the diagram clear) of ellipses, parabolas, and hyperbolas are represented as thin lines in each of the three ranges determined by the previous conics. For ellipses and hyperbolas the other focus (not marked) is on the horizontal line; for parabolas the focal line is perpendicular to this horizontal line. The semilatus rectum of the conic lies on the vertical straight line through the origin; notice in (A) only some hyperbolas do not intersect this line, while in (B) conics which do not intersect the semilatus line include all hyperbolas as well as many parabolas; these are the two generic behaviors, as explained in the text.

Euclidean characteristics that are obtained and discussed in the books of theoretical mechanics, must admit a κ-dependent deformed version appropriate for the general "curved" system. We think that these questions are open problems that must be investigated. We also note that in all of this paper we have only dealt with the two-dimensional case since we assumed that it arises from a reduction of the three-dimensional Kepler problem on S^3 and H^3; this dimensional reduction is worthy of a further study.

Finally, the analysis of the orbits has led us, in a natural way, to the theory of conics on spaces of constant curvature. Notice that, although Secs. III and IV were mainly concerned with dynamical questions, Sec. V was written emphasizing its geometrical character; in fact, it can be considered by itself and independently of the other preceding sections. It is clear that the theory of conics on spaces of constant curvature is a geometrical matter of great importance deserving a deeper study that we hope to present elsewhere. On the one hand, there exist some general points and

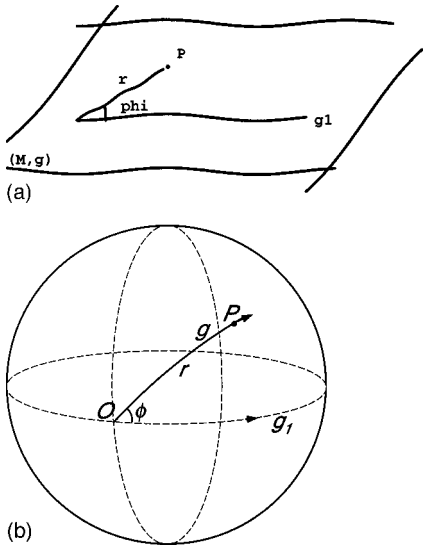

FIG. 7. Polar geodesic coordinates in a two-dimensional Riemannian space (M,g) (A) and in the sphere S^2 (B).

basic properties that, although perfectly known and clearly stated in the Euclidean plane, remain to be studied in the case of spaces of constant curvature; on the other hand, we have already obtained some particular points as, for example, the existence of several different parabolas in the hyperbolic plane, or the possibility of some different alternative ways of defining the eccentricity for a conic in a $\kappa \neq 0$ space, which are really noteworthy. These geometrical questions are also open problems to be investigated.

ACKNOWLEDGMENTS

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APPENDIX: POLAR GEODESIC COORDINATES

A two-dimensional manifold M can be described by using different coordinate systems. If we consider it as an imbedded submanifold of $\mathbb{R}^3$, then the points of M can be characterized by the three external coordinates, as (x,y,z) or (r,ϕ,θ), plus an additional constraint relation. Nevertheless, in differential geometric terms, a more appropriate approach is to develop the study by using two-dimensional systems of coordinates adapted to M.

On any general two-dimensional Riemannian space, not necessarily of constant curvature, there are two distinguished types of local coordinate systems, "geodesic parallel" and "geodesic polar" coordinates. They reduce to the familiar Cartesian and polar coordinates on the Euclidean plane (see Refs. 16 and 42) and both are based on an origin point O and an oriented geodesic g_1 through O.

For any point P in some suitable neighborhood of O, there is a unique geodesic g joining P with O. The (geodesic) polar coordinates (r,ϕ) of P, relative to the origin O and the positive geodesic ray of g_1, are the (positive) distance r between P and O measured along g, and the angle ϕ between g and the positive ray g_1, measured around O (Fig. 7). These coordinates are defined in a neighborhood of O not extending beyond the cut locus of O; polar coordinates are singular at O, and ϕ is discontinuous on the positive ray of g_1.

In the case of M being a space of constant curvature κ, the expression for the differential element of distance ds^2 is given by

$$ds_\kappa^2 = dr^2 + S_\kappa^2(r)d\phi^2,$$

so that we get $ds^2 = dr^2 + r^2\, d\phi^2$ for the particular $\kappa = 0$ Euclidean case.

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Günther's formalism (*k*-symplectic formalism) in classical field theory: Skinner–Rusk approach and the evolution operator

Angel M. Rey[a)]
Departamento de Xeometría e Topoloxía, Facultade de Matemáticas, Universidade de Santiago de Compostela, 15706-Santiago de Compostela, Spain

Narciso Román-Roy[b)]
Departamento de Matemática Aplicada IV, Universidad Politécnica de Cataluña Edificio C-3, Campus Norte, C/ Jordi Girona 1, E-08034 Barcelona, Spain

Modesto Salgado[c)]
Departamento de Xeometría e Topoloxía, Facultade de Matemáticas, Universidade de Santiago de Compostela, 15706-Santiago de Compostela, Spain

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The first aim of this paper is to extend the Skinner–Rusk formalism on classical mechanics for first-order field theories. The second is to generalize the definition and properties of the evolution *K*-operator on classical mechanics for first-order field theories using in both cases Günther's formalism (*k*-symplectic formalism).
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I. INTRODUCTION

The Skinner–Rusk formalism [1] was developed in order to give a geometrical unified formalism for describing mechanical systems. It incorporates all the characteristics of Lagrangian and Hamiltonian descriptions of these systems (including dynamical equations and solutions, constraints, Legendre map, evolution operators, equivalence, etc.).

This formalism has been generalized to time-dependent mechanical systems,[2] and also to the multisymplectic description of first-order field theories.[3,4]

The first aim of this paper is to extend this unified framework to Günther's description of first-order classical field theories,[5] and show how this description comprises the main features of the Lagrangian and Hamiltonian formalisms, both for the regular and singular cases.

Let us point out that Günther's formalism should be also called *k*-symplectic formalism because the base of this formalism are the standard polysymplectic manifolds, introduced by Günther in Ref. 5, which coincide with the *k*-symplectic manifolds introduced by Awane in Refs. 6–8. Günther's paper gives a geometric Hamiltonian formalism for field theories. The crucial device is the introduction of a vector-valued generalization of a symplectic form, called a polysymplectic form. One of the advantages of this formalism is that only the tangent and cotangent bundle of a manifold are required to develop it. In Ref. 9 Günther's formalism was revised and clarified. It was shown that the polysymplectic structures used by Günther to develop his formalism could be replaced by the *k*-symplectic structures defined by Awane.[6–8] So this formalism could be called *k*-symplectic formalism.

The *k*-symplectic formalism is the generalization to field theories of the standard symplectic formalism in mechanics, which is the geometric framework for describing autonomous dynamical systems. In this sense, the *k*-symplectic formalism is used to give a geometric description of

[a)]Electronic mail: angelmrey@edu.xunta.es
[b)]Electronic mail: matnrr@ma4.upc.es
[c)]Electronic mail: modesto@zmat.usc.es

certain kind of field theories: in a local description, those whose Lagrangian does not depend on the coordinates in the basis (in many of them, the space–time coordinates); that is, it is only valid for Lagrangian $L(q^i, v_A^i)$ and Hamiltonian $H(q^i, p_i^A)$ that depends on the field coordinates q^i and on the partial derivatives of the field v_A^i. A natural extension of this formalism is the so-called *k*-cosymplectic formalism, which is the generalization to field theories of the cosymplectic formalism which describes geometrically nonautonomous mechanical systems (this description can be found in Refs. 10 and 11). It is devoted to describing field theories involving the independent parameters $(t^1, \ldots, t^k)$ on the Lagrangian $L(t^A, q^i, v_A^i)$ and on the Hamiltonian $H(t^A, q^i, p_i^A)$.

It is interesting to remark here that the polysymplectic formalism developed by Sardanashvily *et al.*,[12–14] based on a vector valued form on some associated fiber bundle, is a different description of classical field theories of first order than the polysymplectic formalism proposed by Günther. (See also Ref. 15 for more details on the polysymplectic formalism.) In addition, we must remark that the soldering form on the linear frames bundles is a polysymplectic form, and its study and applications to field theory constitute the *n*-symplectic geometry developed by Norris in Refs. 16–20.

The so-called *time-evolution K-operator* in mechanics (also known by some authors as the *relative Hamiltonian vector field* [21]) is a tool which has mainly been developed in order to study the Lagrangian and Hamiltonian formalisms for singular mechanical systems and their equivalence. This operator was introduced in Refs. 22 and 23, and later it was defined geometrically in two different but equivalent ways [24,25] for autonomous dynamical systems. In Ref. 25, a further different geometric construction is given, using a canonical map introduced by Tulczyjew.[26] The *K*-operator relates the sets of solutions of the Euler–Lagrange equations and the Hamilton equations; it also relates constraints on the Lagrangian and Hamiltonian sides, and allows us to obtain a complete classification of constraints;[22] as well as Lagrangian Noether infinitesimal symmetries from a Hamiltonian generator of symmetries.[21,27–29] It is also used for studying Lagrangian systems whose Legendre map has generic singularities.[21,30]

The second aim of this paper is to generalize the definition and properties of this operator for first-order field theories in order to describe the relationship between the Lagrangian and Hamiltonian *k*-symplectic formalisms. In particular we extend the results in Ref. 25, showing how to obtain the solutions of Lagrangian and Hamiltonian field equations by means of this operator. The same idea has been developed in Ref. 31 but using the multisymplectic description of classical field theories.

The organization of the paper is as follows: Section II–IV are devoted to reviewing the main features of Günther's formalism or *k*-symplectic formalism [5,9] of Lagrangian and Hamiltonian field theories.

In particular, in Sec. II the field theoretic phase space is introduced as the Whitney sum $(T_k^1)^*Q = T^*Q \overset{k}{\oplus} \ldots \oplus T^*Q$ of *k*-copies of the cotangent bundle T^*Q of a manifold Q. This space is the canonical example of a polysymplectic manifold. A particular case of polysymplectic manifolds are the *k*-symplectic manifolds (see Refs. 3–5, 8, and 9) which coincide with the standard polysymplectic manifolds.

The field theoretic state space is introduced as the Whitney sum $T_k^1Q = TQ \overset{k}{\oplus} \ldots \oplus TQ$ of *k*-copies of the tangent bundle TQ of a manifold Q. This manifold has a canonical *k*-tangent structure defined by *k* tensor fields of type (1, 1) satisfying certain algebraic properties. The *k*-tangent manifolds were introduced in de León *et al.*,[32,33] and they generalize the tangent manifolds (see Refs. 34–38).

Section III is devoted to giving a geometric interpretation of the second-order partial differential equations. Here we show that these equations can be characterized by using the canonical *k*-tangent structure of T_k^1Q, which generalizes the case of classical mechanics.

The Hamiltonian and Lagrangian formalisms are developed in Sec. IV. Lagrangian formalism is developed using the canonical *k*-tangent structure of T_k^1Q, or the Legendre transformation as in Günther.[5]

In Sec. V we develop the unified formalism for field theories, which is based on the use of the Whitney sum $T^1_kQ\oplus_Q(T^1_k)^*Q$ of T^1_kQ and $(T^1_k)^*Q$. There are canonical presymplectic forms on it (the pull-back of the canonical symplectic form on each T^*Q) and a natural coupling function which is defined by the contraction between vectors and covectors. Then, given a Lagrangian $L\in C^\infty(T^1_kQ)$ we can state a field equation on $T^1_kQ\oplus_Q(T^1_k)^*Q$. This equation has solution only on a submanifold M_L, which is the graph of the Legendre map. Then we prove that if $\mathbf{Z}=(Z_1,\ldots,Z_k)$ is an integrable k-vector field, solution to this equation and tangent to M_L, then the projection onto the first factor T^1_kQ of the integral sections of $\mathbf{Z}$ are solutions of the Euler–Lagrange field equations. If L is regular the converse also holds. Furthermore, we establish the relationship between $\mathbf{Z}$ and the Hamiltonian and the Lagrangian k-vector fields of the k-symplectic formalism, $\mathbf{X_H}$ and $\mathbf{X_L}$.

In Sec. VI we review the definition and the main properties of the evolution operator K for autonomous mechanics. Next we define the field operators which, as a consequence of the field equations on the k-symplectic formalism, are given as a k-vector field along the Legendre transformation FL, associated to the Lagrangian $L:T^1_kQ\to\mathbb{R}$, satisfying certain properties. Finally we finish with similar results for field theories to those obtained in Refs. 25 and 31.

In a forthcoming paper we shall extend the results of this paper to the k-cosymplectic formalism.[10,11]

Manifolds are real, paracompact, connected and C^∞. Maps are C^∞. Sum over crossed repeated indices is understood.

II. GEOMETRIC FRAMEWORK

A. The cotangent bundle of k^1-covelocities of a manifold

Let Q be a differentiable manifold of dimension n and $\tau^*:T^*Q\to Q$ its cotangent bundle. Let us denote by $(T^1_k)^*Q=T^*Q\overset{k}{\oplus}\ldots\oplus T^*Q$ the Whitney sum of k copies of T^*Q, with projection map $\tau^*_Q:(T^1_k)^*Q\to Q$, $\tau^*_Q(\alpha^1_q,\ldots,\alpha^k_q)=q$, for every $(\alpha^1_q,\ldots,\alpha^k_q)\in(T^1_k)^*Q$.

$(T^1_k)^*Q$ can be canonically identified with the vector bundle $J^1(Q,\mathbb{R}^k)_0$ of k^1-covelocities of the manifold Q, that is the vector bundle of 1-jets of maps $\sigma:Q\to\mathbb{R}^k$ with target at $0\in\mathbb{R}^k$ and projection map $\tau^*_Q:J^1(Q,\mathbb{R}^k)_0\to Q$, $\tau^*_Q(j^1_{q,0}\sigma)=q$, say,

$$J^1(Q,\mathbb{R}^k)_0\equiv T^*Q\overset{k}{\oplus}\ldots\oplus T^*Q,$$

$$j^1_{q,0}\sigma\equiv(\mathrm{d}\sigma^1(q),\ldots,\mathrm{d}\sigma^k(q)),$$

where $\sigma^A=\pi^A\circ\sigma:Q\to\mathbb{R}$ is the Ath component of σ, and $\pi^A:\mathbb{R}^k\to\mathbb{R}$ is the canonical projection $1\leqslant A\leqslant k$. For this reason to $(T^1_k)^*Q$ is also called *the bundle of k^1-covelocities of the manifold Q*.

If (q^i) are local coordinates on $U\subseteq Q$, then the induced local coordinates (q^i,p_i), $1\leqslant i\leqslant n$, on $T^*U=(\tau^*)^{-1}(U)$, are given by

$$q^i(\alpha_q)=q^i(q),\quad p_i(\alpha_q)=\alpha_q\left(\left.\frac{\partial}{\partial q^i}\right|_q\right),\quad \alpha_q\in T^*Q,$$

and the induced local coordinates (q^i,p^A_i), $1\leqslant i\leqslant n$, $1\leqslant A\leqslant k$, on $(T^1_k)^*U=(\tau^*_Q)^{-1}(U)$ are given by

$$q^i(\alpha^1_q,\ldots,\alpha^k_q)=q^i(q),\quad p^A_i(\alpha^1_q,\ldots,\alpha^k_q)=\alpha^A_q\left(\left.\frac{\partial}{\partial q^i}\right|_q\right).$$

Let us denote by $\{r_1,\ldots,r_k\}$ the canonical basis of $\mathbb{R}^k$.

Definition 2.1 (Günther [5]): A closed nondegenerate $\mathbb{R}^k$-valued 2-form,

$$\overline{\omega}=\sum_{A=1}^{k}\omega_A\otimes r_A$$

on a manifold M of dimension N is called a polysymplectic form. *The pair* $(M,\overline{\omega})$ *is a* polysymplectic manifold.

The manifold $(T^1_k)^*Q$ is endowed with a *canonical polysymplectic structure*. This canonical structure $\overline{\omega}=\Sigma_{A=1}^{k}(\omega_0)_A\otimes r_A$, on $(T^1_k)^*Q$ is defined by

$$(\omega_0)_A=(\tau_A^*)^*(\omega_0),\quad 1\leqslant A\leqslant k,$$

where $\tau_A^*:(T^1_k)^*Q\to T^*Q$ is the projection on the A^{th}-copy T^*Q of $(T^1_k)^*Q$, and $\omega_0=-\mathrm{d}\theta_0$ is the canonical symplectic structure of T^*Q, θ_0 being the Liouville 1-form defined by

$$\theta_0(\alpha_q)(\tilde{X}_{\alpha_q})=\alpha_q((\tau^*)_*(\alpha_q)(\tilde{X}_{\alpha_q})),\quad \alpha_q\in T^*Q,\quad \tilde{X}_{\alpha_q}\in T_{\alpha_q}(T^*Q).$$

One can also define the 2-forms $(\omega_0)_A$ by $(\omega_0)_A=-d(\theta_0)_A$ where $(\theta_0)_A=(\tau_A^*)^*\theta_0$.

Thus the Liouville 1-form and the canonical symplectic structure on T^*Q are locally given by

$$\theta_0=p_i\,\mathrm{d}q^i,\quad \omega_0=-\,\mathrm{d}\theta_0=\mathrm{d}q^i\wedge\mathrm{d}p_i,$$

and the canonical polysymplectic structure $((\omega_0)_1,\ldots,(\omega_0)_k)$ on $(T^1_k)^*Q$ is locally given by

$$(\omega_0)_A=-\,d(\theta_0)_A=-\,d(p_i^A\,\mathrm{d}q^i)=\mathrm{d}q^i\wedge\mathrm{d}p_i^A. \tag{1}$$

Definition 2.2 (Günther [5]): A polysymplectic form $\overline{\omega}$ *on a manifold M is called standard iff for every point of M there exists a local coordinate system such that* ω_A *is written locally as in (1).*

So the canonical polysymplectic form $\overline{\omega}$ on $(T^1_k)^*Q$ is standard.

Remark 2.1: The *k*-symplectic manifolds were introduced in Refs. 6–8 and they coincide with the *standard polysymplectic manifolds*, as we now shall show.

Definition 2.3 (Awane [6]): A k-symplectic structure on a manifold M of dimension $N=n+kn$ *is a family* $(\omega_A,V;\ 1\leqslant A\leqslant k)$, *where each* ω_A *is a closed* 2*-form and V is an integrable nk-dimensional distribution on M such that*

$$\text{(i) } \omega_{A_{|V\times V}}=0,\quad \text{(ii) } \cap_{A=1}^{k}\ker\omega_A=\{0\}.$$

In this case (M,ω_A,V) *is called a k-symplectic manifold.*

Theorem 2.1 (Awane [6]): *Let* $(\omega_A,V;\ 1\leqslant A\leqslant k)$ *be a k-symplectic structure on M. About every point of M we can find a local coordinate system* (q^i,p_i^A), $1\leqslant i\leqslant n$, $1\leqslant A\leqslant k$, *such that*

$$\omega_A=\mathrm{d}q^i\wedge\mathrm{d}p_i^A,\quad 1\leqslant A\leqslant k. \tag{2}$$

The canonical model of *k*-symplectic manifolds is also $(T^1_k)^*Q$ and the canonical *k*-symplectic structure $(\omega_A,V;\ 1\leqslant A\leqslant k)$, on $(T^1_k)^*Q$ is given by

$$\omega_A=(\omega_0)_A=(\tau_A^*)^*(\omega_0),\quad V(j^1_{q,0}\sigma)=\ker(\tau_Q^*)_*(j^1_{q,0}\sigma).$$

Therefore, the 2-forms of the canonical polysymplectic structure and the canonical *k*-symplectic structure on $(T^1_k)^*Q$ coincide.

From (2) we know that the standard polysymplectic structures and the *k*-symplectic structures coincide. Indeed, if $\overline{\omega}=\Sigma_{A=1}^{k}\omega_A\otimes r_A$ is a standard polysymplectic structure on *M*, given a local adapted coordinate system (q^i,p_i^A) we can define, locally, the distribution *V*, of dimension *nk*, by $\mathrm{d}q^1=\cdots=\mathrm{d}q^n=0$. Then, $(\omega_1,\ldots,\omega_k,V)$ is a *k*-symplectic structure on *M*.

Conversely if $(\omega_1,\ldots,\omega_k,V)$ is a *k*-symplectic structure on *M* then $\overline{\omega}=\Sigma_{A=1}^{k}\omega_A\otimes r_A$ is a standard polysymplectic structure on *M*, because it is trivially standard and is nondegenerate as a consequence of (ii) in Definition 2.3.

As we shall see later, in his Hamiltonian formalism, Günther uses a standard polysymplectic manifold because he needs to have local coordinates (q^i,p_i^A) in the manifold *M* where the Hamiltonian is defined, which is equivalent to considering a *k*-symplectic manifold. For this reason we will call the Günther's formalism, called polysymplectic formalism, *k*-symplectic formalism.

B. The tangent bundle of k^1-velocities of a manifold

Let $\tau: TQ \to Q$ be the tangent bundle of Q. Let us denote by T^1_kQ the Whitney sum $TQ \oplus \overset{k}{\cdots} \oplus TQ$ of k copies of TQ, with projection $\tau_Q: T^1_kQ \to Q$, $\tau_Q(v_{1q}, \ldots, v_{kq}) = q$.

T^1_kQ can be identified with the vector bundle $J^1_0(\mathbb{R}^k, Q)$ of the k^1-velocities of the manifold Q, that is, the vector bundle of 1-jets of maps $\sigma: \mathbb{R}^k \to Q$ with source at $0 \in \mathbb{R}^k$, and projection map $\tau_Q: T^1_kQ \to Q$, $\tau_Q(j^1_{0,q}\sigma) = \sigma(0) = q$, say

$$J^1_0(\mathbb{R}^k, Q) \equiv TQ \oplus \overset{k}{\cdots} \oplus TQ,$$

$$j^1_{0,q}\sigma \equiv (v_{1q}, \ldots, v_{kq}),$$

where $q = \sigma(0)$, and $v_{Aq} = \sigma_*(0)[(\partial/\partial t^A)(0)]$, $1 \leqslant A \leqslant k$. For this reason T^1_kQ is called the *tangent bundle of k^1-velocities of Q*.

If (q^i) are local coordinates on $U \subseteq Q$ then the induced local coordinates (q^i, v^i), $1 \leqslant i \leqslant n$, on $TU = \tau^{-1}(U)$ are given by

$$q^i(v_q) = q^i(q), \quad v^i(v_q) = v_q(q^i), \quad v_q \in TQ,$$

and the induced local coordinates (q^i, v^i_A), $1 \leqslant i \leqslant n$, $1 \leqslant A \leqslant k$, on $T^1_kU = \tau_Q^{-1}(U)$ are given by

$$q^i(v_{1q}, \ldots, v_{kq}) = q^i(q), \quad v^i_A(v_{1q}, \ldots, v_{kq}) = v_{Aq}(q^i).$$

We now introduce the *canonical k-tangent structure* on T^1_kQ.

Definition 2.4: For a vector X_q at Q, and for $1 \leqslant A \leqslant k$, we define its vertical A-lift $(X_q)^A$ as the vector on T^1_kQ given by

$$(X_q)^A(v_{1q}, \ldots, v_{kq}) = \frac{d}{ds}(v_{1q}, \ldots, v_{A-1q}, v_{Aq} + sX_q, v_{A+1q}, \ldots, v_{kq})_{|s=0}$$

for all points $(v_{1q}, \ldots, v_{kq}) \in T^1_kQ$.

In local coordinates we have

$$(X_q)^A = a^i \frac{\partial}{\partial v^i_A}\bigg|_q \tag{3}$$

for a vector $X_q = a^i(\partial/\partial q^i)(q)$.

The *canonical k-tangent structure* on T^1_kQ is the set $(S^1, \ldots, S^k)$ of tensor fields of type (1, 1) defined by

$$S^A(v)(Z_v) = ((\tau_Q)_*(v)(Z_v))^A \quad \text{for all } Z_v \in T_v(T^1_kQ), \quad v = (v_{1q}, \ldots, v_{kq}),$$

for each $1 \leqslant A \leqslant k$.

From (3) we have in local coordinates,

$$S^A = \frac{\partial}{\partial v^i_A} \otimes dq^i. \tag{4}$$

The tensors S^A can be regarded as the $(0, \ldots, 0, \overset{A}{1}, 0, \ldots, 0)$-lift of the identity tensor on Q to T^1_kQ defined by Morimoto.[39]

Remark 2.2: The *k*-tangent manifolds were introduced as a generalization of the tangent manifolds by de León *et al.* [32,33] The canonical model of these manifolds is T^1_kQ with the structure given by $(S^1, \ldots, S^k)$.

To develop later the Lagrangian formalism, we now construct a polysymplectic structure on T^1_kQ, for each regular Lagrangian $L: T^1_kQ \to \mathbb{R}$, , using its canonical *k*-tangent structure.

Definition 2.5: A Lagrangian $L:T^1_kQ\to\mathbb{R}$ *is called regular if and only if*

$$\det\left(\frac{\partial^2 L}{\partial v^i_A\,\partial v^j_B}\right)\neq 0,\quad 1\leqslant i,j\leqslant n,\quad 1\leqslant A,B\leqslant k.$$

Let us consider the 1-forms $(\theta_L)_A=\mathrm{d}L\circ S^A$, $1\leqslant A\leqslant k$. In a local coordinate system (q^i,v^i_A) we have

$$(\theta_L)_A=\frac{\partial L}{\partial v^i_A}\mathrm{d}q^i,\quad 1\leqslant A\leqslant k. \tag{5}$$

Introducing the following 2-forms $(\omega_L)_A=-d(\theta_L)_A$, $1\leqslant A\leqslant k$, one can easily prove the following proposition.

Proposition 2.1: $L:T^1_kQ\to\mathbb{R}$ *is a regular Lagrangian if and only if* $((\omega_L)_1,\ldots,(\omega_L)_k)$ *is a polysymplectic structure on* T^1_kQ.

This polysymplectic structure, associated to L, was also introduced by Günther [5] using the Legendre transformation.

The Legendre map $FL:T^1_kQ\to(T^1_k)^*Q$, was introduced by Günther,[5] and we rewrite it as follows: if $(v_{1q},\ldots,v_{kq})\in(T^1_k)_qQ$,

$$[FL(v_{1q},\ldots,v_{kq})]^A(w_q)=\frac{d}{\mathrm{d}s}L(v_{1q},\ldots,v_{Aq}+sw_q,\ldots,v_{kq})_{|s=0},$$

for each $1\leqslant A\leqslant k$. We deduce that FL is locally given by

$$(q^i,v^i_A)\to\left(q^i,\frac{\partial L}{\partial v^i_A}\right). \tag{6}$$

In fact, from (5) and (6), we easily obtain the following Lemma.

Lemma 2.1: For every $1\leqslant A\leqslant k$, $(\omega_L)_A=(FL)^*(\omega_0)_A$, *where* $(\omega_0)_1,\ldots,(\omega_0)_k$ *are the 2-forms of the canonical polysymplectic structure or canonical k-symplectic structure of* $(T^1_k)^*Q$.

Then, from (6) we get the following.

Proposition 2.2: Let L be a Lagrangian. The following conditions are equivalent.

(1) L is regular. (2) FL is a local diffeomorphism. (3) $((\omega_L)_1,\ldots,(\omega_L)_k)$ *is a polysymplectic structure on* T^1_kQ.

Remark 2.3: If FL is a global diffeomorphism, then L is called a *hyper-regular Lagrangian*.

III. *k*-VECTOR FIELDS. SECOND-ORDER PARTIAL DIFFERENTIAL EQUATIONS ON T^1_kQ

A. *k*-vector fields

Let M be an arbitrary manifold and $\tau_M:T^1_kM\to M$ its tangent bundle of k^1 velocities.

Definition 3.1: A section $\mathbf{X}:M\to T^1_kM$ *of the projection* τ_M *will be called a* k-vector field *on* M.

Since T^1_kM is the Whitney sum $TM\overset{k}{\oplus}\ldots\oplus TM$ of k copies of TM, we deduce that a k-vector field $\mathbf{X}$ defines a family of k vector fields $\{X_1,\ldots,X_k\}$ on M by projecting $\mathbf{X}$ onto every factor. For this reason we will denote a k-vector field $\mathbf{X}$ by $(X_1,\ldots,X_k)$.

Definition 3.2: An integral section *of the k-vector field* $\mathbf{X}=(X_1,\ldots,X_k)$ *passing through a point* $x\in M$ *is a map* $\phi:U_0\subset\mathbb{R}^k\to M$, *defined on some neighborhood* U_0 *of* $0\in\mathbb{R}^k$, *such that*

$$\phi(0)=x,\quad \phi_*(t)\left(\left.\frac{\partial}{\partial t^A}\right|_t\right)=X_A(\phi(t))\quad \textit{for every } t\in U_0,\quad 1\leqslant A\leqslant k,$$

or equivalently, ϕ *satisfies* $\mathbf{X}\circ\phi=\phi^{(1)}$, *where* $\phi^{(1)}$ *is the first prolongation of* ϕ *defined by*

$$\phi^{(1)}: U_0 \subset \mathbb{R}^k \to T_k^1 M,$$

$$t \to \phi^{(1)}(t) = j_0^1 \phi_t, \quad \phi_t(\overline{t}) = \phi(\overline{t} + t),$$

for every $\overline{t}$, $t \in \mathbb{R}^k$ *such that* $\overline{t}+t \in U_0$.

In local coordinates,

$$\phi^{(1)}(t^1,\ldots,t^k) = \left(\phi^i(t^1,\ldots,t^k), \frac{\partial \phi^i}{\partial t^A}(t^1,\ldots,t^k)\right), \quad 1 \leqslant A \leqslant k, \quad 1 \leqslant i \leqslant n. \tag{7}$$

We say that a k-vector field $\mathbf{X}=(X_1,\ldots,X_k)$ on M is integrable if there is an integral section passing through each point of M.

We remark that a k-vector field $\mathbf{X}$ is integrable if, and only if, $\{X_1,\ldots,X_k\}$ define an involutive distribution on M.

B. Second-order partial differential equations in $T_k^1 Q$

The aim of this section is to characterize the integrable k-vector fields on $T_k^1 Q$ such that their integral sections are canonical prolongations of maps from $\mathbb{R}^k$ to Q.

In general, if $F: M \to N$ is a differentiable map, then the induced map $T_k^1(F): T_k^1 M \to T_k^1 N$ defined by $T_k^1(F)(j_0^1 g) = j_0^1(F \circ g)$ is given by

$$T_k^1(F)(v_{1q},\ldots,v_{kq}) = (F_*(q)v_{1q},\ldots,F_*(q)v_{kq}),$$

where $v_{1q},\ldots,v_{kq} \in T_q Q$, $q \in Q$, and $F_*(q): T_q M \to T_{F(q)} N$.

Definition 3.3: A k-vector field on $T_k^1 Q$, *that is, a section* $\mathbf{X}: T_k^1 Q \to T_k^1(T_k^1 Q)$ *of the projection* $\tau_{T_k^1 Q}: T_k^1(T_k^1 Q) \to T_k^1 Q$, *is a* second-order partial differential equation (SOPDE) *if it is also a section of the vector bundle* $T_k^1(\tau_Q): T_k^1(T_k^1 Q) \to T_k^1 Q$; *that is,*

$$T_k^1(\tau_Q) \circ \mathbf{X} = Id_{T_k^1 Q}, \tag{8}$$

where $T_k^1(\tau)$ *is defined by* $T_k^1(\tau_Q)(j_0^1 \gamma) = j_0^1(\tau_Q \circ \gamma)$.

Let (q^i) be a coordinate system on Q and (q^i, v_A^i) the induced coordinate system on $T_k^1 Q$. From a direct computation in local coordinates we obtain that the local expression of a SOPDE $(X_1,\ldots,X_k)$ is

$$X_A(q^i, v_A^i) = v_A^i \frac{\partial}{\partial q^i} + (X_A)_B^i \frac{\partial}{\partial v_B^i}, \quad 1 \leqslant A \leqslant k. \tag{9}$$

If $\varphi: \mathbb{R}^k \to T_k^1 Q$, is an integral section of $(X_1,\ldots,X_k)$ locally given by $\varphi(t) = (\varphi^i(t), \varphi_B^i(t))$ then $X_A(\varphi(t)) = \varphi_*(t)[\partial/\partial t^A(t)]$ and thus

$$\frac{\partial \varphi^i}{\partial t^A}(t) = v_A^i(\varphi(t)) = \varphi_A^i(t), \quad \frac{\partial \varphi_B^i}{\partial t^A}(t) = (X_A)_B^i(\varphi(t)).$$

From (7) we obtain the following.

Proposition 3.1: Let $\mathbf{X}=(X_1,\ldots,X_k)$ *be an integrable* SOPDE. *If* φ *is an integral section then* $\varphi = \phi^{(1)}$ *where* $\phi^{(1)}$ *is the first prolongation of the map* $\phi = \tau_Q \circ \varphi: \mathbb{R}^k \xrightarrow{\varphi} T_k^1 Q \xrightarrow{\tau_Q} Q$, *and satisfies*

$$\frac{\partial \phi^i}{\partial t^A \partial t^B}(t) = (X_A)_B^i(\phi^{(1)}(t)). \tag{10}$$

Conversely, if $\phi: \mathbb{R}^k \to Q$ *is any map satisfying (10) then* $\phi^{(1)}$ *is an integral section of* $(X_1,\ldots,X_k)$.

Definition 3.4: Let $(X_1,\ldots,X_k)$ *be an integrable* SOPDE. *A map* $\phi: \mathbb{R}^k \to Q$ *is said to be a* solution to the SOPDE *if the first prolongation* $\phi^{(1)}$ *is an integral section of* $(X_1,\ldots,X_k)$.

A k-vector field which is an integrable SOPDE *is called a* holonomic *k*-vector field, *and its integral sections* $\varphi=\phi^{(1)}$ *are called* holonomic sections.

Now we show how to characterize the SOPDE using the canonical *k*-tangent structure of T^1_kQ.

Definition 3.5: The Liouville vector field C *on* T^1_kQ *is the infinitesimal generator of the following flow:*

$$\mathbb{R}\times T^1_kQ\to T^1_kQ,$$

$$(s,(v_{1_q},\ldots,v_{k_q}))\to(e^sv_{1_q},\ldots,e^sv_{k_q}),$$

and in local coordinates has the form

$$C=\sum_{i,B}v^i_B\frac{\partial}{\partial v^i_B}. \tag{11}$$

We can write $C=C_1+\cdots+C_k$ where C_A, $1\leqslant A\leqslant k$, are the canonical vector fields on T^1_kQ given by the following flows:

$$\mathbb{R}\times T^1_kQ\to T^1_kQ,$$

$$(s,(v_{1_q},\ldots,v_{k_q}))\to(v_{1_q},\ldots,v_{A-1_q},e^sv_{A_q},v_{A+1_q},\ldots,v_{k_q}).$$

In local coordinates,

$$C_A=\sum_i v^i_A\frac{\partial}{\partial v^i_A}. \tag{12}$$

From (4), (9), (11), and (12) we deduce the following.

Proposition 3.2: A k-vector field $\mathbf{X}=(X_1,\ldots,X_k)$ *on* T^1_kQ *is a* SOPDE *if, and only if,* $S^A(X_A)=C_A$, *for all* $1\leqslant A\leqslant k$, *where* $(S^1,\ldots,S^k)$ *is the canonical k-tangent structure on* T^1_kQ.

IV. HAMILTONIAN AND LAGRANGIAN FORMALISM (Refs. 5 and 9)

A. Hamiltonian formalism

Let (M,ω_A,V) be a *k*-symplectic manifold, and $H:M\to\mathbb{R}$ a Hamiltonian function. Let $\mathbf{X}=(X_1,\ldots,X_k)$ be a *k*-vector field on M that satisfies the equations

$$\sum_{i=1}^{k}\imath_{X_A}\omega_A=\mathrm{d}H. \tag{13}$$

If X_A is locally given by

$$X_A=(X_A)^i\frac{\partial}{\partial q^i}+(X_A)^B_i\frac{\partial}{\partial P^B_i}$$

in a local system of canonical coordinates (q^i,p^A_i) (whose existence is ensured by the Theorem 2.1), then (13) is equivalent to the equations

$$\frac{\partial H}{\partial q^i}=-\sum_{A=1}^{k}(X_A)^A_i,\quad \frac{\partial H}{\partial p^A_i}=(X_A)^i.$$

So if $(X_1,\ldots,X_k)$ is also integrable then its integral sections $\varphi:\mathbb{R}^k\to M$, with $\varphi(t)=(\varphi^i(t),\varphi^A_i(t))$ are solutions to the *Hamilton–De Donder–Weyl field equations*,

$$\frac{\partial H}{\partial q^i} = -\sum_{A=1}^{k} \frac{\partial \varphi_i^A}{\partial t^A}, \quad \frac{\partial H}{\partial p_i^A} = \frac{\partial \varphi^i}{\partial t^A}, \quad 1 \leqslant A \leqslant k, \quad 1 \leqslant i \leqslant n. \tag{14}$$

So, Eq. (13) is a geometric version of the Hamilton–De Donder–Weyl field equations.

B. Lagrangian formalism

In this section, we recall the Lagrangian formalism developed by Günther.[5]

In general, given a Lagrangian function of the form $L=L(q^i, v_A^i)$, and using a variational principle, one obtains the *Euler–Lagrange field equations* for L,

$$\sum_{A=1}^{k} \frac{d}{dt^A}\left(\frac{\partial L}{\partial v_A^i}\right) - \frac{\partial L}{\partial q^i} = 0, \quad v_A^i = \frac{\partial q^i}{\partial t^A}. \tag{15}$$

Then, let $L: T_k^1 Q \to \mathbb{R}$ be a Lagrangian, and let us consider the 2-forms $((\omega_L)_1, \ldots, (\omega_L)_k)$ on $T_k^1 Q$ defined by L, and $E_L = C(L) - L$, C being the Liouville vector field in $T_k^1 Q$. Now, let $\mathbf{X} = (X_1, \ldots, X_k)$ be a k-vector field in $T_k^1 Q$ (that is, a section $\mathbf{X}: T_k^1 Q \to T_k^1(T_k^1 Q)$) of the projection $\tau_{T_k^1 Q}: T_k^1(T_k^1 Q) \to T_k^1 Q$. Then we have the following.

Proposition 4.1: If $\mathbf{X}=(X_1, \ldots, X_k)$ *is an integrable* SOPDE, *and* $\psi \equiv \phi^{(1)}: \mathbb{R}^k \to T_k^1 Q$ *is an integral section of* $\mathbf{X}$, *then* $\mathbf{X}$ *is a solution to the equation*

$$\sum_{A=1}^{k} \imath_{X_A}(\omega_L)_A = dE_L, \tag{16}$$

if, and only if, $\phi: \mathbb{R}^k \to Q$ *is a solution to the Euler–Lagrange equations (15).*

Proof: If each X_A is locally given by

$$X_A = (X_A)^i \frac{\partial}{\partial q^i} + (X_A)_B^i \frac{\partial}{\partial v_B^i}$$

then, from (5), (11), and (16) we deduce that $(X_1, \ldots, X_k)$ is a solution to (16) if, and only if, $(X_A)^i$ and $(X_A)_B^i$ satisfy the system of equations

$$\left(\frac{\partial^2 L}{\partial q^i \partial v_A^j} - \frac{\partial^2 L}{\partial q^j \partial v_A^i}\right)(X_A)^j - \frac{\partial^2 L}{\partial v_A^i \partial v_B^j}(X_A)_B^j = v_A^j \frac{\partial^2 L}{\partial q^i \partial v_A^j} - \frac{\partial L}{\partial q^i}, \tag{17}$$

$$\frac{\partial^2 L}{\partial v_B^j \partial v_A^i}(X_A)^i = \frac{\partial^2 L}{\partial v_B^j \partial v_A^i} v_A^i. \tag{18}$$

But, as $\mathbf{X}$ is a SOPDE, we have

$$(X_A)^i = v_A^i, \tag{19}$$

then (18) holds identically, and (17) is equivalent to

$$\frac{\partial^2 L}{\partial q^j \partial v_A^i} v_A^j + \frac{\partial^2 L}{\partial v_A^i \partial v_B^j}(X_A)_B^j = \frac{\partial L}{\partial q^i}. \tag{20}$$

Now, if $\psi(t) = \phi^{(1)} = (\phi^i(t), \phi_A^i(t))$ is an integral section of $\mathbf{X}$, then

$$(X_A)^i(\psi(t)) = \phi_A^i(t) = \frac{\partial \phi^i}{\partial t^A}, \tag{21}$$

$$(X_A)^i_B(\psi(t)) = \frac{\partial \phi^i_B}{\partial t^A} = \frac{\partial^2 \phi^i}{\partial t^A \partial t^B}, \tag{22}$$

and going to (20) we obtain that

$$\frac{\partial^2 L}{\partial q^i \partial v^j_A}(\phi(t))\frac{\partial \phi^i}{\partial t^A} + \frac{\partial^2 L}{\partial v^i_B \partial v^j_A}(\phi(t))\frac{\partial \phi^i_B}{\partial t^A} = \frac{\partial^2 L}{\partial q^i \partial v^j_A}(\phi(t))\frac{\partial \phi^i}{\partial t^A} + \frac{\partial^2 L}{\partial v^i_B \partial v^j_A}(\phi(t))\frac{\partial^2 \phi^i}{\partial t^A \partial t^B} = \frac{\partial L}{\partial q^i}(\phi(t)) \tag{23}$$

which are the Euler–Lagrange equations for the map ϕ.

Conversely, let $\mathbf{X}$ be an integrable SOPDE having $\psi(t)=\phi^{(1)}=(\phi^i(t),\phi^i_A(t))$ as integral sections, for every $(\phi^i(t))$ solution to the Euler–Lagrange equations. Therefore (21) and (22) hold since $\mathbf{X}$ is a SOPDE, and then (23), which holds because $(\phi^i(t))$ is a solution to the Euler–Lagrange equations, is equivalent to (20). Hence $\mathbf{X}$ is a solution to (16). ■

In this way, Eq. (16) can be considered as a geometric version of the Euler–Lagrange field equations.

Observe that, if the Lagrangian is regular, Eq. (18) leads to conclude that every solution to (16) is a SOPDE. In addition, Eq. (20) leads to defining local solutions to (16) in a neighborhood of each point of T^1_kQ and, using a partition of unity, global solutions to (16).

Now let us suppose that the Lagrangian $L:T^1_kQ\to\mathbb{R}$ is hyper-regular, that is, FL is a diffeomorphism. We consider the Hamiltonian $H:(T^1_k)^*Q\to\mathbb{R}$ defined by $H=E_L\circ FL^{-1}$ where FL^{-1} is the inverse map of FL. Then we have the following.

Theorem 4.1: *(a) If $\mathbf{X}_L=((X_L)_1,\ldots,(X_L)_k)$ is a solution to (16) then $\mathbf{X}_H=((X_H)_1,\ldots,(X_H)_k)$, where $(X_H)_A=FL_*((X_L)_A)$, $1\leqslant A\leqslant k$, is a solution to (13) with $\omega_A=(\omega_0)_A$ and $H=E_L\circ FL^{-1}$.*

(b) If $\mathbf{X}_L=((X_L)_1,\ldots,(X_L)_k)$ is integrable, $\phi^{(1)}$ is an integral section and $\phi=\tau_Q\circ\phi^{(1)}$, then $\varphi=FL\circ\phi^{(1)}$ is an integral section of $\mathbf{X}_H=((X_H)_1,\ldots,(X_H)_k)$ and thus it is a solution to the Hamilton–De Donder–Weyl equations (14) for $H=E_L\circ FL^{-1}$.

Proof: (a) It is an immediate consequence of (13) and (16) using that $FL^*(\omega_0)_A=(\omega_L)_A$ and $E_L=H\circ FL^{-1}$.

(b) It is an immediate consequence of Definition 3.2 of integral section of a k-vector field. ■

Definition 4.1: A singular Lagrangian system $(T^1_kQ,(\omega_L)_1,\ldots,(\omega_L)_k)$ is called almost regular if $\mathcal{P}:=FL(T^1_kQ)$ is a closed submanifold of $(T^1_k)^*Q$ (we will denote the natural imbedding by $j_0:\mathcal{P}\hookrightarrow(T^1_k)^*Q$), FL is a submersion onto its image, and the fibers $FL^{-1}(FL(v))$, for every $v\in T^1_kQ$, are connected submanifolds of T^1_kQ.

In this case there exists $H_0\in\mathrm{C}^\infty(\mathcal{P})$ such that $(FL_0)^*H_0=E_L$, where $FL_0:T^1_kQ\to\mathcal{P}$ is defined by $j_0\circ FL_0=FL$, and the Hamiltonian field equation analogous to (13) is

$$\sum_{i=1}^{k} \imath_{(X_0)_A}\omega^0_A = \mathrm{d}H_0, \tag{24}$$

where $\omega^0_A=j_0^*(\omega_0)_A$, for every $1\leqslant A\leqslant k$, and $\mathbf{X}_0=((X_0)_1,\ldots,(X_0)_k)$ (if it exists) is a k-vector field on $\mathcal{P}$.

V. SKINNER–RUSK FORMULATION

A. The Skinner–Rusk formalism for *k*-symplectic field theories

Let us consider the *Whitney sum* $T^1_kQ\oplus_Q(T^1_k)^*Q$, with coordinates (q^i,v^i_A,p^A_i). It has natural bundle structures over T^1_kQ and $(T^1_k)^*Q$. Let us denote by $pr_1:T^1_kQ\oplus_Q(T^1_k)^*Q\to T^1_kQ$ the projection into the first factor, $pr_1(q^i,v^i_A,p^A_i)=(q^i,v^i_A)$, and $pr_2:T^1_kQ\oplus_Q(T^1_k)^*Q\to(T^1_k)^*Q$ the projection into the second factor, $pr_2(q^i,v^i_A,p^A_i)=(q^i,p^A_i)$.

In this bundle, we have some canonical structures. First, let $((\omega_0)_1,\ldots,(\omega_0)_k)$ be the canonical polysymplectic structure on $(T^1_k)^*Q$. We shall denote by $(\Omega_1,\ldots,\Omega_k)$ the pull-back by pr_2 of these 2-forms to $T^1_kQ\oplus_Q(T^1_k)^*Q$, that is, $\Omega_A=(pr_2)^*(\omega_0)_A$, $1\leqslant A\leqslant k$.

Furthermore, the *coupling function* in $T^1_kQ\oplus_Q(T^1_k)^*Q$, denoted by $\mathcal{C}$, is defined as follows:

$$\mathcal{C}\colon T^1_kQ\oplus_Q(T^1_k)^*Q\to\mathbb{R},$$

$$(v_{1_q},\ldots,v_{kq},\alpha^1_q,\ldots,\alpha^k_q)\mapsto\sum_{A=1}^{k}\alpha^A_q(v_{A_q}).$$

Given a Lagrangian $L\in C^\infty(T^1_kQ)$, we can define the *Hamiltonian function* in $T^1_kQ\oplus_Q(T^1_k)^*Q$, denoted by $\mathcal{H}\in C^\infty(T^1_kQ\oplus_Q(T^1_k)^*Q)$, as

$$\mathcal{H}(v_{1_q},\ldots,v_{k_q},\alpha^1_q,\ldots,\alpha^k_q)=\mathcal{C}(v_{1_q},\ldots,v_{k_q},\alpha^1_q,\ldots,\alpha^k_q)-(pr_1^*L)(v_{1_q},\ldots,v_{k_q},\alpha^1_q,\ldots,\alpha^k_q)$$

which, in local coordinates, is given by

$$\mathcal{H}=\sum_{A=1}^{k}\sum_{i=1}^{n}p^A_iv^i_A-L(q^i,v^i_A). \tag{25}$$

Now, the problem consists in finding the integral sections $\psi\colon\mathbb{R}^k\to T^1_kQ\oplus(T^1_k)^*Q$ of an integrable k-vector field $\mathbf{Z}=(Z_1,\ldots,Z_k)$ on $T^1_kQ\oplus_Q(T^1_k)^*Q$, such that

$$\sum_{A=1}^{k}\imath_{Z_A}\Omega_A=\mathrm{d}\mathcal{H}. \tag{26}$$

Equation (26) gives a different kind of information. In fact, writing locally each Z_A as

$$Z_A=(Z_A)^i\frac{\partial}{\partial q^i}+(Z_A)^i_B\frac{\partial}{\partial v^i_B}+(Z_A)^B_i\frac{\partial}{\partial p^B_i},$$

then, from (1), (25), and (26) we obtain

$$p^A_i=\frac{\partial L}{\partial v^i_A}\circ pr_1, \tag{27}$$

$$(Z_A)^i=v^i_A, \tag{28}$$

$$\sum_{A=1}^{k}(Z_A)^A_i=\frac{\partial L}{\partial q^i}\circ pr_1, \tag{29}$$

where $1\leqslant A\leqslant k, 1\leqslant i\leqslant n$. Then from (28) we have that Z_A is locally given by

$$Z_A=v^i_A\frac{\partial}{\partial q^i}+(Z_A)^i_B\frac{\partial}{\partial v^i_B}+(Z_A)^B_i\frac{\partial}{\partial p^B_i}. \tag{30}$$

So, in particular, we have obtained information of three different classes.

(1) The constraint equations (27), which are algebraic (not differential) equations defining a submanifold M_L of $T^1_kQ\oplus_Q(T^1_k)^*Q$ where the equation (26) has solution. Let us observe that this submanifold is just the graph of the Legendre map FL defined by the Lagrangian L. We denote by $j\colon M_L\to T^1_kQ\oplus_Q(T^1_k)^*Q$ the natural imbedding, and by $pr^0_1\colon M_L\to T^1_kQ$ and $pr^0_2\colon M_L\to(T^1_k)^*Q$ the restricted projections of pr_1 and pr_2.

(2) Equations (28) which are a holonomy condition similar to (19) and, as we will see in the next section (see Theorem 5.1), they force the integral sections of the k-vector field $\mathbf{Z}$ to be lifting

of sections $\phi:\mathbb{R}^k\to Q$. This property is similar to the one in the unified formalism of classical mechanics, and it reflects the fact that the geometric condition in the unified formalism is stronger than the usual one in the Lagrangian formalism.

(3) Equations (29) which, taking into account (27) and (28), are just the classical Euler–Lagrange equations (see Theorem 5.1).

If $\mathbf{Z}=(Z_1,\ldots,Z_k)$ is a solution to (26), then each Z_A is tangent to the submanifold M_L if, and only if, the functions $Z_A(p_j^B-(\partial L/\partial v_B^j)\circ pr_1)$ vanish at the points of M_L, for every $1\leqslant A,\ B\leqslant k$, $1\leqslant j\leqslant n$. Then from (30) we deduce that this is equivalent to the following equations:

$$(Z_A)_j^B=v_A^i\frac{\partial^2 L}{\partial q^i\,\partial v_B^j}+(Z_A)_C^i\frac{\partial^2 L}{\partial v_C^i\,\partial v_B^j}. \tag{31}$$

Thus the problem to be solved is the following.

Statement 5.1: To find an integral section $\psi:\mathbb{R}^k\to M_L\subset T_k^1Q\oplus(T_k^1)^*Q$ of an integrable k-vector field $\mathbf{Z}=(Z_1,\ldots,Z_k)$ on $T_k^1Q\oplus_Q(T_k^1)^*Q$ solution to (26) taking values on M_L. (This means that $\mathbf{Z}$ is tangent to M_L.)

Remark 5.1: (1) Equations (26) do not, in general, have a unique solution. The solutions to (26) are given by $(Z_1,\ldots,Z_k)+\ker\Omega^\sharp$, where $(Z_1,\ldots,Z_k)$ is a particular solution, and $\Omega^\sharp:T_k^1(T_k^1Q\oplus_Q(T_k^1)^*Q)\to T^*(T_k^1Q\oplus_Q(T_k^1)^*Q)$ is defined as $\Omega^\sharp(Y_1,\ldots,Y_k)=\Sigma_{A=1}^k\imath_{Y_A}\Omega_A$.

(2) If L is regular, then taking into account (28) and (29) we can define a local k-vector field $(Z_1,\ldots,Z_k)$ on a neighborhood of each point in M_L which is a solution to (26). Each Z_A is locally given by

$$(Z_A)^i=v_A^i,\quad (Z_A)_i^B=\frac{1}{k}\frac{\partial L}{\partial q^i}\delta_A^B,$$

with $(Z_A)_B^i$ satisfying (31). Now, by using a partition of the unity, one can construct a global k-vector field which is a solution to (26).

When the Lagrangian function L is singular we cannot assure the existence of consistent solutions for Eq. (26). Then we must develop a constraint algorithm for obtaining a constraint submanifold (if it exists) where these solutions exist. Next, we outline this procedure (see also Ref. 4, where a similar algorithm is sketched in the multisymplectic formulation).

First, in order to assure the existence of a Hamiltonian counterpart for the singular Lagrangian system we assume, from now on, that the singular Lagrangians are almost regular.

We begin with $P_0=M_L$. Then, let P_1 be the subset of P_0 made of those points where there exists a solution to (26), that is,

$$P_1=\{z\in P_0\,|\,\exists\,(Z_1\ldots,Z_k)\in(T_k^1)_zP_0 \text{ solution to (26)}\}.$$

If P_1 is a submanifold of P_0, then there exists a section of the canonical projection $\tau_{P_0}:T_k^1P_0\to P_0$ defined on P_1 which is a solution to (26), but that does not define, in general, a k-vector field on P_1. To find solutions taking values into $T_k^1P_1$, we define a new subset P_2 of P_1 as follows:

$$P_2=\{z\in P_1\,|\,\exists\,(Z_1,\ldots,Z_k)\in(T_k^1)_zP_1 \text{ solution to (26)}\}.$$

If P_2 is a submanifold of P_1, then there exists a section of the canonical projection $\tau_{P_1}:T_k^1P_1\to P_1$ defined on P_2 which is a solution to (26), but that does not define, in general, a k-vector field on P_2.

Proceeding further, we get a family of constraint manifolds

$$\cdots\hookrightarrow P_2\hookrightarrow P_1\hookrightarrow P_0=M_L\hookrightarrow T_k^1Q\oplus_Q(T_k^1)^*Q.$$

If there exists a natural number f such that $P_{f+1}=P_f$ and $\dim P_f>k$ then we call P_f the *final constraint submanifold* over which we can find solutions to Eq. (26). Let us observe that the solutions will not be unique (even in the regular case) and, in general, will not be integrable. In

order to find integrable solutions to Eq. (26), a constraint algorithm based on the same idea must be developed.

B. The field equations for sections

M_L being the graph of FL, it is diffeomorphic to T^1_kQ (so pr^0_1 is a diffeomophism). Let $\mathbf{Z}=(Z_1,\ldots,Z_k)$ be an integrable k-vector field solution to (26). Every integral section $\psi: t\in\mathbb{R}^k \to (\psi^j(t),\psi^j_A(t),\ \psi^A_i(t))\in T^1_kQ\oplus_Q(T^1_k)^*Q$ of $\mathbf{Z}$ solution to (26) is of the form $\psi=(\psi_L,\psi_H)$, with $\psi_L=pr_1\circ\psi:\mathbb{R}^k\to T^1_kQ$, and if ψ takes values in M_L then $\psi_H=FL\circ\psi_L$; in fact, from (27) we obtain

$$\psi_H(t)=(pr_2\circ\psi)(t)=(\psi^j(t),\psi^A_i(t))=\left(\psi^j(t),\left.\frac{\partial L}{\partial v^i_A}\right|_{\psi_L(t)}\right)=(FL\circ\psi_L)(t).$$

In this way, every constraint, differential equation, etc., in the unified formalism can be translated to the Lagrangian or the Hamiltonian formalisms by restriction to the first or the second factors of the product bundle. In particular, conditions (27) generate, by pr_2-projection, the primary constraints of the Hamiltonian formalism for singular Lagrangians [i.e., the image of the Legendre transformation, $FL(T^1_kQ)\subset(T^1_k)^*Q$], and they can be called *primary Hamiltonian constraints*.

In this way the main result in this section is the following.

Theorem 5.1: *Let* $\mathbf{Z}=(Z_1,\ldots,Z_k)$ *be an integrable k-vector field in* $T^1_kQ\oplus_Q(T^1_k)^*Q$ *solution to (26) and let* $\psi:\mathbb{R}^k\to M_L\subset T^1_kQ\oplus_Q(T^1_k)^*Q$ *be an integral section of* $\mathbf{Z}=(Z_1,\ldots,Z_k)$, *with* $\psi=(\psi_L,\psi_H)=(\psi_L,FL\circ\psi_L)$. *Then* ψ_L *is the canonical lift* $\phi^{(1)}$ *of the projected section* $\phi=\tau_Q\circ pr_1\circ\psi:\mathbb{R}^k\to Q$, *and* ϕ *is a solution to the Euler–Lagrange field equations (15).*

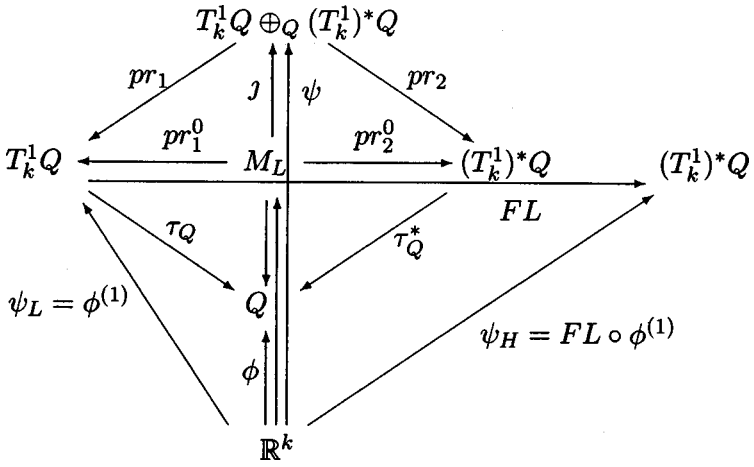

Proof: If $\psi(t)=(\psi^j(t),\psi^j_A(t),\psi^A_i(t))$ is an integral section of $\mathbf{Z}=(Z_1,\ldots,Z_k)$, then

$$Z_A(\psi(t))=\left.\frac{\partial\psi^j}{\partial t^A}(t)\frac{\partial}{\partial q^i}\right|_{\psi(t)}+\left.\frac{\partial\psi^B_i}{\partial t^A}(t)\frac{\partial}{\partial p^B_i}\right|_{\psi(t)}+\left.\frac{\partial\psi^j_B}{\partial t^A}(t)\frac{\partial}{\partial v^i_B}\right|_{\psi(t)}. \tag{32}$$

From (27), (28), and (32) we obtain

$$\psi^j_A(t)=v^i_A(\psi(t))=(Z_A)^i(\psi(t))=\frac{\partial\psi^j}{\partial t^A}(t), \tag{33}$$

$$\psi^A_i(t)=p^A_i(\psi(t))=\left(\frac{\partial L}{\partial v^i_A}\circ pr_1\right)(\psi(t))=\left.\frac{\partial L}{\partial v^i_A}\right|_{\psi_L(t)}, \tag{34}$$

$$\frac{\partial \psi_i^B}{\partial t^A}(t) = (Z_A)_i^B(\psi(t)). \tag{35}$$

Therefore from (29), (34), and (35) we obtain

$$\frac{\partial L}{\partial q^i}(\psi_L(t)) = \sum_{A=1}^{k} (Z_A)_i^A(\psi(t)) = \sum_{A=1}^{k} \frac{\partial \psi_i^A}{\partial t^A}(t) = \sum_{A=1}^{k} \frac{\partial}{\partial t^A}\left(\frac{\partial L}{\partial v_A^i}\bigg|_{\psi_L(t)} \right)$$

and from (33),

$$\psi_A^i(t) = \frac{\partial \psi^i}{\partial t^A}(t).$$

The last two equations are the Euler–Lagrange field equations for the section $\phi(t)=(\psi^i(t))$ $=(\tau\circ pr_1\circ\psi)(t)$, and $\psi_L=\phi^{(1)}$. ■

In addition, for the regular case we can prove the following.

Proposition 5.1: Under the hypothesis of Theorem 5.1, if L is regular then $\psi_H=FL\circ\psi_L$ is a solution to the Hamilton–De Donder–Weyl field equations (14), where the Hamiltonian H is locally given by $H\circ FL=E_L$.

Proof: Since L is regular, FL is a local diffeomorphism and thus we can choose for each point in T_k^1Q an open neighborhood $U\subset T_k^1Q$ such that $FL_{|U}: U\to FL(U)$ is a diffeomorphism. So we can define $H_U: FL(U)\to\mathbb{R}$ as $H_U=(E_L)_{|U}\circ(FL_{|U})^{-1}$.

Denoting by $H\equiv H_U$, $E_L\equiv(E_L)_{|U}$ and $FL\equiv FL_{|U}$, we have $E_L=H\circ FL$ where we provide the identities

$$\frac{\partial H}{\partial p_i^A}\circ FL = v_A^i, \quad \frac{\partial H}{\partial q^i}\circ FL = -\frac{\partial L}{\partial q^i}. \tag{36}$$

Now considering the open subset $V=\psi_L^{-1}(U)\subset\mathbb{R}^k$ we have $\psi_{|V}: V\subset\mathbb{R}^k\to U\oplus FL(U)\subset M_L$, where $(\psi_L)_{|V}: V\subset\mathbb{R}^k\to U\subset T_k^1Q$ and $(\psi_H)_{|V}=FL\circ(\psi_L)_{|V}: V\subset\mathbb{R}^k\to FL(U)\subset(T_k^1)^*Q$.

Therefore from (29), (33), (35), and (36), for every $t\in V\subset\mathbb{R}^k$ we obtain

$$\frac{\partial H}{\partial p_i^A}\bigg|_{\psi_H(t)} = \left(\frac{\partial H}{\partial p_i^A}\circ FL\right)(\psi_L(t)) = v_A^i(\psi_L(t)) = \frac{\partial \psi^i}{\partial t^A}(t)$$

and

$$\frac{\partial H}{\partial q^i}\bigg|_{\psi_H(t)} = \left(\frac{\partial L}{\partial q^i}\circ FL\right)(\psi_L(t)) = -\frac{\partial L}{\partial q^i}\bigg|_{\psi_L(t)} = -\sum_{A=1}^{k}(Z_A)_i^A(\psi(t)) = -\sum_{A=1}^{k}\frac{\partial \psi_i^A}{\partial t^A}(t)$$

from which we deduce that $(\psi_H)_{|V}$ is a solution to the Hamilton–De Donder–Weyl field equations (14). ■

Conversely, we can state the following.

Proposition 5.2: If L is regular and $\mathbf{X}=(X_1,\ldots,X_k)$ is a solution to (16) then

(1) *The k-vector field $\mathbf{Z}=(Z_1,\ldots,Z_k)$ given by $Z_A=(Id_{T_k^1Q}\oplus FL)_*(X_A)$, $1\leqslant A\leqslant k$ is a solution to (26).*
(2) *If $\psi_L:\mathbb{R}^k\to T_k^1Q$ is an integral section of $\mathbf{X}=(X_1,\ldots,X_k)$ (and thus, from Proposition 4.1, a solution to the Euler–Lagrange field equations) then $\psi=(\psi_L, FL\circ\psi_L):\mathbb{R}^k\to M_L\subset T_k^1Q \oplus_Q (T_k^1)^*Q$ is an integral section of $\mathbf{Z}=(Z_1,\ldots,Z_k)$.*

Proof:

(1) If L is regular and $\mathbf{X}=(X_1,\ldots,X_k)$ is a solution to (16), then from Proposition 4.1 we know that X_A is a SOPDE and thus X_A is locally given by

$$X_A = v_A^i \frac{\partial}{\partial q^i} + (X_A)_B^i \frac{\partial}{\partial v_B^i}, \tag{37}$$

where $(X_A)_B^i$ satisfy (20). Since the map $Id_{T_k^1Q} \oplus FL : T_k^1Q \to M_L \subset T_k^1Q \oplus (T_k^1)^*Q$, is locally given by

$$(q^i, v_A^i) \to \left(q^i, v_A^i, \frac{\partial L}{\partial v_A^i} \right), \tag{38}$$

from (37) and (38) we obtain

$$Z_A = (Id_{T_k^1Q} \oplus FL)_*(X_A) = v_A^i \frac{\partial}{\partial q^i} + \left(v_A^i \frac{\partial^2 L}{\partial q^i \, \partial v_C^j} + (X_A)_B^i \frac{\partial^2 L}{\partial v_B^i \, \partial v_C^j} \right) \frac{\partial}{\partial p_j^C} + (X_A)_B^i \frac{\partial}{\partial v_B^i}. \tag{39}$$

Then from (20) and (39) we have that

$$\sum_{A=1}^{k} (Z_A)_j^A = v_A^i \frac{\partial^2 L}{\partial q^i \, \partial v_A^j} + (X_A)_B^i \frac{\partial^2 L}{\partial v_B^i \, \partial v_A^j} = \frac{\partial L}{\partial q^j}, \quad (Z_A)^i = v_A^i, \quad Z_A \left(p_k^B - \frac{\partial L}{\partial v_B^k} \right) = 0,$$

that is, the k-vector field $\mathbf{Z} = (Z_1, \ldots, Z_k)$ is a solution to (26) and each Z_A is tangent to M_L for $A : 1, \ldots, k$.

(2) It follows from Definition 3.2 taking into account that $pr_2 \circ \psi = FL \circ \psi_L$. ■

Remark 5.2: The last result really holds for regular and almost-regular Lagrangians. In the almost-regular case, the proof is the same, but the sections ψ, ψ_L, and ψ_H take values not on M_L, T_k^1Q, and $(T_k^1)^*Q$, but in the final constraint submanifold P_f and on the projection submanifolds $pr_1(P_f) \hookrightarrow T_k^1Q$ and $pr_2(P_f) \hookrightarrow (T_k^1)^*Q$, respectively.

C. The field equations for *k*-vector fields

The aim of this section is to establish the relationship between k-vector fields that are solutions to (16) and k-vector fields that are solutions to (26). The main result is the following.

Theorem 5.2: *Let $\mathbf{Z} = (Z_1, \ldots, Z_k)$ be a k-vector field on M_L solution to (26). Then the k-vector field $\mathbf{X}_L = ((X_L)_1, \ldots, (X_L)_k)$ on T_k^1Q defined by*

$$\mathbf{X}_L \circ pr_1^0 = T_k^1(pr_1^0) \circ \mathbf{Z} \tag{40}$$

is a k-vector field solution to (16) [where $T_k^1(pr_1^0) : T_k^1(M_L) \to T_k^1(T_k^1Q)$ is the natural extension of $(pr_1^0)_*$].

Conversely, every k-vector field $\mathbf{X}_L$ solution to (16) can be recovered in this way from a k-vector field $\mathbf{Z}$ in M_L solution to (26).

Moreover, the k-vector field $\mathbf{Z}$ is integrable iff the k-vector field $\mathbf{X}_L$ is holonomic.

Proof: Since $pr_1^0 : M_L \to T_k^1Q$ is a diffeomorphism, then the k-vector field $\mathbf{X}_L$ on T_k^1Q defined by (40) is given by

$$(X_L)_A = ((pr_1^0)^{-1})^* Z_A, \quad 1 \leqslant A \leqslant k. \tag{41}$$

Now, for every $1 \leqslant A \leqslant k$ we have that

$$j^* \Omega_A = (pr_1^0)^* (\omega_L)_A, \tag{42}$$

which follows from Lemma 2.1,

$$j^* \Omega_A = j^* (pr_2)^* (\omega_0)_A = (pr_2^0)^* (\omega_0)_A = (FL \circ pr_1^0)^* (\omega_0)_A = (pr_1^0)^* FL^* (\omega_0)_A = (pr_1^0)^* (\omega_L)_A.$$

On the other hand we obtain that

$$j^*\mathcal{H} = (pr_1^0)^* E_L, \tag{43}$$

from the following computation:

$$j^*\mathcal{H} = j^*(\mathcal{C} - (pr_1)^* L) = j^*\mathcal{C} - j^*(pr_1)^* L = (pr_1^0)^* CL - (pr_1^0)^* L = (pr_1^0)^* E_L.$$

From (41) and (42) we deduce that

$$\sum_{A=1}^{k} \imath_{Z_A} j^*\Omega_A = \sum_{A=1}^{k} \imath_{(pr_1^0)^*(X_L)_A} (pr_1^0)^*(\omega_L)_A = (pr_1^0)^* \left(\sum_{A=1}^{k} \imath_{(X_L)_A} (\omega_L)_A \right), \tag{44}$$

and from (43) we deduce that

$$\mathrm{d}(j^*\mathcal{H}) = \mathrm{d}((pr_1^0)^* E_L) = (pr_1^0)^* \, \mathrm{d}E_L. \tag{45}$$

Since pr_1^0 is a diffeomorphism, from (44) and (45) we deduce that the k-vector field $\mathbf{Z}$ is a solution to (26) iff the k-vector field $\mathbf{X}_L$ is a solution to (16).

Let us suppose now that the k-vector field $\mathbf{Z}$ is integrable. As a consequence of Theorem 5.1, for every integral section $\psi = (\psi_L, FL \circ \psi_L)$ of $\mathbf{Z}$, $\psi_L = \phi^{(1)}$, for $\phi = \tau \circ pr_1 \circ \psi$. Then

$$(X_L)_A(pr_1^0(\psi(t))) = (pr_1^0)_*(\psi(t))(Z_A(\psi(t))) = (pr_1^0 \circ \psi)_*(t)\left(\frac{\partial}{\partial t^A}\bigg|_q \right) = (\psi_L)_*(t)\left(\frac{\partial}{\partial t^A}\bigg|_q \right).$$

So, $\psi_L = \phi^{(1)}$ is an integral section of $\mathbf{X}_L$, and hence $\mathbf{X}_L$ is holonomic.

Conversely, if $\mathbf{X}_L$ is holonomic then for every integral section $\psi_L = \phi^{(1)}$ with $\phi : \mathbb{R}^k \to Q$, the map $\psi = (\psi_L, FL \circ \psi_L)$ is an integral section of $\mathbf{Z}$. In fact, from (41), for every $1 \leqslant A \leqslant k$,

$$\begin{aligned} Z_A(\psi(t)) = ((pr_1^0)^*(X_L)_A)(\psi(t)) &= ((pr_1^0)^{-1})_*(\psi_L(t))((X_L)_A(\psi_L(t))) \\ &= ((pr_1^0)^{-1})_*(\psi_L(t))\left((\psi_L)_*(t)\left(\frac{\partial}{\partial t^A}(t) \right) \right) \\ &= ((pr_1^0)^{-1} \circ \psi_L)_*(t)\left(\frac{\partial}{\partial t^A}\bigg|_q \right) = \psi_*(t)\left(\frac{\partial}{\partial t^A}\bigg|_q \right). \end{aligned}$$

■

If L is regular, in a neighborhood of each point of $T_k^1 Q$ there exists a local solution $\mathbf{X}_L = ((X_L)_1, \ldots, (X_L)_k)$ to (16). As L is regular, FL is a local diffeomorphism, so this open neighborhood can be chosen in such a way that FL is a diffeomorphism onto its image. Thus in a neighborhood of each point of $FL(T_k^1 Q)$ we can define

$$(X_H)_A = [(FL)^{-1}]^*(X_L)_A, \quad 1 \leqslant A \leqslant k,$$

or equivalently, in terms of k-vector fields

$$T_k^1(FL) \circ X_L = X_H.$$

Proposition 5.3: (1) The local k-vector field $\mathbf{X}_H = ((X_H)_1, \ldots, (X_H)_k)$ is a solution to (13), where the Hamiltonian H is locally given by $H \circ FL = E_L$. (In other words, the local k-vector fields $\mathbf{X}_L$ and $\mathbf{X}_H$ solution to (13) and (16), respectively, are FL related).

(2) Every local integrable k-vector field solution to (13) can be recovered in this way from a local integrable k-vector field $\mathbf{Z}$ in $T_k^1 Q \oplus_Q (T_k^1)^* Q$ solution to (26).

Proof:

(1) This is the local version of Theorem 4.1 (a).

(2) On the other hand, if $\mathbf{X}_H$ is a local integrable k-vector field solution to (13), then we can obtain the FL-related local integrable k-vector field $\mathbf{X}_L$ solution to (16). By Theorem 5.2, we recover $\mathbf{X}_L$ by a local integrable k-vector field $\mathbf{Z}$ solution to (26). ■

VI. FIELD OPERATORS

A. The evolution operator $\mathcal{K}$ in mechanics

The so-called *time-evolution $\mathcal{K}$-operator* in mechanics (also known by some authors as the *relative Hamiltonian vector field* [21]) is a tool which has mainly been developed in order to study the Lagrangian and Hamiltonian formalisms for singular mechanical systems and their equivalence. It was first introduced in a nonintrinsic way in Ref. 22 as an "evolution operator" to connect both formalisms.

In classical mechanics, the evolution operator $\mathcal{K}$ associated with a Lagrangian $L: TQ \to \mathbb{R}$ is a map $\mathcal{K}: TQ \to T(T^*Q)$ satisfying the following conditions (see Ref. 25).

(1) (Structural condition) $\mathcal{K}$ is a vector field along FL, that is, $\tau_{T^*Q} \circ \mathcal{K} = FL$, where FL is the Legendre map defined by L and $\tau_{T^*Q}: T(T^*Q) \to T^*Q$ is the natural projection.
(2) (Dynamical condition) $(FL)^*(\imath_{\mathcal{K}}(\omega \circ FL)) = \mathrm{d}E_L$, where ω is the canonical symplectic form on T^*Q and $E_L = CL - L$, being C the Liouville vector field on TQ.
(3) (Second-order condition) $T(\tau^*) \circ \mathcal{K} = Id_{TQ}$, where $\tau^*: T^*Q \to Q$ is the canonical projection.

The existence and uniqueness of this operator is studied in Ref. 25. Its local expression is

$$\mathcal{K} = v^i \left(\frac{\partial}{\partial q^i} \circ FL \right) + \frac{\partial L}{\partial q^i} \left(\frac{\partial}{\partial p_i} \circ FL \right).$$

By definition $\varphi: \mathbb{R} \to TQ$ is an integral curve of $\mathcal{K}$ if

$$T(FL) \circ \dot{\varphi} = \mathcal{K} \circ \varphi, \tag{46}$$

where $\dot{\varphi}: \mathbb{R} \to T(TQ)$ is the prolongation of φ to the tangent bundle $T(TQ)$ of TQ. So we have the diagram

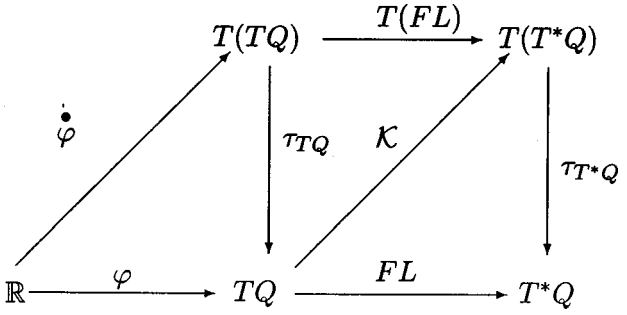

Moreover, (2) $\varphi = \dot{\phi}$, for $\phi: \mathbb{R} \to Q$, that is, φ is holonomic.

The most relevant properties of this operator are the following.

(i) If there exists a Euler–Lagrange vector field X_L on TQ, that is, a solution to the equation $\imath_{X_L}\omega_L = \mathrm{d}E_L$, then $\varphi: \mathbb{R} \to TQ$ is an integral curve of X_L if, and only if, it is an integral curve of $\mathcal{K}$; that is, relation (46) holds.
As a direct consequence of this fact, the relation between $\mathcal{K}$ and X_L is

$$T(FL) \circ X_L = \mathcal{K}. \tag{47}$$

In general, if the dynamical system is singular, the Euler–Lagrange vector fields exist only on a submanifold $S \hookrightarrow TQ$.

(ii) If there exists a Hamilton–Dirac vector field X_H on T^*Q associated with the the Lagrangian system (TQ, ω_L, E_L) (that is, a vector field solution to the Hamilton–Dirac equations in the Hamiltonian formalism), then $\psi: \mathbb{R} \to T^*Q$ is an integral curve of X_H if, and only if,

$$\dot{\psi} = K \circ T(\tau_Q^*) \circ \dot{\psi}. \tag{48}$$

As a consequence, the relation between $\mathcal{K}$ y X_H is

$$X_H \circ FL = \mathcal{K}. \tag{49}$$

(iii) If $\xi \in C^\infty(T^*Q)$ is a Hamiltonian constraint, then $\imath_{\mathcal{K}}(\mathrm{d}\xi \circ FL)$ is a Lagrangian constraint.

Relations (46)–(49) show how the Lagrangian and Hamiltonian descriptions can be unified by means of the operator $\mathcal{K}$.

Some relevant results obtained using this operator are the following.

(i) The equivalence between the Lagrangian and Hamiltonian formalisms is proved by means of this operator in the following way: there is a bijection between the sets of solutions of Euler–Lagrange equations and Hamilton equations, even though the dimensions of the final constraint submanifold in both formalisms are not the same, in general.[22,40]
(ii) The complete classification of constraints is achieved. All the Lagrangian constraints can be obtained from the Hamiltonian ones using the $\mathcal{K}$ operator.[22]
(iii) Noether's theorem is proved and the relation between the generators of gauge and "rigid" symmetries in the Lagrangian and Hamiltonian formalisms is studied.[27–29,41]
(iv) This operator has been applied to studying Lagrangian systems whose Legendre map has *generic singularities*; that is, it degenerates on a hypersurface.[21,30]

B. Field operators $\mathcal{K}$ in field theories

Next we generalize the definition, properties and some of the applications of the evolution operator for the *k*-symplectic formulation of field theories, in order to describe the relationship between the Lagrangian and Hamiltonian formalisms (the generalization for the multisymplectic formulation is given[31]). In particular, we will study how to obtain the solutions of Lagrangian and Hamiltonian field equations by means of this operator, and the relation between them.

Definition 6.1: *A* field operator $\mathcal{K}$ *associated with a Lagrangian* $L: T_k^1Q \to \mathbb{R}$ *is a map*

$$\mathcal{K}: T_k^1Q \to T_k^1((T_k^1)^*Q)$$

satisfying the following conditions.

(1) *Structural condition:* $\mathcal{K}$ *is a k-vector field along FL, that is*

$$\tau_{(T_k^1)^*Q} \circ \mathcal{K} = FL. \tag{50}$$

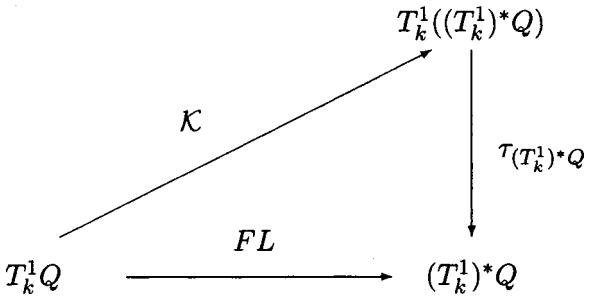

Hence $\mathcal{K} = (\mathcal{K}_1, \ldots, \mathcal{K}_k)$, *where each* $\mathcal{K}_A$, $1 \leqslant A \leqslant k$, *is a vector field along FL.*

(2) *Field equation condition,*

$$\sum_{A=1}^{k} (FL)^*[\imath_{\mathcal{K}_A}(\omega_0)_A \circ FL) = \mathrm{d}E_L. \tag{51}$$

(3) *Second-order condition,*

$$T_k^1(\tau_Q^*)\circ\mathcal{K}=Id_{T_k^1Q}. \tag{52}$$

Now we are going to calculate the local expression of a field operator $\mathcal{K}$. If $v=(v_{1q},\ldots,v_{kq})\in T_k^1Q$ then from (50) we have that

$$\mathcal{K}_A(v)=(\mathcal{K}_A)^i(v)\left.\frac{\partial}{\partial q^i}\right|_{FL(v)}+(\mathcal{K}_A)_i^B(v)\left.\frac{\partial}{\partial p_i^B}\right|_{FL(v)},\quad 1\leqslant A\leqslant k.$$

Taking into account (52) and that the map $T_k^1(\tau_Q^*):T_k^1((T_k^1)^*Q)\to T_k^1Q$ is locally given by $T_k^1(\tau_Q^*)(q^i,p_i^A,(u_A)^i,(u_A)_i^B)=(q^i,(u_A)^i)$, we obtain that

$$(\mathcal{K}_A)^i=v_A^i. \tag{53}$$

Then, writing in local coordinates the expression (51)

$$\sum_{A=1}^k(\omega_0)_A(FL(v))\left(\mathcal{K}_A(v),(FL)_*(v)\left(\left.\frac{\partial}{\partial q^i}\right|_v\right)\right)=\mathrm{d}E_L\left(\left.\frac{\partial}{\partial q^i}\right|_v\right),$$

we obtain that

$$\sum_{A=1}^k\left(v_A^k\frac{\partial^2L}{\partial q^i\,\partial v_A^k}(v)-(\mathcal{K}_A)_j^A(v)\right)=\sum_{A=1}^k v_A^k\frac{\partial^2L}{\partial q^i\,\partial v_A^k}(v)-\frac{\partial L}{\partial q^i}(v).$$

Therefore

$$\sum_{A=1}^k(\mathcal{K}_A)_j^A=(\mathcal{K}_1)_i^1+(\mathcal{K}_2)_i^2+\cdots+(\mathcal{K}_k)_i^k=\frac{\partial L}{\partial q^i}, \tag{54}$$

which means that every field operator $\mathcal{K}_A$ is locally given by

$$\mathcal{K}_A=v_A^i\left(\frac{\partial}{\partial q^i}\circ FL\right)+(\mathcal{K}_A)_i^B\left(\frac{\partial}{\partial p_i^B}\circ FL\right),\quad 1\leqslant A\leqslant k,$$

where the components $(\mathcal{K}_A)_i^B$ satisfy the identity (54).

Equations (53) and (54) lead us to define local solutions in a neighborhood of each point of T_k^1Q satisfying conditions (1), (2), and (3) in Definition 6.1,

$$\mathcal{K}_A=v_A^i\left(\frac{\partial}{\partial q^i}\circ FL\right)+\frac{1}{k}\frac{\partial L}{\partial q^i}\left(\frac{\partial}{\partial p_i^A}\circ FL\right),\quad 1\leqslant A\leqslant k,$$

and, by using a partition of the unity, we obtain global solutions.

Definition 6.2: $\psi:\mathbb{R}^k\to T_k^1Q$ is an integral section of the field operator $\mathcal{K}$ if

$$T_k^1(FL)\circ\psi^{(1)}=\mathcal{K}\circ\psi.$$

Definition 6.2 means that, for every $t\in\mathbb{R}^k$,

$$\mathcal{K}_A(\psi(t))=(FL)_*(\psi(t))\left(\psi_*(t)\left(\left.\frac{\partial}{\partial t^A}\right|_t\right)\right),\quad 1\leqslant A\leqslant k,$$

because

$$(T_k^1(FL)\circ\psi^{(1)})(t)=T_k^1(FL)(j_0^1\psi_t)=j_0^1(FL\circ\psi_t),$$

where $\psi_t(\overline{t})=\psi(t+\overline{t})$. Thus we have the following diagram:

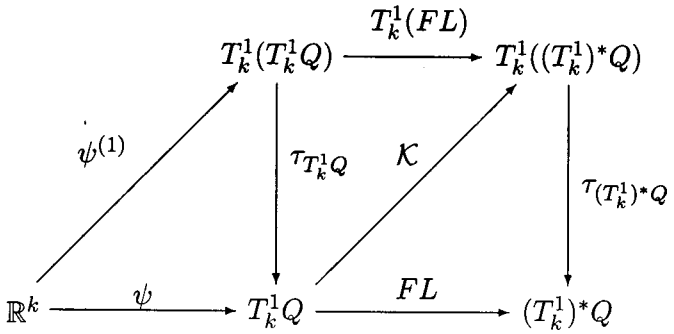

C. Properties of the field operators related to the Lagrangian formalism

In this section we study the properties of the field operator in relation to the Lagrangian field equations. In particular, we generalize the properties of the evolution operator in mechanics given in Eq. (47).

Proposition 6.1: Let $L:T_k^1Q\to\mathbb{R}$ be a Lagrangian. $\psi:\mathbb{R}^k\to T_k^1Q$ is an integral section of $\mathcal{K}$ if, and only if, $\tau_Q\circ\psi:\mathbb{R}^k\overset{\psi}{\to}T_k^1Q\overset{\tau_Q}{\to}Q$ is a solution to the Euler–Lagrange equations (15).

Proof: If $\psi:\mathbb{R}^k\to T_k^1Q$ is locally given by $\psi(t)=(\psi^i(t),\psi_A^i(t))$, then from (6) we obtain that

$$(FL\circ\psi)_*(t)\left(\left.\frac{\partial}{\partial t^A}\right|_t\right)=\frac{\partial\psi^j}{\partial t^A}(t)\left.\frac{\partial}{\partial q^j}\right|_{FL(\psi(t))}+\left(\frac{\partial^2L}{\partial q^i\,\partial v_C^j}(\psi(t))\frac{\partial\psi^i}{\partial t^A}(t)+\frac{\partial\psi_B^j}{\partial t^A}(t)\frac{\partial^2L}{\partial v_B^i\,\partial v_C^j}(\psi(t))\right)\times\left.\frac{\partial}{\partial p_j^C}\right|_{FL(\psi(t))}. \tag{55}$$

On the other hand,

$$\mathcal{K}_A(\psi(t))=v_A^j(\psi(t))\left.\frac{\partial}{\partial q^j}\right|_{FL(\psi(t))}+(\mathcal{K}_A)_j^C(\psi(t))\left.\frac{\partial}{\partial p_j^C}\right|_{FL(\psi(t))}. \tag{56}$$

So if ψ is a solution to $\mathcal{K}$, then from (55) and (56) we obtain the equations

$$\frac{\partial\psi^j}{\partial t^A}(t)=v_A^j(\psi(t))=\psi_A^j(t), \tag{57}$$

and

$$\left.\frac{\partial}{\partial t^A}\right|_t\left(\frac{\partial L}{\partial v_C^j}(\psi(t))\right)=\frac{\partial^2L}{\partial q^i\,\partial v_C^j}(\psi(t))\frac{\partial\psi^i}{\partial t^A}(t)+\frac{\partial^2\psi^i}{\partial t^A\,\partial t^B}(t)\frac{\partial^2L}{\partial v_B^i\,\partial v_C^j}(\psi(t))=(\mathcal{K}_A)_j^C(\psi(t)), \tag{58}$$

for every $A=1,\ldots,k$. Therefore, from (54), (57), and (58) we obtain

$$\sum_{A=1}^k\left.\frac{\partial}{\partial t^A}\right|_t\left(\frac{\partial L}{\partial v_A^i}(\psi(t))\right)=\sum_{A=1}^k(\mathcal{K}_A)_i^A(\psi(t))=\frac{\partial L}{\partial q^i}(\psi(t)),\quad \psi_A^i(t)=\frac{\partial\psi^i}{\partial t^A}(t),$$

that is $(\tau_Q\circ\psi)(t)=(\psi^i(t))$ is a solution to the Euler–Lagrange equations (15).

The proof of the converse follows the same pattern than in the proof of the converse statement of Proposition 4.1. ■

Theorem 6.1: *Let $L:T_k^1Q\to\mathbb{R}$ be a Lagrangian and let $\mathcal{K}$ be a k vector field along the Legendre map $FL:T_k^1Q\to(T_k^1)^*Q$. If $\mathbf{X}_L:T_k^1Q\to T_k^1(T_k^1Q)$ is a k-vector field on T_k^1Q and $j_S:S\hookrightarrow T_k^1Q$ is a submanifold of T_k^1Q such that*

$$T_k^1(FL)\circ \mathbf{X}_L \underset{S}{=} \mathcal{K}, \tag{59}$$

then $\mathcal{K}$ *is a field operator associated with the Lagrangian* L *if, and only if,* $\mathbf{X}_L$ *is a* SOPDE *solution to the equation (16).*

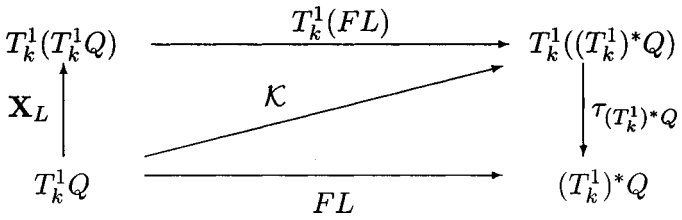

Proof: We must prove that both the second-order condition, and the field equation condition hold for $\mathcal{K}$ if, and only if, they hold for $\mathbf{X}_L$. In this proof all the equalities hold on S.

First, if $\mathcal{K}=(\mathcal{K}_1,\ldots,\mathcal{K}_k)$ and $\mathbf{X}_L=((X_L)_1,\ldots,(X_L)_k)$, then Eq. (59) is equivalent to

$$T(FL)\circ (X_L)_A \underset{S}{=} \mathcal{K}_A, \quad 1\leqslant A\leqslant k.$$

On the other hand $(\omega_L)_A=(FL)^*(\omega_0)_A$ so one easily proves that

$$\imath_{(X_L)_A}(\omega_L)_A \underset{S}{=} (FL)^*(\imath_{\mathcal{K}_A}(\omega_0)_A\circ FL),$$

and for the field equation we obtain

$$\sum_{A=1}^{k}[(FL)^*(\imath_{\mathcal{K}_A}(\omega_A\circ FL)] - \mathrm{d}E_L \underset{S}{=} \sum_{A=1}^{k}[\imath_{X_A}(\omega_L)_A] - \mathrm{d}E_L,$$

hence the field equation condition holds for $\mathcal{K}$ if, and only if, the Lagrangian field equation holds for $\mathbf{X}_L$.

Furthermore, in relation to the second-order condition (see Definition 3.3) we have that

$$T_k^1(\tau_Q^*)\circ\mathcal{K}=Id_{T_k^1Q} \Leftrightarrow T_k^1(\tau_Q^*)\circ T_k^1(FL)\circ\mathbf{X}_L=Id_{T_k^1Q} \Leftrightarrow T_k^1(\tau_Q)\circ\mathbf{X}_L=Id_{T_k^1Q}$$

because FL is a fiber preserving map, that is $\tau_Q^*\circ FL=\tau_Q$, and hence $T_k^1(\tau_Q^*)\circ T_k^1(FL)=T_k^1(\tau_Q)$. Thus the last equality is equivalent to (8), and so the second-order conditions for $\mathcal{K}$ and $\mathbf{X}_L$ are related. ■

Finally, as an immediate consequence of Propositions 4.1 and 6.1, and Theorem 6.1, we have the following.

Corollary 6.1: Under the hypotheses of Theorem 6.1, $\psi:\mathbb{R}^k\to S\subset T_k^1Q$ *is an integral section of the field operator* $\mathcal{K}$ *if, and only if, it is an integral section of the* SOPDE $\mathbf{X}_L$. *(This means that* $\mathcal{K}$ *is integrable if, and only if,* $\mathbf{X}_L$ *is integrable).*

Moreover, every integral section $\psi:\mathbb{R}^k\to S\subset T_k^1Q$ *is a holonomic section.*

D. Properties of the field operators related to the Hamiltonian formalism

Next we analyze the properties of the field operator in relation to the Hamilton–de Donder–Weyl field equations, generalizing the properties of the evolution operator in mechanics given in Eqs. (48) and (49).

Theorem 6.2: *Let* L *be an almost-regular Lagrangian function, and* $\mathcal{K}$ *a field operator associated with* L. *If there exists a k-vector field* $\mathbf{X}_0:\mathcal{P}\to T_k^1\mathcal{P}$, *and a submanifold* $j_S:S\hookrightarrow T_k^1Q$, *such that*

$$T_k^1 j_0\circ\mathbf{X}_0\circ FL_0 \underset{S}{=} \mathcal{K}, \tag{60}$$

then $\mathbf{X}_0$ *is a solution to the equation (24) on* $P=FL_0(S)$.

Conversely, if $\mathbf{X}_0$ *is a k-vector field solution to the equation (24), then the above relation defines a k-vector field* $\mathcal{K}$ *along FL, which satisfy conditions (1) and (2) of Definition 6.1, on S, but not condition (3) (second-order condition) necessarily.*

If L is a hyper-regular Lagrangian function, then the same results hold (with $S=T^1_kQ$*). But in addition, in the converse statements the k-vector field* $\mathcal{K}$ *along FL also satisfies the second-order condition (3) of Definition 6.1, and hence it is a field operator for L.*

Proof: Equation (60) means that

$$(j_0)_*(FL_0(s))((X_0)_A(FL_0(s))) = \mathcal{K}_A(s), \quad s \in S, \quad 1 \leqslant A \leqslant k. \tag{61}$$

Then, since $j_0 \circ FL_0 = FL$ and $(j_0)^*(\omega_0)_A = \omega^0_A$ we deduce from (61) that

$$(FL)^*(\imath_{\mathcal{K}_A}((\omega_0)_A \circ FL)) \underset{S}{=} (FL_0)^*(\imath_{(X_0)_A}\omega^0_A)$$

and since $(FL_0)^*H_0 = E_L$ we obtain

$$\sum_{A=1}^{k} (FL)^*(\imath_{\mathcal{K}_A}((\omega_0)_A \circ FL)) - \mathrm{d}E_L \underset{S}{=} (FL_0)^*\left(\sum_{A=1}^{k} (\imath_{(X_0)_A}\omega^0_A) - \mathrm{d}H_0\right),$$

where all the equalities hold on S. But, as FL_0 is a submersion, we obtain that

$$\sum_{A=1}^{k} (FL)^*(\imath_{\mathcal{K}_A}((\omega_0)_A \circ FL)) - \mathrm{d}E_L \underset{S}{=} 0 \Leftrightarrow \sum_{A=1}^{k} (\imath_{(X_0)_A}\omega^0_A) - \mathrm{d}H_0 \underset{P}{=} 0,$$

hence the field equation condition holds for $\mathcal{K}$ on S if, and only if, the Hamiltonian field equation holds for X_0 on $P=FL_0(S)$.

For hyper-regular systems, the proof of these properties is the same, but taking into acount that now $\mathcal{P}=(T^1_k)^*Q$, and $FL_0=FL$. In addition, the k-vector field $\mathbf{X}_0 \equiv \mathbf{X}$ is defined everywhere in $(T^1_k)^*Q$. Thus, the only addendum is to prove that, if $\mathbf{X}$ is a solution to the equation (24), then its associated k-vector field along $FL, \mathcal{K}$, satisfies the second-order condition. As $\mathbf{X}$ is a k-vector field in $(T^1_k)^*Q$, by definition it is a section of $\tau_{(T^1_k)^*Q}$, thus $\tau_{(T^1_k)^*Q} \circ \mathbf{X} = Id_{(T^1_k)^*Q}$. Then, taking into account that FL is a diffeomorphism, and that (60) reduces to $\mathbf{X} \circ FL = \mathcal{K}$, we have that

$$T^1_k(\tau^*_Q) \circ \mathcal{K} = T^1_k(\tau^*_Q) \circ \mathbf{X} \circ FL = FL^{-1} \circ \tau_{(T^1_k)^*Q} \circ \mathbf{X} \circ FL = Id_{T^1_kQ}$$

which is the second-order condition for $\mathcal{K}$. ■

Then assuming all these relations, we have the following

Theorem 6.3: $\mathcal{K}$ *is integrable if, and only if,* $\mathbf{X}_0$ *is integrable. In particular* we have the following.

(1) *Let* $FL_S: S \to P$ *be the restriction of* FL_0 *to S (that is,* $j_P \circ FL_S = FL_0 \circ j_S$*). If* $\psi: \mathbb{R}^k \overset{\psi_S}{\to} S \overset{j_S}{\hookrightarrow} T^1_kQ$ *is an integral section of* $\mathcal{K}$ *on S, then* $\psi_0: \mathbb{R}^k \overset{\psi_P}{\to} P \overset{j_P}{\hookrightarrow} \mathcal{P}$ *is an integral section of* $\mathbf{X}_0$ *on P, where* $\psi_P := FL_S \circ \psi_S$.

(2) *Conversely, if* $\psi_0: \mathbb{R}^k \overset{\psi_P}{\to} P \overset{j_P}{\hookrightarrow} \mathcal{P}$ *is an integral section of* $\mathbf{X}_0$ *on P, then the section* $\psi: \mathbb{R}^k \overset{\psi_S}{\to} S \overset{j_S}{\hookrightarrow} T^1_kQ$ *is an integral section of* $\mathcal{K}$ *on S, for every* $\psi_S: \mathbb{R}^k \to S \subseteq T^1_kQ$ *such that* $\psi_P = FL_S \circ \psi_S$.

The section ψ_S*, and hence* $\psi := j_S \circ \varphi_S$*, are holonomic if, and only if,* $\mathcal{K}$ *satisfies the second-order condition (and hence it is a field operator).*

Proof: If the system is almost regular, consider the diagram

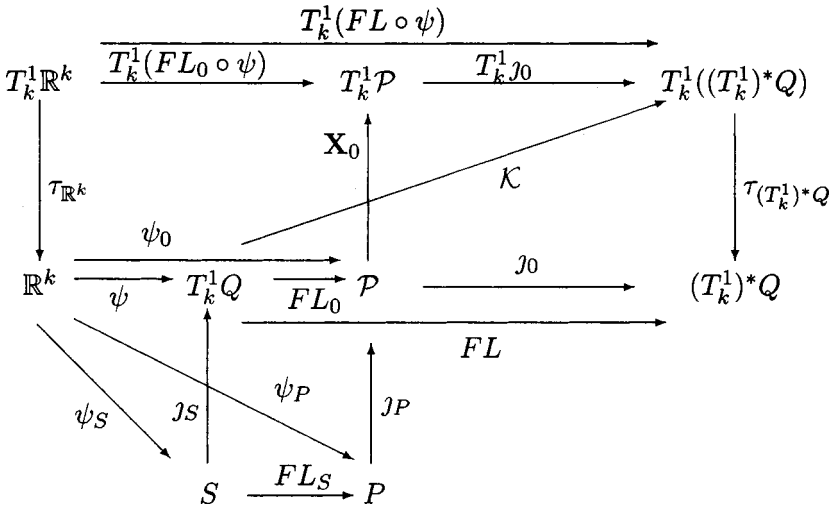

(62)

(where $\mathbf{X}_0$ denotes any extension of the k-vector field solution on P to $\mathcal{P}$).

(1) If ψ is an integral section of $\mathcal{K}$ then

$$\mathcal{K}_A(\psi(t)) = (FL\circ\psi)_*(t)\left(\left.\frac{\partial}{\partial t^A}\right|_t\right), \quad 1\leqslant A\leqslant k, \tag{63}$$

but $FL\circ\psi=j_0\circ\psi_0$ because

$$FL\circ\psi = FL\circ j_S\circ\psi_S = j_0\circ j_P\circ FL_S\circ\psi_S = j_0\circ j_P\circ\psi = j_0\circ\psi_0,$$

therefore (63) is equivalent to

$$\mathcal{K}_A(\psi(t)) = (j_0)_*(\psi_0(t))\left((\psi_0)_*(t)\left(\left.\frac{\partial}{\partial t^A}\right|_t\right)\right), \quad 1\leqslant A\leqslant k. \tag{64}$$

Furthermore, from (61) and taking into account that $FL_0\circ\psi=\psi_0$, we have that

$$\mathcal{K}_A(\psi(t)) = (j_0)_*(FL_0(\psi(t)))(X_0)_A(FL_0(\psi(t))) = (j_0)_*(\psi_0(t))((X_0)_A(\psi_0(t))), \tag{65}$$

then, from (64) and (65), taking into account that j_0 is an imbedding, we deduce

$$(\psi_0)_*(t)\left(\left.\frac{\partial}{\partial t^A}\right|_t\right) = (X_0)_A(\psi_0(t)), \quad 1\leqslant A\leqslant k.$$

Hence, ψ_0 is integral section of $\mathbf{X}_0$.

(2) The converse is proved by reversing the above reasoning. In addition, the sections ψ_S and $\psi:=j_S\circ\psi_S$ are holonomic if, and only if, they are integral sections of a second-order k-vector field along the Legendre map.

If the system is hyper-regular the proof is analogous, but taking $\mathcal{P}=(T_k^1)^*Q$ and $FL_0=FL$. ■

It is important to point out that, if the integrability condition holds only in a submanifold $\mathcal{I}\hookrightarrow S$, then Theorem 6.3 only holds on $\mathcal{I}$ and $FL(\mathcal{I})$ (which is assumed to be a submanifold of P).

Observe also that Theorem 6.3, together with Theorem 6.1, establish the equivalence between the Lagrangian and Hamiltonian formalisms.

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Configurational invariants of Hamiltonian systems

Giuseppe Pucacco[a)]
Dipartimento di Fisica, Università di Roma "Tor Vergata" INFN, Sezione di Roma II, Rome, I-00053, Italy

Kjell Rosquist[b)]
Department of Physics, Stockholm University, Stockholm, Sweden

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In this paper we explore the general conditions in order that a two-dimensional natural Hamiltonian system possess a second invariant which is a polynomial in the momenta and is therefore Liouville integrable. We examine the possibility that the invariant is preserved by the Hamiltonian flow on a given energy hypersurface only (weak integrability) and derive the additional requirement necessary to have conservation at arbitrary energy (strong integrability). Using null complex coordinates, we show that the leading order coefficient of the polynomial is an arbitrary holomorphic function in the case of weak integrability and a polynomial in the coordinates in the strongly integrable one. We review the results obtained so far with strong invariants up to degree four and provide some new examples of weakly integrable systems with linear and quadratic invariants. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1888565]

I. INTRODUCTION

In 1983 Hall[1] published a remarkable paper devoted to a theory of *configurational invariants* of classical Hamiltonian systems. The main virtue of the work consisted in an elegant and powerful technique to solve the equations for the existence of a second polynomial invariant of arbitrary degree in the momenta for two-dimensional Hamiltonian systems. As a result of this approach, Hall was able to get some new examples of integrable systems admitting a second invariant of degree four in the momenta.

Unfortunately, the paper was flawed by a definitely wrong statement and also by many inaccurate arguments and deductions. In fact, Hall purported to remedy supposed oversights in previous works on the search for the second invariant, in particular criticizing the classical account by Whittaker.[2] In Hall's view, Whittaker's (and all others' since then) treatment provides only sufficient conditions for the existence of a second invariant (linear and quadratic in the specific instance), whereas, due to overlooking the link established on phase-space variables by energy conservation, it was not able to find all possible solutions. Actually, as it is, this statement is wrong, in looking for a *strong* second invariant, namely a phase-space function which commutes with the Hamiltonian function, Whittaker's approach is indeed correct and leads to *necessary and sufficient* conditions for its existence. This point was already stressed by Sarlet *et al.*[3] in their criticism to Hall's paper.

Moreover, Hall's discussion contained a confusion between the concept of configurational (or *weak*) invariant, as a function which exactly commutes with the Hamiltonian only on a subset (possibly one) of the energy hypersurfaces (see again Ref. 3 and, e.g., Ref. 4), and the notion of what we may call *formal integral* as it emerges in the analysis of regular portions of the phase space of generic nonintegrable systems (see, e.g., Ref. 5). In particular, the approximate invariants

[a)]Electronic mail: pucacco@roma2.infn.it
[b)]Electronic mail: kr@physto.se

obtained by Hall as a result of his perturbative approach have little to do with those that can be obtained by truncating a normal form expansion.

Nonetheless, in spite of all the above shortcomings, the form in which the problem has been set by Hall and the approach followed for its partial solution deserve attention, since they can still be very useful. Already Hietarinta,[6] in his account of the direct methods for the search of the second invariant, provides a review of all the known systems admitting one or more configurational invariants and works out again the integrability conditions found by Hall for the existence of weak invariants up to degree four. However, in Hietarinta's review, the two settings of weak and strong integrability are still kept well separated. More recently, in a series of works about a unified approach to treat both kinds of invariants,[7–10] the same integrability conditions have been obtained, *supplemented by the additional constraint imposed by strong integrability*. This last step is essential for a neat distinction between the two notions of weak and strong integrability. In these works, this step is a straightforward consequence of the geometric approach in which the existence of the second invariant is addressed by studying the corresponding Killing tensor equations for the Jacobi metric. This metric depends on the mechanical energy as a parameter. Therefore, any tensor object on the corresponding manifold in general depends on the energy. With due care about formal relations between the two approaches, the geometric approach and Hall's approach are equivalent. The essential remark is that, to identify the cases of strong integrability, it is sufficient that in the final results concerning the existence of the invariant, a subset can be isolated which is independent of the energy parameter. In this framework, in Ref. 7, quadratic invariants at arbitrary and fixed energy for two-dimensional Hamiltonian systems were treated in a unified way, whereas in Refs. 8 and 9 the existence of, respectively, *cubic* and *quartic* invariants was discussed accompanied with the discovery of some new examples not given in earlier works (see, e.g., Refs. 10–13). In Ref. 14 the case of Hamiltonian systems with vector potentials is treated, extending previous investigations.[15–20]

The aim of the present paper is to discuss the techniques for solving the equations for a second invariant having a momentum dependence of arbitrary polynomial degree. The analysis is based on a combination of both the above-mentioned approaches, with particular attention dedicated to the conformal transformations used to simplify the equations. The treatment is in general effective for both classes of invariants, configurational (or weak) and strong. After that, we impose the additional condition needed to isolate the class of strongly integrable systems, obtaining the general form of the simplifying family of transformations for each degree of the strong invariant looked for. This in turn implies determining the leading order terms in the invariant itself. An alternative route to this result in the geometric approach is based on the invariance, under conformal transformations, of the conformal part of the Killing tensor. Moreover, a general review of the results obtained so far is provided.

The plan of the paper is as follows: in Sec. II we compare the notion of weak and strong invariants and, working out in detail the quadratic case, we correct Hall's misunderstanding, providing the constraint to be satisfied in order to get strong integrability as a restriction of weak integrability; in Sec. III we recall time reparametrization of the null Hamiltonian and complex ("null") coordinates used to simplify the direct approach; in Sec. IV these tools are exploited to set the general approach to find polynomial invariants of arbitrary degree; in Sec. V we recall the main results concerning invariants of degree up to four; in Sec. VI we present our conclusions and the prospects for future works.

II. CONFIGURATIONAL INVARIANTS VERSUS STRONG INVARIANTS

As it is well known (see, e.g., Ref. 21), to grant the complete integrability of an N-dimensional Hamiltonian system, it is necessary and sufficient to find N independent integrals of motion or *invariants*, for short. In the following, we will limit ourselves to the simplest case of a conservative Hamiltonian system in two dimensions ($N=2$). Since the Hamiltonian itself

$$H = \tfrac{1}{2}(p_x^2 + p_y^2) + V(x,y), \tag{1}$$

is a conserved function, it is enough to find just a second independent invariant.

In his search for polynomial invariants, Hall[1] exploits what is usually called the "direct approach" of Darboux[22] and Whittaker.[2] As an "educated guess" we may start with the working hypothesis of an invariant with a structure analogous to that of the Hamiltonian, namely a second degree polynomial in the momenta. (Since all the work is made in a Hamiltonian context, contrary to the original treatment by Hall, we use canonical phase-space coordinates. However, we have tried to stay as close as possible to his treatment as refers to the procedure and notations.) Clearly, one could start with a polynomial of arbitrary degree or even with a more general expression. In the core part of the paper we will examine the general case. Now, as an introduction aimed at giving the proper settings, we work out in detail the quadratic case. We may then look for a phase-space function of the form

$$I_2(p_x,p_y,x,y) = Ap_x^2 + Bp_xp_y + Cp_y^2 + K, \tag{2}$$

which is preserved along the flow given by Eq. (1), namely

$$\{I_2,H\} = 0. \tag{3}$$

In Eq. (2), A, B, C, and K are each functions of x and y. Actually Hall, probably motivated by his interest in accelerator physics, manages to work out the integrability of Hamiltonians including also a vector potential and henceforth terms which are linear in the momenta. This, in turn, suggests the inclusion of analogous terms in the invariant. However, in the standard case of a Hamiltonian invariant under momentum inversion, $p \to -p$, the equations for the coefficients of even and odd degree terms decouple, greatly reducing the complexity of the system to solve. Therefore, since the main purpose of this paper is to fully clarify the issues of weak and strong integrability, which are unaffected by such generalizations, we prefer to limit ourselves to the standard case of Eq. (1). The treatment of the vector potential is presented elsewhere[14] where new strongly integrable systems with quadratic invariants are presented.

In the direct approach, one inserts the functions (1) and (2) into the Poisson bracket (3). The resulting polynomial in the momenta, of third degree in the present instance, must be identically vanishing. In view of the independence and arbitrariness of the momentum coordinates, each coefficient of the polynomial must vanish, determining in turn the following system of PDEs in the coordinates

$$A_x = 0, \tag{4}$$

$$A_y + B_x = 0, \tag{5}$$

$$B_y + C_x = 0, \tag{6}$$

$$C_y = 0, \tag{7}$$

$$K_x = 2AV_x + BV_y, \tag{8}$$

$$K_y = BV_x + 2CV_y, \tag{9}$$

where, in order to compactify expressions, suffixes denote partial differentiation. As mentioned above, Darboux[22] addressed the problem and the equation ensuing from the integrability condition for K, that is

$$B(V_{yy} - V_{xx}) + 2(A - C)V_{xy} + 3(B_yV_y - B_xV_x) = 0, \tag{10}$$

is known as *Darboux's equation*. Whittaker[2] also analyzed the problem and, for a complete account of the solution of this system, the standard reference is again the review by Hietarinta.[6]

Equations involving only the leading order terms (A, B, and C) in the invariant are readily solved,

$$A = ay^2 + by + c, \tag{11}$$

$$B = -2axy - bx - \mathrm{d}y - e, \tag{12}$$

$$C = ax^2 + \mathrm{d}x + f. \tag{13}$$

Exploiting linear transformations of the coordinates, it can be shown[6,7] that these functions can be reduced to four canonical forms that, inserted into Darboux equation (10), lead to the complete solution of the problem, there exist four fundamental separating coordinate systems (elliptical, polar, parabolic, and Cartesian) in which the potential and the remaining unknown of the invariant, K, can be expressed in terms of combinations of arbitrary functions of each of the separating coordinates. Actually, in his reference to Whittaker's result, Hall mentions only the elliptical solution, but, as shown in Ref. 7 (see also Ref. 23), using conformal transformations, all the separable cases possess the same structure. Moreover, we remark on the additional possibility of complex potentials, which provides four more cases with complex separating coordinates, which are listed in Ref. 6 and can also be obtained with the techniques in Ref. 7.

At this point Hall states that (Ref. 1, p.93) "Whittaker's work $|\cdots|$ was flawed by his failure to recognize that terms in $\dot{x}^2$ and $\dot{y}^2$ are not independent for the purpose of setting the coefficients of their various powers to zero $|\cdots|$. They are related by conservation of energy. Therefore, Whittaker's constraints were over-restrictive; the solutions he found are valid, but others may also exist." On these bases, Hall elaborates a generalized approach that, in his view, provides necessary and sufficient conditions for the existence of the given invariant. Actually, as we will shortly see, Hall fails in recognizing that the possible extension of the family of solutions implies a different status for the additional invariants, they are "fixed energy" or *configurational* invariants.

Configurational (or "conditional" or even "weak") integrals hold for *a specified particular value of the energy constant* and were first investigated by Birkhoff[24] and considered by Fomenko,[25] Kozlov,[26] and others. Weak invariants enjoy weaker properties than their "nobler" cousins, the *strong* invariants, which are constant on *every* energy hypersurface admitted by the dynamics of the system. To clarify this essential point, let us again work with the quadratic case, concretely introducing Hall's argument. This goes as follows: for every value E of the energy, the function (1) defines the hypersurface

$$\tfrac{1}{2}(p_x^2 + p_y^2) + V(x,y) = E. \tag{14}$$

Let us construct the following linear combinations of the squares of the momenta:

$$\Sigma = p_x^2 + p_y^2, \tag{15}$$

$$\Delta = p_x^2 - p_y^2 \tag{16}$$

and observe that, in view of (14), we can impose the constraint

$$\Sigma = 2G(x,y), \tag{17}$$

where we have introduced the *"Jacobi" potential* [the origin of this denomination comes from the close relationship between the picture of a system constrained on the fixed energy surface and the geometric picture of a geodesic flow over a Riemannian manifold endowed with a "Jacobi" metric (see, e.g., Ref. 27)]

$$G = E - V. \tag{18}$$

The quadratic terms in the standard form of the invariant of Eq. (2) can now be written as

$$Ap_x^2 + Bp_xp_y + Cp_y^2 = \tfrac{1}{2}[(A + C)\Sigma + (A - C)\Delta + B\sqrt{\Sigma^2 - \Delta^2}]. \tag{19}$$

Exploiting the energy constraint (17) and redefining coefficients, the quadratic invariant can then be written as

$$I_2(p_x,p_y,x,y) = \tfrac{1}{2}D(p_x^2 - p_y^2) + Bp_xp_y + \tilde{K}, \tag{20}$$

where

$$D = A - C, \tag{21}$$

$$\tilde{K} = K + (A + C)G. \tag{22}$$

Now, we may proceed along the same lines followed above. The commutation relations (3) of the weak invariant (20) with the Hamiltonian reduce to the system

$$D_y + B_x = 0, \tag{23}$$

$$D_x - B_y = 0, \tag{24}$$

$$\tilde{K}_x = BV_y + DV_x - GB_y, \tag{25}$$

$$\tilde{K}_y = BV_x - DV_y - GB_x. \tag{26}$$

The integrability condition for $\tilde{K}$ is now the *generalized Darboux equation*,

$$B(V_{yy} - V_{xx}) + 2DV_{xy} + 3(B_yV_y - B_xV_x) - 2(E - V)D_{xy} = 0, \tag{27}$$

where we have explicitly pointed out the presence of the energy parameter. In practice, since the energy of the system is in general an arbitrary real number, we can write Eq. (27) in the form

$$f_1E + f_0 = 0, \tag{28}$$

where f_1, f_0 are functions of the coordinates, both explicitly and through V and its derivatives.

If we want that the looked for invariant has an identically vanishing Poisson bracket with the Hamilton *regardless of the value of the energy* (in other words that I_2 should be a *strong* invariant), Eq. (28) must be satisfied for every value of the parameter E so that the two equations

$$f_1 = 0, \tag{29}$$

$$f_0 = 0, \tag{30}$$

must separately be satisfied. The first of these equations is simply

$$D_{xy} = 0. \tag{31}$$

As a consequence of this, the second, by a direct comparison, turns out to coincide with the standard Darboux equation (10). This time, the solution of Eq. (31), together with (23) and (24) for the leading order terms (now D and B), gives

$$D = a(y^2 - x^2) + by - \mathrm{d}x + g, \tag{32}$$

$$B = -2axy - bx - dy - e. \tag{33}$$

Recalling (21) and comparing with (11)–(13), we see that we have arrived at a result completely equivalent to that of the standard Darboux–Whittaker approach. In fact, Eq. (30) now coincides with Eq. (10) and, therefore, the same possible separable potentials in two dimensions can be found also following this alternative route.

In our general presentation in Sec. IV, we will see how this strategy reveals to be useful also in the case of higher degree invariants. While used mostly for its pedagogical role in the present instance, what is important to stress is the key role of the integrability condition in the form (28): in the general case of a polynomial invariant of degree M, it turns out that Eq. (28) is a polynomial in E of degree $M/2$ for M even and $(M+1)/2$ for M odd.

In the case of invariance at fixed energy, the problem admits additional solutions. Now we have that Eq. (31) is no more necessary and therefore (23) and (24) are unconstrained Cauchy–Riemann equations. Instead of (32) and (33), the solution is now given by an arbitrary analytic function: its real and imaginary parts, respectively, provide the functions D and B. Because of this feature, we will see in the following how it is more convenient to work with complex variables.

Summarizing, the above procedure shows that the strategy for finding weak invariants is well defined and points out where it must be constrained to get strong invariants. This objective being the most important for applications, it may appear that, going this way, nothing is gained with respect to the usual direct approach. However, the procedure instead proves to be very effective in simplifying the system of equations resulting from implementing the direct approach. This simplification is actually one of the reasons why Hall's work is still useful. At the same time, since the approach based on the constrained invariant ansatz (20), complemented by a correct use of the general Darboux equation (28), provides the same results as the standard approach, we get a simple proof of the invalidity of Hall's criticism towards Whittaker. However, Hall is right in envisaging additional solutions to the problem, in the example we have just seen, it is conceivable to obtain, for *particular* values of E, solutions of Eq. (28) not included in those of (29) and (30). In Ref. 7, we have produced several classes of solutions corresponding to $E=0$.

The investigation of such *weakly integrable systems* (WIS) offers several additional issues to study. We mention some of them.

(i) Possible solutions defined for a continuous but finite range of energy values $E_1 < E < E_2$.
(ii) WIS which are actually SIS (*strongly integrable systems*) with a more general form for the second invariant (examples, the Kepler problem, the Sarlet *et al.* case[3]).
(iii) The main property of the integrable dynamics on the E surface may help in understanding some of the main features in the nonintegrable regime (see, e.g., Ref. 28).

III. THE NULL HAMILTONIAN AND TIME REPARAMETRIZATION

As already put forward by Hietarinta (see Ref. 6, Sec. 7.2), canonical point transformations generated by analytical functions preserve the form of a *null* Hamiltonian. This invariance allows a straightforward way to reduce the set of equations to be solved in the search for a polynomial invariant. In the present section we show how, in the case of two-dimensional systems, the above transformations are actually conformal transformations and are related with the time reparametrization of the dynamics. These tools, exploited in the remaining part of the paper, were implicit in Hall's work.

In general the Hamiltonian itself has the form

$$H = T + V(q) = E, \tag{34}$$

where T is a quadratic form in the momenta. The independent variable, let us say t, is often but not always the time. For any given energy E of the system, to represent the dynamics, we can use the *null* Hamiltonian,

$$H_0 = H - E, \tag{35}$$

provided that we impose the constraint

$$H_0 = 0. \tag{36}$$

For any such zero energy Hamiltonian we can reparametrize the system by introducing a new time variable $\overline{t}$ defined by the relation

$$\mathrm{d}t = N(p,q)\mathrm{d}\overline{t}, \tag{37}$$

together with a redefined Hamiltonian

$$\overline{H_0} = N(p,q)H_0 = NT + N(V - E) = 0. \tag{38}$$

The new Hamiltonian will then give the same equations of motion on the constraint surface $\overline{H_0} = 0$. We shall use the term *lapse function* for $N(p,q)$ which defines the independent variable gauge. This usage is borrowed from cosmological applications where the lapse gives the rate of physical time change relative to coordinate time. The lapse function can be taken as any nonzero function on the phase space.

It is simpler to work with complex, or "null," coordinates,

$$z = x + iy, \quad p_z = p = \tfrac{1}{2}(p_x - ip_y), \tag{39}$$

$$\overline{z} = x - iy, \quad p_{\overline{z}} = \overline{p} = \tfrac{1}{2}(p_x + ip_y). \tag{40}$$

The null Hamiltonian can then be written in the form

$$H_0 = 2p\overline{p} - G(z,\overline{z}) = 0, \tag{41}$$

where G is the function introduced in (18). The equations of motion given by (41) are

$$\frac{\mathrm{d}z}{\mathrm{d}t} = 2\overline{p}, \tag{42}$$

$$\frac{\mathrm{d}p}{\mathrm{d}t} = G_z = -V_z, \tag{43}$$

and corresponding complex conjugates. G and V are always assumed to be real functions. In the following we will spare to mention explicitly to the complex conjugates.

We use a conformal transformation to standardize the frame and coordinate representation of the invariant. To that end we introduce a new complex coordinate w by means of the transformation

$$z = F(w). \tag{44}$$

The conformal transformation

$$z \to w = X + iY, \tag{45}$$

given by the holomorphic function (44) determines the canonical point transformation

$$w = F^{-1}(z), \quad P = F'p, \tag{46}$$

so that (1) transforms into the new null Hamiltonian

$$\widetilde{H}_0 = \frac{2P\overline{P} - \widetilde{G}(w,\overline{w})}{|F'|^2} = 0. \tag{47}$$

Let us introduce the "standard" null Hamiltonian

$$H_S = 2P\overline{P} - \widetilde{G}(w,\overline{w}) = 0, \tag{48}$$

that implies the use of the new "time" s, such that

$$\frac{d}{\mathrm{d}s} = |F'|^2 \frac{d}{\mathrm{d}t}. \tag{49}$$

Equations of motion (42) and (43) becomes

$$\frac{\mathrm{d}w}{\mathrm{d}s} = 2\overline{P}, \tag{50}$$

$$\frac{\mathrm{d}P}{\mathrm{d}s} = \widetilde{G}_w. \tag{51}$$

At the same time, a conserved quantity stays conserved if transformed between the two gauges (47) and (48). In terms of real variables, (48) is given by

$$H_S = \tfrac{1}{2}(P_X^2 + P_Y^2) - \widetilde{G}(X,Y) = 0. \tag{52}$$

IV. INVARIANTS OF ARBITRARY DEGREE

With the choice of polynomial invariants, the time reflection symmetry of Hamiltonian (1) allows a further simplification in the procedure. In fact, it can been proved (see Hietarinta,[6] Sec. 2.3 and Ref. 29) that the algebra of commuting functions with the Hamiltonian, which is an even function with respect to time reflection, has "good" time reflection parity. Therefore, a polynomial second invariant can be either even or odd polynomial in the momenta. We can therefore assume a phase-space function of the following form:

$$I_M = \sum_{k=0}^{[M/2]} \sum_{j=0}^{M-2k} p_x^j p_y^{M-2k-j} A_{(j,M-2k)}(x,y), \tag{53}$$

where the functions $A_{(j,M-2k)}(x,y)$, not necessarily polynomials, must be determined. In the first summation, with $[M/2]$ we denote the greatest integer less than $M/2$, so that if, e.g., $M=1$, k takes only the value zero.

A. The direct approach in the Cartesian frame

The simplest procedure (also called the *direct approach*) is now to compute the Poisson brackets of I_M with H, collect terms with various power of momenta and let vanish their respective coefficients. Using at first the form (53) in the usual Cartesian frame, we then get a system of partial differential equations of the form

$$(j+1)A_{(j+1,k+1)}\partial_x V + (k+1-j)A_{(j,k+1)}\partial_y V = \partial_x A_{(j-1,k-1)} + \partial_y A_{(j,k-1)}, \tag{54}$$

with $j=0,\ldots,k$ and $k=M+1$, $M-1$, $M-3,\ldots,0$ or 1 and it is implicit that $A_{(s,t)}=0$ if $s<0$ or $s>t$ and $t<0$ or $t>M$. In order to simplify formulas, in the present section we reintroduce the standard notation ∂ to denote partial differentiation with respect to the variable in the subscript. The set (54) is a complicated set of PDEs, in general overdetermined: if M is even we have $(M+2)(M+4)/4$ equations for $(M+2)^2/4$ unknowns; if M is odd we have $(M+3)^2/4$ equations for

$(M+1)(M+3)/4$ unknowns. Actually, in the general case, to these figures the potential V enters as an additional unknown.

B. The direct approach in the null frame

Introducing the complex null frame (39) and (40), we have the following generic expression of the invariant:

$$I_M = 2\,\mathrm{Re}\left\{\sum_{k=0}^{M/2} C_{2k}p^{2k}\right\}, \quad M \text{ even}, \tag{55}$$

$$I_M = 2\,\mathrm{Re}\left\{\sum_{k=0}^{(M-1)/2} C_{2k+1}p^{2k+1}\right\}, \quad M \text{ odd}, \tag{56}$$

where the complex functions $C_{2k}, k=0,\ldots,M/2$ or $C_{2k+1}, k=0,\ldots,(M-1)/2$ depend on z, $\overline{z}$ and, with the exclusion of the leading order coefficients C_M, implicitly on E. Their explicit expression in terms of the coefficients of the invariant in Cartesian form are

$$C_{2k}^{(M)} = \sum_{a=0}^{(M/2)-k} \left(\frac{G}{2}\right)^a \times \left\{\sum_{\ell=0}^{2(a+k)} i^{2(a+k)-\ell}\left[\sum_{r=0}^{a}(-1)^r\binom{\ell}{\ell-a+r}\binom{2(a+k)-\ell}{2(a+k)-\ell-r}\right]A_{(\ell,2(a+k))}\right\}, \tag{57}$$

when M is even and

$$C_{2k+1}^{(M)} = \sum_{a=0}^{(M-1)/2-k} \left(\frac{G}{2}\right)^a \times \left\{\sum_{\ell=0}^{2(a+k)+1} i^{2(a+k)+1-\ell}\left[\sum_{r=0}^{a}(-1)^r\binom{\ell}{\ell-a+r}\times\binom{2(a+k)+1-\ell}{2(a+k)+1-\ell-r}\right]A_{(\ell,2(a+k)+1)}\right\}, \tag{58}$$

when M is odd. In these expressions a superscript (M) has been introduced in order to let them apply in general, namely, $C_a^{(M)}$ denotes the ath coefficient of the invariant of degree M. In the following this superscript will not be used unless it is strictly needed to prevent confusion. As usual, in (57) and (58),

$$\binom{n}{k} = \frac{n!}{(n-k)!k!} \tag{59}$$

denotes the binomial coefficient.

The forms (55) and (56) of the invariant do not contain cross terms, namely terms with powers of $p\overline{p}$, since they have been eliminated exploiting the constraint

$$2p\overline{p} = G(z,\overline{z}) \tag{60}$$

dictated by (41). A simple check of this statement can be performed with the quadratic invariant with which we are familiar from Sec. II. Equation (57) with $M=2$ gives

$$C_2^{(2)} = A_{22} - A_{02} + iA_{12}, \tag{61}$$

$$C_0^{(2)} = A_{00} + (A_{02} + A_{22})G. \tag{62}$$

Posing $A_{22}=A$, $A_{12}=B$, $A_{02}=C$, $A_{00}=K$ and $C_2^{(2)}=D+iB$, $C_0^{(2)}=\tilde{K}$ we again find relations (21) and (22) and see that the expression (20) of the invariant is equivalent to

$$I_2(p,\overline{p},z,\overline{z}) = C_2^{(2)}p^2 + \overline{C_2^{(2)}}\overline{p}^2 + \widetilde{K}. \tag{63}$$

The use of the energy constraint leads to the maximal reduction in the number of equations ensuing from the direct approach. However, in the case of integrability at arbitrary energy, to this reduced number one must add the integrability conditions which results in a set of equations generalizing (29). The constraint (60) can also be used to "homogeneize" the polynomial invariant. In this form, used in the geometric framework in connection with the geodesic flow over a Riemannian manifold, the coefficients of the invariant give rise to a symmetric M-rank tensor, known as a *Killing tensor*.

The commutation relation of the functions (55) or (56) with the null Hamiltonian (41) gives the system of equations

$$\partial_{\overline{z}} C_{k-1} + \tfrac{1}{2}(\partial_z C_{k+1})G + \tfrac{1}{2}(k+1)C_{k+1}\partial_z G = 0, \quad k = 0,1,\ldots,M, \tag{64}$$

where it is implicitly assumed that $C_j = 0$ for $j < 0$ and for $j > M$. The set of equation (64) must be supplemented by the closure equations

$$\partial_{\overline{z}} C_M = 0 \tag{65}$$

and

$$\Re\{\partial_z(C_1 G)\} = 0. \tag{66}$$

Clearly, this last condition must be stated only in the case of odd degree, since for M even, a closure condition of the form

$$\Im\{C_0\} = 0 \tag{67}$$

is implicit since C_0 is real by definition.

In both cases, using the null complex coordinates, we have $M+2$ real equations for $M+1$ real unknowns: the substantial reduction of the number of independent equations with respect to that in the Cartesian frame was already remarked by Hietarinta (see Ref. 6, Sec. 7.5). However, he thought that reintroducing the explicit dependence on energy would reestablish the original number, whereas, as we will see, the gain in saving equation still remains when going to the Cartesian frame.

C. Solving the equations for the *M*th-degree invariant

At present a general solution of system (64) is still lacking. In Refs. 7–9 we found the general solutions for $1 \leqslant M \leqslant 4$. In the present section we illustrate the aspect of the procedure which are common to all Mth-degree invariant. The first steps are essentially the same as in the original paper by Hall.

Looking at the system above, we see that Eq. (65) is readily solved,

$$C_M = C_M(z), \tag{68}$$

that is C_M is an arbitrary holomorphic function. The first important result we get is therefore that the leading order coefficient of a polynomial invariant is given by an arbitrary holomorphic function. This fact is already known in the case of homogeneous polynomial invariants (Kolokoltsov,[30] Kozlov[26]) and was obtained by Birkhoff (Ref. 24, Chap. 2) for $M \leqslant 2$. We remark that, in agreement with notations in (57) and (58), here we are referring to $C_M^{(M)}$, that is the leading order coefficient of the polynomial invariant of degree M with various values of M. Therefore, in order to avoid confusion with lower order coefficients in a polynomial with a given M and also to conform with the notation in previous works, in the following we will denote the leading order coefficient with S_M.

In order to attack the remaining equations in (64), we may further simplify them by performing a coordinate transformation. This is a conformal transformation of the form (44), where the generating function $F(w)$ is chosen such that

$$F'(w(z)) = S_M{}^{1/M}. \tag{69}$$

In this case, we see that the first equation of the chain (64) can be rewritten as

$$S_M{}^{(2/M)-1}\partial_{\bar{w}}C_{M-2} + \frac{M}{2}\partial_w \tilde{G} = 0, \tag{70}$$

where, in agreement with (47), the new "conformal" potential

$$\tilde{G}(w,\bar{w}) = |F'(w)|^2 G = (S_M \bar{S_M})^{1/M} G, \tag{71}$$

has been introduced. Defining the function

$$\tilde{C}_{M-2}(w,\bar{w}) = S_M^{(2-M)/M} C_{M-2}, \tag{72}$$

Eq. (70) becomes

$$\partial_{\bar{w}}\tilde{C}_{M-2} + \frac{M}{2}\partial_w \tilde{G} = 0 \tag{73}$$

and, defining in an analogous way,

$$\tilde{C}_{2k}(w,\bar{w}) = S_M^{-2k/M} C_{2k}, \quad k = 0,1,\ldots,[N/2], \tag{74}$$

the rest of the system becomes

$$\partial_{\bar{w}}\tilde{C}_{j-2} + \frac{1}{2\tilde{G}^{j-1}}\partial_w(\tilde{C}_j \tilde{G}^j) = 0, \tag{75}$$

with the ranges $j=4,5,\ldots,N-2$ if N is even and $j=3,4,\ldots,N-2$ if N is odd.

D. The Kähler potential

Equation (70), or better its transformed form (73), plays a special role. In view of the fact that the new potential $\tilde{G}$ is still a real function, (73) can be solved introducing a real function $\mathcal{K}(w,\bar{w})$ such that

$$\tilde{G} = \partial^2_{w\bar{w}}\mathcal{K}, \tag{76}$$

$$\tilde{C}_{M-2} = -\frac{M}{2}\partial^2_{ww}\mathcal{K}. \tag{77}$$

The first equation says that the Jacobi potential is the Laplacian of the function $\mathcal{K}(w,\bar{w})$. Since, in the geometric picture, G is the conformal factor of the metric element, using $\mathcal{K}$ it gives rise to a Hermitian form and therefore it is referred to as the *Kähler potential*. Without loss of generality, in Ref. 9, Sec. IV, it has been shown that the Kähler potential can be assumed to be of the form

$$\mathcal{K} = E[F(w)\bar{F}(\bar{w}) + 2\Re\{\Lambda(z(w))\}] - \Psi, \tag{78}$$

where Λ is an arbitrary holomorphic function independent of E and the real *prepotential* Ψ is such that

$$\partial^2_{w\bar{w}}\Psi = F'\overline{F'}\,\partial^2_{z\bar{z}}\Psi = |F'|^2 V. \tag{79}$$

In the case of invariants up to the fourth degree, $M \leqslant 4$, we see that the closure equations (66) and (67) are themselves expressed only in terms of the Kähler potential. In these cases, to get a complete solution of the problem, it remains *only* to solve an integrability condition for $\mathcal{K}(w,\bar{w})$.

In the cases of linear and quadratic invariants, the integrability condition is linear and we have the general solution depending, respectively, on one and two arbitrary real functions (see Ref. 7). In the higher degree cases, the integrability conditions are nonlinear and a general solution is lacking: moreover, in general, they give rise to an overdetermined system for the unknowns Λ and Ψ. This is consistent with the fact that only isolated cases of integrable Hamiltonian systems with invariant of degree higher than two are known. Failing to work in full generality, a useful approach is to make an ansatz for one of the unknowns (e.g., Λ) and solve for Ψ. In this way several new integrable and superintegrable systems have been found with a cubic[8] and a quartic[9] second invariant.

E. The leading order term of strong invariants

Looking for a strong invariant, so that the integrability condition must be solved for arbitrary values of E, it turns out that the function C_M can no longer be arbitrary. In our previous works we have shown its polynomial structure with degree equal to M for $M \leqslant 4$ and guessed that this is the generic behavior for any value of M. In this section we prove that this conjecture is true by explicitly computing the function with the aid of the already known solution in the Cartesian case.

In Ref. 7 for the linear and quadratic cases we have found, respectively, the conditions

$$\Re\{S_1'(z)\} = 0, \tag{80}$$

$$\Im\{S_2''(z)\} = 0. \tag{81}$$

In Ref. 8, for the cubic case, the condition

$$\Re\left\{\frac{d^3}{dz^3}S_3\right\} = 0 \tag{82}$$

was found, whereas in Ref. 9, for the quartic case, the condition

$$\Im\left\{\frac{d^4}{dz^4}S_4\right\} = 0 \tag{83}$$

was found. Therefore we can guess the general conditions

$$\Re\left\{\frac{d^M}{dz^M}S_M\right\} = 0, \quad M \text{ odd}, \tag{84}$$

$$\Im\left\{\frac{d^M}{dz^M}S_M\right\} = 0, \quad M \text{ even}. \tag{85}$$

Conditions from (80)–(83) have been obtained working on the integrability condition for the Kähler potential $\mathcal{K}$. Since it is not possible to write an explicit expression for the integrability condition at arbitrary M, we prove (84) and (85) by explicitly calculating them. The easiest way to proceed is to exploit the solution in Cartesian coordinates and after that performing the transformation to complex coordinates: the reason for not working directly in the complex frame is that, in (55) and (56), part of the information on the structure of S_M is hidden in the lower order coefficients through the energy constraint, this information could be recovered only having the solution of the complete system of equations for C_k up to the integrability for C_0.

Comparing (55) and (56) with (53) we get the relation

$$S_M(x+iy) \equiv C_M = \sum_{m=0}^{M} i^{M-m} A_{(m,M)}(x,y). \tag{86}$$

As it is natural, the leading order complex coefficient depends only on leading order Cartesian coefficients. Considering (54) with $k=M+1$, we get the equation for the leading order Cartesian coefficients, namely

$$\partial_x A_{(j-1,M)} + \partial_y A_{(j,M)} = 0, \quad j = 0,1,\ldots,M+1, \tag{87}$$

whose solution can be immediately found (see Hietarinta,[6] Sec. 3.0):

$$A_{(m,M)} = \sum_{k=0}^{m} \sum_{j=0}^{M-m} (-1)^k \frac{(j+k)!}{j!k!} a_{(j+k,m-k,M)} x^j y^k, \tag{88}$$

where $a_{(j+k,m-k,M)}$ are *real* integration constants.

From the relation

$$\partial_z = \tfrac{1}{2}(\partial_x - i\partial_y) \tag{89}$$

we have the expression for the rth derivative

$$\partial_z^r = \frac{1}{2^r} \sum_{s=0}^{r} \frac{r!}{(r-s)!s!} (-i)^s \partial_x^{r-s} \partial_y^s. \tag{90}$$

In order to compute the operator (90) we need the following intermediate result:

$$\partial_x^{r-s} \partial_y^s x^j y^k = \frac{j!}{(j-r+s)!} \frac{k!}{(k-s)!} x^{j-r+s} y^{k-s}, \quad \text{for } k \geqslant s \text{ and } j \geqslant r-s, \tag{91}$$

whereas the result is zero if $k<s$ or $j<r-s$. Using it, the action of the operator (90) on the monomial $x^j y^k$ is

$$\partial_z^r x^j y^k = \frac{1}{2^r} \sum_{s=0}^{r} (-i)^s \frac{r!}{(r-s)!s!} \frac{j!k!}{(j-r+s)!(k-s)!} x^{j-r+s} y^{k-s}. \tag{92}$$

Actually, we are interested only in the action of ∂_z^M: in this case, since each derivative corresponds to decreasing the degree of the monomial by one, only the highest degree terms, with $j+k=M$, survive the action of ∂_z^M. Applying (92) we get

$$\partial_z^M x^{M-k} y^k = \frac{1}{2^M} \sum_{s=0}^{M} (-i)^s \frac{M!}{(M-s)!s!} \frac{k!(M-k)!}{(s-k)!(k-s)!} x^{s-k} y^{k-s}. \tag{93}$$

Analogously to those in (91), we have that both conditions $s-k \geqslant 0$ and $k-s \geqslant 0$ must be satisfied. This implies just $s=k$ so that (93) turns out to be simply

$$\partial_z^M x^{M-k} y^k = \frac{1}{2^M} (-i)^k \frac{M!}{(M-k)!k!} k!(M-k)! = (-i)^k \frac{1}{2^M} M!. \tag{94}$$

The same result holds exchanging k with $M-k$,

$$\partial_z^M x^k y^{M-k} = (-i)^k \frac{1}{2^M} M!. \tag{95}$$

Let us now denote with $\hat{A}_{(m,M)}$ the highest degree part of $A_{(m,M)}$,

$$\hat{A}_{(m,M)} = (-1)^m \frac{M!}{(M-m)!m!} a_{(M,0,M)} x^{M-m} y^m. \tag{96}$$

Using (94) we then have

$$\partial_z^M A_{(m,M)} = \partial_z^M \hat{A}_{(m,M)} = \frac{i^m}{2^M} \frac{M!^2}{(M-m)!m!} a_{(M,0,M)}. \tag{97}$$

Remembering (86) we finally get

$$\partial_z^M S_M = \sum_{m=0}^{M} i^{M-m} \partial_z^M A_{(m,M)} \tag{98}$$

$$= \sum_{m=0}^{M} i^{M-m} \frac{i^m}{2^M} \frac{M!^2}{(M-m)!m!} a_{(M,0,M)} \tag{99}$$

$$= \frac{i^m}{2^M} M! a_{(M,0,M)} \sum_{m=0}^{M} \frac{M!}{(M-m)!m!} \tag{100}$$

$$= i^m M! a_{(M,0,M)} \tag{101}$$

which is just what we wanted to prove since it is equivalent to (84) and (85).

V. EXAMPLES

We illustrate the applications of the general approach described so far with a selection of results, many of which are new. In particular, we provide some weakly integrable systems with linear and quadratic invariants and a recipe for higher order examples. In order to compactify formulas, from hereinafter with the subscript we denote the partial derivative with respect to the corresponding variable (except when used to denote a component of momentum).

A. Weakly integrable systems with linear invariants

The ansatz is

$$I_1 = Sp + \overline{S}\overline{p}, \tag{102}$$

where for simplicity we have suppressed the subscript in the S function. The system of equations ensuing from the conservation condition is the following:

$$S_{\bar{z}} = 0, \tag{103}$$

$$\Re\{(GS)_z\} = 0. \tag{104}$$

Equation (103) agrees with (68), confirming that S can be an arbitrary analytic function,

$$S = S(z). \tag{105}$$

According to (69), the conformal transformation is given by

$$\frac{\mathrm{d}z}{\mathrm{d}w} = F'(w) \equiv S(z(w)) \tag{106}$$

or equivalently

$$w = X + iY = \int \frac{dz}{S(z)}. \tag{107}$$

Introducing the "conformal" potential

$$\tilde{G} = |F'|^2 G = |S|^2 G = S\bar{S}G, \tag{108}$$

Eq. (104) reduces to

$$\Re\{\tilde{G}_w\} = 0, \tag{109}$$

which is readily solved in

$$\tilde{G} = g(Y), \tag{110}$$

where g is an arbitrary real function and, according to the definition of the coordinate transformation, Y is the imaginary part of w. In this coordinates, the invariant assumes the normal form

$$I_1 = P + \bar{P} \tag{111}$$

or simply

$$I_1 = P_X. \tag{112}$$

Equation (104), in view of (105) and recalling the definition of G, can be rewritten as

$$\Re\{S'(E - V) - SV_z\} = 0. \tag{113}$$

We recognize the structure of Eq. (28), where now

$$f_1 = \Re\{S'(z)\} = 0 \tag{114}$$

and

$$f_0 = \Re\{(SV)_z\} = 0 \tag{115}$$

and we see that (114) coincides with (80) and solution (110) now applies to V, so that we have

$$V = \frac{g(Y(x,y))}{|S|^2}, \tag{116}$$

with g arbitrary. The general form of the second invariant in the original real coordinates is

$$I_1 = \Re\{S\}p_x + \Im\{S\}p_y. \tag{117}$$

We may provide two interesting classes of weakly integrable systems admitting linear invariants. The first is obtained by the simple observation that, if we choose the level surface $E=0$, it is no longer necessary that condition (114) be satisfied. *Any* analytic function $S=S(z)$ provides a solution through the corresponding conformal transformation. If Y, as above, denotes the new coordinate

$$Y = \mathrm{Im}\left\{\int \frac{dz}{S(z)}\right\}, \tag{118}$$

then the solution is given by the pair (116) and (117), provided we consider only motions at the energy level $E=0$.

The second class of weakly integrable systems is obtained with the following trick. Let us consider the analytic function $f(z)$ and consider then the conformal transformation (106) with $S(z)$ given by

$$S = \frac{1}{a + f'(z)}, \tag{119}$$

with a constant. Recalling definition (108), let us consider the "flat" conformal potential $\widetilde{G}=1$. In this case, relation (108), using (119) gives

$$G = E - V = \frac{1}{|S|^2} = a^2 + a(f' + \overline{f'}) + |f'|^2. \tag{120}$$

We can therefore interpret a^2 as the fixed value of the energy constant and get as a consequence the family of potentials

$$V(z,\overline{z};E) = -\sqrt{E}(f' + \overline{f'}) - |f'|^2. \tag{121}$$

To complete the solution, we must write explicitly the coordinate transformation generated by (119), that is

$$w = \int \frac{\mathrm{d}z}{S(z)} = az + f(z). \tag{122}$$

The invariant is still of the form (117).

B. Weakly integrable systems with quadratic invariants

The ansatz is

$$I_2 = Sp^2 + \overline{S}\overline{p}^2 + \widetilde{K}. \tag{123}$$

The system of equations ensuing from the conservation condition is the following:

$$S_{\overline{z}} = 0, \tag{124}$$

$$\widetilde{K}_{\overline{z}} + SG_z + \tfrac{1}{2}S'G = 0. \tag{125}$$

Equation (124) is already familiar. Since $\widetilde{K}$ is real, Eq. (125) has the following integrability condition:

$$\Im\{S''G + 3S'G_z + 2SG_{zz}\} = 0. \tag{126}$$

However, as above, we can directly simplify Eq. (125). According to (69), the conformal transformation is now given by

$$\frac{\mathrm{d}z}{\mathrm{d}w} = F'(w) \equiv \sqrt{S(z(w))} \tag{127}$$

or equivalently

$$w = \int \frac{\mathrm{d}z}{\sqrt{S(z)}}. \tag{128}$$

With the conformal potential

$$\widetilde{G} = |F'|^2 G = |S|G = \sqrt{S\overline{S}}G, \tag{129}$$

Eq. (125) reduces to

$$\widetilde{K}_{\overline{w}} + \widetilde{G}_w = 0, \tag{130}$$

that is the first example of the set (73). Its integrability condition is

$$\Im\{\widetilde{G}_{ww}\} = 0 \tag{131}$$

which is readily solved by

$$\widetilde{G} = \widetilde{A}(w + \overline{w}) + \widetilde{B}(w - \overline{w}), \tag{132}$$

where $\widetilde{A}$ and $\widetilde{B}$ are arbitrary real functions. Setting this solution in (125) gives

$$\widetilde{K} = \widetilde{B} - \widetilde{A}. \tag{133}$$

Comparing with (129) and using real "separating" coordinates,

$$X = \Re\{w\}, \quad Y = \Im\{w\}, \tag{134}$$

the solution for the original function G is then

$$G = \frac{\widetilde{A}(X;E) + \widetilde{B}(Y;E)}{|S|}. \tag{135}$$

The invariant takes the normal form

$$I_2 = P^2 + \overline{P^2} + \widetilde{B} - \widetilde{A} = \tfrac{1}{2}(P_X^2 - P_Y^2) + \widetilde{B} - \widetilde{A} \tag{136}$$

or, in the original real coordinates,

$$I_2 = \tfrac{1}{2}\,\mathrm{Re}(S)(p_x{}^2 - p_y{}^2) + \mathrm{Im}(S)p_x p_y + \widetilde{B}(Y(x,y)) - \widetilde{A}(X(x,y)). \tag{137}$$

Equation (131) can be rewritten as

$$\Im\{S''(E - V) - 3S'V_z - 2SV_{zz}\} = 0. \tag{138}$$

We again recognize the structure of Eq. (28), where now

$$f_1 = \Im\{S''(z)\} = 0 \tag{139}$$

and

$$f_0 = \Im\{S''V + 3S'V_z + 2SV_{zz}\} = 0 \tag{140}$$

and we see that (139) coincides with (81). It can be proven (see Ref. 28, Sec. II) that this condition, in addition to warrant strong integrability, is also necessary and sufficient in order that the conformal factor $|S|$ can be written as a *sum* of two functions of X and Y, say

$$|S| = S_X(X) + S_Y(Y). \tag{141}$$

Since from (140) we have that solution (135) now applies to V, we get

$$V = \frac{A(X) + B(Y)}{|S|} \tag{142}$$

with suitable A and B. In this case, X and Y are properly referred to as *separable* coordinates. From (135) and (141), we deduce the relations

$$\widetilde{A}(X;E) = ES_X - A(X), \tag{143}$$

$$\widetilde{B}(Y;E) = ES_Y - B(Y), \tag{144}$$

so that, eliminating the energy parameter through the Hamiltonian

$$E = H = \frac{\frac{1}{2}(P_X^2 + P_Y^2) + A + B}{S_X + S_Y}, \tag{145}$$

the general form of the strong quadratic invariant is

$$I_2 = \frac{S_Y(P_X^2 + 2A) - S_X(P_Y^2 + 2B)}{S_X + S_Y}. \tag{146}$$

We mention here some interesting examples of weak integrability with quadratic invariants. Consider first the polynomial function $S(z) = iz^2$. This is the simplest polynomial which gives a potential which is not automatically integrable at arbitrary energy. The corresponding conformal transformation is given by

$$w = 2^{-1/2}(1 - i)\ln z \tag{147}$$

or in terms of the real variables using polar coordinates

$$X = \frac{1}{\sqrt{2}}(\theta + \ln r), \tag{148}$$

$$Y = \frac{1}{\sqrt{2}}(\theta - \ln r). \tag{149}$$

From the relation (135) it then follows that the potential given by

$$V = r^{-2}[A(re^{\theta}) + B(re^{-\theta})], \tag{150}$$

is integrable at zero energy for arbitrary functions A and B. In Ref. 28, the class of systems with

$$A(X) = \tfrac{1}{2}(C - \sin\sqrt{2}X), \tag{151}$$

$$B(Y) = \tfrac{1}{2}(C - \sin\sqrt{2}Y), \tag{152}$$

where C is a real constant, has been investigated. Using polar coordinates, the explicit form of the potential is

$$V(r,\theta) = \frac{C - \sin\theta\cos(\ln r)}{r^2} \tag{153}$$

and that of the second invariant is

$$I_2(p_r, p_\theta, r, \theta) = rp_r p_\theta - \cos\theta\sin(\ln r), \tag{154}$$

where

$$rp_r = xp_x + yp_y, \tag{155}$$

$$p_\theta = xp_y - yp_x. \tag{156}$$

A natural question one can ask is if the system is still integrable at arbitrary energy values. As it is well known, it is possible to answer this question by performing careful numerical investigations, but, on purely analytical grounds, the problem is in general quite difficult. In Ref. 28, this potential has been proven to be nonintegrable at values of the energy $-\epsilon_1 < E < \epsilon_2$, with small

enough $\epsilon_{1,2}$, for every value of C in the interval $(0,1]$. The proof has been obtained by applying the Poincaré nonexistence theorem of additional invariants (see, e.g., Refs. 31 and 32), working in the transformed coordinates X, Y, taking asunperturbed part of the Hamiltonian the integrable system at $E=0$ and as a small perturbation the term associated to the conformal factor.

A second example is that given by a generating function of the form

$$S(z) = z^{-2}. \tag{157}$$

The conformal transformation can then be written in terms of the real variables as

$$X = \tfrac{1}{2}r^2 \cos 2\theta = \tfrac{1}{2}(x^2 - y^2), \tag{158}$$

$$Y = \tfrac{1}{2}r^2 \sin 2\theta = xy. \tag{159}$$

The corresponding potential is

$$V(X,Y) = r^2[A(X) + B(Y)], \tag{160}$$

since the conformal factor is

$$|S(X,Y)| = \frac{1}{2\sqrt{X^2 + Y^2}} = \frac{1}{r^2}. \tag{161}$$

Choosing, for example,

$$A(X) = 4X^2, \tag{162}$$

$$B(Y) = (2 + a)Y^2 + b, \tag{163}$$

where a is a constant such that $0 \leqslant a \leqslant 2$ and $b > 0$, we get the family of potentials

$$V(x,y) = r^2(x^4 + y^4 + ax^2y^2 + b). \tag{164}$$

This potential has a relative maximum at the origin where $V(0,0)=0$, absolute minima placed symmetrically in the four quadrants around the origin and grows as r^6 for $r \to \infty$. It allows bound motion for all the admissible values of the energy. For $a=2$ it is rotationally symmetric and therefore it is "superintegrable" at zero energy. The second invariant is

$$I_2(p_x,p_y,x,y) = \frac{x^2 - y^2}{2r^4}(p_x^2 - p_y^2) - \frac{2xy}{r^4}p_xp_y + x^4 + y^4 - (4 + a)x^2y^2. \tag{165}$$

What is remarkable in this case is that already at energies slightly below or above the integrable level $E=0$, the dynamics is strongly *chaotic*. This shows that identifying weakly integrable systems does not necessarily provide a *nearly* integrable system.

C. Weakly integrable systems with higher-order invariants

Exploiting the results obtained in Refs. 8 and 9, several families of weakly integrable systems admitting cubic and quartic invariants can be obtained. Both cases can be described with a similar approach. The invariants have the form

$$I_3 = 2\,\mathrm{Re}\{S_3p^3 + R_3p\}, \tag{166}$$

$$I_4 = 2\,\mathrm{Re}\{S_4p^4 + R_4p^2\} + C_0. \tag{167}$$

The conformal transformations (69), respectively, give the normal forms

$$I_3 = 2\,\mathrm{Re}\{P^3 + \widetilde{R}_3 P\}, \tag{168}$$

$$I_4 = 2\,\mathrm{Re}\{P^4 + \widetilde{R}_4 P^2\} + C_0, \tag{169}$$

with

$$\widetilde{R}_M = S_M^{(2-M)/M} R_M, \quad M = 3,4, \tag{170}$$

in agreement with definition (72). Introducing the Kähler potential, Eq. (77) provides the solutions for $\widetilde{R}_M$,

$$\widetilde{R}_M = -\frac{M}{2}\mathcal{K}_{ww}. \tag{171}$$

In the cubic case, the closure equation (66) expressed in terms of the Kähler potential gives

$$\Re\{(\mathcal{K}_{ww}\mathcal{K}_{w\bar{w}})_w\} = 0. \tag{172}$$

In the quartic case, the closure equation is that determined by Eq. (75) that, with $j=2$ and the notations adopted here, gives

$$(C_0)_{\bar{w}} = -\frac{1}{2\widetilde{G}}(\widetilde{R}_4\widetilde{G}^2)_w. \tag{173}$$

The reality of C_0 requires the integrability condition

$$\Im\{(\mathcal{K}_{www}\mathcal{K}_{w\bar{w}} + 2\mathcal{K}_{ww\bar{w}}\mathcal{K}_{ww})_w\} = 0. \tag{174}$$

Equations (172) and (174) illustrate the important difference between the previous linear and quadratic cases ($M=1,2$) and the higher order ($M>2$) cases. In the linear [see Eq. (109)] and the quadratic case [see Eq. (131)], the integrability conditions are *linear* differential equations: their solution is in terms of one or two arbitrary functions, respectively. Now, Eqs. (172) and (174) are both *nonlinear* partial differential equations, they appear very complicated and in practice impossible to solve in full generality. Only isolated systems can be identified. Using the general expression (78), we get in both $M=3$ and $M=4$ cases a *quadratic* equation of the form

$$f_2 E^2 + f_1 E + f_0 = 0, \tag{175}$$

where the f_k, $k=0,1,2$ depend on S, Λ, Ψ and their derivatives. Looking for strong invariants, S is determined as above [cf. Eq. (82) and Eq. (83)] and several solutions can be obtained by suitable assumptions on Λ and Ψ.[8,9]

Looking for weak invariants, a large class of solutions can be obtained in the simplest eventuality $E=0$. In fact, in this case the only condition we must satisfy is $f_0=0$ and it can be proven that this equation is a nonlinear PDE in the variable Ψ only. In fact, we get, respectively,

$$\Re\{(\Psi_{ww}\Psi_{w\bar{w}})_w\} = 0, \quad M = 3 \tag{176}$$

and

$$\Im\{(\Psi_{www}\Psi_{w\bar{w}} + 2\Psi_{ww\bar{w}}\Psi_{ww})_w\} = 0, \quad M = 4. \tag{177}$$

Now, *any* solution of these equations in whatever coordinate system can be used to generate a new weakly integrable system (at $E=0$) using an arbitrary conformal transformation not included in the families (82) and (83).

VI. CONCLUSIONS

Much of the structure and ideas presented in this work has come from the geometric formulation using the Jacobi metric as described in Ref. 7 and further developed in Refs. 8 and 9. One of the important results of those earlier works was the unification of the notions of weak and strong integrability in a common framework. Another was the identification of the crucial role of the conformal transformations for analyzing integrability in two dimensions. However, while the geometric picture has been very useful in these and other respects, it is clear from the present work that an approach which is more closely related to the more traditional Hamiltonian picture can also be very effective.

The conformal transformations have provided the clue for finding explicit conditions for the leading order term of strong invariants of arbitrary degree. The conditions, as given in Eqs. (84) and (85), are natural generalizations of the conditions for low order invariants. The examples given in Sec. V provide an illustration of the apparent ease by which it is possible to construct interesting weak invariants. We hope that this work can serve as a starting point for improving the understanding of higher order invariants of both the strong and the weak type.

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Variational principles for locally variational forms

J. Brajerčík[a)]
Department of Mathematics, Prešov University, 08001 Prešov, Slovakia

D. Krupka[b)]
Department of Algebra and Geometry, Palacky University, 77900 Olomouc, Czech Republic and Department of Mathematics, La Trobe University, Melbourne Victoria 3086, Australia

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We present the theory of higher order local variational principles in fibered manifolds, in which the fundamental global concept is a locally variational dynamical form. Any two Lepage forms, defining a local variational principle for this form, differ on intersection of their domains, by a variationally trivial form. In this sense, but in a different geometric setting, the local variational principles satisfy analogous properties as the variational functionals of the Chern–Simons type. The resulting theory of extremals and symmetries extends the first order theories of the Lagrange–Souriau form, presented by Grigore and Popp, and closed equivalents of the first order Euler–Lagrange forms of Haková and Krupková. Conceptually, our approach differs from Prieto, who uses the Poincaré–Cartan forms, which do not have higher order global analogues. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1901323]

I. INTRODUCTION

It is well known that differential equations for critical points of a variational functional in a fibered manifold can be represented by a global differential form, the *Euler–Lagrange form*, whose components are the Euler–Lagrange expressions. It is also well known that there exist differential equations, represented by similar global differential forms, the *dynamical forms*, which are *locally variational*, but do not admit a *global* Lagrangian. A deeper understanding of this phenomenon is provided by the variational bicomplex theory (Vinogradov,[31] Takens,[28] Anderson and Duchamp,[2] Dedecker and Tulczyjew,[6] and Tulczyjew[30]), and the (finite order) variational sequence theory (Krupka,[20] Grigore,[10,11] Vitolo,[32] and Krbek and Musilová[14]).

The corresponding variational principles in the first order field theory have been recently studied by several authors. Grigore and Popp[12] extended the ideas of Souriau[27] on the role of closed 2-forms in mechanics to $(n+1)$-forms in the variational theory for n-dimensional submanifolds of a given manifold. They introduced the *Lagrange–Souriau form*, representing the Euler–Lagrange equations, and proved that this form is equal to the exterior derivative of the *fundamental Lepage form* in the sense of Krupka,[15,18] (see also Betounes[3,4] and Rund[25]). The theory presented by Prieto[23,24]), is based on the existence of the global Poincaré–Cartan form (Sniatycki,[26] Goldschmidt and Sternberg,[9] Krupka,[17,15] and García[8]), and is aimed to extend basic properties of variational principles of the Chern–Simons type (see, e.g., Freed[7]) to fibered manifolds. Haková and Krupková[13] showed that the closed $(n+1)$-forms related to variational systems of first order partial differential equations are exactly the exterior derivative of the fundamental Lepage form.

[a)]Electronic mail: brajerci@unipo.sk
[b)]Electronic mail: krupka@inf.upol.cz

Closed 2-forms in higher order mechanics, equivalent with the Euler–Lagrange forms, were studied by Krupková.[21,22]

This paper is devoted to local variationality in the framework of the *higher order* variational theory on fibered spaces (Krupka[19,15]), and the variational sequence theory. In general, for higher order Lagrangians in field theory a global analogue of the Poincaré–Cartan form does not exist. We show that instead of this form one can use *any* Lepage form; the Poincaré–Cartan form is an example of a first order Lepage form. Any (higher order) Lepage form gives rise, by means of the global variation formula, to the (higher order) *Euler–Lagrange form*. Conceptually, the theory is quite simple and clear. In particular, it is easy to understand, in full generality, that there exist (global) dynamical forms, admitting local higher order Lagrangians, but not a global one.

In Sec. II we give a survey of the higher order variational theory on fibered spaces. Section III is devoted to some new results on infinitesimal symmetries, based on the fundamental Lepage form. In Sec. IV we introduce a *local variational principle* for a *locally variational* dynamical form. We give the *first variation formula* and discuss properties of transformations, leaving invariant the local variational principle, and the locally variational form.

In this paper we suppose that we have a fibered manifold $\pi: Y \to X$, and write $n = \dim X$, and $n+m = \dim Y$. $J^r Y$ is the *r-jet prolongation* of Y, and $\pi^{r,s}: J^r Y \to J^s Y$, $\pi^r: J^r Y \to X$ are the *canonical jet projections*. The *r-jet prolongation* of a section γ is defined to be the mapping $x \to J^r\gamma(x) = J^r_x\gamma$. For any set $W \subset Y$ we denote $W^r = (\pi^{r,0})^{-1}(W)$. Any *fibered chart* (V, ψ), $\psi = (x^i, y^\sigma)$, on Y, induces the *associated charts* on X and on $J^r Y$, denoted by (U, φ), $\varphi = (x^i)$, and (V^r, ψ^r), $\psi^r = (x^i, y^\sigma, y^\sigma_{j_1}, y^\sigma_{j_1 j_2}, \ldots, y^\sigma_{j_1 j_2 \ldots j_r})$, respectively; here $1 \leqslant i \leqslant n$, $1 \leqslant \sigma \leqslant m$, and $V^r = (\pi^{r,0})^{-1}(V)$, $U = \pi^r(V)$. We denote $\omega_0 = \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \cdots \wedge \mathrm{d}x^n$, and

$$\omega_k = i_{\partial/\partial x^k}\omega_0 = (-1)^{k-1}\,\mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \cdots \wedge \mathrm{d}x^{k-1} \wedge \mathrm{d}x^{k+1} \wedge \cdots \wedge \mathrm{d}x^n.$$

We define the *formal derivative operator* by

$$d_i = \frac{\partial}{\partial x^i} + y^\sigma_i \frac{\partial}{\partial y^\sigma} + y^\sigma_{i_1 i} \frac{\partial}{\partial y^\sigma_{i_1}} + \cdots + y^\sigma_{i_1 i_2 \cdots i_r i} \frac{\partial}{\partial y^\sigma_{i_1 i_2 \cdots i_r}}.$$

II. LAGRANGE STRUCTURES

A. Differential forms on jet spaces

For any open set $W \subset Y$, let $\Omega^r_0 W$ be the ring of functions on W^r. The $\Omega^r_0 W$-module of differential q-forms on W^r is denoted by $\Omega^r_q W$, and the exterior algebra of forms on W^r is denoted by $\Omega^r W$. The module of $\pi^{r,0}$-horizontal (π^r-horizontal) q-forms is denoted by $\Omega^r_{q,Y} W$ ($\Omega^r_{q,X} W$, respectively); forms belonging to these spaces are sometimes called $\pi^{r,0}$-semibasic, or π^r-semibasic, respectively.

Let $W \subset Y$ be an open set. The fibered structure of Y induces a morphism of exterior algebras $h: \Omega^r W \to \Omega^{r+1} W$, called the *horizontalization*. In a fibered chart (V, ψ), $\psi = (x^i, y^\sigma)$, h is defined by

$$hf = f \circ \pi^{r+1,r}, \quad h\,\mathrm{d}x^i = \mathrm{d}x^i, \quad h\,\mathrm{d}y^\sigma_{j_1 j_2 \cdots j_p} = y^\sigma_{j_1 j_2 \cdots j_p k}\,\mathrm{d}x^k,$$

where $f: W^r \to \mathbb{R}$ is a function, and $0 \leqslant p \leqslant r$. Note that h can be defined intrinsically: for a k-form $\eta \in \Omega^r_k W$, where $0 \leqslant k \leqslant n$, we define $h\eta$ to be a unique π^{r+1}-horizontal form such that $J^r\gamma^* \eta = J^{r+1}\gamma^* h\eta$ for every section γ of Y (here * denotes the pull-back operation).

We say that a form $\eta \in \Omega^r_k W$ is *contact*, if $h\eta = 0$. For any fibered chart (V, ψ), $\psi = (x^i, y^\sigma)$, the 1-forms

$$\omega^\sigma_{j_1 j_2 \cdots j_p} = \mathrm{d}y^\sigma_{j_1 j_2 \cdots j_p} - y^\sigma_{j_1 j_2 \cdots j_p k}\,\mathrm{d}x^k,$$

where $1 \leqslant p \leqslant r-1$, are examples of contact 1-forms. Note that these forms define a basis of 1-forms on V^r, $(\mathrm{d}x^i, \omega^\sigma_{j_1 j_2 \cdots j_p}, \mathrm{d}y^\sigma_{j_1 j_2 \cdots j_r})$.

It is known that a form $\eta \in \Omega^r_k W$ has a unique decomposition

$$(\pi^{r+1,r})^* \eta = h\eta + p_1\eta + p_2\eta + \cdots + p_k\eta, \tag{1}$$

such that $p_i\eta$ contains, in any fibered chart, exactly i exterior factors $\omega^\sigma_{j_1 j_2 \cdots j_l}$, $1 \leqslant l \leqslant r$. In particular, this gives us a simple formulation of the fact that the forms $\omega^\sigma_{j_1 j_2 \cdots j_l}$ generate an *ideal* in the exterior algebra $\Omega^r V$ (the *contact ideal*).

$h\eta$ ($p_i\eta$) is the *horizontal* (*i*th *contact*) *component* of η. The decomposition (1) is *invariant*, and is called the *canonical decomposition* of η.

η is π^r*-horizontal* if and only if $(\pi^{r+1,r})^*\eta = h\eta$. We say that η is *k-contact*, if $(\pi^{r+1,r})^*\eta = p_k\eta$; in this case k is the *order of contactness* of η.

Let $k \geqslant n+1$. Then for any k-form $\eta \in \Omega^r_k W$, $h\eta = 0$, $p_1\eta = 0$, $p_2\eta = 0, \ldots, p_{k-n-1}\eta = 0$, because each of these forms contains more than n exterior factors $\mathrm{d}x^i$. η is said to be *strongly contact*, if $p_{k-n}\eta = 0$.

B. Lagrangians

A *Lagrangian* (of *order r*) for Y is any π^r-horizontal n-form on some $W^r \subset J^r Y$, i.e., any element of the set $\Omega^r_{n,X} W$. In a fibered chart (V, ψ), $\psi = (x^i, y^\sigma)$, a Lagrangian of order r defined on $V^r = (\pi^{r,0})^{-1}(V)$ has an expression

$$\lambda = \mathcal{L}\omega_0, \tag{2}$$

where $\mathcal{L}: V^r \to \mathbb{R}$ is a function (the *Lagrange function* associated with λ and (V, ψ)). Clearly, in general a Lagrangian cannot be determined by a *globally* defined function unless a volume element on X is specified.

A pair (Y, λ), consisting of a fibered manifold Y and a Lagrangian λ of order r for Y is called a *Lagrange structure* (of order r).

Sometimes it is convenient to use Lagrangians of the form $\lambda = h\eta$, where $\eta \in \Omega^{r-1}_n W$. These Lagrangians have a certain polynomial structure in the highest order variables $y^\sigma_{j_1 j_2 \cdots j_r}$. The assumption $\lambda = h\eta$ appears naturally in the variational sequence theory, but does not restrict the generality.

Note that our definition includes Lagrangians defined over any open subsets $W \subset Y$; we need such a definition to describe phenomena arising in connection with the so-called *local variational principles* for *globally defined* Euler–Lagrange equations. The discussion of this situation is a main objective of this paper.

C. Lepage forms

We now give a formal definition of a Lepage form (Krupka[15]). A principal geometric meaning of this concept consists in the fact, that Lepage forms describe the relationship between the equations for extremals of variational principles on one side, and the exterior derivative operator, acting on differential forms, on the other side.

A differential form $\rho \in \Omega^s_n W$, where $n = \dim X$, is called a *Lepage form*, if $p_1\,\mathrm{d}\rho$ is $\pi^{s+1,0}$-horizontal, i.e., $p_1\,\mathrm{d}\rho \in \Omega^{s+1}_{n+1,Y} W$. A Lepage form ρ is a *Lepage equivalent* of a Lagrangian $\lambda \in \Omega^r_{n,X} W$, if the horizontal component of ρ coincides with λ, i.e., $h\rho = \lambda$ (possibly up to a jet projection).

If ρ is a Lepage equivalent of a Lagrangian $\lambda \in \Omega^r_{n,X} W$, expressed by (2), then one can get by a direct calculation

$$p_1\,\mathrm{d}\rho = E_\sigma(\mathcal{L})\omega^\sigma \wedge \omega_0, \tag{3}$$

where

$$E_\sigma(\mathcal{L}) = \sum_{k=0}^{r} (-1)^k d_{i_1} d_{i_2} \cdots d_{i_k} \frac{\partial \mathcal{L}}{\partial y^\sigma_{i_1 i_2 \cdots i_k}} \tag{4}$$

are the *Euler–Lagrange expressions* associated with the Lagrange function $\mathcal{L}$. In particular, $p_1\,\mathrm{d}\rho$ depends on the Lagrangian λ only. The $(n+1)$-form

$$E_\lambda = p_1\,\mathrm{d}\rho$$

is called the *Euler–Lagrange form* associated with λ.

We give three examples of Lepage equivalents.

(1) Every first order Lagrangian $\lambda \in \Omega^1_{n,X}W$ has a unique Lepage equivalent $\Theta_\lambda \in \Omega^1_{n,Y}W$ whose order of contactness is $\leqslant 1$. If λ is expressed in a fibered chart by $\lambda = \mathcal{L}\omega_0$, then

$$\Theta_\lambda = \mathcal{L}\omega_0 + \frac{\partial \mathcal{L}}{\partial y^\sigma_i}\omega^\sigma \wedge \omega_i.$$

Θ_λ is the *Poincaré–Cartan equivalent* of λ, or the *Poincaré–Cartan form*.

(2) Let $\lambda \in \Omega^1_{n,X}W$ be as above. The *fundamental Lepage equivalent* $\Phi_\lambda \in \Omega^1_{n,Y}W$ of λ is given by

$$\Phi_\lambda = \sum_{k=0}^{n}\left(\frac{1}{k!}\right)^2 \frac{\partial^k \mathcal{L}}{\partial y^{\sigma_1}_{j_1}\partial y^{\sigma_2}_{j_2}\cdots\partial y^{\sigma_k}_{j_k}}\omega^{\sigma_1}\wedge\omega^{\sigma_2}\wedge\cdots\wedge\omega^{\sigma_k}\wedge\omega_{j_1 j_2\cdots j_k}, \tag{5}$$

where

$$i_{\partial/\partial x^{i_k}}\cdots i_{\partial/\partial x^{i_2}} i_{\partial/\partial x^{i_1}}\omega_0 = \omega_{i_1 i_2\cdots i_k}.$$

Φ_λ has the following remarkable properties: (a) $\mathrm{d}\Phi_\lambda = 0$ if and only if $E_\lambda = 0$, and (b) $\lambda = h\eta$ for some $\eta \in \Omega^0_n W$ if and only if E_λ is $\pi^{2,1}$-projectable. The form Φ_λ was introduced for the first time by Krupka,[15,18] and it was rediscovered by Betounes,[3,4] and Rund[25] who wrote Φ_λ in a more simple way as it stands in (5).

(3) Expression

$$\Theta_\lambda = \mathcal{L}\omega_0 + \left(\frac{\partial \mathcal{L}}{\partial y^\sigma_i} - d_p\frac{\partial \mathcal{L}}{\partial y^\sigma_{pi}}\right)\omega^\sigma \wedge \omega_i + \frac{\partial \mathcal{L}}{\partial y^\sigma_{ji}}\omega^\sigma_j \wedge \omega_i \tag{6}$$

generalizes the Poincaré–Cartan form to *second order* Lagrangians $\lambda \in \Omega^2_{n,X}W$ (Krupka[15]), higher order generalizations can be found in Krupka.[19] It can be shown that every Lepage equivalent of a Lagrangian $\lambda = \mathcal{L}\omega_0$ of order r has the chart expression $\rho = \Theta_\lambda + \mathrm{d}\mu + \nu$, where

$$\Theta_\lambda = \mathcal{L}\omega_0 + \sum_{k=0}^{s}\left(\sum_{l=0}^{r-k}(-1)^l d_{i_1} d_{i_2}\cdots d_{i_l}\frac{\partial \mathcal{L}}{\partial y^\sigma_{i_1 i_2\cdots i_l j_1 j_2\cdots j_k}}\right)\omega^\sigma_{j_1 j_2\cdots j_k}\wedge\omega_i, \tag{7}$$

μ is a contact form, and ν is of order of contactness $\geqslant 2$. Expression (6) defines a differential form on J^3Y, but for $r \geqslant 3$, the (local) Lepage equivalents (7) of λ are no longer invariant.

D. Automorphisms, variations

By an *automorphism* of Y we mean a diffeomorphism $\alpha: W \to Y$, where $W \subset Y$ is an open set, such that there exists a diffeomorphism $\alpha_0: \pi(W) \to X$ such that $\pi\alpha = \alpha_0\pi$. If α_0 exists, it is unique, and is called the *π-projection* of α. The *r-jet prolongation* of α is an automorphism $J^r\alpha: W^r \to J^rY$ of J^rY, defined by

$$J^r\alpha(J^r_x\gamma) = J^r_{\alpha_0(x)}(\alpha\gamma\alpha_0^{-1}).$$

Let $U \subset X$ be an open set, and let $\gamma: U \to Y$ be a section. Let ξ be a π-projectable vector field on an open set $W \subset Y$ such that $\gamma(U) \subset W$. If α_t is the local one-parameter group of ξ, and $\alpha_{(0)t}$ is its projection, then since $\pi\alpha_t = \alpha_{(0)t}\pi$,

$$\gamma_t = \alpha_t \gamma \alpha_{(0)t}^{-1}$$

is one-parameter family of sections of Y, depending smoothly on t. γ_t is called the *variation*, or the *deformation* of γ, *induced* by ξ.

We define the *r-jet prolongation* of ξ to be the vector field $J^r\xi$ on J^rY whose local one-parameter group is $J^r_{\alpha_t}$. Thus,

$$J^r\xi(J^r_x\gamma) = \left\{ \frac{\mathrm{d}}{\mathrm{d}t} J^r_{\alpha_{(0)t}(x)}(\alpha_t \gamma \alpha_{(0)t}^{-1}) \right\}_0 .$$

E. Global variational functionals

Let Ω be a piece of X (a compact, n-dimensional submanifold of X with boundary $\partial\Omega$), let $\Gamma_{\Omega,W}(\pi)$ be the set of smooth sections γ over Ω such that $\gamma(\Omega) \subset W$. Suppose that we have a Lagrangian $\lambda \in \Omega^r_{n,X}(W)$. This gives rise to the *variational functional*, or the *action function* associated with λ, $\Gamma_{\Omega,W}(\pi) \ni \gamma \to \lambda_\Omega(\gamma) \in \mathbb{R}$, defined by

$$\lambda_\Omega(\gamma) = \int_\Omega J^r\gamma^*\lambda .$$

Choose a section $\gamma \in \Gamma_{\Omega,W}(\pi)$ and a π-projectable vector field ξ on Y, and consider the induced variation γ_t of γ. Since the domain of γ_t contains Ω for all sufficiently small t, we get a real-valued function on a neighborhood $(-\epsilon, \epsilon)$ of the origin $0 \in \mathbb{R}$,

$$(-\epsilon, \epsilon) \ni t \to \lambda_{\alpha_{(0)t}(\Omega)}(\alpha_t \gamma \alpha_{(0)t}^{-1}) = \int_{\alpha_{(0)t}(\Omega)} J^r(\alpha_t \gamma \alpha_{(0)t}^{-1})^* \lambda \in \mathbb{R}.$$

Differentiating this function at $t=0$ we obtain

$$(\partial_{J^r\xi}\lambda)_\Omega(\gamma) = \int_\Omega J^r\gamma^* \partial_{J^r\xi}\lambda, \tag{8}$$

where $\partial_{J^r\xi}\lambda$ is the Lie derivative of λ by $J^r\xi$. The number (8) is the *variation* of the variational function λ_Ω at γ, *induced* by the vector field ξ. This formula shows, in particular, that the function $\Gamma_{\Omega,W}(\pi) \ni \gamma \to (\partial_{J^r\xi}\lambda)_\Omega(\gamma) \in \mathbb{R}$ is the variational functional (over Ω) associated with the Lagrangian $\partial_{J^r\xi}\lambda$. We call this function the *variational derivative*, or the *first variation* of λ_Ω by ξ.

We now compute the Lie derivative $\partial_{J^r\xi}\lambda$. Choose for this purpose a Lepage equivalent ρ of λ, and denote by s the *order* of ρ. Since $\lambda = h\rho$, or, which is the same, $J^r\gamma^*\lambda = J^s\gamma^*\rho$ for all sections γ, we obtain

$$J^r\gamma^*\partial_{J^r\xi}\lambda = J^s\gamma^*\partial_{J^s\xi}\rho = J^s\gamma^*(i_{J^s\xi}\,\mathrm{d}\rho + \mathrm{d}i_{J^s\xi}\rho).$$

Omitting γ and using the Euler–Lagrange form (3) and (4), we get

$$\partial_{J^r\xi}\lambda = h i_{J^{s+1}\xi} E_\lambda + h\,\mathrm{d}i_{J^s\xi}\rho. \tag{9}$$

This is the *differential first variation formula*; the first term on the right-hand side is the *Euler–Lagrange term*, and the second one is the *boundary term*.

Writing (9) in coordinates, we obtain the well-known classical expressions, standing behind the variation integral.

F. Extremals

Let $\lambda \in \Omega^r_{n,X}W$ be a Lagrangian, and let $\rho \in \Omega^s_n W$ be a Lepage equivalent of λ. We say that a section $\gamma \in \Gamma_{\Omega,W}(\pi)$ is *stable* with respect to a variation ξ of γ, if $(\partial_{J^r\xi}\lambda)_\Omega(\gamma) = 0$. Stable sections with respect to *families* of variations are defined in an obvious way. If γ is stable with respect to

all ξ with support contained in $\pi^{-1}(\Omega)$, we say that γ is an *extremal* of λ_Ω. A section γ which is an extremal of every λ_Ω is called an *extremal* of λ.

The following conditions are equivalent: (1) γ is an extremal of λ, (2) γ satisfies

$$J^s\gamma^* i_{J^s\xi}\,\mathrm{d}\rho = 0$$

for all π-vertical vector fields ξ, and (3) for every fibered chart on Y, γ satisfies the system of partial differential equations

$$E_\sigma(\mathcal{L})\circ J^{2r}\gamma = 0.$$

G. Trivial Lagrangians

A Lagrangian $\lambda \in \Omega^r_{n,X}W$ is called *trivial* (or *variationally trivial*, or *null*) if there exists an $(n-1)$-form $\eta \in \Omega^s_{n-1}W$ such that $\lambda = h\,\mathrm{d}\eta$. λ is called *locally trivial* if there exists an open covering $\{W_\iota\}_{\iota\in I}$ of Y, and to each $\iota \in I$ an $(n-1)$-form $\eta_\iota \in \Omega^s_{n-1}W_\iota$, such that $\lambda = h\,\mathrm{d}\eta_\iota$ over W_ι.

The following is a standard consequence of variational sequence theory.

Theorem 1: *A Lagrangian* λ *is locally trivial if and only if* $E_\lambda = 0$.

H. Locally variational forms

A 1-contact, $\pi^{s,0}$-horizontal form $\varepsilon \in \Omega^s_{n+1,Y}W$ is called a *dynamical form* (Krupková[22]); Takens[28] calls such forms *source forms*. From the definition it follows that in a fibered chart (V,ψ), $\psi=(x^i,y^\sigma)$,

$$\varepsilon = \varepsilon_\sigma \omega^\sigma \wedge \omega_0,$$

where $\varepsilon_\sigma = \varepsilon_\sigma(x^i, y^\sigma, y^\sigma_{j_1}, y^\sigma_{j_1 j_2}, \ldots, y^\sigma_{j_1 j_2 \cdots j_s})$. We say that a dynamical form ε is *variational*, if $\varepsilon = E_\lambda$ for some Lagrangian $\lambda \in \Omega^r_{n,X}W$. ε is said to be *locally variational*, if there are an open covering $\{V_\iota\}_{\iota\in I}$ of Y and a family $\{\lambda_\iota\}_{\iota\in I}$ of Lagrangians $\lambda_\iota \in \Omega^r_{n,X}V_\iota$ such that for every $\iota \in I$,

$$\varepsilon | V_\iota = E_{\lambda_\iota}.$$

Denote

$$H^{j_1 j_2 \cdots j_i}_{\sigma\ \ \ \ \ \ \ \nu}(\varepsilon) = \frac{\partial \varepsilon_\nu}{\partial y^\sigma_{j_1 j_2 \cdots j_i}} - (-1)^i \frac{\partial \varepsilon_\sigma}{\partial y^\nu_{j_1 j_2 \cdots j_i}} - \sum_{k=i+1}^{s} (-1)^k \binom{k}{i} d_{j_{i+1}} d_{j_{i+2}} \cdots d_{j_k} \frac{\partial \varepsilon_\sigma}{\partial y^\nu_{j_1 j_2 \cdots j_1 j_{i+1} \cdots j_k}}$$

and

$$H_\varepsilon = \frac{1}{2}\sum_{i=1}^{s} H^{j_1 j_2 \cdots j_i}_{\sigma\ \ \ \ \ \ \ \nu}(\varepsilon)\,\omega^\sigma_{j_1 j_2 \cdots j_i} \wedge \omega^\nu \wedge \omega_0.$$

The functions $H^{j_1 j_2 \cdots j_i}_{\sigma\ \ \ \ \ \ \ \nu}(\varepsilon)$, called the *Helmholtz expressions*, appeared for the first time in Aldersley;[1] H_ε is the (global) *Helmholtz form* (Anderson,[2] Krupka,[16,20] Krbek and Musilová[14]).

The following is a consequence of the variational sequence theory.

Theorem 2: *A source form* ε *is locally variational if and only if* $H_\varepsilon = 0$.

I. Invariant transformations

An automorphism $\alpha: W \to Y$ of the fibered manifold Y is said to be an *invariant transformation* of a form $\eta \in \Omega^s_p W$, if

$$J^s\alpha^*\eta = \eta.$$

We also say that η is *invariant* with respect to α. Let ξ be a π-projectable vector field on Y. We say that ξ is the *generator* of invariant transformations of η, if

$$\partial_{J^s\xi}\eta = 0.$$

In this case we also say that η is *invariant* with respect to ξ. These definitions include the notions of invariance of *Lagrangians, dynamical forms*, and, in particular, the *Euler–Lagrange forms*.

Note that for *any* π-projectable vector field ξ, and any $\lambda \in \Omega^r_{n,X}W$,

$$\partial_{J^s\xi}E_\lambda = E_{\partial_{J^r\xi}\lambda}, \tag{10}$$

where s is the order of the Euler–Lagrange form E_λ. Thus, E_λ is invariant with respect to ξ if and only if $\partial_{J^r\xi}\lambda$ is a trivial Lagrangian.

The following result is standard.

Theorem 3: *Let ξ be a π-projectable vector field on Y, and let $\lambda \in \Omega^{r+1}_{n,X}W$ be a Lagrangian. The following conditions are equivalent:*

(a) *ξ generates invariant transformations of the Euler–Lagrange form E_λ.*
(b) *There exist an open covering $\{V_\iota\}_{\iota\in I}$ of Y and a system of $(n-1)$-forms $\{\eta_\iota\}_{\iota\in I}$, where $\eta_\iota \in \Omega^r_{n-1}V_\iota$, such that*

$$\partial_{J^{r+1}\xi}\lambda = h\,\mathrm{d}\eta_\iota.$$

The following simple consequence of the first variation formula is known as the *Noether's theorem*.

Theorem 4: *Let $\lambda \in \Omega^{r+1}_{n,X}W$ be a Lagrangian. Let $\rho \in \Omega^s_n W$ be a Lepage equivalent of λ, and let γ be an extremal.*

(a) *For any generator ξ of invariant transformations of λ,*

$$\mathrm{d}J^s\gamma^* i_{J^s\xi}\rho = 0.$$

(b) *For any generator ξ of invariant transformations of E_λ, there exist an open covering $\{V_\iota\}_{\iota\in I}$ of W and a family $\{\eta_\iota\}_{\iota\in I}$ of $(n-1)$-forms $\eta_\iota \in \Omega^r_{n-1}V_\iota$ such that for every $\iota \in I$,*

$$\mathrm{d}J^s\,\gamma^*(i_{J^s\xi}\rho - \eta_\iota) = 0.$$

III. INVARIANCE: FIRST ORDER VARIATIONAL PRINCIPLES

One of specific features of the *first order* Lagrange structures consists in existence of two "simple" Lepage forms (Sec. II C). The first one is the *Poincaré–Cartan form*, whose order of contactness is $\leqslant 1$ (see, e.g., García,[8] Goldschmidt and Sternberg,[9] Krupka,[17] Prieto[24]). The second one is the *fundamental Lepage form*, whose order of contactness is, in general, maximal, i.e., $\leqslant n$. We now compare invariance properties of these forms. Our results extend the usual concepts, based on the use of the Poincaré–Cartan form. For general approach to invariance we refer to Trautman[29] and Krupka.[17,15]

As before, we denote by Φ_λ the fundamental Lepage equivalent, associated with a first order Lagrangian λ, and by Θ_λ the Poincaré–Cartan equivalent.

Theorem 5: *For any automorphism $\alpha: W \to Y$ of Y,*

$$J^1\alpha^*\Phi_\lambda = \Phi_{J^1\alpha^*\lambda}. \tag{11}$$

Proof: (1) Let α_0 be the projection of α, and let (V,ψ), $\psi=(x^i,y^\sigma)$, and $(\overline{V},\overline{\psi})$, $\overline{\psi}=(\overline{x^i},\overline{y^\sigma})$, be two fibered charts such that $\alpha(V)\subset\overline{V}$. Let (U,φ), $\varphi=(x^i)$, and $(\overline{U},\overline{\varphi})$, $\overline{\varphi}=(\overline{x^i})$ be the associated charts on X. Denote

$$\overline{x^i}\alpha_0\varphi^{-1} = f^i, \quad \overline{y^\sigma}\alpha\psi^{-1} = F^\sigma,$$

and

$$x^p \alpha_0^{-1} \overline{\varphi}^{-1} = g^p.$$

Clearly, on the corresponding domains,

$$f^i(g^1(\overline{x^1}, \overline{x^2}, \ldots, \overline{x^n}), g^2(\overline{x^1}, \overline{x^2}, \ldots, \overline{x^n}), \ldots, g^n(\overline{x^1}, \overline{x^2}, \ldots \overline{x^n})) = \overline{x^i},$$

$$g^p(f^1(x^1, x^2, \ldots, x^n), f^2(x^1, x^2, \ldots x^n), \ldots, f^n(x^1, x^2, \ldots, x^n)) = x^p.$$

From these formulas, we can easily derive equations of the mapping $J^1\alpha: W^1 \to J^1Y$ in terms of the associated coordinates. By definition, we have for every $J^1_x\gamma \in W^1$, $J^1\alpha(J^1_x\gamma) = J^1_{\alpha_0(x)}(\alpha\gamma\alpha_0^{-1})$. On $V^1 \subset W^1$,

$$\overline{x^i} J^1\alpha(J^1_x\gamma) = \overline{x^i} J^1_{\alpha_0(x)}(\alpha\gamma\alpha_0^{-1}) = \overline{x^i}\alpha_0(x) = \overline{x^i}\alpha_0\varphi^{-1}(\varphi(x)),$$

$$\overline{y^\sigma} J^1\alpha(J^1_x\gamma) = \overline{y^\sigma} J^1_{\alpha_0(x)}(\alpha\gamma\alpha_0^{-1}) = \overline{y^\sigma}\alpha\psi^{-1}(\psi(\gamma(x))),$$

and

$$\overline{y^\sigma_j} J^1\alpha(J^1_x\gamma) = \overline{y^\sigma_j} J^1_{\alpha_0(x)}(\alpha\gamma\alpha_0^{-1}) = D_j(\overline{y^\sigma}\alpha\gamma\alpha_0^{-1}\overline{\varphi}^{-1})(\overline{\varphi}(\alpha_0(x))).$$

Computing the derivative by the chain rule, we get

$$\begin{aligned} D_j(\overline{y^\sigma}\alpha\gamma\alpha_0^{-1}\overline{\varphi}^{-1})(\overline{\varphi}(\alpha_0(x))) &= D_{1,k}(\overline{y^\sigma}\alpha\psi^{-1})(\psi(\gamma(x)))D_j(x^k\alpha_0^{-1}\overline{\varphi}^{-1})(\overline{\varphi}(\alpha_0(x))) \\ &\quad + D_{2,\nu}(\overline{y^\sigma}\alpha\psi^{-1})(\psi(\gamma(x)))D_k(y^\nu\gamma\varphi^{-1})(\varphi(x)) \\ &\quad \times D_j(x^k\alpha_0^{-1}\overline{\psi}^{-1})(\overline{\psi}(\alpha_0(x))). \end{aligned}$$

We define functions $F^\sigma_j: V^1 \to \mathbb{R}$ by

$$\begin{aligned} F^\sigma_j(x^i(J^1_x\gamma), y^\tau(J^1_x\gamma), y^\tau_p(J^1_x\gamma)) &= D_{1,k}(\overline{y^\sigma}\alpha\psi^{-1})(\psi(\gamma(x)))D_j(x^k\alpha_0^{-1}\overline{\varphi}^{-1})(\overline{\varphi}(\alpha_0(x))) + D_{2,\nu}(\overline{y^\sigma}\alpha\psi^{-1}) \\ &\quad \times(\psi(\gamma(x)))D_k(y^\nu\gamma\varphi^{-1})(\varphi(x))D_j(x^k\alpha_0^{-1}\overline{\varphi}^{-1})(\overline{\varphi}(\alpha_0(x))), \end{aligned}$$

or, which is the same, by

$$\begin{aligned} F^\sigma_j(x^i, y^\tau, y^\tau_p) &= \left(\left(\frac{\partial F^\sigma}{\partial x^k}\right)_{(x^i, y^\tau)} + \left(\frac{\partial F^\sigma}{\partial y^\nu}\right)_{(x^i, y^\tau)} y^\nu_k\right)\left(\frac{\partial g^k}{\partial \overline{x^j}}\right)_{(f^1(x^i), f^2(x^i), \ldots, f^n(x^i))} \\ &= (d_k F^\sigma)(x^i, y^\tau, y^\tau_j)\left(\frac{\partial g^k}{\partial \overline{x^j}}\right)_{(f^1(x^i), f^2(x^i), \ldots f^n(x^i))}. \end{aligned}$$

Then

$$\overline{y^\sigma_j} J^1\alpha(\psi^1)^{-1} = F^\sigma_j.$$

Summarizing, we see that the mapping $J^1\alpha$ is expressed by equations

$$\overline{x^i}\alpha_0\varphi^{-1} = f^i, \quad \overline{y^\sigma}\alpha\psi^{-1} = F^\sigma,$$

$$\overline{y^\sigma_j} J^1\alpha(\psi^1)^{-1} = d_k F^\sigma \cdot \left(\frac{\partial g^k}{\partial \overline{x^j}} \circ \overline{\varphi}\alpha_0\varphi^{-1}\right).$$

(2) We now derive chart expressions for the forms $\alpha_0^* \overline{\omega_0}$ and $\alpha_0^* \overline{\omega}_{i_1 i_2 \cdots i_k}$, where $1 \leqslant k \leqslant n$. We have, with obvious conventions,

$$\alpha_0^*\overline{\omega_0}(x) = \mathrm{d}(\overline{x^1}\alpha_0)(x) \wedge \mathrm{d}(\overline{x^2}\alpha_0)(x) \wedge \cdots \wedge \mathrm{d}(\overline{x^n}\alpha_0)(x) = \det\left(\frac{\partial f^p}{\partial x^q}\right)_{\varphi(x)} \omega_0(x).$$

Analogously, since

$$T_{\alpha_0(x)}\alpha_0^{-1} \cdot \left(\frac{\partial}{\partial \overline{x^i}}\right)_{\overline{\varphi}\alpha_0(x)} = \left(\frac{\partial g^j}{\partial \overline{x^i}}\right)_{\alpha_0(x)} \left(\frac{\partial}{\partial x^j}\right)_x$$

and

$$\alpha_0^*\overline{\omega_i}(x)(\xi_2, \xi_3, \ldots, \xi_n) = \left(\frac{\partial(x^j\alpha_0^{-1}\overline{\varphi}^{-1})}{\partial \overline{x^i}}\right)_{\overline{\varphi}\alpha_0(x)} \det\left(\frac{\partial(\overline{x^p}\alpha_0\varphi^{-1})}{\partial x^q}\right)_{\varphi(x)} \omega_j(x)(\xi_2, \xi_3, \ldots, \xi_n)$$

we have

$$\alpha_0^*\overline{\omega_i}(x) = \left(\frac{\partial g^j}{\partial \overline{x^i}}\right)_{\overline{\varphi}\alpha_0(x)} \det\left(\frac{\partial f^p}{\partial x^q}\right)_{\varphi(x)} \omega_j(x).$$

Continuing in the same way we obtain

$$\alpha_0^*\overline{\omega}_{i_1 i_2 \cdots i_k}(x)(\xi_{k+1}, \xi_{k+2}, \ldots, \xi_n) = \left(\frac{\partial g^{j_1}}{\partial \overline{x^i}_1}\right)_{\overline{\varphi}\alpha_0(x)} \left(\frac{\partial g^{j_2}}{\partial \overline{x^i}_2}\right)_{\overline{\varphi}\alpha_0(x)} \cdots \left(\frac{\partial g^{j_k}}{\partial \overline{x^i}_k}\right)_{\overline{\varphi}\alpha_0(x)} \det\left(\frac{\partial f^p}{\partial x^q}\right)_{\varphi(x)} \times \omega_{j_1 j_2 \cdots j_k}(x)(\xi_{k+1}, \xi_{k+2}, \ldots, \xi_n),$$

i.e.,

$$\alpha_0^*\overline{\omega}_{i_1 i_2 \cdots i_k}(x) = \left(\frac{\partial g^{j_1}}{\partial \overline{x^i}_1}\right)_{\overline{\varphi}\alpha_0(x)} \left(\frac{\partial g^{j_2}}{\partial \overline{x^i}_2}\right)_{\overline{\varphi}\alpha_0(x)} \cdots \left(\frac{\partial g^{j_k}}{\partial \overline{x^i}_k}\right)_{\overline{\varphi}\alpha_0(x)} \det\left(\frac{\partial f^p}{\partial x^q}\right)_{\varphi(x)} \omega_{j_1 j_2 \cdots j_k}(x).$$

(3) Similarly,

$$(J^1\alpha)^*\overline{\omega}^\sigma(J^1_x\gamma) = \left(\frac{\partial F^\sigma}{\partial y^\nu}\right)_{\psi\gamma(x)} \omega^\nu(J^1_x\gamma).$$

(4) We now prove Theorem 5. To simplify our formulas, we sometimes write x, or $\gamma(x)$, instead of $J^1_x\gamma$. Let the Lagrangian λ be expressed over $\overline{V}$ by

$$\lambda = \overline{\mathcal{L}}\,\overline{\omega_0}.$$

Then over V,

$$(J_1\alpha)^*\lambda(J^1_x\gamma) = (\overline{\mathcal{L}} \circ J^1\alpha(J^1_x\gamma))\det\left(\frac{\partial f^p}{\partial x^q}\right)_{\varphi(x)} \omega_0(x).$$

We can express the form $\Phi_{J^1\alpha^*\lambda}$ over V. Taking into account the summand containing k exterior factors ω^σ, we have the form from formula (5),

$$\left(\frac{\partial^k(\overline{\mathcal{L}} \circ J^1\alpha \circ (\psi^1)^{-1})}{\partial y^{\sigma_1}_{j_1} \partial y^{\sigma_2}_{j_2} \cdots \partial y^{\sigma_k}_{j_k}}\right)_{\psi^1(J^1_x\gamma)} \det\left(\frac{\partial f^p}{\partial x^q}\right)_{\varphi(x)} \times \omega^{\sigma_1}(J^1_x\gamma) \wedge \omega^{\sigma_2}(J^1_x\gamma) \wedge \cdots \wedge \omega^{\sigma_k}(J^1_x\gamma) \wedge \omega_{j_1 j_2 \cdots j_k}(J^1_x\gamma). \quad (12)$$

But

$$\left(\frac{\partial(\overline{\mathcal{L}}\circ J^1\alpha\circ(\psi^1)^{-1})}{\partial y^{\sigma_1}_{j_1}}\right)_{\psi^1(J^1_x\gamma)} = \left(\frac{\partial\overline{\mathcal{L}}}{\partial\overline{y}^{\nu_1}_{p_1}}\right)_{\overline{\psi}^1J^1\alpha(J^1_x\gamma)}\left(\frac{\partial F^{\nu_1}}{\partial y^{\sigma_1}}\right)_{\psi\gamma(x)}\left(\frac{\partial g^{j_1}}{\partial\overline{x}^{p_1}}\right)_{\overline{\varphi}\alpha_0(x)},$$

and in the same way

$$\left(\frac{\partial^k(\overline{\mathcal{L}}\circ J^1\alpha\circ(\psi^1)^{-1})}{\partial y^{\sigma_1}_{j_1}\partial y^{\sigma_2}_{j_2}\cdots\partial y^{\sigma_k}_{j_k}}\right)_{\psi^1(J^1_x\gamma)} = \left(\frac{\partial^k\overline{\mathcal{L}}}{\partial\overline{y}^{\nu_1}_{p_1}\partial\overline{y}^{\nu_2}_{p_2}\cdots\partial\overline{y}^{\nu_k}_{p_k}}\right)_{\overline{\psi}^1J^1\alpha(J^1_x\gamma)}\left(\frac{\partial F^{\nu_1}}{\partial y^{\sigma_1}}\right)_{\psi\gamma(x)}\left(\frac{\partial g^{j_1}}{\partial\overline{x}^{p_1}}\right)_{\overline{\varphi}\alpha_0(x)}\left(\frac{\partial F^{\nu_2}}{\partial y^{\sigma_2}}\right)_{\psi\gamma(x)}$$
$$\times\left(\frac{\partial g^{j_2}}{\partial\overline{x}^{p_2}}\right)_{\overline{\varphi}\alpha_0(x)}\cdots\left(\frac{\partial F^{\nu_k}}{\partial y^{\sigma_k}}\right)_{\psi\gamma(x)}\left(\frac{\partial g^{j_k}}{\partial\overline{x}^{p_k}}\right)_{\overline{\varphi}\alpha_0(x)}.$$

Consequently, (12) gives the expression

$$\left(\frac{\partial^k\overline{\mathcal{L}}}{\partial\overline{y}^{\nu_1}_{p_1}\partial\overline{y}^{\nu_2}_{p_2}\cdots\partial\overline{y}^{\nu_k}_{p_k}}\right)_{\overline{\psi}^1J^1\alpha(J^1_x\gamma)}\left(\frac{\partial F^{\nu_1}}{\partial y^{\sigma_1}}\right)_{\psi\gamma(x)}\left(\frac{\partial g^{j_1}}{\partial\overline{x}^{p_1}}\right)_{\overline{\varphi}\alpha_0(x)}\left(\frac{\partial F^{\nu_2}}{\partial y^{\sigma_2}}\right)_{\psi\gamma(x)}\left(\frac{\partial g^{j_2}}{\partial\overline{x}^{p_2}}\right)_{\overline{\varphi}\alpha_0(x)}\cdots\left(\frac{\partial F^{\nu_k}}{\partial y^{\sigma_k}}\right)_{\psi\gamma(x)}$$
$$\times\left(\frac{\partial g^{j_k}}{\partial\overline{x}^{p_k}}\right)_{\overline{\varphi}\alpha_0(x)}\det\left(\frac{\partial f^p}{\partial x^q}\right)_{\varphi(x)}\omega^{\sigma_1}(J^1_x\gamma)\wedge\omega^{\sigma_2}(J^1_x\gamma)\wedge\cdots\wedge\omega^{\sigma_k}(J^1_x\gamma)\wedge\omega_{j_1j_2\cdots j_k}(J^1_x\gamma). \tag{13}$$

On the other hand, consider in Φ_λ the summand

$$\frac{\partial^k\overline{\mathcal{L}}}{\partial\overline{y}^{\sigma_1}_{j_1}\partial\overline{y}^{\sigma_2}_{j_2}\cdots\partial\overline{y}^{\sigma_k}_{j_k}}\overline{\omega}^{\sigma_1}\wedge\overline{\omega}^{\sigma_2}\wedge\cdots\wedge\overline{\omega}^{\sigma_k}\wedge\overline{\omega}_{j_1j_2\cdots j_k} \tag{14}$$

over $\overline{V}$. Computing the pull-back $J^1\alpha^*\Phi_\lambda$, and in particular, the pull-back of the differential form (14), we obtain

$$\left(\frac{\partial^k\overline{\mathcal{L}}}{\partial\overline{y}^{\sigma_1}_{j_1}\partial\overline{y}^{\sigma_2}_{j_2}\cdots\partial\overline{y}^{\sigma_k}_{j_k}}\right)_{\overline{\psi}^1J^1\alpha(J^1_x\gamma)}\left(\frac{\partial F^{\sigma_1}}{\partial y^{\nu_1}}\right)_{\psi\gamma(x)}\left(\frac{\partial F^{\sigma_2}}{\partial y^{\nu_2}}\right)_{\psi\gamma(x)}\cdots\left(\frac{\partial F^{\sigma_k}}{\partial y^{\nu_k}}\right)_{\psi\gamma(x)}\left(\frac{\partial g^{l_1}}{\partial\overline{x}^{l_1}}\right)_{\overline{\varphi}\alpha_0(x)}$$
$$\times\left(\frac{\partial g^{l_2}}{\partial\overline{x}^{l_2}}\right)_{\overline{\varphi}\alpha_0(x)}\cdots\left(\frac{\partial g^{l_k}}{\partial\overline{x}^{l_k}}\right)_{\overline{\varphi}\alpha_0(x)}\det\left(\frac{\partial f^p}{\partial x^q}\right)_{\varphi(x)}\omega^{\nu_1}(J^1_x\gamma)\wedge\omega^{\nu_2}(J^1_x\gamma)$$
$$\wedge\cdots\wedge\omega^{\nu_k}(J^1_x\gamma)\wedge\omega_{l_1l_2\cdots l_k}(J^1_x\gamma). \tag{15}$$

Since (13) and (15) agree, we are done.

Corollary 1: For every π-projectable vector field ξ, the fundamental Lepage form Φ_λ satisfies

$$\partial_{J^1\xi}\Phi_\lambda = \Phi_{\partial_{J^1\xi}\lambda}.$$

Corollary 2: The Poincaré–Cartan form Θ_λ satisfies

$$J^1\alpha^*\Theta_\lambda = \Theta_{J^1\alpha^*\lambda} \tag{16}$$

and

$$\partial_{J^1\xi}\Theta_\lambda = \Theta_{\partial_{J^1\xi}\lambda}. \tag{17}$$

Proof: From the properties of contact forms it follows that the forms of the same order of contactness on the left- and right-hand side of formula (11) agree. Formula (16) means just the equality of forms of order of contactness $\leqslant 1$.

From Theorem 5 we can easily derive, for Lagrangians of order 1, formula (10) of Sec. II I

Corollary 3: The Euler–Lagrange form E_λ satisfies

$$\partial_{J^2\xi} E_\lambda = E_{\partial_{J^1\xi}\lambda}. \tag{18}$$

Proof: From Theorem 5 it follows that

$$\partial_{J^2\xi} p_1\, \mathrm{d}\Phi_\lambda = p_1 \partial_{J^1\xi}\, \mathrm{d}\Phi_\lambda = p_1\, \mathrm{d}\Phi_{\partial_{J^1\xi}\lambda},$$

which is exactly formula (18).

We are now in the position to study symmetries of the first order Lagrange structures. According to the definition used by Prieto,[24] an *infinitesimal symmetry* of a first order Lagrangian λ is a vector field Ξ on J^1Y such that $\partial_\Xi \Theta_\lambda = -\mathrm{d}\eta$ for some $(n-1)$-form η. Clearly, if Ξ is an infinitesimal symmetry, then $\mathrm{d}\partial_\Xi \Theta_\lambda = 0$, and the converse holds locally. In the following theorem we consider infinitesimal symmetries of the form $\Xi = J^1\xi$, where ξ is a π-projectable vector field, and compare them with generators of invariant transformations of the Euler–Lagrange form.

Theorem 6: Let λ *be a first order Lagrangian, and let* ξ *be a* π*-projectable vector field.*

(a) ξ *is the generator of invariant transformations of the Euler–Lagrange form* E_λ *if and only if* $\partial_{J^1\xi}\, \mathrm{d}\Phi_\lambda = 0$.

(b) *If* $\Xi = J^1\xi$ *is an infinitesimal symmetry, then* ξ *generates invariant transformations of* E_λ.

Proof: (a) Suppose that $\partial_{J^2\xi} E_\lambda = 0$. Then from Corollary 3, $E_{\partial_{J^1\xi}\lambda} = 0$, hence $\mathrm{d}\Phi_{\partial_{J^1\xi}\lambda} = 0$ and according to Theorem 5, $\partial_{J^1\xi}\, \mathrm{d}\Phi_\lambda = 0$. The converse is proved by reversing the arguments.

(b) Supposing that $\mathrm{d}\partial_{J^1\xi}\, \mathrm{d}\Theta_\lambda = 0$ we obtain $\mathrm{d}\Theta_{\partial_{J^1\xi}\lambda} = 0$ (Corollary 2) and by definition,

$$p_1\, \mathrm{d}\Theta_{\partial_{J^1\xi}\lambda} = E_{\partial_{J^1\xi}\lambda} = \partial_{J^2\xi} E_\lambda = 0.$$

Remark 1: In Theorem 6, we give some properties of generators of invariant transformations of the Euler–Lagrange form on one side, and infinitesimal symmetries on the other side. Note that for several reasons, the definition of infinitesimal symmetry in its full generality does not seem well motivated. First, variations, induced by general vector fields on J^1Y do not transform sections of the fibered manifold Y into sections of Y; in particular, such variations do not transform solutions of the Euler–Lagrange equations into solutions. Second, according to Theorem 6, infinitesimal symmetries do not include all generators of invariant transformations of the Euler–Lagrange form. The third reason consists in impossibility to generalize the definition of an infinitesimal symmetry to rth order Lagrange structures, because for Lagrangians of order $r \geqslant 3$ we do not have a global analogue of the Poincaré–Cartan form. For these reasons, we prefer, in the theory of local variational principles presented below, the concept of a generator of invariant transformations of the Euler–Lagrange form.

Remark 2: It is not known whether there exists a generalization of the fundamental Lepage form Φ_λ to higher order Lagrange structures.

IV. LOCAL VARIATIONAL PRINCIPLES

A. Local variational principles

Let $\varepsilon \in \Omega^s_{n+1,Y} Y$ be a locally variational form (ε is supposed to be defined globally). According to Sec. II H, the fibered manifold Y can be covered by open sets V_ι, $\iota \in I$, such that to every ι, there exists a Lagrangian λ_ι over V_ι for the form $\varepsilon|_{V_\iota}$; over the intersections $V_\iota \cap V_\kappa$, the Lagrangians λ_ι and λ_κ differ by a trivial Lagrangian. In general, a globally defined Lagrangian for ε need not exist.

In our definition of a local variational principle, we rephrase these properties of locally variational forms in terms of the Lepage forms. We say that a family $\{(V_\iota, \rho_\iota)\}_{\iota \in I}$, in which $\{V_\iota\}_{\iota \in I}$ is an open covering of Y and for every $\iota \in I$, $\rho_\iota \in \Omega^s_n V_\iota$ is a Lepage form, is said to be a *local variational principle*, if for every $\iota, \kappa \in I$,

$$p_1\, \mathrm{d}\rho_\iota = p_1\, \mathrm{d}\rho_\kappa$$

over $V_\iota \cap V_\kappa$. The integer s is called the *order* of the local variational principle $\{(V_\iota, \rho_\iota)\}_{\iota \in I}$.

Suppose that we have a local variational principle $\{(V_\iota, \rho_\iota)\}_{\iota\in I}$ of order s. For every $\iota \in I$, we denote

$$E_\iota = p_1\, \mathrm{d}\rho_\iota.$$

E_ι is the Euler–Lagrange form of the *associated Lagrangian* $\lambda_\iota = h\rho_\iota$, defined over V_ι. Since by definition, $E_\iota = E_\kappa$ for all $\iota, \kappa \in I$, setting

$$E = E_\iota$$

over V_ι, we obtain a global differential form E on $J^{s+1}Y$. This form is called the *Euler–Lagrange form*, associated with the local variational principle $\{(V_\iota, \rho_\iota)\}_{\iota\in I}$. Obviously, the Euler–Lagrange form is dynamical, locally variational form; it is not necessarily (globally) variational.

A local variational principle in another geometric context (i.e., on manifolds without fibration) was formulated by Dedecker.[5] Our definition is close to the Dedecker's approach.

Two local variational principles $\{(V_\iota, \rho_\iota)\}_{\iota\in I}$, $\{(V'_\kappa, \rho'_\kappa)\}_{\kappa\in K}$ are *equivalent*, if the associated Euler–Lagrange forms E, E' coincide, i.e., $E = E'$.

Theorem 7: *A family* $\{(V_\iota, \rho_\iota)\}_{\iota\in I}$, *in which* $\{V_\iota\}_{\iota\in I}$ *is an open covering of* Y *and for every* $\iota \in I$, $\rho_\iota \in \Omega^s_n V_\iota$ *is a Lepage form, is a local variational principle if and only if to every* $\iota, \kappa \in I$, *there exists a form* $\eta_{\iota\kappa} \in \Omega^r_{n-1}(V_\iota \cap V_\kappa)$ *and a contact form* $\chi_{\iota\kappa} \in \Omega^r_n(V_\iota \cap V_\kappa)$ *such that over* $V_\iota \cap V_\kappa$,

$$\rho_\iota - \rho_\kappa = \mathrm{d}\eta_{\iota\kappa} + \chi_{\iota\kappa}. \tag{19}$$

Proof: If $\rho_\iota - \rho_\kappa = \mathrm{d}\eta_{\iota\kappa} + \chi_{\iota\kappa}$, for some $\eta_{\iota\kappa}$ and $\chi_{\iota\kappa}$, then $\mathrm{d}(\rho_\iota - \rho_\kappa) = \mathrm{d}\chi_{\iota\kappa}$. This means that the class of $\chi_{\iota\kappa}$ is a contact Lepage form. Since $p_1\, \mathrm{d}\chi_{\iota\kappa}$ depends on the corresponding Lagrangian only, that is, on $h\chi_{\iota\kappa}$ (see Sec. II C), and this Lagrangian is zero, we have $p_1\, \mathrm{d}\chi_{\iota\kappa} = 0$. Consequently, $p_1\, \mathrm{d}\rho_\iota = p_1\, \mathrm{d}\rho_\kappa$. Conversely, if $p_1\, \mathrm{d}\rho_\iota = p_1\, \mathrm{d}\rho_\kappa$, then the Euler–Lagrange form $E_{h(\rho_\iota - \rho_\kappa)}$ vanishes. This means that the Lagrangian $h(\rho_\iota - \rho_\kappa)$ is trivial, which implies (19).

B. First variation formula, extremals

A basic tool for an analysis of extremals and invariant transformations of a variational functional is the first variation formula. We now give a formulation of the first variation formula for local variational principles.

Let $\{(V_\iota, \rho_\iota)\}_{\iota\in I}$ be a local variational principle of order s. Fix an index $\iota \in I$, and choose a piece $\Omega \subset \pi(V_\iota)$. Then we have the variational functional

$$\Gamma_{\Omega, V_\iota}(\pi) \ni \gamma \to \rho_{\iota,\Omega}(\gamma) = \int_\Omega J^s\gamma^* \rho_\iota \in \mathbb{R}.$$

For any π-projectable vector field ξ on Y, we have the *first variation formula*

$$\partial_{J^s\xi}\rho_\iota = i_{J^s\xi}\, \mathrm{d}\rho_\iota + \mathrm{d}i_{J^s\xi}\rho_\iota.$$

This formula can easily be written by means of the associated Lagrangian $\lambda_\iota = h\rho_\iota$. Since $\partial_{J^{s+1}\xi} h\rho_\iota = h\partial_{J^s\xi}\rho_\iota = hi_{J^s\xi}\, \mathrm{d}\rho_\iota + h\, \mathrm{d}i_{J^s\xi}\rho_\iota$, we have

$$\partial_{J^{s+1}\xi} h\rho_\iota = hi_{J^{s+1}\xi} p\, \mathrm{d}\rho_\iota + h\, \mathrm{d}i_{J^s\xi}\rho_\iota = hi_{J^{s+1}\xi} E + h\, \mathrm{d}i_{J^s\xi}\rho_\iota$$

and

$$\partial_{J^{s+1}\xi}\lambda_\iota = hi_{J^{s+1}\xi} E + h\mathrm{d}i_{J^s\xi}\rho_\iota,$$

where E is the Euler–Lagrange form of $\{(V_\iota, \rho_\iota)\}_{\iota\in I}$. This is another formulation of the first variation formula for the local variational principle $\{(V_\iota, \rho_\iota)\}_{\iota\in I}$.

We have the following simple observation.

Theorem 8: *Let* $\{(V_\iota, \rho_\iota)\}_{\iota\in I}$ *be a local variational principle of order* s. *Let* γ *be a section of*

Y. The following conditions are equivalent:

(a) *For every* $\iota \in I$, $\gamma_\iota = \gamma|_{\pi(V_\iota)}$ *is an extremal of the variational functional* $\rho_{\iota,\Omega}$.
(b) *For every* π*-projectable vector field* ξ, γ *satisfies*

$$J^{s+1}\gamma^* i_{J^{s+1}\xi} E = 0.$$

A section γ, satisfying any of these two equivalent conditions, is called an *extremal* of the local variational principle $\{(V_\iota, \rho_\iota)\}_{\iota \in I}$.

C. Invariant transformations

It is straightforward to extend the theory of invariant transformations as introduced in Sec. II I, to *local variational principles*. The concept of a Lagrangian in this case is defined only locally, but we still have the notions of invariance of the Euler–Lagrange form.

Suppose that we have a local variational principle $\{(V_\iota, \rho_\iota)\}_{\iota \in I}$ of order s, and denote by E its Euler–Lagrange form. Let $\alpha: W \to Y$ be an automorphism of Y. We say that α is an *invariant transformation* of E, if

$$J^{s+1}\alpha^* E = E.$$

A π-projectable vector field ξ on Y is said to be the *generator of invariant transformations* of E, if

$$\partial_{J^{s+1}\xi} E = 0.$$

The following is straightforward.

Theorem 9: *Let* $\{(V_\iota, \rho_\iota)\}_{\iota \in I}$ *be a local variational principle, and let* ξ *be a* π*-projectable vector field. Let E be the Euler–Lagrange form of* $\{(V_\iota, \rho_\iota)\}_{\iota \in I}$. *The following conditions are equivalent:*

(a) ξ *is a generator of invariant transformations of E.*
(b) *There exists a family* $\{\eta_\iota\}_{\iota \in I}$ *of* $(n-1)$*-forms* $\eta_\iota \in \Omega^s_{n-1} V_\iota$ *such that for every* $\iota \in I$,

$$h i_{J^{s+1}\xi} E + h\mathrm{d}(i_{J^s\xi}\rho_\iota - \eta_\iota) = 0. \tag{20}$$

Proof: Let ξ be a generator of invariant transformations of E, let $\iota \in I$. Over V_ι, $E = E_{\lambda_\iota}$, where $\lambda_\iota = h\rho_\iota$, and $\partial_{J^{s+1}\xi} E = E_{\partial_{J^{s+1}\xi}\lambda_\iota} = 0$, hence by Theorem 3, $\partial_{J^{s+1}\xi}\lambda_\iota = h\,\mathrm{d}\,\eta_\iota$ for some $(n-1)$-form η_ι over V_ι. Then

$$\partial_{J^{s+1}\xi}\lambda_\iota = h i_{J^{s+1}\xi} E + h\,\mathrm{d} i_{J^s\xi}\rho_\iota = h\,\mathrm{d}\,\eta_\iota,$$

proving (20).

Consider the Euler–Lagrange form E of the local variational principle $\{(V_\iota, \rho_\iota)\}_{\iota \in I}$, and a vector field ξ on Y. Let (V, ψ), $\psi = (x^i, y^\sigma)$, be a fibered chart on Y such that $V \subset V_\iota$. Suppose that over V,

$$h\rho_\iota = \mathcal{L}_\iota \omega_0$$

and

$$\xi = \xi_0^k \frac{\partial}{\partial x^k} + \xi^\sigma \frac{\partial}{\partial y^\sigma}.$$

Then over V,

$$E = E_\sigma(\mathcal{L}_\iota)\omega^\sigma \wedge \omega_0,$$

where

$$E_\sigma(\mathcal{L}_\iota) = \sum_{k=0}^{r} (-1)^k d_{i_1} d_{i_2} \cdots d_{i_k} \frac{\partial \mathcal{L}_\iota}{\partial y^\sigma_{i_1 i_2 \cdots i_k}}$$

and

$$hi_{J^{s+1}\xi} E = E_\sigma(\mathcal{L}_\iota)(\xi^\sigma - y^\sigma_k \xi^k_0)\omega_0. \tag{21}$$

Formula (21) shows that the Euler–Lagrange equations for extremals are, over V,

$$E_\sigma(\mathcal{L}_\iota) = 0. \tag{22}$$

Thus, if ξ generates invariant transformations of E, we have a *conservation law*

$$\mathrm{d}(i_{J^s\xi}\rho_\iota - \eta_\iota) = 0 \tag{23}$$

(along any extremal). The arising equation (23) should be considered together with Eq. (22).

The set of generators of invariant transformations of the Euler–Lagrange form is a Lie algebra. Indeed, if two π-projectable fields ξ and ζ, satisfy

$$\partial_{J^s\xi} E = 0, \quad \partial_{J^s\zeta} E = 0,$$

then since $J^s[\xi,\zeta]=[J^s\xi, J^s\zeta]$, we have

$$\partial_{J^s[\xi,\zeta]} E = \partial_{J^s\xi}\partial_{J^s\zeta} E - \partial_{J^s\zeta}\partial_{J^s\xi} E = 0.$$

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Group classification of nonlinear wave equations

V. Lahno[a)]
State Pedagogical University, 36000 Poltava, Ukraine

R. Zhdanov[b)]
Institute of Mathematics of NAS of Ukraine, 01601 Kyiv, Ukraine

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We perform complete group classification of the general class of quasilinear wave equations in two variables. This class may be seen as a generalization of the nonlinear d'Alembert, Liouville, sin/sinh-Gordon and Tzitzeica equations. We derive a number of new genuinely nonlinear invariant models with high symmetry properties. In particular, we obtain four classes of nonlinear wave equations that admit five-dimensional invariance groups. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1884886]

INTRODUCTION

More than a century ago Lie introduced the concept of continuous transformation group into mathematical physics and mechanics. His initial motivation was to develop a theory of integration of ordinary differential equations enabling to answer the basic questions, like, why some equations are integrable and others are not. His fundamental results obtained on this way, can be seen as a far reaching generalization of the Galois's and Abel's theory of solubility of algebraic equations by radicals. Since that time the Lie's theory of continuous transformation groups has become applicable to an astonishingly wide range of mathematical and physical problems.

It was Lie who was the first to utilize group properties of differential equations for constructing of their exact solutions. In particular, he computed the maximal invariance group of the one-dimensional heat conductivity equation and applied this symmetry to construct its explicit solutions. Saying it the modern way, he performed symmetry reduction of the heat equation. Since late 1970s symmetry reduction becomes one of the most popular tools for solving nonlinear partial differential equations (PDEs).

By now symmetry properties of the majority of fundamental equations of mathematical and theoretical physics are well known. It turns out that for the most part these equations admit wide symmetry groups. Especially this is the case for linear PDEs and it is this rich symmetry that enables developing a variety of efficient methods for mathematical analysis of linear differential equations. However, linear equations give mathematical description of physical, chemical or biological processes in a first approximation only. To provide a more detailed and precise description a mathematical model must incorporate nonlinear terms. Note that some important differential equations are intrinsically nonlinear and have no linear counterpart.

Hyperbolic type second-order nonlinear PDEs in two independent variables play a fundamental role in modern mathematical physics. Equations of this type are utilized to describe various types of wave propagation. They are used in differential geometry, in various fields of hydrodynamics and gas dynamics, chemical technology, superconductivity, crystal dislocation to mention only a few applications areas. Surprisingly the list of equations utilized is rather narrow. In fact, it is comprised by the Liouville, sine/sinh-Gordon, Goursat, d'Alembert, and Tzitzeica equations and a couple of others. Popularity of these very models has a natural group-theoretical interpretation, namely, all of them have nontrivial Lie or Lie–Bäcklund symmetry. By this very reason some of them are integrable by the inverse problem methods (see, e.g., Refs. 1–3) or linearizable[4–6] and completely integrable.[7,8]

Knowing symmetry group of the equation under study provides us with the powerful equation exploration tool. So it is natural to attempt classifying a reasonably extensive class of nonlinear hyperbolic type PDEs into subclasses of equations enjoying the best symmetry properties. Saying reasonably extensive we mean that (i) this class should contain the above enumerated equations as particular cases, and (ii) it should contain a variety of new invariant models of potential interest for applications. The list of the so obtained invariant equations will contain candidates for realistic nonlinear mathematical models of the physical and chemical processes mentioned above.

The history of group classification methods goes back to Lie itself. Probably, the very first paper on this subject is Ref. 9, where Lie proves that a linear two-dimensional second-order PDE may admit at most a three-parameter invariance group (apart from the trivial infinite-parameter symmetry group, which is due to linearity).

The modern formulation of the problem of group classification of PDEs was suggested by Ovsyannikov in Ref. 10. He developed a regular method (we will refer to it as the Lie–Ovsyannikov method) for classifying differential equations with nontrivial symmetry and performed complete group classification of the nonlinear heat conductivity equation. In a number of subsequent publications more general types of nonlinear heat equations were classified (review of these results can be found in Ref. 11).

However, even a very quick analysis of the papers on group classification of PDEs reveals that an overwhelming majority of them deals with equations whose arbitrary elements (functions) depend on one variable only. The reason for this is that Lie–Ovsyannikov method becomes inefficient for PDEs containing arbitrary functions of several variables. To achieve a complete classification one either needs to specify the transformation group realization or restrict somehow an arbitrariness of the functions contained in the equation under study. We have recently, developed an efficient approach enabling to overcome this difficulty for low dimensional PDEs.[12,13] Utilizing it we have derived the complete group classification of the general quasilinear heat conductivity equation in two independent variables. In this paper we apply the approach in question to perform group classification of the most general quasilinear hyperbolic PDE in two independent variables.

I. GROUP CLASSIFICATION ALGORITHM

While classifying a given class of differential equations into subclasses, one can use different classifying features, like linearity, order, the number of independent or dependent variables, etc. In group analysis of differential equations the principal classifying features are symmetry properties of equations under study. This means that classification objects are equations considered together with their symmetry groups. This point of view is based on the well-known fact that any PDE admits a (possibly trivial) Lie transformation group. And what is more, any transformation group corresponds to a class of PDEs, which are invariant under this group. So the problem of group classification of a class of PDEs reduces to describing all possible (inequivalent) pairs (PDE, maximal invariance group), where PDE should belong to the class of equations under consideration.

We perform group classification of the following class of quasilinear wave equations:

$$u_{tt} = u_{xx} + F(t,x,u,u_x). \tag{1.1}$$

Here F is an arbitrary smooth function, $u=u(t,x)$. Hereafter we adopt notations $u_t=\partial u/\partial t$, $u_x=\partial_u/\partial_x$, $u_{tt}=\partial^2 u/\partial t^2$, etc.

Our aim is describing *all* equations of the form (1.1) that admit nontrivial symmetry groups. The challenge of this task is in the word *all*. If, for example, we somehow constrain the form of invariance group to be found, then the classification problem simplifies enormously. A slightly more cumbersome (but still tractable with the standard Lie–Ovsyannikov approach) is the problem of group classification of equation with arbitrary functions of, at most, one variable.

As equations invariant under similar Lie groups are identical within the group-theoretic framework, it makes sense to consider nonsimilar transformation groups[14,15] only. The important example of similar Lie groups is provided by Lie transformation groups obtained one from another

by a suitable change of variables. Consequently, equations obtained one from another by a change of variables have similar symmetry groups and cannot be distinguished within the group-theoretical viewpoint. That is why, we perform group classification of (1.1) within a change of variables preserving the class of PDEs (1.1).

The problem of group classification of linear hyperbolic type equation

$$u_{tx} + A(t,x)u_t + B(t,x)u_x + C(t,x)u = 0 \tag{1.2}$$

with $u = u(t,x)$, was solved by Lie[9] (see, also, Ref. 16). In view of this fact, we consider only those equations of the form (1.1) which are not (locally) equivalent to the linear equation (1.2).

As we have already mentioned in the Introduction, the Lie–Ovsyannikov method of group classification of differential equations has been suggested in Ref. 10. Utilizing this method enabled solving the group classification problem for a number of important one-dimensional nonlinear wave equations:

$$u_{tt} = u_{xx} + F(u) \quad \text{(Refs. 17–19)},$$

$$u_{tt} = [f(u)u_x]_x \quad \text{(Refs. 20–22)},$$

$$u_{tt} = f(u_x)u_{xx} \quad \text{(Refs. 22,23)},$$

$$u_{tt} = F(u_x)u_{xx} + H(u_x) \quad \text{(Ref. 24)},$$

$$u_{tt} = F(u_{xx}) \quad \text{(Ref. 22)},$$

$$u_{tt} = u_x^m u_{xx} + f(u) \quad \text{(Ref. 25)},$$

$$u_{tt} + f(u)u_t = (g(u)u_x)_x + h(u)u_x \quad \text{(Ref. 26)},$$

$$u_{tt} = (f(x,u)u_x)_x \quad \text{(Ref. 27)}.$$

Analysis of the above list shows that most of all arbitrary elements (=arbitrary functions) depend on one variable. This is not coincidental. As we already mentioned, the Lie–Ovsyannikov approach works smoothly for the case when the arbitrary elements are functions of one variable. The reason for this is that the obtained system of determining equations is still over-determined. So it can be effectively solved within the same techniques used to compute maximal symmetry group of PDEs containing no arbitrary elements.

The situation becomes much more complicated for the case when arbitrary elements are functions of two (or more) arguments. By this very reason the group classification of nonlinear wave equations,

$$u_{tt} + \lambda u_{xx} = g(u,u_x) \quad \text{(Refs. 28,29)},$$

$$u_{tt} = [f(u)u_x + g(x,u)]_x \quad \text{(Ref. 30)},$$

$$u_{tt} = f(x,u_x)u_{xx} + g(x,u_x) \quad \text{(Ref. 31)},$$

is not complete.

We suggest an efficient approach to the problem of group classification of low dimensional PDEs in Refs. 12 and 13. This approach is based on the Lie–Ovsyannikov infinitesimal method

and classification results for abstract finite-dimensional Lie algebras. It enables us to obtain the complete solution of the group classification problem for the general heat equation with a nonlinear source

$$u_t = u_{xx} + F(t,x,u,u_x).$$

Later on, we perform complete group classification of the most general quasilinear evolution equation,[32–34]

$$u_t = f(t,x,u,u_x)u_{xx} + g(t,x,u,u_x).$$

We utilize the above approach to obtain complete solution of the group classification problem for the class of Eqs. (1.1).

Our algorithm of group classification of the class of PDEs (1.1) is implemented in the following three steps (further details can be found in Ref. 34):

(I) Using the infinitesimal Lie method we derive the system of determining equations for coefficients of the first-order operator that generates symmetry group of equation (1.1). (Note that the determining equations which explicitly depend on the function F and its derivatives are called classifying equations.) Integrating equations that do not depend on F we obtain the form of the most general infinitesimal operator admitted by Eq. (1.1) under arbitrary F. Another task of this step is calculating the equivalence group $\mathcal{E}$ of the class of PDEs (1.1).

(II) We construct all realizations of Lie algebras A_n of the dimension $n \leqslant 3$ in the class of operators obtained at the first step within the equivalence relation defined by transformations from the equivalence group $\mathcal{E}$. Inserting the so obtained operators into classifying equations we select those realizations that can be symmetry algebras of a differential equation of the form (1.1).

(III) We compute all possible extensions of realizations constructed at the previous step to realizations of higher dimensional ($n > 3$) Lie algebras. Since extending symmetry algebras results in reducing arbitrariness of the function F, at some point this function will contain either arbitrary functions of at most one variable or arbitrary constants. At this point, we apply the standard classification method (which is due to Lie and Ovsyannikov) to derive the maximal symmetry group of the equation under study. This completes group classification of (1.1).

Performing the above enumerated steps yields the complete list of inequivalent equations of the form (1.1) together with their maximal (in Lie's sense) symmetry algebras.

We say that the group classification problem is completely solved when it is proved that

(1) the constructed symmetry algebras are maximal invariance algebras of the equations under consideration;

(2) the list of invariant equations contains only inequivalent ones, namely, no equation can be transformed into another one from the list by a transformation from the equivalence group $\mathcal{E}$.

II. PRELIMINARY GROUP CLASSIFICATION OF Eq. (1.1)

We look for the infinitesimal operator of symmetry group of equation (1.1) in the form

$$Q = \tau(t,x,u)\partial_t + \xi(t,x,u)\partial_x + \eta(t,x,u)\partial_u, \tag{2.1}$$

where τ, ξ, η are smooth functions defined on an open domain Ω of the space $V = \mathbb{R}^2 \times \mathbb{R}^1$ of independent $\mathbb{R}^2 = \langle t,x \rangle$ and dependent $\mathbb{R}^1 = \langle u \rangle = u(t,x)$ variables.

Operator (2.1) generates one-parameter invariance group of (1.1) iff its coefficients τ, ξ, η, ϵ satisfy the equation (Lie's invariance criterion)

$$\varphi^{tt} - \varphi^{xx} - \tau F_t - \xi F_x - \eta F_u - \varphi^x F_{u_x}\big|_{(1.1)} = 0, \tag{2.2}$$

where

$$\varphi^t = D_t(\eta) - u_t D_t(\tau) - u_x D_t(\xi),$$

$$\varphi^x = D_x(\eta) - u_t D_x(\tau) - u_x D_x(\xi),$$

$$\varphi^{tt} = D_t(\varphi^t) - u_{tt} D_t(\tau) - u_{tx} D_t(\xi),$$

$$\varphi^{xx} = D_x(\varphi^x) - u_{tx} D_x(\tau) - u_{xx} D_x(\xi),$$

and D_t, D_x are operators of total differentiation with respect to the variables t, x. As customary, by writing (1.1) we mean that one needs to replace u_{tt} and its differential consequences with the expression $u_{xx}+F$ and its differential consequences in (2.2).

After a simple transformations algebra we reduce (2.2) to the form

$$\begin{aligned}
&(1) \quad \xi_u = \tau_u = \eta_{uu} = 0,\\
&(2) \quad \tau_t - \xi_x = 0, \quad \xi_t - \tau_x = 0,\\
&(3) \quad 2\eta_{tu} + \tau_x F_{u_x} = 0,\\
&(4) \quad \eta_{tt} - \eta_{xx} - 2u_x \eta_{xu} + [\eta_u - 2\tau_t]\\
&\qquad \times F - \tau F_t - \xi F_x - \eta F_u - [\eta_x + u_x(\eta_u - \xi_x)]F_{u_x} = 0.
\end{aligned} \tag{2.3}$$

The first two groups of PDEs from (2.3) are to be used to derive the form of the most general infinitesimal operator admitted by (1.1). The remaining PDEs are classifying equations.

We prove in Ref. 35 that the following assertion holds.

Theorem 1: *Provided* $F_{u_x u_x} \neq 0$, *the maximal invariance group of equation (1.1) is generated by the following infinitesimal operator:*

$$Q = (\lambda t + \lambda_1)\partial_t + (\lambda x + \lambda_2)\partial_x + [h(x)u + r(t,x)]\partial_u, \tag{2.4}$$

where λ, λ_1, λ_2 *are real constants and* $h=h(x)$, $r=r(t,x)$, $F=F(t,x,u,u_x)$ *are functions obeying the constraint*

$$\begin{aligned}
&r_{tt} - r_{xx} - \frac{\mathrm{d}^2 h}{\mathrm{d}x^2}u - 2\frac{\mathrm{d}h}{\mathrm{d}x}u_x + (h - 2\lambda)F - (\lambda t + \lambda_1)F_t - (\lambda x + \lambda_2)F_x - (hu + r)F_u\\
&\quad - \left(r_x + \frac{\mathrm{d}h}{\mathrm{d}x}u + (h - \lambda)u_x\right)F_{u_x} = 0.
\end{aligned} \tag{2.5}$$

If $F=g(t,x,u)u_x+f(t,x,u)$, $g_u \neq 0$, *then the maximal invariance group of equation (1.1) is generated by infinitesimal operator (2.4), where* λ, λ_1, λ_2 *are real constants* h, r, g, f *are functions satisfying system of two equations*

$$\begin{aligned}
&-2h' - \lambda g = (\lambda t + \lambda_1)g_t + (\lambda x + \lambda_2)g_x + (hu + r)g_u,\\
&-h''u + r_{tt} - r_{xx} + (h - 2\lambda)f = (\lambda t + \lambda_1)f_t + (\lambda x + \lambda_2)f_x + (hu + r)f_u + g(h'u + r_x).
\end{aligned} \tag{2.6}$$

Next, if $F=g(t,x)u_x+f(t,x,u)$, $q \not\equiv 0$, $f_{uu} \neq 0$, *then the infinitesimal operator of the invariance group of equation (1.1) reads as*

$$Q = \tau(t,x)\partial_t + \xi(t,x)\partial_x + (h(t,x)u + r(t,x))\partial_u,$$

where τ, ξ, h, r, g, f are functions satisfying system of PDEs

$$\tau_t - \xi_x = 0, \quad \xi_t - \tau_x = 0,$$

$$2h_t = -\tau_x g, \quad 2h_x = -\tau_t g - \tau g_t - \xi g_x,$$

$$(h_{tt} - h_{xx})u + r_{tt} - r_{xx} + f(h - 2\tau_t) - \tau f_t - \xi f_x - (hu + r)f_u - (h_x u + r_x)g = 0.$$

Finally, if $F = f(t,x,u)$, $f_{uu} \neq 0$, then the maximal invariance group of equation (1.1) is generated by infinitesimal operator

$$Q = [\varphi(\theta) + \psi(\sigma)]\partial_t - [\varphi(\theta) - \psi(\sigma)]\partial_x + [ku + r(t,x)]\partial_u,$$

where $k \in \mathbb{R}$, $\theta = t - x$, $\sigma = t + x$ and functions φ, ψ, r, f and constant k satisfy the following equation:

$$r_{tt} - r_{xx} + [k - 2\varphi' - 2\psi']f - (\varphi + \psi)f_t + (\varphi - \psi)f_x - (ku + r)f_u = 0, \quad \varphi' = \frac{d\varphi}{d\theta}, \quad \psi' = \frac{d\psi}{d\theta}.$$

By virtue of the above theorem the problem of group classification of equation (1.1) reduces to the one of classifying equations of more specific forms,

$$u_{tt} = u_{xx} + F(t,x,u,u_x), \quad F_{u_x u_x} \neq 0, \tag{2.7}$$

$$u_{tt} = u_{xx} + g(t,x,u)u_x + f(t,x,u), \quad g_u \neq 0, \tag{2.8}$$

$$u_{tx} = g(t,x)u_x + f(t,x,u), \quad g_x \neq 0, \quad f_{uu} \neq 0, \tag{2.9}$$

$$u_{tx} = f(t,x,u), \quad f_{uu} \neq 0. \tag{2.10}$$

Note that condition $g_x \neq 0$ is essential, since otherwise (2.9) is locally equivalent (2.10).

Summing up, we conclude that the problem of group classification of (1.1) reduces to classifying more specific classes of PDEs (2.7)–(2.10).

First, we consider equations (2.8)–(2.10).

III. GROUP CLASSIFICATION OF EQ. (2.8)

According to Theorem 1 invariance group of equation (2.8) is generated by infinitesimal operator (2.4). And what is more, the real constants λ, λ_1, λ_2 and functions h, r, g, f satisfy equations (2.6). System (2.6) is to be used to specify both the form of functions f, g from (2.8) and functions h, r and constants λ, λ_1, λ_2 in (2.4). It is called the determining (sometimes classifying) equations.

Efficiency of the Lie method for calculation of maximal invariance group of PDE is essentially based on the fact that routinely system of determining equations is over-determined. This is clearly not the case, since we have only one equation for four (!) arbitrary functions and three of the latter depend on two variables. By this very reason direct application of Lie approach in the Ovsyannikov's spirit is no longer efficient when we attempt classifying PDEs with arbitrary functions of several variables.

Compute the equivalence group E of equation (2.8). This group is generated by invertible transformations of the space V preserving the differential structure of equation (2.8) (see, e.g., Ref. 14). Saying it another way, group transformation from $\mathcal{E}$

$$\overline{t} = \alpha(t,x,u), \quad \overline{x} = \beta(t,x,u), \quad v = U(t,x,u), \quad \frac{D(\overline{t},\overline{x},v)}{D(t,x,u)} \neq 0,$$

should reduce (2.8) to equation of the same form

$$v_{\overline{t}\overline{t}} = v_{\overline{x}\overline{x}} + \tilde{g}(\overline{t},\overline{x},v)v_{\overline{x}} + \tilde{f}(\overline{t},\overline{x},v), \quad \tilde{g}_v \neq 0$$

with possibly different $\tilde{f}$, $\tilde{g}$.

As proved by Ovsyannikov,[14] it is possible to modify the Lie's infinitesimal approach to calculate equivalence group in essentially same way as invariance group. We omit the simple intermediate calculations and present the final result.

Assertion 1: The maximal equivalence group $\mathcal{E}$ of Eq. (2.8) reads as

$$\overline{t} = kt + k_1, \quad \overline{x} = \epsilon kx + k_2, \quad v = X(x)u + Y(t,x), \tag{3.1}$$

where $k \neq 0$, $X \neq 0$, $\epsilon = \pm 1, k, k_1, k_2 \in \mathbb{R}$, and X, Y are arbitrary smooth functions.

This completes the first step of the algorithm.

A. Preliminary group classification of Eq. (2.8)

First, we derive inequivalent classes of equations of the form (2.8) admitting one-parameter invariance groups.

Lemma 1: There exist transformations (3.1) that reduce operator (2.4) to one of the six possible forms,

$$Q = m(t\partial_t + x\partial_x), \quad m \neq 0, \quad Q = \partial_t + \beta\partial_x, \quad \beta \geqslant 0,$$

$$Q = \partial_t + \sigma(x)u\partial_u, \quad \sigma \neq 0, \quad Q = \partial_x, \tag{3.2}$$

$$Q = \sigma(x)u\partial_u, \quad \sigma \neq 0, Q = \theta(t,x)\partial_u, \quad \theta \neq 0.$$

Proof: Change of variables (3.1) reduces operator (2.4) to become

$$\tilde{Q} = k(\lambda t + \lambda_1)\partial_{\overline{t}} + \epsilon k(\lambda x + \lambda_2)\partial_{\overline{x}} + [Y_t(\lambda t + \lambda_1) + (\lambda x + \lambda_2)(X'u + Y_x) + X(hu + r)]\partial_v. \tag{3.3}$$

If $\lambda \neq 0$ in (2.4), then setting $k_1 = \lambda^{-1}\lambda_1 k$, $k_2 = \epsilon\lambda^{-1}\lambda_2 k$, and taking as X, Y ($X \neq 0$) integrals of system of PDEs,

$$X'(\lambda x + \lambda_2) + Xh = 0,$$

$$Y_t(\lambda t + \lambda_1) + Y_x(\lambda x + \lambda_2) + Xr = 0,$$

we reduce (3.3) to the form

$$\tilde{Q} = \lambda(\overline{t}\partial_{\overline{t}} + \overline{x}\partial_{\overline{x}}).$$

Provided $\lambda = 0$ and $\lambda_1 \neq 0$, we similarly obtain

$$\tilde{Q} = \partial_{\overline{t}} + \beta\partial_{\overline{x}}, \quad \beta \geqslant 0, \quad Q = \partial_{\overline{t}} + \sigma(\overline{x})v\partial_v, \quad \sigma \neq 0.$$

Next, if $\lambda = \lambda_1 = 0$, $\lambda_2 \neq 0$ in (2.4), then setting $k = \epsilon\lambda_2^{-1}$, and taking as X, Y ($X \neq 0$) integrals of equations

$$\lambda_2 X' + hX = 0, \quad Y_x + rX = 0,$$

we reduce operator (3.3) to become $\tilde{Q} = \partial_{\overline{x}}$.

Finally, the case $\lambda=\lambda_1=\lambda_2=0$, gives rise to operators $\tilde{Q}=\sigma(\overline{x})v\partial_v$, $\tilde{Q}=\theta(\overline{t,x})\partial_v$.

Rewriting the above operators in the initial variables t, x completes the proof.

Theorem 2: *There are exactly five inequivalent equations of the form (2.8) that admit one-parameter transformation groups. Below we list these equations together with one-dimensional Lie algebras generating their invariance groups (note that we do not present the full form of invariant PDEs we just give the functions f and g),*

$$A_1^1=\langle t\partial_t+x\partial_x\rangle,\quad g=x^{-1}\tilde{g}(\psi,u),$$

$$f=x^{-2}\tilde{f}(\psi,u),\quad \psi=tx^{-1},\quad \tilde{g}_u\neq 0,$$

$$A_1^2=\langle \partial_t+\beta\partial_x\rangle,\quad g=\tilde{g}(\eta,u),\quad f=\tilde{f}(\eta,u),$$

$$\eta=x-\beta t,\quad \beta\geqslant 0,\quad \tilde{g}_u\neq 0,$$

$$A_1^3=\langle \partial_t+\sigma(x)u\partial_u\rangle,\quad g=-2\sigma'\sigma^{-1}\ln|u|+\tilde{g}(\rho,x),$$

$$f=(\sigma'\sigma^{-1})^2u\ln^2|u|-\sigma'\sigma^{-1}\tilde{g}(\rho,x)u\ln|u|-\sigma^{-1}\sigma''u\ln|u|+u\tilde{f}(\rho,x),$$

$$\rho=u\exp(-t\sigma),\quad \sigma\neq 0,$$

$$A_1^4=\langle \partial_x\rangle,\quad g=\tilde{g}(t,u),\quad f=\tilde{f}(t,u),\quad \tilde{g}_u\neq 0,$$

$$A_1^5=\langle \sigma(x)u\partial_u\rangle,\quad g=-2\sigma'\sigma^{-1}\ln|u|+\tilde{g}(t,x),\quad f=(\sigma'\sigma^{-1})^2u\ln^2|u|$$
$$-(\sigma^{-1}\sigma''+\sigma^{-1}\sigma'\tilde{g}(t,x))u\ln|u|+u\tilde{f}(t,x),\quad \sigma'\neq 0.$$

Proof: If Eq. (2.8) admits a one-parameter invariance group, then it is generated by operator of the form (2.4). According to Lemma 1, the latter is equivalent to one of the six operators (3.2). That is why, all we need to do is integrate six systems of determining equations corresponding to operators (2.6). For the first five operators solutions of determining equations are easily shown to have the form given in the statement of the theorem.

We consider in more detail the operator $Q=\theta(t,u)\partial_u$. Determining Eqs. (2.6) for this operator reduce to the form

$$\theta_{tt}-\theta_{xx}=\theta f_u+\theta_x g,\quad \theta g_u=0,$$

whence we get $g_u=0$. Consequently, the system of determining equations is incompatible and the corresponding invariant equation fails to exist.

Nonequivalence of the invariant equations follows from nonequivalence of the corresponding symmetry operators.

The theorem is proved.

Note that in the sequel we give the formulations of theorems omitting routine proofs. The detailed proofs of the most of the statements presented in this paper can be found in Ref. 35.

It is a common knowledge that there exist two inequivalent two-dimensional solvable Lie algebras[36–40]

$$A_{2.1}=\langle e_1,e_2\rangle,\quad [e_1,e_2]=0,$$

$$A_{2.2} = \langle e_1, e_2 \rangle, \quad [e_1, e_2] = e_2.$$

To construct all possible realizations of the above algebras we take as the first basis element one of the realizations of one-dimensional invariance algebras listed in Lemma 1. The second operator is looked for in the generic form (2.4).

Algebra $A_{2.1}$: Let operator e_1 be of the form $\partial_t + x\partial_x$ and operator e_2 read as (2.4). Then it follows from the relation $[e_1, e_2] = 0$ that $\lambda_1 = \lambda_2 = xh' = 0$, $tr_t + xr_x = 0$. Consequently, we can choose basis elements of the algebra in question in the form $\langle t\partial_t + x\partial_x, (mu + r(\psi))\partial_u \rangle$, where $m \in \mathbb{R}$, $\psi = tx^{-1}$. Provided $m = 0$, the operator e_2 becomes $r(\psi)\partial_u$. It is straightforward to verify that this realization does not satisfy the determining equations. Hence, $m \neq 0$. Making the change of variables

$$\overline{t} = t, \quad \overline{x} = x, \quad v = u + m^{-1} r(\psi)$$

reduces the basis operators in question to the form $\overline{t}\partial_{\overline{t}} + \overline{x}\partial_{\overline{x}}$, $mv\partial_v$. That is why we can restrict our considerations to the realization $\langle t\partial_t + x\partial_x, u\partial_u \rangle$.

The second determining equation from (2.6) takes the form $ug_u = 0$. Hence it follows that the realization under consideration does not satisfy the determining equations. Consequently, the realization A_1^1 cannot be extended to a realization of the two-dimensional algebra $A_{2.1}$.

Algebra $A_{2.2}$: If operator e_1 is of the form $t\partial_t + x\partial_x$, then it follows from $[e_1, e_2] = e_2$ that $\lambda = \lambda_1 = \lambda_2 = 0$, $xh' = h$, $tr_t + xr_x = r$.

Next, if e_2 reads as $t\partial_t + x\partial_x$, then we get from $[e_1, e_2] = e_2$ the erroneous equality $1 = 0$.

That is why, the only possible case is when $e_2 = (mxu + xr(\psi))\partial_u$, $m \neq 0$, $\psi = tx^{-1}$, which gives rise to the following realization of the algebra $A_{2.2}$: $\langle t\partial_t + x\partial_x, xu\partial_u \rangle$. This is indeed invariance algebra of an equation from the class (2.8) and the functions f and g read as $g = -2x^{-1} \ln|u| + x^{-1}\tilde{g}(\psi)$, $f = x^{-2}u \ln^2|u| - x^{-2}\tilde{g}(\psi)u \ln|u| + x^{-2}u\tilde{f}(\psi)$, $\psi = tx^{-1}$.

Analysis of the remaining realizations of one-dimensional Lie algebras yields 10 inequivalent $A_{2.1}$- and $A_{2.2}$-invariant equations (see the assertions below). What is more, the obtained (two-dimensional) algebras are maximal symmetry algebras of the corresponding equations.

Theorem 3: *There are, at most, four inequivalent* $A_{2.1}$ *-invariant nonlinear equations (2.8). Below we list the realizations of* $A_{2.1}$ *and the corresponding expressions for* f *and* g.

$$(1) \quad \langle \partial_t, \sigma(x)u\partial_u, \rangle, \quad g = -2\sigma'\sigma^{-1} \ln|u|,$$

$$f = (\sigma'\sigma^{-1})^2 u \ln^2|u| - \sigma^{-1}\sigma' u \ln|u| + u\tilde{f}(x), \quad \sigma' \neq 0,$$

$$(2) \quad \langle \partial_t, \partial_x \rangle, \quad g = \tilde{g}(u), \quad f = \tilde{f}(u), \quad \tilde{g}_u \neq 0,$$

$$(3) \quad \langle \partial_x, \partial_t + u\partial_u \rangle, \quad g = \tilde{g}(\omega), \quad f = \exp(t)\tilde{f}(\omega), \quad \omega = \exp(-t), \quad \tilde{g}_\omega \neq 0,$$

$$(4) \quad \left\langle \sigma(x)u\partial_u, \partial_t - \tfrac{1}{2}k\sigma(x)\psi(x)u\partial_u \right\rangle, \quad g = -2\sigma'\sigma^{-1} \ln|u| + kt + \tilde{g}(x),$$

$$f = (\sigma'\sigma^{-1})^2 u \ln^2|u| - \sigma^{-1}\sigma'' u \ln|u| - \sigma^{-1}\sigma'(kt + \tilde{g}(x))u \ln|u| + u\left[\tfrac{1}{2}k\sigma'\sigma^{-1}t + \tfrac{1}{4}k^2t^2 + \tfrac{1}{2}k\tilde{g}(x) + \tilde{f}(x)\right],$$

$$k \neq 0, \quad \sigma' \neq 0, \quad \psi = \int \sigma^{-1}\, dx.$$

Theorem 4: *There exist, at most, six inequivalent* $A_{2.2}$*-invariant nonlinear equations (2.8). Below we list the realizations of* $A_{2.1}$ *and the corresponding expressions for* f *and* g.

$$(1)\quad \langle t\partial_t + x\partial_x, k^{-1}|x|^k u\partial_u\rangle,\quad g = x^{-1}(-2k\ln|u| + \tilde{g}(\psi)),$$

$$f = x^{-2}u(-k^2\ln^2|u| + k\tilde{g}(\psi)\ln|u| + k(k-1)\ln|u| + \tilde{f}(\psi)),$$

$$k \neq 0,\quad \psi = tx^{-1},$$

$$(2)\quad \langle \partial_t + \beta\partial_x, \exp(\beta^{-1}x)u\partial_u\rangle,\quad g = -2\beta^{-1}\ln|u| + \tilde{g}(\eta),$$

$$f = \beta^{-2}u\ln^2|u| - (\beta^{-2} + \beta^{-1}\tilde{g}(\eta))u\ln|u| + u\tilde{f}(\eta),$$

$$\beta > 0,\quad \eta = x - \beta t,$$

$$(3)\quad \langle -t\partial_t - x\partial_x, \partial_t + \beta\partial_x\rangle,\quad g = \eta^{-1}\tilde{g}(u),\quad f = \eta^{-2}\tilde{f}(u),\quad \beta \geqslant 0,$$

$$\eta = x - \beta t,\quad \tilde{g}_u \neq 0,$$

$$(4)\quad \langle -t\partial_t - x\partial_x, \partial_t + mx^{-1}u\partial_u\rangle,\quad g = x^{-1}(2m\psi + \tilde{g}(\omega)),$$

$$f = x^{-1}[-2m\psi u - 2m\psi - 2 - \tilde{g}(\omega) + \exp(m\psi)\tilde{g}(\omega)],$$

$$m > 0,\quad \omega = u\exp(-m\psi),\quad \psi = tx^{-1},\quad \tilde{g}_\omega \neq 0,$$

$$(5)\quad \langle \partial_x, e^x u\partial_u\rangle,\quad g = -2\ln|u| + \tilde{g}(t),\quad f = u\ln^2|u| - u\ln|u|(1 + \tilde{g}(t)) + u\tilde{f}(t),$$

$$(6)\quad \langle -t\partial_t - x\partial_x, \partial_x\rangle,\quad g = t^{-1}\tilde{g}(u),\quad f = t^{-2}\tilde{f}(u),\quad \tilde{g}_u \neq 0.$$

B. Completing group classification of (2.8)

As the invariant equations obtained in the previous subsection contain arbitrary functions of, at most, one variable, we can now apply the standard Lie–Ovsyannikov routine to complete the group classification of (2.8). We give the computation details for the case of the first $A_{2.1}$-invariant equation, the remaining cases are handled in a similar way.

Setting $g = -2\sigma'\sigma^{-1}\ln|u|$, $f = (\sigma'\sigma^{-1})u\ln^2|u| - \sigma^{-1}\sigma'' u\ln|u| + u\tilde{f}(x)$, $\sigma = \sigma(x)$, $\sigma' \neq 0$ we rewrite the first determining equation to become

$$-2h' + 2\lambda\sigma'\sigma^{-1}\ln|u| = -2(\lambda x + \lambda_2)(\sigma'\sigma^{-1})'_x\ln|u| - 2h\sigma'\sigma^{-1} - 2r\sigma'\sigma^{-1}u^{-1}.$$

As $h = f(x)$, $\sigma = \sigma(x)$, $r = r(t,x)$, λ, $\lambda_2 \in \mathbb{R}$, the above relation is equivalent to the following ones:

$$h' = \sigma'\sigma^{-1}h,\quad r = 0,\quad \lambda\sigma'\sigma^{-1} = -(\lambda x + \lambda_2)(\sigma'\sigma^{-1})'.$$

If σ is an arbitrary function, then $\lambda = \lambda_2 = r = 0$, $h = C\sigma$, $C \in \mathbb{R}$ and we get $\langle \partial_t, \sigma(x)u\partial_u\rangle$ as the maximal symmetry algebra. Hence, extension of the symmetry algebra is only possible when the function $\psi = \sigma'\sigma^{-1}$ is a (nonvanishing identically) solution of the equation

$$(\alpha x + \beta)\psi' + \alpha\psi = 0,\quad \alpha, \beta \in R,\quad |\alpha| + |\beta| \neq 0.$$

If $\alpha \neq 0$, then at the expense of displacements by x we can get $\beta = 0$, so that $\psi = mx^{-1}$, $m \neq 0$. Integrating the remaining determining equations yields

$$g=-2mx^{-1}\ln|u|,\quad f=mx^{-2}[mu\ln^2|u|-(m-1)u\ln|u|+nu],\quad m\neq 0,\quad m,n\in\mathbb{R}.$$

The maximal invariance algebra of the obtained equation is the three-dimensional Lie algebra $\langle\partial_t,|x|^m u\partial_u,t\partial_t+x\partial_x\rangle$ isomorphic to $A_{3.7}$.

Next, if $\alpha=0$, then $\beta\neq 0$ and $\psi=m$, $m\neq 0$. If this is the case, we have

$$g=\ln|u|,\quad f=\tfrac{1}{4}u\ln^2|u|-\tfrac{1}{4}u\ln|u|+nu,\quad n\in\mathbb{R}.$$

The maximal invariance algebra of the above equation reads as

$$\left\langle\partial_t,\partial_x,\exp\left(-\tfrac{1}{2}x\right)u\partial_u\right\rangle.$$

It is isomorphic to $A_{3.2}$.

Similarly, we prove that the list of inequivalent equations of the form (2.8) admitting three-dimensional symmetry algebras is exhausted by the equations given below. Note that the presented algebras are maximal. This means, in particular, that maximal symmetry algebra of Eq. (2.8) is, at most, three dimensional.

$A_{3.2}$-invariant equations,

$$(1)\quad u_{tt}=u_{xx}+u_x\ln|u|+\tfrac{1}{4}u\ln^2|u|-\tfrac{1}{4}u\ln|u|+nu(n\in\mathbb{R}),\left\langle\partial_t,\partial_x,\exp\left(-\tfrac{1}{2}x\right)u\partial_u\right\rangle,$$

$$(2)\quad u_{tt}=u_{xx}+m[\ln|u|-t]u_x+(m^2/4)u[(\ln|u|-t)(\ln|u|-t-1)]+nu(m>0,n\in\mathbb{R}),$$
$$\left\langle\partial_x,\partial_t+u\partial_u,\exp\left(-\tfrac{1}{2}mx\right)u\partial_u\right\rangle.$$

$A_{3.4}$-invariant equations,

$$(1)\quad u_{tt}=u_{xx}+x^{-1}[2\ln|u|+mx^{-1}t+n]u_x+x^{-2}u\ln|u|+(mx^{-1}t+n-2)x^{-2}u\ln|u|+\tfrac{1}{4}m^2x^{-4}t^2u$$
$$+\tfrac{1}{2}m(n-3)x^{-3}tu+px^{-2}u(m\neq 0,n,p\in\mathbb{R}),\quad\langle t\partial_t+x\partial_x,x^{-1}u\partial_u,\partial_t-(m/2)x^{-1}\ln|x|u\partial_u\rangle.$$

$A_{3.5}$-invariant equations,

$$(1)\quad u_{tt}=u_{xx}+|u|^m u_x+n|u|^{1+2m}\quad(m\neq 0,n\in\mathbb{R}),\quad\langle\partial_t,\partial_x,t\partial_t+x\partial_x-m^{-1}u\partial_u\rangle,$$

$$(2)\quad u_{tt}=u_{xx}+e^u u_x+ne^{2u}\quad(n\in\mathbb{R}),\quad\langle\partial_t,\partial_x,t\partial_t+x\partial_x-\partial_u\rangle,$$

$$(3)\quad u_{tt}=u_{xx}-x^{-1}[2\ln|u|-mx^{-1}t-n]u_x+x^{-2}u\ln^2|u|-x^{-2}(mx^{-1}t+n)u\ln|u|+ux^{-2}[(m/4)x^{-2}t^2$$
$$+(m/2)(n-1)x^{-1}t+p](m,n,p\in\mathbb{R}),\quad\langle t\partial_t+x\partial_x,xu\partial_u,\partial_t+(m/4)x^{-1}u\partial_u\rangle.$$

$A_{3.7}$-invariant equations,

$$(1)\quad u_{tt}=u_{xx}-2mx^{-1}u_x\ln|u|+mx^{-2}[mu\ln^2|u|-(m-1)u\ln|u|+nu]$$
$$\times(m\neq 0,1;n\in\mathbb{R}),\quad\langle\partial_t,|x|^m u\partial_u,t\partial_t+x\partial_x\rangle,$$

$$(2)\quad u_{tt}=u_{xx}-x^{-1}[2k+\ln|u|-mx^{-1}t-n]u_x+k^2x^{-2}u\ln^2|u|-kx^{-2}[mtx^{-1}+k+n-1]u\ln|u|+\tfrac{1}{2}m(k$$
$$-2+n)tx^{-3}u+\tfrac{1}{4}m^2t^2x^{-4}u+px^{-2}u\quad(|k|\neq 0,1;m\neq 0,n,p\in\mathbb{R}),$$
$$\langle t\partial_t+x\partial_x,|x|^k u\partial_u,\partial_t+[m/2(1+k)]x^{-1}u\partial_u\rangle.$$

This completes the group classification of nonlinear equations (2.8).

IV. GROUP CLASSIFICATION OF Eq. (2.9)

Omitting calculation details we present below the determining equations for symmetry operators admitted by Eq. (2.9).

Assertion 2: The maximal invariance group of PDE (2.9) is generated by the infinitesimal operator,

$$Q = \tau(t)\partial_t + \xi(x)\partial_x + [h(t)u + r(t,x)]\partial_u, \tag{4.1}$$

where τ, ξ, h, r, f, g are smooth functions satisfying the conditions

$$\begin{gathered} r_{tx} + f[h - \tau_t - \xi_x] = gr_x + \tau f_t + \xi f_x + [hu + r]f_u, \\ h_t = \tau_t g + \tau g_t + \xi g_x. \end{gathered} \tag{4.2}$$

Assertion 3: The equivalence group $\mathcal{E}$ of (2.9) is formed by the following transformations of the space V :

$$(1) \quad \overline{t} = T(t), \quad \overline{x} = X(x), \quad v = U(t)u + Y(t,x), \quad t'X'U \neq 0,$$

$$(2) \quad \overline{t} = T(x), \quad \overline{x} = X(t), \quad v = \Psi(x)\Phi(t,x)u + Y(t,x), \quad t'X'\Psi \neq 0, \tag{4.3}$$

$$\Phi(t,x) = \exp\left(-\int g(t,x)\mathrm{d}t\right), g_x \neq 0.$$

As the direct verification shows, given arbitrary functions g and f, it follows from (4.2) that $\tau = h = \xi = r = 0$. So that in the generic case the maximal invariance group of (2.9) is the trivial group of identical transformations.

We begin classification of (2.9) by constructing equations that admit one-dimensional symmetry algebras. The following assertions hold.

Lemma 2: There exist transformations (4.3) reducing operator (4.1) to one of the seven canonical forms given below

$$\begin{gathered} Q = t\partial_t + x\partial_x, \quad Q = \partial_t, \quad Q = \partial_x + tu\partial_u, \\ Q = \partial_x + \epsilon u\partial_u, \quad \epsilon = 0,1, \quad Q = tu\partial_u, \\ Q = u\partial_u, \quad Q = r(t,x)\partial_u, \quad r \neq 0. \end{gathered} \tag{4.4}$$

Theorem 5: *There exist, at most, three inequivalent nonlinear equations (2.9) that admit one-dimensional invariance algebras. The form of functions f, g and the corresponding symmetry algebras are given below,*

$$A_1^1 = \langle t\partial_t + x\partial_x \rangle, \quad g = t^{-1}\tilde{g}(\omega), \quad f = t^{-2}f(u,\omega), \quad \omega = tx^{-1}, \quad \tilde{g}_\omega \neq 0, \quad f_{uu} \neq 0,$$

$$A_1^2 = \langle \partial_t \rangle, \quad g = \tilde{g}(x), \quad f = \tilde{f}(x,u), \quad \tilde{g}' \neq 0, \quad \tilde{f}_{uu} \neq 0,$$

$$A_1^3 = \langle \partial_x + tu\partial_u \rangle, \quad g = x + \tilde{g}(t), \quad f = e^{tx}\tilde{f}(t,\omega), \quad \omega = e^{-tx}u, \quad \tilde{f}_{\omega\omega} \neq 0.$$

We proceed now to analyzing Eqs. (2.9) admitting two-dimensional symmetry algebras.

Theorem 6: *There exist, at most, three inequivalent nonlinear equations (2.9) that admit two-dimensional symmetry algebras, all of them being $A_{2.2}$-invariant equations. The forms of functions f and g and the corresponding realizations of the Lie algebra $A_{2.2}$ read as*

$$A_{2.2}^1 = \langle t\partial_t + x\partial_x, t^2\partial_t + x^2\partial_x + mut\partial_u \rangle \quad (m \in \mathbb{R}),$$

$$g = [mt + (k-m)x]t^{-1}(t-x)^{-1}, \quad k \neq 0,$$

$$f = |t-x|^{m-2}|x|^{-m}\tilde{f}(\omega),$$

$$\omega = u|t-x|^{-m}|x|^{m}, \quad \tilde{f}_{\omega\omega} \neq 0,$$

$$A^2_{2.2} = \langle t\partial_t + x\partial_x, t^2\partial_t + mtu\partial_u \rangle \quad (m \in \mathbb{R}),$$

$$g = t^{-2}[kx + mt], \quad k \neq 0, \quad f = |t|^{m-2}|x|^{-m}\tilde{f}(\omega),$$

$$\omega = |t|^{-m}|x|^{m}u, \quad \tilde{f}_{\omega\omega} \neq 0,$$

$$A^3_{2.2} = \langle t\partial_t + x\partial_x, x^2\partial_x + tu\partial_u \rangle,$$

$$g = (tx)^{-1}(mx - t)(m \in \mathbb{R}), \quad f = x^{-2}\exp(-tx^{-1})\tilde{f}(\omega),$$

$$\omega = u\exp(tx^{-1}), \quad \tilde{f}_{\omega\omega} \neq 0.$$

Note that if the function $\tilde{f}$ is arbitrary, then the invariance algebras given in the statement of Theorem 6 are maximal.

It turns out that the above theorems provide complete group classification of the class of PDEs (2.9). Namely, the following assertion holds true.

Theorem 7: *A nonlinear equation (2.9) having nontrivial symmetry properties is equivalent to one of the equations listed in Theorems 5 and 6.*

V. GROUP CLASSIFICATION OF Eq. (2.10)

As earlier, we present the results of the first step of our group classification algorithm skipping derivation details.

Assertion 4: Invariance group of equation (2.10) is generated by infinitesimal operator

$$Q = \tau(t)\partial_t + \xi(x)\partial_x + (ku + r(t,x))\partial_u, \tag{5.1}$$

where k is a constant τ, ξ, r, f are functions satisfying the relation

$$r_{tx} + [k - \tau' - \xi']f = \tau f_t + \xi f_x + [ku + r]f_u. \tag{5.2}$$

Assertion 5: Equivalence group $\mathcal{E}$ of the class of equations (2.10) is formed by the following transformations:

$$\begin{aligned} &(1) \quad \bar{t} = T(t), \quad \bar{x} = X(x), \quad v = mu + Y(t,x), \\ &(2) \quad \bar{t} = T(x), \quad \bar{x} = X(t), \quad v = mu + Y(t,x), \quad T'X'm \neq 0. \end{aligned} \tag{5.3}$$

Note that given an arbitrary function f, it follows from (5.2) that $\tau=\xi=k=r=0$, i.e., the group admitted is trivial. To obtain equations with nontrivial symmetry we need to specify properly the function f. To this end we perform classification of equations under study admitting one-dimensional invariance algebras. The following assertions give exhaustive classification of those.

Lemma 3: There exist transformations from the group $\mathcal{E}$ (5.3) that reduce (5.1) to one of the four canonical forms,

$$Q = \partial_t + \partial_x + \epsilon u\partial_u \quad (\epsilon = 0,1),$$

TABLE I. Invariant equations (2.10).

Number	Function f	Symmetry operators	Invariance algebra type
1	$e^t\tilde{f}(\omega)$, $\omega=ue^{-t}$, $\tilde{f}_{\omega\omega}\neq 0$	$\partial_t+u\partial_u$, ∂_x	$A_{2.1}$
2	$e^{t+x}\tilde{f}(\omega)$, $\omega=ue^{-t-x}$, $\tilde{f}_{\omega\omega}\neq 0$	$\partial_t+u\partial_u$, $\partial_x+u\partial_u$	$A_{2.1}$
3	$(t-x)^{-3}\tilde{f}(\omega)$, $\omega=(t-x)u$, $\tilde{f}_{\omega\omega}\neq 0$	$-t\partial_t-x\partial_x+u\partial_u$, $\partial_t+\partial_x$	$A_{2.2}$
4	$x^{-1}\tilde{f}(\omega)$, $\omega=x^{-1}u$, $\tilde{f}_{\omega\omega}\neq 0$	$-t\partial_t-x\partial_x-u\partial_u$, ∂_t	$A_{2.2}$
5	$(t-x)^{-2}\tilde{f}(u)$, $\tilde{f}_{uu}\neq 0$	$\partial_t+\partial_x$, $t\partial_t+x\partial_x$, $t^2\partial_t+x^2\partial_x$	$\mathrm{sl}(2,R)$
6	$\exp(x^{-1}u)$	$-t\partial_t+x\partial_u$, ∂_t, $x\partial_x+u\partial_u$	$A_{2.2}\oplus A_1$
7	$\lambda\lvert x\rvert^{-m-2}\lvert u\rvert^{m+1}$, $\lambda\neq 0$, $m\neq 0$, $-$, $1-2$	∂_t, $t\partial_t-1/mu\partial_u$, $x\partial_x+m+1/mu\partial_u$	$A_{2.2}\oplus A_1$
8	$\tilde{f}(u)$, $\tilde{f}_{uu}\neq 0$	∂_t, ∂_x, $-t\partial_t-x\partial_x$	$A_{3.6}$
9	$\lambda\lvert u\rvert^{n+1}$, $\lambda\neq 0$, $n\neq 0$, -1	$t\partial_t-1/nu\partial_u$, $x\partial_x-1/nu\partial_u$, ∂_t, ∂_x	$A_{2.2}\oplus A_{2.2}$

$$Q=\partial_t+\epsilon u\partial_u \quad (\epsilon=0,1),$$

$$Q=u\partial_u, \quad Q=g(t,x)\partial_u \quad (g\neq 0).$$

Theorem 8: *There exist exactly two nonlinear equations of the form (2.10) admitting one-dimensional invariance algebras. The corresponding expressions for function f and invariance algebras are given below,*

$$A_1^1=\langle \partial_t+\partial_x+\epsilon u\partial_u\rangle \quad (\epsilon=0,1), \quad f=e^{\epsilon t}\tilde{f}(\theta,\omega), \quad \theta=t-x, \quad \omega=e^{-\epsilon t}u, \quad \tilde{f}_{\omega\omega}\neq 0,$$

$$A_1^2=\langle \partial_t+\epsilon u\partial_u\rangle \quad (\epsilon=0,1), \quad f=e^{\epsilon t}\tilde{f}(x,\omega), \quad \omega=e^{-\epsilon t}u, \quad \tilde{f}_{\omega\omega}\neq 0.$$

Our analysis of Eqs. (2.10) admitting higher dimensional invariance algebras yields the following assertion.

Theorem 9: *The Liouville equation $u_{tx}=\lambda e^u$, $\lambda\neq 0$, has the highest symmetry among equations (2.10). Its maximal invariance algebra is infinite-dimensional and is spanned by the following infinite set of basis operators:*

$$Q=h(t)\partial_t+g(x)\partial_x-(h'(t)+g'(x))\partial_u,$$

where h and g are arbitrary smooth functions. Next, there exist exactly nine inequivalent equations of the form (2.10), whose maximal invariance algebras have dimension higher that one. We give these equations and their invariance algebras in Table I.

Details of the proof can be found in Ref. 35.

VI. GROUP CLASSIFICATION OF Eq. (2.7)

The first step of the algorithm of group classification of (2.7),

$$u_{tt} = u_{xx} + F(t,x,u,u_x), \quad F_{u_x u_x} \neq 0,$$

has been partially performed in Sec. II. It follows from Theorem 1 that the invariance group of Eq. (2.7) is generated by infinitesimal operator (2.4). What is more, the real constants λ, λ_1, λ_2 and real-valued functions $h=h(x)$, $r=r(t,x)$, $F=F(t,x,u,u_x)$ obey the relation (2.5). The equivalence group of the class of equations (2.7) is formed by transformations (3.1).

With these facts in hand we can utilize results of group classification of Eq. (2.8) in order to classify Eq. (2.7). In particular, using Lemma 1 and Lemma 2 from Ref. 35 it is straightforward to verify that the following assertions hold true.

Theorem 10: *There are, at most, seven inequivalent classes of nonlinear equations (2.7) invariant under the one-dimensional Lie algebras.*

Below we give the full list of the invariant equations and the corresponding invariance algebras,

$$A_1^1 = \langle t\partial_t + x\partial_x \rangle, \quad F = t^{-2}G(\xi,u,\omega), \quad \xi = tx^{-1}, \quad \omega = xu_x,$$

$$A_1^2 = \langle \partial_t + k\partial_x \rangle \quad (k>0), \quad F = G(\eta,u,u_x), \quad \eta = x - kt,$$

$$A_1^3 = \langle \partial_x \rangle, \quad F = G(t,u,u_x),$$

$$A_1^4 = \langle \partial_t \rangle, \quad F = G(x,u,u_x),$$

$$A_1^5 = \langle \partial_t + f(x)u\partial_u \rangle \quad (f \neq 0),$$

$$F = -tf''u + t^2(f')^2u - 2tf'u_x + e^{tf}G(x,v,\omega),$$

$$v = e^{-tf}u, \quad \omega = u^{-1}u_x - f'f^{-1}\ln|u|,$$

$$A_1^6 = \langle f(x)u\partial_u \rangle \quad (f \neq 0), \quad F = -f^{-1}f''u\ln|u| - 2f^{-1}f'u_x\ln|u| + f^{-2}(f')^2u\ln^2|u| + uG(t,x,\omega),$$

$$\omega = u^{-1}u_x - f'f^{-1}\ln|u|,$$

$$A_1^7 = \langle f(t,x)\partial_u \rangle \quad (f \neq 0), \quad F = f^{-1}(f_{tt} - f_{xx})u + G(t,x,\omega),$$

$$\omega = u_x - f^{-1}f_x u.$$

Note that if the functions F and G are arbitrary, then the presented algebras are maximal (in Lie's sense) symmetry algebras of the respective equations.

Theorem 11: *An equation of the form (2.7) cannot admit Lie algebra which has a subalgebra having nontrivial Levi factor.*

With account of the above facts we conclude that nonlinear equations (2.7) admit a symmetry algebra of the dimension higher than one only if the latter is a solvable real Lie algebra. That is why, we turn to classifying equations (2.7) whose invariance algebras are two-dimensional solvable Lie algebras.

Below we present the list of invariant equations and the corresponding realizations of the two-dimensional invariance algebras.

(I) $A_{2.1}$-invariant equations,

$$A^1_{2.1} = \langle t\partial_t + x\partial_x, u\partial_u\rangle, \quad F = x^{-2}uG(\xi,\omega),$$

$$\xi = tx^{-1}, \quad \omega = u^{-1}xu_x,$$

$$A^2_{2.1} = \langle t\partial_t + x\partial_x, \sigma(\xi)\partial_u\rangle \quad (\sigma \neq 0, \xi = tx^{-1}),$$

$$F = x^{-2}[\sigma^{-1}((1-\xi^2)\sigma'' - 2\xi\sigma')u + G(\xi,\omega)],$$

$$\omega = \xi\sigma' u + \sigma x u_x,$$

$$A^3_{2.1} = \langle \partial_t + k\partial_x, u\partial_u\rangle \quad (k > 0), \quad F = uG(\eta,\omega),$$

$$\eta = x - kt, \quad \omega = u^{-1}u_x,$$

$$A^4_{2.1} = \langle \partial_t + k\partial_x, \varphi(\eta)\partial_u\rangle \quad (k > 0, \eta = x - kt, \varphi \neq 0),$$

$$F = (k^2-1)\varphi''\varphi^{-1}u + G(\eta,\omega), \quad \omega = \varphi u_x - \varphi' u,$$

$$A^5_{2.1} = \langle \partial_t + k\partial_x, \partial_x + u\partial_u\rangle \quad (k > 0),$$

$$F = e^{\eta}G(\omega,v), \quad \eta = x - kt, \quad \omega = ue^{-\eta}, \quad v = u^{-1}u_x,$$

$$A^6_{2.1} = \langle \partial_t, \partial_x\rangle, \quad F = G(u,u_x),$$

$$A^7_{2.1} = \langle \partial_x, u\partial_u\rangle, \quad F = uG(t,\omega), \quad \omega = u^{-1}u_x,$$

$$A^8_{2.1} = \langle \partial_x, \varphi(t)\partial_u\rangle \quad (\varphi \neq 0),$$

$$F = \varphi^{-1}\varphi'' u + G(t,u_x),$$

$$A^9_{2.1} = \langle \partial_t, \partial_u\rangle, \quad F = G(x,u_x),$$

$$A^{10}_{2.1} = \langle \partial_t, f(x)u\partial_u\rangle \quad (f \neq 0),$$

$$F = -u^{-1}u_x^2 + uG(x,\omega),$$

$$\omega = u^{-1}u_x - f' f^{-1}\ln|u|,$$

$$A^{11}_{2.1} = \langle \partial_t + f(x)u\partial_u, g(x)u\partial_u\rangle \quad (\delta = f^{-1}f' - g^{-1}g' \neq 0),$$

$$F = -g^{-1}g''u\ln|u| - 2g^{-1}g'u_x\ln|u| + g^{-2}(g')^2 u\ln^2|u| - 2f\delta t u_x + 2f\delta g' g^{-1}tu\ln|u| + f^2\delta^2 t^2 u + f(g^{-1}g'' - f^{-1}f'')tu + uG(x,\omega),$$

$$\omega = u^{-1}u_x - g'g^{-1}\ln|u| - tf\delta,$$

$$A^{12}_{2.1} = \langle \partial_t + f(x)u\partial_u, e^{tf}\partial_u\rangle \quad (f \neq 0),$$

$$F=[f^2-tf''+t^2(f')^2]u-2tf'u_x+e^{tf}G(x,\omega),$$

$$\omega=e^{-tf}(u_x-tf'u),$$

$$A_{2.1}^{13}=\langle f(x)u\partial_u,g(x)u\partial_u\rangle \quad (\delta=f'g-g'f\neq 0),$$

$$F=-u^{-1}u_x^2-\delta^{-1}\delta'u_x+\delta^{-1}[f''g'-g''f']u\ln|u|+uG(t,x),$$

$$A_{2.1}^{14}=\langle\varphi(t)\partial_u,\psi(t)\partial_u\rangle \quad (\varphi'\psi-\varphi\psi'\neq 0),$$

$$F=\varphi^{-1}\varphi''u+G(t,x,u_x), \quad \varphi''\psi-\varphi\psi''=0.$$

(II) $A_{2.2}$-invariant equations,

$$A_{2.2}^1=\langle t\partial_t+x\partial_x,xu\partial_u\rangle, \quad F=x^{-2}u\ln^2|u|-2x^{-1}u_x\ln|u|+t^{-2}uG(\xi,\omega), \quad \xi=tx^{-1},$$

$$\omega=xu^{-1}u_x-\ln|u|,$$

$$A_{2.2}^2=\langle t\partial_t+x\partial_x,t\varphi(\xi)\partial_u\rangle \quad (\varphi\neq 0,\xi=tx^{-1}),$$

$$F=t^{-2}(1-\xi^2)\varphi^{-1}\xi(2\varphi'+\xi\varphi'')u+t^{-2}G(\xi,\omega),$$

$$\omega=x\varphi u_x+\xi\varphi' u,$$

$$A_{2.2}^3=\langle\partial_t+k\partial_x,\exp(k^{-1}x)u\partial_u\rangle(k>0),$$

$$F=k^{-2}u\ln^2|u|-2k^{-1}u_x\ln|u|-k^{-2}u\ln|u|+uG(\eta,\omega), \quad \eta=x-kt, \quad \omega=u^{-1}u_x-k^{-1}\ln|u|,$$

$$A_{2.2}^4=\langle\partial_t+k\partial_x,e^t\varphi(\eta)\partial_u\rangle \quad (\eta=x-kt,k>0,\varphi\neq 0),$$

$$F=((k^2-1)\varphi''\varphi^{-1}-2k\varphi'\varphi^{-1}+1)u+G(\eta,\omega),$$

$$\omega=\varphi u_x-\varphi' u, \quad \varphi'=\frac{\mathrm{d}\varphi}{\mathrm{d}\eta},$$

$$A_{2.2}^5=\langle -t\partial_t-x\partial_x,\partial_t+k\partial_x\rangle \quad (k>0),$$

$$F=\eta^{-2}G(u,\omega), \quad \eta=x-kt, \quad \omega=u_x\eta,$$

$$A_{2.2}^6=\langle -t\partial_t-x\partial_x+mu\partial_u,\partial_t+k\partial_x\rangle \quad (k>0,m\neq 0),$$

$$F=|\eta|^{-2-m}G(v,\omega), \quad \eta=x-kt,$$

$$\omega=u|\eta|^m, \quad v=u_x|\eta|^{m+1},$$

$$A_{2.2}^7=\langle\partial_x,e^xu\partial_u\rangle, \quad F=u\ln^2|u|-u\ln|u|-2u_x\ln|u|+uG(t,\omega), \quad \omega=u^{-1}u_x-\ln|u|,$$

$$A^{8}_{2.2}=\langle\partial_x,e^x\varphi(t)\partial_u\rangle\quad(\varphi\neq 0),$$

$$F=(\varphi^{-1}\varphi''-1)u+G(t,\omega),\quad \omega=u_x-u,$$

$$A^{9}_{2.2}=\langle -t\partial_t-x\partial_x,\partial_x\rangle,\quad F=t^{-2}G(u,tu_x),$$

$$A^{10}_{2.2}=\langle -t\partial_t-x\partial_x+ku\partial_u,\partial_x\rangle\quad(k\neq 0),$$

$$F=|t|^{-2-k}G(v,\omega),\quad v=|t|^{k}u,\quad \omega=|t|^{k+1}u_x,$$

$$A^{11}_{2.2}=\langle\partial_t,e^t\partial_u\rangle,\quad F=u+G(x,u_x),$$

$$A^{12}_{2.2}=\langle -t\partial_t-x\partial_x,\partial_t\rangle,\quad F=x^{-2}G(u,\omega),\quad \omega=xu_x,$$

$$A^{13}_{2.2}=\langle\partial_t+f(x)u\partial_u,e^{(1+f)t}\partial_u\rangle\quad(f\neq 0),$$

$$F=-(tf''-t^2(f')^2-(1+f^2))u-2tf'u_x+e^{tf}G(x,\omega),\quad \omega=e^{-tf}(u_x-f'(t+f^{-1})u),$$

$$A^{14}_{2.2}=\langle -t\partial_t-x\partial_x,\partial_t+kx^{-1}u\partial_u\rangle\quad(k>0),$$

$$F=-2ktx^{-3}u+k^2t^2x^{-4}u+2ktx^{-2}u_x+x^{-2}\exp(ktx^{-1})G(v,\omega),\quad v=\exp(-kx^{-1}t)u,$$

$$\omega=xu^{-1}u_x+\ln|u|,$$

$$A^{15}_{2.2}=\langle k(t\partial_t+x\partial_x),|x|^{k^{-1}}u\partial_u\rangle\quad(k\neq 0,1),$$

$$F=-k^{-2}(1-k)x^{-2}u\ln|u|-2k^{-1}x^{-1}u_x\ln|u|+k^{-2}x^{-2}u\ln^2|u|+x^{-2}uG(v,\omega),$$

$$v=tx^{-1},\quad \omega=xu^{-1}u_x-k^{-1}\ln|u|,$$

$$A^{16}_{2.2}=\langle k(t\partial_t+x\partial_x),|t|^{k^{-1}}\varphi(\xi)\partial_u\rangle\quad(k\neq 0,1,\varphi\neq 0,\xi=tx^{-1}),\quad F=[k^{-1}(k^{-1}-1)+2\xi(k^{-1}-\xi^2)\varphi^{-1}\varphi'+\xi^2(1-\xi)^2\varphi^{-1}\varphi'']t^{-2}u+t^{-2}G(\xi,\omega),$$

$$\omega=x\varphi u_x+\xi\varphi' u.$$

In the above formulas G stands for an arbitrary smooth function. As customary, the prime denotes the derivative of a function of one variable.

A. Group classification of the equation $u_{tt}=u_{xx}-u^{-1}u_x^2+A(x)u_x+B(x)u\ln|u|+uD(t,x)$

Before analyzing Eqs. (2.7) admitting algebras of the dimension higher than two we perform group classification of the equation

$$u_{tt}=u_{xx}-u^{-1}u_x^2+A(x)u_x+B(x)u\ln|u|+uD(t,x).\tag{6.1}$$

Here $A(x),B(x),D(t,x)$ are arbitrary smooth functions. Note that the above class of PDEs contains $A^{13}_{2.1}$-invariant equation. Importantly, class (6.1) contains a major part of equations of the form (2.7), whose maximal symmetry algebras have dimension three or four. This fact is used to simplify group classification of Eqs. (2.7).

The complete account of symmetry properties of PDE (6.1) is given in the following assertions.

Lemma 4: If A, B, and D are arbitrary, then the maximal invariance algebra of PDE (6.1) is the two-dimensional Lie algebra equivalent to $A_{2.1}^{13}$ *and (6.1) reduces to* $A_{2.1}^{13}$*-invariant equation. Next, if the maximal symmetry algebra of an equation of the form (6.1) is three-dimensional (we denote it as* A_3*), then this equation is equivalent to one of the following ones*:

$$\text{(I) } A_3 \sim A_{3.1}, \quad A_3 = \langle \partial_t, f(x)u\partial_u, \varphi(x)u\partial_u \rangle,$$

$$A = -\sigma^{-1}\sigma', \quad B = \sigma^{-1}\rho, \quad D = 0, \quad \sigma = f'\varphi - f\varphi' \neq 0,$$

$$\rho = \varphi' f'' - \varphi'' f',$$

$$\text{(II) } A_3 \sim A_{3.1}, \quad A_3 = \langle f(x)u\partial_u, \varphi(x)u\partial_u, \partial_t + \psi(x)u\partial_u \rangle,$$

$$A = -\sigma^{-1}\sigma', \quad B = \sigma^{-1}\rho,$$

$$D = t\sigma^{-1}[\sigma'\psi' - \psi\rho - \sigma\psi'],$$

$$\sigma = f'\varphi - \varphi' f \neq 0, \quad \rho = f''\varphi' - \varphi'' f',$$

$$f'\psi - f\psi' \neq 0, \quad \varphi'\psi - \varphi\psi' \neq 0,$$

$$\text{(III) } D = x^{-2}G(\xi), \quad \xi = tx^{-1}, G \neq 0,$$

$$\text{(1) } A_3 \sim A_{3.2}, \; A_3 = \langle t\partial_t + x\partial_x, u\partial_u, |x|^{1-n}u\partial_u \rangle,$$

$$A = nx^{-1} \quad (n \neq 1), \quad B = 0,$$

$$\text{(2) } A_3 \sim A_{3.3}, \quad A_3 = \langle t\partial_t + x\partial_x, u\partial_u, u\ln|x|\partial_u \rangle,$$
$$A = x^{-1}, \quad B = 0,$$

$$\text{(3) } A_3 \sim A_{3.4}, \quad A_3 = \langle t\partial_t + x\partial_x, \sqrt{|x|}u\partial_u, \sqrt{|x|}\ln|x|u\partial_u \rangle,$$

$$A = 0, \quad B = \tfrac{1}{4}x^{-2},$$

$$\text{(4) } A_3 \sim A_{3.9}, \quad A_3 = \left\langle t\partial_t + x\partial_x, \sqrt{|x|}\cos\left(\tfrac{1}{2}\beta\ln|x|\right)u\partial_u, \sqrt{|x|}\sin\left(\tfrac{1}{2}\beta\ln|x|\right)u\partial_u \right\rangle,$$
$$A = 0, \quad B = mx^{-2},$$

$$m > \tfrac{1}{4}, \quad \beta = \sqrt{4m-1},$$

$$\text{(5) } A_3 \sim A_{3.7}, \quad A_3 = \langle t\partial_t + x\partial_x, (\sqrt{|x|})^{1+\beta}u\partial_u, (\sqrt{|x|})^{1-\beta}u\partial_u \rangle,$$

$$A = 0, \quad B = mx^{-2}, \quad m < \tfrac{1}{4}, \quad m \neq 0, \quad \beta = \sqrt{1-4m},$$

(6) $A_3 \sim A_{3.8}$, $A_3 = \langle t\partial_t + x\partial_x, \cos(\sqrt{m}\ln|x|)u\partial_u, \sin(\sqrt{m}\ln|x|)u\partial_u\rangle$,
$A = x^{-1}$, $B = mx^{-2}$, $m > 0$,

(7) $A_3 \sim A_{3.6}$, $A_3 = \langle t\partial_t + x\partial_x, |x|^{\sqrt{|m|}}u\partial_u, |x|^{-\sqrt{|m|}}u\partial_u\rangle$,

$A = x^{-1}$, $B = mx^{-2}$, $m < 0$,

(8) $A_3 \sim A_{3.4}$, $A_3 = \langle t\partial_t + x\partial_x, (\sqrt{|x|})^{1-n}u\partial_u, (\sqrt{|x|})^{1-n} \times \ln|x|u\partial_u\rangle$,
$A = nx^{-1}$ $(n \neq 0,1)$, $B = \frac{1}{4}(n-1)^2x^{-2}$,

(9) $A_3 \sim A_{3.9}$, $A_3 = \left\langle t\partial_t + x\partial_x, (\sqrt{|x|})^{1-n}\cos\left(\frac{1}{2}\beta\ln|x|\right)u\partial_u, (\sqrt{|x|})^{1-n}\sin\left(\frac{1}{2}\beta\ln|x|\right)u\partial_u\right\rangle$,
$A = nx^{-1}$ $(n \neq 0,1)$,

$B = mx^{-2}$ $\left(m > \frac{1}{4}(n-1)^2\right)$, $\beta = \sqrt{4m-(n-1)^2}$,

(10) $A_3 \sim A_{3.7}$, $A_3 = \langle t\partial_t + x\partial_x, (\sqrt{|x|})^{1-\beta-n}u\partial_u, (\sqrt{|x|})^{1-n+\beta} \times u\partial_u\rangle$,
$A = nx^{-1}$ $(n \neq 0,1)$, $B = mx^{-2}$

$\left(m < \frac{1}{4}(n-1)^2, m \neq 0\right)$, $\beta = \sqrt{(n-1)^2-4m}$.

(IV) $D = G(t)$,

(1) $A_3 \sim A_{3.3}$, $A_3 = \langle \partial_x, u\partial_u, xu\partial_u\rangle$,

$A = B = 0$,

(2) $A_3 = A_{3.2}$, $A_3 = \langle \partial_x, u\partial_u, e^x u\partial_u\rangle$,

$A = -1$, $B = 0$,

(3) $A_3 \sim A_{3.8}$, $A_3 = \langle \partial_x, \cos(x)u\partial_u, \sin(x)u\partial_u\rangle$,

$A = 0$, $B = 1$,

(4) $A_3 \sim A_{3.6}$, $A_3 = \langle \partial_x, e^x u\partial_u, e^{-x}u\partial_u\rangle$,

$A = 0$, $B = -1$,

(5) $A_3 \sim A_{3.4}$, $A_3 = \left\langle \partial_x, \exp\left(\frac{1}{2}x\right)u\partial_u, \exp\left(\frac{1}{2}x\right)xu\partial_u\right\rangle$,

$A = -1$, $B = \frac{1}{4}$,

(6) $A_3 \sim A_{3.7}$, $A_3 = \left\langle \partial_x, \exp\left(\frac{1}{2}(1+\beta)x\right)u\partial_u, \exp\left(\frac{1}{2}(1-\beta)x\right)u\partial_u\right\rangle$,

$$A=-1,\quad B=m\quad \left(m<\tfrac{1}{4}\right),\quad m\neq 0,\quad \beta=\sqrt{1-4m},$$

$$(7)\ A_3\sim A_{3.9}, A_3=\left\langle \partial_x, \exp\left(\tfrac{1}{2}x\right)\cos\left(\tfrac{1}{2}\beta x\right)u\partial_u, \exp\left(\tfrac{1}{2}x\right)\sin\left(\tfrac{1}{2}\beta x\right)u\partial_u\right\rangle,$$

$$A=-1,\quad B=m\quad \left(m>\tfrac{1}{4}\right),\quad \beta=\sqrt{4m-1},$$

$$(\mathrm{V})\ D=G(\eta),\quad \eta=x-kt,\quad k>0,$$

$$(1)\ A_3\sim A_{3.3},\quad A_3=\langle \partial_t+k\partial_x, u\partial_u, xu\partial_u\rangle,$$

$$A=B=0,$$

$$(2)\ A_3=A_{3.2},\quad A_3=\langle \partial_t+k\partial_x, u\partial_u, e^x u\partial_u\rangle,$$

$$A=-1,\quad B=0,$$

$$(3)\ A_3\sim A_{3.8},\quad A_3=\langle \partial_t+k\partial_x, \cos(x)u\partial_u, \sin(x)u\partial_u\rangle,$$

$$A=0,\quad B=1,$$

$$(4)\ A_3\sim A_{3.6},\quad A_3=\langle \partial_t+k\partial_x, e^x u\partial_u, e^{-x}u\partial_u\rangle,$$

$$A=n,\quad B=-1,$$

$$(5)\ A_3\sim A_{3.4},\quad A_3=\left\langle \partial_t+k\partial_x, \exp\left(\tfrac{1}{2}x\right)u\partial_u, \exp\left(\tfrac{1}{2}x\right)xu\partial_u\right\rangle,$$

$$A=-1,\quad B=\tfrac{1}{4},$$

$$(6)\ A_3\sim A_{3.7},\quad A_3=\left\langle \partial_t+k\partial_x, \exp\left(\tfrac{1}{2}(1+\beta)x\right)u\partial_u, \exp\left(\tfrac{1}{2}(1-\beta)x\right)u\partial_u\right\rangle,$$

$$A=-1,\quad B=m\quad \left(m<\tfrac{1}{4}\right),\quad m\neq 0,\quad \beta=\sqrt{1-4m},$$

$$(7)\ A_3\sim A_{3.9},\quad A_3=\left\langle \partial_t+k\partial_x, \exp\left(\tfrac{1}{2}x\right)\cos\left(\tfrac{1}{2}\beta x\right)u\partial_u, \exp\left(\tfrac{1}{2}x\right)\sin\left(\tfrac{1}{2}\beta x\right)u\partial_u\right\rangle,$$

$$A=-1,\quad B=m\quad \left(m>\tfrac{1}{4}\right),\quad \beta=\sqrt{4m-1}.$$

Theorem 12: *Equation* $u_{tt}=u_{xx}-u^{-1}u_x^2$ *has the widest symmetry group amongst equations of the form (6.1). Its maximal invariance algebra is the five-dimensional Lie algebra,*

$$A_5^1=\langle \partial_t, \partial_x, t\partial_t+x\partial_x, xu\partial_u, u\partial_u\rangle.$$

There are no equations of the form (6.1) which are inequivalent to the above equation and admit invariance algebra of the dimension higher than four. Inequivalent equations (6.1) admitting four-dimensional algebras are listed below together with their symmetry algebras.

$$(\mathrm{I})\ D=0,$$

$$(1)\ A_4 \sim A_{3.6} \oplus A_1, \quad A_4 = \langle \partial_t, \partial_x, u\,\mathrm{ch}(\beta x)\partial_u, u\,\sinh(\beta x)\partial_u \rangle,$$

$$A = 0, \quad B = -\beta^2, \quad \beta \neq 0,$$

$$(2)\ A_4 \sim A_{3.8} \oplus A_1, \quad A_4 = \langle \partial_t, \partial_x, u\cos(\beta x)\partial_u, u\sin(\beta x)\partial_u \rangle,$$

$$A = 0, \quad B = \beta^2, \quad \beta \neq 0,$$

$$(3)\ A_4 \sim A_{2.1} \oplus A_{2.2}, \quad A_4 = \langle \partial_t, \partial_x, u\partial_u, e^{-x}u\partial_u \rangle, \quad A = 1, \quad B = 0,$$

$$(4)\ A_4 \sim A_{3.4} \oplus A_1, \quad A_4 = \langle \partial_t, \partial_x, e^{-x}u\partial_u, xe^{-x}u\partial_u \rangle, \quad A = 2, \quad B = 1,$$

$$(5)\ A_4 \sim A_{3.9} \oplus A_1, \quad A_4 = \langle \partial_t, \partial_x, ue^{-x}\cos(\beta x)\partial_u, ue^{-x}\sin(\beta x)\partial_u \rangle,$$

$$A = 2, \quad B = m, \quad m > 1, \quad \beta = \sqrt{m-1},$$

$$(6)\ A_4 \sim A_{3.7} \oplus A_1, \quad A_4 = \langle \partial_t, \partial_x, ue^{-x}\,\mathrm{ch}(\beta x)\partial_u, ue^{-x}\,\sinh(\beta x)\partial_u \rangle,$$

$$A = 2, \quad B = m, \quad m > 1, \quad m \neq 0, \quad \beta = \sqrt{1-m},$$

$$(7)\ A_4 \sim A_{4.2}, \quad A_4 = \langle \partial_t, t\partial_t + x\partial_x, \sqrt{|x|}u\partial_u, u\sqrt{|x|}\ln|x|\partial_u \rangle,$$

$$A = 0, \quad B = \tfrac{1}{4}x^{-2},$$

$$(8)\ A_4 \sim A_{4.5}, \quad A_4 = \langle \partial_t, t\partial_t + x\partial_x, |x|^{\frac{1}{2}+\beta}u\partial_u, |x|^{\frac{1}{2}-\beta}u\partial_u \rangle, \quad A = 0,$$

$$B = mx^{-2}, \quad m < \tfrac{1}{4}, \quad m \neq 0, \quad \beta = \sqrt{\tfrac{1}{4}-m},$$

$$(9)\ A_4 \sim A_{4.6}, \quad A_4 = \langle \partial_t, t\partial_t + x\partial_x, \sqrt{|x|}\cos(\beta\ln|x|)u\partial_u, \sqrt{|x|}\sin(\beta\ln|x|)u\partial_u \rangle,$$

$$A = 0, \quad B = mx^{-2}, \quad m > \tfrac{1}{4}, \quad \beta = \sqrt{m-\tfrac{1}{4}},$$

$$(10)\ A_4 \sim A_{4.3}, \quad A_4 = \langle \partial_t, t\partial_t + x\partial_x, u\ln|x|\partial_u, u\partial_u \rangle, \quad A = x^{-1}, \quad B = 0,$$

$$(11)\ A_4 \sim A_{3.7} \oplus A_1, \quad A_4 = \langle \partial_t, t\partial_t + x\partial_x, |x|^{1-n}u\partial_u, u\partial_u \rangle,$$

$$A = nx^{-1}, \quad B = 0, \quad n \neq 0, 1,$$

$$(12)\ A_4 \sim A_{4.5}, \quad A_4 = \langle \partial_t, t\partial_t + x\partial_x, |x|^{\frac{1}{2}(1-n)}u\partial_u, |x|^{\frac{1}{2}(1-n)}u\ln|x|\partial_u \rangle,$$

$$A = nx^{-1}, \quad B = \tfrac{1}{4}(n-1)^2x^{-2}, \quad n \neq 0, 1,$$

$$(13)\ A_4 \sim A_{4.5}, \quad A_4 = \langle \partial_t, t\partial_t + x\partial_x, |x|^{\frac{1}{2}(1-n+\beta)}u\partial_u, |x|^{\frac{1}{2}(1-n-\beta)}u\partial_u \rangle,$$

$$A = nx^{-1}, \quad B = mx^{-2}, \quad m < \tfrac{1}{4}(n-1)^2, \quad m \neq 0, \quad n \neq 0,$$

$$\beta = \sqrt{(n-1)^2 - 4m},$$

(14) $A_4 \sim A_{4.6}$, $A_4 = \langle \partial_t, t\partial_t + x\partial_x, |x|^{\frac{1}{2}(1-n)} \cos(\beta \ln|x|)u\partial_u, |x|^{\frac{1}{2}(1-n)} \sin(\beta \ln|x|)u\partial_u \rangle$,
$A = nx^{-1}$, $B = mx^{-2}$,

$$m \neq 0, \quad n \neq 0, \quad m > \tfrac{1}{4}(n-1)^2, \quad \beta = \sqrt{m - \tfrac{1}{4}(n-1)^2},$$

(II) $D = ktx^{-3}$, $k > 0$,

(1) $A_4 \sim A_{4.1}$, $A_4 = \left\langle \partial_t - \tfrac{1}{2}kx^{-1}u\partial_u, t\partial_t + x\partial_x, xu\partial_u, u\partial_u \right\rangle$, $A = B = 0$,

(2) $A_4 \sim A_{4.2}$, $A_4 = \left\langle \partial_t - \tfrac{4}{9}kx^{-1}u\partial_u, t\partial_t + x\partial_x, \sqrt{|x|}u\partial_u, \sqrt{|x|}\ln|x|u\partial_u \right\rangle$,

$$A = 0, \quad B = \tfrac{1}{4}x^{-2},$$

(3) $A_4 \sim A_{4.5}$, $A_4 = \langle \partial_t - [k/(m+2)]x^{-1}u\partial_u, t\partial_t + x\partial_x, |x|^{\frac{1}{2}+\beta}u\partial_u, |x|^{\frac{1}{2}-\beta}u\partial_u \rangle$,

$$A = 0, \quad B = mx^{-2}, \quad m \neq 0, -2, \quad m < \tfrac{1}{4}, \quad \beta = \sqrt{\tfrac{1}{4} - m},$$

(4) $A_4 \sim A_{4.2}$, $A_4 = \left\langle \partial_t + \tfrac{1}{9}kx^{-1}(1 + 3\ln|x|u)\partial_u, t\partial_t + x\partial_x, x^2u\partial_u, x^{-1}u\partial_u \right\rangle$, $A = 0$, $B = -2x^{-2}$,

(5) $A_4 \sim A_{4.6}$, $A_4 = \langle \partial_t - [k/(m+2)]x^{-1}u\partial_u, t\partial_t + x\partial_x, \sqrt{|x|}u\cos(\beta\ln|x|)\partial_u, \sqrt{|x|}u\sin(\beta\ln|x|)\partial_u \rangle$,
$A = 0$, $B = mx^{-2}$, $m > \tfrac{1}{4}$, $\beta = \sqrt{m - \tfrac{1}{4}}$,

(6) $A_4 \sim A_{4.3}$, $A_4 = \langle \partial_t - kx^{-1}u\partial_u, t\partial_t + x\partial_x, u\partial_u, u\ln|x|\partial_u \rangle$,

$$A = x^{-1}, \quad B = 0,$$

(7) $A_4 \sim A_{3.4} \oplus A_1$, $A_4 = \langle \partial_t + kx^{-1}(1 + \ln|x|)u\partial_u, t\partial_t + x\partial_x, u\partial_u, x^{-1}u\partial_u \rangle$,
$A = 2x^{-1}$, $B = 0$,

(8) $A_4 \sim A_{3.7} \oplus A_1$, $A_4 = \langle \partial_t + [k/(n-2)]x^{-1}u\partial_u, t\partial_t + x\partial_x, u\partial_u, |x|^{1-n}u\partial_u \rangle$,

$$A = nx^{-1}, \quad B = 0, \quad n \neq 0, 1, 2,$$

(9) $A_4 = A_{4.4}$, $A_4 = \left\langle \partial_t - \tfrac{1}{2}kx^{-1}\ln^2|x|u\partial_u, t\partial_t + x\partial_x, x^{-1}u\partial_u, x^{-1}\ln|x|u\partial_u \right\rangle$,
$A = 3x^{-1}$, $B = x^{-2}$,

(10) $A_4 \sim A_{4.2}$, $A_4 = \langle \partial_t - [4k/(n-3)^2]x^{-1}u\partial_u, t\partial_t + x\partial_x, |x|^{\frac{1}{2}(1-n)}u\partial_u, |x|^{\frac{1}{2}(1-n)}\ln|x|u\partial_u \rangle$,
$A = nx^{-1}$, $B = \tfrac{1}{4}(n-1)^2x^{-2}$, $n \neq 0, 3$,

(11) $A_4 \sim A_{4.5}$, $A_4 = \langle t\partial_t + x\partial_x, \partial_t - [k(2-n+m)]x^{-1}u\partial_u, |x|^{\frac{1}{2}(1-n+\beta)}u\partial_u, |x|^{\frac{1}{2}(1-n-\beta)}u\partial_u \rangle$,
$A = nx^{-1}$, $B = mx^{-2}$,

$$n \neq 0,2, \quad m \neq n-2, \quad m < \tfrac{1}{4}(n-1)^2, \quad \beta = \sqrt{(n-1)^2 - 4m},$$

(12) $A_4 \sim A_{4.2}$, $A_4 = \langle t\partial_t + x\partial_x, \partial_t + [k/(3-n)]x^{-1}\ln|x|u\partial_u, x^{-1}u\partial_u, |x|^{2-n}u\partial_u \rangle$,

$$A = nx^{-1}, \quad B = (n-2)x^{-2}, \quad n \neq 0,2,3,$$

(13) $A_4 \sim A_{4.6}$, $A_4 = \langle t\partial_t + x\partial_x, \partial_t - [k/(2-n+m)]x^{-1}u\partial_u,$
$|x|^{\frac{1}{2}(1-n)}u\cos(\beta\ln|x|)\partial_u, |x|^{\frac{1}{2}(1-n)}u\sin(\beta\ln|x|)\partial_u \rangle$,

$$A = nx^{-1}, \quad B = mx^{-2}, \quad n \neq 0, \quad m \neq 0, \quad m > \tfrac{1}{4}(n-1)^2,$$

$$\beta = \sqrt{m - \tfrac{1}{4}(n-1)^2},$$

(III) $D = kt$, $k > 0$,

(1) $A_4 \sim A_{4.1}$, $A_4 = \langle \partial_x, \partial_t - \frac{1}{2}kx^2u\partial_u, xu\partial_u, u\partial_u \rangle$, $A = B = 0$,

(2) $A_4 \sim A_{4.3}$, $A_4 = \langle \partial_x, \partial_t - kxu\partial_u, e^{-x}u\partial_u, u\partial_u \rangle$, $A = 1$, $B = 0$,

(3) $A_4 \sim A_{3.8} \oplus A_1$, $A_4 = \langle \partial_x, \partial_t - k\beta^{-2}u\partial_u, u\cos(\beta x)\partial_u, u\sin(\beta x)\partial_u \rangle$,

$$A = 0, \quad B = \beta^2, \quad \beta \neq 0,$$

(4) $A_4 \sim A_{3.6} \oplus A_1$, $A_4 = \langle \partial_x, \partial_t + k\beta^{-2}u\partial_u, u\,\mathrm{ch}(\beta x)\partial_u, u\sinh(\beta x)\partial_u \rangle$,

$$A = 0, \quad B = -\beta^2, \quad \beta \neq 0,$$

(5) $A_4 \sim A_{3.4} \oplus A_1$, $A_4 = \langle \partial_x, \partial_t - 4ku\partial_u, \exp(-\frac{1}{2}x)u\partial_u, x\exp(-\frac{1}{2}x)u\partial_u \rangle$,

$$A = 1, \quad B = \tfrac{1}{4},$$

(6) $A_4 \sim A_{3.7} \oplus A_1$, $A_4 = \langle \partial_x, \partial_t - km^{-1}u\partial_u, \exp(-\frac{1}{2}(1-\beta)x)u\partial_u, \exp(-\frac{1}{2}(1+\beta)x)u\partial_u \rangle$,

$$A = 1, \quad B = m, \quad m < \tfrac{1}{4}, \quad m \neq 0, \quad \beta = \sqrt{1-4m},$$

(7) $A_4 \sim A_{3.9} \oplus A_1$, $A_4 = \langle \partial_x, \partial_t - km^{-1}u\partial_u, \exp(-\frac{1}{2}x)\cos(\beta x)u\partial_u, \exp(-\frac{1}{2}x)\sin(\beta x)u\partial_u \rangle$,

$$A = 1, \quad B = m, \quad m > \tfrac{1}{4}, \quad \beta = \sqrt{m - \tfrac{1}{4}},$$

(IV) $D = kt^{-2}$, $k \neq 0$,

$$A_4 \sim A_{4.8} \quad (q=-1), \quad A_4 = \langle \partial_x, t\partial_t + x\partial_x, xu\partial_u, u\partial_u \rangle, \quad A = B = 0,$$

$$\text{(V) } D = m(x-kt)^{-2}, \quad k > 0, \quad m \neq 0,$$

$$A_4 \sim A_{4.8} \quad (q=-1), \quad A_4 = \langle \partial_t + k\partial_x, t\partial_t + x\partial_x, xu\partial_u, u\partial_u \rangle, \quad A = B = 0.$$

Proof can be found in Ref. 35.

B. Nonlinear equations (2.7) invariant under three-dimensional Lie algebras

Equations of the form (2.7) cannot be invariant under the algebra which is isomorphic to a Lie algebra with a nontrivial Levi ideal.[35] That is why, to complete the second step of our classification algorithm it suffices to consider three-dimensional solvable real Lie algebras. We begin by considering two decomposable three-dimensional solvable Lie algebras.

Note that while classifying invariant equations (2.7) we skip those belonging to the class (6.1), since the latter has already been analyzed.

1. Invariance under decomposable Lie algebras

As $A_{3.1}=3A_1=A_{2.1}\oplus A_1$, $A_{3.2}=A_{2.2}\oplus A_1$, to construct all realizations of $A_{3.1}$ it suffices to compute all possible extensions of the (already known) realizations of the algebras $A_{2.1}=\langle e_1, e_2\rangle$ and $A_{2.2}=\langle e_1, e_2\rangle$. To this end we need to supplement the latter by a basis operator e_3 of the form (2.4) in order to satisfy the commutation relations

$$[e_1, e_3] = [e_2, e_3] = 0. \tag{6.2}$$

What is more, to simplify the form of e_3 we may use those transformations from $\mathcal{E}$ that do not alter the remaining basis operators of the corresponding two-dimensional Lie algebras.

We skip the full calculation details and give a couple of examples illustrating the main calculation steps needed to extend $A_{2.1}$ to a realization of $A_{3.1}$.

Consider the realization $A^1_{2.1}$. Upon checking commutation relations (6.2), where e_3 is of form (2.4), we get

$$\lambda_1 = \lambda_2 = r(t,x) = 0, \quad h = k = \text{const}.$$

Consequently, e_3 is the linear combination of e_1, e_2, namely, $e_3=\lambda e_1+ke_2$, which is impossible by the assumption that the algebra under study is three dimensional. Hence we conclude that the above realization of $A^1_{2.1}$ cannot be extended to a realization of the algebra $A_{3.1}$.

Turn now to the realization $A^2_{2.1}$. Checking commutation relations (6.2), where e_3 is of form (2.4) yields the following realization of $A_{3.1}$:

$$\langle t\partial_t + x\partial_x, \sigma(\xi)\partial_u, \gamma(\xi)\partial_u \rangle, \quad \xi = tx^{-1},$$

where $\gamma'\sigma - \gamma\sigma' \neq 0$ However, the corresponding invariant equation (2.7) is linear.

Finally, consider the realization $A^3_{2.1}$. Inserting its basis operators and the operator e_3 of the form (2.4) into (6.2) and solving the obtained equations gives the following realization of $A_{3.1}$:

$$\langle \partial_t, \partial_x, u\partial_u \rangle.$$

Inserting the obtained coefficients for e_3 into the classifying equation (2.5) we get invariant equation

$$u_{tt} = u_{xx} + uG(\omega), \quad \omega = u^{-1}u_x,$$

where (to ensure nonlinearity) we need to have $G_{\omega\omega} \neq 0$.

Similar analysis of the realizations $A^i_{2.1}$ $(i=4,5,\ldots,12,14)$ yields three new invariant equations. For two of thus obtained $A_{3.1}$-invariant equations the corresponding three-dimensional algebras are maximal. The other two may admit four-dimensional invariance algebras provided arbitrary elements are properly specified.

Handling in a similar way the extensions of $A_{2.2}$ up to realizations of $A_{3.2}$ gives 10 inequivalent nonlinear equations whose maximal invariance algebras are realizations of the three-dimensional algebra $A_{3.2}$ and four inequivalent equations (2.7) admitting four-dimensional symmetry algebras.

We perform analysis of equations admitting four-dimensional algebras in the next section. Here we present the complete list of nonlinear equations (2.7) whose maximal symmetry algebras are realizations of three-dimensional Lie algebras $A_{3.1}$ and $A_{3.2}$.

$A_{3.1}$-invariant equations,

$$A^1_{3.1}=\langle \partial_t, \partial_x, u\partial_u\rangle,$$

$$F=uG(\omega), \quad \omega=u^{-1}u_x,$$

$$A^2_{3.1}=\langle \partial_x, \varphi(t)\partial_u, \psi(t)\partial_u\rangle,$$

$$\sigma=\psi'\varphi-\psi\varphi'\neq 0, \quad \sigma'=0,$$

$$F=\varphi^{-1}\varphi'' u+G(t,u_x).$$

$A_{3.2}$-invariant equations,

$$A^1_{3.2}=\langle \partial_t, \partial_x, e^x u\partial_u\rangle,$$

$$F=-u^{-1}u_x^2-u\ln|u|+uG(\omega),$$

$$\omega=u^{-1}u_x-\ln|u|,$$

$$A^2_{3.2}=\langle -t\partial_t-x\partial_x, \partial_t+k\partial_x, u\partial_u\rangle \quad (k\geqslant 0),$$

$$F=u\eta^{-2}G(\omega), \quad \eta=x-kt,$$

$$\omega=\eta u^{-1}u_x,$$

$$A^3_{3.2}=\langle -t\partial_t-x\partial_x+mu\partial_u, \partial_t+k\partial_x, |\eta|^{-m}\partial_u\rangle$$

$$(\eta=x-kt,\ k=m=0 \text{ or } k>0,\ m\in\mathbb{R}),$$

$$F=m(k^2-1)(m+1)\eta^{-2}u+|\eta|^{-2-m}G(\omega),$$

$$\omega=|\eta|^m(mu+\eta u_x),$$

$$A^4_{3.2}=\langle \partial_x, e^x u\partial_u, \partial_t+mu\partial_u\rangle \quad (m>0),$$

$$F=-u^{-1}u_x^2-u_x+uG(\omega),$$

$$\omega = u^{-1}u_x - \ln|u| + mt,$$

$$A^5_{3.2} = \langle -t\partial_t - x\partial_x, \partial_x, u\partial_u \rangle,$$

$$F = ut^{-2}G(\omega), \quad \omega = tu^{-1}u_x,$$

$$A^6_{3.2} = \langle -t\partial_t - x\partial_x, \partial_t + kx^{-1}u\partial_u, u\partial_u \rangle \quad (k > 0),$$

$$F = 2ktx^{-2}u_x - 2ktx^{-3}u + k^2t^2x^{-4}u + x^{-2}uG(\omega),$$

$$\omega = xu^{-1}u_x + ktx^{-1},$$

$$A^7_{3.2} = \langle -t\partial_t - x\partial_x, \partial_t + kx^{-1}u\partial_u, \exp(ktx^{-1})\partial_u \rangle \quad (k > 0),$$

$$F = 2ktx^{-2}u_x + (k^2t^2x^{-4} - 2ktx^{-3} + k^2x^{-2})u + x^{-2}\exp(ktx^{-1})G(\omega), \quad \omega = \exp(-ktx^{-1})(xu_x + ktx^{-1}u),$$

$$A^8_{3.2} = \left\langle \frac{1}{2k}(\partial_t + k\partial_x), e^{x+kt}\partial_u, e^{\eta}\partial_u \right\rangle \quad (k > 0,\ \eta = x - kt),$$

$$F = (k^2 - 1)u + G(\eta, \omega), \quad \omega = u_x - u,$$

$$A^9_{3.2} = \langle \partial_t + f(x)u\partial_u, e^{(1+f(x))t}\partial_u, f(x)e^{f(x)t}\partial_u \rangle,$$

$$F = -(tf'' - t^2(f')^2 - (1 + f)^2)u - 2tf'u_x + e^{tf}G(x, \omega),$$

$$\omega = e^{-tf}(u_x - f'(t + f^{-1})u), \quad f'' + 2f^2 + f = 0, \quad f \neq 0,$$

$$A^{10}_{3.2} = \langle k(t\partial_t + x\partial_x), |t|^{k^{-1}}|\xi|^{(k-1)/2k}\partial_u, |\xi|^{(k-1)/2k}\partial_u \rangle \quad (k \neq 0; 1),$$

$$F = \left[\frac{1-k}{k}\xi^2 + \frac{1-k^2}{4k^2}(1 - \xi^2) \right] t^{-2}u + t^{-2}G(\xi, \omega),$$

$$\omega = |\xi|^{(k-1)/2k}\left[xu_x + \frac{k-1}{2k}u \right], \quad \xi = tx^{-1}.$$

2. Invariance under nondecomposable three-dimensional solvable Lie algebras

There exist seven nondecomposable three-dimensional solvable Lie algebras over the field of real numbers. All those algebras contain a subalgebra which is the two-dimensional Abelian ideal. Consequently, we can use the results of classification of $A_{2.1}$-invariant equations in order to describe equations admitting nondecomposable three-dimensional solvable real Lie algebras. We remind that equations of the form (6.1) has already been analyzed and therefore are not considered in the sequel.

Note that there are nonlinear PDEs of the considered form that admits four-dimensional invariance algebras. As four-dimensional algebras will be considered separately in the next section, we give below only those nonlinear invariant equations whose maximal symmetry algebras are three-dimensional nondecomposable solvable real Lie algebras.

$A_{3.3}$-invariant equations,

$$A^1_{3.3} = \langle u\partial_u, \partial_t + k\partial_x, m\partial_t + k^{-1}xu\partial_u \rangle \quad (k > 0, m \neq 0),$$

$$F = -u^{-1}u_x^2 + uG(\omega), \quad \omega = x - kt + mk^2u^{-1}u_x,$$

$$A^2_{3.3} = \langle u\partial_u, \partial_x, m\partial_t + xu\partial_u \rangle \quad (m > 0),$$

$$F = -u^{-1}u_x^2 + uG(\omega), \quad \omega = t - mu^{-1}u_x,$$

$$A^3_{3.3} = \left\langle |t|^{\frac{1}{2}}\partial_u, -|t|^{\frac{1}{2}} \ln|t|\partial_u, t\partial_t + x\partial_x + \tfrac{1}{2}u\partial_u \right\rangle,$$

$$F = -\tfrac{1}{4}t^{-2}u + u_x^3 G(\xi, \omega), \quad \xi = tx^{-1}, \quad \omega = xu_x^2,$$

$$A^4_{3.3} = \langle \partial_u, -t\partial_u, \partial_t + k\partial_x \rangle \quad (k \geqslant 0),$$

$$F = G(\eta, u_x), \quad \eta = x - kt.$$

$A_{3.4}$-invariant equations,

$$A^1_{3.4} = \langle |\eta|^{m-1}\partial_u, \partial_t + k\partial_x, t\partial_t + x\partial_x + (mu + t|\eta|^{m-1})\partial_u \rangle$$

$$(\eta = x - kt,\ k > 0,\ m \neq 1),$$

$$F = (k^2 - 1)(m - 1)(m - 2)\eta^{-2}u - 2k(m - 1)\eta^{m-2} \ln|\eta| + |\eta|^{m-2}G(\omega),$$
$$\omega = [\eta u_x - (m - 1)u]|\eta|^{-m},$$

$$A^2_{3.4} = \langle \partial_u, -t\partial_u, \partial_t + k\partial_x + u\partial_u \rangle \quad (k \geqslant 0),$$

$$F = e^t G(\eta, \omega), \quad \eta = x - kt, \quad \omega = e^{-t}u_x,$$

$$A^3_{3.4} = \left\langle |t|^{\frac{1}{2}}\partial_u, -|t|^{\frac{1}{2}} \ln|t|\partial_u, t\partial_t + x\partial_x + \tfrac{3}{2}u\partial_u \right\rangle,$$

$$F = -\tfrac{1}{4}t^{-2}u + u_x^{-1}G(\xi, \omega), \quad \xi = tx^{-1}, \quad \omega = x^{-1}u_x^2,$$

$$A^4_{3.4} = \langle kx^{-1}u\partial_u, \partial_t - kx^{-1} \ln|x|u\partial_u, t\partial_t + x\partial_x \rangle \quad (k > 0),$$

$$F = -3ktx^{-3}u - 2x^{-2}u \ln|u| - u^{-1}u_x^2 + x^{-2}uG(\omega),$$

$$\omega = xu^{-1}u_x + \ln|u| + ktx^{-1},$$

$$A^5_{3.4} = \langle \exp(ktx^{-1})\partial_u, \partial_t + kx^{-1}u\partial_u, t\partial_t + x\partial_x + (u + t\exp(ktx^{-1}))\partial_u \rangle \quad (k > 0),$$

$$F = k^2x^{-4}u(t^2 + x^2) + 2x^{-1}(ktx^{-1} + 1)u_x + 2k\exp(ktx^{-1})x^{-1} \ln|x| + x^{-1}\exp(ktx^{-1})G(\omega),$$

$$\omega = \exp(-ktx^{-1})(u_x + ktx^{-2}u).$$

$A_{3.5}$-invariant equations,

$$A^1_{3.5} = \langle |\eta|^{m-1}\partial_u, \partial_t + k\partial_x, t\partial_t + x\partial_x + mu\partial_u\rangle \quad (k > 0,\ m \neq 1),$$

$$F = (k^2 - 1)(m - 1)(m - 2)\,\eta^{-2}u + |\eta|^{m-2}G(\omega),$$

$$\omega = |\eta|^{-m}[\eta u_x - (m - 1)u], \quad \eta = x - kt,$$

$$A^2_{3.5} = \langle \partial_t, \partial_x, t\partial_t + x\partial_x\rangle,$$

$$F = u_x^2 G(u),$$

$$A^3_{3.5} = \langle \partial_t, \partial_x, t\partial_t + x\partial_x + mu\partial_u\rangle \quad (m \neq 0),$$

$$F = |u|^{1-(2/m)}G(\omega), \quad \omega = |u_x|^m |u|^{1-m},$$

$$A^4_{3.5} = \langle \partial_t, \partial_x, t\partial_t + x\partial_x + \partial_u\rangle,$$

$$F = e^{-2u}G(\omega), \quad \omega = e^u u_x,$$

$$A^5_{3.5} = \langle \partial_t, x^{-1}u\partial_u, t\partial_t + x\partial_x\rangle,$$

$$F = -u^{-1}u_x^2 - 2x^{-2}u\ln|u| + x^{-2}uG(\omega),$$

$$\omega = xu^{-1}u_x + \ln|u|,$$

$$A^6_{3.5} = \langle \partial_t + kx^{-1}u\partial_u, \exp(ktx^{-1})\partial_u, t\partial_t + x\partial_x + u\partial_u\rangle \quad (k > 0),$$

$$F = kx^{-4}u[kt^2 - 2tx + kx^2] + 2ktx^{-2}u_x + x^{-1}\exp(ktx^{-1})G(\omega),$$

$$\omega = \exp(-ktx^{-1})(u_x + ktx^{-2}u),$$

$$A^7_{3.5} = \langle \varphi(t)\partial_u, \psi(t)\partial_u, \partial_x + u\partial_u\rangle \quad (\varphi'\psi - \varphi\psi' \neq 0),$$

$$F = \varphi^{-1}\varphi'' u + u_x G(t, \omega),$$

$$\omega = e^{-x}u_x, \quad \varphi''\psi - \varphi\psi'' = 0.$$

$A_{3.6}$-invariant equations,

$$A^1_{3.6} = \langle \partial_t + k\partial_x, |\eta|^{m+1}\partial_u, t\partial_t + x\partial_x + mu\partial_u\rangle \quad (k > 0,\ m \neq -1),$$

$$F = m(k^2 - 1)(m + 1)\,\eta^{-2}u + |\eta|^{m-2}G(\omega),$$

$$\omega = |\eta|^{1-m}[u_x - \eta^{-1}(m + 1)u], \quad \eta = x - kt,$$

$$A^2_{3.6} = \langle \partial_t + mx^{-1}u\partial_u, xu\partial_u, t\partial_t + x\partial_x\rangle \quad (m \geqslant 0),$$

$$F = -u^{-1}u_x^2 - 2mtx^{-3}u + x^{-2}uG(\omega),$$

$$\omega = xu^{-1}u_x - \ln|u| + 2mtx^{-1},$$

$$A_{3.6}^3 = \langle \partial_t + kx^{-1}u\partial_u, \exp(ktx^{-1})\partial_u, t\partial_t + x\partial_x - u\partial_u \rangle \quad (k > 0),$$

$$F = x^{-4}[k^2x^2 - 2ktx + k^2t^2]u + 2ktx^{-2}u_x + x^{-3}\exp(ktx^{-1})G(\omega),$$

$$\omega = \exp(-ktx^{-1})(x^2u_x + ktu),$$

$$A_{3.6}^4 = \langle e^{-t}\partial_u, e^t\partial_u, \partial_t + k\partial_x \rangle \quad (k \geqslant 0),$$

$$F = u + G(\eta, u_x), \quad \eta = x - kt,$$

$$A_{3.6}^5 = \left\langle |t|^{-\frac{1}{2}}\partial_u, |t|^{\frac{3}{2}}\partial_u, t\partial_t + x\partial_x + \tfrac{1}{2}u\partial_u \right\rangle,$$

$$F = \tfrac{3}{4}t^{-2}u + |t|^{-3/2}G(\xi, \omega), \quad \xi = tx^{-1}, \quad \omega = x^{-1}u_x^2.$$

$A_{3.7}$-invariant equations,

$$A_{3.7}^1 = \langle \partial_t + k\partial_x, |\eta|^{m-q}\partial_u, t\partial_t + x\partial_x + mu\partial_u \rangle$$

$$(k > 0,\ m \neq q,\ 0 < |q| < 1),$$

$$F = (k^2 - 1)(m - q)(m - q - 1)\eta^{-2}u + |\eta|^{m-2}G(\omega),$$

$$\omega = |\eta|^{1-m}[u_x - (m - q)\eta^{-1}u], \quad \eta = x - kt,$$

$$A_{3.7}^2 = \langle \partial_t + kx^{-1}u\partial_u, \exp(ktx^{-1})\partial_u, t\partial_t + x\partial_x + qu\partial_u \rangle$$

$$(k > 0, 0 < |q| < 1),$$

$$F = [k^2x^{-2} + k^2x^{-4}t^2 - 2ktx^{-3}]u + 2ktx^{-2}u_x + |x|^{q-2}\exp(ktx^{-1})G(\omega),$$

$$\omega = |x|^{1-q}\exp(-ktx^{-1})(u_x + ktx^{-2}u),$$

$$A_{3.7}^3 = \left\langle |t|^{\frac{1}{2}q}\partial_u, |t|^{1-\frac{1}{2}q}\partial_u, t\partial_t + x\partial_x + \left(1 + \tfrac{1}{2}q\right)u\partial_u \right\rangle \quad (q \neq 0, \pm 1),$$

$$F = \tfrac{1}{4}q(q - 2)t^{-2}u + |t|^{\frac{1}{2}(q-2)}G(\xi, \omega),$$

$$\xi = tx^{-1}, \quad \omega = |t|^{-\frac{1}{2}q}u_x,$$

$$A_{3.7}^4 = \left\langle \exp\left(\tfrac{1}{2}(q - 1)t\right)\partial_u, \exp\left(\tfrac{1}{2}(1 - q)t\right)\partial_u, \partial_t + k\partial_x + \tfrac{1}{2}(1 + q)u\partial_u \right\rangle$$

$$(q \neq 0, \pm 1; k \geqslant 0),$$

$$F=\tfrac{1}{4}(q-1)^2u+\exp\left(\tfrac{1}{2}(1+q)t\right)G(\eta,\omega),$$

$$\eta=x-kt,\quad \omega=\exp\left(-\tfrac{1}{2}(1+q)t\right)u_x,$$

$$A^5_{3.7}=\langle\partial_t+kx^{-1}u\partial_u,|x|^{-q}u\partial_u,t\partial_t+x\partial_x\rangle\quad (k\geqslant 0,\ q\neq 0,\pm 1),$$

$$F=-u^{-1}u_x^2-q(q+1)x^{-2}u\ln|u|+k(q-1)(q+2)tx^{-3}u+ux^{-2}G(\omega),$$
$$\omega=xu^{-1}u_x+q\ln|u|+k(1-q)tx^{-1}.$$

$A_{3.8}$-invariant equations

$$A^1_{3.8}=\langle\cos t\partial_u,-\sin t\partial_u,\partial_t+k\partial_x\rangle\quad (k\geqslant 0),$$

$$F=-u+G(\eta,u_x),\quad \eta=x-kt,$$

$$A^2_{3.8}=\left\langle|t|^{\frac{1}{2}}\cos(\ln|t|)\partial_u,-|t|^{\frac{1}{2}}\sin(\ln|t|)\partial_u,t\partial_t+x\partial_x+\tfrac{1}{2}u\partial_u\right\rangle,$$

$$F=-\tfrac{5}{4}t^{-2}u+|t|^{-3/2}G(\xi,\omega),$$

$$\xi=tx^{-1},\quad \omega=|t|^{1/2}u_x.$$

$A_{3.9}$-invariant equations

$$A^1_{3.9}=\langle\sin t\partial_u,\cos t\partial_u,\partial_t+k\partial_x+qu\partial_u\rangle\quad (k\geqslant 0,\ q>0),$$

$$F=-u+e^{qt}G(\eta,\omega),\quad \eta=x-kt,\omega=e^{-qt}u_x,$$

$$A^2_{3.9}=\left\langle|t|^{\frac{1}{2}}\sin(\ln|t|)\partial_u,|t|^{\frac{1}{2}}\cos(\ln|t|)\partial_u,t\partial_t+x\partial_x+\left(\tfrac{1}{2}+q\right)u\partial_u\right\rangle$$

$$(q\neq 0),\quad F=-\tfrac{5}{4}t^{-2}u+|t|^{q-\frac{3}{2}}G(\xi,\omega),$$

$$\xi=tx^{-1},\quad \omega=|t|^{\frac{1}{2}-q}u_x.$$

C. Complete group classification of Eq. (2.7)

The aim of this section is finalizing group classification of (2.7). The majority of invariant equations obtained in the preceding section contain arbitrary functions of one variable. So that we can utilize the standard Lie–Ovsyannikov approach in order to complete their group classification.

1. Equations depending on an arbitrary function of one variable

Note that equations belonging to the already investigated class of (6.1) are not considered. As our computations show, new results could be obtained for the equations,

$$u_{tt}=u_{xx}+uG(\omega),\quad \omega=u^{-1}u_x, \tag{6.3}$$

$$u_{tt}=u_{xx}+G(u_x), \tag{6.4}$$

only. Below we give (without proof) the assertions describing their group properties.

Assertion 6: Equation (6.3) admits wider symmetry group iff it is equivalent to the following equation:

$$u_{tt} = u_{xx} + mu^{-1}u_x^2 \quad (m \neq 0, -1). \tag{6.5}$$

The maximal invariance algebra of (6.5) is the four-dimensional Lie algebra,

$$A_4 \sim A_{3.5} \oplus A_1, \quad A_4 = \langle \partial_t, \partial_x, t\partial_t + x\partial_x, u\partial_u \rangle.$$

Assertion 7: Equation (6.4) admits wider symmetry group iff it is equivalent to one of the following PDEs:

$$u_{tt} = u_{xx} + e^{u_x}, \tag{6.6}$$

$$u_{tt} = u_{xx} + m \ln|u_x|, \quad m > 0, \tag{6.7}$$

$$u_{tt} = u_{xx} + |u_x|^k, \quad k \neq 0, 1. \tag{6.8}$$

The maximal invariance algebras of the above equations are five-dimensional solvable Lie algebras listed below,

$$A_5^2 = \langle \partial_t, \partial_x, \partial_u, t\partial_u, t\partial_t + x\partial_x + (u - x)\partial_u \rangle,$$

$$A_5^3 = \left\langle \partial_t, \partial_x, \partial_u, t\partial_u, t\partial_t + x\partial_x + \left(2u + \tfrac{1}{2}mt^2\right)\partial_u \right\rangle,$$

$$A_5^4 = \left\langle \partial_t, \partial_x, \partial_u, t\partial_u, t\partial_t + x\partial_x + \frac{k-2}{k-1}u\partial_u \right\rangle.$$

Analyzing the remaining equations containing arbitrary functions of one variable we come to conclusion that one of them can admit wider invariance groups iff either

(1) it is equivalent to PDE of the form (6.1), or
(2) it is equivalent to PDE of the form (6.5).

To finalize the procedure of group classification of Eqs. (2.7) we need to consider invariant equations obtained in the preceding section that contain arbitrary functions of two variables.

2. Classification of equations with arbitrary functions of two variables

In the case under study the standard Lie–Ovsyannikov method is inefficient and we apply our classification algorithm. In order to do this we perform extension of three-dimensional solvable Lie algebras to all possible realizations of four-dimensional solvable Lie algebras. The next step will be to check which of the obtained realizations are symmetry algebras of nonlinear equations of the form (2.7). In what follows we use the results of Ref. 41, where all inequivalent (within the action of inner automorphism group) four-dimensional solvable abstract Lie algebras are given.

The computation details can be found in Ref. 35. Here we summarize the obtained results as follows:

(1) If the functions contained in the equations under study are arbitrary, then the corresponding realizations are their maximal invariance algebras, and
(2) Except for Eq. (6.4), all the equations in question do not allow for extension of their symmetry.

Below we give the complete list of PDEs (2.7) invariant under four-dimensional solvable Lie algebras that are obtained through group analysis of equations with arbitrary functions of two variables.

$A_{2.2} \oplus 2A_1$-invariant equations,

$$(1)\ \langle \partial_x, \partial_t + u\partial_u, e^t\partial_u, e^{-t}\partial_u \rangle, \quad F = u + e^t G(\omega), \quad \omega = u^{-t}u_x,$$

$$(2)\ \left\langle \frac{1}{2k}(\partial_t + k\partial_x), e^{x+kt}\partial_u, e^{\eta}\partial_u, \partial_x + u\partial_u \right\rangle \quad (k > 0, \eta = x - kt),$$

$$F = (k^2 - 1)u + e^{\eta}G(\omega), \quad \omega = e^{-\eta}(u_x - u).$$

$2A_{2.2}$-invariant equations,

$$(1)\ \langle \partial_t + \epsilon u\partial_u, \partial_x, e^{x+kt}\partial_u, e^{x-kt}\partial_u \rangle \quad (\epsilon = 0, 1; k > 0),$$

$$F = (k^2 - 1)u + e^{\epsilon t}G(\omega), \quad \omega = e^{-\epsilon t}(u_x - u),$$

$$(2)\ \langle \alpha\partial_x - u\partial_u, \partial_t + k\partial_x, e^{-t}\partial_u, e^t\partial_u \rangle \quad (k \geqslant 0, \alpha > 0),$$

$$F = u + \exp(-\alpha^{-1}\eta)G(\omega), \quad \eta = x - kt, \quad \omega = \exp(\alpha^{-1}\eta)u_x.$$

$A_{3.3} \oplus A_1$-invariant equations,

$$(1)\ \langle \partial_t, \partial_x, \partial_u, t\partial_u \rangle, \quad F = G(u_x).$$

$A_{3.4} \oplus A_1$-invariant equations

$$(1)\ \langle \partial_u, \partial_x, t\partial_t + x\partial_x + (u + x)\partial_u, t\partial_u \rangle,$$

$$F = t^{-1}G(\omega), \quad \omega = u_x - \ln|t|,$$

$$(2)\ \langle \partial_t + u\partial_u, \partial_x, t\partial_u, \partial_u \rangle, \quad F = e^t G(\omega), \omega = e^{-t}u_x,$$

$$(3)\ \langle x^{-1}\partial_u, \partial_x - x^{-1}(u + \ln|x|)\partial_u, t\partial_t + x\partial_x, tx^{-1}\partial_u \rangle,$$

$$F = 2x^{-1}u_x + x^{-2} + t^{-1}x^{-1}G(\omega), \quad \omega = xu_x + u - \ln|tx^{-1}|.$$

$A_{3.5} \oplus A_1$-invariant equations,

$$(1)\ \langle \partial_x, \partial_u, t\partial_t + x\partial_x + u\partial_u, t\partial_u \rangle, \quad F = t^{-1}G(u_x),$$

$$(2)\ \langle x^{-1}\partial_u, \partial_x - x^{-1}u\partial_u, t\partial_t + x\partial_x, tx^{-1}\partial_u \rangle,$$

$$F = -2x^{-2}u + 2t^{-1}(u_x + x^{-1}u)\ln|t(u_x + x^{-1}u)| + t^{-1}(u_x + x^{-1}u)G(\omega), \quad \omega = xu_x + u.$$

$A_{3.6} \oplus A_1$-invariant equations,

$$(1)\ \langle \partial_x, t\partial_u, t\partial_t + x\partial_x, \partial_u \rangle, \quad F = t^{-2}G(\omega), \quad \omega = t^{-1}u_x,$$

$$(2)\ \langle \partial_t, \partial_x, e^t\partial_u, e^{-t}\partial_u \rangle, \quad F = u + G(u_x).$$

$A_{3.7} \oplus A_1$-invariant equations,

$$(1)\ \left\langle \exp\left(-\tfrac{1}{2}(1 - q)t\right)\partial_u, \exp\left(\tfrac{1}{2}(1 - q)t\right)\partial_u, \partial_t + \tfrac{1}{2}(1 + q)u\partial_u, \partial_x \right\rangle$$

$$(q \neq 0, \pm 1), \quad F = \tfrac{1}{4}(1 - q)^2 u + \exp\left(\tfrac{1}{2}(1 + q)t\right)G(\omega),$$

$$\omega = \exp\left(-\tfrac{1}{2}(1+q)t\right)u_x,$$

$$(2)\ \left\langle \partial_x, |t|^{\frac{1}{2}(1-q)}\partial_u, |t|^{\frac{1}{2}(1+q)}\partial_u, t\partial_t + x\partial_x + \tfrac{1}{2}(1+q)u\partial_u \right\rangle$$

$$(q \neq 0, \pm 1), \quad F = \tfrac{1}{4}(q^2-1)t^{-2}u + |t|^{\frac{1}{2}(q-3)}G(\omega),$$

$$\omega = |t|^{\frac{1}{2}(1-q)}u_x,$$

$$(3)\ \left\langle |t|^{-1/q}|\xi|^{(q+1)/2q}\partial_u, \partial_x - \frac{1+q}{2q}x^{-1}u\partial_u, -q(t\partial_t + x\partial_x), |\xi|^{(1+q)/2q}\partial_u \right\rangle$$

$$(q \neq 0, \pm 1), \quad F = \left[\frac{1-q^2}{4q^2}(t^{-2}+x^{-2})\right]u + \frac{1+q}{q}x^{-1}u_x + t^{-2}|\xi|^{(1+q)/2q}G(\omega),$$
$$\xi = tx^{-1}, \quad \omega = |\xi|^{(q-1)/2q}\left[xu_x + \frac{q+1}{2q}u\right].$$

$A_{3.8} \oplus A_1$-invariant equations,

$$(1)\ \langle \sin t\partial_u, \cos t\partial_u, \partial_t, \partial_x \rangle, \quad F = -u + G(u_x).$$

$A_{3.9} \oplus A_1$-invariant equations,

$$(1)\ \langle \sin t\partial_u, \cos t\partial_u, \partial_t + qu\partial_u, \partial_x \rangle \quad (q > 0),$$

$$F = -u + e^{qt}G(\omega), \quad \omega = e^{-qt}u_x.$$

$A_{4.1}$-invariant equations,

$$(1)\ \langle \partial_u, -t\partial_u, \partial_x, \partial_t - tx\partial_u \rangle, \quad F = G(\omega), \quad \omega = u_x + \tfrac{1}{2}t^2,$$

$$(2)\ \left\langle \partial_u, -t\partial_u, \alpha\partial_x + \tfrac{1}{2}t^2\partial_u, \partial_t + kx\partial_x \right\rangle\ (k \geqslant 0, \alpha > 0),$$

$$F = \alpha^{-1}(x - kt) + G(u_x).$$

$A_{4.2}$-invariant equations,

$$(1)\ \left\langle |t|^{1-\frac{1}{2}q}\partial_u, |t|^{\frac{1}{2}q}\partial_u, \partial_x, t\partial_t + x\partial_x + \left[\left(1+\tfrac{1}{2}q\right)u + x|t|^{\frac{1}{2}q}\right]\partial_u \right\rangle$$

$$(q \neq 0, 1), \quad F = \tfrac{1}{4}q(q-2)t^{-2}u + |t|^{\frac{1}{2}(q-3)}G(\omega),$$

$$\omega = |t|^{\frac{1}{2}(1-q)}u_x - 2|t|^{\frac{1}{2}},$$

$$(2)\ \left\langle \partial_x, \sqrt{|t|}\partial_u, \sqrt{|t|}\,\ln|t|\partial_u, t\partial_t + x\partial_x + \left(q+\tfrac{1}{2}\right)u\partial_u \right\rangle$$

$$(q \neq 0), \quad F = -\tfrac{1}{4}t^{-2}u + |t|^{q-\frac{3}{2}}G(\omega), \quad \omega = |t|^{\frac{1}{2}-q}u_x.$$

$A_{4.3}$-invariant equations,

$$(1)\ \left\langle \partial_x, |t|^{\frac{1}{2}}\partial_u, -|t|^{\frac{1}{2}}\ln|t|\partial_u, t\partial_t + x\partial_x + \tfrac{1}{2}u\partial_u \right\rangle,$$

$$F = -\tfrac{1}{4}t^{-2}u + |t|^{-\frac{3}{2}}G(\omega), \quad \omega = |t|^{\frac{1}{2}}u_x,$$

$$(2)\ \langle \partial_x, t\partial_u, \partial_u, t\partial_t + x\partial_x \rangle, \quad F = t^{-2}G(\omega), \omega = tu_x,$$

$$(3)\ \langle e^{kt}\partial_u, \partial_t + ku\partial_u, \beta\partial_x + te^{kt}\partial_u, e^{-kt}\partial_u \rangle \quad (k \neq 0, \beta > 0),$$

$$F = k^2u + 2k\beta^{-1}xe^{kt} + e^{kt}G(\omega), \quad \omega = e^{-kt}u_x,$$

$$(4)\ \langle e^{x+kt}\partial_u, e^{\eta}\partial_u, \alpha(\partial_x + u\partial_u) + 2kte^{\eta}\partial_u, -(1/2k)(\partial_t + k\partial_x) \rangle$$

$$(\alpha \neq 0,\ k > 0), \quad F = (k^2 - 1)u - 4k^2\alpha^{-1}\eta e^{\eta} + e^{\eta}G(\omega),$$

$$\omega = e^{-\eta}(u_x - u), \quad \eta = x - kt.$$

$A_{4.4}$-invariant equations,

$$(1)\ \left\langle |t|^{\frac{1}{2}}\partial_u, -|t|^{\frac{1}{2}}\ln|t|\partial_u, \partial_x, t\partial_t + x\partial_x + \left[\tfrac{3}{2}u - x|t|^{\frac{1}{2}}\ln|t|\right]\partial_u \right\rangle,$$

$$F = \tfrac{1}{4}t^{-2}u + |t|^{-\frac{1}{2}}G(\omega), \omega = |t|^{-\frac{1}{2}}u_x + \tfrac{1}{2}\ln^2|t|.$$

$A_{4.5}$-invariant equations,

$$(1)\ \langle \partial_x, |t|^{m-\alpha}\partial_u, |t|^{1-m+\alpha}\partial_u, t\partial_t + x\partial_x + mu\partial_u \rangle$$

$$\left(m \neq \tfrac{1}{2}(1+\alpha), \tfrac{1}{2} + \alpha; \alpha \neq 0\right),$$

$$F = (m - \alpha)(m - \alpha - 1)t^{-2}u + |t|^{m-2}G(\omega), \quad \omega = |t|^{1-m}u_x.$$

$A_{4.6}$-invariant equations,

$$(1)\ \left\langle \partial_x, |t|^{\frac{1}{2}}\sin(q^{-1}\ln|t|)\partial_u, |t|^{\frac{1}{2}}\cos(q^{-1}\ln|t|)\partial_u, qt\partial_t + qx\partial_x + \left(\tfrac{1}{2}q + p\right)u\partial_u \right\rangle \quad (q \neq 0, p \geqslant 0),$$

$$F = -\left(\tfrac{1}{4} + q^{-2}\right)t^{-2}u + |t|^{q^{-1}\left(p - \frac{3}{2}q\right)}G(\omega), \quad \omega = |t|^{q^{-1}\left(\frac{1}{2}q - p\right)}u_x.$$

$A_{4.7}$-invariant equations,

$$(1)\ \left\langle \partial_u, -t\partial_u, \partial_t + k\partial_x, t\partial_t + x\partial_x + \left(2u - \tfrac{1}{2}t^2\right)\partial_u \right\rangle \quad (k \geqslant 0),$$

$$F = -\ln|\eta| + G(\omega), \quad \omega = \eta^{-1}u_x, \quad \eta = x - kt.$$

$A_{4.8}$-invariant equations,

$$(1)\ \langle \partial_t + \epsilon u\partial_u, \partial_x, e^x\partial_u, te^x\partial_u \rangle \quad (\epsilon = 0; 1),$$

$$F = -u + e^{\epsilon t}G(\omega), \quad \omega = e^{-\epsilon t}(u_x - u),$$

$$(2)\ \langle |x|^{m-q}\partial_u, \partial_t, t|x|^{m-q}\partial_u, t\partial_t + x\partial_x + mu\partial_u \rangle \quad (q \neq 0,\ m \in \mathbb{R}),$$

$$F = -(m-q)(m-q-1)x^{-2}u + |x|^{m-2}G(\omega),$$

$$\omega = |x|^{1-m}[u_x - (m-q)x^{-1}u],$$

$$(3)\ \langle \partial_t + k\partial_x, \partial_u, t\partial_u, t\partial_t + x\partial_x + qu\partial_u \rangle \quad (k > 0,\ q \in \mathbb{R}),$$

$$F = |\eta|^{q-2}G(\omega), \quad \omega = |\eta|^{1-q}u_x, \quad \eta = x - kt,$$

$$(4)\ \langle x^{-1}\partial_u, \partial_t + \partial_x - x^{-1}u\partial_u, tx^{-1}\partial_u, t\partial_t + x\partial_x \rangle,$$

$$F = 2x^{-1}u_x + x^{-1}(t-x)^{-1}G(\omega), \quad \omega = xu_x + u,$$

$$(5)\ \langle \partial_u, -t\partial_u, \partial_t + k\partial_x + u\partial_u, \alpha\partial_x + u\partial_u \rangle \quad (\alpha \neq 0,\ k \geqslant 0),$$

$$F = \exp(\alpha^{-1}\eta + t)G(\omega), \quad \omega = \exp(-\alpha^{-1}\eta - t)u_x, \quad \eta = x - kt.$$

$A_{4.10}$-invariant equations,

$$(1)\ \langle \sin t\partial_u, \cos t\partial_u, \partial_x + u\partial_u, \partial_t + k\partial_x \rangle \quad (k \geqslant 0),$$

$$F = -u + e^{\eta}G(\omega), \quad \omega = e^{-\eta}u_x, \quad \eta = x - kt.$$

In the above formulas $G = G(\omega)$ is an arbitrary function satisfying the condition $F_{u_x u_x} \neq 0$.

CONCLUDING REMARKS

Let us briefly summarize the results obtained in this paper.

We prove that the problem of group classification of the general quasilinear hyperbolic type equation (1.1) reduces to classifying equations of more specific forms,

$$\text{(I)}\ u_{tt} = u_{xx} + F(t,x,u,u_x), \quad F_{u_x u_x} \neq 0,$$

$$\text{(II)}\ u_{tt} = u_{xx} + g(t,x,u)u_x + f(t,x,u), \quad g_u \neq 0,$$

$$\text{(III)}\ u_{tx} = g(t,x)u_x + f(t,x,u), \quad g_x \neq 0, \quad f_{uu} \neq 0,$$

$$\text{(IV)}\ u_{tx} = f(t,x,u), \quad f_{uu} \neq 0.$$

If we denote as $\mathcal{DE}$ the set of PDEs (II)–(III), then the results of application of our algorithm for group classification of equations (I)–(IV) can be summarized as follows.

(1) We perform complete group classification of the class $\mathcal{DE}$. We prove that the Liouville equation has the highest symmetry properties among equations from $\mathcal{DE}$. Next, we prove that the only equation belonging to this class and admitting the four-dimensional invariance algebra is the nonlinear d'Alembert equations. It is established that there are 12 inequivalent equations from $\mathcal{DE}$ invariant under three-dimensional Lie algebras. We give the lists of all inequivalent equations from $\mathcal{DE}$ that admit one- and two-dimensional symmetry algebras.

(2) We have studied the structure of invariance algebras admitted by nonlinear equations from the class (I). It is proved, in particular, that their invariance algebras are necessarily solvable.

(3) We perform complete group classification of nonlinear equations from the class of PDEs (I). We prove that the highest symmetry algebras admitted by those equations are five dimen-

sional and construct all inequivalent classes of equations invariant with respect to five-dimensional Lie algebras. We also construct all inequivalent equations of the form (I) admitting one-, two-, three-, and four-dimensional Lie algebras.

In one of our future papers we intend to exploit the obtained classification results to construct exact solutions of nonlinear wave equations (I)–(IV).

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A cluster expansion for the decay of correlations of light-mass quantum crystals and some stochastic models under intense noise

Rafael S. Thebaldi[a] and Emmanuel Pereira[b]
Departamento de Física-ICEx, Universidade Federal de Minas Gerais, C.P. 702, 30.161-970 Belo Horizonte MG, Brazil

Aldo Procacci[c]
Departamento de Matemática - ICEx, Universidade Federal de Minas Gerais, C.P. 702, 30.161-970 Belo Horizonte MG, Brazil

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We analyze the two- and four-point truncated function of a lattice system of unbounded continuous spin variables describing a large class of light-mass quantum anharmonic crystals and some stochastic Ginzburg–Landau-type models under intense noise. We develop a cluster expansion and use it to obtain the decay of the two-point truncated function (which gives information about the one-particle excitations), for the interactions with finite range or with polynomial decay. Moreover, using a Bethe–Salpeter equation, we investigate the four-point truncated in a perturbative approach (whose reliability is supported by the convergence of the cluster expansion), and establish a condition for the existence of a two-particle bound state in the low-lying spectrum of the system. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1895845]

I. INTRODUCTION

In this paper we develop a cluster expansion and investigate the low-lying spectrum of some systems related to commonly used physical models, namely, to light-mass quantum crystals and to stochastic Ginzburg–Landau- (GL) type models submitted to intense noise.

The interest of such problems is well known. The study of the basic properties of the quantum crystals, for example, is an old problem in physics. For these crystal models we mean a system of unbounded continuous spin variables $\varphi_i \in \mathbb{R}$, in a lattice space with Hamiltonian given by

$$H = \sum_{i \in \mathbb{Z}^d} -\frac{1}{2m}\frac{\partial^2}{\partial \varphi_i^2} + \frac{1}{2}\sum_{i,j \in \mathbb{Z}^d} \varphi_i J_{ij} \varphi_j + \sum_{i \in \mathbb{Z}^d} V(\varphi_i), \tag{1}$$

where $J_{i,j}$ is usually taken as a positive operator (e.g., the lattice Laplacian; i.e., in some recent rigorous works the pair interaction is restricted to the ferromagnetic case), and V is given, e.g., by $V(\varphi_i) = a\varphi_i^2 + b\varphi_i^4$. In the present paper, we consider more general cases, we do not restrict the quadratic interaction to ferromagnetic cases and neither the anharmonic potential to a local interaction. We give details later. Recently, several works have been devoted to a rigorous analysis of the small mass behavior of such lattice models (light-mass means that the system is strongly quantum). For example, in Refs. 1 and 2 the fact that small mass implies uniqueness of Gibbs states of a quantum crystal is rigorously established (there, for the ferromagnetic case and with local anharmonicity), an important result about the influence of quantum effects on structural

[a]Electronic mail: rafaelst@fisica.ufmg.br
[b]Electronic mail: emmanuel@fisica.ufmg.br
[c]Electronic mail: aldo@mat.ufmg.br

phase transitions. See also Ref. 3 and references therein for more recent results. Effects of nonlocality in the anharmonicity on the spectral properties of quantum crystals (in the regime of large mass) are presented in Ref. 4. In the present paper, besides other results, such as the uniqueness of a phase given by the convergence of the cluster expansion, we will establish conditions for the existence of a two-particle bound state in the excitation spectrum of these light-mass quantum crystals, showing that the system, although in a single phase region, may have nontrivial spectral excitations.

The stochastic GL-type models are also extensively investigated in physics, in particular, in the study of dynamical critical phenomena. The spectrum of the generator of the dynamics gives information about, e.g., the relaxation rates of the correlation functions, and so, it is of direct physical interest. Recently, several works have been devoted to detailed investigations on the spectral properties of such systems. For the weakly coupled GL model, the existence of an isolated one-particle and two-particle bound states have been established perturbatively in Ref. 5, and rigorously in Ref. 6. Effects on the spectrum due to changes in the noise strength are presented in Refs. 7–9, for the small noise regime, and in Ref. 10 for intense noise. In Ref. 11, the one-particle state is rigorously established for a particular case of these GL-type models under intense noise.

In order to make clear the relation between the stochastic GL system and the anharmonic quantum crystal, we present below a brief technical description of the dynamics generator of the stochastic model.

Consider a system of unbounded continuous spin variables $\phi_{\vec{x},t} \in \mathbb{R}$, in a lattice space box $\vec{x} \in V \subset \mathbb{Z}^d$ (the thermodynamic limit is considered when $V \to \mathbb{Z}^d$), with time evolution (Langevin dynamics) given by

$$\frac{\partial}{\partial t}\phi_{\vec{x},t} = -\frac{1}{2}\nabla S(\phi_{\vec{x},t}) + \eta_{\vec{x},t}, \quad \phi_{\vec{x},t=0} = \psi_{\vec{x}}, \tag{2}$$

where $\nabla S = \delta S / \delta \phi$, and the GL (spatial) interaction is

$$S(\phi) = \frac{1}{2}\sum_{\vec{x},\vec{y}\in V} J_{\vec{x},\vec{y}}\phi_{\vec{x}}\phi_{\vec{y}} + \lambda \sum_{\vec{x}\in V} \mathcal{P}(\phi_{\vec{x}}), \tag{3}$$

$\lambda > 0$, $\mathcal{P}$ is a polynomial bounded from below; η is a family of Gaussian white-noise processes with expectations

$$E(\eta_{\vec{x},t}) = 0, \quad E(\eta_{\vec{x},t}\eta_{\vec{y},t'}) = \gamma\delta_{\vec{x},\vec{y}}\delta(t-t'), \tag{4}$$

$\vec{x} \in V$, $t \in [0,\infty)$ (in principle, we extend the time interaction to $-t$ and introduce a time regularizer that makes t discrete later); $\gamma > 0$ is the noise strength, we will treat the regime $\gamma \gg 1$. $J_{\vec{x},\vec{y}}$ is an arbitrary summable spatial interaction, i.e., we assume that $J_{\vec{x},\vec{y}}$ is symmetric, translational invariant with

$$\sup_{\vec{x}\in\mathbb{Z}^d} \sum_{\vec{y}\in\mathbb{Z}^d} |J_{\vec{x},\vec{y}}| < \infty. \tag{5}$$

Note that the pair potential $J(\vec{x},\vec{y})$ does not have to be positive.

The time evolution of functions f of the spin configuration ϕ for such systems is defined by

$$f_t(\psi) = E(f(\phi_t)),$$

where $\psi = \phi_{t=0}$ is some initial condition. From Itô calculus, it follows that

$$f_t(\psi) = e^{-t\mathcal{H}_V^0} f(\psi), \quad \mathcal{H}_V^0 f = \left\{ \sum_{\vec{x}\in V} -\frac{1}{2}\gamma \frac{\partial^2}{\partial \phi_{\vec{x}}^2} + \frac{1}{2}\frac{\partial S}{\partial \phi_{\vec{x}}}\frac{\partial}{\partial \phi_{\vec{x}}} \right\} f. \tag{6}$$

The generator $\mathcal{H}_V^0$ of the strongly continuous semigroup describing the Markov dynamics above is Hermitian and positive in the Hilbert space $L^2(\mathrm{d}\sigma_V^0)$, where $\mathrm{d}\sigma_V^0$ is the invariant measure given by the Gibbs probability distribution

$$\mathrm{d}\sigma_V^0 = e^{-S(\phi)/\gamma}\, \mathrm{d}\phi_V/\text{normalization}, \quad \text{where } \mathrm{d}\phi_V = \prod_{\vec{x}\in V} \mathrm{d}\phi_{\vec{x}}. \tag{7}$$

The ground state of $\mathcal{H}_V^0$ is the eigenfunction $f \equiv 1$ with eigenvalue zero. We note that $\mathcal{H}_V^0$ is unitarily equivalent to a Schrödinger operator with a potential going to infinity, defining the unitary operator U_V^0 from $L^2(\mathrm{d}\sigma_V^0) \to L^2(\mathrm{d}\phi_V)$ as

$$(U_V^0 f)(\phi) = Z_V^{-1/2} e^{-(1/2\gamma)S} f(\phi),$$

where Z_V is the normalization in $\mathrm{d}\sigma_V^0$, a straightforward calculation gives us

$$H_V^0 = U_V^0 \mathcal{H}_V^0 (U_V^0)^{-1} = \sum_{\vec{x}\in V} -\frac{1}{2}\gamma \frac{\partial^2}{\partial \phi_{\vec{x}}^2} + \frac{1}{4}\sum_{\vec{x}\in V}\left[\frac{1}{2\gamma}\left(\frac{\partial S}{\partial \phi_{\vec{x}}} \right)^2 - \frac{\partial^2 S}{\partial \phi_{\vec{x}}^2} \right]. \tag{8}$$

Performing the derivatives, we get

$$\begin{aligned} H_V^0 = &-\frac{1}{2}\gamma \sum_{\vec{x}\in V} \frac{\partial^2}{\partial \phi_{\vec{x}}^2} + \frac{1}{8\gamma}\sum_{\vec{x},\vec{y}\in V} [J * J]_{\vec{x},\vec{y}} \phi_{\vec{x}} \phi_{\vec{y}} + \frac{\lambda}{4\gamma}\sum_{\vec{x},\vec{y}\in V} J_{\vec{x},\vec{y}} \mathcal{P}'(\phi_{\vec{x}})\phi_{\vec{y}} \\ &+ \sum_{\vec{x}\in V}\left[\frac{\lambda^2}{8\gamma}\mathcal{P}'(\phi_{\vec{x}})^2 - \frac{\lambda}{4}\mathcal{P}''(\phi_{\vec{x}}) + c \right], \end{aligned} \tag{9}$$

where c is a constant (depending of J and d), and $[J*J]_{\vec{x},\vec{y}} = \Sigma_{\vec{z}\in V} J_{\vec{x},\vec{z}} J_{\vec{z},\vec{y}}$ is the spatial convolution.

The relation between the spectral properties of the generator of the stochastic dynamics and the study of the excitation spectrum of the quantum anharmonic crystals becomes evident from the expression for H_V^0 above, as we have recalled, note that the large noise intensity γ above represents the inverse of small mass m of the particles for the anharmonic oscillators in (1); note also that the stochastic "potential" is more intricate.

It is useful to construct a Feynman–Kac integral formalism associated to H_V^0 [or to H (1)]. It follows from standard procedures.[12] If $f_1, \ldots, f_n$ are functions of the spin configuration in V, $\Omega(\phi) = 1$ is the ground state of $\mathcal{H}_V^0$ and for $t_1 \leqslant t_2 \leqslant \cdots t_n \in \mathbb{R}$, now $t_i \in [-T, T]$, then we have

$$\begin{aligned} (\Omega, f_1 e^{-(t_2-t_1)\mathcal{H}_V^0} f_2 \cdots e^{-(t_n-t_{n-1})\mathcal{H}_V^0} f_n \Omega)_{L^2(\mathrm{d}\sigma_V^0)} &= (U_V^0\Omega, f_1 e^{-(t_2-t_1)H_V^0} f_2 \cdots e^{-(t_n-t_{n-1})H_V^0} f_n U_V^0 \Omega)_{L^2(\mathrm{d}\phi_V)} \\ &= \int f_1(\phi(t_1)) \cdots f_n(\phi(f_n)) \mathrm{d}\rho_V^0, \end{aligned} \tag{10}$$

where the path space measure $\mathrm{d}\rho_V^0$ is the weak limit $T \to \infty$ of

$$\mathrm{d}\rho_\Lambda^0 = \frac{e^{-W_\Lambda^0(\phi)}\, \mathrm{d}\omega_\Lambda^0}{\displaystyle\int e^{-W_\Lambda^0(\phi)}\, \mathrm{d}\omega_\Lambda^0}, \tag{11}$$

with $\Lambda \equiv ([-T, T], V)$ and

$$W_\Lambda^0(\phi) = \int_{-T}^{T} \mathrm{d}t \left\{ \frac{\lambda}{4\gamma}\sum_{\vec{x},\vec{y},\in V} J_{\vec{x},\vec{y}} \mathcal{P}'(\phi_{\vec{x}})\phi_{\vec{y}} + \sum_{\vec{x}\in V}\left[\frac{\lambda^2}{8\gamma}\mathcal{P}'(\phi_{\vec{x}})^2 - \frac{\lambda}{4}\mathcal{P}''(\phi_{\vec{x}}) \right] \right\}, \tag{12}$$

and $\mathrm{d}\omega_\Lambda^0$ is a Gaussian measure with mean zero and variance given by

$$\gamma C_\Lambda(t,\vec{x};t',\vec{y}) = \int \phi_{t,\vec{x}}\phi_{t',\vec{y}}\,\mathrm{d}\omega_\Lambda^0 = \frac{\gamma}{2\pi|V|}\int_{-\infty}^{\infty}\mathrm{d}p_0 \sum_{\vec{p}\in\tilde{V}} \frac{e^{ip_0(t-t')}e^{i\vec{p}\cdot(\vec{x}-\vec{y})}}{p_0^2+[\tilde{J}(\vec{p})]^2/4}, \tag{13}$$

where $\tilde{J}(\vec{p})$ is the Fourier transform of $J_{\vec{x},\vec{y}}$; $|V|$ is the number of points in V; $\tilde{V}$ is the Fourier dual lattice; $\vec{p}=(p_1,\ldots,p_d)\in\tilde{V}$ and $\vec{p}\cdot(\vec{x}-\vec{y})=\Sigma_{i=1}^d p_i(x_i-y_i)$.

The Feynman–Kac formula above and the spectral theorem for Hermitian operators give us the connection between the spectrum of the generator of the dynamics and the behavior of the correlation functions. For example, for the truncated two-point function $S_2(x;y)\equiv\langle\phi_x\phi_y\rangle-\langle\phi_x\rangle\times\langle\phi_y\rangle\equiv\int\phi_x\phi_y\,\mathrm{d}\rho_V^0-\int\phi_x\,\mathrm{d}\rho_V^0\int\phi_y\,\mathrm{d}\rho_V^0$, $x\equiv(x_0,\vec{x})$, $x_0\equiv t\in\mathbb{R}$, $\vec{x}\in\mathbb{Z}^d$ (let us assume the thermodynamic limit in this short comment), direct calculations lead to

$$\tilde{S}_2(p) = \int_0^\infty \int_{\mathbf{T}^d} \frac{2E}{E^2+(p_0)^2}(2\pi)^d\delta(\vec{q}-\vec{p})d(\Omega,\phi\mathcal{E}(E,\vec{q})\phi\Omega), \tag{14}$$

where $\tilde{S}_2$ is the Fourier transform of S_2, $\mathcal{E}(E,\vec{p})$ is the spectral projection associated with the operators $(H,\vec{P})$ (the momentum operator $\vec{P}$ is the space translation generator), the integral over E runs from 0 to ∞ and that over $\vec{q}$ runs in T^d. Hence, a singularity in $\tilde{S}_2$ for imaginary $p_0=ik_0$ gives a point in the spectrum (one-particle sector) of the generator of the dynamics, and, by the Paley–Wiener theorem, the singularity in $\tilde{S}_2$ is related to the decay of S_2. Similarly, the decay of the truncated four-point function gives us information about, e.g., the existence of two-particle bound states. More details and comments are presented in Ref. 6 and references therein.

The rest of the paper is organized as follows.

In Sec. II we introduce the model to be treated here, describe a formalism for the correlations (a Feynman–Kac-type integral formalism) and list the main results of the paper. In Sec. III we present the cluster expansion, whose convergence is proved in Sec. IV. Section V is devoted to the study of the decay of the two-point truncated correlation, and Sec. VI to the analysis of the four-point truncated function.

II. THE MODEL AND MAIN RESULTS

In the present paper we will analyze in detail the model of unbounded continuous scalar field variables with (say) Hamiltonian

$$H_V = \sum_{\vec{x}\in V} -\frac{1}{2}\gamma\frac{\partial^2}{\partial\phi_{\vec{x}}^2} + \frac{1}{2}\sum_{\vec{x},\vec{y}\in V}\phi_{\vec{x}}J_{\vec{x},\vec{y}}\phi_{\vec{y}} + \lambda\sum_{\vec{x}\in V}Q(\phi_{\vec{x}}), \tag{15}$$

where

$$Q(\phi_{\vec{x}}) = P(\phi_{\vec{x}}) + \sum_{i=1}^{c}\sum_{\vec{y}\in V}\phi_{\vec{x}}^{a_i}D_{\vec{x},\vec{y}}^{(i)}\phi_{\vec{y}}^{b_i}, \tag{16}$$

$\phi_{\vec{x}}\in\mathbb{R}$, $V\subset\mathbb{Z}^d$, $\gamma>0$, $\lambda>0$, P is a polynomial bounded from below of degree $2m$, $c>0$ is an integer, a_i,b_i with $i=1,2,\ldots,c$, are integers such that $1\leqslant a_i,\ b_i\leqslant m$. $J_{\vec{x},\vec{y}}$ and $D_{\vec{x},\vec{y}}^{(i)}$ are symmetric spatial interactions, translational invariant and such that, $\forall_i=1,2,\ldots,c$,

$$\sup_{\vec{x}\in\mathbb{Z}^d}\sum_{\vec{y}\in\mathbb{Z}^d}|J_{\vec{x},\vec{y}}| \equiv J_M<\infty, \quad \sup_{\vec{x}\in\mathbb{Z}^d}\sum_{\vec{y}\in\mathbb{Z}^d}|D_{\vec{x},\vec{y}}^{(i)}| \equiv D_M^{(i)}<\infty. \tag{17}$$

Analyzing these specific models, we will get properties of a large class of anharmonic quantum crystals as well as of some stochastic GL models.

The spectral results to be presented are supported by a cluster expansion which we develop here. To obtain these results, in a rough resume, we start from the dynamics generator (or Hamiltonian), establish a lattice Feynman–Kac integral formula for the correlation functions, relating the

initial problem to a spatially nonlocal imaginary time quantum field theory. Then, we study the decay of some truncated correlation functions using our "high temperature" cluster expansion for unbounded spin systems, which is related to that recently proposed in Ref. 13. Information on the two-particle spectrum (related to the four-point correlation functions) is obtained in a perturbative analysis only, we use the Bethe–Salpeter (BS) equation with the BS kernel in a ladder approximation (details ahead). The reliability of the perturbative result is supported (again) by the convergence of the cluster expansion.

The Feynman–Kac functional integral associated to H_V follows, as said, from standard procedures. If $f_1,\ldots,f_n$ are functions of the spin configuration in V, $t_1\leqslant t_2\leqslant\cdots t_n\in\mathbb{R}$, as described in the introduction, we have an integral representation for the correlations

$$\int f_1(\phi(t_1))\cdots f_n(\phi(t_n))\mathrm{d}\rho_V, \tag{18}$$

where, now, the path space measure $\mathrm{d}\rho_V$ is the weak limit $T\to\infty$ of

$$\mathrm{d}\rho_\Lambda=\frac{e^{-W_\Lambda(\phi)}\,\mathrm{d}\omega_\Lambda}{\displaystyle\int e^{-W_\Lambda(\phi)}\,\mathrm{d}\omega_\Lambda}, \tag{19}$$

with $\Lambda\equiv([-T,T],V)$ and

$$W_\Lambda(\phi)=\int_{-T}^{T}\mathrm{d}t\,\lambda\sum_{\vec{x}\in V}Q(\phi_{t,\vec{x}})=\int_{-T}^{T}\mathrm{d}t\,\lambda\left[\sum_{\vec{x}\in V}P(\phi_{t,\vec{x}})+\sum_{i=1}^{c}\sum_{\vec{x},\vec{y}\in V}\phi_{t,\vec{x}}^{a_i}D_{\vec{x},\vec{y}}^{(i)}\phi_{t,\vec{y}}^{b_i}\right], \tag{20}$$

and $\mathrm{d}\omega_\Lambda$ is a Gaussian measure with mean zero and variance given by

$$\gamma C_\Lambda(t,\vec{x};t',\vec{y})=\int\phi_{t,\vec{x}}\phi_{t',\vec{y}}\,\mathrm{d}\omega_\Lambda=\frac{\gamma}{2\pi|V|}\int_{-\infty}^{\infty}\mathrm{d}p_0\sum_{\vec{p}\in\tilde{V}}\frac{e^{ip_0(t-t')}e^{i\vec{p}\cdot(\vec{x}-\vec{y})}}{p_0^2+\gamma\tilde{J}(\vec{p})}, \tag{21}$$

where $\tilde{J}(\vec{p})$ is the Fourier transform of $J_{\vec{x},\vec{y}}$; $|V|$ is the number of points in V; $\tilde{V}$ is the Fourier dual lattice; $\vec{p}=(p_1,\ldots,p_d)\in\tilde{V}$ and $\vec{p}\cdot(\vec{x}-\vec{y})=\sum_{i=1}^{d}p_i(x_i-y_i)$.

For technical reasons, we will consider a time regularized version of the measure $\mathrm{d}\rho_\Lambda$. Precisely, from now on, we consider only the values of t in $\mathbb{Z}\cap[-T,T]$, so that our Feynman–Kac integral formula (18) becomes, say, the description of continuous spin system in a finite box $\Lambda\equiv(\mathbb{Z}\cap[-T,T],V)$ in $\mathbb{Z}^{d+1}$ (with periodic boundary conditions in space and free boundary conditions in time). Recall from field theory that such a (ultraviolet) cutoff shall not change the low-lying spectrum. We also will use the notation $x=(x_0,\vec{x})\in\mathbb{Z}^{d+1}$ with $x_0\in\mathbb{Z}\cap[-T,T]$ being the discrete time coordinate and $\vec{x}\in V$ the space coordinate. We define $\beta\equiv1/\gamma$, and so, intense noise regime $\gamma\gg1$ corresponds to the small β regime. Hence, from the path space measure $\mathrm{d}\rho_\Lambda$ with discrete time, we introduce the "Gibbs measure" for such system,

$$\begin{aligned}\mu_\Lambda(\cdot)&=\left[\int e^{-W_\Lambda(\phi)}\,\mathrm{d}\omega_\Lambda\right]^{-1}\int(\cdot)e^{-W_\Lambda(\phi)}\,\mathrm{d}\omega_\Lambda=\frac{1}{Z_\Lambda}\int(\cdot)\exp\left\{-\lambda\sum_{x\in\Lambda}Q(\phi_x)\right\}\\&\quad\times\exp\left\{-\frac{1}{2\gamma}\sum_{x,y\in\Lambda}\phi_xC_\Lambda^{-1}(x,y)\phi_y\right\}\prod_{x\in\Lambda}\mathrm{d}\phi_x,\end{aligned} \tag{22}$$

where

$$\sum_{x\in\Lambda} Q(\phi_x) = \sum_{x\in\Lambda} P(\phi_x) + \sum_{i=1}^{c}\sum_{x,y\in\Lambda} \phi_x^{a_i} D^{(i)}_{\vec{x},\vec{y}} \phi_y^{b_i} \delta_{x_0,y_0}[\delta_{\vec{x},\vec{y}} + (1-\delta_{\vec{x},\vec{y}})] = \sum_{x\in\Lambda}\left[P(\phi_x) + \sum_{i=1}^{c} D^{(i)}_{\vec{x},\vec{x}} \phi^{a_i+b_i}\right]$$
$$+ \sum_{i=1}^{c}\sum_{x,y\in\Lambda} \phi_x^{a_i} D^{(i)}_{\vec{x},\vec{y}} \phi_y^{b_i} \delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}}), \tag{23}$$

$$\sum_{x,y\in\Lambda} \phi_x C^{-1}_{\Lambda}(x,y)\phi_y = \sum_{x,y\in\Lambda} \phi_x(-\delta_{\vec{x},\vec{y}}\Delta_t + \gamma J_{\vec{x},\vec{y}}\delta_{x_0,y_0})\phi_y = \sum_{x,y\in\Lambda} \phi_x\{\delta_{\vec{x},\vec{y}}(2\delta_{x_0,y_0} - \delta_{|x_0-y_0|,1})$$
$$+ \gamma J_{\vec{x},\vec{y}}\delta_{x_0,y_0}[\delta_{\vec{x},\vec{y}} + (1-\delta_{\vec{x},\vec{y}})]\}\phi_y = \sum_{x\in\Lambda}[2\phi_x^2 + \gamma J_{\vec{x},\vec{x}}\phi_x^2]$$
$$+ \sum_{x,y\in\Lambda} \phi_x[-\delta_{\vec{x},\vec{y}}\delta_{|x_0-y_0|,1} + \gamma J_{\vec{x},\vec{y}}\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}})]\phi_y. \tag{24}$$

We used above that, due to the discrete time, $-\Delta_t = 2\delta_{x_0,y_0} - \delta_{|x_0-y_0|,1}$. In short, we have

$$\mu_\Lambda(\cdot) = \frac{1}{Z_\Lambda}\int \prod_{x\in\Lambda} \mathrm{d}\phi_x\, e^{-\beta U(\phi_x)} \prod_{\{x,y\}\subset\Lambda} e^{\beta G_{xy}(\phi_x,\phi_y)}(\cdot), \tag{25}$$

where $\mathrm{d}\phi_x$ is the Lebesgue measure in $\mathbb{R}$ and the partition function Z_Λ is defined by

$$Z_\Lambda \equiv \int \prod_{\{x,y\}\subset\Lambda} e^{\beta G_{xy}(\phi_x,\phi_y)} \prod_{x\in\Lambda} \mathrm{d}\phi_x\, e^{-\beta U(\phi_x)}. \tag{26}$$

Here, $U(\phi)$ is a local polynomial function (on site potential) bounded from below and given by

$$U(\phi) = \frac{\lambda}{\beta}P(\phi) + \frac{J(0)}{2\beta}\phi^2 + \phi^2 + \frac{\lambda}{\beta}\sum_{i=1}^{c}\phi^{a_i+b_i}D_i(0), \tag{27}$$

with $J(0)\equiv J(\vec{x},\vec{x})$ and $D_i(0)\equiv D^{(i)}(\vec{x},\vec{x})$; we assume that $J(\vec{x},\vec{y})$ and $D^{(i)}(\vec{x},\vec{y})$ are translational invariant and $J(\vec{x},\vec{y}) = J(|\vec{y}-\vec{x}|)$, $D^{(i)}(\vec{x},\vec{y}) = D^{(i)}(|\vec{y}-\vec{x}|)$. The coupling term is given by

$$G_{xy}(\phi_x,\phi_y) = -\left[\frac{1}{\beta}J_{\vec{x},\vec{y}}\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}}) - \delta_{\vec{x},\vec{y}}\delta_{|x_0-y_0|,1}\right]\frac{\phi_x\phi_y}{2} - \frac{\lambda}{\beta}\sum_{i=1}^{c} D^{(i)}_{\vec{x},\vec{y}}\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}})\phi_x^{a_i}\phi_y^{b_i}$$
$$= A^{(1)}_{xy}\phi_x\phi_y + \sum_{i=1}^{c} A^{(i+1)}_{xy}\phi_x^{a_i}\phi_y^{b_i} = \sum_{s=1}^{c+1} A^{(s)}_{xy}\phi_x^{a_{s-1}^{(1-\delta_{s,1})}}\phi_y^{b_{s-1}^{(1-\delta_{s,1})}}, \tag{28}$$

where we define $a_0\equiv 1$, $b_0\equiv 1$, and for $s=2,3,\ldots,(c+1)$.

$$A^{(1)}_{xy} \equiv -\frac{1}{2}\left[\frac{1}{\beta}J_{\vec{x},\vec{y}}\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}}) - \delta_{\vec{x},\vec{y}}\delta_{|x_0-y_0|,1}\right], \quad A^{(s)}_{xy} \equiv -\frac{\lambda}{\beta}D^{(s-1)}_{\vec{x},\vec{y}}\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}}). \tag{29}$$

Note that our problem involves, say, an unusual high temperature spin system, we have a nonlocal anharmonic potential and the interaction decay depends on the direction (polynomial in space, and short range in "time").

The two-point truncated function is given by

$$S_2(x;y) = \mu_\Lambda(\phi_x\phi_y) - \mu_\Lambda(\phi_x)\mu_\Lambda(\phi_y). \tag{30}$$

In the next section we will develop a polymer expansion for such model, which will permit us to show that $S_2(x;y)$ is analytic in β and admits upper and lower bounds uniform in Λ.

Now, let us state our main results.

Theorem 1: *The two-point truncated function $S_2(x;y)$, written as series in β, converges*

absolutely, uniformly in the volume $|\Lambda|$, *for* β, J_M *and* λ *small enough. Moreover,* $S_2(x;y)$ *has the following bounds:*

$$|S_2(x;y)| \leq C' e^{-m|x_0-y_0|-m_s|\vec{x}-\vec{y}|},$$

if $J_{\vec{x},\vec{y}}$ *and* $D^{(i)}_{\vec{x},\vec{y}}$ *are finite range (i.e., if* $\exists\, r>0$ *such that* $J_{\vec{x},\vec{y}}=0$ *for* $|\vec{x}-\vec{y}|>r$, *and the same for* $D^{(i)}_{\vec{x},\vec{y}}$, *where* C' *is a constant uniform in* β, J_M *and* $\lambda D^{(i)}_M$; *or*

$$|S_2(x;y)| \leq C'' e^{-m'|x_0-y_0|}\left(\frac{1-\delta_{\vec{x},\vec{y}}}{|\vec{x}-\vec{y}|^p}+\delta_{\vec{x},\vec{y}}\right),$$

if $J_{\vec{x},\vec{y}}$ *and* $D^{(i)}_{\vec{x},\vec{y}}$ *have polynomial decay, i.e., for* $\vec{x}\neq\vec{y}$, $J_{\vec{x},\vec{y}}\leq J/|\vec{x}-\vec{y}|^p$ *and* $D^{(i)}_{\vec{x},\vec{y}}\leq D_i/|\vec{x}-\vec{y}|^p$; *where* C'' *is a constant uniform in* β, J_M *and* $\lambda D^{(i)}_M$.

Remarks:

(1) The upper bound described in Theorem 1 shall give, essentially, the asymptotic behavior of the two-point truncated correlation. Namely, assuming that we still have lower bounds for the interactions, e.g., $J'/|\vec{x}-\vec{y}|^p \leq |J_{\vec{x},\vec{y}}| \leq J/|\vec{x}-\vec{y}|^p$ and $D'_i/|\vec{x}-\vec{y}|^p \leq |D^{(i)}_{\vec{x},\vec{y}}| \leq D_i/|\vec{x}-\vec{y}|^p$, $\vec{x}\neq\vec{y}$, it follows that we shall also obtain a lower bound for $S_2(x;y)$ involving $C'''/|\vec{x}-\vec{y}|^p$ (see, e.g., Ref. 13).

(2) The one-particle mass M is directly related to the "time" decay of S_2, i.e., $m'<M<\tilde{m}$, where m' is the term in upper bound above, and $\tilde{m}$ the similar one in a possible lower bound. A more precise estimate of M is possible by adopting standard techniques of constructive field theory, developed to study analyticity properties of one-particle irreducible Green's functions,[12] taking as input the cluster expansion developed here. We do not carry out these calculations here, but we go further on the mass spectrum and investigate the existence of two-particle bound states. To get the results, we analyze the "time" decay of the truncated four-point function in terms of a BS equation, and carry out the computation considering the BS kernel up to dominant order in β only (ladder approximation). The convergence of the cluster expansion (leading, e.g., to a convergent series in β for S_2, as described in Theorem 1) supports such a perturbative analysis. We emphasize that in some related spectral problems (e.g., Refs. 6,14,15), where a complete study has been established, the rigorous results show that the spectral properties (e.g., one-particle and two-particle bound state masses) are given as small corrections of those obtained by similar perturbative approximations. For clearness, we summarize these results on the two-particle bound states in the proposition below.

Proposition 1: Concerning the low-lying energy-momentum spectrum of the model, for the case of the interactions restricted to even functions of the spin variable ϕ, *for* β, J_M, *and* λ *small enough, considering the ladder approximation for the Bethe–Salpeter kernel, there is an isolated two-particle bound state with mass* $M^*=2M+\log(1-\zeta)$, *if* $\zeta>0$, *where* M *is the one-particle mass and* $\zeta=[\langle\phi^4\rangle-3\langle\phi^2\rangle]/[\langle\phi^4\rangle-\langle\phi^2\rangle]$, $\langle\cdot\rangle$ *is the expectation with respect to the single spin distribution* $d\nu(\phi)$ *(31).*

III. THE POLYMER EXPANSION

We now rewrite the expression for the partition function in terms of a polymer expansion. First we define the single spin distribution (SSD),

$$d\nu(\phi)=\frac{e^{-\beta U(\phi)}}{C(\lambda,\beta)}d\phi, \quad C(\lambda,\beta)=\int e^{-\beta U(\phi)}\,d\phi, \tag{31}$$

$d\nu(\phi)$ is a probability measure and (as usual) the partition function (26) can be rewritten as

$$Z_\Lambda = C^{|\Lambda|} \prod_{x\in\Lambda} \int \mathrm{d}\nu(\phi_x) \prod_{\{x,y\}\subset\Lambda} (e^{\beta G_{xy}(\phi_x,\phi_y)} - 1 + 1) = C^{|\Lambda|}\Xi_\Lambda, \tag{32}$$

with

$$\Xi_\Lambda = 1 + \sum_{n\geqslant 1} \frac{1}{n!} \sum_{\substack{R_1,\dots,R_n\subset\Lambda \\ R_i\cap R_j=\emptyset, |R_i|\geqslant 2}} \rho(R_1)\cdots\rho(R_n), \tag{33}$$

where $R_1,\dots,R_n\subset\Lambda$ is a collection of subsets of Λ with cardinality greater than 1, with associated activities $\rho(R)$ given by

$$\rho(R) = \prod_{x\in R} \int \mathrm{d}\nu(\phi_x) \sum_{g\in G_R} \prod_{\{x,y\}\subset\Lambda} (e^{\beta G_{xy}(\phi_x,\phi_y)} - 1), \tag{34}$$

where $\Sigma_{g\in G_R}$ is the sum over the connected graphs on the set R. Given a finite set A, we define a graph g in A as a collection $\{\gamma_1,\dots,\gamma_m\}$ of distinct pairs of A, i.e., $\gamma_i=\{x_i,y_i\}\subset A$ with $x_i\neq y_i$. A graph $g=\{\gamma_1,\dots,\gamma_m\}$ in A is connected if for any B,C of subsets of A such that $B\cup C=A$ and $B\cap C=\emptyset$, there is a $\gamma_i\in g$ such that $\gamma_i\cap B\neq\emptyset$ and $\gamma_i\cap C\neq\emptyset$. The pairs γ_i are called links of the graph. We denote by $|g|$ the number of links in g.

By standard arguments one can expand $\log\Xi_\Lambda$ as

$$\log\Xi_\Lambda = \sum_{n\geqslant 1} \frac{1}{n!} \sum_{\substack{R_1,\dots,R_n\subset\Lambda \\ |R_i|\geqslant 2}} \phi^T(R_1,\dots,R_n)\rho(R_1)\cdots\rho(R_n), \tag{35}$$

with

$$\phi^T(R_1,\dots,R_n) = \begin{cases} 1, & \text{if } n=1, \\ \displaystyle\sum_{\substack{f\in G_n \\ f\subset g(R_1,\dots,R_n)}} (-1)^{|f|}, & \text{if } n\geqslant 2 \text{ and } g(R_1,\dots,R_n)\in G_n, \\ 0, & \text{if } g(R_1,\dots,R_n)\notin G_n, \end{cases} \tag{36}$$

where G_n above denotes the set of the connected graphs on $\{1,\dots,n\}$, and $g(R_1,\dots,R_n)$ denotes the graph in $\{1,2,\dots,n\}$ which has the link $\{i,j\}$ if and only if $R_i\cap R_j\neq\emptyset$. The series (35) is known to converge absolutely, uniformly in Λ, if the activity $\rho(R)$ is sufficiently small,[16] e.g., if

$$\sup_{x\in\Lambda} \sum_{R\ni x} |\rho(R)| e^{a|R|} < a, \tag{37}$$

for some $a>0$. The two-point truncated correlation (30) can now be rewritten as

$$S_2(x_1;x_2) = \left.\frac{\partial^2}{\partial\alpha_1\,\partial\,\alpha_2} \log\tilde{\Xi}_\Lambda(\alpha_1,\alpha_2)\right|_{\alpha=0}, \tag{38}$$

where

$$\tilde{\Xi}_\Lambda(\alpha_1,\alpha_2) = \prod_{x\in\Lambda} \int \mathrm{d}\nu(\phi_x) e^{\beta G_{xy}(\phi_x,\phi_y)} (1+\alpha_1\phi_{x_1})(1+\alpha_2\phi_{x_2}). \tag{39}$$

Note that $\tilde{\Xi}_\Lambda(\alpha_1=0,\alpha_2=0)=\Xi_\Lambda$. Let us expand $\tilde{\Xi}_\Lambda(\alpha_1,\alpha_2)$ in terms of polymers. For any $R\subset\Lambda$, let us denote by I_R the subset (possibly empty) of $\{1, 2\}$ such that $i\in I_R$ iff $x_i\in R$, where $i=1, 2$. We get

$$\Xi_\Lambda(\alpha_1,\alpha_2) = 1 + \sum_{n\geqslant 1} \frac{1}{n!} \sum_{\substack{R_1,\dots R_n\subset\Lambda \\ R_i\cap R_j=\emptyset \mid R_i\mid\geqslant 1}} \tilde{\rho}(R_1,\alpha)\cdots\tilde{\rho}(R_n,\alpha), \tag{40}$$

where

$$\tilde{\rho}(R,\alpha) = \begin{cases} \displaystyle\prod_{x\in R}\int \mathrm{d}\nu(\phi_x)\prod_{i\in I_R}(1+\alpha_i\phi_{x_i})\sum_{g\in G_R}\prod_{\{x,y\}\in g}(e^{\beta G_{xy}(\phi_x,\phi_y)}-1) & \text{for } |R|\geqslant 2, \\ \displaystyle\prod_{x\in R}\int \mathrm{d}\nu(\phi_x)\prod_{i\in I_R}\alpha_i\phi_{x_i} & \text{for } I_R\neq\emptyset, |R|=1, \\ 0 \quad \text{for } I_R=\emptyset, |R|=1. \end{cases} \tag{41}$$

Note that the one-body polymers $R=\{x\}$ can also contribute to the partition function (40), but only if $x=x_i$ for some $i\in\{1,2\}$.

Taking the log of (40) and noting, from (38), that only the terms proportional to $\alpha_1\alpha_2$ give a nonvanishing contribution to the two-point truncated correlation function, we get

$$S_2(x_1;x_2) = \sum_{n\geqslant 1}\frac{1}{n!}\sum_{i_1,i_2=1}^{n}\sum_{\substack{R_1,\dots,R_n\subset\Lambda,|R_j|\geqslant 2 \\ R_{i_1}\ni x_1 R_{i_2}\ni x_2}} \phi^T(R_1,\dots,R_n)\tilde{\rho}(R_1)\cdots\tilde{\rho}(R_n), \tag{42}$$

where

$$\tilde{\rho}(R_i) = \prod_{x\in R_i}\int \mathrm{d}\nu(\phi_x)(\phi_{x_1}^{\beta_i^1}+\beta_i^1 l)(\phi_{x_2}^{\beta_i^2}+\beta_i^2 l)\sum_{g\in G_R}\prod_{\{x,y\}\in g}(e^{\beta G_{xy}(\phi_x,\phi_y)}-1), \tag{43}$$

with $\beta_i^j=0$ if $i\neq i_j$, or 1 if $i=i_j$ and $l=\int \mathrm{d}\nu(\phi)\phi$.

Note that the one-body polymers are absorbed in the activity of the many-body polymers (in the terms proportional to l), due to the fact that $R_1,\dots,R_n$ must be connected, and so each one-body polymer (if any) is always contained in (at least) one many-body polymer.

IV. CONVERGENCE OF THE POLYMER EXPANSION

We will treat in detail here the case where the pair potential $J_{\vec{x},\vec{y}}$ and $D^{(i)}_{\vec{x},\vec{y}}$ decays polynomially (the more complicated one). That is, we will assume that, $\forall i=1,2,\dots,c$, $\vec{x}\neq\vec{y}$,

$$J_{\vec{x},\vec{y}} \leqslant \frac{J}{|\vec{x}-\vec{y}|^p}, \quad D^{(i)}_{\vec{x},\vec{y}} \leqslant \frac{D_i}{|\vec{x}-\vec{y}|^p}, \tag{44}$$

$J, D_i\in\mathbb{R}$ are constants. We will treat the cases where $p\geqslant d+\varepsilon$ with $\varepsilon>0$.

The cases of $J_{\vec{x},\vec{y}}$ and $D^{(i)}_{\vec{x},\vec{y}}$ with finite range or with exponential decay are easier and can be treated in a similar way.

In order to ensure the convergence condition (37) we will bound the factor

$$\varepsilon_n(z,z') = \sum_{\substack{R\subset\Lambda:|R|=n \\ z,z'\in R}} |\rho(R)|, \tag{45}$$

and show that $\varepsilon_n(z,z')\leqslant[f(\beta,J,\lambda D_1,\dots,\lambda D_c)]^n$, where $f(\beta,J,\lambda D_1,\dots,\lambda D_c)\to 0$ as $\beta,J,\lambda D_1,\dots,\lambda D_c\to 0$.

In order to get an efficient bound for the factor

$$\sum_{g\in G_R}\prod_{\{x,y\}\subset\Lambda}(e^{\beta G_{xy}(\phi_x,\phi_y)}-1) \tag{46}$$

that appears in $\rho(R)$, we use a standard cluster expansion result, namely, the Brydges–Battle–Federbush tree graph inequality, which can be resumed in the following lemma.

Lemma 1: Let R be a finite set with cardinality $|R|$ *and let* $\{V_{xy}:\{x,y\}\in\mathbb{R}\}$ *a set with* $|R|(|R|-1)/2$ *real numbers (with* $\{x,y\}$ *unordered pair in R). Suppose now that there exist* $|R|$ *positive numbers* V_x *(with* $x\in R$ *such that, for any subset* $S\subset R$,

$$\sum_{x\in S}V_x+\sum_{\{x,y\}\in S}V_{xy}\geqslant 0. \tag{47}$$

Then

$$\left|\sum_{g\in G_R}\prod_{\{x,y\}\in g}(e^{-V_{xy}}-1)\right|\leqslant e^{\sum_{x\in R}V_x}\sum_{\tau\in T_R}\prod_{\{x,y\}\in\tau}|V_{xy}|, \tag{48}$$

where T_R *denotes the set of the tree graphs on R.*

For the proof of this lemma see, e.g., Refs. 17,18.

For any $\varphi,\phi\in\mathbb{R}$, we have $2|\varphi\phi|\leqslant|\varphi|^2+|\phi|^2$ and $|\varphi|^a|\phi|^b\leqslant|\varphi|^{a+b}+|\phi|^{a+b}$. Then, for any $R\subset\Lambda$, it follows that

$$\begin{aligned}\sum_{\{x,y\}\subset R}|G_{xy}(\phi_x,\phi_y)|&\leqslant\sum_{\{x,y\}\subset R}\left|\frac{1}{\beta}J_{\vec{x},\vec{y}}\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}})+\delta_{\vec{x},\vec{y}}\delta_{|x_0-y_0|,1}\right|\frac{|\phi_x\phi_y|}{2}+\sum_{i=1}^{c}\left|\frac{\lambda}{\beta}D^{(i)}_{\vec{x},\vec{y}}\delta_{x_0,y_0}(1\right.\\&\left.-\delta_{\vec{x},\vec{y}})\right||\phi_x^{a_i}\phi_y^{b_i}|\leqslant\sum_{\{x,y\}\subset R}\left|\frac{1}{\beta}J_{\vec{x},\vec{y}}\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}})+\delta_{\vec{x},\vec{y}}\delta_{|x_0-y_0|,1}\right|\frac{1}{4}(|\phi_x|^2+|\phi_y|^2)\\&+\sum_{i=1}^{c}\left|\frac{\lambda}{\beta}D^{(i)}_{\vec{x},\vec{y}}\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}})\right|(|\phi_x|^{a_i+b_i}+|\phi_y|^{a_i+b_i})\\&\leqslant\sum_{x\in R}\frac{|\phi_x|^2}{2}\sum_{y\in R}\left|\frac{1}{\beta}J_{\vec{x},\vec{y}}\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}})+\delta_{\vec{x},\vec{y}}\delta_{|x_0-y_0|,1}\right|\\&+\sum_{i=1}^{c}\sum_{x\in R}|\phi_x|^{a_i+b_i}\sum_{y\in R}\left|\frac{2\lambda}{\beta}D^{(i)}_{\vec{x},\vec{y}}\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}})\right|.\end{aligned}$$

Note that

$$\sum_{y\in R}\delta_{\vec{x},\vec{y}}\delta_{|x_0-y_0|,1}\leqslant\sum_{y_0\in\mathbb{Z}}\delta_{|x_0-y_0|,1}\leqslant 2,$$

$$\sum_{y\in R}|J_{\vec{x},\vec{y}}|\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}})\leqslant\sup_{\vec{x}\in\mathbb{Z}^d}\sum_{\vec{y}\in\mathbb{Z}^d}|J_{\vec{x},\vec{y}}|\leqslant J_M,$$

$$\sum_{y\in R}|D^{(i)}_{\vec{x},\vec{y}}|\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}})\leqslant\sup_{\vec{x}\in\mathbb{Z}^d}\sum_{\vec{y}\in\mathbb{Z}^d}|D^{(i)}_{\vec{x},\vec{y}}|\leqslant D^{(i)}_M.$$

Hence,

$$\sum_{\{x,y\}\subset R}|G_{xy}(\phi_x,\phi_y)|\leqslant\sum_{x\in R}\left[\left(\frac{J_M}{2\beta}+1\right)|\phi_x|^2+\sum_{i=1}^{c}\frac{2\lambda D^{(i)}_M}{\beta}|\phi_x|^{a_i+b_i}\right].$$

As $|\phi|^2\leqslant|\phi|^{a_i+b_i}\leqslant|\phi|^{a_i+b_i}+1$ if $|\phi|\geqslant 1$ and $|\phi|^2\leqslant 1\leqslant|\phi|^{a_i+b_i}+1$ if $|\phi|\leqslant 1$ and, defining $(a,b)\equiv(a_j,b_j)$ for j such that $a_j+b_j=\max\{a_1+b_1,\ldots,a_c+b_c\}$, it follows that

$$\sum_{\{x,y\}\subset R} |G_{xy}(\phi_x,\phi_y)| \leqslant \sum_{x\in R} (C_1\phi_x^{a+b} + C_2),$$

where

$$C_1 \equiv \frac{J_M}{2\beta} + 1 + \sum_{i=1}^{c} \frac{2\lambda D_M^{(i)}}{\beta}, \quad C_2 \equiv \frac{J_M}{2\beta} + 1. \tag{49}$$

Using Lemma 1 we get

$$\left| \sum_{g\in G_R} \prod_{\{x,y\}\in g} (e^{\beta G_{xy}(\phi_x,\phi_y)} - 1) \right| \leqslant \prod_{x\in R} e^{\beta(C_1\phi_x^{a+b}+C_2)} \sum_{\tau\in T_R} \prod_{\{x,y\}\in\tau} |\beta G_{xy}(\phi_x,\phi_y)|, \tag{50}$$

and so,

$$\sum_{\substack{R\subset\Lambda:|R|\geqslant 2\\ z,z'\in R}} |\rho(R)|e^{|R|} = \sum_{n\geqslant 2} e^n \sum_{\substack{R\subset\Lambda:|R|=n\\ z,z'\in R}} |\rho(R)| = \sum_{n\geqslant 2} \frac{e^n}{(n-2)!} \sum_{\substack{x_1,\ldots,x_n\in\Lambda:\\ x_1=z,x_2=z',x_1\neq x_j}} |\rho(R=\{x_1,\ldots,x_n\})|$$

$$\leqslant \sum_{n\geqslant 2} \frac{e^n}{(n-2)!} \sum_{\substack{x_1,\ldots,x_n\in\Lambda:\\ x_1=z,x_2=z',x_i\neq x_j}} \int \prod_{i=1}^{n} \mathrm{d}\nu(\phi_{x_i}) e^{\beta(C_1\phi_{x_i}^{a+b}+C_2)} \sum_{\tau\in T_n} \prod_{\{i,j\}\in\tau} |\beta G_{x_iy_j}(\phi_{x_i}\phi_{x_j})|.$$

Recall now (28) and (29), and that $|\tau| = n-1$. Hence, fixing $\tau\in T_n$, we have

$$\prod_{\{i,j\}\in\tau} |G_{x_iy_j}(\phi_{x_i}\phi_{x_j})| \leqslant \prod_{\{i,j\}\in\tau} \sum_{s=1}^{c+1} |A_{x_ix_j}^{(s)}| |\phi_{x_i}^{a_{s-1}^{(1-\delta_{s,1})}}| |\phi_{x_j}^{b_{s-1}^{(1-\delta_{s,1})}}| \leqslant \sum_{\{i,j\}\in\tau} \sum_{s_{ij}=1}^{c+1} \prod_{k=1}^{n} |\phi_{x_k}|^{n_k(s)} \prod_{\{i,j\}\in\tau} |A_{x_ix_j}^{(s_{ij})}|,$$

where $n_k(s)$ depends on $a_1,\ldots,a_c$, $b_1,\ldots,b_c$ and on the sequence $\{s_{ij}\}_{\{i,j\}\in\tau}$. In any case, we have $d_k \leqslant n_k(s) \leqslant d_k \cdot \max\{a_1,\ldots,a_c,b_1,\ldots,b_c\} \leqslant md_k$, where $2m$ is the degree of the polynomial $P(\phi)$, and $\{d_k\}_{k=1}^n$ are the incidence indices of the tree $\tau\in T_n$, with $1\leqslant d_k\leqslant n-1$ and $\Sigma_{k=1}^n d_k = 2n-2$. Then

$$\sum_{\substack{R\subset\Lambda:|R|\geqslant 2\\ z,z'\in R}} |\rho(R)|e^{|R|} \leqslant \sum_{n\geqslant 2} \frac{e^n e^{n\beta C_2}\beta^{n-1}}{(n-2)!} \sum_{\substack{x_1,\ldots,x_n\in\Lambda:\\ x_1=z,x_2=z',x_i\neq x_j}} \int \prod_{i=1}^{n} \mathrm{d}\nu(\phi_{x_i}) e^{\beta C_1\phi_{x_i}^{a+b}}$$

$$\times \sum_{\tau\in T_n} \sum_{\{i,j\}\in\tau} \sum_{s_{ij}=1}^{c+1} \prod_{k=1}^{n} |\phi_{x_k}|^{n_k(s)} \prod_{\{i,j\}\in\tau} |A_{x_ix_j}^{(s_{ij})}| \leqslant \sum_{n\geqslant 2} \frac{e^n e^{n\beta C_2}\beta^{n-1}}{(n-2)!} \sum_{\substack{x_1,\ldots,x_n\in\Lambda:\\ x_1=z,x_2=z',x_i\neq x_j}}$$

$$\times \sum_{\tau\in T_n} \sum_{\{i,j\}\in\tau} \sum_{s_{ij}=1}^{c+1} \prod_{k=1}^{n} \left(\int \mathrm{d}\nu(\phi_{x_k}) e^{\beta C_1\phi_{x_k}^{a+b}} |\phi_{x_k}|^{n_k(s)} \right) \prod_{\{i,j\}\in\tau} |A_{x_ix_j}^{(s_{ij})}|.$$

Lemma 2: If $a\leqslant m$ and $b\leqslant m$, then $\forall\alpha>0$, $\alpha\in\mathbb{R}$, we have

$$\int \mathrm{d}\nu(\phi) e^{\beta C_1\phi^{a+b}} |\phi|^{\alpha} \leqslant \frac{e^{C_4-C_6} C_3^{1/2m}}{C_5^{(\alpha+1)/2m}} \left[\Gamma\left(\frac{1}{2m}\right) \right]^{-1} \Gamma\left(\frac{\alpha+1}{2m}\right),$$

where C_3, C_4, C_5, and *C_6 are constants such that, $\forall\phi\in\mathbb{R}$,*

$$\beta U(\phi) \leqslant C_3\phi^{2m} + C_4, \quad \beta U(\phi) - \beta C_1\phi^{a+b} \geqslant C_5\phi^{2m} + C_6.$$

Proof: As $P(\phi)$ is a polynomial of degree $2m$ bounded from below, there exist contants A_1, A_2, A_3, and A_4 (with A_1 and $A_3>0$) such that

$$A_1\phi^{2m} + A_2 \leqslant P(\phi) \leqslant A_3\phi^{2m} + A_4.$$

Then, as $\phi^2 \leqslant \phi^{a+b}+1$ and $\phi^{a_i+b_i} \leqslant \phi^{a+b} \leqslant \phi^{2m}$ since $a_i+b_i \leqslant a+b \leqslant 2m$, we obtain

$$\beta U(\phi) = \lambda P(\phi) + \frac{J(0)}{2}\phi^2 + \beta\phi^2 + \lambda\sum_{i=1}^{c} \phi^{a_i+b_i} D_i(0) \leqslant \lambda(A_3\phi^{2m} + A_4) + \frac{J(0)}{2}(\phi^{m2}+1) + \beta(\phi^{2m}+1)$$
$$+ \lambda\phi^{2m}\sum_{i=1}^{c} D_i(0) \leqslant C_3\phi^{2m} + C_4,$$

where

$$C_3 \equiv \lambda A_3 + \frac{J(0)}{2} + \beta + \lambda\sum_{i=1}^{c} D_i(0), \quad C_4 \equiv \lambda A_4 + \frac{J(0)}{2} + \beta + \lambda\sum_{i=1}^{c} D_i(0).$$

We also have

$$\beta U(\phi) - \beta C_1\phi^{a+b} = \lambda P(\phi) + \frac{J(0)}{2}\phi^2 + \beta\phi^2 + \lambda\sum_{i=1}^{c} \phi^{a_i+b_i} D_i(0) - \beta C_1\phi^{a+b} \geqslant \lambda(A_1\phi^{2m} + A_2)$$
$$+ \lambda\sum_{i=1}^{c} \phi^{a_i+b_i} D_i(0) - \beta C_1\phi^{a+b}.$$

If $a+b=2m$, we have

$$\beta U(\phi) - \beta C_1\phi^{a+b} \geqslant \left[\lambda A_1 - \beta C_1 + \lambda \sum_{i:a_i+b_i=2m}^{c} D_i(0)\right]\phi^{2m} + \lambda A_2 \geqslant C_5\phi^{2m} + C_6.$$

If $a+b<2m$, then $\phi^{a+b} \leqslant \phi^{2m}+1$ and it follows that

$$\beta U(\phi) - \beta C_1\phi^{a+b} \geqslant (\lambda A_1 - \beta C_1)\phi^{2m} + \lambda A_2 - \beta C_1 \geqslant C_5\phi^{2m} + C_6.$$

Hence, $C_5=\lambda A_1-\beta C_1+\lambda\Sigma^{c}_{i:a_i+b_i=2m}D_i(0)$ if $a+b=2m$, or $C_5=\lambda A_1-\beta C_1$ if $a+b<2m$. $C_6=\lambda A_2$ if $a+b=2m$, or $C_6=\lambda A_2-\beta C_1$ if $a+b<2m$. From the definition of the SSD $\mathrm{d}\nu(\phi)$, we have

$$\int \mathrm{d}\nu(\phi) e^{\beta C_1\phi^{a+b}} |\phi|^{\alpha} = \frac{1}{C(\lambda,\beta)} \int e^{-\beta U(\phi)} e^{\beta C_1\phi^{a+b}} |\phi|^{\alpha}\, \mathrm{d}\phi.$$

Hence,

$$C(\lambda,\beta) = \int_{\mathbb{R}} e^{-\beta U(\phi)}\, \mathrm{d}\phi \geqslant e^{-C_4}\int_{\mathbb{R}} e^{-C_3\phi^{2m}}\, \mathrm{d}\phi \geqslant e^{-C_4}\frac{1}{mC_3^{1/2m}}\Gamma\left(\frac{1}{2m}\right),$$

$$\int e^{-\beta U(\phi)} e^{\beta C_1\phi^{a+b}} |\phi|^{\alpha}\, \mathrm{d}\phi \leqslant e^{-C_6}\int_{\mathbb{R}} e^{-C_5\phi^{2m}} |\phi|^{\alpha}\, \mathrm{d}\phi \leqslant e^{-C_6}\frac{1}{mC_5^{(\alpha+1)/2m}}\Gamma\left(\frac{\alpha+1}{2m}\right),$$

where we used that $C_5>0$ for β small enough. Lemma 2 follows from these two bounds. ■

Recalling that $1 \leqslant d_k \leqslant n_k(s) \leqslant md_k$, we get $[n_k(s)+1]/2m \leqslant 2n_k(s)/2m \leqslant d_k$, and so, using Lemma 2, we obtain

$$\sum_{\substack{R\subset\Lambda:|R|\geqslant 2\\ z,z'\in R}}|\rho(R)|e^{|R|}\leqslant\sum_{n\geqslant 2}\frac{e^n e^{n\beta C_2}\beta^{n-1}}{(n-2)!}\sum_{\substack{x_1,\ldots,x_n\in\Lambda:\\ x_1=z,x_2=z',x_{i\neq}x_j}}\sum_{\tau\in T_n}\sum_{\{i,j\}\in\tau}\sum_{s_{ij}=1}^{c+1}$$

$$\times\prod_{k=1}^{n}\left\{\frac{e^{C_4-C_6}C_3^{1/2m}}{C_5^{d_k}}\left[\Gamma\left(\frac{1}{2m}\right)\right]^{-1}\Gamma(d_k)\right\}\prod_{\{i,j\}\in\tau}|A_{x_i x_j}^{(s_{ij})}|$$

$$\leqslant\sum_{n\geqslant 2}\frac{e^n e^{n\beta C_2}\beta^{n-1}}{(n-2)!}\frac{(e^{C_4-C_6}C_3^{1/2m})^n}{C_5^{2(n-1)}}\left[\Gamma\left(\frac{1}{2m}\right)\right]^{-n}\sum_{\tau\in T_n}\sum_{\{i,j\}\in\tau}\sum_{s_{ij}=1}^{c+1}$$

$$\times\prod_{k=1}^{n}\Gamma(d_k)\sum_{\substack{x_1,\ldots,x_n\in\Lambda:\\ x_1=z,x_2=z',x_i\neq x_j}}\prod_{\{i,j\}\in\tau}|A_{x_i x_j}^{(s_{ij})}|, \tag{51}$$

where we use that $\Pi_{k=1}^{n}C_5^{d_k}=C_5^{(d_1+d_2+\cdots+d_n)}=C_5^{2(n-1)}$.

We note that for any $\tau\in T_n$, there is a unique path $\overline{\tau}$ in τ which joins vertex 1 to vertex 2. Fixing $\tau\in T_n$, let $\overline{\tau}\equiv\{1,i_1\},\{i_1,i_2\},\{i_2,i_3\},\ldots,\{i_{k-1},i_k\},\{i_k,2\}$ and $I_\tau\equiv\{1,i_1,i_2,\ldots,i_k,2\}$ the subset of $\{1,2,3,\ldots,n\}$ whose elements are the vertices of the path $\overline{\tau}$. Hence, $|\tau|=n-1$, $|\overline{\tau}|=k+1$, and $|\tau\backslash\overline{\tau}|=n-k-2$.

From the definitions (29) of $|A_{xy}^{(s)}|:s=1,\ldots,(c+1)$, we see that all the terms vanish if $|x_0-y_0|>1$. Hence, fixing $\tau\in T_n$, if $\exists\{i,j\}\in\tau$ such that $|(x_i)_0-(x_j)_0|>1$ we have $|A_{x_i x_j}^{(s)}|=0\,\forall\, s=1,\ldots,(c+1)$, and so, this tree τ does not contribute to the sum (51). Then, given $|(x_1)_0-(x_2)_0|$, as $|\overline{\tau}|=k+1$, if $|(x_1)_0-(x_2)_0|>k+1$ then $\exists\{i,j\}\in\overline{\tau}$ such that $|(x_i)_0-(x_j)_0|>1$, and so, τ do not contribute to (51). As $\overline{\tau}\subset\tau$ we have $n-1\geqslant k+1$. Therefore, any tree $\tau\in T_n$ such that $|(x_1)_0-(x_2)_0|>n-1\geqslant k+1$ do not contribute to (51), in other words, $\rho(R)$ vanishes if $|(x_1)_0-(x_2)_0|>|R|-1$, i.e., if $|R|<|(x_1)_0-(x_2)_0|+1$.

So, we define $N\equiv|z_0-z'_0|+1$, and we have

$$\sum_{\substack{R\subset\Lambda:|R|\geqslant 2\\ z,z'\in R}}|\rho(R)|e^{|R|}\leqslant\sum_{\substack{R\subset\Lambda:|R|\geqslant N\\ z,z'\in R}}|\rho(R)|e^{|R|}. \tag{52}$$

Now, we note that

$$\delta_{\vec{x},\vec{y}}\delta_{|x_0-y_0|,1}\leqslant\delta_{\vec{x},\vec{y}}e^{-|x_0-y_0|+1},\quad \delta_{x_0,y_0}\leqslant e^{-|x_0-y_0|}.$$

Then,

$$|A_{xy}^{(1)}|=\frac{1}{2}\left|\frac{1}{\beta}J_{\vec{x},\vec{y}}\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}})-\delta_{\vec{x},\vec{y}}\delta_{|x_0-y_0|,1}\right|\leqslant\frac{e^{-|x_0-y_0|}}{2}\left[\frac{1}{\beta}\frac{J}{|\vec{x}-\vec{y}|^p}(1-\delta_{\vec{x},\vec{y}})+e\,\delta_{\vec{x},\vec{y}}\right],$$

$$|A_{xy}^{(s)}|=\left|\frac{\lambda}{\beta}D_{\vec{x},\vec{y}}^{(s-1)}\delta_{x_0,y_0}(1-\delta_{\vec{x},\vec{y}})\right|\leqslant\frac{\lambda D_{s-1}}{\beta|\vec{x}-\vec{y}|^p}(1-\delta_{\vec{x},\vec{y}})e^{-|x_0-y_0|}.$$

Hence, $\forall s=1,\ldots,(c+1)$,

$$|A_{xy}^{(s)}|\leqslant Ke^{-|x_0-y_0|}\left[\frac{1}{|\vec{x}-\vec{y}|^p}(1-d_{\vec{x},\vec{y}})+\frac{e}{2}\delta_{\vec{x},\vec{y}}\right]\leqslant eKe^{-|x_0-y_0|}\left[\frac{(1-\delta_{\vec{x},\vec{y}})}{|\vec{x}-\vec{y}|^p}+\delta_{\vec{x},\vec{y}}\right]\leqslant eKF_{xy}^{(1)},$$

$$\sup_{x\in\Lambda}\sum_{y\in\Lambda}|A_{xy}^{(s)}|\leqslant e\mathcal{O}(1)K,$$

where, we define

$$K \equiv \frac{1}{\beta}\max\left\{\frac{J}{2}, \lambda D_1, \lambda D_2 \ldots, \lambda D_c\right\}, \tag{53}$$

and, for $w \in \mathbb{R}$, $w > 0$,

$$F_{xy}^{(w)} \equiv e^{-w|x_0 - y_0|}\left[\frac{(1 - \delta_{\vec{x},\vec{y}})}{|\vec{x} - \vec{y}|^p} + \delta_{\vec{x},\vec{y}}\right].$$

Then, fixing $\tau \in T_n$ and the sequence $\{s_{ij}\}$, we get

$$\begin{aligned}
\sum_{\substack{x_1,\ldots,x_n \in \Lambda: \\ x_1 = z, x_2 = z', x_i \neq x_j}} \prod_{\{i,j\} \in \tau} |A_{x_i x_j}^{(s_{ij})}| &= \sum_{\substack{x_1,\ldots,x_n \in \Lambda: \\ x_1 = z, x_2 = z', x_i \neq x_j}} \prod_{\{i,j\} \in \tau \setminus \overline{\tau}} |A_{x_i x_j}^{(s_{ij})}| \prod_{\{i,j\} \in \overline{\tau}} |A_{x_i x_j}^{(s_{ij})}| \\
&\leqslant [e\mathcal{O}(1)K]^{(n-k-2)} \sum_{\substack{x_{i_1},\ldots,x_{i_k} \in \Lambda: \\ x_{i_r} \neq x_{i_q}\ \forall r,q = 1,\ldots,k}} \prod_{\{i,j\} \in \overline{\tau}} |A_{x_i x_j}^{(s_{ij})}| \\
&\leqslant [e\mathcal{O}(1)K]^{(n-k-2)} \sum_{\substack{x_{i_1},\ldots,x_{i_k} \in \Lambda: \\ x_{i_r} \neq x_{i_q}\ \forall r,q = 1,\ldots,k}} eKF_{x_1 x_{i_1}}^{(1)}\, eKF_{x_{i_1} x_{i_2}}^{(1)} \cdots eKF_{x_{i_{k-1}} x_{i_k}}^{(1)}\, eKF_{x_{i_k} x_2}^{(1)}.
\end{aligned}$$

Applying iteratively the inequality (for $w_1 < w_2$)

$$\sum_{\substack{x_i \in \Lambda: \\ x_i \neq x, y}} F_{x x_i}^{(w_1)} F_{x_i y}^{(w_2)} \leqslant \mathcal{O}(1) F_{xy}^{(w_1)}, \tag{54}$$

which follows from

$$\sum_{\substack{\vec{x}_i \in \mathbb{Z}^d: \\ \vec{x}_i \neq \vec{x}, \vec{y}}} \frac{1}{|\vec{x} - \vec{x}_i|^p} \frac{1}{|\vec{x}_i - \vec{y}|^p} \leqslant \frac{\mathcal{O}(1)}{|\vec{x} - \vec{y}|^p}, \qquad \sum_{\substack{z_0 \in \mathbb{R}: \\ z_0 \neq x_0, y_0}} e^{-w_1|x_0 - z_0|} e^{-w_2|z_0 - y_0|} \leqslant \mathcal{O}(1) e^{-w_1|x_0 - y_0|}$$

(the formula is valid for any $w_1 < w_2$, specific for $w_1 = 2/3$ and $w_2 = 1$, which we will take here), we get

$$\sum_{\substack{x_1,\ldots,x_n \in \Lambda: \\ x_1 = z, x_2 = z', x_i \neq x_j}} \prod_{\{i,j\} \in \tau} |A_{x_i x_j}^{(s_{ij})}| \leqslant [e\mathcal{O}(1)K]^{(n-1)} F_{zz'}^{(2/3)}. \tag{55}$$

Recall that

$$\sum_{\tau \in T_n} 1 = \sum_{\substack{d_1 + \cdots + d_n = 2n+2 \\ d_i \geqslant 1}} \sum_{\substack{\tau \in T_n: \\ \tau \approx (d1,\ldots,d_n)}} 1, \tag{56}$$

where the notation $\tau \approx (d_1, \ldots, d_n)$ means that the last sum above runs over the trees $\tau \in T_n$ that have fixed incidence indices $(d_1, \ldots, d_n)$. From the Cayley formula

$$\sum_{\substack{\tau \in T_n: \\ \approx (d1,\ldots,d_n)}} 1 = \frac{(n-2)!}{\prod_{i=1}^{n} (d_i - 1)!},$$

and, fixing $\tau \in T_n$, we have

$$\sum_{\{i,j\}\in\tau}\sum_{s_{ij}=1}^{c+1}1=(c+1)^{(n-1)}.$$

Hence, using (52), we get

$$\sum_{\substack{R\subset\Lambda:|R|\geqslant 2\\ z,z'\in R}}|\rho(R)|e^{|R|}\leqslant\sum_{n\geqslant N}\frac{e^n e^{n\beta C_2}\beta^{n-1}}{(n-2)!}\frac{(e^{C_4-C_6}C_3^{1/2m})^n}{C_5^{2(n-1)}}\left[\Gamma\left(\frac{1}{2m}\right)\right]^{-n}\times\sum_{\tau\in T_n}\sum_{\{i,j\}\in\tau}\sum_{s_{ij}=1}^{c+1}\prod_{k=1}^{n}\Gamma(d_k)$$

$$\times[e\mathcal{O}(1)K]^{(n-1)}F_{zz'}^{(2/3)}$$

$$\leqslant\sum_{n\geqslant N}\frac{e^n e^{n\beta C_2}\beta^{n-1}}{(n-2)!}\frac{(e^{C_4-C_6}C_3^{1/2m})^n}{C_5^{2(n-1)}}\left[\Gamma\left(\frac{1}{2m}\right)\right]^{-n}[e\mathcal{O}(1)K]^{(n-1)}\times F_{zz'}^{(2/3)}(c+1)^{(n-1)}\sum_{\substack{d_1+\cdots+d_n=2n+2\\ d_i\geqslant 1}}\prod_{k=1}^{n}(d_k-1)!\,\frac{(n-2)!}{\prod_{i=1}^{n}(d_i-1)!}$$

$$\leqslant\sum_{n\geqslant N}e^n e^{n\beta C_2}\beta^{n-1}\frac{(e^{C_4-C_6}C_3^{1/2m})^n}{C_5^{2(n-1)}}\left[\Gamma\left(\frac{1}{2m}\right)\right]^{-n}[e\mathcal{O}(1)K]^{(n-1)}F_{zz'}^{(2/3)}(c+1)^{(n-1)}4^n,$$

where we used the inequality

$$\sum_{\substack{d_1+\cdots+d_n=2n+2\\ d_i\geqslant 1}}1\leqslant 4^n.$$

Hence,

$$\sum_{\substack{R\subset\Lambda:|R|\geqslant 2\\ z,z'\in R}}|\rho(R)|e^{|R|}\leqslant e^N e^{N\beta C_2}\beta^N\frac{(e^{C_4-C_6}C_3^{1/2m})^N}{C_5^{2N}}\left[\Gamma\left(\frac{1}{2m}\right)\right]^{-N}[e\mathcal{O}(1)K]^N F_{zz'}^{(2/3)}$$

$$\times(c+1)^N 4^N\sum_{n\geqslant 0}\left\{e^2e^{\beta C_2}\beta\frac{(e^{C_4-C_6}C_3^{1/2m})}{C_5^2}\left[\Gamma\left(\frac{1}{2m}\right)\right]^{-1}\mathcal{O}(1)4(c+1)K\right\}^n.$$

In short, we have proved the following result.

Lemma 3: If β and $\beta K=\max\{J/2,\lambda D_1,\ldots,\lambda D_c\}$ are sufficiently small such that

$$\varepsilon(\beta,K)\equiv e^2e^{\beta C_2}4(c+1)\beta K\frac{(e^{C_4-C_6}C_3^{1/2m})}{C_5^2}\left[\Gamma\left(\frac{1}{2m}\right)\right]^{-1}\mathcal{O}(1)<1,$$

then, $\varepsilon(\beta,K)$ is a positive function and, for any $z\in\Lambda$, $z'\in\Lambda$ with $z\neq z'$,

$$\sum_{\substack{R\subset\Lambda:|R|\geqslant 2\\ z,z'\in R}}|\rho(R)|e^{|R|}\leqslant[\varepsilon(\beta,K)]^N F_{zz'}^{(2/3)}=[\varepsilon(\beta,K)]^{|z_0-z'_0|+1}F_{zz'}^{(2/3)}. \tag{57}$$

From Lemma 3, we obtain the following.

Corollary 4:

$$\sup_{x\in\mathbb{Z}^{d+1}}\sum_{R:x\in R}|\rho(R)|e^{|R|}\leqslant\mathcal{O}(1)\varepsilon(\beta,K).$$

Proof: In fact, as $\rho(R)=0$ if $|R|=1$, we have

$$\sup_{x\in\mathbb{Z}^{d+1}}\sum_{R:x\in R}|\rho(R)|e^{|R|}=\sup_{x\in\mathbb{Z}^{d+1}}\sum_{\substack{R:x\in R\\|R|\geqslant 2}}|\rho(R)|e^{|R|}\leqslant\sup_{x\in\mathbb{Z}^{d+1}}\sum_{\substack{z\in\mathbb{Z}^{d+1}:\\ z\neq x}}\sum_{\substack{R:|R|\geqslant 2\\ x,z\in R}}|\rho(R)|e^{|R|}$$

$$\leqslant\sup_{x\in\mathbb{Z}^{d+1}}\sum_{z\in\mathbb{Z}^{d+1}:z\neq x}[\varepsilon(\beta,K)]^{|x_0-z_0|+1}F_{xz}^{(2/3)}\leqslant\mathcal{O}(1)\varepsilon(\beta,K),$$

since, for $w>0$,

$$\sum_{z\in\mathbb{Z}^{d+1}:z\neq x}e^{-w|x_0-z_0|}\left[\frac{(1-\delta_{\vec{x},\vec{z}})}{|\vec{x}-\vec{z}|^p}+\delta_{\vec{x},\vec{z}}\right]=\mathcal{O}(1),$$

and so $\Sigma_{z\in\mathbb{Z}^{d+1}:z\neq x}F_{xz}^{(2/3)}\leqslant\mathcal{O}(1)$. ■

The results above establish the convergence of the cluster expansion for $\varepsilon(\beta,K)$ small enough such that $\mathcal{O}(1)\varepsilon(\beta,K)<1$ [see condition (37)].

V. DECAY OF TWO-POINT TRUNCATED CORRELATION

As it is well known, the convergence of the cluster expansion assures the decay of the correlation functions and lead to direct estimates. We present the main technical details related to the behavior of the truncated two-point function below.

Turning to the expression (43) which defines $\tilde{\rho}(R_i)$, we note that the index i of the term β_i^j is the same of the polymer R_i, and so $i\in\{1,2,3,\ldots,n\}$ as $j\in\{1,2\}$.

Consider the expression (30) for $S_2(x_1;x_2)$, and recall that $i_1,i_2\in\{1,2,3,\ldots,n\}$. Then, we have two distinct cases, $i_1=i_2$ or $i_1\neq i_2$. If $i_1=i_2$, then $\{x_1,x_2\}\subset R_{i_1}$, $\{x_1,x_2\}\cap R_i=\emptyset\ \forall i\neq i_1$ and $\beta_{i_1}^1=\beta_{i_1}^1=\beta_{i_2}^2=\beta_{i_2}^2=1$. If $i_1\neq i_2$, then $x_1\in R_{i_1}$, $x_1\notin R_{i_2}$, $x_2\in R_{i_2}$, $x_2\notin R_{i_1}$, $\{x_1,x_2\}\cap R_i=\emptyset\ \forall i\notin\{i_1,i_2\}$, $\beta_{i_1}^1=\beta_{i_2}^2=1$, and $\beta_{i_1}^2=\beta_{i_2}^1=0$.

Hence, as $1=(1-\delta_{i_1,i_2})+\delta_{i_1,i_2}$ we rewrite

$$S_2(x_1;x_2)=A_1(x_1,x_2)+A_2(x_1,x_2),$$

where

$$A_1(x_1,x_2)\equiv\sum_{n\geqslant 1}\frac{1}{n!}\sum_{i_1,i_2=1}^{n}(1-\delta_{i_1,i_2})\sum_{\substack{R_1,\ldots,R_n\subset\Lambda,|R_j|\geqslant 2\\ R_{i_1}\ni x_1 R_{i_2}\ni x_2}}\phi^T(R_1,\ldots,R_n)\tilde{\rho}(R_1)\cdots\tilde{\rho}(R_n)$$

$$=\sum_{n\geqslant 2}\frac{1}{(n-2)!}\sum_{\substack{R_1,\ldots,R_n\subset\Lambda,|R_j|\geqslant 2\\ R_1\ni x_1 R_2\ni x_2}}\phi^T(R_1,\ldots,R_n)\tilde{\rho}(R_1)\cdots\tilde{\rho}(R_n),$$

$$A_2(x_1,x_2)\equiv\sum_{n\geqslant 1}\frac{1}{n!}\sum_{i_1,i_2=1}^{n}\delta_{i_1,i_2}\sum_{\substack{R_1,\ldots,R_n\subset\Lambda,|R_j|\geqslant 2\\ R_{i_1}\ni x_1 R_{i_2}\ni x_2}}\phi^T(R_1,\ldots,R_n)\tilde{\rho}(R_1)\cdots\tilde{\rho}(R_n)$$

$$=\sum_{n\geqslant 1}\frac{1}{(n-1)!}\sum_{\substack{R_1,\ldots,R_n\subset\Lambda,|R_j|\geqslant 2\\ R_1\supset\{x_1,x_2\}}}\phi^T(R_1,\ldots,R_n)\tilde{\rho}(R_1)\cdots\tilde{\rho}(R_n),$$

since, in $A_1(x_1,x_2)$ when $n=1$ we have $\Sigma_{i_1,i_2=1}^1(1-\delta_{i_1,i_2})=0$ and, for any $n>2$ the sum $\Sigma_{i_1,i_2=1}^n(1-\delta_{i_1,i_2})$ leads to $n(n-1)$ equal terms. And, in $A_2(x_1,x_2)$ the sum $\Sigma_{i_1,i_2=1}^n\delta_{i_1,i_2}$ gives n equal terms.

Thus,

$$|S_2(x_1;x_2)|\leqslant|A_1(x_1,x_2)|+|A_2(x_1,x_2)|.$$

Comparing (34) and (43), we note that if $R_i \cap \{x_1, x_2\} = \emptyset$ then $\tilde{\rho}(R_i) = \rho(R_i)$. If $R_i \cap \{x_1, x_2\} \neq \emptyset$, we can obtain the result (57) of Lemma 3 for $\tilde{\rho}(R_i)$ by changing $n_k(s)$ by $n_k(s)+1$. With such result, we change $\Gamma(d_k)$ by $\Gamma(d_k+1)$ in (51) and obtain an extra $\Pi_{k=1}^{n} d_k$, which is bounded by $e^{2(n-1)}$. We use Lemma 2 to bound the factor $l = \int \mathrm{d}\nu(\phi)\phi$ in (43). Hence, we can apply Lemma 3 and Corollary 4 to estimate $\tilde{\rho}(R_i)$ (changing some multiplicative constants).

Now, let us find an upper bound for the term $|A_1(x_1, x_2)|$. We have

$$|A_1(x_1,x_2)| \leqslant \sum_{n \geqslant 2} \frac{1}{(n-2)!} B_n(x_1,x_2),$$

where

$$B_n(x_1,x_2) = \sum_{\substack{R_1,\ldots,R_n \subset \Lambda \\ |R_i| \geqslant 2, x_1 \in R_1, x_2 \in R_2}} |\phi^T(R_1,R_2,\ldots,R_n)| \tilde{\rho}(R_1) \| \tilde{\rho}(R_2) \| \tilde{\rho}(R_3) \cdots \tilde{\rho}(R_n)|.$$

Note that in (36), for $n \geqslant 2$, $\phi^T(R_1,\ldots,R_n) > 0$ only if $g(R_1,\ldots,R_n) \in G_n$. Thus,

$$\sum_{\substack{R_1,\ldots,R_n \subset \Lambda \\ |R_i| \geqslant 2, x_1 \in R_1, x_2 \in R_2}} |\phi^T(R_1,R_2,\ldots,R_n)|[\cdot] = \sum_{g \in G_n} \left| \sum_{\substack{f \in G_n \\ \subset g}} (-1)^{|f|} \right| \sum_{\substack{R_1,\ldots,R_n \subset \Lambda : |R_i| \geqslant 2 \\ g(R_1,\ldots,R_n) = g, x_1 \in R_1, x_2 \in R_2}} [\cdot].$$

By the Rota formula,[19] we have

$$\left| \sum_{\substack{f \in G_n \\ f \subset g}} (-1)^{|f|} \right| \leqslant \sum_{\tau \in T_n : \tau \subset g} 1 \equiv N(g).$$

A proof of the Rota formula above can be found, e.g., in Refs. 19 and 20.

We recall now that

$$\sum_{g \in G_n} [\cdot] = \sum_{\tau \in T_n} \sum_{g : \tau \subset g} \frac{1}{N(g)} [\cdot],$$

since in the double sum $\Sigma_\tau \Sigma_{g \supset t}$ each g will be repeated exactly $N(g)$ times.

Thus,

$$B_n(x_1,x_2) \leqslant \sum_{\tau \in T_n} w_n(\tau, x_1, x_2),$$

where we have defined

$$w_n(\tau,x_1,x_2) \equiv \sum_{\substack{R_1,\ldots,R_n \subset \Lambda : |R_i| \geqslant 2 \\ g(R_1,R_2,\ldots,R_n) \supset \tau, x_1 \in R_1, x_2 \in R_2}} |\tilde{\rho}(R_1)\| \tilde{\rho}(R_2)\| \tilde{\rho}(R_3) \cdots \tilde{\rho}(R_n)|.$$

Using now the obvious bound

$$\sum_{R : R \cap R' \neq \emptyset} |\cdot| \leqslant |R'| \sup_{x \in R'} \sum_{R : x \in R} |\cdot|,$$

and denoting again as $\overline{\tau}$ the subtree of τ which is the unique path joining vertex 1 to vertex 2, and denoting as $I_\tau = \{1, i_1, \ldots, i_k, 2\}$ the ordered set of the vertices of $\overline{\tau}$, one can easily check that

$$w_n(\tau,x_1,x_2) \leqslant \prod_{i\notin I_\tau}\left[\sup_{x\in Z^d}\sum_{R_i:x\in R_i}|R_i|^{d_i-1}|\tilde{\rho}(R_i)|\right]$$
$$\times \sum_{\substack{R_1,R_{i_1},\dots,R_{i_k},R_2:x_1\in R_1,x_2\in R_2\\ R_1\cap R_{i_1}\neq\emptyset,\dots R_{i_k}\cap R_2\neq\emptyset}} |R_1|^{d_1-1}|\tilde{\rho}(R_1)||R_2|^{d_2-1}|\tilde{\rho}(R_2)|\prod_{\substack{i\in I_\tau\\ i\neq 1,2}}^{n}|R_i|^{d_i-2}|\tilde{\rho}(R_i)|$$
$$\leqslant \prod_{i\notin I_\tau}\left[\sup_{x\in Z^d}\sum_{R_i:x\in R_i}(d_i-1)!\,|\tilde{\rho}(R_i)|e^{|R_i|}\right](d_1-1)!\,(d_2-1)!$$
$$\times \sum_{\substack{R_1,R_{i_1},\dots,R_{i_k},R_2:x_1\in R_1,x_2\in R_2\\ R_1\cap R_{i_1}\neq\emptyset,\dots,R_{i_k}\cap R_2\neq\emptyset}} |\tilde{\rho}(R_1)|e^{|R_1|}|\tilde{\rho}(R_2)|e^{|R_2|}\prod_{\substack{i\in I_\tau\\ i\neq 1,2}}(d_i-2)!\,|\tilde{\rho}(R_i)|e^{|R_i|},$$

since $|R|^n\leqslant n!\,e^{|R|}$. Now, note that

$$\sum_{\substack{R_1,R_{i_1},\dots,R_{i_k},R_2:x_1\in R_1,x_2\in R_2\\ R_1\cap R_{i_1}\neq\emptyset,\dots,R_{i_k}\cap R_2\neq\emptyset}} \leqslant \sum_{x_{i_0}\in Z^d}\sum_{x_{i_1}\in Z^d}\cdots\sum_{x_{i_k}\in Z^d}\sum_{\substack{R_1\\ x_1,x_{i_0}\in R_1}}\sum_{\substack{R_{i_1}\\ x_{i_0},x_{i_1}\in R_{i_1}}}\cdots\sum_{\substack{R_{i_k}\\ x_{i_{k-1}},x_{i_k}\in R_{i_k}}}\sum_{\substack{R_2\\ x_{i_k},x_2\in R_2}}.$$

Hence, recalling (57) and applying iteratively the inequality (54) with $w_1=1/2$ and $w_2=2/3$,

$$\sum_{\substack{R_1,R_{i_1},\dots,R_{i_k},R_2:x_1\in R_1,x_2\in R_2\\ R_1\cap R_{i_1}\neq\emptyset,\dots,R_{i_k}\cap R_2\neq\emptyset}} |\tilde{\rho}(R_1)|e^{|R_1|}|\tilde{\rho}(R_2)|e^{|R_2|}\prod_{i\in I_\tau}|\tilde{\rho}(R_i)|e^{|R_i|}$$
$$\leqslant \sum_{x_{i_0}\in Z^d}\sum_{x_{i_1}\in Z^d}\cdots\sum_{x_{i_k}\in Z^d}[\varepsilon(\beta,K)]^{|(x_1)_0-(x_{i_0})_0|+1}F^{(2/3)}_{x_1x_{i_0}}\cdots[\varepsilon(\beta,K)]^{|(x_{i_k})_0-(x_2)_0|+1}F^{(2/3)}_{x_{i_k}x_2}$$
$$\leqslant [\mathcal{O}(1)]^{k+1}[\varepsilon(\beta,K)]^{|(x_1)_0-(x_2)_0|+(k+2)}F^{(1/2)}_{x_1x_2},$$

since $\varepsilon(\beta,K)<1$ and $|(x_1)_0-(x_2)_0|\leqslant|(x_1)_0-(x_{i_0})_0|+|(x_{i_0})_0-(x_{i_1})_0|+\cdots+|(x_{i_k})_0-(x_2)_0|$.

Thus, using Corollary 4 and noting that $|\{1,\dots,n\}\backslash I_\tau|=n-k-2$,

$$w_n(\tau,x_1,x_2)\leqslant(d_1-1)!\,(d_2-1)!\left[\prod_{i\notin I_\tau}^{n}\sup_{x\in Z^d}\sum_{R_i:x\in R_i}(d_i-1)!\,|\rho(R_i)|e^{|R_i|}\right]$$
$$\times\left[\prod_{\substack{i\in I_\tau\\ i\neq 1,2}}^{n}(d_i-2)!\right][\varepsilon(\beta,K)]^{|(x_1)_0-(x_2)_0|+(k+2)}[\mathcal{O}(1)]^{k+1}F^{(1/2)}_{x_1x_2}$$
$$\leqslant[\mathcal{O}(1)]^n[\varepsilon(\beta,K)]^{|(x_1)_0-(x_2)_0|+n}F^{(1/2)}_{x_1x_2}\prod_{i=1}^{n}(d_i-1)!\,.$$

Finally, carrying out the sum over τ (and using, once again, the Cayley formula) we obtain

$$B_n(x_1,x_2)\leqslant(n-2)!\,[4\mathcal{O}(1)]^n[\varepsilon(\beta,K)]^{|(x_1)_0-(x_2)_0|+n}F^{(1/2)}_{x_1x_2}.$$

Taking β,K small enough to make $4\mathcal{O}(1)\varepsilon(\beta,K)<1$, for the contribution of A_1 to the correlations, we get the following bound:

$$|A_1(x_1,x_2)|\leqslant\sum_{n\geqslant 2}[4\mathcal{O}(1)]^n[\varepsilon(\beta,K)]^{|(x_1)_0-(x_2)_0|+n}F^{(1/2)}_{x_1x_2}\leqslant\mathcal{O}(1)[\varepsilon(\beta,K)]^{|(x_1)_0-(x_2)_0|+2}F^{(1/2)}_{x_1x_2}.$$

In a similar and much easier way one can also prove a completely analogous bound for $|A_2(x_1,x_2)|$,

$$|A_2(x_1,x_2)| \leqslant \mathcal{O}(1)[\varepsilon(\beta,K)]^{|(x_1)_0-(x_2)_0|+1} F^{(1/2)}_{x_1x_2}.$$

Hence,

$$|S_2(x;y)| \leqslant \mathcal{O}(1)[\varepsilon(\beta,K)]^{|x_0-y_0|} F^{(1/2)}_{xy} \leqslant \mathcal{O}(1)[\varepsilon(\beta,K)]^{|x_0-y_0|} e^{-|x_0-y_0|/2}\left(\frac{1-\delta_{\vec{x},\vec{y}}}{|\vec{x}-\vec{y}|^p}+\delta_{\vec{x},\vec{y}}\right)$$

$$\leqslant \mathcal{O}(1) e^{-m'(\beta,K)|x_0-y_0|}\left(\frac{1-\delta_{\vec{x},\vec{y}}}{|\vec{x}-\vec{y}|^p}+\delta_{\vec{x},\vec{y}}\right),$$

where, since $\varepsilon(\beta,K)<1$, we write above

$$m'(\beta,K) \equiv -\log\{\varepsilon(\beta,K)\} + 1/2 > 0.$$

These results prove part 2 of Theorem 1 (the part 1 is a simpler case and may be proved in a similar way).

A lower bound can be obtained, as said, by analogous procedures (see, e.g., Ref. 13).

VI. FOUR-POINT TRUNCATED CORRELATION

Now we analyze the "time" decay of the partially truncated four-point function in order to determine the mass spectrum in the interval $(M,2M)$, where M is the one-particle mass. In this section, we restrict the interaction to even function of the spin variable ϕ.

We use the BS equation, and omit several technical details (related to those presented, e.g., in Ref. 6). The computation is carried out in a perturbative approach, we keep only the dominant term in a β expansion of the BS kernel.

Roughly, we show that, for the model considered here, in the intense noise regime $\beta \ll 1$, if the polynomial $U(\phi)$ is such that $\langle\phi^4\rangle > 3\langle\phi^2\rangle^2$, where $\langle\cdot\rangle$ is the expectation with respect to the single spin distribution $\mathrm{d}\nu(\phi)$ (31), there is an isolated two-particle bound state with mass $M^*=2M+\log(1-\zeta)+\mathcal{O}(\beta)$, where $\zeta=[\langle\phi^4\rangle-3\langle\phi^2\rangle]/[\langle\phi^4\rangle-\langle\phi^2\rangle]$.

Sketch of the proof: We use the BS equation which writes the truncated four-point function $D(x_1,x_2;x_3,x_4)=S_4(x_1,x_2,x_3,x_4)-S_2(x_1,x_2)S_2(x_3,x_4)$ as

$$D(x_1,x_2;x_3,x_4) = D_0(x_1,x_2;x_3,x_4) + \sum_{y_1,y_2,y_3,y_4} D(x_1,x_2;y_1,y_2)K(y_1,y_2;y_3;y_4)D_0(y_3,y_4;x_3,x_4),$$

where $D_0(x_1,x_2;x_3,x_4) \equiv S_2(x_1,x_3)S_2(x_2,x_4)+S_2(x_1,x_4)S_2(x_2,x_3)$.

Due to translation invariance, D depends only on difference variable, i.e., $D=D(\xi,\eta,\tau)$, where here we take $\xi=x_2-x_1$, $\eta=x_4-x_3$, and $\tau=x_3-x_2$. Using p,q, and k, the conjugate variable (the Fourier transform) of ξ,η,τ, the BS equation becomes

$$\tilde{D}(p,q,k) = \tilde{D}_0(p,q,k) + \frac{1}{(2\pi)^{2(d+1)}}\int_{T^{d+1}} \mathrm{d}^{d+1}p'\,\mathrm{d}^{d+1}q'\,\tilde{D}(p,p',k)\tilde{K}(p',q',k)\tilde{D}_0(q',q,k),$$

or using the notation $(\tilde{D}(k)f)(p) \equiv \int_{T^{d+1}} \mathrm{d}^{d+1}q\ \tilde{D}(p,q,k)f(q)$,

$$\tilde{D}(k) = \tilde{D}_0(k) + \frac{1}{(2\pi)^{2(d+1)}}\tilde{D}(k)\tilde{K}(k)\tilde{D}_0(k) = \tilde{D}_0(k)[1-(2\pi)^{-2(d+1)}\tilde{K}(k)\tilde{D}_0(k)]^{-1}.$$

We restrict the analysis to the mass spectrum, i.e., we take $k=(k_0,\vec{k}=\vec{0})$, and consider $f(p)$ depending only on $\vec{p}$. From the definition of D_0, we get

$$\tilde{D}_0(p,q,k) = (2\pi)^{d+1}[\tilde{S}_2(p)\tilde{S}_2(q)\,\delta(k-p-q) + \tilde{S}_2(p)\tilde{S}_2(k-p)\,\delta(q-p)]. \tag{58}$$

Hence, $(\tilde{D}_0(k_0)f)(p) = (2\pi)^{d+1}\tilde{S}_2(p)\tilde{S}_2(k-p)[f(\vec{p})+f(-\vec{p})]$. For $f(\vec{p})=f(-\vec{p})$, we obtain

$$(\tilde{f},\tilde{D}(k_0)\tilde{f}) = \int \tilde{f}(\vec{p})\left\{2(2\pi)^{d+1}\int \mathrm{d}p_0\, \tilde{S}_2(p)\tilde{S}_2(k_0-p_0,-\vec{p})\right\} \times \left(\left[1-\frac{1}{(2\pi)^{2(d+1)}}\tilde{K}(k_0)\tilde{D}_0(k_0)\right]^{-1}\tilde{f}\right) \times(\vec{p})\mathrm{d}^d p. \tag{59}$$

As $\{\cdots\}(k_0,\vec{p})$ above is analytic in $|\mathrm{Im}\, k_0|<2M$, the singularities in such region come from where the inverse of $1-(2\pi)^{-2(d+1)}\tilde{K}(k_0)\tilde{D}_0(k_0)$ does not exist.

Now we follow replacing $\tilde{K}$ by the leading term in the perturbation expansion (in terms of β), which is named ladder approximation. We remark (once more time), as a comment on the reliability of such procedure, that in Refs. 6,14 and 15 a rigorous analysis (in similar "field theory") shows that the spectral properties calculated in the ladder approximation are maintained.

Using $K=D_0^{-1}-D^{-1}$ we obtain

$$\tilde{K}(p,q,k)_{\mathcal{O}(\beta=0)} = \frac{\langle\phi^4\rangle-3\langle\phi^2\rangle^2}{2\langle\phi^2\rangle^2[\langle\phi^4\rangle-\langle\phi^2\rangle^2]} = R, \tag{60}$$

i.e., constant (not depending on β), local in space and time. Writing $[1-A]^{-1}=1+[1-A]^{-1}A$ we get

$$(\tilde{f},\tilde{D}_0(k_0)\tilde{f}) = \int \overline{\tilde{f}}(\vec{p})\tilde{D}_0(p,q,k_0)\tilde{f}(\vec{q})\mathrm{d}p\ \mathrm{d}q + \frac{R'}{1-R'I_D}\left(\int \overline{\tilde{f}}(\vec{p})\tilde{D}_0(p,q,k_0)\mathrm{d}p\ \mathrm{d}q\right) \times\left(\int \tilde{D}_0(p',q',k_0)\tilde{f}(\vec{q}')\mathrm{d}p'\ \mathrm{d}q\right), \tag{61}$$

where $\mathrm{d}p\equiv\mathrm{d}^{d+1}p$, etc., $R'=R/(2\pi)^{2(d+1)}$ and

$$I_D = \int \mathrm{d}q'\ \mathrm{d}q\ \tilde{D}_0(q',q,k_0) = 2(2\pi)^{d+1}\int \mathrm{d}p\ \tilde{S}_2(p)\tilde{S}_2(k_0-p_0,-\vec{p}).$$

Thus, the singularity, and so the bound state, comes for $R'I_D=1$. We follow the calculations separating in the expression for $\tilde{S}_2(p)$ the dominant one-particle contribution (as usual, we take the Lehmann spectral representation, see, e.g., Refs. 6 and 12),

$$\tilde{S}_2(p) = (2\pi)^d\tilde{c}_2(\vec{p})\frac{\sinh M(\vec{p})}{\cosh M(\vec{p})-\cos p_0} + \int_{3M-\varepsilon}^{\infty}\frac{\sinh E}{\cosh E-\cos p_0}\mathrm{d}\eta(E,\vec{p}),$$

where $\tilde{c}_2(\vec{p})=\partial\tilde{\Gamma}(p_0=i\xi,\vec{p})/\partial\xi|_{\xi=M(\vec{p})}$. We have, for the (first) dominant term, $\tilde{c}_2(\vec{p})=[\langle\phi^2\rangle/(2\pi)^d]+\mathcal{O}(\beta)$. Thus, for the computation of (the leading part of) I_D we use $\tilde{S}_2(p)=\langle\phi^2\rangle\times\{\sinh M(\vec{p})/[\cosh M(\vec{p})-\cos p_0]\}$. Hence,

$$I_D = 2(2\pi)^{d+1}\int \mathrm{d}p\langle\phi^2\rangle^2\frac{(e^{M(\vec{p})}-e^{-M(\vec{p})})^2}{(e^{M(\vec{p})}+e^{-M(\vec{p})}-e^{ip_0}-e^{-ip_0})(e^{M(\vec{p})}+e^{-M(\vec{p})}-e^{ik_0-ip_0}-e^{-ik_0+ip_0})}.$$

Writing $ik_0=2M-\varepsilon$, we get (taking the leading term $\beta=0$) $I_D=2(2\pi)^{2(d+1)}\langle\phi^2\rangle^2/(1-e^{-\varepsilon})$. And for the eigenvalue equation $R'I_D=1$ we obtain

$$1-e^{-\varepsilon} = \frac{\langle\phi^4\rangle-3\langle\phi^2\rangle^2}{\langle\phi^4\rangle-\langle\phi^2\rangle^2} \equiv \zeta, \tag{62}$$

which leads, if $\zeta>0$, to the bound state mass

$$M^* = 2M+\ln(1-\zeta). \tag{63}$$

■

We have the same bound state mass expression of Ref. 15, calculated there for a ferromagnetic system with continuous spin, nearest neighbor interaction, and even single spin distribution.

As a final comment, let us say that we expect to apply the techniques presented here in the analysis of the correlation functions of other stochastic dynamical systems, such as those described by an anharmonic chain of oscillators, with conservative dynamics and different stochastic reservoirs[21] (in our case, for the intense noise, i.e., "high temperature" regime).

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Propagators weakly associated to a family of Hamiltonians and the adiabatic theorem for the Landau Hamiltonian with a time-dependent Aharonov–Bohm flux

J. Asch
Centre de Physique Théorique, CNRS, Luminy, Case 907, Marseille Cedex 9, France and CPT-PhyMat, Université du Sud Toulon-Var, BP 20132, F-83957 La Garde Cedex, France

I. Hradecký and P. Šťovíček
Department of Mathematics, Faculty of Nuclear Science, Czech Technical University, Trojanova 13, 120 00 Prague, Czech Republic

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We study the dynamics of a quantum particle moving in a plane under the influence of a constant magnetic field and driven by a slowly time-dependent singular flux tube through a puncture. The known standard adiabatic results do not cover directly these models as the Hamiltonian has time-dependent domain. We give a meaning to the propagator and prove an adiabatic theorem. To this end we introduce and develop the new notion of a propagator weakly associated to a time-dependent Hamiltonian. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1895865]

I. INTRODUCTION

The model under consideration originates from Laughlin's[12] and Halperin's[9] discussion of the integer quantum Hall effect. In the mathematical physics literature Bellissard *et al.*[5] and Avron *et al.*[3] used an adiabatic limit of the model (with additional randomness) to introduce indices. The indices explain the quantization of charge transport observed in the experiments.[14]

In this paper we discuss some mathematical aspects of the existence of the propagator and the validity of the adiabatic approximation and propose how to overcome the difficulties originating from the strong singularity of the external field.

Let us specify the model, summarize our results and introduce the notation. The configuration space is $\mathbb{R}^2\backslash\{(0,0)\}$ and the model is considered in polar coordinates (r,θ). The vector potential A is the sum of a part for the homogeneous magnetic field of strength $B>0$,

$$\frac{B}{2}(x_1\,\mathrm{d}x_2 - x_2\,\mathrm{d}x_1) = \frac{Br^2}{2}\mathrm{d}\theta,$$

plus a part describing the flux Φ which varies in time,

$$\frac{\Phi}{2\pi}\frac{1}{|\vec{x}|^2}(x_1\,\mathrm{d}x_2 - x_2\,\mathrm{d}x_1) = \frac{\Phi}{2\pi}\mathrm{d}\theta;$$

the real-valued function Φ is assumed to be monotonous and C^2. With the metric coefficients $g_{11}=1$, $g_{22}=r^2$, $g_{12}=0$, the differential expression of the Hamiltonian acting in $L^2(\mathbb{R}_+\times[0,2\pi[,r\,\mathrm{d}r\,\mathrm{d}\theta)$ is

$$\frac{1}{2m}\left(-i\hbar\partial_j - \frac{e}{c}A_j\right)\sqrt{g}g^{jk}\left(-i\hbar\partial_k - \frac{e}{c}A_k\right) = \frac{\hbar^2}{2m}\left(-\frac{1}{r}\partial_r r\partial_r + \frac{1}{r^2}\left(-i\partial_\theta - \frac{e}{\hbar c}\frac{Br^2}{2} - \frac{e}{hc}\Phi\right)^2\right).$$

Our purpose is to study the response of the system if flux quanta hc/e are added adiabatically, i.e., the flux function is of the form $t\mapsto\Phi(t/\tau)$ with the time t varying in $[0,\tau]$ for some $\tau\gg 1$.

In a first step we analyze the case when Φ is linear. Furthermore, we fix an angular momentum sector defined by $-i\partial_\theta e^{im\theta}=me^{im\theta}$ ($m\in\mathbb{Z}$), and use a slow time s, i.e., the substitution $s=-m+e/(hc)\Phi(t/\tau)$. Also we are not interested here in keeping track of the behavior in the physical parameters e, $\hbar$, c, $2m$, so we set them all equal to one. This is our motivation to consider the operator

$$H(s)=-\frac{1}{r}\partial_r r\partial_r+\frac{1}{r^2}\left(s+\frac{Br^2}{2}\right)^2 \quad \text{in } L^2(\mathbb{R}_+,r\,\mathrm{d}r). \tag{1}$$

In a second step we shall then show that our analysis generalizes to Hamiltonians of the form $H(\zeta(s))$ where $\zeta\in C^2$ is a monotone function.

$H(s)$ is essentially self-adjoint on $C_0^\infty(]0,\infty[)$ iff $s^2\geqslant 1$.[13] For $0<s^2<1$ we impose the regular boundary condition as $r\to 0+$ [i.e., a wave function belongs to the domain if it has no part proportional to the (square integrable) singularity $r^{-|s|}$]. This is in fact the most common choice, see Ref. 8 for a detailed discussion. The case $s=0$ is particular since the singularity in question is logarithmic but otherwise the situation is similar, see Ref. 1. The Hamiltonian $H(s)$ is unambiguously determined by specifying a complete set of eigenfunctions with corresponding eigenvalues, see below.

The dynamics of the model should be defined by

$$i\partial_s U_\tau(s,s_0)\psi=\tau H(s)U_\tau(s,s_0)\psi, \quad U_\tau(s_0,s_0)\psi=\psi, \tag{2}$$

where U_τ is unitary and ψ is an arbitrary initial condition from the domain of $H(s_0)$. The existence of a propagator in this sense is, however, uncertain. The problem arises from the fact that the domain of $H(s)$ is not constant in s, respectively, that $\dot{H}(s)$ is not relatively bounded with respect to $H(s)$. Thus the usual theorems which assure the existence of the propagator[13] and the validity of the adiabatic approximation[4,2] are not directly applicable.

A convenient way to see this is to consider the eigenfunctions. The operator $H(s)$ has a simple discrete spectrum; the eigenvalues are

$$\lambda_n(s)=B(s+|s|+2n+1), \quad n\in\{0,1,2,\ldots\}, \tag{3}$$

with the corresponding normalized eigenfunctions

$$\varphi_n(s;r)=c_n(s)r^{|s|}L_n^{(|s|)}\left(\frac{Br^2}{2}\right)\exp\left(-\frac{Br^2}{4}\right),$$

where

$$c_n(s)=\left(\frac{B}{2}\right)^{(|s|+1)/2}\left(\frac{2n!}{\Gamma(n+|s|+1)}\right)^{1/2}$$

are the normalization constants and $L_n^{(|s|)}$ are the generalized Laguerre polynomials (see, for example, Ref. 8).

The derivative of $H(s)$ equals

$$\dot{H}(s)=\frac{2s}{r^2}+B.$$

Notice that if $|s|\leqslant 1$ then $\varphi_n(s)$ cannot belong to the domain $\mathrm{Dom}\,\dot{H}(s)$ since $\dot{H}(s)\varphi_n(s)\sim r^{-2+|s|}$ for $r\to 0+$. This means that $\dot{H}(s)$ is not relatively bounded with respect to $H(s)$.

Remark that, on the other hand, the quadratic expression

$$\int_0^\infty \varphi_m(s;r)\dot{H}(s)\varphi_n(s;r)r\,\mathrm{d}r$$

makes good sense. In order to avoid a complicated notation we shall denote it by the symbol $\langle\varphi_m(s),\dot{H}(s)\varphi_n(s)\rangle$ even though the symbol cannot be taken literally and is therefore somewhat misleading. Furthermore, the derivative of the eigenfunction, $\dot{\varphi}_n(s)$, belongs to $L^2(\mathbb{R}_+,r\,\mathrm{d}r)$. Since the eigenfunctions are chosen to be real valued it holds true that

$$\langle\varphi_n(s),\dot{\varphi}_n(s)\rangle = 0.$$

Let us also note that, similarly, if $|s|\leqslant 1$ and $s^2\neq s'^2$ then the eigenfunction $\varphi_n(s)$ cannot belong to $\mathrm{Dom}\,H(s')$. It is so because (as formal expressions) $H(s')-H(s)=(s'^2-s^2)/r^2+B(s'-s)$ and $H(s')\varphi_n(s;r)$ has a nonintegrable singularity at $r=0$. Hence $\mathrm{Dom}\,H(s)$ depends on s.

It turns out that, following the strategy of Born and Fock,[6] the problems of existence and adiabatic approximation can both be handled.

Denote the eigenprojector onto $\mathbb{C}\varphi_n(s)$ by $P_n(s)$; it is differentiable as a bounded operator. The hard part of our work consists in showing that

$$i\sum_{k=0}^{\infty}\dot{P}_k(s)P_k(s)$$

is a bounded operator. This is stated in Lemma 6. It requires work because its matrix elements have bad off-diagonal decay, see Lemma 4 (which is formulated for the unitarily equivalent operator Q).

Now

$$H_{AD}(s):=H(s)+\frac{i}{\tau}\sum_{n=0}^{\infty}\dot{P}_n(s)P_n(s)$$

has a propagator which is well defined in the usual way, i.e.,

$$i\partial_s U_{AD}(s,s_0)\psi=\tau H_{AD}(s)U_{AD}(s,s_0)\psi,\quad U_{AD}(s_0,s_0)\psi=\psi, \tag{4}$$

for $\psi\in\mathrm{Dom}(H_{AD}(s_0))$. To see this notice that U_{AD} can be computed by its action on the eigenbasis,

$$U_{AD}(s,s_0)\varphi_n(s_0)=e^{-i\tau\int_{s_0}^{s}\lambda_n(u)\mathrm{d}u}\varphi_n(s).$$

Furthermore, $\lambda_n(s)-\lambda_n(0)$ is bounded in n and so

$$U_{AD}(s,s_0)\mathrm{Dom}\,H_{AD}(s_0)=\mathrm{Dom}\,H_{AD}(s).$$

Since $H(s)-H_{AD}(s)$ is bounded the domains of $H(s)$ and $H_{AD}(s)$ are identical. By time-dependent transformation a natural candidate for the propagator of $H(s)$ is

$$U_\tau(s,s_0):=U_{AD}(s,0)C(s,s_0)U_{AD}(0,s_0), \tag{5}$$

where $C(s,s_0)$ is defined by

$$i\partial_s C(s,s_0)=-Q_\tau(s)C(s,s_0),\quad C(s_0,s_0)=\mathbb{I}, \tag{6}$$

with

$$Q_\tau(s):=U_{AD}(0,s)\left(i\sum_{k=0}^{\infty}\dot{P}_k(s)P_k(s)\right)U_{AD}(s,0). \tag{7}$$

Since $\|Q_\tau(s)\|$ is locally bounded the propagator $C(s,s_0)$ is well defined by the Dyson formula.

The adiabatic approximation problem is settled in Proposition 11 where it is shown that

$$\|U_\tau(s,0) - U_{AD}(s,0)\| = O\left(\frac{1}{\tau}\right).$$

It remains unclear, however, whether $C(s,s_0)$ preserves the domain of $H(0)$ and therefore whether the propagator $U_\tau(s,s_0)$ is actually related to the Hamiltonian $H(s)$ in the usual sense. To handle this problem we develop the general concept of weak association of a propagator and a time-dependent Hamiltonian. We can show that U_τ is weakly associated to $H(s)$ and that the Schrödinger equation (2) is fulfilled in the sense of distributions.

We shall use the following notation. The symbol $V(s)$ stands for the unitary operator which sends all eigenstates at time 0 to the corresponding eigenstates at time s, i.e.,

$$V(s)\varphi_n(0) = \varphi_n(s) \quad \forall\, n \in \mathbb{Z}_+ \tag{8}$$

(here and everywhere in what follows $\mathbb{Z}_+$ stands for the set of non-negative integers). Further set

$$W(s) = V(s)^{-1}H(s)V(s) = \sum_{n=0}^{\infty} \lambda_n(s)P_n(0) \tag{9}$$

and

$$\Omega(s) = \sum_{n=0}^{\infty} \omega_n(s)P_n(0), \tag{10}$$

where

$$\omega_n(s) = \int_0^s \lambda_n(u)\mathrm{d}u.$$

Remark that the adiabatic propagator decomposes as

$$U_{AD}(s,s_0) = V(s)e^{-i\tau(\Omega(s)-\Omega(s_0))}V(s_0)^{-1}.$$

The paper is organized as follows. In Secs. II and III we do the analysis necessary to prove the boundedness result stated in Lemma 6. Section IV is devoted to the existence problem for the propagator. In Sec. V we prove the adiabatic theorem in Proposition 11. The result is then extended to a more general time dependence in Sec. VI.

A rather independent part of the paper is the Appendix where we propose the notion of a propagator weakly associated to a time-dependent Hamiltonian. We indicate cases where the weak association can be verified while the usual relationship between a propagator and a Hamiltonian is unclear or even is not valid. In particular, this concept was inspired by the situation we encountered in the present model. We believe, however, that this idea need not be restricted to this case only and that it might turn out to be useful in resolving this type of difficulties in other models as well.

II. AUXILIARY ESTIMATES OF MATRIX OPERATORS

Here we derive some auxiliary estimates that will be useful later when verifying assumptions of the adiabatic theorem.

Lemma 1: *Let $A(\sigma)$ be an operator in $l^2(\mathbb{N})$ depending on a parameter $\sigma \geqslant 0$ whose matrix entries in the standard basis equal*

$$A(\sigma)_{mn} = \begin{cases} 0 & \text{for } m = n, \\ -\frac{i}{n}\left(\frac{m}{n}\right)^{\sigma} & \text{for } m < n, \\ \frac{i}{m}\left(\frac{n}{m}\right)^{\sigma} & \text{for } m > n. \end{cases}$$

Then $A(\sigma)$ is bounded, uniformly in σ, and its norm satisfies the estimate

$$\|A(\sigma)\| \leqslant 24.$$

Proof: The proof will be done in several steps.

(i) Let $K(\sigma)$ be an integral operator acting in $L^2(\mathbb{R}_+, \mathrm{d}x)$ with the integral kernel

$$\mathcal{K}_{\sigma}(x,y) = \begin{cases} -\frac{i}{y}\left(\frac{x}{y}\right)^{\sigma} & \text{for } x < y, \\ \frac{i}{x}\left(\frac{y}{x}\right)^{\sigma} & \text{for } x > y. \end{cases}$$

Let us show that

$$\|K(\sigma)\| = \frac{2}{2\sigma + 1}.$$

First we apply the unitary transform

$$U{:}L^2(\mathbb{R}_+, \mathrm{d}x) \to L^2(\mathbb{R}, \mathrm{d}y), \quad U\psi(y) = e^{y/2}\psi(e^y). \tag{11}$$

The inverse transform reads $U^{-1}\hat{\psi}(x) = x^{-1/2}\hat{\psi}(\ln x)$. Set

$$\widetilde{K}(\sigma) = UK(\sigma)U^{-1}.$$

One finds that $\widetilde{K}(\sigma)$ is again an integral operator with the integral kernel

$$\widetilde{\mathcal{K}}_{\sigma}(y,z) = i\,\mathrm{sgn}(y - z)e^{-(\sigma+1/2)|y-z|}.$$

Hence $\widetilde{K}(\sigma)$ is a convolution operator and it is therefore diagonalizable with the aid of the Fourier transform $\mathcal{F}$ on $\mathbb{R}$. This means that

$$(\mathcal{F}\widetilde{K}(\sigma)\mathcal{F}^{-1}\psi)(z) = \hat{q}(z)\psi(z),$$

where

$$\hat{q}(z) = \int_{\mathbb{R}} e^{izy}\,\mathrm{sgn}(y)e^{-(\sigma+1/2)|y|}\,\mathrm{d}y = \frac{2iz}{\left(\sigma + \frac{1}{2}\right)^2 + z^2}.$$

It follows that

$$\|K(\sigma)\| = \|\mathcal{F}\widetilde{K}(\sigma)\mathcal{F}^{-1}\| = \|\hat{q}\|_{\infty} = \frac{1}{\sigma + \frac{1}{2}}. \tag{12}$$

(ii) Suppose that $\{\psi\}_{n=1}^{\infty}$ is an orthogonal system in $L^2(\mathbb{R}_+, \mathrm{d}x)$ such that

$$\forall m,n \in \mathbb{N}, \quad \langle \psi_m, K(\sigma)\psi_n \rangle = A(\sigma)_{mn}$$

and

$$\forall n \in \mathbb{N}, \quad \|\psi_n\|^2 = \kappa > 0.$$

Let P_+ be the orthogonal projector onto span $\{\psi_n\}_{n=1}^{\infty}$ in $L^2(\mathbb{R}_+, \mathrm{d}x)$. Then one can identify $P_+K(\sigma)P_+$ with $\kappa^{-1}A(\sigma)$. Hence

$$\|A(\sigma)\| = \kappa\|P_+K(\sigma)P_+\| \leqslant \kappa\|K(\sigma)\|. \tag{13}$$

(iii) We shall construct an orthogonal system $\{\psi_n\}_{n=1}^{\infty}$ described in the preceding point as follows. Consider the natural embedding $L^2([n,n+1],\mathrm{d}x)\subset L^2(\mathbb{R}_+,\mathrm{d}x)$, $n\in\mathbb{N}$. We seek $\psi_n\in L^2([n,n+1],\mathrm{d}x)$ in the form

$$\psi_n = \alpha_n u_n + \beta_n v_n + f_n,$$

where α_n, $\beta_n\in\mathbb{R}$, u_n, v_n, $f_n\in L^2([n,n+1],\mathrm{d}x)$,

$$u_n(x) = x^{\sigma}, \quad v_n(x) = x^{-\sigma-1} \quad \text{for } x\in[n,n+1],$$

and $f_n\perp u_n$, $f_n\perp v_n$. Suppose for definiteness that $m<n$. Then

$$\langle\psi_m,K(\sigma)\psi_n\rangle = \int_m^{m+1}\mathrm{d}x\int_n^{n+1}\mathrm{d}y\ \mathcal{K}_\sigma(x,y)\psi_m(x)\psi_n(y) = -i\langle u_m,\psi_m\rangle\langle v_n,\psi_n\rangle.$$

Furthermore,

$$\langle\psi_n,K(\sigma)\psi_n\rangle = \int_n^{n+1}\int_n^{n+1}\mathcal{K}_\sigma(x,y)\psi_n(x)\psi_n(y)\mathrm{d}x\,\mathrm{d}y = 0$$

since $\mathcal{K}_\sigma(x,y)$ is antisymmetric, $\mathcal{K}_\sigma(y,x)=-\mathcal{K}_\sigma(x,y)$. Consequently, it suffices to choose the real coefficients α_n, β_n so that

$$\forall n\in\mathbb{N},\langle u_n,\psi_n\rangle = n^{\sigma}, \quad \langle v_n,\psi_n\rangle = n^{-\sigma-1}.$$

This system has a unique solution (α_n,β_n). The function f_n can be arbitrary. Its only purpose is to adjust the norms of the functions ψ_n so that they are all equal. Set

$$N_n(\sigma) = \|\alpha_n u_n + \beta_n v_n\|^2 = \int_n^{n+1}(\alpha_n x^{\sigma} + \beta_n x^{-\sigma-1})^2\,\mathrm{d}x$$

and

$$\kappa(\sigma) = \sup_{n\in\mathbb{N}} N_n(\sigma).$$

One can choose the orthogonal system $\{\psi_n\}_{n=1}^{\infty}$ so that $\|\psi_n\|^2=\kappa(\sigma)$ for all n. According to (12) and (13) we have

$$\|A(\sigma)\| \leqslant \frac{2\kappa(\sigma)}{2\sigma+1}. \tag{14}$$

(iv) It remains to find an upper bound on $\kappa(\sigma)$. Set

$$\xi_n = n^{\sigma}, \quad \eta_n = n^{-\sigma-1}.$$

Simple algebraic manipulations yield

$$N_n(\sigma) = \frac{\langle v_n,v_n\rangle\xi_n^2 - 2\langle u_n,v_n\rangle\xi_n\eta_n + \langle u_n,u_n\rangle\eta_n^2}{\langle u_n,u_n\rangle\langle v_n,v_n\rangle - \langle u_n,v_n\rangle^2}.$$

Here

$$\langle u_n,v_n\rangle = \ln\left(1+\frac{1}{n}\right),$$

$$\langle u_n, u_n\rangle = \frac{1}{2\sigma+1}((n+1)^{2\sigma+1} - n^{2\sigma+1}),$$

$$\langle v_n, v_n\rangle = \frac{1}{2\sigma+1}(n^{-2\sigma-1} - (n+1)^{-2\sigma-1}).$$

Set

$$w = \left(\sigma + \frac{1}{2}\right)\ln\left(1 + \frac{1}{n}\right).$$

One can rewrite the expression for $N_n(\sigma)$ as follows:

$$N_n(\sigma) = \frac{2\sigma+1}{n}\frac{\sinh(w)\cosh(w) - w}{\sinh^2(w) - w^2}.$$

Using an elementary analysis one can show that

$$\frac{\sinh(w)\cosh(w) - w}{\sinh^2(w) - w^2} \leqslant \frac{\sinh(w)\cosh(w) - w}{\sinh(w)(\sinh(w) - w)} \leqslant 4\,\mathrm{cotgh}(w).$$

Hence

$$N_n(\sigma) \leqslant \frac{4(2\sigma+1)}{n}\frac{\left(1 + \frac{1}{n}\right)^{2\sigma+1} + 1}{\left(1 + \frac{1}{n}\right)^{2\sigma+1} - 1} \leqslant 12(2\sigma+1).$$

Consequently,

$$\kappa(\sigma) \leqslant 12(2\sigma+1). \tag{15}$$

From (14) and (15) it follows that $\|A(\sigma)\| \leqslant 24$. □

Lemma 2: *Let $A(\sigma)$ be an operator in $l^2(\mathbb{N})$ whose matrix entries in the standard basis equal*

$$A(\sigma)_{mn} = \begin{cases} 0 & \text{for } m = n, \\ -\frac{i}{n} f_\sigma\left(\frac{m}{n}\right) & \text{for } m < n, \\ \frac{i}{m} f_\sigma\left(\frac{n}{m}\right) & \text{for } m > n, \end{cases}$$

where

$$f_\sigma(u) = \frac{1 - u^\sigma}{1 - u}, \qquad u \in]0,1[,$$

and $\sigma \in [0,1]$ is a parameter. Then $A(\sigma)$ is bounded and its norm satisfies the estimate

$$\|A(\sigma)\| \leqslant \left(\frac{\sqrt{2}}{3} + 4\right)\pi^2\sigma.$$

Proof: The proof will be done in several steps.

(i) Let $K(\sigma)$ be an integral operator acting in $L^2(\mathbb{R}_+, \mathrm{d}x)$ with the integral kernel

$$\mathcal{K}_\sigma(x,y) = \begin{cases} -\frac{i}{y} f_\sigma\left(\frac{x}{y}\right) & \text{for } x < y, \\ \frac{i}{x} f_\sigma\left(\frac{y}{x}\right) & \text{for } x > y. \end{cases}$$

Let us show that

$$\|K(\sigma)\| \leqslant \pi^2\sigma. \tag{16}$$

This step is quite analogous to the proof of point (i) in Lemma 1. First we apply the unitary transform U defined in (11). Set

$$\widetilde{K}(\sigma) = UK(\sigma)U^{-1}.$$

One finds that $\widetilde{K}(\sigma)$ is again an integral operator with the integral kernel,

$$\widetilde{\mathcal{K}}_\sigma(y,z) = i\,\mathrm{sgn}(y-z) f_\sigma(e^{-|y-z|}) e^{-|y-z|/2}.$$

Thus $\widetilde{K}(\sigma)$ is a convolution operator which is diagonalizable with the aid of the Fourier transform $\mathcal{F}$ on $\mathbb{R}$. This means that $(\mathcal{F}\widetilde{K}(\sigma)\mathcal{F}^{-1}\psi)(z) = \hat{q}(z)\psi(z)$ where

$$\hat{q}(z) = \int_{\mathbb{R}} e^{izy}\,\mathrm{sgn}(y) f_\sigma(e^{-|y|}) e^{-|y|/2}\,\mathrm{d}y.$$

A standard estimate yields

$$|\hat{q}(z)| \leqslant 2\int_0^\infty \frac{1-e^{-\sigma y}}{1-e^{-y}} e^{-y/2}\,\mathrm{d}y \leqslant \sigma\int_0^\infty \frac{y}{\sinh(y/2)}\mathrm{d}y = \pi^2\sigma.$$

It follows that

$$\|K(\sigma)\| = \|\mathcal{F}\widetilde{K}(\sigma)\mathcal{F}^{-1}\| = \|\hat{q}\|_\infty \leqslant \pi^2\sigma.$$

(ii) Let $\chi_n(x)$ be the characteristic function of the interval $]n, n+1[$. The linear mapping

$$J: l^2(\mathbb{N}) \to L^2(\mathbb{R}_+, \mathrm{d}x): \{\xi_n\} \mapsto \sum_{n=1}^{\infty} \xi_n \chi_n$$

is an isometry. The adjoint mapping reads

$$J^*: L^2(\mathbb{R}_+, \mathrm{d}x) \to l^2(\mathbb{N}): \psi \mapsto \{\langle \chi_n, \psi\rangle\}_{n=1}^{\infty}.$$

Set

$$L(\sigma) = JA(\sigma)J^*.$$

$L(\sigma)$ is an integral operator with the kernel

$$\mathcal{L}_\sigma(x,y) = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} A(\sigma)_{mn}\chi_m(x)\chi_n(y).$$

This can be rewritten as

$$\mathcal{L}_\sigma(x,y) = \begin{cases} -\frac{i}{[y]} f_\sigma\left(\frac{[x]}{[y]}\right) & \text{if } 0 < [x] < [y], \\ \frac{i}{[x]} f_\sigma\left(\frac{[y]}{[x]}\right) & \text{if } 0 < [y] < [x], \\ 0 & \text{otherwise.} \end{cases}$$

Here $[x]$ denotes the integer part of x. Notice that J^*J is the identity on $l^2(\mathbb{N})$ and so $L(\sigma)J = JA(\sigma)$. Consequently,

$$\|A(\sigma)\| = \|JA(\sigma)\| = \|L(\sigma)J\| \leqslant \|L(\sigma)\|. \tag{17}$$

(iii) Denote by $\widetilde{P}_n$, $n \in \mathbb{Z}_+$, the orthogonal projector onto $\mathbb{C}\chi_n$ in $L^2(\mathbb{R}_+, \mathrm{d}x)$. Set

$$K^{\mathrm{off}}(\sigma) = K(\sigma) - \widetilde{P}_0 K(\sigma) - K(\sigma)\widetilde{P}_0 + \widetilde{P}_0 K(\sigma)\widetilde{P}_0 - \sum_{n=1}^{\infty} \widetilde{P}_n K(\sigma)\widetilde{P}_n.$$

In other words, we subtract from $K(\sigma)$ the diagonal as well as the first row and the first column (i.e., with index 0) with respect to the orthogonal system $\{\chi_n\}_{n=0}^{\infty}$. We can say also that the integral kernel $\mathcal{K}_\sigma^{\mathrm{off}}(x,y)$ vanishes if $[x]=[y]$ or $[x]=0$ or $[y]=0$ and otherwise it coincides with $\mathcal{K}_\sigma(x,y)$. Since

$$\left\| \widetilde{P}_0 K(\sigma)\widetilde{P}_0 - \sum_{n=1}^{\infty} \widetilde{P}_n K(\sigma)\widetilde{P}_n \right\| = \sup_{n\in\mathbb{Z}_+} \|\widetilde{P}_n K(\sigma)\widetilde{P}_n\| \leqslant \|K(\sigma)\|,$$

we have

$$\|K^{\mathrm{off}}(\sigma)\| \leqslant 4\|K(\sigma)\|. \tag{18}$$

(iv) It remains to estimate the norm of the difference $L(\sigma) - K^{\mathrm{off}}(\sigma)$. This is a Hermitian integral operator whose kernel does not vanish only if $0<[x]<[y]$ or $0<[y]<[x]$. Suppose for definiteness that $0<[x]<[y]$. Then the kernel equals, up to the multiplier $-i$,

$$\frac{1}{[y]} f_\sigma\left(\frac{[x]}{[y]}\right) - \frac{1}{y} f_\sigma\left(\frac{x}{y}\right) = \left(\frac{1}{[y]^\sigma} - \frac{1}{y^\sigma}\right)\frac{[y]^\sigma - [x]^\sigma}{[y]-[x]} + \frac{1}{y^\sigma}\left(\frac{[y]^\sigma - [x]^\sigma}{[y]-[x]} - \frac{y^\sigma - x^\sigma}{y-x}\right).$$

Let us show that

$$0 \leqslant \frac{1}{[y]} f_\sigma\left(\frac{[x]}{[y]}\right) - \frac{1}{y} f_\sigma\left(\frac{x}{y}\right) \leqslant \frac{2\sigma}{[x]([y]-[x])}. \tag{19}$$

First notice that

$$0 \leqslant \frac{1}{[y]^\sigma} - \frac{1}{y^\sigma} = -\sigma \int_y^{[y]} z^{-\sigma-1}\, \mathrm{d}z \leqslant \frac{\sigma(y-[y])}{[y]^{\sigma+1}}$$

and so

$$0 \leqslant \left(\frac{1}{[y]^\sigma} - \frac{1}{y^\sigma}\right)\frac{[y]^\sigma - [x]^\sigma}{[y]-[x]} \leqslant \frac{\sigma}{[y]([y]-[x])}. \tag{20}$$

Further set temporarily

$$D = \frac{[y]^\sigma - [x]^\sigma}{[y]-[x]} - \frac{y^\sigma - x^\sigma}{y-x} = \sigma \int_0^1 (([x](1-t) + [y]t)^{\sigma-1} - (x(1-t)+yt)^{\sigma-1})\mathrm{d}t.$$

The integrand in the last integral equals

$$\sigma(1-\sigma)\xi_t^{\sigma-2}((x-[x])(1-t) + (y-[y])t),$$

where ξ_t is a real number lying between $[x](1-t)+[y]t$ and $x(1-t)+yt$. Notice that

$$0 \leqslant (x-[x])(1-t) + (y-[y])t \leqslant 1.$$

We assume that $0 \leqslant \sigma \leqslant 1$. Therefore

$$0 \leqslant D \leqslant \sigma(1-\sigma)\int_0^1 ([x](1-t)+[y]t)^{\sigma-2}\,\mathrm{d}t = -\sigma\frac{[y]^{\sigma-1} - [x]^{\sigma-1}}{[y]-[x]}$$

and so

$$0 \leqslant \frac{1}{y^\sigma} D \leqslant \frac{\sigma [x]^{\sigma-1}}{y^\sigma([y]-[x])} \leqslant \frac{\sigma}{[x]([y]-[x])}. \tag{21}$$

Inequalities (20) and (21) jointly imply (19).

(v) From estimate (19) one can deduce that $L(\sigma)-K^{\mathrm{off}}(\sigma)$ is a Hilbert–Schmidt operator and

$$\|L(\sigma)-K^{\mathrm{off}}(\sigma)\|_{\mathrm{HS}} \leqslant \frac{\sqrt{2}\pi^2}{3}\sigma. \tag{22}$$

Actually,

$$\|L(\sigma)-K^{\mathrm{off}}(\sigma)\|_{\mathrm{HS}}^2 = 2\int_1^\infty \mathrm{d}x \int_{[x]+1}^\infty \mathrm{d}y |\mathcal{L}_\sigma(x,y)-\mathcal{K}_\sigma^{\mathrm{off}}(x,y)|^2 \leqslant 8\sigma^2 \int_1^\infty \mathrm{d}x \frac{1}{[x]^2}\int_{[x]+1}^\infty \mathrm{d}y \frac{1}{([y]-[x])^2}$$
$$= 8\sigma^2\left(\sum_{k=1}^\infty \frac{1}{k^2}\right)^2.$$

(vi) Inequalities (17), (18), (16), and (22) imply that

$$\|A(\sigma)\| \leqslant \|L(\sigma)\| \leqslant \|K^{\mathrm{off}}(\sigma)\| + \|L(\sigma)-K^{\mathrm{off}}(\sigma)\| \leqslant 4\pi^2\sigma + \frac{\sqrt{2}\pi^2}{3}\sigma.$$

This shows the lemma. □

Lemma 3: *Let $A(\sigma)$ be an operator in $l^2(\mathbb{N})$ with the matrix entries in the standard basis*

$$A(\sigma)_{mn} = \begin{cases} 0 & \text{for } m=n, \\ \frac{i}{n-m}\min\left\{\left(\frac{m}{n}\right)^\sigma, \left(\frac{n}{m}\right)^\sigma\right\} & \text{for } m \neq n. \end{cases}$$

Then $A(\sigma)$ is bounded for all $0 \leqslant \sigma$ and its norm satisfies the estimate

$$\|A(\sigma)\| \leqslant \pi + \left(\frac{\sqrt{2}}{3}+4\right)\pi^2\sigma.$$

Proof: Let us first show that

$$\|A(0)\| \leqslant \pi.$$

For $\sigma=0$ we get

$$A(0)_{mn} = \frac{i}{n-m} \quad \text{if } m \neq n.$$

Considering the natural embedding $l^2(\mathbb{N}) \subset l^2(\mathbb{Z})$ let us denote by P_+ the orthogonal projector onto $l^2(\mathbb{N})$ in $l^2(\mathbb{Z})$. Let B be an operator in $l^2(\mathbb{Z})$ with the matrix

$$B_{mn} = q(n-m) \quad \text{where } q(n) = \begin{cases} 0 & \text{for } n=0, \\ \frac{i}{n} & \text{for } n \neq 0. \end{cases}$$

One can identify $A(0)$ with P_+BP_+. B is a convolution operator and therefore it is diagonalizable by the Fourier transform $\mathcal{F}: l^2(\mathbb{Z}) \to L^2([0,2\pi], \mathrm{d}\theta)$. In more detail,

$$(\mathcal{F}B\mathcal{F}^{-1}\psi)(\theta) = \hat{q}(\theta)\psi(\theta) \quad \text{where } \hat{q}(\theta) = \sum_{n\in\mathbb{Z}} q(n)e^{in\theta}.$$

One finds that $\hat{q}(\theta) = -\pi + \theta$. Consequently,

$$\|A(0)\| = \|P_+ B P_+\| \leqslant \|B\| = \|\mathcal{F} B \mathcal{F}^{-1}\| = \max_{0\in[0,2\pi]} |\hat{q}(\theta)| = \pi.$$

Suppose now that $0<m<n$. Notice that

$$(A(\sigma+1) - A(\sigma))_{mn} = -\frac{i}{n}\left(\frac{m}{n}\right)^{\sigma}$$

and

$$(A(\sigma) - A(0))_{mn} = -\frac{i}{n} f_{\sigma}\left(\frac{m}{n}\right).$$

Using Lemma 1 and Lemma 2 one can estimate

$$\begin{aligned}\|A(\sigma)\| &\leqslant \|A(0)\| + \|A(\sigma - [\sigma]) - A(0)\| + \|A(\sigma - [\sigma] + 1) - A(\sigma - [\sigma])\| + \cdots + \|A(\sigma) - A(\sigma - 1)\| \\ &\leqslant \pi + \left(\frac{\sqrt{2}}{3} + 4\right)\pi^2(\sigma - [\sigma]) + 24[\sigma] \leqslant \pi + \left(\frac{\sqrt{2}}{3} + 4\right)\pi^2\sigma.\end{aligned}$$

This proves the lemma. □

III. BOUNDEDNESS OF THE OPERATOR $i\Sigma_{k=0}^{\infty}\dot{P}_k(s)P_k(s)$

We consider $i\Sigma_{k=0}^{\infty}\dot{P}_k(s)P_k(s)$ in the time independent frame, i.e., the operator $Q(s)$ defined by

$$Q(s) = iV(s)^*\sum_{k=0}^{\infty}\dot{P}_k(s)P_k(s)V(s) = -i\dot{V}(s)^*V(s) = iV(s)^*\dot{V}(s). \tag{23}$$

The operator $V(s)$ is defined in (8). $Q(s)$ is symmetric and its matrix entries in the basis $\{\varphi_n(0)\}$ are

$$\langle\varphi_m(0), Q(s)\varphi_n(0)\rangle = i\langle\varphi_m(s), \dot{\varphi}_n(s)\rangle.$$

Since $\varphi_n(s)$ depends on s only through the absolute value it holds true that $Q(-s)=-Q(s)$ for $s\neq 0$. For $s=0$ the operator-valued function $Q(s)$ has a discontinuity. The goal of this section is to show that the operator $Q(s)$ is in fact bounded.

To compute the matrix entries one can use the identity

$$\langle\varphi_m(s), \dot{\varphi}_n(s)\rangle = \frac{\langle\varphi_m(s), \dot{H}(s)\varphi_n(s)\rangle}{\lambda_n(s) - \lambda_m(s)}. \tag{24}$$

Let us emphasize once more that the scalar product on the right-hand side should be interpreted as a quadratic form since, in general, $\varphi_n(s) \notin \mathrm{Dom}\,\dot{H}(s)$. The derivation goes through basically as usual even though one cannot use the scalar product directly. Differentiating the equation on eigenvalues one arrives at the equality

$$H(s)\dot{\varphi}_n(s;r) + \dot{H}(s)\varphi_n(s;r) = \dot{\lambda}_n(s)\varphi_n(s;r) + \lambda_n(s)\dot{\varphi}_n(s;r),$$

valid for any $r>0$, in which one should substitute for $H(s)$ and $\dot{H}(s)$ the corresponding formal differential operators. Next one multiplies the equality by $r\varphi_m(s;r)$ and integrates the both sides from ε to infinity for some $\varepsilon>0$. In the integral

$$-\int_{\varepsilon}^{\infty}\varphi_m(s;r)\partial_r r\partial_r\dot{\varphi}_n(s;r)\mathrm{d}r$$

occurring on the left-hand side one integrates twice by parts. Checking the asymptotic behavior of the eigenfunctions near the origin,

$$\varphi_n(s;r) \sim \left(\frac{B}{2}\right)^{(|s|+1)/2}\left(\frac{2n!}{\Gamma(n+|s|+1)}\right)^{1/2} r^{|s|}(1+O(r^2)) \quad \text{for } r \to 0+, \tag{25}$$

one finds that

$$\lim_{r\to 0+} r\varphi_m(s;r)\partial_r\dot{\varphi}_n(s;r) = \lim_{r\to 0+} r(\partial_r\varphi_m(s;r))\dot{\varphi}_n(s;r) = 0.$$

Hence sending ε to 0 actually leads to equality (24).

Lemma 4: *The matrix entries of the operator $Q(s)$ for $s \neq 0$ are given by the formulas*

$$\langle \varphi_m(0), Q(s)\varphi_n(0)\rangle = 0 \quad \text{for } m = n,$$

and

$$\langle \varphi_m(0), Q(s)\varphi_n(0)\rangle = \frac{i\,\mathrm{sgn}(s)}{2(n-m)}\min\left\{\frac{\gamma_m(s)}{\gamma_n(s)}, \frac{\gamma_n(s)}{\gamma_m(s)}\right\} \quad \text{for } m \neq n,$$

where

$$\gamma_n(s) = \left(\frac{\Gamma(n+|s|+1)}{n!}\right)^{1/2}. \tag{26}$$

Proof: Assume that $m<n$ and $s>0$. Using the explicit expression for the generalized Laguerre polynomials,

$$L_n^{(\alpha)}(x) = \sum_{k=0}^{n} (-1)^k \binom{n+\alpha}{n-k}\frac{1}{k!}x^k,$$

one finds that

$$\begin{aligned}\langle \varphi_m(s), \dot{H}(s)\varphi_n(s)\rangle &= 2sc_m(s)c_n(s)\int_0^\infty r^{2s-1}L_m^{(s)}\left(\frac{Br^2}{2}\right)L_n^{(s)}\left(\frac{Br^2}{2}\right)\exp\left(-\frac{Br^2}{2}\right)dr \\ &= sc_m(s)c_n(s)\left(\frac{2}{B}\right)^s S_{m,n},\end{aligned}$$

where

$$S_{m,n} = \sum_{k=0}^{m}\sum_{\ell=0}^{n}(-1)^{k+\ell}\frac{\Gamma(m+s+1)\Gamma(n+s+1)\Gamma(k+\ell+s)}{\Gamma(k+s+1)\Gamma(\ell+s+1)m!n!}\binom{m}{k}\binom{n}{\ell}.$$

In this expression only the summand with $k=0$ does not vanish since

$$\sum_{\ell=0}^{n}(-1)^\ell\binom{n}{\ell}\ell^j = 0 \quad \text{for } j = 0,1,\ldots,n-1.$$

Hence

$$\begin{aligned}S_{m,n} &= \frac{\Gamma(m+s+1)\Gamma(n+s+1)}{\Gamma(s+1)m!n!}\sum_{\ell=0}^{n}(-1)^\ell\frac{\Gamma(\ell+s)}{\Gamma(\ell+s+1)}\binom{n}{\ell} = \frac{\Gamma(m+s+1)\Gamma(n+s+1)}{\Gamma(s+1)m!n!}B(s,n+1) \\ &= \frac{\Gamma(m+s+1)}{sm!}.\end{aligned}$$

Furthermore, $\lambda_n(s)-\lambda_m(s)=2B(n-m)$ and so

$$\langle \varphi_m(0), Q(s)\varphi_n(0)\rangle = i\left(\frac{2}{B}\right)^s \frac{c_m(s)c_n(s)}{2B(n-m)} \frac{\Gamma(m+s+1)}{m!}.$$

Now it suffices to plug in the explicit expressions for the normalization constants $c_m(s)$ and $c_n(s)$. □

Using the Stirling formula one can check the asymptotic behavior of the matrix entries of the operator $Q(s)$ for m and n large. It turns out that the operator $Q(s)$ is in some sense close to a Hermitian operator $A(s)$ in $L^2(\mathbb{R}_+, r\,\mathrm{d}r)$ with the matrix entries

$$\langle \varphi_m(0), A(s)\varphi_n(0)\rangle = 0 \quad \text{for } m = n, \tag{27}$$

and

$$\langle \varphi_m(0), A(s)\varphi_n(0)\rangle = \frac{i\,\mathrm{sgn}(s)}{2(n-m)} \min\left\{\left(\frac{m+1}{n+1}\right)^{|s|/2}, \left(\frac{n+1}{m+1}\right)^{|s|/2}\right\} \text{for } m \neq n. \tag{28}$$

Note that $A(0+) = Q(0+)$. We shall also write $Q(s)_{mn}$ instead of $\langle \varphi_m(0), Q(s)\varphi_n(0)\rangle$, and similarly for $A(s)$.

Lemma 5: *Let $A(s)$ be the Hermitian operator in $L^2(\mathbb{R}_+, r\,\mathrm{d}r)$ defined by relations* (27) and (28). *Then $Q(s) - A(s)$ is a Hilbert–Schmidt operator and it holds true that*

$$\|Q(s) - A(s)\|_{\mathrm{HS}} \leqslant \tfrac{1}{2}|s|(1+|s|)^{(3+|s|)/2}.$$

Proof: Let us suppose for definiteness that $s > 0$ and $m < n$. For $x \geqslant 1$ set

$$g_s(x) = \frac{\Gamma(x+s)}{x^s \Gamma(x)}.$$

One can express

$$\begin{aligned} |Q(s)_{mn} - A(s)_{mn}| &= \frac{1}{2(n-m)} |g_s(m+1)^{1/2} - g_s(n+1)^{1/2}| \left(\frac{m+1}{n+1}\right)^{s/2} g_s(n+1)^{-1/2} \\ &\leqslant \frac{1}{4} g_s(n+1)^{-1/2} \int_0^1 g_s(m+1+(n-m)t)^{-1/2} |g_s'(m+1+(n-m)t)|\,\mathrm{d}t. \end{aligned}$$

Notice that

$$\frac{g_s'(x)}{g_s(x)} = \frac{\Gamma'(x+s)}{\Gamma(x+s)} - \frac{\Gamma'(x)}{\Gamma(x)} - \frac{s}{x}.$$

Using the well-known formula for the logarithmic derivative of the gamma function,

$$-\frac{\Gamma'(z)}{\Gamma(z)} = \frac{1}{z} + \gamma + \sum_{n=1}^{\infty} \left(\frac{1}{n+z} - \frac{1}{n}\right), \tag{29}$$

one finds that

$$\frac{g_s'(x)}{g_s(x)} = s\left(\sum_{n=0}^{\infty} \frac{1}{(n+x)(n+x+s)} - \frac{1}{x}\right) \leqslant s\left(\sum_{n=0}^{\infty} \frac{1}{(n+x)^2} - \frac{1}{x}\right) \leqslant s\left(\frac{1}{x^2} + \int_x^{\infty} \frac{\mathrm{d}y}{y^2} - \frac{1}{x}\right) = \frac{s}{x^2}.$$

Similarly,

$$\frac{g_s'(x)}{g_s(x)} \geqslant s\left(\int_x^{\infty} \frac{\mathrm{d}y}{y(y+s)} - \frac{1}{x}\right) = \ln\left(1+\frac{s}{x}\right) - \frac{s}{x} \geqslant -\frac{s^2}{2x^2}.$$

In particular,

$$|g_s'(x)| \leqslant \frac{s(s+1)}{x^2} g_s(x).$$

From here one derives the estimates, for $t \in [0,1]$,

$$\frac{g_s(m+1+(n-m)t)}{g_s(n+1)} = \exp\left(-\int_{m+1+(n-m)t}^{n+1} \frac{g_s'(y)}{g_s(y)}\mathrm{d}y\right) \leqslant \exp\left(\int_{m+1}^{n+1}\left(\frac{s}{y} - \ln\left(\frac{y+s}{y}\right)\right)\mathrm{d}y\right)$$
$$= \exp\left((m+1+s)\ln\left(1+\frac{s}{m+1}\right) - (n+1+s)\ln\left(1+\frac{s}{n+1}\right)\right) \leqslant (1+s)^{1+s}$$

and

$$|Q(s)_{mn} - A(s)_{mn}| \leqslant \frac{s(s+1)}{4g_s(n+1)^{1/2}} \int_0^1 \frac{g_s(m+1+(n-m)t)^{1/2}}{(m+1+(n-m)t)^2}\mathrm{d}t$$
$$\leqslant \frac{1}{4}s(1+s)^{(3+s)/2} \int_0^1 \frac{\mathrm{d}t}{(m+1+(n-m)t)^2}.$$

Let $F(t)$ be a Hermitian operator in $L^2(\mathbb{R}_+, r\,\mathrm{d}r)$ with the following matrix entries in the basis $\{\varphi_n(0)\}$:

$$F(t)_{mn} = 0 \quad \text{for } m = n$$

and

$$F(t)_{mn} = (m+1+(n-m)t)^{-2} \quad \text{for } m < n.$$

Then $F(t)$ is a Hilbert–Schmidt operator and

$$\|F(t)\|_{\mathrm{HS}}^2 = 2\sum_{m=0}^{\infty}\sum_{n=m+1}^{\infty}(m+1+(n-m)t)^{-4} \leqslant 2\sum_{m=0}^{\infty}\int_0^{\infty}\frac{\mathrm{d}y}{(m+1+ty)^4} = \frac{2}{3t}\sum_{m=0}^{\infty}\frac{1}{(m+1)^3} \leqslant \frac{1}{t}.$$

Hence

$$\|Q(s) - A(s)\|_{\mathrm{HS}} \leqslant \frac{1}{4}s(1+s)^{(3+s)/2}\int_0^1 \|F(t)\|_{\mathrm{HS}}\,\mathrm{d}t \leqslant \frac{1}{2}s(1+s)^{(3+s)/2}.$$

This proves the lemma. □

Combining Lemma 3 and Lemma 5 we deduce that the operator $Q(s)$ is actually bounded.

Lemma 6: *The operator $Q(s)$ is bounded and its norm satisfies the estimate*

$$\|Q(s)\| \leqslant \frac{\pi}{2} + 12|s| + \frac{1}{2}|s|(1+|s|)^{(3+|s|)/2}.$$

Proof: Let $A(s)$ be the Hermitian operator in $L^2(\mathbb{R}_+, r\,\mathrm{d}r)$ defined by relations (27) and (28). According to Lemma 3 it holds true that

$$\|A(s)\| \leqslant \frac{1}{2}\left(\pi + \left(\frac{\sqrt{2}}{3} + 4\right)\pi^2\frac{|s|}{2}\right).$$

Lemma 5 leads to the estimate

$$\|Q(s)\| \leqslant \|A(s)\| + \|Q(s) - A(s)\| \leqslant \frac{1}{2}\left(\pi + \left(\frac{1}{3\sqrt{2}} + 2\right)\pi^2|s| + |s|(1+|s|)^{(3+|s|)/2}\right).$$

Since $(1+1/(6\sqrt{2}))\pi^2 < 12$ the lemma follows. □

IV. THE MEANING OF THE PROPAGATOR $U_\tau(s,s_0)$

As already discussed in the Introduction the natural propagator $U_\tau(s,s_0)$ defined in (5) is not related in the standard way to the Hamiltonian $\tau H(s)$ defined in (1). In particular it is not clear if $U_\tau(s,s_0)$ maps the domain Dom $H(s_0)$ into Dom $H(s)$. This is why we propose in the Appendix the notion of a propagator weakly associated to a Hamiltonian, see Definition A.3. We should like to emphasize that this relationship is unique, i.e., at most one propagator can be weakly associated to a Hamiltonian.

In this section we show that U_τ is weakly associated to τH and that $(s,r)\mapsto U_\tau(s,s_0)\psi_0(r)$ satisfies the Schrödinger equation as a distribution for all $\psi_0\in L^2(\mathbb{R}_+, r\,\mathrm{d}r\,\mathrm{d}\varphi)$.

Proposition 7: *The propagator $U_\tau(s,s_0)$ is weakly associated to $\tau H(s)$.*

Proof: Relation (5) means that

$$U_\tau(s,s_0) = V(s)e^{-i\tau\Omega(s)}C(s,s_0)e^{i\tau\Omega(s_0)}V(s_0)^{-1}.$$

So starting from $C(s,s_0)$ one can reach $U_\tau(s,s_0)$ by two consecutive unitary transformations. The propagator $C(s,s_0)$ was defined in (6). It corresponds to the Hamiltonian $-Q_\tau(s)$ defined in (7). According to Lemma 6 the function $\|Q_\tau(s)\|=\|Q(s)\|$ is locally bounded and thus $C(s,s_0)$ is given by the Dyson formula, see relation (31) in Sec. V.

First we apply Proposition A.4 in which we set

$$A(t) = -Q_\tau(t),\ D = \mathrm{Dom}\,H(0),\ T(t) = \exp(-i\tau\Omega(t)),$$

and

$$X(t) = i(\partial_t e^{-i\tau\Omega(t)})e^{i\tau\Omega(t)} = \tau W(t).$$

We conclude that the propagator $e^{-i\tau\Omega(s)}C(s,s_0)e^{i\tau\Omega(s_0)}$ is weakly associated to

$$\tau W(s) - e^{-i\tau\Omega(s)}Q_\tau(s)e^{i\tau\Omega(s)} = \tau W(s) - Q(s).$$

Next we apply Proposition A.6 in which we set $\widetilde{H}(t)=\tau W(t)-Q(t)$ and $\widetilde{U}(t,s)=e^{-i\tau\Omega(t)}C(t,s)e^{i\tau\Omega(s)}$. Recall further that $V(t)$ was defined in Eq. (8). We conclude that $U_\tau(s,s_0)=V(s)\widetilde{U}(s,s_0)V(s_0)^{-1}$ is weakly associated to

$$\tau V(s)W(s)V(s)^{-1} - V(s)Q(s)V(s)^{-1} + i\dot{V}(s)V(s)^{-1} = \tau H(s).$$

The proposition is proven. □

In the studied model $\mathcal{H}=L^2(\mathbb{R}_+, r\,\mathrm{d}r)$ and so

$$\mathcal{K} = L^2(\mathbb{R},\mathcal{H},\mathrm{d}s) = L^2(\mathbb{R}\times\mathbb{R}_+, r\,\mathrm{d}s\,\mathrm{d}r).$$

Let $\mathfrak{H}=\int_{\mathbb{R}}^{\oplus}H(s)\mathrm{d}s$ be the direct integral of the family of self-adjoint operators $H(s)$ which is nothing but a multiplication operator in $\mathcal{K}$. Let K_τ be the quasienergy operator associated to the propagator $U_\tau(s,s_0)$ (see Appendix). According to Proposition 7 it holds true that

$$K_\tau = \overline{-i\partial_s + \tau\mathfrak{H}}. \tag{30}$$

To an initial condition $\psi_0\in\mathcal{H}$ we relate the function $\psi(s,r)=(U_\tau(s,0)\psi_0)(r)$ which is a locally square integrable function in the variables s and r. We now show that $\psi(s,r)$ fulfills the Schrödinger equation in the space of distributions $\mathcal{D}'(\mathbb{R}\times]0,\infty[)$. Let us note that for the proof it suffices to know that $-i\partial_s+\tau\mathfrak{H}\subset K_\tau$, the stronger property Eq. (30) is not necessary.

Proposition 8: *For every $\psi_0\in\mathcal{H}$, the function $\psi(s,r)=(U_\tau(s,0)\psi_0)(r)$ satisfies the Schrödinger equation in the sense of distributions.*

Proof: Let $\xi\in C_0^\infty(\mathbb{R}\times]0,+\infty[)$ be an arbitrary real-valued test function. Set $g(s,r)=\xi(s,r)/r$. Clearly, $g\in\mathrm{Dom}(-i\partial_s+\tau\mathfrak{H})\subset\mathrm{Dom}\,K_\tau$. Let $[a,b]\times[c,d]$ be a rectangle containing supp ξ and choose $\eta\in C_0^\infty(\mathbb{R})$ so that $\eta\equiv 1$ on a neighborhood of the interval $[a,b]$. From Proposition A.2 we know that $K_\tau(\eta(s)\psi(s,r))=-i\eta'(s)\psi(s,r)$. From the choice of η it follows that

$$0 = -i\langle g, \eta'\psi\rangle_{\mathcal{K}} = \langle g, K_\tau(\eta\psi)\rangle_{\mathcal{K}} = \langle(-i\partial_s + \tau\mathfrak{H})g, \eta\psi\rangle_{\mathcal{K}}.$$

The last term equals

$$\int_{\mathbb{R}\times\mathbb{R}_+}\left(i\partial_s\frac{1}{r}\xi(s,r) + \tau H(s)\frac{1}{r}\xi(s,r)\right)\eta(s)\psi(s,r)r\,\mathrm{d}s\,\mathrm{d}r$$
$$= \int_{\mathbb{R}\times\mathbb{R}_+}\left(i\partial_s\xi(s,r) + \tau\left(-\partial_r r\partial_r\frac{1}{r} + \frac{1}{r^2}\left(s + \frac{Br^2}{2}\right)^2\right)\xi(s,r)\right)\psi(s,r)\mathrm{d}s\,\mathrm{d}r.$$

This means that

$$-i\partial_s\psi(s,r) + \tau\left(-\frac{1}{r}\partial_r r\partial_r + \frac{1}{r^2}\left(s + \frac{Br^2}{2}\right)^2\right)\psi(s,r) = 0$$

in the domain $\mathbb{R}\times]0,+\infty[$ in the sense of distributions. □

V. PROOF OF THE ADIABATIC THEOREM

We follow the strategy explained in the Introduction. The adiabatic propagator U_{AD} [see (4)] and the propagator U_τ defined in (5) differ by C defined by (6). Since $Q_\tau(s) = e^{i\tau\Omega(s)}Q(s)e^{-i\tau\Omega(s)}$, defined in (7), is unitarily equivalent to $Q(s)$ it is bounded, uniformly in s on every bounded interval $[0,S]$. Hence $C(s,s_0)$ exists and is given by the Dyson formula

$$C(s,s_0) = \mathbb{I} + \sum_{n=1}^{\infty} i^n \int_{s_0}^{s}\mathrm{d}s_1\int_{s_0}^{s_1}\mathrm{d}s_2\cdots\int_{s_0}^{s_{n-1}}\mathrm{d}s_n\, Q_\tau(s_1)Q_\tau(s_2)\cdots Q_\tau(s_n). \tag{31}$$

The task is to estimate the norm of the integral of Q_τ. This will be done by the integration by parts technique developed in the following two lemmas.

The first step is to find a bounded differentiable solution $X(s)$ of the commutation equation

$$Q(s) = i[W(s), X(s)].$$

The operator $W(s)$ was defined in (9). The off-diagonal entries of the $X(s)$ are determined unambiguously,

$$\langle\varphi_m(0), X(s)\varphi_n(0)\rangle = -i\frac{\langle\varphi_m(0), Q(s)\varphi_n(0)\rangle}{\lambda_m(s) - \lambda_n(s)}$$
$$= -\frac{\mathrm{sgn}(s)}{4B(n-m)^2}\min\left\{\frac{\gamma_m(s)}{\gamma_n(s)}, \frac{\gamma_n(s)}{\gamma_m(s)}\right\} \quad \text{for } m \neq n, \tag{32}$$

with $\gamma_n(s)$ defined in (26). We set

$$\langle\varphi_m(0), X(s)\varphi_n(0)\rangle = 0 \quad \text{for } m = n, \tag{33}$$

and write again $X(s)_{mn}$ instead of $\langle\varphi_m(0), X(s)\varphi_n(0)\rangle$.

Lemma 9: *The operator $X(s)$ defined by relations (33) and (32) is bounded and its norm satisfies the estimate*

$$\|X(s)\| \leqslant \frac{\pi^2}{12B}.$$

The derivative $\dot{X}(s)$ exists in the operator norm and satisfies the estimate

$$\|\dot{X}(s)\| \leqslant \frac{(1+\sqrt{2})\pi^2}{48B}.$$

Proof: The operator norm of $X(s)$ is bounded from above by the Shur–Holmgren norm,

$$\|X(s)\| \leqslant \|X(s)\|_{\mathrm{SH}} = \sup_{m\in\mathbb{Z}_+} \sum_{n=0}^{\infty} |X(s)_{mn}| \leqslant \frac{1}{2B}\sum_{k=1}^{\infty}\frac{1}{k^2} = \frac{\pi^2}{12B}.$$

Suppose that $s>0$ and $m<n$. Let us estimate the derivative of $X(s)_{mn}$. Using (29) one finds that

$$\left(\frac{\gamma_m(s)}{\gamma_n(s)}\right)' = \frac{\gamma_m(s)}{2\gamma_n(s)}\left(\frac{\Gamma'(m+s+1)}{\Gamma(m+s+1)} - \frac{\Gamma'(n+s+1)}{\Gamma(n+s+1)}\right)$$

$$= \frac{\gamma_m(s)}{2\gamma_n(s)}\sum_{k=0}^{\infty}\frac{n-m}{(k+m+s+1)(k+n+s+1)}.$$

Hence

$$\left|\frac{\mathrm{d}}{\mathrm{d}s}X(s)_{mn}\right| \leqslant \frac{1}{8B(n-m)}\left(\frac{1}{(m+1)(n+1)} + \int_1^{\infty}\frac{\mathrm{d}y}{(y+m)(y+n)}\right) = \frac{1}{8B(n-m)}\left(\frac{1}{(m+1)(n+1)} + \frac{1}{n-m}\ln\left(\frac{n+1}{m+1}\right)\right).$$

Thus we get, for $m\neq n$,

$$\left|\frac{\mathrm{d}}{\mathrm{d}s}X(s)_{mn}\right| \leqslant \frac{1}{8B}\left(\frac{1}{(m+1)(n+1)} + \frac{1}{|n-m|\min\{m+1,n+1\}}\right). \tag{34}$$

Let $\dot{X}(s)$ be a Hermitian operator in $L^2(\mathbb{R}_+, r\,\mathrm{d}r)$ with the matrix entries $\mathrm{d}X(s)_{mn}/\mathrm{d}s$. From the estimate (34) we deduce that $\dot{X}(s)$ is a Hilbert–Schmidt operator and

$$\|\dot{X}(s)\|_{\mathrm{HS}} \leqslant \frac{1}{8B}\left(\sum_{m=0}^{\infty}\frac{1}{(m+1)^2}\sum_{n=0}^{\infty}\frac{1}{(n+1)^2}\right)^{1/2} + \frac{1}{8B}\left(2\sum_{m=0}^{\infty}\frac{1}{(m+1)^2}\sum_{n=m+1}^{\infty}\frac{1}{(n-m)^2}\right)^{1/2}$$

$$= \frac{(1+\sqrt{2})\pi^2}{48B}.$$

Furthermore, since estimate (34) is uniform in s one can apply the Lebesgue dominated convergence theorem to conclude that

$$\lim_{\varepsilon\to 0}\left\|\frac{1}{\varepsilon}(X(s+\varepsilon)-X(s)) - \dot{X}(s)\right\|_{\mathrm{HS}} = 0.$$

Hence the derivative of the operator-valued function $X(s)$ exists in the operator norm and equals $\dot{X}(s)$. □

The matrix entries of the operator $Q_\tau(s)$ defined in (7) equal

$$\langle\varphi_m(0), Q_\tau(s)\varphi_n(0)\rangle = ie^{i\tau(\omega_m(s)-\omega_n(s))}\langle\varphi_m(s), \dot{\varphi}_n(s)\rangle.$$

Notice that the both operators $\Omega(s)$ and $W(s)=\Omega'(s)$ are diagonal in the basis $\{\varphi_n(0)\}$ and therefore they commute.

Lemma 10: *It holds true that*

$$\left\| \int_0^s Q_\tau(u)\mathrm{d}u \right\| \leqslant \left(1 + \frac{1+\sqrt{2}}{8}|s|\right)\frac{\pi^2}{6B\tau}.$$

Proof: Suppose that $s>0$. The integral can be rewritten as follows:

$$\int_0^s Q_\tau(u)\mathrm{d}u = i\int_0^s e^{i\pi\Omega(u)}[W(u),X(u)]e^{-i\pi\Omega(u)}\,\mathrm{d}u$$

$$=\frac{1}{\tau}\int_0^s ((e^{i\pi\Omega(u)})'X(u)e^{-i\pi\Omega(u)} + e^{i\pi\Omega(u)}X(u)(e^{-i\pi\Omega(u)})')\mathrm{d}u$$

$$=\frac{1}{\tau}\int_0^s ((e^{i\pi\Omega(u)}X(u)e^{-i\pi\Omega(u)})' - e^{i\pi\Omega(u)}\dot{X}(u)e^{-i\pi\Omega(u)})\mathrm{d}u.$$

Consequently,

$$\int_0^s Q_\tau(u)\mathrm{d}u = \frac{1}{\tau}\left(e^{i\pi\Omega(s)}X(s)e^{-i\pi\Omega(s)} - X(0) - \int_0^s e^{i\pi\Omega(u)}\dot{X}(u)e^{-i\pi\Omega(u)}\,\mathrm{d}u\right).$$

More precisely, the derivation of this equality was rather formal but it becomes rigorous when sandwiching the both sides with the scalar product $\langle\varphi_m(0),\cdot\varphi_n(0)\rangle$. This is to say that the both sides have the same matrix entries in the basis $\{\varphi_n(0)\}$. But since the equality concerns bounded operators it holds true.

Using Lemma 9 one arrives at the estimate

$$\left\| \int_0^s Q_\tau(u)\mathrm{d}u \right\| \leqslant \frac{1}{\tau}\left(\|X(s)\| + \|X(0)\| + \int_0^s \|\dot{X}(u)\|\mathrm{d}u\right) \leqslant \frac{\pi^2}{B\tau}\left(\frac{1}{6} + \frac{1+\sqrt{2}}{48}s\right).$$

The lemma is proven. □

We can now show that the adiabatic propagator $U_{AD}(s,0)$ [see (4)] is close to the propagator $U_\tau(s,0)=U_{AD}(s,0)C(s,0)$ defined in (5) provided the adiabatic parameter τ is large.

Proposition 11: *It holds true that*

$$\|U_\tau(s,0) - U_{AD}(s,0)\| \leqslant M(s)e^{|s|M(s)}\frac{\pi}{3B\tau},$$

where

$$M(s) = \frac{\pi}{2} + 12|s| + \frac{1}{2}|s|(1+|s|)^{(3+|s|)/2}. \tag{35}$$

Proof: According to Lemma 6, $\|Q(s)\|\leqslant M(s)$, and from Lemma 10 one easily deduces that

$$\left\| \int_0^s Q_\tau(u)\mathrm{d}u \right\| \leqslant \frac{\pi}{3B\tau}M(s).$$

Using formula (5) one can estimate

$$\|U_\tau(s,0) - U_{AD}(s,0)\| = \|C(s,0) - \mathbb{I}\| \leqslant \sum_{n=1}^{\infty}\int_0^{|s|}\mathrm{d}s_1\cdots\int_0^{s_{n-2}}\mathrm{d}s_{n-1}\|Q_\tau(s_1)\|\cdots\|Q_\tau(s_{n-1})\|$$
$$\times\left\|\int_0^{s_{n-1}}\mathrm{d}s_n\,Q_\tau(s_n)\right\| \leqslant \frac{\pi}{3B\tau}\sum_{n=1}^{\infty}M(s)^n\int_0^{|s|}\mathrm{d}s_1\cdots\int_0^{s_{n-2}}\mathrm{d}s_{n-1}$$

$$= \frac{\pi}{3B\tau} \sum_{n=1}^{\infty} M(s)^n \frac{|s|^{n-1}}{(n-1)!}.$$

The proposition is proven. □

VI. THE GENERAL DEPENDENCE ON TIME

Here we show that the adiabatic theorem extends to Hamiltonians of the form

$$H^\zeta(s) = H(\zeta(s))$$

where $H(s)$ is defined in (1) and $\zeta \in C^2(\mathbb{R})$ is a real-valued function. In order to simplify the discussion and to avoid considering discontinuities [recall that $Q(s)$ is discontinuous at $s=0$] we shall further assume that $\zeta'(s) > 0$ and $\zeta(0) = 0$.

Set

$$V^\zeta(s) = V(\zeta(s)), \quad W^\zeta(s) = W(\zeta(s)), \quad \Omega^\zeta(s) = \int_0^s W^\zeta(u) \mathrm{d}u.$$

Let $C^\zeta(s, s_0)$ be the propagator related via the Dyson formula to the Hamiltonian $-Q_\tau^\zeta(s)$, where

$$Q_\tau^\zeta(s) = \exp(i\tau\Omega^\zeta(s)) Q^\zeta(s) \exp(-i\tau\Omega^\zeta(s)), \quad Q^\zeta(s) = \zeta'(s) Q(\zeta(s)).$$

Exactly in the same way as in the proof of Proposition 7 one can show that the propagator

$$U_\tau^\zeta(s, s_0) = V^\zeta(s) \exp(-i\tau\Omega^\zeta(s)) C^\zeta(s, s_0) \exp(i\tau\Omega^\zeta(s_0)) V^\zeta(s_0)^{-1}$$

is weakly associated to the Hamiltonian $H^\zeta(s)$. The adiabatic propagator now reads

$$U_{AD}^\zeta(s, s_0) = V^\zeta(s) \exp(-i\tau(\Omega^\zeta(s) - \Omega^\zeta(s_0))) V^\zeta(s_0)^{-1}.$$

Proposition 12: *Assume that* $\zeta \in C^2(\mathbb{R})$, $\zeta'(s) > 0$ *and* $\zeta(0) = 0$. *Then there exists a locally bounded function* $m^\zeta(s)$ *such that*

$$\forall s \in \mathbb{R}, \quad \| U_\tau^\zeta(s, 0) - U_{AD}^\zeta(s, 0) \| \leqslant \frac{m^\zeta(s)}{B\tau}.$$

Proof: Suppose for definiteness that $s > 0$. Recall that $\|Q(s)\| \leqslant M(s)$ where $M(s)$ was defined in (35). The operator-valued function

$$X^\zeta(s) = \zeta'(s) X(\zeta(s)),$$

with $X(s)$ being defined in (32) and (33), satisfies the commutation equation

$$Q^\zeta(s) = i[W^\zeta(s), X^\zeta(s)].$$

Quite analogously as in the proof of Lemma 10 one derives the estimate

$$\left\| \int_0^s Q_\tau^\zeta(u) \mathrm{d}u \right\| \leqslant \frac{1}{\tau} \left(\|X^\zeta(s)\| + \|X^\zeta(0)\| + \int_0^s \|\dot{X}^\zeta(u)\| \mathrm{d}u \right).$$

In virtue of Lemma 9 we have

$$\|X^\zeta(s)\| \leqslant \frac{\pi^2}{12B} \zeta'(s)$$

and

$$\int_0^s \|\dot{X}^\zeta(u)\|\mathrm{d}u \leqslant \frac{\pi^2}{12B}\int_0^s |\zeta''(u)|\mathrm{d}u + \frac{(1+\sqrt{2})\pi^2}{48B}\int_0^s \zeta'(u)^2\,\mathrm{d}u.$$

Hence

$$\left\| \int_0^s Q_\tau^\zeta(u)\mathrm{d}u \right\| \leqslant \frac{q^\zeta(s)}{B\tau},$$

where

$$q^\zeta(s) = \frac{\pi^2}{12}\left(\zeta'(0) + \sup_{0\leqslant u\leqslant s}\zeta'(u) + \int_0^s |\zeta''(u)|\mathrm{d}u + \frac{1+\sqrt{2}}{4}\int_0^s \zeta'(u)^2\,\mathrm{d}u\right).$$

Finally one can proceed similarly as in the proof of Proposition 11 to derive the estimate

$$\|U_\tau^\zeta(s,0) - U_{AD}^\zeta(s,0)\| = \|C^\zeta(s,0) - \mathbb{I}\| \leqslant \exp\left(\int_0^{\zeta(s)} M(v)\mathrm{d}v\right)\frac{q^\zeta(s)}{B\tau}.$$

This completes the proof.

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APPENDIX: PROPAGATOR WEAKLY ASSOCIATED TO A HAMILTONIAN

By a propagator $U(t,s)$ we mean a family of unitary operators in a separable Hilbert space $\mathcal{H}$ depending on t, $s\in\mathbb{R}$ which satisfies the following conditions:

(i) $U(t,s)$ is strongly continuous jointly in t, s,
(ii) the Chapman–Kolmogorov equality is satisfied, i.e.,

$$\forall\, t,s,r \in \mathbb{R}, \quad U(t,r)U(r,s) = U(t,s).$$

Let $H(t)$, $t\in\mathbb{R}$, be a family of self-adjoint operators in $\mathcal{H}$. The domain may depend on t. The standard way how one relates a propagator $U(t,s)$ to $H(t)$ is based on the following two requirements:

(i) $\forall t,s\in\mathbb{R}, \quad U(t,s)(\mathrm{Dom}\,H(s)) = \mathrm{Dom}\,H(t)$,
(ii) $\forall \psi\in\mathrm{Dom}\,H(s), \quad \forall\, t\in\mathbb{R}, \quad i\partial_t U(t,s)\psi = H(t)U(t,s)\psi$.

Clearly, if a propagator exists then it is unique. In some situations, however, these requirements may turn out to be unnecessarily strong. In particular this is true for the model studied in the current paper. The heart of the problem is illustrated on the following example.

Let $A(t)$ be a family of bounded Hermitian operators in $\mathcal{H}$ which is uniformly bounded. Then the propagator exits and is given by the Dyson formula. Let us call it $C(t,s)$. Let $D\subset\mathcal{H}$ be a dense linear subspace, and let $T(t)$ be a strongly continuous family of unitary operators such that D is invariant with respect to $T(t)$ and for every $\psi\in D$ there exists the derivative $\partial_t T(t)\psi$. Furthermore, suppose that $X(t) = i\dot{T}(t)T(t)^{-1}$, with $\mathrm{Dom}\,X(t) = D$, is a self-adjoint operator for all t (the dot designates the derivative). A formal computation gives

$$T(t)(-i\partial_t + A(t))T(t)^{-1} = -i\partial_t + X(t) + T(t)A(t)T(t)^{-1}.$$

If $C(t,s)$ preserved the domain D then the propagator $T(t)C(t,s)T(s)^{-1}$ would solve the Schrödinger equation for $X(t)+T(t)A(t)T(t)^{-1}$ on D. Thus it is natural to associate it to this family of self-adjoint operators. The hypothesis on $C(t,s)$ need not be, however, satisfied since $A(t)$ is an arbitrary family of bounded operators and so $C(t,s)$ will in general not preserve this domain.

In this appendix we propose a way how to associate a propagator to a given time-dependent Hamiltonian in a weak sense. This association is more general than the standard one (which supposes a constant domain and solving the Schrödinger equation in the strong sense) and it is still unique (i.e., there is at most one propagator weakly associated to a given time-dependent Hamiltonian).

Here we develop this approach only to an extent which makes it possible to apply these ideas to the studied model with a time-dependent Aharonov–Bohm flux. In particular, the described example is covered by Proposition A.4 below.

Let $\mathcal{X}$ be a Banach space. We shall say that a vector-valued function $f:\mathbb{R}\to\mathcal{X}$ is absolutely continuous on $\mathbb{R}$ if it is absolutely continuous on every compact interval $I\subset\mathbb{R}$. By the symbol $\widetilde{AC}(\mathbb{R},\mathcal{X})$ (or just $\widetilde{AC}$ if there is no danger of misunderstanding) we shall denote the space of all absolutely continuous vector-valued functions $f(t)$ such that the derivative $f'(t)$ exists almost everywhere on $\mathbb{R}$. In such a case the function $\|f'(t)\|$ is locally integrable and $f(t)=f(0)+\int_0^t f'(s)\mathrm{d}s$ (Ref. 10 Theorem 3.8.6). If the Banach space $\mathcal{X}$ has the Radon–Nikodym property then the space $\widetilde{AC}(\mathbb{R},\mathcal{X})$ coincides with the space of absolutely continuous vector-valued functions $AC(\mathbb{R},\mathcal{X})$. Let us recall that $\mathcal{X}$ is said to have the Radon–Nikodym property if the fundamental theorem of calculus holds, i.e., if any absolutely continuous function is the antiderivative of a Bochner integrable function. For example, separable Hilbert spaces are known to have the Radon–Nikodym property.[7]

Clearly, if $f,g\in AC(\mathbb{R},\mathcal{H})$ then the function $\langle f(t),g(t)\rangle$ is absolutely continuous and

$$\partial_t\langle f(t),g(t)\rangle = \langle f'(t),g(t)\rangle + \langle f(t),g'(t)\rangle \text{ a.e.}$$

Similarly, if $A\in\widetilde{AC}(\mathbb{R},\mathcal{B}(\mathcal{H}))$ and $f\in AC(\mathbb{R},\mathcal{H})$ then $A(t)f(t)\in AC(\mathbb{R},\mathcal{H})$ and

$$\partial_t A(t)f(t) = \dot{A}(t)f(t) + A(t)f'(t) \text{ a.e.}$$

Let $\{e_k\}$ be an orthonormal basis in $\mathcal{H}$. A vector-valued function $f(t)=\Sigma\,\eta_k(t)e_k$ belongs to $AC(\mathbb{R},\mathcal{H})$ if and only if the following two conditions are satisfied:

(i) $\exists a\in\mathbb{R}$ such that $\Sigma_k|\eta_k(a)|^2<\infty$,
(ii) $\forall k$, $\eta_k\in AC$, and $(\Sigma_k|\eta_k'(t)|^2)^{1/2}\in L^1_{\mathrm{loc}}(\mathbb{R})$.

From here one easily derives the following criterion [alternatively, one can again consult (Ref. 10, Theorem 3.8.6)].

Lemma A.1: *A vector-valued function $f:\mathbb{R}\to\mathcal{H}$ belongs to $AC(\mathbb{R},\mathcal{H})$ if and only if the following two conditions are satisfied:*

(i) *there exists a total set $\mathcal{T}\subset\mathcal{H}$ such that for all $\psi\in\mathcal{T}$, $\langle\psi,f(t)\rangle$ is absolutely continuous,*
(ii) *the derivative $f'(t)$ exists almost everywhere and $\|f'(t)\|\in L^1_{\mathrm{loc}}(\mathbb{R})$.*

Set $\mathcal{K}=L^2(\mathbb{R},\mathcal{H},\mathrm{d}t)$. Let us recall that to every propagator $U(t,s)$ on $\mathcal{H}$ one can relate a unique self-adjoint operator K in $\mathcal{K}$ which is the generator of the one-parameter group of unitary operators $\exp(-i\sigma K)$, $\sigma\in\mathbb{R}$, defined by[11]

$$(e^{-i\sigma K}f)(t) = U(t,t-\sigma)f(t-\sigma).$$

K is called the quasienergy operator. Equivalently,

$$K = \mathfrak{U}(-i\partial_t)\mathfrak{U}^*, \quad \text{where } \mathfrak{U} = \int_{\mathbb{R}}^{\oplus} U(t,0)\mathrm{d}t. \tag{A1}$$

So $f \in \mathrm{Dom}\, K$ if and only if $U(t,0)^{-1}f(t) \in \mathrm{Dom}(-i\partial_t)$ which means that $f \in L^2$, $U(t,0)^{-1}f(t) \in AC$ and $(U(t,0)^{-1}f(t))' \in L^2$.

From (A1) one concludes that the spectrum of K is purely absolutely continuous and coincides with $\mathbb{R}$. So the kernel of K is always trivial. It seems to be natural, however, to introduce a generalized kernel of K, called $\mathrm{Ker}_0\, K$, as follows:

$$\mathrm{Ker}_0\, K = \{f \in L^2_{\mathrm{loc}}(\mathbb{R},\mathcal{H},\mathrm{d}t);\ \forall\ \eta \in C_0^\infty(\mathbb{R}), \quad \eta f \in \mathrm{Dom}\, K \text{ and } K(\eta f) = -i\eta' f\}.$$

Since K can be very roughly imagined as the formal operator $-i\partial_t + H(t)$ the elements of $\mathrm{Ker}_0\, K$ can be regarded as solutions of the Schrödinger equation in a weak sense.

Proposition A.2: *Let $U(t,s)$ be a propagator and let K be the quasienergy operator associated to it. Then it holds*

$$\mathrm{Ker}_0\, K = \{U(t,0)\psi; \psi \in \mathcal{H}\}.$$

Proof: If $f(t) = U(t,0)\psi$, with $\psi \in \mathcal{H}$, and $\eta \in C_0^\infty(\mathbb{R})$ then, in $\mathcal{K}$, there exists the derivative

$$i\frac{\mathrm{d}}{\mathrm{d}\sigma}(e^{-i\sigma K}\eta f)(t)\bigg|_{\sigma=0} = i\frac{\mathrm{d}}{\mathrm{d}\sigma}(\eta(t-\sigma)U(t,0)\psi)\bigg|_{\sigma=0} = -i\eta'(t)f(t).$$

Hence, by the Stone theorem, $\eta f \in \mathrm{Dom}\, K$ and $K(\eta f) = -i\eta' f$.

Conversely, suppose that $f \in \mathrm{Ker}_0\, K$ and set $g(t) = U(t,0)^{-1}f(t)$. Let η be a test function. From (A1) one deduces that $\eta g \in \mathrm{Dom}(-i\partial_t)$ and

$$\partial_t(\eta(t)g(t)) = \eta'(t)g(t) \text{ a.e.}$$

Since $\eta \in C_0^\infty(\mathbb{R})$ is arbitrary this implies that $g(t) \in AC(\mathbb{R},\mathcal{H})$ and $g'(t) = 0$a.e. Consequently, $g(t) = \psi \in \mathcal{H}$ is a constant vector-valued function and $f(t) = U(t,0)\psi$. □

It is known that the correspondence between the propagators and the quasienergy operators is one-to-one [Ref. 11, Remark (1) on p. 321]. On the one hand, by the very definition, K is unambiguously determined by $U(t,s)$. On the other hand, if $U(t,s)$ and $U_1(t,s)$ are two propagators with equal quasienergy operators, $K = K_1$, then $U(t,s) = U_1(t,s)$. This uniqueness result is also a straightforward corollary of Proposition A.2. Actually, Proposition A.2 implies that for every $\psi \in \mathcal{H}$ there exists $\psi_1 \in \mathcal{H}$ such that $U(t,0)\psi = U_1(t,0)\psi_1$ for all t (we use the strong continuity of the propagators). By setting $t = 0$ one finds that $\psi = \psi_1$. Hence $U(t,0)\psi = U_1(t,0)\psi$ for all $\psi \in \mathcal{H}$. Consequently,

$$U(t,s) = U(t,0)U(s,0)^{-1} = U_1(t,0)U_1(s,0)^{-1} = U_1(t,s).$$

For a family of self-adjoint operators $H(t)$, $t \in \mathbb{R}$, set $\mathfrak{H} = \int_{\mathbb{R}}^{\oplus} H(t)\mathrm{d}t$. This means that $f \in \mathcal{K}$ belongs to $\mathrm{Dom}\, \mathfrak{H}$ if and only if $f(t) \in \mathrm{Dom}\, H(t)$a.e. and $\|H(t)f(t)\| \in L^2(\mathbb{R},\mathrm{d}t)$. Then $\mathfrak{H}$ is a self-adjoint operator in $\mathcal{K}$. In what follows we shall always suppose that the intersection $\mathrm{Dom}(-i\partial_t) \cap \mathrm{Dom}\, \mathfrak{H}$ is dense in $\mathcal{K}$. For example, this is true in the case when the domain $\mathrm{Dom}\, H(t)$ is independent of t. Consequently, $-i\partial_t + \mathfrak{H}$ is a densely defined symmetric operator.

Definition A.3: *We shall say that a propagator $U(t,s)$ is* weakly associated to $H(t)$ *if*

$$K = \overline{-i\partial_t + \mathfrak{H}}. \tag{A2}$$

Notice that equality (A2) is equivalent to the following two conditions:

(i) $-i\partial_t + \mathfrak{H} \subset K$,
(ii) $-i\partial_t + \mathfrak{H}$ is essentially self-adjoint.

Furthermore, it is important to note that this definition still guarantees the uniqueness, i.e., to $H(t)$ one can weakly associate at most one propagator $U(t,s)$. Actually, if $U(t,s)$ and $U_1(t,s)$ are weakly associated to $H(t)$ then $K=K_1$ according to equality (A2). But due to the one-to-one correspondence between the propagators and the quasienergy operators we have $U(t,s)=U_1(t,s)$.

Now we are ready to formulate and prove two propositions which are directly applicable to the model studied in this paper.

Proposition A.4: *Let $A(t)$ be a family of bounded self-adjoint operators in $\mathcal{H}$ which is locally bounded. Let $C(t,s)$ be the propagator associated to $A(t)$ via the Dyson formula. Let $D\subset\mathcal{H}$ be a dense linear subspace and let $T(t)$ be a strongly continuous family of unitary operators in $\mathcal{H}$ obeying the following conditions:*

(i) $\forall t\in\mathbb{R}$, $T(t)D=D$,
(ii) $\forall\psi\in D$, $T(t)\psi$ *is continuously differentiable,*
(iii) $\forall t\in\mathbb{R}$, $X(t)=i\dot{T}(t)T(t)^{-1}$, *with* $\mathrm{Dom}\,X(t)=D$, *is a self-adjoint operator.*

Then the propagator $T(t)C(t,s)T(s)^{-1}$ is weakly associated to the family

$$X(t)+T(t)A(t)T(t)^{-1}.$$

Proof: Set

$$Y(t)=X(t)+T(t)A(t)T(t)^{-1},\quad \mathfrak{Y}=\int_{\mathbb{R}}^{\oplus}Y(t)\mathrm{d}t,\quad \mathfrak{T}=\int_{\mathbb{R}}^{\oplus}T(t)\mathrm{d}t.$$

Let K_Y be the quasienergy operator associated to the propagator $T(t)C(t,s)T(s)^{-1}$. Set

$$C(t)=C(t,0),\quad \mathfrak{C}=\int_{\mathbb{R}}^{\oplus}C(t)\mathrm{d}t.$$

$C(t)$ is a family of unitary operators which satisfies $C(t)\in\widetilde{AC}(\mathbb{R},\mathfrak{B}(\mathcal{H}))$ and $A(t)=i\dot{C}(t)C(t)^{-1}$.

(i) Let us verify that

$$-i\partial_t+\mathfrak{Y}\subset K_Y=\mathfrak{T}\mathfrak{C}(-i\partial_t)\mathfrak{C}^{-1}\mathfrak{T}^{-1}.$$

Suppose that a vector-valued function $f:\mathbb{R}\to\mathcal{H}$ belongs to $\mathrm{Dom}(-i\partial_t+\mathfrak{Y})$. This happens if and only if f obeys the following conditions: $f\in L^2$, $f\in AC$, $f'\in L^2$, $f(t)\in D$ a.e. and $Y(t)f(t)\in L^2$. In that case the function $T(t)^{-1}f(t)$ is differentiable almost everywhere and the derivative

$$(T(t)^{-1}f(t))'=T(t)^{-1}(f'(t)+iX(t)f(t))$$

is square integrable. Moreover, if $\psi\in D$ then the function $\langle\psi,T(t)^{-1}f(t)\rangle=\langle T(t)\psi,f(t)\rangle$ is absolutely continuous. According to Lemma A.1 this implies that $T(t)^{-1}f(t)\in AC(\mathbb{R},\mathcal{H})$ and consequently $C(t)^{-1}T(t)^{-1}f(t)\in AC$ as well. Furthermore, a straightforward computation yields

$$Y(t)f(t)=i(\dot{T}(t)T(t)^{-1}f(t)+T(t)\dot{C}(t)C(t)^{-1}T(t)^{-1}f(t))$$

$$=i(T(t)C(t))'C(t)^{-1}T(t)^{-1}f(t)$$

$$=if'(t)-iT(t)C(t)(C(t)^{-1}T(t)^{-1}f(t))'.$$

Hence $(C(t)^{-1}T(t)^{-1}f(t))'\in L^2$, $f\in\mathrm{Dom}\,K_Y$ and $-if'(t)+Y(t)f(t)=K_Yf(t)$.

(ii) Let us verify that $-i\partial_t+\mathfrak{Y}$ is essentially self-adjoint. Suppose that $g\in\mathrm{Dom}(-i\partial_t+\mathfrak{Y})^*$ satisfies $(-i\partial_t+\mathfrak{Y})^*g=zg$ with $\mathrm{Im}(z)\neq 0$. This means that

$$\forall f \in \mathrm{Dom}(-i\partial_t + \mathfrak{Y}), \quad \langle(-i\partial_t + \mathfrak{Y})f, g\rangle_{\mathcal{K}} = z\langle f, g\rangle_{\mathcal{K}}.$$

Choose $f(t) = \eta(t)T(t)\psi$ where $\psi \in D$ and $\eta \in C_0^\infty(\mathbb{R})$ is real valued. Then $f \in \mathrm{Dom}(-i\partial_t + \mathfrak{Y})$ and an easy computation shows that

$$(-i\partial_t + \mathfrak{Y})f(t) = -i\eta'(t)T(t)\psi + \eta(t)T(t)A(t)\psi.$$

Hence for all $\eta \in C_0^\infty(\mathbb{R})$ we have

$$\int_{\mathbb{R}} (i\eta'(t)\langle T(t)\psi, g(t)\rangle + \eta(t)\langle T(t)A(t)\psi, g(t)\rangle)\mathrm{d}t = z\int_{\mathbb{R}} \eta(t)\langle T(t)\psi, g(t)\rangle \mathrm{d}t.$$

Setting

$$F(t) = \langle T(t)\psi, g(t)\rangle, \quad G(t) = \langle T(t)A(t)\psi, g(t)\rangle,$$

we find that

$$-i\partial_t F(t) + G(t) = zF(t) \tag{A3}$$

in the sense of distributions. Since both $F(t)$ and $G(t)$ are locally integrable, a standard result from the theory of distributions tells us that $F(t)$ is absolutely continuous and equality (A3) holds true in the usual sense. Moreover, equality (A3) implies that

$$\partial_t(e^{2\,\mathrm{Im}(z)t}|F(t)|^2) = 2e^{2\,\mathrm{Im}(z)t}\,\mathrm{Im}(\overline{F(t)}G(t)).$$

Let us now choose an orthonormal basis $\{\psi_k\}$ whose elements all belong to the domain D. Let us write F_k instead of F and G_k instead of G when replacing ψ by ψ_k. We have derived the equality

$$|F_k(t)|^2 = e^{-2\,\mathrm{Im}(z)(t-a)}|F_k(a)|^2 + 2\int_a^t e^{-2\,\mathrm{Im}(z)(t-s)}\,\mathrm{Im}(\overline{F_k(s)}G_k(s))\mathrm{d}s \tag{A4}$$

which is valid for all k and all a, $t \in \mathbb{R}$. Observe that

$$\sum_k |F_k(t)|^2 = \|g(t)\|^2 \quad \text{a.e.},$$

$$\sum_k |F_k(s)||G_k(s)| \leqslant \|g(s)\|\|A(s)T(s)^{-1}g(s)\| \in L^1_{\mathrm{loc}}(\mathbb{R}, \mathrm{d}s) \quad \text{a.e.},$$

and

$$\sum_k \overline{F_k(s)}G_k(s) = \langle g(s), T(s)A(s)T(s)^{-1}g(s)\rangle \in \mathbb{R} \quad \text{a.e.}$$

Summing in k in equality (A4) we find that

$$\|g(t)\| = e^{-\mathrm{Im}(z)(t-a)}\|g(a)\|$$

for almost all a, $t \in \mathbb{R}$. Since $\|g(t)\|$ is square integrable this is possible only if $g(t) = 0$ a.e. □

Proposition A.4 has a corollary justifying the adverb "weakly" in Definition A.3.

Corollary A.5: *Assume that a propagator $U(t, t_0)$ is associated as a strong solution of the Schrödinger equation to a time-dependent Hamiltonian $H(t)$ which has, however, a time-independent domain (i.e., the relationship between the propagator and the Hamiltonian is the usual one). Then $U(t, t_0)$ is weakly associated to $H(t)$.*

Proof: In Proposition A.4 it suffices to set $D = \mathrm{Dom}\, H(0)$, $T(t) = U(t, 0)$ and $A(t) = 0$. Then $X(t) = H(t)$, $C(t, s) = \mathbb{I}$, and $T(t)C(t, s)T(s)^{-1} = U(t, s)$. □

Proposition A.6: *Suppose that $V(t)$, $t \in \mathbb{R}$, is a family of unitary operators which is continu-*

ously differentiable in the strong sense. Let $\tilde{H}(t)$, $t\in\mathbb{R}$, *be a family of self-adjoint operators such that* $\mathrm{Dom}\,\tilde{H}(t)=D$ *for all* $t\in\mathbb{R}$. *Set*

$$H(t) = V(t)\tilde{H}(t)V(t)^{-1} + i\dot{V}(t)V(t)^{-1}.$$

If the propagator $\tilde{U}(t,s)$ *is weakly associated to* $\tilde{H}(t)$ *then the propagator* $U(t,s)=V(t)\tilde{U}(t,s)V(s)^{-1}$ *is weakly associated to* $H(t)$.

Proof: Set

$$\tilde{U}(t) = \tilde{U}(t,0), \quad \tilde{\mathfrak{U}} = \int_{\mathbb{R}}^{\oplus} \tilde{U}(t)\mathrm{d}t, \quad \mathfrak{V} = \int_{\mathbb{R}}^{\oplus} V(t)\mathrm{d}t.$$

By the assumption, $\tilde{\mathfrak{U}}(-i\partial_t)\tilde{\mathfrak{U}}^{-1}=\overline{-i\partial_t+\tilde{\mathfrak{H}}}$. We must show that

$$\mathfrak{V}\tilde{\mathfrak{U}}(-i\partial_t)\tilde{\mathfrak{U}}^{-1}\mathfrak{V}^{-1} = \overline{-i\partial_t+\mathfrak{H}}.$$

Since

$$\mathfrak{V}\tilde{\mathfrak{U}}(-i\partial_t)\tilde{\mathfrak{U}}^{-1}\mathfrak{V}^{-1} = \mathfrak{V}\overline{(-i\partial_t+\tilde{\mathfrak{H}})}\mathfrak{V}^{-1} = \overline{\mathfrak{V}(-i\partial_t+\tilde{\mathfrak{H}})\mathfrak{V}^{-1}}$$

it is sufficient to verify that

$$\mathfrak{V}(-i\partial_t+\tilde{\mathfrak{H}})\mathfrak{V}^{-1} = -i\partial_t+\mathfrak{H}.$$

This would also imply that $\mathrm{Dom}(-i\partial_t)\cap\mathrm{Dom}(\mathfrak{H})$ is dense in $\mathcal{K}$.

A vector-valued function $f:\mathbb{R}\to\mathcal{H}$ belongs to $\mathrm{Dom}(\mathfrak{V}(-i\partial_t+\tilde{\mathfrak{H}})\mathfrak{V}^{-1})$ if and only if it satisfies the following conditions: $f\in L^2$, $V(t)^{-1}f(t)\in AC$, $(V(t)^{-1}f(t))'\in L^2$, $V(t)^{-1}f(t)\in D$ a.e. and $\tilde{H}(t)V(t)^{-1}f(t)\in L^2$. Let us note that from the continuous differentiability of $V(t)$ in the strong sense and from the uniform boundedness principle it follows that $\dot{V}(t)$, $t\in\mathbb{R}$, is a family of bounded operators which is locally bounded. Furthermore, $V(t)^*=V(t)^{-1}$ is continuously differentiable in the strong sense as well and $V(t)^{-1}\psi\in AC$ for all $\psi\in\mathcal{H}$. Suppose that $f\in L^2$. If $V(t)^{-1}f(t)\in AC$ then $f'(t)$ exists almost everywhere and $\|f'(t)\|$ is locally integrable, the function $\langle\psi,f(t)\rangle=\langle V(t)^{-1}\psi,V(t)^{-1}f(t)\rangle$ is absolutely continuous for all $\psi\in\mathcal{H}$ and therefore, by Lemma A.1, $f(t)\in AC$. Similarly, the converse is also true. If $f(t)\in AC$ then $V(t)^{-1}f(t)\in AC$.

Using these facts and the relation between $\tilde{H}(t)$ and $H(t)$ [including that $\mathrm{Dom}\,H(t)=V(t)D$] one easily finds that the domains of $\mathfrak{V}(-i\partial_t+\tilde{\mathfrak{H}})\mathfrak{V}^{-1}$ and $-i\partial_t+\mathfrak{H}$ coincide and that

$$V(t)(-i\partial_t+\tilde{H}(t))V(t)^{-1}f(t) = -if'(t)+H(t)f(t)$$

for every $f\in\mathrm{Dom}(-i\partial_t+\mathfrak{H})$. □

Remark: Proposition A.6 can be easily extended to the case when the family of unitary operators $V(t)$ is continuous and piecewise continuously differentiable in the strong sense and in each point of discontinuity there exist the limits of the derivative both from the left and from the right.

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An approach to the problem of phase transitions in the continuum

Alejandro Mesón[a] and Fernando Vericat[b]
Instituto de Física de Líquidos y Sistemas Biológicos, CONICET-UNLP-CICPBA and Grupo de Aplicaciones Matemáticas y Estadísticas de la Facultad de Ingeniería, UNLP, La Plata, Argentina

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Based on the spectral properties of Ruelle transfer operators, we establish conditions for the absence of phase transitions in the continuum. Our approach differs in several aspects from those which use Kirkwood–Salsburg and Kirkwood–Ruelle operators. In particular the results follow in a concise and relatively direct way. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1897163]

I. INTRODUCTION

The analysis of the equilibrium behavior of systems can be done by studying thermodynamical properties. One main aspect is the coexistence of two or more pure phases for "physically acceptable" interactions. In order to investigate the uniqueness of phases it is important to analyze the variation of some macroscopic quantities when thermodynamical parameters, such as the temperature, are changed.

Numerical studies show that restrictions on the configuration space favor the disappearance of phase transitions. The well known fact, stated by van Hove theorem,[2,15] that when the dimension is reduced to one is more difficult to observe phase transitions, would confirm those claims. In this vein, instead of reducing the dimension we could consider as well the confinement of the system configurations to a compact set. This can be achieved by considering special potentials between pairs of particles or adequate external fields.

In this paper we shall give conditions for ensuring the absence of phase transition in more general system of particles, in the sense that they are not necessarily confined. The systems we are thinking of consist of N particles into a container $\Omega \subset \mathbf{R}^d$, $|\Omega| = \mathrm{mes}(\Omega) \leqslant \infty$, interacting *via* a potential map $V_N : \Omega^N \to \mathbf{R}$ of the form

$$V_N(x_0, x_1, \ldots, x_{N-1}) = \sum_{i<j} \varphi(x_i, x_j) + \sum_i \psi(x_i), \tag{1}$$

where $\varphi : \Omega \times \Omega \to \mathbf{R}$ and $\psi : \Omega \to \mathbf{R}$ are maps that represent the pair potential and an external field, respectively.

The problem of the absence of phase transitions has been frequently treated by using spectral properties of the Kirkwood–Salsburg (KS) and Kirkwood–Ruelle (KR) operators. Historically the first contribution in that direction is the article by Pastur.[10] For further contributions see for instance Refs. 3 and 4 and 17–19. The analysis began with the consideration of confined systems in a bounded set Λ and then taking the thermodynamic limit to reach an infinite volume set. Here we propose an alternative way. In the first place, as we mentioned above, we considered a not necessarily bounded container for the particles, and so we do not need to take the thermodynamic limit. On the other hand, we use the Grothendieck theory of nuclear operators instead of the KR

[a]Electronic mail: meson@iflysib.unlp.edu.ar
[b]Electronic mail: vericat@iflysib.unlp.edu.ar

and KS operators. This approach allows to get a relationship between the spectral radius of the operators and the free energy, for any value of the temperature. The conclusions follow in a relatively direct manner from Grothendieck results.

From the mathematical point of view the absence of phase transition is established by means of the uniqueness of the *Gibbs states*, which are special probability measures on Ω. The set $\mathcal{G}$ of the Gibbs states is convex[12] so, any element of it can be written as a convex combination (*mixture*) of the extremal points of $\mathcal{G}$. The extremal Gibbs states are interpreted as *pure homogenous phases* and any Gibbs state admits a unique integral decomposition in terms of pure phases.

Recently, Franzosi *et al.*[1] have given sufficient conditions for the existence of just one phase in systems interacting via a general class of confined potentials in any dimension. These conditions include the extra hypothesis that each equipotential surface is C^∞-diffeomorphic to the others. This hypothesis, together with Morse theory of critical points, leads to differentiability of the free energy.

In this paper, we study the behavior of the phases when the inverse temperature q is varied. We use a formalism in which a "free energy function" $T(q)$ is identified with the limit of the logarithm of a partition function over the total particle number. From the Ruelle thermodynamic formalism,[12] which we can adapt for the continuous case, it is known that the Gibbs states are functional tangents to $T(q)$ and hence a phase transition is detected when this function has a singularity. In order to demonstrate the uniqueness of Gibbs states, we shall introduce adequate *transfer operators* and we will prove that $\exp(T(q))$ is an isolated eigenvalue of these operators. This kind of analysis, for one dimensional lattices, was already done by Ruelle[11,12] and Sinai.[13] In Ref. 9 we extended Sinai–Ruelle approaches in some directions. Instead of a symbolic space (a one dimensional lattice in the statistical mechanics terminology), we have considered a compact submanifold $X \subset \mathbf{R}^d$. On the other hand, the dynamics were more generally given by continuous maps $f: X \to X$ and we introduced a free energy $T(q)$ adequate to that context. In that case the partition function is defined by summing over the set of microstates (the periodic points of f), which will be finite by the conditions imposed on the dynamics.

Under the conditions assumed here, the states belong to a continuum, so that partition functions must be defined by mean of integrals. Moreover we emphasize the statistical mechanical more than the dynamic character of the system under study. Also, in our previous paper[9] we have considered systems which can be "discretized" and, because of this, the transfer operators are defined as sums. Here, the discretization property is relaxed and the operators are integral ones.

The paper layout is as follows: in the next section we review the concept of Gibbs states, in any dimension and introduce the formalism to define the partition functions and free energy functions. In Sec. III we use the transfer operators and prove the absence of phase transition in the models considered.

II. THE FREE ENERGY FUNCTION AND GIBBS STATES

Let us denote by $\mathcal{G}(q)$ the space of the *Gibbs states* for a system at inverse temperature q and described by a total potential of the form of Eq. (1). It is constituted by the probability measures μ_q which are infinite volume limits as $N \to \infty$ of the finite volume ensembles,

$$\mu_{q,N}(x_0, x_1, \ldots, x_{N-1}) = \frac{\exp(-qV_N)}{Z_N(q)} \delta_{(x_0, x_1, \ldots, x_{N-1})}. \tag{2}$$

Here δ_x is the point mass measure in x and the configurational partition function for the system reads

$$Z_N(q) = \int_{\Omega^N} \exp(-qV_N) \mathrm{d}x_0 \, \mathrm{d}x_1 \cdots \mathrm{d}x_{N-1}. \tag{3}$$

Therefore the *free energy function per particle* is, provided the limit exists,

$$T(q) = \lim_{N\to\infty} \frac{1}{N} \log Z_N(q). \tag{4}$$

It may be interesting to notice how this formalism could read in the context of dynamical systems. Let us consider a pair (X,f) with X be a compact subset of $\mathbf{R}^d$ $(d>0)$ and $f:X\to X$, a continuous map. For a potential $\varphi \in C(X)$ we define the *statistical sum* by

$$S_N(x) = \sum_{i=0}^{N-1} \varphi(f^i(x)). \tag{5}$$

Let us assume that the dynamical map f be *expansive*, i.e., there is a constant $\delta>0$, such that $d(f^N(x), f^N(y)) < \delta$, for any integer N implies $x=y$. Under these conditions the set of periodic points, $P_N(f) := \{x: f^N x = x\}$, is (N,δ)-separated and, since X is compact, then it is finite (these are standard facts in topological dynamics, see Ref. 16 or Ref. 7). Now, as a set of "microstates," we can consider the whole set of periodic points. The configurations can be given by the orbits of the points $x \in X$, i.e., $x_i = f^i(x)$, $i=0,1,\ldots,N-1$, and so the "Hamiltonian of a dynamical system of N particles" can be defined as the statistical sum $V_N = S_N$. A construction of a Gibbs state in this context can be done by defining the ensembles supported on periodic points of f,[7,14]

$$\mu_{q,N} = \frac{\exp(-qV_N(x))\delta_x}{Z_N(q)}, \tag{6}$$

with the corresponding partition function given by

$$Z_N(q) = \sum_{x\in P_N(f)} \exp(-qV_N(x)). \tag{7}$$

III. ANALYSIS OF PHASE TRANSITIONS

By $\mathcal{A}_\infty(U)$, $U \subset \mathbf{C}^d$, we denote the space of functions holomorphic in U and bounded on the closure of U (with the supreme norm). We consider the Gibbs–Boltzmann factor,

$$G(x,y) = \exp[-\varphi(x,y)]\exp\left(-\tfrac{1}{2}[\psi(x)+\psi(y)]\right)$$

and impose the following condition.

There exists an open neighborhood W of Ω such that $G:\Omega\times\Omega\to\mathbf{R}$ has an analytic extension to a map $\hat{G}:U\times U\to\mathbf{C}$, where U is a complex open neighborhood of W in $\mathbf{C}^d$ and such that $\hat{G}$ belong to $\mathcal{A}_\infty(U\times U)$. This requirement is of course fulfilled if $\varphi:\Omega\times\Omega\to\mathbf{R}$ satisfies such analytic extension and $\psi:\Omega\to\mathbf{R}$ also does.

We introduce next the transfer operators, in the sense of Ruelle thermodynamic formalism. They will be defined on the space of functions $\mathcal{A}_\infty(U)$, for an adequate domain U.

For any value of the temperature parameter q, let us introduce the *transfers operators* $\mathcal{L}_q:\mathcal{A}_\infty(U)\to\mathcal{A}_\infty(U)$ according to

$$\mathcal{L}_q(\varkappa)(z) = \int_\Omega \exp[-q\varphi(z,w)]\exp\left(-\frac{q}{2}[\psi(z)+\psi(w)]\right)\chi(w)\mathrm{d}w. \tag{8}$$

Lemma 1: The spectral radius $\rho(\mathcal{L}_q)$ of operators $\mathcal{L}_q$ equals $\exp(T(q))$.

Proof: Let E_q be the maximal eigenvalue, in modulus, of $\mathcal{L}_q$, so we have for any function $\xi \in C(\Omega): \lim_{N\to\infty} E_q^{-N} \log \mathcal{L}_q^N = \upsilon_q(\xi)\psi_q$, where υ_q is some functional on $C(\Omega)$ and ψ_q is the eigenfunction corresponding to E_q. If there is a unique Gibbs state μ_q associate to $q\varphi$ then υ_q is precisely μ_q, seen in this case as a functional. This arises from an adaptation of the Ruelle–Perron–Frobenius theorem. Now taking $\xi \equiv 1$, we obtain

$$\log E_q = \lim_{N\to\infty}\frac{1}{N}\log \mathcal{L}_q^N(1)(x_0,x_1,\ldots,x_{N-1}) = \lim_{N\to\infty}\frac{1}{N}\log\int_{\Omega^N}\exp(-qV_N)\mathrm{d}x_0\,\mathrm{d}x_1\ldots\mathrm{d}x_{N-1}$$

$$= \lim_{N\to\infty}\frac{1}{N}\log Z_N(q) = T(q).$$

Therefore $\rho(\mathcal{L}_q)=\exp(T(q))$.

■

One main fact about these operators is that they are *nuclear.* Let us recall that a map $\mathcal{L}$ acting on a Banach space B is nuclear if there exist sequences $(x_n)\subset B$, $(f_n)\subset B^*$ (the dual space of B) with $\|x_n\|=1$, $\|f_n\|=1$ and numbers (ρ_n) with $\Sigma_{n=0}^{\infty}|\rho_n|<\infty$ such that $\mathcal{L}(x)=\Sigma_{n=0}^{\infty}\rho_n f_n(x)x_n$ for every $x\in B$. This notion can be generalized to maps from complete metric topological spaces (Frechet spaces) to Banach spaces. For more details see Refs. 5 and 8. There is a particular class $\mathcal{F}$ of Frechet spaces with the property that any bounded map $\mathcal{L}:\mathcal{F}\to B$, with B an arbitrary Banach space is nuclear. Such spaces are also called nuclear.

Proposition 2: The transfer operators $\mathcal{L}_q:\mathcal{A}_\infty(U)\to\mathcal{A}_\infty(U)$, for a domain $U\subset\mathbf{C}^d$, are nuclear for any q.

Proof: The demonstration is an application of the Grothendieck theory.[5,6] We analyze the kernel of these operators which are operators of the following type:

$$P_{\hat{G}}(\chi)(z) = \hat{G}(z)\chi(z).$$

We shall consider an adequate nuclear space $\mathcal{F}$ and we prove that $P_{\hat{G}}$ defined on $\mathcal{F}$ is bounded. This space will be $\mathcal{H}(U)$ equal to the space of holomorphic functions in a domain $U\subset\mathbf{C}^d$ equipped with the seminorm $\|f\|_K=\sup_{z\in K}|f(z)|$, K is a compact subset of $\mathbf{C}^d$. It is known that the space $\mathcal{H}(U)$ with the topology of the seminorms $\|\bullet\|_K$ is nuclear.[8] Now by proving that the operators $P_{\hat{G}}:\mathcal{H}(U)\to\mathcal{A}_\infty(U)$ are bounded in the space $\mathcal{H}(U)$ we ensure that they are nuclear.

Let K be a compact subset of U, such that $\hat{G}(\overline{U})\subset K\subset U$, and we set $B_M:=\{f\in\mathcal{H}(U):\|f\|_K<M\}$. Thus $\|P_{\hat{G}}(\chi)\|=\sup_{z\in\overline{U}}\{|\hat{G}(z)\chi(z)|\}\leqslant\|\hat{G}\|_K\|\chi\|_K<M^2$.

So that the set B_M is carried by $P_{\hat{G}}$ in a bounded set in $\mathcal{A}_\infty(U)$. To show that $P_{\hat{G}}$ is defined on $\mathcal{A}_\infty(U)$ we change the composition of $P_{\hat{G}}$ with the canonical injection $\iota:\mathcal{A}_\infty(U)\hookrightarrow\mathcal{H}(U)$. Thus $P_{\hat{G}}\circ\iota:\mathcal{A}_\infty(D)\to\mathcal{A}_\infty(D)$ is nuclear.

■

Let us recall that the *Fredholm determinant* of $\mathcal{L}_q$ is

$$\det(1-z\mathcal{L}_q) = \exp\left(-\sum_{N=1}^{\infty}\frac{z^N}{N}\operatorname{Tr}(\mathcal{L}_q^N)\right),\quad z\in\mathbf{C}.$$

From the fact that $\mathcal{L}_q$ is nuclear it follows that the function $\det(1-z\mathcal{L}_q)$ is entire in both two variables z, q. Besides the set of zeros z of the Fredholm determinant agree with the set of the nonzero eigenvalues of $\mathcal{L}_q$.

The following formula[8] is useful to obtain a development of $\operatorname{Tr}(\mathcal{L}_q^N)$,

$$\det(1-\mathcal{L}) = \sum_{\kappa=0}^{d}(-1)^\kappa\operatorname{Tr}(\wedge_\kappa\mathcal{L}),$$

here $\wedge_\kappa\mathcal{L}$ is the κ-fold exterior product. Then we can define operators $\mathcal{L}_q^{(k)}$, $\wedge_k\mathcal{F}(U)\to\wedge_k\mathcal{F}(U)$, where $\wedge_k\mathcal{F}(U)$ denotes the Banach space of differential k-forms holomorphic in U. Now the operators are defined as

$$\mathcal{L}_q^{(k)}(\omega_k)(z) = \int_\Omega\exp[-q\varphi(z,w)]\exp\left(-\frac{q}{2}[\psi(z)+\psi(w)]\right)\wedge_k D(\varphi(z,w)+\psi(z)+\psi(w))(\omega_k)\mathrm{d}w$$

Here $\wedge_k D\phi$ means the k-fold exterior product of the linear operator $D\phi$.

The Fredholm determinant is related with the *Ruelle zeta function*[12] which is defined as

$$\zeta(z,q) = \exp\left(\sum_{n=1}^{\infty} \frac{z^N}{N} Z_N(q)\right).$$

This series converges in $\{z:|z|<\exp(-T(q))\}$. The Fredholm determinant is used to show that the Ruelle zeta function may have a meromorphic extension to the whole complex plane. For instance if $k=1$ holds,[8]

$$\zeta(z,q) = \frac{\det(1 - z\mathcal{L}_q^{(1)})}{\det(1 - z\mathcal{L}_q^{(0)})}.$$

Therefore the z poles of $\zeta(z,q)$ are found among the z zeros of $\det(1-z\mathcal{L}_q^{(0)})$, i.e., the nonzero eigenvalues of $\mathcal{L}_q^{(0)} \equiv \mathcal{L}_q$. The zeta function has a pole localized in $\exp(T(q))$, i.e., in the leading eingenvalue of $\mathcal{L}_q$. Then since $\exp(T(q))$ is an isolated singularity of the map ζ the leading eigenvalue of $\mathcal{L}_q$ is isolated. As we pointed out in the introduction, in this way the nonexistence of phase transition is proved.

From the above results and considerations we can state the following.

Theorem 3: For systems of particles in $\mathbf{R}^d$ with a Gibbs–Boltzmann factor belonging to the class $\mathcal{A}_\infty(U\times U)$, for some domain $U\subset \mathbf{C}^d$, and with transfer operators acting on $\mathcal{A}_\infty(U)$ there is no phase transition.

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Geometry of contours and Peierls estimates in $d=1$ Ising models with long range interactions

Marzio Cassandro[a)]
Dipartimento di Fisica, Università di Roma la Sapienza and INFM Sezione di Roma, 00185 Rome, Italy

Pablo Augusto Ferrari[b)]
Departamento de Estatistica, Universidade de São Paulo, Brazil

Immacolata Merola[c)] and Errico Presutti[d)]
Dipartimento di Matematica, Università di Roma Tor Vergata, 00133 Rome, Italy

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Following Fröhlich and Spencer, we study one dimensional Ising spin systems with ferromagnetic, long range interactions which decay as $|x-y|^{-2+\alpha}$, $0\leqslant\alpha\leqslant 1/2$. We introduce a geometric description of the spin configurations in terms of triangles which play the role of contours and for which we establish Peierls bounds. This in particular yields a direct proof of the well-known result by Dyson about phase transitions at low temperatures. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1897644]

I. INTRODUCTION

A rigorous proof of liquid–vapor phase transitions is a long standing challenge for mathematical physicists. A clear understanding of the phenomenon goes back to van der Waals, but a mathematically consistent theory is still lacking. Lebowitz, Mazel, and Presutti,[14] have tried to capture van der Waals ideas by considering an Hamiltonian which has a term given by an attractive, two-body Kac potential. The effort was to study the model without taking the Kac scaling parameter $\gamma\to 0$, as in the original works of Kac, Uhlenbeck, and Hemmer,[13] and Lebowitz and Penrose.[15] Technically, the idea was to study the system as a perturbation of mean field, which corresponds to the limit case $\gamma=0$, and to adapt to such a context the Pirogov–Sinai theory of finite temperature perturbations of ground states. To carry through the program, one needs a good control of an approximate model where the Kac potential term in the Hamiltonian is replaced by a self-consistent, external one-body field, whose intensity depends on the true value of the order parameter (the particles density) at equilibrium. In the continuum, the Hamiltonian cannot consist of just the attractive Kac potential (as in Ising models with Kac potentials) and a repulsive force is needed to prevent a collapse of matter. The natural choice (as proposed originally by Kac *et al.* [13]) is then to add a hard-core interaction, but, at the required values of the particles density, the cluster expansion results for the system with only hard cores are not valid and the implementation of the Pirogov–Sinai methods collapses. In Ref. 14 the problem has been avoided by using repulsive forces which are also given by Kac potentials, in particular four-body positive interactions. The escamotage is physically not totally satisfactory, as the phase transition should arise from a competition between the short range repulsive and the much longer range attractive intermolecular forces. Several efforts to extend[14] to such a context and in particular to the model with hard core plus attractive two-body Kac potentials have failed.

[a)]Electronic mail: marzio.cassandro@roma1.infn.it
[b)]Electronic mail: pablo@ime.usp.br
[c)]Electronic mail: merola@mat.uniroma2.it
[d)]Electronic mail: presutti@mat.uniroma2.it

There is however some margin left if we restrict to one dimensions, because the pure hard rods system is isomorphic to an ideal gas. Unfortunately, there is a price to pay, to have a phase transition in $d=1$, we need to consider long range forces (potentials which decay as $|x-y|^{-2+\alpha}$, $\alpha\in[0,1)$) which are not covered by the traditional Pirogov–Sinai theory. Prior to Ref. 14, the problem of phase transition in the continuum in $d=1$ with such long range interactions had already been considered by Johansson,[11,12] who studied the system in the canonical ensemble, proving phase transition for the thermodynamic potentials. The existence of distinct DLR measures at the proper values of chemical potential and temperature remains however open.

The Pirogov–Sinai theory seems the natural way to answer these questions, as it provides powerful tools for investigating phase transitions at low temperatures and at low effective temperatures as well, with a quite satisfactory description of systems in dimensions larger or equal to two. In view of the desired applications to continuum particle models, our mid-term program is to extend Pirogov–Sinai to one-dimensional spin systems with long range interactions. The content of this paper will be the definition of contours and the establishment of Peierls estimates, as a preliminary step in this direction. After the papers by Dyson,[6,7] on a model with hierarchical interactions (which, by ferromagnetic inequalities, prove phase transitions in Ising systems as well), we find in the literature the fundamental paper by Fröhlich and Spencer,[8] where the critical case $\alpha=0$ is studied by deriving Peierls estimates for suitably defined contours. A further step forward has then been done by Imbrie,[9] who proved the validity of the cluster expansion for this gas of contours. A different approach, based on inequalities, has instead been followed by Dümcke and Spohn,[5] and Spohn,[18] to prove phase transitions for systems of ±1 spins on $\mathbb{R}$ with long range interactions, $\alpha\in[0,1)$. The results were used in the analysis of ground states for some quantum systems.

In this paper we revisit Fröhlich and Spencer[8] and extend it to the case $\alpha\in(0,1/2]$. In particular we prove that the probability of occurrence of a droplet of the opposite phase is depressed at least by $c\exp\{-\beta\zeta L^{\alpha}\}$, c and ζ positive constants, L the length of the droplet. The analogy with $d>1$ where the bound goes as $c\exp\{-\beta\zeta L^{(d-1)/d}\}$, is evident (our proof applies essentially unchanged through $\alpha=0$, where it yields the bound $c\exp\{-\beta\zeta\ln L\}$, losing however the analogy with $d>1$). Comforted by these results and the analogy with $d>1$, we plan, in the future, to extend the analysis to Ising systems with Kac potentials and then, hopefully, to prove phase transitions for hard rods with attractive Kac potentials, at least for $\alpha>0$.

The bibliography on the subject should also include the papers,[1,2,16,10,17] which refer to $d=1$, long range percolation. In fact, using the Fortuin and Kasteleyn (FK) representation, the results can be transferred to Ising systems, but it is not clear whether the approach could extend to the continuum particle systems where ferromagnetic inequalities are absent.

The techniques which have been developed in Ref. 8 and in the successive papers mentioned above can be used to prove the occurrence of a phase transition at large β also in the model we consider here ($\alpha>0$). In Ref. 8 Fröhlich and Spencer consider the sets of local fluctuations with the same energy and estimate their entropy. The hard part of the proof is to get a suitable lower bound for the energy.

Our approach based on a graphical representation of the spin configurations, gives a geometrical picture of the local fluctuations and allows to derive in easy and transparent way, estimates for their contribution to the total energy.

This more detailed description, that we developed for future applications, implies longer and more complex estimates but makes explicit hierarchical structure of the model and its relation with the original analysis of Dyson.[6,7]

Thus, the model we consider here is an Ising ferromagnet on a one dimensional lattice, with total energy

$$h(\sigma)=\frac{1}{2}\sum_{x,y\in\mathbb{Z}}J(|x-y|)\mathbf{1}_{\sigma(x)\neq\sigma(y)}, \tag{1.1}$$

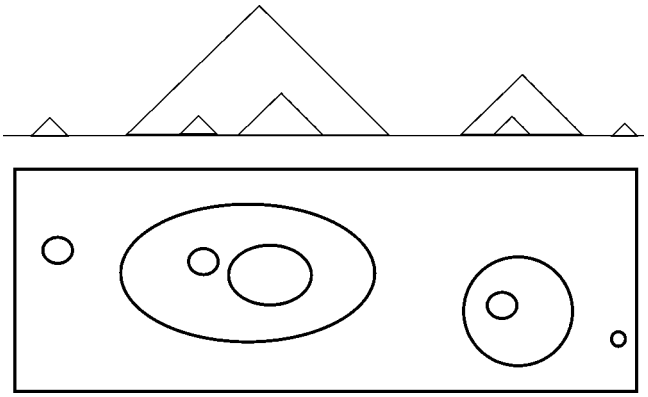

FIG. 1. External and internal interfaces in $d=1$ and $d=2$.

$$J(n) = \begin{cases} J(1) \gg 1 & \text{with } \alpha \in [0,1/2], \\ \dfrac{1}{n^{2-\alpha}} & \text{if } n > 1. \end{cases} \tag{1.2}$$

which will be studied at equilibrium with $\beta \gg 1$. In the sequel, for notational convenience, we restrict $\alpha \in (0,1/2]$, the analysis of the case $\alpha=0$ is analogous and treated in Appendixes A, E, and F.

In this paper we will show that the equilibrium configurations for the system associated to the Hamiltonian (1.1) can be described in terms of contours whose weights satisfy a Peierls bound. These contours (as in Pirogov–Sinai) are defined as regions which collect close-by deviations from the ground states. The Peierls bound follows from the fact that the excess energy of the associated interfaces is bounded from below proportionally to the size of the region to a positive power. To illustrate this point consider the simple case of three contiguous intervals B^-, A, and B^+. Let A be of size L and $B^\pm$ of size larger or equal to L and call $\mathcal{C}$ the set of configurations so that $\sigma=+1$ for all sites belonging to A and $\sigma=-1$ for all sites belonging to $B^\pm$. An explicit calculation, see Appendix A, shows that for all configurations in $\mathcal{C}$ the variation of energy obtained by flipping the spins inside A (thus getting all spins equal to $+1$ in $A \sqcup B^+ \sqcup B^-$) is bounded from below by $\zeta_\alpha L^\alpha$, with $\zeta_\alpha > 0$ for $\alpha \in (0,1/2]$ and if $J(1)$ is large enough.

In Sec. II we give a graphical description of a spin configuration in terms of a configuration of triangles, which allows to introduce the notion of internal and external interfaces (like in $d > 1$ dimensions), see Fig. 1 in Sec. II.

In Sec. III we introduce the notion of contours as clusters of nearby triangles and prove Peierls bounds for their energy. Our definition is very similar to that in Ref. 8, but our aim is to get a geometric representation of the contours more explicit and better suited for further generalizations.

In Sec. IV we prove that for β large enough the Peierls estimates on the energy of contours enable to control their entropy.

The approach we use can be generalized to a larger class of long range attractive forces where the assumption $J(1) \gg 1$ is dropped and $\alpha \in (0,1)$. We will discuss this point in a forthcoming paper together with a characterization of the typical configurations for slow decreasing ferromagnetic Kac potentials. As mentioned the ultimate goal is the extension to a one-dimensional system of hard-core particles interacting via such long range attractive forces, but at the moment we do not have concrete results in this direction.

II. SPIN AND TRIANGLE CONFIGURATIONS

We will consider in this paper homogeneous boundary conditions, i.e., the spins in the boundary conditions are either all $+1$ or all -1. By the spin–flip symmetry, we may and will restrict to the former, so that we will only study configurations $\sigma=\{\sigma_x, x \in \mathbb{Z}\} \in \mathcal{X}_+$, namely such that σ_x

$=1$ for all $|x|$ large enough. Our aim here is to recover a picture as in $d>1$, where the configurations are described by a collection of interfaces. In one dimensions, an interface at $(x,x+1)$ means $\sigma_x\sigma_{x+1}=-1$. The precise location of the interface in the interval is immaterial and we will use it to our advantage by choosing a point in each interval $(x+1/2)\pm\delta(\delta\in(0,1/4))$, $x\in\mathbb{Z}$, with the property that for any four distinct points r_i, $i=1,\ldots,4$, $|r_1-r_2|\neq|r_3-r_4|$. We suppose the choice done once for all, so that hereafter an interface point between x and $x+1$ is uniquely fixed. This will avoid ambiguities in the construction that follows.

Any interface point, by its definition, represents a change of phase so that after the first interface point (coming from the left), the second one corresponds to a reestablishing of the original phase, and so on. However, this is not the most convenient way to look at the spin configurations. Our construction is similar to that in Ref. 8 (where interface points were called spin–flip points) and it is based on suitably coupling together pairs of interface points. To this end we will use the criterion of minimal distance, which will be made geometrically intuitive by using a graphical representation where each spin configuration is mapped into a set of triangles. The endpoints of the triangles will be the pairs of coupled interface points.

Due to the above choice of the boundary conditions, any $\sigma\in\mathcal{X}_+$ has a finite, even number of interface points. We then let each interface point evolve into two trajectories represented in the (r,t) plane by the two lines $r\pm t$, $t\geqslant 0$. We have thus a bunch of growing v-lines each one emanating from an interface point. Once two v-lines meet, they are frozen and stop their growth, while the others are undisturbed and keep growing. Our choice of the location of the interface points ensure that collisions occur one at a time so that the above definition is unambiguous.

The collision of two points is represented graphically in the (r,t) plane by a triangle whose basis is the line joining the two interface points and whose sides are the two arms of the v-lines which enter into contact at the time of collision. Triangles will be usually denoted by T and we will write

$$|T| = \text{cardinality of } T\sqcap\mathbb{Z}, \quad \text{dist}(T,T') = \text{cardinality of } I\sqcap\mathbb{Z}, \tag{2.1}$$

where I is the interval between T and T' if T and T' are disjoint; if T and T' are one contained in the other (no other possibility may arise in the above construction) then I denotes the minimal interval between the two.

We have thus represented a configuration $\sigma\in\mathcal{X}_+$ as a collection $\underline{T}=(T_1,\ldots,T_n)$ of triangles in the (r,t) plane. The set of configurations of triangles obtained in this way are denoted by $\{\underline{T}\}$, and the above construction defines a one-to-one map from $\mathcal{X}_+$ onto $\{\underline{T}\}$. It is easy to see that a triangle configuration $\underline{T}$ belongs to $\{\underline{T}\}$ iff for any pair T and T' in $\underline{T}$,

$$\text{dist}(T,T')\geqslant\min\{|T|,|T'|\}. \tag{2.2}$$

The two endpoints of a triangle play the role which has the interface in higher dimensions and we thus have, also in $d=1$, a notion of external and internal interfaces (see Fig. 1).

Figure 1 is taken from a model for $d=1$ coarsening, see Derrida,[4] Carr and Pego,[3] and also some old, unpublished notes of two of the present authors (P.F. and E.P.). The general context is "spinodal decomposition," namely the phenomena which occur when an initial unstable state develops into a state where the stable state nucleate into droplets. Coarsening describes the evolution of these droplets where some of them grow to the expenses of the others. In $d=1$ this process is extremely slow and it is often a good approximation to say that in a given sequence of intervals of alternating phases, the shortest one disappears first, while all the others are unchanged. The dynamics is then described in terms of triangles by calling the first interval which disappears as the basis of the smallest triangle and then iterating the procedure. The interesting setup when studying coarsening is to have initially infinitely many phase changes and one of the aims is to understand if and which are the self-similar structures which emerge from the triangles picture. Here our task is simpler, we have finitely many phase changes and want to prove that each one of them has a small Gibbs weight.

Writing

$$H(\underline{T}) = h(\sigma), \quad \sigma \in \mathcal{X}_+ \Leftrightarrow \underline{T} \in \{\underline{T}\}, \tag{2.3}$$

and calling $\underline{T}=(T_1,\dots,T_n)$ with $|T_i| \leqslant |T_{i+1}|$, we have

$$H(\underline{T}) = H(T_1|\underline{T}\setminus T_1) + H(\underline{T}\setminus T_1), \quad H(\underline{S}|\underline{T}) := H(\underline{S}\sqcup\underline{T}) - H(\underline{T}). \tag{2.4}$$

In fact if $\underline{T}\in\{\underline{T}\}$, and $T\in\underline{T}$, then $\underline{T}\setminus T$ obviously satisfies (2.2) and therefore it is in $\{\underline{T}\}$. $\underline{T}\setminus T$ is obtained from the configuration σ corresponding to $\underline{T}$ by flipping all the spins inside the basis of T. By iteration,

$$H(\underline{T}) = \sum_{i=1}^{n} H(T_i|\underline{T}\setminus[T_1\sqcup\cdots\sqcup T_i]). \tag{2.5}$$

Lemma 2.1: *For any i,*

$$H(T_i|\underline{T}\setminus[T_1\sqcup\cdots\sqcup T_i]) \geqslant W(|T_i|), \tag{2.6}$$

where

$$W(L) = \sum_{x=1}^{L}\left(\sum_{\substack{y\in[L+1,2L]\\ y\in[-L+1,0]}} J(|x-y|) - \sum_{\substack{y\in[2L+1,\infty]\\ y\in[-\infty,-L]}} J(|x-y|)\right). \tag{2.7}$$

Proof: Call $I_i^{\pm}$ the two intervals in $\mathbb{Z}$ which are to the right and to the left of T_i, each one consisting of $|T_i|$ sites. There is no interface point inside T_i, and inside $I_i^{\pm}$ as well, because $|T_i|$ is the minimal length in $\underline{T}\setminus[T_1\sqcup\cdots\sqcup T_{i-1}]$ and all T_j, $j>i$, have distance from T_i which is $\geqslant|T_i|$. Then, if σ corresponds to $\underline{T}\setminus[T_1\sqcup\cdots\sqcup T_{i-1}]$, the spins in $T_i\sqcap\mathbb{Z}$ are all equal to each other and opposite to those in $I_i^{\pm}$. Instead, in the configuration σ' which corresponds to $\underline{T}\setminus[T_1\sqcup\cdots\sqcup T_i]$, the spins are all the same in $(T_i\sqcap\mathbb{Z})\sqcup I_i^{+}\sqcup I_i^{-}$. By (2.4), $H(T_i|\underline{T}\setminus[T_1\sqcup\cdots\sqcup T_i]) = h(\sigma)-h(\sigma')$, so that (2.6) and the lemma are proved. □

In Lemma A.1 it is proved that for $J(1)$ large enough, there is $\zeta>0$ so that

$$W(L) \geqslant \zeta h_\alpha(L) \quad \text{where } h_\alpha(L) := \begin{cases} L^\alpha, & \alpha\in(0,1/2],\\ \ln L + 4, & \alpha = 0 \end{cases} \tag{2.8}$$

in the sequel we fix our attention on the case $\alpha\in(0,1/2]$, and discuss the case $\alpha=0$ in Appendixes A, E, and F. Thus

$$H(\underline{T}) \geqslant \zeta\sum_{i=1}^{n} |T_i|^\alpha, \quad \underline{T} = (T_1,\dots,T_n). \tag{2.9}$$

The inequality must be seen as an analogue of the Peierls estimate in $d>1$ where the excess energy of a configuration of interfaces is bounded from below proportionally to the surface area of such interfaces. Since $|T_i|$ is the volume surrounded by the interface, α is identified to the ratio $(d-1)/d$, with d an "effective dimension" of the system.

This is however only an analogy. To really implement a Peierls bound in our setup, we need to "localize the estimates," being able to compute the weight of a given triangle in a generic configuration. The previous bound was easy, because we could estimate successively the weights of the triangles in the same order as their lengths. If we want to bound the energy of a generic triangle T in configuration $\underline{T}$, $|T|$ may not be the smallest length so that we are confronted with cases where there are other triangles in $T\sqcup I^+\sqcup I^-$ (see Lemma 2.1 for notation). Indeed, we could add to T smaller triangles T' in $T\sqcup I^+\sqcup I^-$ without violating (2.2). Our approach will be • to "connect" triangles if they are "dangerously close" to each other, • to define contours as "connected clusters" of triangles, and • to compute probabilities of contours rather than of single

triangles. To compute the probability of a contour, we first order increasingly the triangles in the contour, according to their lengths. Then the previous argument can be generalized, exploiting the fact that the triangles which are not in the contour are "sufficiently far away" (by the way contours are defined). In the next section we will see how triangles can be clustered into contours and then extend Lemma 2.1 to contours, thus concluding the analysis of the energy of contours; in Sec. IV we will prove entropy bounds (on the number of contours), which show that for β large enough, energy wins against entropy.

III. CONTOURS AND PEIERLS ESTIMATES

In Sec. III A we will define a function $\mathcal{R}$ which associates to any configuration $\underline{T}\in\{\underline{T}\}$ a configuration $\{\Gamma_j\}$ of contours, each Γ_j being a subset of triangles in $\underline{T}$. The crucial point in the definition is that the triangles in a contour are "close to each other," while all the other triangles are "far away;" using such a property we will be able to extend to contours the energy estimate of the preceding section, thus deriving the Peierls estimates of Sec. III B. In Sec. III C we will recall the classical argument for existence of a phase transition, using the Peierls bound proved in Sec. III B and the entropy estimates which will be proved in Sec. IV.

A. Contours

A contour Γ is a collection $\underline{T}$ of triangles ($\underline{T}$ in this section will always, and sometimes tacitly, denote an element in $\{\underline{T}\}$) joined together by a hierarchical network of connections, under which all the triangles of a contour become mutually connected. The structure has a self-similar property which we will exploit when counting the contours. The coarsest picture of a contour Γ is the pair $\{T(\Gamma),|\Gamma|\}$, $T(\Gamma)$ a triangle, $|\Gamma|$ its mass. $T(\Gamma)$ is the triangle whose basis is the smallest interval which contains all the triangles of the contour, the right and left endpoints of $T(\Gamma)\sqcap\mathbb{Z}$ are denoted by $x_{\pm}(\Gamma)|\Gamma|$, the mass of the contour, is the sum of the masses of all the triangles in Γ, the mass $|T_i|$ of a triangle being defined in (2.1).

Our aim is to define an algorithm $\mathcal{R}(\underline{T})$ on $\{\underline{T}\}$, which associates to any configuration $\underline{T}$ a configuration $\{\Gamma_j\}$ of contours with the following properties.

P.0. *Let* $\mathcal{R}(\underline{T})=(\Gamma_1,\cdots,\Gamma_n)$, $\Gamma_i=\{T_{j,i},1\leqslant j\leqslant k_i\}$, *then* $\underline{T}=\{T_{j,i},1\leqslant i\leqslant n,1\leqslant j\leqslant k_i\}$.

P.1. *Contours are well separated from each other.* Any pair $\Gamma\neq\Gamma'$ in $\mathcal{R}(\underline{T})$ verifies one of the following two alternatives: (i) $T(\Gamma)\sqcap T(\Gamma')=\emptyset$, in which case

$$\operatorname{dist}(\Gamma,\Gamma')>c\min\{|\Gamma|^3,|\Gamma'|^3\}, \tag{3.1}$$

where c is as in (3.15) below and $\operatorname{dist}(\cdot,\cdot)$ means distance as defined in (2.1) between the set of all the triangles in Γ from the corresponding set in Γ',

$$\operatorname{dist}(\Gamma,\Gamma'):=\min_{\substack{T\in\Gamma\\ T'\in\Gamma'}}\operatorname{dist}(T,T')$$

[which in the present case is equal to the distance between the two triangles $T(\Gamma)$ and $T(\Gamma')$].

(ii) $T(\Gamma)\sqcap T(\Gamma')\neq\emptyset$, then either $T(\Gamma)\sqsubset T(\Gamma')$ or $T(\Gamma')\sqsubset T(\Gamma)$; moreover, supposing for instance that the former case is verified (in which case we call Γ an inner contour), then for any triangle $T'_i\in\Gamma'$, either $T(\Gamma)\sqsubset T'_i$ or $T(\Gamma)\sqcap T'_i=\emptyset$; and

$$\operatorname{dist}(\Gamma,\Gamma')>c|\Gamma|^3,\quad \text{if } T(\Gamma)\sqsubset T(\Gamma'). \tag{3.2}$$

P.2. *Independence:* Let $\{\underline{T}^{(1)},\ldots,\underline{T}^{(k)}\}$, be $k>1$ configurations of triangles; $\mathcal{R}(\underline{T}^{(i)})=\{\Gamma_j^{(i)},j=1,\ldots,n_i\}$ the contours of the configuration $\underline{T}^{(i)}$. Then, if any distinct pair $\Gamma_j^{(i)}$ and $\Gamma_{j'}^{(i')}$ satisfies P.1,

$$\mathcal{R}(\underline{T}^{(1)}\ldots,\underline{T}^{(k)})=\{\Gamma_j^{(i)},j=1,\ldots,n_i;i=1,\ldots,k\}. \tag{3.3}$$

It is a nice fact of life that not only P.0, P.1, and P.2 can be actually implemented by some algorithm $\mathcal{R}$, but also that such an algorithm is unique. In Appendix B we will prove the following theorem.

Theorem 3.1: (Existence and uniqueness) *There is a unique algorithm $\mathcal{R}(\underline{T})$ which satisfies P.0, P.1, and P.2.*

B. Peierls estimates

The idea behind the proof of the Peierls estimates, Theorem 3.2 below, is that the property P.1 will ensure that the triangles which do not belong to a contour are so far away that, to leading order, they can be neglected and the bond (2.6) can be extended to contours.

Theorem 3.2: *Let the constant c in the definition of the contours (see P.1) be so large that* (3.15) *below holds. For any $\underline{T}\in\{\underline{T}\}$, let $\Gamma_0\in\mathcal{R}(\underline{T})$, $\underline{T}^{(0)}$ the triangles in Γ_0, $\zeta>0$ as in* (2.8). *Then*

$$H(\underline{T}^{(0)}|\underline{T}/\underline{T}^{(0)}) \leqslant \frac{\zeta}{2}\sum_{T\in\underline{T}^{(0)}}|T|^{\alpha} \tag{3.4}$$

[*for* $\alpha=0$, (3.4) *holds with* $|T|^{\alpha}$ *replaced by* $\log|T|+4$].

Proof: Calling $\underline{T}^{(0)}=(T_1,\dots,T_k)$, $|T_i|\leqslant|T_{i+1}|$, $i=1,\dots,k-1$,

$$H(\underline{T}^{(0)}|\underline{T}\setminus\underline{T}^{(0)}) = \sum_{i=1}^{k} H(T_i|\underline{T}\setminus\{T_1,\dots,T_i\}). \tag{3.5}$$

As a difference with Sec. II, here we may have triangles in $I_i^{\pm}$, but, by the argument after (2.4),

$$(I_i^{+}\sqcup I_i^{-})\sqcap T_j=\emptyset, \quad \text{for all } j>i T_j\not\perp T_i. \tag{3.6}$$

We also have, calling $\{\Gamma_j, j\geqslant 1\}$, the other contours of $\underline{T}$, different from Γ_0,

$$(I_i^{+}\sqcup I_i^{-})\sqcap T=\emptyset, \quad \text{for all } T\in\Gamma_j, \quad T\not\perp T_i, \quad j\geqslant 1 \text{ such that } |\Gamma_j|\geqslant|\Gamma_0| \tag{3.7}$$

because, by property P.1 of Sec. IV, $\operatorname{dist}(T_i,\Gamma_j)\geqslant \operatorname{dist}(\Gamma_0,\Gamma_j)\geqslant c|\Gamma_0|^3\geqslant|T_i|$.

Finally, using again P.1,

$$\operatorname{dist}(T_i,T)>c|\Gamma_j|^3, \quad \text{for all } T\in\Gamma_j, \quad j\geqslant 1 \text{ and such that } |\Gamma_j|<|\Gamma_0|. \tag{3.8}$$

With the notation introduced after (2.6), and with

$$A(T_i;\Gamma_j)=\bigsqcup_{T\in\Gamma_j, T_i\not\perp T} T\sqcap\mathbb{Z}, \quad |\Gamma|=\sum_{T\in\Gamma}|T| \tag{3.9}$$

we claim that

$$H(T_i|\underline{T}\setminus[T_1\sqcup\cdots\sqcup T_i])\geqslant W(|T_i|)-2\sum_{M}\sum_{j=1}^{n}\mathbf{1}_{|\Gamma_j|=M}\sum_{x\in T_i\sqcap\mathbb{Z}}\sum_{y\in I_i^{\pm}}J(|x-y|)(\mathbf{1}_{y\in A(T_i;\Gamma_j)}+\mathbf{1}_{x\in A(T_i;\Gamma_j)}). \tag{3.10}$$

To prove (3.10), we observe that the contribution of σ_x and σ_y [x and y as in (3.10)] is the same as in $W(|T_i|)$ whenever $\sigma_x\sigma_y=-1$; on the other hand, if $\sigma_x=\sigma_y$ then there must exist a triangle distinct from T_i which contains one site and not the other one. We thus automatically exclude the triangles which contain T_i, as, by (2.2), they will also contain $I_i^{\pm}$; by (3.6), $(T_{i+1},\dots,T_k)$ are also excluded. Then (3.10) follows after noticing that if $\sigma_x=\sigma_y$, the pair σ_x,σ_y contributes with the opposite sign to the energy as for $W(|T_i|)$, hence the factor 2 in the second term on the right-hand side (rhs) of (3.10). In (3.10) we have also split the sum over all contours setting together contours with the same mass, the mass of a contour Γ being defined in (3.9).

Call y_0 the rightmost point of $\mathbb{Z}$ in T_i, $y_1 \in I_i^+$ the point, if it exists, separated from y_0 by $[cM^3]$ sites, $[\cdot]$ the integer part of $\cdot$. By (3.7) and (3.8) the following holds: any Γ_j with $|\Gamma_j| = M$ is such that all its triangles which do not contain T_i and are to its right, have their left endpoint to the right of y_1. After changing labels, let Γ_1 be the contour of mass M with the closest triangle to y_1 (and to its right). The triangles in Γ_j, $j>1$, with mass M, cannot be closer than $y_2 \in I_i^+$, where y_2 (if it exists) is separated from y_1 by $[cM^3]$ sites. By iteration we define y_j, $j>2$, and have that the nth closest contour to T_i of mass M and to its right, is to the right of y_j. Calling y_n the last of such points in I_i^+, we have, for any $x \in T_i$,

$$\sum_{j=1}^{n} \mathbf{1}_{|\Gamma_j|=M} \sum_{y \in I_i^+} J(|x-y|) \mathbf{1}_{y \in A(T;\Gamma_j)} \leqslant M \sum_{k=1}^{n} J(|x-y_k|) \tag{3.11}$$

because $J(|x-y|) = J(y-x)$ is a decreasing function of y and the total number of sites in the triangles of a contour Γ is not larger than $|\Gamma|$ (not necessarily equal because a triangle might be contained in another one). Moreover, by monotonicity,

$$J(|x-y_k|) \leqslant \frac{1}{[cM^3]} \sum_{y \in (y_{k-1}, y_k)} J(|x-y|) \tag{3.12}$$

so that

$$\sum_{j=1}^{n} \mathbf{1}_{|\Gamma_j|=M} \sum_{y \in I_i^+} J(|x-y|) \mathbf{1}_{y \in A(T;\Gamma_j)} \leqslant \frac{M}{[cM^3]} \sum_{y \in I_i^+} J(|x-y|). \tag{3.13}$$

The sum is the same as in $W(|T_i|)$. Repeating the same procedure for T_i and I_i^- we finally get

$$H(T_i | \underline{T} \setminus [T_1 \sqcup \cdots \sqcup T_i]) \geqslant W(|T_i|) \left(1 - \sum_M \frac{4M}{[cM^3]} \right). \tag{3.14}$$

By choosing c so large that

$$\sum_M \frac{4M}{[cM^3]} \geqslant \frac{1}{2} \tag{3.15}$$

and recalling (2.8) we then prove the theorem. □

C. Phase transitions

To prove phase transitions we follow the well-known argument for $d>1$. Let Λ be an interval containing the origin, μ_Λ^+ the Gibbs measure in Λ with $+$ boundary conditions. Then

$$\mu_\Lambda^+(\sigma_0 = -1) \leqslant \mu_\Lambda^+(\{0 \in \Gamma\}), \tag{3.16}$$

where $\{0 \in \Gamma\}$ denotes the event that there is a contour Γ which has a triangle T which contains the origin. Then

$$\mu_\Lambda^+(\{0 \in \Gamma\}) = \frac{1}{Z_\Lambda^+} \sum_{\Gamma \ni 0} \sum_{\underline{T}: \Gamma \in \mathcal{R}(\underline{T})} e^{-\beta H(\underline{T})}.$$

Calling $\underline{T}^{(0)}$ the collection of triangles in Γ, $\mathcal{R}(\underline{T}^{(0)}) = \Gamma$, by Theorem 3.2,

$$e^{-\beta H(\underline{T})} \leqslant e^{-\beta H(\underline{T} \setminus \underline{T}^{(0)})} w_{\zeta\beta/2}(\Gamma), \tag{3.17}$$

where, for $b>0$,

$$w_b(\Gamma) := \prod_{T\in\Gamma} e^{-b|T|^\alpha}, \tag{3.18}$$

$w_b(\Gamma)$ is called the b-weight of the contour Γ. Then, using (3.17),

$$\mu_\Lambda^+(\{0\in\Gamma\}) \leqslant \sum_{\Gamma\ni 0} w_{\zeta\beta/2}(\Gamma) = \sum_m \sum_{\Gamma:|\Gamma|=m,0\in\Gamma} w_{\zeta\beta/2}(\Gamma) \tag{3.19}$$

and, by (4.1) below, valid for β large enough,

$$\mu_\Lambda^+(\{0\in\Gamma\}) \leqslant 2\sum_m m e^{-\zeta\beta m^\alpha/2}. \tag{3.20}$$

Since the sum starts from $m\geqslant 1$, the right-hand side (rhs) is $<1/2$ if β is large enough, hence the spin–flip symmetry is broken and there is a phase transition.

IV. ENTROPY OF CONTOURS

The main result in this section is Theorem 4.1 below, where we prove (3.20), and hence that, for β large, entropy is controlled by energy and a phase transition occurs.

Theorem 4.1: *For any b large enough and any* $m>0$,

$$\sum_{\Gamma:|\Gamma|=m,0\in\Gamma} w_b(\Gamma) \leqslant 2me^{-bm^\alpha}, \tag{4.1}$$

where $w_b(\Gamma)$ has been defined in (3.18).

The theorem is proved in Secs. IV C, by exploiting a self-similarity property of the contours which is the argument of the next two sections.

A. An auxiliary branching process

Contours can be described in terms of trees with a self-similar, hierarchical structure. We will first describe abstractly the trees and then relate them to the contours.

The nodes of the tree are "individuals" of two species, heavy triangles, h-triangles in short, and spheres; the h-triangles can be either black or white. Only black triangles can procreate and their offsprings contain at least two h-triangles. The offsprings in a branching are ordered, the h-triangles are drawn sequentially, the spheres, also drawn sequentially, can lie in each one of the intervals in between two consecutive h-triangles, but also "inside" the white triangles, the latter will be called "attached" to the white triangle in which they are contained.

Finally the tree has a root which consists either of a single black triangle or of a single white triangle with possibly spheres inside the white triangle. In the second alternative the tree consists of only its root, as white triangles and spheres cannot procreate. An example of tree is drawn in Fig. 2.

We will construct an algorithm which associates to any contour a tree with the above properties and later use such a correspondence to prove (4.1). We will in fact organize the sum over contours in (4.1) by summing over trees after having summed over all contours which produce the same tree. The identification of the nodes of the tree in terms of contours will allow for an inductive procedure which greatly reduces the complexity of the computation. We describe here the main features of the algorithm, which are those used in the proof of (4.1), while the existence of the algorithm itself will be proved in Sec. IV B, by exploiting a graphical representation of contours.

We will restrict in the sequel to configurations $\underline{T}$ such that $\mathcal{R}(\underline{T})$ is a singleton. As mentioned, the basic property of the algorithm which associates a tree to $\underline{T}$, is that each node of the tree is representative of a subset $\underline{T}'$ of $\underline{T}$ such that $\mathcal{R}(\underline{T}')$ is a singleton.

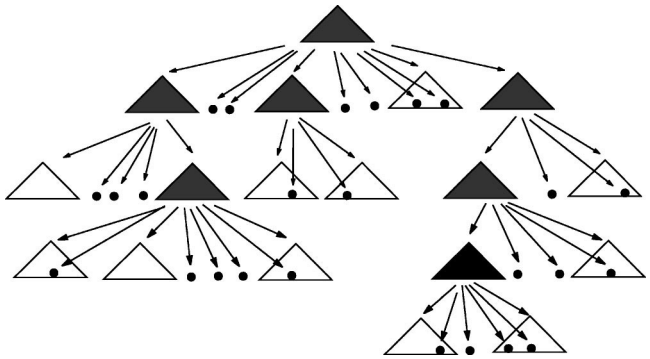

FIG. 2. Example of tree.

The root corresponds to the full $\underline{T}$. Moreover the collection of all the triangles associated to all the individuals of an offspring is the same as the set of triangles associated to the parent, so that a branching is nothing else than a partition of the triangles present in the branching node. In particular mass is conserved in a branching.

White triangles are associated to contours consisting of a single triangle, such triangle must be maximal, i.e., not contained in any other triangle of $\underline{T}$. Take notice, however, that the converse may not be true, as it may happen that a maximal triangle is one of the triangles associated to a black triangle or a sphere. If a maximal triangle T corresponds to a white triangle, then the spheres in the white triangle are associated to the contours of the configuration $\underline{T}'$ made of all the triangles of $\underline{T}$ which are contained in T.

The next properties we mention establish a quantitative relation between the ordering of the offsprings in the tree and the location of the corresponding triangles. If a black triangle generates $n \geqslant 2$ h-triangles labeled consecutively, call Γ_i, $1 \leqslant i \leqslant n$, the triangle associated to the ith h-triangle (by itself each Γ_i is a contour, hence the notation). Then the triangles $\{T(\Gamma_i)\}$ [recall that $T(\Gamma)$ is the minimal triangle which contains all the triangles forming Γ] are consecutive from left to right and

$$\operatorname{dist}(T(\Gamma_i), T(\Gamma_{i+1})) \leqslant c \min\{|\Gamma_i|^3, |\Gamma_{i+1}|^3\}, \quad i = 1, \ldots, n-1. \tag{4.2}$$

Moreover, if there are k_i spheres between the ith and $(i+1)$th h-triangle, call $\Gamma_j^{(i)}$, $j = 1, \ldots, k_i$, the contours associated to these spheres. Then all $T(\Gamma_j^{(i)})$ are in between $T(\Gamma_i)$ and $T(\Gamma_{i+1})$, $\{T(\Gamma_j^{(i)})\}$ is sequential and the following constraint on their mutual distances holds. Letting $x_\pm(\Gamma)$ as in the beginning of Sec. III A, the set of endpoints $\{x_\pm(\Gamma_j^{(i)}), a = x_+(\Gamma_i), b = x_-(\Gamma_{i+1})\}$ is such that there is p_i, $0 \leqslant p_i \leqslant k_i$ so that

$$0 \leqslant x_-(\Gamma_1^{(i)}) - a \leqslant c|\Gamma_1^{(i)}|^3 + 1,$$

$$0 \leqslant x_-(\Gamma_2^{(i)}) - x_+(\Gamma_1^{(i)}) \leqslant c|\Gamma_2^{(i)}|^3 + 1, \ldots, \ldots, x_-(\Gamma_{p_i}^{(i)}) - x_+(\Gamma_{p_i-1}^{(i)}) \leqslant c|\Gamma_{p_i}^{(i)}|^3 + 1,$$

$$0 \leqslant b - x_+(\Gamma_{k_i}^{(i)}) \leqslant c|\Gamma_{k_i}^{(i)}|^3 + 1,$$

$$0 \leqslant x_+(\Gamma_{k_i}^{(i)}) - x_-(\Gamma_{k_i-1}^{(i)}) \leqslant c|\Gamma_{k_i-1}^{(i)}|^3 + 1, \ldots, \ldots, x_+(\Gamma_{p_i+1}^{(i)}) - x_-(\Gamma_{p_i+2}^{(i)}) \leqslant c|\Gamma_{p_i+1}^{(i)}|^3 + 1. \tag{4.3}$$

Finally if Γ_j, $j = 1, \ldots, k$, are the sets of triangles associated to the spheres inside a white triangle, represented by T, then the triangles $T(\Gamma_j)$ satisfy the analogue of (4.3) with $a = x_-(T) + 1$ and $b = x_+(T) - 1$. These are the only properties on the structure of contours that we will use in the proof of (4.1) in Sec. IV C, the next section is only an existence proof of the algorithm for associating

a tree to a contour with the properties we have been describing so far, and, to a first reading, it may be skipped.

B. Graphical construction

We will construct here an algorithm which associates a tree (with the properties described in the preceding section) to any $\underline{T}$ such that $\mathcal{R}(\underline{T})$ is a single contour. The algorithm is obtained via a graphical representation of $\underline{T}$, where we draw at any integer time $t \in \{0,1,\ldots\}$ a configuration of mutually disjoint squares with a side in $\mathbb{R}$, called the basis of the square. Each square S is representative of a cluster $\{\underline{T}\}_S$ of triangles in $\underline{T}$, with the property that $\mathcal{R}(\{\underline{T}\}_S)$ is a singleton; the name "squares" is just to avoid confusion with the original triangles and the h-triangles of the tree. The mass of a square S equals the sum of the masses of the triangles in $\{\underline{T}\}_S$ (the mass of a triangle being the number of integers contained in its basis). The configurations of squares at the different times will be viewed as the successive applications of a renormalization group transformation.

1. The time $t=0$ configuration

This is obtained by associating to each "maximal" triangle of $\underline{T}$ a square with the same basis, $T \in \underline{T}$ is maximal if it is not contained in any other triangle of $\underline{T}$. By definition of maximality the set of maximal triangles, hence of squares, is sequential. The cluster of triangles $\{\underline{T}\}_S$ represented by the square S consists of a maximal triangle T and of all the triangles contained in T. The mass of S, according to the general rule, is then the sum of all the masses in $\{\underline{T}\}_S$. Statement (ii) in Lemma 4.2 below, proves that these squares verify the property that the sets $\{\underline{T}\}_S$ form a single contour, thus our definition of the square configuration at $t=0$ is well posed. In Appendix C we will prove the following.

Lemma 4.2: *Let S be a square corresponding to a maximal triangle T. Then (i) $\mathcal{R}(\{\underline{T}\}_S \setminus T) = \{\Gamma_j\}$ is sequential and the sequence $\{T(\Gamma_j)\}$ satisfies the analogue of* (4.3) *with $a = x_-(T)$ and $b = x_+(T)$; moreover, (ii) $\mathcal{R}(\{\underline{T}\}_S)$ consists of a single contour.*

By (i) the sequence $\{T(\Gamma_j)\}$ satisfies the same properties as the sequence of triangles obtained from the spheres attached to a white triangle, as described in the preceding section. Together with (ii), this shows that each one of the squares at time $t=0$ is a candidate for being a white triangle. Whether this will really happen, does depend in a complex way on the relative positions of the other triangles of $\underline{T}$, as we will see after completing the construction of the square process.

2. The next time-step configuration

The construction of the configuration of squares at time $t=n+1$ only depends on the configuration at time $t=n$, namely on the location of the squares in the configuration and on their masses. Like at time $t=0$, each square S is representative of a collection $\{\underline{T}\}_S$ of triangles in $\underline{T}$, more and more complex as time increases, but, as said, the construction of the configurations at the successive time will only depend on locations and masses of the squares, the latter being the sum of all the masses of the triangles represented. The rule for constructing the configuration at time $t=n+1$ given the one at time $t=n$, defines the action of the renormalization group transformation mentioned at the beginning of this section.

We start by drawing oriented arrows between pairs of squares, we set an arrow (S,S') from S to S' if $|S| \leqslant |S'|$, $|S|$ the mass of the square S (in case of equality if S is before S', going from left to right) and if the distance between S and S' is $\leqslant c|S|^3$. Arrows define a connection, which will be referred to as a-connection (a represents arrow), to distinguish it from the connection used in the definition of contours. Two squares are a-connected if they can be joined via a chain of pairs of squares, each pair linked by an arrow (independently of the direction of the arrow).

To each a-connected component we associate a protosquare, which is the minimal square which contains all the squares in that component, we call them protosquares because some of the protosquares will become a square in the configuration at time $t=n+1$. We will prove below that any two such protosquares are either disjoint or one contained in the other. We call maximal those which are not contained in any other one. *The maximal protosquares are the squares at time*

$t=n+1$. The set $\{\underline{T}\}_S$ represented by a maximal protosquare S, is the collection of all $\{\underline{T}\}_{S'}$, with S' running over all the squares at time $t=n$ which are contained in S. By maximality the new squares at time $t=n+1$ are sequential. In Lemma C.2, we will prove that $\mathcal{R}(\{\underline{T}\}_S)$ consists of a single contour, thus legitimating the present definition of the square configuration at time $t=n+1$.

We next state some features of the construction needed later for the identification of a tree structure. To this end it is convenient to erase some arrows, thus we will call "old arrows" the arrows defined so far and (old a)-connected squares connected by old arrows. Old arrows are erased with the following rule: if there are several arrows emanating from the same square, all in the same direction (i.e., right or left), we keep only the minimal one and erase all the others. This is done for all squares and all directions. The arrows which are left are the new arrows, and we will call (new a)-connected, squares connected by the new arrows. In Lemma D.1, it is proved that a set is (new a)-connected iff it is (old a)-connected. We will hereafter in this section call arrows the new arrows and a-connected, (new a)-connected sets.

The "*shadow*" of the arrow (S,S') is the interval between the two endpoints of S and S' which face each other. If two shadows have nonempty intersection, they must be one contained in the other, Lemma D.2; such a statement proves the above property about the fact that the protosquares are either disjoint or one contained in the other.

We then call *primary* an arrow with maximal shadow, i.e., which is not contained in any other shadow, and *primary* the two squares connected by a *primary* arrow. The set $\{\underline{T}'\}$ of all triangles in $\underline{T}$ whose basis are contained in the shadow (a,b) of a primary arrow (S_1,S_2) is such that we have the following.

Lemma 4.3: *With the above notation, (i)* $\mathcal{R}(\underline{T}')=\{\Gamma_j\}$ *and* $\{T(\Gamma_j)\}$ *is a sequence which satisfies the analogue of* (4.3) *with* $a=x_+(S_1)$ *and* $b=x_-(S_2)$ *supposing for instance that* S_1 *is before* S_2*; moreover, (ii)* $\mathcal{R}(\underline{T}'')$ *consists of a single contour,* $\underline{T}''$ *being the union of all triangles in* $\underline{T}'$ *and those associated to* S_1 *and* S_2.

Lemma 4.3 is proved in Appendix C. The primary squares may thus become h-triangles, as they form a sequence which satisfy (4.2), while all the squares in a shadow, called *secondary*, are eligible for being the spheres which lie between two h-triangles in the tree.

We finally observe that after a finite number of iterations the process stabilizes, the final configuration consisting of a single square S, $\{\underline{T}\}_S=\underline{T}$, its mass therefore being the sum of all $|T|$ over $\underline{T}$; the basis of S is $T(\Gamma)$, the triangle representative of the contour $\Gamma=\mathcal{R}(\underline{T})$. Any other final state would in fact contradict the assumption that $\mathcal{R}(\underline{T})$ consists of a single contour.

3. The tree structure

We have constructed so far, for any contour, a process, called the square process, evolving at integer times, whose state space is a square configuration, each square with its own mass. The evolution consists of a clustering mechanism, for which a cluster of squares at time t becomes a single square at time $t+1$. We have also distinguished in a forming cluster some squares which are primary, the others being called secondary. Our purpose now is to identify a tree structure from $\underline{T}$ via the realization of the square process. To this end, let t_f be the first time when the final configuration, consisting of a single square, is reached. This is identified to the root of the tree we are going to construct. If $t_f=0$ the root is a white triangle, otherwise it is black. In the former case, the configuration at time 0 has only one square, S, which, recalling the definition, means that there is a unique maximal triangle, T, in $\underline{T}$, and S has the same basis as T. The spheres attached to the white triangle root of the tree, are identified to the contours $\mathcal{R}(\underline{T}\backslash T)$, by Lemma 4.2 such an identification respects the requests of Sec. IV A. Notice that the identification of the spheres attached to a white triangle requires the knowledge of $\underline{T}$ and cannot be read only from the square process, which, as we will see, only identifies white and black triangles and spheres between h-triangles, all with their masses, but it does not give any information on the structure of the spheres inside the white triangles, except for their masses.

If $t_f>0$, the root is a black triangle and its offspring is the configuration at time t_f-1, identifying primary squares with h-triangles and secondary squares with spheres, consistently with the properties of such objects, by Lemma 4.3. Let S be one of the primary squares and $t_S<t_f$

-1 the time in the square process when there is a cluster of more than one square which at time t_S+1 becomes S; if such a time does not exist, then S was present also at time 0, and it is identified to a white triangle with the same procedure as above. Otherwise S is identified to a black triangle, whose offspring is determined by the configuration of squares at time t_S which merge into S at time t_S+1, with the same rules as those described for the branching of the root. By iterating the procedure we complete the identification of the tree.

C. Proof of Theorem 4.1

Since the number of translates of a contour with the property $0\in\Gamma$, is bounded by $|\Gamma|$, the proof of Theorem 4.1 reduces to proving that for any $b>0$ large enough and any $m>0$,

$$G_m := \sum_{\Gamma:|\Gamma|=m,x_-(\Gamma)=0} w_b(\Gamma) \leqslant 2e^{-bm^\alpha}. \tag{4.4}$$

The proof is by induction on the mass m of the contour, recall that the mass of a contour is necessarily an integer. We thus suppose (4.4) proved whenever $m\leqslant M-1$ and want to prove it for M. We have

$$G_M = G'_M + G''_M, \tag{4.5}$$

$$G'_M = \sum_{\substack{|\Gamma|=M,x_-(\Gamma)=0\\ \text{root of } \Gamma \text{ is white}}} w_b(\Gamma), \quad G''_M = \sum_{\substack{|\Gamma|=M,x_-(\Gamma)=0\\ \text{root of } \Gamma \text{ is black}}} w_b(\Gamma). \tag{4.6}$$

We start by bounding G'_M. We call $\ell=|T(\Gamma)|$, n the number of contours (spheres) attached to the white triangle; $m_1,\dots,m_n$ their masses. These variables are not independent, as, for instance, we must have $m_1+\cdots+m_n+\ell=M$. We organize the sum in (4.6) by fixing ℓ, n, $m_1,\dots,m_n$, then summing over all the contours compatible with such specifications and with (4.3) and finally summing over the specifications ℓ, n, $m_1,\dots,m_n$.

Let $\Gamma_1,\dots,\Gamma_n$ be n contours whose masses are $m_1,\dots,m_n$ and all with $x_-(\Gamma_i)=0$. We call $X_n(\ell,\Gamma_1,\dots,\Gamma_n)$ the set of all $(x_1,\dots,x_n)$ such that the collection $\{S_{x_i}(\Gamma_i)\}$, S_x denoting translation by x, fulfills (4.3) with $a=0$, $b=\ell$, and $k_i=n$. We then have

$$G'_M \leqslant \sum_{\ell>0} e^{-b\ell^\alpha} \sum_{n\geqslant 0} \sum_{\substack{m_1,\dots,m_n\\ m_1+m_2+\cdots+m_n+\ell=M}} \sum_{\substack{\Gamma_1,\dots,\Gamma_n\\ |\Gamma_i|=m_i,x_-(\Gamma_i)=0}} |X_n(\ell,\Gamma_1,\dots,\Gamma_n)| \prod_{i=1}^n w_b(\Gamma_i).$$

Writing $[a\wedge b] := \min\{a,b\}$, we have

$$|X_n(\ell,\Gamma_1,\dots,\Gamma_n)| \leqslant (n+1)\prod_{i=1}^n [cm_i^3 \wedge \ell\,],$$

where $n+1$ counts the number of values that p_i can take when $k_i=n$ in (4.3). Using the induction assumption we then get

$$G'_M \leqslant \sum_{\ell>0}\sum_{n\geqslant 0} \sum_{\substack{m_1,\dots,m_n\\ m_1+m_2+\cdots+m_n+\ell=M}} 2^n e^{-b(\ell^\alpha+m_1^\alpha+\cdots+m_n^\alpha)}(n+1)\prod_{i=1}^n [cm_i^3\wedge\ell].$$

To select the maximal among all masses, we rewrite the above as

$$G'_M \leqslant \sum_{\ell>0}\sum_{n\geqslant 0} 2^n(n+1) \sum_{\substack{m_1,\dots,m_n \\ m_1+m_2+\cdots+m_n+\ell=M}} e^{-b(\ell^\alpha+m_1^\alpha+\cdots+m_n^\alpha)}\prod_{i=1}^{n}[cm_i^3\wedge\ell]\times\Big[\mathbf{1}_{\{\ell\geqslant m_i\forall i\}}+\mathbf{1}\begin{Bmatrix} m_1\geqslant m_i\forall i\neq 1 \\ m_1\geqslant\ell\end{Bmatrix}$$
$$+\cdots+\mathbf{1}\begin{Bmatrix} m_n\geqslant m_i\forall i\neq n \\ m_n\geqslant\ell\end{Bmatrix}\Big]. \tag{4.7}$$

In the term where the maximum is m_i, we bound $[cm_i^3\wedge\ell]=\ell\leqslant c\ell^3$ and get

$$G'_M \leqslant \sum_{n\geqslant 0} 2^n(n+1)^2 \sum_{\substack{x_1+\cdots+x_n+y=M \\ 0\leqslant x_i\leqslant y}} e^{-by^\alpha}\prod_{i=1}^{n}[e^{-bx_i^\alpha}(cx_i^3)] \leqslant \sum_{n\geqslant 0}(n$$
$$+1)^2(2c)^n \sum_{\substack{x_1+\cdots+x_n+y=M \\ 0\leqslant x_i\leqslant y}} e^{-by^\alpha+\sum_i^n (b-a)x_i^\alpha}\prod_{i=1}^{n}[e^{-ax_i^\alpha}x_i^3]. \tag{4.8}$$

By Lemma E.1, if b/a is large enough,

$$\exp\left\{-by^\alpha+\sum_i^n (b-a)x_i^\alpha\right\} \leqslant \exp\{-b[y+x_1+\cdots+x_n]^\alpha\}, \tag{4.9}$$

so that

$$G'_M \leqslant e^{-bM^\alpha}\sum_{n>0}(n+1)^2(2c)^n\Big(\sum_x e^{-ax^\alpha}x^3\Big)^n.$$

Calling $\delta(a)$ the sum in the last parentheses and noticing that $\delta(a)\to 0$ as $a\to\infty$, for a large enough,

$$G'_M \leqslant e^{-bM^\alpha}\Big(1+\sum_{n\geqslant 1}(n+1)^2(2c)^n[\delta(a)]^n\Big) \leqslant \frac{3}{2}e^{-bM^\alpha}.$$

Bound on G''_M: We now call $n\geqslant 2$ the number of (black and white) triangles generated by the root, m_i their masses. We fix all the contours with such specifications and sum over the spheres between two consecutive triangles. Denote by $k_i\geqslant 0$ the number of spheres between the ith and $(i+1)$th triangles, m_j^i their masses. The space interval where such spheres can be located is determined by the position of the triangles i and $i+1$, by (4.2) its length is bounded by $cm_{i,i+1}^3$, where $m_{i,i+1}:=[m_i\wedge m_{i+1}]$. Then the sum over the spheres, once their number and masses are fixed, is bounded as in (4.7). We can also sum over all possible realizations of the n black and white triangles, given their number and masses using (4.2) and the induction assumption. We then get (with an extra 2^n factor counting the number of ways to color, either black or white, the n triangles)

$$G''_M \leqslant \sum_{n\geqslant 2} 2^n \sum_{\substack{m_1,\dots,m_n \\ m_i>0}} \Big\{\prod_{i=1}^{n-1} cm_{i,i+1}^3\Big\}\Big\{\prod_{i=1}^{n}[2e^{-bm_i^\alpha}]\Big\}\times\sum_{k_1\geqslant 0}\sum_{\substack{m_1^1\dots,m_{k_1}^1 \\ m_j^1>0}}\Big\{(k_1+1)\prod_{j=1}^{k_1} c[(m_j^1)^3\wedge m_{1,2}^3]\Big\}$$
$$\times\Big\{\prod_{j=1}^{k_1}[2e^{-b(m_j^1)^\alpha}]\Big\}\times\cdots\sum_{k_{n-1}\geqslant 0}\sum_{\substack{m_1^{n-1}\cdots m_{k_1}^{n-1} \\ m_j^{n-1}>0}}\Big\{(k_{n-1}+1)\prod_{j=1}^{k_{n-1}} c[(m_j^{n-1})^3\wedge m_{n-1,n}^3]\Big\}$$
$$\times\Big\{\prod_{j=1}^{k_{n-1}}[2e^{-b(m_j^{k_{n-1}})^\alpha}]\Big\}\mathbf{1}_{\{\sum_i m_i+\sum_{k,l} m_k^l=M\}}.$$

We fix $n,k_1,\dots,k_{n-1}$ and sum over all masses. As in (4.8) we split the sum by fixing which one of the masses is larger. This will give a factor $(n+k_1+\cdots+k_{n-1})$ equal to the number of masses which are present. Except for the largest mass we write the generic factor $e^{-bm^\alpha}=e^{-(b-a)m^\alpha}e^{-am^\alpha}$. In order to apply Lemma E.1 and get the analogue of (4.9), we must check that there is not a term with the maximal mass to the cube. If the maximal is one of the masses m_i, then it does not appear because we have products of $m^3_{i,i+1}$ which automatically select the smaller and avoid the larger. If the maximal mass is one of those relative to spheres, say m^i_j, we use the same trick as for G'_M and bound $[(m^i_j)^3\wedge m^3_{i,i+1}]\leqslant m^3_{i,i+1}$, so that the term $(m^i_j)^3$ does not appear. Notice that in this way there could be factors $m^6_{i,i+1}$. We then get

$$\leqslant e^{-bM^\alpha}\sum_{n\geqslant 2}2^n\sum_{k_1\geqslant 0,\dots,k_{n-1}\geqslant 0}(n+k_1+\cdots+k_{n-1})(k_1+1)\times\cdots(k_{n-1}+1)$$
$$\times\left(\sum_{x\geqslant 1}e^{-ax^\alpha}(2c)x^6\right)^{(n-1+k_1+\cdots+k_{n-1})},$$

calling $\delta=\Sigma_{x\geqslant 1}e^{-ax^\alpha}(2c)x^6$,

$$\leqslant e^{-bM^\alpha}\sum_{n\geqslant 2}2^n\delta^{n-1}\sum_{k_1\geqslant 0}\delta^{k_1}(k_1+1)\cdots\sum_{k_{n-1}\geqslant 0}\delta^{k_{n-1}}\times(k_{n-1}+1)(n+k_1+\cdots+k_{n-1}).$$

Since $(n+k_1+\cdots+k_{n-1})=[(k_1+1)+\cdots+(k_{n-1}+1)+1]\leqslant 2[(k_1+1)+\cdots+(k_{n-1}+1)]$,

$$\leqslant e^{-bM^\alpha}\sum_{n\geqslant 2}2^n\delta^{n-1}2n\left(\sum_{k\geqslant 0}\delta^k(k+1)^2\right)^n$$

$$\leqslant e^{-bM^\alpha}\sum_{n\geqslant 2}\delta^{n-1}2^{2n+1}n\leqslant\frac{e^{-bM^\alpha}}{2}$$

because for a large enough

$$\sum_{k\geqslant 0}\delta^k(k+1)^2\leqslant 2,\quad \sum_{n\geqslant 2}\delta^{n-1}2^{2n+1}n\leqslant 1/2.$$

We have thus proved that

$$G_M=G'_M+G''_M\leqslant\left(\tfrac{3}{2}+\tfrac{1}{2}\right)e^{-bM^\alpha},$$

hence (4.4) and Theorem 4.1 are proved.

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APPENDIX A

In this appendix we will prove (2.8) identifying the value of the parameter ζ. We set

$$\zeta_\alpha:=1-2(2^\alpha-1)>0,\quad 0<\alpha<\alpha_+:=\frac{\ln 3}{\ln 2}-1 \tag{A1}$$

observing that $\alpha_+>1/2$. We call $W_\alpha(L)$ the rhs of (2.7), the subscript underlining the dependence on α.

Lemma A.1: *Given* $\alpha\in[0,\alpha_+)$, *for* $J(1)$ *large enough*

$$W_\alpha(L)\geqslant\begin{cases}\zeta_\alpha L^\alpha, & \text{if } \alpha>0,\\ 2\ln L+8, & \text{if } \alpha=0.\end{cases}\tag{A2}$$

Proof: We first consider the case $\alpha>0$ and call $W'_\alpha(L)=W_\alpha(L)-2(J(1)-1)$. Using (1.2) and (2.7) reads

$$W'_\alpha(L)=\sum_{x=1}^{L}\left(\sum_{\substack{y\in[L+1,2L]\\ y\in[-L+1,0]}}\frac{1}{|x-y|^{2-\alpha}}-\sum_{\substack{y\in[2L+1,\infty]\\ y\in[-\infty,-L]}}\frac{1}{|x-y|^{2-\alpha}}\right)=2\sum_{x=1}^{L}\left(\sum_{y=L+1}^{2L}\frac{1}{|x-y|^{2-\alpha}}\right.$$
$$\left.-\sum_{y=2L+1}^{\infty}\frac{1}{|x-y|^{2-\alpha}}\right)=2\sum_{x=1}^{L}\left(\sum_{y=L+1-x}^{2L-x}\frac{1}{y^{2-\alpha}}-\sum_{y=2L+1-x}^{\infty}\frac{1}{y^{2-\alpha}}\right)$$

and using monotonicity to replace sums by integrals,

$$\geqslant 2\sum_{x=1}^{L}\left[\int_{L+1-x}^{2L+1-x}\frac{dz}{z^{2-\alpha}}-\int_{2L-x}^{\infty}\frac{dz}{z^{2-\alpha}}\right]\geqslant 2\sum_{x=1}^{L}\frac{1}{\alpha-1}\{[(2L-x)^{\alpha-1}-(L+1-x)^{\alpha-1}]+(2L-x)^{\alpha-1}\}$$
$$\geqslant 2\sum_{x=1}^{L}\frac{1}{1-\alpha}\{[-2(2L-x)^{\alpha-1}+(L+1-x)^{\alpha-1}]\}\geqslant\frac{2}{1-\alpha}\left[-2\sum_{y=0}^{L-1}(L+y)^{\alpha-1}+\sum_{y=0}^{L-1}(y+1)^{\alpha-1}\right]$$
$$\geqslant\frac{2}{1-\alpha}\left[-2\int_{y=-1}^{L-1}(L+y)^{\alpha-1}+\int_{y=0}^{L}(y+1)^{\alpha-1}\right]\geqslant\frac{2}{\alpha(1-\alpha)}[-2[(2L-1)^\alpha-(L-1)^\alpha]$$
$$+(L+1)^\alpha-1]$$

hence, recalling that $W_\alpha(L)=W'_\alpha(L)+2(J(1)-1)$ and that $\alpha\in(0,\alpha_+)$, we get $W_\alpha(L)\geqslant\zeta_\alpha L^\alpha$ for L large enough, and for all L, if $J(1)$ is large enough.

In the case $\alpha=0$ we can repeat the same computations obtaining

$$W_0(L)\geqslant 2\ln(L+2)+[2J(1)-4\ln(3)-2]\geqslant 2\ln L+8$$

for $J(1)$ large enough. The lemma is proved. □

APPENDIX B

We start by a preliminary lemma.

Lemma B.1: *Let* $\mathcal{R}(\underline{T})$ *satisfy P.0, P.1, and P.2,* $\Gamma\in\mathcal{R}(\underline{T})$ *and* $\underline{T}'$ *the configuration of triangles in* Γ. *Then* $\mathcal{R}(\underline{T}')=\{\Gamma\}$.

Proof: Writing $\mathcal{R}(\underline{T})=\{\Gamma_i, i=1,\dots,n\}$, denote by $\underline{T}^{(i)}$ the triangles in Γ_i and write

$$\mathcal{R}(\underline{T}^{(i)})=\{\Gamma_1^{(i)},\dots,\Gamma_{n_i}^{(i)}\}.$$

Each pair (Γ_i,Γ_j), $i\neq j$, verifies P.1, we want to show that P.1 is also verified by each distinct pair $\Gamma_j^{(i)}$, $\Gamma_{j'}^{(i')}$. This is by definition if $i=i'$, let us then suppose $i\neq i'$. If $T(\Gamma_i)\sqcap T(\Gamma_{i'})=\emptyset$, then the same holds for $T(\Gamma_j^{(i)})$ and $T(\Gamma_{j'}^{(i')})$ and (3.1) holds. If instead $T(\Gamma_i)\sqsubset T(\Gamma_{i'})$ (or vice versa), if instead $T(\Gamma_i)\sqsubset T(\Gamma_{i'})$ (or vice versa) then $\operatorname{dist}(\Gamma_j^{(i)},\Gamma_{j'}^{(i')})\geqslant\operatorname{dist}(\Gamma_j^{(i)},\Gamma_{i'})\geqslant\operatorname{dist}(\Gamma_i,\Gamma_{i'})\geqslant c|\Gamma_i|^3$ $\geqslant c|\Gamma_j^{(i)}|^3\geqslant c\min\{|\Gamma_j^{(i)}|^3,|\Gamma_{j'}^{(i')}|^3\}$ so that $\Gamma_j^{(i)}$, $\Gamma_{j'}^{(i')}$ verifies P.1.

By applying P.2, $\mathcal{R}(\underline{T})=\{\Gamma_j^{(i)}\}$ which must therefore coincide with $\{\Gamma_i\}$. Hence the decomposition of each Γ_i into $\Gamma_j^{(i)}$ is trivial, i.e., $n_i=1$ and $\Gamma_1^{(i)}=\gamma_i$. The lemma is proved. □

Proof of Theorem 3.1: *Uniqueness:* Suppose there are two algorithms, $\mathcal{R}^{(i)}$, $i=1,2$ which both satisfy P.1 and P.2 and let $\mathcal{R}^{(i)}(\underline{T})=\{\Gamma_j^{(i)}, j=1,\dots,n_i\}$. Let

$$A_h^{(1)} = \Gamma_1^{(1)} \sqcap \Gamma_h^{(2)} \tag{B1}$$

be the collection of those triangles which are both in $\Gamma_1^{(1)}$ and $\Gamma_h^{(2)}$. Of course the union of $A_h^{(1)}$ over h is equal to $\Gamma_1^{(1)}$.

Call $\{K_{h,j}^{(1)}, j=1,\ldots,m_h\}=\mathcal{R}^{(1)}(A_h^{(1)})$. Each distinct pair $K_{h,j}^{(1)}$, $K_{h',j'}^{(1)}$ verifies P.1, by an argument similar to that used in the proof of Lemma B.1 and which is omitted. Then, by P.2, $\{K_{h,j}^{(1)}, h=1,\ldots,n_2, j=1,\ldots,m_h\}=\mathcal{R}^{(1)}(\underline{T}^{(1)})$, $\underline{T}^{(1)}$ the collection of all triangles in $\Gamma_1^{(1)}$. By Lemma B.1 the decomposition is then trivial, which means that $\Gamma_1^{(1)}=\Gamma_i^{(2)}$ for some i. By iteration we then conclude that the two systems of contours $\{\Gamma_j^{(1)}\}$ and $\{\Gamma_i^{(2)}\}$ are identical. Thus $\mathcal{R}^{(1)}=\mathcal{R}^{(2)}$.

Existence: Given a configuration $\underline{T}$ of triangles, we call $\mathcal{C}$ the collection of all partitions $\underline{C}=(C_1,\ldots,C_n)$ of $\underline{T}$ so that each pair (C_i,C_j), $i\neq j$, verifies P.1 and P.0 (relative to $\underline{T}$). $\mathcal{C}$ is nonempty as the trivial partition in a single atom verifies P.0 and P.1 (as in that case there is nothing to check). We order $\mathcal{C}$ by setting $\underline{C}\geqslant\underline{C}'$ if the partition $\underline{C}$ is finer than $\underline{C}'$. We claim that $\mathcal{C}$ has a unique maximal element, which will be called $\mathcal{M}(\underline{T})$; we will then prove that $\mathcal{M}(\cdot)$ satisfies P.1 and P.2 and conclude the proof of existence.

The claim will follow from showing that the partition

$$\underline{C}\vee\underline{C}'=\{C_i\sqcap C_j'\},\quad \underline{C}=(C_1,\ldots,C_n),\quad \underline{C}'=(C_1',\ldots,C_m')$$

is in $\mathcal{C}$, if also $\underline{C}$ and $\underline{C}'$ are in $\mathcal{C}$.

Without loss of generality we must thus prove that any distinct pair $(C_i\sqcap C_j', C_{i'}\sqcap C_{j'}')$ verifies the alternatives in P.1. By symmetry between the two clusters, we may suppose $i\neq i'$. If $T(C_i)\sqcap T(C_{i'})=\emptyset$, then also $T(C_i\sqcap C_j')\sqcap T(C_{i'}\sqcap C_{j'}')=\emptyset$ and (3.1) holds. Let us suppose (again without loss of generality) that $T(C_i)\sqsubset T(C_{i'})$, then for any $T_k\in C_{i'}$, either $T(C_i)\sqsubset T_k$ or $T(C_i)\sqcap T_k=\emptyset$. If $T_k\in C_{j'}'$, in correspondence with the previous alternative, either $T(C_i\sqcap C_j')\sqsubset T_k$ or $T(C_i\sqcap C_j')\sqcap T_k=\emptyset$. If instead $T_k\notin C_{j'}'$, then $T_k\notin C_{i'}\sqcap C_{j'}'$ and there is nothing to check. In conclusion the pair $(C_i\sqcap C_j', C_{i'}\sqcap C_{j'}')$ verifies the alternatives (i) and (ii) and in case the latter is verified, (3.2) holds.

To complete the proof we must show that $\mathcal{M}(\underline{T})$ satisfies P.2. Let $\underline{T}$ and $\underline{T}^{(i)}$: $\sqcup\underline{T}^{(i)}=\underline{T}$ be as in P.2 and suppose that the elements of $\{\mathcal{M}(\underline{T}^{(i)}), i=1,\ldots,k\}$ satisfy (3.1) and (3.2). Suppose by contradiction that $\mathcal{M}(\underline{T})$ is not equal to $\{\mathcal{M}(\underline{T}^{(i)}), i=1,\ldots,k\}$, since the latter is in $\mathcal{C}$ (relative to $\underline{T}$), $\mathcal{M}(\underline{T})$ must then be finer than $\{\mathcal{M}(\underline{T}^{(i)}), i=1,\ldots,k\}$. But then we would have a finer partition of $\underline{T}^{(i)}$, for some i, which still verifies P.1. We have thus reached a contradiction.

The theorem is proved. □

As a consequence of P.1 and P.2 we have the following obvious property, namely that by adding triangles it cannot happen that contours split; the new triangles can either form separate contours or join other preexistent ones and possibly cause them to merge.

Lemma B.2: *Monotonicity*.

Let $\underline{T}$, $\underline{T}'$ be two configurations of triangles, $\underline{T}\sqsubset\underline{T}'$, then for any $\Gamma\in\mathcal{R}(\underline{T})$, there is $\Gamma'\in\mathcal{R}(\underline{T}')$ so that $\Gamma\sqsubset\Gamma'$.

Proof: Let $\Gamma_0\in\mathcal{R}(\underline{T})$, $\mathcal{R}(\underline{T}')=\{\Gamma_j'\}$ and [recalling the notation in (B1)] $A_j:=\Gamma_0\sqcap\Gamma_j'$. We must prove that for any j, either $A_j=\emptyset$ or $A_j=\Gamma_0$. Suppose by contradiction that this is not the case. We then consider the new partition of $\underline{T}$:$\underline{C}:=[\mathcal{R}(\underline{T})\vee\{(\mathcal{R}(\underline{T})\setminus\Gamma_0), A_1,\ldots,A_m\}]$. $\underline{C}$ is then in $\mathcal{C}$ (relative to $\underline{T}$) and is finer than $\mathcal{R}(\underline{T})$, which contradicts the fact that $\mathcal{R}(\underline{T})$ is the unique, finest partition of $\underline{T}$ verifying P.0, P.1, and P.2. The lemma is proved. □

APPENDIX C

An interval $[a,b]$ is compatible with $\underline{T}$ if a is an endpoint of a triangle of $\underline{T}$, b is also an endpoint of a triangle of $\underline{T}$ and for all $T\in\underline{T}$, $T\sqcap(a,b)$ is either void or equal to (a,b).

Lemma C.1: *Let $\underline{T}''\sqsubset\underline{T}$, with $\mathcal{R}(\underline{T}'')$ a singleton; $[a,b]$ a $\underline{T}''$-compatible interval; $\underline{T}'$ the collection of all triangles of $\underline{T}$ with basis in (a,b). Then if $\mathcal{R}(\underline{T}',\underline{T}'')$ is not a singleton, also $\mathcal{R}(\underline{T})$ is not a singleton.*

Proof: Since $\mathcal{R}(\underline{T}'')$ is a singleton, by Lemma B.2 there is a contour Γ_0 in $\mathcal{R}(\underline{T}',\underline{T}'')$ which contains $\underline{T}''$. In order to prove the lemma we must consider the case

$$\mathcal{R}(\underline{T}',\underline{T}'')=\{\Gamma_0,\ldots,\Gamma_n\},\quad n\geqslant 1.$$

Since Γ_i, $i\geqslant 1$, is distinct from Γ_0, it is a subset of $\underline{T}'$ and therefore $T(\Gamma_i)$ is strictly contained in (a,b). Let

$$\mathcal{R}(\{\underline{T}\setminus\underline{T}'\}\sqcup\Gamma_0)=\{\Gamma_1'\cdots\Gamma_k'\}.$$

We claim that

$$\mathcal{R}(\underline{T})=\{\Gamma_1,\ldots,\Gamma_n,\Gamma_1'\cdots\Gamma_k'\} \tag{C1}$$

hence $\mathcal{R}(\underline{T})$ is not a singleton and the lemma is proved.

To prove (C1), it is enough to show that $\{\Gamma_1,\ldots,\Gamma_n,\Gamma_1'\cdots\Gamma_k'\}$ satisfy properties P.0 and P.1 in the definition of contours, see Sec. III, because (C1) would then follow from P.2.

P.0 is obviously satisfied. Pairs Γ_i, Γ_j and Γ_i', Γ_j' satisfy P.1 by definition, it thus remains to check P.1 for pairs Γ_i, Γ_j'. By Lemma B.2, Γ_0 is contained in one of the contours Γ_j', say Γ_1', and let us start from this case. Then $\mathrm{dist}(\Gamma_i,\Gamma_1')=\mathrm{dist}(\Gamma_i,\Gamma_0)$ [because the triangles in $\Gamma_1'\setminus\Gamma_0$ are outside $[a,b]$, while Γ_0 contains triangle(s) whose endpoints are a, b and Γ_i has support inside (a,b)]. Since the pair Γ_i, Γ_0 satisfies P.1 then also Γ_i, Γ_1' satisfies P.1. For the same reason as before, also for $j>1$, $\mathrm{dist}(\Gamma_i,\Gamma_j')\geqslant\mathrm{dist}(T(\Gamma_i),\{a,b\})=\mathrm{dist}(\Gamma_i,\Gamma_0)>c|\Gamma_i|^3$ [the latter inequality by (ii) of P.1]. Hence $\mathrm{dist}(\Gamma_i,\Gamma_j')>c\ \min\{|\Gamma_i|^3,|\Gamma_j'|^3\}$. We have thus completed the proof of P.1, (C1) and Lemma C.1 are thus proved. □

Proof of (ii) of Lemma 4.2: We apply Lemma C.1 with $\underline{T}''=T$ (the maximal triangle), a, b the endpoints of T. Since $\mathcal{R}(\underline{T}'')=T$, $\mathcal{R}(\underline{T}'')$ is a singleton; $\underline{T}'=\{\underline{T}\}_S\setminus T$. By assumption $\mathcal{R}(\underline{T})$ is a singleton, then, by Lemma C.1, also $\mathcal{R}(\underline{T}',\underline{T}'')$ is a singleton, hence (ii) of Lemma 4.2 because $\mathcal{R}(\underline{T}',\underline{T}'')=\mathcal{R}(\{\underline{T}\}_S)$. □

Proof of (ii) of Lemma 4.3: $\mathcal{R}(\{\underline{T}\}_{S_i})$, $i=1,2$, are singletons (by definition of squares); then $\mathcal{R}(\{\underline{T}\}_{S_1},\{\underline{T}\}_{S_2})$ is a singleton as well, because S_1 and S_2 are a-connected. We then apply Lemma C.1, identifying $T''=\{\{\underline{T}\}_{S_1},\{\underline{T}\}_{S_2}\}$ and a, b as the endpoints of the squares S_1, S_2 which face each other. The argument is hereafter the same as in the proof of (ii) of Lemma 4.2. □

Lemma C.2: *Let $\underline{S}$ be the square configuration at time $t=n$. Call $\underline{S}'$ the collection of squares in a maximal a-connected component of $\underline{S}$, $(\{\underline{T}\}_{\underline{S}'})$ the set of triangles represented by the squares in $\underline{S}'$. Then $\mathcal{R}(\{\underline{T}\}_{\underline{S}'})$ is a singleton and $\underline{S}'$ will be represented by a square in the square configuration at time $t=n+1$.*

Proof: Suppose $\underline{S}'$ is not a singleton (otherwise the statement of the lemma would trivially hold). If $S_1\in\underline{S}'$ there must be $S_2\in\underline{S}'$ with S_1 and S_2 endpoints of an arrow. Then either S_1 is an endpoint of a primary arrow, or it is in a shadow of a primary arrow. By the assumed maximality of $\underline{S}'$ it then follows that $\underline{S}'$ is made of a sequence of squares each one connected by a primary arrow to the successive one and all other squares contained in the shadow of these primary arrows.

By (ii) of Lemma 4.3, the collection of all the triangles in the shadow of a primary arrow and those in the two squares connected by the primary arrow form a single contour. The statement of the lemma then follows by monotonicity, Lemma B.2.

Proof of (i) of Lemma 4.2: We will first prove that $\Gamma_1,\ldots,\Gamma_n$ are sequential, where

$$\{\Gamma_1,\ldots,\Gamma_n\}=\mathcal{R}(\{\underline{T}\}_S\setminus T). \tag{C2}$$

Suppose by contradiction that $T(\Gamma_i)\sqsubset T(\Gamma_j)$, $i\neq j$. By property P.1 in the definition of contours, there is a minimal contour Γ_k distinct from Γ_i such that $T(\Gamma_i)\sqsubset T(\Gamma_k)$. Let $[a,b]$ be the smallest interval containing $T(\Gamma_i)$ and compatible with Γ_k. Let $\underline{T}'$ be the collection of triangles with basis in (a,b). Then $\mathcal{R}(\underline{T}',\Gamma_k)$ contains at least Γ_i and Γ_k (by Lemma B.2), so that, by Lemma C.1, $\mathcal{R}(\underline{T})$ is not a singleton, against the assumption. Therefore $\Gamma_1,\ldots,\Gamma_n$ are sequential.

We will next prove the analogue of (4.3), calling a^*, b^* the endpoints of T, shorthanding $\{\Gamma_i\}:=\{\Gamma_1,\dots,\Gamma_n\}$ and labelling the contours so that Γ_i is before Γ_j when $i<j$ (we have already proved that $\{\Gamma_i\}$ is sequential). There is Γ_j such that $\mathrm{dist}(\Gamma_j,\{a^*,b^*\})\equiv\mathrm{dist}(T(\Gamma_j),\{a^*,b^*\})\leqslant c|\Gamma_j|^3$, otherwise all Γ_i would be contours in $\mathcal{R}(\underline{T})$, by the argument already used several times above. Supposing for the sake of definiteness that $\mathrm{dist}(\Gamma_j,a^*)\leqslant c|\Gamma_j|^3$, we then claim that

$$\mathrm{dist}(\Gamma_1,a^*)\leqslant c|\Gamma_1|^3. \tag{C3}$$

Suppose by contradiction that there is $1<k\leqslant j$ so that for any $i<k$, $\mathrm{dist}(\Gamma_i,a^*)>c|\Gamma_i|^3$ while $\mathrm{dist}(\Gamma_k,a^*)\leqslant c|\Gamma_k|^3$. This would imply that, for any $i<k$, $c|\Gamma_i|^3<\mathrm{dist}(\Gamma_i,a^*)\leqslant\mathrm{dist}(\Gamma_k,a^*)\leqslant c|\Gamma_k|^3$. Thus $|\Gamma_i|\leqslant|\Gamma_k|$ for any $i\leqslant k$. Since $\{\Gamma_1,\dots,\Gamma_n\}$ are distinct contours, $\mathrm{dist}(\Gamma_i,\Gamma_k)>c\min\{|\Gamma_i|^3,|\Gamma_k|^3\}=c|\Gamma_i|^3$, for any $i<k$.

Call $\underline{T}'$ the collection of all triangles in $\{\Gamma_1,\dots,\Gamma_{k-1}\}$, $[a,b]=[a^*,x_-(\Gamma_k)]$, $\underline{T}''=\{T,\Gamma_k\}$. We can then apply Lemma C.1 because $\mathcal{R}(\underline{T}'')$ is a singleton, since $\mathrm{dist}(\Gamma_k,a^*)\leqslant c|\Gamma_k|^3$: then $\{\Gamma_1,\dots,\Gamma_{k-1}\}$ are contours for $\mathcal{R}(\underline{T})$ which contradicts the assumption that the latter is a singleton. Equation (C3) is proved.

By (C3), $\mathcal{R}(\{T\}_{\Gamma_1},T)$ is a singleton, so that the previous analysis applies again with T replaced by $\{\Gamma_1,T\}$ and a^* replaced by $a_1^*=x_+(\Gamma_1)$, showing that if $\mathrm{dist}(\Gamma_j,a^*)\leqslant c|\Gamma_j|^3$ with $j>2$, then $\mathrm{dist}(\Gamma_2,a_1^*)\leqslant c|\Gamma_2|^3$. By iterating the argument we then conclude the proof of (i) of Lemma 4.2.□

Proof of (i) of Lemma 4.3: Since $\mathcal{R}(\{S_1,S_2\})$ is a singleton [see the proof above of (ii) of Lemma 4.3] the previous applies unchanged with a^* and b^* the endpoints of S_1 and S_2 which face each other. □

APPENDIX D

Lemma D.1: *A squares configuration $\underline{S}$ is (new a)-connected iff it is (old a)-connected.*

Proof: If $\underline{S}$ is (new a)-connected, then it is also (old a)-connected, as the new arrows are also old arrows. We thus only need to prove the reverse implication, we suppose $\underline{S}$ (old a)-connected but not (new a)-connected and want to show that this leads to a contradiction.

We call "odd" a pair S and S' of squares when there is an old arrow between S and S' [denoted by $(S,S')_{\mathrm{old}}$] while S and S' are not (new a)-connected. We will first show that if $\underline{S}$ is (old a)-connected but not (new a)-connected then there exist odd pairs; we will then prove that odd pairs "can be shortened" in the sense that if S and S' is an odd pair, then there is another square S'' in between S and S' such that either S and S'' or S' and S'' is an odd pair. The endless iteration of the argument leads to a contradiction.

Existence of odd pairs: If $\underline{S}$ is not (new a)-connected, there are two squares S and S' which are not (new a)-connected; since S and S' are (old a)-connected, there is a sequence $\{S_{\ell_i},i=1,\dots,j\}$ such that each pair $S_{\ell_i},S_{\ell_{i+1}}$ is connected by an old arrow, and $S_{\ell_1}=S$ and $S_{\ell_j}=S'$. Then one of the pairs $S_{\ell_i},S_{\ell_{i+1}}$ must be odd, otherwise S and S' would be (new a)-connected.

Shortening odd pairs: Writing $S\prec S'$ if the square S is before S' (recall that a square configuration is sequential), we label $\underline{S}$ so that $S_1\prec S_2\prec\cdots\prec S_n$. Let S_k, S_m be an odd pair and suppose, without loss of generality, that $S_k\prec S_m$ and that the old arrow which connects them goes from S_k to S_m. The old arrow which connects S_k to S_m is not a new arrow, otherwise S_k and S_m would be (new a)-connected, therefore there exists $S_\ell: S_k\prec S_\ell\prec S_m$; $|S_\ell|\geqslant|S_k|$ such that there is a new arrow from S_k to S_ℓ. Consider separately the two possible cases (1) $|S_\ell|\leqslant|S_m|$ and (2) $|S_\ell|>|S_m|$.

(1) Since $c|S_\ell|^3\geqslant c|S_k|^3\geqslant\mathrm{dist}(S_k,S_m)>\mathrm{dist}(S_m,S_\ell)$, there is an old arrow connecting S_ℓ and S_m; on the other hand, by definition, S_ℓ and S_k are (new a)-connected, hence S_ℓ and S_m cannot be (new a)-connected, hence S_ℓ, S_m is an odd pair.

(2) As in (1), $c|S_m|^3>\mathrm{dist}(S_m,S_\ell)$, which implies that there is an old arrow from S_m to S_ℓ, as well as an old arrow from S_k to S_ℓ. There are two subcases, (a) S_m and S_ℓ are also connected by a new arrow or else (b) they are not. In subcase (a), S_ℓ is (new a)-connected to S_m, hence it cannot be (new a)-connected to S_k, thus S_k, S_ℓ is an odd pair. In subcase (b), there is $S_h: S_\ell\prec S_h$

$<S_m; |S_h| \geq |S_m|$, such that there is a new arrow from S_m to S_h. Again, as S_h is (new a)-connected to S_m, it is not (new a)-connected to S_k. On the other hand, $|S_h| \geq |S_m| \geq |S_k|$, hence there is an old arrow from S_k to S_h, thus S_k, S_h is an odd pair.

This concludes the analysis of case (2), and the proof of the shortening property of odd pairs. Thus the lemma is proved. □

Proposition D.2: *The shadows of two new arrows have either empty intersection or else, one is contained in the other.*

Proof: Suppose by contradiction that there are four squares $S_a < S_u < S_b < S_z$, with the crossing arrows $\vec{\xi}_{ab}$ (denoting a new arrow from a to b) and $\vec{\xi}_{uz}$. By definition of new arrow, this implies that there is no arrow $\vec{\xi}_{au}$ (there could be however an arrow in the opposite direction $\vec{\xi}_{ua}$) and that $\mathrm{dist}(S_a, S_b) \leq c|S_a|^3$. Recalling that $S_u < S_b$ the only compatible sizes with the new arrow $\vec{\xi}_{a,b}$ are $|S_u| < |S_a| < |S_b|$. On the other hand, $\mathrm{dist}(S_u, S_b) < \mathrm{dist}(S_u, S_z) \leq c|S_u|^3$ then, being $|S_b| > |S_u|$ there should be an arrow $\vec{\xi}_{u,b}: S_u \to S_b$ contradicting the fact $\vec{\xi}_{uz}$ is a new arrow (i.e., that S_z is the first square connected with S_u).

Consider now the case in which the crossing arrows are $\vec{\xi}_{b,a}$ and $\vec{\xi}_{u,z}$ (that implies that $|S_b| > |S_a|$ and $|S_z| > |S_u|$). The existence of these arrows implies that there are no arrows $\vec{\xi}_{b,u}$ and $\vec{\xi}_{u,b}$, and, since $\mathrm{dist}(S_b, S_u) < \mathrm{dist}(S_a, S_b) \leq c|S_b|^3$, this implies that $|S_u| \leq c|S_b|$. We get a contradiction by observing that, since $\mathrm{dist}(S_u, S_b) \leq \mathrm{dist}(S_u, S_z) \leq |S_u|^3$, there should be an arrow $\vec{\xi}_{u,b}$ that is incompatible with $\vec{\xi}_{u,z}$.

The other possible crossing cases are reduced to those above by reflection and the proposition is proved. □

APPENDIX E

Lemma E.1: *Let $\alpha \in [0, 1/2]$, a and b positive and b/a large enough. Then for any $n \geq 2$, any $x_1, \ldots, x_{n-1}$, y such that $1 \leq x_i \leq y$,*

$$bh_\alpha(y) + (b-a)\sum_{i=1}^{n-1} h_\alpha(x) \geq bh_\alpha\left(\sum_{i=1}^{n-1} x_i + y\right), \tag{E1}$$

where $h_\alpha(L)$ is defined in (2.8).

Proof: We will prove (E1) by induction on $n \geq 2$ showing that

$$f_n(x_1, \ldots, x_{n-1}, y) := \frac{b}{b-a} h_\alpha(y) + \sum_{i=1}^{n-1} h_\alpha(x) - \frac{b}{b-a} h_\alpha\left(y + \sum_{i=1}^{n-1} x_i\right)$$

is non-negative in the set $1 \leq x_i \leq y$.

We start the induction by supposing that for $n > 2$, for any $2 \leq m \leq n$, $f_m \geq 0$ and want to prove that $f_{n+1}(x_1, \ldots, x_n, y) \geq 0$. Since f_{n+1} is symmetric in the first n variables, we may suppose, without loss of generality, that $x_i \leq x_n \leq y \leq x_1 + \cdots + x_{n-1} + y =: L$. Then

$$f_{n+1}(x_1, \ldots, x_n, y) = f_n(x_1, \ldots, x_{n-1}, y) + h_\alpha(x_n) + \frac{b}{b-a} h_\alpha(L) - \frac{b}{b-a} h_\alpha(L + x_n) = f_n(x_1, \ldots, x_{n-1}, y)$$
$$+ f_2(x_n, L) \geq 0.$$

To complete the induction we need to prove that $f_2(x, y) \geq 0$.

The case $\alpha > 0$. We have $f_2(x, y) = y^\alpha g(x/y)$ where

$$g(x) := x^\alpha + \frac{b}{b-a} - \frac{b}{b-a}(x+1)^\alpha, \quad 0 \leq x \leq 1.$$

If b/a is large enough, $g'(x) > 0$ and $g(x) \geq g(0) = 0$ and the induction is proved. Thus (E1) is proved in the case $\alpha > 0$.

The case $\alpha=0$.
Let

$$p := \frac{b}{b-a}, \quad \text{choose } a \text{ so that } 1 < p < 2.$$

We have

$$f_2(x,y) = p(\ln y + 4) + (\ln x + 4) - p(\ln[x+y] - 4) = -p\ln(1+x/y) + \ln x + 4 \geqslant -2p + 4 + \ln x \geqslant 0$$

because $x \geqslant 1$ and $p < 2$. □

APPENDIX F

In this appendix we sketch the proof of the analogue of (4.1) in the case $\alpha=0$, namely that

$$\sum_{\Gamma:|\Gamma|=m,0\in\Gamma} w_b^0(\Gamma) \leqslant 2me^{-b(\ln m+4)}, \tag{F1}$$

where

$$w_b^0(\Gamma) := \prod_{T\in\Gamma} e^{-b(\ln(|T|+4))} = \prod_{T\in\Gamma} (|T|^{-b}e^{-4b}).$$

Equation (F1) yields the analogue of (3.20), i.e.,

$$\mu_\Lambda^+(\{0\in\Gamma\}) \leqslant 2\sum_{m\geqslant 1} me^{-\beta(\ln(m)+4)} = 2e^{-4\beta}\sum_{m\geqslant 1} m^{1-\beta}. \tag{F2}$$

The sum in (F1) is bounded using the same iterative procedure as when $\alpha\in(0,1/2]$, with the fundamental inequality (4.9) replaced by the "convexity" inequality

$$bh_0(y) + (b-a)\sum_{i=1}^{n-1} h_0(x) \geqslant bh_0\left(\sum_{i=1}^{n-1} x_i + y\right)$$

proved in Appendix D for $0<a<b/2$. The proof of (F1) then follows closely that of (4.1) for $\alpha>0$, and it is omitted. □

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Multispecies extension of the solvable partially asymmetric reaction–diffusion processes

M. Alimohammadi[a] and Y. Naimi
Department of Physics, University of Tehran, North Karegar Ave., Tehran, Iran

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By considering the master equation of the partially asymmetric diffusion process on a one-dimensional lattice, the most general boundary condition (i.e., interactions) for the multispecies reaction–diffusion processes is considered. The resulting system has various interactions including diffusion to the left and right, two-particle interactions $A_\alpha A_\beta \rightarrow A_\gamma A_\delta$, and the extended n-particle drop–push interactions to the left and right. We obtain three distinct new models. The conditions on reaction rates to ensure the solvability of the resulting models are obtained. The two-particle conditional probabilities are calculated exactly. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1897664]

I. INTRODUCTION

The understanding of nonequilibrium statistical physics is still much more incomplete than that of equilibrium theory, due to the absence of an analogue of the Boltzman–Gibbs approach and in spite of considerable recent progress.[1] Therefore nonequilibrium systems must be specified by some defining dynamical rules which are then analyzed. The topic has received a lot of attention and many reviews exist, e.g., Refs. 2–7.

One of the interesting and important examples of the nonequilibrium systems is the one-dimensional reaction–diffusion processes, which have application in various fields of physics like study of the shocks,[8] noisy Burgers equation,[9] polymers in random media,[10] traffic models,[11] and biopolymerization.[12] As these systems are interacting systems with N-particle, even simple models may pose a formidable problem if one wants to approach them analytically. See Refs. 13–16 for more recent references.

The simplest reaction–diffusion process is the totally asymmetric simple exclusion process (TASEP). In this model, each lattice site is occupied by at most one particle and all particles can only hop with equal rate to their right-neighboring sites, if these sites are not occupied. TASEP has been studied in Ref. 17 by introducing a master equation which describes the evolution equation of the particles when they are not in neighboring sites, and a so-called boundary condition, which specifies the situation in which the probabilities go outside the physical regions. This happens when some of the particles are in adjacent sites and the master equation cannot be applied to them. It has been shown that the model is integrable in the sense that the N-particle S-matrix is factorized into a product of two-particle S-matrices. The coordinate Bethe ansatz has been used in this proof.

The interesting observation is that if one chooses other boundary conditions, with the same master equation, one can in principle introduce other interactions (besides diffusion to right-neighboring sites), which may be integrable in the above-mentioned sense. This is what is first done in Ref. 18, in which the so-called drop–push model has been studied by this method. In this model the particle hops to the next right site, even if it is occupied. It can hop by pushing all the neighboring particles to their next right sites, with a rate depending on the number of these particles. Some other generalization of TASEP can be found in Refs. 19–21.

[a]Electronic mail: alimohmd@ut.ac.ir

The generalization of one-species reaction–diffusion processes to p-species is an important task. The main problem in this generalization, besides introducing a set of suitable boundary conditions to model an interacting system, arises from the above-mentioned factorization of N-particle scattering matrix. It was shown in Ref. 22 that in order that a more-than-one species system to be solvable, in the sense of the Bethe ansatz, certain relations should be satisfied between the rates. These relations can be written as some kind of a spectral Yang–Baxter (SYB) equation. By this method, all the solvable two-species reaction–diffusion models, without annihilation and creation reactions and with equal reaction rates, have been obtained in Ref. 22.

The multispecies generalization of the reactions considered in Ref. 22 has been studied in Ref. 23, and the drop–push reaction of Ref. 18 has been generalized to p-species in Ref. 24. The most general totally asymmetric reaction–diffusion processes have been recently studied in Ref. 25. These processes are

$$\begin{aligned} &A_\alpha \emptyset \to \emptyset A_\alpha \quad \text{with rate } D_R, \\ &A_\alpha A_\beta \to A_\gamma A_\delta \quad \text{with rate } c_{\gamma\delta}^{\alpha\beta}, \\ &A_\alpha A_\beta \emptyset \to \emptyset A_\gamma A_\delta \quad \text{with rate } b_{\gamma\delta}^{\alpha\beta}, \\ &\cdots, \end{aligned} \tag{1}$$

where the dots indicate the other drop–push reactions with n-adjacent particles, in which in the mean time the types of the particles can also be changed. These latter reactions are called the extended drop–push processes. It has been shown that the reaction rates of processes (1) must satisfy some specific constraints, in order that we have a set of consistent evolution equations. Also the corresponding two-particle S-matrices must satisfy the SYB equation. Some classes of the solutions of these equations have been discussed in Ref. 25.

In all of the above studies, only the totally asymmetric exclusion processes have been considered, i.e., the particles can only diffuse to their next right neighboring sites. If one wants to consider the left and right diffusions simultaneously, one must consider a more general master equation with suitable boundary conditions and then seek the situations in which the model is integrable. In Ref. 17, one-species model with only simple diffusion to left and right (i.e., partially asymmetric) has been considered, and in Ref. 26, the one-species partially asymmetric drop–push model has been studied. Finally a two-species model in which the particles, besides diffusion to the left and right, have exchange-reaction has been studied in Ref. 27.

In this paper we want to study the most general p-species integrable models with partially asymmetric reaction–diffusion processes, which all the previous studied models are the special cases of them. These general models may have some or all of the following reactions:

$$A_\alpha \emptyset \to \emptyset A_\alpha \quad \text{with rate } D_R, \tag{2}$$

$$\emptyset A_\alpha \to A_\alpha \emptyset \quad \text{with rate } D_L, \tag{3}$$

$$A_\alpha A_\beta \to A_\gamma A_\delta \quad \text{with rate } E_{\gamma\delta}^{\alpha\beta}, \tag{4}$$

$$A_\alpha A_\beta \emptyset \to \emptyset A_\gamma A_\delta \quad \text{with rate } R_{\gamma\delta}^{\alpha\beta}, \tag{5}$$

$$\cdots$$

and

$$\emptyset A_\alpha A_\beta \to A_\gamma A_\delta \emptyset \quad \text{with rate } L_{\gamma\delta}^{\alpha\beta}, \tag{6}$$

$$\cdots .$$

In the above equations $\alpha,\beta,\ldots=(1,\ldots,p),\emptyset$ stands for vacancy, and dots in Eqs. (5) and (6) indicate the drop–push of n-adjacent particles to the right and left sites, respectively, in which in the mean time the types of the particles can also be changed. We call interactions (5) and (6) as right-drop–pushing and left-drop–pushing, respectively. We show that there are three distinct models which are integrable and each of these models contains reactions (2) and (3) and one or two of the reactions (4)–(6).

The scheme of the paper is as follows. There are two kinds of boundary conditions that can be generalized to p-species cases. In Sec. II, we generalize the first kind of boundary condition, which was introduced in Ref. 26, to the most general p-species case. Using the law of conservation of the number of particles, it is shown that there exists five constraints that must be satisfied by reaction rates of Eqs. (2)–(6), in order to have a set of consistent evolution equations to express the interactions (2)–(6). But it is seen that there is no solution for these constraints. The situation does not change even if we relax one of the constraints by including the annihilation processes. Therefore one cannot explain all the reactions (2)–(6) by this method. But it will be shown that we can have two distinct models. In the first type model the reactions are Eqs. (2)–(5) and in the second type the reactions are Eqs. (2)–(4) and (6).

The second kind of boundary condition, which was used in Refs. 17 and 27, is generalized to the most general p-species case in Sec. III. We show that the resulting consistent boundary condition can explain the reactions (2)–(4). This is the type 3 model. It must be mentioned that the type 3 model is not a subclass of types 1 and 2 and is a new distinct one. In Sec. IV we investigate the Bethe ansatz solution for these models and discuss the solutions of the corresponding SYB equations. We see that the S-matrix of type 3 model is much more involved than two other ones and therefore only some special classes of solutions of its SYB equation can be obtained. Finally we study the conditional probabilities of these models and in special two-particle sector, we obtain the exact expressions.

II. FIRST KIND GENERALIZATION

Consider a p-species system with particles $A_1,A_2,\ldots,A_p$. The basic objects we are interested in are the probabilities $P_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_N;t)$ for finding at time t the particle of type α_1 at site x_1, particle of type α_2 at site x_2, etc. We take the physical region of coordinates as $x_1<x_2<\cdots<x_N$. The master equation for a partially asymmetric exclusion process is

$$\begin{aligned}\frac{\partial}{\partial t}P_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_N;t) &= D_R\sum_{i=1}^{N} P_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_{i-1},x_i-1,x_{i+1},\ldots,x_N;t)\\ &\quad + D_L\sum_{i=1}^{N} P_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_{i-1},x_i+1,x_{i+1},\ldots,x_N;t)\\ &\quad - NP_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_N;t). \qquad (7)\end{aligned}$$

This equation describes a collection of N particles, diffusing to the next-right sites by rate D_R and to the next-left sites by rate D_L. In Eq. (7) we have used a time scale so that

$$D_R+D_L\equiv 1. \qquad (8)$$

This master equation is only valid for $x_i<x_{i+1}-1$. For $x_i=x_{i+1}-1$, there will be some terms with $x_i=x_{i+1}$ in the right-hand side of Eq. (7) which are out of the physical region. But one can assume that (7) is valid for all the physical regions $x_i<x_{i+1}$ by imposing certain boundary conditions for $x_i=x_{i+1}$. Different boundary condition introduces different interactions for particles. Following the argument given in Ref. 25, it can be easily seen that the master equation (7) leads to the following relation for two-particle probabilities:

$$\frac{\partial}{\partial t}\sum_{x_2}\sum_{x_1<x_2} P_{\alpha_1\alpha_2}(x_1,x_2;t) = \sum_x [D_R P_{\alpha_1\alpha_2}(x,x;t) + D_L P_{\alpha_1\alpha_2}(x+1,x+1;t)] - \sum_x P_{\alpha_1\alpha_2}(x,x+1;t)$$
$$= \sum_x P_{\alpha_1\alpha_2}(x,x;t) - \sum_x P_{\alpha_1\alpha_2}(x,x+1;t). \tag{9}$$

This equation leads us to take $P_{\alpha_1\alpha_2}(x,x;t)$ as linear combination of $P_{\beta_1\beta_2}(x,x+1;t)$ and $P_{\beta_1\beta_2}(x-1,x;t)$'s as the only choice for having a consistent set of evolution equations in more-than-two-particle sectors.[25] Therefore the most general boundary condition is

$$P_{\alpha_1\alpha_2}(x,x) = \sum_\beta b^{\beta_1\beta_2}_{\alpha_1\alpha_2} P_{\beta_1\beta_2}(x-1,x) + \sum_\beta c^{\beta_1\beta_2}_{\alpha_1\alpha_2} P_{\beta_1\beta_2}(x,x+1). \tag{10}$$

β stands for $(\beta_1\beta_2)$ and b and c are $p^2\times p^2$ matrices which determine the interactions. In the probabilities of Eq. (10), we have suppressed all the other coordinates and the time t for simplicity. In fact $P_{\alpha_1\alpha_2}(x,x) \equiv P_{\gamma_1\cdots\gamma_i\alpha_1\alpha_2\gamma_{i+3}\cdots\gamma_N}(x_1,\ldots,x_i,x,x,x_{i+3},\ldots,x_N)$. In the first step, let us exclude the creation and annihilation processes (it can be shown that one cannot study the creation processes by this method, so in fact in this step, we exclude the annihilation processes). Since the number of particles is constant in time, summing over α_1 and α_2 makes the left-hand side of (9) zero and results in

$$-\sum_x\sum_\alpha P_{\alpha_1\alpha_2}(x,x+1) + \sum_x\sum_\beta\left(\sum_\alpha (b+c)^{\beta_1\beta_2}_{\alpha_1\alpha_2}\right) P_{\beta_1\beta_2}(x,x+1) = 0, \tag{11}$$

in which Eq. (10) has been used. Clearly Eq. (11) gives

$$\sum_\alpha (b+c)^{\beta_1\beta_2}_{\alpha_1\alpha_2} = 1 \quad \text{constraint (I)}. \tag{12}$$

Note that in $p=1$, the boundary condition (10) and constraint (12) reduce to those considered in Ref. 26. Also in the case of totally asymmetric processes in which $D_L=0$, our problem reduces to one considered in Ref. 25. Following the same steps as Ref. 25, we first consider $\dot{P}_{\alpha_1\alpha_2}(x,x+1)$. Using Eqs. (7) and (10), it is found

$$\dot{P}_{\alpha_1\alpha_2}(x,x+1) = D_R P_{\alpha_1\alpha_2}(x-1,x+1) + D_L P_{\alpha_1\alpha_2}(x,x+2) + D_R\sum_\beta b^{\beta_1\beta_2}_{\alpha_1\alpha_2} P_{\beta_1\beta_2}(x-1,x)$$
$$+ D_L\sum_\beta c^{\beta_1\beta_2}_{\alpha_1\alpha_2} P_{\beta_1\beta_2}(x+1,x+2) + \left(D_R\sum_\beta c^{\beta_1\beta_2}_{\alpha_1\alpha_2} + D_L\sum_\beta b^{\beta_1\beta_2}_{\alpha_1\alpha_2}\right) P_{\beta_1\beta_2}(x,x+1)$$
$$-2P_{\alpha_1\alpha_2}(x,x+1) = D_R P_{\alpha_1\alpha_2}(x-1,x+1) + D_L P_{\alpha_1\alpha_2}(x,x+2) + D_R\sum_\beta b^{\beta_1\beta_2}_{\alpha_1\alpha_2} P_{\beta_1\beta_2}$$
$$(x-1,x) + D_L\sum_\beta c^{\beta_1\beta_2}_{\alpha_1\alpha_2} P_{\beta_1\beta_2}(x+1,x+2) + \sum_{\beta\neq\alpha}(D_R c^{\beta_1\beta_2}_{\alpha_1\alpha_2} + D_L b^{\beta_1\beta_2}_{\alpha_1\alpha_2}) P_{\beta_1\beta_2}(x,x+1)$$
$$-\left[D_R + D_L + \sum_{\beta\neq\alpha}(D_R c^{\alpha_1\alpha_2}_{\beta_1\beta_2} + D_L b^{\alpha_1\alpha_2}_{\beta_1\beta_2}) + \sum_\beta (D_R b^{\alpha_1\alpha_2}_{\beta_1\beta_2} + D_L c^{\alpha_1\alpha_2}_{\beta_1\beta_2})\right] P_{\alpha_1\alpha_2}(x,x+1), \tag{13}$$

in which we use Eqs. (8) and (12). The latter can be written as

$$c^{\alpha_1\alpha_2}_{\alpha_1\alpha_2} = 1 - \sum_\beta b^{\alpha_1\alpha_2}_{\beta_1\beta_2} - \sum_{\beta\neq\alpha} c^{\alpha_1\alpha_2}_{\beta_1\beta_2} \tag{14}$$

or

$$b_{\alpha_1\alpha_2}^{\alpha_1\alpha_2} = 1 - \sum_{\beta\neq\alpha} b_{\beta_1\beta_2}^{\alpha_1\alpha_2} - \sum_{\beta} c_{\beta_1\beta_2}^{\alpha_1\alpha_2}. \tag{15}$$

It is seen that the evolution equation (13) describes the following two-particle interactions:

$$\begin{gathered} A_\alpha\emptyset \to \emptyset A_\alpha \quad \text{with rate } D_R, \\ \emptyset A_\alpha \to A_\alpha\emptyset \quad \text{with rate } D_L, \\ A_\alpha A_\beta \to A_\gamma A_\delta \quad \text{with rate } D_R c_{\gamma\delta}^{\alpha\beta} + D_L b_{\gamma\delta}^{\alpha\beta}, \\ A_\alpha A_\beta \emptyset \to \emptyset A_\gamma A_\delta \quad \text{with rate } D_R b_{\gamma\delta}^{\alpha\beta}, \\ \emptyset A_\alpha A_\beta \to A_\gamma A_\delta \emptyset \quad \text{with rate } D_L c_{\gamma\delta}^{\alpha\beta}. \end{gathered} \tag{16}$$

To study the consistency of our formalism and also deriving the more-than-two particle interactions, we consider $\dot{P}_{\alpha_1\cdots\alpha_n}(x,x+1,\ldots,x+n-1)$. In $n=3$, we encounter two boundary terms $P_{\alpha_1\alpha_2\alpha_3}(x,x+1,x+1)$ and $P_{\alpha_1\alpha_2\alpha_3}(x+1,x+1,x+2)$. Using (10), the first one becomes

$$\begin{aligned} P_{\alpha_1\alpha_2\alpha_3}(x,x+1,x+1) = &\sum_{\beta\gamma} b_{\alpha_2\alpha_3}^{\beta_2\beta_3}[b_{\alpha_1\beta_2}^{\gamma_1\gamma_2} P_{\gamma_1\gamma_2\beta_3}(x-1,x,x+1) + c_{\alpha_1\beta_2}^{\gamma_1\gamma_2} P_{\gamma_1\gamma_2\beta_3}(x,x+1,x+1)] \\ &+ \sum_{\beta} c_{\alpha_2\alpha_3}^{\beta_2\beta_3} P_{\alpha_1\beta_2\beta_3}(x,x+1,x+2) \end{aligned} \tag{17}$$

which describes the boundary term $P_{\alpha_1\alpha_2\alpha_3}(x,x+1,x+1)$ as a linear combination of other boundary terms, i.e., $P_{\gamma_1\gamma_2\beta_3}(x,x+1,x+1)$'s. As has been shown in Ref. 25, the only consistent solution to this problem is the vanishing of these terms on the right-hand side of Eq. (17), which results in

$$\sum_{\beta_2} c_{\alpha_1\beta_2}^{\gamma_1\gamma_2} b_{\alpha_2\alpha_3}^{\beta_2\beta_3} = 0 \quad \text{constraint (II)} \tag{18}$$

or

$$(1\otimes b)(c\otimes 1) = 0, \tag{19}$$

in which 1 stands for the $p\times p$ identity matrix. The second boundary term is

$$\begin{aligned} P_{\alpha_1\alpha_2\alpha_3}(x+1,x+1,x+2) = &\sum_{\beta} b_{\alpha_1\alpha_2}^{\beta_1\beta_2} P_{\beta_1\beta_2\alpha_3}(x,x+1,x+2) + \sum_{\beta\gamma} c_{\alpha_1\alpha_2}^{\beta_1\beta_2}[b_{\beta_2\alpha_3}^{\gamma_2\gamma_3} P_{\beta_1\gamma_2\gamma_3} \\ &(x+1,x+1,x+2) + c_{\beta_2\alpha_3}^{\gamma_2\gamma_3} P_{\beta_1\gamma_2\gamma_3}(x+1,x+2,x+3)], \end{aligned} \tag{20}$$

which again leads us to take

$$\sum_{\beta_2} c_{\alpha_1\alpha_2}^{\beta_1\beta_2} b_{\beta_2\alpha_3}^{\gamma_2\gamma_3} = 0 \quad \text{constraint (III)}, \tag{21}$$

or

$$(c\otimes 1)(1\otimes b) = 0. \tag{22}$$

Assuming constraints (18) and (21) and using Eqs. (7) and (10), $\dot{P}_{\vec{\alpha}}(x,x+1,x+2)$ is

$$\dot{P}_{\vec{\alpha}}(x,x+1,x+2) = D_R P_{\vec{\alpha}}(x-1,x+1,x+2) + D_L P_{\vec{\alpha}}(x,x+1,x+3) + D_R \sum_{\beta} b^{\beta_1\beta_2}_{\alpha_1\alpha_2} P_{\beta_1\beta_2\alpha_3}$$
$$(x-1,x,x+2) + D_L \sum_{\beta} c^{\beta_2\beta_3}_{\alpha_2\alpha_3} P_{\alpha_1\beta_2\beta_3}(x,x+2,x+3) + \sum_{\beta\neq\alpha} (D_R c^{\beta_1\beta_2}_{\alpha_1\alpha_2}$$
$$+ D_L b^{\beta_1\beta_2}_{\alpha_1\alpha_2}) P_{\beta_1\beta_2\alpha_3}$$
$$(x,x+1,x+2) + \sum_{\beta\neq\alpha} (D_R c^{\beta_2\beta_3}_{\alpha_2\alpha_3} + D_L b^{\beta_2\beta_3}_{\alpha_2\alpha_3}) P_{\alpha_1\beta_2\beta_3}(x,x+1,x+2) + D_R \sum_{\gamma} b^{\vec{\gamma}}_{\vec{\alpha}} P_{\vec{\gamma}}$$
$$(x-1,x,x+1) + D_L \sum_{\gamma} c^{\vec{\gamma}}_{\vec{\alpha}} P_{\vec{\gamma}}(x+1,x+2,x+3) - \Bigg[D_R + D_L + D_R \sum_{\beta} b^{\alpha_1\alpha_2}_{\beta_1\beta_2}$$
$$+ D_L \sum_{\beta} c^{\alpha_1\alpha_2}_{\beta_1\beta_2} + D_R \sum_{\beta} b^{\alpha_2\alpha_3}_{\beta_2\beta_3} + D_L \sum_{\beta} c^{\alpha_2\alpha_3}_{\beta_2\beta_3} + \sum_{\beta\neq\alpha} (D_R c^{\alpha_1\alpha_2}_{\beta_1\beta_2} + D_L b^{\alpha_1\alpha_2}_{\beta_1\beta_2})$$
$$+ \sum_{\beta\neq\alpha} (D_R c^{\alpha_2\alpha_3}_{\beta_2\beta_3} + D_L b^{\alpha_2\alpha_3}_{\beta_2\beta_3}) \Bigg] P_{\vec{\alpha}}(x,x+1,x+2), \tag{23}$$

in which we have used Eqs. (14) and (15) for diagonal elements of matrix $D_R c + D_L b$. $b^{\vec{\gamma}}_{\vec{\alpha}}$ and $c^{\vec{\gamma}}_{\vec{\alpha}}$ are defined as follows:

$$b^{\vec{\gamma}}_{\vec{\alpha}} = \sum_{\gamma} b^{\gamma_1\gamma_2}_{\alpha_1\beta} b^{\beta\gamma_3}_{\alpha_2\alpha_3}, \tag{24}$$

$$c^{\vec{\gamma}}_{\vec{\alpha}} = \sum_{\gamma} c^{\gamma_1\beta}_{\alpha_1\alpha_2} c^{\gamma_2\gamma_3}_{\beta\alpha_3}. \tag{25}$$

Looking at source terms of Eq. (23), it is obvious that they describe the reactions (16) and the following three-particle drop–push reactions:

$$A_{\gamma_1} A_{\gamma_2} A_{\gamma_3} \emptyset \to \emptyset A_{\alpha_1} A_{\alpha_2} A_{\alpha_3} \quad \text{with rate } D_R b^{\vec{\gamma}}_{\vec{\alpha}} \tag{26}$$

and

$$\emptyset A_{\gamma_1} A_{\gamma_2} A_{\gamma_3} \to A_{\alpha_1} A_{\alpha_2} A_{\alpha_3} \emptyset \quad \text{with rate } D_L c^{\vec{\gamma}}_{\vec{\alpha}}. \tag{27}$$

The sink terms are consistent with this description, provided

$$\sum_{\beta} b^{\vec{\alpha}}_{\vec{\beta}} = \sum_{\beta\gamma} b^{\alpha_1\alpha_2}_{\beta_1\gamma} b^{\gamma\alpha_3}_{\beta_2\beta_3} = \sum_{\beta} b^{\alpha_1\alpha_2}_{\beta_1\beta_2} \quad \text{constraint (IV)} \tag{28}$$

and

$$\sum_{\beta} c^{\vec{\alpha}}_{\vec{\beta}} = \sum_{\beta\gamma} c^{\alpha_1\gamma}_{\beta_1\beta_2} c^{\alpha_2\alpha_3}_{\gamma\beta_3} = \sum_{\beta} c^{\alpha_2\alpha_3}_{\beta_2\beta_3} \quad \text{constraint (V)}. \tag{29}$$

By calculating other $\dot{P}_{\vec{\alpha}}(x,x+1,\ldots,x+n-1)$'s it can be shown that we do not need any more constraints and therefore the master equation (7) with boundary condition (10) and five constraints (I)–(V) can consistently describe the following reactions:

$$A_\alpha \emptyset \to \emptyset A_\alpha \quad \text{with rate } D_R, \tag{30}$$

$$\emptyset A_\alpha \to A_\alpha \emptyset \quad \text{with rate } D_L, \tag{31}$$

$$A_\alpha A_\beta \to A_\gamma A_\delta \quad \text{with rate } D_R c^{\alpha\beta}_{\gamma\delta} + D_L b^{\alpha\beta}_{\gamma\delta}, \tag{32}$$

$$A_{\alpha_0}\cdots A_{\alpha_n}\emptyset \to \emptyset A_{\gamma_0}\cdots A_{\gamma_n} \quad \text{with rate } D_R(b_{n-1,n}\cdots b_{0,1})^{\alpha_0\cdots\alpha_n}_{\gamma_0\cdots\gamma_n}, \tag{33}$$

$$\emptyset A_{\alpha_0}\cdots A_{\alpha_n} \to A_{\gamma_0}\cdots A_{\gamma_n}\emptyset \quad \text{with rate } D_L(c_{0,1}\cdots c_{n-1,n})^{\alpha_0\cdots\alpha_n}_{\gamma_0\cdots\gamma_n}. \tag{34}$$

In the above equations we use the following definition for $b_{k,k+1}$ and $c_{k,k+1}$:

$$a_{k,k+1} = 1 \otimes \cdots \otimes 1 \otimes \underbrace{a}_{k,k+1} \otimes 1 \otimes \cdots \otimes 1. \tag{35}$$

Note that for $D_L=0$, the five classes of the above reactions reduce to three classes discussed in Ref. 25. In Ref. 25, the constraints between reaction rates are three relations (I), (II), and (IV). Note that at $D_L=0$, the constraints (III) and (V) do not appear since the multiplication factors of their corresponding terms in evolution equation is D_L, which is zero.

To find the set of solutions of five constraints (I)–(V), one can consider the solutions of equations (I), (II), and (IV), that is the solutions derived in Ref. 25, and then considers the subset of them satisfies (III) and (V). We must note that in our models, the diagonal elements of matrix c are the reaction rates of the last line of Eq. (16) and must be positive. This is in contrast to the case studied in Ref. 25 in which the diagonal elements of c can be negative.

We can also follow another approach. That is trying to find the solution of equations (II)–(IV) and then seek ones which satisfy relation (I). As these relations are rather complex, we cannot completely solve them for arbitrary p, but we try them as much as possible.

As all the matrix elements of matrices b and c are reaction rates, they cannot be negative, so the only solution of Eq. (18) is

$$c^{\gamma_1\gamma_2}_{\alpha_1\beta_2} b^{\beta_2\beta_3}_{\alpha_2\alpha_3} = 0 \quad (\text{without sum over } \beta_2). \tag{36}$$

This relation has the two following solutions (for each β_2):

$$c^{\gamma_1\gamma_2}_{\alpha_1\beta_2} = 0 \quad \text{and } b^{\beta_2\beta_3}_{\alpha_2\alpha_3} = 0. \tag{37}$$

So for each β_2 we have two solutions, and as β_2 runs from 1 to p, we have 2^p-2 set of solutions for constraint (II). We exclude two of the solutions in which all of the elements of c or b is zero, since we look for the situations in which $b\neq 0$ and $c\neq 0$. We will later study the cases $b=0$ or $c=0$ in which the number of independent classes of reactions (30)–(34) reduces to four. By the same argument, the solutions of Eq. (21) are (for each β_2)

$$c^{\beta_1\beta_2}_{\alpha_1\alpha_2} = 0 \quad \text{and } b^{\gamma_2\gamma_3}_{\beta_2\alpha_3} = 0, \tag{38}$$

and therefore we again have 2^p-2 set of solutions for constraint (III). Note that from 2^p-2 solutions of constraints (II) [and (III)] only $(p-1)$ of them are independent, that is, does not transform to each other under interchanging of the labels of the species of the particles. So the number of independent solutions of constraints (II) and (III) are $(p-1)(2^p-2)$. For example, in $p=2$, the independent solutions of (II) and (III) are

$$\begin{aligned} &\{c^{\gamma_1\gamma_2}_{\alpha_1 1} = 0, b^{2\beta_3}_{\alpha_2\alpha_3} = 0, c^{\beta_1 1}_{\alpha_1\alpha_2} = 0, b^{\gamma_2\gamma_3}_{2\alpha_3} = 0\}, \\ &\{c^{\gamma_1\gamma_2}_{\alpha_1 1} = 0, b^{2\beta_3}_{\alpha_2\alpha_3} = 0, c^{\beta_1 2}_{\alpha_1\alpha_2} = 0, b^{\gamma_2\gamma_3}_{1\alpha_3} = 0\}, \end{aligned} \tag{39}$$

which can be written as

$$b=\begin{pmatrix} b_{11} & b_{12} & 0 & 0 \\ b_{21} & b_{22} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad c=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & c_{22} & 0 & c_{24} \\ 0 & 0 & 0 & 0 \\ 0 & c_{42} & 0 & c_{44} \end{pmatrix} \tag{40}$$

and

$$b=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ b_{31} & b_{32} & 0 & 0 \\ b_{41} & b_{42} & 0 & 0 \end{pmatrix}, \quad c=\begin{pmatrix} 0 & 0 & 0 & 0 \\ c_{21} & 0 & c_{23} & 0 \\ 0 & 0 & 0 & 0 \\ c_{41} & 0 & c_{43} & 0 \end{pmatrix}, \tag{41}$$

respectively. We label the states as $|1\rangle=(1,1)$, $|2\rangle=(1,2)$, $|3\rangle=(2,1)$ and $|4\rangle=(2,2)$. Setting Eqs. (40) and (41) into the constraints (IV) and (V) [Eqs. (28) and (29)] results in

$$b=\begin{pmatrix} 1 & 1 & 0 & 0 \\ b_{21} & b_{21} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad c=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & c_{22} & 0 & c_{22} \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix} \tag{42}$$

and

$$b=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ b_{41} & b_{41} & 0 & 0 \end{pmatrix}, \quad c=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ c_{41} & 0 & c_{41} & 0 \end{pmatrix}, \tag{43}$$

respectively. Now Eq. (12) [constraint (I)] says that the sum of the elements of each column of matrix $(b+c)$ must be one, which unfortunately does not satisfy by (42) and (43). The sum of the elements of the second column of $(b+c)$ of Eq. (42) and the first column of Eq. (43) are greater than (or equal to) 2. So reactions (30)–(34) have not any representation in $p=2$, the situation which we expect to be true for other p's. For example, in $p=3$, constraints (II) and (III) have 12 independent solutions, which are in two categories, the number of constraints on ${b_i}^j$ and ${c_k}^l$'s are equal (three on ${b_i}^j$ and three on ${c_k}^l$), and one which these numbers differ, i.e., 4 and 2. As an example of the first category, we consider the case in which ${c_{\alpha 1}}^j=0$, ${c_{\alpha 2}}^j=0$, ${c_i}^{\beta 1}=0$, ${b_k}^{3\gamma}=0$, ${b_{1\alpha}}^k=0$, ${b_{3\alpha}}^k=0$. It means that in matrix c, the rows 1,2,4,5,7,8 and columns 2,5, and 8 are zero, so it has 18 nonzero elements, and b is a matrix in which the rows 1,2,3,7,8,9 and columns 7,8, and 9 are zero so it also has 18 nonzero elements. Setting these b and c matrices in constraints (IV) and (V) results in two of the following solutions for each b and c:

$$\begin{aligned} &c_1{:}\{c_{31}=c_{34}=c_{37}=1, c_{33} \text{ and } c_{36} \text{ arbitrary}\}, \\ &c_2{:}\{c_{93}=c_{96}=c_{99}=1, c_{91} \text{ and } c_{94} \text{ arbitrary}\}, \\ &b_1{:}\{b_{41}=b_{42}=b_{43}=1, b_{44} \text{ and } b_{45} \text{ arbitrary}\}, \\ &b_2{:}\{b_{54}=b_{55}=b_{56}=1, b_{51} \text{ and } b_{52} \text{ arbitrary}\}, \end{aligned} \tag{44}$$

in which we only write down the nonzero elements. It can be easily seen that none of the combinations b_1+c_1, b_1+c_2, b_2+c_1, b_2+c_2 are acceptable in the sense of constraint (I), as at least the sum of the elements of one of the columns of these matrices are greater than (or equal to) 2. We have checked that the same situation arises in other 11 solutions. So again in $p=3$, we have no

representation. We cannot generally prove this, but we believe that the set of constraints (I)–(V) have no solution for arbitrary p.

One may suppose that if we somehow change the constraint (I), then it may be possible to find some solution for our equations. So we add the annihilation processes to our previous interactions. Note that these interactions appear only in the sink terms of the evolution equation, as if we consider the initial state with n particles, no annihilation processes can lead to a n-particle state at any other time t. So if we change the constraint (I) to (as we do not have the conservation of particles)

$$\sum_{\alpha} (b+c)^{\beta_1\beta_2}_{\alpha_1\alpha_2} = 1 - \lambda_{\beta_1\beta_2}, \tag{45}$$

and using it in the calculation of $\dot{P}_{\alpha_1\alpha_2}(x,x+1)$, we find the same equation as (13), except an extra term $\lambda_{\alpha_1\alpha_2}\dot{P}_{\alpha_1\alpha_2}(x,x+1)$ which is added to sink terms. So $\lambda_{\alpha_1\alpha_2}$ is the sum of the rates of all annihilation processes with initial state $(\alpha_1\alpha_2)$ and therefore is a positive quantity. Therefore adding the annihilation processes to interactions (30)–(34) means that the sum of the elements of each column of $(b+c)$ can now be less than or equal to 1. But as we have shown in Eqs. (42)–(44), the sum of the elements of some of the columns of $(b+c)$ in these examples are at least 2, which differs from what is suggested by Eq. (45). In brief, including the annihilation processes cannot alter our result and the set of processes (30)–(34) have no representation, with or without adding the annihilation processes.

Now it is interesting to note that even if one of the matrices b or c is equal to zero, we have yet all four desired reactions, diffusion to left *and* right, two-particle reactions $A_\alpha A_\beta \to A_\gamma A_\delta$, and the extended drop–push reactions, which the latter occur only on one side (left *or* right). These are almost the general reactions that one can study in this framework. Let us check the constraints in these cases.

A. Type 1 model

Take $c=0$. Equation (12) becomes

$$\sum_{\alpha} b^{\beta_1\beta_2}_{\alpha_1\alpha_2} = 1. \tag{46}$$

Constraints (II), (III), and (V) are satisfied trivially and constraint (IV) is also satisfied: using Eq. (46), both sides of constraint (IV) become one. Therefore master equation (7) with boundary condition

$$P_{\alpha_1\alpha_2}(x,x) = \sum_{\beta} b^{\beta_1\beta_2}_{\alpha_1\alpha_2} P_{\beta_1\beta_2}(x-1,x), \tag{47}$$

and constraint (46), describe consistently the following reactions:

$$\begin{gathered} A_\alpha \emptyset \to \emptyset A_\alpha \quad \text{with rate } D_R, \\ \emptyset A_\alpha \to A_\alpha \emptyset \quad \text{with rate } D_L, \\ A_\alpha A_\beta \to A_\gamma A_\delta \quad \text{with rate } D_L b^{\alpha\beta}_{\gamma\delta}, \\ A_{\alpha_0}\cdots A_{\alpha_n}\emptyset \to \emptyset A_{\gamma_0}\cdots A_{\gamma_n} \quad \text{with rate } D_R (b_{n-1,n}\cdots b_{0,1})^{\alpha_0\cdots\alpha_n}_{\gamma_0\cdots\gamma_n}. \end{gathered} \tag{48}$$

B. Type 2 model

In the same way, for $b=0$ it can be seen that the master equation (7) with boundary condition

$$P_{\alpha_1\alpha_2}(x,x) = \sum_{\beta} c^{\beta_1\beta_2}_{\alpha_1\alpha_2} P_{\beta_1\beta_2}(x,x+1), \tag{49}$$

and constraint

$$\sum_{\alpha} c^{\beta_1\beta_2}_{\alpha_1\alpha_2} = 1, \tag{50}$$

describe successfully the reactions

$$\begin{aligned} A_\alpha \emptyset &\to \emptyset A_\alpha \quad \text{with rate } D_R, \\ \emptyset A_\alpha &\to A_\alpha \emptyset \quad \text{with rate } D_L, \\ A_\alpha A_\beta &\to A_\gamma A_\delta \quad \text{with rate } D_R c^{\alpha\beta}_{\gamma\delta}, \end{aligned} \tag{51}$$

$$\emptyset A_{\alpha_0} \cdots A_{\alpha_n} \to A_{\gamma_0} \cdots A_{\gamma_n} \emptyset \quad \text{with rate } D_L (c_{0,1} \cdots c_{n-1,n})^{\alpha_0 \cdots \alpha_n}_{\gamma_0 \cdots \gamma_n}.$$

The condition of solvability of these models will be discussed in the next sections.

III. SECOND KIND GENERALIZATION

By noting the first line of Eq. (9), it is seen that Eq. (10) is not the only possible p-species boundary condition. In fact, one can instead consider the following boundary condition:

$$D_R P_{\alpha_1\alpha_2}(x,x) + D_L P_{\alpha_1\alpha_2}(x+1,x+1) = \sum_{\beta} b^{\beta_1\beta_2}_{\alpha_1\alpha_2} P_{\beta_1\beta_2}(x-1,x) + \sum_{\beta} c^{\beta_1\beta_2}_{\alpha_1\alpha_2} P_{\beta_1\beta_2}(x,x+1). \tag{52}$$

This is the multispecies generalization of the boundary condition considered in Refs. 17 and 27.

To study the interactions introduced by (7) and (52), we must again consider $\dot{P}_{\alpha_1\cdots\alpha_n}(x,x+1,\ldots,x+n-1)$. In $n=3$, we encounter the boundary term $D_R P_{\alpha_1\alpha_2\alpha_3}(x,x+1,x+1) + D_L P_{\alpha_1\alpha_2\alpha_3}(x,x+2,x+2)$, where using (52) results in $\Sigma_\beta b^{\beta_2\beta_3}_{\alpha_2\alpha_3} P_{\alpha_1\beta_2\beta_3}(x,x,x+1) + \Sigma_\beta c^{\beta_2\beta_3}_{\alpha_2\alpha_3} P_{\alpha_1\beta_2\beta_3}(x,x+1,x+2)$. But the first term $P_{\alpha_1\beta_2\beta_3}(x,x,x+1)$ cannot be written in terms of physical probabilities, since in this case only the linear combination $D_R P_{\alpha_1\alpha_2\cdots}(x,x,\ldots) + D_L P_{\alpha_1\alpha_2\cdots}(x+1,x+1,\ldots)$ can be written in terms of physical function [Eq. (52)]. This is in contrast with the case studied in Sec. II. The only solution to this problem is taking

$$b = 0. \tag{53}$$

So our second kind p-species model is defined through the master equation (7) and the following boundary condition:

$$D_R P_{\alpha_1\alpha_2}(x,x) + D_L P_{\alpha_1\alpha_2}(x+1,x+1) = \sum_{\beta} c^{\beta_1\beta_2}_{\alpha_1\alpha_2} P_{\beta_1\beta_2}(x,x+1). \tag{54}$$

Conservation of the number of particles gives

$$\sum_{\alpha} c^{\beta_1\beta_2}_{\alpha_1\alpha_2} = 1, \tag{55}$$

and calculating $\dot{P}_{\alpha_1\alpha_2}(x,x+1)$ results in

$$\dot{P}_{\alpha_1\alpha_2}(x,x+1) = D_R P_{\alpha_1\alpha_2}(x-1,x+1) + D_L P_{\alpha_1\alpha_2}(x,x+2) + \sum_{\beta\neq\alpha} c^{\beta_1\beta_2}_{\alpha_1\alpha_2} P_{\beta_1\beta_2}(x,x+1)$$
$$- \left(D_R + D_L + \sum_{\beta\neq\alpha} c^{\alpha_1\alpha_2}_{\beta_1\beta_2}\right) P_{\alpha_1\alpha_2}(x,x+1). \tag{56}$$

This equation describes the following reactions as source and sink terms:

$$A_\alpha\emptyset \to \emptyset A_\alpha \quad \text{with rate } D_R,$$
$$\emptyset A_\alpha \to A_\alpha\emptyset \quad \text{with rate } D_L, \tag{57}$$
$$A_\alpha A_\beta \to A_\gamma A_\delta \quad \text{with rate } c^{\alpha\beta}_{\gamma\delta}.$$

Calculating other $\dot{P}_{\alpha_1\cdots\alpha_n}(x,x+1,\ldots,x+n-1)$'s confirms these reactions without any further constraint. So the **type 3 model** is defined by the master equation (7), boundary condition (54), constraint (55), and reactions (57).

IV. BETHE ANSATZ SOLUTION

Until now, we have constructed a consistent formalism to study some reaction–diffusion processes. Now we want to solve the resulting evolution equations and check the solvability of these models. To solve the master equation (7), we consider the following Bethe ansatz:

$$P_{\alpha_1\cdots\alpha_N}(\mathbf{x};t) = e^{-E_N t}\psi_{\alpha_1\cdots\alpha_N}(\mathbf{x}), \tag{58}$$

with

$$\Psi(\mathbf{x}) = \sum_\sigma \mathbf{A}_\sigma e^{i\sigma(\mathbf{p})\cdot\mathbf{x}}. \tag{59}$$

Ψ is a tensor of rank N with components $\psi_{\alpha_1\cdots\alpha_N}(\mathbf{x})$ and the summation runs over the elements of the permutation group of N objects.[28,29] Inserting (58) in (7), results in

$$E_N = \sum_{k=1}^{N} (1 - D_R e^{-ip_k} - D_L e^{ip_k}). \tag{60}$$

Inserting (58) in boundary condition (47) gives

$$\Psi(\ldots,x_k = x, x_{k+1} = x, \ldots) = b_{k,k+1}\Psi(\ldots,x_k = x-1, x_{k+1} = x, \ldots), \tag{61}$$

which using (59) results

$$[1 - e^{-i\sigma(p_k)}b_{k,k+1}]\mathbf{A}_\sigma + [1 - e^{-i\sigma(p_{k+1})}b_{k,k+1}]\mathbf{A}_{\sigma\sigma_k} = 0. \tag{62}$$

σ_k is an element of permutation group which only interchanges p_k and p_{k+1},

$$\sigma_k:(p_1,\ldots,p_k,p_{k+1},\ldots,p_N) \to (p_1,\ldots,p_{k+1},p_k,\ldots,p_N). \tag{63}$$

Equation (62) gives $\mathbf{A}_{\sigma\sigma_k}$ in terms of $\mathbf{A}_\sigma$ as follows:

$$\mathbf{A}_{\sigma\sigma_k} = S^{(1)}_{k,k+1}(\sigma(p_k),\sigma(p_{k+1}))\mathbf{A}_\sigma, \tag{64}$$

where

$$S^{(1)}_{k,k+1}(z_1,z_2) = 1 \otimes \cdots \otimes 1 \otimes \underbrace{S^{(1)}(z_1,z_2)}_{k,k+1} \otimes 1 \otimes \cdots \otimes 1, \tag{65}$$

and $S^{(1)}(z_1,z_2)$ is the following $p^2 \times p^2$ matrix:

$$S^{(1)}(z_1,z_2) = -(1-z_2^{-1}b)^{-1}(1-z_1^{-1}b), \tag{66}$$

in which $z_k = e^{ip_k}$. The same procedure for boundary conditions (49) and (54), i.e., the type 2 and type 3 models, results in

$$S^{(2)}(z_1,z_2) = -(1-z_1c)^{-1}(1-z_2c) \tag{67}$$

and

$$S^{(3)}(z_1,z_2) = -(D_R + z_1z_2D_L - z_1c)^{-1}(D_R + z_1z_2D_L - z_2c), \tag{68}$$

respectively. Equation (64) allows one to compute all $\mathbf{A}_\sigma$'s in terms of $\mathbf{A}_1$ (which is set to unity).

As the generators of permutation group satisfy $\sigma_k\sigma_{k+1}\sigma_k = \sigma_{k+1}\sigma_k\sigma_{k+1}$, so one also needs

$$\mathbf{A}_{\sigma_k\sigma_{k+1}\sigma_k} = \mathbf{A}_{\sigma_{k+1}\sigma_k\sigma_{k+1}}. \tag{69}$$

This, in terms of S-matrices becomes

$$S_{12}(z_2,z_3)S_{23}(z_1,z_3)S_{12}(z_1,z_2) = S_{23}(z_1,z_2)S_{12}(z_1,z_3)S_{23}(z_2,z_3). \tag{70}$$

In the terms of R-matrix defined through

$$S_{k,k+1} =: \Pi_{k,k+1}R_{k,k+1}, \tag{71}$$

where Π is the permutation matrix, Eq. (70) is transformed to

$$R_{23}(z_2,z_3)R_{13}(z_1,z_3)R_{12}(z_1,z_2) = R_{12}(z_1,z_2)R_{13}(z_1,z_3)R_{23}(z_2,z_3). \tag{72}$$

This is the spectral Yang–Baxter equation.

The Bethe ansatz solution exists, if the scattering matrix satisfies (70). In other words, the matrix b in (66) and c in (67) and (68) is acceptable only if the resulting S-matrices satisfy (70). This is a very restricted condition and needed for having the solvability.

The S-matrices (66) and (67) are exactly the ones considered in Refs. 24 and 23, respectively. Using the fact that $S^{(1)}$ is a binomial of degree one with respect to $z_1^{-1} = e^{-ip_1}$ and $S^{(2)}$ is of degree one with respect to z_2, it can be shown that SYB equation (70) for $S^{(1)}$ and $S^{(2)}$ reduces to

$$b_{23}[b_{23},b_{12}] = [b_{23},b_{12}]b_{12} \tag{73}$$

and

$$c_{12}[c_{12},c_{23}] = [c_{12},c_{23}]c_{23}, \tag{74}$$

respectively.[23,24] Note that although the above equations are much simpler than Eq. (70), but they are very complicated yet. In p-species, each one is an equality between two $p^3\times p^3$ matrices which results a system of p^6 equations to be solved for p^4-p^2 elements of b (or c), which may or may not have solution [Eq. (46) and (50) reduce the number of independent elements of b and c to p^4-p^2]. The general properties of the solutions of Eq. (73) and Eq. (74) have been discussed in Refs. 24 and 23, respectively, which can be directly used here. In other words, for every solution of Eq. (74), there exists a corresponding solvable model which has been discussed in Ref. 23, i.e.,

$$\begin{aligned} A_\alpha\emptyset &\to \emptyset A_\alpha \quad \text{with rate 1},\\ A_\alpha A_\beta &\to A_\gamma A_\delta \quad \text{with rate } c_{\gamma\delta}^{\alpha\beta}. \end{aligned} \tag{75}$$

and a type 2 model with reactions written in Eq. (51) [note that the reactions (75) are a subset of (51) with $D_L=0$]. The same is true for solutions of (73). They can describe the following solvable model (discussed in Ref. 24):

$$A_\alpha\emptyset \to \emptyset A_\alpha \quad \text{with rate 1},$$

$$A_{\alpha_0}\cdots A_{\alpha_n}\emptyset \to \emptyset A_{\gamma_0}\cdots A_{\gamma_n} \quad \text{with rate } (b_{n-1,n}\cdots b_{0,1})^{\alpha_0\cdots\alpha_n}_{\gamma_0\cdots\gamma_n}, \tag{76}$$

and a type 1 model with reaction (48) [again at $D_L=0$, (48) reduces to (76)].

The reasoning which leads the SYB equations of $S^{(1)}$ and $S^{(2)}$ to (73) and (74) does not work for $S^{(3)}$ since it is not a binomial of degree one with respect to z_1 or z_2, in fact it contains all powers of z_1 and z_2. So obtaining the solutions of (70) for $S^{(3)}$ is more difficult than for $S^{(1)}$ and $S^{(2)}$, even in the simplest case $p=2$. In the $p=2$ case we encounter a system of 64 equations that must be solved for 12 nondiagonal elements of c [the diagonal elements are determined by Eq. (55)]. The solution must be momentum independent (independent of z_1, z_2, and z_3) and non-negative. We cannot solve this equation generally (taking all $c_{ij}\neq 0$) by standard mathematical softwares and therefore restrict ourselves to some specific cases. For example, taking

$$c=\begin{pmatrix} c_{11} & 0 & 0 & c_{14} \\ c_{21} & 1 & 0 & c_{24} \\ 1-c_{11}-c_{21} & 0 & 1 & 1-c_{14}-c_{24} \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{77}$$

or

$$c=\begin{pmatrix} 0 & 0 & 0 & 0 \\ c_{21} & 1 & 0 & c_{24} \\ c_{31} & 0 & 1 & c_{34} \\ 1-c_{21}-c_{31} & 0 & 0 & 1-c_{24}-c_{34} \end{pmatrix}, \tag{78}$$

which are the four-parameters cases, one obtains two solutions

$$c=\begin{pmatrix} 0 & 0 & 0 & 0 \\ D_R & 1 & 0 & D_L \\ D_L & 0 & 1 & D_R \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{79}$$

and one with $D_L \leftrightarrow D_R$. Taking

$$c=\begin{pmatrix} 1-c_{41} & 1-c_{42} & 1-c_{43} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ c_{41} & c_{42} & c_{43} & 1 \end{pmatrix} \tag{80}$$

or

$$c=\begin{pmatrix} 1 & 1-c_{42} & 1-c_{43} & 1-c_{44} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & c_{42} & c_{43} & c_{44} \end{pmatrix}, \tag{81}$$

as some three-parameters cases, we find four solutions

$$c = \begin{pmatrix} 1 & 1-c_{42} & 1-c_{43} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & c_{42} & c_{43} & 1 \end{pmatrix}, \tag{82}$$

where each of c_{42} and c_{43} are either D_R or D_L. Taking $A_1 \equiv A$ and $A_2 \equiv B$, the interactions introduced by (79), for instance, are

$$\begin{aligned} A\emptyset &\xrightarrow{D_R} \emptyset A, \\ B\emptyset &\xrightarrow{D_R} \emptyset B, \\ \emptyset A &\xrightarrow{D_L} A\emptyset, \\ \emptyset B &\xrightarrow{D_L} B\emptyset, \\ AA &\xrightarrow{D_R} AB, \\ BB &\xrightarrow{D_L} AB, \\ AA &\xrightarrow{D_L} BA, \\ BB &\xrightarrow{D_R} BA. \end{aligned} \tag{83}$$

The model built on the reactions (83) is integrable.

Assuming that the solvability condition (70) is satisfied, it is easy to see that the conditional probability (the propagator) is

$$U(\mathbf{x};t|\mathbf{y};0) = \int \frac{d^N p}{(2\pi)^N} e^{-E_N t} e^{-i\mathbf{p}.\mathbf{y}} \sum_{\sigma} \mathbf{A}_{\sigma} e^{i\sigma(\mathbf{p})\cdot\mathbf{x}}, \tag{84}$$

where the integration region for each p_i is $[0, 2\pi]$ and $A_1 = 1$. The singularity in A_σ is removed by setting $p_j \to p_j + i\varepsilon$, where one should consider the limit $\varepsilon \to 0^+$. Using this propagator, one can write the probability at the time t in terms of the initial value of probability,

$$|P(\mathbf{x};t)\rangle = \sum_{y} U(\mathbf{x};t|\mathbf{y};0)|P(\mathbf{y};0)\rangle. \tag{85}$$

Note that although $S^{(1)}$ and $S^{(2)}$ are similar to ones considered in Refs. 24 and 23, the propagators $U^{(1)}$ and $U^{(2)}$ are different since the energy spectrum of our models differs from those considered there. In $D_L = 0$, our results must coincide with those obtained in Refs. 23 and 24.

For the two-particle sector, there is only one matrix in the expression of $U^{(i)}$s (b in $U^{(1)}$ and c in $U^{(2)}$ and $U^{(3)}$). So it can be treated as a c-number. Using calculation similar to what has been done in Refs. 23–25, one arrives at

$$U^{(1)}(x_1,x_2;t|y_1,y_2;0) = e^{-2t}\sum_{n,m=0}^{\infty}\left\{\frac{D_L^n D_R^{x_1-y_1+n}t^{x_1-y_1+2n}}{n!(x_1-y_1+n)!}\frac{D_L^m D_R^{x_2-y_2+m}t^{x_2-y_2+2m}}{m!(x_2-y_2+m)!}\right.$$
$$+\sum_{l=0}^{\infty}\frac{D_L^n D_R^{x_2-y_1+n}t^{x_2-y_1+2n}}{n!(x_2-y_1+n)!}\frac{D_L^m D_R^{x_1-y_2-l+m}t^{x_1-y_2-l+2m}}{m!(x_1-y_2-l+m)!}$$
$$\left.\times b^l\left[-1+\frac{x_2-y_1+n}{D_R t}b\right]\right\}, \tag{86}$$

and

$$U^{(2)}(x_1,x_2;t|y_1,y_2;0) = e^{-2t}\sum_{n,m=0}^{\infty}\left\{\frac{D_L^n D_R^{x_1-y_1+n}t^{x_1-y_1+2n}}{n!(x_1-y_1+n)!}\frac{D_L^m D_R^{x_2-y_2+m}t^{x_2-y_2+2m}}{m!(x_2-y_2+m)!}\right.$$
$$+\sum_{l=0}^{\infty}\frac{D_L^n D_R^{x_2-y_1+l+n}t^{x_2-y_1+l+2n}}{n!(x_2-y_1+l+n)!}\frac{D_L^m D_R^{x_1-y_2+m}t^{x_1-y_2+2m}}{m!(x_1-y_2+m)!}$$
$$\left.\times c^l\left[-1+\frac{D_R t}{x_1-y_2+m+1}c\right]\right\}. \tag{87}$$

Similarly one can obtain a more lengthy expression for $U^{(3)}$. Note that at $D_L=0$, Eqs. (86) and (87) lead Eqs. (38) of Ref. 24 and (30) of Ref. 23, respectively.

To investigate the large-time behaviors of the probabilities $U^{(1)}$, $U^{(2)}$, and $U^{(3)}$, it is useful to decompose the vector spaces on which b (in type 1 model) and c (in types 2 and 3 models) act, in two subspaces invariant under the action of $b(c)$, the first subspace corresponding to eigenvalues with modulus one, and another invariant subspace. For types 1 and 2 models with conditions (46) and (50), as all the elements of matrix $b(c)$ are non-negative, the second subspace corresponds to eigenvalues with modulus less than 1. By focusing on type 1 model, this decomposition can be done by introducing two projectors Q and R, satisfying

$$Q+R=1,$$
$$QR=RQ=0, \tag{88}$$
$$[b,Q]=[b,R]=0.$$

Q projects on the first subspace and R projects on the second. Following Ref. 23, we multiply $U^{(1)}$ by $Q+R=1$:

$$U^{(1)}(\mathbf{x};t|\mathbf{y};0) = U^{(1)}Q + U^{(1)}R. \tag{89}$$

In the terms multiplied by R, one can treat b as a number with modulus different from 1. So the integrand in (84) is nonsingular at points $p_j=0$, which have the main contributions at large times. Setting $p_j=0$, we have $S^{(1)}\approx -1$ and $\mathbf{A}_\sigma \approx (-1)^{[\sigma]}$, and Eq. (84) results in

$$\text{the second term of } U^{(1)} = \frac{1}{2\pi t}\{e^{-\{[x_1-y_1-(D_R-D_L)t]^2+[x_2-y_2-(D_R-D_L)t]^2\}/(2t)}$$
$$-e^{-\{[x_1-y_2-(D_R-D_L)t]^2+[x_2-y_1-(D_R-D_L)t]^2\}/(2t)}\}R, \quad t\to\infty, \tag{90}$$

which is independent of b. So at large time, the second term of $U^{(1)}$ tends to zero faster than t^{-1} and the leading term in $U^{(1)}$, which is order t^{-1}, does not involve the second term.

If the only eigenvalue of b with modulus 1 is 1, then $bQ=Q$ and $U^{(1)}$ has a simple behavior at $t\to\infty$,

$$U^{(1)}(x_1,x_2;t|y_1,y_2;0) = e^{-2t}\sum_{n,m=0}^{\infty}\left\{\frac{D_L^n D_R^{x_1-y_1+n}t^{x_1-y_1+2n}}{n!(x_1-y_1+n)!}\frac{D_L^m D_R^{x_2-y_2+m}t^{x_2-y_2+2m}}{m!(x_2-y_2+m)!}\right.$$
$$+\sum_{l=0}^{\infty}\frac{D_L^n D_R^{x_2-y_1+n}t^{x_2-y_1+2n}}{n!(x_2-y_1+n)!}\frac{D_L^m D_R^{x_1-y_2-l+m}t^{x_1-y_2-l+2m}}{m!(x_1-y_2-l+m)!}$$
$$\left.\times\left[-1+\frac{x_2-y_1+n}{D_R t}\right]\right\}Q. \tag{91}$$

This is simply the propagator of a single-species model with diffusions to the right and left and drop–push to the right (i.e., the $\lambda=0$ case of the reactions studied in Refs. 26 and 30), multiplied by Q. In fact Eq. (91) is $\lambda=0$ case of Eq. (30) of Ref. 26, times Q.

For $U^{(2)}$, the same decomposition leads to Eq. (90) for its second term and in the case $cQ=Q$, $U^{(2)}$ tends to (87), with $c=1$, times Q, at $t\to\infty$. The resulting one-species model is the $\mu=0$ case of the reactions studied in Refs. 26 and 30. For $U^{(3)}$, we again find (90) and the one-species partially asymmetric simple exclusion process of Ref. 17.

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Global existence to Boltzmann equation with external force in infinite vacuum

Renjun Duan
Laboratory of Nonlinear Analysis, Department of Mathematics, Central China Normal University, Wuhan 430079, People's Republic of China

Tong Yang
Department of Mathematics, City University of Hong Kong, Kowloon, Hong Kong, People's Republic of China

Changjiang Zhu[a)]
Laboratory of Nonlinear Analysis, Department of Mathematics, Central China Normal University, Wuhan 430079, People's Republic of China

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In this paper, we give a condition on the bicharacteristic which guarantees the global existence of the mild solution to the Boltzmann equation with an external force for the hard-sphere model and potentials with angular cutoff in infinite vacuum. This generalizes the previous results to the case when the force can have arbitrary strength. The constructive condition on the bicharacteristic is used to obtain the pointwise estimates on the collision operator so that the global existence comes from the contraction mapping theorem. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1899985]

I. INTRODUCTION

The purpose of this paper is to study the global existence of mild solutions to the initial value problem for the Boltzmann equation with an external force for the hard-sphere model and some angle cutoff potential. Let $f=f(t,x,v)$ be the density distribution function of the interacting gas particles at time $t\geqslant 0$ and position $x\in\mathbf{R}^3$ with velocity $v\in\mathbf{R}^3$ for rarefied gases. In the presence of external forces depending only on space and time variables, the evolution of f is described by the Boltzmann equation

$$f_t = v\cdot\nabla_x f + E(t,x)\cdot\nabla_v f = Q[f], \tag{1.1}$$

with initial data

$$f(0,x,v) = f_0(x,v), \tag{1.2}$$

where $E(t,x)\in\mathbf{R}^3$ is an external force and Q is a nonlinear collision operator capturing the binary collisions between particles whose specific form will be given below.

Let (v,v_*) and (v',v_*') be velocities before and after the collision, respectively. Under the assumption of elastic collision, the conservation of the momentum and energy:

$$v+v_* = v'+v_*',$$

$$|v|^2+|v_*|^2 = |v'|^2+|v_*'|^2,$$

yields

[a)]Author to whom correspondence should be addressed. Electronic mail: cjzhu@mail.ccnu.edu.cn

$$v' = v - [(v - v_*) \cdot \omega]\omega, \quad v'_* = v_* + [(v - v_*) \cdot \omega]\omega, \tag{1.3}$$

where $\omega \in S^2_+ = \{\omega \in S^2 : (v - v_*) \cdot \omega \geqslant 0\}$. Moreover, the collision term $Q[f]$ takes the form

$$Q[f](v) = \frac{1}{\varepsilon} \int_{\mathbf{R}^3 \times S^2_+} B(|v - v_*|, \theta)\{f(v')f(v'_*) - f(v)f(v_*)\} \mathrm{d}v_* \, \mathrm{d}\omega, \tag{1.4}$$

where ε is the Knudsen number proportional to the mean free path. For simplicity of notation, we sometimes use $f(v)$ to denote $f(t,x,v)$ without any ambiguity. In (1.4), the function $B(|v - v_*|, \theta)$ is the collision cross section with

$$\theta = \cos^{-1}\left(\frac{(v - v_*) \cdot \omega}{|v - v_*|} \right) \in \left[0, \frac{\pi}{2} \right] \tag{1.5}$$

being the scattering angle between $v - v_*$ and ω. The definition of B depends on the physics of collision. In fact, for the inverse power interaction potential, B takes the form of

$$B(|v - v_*|, \theta) = b_\gamma(\theta)|v - v_*|^\gamma, \quad -3 < \gamma < 1, \tag{1.6}$$

with $\gamma = 0$ corresponding to the Maxwellian molecules, $\gamma > 0$ corresponding to the hard interaction and $\gamma < 0$ corresponding to the soft interaction. Moreover, the hard-sphere model satisfies $B(|v - v_*|, \theta) = \sigma |v - v_*| \cos\theta$ with σ being the radius of the hard sphere.

For later use, as in Ref. 11 we denote $u = v - v_*$, $u_\parallel = (u \cdot \omega)\omega$ and $u_\perp = u - u_\parallel$ so that

$$v' = v - u_\parallel, \quad v'_* = v - u_\perp. \tag{1.7}$$

Then the collision term $Q[f]$ becomes

$$Q[f](v) = \frac{1}{\varepsilon} \int_{\mathbf{R}^3 \times S^2_+} B(|u|, \theta)\{f(v')f(v'_*) - f(v)f(v - u)\} \mathrm{d}u \, \mathrm{d}\omega, \tag{1.8}$$

where v' and v'_* are given by (1.7). Furthermore, let us denote the collision operator

$$Q(f,g) = Q^+(f,g) - Q^-(f,g) \tag{1.9}$$

with the gain term Q^+ and the loss term Q^- given by

$$Q^+(f,g)(t,x,v) = \frac{1}{\varepsilon} \int_{\mathbf{R}^3 \times S^2_+} B(|u|, \theta) f(t,x,v') g(t,x,v'_*) \mathrm{d}u \, \mathrm{d}\omega \tag{1.10}$$

and

$$Q^-(f,g)(t,x,v) = \frac{1}{\varepsilon} \int_{\mathbf{R}^3 \times S^2_+} B(|u|, \theta) f(t,x,v) g(t,x,v - u) \mathrm{d}u \, \mathrm{d}\omega. \tag{1.11}$$

Clearly,

$$Q[f] = Q(f,f). \tag{1.12}$$

For any fixed point (t,x,v) in $\mathbf{R}^+ \times \mathbf{R}^3 \times \mathbf{R}^3$, we now consider the bicharacteristic equations of (1.1) in $\mathbf{R}^3 \times \mathbf{R}^3$,

$$\frac{\mathrm{d}X}{\mathrm{d}s} = V, \quad \frac{\mathrm{d}V}{\mathrm{d}s} = E(s,X), \qquad (X,V)|_{s=t} = (x,v). \tag{1.13}$$

Suppose that the above ODE system have smooth solutions globally in time denoted by

$$[X(s;t,x,v),V(s;t,x,v)] \tag{1.14}$$

for any $(t,x,v)\in\mathbf{R}^+\times\mathbf{R}^3\times\mathbf{R}^3$. Then integrating (1.1) along the bicharacteristic, we obtain the representation of the mild solution to the Boltzmann equation,

$$f(t,x,v)=f_0(X(0;t,x,v),V(0;t,x,v))+\int_0^t Q(f,f)(s,X(s;t,x,v),V(s;t,x,v))\mathrm{d}s. \tag{1.15}$$

In fact, the mild solution can be defined as follows:

Definition 1.1: *A non-negative function* $f(t,x,v)\in C([0,T);L^1_+(\mathbf{R}^3\times\mathbf{R}^3))$ *is a mild solution to* (1.1) *with a non-negative initial data* f_0 *if and only if* f *satisfies the integral equation* (1.15) *for all* $t\in[0,T)$ *and a.e.* $(x,v)\in\mathbf{R}^3\times\mathbf{R}^3$.

The function spaces on $\mathbf{R}^+\times\mathbf{R}^3\times\mathbf{R}^3$ for the solutions constructed later can be defined in the following. For any $p>0,q>0$, let $S_{p,q}$ be the completion of the set consisting of the continuous functions of compact support with respect to the norm

$$|||f|||=\sup_{t,x,v}(1+|X(0;t,x,v)|^2)^p\exp\{q|V(0;t,x,v)|^2\}|f(t,x,v)|. \tag{1.16}$$

And for any fixed time t, define the norm

$$\|f(t)\|=\sup_{x,v}(1+|X(0;t,x,v)|^2)^p\exp\{q|V(0;t,x,v)|^2\}|f(t,x,v)|, \tag{1.17}$$

in particular,

$$\|f_0\|_{p,q}=\sup_{x,v}(1+|x|^2)^p e^{q|v|^2}|f_0(x,v)|. \tag{1.18}$$

Throughout this paper, the assumptions on p,q, the collision kernel and the external force can be summarized as follows:

(A1) $p>\frac{1}{2}$.

(A2) The cross section B is in the form of (1.6) with $-2<\gamma\leqslant 1$ satisfying

$$\int_0^{\pi/2} b_\gamma(\theta)(1+\tan\theta)\mathrm{d}\theta\leqslant b_0, \tag{1.19}$$

where b_0 is a positive constant.

(A3) The external force $E(t,x)$ is C^0 in (t,x). Furthermore, for any fixed point $(t,x,v)\in\mathbf{R}^+\times\mathbf{R}^3\times\mathbf{R}^3$, the first order ODE system (1.13) has global smooth solutions (1.14) satisfying the following constructive condition:

$$\begin{aligned} X(0;s,X(s;t,x,v),V(s;t,x,v)-\xi)&=X(0;t,x,v)+\alpha_1(s;t,x,v)\xi,\\ V(0;s,X(s;t,x,v),V(s;t,x,v)-\xi)&=V(0;t,x,v)-\alpha_2(s;t,x,v)\xi, \end{aligned} \tag{1.20}$$

for any $s\in\mathbf{R}^+$ and $\xi\in\mathbf{R}^3$, where $\alpha_1(s;t,x,v),\alpha_2(s;t,x,v)\in C^1(s)$ satisfy the following inequalities:

$$\alpha_i(s;t,x,v)>0,\quad i=1,2,$$

$$\alpha(s;t,x,v)\equiv\alpha_1'(s;t,x,v)\alpha_2(s;t,x,v)-\alpha_1(s;t,x,v)\alpha_2'(s;t,x,v)>0, \tag{1.21}$$

$$(\alpha_2(s;t,x,v))^{\gamma+1}\alpha(s;t,x,v)\geqslant\alpha_0>0,$$

where α_0 is a positive constant independent of s and (t,x,v). Here and in the sequel $\alpha_i'(s;t,x,v)$ represent the derivative with respect to s.

Now we can state the main result of this paper as follows:

Theorem 1.2: *Under the assumptions (A1)–(A3), there is a sufficiently small positive constant* $\delta_0>0$ *such that if* $0\leqslant f_0(x,v)$ *and* $\|f_0\|_{p,q}\leqslant\varepsilon\delta_0$, *then there exists a unique global in time mild solution* $f(t,x,v)$ *to the initial value problem* (1.1) and (1.2) *satisfying* $|||f|||\leqslant 2\varepsilon\delta_0$.

Remark 1.3: For the moment let us discuss the assumptions (A1)–(A3). First, (A1) means that initial data decays with algebraic rate in the space variable x, and decays with exponential rate in the velocity variable v. Then (A2) holds for the collision kernels satisfying the inverse power law with an angular cutoff assumption and the hard-sphere model. Finally, (A3) is a constructive assumption on the external forces which can be satisfied by forces without decay or smallness assumption on their strength. In the following, we will give two examples of external forces satisfying (A3). Even though in general the assumption (A3) is difficult to verify and is in some sense unsatisfactory, it can be viewed as the improvement of the previous results on the study on the Boltzmann equation with the external force.

Remark 1.4: Based on the estimates on the cross section from Refs. 2 and 22, similar argument in this paper holds for the polynomial decay norm in the velocity. That is, define

$$|||f|||' = \sup_{t,x,v,}(1+|X(0;t,x,v)|^2)^p(1+|V(0;t,x,v,)|^2)^q|f(t,x,v)|$$

and

$$\|f_0\|'_{p,q} = \sup_{x,v}(1+|x|^2)^p(1+|v|^2)^q|f_0(x,v)|.$$

Moreover, instead of the assumptions (A1) and (A2), we assume the following:

(A1)′ $p>\frac{1}{2}$ and $q>\frac{3}{2}$.

(A2)′ The cross section B is in the form of (1.6) with $-2<\gamma\leqslant 1$ and satisfying

$$\left|\frac{b_\gamma(\theta)}{\cos\theta}\right|\leqslant b_0',$$

where b_0' is some positive constant.

Then similar to Theorem 1.2, we also have that under the assumptions (A1)′, (A2)′, and (A3), there is a sufficiently small positive constant $\delta_0'>0$ such that if $0\leqslant f_0(x,v)$ and $\|f_0\|'_{p,q}\leqslant\varepsilon\delta_0'$, then there exists a unique global in time mild solution $f(t,x,v)$ to the initial value problem (1.1) and (1.2) satisfying $|||f|||'\leqslant 2\varepsilon\delta_0'$.

Now to understand the assumption (A3), we give the following two examples:

Example 1.4: Let $E(t,x)\equiv E(t)$. For any fixed (t,x,v), the bicharacteristic equations (1.13) have solutions

$$X(s;t,x,v) = x+v(s-t)+\int_t^s\int_t^\eta E(\tau)\mathrm{d}\tau\,\mathrm{d}\eta,$$

$$V(s;t,x,v) = v+\int_t^s E(\tau)\mathrm{d}\tau.$$

Hence,

$$X(0;t,x,v) = x-vt-\int_0^t\int_t^\eta E(\tau)\mathrm{d}\tau\,\mathrm{d}\eta,$$

$$V(0;t,x,v) = v-\int_0^t E(\tau)\mathrm{d}\tau.$$

Therefore, (A3) holds with

$$\alpha_1(s;t,x,v) = s \quad \text{and } \alpha_2(s;t,x,v) = 1,$$

when $0 < \alpha_0 \leqslant 1$ and $-2 < \gamma \leqslant 1$.

In fact, notice that for this case when external forces depend only on the time t, the Boltzmann equation with external forces can be rewritten to the Boltzmann equation without forces by the following transformation of independent variables, cf. Ref. 8:

$$\tilde{t} = t,$$

$$\tilde{x} = x - \int_0^t \int_0^\eta E(\tau)\mathrm{d}\tau\,\mathrm{d}\eta, \tag{1.22}$$

$$\tilde{v} = v - \int_0^t E(\tau)\mathrm{d}\tau.$$

Therefore, the existence of mild and classical solutions and L^1 stability around vacuum to the Boltzmann equation without forces, cf. Refs. 13, 25, and 12, can be applied to this case without any difficulty.

Example 1.5: Let $E(t,x) = a^2x + E_0(t)$, with $a > 0$ being a constant. For any fixed (t,x,v), the bicharacteristic equations (1.13) have solutions

$$X(s;t,x,v) = \frac{ax+v}{2a}e^{a(s-t)} + \frac{ax-v}{2a}e^{-a(s-t)} - \frac{E_2(t)}{2a}e^{a(s-t)} + \frac{E_3(t)}{2a}e^{-a(s-t)} + E_1(s),$$

$$V(s;t,x,v) = \frac{ax+v}{2}e^{a(s-t)} - \frac{ax-v}{2}e^{-a(s-t)} - \frac{E_2(t)}{2}e^{a(s-t)} - \frac{E_3(t)}{2}e^{-a(s-t)} + E_1'(s),$$

where $E_1(s)$ is some special solution to the second order linear ODE,

$$\frac{d^2E_1(s)}{\mathrm{d}s^2} = a^2E_1(s) + E_0(s),$$

and $(E_2(t), E_3(t))$ are defined by

$$E_2(t) = E_1'(t) + aE_1(t),$$

$$E_3(t) = E_1'(t) - aE_1(t).$$

Hence,

$$X(0;t,x,v) = \frac{ax+v}{2a}e^{-at} + \frac{ax-v}{2a}e^{at} - \frac{E_2(t)}{2a}e^{-at} + \frac{E_3(t)}{2a}e^{at} + E_1(0),$$

$$V(0;t,x,v) = \frac{ax+v}{2}e^{-at} - \frac{ax-v}{2}e^{at} - \frac{E_2(t)}{2}e^{-at} - \frac{E_3(t)}{2}e^{at} + E_1'(0).$$

Straightforward calculation shows that

$$\alpha_1(s;t,x,v) = \frac{1}{2a}(e^{as} - e^{-as}) \quad \text{and } \alpha_2(s;t,x,v,) = \frac{1}{2}(e^{as} + e^{-as}).$$

Thus,

$$\alpha(s;t,x,v) = \alpha_1'(s;t,x,v)\alpha_2(s;t,x,v) - \alpha_1(s;t,x,v)\alpha_2'(s;t,x,v) \equiv 1 > 0$$

and

$$\alpha_2(s;t,x,v) \geqslant 1.$$

If $0 < \alpha_0 \leqslant 1$ and $-1 \leqslant \gamma \leqslant 1$, then (A3) holds.

Notice that the positive coefficient in front of x in the force term of Example 1.5 implies that the bicharacteristic curves go to infinity in space as time tends to infinity. If the coefficient is negative, then the bicharacteristic is oscillating in the space of (X,V) and there is no known existence results on this interesting case for the nonlinear Boltzmann equation. However, for the linearized Boltzmann equation, the case when $E(t,x) = -x$ was studied by Tabata[20] using the semigroup approach. This result was later generalized in Ref. 21 to the case of linearized Boltzmann equation with an unbounded external force potential that is spherically symmetric and satisfies some differential inequalities.

Now we compare Theorems 1.2 with the previous related work. First, if $p > 3/2$, the bound on the initial data f_0 implies the total mass satisfies

$$\int_{\mathbf{R}^3 \times \mathbf{R}^3} |f_0(x,v)| \mathrm{d}x\, \mathrm{d}v \leqslant C\varepsilon\delta_0,$$

where C is a generic positive constant. This requires that the mean free path is sufficient large if total mass is finite because δ_0 is sufficiently small. This is exactly the requirement on the Boltzmann equation without forces in infinite vacuum considered by Illner and Shinbrot in Ref. 13. On the other hand, as in Ref. 2, if $1/2 < p \leqslant 3/2$, then the initial total mass can be infinite. For the method of proof, as in Refs. 11 and 25. Theorem 1.2 is obtained by using the contraction mapping theorem. Precisely, we obtain the following estimates:

$$\begin{aligned} |||\mathbf{T}f||| &\leqslant C\|f_0\|_{p,q} + C|||f|||^2, \\ |||\mathbf{T}f - \mathbf{T}g||| &\leqslant C(|||f||| + |||g|||)|||f - g|||, \end{aligned} \tag{1.23}$$

where $\mathbf{T}$ is a mapping from $S_{p,q}$ to $S_{p,q}$ defined by (3.18) in Sec. III. In order to prove (1.23), we need to control the time integration of the collision term $Q(f,g)$ along the bicharacteristic,

$$\int_0^t Q(f,g)(s, X(s;t,x,v), V(s;t,x,v))\mathrm{d}s.$$

The estimation on this integral is based on the constructive assumption (A3) and is given in Lemma 3.1 of Sec. III.

There have been extensive studies on the mathematical aspects on the Boltzmann equation, see Refs. 2, 4, and 5. For the Boltzmann equation in the absence of an external force in infinite vacuum, the global existence of mild solutions to (1.1) was first given by Illner–Shinbrot[13] following the work on local existence by Kaniel–Shinbrot in Ref. 14. For perturbation of a global Maxwellian, Ukai,[24] Nishida–Imai,[16] Shizuta–Asano,[19] and Uaki–Asano,[26] and others showed the global existence of solutions to the initial or initial boundary value problem of the Boltzmann equation in various situations. For other interesting issues, such as large data existence theory, stability and convergence to the Maxwellian, see Refs. 6, 15, 18, and 23, and references therein.

However, there are fewer works done for the Boltzmann equation with an external force. Glikson[9,10] obtained the unique local existence of solutions to the initial value problem for sufficiently small initial data. When the initial data was arbitrary large, the local existence of solutions to the initial and initial boundary value problem was obtained by Asano.[1] And a general framework on the global existence solutions in infinite vacuum is given in Ref. 3. Recently, Guo[11] proved the global existence of classical solutions with small amplitude to the initial value problem for the Boltzmann equation with an external force and a "soft" potential when the external force

decays in time (see also Ref. 7). Moreover, the global existence and stability of the stationary solutions to time independent potential force was obtained by Ukai–Yang–Zhao in Ref. 27 through the energy method. Our result is new in the sense that a constructive condition is given for the global existence of mild solutions in infinite vacuum when external force can be arbitrary large.

The rest of this paper is organized as follows. In Sec. II, we give some preliminary estimates for later use. In Sec. III, we study the integration of the collision term to obtain the global in time estimate. And then the existence of the mild solution to the initial value problem (1.1) and (1.2) follows from the contraction mapping theorem.

II. PRELIMINARIES

In this section, we give some preliminary lemmas which will be used in the proof of the global existence of solutions in the next section. First we borrow three lemmas from Refs. 12 and 17 for the completeness of the paper. Interested readers please refer to these two papers for their proofs.

Lemma 2.1: *For any* $z \in \mathbf{R}^3$, $\eta \in \mathbf{R}$ *and* $(u_\parallel, u_\perp) \in \mathbf{R}^3 \times \mathbf{R}^3$ *with* $u_\parallel \cdot u_\perp = 0$, *we have*

$$|z + \eta u_\parallel|^2 + |z + \eta u_\perp|^2 = |z|^2 + |z + \eta(u_\parallel + u_\perp)|^2. \tag{2.1}$$

Lemma 2.2: *For any* $p > \frac{1}{2}$ *and* $(z,u) \in \mathbf{R}^3 \times \mathbf{R}^3$ *with* $u \neq 0$, *we have*

$$\int_0^\infty (1 + |z + \eta u|^2)^{-p} \, \mathrm{d}\eta \leqslant \frac{4p}{|u|(2p-1)}. \tag{2.2}$$

Moreover, for any $q > 0, -2 < \gamma \leqslant 1$ *and* $z \in \mathbf{R}^3$, *we have*

$$\int_{\mathbf{R}^3} |u|^{\gamma - 1} \exp\{-q|z-u|^2\} \mathrm{d}u \leqslant I^1_{\gamma,q}, \tag{2.3}$$

where

$$I^1_{\gamma,q} = \frac{4\pi}{\gamma + 2} + \frac{\pi}{q^{3/2}}, \tag{2.4}$$

is a positive constant depending only on γ *and* q.

Lemma 2.3: *For any* $p > 0$, $z \in \mathbf{R}^3$, $s \in \mathbf{R}^+$ *and* $(u_\parallel, u_\perp) \in \mathbf{R}^3 \times \mathbf{R}^3$ *with* $u_\parallel \cdot u_\perp = 0$, *we have that*

$$\begin{aligned}(1 + |z + su_\parallel|^2)^{-p}(1 + |z + su_\perp|^2)^{-p} \leqslant (1 + |z|^2)^{-p}\{&(1 + |z + su_\parallel|^2)^{-p} \\ &+ (1 + |z + su_\perp|^2)^{-p} + (1 + |z + s(u_\parallel + u_\perp)|^2)^{-p}\}.\end{aligned} \tag{2.5}$$

In order to control the integration of the collision term $Q(f,g)$ along the bicharacteristic

$$\int_0^t \int_{\mathbf{R}^3 \times S^2_+} (\cdots)(s, X(s;t,x,v), V(s;t,x,v)) \mathrm{d}u \, \mathrm{d}\omega \, \mathrm{d}s,$$

we consider the following two integrals:

$$\begin{aligned}I^{2,1}(z_1, z_2, t, x, v) = \int_0^\infty \int_{\mathbf{R}^3 \times S^2_+} &b_\gamma(\theta)|u|^\gamma (1 + |z_1 + \alpha_1(s;t,x,v)u|^2)^{-p} \\ &\times \exp\{-q|z_2 - \alpha_2(s;t,x,v)u|^2\} \mathrm{d}u \, \mathrm{d}\omega \, \mathrm{d}s\end{aligned} \tag{2.6}$$

and

$$I^{2,2}(z_1,z_2,t,x,v)=\int_0^\infty\int_{\mathbf{R}^3\times S_+^2} b_\gamma(\theta)|u|^\gamma\{(1+|z_1+\alpha_1(s;t,x,v)u_\parallel|^2)^{-p}+(1+|z_1+\alpha_1(s;t,x,v)u_\perp|^2)^{-p}\}$$
$$\times\exp\{-q|z_2-\alpha_2(s;t,x,v)u|^2\}\mathrm{d}u\,\mathrm{d}\omega\,\mathrm{d}s, \tag{2.7}$$

for any $(z_1,z_2)\in\mathbf{R}^3\times\mathbf{R}^3$ and $(t,x,v)\in\mathbf{R}^+\times\mathbf{R}^3\times\mathbf{R}^3$. Here $\alpha_1(s;t,x,v)$ and $\alpha_2(s;t,x,v)$ satisfy the assumption (A3). The estimates on (2.6) and (2.7) are given in the following lemma:

Lemma 2.4: *Under the assumptions (A1)–(A3), it holds that*

$$\sup I^{2,i}(z_1,z_2,t,x,v)\leqslant I^2_{\gamma,p,q},\ i=1,2, \tag{2.8}$$

where

$$I^2_{\gamma,p,q}=\frac{8\pi p b_0 I^1_{\gamma,q}}{\alpha_0(2p-1)}, \tag{2.9}$$

is a positive constant depending only on γ,p,q,α_0, *and* b_0.

Proof: For $i=1$, fix $(z_1,z_2)\in\mathbf{R}^3\times\mathbf{R}^3$ and $(t,x,v)\in\mathbf{R}^+\times\mathbf{R}^3\times\mathbf{R}^3$. Since $\alpha_2(s;t,x,v)>0$, we let

$$\alpha_2(s;t,x,v)u=\overline{u},$$

to obtain

$$I^{2,1}(z_1,z_2,t,x,v)=\int_0^\infty\int_{\mathbf{R}^3\times S_+^2} b_\gamma(\theta)|\overline{u}|^\gamma(\alpha_2(s;t,x,v))^{-\gamma-3}\left(1+\left|z_1+\frac{\alpha_1(s;t,x,v)}{\alpha_2(s;t,x,v)}\overline{u}\right|^2\right)^{-p}$$
$$\times\exp\{-q|z_2-\overline{u}|^2\}\mathrm{d}\overline{u}\,\mathrm{d}\omega\,\mathrm{d}s. \tag{2.10}$$

Since

$$\frac{d}{\mathrm{d}s}\left(\frac{\alpha_1(s;t,x,v)}{\alpha_2(s;t,x,v)}\right)=\frac{\alpha_1'(s;t,x,v)\alpha_2(s;t,x,v)-\alpha_1(s;t,x,v)\alpha_2'(s;t,x,v)}{(\alpha_2(s;t,x,v))^2}=\frac{\alpha(s;t,x,v)}{(\alpha_2(s;t,x,v))^2}>0,$$

by the assumption (A3), we can let variable

$$\eta=\frac{\alpha_1(s;t,x,v)}{\alpha_2(s;t,x,v)},$$

to have

$$I^{2,1}(z_1,z_2,t,x,v)\leqslant\int_0^\infty\int_{\mathbf{R}^3\times S_+^2} b_\gamma(\theta)|\overline{u}|^\gamma\frac{1}{(\alpha_2(s;t,x,v))^{\gamma+1}\alpha(s;t,x,v)}(1+|z_1+\eta\overline{u}|^2)^{-p}$$
$$\times\exp\{-q|z_2-\overline{u}|^2\}\mathrm{d}\overline{u}\,\mathrm{d}\omega\,\mathrm{d}\eta\leqslant\frac{1}{\alpha_0}\int_0^\infty\int_{\mathbf{R}^3\times S_+^2} b_\gamma(\theta)|\overline{u}|^\gamma(1+|z_1+\eta\overline{u}|^2)^{-p}$$
$$\times\exp\{-q|z_2-\overline{u}|^2\}\mathrm{d}\overline{u}\,\mathrm{d}\omega\,\mathrm{d}\eta. \tag{2.11}$$

Then it follows from the Lemma 2.2 and the assumption (A2) that

$$I^{2,1}(z_1,z_2,t,x,v) \leqslant \frac{4p}{\alpha_0(2p-1)}\int_{\mathbf{R}^3\times S_+^2} b_\gamma(\theta)|\overline{u}|^{\gamma-1}\exp\{-q|z_2-\overline{u}|^2\}\mathrm{d}\overline{u}\,\mathrm{d}\omega$$
$$= \frac{8\pi p}{\alpha_0(2p-1)}\int_0^{\frac{\pi}{2}} b_\gamma(\theta)\sin\theta\,\mathrm{d}\theta\int_{\mathbf{R}^3}|\overline{u}|^{\gamma-1}\exp\{-q|z_2-\overline{u}|^2\}\mathrm{d}\overline{u} \leqslant \frac{8\pi p b_0 I^1_{\gamma,q}}{\alpha_0(2p-1)}. \tag{2.12}$$

This completes the proof for $i=1$.

For the case of $i=2$, similar to (2.11) and (2.12), we have

$$I^{2,2}(z_1,z_2,t,x,v) \leqslant \frac{4p}{\alpha_0(2p-1)}\int_{\mathbf{R}^3\times S_+^2} b_\gamma(\theta)|\overline{u}|^\gamma\left(\frac{1}{|\overline{u}_\parallel|}+\frac{1}{|\overline{u}_\perp|}\right)\exp\{-q|z_2-\overline{u}|^2\}\mathrm{d}\overline{u}\,\mathrm{d}\omega$$
$$= \frac{8\pi p}{\alpha_0(2p-1)}\int_{\mathbf{R}^3}\int_0^{\pi/2} b_\gamma(\theta)|\overline{u}|^\gamma\left(\frac{1}{|\overline{u}|\cos\theta}+\frac{1}{|\overline{u}|\sin\theta}\right)\exp\{-q|z_2-\overline{u}|^2\}\sin\theta\,\mathrm{d}\overline{u}\,\mathrm{d}\theta$$
$$= \frac{8\pi p}{\alpha_0(2p-1)}\int_0^{\pi/2} b_\gamma(\theta)(1+\tan\theta)\mathrm{d}\theta\int_{\mathbf{R}^3}|\overline{u}|^{\gamma-1}\exp\{-q|z_2-\overline{u}|^2\}\mathrm{d}\overline{u} \leqslant \frac{8\pi p b_0 I^1_{\gamma,q}}{\alpha_0(2p-1)}. \tag{2.13}$$

Hence, (2.12) and (2.13) yields the proof of Lemma 2.4.

III. EXISTENCE OF THE MILD SOLUTION

In this section, we give the crucial estimate for the global existence of the solution by the contraction mapping theorem.

First, similar to (1.9)–(1.11), denote

$$N(f,g) = N^+(f,g) - N^-(f,g), \tag{3.1}$$

by

$$N^+(f,g)(t,x,v) = \int_0^t Q^+(f,g)(s,X(s;t,x,v),V(s;t,x,v))\mathrm{d}s$$
$$= \frac{1}{\varepsilon}\int_0^t\int_{\mathbf{R}^3 S_+^2} b_\gamma(\theta)|u|^\gamma f(s,X(s;t,x,v),V(s;t,x,v)-u_\parallel)g(s,X(s;t,x,v),$$
$$\times V(s;t,x,v)-u_\perp)\mathrm{d}u\,\mathrm{d}\omega\,\mathrm{d}s \tag{3.2}$$

and

$$N^-(f,g)(t,x,v) = \int_0^t Q^-(f,g)(s,X(s;t,x,v),V(s;t,x,v))\mathrm{d}s$$
$$= \frac{1}{\varepsilon}\int_0^t\int_{\mathbf{R}^3 S_+^2} b_\gamma(\theta)|u|^\gamma f(s,X(s;t,x,v),V(s;t,x,v))g(s,X(s;t,x,v),$$
$$\times V(s;t,x,v)-u)\mathrm{d}u\,\mathrm{d}\omega\,\mathrm{d}s. \tag{3.3}$$

From (1.9), we have

$$N(f,g)(t,x,v) = \int_0^t Q(f,g)(s,X(s;t,x,v),V(s;t,x,v))\mathrm{d}s. \tag{3.4}$$

Lemma 3.1: *Under the assumptions (A1)–(A3), it holds that*

$$|||N(f,g)||| \leqslant \frac{1}{\varepsilon} I_{\gamma,p,q} |||f||| \times |||g|||, \tag{3.5}$$

where $I_{\gamma,p,q}$ is a positive constant.

Proof: We first estimate the loss term $N^-(f,g)$ in (3.1). Let (t,x,v) fixed. From the definition (1.17) of the norm $\|\cdot\|$ and the assumption (A3), we have for any s in $(0,t)$,

$$\begin{aligned}
&|f(s,X(s;t,x,v),V(s;t,x,v))| \\
&\qquad \leqslant \|f(s)\|(1+|X(0;s,X(s;t,x,v),V(s;t,x,v))|^2)^{-p} \\
&\qquad\quad \times \exp\{-q|V(0;s,X(s;t,x,v),V(s;t,x,v))|^2\} \\
&\qquad = \|f(s)\|(1+|X(0;t,x,v)|^2)^{-p} \exp\{-q|V(0;t,x,v)|^2\}
\end{aligned} \tag{3.6}$$

and

$$\begin{aligned}
&|g(s,X(s;t,x,v),V(s;t,x,v)-u)| \\
&\qquad \leqslant \|g(s)\|(1+|X(0;s,X(s;t,x,v),V(s;t,x,v)-u)|^2)^{-p} \\
&\qquad\quad \times \exp\{-q|V(0;s,X(s;t,x,v),V(s;t,x,v)-u)|^2\} \\
&\qquad = \|g(s)\|(1+|X(0;t,x,v)+\alpha_1(s;t,x,v)u|^2)^{-p} \times \exp\{-q|V(0;t,x,v) \\
&\qquad\quad -\alpha_2(s;t,x,v)u|^2\}.
\end{aligned} \tag{3.7}$$

Hence, from (3.3), we have

$$\begin{aligned}
|N^-(f,g)(t,x,v)| &\leqslant \frac{1}{\varepsilon}\int_0^t \int_{\mathbf{R}^3\times S^2_+} b_\gamma(\theta)|u|^\gamma \|f(s)\|\|g(s)\|(1+|X(0;t,x,v)|^2)^{-p}\exp\{-q|V(0;t,x,v)|^2\} \\
&\quad \times(1+|X(0;t,x,v)+\alpha_1(s;t,x,v)u|^2)^{-p}\exp\{-q|V(0;t,x,v) \\
&\quad -\alpha_2(s;t,x,v)u|^2\}\mathrm{d}u\,\mathrm{d}\omega\,\mathrm{d}s \leqslant \frac{1}{\varepsilon}(1+|X(0;t,x,v)|^2)^{-p}\exp\{-q|V(0;t,x,v)|^2\} \\
&\quad \times|||f|||||g|||\int_0^\infty \int_{\mathbf{R}^3\times S^2_+} b_\gamma(\theta)|u|^\gamma(1+|X(0;t,x,v)+\alpha_1(s;t,x,v)u|^2)^{-p} \\
&\quad \times \exp\{-q|V(0;t,x,v)-\alpha_2(s;t,x,v)u|^2\}\mathrm{d}u\,\mathrm{d}\omega\,\mathrm{d}s.
\end{aligned} \tag{3.8}$$

By Lemma 2.4, we have

$$|N^-(f,g)(t,x,v)| \leqslant \frac{1}{\varepsilon} I^2_{\gamma,p,q}(1+|X(0;t,x,v)|^2)^{-p}\exp\{-q|V(0;t,x,v)|^2\}|||f||| \times |||g|||. \tag{3.9}$$

Multiplying (3.9) by $(1+|X(0;t,x,v)|^2)^p \exp\{q|V(0;t,x,v)|^2\}$ and taking the supremum with respect to (t,x,v) in $\mathbf{R}^+\times\mathbf{R}^3\times\mathbf{R}^3$, we have by (1.16) that

$$|||N^-(f,g)||| \leqslant \frac{1}{\varepsilon} I^2_{\gamma,p,q}|||f||| \times |||g|||. \tag{3.10}$$

Next for the gain term $N^+(f,g)$, similar to (3.6) and (3.7), we have for any s in $(0,t)$,

$$
\begin{aligned}
&|f(s,X(s;t,x,v),V(s;t,x,v)-u_{\|})| \\
&\qquad \leqslant \|f(s)\|(1+|X(0;s,X(s;t,x,v),V(s;t,x,v)-u_{\|})|^2)^{-p}\times\exp\{ \\
&\qquad\quad -q|V(0;s,X(s;t,x,v),V(s;t,x,v)-u_{\|})|^2\} \\
&\qquad = \|f(s)\|(1+|X(0;t,x,v)+\alpha_1(s;t,x,v)u_{\|}|^2)^{-p}\exp\{-q|V(0;t,x,v) \\
&\qquad\quad -\alpha_2(s;t,x,v)u_{\|}|^2\} \qquad (3.11)
\end{aligned}
$$

and

$$
\begin{aligned}
&|g(s,X(s;t,x,v),V(s;t,x,v)-u_{\perp})| \\
&\qquad \leqslant \|g(s)\|(1+|X(0;s,X(s;t,x,v),V(s;t,x,v)-u_{\perp})|^2)^{-p} \\
&\qquad\quad \times\exp\{-q|V(0;s,X(s;t,x,v),V(s;t,x,v)-u_{\perp})|^2\} \\
&\qquad = \|g(s)\|(1+|X(0;t,x,v)+\alpha_1(s;t,x,v)u_{\perp}|^2)^{-p} \\
&\qquad\quad \times\exp\{-q|V(0;t,x,v)-\alpha_2(s;t,x,v)u_{\perp}|^2\}. \qquad (3.12)
\end{aligned}
$$

Setting (3.11) and (3.12) into (3.2), we have that

$$
\begin{aligned}
|N^+(f,g)(t,x,v)| &\leqslant \frac{1}{\varepsilon}\int_0^t\int_{\mathbf{R}^3\times S_+^2} b_\gamma(\theta)|u|^\gamma\|f(s)\|\|g(s)\|(1+|X(0;t,x,v)+\alpha_1(s;t,x,v)u_{\|}|^2)^{-p} \\
&\quad\times(1+|X(0;t,x,v)+\alpha_1(s;t,x,v)u_{\perp}|^2)^{-p}\times\exp\{-q|V(0;t,x,v)-\alpha_2(s;t,x,v)u_{\|}|^2 \\
&\quad -q|V(0;t,x,v)-\alpha_2(s;t,x,v)u_{\perp}|^2\}\mathrm{d}u\,\mathrm{d}\omega\,\mathrm{d}s \leqslant \frac{1}{\varepsilon}|||f|||\times|||g|||\int_0^\infty\int_{\mathbf{R}^3\times S_+^2} b_\gamma(\theta) \\
&\quad\times|u|^\gamma(1+|X(0;t,x,v)+\alpha_1(s;t,x,v)u_{\|}|^2)^{-p}\times(1+|X(0;t,x,v) \\
&\quad +\alpha_1(s;t,x,v)u_{\perp}|^2)^{-p}\times\exp\{-q|V(0;t,x,v)-\alpha_2(s;t,x,v)u_{\|}|^2-q|V(0;t,x,v) \\
&\quad -\alpha_2(s;t,x,v)u_{\perp}|^2\}\mathrm{d}u\,\mathrm{d}\omega\,\mathrm{d}s. \qquad (3.13)
\end{aligned}
$$

By Lemmas 2.1 and 2.3, we have

$$
\begin{aligned}
|N^+(f,g)(t,x,v)| &\leqslant \frac{1}{\varepsilon}|||f|||\times|||g|||\int_0^\infty\int_{\mathbf{R}^3\times S_+^2} b_\gamma(\theta)|u|^\gamma(1+|X(0;t,x,v)|^2)^{-p} \\
&\quad\times\{(1+|X(0;t,x,v)+\alpha_1(s;t,x,v)u_{\|}|^2)^{-p}+(1+|X(0;t,x,v)+\alpha_1(s;t,x,v)u_{\perp}|^2)^{-p} \\
&\quad +(1+|X(0;t,x,v)+\alpha_1(s;t,x,v)u|^2)^{-p}\}\times\exp\{-q|V(0;t,x,v)|^2-q|V(0;t,x,v) \\
&\quad -\alpha_2(s;t,x,v)u|^2\}\mathrm{d}u\,\mathrm{d}\omega\,\mathrm{d}s \leqslant \frac{1}{\varepsilon}(1+|X(0;t,x,v)|^2)^{-p}\exp\{-q|V(0;t,x,v)|^2\}|||f||| \\
&\quad\times|||g|||\times\int_0^\infty\int_{\mathbf{R}^3\times S_+^2} b_\gamma(\theta)|u|^\gamma\{(1+|X(0;t,x,v)+\alpha_1(s;t,x,v)u_{\|}|^2)^{-p}+(1 \\
&\quad +|X(0;t,x,v)+\alpha_1(s;t,x,v)u_{\perp}|^2)^{-p}+(1+|X(0;t,x,v)+\alpha_1(s;t,x,v)u|^2)^{-p}\} \\
&\quad\times\exp\{-q|V(0;t,x,v)-\alpha_2(s;t,x,v)u|^2\}\mathrm{d}u\,\mathrm{d}\omega\,\mathrm{d}s. \qquad (3.14)
\end{aligned}
$$

Thus, it follows from Lemma 2.4 that

$$
|N^+(f,g)(t,x,v)| \leqslant \frac{2}{\varepsilon}I^2_{\gamma,p,q}(1+|X(0;t,x,v)|^2)^{-p}\exp\{-q|V(0;t,x,v)|^2\}|||f|||\times|||g|||,
$$

That is,

$$|||N^+(f,g)||| \leqslant \frac{2}{\varepsilon} I_{\gamma,p,q}^2 |||f||| \times |||g|||. \tag{3.15}$$

Combining (3.10) and (3.15), we have

$$|||N(f,g)||| \leqslant |||N^+(f,g)||| + |||N^-(f,g)||| \leqslant \frac{3}{\varepsilon} I_{\gamma,p,q}^2 |||f||| \times |||g|||. \tag{3.16}$$

Take $I_{\gamma,p,q}=3I_{\gamma,p,q}^2$ and then it follows from (2.4) and (2.9) that

$$I_{\gamma,p,q} = \frac{24\pi p b_0 I_{\gamma,q}^1}{\alpha_0(2p-1)} = \frac{24\pi p b_0}{\alpha_0(2p-1)}\left(\frac{4\pi}{\gamma+2} + \frac{\pi}{q^{3/2}}\right). \tag{3.17}$$

Therefore, (3.16) yields (3.5) and this completes the proof of Lemma 3.1.

Finally, we prove Theorem 1.2. For this purpose, we define the mapping $\mathbf{T}: S_{p,q} \to S_{p,q}$ by

$$\mathbf{T}f(t,x,v) = f_0(X(0;t,x,v), V(0;t,x,v)) + N(f,f)(t,x,v) \tag{3.18}$$

for any $f \in S_{p,q}$. For the mapping $\mathbf{T}$, we have the following lemma.

Lemma 3.2: *For any f, $g \in S_{p,q}$, it holds that*

$$\begin{aligned} |||\mathbf{T}f||| &\leqslant \|f_0\|_{p,q} + \frac{1}{\varepsilon} I_{\gamma,p,q} |||f|||^2, \\ |||\mathbf{T}f - \mathbf{T}g||| &\leqslant \frac{1}{\varepsilon} I_{\gamma,p,q} (|||f||| + |||g|||) |||f-g|||, \end{aligned} \tag{3.19}$$

where $I_{\gamma,p,q}$ is defined by (3.17).

Proof: Fix $f \in S_{p,q}$. Multiplying (3.18) by $(1+|X(0;t,x,v)|^2)^p \exp\{q|V(0;t,x,v)|^2\}$ and taking the supremum with respect to (t,x,v) over $\mathbf{R}^+ \times \mathbf{R}^3 \times \mathbf{R}^3$, by Lemma 3.1, we obtain the first estimate in (3.19). Then, notice that

$$\mathbf{T}f - \mathbf{T}g = N(f-g,f) + N(g,f-g). \tag{3.20}$$

The second estimate in (3.19) follows similarly.

Proof of Theorem 1.2: We only need to show that $\mathbf{T}$ has a fixed point by the contraction mapping theorem. In fact, let us denote the closed subset S_0 of $S_{p,q}$ by

$$S_0 = \{f \in S_{p,q} : |||f||| \leqslant 2\varepsilon\delta_0\}, \tag{3.21}$$

where δ_0 is a sufficiently small positive constant such that

$$\lambda_0 \equiv 4\delta_0 I_{\gamma,p,q} < 1. \tag{3.22}$$

Let $\|f_0\|_{p,q} \leqslant \varepsilon\delta_0$ and then we have from Lemma 3.2 that

$$\mathbf{T}f \in S_0 \quad \text{and } |||\mathbf{T}f - \mathbf{T}g||| \leqslant \lambda_0 |||f-g|||, \tag{3.23}$$

for any f, $g \in S_0$. Thus the mapping $\mathbf{T}: S_0 \to S_0$ is a contraction and hence has a fixed point f in $S_0 = \{f \in S_{p,q} : |||f||| \leqslant 2\varepsilon\delta_0\}$. This implies that the initial value problem (1.1) and (1.2) has a unique solution f such that $|||f||| \leqslant 2\varepsilon\delta_0$. It then follows from the same argument as the one in Ref. 25 that if $f_0(x,v) \geqslant 0$ then $f(t,x,v) \geqslant 0$. Hence, the proof of Theorem 1.2 is complete.

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Hyperbolic Kac–Moody superalgebras

L. Frappat
Laboratoire d'Annecy-le-Vieux de Physique Théorique, CNRS, UMR 5108, associée à l'Université de Savoie, BP 110, F-74941 Annecy-le-Vieux Cedex, France

A. Sciarrino
Dipartimento di Scienze Fisiche, Università di Napoli "Federico II" and INFN, Sezione di Napoli, Complesso Universitario di Monte S. Angelo, Via Cintia, I-80126 Napoli, Italy

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We present a classification of the hyperbolic Kac–Moody (HKM) superalgebras. The HKM superalgebras of rank $r \geqslant 3$ are finite in number (213) and limited in rank (6). The Dynkin–Kac diagrams and the corresponding simple root systems are determined. We also discuss a class of singular sub(super)algebras obtained by a folding procedure. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Affine Kac–Moody are presently well established tools of theoretical physics. The indefinite Kac–Moody (KM) algebras[1] form a so general set of algebras that they defy any general classification. A subclass of these KM algebras, called hyperbolic, which are defined by the property that the diagrams (generally disconnected) obtained taking away a dot from their defining diagrams define a direct sum of finite and/or affine KM algebras have been classified in Refs. 2 and 3. It has been found that these algebras are finite in number (238 in which 142 have a symmetric or symmetrizable Cartan matrix) and bounded in rank (10). These algebras have in the last decade attracted the attention of physicists, as they appear in a variety of physical models in two-dimensional field theories (supergravity, string theory, cosmological billiards).[4–7] Therefore it seems natural to study the corresponding partners in the realm of Kac–Moody superalgebras.[8–10] From these motivations, the authors of Ref. 11 have recently classified hyperbolic Kac–Moody (HKM) superalgebras by a procedure quite close to that followed to classify the hyperbolic Kac–Moody ones, showing that they are limited in rank, now the maximum rank being 6, and that they are finite in number (for rank >2). However, as we remarked that many diagrams are missing, while some of the proposed Dynkin–Kac diagrams correspond in fact to diagrams of untwisted or twisted affine Lie superalgebras (sometimes in the not distinguished basis), we present here a, hopefully exhaustive, classification of HKM superalgebras, together with a corresponding simple roots basis and we discuss a class of singular subalgebras.

The paper is organized as follows: in Sec. II we recall the definition of a superalgebra, the relation between Dynkin–Kac diagrams and generalized Cartan matrices, the action of the (super)Weyl or generalized Weyl transformations on the simple roots systems and the structure of the supplementary or non-Serre relations. Although most of the material is not new, we believe it is worthwhile to report it in some details for several reasons: (i) the standard rules of translating matrices in diagrams must be slightly and suitably defined to include the case of indefinite, in particular hyperbolic, KM superalgebras; (ii) the deformation of the Dynkin–Kac diagrams must be carefully handled, otherwise one is lead to naively include diagrams for HKM superalgebras, which really correspond to more general indefinite KM superalgebras; (iii) the action of the generalized Weyl transformations, which provides also in the case of HKM superalgebras all the not equivalent simple roots systems, allows one not to be worried about the appearance of new non-Serre relations. In Sec. III and the related appendixes we present the diagrams corresponding to HKM superalgebras, together with their (not unique) system of simple roots and with their

maximal regular subalgebras; in Sec. IV we list the singular subalgebras, obtained by the procedure of folding.

II. KAC–MOODY SUPERALGEBRAS

A. Generalized Cartan matrices and Dynkin diagrams

Let A be a $r\times r$ matrix and $\{i_1,\ldots,i_p\}$ be a subset of indices of $I=\{1,\ldots,r\}$. The principal $\{i_1,\ldots,i_p\}$-submatrix of A, of order $r-p$, is a matrix obtained from A by deleting the rows and columns labelled by $i_1,\ldots,i_p$. A principal submatrix of order $r-1$ is called leading.

We start by defining the notion of the generalized Cartan matrix. In the case of $\mathbb{Z}_2$-graded algebras, it is convenient to deal with a recursive definition.

Definition 2.1: *A $r\times r$ matrix A with integral entries a_{ij} is called a* generalized Cartan matrix *if for each $i\in\{1,\ldots,r\}$, the leading principal $\{i\}$-submatrix of A is a generalized Cartan matrix (which may be of block diagonal form).*

The Cartan matrices of the simple Lie algebras—A_n, B_n, C_n, D_n, $E_{6,7,8}$, F_4, and G_2—and of the basic Lie superalgebras—$A(m,n)$, $B(m,n)$, $C(n+1)$, $D(m,n)$, $F(4)$, $G(3)$, and $D(2,1,\alpha)$—are generalized Cartan matrices.

The matrix A is called symmetrizable *if it exists an invertible diagonal matrix D such that DA is a symmetric matrix. The matrix A is called* indecomposable *if it cannot be reduced to a block diagonal form by reordering rows and columns.*

We will only consider generalized Cartan matrices which are indecomposable and symmetrizable. Moreover, we assume that the generalized Cartan matrices are properly normalized, i.e., $a_{ii}=2$ or $a_{ii}=0$ for each i. If one defines the matrix $D_{ij}=d_i\delta_{ij}$ where the rational coefficients d_i satisfy $d_ia_{ij}=d_ja_{ji}$, the symmetric Cartan matrix A' is given from the generalized Cartan matrix A by $A'=DA$. Note that, due to the fact that off-diagonal entries of a row of a Cartan matrix corresponding to $a_{ii}=0$ may have different signs, the diagonal entries of the symmetric Cartan matrices are not necessarily positive.

Remark 2.1: It follows from the definition that the Cartan matrices of the affine (untwisted or twisted) Kac–Moody algebras and superalgebras are generalized Cartan matrices.

Definition 2.2: *Let τ be a subset of $I=\{1,\ldots,r\}$. To a given generalized Cartan matrix A and subset τ, we associate a complex contragradient Lie superalgebra $\mathcal{G}(A,\tau)$—called Kac–Moody superalgebra—with $3r$ generators h_i, $e_i^{\pm}$ and $\mathbb{Z}_2$-gradation defined by* $\deg e_i^{\pm}=\bar{0}$ *if $i\notin\tau$,* $\deg e_i^{\pm}=\bar{1}$ *if $i\in\tau$ and* $\deg h_i=\bar{0}$ *for all i. The generators h_i and $e_i^{\pm}$ are subject to the following set of relations:*

$$[h_i,h_j]=0, \tag{2.1}$$

$$[h_i,e_j^{\pm}]=\pm a_{ij}e_j^{\pm}, \tag{2.2}$$

$$[\![e_i^{+},e_j^{-}]\!]=\delta_{ij}h_i, \tag{2.3}$$

$$[\![e_i^{\pm},e_i^{\pm}]\!]=0 \quad \text{if } a_{ii}=0 \tag{2.4}$$

and

$$(\mathrm{ad}\, e_i^{\pm})^{1-\tilde{a}_{ij}}e_j^{\pm}=0 \tag{2.5}$$

where the matrix $\tilde{A}=(\tilde{a}_{ij})$ is deduced from the Cartan matrix $A=(a_{ij})$ of $\mathcal{G}(A,\tau)$ by replacing all its positive off-diagonal entries by -1. Here ad *denotes the adjoint action*

$$(\mathrm{ad}\, X)Y=[\![X,Y]\!]=XY-(-1)^{\deg X\cdot\deg Y}YX. \tag{2.6}$$

We denote by $\mathcal{G}_{\bar{0}}$ and $\mathcal{G}_{\bar{1}}$ the even and odd parts of the Kac–Moody superalgebra $\mathcal{G}(A,\tau)$. Let $\mathcal{H}\subset\mathcal{G}_{\bar{0}}$ be the subalgebra of $\mathcal{G}$ generated by the h_i (Cartan subalgebra). The superalgebra $\mathcal{G}(A,\tau)$ can be decomposed as $\mathcal{G}=\oplus_\alpha\mathcal{G}_\alpha$ where $\mathcal{G}_\alpha=\{x\in\mathcal{G}\,|\,[h,x]=\alpha(h)x, h\in\mathcal{H}\}$. By definition, the root system of $\mathcal{G}$ is the set $\Delta=\{\alpha\in\mathcal{H}^*\,|\,\mathcal{G}_\alpha\neq 0\}$. A root α is called even (respectively, odd) if $\mathcal{G}_\alpha\cap\mathcal{G}_{\bar{0}}\neq\emptyset$ (respectively, $\mathcal{G}_\alpha\cap\mathcal{G}_{\bar{1}}\neq\emptyset$). The set of even (respectively, odd) roots is denoted by $\Delta_{\bar{0}}$

(respectively, $\Delta_{\bar{1}}$). Since $\mathcal{G}(A,\tau)$ clearly admits a Borel decomposition, one defines as usual the notion of simple root system.[8,12]

To each superalgebra $\mathcal{G}(A,\tau)$ can be associated a Dynkin diagram according to the following rules.[12] We will always assume that $i\in\tau$ if $a_{ii}=0$.

(1) Using the generalized Cartan matrix A,

(a) one associates to each i such that $a_{ii}=2$ and $i\notin\tau$ a white dot, to each i such that $a_{ii}=2$ and $i\in\tau$ a black dot, to each i such that $a_{ii}=0$ and $i\in\tau$ a grey dot,

white dot ○ black dot ● grey dot ⊗ .

(b) The ith and jth dots will be joined by η_{ij} lines where

$$\eta_{ij}=\max(|a_{ij}|,|a_{ji}|) \quad \text{if } a_{ii}\neq 0 \text{ or/and } a_{jj}\neq 0 \text{ and } |a_{ij}a_{ji}|\leqslant 4,$$

$$\eta_{ij}=|a_{ij}|=|a_{ij}| \quad \text{if } a_{ii}=a_{jj}=0 \text{ and } |a_{ij}|,|a_{ji}|\leqslant 4.$$

Otherwise, the ith and jth dots will be joined by a boldface line equipped with an ordered pair of integers $(|a_{ij}|,|a_{ji}|)$. Note that this latter case does not appear for finite or affine Kac–Moody superalgebras.

(c) We add an arrow on the lines connecting the ith and jth dots when $\eta_{ij}>1$ and $|a_{ij}|\neq|a_{ji}|$, pointing from j to i if $|a_{ij}|>1$.

(d) For $D(2,1;\alpha)$, $\eta_{ij}=1$ if $a_{ij}\neq 0$ and $\eta_{ij}=0$ if $a_{ij}=0$. No arrow is set on the Dynkin diagram.

(2) Using the symmetric Cartan matrix A',

(a) one associates to each i such that $a'_{ii}\neq 0$ and $i\notin\tau$ a white dot, to each i such that $a'_{ii}\neq 0$ and $i\in\tau$ a black dot, to each i such that $a'_{ii}=0$ and $i\in\tau$ a grey dot (see pictures above).

(b) The ith and jth dots will be joined by η_{ij} lines where

$$\eta_{ij}=\frac{2|a'_{ij}|}{\min(|a'_{ii}|,|a'_{jj}|)} \quad \text{if } a'_{ii}\cdot a'_{jj}\neq 0 \text{ and } a'^{2}_{ij}\leqslant|a'_{ii}\cdot a'_{jj}|,$$

$$\eta_{ij}=\frac{2|a'_{ij}|}{\min(|a'_{ii}|,2)} \quad \text{if } a'_{ii}\neq 0,\ a'_{jj}=0 \text{ and } \eta_{ij}\leqslant 4,$$

$$\eta_{ij}=|a'_{ij}| \quad \text{if } a'_{ii}=a'_{jj}=0 \text{ and } |a'_{ij}|\leqslant 4.$$

Otherwise, the ith and jth dots will be joined by a boldface line equipped with an ordered pair of integers $(|a_{ij}|,|a_{ji}|)$.

(c) We add an arrow on the lines connecting the ith and jth dots when $\eta_{ij}>1$, pointing from i to j if $a'_{ii}\cdot a'_{jj}\neq 0$ and $|a'_{ii}|>|a'_{jj}|$ or if $a'_{ii}=0$, $a'_{jj}\neq 0$, $|a'_{jj}|<2$, and pointing from j to i if $a'_{ii}=0$, $a'_{jj}\neq 0$, $|a'_{jj}|>2$.

(d) For $D(2,1;\alpha)$, $\eta_{ij}=1$ if $a'_{ij}\neq 0$ and $\eta_{ij}=0$ if $a'_{ij}=0$. No arrow is set on the Dynkin diagram. Although the rules seem more complicated when using the symmetric Cartan matrix A', the computation of the Cartan matrix A is often more involved than the symmetric Cartan matrix A'.

Remark 2.2: The entries of the symmetric Cartan matrices A' can be obtained as the scalar products of the simple roots, i.e., $a'_{ij}=(\alpha_i,\alpha_j)$ (up to a multiplication by a suitable factor in order to get integer entries).

Remark 2.3: The above rules imply that two white/black dots of square length L and scalar product S are connected by $|2S/L|$ lines. With this convention, the Dynkin diagram of the affine Kac–Moody algebra $A_1^{(1)}$ is simply given by two white dots connected by two lines without any arrow.

Note that for superalgebras Dynkin–Kac diagrams with the same "topology" may be different. For example the diagrams drawn below represent, respectively, the superalgebras sl(2|2), osp(4|2), osp(4|4) and a hyperbolic Kac–Moody superalgebra of rank four (see Definition 3.1). The root systems are described in terms of the orthogonal vectors ε_i, δ_i, and $K^{\pm}$ (see Appendix B for conventions),

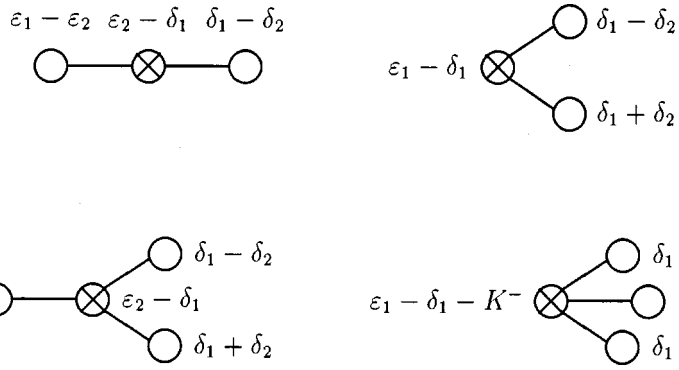

B. Non-Serre-type relations and generalized Weyl transformations

In the case of finite and affine Kac–Moody superalgebras, it is known that the description given by the Serre relations (2.1) to (2.4) may lead to superalgebras with nontrivial ideals.[13,14] In order to obtain a simple superalgebra, it is necessary to write supplementary relations involving more than two generators, in order to quotient the bigger superalgebra. These supplementary non-Serre-type conditions appear when one deals with isotropic odd roots (that is $a_{ii}=0$).

The supplementary conditions depend on the different kinds of vertices which appear in the Dynkin diagrams. The vertices for finite and affine superalgebras can be of the following type:

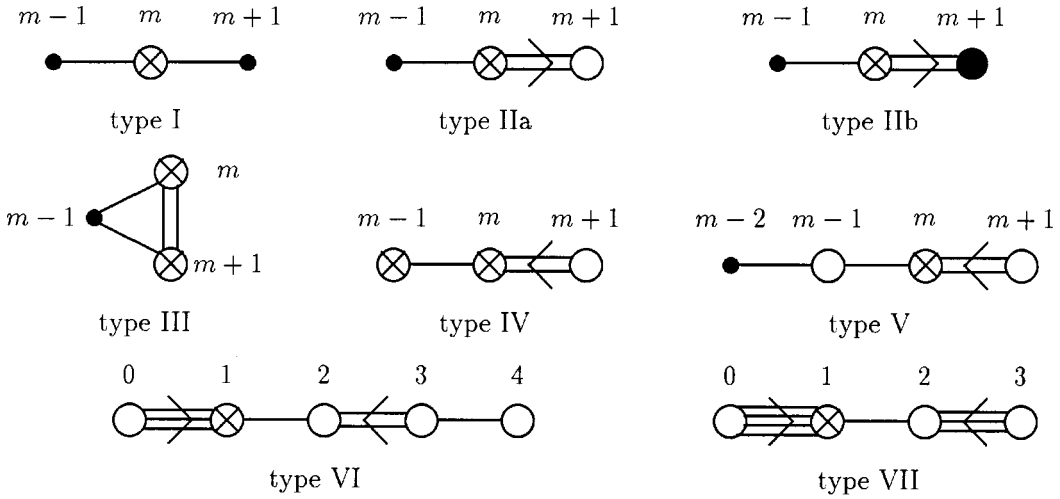

where the small black dots represent either white dots associated to even roots or grey dots associated to isotropic odd roots. Hyperbolic superalgebras exhibit also more complicated vertices.

The supplementary conditions take the following form:[13–15]

$$\text{type I, IIa, and IIb vertices,} \quad [[e_m^{\pm},[[e_{m+1}^{\pm},[[e_m^{\pm},e_{m-1}^{\pm}]]]]]=0,$$

$$\text{type III vertex,} \quad [[e_m^{\pm},[[e_{m+1}^{\pm},e_{m-1}^{\pm}]]]-[[e_{m+1}^{\pm},[[e_m^{\pm},e_{m-1}^{\pm}]]]=0,$$

$$\text{type IV vertex,} \quad [[e_m^{\pm},[[[[e_{m+1}^{\pm},[[e_m^{\pm},e_{m-1}^{\pm}]]],[[e_m^{\pm},e_{m-1}^{\pm}]]]]=0,$$

$$\text{type V vertex,} \quad [[e_m^{\pm},[[e_{m-1}^{\pm},[[e_m^{\pm},[[e_{m+1}^{\pm},[[e_m^{\pm},[[e_{m-1}^{\pm},e_{m-2}^{\pm}]]]]]]]]]]]=0,$$

$$\text{type VI vertex,} \quad [[e_2^\pm,[[e_1^\pm,[[e_3^\pm,[[e_2^\pm,[[e_1^\pm,e_0^\pm]]]]]]]]] - 2[[e_1^\pm,[[e_2^\pm,[[e_3^\pm,[[e_2^\pm,[[e_1^\pm,e_0^\pm]]]]]]]]] = 0,$$

$$\text{type VII vertex,} \quad 2\,[[e_2^\pm,[[e_1^\pm,[[e_3^\pm,[[e_2^\pm,[[e_1^\pm,e_0^\pm]]]]]]]]] - 3[[e_1^\pm,[[e_2^\pm,[[e_3^\pm,[[e_2^\pm,[[e_1^\pm,e_0^\pm]]]]]]]]] = 0.$$

For Kac–Moody superalgebras, there are in general many inequivalent simple root systems (when they contain isotropic odd roots), up to a transformation of the Weyl group $W(\mathcal{G})$ of $\mathcal{G}$. Following Ref. 16, the Weyl group $W(\mathcal{G})$ is extended by adding the following transformations (called generalized Weyl transformations) associated to the isotropic odd roots of $\mathcal{G}$. For $\alpha \in \Delta_{\bar{1}}$, one defines

$$w_\alpha(\beta) = \beta - 2\frac{(\alpha,\beta)}{(\alpha,\alpha)}\alpha \quad \text{if } (\alpha,\alpha) \neq 0,$$

$$w_\alpha(\beta) = \beta + \alpha \quad \text{if } (\alpha,\alpha) = 0 \text{ and } (\alpha,\beta) \neq 0,$$

$$w_\alpha(\beta) = \beta \quad \text{if } (\alpha,\alpha) = 0 \text{ and } (\alpha,\beta) = 0,$$

$$w_\alpha(\alpha) = -\alpha. \tag{2.7}$$

The transformation associated to an isotropic odd root α cannot be lifted to an automorphism of the superalgebra since w_α transforms even roots into odd ones, and vice versa, and the $\mathbb{Z}_2$-gradation would not be respected.

Let Δ^0 be a simple root system of $\mathcal{G}$ and α an isotropic odd root. Then one has for any root $\gamma \neq n_\alpha \alpha$,

$$\gamma = \sum_{\substack{\beta \neq \alpha \in \Delta^0 \\ a_{\alpha\beta} \neq 0}} n_\beta \beta + \sum_{\substack{\beta \neq \alpha \in \Delta^0 \\ a_{\alpha\beta} = 0}} n_\beta \beta + n_\alpha \alpha = \sum_{\beta \neq \alpha \in \Delta^0} n_\beta w_\alpha(\beta) + s_\gamma w_\alpha(\alpha), \tag{2.8}$$

where the coefficients n_α, $n_\beta \in \mathbb{Z}_{\geqslant 0}$ and s_γ is given by

$$s_\gamma = \sum_{\substack{\beta \neq \alpha \in \Delta^0 \\ a_{\alpha\beta} \neq 0}} n_\beta - n_\alpha. \tag{2.9}$$

Then, by induction on the height of the root γ, one can prove that s_γ is a non-negative number, which shows that the transformed simple root system $w_\alpha(\Delta^0)$ is again a simple root system.[16] The generalization of the Weyl group gives a method for constructing all the simple root systems of $\mathcal{G}$ and hence all the inequivalent Dynkin diagrams. A simple root system Δ^0 being given, from any isotropic odd root $\alpha \in \Delta^0$, one constructs the simple root system $w_\alpha(\Delta^0)$ where w_α is the generalized Weyl reflection with respect to α and one repeats the procedure on the obtained system until no new basis arises.

Note that this procedure is in fact very general and apply for any Kac–Moody superalgebra whose simple root systems contain isotropic odd roots. However, for Kac–Moody superalgebras which are neither of finite type nor of affine one, one may obtain in certain cases simple root systems containing even or odd root(s) of very large negative length. We will comment this point in the next section in the peculiar case of hyperbolic KM superalgebras.

III. HYPERBOLIC KAC–MOODY SUPERALGEBRAS

A. Definition

Let $\mathcal{G}(A,\tau)$ be a Kac–Moody superalgebra with generalized Cartan matrix A and $\mathbb{Z}_2$-gradation τ. By convention, it will be called indefinite Kac–Moody superalgebra if it is neither of finite nor of affine type. Of course, when the $\mathbb{Z}_2$-gradation τ is trivial, one recovers the usual classification of the Kac–Moody algebras.

Definition 3.1: *Let $\mathcal{G}(A,\tau)$ be an indefinite Kac–Moody superalgebra with generalized Cartan*

matrix A and nontrivial $\mathbb{Z}_2$*-gradation* τ *corresponding to a connected Dynkin–Kac diagram.* $\mathcal{G}(A,\tau)$ *is called a* hyperbolic Kac–Moody (HKM) *superalgebra if every leading principal submatrix of A decomposes into constituents of finite or affine type, or equivalently, if deleting a vertex of the Dynkin diagram, one gets Dynkin diagrams of finite or affine type.*

The hyperbolic superalgebras are divided into the following classes:

(1) strictly hyperbolic if every leading principal submatrix of A decomposes into constituents of finite type,
(2) purely hyperbolic if every leading principal submatrix of A decomposes into constituents of affine type,
(3) hyperfinite if at least one leading principal submatrix of A decomposes into constituents of finite type,
(4) hyperaffine if at least one leading principal submatrix of A decomposes into constituents of affine type.

Theorem 3.2: *The hyperbolic Kac–Moody superalgebras of rank* $r \geqslant 3$ *are finite in number (213) and limited in rank (6). They are listed in Appendix A.*

Remark 3.1: As in the algebraic case, the HKM superalgebras are *not* of finite growth.[10,17] Let us remind the notion of growth: let $\mathcal{G}(A,\tau)$ be a Kac–Moody superalgebra and $\mathcal{I} \subset \mathcal{G}$ a finite subset of $\mathcal{G}$. The growth of $\mathcal{G}$ is by definition the number

$$r(\mathcal{G}) = \sup_{\mathcal{I}} \overline{\lim_{n\to\infty}} (\ln d(\mathcal{I},n)/\ln n), \tag{3.1}$$

where $\mathcal{I}$ runs over all finite subsets of $\mathcal{G}$ and $d(\mathcal{I},n)$ is the dimension of the linear span of the commutators of length at most n of elements of $\mathcal{I}$. The superalgebra $\mathcal{G}$ is of finite growth if $r(\mathcal{G}) < \infty$.

By applying the Definition 3.1, one gets a Dynkin diagram for a given HKM superalgebra. The other Dynkin diagrams are obtained by means of generalized Weyl transformations. Generally, the transformed Dynkin diagrams do not satisfy the Definition 3.1 (see example below). We conjecture that it always exists only one Dynkin diagram with the minimal number of odd roots satisfying Definition 3.1. Such a Dynkin diagram will be called distinguished.

B. Example

As an illustration of the generalized Weyl transformations procedure, we give below the different inequivalent simple root systems with the corresponding Dynkin diagrams and symmetric Cartan matrices of a HKM superalgebra of rank 6. Let $(\varepsilon_+ = K^+, \varepsilon_- = K^-, \varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \varepsilon_5 = \delta)$ be a basis of $\mathbb{R}^{(5,2)}$ with metric $g_{ij} = (\varepsilon_i, \varepsilon_j)$ such that $g_{+-} = g_{-+} = g_{11} = g_{22} = g_{33} = g_{44} = -g_{55} = 1$ and all other values are zero.

(i) Simple root system $\Delta^0 = \{\alpha_1 = \delta - \varepsilon_1 - K^-, \alpha_2 = \varepsilon_1 - \varepsilon_2, \alpha_3 = \varepsilon_2 - \varepsilon_3, \alpha_4 = \varepsilon_3 - \varepsilon_4, \alpha_5 = \varepsilon_3 + \varepsilon_4, \alpha_6 = K^+ - \varepsilon_1 - \varepsilon_2\}$,

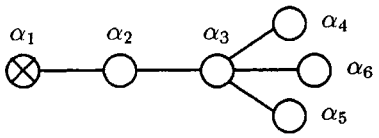

$$\begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & -1 & -1 \\ 0 & 0 & -1 & 2 & 0 & 0 \\ 0 & 0 & -1 & 0 & 2 & 0 \\ 0 & 0 & -1 & 0 & 0 & 2 \end{pmatrix}.$$

(ii) Simple root system $\Delta^0 = \{\alpha_1 = K^- - \delta + \varepsilon_1, \alpha_2 = \delta - \varepsilon_2 - K^-, \alpha_3 = \varepsilon_2 - \varepsilon_3, \alpha_4 = \varepsilon_3 - \varepsilon_4, \alpha_5 = \varepsilon_3 + \varepsilon_4, \alpha_6 = K^+ - \varepsilon_1 - \varepsilon_2\}$,

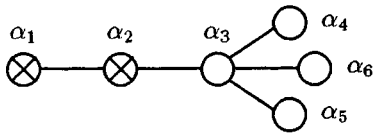

$$\begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & -1 & -1 \\ 0 & 0 & -1 & 2 & 0 & 0 \\ 0 & 0 & -1 & 0 & 2 & 0 \\ 0 & 0 & -1 & 0 & 0 & 2 \end{pmatrix}.$$

(iii) Simple root system $\Delta^0=\{\alpha_1=\varepsilon_1-\varepsilon_2, \alpha_2=K^- -\delta+\varepsilon_2, \alpha_3=\delta-\varepsilon_3-K^-, \alpha_4=\varepsilon_3-\varepsilon_4, \alpha_5=\varepsilon_3+\varepsilon_4, \alpha_6=K^+-\varepsilon_1-\varepsilon_2\}$,

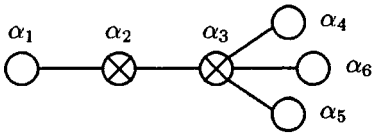

$$\begin{pmatrix} 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & -1 & -1 \\ 0 & 0 & -1 & 2 & 0 & 0 \\ 0 & 0 & -1 & 0 & 2 & 0 \\ 0 & 0 & -1 & 0 & 0 & 2 \end{pmatrix}.$$

(iv) Simple root system $\Delta^0=\{\alpha_1=\varepsilon_1-\varepsilon_2, \alpha_2=\varepsilon_2-\varepsilon_3, \alpha_3=K^- -\delta+\varepsilon_3, \alpha_4=\delta-\varepsilon_4-K^-, \alpha_5=\delta+\varepsilon_4-K^-, \alpha_6=K^+-K^-+\delta-\varepsilon_1-\varepsilon_2-\varepsilon_3\}$,

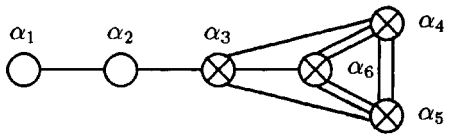

$$\begin{pmatrix} 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & -2 & -2 \\ 0 & 0 & 1 & -2 & 0 & -2 \\ 0 & 0 & 1 & -2 & -2 & 0 \end{pmatrix}.$$

(v) Simple root system $\Delta^0=\{\alpha_1=\varepsilon_1-\varepsilon_2, \alpha_2=\varepsilon_2-\varepsilon_3, \alpha_3=\varepsilon_3-\varepsilon_4, \alpha_4=K^- -\delta+\varepsilon_4, \alpha_5=2\delta-2K^-, \alpha_6=K^+-2K^-+2\delta-\varepsilon_1-\varepsilon_2-\varepsilon_3-\varepsilon_4\}$

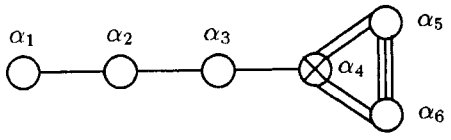

$$\begin{pmatrix} 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 2 & 2 \\ 0 & 0 & 0 & 2 & -4 & -6 \\ 0 & 0 & 0 & 2 & -6 & -4 \end{pmatrix}.$$

The explicit form of the non-Serre-type supplementary relations for HKM superalgebras is not known yet, at least for the vertices which are not of finite nor of affine type. However, another alternative way of describing the HKM superalgebras is to consider *all* inequivalent Dynkin diagrams and write the usual Serre relations (2.1) and (2.2) (of course this leads to redundant information). Indeed, the non-Serre-type relations become Serre relations after a generalized Weyl reflection with respect to an appropriate isotropic odd root.[18]

Note nevertheless that in the case of HKM superalgebras, one may produce by generalized Weyl transformations some exotic simple root systems corresponding to Cartan matrices with noninteger (rational) entries associated to weird nonstandard Dynkin diagrams (this was *not* the

case in the above example). As in the usual case, one gets supplementary non-Serre-type relations, but now also associated to nonisotropic even simple roots.

C. Rank two HKM superalgebras

Clearly any rank 2 HKM superalgebra is described by a Dynkin–Kac diagram of the form

where the dot can be a white, black or grey dot. Both dots cannot be either white, as this diagram describes KM algebras, or grey, as this diagram is isomorphic to the diagram, in the nondistinguished basis, of sl(1/2). The Dynkin–Kac diagrams corresponding to rank 2 finite and affine KM superalgebras, up to generalized Weyl transformations, are listed below

$$\mathrm{osp}(1|4) \quad \begin{pmatrix} 2 & -1 \\ -2 & 2 \end{pmatrix},$$

$$\mathrm{sl}(1|3)^{(4)} \quad \begin{pmatrix} 2 & -2 \\ -2 & 2 \end{pmatrix},$$

$$\mathrm{sl}(1|2) \quad \begin{pmatrix} 0 & 1 \\ -1 & 2 \end{pmatrix},$$

$$\mathrm{osp}(1|2)^{(1)} \quad \begin{pmatrix} 2 & -1 \\ -4 & 2 \end{pmatrix},$$

$$\mathrm{osp}(2|2)^{(2)} \quad \begin{pmatrix} 2 & -2 \\ -2 & 2 \end{pmatrix},$$

$$\mathrm{osp}(3|2) \quad \begin{pmatrix} 0 & 1 \\ -2 & 2 \end{pmatrix},$$

In Refs. 17 and 10, it is proven that any superalgebra associated to a 2×2 matrix not appearing in the above list is of *infinite growth*. It follows.

Theorem 3.3: *The hyperbolic Kac–Moody superalgebras of rank two are infinite in number. Their generalized Cartan matrix and Dynkin diagram are, up to generalized Weyl transformations, reducible to one of the following list:*

(i) *with* $\mathbb{Z}_2$*-gradation* $\tau=\{1\}$,

$$\begin{pmatrix} 2 & -k \\ -k' & 2 \end{pmatrix} \quad \text{with } (k,k')=(1,k'), \quad k'\leqslant 4, \quad (k,k')=(3,1) \text{ or } k,k'\in\mathbb{Z}_{>0}, \quad kk'>4,$$

$$\begin{pmatrix} 0 & 1 \\ -k & 2 \end{pmatrix} \quad \text{with } k\in\mathbb{Z}_{>0}, \quad k>2,$$

(ii) *with* $\mathbb{Z}_2$*-gradation* $\tau=\{1,2\}$,

$$\begin{pmatrix} 2 & -k \\ -k' & 2 \end{pmatrix} \quad \text{with } (k,k')=(1,k'), \quad k'\leqslant 4 \text{ or } k,k'\in\mathbb{Z}_{>0}, \quad kk'>4,$$

$$\begin{pmatrix} 0 & 1 \\ -k & 2 \end{pmatrix} \quad \text{with } k\in\mathbb{Z}_{>0}, \quad k\neq 2.$$

We denote them as $BW(k,k')$, $GW(k)$, $BB(k,k')$, and $GB(k)$, with corresponding Dynkin diagrams,

Note that in order to write only one type of diagram, we have not strictly followed the rules given in Sec. II.

The simple root systems of the HKM superalgebras $BW(k,k')$ and $BB(k,k')$ are given by

$$\alpha = \sum_{i=1}^{n} k_i \varepsilon_i + k_\alpha K^+ \quad \text{and} \quad \alpha' = -\sum_{i=1}^{n'} k'_i \varepsilon_i - k'_\alpha K^-, \tag{3.2}$$

where k_i, k'_i, k_α, $k'_\alpha \in \mathbb{Z}_{\geqslant 0}$ satisfy $kk' = k_\alpha k'_\alpha + \Sigma_{i=1}^{\min(n,n')} k_i k'_i$, $k^2 = \Sigma_{i=1}^{n} k_i^2$, and $k'^2 = \Sigma_{i=1}^{n'} k_i'^2$, while for the HKM superalgebras $GW(k)$ and $GB(k)$ the simple roots are $\alpha = -kK^-$ and $\alpha' = \varepsilon_1 - \varepsilon_2 + K^+$.

IV. SUBALGEBRAS OF HYPERBOLIC KM SUPERALGEBRAS

Let $\mathcal{G}$ be a Kac–Moody superalgebra, and consider its canonical root decomposition

$$\mathcal{G} = \mathcal{H} \oplus \bigoplus_{\alpha \in \Delta} \mathcal{G}_\alpha,$$

where $\mathcal{H}$ is the Cartan subalgebra of $\mathcal{G}$ and Δ its corresponding root system. A sub(super)algebra $\mathcal{G}'$ of $\mathcal{G}$ is called regular if $\mathcal{G}'$ has the root decomposition

$$\mathcal{G}' = \mathcal{H}' \oplus \bigoplus_{\alpha' \in \Delta'} \mathcal{G}'_{\alpha'},$$

where $\mathcal{H}' \subset \mathcal{H}$ and $\Delta \subset \Delta'$.

Consider a HKM superalgebra $\mathcal{G}$. Deleting a dot in the distinguished Dynkin diagram of $\mathcal{G}$ leads to regular sub(super)algebras of $\mathcal{G}$ of finite or affine type by definition. In Appendix C, we list these regular sub(super)algebras corresponding to the Dynkin diagrams of Appendix A. Note that in several cases, the diagram of the subsuperalgebra is not the distinguished one.

A sub(super)algebra $\mathcal{G}'$ of $\mathcal{G}$ is called singular if it is not regular. The folding method allows one to obtain some singular sub(super)algebras of the HKM superalgebras. Let $\mathcal{G}$ be a HKM superalgebra with a distinguished Dynkin diagram exhibiting a $\mathbb{Z}_N$ symmetry. This $\mathbb{Z}_N$ symmetry is generated by an automorphism τ of order $N(\tau^N = 1)$ acting on the root system. The automorphism τ can be lifted at the algebra level by setting $\tau(e_\alpha) = e_{\tau(\alpha)}$ for a generator e_α associated to a simple root α. The symmetry of the Dynkin diagram induces a direct construction of the sub(super)algebra $\mathcal{G}'$ invariant under the $\mathcal{G}$ automorphism associated to τ. Indeed, if the simple root α is transformed into $\tau(\alpha)$, then $\alpha' = \alpha + \tau(\alpha) + \cdots + \tau^{N-1}(\alpha)$ is τ-invariant since $\tau^N = 1$, and appears as a simple root of $\mathcal{G}'$ associated to the generator $e_{\alpha'} = e_\alpha + e_{\tau(\alpha)} + \cdots + e_{\tau^{N-1}(\alpha)}$, where $e_{\tau^k(\alpha)}$ is the generator corresponding to the root $\tau^k(\alpha)$ $(k = 0, \ldots, N-1)$. A Dynkin diagram of $\mathcal{G}'$ will therefore be obtained by folding the $\mathbb{Z}_N$-symmetric Dynkin diagram of $\mathcal{G}$, that is by transforming each N-uple $(\alpha, \tau(\alpha), \ldots, \tau^{N-1}(\alpha))$ into the root $\alpha' = \alpha + \tau(\alpha) + \cdots + \tau^{N-1}(\alpha)$ of $\mathcal{G}'$. It is easy to convince oneself that for $\mathcal{G}'$ the defining relations (2.1)–(2.5) of a HKM superalgebra hold [be aware that, in particular for the Serre relations (2.5), the entries of the Cartan matrix are now those of $\mathcal{G}'$].

We present in Table I the list of HKM superalgebras $\mathcal{G}$ to which the folding procedure can be applied and the corresponding singular subsuperalgebras $\mathcal{G}'$. Note that in general the obtained singular subsuperalgebras are also HKM superalgebras. However, in the case of the HKM superalgebra #6 of rank 6, one obtains for $\mathcal{G}'$ the simple Lie superalgebra $F(4)$ [note that for affine Lie (super)algebras the folding procedure always leads to (super)algebras of affine type]. This is due to the fact that for HKM superalgebras the root system contains *two* isotropic roots whose scalar product is not trivial.

Remark 4.1: The folding procedure cannot be applied to the rank four HKM superalgebras labelled by the numbers #59 to #62, despite the apparent $\mathbb{Z}_2$-symmetry of the distinguished Dynkin diagram, as the $\mathbb{Z}_2$-grading of the invariant generators would not be respected.

TABLE I. Folding of the HKM superalgebras.

Rank of $\mathcal{G}$	$\mathcal{G}$ label	Order of τ	Rank of $\mathcal{G}'$	$\mathcal{G}'$ label
3	#24	2	2	$BW(4,2)$
3	#25	2	2	$BW(2,4)$
3	#27	2	2	$BB(2,4)$
3	#28	2	2	$BB(4,2)$
3	#31	2	2	$BW(8,1)$
4	#33	2	4	#37
4	#34	2	4	#39
4	#40	2	3	#57
4	#41	2	3	#5
4	#42	2	3	#21
4	#44	2	3	#26
4	#45	2	3	#15
4	#46	2	3	#13
4	#47	2	3	#14
4	#48	2	3	#34
4	#55	2	3	#52
4	#56	2	3	#54
4	#57	2	3	#53
4	#58	2	3	#47
4	#63	2	3	#37
4	#64	2	3	#5
4	#65	2	3	#1
4	#66	2	3	#9
4	#67	2	3	#6
4	#68	2	3	#24
4	#68	2	4	#28
4	#69	2	4	#7
4	#70	2	4	#42
4	#71	2	4	#51
4	#72	2	4	#50
4	#73	2	4	#58
5	#28	2	4	#14
5	#30	2	4	#8
5	#31	2	4	#9
5	#32	2	4	#11
5	#33	2	4	#5
5	#34	2	4	#7
5	#35	3	3	#2
5	#36	2	4	#1
5	#37	2	4	#13
5	#38	3	3	#36
6	#6	2	4	F(4)
6	#12	2	4	#1
6	#14	3	4	#21
6	#15	3	4	#26

APPENDIX A: DYNKIN DIAGRAMS OF THE HYPERBOLIC SUPERALGEBRAS

Rank 3 hyperbolic superalgebras (87 diagrams):

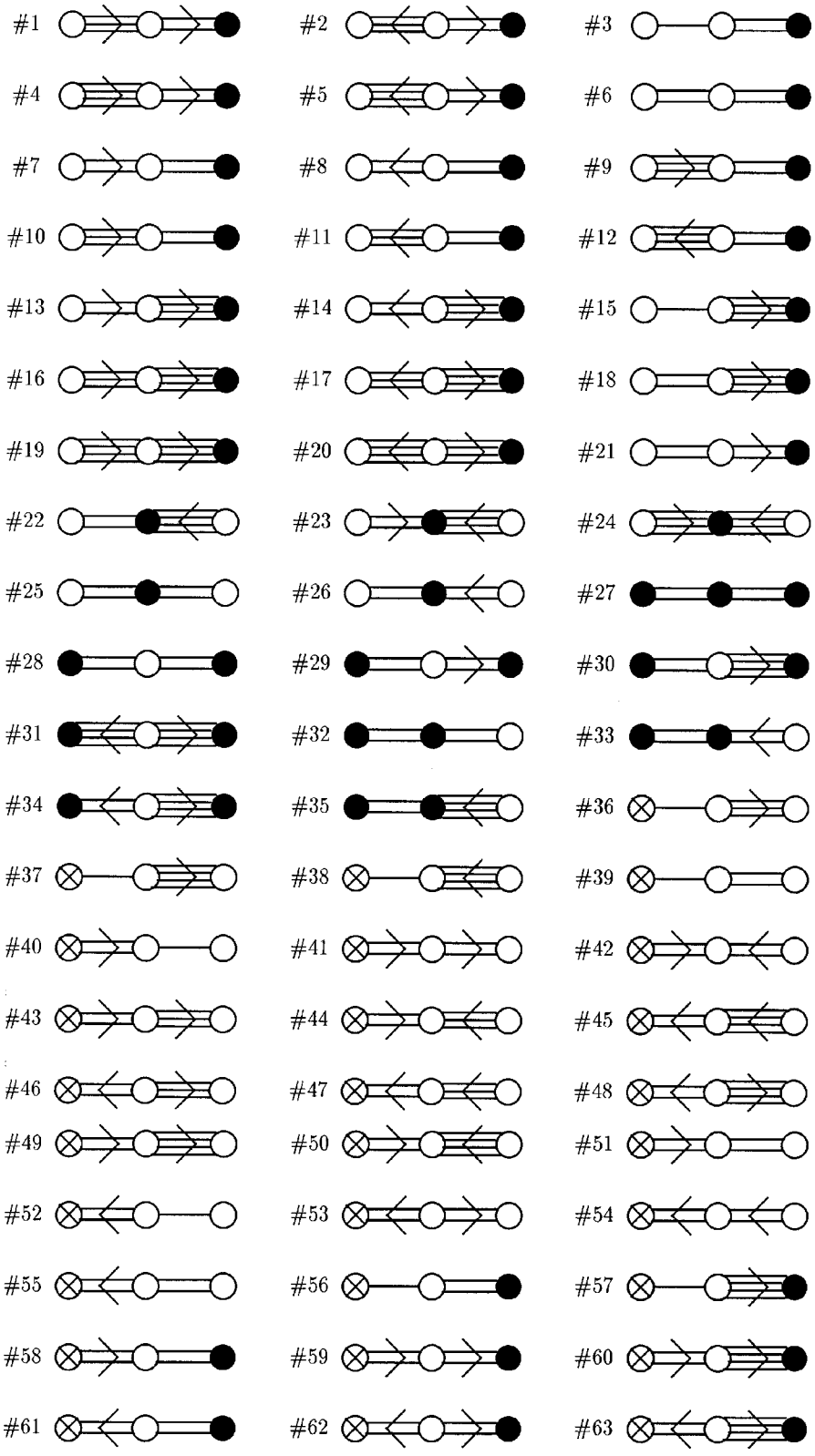

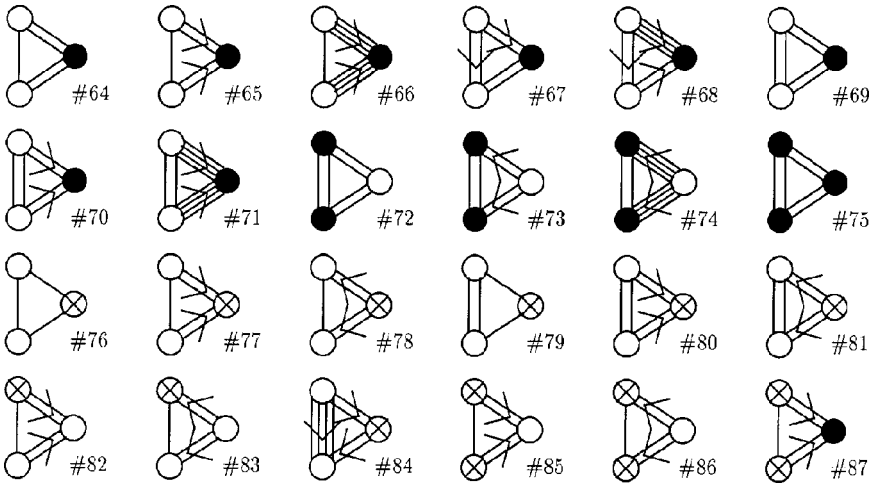

Rank 4 hyperbolic superalgebras (73 diagrams):

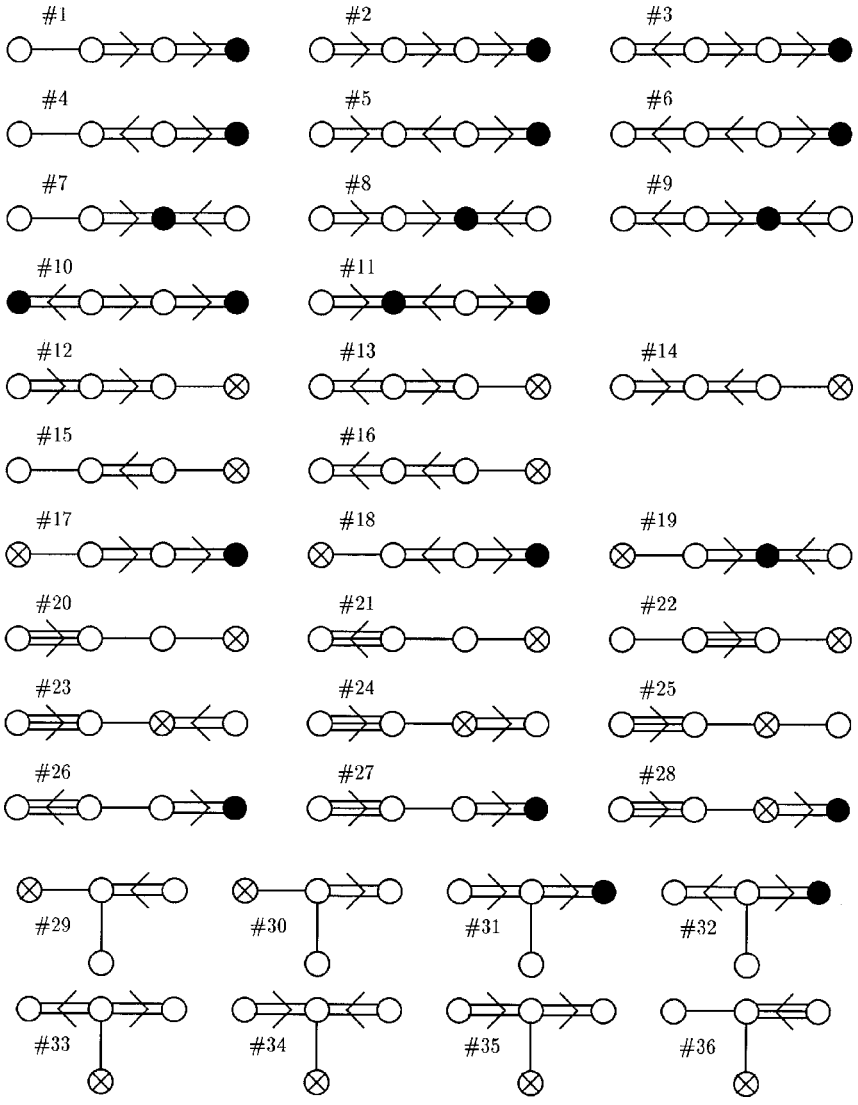

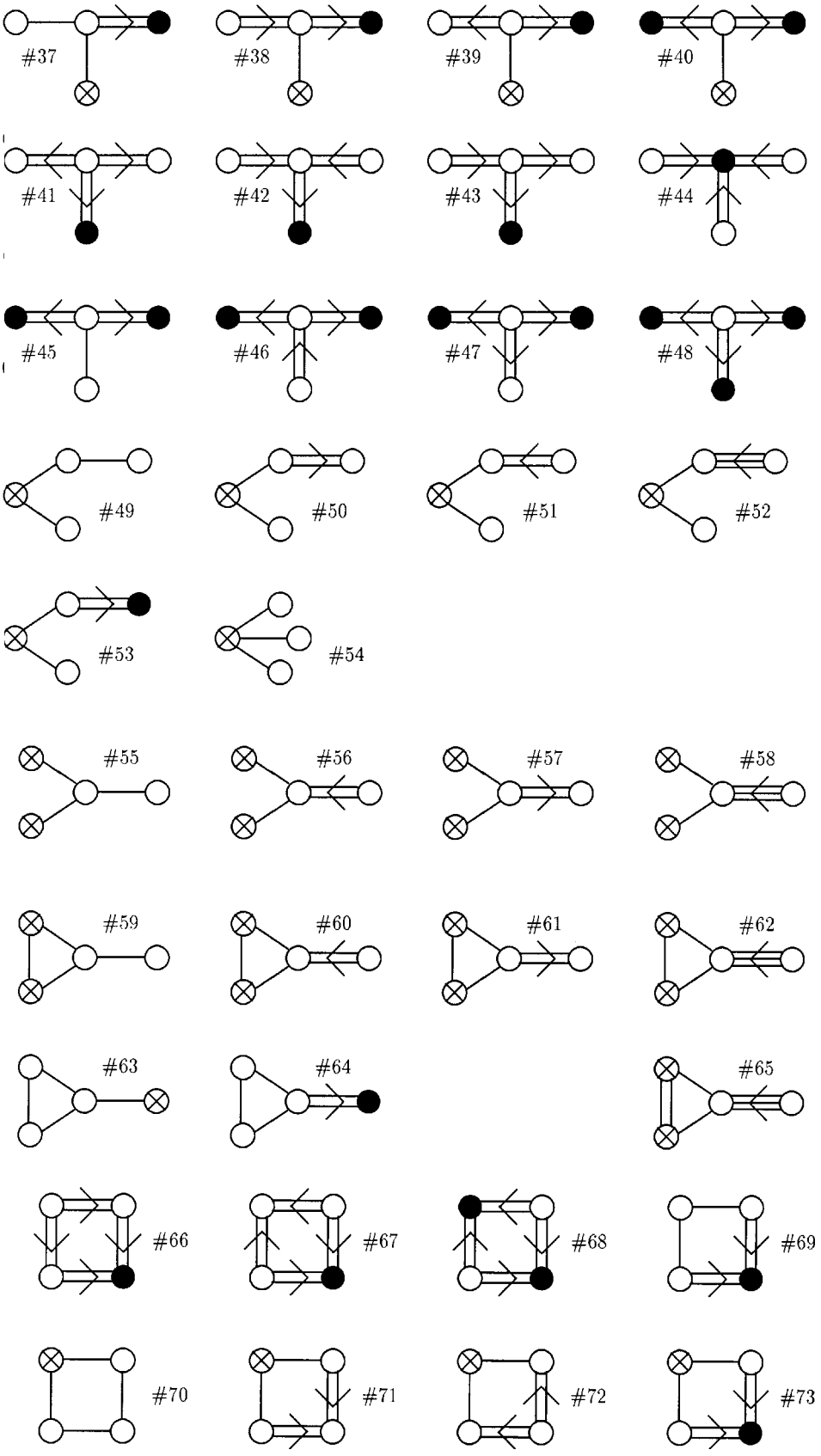
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Rank 5 hyperbolic superalgebras (38 diagrams):

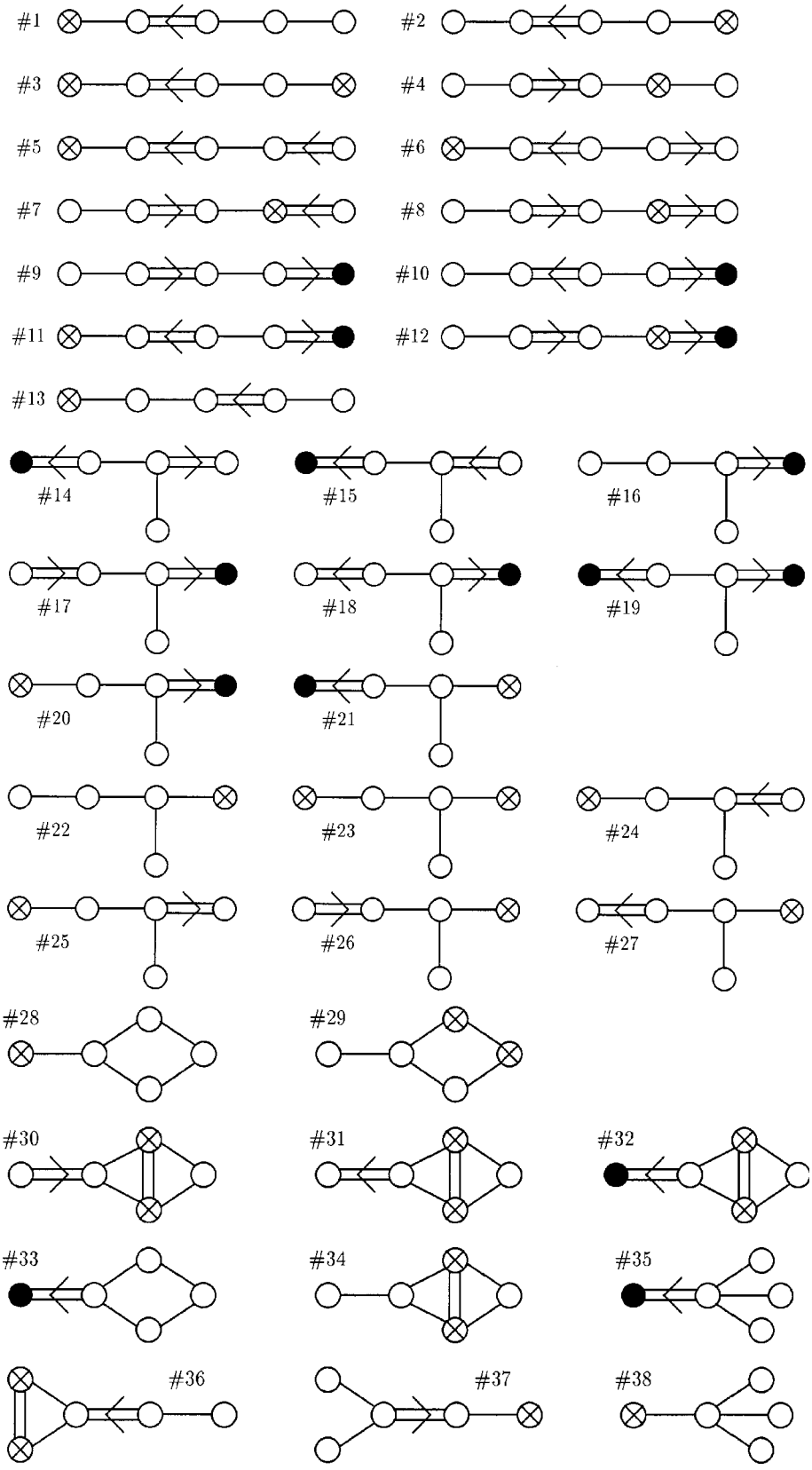

Rank 6 hyperbolic superalgebras (15 diagrams):

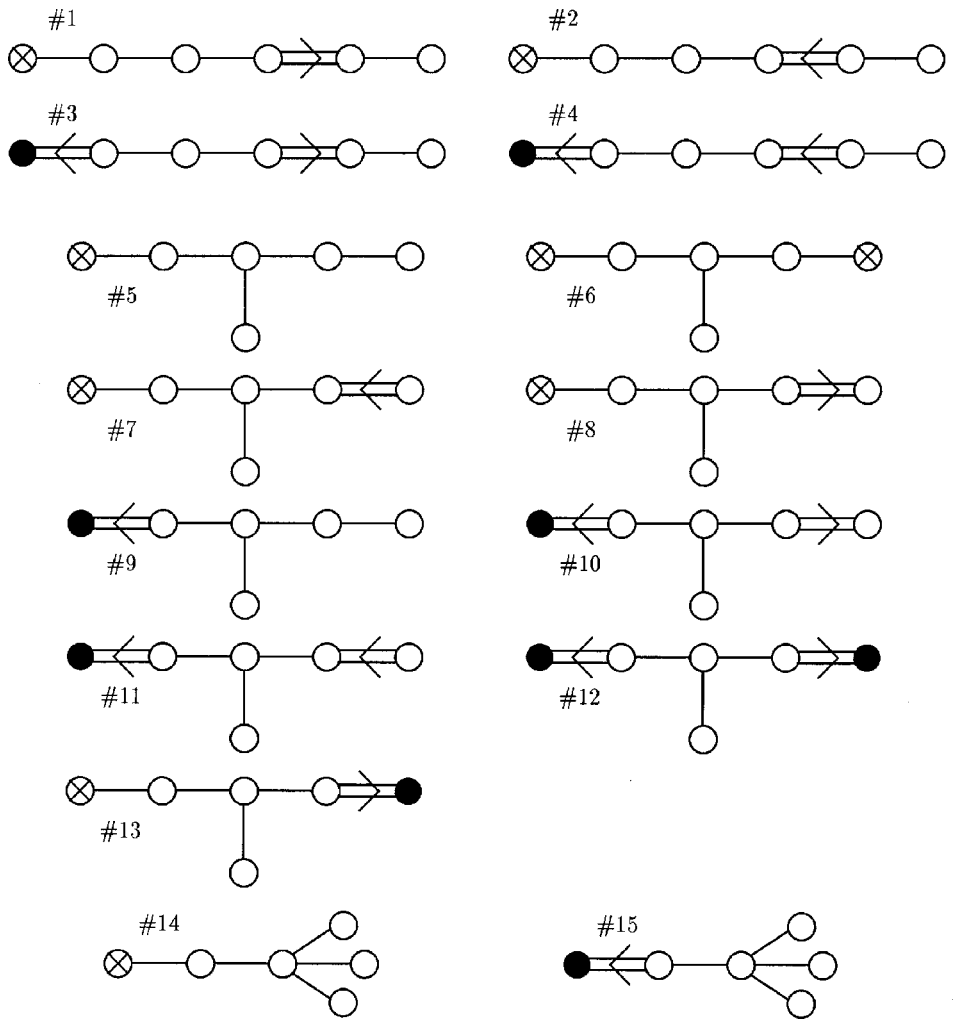

APPENDIX B: SIMPLE ROOT SYSTEMS

We describe in this section the simple root systems corresponding to the Dynkin diagrams of Appendix A (as usual, the parametrization is not unique). We give below the conventions used to describe the simple root systems depending on the topology of the considered Dynkin diagrams. In any case, the simple roots are written in terms of orthogonal vectors ε_i, δ_i, K^+, and K^- such that $(\varepsilon_i,\varepsilon_j)=1$, $(\delta_i,\delta_j)=-1$, $(K^+,K^-)=1$ and all other scalar products are zero. It is also convenient to introduce $\tilde{\delta}=\delta_1+\delta_2+\delta_3$ which satisfies $(\tilde{\delta},\tilde{\delta})=-3$ and $(\tilde{\delta},\varepsilon_i)=(\tilde{\delta},K^+)=(\tilde{\delta},K^-)=0$.

Rank 3 hyperbolic superalgebras: Conventions for the simple root systems $\Delta^0=\{\alpha_1,\alpha_2,\alpha_3\}$,

$$\#1{:}\Delta^0 = \{2\varepsilon_1 - \varepsilon_2 - \varepsilon_3 - K^-, \varepsilon_2 - \varepsilon_1, 2K^+ + \varepsilon_1\},$$

$$\#2{:}\Delta^0 = \left\{\tfrac{1}{3}(2\varepsilon_1 - \varepsilon_2 - \varepsilon_3) - K^-, \varepsilon_2 - \varepsilon_1, \tfrac{2}{3}K^+ + \varepsilon_1\right\},$$

$$\#3{:}\Delta^0 = \left\{-\tfrac{1}{2}(\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4) - K^-, \varepsilon_1, -\varepsilon_1 + \tfrac{1}{2}K^+\right\},$$

$$\#4{:}\Delta^0 = \{-2\varepsilon_1 + 2\varepsilon_2 - K^-, \varepsilon_1 - \varepsilon_2, 2K^+ + \varepsilon_2\},$$

$$\#5{:}\Delta^0 = \left\{-\tfrac{1}{2}(\varepsilon_1 - \varepsilon_2) - K^-, \varepsilon_1 - \varepsilon_2, \tfrac{1}{2}K^+ + \varepsilon_2\right\},$$

$$\#6{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1, -\varepsilon_1 + K^+\},$$

$$\#7{:}\Delta^0 = \{-\varepsilon_1 + \varepsilon_2 - K^-, \varepsilon_1, -\varepsilon_1 + K^+\},$$

$$\#8{:}\Delta^0 = \left\{\tfrac{1}{2}(-\varepsilon_1 + \varepsilon_2) - K^-, \varepsilon_1, -\varepsilon_1 + \tfrac{1}{2}K^+\right\},$$

$$\#9{:}\Delta^0 = \{-2\varepsilon_1 - K^-, \varepsilon_1, -\varepsilon_1 + 2K^+\},$$

$$\#10{:}\Delta^0 = \left\{-\tfrac{1}{2}(3\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4) - \tfrac{3}{2}K^-, \varepsilon_1, -\varepsilon_1 + K^+\right\},$$

$$\#11{:}\Delta^0 = \left\{-\tfrac{1}{6}(3\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4) - \tfrac{1}{2}K^-, \varepsilon_1, -\varepsilon_1 + K^+\right\},$$

$$\#12{:}\Delta^0 = \left\{-\tfrac{1}{2}\varepsilon_1 - K^-, \varepsilon_1, -\varepsilon_1 + \tfrac{1}{2}K^+\right\},$$

$$\#13{:}\Delta^0 = \{2\varepsilon_1 - 2\varepsilon_2 - K^-, 2\varepsilon_2, 2K^+ - \varepsilon_2\},$$

$$\#14{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - K^-, 2\varepsilon_2, K^+ - \varepsilon_2\},$$

$$\#15{:}\Delta^0 = \{\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 - K^-, -2\varepsilon_1, K^+ + \varepsilon_1\},$$

$$\#16{:}\Delta^0 = \left\{2\varepsilon_1 - \varepsilon_2 - \varepsilon_3 - K^-, \varepsilon_2 - \varepsilon_1, \tfrac{3}{2}K^+ + \tfrac{1}{2}(\varepsilon_1 - \varepsilon_2)\right\},$$

$$\#17{:}\Delta^0 = \left\{\tfrac{1}{3}(2\varepsilon_1 - \varepsilon_2 - \varepsilon_3) - K^-, \varepsilon_2 - \varepsilon_1, \tfrac{1}{2}K^+ + \tfrac{1}{2}(\varepsilon_1 - \varepsilon_2)\right\},$$

$$\#18{:}\Delta^0 = \{2\varepsilon_1 - K^-, -2\varepsilon_1, 2K^+ + \varepsilon_1\},$$

$$\#19{:}\Delta^0 = \{-4\varepsilon_1 - K^-, 2\varepsilon_1, -\varepsilon_1 + 4K^+\},$$

$$\#20{:}\Delta^0 = \{-\varepsilon_1 - K^-, 2\varepsilon_1, K^+ - \varepsilon_1\},$$

$$\#21{:}\Delta^0 = \{-\varepsilon_1 + \varepsilon_2 - K^-, \varepsilon_1 - \varepsilon_2, K^+ + \varepsilon_2\},$$

$$\#22{:}\Delta^0 = \{-\varepsilon_1 - 2K^-, \varepsilon_1, -2\varepsilon_1 + K^+\},$$

$$\#23{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - 2K^-, \varepsilon_2, K^+ - 2\varepsilon_2\},$$

$$\#24{:}\Delta^0 = \{-2\varepsilon_1 - 2K^-, \varepsilon_1, 2K^+ - 2\varepsilon_1\},$$

$$\#25{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1, -\varepsilon_1 + K^+\},$$

$$\#26{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1, -\varepsilon_1 + \varepsilon_2 + K^+\},$$

$$\#27{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1, -\varepsilon_1 + K^+\},$$

$$\#28{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1, -\varepsilon_1 + K^+\},$$

$$\#29{:}\Delta^0 = \left\{-\varepsilon_1 - \tfrac{1}{2}K^-, \varepsilon_1, -\tfrac{1}{2}(\varepsilon_1 - \varepsilon_2) + K^+\right\},$$

$$\#30{:}\Delta^0 = \left\{-\varepsilon_1 - \tfrac{1}{2}K^-, \varepsilon_1, -\tfrac{1}{2}\varepsilon_1 + K^+\right\},$$

$$\#31{:}\Delta^0 = \{-\varepsilon_1 - K^-, 2\varepsilon_1, K^+ - \varepsilon_1\},$$

$$\#32{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1, -\varepsilon_1 + K^+\},$$

$$\#33{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1, -\varepsilon_1 + \varepsilon_2 + K^+\},$$

$$\#34{:}\Delta^0 = \left\{-\varepsilon_1 - \tfrac{1}{2}K^-, \varepsilon_1 - \varepsilon_2, -\tfrac{1}{2}(\varepsilon_1 - \varepsilon_2) + K^+\right\},$$

$$\#35{:}\Delta^0 = \{-\varepsilon_1 - 2K^-, \varepsilon_1, -2\varepsilon_1 + K^+\},$$

$$\#36{:}\Delta^0 = \left\{\delta_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_1, \tfrac{1}{3}K^+ + \tfrac{1}{3}(2\varepsilon_1 - \varepsilon_2 - \varepsilon_3)\right\},$$

$$\#37{:}\Delta^0 = \left\{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, -\tfrac{1}{2}(\varepsilon_1 - \varepsilon_2) + \tfrac{1}{2}K^+\right\},$$

$$\#38{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, -2\varepsilon_1 + 2\varepsilon_2 + 2K^+\},$$

$$\#39{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, -\varepsilon_1 + \varepsilon_2 + K^+\},$$

$$\#40{:}\Delta^0 = \left\{\varepsilon_1 - \delta_1 - K^-, -\varepsilon_1, \tfrac{1}{2}(\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4) + \tfrac{1}{2}K^+\right\},$$

$$\#41{:}\Delta^0 = \left\{\varepsilon_1 - \delta_1 - K^-, -\varepsilon_1, \tfrac{1}{2}(\varepsilon_1 - \varepsilon_2) + \tfrac{1}{2}K^+\right\},$$

$$\#42{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - K^-, -\varepsilon_1, \varepsilon_1 - \varepsilon_2 + K^+\},$$

$$\#43{:}\Delta^0 = \left\{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1, -\tfrac{1}{2}\varepsilon_1 + \tfrac{1}{6}(\varepsilon_2 + \varepsilon_3 + \varepsilon_4) + \tfrac{1}{2}K^+\right\},$$

$$\#44{:}\Delta^0 = \left\{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1, -\tfrac{3}{2}\varepsilon_1 + \tfrac{1}{2}(\varepsilon_2 + \varepsilon_3 + \varepsilon_4) + \tfrac{3}{2}K^+\right\},$$

$$\#45{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - 4K^-, -2\varepsilon_1, 4\varepsilon_1 + K^+\},$$

$$\#46{:}\Delta^0 = \left\{\delta_1 - \varepsilon_1 - K^-, 2\varepsilon_1, -\varepsilon_1 + \tfrac{1}{3}(\varepsilon_2 + \varepsilon_3 + \varepsilon_4) + K^+\right\},$$

$$\#47{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1, -3\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 + 3K^+\},$$

$$\#48{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - K^-, -2\varepsilon_1, \varepsilon_1 + K^+\},$$

$$\#49{:}\Delta^0 = \left\{\varepsilon_1 - \delta_1 - \tfrac{1}{2}K^-, -\varepsilon_1, \tfrac{1}{2}\varepsilon_1 + K^+\right\},$$

$$\#50{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - 2K^-, -\varepsilon_1, 2\varepsilon_1 + K^+\},$$

$$\#51{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - \delta_1 + \delta_2 - 2K^-, -\varepsilon_1 + \varepsilon_2, \varepsilon_1 - \varepsilon_2 + K^+\},$$

$$\#52{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - K^-, -2\varepsilon_1, \varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 + K^+\},$$

$$\#53{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - K^-, -2\varepsilon_1, \varepsilon_1 - \varepsilon_2 + K^+\},$$

$$\#54{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - 2K^-, -2\varepsilon_1, 2\varepsilon_1 - 2\varepsilon_2 + K^+\},$$

$$\#55{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - 2K^-, -2\varepsilon_1, 2\varepsilon_1 + K^+\},$$

$$\#56{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, -\varepsilon_1 + \varepsilon_2 + K^+\},$$

$$\#57{:}\Delta^0 = \left\{\delta_1 - \varepsilon_1 - \tfrac{1}{2}K^-, \varepsilon_1 - \varepsilon_2, -\tfrac{1}{2}(\varepsilon_1 - \varepsilon_2) + K^+\right\},$$

$$\#58{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - K^-, -\varepsilon_1, \varepsilon_1 + K^+\},$$

$$\#59{:}\Delta^0 = \left\{\varepsilon_1 - \delta_1 - K^-, -\varepsilon_1, \tfrac{1}{2}(\varepsilon_1 - \varepsilon_2) + \tfrac{1}{2}K^+\right\},$$

$$\#60{:}\Delta^0 = \left\{\varepsilon_1 - \delta_1 - \tfrac{1}{2}K^-, -\varepsilon_1, \tfrac{1}{2}\varepsilon_1 + K^+\right\},$$

$$\#61{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - 2K^-, -2\varepsilon_1, 2\varepsilon_1 + K^+\},$$

$$\#62{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - K^-, -2\varepsilon_1, \varepsilon_1 - \varepsilon_2 + K^+\},$$

$$\#63{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - K^-, -2\varepsilon_1, \varepsilon_1 - \varepsilon_2 + K^+\},$$

$$\#64{:}\Delta^0 = \{-\varepsilon_1 + \varepsilon_2 - 3K^-, -\varepsilon_1 + \varepsilon_2 + K^+, \varepsilon_1 - \varepsilon_2\},$$

$$\#65{:}\Delta^0 = \{\varepsilon_1 + \varepsilon_2 - 3K^-, \varepsilon_1 + \varepsilon_2 + K^+, -\varepsilon_1\},$$

$$\#66{:}\Delta^0 = \{-2\varepsilon_1 - 3K^-, -2\varepsilon_1 + 2K^+, \varepsilon_1\},$$

$$\#67{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - 2K^-, -\varepsilon_2 + K^+, \varepsilon_2\},$$

$$\#68{:}\Delta^0 = \{-2\varepsilon_2 - 2K^-, \varepsilon_1 - \varepsilon_2 + 2K^+, \varepsilon_2\},$$

$$\#69{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - 2K^-, \varepsilon_1 - \varepsilon_2 + 2K^+, -\varepsilon_1 + \varepsilon_2\},$$

$$\#70{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - 2K^-, \varepsilon_1 - \varepsilon_2 + 2K^+, -\varepsilon_1\},$$

$$\#71{:}\Delta^0 = \left\{\varepsilon_1 - \varepsilon_2 - 2K^-, \varepsilon_1 - \varepsilon_2 + 2K^+, -\tfrac{1}{2}(\varepsilon_1 - \varepsilon_2)\right\},$$

$$\#72{:}\Delta^0 = \{\varepsilon_1 - 2K^-, \varepsilon_1 + K^+, -\varepsilon_1\},$$

$$\#73{:}\Delta^0 = \{\varepsilon_1, -\varepsilon_1 - 2K^-, \varepsilon_2 - \varepsilon_1 + K^+\},$$

$$\#74{:}\Delta^0 = \{\varepsilon_1, -\varepsilon_1 - 2K^-, -2\varepsilon_1 + 2K^+\},$$

$$\#75{:}\Delta^0 = \{\varepsilon_1 - 2K^-, \varepsilon_1 + K^+, -\varepsilon_1\},$$

$$\#76{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - K^-, \varepsilon_1 + \varepsilon_2 + K^+, \delta_1 - \varepsilon_1\},$$

$$\#77{:}\Delta^0 = \{2\varepsilon_1 - 3K^-, 2\varepsilon_1 + 2K^+, \delta_1 - \varepsilon_1\},$$

$$\#78{:}\Delta^0 = \left\{\varepsilon_1 - \tfrac{3}{2}K^-, \varepsilon_1 + K^+, \delta_1 - \varepsilon_1\right\},$$

$$\#79{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - 2K^-, \varepsilon_1 - \varepsilon_2 + 2K^+, \delta_1 - \varepsilon_1\},$$

$$\#80{:}\Delta^0 = \{2\varepsilon_1 - 4K^-, 2\varepsilon_1 + 2K^+, \delta_1 - \varepsilon_1\},$$

$$\#81{:}\Delta^0 = \{\varepsilon_1 - 2K^-, \varepsilon_1 + K^+, \delta_1 - \varepsilon_1\},$$

$$\#82{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - 2K^-, \varepsilon_1 - \varepsilon_2 + K^+, -\varepsilon_1\},$$

$$\#83{:}\Delta^0 = \{\varepsilon_1 - \delta_1 - 2K^-, \varepsilon_1 - \varepsilon_2 + K^+, -2\varepsilon_1\},$$

$$\#84{:}\Delta^0 = \{2\varepsilon_1 - 2K^-, \varepsilon_1 + 2K^+, \delta_1 - \varepsilon_1\},$$

$$\#85{:}\Delta^0 = \{\varepsilon_1 - \delta_1 + K^-, \varepsilon_1 - \delta_1 + K^+, -\varepsilon_1\},$$

$$\#86{:}\Delta^0 = \{\varepsilon_1 - \delta_1 + K^-, \varepsilon_1 - \delta_1 + K^+, -2\varepsilon_1\},$$

$$\#87{:}\Delta^0 = \{\varepsilon_1 + \delta_1 - K^-, \varepsilon_1 + \delta_1 + K^+, -\varepsilon_1\}.$$

Rank 4 hyperbolic superalgebras: Conventions for the simple root systems $\Delta^0 = \{\alpha_1, \alpha_2, \alpha_3, \alpha_4\}$

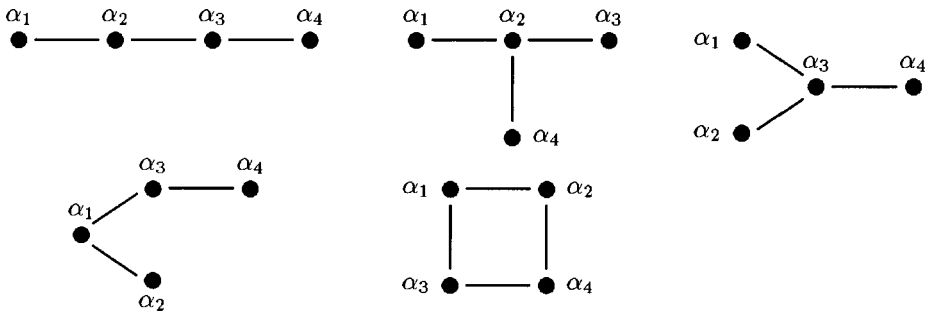

$$\#1{:}\Delta^0 = \{\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 - K^-, -2\varepsilon_1, \varepsilon_1 - \varepsilon_2, K^+ + \varepsilon_2\},$$

$$\#2{:}\Delta^0 = \{2\varepsilon_1 + 2\varepsilon_2 - K^-, -2\varepsilon_1, \varepsilon_1 - \varepsilon_2, 2K^+ + \varepsilon_2\},$$

$$\#3{:}\Delta^0 = \{\varepsilon_1 + \varepsilon_2 - K^-, -2\varepsilon_1, \varepsilon_1 - \varepsilon_2, K^+ + \varepsilon_2\},$$

$$\#4{:}\Delta^0 = \left\{\tfrac{1}{2}(\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4) - K^-, -\varepsilon_1, \varepsilon_1 - \varepsilon_2, \tfrac{1}{2}K^+ + \varepsilon_2\right\},$$

$$\#5{:}\Delta^0 = \{\varepsilon_1 + \varepsilon_2 - K^-, -\varepsilon_1, \varepsilon_1 - \varepsilon_2, K^+ + \varepsilon_2\},$$

$$\#6{:}\Delta^0 = \left\{\tfrac{1}{2}(\varepsilon_1 + \varepsilon_2) - K^-, -\varepsilon_1, \varepsilon_1 - \varepsilon_2, \tfrac{1}{2}K^+ + \varepsilon_2\right\},$$

$$\#7{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_3, K^+ - \varepsilon_2 - \varepsilon_3\},$$

$$\#8{:}\Delta^0 = \{-2\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, 2K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#9{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#10{:}\Delta^0 = \{\varepsilon_1 + \varepsilon_2 - K^-, -2\varepsilon_1, \varepsilon_1 - \varepsilon_2, K^+ + \varepsilon_2\},$$

$$\#11{:}\Delta^0 = \{\varepsilon_1 + \varepsilon_2 - K^-, -\varepsilon_1, \varepsilon_1 - \varepsilon_2, K^+ + \varepsilon_2\},$$

$$\#12{:}\Delta^0 = \{-2\varepsilon_1 - 2\varepsilon_2 - K^-, 2\varepsilon_2, \varepsilon_1 - \varepsilon_2, \delta_1 - \varepsilon_1 + 2K^+\},$$

$$\#13{:}\Delta^0 = \{-\varepsilon_1 - \varepsilon_2 - K^-, 2\varepsilon_2, \varepsilon_1 - \varepsilon_2, \delta_1 - \varepsilon_1 + K^+\},$$

$$\#14{:}\Delta^0 = \{-\varepsilon_1 - \varepsilon_2 - K^-, \varepsilon_2, \varepsilon_1 - \varepsilon_2, K^+ + \delta_1 - \varepsilon_1\},$$

$$\#15{:}\Delta^0 = \left\{-\tfrac{1}{2}(\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4) + K^-, \varepsilon_2, \varepsilon_1 - \varepsilon_2, \tfrac{1}{2}K^+ + \varepsilon_2 - \delta_1\right\},$$

$$\#16{:}\Delta^0 = \left\{\tfrac{1}{2}(\varepsilon_1 + \varepsilon_2) - K^-, -\varepsilon_1, \varepsilon_1 - \varepsilon_2, \tfrac{1}{2}K^+ + \varepsilon_2 - \delta_1\right\},$$

$$\#17{:}\Delta^0 = \left\{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, -\tfrac{1}{2}(\varepsilon_1 + \varepsilon_2) + \tfrac{1}{2}K^+\right\},$$

$$\#18{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, 2\varepsilon_2, -\varepsilon_1 - \varepsilon_2 + K^+\},$$

$$\#19{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#20{:}\Delta^0 = \{2\varepsilon_3 - \varepsilon_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_1 - \varepsilon_2, K^+ - \varepsilon_1 + \delta_1\},$$

$$\#21{:}\Delta^0 = \left\{\tfrac{1}{3}(2\varepsilon_3 - \varepsilon_1 - \varepsilon_2) - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_1 - \varepsilon_2, \tfrac{1}{3}K^+ - \varepsilon_1 + \delta_1\right\},$$

$$\#22{:}\Delta^0 = \{2\varepsilon_3 - \varepsilon_1 - \varepsilon_2 - K^-, 2\varepsilon_2 - \varepsilon_1 - \varepsilon_3 - K^-, \varepsilon_1 - \varepsilon_2, \delta_1 - \varepsilon_1 + K^+\},$$

$$\#23{:}\Delta^0 = \{2\varepsilon_2 - \varepsilon_1 - \varepsilon_3 - K^-, \varepsilon_1 - \varepsilon_2, \delta_1 - \varepsilon_1 + K^+, -2\delta_1\},$$

$$\#24{:}\Delta^0 = \{2\varepsilon_2 - \varepsilon_1 - \varepsilon_3 - K^-, \varepsilon_1 - \varepsilon_2, \delta_1 - \varepsilon_1 + K^+, -\delta_1\},$$

$$\#25{:}\Delta^0 = \{2\varepsilon_2 - \varepsilon_1 - \varepsilon_3 - K^-, \varepsilon_1 - \varepsilon_2, \delta_1 - \varepsilon_1 + K^+, \delta_2 - \delta_1\},$$

$$\#26{:}\Delta^0 = \left\{\tfrac{1}{3}(2\varepsilon_3 - \varepsilon_1 - \varepsilon_2) - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_1 - \varepsilon_2, \tfrac{1}{3}K^+ - \varepsilon_1\right\},$$

$$\#27{:}\Delta^0 = \{2\varepsilon_3 - \varepsilon_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_1 - \varepsilon_2, K^+ - \varepsilon_1\},$$

$$\#28{:}\Delta^0 = \{2\varepsilon_2 - \varepsilon_1 - \varepsilon_3 - K^-, \varepsilon_1 - \varepsilon_2, \delta_1 - \varepsilon_1 + K^+, -\delta_1\},$$

$$\#29{:}\Delta^0 = \{\delta_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, 2\varepsilon_3, K^+ + \varepsilon_1 - \varepsilon_2\},$$

$$\#30{:}\Delta^0 = \{\delta_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_3, K^+ + \varepsilon_1 - \varepsilon_2\},$$

$$\#31{:}\Delta^0 = \{-2\varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_3, 2K^+ + \varepsilon_1 - \varepsilon_2\},$$

$$\#32{:}\Delta^0 = \{-\varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_3, K^+ + \varepsilon_1 - \varepsilon_2\},$$

$$\#33{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, K^+ + \delta_1 - \varepsilon_1\},$$

$$\#34{:}\Delta^0 = \{-2\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, 2\varepsilon_2, 2K^+ + \delta_1 - \varepsilon_1\},$$

$$\#35{:}\Delta^0 = \{-2\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, 2K^+ + \delta_1 - \varepsilon_1\},$$

$$\#36{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, 2\varepsilon_3 - \varepsilon_1 - \varepsilon_2 - K^-, 2K^+ + \varepsilon_3 - \delta_1\},$$

$$\#37{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_3, K^+ + \delta_1 - \varepsilon_2\},$$

$$\#38{:}\Delta^0 = \{-2\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, 2K^+ + \delta_1 - \varepsilon_1\},$$

$$\#39{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, K^+ + \delta_1 - \varepsilon_1\},$$

$$\#40{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, K^+ + \delta_1 - \varepsilon_1\},$$

$$\#41{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, K^+ - \varepsilon_1\},$$

$$\#42{:}\Delta^0 = \{-2\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, 2\varepsilon_2, 2K^+ - \varepsilon_1\},$$

$$\#43{:}\Delta^0 = \{-2\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, 2K^+ - \varepsilon_1\},$$

$$\#44{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - K^-, \varepsilon_2, -\varepsilon_1 - \varepsilon_2, 2K^+ + \varepsilon_1 - \varepsilon_2\},$$

$$\#45{:}\Delta^0 = \{-\varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_3, K^+ + \varepsilon_1 - \varepsilon_2\},$$

$$\#46{:}\Delta^0 = \{-\varepsilon_1 - 2K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, K^+ - 2\varepsilon_1\},$$

$$\#47{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, K^+ - \varepsilon_1\},$$

$$\#48{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2, K^+ - \varepsilon_1\},$$

$$\#49{:}\Delta^0 = \{\delta_1 - \varepsilon_1, \varepsilon_1 + \varepsilon_2 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3 + K^+\},$$

$$\#50{:}\Delta^0 = \{\delta_1 - \varepsilon_1, \varepsilon_1 + \varepsilon_2 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 + K^+\},$$

$$\#51{:}\Delta^0 = \{\delta_1 - \varepsilon_1, \varepsilon_1 + \varepsilon_2 - 2K^-, \varepsilon_1 - \varepsilon_2, 2\varepsilon_2 + K^+\},$$

$$\#52{:}\Delta^0 = \{\delta_1 - \varepsilon_1, \varepsilon_1 + \varepsilon_2 - K^-, \varepsilon_1 - \varepsilon_2, 2\varepsilon_2 - \varepsilon_1 - \varepsilon_3 + K^+\},$$

$$\#53{:}\Delta^0 = \{\delta_1 - \varepsilon_1, \varepsilon_1 + \varepsilon_2 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 + K^+\},$$

$$\#54{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_1 + \varepsilon_2, \varepsilon_3 - \varepsilon_4 + K^+\},$$

$$\#55{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \delta_2 - \varepsilon_1 + K^+, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3\},$$

$$\#56{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \delta_2 - \varepsilon_1 + K^+, \varepsilon_1 - \varepsilon_2, 2\varepsilon_2\},$$

$$\#57{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \delta_2 - \varepsilon_1 + K^+, \varepsilon_1 - \varepsilon_2, \varepsilon_2\},$$

$$\#58{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, -\delta_2 + \varepsilon_2 - 2K^-, \varepsilon_1 - \varepsilon_2, K^+ + 2\varepsilon_2 - \varepsilon_1 - \varepsilon_3\},$$

$$\#59{:}\Delta^0 = \{\delta_1 - \varepsilon_1, \varepsilon_2 - \delta_1 - K^-, \varepsilon_1 - \varepsilon_2, K^+ + \varepsilon_2 - \varepsilon_3\},$$

$$\#60{:}\Delta^0 = \{\delta_1 - \varepsilon_1, \varepsilon_2 - \delta_1 - 2K^-, \varepsilon_1 - \varepsilon_2, K^+ + 2\varepsilon_2\},$$

$$\#61{:}\Delta^0 = \{\delta_1 - \varepsilon_1, \varepsilon_2 - \delta_1 - K^-, \varepsilon_1 - \varepsilon_2, K^+ + \varepsilon_2\},$$

$$\#62{:}\Delta^0 = \{\delta_1 - \varepsilon_2 - K^-, \varepsilon_3 - \delta_1 - 2K^-, \varepsilon_2 - \varepsilon_3, K^+ + 2\varepsilon_3 - \varepsilon_1 - \varepsilon_2\},$$

$$\#63{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2, \varepsilon_3 - \varepsilon_1 - K^-, \varepsilon_2 - \varepsilon_3, K^+ + \varepsilon_3 - \delta_1\},$$

$$\#64{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2, \varepsilon_3 - \varepsilon_1 - K^-, \varepsilon_2 - \varepsilon_3, K^+ + \varepsilon_3\},$$

$$\#65{:}\Delta^0 = \{\delta_1 - \varepsilon_2 - K^-, -\delta_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, K^+ + 2\varepsilon_3 - \varepsilon_1 - \varepsilon_2\},$$

$$\#66{:}\Delta^0 = \{-2\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_1 + \varepsilon_2, 2K^+ - \varepsilon_1\},$$

$$\#67{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_1 + \varepsilon_2, K^+ - \varepsilon_1\},$$

$$\#68{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_1 + \varepsilon_2, K^+ - \varepsilon_1\},$$

$$\#69{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_2 + \varepsilon_3, K^+ - \varepsilon_2\},$$

$$\#70{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_1 + \varepsilon_2, K^+ - \varepsilon_1 + \varepsilon_3\},$$

$$\#71{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_1 + \varepsilon_2, K^+ - \varepsilon_1\},$$

$$\#72{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - 2K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_1 + \varepsilon_2, K^+ - 2\varepsilon_1\},$$

$$\#73{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_1 + \varepsilon_2, K^+ - \varepsilon_1\}.$$

Rank 5 hyperbolic superalgebras: Conventions for the simple root systems $\Delta^0 = \{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5\}$,

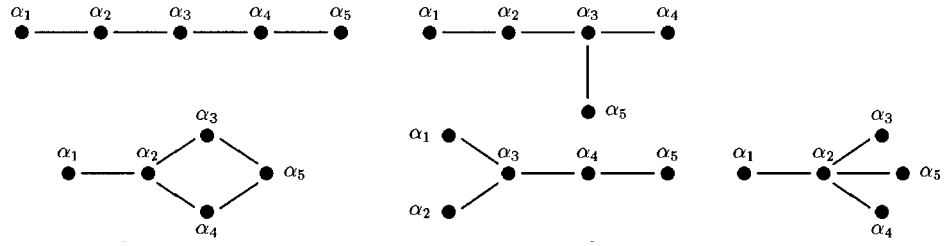

$$\#1{:}\Delta^0 = \left\{\tfrac{1}{2}(\tilde{\delta} - \varepsilon_1 - \varepsilon_2 - \varepsilon_3) - K^-, \varepsilon_3, \varepsilon_2 - \varepsilon_3, \varepsilon_1 - \varepsilon_2, \tfrac{1}{2}K^+ + \varepsilon_4 - \varepsilon_1\right\},$$

$$\#2{:}\Delta^0 = \left\{\tfrac{1}{2}(\varepsilon_4 - \varepsilon_1 - \varepsilon_2 - \varepsilon_3) - K^-, \varepsilon_3, \varepsilon_2 - \varepsilon_3, \varepsilon_1 - \varepsilon_2, \tfrac{1}{2}K^+ - \varepsilon_1 + \delta_1\right\},$$

$$\#3{:}\Delta^0 = \left\{\tfrac{1}{2}(\tilde{\delta} - \varepsilon_1 - \varepsilon_2 - \varepsilon_3) - K^-, \varepsilon_3, \varepsilon_2 - \varepsilon_3, \varepsilon_1 - \varepsilon_2, \tfrac{1}{2}K^+ + \delta_4 - \varepsilon_1\right\},$$

$$\#4{:}\Delta^0 = \left\{\varepsilon_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_3, \tfrac{1}{2}(\tilde{\delta} - \varepsilon_1 - \varepsilon_2 - \varepsilon_3), K^+ + \varepsilon_1\right\},$$

$$\#5{:}\Delta^0 = \left\{\tfrac{1}{2}(\tilde{\delta} - \varepsilon_1 - \varepsilon_2 - \varepsilon_3) - K^-, \varepsilon_3, \varepsilon_2 - \varepsilon_3, \varepsilon_1 - \varepsilon_2, K^+ - 2\varepsilon_1\right\},$$

$$\#6{:}\Delta^0 = \left\{\tfrac{1}{2}(\tilde{\delta} - \varepsilon_1 - \varepsilon_2 - \varepsilon_3) - K^-, \varepsilon_3, \varepsilon_2 - \varepsilon_3, \varepsilon_1 - \varepsilon_2, \tfrac{1}{2}K^+ - \varepsilon_1\right\},$$

$$\#7{:}\Delta^0 = \{\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 - K^-, -2\varepsilon_1, \varepsilon_1 - \varepsilon_2, K^+ + \varepsilon_2 - \delta_1, 2\delta_1\},$$

$$\#8{:}\Delta^0 = \{\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 - K^-, -2\varepsilon_1, \varepsilon_1 - \varepsilon_2, K^+ + \varepsilon_2 - \delta_1, \delta_1\},$$

$$\#9{:}\Delta^0 = \{\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 - K^-, -2\varepsilon_1, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, K^+ + \varepsilon_3\},$$

$$\#10{:}\Delta^0 = \left\{\tfrac{1}{2}(\varepsilon_4 - \varepsilon_1 - \varepsilon_2 - \varepsilon_3) - K^-, \varepsilon_3, \varepsilon_2 - \varepsilon_3, \varepsilon_1 - \varepsilon_2, \tfrac{1}{2}K^+ - \varepsilon_1\right\},$$

$$\#11{:}\Delta^0 = \left\{\tfrac{1}{2}(\tilde{\delta} - \varepsilon_1 - \varepsilon_2 - \varepsilon_3) - K^-, \varepsilon_3, \varepsilon_2 - \varepsilon_3, \varepsilon_1 - \varepsilon_2, \tfrac{1}{2}K^+ - \varepsilon_1\right\},$$

$$\#12{:}\Delta^0 = \{\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 - K^-, -2\varepsilon_1, \varepsilon_1 - \varepsilon_2, K^+ + \varepsilon_2 - \delta_1, \delta_1\},$$

$$\#13{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, 2\varepsilon_3, K^+ - \varepsilon_1 - \varepsilon_2 - \varepsilon_3 - \varepsilon_4\},$$

$$\#14{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#15{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, 2\varepsilon_3, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#16{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_4, K^+ - \varepsilon_2 - \varepsilon_3\},$$

$$\#17{:}\Delta^0 = \{-2\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3, 2K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#18{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#19{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#20{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#21{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \delta_1, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#22{:}\Delta^0 = \{\varepsilon_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_4 - \delta_1, K^+ - \varepsilon_2 - \varepsilon_3\},$$

$$\#23{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \delta_2, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#24{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, 2\varepsilon_3, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#25{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#26{:}\Delta^0 = \{-2\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \delta_1, 2K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#27{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \delta_1, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#28{:}\Delta^0 = \{\varepsilon_4 - \delta_1 - K^-, \varepsilon_3 - \varepsilon_4, \varepsilon_2 - \varepsilon_3, K^+ + \varepsilon_4 - \varepsilon_1, \varepsilon_1 - \varepsilon_2\},$$

$$\#29{:}\Delta^0 = \{-\varepsilon_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \delta_1, \varepsilon_1 - \varepsilon_2, K^+ + \delta_1 - \varepsilon_1\},$$

$$\#30{:}\Delta^0 = \{-2\varepsilon_2 - K^-, \varepsilon_1 + \varepsilon_2, \delta_1 - \varepsilon_1, -\delta_1 - \varepsilon_1, 2K^+ + \varepsilon_1 - \varepsilon_2\},$$

$$\#31{:}\Delta^0 = \{-\varepsilon_2 - K^-, \varepsilon_1 + \varepsilon_2, \delta_1 - \varepsilon_1, -\delta_1 - \varepsilon_1, K^+ + \varepsilon_1 - \varepsilon_2\},$$

$$\#32{:}\Delta^0 = \{-\varepsilon_2 - K^-, \varepsilon_1 + \varepsilon_2, \delta_1 - \varepsilon_1, -\delta_1 - \varepsilon_1, K^+ + \varepsilon_1 - \varepsilon_2\},$$

$$\#33{:}\Delta^0 = \{\varepsilon_4 - K^-, \varepsilon_3 - \varepsilon_4, \varepsilon_2 - \varepsilon_3, K^+ + \varepsilon_4 - \varepsilon_1, \varepsilon_1 - \varepsilon_2\},$$

$$\#34{:}\Delta^0 = \{\varepsilon_3 - \varepsilon_2 - K^-, \varepsilon_1 + \varepsilon_2, \delta_1 - \varepsilon_1, -\delta_1 - \varepsilon_1, K^+ + \varepsilon_1 - \varepsilon_2\},$$

$$\#35{:}\Delta^0 = \{-\varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_3 + \varepsilon_4, K^+ + \varepsilon_1 - \varepsilon_2\},$$

$$\#36{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, -\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, 2\varepsilon_2, -\varepsilon_1 - \varepsilon_2 - \varepsilon_3 - \varepsilon_4 + K^+\},$$

$$\#37{:}\Delta^0 = \left\{\varepsilon_1 - \varepsilon_2, K^+ - \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3, \tfrac{1}{2}(\tilde{\delta} - \varepsilon_1 - \varepsilon_2 - \varepsilon_3) - K^-\right\},$$

$$\#38{:}\Delta^0 = \{\delta_1 - \varepsilon_2 - K^-, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_3 + \varepsilon_4, K^+ + \varepsilon_1 - \varepsilon_2\}.$$

Rank 6 hyperbolic superalgebras: Conventions for the simple root systems $\Delta^0 = \{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_6\}$,

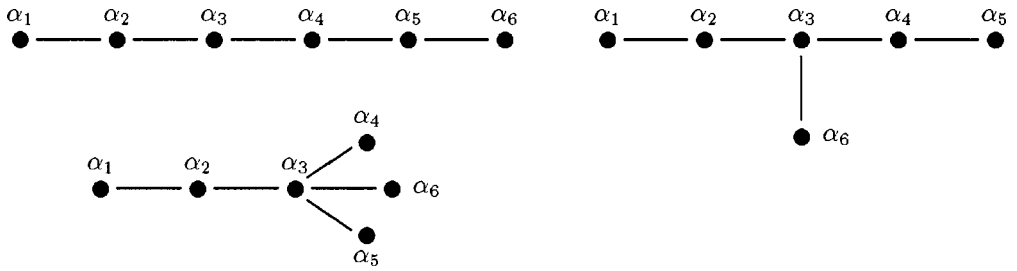

$$\#1{:}\Delta^0 = \left\{-\varepsilon_1 + \delta_1 - \tfrac{1}{2}K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_4, K^+ - \tfrac{1}{2}(\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4)\right\},$$

$$\#2{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, 2\varepsilon_4, K^+ - (\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4)\},$$

$$\#3{:}\Delta^0 = \left\{-\varepsilon_1 - \tfrac{1}{2}K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_4, K^+ - \tfrac{1}{2}(\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4)\right\},$$

$$\#4{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, 2\varepsilon_4, K^+ - (\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4)\},$$

$$\#5{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_4 - \varepsilon_5, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#6{:}\Delta^0 = \left\{\tfrac{1}{2}(\tilde{\delta} - \varepsilon_1 - \varepsilon_2 - \varepsilon_3) - 3K^-, \varepsilon_3 + \varepsilon_4, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \tfrac{1}{2}(-\tilde{\delta} - \varepsilon_1 - \varepsilon_2 - \varepsilon_3) + \tfrac{1}{2}K^+, \varepsilon_1 - \varepsilon_2\right\},$$

$$\#7{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, 2\varepsilon_4, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#8{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_4, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#9{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_4 - \varepsilon_5, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#10{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_4, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#11{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, 2\varepsilon_4, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#12{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_4, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#13{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_4, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#14{:}\Delta^0 = \{\delta_1 - \varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_3 + \varepsilon_4, K^+ - \varepsilon_1 - \varepsilon_2\},$$

$$\#15{:}\Delta^0 = \{-\varepsilon_1 - K^-, \varepsilon_1 - \varepsilon_2, \varepsilon_2 - \varepsilon_3, \varepsilon_3 - \varepsilon_4, \varepsilon_3 + \varepsilon_4, K^+ - \varepsilon_1 - \varepsilon_2\}.$$

APPENDIX C: SUBALGEBRAS OF THE HYPERBOLIC KM SUPERALGEBRAS

Rank 3 hyperbolic superalgebras:

#1: $G_2, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{osp}(1|4)$
#2: $G_2, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{osp}(1|4)$
#3: $\mathrm{sl}(1|3)^{(4)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sl}(3)$
#4: $\mathrm{osp}(1|4), \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sl}(3)^{(2)}$
#5: $\mathrm{osp}(1|4), \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sl}(3)^{(2)}$
#6: $\mathrm{sl}(1|3)^{(4)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sl}(2)^{(1)}$
#7: $\mathrm{sl}(1|3)^{(4)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sp}(4)$
#8: $\mathrm{sl}(1|3)^{(4)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sp}(4)$
#9: $\mathrm{sl}(1|3)^{(4)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sl}(3)^{(2)}$
#10: $\mathrm{sl}(1|3)^{(4)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), G_2$
#11: $\mathrm{sl}(1|3)^{(4)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), G_2$
#12: $\mathrm{sl}(1|3)^{(4)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sl}(3)^{(2)}$
#13: $\mathrm{osp}(1|2)^{(1)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sp}(4)$
#14: $\mathrm{osp}(1|2)^{(1)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sp}(4)$
#15: $\mathrm{osp}(1|2)^{(1)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sl}(3)$
#16: $\mathrm{osp}(1|2)^{(1)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), G_2$
#17: $\mathrm{osp}(1|2)^{(1)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), G_2$
#18: $\mathrm{osp}(1|2)^{(1)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sl}(2)^{(1)}$
#19: $\mathrm{osp}(1|2)^{(1)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sl}(3)^{(2)}$
#20: $\mathrm{osp}(1|2)^{(1)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sl}(3)^{(2)}$
#21: $\mathrm{osp}(1|4), \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{sl}(2)^{(1)}$
#22: $\mathrm{osp}(1|2)^{(1)}, 2\mathrm{sl}(2), \mathrm{sl}(1|3)^{(4)}$
#23: $\mathrm{osp}(1|2)^{(1)}, 2\mathrm{sl}(2), \mathrm{osp}(1|4)$
#24: $\mathrm{osp}(1|2)^{(1)}, 2\mathrm{sl}(2)$
#25: $\mathrm{sl}(1|3)^{(4)}, 2\mathrm{sl}(2)$
#26: $\mathrm{sl}(1|3)^{(4)}, 2\mathrm{sl}(2), \mathrm{osp}(1|4)$
#27: $\mathrm{osp}(2|2)^{(2)}, 2\mathrm{osp}(1|2)$
#28: $\mathrm{sl}(1|3)^{(4)}, 2\mathrm{osp}(1|2)$
#29: $\mathrm{osp}(1|4), 2\mathrm{osp}(1|2), \mathrm{sl}(1|3)^{(4)}$
#30: $\mathrm{osp}(1|2)^{(1)}, 2\mathrm{osp}(1|2), \mathrm{sl}(1|3)^{(4)}$
#31: $\mathrm{osp}(1|2)^{(1)}, 2\mathrm{osp}(1|2)$
#32: $\mathrm{sl}(1|3)^{(4)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{osp}(2|2)^{(2)}$
#33: $\mathrm{osp}(1|4), \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{osp}(2|2)^{(2)}$
#34: $\mathrm{osp}(1|2)^{(1)}, 2\mathrm{osp}(1|2), \mathrm{osp}(1|4)$
#35: $\mathrm{osp}(1|2)^{(1)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(2), \mathrm{osp}(2|2)^{(2)}$
#36: $G_2, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{sl}(1|2)$
#37: $\mathrm{sl}(3)^{(2)}, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{sl}(1|2)$
#38: $\mathrm{sl}(3)^{(2)}, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{sl}(1|2)$
#39: $\mathrm{sl}(2)^{(1)}, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{sl}(1|2)$
#40: $\mathrm{sl}(3), \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(3|2)$
#41: $\mathrm{sp}(4), \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(3|2)$
#42: $\mathrm{sp}(4), \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(3|2)$
#43: $G_2, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(3|2)$
#44: $G_2, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(3|2)$
#45: $\mathrm{sl}(3)^{(2)}, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(2|2)$
#46: $G_2, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(2|2)$
#47: $G_2, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(2|2)$
#48: $\mathrm{sl}(3)^{(2)}, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(2|2)$
#49: $\mathrm{sl}(3)^{(2)}, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(3|2)$
#50: $\mathrm{sl}(3)^{(2)}, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(3|2)$
#51: $\mathrm{sl}(2)^{(1)}, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(3|2)$
#52: $\mathrm{sl}(3), \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(2|2)$
#53: $\mathrm{so}(5), \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(2|2)$
#54: $\mathrm{sp}(4), \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(2|2)$
#55: $\mathrm{sl}(2)^{(1)}, \mathrm{sl}(1|1) \oplus \mathrm{sl}(2), \mathrm{osp}(2|2)$
#56: $\mathrm{sl}(1|3)^{(4)}, \mathrm{sl}(1|1) \oplus \mathrm{osp}(1|2), \mathrm{sl}(1|2)$
#57: $\mathrm{osp}(1|2)^{(1)}, \mathrm{sl}(1|1) \oplus \mathrm{osp}(1|2), \mathrm{sl}(1|2)$
#58: $\mathrm{sl}(1|3)^{(4)}, \mathrm{sl}(1|1) \oplus \mathrm{osp}(1|2), \mathrm{osp}(3|2)$
#59: $\mathrm{osp}(1|4), \mathrm{osp}(1|2) \oplus \mathrm{sl}(1|1), \mathrm{osp}(3|2)$
#60: $\mathrm{osp}(1|2)^{(1)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(1|1), \mathrm{osp}(3|2)$
#61: $\mathrm{sl}(1|3)^{(4)}, \mathrm{sl}(1|1) \oplus \mathrm{osp}(1|2), \mathrm{osp}(2|2)$
#62: $\mathrm{osp}(1|4), \mathrm{osp}(1|2) \oplus \mathrm{sl}(1|1), \mathrm{osp}(2|2)$
#63: $\mathrm{osp}(1|2)^{(1)}, \mathrm{osp}(1|2) \oplus \mathrm{sl}(1|1), \mathrm{osp}(2|2)$
#64: $\mathrm{sl}(1|3)^{(4)}, \mathrm{sl}(3)$
#65: $\mathrm{osp}(1|4), \mathrm{sl}(3)$
#66: $\mathrm{osp}(1|2)^{1)}, \mathrm{sl}(3)$
#67: $\mathrm{osp}(1|4), \mathrm{sp}(4), \mathrm{sl}(1|3)^{(4)}$
#68: $\mathrm{osp}(1|4), \mathrm{osp}(1|2)^{(1)}, \mathrm{sp}(4)$
#69: $\mathrm{sl}(1|3)^{(4)}, \mathrm{sl}(2)^{(1)}$
#70: $\mathrm{osp}(1|4), \mathrm{sl}(2)^{(1)}$
#71: $\mathrm{osp}(1|2)^{(1)}, \mathrm{sl}(2)^{(1)}$
#72: $\mathrm{osp}(2|2)^{(2)}, \mathrm{sl}(1|3)^{(4)}$
#73: $\mathrm{osp}(2|2)^{(2)}, \mathrm{osp}(1|4)$
#74: $\mathrm{osp}(2|2)^{(2)}, \mathrm{osp}(1|2)^{(1)}$
#75: $\mathrm{osp}(2|2)^{(2)}$
#76: $\mathrm{sl}(1|2), \mathrm{sl}(3)$
#77: $\mathrm{osp}(2|2), \mathrm{sl}(3)$
#78: $\mathrm{osp}(3|2), \mathrm{sl}(3)$

#79: $sl(1|2), sl(2)^{(1)}$
#80: $osp(2|2), sl(2)^{(1)}$
#81: $osp(3|2), sl(2)^{(1)}$
#82: $so(5), sl(1|2), osp(3|2)$
#83: $sp(4), sl(1|2), osp(2|2)$
#84: $sl(3)^{(2)}, osp(3|2), osp(2|2)$
#85: $osp(3|2), sl(1|2)$
#86: $osp(2|2), sl(1|2)$
#87: $osp(3|2), sl(1|2)$

Rank 4 hyperbolic superalgebras:

$$\#1{:}\,osp(1|4)^{(1)}, sl(2) \oplus osp(1|4), sl(3) \oplus osp(1|2), so(7),$$

$$\#2{:}\,osp(1|4)^{(1)}, sl(2) \oplus osp(1|4), so(5) \oplus osp(1|2), sl(5)^{(2)},$$

$$\#3{:}\,osp(1|4)^{(1)}, sl(2) \oplus osp(1|4), sp(4) \oplus osp(1|2), sl(4)^{(2)},$$

$$\#4{:}\,sl(1|5)^{(4)}, sl(2) \oplus osp(1|4), sl(3) \oplus osp(1|2), sp(6),$$

$$\#5{:}\,sl(1|5)^{(4)}, sl(2) \oplus osp(1|4), sp(4) \oplus osp(1|2), sp(4)^{(1)},$$

$$\#6{:}\,sl(1|5)^{(4)}, sl(2) \oplus osp(1|4), sp(4) \oplus osp(1|2), sl(5)^{(2)},$$

$$\#7{:}\,sl(1|4)^{(2)}, sl(2) \oplus osp(1|4), sl(3) \oplus sl(2), osp(1|6),$$

$$\#8{:}\,sl(1|4)^{(2)}, sl(2) \oplus osp(1|4), sp(4) \oplus sl(2), osp(1|4)^{(1)},$$

$$\#9{:}\,sl(1|4)^{(2)}, sl(2) \oplus osp(1|4), sp(4) \oplus sl(2), sl(1|5)^{(4)},$$

$$\#10{:}\,osp(1|4)^{(1)}, osp(1|2) \oplus osp(1|4), sl(1|5)^{(4)},$$

$$\#11{:}\,osp(2|4)^{(2)}, sl(2) \oplus osp(1|4), osp(1|4) \oplus osp(1|2), sl(1|4)^{(2)},$$

$$\#12{:}\,osp(2|4), sl(2) \oplus sl(1|2), sp(4) \oplus sl(1|1), sl(5)^{(2)},$$

$$\#13{:}\,osp(2|4), sl(2) \oplus sl(1|2), so(5) \oplus sl(1|1), sl(4)^{(2)},$$

$$\#14{:}\,osp(5|2), sl(2) \oplus sl(1|2), sp(4) \oplus sl(1|1), sp(4)^{(1)},$$

$$\#15{:}\,osp(5|2), sl(2) \oplus sl(1|2), sl(3) \oplus sl(1|1), sp(6),$$

$$\#16{:}\,osp(5|2), sl(2) \oplus sl(1|2), sp(4) \oplus sl(1|1), sl(5)^{(2)},$$

$$\#17{:}\,osp(1|4)^{(1)}, sl(1|1) \oplus osp(1|4), sl(1|2) \oplus osp(1|2), osp(5|2),$$

$$\#18{:}\,sl(1|5)^{(4)}, sl(1|1) \oplus osp(1|4), sl(1|2) \oplus osp(1|2), osp(2|4),$$

$$\#19{:}\,sl(1|4)^{(2)}, sl(1|1) \oplus osp(1|4), sl(1|2) \oplus sl(2), osp(3|4),$$

$$\#20{:}\,sl(1|3), sl(2) \oplus sl(1|2), G_2 \oplus sl(1|1), D_4^{(3)},$$

$$\#21{:}\mathrm{sl}(1|3),\mathrm{sl}(2)\oplus\mathrm{sl}(1|2),G_2\oplus\mathrm{sl}(1|1),G_2^{(1)},$$

$$\#22{:}G(3),\mathrm{sl}(2)\oplus\mathrm{sl}(1|2),\mathrm{sl}(3)\oplus\mathrm{sl}(1|1),G_2^{(1)},$$

$$\#23{:}\mathrm{osp}(4|2),\mathrm{sl}(2)\oplus\mathrm{osp}(2|2),G_2\oplus\mathrm{sl}(2),G(3),$$

$$\#24{:}\mathrm{osp}(3|4),\mathrm{sl}(2)\oplus\mathrm{osp}(3|2),G_2\oplus\mathrm{sl}(2),G(3),$$

$$\#25{:}\mathrm{sl}(2|2),\mathrm{sl}(2)\oplus\mathrm{sl}(1|2),G_2\oplus\mathrm{sl}(2),G(3),$$

$$\#26{:}\mathrm{osp}(1|6),\mathrm{sl}(2)\oplus\mathrm{osp}(1|4),G_2\oplus\mathrm{osp}(1|2),G_2^{(1)},$$

$$\#27{:}\mathrm{osp}(1|6),\mathrm{sl}(2)\oplus\mathrm{osp}(1|4),G_2\oplus\mathrm{osp}(1|2),D_4^{(3)},$$

$$\#28{:}\mathrm{osp}(5|2),\mathrm{sl}(2)\oplus\mathrm{osp}(3|2),G_2\oplus\mathrm{osp}(1|2),G(3),$$

$$\#29{:}\mathrm{sp}(6),\mathrm{sl}(1|1)\oplus 2\ \mathrm{sl}(2),\mathrm{sl}(1|3),\mathrm{osp}(2|4),$$

$$\#30{:}\mathrm{so}(7),\mathrm{sl}(1|1)\oplus 2\ \mathrm{sl}(2),\mathrm{sl}(1|3),\mathrm{osp}(5|2),$$

$$\#31{:}\mathrm{osp}(1|6),\mathrm{osp}(1|2)\oplus 2\ \mathrm{sl}(2),\mathrm{sp}(6),\mathrm{osp}(1|4)^{(1)},$$

$$\#32{:}\mathrm{osp}(1|6),\mathrm{osp}(1|2)\oplus 2\ \mathrm{sl}(2),\mathrm{so}(7),\mathrm{sl}(1|5)^{(4)},$$

$$\#33{:}\mathrm{osp}(5|2),\mathrm{sl}(1|1)\oplus 2\ \mathrm{sl}(2),\mathrm{sl}(4)^{(2)},$$

$$\#34{:}\mathrm{osp}(2|4),\mathrm{sl}(1|1)\oplus 2\ \mathrm{sl}(2),\mathrm{sp}(4)^{(1)},$$

$$\#35{:}\mathrm{osp}(2|4),\mathrm{sl}(1|1)\oplus 2\ \mathrm{sl}(2),\mathrm{osp}(5|2),\mathrm{sl}(5)^{(2)},$$

$$\#36{:}G(3),\mathrm{sl}(1|1)\oplus 2\ \mathrm{sl}(2),\mathrm{sl}(1|3),D_4^{(3)},$$

$$\#37{:}\mathrm{osp}(3|4),\mathrm{osp}(1|2)\oplus\mathrm{sl}(1|1)\oplus\mathrm{sl}(2),\mathrm{sl}(1|3),\mathrm{osp}(1|6),$$

$$\#38{:}\mathrm{osp}(3|4),\mathrm{osp}(1|2)\oplus\mathrm{sl}(1|1)\oplus\mathrm{sl}(2),\mathrm{osp}(2|4),\mathrm{osp}(1|4)^{(1)},$$

$$\#39{:}\mathrm{osp}(3|4),\mathrm{osp}(1|2)\oplus\mathrm{sl}(1|1)\oplus\mathrm{sl}(2),\mathrm{osp}(5|2),\mathrm{sl}(1|5)^{(4)},$$

$$\#40{:}\mathrm{osp}(3|4),2\ \mathrm{osp}(1|2)\oplus\mathrm{sl}(1|1),\mathrm{osp}(2|4)^{(2)},$$

$$\#41{:}\mathrm{sl}(1|5)^{(2)},\mathrm{osp}(1|2)\oplus 2\ \mathrm{sl}(2),\mathrm{sl}(4)^{(2)},$$

$$\#42{:}\mathrm{osp}(1|4)^{(1)},\mathrm{osp}(1|2)\oplus 2\ \mathrm{sl}(2),\mathrm{sp}(4)^{(1)},$$

$$\#43{:}\mathrm{osp}(1|4)^{(1)},\mathrm{osp}(1|2)\oplus 2\ \mathrm{sl}(2),\mathrm{sl}(1|5)^{(4)},\mathrm{sl}(5)^{(2)},$$

$$\#44{:}\mathrm{sl}(1|4)^{(2)},3\ \mathrm{sl}(2),$$

$$\#45{:}\mathrm{osp}(1|6),2\ \mathrm{osp}(1|2)\oplus\mathrm{sl}(2),\mathrm{sl}(1|5)^{(4)},$$

$$\#46{:}\mathrm{osp}(1|4)^{(1)},2\ \mathrm{osp}(1|2)\oplus\mathrm{sl}(2),\mathrm{sl}(1|5)^{(4)},$$

$$\#47{:}\mathrm{osp}(2|4)^{(2)},2\ \mathrm{osp}(1|2)\oplus\mathrm{sl}(2),\mathrm{sl}(1|5)^{(4)},$$

$$\#48{:}\mathrm{sl}(1|5)^{(4)},3\ \mathrm{osp}(1|2),$$

$$\#49{:}\mathrm{sl}(1|3),\mathrm{sl}(2)\oplus\mathrm{sl}(3),\mathrm{sl}(1|2)\oplus\mathrm{sl}(2),\mathrm{osp}(4|2),$$

$$\#50{:}\mathrm{osp}(5|2),\mathrm{sl}(2)\oplus\mathrm{so}(5),\mathrm{sl}(1|2)\oplus\mathrm{sl}(2),\mathrm{osp}(4|2),$$

$$\#51{:}\mathrm{osp}(2|4),\mathrm{sl}(2)\oplus\mathrm{sp}(4),\mathrm{sl}(1|2)\oplus\mathrm{sl}(2),\mathrm{osp}(4|2),$$

$$\#52{:}G(3),\mathrm{sl}(2)\oplus G_2,\mathrm{sl}(1|2)\oplus\mathrm{sl}(2),\mathrm{osp}(4|2),$$

$$\#53{:}\mathrm{osp}(3|4),\mathrm{sl}(2)\oplus\mathrm{osp}(1|4),\mathrm{sl}(1|2)\oplus\mathrm{osp}(1|2),\mathrm{osp}(4|2),$$

$\#54{:}\,\mathrm{osp}(4|2),3\ \mathrm{sl}(2),$
$\#55{:}\,\mathrm{sl}(1|3),\mathrm{sl}(2)\oplus 2\ \mathrm{sl}(1|1),\mathrm{sl}(2|2),$
$\#56{:}\,\mathrm{osp}(2|4),\mathrm{sl}(2)\oplus 2\ \mathrm{sl}(1|1),\mathrm{sl}(2|2),$
$\#57{:}\,\mathrm{osp}(5|2),\mathrm{sl}(2)\oplus 2\ \mathrm{sl}(1|1),\mathrm{sl}(2|2),$
$\#58{:}\,G(3),\mathrm{sl}(2)\oplus 2\ \mathrm{sl}(1|1),\mathrm{sl}(2|2),$
$\#59{:}\,\mathrm{sl}(1|2)^{(1)},\mathrm{sl}(1|2)\oplus\mathrm{sl}(2),\mathrm{sl}(1|3),$
$\#60{:}\,\mathrm{sl}(1|2)^{(1)},\mathrm{sl}(1|2)\oplus\mathrm{sl}(2),\mathrm{osp}(2|4),$
$\#61{:}\,\mathrm{sl}(1|2)^{(1)},\mathrm{sl}(1|2)\oplus\mathrm{sl}(2),\mathrm{osp}(5|2),$
$\#62{:}\,\mathrm{sl}(1|2)^{(1)},\mathrm{sl}(1|2)\oplus\mathrm{sl}(2),G(3),$
$\#63{:}\,\mathrm{sl}(3)^{(1)},\mathrm{sl}(3)\oplus\mathrm{sl}(1|1),\mathrm{sl}(1|3),$
$\#64{:}\,\mathrm{sl}(3)^{(1)},\mathrm{sl}(3)\oplus\mathrm{osp}(1|2),\mathrm{osp}(1|6),$
$\#65{:}\,\mathrm{osp}(2|4),\mathrm{osp}(2|2)\oplus\mathrm{sl}(2),G(3),$
$\#66{:}\,\mathrm{sl}(1|4)^{(2)},\mathrm{osp}(1|4)^{(1)},\mathrm{sl}(4)^{(2)},$
$\#67{:}\,\mathrm{sl}(1|4)^{(2)},\mathrm{sl}(1|5)^{(4)},\mathrm{sp}(4)^{(1)},$
$\#68{:}\,\mathrm{sl}(1|4)^{(2)},\mathrm{osp}(2|4)^{(2)},$
$\#69{:}\,\mathrm{sl}(1|4)^{(2)},\mathrm{osp}(1|6),\mathrm{sl}(4),$
$\#70{:}\,\mathrm{sl}(4),\mathrm{sl}(1|3),\mathrm{sl}(2|2),$
$\#71{:}\,\mathrm{sp}(4)^{(1)},\mathrm{osp}(5|2),\mathrm{osp}(4|2),$
$\#72{:}\,\mathrm{sl}(4)^{(2)},\mathrm{osp}(2|4),\mathrm{osp}(4|2).$
$\#73{:}\,\mathrm{sl}(1|4)^{(2)},\mathrm{sl}(2|2),\mathrm{osp}(3|4),$

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Rank 5 hyperbolic superalgebras:

$$\#1{:}\mathrm{so}(9),\mathrm{sl}(4)\oplus\mathrm{sl}(1|1),\mathrm{sl}(3)\oplus\mathrm{sl}(1|2),\mathrm{osp}(2|4)\oplus\mathrm{sl}(2),F(4),$$

$$\#2{:}\mathrm{osp}(7|2),\mathrm{sl}(2)\oplus\mathrm{sl}(1|3),\mathrm{sl}(3)\oplus\mathrm{sl}(1|2),\mathrm{sp}(6)\oplus\mathrm{sl}(1|1),F_4,$$

$$\#3{:}\mathrm{osp}(7|2),\mathrm{sl}(1|3)\oplus\mathrm{sl}(1|1),2\ \mathrm{sl}(1|2),\mathrm{osp}(2|4)\oplus\mathrm{sl}(1|1),F(4),$$

$$\#4{:}\mathrm{osp}(4|4),\mathrm{sl}(2|2)\oplus\mathrm{sl}(2),\mathrm{sl}(3)\oplus\mathrm{sl}(1|2),\mathrm{so}(7)\oplus\mathrm{sl}(2),F(4),$$

$$\#5{:}\mathrm{sl}(7)^{(2)},\mathrm{sp}(6)\oplus\mathrm{sl}(1|1),\mathrm{sp}(4)\oplus\mathrm{sl}(1|2),\mathrm{osp}(2|4)\oplus\mathrm{sl}(2),F(4),$$

$$\#6{:}\mathrm{so}(8)^{(2)},\mathrm{so}(7)\oplus\mathrm{sl}(1|1),\mathrm{so}(5)\oplus\mathrm{sl}(1|2),\mathrm{osp}(2|4)\oplus\mathrm{sl}(2),F(4),$$

$$\#7{:}\mathrm{sl}(2|4)^{(2)},\mathrm{osp}(4|2)\oplus\mathrm{sl}(2),\mathrm{osp}(2|2)\oplus\mathrm{sl}(3),\mathrm{so}(7)\oplus\mathrm{sl}(2),F(4),$$

$$\#8{:}\mathrm{osp}(3|4)^{(1)},\mathrm{osp}(3|4)\oplus\mathrm{sl}(2),\mathrm{osp}(3|2)\oplus\mathrm{sl}(3),\mathrm{so}(7)\oplus\mathrm{sl}(2),F(4),$$

$$\#9{:}\mathrm{osp}(1|6)^{(1)},\mathrm{osp}(1|6)\oplus\mathrm{sl}(2),\mathrm{osp}(1|4)\oplus\mathrm{sl}(3),\mathrm{osp}(1|2)\oplus\mathrm{so}(7),F_4,$$

$$\#10{:}\mathrm{sl}(1|7)^{(4)},\mathrm{osp}(1|6)\oplus\mathrm{sl}(2),\mathrm{osp}(1|4)\oplus\mathrm{sl}(3),\mathrm{osp}(1|2)\oplus\mathrm{sp}(6),F_4,$$

$$\#11{:}\mathrm{sl}(1|7)^{(4)},\mathrm{osp}(1|6)\oplus\mathrm{sl}(1|1),\mathrm{osp}(1|4)\oplus\mathrm{sl}(1|2),\mathrm{osp}(2|4)\oplus\mathrm{osp}(1|2),F(4),$$

$$\#12{:}\mathrm{sl}(5|2)^{(2)},\mathrm{osp}(5|2)\oplus\mathrm{sl}(2),\mathrm{osp}(3|2)\oplus\mathrm{sl}(3),\mathrm{so}(7)\oplus\mathrm{osp}(1|2),F(4),$$

$$\#13{:}F_4,\mathrm{so}(7)\oplus\mathrm{sl}(1|1),\mathrm{sl}(3)\oplus\mathrm{sl}(1|2),\mathrm{sl}(2)\oplus\mathrm{sl}(1|3),\mathrm{osp}(2|6),$$

$$\#14{:}\mathrm{so}(7)^{(1)},\mathrm{so}(7)\oplus\mathrm{osp}(1|2),\mathrm{osp}(1|4)\oplus 2\mathrm{sl}(2),\mathrm{osp}(1|8),\mathrm{sl}(1|7)^{(4)},$$

$$\#15{:}\mathrm{sl}(6)^{(2)},\mathrm{sp}(6)\oplus\mathrm{osp}(1|2),\mathrm{osp}(1|4)\oplus 2\mathrm{sl}(2),\mathrm{osp}(1|8),\mathrm{osp}(1|6)^{(1)},$$

$$\#16{:}\mathrm{sl}(1|6)^{(2)},\mathrm{osp}(1|6)\oplus\mathrm{sl}(2),\mathrm{sl}(3)\oplus\mathrm{sl}(2)\oplus\mathrm{osp}(1|2),\mathrm{sl}(5),\mathrm{osp}(1|8),$$

$$\#17{:}\mathrm{sl}(1|6)^{(2)},\mathrm{osp}(1|6)\oplus\mathrm{sl}(2),\mathrm{sp}(4)\oplus\mathrm{osp}(1|2)\oplus\mathrm{sl}(2),\mathrm{sp}(8),\mathrm{osp}(1|6)^{(1)},$$

$$\#18{:}\mathrm{sl}(1|6)^{(2)},\mathrm{osp}(1|6)\oplus\mathrm{sl}(2),\mathrm{so}(5)\oplus\mathrm{osp}(1|2)\oplus\mathrm{sl}(2),\mathrm{so}(9),\mathrm{sl}(1|7)^{(4)},$$

$$\#19{:}\mathrm{sl}(1|6)^{(2)},\mathrm{osp}(1|6)\oplus\mathrm{osp}(1|2),\mathrm{osp}(1|4)\oplus\mathrm{osp}(1|2)\oplus\mathrm{sl}(2),\mathrm{osp}(1|8),\mathrm{osp}(2|6)^{(2)},$$

$$\#20{:}\mathrm{sl}(1|6)^{(2)},\mathrm{osp}(1|6)\oplus\mathrm{sl}(1|1),\mathrm{sl}(1|2)\oplus\mathrm{osp}(1|2)\oplus\mathrm{sl}(2),\mathrm{sl}(1|4),\mathrm{osp}(3|6),$$

$$\#21{:}\mathrm{osp}(6|2),\mathrm{osp}(1|2)\oplus\mathrm{sl}(1|3),\mathrm{osp}(1|4)\oplus\mathrm{sl}(1|1)\oplus\mathrm{sl}(2),\mathrm{osp}(1|8),\mathrm{osp}(3|6),$$

$$\#22{:}\mathrm{osp}(6|2),\mathrm{sl}(2)\oplus\mathrm{sl}(1|3),\mathrm{sl}(3)\oplus\mathrm{sl}(2)\oplus\mathrm{sl}(1|1),\mathrm{sl}(5),\mathrm{sl}(1|4),$$

$$\#23{:}\mathrm{osp}(6|2),\mathrm{sl}(1|3)\oplus\mathrm{sl}(1|1),\mathrm{sl}(1|2)\oplus\mathrm{sl}(1|1)\oplus\mathrm{sl}(2),\mathrm{sl}(1|4),\mathrm{sl}(2|3),$$

$$\#24{:}\mathrm{sl}(6)^{(2)},\mathrm{sp}(6)\oplus\mathrm{sl}(1|1),\mathrm{sl}(1|2)\oplus 2\mathrm{sl}(2),\mathrm{sl}(1|4),\mathrm{osp}(2|6),$$

$$\#25{:}\mathrm{so}(7)^{(1)},\mathrm{so}(7)\oplus\mathrm{sl}(1|1),\mathrm{sl}(1|2)\oplus 2\mathrm{sl}(2),\mathrm{sl}(1|4),\mathrm{osp}(7|2),$$

$$\#26{:}\mathrm{osp}(6|2),\mathrm{sl}(2)\oplus\mathrm{sl}(1|3),\mathrm{sp}(4)\oplus\mathrm{sl}(2)\oplus\mathrm{sl}(1|1),\mathrm{sp}(8),\mathrm{osp}(2|6),$$

$$\#27{:}\mathrm{osp}(6|2),\mathrm{sl}(2)\oplus\mathrm{sl}(1|3),\mathrm{so}(5)\oplus\mathrm{sl}(2)\oplus\mathrm{sl}(1|1),\mathrm{so}(9),\mathrm{osp}(7|2),$$

$$\#28{:}\mathrm{sl}(4)^{(1)},\mathrm{sl}(4)\oplus\mathrm{sl}(1|1),\mathrm{sl}(1|4),\mathrm{osp}(6|2),$$

$$\#29{:}\mathrm{sl}(1|3)^{(1)},\mathrm{sl}(1|3)\oplus\mathrm{sl}(2),\mathrm{sl}(1|4),\mathrm{osp}(6|2),$$

$$\#30{:}\mathrm{sl}(2|4)^{(2)},\mathrm{osp}(2|4)\oplus\mathrm{sl}(2),\mathrm{osp}(4|4),\mathrm{osp}(2|4)^{(1)},$$

$$\#31{:}\mathrm{sl}(2|4)^{(2)},\mathrm{osp}(2|4)\oplus\mathrm{sl}(2),\mathrm{osp}(5|4),\mathrm{sl}(5|2)^{(2)},$$

$$\#32{:}\mathrm{sl}(2|4)^{(2)},\mathrm{osp}(2|4)\oplus\mathrm{osp}(1|2),\mathrm{osp}(5|4),\mathrm{osp}(3|4)^{(1)},$$

$$\#33{:}\mathrm{sl}(4)^{(1)},\mathrm{sl}(4)\oplus\mathrm{osp}(1|2),\mathrm{sl}(1|6)^{(2)},\mathrm{osp}(1|8),$$

$$\#34{:}\mathrm{sl}(2|4)^{(2)},\mathrm{osp}(2|4)\oplus\mathrm{sl}(2),\mathrm{sl}(2|3),\mathrm{osp}(2|6),$$

$$\#35{:}\mathrm{so}(8),\mathrm{osp}(1|2)\oplus 3\ \mathrm{sl}(2),\mathrm{sl}(1|6)^{(2)},$$

$$\#36{:}F(4),\mathrm{osp}(2|2)\oplus\mathrm{sl}(3),\mathrm{osp}(2|4)\oplus\mathrm{sl}(2),\mathrm{osp}(2|4)^{(1)},$$

$$\#37{:}F(4),\mathrm{sl}(1|2)\oplus 2\mathrm{sl}(2),\mathrm{sl}(4)\oplus\mathrm{sl}(1|1),\mathrm{so}(7)^{(1)},$$

$$\#38{:}\mathrm{so}(8),\mathrm{osp}(6|2),\mathrm{sl}(1|1)\oplus 3\ \mathrm{sl}(2),$$

Rank 6 hyperbolic superalgebras:

$$\#1{:}F_4^{(1)},\mathrm{sl}(1|1)\oplus F_4,\mathrm{sl}(1|2)\oplus\mathrm{sp}(6),\mathrm{sl}(1|3)\oplus\mathrm{sl}(3),\mathrm{sl}(1|4)\oplus\mathrm{sl}(2),\mathrm{osp}(9|2),$$

$$\#2{:}E_6^{(2)},\mathrm{sl}(1|1)\oplus F_4,\mathrm{sl}(1|2)\oplus\mathrm{so}(7),\mathrm{sl}(1|3)\oplus\mathrm{sl}(3),\mathrm{sl}(1|4)\oplus\mathrm{sl}(2),\mathrm{osp}(2|8),$$

$$\#3{:}F_4^{(1)},\mathrm{osp}(1|2)\oplus F_4,\mathrm{osp}(1|4)\oplus\mathrm{sp}(6),\mathrm{osp}(1|6)\oplus\mathrm{sl}(3),\mathrm{osp}(1|8)\oplus\mathrm{sl}(2),\mathrm{sl}(1|9)^{(4)},$$

$$\#4{:}E_6^{(2)},\mathrm{osp}(1|2)\oplus F_4,\mathrm{osp}(1|4)\oplus\mathrm{so}(7),\mathrm{osp}(1|6)\oplus\mathrm{sl}(3),\mathrm{osp}(1|8)\oplus\mathrm{sl}(2),\mathrm{osp}(1|8)^{(1)},$$

$$\#5{:}\mathrm{so}(10),\mathrm{sl}(1|1)\oplus\mathrm{sl}(5),\mathrm{sl}(1|2)\oplus\mathrm{sl}(3)\oplus\mathrm{sl}(2),\mathrm{sl}(1|4)\oplus\mathrm{sl}(2),\mathrm{osp}(8|2),\mathrm{sl}(1|5),$$

$$\#6{:}\mathrm{osp}(8|2),\mathrm{sl}(1|1)\oplus\mathrm{sl}(1|4),\mathrm{sl}(2)\oplus 2\mathrm{sl}(1|2),\mathrm{sl}(2|4),$$

$$\#7{:}\mathrm{sl}(8)^{(2)},\mathrm{sl}(1|1)\oplus\mathrm{sp}(8),\mathrm{sl}(1|2)\oplus\mathrm{sl}(2)\oplus\mathrm{sp}(4),\mathrm{sl}(1|4)\oplus\mathrm{sl}(2),\mathrm{osp}(8|2),\mathrm{osp}(2|8),$$

$$\#8{:}\mathrm{so}(9)^{(1)},\mathrm{sl}(1|1)\oplus\mathrm{so}(9),\mathrm{sl}(1|2)\oplus\mathrm{sl}(2)\oplus\mathrm{so}(5),\mathrm{sl}(1|4)\oplus\mathrm{sl}(2),\mathrm{osp}(8|2),\mathrm{osp}(9|2),$$

$$\#9{:}\mathrm{so}(10),\mathrm{osp}(1|2)\oplus\mathrm{sl}(5),\mathrm{sl}(2)\oplus\mathrm{sl}(3)\oplus\mathrm{osp}(1|4),\mathrm{sl}(2)\oplus\mathrm{osp}(1|8),\mathrm{sl}(1|8)^{(2)},\mathrm{osp}(1|10),$$

$$\#10{:}\mathrm{so}(9)^{(1)},\mathrm{osp}(1|2)\oplus\mathrm{so}(9),\mathrm{osp}(1|4)\oplus\mathrm{sl}(2)\oplus\mathrm{so}(5),\mathrm{osp}(1|8)\oplus\mathrm{sl}(2),\mathrm{sl}(1|8)^{(2)},\mathrm{sl}(1|9)^{(4)},$$

$$\#11{:}\mathrm{sl}(8)^{(2)},\mathrm{osp}(1|2)\oplus\mathrm{sp}(8),\mathrm{osp}(1|4)\oplus\mathrm{sl}(2)\oplus\mathrm{sp}(4),\mathrm{osp}(1|8)\oplus\mathrm{sl}(2),\mathrm{sl}(1|8)^{(2)},\mathrm{osp}(1|8)^{(1)},$$

$$\#12{:}\mathrm{sl}(1|8)^{(2)},\mathrm{osp}(1|2)\oplus\mathrm{osp}(1|8),\mathrm{osp}(1|4)\oplus\mathrm{sl}(2)\oplus\mathrm{osp}(1|4),\mathrm{osp}(2|8)^{(2)},$$

$$\#13{:}\mathrm{sl}(1|8)^{(2)},\mathrm{sl}(1|1)\oplus\mathrm{osp}(1|8),\mathrm{sl}(1|2)\oplus\mathrm{sl}(2)\oplus\mathrm{osp}(1|4),\mathrm{sl}(1|4)\oplus\mathrm{osp}(1|2),\mathrm{osp}(8|2),\mathrm{osp}(3|8),$$

$$\#14{:}\mathrm{so}(8)^{(1)},\mathrm{sl}(1|1)\oplus\mathrm{so}(8),\mathrm{sl}(1|2)\oplus 3\ \mathrm{sl}(2),\mathrm{osp}(8|2),$$

$$\#15{:}\mathrm{so}(8)^{(1)},\mathrm{osp}(1|2)\oplus\mathrm{so}(8),\mathrm{osp}(1|4)\oplus 3\ \mathrm{sl}(2),\mathrm{sl}(1|8)^{(2)}\ .$$

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On unitary, irreducible representations of the proper, orthochronous Lorentz group

J. Kubieniec[a)]
Marian Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, 30-059 Kraków, Poland

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The theory of unitary, irreducible representations of the proper, orthochronous Lorentz group is presented by means of the usual tensor calculus in Minkowski space–time. This makes all steps manifestly Lorentz invariant. Explicit expressions for spherically symmetric eigenfunctions of the first Casimir operator C_1 of the proper, orthochronous Lorentz group are calculated and their completeness is proved. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1869537]

I. INTRODUCTION

Unitary, irreducible representations of the proper, orthochronous Lorentz group were discovered simultaneously and independently by Gelfand and Neumark,[1] Bargmann,[2] and Harish-Chandra.[3] They are described in several textbooks, both mathematical[4,5] and physical.[6,7] In all those textbooks the functions spanning the representation space depend on one complex variable. The connection with the Lorentz group arises from the well-known isomorphism between the group of proper, orthochronous Lorentz transformations of null directions and the group of homographic transformations of the complex plane. However, the existence of this isomorphism allows only to check the Lorentz invariance, which in the tensor calculus in Minkowski space–time is manifest.

In this paper we shall construct the representations of the proper, orthochronous Lorentz group by analogy with the representations of the rotation group SO(3). The spherical functions Y_{lm}, which span the unitary, irreducible representations of the rotation group SO(3), can be obtained as the solutions of the Laplace equation

$$\Delta f \equiv \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} = 0, \tag{1}$$

which have a fixed degree of homogeneity d,

$$f(\lambda x, \lambda y, \lambda z) = \lambda^d f(x,y,z) \quad \text{for each } \lambda > 0. \tag{2}$$

Solving the Laplace equation we obtain

$$f(x,y,z) = r^l Y_{lm}(\theta, \varphi), \tag{3}$$

where r, θ, and φ are the usual spherical coordinates, $l=0,1,2,\ldots$ and $m=-l,\ldots,l$. Thus $d=l=0,1,2,\ldots$.

By analogy, we shall consider the solutions of the d'Alembert equation ($c=1$),

a)Electronic mail: jakub@th.if.uj.edu.pl

$$\Box f \equiv \frac{\partial^2 f}{\partial t^2} - \frac{\partial^2 f}{\partial x^2} - \frac{\partial^2 f}{\partial y^2} - \frac{\partial^2 f}{\partial z^2} = 0, \tag{4}$$

which have a fixed degree of homogeneity d,

$$f(\lambda t, \lambda x, \lambda y, \lambda z) = \lambda^d f(t,x,y,z) \quad \text{for each } \lambda > 0. \tag{5}$$

This approach allows to use the tensor calculus in Minkowski space–time, thus making the Lorentz invariance manifest at each step. Moreover, it reveals the spatiotemporal shape of solutions which is completely absent in the standard expositions mentioned above.

We use units in which $\hbar = 1 = c$. We use the metric tensor $g_{\mu\nu}$ such that $xx = g_{\mu\nu}x^\mu x^\nu \equiv (x^0)^2 - (x^1)^2 - (x^2)^2 - (x^3)^2$. Finally, we restrict our treatment to the spinless case $C_2 = 0$, where C_2 is the second Casimir operator of the proper, orthochronous Lorentz group. The reason is that $C_2 = 0$ for the so-called supplementary series, which is the hardest case from the point of view of the Lorentz invariance and quantum-mechanical significance.

II. THE INTERNAL GEOMETRY OF THE LIGHT CONE

We describe the internal geometry of the light cone, following Gelfand, Graev, and Vilenkin[4] (cf. p. 426), and Staruszkiewicz.[8]

The upper light cone (here in the momentum space) is a figure formed by positive frequency null vectors $kk = 0$, $k^0 > 0$. It consists of null directions. A null direction is a set of null vectors parallel to a given null vector. Null directions generate two Lorentz invariant measures on the upper light cone, the projective distance along the null directions,

$$\left.\frac{\mathrm{d}k^0}{k^0}\right| \; k^1 : k^2 : k^3 = \text{const} \tag{6}$$

and the volume of the set of null directions

$$\mathrm{d}^2 k = \frac{k^1\, \mathrm{d}k^2 \wedge \mathrm{d}k^3 + k^2\, \mathrm{d}k^3 \wedge \mathrm{d}k^1 + k^3\, \mathrm{d}k^1 \wedge \mathrm{d}k^2}{k^0}. \tag{7}$$

Here $\wedge$ denotes the outer product. The well-known Lorentz invariant volume of the upper light cone

$$\mathrm{d}k = \frac{\mathrm{d}k^1 \wedge \mathrm{d}k^2 \wedge \mathrm{d}k^3}{k^0} \tag{8}$$

can be written as the outer product of the projective distance along the null directions and the volume of the set of null directions,

$$\mathrm{d}k = \frac{\mathrm{d}k^0}{k^0} \wedge \mathrm{d}^2 k. \tag{9}$$

The Lorentz invariant measure $\mathrm{d}^2 k$ is applicable when one integrates a homogeneous of degree -2 function of k because then one obtains a manifestly Lorentz invariant integral. This allows, e.g., to calculate many difficult integrals in a simple way.[8]

Consider, for example, the simplest integral of this form

$$I(u) = \int \frac{\mathrm{d}^2 k}{(uk)^2}, \tag{10}$$

where u is a timelike vector $uu > 0$. In the spherical coordinates,

$$k^0 = \omega,$$

$$k^1 = \omega \sin\theta \cos\varphi,$$

$$k^2 = \omega \sin\theta \sin\varphi,$$

$$k^3 = \omega \cos\theta, \tag{11}$$

$\mathrm{d}^2k = \omega^2 \sin\theta\, \mathrm{d}\theta \wedge \mathrm{d}\varphi$. The integral $I(u)$ is manifestly Lorentz invariant and therefore can be calculated in the rest frame of u, in which it is equal to

$$I(u) = \int \frac{\omega^2 \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\varphi}{(u^0)^2\omega^2} = \frac{4\pi}{(u^0)^2} = \frac{4\pi}{uu}. \tag{12}$$

Someone who does not know that the integral $I(u)$ is Lorentz invariant will use only its rotational invariance and will have to take an additional integral over θ. In this case the use of the Lorentz invariance is a matter of convenience but in more complicated cases it makes a difference between what can and what cannot be done.

III. SOLUTIONS OF THE D'ALEMBERT EQUATION WITH A FIXED DEGREE OF HOMOGENEITY

The generators of the proper, orthochronous Lorentz group for the spinless case in Minkowski space–time written in a manifestly Lorentz covariant form are

$$M_{\mu\nu} = x_\mu p_\nu - x_\nu p_\mu = i\left(x_\mu \frac{\partial}{\partial x^\nu} - x_\nu \frac{\partial}{\partial x^\mu}\right). \tag{13}$$

The Casimir operators of the proper, orthochronous Lorentz group for the spinless case in Minkowski space–time written in a manifestly Lorentz invariant form are

$$C_1 = -\tfrac{1}{2} M_{\mu\nu}M^{\mu\nu} = xx\Box - x^\mu \frac{\partial}{\partial x^\mu}\left(x^\nu \frac{\partial}{\partial x^\nu} + 2\right), \tag{14}$$

$$C_2 = \tfrac{1}{8}\epsilon^{\mu\nu\rho\sigma} M_{\mu\nu}M_{\rho\sigma} \equiv 0. \tag{15}$$

Here $\Box$ denotes the d'Alembert operator, $\epsilon^{\mu\nu\rho\sigma}$ denotes the Levi–Civita symbol, $\epsilon^{0123} = 1$.

Assume that f is a solution of the d'Alembert equation $\Box f = 0$ with a fixed degree of homogeneity d. The Euler theorem on homogeneous functions states that

$$x^\mu \frac{\partial}{\partial x^\mu} f = df. \tag{16}$$

Then

$$C_1 f = -d(d+2)f, \tag{17}$$

which shows that the degree of homogeneity d fixes the eigenvalue of the Casimir operator C_1. Hence irreducible representations can be classified according to the degree of homogeneity.

To have unitarity we need a positive definite scalar product. It is well known that such a scalar product is obtained when the standard sesquilinear, Hermitian form

$$(f,f) = i\int_{\mathrm{CS}} \mathrm{d}\Sigma^\mu \left(\bar{f}\frac{\partial f}{\partial x^\mu} - \frac{\partial \bar{f}}{\partial x^\mu} f\right), \tag{18}$$

where CS is an arbitrary Cauchy surface and $\mathrm{d}\Sigma^\mu$ is the volume element on this surface, is restricted to positive frequency solutions, i.e., to solutions whose Fourier transform has the support on the upper light cone in the momentum space.

This closes our construction for the so-called main series.

IV. THE MAIN SERIES

The Casimir operator C_1 for the main series has values[4] $C_1=1+\nu^2\geqslant 1$, which means that the degree of homogeneity $d=-1-i\nu$ with ν real. Positive frequency solutions of the d'Alembert equation, which are homogeneous of degree $-1-i\nu$ can be represented by the Fourier transform

$$f(x)=\int \mathrm{d}k\, e^{-ikx}f(k), \tag{19}$$

where the function $f(k)$, defined on the upper light cone in the momentum space, is homogeneous of degree $-1+i\nu$. Expressing the sesquilinear, Hermitian form (f,f) from the preceding section by the Fourier transform $f(k)$ we obtain

$$(f,f)=2(2\pi)^3\int_0^\infty \frac{\mathrm{d}k^0}{k^0}\cdot\int \mathrm{d}^2k\,\overline{f(k)}f(k). \tag{20}$$

Dropping the infinite constant $2(2\pi)^3\int_0^\infty \mathrm{d}k^0/k^0$ we have the local scalar product in the momentum space appropriate for the main series

$$\langle f|f\rangle=\int \mathrm{d}^2k\,\overline{f(k)}f(k), \tag{21}$$

which is manifestly Lorentz invariant and positive definite. In this manner we obtain a Hilbert space, in which irreducible representations of the proper, orthochronous Lorentz group are unitary. The functions belonging to this Hilbert space are square integrable.

It is clear that a spherically symmetric function $f(k)$ must be proportional to

$$(k^0)^{-1+i\nu}. \tag{22}$$

This gives spherically symmetric solutions $f(x)$ in Minkowski space–time proportional to (see Appendix A)

$$\frac{1}{r}\left\{\left[\cosh\left(\frac{\pi}{2}\nu\right)+\mathrm{sign}(t-r)\sinh\left(\frac{\pi}{2}\nu\right)\right]|t-r|^{-i\nu}-\left[\cosh\left(\frac{\pi}{2}\nu\right)+\mathrm{sign}(t+r)\sinh\left(\frac{\pi}{2}\nu\right)\right]|t+r|^{-i\nu}\right\}, \tag{23}$$

where $t=x^0$, $r=\sqrt{(x^1)^2+(x^2)^2+(x^3)^2}$, sign is the signum function.

The functions belonging to the main series form a complete set (see Appendix B). Thus someone who knows quantum mechanics would suspect that these are all representations. There exists, nevertheless, the supplementary series.

V. THE SUPPLEMENTARY SERIES

The existence of the supplementary series, undoubtedly surprising from the point of view of quantum mechanics, can be inferred as follows. Consider the hyperboloid $xx=-1$. This hyperboloid is a three-dimensional space–time analogous to the four-dimensional de Sitter space–time used sometimes in cosmology. The operator $-C_1=(1/2)M_{\mu\nu}M^{\mu\nu}$, given by Eq. (14), is the d'Alembert operator in this space–time. Therefore the eigenequation

$$C_1 f=-d(d+2)f \tag{24}$$

is the Klein–Gordon equation in the three-dimensional de Sitter space–time $xx=-1$. For the main series the square of the "mass" $-d(d+2)=1+\nu^2\geqslant 1$. Physically this is of course the square of the product of physical mass and radius; the condition $-d(d+2)=1+\nu^2\geqslant 1$ means simply that the square of this product is bigger than the critical value equal to 1. There is no reason, however, to

assume the condition $-d(d+2) \geqslant 1$. Space–time, in this case the three-dimensional de Sitter space–time $xx=-1$, is simply a container in which we should be able to place a quantum particle of arbitrary real and positive physical mass. Using this physically obvious principle we set[4]

$$\nu = i\sigma, \quad 0 < \sigma < 1, \tag{25}$$

which means that $0 < C_1 = -d(d+2) = 1-\sigma^2 < 1$ and $f(x)$ is now homogeneous of degree $-1+\sigma$ while $f(k)$ is homogeneous of degree $-1-\sigma$.

The de Sitter space–time $xx=-1$ has a compact Cauchy surface which means that the standard sesquilinear, Hermitian form

$$(f,f) = i\int_{\mathrm{CS}} \mathrm{d}\Sigma^k \left(\bar{f}\frac{\partial f}{\partial \xi^k} - \frac{\partial \bar{f}}{\partial \xi^k} f \right), \tag{26}$$

where ξ^1, ξ^2, ξ^3 are arbitrary internal coordinates in this space–time, is always perfectly well defined. We assume the definition of a positive frequency solution in the de Sitter space–time $xx=-1$ first given by Staruszkiewicz:[9] a solution of the Klein–Gordon equation with the square of the "mass" $-d(d+2)$ in the de Sitter space–time $xx=-1$ is a positive frequency one if it is a restriction to the hyperboloid $xx=-1$ of a homogeneous of degree d, positive frequency solution of the d'Alembert equation in Minkowski space–time. Thus we obtain a Lorentz invariant and positive definite scalar product, which we need to have a unitary representation.

Let us express the sesquilinear, Hermitian form (f,f) by the Fourier transform $f(k)$ which now is homogeneous of degree $-1-\sigma$. Since (f,f) is a Lorentz invariant scalar product, there is a function $K(\sigma)$ such that

$$(f,f) = \int \frac{\mathrm{d}^2k\, \mathrm{d}^2l}{(kl)^{1-\sigma}} \overline{f(k)} f(l) \cdot K(\sigma). \tag{27}$$

Dropping the irrelevant function $K(\sigma)$ we have the nonlocal scalar product in the momentum space appropriate for the supplementary series

$$\langle f|f\rangle_\sigma = \int \frac{\mathrm{d}^2k\, \mathrm{d}^2l}{(kl)^{1-\sigma}} \overline{f(k)} f(l), \tag{28}$$

which is manifestly Lorentz invariant. The reader is invited to compare this expression with the same scalar product given by Mukunda and Simon[10] in Eq. (5.4) of their paper to see the improvement brought about by the use of the Lorentz invariant measure d^2k. In this manner we obtain a Hilbert space, in which irreducible representations of the proper, orthochronous Lorentz group are unitary.

It is clear that a spherically symmetric function $f(k)$ must be proportional to

$$(k^0)^{-1-\sigma}. \tag{29}$$

This gives spherically symmetric solutions $f(x)$ in Minkowski space–time proportional to (see again Appendix A)

$$\frac{1}{r}\left\{ \left[\cos\left(\frac{\pi}{2}\sigma\right) + i\,\mathrm{sign}(t-r)\sin\left(\frac{\pi}{2}\sigma\right) \right] |t-r|^\sigma - \left[\cos\left(\frac{\pi}{2}\sigma\right) + i\,\mathrm{sign}(t+r)\sin\left(\frac{\pi}{2}\sigma\right) \right] |t+r|^\sigma \right\}. \tag{30}$$

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APPENDIX A: THE USEFUL INTEGRAL

Let us consider the integral analytic in the lower half-plane of complex time $\mathrm{Im}\, x^0 < 0$,

$$\int \mathrm{d}k\, e^{-ikx}(k^0)^{-1-C}, \tag{A1}$$

which is to be understood as the limit of the integral

$$\int \mathrm{d}k\, e^{-ik(x-i\varepsilon)}(k^0)^{-1-C}, \tag{A2}$$

where ε is an infinitesimal future oriented timelike vector $\varepsilon\varepsilon > 0$, $\varepsilon^0 > 0$. The last integral is convergent for $\mathrm{Re}\, C < 1$ and in the limit it equals[11]

$$\frac{2\pi\Gamma(-C)}{i}\frac{1}{r}\left\{\left[\cos\left(\frac{\pi}{2}C\right) + i\,\mathrm{sign}(t-r)\sin\left(\frac{\pi}{2}C\right)\right]|t-r|^C - \left[\cos\left(\frac{\pi}{2}C\right) + i\,\mathrm{sign}(t+r)\sin\left(\frac{\pi}{2}C\right)\right]|t+r|^C\right\}, \tag{A3}$$

where $t = x^0$, $r = \sqrt{(x^1)^2 + (x^2)^2 + (x^3)^2}$, Γ is the gamma function, sign is the signum function.

APPENDIX B: PROOF OF COMPLETENESS

All functions defined on the upper light cone in the momentum space with a given degree of homogeneity can be obtained from the spherically symmetric function by application of Lorentz "boosts." Thus, in order to prove that the functions belonging to the main series form a complete set, it is sufficient to show that spherically symmetric ones form a complete set in the subspace of spherically symmetric functions.

It is easy to calculate that

$$\int \mathrm{d}k\overline{(k^0)^{-1+i\mu}}(k^0)^{-1+i\nu} = 8\pi^2\delta(\mu-\nu). \tag{B1}$$

Using this result we get the decomposition of an arbitrary spherically symmetric function $\psi(k^0)$ defined on the upper light cone in the momentum space,

$$\begin{aligned}\psi(k^0) &= \int_{-\infty}^{+\infty}\mathrm{d}\nu(k^0)^{-1+i\nu}\psi(\nu),\\ \psi(\nu) &= \frac{1}{2\pi}\int_0^{\infty}\mathrm{d}k^0(k^0)^{-i\nu}\psi(k^0),\end{aligned} \tag{B2}$$

which boils down to the pair of Mellin transforms and gives all the results known for this pair. Thus we see that spherically symmetric functions from the main series form a complete set in the subspace of spherically symmetric functions.

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Semiclassical states for NLS equations with magnetic potentials having polynomial growths

Silvia Cingolani[a)]
Dipartimento di Matematica del Politecnico di Bari, via Amendola 126/B I-70126 Bari, Italy

Simone Secchi[b)]
Dipartimento di Matematica, Università di Milano, via Saldini 50, I-20133 Milano, Italy

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We prove existence of standing wave solutions for a nonlinear Schrödinger equation on $\mathbb{R}^3$ under the influence of an external magnetic field B. In particular we deal with the physically meaningful case of a constant magnetic field $B=(0,0,b)$ having source in the potential $A(x)=(b/2)(-x_2,x_1,0)$ corresponding to the Lorentz gauge. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1874333]

I. INTRODUCTION

In quantum mechanics the introduction of an external magnetic field $B:\mathbb{R}^3\to\mathbb{R}^3$ involves replacing the gradient operator ∇ with $\nabla+iA(x)$ where A is a vector (or magnetic) potential and satisfies curl $A(x)=B(x)$. The Schrödinger operator with a magnetic field having source in A and a scalar (electric) potential W has the following expression:

$$L^{\hbar}_{A,W}=\left(\frac{\hbar}{i}\nabla-A\right)^2+W(x)=-\hbar^2\Delta-\frac{2\hbar}{i}A\cdot\nabla+|A|^2-\frac{\hbar}{i}\operatorname{div}A+W(x), \tag{1}$$

where $i^2=-1$ and $\hbar$ is the Planck constant. We notice that if we replace the magnetic potential A by $\tilde{A}(x)=A(x)+\nabla\varphi(x)$ for some real-valued C^2 function φ then $\tilde{B}(x)=\operatorname{curl}\tilde{A}(x)=\operatorname{curl}A(x)=B(x)$ and

$$e^{-i\varphi}\left[\left(\frac{1}{i}\nabla-\tilde{A}(x)\right)^2+W(x)\right]e^{i\varphi}=\left(\frac{1}{i}\nabla-A(x)\right)^2+W(x),$$

so that the spectral properties of $L^{\hbar}_{A,W}$ and $L^{\hbar}_{\tilde{A},W}$ are the same. The above properties is called the *gauge invariance* of the magnetic Schrödinger operator and it is in accordance with the fact that the physically relevant quantity is the magnetic field B and not its vector potential A (cf. Ref. 6).

Motivated by the theory of superconductivity, a lot of papers are devoted to the analysis of the spectrum of $L^{\hbar}_{A,W}$ in a semiclassical regime, namely as, $\hbar\to 0$. We quote in particular the works by Bernoff-Stenberg,[7] Del Pino–Felmer–Stenberg,[16] Lu–Pan,[7,26] devoted to the analysis, in a semiclassical regime, of the lowest eigenvalue of the magnetic Schrödinger operator. Finally we mention a recent paper by Helffer and Morame,[20] concerning the localization of the ground state in the case of a constant magnetic field.

[a)]Supported by MIUR, national project Variational and topological methods in the study of nonlinear phenomena. Electronic mail: cingolan@poliba.it
[b)]Supported by MIUR, national project Variational methods and Nonlinear differential equations. Electronic mail: secchi@mat.unimi.it

In the present work we study, in a semiclassical regime, a nonlinear Schrödinger equation with an additional cubic term, which arises in many fields of physics, in a particular condensed matter physics and nonlinear optics (see Ref. 33). More precisely, we are looking for stationary states to the evolution equation

$$i\hbar\frac{\partial\psi}{\partial t} = L^{\hbar}_{A,W}\psi - |\psi|^2\psi \quad \text{in } \mathbb{R}^+ \times \mathbb{R}^3, \tag{2}$$

as $\hbar \to 0$. The *ansatz* that the solution $\psi(x,t)$ to (2) is a standing wave of the form

$$\psi(t,x) = e^{-iE\hbar^{-1}t}u(x),$$

with $E \in \mathbb{R}$ and u: $\mathbb{R}^3 \to \mathbb{C}$, leads us to solve the semilinear elliptic equation

$$L^{\hbar}_{A,W}u = Eu + |u|^2u \quad \text{in } \mathbb{R}^3. \tag{3}$$

In the work we consider an electric potential $W(x)$ which is bounded from below on $\mathbb{R}^3$, and we choose E such that $V(x) = W(x) - E$ is strictly positive. Hence Eq. (3) becomes

$$L^{\hbar}_{A,V}u = |u|^2u \quad \text{in } \mathbb{R}^3, \tag{4}$$

where V is a strictly positive potential.

While there is an extensive literature dealing with (4) in the case $A=0$ (see Refs. 3, 4, 9, 10, 13, 15, 14, 19, 24, 27, and 29), there are few papers concerning the nonlinear Schrödinger equation with magnetic fields.

To our knowledge, the first paper, in which semilinear Schrödinger equation (4) with external magnetic field is considered, is by Esteban and Lions.[18] The authors proved the existence of standing wave solutions to (4), by a constrained minimization in the case $V(x)=1$ on $\mathbb{R}^3$ and $\hbar > 0$ is fixed. Concentration and compactness arguments are applied to solve such minimization problems for special classes of magnetic fields.

Afterward, in Ref. 21, Kurata has proved the existence of least energy solutions to (4) for any fixed $\hbar > 0$, under some assumptions linking the magnetic field B and the electric potential V (see also Ref. 32).

A first multiplicity result for standing wave solutions to (4), as $\hbar \to 0$, has been proved by Cingolani in Ref. 8, using topological arguments that allow to relate the number of standing wave solutions to (4) to the *topology* of the set of global minima of V. This result covers the case of magnetic potentials having polynomial growths, having special physical interest, but the used approach works only near global minima of V.

In a recent paper,[11] the more general case, in which the electric potential V has a manifold M of stationary points, not necessarily global minima, has been considered. For bounded electric and magnetic potentials, it has been proved a multiplicity result of semiclassical standing waves of (4), following the new perturbation approach contained in the paper[4] by Ambrosetti, Malchiodi, and Secchi (see also Refs. 2 and 3). Precisely, by means of a finite dimensional reduction, the complex-valued solutions to (4) are found near least energy solutions of the complex-valued limiting equation

$$\left(\frac{\nabla}{i} - A(\hbar\xi)\right)^2 u + u + V(\hbar\xi)u = |u|^2u \quad \text{in } \mathbb{R}^3, \tag{5}$$

where $\hbar\xi$ belongs to a neighborhood of M. We remark that in Ref. 11 the boundedness of the scalar and magnetic potentials on $\mathbb{R}^3$ is a crucial assumption to guarantee that the variational framework, in which problem (4) is set up, becomes *equivalent* to the space $H^1(\mathbb{R}^3,\mathbb{C})$, which is the variational setting of the limiting problem (5), independently of the vector potential A.

Concerning other papers on this topic, we mention a recent work[31] by Secchi and Squassina in which the authors have established necessary conditions for a sequence of standing wave solutions

to (4) to concentrate, in different senses, around a given point. Finally we quote the paper by Arioli and Szulkin[5] where existence of infinitely many solutions of (5) is proved assuming that V and B are periodic and $\hbar$ fixed.

In the present work we are concerned with the study of standing wave solutions to (4) in a semiclassical regime, in the presence of a magnetic field, having source in a vector potential A possibly unbounded on $\mathbb{R}^3$. This is a relevant case in physics, since constant magnetic fields B lead to vector potentials A, having polynomial growths on $\mathbb{R}^3$. For instance, if B is the constant magnetic field $(0,0,b)$, then a suitable vector field is given by $A(x)=(b/2)(-x_2,x_1,0)$. In physical literature the potential A corresponds to the so-called *Lorentz gauge* (see Ref. 18).

In Main Theorem, which is the main result, we prove that for each topologically nontrivial critical point x_0 of the scalar potential V, there exists a standing wave solution $\psi_\hbar$ of (2) whose modulus concentrates at x_0 for $\hbar$ small. The magnetic field only influences the phase factor of the standing wave as $\hbar$ is small.

The used approach is variational and is based on a penalization procedure, introduced by Del Pino and Felmer in Ref. 13 for studying nonlinear Schrödinger equations with $A(x)=0$ in the semiclassical limit.

We point out that in the presence of a magnetic field new difficulties arise in order to carry out a penalization procedure as in Ref. 13. First, the problem is complex valued (unless $A\equiv 0$) and the penalization acts only on the modulus of the functions. Moreover differently from Refs. 11 and 13, if A is an unbounded function on $\mathbb{R}^3$, there is no kind of relationship between the variational setting $H^\hbar_{A,V}$ associated to problem (4), and the limit space $H^1(\mathbb{R}^3,\mathbb{C})$ as $\hbar\to 0$ (see Remark 3.1). Kato's inequality for magnetic fields and delicate subsolution estimates will provide the tools to extend the results in Ref. 13 for nonlinear Schrödinger equations in presence of an external magnetic field.

We use the following notations:

(1) The complex conjugate of any number $z\in\mathbb{C}$ will be denoted by $\bar{z}$.
(2) The real part of a number $z\in\mathbb{C}$ will be denoted by $\mathrm{Re}\, z$.
(3) The ordinary inner product between two vectors $a,b\in\mathbb{R}^3$ will be denoted by $a\cdot b$.
(4) From time to time, when no confusion can arise, we omit the symbol dx in integrals over $\mathbb{R}^3$.
(5) The letter C denotes a generic positive constant, which may vary inside a chain of inequalities.
(6) We use the Landau symbols. For example, $O(\varepsilon)$ is a generic function such that $\limsup_{\varepsilon\to 0}[O(\varepsilon)/\varepsilon]<\infty$, and $o(\varepsilon)$ is a function such that $\lim_{\varepsilon\to 0}[o(\varepsilon)/\varepsilon]=0$.

II. STATEMENT OF THE MAIN RESULT

In the work we consider, more generally, with the semilinear elliptic equation

$$\left(\frac{\hbar}{i}\nabla - A(x)\right)^2 u + V(x)u = f(|u|^2)u \quad \text{in } \mathbb{R}^3, \tag{6}$$

where $\hbar$ is regarded as a small parameter and $f:[0,+\infty[\to\mathbb{R}$ satisfies the following assumptions.

(f1) f is of class C^1 increasing, $f(0)=0$ and

$$\lim_{s\to\infty}\frac{f(s)}{s^{\frac{p-1}{2}}}=0 \quad \text{and } 0<\vartheta F(s)\leqslant f(s)s$$

for some $p\in(1,5)$ and $\vartheta>2$, where $F(s)=\frac{1}{2}\int_0^s f(t)dt$, for $s\in\mathbb{R}^+$.

(f2) For each $a>0$, the limiting functional $I_a:H^1(\mathbb{R}^3,\mathbb{R})\to\mathbb{R}$, defined as

$$I_a(v) = \frac{1}{2}\int_{\mathbb{R}^3} [|\nabla v|^2 + a|v|^2] - \int_{\mathbb{R}^3} F(|v|^2), \tag{7}$$

possesses a unique critical point, whose critical value is denoted by b^a.

Throughout the paper we also make the following mild assumptions on the vector and scalar potentials.

(A1) A: $\mathbb{R}^3 \to \mathbb{R}^3$ is a C^1-vector field such that, for some positive constants C and γ,

$$|J_A(x)| \leqslant Ce^{\gamma|x|}, \tag{8}$$

where $J_A(x)$ denotes the Jacobian matrix of A at x.

(V1) $V: \mathbb{R}^3 \to \mathbb{R}$ is a positive C^1 function such that $\inf_{x\in\mathbb{R}^3} V(x) = V_0 > 0$ and for some positive constants C_1 and γ_1,

$$|\nabla V(x)| \leqslant C_1 e^{\gamma_1|x|}. \tag{9}$$

(V2) There is an open, bounded set $\Lambda \subset \mathbb{R}^3$ with smooth boundary and there exist closed subsets B, B_0 of Λ such that B is connected and $B_0 \subset B$. Let Γ be the family of all continuous functions ϕ: $B \to \Lambda$ with the property that $\phi(x) = x$ whenever $x \in B_0$. Define

$$c = \inf_{\phi\in\Gamma} \max_{x\in B} V(\phi(x)). \tag{10}$$

Moreover we assume that $\sup_{x\in B_0} V(x) < c$ and for all $\phi \in \Gamma$,

$$c \leqslant \inf_{x\in B} V(\phi(x)).$$

(V3) For all $x \in \partial\Lambda$ such that $V(x) = c$, there holds $\partial_\tau V(x) \neq 0$, where ∂_τ stands for the tangential derivative.

We notice that assumptions (V2) and (V3) express a local linking for V in Λ (see for instance Ref. 14) and guarantee the existence of a critical point for V inside Λ at level c. Particular cases of local linking of V in Λ are local maxima, local minima or saddle points for V inside Λ.

We can state the main result of this work, which is going to be proved in the last section.

Main Theorem: *Assume* (f1) and (f2), (A1), (V1)–(V3). *Then there is a number* $\hbar_0 > 0$ *such that for all* $0 < \hbar < \hbar_0$, *there exists a solution* $u_\hbar$ *to Eq.* (6) *such that*

$$\int_{\mathbb{R}^3} \left| \left(\frac{\hbar}{i}\nabla - A(x) \right) u_\hbar \right|^2 \mathrm{d}x + \int_{\mathbb{R}^3} V(x)|u_\hbar|^2 \,\mathrm{d}x < +\infty. \tag{11}$$

Furthermore $u_\hbar \in C^{2,\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$, *with* $\alpha \in (0,1)$.

We remark that assumption (f1) is clearly satisfied if the nonlinear term in (6) is homogeneous, namely $f(t) = |t|^{(p-2)/2}$. In this case, assumption (f2) is also satisfied by the uniqueness results in Ref. 22. By Main Theorem, we deduce the following corollary.

Corollary 2.1: Assume (A1), (V1)–(V3). *Then there is a number* $\hbar_0 > 0$ *such that for all* $0 < \hbar < \hbar_0$, *there exists a solution* $u_\hbar$ *to Eq.* (4) *such that* (11) *holds. Furthermore* $u_\hbar \in C^{2,\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$, *with* $\alpha \in (0,1)$.

We remark that in Main Theorem we deal with a nonlinear Schrödinger equation in $\mathbb{R}^3$ as this is the main relevant case in quantum mechanics. Actually, the result of Main Theorem also holds for nonlinear Schrödinger equations in $\mathbb{R}^N$, assuming the following.

(f2′) The nonlinearity f is of class C^1, increasing, $f(0) = 0$ and

$$\lim_{s\to\infty}\frac{f(s)}{s^{\frac{p-1}{2}}}=0 \quad \text{and } 0<\vartheta F(s)\leqslant f(s)s$$

for some $p>1$ if $N=1$, 2 and $p\in\left[1,(N+2)\big/(N-2)\right]$ if $N\geqslant 3$ and $\vartheta>2$, where $F(s)=\frac{1}{2}\int_0^s f(t)\mathrm{d}t$, for $s\in\mathbb{R}^+$.

III. MAGNETIC FIELDS: THE SPACE H_A

In this section we recall some classical results on Schrödinger operators with magnetic field, which are useful in the proof of Main Theorem.

We consider the space $H_A(\mathbb{R}^3,\mathbb{C})$ consisting of all the function $u\in L^2(\mathbb{R}^3,\mathbb{C})$ with $(\partial_j+iA_j)u\in L^2(\mathbb{R}^3,\mathbb{C})$ for any $j=1,2,3$ endowed with the norm

$$\|u\|_{H_A}^2=\int_{\mathbb{R}^3}|(\nabla+iA)u|^2\,\mathrm{d}x+\int_{\mathbb{R}^3}|u|^2\,\mathrm{d}x.$$

Remark 3.1: We do not assume that ∇u or Au are separately in $L^2(\mathbb{R}^3,\mathbb{C})$. Therefore, in general, there is no relationship between the spaces $H_A(\mathbb{R}^3,\mathbb{C})$ and $H^1(\mathbb{R}^3,\mathbb{C})$, namely $H_A(\mathbb{R}^3,\mathbb{C})\not\subset H^1(\mathbb{R}^3,\mathbb{C})$ or $H^1(\mathbb{R}^3,\mathbb{C})\not\subset H_A^{\hbar}(\mathbb{R}^3,\mathbb{C})$ (see Ref. 18).

Theorem 3.2: *Let A: $\mathbb{R}^3\to\mathbb{R}^3$ be in $L^2_{\mathrm{loc}}(\mathbb{R}^3)$ and let $u\in H_A^1(\mathbb{R}^3,\mathbb{C})$. Then $|u|\in H^1(\mathbb{R}^3,\mathbb{R})$ and the diamagnetic inequality*

$$|\nabla|u|(x)|\leqslant|(\nabla+iA)u(x)| \tag{12}$$

holds for almost every $x\in\mathbb{R}^3$.

By the diamagnetic inequality, the following result follows (see Ref. 18).

Theorem 3.3: *The space $C_0^\infty(\mathbb{R}^3,\mathbb{C})$ is dense in $H_A^1(\mathbb{R}^3,\mathbb{C})$.*

Furthermore we recall the following Kato's inequality (see Ref. 30).

Theorem 3.4: *Let $u\in L^1_{\mathrm{loc}}(\mathbb{R}^3,\mathbb{C})$ with $\nabla u\in L^1_{\mathrm{loc}}(\mathbb{R}^3,\mathbb{C})$. Define*

$$(\operatorname{sign} u)(x)=\begin{cases}\dfrac{\overline{u(x)}}{|u(x)|} & \text{if } u(x)\neq 0,\\ 0 & \text{if } u(x)=0,\end{cases} \tag{13}$$

we have that $\operatorname{sign} u\in L^\infty(\mathbb{R}^3)$ *and* $(\operatorname{sign} u)\nabla u(x)$ *is locally L^1 and hence a distribution. Moreover we have*

$$\Delta|u|\geqslant\operatorname{Re}[(\operatorname{sign} u)\Delta u].$$

We furthermore recall the application of Kato's inequality to the Schrödinger operator with magnetic field (see Ref. 30).

Theorem 3.5: *Let A: $\mathbb{R}^3\to\mathbb{R}^3$ be a C^1 real vector valued function. Let $D_k u=(1/i)(\partial u/\partial x_k)-A_k u$, for any $k=1,2,3$ and $D_A^2=\Sigma_{k=1}^3 D_k^2$. Then for any $u\in L^1_{\mathrm{loc}}(\mathbb{R}^3,\mathbb{C})$ and $D^2u\in L^2_{\mathrm{loc}}(\mathbb{R}^3,\mathbb{C})$ we have*

$$\Delta|u|\geqslant-\operatorname{Re}[(\operatorname{sign} u)D_A^2u].$$

Throughout the paper, we set $\hbar=\varepsilon$ and denote by D_ε and D^ε for each $\varepsilon>0$ the (formal) differential operators

$$D_\varepsilon=\frac{\varepsilon}{i}\nabla-A(x), \tag{14}$$

$$D^{\varepsilon} = \frac{\nabla}{i} - A(\varepsilon x). \tag{15}$$

As in Sec. II, we introduce the real Hilbert space $H^{\varepsilon}_{A,V}$ as the completion of $C_0^{\infty}(\mathbb{R}^3, \mathbb{C})$ with respect to the inner product

$$\langle u, v\rangle_{H^{\varepsilon}_{A,V}} = \mathrm{Re}\int_{\mathbb{R}^3} D_{\varepsilon}u \cdot \overline{D_{\varepsilon}v}\, \mathrm{d}x + \mathrm{Re}\int_{\mathbb{R}^3} V(x)u\overline{v}\, \mathrm{d}x. \tag{16}$$

As remarked above, this space has in general no relationship with $H^1(\mathbb{R}^3, \mathbb{C})$. Anyway, by Theorem 3.2, we have the following *diamagnetic inequality*:

$$\int_{\mathbb{R}^3} \varepsilon^2 |\nabla |u||^2\, \mathrm{d}x \leqslant \int_{\mathbb{R}^3} |D_{\varepsilon}u|^2\, \mathrm{d}x, \quad \text{for every } u \in H^{\varepsilon}_{A,V}. \tag{17}$$

It is easy to check that, under our assumptions, the functional

$$\mathcal{F}_{\varepsilon}(u) = \frac{1}{2}\int_{\mathbb{R}^3} |D_{\varepsilon}u|^2\, \mathrm{d}x + \int_{\mathbb{R}^3} V(x)|u|^2\, \mathrm{d}x - \int_{\mathbb{R}^3} F(|u|^2)\mathrm{d}x \tag{18}$$

is of class C^2, so that solutions to (6) correspond to critical points of $\mathcal{F}_{\varepsilon}$.

IV. A PENALIZATION ACTING ON THE MODULUS

In this section we perform a penalization of the Euler functional $\mathcal{F}_{\varepsilon}$, inspired by Refs. 13 and 14. To this order, we begin to assume, without loss of generality, that the infimum of V in $\overline{\Lambda}$ is very close to c. Let $\delta > 0$ be a small but fixed number, we can assume that $\Lambda = \{x \,|\, V(x) > c - \delta\}$ and

$$B \subset \{x \in \Lambda \,|\, V(x) \geqslant c(\varepsilon)\}, \quad B_0 \subset \{x \in \Lambda \,|\, V(x) = c(\varepsilon)\},$$

where $c - \delta < c(\varepsilon) < c$, $\lim_{\varepsilon \to 0} c(\varepsilon) = c - \delta$ and $\mathrm{dist}(B_0, \partial\Lambda) = \sqrt{\varepsilon}$. In fact as in Ref. 14, we can redefine $\Lambda_{\delta} = \Lambda \cap \{x \,|\, V(x) > c - \delta\}$ and

$$B^{\delta,\varepsilon} = B \cap \{x | V(x) \geqslant c(\varepsilon)\}, \tag{19}$$

$$B_0^{\delta,\varepsilon} = B_0 \cap \{x | V(x) = c(\varepsilon)\}, \tag{20}$$

where

$$c(\varepsilon) = \inf\{\xi | \mathrm{dist}(\{x \in \Lambda | V(x) = \xi\}, \Lambda_{\delta}) \geqslant \sqrt{\varepsilon}\}$$

without affecting condition (V3) in the definition of linking. We notice that the set $B_0^{\delta,\varepsilon}$ is not empty as B is connected. Then if ϕ: $B^{\delta,\varepsilon} \to \Lambda_{\delta}$ is a continuous map with $\phi(x) = x$ for every $x \in B_0^{\delta,\varepsilon}$, we can define its extension $\tilde{\phi}$ as the identity on $B \setminus B^{\delta,\varepsilon}$. Thus $\tilde{\phi}$: $B \to \Lambda$ and $\sup_{x \in B} V(\tilde{\phi}) = \sup_{x \in B^{\delta,\varepsilon}} V(\tilde{\phi}) \geqslant c$.

We consider a modification of the nonlinear term in (6), that will prevent concentration outside Λ. We remark that differently from Ref. 13, as our problem is complex valued, the penalization affects only the modulus of the functions.

Let ϑ be the number defined in (f1) and choose $k > 0$ such that $k > \vartheta/(\vartheta - 2)$. Since f is increasing, we can fix a number $a > 0$ with $f(a) = V_0/k$. Set

$$\tilde{f}(s) = \begin{cases} f(s) & \text{if } s \leqslant a, \\ V_0/k & \text{if } s > a, \end{cases} \tag{21}$$

we define g: $\mathbb{R}^3 \times \mathbb{R}^+ \to \mathbb{R}$ by

$$g(x,s) = \chi_\Lambda(x) f(s) + (1 - \chi_\Lambda(x))\tilde{f}(s), \tag{22}$$

where χ_Λ is the characteristic function of the set Λ and we consider the modified equation

$$\left(\frac{\varepsilon}{i}\nabla - A(x)\right)^2 u + V(x)u = g(x,|u|^2)u \quad \text{in } \mathbb{R}^3. \tag{23}$$

Weak solutions of Eq. (23) correspond to critical points of the C^1 functional J_ε: $H^\varepsilon_{A,V} \to \mathbb{R}$,

$$J_\varepsilon(u) = \frac{1}{2}\int_{\mathbb{R}^3} |D_\varepsilon u|^2 + V(x)|u|^2 - \int_{\mathbb{R}^3} G(x,|u|^2)\mathrm{d}x, \tag{24}$$

where $G(x,s) = \frac{1}{2}\int_0^s g(x,t)\mathrm{d}t$.

For the sake of convenience, we highlight some obvious properties of g, which follow directly from (f1) and (f2).

(g1) $\lim_{s\to 0^+} g(x,s) = 0$, uniformly with respect to $x \in \mathbb{R}^3$.

(g2) There exist a bounded subset K of $\mathbb{R}^3$ and a number $\vartheta > 2$ such that

$$0 < \vartheta G(x,s) \leqslant g(x,s)$$

for all $x \in K$.

(g3) For all $s \geqslant 0$, $x \notin K$,

$$0 \leqslant 2G(x,s) \leqslant g(x,s) \leqslant \frac{1}{k}V(x)$$

with a constant $k > \vartheta/(\vartheta - 2)$.

We begin to show that the penalized functional J_ε satisfies the Palais–Smale condition. This may not be true for the functional $\mathcal{F}_\varepsilon$.

Lemma 4.1: For any $\varepsilon > 0$ fixed, the penalized functional J_ε satisfies the Palais–Smale condition at all positive levels.

Proof: Let $\varepsilon > 0$ be fixed. Let $\{u_n\}$ be a sequence in $H^\varepsilon_{A,V}$ such that $\{J_\varepsilon(u_n)\}$ is bounded and $J'_\varepsilon(u_n) \to 0$. First we prove that $\{u_n\}$ is bounded. By (g3), it follows that

$$\frac{1}{2}\int_K g(x,|u_n|^2)|u_n|^2 + o(\|u_n\|) \leqslant \frac{1}{2}\int_{\mathbb{R}^3} |D_\varepsilon u_n|^2 + V|u_n|^2 \leqslant \int_K G(x,|u_n|^2) + \frac{1}{2k}\int_{\mathbb{R}^3\setminus K} V|u_n|^2 + O(1),$$

where $\|\cdot\|$ denotes the norm in $H^\varepsilon_{A,V}$ induced by the scalar product in (16). Thus the above inequality and (g2) imply

$$\left(\frac{\vartheta}{2} - 1\right)\int_{\mathbb{R}^3} |D_\varepsilon u_n|^2 + V|u_n|^2 \leqslant \frac{\vartheta}{2k}\int_{\mathbb{R}^3\setminus K} V|u_n|^2 + o(\|u_n\|) + O(1).$$

In particular, it follows that $\{u_n\}$ is bounded in $H^\varepsilon_{A,V}$. We choose a subsequence, still denoted by $\{u_n\}$ for simplicity, that converges weakly to some u in $H^\varepsilon_{A,V}$. we claim that $u_n \to u$ strongly in $H^\varepsilon_{A,V}$. To this aim, it suffices to show that for any given $\delta > 0$ there exists $R > 0$ such that

$$\limsup_{n\to\infty} \int_{|x|>R} (|D_\varepsilon u_n|^2 + V(x)|u_n|^2)\mathrm{d}x < \delta.$$

Without loss of generality, we can take R so large that $K \subset B_{R/2}$. Fix a smooth cutoff function η_R such that $\eta_R = 0$ on $B_{R/2}$, $\eta_R = 1$ outside $B_{R/2}$, $0 \leqslant \eta_R \leqslant 1$ and $|\nabla \eta_R| \leqslant c/R$ for some constant $c > 0$. Since $\{u_n\}$ is a bounded Palais–Smale sequence, we have

$$J'(u_n)[\eta_R u_n] = o(1),$$

so that

$$\int_{\mathbb{R}^3} (|D_\varepsilon u_n|^2 + V|u_n|^2)\,\eta_R + \mathrm{Re}\int_{\mathbb{R}^3} u_n D_\varepsilon u_n \cdot \overline{D_\varepsilon \eta_R} = \mathrm{Re}\int_{\mathbb{R}^3} g(x,|u_n|^2)\,\eta_R |u_n|^2 + o(1)$$

$$\leqslant \frac{1}{k}\int_{\mathbb{R}^3} V|u_n|^2\,\eta_R + o(1).$$

We conclude that

$$\int_{|x|>R} |D_\varepsilon u_n|^2 + V(x)|u_n|^2 \leqslant \frac{C}{R}\|u_n\|_{L^2}\|D_\varepsilon u_n\|_{L^2} + o(1),$$

which clearly proves the claim. □

V. THE MINIMAX SCHEME

By assumption (f2) the limiting functional I_a defined in (7) has a unique critical value, which we can characterize as

$$b^a = \inf_{v\in H^1(\mathbb{R}^3)\setminus\{0\}} \sup_{t>0} I_a(tv). \tag{25}$$

It can be shown that the map $a \mapsto b^a$, with $a>0$, is strictly increasing and continuous. Associated to the critical value b^a there exists a radially symmetric solution $\omega_a \in H^1(\mathbb{R}^3,\mathbb{R})$ of the scalar equation

$$\Delta\omega - a\omega + f(|\omega|^2)\omega = 0. \tag{26}$$

Fix a small number $\delta_0>0$. For each $y\in\mathbb{R}^3$ with $\mathrm{dist}(y,\partial\Lambda)>\delta_0$ we denote by w_ε^y the function in $H^\varepsilon_{A,V}$ given by

$$w_\varepsilon^y(x) = e^{iA(y)[(y-x)/\varepsilon]}\eta(|x-y|/\delta_0)\,\omega_{V(y)}\left(\frac{y-x}{\varepsilon}\right), \tag{27}$$

where η is a smooth cutoff function that equals 1 on (0, 1) and 0 on $(2,+\infty)$.

Define now the class Γ_ε of all continuous maps ϕ: $B^\varepsilon \to \mathcal{M}_\varepsilon$ such that

$$\phi(y) = t(\varepsilon,y)w_\varepsilon^y \quad \text{for all } y\in B_0^\varepsilon, \tag{28}$$

where

$$\mathcal{M}_\varepsilon = \left\{ u\in H^\varepsilon_{A,V}\setminus\{0\} \middle| \int_{\mathbb{R}^3} |D_\varepsilon u|^2 + V(x)|u|^2 = \int_{\mathbb{R}^3} g(x,|u|^2)|u|^2 \right\}$$

is the Nehari manifold associated to the polarized functional J_ε and $t(\varepsilon,y)$ is the unique positive number such that $t(\varepsilon,y)w_\varepsilon^y \in \mathcal{M}_\varepsilon$. We define a minimax value as follows:

$$\gamma_\varepsilon = \inf_{\phi\in\Gamma_\varepsilon} \sup_{y\in B^\varepsilon} J_\varepsilon(\phi(y)). \tag{29}$$

By slightly deforming w_ε^y and recalling the definitions of B^ε and B_0^ε, one can show that

$$b^c \geqslant \limsup_{\varepsilon\to 0} \varepsilon^{-3}\gamma_\varepsilon \geqslant \liminf_{\varepsilon\to 0} \varepsilon^{-3}\gamma_\varepsilon \geqslant b^{c-\delta}. \tag{30}$$

We show that the last inequality in (30) is strict. We begin to prove the following useful lemma, which generalizes Lemma 2.3 in Ref. 14 (see also Ref. 17) to the case of a complex valued equation.

Lemma 5.1: Let $v \in H^1(\mathbb{R}^3,\mathbb{C}) \cap C(\mathbb{R}^3)$ *be a weak solution of the equation*

$$\Delta v - V(\xi)v + \chi_{\{x_1<0\}} f(|v|^2)v + \chi_{\{x_1>0\}} \tilde{f}(|v|^2)v = 0, \tag{31}$$

where $\xi \in \mathbb{R}^3$. *Then* $|v| \leqslant \sqrt{a}$ *for any* $x_1 > 0$ *and* v *actually solves the equation*

$$\Delta v - V(\xi)v + f(|v|^2)v = 0.$$

Proof: We test Eq. (31) by $\overline{\partial v}/\partial x_1$ and we derive [x' stands for $=(x^2,x^3)$]

$$\int_{\mathbb{R}^2} dx' \int_{-\infty}^{\infty} \frac{\partial}{\partial x_1}[|\nabla v|^2 + V(\xi)|v|^2]dx_1 + \int_{\mathbb{R}^2} \left[F(|v(0,x')|^2) - \tilde{F}(|v(0,x')|^2)\right]dx' = 0. \tag{32}$$

We notice that $F(s) \geqslant \tilde{F}(s)$ with inequality if $s \leqslant a$. Thus $|v(0,x')| \leqslant \sqrt{a}$. Finally we show that $|v(x_1,x')|^2 \leqslant \sqrt{a}$ for any $x_1 > 0$.

By Kato's inequality we derive that

$$\Delta|v| \geqslant V(\xi)|v| - \chi_{\{x_1<0\}} f(|v|^2)|v| - \chi_{\{x_1>0\}} \tilde{f}(|v|^2)|v|. \tag{33}$$

Now we can test (33) by $\phi = \chi_{\{x_1>0\}}(|v| - \sqrt{a})_+ \in H^1(\mathbb{R}^3,\mathbb{R})$ and we derive

$$\int_{\mathbb{R}^3} \chi_{\{x_1>0\}} |\nabla(|v| - \sqrt{a})_+|^2 + q(x)\chi_{\{x_1>0\}}(|v| - \sqrt{a})_+^2 + \sqrt{aq}(x)\chi_{\{x_1>0\}}(|v| - \sqrt{a})_+ \leqslant 0, \tag{34}$$

where

$$q(x) = V(\xi) - \tilde{f}(|v|^2)\chi_{\{x_1>0\}}.$$

For $s \geqslant a$, $\tilde{f}(s) = (V_0/k) < V(\xi)$, so that $q(x) > 0$ and all the terms in (34) are necessarily zero, and $\phi = \chi_{\{x_1>0\}}(|v| - \sqrt{a})_+ = 0$. We conclude that

$$|v(x_1,x')| \leqslant \sqrt{a} \quad \forall\, x_1 > 0,\ \ x' \in \mathbb{R}^2.$$

□

Lemma 5.2: There results

$$\liminf_{\varepsilon \to 0} \varepsilon^{-3} \gamma_\varepsilon > b^{c-\delta}. \tag{35}$$

Proof: We argue by contradiction, following arguments strictly related to Ref. 14, Lemma 1.1. If (35) is not true, then there exists a sequence $\varepsilon_n \to 0$ such that

$$\varepsilon_n^{-3} \gamma_{\varepsilon_n} \leqslant b^{c-\delta} + o(1).$$

Fix some $\phi_n \in \Gamma_{\varepsilon_n}$ with the property that

$$\varepsilon_n^{-3} \sup_{y \in B^{\varepsilon_n}} J_{\varepsilon_n}(\phi_n(y)) \leqslant b^{c-\delta} + o(1). \tag{36}$$

For the reader's convenience, we split the proof in several steps.

Step I: Setting $\Lambda_n = \{x \in \mathbb{R}^3 | \operatorname{dist}(x,\Lambda) < \sqrt{\varepsilon_n}\}$, we claim that

$$\lim_{n\to\infty} \varepsilon_n^{-3} \sup_{y\in B^{\varepsilon_n}} \int_{\mathbb{R}^3\setminus\Lambda_n} |\phi_n(x)|^2 = 0. \tag{37}$$

To prove this claim, we fix $y_n \in B^{\varepsilon_n}$ and simplify notation by introducing $u_n = \phi_n(y_n)$.

Since $u_n \in \mathcal{M}_{\varepsilon_n}$, we have

$$J_{\varepsilon_n}(u_n) \geqslant J_{\varepsilon_n}(tu_n)$$

for any $t>0$. Let us set

$$E_n(v) = \frac{1}{2}\int_{\Lambda_n} |D_{\varepsilon_n} v|^2 + V(x)|v|^2 - \int_{\Lambda_n} G(x,|v|^2)\mathrm{d}x,$$

and choose numbers $t_n>0$ with the property that

$$E_n(t_n u_n) = \max_{t>0} E_n(tu_n).$$

Now, from the properties of the penalization g, it follows that

$$\frac{V(x)}{2} - G(x,s) \geqslant \gamma \quad \text{for all } x \in \mathbb{R}^3 \setminus \Lambda \text{ and } s>0.$$

This and Eq. (36) imply that

$$E_n(t_n u_n) + \gamma t_n^2 \int_{R^3\setminus\Lambda_n} |u_n|^2 \leqslant \varepsilon_n^3 (b^{c-\delta} + o(1))$$

with an error $o(1)$ uniform with respect to $\{y_n\}$. Furthermore, we claim that there exists $\sigma>0$ such that

$$\inf_{n\geqslant 1} t_n \geqslant \sigma. \tag{38}$$

First we notice that from the relation $J_{\varepsilon_n}(u_n) \leqslant C\varepsilon_n^3$, the diamagnetic inequality and again the properties of g, the existence of a constant C_0, independent of $\{y_n\}$, such that

$$\int_{\mathbb{R}^3} |D_{\varepsilon_n} u_n|^2 + |u_n|^2 \leqslant C_0 \varepsilon_n^3 \tag{39}$$

follows easily. Set now $v_n(x) = t_n u_n(\varepsilon_n x)$ and $\tilde{\Lambda}_n = \varepsilon_n^{-1}\Lambda_n$. The definition of t_n implies

$$\int_{\tilde{\Lambda}_n} |D^{\varepsilon_n} v_n|^2 + V(\varepsilon_n x)|v_n|^2 = \int_{\tilde{\Lambda}_n} g(\varepsilon_n x, |v_n|^2)|v_n|^2 \,\mathrm{d}x \leqslant \int_{\tilde{\Lambda}_n} C_0|v_n|^{p+1} + \rho|v_n|^2, \tag{40}$$

where $\rho>0$ can be fixed as small as we please. We can deduce from the Sobolev embedding theorem as stated in Ref. 1, Lemma 5.10 that there exists a constant $\overline{C}>0$, independent of n, such that

$$\int_{\tilde{\Lambda}_n} |v_n|^{p+1} \leqslant \overline{C}\left(\int_{\tilde{\Lambda}_n} |\nabla |v_n||^2 + |v_n|^2\right)^{(p+1)/2} \leqslant \overline{C}\left(\int_{\tilde{\Lambda}_n} |D^{\varepsilon_n} v_n|^2 + |v_n|^2\right)^{(p+1)/2}. \tag{41}$$

By combining (41) with Eq. (40), we see that

$$\int_{\tilde{\Lambda}_n} |v_n|^{p+1} \geqslant \sigma > 0,$$

and in particular $\int_{\tilde{\Lambda}_n} |D^{\varepsilon_n} v_n|^2 + |v_n|^2 \geqslant \sigma > 0$ for a suitable $\sigma > 0$ independent of n, and so

$$t_n^2 \int_{\Lambda_n} (|D_{\varepsilon_n} u_n|^2 + |u_n|^2) \geqslant \sigma \varepsilon_n^3.$$

This proves (38).

Observe now that, from the definition of t_n and from the diamagnetic inequality, we get

$$E_n(t_n u_n) \geqslant \inf_{u \in H^1(\Lambda_n)} \sup_{t>0} E_n(tu) \equiv b_n.$$

If we prove that

$$\lim_{n \to \infty} \varepsilon_n^{-3} b_n = b^{c-\delta}, \tag{42}$$

then Eq. (37) follows from our previous arguments.

Step II: We prove that identity (42) holds.

We follow Ref. 15, with minor changes. By a deformation argument, it is easy to see that

$$b_n \leqslant (b^{c-\delta} + o(1))\varepsilon_n^3. \tag{43}$$

We prove the opposite inequality. Since the functional E_n satisfies (PS), by standard Critical Point Theory, the number b_n is a critical value for E_n. Let $w_n \in H^1(\Lambda_n)$ be an associated critical point. As such, it satisfies the equation

$$\begin{cases} \left(\dfrac{\varepsilon_n}{i} \nabla - A \right)^2 w_n + V w_n = g(x, |w_n|^2) w_n \quad \text{in } \Lambda_n, \\ \dfrac{\partial w_n}{\partial \nu} = 0 \quad \text{on } \partial \Lambda_n. \end{cases}$$

In particular, by Kato's inequality, $|w_n|$ solves the differential inequality

$$\begin{cases} \varepsilon_n^2 \Delta |w_n| - V(x)|w_n| + g(x, |w_n|^2)|w_n|^2 \geqslant 0 \quad \text{in } \Lambda_n, \\ \dfrac{\partial w_n}{\partial \nu} = 0 \quad \text{on } \partial \Lambda_n. \end{cases} \tag{44}$$

By the maximum principle, $|w_n|$ cannot attain a local maximum inside $\overline{\Lambda_n} \setminus \Lambda$, thanks to the Neumann boundary condition in (44). If x_n is a maximum of $|w_n|$, then necessarily $x_n \in \overline{\Lambda}$. Moreover, $\inf_n \max_{\Lambda_n} |w_n| > 0$. Assume, without loss of generality, that $x_n \to x^* \in \overline{\Lambda}$. Scaling w_n to a map on $\Omega_n \equiv \varepsilon_n^{-1}(\Lambda_n - x_n)$ defined by $v_n(x) = w_n(x_n + \varepsilon_n x)$, we have that v_n satisfies the equation

$$\begin{aligned} &-\Delta v_n - \frac{2}{i} A(x_n + \varepsilon_n x) \cdot \nabla v_n + |A(x_n + \varepsilon_n x)|^2 v_n - \frac{\varepsilon_n}{i} \operatorname{div} A(x_n + \varepsilon_n x) v_n \\ &\quad + V(x_n + \varepsilon_n x) v_n = g(x_n + \varepsilon_n x, |v_n|^2) v_n \quad \text{in } \Omega_n \end{aligned} \tag{45}$$

with Neumann boundary condition, and, again by Kato's inequality,

$$\Delta |v_n| \geqslant V(x_n + \varepsilon_n x)|v_n| - g(x_n + \varepsilon_n x, |v_n|^2)|v_n| \quad \text{in } \Omega_n.$$

From (43) we deduce that

$$\sup_{n\geqslant 1}\int_{\Omega_n}[|D^{\varepsilon_n}v_n|^2\,\mathrm{d}x+V_n|v_n|^2]\mathrm{d}x<+\infty,$$

where $A_n(x)=A(x_n+\varepsilon_n x)$ and $V_n(x)=V(x_n+\varepsilon_n x)$. Take an arbitrary open set Ω, relatively compact in $\mathbb{R}^3$. Since we may assume that $\Omega\subset\Omega_n$ for all n sufficiently large, Eq. (43) and the diamagnetic inequality (12), entail that the sequence $\{|v_n|\}$ is bounded in $H^1(\Omega,\mathbb{R})$ and, up to subsequences, converges weakly in $H^1(\Omega,\mathbb{R})$ and strongly in $L^q(\Omega,\mathbb{R})$ with $q<5$ to some $v^*\in H^1(\Omega,\mathbb{R})$. Moreover $\{v_n\}$ is a bounded sequence in $H^1(\Omega,\mathbb{C})$. Since Ω is arbitrary, the limit v^* can be extended to a function defined on $\mathbb{R}^3$. Thus by applying the subsolution estimates (see Theorems 13.1, 14.1 in Ref. 23) we infer that the sequence $\{v_n\}$ is bounded in $L^\infty(\Omega)$. By Schauder estimates, the sequence $\{v_n\}$ is bounded in $C^{2,\alpha}(K)$ for some $\alpha\in(0,1)$ and thus, up to subsequences, v_n converges to v in $C^2_{\mathrm{loc}}(\mathbb{R}^3)$ and also weakly in $L^q(\mathbb{R}^3,\mathbb{R})$ with $q<5$. It follows that $|v|=v^*\in H^1(\mathbb{R}^3,\mathbb{R})$ and $v\neq 0$ as $\inf_n|v_n(0)|\geqslant b>0$. Therefore,

$$-\Delta v-\frac{2}{i}A(x^*)\cdot\nabla v+|A(x^*)|^2v+V(x^*)v=\bar{g}(x,|v|^2)v\quad\text{in }\mathbb{R}^3,\tag{46}$$

in the sense of distributions, where $\bar{g}(x,s)=\chi(x)f(s)+(1-\chi(x))\tilde{f}(s)$ and χ is the weak * limit of the sequence $\{\chi_\Lambda(x_n+\varepsilon_n)\}_{n\geqslant 1}$ in $L^\infty(\mathbb{R}^3)$. Since $|v|\in H^1(\mathbb{R}^3,\mathbb{R})$ and by definition of $\bar{g}$, we deduce that $\int_{\mathbb{R}^3}\bar{g}(x,|v|^2)|v|^2\,\mathrm{d}x$ is finite and by (46) we have $v\in H^1(\mathbb{R}^3,\mathbb{C})$ and thus v solves (46) in weak sense. By performing a rotation, Lemma 5.1 can be applied to prove that the function $v(x)=e^{-\mathrm{i}A(x^*)\cdot x}\tilde{v}(x)$ satisfies

$$\Delta v-V(x^*)v+f(|v|^2)v=0.$$

We must have

$$\liminf_{n\to\infty}\varepsilon_n^{-3}E_n(w_n)=\liminf_{n\to\infty}E_n(v_n)\geqslant I_{V(x^*)}(v).$$

Indeed, as v_n converges to v in $C^2_{\mathrm{loc}}(\mathbb{R}^3)$, we derive that

$$\lim_{n\to+\infty}\int_{B_R}\sigma_n=\frac{1}{2}\int_{B_R}\left|\left(\frac{\nabla}{i}-A(x^*)\right)v\right|^2+\frac{V(x^*)}{2}\int_{B_R}|v|^2-\int_{B_R}\bar{G}(x,|v|^2),\tag{47}$$

where

$$\sigma_n(x)=\frac{1}{2}\left[\left|\left(\frac{\nabla}{i}-A_n(x)\right)v_n\right|^2+V_n(x)|v_n|^2\right]-\bar{G}(x,|v_n|^2).$$

Since $v\in H^1(\mathbb{R}^N,\mathbb{C})$, we have that for each $\delta>0$ there exists $R>0$ so large that

$$\lim_{n\to+\infty}\int_{B_R}\sigma_n\geqslant I_{V(x^*)}(v)-\delta.$$

To complete the proof, we need to show that

$$\liminf_{n\to\infty}\int_{\varepsilon_n^{-1}(\Lambda_n-x_n)\setminus B_R}\sigma_n(x)\mathrm{d}x\geqslant-\delta\tag{48}$$

for R sufficiently large. Choose a smooth cutoff function η such that $\eta=0$ on B_{R-1}, $\eta=1$ on $\mathbb{R}^3\setminus B_R$, and $|\nabla\eta|\leqslant C$ where C is a positive constant, independent of R and n. Now test the identity $J_n'(v_n)=0$ against the function $\eta\bar{v}_n\in H^1_{A_n,V_n}$ to obtain

$$0 = J_n'(v_n)[\eta\overline{v_n}] = H_n + \int_{\varepsilon_n^{-1}(\Lambda_n - x_n)\setminus B_R} (2\sigma_n + g_n)$$

with $g_n(x) = 2G(x_n + \varepsilon_n x, |v_n|^2) - g(x_n + \varepsilon_n x, |v_n|^2)|v_n|^2$ and

$$H_n = \mathrm{Re}\int_{B_R\setminus B_{R-1}} \nabla v_n \cdot \overline{\nabla(\eta v_n)} + \int_{B_R\setminus B_{R-1}} |A(x_n + \varepsilon_n x)|^2 \eta |v_n|^2 - \mathrm{Re}\frac{2}{i}\int_{B_R\setminus B_{R-1}} A(x_n + \varepsilon_n x)\cdot \nabla v_n \eta\overline{v_n}$$
$$+ \int_{B_R\setminus B_{R-1}} V(x_n + \varepsilon_n x)\,\eta |v_n|^2 - \int_{B_R\setminus B_{R-1}} g(x_n + \varepsilon_n x, |v_n|^2)\,\eta |v_n|^2.$$

From the local C^1 convergence of $\{v_n\}$ to v and the fact that $v \in H^1(\mathbb{R}^N, \mathbb{C})$, we deduce that there exists $R > 0$ so large that $\lim_{n\to\infty} |H_n| \leqslant \delta$. Recalling that $g_n \leqslant 0$ because of the properties of g, one easily gets (48). But $V(x^*) \geqslant c - \delta$ so that $I_{V(x^*)}(v) \geqslant b^{c-\delta}$. We conclude that $b_n \geqslant (b^{c-\delta} + o(1))\varepsilon^3$. Equation (37) follows easily from (42) and (38).

Step III: We now introduce the well-known tool of the *center of mass* for an L^2 function, and apply it to our ϕ_n.

Let $u \in L^2(\mathbb{R}^3)$ be a given map. We define its center of mass $\beta(u) \in \mathbb{R}^3$ as

$$\beta(u) = \frac{\int_{\Lambda^+} x|u(x)|^2\,\mathrm{d}x}{\int_{R^2} |u(x)|^2\,\mathrm{d}x},$$

where Λ^+ is a fixed small neighborhood of $\overline{\Lambda}$. We may of course assume that $\delta_0 < \mathrm{dist}(\partial\Lambda^+, \overline{\Lambda})$ where δ_0 is fixed in (27). We claim that

$$\beta(\phi_n(y)) \in \Lambda^+ \cap \left\{ x \in \mathbb{R}^3 \,\middle|\, V(x) \leqslant c - \frac{\delta}{2} \right\} \quad \text{for all } y \in B^{\varepsilon_n}. \tag{49}$$

Again, the proof of this fact is by contradiction. If (49) is false, then, passing to some subsequence, the existence of $y_n \in B^{\varepsilon_n}$ is assured, such that

$$\beta(\phi_n(y_n)) \notin \Lambda^+ \cap \left\{ x \in \mathbb{R}^3 \,\middle|\, V(x) \leqslant c - \frac{\delta}{2} \right\} \tag{50}$$

for all $n \in N$. If we set $u_n = \phi_n(y_n)$ and $v_n(x) = u_n(\varepsilon_n x)$, we have

$$\sup_{t>0} I_{c-\delta}(t|v_n|) \leqslant b^{c-\delta} + o(1). \tag{51}$$

This inequality is proved as follows: it is already known from (36) and (17) that $\{|v_n|\}$ is bounded in $H^1(\mathbb{R}^3, \mathbb{R})$. Moreover, it follows from

$$\int_{\mathbb{R}^3} (|D^{\varepsilon_n} v_n|^2 + V(\varepsilon_n x)|v_n|^2)\mathrm{d}x = \int_{\mathbb{R}^3} g(\varepsilon_n x, |v_n|^2)|v_n|^2 \leqslant \int_{\mathbb{R}^3} f(|v_n|^2)|v_n|^2$$

that

$$\inf_n \int_{\mathbb{R}^3} |v_n|^{p+1} = \sigma > 0.$$

By virtue of Lions' vanishing lemma (Ref. 25, Lemma I.1) we may find a sequence $\{B_n\}$ of balls of fixed radius (say 1) with

$$\inf_n \int_{B_n} |v_n|^2 \geqslant \sigma > 0.$$

For each n, select a number $t_n > 0$ such that $I_{c-\delta}(t_n|v_n|) = \sup_{t>0} I_{c-\delta}(t|v_n|)$. From the boundedness of $\{|v_n|\}$ in $H^1(\mathbb{R}^3, \mathbb{R})$, we get

$$Ct_n^2 - \int_{R^3} F(|t_n v_n|^2) \geqslant I_{c-\delta}(t_n|v_n|) \geqslant b^{c-\delta}.$$

Recalling assumption (H2), we have

$$t_n^{\vartheta-2} \int_{R^3} |v_n|^{\vartheta} \leqslant C$$

with $2 < \vartheta < 5$. Thus $\{t_n\}$ is bounded, and from (37) we have

$$\lim_{n\to\infty} \int_{\mathbb{R}^3 \setminus (\varepsilon_n^{-1}\Lambda^+)} |t_n v_n|^2 = 0. \tag{52}$$

Finally, from (36) we have

$$b^{c-\delta} + o(1) \geqslant \varepsilon_n^{-3} J_{\varepsilon_n}(t_n u_n) \geqslant I_{c-\delta}(t_n|v_n|) - \frac{t_n^2}{2} \int_{\mathbb{R}^3 \setminus (\varepsilon_n^{-1}\Lambda^+)} (c - \delta + o(1))|v_n|^2,$$

and (51) follows from (52).

Set now $w_n = t_n|v_n|$, with the same t_n as before. The function w_n belongs to the Nehari manifold of $I_{c-\delta}$ and (51) implies that w_n is a minimizing sequence of $I_{c-\delta}$ constrained on the Nehari manifold. A standard application of Ekeland's variational principle yields a (PS) sequence $\{\tilde{w}_n\}$ for $I_{c-\delta}$ such that $|w_n| - \tilde{w}_n \to 0$ in $H^1(\mathbb{R}^3, \mathbb{R})$. By concentration-compactness arguments, there exists a sequence $\{z_n\}$ of points in $\mathbb{R}^3$ such that $w_n(\cdot - z_n)$ converges in H^1 to some w which solves

$$\Delta w - (c - \delta)w + f(|w|^2)w = 0 \quad \text{in } \mathbb{R}^3.$$

Denote $\bar{y}_n = \varepsilon_n z_n$. From (37), we can assume that, up to a subsequence, $\bar{y}_n \to \bar{y}$ in $\overline{\Lambda}$. Since

$$b^{c-\delta} \geqslant \lim_{n\to\infty} \varepsilon_n^{-3} J_{\varepsilon_n}(t_n u_n) \geqslant \lim_{n\to\infty} I(t_n|v_n|) = I_{V(\bar{y})}(\omega),$$

we have $b^{c-\delta} \geqslant b^{V(\bar{y})}$, so that $V(\bar{y}) \leqslant c - \delta$. But $\beta(u_n) \to \bar{y} \in \overline{\Lambda}$ and (50) implies $V(\bar{y}) > c - \delta/2$. This contradiction proves (49).

Step IV: We are going to find a contradiction that proves (35), which will complete the proof. Recall the validity of (49). Let $\varphi_n(y) = \pi(\beta(\phi_n(y)))$ where π: $\Lambda^+ \to \Lambda$ is a continuous mapping that equals the identity on Λ and Λ^+ is a fixed small neighborhood of Λ fixed in Step III. Now, $\phi_n(y) = w^w_{\varepsilon_n}$ for each $y \in B_0^{\varepsilon_n}$, and $w^y_{\varepsilon_n}$ is radially symmetric with respect to the point y. Therefore ϕ_n acts as the identity on $B_0^{\varepsilon_n}$. As such, map ϕ_n is admissible in the class of functions that defines the level c. Assumption (V2) implies now that $c \leqslant \sup_{y \in B_0^{\epsilon_n}} V(\varphi_n(y))$ for all $n \geqslant 1$. If n is large enough, this contradicts (49), and we have proved that (35) is true. □

Proposition 5.3: For each ε sufficiently small, the number γ_ε defined by (29) is a critical value for the functional J_ε. As a consequence, there exists a solution $u_\varepsilon \in H^\varepsilon_{A,V}$ to Eq. (23) such that $J_\varepsilon(u_\varepsilon) = \gamma_\varepsilon$. Furthermore $u_\varepsilon \in C^{2,\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$, with $\alpha \in (0,1)$.

Proof: We already know from Lemma 4.1 that J_ε satisfies the (PS) condition, provided ε is small enough. Moreover, the last lemma implies that $\varepsilon^{-3}\gamma_\varepsilon \geqslant b^{c-\delta} + o(1)$ for all ε small. If $\phi \in \Gamma_\varepsilon$, then $\phi(y) = w^y_\varepsilon$ whenever $y \in B_0^\varepsilon$. This entails that

$$\sup_{y\in B_0^\varepsilon} \varepsilon^{-3} J_\varepsilon(\phi(y)) \leqslant b^{c-\delta} + o(1).$$

The proof is completed by a standard deformation argument. By standard regularity results, $u_\varepsilon \in C^{2,\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$. □

VI. PROOF OF THE MAIN THEOREM

First we derive the following proposition in which the asymptotic behavior of $\max_{\partial\Lambda}|u_\varepsilon|$ is described.

Proposition 6.1: Let

$$m_\varepsilon = \max_{x\in\partial\Lambda} |u_\varepsilon(x)|,$$

then

$$\lim_{\varepsilon\to 0} m_\varepsilon = 0. \tag{53}$$

Proof: We split again the proof.

Step I: We begin to establish the following fact: if $\varepsilon_n \to 0$ and $x_n \in \overline{\Lambda}$ are such that $|u_{\varepsilon_n}(x_n)| \geqslant b > 0$, then

$$\limsup_{n\to\infty} V(x_n) \leqslant c.$$

By contradiction, we assume, up to a subsequence, that $x_n \to x^* \in \overline{\Lambda}$ and $V(x^*) > c$. Set $v_n(x) = u_{\epsilon_n}(x_n + \epsilon_n x)$, we have that v_n satisfies the equation

$$-\Delta v_n - \frac{2}{i} A(x_n + \varepsilon_n x)\cdot \nabla v_n + |A(x_n+\epsilon_n x)|^2 v_n - \frac{\varepsilon_n}{i}\operatorname{div} A(x_n+\varepsilon_n x) v_n + V(x_n+\varepsilon_n x) v_n = g(x_n+\varepsilon_n x, |v_n|^2) v_n \quad \text{in } \mathbb{R}^3 \tag{54}$$

By reasoning as in Step II of Lemma 2, $\{v_n\}$ converges in $C^2_{\mathrm{loc}}(\mathbb{R}^3)$ to some v. Let χ be the weak * limit in $L^\infty(\mathbb{R}^3)$ of the sequence $\{\chi_\Lambda(x_n+\varepsilon_n\cdot)\}$, $v \in C^2_{\mathrm{loc}}(\mathbb{R}^3)$ solves the equation in each compact set

$$-\Delta v - \frac{2}{i} A(x^*)\cdot \nabla v + |A(x^*)|^2 v + V(x^*) v = \bar{g}(x, |v|^2) v \quad \text{in } \mathbb{R}^3, \tag{55}$$

where $\bar{g}(x,s) = \chi(x) f(s) + (1-\chi(x))\tilde{f}(s)$ and $0 \leqslant \chi \leqslant 1$. Since $v \in H^1(\mathbb{R}^3, \mathbb{C})$, we infer v solves (46) in weak sense. Setting $\tilde{v}(x) = e^{-iA(x^*)\cdot x} v(x)$, we see that $\tilde{v}$ weakly solves

$$-\Delta \tilde{v} + V(x^*)\tilde{v} = \bar{g}(x, |\tilde{v}|^2)\tilde{v} \quad \text{in } \mathbb{R}^3 \tag{56}$$

Let $\bar{J}$: $H^1(\mathbb{R}, \mathbb{C}) \to R$ be the functional defined by

$$\bar{J}(u) = \frac{1}{2}\int_{\mathbb{R}^3} |\nabla u|^2 + V(x^*)|u|^2 - \int_{\mathbb{R}^3} \bar{G}(x, |u|^2),$$

where $\bar{G}(x,s) = \int_0^s \bar{g}(x,t)\mathrm{d}t$, we observe that $\tilde{v}$ is a critical point of $\bar{J}$. Following Step II of Lemma 5.2, one can prove that

$$\bar{J}(\tilde{v}) \leqslant \liminf_{n\to\infty} J_{\varepsilon_n}(v_n). \tag{57}$$

By (57) and taking into account (30) we deduce that $b^c \geqslant \bar{J}(\tilde{v})$. Since $h(s) \geqslant \tilde{h}(s)$ for all s we derive

$$b^c \geqslant \bar{J}(\tilde{v}) = \max_{\tau \geqslant 0} \bar{J}(\tau v) \geqslant \max_{\tau \geqslant 0} I_{V(x^*)}(tv) \geqslant b^{V(x^*)},$$

where

$$I_{V(x^*)}(u) = \frac{1}{2}\int_{\mathbb{R}^3} |\nabla u|^2 + V(x^*)|u|^2 - \int_{\mathbb{R}^3} F(|u|^2).$$

It follows that $V(x^*) \leqslant c$, which contradicts the fact that $V(x^*) > c$.

Step II: Now we pass to prove (53). By contradiction, we assume, up to a subsequence, that there exists a sequence $x_n \in \partial\Lambda$ such that $x_n \to \bar{x} \in \overline{\partial\Lambda}$ and

$$|u_{\varepsilon_n}(x_n)| \geqslant \gamma > 0. \tag{58}$$

It follows that $V(\bar{x}) \leqslant c$. We claim that $V(\bar{x}) > c - \delta$. By contradiction, we suppose that $V(\bar{x}) = c - \delta$.

Arguing as before, we can consider the scaled sequence $v_n(x) = u_{\varepsilon_n}(x_n + \varepsilon_n x)$, and we can deduce that v_n solves (45) and it converges to some $v \in H^1(\mathbb{R}^3, \mathbb{C})$ in $C^2_{\mathrm{loc}}(\mathbb{R}^3)$, up to subsequences and $v \neq 0$. Moreover v weakly solves the equation

$$-\Delta v - \frac{2}{i}A(\bar{x}) \cdot \nabla v + |A(\bar{x})|^2 v + V(\bar{x})v = \bar{g}(x, |v|^2)v \quad \text{in } \mathbb{R}^3, \tag{59}$$

where $\bar{g}(x,s) = \chi(x)f(s) + (1 - \chi(x))\tilde{f}(s)$.

Setting $\tilde{v}(x) = e^{-iA(\bar{x})\cdot x}v(x)$, we see that $\tilde{v}$ weakly solves

$$-\Delta \tilde{v} + V(\bar{x})\tilde{v} = \bar{g}(x, |\tilde{v}|^2)\tilde{v} \quad \text{in } \mathbb{R}^3 \tag{60}$$

and thus $\tilde{v}$ is a critical point of the functional $\bar{I}$: $H^1(\mathbb{R}^3, \mathbb{C}) \to \mathbb{R}$ defined by

$$\bar{I}(u) = \frac{1}{2}\int_{\mathbb{R}^3} |\nabla u|^2 + V(\bar{x})|u|^2 - \int_{\mathbb{R}^3} \bar{G}(x, |u|^2),$$

where $\bar{G}(x,s) = \int_0^s \bar{g}(x,t)\mathrm{d}t$.

Now for any $n \in N$ we consider the positive measure $\mu_n(\Omega) = \int_\Omega |\nabla |v_n||^2 + V(x_n + \varepsilon_n x)|v_n|$. We have that the sequence $\{\mu_n(\mathbb{R}^3)\}_n$ is bounded and, up to subsequences, μ_n tends to some $\tilde{c}$.

Therefore there exists a subsequence of $\{\mu_n\}_n$ (without relabelling) for which one of the three possibilities of Lions' concentration-compactness lemma (see Ref. 25) holds. First we notice that vanishing cannot occur, as $|v(0)| > 0$.

If we have tightness, we derive that there exists z_n with the following property: for any $\gamma > 0$ there exists $\rho > 0$ such that

$$\int_{B_\rho(z_n)} |\nabla |v_n||^2 + V(x_n + \varepsilon_n x)|v_n| \geqslant \tilde{c} - \gamma.$$

If $\varepsilon_n z_n$ tends to some point $y \in \mathbb{R}^3$, then we derive that $|v_n|$ tends to $|v|$ strongly in $H^1(\mathbb{R}^3, \mathbb{R})$ and thus $|v_n|$ tends to $|v|$ strongly in $L^q(\mathbb{R}^3, \mathbb{R})$ with $q < 5$.

Testing Eq. (45) we get that

$$\int_{\mathbb{R}^3} \left| \left(\frac{\nabla}{i} - A_n(x) \right) v_n \right|^2 + V_n(x)|v_n|^2 = \int_{\mathbb{R}^3} \bar{g}(x, |v_n|^2)|v_n|^2$$

and, since $\int \bar{g}(x, |v_n|^2)|v_n|^2 \to \int \bar{g}(x, |v|^2)|v|^2$ and v solves (60) we deduce

$$\int_{R^3}\left|\left(\frac{\nabla}{i}-A_n(x)\right)v_n\right|^2+V_n(x)|v_n|^2\to\int_{R^3}\left|\left(\frac{\nabla}{i}-A(\bar{x})\right)v\right|^2+V(\bar{x})|v|^2 \tag{61}$$

and so

$$b^c\geqslant\lim_n\varepsilon_n^{-3}J_{\varepsilon_n}(u_n)=\bar{I}(\tilde{v}).$$

After a rotation, by Lemma 5.1, $\tilde{v}$ solves

$$-\Delta\tilde{v}+V(\bar{x})\tilde{v}=f(|\tilde{v}|^2)\tilde{v}$$

and since we have assumed $V(\bar{x})=c-\delta$, we get $\bar{I}(\tilde{v})=b^{c-\delta}$. This is a contradiction to (35).

Conversely, if $|\varepsilon_n z_n|\to\infty$, we can conclude that

$$b^c\geqslant\lim_n\varepsilon_n^{-3}J_{\varepsilon_n}(u_n)=b^{c-\delta}+b^{V_0}$$

which, by the continuity of $a\mapsto b^a$, is not possible if δ is chosen sufficiently small. In a similar way we can infer that dichotomy cannot occur.

Therefore $V(\bar{x})>c-\delta$ and $|v_n|\to|v|$ strongly in $H^1(\mathbb{R}^3,\mathbb{R})$ as $n\to+\infty$.

Step III: Observe that we can assume that δ was fixed so that $\bar{x}$ lies in a region where $\partial\Lambda$ is smooth and $\partial_\tau V(\bar{x})\neq 0$.

Arguing as in Ref. 14 we can assume $\bar{x}=0$ and the domain Λ can be described as

$$\Lambda\cap B(0,2\rho)=\{(x,x')\in B(0,2\rho)|x'\in\mathbb{R}^2,\ x_3<\psi(x')\},$$

where ψ is a smooth function such that $\psi(0)=0$ and $\nabla\psi(0)=0$. So we have that in $B(0,\rho/\varepsilon_n)v_n$ satisfies

$$\begin{aligned}&-\Delta v_n-\frac{2}{i}A(x_n+\varepsilon_n x)\cdot\nabla v_n+|A(x_n+\varepsilon_n x)|^2v_n-\frac{\varepsilon_n}{i}\operatorname{div}A(x_n+\varepsilon_n x)v_n+V(x_n+\varepsilon_n x)v_n\\&=\chi_{\{z_3<\varepsilon^{-1}\psi(\varepsilon z')\}}f(|v_n|^2)v_n+\chi_{\{z_3>\varepsilon^{-1}\psi(\varepsilon z')\}}\tilde{f}(|v_n|^2)v_n.\end{aligned} \tag{62}$$

Since $|v_n|$ converges to $|v|$ strongly in $H^1(\mathbb{R}^3,\mathbb{R})$, arguing as in Ref. 21 or in Ref. 31 we derive that $|v_n(z)|\leqslant Ce^{-\beta|z|}$ for some constants C, β independent of n. Recalling that each v_n is complex valued, it is not so easy to prove a similar decaying behavior for the gradients ∇v_n, too. Hence we need to modify the proof in Ref. 14. The main tool is a kind of variational identity inspired to the celebrated Pucci–Serrin identity in Ref. 28 (see also Ref. 12). Since all the details for deriving this identity for complex-valued solutions to the Schrödinger equation with magnetic field can be found in Ref. 31, we will be rather sketchy. Fix the index $n\geqslant 1$, and choose a sequence $\{\psi_h\}_{h\in\mathbb{N}}$ of functions from $C_0^\infty(B(0,\rho/\varepsilon_n))$ such that their supports converge to $B(0,\rho/\varepsilon_n)$ as $h\to+\infty$. Now multiply equation (62) by $\psi_h(\partial v_n/\partial x_k)$ $(k=1,2)$ and integrate by parts. By reasoning as in Ref. 31 and exploiting (8) and (9), we can show that it is possible to take first the limit as $h\to\infty$ and then the limit $n\to\infty$, finally deducing that

$$\begin{aligned}&\int_{\mathbb{R}^3}\frac{\partial A}{\partial x_k}(0)\cdot A(0)|v|^2\,\mathrm{d}x-\mathrm{Re}\frac{1}{i}\int_{\mathbb{R}^3}\nabla v\cdot\frac{\partial A}{\partial x_k}(0)\bar{v}\,\mathrm{d}x+\frac{\partial V}{\partial x_k}(0)\int_{\mathbb{R}^3}\frac{|v|^2}{2}\mathrm{d}x\\&=\int_{\mathbb{R}^2}\left[F(|v|^2)-\tilde{F}(|v|^2)\right]z'\cdot\nabla\frac{\partial\psi}{\partial x_k}(0)\mathrm{d}z'.\end{aligned}$$

If we define U_0 by $v(x)=e^{iA(0)\cdot x}U_0(x)$, then $U_0\in H^1(\mathbb{R}^3,\mathbb{C})$ satisfies the identity

$$-\Delta U_0 + V(0)U_0 = \chi_{\{z_3<\psi(0)\}} f(|U_0|^2)U_0 + \chi_{\{z_3>\psi(0)\}} \tilde{f}(|U_0|^2)U_0.$$

Hence by Lemma 5.1 (after a suitable rotation) and an elementary calculation we conclude that

$$\frac{\partial A}{\partial x_k}(0) \cdot \int_{\mathbb{R}^3} \mathrm{Re}(i\overline{U}_0 \nabla U_0)\mathrm{d}x + \frac{\partial V}{\partial x_k}(0) \int_{\mathbb{R}^3} \frac{|U_0|^2}{2}\mathrm{d}x = 0.$$

But by the uniqueness of critical points for the functional I_a [see assumption (f2) and the arguments in Ref. 31], $\mathrm{Re}(i\overline{U}_0 \nabla U_0)=0$ a.e. in $\mathbb{R}^3$. This immediately implies that $(\partial V/\partial x_k)(0)=0$ for $k=1,2$ and so $\partial_\tau V(\bar{x})=0$. This contradiction complete the proof. □

Finally we prove the main result. For the reader's convenience, we repeat its statement below.

Main Theorem: *Under assumptions* (f1) and (f2), (A1), (V1–V3), *there is a number* $\varepsilon_0>0$ *such that for all* $\varepsilon<\varepsilon_0$, *there exists a solution* $u_\varepsilon \in H^\varepsilon_{A,V}$ *of* Eq. (6). *Furthermore* $u_\varepsilon \in C^{2,\alpha}_{\mathrm{loc}}(\mathbb{R}^3)$ *with* $\alpha \in (0,1)$.

Proof: By Proposition 6.1, for all ε small enough,

$$|u_\varepsilon(x)| < \sqrt{a} \quad \text{for all } x \in \partial\Lambda.$$

The function u_ε satisfies the equation

$$\left(\frac{\varepsilon}{i}\nabla - A\right)^2 u_\varepsilon + Vu_\varepsilon = g(x,|u_\varepsilon|^2)u_\varepsilon \quad \text{in } \mathbb{R}^3. \tag{63}$$

Therefore we can test (63) against $(|u_\varepsilon|-\sqrt{a})_+$, and recalling Kato's inequality we find

$$\int_{\mathbb{R}^3\setminus\Lambda} \varepsilon^2 |\nabla (|u_\varepsilon| - \sqrt{a})_+|^2 + c(x)(|u_\varepsilon| - \sqrt{a})_+^2 + c(x)\sqrt{a}(|u_\varepsilon| - \sqrt{a})_+ \leqslant 0, \tag{64}$$

where

$$c(x) = V(x) - g(x,|u_\varepsilon(x)|^2).$$

By definition of g, we have $c>0$ in $\mathbb{R}^3\setminus\Lambda$. Hence all terms in (64) are necessarily zero, and in particular

$$|u_\varepsilon(x)| \leqslant \sqrt{a} \quad \text{for all } x \in \mathbb{R}^3 \setminus \Lambda.$$

This, of course, implies that u_ε is a solution of (6). □

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On reflection algebras and twisted Yangians

Anastasia Doikou[a)]
Laboratoire d'Annecy-le-Vieux de Physique Théorique, LAPTH, CNRS, UMR 5108, Université de Savoie, B.P. 110, F-74941 Annecy-le-Vieux Cedex, France

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It is well known that integrable models associated to rational R matrices give rise to certain non-Abelian symmetries known as Yangians. Analogously boundary symmetries arise when general but still integrable boundary conditions are implemented, as originally argued by Delius, Mackay, and Short from the field theory point of view, in the context of the principal chiral model on the half-line. In the present study we deal with a discrete quantum mechanical system with boundaries, that is the N site gl(n) open quantum spin chain. In particular, the open spin chain with two distinct types of boundary condition known as soliton preserving and soliton nonpreserving is considered. For both types of boundaries we present a unified framework for deriving the corresponding boundary nonlocal charges directly at the quantum level. The nonlocal charges are simply coproduct realizations of particular boundary quantum algebras called boundary or twisted Yangians, depending on the choice of boundary conditions. Finally, with the help of linear intertwining relations between the solutions of the reflection equation and the generators of the boundary or twisted Yangians we are able to exhibit the exact symmetry of the open spin chain, namely we show that a number of the boundary nonlocal charges are in fact conserved quantities. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1888029]

I. INTRODUCTION

Symmetry breaking mechanisms have been the subject of immense interest in modern physics. A well-known symmetry breaking process in the context of two dimensional integrable systems is the implementation of general boundaries that preserve however integrability.[1,2] The presence of general integrable boundaries usually reduces the original symmetry of the system giving rise to boundary algebraic structures known as boundary quantum groups (algebras) (see, e.g., Refs. 3–6). The boundary quantum groups are essentially subalgebras of the usual quantum groups,[7–10] and they provide the underlying algebraic structures in the reflection equation[1] exactly as quantum groups do in the Yang–Baxter equation.[11–13] As is well known the Yang–Baxter and reflection equations are collections of algebraic constraints ruling two dimensional integrable models with boundaries. The study of such boundary symmetries for a particular class of integrable systems will be the main objective of this investigation.

The present work may be seen as the continuation of the investigation undertaken in Ref. 6, where the boundary quantum group generators for the open XXZ spin chain, were constructed by studying the asymptotics of the open spin chain. Historically, boundary quantum group generators were obtained for the first time in the context of the sine-Gordon model in the free fermion point,[3] whereas in Ref. 14 realizations of such generators were constructed for models associated to higher rank algebras. In Ref. 4 the boundary quantum group was derived for the affine Toda field theories on the half-line, and solutions of the reflection equation associated to a certain type of boundary conditions were found. Also, boundary nonlocal charges were constructed classically, in

[a)]Electronic mail: doikou@lapp.in2p3.fr

the framework of the principal chiral model on the half-line,[5] for two distinct types of boundary conditions known as soliton preserving (SP) (Refs. 15–18) and soliton nonpreserving (SNP).[19–22]

In this paper we focus on the quantum mechanical system that is the N site gl(n) open quantum spin chain, and we consider two types of boundary conditions, i.e., SP and SNP. For both types of boundaries the corresponding nonlocal charges are constructed in a systematic way by studying the asymptotics of the gl(n) open spin chain. It turns out that the nonlocal charges are simply coproducts of certain boundary quantum algebras called boundary or twisted Yangians,[23–25] depending on the choice of boundary conditions. It is worth remarking that in Ref. 5 linear intertwining relations involving the boundary algebra generators were used as the starting point for deriving solutions of the reflection equation for both types of boundary conditions. In the present study on the other hand we start our analysis having at our disposal c-number solutions of the reflection equation, and we simply exploit the existence of the intertwining relations in order to derive the symmetry of the open spin chain (see also Ref. 6). In fact, we show explicitly that a set of the boundary nonlocal charges are conserved quantities, that is they commute with the transfer matrix of the open spin chain. It should be pointed out that our results rely on purely algebraic grounds, and therefore they are independent of the choice of representation.

II. THE UNDERLYING ALGEBRAS

In general, two types of spin chains exist known as closed (e.g., periodic boundary conditions) and open. To construct and study a periodic spin chain one must first introduce the basic building block, namely the $R(\mathcal{L})$ matrix satisfying the Yang–Baxter equation.[11–13] The construction of an open spin chain on the other hand requires the consideration of one more fundamental object called the $\mathcal{K}$ matrix, which satisfies another set of algebraic constraints known as the reflection equation.[1] The main objective of the two subsequent sections is to introduce the aforementioned fundamental objects, and also briefly describe the corresponding algebraic framework.

A. The Yang–Baxter equation

Let us first introduce the gl(n)R matrix, which is a solution of the Yang–Baxter equation,[11–13]

$$R_{12}(\lambda_1-\lambda_2)R_{13}(\lambda_1)R_{23}(\lambda_2)=R_{23}(\lambda_2)R_{13}(\lambda_1)R_{12}(\lambda_1-\lambda_2), \tag{2.1}$$

acting on $\mathbb{V}\otimes\mathbb{V}\otimes\mathbb{V}$, and as usual $R_{12}=R\otimes\mathbb{I}$, $R_{23}=\mathbb{I}\otimes R$, and so on. The R matrix may be written in the following compact form:

$$R(\lambda)=\mathbb{I}+\frac{i}{\lambda}\mathcal{P}, \tag{2.2}$$

where $\mathcal{P}$ is the permutation operator, acting on $(\mathbb{C}^n)^{\otimes 2}$ with

$$\mathcal{P}(a\otimes b)=b\otimes a \quad \text{and } \mathcal{P}^2=\mathbb{I}. \tag{2.3}$$

In addition, the R matrix satisfies the unitarity condition,

$$R(\lambda)\hat{R}(-\lambda)\propto\mathbb{I} \quad \text{where } \hat{R}(\lambda)=\mathcal{P}\,R(\lambda)\mathcal{P}. \tag{2.4}$$

Notice that $R(\lambda)\in\mathrm{End}(\mathbb{C}^n\otimes\mathbb{C}^n)$, however in general one may define the object $\mathcal{L}(\lambda)\in\mathrm{End}(\mathbb{C}^n)\otimes\mathcal{Y}[\lambda^{-1}]$, where the second space is not represented, but it is occupied by elements of the algebra $\mathcal{Y}$ called the gl(n) Yangian,[8,9] and defined by the following fundamental algebraic relation:

$$R_{12}(\lambda_1-\lambda_2)\mathcal{L}_{13}(\lambda_1)\mathcal{L}_{23}(\lambda_2)=\mathcal{L}_{23}(\lambda_2)\mathcal{L}_{13}(\lambda_1)R_{12}(\lambda_1-\lambda_2). \tag{2.5}$$

It is worth pointing out that the asymptotic expansion of $\mathcal{L}(\lambda)$ to powers of λ^{-1} yields the generators of the Yangian, which satisfy exchange relations dictated by (2.5). A more detailed analysis on the Yangian will be presented in Sec. III. A solution of the fundamental equation (2.5), which we shall use hereafter, may take the following simple form:

$$\mathcal{L}(\lambda) = \mathbb{I} + \frac{i}{\lambda}\mathbb{P}. \tag{2.6}$$

$\mathbb{P}$ is an $n \times n$ matrix with entries $\mathbb{P}_{ab} \in \mathrm{gl}(n)$.

The Yangian (2.5) is a Hopf algebra equipped with a coproduct $\Delta : \mathcal{Y} \to \mathcal{Y} \otimes \mathcal{Y}$,

$$(\mathrm{id} \otimes \Delta)\mathcal{L}(\lambda) = \mathcal{L}_{13}(\lambda)\mathcal{L}_{12}(\lambda), \tag{2.7}$$

and by treating $\mathcal{L}$ as an $n \times n$ matrix with entries $\mathcal{L}_{ab}$ being elements of $\mathcal{Y}$, we conclude that

$$\Delta(\mathcal{L}_{ab}(\lambda)) = \sum_{c=1}^{n} \mathcal{L}_{cb}(\lambda) \otimes \mathcal{L}_{ac}(\lambda), \quad a,b \in \{1,\ldots,n\}. \tag{2.8}$$

It will be helpful for the following to also introduce $\Delta' : \mathcal{Y} \to \mathcal{Y} \otimes \mathcal{Y}$ obtained from Δ by permutation. In particular, let Π be the shift operator $\Pi : \mathcal{O}_1 \otimes \mathcal{O}_2 \to \mathcal{O}_2 \otimes \mathcal{O}_1$ then one may write

$$\Delta'(x) = \Pi \circ \Delta(x), \quad x \in \mathcal{Y}. \tag{2.9}$$

Also, by iteration the l coproduct $\Delta^{(l)} : \mathcal{Y} \to \mathcal{Y}^{\otimes(l)}$ may be written as

$$\Delta^{(l)} = (\mathrm{id} \otimes \Delta^{(l-1)})\Delta. \tag{2.10}$$

By considering tensor products of $\mathcal{Y}$ one may construct the periodic spin chain. Let us first define the algebraic monodromy matrix T as tensor product of N $\mathcal{L}$ matrices, i.e.,

$$T_0(\lambda) = (\mathrm{id} \otimes \Delta^{(N)})\mathcal{L}(\lambda) = \mathcal{L}_{0N}(\lambda) \cdots \mathcal{L}_{01}(\lambda), \tag{2.11}$$

the monodromy matrix $T \in \mathrm{End}(\mathbb{C}^n) \otimes \mathcal{Y}^{\otimes N}$ is also a solution of (2.5). Traditionally the indices $i \in \{1,\ldots,N\}$ are associated to the quantum spaces and they are suppressed from the monodromy matrix (2.11), whereas the index 0 corresponds to the so-called auxiliary space. Finally, the transfer matrix of the periodic spin chain is derived by simply taking the trace over the auxiliary space,

$$t(\lambda) = Tr_0 T_0(\lambda), \tag{2.12}$$

and it is clear that $t(\lambda) \in \mathcal{Y}^{\otimes N}$. It follows immediately from (2.5) that the transfer matrix (2.12) provides a family of commuting operators,

$$[t(\lambda), t(\lambda')] = 0, \tag{2.13}$$

ensuring the integrability of the model. Each quantum space in (2.11) and (2.12) is associated to a copy of $\mathcal{Y}$, and the corresponding sequence of N copies of $\mathcal{Y}$ described by (2.11) and (2.12) is a purely algebraic construction. It acquires a physical meaning as a spin chain once the quantum spaces are mapped to finite or infinite dimensional spaces. Then the spectrum of the transfer matrix and the corresponding Bethe ansatz equations can be derived and the physically relevant quantities may be computed.[26]

B. The reflection equation

In the following two distinct types of boundary conditions SP, SNP are described using a unified framework, and the corresponding spin chains are constructed. As mentioned, in order to build the open spin chain an additional fundamental object needs to be considered, that is the $\mathcal{K}^*$ matrix, which is a solution of the reflection equation[1]

$$R_{12}(\lambda_1 - \lambda_2)\mathcal{K}_1^*(\lambda_1)R_{21}^*(\lambda_1 + \lambda_2)\mathcal{K}_2^*(\lambda_2) = \mathcal{K}_2^*(\lambda_2)R_{12}^*(\lambda_1 + \lambda_2)\mathcal{K}_1^*(\lambda_1)R_{21}(\lambda_1 - \lambda_2) \tag{2.14}$$

acting on $\mathbb{V} \otimes \mathbb{V}$, and as customary $\mathcal{K}_1^* = \mathcal{K}^* \otimes \mathbb{I}$, $\mathcal{K}_2^* = \mathbb{I} \otimes \mathcal{K}^*$. We also introduce the notation,

$$\mathcal{K}^*(\lambda) = \mathcal{K}(\lambda), \quad R^*(\lambda) = R(\lambda) \quad \text{for SP b . c . ,}$$

$$\mathcal{K}^*(\lambda) = \overline{\mathcal{K}}(\lambda), \quad R^*(\lambda) = \overline{R}(\lambda) \quad \text{for SNP bc . ,} \tag{2.15}$$

and we define

$$\overline{R}_{12}(\lambda) = f(\lambda)V_1 R_{12}^{t_2}(-\lambda - i\rho)V_1 = f(\lambda)V_2^{t_2}R_{12}^{t_1}(-\lambda - i\rho)V_2^{t_2},$$

$$\rho = \frac{n}{2}, \quad f(\lambda) = \frac{\lambda + i\rho}{\lambda}, \tag{2.16}$$

$\overline{R}_{21}(\lambda) = \overline{R}_{12}(\lambda)^{t_1 t_2}$, t_i denotes the transposition on the ith space. V is the charge conjugation being of the form

$$V = \text{antidiag}(1,1,\ldots,1,1), \quad n \quad \text{odd and even, or}$$

$$V = \text{antidiag}(i,-i,\ldots,i,-i), \quad n \quad \text{even only.} \tag{2.17}$$

The $\overline{R}$ matrix may be also written in a compact form as

$$\overline{R}(\lambda) = \frac{\lambda + i\rho}{\lambda}\mathbb{I} - \frac{i}{\lambda}K = \mathbb{I} + \frac{i}{\lambda}\check{\mathcal{P}}, \tag{2.18}$$

where K is a one-dimensional projector satisfying

$$K\,\mathcal{P} = \mathcal{P}, \quad K = \pm K, \quad K^2 = nK, \tag{2.19}$$

and consequently $\check{\mathcal{P}}^2 = \rho^2\mathbb{I}$. For the special case $n=2$, it is clear that $\check{\mathcal{P}} = \mathcal{P}$. Relation (2.14) defines the so-called reflection algebra (boundary Yangian)[2,27–30] or the twisted Yangian[23–25] depending on the action of $*$ (2.15). Let us denote the boundary or twisted Yangian as $\mathbb{B}^*$, more specifically

$$\mathbb{B}^* = \mathbb{B} \text{ boundary Yangian for SP b . c . , } \quad \mathbb{B}^* = \overline{\mathbb{B}} \text{ twisted Yangian for SNP b . c.} \tag{2.20}$$

It should be noted that from the physical point of view SP b.c. describe the reflection of a soliton to a soliton, while SNP b.c. describe the reflection of a soliton to an antisoliton.

The general form of the gl(n)c-number $\mathcal{K}^*$ matrix is given by[1]

$$\mathcal{K}^*(\lambda) = \lambda k^* + f^*, \tag{2.21}$$

where f^*, k^* are $n \times n$ λ independent matrices with $f^* = f$ or $\overline{f}$ and $k^* = k$ or $\overline{k}$ for SP and SNP bc., respectively. For SP b

c. in particular, $f = i\xi\mathbb{I}$ and k is a $n \times n$ λ independent matrix with nonzero entries given by[17]

$$k_{11}(\lambda) = -1, \quad k_{nn}(\lambda) = 1, \quad k_{1n}(\lambda) = k_{n1}(\lambda) = 2\kappa,$$

$$k_{jj}(\lambda) = 1 + 2c, \quad j = 2,\ldots,n-1, \tag{2.22}$$

with ξ arbitrary constant, and c, κ constants satisfying $\kappa^2 = c(c+1)$ (see also Ref. 17), so there are two arbitrary boundary parameters ξ and κ. Notice that the entries of the $\mathcal{K}$ matrix are simply c numbers and this is the reason why (2.22) is called a c-number solution of the reflection equation.

Although certain solutions $\overline{\mathcal{K}}$ (SNP) of (2.14) have been derived for the trigonometric[4,20] and rational case,[5,22] the situation is not completely clear yet for this type of boundary conditions. Nevertheless, assuming the general form (2.21) for the c-number $\overline{\mathcal{K}}$ matrix is sufficient for our analysis. It is evident that the gl(2) case is rather special, because $R_{12} - \overline{R}_{12}$ [by choosing the second V in (2.17)], and consequently $\mathcal{K} = \overline{\mathcal{K}}$.

Having at our disposal *c*-number solutions of (2.14) we may build the more general form of solution. To do so it is first necessary to define the following objects:

$$\hat{\mathcal{L}}_{12}(\lambda) = \mathcal{L}_{12}^{-1}(-\lambda), \quad \overline{\mathcal{L}'}(\lambda) = f(\lambda) V_1^{t_1} \mathcal{L}_{12}^{t_1}(-\lambda - i\rho) V_1^{t_1} \tag{2.23}$$

and

$$\mathcal{L}^*(\lambda) = \hat{\mathcal{L}}(\lambda), \quad \text{for SP b . c . }, \quad \mathcal{L}^*(\lambda) = \overline{\mathcal{L}'}(\lambda) \quad \text{for SNP b . c.} \tag{2.24}$$

It will be instructive for the following to present explicit expressions of the $\mathcal{L}^*$. Although the expressions for $\mathcal{L}^{-1}$ and consequently $\hat{\mathcal{L}}$ are quite intricate, fortunately for our purposes it is only necessary to consider the asymptotic behavior as $\lambda \to \infty$, keeping terms up to $1/\lambda^2$,

$$\hat{\mathcal{L}}_{12}(\lambda \to \infty) \propto \mathbb{I} + \frac{i}{\lambda}\mathbb{P}_{12} - \frac{1}{\lambda^2}\mathbb{P}_{12}^2 + \mathcal{O}\left(\frac{1}{\lambda^3}\right) \quad \text{and} \quad \overline{\mathcal{L}'}_{12}(\lambda) = \mathbb{I} + \frac{i}{\lambda}\check{\mathbb{P}}_{12}, \tag{2.25}$$

where

$$\check{\mathbb{P}}_{12} = \rho\mathbb{I} - V_1^{t_1}\mathbb{P}_{12}^{t_1}V_1^{t_1}. \tag{2.26}$$

And more specifically, $\hat{R}(\lambda)$ is provided by (2.4), and $\overline{R'}(\lambda) = \mathcal{P}\,\overline{R}(\lambda)\mathcal{P}$.

The more general solution of (2.14) is then given by[2]

$$\mathbb{K}^*(\lambda) = \mathcal{L}(\lambda - \Theta)(\mathcal{K}^*(\lambda) \otimes \mathbb{I})\mathcal{L}^*(\lambda + \Theta). \tag{2.27}$$

Θ some times is called inhomogeneity and henceforth for simplicity we shall consider it to be zero. The entries of $\mathbb{K}^*$ are elements of the $\mathbb{B}^*$ algebra defined by (2.14). It is clear that the general solution (2.27) allows the expansion in powers of λ^{-1} as we shall see in subsequent sections, providing the generators of the boundary Yangian (for SP) or the twisted Yangian (for SNP), which obey commutation relations dictated by the defining algebraic relations (2.14). The algebra $\mathbb{B}^*$ is also endowed with a coproduct inherited essentially from the Yangian. In particular, let us first derive the coproduct for $\mathcal{L}^*$, i.e.,

$$(\mathrm{id} \otimes \Delta)\mathcal{L}^*(\lambda) = \mathcal{L}_{12}^*(\lambda)\mathcal{L}_{13}^*(\lambda) \to \Delta(\mathcal{L}_{ab}^*(\lambda)) = \sum_{c=1}^{n} \mathcal{L}_{ac}^*(\lambda) \otimes \mathcal{L}_{cb}^*(\lambda), \quad a,b \in \{1,\ldots,n\}. \tag{2.28}$$

Then it is clear from (2.8) and (2.28) that the elements of $\mathbb{B}^*$ form coproducts $\Delta : \mathbb{B}^* \to \mathbb{B}^* \otimes \mathcal{Y}$, such that (see also Refs. 4 and 5)

$$\Delta(\mathbb{K}_{ab}^*(\lambda)) = \sum_{k,l=1}^{n} \mathbb{K}_{kl}^*(\lambda) \otimes \mathcal{L}_{ak}(\lambda)\mathcal{L}_{lb}^*(\lambda), \quad a,b \in \{1,\ldots,n\}. \tag{2.29}$$

Our final aim of course is to build the corresponding quantum system that is the open quantum spin chain. For this purpose we shall need tensor product realizations of the general solution (2.27). We define

$$T_0^*(\lambda) = (\mathrm{id} \otimes \Delta^{(N)})\mathcal{L}^*(\lambda) = \mathcal{L}_{01}^*(\lambda) \cdots \mathcal{L}_{0N}^*(\lambda) \tag{2.30}$$

then the general tensor type solution of the (2.14) takes the form

$$\mathcal{T}_0^*(\lambda) = T_0(\lambda)\mathcal{K}_0^*(\lambda)T_0^*(\lambda), \tag{2.31}$$

with entries being clearly coproducts of the $\mathbb{B}^*$ algebra, namely

$$\mathcal{T}^{*}_{ab}(\lambda) = \Delta^{(N)}(\mathbb{K}_{ab}(\lambda)) \tag{2.32}$$

recall that $\Delta^{(N)}$ is defined via (2.10), and $\Delta(\mathbb{K}_{ab})$ is given in (2.29). Finally, we introduce the transfer matrix of the open spin chain,[2] which may be written as

$$t^{*}(\lambda) = Tr_0 \mathcal{K}^{(+)*}_0(\lambda)\mathcal{T}^{*}_0(\lambda), \tag{2.33}$$

$\mathcal{K}^{(+)*}(\lambda) = \mathcal{K}^{(l)*}(-\lambda - i\rho)$, where $\mathcal{K}^{(l)*}(\lambda)$ is also a solution of (2.14), but here for simplicity is considered to be $\mathbb{I}$. The $*$ notation for the aforementioned objects is applied as follows:

$$T^{*}(\lambda) = \hat{T}(\lambda), \quad \mathcal{T}^{*}(\lambda) = \mathcal{T}(\lambda), \quad t^{*}(\lambda) = t(\lambda), \quad \text{for SP b . c . ,}$$

$$T^{*}(\lambda) = \overline{T}(\lambda), \quad \mathcal{T}^{*}(\lambda) = \overline{\mathcal{T}}(\lambda), \quad t^{*}(\lambda) = \overline{t}(\lambda), \quad \text{for SNP b . c.} \tag{2.34}$$

It can be shown,[2,21] using the fact that $\mathcal{T}^{*}$ is a solution of the reflection equation (2.14), that the transfer matrices (2.33) provide families of commuting operators, i.e.,

$$[t^{*}(\lambda), t^{*}(\lambda')] = 0. \tag{2.35}$$

The latter commutation relations (2.35) ensure the integrability of the relevant models.

III. MORE ON YANGIANS

It is instructive for what follows to recall in more detail the basic definitions associated to Yangians[8,31] (for a review on Yangians see, e.g., Ref. 32). The gl(n) Yangian $\mathcal{Y}$, is a non-Abelian algebra—a quantum group[9,10]—with generators $\mathcal{Q}^{(p)}_{ab}$ and defining relations given below

$$[\mathcal{Q}^{(0)}_{ab}, \mathcal{Q}^{(0)}_{cd}] = i\delta_{cb}\mathcal{Q}^{(0)}_{ad} - i\delta_{ad}\mathcal{Q}^{(0)}_{cb},$$

$$[\mathcal{Q}^{(0)}_{ab}, \mathcal{Q}^{(1)}_{cd}] = i\delta_{cb}\mathcal{Q}^{(1)}_{ad} - i\delta_{ad}\mathcal{Q}^{(1)}_{cb},$$

$$[\mathcal{Q}^{(1)}_{ab}, \mathcal{Q}^{(1)}_{cd}] = i\delta_{cb}\mathcal{Q}^{(2)}_{ad} - i\delta_{ad}\mathcal{Q}^{(2)}_{cb} + \frac{ih^2}{4}\mathcal{Q}^{(0)}_{ad}\left(\sum_e \mathcal{Q}^{(0)}_{ce}\mathcal{Q}^{(0)}_{eb}\right) - \frac{ih^2}{4}\left(\sum_e \mathcal{Q}^{(0)}_{ae}\mathcal{Q}^{(0)}_{ed}\right)\mathcal{Q}^{(0)}_{cb},$$

$$a, b \in \{1, \ldots, n\}, \tag{3.1}$$

and also relations

$$[\mathcal{Q}^{(0)}_{ab}, [\mathcal{Q}^{(1)}_{cd}, \mathcal{Q}^{(1)}_{ef}]] - [\mathcal{Q}^{(1)}_{ab}, [\mathcal{Q}^{(0)}_{cd}, \mathcal{Q}^{(1)}_{ef}]] = \frac{h^2}{4}\sum_{p,q}([\mathcal{Q}^{(0)}_{ab}, [\mathcal{Q}^{(0)}_{cp}\mathcal{Q}^{(0)}_{pd}, \mathcal{Q}^{(0)}_{eq}\mathcal{Q}^{(0)}_{qf}]] - [\mathcal{Q}^{(0)}_{ap}\mathcal{Q}^{(0)}_{pd}, [\mathcal{Q}^{(0)}_{cd}, \mathcal{Q}^{(0)}_{eq}\mathcal{Q}^{(0)}_{qf}]]). \tag{3.2}$$

As already mentioned (2.8) the Yangian is endowed with a coproduct $\Delta : \mathcal{Y} \to \mathcal{Y} \otimes \mathcal{Y}$. In particular, the coproducts of the generators $\mathcal{Q}^{(p)}_{ab}$ may be written as

$$\Delta(\mathcal{Q}^{(0)}_{ab}) = \mathcal{Q}^{(0)}_{ab} \otimes \mathbb{I} + \mathbb{I} \otimes \mathcal{Q}^{(0)}_{ab},$$

$$\Delta(\mathcal{Q}^{(1)}_{ab}) = \mathcal{Q}^{(1)}_{ab} \otimes \mathbb{I} + \mathbb{I} \otimes \mathcal{Q}^{(1)}_{ab} + \frac{h}{2}\sum_{d=1}^{n}(\mathcal{Q}^{(0)}_{ad} \otimes \mathcal{Q}^{(0)}_{db} - \mathcal{Q}^{(0)}_{db} \otimes \mathcal{Q}^{(0)}_{ad}), \tag{3.3}$$

also for Δ' similar expressions may be deduced. In fact the only difference between expressions Δ and Δ' is a minus sign in front of h in the coproduct of $\mathcal{Q}^{(1)}_{ab}$. Using (2.10) we can get explicit expression for the l coproducts,

$$\Delta^{(l)}(\mathcal{Q}_{ab}^{(0)}) = \sum_{i=1}^{l} (\mathcal{Q}_{ab}^{(0)})_i,$$

$$\Delta^{(l)}(\mathcal{Q}_{ab}^{(1)}) = \sum_{i=1}^{l} (\mathcal{Q}_{ab}^{(1)})_i + \frac{h}{2} \sum_{j>i=1}^{l} \sum_{d=1}^{n} ((\mathcal{Q}_{ad}^{(0)})_i \otimes (\mathcal{Q}_{db}^{(0)})_j - (\mathcal{Q}_{db}^{(0)})_i \otimes (\mathcal{Q}_{ad}^{(0)})_j), \tag{3.4}$$

where the indices i,j denote the site in the l coproduct sequence. We may also define $\Delta'^{(l)}: \mathcal{Y} \to \mathcal{Y}^{\otimes(l)}$ as

$$\Delta'^{(l)} = (\mathrm{id} \otimes \Delta^{(l-1)})\Delta'. \tag{3.5}$$

Note that there also exists the opposite coproduct $\Delta^{\mathrm{op}(l)} = (\mathrm{id} \otimes \Delta^{\mathrm{op}(l-1)})\Delta^{\mathrm{op}}$ with $\Delta^{\mathrm{op}} = \Delta'$. For generic values of l, $\Delta^{\mathrm{op}(l)} \neq \Delta'^{(l)}$ and they only coincide for $l=2$. Expressions similar to (3.4) may be derived for $\Delta'^{(l)}$, but we omit them here for brevity.

Realizations of Yangian generators: As is known the asymptotic behavior of the monodromy matrix T (2.11) as $\lambda \to \infty$ provides tensor product representations of $\mathcal{Y}$. Let us briefly review how this process works. Recall that the operators $\mathcal{L}$ and T are treated as $n \times n$ matrices with entries being elements of $\mathcal{Y}, \mathcal{Y}^{\otimes N}$, respectively. The monodromy matrix T as $\lambda \to \infty$ may be written as (for simplicity we suppress the auxiliary space index 0 from T in the following)

$$T(\lambda \to \infty) \propto \mathbb{I} + \sum_{m=0}^{\infty} \lambda^{-m-1} t^{(m)}. \tag{3.6}$$

Exchange relations among the charges $t_{ab}^{(m)}$ (the entries of $t^{(m)}$) may be derived by virtue of the fundamental algebraic relation (2.5), as $\lambda_i \to \infty$. To extract the Yangian generators we study the asymptotic expansion (3.6) keeping higher orders in the $1/\lambda$ expansion. Recalling the form of $\mathcal{L}$ (2.6) and T (2.11) we conclude that

$$T(\lambda \to \infty) \propto \mathbb{I} + \frac{i}{\lambda} \sum_{i=1}^{N} \mathbb{P}_{0i} - \frac{1}{\lambda^2} \sum_{i>j=1}^{N} \mathbb{P}_{0i}\mathbb{P}_{0j} + \mathcal{O}\left(\frac{1}{\lambda^3}\right). \tag{3.7}$$

Now consider the quantities below written as combinations of $t^{(p)}$, $p \in \{0,1\}$,

$$Q^{(0)} = t^{(0)}, \quad Q^{(1)} = t^{(1)} - \tfrac{1}{2} Q^{(0)} Q^{(0)}, \tag{3.8}$$

where the form of $t^{(p)}$ is defined by (3.6) and (3.7). Then $Q^{(p)}$ may be written as combinations of the operators $\mathbb{P}_{0i}$, each acting on $\mathbb{C}^n \otimes \mathcal{Y}$, namely [from now on we consider $h=-1$ in (3.3)]

$$Q^{(0)} = i \sum_{i=1}^{N} \mathbb{P}_{0i}, \quad Q^{(1)} = \frac{1}{2} \sum_{i=1}^{N} \mathbb{P}_{0i}^2 + \frac{1}{2} \sum_{j>i=1}^{N} (\mathbb{P}_{0i}\mathbb{P}_{0j} - \mathbb{P}_{0j}\mathbb{P}_{0i}). \tag{3.9}$$

Note that for simplicity both quantum and auxiliary indices in $Q^{(p)}$ (3.9) are omitted. The entries of the matrices $Q^{(p)}$ are the nonlocal charges $Q_{ab}^{(p)} \in \mathcal{Y}^{\otimes N}$ being coproduct realizations of the Yangian, i.e.,

$$Q_{ab}^{(p)} = \Delta^{(N)}(\mathcal{Q}_{ab}^{(p)}), \quad p \in \{0,1\}, \quad a,b \in \{1,\ldots,n\}. \tag{3.10}$$

The charges $Q_{ab}^{(0)}$ in particular, are coproducts of the generators of the gl(n) Lie algebra. It is also apparent from (3.10) that for $N=1$, $Q_{ab}^{(p)} \to \mathcal{Q}_{ab}^{(p)}$.

IV. BOUNDARY AND TWISTED YANGIAN GENERATORS

After the brief review on Yangians we are in the position to deal with realizations of boundary or twisted Yangians. As already mentioned two different types of boundary conditions, the SP and

the SNP[19–22,33] will be investigated using a unified framework. The SNP boundary conditions were studied for the first time in the context of integrable lattice models in Ref. 21, whereas a generalized description of these boundaries is presented in Ref. 33.

As we have seen in Sec. II B the entries of $\mathcal{T}^*$ are coproducts of the $\mathbb{B}^*$ algebra. The main objective now is to obtain, as in the case of Yangians, the exact form of tensor products of the generators of $\mathbb{B}^*$ via the asymptotic expansion of $\mathcal{T}^*$. Again $\mathcal{L}(\mathcal{L}^*)$, $T(T^*)$, and consequently $\mathcal{T}^*$ (2.33) are treated as $n\times n$ matrices with entries being elements of $\mathcal{Y},\mathcal{Y}^{\otimes N}$, respectively. Recall also that $\mathcal{K}^*$ (2.22) is a $n\times n$ matrix with c-number entries. The expansion of $\mathcal{T}^*$ (2.33) as $\lambda\to\infty$ reads (again for simplicity we suppress the auxiliary space index 0 from T,T^*, and $\mathcal{T}^*$ in the following)

$$\mathcal{T}^*(\lambda\to\infty)\propto\mathbb{I}+\sum_{m=0}^{\infty}\lambda^{-m-1}\tilde{t}^{(m)}, \tag{4.1}$$

while exchange relations among the charges $\tilde{t}_{ab}^{(m)}$ may be now found by virtue of the algebraic relations (2.14).

As in the bulk case to extract the boundary or twisted Yangian generators we shall keep higher order terms in the expansion (4.1). We need first the asymptotic behavior of the matrices T,T^* as well as $\mathcal{K}^*$. The expansion of T is given by (3.7), while T^* reads as $\lambda\to\infty$,

$$T^*(\lambda\to\infty)\propto\mathbb{I}+\frac{i}{\lambda}\sum_{i=1}^{N}\mathbb{P}_{0i}^*-\frac{1}{\lambda^2}\left(\sum_{i<j=1}^{N}\mathbb{P}_{0i}^*\mathbb{P}_{0j}^*+Y^*\right)+\mathcal{O}\left(\frac{1}{\lambda^3}\right), \tag{4.2}$$

where

$$\mathbb{P}^*=\mathbb{P}\quad\text{for SP b . c . ,}\quad \mathbb{P}^*=\check{\mathbb{P}}\quad\text{for SNP b . c,} \tag{4.3}$$

and

$$Y^*=\sum_{i=1}^{N}\mathbb{P}_{0i}^2\quad\text{for SP b . c . ,}\quad Y^*=0\quad\text{for SNP b . c.}$$

Before we continue with the asymptotics of $\mathcal{T}^*$ it is necessary for our purposes to derive the charges from the expansion of $\overline{T}$ as $\lambda\to\infty$ [the expansion of $\hat{T}$ yields the same charges as in (3.9)]. Note that $\overline{T}$ also satisfies the defining relation of the Yangian (2.5), therefore the corresponding charges are expected to be coproducts of the Yangian generators. In fact, the asymptotic expansion of $\overline{T}$ (up to $1/\lambda^2$) provides the following operators:

$$\check{Q}^{(0)}=i\sum_{i=1}^{N}\check{\mathbb{P}}_{0i},\quad \check{Q}^{(1)}=-\frac{1}{2}\sum_{i=1}^{N}\check{\mathbb{P}}_{0i}^2+\frac{1}{2}\sum_{j>i=1}^{N}(\check{\mathbb{P}}_{0i}\check{\mathbb{P}}_{0j}-\check{\mathbb{P}}_{0j}\check{\mathbb{P}}_{0i}). \tag{4.4}$$

The entries of the matrices (4.4) may be indeed written as coproducts of an alternative set of generators of the Yangian $\check{\mathcal{Q}}_{ab}^{(p)}$,

$$\check{Q}_{ab}^{(p)}=\Delta^{(N)}(\check{\mathcal{Q}}_{ab}^{(p)}),\quad p\in\{0,1\},\quad a,b\in\{1,\ldots,n\}, \tag{4.5}$$

where $\check{\mathcal{Q}}_{ab}^{(p)}$ are the entries of the matrices derived in (4.4) for $N=1$. The generators $\check{\mathcal{Q}}_{ab}^{(p)}$ are isomorphic to $\mathcal{Q}_{ab}^{(p)}$, and their exact correspondence may be found by exploiting the relation between $\mathbb{P}$ and $\check{\mathbb{P}}$ given by (2.26).

Recall also that the $\mathcal{K}^*$ matrix is given by the general form (2.21) for any solution of the reflection equation (2.14), associated to the gl(n)R matrix. Having derived the expansions of T, T^*, and $\mathcal{K}^*$ we may now come to the asymptotic behavior of $\mathcal{T}^*$ as $\lambda\to\infty$ (we keep here up to $1/\lambda^2$ terms), i.e.,

$$\mathcal{T}^*(\lambda\to\infty)\propto k^*+\frac{1}{\lambda}\left(f^*+ik^*\sum_{i=1}^{N}\mathbb{P}_{0i}^*+i\sum_{i=1}^{N}\mathbb{P}_{0i}k^*\right)+\frac{1}{\lambda^2}\left(-k^*\sum_{i<j=1}^{N}\mathbb{P}_{0i}^*\mathbb{P}_{0j}^*-\sum_{i>j=1}^{N}\mathbb{P}_{0i}\mathbb{P}_{0j}k^*\right.$$
$$\left.-\sum_{i,j=1}^{N}\mathbb{P}_{0i}k^*\mathbb{P}_{0j}^*+if^*\sum_{i=1}^{N}\mathbb{P}_{0i}^*+i\sum_{i=1}^{N}\mathbb{P}_{0i}f^*-k^*Y^*\right)+\mathcal{O}\left(\frac{1}{\lambda^3}\right), \tag{4.6}$$

which provides the form of $\tilde{t}^{(p)}$, $p\in\{0,1\}$ (4.1). Consider now the following combinations of $\tilde{t}^{(p)}$:

$$\tilde{Q}^{(0)}=\tilde{t}^{(0)}-f^*,\quad \tilde{Q}^{(1)}=\tilde{t}^{(1)}-\tfrac{1}{2}\tilde{Q}^{(0)}(k^*)^{-1}\tilde{Q}^{(0)}, \tag{4.7}$$

where for the general gl(n) solution (2.22) $k^{-1}=[1/(1+4\kappa^2)]k$, and $\overline{k}$ (SNP b.c.) is also invertible (see, e.g., Ref. 20). Let us also introduce the following objects:

$$\mathcal{D}=(\mathbb{P}k^*-k^*\mathbb{P}^*),\quad \mathcal{S}=(k^*\mathbb{P}^*+\mathbb{P}k^*), \tag{4.8}$$

$$Q^{*(p)}=Q^{(p)}\quad \text{for SP b.c.},\quad Q^{*(p)}=\check{Q}^{(p)}\ \text{for SNP b.c.} \tag{4.9}$$

Then according to (3.9), (4.4), (4.7), and (4.8) the matrices $\tilde{Q}^{(p)}$ may be written as

$$\tilde{Q}^{(0)}=i\sum_{i=1}^{N}\mathcal{S}_{0i},$$

$$\tilde{Q}^{(1)}=f^*Q^{*(0)}+Q^{(0)}f^*+\frac{1}{2}\sum_{i<j=1}^{N}(\mathcal{S}_{0i}(k^*)^{-1}\mathcal{D}_{0j}-\mathcal{D}_{0j}(k^*)^{-1}\mathcal{S}_{0i})-k^*Y^*+\frac{1}{2}k^*\sum_{i=1}^{N}\mathbb{P}_{0i}^{*2}+\frac{1}{2}\sum_{i=1}^{N}\mathbb{P}_{0i}^2k^*$$
$$+\frac{1}{2}\sum_{i=1}^{N}(k^*\mathbb{P}_{0i}^*(k^*)^{-1}\mathbb{P}_{0i}k^*-\mathbb{P}_{0i}k^*\mathbb{P}_{0i}^*). \tag{4.10}$$

The corresponding entries $\tilde{Q}_{ab}^{(p)}$ $a,b\in\{1,\ldots,n\}$ are the boundary nonlocal charges. Notice that the two last terms in (4.10) vanish for the special case of SP where $k=\mathbb{I}$. $\mathcal{K}^*=\mathbb{I}$ ($k^*=\mathbb{I}$, $f^*=0$) is a valid solution of (2.14) for both boundary conditions. We should point out that for $\mathcal{K}=\mathbb{I}$ (SP b.c.) $\tilde{Q}_{ab}^{(1)}=0$ (4.10), so the only charges that survive are the $\tilde{Q}_{ab}^{(0)}\propto Q_{ab}^{(0)}$. There exist of course higher nonlocal charges that may be obtained by keeping higher order terms in the asymptotic expansion (4.6). This is a significant investigation, which will be undertaken however in a forthcoming work.

The nonlocal charges $\tilde{Q}_{ab}^{(p)}$ (4.10) may be written as combinations of the Yangian coproducts $Q_{ab}^{(p)},\check{Q}_{ab}^{(p)}$ (3.9) and (4.4),

$$\tilde{Q}_{ab}^{(0)}=k_{ac}^*Q_{cb}^{*(0)}+Q_{ac}^{(0)}k_{cb}^*,$$

$$\tilde{Q}_{ab}^{(1)}=-k_{ac}^*Q_{cb}^{*(1)}+Q_{ac}^{(1)}k_{cb}^*+f_{ac}^*Q_{cb}^{*(0)}+Q_{ac}^{(0)}f_{cb}^*-\tfrac{1}{2}(k_{ac}^*Q_{cd}^{*(0)}(k^*)_{de}^{-1}Q_{ef}^{(0)}k_{fb}^*-Q_{ac}^{(0)}k_{cd}^*Q_{db}^{*(0)}),$$
$$a,b\in\{1,\ldots,n\}. \tag{4.11}$$

Note that the summation over repeated indices is omitted from now on. The quantities k_{ab}^*,f_{ab}^* are c numbers (the entries of the matrices k^*,f^*), $Q_{ab}^{(p)}$ are given by (3.9) and $Q_{ab}^{*(p)}$ by (4.9). The derivation of the boundary nonlocal charges (4.11) is one of the main results of this study. It is worth emphasizing that the nonlocal charges (4.11) were derived independently of the choice of representation.

V. THE SYMMETRY

Our ultimate goal is to study the symmetry of the open spin chain, namely to derive conserved quantities commuting with the open transfer matrix. This may be achieved by using linear intertwining relations between representations of the boundary Yangian generators and the solutions of the reflection equation.

In the preceding section we derived the boundary nonlocal charges (4.11) as coproducts of the boundary or twisted Yangian generators. It is evident that from the expressions (4.11) for $N=1$, one may write down the corresponding abstract generators of $\mathbb{B}^*$,

$$\tilde{\mathcal{Q}}^{(0)}_{ab} = k^*_{ac}\mathcal{Q}^{*(0)}_{cb} + \mathcal{Q}^{(0)}_{ac}k^*_{cb},$$

$$\tilde{\mathcal{Q}}^{(1)}_{ab} = -k^*_{ac}\mathcal{Q}^{*(1)}_{cb} + \mathcal{Q}^{(1)}_{ac}k^*_{cb} + f^*_{ac}\mathcal{Q}^{*(0)}_{cb} + \mathcal{Q}^{(0)}_{ac}f^*_{cb} - \tfrac{1}{2}(k^*_{ac}\mathcal{Q}^{*(0)}_{cd}(k^*)^{-1}_{de}\mathcal{Q}^{(0)}_{ef}k^*_{fb} - \mathcal{Q}^{(0)}_{ac}k^*_{cd}\mathcal{Q}^{*(0)}_{db}),$$
$$a,b \in \{1,\ldots,n\}. \tag{5.1}$$

The quantities $\tilde{\mathcal{Q}}^{(0)}_{ab}$ are simply linear combinations of the generators of the gl(n) Lie algebra. For SNP b.c. in particular the conjugate generators $\check{\mathcal{Q}}^{(0)}_{ab}$ are combined together with $\mathcal{Q}^{(0)}_{ab}$ in the expression (5.1) for $\tilde{\mathcal{Q}}^{(0)}_{ab}$, a fact that implies the folding of the gl(n) algebra for $k^*=\mathbb{I}$ (for more details on this subject see, e.g., Refs. 21 and 33).

As an immediate consequence of (3.10), (4.11), and (5.1) the boundary nonlocal charges may be written in a more compact form as

$$\tilde{Q}^{(p)}_{ab} = \Delta^{(N)}(\tilde{\mathcal{Q}}^{(p)}_{ab}), \quad p \in \{0,1\}. \tag{5.2}$$

The main advantage when deriving generators of $\mathbb{B}^*$ via the asymptotics of the spin chain is that one directly obtains the explicit form of the coproducts of $\mathbb{B}^*$ generators (3.10) and (4.11). Bearing in mind the coproducts of the Yangian generators (3.3) and also equations (3.10) and (4.11) for $N=2$ one may derive the following more convenient expressions for $\Delta:\mathbb{B}^*\to\mathbb{B}^*\otimes\mathcal{Y}$:

$$\Delta(\tilde{\mathcal{Q}}^{(0)}_{ab}) = \mathbb{I}\otimes\tilde{\mathcal{Q}}^{(0)}_{ab} + \tilde{\mathcal{Q}}^{(0)}_{ab}\otimes\mathbb{I},$$

$$\Delta(\tilde{\mathcal{Q}}^{(1)}_{ab}) = \mathbb{I}\otimes\tilde{\mathcal{Q}}^{(1)}_{ab} + \tilde{\mathcal{Q}}^{(1)}_{ab}\otimes\mathbb{I} - \frac{(k^*)^{-1}_{cd}}{2}(\tilde{\mathcal{Q}}^{(0)}_{ac}\otimes\tilde{\mathcal{Q}}^{(0)^-}_{db} - \tilde{\mathcal{Q}}^{(0)}_{db}\otimes\tilde{\mathcal{Q}}^{(0)^-}_{ac}), \tag{5.3}$$

where

$$\tilde{\mathcal{Q}}^{(0)^-}_{ab} = \mathcal{Q}^{(0)}_{ac}k^*_{cb} - k^*_{ac}\mathcal{Q}^{*(0)}_{cb}. \tag{5.4}$$

Similarly, with the help of (2.9) one obtains $\Delta':\mathbb{B}^*\to\mathcal{Y}\otimes\mathbb{B}^*$,

$$\Delta'(\tilde{\mathcal{Q}}^{(1)}_{ab}) = \mathbb{I}\otimes\tilde{\mathcal{Q}}^{(1)}_{ab} + \tilde{\mathcal{Q}}^{(1)}_{ab}\otimes\mathbb{I} + \frac{(k^*)^{-1}_{cd}}{2}(\tilde{\mathcal{Q}}^{(0)^-}_{ac}\otimes\tilde{\mathcal{Q}}^{(0)}_{db} - \tilde{\mathcal{Q}}^{(0)^-}_{db}\otimes\tilde{\mathcal{Q}}^{(0)}_{ac}), \tag{5.5}$$

and the l coproducts are deduced in a straightforward manner via (2.10) and (3.5). Note that expressions similar to (5.1), (5.3), and (5.5), but not exactly the same, were also derived in Ref. 5 from a field theoretical point of view.

Consider now the evaluation representation $\pi_\lambda:\mathcal{Y}\to\mathrm{End}(\mathbb{C}^n)$ such that

$$\pi_\lambda(\mathcal{Q}^{*(1)}_{ab}) = i\lambda\mathcal{P}^*_{ab}, \quad \pi_\lambda(\mathcal{Q}^{*(0)}_{ab}) = i\mathcal{P}^*_{ab}, \quad a,b \in \{1,\ldots,n\}. \tag{5.6}$$

$\mathcal{P}^*$ is an $n\times n$ matrix, with entries $\mathcal{P}^*_{ab}$ being operators which act on $\mathbb{C}^n$. The generators (5.1) are then expressed in terms of the operators $\mathcal{P}^*_{ab}$ as

$$\pi_\lambda(\tilde{\mathcal{Q}}^{(0)}_{ab}) = ik^*_{ac}\mathcal{P}^*_{cb} + i\mathcal{P}_{ac}k^*_{cb},$$

$$\pi_\lambda(\tilde{\mathcal{Q}}^{(1)}_{ab}) = -i\lambda k^*_{ac}\mathcal{P}^*_{cb} + i\lambda\mathcal{P}_{ac}k^*_{cb} + if^*_{ac}\mathcal{P}^*_{cb} + i\mathcal{P}_{ac}f^*_{cb} + \tfrac{1}{2}(k^*_{ac}\mathcal{P}^*_{cd}(k^*)^{-1}_{de}\mathcal{P}_{ef}\,k^*_{fb} - \mathcal{P}_{ac}k^*_{cd}\mathcal{P}^*_{db}). \tag{5.7}$$

We shall henceforth restrict our attention to SP boundary conditions only, and we shall derive certain intertwining relations between the charges (5.7) and the $\mathcal{K}$ matrix (2.22). More specifically, it may be directly deduced from the reflection equation (2.14) that all the elements of the algebra $\mathbb{B}$ commute with the $\mathcal{K}$ matrix (see also Refs. 4 and 5). Indeed, by acting with the evaluation representation on the second space of (2.27) we obtain

$$(\mathrm{id}\otimes\pi_{\pm\lambda})\mathbb{K}(\lambda') = R(\lambda'\mp\lambda)(\mathcal{K}(\lambda')\otimes\mathbb{I})\hat{R}(\lambda\pm\lambda'). \tag{5.8}$$

Now recalling the reflection equation (2.14) and because of the form of the above expressions it is straightforward to show that

$$(\mathrm{id}\otimes\pi_\lambda)\mathbb{K}(\lambda')(\mathbb{I}\otimes\mathcal{K}(\lambda)) = (\mathbb{I}\otimes\mathcal{K}(\lambda))(\mathrm{id}\otimes\pi_{-\lambda})\mathbb{K}(\lambda'). \tag{5.9}$$

As a consequence the entries of $\mathbb{K}$ in the evaluation representation commute with the *c*-number $\mathcal{K}$ matrix (2.22),

$$\pi_\lambda(\mathbb{K}_{ab}(\lambda'))\mathcal{K}(\lambda) = \mathcal{K}(\lambda)\pi_{-\lambda}(\mathbb{K}_{ab}(\lambda')), \quad a,b\in\{1,\ldots,n\}. \tag{5.10}$$

In addition, as we have seen from the analysis of the preceding section, the elements $\mathbb{K}_{ab}(\lambda'\to\infty)$ provide essentially the generators (5.1), and therefore we conclude that

$$\pi_\lambda(\tilde{\mathcal{Q}}^{(p)}_{ab})\mathcal{K}(\lambda) = \mathcal{K}(\lambda)\pi_{-\lambda}(\tilde{\mathcal{Q}}^{(p)}_{ab}). \tag{5.11}$$

Note that we also verified by inspection, taking into account the form of the $\mathrm{gl}(n)\mathcal{K}$ matrices (2.21), (2.22), and (5.7), that the latter relations (5.11) are indeed satisfied.

Equations (5.11) are the boundary analogues of the bulk intertwining relations for the $\mathcal{L}$ matrix, i.e.,

$$(\pi_\lambda\otimes\mathrm{id})\Delta'(\mathcal{Q}^{(p)}_{ab})\mathcal{L}(\lambda) = \mathcal{L}(\lambda)(\pi_\lambda\otimes\mathrm{id})\Delta(\mathcal{Q}^{(p)}_{ab}),$$

$$(\pi_{-\lambda}\otimes\mathrm{id})\Delta(\mathcal{Q}^{(p)}_{ab})\hat{\mathcal{L}}(\lambda) = \hat{\mathcal{L}}(\lambda)(\pi_{-\lambda}\otimes\mathrm{id})\Delta'(\mathcal{Q}^{(p)}_{ab}). \tag{5.12}$$

Relations of the form (5.11) should also hold for solutions $\overline{\mathcal{K}}$ of (2.14) for the general $\mathrm{gl}(n)$ case, which however merits further study and it will be the subject of a forthcoming work. It is worth remarking that in Refs. 4 and 5 intertwining relations such as in (5.11) were used as a starting point for deriving solutions of the reflection equation.

Expressions of the type (5.11) may be obtained for $\mathcal{T}$ (2.31) as well (see also Ref. 6). To derive the generalized intertwining relations for the $\mathcal{T}$ matrix we first need to show relations similar to (5.12) for the monodromy matrices T and $\hat{T}$. Indeed, it immediately follows by induction using (5.12) and the definitions (2.11) and (2.30) that

$$(\pi_\lambda\otimes\mathrm{id}^{\otimes N})\Delta'^{(N+1)}(\mathcal{Q}^{(p)}_{ab})T(\lambda) = T(\lambda)(\pi_\lambda\otimes\mathrm{id}^{\otimes N})\Delta^{(N+1)}(\mathcal{Q}^{(p)}_{ab}),$$

$$(\pi_{-\lambda}\otimes\mathrm{id}^{\otimes N})\Delta^{(N+1)}(\mathcal{Q}^{(p)}_{ab})\hat{T}(\lambda) = \hat{T}(\lambda)(\pi_{-\lambda}\otimes\mathrm{id}^{\otimes N})\Delta'^{(N+1)}(\mathcal{Q}^{(p)}_{ab}), \quad p\in\{0,1\}. \tag{5.13}$$

It should be stressed that the latter relations provide also an effective means for studying the symmetry of the periodic $\mathrm{gl}(n)$ spin chain. From (5.11) and because of the form of the coproducts (5.3) we conclude also that

$$(\pi_\lambda \otimes \mathrm{id}^{\otimes N})\Delta^{(N+1)}(\tilde{\mathcal{Q}}_{ab}^{(p)})\mathcal{K}(\lambda) = \mathcal{K}(\lambda)(\pi_{-\lambda} \otimes \mathrm{id}^{\otimes N})\Delta^{(N+1)}(\tilde{\mathcal{Q}}_{ab}^{(p)}). \tag{5.14}$$

Recalling that the generators of $\mathbb{B}$ (5.1) are written exclusively in terms of $\mathcal{Q}_{ab}^{(p)}$ we conclude that the intertwining relations (5.13) hold also for $\tilde{\mathcal{Q}}_{ab}^{(p)}$. Then taking into account relations (5.13) for $\tilde{\mathcal{Q}}_{ab}^{(p)}$, (5.14), and also (2.31), we may derive the following relations:

$$(\pi_\lambda \otimes \mathrm{id}^{\otimes N})\Delta'^{(N+1)}(\tilde{\mathcal{Q}}_{ab}^{(p)})\mathcal{T}(\lambda) = \mathcal{T}(\lambda)(\pi_{-\lambda} \otimes \mathrm{id}^{\otimes N})\Delta'^{(N+1)}(\tilde{\mathcal{Q}}_{ab}^{(p)}), \tag{5.15}$$

which hold for the general gl(n) case. The derivation of the representations (5.7) and the intertwining relations (5.11) and (5.15) are also among the main results of this paper. The latter relations (5.15) in particular are of great significance as we shall see below, because they facilitate the study of the exact symmetry of the open spin chain.

Before we continue with the investigation of the symmetry it will be instructive to write explicitly the following coproducts, which are valid for the gl(n) case [see also (2.10), (3.5), (5.2), (5.3), and (5.5)]:

$$(\pi_\lambda \otimes \mathrm{id}^{\otimes N})\Delta^{(N+1)}(\tilde{\mathcal{Q}}_{ab}^{(0)}) = \pi_\lambda(\tilde{\mathcal{Q}}_{ab}^{(0)}) \otimes \mathbb{I} + \mathbb{I} \otimes \tilde{Q}_{ab}^{(0)},$$

$$(\pi_\lambda \otimes \mathrm{id}^{\otimes N})\Delta^{(N+1)}(\tilde{\mathcal{Q}}_{ab}^{(1)}) = \pi_\lambda(\tilde{\mathcal{Q}}_{ab}^{(1)}) \otimes \mathbb{I} + \mathbb{I} \otimes \tilde{Q}_{ab}^{(1)} - \frac{(k^*)_{cd}^{-1}}{2}(\pi_\lambda(\tilde{\mathcal{Q}}_{ac}^{(0)}) \otimes \tilde{Q}_{db}^{(0)-} - \pi_\lambda(\tilde{\mathcal{Q}}_{db}^{(0)}) \otimes \tilde{Q}_{ac}^{(0)-}),$$

$$(\pi_\lambda \otimes \mathrm{id}^{\otimes N})\Delta'^{(N+1)}(\tilde{\mathcal{Q}}_{ab}^{(1)}) = \pi_\lambda(\tilde{\mathcal{Q}}_{ab}^{(1)}) \otimes \mathbb{I} + \mathbb{I} \otimes \tilde{Q}_{ab}^{(1)} + \frac{(k^*)_{cd}^{-1}}{2}(\pi_\lambda(\tilde{\mathcal{Q}}_{ac}^{(0)-}) \otimes \tilde{Q}_{db}^{(0)} - \pi_\lambda(\tilde{\mathcal{Q}}_{db}^{(0)-}) \otimes \tilde{Q}_{ac}^{(0)}), \tag{5.16}$$

where

$$\tilde{Q}_{ab}^{(0)-} = \Delta^{(N)}(\tilde{\mathcal{Q}}_{ab}^{(0)-}). \tag{5.17}$$

The crucial point is that Eqs. (5.15) bear algebraic relations between the entries of the operator $\mathcal{T}$ and the boundary nonlocal charges (4.11). For simplicity we use the XXX (gl(2)) model to exhibit the symmetry of the open transfer matrix (2.33), although the following procedure may be easily generalized for the gl(n) case. Note that the gl(2) case is quite special, because the twisted Yangian coincides essentially with the boundary Yangian, recall that $R_{12}(\lambda) = \overline{R}_{12}(\lambda)$ (and $\mathcal{P} = \check{\mathcal{P}}$), nevertheless it provides an illuminating paradigm. Let

$$\mathcal{T}_0(\lambda) = \begin{pmatrix} \mathcal{A}_1 & \mathcal{B} \\ \mathcal{C} & \mathcal{A}_2 \end{pmatrix} \quad \text{and } t(\lambda) = \mathcal{A}_1 + \mathcal{A}_2 \tag{5.18}$$

then from the commutation relations (5.15) and also (5.1), (5.6), and (5.16) we obtain

$$[\tilde{Q}_{aa}^{(0)}, \mathcal{A}_1] = 2i\kappa(\mathcal{B} - \mathcal{C}), \quad [\tilde{Q}_{aa}^{(0)}, \mathcal{A}_2] = -2i\kappa(\mathcal{B} - \mathcal{C}), \quad a \in \{1,2\},$$

$$[\tilde{Q}_{ab}^{(0)}, \mathcal{A}_1] = [\tilde{Q}_{ab}^{(0)}, \mathcal{A}_2] = [\tilde{Q}_{ab}^{(0)}, \mathcal{B}] = [\tilde{Q}_{ab}^{(0)}, \mathcal{C}] = 0, \quad a \neq b,$$

$$[\tilde{Q}_{aa}^{(0)}, \mathcal{B}] = 2i\kappa(\mathcal{A}_1 - \mathcal{A}_2) + 2i\mathcal{B}, \quad [\tilde{Q}_{aa}^{(0)}, \mathcal{C}] = -2i\kappa(\mathcal{A}_1 - \mathcal{A}_2) - 2i\mathcal{C}, \tag{5.19}$$

and it follows that

$$[t(\lambda), \tilde{Q}_{ab}^{(0)}] = 0, \quad a,b \in \{1,2\}. \tag{5.20}$$

From the intertwining relations (5.15) and with the help of (5.19) it also follows that

$$[t(\lambda),\tilde{Q}_{11}^{(1)}]=-[t(\lambda),\tilde{Q}_{22}^{(1)}]=[t(\lambda),\kappa(\tilde{Q}_{12}^{(1)}+\tilde{Q}_{21}^{(1)})]=4\kappa i(\lambda+i)(\mathcal{B}-\mathcal{C}), \tag{5.21}$$

and consequently

$$[t(\lambda),\tilde{Q}_{11}^{(1)}+\tilde{Q}_{22}^{(1)}]=[t(\lambda),\kappa(\tilde{Q}_{12}^{(1)}+\tilde{Q}_{21}^{(1)})+(-)^a\tilde{Q}_{aa}^{(1)}]=0. \tag{5.22}$$

It should be pointed out that the combinations of nonlocal charges appearing in (5.22) are expressed solely in terms of $\tilde{Q}_{ab}^{(0)}$'s, which means that the only conserved charges entailed so far are the $\tilde{Q}_{ab}^{(0)}$'s. In fact the first combination is trivial, because $\tilde{Q}_{11}^{(1)}+\tilde{Q}_{22}^{(1)}\propto\mathbb{I}$, and it is also expected from the commutation relation (2.35) as $\lambda'\to\infty$. The existence of higher nontrivial conserved charges is an intriguing question that will be examined in detail elsewhere. It is clear that generalized commutation relations between the generators $\tilde{Q}_{ab}^{(p)}, a,b\in\{1,\ldots,n\}$ and the entries of the $\mathrm{gl}(n)\mathcal{T}$ matrix may be now deduced in an analogous, although technically more complicated way.

It is finally worth emphasizing that the general intertwining relations (5.15) and the discovered symmetry (5.20) and (5.22) are independent of the choice of representation on the quantum spaces, and therefore they are universal results. In the special case where the quantum spaces are mapped via the evaluation representation (5.6), and $\mathcal{L}\to R$ the relations (5.15), (5.16), (5.20), and (5.22) are of course still valid, but with $\mathrm{id}^{\otimes N}\to\pi_0^{\otimes N}$.

VI. DISCUSSION

Let us briefly review the main results of this investigation. The main objective of this work was the study of the remaining symmetries of rational integrable spin chains ($\mathrm{gl}(n)$) once nondiagonal integrable boundaries are implemented. We considered two types of boundary conditions known as soliton preserving and soliton nonpreserving. For both types of boundaries nonlocal charges (4.11) were derived explicitly by means of the study of the asymptotic behavior of the coproduct type solution of the reflection equation $\mathcal{T}$. The nonlocal charges (4.11) were simply coproducts of generators of the boundary or twisted Yangian (5.1) depending on the choice of boundary conditions (2.14). Furthermore, by using the intertwining relations (5.11) and (5.15) we were able to derive the symmetry of the open spin chain (5.20). Relations of the form (5.11) provide also an alternative way of finding solutions of the reflection equation (2.14) (see, e.g., Refs. 4 and 5), although there exist other effective algebraic techniques allowing the solution of the reflection equation (see, e.g., Ref. 34).

It should be finally emphasized that R matrices associated to, e.g., $\mathrm{o}(n)$, $\mathrm{sp}(n)$ algebras enjoy crossing symmetry, i.e., $R_{12}(\lambda)=\overline{R}_{12}(\lambda)$ (2.16), and therefore in this case the boundary Yangian coincides with the twisted Yangian (see also Refs. 29 and 35).

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A Weyl-covariant tensor calculus

Nicolas Boulanger[a)]
Université de Mons-Hainaut, Mécanique et Gravitation, 6, Avenue du Champ de Mars, 7000 Mons, Belgium

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On a (pseudo-) Riemannian manifold of dimension $n \geqslant 3$, the space of tensors which transform covariantly under Weyl rescalings of the metric is built. This construction is related to a Weyl-covariant operator $\mathcal{D}$ whose commutator $[\mathcal{D},\mathcal{D}]$ gives the conformally invariant Weyl tensor plus the Cotton tensor. So-called generalized connections and their transformation laws under diffeomorphisms and Weyl rescalings are also derived. These results are obtained by application of Becchi Rouet Stora Tyutin techniques. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1896381]

I. INTRODUCTION

Recently,[1] a purely algebraic method was used to solve the problem of constructing and classifying all the local scalar invariants of a conformal structure on a (pseudo-) Riemannian manifold of dimension $n=8$. The approach, however, is not confined to $n=8$, and one of the purposes of this paper is to explain the derivation of the so-called Weyl-covariant tensors, the building blocks of the local conformal invariants in arbitrary dimension $n \geqslant 3$.

In the context of local gauge field theory, the determination of quantities which are invariant under a given set of gauge transformations can be rephrased in terms of local Becchi Rouet Stora Tyutin (BRST) cohomology. Within the BRST framework, the gauge symmetry and its algebra are encoded in a single differential s.[2–5] Powerful techniques for the computation of BRST cohomologies are proposed in Ref. 6 (see also Ref. 7), that apply to a large class of gauge theories and relate the BRST cohomology to an underlying gauge covariant algebra. At the core of this analysis is a definition of tensor fields and connections on which an underlying gauge covariant algebra is realized. Such a characterization of tensor fields, connections and the corresponding transformation laws has the advantage that it is purely algebraic and does not invoke any concept in addition to the BRST cohomology itself.

In the present paper, we consider theories where the only classical field is the metric $g_{\mu\nu} = g_{\nu\mu}$ and the gauge symmetries are diffeomorphisms plus Weyl rescalings. Explicitly, the infinitesimal gauge transformations read

$$\delta g_{\mu\nu} = \mathcal{L}_\xi g_{\mu\nu} + \delta^W_\phi g_{\mu\nu} = \xi^\rho \partial_\rho g_{\mu\nu} + \partial_\mu \xi^\rho g_{\rho\nu} + \partial_\nu \xi^\rho g_{\mu\rho} + 2\phi g_{\mu\nu}. \tag{1}$$

Our aim is to construct the space $\mathcal{W}$ of tensors and generalized connections that transform covariantly with respect to diffeomorphisms and Weyl transformations. The latter property means that, under Weyl rescalings, the tensors belonging to $\mathcal{W}$ will make appear at most the first derivative $\partial_\mu \phi$ of the Weyl parameter ϕ, and no derivative $\partial_{\mu_1} \cdots \partial_{\mu_k} \phi$ with $k \geqslant 2$.

Knowing the space $\mathcal{W}$, we are able to define an operator $\mathcal{D}$ acting in $\mathcal{W}$ and such that $[\mathcal{D},\mathcal{D}] \sim C + \tilde{C}$, where C and $\tilde{C}$, respectively, denote the conformally invariant Weyl tensor and the Cotton tensor. The Weyl-covariant derivative $\mathcal{D}$ generates the whole space of tensor fields belonging to $\mathcal{W}$ by successive applications on C (and $\tilde{C}$ in $n=3$). The rule for the commutator $[\mathcal{D},\mathcal{D}]$ is

[a)]Chargé de recherches du FNRS (Belgium). Electronic mail: nicolas.boulanger@umh.ac.be

at the basis of the Weyl-covariant tensor calculus utilized in Ref. 1. Other useful relations are obtained which are nothing but the Jacobi identities for the underlying gauge covariant algebra alluded to before.

The generalized connections play no role in the construction of local Weyl invariants, but are of prime importance in many other issues, like for example in the determination of the counterterms, the consistent interactions and the conservation laws that a gauge theory admits. They are also relevant for the classification of the Weyl anomalies, the solutions of the Wess–Zumino consistency condition for a theory describing conformal massless matter fields in an external gravitational background.

II. BRST FORMULATION

A. Some definitions

As mentioned above, the derivation of the space $\mathcal{W}$ of Weyl-covariant tensors and generalized connections is purely algebraic and requires no dynamical information. As a consequence, all that we need is contained in Eq. (1) and the BRST differential s reduces to γ, the differential along the gauge orbits. We refer to Refs. 8 and 9 for more details on the BRST formalism as used throughout the present work. For an application of this formalism in the context of Weyl gravity, see Ref. 10.

A $\mathbb{Z}$-grading called *ghost number* is associated to the differential γ. The latter raises the ghost number by one unit and is decomposed according to the degree in the Weyl ghost (the fermionic field associated to the Weyl parameter), $\gamma=\gamma_0+\gamma_1$. The first part γ_0 contains the information about the diffeomorphisms. The second part, γ_1, corresponds to Weyl rescalings of the metric and increases the number of (possibly differentiated) Weyl ghosts by 1.

The action of γ on the fields Φ^A (including the ghosts) is given as follows:

$$\gamma_0 g_{\mu\nu}=\xi^\rho\partial_\rho g_{\mu\nu}+\partial_\mu\xi^\rho g_{\rho\nu}+\partial_\nu\xi^\rho g_{\mu\rho},\quad \gamma_1 g_{\mu\nu}=2\omega g_{\mu\nu}, \tag{2a}$$

$$\gamma_0\xi^\mu=\xi^\rho\partial_\rho\xi^\mu,\quad \gamma_0\omega=\xi^\rho\partial_\rho\omega,\quad \gamma_1\xi^\mu=0,\quad \gamma_1\omega=0. \tag{2b}$$

The field ω is the Weyl ghost, the anticommuting field associated to the Weyl parameter ϕ, while ξ^μ is the anticommuting diffeomorphisms ghost associated to the vector field ζ^μ of Eq. (1). By definition, the Grassmann-odd fields ω and ξ^μ have ghost number +1. The last equality of (2b) reflects the Abelian nature of the algebra of Weyl transformations. From the above equations and by using the fact that γ is an odd derivation, it is easy to check that γ is indeed a differential.

One unites the BRST differential γ and the total exterior derivative d into a single differential $\tilde{\gamma}=\gamma+d$. Then, the Wess–Zumino consistency condition and its descent are encapsulated in

$$\tilde{\gamma}\tilde{a}=0,\quad \tilde{a}\neq\tilde{\gamma}\tilde{b}+\text{constant} \tag{3}$$

for the local total forms $\tilde{a}$ and $\tilde{b}$ of total degrees $G=n+1$ and $G=n$.[6] Total local forms are by definition formal sums of local forms with different form degrees and ghost numbers, $\tilde{a}=\sum_{p=0}^{n}a_p^{G-p}$, where subscripts (respectively, superscripts) denote the form degree (respectively, the ghost number). A local p-form ω_p depends on the fields Φ^A and their derivatives up to some finite (but otherwise unspecified) order, which is denoted by $\omega_p=(1/p!)\mathrm{d}x^{\mu_1}\cdots\mathrm{d}x^{\mu_p}\,\omega_{\mu_1\cdots\mu_p}(x,[\Phi^A])$.

The relations (3) imply that $\tilde{a}$ is a nontrivial element of the cohomology group $H(\tilde{\gamma})$ in the algebra of total local forms. As shown in Ref. 6, the cohomology of γ in the space of local functionals (integrals of local n forms) is indeed locally isomorphic to the cohomology of $\tilde{\gamma}$ in the space of local total forms. In other words, the solutions a_n^g of the Wess–Zumino consistency condition

$$\gamma a_n^g+\mathrm{d}a_{n-1}^{g+1}=0,\quad a_n^g\neq\gamma b_n^{g-1}+\mathrm{d}b_{n-1}^g \tag{4}$$

correspond one-to-one (modulo trivial solutions) to the solutions $\tilde{a}$ of (3) at total degree $G=g+n$, $\mathrm{tot\,deg}(\tilde{a})=g+n$.

The solutions of (3) or (4) determine the general structure of the counterterms that an action admits, the possible gauge anomalies, the conserved currents, the consistent interactions, etc.[9] In the next sections and in the appendix, we determine the restricted space $\mathcal{W}$ of the space of total local forms in which these solutions naturally appear, for a gravity theory invariant under the transformations (1).

We close this section with some more definitions and conventions. The conformally invariant Weyl tensor $C^{\beta}{}_{\gamma\delta\varepsilon}$, the tensor $K_{\alpha\beta}$ and the Cotton tensor $\widetilde{C}_{\alpha\mu\nu}$ are given by

$$C^{\alpha}{}_{\beta\gamma\delta} := R^{\alpha}{}_{\beta\gamma\delta} - 2(\delta^{\alpha}_{[\gamma} K_{\delta]\beta} - g_{\beta[\gamma} K_{\delta]}{}^{\alpha}), \tag{5a}$$

$$K_{\alpha\beta} := \frac{1}{n-2}\left(R_{\alpha\beta} - \frac{1}{2(n-1)} g_{\alpha\beta} R\right), \tag{5b}$$

$$\widetilde{C}_{\alpha\mu\nu} := \tfrac{1}{2}\nabla_{[\nu} K_{\mu]\alpha}. \tag{5c}$$

The Ricci tensor is $R_{\beta\delta}=R^{\alpha}{}_{\beta\alpha\delta}$, where $R^{\alpha}{}_{\beta\gamma\delta}=(\partial_{\gamma}\Gamma_{\beta\delta}{}^{\alpha}+\Gamma_{\gamma\lambda}{}^{\alpha}\Gamma_{\beta\delta}{}^{\lambda})-(\gamma\leftrightarrow\delta)$ is the Riemann tensor. The Christoffel symbols are given by $\Gamma_{\alpha\beta}{}^{\gamma}=\frac{1}{2}g^{\gamma\lambda}(\partial_{\alpha}g_{\beta\lambda}+\partial_{\beta}g_{\alpha\lambda}-\partial_{\lambda}g_{\alpha\beta})$. Curved brackets denote strength-one complete symmetrization, whereas square brackets denote strength-one complete antisymmetrization. We have $\nabla_{\mu}g_{\alpha\beta}=0$, where the symbol ∇ denotes the usual torsion-free covariant derivative associated to $\Gamma_{\alpha\beta}{}^{\gamma}$. Finally, the derivative $\partial_{\alpha}\omega$ of the Weyl ghost will sometimes be noted $\omega_{\alpha}\equiv\partial_{\alpha}\omega$.

B. Contracting homotopy

A well-known technique in the study of cohomologies is the use of contracting homotopies. The idea is to construct contracting homotopy operators which allow to eliminate certain local jet coordinates, called *trivial pairs*, from the cohomological analysis. This reduces the cohomological problem to an analogous one involving only the remaining jet coordinates. For that purpose one needs to construct suitable sets of jets coordinates replacing the fields, the ghosts and all their derivatives and satisfying appropriate requirements.

The following lemma is at the basis of the contracting homotopy techniques. We use the notations of Ref. 6 to which we refer for more details.

Lemma 1. Suppose there is a set of local jet coordinates,

$$\mathcal{B}=\{\mathcal{U}^{\ell},\mathcal{V}^{\ell},\mathcal{W}^{\Lambda}\},$$

such that the change of coordinates from $\mathcal{J}=\{[\Phi^{A}],x^{\mu},\mathrm{d}x^{\mu}\}$ *to* $\mathcal{B}$ *is local and locally invertible and*

$$\tilde{\gamma}\mathcal{U}^{\ell}=\mathcal{V}^{\ell}\ \forall\ \ell, \tag{6a}$$

$$\tilde{\gamma}\mathcal{W}^{\Lambda}=\mathcal{R}^{\Lambda}(\mathcal{W})\ \forall\ \Lambda. \tag{6b}$$

Then, locally the $\mathcal{U}$*'s and* $\mathcal{V}$*'s can be eliminated from the* $\tilde{\gamma}$*-cohomology, i.e., the latter reduces locally to the* $\tilde{\gamma}$*-cohomology on total local forms depending only on the* $\mathcal{W}$*'s.*

Note that both (6a) and (6b) must hold in order to eliminate the $\mathcal{U}$'s and $\mathcal{V}$'s from the cohomology. It is important to stress that the existence of a pair of jet coordinates satisfying (6a) does in general *not* guarantee the existence of complementary $\mathcal{W}$'s satisfying (6b). Clearly, the aim is to construct a set of local jet coordinates containing as many trivial pairs as possible. The difficulty of this construction is in general *not* the finding of pairs satisfying (6a), but the construction of complementary $\mathcal{W}$'s satisfying (6b). There is no general rule to deal with the latter, nontrivial problem.

To our knowledge, the $\mathcal{U}$-$\mathcal{V}$-$\mathcal{W}$ decomposition had never been done in the context of Weyl gravity theories in arbitrary dimension $n \geqslant 3$. Here, we fill this gap and compactly summarize our main results in the following proposition.

Proposition 1: Let $\mathcal{J}$ be the jet space $\mathcal{J}=\{[g_{\mu\nu}],[\omega],[\xi^\mu],x^\mu,\mathrm{d}x^\mu\}$ and $\tilde{\gamma}=\gamma_0+\gamma_1+d$ the differential acting on $\mathcal{J}$ according to

$$\gamma_0 g_{\mu\nu} = \xi^\rho \partial_\rho g_{\mu\nu} + \partial_\mu \xi^\rho g_{\rho\nu} + \partial_\nu \xi^\rho g_{\mu\rho}, \quad \gamma_1 g_{\mu\nu} = 2\omega g_{\mu\nu},$$
$$\gamma_0 \xi^\mu = \xi^\rho \partial_\rho \xi^\mu, \quad \gamma_0 \omega = \xi^\rho \partial_\rho \omega, \quad \gamma_1 \xi^\mu = 0, \quad \gamma_1 \omega = 0. \tag{7}$$

Then, the $\{\mathcal{U},\mathcal{V},\mathcal{W}\}$-decomposition of $\mathcal{J}$ corresponding to $\tilde{\gamma}$ is

$$\{\mathcal{U}^\ell\} = \{x^\mu, \partial_{(\mu_1\cdots\mu_k} \Gamma^{\nu}{}_{\mu_{k+1}\mu_{k+2})}, \nabla_{(\mu_1\cdots\mu_k} K_{\mu_{k+1}\mu_{k+2})}, k \in \mathbb{N}\},$$

$$\{\mathcal{V}^\ell\} = \{\tilde{\gamma}\mathcal{U}^\ell\}, \quad \{\mathcal{W}^\Lambda\} = \{\mathcal{T}^i, \tilde{C}^N\},$$

$$\{\mathcal{T}^i\} = \{g_{\mu\nu}, \mathcal{D}_{(\mu_1} \cdots \mathcal{D}_{\mu_k} C^\beta{}_{\gamma\delta)\varepsilon}, k \in \mathbb{N}\}, \tag{8a}$$

$$\{\tilde{C}^N\} = \{2\omega, \tilde{\xi}^\nu, \tilde{C}_\nu{}^\rho, \tilde{\omega}_\alpha\}, \tag{8b}$$

$$\tilde{\xi}^\nu := \xi^\nu + \mathrm{d}x^\nu, \quad \tilde{C}_\nu{}^\rho := \partial_\nu \xi^\rho + \tilde{\xi}^\alpha \Gamma_{\alpha\nu}{}^\rho, \quad \tilde{\omega}_\alpha := \omega_\alpha - \tilde{\xi}^\beta K_{\alpha\beta}.$$

The rest of the paper contains the definition of the operator $\mathcal{D}$ together with the $\tilde{\gamma}$-transformation rules for the elements of $\mathcal{W}$. A remark will also be made for the case $n=3$. In order to derive the results of Proposition 1, we used the fact that every function of the Riemann tensor and its covariant derivatives can be written as a function of the Weyl tensor, its covariant derivatives and the completely symmetric tensors $\nabla_{(\lambda_1\lambda_2\cdots\lambda_k} K_{\alpha\beta)}$. A proof of the latter statement can be found in the appendix of Ref. 1. The same proof can be used to show that, in $n=3$, every function of the Ricci tensor and its covariant derivatives can be written as a function of the Cotton tensor, its covariant derivatives and the completely symmetric tensors $\nabla_{(\lambda_1\lambda_2\cdots\lambda_k} K_{\alpha\beta)}$.

It is understood that only the algebraically independent components of $g_{\mu\nu}$ and $C^\beta{}_{\gamma\delta\varepsilon}$ enter into (8a). [Together with the symmetrization of the indices in (8a), this guarantees the absence of algebraic identities between the generators $\mathcal{T}^i$, taking into account the second equation of (13c) and the Bianchi identity (14b).]

The tensor fields $\{\mathcal{T}^i\}$ have total degree zero whereas the generalized connections $\{\tilde{C}^N\}$ have total degree 1. They decompose into two parts, the first of ghost number 1 and form degree zero, the second of ghost number zero and form degree 1,

$$\mathrm{tot\,deg}(\mathcal{T}^i) = 0, \quad \mathrm{tot\,deg}(\tilde{C}^N) = 1, \quad \tilde{C}^N = \hat{C}^N + \mathcal{A}^N,$$

$$\mathrm{gh}(\hat{C}^N) = 1 = \mathrm{form\,deg}(\mathcal{A}^N), \quad \mathrm{gh}(\mathcal{A}^N) = 0 = \mathrm{form\,deg}(\hat{C}^N),$$

where, from (8b),

$$\{\hat{C}^N\} = \{2\omega, \xi^\nu, \hat{C}_\nu{}^\rho := \partial_\nu \xi^\rho + \xi^\alpha \Gamma_{\alpha\nu}{}^\rho, \hat{\omega}_\alpha := \omega_\alpha - \xi^\mu K_{\mu\alpha}\}, \tag{9a}$$

$$\{\mathcal{A}^N\} = \{0, \mathrm{d}x^\mu\, \delta_\mu^\nu, \mathrm{d}x^\mu\, \Gamma_{\mu\nu}{}^\rho, -\mathrm{d}x^\mu\, K_{\mu\alpha}\}. \tag{9b}$$

The $\mathcal{A}^N$'s and $\hat{C}^N$'s are called, respectively, connection 1-forms and covariant ghosts.[6] Since $\tilde{\gamma}$ raises the total degree by one unit, we have

$$\tilde{\gamma}\mathcal{T}^i = \tilde{C}^N \Delta_N \mathcal{T}^i \Leftrightarrow \begin{cases} \gamma\mathcal{T}^i = \hat{C}^N \Delta_N \mathcal{T}^i, \\ d\mathcal{T}^i = \mathcal{A}^N \Delta_N \mathcal{T}^i, \end{cases} \tag{10a}$$

$$\{\Delta_N\} = \{\Delta, \mathcal{D}_\nu, \Delta_\rho{}^\nu, \mathbf{\Gamma}^\alpha\}. \tag{10b}$$

C. BRST covariant algebra for Weyl gravity

The Weyl-covariant derivative $\mathcal{D}$ is given by

$$\mathcal{D}_\mu := \partial_\mu - \Gamma_{\mu\nu}{}^\rho \Delta_\rho{}^\nu + K_{\mu\alpha}\mathbf{\Gamma}^\alpha. \tag{11}$$

The aim of this section is to make precise the above definition by explicitly defining the three operators $\{\Delta, \Delta_\rho{}^\nu, \mathbf{\Gamma}^\alpha\}$ introduced in (10). An underlying gauge covariant algebra will be exhibited, which provides a compact formulation of the BRST algebra on tensor fields and generalized connections.

(1) The operator Δ corresponds to the dimension operator. It counts the number of metrics that explicitly appear in a given expression,

$$\Delta := g_{\mu\nu}\frac{\partial^{\text{expl}}}{\partial g_{\mu\nu}}.$$

For example, $\Delta(g^{\gamma\mu_2}g^{\lambda\mu_1}\mathcal{D}_{\mu_1}C^\beta{}_{\gamma\delta\varepsilon}) = -2(g^{\gamma\mu_2}g^{\lambda\mu_1}\mathcal{D}_{\mu_1}C^\beta{}_{\gamma\delta\varepsilon})$ and $\Delta(g_{\alpha\beta}g^{\gamma\delta}) = 0$. As a consequence of (10a), (10b), and (9a), we can write $\gamma_1\sqrt{|g|} = 2\omega\Delta\sqrt{|g|} = 2\omega[(n/2)\sqrt{|g|}] = n\omega\sqrt{|g|}$, where $|g|$ denotes the absolute value of the determinant of $g_{\mu\nu}$ (supposed invertible).

(2) The operator $\Delta_\mu{}^\rho$ generates GL(n)-transformations of world indices according to

$$\Delta_\mu{}^\nu T^\beta_\alpha = \delta^\nu_\alpha T^\beta_\mu - \delta^\beta_\mu T^\nu_\alpha,$$

where T^β_α is a (1,1)-type tensor under GL(n) transformations. The usual torsion-free covariant derivative can thus be written $\nabla_\mu = \partial_\mu - \Gamma_{\mu\nu}{}^\rho \Delta_\rho{}^\nu$. Note that this expression must be completed by $p\Gamma_{\mu\alpha}{}^\alpha$ if one takes the covariant derivative ∇_μ of a weight-p tensor density, so $\nabla = \mathrm{d}x^\mu \nabla_\mu = \mathrm{d}x^\mu \partial_\mu - \tilde{C}_\nu{}^\rho \Delta_\rho{}^\nu + p\tilde{C}_\mu{}^\mu$.

(3) In order to conveniently define the action of the generator $\mathbf{\Gamma}^\alpha$, we first define the so-called W-tensors carrying superindices Ω_k,

$$W_{\Omega_0} := C^\beta{}_{\gamma\delta\varepsilon}, \quad W_{\Omega_1} := \mathcal{D}_{\alpha_1} C^\beta{}_{\gamma\delta\varepsilon}, \ \dots,$$

$$W_{\Omega_k} := \mathcal{D}_{\alpha_k}\mathcal{D}_{\alpha_{k-1}} \cdots \mathcal{D}_{\alpha_2}\mathcal{D}_{\alpha_1} C^\beta{}_{\gamma\delta\varepsilon}.$$

Then, we can write $\{\mathcal{T}^i\} \subset \{g_{\mu\nu}, \{W_{\Omega_k}\} : k = 0, 1, \dots\}$ and the operator $\mathbf{\Gamma}^\alpha$ acts on space of the W-tensors according to

$$\mathbf{\Gamma}^\alpha W_{\Omega_j} = [T^\alpha]_{\Omega_j}{}^{\Omega_{j-1}} W_{\Omega_{j-1}}, \quad \mathbf{\Gamma}^\alpha := [T^\alpha]_{\Omega_i}{}^{\Omega_{i-1}} \Delta_{\Omega_{i-1}}{}^{\Omega_i}, \tag{12}$$

where $\Delta_{\Omega_j}{}^{\Omega_k} W_{\Omega_i} = \delta^{\Omega_k}_{\Omega_i} W_{\Omega_j}$ and where the symbol $\delta^{\Omega_k}_{\Omega_i}$ is such that $\delta^{\Omega_k}_{\Omega_i} W_{\Omega_k} = W_{\Omega_i}$. We use Einstein's summation conventions for the W-tensor superindices Ω_i. The matrices $[T^\alpha]_{\Omega_j}{}^{\Omega_{j-1}}$ are obtained by recursion in the appendix, with $[T^\alpha]_{\Omega_j}{}^{\Omega_{j-1}} = 0 \ \forall j \leqslant 0$. The action of $\mathbf{\Gamma}^\alpha$ gives zero on everything but the W tensors. In particular, $\mathbf{\Gamma}^\alpha g_{\mu\nu} = 0$.

The W-tensors transform under $\tilde{\gamma}$ according to (10) and (9). They are the building blocks for the construction of Weyl invariants.[1] Note that the Bach tensor is nothing but the following double trace of W_{Ω_2}:

$$B_{\mu\nu} \equiv \nabla^{\alpha}\tilde{C}_{\mu\nu\alpha} - K^{\lambda\rho}C_{\lambda\mu\nu} = \frac{1}{(3-n)}g^{\alpha\rho}\mathcal{D}_{\alpha}\mathcal{D}_{\beta}C^{\beta}{}_{\mu\nu\rho}.$$

For the action of $\tilde{\gamma}$ on the generalized connections, we find

$$\tilde{\gamma}\omega = \tilde{\xi}^{\mu}\tilde{\omega}_{\mu},$$

$$\tilde{\gamma}\tilde{\xi}^{\mu} = \tilde{\xi}^{\rho}\tilde{C}_{\rho}{}^{\mu},$$

$$\tilde{\gamma}\tilde{C}_{\mu}{}^{\nu} = \tilde{C}_{\mu}{}^{\alpha}\tilde{C}_{\alpha}{}^{\nu} + \tfrac{1}{2}\tilde{\xi}^{\rho}\tilde{\xi}^{\sigma}C^{\nu}{}_{\mu\rho\sigma} + \mathcal{P}^{\alpha\nu}_{\mu\beta}\tilde{\omega}_{\alpha}\tilde{\xi}^{\beta},$$

$$\tilde{\gamma}\tilde{\omega}_{\alpha} = \tfrac{1}{2}\tilde{\xi}^{\rho}\tilde{\xi}^{\sigma}\tilde{C}_{\alpha\rho\sigma} + \tilde{C}_{\alpha}{}^{\beta}\tilde{\omega}_{\beta},$$

where $\mathcal{P}^{\alpha\nu}_{\mu\beta} := (-g^{\alpha\nu}g_{\mu\beta} + \delta^{\alpha}_{\mu}\delta^{\nu}_{\beta} + \delta^{\alpha}_{\beta}\delta^{\nu}_{\mu})$. Note the relations $C^{\mu}{}_{\nu\alpha\beta} = R^{\mu}{}_{\nu\alpha\beta} - 2\mathcal{P}^{\mu\rho}_{\nu[\alpha}K_{\beta]\rho}$ and $\gamma_1\Gamma_{\mu\beta}{}^{\nu} = \mathcal{P}^{\alpha\nu}_{\mu\beta}\omega_{\alpha}$.

From $\tilde{\gamma}^2\mathcal{T}^i = 0$, we derive the gauge covariant algebra generated by $\{\Delta, \mathcal{D}_{\nu}, \Delta_{\rho}{}^{\nu}, \mathbf{\Gamma}^{\alpha}\}$,

$$[\Delta_{\nu}{}^{\rho}, \mathbf{\Gamma}^{\alpha}] = -\delta^{\alpha}_{\nu}\mathbf{\Gamma}^{\rho}, \quad [\mathbf{\Gamma}^{\alpha}, \mathbf{\Gamma}^{\beta}] = 0, \tag{13a}$$

$$[\Delta_{\nu}{}^{\rho}, \mathcal{D}_{\mu}] = \delta^{\rho}_{\mu}\mathcal{D}_{\nu}, \quad [\Delta_{\mu}{}^{\rho}, \Delta_{\nu}{}^{\sigma}] = \delta^{\rho}_{\nu}\Delta_{\mu}{}^{\sigma} - \delta^{\rho}_{\nu}\Delta_{\mu}{}^{\sigma}, \tag{13b}$$

$$[\mathbf{\Gamma}^{\alpha}, \mathcal{D}_{\beta}] = -\mathcal{P}^{\alpha\nu}_{\mu\beta}\Delta_{\nu}{}^{\mu}, \quad [\mathcal{D}_{\mu}, \mathcal{D}_{\nu}] = C_{\mu\nu\rho}{}^{\sigma}\Delta_{\sigma}{}^{\rho} - \tilde{C}_{\alpha\mu\nu}\mathbf{\Gamma}^{\alpha}, \tag{13c}$$

where the operator Δ commutes with everything. The second equality of (13a) reflects the Abelian nature of the Weyl transformations, while the second equality of (13c) displays the commutator of two Weyl-covariant derivatives in terms of the Weyl tensor and the Cotton tensor. Note that the commutator of two covariant derivatives reads $[\nabla_{\mu}, \nabla_{\nu}] = R_{\mu\nu\rho}{}^{\sigma}\Delta_{\sigma}{}^{\rho}$.

From $\tilde{\gamma}^2\tilde{C}^N = 0$, we find the following set of Bianchi identities:

$$\tilde{\gamma}^2\omega = 0 \Rightarrow \tilde{C}_{[\mu\rho\sigma]} = 0, \tag{14a}$$

$$\tilde{\gamma}^2\tilde{C}_{\mu}{}^{\nu} = 0 \Rightarrow \nabla_{[\gamma}C_{\delta\varepsilon]\alpha\beta} - \tilde{C}_{\alpha[\gamma\delta}g_{\varepsilon]\beta} + \tilde{C}_{\beta[\gamma\delta}g_{\varepsilon]\alpha} = 0, \tag{14b}$$

$$\tilde{\gamma}^2\tilde{\xi}^{\mu} = 0 \Rightarrow \begin{cases} \mathcal{P}^{\alpha\mu}_{[\rho\nu]} = 0, \\ C^{\mu}{}_{[\nu\rho\sigma]} = 0, \end{cases} \tag{14c}$$

$$\tilde{\gamma}^2\tilde{\omega}_{\alpha} = 0 \Rightarrow \begin{cases} \mathbf{\Gamma}^{\alpha}\tilde{C}_{\beta\rho\sigma} + C^{\alpha}{}_{\beta\rho\sigma} = 0, \\ \mathcal{D}_{[\beta}\tilde{C}_{\rho\sigma]\alpha} = 0 \end{cases} \tag{14d}$$

which are nothing but the Jacobi identities for the algebra (13).

Note that the case $n=3$ proceeds in exactly the same way, provided one sets $C^{\mu}{}_{\nu\rho\sigma}$ to zero and one defines $W^{(3)}_{\Omega_0} := \tilde{C}_{\alpha\rho\sigma}$. In other words, the relations (13) and (14) still hold, setting $C^{\mu}{}_{\nu\rho\sigma} = 0$. The representation matrices $\mathbf{\Gamma}^{\alpha}$ and the Weyl-covariant derivative (11) are unchanged as well. More explicitly, we have

$$n \geqslant 4, \quad \gamma_1\mathcal{D}_{\alpha_1}C^{\beta}{}_{\gamma\delta\varepsilon} = \omega_{\alpha}(-\mathcal{P}^{\alpha\nu}_{\mu\alpha_1}\Delta_{\nu}{}^{\mu})C^{\beta}{}_{\gamma\delta\varepsilon} \rightsquigarrow \gamma_1 W_{\Omega_1} = \omega_{\alpha}\mathbf{\Gamma}^{\alpha}W_{\Omega_1},$$

$$n=3, \quad \gamma_1 \mathcal{D}_{\alpha_1} \widetilde{C}_{\gamma\delta\varepsilon} = \omega_\alpha (-\mathcal{P}^{\alpha\nu}_{\mu\alpha_1} \Delta_\nu{}^\mu) \widetilde{C}_{\gamma\delta\varepsilon} \rightsquigarrow \gamma_1 W^{(3)}_{\Omega_1} = \omega_\alpha \mathbf{\Gamma}^\alpha_{(3)} W^{(3)}_{\Omega_1},$$

which shows that the representation matrices $\mathbf{\Gamma}^\alpha$ and $\mathbf{\Gamma}^\alpha_{(3)}$ are essentially the same. Indeed, the iterative procedure given in the appendix reproduces itself in exactly the same way when $n=3$, with the convention that $W^{(3)}_{\Omega_0} \equiv \widetilde{C}_{\alpha\rho\sigma}$.

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APPENDIX: *W*-TENSORS AND THEIR TRANSFORMATIONS

The *W*-tensors are computed iteratively, together with their transformation laws under Weyl rescalings of the metric.

(A) First, we have $\gamma_1 W_{\Omega_0} = \omega_\alpha \mathbf{\Gamma}^\alpha W_{\Omega_0} = 0$. Then, we form $W_{\Omega_1} = \nabla_{\alpha_1} W_{\Omega_0}$. Taking the Weyl variation gives

$$\gamma_1 W_{\Omega_1} = \gamma_1 [(\partial_{\alpha_1} - \Gamma_{\alpha_1\mu}{}^\nu \Delta_\nu{}^\mu) W_{\Omega_0}] = -\omega_\lambda \mathcal{P}^{\lambda\nu}_{\mu\alpha_1} \Delta_\nu{}^\mu W_{\Omega_0} = \omega_\lambda [T^\lambda]_{\Omega_1}{}^{\Omega_0} W_{\Omega_0},$$

where the last equality serves as a definition for the tensor $[T^\lambda]_{\Omega_1}{}^{\Omega_0}$, which satisfies $\gamma_1 [T^\lambda]_{\Omega_1}{}^{\Omega_0} = 0 = \nabla_\mu [T^\lambda]_{\Omega_1}{}^{\Omega_0}$. We also use the notation $\gamma_1 W_{\Omega_1} = \omega_\alpha \mathbf{\Gamma}^\alpha W_{\Omega_0}$, cf. Eq. (12).

Continuing, we compute the Weyl variation of $\nabla_{\alpha_2} W_{\Omega_1}$,

$$\begin{aligned}\gamma_1 \nabla_{\alpha_2} W_{\Omega_1} &= \nabla_{\alpha_2} (\omega_\lambda [T^\lambda]_{\Omega_1}{}^{\Omega_0} W_{\Omega_0}) - \omega_\lambda \mathcal{P}^{\lambda\nu}_{\mu\alpha_2} \Delta_\nu{}^\mu W_{\Omega_1} \\ &= (-\gamma_1 K_{\lambda\alpha_2}) [T^\lambda]_{\Omega_1}{}^{\Omega_0} W_{\Omega_0} + \omega_\lambda [T^\lambda]_{\Omega_1}{}^{\Omega_0} \nabla_{\alpha_2} W_{\Omega_0} - \omega_\lambda \mathcal{P}^{\lambda\nu}_{\mu\alpha_2} \Delta_\nu{}^\mu W_{\Omega_1}.\end{aligned}$$

Using $\gamma_1([T^\lambda]_{\Omega_1}{}^{\Omega_0} W_{\Omega_0}) = 0$, we obtain

$$\gamma_1 (\nabla_{\alpha_2} W_{\Omega_1} + K_{\lambda\alpha_2} [T^\lambda]_{\Omega_1}{}^{\Omega_0} W_{\Omega_0}) = \omega_\lambda (\delta^{\Omega'}_{\alpha_2\Omega_0}{}^1 [T^\lambda]_{\Omega_1}{}^{\Omega_0} - \delta^{\Omega'}_{\Omega_1}{}^1 \mathcal{P}^{\lambda\nu}_{\mu\alpha_2} \Delta_\nu{}^\mu) W_{\Omega'_1}$$

which we rewrite

$$\gamma_1 W_{\Omega_2} = \omega_\lambda [T^\lambda]_{\Omega_2}{}^{\Omega_1} W_{\Omega_1} = \omega_\alpha \mathbf{\Gamma}^\alpha W_{\Omega_2},$$

where $W_{\Omega_2} \equiv \mathcal{D}_{\alpha_2} W_{\Omega_1} = \nabla_{\alpha_2} W_{\Omega_1} + K_{\lambda\alpha_2} [T^\lambda]_{\Omega_1}{}^{\Omega_0} W_{\Omega_0}$.

Calculating $\gamma_1 \gamma_1 W_{\Omega_2}$, we find $0 = \omega_\alpha \omega_\beta \mathbf{\Gamma}^\alpha \mathbf{\Gamma}^\beta W_{\Omega_2}$, or $[\mathbf{\Gamma}^\alpha, \mathbf{\Gamma}^\beta] = 0$, cf. second equation of (13a). Also, since

$$W_{\Omega_2} \equiv \mathcal{D}_{\alpha_2} W_{\Omega_1} \equiv \mathcal{D}_{\alpha_2} \mathcal{D}_{\alpha_1} W_{\Omega_0} = (\nabla_{\alpha_2} \nabla_{\alpha_1} + K_{\lambda\alpha_2} [T^\lambda]_{\Omega_1}{}^{\Omega_0}) W_{\Omega_0},$$

we find that

$$[\mathcal{D}_{\alpha_2}, \mathcal{D}_{\alpha_1}] W_{\Omega_0} = C_{\alpha_2\alpha_1\mu}{}^\nu \Delta_\nu{}^\mu W_{\Omega_0},$$

in agreement with the second equation of (13c) and $\mathbf{\Gamma}^\alpha W_{\Omega_0} = 0$ (equivalent to $\gamma_1 W_{\Omega_0} = 0$).

(B) Suppose that we have $W_{\Omega_k} \equiv \mathcal{D}_{\alpha_k} \cdots \mathcal{D}_{\alpha_2} \mathcal{D}_{\alpha_1} W_{\Omega_0}$, $k \geqslant 2$. In other words, we know that

$$W_{\Omega_k} = (\nabla_{\alpha_k} + K_{\lambda\alpha_k} \mathbf{\Gamma}^\lambda) W_{\Omega_{k-1}},$$

$$\gamma_1 W_{\Omega_k} = \omega_\alpha \mathbf{\Gamma}^\alpha W_{\Omega_k} = \omega_\alpha [T^\alpha]_{\Omega_k}{}^{\Omega_{k-1}} W_{\Omega_{k-1}},$$

and

$$\mathbf{\Gamma}^{[\alpha}\,\mathbf{\Gamma}^{\beta]} W_{\Omega_k} = 0.$$

We want to obtain the next tensor, $W_{\Omega_{k+1}} \equiv \mathcal{D}_{\alpha_{k+1}} W_{\Omega_k}$, and its transformation rule.

As before, we first compute the Weyl transformation of $\nabla_{\alpha_{k+1}} W_{\Omega_k}$,

$$\begin{aligned}\gamma_1 \nabla_{\alpha_{k+1}} W_{\Omega_k} &= \nabla_{\alpha_{k+1}} (\omega_\alpha \mathbf{\Gamma}^\alpha W_{\Omega_k}) - \omega_\alpha \mathcal{P}^{\alpha\mu}_{\nu\alpha_{k+1}} \Delta_\mu{}^\nu W_{\Omega_k} \\ &= (-\gamma_1 K_{\alpha\alpha_{k+1}}) \mathbf{\Gamma}^\alpha W_{\Omega_k} + \omega_\alpha [T^\alpha]_{\Omega_k}{}^{\Omega_{k-1}} \nabla_{\alpha_{k+1}} W_{\Omega_{k-1}} - \omega_\alpha \mathcal{P}^{\alpha\mu}_{\nu\alpha_{k+1}} \Delta_\mu{}^\nu W_{\Omega_k}.\end{aligned}$$

Hence, we get

$$\gamma_1 (\nabla_{\alpha_{k+1}} W_{\Omega_k} + K_{\alpha\alpha_{k+1}} \mathbf{\Gamma}^\alpha W_{\Omega_k}) = K_{\alpha\alpha_{k+1}} \omega_\beta \mathbf{\Gamma}^\alpha \mathbf{\Gamma}^\beta W_{\Omega_k} - \omega_\alpha \mathcal{P}^{\alpha\mu}_{\nu\alpha_{k+1}} \Delta_\mu{}^\nu W_{\Omega_k} + \omega_\alpha [T^\alpha]_{\Omega_k}{}^{\Omega_{k-1}} \nabla_{\alpha_{k+1}} W_{\Omega_{k-1}}.$$

Using

$$\nabla_{\alpha_{k+1}} W_{\Omega_{k-1}} = \mathcal{D}_{\alpha_{k+1}} W_{\Omega_{k-1}} - K_{\beta\alpha_{k+1}} \mathbf{\Gamma}^\beta W_{\Omega_{k-1}}$$

and posing

$$\mathcal{D}_{\alpha_{k+1}} W_{\Omega_k} = \nabla_{\alpha_{k+1}} W_{\Omega_k} + K_{\alpha_{k+1}\lambda} \mathbf{\Gamma}^\lambda W_{\Omega_k},$$

we find

$$\begin{aligned}\gamma_1 \mathcal{D}_{\alpha_{k+1}} W_{\Omega_k} &= K_{\alpha\alpha_{k+1}} \omega_\beta \mathbf{\Gamma}^\alpha \mathbf{\Gamma}^\beta W_{\Omega_k} - K_{\beta\alpha_{k+1}} \omega_\alpha \mathbf{\Gamma}^\alpha \mathbf{\Gamma}^\beta W_{\Omega_k} - \omega_\alpha \mathcal{P}^{\alpha\mu}_{\nu\alpha_{k+1}} \Delta_\mu{}^\nu W_{\Omega_k} \\ &\quad + \omega_\alpha \delta^{\Omega'_k}_{\alpha_{k+1}\Omega_{k-1}} [T^\alpha]^{\Omega_{k-1}}_{\Omega_k} W_{\Omega'_k} \\ &= \omega_\lambda (\delta^{\Omega'_k}_{\alpha_{k+1}\Omega_{k-1}} [T^\alpha]^{\Omega_{k-1}}_{\Omega_k} - \delta^{\Omega'_k}_{\Omega_k} \mathcal{P}^{\lambda\mu}_{\nu\alpha_{k+1}} \Delta_\mu{}^\nu) W_{\Omega'_k} = \omega_\lambda [T^\alpha]^{\Omega'_k}_{\alpha_{k+1}\Omega_k} W_{\Omega'_k},\end{aligned}$$

where we used $\mathbf{\Gamma}^{[\alpha}\,\mathbf{\Gamma}^{\beta]} W_{\Omega_k} = 0$. □

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Second-order superintegrable systems in conformally flat spaces. I. Two-dimensional classical structure theory

E. G. Kalnins
Department of Mathematics and Statistics, University of Waikato, Hamilton, New Zealand

J. M. Kress[a)]
School of Mathematics, The University of New South Wales, Sydney NSW 2052, Australia

W. Miller, Jr.
School of Mathematics, University of Minnesota, Minneapolis, Minnesota 55455

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This paper is the first in a series that lays the groundwork for a structure and classification theory of second-order superintegrable systems, both classical and quantum, in conformally flat spaces. Many examples of such systems are known, and lists of possible systems have been determined for constant curvature spaces in two and three dimensions, as well as few other spaces. Observed features of these systems are multiseparability, closure of the quadratic algebra of second-order symmetries at order 6, use of representation theory of the quadratic algebra to derive spectral properties of the quantum Schrödinger operator, and a close relationship with exactly solvable and quasi-exactly solvable systems. Our approach is, rather than focus on particular spaces and systems, to use a general theoretical method based on integrability conditions to derive structure common to all systems. In this first paper we consider classical superintegrable systems on a general two-dimensional Riemannian manifold and uncover their common structure. We show that for superintegrable systems with nondegenerate potentials there exists a standard structure based on the algebra of 2×2 symmetric matrices, that such systems are necessarily multiseparable and that the quadratic algebra closes at level 6. Superintegrable systems with degenerate potentials are also analyzed. This is all done without making use of lists of systems, so that generalization to higher dimensions, where relatively few examples are known, is much easier. [DOI: 10.1063/1.1897183]

I. INTRODUCTION AND EXAMPLES

The goal of this series of papers is a structure and classification theory of second-order superintegrable systems, both classical and quantum, in conformally flat spaces. A classical superintegrable system $\mathcal{H}=\Sigma_{ij}g^{ij}p_ip_j+V(\mathbf{x})$ on an n-dimensional local Riemannian manifold is one that admits $2n-1$ functionally independent symmetries (i.e., constants of the motion) $\mathcal{S}_k$, $k=1,\ldots,2n-1$ with $\mathcal{S}_1=\mathcal{H}$. That is, $\{\mathcal{H},\mathcal{S}_k\}=0$ where

$$\{f,g\}=\sum_{j=1}^{n}(\partial_{x_j}f\partial_{p_j}g-\partial_{p_j}f\partial_{x_j}g))$$

is the Poisson bracket for functions $f(\mathbf{x},\mathbf{p}),g(\mathbf{x},\mathbf{p})$ on phase space.[1–8] Note that $2n-1$ is the maximum possible number of functionally independent symmetries and, locally, such symmetries always exist. The main interest is in symmetries that are polynomials in the p_k and are globally

[a)]Electronic mail: j.kress@unsw.edu.au

defined, except for lower dimensional singularities such as poles and branch points. Many tools in the theory of Hamiltonian systems have been brought to bear on superintegrable systems, such as R-matrix theory, Lax pairs, exact solvability, quasi-exact solvability, and the Jacobi metric.[9–13] However, the most detailed and complete results are obtained from separation of variables methods in those cases where they are applicable. Standard orthogonal separation of variables techniques are associated with second-order symmetries, e.g., Refs. 14–20 and multiseparable Hamiltonian systems provide numerous examples of superintegrability. In these papers we shall concentrate on second-order superintegrable systems, that is, those in which the symmetries take the form $\mathcal{S}=\Sigma a^{ij}(\mathbf{x})p_ip_j+W(\mathbf{x})$, quadratic in the momenta.

There is an analogous definition for second-order quantum superintegrable systems with Schrödinger operator

$$H=\Delta+V(\mathbf{x}),\quad \Delta=\frac{1}{\sqrt{g}}\sum_{ij}\partial_{x_i}(\sqrt{g}g^{ij})\partial_{x_j},$$

where Δ is the Laplace–Beltrami operator on a Riemannian manifold, expressed in local coordinates x_j.[15] Here there are $2n-1$ second-order symmetry operators

$$S_k=\frac{1}{\sqrt{g}}\sum_{ij}\partial_{x_i}(\sqrt{g}a^{ij}_{(k)})\partial_{x_j},\quad k=1,\ldots,2n-1$$

with $S_1=H$ and $[H,S_k]\equiv HS_k-S_kH=0$. Again multiseparable systems yield many examples of superintegrability. However, as we shall show, not all multiseparable systems are superintegrable and not all second-order superintegrable systems are multiseparable. There is also a quantization problem in extending the results for classical systems to operator systems. This problem turns out to be very easily solved in two dimensions and not difficult in higher dimensions for nondegenerate systems.

Superintegrable systems can (1) be solved explicitly, and (2) they can be solved in multiple ways. It is the information gleaned from comparing the distinct solutions and expressing one solution set in terms of another that is a primary reason for their interest.

To illustrate some of the main features of superintegrable systems we give a simple example in real Euclidean space. (To make clearer the connection with quantum theory and Hilbert space methods we shall, for this example alone, adopt standard physical normalizations, such as using the factor $-\frac{1}{2}$ in front of the free Hamiltonian.) Consider the Schrödinger eigenvalue equation $H\Psi=E\Psi$ or

$$-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\Psi+\frac{1}{2}\left(\omega^2(x^2+y^2)+\frac{k_1^2-\frac{1}{4}}{x^2}+\frac{k_2^2-\frac{1}{4}}{y^2}\right)\Psi=E\Psi. \tag{1}$$

This equation separates in three systems: *Cartesian* coordinates (x,y); *polar* coordinates $x=r\cos\theta$, $y=r\sin\theta$, and *elliptical* coordinates

$$x^2=c^2\frac{(u_1-e_1)(u_2-e_1)}{(e_1-e_2)},\quad y^2=c^2\frac{(u_1-e_2)(u_2-e_2)}{(e_2-e_1)}.$$

The bound states are degenerate with energies given by $E_n=\omega(2n+2+k_1+k_2)$ for integer n. The corresponding wave functions are (1) *Cartesian:*

$$\Psi_{n_1,n_2}(x,y)=2\omega^{(1/2)(k_1+k_2+2)}\sqrt{\frac{n_1!n_2!}{\Gamma(n_1+k_1+1)\Gamma(n_2+k_2+1)}}x^{(k_1+1/2)}y^{(k_2+1/2)}e^{-(\omega/2)(x^2+y^2)}L_{n_1}^{k_1}(\omega x^2)$$
$$\times L_{n_2}^{k_2}(\omega y^2),\quad n=n_1+n_2, \tag{2}$$

and the $L_n^k(x)$ are Laguerre polynomials.[21] (2) *Polar:*

$$\Psi(r,\theta)=\Phi_q^{(k_1,k_2)}(\theta)\omega^{(1/2)(2q+k_1+k_2+1)}\sqrt{\frac{2m!}{\Gamma(m+2q+k_1+k_2+1)}}e^{(-\omega r^2/2)}r^{(2q+k_1+k_2+1)}L_m^{2q+k_1+k_2+1}(\omega r^2),$$
$$n=m+q, \tag{3}$$

$$\Phi_q^{(k_1,k_2)}(\theta)=\sqrt{2(2q+k_1+k_2+1)\frac{q!\Gamma(k_1+k_2+q+1)}{\Gamma(k_2+q+1)\Gamma(k_1+q+1)}}(\cos\theta)^{k_1+(1/2)}(\sin\theta)^{k_2+(1/2)}P_q^{(k_1,k_2)}\times(\cos 2\theta), \tag{4}$$

and the $P_q^{(k_1,k_2)}(\cos 2\theta)$ are Jacobi polynomials.[21] (3) *Elliptical:*

$$\Psi=e^{-\omega(x^2+y^2)}x^{k_1+1/2}y^{k_2+1/2}\prod_{m=1}^{n}\left(\frac{x^2}{\theta_m-e_1}+\frac{y^2}{\theta_m-e_2}-c^2\right)$$

where

$$\frac{x^2}{\theta-e_1}+\frac{y^2}{\theta-e_2}-c^2=-c^2\frac{(u_1-\theta)(u_2-\theta)}{(\theta-e_1)(\theta-e_2)} \tag{5}$$

are ellipsoidal wave functions.[22,23] A basis for the second-order symmetry operators is

$$L_1=\partial_x^2+\frac{\left(\frac{1}{4}-k_1^2\right)}{x^2}-\omega^2x^2,\quad L_2=\partial_y^2+\frac{\left(\frac{1}{4}-k_2^2\right)}{y^2}-\omega^2y^2,$$
$$L_3=(x\partial_y-y\partial_x)^2+\left(\frac{1}{4}-k_1^2\right)\frac{y^2}{x^2}+\left(\frac{1}{4}-k_2^2\right)\frac{x^2}{y^2}-\frac{1}{2}. \tag{6}$$

(Note that $-2H=L_1+L_2$.) The separable solutions are eigenfunctions of the symmetry operators L_1, L_3 and $L_3+e_2L_1+e_1L_2$ with eigenvalues

$$\lambda_c=-\omega(2n_1+k_1+1),\quad \lambda_p=(2q+k_1+k_2+1)^2+(1+k_1^2+k_2^2),$$

$$\lambda_e=2(1-k_1)(1-k_2)-2e_2\omega(k_1+1)-2e_1\omega(k_2+1)-\omega^2e_1e_2-4\sum_{m=1}^{q}\left[e_2\frac{k_1+1}{\theta_m-e_1}+e_1\frac{k_2+1}{\theta_m-e_2}\right],$$

respectively. The algebra constructed by repeated commutators is

$$[L_1,L_3]=[L_3,L_2]\equiv R,\quad [L_i,R]=-4\{L_i,L_j\}+16\omega^2L_3,\quad i\neq j,\quad i,j=1,2,$$

$$[L_3,R]=4\{L_1,L_3\}-4\{L_2,L_3\}+8(1-k_2^2)L_1-8(1-k_1^2)L_2,$$

$$R^2=\tfrac{8}{3}\{L_1,L_2,L_3\}+\tfrac{64}{3}\{L_1,L_2\}+16\omega^2L_3^2-16(1-k_2^2)L_1^2-16(1-k_1^2)L_2^2-\tfrac{128}{3}\omega^2L_3-64\omega^2(1-k_1^2)(1-k_2^2). \tag{7}$$

Note that these relations are quadratic. Here $\{A,B\}=AB+BA$, is a double symmetrizer and there is a corresponding definition for the triple symmetrizer. The important fact to observe about the algebra generated by L_1,L_2,L_3, R is that it is *closed under commutation*.[24,25] This is a remarkable fact, but typical of superintegrable systems with nondegenerate potentials, as we shall show. Indeed the closure is at level 6, since we have to express the square of the third-order operator R

in terms of the L_j basis of second-order operators. Note that the degeneracy of the energy eigenspace is broken by the alternate separated bases of eigenfunctions. The eigenfunctions of one separable system can be expanded in terms of the eigenfunctions of another, and this is the source of nontrivial special function expansion theorems.[26] The symmetry operators are in formal self-adjoint form and suitable for spectral analysis. Also, the quadratic algebra identities allow us to relate eigenbases and eigenvalues of one symmetry operator to those of another. Indeed the representation theory of the abstract quadratic algebra can be used to derive spectral properties of the generators L_j, in a manner analogous to the use of Lie algebra representation theory to derive spectral properties of quantum systems that admit Lie symmetry algebras.[26–29] (Note however that for superintegrable systems with nondegenerate potential, there is no first-order Lie symmetry.)

A common feature of quantum superintegrable systems, exhibited in the above-given example, is that after splitting off a multiplicative functional factor, $x^{(k_1+1/2)}y^{(k_2+1/2)}e^{-(\omega/2)(x^2+y^2)}$ in the example, the Schrödinger and symmetry operators are acting on a space of polynomials.[30] This is closely related to the theory of exactly and quasi-exactly solvable systems.[11,31,32] In the example the one-dimensional ordinary differential equations (ODEs) obtained by separation in the Cartesian and polar systems are exactly solvable, in terms of hypergeometric functions, i.e., there is an infinite set of nested invariant subspaces under the Cartesian or polar separated ODEs, and the energy eigenvalues are easily obtained. The elliptic system separated equations are quasi-exactly solvable, i.e., there is a single invariant finite dimensional subspace of a separated ODE and only for certain parameter choices, and polynomial solutions are obtained for only particular values of E. However, these values are just the energy eigenvalues obtained in the Cartesian and polar systems. This characterization of quasi-exactly solvable systems as embedded in PDE superintegrable systems provides insight into the nature of these phenomena.

The classical analog of the above-given example is obtained by the replacements $\partial_x \to p_x$, $\partial_y \to p_y$. Commutators go over to Poisson brackets. The operator symmetries become second-order constants of the motion. Symmetrized operators become products of functions. The quadratic algebra relations simplify: the highest order terms agree with the operator case but there are fewer nonzero lower order terms. Indeed, the classical algebra has basis

$$\mathcal{S}_1 = p_x^2 + \frac{\frac{1}{4} - k_1^2}{x^2} - \omega^2 x^2, \quad \mathcal{S}_2 = p_y^2 + \frac{\frac{1}{4} - k_2^2}{y^2} - \omega^2 y^2,$$
$$\mathcal{S}_3 = (xp_y - yp_x)^2 + \left(\frac{1}{4} - k_1^2\right)\frac{y^2}{x^2} + \left(\frac{1}{4} - k_2^2\right)\frac{x^2}{y^2}, \quad -2\mathcal{H} = \mathcal{S}_1 + \mathcal{S}_2. \tag{8}$$

The classical quadratic algebra relations are

$$\{\mathcal{S}_1, \mathcal{S}_3\} = \{\mathcal{S}_3, \mathcal{S}_2\} \equiv \mathcal{R}, \quad \{\mathcal{S}_i, \mathcal{R}\} = 8\mathcal{S}_i\mathcal{S}_j + 16\omega^2\mathcal{S}_3, \quad i \neq j, \quad i,j = 1,2,$$
$$\{\mathcal{S}_3, \mathcal{R}\} = 8\mathcal{S}_1\mathcal{S}_3 - 8\mathcal{S}_2\mathcal{S}_3 + (4 - 16k_2^2)\mathcal{S}_1 - (4 - 16k_1^2)\mathcal{S}_2, \tag{9}$$
$$\mathcal{R}^2 = 16\mathcal{S}_1\mathcal{S}_2\mathcal{S}_3 - 16\omega^2\mathcal{S}_3^2 + (4 - 16k_2^2)\mathcal{S}_1^2 - (4 - 16k_1^2)\mathcal{S}_2^2 + 4\omega^2(1 - 4k_1^2)(1 - 4k_2^2).$$

In the example the potential

$$V(x,y) = \frac{1}{2}\left(\omega^2(x^2 + y^2) + \frac{k_1^2 - \frac{1}{4}}{x^2} + \frac{k_2^2 - \frac{1}{4}}{y^2}\right)$$

is *nondegenerate* in the sense that at any point x_0, y_0 where the potential is defined and analytic and the $\mathcal{S}_k$ are functionally independent, we can prescribe the values of $V_1(x_0,y_0), V_2(x_0,y_0), V_{11}(x_0,y_0)$ arbitrarily by choosing appropriate values for the parameters

ω, k_1, k_2. Here, $V_1 = \partial V/\partial x$, $V_2 = \partial V/\partial y$, etc. [Another way to look at this is to say that

$$V_1(x_0,y_0), V_2(x_0,y_0), V_{11}(x_0,y_0)$$

are the parameters.] This is in addition to the trivial constant that we can always add to a potential. As we shall show, this requirement for a superintegrable system implies that the potential is any solution of a system of coupled PDEs of the form

$$V_{22} = V_{11} + A^{22}(x,y)V_1 + B^{22}(x,y)V_2, \quad V_{12} = A^{12}(x,y)V_1 + B^{12}(x,y)V_2,$$

where the functions A^{ij}, B^{ij} are subject to certain compatibility conditions, so that the solution space is of dimension four. In $n \geqslant 2$ dimensions the analogous nondegenerate potentials depend on $n+2$ parameters. Systems with nondegenerate potentials have the most beautiful properties but there are also superintegrable systems with degenerate potentials depending on $<n+2$ parameters. For $n=2$ we will show that all of these systems depending on two or three parameters are in a certain sense specializations of the nondegenerate systems. (For degenerate systems, first-order symmetries may exist.) However, superintegrable systems with one parameter (i.e., constant) potentials are in general not restrictions of systems with nondegenerate potentials. [Note that in the classical case the symmetries corresponding to a constant potential are just Killing tensors.[15]] Indeed superintegrable systems with constant potential do not necessarily have a closed quadratic algebra. See Ref. 44 for a counterexample.

Many examples of such systems are known, and lists of possible systems have been determined for constant curvature spaces in two and three dimensions, as well as a few other spaces.[33–38] Here, rather than focus on particular spaces and systems, we employ a theoretical method based on integrability conditions to derive structure common to all such systems. In this paper we consider classical superintegrable systems on a general two-dimensional (2D) Riemannian manifold, real or complex, and uncover their common structure. We show that for superintegrable systems with nondegenerate potentials there exists a standard structure based on the algebra of 2×2 symmetric matrices, that such systems are necessarily multiseparable, and that the quadratic algebra closes at level 6. Superintegrable systems with degenerate potentials are also analyzed. This is all done without making use of lists of such systems, so that generalization to higher dimensions, where relatively few examples are known,[38] is much easier.

In the next paper in this series we will study the Stäckel transform, or coupling constant metamorphosis,[39,40] for 2D classical superintegrable systems. This is a conformal transformation of a superintegrable system on one space to a superintegrable system on another space. We will prove that all nondegenerate 2D superintegrable systems are Stäckel transforms of constant curvature systems and give a complete classification of all 2D superintegrable systems. The following papers will extend these results to three-dimensional (3D) systems and the quantum analogs of 2D and 3D classical systems.

II. SECOND-ORDER KILLING TENSORS FOR 2D COMPLEX RIEMANNIAN MANIFOLDS

Before proceeding to the study of superintegrable systems with potential, we review some basic facts about second-order symmetries (without potential) of the underlying 2D complex Riemannian spaces, i.e., second-order Killing tensors.[15] These were worked out by Koenigs,[41] though here we make an alternate presentation suggested by Refs. 42, 43, and 17. It is always possible to find a local coordinate system $(x,y) \equiv (x_1,x_2)$ defined in a neighborhood of (0,0) on the manifold such that the metric is

$$ds^2 = \lambda(x,y)(dx^2 + dy^2) = \lambda\, dz\, d\overline{z}, \quad z = x + iy, \quad \overline{z} = x - iy,$$

and the Hamiltonian is $H_0 = (p_1^2 + p_2^2)/\lambda$. We can consider a second-order Killing tensor (symmetry) as a quadratic form $\mathcal{L} = \Sigma_{i,j=1}^2 a^{ij}(x,y)p_i p_j$, $a^{ij} = a^{ji}$, that is in involution with the free Hamiltonian H_0: $\{H_0, \mathcal{L}\} = 0$. The conditions are

$$a_i^{ii} = -\frac{\lambda_1}{\lambda}a^{i1} - \frac{\lambda_2}{\lambda}a^{i2}, \quad i = 1,2,$$
$$2a_i^{ij} + a_j^{ii} = -\frac{\lambda_1}{\lambda}a^{j1} - \frac{\lambda_2}{\lambda}a^{j2}, \quad i,j = 1,2, \quad i \neq j. \tag{10}$$

From these conditions we easily obtain the requirements

$$2a_1^{12} = -(a^{11} - a^{22})_2, \quad 2a_2^{12} = (a^{11} - a^{22})_1.$$

From the integrability conditions for these last equations we see that

$$\Delta a^{12} = 0, \quad \Delta(a^{11} - a^{22}) = 0, \quad \Delta = \partial_x^2 + \partial_y^2$$

and that there exist analytic functions $f(z)$, $g(\overline{z})$ such that

$$2a^{12} = f(z) + g(\overline{z}), \quad a^{11} - a^{22} = i(f(z) - g(\overline{z})).$$

Substituting these results in the remaining equations we find

$$(a^{11}\lambda)_1 = -\tfrac{1}{2}\lambda_2(f+g), \quad (a^{22}\lambda)_2 = -\tfrac{1}{2}\lambda_1(f+g).$$

The integrability condition for these last equations is

$$\partial_{12}((\lambda(f-g)) + \frac{i}{2}\partial_1((\lambda_1(f+g)) - \frac{i}{2}\partial_2((\lambda_2(f+g)) = 0$$

or

$$f'' + 3f'\frac{\lambda_z}{\lambda} + 2f\frac{\lambda_{zz}}{\lambda} = -g'' - 3g'\frac{\lambda_{\overline{z}}}{\lambda} - 2g\frac{\lambda_{\overline{zz}}}{\lambda}. \tag{11}$$

If the space admits at least one Killing tensor independent of the Hamiltonian, then we can always assume that it is of the form $(f,g)=(1,1)$, i.e., we can make the change of coordinates $Z = \int dz/\sqrt{f(z)}$, $\overline{Z} = \int d\overline{z}/\sqrt{g(\overline{z})}$ so that (11) implies

$$\lambda_{zz} = \lambda_{\overline{zz}}.$$

Prescribing the values of $g(0), g'(0), g''(0), f(0), f'(0)$, we can use (11) to compute $f''(0)$. Differentiating this equation successively with respect to z and $\overline{z}$ we can compute all derivatives of f and g. Thus any solution (f,g) of the integrability conditions is uniquely determined by the five prescribed values. Once f and g are given, the Killing tensor a^{ij} is determined to within addition of an arbitrary multiple of the Hamiltonian H_0. Thus the maximum dimension of the space of second-order Killing tensors is six. As is very well known, this maximum is actually achieved for flat space and spaces of nonzero constant curvature. Recall that a 2D manifold is of constant curvature if and only if $k = (\partial_{z\overline{z}}\ln\lambda)/\lambda$ is a constant. The space is flat if and only if $k \equiv 0$.

Note that the maximum dimension of six is achieved if and only if the integrability conditions for (11) are themselves satisfied identically. Applying the operator $\partial_{z\overline{z}}$ to both sides of this expression we find

$$3\partial_{\overline{z}}\left(\frac{\lambda_z}{\lambda}\right)f'' + \left(2\partial_{\overline{z}}\left(\frac{\lambda_{zz}}{\lambda}\right) + 3\partial_{z\overline{z}}\left(\frac{\lambda_z}{\lambda}\right)\right)f' + 2\partial_{z\overline{z}}\left(\frac{\lambda_{zz}}{\lambda}\right)f$$
$$= -3\partial_z\left(\frac{\lambda_{\overline{z}}}{\lambda}\right)g'' - \left(2\partial_z\left(\frac{\lambda_{\overline{zz}}}{\lambda}\right) + 3\partial_{z\overline{z}}\left(\frac{\lambda_{\overline{z}}}{\lambda}\right)\right)g' - 2\partial_{z\overline{z}}\left(\frac{\lambda_{\overline{zz}}}{\lambda}\right)g. \tag{12}$$

If dimension six is achieved then this last condition on f and g cannot be independent of (11). Hence, either the coefficients of f'',f',f,g'',g',g all vanish identically, in which case $\partial_{z\bar{z}}\ln\lambda \equiv 0$ and the space is flat, or $\partial_{z\bar{z}}\ln\lambda \neq 0$ and (12) is obtained from (11) through multiplication by $\partial_{z\bar{z}}\ln\lambda$. In the second case one can easily see that

$$\partial_z\left(\frac{\partial_{z\bar{z}}\ln\lambda}{\lambda}\right) = \partial_{\bar{z}}\left(\frac{\partial_{z\bar{z}}\ln\lambda}{\lambda}\right) = 0$$

so the space is of nonzero constant curvature.

If the dimension of the space of symmetries is less than six then (12) is independent of (11). In this case we can eliminate f'' and g'' between these two equations and obtain a condition relating only f',f,g',g:

$$\left[2\left(\frac{\lambda_{zz}}{\lambda}\right)_{\bar{z}} - 9k\lambda_z + 3\left(\frac{\lambda_z}{\lambda}\right)_{z\bar{z}}\right]f' + \left[2\left(\frac{\lambda_{zz}}{\lambda}\right)_{z\bar{z}} - 6k\lambda_{zz}\right]f$$
$$= -\left[2\left(\frac{\lambda_{zz}}{\lambda}\right)_{z} - 9k\lambda_z + 3\left(\frac{\lambda_z}{\lambda}\right)_{z\bar{z}}\right]g' - \left[2\left(\frac{\lambda_{\bar{z}\bar{z}}}{\lambda}\right)_{z\bar{z}} - 6k\lambda_{zz}\right]g. \tag{13}$$

Thus the remaining systems have spaces of symmetries of dimensions $\leqslant 4$. A straightforward computation shows that this last equation can be rewritten as

$$[5\lambda k_z]f + [2\lambda k_{zz} + 8\lambda_z k_z]f' = -[5\lambda k_{\bar{z}}]g' - [2\lambda k_{\bar{z}\bar{z}} + 8\lambda_{\bar{z}} k_{\bar{z}}]g \tag{14}$$

where $2\lambda k_{zz} + 8\lambda_z k_z = 2\lambda k_{\bar{z}\bar{z}} + 8\lambda_{\bar{z}} k_{\bar{z}}$. If the space of symmetries is of dimension four then the integrability conditions for this last equation are satisfied identically. The systems with dimension four (which we call the Darboux spaces) were classified by Koenigs and are four in number.[41] If the equations are not satisfied identically, then we can repeat this procedure and find integrability conditions for the spaces of symmetries of dimension three. These spaces were also classified by Koenigs. In the next paper in this series we will find an alternate, much simpler derivation of these spaces that shows that they all admit superintegrable systems with nondegenerate potentials.

Functional independence and functional linear independence of superintegrable systems. Suppose we have a Hamiltonian $H=H_0+V=\Sigma_{i,j=1}^2 g^{ij}p_ip_j+V(x,y)$ and constants of the motion $L_k = \mathcal{L}_k + W^{(k)} = \Sigma_{i,j=1}^2 a_{(k)}^{ij}p_ip_j + W^{(k)}(x,y)$, for $k=1,2$. We say that such a system is *superintegrable* provided the two functions L_h together with H are functionally independent in the four-dimensional phase space. (Here the possible V will always be assumed to form a vector space and we require functional independence for each such V and the associated $W^{(k)}$. This means that we require that the three quadratic forms $\mathcal{L}_k, H_0$ are functionally independent.)

In the work to follow it will be important that the functionally independent symmetries also be functionally linearly independent. It is clear that there are no constants α,β,γ not all 0 such that $\alpha\mathcal{L}_1+\beta\mathcal{L}_2+\gamma H_0 \equiv 0$. However such a relation is possible if α,β,γ are functions. Indeed we have the example

$$H_0 = p_zp_{\bar{z}} + V(\bar{z}), \quad \mathcal{L}_1 = p_z^2, \quad \mathcal{L}_2 = p_z(zp_z - \bar{z}p_{\bar{z}}),$$

$$W^{(1)} = 0, \quad W^{(2)} = W^{(2)}(\bar{z}), \tag{15}$$

where $-\bar{z}V_{\bar{z}} = W_{\bar{z}}^{(2)}$. Here $\mathcal{L}_2 = z\mathcal{L}_1 - \bar{z}H_0$. (This superintegrable system is in Lie form.[41] It is not multiseparable.) The following result shows that this example is unique.

Theorem 1: *The flat space system* (15) *is the only superintegrable system in a 2D complex Riemannian space such that the functionally independent symmetries are functionally linearly dependent*.

Proof: Suppose L_1,L_2,H are functionally independent symmetries that are functionally linearly dependent. Without loss of generality we can assume that

$$\mathcal{L}_2 = f(x,y)\mathcal{L}_1 + g(x,y)H, \quad df \neq 0, \quad dg \neq 0.$$

Since L_2 is a symmetry we have the condition $\{f,H_0\}\mathcal{L}_1+\{g,H_0\}H_0=0$ or

$$\begin{gathered} f_x a^{11} + g_x/\lambda = 0, \\ f_y a^{22} + g_y/\lambda = 0, \\ f_y a^{11} + 2f_x a^{12} + g_y/\lambda = 0, \\ f_x a^{22} + 2f_y a^{12} + g_x/\lambda = 0. \end{gathered} \tag{16}$$

Thus $g_x=-\lambda f_x a^{11}$, $g_y=-\lambda f_y a^{22}$ and the remaining conditions take the form

$$\begin{pmatrix} 2a^{12} & a^{11}-a^{22} \\ a^{22}-a^{11} & 2a^{12} \end{pmatrix}\begin{pmatrix} f_x \\ f_y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Since $df\neq 0$ the determinant of the 2×2 matrix must be zero:

$$4(a^{12})^2 + (a^{22}-a^{11})^2 = 0.$$

We consider the case $a^{22}-a^{11}=-2ia^{12}$. Then $f_x=-if_y$, so $f=f(z)$. From the Killing equations (10) we see that $a_2^{12}=ia_1^{12}$ so, $a^{12}=a^{12}(z)$. The symmetry conditions for $V,W^{(1)},W^2$ are $W_k^{(j)}=a^{k1}V_1+a^{k2}V_2$, $j,k=1,2$ and the integrability conditions for these equations are the Bertrand–Darboux (BD) conditions $(W_1^{(j)})_2=(W_2^{(j)})_1$, $j=1,2$, which in this case simplify to

$$V_{22}-V_{11}+2iV_{12} = -\left[3\frac{a_2^{12}}{a^{12}} + 2i\frac{\lambda_1}{\lambda} + 2\frac{\lambda_2}{\lambda}\right](V_2+iV_1),$$

$$V_{22}-V_{11}+2iV_{12} = -\left[3\frac{a_2^{12}}{a^{12}} + 2i\frac{\lambda_1}{\lambda} + 2\frac{\lambda_2}{\lambda}\right](V_2+iV_1) - 3\frac{f_2}{f}(V_2+iV_1).$$

Subtracting the second BD equation from the first, we find $V_1-iV_2=0$ or $V=V(\overline{z})$. The remaining Killing tensor equations are

$$(a^{11}\lambda)_1 = -\lambda_2 a^{12}, \quad (a^{11}\lambda)_2 = 2i(a^{12}\lambda)_2 - \lambda_1 a^{12},$$

with integrability condition

$$-(\lambda_2 a^{12})_2 = 2i(\lambda a^{12})_{12} - (\lambda_1 a^{12})_1.$$

At this point it is useful to write all equations in terms of the variables $z,\overline{z}$. Then the Killing tensor equations become

$$\lambda_{zz}=0, \quad \left(\lambda\left[a^{11}-\frac{i}{2}\right]\right)_z = 0 \tag{17}$$

and the previous integrability condition becomes

$$s'' + 3s'\frac{\lambda_{zz}}{\lambda} + 2\frac{\lambda_{zz}}{\lambda} = 0,$$

where

$$2a^{12} = s(z),\ a^{11} - a^{22} = is(z).$$

We can change to new variables $Z(z),\overline{Z(\overline{z})}=\overline{z}$ such that this last equation becomes $s(Z)\equiv 1$, $\lambda_{ZZ}=0$. From now on, we assume that the original coordinates $z,\overline{z}$ were chosen so that $\lambda_{zz}=0$, $2a^{12}=1$, $a^{11}-a^{22}=i$. In the new coordinates we have

$$H_0 = 2\frac{p_z p_{\overline{z}}}{\lambda},\quad \mathcal{L}_1 = 2ip_z^2 + 4\left(a^{11} - \frac{i}{2}\right)p_z p_{\overline{z}},\quad g_{\overline{z}} = -i\lambda f'(z),$$

$$g_z = -2\lambda\left(a^{11} - \frac{i}{2}\right)f'(z),$$

so the integrability equation for g is

$$-i\lambda_z f' - i\lambda f'' = -2\lambda_{\overline{z}} f\left(a^{11} - \frac{i}{2}\right)f' - 2\lambda a_z^{11} f',$$

which simplifies to $(\lambda f'(z))_z = 0$. From (17) we see that there are functions $M(\overline{z}),N(\overline{z})$ such that

$$\lambda = izM'(\overline{z}) + N(\overline{z}),\quad a^{11} - \frac{i}{2} = \frac{M(\overline{z})}{izM'(\overline{z}) + N(\overline{z})}.$$

If $M'(\overline{z})\neq 0$ then we can choose a new variable $\overline{Z(\overline{z})}$ such that $M'(\overline{Z})=-i$. Assume that we have made this choice for $\overline{z}$ from the beginning. Then the equation $(\lambda f'(z))_z=0$ implies $zf'(z) + N(\overline{z})f'(z) = Q(\overline{z})$, so $N'(\overline{z})f''(z)=0$. If $f''(z)=0$ then f is linear in z and this is impossible unless f is constant, a contradiction. Thus $L'=0$ and we can take $\lambda=z$, $f(z)=\ln(z)$, $a^{11}-i/2=-i\overline{z}/z$ which implies that the space is flat. Further we can introduce a new variable $Z(z)$ such that in the new variables $\lambda=1$. If on the other hand $M'(\overline{z})\equiv 0$, then again the space is flat and we can introduce a new variable $\overline{Z(\overline{z})}$ such that $\lambda=1$ with respect to the new variables. In the case that $a^{22}-a^{11} = +2ia^{12}$ the argument is the same, but with the roles of z and $\overline{z}$ interchanged. Q.E.D.

III. MAXIMUM DIMENSIONS OF THE SPACES OF POLYNOMIAL CONSTANTS IN 2D FOR TWO-PARAMETER POTENTIALS

In order to demonstrate the existence and structure of quadratic algebras for 2D superintegrable systems, it is important to compute the dimensions of the spaces of symmetries of these systems that are of orders 2, 3, 4, and 6. These symmetries are necessarily of a special type. The highest order terms in the momenta are independent of the parameters in the potential, while the terms of order 2 less in the momenta are linear in these parameters, those of order 4 less are quadratic, and those of order 6 less are cubic. We will obtain these dimensions exactly, but first we need to establish sharp upper bounds.

Consider a Hamiltonian in a general two-dimensional space of the form

$$H = \frac{p_1^2 + p_2^2}{\lambda} + \alpha_1 V^1 + \alpha_2 V^2. \tag{18}$$

Here, λ and the terms in the potential V^i depend on the coordinates x_i while the α_i are arbitrary parameters. We say that V is a *two-parameter potential* if the gradients of V^1 and V^2 are linearly independent, that is $V_1^1V_2^2 - V_2^1V_1^2 \neq 0$. We are free to redefine V^1 and V^2 by taking linear combinations and so we will also assume that $V_1^1\neq 0$ and $V_2^2\neq 0$.

A. Quadratic constants

We wish to determine how large the space of second-order constants of the motion can be when V is a two-parameter superintegrable potential, i.e., it admits three functionally independent constants of the motion. The general constant of second order in the momenta is

$$L = a^{11}p_1^2 + a^{22}p_2^2 + 2a^{12}p_1p_2 + \alpha_1 b^1 + \alpha_2 b^2 \tag{19}$$

with a^{ij} and b^i being functions of the coordinates alone.

Since $\{H,L\}$ is polynomial in p_1, p_2, α_1 and α_2, and the a^{ij}, b^i and V^i depend only on the coordinates x_1 and x_2, the vanishing of $\{H,L\}$ gives eight equations for the derivatives of a^{ij} and b^i. Introducing two new symbols, $c^1=a_1^{12}$ and $c^2=a_2^{12}$, we solve these equations to obtain

$$a_1^{11} = -\frac{\lambda_1}{\lambda}a^{11} - \frac{\lambda_2}{\lambda}a^{12}, \quad b_1^1 = V_1^1\lambda a^{11} + V_2^1\lambda a^{12},$$

$$a_2^{11} = -2c^1 - \frac{\lambda_2}{\lambda}a^{22} - \frac{\lambda_1}{\lambda}a^{12}, \quad b_2^1 = V_1^1\lambda a^{12} + V_2^1\lambda a^{22},$$

$$a_1^{22} = -2c^2 - \frac{\lambda_1}{\lambda}a^{11} - \frac{\lambda_2}{\lambda}a^{12}, \quad b_1^2 = V_1^2\lambda a^{11} + V_2^2\lambda a^{12},$$

$$a_2^{22} = -\frac{\lambda_2}{\lambda}a^{22} - \frac{\lambda_1}{\lambda}a^{12}, \quad b_2^2 = V_1^2\lambda a^{12} + V_2^2\lambda a^{22}. \tag{20}$$

Without expressions for the derivatives of c^1 and c^2 the system is not involutive. However, the integrability conditions for b^1 and b^2 give equations (the Bertrand–Darboux equations) that can be used to express c^1 and c^2 entirely in terms of the a^{ij}. Calculating each of b_{12}^1 and b_{12}^2 in two different ways and replacing derivatives of the form a_j^{ii} with the above-given expressions leads to two equations for c^1 and c^2,

$$\begin{aligned} -3V_1^1\lambda c^1 + 3V_2^1\lambda c^2 &= (V_1^1\lambda_2 + V_2^1\lambda_1 + \lambda V_{12}^1)(a^{22}-a^{11}) + (V_1^1\lambda_1 + V_{11}^1\lambda - V_2^1\lambda_2 - V_{22}^1\lambda)a^{12}, \\ -3V_1^2\lambda c^1 + 3V_2^2\lambda c^2 &= (V_1^2\lambda_2 + V_2^2\lambda_1 + \lambda V_{12}^2)(a^{22}-a^{11}) + (V_1^2\lambda_1 + V_{11}^2\lambda - V_2^2\lambda_2 - V_{22}^2\lambda)a^{12}. \end{aligned} \tag{21}$$

These can be solved for c^1 and c^2 since the gradients of V^1 and V^2 are linearly independent.

Since all of the derivatives of a^{11}, a^{22}, and a^{12} can be expressed in terms of the a^{ij}, at any regular point, the second-order part of L is determined by three numbers.

Theorem 2: *The space of second-order constants for a 2D superintegrable potential with two parameters is exactly three-dimensional.*

B. Cubic constants

Theorem 3: *The space of third-order constants for a 2D superintegrable potential with two parameters is at most one-dimensional.*

Proof: The general constant of third order in the momenta has the form

$$L = a^{111}p_1^3 + a^{222}p_2^3 + 3a^{112}p_1^2p_2 + 3a^{122}p_1p_2^2 + (\alpha_1 b^{11} + \alpha_2 b^{12})p_1 + (\alpha_1 b^{21} + \alpha_2 b^{22})p_2. \tag{22}$$

As for the second-order constants, we demand that the coefficients of p_1, p_2, α_1, and α_2 vanish. The terms of zeroth order in the momenta lead to

$$V_1^1 b^{11} + V_2^1 b^{21} = 0, \quad V_1^2 b^{12} + V_2^2 b^{22} = 0, \tag{23}$$

$$V_1^1 b^{12} + V_2^1 b^{22} + V_1^2 b^{11} + V_2^2 b^{21} = 0.$$

Since we have chosen V^1 and V^2 such that $V_2^2 \neq 0$, we can solve for b^{11}, b^{22}, and b^{21} in terms of b^{12}, and find

$$b^{11} = -\frac{V_2^1}{V_2^2} b^{12}, \quad b^{22} = \frac{V_2^1}{V_2^2} b^{12}, \quad b^{21} = -\frac{V_1^1}{V_2^2} b^{12}. \tag{24}$$

The coefficients in $\{H,L\}$ that are first order in the momenta give the six equations,

$$\begin{aligned}
3V_1^1 a^{111} + 3V_2^1 a^{112} &= \frac{2}{\lambda} b_1^{11} + \frac{\lambda_1}{\lambda^2} b^{11} + \frac{\lambda_2}{\lambda^2} b^{21}, \\
3V_1^2 a^{111} + 3V_2^2 a^{112} &= \frac{2}{\lambda} b_1^{12} + \frac{\lambda_1}{\lambda^2} b^{12} + \frac{\lambda_2}{\lambda^2} b^{22}, \\
3V_1^2 a^{122} + 3V_2^2 a^{222} &= \frac{2}{\lambda} b_2^{22} + \frac{\lambda_1}{\lambda^2} b^{12} + \frac{\lambda_2}{\lambda^2} b^{22}, \\
3V_1^1 a^{122} + 3V_2^1 a^{222} &= \frac{2}{\lambda} b_2^{21} + \frac{\lambda_1}{\lambda^2} b^{11} + \frac{\lambda_2}{\lambda^2} b^{21}, \\
3V_1^1 a^{112} + 3V_2^1 a^{122} &= \frac{2}{\lambda} b_1^{21} + \frac{2}{\lambda} b_2^{11}, \\
3V_1^2 a^{112} + 3V_2^2 a^{122} &= \frac{2}{\lambda} b_1^{22} + \frac{2}{\lambda} b^{12}.
\end{aligned} \tag{25}$$

The first four of these, together with (24), allow a^{111}, a^{222}, a^{112}, and a^{122} to be expressed in terms of b^{12} and its derivatives, provided that, as assumed, $V_1^1 V_2^2 - V_2^1 V_1^2 \neq 0$. Then, substituting these expressions and (24) into the last two equations we obtain two equations for b_1^{12} and b_2^{12} of the form

$$-V_1^1 b_1^{12} + V_2^1 b_2^{12} = \frac{f_1(\lambda, \lambda_i, V_k^j)}{\lambda (V_1^1 V_2^2 - V_2^1 V_1^2) V_2^2} b^{12}, \tag{26}$$

$$-V_1^2 b_1^{12} + V_2^2 b_2^{12} = \frac{f_2(\lambda, \lambda_i, V_k^j)}{\lambda (V_1^1 V_2^2 - V_2^1 V_1^2) V_2^2} b^{12}, \tag{27}$$

where the two functions $f_m(\lambda, \lambda_i, V_k^j)$ are polynomial in their arguments. So the derivatives of b^{12} are multiples of b^{12} provided $V_1^1 V_2^2 - V_2^1 V_1^2 \neq 0$ and $V_2^2 \neq 0$. Hence at any regular point, all of the a^{ijk} and b^{ij} are determined by one number and so the space of third-order constants is at most one-dimensional. Q.E.D.

C. Fourth- and sixth-order constants

Theorem 4: *The space of fourth-order constants for a 2D superintegrable potential with two parameters is at most six-dimensional.*

Proof: The general constant of fourth order has the form

$$L = \sum_{i,j,k,l=1,2} a^{ijkl} p_i p_j p_k p_l + \sum_{i,j,k=1,2} b^{ij,k} \alpha_k p_i p_j + \sum_{i,j=1,2} c^{,ij} \alpha_i \alpha_j. \tag{28}$$

The vanishing of the coefficients of p_i in $\{H,L\}$ allow all of the derivative of the $c^{,ij}$ to be expressed in terms of the $b^{ij,k}$,

$$\begin{aligned}
c_1^{,11} &= \lambda V_1^1 b^{11,1} + \lambda V_2^1 b^{12,1},\\
c_2^{,11} &= \lambda V_1^1 b^{12,1} + \lambda V_2^1 b^{22,1},\\
c_1^{,12} &= \lambda V_1^1 b^{11,2} + \lambda V_2^1 b^{12,2} + \lambda V_1^2 b^{11,1} + \lambda V_2^2 b^{12,1},\\
c_2^{,12} &= \lambda V_1^1 b^{12,2} + \lambda V_2^1 b^{12,2} + \lambda V_1^2 b^{11,1} + \lambda V_2^2 b^{12,1},\\
c_1^{,22} &= \lambda V_1^2 b^{11,2} + \lambda V_2^2 b^{12,2},\\
c_2^{,22} &= \lambda V_1^2 b^{12,2} + \lambda V_1^2 b^{22,2}.
\end{aligned} \tag{29}$$

The integrability conditions of these equations, that is, equations of the form $c_{12}^{,ij} = c_{21}^{,ij}$, along with terms from $\{H,L\}$ that are cubic in the momenta, provide eleven equations for the twelve derivatives of the $b^{ij,k}$. If we define $\mathbf{b} = (b_1^{11,1}, b_2^{11,1}, b_1^{11,2}, b_2^{11,2}, b_1^{12,1}, b_1^{12,2}, b_2^{12,2}, b_1^{22,1}, b_2^{22,1}, b_1^{22,2}, b_2^{22,2})$, i.e., all of the derivatives of the b's excluding $b_2^{12,1}$, then when these equations are written in matrix form as $\mathbf{Ab} = \mathbf{B}$, the coefficient matrix $\mathbf{A}$ has determinant that is a constant multiple of $\lambda^{-5} V_1^1 (V_1^1 V_2^2 - V_2^1 V_1^2)$. Hence all of the derivative of the b's except $b_2^{12,1}$ can be expressed in terms of the $b^{ij,k}$ and the a^{ijkl} provided that $V_1^1 \neq 0$ and $V_1^1 V_2^2 - V_2^1 V_1^2 \neq 0$. For the remaining derivative, we define $d^1 = b_2^{12,1}$.

Now, the integrability conditions for the $b^{ij,k}$ and the equations obtained from the terms of $\{H,L\}$ that are of fifth order in the momenta give twelve equations for the ten derivatives of $a^{ijkl,m}$ and the two derivatives d_1^1 and d_2^1. The coefficient matrix of these terms in the equations has determinant that is a constant multiple of $(V_1^1 V_2^2 - V_2^1 V_1^2)^3 (\lambda V_1^1)^{-2}$, hence these equations can be solved provided $V_1^1 V_2^2 - V_2^1 V_1^2 \neq 0$ and $V_1^1 \neq 0$.

So, the 5 a^{ijkl}, 6 $b^{ij,k}$, 3 $c^{,ij}$ and d^1 form an involutive system. Each of these symbols can be specified arbitrarily at a point. The three $c^{,ij}$ give rise to three zeroth-order constants, the six $b^{ij,k}$ give rise to six quadratic constants (three multiplied by α_1 and three multiplied by α_2), and so there are at most $5+1=6$ genuinely fourth-order constants. Q.E.D.

For the general sixth-order constant

$$\begin{aligned}
L = &\sum_{i,j,k,l,m,n=1,2} a^{ijklmn} p_i p_j p_k p_l p_m p_n + \sum_{i,j,k,l,m=1,2} b^{ijkl,m} \alpha_m p_i p_j p_k p_l + \sum_{i,j,k,l=1,2} c^{ij,kl} \alpha_k \alpha_l p_i p_j\\
&+ \sum_{i,j,k=1,2} d^{,ijk} \alpha_i \alpha_j \alpha_k
\end{aligned} \tag{30}$$

the argument proceeds similarly.

Theorem 5: *The space of sixth-order constants for a 2D superintegrable potential with two parameters is at most ten-dimensional.*

We will show that the space is exactly ten-dimensional.

IV. NONDEGENERATE SUPERINTEGRABLE SYSTEMS IN TWO DIMENSIONS

Now we take up our main topic: a nondegenerate superintegrable system on a two-dimensional manifold. In earlier work we have classified the possible superintegrable systems on

2D complex flat space, the two-sphere, and on Darboux spaces.[44,45,34–36]. The theory we present here applies to all 2D spaces and adds greater understanding of the structure of these systems. The Hamiltonian system is

$$H = \frac{p_1^2 + p_2^2}{\lambda(x,y)} + V(x,y) \tag{31}$$

in local orthogonal coordinates. We say that the system is *second-order superintegrable* with *nondegenerate potential* if it admits three functionally independent second-order symmetries and the potential is three-parameter (in addition to the usual additive parameter). That is, at each point where the potential is defined and analytic (a regular point), we can prescribe the value of V_1, V_2 and V_{11} for some unique choice of parameters. Using the two Bertrand–Darboux equations satisfied by the potential (coming from the two symmetries other than the Hamiltonian) we can solve for $V_{22}-V_{11}$ and V_{12} in terms of the first derivatives of V.

Thus a nondegenerate potential $V(x,y)$ obeys

$$\begin{aligned} V_{22} &= V_{11} + A^{22}V_1 + B^{22}V_2, \\ V_{12} &= A^{12}V_1 + B^{12}V_2. \end{aligned} \tag{32}$$

Here, V_1,V_2,V_{11} can be prescribed arbitrarily at a fixed regular point.

A seemingly weaker requirement for a superintegrable system is that, as usual, it admits three functionally independent constants of the motion, but only for a two-parameter family of potentials $V(x,y)=\alpha V^{(1)}(x,y)+\beta V^{(2)}(x,y)$, where the gradients of $V^{(1)},V^{(2)}$ are linearly independent.

Lemma 1: "Two implies three." If the system (31) admits three functionally independent constants of the motion and a two-parameter family of potentials, then it admits a three-parameter family (32).

Proof: The system admits a symmetry $\Sigma a^{ij}p_ip_j+W$ if and only if the Bertrand–Darboux equation is satisfied. This is $\partial_j W_i=\partial_i W_j$ or

$$(V_{22}-V_{11})a^{12} + V_{12}(a^{11}-a^{22}) = \left[\frac{(\lambda a^{12})_1 - (\lambda a^{11})_2}{\lambda}\right]V_1 + \left[\frac{(\lambda a^{22})_1 - (\lambda a^{12})_2}{\lambda}\right]V_2.$$

We can always find a symmetry such that a^{11},a^{12},a^{22} take on any prescribed values at a regular point $\mathbf{x}_0$. Thus we can solve the three Bertrand–Darboux equations for the potential to obtain the system

$$V_{22} = V_{11} + A^{22}V_1 + B^{22}V_2,$$

$$V_{12} = A^{12}V_1 + B^{12}V_2,$$

$$0 = A^3V_1 + B^3V_2.$$

Case 1. $A^3\equiv B^3\equiv 0$. Then the equations are (32) and the system admits a three-parameter family of potentials.

Case 2. $A^3\not\equiv 0$. Then $V_1=D^4V_2$ so we find $V_{11}=D^5V_2$, $V_{22}=D^6V_2$, $V_{12}=D^7V_2$. Thus V depends on only one parameter. Impossible!

Case 3. $B^3\not\equiv 0$. Then $V_2=E^4V_1$ so we find $V_{11}=E^5V_1$, $V_{22}=E^6V_1$, $V_{12}=E^7V_1$. Thus V depends on only one parameter. Impossible! Q.E.D.

[Note added in proof. There is a fourth case to consider. It could be that V satisfies (32) but that the integrability conditions are not satisfied indentically, and this yields a further condition $V_{11}=A^{11}V_1+B^{11}V_2$. The lemma still holds but the proof for this case requires the Stäckel transform and will be given later in this series.]

To obtain the integrability conditions for Eq. (32) we introduce the dependent variables $W^{(1)}=V_1$, $W^{(2)}=V_2$, $W^{(3)}=V_{11}$, the vector

$$\mathbf{w} = \begin{pmatrix} W^{(1)} \\ W^{(2)} \\ W^{(3)} \end{pmatrix}, \tag{33}$$

and the matrices

$$\mathbf{A}^{(1)} = \begin{pmatrix} 0 & 0 & 1 \\ A^{12} & B^{12} & 0 \\ A^{13} & B^{13} & B^{12} - A^{22} \end{pmatrix}, \tag{34}$$

$$\mathbf{A}^{(2)} = \begin{pmatrix} A^{12} & B^{12} & 0 \\ A^{22} & B^{22} & 1 \\ A^{23} & B^{23} & A^{12} \end{pmatrix}, \tag{35}$$

where

$$A^{13} = A_2^{12} - A_1^{22} + B^{12}A^{22} + A^{12}A^{12} - B^{22}A^{12},$$

$$B^{13} = B_2^{12} - B_1^{22} + A^{12}B^{12}, \tag{36}$$

$$A^{23} = A_1^{12} + B^{12}A^{12}, \quad B^{23} = B_1^{12} + B^{12}B^{12}. \tag{37}$$

Then the integrability conditions for the system

$$\partial_{x_j}\mathbf{w} = \mathbf{A}^{(j)}\mathbf{w}, \quad j = 1,2, \tag{38}$$

must hold. These conditions are

$$A_i^{(j)} - A_j^{(i)} = A^{(i)}A^{(j)} - A^{(j)}A^{(i)} \equiv [A^{(i)},A^{(j)}]. \tag{39}$$

If and only if these conditions hold, the system has a solution V depending on three parameters.

From the conditions that

$$L = \sum_{k,j=1}^{2} a^{kj}(x,y)p_k p_j + W(x,y), \quad a^{kj} = a^{jk},$$

be a symmetry of the Hamiltonian and relations (32) we can solve for all of the first partial derivatives $\partial_i(\lambda a^{jk})$ to obtain

$$\partial_1(\lambda a^{11}) = -\frac{\lambda_2}{\lambda}(\lambda a^{12}), \quad \partial_2(\lambda a^{22}) = -\frac{\lambda_1}{\lambda}(\lambda a^{12}),$$

$$3\partial_2(\lambda a^{12}) = (\lambda a^{11} - \lambda a^{22})\left(-B^{12} - \frac{\lambda_1}{\lambda}\right) + (\lambda a^{12})\left(-B^{22} + \frac{\lambda_2}{\lambda}\right),$$

$$3\partial_1(\lambda a^{22}) = (\lambda a^{11} - \lambda a^{22})\left(2B^{12} - \frac{\lambda_1}{\lambda}\right) + (\lambda a^{12})\left(2B^{22} + \frac{\lambda_2}{\lambda}\right), \tag{40}$$

$$3\partial_1(\lambda a^{12}) = (\lambda a^{11} - \lambda a^{22})\left(A^{12} + \frac{\lambda_2}{\lambda}\right) + (\lambda a^{12})\left(A^{22} + \frac{\lambda_1}{\lambda}\right),$$

$$3\partial_2(\lambda a^{11}) = (\lambda a^{11} - \lambda a^{22})\left(-2A^{12} + \frac{\lambda_2}{\lambda}\right) + (\lambda a^{12})\left(-2A^{22} + \frac{\lambda_1}{\lambda}\right).$$

This system closes, so the space of solutions is at most three dimensional. However, by the assumption of superintegrability there are at least three functionally independent symmetries. Hence the space of second-order symmetries is exactly three dimensional. A symmetry is uniquely determined by the 2×2 symmetric matrix $(A^{ij}(\mathbf{x}_0))$ of its values at a regular point $\mathbf{x}_0$, and any such matrix corresponds to a symmetry.

To determine the integrability conditions for system (40) we define the vector-valued function

$$\mathbf{h}(x,y,z) = \begin{pmatrix} a^{11} \\ a^{12} \\ a^{22} \end{pmatrix}$$

and directly compute the 3×3 matrix functions $\mathcal{A}(j)$ to get the first-order system

$$\partial_{x_j}\mathbf{h} = \mathcal{A}^{(j)}\mathbf{h}, \quad j = 1,2. \tag{41}$$

The integrability conditions for this system are

$$\mathcal{A}_1^{(2)} - \mathcal{A}_2^{(1)} = \mathcal{A}^{(1)}\mathcal{A}^{(2)} - \mathcal{A}^{(2)}\mathcal{A}^{(1)} \equiv [\mathcal{A}^{(1)}, \mathcal{A}^{(2)}]. \tag{42}$$

Now we investigate the space of third-order constants of the motion:

$$K = \sum_{k,j,i=1}^{2} a^{kji}(x_1,x_2)p_k p_j p_i + b^{\ell}(x_1,x_2)p_{\ell}, \tag{43}$$

which must satisfy $\{H,K\}=0$. Here a^{kji} is symmetric in the indices k,j,i.

The conditions are

$$2\frac{\partial a^{iii}}{\partial x_i} = -3\left(\frac{\partial \ln\lambda}{\partial_{x_i}}a^{iii} + \frac{\partial \ln\lambda}{\partial_{x_j}}a^{jii}\right), \quad i \neq j,$$

$$3\frac{\partial a^{jii}}{\partial x_i} + \frac{\partial a^{iii}}{\partial x_j} = 3\left(-\frac{\partial \ln\lambda}{\partial_{x_i}}a^{iij} - \frac{\partial \ln\lambda}{\partial_{x_j}}a^{ijj}\right), \quad i \neq j,$$

$$2\left(\frac{\partial a^{122}}{\partial x_1} + \frac{\partial a^{112}}{\partial x_2}\right) = -\frac{\partial \ln\lambda}{\partial_{x_1}}a^{122} - \frac{\partial \ln\lambda}{\partial_{x_1}}a^{111} - \frac{\partial \ln\lambda}{\partial_{x_2}}a^{222} - \frac{\partial \ln\lambda}{\partial_{x_2}}a^{112}, \tag{44}$$

$$\frac{\partial b^1}{\partial x_2}+\frac{\partial b^2}{\partial x_1}=3\sum_{s=1}^{2}\lambda a^{s21}\frac{\partial V}{\partial x_s},$$

$$\frac{\partial b^j}{\partial x_j}=\frac{3}{2}\sum_{s=1}^{2}a^{sjj}\frac{\partial V}{\partial x_s}-\frac{1}{2}\sum_{s=1}^{2}\frac{\partial \ln\lambda}{\partial x_s}b^s,\quad j=1,2, \tag{45}$$

and

$$\sum_{s=1}^{2}b^s\frac{\partial V}{\partial x_s}=0. \tag{46}$$

The general solution for the terms third order in the p_j is a sum of third-order monomials in the p_j and $J_3=x_1p_2-x_2p_1$. The a^{kji} is just a third-order Killing tensor. We require the potential V to be superintegrable and nondegenerate, and that the highest order terms, the a^{kji} in the constant of the motion, be independent of the three parameters in V. The b^ℓ must depend on these parameters linearly. We set

$$b^\ell(x_1,x_2)=\sum_{j=1}^{2}f^{\ell,j}(x_1,x_2)\frac{\partial V}{\partial x_j}(x_1,x_2).$$

(We are excluding the purely first order symmetries.) Substituting this expression into (46) we see that

$$f^{\ell,j}+f^{j,\ell}=0,\quad 1\leqslant \ell,j\leqslant 2.$$

Further

$$b_1^1=f_1^{1,2}V_2+f^{1,2}V_{12},\quad b_2^1=f_2^{1,2}V_2+f^{1,2}V_{22},$$

$$b_1^2=f_1^{2,1}V_1+f^{2,1}V_{11},\quad b_2^2=f_2^{2,1}V_1+f^{2,1}V_{12},$$

where the subscript j denotes the partial derivative with respect to x_j. Substituting these results and expressions (32) into the defining equations (45) and equating coefficients of V_1, V_2, V_{11}, respectively, we obtain the independent conditions:

$$\begin{gathered}\lambda a^{111}=\tfrac{1}{3}f^{1,2}(2A^{12}-(\ln\lambda)_2),\\ \lambda a^{222}=\tfrac{1}{3}f^{1,2}(-2B^{12}+(\ln\lambda)_1),\\ \lambda a^{112}=\tfrac{1}{9}f^{1,2}(2A^{22}+2B^{12}+(\ln\lambda)_1),\\ \lambda a^{122}=\tfrac{1}{9}f^{1,2}(-2A^{12}+2B^{22}-(\ln\lambda)_2),\end{gathered} \tag{47}$$

$$\begin{gathered}f_1^{1,2}=\tfrac{1}{3}f^{1,2}(A^{22}-2B^{12}-(\ln\lambda)_1),\\ f_2^{1,2}=\tfrac{1}{3}f^{1,2}(-2A^{12}-B^{22}+(\ln\lambda)_2),\end{gathered} \tag{48}$$

Note that (47) yields expressions for all a^{ijk} in terms of $f^{1,2}$ and the A^{ij},B^{ij}, functions. Similarly (48) yields expressions for $f_k^{1,2}$ in terms of $f^{1,2}$ and the $A^{k\ell}$,$B^{k\ell}$ functions. Thus we have an involutive system for $f^{1,2}$, possibly subject to additional conditions from (45). Thus any third-order

constant of the motion defined by $f^{1,2}(x,y)$ is uniquely determined by its value $f^{1,2}(x_0,y_0)$ at some regular point (x_0,y_0). This means that the space of third-order constants of the motion is at most one-dimensional.

There are two cases to consider.

Case 1: $2A^{12}=B^{22}=(\ln\lambda)_2$, $2B^{12}=-A^{22}=(\ln\lambda)_1$. Then it follows from (47) that all $a^{ijk}\equiv 0$. The integrability conditions require $(\ln\lambda)_{11}+(\ln\lambda)_{22}=0$, which is the condition for flat space, Thus by an appropriate orthogonal change of coordinates we can assume that $\lambda\equiv 1$. In these new coordinates we see that $A^{ij}=B^{ij}\equiv 0$ for all i,j. The general solution is

$$f^{1,2}=c_1,$$

where c_1, is a constant. This is the *homogeneous isotropic oscillator:*

$$V(x,y)=\alpha x+\beta y+\gamma(x^2+y^2). \tag{49}$$

Note that for this very special case a nonzero Poisson bracket of two second-order constants of the motion must be first order.

Case 2: The conditions for Case 1 do not hold for all A^{ij},B^{ij}. Now (47) yield expressions for all a^{ijk} in terms of f^{12} and the A^{ij},B^{ij} functions and not all a^{ijk} vanish. Similarly (48) yields expressions for all $f_i^{1,2}$ in terms of $f^{1,2}$ and the $A^{k\ell},B^{k\ell}$ functions. We will show that the space of symmetries is exactly one dimensional.

Theorem 6: *Let K be a third-order constant of the motion for a superintegrable system with nondegenerate potential V*:

$$K=\sum_{k,j,i=1}^{2} a^{kji}(x,y)p_kp_jp_i+\sum_{\ell=1}^{2} b^{\ell}(x,y)p_{\ell}.$$

Then

$$b^{\ell}(x,y)=\sum_{j=1}^{2} f^{\ell,j}(x,y)\frac{\partial V}{\partial x_j}(x,y) \tag{50}$$

with

$$f^{\ell,j}+f^{j,\ell}=0,\quad 1\leqslant \ell,j\leqslant 2,$$

and the a^{ijk}, b^{ℓ} are uniquely determined by the number $f^{1,2}(x_0,y_0)$ at some regular point (x_0,y_0) of V.

Let

$$L_1=\sum a^{kj}_{(1)}p_kp_j+W_{(1)},\quad L_2=\sum a^{kj}_{(2)}p_kp_j+W_{(2)}$$

be second-order constants of the the motion for a superintegrable system with nondegenerate potential and let $\mathcal{A}_{(i)}(x,y)=\{a^{kj}_{(i)}(x,y)\}$, $i=1,2$ be 2×2 matrix functions. Then the Poisson bracket of these symmetries is given by

$$\{L_1,L_2\}=\sum_{k,j,i=1}^{2} a^{kji}(x,y)p_kp_jp_i+b^{\ell}(x,y)p_{\ell} \tag{51}$$

where

$$f^{k,\ell}=2\lambda\sum_j (a^{kj}_{(2)}a^{j\ell}_{(1)}-a^{kj}_{(1)}a^{j\ell}_{(2)}). \tag{52}$$

Thus $\{L_1,L_2\}$ is uniquely determined by the skew-symmetric matrix

$$[\mathcal{A}_{(2)},\mathcal{A}_{(1)}] \equiv \mathcal{A}_{(2)}\mathcal{A}_{(1)} - \mathcal{A}_{(1)}\mathcal{A}_{(2)}, \tag{53}$$

hence by the constant matrix $[\mathcal{A}_{(2)}(x_0,y_0),\mathcal{A}_{(1)}(x_0,y_0)]$ evaluated at a regular point.

Corollary 1: Let V be a superintegrable nondegenerate potential. The space of third-order constants of the motion is one-dimensional and is spanned by Poisson brackets of the second-order constants of the motion.

Corollary 2: Let V be a superintegrable nondegenerate potential and L_1,L_2 *be second-order constants of the motion with matrices* $\mathcal{A}_{(1)},\mathcal{A}_{(2)}$*, respectively. Then*

$$\{L_1,L_2\} \equiv 0 \Leftrightarrow [\mathcal{A}_{(1)},\mathcal{A}_{(2)}] \equiv 0 \Leftrightarrow [\mathcal{A}_{(1)}(\mathbf{x}_0),\mathcal{A}_{(2)}(\mathbf{x}_0)] = 0$$

at a regular point $\mathbf{x}_0$.

A. A standard form for 2D superintegrable systems

For superintegrable nondegenerate potentials there is a standard structure allowing the identification of the space of second-order constants of the motion with the space of 2×2 symmetric matrices, as well as identification of the space of third-order constants of the motion with the space of 2×2 skew-symmetric matrices. Indeed, if $\mathbf{x}_0$ is a regular point then there is a $1-1$ linear correspondence between second-order operators L and their associated symmetric matrices $\mathcal{A}(\mathbf{x}_0)$. Let $\{L_1,L_2\}' = \{L_2,L_1\}$ be the reversed Poisson bracket. Then the map

$$\{L_1,L_2\}' \Leftrightarrow [\mathcal{A}_{(1)}(\mathbf{x}_0),\mathcal{A}_{(2)}(\mathbf{x}_0)]$$

is an algebraic isomorphism. Here, L_1,L_2 are in involution if and only if matrices $\mathcal{A}_{(1)}(\mathbf{x}_0)$, $\mathcal{A}_{(2)}\times(\mathbf{x}_0)$ commute. If $\{L_1,L_2\}\neq 0$ then it is a third-order symmetry and can be uniquely associated with the skew-symmetric matrix $[\mathcal{A}_{(1)}(\mathbf{x}_0),\mathcal{A}_{(2)}(\mathbf{x}_0)]$. Since commutators of second-order constants of the motion span the space of third-order constants, we can identify these $1-1$ with 2×2 skew-symmetric matrices. Let $\mathcal{E}^{ij}$ be the 2×2 matrix with a 1 in row i, column j and 0 for every other matrix element. Then the symmetric matrices

$$\mathcal{A}^{(ij)} = \tfrac{1}{2}(\mathcal{E}^{ij} + \mathcal{E}^{ji}) = \mathcal{A}^{(ji)}, \quad i,j = 1,2 \tag{54}$$

form a basis for the three-dimensional space of symmetric matrices. Moreover,

$$[\mathcal{A}^{(ij)},\mathcal{A}^{(k\ell)}] = \tfrac{1}{2}(\delta_{jk}\mathcal{B}^{(i\ell)} + \delta_{j\ell}\mathcal{B}^{(ik)} + \delta_{ik}\mathcal{B}^{(j\ell)} + \delta_{i\ell}\mathcal{B}^{(jk)}) \tag{55}$$

where

$$\mathcal{B}^{(ij)} = \tfrac{1}{2}(\mathcal{E}^{ij} - \mathcal{E}^{ji}) = -\mathcal{B}^{(ji)}, \quad i,j = 1,2.$$

Here $\mathcal{B}^{(ii)}=0$ and $\mathcal{B}^{(12)}$ forms a basis for the space of skew-symmetric matrices. Thus (55) gives the commutation relations for the second-order symmetries. If V is the isotropic oscillator then there is no truly third-order symmetry. For any other nondegenerate potential, the space of symmetries is exactly one dimensional.

To gain a deeper understanding of this structure, it is useful to reformulate the problem of determining the second-order symmetries of (31). We set

$$W(x) = f^1V_1 + f^2V_2 + f^{11}V_{11}$$

and substitute this result into $W_i = \lambda\Sigma_{j=1}^2 a^{ij}V_j$. Additionally we must impose the Killing tensor conditions

$$a_i^{ii} = -(\ln\lambda)_1 a^{1i} - (\ln\lambda)_2 a^{2i}, \quad 2a_i^{ij} + a_j^{ii} = -(\ln\lambda)_1 a^{1j} - (\ln\lambda)_2 a^{2j}, \quad i\neq j.$$

From the expressions for W_i we obtain the equations for the a^{ij}:

$$\lambda a^{11} = f_1^1 + f^2 A^{12} + f^{11} A^{13},$$

$$\lambda a^{12} = f_2^1 + f^1 A^{12} + f^2 A^{22}, \tag{56}$$

$$\lambda a^{22} = f_2^2 + f^1 B^{12} + f^2 B^{22}$$

and the condition on the first derivatives of the f^i:

$$f_2^1 - f_1^2 = -f^1 A^{12} + f^2 (A^{22} - B^{12}) - f^{11} B^{13}. \tag{57}$$

Note the expressions for f_1^{11} and f_2^{11} in terms of f^1, f^2, f^{11}:

$$f_1^{11} + f^1 + f^{11}(B^{12} - A^{22}) = 0, \quad f_2^{11} + f^2 + f^{11} A^{12} = 0.$$

Differentiating (57) with respect to each of x_1 and x_2 and substituting (56) into the Killing equations we see that we can express each of the second derivatives of f^1, f^2 in terms of lower order derivatives of f^1, f^2, f^{11}. Thus the system is in involution at the second derivative level, but not at the first derivative level because we have only one condition for the six derivatives $f_1^1, f_2^1, f_1^2, f_2^2$. We can uniquely determine a symmetry at a regular point by choosing the six parameters $(f^1, f^2, f^{11}, f_1^1, f_2^1, f_2^2)$. The values of f^1, f^2, f^{11} at the regular point are analogous to the three parameters that we can add to the potentials in the three parameter family. For our standard basis, we fix $(f^1, f^2, f^{11})_{\mathbf{x}_0} = (0,0,0)$. Then from (56) and (57) we have

$$\begin{pmatrix} f_1^1 & f_2^1 \\ f_1^2 & f_2^2 \end{pmatrix} = \lambda \begin{pmatrix} a^{11} & a^{12} \\ a^{21} & a^{22} \end{pmatrix}.$$

Thus we can define a standard set of basis symmetries $\mathcal{S}^{(jk)} = \Sigma_{i,h} a^{ih}_{(jk)}(\mathbf{x}) p_i p_h + W^{(jk)}(\mathbf{x})$ corresponding to a regular point $\mathbf{x}_0$ by

$$\begin{pmatrix} f_1^1 & f_2^1 \\ f_1^2 & f_2^2 \end{pmatrix}_{\mathbf{x}_0} = \lambda(\mathbf{x}_0) \begin{pmatrix} a^{11} & a^{12} \\ a^{21} & a^{22} \end{pmatrix}_{\mathbf{x}_0} = \lambda(\mathbf{x}_0) \mathcal{A}^{(jk)}, \quad W^{(jk)}(\mathbf{x}_0) = 0.$$

The condition on $W^{(jk)}$ is actually three conditions since $W^{(jk)}$ depends on three parameters.

B. Multiseparability of 2D systems

From the general theory of variable separation for Hamilton–Jacobi equations[19,20] we know that a second-order symmetry L defines a separable system for

$$H = \frac{p_x^2 + p_y^2}{\lambda(x,y)} + V(x,y) = E$$

if and only if

1. The symmetries H, L form a linearly independent set as quadratic forms.
2. The two quadratic forms have a common eigenbasis of differential forms.

This last requirement means that, expressed in Cartesian coordinates, the matrix $\mathcal{A}(\mathbf{x})$ can be diagonalized by conjugacy transforms in a neighborhood of a regular point.

Corollary 3: Let V be a superintegrable nondegenerate potential and L be a second-order constant of the motion with matrix function $\mathcal{A}(\mathbf{x})$. If at some regular point $\mathbf{x}_0$ the matrix $\mathcal{A}(\mathbf{x}_0)$ has two distinct eigenvalues, then H,L characterize an orthogonal separable coordinate system.

Note: Since a generic 2×2 symmetric matrix has distinct roots, it follows that any superintegrable nondegenerate potential is multiseparable.

C. The quadratic algebra

Next we investigate the space of fourth-order constants of the motion for 2D systems in some detail. We already know that the dimension of this space is at most 6. Here a constant of the motion

$$F=\sum_{\ell,k,j,i=1}^{2} a^{\ell kji}(x,y,z)p_\ell p_k p_j p_i+\sum_{m,q=1}^{2} b^{mq}(x,y,z)p_m p_q+W(x,y,z), \tag{58}$$

must satisfy $\{H,F\}=0$. Again $a^{\ell kji}$, b^{mq} are symmetric in all indices.

The conditions are

$$\frac{\partial a^{iiii}}{\partial x_i}=-2\sum_{s=1}^{2} a^{siii}\frac{\partial \ln \lambda}{\partial x_s}, \tag{59}$$

$$4\frac{\partial a^{jiii}}{\partial x_i}+\frac{\partial a^{iiii}}{\partial x_j}=-6\sum_{s=1}^{2} a^{siij}\frac{\partial \ln \lambda}{\partial x_s}, \quad i\neq j, \tag{60}$$

$$3\frac{\partial a^{jjii}}{\partial x_i}+2\frac{\partial a^{iiij}}{\partial x_j}=-\sum_{s=1}^{2} a^{siii}\frac{\partial \ln \lambda}{\partial x_s}-3\sum_{s=1}^{2} a^{sijj}\frac{\partial \ln \lambda}{\partial x_s}, \quad i\neq j,$$

$$2\frac{\partial b^{ij}}{\partial x_i}+\frac{\partial b^{ii}}{\partial x_j}=6\lambda\sum_{s=1}^{3} a^{sjii}\frac{\partial V}{\partial x_s}-\sum_{s=1}^{2} b^{sj}\frac{\partial \ln \lambda}{\partial x_s}, \quad i\neq j,$$

$$\frac{\partial b^{ii}}{\partial x_i}=2\lambda\sum_{s=1}^{3} a^{siii}\frac{\partial V}{\partial x_s}-\sum_{s=1}^{2} b^{sj}\frac{\partial \ln \lambda}{\partial x_s}, \tag{61}$$

and

$$\lambda\sum_{s=1}^{3} b^{si}\frac{\partial V}{\partial x_s}=\frac{\partial W}{\partial x_i}. \tag{62}$$

Note that the $a^{\ell kji}$ is a fourth-order Killing tensor. We require the potential V to be superintegrable and nondegenerate and that the highest order terms, the $a^{\ell kji}$ in the constant of the motion, be independent of the three parameters in V. The b^{mq} must depend linearly and W quadratically on these parameters.

We set

$$b^{jk}=\sum_{\alpha=1}^{3} f^{jk,\alpha}W^{(\alpha)}, \quad f^{jk,\alpha}=f^{kj,\alpha},$$

where $W^{(\alpha)}$ is defined by

$$\begin{pmatrix} W^{(1)} \\ W^{(2)} \\ W^{(3)} \end{pmatrix}=\begin{pmatrix} V_1 \\ V_2 \\ V_{11} \end{pmatrix}.$$

Then conditions (61) become

$$\frac{\partial}{\partial_{x_h}}f^{jk,\alpha}+\frac{\partial}{\partial_{x_k}}f^{hj,\alpha}+\frac{\partial}{\partial_{x_j}}f^{kh,\alpha}-2\lambda a^{\alpha hjk}=-\sum_{\gamma=1}^{3}(f^{jk,\gamma}A^{(h)}_{\gamma\alpha}+f^{hj,\gamma}A^{(k)}_{\gamma\alpha}+f^{kh,\gamma}A^{(j)}_{\gamma\alpha})$$
$$-\sum_{s=1}^{2}(f^{sk,\alpha}\delta_{hk}+f^{sj,\alpha}\delta_{kh}+f^{sh,\alpha}\delta_{jk})\frac{\partial}{\partial_{x_s}}\ln\lambda, \qquad (63)$$

where $1\leqslant j,k,h\leqslant 2$ and we set $a^{3hjk}\equiv 0$. From the integrability conditions $(\partial/\partial_{x_j})(\partial W/\partial x_i)=(\partial/\partial_{x_i})(\partial W/\partial x_j)$, $i\neq j$ for Eq. (62) we obtain the conditions

$$\partial_{x_j}f^{\beta k,\alpha}+\partial_{x_j}f^{\alpha k,\beta}-\partial_{x_k}f^{\beta j,\alpha}-\partial_{x_k}f^{\alpha j,\beta}=\sum_{s=1}^{2}(A^{(k)}_{\beta s}f^{sj,\alpha}+A^{(k)}_{\alpha s}f^{sj,\beta}-A^{(j)}_{\beta s}f^{sk,\alpha}-A^{(j)}_{\alpha s}f^{sk,\beta})$$
$$+\sum_{\gamma=1}^{3}(f^{\beta j,\gamma}A^{(k)}_{\gamma\alpha}+f^{\alpha j,\gamma}A^{(k)}_{\gamma\beta}-f^{\beta k,\gamma}A^{(j)}_{\gamma\alpha}-f^{\alpha k,\gamma}A^{(j)}_{\gamma\beta})$$
$$-(f^{\beta k,\alpha}+f^{\alpha k,\beta})\frac{\partial}{\partial_{x_j}}\ln\lambda+(f^{\beta j,\alpha}+f^{\alpha j,\beta})\frac{\partial}{\partial_{x_k}}\ln\lambda, \qquad (64)$$

where $j\neq k$, $1\leqslant\alpha,\ \beta\leqslant 3$ and we set $f^{3j,\alpha}\equiv 0$.

There are eight independent equations (63) with $\alpha\neq 3$ and we use five of these to define the five components a^{ihjk} as linear combinations of $(\partial/\partial_{x_h})f^{jk,\alpha}$ and $f^{jk,\alpha}$. We can then eliminate the a^{ihjk} from the remaining three equations to obtain three conditions relating $(\partial/\partial_{x_h})f^{jk,\alpha}$ and $f^{jk,\alpha}$. There are six terms of the form $(\partial/\partial_{x_h})f^{jk,3}$. Equation (64) with $\alpha=\beta=3$ is satisfied identically. There are two equations (64) with $\beta=3$, $1\leqslant\alpha\leqslant 2$ and four equations (63) with $\alpha=3$. Thus all six terms of the form $(\partial/\partial_{x_h})f^{jk,3}$ can be expressed as linear combinations of $f^{jk,\alpha}$. There are a total of twelve distinct terms of the form $(\partial/\partial_{x_h})f^{jk,m}$, $1\leqslant h,j,k,m\leqslant 2$. We have seen that there are three conditions on these terms remaining from (63); there are an additional three such conditions from (64) with $\alpha,\beta\neq 3$. Thus there is a shortfall of six conditions on the first derivatives $(\partial/\partial_{x_h})f^{jk,m}$.

There are a total of eighteen distinct terms of the form $(\partial^2/\partial_{x_h}\partial_{x_\ell})f^{jk,m}$ with $1\leqslant h,j,k,\ell,m\leqslant 2$. Differentiating with respect to x_1,x_2 the three first-order conditions of (63), from which the a^{ihjk} have been eliminated, we obtain six independent conditions on these second derivatives. Differentiating each of our expressions for the a^{ihjk} and substituting into Eq. (59) we find six additional conditions on the second derivatives. Also, we can differentiate the three equations from (62) with $\alpha,\beta\neq 3$ to obtain six additional conditions on the second derivatives. This allows us to express each second-order derivative as a linear combination of lower order derivatives, Thus the system is in involution.

We conclude that any fourth-order symmetry is uniquely determined by the values $f^{jk,\alpha}(\mathbf{x}_0)$ and a subset of six of the values $(\partial/\partial_{x_h})f^{jk,m}(\mathbf{x}_0)$ at a regular point $\mathbf{x}_0$. Note that by adding an appropriate linear combination of purely second-order symmetries to the fourth-order symmetry we can achieve $f^{jk,\alpha}(\mathbf{x}_0)=0$ for all j,k,α, so the maximum possible dimension of the space of purely fourth-order symmetries is six. However any second-order polynomial in the second-order symmetries is a fourth-order symmetry, and the subspace of polynomial symmetries is at least five and at most six. We show that it is exactly six.

Theorem 7: *The six distinct monomials*

$$(\mathcal{S}^{(11)})^2,\quad (\mathcal{S}^{(22)})^2,\quad (\mathcal{S}^{(12)})^2,\quad \mathcal{S}^{(11)}\mathcal{S}^{(22)},\quad \mathcal{S}^{(11)}\mathcal{S}^{(12)},\quad \mathcal{S}^{(12)}\mathcal{S}^{(22)},$$

form a basis for the space of fourth order symmetries.

Proof: Since the three symmetries $\mathcal{S}^{(11)}$, $\mathcal{S}^{(22)}$, $\mathcal{S}^{(12)}$ are functionally independent, the six monomials listed above are linearly independent. Hence they form a basis. Q.E.D.

We can use this result to explicitly expand a general fourth-order symmetry

$$F = \sum_{\ell,k,j,i=1}^{2} a^{\ell kji}(x,y,z)p_\ell p_k p_j p_i + \sum_{m,q=1}^{2} b^{mq}(x,y,z)p_m p_q + W(x,y,z)$$

in terms of the standard basis. Without loss of generality we can assume that $(0,0)=\mathbf{0}$ is a regular point. Then F is uniquely determined by the data $a^{\ell kji}(\mathbf{0})$, $\partial_m a^{\ell kji}(\mathbf{0})$, $b^{mq}(\mathbf{0})$, $W(\mathbf{0})$. We can uniquely match the data $a^{\ell kji}(\mathbf{0})$ by taking a linear combination of the basis symmetries

$$(\mathcal{S}^{(11)})^2, \quad (\mathcal{S}^{(22)})^2, \quad (\mathcal{S}^{(12)})^2, \quad \mathcal{S}^{(11)}\mathcal{S}^{(12)}, \quad \mathcal{S}^{(12)}\mathcal{S}^{(22)}.$$

This leaves the symmetry $\mathcal{S}^{(11)}\mathcal{S}^{(22)}-(\mathcal{S}^{(12)})^2$, whose leading order terms vanish at the regular point. The expansion coefficient for this term is obtained uniquely from the derivative data $\partial_m a^{\ell kji}(\mathbf{0})$. Now we have matched all of the fourth order terms in F with an expansion of the form $\mathcal{F}=\Sigma\xi_{ijk\ell}\mathcal{S}^{(ij)}\mathcal{S}^{(k\ell)}$. The difference $F-\mathcal{F}$ is a second-order symmetry. It is uniquely determined by the data $b^{mq}(\mathbf{0}),W(\mathbf{0})$, which has not changed since $W^{(ij)}(\mathbf{0})=0$ for all terms in the standard basis, Thus $F-\mathcal{F}=\Sigma b^{mq}(\mathbf{0})\mathcal{S}^{(mq)}+W(\mathbf{0})$ and we have expanded the original symmetry in terms of second-order polynomials in the standard basis.

Similarly we see that the maximal dimension of ten sixth-order symmetries is achieved by monomials in the second order symmetries.

Theorem 8: *The ten distinct monomials*

$$(\mathcal{S}^{(ii)})^3, \quad (\mathcal{S}^{(ij)})^3, \quad (\mathcal{S}^{(ii)})^2\mathcal{S}^{(jj)}, \quad (\mathcal{S}^{(ii)})^2\mathcal{S}^{(ij)}, \quad (\mathcal{S}^{(ij)})^2\mathcal{S}^{(ii)}, \quad \mathcal{S}^{(11)}\mathcal{S}^{(12)}\mathcal{S}^{(22)},$$

for $i,j=1,2$, $i\neq j$ *form a basis for the space of sixth-order symmetries*.

Proof: Since the three symmetries $\mathcal{S}^{(11)}$, $\mathcal{S}^{(22)}$, $\mathcal{S}^{(12)}$ are functionally independent, the ten monomials listed above are linearly independent. Hence they form a basis. Q.E.D.

These theorems establish the closure of the quadratic algebra for 2D superintegrable potentials: All fourth-order and sixth-order symmetries can be expressed as polynomials in the second-order symmetries.

Again, we can use these results to explicitly expand a general sixth-order symmetry

$$G = \sum_{i,j,k,l,m,n=1,2} a^{ijklmn}p_i p_j p_k p_l p_m p_n + \sum_{i,j,k,l=1,2} b^{ijkl}p_i p_j p_k p_l + \sum_{i,j=1,2} c^{ij}p_i p_j + W \tag{65}$$

in terms of the standard basis. Without loss of generality we can assume that $(0,0)=\mathbf{0}$ is a regular point. Then G is uniquely determined by the data $a^{ijklmn}(\mathbf{0})$, $\partial_q a^{ijklmn}(\mathbf{0})$, $b^{ijkl}(\mathbf{0})$, $\partial_m b^{ijkl}(\mathbf{0})$, $W(\mathbf{0})$. We can uniquely match the data $a^{ijklmn}(\mathbf{0})$ by taking a linear combination of the seven symmetries

$$(\mathcal{S}^{(ii)})^3, \quad (\mathcal{S}^{(ij)})^3, \quad (\mathcal{S}^{(ii)})^2\mathcal{S}^{(jj)}, \quad (\mathcal{S}^{(ii)})^2\mathcal{S}^{(ij)},$$

for $i,j=1,2$, $i\neq j$. This leaves the three symmetries

$$\mathcal{S}^{(11)}(\mathcal{S}^{(11)}\mathcal{S}^{(22)}-(\mathcal{S}^{(12)})^2), \quad \mathcal{S}^{(12)}(\mathcal{S}^{(11)}\mathcal{S}^{(22)}-(\mathcal{S}^{(12)})^2), \quad \mathcal{S}^{(22)}(\mathcal{S}^{(11)}\mathcal{S}^{(22)}-(\mathcal{S}^{(12)})^2)$$

whose leading order terms vanish at the regular point. The expansion coefficients for these three terms are obtained uniquely from the derivative data $\partial_q a^{ijklmn}$. Now we have matched all of the sixth order terms in G with an expansion of the form $\mathcal{G}=\Sigma\xi_{ijklmn}\mathcal{S}^{(ij)}\mathcal{S}^{(kl)}\mathcal{S}^{(mn)}$. The difference $G-\mathcal{G}$ is a fourth-order symmetry. It is uniquely determined by the data $b^{ijkl}(\mathbf{0})$, $W(\mathbf{0})$ $b^{mq}(\mathbf{0})$, $W(\mathbf{0})$ [which has not changed since $W^{(ij)}(\mathbf{0})=0$ for all terms in the standard basis], and the data $\partial_m\tilde{b}^{ijkl}(\mathbf{0})$ which has changed. Now we can use the argument presented above to expand this fourth-order symmetry in terms of polynomials in the standard basis.

Example: We indicate, briefly, how the example that we started with, (1), fits into the present structure. In the example the potential is

$$V(x,y)=\frac{1}{2}\left(\omega^2(x^2+y^2)+\frac{k_1^2-\frac{1}{4}}{x^2}+\frac{k_2^2-\frac{1}{4}}{y^2}\right),$$

where ω, k_1 and k_2 are arbitrary parameters. It is easy to verify that, apart from an additve constant, this is the general solution of the system

$$V_{22}-V_{11}=\frac{3}{x}V_1-\frac{3}{y}V_2,\quad V_{12}=0.$$

Hence we have a nondegenerate potential with

$$A^{22}=\frac{3}{x},\quad B^{22}=-\frac{3}{y},\quad A^{12}=B^{12}=0.$$

A natural basis of functionally independent second-order symmetries is $\{\mathcal{S}_1,\mathcal{S}_2,\mathcal{S}_3\}$, (8). To apply the above results directly, we need to choose a standard basis at a regular point. We choose the regular point $\mathbf{x}_0=(1,1)$. Then the standard second-order symmetries $\mathcal{S}^{(11)}$, $\mathcal{S}^{(22)}$, $\mathcal{S}^{(12)}$ are the unique symmetries that restrict to p_x^2, p_y^2, p_xp_y, respectively, at $\mathbf{x}_0$. Thus

$$\mathcal{S}^{(11)}=p_x^2+\left(\frac{1}{4}-k_1^2\right)\left(\frac{1}{x^2}-1\right)+\omega^2(1-x^2),$$

$$\mathcal{S}^{(22)}=p_y^2+\left(\frac{1}{4}-k_2^2\right)\left(\frac{1}{y^2}-1\right)+\omega^2(1-y^2),$$

$$\mathcal{S}^{(12)}=\frac{1}{2}(p_x^2+p_y^2-(xp_y-yp_x)^2)+\frac{1}{2}\left(\left(\frac{1}{4}-k_1^2\right)\frac{1-y^2}{x^2}+\left(\frac{1}{4}-k_2^2\right)\left(\frac{1-x^2}{y^2}\right)\right)+\omega^2(2-x^2-y^2).$$

The bases are related by

$$\mathcal{S}_1=\mathcal{S}^{(11)}+\omega^2+k_1^2-\tfrac{1}{4},\quad \mathcal{S}_2=\mathcal{S}^{(22)}+\omega^2+k_2^2-\tfrac{1}{4},$$

$$\mathcal{S}_3=\mathcal{S}^{(11)}+\mathcal{S}^{(22)}-2\mathcal{S}^{(12)}+\tfrac{1}{2}-k_1^2-k_2^2.$$

Using these relations and our theory we can verify the quadratic algebra structure for (8).

V. FINE STRUCTURE FOR 2D SUPERINTEGRABLE SYSTEMS: A ONE-PARAMETER POTENTIAL

Here we consider a superintegrable system that admits three functionally independent constants of the motion, but only for a one-parameter family of potentials $V(x,y)=\alpha V^{(0)}(x,y)$, where the gradient of $V^{(0)}$ is nonzero. If the one-parameter family of potentials cannot be extended to a two-parameter family, then by the proof of Lemma 1 the system must admit a four-dimensional family of symmetries $\Sigma a_{(k)}^{ij}p_ip_j+W^{(k)}$, $k=1,\ldots,4$. The Bertrand–Darboux equations for the potential are equivalent to a single first-order equation that, without loss of generality, we can write as

$$V_1+DV_2=0. \tag{66}$$

We change variables to a new orthogonal coordinate system $\{u,v\}$ so that (66) transforms to $\partial_u V=0$. In these coordinates the Bertrand–Darboux equation for a symmetry becomes

$$-V_{vv}\lambda a^{12}=[(\lambda a^{12})_v-(\lambda a^{22})_u]V_v \tag{67}$$

where

$$-\lambda a^{12}A(v) = (\lambda a^{12})_v - (\lambda a^{22})_u$$

for all symmetries a^{ij}. Thus the equation for the potential $V(v)$ becomes $V_{vv}=A(v)V_v$.

The equations for a second-order symmetry are now

$$(\lambda a^{11})_u = -\lambda_v a^{12},$$

$$(\lambda a^{22})_u = \tfrac{2}{3}A(v)\lambda a^{12} + \tfrac{1}{3}\lambda_v a^{12} + \tfrac{1}{3}\lambda_u(a^{22} - a^{11}),$$

$$(\lambda a^{22})_v = -\lambda_u a^{12}, \tag{68}$$

$$(\lambda a^{12})_v = -\tfrac{1}{3}A(v)\lambda a^{12} + \tfrac{1}{3}\lambda_v a^{12} + \tfrac{1}{3}\lambda_u(a^{22} - a^{11}),$$

$$2(\lambda a^{12})_u + (\lambda a^{11})_v = \lambda_u a^{12} + \lambda_v(a^{11} - a^{22}).$$

From the integrability condition $\partial_u(\lambda a^{22})_v = \partial_v(\lambda a^{22})_u$ and (68) we can derive an equation of the form $\lambda_u a_v^{22}=\cdots$ where the right-hand side does not depend on the derivatives of the a^{ij}. If $\lambda_u \neq 0$ then we have an involutory system $a_u^{ij}=\cdots$, $a_v^{ij}=\cdots$ at the first derivative level. Hence the space of symmetries would be at most three-dimensional. This is a contradiction, so we must have $\lambda_u = 0$. This implies that the system admits the first-order symmetry $L=p_u$ as well as a second-order symmetry p_u^2.

Introducing these simplifications into (68) and setting $a_v^{11}=s$ we obtain the involutive system

$$a_u^{11} = -\frac{\lambda'}{\lambda}a^{12},$$

$$a_u^{22} = \frac{2}{3}A(v)a^{12} + \frac{1}{3}\frac{\lambda'}{\lambda}a^{12},$$

$$a_v^{22} = -\frac{\lambda'}{\lambda}a^{22},$$

$$a_v^{12} = -\left(\frac{1}{3}A(v) + \frac{2}{3}\frac{\lambda'}{\lambda}\right)a^{12}, \tag{69}$$

$$a_u^{12} = -\frac{1}{2}\left(\frac{\lambda'}{\lambda}a^{22} + s\right),$$

$$s_u = \left(-\left(\frac{\lambda'}{\lambda}\right)' + \frac{1}{3}\frac{\lambda'}{\lambda}\left(2\frac{\lambda'}{\lambda} + A(v)\right)\right)a^{12},$$

$$s_v = \frac{1}{3}\left(2\frac{\lambda'}{\lambda} + A(v)\right)\left(-\frac{\lambda'}{\lambda}a^{22} - s\right) + \left(\left(\frac{\lambda'}{\lambda}\right)^2 - \left(\frac{\lambda'}{\lambda}\right)'\right)a^{22},$$

where $\lambda=\lambda(v)$. This system can depend on at most four constants a^{11}, a^{12}, a^{22}, s at a regular point. Since the system is at least four-dimensional, we see that it is *exactly* four-dimensional and that the integrability conditions must be satisfied. (Thus the system corresponds to a Darboux space.[41,35,36]) The only nontrivial integrability condition is $\partial_u a_v^{22} = \partial_v a_u^{22}$ or

$$2A' - \frac{2}{3}A^2 + \frac{1}{3}A\frac{\lambda'}{\lambda} + \frac{1}{3}\left(\frac{\lambda'}{\lambda}\right)^2 + \left(\frac{\lambda'}{\lambda}\right)' = 0. \tag{70}$$

In terms of the potential function V, this condition can be expressed as

$$\frac{\lambda'}{\lambda} + 2\frac{V''}{V'} = \alpha\lambda^{-1/3}(V')^{1/3}$$

for α a constant.

Theorem 9: *Every system with a one-parameter potential and three functionally independent second-order symmetries is the restriction of some three-parameter potential to a single parameter, such that the restricted potential is annihilated by some first-order symmetry of the Darboux space*.

Proof: From the discussion above, we can pass to coordinates u,v such that the system takes the form

$$H = \frac{p_u^2 + p_v^2}{\lambda(v)} + \gamma V(v).$$

The Poisson bracket $\{p_u, S\}$ for any second-order symmetry $S=\Sigma a^{ij}p_ip_j+W$ of our system is also a second-order symmetry $\Sigma a_u^{ij}p_ip_j+W_u$. Thus the linear operation of differentiating with respect to u leaves the four-dimensional space of second-order symmetries invariant. We can get more detailed information about this space by choosing a basis in which ∂_u is in Jordan canonical form. A two-dimensional subspace of the symmetries is spanned by H and p_u^2, which are in the null space of ∂_u. Thus the possible Jordan forms for ∂_u are

$$(i):\begin{pmatrix} \xi_1 & 0 & 0 & 0 \\ 0 & \xi_2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (ii):\begin{pmatrix} \xi & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$(iii):\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (iv):\begin{pmatrix} \xi & 1 & 0 & 0 \\ 0 & \xi & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$(v):\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

where ξ and ξ_1 are nonzero.

We will use these canonical forms to show that there always exists a three-dimensional subspace of the four parameter subspace of second-order symmetries and a nondegenerate potential $\tilde{V}$, containing, V as a special case, such that the subspace is spanned by $\tilde{H}=(p_u^2+p_v^2)/\lambda+\tilde{V}$, $p_u^2+\tilde{W}_1$, and $\Sigma a^{ij}p_ip_j+\tilde{W}_2$ where $\Sigma a^{ij}p_ip_j+W_k$ is one of the symmetries of the one-parameter system. First note from the Bertrand–Darboux equations and Eq. (69) that the defining equations for the nondegenerate potential associated to these three symmetries must be

$$\tilde{V}_{vv} = \tilde{V}_{uu} + 3(\ln a^{12})_u \tilde{V}_u + A(v)\tilde{V}_v,$$
$$\tilde{V}_{uv} = -\frac{\lambda'}{\lambda}\tilde{V}_u. \tag{71}$$

Here $(\ln a^{12})_{uv} = 0$ and $\Sigma a^{ij}p_i p_j + W_k$ is the third symmetry. The integrability conditions for Eq. (71) reduce to the single requirement

$$A\left(\frac{\lambda'}{\lambda}\right)' + A'\left(\frac{\lambda'}{\lambda}\right) + 2\left(\frac{\lambda'}{\lambda}\right)\left(\frac{\lambda'}{\lambda}\right)' - \left(\frac{\lambda'}{\lambda}\right)'' = 0. \tag{72}$$

Consider the case where ∂_u acting on the space of second-order symmetries has an eigenvector S with eigenvalue $\xi \neq 0$. Then this symmetry must have the form

$$a^{11} = b^{11}(v)e^{\xi u}, \quad a^{12} = b^{12}(v)e^{\xi u}, \quad a^{22} = b^{22}(v)e^{\xi u}.$$

Substituting these expressions into Eq. (69) we obtain the conditions

$$2\xi^2 - \left(\frac{\lambda'}{\lambda}\right)' + \left(\frac{\lambda'}{\lambda}\right)^2 + A\frac{\lambda'}{\lambda} = 0, \quad (\ln a^{12})_u = \xi \tag{73}$$

which, together with (70), implies (72). Further, the integrability conditions for the three symmetries $\tilde{H}$, $p_u^2 + \tilde{W}$, S to correspond to a nondegenerate potential are

$$18\xi^2 = 12\left(\frac{\lambda'}{\lambda}\right)' - 8\left(\frac{\lambda'}{\lambda}\right)^2 - 8A\frac{\lambda'}{\lambda} + 6A' - 2A^2, \quad 2\xi^2 = \left(\frac{\lambda'}{\lambda}\right)' - \left(\frac{\lambda'}{\lambda}\right)^2 - A\frac{\lambda'}{\lambda}, \tag{74}$$

and these are also implied by (73) and (70).

For the remaining systems there is a second-order symmetry whose quadratic terms are $S_2 = \Sigma a^{ij}p_i p_j$ such that the quadratic terms in $S_1 = \partial_u S_2$ also correspond to a symmetry, and $\partial_u S_1 \equiv 0$. Clearly, there are constants α,β with $|\alpha|^2 + |\beta|^2 > 0$ and

$$S_1 = \alpha\frac{p_u^2 + p_v^2}{\lambda} + \beta p_u^2, \quad S_2 = uS_1 + T_2(v),$$

where T_2 is a quadratic form in p_u, p_v that depends only on v. From conditions (69) it is straightforward to compute that

$$a^{12} = b^{12}(v), \quad a^{22} = \frac{\alpha u + \beta}{\lambda}, \quad a^{11} = -\frac{\lambda'}{\lambda}b^{12}(v)u + c^{12}(v),$$

and, finally, that

$$-\left(\frac{\lambda'}{\lambda}\right)' + \left(\frac{\lambda'}{\lambda}\right)^2 + A\frac{\lambda'}{\lambda} = 0, \quad (\ln a^{12})_u = \xi. \tag{75}$$

The integrability conditions for the three symmetries $\tilde{H}$, $p_u^2 + \tilde{W}$, $S_2 + \tilde{W}_2$ to correspond to a nondegenerate potential are

$$0 = 12\left(\frac{\lambda'}{\lambda}\right)' - 8\left(\frac{\lambda'}{\lambda}\right)^2 - 8A\frac{\lambda'}{\lambda} + 6A' - 2A^2, \quad 0 = \left(\frac{\lambda'}{\lambda}\right)' - \left(\frac{\lambda'}{\lambda}\right)^2 - A\frac{\lambda'}{\lambda}, \tag{76}$$

and these, as well as (72) are implied by (73) and (70). Q.E.D.

Remark: It is easy to show using conditions (69) that the Jordan form (iv) does not, in fact, occur.

VI. CONCLUSIONS AND FURTHER WORK

In this paper we have uncovered the structure of 2D classical superintegrable systems with nondegenerate potential and verified the existence of a quadratic algebra of symmetries for all such systems. We have shown how to compute the quadratic algebra relations in general. We have shown that superintegrable systems with degenerate one and two parameter potentials (in addition to the trivial added constant) can be considered as restrictions of nondegenerate systems. We have verified that, with one exception, all nondegenerate superintegrable 2D systems are multiseparable. In the next paper in this series we will develop the properties of the Stäckel transform between superintegrable systems and verify that all nondegenerate 2D systems are Stäckel transforms of 2D constant curvature systems (already classified[44,45]). This will lead to a simple classification of all 2D nondegenerate superintegrable systems. Koenigs[41] in a remarkable paper has already classified all 2D (zero potential) spaces that admit three second-order Killing tensors. Our classification, considerably simpler than Koenigs', will show that all of his spaces also admit nondegenerate potentials. The next papers will extend these results to the case $n=3$, a prelude to a treatment for general n. The case $n=2$ is very special and new techniques have to be developed for higher n. However the basic conclusions and structure theorems can be generalized. We will also show how to solve the quantization problem and carry over the structure theory to the operator case.

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Second order superintegrable systems in conformally flat spaces. II. The classical two-dimensional Stäckel transform

E. G. Kalnins
Department of Mathematics and Statistics, University of Waikato, Hamilton, New Zealand

J. M. Kress[a)]
School of Mathematics, The University of New South Wales, Sydney NSW 2052, Australia

W. Miller, Jr.
School of Mathematics, University of Minnesota, Minneapolis, Minnesota, 55455

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This paper is one of a series that lays the groundwork for a structure and classification theory of second order superintegrable systems, both classical and quantum, in conformally flat spaces. Here we study the Stäckel transform (or coupling constant metamorphosis) as an invertible mapping between classical superintegrable systems on different spaces. Through the use of this tool we derive and classify for the first time all two-dimensional (2D) superintegrable systems. The underlying spaces are exactly those derived by Koenigs in his remarkable paper giving all 2D manifolds (with zero potential) that admit at least three second order symmetries. Our derivation is very simple and quite distinct. We also show that every superintegrable system is the Stäckel transform of a superintegrable system on a constant curvature space. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1894985]

I. INTRODUCTION

This is a sequel to our first paper.[1] Our purpose is to lay the groundwork for a structure and classification theory of second order superintegrable systems, both classical and quantum, in complex conformally flat spaces. Real spaces are considered as restrictions of these to the various real forms. In Ref. 1 we have given examples, described the background as well as the interest and importance of these systems in mathematical physics and given many relevant references. Observed features of the systems are multiseparability, closure of the quadratic algebra of second order symmetries at order 6, use of representation theory of the quadratic algebra to derive spectral properties of the quantum Schrödinger operator, and a close relationship with exactly solvable and quasiexactly solvable problems.[2–9] Our approach is, rather than focus on particular spaces and systems, to use a general theoretical method based on integrability conditions to derive structure common to all systems.

In this paper we study the Stäckel transform, or coupling constant metamorphosis,[10,11] for two-dimensional(2D) classical superintegrable systems. Recall that for a classical 2D system on a Riemannian manifold we can always choose local coordinates x,y, not unique, such that the Hamiltonian takes the form

$$H=\frac{p_1^2+p_2^2}{\lambda(x,y)}+V(x,y).$$

a)Electronic mail: j.kress@unsw.edu.au

This system is *second order superintegrable* with *nondegenerate* potential $V=V(x,y,\alpha,\beta,\gamma)$ if it admits three functionally independent quadratic constants of the motion

$$S_k = \sum_{ij} a^{ij}_{(k)} p_i p_j + W_{(k)}(x,y,\alpha,\beta,\gamma).$$

(We also refer to these constants of the motion as symmetries because; each leads to a conserved quantity for the associated physical system; their Poisson brackets with the Hamiltonian vanish, so that they are generalized symmetries in the Lie sense; and their quantizations lead to second order partial differential operators that commute with the Schrödinger operator, so are again generalized symmetries in the Lie sense.) The potential V is nondegenerate in the sense that at any regular point x_0,y_0 where the potential is defined and analytic and the S_k are functionally independent, we can prescribe the values of $V_1(x_0,y_0),V_2(x_0,y_0),V_{11}(x_0,y_0)$ arbitrarily by choosing appropriate values for the parameters α,β,γ. Here, $V_1=\partial V/\partial x$, $V_2=\partial V/\partial y$, etc. [Another way to look at this is to say that $V_1(x_0,y_0),V_2(x_0,y_0),V_{11}(x_0,y_0)$ are the parameters.] This is in addition to the trivial constant that we can always add to a potential. This requirement implies that the potential satisfies a system of coupled PDEs of the form

$$V_{22} = V_{11} + A^{22}(x,y)V_1 + B^{22}(x,y)V_2, \quad V_{12} = A^{12}(x,y)V_1 + B^{12}(x,y)V_2.$$

The Stäckel transform is a conformal transformation of a superintegrable system on one space to a superintegrable system on another space. We prove that all nondegenerate 2D superintegrable systems are Stäckel transforms of constant curvature systems and give a complete and simple classification of all 2D superintegrable systems. The following papers will extend these results to three-dimensional (3D) systems and the quantum analogs of 2D and 3D classical systems.

II. THE STÄCKEL TRANSFORM FOR TWO-DIMENSIONAL SYSTEMS

The Stäckel transform[10] or coupling constant metamorphosis[11] plays a fundamental role in relating superintegrable systems on different manifolds. The basic idea behind this transform has long been observed in various important classical and quantum mechanical systems. One of the most familiar is the Hamilton–Jacobi equation for the classical Coulomb problem $H\equiv p_1^2+p_2^2+p_3^2+Z/r=E$ where r is the radial coordinate and Z is the charge. Division of the equation by the potential term r^{-1} converts it into the pseudo-Coulomb problem $H'\equiv r(p_1^2+p_2^3+p_3^2)-Er=-Z$, much easier to solve from a group theoretic point of view, where the space has changed and the energy and charge have switched roles. In Ref. 11 it was pointed out that if $H+ZV(\mathbf{x})=E$ is an integrable Hamiltonian system for some additive potential V and all values of the parameters Z,E, then the system $H/V-E/V=Z$ is also integrable, where the parameters E and Z have changed roles. This general transformation was called coupling constant metamorphosis. Independently in Ref. 10 it was observed that if the Hamilton–Jacobi equations $\Sigma g^{ij}p_1p_j+V(\mathbf{q})=E$, $\Sigma g^{ij}p_1p_j+U(\mathbf{q})=E$ each admit a complete integral via separation of variables in the orthogonal coordinates $\mathbf{q}$, where U is nonzero, then the system $U^{-1}\Sigma g^{ij}p_1p_j+U^{-1}V(\mathbf{q})=E'$ also admits a complete integral via separation in the same coordinates, but on a different manifold. The second order constants of the motion that describe the separation and the corresponding Stäckel matrices are mapped into one another by the transformation. We called this the Stäckel transform since it preserved the Stäckel form of the separable system. All of these observations have straightforward extensions to n dimensions and to the corresponding quantum mechanical operators.

Suppose we have a superintegrable system

$$H = \frac{p_1^2+p_2^2}{\lambda(x,y)} + V(x,y) \tag{1}$$

in local orthogonal coordinates, with nondegenerate potential $V(x,y)$,

$$V_{22} = V_{11} + A^{22}V_1 + B^{22}V_2,$$
$$V_{12} = A^{12}V_1 + B^{12}V_2 \tag{2}$$

and suppose $U(x,y)$ is a particular solution of equations (2), nonzero in an open set. Then the transformed system

$$\tilde{H} = \frac{p_1^2 + p_2^2}{\tilde{\lambda}(x,y)} + \tilde{V}(x,y) \tag{3}$$

with nondegenerate potential $\tilde{V}(x,y)$,

$$\tilde{V}_{22} = \tilde{V}_{11} + \tilde{A}^{22}\tilde{V}_1 + \tilde{B}^{22}\tilde{V}_2,$$
$$\tilde{V}_{12} = \tilde{A}^{12}\tilde{V}_1 + \tilde{B}^{12}\tilde{V}_2 \tag{4}$$

is also superintegrable, where

$$\tilde{\lambda} = \lambda U, \quad \tilde{V} = \frac{V}{U},$$

$$\tilde{A}^{12} = A^{12} - \frac{U_2}{U}, \quad \tilde{A}^{22} = A^{22} + 2\frac{U_1}{U}, \quad \tilde{B}^{12} = B^{12} - \frac{U_1}{U}, \quad \tilde{B}^{22} = B^{22} - 2\frac{U_2}{U}.$$

Let $S=\Sigma a^{ij}p_ip_j+W=S_0+W$ be a second order symmetry of H and $S_U=\Sigma a^{ij}p_ip_j+W_U=S_0+W_U$ be the special case of this that is in involution with $p_1^2+p_2^2/\lambda+U$. Then

$$\tilde{S} = S_0 - \frac{W_U}{U}H + \frac{1}{U}H$$

is the corresponding symmetry of $\tilde{H}$. Since one can always add a constant to a nondegenerate potential, it follows that $1/U$ defines an inverse Stäckel transform of $\tilde{H}$ to H. See Refs. 10 and 12 for many examples of this transform. We say that two superintegrable systems are Stäckel equivalent if one can be obtained from the other by a Stäckel transform.

A. A Stäckel transform approach to the classification of nondegenerate superintegrable systems

Through the use the Stäckel transform we can develop a method for classifying 2D nondegenerate superintegrable systems that is differential equations based. (In particular it is distinct from the Koenigs analytic function approach to finding spaces that admit at least three second order Killing tensors.) Let

$$ds^2 = \lambda(x,y)(dx^2 + dy^2)$$

be a metric for a nondegenerate superintegrable system. We recall from Sec. 2 of Ref. 1 that necessary and sufficient conditions for a^{ij} to be a second order Killing tensor for λ are that

$$\Delta a^{12} = 0, \quad \Delta(a^{11} - a^{22}) = 0, \quad \Delta = \partial_x^2 + \partial_y^2,$$

where

$$(a^{22} - a^{11})_2 = 2a_1^{12}, \quad (a^{22} - a^{11})_1 = -2a_2^{12},$$

and the a^{ij} satisfy the integrability condition

$$(\lambda_{22}-\lambda_{11})a^{12}-\lambda_{12}(a^{22}-a^{11})=3\lambda_1 a_1^{12}-3\lambda_2 a_2^{12}+(a_{11}^{12}-a_{22}^{12})\lambda. \tag{5}$$

Since λ is nondegenerate superintegrable we have three independent symmetries of the form $\mathcal{S}=\Sigma a^{ij}p_ip_j+W$ and a nondegenerate potential V satisfying the Bertrand–Darboux equations

$$(V_{22}-V_{11})a^{12}+V_{12}(a^{11}-a^{22})=\left[\frac{(\lambda a^{12})_1-(\lambda a^{11})_2}{\lambda}\right]V_1+\left[\frac{(\lambda a^{22})_1-(\lambda a^{12})_2}{\lambda}\right]V_2 \tag{6}$$

for all symmetries with quadratic terms a^{ij}.

For a superintegrable system we can always use the independent symmetries to solve equations (6) for $V_{22}-V_{11}, V_{12}$ in the form (2). If these two equations are the only conditions on the potential function V then it will depend on four parameters, the maximum number possible. Thus we can prescribe the derivatives V_1, V_2, V_{11} and the value of V at a fixed point. This is the case of a nondegenerate potential. If, however, the equations (6) put additional conditions on the potential then there will be a restriction on the first derivatives and the potential will depend on fewer parameters than four. In this case the potential is degenerate. In Ref. 1 we showed that superintegrable systems with three and two parameter potentials were, essentially, just restrictions of the four parameter nondegenerate potentials. One parameter potentials (i.e., constant potentials) are different. They in general are not restrictions of nondegenerate potentials and, indeed, the quadratic algebra structure may not hold. See Ref. 13 for a counterexample.

Returning to our nondegeneracy assumption, the system of equations (6) has a four parameter family of solutions V, counting the addition of a scalar to V as a parameter. Also, every Stäckel transform of this system to a system with metric μ must be of the form $\hat{V}=\mu/\lambda$ where $V=\hat{V}$ is some particular solution of the equations (6). Thus it is of interest to determine the equations that characterize μ.

To simplify the computations to follow, we recall that we can choose our orthogonal coordinates x,y such that one of our symmetries takes the form $a^{12}\equiv 0$, $a^{22}-a^{11}=1$. In this system the symmetry and (5) imply $\lambda_{12}=0$, and, as we will see, $\mu_{12}=0$. A second symmetry is defined by the Hamiltonian itself, $a^{11}=a^{22}=1/\lambda$, $a^{12}=0$, which clearly always satisfies equations (5) and (6). Due to nondegeneracy, for the third symmetry we must have $a^{12}\neq 0$ and it is on this third symmetry that we will focus our attention in the following. Now the fundamental integrability conditions can be rewritten as

$$\lambda_{12}=0, \quad \lambda_{22}-\lambda_{11}=3\lambda_1 A_1-3\lambda_2 A_2+(A_{11}+A_1^2-A_{22}-A_2^2)\lambda, \tag{7}$$

where $A=\ln a^{12}$ and the subscripts denote differentiation. Similarly, using this result and (6) we find that the equations characterizing μ are

$$\mu_{12}=0, \quad \mu_{22}-\mu_{11}=3\mu_1 A_1-3\mu_2 A_2+(A_{11}+A_1^2-A_{22}-A_2^2)\mu. \tag{8}$$

Note that these two equations appear identical. However they have different interpretations. The fixed metric λ satisfies (7) and is a special solution of (8). Here μ designates a four-parameter family of solutions, of which λ is a particular special case. It follows that A satisfies the integrability conditions for this system.

Let us apply ∂_{12} to both sides of (8). The result, using $\mu_{12}=0$ and $\Delta a^{12}=0$, is

$$0=3A_{12}(\mu_{11}-\mu_{22})+(3A_{112}+2[A_{11}+A_1^2]_2)\mu_1+(-3A_{122}+2[A_{11}+A_1^2]_1)\mu_2+2\mu(A_{11}+A_1^2)_{12}. \tag{9}$$

There are two possibilities here.

(1) *Case I:* $A_{12}=0$. Then every term in the preceding equation vanishes identically. We conclude that a^{12} factors as $a^{12}=X(x)Y(y)$, where $\Delta a^{12}=0$. Thus there is a constant α such that

$$X'' = \alpha^2 X, \quad Y'' = -\alpha^2 Y.$$

We have solutions

$$X(x) = \beta_1 e^{\alpha x} + \beta_2 e^{-\alpha_2 x}, \quad Y(y) = \gamma_1 e^{i\alpha y} + \gamma_1 e^{-i\alpha y}.$$

Variables separate in the equations for μ into two ODEs. Thus for every choice of a^{12} we can find all solutions μ explicitly.

(2) *Case II:* $A_{12} \neq 0$. Now the coefficients of μ_{11}, μ_{22} in (9) are nonvanishing. The equation can be rewritten as

$$\mu_{22} - \mu_{11} = \mu_1 \left[\frac{3A_{112} + 2(A_{11} + A_1^2)_2}{3A_{12}} \right] + \mu_2 \left[\frac{-3A_{122} + 2(A_{11} + A_1^2)_1}{3A_{12}} \right] + 2\mu(A_{11} + A_1^2)_{12}.$$

Since μ is a four-parameter solution, the coefficients of μ_1, μ_2, and μ can be equated. Thus we have three new identities, which together with $\Delta a^{12} = 0$ give

$$\begin{gathered} \text{(i) } 9A_1A_{12} = 3A_{112} + 2(A_{11} + A_1^2)_2, \quad \text{(ii) } 9A_2A_{12} = 3A_{122} + 2(A_{22} + A_2^2)_1, \\ \text{(iii) } 3(A_{11} + A_1^2)A_{12} = (A_{11} + A_1^2)_{12}, \quad \text{(iv) } A_{11} + A_1^2 + A_{22} + A_2^2 = 0. \end{gathered} \tag{10}$$

The first two identities imply $A_{12} = Ce^A$ for some nonzero constant C. This is the Liouville equation with general solution

$$a^{12} = e^A = \frac{2X'(x)Y'(y)}{C(X(x) + Y(y))^2},$$

where $X(x)$ and $Y(y)$ are functions such that $X'(x)Y'(y) \neq 0$. At this point it is convenient to use X, Y as new coordinates. Thus there are functions $F(X), G(Y)$ such that

$$(X')^2 = F(X), \quad X'' = \tfrac{1}{2}F'(X), \quad (Y')^2 = G(Y), \quad Y'' = \tfrac{1}{2}G'(Y).$$

Substituting these expressions into the identities (i)–(iv) we obtain a system of functional differential equations for F, G with the general solution

$$F(X) = \frac{\alpha}{24}X^4 + \frac{\gamma_1}{6}X^3 + \frac{\gamma_2}{2}X^2 + \gamma_3 X + \gamma_4,$$

$$G(Y) = -\frac{\alpha}{24}Y^4 + \frac{\gamma_1}{6}Y^3 - \frac{\gamma_2}{2}Y^2 + \gamma_3 Y - \gamma_4,$$

where α, γ_j are constants. Note that the equations for x, y in terms of X, Y take the form of elliptic integrals,

$$x = \int \frac{dX}{\sqrt{\frac{\alpha}{24}X^4 + \frac{\gamma_1}{6}X^3 + \frac{\gamma_2}{2}X^2 + \gamma_3 X + \gamma_4}},$$

$$y = \int \frac{dY}{\sqrt{\frac{-\alpha}{24}Y^4 + \frac{\gamma_1}{6}Y^3 - \frac{\gamma_2}{2}Y^2 + \gamma_3 Y - \gamma_4}}.$$

Again, variables separate into two ODEs in the equations for μ. Thus for every choice of a^{12} we can find all solutions μ explicitly.

Theorem 1: If $ds^2 = \lambda(dx^2 + dy^2)$ is the metric of a nondegenerate superintegrable system (expressed in coordinates x, y such that $\lambda_{12} = 0$) then $\lambda = \mu$ is a solution of the system

$$\mu_{12}=0, \quad \mu_{22}-\mu_{11}=3\mu_1(\ln a^{12})_1-3\mu_2(\ln a^{12})_2+\left(\frac{a_{11}^{12}-a_{22}^{12}}{a^{12}}\right)\mu, \tag{11}$$

where either

$$\text{(I) } a^{12}=X(x)Y(y), \quad X''=\alpha^2 X, \quad Y''=-\alpha^2 Y,$$

or

$$\text{(II) } a^{12}=\frac{2X'(x)Y'(y)}{C(X(x)+Y(y))^2},$$

$$(X')^2=F(X), \quad X''=\frac{1}{2}F'(X), \quad (Y')^2=G(Y), \quad Y''=\frac{1}{2}G'(Y),$$

where

$$F(X)=\frac{\alpha}{24}X^4+\frac{\gamma_1}{6}X^3+\frac{\gamma_2}{2}X^2+\gamma_3 X+\gamma_4,$$

$$G(Y)=-\frac{\alpha}{24}Y^4+\frac{\gamma_1}{6}Y^3-\frac{\gamma_2}{2}Y^2+\gamma_3 Y-\gamma_4.$$

Conversely, every solution λ of one of these systems defines a nondegenerate superintegrable system. If λ is a solution then the remaining solutions μ are exactly the nondegenerate superintegrable systems that are Stäckel equivalent to λ.

This result provides the basis for a simple classification of all nondegenerate superintegrable systems. In fact the spaces that arise correspond one-to-one with Koenigs' tables of 2D spaces that admit at least three second order symmetries. Indeed, from the fact that $F(X)$ and $G(Y)$ are fourth order polynomials we can determine which solutions of the functions $X(x)$ and $Y(y)$ yield the lists drawn up by Koenigs in his two tables. (We give the details of these tables in Sec. II B.)

To understand more clearly the significance of cases (I) and (II) in the preceding theorem, we make use of the symmetry of equations (8), first exploited by Koenigs. We write the system in the form

$$a_{11}^{12}+a_{22}^{12}=0, \quad \mu_{12}=0, \quad a^{12}(\mu_{11}-\mu_{22})+3\mu_1 a_1^{12}-3\mu_2 a_2^{12}+(a_{11}^{12}-a_{22}^{12})\mu=0, \tag{12}$$

Lemma 1: Suppose $\mu=\lambda(x,y)$, $a^{12}=a(x,y)$ satisfy (12). Then $\mu=\tilde{a}(x,y)$, $a^{12}=\tilde{\lambda}(x,y)$ also satisfy (12) where

$$\tilde{a}(x,y)=a(x+y,ix-iy), \quad \tilde{\lambda}(x,y)=\lambda(x-iy,y-ix).$$

This transformation is invertible.

Proof: It is straightforward to check that $\tilde{a}_{12}=0$, $\tilde{\lambda}_{11}+\tilde{\lambda}_{22}=0$. The symmetry of the third equation under this invertible transform is obvious. Q.E.D.

Theorem 2: System (12) characterizes a nondegenerate superintegrable system if and only if the metric $\tilde{a}^{12}(x,y)$ is of constant curvature. Equivalently, the system (12) characterizes a nondegenerate superintegrable system if and only if the symmetry a^{12} is the image $a^{12}=\tilde{\lambda}$ where the metric λ (with $\lambda_{12}=0$ is of constant curvature).

Proof: System (12) characterizes a nondegenerate superintegrable system if and only if the symmetry a^{12} satisfies the Liouville equation $(\ln a^{12})_{12}=Ca^{12}$ for some constant C. [If $C=0$ we have case (I), and if $C\neq 0$ we have case (II).] It is straightforward to check that this means that

$$\frac{\tilde{a}^{12}_{11}+\tilde{a}^{12}_{22}}{(\tilde{a}^{12})^2}-\frac{(\tilde{a}^{12}{}_1)^2+(\tilde{a}^{12}_2)^2}{(\tilde{a}^{12})^3}=4iC,$$

so the scalar curvature of metric $\tilde{a}^{12}(dx^2+dy^2)$ is constant. Similarly, if λ is of constant curvature then $\tilde{\lambda}$ satisfies Liouville's equation. Q.E.D.

Theorem 3: Every nondegenerate superintegrable 2D system is Stäckel equivalent to a nondegenerate superintegrable system on a constant curvature space.

Proof: Every nondegenerate superintegrable 2D system with metric $\lambda(dx^2+dy^2)$ corresponds to a function a^{12}_0 and a system of equations (12) (with $a^{12}=a^{12}_0$) where $\mu=\lambda$ is a solution and the integrabilty conditions are satisfied identically, so that the space of solutions μ is four dimensional. From Theorem 1 we see that a^{12}_0 must satisfy the Liouville equation, so by Theorem 2 the metric $\xi=\tilde{a}^{12}_0$ is of constant curvature. Recall that the space of second order symmetries of a constant curvature space is six dimensional. Consider the possible symmetries a^{12} such that standard equations

$$a^{12}_{11}+a^{12}_{22}=0,\quad a^{12}(\xi_{11}-\xi_{22})+3\xi_1 a^{12}_1-3\xi_2 a^{12}_2+(a^{12}_{11}-a^{12}_{22})\xi=0$$

are satisfied. One constant curvature space symmetry with $a^{12}=0$ determines the separable coordinates $\{x,y\}$ and one symmetry is the Hamiltonian $(p_1^2+p_2^2)/\lambda$. A basis for the remaining symmetries consists of four linearly independent symmetries with a^{12} harmonic and nonzero. It is clear that the Koenig duality mapping $\tilde{\mu}$ for μ a solution of system (12) maps the four-dimensional space of solutions μ (except $\mu=0$) one-to-one onto the constant curvature space symmetries with a^{12} harmonic and nonzero. For constant curvature spaces we know that there are symmetries a^{12} that define nondegenerate superintegrable systems (the systems on flat space and the 2-sphere.) Let $a^{12}=b^{12}$ be one such symmetry. By Theorem 1 b^{12} satisfies the Liouville equation. Since the Koenigs duality map is onto, there must exist a solution $\mu=\nu$ of system (12) such that $\tilde{\nu}=b^{12}$. By Theorem 2 ν is the metric of a constant curvature space. This means that the system with metric λ is Stäckel equivalent to the constant curvature system with metric ν. Q.E.D.

B. Examples and relationship with the Koenigs tables

In a tour de force, Koenigs[14] has classified all 2D manifolds that admit exactly three second order Killing tensors and listed them in two tables, Table VI and Table VII.

In each case Koenigs gave the terms that give rise to the leading coefficients of the additional quadratic constant of the motion not implicitly defined by the Liouville form of the metric. We have given these metrics in a symmetric orthogonal form.

We can now reproduce the tables via the duality between separable coordinate systems on spaces of constant curvature and the form of the Killing tensors admitted in these particular coordinate systems.

For example, taking $\alpha=1$ in case (I), a solution for a^{12} is

$$X(x)=\sin x,\quad Y(y)=\sinh y\Rightarrow a^{12}=\sin x\sinh y.$$

Now $\mu_{12}=0\Rightarrow\mu=f(x)+g(y)$ and so Eq. (11) for μ becomes

$$g''-f''=3f'\cot x-3g'\coth x-2(f+g)$$

which separates into a pair of ordinary differential equations,

$$g''+3\coth y g'+2g=K,\quad f''+\cot x f'-2f=K,$$

for some separation constant K. These equations have solutions

$$f(x)=\frac{c_1\cos x+c_2}{\sin^2 x}-\frac{1}{2}K,\quad g(y)=\frac{c_3\cosh y+c_4}{\sinh^2 y}+\frac{1}{2}K$$

and so

$$\mu = \frac{c_1 \cos x + c_2}{\sin^2 x} + \frac{c_3 \cosh y + c_4}{\sin^2 y}. \tag{13}$$

In the preceding, we have used coordinates in which the metric was a multiple of $dx^2 + dy^2$, while Koenigs used coordinates in which the metric was a multiple of $dx\, dy$. To bridge this gap, we make the change of coordinates $x \to a$, $y \to ib$ to obtain (with a trivial redefinition of the parameters c_i) the first metric in Table VI.

The remaining metrics in Table VI are obtained by similar calculations using the following particular solutions to the case (I) equations in Theorem 1:

(1) $X = \sin x, \quad Y = \sinh y,$

(2) $X = \sinh x, \quad Y = e^{iy},$

(3) $X = e^x, \quad Y = e^{iy},$

(4) $X = x, \quad Y = y,$

(5) $X = x, \quad Y = 1,$

(6) $X = Y = 1,$

The metrics in Table VII are obtained from particular solutions to the case (II) equations in Theorem 1 in the same way as described for Table VI.

(1) Both $F(X)$ and $G(Y)$ are general fourth order polynomials,

(2) $$\left.\begin{aligned} 4F(X) &= 1 - X^2 \\ 4G(Y) &= Y^2 - 1 \end{aligned}\right\} \Rightarrow \begin{cases} X = -2\cos 2x, \\ Y = \cosh 2y, \end{cases}$$

(3) $$\left.\begin{aligned} F(X) &= X^2(X-1)^2 \\ G(Y) &= -Y^2(Y+1)^2 \end{aligned}\right\} \Rightarrow \begin{cases} X = \dfrac{1}{1+e^x}, \\ Y = \dfrac{1}{-1+e^{iy}}, \end{cases}$$

(4) $$\left.\begin{aligned} F(X) &= X^3(X-1) \\ G(Y) &= -Y^3(Y+1) \end{aligned}\right\} \Rightarrow \begin{cases} X = \dfrac{1}{1-\frac{1}{4}x^2}, \\ Y = -\dfrac{1}{1+\frac{1}{4}y^2}, \end{cases}$$

$$(5)\qquad \left.\begin{aligned} F(X) &= 1 \\ G(Y) &= 1 \end{aligned}\right\} \Rightarrow \begin{cases} X = x, \\ Y = y, \end{cases}$$

There are clearly other choices possible for X and Y but they revert to various versions of the cases given in Koenigs' tables. Since a single space may have more than one nondegenerate potential, our classification may include a space more than once.

Next, we examine each of his spaces and show in detail what was proved in the last section: that every superintegrable system on the space can be obtained as the Stäckel transform of a constant curvature space with respect to Koenigs Table VI,

$$(1)\qquad ds^2 = \left[\frac{c_1\cos a + c_2}{\sin^2 a} + \frac{c_3\cos b + c_4}{\sin^2 b}\right](da^2 - db^2)$$

$$(2)\qquad ds^2 = \left[\frac{c_1\cosh a + c_2}{\sinh^2 a} + \frac{c_3 e^b + c_4}{e^{2b}}\right](da^2 - db^2)$$

$$(3)\qquad ds^2 = \left[\frac{c_1 e^a + c_2}{e^{2a}} + \frac{c_3 e^b + c_4}{e^{2b}}\right](da^2 - db^2)$$

$$(4)\qquad ds^2 = \left[c_1(a^2 - b^2) + \frac{c_2}{a^2} + \frac{c_3}{b^2} + c_4\right](da^2 - db^2)$$

$$(5)\qquad ds^2 = \left[c_1(a^2 - b^2) + \frac{c_2}{a^2} + c_3 b + c_4\right](da^2 - db^2)$$

$$(6)\qquad ds^2 = [c_1(a^2 - b^2) + c_2 a + c_3 b + c_4](da^2 - db^2)$$

and Koenigs Table VII,

$$(1)\qquad ds^2 = \left[c_1\left(\frac{1}{\mathrm{sn}^2(a,k)} - \frac{1}{\mathrm{sn}^2(b,k)}\right) + c_2\left(\frac{1}{\mathrm{cn}^2(a,k)} - \frac{1}{\mathrm{cn}^2(b,k)}\right) + c_3\left(\frac{1}{\mathrm{dn}^2(a,k)} - \frac{1}{\mathrm{dn}^2(b,k)}\right) + c_4(\mathrm{sn}^2(a,k) - \mathrm{sn}^2(b,k))\right](da^2 - db^2)$$

$$(2)\qquad ds^2 = \left[c_1\left(\frac{1}{\sin^2 a} - \frac{1}{\sin^2 b}\right) + c_2\left(\frac{1}{\cos^2 a} - \frac{1}{\cos^2 b}\right) + c_3(\cos 2a - \cos 2b) + c_4(\cos 4a - \cos 4b)\right](da^2 - db^2)$$

$$(3)\qquad ds^2 = [c_1(\sin 4a - \sin 4b) + c_2(\cos 4a - \cos 4b) + c_3(\sin 2a - \sin 2b) + c_4(\cos 2a - \cos 2b)](da^2 - db^2)$$

$$(4)\qquad ds^2 = \left[c_1\left(\frac{1}{a^2} - \frac{1}{b^2}\right) + c_2(a^2 - b^2) + c_3(a^4 - b^4) + c_4(a^6 - b^6)\right](da^2 - db^2)$$

$$(5)\qquad ds^2 = [c_1(a - b) + c_2(a^2 - b^2) + c_3(a^3 - b^3) + c_4(a^4 - b^4)](da^2 - db^2)$$

to a nondegenerate superintegrable potential. In Refs. 3–16 the authors have computed all the

nondegenerate (and degenerate) superintegrable potentials for complex 2D flat space, potentials [**E1**]–[**E20**], and nonzero constant curvature space, potentials [**S1**]–[**S9**], and we identify the relevant potentials on the list that is given in Ref. 16.

1. Table VI

(1) In this case the infinitesimal distance has the form

$$ds^2 = \left(\frac{c_1\cos a + c_2}{\sin^2 a} + \frac{c_3\cos b + c_4}{\sin^2 b}\right)(da^2 - db^2).$$

If we rewrite the Hamilton–Jacobi equation on the sphere,

$$H = p_1^2 + p_2^2 + p_3^2 + \hat{c}_1 + \frac{i\hat{c}_2 s_3}{\sqrt{s_1^2 + s_2^2}} + \frac{\hat{c}_3 s_2}{s_1^2\sqrt{s_1^2 + s_2^2}} + \frac{\hat{c}_4}{s_1^2} = E,$$

using a variant of spherical coordinates

$$s_1 = \frac{\sin b}{\sin a}, \quad s_2 = \frac{\cos b}{\sin a}, \quad s_3 = -i\frac{\cos a}{\sin a}$$

we obtain the form

$$p_b^2 - p_a^2 - \frac{E + \hat{c}_1}{\sin^2 a} - \frac{\hat{c}_2\cos a}{\sin^2 a} - \frac{\hat{c}_3\cos b}{\sin^2 b} - \frac{\hat{c}_4}{\sin^2 b} = 0.$$

Thus the potential from which this metric has been derived via Stäckel transform is [**S7**].

(2) In this case the metric is

$$ds^2 = \left(\frac{c_1\cosh a + c_2}{\sinh^2 a} + c_3 e^{-b} + c_4 e^{-2b}\right)(da^2 - db^2)$$

Choosing Euclidean space coordinates of the form

$$x = \exp\left(-\tfrac{1}{2}u\right)\cosh\left(\tfrac{1}{2}v\right), \quad y = i\exp\left(-\tfrac{1}{2}u\right)\sinh\left(\tfrac{1}{2}v\right)$$

and substituting into the Hamilton–Jacobi equation

$$H = p_x^2 + p_y^2 + \hat{c}_1(x^2 + y^2) + \frac{\hat{c}_2}{x^2} + \frac{\hat{c}_3}{y^2} + \hat{c}_4 = E$$

we obtain the form

$$p_u^2 - p_v^2 + \frac{1}{4}\hat{c}_1 e^{-2u} + \mathcal{C}_2\frac{\cosh v}{\sinh^2 v} + \mathcal{C}_3\frac{1}{\sinh^2 v} + \frac{1}{4}(\hat{c}_4 - E)e^{-u},$$

where $\mathcal{C}_2 = \frac{1}{2}(\hat{c}_2 + \hat{c}_3)$ and $\mathcal{C}_3 = \frac{1}{2}(\hat{c}_3 - \hat{c}_2)$. From this it follows that the potential from which this metric is derived via Stäckel transform is [**E1**].

(3) In this case the infinitesimal distance has the form

$$ds^2 = (c_1 e^{-a} + c_2 e^{-2a} + c_3 e^{-b} + c_4 e^{-2b})(da^2 - db^2).$$

In the variables

$$x = e^{-a}\cosh b, \quad y = -ie^{-a}\sinh b$$

this metric assumes the form

$$ds^2 = \left(\frac{c_1}{\sqrt{x^2 + y^2}} + c_2 + \frac{c_3}{\sqrt{x^2 + y^2}(x + iy)} + \frac{c_4}{(x + iy)^2}\right)(dx^2 - dy^2).$$

We recognize this as arising via Stäckel transform from [**E17**]. Indeed note that if we write out the equation $H=E$ in suitable coordinates we obtain

$$p_1^2 + p_2^2 + \frac{\hat{c}_1}{\sqrt{x^2+y^2}} + \frac{\hat{c}_2}{(x+iy)^2} + \frac{\hat{c}_3}{\sqrt{x^2+y^2}(x+iy)} - E = 0$$

from which we can clearly see the identification.

(4) In this case the infinitesimal distance is

$$ds^2 = \left(c_1(a^2-b^2) + \frac{c_2}{a^2} + \frac{c_3}{b^2} + c_4\right)(da^2 - db^2),$$

and by setting $a=x$, $b=iy$ this metric can be clearly related to a Stäckel transform from the potential [**E1**].

(5) Here

$$ds^2 = \left(c_1(a^2-b^2) + \frac{c_2}{a^2} + c_3 b + c_4\right)(da^2 - db^2).$$

It is clear that this metric is derived by Stäckel transform from the potential

$$V = \hat{c}_1(x^2+y^2) + \frac{\hat{c}_2}{x^2} + \hat{c}_3 y + \hat{c}_4,$$

where $a=x$, $b=iy$. As we do not distinguish the use of Cartesian coordinates in any way it is always possible to rotate and translate them. If we do this then for the various choices of $\hat{c}_i$ we have the following potentials from our complete list.

(i) $\hat{c}_1 \neq 0$: We can translate with respect to y and make $\hat{c}_3=0$ to obtain a special case of [**E1**]. If further $\hat{c}_2=0$ then we obtain [**E3**].

(ii) $\hat{c}_1=0$: We have a special case of [**E2**] if $\hat{c}_2, \hat{c}_3 \neq 0$. If $\hat{c}_3=0$ we obtain [**E6**], and if $\hat{c}_2=0$ we obtain [**E5**].

(6) Here

$$ds^2 = (c_1(a^2-b^2) + c_2 a + c_3 b + c_4)(da^2 - db^2)$$

and this is easily recognized to be in the form corresponding to the potential

$$V = \hat{c}_1(x^2+y^2) + \hat{c}_2 x + \hat{c}_3 y + \hat{c}_4.$$

This can easily be interpreted. If $\hat{c}_1 \neq 0$ then we can take $\hat{c}_2$ and $\hat{c}_3=0$ by suitable translations and relate our system to a Stäckel transform of [**E3**]. If $\hat{c}_1=0$ then V can take one of the two forms

(i) $V=\alpha(x+iy)+\beta$ corresponding to [**E4**] or

(ii) $V=\alpha x$ corresponding to [**E6**].

2. Table VII

(1) Here the metric has the form

$$ds^2 = c_1(P(a)-P(b)) + c_2(P(a+\omega_1)-P(b+\omega_1)) + c_3(P(a+\omega_2)-P(b+\omega_2)) + c_4(P(a+\omega_3)-P(b+\omega_3))(da^2-db^2),$$

where $P(a)$ is the Weierstrass function.[17] If we make the choice $e_1=1/k^2$, $e_2=1$, and $e_3=0$ in the standard formulas for these functions we can relate them directly to the Jacobi elliptic functions,[17] via the formulas

$$P(kz) = \frac{1}{k^2\,\mathrm{sn}^2(z,k)}, \quad P(kz+\omega_1) = \frac{1}{k^2} - \frac{k'^2\,\mathrm{sn}^2(z,k)}{k^2\,\mathrm{cn}^2(z,k)},$$

$$P(kz+\omega_2) = \mathrm{sn}^2(z,k), \quad P(kz+\omega_3) = 1 - k'^2\frac{\mathrm{sn}^2(z,k)}{\mathrm{cn}^2(z,k)}.$$

With these formulas the relationship to a constant curvature superintegrable system becomes clear. Indeed if we write the Hamilton–Jacobi equation

$$H = p_1^2 + p_2^2 + p_3^2 + \frac{\hat{c}_1}{s_1^2} + \frac{\hat{c}_2}{s_2^2} + \frac{\hat{c}_3}{s_3^2} + \hat{c}_4 = E$$

using conical coordinates in Jacobi elliptic function form,[17] viz.

$$s_1 = k\,\mathrm{sn}(\alpha,k)\mathrm{sn}(\beta,k), \quad s_2 = i\frac{k'}{k}\mathrm{cn}(\alpha,k)\mathrm{cn}(\beta,k),$$

$$s_3 = \frac{k'}{k}\mathrm{dn}(\alpha,k)\mathrm{dn}(\beta,k), \quad s_1^2 + s_2^2 + s_3^2 = 1,$$

then it becomes

$$p_\alpha^2 + p_\beta^2 + \frac{\hat{c}_1}{k^2}\left(\frac{1}{\mathrm{sn}^2(\alpha,k)} - \frac{1}{\mathrm{sn}^2(\beta,k)}\right) + \frac{\hat{c}_2 k'^2}{k^2}\left(\frac{1}{\mathrm{cn}^2(\alpha,k)} - \frac{1}{\mathrm{cn}^2(\beta,k)}\right)$$
$$+ \frac{\hat{c}_3 k'^2}{k^2}\left(\frac{1}{\mathrm{dn}^2(\alpha,k)} - \frac{1}{\mathrm{dn}^2(\beta,k)}\right) + (\hat{c}_4 - E)(\mathrm{sn}^2(\alpha,k) - \mathrm{sn}^2(\beta,k)) = 0$$

which has the form we expect. This system is therefore related to [**S9**] on the sphere, via a Stäckel transform.

(2) In this case

$$\mathrm{d}s^2 = \left(c_1\left(\frac{1}{\sin^2 a} - \frac{1}{\sin^2 b}\right) + c_2\left(\frac{1}{\cos^2 a} - \frac{1}{\cos^2 b}\right) + c_3(\cos 2a - \cos 2b)\right.$$
$$\left. + c_4(\cos 4a - \cos 4b)\right)(\mathrm{d}a^2 - \mathrm{d}b^2).$$

If we write out the Hamilton–Jacobi equation

$$H = p_1^2 + p_2^2 + \hat{c}_1(x^2 + y^2) + \frac{\hat{c}_2}{x^2} + \frac{\hat{c}_3}{y^2} + \hat{c}_4 = E$$

using coordinates $x = \cos a \cos b$, $y = i \sin a \sin b$ we obtain

$$p_a^2 - p_b^2 + \hat{c}_1(\cos^4 b - \cos^4 b) + \hat{c}_2\left(\frac{1}{\cos^2 a} - \frac{1}{\cos^2 b}\right) + \hat{c}_3\left(\frac{1}{\sin^2 a} - \frac{1}{\sin^2 b}\right)$$
$$+ (\hat{c}_4 - E)(\cos^2 b - \cos^2 a) = 0.$$

The potential for this case arises from [**E1**] via the choice of elliptic coordinates. This is clear from the usual multiplication formulas

$$\cos 2x = 2\cos^2 x - 1, \quad \cos 4x = 8\cos^4 x - 8\cos^2 x + 1.$$

(3) Here

$$ds^2 = (c_1(\sin 4a - \sin 4b) + c_2(\cos 4a - \cos 4b) + c_3(\sin 2a - \sin 2b) + c_4(\cos 2a - \cos 2b))(da^2 - db^2).$$

If we write the Hamilton–Jacobi equation

$$H = p_1^2 + p_2^2 + \hat{c}_1 + \frac{\hat{c}_2(x - iy)}{\sqrt{(x - iy)^2 + 4}} + \frac{\hat{c}_3(x + iy)}{((x - iy)^2 + 4)(x - iy + \sqrt{(x - iy)^2 + 4})^2} + \hat{c}_4(x^2 + y^2) = E,$$

using the coordinates $x = 2i \cos u \cos v$, $y = 2 \sin u \sin v$ we obtain

$$p_u^2 - p_v^2 + 2(\hat{c}_1 - 2E)(\cos 2u - \cos 2v) + \hat{c}_2(\sin 2u - \sin 2v) + \tfrac{1}{4}\hat{c}_3(\cos 4u + i \sin 4u - \cos 4v - i \sin 4v) + 2\hat{c}_4(\cos 4v - \cos 4u) = 0$$

which gives rise to a metric of this type. This corresponds to system [**E7**].

(4) Here

$$ds^2 = \left(c_1\left(\frac{1}{a^2} - \frac{1}{b^2}\right) + c_2(a^2 - b^2) + c_3(a^4 - b^4) + c_4(a^6 - b^6)\right)(da^2 - db^2).$$

In the coordinates $x = \frac{1}{2}(\xi^2 + \eta^2)$, $y = i\xi\eta$ the Hamilton–Jacobi equation

$$p_1^2 + p_2^2 + \hat{c}_1(4x^2 + y^2) + \hat{c}_2 x + \frac{\hat{c}_3}{y^2} + \hat{c}_4 = E$$

is equivalent to

$$p_\xi^2 - p_\eta^2 + (\hat{c}_4 - E)(\xi^2 - \eta^2) + \hat{c}_1(\xi^6 - \eta^6) + \frac{1}{2}\hat{c}_2(\xi^4 - \eta^4) + \hat{c}_3\left(\frac{1}{\xi^2} - \frac{1}{\eta^2}\right) = 0,$$

from which we see that this system is obtained from [**E2**].

(5) The infinitesimal distance has the form

$$ds^2 = (c_1(a^4 - b^4) + c_2(a^3 - b^3) + c_3(a^2 - b^2) + c_4(a - b))(da^2 - db^2).$$

Consider the Hamilton–Jacobi equation

$$H = p_z p_{\bar{z}} + \hat{c}_1 + \hat{c}_2 z + \hat{c}_3\left(\bar{z} - \frac{3}{8}iz^2\right) - \frac{i}{8}\hat{c}_4(z^3 + 8iz\bar{z}) = E,$$

where $z = x + iy$, $\bar{z} = x - iy$. In coordinates $z = 4i(u + w)$, $\bar{z} = 2i(u - w)^2$ this equation is equivalent to

$$p_u^2 - p_w^2 + 16(\hat{c}_1 - E)(u - w) + 64i\hat{c}_2(u^2 - w^2) + 128i\hat{c}_3(u^3 - w^3) - 256\hat{c}_4(u^4 - w^4) = 0$$

from which we see that this system is Stäckel equivalent to [**E10**] with some minor corrections.

In the last section we gave a simple derivation of all 2D superintegrable systems with nondegenerate potential. Such systems must admit at least three second order Killing tensors. Koenigs solved a different and more general problem. He found all spaces that admit at least three second order Killing tensors. It is a remarkable fact that the lists are the same. Thus from our point of view the Koenigs derivation is a proof of the following result.

Theorem 4: Every 2D Riemannian space with at least three linearly independent second order Killing tensors admits a superintegrable system with nondegenerate potential.

Corollary 1: Necessary and sufficient conditions for a superintegrable system with nondegenerate potential on a 2D Riemannian manifold are that there are local orthogonal coordinates x, y such that the system takes the form $H/U(x, y)$ where

$$H = \frac{p_x^2 + p_y^2}{\lambda(x,y)} + V(x,y)$$

is a superintegrable system on a constant curvature space with nondegenerate potential

$$V(x,y) = \alpha V^{(1)}(x,y) + \beta V^{(2)}(x,y) + \gamma V^{(3)}(x,y) + \delta$$

and

$$U(x,y) = \alpha_0 V^{(1)}(x,y) + \beta_0 V^{(2)}(x,y) + \gamma_0 V^{(3)}(x,y) + \delta_0.$$

Corollary 2: Necessary and sufficient conditions for a 2D Riemannian manifold to admit a three dimensional space of second order Killing tensors are that there are local orthogonal coordinates x,y such that the metric takes the form $ds^2 = \lambda(x,y)U(x,y)(dx^2 + dy^2)$ where $\lambda(x,y)(dx^2 + dy^2)$ is a metric on a constant curvature space with nondegenerate potential,

$$V(x,y) = \alpha V^{(1)}(x,y) + \beta V^{(2)}(x,y) + \gamma V^{(3)}(x,y) + \delta$$

and

$$U(x,y) = \alpha_0 V^{(1)}(x,y) + \beta_0 V^{(2)}(x,y) + \gamma_0 V^{(3)}(x,y) + \delta_0.$$

III. CONCLUSIONS AND FURTHER WORK

In this paper we have shown that every 2D nondegenerate superintegrable system is Stäckel equivalent (or equivalent via coupling constant metamorphosis) to a 2D nondegenerate superintegrable system on a constant curvature space. We found a simple derivation of all such spaces and potentials. We found that the list of spaces with nondegenerate potentials coincided with the Koenigs list of all 2D manifolds with three linearly independent second order Killing tensors. Thus any 2D space with three second order Killing tensors necessarily admits a nondegenerate potential.

In a forthcoming paper we will extend these results to 2D quantum systems, where the same spaces and potentials will occur. We will uncover the structure of the quantum quadratic algebra generated by the second order symmetry operators and show how to compute it in general.

Extension of our results to 3D systems is more challenging. Here the spaces we consider are conformally flat, since the Stäckel transform is conformal and the best known examples of superintegrable systems are in constant curvature spaces. Now for a superintegrable system we must have five functionally independent symmetries. Although several technical problems related to dimension must be overcome, we will be able to show that the structure theory for the quadratic algebras works in analogy to the 2D case. The extension to the quantum case is again more challenging, but the basic structure results for the quadratic algebra carry over for suitably modified potentials.

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Exact solution for the hypergeometric Green's function describing spectral formation in x-ray pulsars

Peter A. Becker[a)]
Center for Earth Observing and Space Research, School of Computational Sciences, George Mason University, Fairfax, Virginia 22030-4444

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An eigenfunction expansion method involving hypergeometric functions is used to solve the partial differential equation governing the transport of radiation in an x-ray pulsar accretion column containing a radiative shock. The procedure yields the exact solution for the Green's function, which describes the scattering of monochromatic radiation injected into the column from a source located near the surface of the star. Collisions between the injected photons and the infalling electrons cause the radiation to gain energy as it diffuses through the gas and gradually escapes by passing through the walls of the column. The presence of the shock enhances the energization of the radiation and creates a power-law spectrum at high energies, which is typical for a Fermi process. The analytical solution for the Green's function provides important physical insight into the spectral formation process in x-ray pulsars, and it also has direct relevance for the interpretation of spectral data for these sources. Additional interesting mathematical aspects of the problem include the establishment of a closed-form expression for the quadratic normalization integrals of the orthogonal eigenfunctions, and the derivation of a new summation formula involving products of hypergeometric functions. By taking various limits of the general expressions, we also develop new linear and bilinear generating functions for the Jacobi polynomials. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1894965]

I. INTRODUCTION

In this paper, methods of classical analysis are employed to obtain the exact solution for the Green's function describing the spectrum of radiation emitted by an x-ray pulsar. Beyond the direct physical relevance of the Green's function, the method of solution also yields several additional results of mathematical interest, including a new summation formula involving products of two hypergeometric functions, as well as new linear and bilinear generating functions for the Jacobi polynomials. We also obtain an exact expression for the quadratic normalization integrals of the orthogonal hypergeometric eigenfunctions. Before proceeding with the main derivation, some physical background is called for. The radiation produced in bright x-ray pulsars is powered by the gravitational accretion (inflow) of ionized gas that is channeled onto the poles of a rotating neutron star by the strong magnetic field. In these sources, the radiation pressure greatly exceeds the gas pressure, and therefore the pressure of the photons governs the dynamical structure of the accretion flow. It follows that the gas must pass through a radiation-dominated shock on its way to the stellar surface, and the kinetic energy of the gas is carried away by the high-energy radiation that escapes from the column.[1] The strong gradient of the radiation pressure decelerates the material to rest at the surface of the star, and the compression of the infalling gas drives its temperatures up to a few million Kelvins. The gas therefore radiates x-rays, which appear to

[a)]Electronic mail: pbecker@gmu.edu

pulsate due to the star's spin. However, the observed x-ray spectrum is nonthermal, indicating that nonequilibrium processes are playing an important role in the formation of the radiation distribution.

The nonthermal shape of the spectrum is primarily due to the flow compression, which causes Fermi energization of the photons as they collide with infalling electrons in the column, until the radiation escapes from the column into space. Our primary goal in this paper is to obtain an exact solution for the Green's function describing the upscattering of soft, monoenergetic photons injected by a source located in the base of the accretion column, near the surface of the star. The Green's function contains a complete representation of the fundamental physics governing the propagation of the photons in the physical and energy spaces. Since the transport equation governing the radiation spectrum is linear, we can compute the solution associated with an arbitrary source distribution via convolution. Hence the Green's function provides the most direct means for exploring the relationship between the physics occurring in the accretion shock and the production of the observed nonthermal x radiation.

II. FUNDAMENTAL EQUATIONS

We assume that the accretion column is cylindrical, and we define x as the spatial coordinate measured along the column axis. The gas flows through the column onto the stellar surface with velocity v. We define the Green's function, $f_{\mathrm{G}}(x_0,x,\epsilon_0,\epsilon)$, as the radiation distribution at location x and energy ϵ resulting from the injection of $\dot{N}_0$ photons per second with energy ϵ_0 from a monochromatic source at location x_0 inside the column. In a steady-state situation, f_{G} satisfies the transport equation[2,3]

$$v\frac{\partial f_{\mathrm{G}}}{\partial x}=\frac{\mathrm{d}v}{\mathrm{d}x}\frac{\epsilon}{3}\frac{\partial f_{\mathrm{G}}}{\partial\epsilon}+\frac{\partial}{\partial x}\left(\frac{c}{3n_e\sigma_{\parallel}}\frac{\partial f_{\mathrm{G}}}{\partial x}\right)+\frac{\dot{N}_0\delta(\epsilon-\epsilon_0)\delta(x-x_0)}{\pi r_0^2\epsilon_0^2}-\frac{f_{\mathrm{G}}}{t_{\mathrm{esc}}}-\beta v_0\delta(x-x_0)f_{\mathrm{G}},\tag{1}$$

where n_e is the electron number density, $\sigma_{\parallel}$ is the electron scattering cross section for photons propagating parallel to the x axis, r_0 is the radius of the column, v_0 is the flow speed at the source location, c is the speed of light, and t_{esc} is the mean time photons spend in the column before escaping through the walls into space. The total radiation number and energy densities associated with the distribution function f_{G} are, respectively,

$$n_{\mathrm{G}}(x)\equiv\int_0^{\infty}\epsilon^2 f_{\mathrm{G}}\,\mathrm{d}\epsilon,\quad U_{\mathrm{G}}(x)\equiv\int_0^{\infty}\epsilon^3 f_{\mathrm{G}}\,\mathrm{d}\epsilon.\tag{2}$$

The terms in (1) represent, from left to right, the comoving (convective) time derivative, first-order Fermi energization ("bulk comptonization") of the radiation in the converging flow, spatial diffusion of the photons parallel to the column axis, the monochromatic photon source, escape of radiation from the column, and the possible absorption of radiation at the source location, respectively. In physical terms, the first-order Fermi energization corresponds to the $P\,\mathrm{d}V$ work done on the radiation by the compression of the background plasma as it accretes onto the stellar surface.[3] The dimensionless constant β expresses the strength of the absorption (if any) occurring at the source location, and the mean escape time is given by

$$t_{\mathrm{esc}}=\frac{r_0^2 n_e\sigma_{\perp}}{c},\tag{3}$$

where $\sigma_{\perp}$ is the electron scattering cross section for photons propagating perpendicular to the column axis. In general, $\sigma_{\parallel}\neq\sigma_{\perp}$ due to the influence of the strong magnetic field, which is directed parallel to the axis of the column. Absorption at the source location is expected if the photons are produced in a black-body "mound" of dense gas near the base of the accretion column,[1] because a perfect black body acts as both a source and a sink of radiation.[4]

The flux of electrons flowing down the column is denoted by $J \equiv n_e v$. In our cylindrical, steady-state problem, J maintains a constant value. Becker[5] demonstrated that in order for the inflowing matter to come to rest at the stellar surface as required, the parameters r_0, J, $\sigma_\parallel$, and $\sigma_\perp$ must satisfy the dynamical constraint

$$r_0^2 J^2 \sigma_\perp \sigma_\parallel = \tfrac{3}{4} c^2. \tag{4}$$

In general, radiation-dominated shocks are continuous velocity transitions, with an overall thickness of a few Thomson scattering lengths, unlike standard (discontinuous) gas-mediated shocks.[6] The exact solution for the inflow velocity v as a function of the spatial coordinate x is given by[5,7]

$$\frac{v(x)}{v_c} = \frac{7}{4}\left[1 - \left(\frac{7}{3}\right)^{-1+x/x_{\rm st}}\right], \tag{5}$$

where v_c is the flow velocity at the sonic point, which is related to the stellar mass M_*, the stellar radius R_*, and the gravitational constant G via[5]

$$v_c = \frac{4}{7}\left(\frac{2GM_*}{R_*}\right)^{1/2}. \tag{6}$$

The quantity $x_{\rm st}$ appearing in (5) is the distance between the sonic point and the stellar surface, which can be evaluated using Eq. (4.16) from Ref. 5 to obtain

$$x_{\rm st} = \frac{r_0}{2\sqrt{3}}\left(\frac{\sigma_\perp}{\sigma_\parallel}\right)^{1/2} \ln\left(\frac{7}{3}\right). \tag{7}$$

According to (5), the flow does come to rest at the surface of the star as required, since $v(x_{\rm st}) = 0$. Furthermore, the constancy of the electron flux J in our cylindrical, steady-state problem implies that the electron number density n_e is a function of x because v varies with the height inside the column [see Eq. (5)].

Further simplification is possible if we work in terms of the new spatial variable y, defined by

$$y(x) \equiv \left(\frac{7}{3}\right)^{-1+x/x_{\rm st}}. \tag{8}$$

Note that $y \to 0$ in the far upstream region ($x \to -\infty$), and $y \to 1$ at the surface of the star ($x \to x_{\rm st}$). Based on (5) and (8), we find that the variation of the velocity v as a function of the new variable y is given by the simple expression

$$\frac{v(y)}{v_c} = \frac{7}{4}(1-y). \tag{9}$$

By combining (3), (4), and (9) with the derivative relation

$$\frac{{\rm d}x}{{\rm d}y} = \frac{r_0}{2\sqrt{3}}\left(\frac{\sigma_\perp}{\sigma_\parallel}\right)^{1/2} y^{-1}, \tag{10}$$

we can transform the transport equation (1) for $f_{\rm G}$ from x to y to obtain

$$y(1-y)\frac{\partial^2 f_{\rm G}}{\partial y^2} + \left(\frac{1-5y}{4}\right)\frac{\partial f_{\rm G}}{\partial y} - \frac{\epsilon}{4}\frac{\partial f_{\rm G}}{\partial \epsilon} + \left(\frac{y-1}{4y}\right) f_{\rm G} = \frac{3\beta v_0 \delta(y-y_0) f_{\rm G}}{7 v_c} - \frac{3\dot{N}_0 \delta(\epsilon-\epsilon_0)\delta(y-y_0)}{7\pi r_0^2 \epsilon_0^2 v_c}, \tag{11}$$

where $y_0 \equiv y(x_0)$ denotes the value of y at the source location. According to (9), the flow velocity at the source, v_0, is related to v_c and y_0 by

$$\frac{v_0}{v_c} = \frac{7}{4}(1 - y_0). \tag{12}$$

Note that we can write the Green's function as either $f_G(x_0, x, \epsilon_0, \epsilon)$ or $f_G(y_0, y, \epsilon_0, \epsilon)$ since the parameters (x, x_0) and (y, y_0) are interchangeable via (8).

III. SOLUTION FOR THE GREEN'S FUNCTION

The physical model considered here includes Fermi energization, which tends to boost the energy of the injected photons as they collide with high-energy electrons streaming down through the accretion column towards the surface of the neutron star. Moreover, since no process that can lower the photon energy is included in the model, all of the photons injected from a source of monochromatic radiation with energy $\epsilon = \epsilon_0$ must at later times have energy $\epsilon > \epsilon_0$. It follows that $f_G = 0$ for $\epsilon < \epsilon_0$. When $\epsilon > \epsilon_0$, (11) is separable in energy and space using the functions

$$f_\lambda(\epsilon, y) = \epsilon^{-\lambda} g(\lambda, y), \tag{13}$$

where λ is the separation constant, and the spatial function g satisfies the differential equation

$$y(1 - y)\frac{d^2 g}{dy^2} + \left(\frac{1 - 5y}{4}\right)\frac{dg}{dy} + \left(\frac{\lambda y + y - 1}{4y}\right)g = \frac{3\beta v_0 \delta(y - y_0)}{7 v_c} g. \tag{14}$$

In order to avoid an infinite spatial diffusion flux at $y = y_0$, the function g must be continuous there, and consequently we obtain the condition

$$\Delta[g(\lambda, y)]\big|_{y=y_0} \equiv \lim_{\varepsilon \to 0} g(\lambda, y_0 + \varepsilon) - g(\lambda, y_0 - \varepsilon) = 0. \tag{15}$$

We can also derive a jump condition for the derivative dg/dy at the source location by integrating (14) with respect to y in a small region around $y = y_0$. The result obtained is

$$\Delta\left[\frac{dg}{dy}\right]\Bigg|_{y=y_0} = \frac{3\beta}{4y_0} g(\lambda, y_0), \tag{16}$$

where we have used (12) to substitute for v_0.

The homogeneous version of (14) obtained when $y \neq y_0$ has fundamental solutions given by

$$\varphi_1(\lambda, y) \equiv y F(a, b; c; y), \tag{17}$$

$$\varphi_1^*(\lambda, y) \equiv y^{-1/4} F(a - 5/4, b - 5/4; 2 - c; y), \tag{18}$$

where $F(a, b; c; z)$ denotes the hypergeometric function,[8] and the parameters a, b, and c are defined by

$$a \equiv \frac{9 - \sqrt{17 + 16\lambda}}{8}, \quad b \equiv \frac{9 + \sqrt{17 + 16\lambda}}{8}, \quad c \equiv \frac{9}{4}, \tag{19}$$

and therefore $a + b = c$.

A. Asymptotic analysis

The source photons injected into the flow are unable to diffuse very far upstream due to the high speed of the inflowing electrons. Most of the photons escape through the walls of the column within a few scattering lengths of the source, and therefore we conclude that the function g must *vanish* in the upstream limit, $y \to 0$. Asymptotic analysis indicates that the function $\varphi_1(\lambda, y) \to 0$ in the limit $y \to 0$ as required, but $\varphi_1^*(\lambda, y)$ diverges and therefore it cannot be utilized in the upstream region $(y \leqslant y_0)$. Hence g must be given by φ_1 for $y \leqslant y_0$. Conversely, in the downstream limit, the gas settles onto the surface of the star and therefore g should approach a constant as $y \to 1$. These

conditions are satisfied if λ is equal to one of the eigenvalues, λ_n, which are associated with the spatial eigenfunctions, $g_n(y)$, defined by

$$g_n(y) \equiv g(\lambda_n, y). \tag{20}$$

In order to obtain a complete understanding of the global behavior of the eigenfunctions, we must also consider the asymptotic behaviors of the two functions φ_1 and φ_1^* in the downstream region, which are discussed below.

The hypergeometric functions appearing in (17) and (18) can be evaluated at $y=1$ using Eq. (15.1.20) from Abramowitz and Stegun,[8] which gives for general values of a, b, and c,

$$F(a,b;c;1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}. \tag{21}$$

However, for the values of a, b, and c in (17) and (18), we find that [see Eq. (19)]

$$c - a - b = 0, \tag{22}$$

and therefore the hypergeometric functions $F(a,b;c;y)$ and $F(a-5/4, b-5/4; 2-c; y)$ each *diverge* in the downstream limit $y \to 1$. Since the eigenfunction g_n should approach a constant as $y \to 1$ based on physical considerations, we conclude that in the downstream region ($y \geqslant y_0$), g_n must be represented by a suitable linear combination of φ_1 and φ_1^* that remains *finite* as $y \to 1$. In order to make further progress, we need to employ Eq. (15.3.10) from Abramowitz and Stegun,[8] which yields for general a, b, and y,

$$F(a,b;a+b;y) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(n!)^2} [2\Psi(n+1) - \Psi(a+n) - \Psi(b+n) - \ln(1-y)](1-y)^n, \tag{23}$$

where

$$\Psi(z) \equiv \frac{1}{\Gamma(z)} \frac{d\Gamma(z)}{dz}. \tag{24}$$

Asymptotic analysis of this expression reveals that in the limit $y \to 1$, the logarithmic divergences of the two functions φ_1 and φ_1^* can be balanced by creating the new function

$$\varphi_2(\lambda, y) \equiv \frac{\Gamma(b)}{\Gamma(c)\Gamma(1-b)} \varphi_1(\lambda, y) - \frac{\Gamma(1-a)}{\Gamma(2-c)\Gamma(a)} \varphi_1^*(\lambda, y), \tag{25}$$

which remains finite as $y \to 1$. Hence φ_2 represents the fundamental solution for g_n in the region downstream from the source. We can use the asymptotic behaviors of φ_1 and φ_1^* to show that

$$\lim_{y \to 1} \varphi_2(\lambda, y) = \frac{\pi[\cot(\pi a) + \cot(\pi b)]}{\Gamma(a)\Gamma(1-b)}. \tag{26}$$

Since the solutions φ_1 and φ_2 are applicable in the upstream and downstream regions, respectively, the global expression for the eigenfunction g_n is therefore given by

$$g_n(y) = \begin{cases} \varphi_1(\lambda_n, y), & y \leqslant y_0, \\ B_n \varphi_2(\lambda_n, y), & y \geqslant y_0, \end{cases} \tag{27}$$

where the constant B_n is evaluated using the continuity condition [Eq. (15)], which yields

$$B_n = \frac{\varphi_1(\lambda_n, y_0)}{\varphi_2(\lambda_n, y_0)}. \tag{28}$$

It follows from (26)–(28) that the downstream value of g_n is given by

$$\lim_{y\to 1} g_n(y) = \frac{\pi[\cot(\pi a) + \cot(\pi b)]}{\Gamma(a)\Gamma(1-b)} \frac{\varphi_1(\lambda_n, y_0)}{\varphi_2(\lambda_n, y_0)}. \tag{29}$$

Conversely, in the upstream region, $\varphi_1 \to y$, and therefore we have the asympototic behavior

$$\lim_{y\to 0} \frac{g_n(y)}{y} = 1. \tag{30}$$

B. Eigenvalue equation

We can combine (16), (27), and (28) to show that the eigenvalues λ_n satisfy the equation

$$W(\lambda_n, y_0) - \frac{3\beta\varphi_1(\lambda_n, y_0)\varphi_2(\lambda_n, y_0)}{4y_0} = 0, \tag{31}$$

where the Wronskian of the two functions φ_1 and φ_2 is defined for general values of λ and y by

$$W(\lambda, y) \equiv \varphi_1 \frac{d\varphi_2}{dy} - \varphi_2 \frac{d\varphi_1}{dy}. \tag{32}$$

Further progress can be made by deriving an analytical expression for the Wronskian. We begin by writing the differential equation (14) governing the two functions φ_1 and φ_2 in the self-adjoint form

$$\frac{d}{dy}\left[y^{1/4}(1-y)\frac{d\varphi}{dy} \right] + \frac{\lambda}{4y^{3/4}}\varphi - T\varphi = 0, \tag{33}$$

where

$$T \equiv \frac{1-y}{4y^{7/4}} + \frac{3\beta v_0 \delta(y-y_0)}{7v_c y^{3/4}}. \tag{34}$$

By applying (33) to the function φ_2 and multiplying the result by φ_1, and then subtracting from this the same expression with φ_1 and φ_2 interchanged, we obtain

$$\varphi_1 \frac{d}{dy}\left[y^{1/4}(1-y)\frac{d\varphi_2}{dy} \right] - \varphi_2 \frac{d}{dy}\left[y^{1/4}(1-y)\frac{d\varphi_1}{dy} \right] = 0, \tag{35}$$

which can be rewritten as

$$y^{1/4}(1-y)\frac{dW}{dy} + W\frac{d}{dy}[y^{1/4}(1-y)] = 0, \tag{36}$$

where we have made use of the result

$$\frac{dW}{dy} = \varphi_1 \frac{d^2\varphi_2}{dy^2} - \varphi_2 \frac{d^2\varphi_1}{dy^2}. \tag{37}$$

Equation (36) can be rearranged in the form

$$\frac{\mathrm{d}\ln W}{\mathrm{d}y} = -\frac{\mathrm{d}}{\mathrm{d}y}\ln[y^{1/4}(1-y)], \tag{38}$$

which can be integrated to obtain the exact solution

$$W(\lambda,y) = \frac{D(\lambda)}{y^{1/4}(1-y)}, \tag{39}$$

where $D(\lambda)$ is an integration constant that depends on λ but not on y. The exact dependence of D on λ can be derived by analyzing the behaviors of the functions φ_1 and φ_2 in the limit $y\to 0$. For small values of y, we have the asymptotic expressions[8]

$$\varphi_1 \to y, \quad y \to 0,$$

$$\varphi_2 \to -\frac{\Gamma(1-a)}{\Gamma(a)\Gamma(2-c)}y^{-1/4}, \quad y \to 0. \tag{40}$$

Combining (32) and (40), we find that asymptotically,

$$W \to \frac{5}{4}\frac{\Gamma(1-a)}{\Gamma(a)\Gamma(2-c)}y^{-1/4}, \quad y \to 0. \tag{41}$$

Comparing this result with (39), we conclude that

$$D(\lambda) = \frac{5}{4}\frac{\Gamma(1-a)}{\Gamma(a)\Gamma(2-c)}, \tag{42}$$

and therefore the exact solution for the Wronskian for general values of λ and y is given by

$$W(\lambda,y) = \frac{5}{4}\frac{\Gamma(1-a)}{\Gamma(a)\Gamma(2-c)}\frac{y^{-1/4}}{1-y}. \tag{43}$$

Substituting for W in (31) using (43), we can rewrite the eigenvalue equation in the equivalent form

$$\frac{5}{3}\frac{\Gamma(1-a)}{\Gamma(a)\Gamma(2-c)}\frac{y_0^{3/4}}{1-y_0} = \beta\varphi_1(\lambda_n,y_0)\varphi_2(\lambda_n,y_0), \tag{44}$$

where a and b are functions of λ_n by virtue of (19), and $c=9/4$. The roots of this expression are the eigenvalues λ_n, and the associated eigenfunctions are evaluated using (27). The first eigenvalue, λ_0, is especially important because it determines the power-law shape of the high-energy portion of the Green's function [see Eq. (13)].

In Fig. 1 we plot the first eigenvalue λ_0 as a function of the dimensionless parameters β and y_0. Note that λ_0 is a double-valued function of y_0 for fixed β, which is a consequence of the imposed velocity profile [Eq. (5)]. Physically, this behavior reflects the fact that it is always possible to achieve a desired amount of compression (first-order Fermi energization) by placing the source in a specific location in either the upstream or downstream regions of the flow. We also observe that if we increase the absorption parameter β while holding y_0 fixed, then λ_0 increases monotonically, and therefore the high-energy spectrum becomes progressively steeper. This behavior is expected physically because as the absorption parameter is increased, the injected photons spend less time on average being energized by collisions with electrons before either escaping from the column or being absorbed at the source location. The decreased amount of energization naturally leads to a steepening of the radiation spectrum. When $\beta=0$, no absorption occurs, and the index λ_0 achieves its minimum (limiting) value of 4. This limit is, however, unphysical since

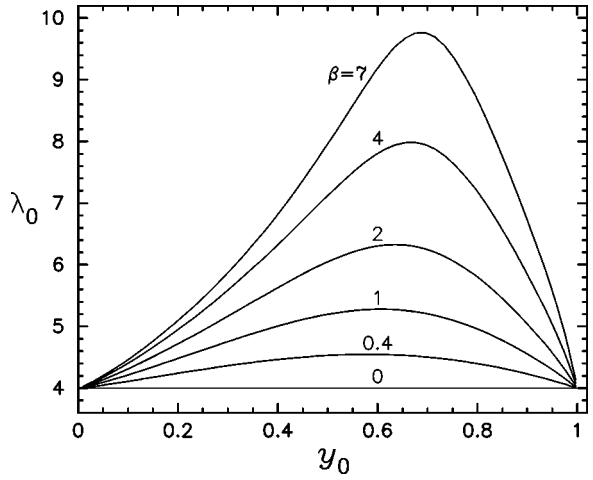

FIG. 1. First eigenvalue λ_0 of the Green's function expansion plotted as a function of the source location y_0 for the indicated values of the absorption parameter β. Note the steepening of the radiation spectrum that occurs when β is increased for a fixed value of y_0, which reflects the decreasing residence time for the photons in the plasma (see the discussion in the text).

it yields a divergent result for the total photon energy density U_G according to (2). Nonetheless, the case with $\beta=0$ is interesting from a mathematical viewpoint, and for that reason it is further discussed in Sec. V.

C. Orthogonality of the eigenfunctions

We shall next demonstrate that the eigenfunctions $g_n(y)$ form an orthogonal set, which is an extremely useful property. This is a standard Sturm–Liouville problem and therefore we follow the usual procedure. Let us suppose that $g_n(y)$ and $g_m(y)$ are two eigenfunctions corresponding to the distinct eigenvalues λ_n and λ_m, respectively. The functions g_n and g_m each satisfy the differential equation (14), and therefore we can utilize the self-adoint form to write [cf. Eq. (33)]

$$g_m\left\{\frac{\mathrm{d}}{\mathrm{d}y}\left[y^{1/4}(1-y)\frac{\mathrm{d}g_n}{\mathrm{d}y}\right]+\frac{\lambda_n}{4y^{3/4}}g_n-Tg_n\right\}=0 \tag{45}$$

and

$$g_n\left\{\frac{\mathrm{d}}{\mathrm{d}y}\left[y^{1/4}(1-y)\frac{\mathrm{d}g_m}{\mathrm{d}y}\right]+\frac{\lambda_m}{4y^{3/4}}g_m-Tg_m\right\}=0, \tag{46}$$

where T is given by (34). Subtracting the second equation from the first yields, after integrating by parts with respect to y from $y=0$ to $y=1$,

$$(\lambda_n-\lambda_m)\int_0^1 y^{-3/4}g_n(y)g_m(y)\mathrm{d}y=4y^{1/4}(1-y)\left[g_n\frac{\mathrm{d}g_m}{\mathrm{d}y}-g_m\frac{\mathrm{d}g_n}{\mathrm{d}y}\right]\Bigg|_0^1. \tag{47}$$

Based on the asymptotic behaviors of the eigenfunctions g_n and g_m given by (29) and (30), we find that the right-hand side of (47) vanishes exactly, and therefore we obtain

$$(\lambda_n-\lambda_m)\int_0^1 y^{-3/4}g_n(y)g_m(y)\mathrm{d}y=0, \tag{48}$$

which establishes the orthogonality of the eigenfunctions. The set of eigenfunctions is also complete according to the Sturm–Liouville theorem. Since the eigenfunctions are orthogonal, the Green's function can be expressed as the infinite series

$$f_G(y_0,y,\epsilon_0,\epsilon)=\sum_{n=0}^{\infty}A_n\left(\frac{\epsilon}{\epsilon_0}\right)^{-\lambda_n}g_n(y), \tag{49}$$

for $\epsilon \geqslant \epsilon_0$, where the expansion coefficients A_n are computed by employing the orthogonality of the eigenfunctions along with the condition

$$f_G(y_0,y,\epsilon_0,\epsilon)|_{\epsilon=\epsilon_0}=\frac{12\dot{N}_0}{7\pi r_0^2\epsilon_0^3 v_c}\delta(y-y_0), \tag{50}$$

which is obtained by integrating the transport equation (11) with respect to ϵ in a small range surrounding the injection energy ϵ_0. The result obtained for the nth expansion coefficient is

$$A_n=\frac{12\dot{N}_0 y_0^{-3/4}g_n(y_0)}{7\pi r_0^2\epsilon_0^3 v_c \mathfrak{C}_n}, \tag{51}$$

where the quadratic normalization integrals, $\mathfrak{C}_n$, are defined by

$$\mathfrak{C}_n \equiv \int_0^1 y^{-3/4}g_n^2(y)\mathrm{d}y. \tag{52}$$

As an alternative to numerical integration, in Sec. III D we derive a closed-form expression for evaluating the normalization integrals based directly on the associated differential equation.

D. Quadratic normalization integrals

The direct computation of the normalization integrals $\mathfrak{C}_n$ via numerical integration is costly and time consuming, and therefore it is desirable to have an alternative procedure available for their evaluation. In fact, it is possible to derive an analytical expression for the normalization integrals based on manipulation of the fundamental differential equation (14) governing the eigenfunctions $g_n(y)$.

Let us suppose that $g(\lambda,y)$ is a general solution to (14) for an arbitrary value of λ (i.e., not necessarily an eigenvalue) with the asymptotic (upstream) behavior

$$g(\lambda,y)\to y, \quad y\to 0, \tag{53}$$

which is the same as the upstream behavior of the eigenfunction $g_n(y)$ [see Eq. (30)]. We also stipulate that g must be continuous at $y=y_0$, and that it satisfies the derivative jump condition given by (16). After a bit of algebra, we find that the global solution for g consistent with these requirements can be expressed as

$$g(\lambda,y)=\begin{cases}\varphi_1(\lambda,y), & y\leqslant y_0,\\ (1+\hat{a})\varphi_1(\lambda,y)+\hat{b}\varphi_2(\lambda,y), & y\geqslant y_0,\end{cases} \tag{54}$$

where the coefficients $\hat{a}$ and $\hat{b}$ are are given by

$$\hat{a}=-\frac{3\beta\varphi_1(\lambda,y_0)\varphi_2(\lambda,y_0)}{4y_0W(\lambda,y_0)}, \quad \hat{b}=\frac{3\beta\varphi_1^2(\lambda,y_0)}{4y_0W(\lambda,y_0)}, \tag{55}$$

and the Wronskian W is evaluated using (43).

Comparing the general solution for $g(\lambda,y)$ with the solution for the eigenfunction $g_n(y)$ given by (27), we note that

$$\lim_{\lambda\to\lambda_n}\hat{a}=-1, \quad \lim_{\lambda\to\lambda_n}\hat{b}=B_n. \tag{56}$$

We can now use the self-adoint form of (14) to write [cf. Eqs. (45) and (46)]

$$g_n\left\{\frac{\partial}{\partial y}\left[y^{1/4}(1-y)\frac{\partial g}{\partial y}\right]+\frac{\lambda}{4y^{3/4}}g-Tg\right\}=0 \tag{57}$$

and

$$g\left\{\frac{\mathrm{d}}{\mathrm{d}y}\left[y^{1/4}(1-y)\frac{\mathrm{d}g_n}{\mathrm{d}y}\right]+\frac{\lambda_n}{4y^{3/4}}g_n-Tg_n\right\}=0, \tag{58}$$

where T is defined by (34). Subtracting the second equation from the first and integrating by parts from $y=0$ to $y=1$ yields

$$(\lambda-\lambda_n)\int_0^1 y^{-3/4}g(\lambda,y)g_n(y)\mathrm{d}y=4y^{1/4}(1-y)\left[g(\lambda,y)\frac{\mathrm{d}g_n}{\mathrm{d}y}-g_n(y)\frac{\partial g}{\partial y}\right]\Bigg|_0^1. \tag{59}$$

Since $g\to y$ and $g_n\to y$ as $y\to 0$, we conclude that the evaluation at the lower bound $y=0$ on the right-hand side yields zero, and consequently in the limit $\lambda\to\lambda_n$ we obtain for the quadratic normalization integral $\mathfrak{C}_n$ [see Eq. (52)],

$$\mathfrak{C}_n=\int_0^1 y^{-3/4}g_n^2(y)\mathrm{d}y=\lim_{\lambda\to\lambda_n}\frac{4y^{1/4}(1-y)[g(\lambda,y)(\mathrm{d}g_n/\mathrm{d}y)-g_n(y)(\partial g/\partial y)]}{\lambda-\lambda_n}\Bigg|_{y=1}. \tag{60}$$

The numerator and denominator on the right-hand side of (60) each vanish in the limit $\lambda\to\lambda_n$, and therefore we can employ L'Hôpital's rule to show that (e.g., Becker[9])

$$\mathfrak{C}_n=\lim_{\lambda\to\lambda_n}4y^{1/4}(1-y)\left[\frac{\partial g}{\partial y}\frac{\mathrm{d}g_n}{\mathrm{d}y}-g_n\frac{\partial^2 g}{\partial y\partial\lambda}\right]\Bigg|_{y=1}. \tag{61}$$

Substituting the analytical forms for $g_n(y)$ and $g(\lambda,y)$ given by (27) and (54), respectively, we find that (61) can be rewritten as

$$\mathfrak{C}_n=\lim_{y\to 1}4y^{1/4}(1-y)B_n\left[W(\lambda,y)\frac{\mathrm{d}\hat{a}}{\mathrm{d}\lambda}+B_n\frac{\partial\varphi_2}{\partial\lambda}\frac{\partial\varphi_2}{\partial y}-B_n\varphi_2(\lambda,y)\frac{\partial^2\varphi_2}{\partial y\partial\lambda}\right]\Bigg|_{\lambda=\lambda_n}, \tag{62}$$

where we have also utilized (32) and (56). Based on the asymptotic behavior of φ_2 [see (26)], we conclude that the final two terms on the right-hand side of (62) contribute nothing in the limit $y\to 1$, and therefore our expression for $\mathfrak{C}_n$ reduces to

$$\mathfrak{C}_n=\lim_{y\to 1}4y^{1/4}(1-y)B_nW(\lambda,y)\left.\frac{\mathrm{d}\hat{a}}{\mathrm{d}\lambda}\right|_{\lambda=\lambda_n}. \tag{63}$$

Since $y=1$ is a singular point of the differential equation (14), it is convenient to employ the relation [see Eq. (39)]

$$W(\lambda,y)y^{1/4}(1-y)=W(\lambda,y_0)y_0^{1/4}(1-y_0), \tag{64}$$

which allows us to transform the evaluation in (63) from $y=1$ to $y=y_0$ to obtain the equivalent result

$$\mathfrak{C}_n=4y_0^{1/4}(1-y_0)\hat{a}W(\lambda,y_0)\frac{\varphi_1(\lambda_n,y_0)}{\varphi_2(\lambda_n,y_0)}\left.\frac{\mathrm{d}\ln\hat{a}}{\mathrm{d}\lambda}\right|_{\lambda=\lambda_n}, \tag{65}$$

where we have also substituted for B_n using (28). The derivative on the right-hand side can be evaluated using (55), which yields

$$\frac{\mathrm{d}\ln \hat{a}}{\mathrm{d}\lambda} = \frac{\partial \ln \varphi_1}{\partial \lambda} + \frac{\partial \ln \varphi_2}{\partial \lambda} - \frac{\partial \ln W}{\partial \lambda}, \tag{66}$$

where the derivative of the Wronskian is given by [see Eqs. (19) and (43)]

$$\frac{\partial \ln W}{\partial \lambda} = \frac{\Psi(a) + \Psi(1-a)}{(17+16\lambda)^{1/2}} \tag{67}$$

and

$$\Psi(z) \equiv \frac{1}{\Gamma(z)} \frac{\mathrm{d}\Gamma(z)}{\mathrm{d}z}. \tag{68}$$

Combining (55) and (65)–(67), we find that the quadratic normalization integrals can be evaluated using the closed-form expression

$$\mathfrak{C}_n = K(\lambda_n, y_0), \tag{69}$$

where

$$K(\lambda,y) \equiv 3\beta y^{-3/4}(1-y)\varphi_1^2(\lambda,y)\left[\frac{\Psi(a)+\Psi(1-a)}{(17+16\lambda)^{1/2}} - \frac{\partial \ln \varphi_1}{\partial \lambda} - \frac{\partial \ln \varphi_2}{\partial \lambda}\right]. \tag{70}$$

This formula provides an extremely efficient alternative to numerical integration for the computation of $\mathfrak{C}_n$.

E. Numerical examples

In this section we illustrate the computational method by examining the dependence of the Green's function $f_{\mathrm{G}}(y_0, y, \epsilon_0, \epsilon)$ on the spatial location y and the energy ϵ. We remind the reader that the solution for the Green's function represents the photon spectrum inside the accretion column at the specified position and energy, resulting from the injection of monochromatic photons with energy ϵ_0 from a source located at y_0. Hence analysis of f_{G} allows us to explore the competing effects of Fermi energization and diffusion as photons travel through the column. The Green's function can be computed by combining (49), (51), and (69) once the eigenvalues λ_n have been determined using (44). The eigenfunction expansion for f_{G} converges fairly rapidly, and in general one obtains at least five decimal digits of accuracy if the series in (49) is terminated after the first 20 terms.

The Green's function $f_{\mathrm{G}}(y_0, y, \epsilon_0, \epsilon)$ is plotted as a function of the energy ratio ϵ/ϵ_0 and the location y in Fig. 2 for the parameter values $\beta = 0.4$ and $y_0 = 0.9$. In this case the first eigenvalue is given by $\lambda_0 = 4.231$ (see Fig. 1), which is equal to the high-energy slope of the Green's function in the log–log plots in Fig. 2. The selected value of y_0 corresponds to a source located near the bottom of the accretion column, just above the stellar surface. At the source location, $y = y_0 = 0.9$, the energy spectrum extends down to the injection energy, ϵ_0. However, at all other radii the spectrum displays a steep turnover above that energy because all of the photons have experienced Fermi energization due to collisions with the infalling electrons. The photons with energy $\epsilon = \epsilon_0$ at the source location have been injected so recently that they have not yet experienced significant energization. Note that in the far upstream region (i.e., for small values of y), the spectrum is greatly attenuated due to the inability of the photons to diffuse upstream through the rapidly infalling plasma. In this example, the average photon energy achieves its maximum value in the upstream region because these are the photons that have resided in the flow the longest and therefore experienced the most energy amplification. However, due to the attenuation mentioned above, there are not many of these photons.

In Fig. 3 we plot the Green's function f_{G} for the case with $\beta = 4$ and $y_0 = 0.4$, which yields for the first eigenvalue $\lambda_0 = 6.325$. The source is now located in the upstream region and the absorption is stronger, and consequently the behavior is somewhat different from that displayed in Fig. 2. In

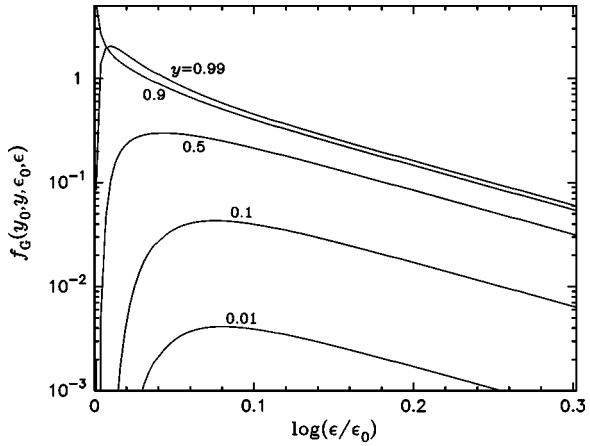

FIG. 2. Green's function $f_G(y_0,y,\epsilon_0,\epsilon)$ [Eq. (49)] plotted in units of $\dot{N}_0/(r_0^2\epsilon_0^3 v_c)$ as a function of the photon energy ratio ϵ/ϵ_0 for the indicated values of the spatial variable y. In this example we have set the absorption constant $\beta=0.4$ and the source location parameter $y_0=0.9$, so that the source is located near the base of the accretion column.

particular, the photons experience less overall compression in the flow and therefore the spectrum is steeper at high energies, as evidenced by the increase in the primary eigenvalue λ_0. This is mainly due to the larger value of β, which causes the photons to spend less time on average in the flow being energized by collisions with the electrons before they escape from the column or are "recycled" by absorption. We also note that in this case the average radiation energy displays its maximum value in the downstream region. This is the reverse of the behavior displayed in Fig. 2 because in the present situation, the source is located in the upstream region and therefore the photons that diffuse further upstream do not experience as much energization as those considered in Fig. 2. The radiation distribution in the far upstream region is greatly attenuated due to diffusion against the current of infalling electrons, as in Fig. 2. The analytical results for the Green's function obtained here provide the basis for the consideration of any source distribution since the fundamental differential equation (1) is linear. This is further discussed in Sec. IV.

IV. HYPERGEOMETRIC SUMMATION FORMULA

We can derive two interesting summation formulas for the hypergeometric eigenfunctions by using the transport equation (11) to study the behavior of the "energy moments," I_ℓ, defined by

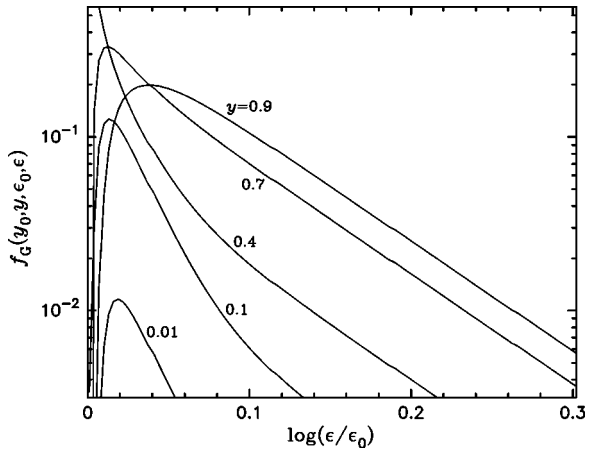

FIG. 3. Same as Fig. 2, except $\beta=4.0$ and $y_0=0.4$. In this case the source is located in the upstream region, and the average photon energy achieves its maximum value in the downstream region.

$$I_\ell(y) \equiv \int_{\epsilon_0}^{\infty} \epsilon^\ell f_G \mathrm{d}\epsilon. \tag{71}$$

The lower bound of ϵ_0 is chosen because $f_G=0$ for $\epsilon<\epsilon_0$ as explained in the discussion preceding (13). Note that according to (2), the number and energy densities are given by $n_G=I_2$ and $U_G=I_3$, respectively. The differential equation satisfied by I_ℓ is obtained by operating on (11) with $\int \epsilon^\ell \, d\epsilon$, which yields

$$y(1-y)\frac{\mathrm{d}^2 I_\ell}{\mathrm{d}y^2} + \left(\frac{1-5y}{4}\right)\frac{\mathrm{d}I_\ell}{\mathrm{d}y} + \left(\frac{\ell y + 2y - 1}{4y}\right) I_\ell = \frac{3\beta v_0 \delta(y-y_0) I_\ell}{7 v_c} - \frac{3\dot{N}_0 \epsilon_0^{\ell-2}\delta(y-y_0)}{7\pi r_0^2 v_c}. \tag{72}$$

The energy moment I_ℓ must be continuous at $y=y_0$ in order to avoid generating an infinite spatial diffusion flux there, and consequently we have

$$\Delta\,[I_\ell(y)]|_{y=y_0} = 0. \tag{73}$$

By integrating (72) in a small region around $y=y_0$, we can show that I_ℓ also satisfies the derivative jump condition

$$\Delta \left[\frac{\mathrm{d}I_\ell}{\mathrm{d}y}\right]\Bigg|_{y=y_0} = \frac{3\beta I_\ell(y_0)}{4y_0} - \frac{3\dot{N}_0 \epsilon_0^{\ell-2}}{7\pi r_0^2 v_c y_0 (1-y_0)}, \tag{74}$$

where we have also utilized (12).

The homogeneous version of (72) obtained when $y \neq y_0$ is equivalent to (14) for g if we replace λ with $\ell+1$. Since the energy moments I_ℓ must satisfy the same upstream and downstream boundary conditions that apply to the separation eigenfunctions g_n, we can therefore write the general solution for I_ℓ as

$$I_\ell(y) = \begin{cases} C_\ell \varphi_1(\ell+1, y), & y \leqslant y_0, \\ D_\ell \varphi_2(\ell+1, y), & y \geqslant y_0, \end{cases} \tag{75}$$

where the constants C_ℓ and D_ℓ are computed by satisfying the continuity and derivative jump conditions given by (73) and (74). Upon substitution, we obtain after some algebra

$$C_\ell = \frac{12\dot{N}_0 \epsilon_0^{\ell-2}}{7\pi v_c r_0^2} \frac{(1-y_0)^{-1}\varphi_2(\ell+1, y_0)}{3\beta\varphi_1(\ell+1, y_0)\varphi_2(\ell+1, y_0) - 4y_0 W(\ell+1, y_0)}, \tag{76}$$

$$D_\ell = \frac{12\dot{N}_0 \epsilon_0^{\ell-2}}{7\pi v_c r_0^2} \frac{(1-y_0)^{-1}\varphi_1(\ell+1, y_0)}{3\beta\varphi_1(\ell+1, y_0)\varphi_2(\ell+1, y_0) - 4y_0 W(\ell+1, y_0)}, \tag{77}$$

where $W(\ell+1, y_0)$ is computed using [cf. Eq. (43)]

$$W(\ell+1, y_0) = \frac{5}{4}\frac{\Gamma(1-a_\ell)}{\Gamma(a_\ell)\Gamma(-1/4)}\frac{y_0^{-1/4}}{1-y_0} \tag{78}$$

and

$$a_\ell \equiv \frac{9 - \sqrt{33+16\ell}}{8}. \tag{79}$$

The energy moments $I_\ell(y)$ can also be calculated by substituting for the Green's function in the fundamental integral (71) using (49). Reversing the order or summation and integration yields

$$I_\ell(y) = \epsilon_0^{\ell+1} \sum_{n=0}^{\infty} A_n (\lambda_n - \ell - 1)^{-1} g_n(y), \tag{80}$$

where $g_n(y)$ and A_n are given by (27) and (51), respectively. Note that the expression for $g_n(y)$ can be rewritten as

$$g_n(y) = \frac{\varphi_1(\lambda_n, y_{\min}) \varphi_2(\lambda_n, y_{\max})}{\varphi_2(\lambda_n, y_0)}, \tag{81}$$

where

$$y_{\min} \equiv \min(y, y_0), \quad y_{\max} \equiv \max(y, y_0). \tag{82}$$

Eliminating $I_\ell(y)$ between (75) and (80) and making use of (51), (76), (77), and (81), we find after some simplification that

$$\sum_{n=0}^{\infty} \frac{\varphi_1(\lambda_n, y_0)}{\varphi_2(\lambda_n, y_0)} \frac{\varphi_1(\lambda_n, y_{\min}) \varphi_2(\lambda_n, y_{\max})}{(\lambda_n - \ell - 1) \mathfrak{C}_n} = \frac{y_0^{3/4} (1 - y_0)^{-1} \varphi_1(\ell + 1, y_{\min}) \varphi_2(\ell + 1, y_{\max})}{3\beta \varphi_1(\ell + 1, y_0) \varphi_2(\ell + 1, y_0) - 4 y_0 W(\ell + 1, y_0)}, \tag{83}$$

where the eigenvalues λ_n are computed using (44). Equation (83) is a new hypergeometric summation formula that has not appeared previously in the literature. This relation holds for all real values of ℓ.

V. LINEAR AND BILINEAR GENERATING FUNCTIONS

The case with $\beta = 0$ is interesting from a mathematical point of view because in this limit, the hypergeometric eigenfunctions reduce to Jacobi polynomials. We can therefore combine various results from Secs. III and IV to obtain two new summation formulas (i.e., linear and bilinear generating functions) for the Jacobi polynomials that have not appeared previously in the literature. In the limit $\beta \to 0$, the eigenvalue equation (31) reduces to

$$W(\lambda_n, y_0) = \frac{5}{4} \frac{\Gamma(1 - a)}{\Gamma(a) \Gamma(-1/4)} \frac{y_0^{-1/4}}{1 - y_0} = 0, \tag{84}$$

where we have also made use of (43). Roots of this expression occur where $|\Gamma(a)| \to \infty$, which corresponds to

$$a = -n, \quad n = 0, 1, 2, \ldots . \tag{85}$$

In this situation, we can use (19) to demonstrate that the exact solution for the eigenvalues λ_n is given by

$$\lambda_n = 4n^2 + 9n + 4. \tag{86}$$

Next we note that $a + b = 9/4$ in general according to (19), and therefore we find that

$$b = \tfrac{9}{4} + n. \tag{87}$$

The corresponding expression for the fundamental upstream eigensolution, $\varphi_1(\lambda_n, y)$, is given in this case by the polynomial [see Eq. (17)]

$$\varphi_1(\lambda_n, y) = y F\left(-n, \tfrac{9}{4} + n; \tfrac{9}{4}; y\right), \tag{88}$$

and the fundamental eigensolution in the downstream region, $\varphi_2(\lambda_n, y)$, likewise reduces to [see Eq. (25)]

$$\varphi_2(\lambda_n,y) = \frac{\Gamma(n+9/4)}{\Gamma(9/4)\Gamma(-n-5/4)}\varphi_1(\lambda_n,y). \tag{89}$$

Hence the two eigensolutions $\varphi_1(\lambda_n,y)$ and $\varphi_2(\lambda_n,y)$ are *linearly dependent functions* in this case, which is expected since the Wronskian $W(\lambda_n,y_0)=0$ according to (84). This in turn reflects the fact that there is no derivative jump in the global separation eigenfunction $g_n(y)$ at $y=y_0$ when $\beta=0$ [see Eq. (16)].

Due to the linear dependence of $\varphi_1(\lambda_n,y)$ and $\varphi_2(\lambda_n,y)$, Eq. (81) for the global eigenfunction $g_n(y)$ now simplifies to

$$g_n(y) = \varphi_1(\lambda_n,y), \tag{90}$$

and therefore the summation formula presented in (83) can be rewritten in the $\beta=0$ case as

$$\sum_{n=0}^{\infty} \frac{\varphi_1(\lambda_n,y_0)\varphi_1(\lambda_n,y)}{(\lambda_n-\ell-1)\mathfrak{C}_n} = -\frac{\varphi_1(\ell+1,y_{\min})\varphi_2(\ell+1,y_{\max})}{4y_0^{1/4}(1-y_0)W(\ell+1,y_0)}, \tag{91}$$

where $y_{\min}$ and $y_{\max}$ are defined by (82) and $W(\ell+1,y_0)$ is computed using (78).

We are now in a position to derive an interesting summation formula for products of Jacobi polynomials. Using Eq. (15.4.6) from Abramowitz and Stegun,[8] our expression for the eigensolution $\varphi_1(\lambda_n,y)$ can be rewritten as

$$\varphi_1(\lambda_n,y) = \frac{n!}{(9/4)_n} y P_n^{(5/4,0)}(1-2y), \tag{92}$$

where

$$P_n^{(5/4,0)}(1-2y) = \frac{(9/4)_n}{n!} F\left(-n,\frac{9}{4}+n;\frac{9}{4};y\right) \tag{93}$$

represents the Jacobi polynomial, and $(a)_n$ denotes the Pochhammer symbol, defined by[8]

$$(a)_n \equiv \frac{\Gamma(a+n)}{\Gamma(a)}. \tag{94}$$

In the present application, with $\beta=0$, we can combine (52), (90), and (92) to express the quadratic normalization integrals, $\mathfrak{C}_n$, as

$$\mathfrak{C}_n = \left[\frac{n!}{(9/4)_n}\right]^2 \int_0^1 y^{5/4}[P_n^{(5/4,0)}(1-2y)]^2\,dy, \tag{95}$$

which can be evaluated using Eq. (7.391.1) from Gradshteyn and Ryzhik[10] to obtain

$$\mathfrak{C}_n = \left[\frac{n!}{(9/4)_n}\right]^2 \left(2n+\frac{9}{4}\right)^{-1}. \tag{96}$$

Equations (78), (86), (91), (92), and (96) can be combined to derive a new *bilinear generating function* for the Jacobi polynomials, which can be written as

$$\sum_{n=0}^{\infty} (9+8n)\frac{P_n^{(5/4,0)}(1-2y_0)P_n^{(5/4,0)}(1-2y)}{4n^2+9n+3-\ell} = \frac{16}{5}\frac{\Gamma(3/4)\Gamma(a_\ell)}{\Gamma(1-a_\ell)}\frac{\varphi_1(\ell+1,y_{\min})\varphi_2(\ell+1,y_{\max})}{yy_0}, \tag{97}$$

where a_ℓ is defined by (79). Note that the functions $\varphi_1(\ell+1,y_{\min})$ and $\varphi_2(\ell+1,y_{\max})$ appearing on the right-hand side of (97) are *not* eigenfunctions since in general the quantity $\ell+1$ is not equal to one of the eigenvalues λ_n.

An interesting special case occurs in the limit $y_0 \to 0$. Making use of the relation [see Eq. (93)]

$$P_n^{(5/4,0)}(1) = \frac{(9/4)_n}{n!}, \tag{98}$$

and the identity

$$\Gamma\left(\tfrac{3}{4}\right)\Gamma\left(\tfrac{9}{4}\right) = \tfrac{5}{16}\pi 2^{1/2}, \tag{99}$$

we now find that (97) reduces to the *linear generating function*

$$\sum_{n=0}^{\infty} \frac{(9+8n)\Gamma(n+9/4)}{(4n^2+9n+3-\ell)n!} P_n^{(5/4,0)}(1-2y) = \frac{\pi 2^{1/2}\Gamma(a_\ell)}{\Gamma(1-a_\ell)} \frac{\varphi_2(\ell+1,y)}{y}, \tag{100}$$

which is valid for all real values of ℓ. Equations (97) and (100) are new results that are useful for the evaluation of infinite sums containing either products of Jacobi polynomials or single Jacobi polynomials, respectively.

VI. CONCLUSION

In this paper we have employed methods of classical analysis to obtain the exact solution for the Green's function describing the Fermi energization of photons scattered by infalling electrons in a pulsar accretion column. This process is of central importance in the development of theoretical models for the production of the x-ray spectra observed from these objects, which are among the brightest sources in the Milky Way galaxy. As demonstrated in Fig. 1 and Eq. (49), the Green's function is characterized by a power-law shape at high photon energies, which is typical for a Fermi process. In this scenario, photons gain their energy by diffusing back and forth across the shock many times. The probability of multiple shock crossings decreases exponentially with the number of crossings, and the mean energy of the photons increases exponentially with the number of crossings. This combination of factors naturally gives rise to a power-law energy distribution.[11] Hence shock energization in the pulsar accretion column provides a simple explanation for the spectrum of the high-energy radiation produced by x-ray pulsars. Specific examples of the Green's function are plotted in Figs. 2 and 3.

Due to the linearity of the transport equation (1), we can employ the Green's function to calculate the radiation spectrum inside the accretion column resulting from an arbitrary source spectrum using the convolution[12]

$$f(y_0,y,\epsilon) = \int_0^{\infty} j(\epsilon_0) \frac{f_G(y_0,y,\epsilon_0,\epsilon)}{\dot{N}_0} \mathrm{d}\epsilon_0, \tag{101}$$

where $j(\epsilon_0)\mathrm{d}\epsilon_0$ represents the number of photons injected per unit time into the accretion column at location y_0 with energy between ϵ_0 and $\epsilon_0+\mathrm{d}\epsilon_0$. The source distribution of greatest astrophysical interest is the "thermal mound" source located near the base of the accretion column, where the gas has decelerated almost to rest and is therefore extremely dense. This hot plasma is in full thermodynamic equilibrium, and consequently it radiates a black-body spectrum.[1] The absorption parameter β has been included in the transport equation (1) in order to account for the fact that a black body acts as both a source and a sink of radiation.[4] The fundamental results for the Green's function obtained in the present paper will be used to study the reprocessing of the black-body radiation emitted from the thermal mound in a subsequent paper.

In addition to the analytical results for the Green's function, we have also obtained an interesting formula for the evaluation of an infinite series involving products of the orthogonal hypergeometric eigenfunctions [see Eq. (83)]. This derivation was based on the simultaneous calculation of the energy moments $I_\ell(y)$ using both an expression based on term-by-term integration of the Green's function expansion (49), and an independent solution developed via direct integration of the fundamental transport equation (1). In the special case $\beta \to 0$, which corresponds physically

to the neglect of absorption at the source location, our general formula for the hypergeometric summation reduces to a bilinear generating function for the Jacobi polynomials given by (97). This relation in turn simplifies to yield a linear generating function for the Jacobi polynomials in the limit $y_0 \to 0$, which corresponds physically to a source located in the far upstream region [see Eq. (100)].

The results derived in this paper for the linear and bilinear generating functions of Jacobi polynomials are related to various similar expressions obtained previously by Chen and Srivastava,[13,14] Srivastava,[15] Rangarajan,[16] and Pittaluga, Sacripante, and Srivastava.[17] However, our results are not identical to any of their formulas and therefore they represent an interesting new family of relations. Although the linear and bilinear generating functions developed here relate specifically to the properties of the polynomials $P_n^{(5/4,0)}(1-2y)$, we expect that some level of generalization may be possible. We plan to pursue this question in future work.

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Hecke transformation and the generalized theta function

Indranil Biswas[a)]
School of Mathematics, Tata Institute of Fundamental Research, Homi Bhabha Road, Bombay, 400005, India

A. K. Raina[b)]
Tata Institute of Fundamental Research, Theoretical Physics Department, Homi Bhabha Road, Colaba, Mumbai, Bombay 400 005, India

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We describe the behavior of the generalized theta function with respect to the Hecke transformations. Let E be a holomorphic vector bundle over rank r and degree $r(g-1)$ over a compact Riemann surface X of genus g. Let $P(E)$ [respectively, $\mathbb{P}(E)$] be the space of all lines (respectively, hyperplanes) in the fibers of E. Certain Zariski open subsets of $\mathbb{P}(E)\times\times P(E)$ and $\mathbb{P}(E)\times\mathbb{P}(E)\times P(E)\times P(E)$ parametrize holomorphic families of vector bundles over X of rank r and degree $r(g-1)$. We describe the generalized theta line bundle for these families. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1879082]

I. INTRODUCTION

In a well known paper, Hawley and Schiffer [5]generalized the notion of a Szegö kernel from a domain in the complex plane (with smooth boundary) to a compact connected Riemann surface X of arbitrary genus g. More recently, it was observed by physicists that the Szegö kernel could be identified as the "two-point function" of a model two-dimensional quantum field theory appearing in conformal field theory and string theory (see Ref. 10 for references). It was shown by Raina[10,11] that the physics could be in a natural way reformulated in the language of algebraic geometry. Given a line bundle α on X of degree $g-1$ lying outside the theta divisor, i.e., a holomorphic line bundle α with $H^0(X,\alpha)=0=H^1(X,\alpha)$, a "$2n$-point function" is interpreted as a meromorphic section with certain physically required zeros and poles of the line bundle over X^{2n} which is constructed using the (external) tensor product of n copies of α and n copies of its Serre dual $K_X\otimes\alpha^{-1}$. The line bundle K_X is the holomorphic cotangent bundle of X. A proof of the uniqueness of the $2n$-point functions and an application of a "Riemann lemma" enabled the explicit determination of these sections in terms of theta functions associated with the Riemann surface. In the case of the four-point function, this led to a proof of the trisecant identity for theta functions associated to a Jacobian.[10]

A subject of much speculation has been whether there is an interesting analog of these results when the line bundle α is replaced by a vector bundle E of rank r and degree $r(g-1)$. Indeed, it was remarked by Raina (see Ref. 10, Remark 5.7) that the proof of the uniqueness of the $2n$-point function remained valid if E has no holomorphic sections and is simple. However, the interesting question is to relate the sections to *generalized theta functions* and possibly to arrive at a corresponding generalization of the trisecant identity. We shall carry out the first part and give indications towards the second. In a recent paper,[2] David Ben-Zvi and one of us (I.B.) studied the corresponding Szegö kernel and its relationship with generalized theta functions. We remark that, while there have been other works thematically related to the present one, (see Refs. 3 and 8), the present work is quite different from these. While in Polishchuk[8], the approach to the higher rank

[a)]E-mail: indranil@math.tifr.res.in
[b)]E-mail: raina@tifr.res.in

generalization of the trisecant identity is through generalized determinants, and in Gómez and González[3], the natural embedding of $X\times X$ in the moduli space of vector bundles over X defined by $(x,y)\mapsto E\otimes\mathcal{O}_X(x-y)$ is investigated (just as done in the case of line bundles), the aim here is to investigate the relationship between the Hecke transformations and the Quillen determinant line bundle. The relationships between them established here turn out to suggest a possible approach to the higher rank generalization of the trisecant identity.

Remark 5.7 of Ref. 10 also provided motivation for the construction of a higher rank analog of the *bc*-system carried out by Schork.[12,13] The generalized theta functions on the parameter spaces considered here are related to the correlation functions of that system.

To describe the results proved here, let E be a holomorphic vector bundle of rank r and degree $r(g-1)$ over X, with $P(E)$ [respectively, $\mathbb{P}(E)$] being the space of all lines (respectively, hyperplanes) in the fibers of E. Given a line ℓ or a hyperplane H in the fiber E_x of E over $x\in X$, the Hecke transformation gives vector bundles defined by the exact sequences

$$0\to V\to E\to E_x/\ell\to 0$$

and

$$0\to W\to E\to E_x/H\to 0.$$

So V and W are canonically identified with E over $X\backslash\{x\}$.

Now, given a point of $P(E)$ and a point of $\mathbb{P}(E)$, a new vector bundle over X can be constructed by combining the above constructions. Therefore, we have a family of vector bundles over X parametrized by a Zariski open dense subset $\mathcal{U}\subset\mathbb{P}(E)\times P(E)$. This construction does not give a vector bundle if the hyperplane contains the line in the fiber of E; therefore, that family is actually parametrized by an open subset of $\mathbb{P}(E)\times P(E)$.

In Lemma 2.1 we identify the generalized theta line bundle (= determinant line bundle) for this family. Since the complement of $\mathcal{U}$ in $\mathbb{P}(E)\times P(E)$ is of codimension at least two, the generalized theta line bundle as well as its section given by the generalized theta function extend to $\mathbb{P}(E)\times P(E)$.

A family of vector bundles over X can similarly be constructed which is parametrized by a Zariski open dense subset

$$\mathcal{U}_2\subset\mathbb{P}(E)\times\mathbb{P}(E)\times P(E)\times P(E).$$

For any point $(y_1,y_2,z_1,z_2)\in\mathcal{U}_2$, the corresponding vector bundle over X is constructed by performing Hecke transformations using the lines z_1, z_2 as well as the hyperplanes y_1, y_2. In Lemma 2.3 we identify the determinant line bundle over $\mathcal{U}_2$ for this family. In Theorem 3.1 it is shown that this line bundle over $\mathcal{U}_2$ has the property that the space of its global holomorphic sections is one dimensional, provided $\dim H^0(X,E)=0=\dim H^0(X,\mathrm{End}(E))-1$.

For any vector bundle E satisfying the above cohomology conditions, let ϑ and ϑ_2 be the generalized theta functions on $\mathbb{P}(E)\times P(E)$ and $\mathbb{P}(E)\times\mathbb{P}(E)\times P(E)\times P(E)$, respectively, for the above families of vector bundles over X (the functions extend). Consider $q_{13}^*\vartheta\otimes q_{24}^*\vartheta-q_{14}^*\vartheta\otimes q_{23}^*\vartheta$, where q_{ij}, $1\leqslant i<j\leqslant 4$, is the projection of $\mathbb{P}(E)\times\mathbb{P}(E)\times P(E)\times P(E)$ to the product of the ith and jth factor, that is, $q_{ij}(a_1,a_2,a_3,a_4)=(a_i,a_j)$. If $r=1$, then $\mathbb{P}(E)\cong X\cong P(E)$, and hence this section vanishes over the two images of X^3 in X^4 defined by $(x,y,z)\mapsto(x,x,y,z)$ and $(x,y,z)\mapsto(x,y,z,z)$. This immediately implies that the above defined section coincides with ϑ_2. This equality of sections is the trisecant identity. However, if $r>1$, then we do not know if the section vanishes over the two images of X^3. If it does, then a similar identity for the generalized function would follow immediately.

II. THE DETERMINANT LINE BUNDLE

Let X be a compact connected Riemann surface, or equivalently, a connected smooth projective curve defined over $\mathbb{C}$. The genus of X will be denoted by g.

Fix a holomorphic vector bundle E over X of rank r and degree $r(g-1)$. Let $\mathbb{P}(E)$ [respectively, $P(E)$] be the projective bundle over X parametrizing all hyperplanes (respectively, lines) in the fibers of E. Let $\mathcal{O}_{\mathbb{P}(E)}(1)$ [respectively, $\mathcal{O}_{P(E)}(1)$] be the tautological line bundle over $\mathbb{P}(E)$ [respectively, $P(E)$] whose fiber over any point is the quotient by the hyperplane (respectively, dual of the line) represented by the point.

For notational simplicity, the variety $\mathbb{P}(E)$ [respectively, $P(E)$] will be denoted by Y (respectively, Z). For the same reason, the line bundle $\mathcal{O}_{\mathbb{P}(E)}(1)$ [respectively, $\mathcal{O}_{P(E)}(1)$] will be denoted by ζ (respectively, η).

Let $f_2\colon Z\to X$ be the natural projection. Note that we have a natural inclusion of $\mathcal{O}_{P(E)}(-1) := \eta^*$ in f_2^*E as a subbundle. Let Q be the vector bundle over $P(E)=Z$ of rank $r-1$ that fits in the following exact sequence of vector bundles

$$0 \to \mathcal{O}_{P(E)}(-1) = \eta^* \to f_2^*E \to Q \to 0 \tag{2.1}$$

over Z.

Let $f_1\colon Y\to X$ be the natural projection. Note that the vector bundle f_1^*E has a natural projection to the line bundle ζ. Let Q' (respectively, ζ') over $X\times Z$ (respectively, $X\times Y$) be the direct image of Q (respectively, ζ) by the embedding that sends any point $z\in Z$ (respectively, $y\in Y$) to $(f_2(z),z)\in X\times Z$ [respectively, $(f_1(y),y)\in X\times Y$]. So both Q' and ζ' are torsion sheaves.

Consider the Cartesian product $X\times Y\times Z$, which is a projective variety of dimension $2r+1$. Let

$$p_1\colon X\times Y\times Z\to X$$

be the projection to the first factor. So we have a homomorphism

$$\alpha=\alpha_1\oplus\alpha_2\colon p_1^*E\to p_{12}^*\zeta'\oplus p_{13}^*Q', \tag{2.2}$$

where p_{12} (respectively, p_{13}) is the projection $X\times Y\times Z$ to $X\times Y$ (respectively, $X\times Z$); the homomorphism α_2 is the pullback of the projection map in (2.1), and α_1 is the pullback of the projection $f_1^*E\to\zeta$. Let p_Y and p_Z be the projections of $Y\times Z$ to Y and Z, respectively.

We note that $p_{12}^*\zeta'$ (respectively, p_{13}^*Q') is identified with the direct image of $p_Y^*\zeta$ (respectively, p_Z^*Q) by the embedding of $Y\times Z$ in $X\times Y\times Z$ that sends any point (y,z) to $(f_1(y),y,z)$ [respectively, $(f_2(z),y,z)$].

Let

$$\mathcal{E}' := \text{kernel}(\alpha)\subset f^*E \tag{2.3}$$

be the kernel of the homomorphism α defined in (2.2) (see Ref. 7, Sec. 4 for this construction which is known as the Hecke transformation). The torsionfree coherent sheaf $\mathcal{E}'$ on $X\times Y\times Z$ is not locally free in general. The projection of $X\times Y\times Z$ to $Y\times Z$ will be denoted by p_{23}. Consider the closed subvariety $S\subset Y\times Z$ defined by all points of the form (y,z) satisfying the two conditions that $f_1(y)=f_2(z)$ and the hyperplane in the fiber $E_{f_1(y)}$ defined by y contains the line in $E_{f_2(z)}$ defined by z. Let

$$\mathcal{U} := (Y\times Z)\setminus S \tag{2.4}$$

be the complement. The coherent sheaf $\mathcal{E}'$ is locally free over $p_{23}^{-1}(\mathcal{U})\subset X\times Y\times Z$. Indeed, this follows from the fact that for any $(y,z)\in\mathcal{U}$, the two subspaces of $E_{f_1(y)}$, namely $\eta_{f_2(z)}$ and the kernel of the projection $E_{f_1(y)}\to\zeta_{f_1(y)}$, are transversal. Note that the codimension of S in $Y\times Z$ is two if $\text{rank}(E)\geqslant 2$, and if E is a line bundle, then S is the empty set. Although we do not need it, it may be mentioned that $\mathcal{E}'$ fails to be locally free exactly over the subvariety of $X\times Y\times Z$ defined by all points (x,y,z) satisfying the two conditions that $(y,z)\in S$ and $x=f_1(y)$.

Since $\mathcal{E}'$ is a vector bundle over $p_{23}^{-1}(\mathcal{U})$, we can—and we will—consider $\mathcal{E}'|_{p_{23}^{-1}(\mathcal{U})}$ as an algebraic family of vector bundles over X parametrized by $\mathcal{U}$. Note that for any point $(y,z)\in\mathcal{U}$

with $f_1(y)=f_2(z)$, the corresponding vector bundle over X for this family (that is, the restriction of $\mathcal{E}'$ to $X\times\{y\}\times\{z\}$) is canonically identified with the vector bundle $E\otimes\mathcal{O}_X(-f_1(y))$.

Let p_i, $i=1,2,3$, be the projection of $X\times Y\times Z$ to the ith factor (the projection p_1 was defined earlier). So then $p_{1j}=p_1\times p_j$, where $j=2,3$, and we also have $p_2=p_Y\circ p_{23}$ and $p_3=p_Z\circ p_{23}$.

Let $\Delta\subset X\times X$ be the (reduced) diagonal divisor defined by all points of the form (x,x), where $x\in X$. Let

$$L_\Delta := (p_1\times(f_2\circ p_3))^*\mathcal{O}_{X\times X}(\Delta) \tag{2.5}$$

be the line bundle over $X\times Y\times Z$.

Define the vector bundle

$$\mathcal{E} := \mathcal{E}'\otimes L_\Delta \tag{2.6}$$

over $p_{23}^{-1}(\mathcal{U})\cong X\times\mathcal{U}$, where $\mathcal{E}'$ is defined in (2.3) and L_Δ is defined in (2.5). We will consider $\mathcal{E}$ as an algebraic family of vector bundles over X parametrized by $\mathcal{U}$. For any point $t\in\mathcal{U}$, the vector bundle over X obtained by restricting $\mathcal{E}$ to $X\times\{t\}$ will be denoted by $\mathcal{E}_t$. Note that if $f_1\circ p_Y(t)=f_2\circ p_Z(t)\in X$, where $t\in\mathcal{U}$, then $\mathcal{E}_t$ is identified with E. Indeed, this follows from the earlier observation that $\mathcal{E}'|_{X\times\{y\}\times\{z\}}\cong E\otimes\mathcal{O}_X(-f_1(y))$.

Let

$$\mathcal{L} := d(\mathcal{E}) \tag{2.7}$$

be the determinant line bundle over $\mathcal{U}$ for the family of vector bundles over X defined by $\mathcal{E}$ (see Refs. 9 and 1 for the determinant line bundle). So, for any point $t\in\mathcal{U}$ the fiber $\mathcal{L}_t$ is canonically identified with the line $(\wedge^{\text{top}}H^0(X,\mathcal{E}_t)^*)\otimes(\wedge^{\text{top}}H^1(X,\mathcal{E}_t))$. These lines fit together in a natural fashion to define a holomorphic line bundle over the parameter space (namely, $\mathcal{U}$).

For a holomorphic vector bundle F over X, we will denote by $d(F)$ the complex line $(\wedge^{\text{top}}H^0(X,F)^*)\otimes(\wedge^{\text{top}}H^1(X,F))$.

Lemma 2.1: The determinant line bundle $\mathcal{L}$ over $\mathcal{U}$ is canonically isomorphic to the restriction to $\mathcal{U}\subset Y\times Z$ of $p_Y^*\zeta\otimes p_Z^*(\eta^*\otimes f_2^*K_X)\otimes(f_1\times f_2)^*\mathcal{O}_{X\times X}(\Delta)\otimes l$, where K_X is the holomorphic cotangent bundle of X and l is the trivial line bundle over $Y\times Z$ with fiber $d(E)$, where $d(E)$ is the line defined above.

Proof: The natural isomorphism between $p_Y^*\zeta\otimes p_Z^*(\eta^*\otimes f_2^*K_X)\otimes(f_1\times f_2)^*\mathcal{O}_{X\times X}(\Delta)\otimes l$ and $\mathcal{L}$ over $\mathcal{U}$ asserted in the lemma is produced by identifying the fibers of the two line bundles.

Take any point $t=(y,z)\in\mathcal{U}\subset Y\times Z$. Set $x_1=f_1(y)$ and $x_2=f_2(z)$. The vector bundle $\mathcal{E}_t$ is identified with the kernel of the subjective homomorphism

$$E\otimes_{\mathcal{O}_X}\mathcal{O}_X(x_2)\to(\zeta_y\otimes\mathcal{O}_X(x_2)_{x_1})\oplus(Q_z\otimes\mathcal{O}_X(x_2)_{x_2}), \tag{2.8}$$

where $\mathcal{O}_X(x_2)_x$ is the fiber of the line bundle $\mathcal{O}_X(x_2)$ over x. Note that this description of $\mathcal{E}_t$ implies that if $x_1=x_2$, then $\mathcal{E}_t$ is identified with E. Indeed, in that case the fiber $E_{x_2}\otimes\mathcal{O}_X(x_2)_{x_2}$ is mapped isomorphically to $(\zeta_y\otimes\mathcal{O}_X(x_2)_{x_1})\oplus(Q_z\otimes\mathcal{O}_X(x_2)_{x_2})$ by the homomorphism defined in (2.8). Consequently, the kernel of the homomorphism in (2.8) is identified with the image of E in $E\otimes_{\mathcal{O}_X}\mathcal{O}_X(x_2)$ by the inclusion map.

For an exact sequence of coherent sheaves

$$0\to A\to B\to C\to 0$$

over X, where A and B are locally free (vector bundles) and C is a torsion sheaf supported over a point with $\dim_{\mathbb{C}}C=n$, we have an isomorphism

$$d(A)\cong d(B)\otimes\wedge^n C \tag{2.9}$$

(recall that $d(F):=\wedge^{\text{top}}H^0(X,F)^*\otimes\wedge^{\text{top}}H^1(X,F)$). Consequently, setting $A=E$ and $B=E\otimes_{\mathcal{O}_X}\mathcal{O}_X(x_2)$ we obtain

$$d(E\otimes_{\mathcal{O}_X}\mathcal{O}_X(x_2))\cong d(E)\otimes\wedge^r(E_{x_2}\otimes T_{x_2}X)^*, \tag{2.10}$$

where $r=\mathrm{rank}(E)$.

Let V be the vector bundle over X defined by the exact sequence of coherent sheaves

$$0\to V\to E\otimes_{\mathcal{O}_X}\mathcal{O}_X(x_2)\to Q_z\otimes\mathcal{O}_X(x_2)_{x_2}\to 0,$$

where Q_z is the quotient of E_{x_2} defined by the point $z\in Z$. Using (2.9) and (2.10) it follows that

$$d(V)\cong d(E)\otimes K_{x_2}\otimes\eta_z, \tag{2.11}$$

where K_{x_2} is the fiber over x_2 of the holomorphic cotangent bundle K_X.

The vector bundle $\mathcal{E}_t$ over X (recall that $t=(y,z)$) fits in the exact sequence

$$0\to\mathcal{E}_t\to V\to\zeta_y\otimes\mathcal{O}_X(x_2)_{x_1}\to 0.$$

Therefore, using (2.9) and (2.11) we have

$$d(\mathcal{E}_t)\cong d(V)\otimes\zeta_y\otimes\mathcal{O}_X(x_2)_{x_1}\cong d(E)\otimes K_{x_2}\otimes\eta_z\otimes\zeta_y\otimes\mathcal{O}_{X\times X}(\Delta)_{(x_1,x_2)}$$

as $\mathcal{O}_X(x_2)_{x_1}$ is identified with the fiber over the point $(x_1,x_2)\subset X\times X$ of the line bundle $\mathcal{O}_{X\times X}(\Delta)$. This completes the proof of the lemma. □

Since we have $\chi(E)=0$, the determinant line bundle $d(\mathcal{E})$ in (2.7) has a canonical section, which is know as the *generalized theta function*[1,9]. This section vanishes at a point $u\in\mathcal{U}$ if and only if $H^0(X,\ \mathcal{E}|_{X\times\{u\}})\neq 0$. Let

$$\theta\in H^0(\mathcal{U},d(\mathcal{E})) \tag{2.12}$$

be the generalized theta function. We recall that θ vanishes at a point $t\in\mathcal{U}$ if and only if $H^0(X,\mathcal{E}_t)\neq 0$. In particular, if $\mathcal{E}_t$ is not semistable, then $\theta(t)=0$.

Let

$$\vartheta\in H^0(\mathcal{U},p_Y^*\zeta\otimes p_Z^*(\eta^*\otimes f_2^*K_X)\otimes(f_1\times f_2)^*\mathcal{O}_{X\times X}(\Delta)\otimes l) \tag{2.13}$$

be the section over $\mathcal{U}$ defined by θ [in (2.12)] using the isomorphism in Lemma 2.1. Note that the complement of $\mathcal{U}$ in $Y\times Z$ is of codimension at least two. Therefore, ϑ extends to $Y\times Z$; the extended section will also be denoted by ϑ.

We will now identify the determinant line bundle over $Y\times Y\times Z\times Z$ for a family of vector bundles constructed also using Hecke transformation.

Let $\Delta_Y\subset Y\times Y$ and $\Delta_Z\subset Z\times Z$ be the diagonals. Let q_{ij}, $1\leqslant i<j\leqslant 4$, be the projection $Y\times Y\times Z\times Z$ to the product of the ith and the jth factor. Therefore, q_{ij} sends any point (x_1,x_2,x_3,x_4) of $Y\times Y\times Z\times Z$ to (x_i,x_j). Set

$$S_2:=q_{12}^{-1}(\Delta_Y)\cup q_{34}^{-1}(\Delta_Z)\bigcup_{i=1,2;j=3,4}q_{ij}^{-1}(S)\subset Y\times Y\times Z\times Z, \tag{2.14}$$

where $S\subset Y\times Z$ is the subvariety in (2.4). Let

$$\mathcal{U}_2:=S_2^c=(Y\times Y\times Z\times Z)\setminus S_2\subset Y\times Y\times Z\times Z \tag{2.15}$$

be the complement of S_2 [defined in (2.14)], which is a Zariski open dense subset.

As before, there is a natural family of vector bundles over X parametrized by $\mathcal{U}_2$. We will describe this family.

Let ϕ_i, $1\leqslant i\leqslant 5$, be the projection of $X\times Y\times Y\times Z\times Z$ to the ith factor. The projection of $X\times Y\times Y\times Z\times Z$ to the product of the ith factor and the jth factor, where $1\leqslant i<j\leqslant 5$, will be denoted by ϕ_{ij}. So ϕ_i (respectively, ϕ_{ij}) sends any point (x_1,x_2,x_3,x_4,x_5) of $X\times Y\times Y\times Z\times Z$ to x_i [respectively, (x_i,x_j)].

Consider the homomorphism

$$\beta := (\beta_{11} \oplus \beta_{12}) \oplus (\beta_{21} \oplus \beta_{22}) : \phi_1^* E \to (\phi_1 \times \phi_{24})^* (p_{12}^* \zeta' \oplus p_{13}^* Q') \oplus (\phi_1 \times \phi_{35})^* (p_{12}^* \zeta' \oplus p_{13}^* Q') \tag{2.16}$$

over $X \times Y \times Y \times Z \times Z$, where β_{ij}, $i,j \in \{1,2\}$, is the pullback to $X \times Y \times Y \times Z \times Z$ of the homomorphism α_j in (2.2). Thus $\beta_{11} : \phi_1^* E \to (\phi_1 \times \phi_{24})^* p_{12}^* \zeta'$ and $\beta_{21} : \phi_1^* E \to (\phi_1 \times \phi_{35})^* p_{12}^* \zeta'$ are the pullbacks of α_1 [defined in (2.2)] using the projections $\phi_1 \times \phi_{24}$ and $\phi_1 \times \phi_{35}$, respectively. The homomorphisms β_{12} and β_{22} are constructed from α_2 in a similar fashion.

Proposition 2.2: The kernel of the homomorphism β constructed in (2.16) is locally free over $X \times \mathcal{U}_2$, where $\mathcal{U}_2$ is defined in (2.15).

Proof: Let Δ_1 (respectively, Δ_2) be the reduced divisor on $X \times Y \times Y \times Z \times Z$ defined by all points $(x_1, x_2, x_3, x_4, x_5)$ with $f_1(x_2) = x_1$ (respectively, $f_1(x_3) = x_1$), where, as before, f_1 is the projection of Y to X. On Δ_i, $i = 1,2$, we have a subbundle $V_i \subset (\phi_1^* E)|_{\Delta_i}$ of rank $r-1$ defined as the kernel of the natural projection of $(\phi_1^* E)|_{\Delta_i}$ to $(\phi_{i+1}|_{\Delta_i})^* \zeta$.

Similarly, define Δ_3 (respectively, Δ_4) to be the reduced divisor on $X \times Y \times Y \times Z \times Z$ defined by all points $(x_1, x_2, x_3, x_4, x_5)$ with $f_2(x_4) = x_1$ [respectively, $f_2(x_5) = x_1$], where f_2 is the projection of Z to X. Let $V_i = (\phi_{i+1}|_{\Delta_i})^* \eta^*$, $i = 3,4$, be the line subbundle of $(\phi_1^* E)|_{\Delta_i}$ defined using (2.1).

The union

$$\overline{\Delta} := \sum_{i=1}^{4} \Delta_i$$

constitutes a normal crossing divisor on $X \times Y \times Y \times Z \times Z$. Over any connected component of $\Delta_i \cap \Delta_j \cap (X \times \mathcal{U}_2)$, where $1 \leqslant i < j \leqslant 4$, the intersection of the two subbundles V_i and V_j is again a subbundle of $(\phi_1^* E)|_{\Delta_i \cap \Delta_j \cap (X \times \mathcal{U}_2)}$. In other words, the dimension of $(V_i)_y \cap (V_j)_y \subset (\phi_1^* E)_y$ is independent of y, where y runs over a connected component of $\Delta_i \cap \Delta_j \cap (X \times \mathcal{U}_2)$.

The same assertion holds for each connected component of each triple intersection $\Delta_i \cap \Delta_j \cap \Delta_l \cap (X \times \mathcal{U}_2)$, where $1 \leqslant i < j < k \leqslant 4$, that is, $\dim (V_i)_y \cap (V_j)_y \cap (V_k)_y$ does not change while y runs over a connected component. This also holds for the total intersection $\cap_{i=1}^4 \Delta_i$.

These observations immediately imply that the kernel of the homomorphism β is locally free over $X \times \mathcal{U}_2$, completing the proof of the proposition. □

Thus kernel(β) [as in (2.16)] defines a vector bundle over $X \times \mathcal{U}_2$; this vector bundle will be denoted by $\mathcal{E}_2'$.

Now, define the vector bundle

$$\mathcal{E}_2 := \mathcal{E}_2' \otimes (\phi_1 \times \phi_{24})^* L_\Delta \otimes (\phi_1 \times \phi_{35})^* L_\Delta \tag{2.17}$$

over $X \times \mathcal{U}_2$, where L_Δ is the line bundle over $X \times Y \times Z$ defined in (2.5). Note that both $(\phi_1 \times \phi_{24})^* L_\Delta$ and $(\phi_1 \times \phi_{35})^* L_\Delta$ are pullbacks to $X \times Y \times Y \times Z \times Z$ of line bundles over $X \times Y \times Z$.

Let

$$\mathcal{L}_2 := d(\mathcal{E}_2) \tag{2.18}$$

be the determinant line bundle over $\mathcal{U}_2$ for the algebraic family, defined by $\mathcal{E}_2$, of vector bundles over X parametrized by $\mathcal{U}_2$. We will identify the line bundle $d(\mathcal{E}_2)$ in the spirit of Lemma 2.1.

Let

$$\delta := p_Y^* \zeta \otimes p_Z^* (\eta^* \otimes f_2^* K_X) \otimes (f_1 \times f_2)^* \mathcal{O}_{X \times X}(\Delta) \tag{2.19}$$

be the line bundle over $Y \times Z$ (see Lemma 2.1). Let

$$L_Y := (f_1 \times f_1)^* \mathcal{O}_{X \times X}(\Delta)$$

be the line bundle over $Y \times Y$. Similarly, define the line bundle $L_Z := (f_2 \times f_2)^* \mathcal{O}_{X \times X}(\Delta)$ over $Z \times Z$. Let

$$L' := (f_1 \times f_2)^* \mathcal{O}_{X\times X}(\Delta) \tag{2.20}$$

be the line bundle over $Y \times Z$.

Lemma 2.3: The determinant line bundle $\mathcal{L}_2$ over $\mathcal{U}_2$ [defined in (2.18)] is canonically identified with the line bundle

$$l_2 \otimes q_{13}^* \delta \otimes q_{24}^* \delta \otimes (q_{12}^* L_Y \otimes q_{34}^* L_Z)^* \otimes q_{14}^* L' \otimes q_{23}^* L'$$

where l_2 is the trivial line bundle over $\mathcal{U}_2$ with fiber $d(E)$; the line bundles δ and L' are defined, respectively, in (2.19) and (2.20), and L_Y, L_Z are defined above.

Proof: The proof of this lemma is very similar to the proof of Lemma 2.1. However, for the sake of completeness, we give the details.

Take a point $t=(y_1,y_2,z_1,z_2) \in \mathcal{U}_2$. Set $x_i=f_2(z_i)$, $i=1,2$. Consider the vector bundle W over X defined by the exact sequence

$$0 \to E \to W \to A_1 \to 0$$

of coherent sheaves, where A_1 is a torsion sheaf of dimension one supported at the (reduced) point x_1, and the kernel of the homomorphism $E_{x_1} \to W_{x_1}$ is the line in E_{x_1} represented by z_1. Note that since $z_2 \neq z_1$, the line in the fiber E_{x_2} represented by z_2 defines a line in W_{x_2}. Let W' be the vector bundle over X defined by the exact sequence

$$0 \to W \to W' \to A_2 \to 0$$

of coherent sheaves, where A_2 is a torsion sheaf of dimension one supported at the (reduced) point x_2, and the kernel of the homomorphism $W_{x_2} \to W'_{x_2}$ is the line defined by z_2.

From the definition of W and W' it follows immediately that $A_1 \cong \eta_{z_1} \otimes T_{x_1}X$ and

$$A_2 \cong \eta_{z_2} \otimes T_{x_2}X \otimes \mathcal{O}_{X\times X}(\Delta)_{(x_1,x_2)}$$

as the fiber $\mathcal{O}_{X\times X}(\Delta)_{(x_1,x_2)}$ of the line bundle $\mathcal{O}_{X\times X}(\Delta)$ over the point (x_1,x_2) is identified with the fiber of $\mathcal{O}_X(x_1)$ over x_2. Now using the isomorphism in (2.9) we conclude that

$$d(W') \cong d(E) \otimes \eta_{z_1}^* \otimes K_{x_1} \otimes \eta_{z_2}^* \otimes K_{x_2} \otimes \mathcal{O}_{X\times X}(-\Delta)_{(x_1,x_2)}, \tag{2.21}$$

where K_x is the fiber over the point x of the holomorphic cotangent bundle of X.

Set $x_1^0=f_1(y_1) \in X$. Let V be the vector bundle over X defined by the exact sequence

$$0 \to V \to W' \to \zeta_{y_1} \otimes_{\mathbb{C}} \mathcal{O}_X(x_1+x_2) \to 0.$$

Note that $\zeta_{y_1} \otimes_{\mathbb{C}} \mathcal{O}_X(x_1+x_2)$ is a torsion sheaf of dimension one supported on the reduced point x_1^0. The projection of W' to $\zeta_{y_1} \otimes_{\mathbb{C}} \mathcal{O}_X(x_1+x_2)$ is defined by the natural projection $E_{x_1^0} \to \zeta_{y_1}$. The identity (2.9) for this exact sequence gives

$$d(V) \cong d(W') \otimes \zeta_{y_1} \otimes \mathcal{O}_{X\times X}(\Delta)_{(x_1^0,x_1)} \otimes \mathcal{O}_{X\times X}(\Delta)_{(x_1^0,x_2)}. \tag{2.22}$$

Similarly, set $x_2^0=f_1(y_2) \in X$. The vector bundle $\mathcal{E}_2|_t$ over X, obtained by restricting $\mathcal{E}_2$ to $X \times \{t\} \subset X \times Y \times Y \times Z \times Z$, fits in the following exact sequence

$$0 \to \mathcal{E}_2|_t \to V \to \zeta_{y_2} \otimes_{\mathbb{C}} \mathcal{O}_X(x_1+x_2-x_1^0) \to 0,$$

where $\zeta_{y_2} \otimes_{\mathbb{C}} \mathcal{O}_X(x_1+x_2-x_1^0)$ is the torsion sheaf of dimension one supported on x_2^0, and the projection of V to $\zeta_{y_2} \otimes_{\mathbb{C}} \mathcal{O}_X(x_1+x_2-x_1^0)$ is defined by the natural projection $E_{x_2^0} \to \zeta_{y_2}$. The identity (2.9) gives

$$d(\mathcal{E}_2|_t) \cong d(V) \otimes \zeta_{y_1} \otimes \mathcal{O}_{X\times X}(\Delta)_{(x_2^0,x_1)} \otimes \mathcal{O}_{X\times X}(\Delta)_{(x_2^0,x_2)} \otimes \mathcal{O}_{X\times X}(-\Delta)_{(x_2^0,x_1^0)}. \tag{2.23}$$

Finally, (2.21)–(2.23) together complete the proof of the lemma.

□

Let

$$\theta_2 \in H^0(\mathcal{U}_2, \mathcal{L}_2) \tag{2.24}$$

be the generalized theta function for the family of vector bundles over X defined by $\mathcal{E}_2$. Set

$$L_2 := l_2 \otimes q_{13}^*\delta \otimes q_{24}^*\delta \otimes (q_{12}^*L_Y \otimes q_{34}^*L_Z)^* \otimes q_{14}^*L' \otimes q_{23}^*L' \tag{2.25}$$

to be the line bundle over $Y\times Y\times Z\times Z$, where l_2 as before is the trivial line bundle with fiber $d(E)$ (see Lemma 2.3). Let

$$\vartheta_2 \in H^0(\mathcal{U}_2,\, L_2|_{\mathcal{U}_2}) \tag{2.26}$$

be the section defined by θ_2 using the isomorphism in Lemma 2.3.

Assume that $r=\mathrm{rank}(E)\geqslant 2$. Consequently, the codimension of the subvariety S_2 defined in (2.14) is at least two. (Note that if $r=1$, then both Δ_Y and Δ_Z coincide with the diagonal divisor in $X\times X$.) Therefore, ϑ_2 extends to a section of L_2 over $Y\times Y\times Z\times Z$. This extended section will also be denoted by ϑ_2.

If $r=1$, then $\mathcal{E}_2$ extends naturally to $X\times Y\times Y\times Z\times Z$ as a line bundle. So even in the case $r=1$, the section ϑ_2 is defined over $Y\times Y\times Z\times Z$ (see Ref. 6, Chap. 11, p. 357, Proposition 10.2).

In the next section we will describe ϑ_2 using the section ϑ over $Y\times Z$ constructed in (2.13).

III. SECTIONS OF THE PULLBACK BUNDLE

Assume that $H^0(X,E)=0$. Consequently, $H^1(X,E)=0$, as $\mathrm{degree}(E)=r(g-1)$. Note that the condition $H^0(X,E)=0$ implies that the vector bundle E is semistable. Let

$$\xi := L_2 \otimes l_2^* = q_{13}^*\delta \otimes q_{24}^*\delta \otimes (q_{12}^*L_Y \otimes q_{34}^*L_Z)^* \otimes q_{14}^*L' \otimes q_{23}^*L' \tag{3.1}$$

be the line bundle over $Y\times Y\times Z\times Z$, where L_2 is defined in (2.25).

Theorem 3.1: *Let E be a holomorphic vector bundle with $H^i(X,E)=0$, $i=0,1$, and $H^0(X,\mathrm{End}(E))\cong\mathbb{C}$. Then we have*

$$\dim H^0(Y\times Y\times Z\times Z,\xi)=1,$$

where ξ is the line bundle defined above.

Proof: Let

$$F: Y\times Y\times Z\times Z \to X^4$$

be the natural projection defined by

$$(y_1,y_2,z_1,z_2)\mapsto (f_1(y_1),f_1(y_2),f_2(z_1),f_2(z_2)).$$

The fibers of F are products of projective spaces. Note that for any point $x\in X^4$, we have $H^i(F^{-1}(x),\, \xi|_{F^{-1}(x)})=0$ for each $i\geqslant 1$. Indeed, this follows from the Künneth formula and the fact that ξ is relatively ample for the projection F.

Therefore, we have

$$H^0(Y\times Y\times Z\times Z,\xi)\cong H^0(X^4,F_*\xi). \tag{3.2}$$

Let $\psi_i: X^4\to X$, $1\leqslant i\leqslant 4$, be the projection to the ith factor. For $1\leqslant i<j\leqslant 4$, let $\psi_{ij}=\psi_i\times\psi_j$ be the projection of X^4 to X^2. The divisor $\psi_{ij}^{-1}(\Delta)\subset X^4$ will be denoted by Δ_{ij}.

Since $f_{1*}\zeta\cong E$ and $f_{2*}\eta\cong E^*$, we have

$$F_*\xi \cong \mathcal{W}_E := \psi_1^*(E) \otimes \psi_2^*(E) \otimes \psi_3^*(E^* \otimes K_X) \otimes \psi_4^*(E^* \otimes K_X) \otimes \mathcal{O}_{X^4}(\Delta_{13} + \Delta_{24} + \Delta_{14} + \Delta_{23} - \Delta_{12} - \Delta_{34})$$

over X^4.

Now, $\dim H^0(X^4, \mathcal{W}_E) = 1$ as $\dim H^0(X, \mathrm{End}(E)) = 1$ [see Ref. 10, p. 239, Remark 5.7]. As noted in Ref. 10, Remark 5.7, the proof of Theorem 5.5 in Ref. 10, p. 239 (which is for line bundles) goes through for vector bundles under that assumption that the vector bundle is simple. This completes the proof of the theorem. □

Note that X admits a stable vector bundle E of rank at least two with $H^0(X, \mathrm{End}(E)) \cong \mathbb{C}$ if and only if the genus of X is at least two.

For any vector bundle E with $H^0(X,E) = 0 = H^1(X,E)$, the line

$$d(E) := \wedge^{\mathrm{top}} H^0(X,E)^* \otimes \wedge^{\mathrm{top}} H^1(X,E)$$

is canonically identified with $\mathbb{C}$, as the condition $H^i(X,E) = 0$ gives a nonzero element in $d(E)$. Let

$$\vartheta \in H^0(Y \times Z, p_Y^*\zeta \otimes p_Z^*(\eta^* \otimes f_2^* K_X) \otimes (f_1 \times f_2)^* \mathcal{O}_{X \times X}(\Delta))$$

be the section constructed using this identification of $d(E)$ with $\mathbb{C}$ from the section defined in (2.13) (recall that the section in (2.13) extends to $Y \times Z$).

Note that both the tensor products $q_{13}^*\vartheta \otimes q_{24}^*\vartheta$ and $q_{14}^*\vartheta \otimes q_{23}^*\vartheta$ are sections of

$$q_{13}^*\delta \otimes q_{24}^*\delta \otimes q_{14}^*L' \otimes q_{23}^*L' \cong \xi \otimes q_{12}^*L_Y \otimes q_{34}^*L_Z$$

over $Y \times Y \times Z \times Z$, where ξ is defined in (3.1); the line bundles δ and L' are defined in (2.19) and (2.20), respectively, and the projections q_{ij} are as in (2.14). Hence

$$q_{13}^*\vartheta \otimes q_{24}^*\vartheta - q_{14}^*\vartheta \otimes q_{23}^*\vartheta \in H^0(Y \times Y \times Z \times Z, \xi \otimes q_{12}^*L_Y \otimes q_{34}^*L_Z). \tag{3.3}$$

Since the line bundle $q_{12}^*L_Y \otimes q_{34}^*L_Z$ is defined by the effective divisor $((f_1 \times f_1) \circ q_{12})^{-1}(\Delta) + ((f_2 \times f_2) \circ q_{34})^{-1}(\Delta)$, there is a natural inclusion of $H^0(Y \times Y \times Z \times Z, \xi)$ in $H^0(Y \times Y \times Z \times Z, \xi \otimes q_{12}^*L_Y \otimes q_{34}^*L_Z)$.

Assume that $\dim H^0(X, \mathrm{End}(E)) = 1$. If the section in (3.3) is contained in the image

$$H^0(Y \times Y \times Z \times Z, \xi) \hookrightarrow H^0(Y \times Y \times Z \times Z, \xi \otimes q_{12}^*L_Y \otimes q_{34}^*L_Z)$$

by the above inclusion map, then it is easy to check that the section in (3.3) coincides with the section ϑ_2 [constructed in (2.26)] after using the isomorphism of $d(E)$ with $\mathbb{C}$. Note that from Theorem 3.1 it follows that the section in (3.3) must be a constant scalar multiple of ϑ_2 [if the section in (3.3) comes from a section of ξ].

If $r = 1$, then clearly the section in (3.3) comes from a section of ξ. Therefore, it coincides with ϑ_2 (if $r = 1$). The equality of ϑ_2 with the section in (3.3) is the well known trisecant identity (for $r = 1$); see Ref. 6, Chap. 11, p. 357, Proposition 10.2, and Ref. 10 for the details.

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The Parr formula for the superheating field in a semi-infinite film

Pierre Del Castillo[a)]
Laboratoire Amiénois de Mathématiques Fondamentales et Appliquées, CNRS UMR 6140, Université de Picardie Jules Verne, 33 r. Saint-Leu, 80039 Amiens Cedex 1, France

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Di Bartolo, Dolgert, and Dorsey [Phys. Rev. B **53**, 5650–5660 (1996)] have constructed asymptotic matched solutions at order 2 for the half-space Ginzburg–Landau model in the weak-κ limit. These authors deduced a formal expansion for the superheating field $h^{\mathrm{sh}}(\kappa)$ up to order 4, extending the de Gennes formula [Proceedings of the Eighth Latin American School of Physics, Caracas, 1966] and the two terms in Parr's formula [Z. Phys. B **25**, 359–361 (1976)]. On the other hand, the present author [Eur. J. Appl. Math **13**, 519–547 (2002)] obtained two terms in the lower bound for $h^{\mathrm{sh}}(\kappa)$. In this paper, we prove rigorously that the second term of the expansion of $h^{\mathrm{sh}}(\kappa)$ is of the order of $\mathcal{O}(\kappa^{1/2})$ and we get the Parr formula. We improve the upper bound obtained by Bolley and Helffer [Ann. Inst. Henri Poincaré, Anal. Non Linéaire **14**, 597–613 (1997)] and we get $\kappa(h^{\mathrm{sh}}(\kappa))^2 \leqslant 2^{-3/2} + \frac{15}{32}\kappa + \mathcal{O}(\kappa^{1+\rho})$, $\rho > 0$. The proof is based on new estimates for f', A, and A'. To achieve this, we are guided by the analysis of the properties of the approximate solution constructed previously in [Del Castillo, Math Modell. Numer. Anal. **36**, 971–973 (2002); J. Math. Phys. **44**, 2416–2450 (2003); Dolgert *et al.*, Phys. Rev. B **53**, 5650–5660 (1996)]. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The states of a superconducting material in an exterior magnetic field are described by the Ginzburg–Landau theory which introduces a functional depending in particular on a complex wave function and on the magnetic potential A. These states are characterized as global or local minima of this functional. When the sample is a film and the exterior magnetic field is parallel to the surface, the Ginzburg–Landau model reduces to a one-dimensional problem where the wave function is real (and denoted by f) and where the functional is the following:

$$\varepsilon_d(f,A;h) = \int_{-d/2}^{d/2} \left[\frac{1}{2}(1-f(x)^2)^2 - \frac{1}{2} + \kappa^{-2} f'(x)^2 + f(x)^2 A(x)^2 + (A'(x)-h)^2 \right] \mathrm{d}x,$$

with $(f,A) \in (H^1([-d/2,d/2]))^2$. Here, d is proportional to the thickness of the film, h is proportional to the exterior magnetic field, and κ is the Ginzburg–Landau (GL) parameter characterizing the properties of the material. The value of κ determines the type of superconductor according to the type of phase transition which takes place between the normal phase and the superconducting phase. κ small describes what is known as a type I superconductor and κ large as a type II. More precisely, for a type I superconductor, there is a critical magnetic field h_c such that $h < h_c$, the material is entirely superconducting, and the magnetic field is expelled from the sample apart from a boundary layer of size λ. This is called the Meissner effect. If $h > h_c$, superconductivity is

a)Electronic mail: pierre.delcastillo@u-picardie.fr

destroyed and the material is in the normal state, that is $f \equiv 0$ and $A' \equiv h$. For a type II superconductor, the phase transition is different and there are two critical field h_{c_1} and h_{c_2}. For $h < h_{c_1}$, the exterior magnetic field is expelled from the sample and there is a Meissner effect as for type I superconductors. When h increases above h_{c_1}, superconductivity is not destroyed straight away, since the superconducting and the normal phase coexist under the form of filaments or vortices. As h increases further, the vortices become more numerous until the critical value h_{c_2} is reached at which superconductivity is destroyed. For $h > h_{c_2}$, the material is in the normal state. The way superconductivity is nucleated is highly dependent on d and κ (see, for example, Ref. 25).

In the following, we restrict ourselves to the research of *symmetric solutions*. By symmetric solutions, we mean solutions (f,A) such that f is even and A is odd. Hence, we reduce the study of ε_d to the interval $]-d,0[$ and then to $]0,d[$ by a translation (the edge of the film is then at 0). A reduced GL functional is then defined by

$$\varepsilon_d(f,A;h) = \int_0^d \left[\frac{1}{2} f^4 - f^2 + \kappa^{-2}(f')^2 + f^2 A^2 + (A' - h)^2 \right] \mathrm{d}x, \tag{1}$$

for the pairs (f,A) of $H^1(]0,d[)^2$ such that $A(d)=0$.

When the width d of the film is large (in the sense that κd is large), a slightly different modelization is considered, which was first introduced by Ginzburg and which is usually called the superconducting half-space. To get formally the limiting problem on the interval $[0,+\infty[$, we put $d=+\infty$ in the definition of the GL functional (1) after a renormalization obtained by adding the term $(h^2-\frac{1}{2})d$. We then get

$$\varepsilon_\infty(f,A) = \int_0^{+\infty} \left[\frac{1}{2}(1 - f(x)^2)^2 + \kappa^{-2} f'(x)^2 + f(x)^2 A(x)^2 + A'(x)^2 \right] \mathrm{d}x + 2hA(0), \tag{2}$$

defined for $(f,A) \in E_\infty = \{(f,A); (1-f) \in H^1(]0,+\infty[), A \in H^1(]0,+\infty[)\}$. The corresponding Ginzburg–Landau equations expressing the necessary conditions for minima are then

$$(\mathrm{GL})_\infty \begin{cases} (a) & -\kappa^{-2} f'' - f + f^3 + fA^2 = 0 \quad \text{on } [0,+\infty[, \\ (b) & -A'' + Af^2 = 0 \quad \text{on } [0,+\infty[, \end{cases} \tag{3}$$

with the boundary conditions

$$f'(0) = 0, \quad A'(0) = h. \tag{4}$$

The problem $(\mathrm{GL})_\infty$ is called the half-space model and was studied in Refs. 18 and 19 where numerical solutions are given.

We consider the set $\mathcal{H}_\infty \subset \mathbb{R}^+$ of the h's such that there exist solutions of the (GL) system with $f > 0$. We know that $\mathcal{H}_\infty$ is a bounded interval $[0,h^+)$ (see Ref. 4, Proposition 2.1) and we then introduce the superheating field $h^{\mathrm{sh}}(\kappa)$, defined as the supremum of the interval $\mathcal{H}_\infty$. This critical field is very important for many applications. For instance, measuring the superheating field provides one of the few methods of experimentally determining the Ginzburg–Landau parameter κ in type-I superconductors (see Ref. 10 and also Ref. 1 for other properties and developments).

P. G. de Gennes[12] (see also Ref. 22) has proposed the formula

$$\lim_{\kappa \to 0} \kappa (h^{\mathrm{sh}}(\kappa))^2 = 2^{-3/2}. \tag{5}$$

In Refs. 4 and 6, Bolley and Helffer have rigorously proved (5). To get an upper bound for $A'(0)$, these authors have proved the following estimates, for any pairs (f,A) solutions of $(\mathrm{GL})_\infty$:

$$A'(0)^2 \leqslant \sqrt{2}[(1 - f(0)^2) f(0)^2 \kappa^{-1} - 5A(0) f(0)^{-1}], \tag{6}$$

$$\kappa A'(0)^2 \geqslant \sqrt{2}(1-f(0)^2)f(0)^2. \tag{7}$$

On the other hand, in Ref. 9 (see Proposition 3, p. 361), these authors have proved the following estimate:

Proposition 1.1: There exist κ_0 *and* C *such that, for all* $\kappa \leqslant \kappa_0$ *and any solution* (f,A) *of* $(GL)_\infty$, *we have*

$$A'(0)^2 = h^2 \leqslant \frac{1}{2} + C\frac{f(0)}{\kappa}. \tag{8}$$

From (6), taking the maximum of $(1-f(0)^2)f(0)^2$ on the interval $[0,1]$, and from (8), they have deduced the upperbound

$$\kappa h^2 \leqslant 2^{-3/2} + \mathcal{O}(\kappa^{1/2}), \tag{9}$$

for all $h \in \mathcal{H}_\infty$ and for κ small enough.

Parr[23] has proposed on the basis of some heuristic computations, the more general formula

$$\kappa(h^{\mathrm{sh}}(\kappa))^2 = 2^{-3/2} + \tfrac{15}{32}\kappa + o(\kappa). \tag{10}$$

In Ref. 17, using the method of matched asymptotic expansions,[21–26] Dorsey, Di Bartolo, and Dolgert have obtained a formal expansion in powers of $\kappa^{1/2}$ up to order 4 for the superheating field $h^{\mathrm{sh}}(\kappa)$, recovering in particular formula (10) at a formal level. On the other hand, in Ref. 8, Bolley and Helffer have shown that numerical computations fit very well with the Parr formula.

Constructing subsolutions and supersolutions of $(\mathrm{GL})_\infty$ based on the existence of formal solutions of the half-space Ginzburg–Landau model obtained in Ref. 17, we have proved in Ref. 14 the following theorem:

Theorem 1.2: *There exist* $\kappa_0 > 0$ *and* C *such that, for all* $\kappa \leqslant \kappa_0$, *we have*

$$\kappa(h^{\mathrm{sh}}(\kappa))^2 \geqslant 2^{-3/2} + \tfrac{15}{32}\kappa + C\kappa^2. \tag{11}$$

In this paper, to get a complete and rigorous proof of the Parr formula, we prove the following theorem:

Theorem 1.3: *There exist* κ_0 *and* $\rho > 0$, *such that, for all pairs* (f,A) *solution of* $(GL)_\infty$, *for all* $\kappa \leqslant \kappa_0$, *we have*

$$\kappa A'(0)^2 = \kappa h^2 \leqslant 2^{-3/2} + \tfrac{15}{32}\kappa + \mathcal{O}(\kappa^{1+\rho}). \tag{12}$$

The approach proposed by the physicists Dorsey, Di Bartolo, and Dolgert and the approach exposed here are distinct. The first uses the method of asymptotic matched expansions and leads in particular to a formal proof of the Parr formula. The second one is essentially based on the maximum principle and leads to a rigorous proof of this formula. Nevertheless, we are guided in our analysis by the structure of the formal construction.

The key of Theorem 1.3 is the improvement of estimates for f', A, and A' obtained in Refs. 4 and 5. Notably, we get an estimate for f' on $[0,\kappa^{-\rho}]$, $\rho > 0$ coinciding with the formal estimate given in Ref. 17.

The plan of this paper is the following. In Sec. II, we first recall some estimates for the functions f, A, f' and, A' obtained in Refs. 4 and 6. We get new estimates for A and A'. In Sec. III, we analyze the estimate for $A'(0)=h$ obtained by Bolley and Helffer in Ref. 6. We get the estimate for f'. In Sec. IV, we improve the upper bound for $A'(0)$ given in (6) and get Theorem 1.3. We deduce the Parr formula (10).

II. PROPERTIES OF SOLUTIONS OF $(GL)_\infty$

A. General properties of the Ginzburg–Landau equations

Let us recall some properties of the functions f, A, f', and A' obtained in Refs. 4 and 5.

Proposition 2.1: Let (f,A) be a solution of $(GL)_\infty$.

1. *f is increasing on $\mathbb{R}^+$ and we have*

$$0 < f(x) \leqslant \tanh\left(\frac{\kappa x}{\sqrt{2}} + x_0\right), \quad \tanh(x_0) = f(0). \tag{13}$$

2. *A is strictly increasing on $[0,+\infty[$ and we have*

$$0 \leqslant A'(x) \leqslant h, \quad \forall\, x \in [0,+\infty[. \tag{14}$$

3. *f' satisfies the inequalities*

$$0 \leqslant f'(x) \leqslant \frac{\kappa}{\sqrt{2}}, \quad \forall\, x \in [0,+\infty[. \tag{15}$$

4. *The pair (f,A) satisfies the following energy conservation:*

$$\kappa^{-2} f'(x)^2 + A'(x)^2 = A(x)^2 f(x)^2 + \frac{(1-f(x)^2)^2}{2}, \quad \forall\, x \in [0,+\infty[. \tag{16}$$

5. *The pair (f,A) satisfies the inequalities*

$$0 < -Af \leqslant A', \quad \forall\, x \in [0,+\infty[. \tag{17}$$

Remark 2.2: From Proposition 2.1 [see (13)], we deduce that in a region $[0,\kappa^{-\rho}]$, $\rho>0$, we have for some $c>0$,

$$f(0) \leqslant f(x) \leqslant f(0) + c\kappa^{1-\rho}. \tag{18}$$

B. New estimates for f', A, and A'

In the next sections, we use two useful versions of the maximum principle (cf. Refs. 6 and 3).

Lemma 2.3: Let $d \in \mathbb{R}^+ \cup \{+\infty\}$. Let C be a bounded function on $]0,d[$ such that

$$C(x) \geqslant 0, \quad \forall\, x \in\ ]0,d[,$$

and let $u \in C^2([0,d])$ be a function such that

$$\begin{gathered} -u(x)'' + C(x)u(x) \leqslant 0 \quad \text{on }]0,d[, \\ u'(0) \geqslant 0. \end{gathered} \tag{19}$$

If $d \in \mathbb{R}^+$, we assume that $u(d) \leqslant 0$, and if $d=+\infty$, $u'(x) \to 0$ when $x \to +\infty$.

Then, in these two cases,

$$u(x) \leqslant 0 \quad \text{on }]0,d[.$$

From Proposition 1.1, we deduce that Inequality (12) is true for any pairs (f,A) solutions of $(GL)_\infty$ such that $f(0) \leqslant 1/10C$. In all the following sections, we will restrict ourselves to the pairs (f,A) such that

$$f(0) \geqslant \frac{1}{10C}. \tag{20}$$

Some inequalities on the functions f', A, and A' are not optimal in $[0, \kappa^{-\rho}]$. In this section, we get a better control on A and A'. Let us recall that in Ref. 4, Bolley and Helffer have obtained the following control for A:

$$h \exp(-x) \leqslant -A \leqslant \frac{h}{f(0)} \exp(-f(0)x), \quad \forall x \in \mathbb{R}^+. \tag{21}$$

In Ref. 15 (see also Refs. 13 and 17), we have constructed an asymptotic matched solution $(f^{\mathrm{vd},(n)}, A^{\mathrm{vd},(n)})$ of $(\mathrm{GL})_\infty$. Let us recall that

$$f^{\mathrm{vd},(0)}(x) = \tanh\left(\frac{\kappa x}{\sqrt{2}} + x_0\right), \tag{22}$$

and

$$\kappa^{1/2} A^{\mathrm{vd},(0)}(x) = -2^{1/4}(1 - A_0^2)^{1/2} \exp(-A_0 x), \tag{23}$$

where $A_0 = \tanh(x_0)$, $x_0 \geqslant 0$.

The comparison with the behavior of the formal solution suggests that the lower bound for $-A$ is not optimal in the interval $[0, \kappa^{-\rho}]$. We get a better lower bound for $-A$ in the following proposition:

Proposition 2.4: Let $\rho \in]0, \frac{1}{2}[$. *There exist* $\kappa_0 > 0$ *and* $C > 0$ *such that, for all* $\kappa \leqslant \kappa_0$, *for all pairs* (f, A) *solutions of* $(\mathrm{GL})_\infty$ *satisfying (20), the function A satisfies the inequality*

$$\forall x \in [0, \kappa^{-\rho}], \quad -A \geqslant \frac{h}{f(0)}(1 - C\kappa^{1-2\rho}) \exp -(f(0)x). \tag{24}$$

Proof: We set

$$v_2(x) := \tanh\left(\frac{\kappa x}{\sqrt{2}} + x_0\right), \quad \tanh(x_0) = f(0). \tag{25}$$

From (13), we get

$$f \leqslant v_2. \tag{26}$$

Let us consider the unique solution in $H^2(]0, +\infty[)$ of the problem

$$\begin{aligned} -W'' + v_2^2 W &= 0, \\ W'(0) &= h. \end{aligned} \tag{27}$$

From (27), and applying Lemma 2.3 with $d = +\infty$, $C = v_2^2$, and $u = W$, we get $W \leqslant 0$ on $\mathbb{R}^+$. From $(3)_b$, (26) and (27), we get $-(A-W)'' + f^2(A-W) \leqslant 0$. Applying again Lemma 2.3 with $d = +\infty$, $C = f^2$, and $u = A - W$, we get

$$A \leqslant W. \tag{28}$$

We set

$$\phi(x) := \int_0^x (v_2 + c_1 \kappa) \mathrm{d}t, \tag{29}$$

where c_1 is a strictly positive parameter, which will be determined later. We consider

$$z(x) = z(0)\exp(-\phi(x)), \tag{30}$$

where $z(0)$ is determined by the condition $z'(0)=h$. We get $z'(0)=-(v_2(0)+c_1\kappa)z(0)=h$. Hence, from (25), it derives that

$$z(0) = -\frac{h}{f(0)+c_1\kappa}. \tag{31}$$

We have

$$-(W-z)''+v_2^2(W-z) = z(0)\exp(-\phi(x))\left(-\frac{\kappa}{\sqrt{2}}\frac{1}{\cosh^2((\kappa x/\sqrt{2})+x_0)}+2v_2c_1\kappa+c_1^2\kappa^2\right). \tag{32}$$

From the definition of the function v_2, we get

$$-\frac{1}{\sqrt{2}}\cosh^{-2}\left(\frac{\kappa x}{\sqrt{2}}+x_0\right)+2v_2c_1+c_1^2\kappa \geqslant 2c_1\tanh(x_0)-\frac{1}{\sqrt{2}}\cosh^{-2}(x_0). \tag{33}$$

We choose c_1 such that

$$c_1 > \frac{1}{2\sqrt{2}}(\sinh(x_0)\cosh(x_0))^{-1}. \tag{34}$$

From (31), as $z(0)<0$ and according to (32)–(34), we get $-(W-z)''+v_2^2(W-z)<0$. Applying Lemma 2.3 on $[0,+\infty[$ with $C=v_2^2$ and $u=W-z$, we deduce that $W-u\leqslant 0$. From (30) and (31), it results that

$$-W \geqslant -z = \frac{h}{f(0)+c_1\kappa}\exp(-\phi(x)). \tag{35}$$

From (29), we get

$$\phi(x) = \phi'(0)x + x^2\int_0^1 \phi''(\theta x)\mathrm{d}\theta.$$

According to (25) and (29) it derives that there exists $\rho>0$ such that

$$\forall x \in [0,\kappa^{-\rho}], \quad \phi(x) \leqslant (f(0)+c_1\kappa)x + \frac{\kappa^{1-2\rho}}{\sqrt{2}}. \tag{36}$$

Finally, from (28), (35), and (36), we get the inequality

$$-A \geqslant -W \geqslant \frac{h}{f(0)+c_1\kappa}\exp\left(-f(0)x-c_1\kappa x-\frac{\kappa^{1-2\rho}}{\sqrt{2}}\right).$$

From (20), we deduce that there exist $C>0$ and κ_0, such that, for all $\kappa \in]0,\kappa_0]$, for all $x \in [0,\kappa^{-\rho}]$, we have the inequality

$$-A \geqslant \frac{h}{f(0)}(1-C\kappa^{1-2\rho})\exp(-f(0)x).$$

The proof of Proposition 2.4 follows.

We also have to get a lower bound and an upper bound for A'. In Ref. 4, Bolley and Helffer get in Proposition 2.4 the following estimate for A':

$$h\exp(-x) \leqslant A'(x) \leqslant \frac{h}{f(0)}\exp(-f(0)x), \quad \forall\, x \in \mathbb{R}^+. \tag{37}$$

Equalities (22) and (23) suggest that these estimates are not optimal in $[0,\kappa^{-\rho}]$. We get a better control for A' in the following proposition:

Proposition 2.5: Let $\rho \in \left[0,\frac{1}{4}\right]$. *There exists* $\kappa_0 > 0$ *such that, for all* $\kappa \leqslant \kappa_0$ *and for all* (f,A) *solutions of* $(GL)_\infty$ *satisfying (20), we have the following estimate for* A':

$$A' = (h + \mathcal{O}(\kappa^{1/2-2\rho}))\exp(-f(0)x), \quad \forall\, x \in [0,\kappa^{-\rho}]. \tag{38}$$

Proof: From $(3)_b$, the function A' satisfies

$$-(A')'' + f^2A' = -2f'fA, \quad A''(0) = A(0)f(0)^2. \tag{39}$$

From (13), (15), and (21), we get the inequality

$$-2f'fA \leqslant \frac{2\kappa h}{\sqrt{2}f(0)}\exp(-f(0)x), \quad \forall\, x \in \mathbb{R}^+. \tag{40}$$

We can compare A' with the unique solution in $H^2(\mathbb{R}^+)$ of

$$\begin{aligned} -y'' + f(0)^2y &= \frac{\sqrt{2}\kappa h}{f(0)}\exp(-f(0)x), \\ y'(0) &= A(0)f(0)^2, \end{aligned} \tag{41}$$

given by

$$y(x) = \left(-A(0)f(0) + \frac{\sqrt{2}\kappa h(1+f(0)x)}{2f(0)^3}\right)\exp(-f(0)x). \tag{42}$$

According to (39)–(41), we get $-(A'-y)''+f^2A'-f(0)^2y \leqslant 0$. Applying the principle maximum (see Lemma 2.3) with $d=+\infty$, $C(x)=f(0)^2$, and $u=A'-y$, we get $A' \leqslant y$ on $\mathbb{R}^+$. From (17) at the point $x=0$, it results that $-A(0)f(0) \leqslant h$. From (9), we have $h=\mathcal{O}(\kappa^{-1/2})$. As $1/10C \leqslant f(0) \leqslant 1$, for $x \in [0,\kappa^{-\rho}]$, we deduce the estimate

$$\frac{\sqrt{2}\kappa h(1+f(0)x)}{2f(0)^3} = \mathcal{O}(\kappa^{1/2-\rho}).$$

As $A' \leqslant y$, and from (42), it results that

$$A' \leqslant (h + \mathcal{O}(\kappa^{1/2-\rho}))\exp(-f(0)x). \tag{43}$$

To get a lower bound for A', we proceed as in Proposition 2.4. We compare A' solution of (39) with the unique solution in $H^2(]0,+\infty[)$ of

$$\begin{aligned} -W'' + v_2^2W &= 0, \\ W'(0) &= A(0)f(0)^2, \end{aligned} \tag{44}$$

where v_2 is defined in (25). From Lemma 2.3 with $u=-W$ and $C=v_2^2$, let us remark that we have $W \geqslant 0$ on $\mathbb{R}^+$. Applying again this lemma with $d=+\infty$, $C=f^2$, and $u=W-A'$, we deduce $W \leqslant A'$. Now, we compare W with the function z defined in (30) and satisfying $z'(0)=A(0)f(0)^2$. The function $z-W$ satisfies (32) [replacing $z(0)$ with $-z(0)$] and taking c_1 as in (34), we get $-(z-W)''+v_2^2(z-W) < 0$. Applying Lemma 2.3 with $d=+\infty$, $u=z-W$, and $C=v_2^2$, we get

$$z(x) = -\frac{A(0)f(0)^2}{f(0)+c_1\kappa}\exp(-\phi(x)) \leqslant W(x).$$

Following Proposition 2.4, for $x \in [0, \kappa^{-\rho}]$, we get

$$-\frac{A(0)f(0)^2}{f(0)+c_1\kappa}\exp\left(-f(0)x - c_1\kappa - \frac{\kappa^{1-2\rho}}{\sqrt{2}}\right) \leqslant z(x).$$

It derives that

$$-A(0)f(0)(1-C\kappa^{1-2\rho})\exp(-f(0)x) \leqslant A'. \tag{45}$$

From (24) at the point $x=0$, we get

$$h(1-C\kappa^{1-2\rho}) \leqslant -A(0)f(0).$$

From (45), it results that

$$h(1-C\kappa^{1-2\rho})\exp(-f(0)x) \leqslant A'. \tag{46}$$

According to (43) and (46), the proof of Proposition 2.5 follows.

III. ESTIMATES FOR $A'(0)$

A. Preliminaries

First, we show that Inequality (12) is true for some pairs (f,A) such that

$$f(0) \in \left[0, \frac{1}{\sqrt{2}} - \alpha\kappa^{\gamma}\right] \cup \left[\frac{1}{\sqrt{2}} + \alpha\kappa^{\gamma}, 1\right], (\alpha,\gamma) \in (\mathbb{R}^+)^2.$$

Lemma 3.1: There exist $\alpha>0$ and κ_0, such that, for all $\kappa \leqslant \kappa_0$, for all pairs (f,A) solutions of $(GL)_\infty$ such that

$$f(0) \in \left[0, \frac{1}{\sqrt{2}} - \alpha\kappa^{1/4}\right] \cup \left[\frac{1}{\sqrt{2}} + \alpha\kappa^{1/4}, 1\right],$$

we have

$$\kappa(A'(0))^2 \leqslant 2^{-3/2}. \tag{47}$$

Proof: We set

$$\phi_0(y) = \sqrt{2}y^2(1-y^2). \tag{48}$$

This function achieves its unique maximum on $[0,1]$ at the point $y=1/\sqrt{2}$, and $\phi_0(1/\sqrt{2})=2^{-3/2}$. We have seen that Inequality (47) is satisfied for $f(0) \leqslant 1/10C$. If $f(0) \geqslant 1/10C$, then from (38), we have

$$\frac{A'(0)}{f(0)} = \mathcal{O}(\kappa^{-1/2}).$$

From (6), with the choice $f(0)=1/\sqrt{2}+\alpha\kappa^{1/4}$, we get for some $\widetilde{C}$,

$$\kappa(A'(0))^2 \leqslant 2^{-3/2} + \frac{1}{2}\phi_0''\left(\frac{1}{\sqrt{2}}\right)\alpha^2\kappa^{1/2} + \widetilde{C}\kappa^{1/2} + \mathcal{O}_\alpha(\kappa^{3/4}).$$

We choose first α such that $\frac{1}{2}\phi_0''(1/\sqrt{2})\alpha^2 + \widetilde{C} \leqslant -1$ and then $\kappa \leqslant \kappa_0$ for κ_0 small enough. The proof of Lemma 3.1 follows.

From now on, α is fixed according to Lemma 3.1 and we assume that

$$f(0) \in \left[\frac{1}{\sqrt{2}} - \alpha\kappa^{1/4}, \frac{1}{\sqrt{2}} + \alpha\kappa^{1/4} \right], \quad \alpha > 0. \tag{49}$$

From (7), for all pairs (f,A) solution of $(\mathrm{GL})_\infty$ satisfying (49), we have

$$\kappa h^2 \geqslant 2^{-3/2} + \mathcal{O}(\kappa^{1/4}). \tag{50}$$

From (9) and (50), we deduce that

$$\kappa h^2 = 2^{-3/2} + \mathcal{O}(\kappa^{1/4}), \tag{51}$$

for all pairs (f,A) solution of $(\mathrm{GL})_\infty$ satisfying (49). In order to get Inequality (12), let us analyze the proof by Bolley and Helffer of the De Gennes formula (Ref. 6, p. 604), and improve some of their estimates. For doing this, we are guided by the analysis of the properties of the approximate solution constructed in Ref. 15. To get an upper bound on $A'(0)$, Bolley and Helffer start by the identity

$$h^2 = -2\int_0^{+\infty} A'(t)A''(t)\mathrm{d}t.$$

Then, from $(3)_{(b)}$, they get

$$h^2 = 2\int_0^{+\infty} A'(t)(-A(t)f(t)^2)\mathrm{d}t. \tag{52}$$

Then, using Inequality (17), they obtain

$$h^2 \leqslant 2\int_0^{+\infty} f(t)A'(t)^2\mathrm{d}t. \tag{53}$$

We suspect that something has been lost when writing

$$-Af \leqslant A'.$$

Then, using $(3)_{(a)}$ and the energy conservation (16), they get

$$h^2 \leqslant 2\int_0^{+\infty} f(t)A'(t)^2\mathrm{d}t = \int_0^{+\infty} f(x)(1-f(x)^4)\mathrm{d}x - 6\kappa^{-2}\int_0^{+\infty} f(x)f'(x)^2\mathrm{d}x. \tag{54}$$

In order to get the control of the right-hand side of Inequality (54), in particular the two terms f' and $1-f^2$, they use the conservation law (16). If we rewrite the energy conservation in the form

$$(\kappa^{-1}f'(x) + A'(x))^2 = A(x)^2f(x)^2 + 2\kappa^{-1}f'(x)A'(x) + \tfrac{1}{2}(1-f(x)^2)^2,$$

we observe that these authors have neglected the positive term $A(x)^2f(x)^2+2\kappa^{-1}f'(x)A'(x)$ for getting the inequality

$$\kappa^{-1}f'(x) + A'(x) \geqslant \frac{1}{\sqrt{2}}(1-f(x)^2).$$

To improve Inequality (54), in the next sections, we get an upper bound and a lower bound for the difference $(A')^2-A^2f^2$. Moreover, we improve the control on f' given in (15). This is the object of the following subsection.

B. Estimate for f'

In order to get an estimate on f' on the interval $[0,\kappa^{-\rho}]$, we establish the following lemma:

Lemma 3.2: Let $\rho\in\left[0,\frac{1}{4}\right]$. *There exists* κ_0 *such that, for all* $\kappa\leqslant\kappa_0$, *for all pairs* (f,A) *solutions of* $(GL)_\infty$ *satisfying (49), we have the following estimate:*

$$A'f'=\frac{\kappa^2h^3}{2f(0)^2}\exp(-f(0)x)(1-\exp(-2f(0)x)+\mathcal{O}(\kappa^\rho)),\quad\forall\, x\in[0,\kappa^{-\rho}]. \tag{55}$$

Proof: Step 1: Estimate for $A'f'$ *at the point* $x=\kappa^{-\rho}$. Let $\rho\in\left[0,\frac{1}{4}\right]$. We set $Y=A'f'$. As $f'\geqslant 0$ and $A'\geqslant 0$, we have $Y\geqslant 0$. In order to use Lemma 2.3 with $d=\kappa^{-\rho}$, we estimate $A'f'$ at the point $x=\kappa^{-\rho}$. From (13) and (16) at the point $x=\kappa^{-\rho}$ and (17), we deduce that

$$f'(\kappa^{-\rho})\leqslant\frac{\kappa}{\sqrt{2}}(1-f(\kappa^{-\rho})^2)\leqslant\frac{\kappa}{\sqrt{2}}(1-\tanh(x_0)^2).$$

According to (38), and as $\tanh(x_0)=f(0)$ with

$$f(0)\in\left[\frac{1}{\sqrt{2}}-\alpha\kappa^{1/4},\frac{1}{\sqrt{2}}+\alpha\kappa^{1/4}\right],$$

we deduce that there exists $\hat{C}$ such that

$$(A'f')(\kappa^{-\rho})\leqslant\left(\frac{\kappa h}{2\sqrt{2}}+\hat{C}\kappa^{3/4}\right)\exp(-f(0)\kappa^{-\rho}). \tag{56}$$

To get a lower bound for $(A'f')(\kappa^{-\rho})$, let us remark that, from (21) and (37) at the point $x=\kappa^{-\rho}$, for κ small, we have $(A^2f^2-A'^2)(\kappa^{-\rho})=\mathcal{O}(\kappa^{-1})\exp(-f(0)\kappa^{-\rho})=\mathcal{O}(\kappa^2)$. From (16) at the point $x=\kappa^{-\rho}$, we deduce that

$$\kappa^{-2}f'(\kappa^{-\rho})^2=\frac{(1-f(\kappa^{-\rho})^2)^2}{2}+\mathcal{O}(\kappa^2)\geqslant\frac{1}{2}\left(1-\tanh^2\left(\frac{\kappa^{1-\rho}}{\sqrt{2}}+x_0\right)\right)^2+\mathcal{O}(\kappa^2).$$

Hence, from (49), we get

$$f'(\kappa^{-\rho})\geqslant\frac{\kappa}{2\sqrt{2}}(1+\mathcal{O}(\kappa^{3/4})).$$

According to (38), it results that there exists $\tilde{C}$ such that

$$\left(\frac{\kappa h}{2\sqrt{2}}+\tilde{C}\kappa^{3/4}\right)\exp(-f(0)\kappa^{-\rho})\leqslant(A'f')(\kappa^{-\rho}). \tag{57}$$

Step 2: Upper bound for Y. Using the Ginzburg–Landau equations (3), we get

$$Y'=Af^2f'+\kappa^2A'(-f+f^3+A^2f).$$

We observe that $Y'(0)=hf''(0)$. Differentiating once more and using (3), we deduce that the function Y is the unique solution in $H^2(\mathbb{R}^+)$ of the problem

$$Y''-f^2Y=2ff'^2A+2\kappa^2Af^2(-f+f^3+A^2f)+\kappa^2A'(-f'+3f'f^2)+2\kappa^2A'^2Af+2\kappa^2A'A^2f',$$

$$Y'(0)=hf''(0).$$

Hence, we get

$$-Y''+GY=-2ff'^2A-2\kappa^2Af^2(f^3-f)-2\kappa^2A^3f^3-2\kappa^2A'^2Af,$$

$$Y'(0) = hf''(0), \tag{58}$$

where

$$G := f^2 + \kappa^2(-1 + 3f^2 + A^2). \tag{59}$$

According to (18) and (21), for $x \in [0, \kappa^{-\rho}]$, we get

$$f(0)^2 \leqslant G(x) \leqslant f(0)^2 + \mathcal{O}(\kappa^{1-\rho}). \tag{60}$$

In order to get an upper bound for Y, we look for an upper bound of the right-hand side of (58). First, let us analyze the main term of (58) which is given by $-2\kappa^2 Af(A^2f^2+A'^2)$. According to (18) and (21), it derives that there exists C_2 such that, for $x \in [0, \kappa^{-\rho}]$, we get

$$-2\kappa^2 Af(A^2f^2 + A'^2) \leqslant (4\kappa^2h^3 + C_2\kappa^{1-\rho})\exp(-3f(0)x).$$

As $0 \leqslant f \leqslant 1$ and $A < 0$ on $\mathbb{R}^+$, we get

$$-2ff'^2A - 2\kappa^2Af^2(f^3 - f) \leqslant -2ff'^2A.$$

As $h = \mathcal{O}(\kappa^{-1/2})$ [see (9)], and from (15), (21), (38), and (49), there exists C_1 such that, for all $x \in [0, \kappa^{-\rho}]$, we get

$$-2ff'^2A \leqslant C_1\kappa^{3/2}\exp(-f(0)x).$$

Then, to get an upper bound for Y, we compare this function with the solution in $H^2([0, \kappa^{-\rho}])$ of

$$-y_1'' + f(0)^2y_1 = (4\kappa^2h^3 + C_2\kappa^{1-\rho})\exp(-3f(0)x) + C_1\kappa^{3/2}\exp(-f(0)x), \tag{61}$$

satisfying

$$y_1'(0) = Y'(0), \quad y_1(\kappa^{-\rho}) = \left(\frac{\kappa h}{2\sqrt{2}} + \hat{C}\kappa^{3/4}\right)\exp(-f(0)\kappa^{-\rho}). \tag{62}$$

From (60) and as $Y \geqslant 0$, we have

$$-(Y - y_1)'' + f(0)^2(Y - y_1) \leqslant -(Y - y_1)'' + GY - f(0)^2y_1 \leqslant 0.$$

From (56) and (62), we have $(Y-y_1)'(0) = 0$ and $(Y-y_1)(\kappa^{-\rho}) \leqslant 0$. Applying Lemma 2.3 with $d = \kappa^{-\rho}$, $C = f(0)^2$, and $u = Y - y_1$, for $x \in [0, \kappa^{-\rho}]$, we get $Y \leqslant y_1$ on $[0, \kappa^{-\rho}]$. The solution of (61) is given by

$$\begin{aligned} y_1(x) = {} & \widetilde{C}_1(\kappa)\exp(-f(0)x) + \widetilde{C}_2(\kappa)\exp(f(0)x) - \frac{1}{8f(0)^2}\exp(-3f(0)x)(4\kappa^2h^3 + C_2\kappa^{1-\rho}) \\ & + \exp(-f(0)x)\left(\frac{C_1}{4f(0)^2}\kappa^{3/2}(1 + 2f(0)x)\right). \end{aligned} \tag{63}$$

For $x \in [0, \kappa^{-\rho}]$, $\left(\rho \leqslant \frac{1}{4}\right)$, we have $\kappa^{3/2}(1+2f(0)x) = \mathcal{O}(\kappa)$. Hence, from (62) and (63), we get

$$y_1(\kappa^{-\rho}) = \widetilde{C}_2(\kappa)\exp(f(0)\kappa^{-\rho}) + (\widetilde{C}_1(\kappa) + \mathcal{O}(\kappa))\exp(-f(0)\kappa^{-\rho}) = \left(\frac{\kappa h}{2\sqrt{2}} + \hat{C}\kappa^{3/4}\right)\exp(-f(0)\kappa^{-\rho}). \tag{64}$$

As $\kappa h = \mathcal{O}(\kappa^{1/2})$, from (64), it results that

$$\widetilde{C}_2(\kappa) = (-\widetilde{C}_1(\kappa) + \mathcal{O}(\kappa^{1/2}))\exp(-2f(0)\kappa^{-\rho}). \tag{65}$$

From (63), we have

$$y_1'(0) = f(0)\widetilde{C}_2(\kappa) - f(0)\widetilde{C}_1(\kappa) + \frac{1}{8f(0)}(12\kappa^2h^3 - 2C_1\kappa^{3/2} + 3C_2\kappa^{1-\rho}).$$

From (65) and the condition $y_1'(0)=Y'(0)=hf''(0)$, we get for κ small

$$\widetilde{C}_1(\kappa) = -\frac{hf''(0)}{f(0)} + \frac{3}{2}\frac{\kappa^2h^3}{2(0)^2} + \mathcal{O}(\kappa^{1-\rho}).$$

From (3), (21), and (24), we get

$$f''(0) = \frac{\kappa^2h^2}{f(0)} + \mathcal{O}(\kappa^2). \tag{66}$$

Hence, we get

$$\widetilde{C}_1(\kappa) = \frac{\kappa^2h^3}{2f(0)^2} + \mathcal{O}(\kappa^{1-\rho}). \tag{67}$$

According to (63) and (65), for $x \in [0, \kappa^{-\rho}]$, we get

$$y_1(x) = -\frac{\kappa^2h^3}{2f(0)^2}\exp(-3f(0)x) + \exp(-f(0)x)[\widetilde{C}_1(\kappa) + (-\widetilde{C}_1(\kappa) + \mathcal{O}(\kappa^{1/2}))\exp(2f(0)(x-\kappa^{-\rho}))]. \tag{68}$$

From (67), we have $\widetilde{C}_1(\kappa)=\mathcal{O}(\kappa^{1/2})$. Let us remark that, for $x \in [0, \kappa^{-\rho}/2]$, for all $n \in \mathbb{N}$, we have

$$(-\widetilde{C}_1(\kappa) + \mathcal{O}(\kappa^{1/2}))\exp(2f(0)(x-\kappa^{-\rho})) = \mathcal{O}(\kappa^n).$$

From (67) and (68), for $x \in [0, \kappa^{-\rho}/2]$, it results that

$$Y \leqslant y_1(x) = -\frac{\kappa^2h^3}{2f(0)^2}\exp(-3f(0)x) + \left(\frac{\kappa^2h^3}{2f(0)^2} + \mathcal{O}(\kappa^{1-\rho})\right)\exp(-f(0)x). \tag{69}$$

If we make κ_0 smaller, we get (55) on $[0, \kappa^{-\rho}]$.

Step 3: Lower bound for Y. According to (13), (15), and (21), and as $A' \geqslant 0$ and $A < 0$, we deduce that there exists C_3 such that, for $x \in [0, \kappa^{-\rho}]$, we get

$$-2ff'^2A + 2\kappa^2Af^2(f-f^3) \geqslant 2\kappa^2Af^2(f-f^3) \geqslant C_3\kappa^{3/2}\exp(-f(0)x).$$

On the other hand, from (24) and (38), it results that there exists C_4 such that

$$-2\kappa^2Af(A^2f^2 + A'^2) \geqslant (4\kappa^2h^3 + C_4\kappa^{1-\rho})\exp(-3f(0)x), \quad \forall\, x \in [0, \kappa^{-\rho}].$$

From Remark 2.2, we can compare Y with the solution in $H^2([0, \kappa^{-\rho}])$ of

$$-y_2'' + (f(0)^2 + C_5\kappa^{1-\rho})y_2 = (4\kappa^2h^3 + C_4\kappa^{1-\rho})\exp(-3f(0)x) - C_3\kappa^{3/2}\exp(-f(0)x) \tag{70}$$

satisfying the conditions

$$y_2'(0) = Y'(0), \quad y_2(\kappa^{-\rho}) = \left(\frac{\kappa h}{2\sqrt{2}} + \widetilde{C}\kappa^{3/4}\right)\exp(-f(0)\kappa^{-\rho}). \tag{71}$$

According to (57), (70), and (71), Lemma 2.3 with $d=\kappa^{-\rho}$, $C(x)=f(0)^2+C_5\kappa^{1-\rho}$, and $u=y_2-Y$, we get $y_2 \leqslant Y$ on $[0, \kappa^{-\rho}]$. We set $\bar{C} := \sqrt{f(0)^2+C_5\kappa^{1-\rho}}$. The solution of (70) is given by

$$y_2(x) = \hat{C}_1(\kappa)\exp(-\bar{C}x) + \hat{C}_2(\kappa)\exp(\bar{C}x) + F(x)\exp(-f(0)x), \tag{72}$$

where

$$F(x) = -\frac{4\kappa^2 h^3 \exp(-2f(0)x) + 8\frac{C_3}{C_5}\kappa^{1/2+\rho} f(0)^2 - C_3\kappa^{3/2} + C_4\kappa^{1-\rho}\exp(-2f(0)x)}{8f(0)^2 - C_5\kappa^{1-\rho}} \exp(-f(0)x).$$

From (51), we have $\kappa^2 h^3 = \mathcal{O}(\kappa^{1/2})$, hence

$$F(\kappa^{-\rho}) = \mathcal{O}(\kappa^{1/2+\rho}).$$

From (70) and (72) at the point $x = \kappa^{-\rho}$, it results that

$$\hat{C}_2(\kappa) = -\hat{C}_1(\kappa)\exp(-2\bar{C}\kappa^{-\rho}) + \mathcal{O}(\kappa^{1/2})\exp(-(\bar{C} + f(0))\kappa^{-\rho}). \tag{73}$$

From (72), we get

$$y_2'(0) = -\frac{8\frac{C_3}{C_5}\kappa^{1/2+\rho} f(0)^3 + 12\kappa^2 h^3 f(0) + 3\kappa^{1-\rho} C_4 f(0) - f(0) C_3 \kappa^{3/2}}{(-8f(0)^2 + C_5\kappa^{1-\rho})} + \bar{C}(\hat{C}_2(\kappa) - \hat{C}_1(\kappa)).$$

The condition $y_2'(0) = hf''(0)$, (66) and (73) lead to

$$-\hat{C}_1(\kappa)\bar{C} + \frac{3\kappa^2 h^3}{2f(0)} + \mathcal{O}(\kappa^{1/2+\rho}) = hf''(0),$$

hence, as $\bar{C} = \sqrt{f(0)^2 + C_5\kappa^{1-\rho}}$,

$$\hat{C}_1(\kappa) = -\frac{hf''(0)}{f(0)} + \frac{3\kappa^2 h^3}{2f(0)^2} + \mathcal{O}(\kappa^{1/2+\rho}).$$

Following step 1, we restrict ourselves to $[0, \kappa^{-\rho}/2]$ and from (66), we get

$$Y(x) \geqslant \frac{\kappa^2 h^3}{2f(0)^2}\exp(-f(0)x)(1 - \exp(-2f(0)x) + \mathcal{O}(\kappa^{\rho})). \tag{74}$$

From (69) and (74), we deduce that there exists κ_0 such that, for all $\kappa \leqslant \kappa_0$, for all pairs (f, A) satisfying (49), Estimate (55) is true on $[0, \kappa^{-\rho}]$. The proof of Lemma 3.2 follows.

From Lemma 3.2, we deduce an estimate for f' in the following proposition:

Proposition 3.3: Let $\rho \in \left[0, \frac{1}{8}\right]$. *There exists* κ_0 *such that, for all* $\kappa \leqslant \kappa_0$, *for all pairs* (f, A) *solutions of* $(GL)_\infty$ *satisfying (49), we have the estimate*

$$f'(x) = \kappa^2 h^2 (1 - \exp(-\sqrt{2}x) + \mathcal{O}(\kappa^{\rho})), \quad \forall\, x \in [0, \kappa^{-\rho}]. \tag{75}$$

Proof: According to Proposition 2.5 and Lemma 3.2, we get

$$f'(x) = \frac{\kappa^2 h^3}{2f(0)^2}(1 - \exp(-2f(0)x) + \mathcal{O}(\kappa^{\rho})) \cdot \left(\frac{1}{h} + \mathcal{O}(\kappa^{3/2-2\rho})\right).$$

For

$$f(0) = \frac{1}{\sqrt{2}} + \mathcal{O}(\kappa^{1/4}),$$

and for $x \in [0, \kappa^{-\rho}]$, we have $\exp(-2f(0)x) = \exp(-\sqrt{2}x) + \mathcal{O}(\kappa^{1/4-\rho})$. As $\rho \in \left[0, \frac{1}{8}\right]$, Estimate (75) follows and this achieves the proof of Proposition 3.3.

Remark 3.4: For $n = 1$, *at the superheating field, we have shown in Ref. 15 (see also Ref. 17) that*

$$f^{\mathrm{vd},(1)}(x) = \tanh\left(\frac{\kappa x}{\sqrt{2}} + x_0\right) + \frac{\kappa}{4}\exp(-\sqrt{2}x), \tag{76}$$

where

$$\tanh(x_0) = \frac{1}{\sqrt{2}}.$$

From (76), it results that, for $x \in [0, \kappa^{-\rho}]$, *we have*

$$(f^{\mathrm{vd},(1)})'(x) = \frac{\sqrt{2}}{4}\kappa(1 - \exp(-\sqrt{2}x)) + \mathcal{O}(\kappa^{2-\rho}). \tag{77}$$

According to (7) and (8) with $f(0) = 1/\sqrt{2}$, *the main term of Estimate (75) is the one of Estimate (77). Therefore, we suspect that Estimate (75) is optimal.*

C. Estimate for $A' + Af$

To get an estimate for $A' + Af$, we use Lemma 2.3 and estimates for A', A, f', and f obtained in Propositions 2.4 and 2.5.

Lemma 3.5: Let $\rho \in \left[0, \frac{1}{8}\right]$. *There exists* κ_0 *such that, for all* $\kappa \leqslant \kappa_0$, *for all pairs* (f, A) *solutions of* $(GL)_\infty$ *satisfying (49), we have the following estimate:*

$$A' + Af = \frac{1}{2}\exp\left(-\frac{1}{\sqrt{2}}x\right)\left(-\kappa^2 h^3 \exp(-\sqrt{2}x) - \frac{1}{8h} + 3\kappa^2 h^3 + \mathcal{O}(\kappa^{1/2+\rho})\right), \quad \forall\, x \in [0, \kappa^{-\rho}]. \tag{78}$$

Proof: Step 1: Upper bound for $A' + Af$. We introduce the function $Z := A' + Af$. From (17), this function is positive. At the point $x = \kappa^{-\rho}$, from (21), (24), and (38), we deduce that there exist $\hat{C}$ and $\widetilde{C}$ such that

$$\hat{C}\kappa^{1/2-2\rho}\exp(-f(0)\kappa^{-\rho}) \leqslant Z(\kappa^{-\rho}) = (A' + Af)(\kappa^{-\rho}) \leqslant \widetilde{C}\kappa^{1/2-2\rho}\exp(-f(0)\kappa^{-\rho}). \tag{79}$$

From $(3)_{(b)}$, we have

$$Z' = Af^2 + A'f + Af'.$$

Differentiating more, and using the GL equations, we get

$$Z'' = A'f^2 + 2Af'f + Af^3 + 2A'f' + \kappa^2 A(-f + f^3 + A^2 f).$$

It results that the function Z satisfies

$$-Z'' + (f^2 + 2f')Z = -\kappa^2 A(-f + f^3 + A^2 f). \tag{80}$$

Let us estimate $Z'(0)$. As $f'(0) = 0$ and from (16) at the point $x = 0$, we get

$$Z'(0) = f(0)(h + A(0)f(0)) = \frac{f(0)(1 - f(0)^2)^2}{2(h - A(0)f(0))}.$$

From (17) and (24) at the point $x = 0$, we get $h(2 + \mathcal{O}(\kappa^{3/2-2\rho})) \leqslant h - A(0)f(0) \leqslant 2h$. It results that

$$\frac{f(0)(1 - f(0)^2)^2}{4h} \leqslant Z'(0) \leqslant \frac{f(0)(1 - f(0)^2)^2}{4h(1 + \mathcal{O}(\kappa^{3/2-2\rho}))}.$$

Hence, as

$$f(0) = \frac{1}{\sqrt{2}} + \mathcal{O}(\kappa^{1/4}),$$

we get

$$Z'(0) = \frac{1}{16\sqrt{2}h}(1 + \mathcal{O}(\kappa^{1/4})). \tag{81}$$

Now, we can estimate the term $-\kappa^2 A(-f+f^3+A^2 f)$. First, for $x \in \mathbb{R}^+$, as $A<0$ and $0 \leqslant f \leqslant 1$, we have $-\kappa^2 A(-f+f^3)<0$. According to (18) and (21) and using

$$f(0) = \frac{1}{\sqrt{2}} + \mathcal{O}(\kappa^{1/4}),$$

we deduce that there exists C_6 such that, for $x \in [0, \kappa^{-\rho}]$, we get the estimate

$$-\kappa^2 A^3 f \leqslant (2\kappa^2 h^3 + C_6 \kappa^{3/4}) \exp(-3f(0)x).$$

To get an upper bound for Z, as $f^2+2f' \geqslant f(0)^2$, we compare this function with the solution in $H^2([0, \kappa^{-\rho}])$ of

$$-V'' + f(0)^2 V = (2\kappa^2 h^3 + C_6 \kappa^{3/4}) \exp(-3f(0)x), \tag{82}$$

and satisfying

$$V'(0) = Z'(0), \quad V(\kappa^{-\rho}) = \widetilde{C} \kappa^{1/2-2\rho} \exp(-f(0)\kappa^{-\rho}). \tag{83}$$

According to (79), (80), (82), and (83) and as $Z \geqslant 0$, we can apply Lemma 2.3 with $d=\kappa^{-\rho}$, $C=f(0)^2$ and $u=Z-V$ and we get $Z \leqslant V$. For $x \in [0, \kappa^{-\rho}]$, the solution of (82) is given by

$$V(x) = \widetilde{C}_3(\kappa)\exp(-f(0)x) + \widetilde{C}_4(\kappa)\exp(f(0)x) - \left(\frac{\kappa^2 h^3}{4f(0)^2} + \frac{C_6}{8f(0)^2}\kappa^{3/4}\right)\exp(-3f(0)x). \tag{84}$$

From (83) and (84), we get

$$\widetilde{C}_4(\kappa) = (-\widetilde{C}_3(\kappa) + \mathcal{O}(\kappa^{1/2-2\rho}))\exp(-2f(0)\kappa^{-\rho}). \tag{85}$$

From (84), we deduce that

$$V'(0) = -f(0)\widetilde{C}_3(\kappa) + f(0)\widetilde{C}_4(\kappa) + \frac{3\kappa^2 h^3}{4f(0)} + \frac{3C_6}{8f(0)}\kappa^{3/4}.$$

From (85) and taking account the condition $V'(0)=Z'(0)$ (see (81)) and replacing $f(0)$ with

$$\frac{1}{\sqrt{2}} + \mathcal{O}(\kappa^{1/4}),$$

we get

$$\widetilde{C}_3(\kappa) = -\frac{1}{16h}(1 + \mathcal{O}(\kappa^{1/4})) + \frac{3\kappa^2 h^3}{2}. \tag{86}$$

We have

$$\exp(-f(0)) = \exp\left(-\frac{1}{\sqrt{2}}x\right)(1 + \mathcal{O}(\kappa^{1/4-\rho}))$$

on $[0, \kappa^{-\rho}]$. From (84)–(86), we get the estimate, for $x \in [0, \kappa^{-\rho}/2]$ and for κ small enough

$$Z \leqslant V(x) = \frac{1}{2}\exp\left(-\frac{1}{\sqrt{2}}x\right)\left(-\kappa^2 h^3 \exp(-\sqrt{2}x) - \frac{1}{8h} + 3\kappa^2 h^3 + \mathcal{O}(\kappa^{3/4-\rho})\right). \tag{87}$$

Step 2: Lower bound for $A'+Af$. First, from (24), we remark that there exists C_7 such that, for $x \in [0, \kappa^{-\rho}]$,

$$-\kappa^2 A(-f+f^3) \geqslant C_7 \kappa^{3/2}\exp(-f(0)x).$$

According to (15) and (18), we deduce that there exists C_8 such that $f^2+2f' \leqslant f(0)^2 + C_8\kappa^{1-\rho}$. To get a lower bound, we compare Z with the solution of

$$\begin{gathered} -W'' + (f(0)^2 + C_8\kappa^{1-\rho})W = (2\kappa^2 h^3 + C_6\kappa^{3/4})\exp(-3f(0)x) + C_7\kappa^{3/2}\exp(-f(0)x), \\ W'(0) = Z'(0), \quad W(\kappa^{-\rho}) = \hat{C}\kappa^{1/2-2\rho}\exp(-f(0)\kappa^{-\rho}). \end{gathered} \tag{88}$$

Following Step 1, we apply Lemma (2.3) with $d=\kappa^{-\rho}$, $C=(f(0)^2+C_8\kappa^{1-\rho})$, and $u=W-Z$, and we get $W \leqslant Z$ on $[0, \kappa^{-\rho}]$. Following Step 2, in the proof of Lemma 3.2, one can prove that

$$W(x) = \frac{1}{2}\exp\left(-\frac{1}{\sqrt{2}}x\right)\left(-\kappa^2 h^3 \exp(-\sqrt{2}x) - \frac{1}{8h} + 3\kappa^2 h^3 + \mathcal{O}(\kappa^{1/2+\rho})\right) \leqslant Z(x). \tag{89}$$

Taking into account (87) and (89), we deduce that there exists κ_0 such that, for all $\kappa \leqslant \kappa_0$, for all pairs (f,A) satisfying (49), we get Estimate (78) on $[0, \kappa^{-\rho}]$. The proof of Lemma 3.5 follows.

Then, from Lemma 3.5, we can improve Inequality (17) and get the following proposition:

Proposition 3.6: There exists κ_0 such that, for all $\kappa \leqslant \kappa_0$, for all pairs (f,A) solutions of $(GL)_\infty$ satisfying (49), we have the following estimate:

$$-Af = A' - B, \quad \forall\, x \in [0, \kappa^{-\rho}], \tag{90}$$

where B is defined by

$$B(x) := \frac{1}{2}\exp\left(-\frac{1}{\sqrt{2}}x\right)\left(-\kappa^2 h^3 \exp(-\sqrt{2}x) - \frac{1}{8h} + 3\kappa^2 h^3 + \mathcal{O}(\kappa^{1/2+\rho})\right). \tag{91}$$

D. Control of the function $S := \sqrt{(A')^2 - A^2 f^2}$

In all the following sections, we set

$$S^2 := (A')^2 - A^2 f^2. \tag{92}$$

From Proposition 3.5, we can state the following proposition:

Proposition 3.7: Let $\rho \in [0, \frac{1}{8}]$ and S^2 be the function defined in (92). There exists κ_0 such that, for all $\kappa \leqslant \kappa_0$, for all pairs (f,A) solutions of $(\mathrm{GL})_\infty$ satisfying (49), we have the following estimate:

$$S^2 = \tfrac{1}{8}(-8\kappa^2 h^4 \exp(-\sqrt{2}x) - 1 + 24\kappa^2 h^4 + \mathcal{O}(\kappa^\rho))\exp(-\sqrt{2}x), \quad \forall\, x \in [0, \kappa^{-\rho}]. \tag{93}$$

Proof: According to (21), (24), (37), and (38), for $x \in [0, \kappa^{-\rho}]$, we deduce the estimate

$$A' - Af = 2(h + \mathcal{O}(\kappa^{1/2-2\rho}))\exp(-f(0)x). \tag{94}$$

From (94) and Lemma 3.5 [see (78)], we can write

$$S^2 = (A' - Af)\,.\,(A' + Af) = \tfrac{1}{8}(-8\kappa^2 h^4 \exp(-\sqrt{2}x) - 1 + 24\kappa^2 h^4 + \mathcal{O}(\kappa^\rho))\exp(-\sqrt{2}x).$$

The proof of Proposition 3.7 follows.

IV. PROOF OF THE PARR FORMULA

In this section, first, using Propositions 3.3, 3.6, and 3.7, we get Inequality (12) for all pairs (f,A) solution of $(\mathrm{GL})_\infty$ such that

$$f(0) \in \left[\frac{1}{\sqrt{2}} - \alpha\kappa^{1/4}, \frac{1}{\sqrt{2}} + \alpha\kappa^{1/4} \right].$$

In the following, we use the elementary equality, for $a>0$ and $b>0$,

$$\sqrt{a^2+b^2} = a + b - \frac{2ab}{a+b+\sqrt{a^2+b^2}}. \tag{95}$$

Proof of Inequality (12): Step 1: New estimate for $A'(0)$. According to (52) and Proposition 3.6 [see (90)], we get the upper bound for $A'(0)^2$,

$$h^2 \leqslant 2\int_0^\infty f(t)A'(t)^2 \mathrm{d}t - 2\int_0^{\kappa^{-\rho}} A'(t)f(t)B(t)\mathrm{d}t,$$

where B is defined in (91). From (54), we get

$$h^2 \leqslant -2\int_0^{\kappa^{-\rho}} A'(t)f(t)B(t)\mathrm{d}t + \int_0^{+\infty} f(x)(1-f(x)^4)\mathrm{d}x - 6\kappa^{-2}\int_0^{+\infty} f(x)f'(x)^2\mathrm{d}x. \tag{96}$$

According to (16) and (95) with the choice $a=\kappa^{-1}f'$ and $b=S$, the following equality results:

$$\frac{1}{\sqrt{2}}(1-f^2) = \kappa^{-1}f' + S - T, \tag{97}$$

where T is defined on $\mathbb{R}^+$ by

$$T(x) := \frac{2\kappa^{-1}f'S}{S+\kappa^{-1}f'+\sqrt{S^2+\kappa^{-2}(f')^2}}. \tag{98}$$

From (97) and following Ref. 6 (see Proposition 3.1, p. 604), we get

$$\int_0^\infty (1-f^4(x))f(x)\mathrm{d}x = \frac{1}{2\sqrt{2}}\kappa^{-1}(1-f(0)^2)(3+f(0)^2) + \sqrt{2}\int_0^\infty f(x)(1+f(x)^2)\,.\,S(x)\mathrm{d}x$$
$$-\sqrt{2}\int_0^\infty f(x)(1+f(x)^2)T(x)\mathrm{d}x,$$

and

$$\int_0^\infty f(x)f'(x)^2\mathrm{d}x = \frac{\kappa}{4\sqrt{2}}(1-f(0)^2)^2 - \kappa\int_0^\infty f(x)f'(x)S(x)\mathrm{d}x + \kappa\int_0^\infty f(x)f'(x)T(x)\mathrm{d}x.$$

Hence, from (96) we get

$$h^2 \leqslant \kappa^{-1}\phi_0(f(0)) + I_1 + I_2 + I_3,$$

where ϕ_0 is defined in (48),

$$I_1 := -2\int_0^{\kappa^{-\rho}} A'(t)f(t)B(t)\mathrm{d}t, \tag{99}$$

$$I_2 := \sqrt{2}\int_0^\infty f(x)(1+f(x)^2)S(x)\mathrm{d}x + 6\kappa^{-1}\int_0^\infty f(x)f'(x)S(x)\mathrm{d}x, \tag{100}$$

$$I_3 := -\sqrt{2}\int_0^\infty f(x)(1+f(x)^2)T(x)\mathrm{d}x - 6\kappa^{-1}\int_0^\infty f(x)f'(x)T(x)\mathrm{d}x. \tag{101}$$

For all $f(0)\in\,]0,1]$, we have $\phi_0(f(0))\leqslant 2^{-3/2}$. Then, we get

$$h^2 \leqslant \kappa^{-1}2^{-3/2} + I_1 + I_2 + I_3. \tag{102}$$

For $\rho\in\,]0,\frac{1}{8}[$, we cut the integration interval in $[0,\kappa^{-\rho}]$ and $[\kappa^{-\rho},+\infty[$. As the functions f and f' are bounded and the function S admits for upper bound and lower bound an exponential polynomial in the form of $P(x)\exp(-\sqrt{2}x)$, the integrals in (100) and (101) on the interval $[\kappa^{-\rho},+\infty[$ are equal to $\mathcal{O}(\kappa^n)$ for all $n\in\mathbb{N}$. According to (18), (38), and (91), we get

$$-2\int_0^{\kappa^{-\rho}} A'(t)f(t)B(t)\mathrm{d}t \leqslant -f(0)\int_0^{\kappa^{-\rho}} \exp(-\sqrt{2}x)\left(\kappa^2h^4\exp(-\sqrt{2}x) - \frac{1}{8} + 3\kappa^2h^4 + \mathcal{O}(\kappa^\rho)\right)\mathrm{d}x.$$

From (51) and as $e^{-\sqrt{2}\kappa^{-\rho}}=\mathcal{O}(\kappa^n)$ for κ small, it results that

$$I_1 \leqslant -\tfrac{3}{32} + \mathcal{O}(\kappa^\rho). \tag{103}$$

Step 2: Estimate for I_2. On the other hand, using Proposition 3.7, and making the scaling $u=\exp(-\sqrt{2}x)$, we get

$$\begin{aligned}\int_0^{\kappa^{-\rho}} S(x)\mathrm{d}x &= \frac{1}{4}\int_{e^{-\sqrt{2}\kappa^{-\rho}}}^1 \frac{\sqrt{2u-u^2}}{u}\mathrm{d}u + \mathcal{O}(\kappa^\rho)\\ &= \left[\frac{1}{4}\sqrt{2u-u^2} + \frac{1}{4}\arcsin(u-1)\right]_{e^{-\sqrt{2}\kappa^{-\rho}}}^1 + \mathcal{O}(\kappa^\rho)\end{aligned}$$

hence, for κ small

$$\int_0^{\kappa^{-\rho}} S(x)\mathrm{d}x = \frac{\pi}{8} + \frac{1}{4} + \mathcal{O}(\kappa^\rho). \tag{104}$$

From (18) and (104) and Proposition 3.3 [see (75)], it results that

$$6\kappa^{-1}\int_0^{\kappa^{-\rho}} f(x)f'(x)S(x)\mathrm{d}x \leqslant 6\kappa^{-1}(f(0)+c\kappa^{1-\rho})\int_0^{\kappa^{-\rho}} \kappa^2h^2(1-\exp(-\sqrt{2}x))\,.\,S(x)\mathrm{d}x.$$

From (51) and making the scaling $u=\exp(-\sqrt{2}x)$, we get

$$\begin{aligned}\int_0^{\kappa^{-\rho}} (1-\exp(-\sqrt{2}x))\,.\,S(x)\mathrm{d}x &= \frac{1}{4}\int_{e^{-\sqrt{2}\kappa^{-\rho}}}^1 \frac{(1-u)}{u}\sqrt{2u-u^2}\mathrm{d}u + \mathcal{O}(\kappa^\rho)\\ &= \left[\left(\frac{3}{8}-\frac{u}{8}\right)\sqrt{2u-u^2} + \frac{1}{8}\arcsin(u-1)\right]_{e^{-\sqrt{2}\kappa^{-\rho}}}^1 + \mathcal{O}(\kappa^\rho),\end{aligned}$$

hence

$$\int_0^{\kappa^{-\rho}} (1-\exp(-\sqrt{2}x))\,.\,S(x)\mathrm{d}x = \frac{\pi}{16} + \frac{1}{4} + \mathcal{O}(\kappa^\rho).$$

From (49) and (51), we get

$$6\kappa^{-1}\int_0^{\kappa^{-\rho}} f(x)f'(x)S(x)\mathrm{d}x \leqslant \frac{3}{2}\left(\frac{\pi}{16}+\frac{1}{4}\right)+\mathcal{O}(\kappa^{\rho}). \tag{105}$$

According to (18) and (104), we deduce that

$$\sqrt{2}\int_0^{\kappa^{-\rho}} f(x)(1+f(x)^2)S(x)\mathrm{d}x \leqslant \sqrt{2}(f(0)+c\kappa^{1-\rho})(1+(f(0)+c\kappa^{1-\rho})^2)\int_0^{\kappa^{-\rho}} S(x)\mathrm{d}x.$$

From (104), we get

$$\sqrt{2}\int_0^{\kappa^{-\rho}} f(x)(1+f(x)^2)S(x)\mathrm{d}x \leqslant \frac{3}{2}\left(\frac{\pi}{8}+\frac{1}{4}\right)+\mathcal{O}(\kappa^{\rho}). \tag{106}$$

According to (100), (105), and (106), we get

$$I_2 \leqslant \frac{9\pi}{32}+\frac{3}{4}+\mathcal{O}(\kappa^{\rho}). \tag{107}$$

Step 3: Estimate for I_3. From Proposition 3.3 [see (75)] and (51), on the interval $[0,\kappa^{-\rho}]$, we have

$$T \geqslant U := \frac{B}{C}, \tag{108}$$

where

$$B(x) := \frac{\sqrt{2}}{2}(1-\exp(-\sqrt{2}x)+\mathcal{O}(\kappa^{\rho}))\,.\,S, \tag{109}$$

and

$$C(x) := S+\frac{\sqrt{2}}{4}(1-\exp(-\sqrt{2}x)+\mathcal{O}(\kappa^{\rho}))\,.\,S+\sqrt{S^2+\frac{1}{8}(1-\exp(-\sqrt{2}x)+\mathcal{O}(\kappa^{\rho}))^2}. \tag{110}$$

As the functions f' and S are positive on $\mathbb{R}^+$, from (98), we deduce that $T \geqslant 0$. Thus, from (18) and (108), we get

$$-\sqrt{2}\int_0^{\infty} f(x)(1+f(x)^2)T(x)\mathrm{d}x \leqslant -\frac{3}{2}\int_0^{\kappa^{-\rho}} U(x)\mathrm{d}x+\mathcal{O}(\kappa^{\rho}). \tag{111}$$

Moreover, we have

$$-6\kappa^{-1}\int_0^{\infty} f(x)f'(x)T(x)\mathrm{d}x \leqslant -\frac{3}{2}\int_0^{\kappa^{-\rho}} (1-\exp(-\sqrt{2}x))\,.\,U(x)\mathrm{d}x+\mathcal{O}(\kappa^{\rho}). \tag{112}$$

Making the scaling $u=\exp(-\sqrt{2}x)$, from (51) and (108)–(110), we get

$$\int_0^{\kappa^{-\rho}} U(x)\mathrm{d}x = \frac{1}{\sqrt{2}}\int_{e^{-\sqrt{2}\kappa^{-\rho}}}^1 \frac{1}{\sqrt{2}u}\frac{\sqrt{u(2-u)}(u-1)}{u-2-\sqrt{u(2-u)}}\mathrm{d}u+\mathcal{O}(\kappa^{\rho}), \tag{113}$$

and

$$\int_0^{\kappa^{-\rho}} (1-\exp(-\sqrt{2}x))\,.\,U(x)\mathrm{d}x = \frac{1}{\sqrt{2}}\int_{e^{-\sqrt{2}\kappa^{-\rho}}}^1 -\frac{1}{\sqrt{2}u}\frac{\sqrt{u(2-u)}(u-1)^2}{u-2-\sqrt{u(2-u)}}\mathrm{d}u+\mathcal{O}(\kappa^{\rho}). \tag{114}$$

For $u \in]0,2[$, we have

$$\int \frac{1}{\sqrt{2}u}\frac{\sqrt{u(2-u)}(u-1)}{u-2-\sqrt{u(2-u)}}\mathrm{d}u = \frac{\sqrt{2}}{4}(\arcsin(u-1)-u+\sqrt{2u-u^2}),$$

and

$$\int -\frac{1}{\sqrt{2}u}\frac{\sqrt{u(2-u)}(u-1)^2}{u-2-\sqrt{u(2-u)}}\mathrm{d}u = \frac{1}{8}\arcsin(u-1)+\frac{\sqrt{2}}{8}\sqrt{2u-u^2}(3-u)-\frac{\sqrt{2}}{4}u\left(1-\frac{u}{2}\right).$$

From (113), it results that

$$\int_0^{\kappa^{-\rho}} U(x)\mathrm{d}x = \frac{\pi}{8}+\mathcal{O}(\kappa^{\rho}). \tag{115}$$

Moreover, from (114), we get

$$\int_0^{\kappa^{-\rho}} (1-\exp(-\sqrt{2}x))\,.\,U(x)\mathrm{d}x = \frac{1}{8}\left(1+\frac{\pi}{2}\right)+\mathcal{O}(\kappa^{\rho}). \tag{116}$$

From (111), (112), (115), and (116), we get

$$I_3 \leqslant -\frac{9\pi}{32}-\frac{3}{16}+\mathcal{O}(\kappa^{\rho}). \tag{117}$$

Step 4: Upper bound for $A'(0)$. According to (102), (103), (107), and (117), we deduce that there exists κ_0, such that, for all $\kappa \leqslant \kappa_0$ and all pairs (f,A) solutions of $(\mathrm{GL})_\infty$ satisfying (49), we have

$$h^2 \leqslant \kappa^{-1}2^{-3/2}+\tfrac{15}{32}+\mathcal{O}(\kappa^{\rho}). \tag{118}$$

From Lemma 3.1 and (118), the proof of Theorem 1.3 follows.

According to (11) and Theorem 1.3, we deduce the Parr formula (10).

Theorem 4.1 *(Parr formula): There exists* κ_0 *such that, for all* $\kappa_0 \leqslant \kappa$, *we have*

$$\kappa(h^{\mathrm{sh}}(\kappa))^2 = 2^{-3/2}+\frac{15}{32}\kappa+o(\kappa).$$

Remark 4.2: In Ref. 2, Bolley and the authors have proved that the set $\{(f_0,h)\in\,]0,1]\times[0,+\infty[\ \text{s.t.}\ \exists(f,A)$ *solution of* $(GL)_\infty$ *with* $f(0)=f_0\}$ *is a graph of a map* σ *from* $]0,1]$ *into* $[0,+\infty[$. *From Theorem 1.3, we deduce an upper bound for the maximum of* σ *on* $]0,1]$.

V. CONCLUSION

In the weak-κ limit, we have rigorously proved that the second term in the expansion of $\kappa^{1/2}h^{\mathrm{sh}}(\kappa)$ is of order of $\mathcal{O}(\kappa)$ and we have recovered the constant of Parr. In Ref. 23, this author associated the initial condition

$$f_0 = \frac{1}{\sqrt{2}}-\frac{7}{32}\kappa$$

to the superheating field. An open problem is to prove that the second term in the expansion of f_0 is of the order of $\mathcal{O}(\kappa)$. Consequently, we will prove the following conjecture introduced in Ref. 15 (see also Ref. 24). At the superheating field, there exists κ_0 such that, for all $\kappa \leqslant \kappa_0$, we have the asymptotic expansion

$$-\frac{A_\kappa(0)}{A'_\kappa(0)} = \sqrt{2} + \frac{3}{16}\kappa + \mathcal{O}(\kappa^2). \tag{119}$$

More generally, in Ref. 15 (see also Ref. 17), as a consequence of the construction of an asymptotic matched solution, we have obtained a complete expansion for the superheating field, denoted by $h^{\mathrm{sh},f}(\kappa) = \kappa^{-1/2}\Sigma_{i=0}^{\infty} h_i \kappa^i$. In Ref. 16, we have rigorously proved that for all $n \in \mathbb{N}$, there exist κ_0 and C such that, for all $\kappa \leqslant \kappa_0$, we have

$$\kappa^{1/2} h^{\mathrm{sh}}(\kappa) \geqslant \sum_{i=0}^{n} h_i \kappa^i + C\kappa^{n+1}.$$

An open problem is to prove that for all $n \in \mathbb{N}$, we have

$$\kappa^{1/2} h^{\mathrm{sh}}(\kappa) = \sum_{i=0}^{n} h_i \kappa^i + o(\kappa^n). \tag{120}$$

It seems difficult to extend the approach presented here to obtain the coefficients of higher order terms. It is necessary to recover the asymptotic matched solution at all orders constructed in Ref. 15 to get these terms.

In the large-κ limit, using a method of matched asymptotic expansions, Chapman[11] (see also Refs. 7 and 20) has formally proved the formula

$$h^{\mathrm{sh}}(\kappa) = \frac{1}{\sqrt{2}} + C\kappa^{-4/3} + o(\kappa^{-4/3}) \tag{121}$$

for some $C \sim 0.3$. This suggests that the superheating field $h^{\mathrm{sh}}(\kappa)$ admits an expansion in powers of $\kappa^{-4/3}$ when κ is large. The rigorous proof of formula (121) is also an open problem.

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Discrete and continuous cosine transform generalized to Lie groups SU(2)×SU(2) and O(5)

J. Patera[a] and A. Zaratsyan[b]
Centre de Recherches Mathématiques, Université de Montréal, C.P. 6128 SUCC. Centre-Ville, Montréal, Québec, Canada H3C 3J7

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We develop and describe continuous and discrete transforms of class functions on compact semisimple Lie group G as their expansions into series of uncommon special functions, called here C-functions in recognition of the fact that the functions generalize cosine to any dimension $n<\infty$. A uniform discretization of the problem on lattices of any density is described. Continuous and discrete orthogonality of C-functions is shown. Discrete transform is known in the case $n=1$ as the cosine transform. Continuous extension of the discrete transform is described. In general, C-functions are the contributions to irreducible characters from just one orbit of the Weyl group of G. Their products are fully decomposable to the sums of C-functions, so are the reductions to subgroups of the Lie group. They are eigenfunctions of Laplace operator, satisfying Neumann conditions at the boundary of the fundamental region of G, etc. A ready-to-use presentation is made of two of the four variants of the two-dimensional transforms. Both variants have in common exploitation of square lattices for the discrete version of the transforms. They are based on the compact Lie groups SU(2)×SU(2) and O(5), or, equivalently, Sp(4). Remaining two groups, SU(3) and G(2), involve triangular lattices. They are considered separately. Processing digital data, sampled on square lattices, is our motivating application.
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I. INTRODUCTION

This is the first in the series of three papers[1,2] dealing with two families of special functions, called here C- and S-functions, whose many properties, very useful for applications, apparently went mostly unnoticed, although the functions have been known in Lie theory for decades. The C-functions were called "orbit functions" or "orbit sums" since Ref. 3, while the S-functions appear in Weyl's character formula under the name "characteristic functions."

The aim of the series is twofold, (i) to formulate, derive, and bring forward practically useful properties of these functions and their discretization in general, and (ii) to work out all the details of all the four variants in two dimensions.

In this paper we consider two of the four variants of C-functions, since both of them involve rectangular lattices. Two other cases, which involve triangular lattices, are given in Ref. 1. The S-functions for all four cases are described in Ref. 2.

The present approach can be viewed as originating from three sources. First it is the traditional theory of compact semisimple Lie groups and their finite dimensional representations. Indeed, from there we take the definition of C- and S-functions (though under different names and to be used for a very different purpose), second is the general discretization of the Fourier-like trans-

[a]Electronic mail: patera@crm.umontreal.ca
[b]Electronic mail: zaratsyan@crm.umontreal.ca

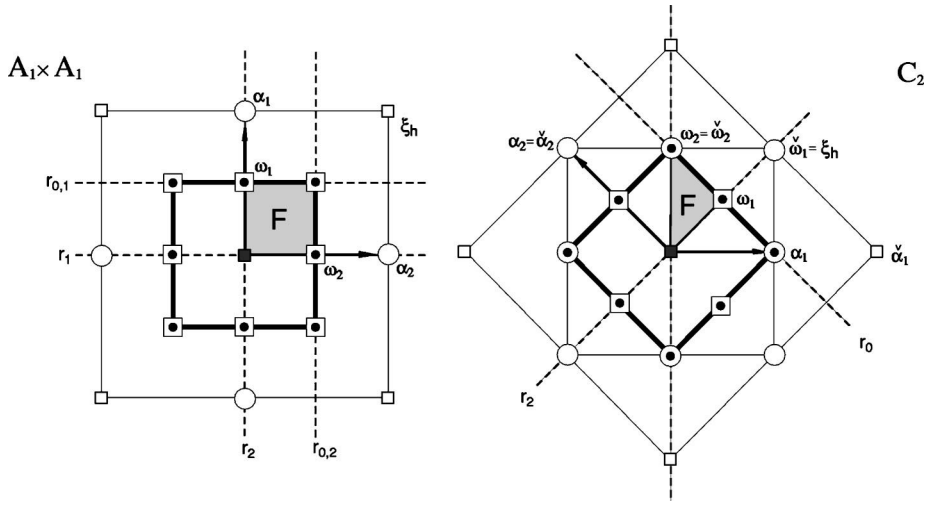

FIG. 1. The simple roots, the fundamental weights, along with their duals, and the fundamental region for the cases $A_1 \times A_1$ and C_2.

forms involving C-functions,[3] and finally it is the observation, made in Ref. 4, that the continuous extensions of discrete C-expansions interpolates smoothly between points where digital data are given.

Two and three dimensional digital data is often collected in physical experiments, the largest and, probably, the most costly of them being the elaborate batteries of particle counters in high-energy experimental astrophysics and particle physics. In the recent years digital images have also been generated in innumerable applications. Quite often processing such data involves Fourier analysis and discrete transforms.[5]

In this paper we describe a new versatile approach to the treatment of such data, which has been mostly unexplored so far. One of our objectives is to make the approach as ready to use as possible. Its one-dimensional (discrete) version was discovered some 30 years ago and is extensively used ever since under the name of the cosine transform.[6,7] Its straightforward generalization to two dimensions is, in our notation, the (discrete) case of $A_1 \times A_1$ [equivalently SU(2) $\times$ SU(2)]. Apparently, the first exploitation of the case A_2 [equivalently SU(3)] is quite recent,[4,8,9] although the problem of processing the digital data sampled on triangular lattices is not new.[10]

The important difference between the presented method and the traditional decomposition into Fourier series is not in that here we consider other compact semisimple Lie groups of rank 2 rather than the traditional SU(2) $\times$ SU(2). This is merely a technicality; the reason for the approach lies elsewhere. Traditionally, in any dimension $1 \leqslant n \leqslant \infty$, one uses the periodicity of the functions (the functions to be decomposed as well as the expansion functions). The underlying group in that case is the U(1) of our example (2.2), or a product of n of them. Thus, the involved group is the group of discrete translations. In our method a larger group is involved, the affine Weyl group, which contains the translations as its subgroup. It requires the use of more complicated functions (the C-functions or S-functions), but, in comparison, it involves lower harmonics in the expansions, which in turn results in much smoother interpolation between digital points during the continuous extension of the method,[4] etc.

As a quantitative measure of the difference between the two methods (the number of "harmonics," for example), we can take the comparison of the area of the fundamental region for the affine Weyl group and for its translation subgroup, assuming we have the grids of comparable densities. The fundamental regions F of the affine groups are shown in Fig. 1, the fundamental region of the translation subgroup is the Voronoi domain[11] (also called the proximty cell) of the corresponding root lattice. For A_1 the ratio is 1 : 2, for $A_1 \times A_1, A_2, C_2$, and G_2 the ratio is 1 : 4, 1 : 6, 1 : 8, and 1 : 12, respectively.

There are three compact simple Lie groups of rank 2, namely the following: SU(3), O(5) or Sp(4), and G(2). There is only one nonsimple but semisimple compact Lie group, SU(2) ×SU(2). In this paper, we use the notation more familiar in Lie algebra theory,

$$A_1 \leftrightarrow \mathrm{SU}(2),$$

and

$$\begin{gathered} A_1 \times A_1 \leftrightarrow \mathrm{SU}(2) \times \mathrm{SU}(2), \\ A_2 \leftrightarrow \mathrm{SU}(3), \\ C_2 \leftrightarrow \mathrm{O}(5) \text{or } \mathrm{Sp}(4), \\ G_2 \leftrightarrow \mathrm{G}(2). \end{gathered} \tag{1.1}$$

In principle, one could also consider the compact Lie groups of rank 2, U(1)×U(1) and U(1) ×SU(2), which are not semisimple. In view of (2.2), that would lead to the traditional Fourier decompositions. Here we disregard those cases.

In Sec. II, our general goals are compared with the traditional approach, namely, with the decomposition of a class function f into series irreducible characters. It is pointed out that our expansion functions are different, and that we are considering in parallel continuous f as well as f sampled on a discrete lattice of any density. Section III deals with the one-dimensional case, both continuous and discrete. It serves as a didactic illustration and an introduction to higher rank cases. General continuous case of any semisimple compact Lie group is presented in a uniform way in Sec. IV. Properties of C-functions are our main target. Sections V and VI contain, respectively, all the details for exploitation of the method for $A_1 \times A_1$ and C_2. Discretization of two-dimensional cases in general, as well as the specialization to $A_1 \times A_1$ and C_2 is the subject of Sec. VII. Examples are shown. Concluding remarks and related problems are brought forward in Sec. VIII.

Let us underline some notations used throughout the paper. The symbols $\mathbb{R}, \mathbb{Z}$, and $\mathbb{N}$ denote the real numbers, integers, and positive integers, respectively. The scalar product of $a, b \in \mathbb{R}^2$ in a real Euclidean space $\mathbb{R}^n$ of dimension n, is denoted by $\langle a|b\rangle$. The same notation is used for the Hermitian product of the class functions in the functional space spanned by irreducible characters (or C-functions).

II. GENERAL GOALS

The standard general problem of harmonic analysis on a compact Lie group G, is to consider the functions depending on conjugacy classes of elements of the group, i.e., such that

$$f(g') = f(g_0 g\, g_0^{-1}), \quad \text{for all } g, g_0 \in G,$$

and to find their expansions, along with their inversions

$$f(g) = \sum_{\lambda} \mathrm{d}_\lambda \chi_\lambda(g), \quad \mathrm{d}_\lambda = \int_F f(g)\overline{\chi_\lambda(g)}\mathrm{d}g, \tag{2.1}$$

in terms of irreducible characters χ_λ. The inversion is possible due to the orthogonality of the characters when integrated over the fundamental region F of the group.

The simplest example of (2.1) is the case when G is the 1-parametric compact Lie group U(1). In this case the irreducible characters are the exponential functions,

$$\chi_m(\theta) = e^{2\pi i m\theta}, \quad \text{where } m \in \mathbb{Z} \text{ and } \theta \in \mathbb{R}. \tag{2.2}$$

We take a similar problem, but it differs from (2.1) in two important ways.

(i) Our expansions are into series of C-functions (4.7), rather than irreducible characters of compact semisimple Lie groups. It offers a considerable practical advantage, since the C-functions, unlike the characters, do not get more complicated as λ increases. The second advantage has yet to be utilized, the C-functions are the eigenfunctions of the corresponding Laplace operator[12] and their eigenvalues are explicitly known.

(ii) We are interested in discrete expansions (7.7) besides the continuous ones. That is, expansions of functions given digitally by their values on a discrete grid of points F_M in F. Those functions are then expanded into a series in terms of C-functions given on the same grid. Inversion of such expansions is possible because of the discrete orthogonality of C-functions (7.4) established in Ref. 13 for any semisimple compact Lie group. Practically useful appears to be subsequent continuous extensions of discrete expansions (7.9).

Also it is difficult to overestimate the versatility of different choices of the grid F_M in F offered by our approach, which are equivalent to choosing, for each $M \in \mathbb{N}$, the finite Abelian subgroup of the maximal torus of the Lie group generated by all elements of order M.

III. DISCRETIZATION IN THE CASE OF A_1

Leaving aside the simplest case (2.2), there remains only one other compact Lie group of rank 1, namely A_1. One can recognize a familiar situation in this one-dimensional setup, without any group theory, once the C-functions $\Omega_m(\theta)$ are explicitly written below, in (3.1). In spite of that, it is useful to go through it using terms and notions that are indispensable in the case of higher ranks.

A. The continuous case

The Weyl group of A_1 has two elements $W=\{1,r\}$, where r is the reflection in the origin. The weight lattice $P(A_1)$ consists of all the points $x=\mathbb{Z}\omega$, where $\mathbb{Z}$ stands for any integer, while the root lattice $Q(A_1)$ consists of the even points of P. Symbolically, we write it as

$$Q(A_1) = \mathbb{Z}\alpha = 2\mathbb{Z}\omega,$$

$$P(A_1) = \mathbb{Z}\omega = Q(A_1) \cup (\omega + Q(A_1)).$$

Here α is called the simple root of A_1 and ω is the fundamental weight. Hence the relative lengths of the basis vectors of Q and P are fixed, $\alpha=2\omega$. We fix also their absolute length by choosing the value of the scalar product $\langle\alpha|\alpha\rangle=4\langle\omega|\omega\rangle=2$. The root system, $\Delta(A_1)=\{\pm\alpha\}$ has just two roots.

Given a point $\lambda=m\omega\in P$, its Weyl group orbit W_λ is the following:

$$W_\lambda \equiv W_m = \begin{cases} \{0\}, & \text{if } m = 0, \\ \{m\omega, -m\omega\}, & \text{if } 0 \neq m \in \mathbb{Z}. \end{cases}$$

The A_1 C-function $\Omega_\lambda(z)\equiv\Omega_m(\theta)$ is defined for $\theta\in\mathbb{R}$ as

$$\Omega_m(\theta) \overset{\text{def}}{=} \sum_{\mu\in W_\lambda} e^{2\pi i\langle\mu|z\rangle} = \begin{cases} 1, & \text{for } m = 0, \\ 2\cos\pi m\theta, & \text{for } m \in \mathbb{N}. \end{cases} \tag{3.1}$$

Here we have used $\langle\mu|z\rangle=\pm m\theta\langle\omega|\omega\rangle=\pm\frac{1}{2}m\theta$. Sometimes it is convenient to introduce a different normalization of the C-functions, namely the following one:

$$\Phi_m(\theta) = 2\cos\pi m\theta, \quad \text{for all } m \in \mathbb{Z}^{\geqslant 0}. \tag{3.2}$$

The fundamental region $F(A_1)$ is the closed segment with the end points 0 and ω. Its length is $|\omega|=1/\sqrt{2}$. Hence $0\leqslant\theta\leqslant 1$ within $F(A_1)$.

It is straightforward to verify the decomposition of the products,

$$\Phi_m(\theta)\Phi_{m'}(\theta) = \Phi_{m+m'}(\theta) + \Phi_{m-m'}(\theta), \quad \text{for } m,m' \in \mathbb{Z}^{\geqslant 0}.$$

Any two functions $\Omega_m(\theta), \Omega_{m'}(\theta)$, where $m \neq m'$, are orthogonal, i.e.,

$$\int_0^1 \Omega_m(\theta)\Omega_{m'}(\theta)\mathrm{d}\theta = \begin{cases} 0, & \text{if } m \neq m', \\ 1, & \text{if } m = m' = 0, \\ 2, & \text{if } m = m' > 0. \end{cases} \tag{3.3}$$

It is useful to notice the special case of (3.3) arising for $m>0$ and $m'=0$,

$$\int_0^1 \Omega_m(\theta)\mathrm{d}\theta = 0, \quad \text{for any } m \in \mathbb{N}.$$

The orthogonality can be used to invert the Fourier series (2.1) on $F(A_1)$ in the traditional way.

Every element of the group A_1 is conjugate to an element of its torus. Elements of the torus are parametrized by points of a circle. Every point of F stands for one conjugacy class of the elements of A_1.

B. Discretization of A_1

The objective of this section is the description of the A_1 version of the discrete orthogonality (7.4) of the C-functions.

Here we are interested in the elements $s\omega \in F$ with rational values of s. They are specified by two non-negative integers s_0 and s_1. It is convenient to set it up as follows:

$$F \ni s\omega = \frac{s_1}{M}\omega, \quad \text{where } s_0 + s_1 = M > 0, \quad s_0, s_1 \in \mathbb{Z}^{\geqslant 0}.$$

Fixing M determines an equidistant grid of $M+1$ points $s\omega \in F$. The set F_M of their coordinates is

$$F_M \overset{\text{def}}{=} \left\{ 0, \frac{1}{M}, \frac{2}{M}, \frac{3}{M}, \ldots, \frac{M-1}{M}, 1 \right\}.$$

C. Scalar product on the grid F_M

The points of F are in one-to-one correspondence with conjugacy classes of elements of A_1. They represent the conjugacy classes of elements of orders equal to M, as well as all the divisors of M.

In general, one introduces a scalar product in the space of functions defined digitally on F_M,

$$\langle f|h\rangle_M \overset{\text{def}}{=} \sum_{s \in T_M} f(s)h(s) = \sum_{s \in F_M} c_s f(s)h(s). \tag{3.4}$$

Here T_M stands for the Abelian subgroup of the maximal torus of A_1, which is generated by all the elements of order M. The coefficients c_s in the sum over F_M count the number of points in the torus that are conjugate to s. One has

$$c_0 = c_1 = 1, \quad \text{and } c_{1/M} = c_{2/M} = \cdots = c_{(M-1)/M} = 2. \tag{3.5}$$

The C-functions take the following values on the points of the grid:

$$\Omega_0(s) = 1, \quad \Omega_m(s) = 2\cos \pi m s, \quad \text{for } s \in F_M \text{ and } m \in \mathbb{N}. \tag{3.6}$$

In order to reduce the number of calculations, it is more convenient to utilize in the discretization the normalized form of the C-functions given in (3.2).

TABLE I. Values of several normalized C-functions of A_1 on the points of the grid F_M with $M=3$. Note that only the first four C-functions are pairwise orthogonal. The higher ones repeat the values of the lowest four. c_s are the coefficients from ((3.5)).

s	0	$\frac{1}{3}$	$\frac{2}{3}$	1
$\Phi_0(s)$	2	2	2	2
$\Phi_1(s)$	2	1	−1	−2
$\Phi_2(s)$	2	−1	−1	2
$\Phi_3(s)$	2	−2	2	−2
$\Phi_4(s)$	2	−1	−1	2
$\Phi_5(s)$	2	1	−1	−2
$\Phi_6(s)$	2	2	2	2
c_s	1	2	2	1

$$\Phi_m(s) = 2\cos \pi m s, \quad \text{for } s \in F_M \text{ and all } m \in \mathbb{Z}^{\geqslant 0}. \tag{3.7}$$

The crucial discrete orthogonality property of the normalized C-functions over F_M is the following:

$$\langle \Phi_m | \Phi_{m'} \rangle_M = \begin{cases} 8M, & \text{if } m = m' = 0 \mod M, \\ 4M, & \text{if } m = m' \neq 0 \mod M, \\ 0, & \text{if } m \neq m' \mod M. \end{cases} \tag{3.8}$$

Note that the orthogonality (3.8) is valid not only when m and m' are constrained to the range $\{0,1,\ldots,M\}$.

Examples of several A_1 normalized C-functions on the grid F_3 are given in the Table I.

Our aim in the development of the formalism so far is to use it for the expansion in terms of the C-functions of any function $f(s)$, given by its values on the grid F_M.

More precisely, a function $f(s)$, with known real values on F_M, can be decomposed as follows:

$$f(s) = \sum_{k=0}^{M} d_k \Phi_k(s), \quad s \in F_M. \tag{3.9}$$

Then we can compute the coefficients d_k from

$$\langle f | \Phi_k \rangle_M = \sum_{s \in F_M} c_s f(s) \Phi_k(s) = \begin{cases} 8M d_k, & \text{if } k = 0 \text{ or } k = M, \\ 4M d_k, & \text{if } k = 1,2,\ldots,M-1. \end{cases} \tag{3.10}$$

After the coefficients d_k have been calculated, one can replace s in (3.9) by the continuous variable θ,

$$f_{\text{cont}}(\theta) \overset{\text{def}}{=} \sum_{k=0}^{M} d_k \Phi_k(\theta), \quad \text{where } \theta \in \mathbb{R}. \tag{3.11}$$

At $\theta = s \in F_M$, the continuous function $f_{\text{cont}}(\theta)$ coincides with $f(s)$.

The all-important property that distinguishes (3.11) from the standard Fourier transform and that was apparently established only recently,[4] is the smoothness of the interpolation of f_{cont} between the points of the grid F_M.

IV. HIGHER RANK CASES IN GENERAL

The basic tools that we need, in order to develop the formalism of every case, can be introduced equally simply for all the cases at once and for any rank $n<\infty$. Thus, we do not always require that $n=2$. The rank of the Lie group is the dimension of the decomposition problem, i.e., the number of variables in a C-function.

A. The α and ω bases and their dual bases

The root system $\Delta \in \mathbb{R}^n$ contains k distinct vectors/roots. A suitable basis $\Pi = \{\alpha_1, \ldots, \alpha_n\} \subset \Delta$ consists of the simple roots (α basis). For any simple Lie algebra, its simple roots are of at most of two different lengths.

Relative lengths and angles between simple roots of the basis Π are concisely specified in terms of the elements of the Cartan matrix C,

$$C_{jk} = \frac{2\langle \alpha_j | \alpha_k \rangle}{\langle \alpha_k | \alpha_k \rangle} = \langle \alpha_j | \hat{\alpha}_k \rangle, \quad \text{for } j,k = 1, \ldots, n, \tag{4.1}$$

where $\hat{\alpha}_k$ is the simple root of the dual root system $\hat{\Delta}$. Adopting the standard convention for the lengths of the long root of Π, namely $\langle \alpha_l | \alpha_l \rangle = 2$, the elements of the Cartan matrix become the smallest possible integers. During the dualization,

$$\alpha \leftrightarrow \hat{\alpha} = \frac{2\alpha}{\langle \alpha | \alpha \rangle} \quad \text{of } \alpha \in \Delta,$$

the long roots do not change, while the short ones become long (see Fig. 1).

In addition to the α and $\hat{\alpha}$ bases, we introduce the basis of the fundamental weights and its dual basis, called ω and $\hat{\omega}$ basis, respectively. In the matrix form, using (4.1), we have

$$\alpha = C\omega, \quad \omega = C^{-1}\alpha, \quad \hat{\alpha} = C^T \hat{\omega}, \quad \hat{\omega} = C^{T-1}\hat{\alpha}. \tag{4.2}$$

Given a specific Cartan matrix, one can verify the following frequently used multiplication rules:

$$\langle \hat{\alpha}_j | \omega_k \rangle = \langle \alpha_j | \hat{\omega}_k \rangle = \frac{2\langle \alpha_j | \omega_k \rangle}{\langle \alpha_j | \alpha_j \rangle} = \delta_{jk}. \tag{4.3}$$

B. Reflections of the finite Weyl group

For each $\xi \in \Delta$ there are reflections r_ξ, which act in $\mathbb{R}^n$ according to

$$r_\xi x = x - \frac{2\langle x | \xi \rangle}{\langle \xi | \xi \rangle} \xi, \quad \text{where } \xi \in \Delta,\ x \in \mathbb{R}^n. \tag{4.4}$$

Those with $\xi \in \Pi$ generate the finite Weyl group W.

Observe that r_ξ does depend on the direction of ξ, but not on its length or orientation along that direction. In particular, it is easy to check that $r_\xi \xi = -\xi$ and also that

$$r_\xi r_\xi x = r_\xi \left(x - \frac{2\langle x | \xi \rangle}{\langle \xi | \xi \rangle} \xi \right) = r_\xi x - \frac{2\langle x | \xi \rangle}{\langle \xi | \xi \rangle} r_\xi \xi = x.$$

The application of W to the basis Π yields the root system, $W\Pi = \Delta$. Consequently, one has the W invariance, $\Delta = W\Delta$. Thus, a root is transformed into a root of the same system by any element of W. Each root appears exactly once in Δ. It is known that for simple Lie groups the root system is obtained by applying W to either one, or at most two roots of the basis Π.

C. The affine Weyl group

The group W contains the reflections r_ξ in mirrors, which are orthogonal to any $\xi \in \Delta$ and pass through the origin. The affine Weyl group W^{aff} contains all the reflections $R_{N\xi}$ in mirrors, which are orthogonal to ξ and displaced from the origin by any $N\xi$, where $N \in \mathbb{Z}$. Hence W^{aff} is of infinite order, and $W \subset W^{\text{aff}}$.

One has the affine reflections $R_{N\xi}$,

$$R_{N\xi}x \overset{\text{def}}{=} N\xi + r_\xi x, \quad \text{where } x \in \mathbb{R}^n,\ N \in \mathbb{Z} \text{ and } \xi \in \Delta. \tag{4.5}$$

Note that $R_{0\xi} = r_\xi$ and that $R_{N\xi} \neq R_{-N\xi}$. In particular, $R_{N\xi}0 = N\xi$ is the reflection of the origin in the midpoint $\frac{1}{2}N\xi$, and $R_{N\xi}(N\xi) = 0$. In general, one has

$$R_{N\xi}R_{N\xi}x = R_{N\xi}(N\xi + r_\xi x) = N\xi + r_\xi(N\xi + r_\xi x) = N(\xi + r_\xi\xi) + r_\xi r_\xi x = x.$$

It is useful to note the presence of a translation subgroup $T \subset W^{\text{aff}}$. It is an Abelian subgroup of W^{aff}, whose elements are all the translations $t_{N\xi}$, $N \in \mathbb{Z}$,

$$t_{N\xi}x \overset{\text{def}}{=} R_{N\xi}r_\xi x = r_\xi R_{-N\xi}x = (N\xi + r_\xi^2 x) = x + N\xi, \quad \text{where } N \in \mathbb{Z},\ \xi \in \Delta \text{ and } x \in \mathbb{R}^n. \tag{4.6}$$

As an example, one may verify that $t_{-N\xi}x = r_\xi R_{N\xi}x$.

In general, W^{aff} can be defined as the semidirect product $W \ltimes T$.

D. Root and weight lattice

The root lattice Q consists of all the elements that can be written symbolically as

$$\mathbb{Z}\alpha_1 + \cdots + \mathbb{Z}\alpha_n \in Q, \quad \text{where } \alpha_1, \ldots, \alpha_n \in \Pi,$$

in which $\mathbb{Z}$ stands for any integer chosen independently in each term of the sum. In particular, $\Delta \subset Q$.

We will mainly consider the weight lattice P and its positive chamber P^+,

$$\mathbb{Z}\omega_1 + \cdots + \mathbb{Z}\omega_n \in P, \quad \text{and } \mathbb{Z}^{\geqslant 0}\omega_1 + \cdots + \mathbb{Z}^{\geqslant 0}\omega_n \in P^+.$$

In all cases $Q \subseteq P$.

In addition to the root and weight lattices Q and P, we have also their dual latices, $\hat{Q}$ and $\hat{P}$, each along with its basis, namely the $\alpha, \omega, \hat{\alpha}, \hat{\omega}$ basis, respectively.

E. Weyl group orbits

Let $\lambda \in P \subset \mathbb{R}^n$. The Weyl group orbit W_λ of λ is the set of distinct elements of P obtained by all possible applications of W to λ. We write $W\lambda = W_\lambda$. In a similar way, one defines $W_\lambda^{\text{aff}} = W^{\text{aff}}\lambda$. The orbit W_λ is always finite, while W_λ^{aff} is infinite. The size $|W_\lambda|$ of W_λ is the number of distinct points which are generated from λ by W. The maximal value of $|W_\lambda|$ equals to the order $|W|$ of the Weyl group. Other possible values of $|W_\lambda|$ are some of the divisors of $|W|$.

In particular, we are interested in the following properties:

$$W0 = 0 \quad \text{and } W\Pi = \Delta.$$

In general, P is a union of several W^{aff} orbits.

Each $\lambda \in P$ is contained in precisely one W-orbit W_λ. Elements of W_λ are called weights. Each W orbit contains a unique element belonging to P^+, called the dominant weight of W_λ. The dominant weight is easy to recognize since its coordinates in ω basis are non-negative integers. It is then usually taken as the λ to be used in the symbol W_λ.

F. C-functions

The definition of a C-function $\Omega_\lambda(z)$ involves $\lambda \in P^+$ and $z \in \mathbb{R}^n$. It requires also the W-orbit W_λ of λ. The compact semisimple Lie group figures only through its Weyl group. One has

$$\Omega_\lambda(z) \overset{\text{def}}{=} \sum_{\mu \in W_\lambda} e^{2\pi i \langle \mu | z \rangle}, \quad \text{where } \lambda \in P^+ \text{ and } z \in \mathbb{R}^n. \tag{4.7}$$

The number of summands in (4.7) is the number $|W_\lambda|$ of weights in W_λ,

$$|W_\lambda| = \frac{|W|}{|\mathrm{Stab}_W(\lambda)|},$$

where $\mathrm{Stab}_W(\lambda)$ is the stabilizer of λ in W, the subgroup of W generated by reflections which do not move λ.

A different normalization of C-functions than (4.7) may occasionally be more convenient. We will use the following one:

$$\Phi_\lambda(z) \overset{\text{def}}{=} |\mathrm{Stab}_W(\lambda)| \Omega_\lambda(z). \tag{4.8}$$

All C-functions, renormalized in such way, take the same value at the origin,

$$\Phi_\lambda(0) = \Phi_{\lambda'}(0), \quad \text{for all } \lambda, \lambda' \in P^+.$$

In order to make explicit the dependencies of C-functions on λ and z, one needs to fix a particular semisimple Lie group, or, equivalently, a Weyl group, choose the weight λ, and provide more details on how to calculate the products $\langle \mu | z \rangle$. That is, in which bases one has z and λ. In the rest of this paper it is done explicitly for the cases of interest, where $n=2$. Most often λ is given relative to either ω or α basis, while z is taken relative to $\hat{\omega}$ basis.

G. Other properties of C-functions

Important symmetry properties of C-functions are the following:

$$\Omega_{(a,b)}(z) = \Omega_{(a,b)}(wz),$$

$$\Omega_{(a,b)}(z) = \Omega_{(a,b)}(R_{N\gamma} z) = \Omega_{(a,b)}(r_\gamma z + N\gamma) = \Omega_{(a,b)}(r_\gamma z), \tag{4.9}$$

$$\Omega_{(a,b)}(z) = \Omega_{(a,b)}(r_\gamma R_{N\gamma} z) = \Omega_{(a,b)}(R_{N\gamma} r_\gamma z) = \Omega_{(a,b)}(z \pm N\gamma),$$

where $w \in W$, $\gamma \in \hat{\Delta}$, and $N \in \mathbb{Z}^{>0}$.

In view of (4.3), $\langle \lambda | \gamma \rangle$ for all $\gamma \in \hat{Q}$, $\lambda \in P$ take integer values. Hence, they do not change the value of a C-function (4.7). The first property in (4.9) follows from $\langle \eta | z \rangle = \langle w\eta | wz \rangle$ for all $w \in W$ and $\eta \in W_\lambda$.

Another useful property of C-functions is the complete decomposability of their products into a linear combination of C-functions with positive integer coefficients,

$$\Omega_\lambda \Omega_{\lambda'} = \Omega_{\lambda+\lambda'} + \cdots . \tag{4.10}$$

The problem of finding the remaining terms of the sum and their multiplicities is a question of computation. Many examples are found in Refs. 14,15.

H. The fundamental region

The fundamental region F of a group, in general, is a finite region, where every conjugacy class of the elements of the group is represented precisely by one point. For a compact simple Lie

group of rank n, F is a simplex in $\mathbb{R}^n$. When $n=2$, it forms a triangle. For a nonsimple group, it is a Cartesian product of corresponding simplexes. Thus, for A_1, F is a segment, for $A_1 \times A_1$, a square.

The definition (4.7) of the C-function clearly allows one to consider z in the entire space $\mathbb{R}^n$. However, due to the symmetries (4.9), we are mainly interested in the C-functions with z in the fundamental region of the corresponding semisimple Lie group.

The fundamental region of a simple Lie group consists of the points x such that $0 \leqslant \langle x | \xi_h \rangle \leqslant 1$, where ξ_h is the highest root of Δ. Suppose,

$$\xi_h = q_1\alpha_1 + q_2\alpha_2 + \cdots + q_n\alpha_n, \tag{4.11}$$

where $q_1, \ldots, q_n$ are well-known positive integers for each root system. Then the vertices of the simplex F are the following:

$$F: \left\{ 0, \frac{1}{q_1}\hat{\omega}_1, \frac{1}{q_2}\hat{\omega}_2, \ldots, \frac{1}{q_n}\hat{\omega}_n \right\}. \tag{4.12}$$

I. C-functions and irreducible characters

The character χ_λ of a finite-dimensional irreducible representation of a group G is a linear combination of C-functions,

$$\chi_\lambda(z) = \sum_\mu m_{\lambda\mu}\Omega_\mu(z), \tag{4.13}$$

where the summation extends over the set of distinct dominant weights in the weight system V_λ of the representation labeled by λ. Coefficients $m_{\lambda\mu}$ are the multiplicities of the dominant weights in V_λ. It is a well-known computational problem in Lie theory to find the multiplicities $m_{\lambda\mu}$ for a given λ, see, for example, the tables[16] and references therein. The matrix $(m_{\lambda\mu})$ is nonsingular. A suitable ordering of the dominant weights makes it triangular. Hence, it can be inverted, so that one has

$$\Omega_\lambda(z) = \sum_\mu n_{\lambda\mu}\chi_\mu(z), \tag{4.14}$$

where $n_{\lambda\mu}$ are the (integer) matrix elements of the inverse matrix of dominant weight multiplicities. The summation in (4.14) ranges over the same finite set of dominant weights as in (4.13).

Consequently, C-functions form another basis in the space spanned by irreducible characters of G.

J. Orthogonality of C-functions

The orthogonality property of C-functions,

$$\int_F \Omega_\lambda(z)\overline{\Omega_{\lambda'}(z)}\mathrm{d}F = 0, \quad \text{where } \lambda, \lambda' \in P^+ \text{ and } \lambda \neq \lambda', \tag{4.15}$$

is a consequence of the orthogonality of characters of irreducible representations and the decomposability of products (4.10) of C-functions. Indeed, let the zero weight be denoted 0 for any rank. Because $W0=0$, one has $\Omega_0(z)=1$ for every group and all $z \in \mathbb{R}^n$. Setting $\lambda'=0$ in (4.15), we have

$$\int_F \Omega_\lambda(z)\mathrm{d}F = 0, \quad \text{for any } 0 \neq \lambda \in P^+. \tag{4.16}$$

Complex conjugate $\overline{\Omega_\lambda}$ is a C-function with another (contragredient) dominant weight, say $\overline{\lambda'}$. Therefore $\Omega_\lambda(z)\overline{\Omega_{\lambda'}(z)}$ decomposes according to (4.10). The decomposition contains Ω_0 precisely if $\overline{\lambda'}=\overline{\lambda}$. Therefore, only in that case, the integral (4.15) is not zero.

K. Eigenfunctions of the Laplace operator

Consider the differential operator

$$L=(\alpha_1\partial_1+\alpha_2\partial_2+\cdots+\alpha_n\partial_n)^2. \tag{4.17}$$

Since the matrix of scalar products of simple roots is positive definite, by a suitable choice of basis, the operator can be brought to the sum of second derivatives with positive coefficients. Hence, one is justified in calling L the Laplace operator.

Subsequently, we will verify the validity of the eigenvalue equation[17]

$$L\Omega_\lambda(z)=-4\pi\langle\lambda|\lambda\rangle\Omega_\lambda(z),\quad \text{for all } \lambda\in P^+ \text{ and } z\in\mathbb{R}^n. \tag{4.18}$$

From (4.7) it is clear that C-functions are continuous functions with continuous derivatives of all orders in $\mathbb{R}^n$. Then it follows from (4.9) that their derivatives, normal to the boundary of the fundamental region, must be equal to zero (Newmann boundary value condition).

V. THE CASE $A_1\times A_1$

This is a simple concatenation of two cases of A_1 described in Sec. III.

A. Roots and weights

Relative length and angles of the simple roots are given by the scalar products,

$$\langle\alpha_1|\alpha_2\rangle=0,\quad \langle\alpha_1|\alpha_1\rangle=\langle\alpha_2|\alpha_2\rangle=2.$$

The Cartan matrix and its inverse are the following:

$$C=\begin{pmatrix}2&0\\0&2\end{pmatrix}\quad\text{and } C^{-1}=\begin{pmatrix}\frac{1}{2}&0\\0&\frac{1}{2}\end{pmatrix}.$$

Consequently, $\alpha_1=2\omega_1$ and $\alpha_2=2\omega_2$. Their duals $\hat{\alpha}_k$ and $\hat{\omega}_j$ coincide with α_k and ω_j. The root system $\Delta=\{\pm\alpha_1,\pm\alpha_2\}$ geometrically represents the vertices of a square of a side length $2\sqrt{2}$.

B. Weyl group orbits

Suppose $\lambda=a\omega_1+b\omega_2\in P$. Then the Weyl group orbit W_λ is given by

$$W_\lambda\equiv W_{(a,b)}=\begin{cases}\{(0,0)\}, & \text{if } a,b=0,\\ \{\pm(a,0)\}, & \text{if } a\neq 0 \text{ and } b=0,\\ \{\pm(0,b)\}, & \text{if } a=0 \text{ and } b\neq 0,\\ \{\pm(a,b),\pm(a,-b)\}, & \text{if } a,b\neq 0.\end{cases}$$

C. C-functions

The C-functions of $A_1\times A_1$, with $\lambda=a\omega_1+b\omega_2$ and $z=x\omega_1+y\omega_2$, are products of two A_1 C-functions,

$$\Omega_{a.b}(x,y)=\Omega_a(x)\Omega_b(y).$$

They are the following:

$$\Omega_{(0,0)}(x,y)=1,$$

$$\Omega_{(a,0)}(x,y) = 2\cos(\pi a x),$$

$$\Omega_{(0,b)}(x,y) = 2\cos(\pi b y),$$

$$\Omega_{(a,b)}(x,y) = 4\cos(\pi a x)\cos(\pi b y). \tag{5.1}$$

The C-functions, normalized as in (4.8), are written for all $a,b \in \mathbb{Z}^{\geqslant 0}$ in one expression,

$$\Phi_{(a,b)}(x,y) = 4\cos(\pi a x)\cos(\pi b y).$$

D. Orthogonality of C-functions

The fundamental region of $A_1 \times A_1$ here is

$$F(A_1 \times A_1) = \{x\omega_1 + y\omega_2 \mid 0 \leqslant x,y \leqslant 1\},$$

its vertices being 0, ω_1, ω_2, and ω_1, ω_2 (see Fig. 1). Hence its sides have length $|\omega_1| = |\omega_2| = 1/\sqrt{2}$.

Orthogonality of the functions is readily verified directly,

$$\int_F \Omega_{(a,b)}(x,y)\Omega_{(c,d)}(x,y)\mathrm{d}F = \frac{1}{2}\int_0^1 \mathrm{d}x \int_0^1 \Omega_{(a,b)}(x,y)\Omega_{(c,d)}(x,y)\mathrm{d}y$$
$$= \begin{cases} 0, & \text{if } a \neq c \text{ and } b \neq d, \\ \frac{1}{2}, & \text{if } a = b = c = d = 0, \\ 1, & \text{if } a = c > 0 \text{ and } b = d = 0, \\ & \text{or } a = c = 0 \text{ and } b = d > 0, \\ 2, & \text{if } a = b > 0 \text{ and } c = d > 0. \end{cases} \tag{5.2}$$

E. Laplace operator

The Laplace operator in this case is

$$L = 2\partial_{xx} + 2\partial_{yy}.$$

The C-functions are its eigenfunctions, and

$$L\Omega_\lambda = -4\pi^2\langle\lambda|\lambda\rangle\Omega_\lambda = -2\pi^2(a^2+b^2)\Omega_\lambda,$$

where the scalar product for $\lambda = a\omega_1 + b\omega_2$ is computed using the inverse Cartan matrix C^{-1}:

$$\langle\lambda|\lambda\rangle = (a\ b)C^{-1}\begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{2}(a^2+b^2).$$

VI. THE CASE C_2

A. Roots and weights

Relative length and angles of the simple roots of C_2 are given by

$$\langle\alpha_1|\alpha_2\rangle = -1, \quad \langle\alpha_1|\alpha_1\rangle = 1, \quad \langle\alpha_2|\alpha_2\rangle = 2.$$

The Cartan matrix and its inverse are

$$C=\begin{pmatrix}2 & -1\\ -2 & 2\end{pmatrix} \quad \text{and } C^{-1}=\begin{pmatrix}1 & \frac{1}{2}\\ 1 & 1\end{pmatrix}.$$

Consequently,

$$\alpha_1=2\omega_1-\omega_2,\quad \omega_1=\alpha_1+\tfrac{1}{2}\alpha_2,\quad \hat{\alpha}_1=2\alpha_1,\quad \hat{\omega}_1=\hat{\alpha}_1+\hat{\alpha}_2,$$

$$\alpha_2=-2\omega_2+2\omega_2,\quad \omega_2=\alpha_1+\alpha_2,\quad \hat{\alpha}_2=\alpha_2,\quad \hat{\omega}_2=\tfrac{1}{2}\hat{\alpha}_1+\hat{\alpha}_2.$$

The root system $\Delta=\{\pm\alpha_1,\pm\alpha_2,\pm(\alpha_1+\alpha_2),\pm(2\alpha_1+\alpha_2)\}$ geometrically represents the vertices and midpoints of a square. The highest root is $\xi_h=2\alpha_1+\alpha_2$.

B. Weyl group orbits

Let $\lambda=a\omega_1+b\omega_2\in P^+$. Then the Weyl group orbit $W_\lambda\equiv W_{(a,b)}$ contains one, four, or eight points. More precisely,

$$W_{(a,b)}=\begin{cases}\{(0,0)\}, & \text{if } a=b=0,\\ \{\pm(a,0),\pm(-a,a)\}, & \text{if } a\neq 0 \text{ and } b=0,\\ \{\pm(0,b),\pm(2b,-b)\}, & \text{if } a=0 \text{ and} b\neq 0,\\ \{\pm(a,b),\pm(-a,a+b),\pm(a+2b,-b),\pm(a+2b,-a-b)\}, & \text{if } a,b\neq 0.\end{cases}$$

In particular, $\Delta=W_{(2,0)}\cup W_{(0,1)}$.

C. C-functions

The C-functions of C_2, with $\lambda=a\omega_1+b\omega_2$ and $z=x\hat{\omega}_1+y\hat{\omega}_2$, are the following:

$$\Omega_{(0,0)}(x,y)=1,$$

$$\Omega_{(a,0)}(x,y)=2\cos(\pi ay)+2\cos(\pi a(2x+y)),$$

$$\Omega_{(0,b)}(x,y)=2\cos(2\pi bx)+2\cos(2\pi b(x+y)),$$

$$\begin{aligned}\Omega_{(a,b)}(x,y)&=2\cos(\pi(2bx+(a+2b)y))+2\cos(\pi((2a+2b)x+(a+2b)y))\\ &\quad+2\cos(\pi(ay+(2a+2b)x))+2\cos(\pi(2bx-ay)),\quad \text{where } a,b>0.\end{aligned}\tag{6.1}$$

C-functions, normalized as in (4.8), are written for all $a,b\in\mathbb{Z}^{\geqslant 0}$ in one expression,

$$\begin{aligned}\Phi_{(a,b)}(x,y)&=2\cos(\pi(2bx+(a+2b)y))+2\cos(\pi((2a+2b)x+(a+2b)y))\\ &\quad+2\cos(\pi(ay+(2a+2b)x))+2\cos(\pi(2bx-ay)).\end{aligned}$$

D. Decomposition of products of C-functions

Products of the C-functions decompose into sums of C-functions (4.10). For example, one has

$$\Omega_{(0,a)}\Omega_{(0,b)}=\Omega_{(0,a+b)}+\Omega_{(2a,b-a)}+\Omega_{(0,b-a)},\quad \text{when } a<b,$$

$$\Omega_{(0,a)}\Omega_{(b,0)}=\Omega_{(b,a)}+\Omega_{(2a-b,b-a)},\quad \text{when } a<b<2a,$$

$$\Omega_{(a,0)}\Omega_{(0,b)}=\Omega_{(a,b)}+\Omega_{(a,b-2a)},\quad \text{when } b>2a.$$

It is possible to build up recursively the higher C-functions, starting from the lowest three, namely, $\Omega_{(0,0)}, \Omega_{(1,0)}$, and $\Omega_{(0,1)}$,

$$\Omega_{(1,1)} = \Omega_{(1,0)}\Omega_{(0,1)} - 2\Omega_{(1,0)},$$

$$\Omega_{(2,0)} = \Omega_{(1,0)}\Omega_{(1,0)} - 4\Omega_{(0,0)} - 2\Omega_{(0,1)},$$

$$\Omega_{(0,2)} = \Omega_{(0,1)}\Omega_{(0,1)} - 4\Omega_{(0,0)} - 2\Omega_{(2,0)},$$

$$\Omega_{(2,1)} = \Omega_{(0,1)}\Omega_{(2,0)} - 2\Omega_{(0,1)},$$

$$\Omega_{(3,0)} = \Omega_{(1,0)}\Omega_{(2,0)} - \Omega_{(1,0)} - \Omega_{(1,1)},$$

$$\Omega_{(1,2)} = \Omega_{(0,1)}\Omega_{(1,1)} - 2\Omega_{(1,0)} - \Omega_{(1,1)} - 2\Omega_{(3,0)},$$

$$\cdots .$$

E. Orthogonality of C-functions

The fundamental region $F(C_2)$ is defined as follows:

$$F(C_2) = \{x\hat{\omega}_1 + y\hat{\omega}_2 \mid x,y \geqslant 0 \text{ and } 2x + y \leqslant 1\}.$$

Therefore, its vertices are 0, $\hat{\omega}_1/2$, and $\hat{\omega}_2$. Geometrically it is a triangle with angles $\pi/2, \pi/4$, and $\pi/4$ (see Fig. 1).

Orthogonality of C-functions of C_2 can be verified, if somewhat laboriously, by using (6.1) in (4.15),

$$\int_F \Omega_{(a,b)}(x,y)\Omega_{(c,d)}(x,y)\mathrm{d}F = \int_0^{\frac{1}{2}} \mathrm{d}x \int_0^{1-2x} \Omega_{(a,b)}(x,y)\Omega_{(c,d)}(x,y)\mathrm{d}y$$
$$= \begin{cases} 0, & \text{if } a \neq c \text{ and } b \neq d, \\ \frac{1}{4}, & \text{if } a = b = c = d = 0, \\ 1, & \text{if } a = c > 0 \text{ and } b = d = 0, \\ & \text{or } a = c = 0 \text{ and } b = d > 0, \\ 2, & \text{if } a = c > 0 \text{ and } b = d > 0. \end{cases} \tag{6.2}$$

In particular, we have for any $(a,b) \neq (0,0)$ and $(c,d) = (0,0)$

$$\int_F \Omega_{(a,b)}(x,y)\mathrm{d}F = 0.$$

F. Laplace operator

The Laplace operator (4.17) specializes to C_2 as follows:

$$L = (\alpha_1\partial_x + \alpha_2\partial_y)^2 = \partial_{xx} - 2\partial_{xy} + 2\partial_{yy}.$$

Applying L to C-functions, we see that they are its eigenfunctions,

TABLE II. Examples of the decomposition of C-functions of C_2 (left column) into C-functions of the maximal subgroup $A_1\times A_1^{\subset}$ (middle column) and of the maximal subjoint group $A_1\times A_1^{<}$ (right column).

C_2	$A_1\times A_1^{\subset}$	$A_1\times A_1^{<}$
$\Omega_{(0,0)}$	$\Omega_{(0,0)}$	$\Omega_{(0,0)}$
$\Omega_{(1,0)}$	$\Omega_{(1,0)}+\Omega_{(0,1)}$	$\Omega_{(1,1)}$
$\Omega_{(0,1)}$	$\Omega_{(1,1)}$	$\Omega_{(2,0)}+\Omega_{(0,2)}$
$\Omega_{(2,0)}$	$\Omega_{(2,0)}+\Omega_{(0,2)}$	$\Omega_{(2,2)}$
$\Omega_{(1,1)}$	$\Omega_{(2,1)}+\Omega_{(1,2)}$	$\Omega_{(3,1)}+\Omega_{(1,3)}$
$\Omega_{(0,2)}$	$\Omega_{(2,2)}$	$\Omega_{(4,0)}+\Omega_{(0,4)}$
$\Omega_{(3,0)}$	$\Omega_{(3,0)}+\Omega_{(0,3)}$	$\Omega_{(3,3)}$
$\Omega_{(2,1)}$	$\Omega_{(3,1)}+\Omega_{(1,3)}$	$\Omega_{(4,2)}+\Omega_{(2,4)}$
$\Omega_{(1,2)}$	$\Omega_{(3,2)}+\Omega_{(2,3)}$	$\Omega_{(5,1)}+\Omega_{(1,5)}$
$\Omega_{(0,3)}$	$\Omega_{(3,3)}$	$\Omega_{(6,0)}+\Omega_{(0,6)}$
$\Omega_{(4,0)}$	$\Omega_{(4,0)}+\Omega_{(0,4)}$	$\Omega_{(4,4)}$

$$L\Omega_\lambda = -4\pi^2\langle\lambda|\lambda\rangle\Omega_\lambda = -2\pi^2(a^2+2ab+2b^2)\Omega_\lambda,$$

where the scalar product $\langle\lambda|\lambda\rangle$ is computed for $\lambda=(a\omega_1+b\omega_2)\equiv(a\ b)$, using the quadrature matrix Q,

$$\langle\lambda|\lambda\rangle = \lambda Q\lambda^T = \frac{1}{2}(a\ b)\begin{pmatrix}1 & 1\\ 1 & 2\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = \frac{1}{2}a^2+ab+b^2.$$

G. The branching rules for C-functions of C_2 to the subgroup $A_1\times A_1$

The problem considered here is to calculate the "branching rules" for C-functions. There are two rather different ways how a semisimple Lie group of rank 2 is related to C_2. In both cases the group is of type $A_1\times A_1$. In order to distinguish the two cases we use the notations $A_1\times A_1^{\subset}$ and $A_1\times A_1^{<}$. The C-functions of C_2 are completely reducible with respect to either of $A_1\times A_1$. The possibility of such reduction is a direct consequence of the corresponding reduction of W orbits.[15]

The first case is the maximal subgroup $A_1\times A_1^{\subset}$ of C_2. Its root system is the subset of long roots of C_2. In the second case, $A_1\times A_1^{<}$ is not a subgroup. It is the maximal subjoint group $A_1\times A_1$ to C_2. Its root system consists of the short roots of C_2. For more about subjoining, see Refs. 18 and 19.

Using the matrices

$$B_1 = \begin{pmatrix}0 & \frac{1}{2}\\ 1 & -\frac{1}{2}\end{pmatrix} \quad \text{and } B_2 = \begin{pmatrix}1 & -1\\ 0 & 1\end{pmatrix}$$

to transform the variables in the C-functions of C_2, we can obtain the decompositions of C_2 C-functions into C-functions of its subgroup and subjoint group, demonstrated in Table II. The general rules for such decompositions are given by

$$[\Omega_{(a,b)}]_{C_2} = [\Omega_{(a+b,b)} + (1-\delta_{a,0})\Omega_{(b,a+b)}]_{A_1\times A_1^{\subset}} \tag{6.3}$$

and

$$[\Omega_{(a,b)}]_{C_2} = [\Omega_{(a+2b,a)} + (1-\delta_{b,0})\Omega_{(a,a+2b)}]_{A_1\times A_1^{<}}. \tag{6.4}$$

VII. DISCRETIZATION OF TWO-DIMENSIONAL TRANSFORMS

In this section we describe all the necessary tools, which allow one to decompose a function $f(s)$, given by its values on points s of certain two-dimensional grids F_M, $M=1,2,\ldots<\infty$, in terms of finite series of C-functions. Such decomposition is possible, due to the discrete orthogonality of C-functions on the points of F_M, i.e., its coefficients can be computed.

A. Equidistant grids of points in the fundamental region

The fundamental region F can be used to tile the entire plane by its copies, $W^{\text{aff}}F=\mathbb{R}^2$. Our next task is to describe grids F_M of discrete points in F of any density, specified by a positive integer M, which extends into a lattice with the tiling of $\mathbb{R}^2$ by copies of F.

The points s of F_M are conveniently described in barycentric coordinates. That is, by three non-negative integers, $[s_0,s_1,s_2]$. A point s belongs the grid F_M, provided

$$s=\frac{s_1}{M}\hat{\omega}_1+\frac{s_2}{M}\hat{\omega}_2, \quad \text{where } s_0,s_1,s_2\in\mathbb{Z}^{\geqslant 0} \text{ and } M=s_0+q_1s_1+q_2s_2>0. \tag{7.1}$$

Here q_1 and q_2 are positive integers, specific for each Lie group. They are the coefficients of the highest root of Δ in α basis. Equivalently, we write

$$F_M\overset{\text{def}}{=}\left\{\left(\frac{s_1}{M},\frac{s_2}{M}\right)\mid s_0,s_1,s_2\in\mathbb{Z}^{\geqslant 0},s_0+q_1s_1+q_2s_2=M>0\right\}. \tag{7.2}$$

B. Bilinear form on F_M

Given the set of points F_M in the fundamental region, and two functions $f(s)$ and $h(s)$, given by their values at the points $s\in F_M$, one defines a Hermitian form as follows:[3]

$$\langle f|h\rangle_M\overset{\text{def}}{=}\sum_{s\in F_M}c_sf(s)\overline{h(s)}. \tag{7.3}$$

The line over $h(s)$ stands for complex conjugation. The coefficients c_s are positive integer numbers for each Lie group. They are given below for the groups of rank 2, for a general case, see Ref. 3.

C. Discrete orthogonality of C-functions

For a fixed value of $M\in\mathbb{N}$, the discrete orthogonality of C-functions on $F_M\subset F$ is crucial for this study,

$$\langle\Phi_{(a,b)}|\Phi_{(a',b')}\rangle_M=\sum_{s\in F_M}c_s\Phi_{(a,b)}(s)\overline{\Phi_{(a',b')}(s)}=\delta_{a,a'}\delta_{b,b'}\langle\Phi_{(a,b)}|\Phi_{(a,b)}\rangle_M. \tag{7.4}$$

The orthogonality (7.4) holds for $\Phi_{(a,b)},\Phi_{(a',b')}$ from a finite subset S_M of C-functions.

In general, for all cases of rank 2, we can construct (infinitely many) such subsets S_M by using the following:

$$S_M\overset{\text{def}}{=}\left\{\Phi_{(a,b)}|\left(\frac{b}{M},\frac{a}{M}\right)=r\left(\frac{s_1}{M},\frac{s_2}{M}\right),\ \text{where}\left(\frac{s_1}{M},\frac{s_2}{M}\right)\in F_M \text{ and } r\in W^{\text{aff}}\right\}. \tag{7.5}$$

As an easy example, one can obtain the set of the lowest $\Phi_{(a,b)}\in S_M$, by taking $r=1$ and a,b that satisfy the inequality

$$aq_2+bq_1\leqslant M\Rightarrow\Phi_{(a,b)}\in S_M, \tag{7.6}$$

where q_1,q_2 are the same as in (4.11).

From the definition of S_M it is easy to see that

$$|S_M| = |F_M|.$$

The numbers $\langle \Phi_{(a,b)} | \Phi_{(a,b)} \rangle_M$ in (7.4) take only a few integer values for each M. Subsequently, we will provide them for all $0 \leqslant a,b < \infty$, for all the cases considered in this paper.

D. Decomposition into C-functions and continuous extension

A function $f(s)$, with known values on points of the grid F_M, can be decomposed as follows:

$$f(s) = \sum_{\Phi_{(a,b)} \in S_M} d_{(a,b)} \Phi_{(a,b)}(s), \quad s \in F_M. \tag{7.7}$$

Orthogonality (7.4) makes it possible to compute the coefficients $d_{(a,b)}$ from

$$d_{(a,b)} = \frac{\langle f | \Phi_{(a,b)} \rangle_M}{\langle \Phi_{(a,b)} | \Phi_{(a,b)} \rangle_M}, \quad \text{where } \langle f | \Phi_{(a,b)} \rangle_M = \sum_{s \in F_M} c_s f(s) \overline{\Phi_{(a,b)}(s)}. \tag{7.8}$$

After $d_{(a,b)}$ have been calculated, one can replace s in (7.7) by the continuous variables x and y,

$$f_{\text{cont}}(x,y) \overset{\text{def}}{=} \sum_{\Phi_{(a,b)} \in S_M} d_{(a,b)} \Phi_{(a,b)}(x,y), \quad x,y \in \mathbb{R}. \tag{7.9}$$

The function $f_{\text{cont}}(x,y)$ is the continuous extension of the decomposition (7.7). Both functions coincide at the points $(x,y) = (s_1/M, s_2/M) = s \in F_M$.

E. Discretization in the case of $A_1 \times A_1$

The fundamental region in the case of $A_1 \times A_1$ is a Cartesian product of two fundamental regions of A_1. It forms a square described by the following:

$$F = \{ x\omega_1 + y\omega_2 \mid 0 \leqslant x,y \leqslant 1 \}.$$

A square lattice F_M of order M is a Cartesian product of two lattices $F_M(A_1)$, built on F the following way:

$$F_M \overset{\text{def}}{=} \left\{ \left(\frac{s_1}{M}, \frac{s_2}{M} \right) \mid s_1, s_2 \in \mathbb{Z}^{\geqslant 0}, \quad s_1, s_2 \leqslant M \in \mathbb{N} \right\}.$$

Coefficients c_s are in this case

$$c_s \equiv c_{(s_1/M, s_2/M)} = \begin{cases} 1, & \text{if } s_2 = s_2 = 0, \\ & \quad \text{or } s_1 = s_2 = M, \\ & \quad \text{or } s_1 = 0 \text{ and } s_2 = M, \\ & \quad \text{or } s_1 = M \text{ and } s_2 = 0, \\ 2, & \text{if } s_1 = 0 \text{ and } 0 < s_2 < M, \\ & \quad \text{or } s_2 = 0 \text{ and } 0 < s_1 < M, \\ & \quad \text{or } s_1 = M \text{ and } 0 < s_2 < M, \\ & \quad \text{or } s_2 = M \text{ and } 0 < s_1 < M, \\ 4, & \text{if } 0 < s_1, s_2 < M. \end{cases}$$

The C-functions are orthogonal,

$$\langle \Phi_{(a,b)} | \Phi_{(a',b')} \rangle_M = 0, \quad \text{if } a \neq a' \text{ and } b \neq b',$$

otherwise, for the set of the lowest pairwise orthogonal normalized C-functions,

$$\langle\Phi_{(a,b)}|\Phi_{(a,b)}\rangle_M = 16M^2 \times \begin{cases} 1, & \text{if } 0 < a,b < M, \\ 2, & \text{if } 0 < a < M \text{ and } b = 0, \\ & \text{or } a = 0 \text{ and } 0 < b < M, \\ & \text{or } 0 < a < M \text{ and } b = M, \\ & \text{or } a = M \text{ and } 0 < b < M, \\ 4, & \text{if } a = b = 0, \\ & \text{or } a = 0 \text{ and } b = M, \\ & \text{or } a = M \text{ and } b = 0, \\ & \text{or } a = b = M, \end{cases}$$

with the higher C-functions repeating the values of the lowest ones. (See Fig. 2.)

For example, F_2 consists of the nine points given as $[s_1,s_2]=(s_1/2,s_2/2)$,

$$[0,0]=(0,0), \quad [0,1]=\left(0,\tfrac{1}{2}\right), \quad [0,2]=(0,1),$$

$$[1,0]=\left(\tfrac{1}{2},0\right), \quad [1,1]=\left(\tfrac{1}{2},\tfrac{1}{2}\right), \quad [1,2]=\left(\tfrac{1}{2},1\right), \tag{7.10}$$

$$[2,0]=(1,0), \quad [2,1]=\left(1,\tfrac{1}{2}\right), \quad [2,2]=(1,1),$$

while F_1 has only four points,

$$[0,0]=(0,0), \quad [0,1]=(0,1), \quad [1,0]=(1,0), \quad [1,1]=(1,1).$$

F. Discretization in the case of C_2

The highest root of C_2 is $2\alpha_1+\alpha_2$. Therefore,

$$F_M \overset{\text{def}}{=} \left\{ \left(\frac{s_1}{M}, \frac{s_2}{M} \right) \mid s_0,s_1,s_2 \in \mathbb{Z}^{\geqslant 0}, \quad s_0 + 2s_1 + s_2 = M > 0 \right\}.$$

Vertices of F are (0,0), (0,1), $\left(\frac{1}{2},0\right)$, relative to $\hat{\omega}$ basis. (See Fig. 3.) Coefficients c_s are in this case,

$$c_s \equiv c_{(s_1/M,s_2/M)} = \begin{cases} 1, & \text{if } s_1 = 0 \text{ and } s_2 = 0, \\ & \text{or } s_1 = 0 \text{ and } s_2 = M, \\ 2, & \text{if } s_1 = 0 \text{ and } s_2 = \frac{M}{2}, \\ 4, & \text{if } s_1 = 0 \text{ and } 0 < s_2 < M, \\ & \text{or } s_2 = 0 \text{ and } 0 < s_1 < M, \\ & \text{or } s_1,s_2 > 0 \text{ and } 2s_1 + s_2 = M, \\ 8, & \text{if } s_1,s_2 > 0 \text{ and } 2s_1 + s_2 < M. \end{cases} \tag{7.11}$$

The discrete orthogonality,

$$\langle\Phi_{(a,b)}|\Phi_{(a',b')}\rangle_M = 0, \quad \text{if } a \neq a' \text{ and } b \neq b',$$

otherwise, for the set of the lowest pairwise orthogonal normalized C-functions,

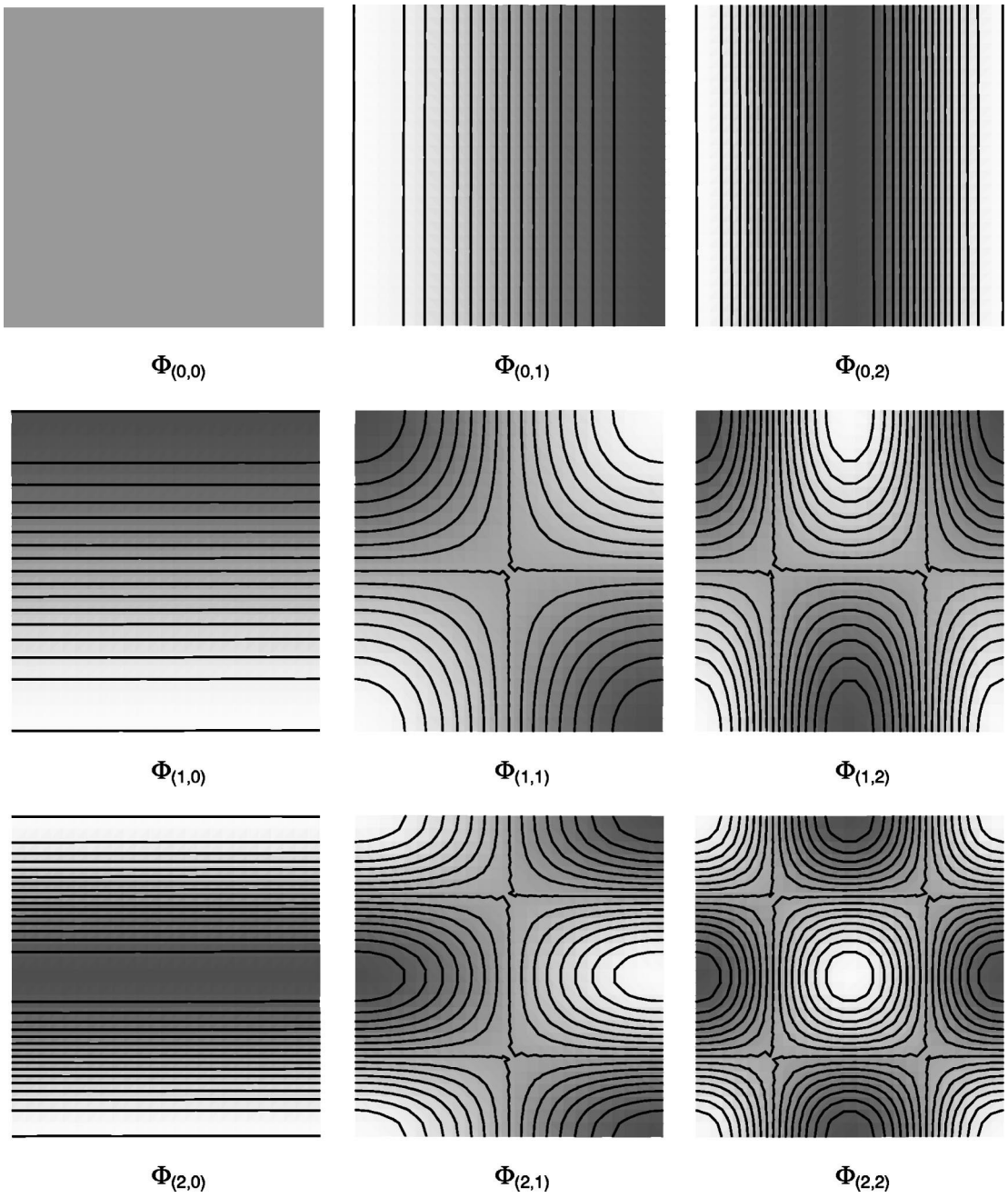

FIG. 2. The set of nine lowest pairwise orthogonal normalized C-functions of $A_1 \times A_1$ for the grid F_2.

$$\langle \Phi_{(a,b)} | \Phi_{(a,b)} \rangle_M = 16M^2 \times \begin{cases} 1, & \text{if } 0 < a,b \text{ and } a + 2b < M, \\ 2, & \text{if } 0 < a < M \text{ and } b = 0, \\ & \quad \text{or } a = 0 \text{ and } 0 < 2b < M, \\ & \quad \text{or } 0 < a,b \text{ and } a + 2b = M, \\ 4, & \text{if } a = 0 \text{ and } 2b = M, \\ 8, & \text{if } a = b = 0, \\ & \quad \text{or } a = M \text{ and } b = 0, \end{cases}$$

with the higher C-functions repeating the values of the lowest ones. (See Fig. 4.)

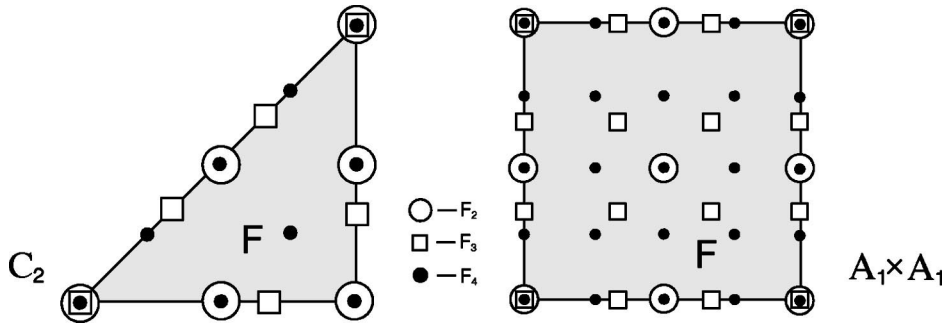

FIG. 3. The lattice points of F_2, F_3, and F_4 in the fundamental region F for the cases C_2 and $A_1 \times A_1$.

For example, F_3 consists of the six points given as $[s_0, s_1, s_2] = (s_1/M, s_2/M)$,

$$[1,0,0] = (0,0), \quad [0,0,1] = (0,1), \quad [1,1,0] = \left(\tfrac{1}{3}, 0\right),$$
$$[0,1,1] = \left(\tfrac{1}{3}, \tfrac{1}{3}\right), \quad [1,0,2] = \left(0, \tfrac{2}{3}\right), \quad [2,0,1] = \left(0, \tfrac{1}{3}\right), \tag{7.12}$$

while F_2 has only four points,

$$[1,0,0] = (0,0), \quad [0,0,1] = (0,1), \quad [0,1,0] = \left(\tfrac{1}{2}, 0\right), \quad [1,0,1] = \left(0, \tfrac{1}{2}\right).$$

As an example, the values of C_2 normalized orbit functions on the grid F_3 are given in Table III.

VIII. MOTIVATING EXAMPLES

Comparison of expansions of into series of both groups considered here, as well as the two additional groups of Ref. 1, will require further study. Related questions are illustrated by the following examples.

There are two examples shown in this section, involving decomposition of the same function $f(x,y)$ into series of C-functions of $A_1 \times A_1$ and C_2. Goal of the examples is (i) to illustrate discrete decomposition of a given function followed by the continuous extension, and (ii) to compare the continuous extensions in both cases.

We choose for $f(x,y)$ the square step function with sharp edges,

$$f(x,y) = \begin{cases} 1 & \text{for } 0.30 < x < 0.45, \quad \text{and } 0.05 < y < 0.20, \\ 0 & \text{elsewhere in } F. \end{cases} \tag{8.1}$$

In order to make the comparison, we set up the vertices of the two fundamental regions as follows (relative to an orthonormal basis):

$$F(A_1 \times A_1) = \left\{(0,0), \left(\tfrac{1}{2}, 0\right), \left(0, \tfrac{1}{2}\right), \left(\tfrac{1}{2}, \tfrac{1}{2}\right)\right\}, \tag{8.2}$$

$$F(C_2) = \left\{(0,0), \left(\tfrac{1}{2}, 0\right), \left(\tfrac{1}{2}, \tfrac{1}{2}\right)\right\}. \tag{8.3}$$

Thus $F(C_2)$ is exactly half of $F(A_1 \times A_1)$ with three vertices in common. In order to have the grid of the same density in both regions, one must make sure that there is the same number of points along the edges of sides of F adjacent to angle $\pi/2$.

Suppose M is fixed. Then each side of $F(A_1 \times A_1)$ contains $M+1$ points each. For a given M', the $F(C_2)$-edge $(0,0)$, $\left(\tfrac{1}{2}, 0\right)$ contains $[M'/2]$ points, where $[M'/2]$ stands for the integer part of $M'/2$. Consequently, to have the same density of the grid in both cases, we have to have $M+1 = [M'/2]$.

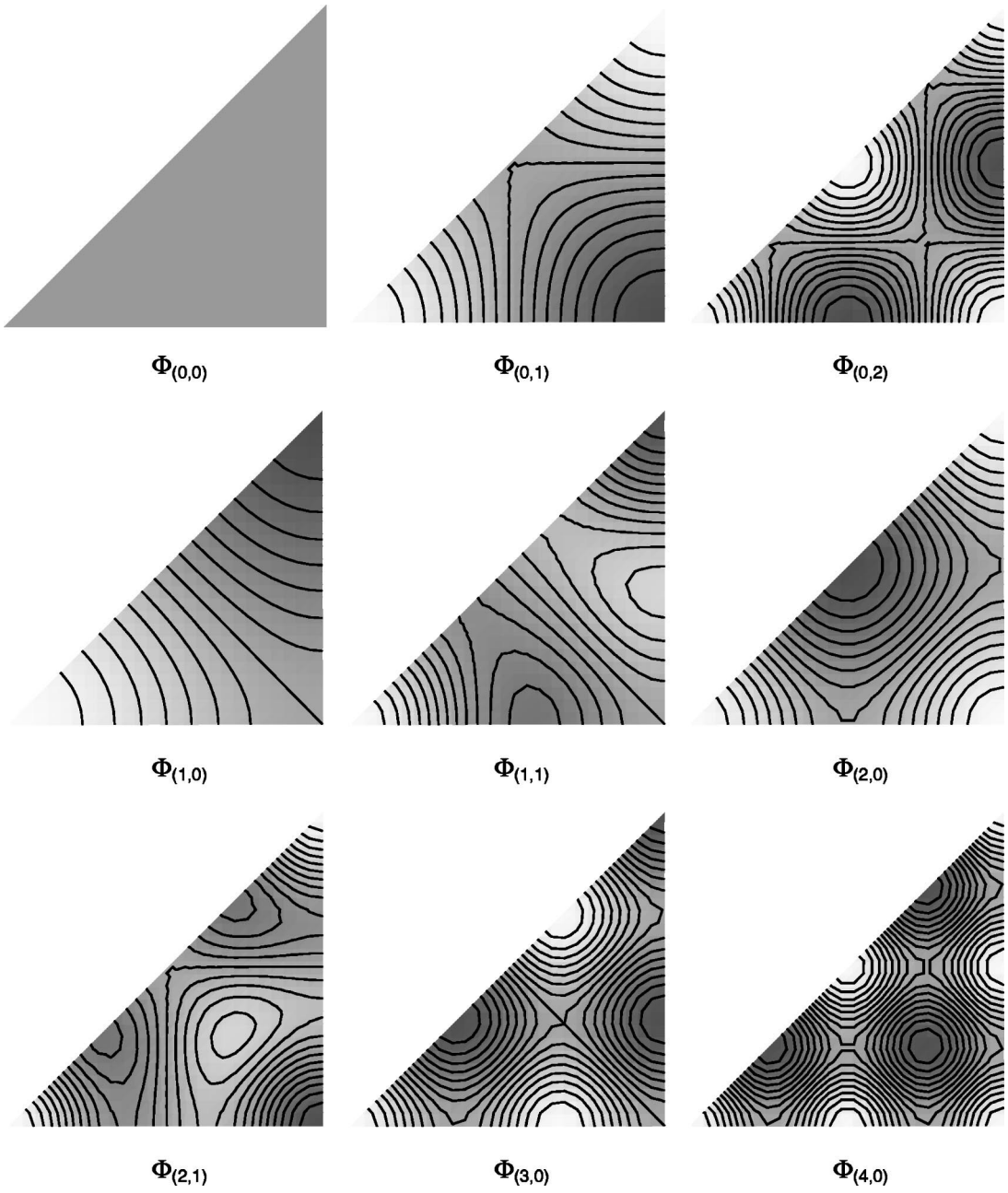

FIG. 4. The set of nine lowest pairwise orthogonal normalized C-functions of C_2 for the grid F_4.

Figures 5 and 6 contain results of our two examples. The same function $f(x,y)$ of (8.1) is placed into the fundamental regions F of the two groups, their values are sampled at the points s of the grids F_M (7.2) and taken as our digital data $f(s)$. Then the functions are expanded (7.7) into C-functions of $A_1 \times A_1$ and of C_2 on the corresponding grid F_M, i.e., expansion coefficients are calculated (7.8). After that, continuous extensions of the discrete expansions of $f(s)$ are made (7.9) by replacing the C-functions of the discrete argument s in the expansions by the same functions of the continuous argument, while keeping the expansion coefficients unchanged. Each figure shows the function $f_{\text{cont}}(x,y)$ resulting from the continuous extension of discrete expansions. More precisely, four different continuous extensions are shown in each figure. They differ by the densities

TABLE III. Values of several normalized C-functions of C_2 at the points of the grid F_3. Note that only the first six C-functions are pairwise orthogonal. The higher ones repeat the values of the lowest six. The c_s are the coefficients from ((7.11)).

s	$(0, 0)$	$(0, \frac{1}{3})$	$(0, \frac{2}{3})$	$(\frac{1}{3}, 0)$	$(\frac{1}{3}, \frac{1}{3})$	$(0, 1)$
$\Phi_{(0,0)}(s)$	8	8	8	8	8	8
$\Phi_{(0,1)}(s)$	8	2	2	−4	−4	8
$\Phi_{(1,0)}(s)$	8	4	−4	2	−2	−8
$\Phi_{(1,1)}(s)$	8	−2	2	−4	4	−8
$\Phi_{(2,0)}(s)$	8	−4	−4	2	2	8
$\Phi_{(3,0)}(s)$	8	−8	8	8	−8	−8
$\Phi_{(2,1)}(s)$	8	−4	−4	2	2	8
$\Phi_{(3,1)}(s)$	8	−2	2	−4	4	−8
$\Phi_{(1,2)}(s)$	8	4	−4	2	−2	−8
$\Phi_{(0,2)}(s)$	8	2	2	−4	−4	8
$\Phi_{(0,3)}(s)$	8	8	8	8	8	8
c_s	1	4	4	4	4	1

of the grid F_M, namely $M=4$, 8, 16, and 32, from which the continuous extension is made. For the same value of M, the densities of grids of $A_1 \times A_1$ and C_2 are the same. The points of the grids are not shown in the figures.

Inspecting and comparing the two figures, one readily observes the following:

(i) Increasing density of the grid, i.e., increasing the value of M, makes the continuous extension to match more closely the given model function $f(x,y)$ of (8.1).

(ii) Quality of the extension, i.e., the match between the continuous extension $f_{\text{cont}}(x,y)$ and the original function $f(x,y)$, is comparable for the same density of the grid in both cases, though C_2 expansion may be slightly superior, as noticeable by comparing the two at $M=32$.

The observations have important consequences.

The number of points of $F_M(A_1 \times A_1)$ and $F_M(C_2)$ are approximately in the ratio 2:1, due to the ration of the areas of the fundamental regions (see Fig. 1) and to the equal density of the points in both cases.

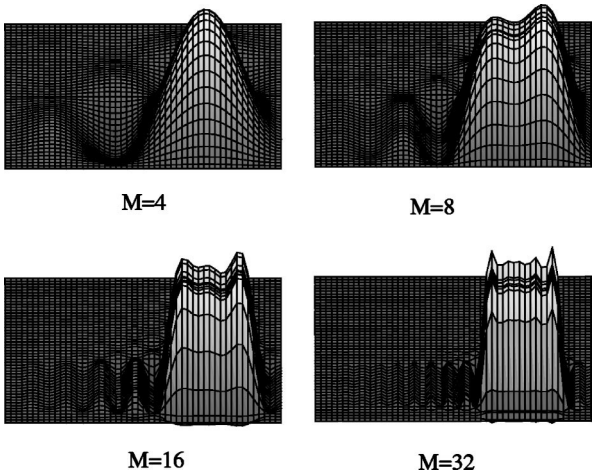

FIG. 5. Decomposition and continuous extension of a square step function placed in the fundamental region of $A_1 \times A_1$ on the grids of orders $M=4$, 8, 16, and 32.

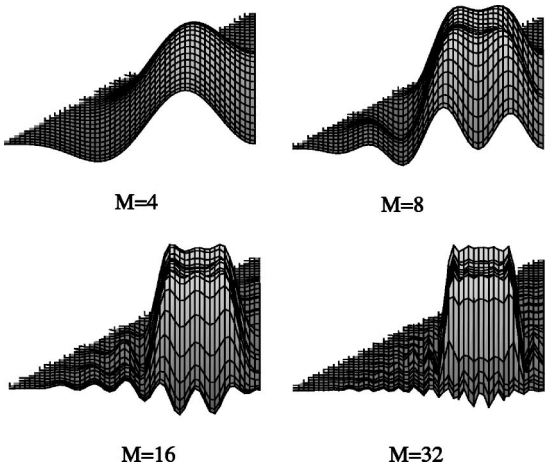

FIG. 6. Decomposition and continuous extension of a square step function placed in the fundamental region of C_2 on the grids of orders $M=4$, 8, 16, and 32.

The number of terms in the expansions equals the number of points in the corresponding F_M. Hence the C_2 expansions are half as long as those of $A_1\times A_1$ for the same quality of continuous expansion.

Consequently, as much as one can draw a conclusion from an example of using only one function $f(x,y)$, it appears that the C_2 expansions are considerably more efficient than the $A_1\times A_1$ ones.

In a way of objection to the conclusion just made, one may point out that C-functions of C_2 are formed as sums of twice as many exponential functions (up to eight), in comparison with C-functions of $A_1\times A_1$ (sums of up to four exponentials). Consequently, computing the values of more complicated C-functions of C_2 on half as many points of its grid, may require comparable computational efforts to those for the simpler C-functions of $A_1\times A_1$ on larger number of points. Although such an objection is undoubtedly true, it is hardly pertinent. Indeed, in any extensive computations of the expansions, the values of C-functions at the grid points would be calculated in advance, and used as a look-up table during the actual expansions. Size of such a look-up table is given by the number of points in F_M, and by, what is the same, the number of discretely orthogonal C-functions in the set S_M. Moreover, the same table should be used for expansion of any function on the same grid.

IX. CONCLUDING REMARKS

(1) In general terms, the families of C- and S-functions, based on any compact semisimple Lie group, have all the properties of traditional special functions, and more.[12] Indeed, discretization, as demonstrated in this paper and generally in Ref. 3, is not a standard feature of traditional special functions.

(2) The application, which mostly motivated our interest in rank-2 group transforms, like the two considered in this paper, is the decomposition of functions sampled on two-dimensional lattices into finite sums of discretized C-functions. The remaining two cases, the groups A_2 and G_2, are considered in a similar manner in Ref. 1.

(3) Recently it was recognized[4] that the continuous extension of the decompositions on the grid F_M is particularly useful. Once coefficients of a discrete expansion are found, one replaces in the expansion the C-functions, sampled on F_M, by their continuous versions. Unlike similar extension of conventional Fourier expansions, continuous extensions of C-function expansions smoothly interpolate between grid points of F_M. This property is likely to turn out extremely useful for various methods of image enhancement and data compression.[4,8]

(4) In parallel with cosine transform, there exists a sine transform (see for example, Ref. 20). Similarly, as C-function transforms generalize cosine transform to any compact semisimple

Lie group, the sine transforms generalize as S-function transforms[2] (continuous and discrete). Most of the properties of C-transforms carry over as properties of S-transforms, one of the noticeable differences being their behaviors at the boundary of F.

(5) In our opinion, independent interest represents the construction of the lattices in $\mathbb{R}^n$ through the grids in F_M, even without the problem of expansion of functions on F,. The flexibility and uniformity of its construction for any density specified by just one natural number M, should be exploited in other applications. Let us also single out the fact that the grid F_M, for any M, is group-theoretically defined. It represents an Abelian subgroup of the maximal torus generated by the elements of order M. Each point $s \in F_M$ is a representative of a conjugacy class of elements of finite order in the Lie group.

(6) Among problems of interest related to this paper and to Refs. 1 and 2, one can point out the following ones:

(i) The fact, that the C- and S-functions are the eigenfunctions of the Laplace operator with known eigenvalues and known value at the boundary of F, should find a number of useful applications in physics. That property, along with their relative simplicity, distinguishes them from the irreducible characters. Equally useful should prove to be the fact that they form bases for lattice problems.

(ii) Also, we are interested in the question of identification of the types of functions on F, which are most efficiently decomposed into C- and/or S-function series for each of the four semisimple Lie groups of rank 2. Examples of comparison are given in Sec. VIII and in Ref. 1, but more conclusive and more definite results would be interesting.

(iii) Practical processing of two-dimensional digital data often involves grids with millions of points. The question of computational efficiency in large scale applications needs to be investigated. Furthermore, rational coordinates of points $s \in F_M$ make C-functions into linear combinations of Mth roots of unity. It was shown in Ref. 3 that some, even very large, decomposition problems can be reformulated and done entirely in integers, for example, Ref. 14.

(iv) There exists a similarity to fast Fourier transform, which merits further investigation. Indeed, one has the freedom to work with series of gradually refining grids, for example, $F_2 \subset F_{2^2} \subset \cdots \subset F_{2^k} \subset \cdots$.

(7) Every C- or S-function is a sum of a finite number of exponential functions. In rank 2, that is

$$e^{2\pi i\langle \lambda | z\rangle} = e^{2\pi i(A/|C|)\theta_1 + 2\pi i(B/|C|)\theta_2},$$

where A and B are integers and $|C|$ is the determinant of the corresponding Cartan matrix. The substitution

$$e^{2\pi i(\theta_1/|C|)} \to x, \quad e^{2\pi i(\theta_2/|C|)} \to y$$

transforms any C- and S-function into a polynomial in x and y. Indeed, one gets $e^{2\pi i\langle \lambda | z\rangle} = x^A y^B$.

Thus, C- and S-functions are families of orthogonal polynomials, each related to a particular semisimple Lie group and to a particular W orbit, in as many variables as is the rank of the group.

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Continuous spin representations from group contraction

Abu M. Khan[a] and Pierre Ramond[b]
Institute for Fundamental Theory, Department of Physics, University of Florida, Gainesville, Florida 32611

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We consider how the continuous spin representation (CSR) of the Poincaré group in four dimensions can be generated by dimensional reduction. The analysis uses the front-form little group in five dimensions, which must yield the Euclidean group $E(2)$, the little group of the CSR. We consider two cases, one is the single spin massless representation of the Poincaré group in five dimensions, the other is the infinite component Majorana equation, which describes an infinite tower of massive states in five dimensions. In the first case, the double singular limit $j, R \to \infty$, with j/R fixed, where R is the Kaluza–Klein radius of the fifth dimension, and j is the spin of the particle in five dimensions, yields the CSR in four dimensions. It amounts to the Inönü–Wigner contraction, with the inverse Kaluza–Klein radius as contraction parameter. In the second case, the CSR appears only by taking a triple singular limit, where an internal coordinate of the Majorana theory goes to infinity, while leaving its ratio to the Kaluza–Klein radius fixed. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1897663]

I. INTRODUCTION

As shown in Wigner's classic work[1] in four dimensions, there are four types of irreducible representations of the Poincaré group. Two describe massless and massive elementary particles with definite helicity and spin, respectively. However, nature does not seem to use the other two, one that describes particles with spacelike momenta,[2] tachyons which move faster than the speed of light, and the others that describe massless states with an infinite number of integer or half-odd integer unit-spaced helicities, dubbed by Wigner continuous spin representations (CSRs).

When tachyons occur in field and string theories, it is as symptoms of an unstable theory, a malady whose cure is known, by shifting the vacuum through spontaneous symmetry breaking as in field and string field theory, or by extending to supersymmetry as in string theory.

There is no analogous cure for the CSR, for which the obstacles are indeed formidable, negative norm states, nonlocality, and acausality,[3] and according to Wigner himself,[4] infinite heat capacity of the vacuum.

The bosonic CSR necessarily contains one massless graviton, but accompanied by an infinite tower of massless helicity states. Therefore it should be viewed in the context of theories that extend general relativity, such as M- or string theories, where a naive application of the infinite slope limit to their spectrum leads to an infinite array of massless states with unit-spaced helicities. Like the tachyonic representation, the CSR may also be symptomatic of a diseased theory, but is there a cure for it?

Such considerations merit further studies. In a previous paper,[5] Wigner's bosonic and fermionic CSR in four dimensions were found to be supersymmetric partners of one another. Interestingly, the supersymmetric CSR does not have infinite heat capacity as it cancels between bosons

[a]Electronic mail: amas@phys.ufl.edu
[b]Electronic mail: ramond@phys.ufl.edu

and fermions. We also showed how to generalize them to higher dimensions by using Dirac's front form (also known as light cone) where the CSRs are linked to representations of the Euclidian group in the transverse plane in any dimensions.

The purpose of this paper is to seek CSR's in familiar mathematical structures which contain the Poincaré group in four dimensions: the conformal group SO(4,2), the Poincaré group in higher dimensions, and in the de Sitter and anti-de Sitter groups in five dimensions. The latter require group contraction, introduced by Inönü and Wigner (IW),[6] in order to generate the Euclidean group from the rotation group. We show that, while the CSR do not appear as representations of the conformal group,[7,8] they can be generated from the five-dimensional Poincaré group by a combination of group contraction and Kaluza–Klein[9] dimensional reduction. We apply the same procedure to a more complicated theory, Majorana's infinite component wave equation[10] in five dimensions. We do not consider how string theories in higher dimension can yield CSR's in lower dimensions, our considerations indicate a connection between group contraction and their infinite slope limit.

II. FRONT FORMS OF THE POINCARÉ AND CONFORMAL ALGEBRAS

In this section, we briefly review the light-cone forms of the Poincaré and conformal algebras in arbitrary dimensions.

A. Poincaré algebra

In d dimensions, the generators of the Poincaré algebra satisfy the commutation relations

$$[P^\mu, P^\nu] = 0,$$

$$[M^{\mu\nu}, P^\sigma] = i(\eta^{\mu\sigma}P^\nu - \eta^{\nu\sigma}P^\mu),$$

$$[M^{\mu\nu}, M^{\alpha\beta}] = i(\eta^{\mu\alpha}M^{\nu\beta} + \eta^{\alpha\nu}M^{\beta\mu} + \eta^{\nu\beta}M^{\mu\alpha} + \eta^{\beta\mu}M^{\alpha\nu}),$$

where $\eta_{\mu\nu}=(-1,1,\ldots,1)$ and $\mu,\nu,\alpha,\beta=0,\ldots,(d-1)$.

Introduce the light-cone coordinates,[11,5]

$$x^\pm = \frac{1}{\sqrt{2}}(t \pm x^{d-1}) \quad \text{and } p^\pm = \frac{1}{\sqrt{2}}(p^0 \pm p^{d-1}),$$

where $i,j=1,2,\ldots,(d-2)$ are the transverse directions. The commutation relations satisfied by the momenta and positions are

$$[x^-, p^+] = -i \quad \text{and } [x^i, p^j] = i\eta^{ij}.$$

Following Dirac, we set $x^+=0$ and use the mass-shell condition to express its conjugate variable p^- in terms of the remaining variables. The translation generators become

$$P^- = \frac{p^i p^i + M^2}{2p^+}, \quad P^+ = p^+, \quad P^i = p^i;$$

P^- is called the light-cone Hamiltonian. The Lorentz generators are given by

$$M^{+i} = -x^i p^+, \tag{1}$$

$$M^{+-} = -x^- p^+, \tag{2}$$

$$M^{ij} = x^i p^j - x^j p^i + S^{ij}, \tag{3}$$

$$M^{-i} = x^- p^i - \frac{1}{2}\{x^i, P^-\} + \frac{1}{p^+}(T^i - p^j S^{ij}). \tag{4}$$

The generators, S^{ij}, form the SO$(d-2)$ transverse light-cone little group and obey,

$$[S^{ij}, S^{kl}] = i(\eta^{ik}S^{jl} + \eta^{kj}S^{li} + \eta^{jl}S^{ik} + \eta^{li}S^{kj}). \tag{5}$$

The T^i's transform as SO$(d-2)$ vectors, called the light-cone translation vectors and satisfy

$$[S^{ij}, T^k] = i(\eta^{ik}T^j - \eta^{jk}T^i), \tag{6}$$

$$[T^i, T^j] = iM^2 S^{ij}. \tag{7}$$

The difference between the various representations is easily understood in terms of these variables.

(i) When $M \neq 0$, we can divide Eq. (7) by M, so that

$$S^{ij} \quad \text{and} \quad \frac{T^i}{M}$$

generate the massive little group SO$(d-1)$. The representations are therefore labelled by the massive little group.

(ii) When $M=0$, the T^i's are still SO$(d-2)$ vectors, but they commute with one another. This leads us to consider two cases.

(1) $T^i=0$, yields the regular massless representation labelled by a representation of the SO$(d-2)$ little group generated by S^{ij}, with a finite number of helicity states.

(2) $T^i \neq 0$. In this case, the S^{ij} and T^i's form the inhomogeneous light-cone little group in $(d-2)$ dimensions, which has infinite-dimensional representations, yielding the continuous spin massless representations of the Poincaré group.

B. Conformal algebra

The Poincaré group is a subgroup of the conformal group SO$(d,2)$ which contains dilatation and conformal transformations. The concept of mass makes sense in the conformal sense only if it is zero, to preserve scale invariance. Thus one expects massless representations of the Poincaré group to appear naturally in those of the conformal group.

It has been known[7,8] for some time that the CSR do not appear in this decomposition. We can show it elegantly using light-cone coordinates, and expressing the generators of the conformal algebra using the same variables as for the Poincaré algebra. We need to add to the Poincaré generators the dilatation generator

$$D = \tfrac{1}{2}(x \cdot p + p \cdot x), \tag{8}$$

for the scale transformation and the special conformal transformations generated by

$$K^\mu = 2x_\nu M^{\mu\nu} + x^2 p^\mu = 2x^\mu D - x^2 p^\mu + 2x^\nu S^{\mu\nu}, \tag{9}$$

where $\mu=0,1,\ldots(d-1)$, and

$$M^{\mu\nu} = x^\mu p^\nu - x^\nu p^\mu + S^{\mu\nu}. \tag{10}$$

In addition to those of the Poincaré algebra, these two generators satisfy the following commutation relations:

$$[M^{\mu\nu}, D] = 0, \quad [D, p^\mu] = ip^\mu, \quad [D, K^\mu] = -iK^\mu,$$

$$[M^{\mu\nu},K^{\alpha}]=i(\eta^{\mu\alpha}K^{\nu}-\eta^{\nu\alpha}K^{\mu}),\quad [p^{\mu},K^{\nu}]=-2i(\eta^{\mu\nu}D-M^{\mu\nu}).$$

To obtain the light-cone forms of the dilatation and the conformal translation generators, we first express the dilation and conformal generators in light-cone coordinates,

$$D=\tfrac{1}{2}(-\{x^{-},p^{+}\}-\{x^{+},p^{-}\}+\{x^{i},p^{i}\}),$$

$$K^{+}=-2x^{+}M^{+-}+x^{2}p^{+}+2x^{i}M^{+i},$$

$$K^{-}=2x^{-}M^{+-}+2x^{i}M^{-i}+x^{2}p^{-},$$

$$K^{i}=2x^{-}M^{+i}+2x^{+}M^{-i}+2x^{j}M^{ij}+x^{2}p^{i},$$

where $i,j=1,\ldots,(d-2)$. Using the light-cone forms of the Poincaré generators from Eqs. (1)–(4) and setting $x^{+}=0$, K^{-}, and K^{i} can be written as

$$K^{-}=2x^{-}(-x^{-}p^{+}+x^{i}p^{i})-x^{i}x^{i}p^{-}+\frac{2}{p^{+}}(x^{i}T^{i}-x^{i}p^{j}S^{ij}), \tag{11}$$

$$K^{i}=2x^{i}(-x^{-}p^{+}+x^{i}p^{i})-x^{j}x^{j}p^{i}+2x^{j}S^{ij}. \tag{12}$$

To check if these satisfy the algebra, we calculate the commutators $[P^{-},K^{i}]$ and $[p^{i},K^{-}]$. Substituting the light-cone forms, we find

$$[P^{-},K^{i}]=2i\left(x^{-}p^{i}-\frac{1}{2}\{x^{i},P^{-}\}-\frac{p^{j}}{p^{+}}S^{ij}\right), \tag{13}$$

$$-[p^{i},K^{-}]=2i\left(x^{-}p^{i}-\frac{1}{2}\{x^{i},P^{-}\}+\frac{1}{p^{+}}(T^{i}-p^{j}S^{ij})\right). \tag{14}$$

But to satisfy the conformal algebra, these two commutators must be equal, requiring $T^{i}=0$. Therefore, the front forms of the conformal generators are

$$K^{+}=-x^{i}x^{i}p^{+},\quad K^{i}=2x^{i}D-x^{j}x^{j}p^{i}+2x^{j}S^{ij}, \tag{15}$$

$$K^{-}=2x^{-}D-x^{i}x^{i}p^{-}-\frac{2}{p^{+}}x^{i}p^{j}S^{ij}, \tag{16}$$

$$D=\tfrac{1}{2}(-\{x^{-},p^{+}\}+\{x^{i},p^{i}\}). \tag{17}$$

This shows that $T^{i}=0$, which imply regular massless representations, not the CSR.

We conclude that in order to generate a CSR by embedding the Poincaré algebra into larger algebraic structures, we must consider singular limits. The CSRs require the transverse little group to be the Euclidean group $E(2)$, the semidirect product of translations and rotations. It is the very same group that Inönü and Wigner[6] obtained by contracting the homogeneous SO(3) group. As this group is the massless transverse little group in five dimensions, we are led to consider dimensional reduction as well as group contraction of the Poincaré group in higher dimensions.

III. KALUZA–KLEIN REDUCTION OF THE 5D POINCARÉ ALGEBRA

Kaluza and Klein[9] reduced one dimension by setting it on to a circle of finite radius. We apply it to the five-dimensional Poincaré algebra, by setting the third direction on to a circle of radius R,

$$x^3 = x^3 + 2\pi R.$$

The generators act on functions of the form

$$\Phi(x) = \sum_n \Phi_n(x^\mu) e^{inx^3/R}, \tag{18}$$

where $\mu = +, -, 1, 2$ and n is the mode number. The momentum along the third direction is quantized

$$p^3 = \frac{n}{R}, \tag{19}$$

and the light-cone Hamiltonian becomes

$$P^- = \frac{p^i p^i + (p^3)^2 + M^2}{2p^+} \equiv \frac{p^i p^i + M_n^2}{2p^+}, \tag{20}$$

where

$$M_n^2 = M^2 + \frac{n^2}{R^2}, \tag{21}$$

is the Kaluza–Klein (KK) mass. The single state of mass M in five dimensions generates an equally spaced tower of states of mass M_n. To find their spin, observe that the two transverse boost generators are

$$M^{-i} = x^- p^i - \frac{1}{2}\{x^i, P^-\} + \frac{1}{p^+}\left(T^i + \frac{n}{R} S^{3i} - p^j S^{ij}\right), \tag{22}$$

for $i = 1, 2$, leading us to define new light-cone translation vectors

$$\hat{T}^i = T^i + \frac{n}{R} S^{3i}, \tag{23}$$

which satisfy the algebra

$$[S^{ij}, \hat{T}^k] = i(\eta^{jk}\hat{T}^j - \eta^{jk}\hat{T}^i), \quad [\hat{T}^i, \hat{T}^j] = iM_n^2 S^{ij}. \tag{24}$$

The generators

$$S^{12}, \quad \frac{\hat{T}^i}{M_n},$$

form the SO(3) light-cone little group in four dimensions. Analyzing the mass term, the mass M_n increases with the mode number and gives the well-known infinite (KK) tower of masses starting at $M_0 = M$. The remaining Lorentz generators of the four-dimensional group, M^{+-}, M^{12}, and M^{+i} for $i = 1, 2$ are not changed. Note that when evaluated at $x^3 = 2\pi R$, the generators that rotate into the third direction become (for large R) like the momenta

$$\frac{M^{-3}}{R} = \frac{n}{R^2} x^- - 2\pi p^- + \frac{1}{Rp^+}(T^3 - p^i S^{3i}), \tag{25}$$

$$\frac{M^{3i}}{R} = 2\pi p^i - \frac{nx^i}{R^2} + \frac{1}{R} S^{3i}, \tag{26}$$

$$\frac{M^{+3}}{R} = -2\pi p^{+}. \tag{27}$$

When the starting representation is massive ($M \neq 0$), the KK procedure yields massive representations in lower dimensions, but even if $M=0$, the ground floor of a KK tower is the usual massless representation in four dimensions, not the CSR. In the simple limit $R \to \infty$, the KK mass tower collapses without any sign of a CSR.

IV. INÖNÜ–WIGNER CONTRACTION

This section presents the original Inönü–Wigner[6] contraction procedure. Starting from the homogeneous SO(3) group, they generated the Euclidean group $E(2)$, in a singular limit with an arbitrary contraction parameter that tends to zero. They considered the algebra's generators, identifying those which are well defined under contraction, as well as to the two-dimensional wave function on which the Euclidean translation vectors act, which they show to be Bessel's functions J_n.

They begin with the SO(3) generators L_i in the $(2l+1)$-dimensional representation, which satisfy

$$[L_i, L_j] = i\epsilon_{ijk}L_k, \quad L_iL_i = l(l+1), \quad L_3 = m.$$

They introduce a contraction parameter ϵ and the vectors

$$T_i \equiv \epsilon L_i. \tag{28}$$

They observe that in the limit $\epsilon \to 0$, these, together with L_3, satisfy the commutation relations of the Euclidean algebra

$$[L_3, T_i] = \epsilon_{ij}T_j, \quad [T_i, T_j] = 0. \tag{29}$$

Multiplying the Casimir operator with ϵ^2 yields

$$(\epsilon m)^2 + T_1^2 + T_2^2 = \epsilon^2 l(l+1). \tag{30}$$

The Inönü–Wigner contraction is the double limit

$$l \to \infty, \quad \epsilon \to 0, \quad \epsilon l \equiv \Xi \text{ fixed}, \tag{31}$$

in which the Euclidean translations have a finite length

$$T_1^2 + T_2^2 = \Xi^2. \tag{32}$$

In their original paper, Inönü and Wigner applied their method to the Poincaré group, using the inverse of the speed of light as a contraction parameter, and find it to contract to the nonrelativistic Galilei group (*but only if the starting point is the tachyonic representation*).

The representation function of $E(2)$ in a space labelled by the polar coordinates ρ and θ are of the form

$$\sum_n c_n J_n(\Xi\rho)e^{in\theta}. \tag{33}$$

In the Appendix we show how to obtain these results directly by imposing periodic boundary conditions à la Kaluza–Klein.

V. THE CSR À LA KALUZA–KLEIN–INÖNÜ–WIGNER

The results of the preceding two sections hints on how to proceed. The contraction parameter ϵ is simply the inverse of the Kaluza–Klein radius. We start from the usual massless Poincaré group in five dimensions, and apply the KK procedure to the third direction. The dynamical boosts are

$$M^{-i} = x^- p^i - \frac{1}{2}\{x^i, P^-\} + \frac{1}{p^+}\left(\frac{n}{R}S^{3i} - p^j S^{ij}\right). \tag{34}$$

Comparison with the results of the preceding section leads us to identify the IW contraction parameter as

$$\epsilon = \frac{n}{R}. \tag{35}$$

This yields the CSR boosts, where the translations are given by

$$\hat{T}^i = \frac{n}{R}S^{3i}. \tag{36}$$

We mimic the IW procedure and consider the Casimir operator of the SO(3) light-cone little group, where j is the spin of the massless particle in five dimensions,

$$(S^{12})^2 + (S^{23})^2 + (S^{31})^2 = j(j+1).$$

Dividing both sides by R^2, we obtain

$$(\hat{T}^1)^2 + (\hat{T}^2)^2 = \frac{n^2 j^2}{R^2} \equiv \Xi^2 \neq 0. \tag{37}$$

The length of the translation vector is nothing but the Pauli–Lubanski Casimir operator of the Poincaré group. This shows that it is possible to generate the CSR as long as one takes the double limit

$$R \to \infty, \quad j \to \infty, \quad \frac{j}{R} \text{ fixed}. \tag{38}$$

In the next section, we apply the same method to a more complicated theory.

VI. CSR FROM MAJORANA'S THEORY

In this section, we consider the contraction of the five-dimensional massive representations. A simple, yet nontrivial model for the massive relativistic particle is the infinite component Majorana theory, introduced by Majorana long ago.[10] Its spectrum can be inferred from Poincaré generators with a massive SO(4) little group. Amusingly the mathematics of this SO(4) are exactly the same as those of Bohr's nonrelativistic hydrogen atom. We want to apply contraction to this theory and investigate under what circumstances a CSR can be generated.

In the following, we construct the mass operator and other generators of the little group in terms of internal coordinates. This can be thought of as the nonlinear realization of the homogeneous SO(4) group. We start with applying the contraction to the SO(4) little group algebra and find the Casimirs in five and four dimensions which label the representations. We will then find the conditions necessary for the existence of the CSRs. We will also find the representation of the wave functions in four dimensions and compare with the IW paper.

A. Majorana's theory

We start with the five dimensional light-cone realization of the dynamical Poincaré boosts

$$M^{-i} = x^- p^i - \frac{1}{2}\{x^i, P^-\} + \frac{1}{p^+}(T^i - p^j S^{ij}),$$

with $i, j = 1,2,3$.

The little group generators are built in terms of three "internal variables" η^j and their conjugates π^j,

$$[\eta^j, \pi^j] = i\delta^{ij}, \quad i,j = 1,2,3, \tag{39}$$

in the form

$$S^{ij} = \epsilon^{ijk} L^k = \eta^i \pi^j - \eta^j \pi^i, \tag{40}$$

and with the nonlinear Laplace–Runge–Lenz (LRL) vectors

$$T^i = \epsilon^{ijk} \pi^j L^k - \mu \frac{\eta^j}{\eta} - i\pi^j, \tag{41}$$

where $\eta = \sqrt{\eta^j \eta^j}$ and μ is a mass parameter (we have set the "electron charge" to one). They obey the commutation relations

$$[T^i, T^j] = i(-2\mu H)\epsilon^{ijk} L^k, \tag{42}$$

where H is the same as Bohr's Hamiltonian

$$H = \frac{\pi^i \pi^i}{2\mu} - \frac{1}{\eta}. \tag{43}$$

[In Bohr's case, of course, the SO(4) generators are written in terms of coordinates and momenta in real three-dimensional space.]

Comparison between Eqs. (7) and (42) yields the mass squared operator

$$M^2 = -2\mu H, \tag{44}$$

which must then appear in the light-cone Hamiltonian,

$$P^- = \frac{p^i p^i + M^2}{2p^+} = \frac{p^i p^i - 2\mu H}{2p^+}.$$

Each mass level has the same degeneracy as that of the hydrogen atom. Two commuting SO(3)'s are generated by the combinations

$$\frac{1}{2}\left(L^k + \frac{T^k}{\sqrt{-2\mu H}}\right), \quad \frac{1}{2}\left(L^k - \frac{T^k}{\sqrt{-2\mu H}}\right),$$

corresponding to $\mathrm{SO}(4) \sim \mathrm{SO}(3) \times \mathrm{SO}(3)$. Since

$$L^k T^k = T^k L^k = 0, \tag{45}$$

they have the same Casimir operator

$$C_2 = \frac{1}{4}\left(L^k L^k - \frac{T^k T^k}{2\mu H}\right) = j(j+1), \tag{46}$$

where j is related to the mass operator by

$$M_j^2 = \frac{\mu^2}{4C_2 + 1} = \frac{\mu^2}{(2j+1)^2}, \tag{47}$$

so that $(2j+1)$ is Bohr's principal quantum number. At each mass level, these states assemble in a representation of SO(4) and generate the spectrum of the infinite component Majorana wave equation. Since $\mathrm{SO}(4) \supset \mathrm{SO}(3) \supset \mathrm{SO}(2)$, we need to contract at least twice to obtain a CSR in four dimensions. One contraction parameter is of course the inverse radius of the compactified direction and the other one is not yet defined. There are two ways to proceed with the contractions.

(1) We contract, staying in five dimensions first, and then use KK reduction and contract to four dimensions, i.e.,

$$\mathrm{SO}(4) \xrightarrow[\text{contraction}]{\text{1st}} E(3) \xrightarrow[\text{reduction}]{\text{KK}} \mathrm{SO}(3) \xrightarrow[\text{contraction}]{\text{2nd}} E(2).$$

(2) We apply the KK reduction first and then contract, i.e.,

$$\mathrm{SO}(4) \xrightarrow[\text{reduction}]{\text{KK}} \mathrm{SO}(3) \xrightarrow[\text{contraction}]{\text{Double}} E(2).$$

We consider both cases in the following and find the conditions for these procedures to lead to the CSR in four dimensions.

1. Case 1: Contraction to E(3)

In the Majorana theory, the degeneracy at each mass level is generated by the addition of two angular momenta j. The states are eigenstates of their SO(3) diagonal subgroup (the angular momentum in Bohr's model), so that

$$L^k L^k = l(l+1), \tag{48}$$

where $l = 0, 1, 2, \ldots, 2j$. This is the analog of the magnetic quantum number in the $\mathrm{SO}(3) \to E(2)$ contraction process, its range goes to infinity while its value remains finite. This leads us to consider the contraction where all three L^k that generate SO(3) remain finite as $j \to \infty$.

In that limit, the mass vanishes and the T^k become commuting translations

$$M_j = \frac{\mu}{2j+1} \to 0, \quad [T^i, T^k] \to 0, \tag{49}$$

producing $E(3)$, the Euclidean group in three dimensions. This contraction of the transverse little group yields a CSR in five dimensions. To see this explicitly, we multiply the SO(4) Casimir operator by the contraction parameter ϵ,

$$(\epsilon L^k)(\epsilon L^k) + \frac{\epsilon^2}{M_j^2} T^k T^k = 4\epsilon^2 j(j+1).$$

As $\epsilon \to 0$ and $j \to \infty$, for fixed ϵj we get

$$T^k T^k = \mu^2, \tag{50}$$

so that the length of the translation vector is fixed.

In five dimensions, the Poincaré group has three Casimir operators, the momentum squared (zero in this case),

$$W_{\mu\nu} W^{\mu\nu} \quad \text{and } W = \epsilon_{\rho\mu\nu\sigma\lambda} P^\rho M^{\mu\nu} M^{\sigma\lambda}, \tag{51}$$

where

$$W_{\mu\nu} = \epsilon_{\mu\nu\rho\sigma\lambda} P^{\rho} M^{\sigma\lambda}. \tag{52}$$

In this case,

$$W_{\mu\nu} W^{\mu\nu} = \mu^2 \quad \text{and } W = T_k L_k = 0. \tag{53}$$

These two Casimirs characterize a unique CSR in five dimensions. The dimensionality of space–time does not change, but the contraction parameter ϵ does not have an obvious physical meaning.

We can use this contracted theory as a starting point to obtain a four-dimensional theory. So we apply the KK reduction to the $E(3)$ algebra to get down to four dimensions. The mass operator and the light-cone vector now takes the following form:

$$M_n^2 = \frac{n^2}{R^2} \quad \text{and } \hat{T}^a = T^a + \frac{n}{R} S^{3a}, \quad a = 1,2, \tag{54}$$

which can be checked by analyzing the light-cone Hamiltonian and the dynamical boosts, respectively. The generators S^{12} and $\hat{T}^a$ now form SO(3), the massive little group in four dimensions. The contraction parameter is now $\epsilon' = 1/R$. Let $\tilde{j}(\tilde{j}+1)$ be the eigenvalue of this SO(3) angular momentum algebra. It is quite clear that to get a CSR, we take the limits,

$$R \to \infty, \quad \tilde{j} \to \infty \quad \text{with } \frac{\tilde{j}}{R} \text{ fixed}.$$

Therefore we obtain,

$$\hat{T}^a \hat{T}^a = \frac{n^2 \tilde{j}^2}{R^2} \equiv \tilde{\Xi}^2, \tag{55}$$

which is the Casimir of the $E(2)$ algebra. The other Casimir is of course the mass squared which is zero. These two uniquely determines the CSR in four dimensions.

Notice that the first contraction parameter could have been identified with $1/j$ or μ; both would have yielded a zero mass, but it is only the first case that leads to the CSR; the other $\mu \to 0$ generates a normal massless representation of definite helicity.

2. Case 2: KK reduction first

In this case, we apply the KK reduction first. The massive SO(4) little group in five dimensions now reduces to the massive little group in four dimensions. The light-cone Hamiltonian becomes

$$P^- = \frac{1}{2p^+}(p^a p^a + M_{jn}^2), \tag{56}$$

for $a = 1, 2$, with

$$M_{jn}^2 = \frac{\mu^2}{(2j+1)^2} + \frac{n^2}{R^2}, \tag{57}$$

using Eq. (19). The generators of the SO(3) little group are

$$L^3 \quad \text{and } \hat{T}^a = \left(T^a + \frac{n}{R} S^{3a} \right), \quad a = 1,2 \tag{58}$$

deduced by looking at M^{-a}.

The quadratic Casimir is

$$(L^3)^2 + \frac{1}{M_{jn}^2}\left(T^a + \frac{n}{R}S^{3a}\right)\left(T^a + \frac{n}{R}S^{3a}\right) = j'(j'+1). \tag{59}$$

The mass operator in Eq. (57) clearly shows that we need to take the double limit $j,R\to\infty$ to obtain the massless case. However this is not enough to get a CSR, because from Eq. (59), it is also clear that the ratio j'/R must also remain finite and nonzero. To see it explicitly, we divide Eq. (59) by R^2 and rearrange to get

$$\hat{T}^a\hat{T}^a = \left(\frac{\mu^2}{(2j+1)^2/R^2} + n^2\right)\left(\frac{j'}{R}\right)^2 - M_{jn}^2 m^2, \tag{60}$$

where we have used $L^3 = m$. The double limit certainly does not give any nonzero value, but the following triple limit,

$$j,j',R\to\infty, \quad \text{such that } \frac{j}{R},\frac{j'}{R} \text{ remain finite (nonzero)}, \tag{61}$$

does give a finite value. Therefore, in this triple limit, we find,

$$(\hat{T}^a)^2 = \left(\frac{\mu^2}{(2j/R)^2} + n^2\right)\left(\frac{j'}{R}\right)^2 \equiv \Xi'^2, \tag{62}$$

which is the Casimir in four dimensions. This and the mass squared (which is zero) uniquely labels the representation. The difference between Case 1 and Case 2 is the length of the light-cone vector. This feature is what we expected, because the generator S^{12} was not affected by any of the reduction and/or contraction processes. The contraction only affected the quadratic Casimir eigenvalues which sets the range of quadratic Casimir of its maximal subgroup. Therefore, the representations of the contracted algebra of these two cases should differ by the length of the light-cone vectors and that is what we have found. These representations are also consistent with Inönü and Wigner's result with different lengths of the Euclidean light-cone vectors.

B. Representation of the wave function

Since we have the form of the T^i's in terms of the internal variables, we can explicitly find the representation of the wave function for the light-cone vectors $\hat{T}^a$. First note that in $\hat{T}^a$ the contraction parameter j is not explicitly present. Therefore if we apply the contraction it will only include the $R\to\infty$ limit, not the $j\to\infty$. As a result we will not obtain a commuting vector which is required to obtain the CSR. Since the contraction parameter j appears through the Hamiltonian when it acts on the wave function, we rewrite T^i in terms of the Hamiltonian as in the following:

$$T^i = \epsilon_{ijk}\pi^j L^k - \frac{\mu\eta^i}{\eta} - i\pi^i = \eta^i\left(2\mu H + \frac{\mu}{\eta}\right) - (\eta\cdot\pi - i)\pi^i, \tag{63}$$

where we used H as given by Eq. (43). Therefore the light-cone vector, $\hat{T}^a$, can be expressed as

$$\hat{T}^a = \left(2\mu\eta^a H + \frac{\mu\eta^a}{\eta} - \frac{n}{R}\eta^a\pi^3 - \mu[\eta^a,H]\right) + (y + 2i - \eta\cdot\pi)\pi^a, \tag{64}$$

where

$$y = \frac{n\eta^3}{R}. \tag{65}$$

The first term is dependent on the contraction parameters whereas the second term is independent and also both terms are separately Hermitian. Since $H\sim\mathcal{O}(1/j^2)$ and $1/\eta\sim\mathcal{O}(1/R)$, the first term vanishes as $j,\ R\to\infty$.

It should be noted that if we evaluate the commutator in the first term in Eq. (64) and then consider the contraction, the resulting light-cone vector becomes non-Hermitian and the whole analysis becomes physically meaningless. It is not well understood why this happens, but to maintain the hermiticity, we must consider the contraction without computing the commutator. Using

$$\eta \cdot \pi = \eta^a \pi^a - iy\frac{\partial}{\partial y},$$

and dropping the first term, the light-cone vector becomes

$$\hat{T}^a = \left(y + 2i + iy\frac{\partial}{\partial y} - \eta^b \pi^b\right)\pi^a. \tag{66}$$

It can be easily checked that the above form satisfies the $E(2)$ algebra,

$$[\hat{T}^a, \hat{T}^b] = 0 \quad \text{and } [S^{ab}, \hat{T}^c] = i(\eta^{ac}\hat{T}^b - \eta^{bc}\hat{T}^a),$$

which is required to obtain any CSR in four dimensions. We now find the representation of the wave function for this $E(2)$ algebra.

The square of the light-cone vector is

$$(\hat{T}^a)^2 = \left[(\eta^b \pi^b)^2 - i\eta^b \pi^b\left(-2iy + 5 + 2y\frac{d}{dy}\right) - \left(y^2\frac{d^2}{dy^2} - (2iy^2 - 6y)\frac{d}{dy} - (y^2 + 6iy - 6)\right)\right](\pi^2).$$

On a wave function of the form,

$$\Phi(\eta^i) = e^{iy}\phi(\eta^a, y),$$

this gives the following form of the differential equation:

$$\left[(\eta^b \pi^b)^2 - i\eta^b \pi^b\left(5 + 2y\frac{d}{dy}\right) - \left(y^2\frac{d^2}{dy^2} + 6y\frac{d}{dy} + 6\right)\right](\pi^2) = \Xi^2, \tag{67}$$

where $\Xi = \tilde{\Xi}$ or Ξ' corresponding to Case 1 and Case 2, respectively. To solve the above equation, let

$$(\pi^a)^2 = \Pi^2(y) \tag{68}$$

when it acts on $\phi(\eta^a, y)$, that is the representation of the η^a dependent part of the wave function is the Bessel function, namely,

$$\phi(\eta^a, y) = J_m(\Pi(y)\rho)e^{im\theta}F(y),$$

where $F(y)$ is a real function and we used the polar coordinates, $\eta^1 = \rho\cos\theta$ and $\eta^2 = \rho\sin\theta$. In polar coordinates, we use,

$$-i\eta^a \pi^a = -\rho\frac{d}{d\rho},$$

$$(\eta^a \pi^a)^2 = -\left(\rho^2\frac{d^2}{d\rho^2} + \rho\frac{d}{d\rho}\right),$$

and we rewrite Eq. (67) as

$$\left[\rho^2\frac{d^2}{d\rho^2}+\left(6+2y\frac{d}{dy}\right)\rho\frac{d}{d\rho}+\left(y^2\frac{d^2}{dy^2}+6y\frac{d}{dy}+6\right)\right](\Pi^2 J_m F)=-\Xi^2 J_m F. \tag{69}$$

Making use of the following identities:

$$\frac{d}{d\rho}J_m(\Pi(y)\rho)=\frac{\Pi}{2}(J_{m-1}-J_{m+1}), \tag{70}$$

$$\frac{d}{dy}J_m(\Pi(y)\rho)=\frac{\rho}{2}\frac{d\Pi}{dy}(J_{m-1}-J_{m+1}), \tag{71}$$

and after straightforward algebra, the left-hand side of Eq. (69) can be expressed as a linear combination of Bessel function of different orders,

$$\begin{aligned}
&\left(\frac{\rho^2\Pi^4 F}{4}+\frac{\rho^2 y\Pi^3\Pi' F}{2}+\frac{\rho^2 y^2\Pi^2\Pi'^2 F}{4}\right)(J_{m-2}+J_{m+2})\\
&+\left(3\rho\Pi^3 F+6\rho y\Pi^2\Pi' F+\rho y\Pi^3 F'+2\rho y^2\Pi\Pi'^2 F+\rho y^2\Pi^2\Pi' F'+\frac{\rho y^2\Pi^2\Pi'' F}{2}\right)(J_{m-1}-J_{m+1})\\
&+\left(-\frac{\rho^2\Pi^4 F}{2}-\rho^2 y\Pi^3\Pi' F+2y^2\Pi'^2 F+2y^2\Pi\Pi\Pi'' F+4y^2\Pi\Pi' F'+y^2\Pi^2 F''\right.\\
&\left.-\frac{\rho^2 y^2\Pi^2\Pi'^2 F}{2}+12y\Pi\Pi' F+6y\Pi^2 F'+6\Pi^2 F\right)J_m,
\end{aligned}$$

where the prime denotes derivative with respect to the argument. By matching the coefficients of Bessel functions of different order with the right-hand side of Eq. (69), we get three constraints. Equating the coefficient of $J_{m\pm2}$ to zero gives the first constraint,

$$\frac{\rho^2\Pi^2}{4}\left(\Pi^2+2y\Pi\frac{d\Pi}{dy}+y^2\left(\frac{d\Pi}{dy}\right)^2\right)F(y)=0,$$

which is satisfied if

$$\Pi^2+2y\Pi\frac{d\Pi}{dy}+y^2\left(\frac{d\Pi}{dy}\right)^2=0. \tag{72}$$

The solution to this equation is given by

$$\Pi(y)=\frac{\Pi_0}{y}, \tag{73}$$

where Π_0 is a constant. The constraint obtained by equating the coefficients of $J_{m\pm1}$ provides no new result. Finally the remaining constraint is from the coefficients of J_m which gives a differential equation for $F(y)$,

$$\frac{d^2F}{dy^2}+\frac{2}{y}\frac{dF}{dy}+\frac{\Xi^2}{\Pi_0^2}F=0, \tag{74}$$

where we used $\Pi(y)=\Pi_0/y$ and its derivatives. The solution is given by

$$F(y)=\frac{1}{y}\left(A\sin\left(\frac{\Xi y}{\Pi_0}\right)+B\cos\left(\frac{\Xi y}{\Pi_0}\right)\right), \tag{75}$$

where A and B are constants, and the regularity condition at $y=0$ implies $B=0$. Therefore the complete wave function can be written as

$$\Phi(\rho,\theta,y)=\sum_m N_m\left(\frac{e^{iy}}{y}\sin\left(\frac{\Xi y}{\Pi_0}\right)\right)e^{im\theta}J_m\left(\frac{\Pi_0\rho}{y}\right), \tag{76}$$

where N_m is the overall normalization constant.

In their paper,[6] IW found the following wave function for the $E(2)$ algebra,

$$\Phi_{\mathrm{IW}}(\rho,\theta)=\sum_m c_m e^{im\theta}J_m(\Xi\rho), \tag{77}$$

where Ξ^2, the square of the Pauli–Lubanski vector, is the second Casimir of the Poincaré group, and labels the CSR in four dimensions. The Euclidean vector is linear in π^a and as a result its length appeared as a scale factor in the Bessel function. In four dimensions there are only two types of CSRs, fermionic and bosonic types corresponding to half-odd and integer values of m. The amplitude is also constant.

Although similar in form, there are differences between Eq. (76) and the IW form in Eq. (77). In our case, the internal momentum [Eq. (73)] and amplitude are not constant, but functions of y which is the ratio of the internal and external coordinates. It is due to the fact that the Euclidean light-cone vector $\hat{T}^a$ is not linear in π^a (in addition to the y dependence). Moreover, unlike the IW case, the length of the light-cone vector does not appear as a scale factor in the Bessel function, even though it is the CSR. To find how our CSR is related to IW's CSR, we must find a relation between Π and Ξ. Let us assume $\Pi=\Xi=\Pi_0/y$. The only solution we get, following Eq. (72), is $\Xi=0$ which corresponds to the regular massless representation, not the CSR. Therefore $\Pi\neq\Xi$ is the only possibility and these are quite new. On the other hand, we may assume that, instead of Π, $\Pi_0=\Xi$. Substituting this into Eq. (76) and setting $y=1$, the solution becomes exactly the same as that of Wigner's CSR apart from the overall phase factor which has no physical effect (the overall constant factor can be absorbed into the normalization factor). For any other values of y, we have a different kind of CSR because of the nonequality between the scale factor and length of the Euclidean vector. There is no physical reason for Π_0 and Ξ to be equal and $y=1$, but this is the only condition to obtain IW's result.

Finally, the raising and lowering operators are defined as

$$\hat{T}^{\pm}=\hat{T}^1\pm i\hat{T}^2.$$

In polar coordinates, these become

$$\hat{T}^{+}=e^{i\theta}\left(2+y\frac{d}{dy}+\rho\frac{d}{d\rho}\right)\left(\frac{d}{d\rho}+\frac{i}{\rho}\frac{d}{d\theta}\right), \tag{78}$$

$$\hat{T}^{-}=e^{-i\theta}\left(2+y\frac{d}{dy}+\rho\frac{d}{d\rho}\right)\left(\frac{d}{d\rho}-\frac{i}{\rho}\frac{d}{d\theta}\right), \tag{79}$$

which acts on $\phi(\rho,\theta,y)$. It is quite obvious that the states $\hat{T}^{+}|>$ and $\hat{T}^{-}|>$ have helicities $(m+1)$ and $(m-1)$, respectively. The remaining generator T^3/R becomes

$$\frac{T^3}{R}=(\pi^a)^2,$$

under contraction. The complete Poincaré wave function is

$$\Phi(x^{+},x^{a};\rho,\theta,y)=\sum_m N_m\frac{e^{iy}}{y}\sin\left(\frac{\Xi y}{\Pi_0}\right)e^{-i(x^{-}p^{+}-x^{a}p^{a})}e^{im\theta}J_m\left(\frac{\Pi_0\rho}{y}\right).$$

The physical meaning of the new parameter y is not clear to us, but it links the external to the internal coordinates of the Majorana theory. This type of limit links the internal structure to that of

space–time. If we view, as we have, the Majorana theory as a warm-up for string theory, it may correspond to compactifying a string with its vibrational modes stuck along an extra dimension. This may help define the infinite slope limit of string theory.

VII. CONCLUSION

In this paper, we showed that if we dimensionally reduce from five to four dimensions, the compactified algebra is the regular representation of the Poincaré group in four dimensions with mass M_n for all modes. For the infinite radius limit, we find that the KK mass spectra collapses to the lowest mass state and gives the regular representation of the Poincaré group in four dimensions. Only for nonzero modes and infinite radius limit, we obtain CSR if the j/R remains constant as $R\to\infty$, otherwise we will get the regular representation.

We constructed explicitly the representation of the Euclidean group in a system with periodic boundary condition for internal coordinates and found the condition to obtain nonzero Euclidean vectors using IW contraction method. We found that for nonzero and finite Euclidean vector, the eigenvalue of the uncontracted group must be proportional to the radius of the compactified direction. This condition is similar to that of the CSR where the spin is proportional to the radius, apart from the mode number. Therefore finding the representations of any Euclidean group provides the representations of the inhomogeneous light-cone little group which is the CSR.

We have applied the contraction technique to both regular massless and massive representations in five dimensions. In the regular massless case, the contraction yields the $E(2)$ little group under the double limits j, $R\to\infty$, keeping j/R finite and nonzero.

The massive case is not as straightforward as the regular massless case. We have considered Majorana theory as a model in the five-dimensional massive case. We have found that the double limits are not enough to get a CSR, even though the mass operator vanishes. We must consider triple singular limits j, j', $R\to\infty$ such that both j/R and j'/R remain fixed and nonzero. There are two ways to consider the contraction limits, in the sequence of contraction, KK reduction and contraction, or KK reduction and double contraction. Both of these yield the CSR in four dimensions. The difference is in the length of the light-cone vector. The representation wave function of the contracted algebra is the Bessel function, however as in Wigner's solution, the length of the light cone vector does not appear as a scale factor in the Bessel factor. In our case both the amplitude and the scale factor are a function of the parameter y which is a ratio of the internal and external coordinates. We have found that the contracted algebra is identical to that of Wigner's CSR only if Π_0 which is the magnitude of the internal momenta at $y=1$, equals the length of the light-cone vector (apart from an overall phase factor).

Thus, the CSR can arise in the Majorana theory, but with an extra variable. Its physical interpretation may provide clues when we apply our techniques to string theory in the hope of identifying the CSR with its infinite slope limit.

Our technique may also prove useful when the starting point is curved space in higher dimensions, particularly anti-de-Sitter. There the starting group is the conformal, not the Poincaré group. This possibility, though interesting in its own right, will not be discussed here.

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APPENDIX: INÖNÜ–WIGNER À LA KALUZA–KLEIN

In this Appendix we reproduce their results by a different method. We consider the full SO(3) algebra which acts on three-dimensional vector space with periodic boundary condition along one direction The contraction parameter is in the inverse radius of that direction. After the contraction, the three-dimensional wave function reduces to Bessel functions in the radial coordinate. In the following we retrace IW's steps, stressing the geometrical picture of the contraction procedure.

The IW contraction of SO(3) to $E(2)$ amounts to the study of a dynamical system with SO(3) symmetry restrained to a space whose boundary condition breaks that symmetry. We switch to cylindrical coordinates, and seek solutions which are periodic in z,

$$z \to z + 2\pi R, \tag{A1}$$

$$\Phi(\rho, \theta, z) = \sum_n \Phi_n(\rho, \theta) e^{inz/R}, \tag{A2}$$

where n is the mode number. In the following we will use $1/R$ as the contraction parameter. The angular momentum operators are given by

$$S^{12} = -i\frac{\partial}{\partial \theta}, \tag{A3}$$

$$S^{23} = -i\left(-z\sin\theta\frac{\partial}{\partial \rho} + \rho\sin\theta\frac{\partial}{\partial z} - \frac{z\cos\theta}{\rho}\frac{\partial}{\partial \theta}\right), \tag{A4}$$

$$S^{31} = -i\left(z\cos\theta\frac{\partial}{\partial \rho} - \rho\cos\theta\frac{\partial}{\partial z} - \frac{z\sin\theta}{\rho}\frac{\partial}{\partial \theta}\right). \tag{A5}$$

Acting on the wave function, the factor $\partial/\partial z$ can be replaced by in/R. When R is very large (ultimately we will take it to ∞), we drop all terms proportional to $\partial/\partial z$, yielding

$$S^{31} \to -iz\left(\cos\theta\frac{\partial}{\partial \rho} - \frac{\sin\theta}{\rho}\frac{\partial}{\partial \theta}\right), \tag{A6}$$

$$S^{32} \to iz\left(-\sin\theta\frac{\partial}{\partial \rho} - \frac{\cos\theta}{\rho}\frac{\partial}{\partial \theta}\right). \tag{A7}$$

However z is no longer well defined on the wave function. The Casimir operator now becomes

$$(S^{12})^2 + (S^{31})^2 + (S^{32})^2 = j(j+1), \tag{A8}$$

$$\to -z^2\left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} + \left(\frac{1}{\rho^2} + \frac{1}{z^2}\right)\frac{\partial^2}{\partial \theta^2}\right). \tag{A9}$$

The wave function on which this differential operator acts is of the form

$$\Phi(\rho, \theta) = \mathcal{R}(\rho)\Theta(\theta),$$

with eigenvalue s^2. Since there is no mode dependence, we have dropped the subscript n from the wave function. For the above form of the wave function, the angular part decouples from the radial part and can be written as

$$\frac{1}{\Theta}\frac{\mathrm{d}^2\Theta}{\mathrm{d}\theta^2} \equiv -m^2, \tag{A10}$$

where m, the azimuthal quantum number, is an integer or half-odd integer depending on whether the wave function is single or double valued. Let us also define the dimensionless variable

$$\tilde{\rho} = \frac{\sqrt{s^2 - m^2}}{z}\rho \equiv q(s,m)\rho.$$

Substituting the angular part, the eigenvalue equation for the differential operator in Eq. (A9) becomes Bessel's differential equation

$$\tilde{\rho}^2 \frac{\mathrm{d}^2\mathcal{R}}{\mathrm{d}\tilde{\rho}^2} + \tilde{\rho}\frac{\mathrm{d}\mathcal{R}}{\mathrm{d}\tilde{\rho}} + (\tilde{\rho}^2 - m^2)\mathcal{R} = 0, \tag{A11}$$

whose solutions are well known. The regularity condition at the origin implies that the physically relevant solution is the Bessel function $J_m(\tilde{\rho})$. Therefore the wave functions for the $E(2)$ group are linear combinations of the form

$$\Phi(\rho,\theta) = J_m(q\rho)e^{im\theta}. \tag{A12}$$

We let

$$T^a \equiv \lim_{R\to\infty} \frac{S^{3a}}{R}, \tag{A13}$$

that is

$$T^1 = \left(\cos\theta\frac{\partial}{\partial\rho} - \frac{\sin\theta}{\rho}\frac{\partial}{\partial\theta}\right), \quad T^2 = \left(-\sin\theta\frac{\partial}{\partial\rho} - \frac{\cos\theta}{\rho}\frac{\partial}{\partial\theta}\right).$$

It can easily be checked that the T^a, $a=1, 2$, commute and that they transform as a 2-vector under S[12], forming a representation of the $E(2)$ algebra. The length of the Euclidean vector is now

$$\xi^2 \equiv T^a T^a = -\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}\right). \tag{A14}$$

The wave function for the above differential equation is the same as in Eq. (A12) with scale factor q defined as

$$q(\xi) = \frac{\xi}{z/R}. \tag{A15}$$

Since in the infinite radius limit these two scale factors are the same, the eigenvalues, ξ and s, must be related by

$$\xi = 2\pi q = \frac{s}{R}. \tag{A16}$$

This solution is of course the same as that of Inönü and Wigner, because s and j are the same when both are large. The generalization of the above construction to any dimensions is also quite straightforward.

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Quantum integrability of quadratic Killing tensors

C. Duval[a)]
Centre de Physique Théorique, CNRS, Luminy, Case 907, F-13288 Marseille Cedex 9, France[b)]

G. Valent[c)]
Laboratoire de Physique Théorique et des Hautes Energies, 2, Place Jussieu, F-75251 Paris Cedex 5, France[d)]

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Quantum integrability of classical integrable systems given by quadratic Killing tensors on curved configuration spaces is investigated. It is proven that, using a "minimal" quantization scheme, quantum integrability is ensured for a large class of classic examples. © *2005 American Institute of Physics.*
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I. INTRODUCTION

One of the main goals of this paper is to present a somewhat general framework for the quantization of classical observables on a cotangent bundle which are polynomials at most cubic in momenta. This approach enables us to investigate the quantization of classically Poisson-commuting observables, and hence to tackle the problem of quantum integrability for a reasonably large class of dynamical systems.

What should actually be the definition of quantum integrability is a long standing issue, see, e.g., Ref. 37. The point of view espoused in this paper is the following. Start with a complete set of independent Poisson-commuting classical observables, and use some quantization rule to get a corresponding set of quantum observables; if these operators appear to be still in involution with respect to the commutator, the system will be called integrable at the quantum level.

Our work can be considered as a sequel to earlier and pioneering contributions[11,4,5,22,34] that provide worked examples of persistence of integrability from the classical to the quantum regime. The general approach we deal with in this paper helps us to highlight the general structure of quantum corrections and to show that the latter actually vanish in most, yet not all, interesting examples.

Returning to the general issue of quantization, let us mention that our choice of quantization procedure, which we might call "minimal," does not stem from first principles, e.g., from invariance or equivariance requirements involving some specific symmetry. Although this "minimal" quantization only applies to low degree polynomials on cotangent bundles, it has the virtue of leading automatically to the simplest symmetric operators that guarantee quantum integrability in many cases. In order to provide the explicit form of the quantization scheme, hence of the quantum corrections, we need a symmetric linear connection to be given on the base of our cotangent bundle. In most examples where a (pseudo-)Riemannian metric is considered from the outset, this connection will be chosen as the Levi-Civita connection.

To exemplify our construction, we consider a number of examples of classical integrable systems together with their quantization. For instance, our approach for dealing with quantum

[a)]Electronic mail: duval@cpt.univ-mrs.fr
[b)]UMR 6207 du CNRS associée aux Universités d'Aix-Marseille I et II Université du Sud Toulon-Var; Laboratoire affilié à la FRUMAM-FR2291.
[c)]Electronic mail: gvalent@lumimath.univ-mrs.fr
[d)]UMR 7589 du CNRS associée aux Universités Paris VI et Paris VII.

integrability in somewhat general terms allowed us to deduce the quantum integrability of the Hamiltonian flow for the generalized Kerr–Newman solution of the Einstein–Maxwell equations with a cosmological constant first discovered by Carter.[9–11] Also our quantization scheme leads us to an independent proof of the quantum integrability for Stäckel systems originally due to Benenti, Chanu, and Rastelli.[4,5]

The paper is organized as follows. In Sec. II we gather the definitions of the Schouten bracket of symmetric contravariant tensor fields on configuration space, M. We make use of Souriau's procedure to present, in a manifestly gauge invariant fashion, the minimal coupling to an external electromagnetic field; this enables us to provide a geometric definition of the so-called Schouten–Maxwell bracket. The related definitions of Killing and Killing–Maxwell tensors follow naturally and will be used throughout the rest of the article. We recall the basics of classical integrable systems, with emphasis on the Stäckel class. The main objective of the present section is then to revisit some classic examples of integrable systems involving Killing tensors. Naturally starting with the Jacobi system on the ellipsoid, we prove, *en passant*, that it is locally of the Stäckel type, even allowing for an extra harmonic potential. This extends previous work of Benenti[3] related to the geodesic flow of the ellipsoid. Similarly, we show that the Neumann system is also locally Stäckel. A number of additional examples, not of Stäckel type, e.g., the Di Pirro system, and the geodesic flow on various (pseudo-)Riemannian manifolds such as the Kerr–Newman–de Sitter solution and the multi-center solution are also considered.

We introduce, in Sec. III, a specific "minimal" quantization scheme for observables at most cubic in momenta on the cotangent bundle T^*M of a smooth manifold M endowed with a symmetric connection ∇, extending a previous proposal.[11] This quantization mapping is shown to be equivariant with respect to the affine group of (M,∇). The computation of the commutators of quantum observables is then carried out and yields explicit expressions for quantum corrections. We also provide the detailed analysis of quantum integrability for a wide class of examples within the above-mentioned list.

The concluding section includes a discussion and brings together several remarks about the status of the "minimal" quantization that has been abstracted from the various examples dealt with in this paper. It also opens some prospects for future investigations related to quantum integrability in the spirit of this work.

II. CLASSICAL INTEGRABLE SYSTEMS

A. Killing tensors

Let us start with the definition of the Schouten bracket of two polynomial functions on the cotangent bundle $(T^*M,\omega=\mathrm{d}\xi_i\wedge\mathrm{d}x^i)$ of a smooth manifold M. Consider two such homogeneous polynomials $P=P^{i_1\ldots i_k}(x)\xi_{i_1}\ldots\xi_{i_k}$ and $Q=Q^{i_1\ldots i_\ell}(x)\xi_{i_1}\ldots\xi_{i_\ell}$ of degree k and ℓ, respectively; we will identify these polynomials with the corresponding smooth symmetric contravariant tensor fields $P^\sharp=P^{i_1\ldots i_k}(x)\partial_{i_1}\otimes\cdots\otimes\partial_{i_k}$ and $Q^\sharp=Q^{i_1\ldots i_\ell}(x)\partial_{i_1}\otimes\cdots\otimes\partial_{i_\ell}$.

The Schouten bracket $[P^\sharp,Q^\sharp]_S$ of the two contravariant symmetric tensors $P^\sharp$ and $Q^\sharp$ (of degree k and ℓ, respectively) is the symmetric contravariant $(k+\ell-1)$-tensor corresponding to the Poisson bracket of P and Q, namely

$$[P^\sharp,Q^\sharp]_S=\{P,Q\}^\sharp. \tag{2.1}$$

Using the Poisson bracket $\{P,Q\}=\partial_{\xi_i}P\partial_iQ-\partial_{\xi_i}Q\partial_iP$, and (2.1), we readily get the local expression of the Schouten bracket of $P^\sharp$ and $Q^\sharp$. If the manifold M is endowed with a symmetric connection ∇, the latter can be written as

$$[P^\sharp,Q^\sharp]_S^{i_1\ldots i_{k+\ell-1}}=kP^{i(i_1\ldots i_{k-1}}\nabla_iQ^{\,i_k\ldots i_{k+\ell-1})}-\ell Q^{i(i_1\ldots i_{\ell-1}}\nabla_iP^{\,i_\ell\ldots i_{k+\ell-1})}. \tag{2.2}$$

[In this paper the round (respectively, square) brackets will denote symmetrization (respectively, skew-symmetrization) with the appropriate combinatorial factor.] If M is, in addition, equipped with a (pseudo-)Riemannian metric, g, we denote by

$$H = \tfrac{1}{2} g^{ij} \xi_i \xi_j \tag{2.3}$$

the Hamiltonian function associated with this structure. The Hamiltonian flow associated with H is nothing but the geodesic flow on T^*M.

A symmetric contravariant tensor field $P^\sharp$ of degree k satisfying $\{H,P\}=0$ is called a Killing (or Killing–Stäckel) tensor; now using the Levi-Civita connection ∇ in (2.2), this condition reads

$$\nabla^{(i} P^{i_1 \dots i_k)} = 0. \tag{2.4}$$

B. Killing–Maxwell tensors

1. Souriau's coupling

In the presence of an electromagnetic field, F, Souriau[33] has proposed to replace the canonical symplectic structure, ω, of T^*M by the twisted symplectic structure $\omega_F = \mathrm{d}\xi_i \wedge \mathrm{d}x^i + \frac{1}{2} F_{ij} \mathrm{d}x^i \wedge \mathrm{d}x^j$. The (gauge-invariant) Poisson bivector now reads

$$\pi_F = \partial_{\xi_i} \wedge \partial_i - \tfrac{1}{2} F_{ij} \partial_{\xi_i} \wedge \partial_{\xi_j}.$$

The Poisson bracket of two observables P, Q of T^*M is now

$$\{P,Q\}_F = \pi_F(dP, dQ) = \partial_{\xi_i} P \partial_i Q - \partial_{\xi_i} Q \partial_i P - F_{ij} \partial_{\xi_i} P \wedge \partial_{\xi_j} Q, \tag{2.5}$$

and the Schouten–Maxwell bracket of two polynomials P and Q is then defined by

$$[P^\sharp, Q^\sharp]_{S,F} = \{P,Q\}_F^\sharp.$$

If the manifold M is endowed with a symmetric connection ∇, the Schouten–Maxwell bracket takes on the following form:

$$[P^\sharp, Q^\sharp]_{S,F} = [P^\sharp, Q^\sharp]_S^{i_1 \dots i_{k+\ell-1}} \partial_{i_1} \otimes \cdots \otimes \partial_{i_{k+\ell-1}} - k\ell F_{ij} P^{i(i_1 \dots i_{k-1}} Q^{i_k \dots i_{k+\ell-2})j} \partial_{i_1} \otimes \cdots \otimes \partial_{i_{k+\ell-2}} \tag{2.6}$$

with the expression (2.2) of the Schouten bracket $[\cdot,\cdot]_S$.

Suppose now that the manifold M is endowed with a metric g; the Hamiltonian vector field on (T^*M, ω_F) for the Hamiltonian H given by (2.3) yields the Lorentz equations of motions for a charged test particle moving on (M,g) under the influence of an external electromagnetic field F.

A symmetric contravariant tensor field $P^\sharp$ of degree k on (M,g) is now called a Killing–Maxwell tensor if $\{H,P\}_F=0$. The Killing–Maxwell equations then read, using (2.6),

$$\nabla^{(i} P^{i_1 \dots i_k)} = 0, \quad P^{i(i_1 \dots i_{k-1}} F_i^{\ i_k)} = 0, \tag{2.7}$$

where $F_i^j = g^{jm} F_{mi}$, in accordance with previous results[11] obtained with a slightly different standpoint.

The conditions (2.7) are of special importance for proving the classical and quantum integrability of the equations of motion of a charged test particle in the generalized Kerr–Newman background.

2. Standard electromagnetic coupling

A more traditional, though equivalent, means to deal with the coupling to an electromagnetic field, $F=\mathrm{d}A$ (locally), is to keep the canonical one-form, $\alpha = \xi_i \mathrm{d}x^i$, on T^*M unchanged, and hence to work with the original Poisson bracket $\{\cdot,\cdot\}$, but to replace the Hamiltonian (2.3) by

$$\tilde{H} = \tfrac{1}{2} \mathrm{g}^{ij} (\xi_i - A_i)(\xi_j - A_j), \tag{2.8}$$

where the tilde makes it clear that the expressions to consider are actually polynomials in the variables $\xi_i - A_i$, for $i=1,\dots,n$; for example, if $P = P^{i_1 \cdots i_k} \xi_{i_1} \dots \xi_{i_k}$, then

$$\widetilde{P} = P^{i_1\cdots i_k}(\xi_{i_1} - A_{i_1}) \ldots (\xi_{i_k} - A_{i_k}). \tag{2.9}$$

The equations of motion given by the Hamiltonian vector field for the Hamiltonian (2.8) on $(T^*M, \mathrm{d}\alpha)$ are, again, the Lorentz equations of motion.

The Schouten–Maxwell brackets and Schouten brackets for the electromagnetic coupling are related as follows via the corresponding Poisson brackets, viz.

$$\{P,Q\}_F = \{\widetilde{P},\widetilde{Q}\}.$$

In this framework, a Killing–Maxwell tensor, $P^\sharp$, of degree k on (M,g) is defined by the equation $\{\widetilde{H},\widetilde{P}\}=0$. The resulting constraints are, again, given by (2.7).

From now on, and in order to simplify the notation, we will omit the $\sharp$-superscript and use the same symbol for symmetric contravariant tensors and the corresponding polynomial functions on T^*M.

C. General definition of classical integrability

Let us recall that a dynamical system $(\mathcal{M},\omega,H)$ is (Liouville) integrable if there exist $n = \frac{1}{2}\dim\mathcal{M}$ independent Poisson-commuting functions $P_1,\ldots,P_n \in C^\infty(\mathcal{M})$—that is $\mathrm{d}P_1\wedge\cdots\wedge\mathrm{d}P_n \neq 0$ and $\{P_k,P_\ell\}=0$ for all $k,\ell=1,\ldots,n$—such that $P_1=H$.

We will, in the sequel, confine considerations to the case of cotangent bundles, $(\mathcal{M}=T^*M,\omega=\mathrm{d}\theta)$ where θ is the canonical one-form, and of polynomial functions, $P_1,\ldots,P_n$, on T^*M, that is to the case of n Schouten-commuting Killing tensors. Moreover, all examples that we will consider will be given by polynomials of degree two or three.

D. The Stäckel systems

These systems on $(T^*M,\omega=\mathrm{d}\xi_i\wedge\mathrm{d}x^i)$ are governed by the Hamiltonians

$$H = \sum_{i=1}^{n} a^i(x)\left(\tfrac{1}{2}\xi_i^2 + f_i(x^i)\right) \tag{2.10}$$

where the ith function f_i depends on the coordinate x^i only, and the functions a^i are defined as follows. Let B denote a $\mathrm{GL}(n,\mathbf{R})$-valued function defined on M and such that

$$B(x) = (B_1(x^1)B_2(x^2)\ldots B_n(x^n)),$$

where the ith column $B_i(x^i)$ depends on x^i only $(i=1,\ldots,n)$; such a matrix will be called a Stäckel matrix. Then take

$$a(x) = \begin{pmatrix} a^1(x) \\ \vdots \\ a^n(x) \end{pmatrix}$$

to be the first column $A_1(x)$ of the matrix $A(x)=B(x)^{-1}$.

The integrability of such a system follows from the existence of n quadratic polynomials

$$I_\ell = \sum_{i=1}^{n} A^i_\ell(x)\left(\tfrac{1}{2}\xi_i^2 + f_i(x^i)\right), \quad \ell = 1,\ldots,n, \quad H = I_1. \tag{2.11}$$

We call Stäckel potential every function of the form

$$U_\ell(x) = \sum_{i=1}^{n} A_\ell^i(x) f_i(x^i), \quad \ell = 1, \ldots, n; \tag{2.12}$$

the potential appearing in the Hamiltonian is just U_1.

One can check (see, e.g., Ref. 28, p. 101) that the n independent quantities I_ℓ are such that

$$\{I_\ell, I_m\} = \sum_{s,t=1}^{n} (A_\ell^s \partial_s A_m^t - A_m^s \partial_s A_\ell^t) \xi_s \left(\frac{1}{2} \xi_t^2 + f_t \right), \quad \ell \neq m.$$

The relation $A = B^{-1}$, gives the useful identity (the Einstein summation convention is not used)

$$\partial_k A_j^i = - C_k^i A_j^k, \quad C_k^i = \sum_{s=1}^{n} A_s^i \frac{dB_k^s}{dx^k}, \tag{2.13}$$

which implies

$$A_\ell^s \partial_s A_m^t - A_m^s \partial_s A_\ell^t = 0, \quad \ell \neq m, \quad s,t = 1, \ldots, n \tag{2.14}$$

and therefore the so-defined Stäckel systems are classically integrable.

Remark 2.1: Let us mention an interesting result due to Pars (see Ref. 28, p. 102): for a system whose Hamiltonian is of the form (2.10), the Hamilton–Jacobi equation is separable if and only if this system is Stäckel.

Although these systems constitute quite a large class of integrable systems, they do not exhaust the full class. A simple example of a non-Stäckel integrable system was produced by Di Pirro (see Sec. II I).

E. The Jacobi integrable system on the ellipsoid

Let $\mathcal{E} \subset \mathbf{R}^{n+1}$ be the n-dimensional ellipsoid defined by the equation $Q_0(y,y) = 1$ where we define, for $y, z \in \mathbf{R}^{n+1}$,

$$Q_\lambda(y,z) = \sum_{\alpha=0}^{n} \frac{y_\alpha z_\alpha}{a_\alpha - \lambda}, \tag{2.15}$$

with $0 < a_0 < a_1 < \ldots < a_n$; the equations $Q_\lambda(y,y) = 1$ define a family of confocal quadrics.

It has been proved by Jacobi (in the case $n=2$) that the differential equations governing the geodetic motions on the ellipsoid, $\mathcal{E}$, form an integrable system. The same remains true if a quadratic potential is admitted (see Ref. 27). The Hamiltonian of the system, prior to reduction, reads

$$H(p,y) = \frac{1}{2} \sum_{\alpha=0}^{n} p_\alpha^2 + \frac{a}{2} \sum_{\alpha=0}^{n} y_\alpha^2 \tag{2.16}$$

where $p, y \in \mathbf{R}^{n+1}$ and a is some real parameter.

Moser has shown[26] that the following polynomial functions

$$F_\alpha(p,y) = p_\alpha^2 + a y_\alpha^2 + \sum_{\beta \neq \alpha} \frac{(p_\alpha y_\beta - p_\beta y_\alpha)^2}{a_\alpha - a_\beta} \quad \text{with} \quad \alpha = 0,1, \ldots, n, \tag{2.17}$$

are in involution on $(T^*\mathbf{R}^{n+1}, \Sigma_{\alpha=0}^n \mathrm{d}p_\alpha \wedge \mathrm{d}y_\alpha)$. Those will generate the commuting first integrals of the Jacobi dynamical system on the cotangent bundle $T^*\mathcal{E}$ of the ellipsoid.

Our goal is to deduce from the knowledge of (2.17) the independent quantities in involution $I_1, \ldots, I_n$ on $(T^*\mathcal{E}, \mathrm{d}\xi_i \wedge \mathrm{d}x^i)$ from the symplectic embedding

$$\iota: T^*\mathcal{E} \hookrightarrow T^*\mathbf{R}^{n+1}$$

given by $Z_1(p,y)=Q_0(y,y)-1=0$ and $Z_2(p,y)=Q_0(p,y)=0$.

Proposition 2.2: The restrictions $F_\alpha|_{T^*\mathcal{E}}=F_\alpha\circ\iota$ *of the functions (2.17) Poisson-commute on* $T^*\mathcal{E}$.

Proof: We get, using Dirac brackets,

$$\{F_\alpha|_{T^*\mathcal{E}}, F_\beta|_{T^*\mathcal{E}}\} = \{F_\alpha,F_\beta\}|_{T^*\mathcal{E}} - \frac{1}{\{Z_1,Z_2\}}[\{Z_1,F_\alpha\}\{Z_2,F_\beta\} - \{Z_1,F_\beta\}\{Z_2,F_\alpha\}]|_{T^*\mathcal{E}} \tag{2.18}$$

for second-class constraints. Now, the denominator $\{Z_1,Z_2\}=-2\Sigma_{\alpha=0}^n(y_\alpha/a_\alpha)^2$ does not vanish while $\{Z_1,F_\alpha\}=4(p_\alpha y_\alpha/a_\alpha)Z_1-4(y_\alpha^2/a_\alpha)Z_2$ is zero on $T^*\mathcal{E}$, for all $\alpha=0,\ldots,n$. The fact that $\{F_\alpha,F_\beta\}=0$ completes the proof. □

The reduced Hamiltonian for the Jacobi system on the ellipsoid $\mathcal{E}$ is plainly

$$H=\frac{1}{2}\sum_{\alpha=0}^n (p_\alpha^2+ay_\alpha^2)|_{T^*\mathcal{E}} = \frac{1}{2}\sum_{\alpha=0}^n F_\alpha|_{T^*\mathcal{E}}. \tag{2.19}$$

In order to provide explicit expressions for the function in involution $I_1,\ldots,I_n$, we resort to Jacobi ellipsoidal coordinates $x^1,\ldots,x^n$ on $\mathcal{E}$. Those are defined by

$$Q_\lambda(y,y) = 1 - \frac{\lambda U_x(\lambda)}{V(\lambda)}, \tag{2.20}$$

where

$$U_x(\lambda)=\prod_{i=1}^n(\lambda-x^i), \quad V(\lambda)=\prod_{\alpha=0}^n(\lambda-a_\alpha) \tag{2.21}$$

and are such that $a_0<x^1<a_1<x^2<\ldots<x^n<a_n$. The induced metric, $g=\Sigma_{i,j=1}^n g_{ij}(x)\mathrm{d}x^i\mathrm{d}x^j$, of the ellipsoid $\mathcal{E}$ is given by

$$g_{ij}(x)=\frac{1}{4}\sum_{\alpha=0}^n\frac{y_\alpha^2}{(a_\alpha-x^i)(a_\alpha-x^j)}$$

and retains the form[26]

$$g=\sum_{i=1}^n g_i(x)(\mathrm{d}x^i)^2 \quad \text{where} \quad g_i(x)=-\frac{x^i}{4}\frac{U_x'(x^i)}{V(x^i)}, \tag{2.22}$$

which is actually Riemannian because of the previous inequalities. We put for convenience $g^i(x)=1/g_i(x)$.

Using (2.20) and (2.21), we find the local expressions $y_\alpha(x)$ via the formula

$$y_\alpha^2 = a_\alpha\frac{\prod_{i=1}^n(a_\alpha-x^i)}{\prod_{\beta\neq\alpha}(a_\alpha-a_\beta)} \tag{2.23}$$

and then obtain the constrained coordinate functions

$$p_\alpha(\xi,x) = -\frac{1}{2}y_\alpha\sum_{i=1}^n\frac{g^i(x)\xi_i}{(a_\alpha-x^i)} \tag{2.24}$$

given by the induced canonical one-form $\Sigma_{i=1}^n\xi_i\mathrm{d}x^i=\iota^*(\Sigma_{\alpha=0}^n p_\alpha\mathrm{d}y_\alpha)$.

The Hamiltonian (2.19) on $(T^*\mathcal{E}, \mathrm{d}\xi_i \wedge \mathrm{d}x^i)$ is then found to be

$$H = \frac{1}{2}\sum_{i=1}^{n} g^i(x)\xi_i^2 + \frac{a}{2}\left[\sum_{\alpha=0}^{n} a_\alpha - \sum_{i=1}^{n} x^i\right]. \tag{2.25}$$

Note that the potential term is obtained from the large λ behavior

$$Q_\lambda(y,y) \sim \frac{1}{\lambda}\sum_{\alpha=0}^{n} y_\alpha^2 + \frac{1}{\lambda^2}\sum_{\alpha=0}^{n} a_\alpha y_\alpha^2 + \cdots,$$

which can be computed using relation (2.20). One gets

$$Q_\lambda(y,y) \sim \frac{1}{\lambda}\left[\sum_{\alpha=0}^{n} a_\alpha - \sum_{i=1}^{n} x^i\right] + \cdots .$$

One relates the conserved quantities (2.17) to their reduced expressions on $T^*\mathcal{E}$ by computing, using (2.24) and (2.23), the expression of $F_\alpha|_{T^*\mathcal{E}}$. One gets

Proposition 2.3: The Moser conserved quantities $(F_\alpha|_{T^*\mathcal{E}})_{\alpha=0,\ldots,n}$ *retain the form*

$$F_\alpha|_{T^*\mathcal{E}} = \frac{a_\alpha G_{a_\alpha}(\xi,x)}{\prod_{\beta\neq\alpha}(a_\alpha - a_\beta)}$$

where

$$G_\lambda(\xi,x) = \sum_{i=1}^{n} g^i(x)\prod_{j\neq i}(\lambda - x^j)\xi_i^2 + a\prod_{i=1}^{n}(\lambda - x^i). \tag{2.26}$$

It is useful to introduce the notation $\sigma_k^i(x)$ for the symmetric functions of order $k = 0,1,\ldots,n-1$ of the variables $(x^1,\ldots,x^n)$, with the exclusion of index i, namely

$$\prod_{j\neq i}(\lambda - x^j) = \sum_{k=1}^{n}(-1)^{k-1}\lambda^{n-k}\sigma_{k-1}^i(x). \tag{2.27}$$

We note that, from the above definition, $\sigma_0^i(x) = 1$.

It is also worthwhile to introduce other symmetric functions, $\sigma_k(x)$, via

$$\prod_{j=1}^{n}(\lambda - x^j) = \sum_{k=0}^{n}(-1)^k\lambda^{n-k}\sigma_k(x). \tag{2.28}$$

We thus have

$$G_\lambda(\xi,x) = \sum_{i=1}^{n}(-1)^{i-1}\lambda^{n-i}I_i(\xi,x) + a(-\lambda)^n, \tag{2.29}$$

where the independent functions I_i $(i = 1,\ldots,n)$ are in involution and can be written as

$$I_i(\xi,x) = \sum_{j=1}^{n} A_i^j(x)\xi_j^2 - a\sigma_i(x) \quad \text{with} \quad A_i^j(x) = g^j(x)\sigma_{i-1}^j(x). \tag{2.30}$$

In the case $i = 1$, we recover the Hamiltonian (2.25), i.e.,

$$H = \frac{1}{2}I_1 + \frac{a}{2}\sum_{\alpha=0}^{n} a_\alpha.$$

Proposition 2.4: The Jacobi system on $T^\star\mathcal{E}$ defines a Stäckel system, with Stäckel matrix

$$B_k^i(x^k) = (-1)^i \frac{(x^k)^{n+1-i}}{4V(x^k)} \tag{2.31}$$

and potential functions

$$f_k(x^k) = a\frac{(x^k)^{n+1}}{4V(x^k)} \tag{2.32}$$

for $i,k=1,\ldots,n$.

Proof: It is obvious from its definition that B is a Stäckel matrix. We just need to prove that $A=B^{-1}$. To this aim we first prove a useful identity. Let us consider the integral in the complex plane

$$\frac{1}{2i\pi}\int_{|z|=R} \frac{z^{n-i}}{(z-\lambda)}\frac{U_x(\lambda)}{U_x(z)}\mathrm{d}z.$$

When $R\to\infty$ the previous integral vanishes because the integrand vanishes as $1/R^2$ for large R. We then compute this integral using the theorem of residues and we get the identity

$$\sum_{k=1}^{n} \frac{(x^k)^{n-i}}{U_x'(x^k)}\prod_{j\neq k}(\lambda - x^j) = \lambda^{n-i}. \tag{2.33}$$

Equipped with this identity let us now prove that

$$\sum_{k=1}^{n} B_k^i A_j^k = \delta_j^i.$$

Multiplying this relation by $(-1)^{j-1}\lambda^{n-j}$ and summing over j from 1 to n, we get the equivalent relation

$$\sum_{k=1}^{n} B_k^i \sum_{j=1}^{n} (-1)^{j-1}\lambda^{n-j}A_j^k = (-1)^{i-1}\lambda^{n-i},$$

which becomes, using (2.30) and (2.27):

$$\sum_{k=1}^{n} B_k^i g^k(x)\prod_{j\neq k}(\lambda - x^j) = (-1)^{i-1}\lambda^{n-i}.$$

Using the explicit form of $g^k(x)$ given in (2.22) and of the matrix B, this relation reduces to the identity (2.33) and this completes the derivation of (2.31).

In order to get the functions $f_i(x^i)$ as in (2.10), let us resort to (2.30) and solve, for the unknown f_i, the following

$$-a\sigma_i(x) = \sum_{j=1}^{n} A_i^j(x) f_j.$$

Multiplying both sides by B_k^i, summing over i from 1 to n, and using (2.31) we get

$$f_k = -a\sum_{i=1}^{n} B_k^i\sigma_i(x) = -\frac{a}{4V(x^k)}\sum_{i=1}^{n}(-1)^i(x^k)^{n+1-i}\sigma_i(x) = -\frac{a}{4V(x^k)}\left[\sum_{i=0}^{n}(-1)^i(x^k)^{n+1-i}\sigma_i(x) - (x^k)^{n+1}\right].$$

In view of (2.28), we have $\Sigma_{i=0}^{n}(-1)^i(x^k)^{n-i}\sigma_i(x) = \Pi_{j=1}^{n}(x^k - x^j) = 0$, which completes the proof. □

Remark 2.5: 1. The fact that the geodesic flow on $T^\star\mathcal{E}$ is a Stäckel system was first proved by

Benenti in Ref. 3. We have given here a new derivation, which makes the link between Moser's conserved quantities on $T^*\mathbf{R}^{n+1}$ and the Stäckel conserved quantities on $T^*\mathcal{E}$. We have extended this link to the case where Jacobi's potential is admitted.

2. Checking that the unconstrained observables I_i are in involution is most conveniently done using their generating function (2.26). Indeed it is easy to verify the relation

$$\{G_\lambda(\xi,x),G_\mu(\xi,x)\}=0, \quad \lambda,\mu\in\mathbf{R},$$

which implies, via (2.29), and upon expansion in powers of λ and μ, the relations $\{I_i,I_j\}=0$ for any $i,j=1,\ldots,n$.

3. Some authors[2,22] have quantized the full set of commuting observables for the geodesic flow of the ellipsoid $\mathcal{E}\subset\mathbf{R}^{n+1}$ in its unconstrained form, namely on $T^*\mathbf{R}^{n+1}$. Notice though that in the reduction process from $T^*\mathbf{R}^{n+1}$ to $T^*\mathcal{E}$ quantum corrections may prove necessary in order to ensure self-adjointness of the quantized observables. Our point of view will be to perform the classical reduction in the first place and then to quantize the observables directly on $T^*\mathcal{E}$ via a specific procedure that will be described in Sec. III.

F. The Neumann system

The Neumann Hamiltonian on $(T^*\mathbf{R}^{n+1},\Sigma_{\alpha=0}^n \mathrm{d}p_\alpha\wedge\mathrm{d}y_\alpha)$ is[1]

$$H=\frac{1}{2}\sum_{\alpha=0}^{n}(p_\alpha^2+a_\alpha y_\alpha^2) \tag{2.34}$$

with the real parameters $0<a_0<a_1<\ldots<a_n$. Under the symplectic reduction, with the second class constraints

$$Z_1(p,y)=\sum_{\alpha=0}^{n}y_\alpha^2-1=0, \quad Z_2(p,y)=\sum_{\alpha=0}^{n}p_\alpha y^\alpha=0, \tag{2.35}$$

it becomes a dynamical system on $(T^*S^n,\mathrm{d}\xi_i\wedge\mathrm{d}x^i)$.

This system is classically integrable, with the following commuting first integrals of the Hamiltonian flow in $T^*\mathbf{R}^{n+1}$:

$$F_\alpha(p,y)=y_\alpha^2+\sum_{\beta\neq\alpha}\frac{(p_\alpha y_\beta-p_\beta y_\alpha)^2}{a_\alpha-a_\beta} \quad \text{with} \quad \alpha=0,1,\ldots,n. \tag{2.36}$$

The symplectic embedding

$$\iota:T^*S^n\hookrightarrow T^*\mathbf{R}^{n+1}$$

given by $Z_1(p,y)=0$ and $Z_2(p,y)=0$ preserves the previous conservation laws. Indeed the Poisson brackets of the restrictions $F_\alpha|_{T^*\mathcal{E}}=F_\alpha\circ\iota$ of the functions F_α are still given by the Dirac brackets (2.18) of the second class constraints (2.35). This time we have

$$\{Z_1,Z_2\}=-2\sum_{\alpha=0}^{n}y_\alpha^2\neq 0, \quad \{Z_1,F_\alpha\}=0,$$

which gives again

$$\{F_\alpha|_{T^*\mathcal{E}},F_\beta|_{T^*\mathcal{E}}\}=0.$$

Let us introduce an adapted coordinate system on $(T^*S^n,\mathrm{d}\xi_i\wedge\mathrm{d}x^i)$ much in the same manner as for the ellipsoid.

We start with the following definition[26] of a coordinate system $(x^1,\ldots,x^n)$ on S^n:

$$Q_\lambda(y,y) = \sum_{\alpha=0}^{n} \frac{y_\alpha^2}{a_\alpha - \lambda} = -\frac{\prod_{i=1}^{n}(\lambda - x^i)}{\prod_{\alpha=0}^{n}(\lambda - a_\alpha)}.$$

The following inequalities hold: $0 < a_0 < x^1 < a_1 < \ldots < x^n < a_n$. We get, in the same way as before,

$$y_\alpha^2 = \frac{\prod_{i=1}^{n}(a_\alpha - x^i)}{\prod_{\beta\neq\alpha}(a_\alpha - a_\beta)} \tag{2.37}$$

together with the following expression of the round metric $g = \Sigma_{\alpha=0}^{n} \mathrm{d}y_\alpha^2|_{S^n}$ in terms of the newly introduced coordinates, namely

$$g = \sum_{i=1}^{n} g_i(x)(\mathrm{d}x^i)^2 \quad \text{with } \mathrm{g}_i(x) = -\frac{U_x'(x^i)}{4V(x^i)} \tag{2.38}$$

with the notation (2.21). Again, we put for convenience $g^i(x) = 1/g_i(x)$.

Our goal is to deduce from the knowledge of (2.36) the independent quantities in involution $I_1, \ldots, I_n$ on $(T^*S^n, \mathrm{d}\xi_i \wedge \mathrm{d}x^i)$. The formula (2.24) relating unconstrained and constrained momenta still holds and yields

Proposition 2.6: The Neumann system $(F_\alpha|_{T^*S^n})_{\alpha=0,\ldots,n}$ *retains the following form:*

$$F_\alpha|_{T^*S^n} = -\frac{G_{a_\alpha}(\xi,x)}{\prod_{\beta\neq\alpha}(a_\alpha - a_\beta)},$$

where

$$G_\lambda(\xi,x) = \sum_{i=1}^{n} g^i(x) \prod_{j\neq i} (\lambda - x^j)\xi_i^2 + \prod_{j=1}^{n} (\lambda - x^j).$$

Let us, again, posit

$$G_\lambda(\xi,x) = \sum_{i=1}^{n} (-1)^{i-1} \lambda^{n-i} I_i(\xi,x) + \lambda^n$$

where the independent functions I_i $(i = 1, \ldots, n)$ are in involution and can be written as

$$I_i(\xi,x) = \sum_{j=1}^{n} A_i^j(x)\xi_j^2 - \sigma_i(x) \quad \text{with } A_i^j(x) = g^j(x)\sigma_{i-1}^j(x), \tag{2.39}$$

where the symmetric functions $\sigma_i(x)$ are as in (2.28).

Using the relations

$$\sigma_1(x) = \sum_{i=1}^{n} x^i, \quad \sum_{\alpha=0}^{n} a_\alpha y_\alpha^2 = \sum_{\alpha=0}^{n} a_\alpha - \sum_{i=1}^{n} x^i,$$

one can check that the Hamiltonian (2.34) is $H = \frac{1}{2} I_1$.

Proposition 2.7: The Neumann flow on (T^*S^n, H) *defines a Stäckel system, with Stäckel matrix*

$$B_k^i(x^k) = (-1)^i \frac{(x^k)^{n-i}}{4V(x^k)}$$

and potential functions

$$f_k(x^k) = \frac{(x^k)^n}{4V(x^k)} \tag{2.40}$$

for $i,k=1,\ldots,n$.

Proof: To check that $A=B^{-1}$, it is enough to use the identity (2.33). The computation of the potential functions f_k proceeds along the same lines as in the proof of Proposition 2.4. □

Remark 2.8: The involution property $\{I_i,I_j\}=0$ for $i,j=1,\ldots,n$, similar to the case of the ellipsoid, is seen to follow from the relation $\{G_\lambda(\xi,x),G_\mu(\xi,x)\}=0$.

G. Test particles in generalized Kerr–Newman background

Plebanski and Demianski have constructed in Refs. 29 and 30 a class of metrics generalizing the Kerr–Newman solution in four-dimensional space-time. The former are also known as the Kerr–Newman–Taub–NUT–de Sitter solutions of the Einstein–Maxwell equations. The metric, in the coordinate system $(x^1,x^2,x^3,x^4)=(p,q,\sigma,\tau)$, retains the form

$$g = \frac{X}{p^2+q^2}(\mathrm{d}\tau + q^2\mathrm{d}\sigma)^2 - \frac{Y}{p^2+q^2}(\mathrm{d}\tau - p^2\mathrm{d}\sigma)^2 + \frac{p^2+q^2}{X}\mathrm{d}p^2 + \frac{p^2+q^2}{Y}\mathrm{d}q^2 \tag{2.41}$$

with

$$X = \gamma - g^2 + 2np - \epsilon p^2 - \frac{\Lambda}{3}p^4, \quad Y = \gamma + e^2 - 2mq + \epsilon q^2 - \frac{\Lambda}{3}q^4, \tag{2.42}$$

where (m,γ) are related to the mass and angular momentum of the Kerr black hole, (e,g) to the electric and magnetic charge; n is the NUT charge, and Λ the cosmological constant. The remaining parameter ϵ can be scaled out to ± 1 or 0.

This metric, g, together with the electromagnetic field, locally given by $F=dA$ where

$$A = \frac{1}{p^2+q^2}[(eq+gp)\mathrm{d}\tau + pq(gq-ep)\mathrm{d}\sigma], \tag{2.43}$$

provide an exact solution of the Einstein–Maxwell equations with cosmological constant Λ. Let us notice for further use that

$$\nabla_i A^i = 0. \tag{2.44}$$

Upon defining the one-forms

$$K = \sqrt{\frac{Y}{2(p^2+q^2)}}(\mathrm{d}\tau - p^2\mathrm{d}\sigma) + \sqrt{\frac{p^2+q^2}{2Y}}\mathrm{d}q,$$

$$L = \sqrt{\frac{Y}{2(p^2+q^2)}}(\mathrm{d}\tau - p^2\mathrm{d}\sigma) - \sqrt{\frac{p^2+q^2}{2Y}}\mathrm{d}q,$$

$$M_1 = \sqrt{\frac{p^2+q^2}{X}}\mathrm{d}p,$$

$$M_2 = \sqrt{\frac{X}{p^2+q^2}}(\mathrm{d}\tau + q^2\mathrm{d}\sigma),$$

one constructs the two-form

$$\mathcal{Y} = pK \wedge L - qM_1 \wedge M_2. \tag{2.45}$$

One can check that the twice-symmetric tensor $P=-\mathcal{Y}^2$, namely $P_{ij}=-\mathcal{Y}_{ik}\mathcal{Y}_{\ell j}\mathrm{g}^{k\ell}$, is a Killing–Maxwell tensor [see (2.7)], given by

$$P = p^2(K\otimes L + L\otimes K) + q^2(M_1\otimes M_1 + M_2\otimes M_2). \tag{2.46}$$

We thus recover Carter's result[11] about the integrability of the Hamiltonian flow for a charged test particle in the generalized Kerr–Newman background in a different manner.

Remark 2.9: The two-form $\mathcal{Y}$ in (2.45) defines what is usually called a Killing–Yano tensor.[20,8]

The four conserved quantities in involution for the generalized Kerr–Newman system are, respectively,

$$\widetilde{H} = \tfrac{1}{2}g^{ij}(\xi_i - A_i)(\xi_j - A_j), \quad \widetilde{P} = P^{ij}(\xi_i - A_i)(\xi_j - A_j) \tag{2.47}$$

where P is as in (2.46), and

$$\widetilde{S} = \xi_3 - A_3, \quad \widetilde{T} = \xi_4 - A_4. \tag{2.48}$$

H. The multi-center geodesic flow

The class of multi-center Euclidean metrics in four dimensions retain, in a local coordinate system $(x^i)=(t,(y^a)) \in \mathbf{R}\times\mathbf{R}^3$, the form

$$\mathrm{g} = \frac{1}{V(y)}(\mathrm{d}t + A_a(y)\mathrm{d}y^a)^2 + V(y)\gamma \tag{2.49}$$

with $\gamma=\delta_{ab}\mathrm{d}y^a\mathrm{d}y^b$ the flat Euclidean metric in three-space, and $\mathrm{d}V=\pm\star(\mathrm{d}A)$ where $\star$ is the Hodge star for γ. These conditions ensure that the metric (2.49) is Ricci-flat.

For some special potentials $V(y)$, the geodesic flow is integrable as shown in Refs. 21, 13, and 35. The four conserved quantities in involution are given by

$$H = \tfrac{1}{2}\mathrm{g}^{ij}\xi_i\xi_j, \quad K = K^i\xi_i, \quad L = L^i\xi_i, \quad P = P^{ij}\xi_i\xi_j, \tag{2.50}$$

where K and L are two commuting Killing vectors and P a Killing two-tensor whose expressions can be found in the previous references.

I. The Di Pirro system

Di Pirro has proved (see, e.g., Ref. 28, p. 113) that the Hamiltonian on $T^*\mathbf{R}^3$,

$$H = \frac{1}{2(\gamma(x^1,x^2)+c(x^3))}[a(x^1,x^2)\xi_1^2 + b(x^1,x^2)\xi_2^2 + \xi_3^2] \tag{2.51}$$

admits one and only one additional first integral given by

$$P = \frac{1}{(\gamma(x^1,x^2)+c(x^3))}[c(x^3)(a(x^1,x^2)\xi_1^2 + b(x^1,x^2)\xi_2^2) - \gamma(x^1,x^2)\xi_3^2]. \tag{2.52}$$

In the case where the metric defined by H in (2.51) possesses a Killing vector, the system becomes integrable though not of Stäckel type. This happens, e.g., if (i) $c(x^3)=$const., or (ii) $a=b$ and γ depend on $r=\sqrt{(x^1)^2+(x^2)^2}$ only.

III. A QUANTIZATION SCHEME FOR INTEGRABLE SYSTEMS

We wish to deal now with the quantum version of the preceding examples. Let us start with some preliminary considerations:

1. There is no universally accepted procedure of quantization, i.e., of a linear identification, $\mathcal{Q}$, of a space of classical observables with some space of linear symmetric operators on a Hilbert space. One—among many—of the pathways to construct such a quantization mapping has been to demand that the mapping $\mathcal{Q}$ be equivariant with respect to some Lie group of symplectomorphisms of classical phase space.
2. Similarly, there is no universally accepted notion of quantum integrability. However, given a classical integrable system $P_1,\ldots,P_n$ on a symplectic manifold $(\mathcal{M},\omega)$, and a quantization mapping $\mathcal{Q}:P_i\mapsto\hat{P}_i$, we will say that such a system is integrable in the quantum sense if $[\hat{P}_i,\hat{P}_j]=0$ for all $i,j=1,\ldots,n$.
3. A large number of integrable systems involve *quadratic* observables. We will thus choose to concentrate on this important—yet very special—case, both from the classical and quantum viewpoint.
4. Among all possible quantization procedures, the search for integrability-preserving ones (if any) should be of fundamental importance. The quantization of quadratic observables we will present in the following might serve as a starting point for such a program.

A. Quantizing quadratic and cubic observables

Let us recall that the space $\mathcal{F}_\lambda(M)$ of λ-densities on M is defined as the space of sections of the complex line bundle $|\Lambda^n T^*M|^\lambda\otimes\mathbf{C}$. In the case where the configuration manifold is orientable, (M,vol), such a λ-density can be, locally, cast into the form $\phi=f|\mathrm{vol}|^\lambda$ with $f\in C^\infty(M)$ which means that ϕ transforms under the action of $a\in\mathrm{Diff}(M)$ according to $f\mapsto a_*f|(a_*\mathrm{vol})/\mathrm{vol}|^\lambda$.

The completion $\mathcal{H}(M)$ of the space of compactly supported half-densities, $\lambda=\frac{1}{2}$, is a Hilbert space canonically attached to M that will be used throughout this paper. The scalar product of two half-densities reads

$$\langle\phi,\psi\rangle=\int_M\overline{\phi}\psi,$$

where the bar stands for complex conjugation.

We will assume that configuration space is endowed with a (pseudo-)Riemannian structure, (M,g); and denote by $|\mathrm{vol}_g|$ the corresponding density and by Γ^k_{ij} the associated Christoffel symbols.

The quantization now introduced is a linear invertible mapping from the space of quadratic observables $P=P_2^{jk}(x)\xi_j\xi_k+P_1^j(x)\xi_j+P_0(x)$ to the space of second-order differential operators on $\mathcal{H}(M)$, viz. $A=\hat{P}=A_2^{jk}(x)\nabla_j\nabla_k+A_1^j(x)\nabla_j+A_0(x)\mathbf{1}$ where the covariant derivative of half-densities $\nabla_j\phi=\partial_j\phi-\frac{1}{2}\Gamma^k_{jk}\phi$ (or, locally, $\nabla_j\phi=(\partial_j f)|\mathrm{vol}_g|^{1/2}$) has been used. We furthermore require that the principal symbol be preserved [see in the following (3.1)–(3.3)], and that $\hat{P}$ be formally self-adjoint, i.e., $\langle\phi,\hat{P}\psi\rangle=\langle P\phi,\psi\rangle$ for all compactly supported $\phi,\psi\in\mathcal{F}_{1/2}(M)$.

The quantization reads

$$A_2^{jk}=-P_2^{jk}, \tag{3.1}$$

$$A_1^j=iP_1^j-\nabla_kP_2^{jk}, \tag{3.2}$$

$$A_0 = P_0 + \frac{i}{2}\nabla_j P_1^j \tag{3.3}$$

and admits the alternative form

$$P = -\nabla_j \circ P_2^{\mathrm{jk}} \circ \nabla_k + \frac{i}{2}(P_1^j \circ \nabla_j + \nabla_j \circ P_1^j) + P_0\mathbf{1}, \tag{3.4}$$

which makes clear the symmetry of the quantum operators.

Remark 3.1: The formula (3.4) was originally used by Carter[11] for proving the quantum integrability of the equations of motion of charged test particles in the Kerr–Newman solution.

Remark 3.2: It is worth mentioning that formula (3.4) actually corresponds at the same time to the projectively equivariant quantization[24,17] and to the conformally equivariant quantization[15,16] $\mathcal{Q}_{0,1}(P):\mathcal{F}_0(M)\to\mathcal{F}_1(M)$ restricted to quadratic polynomials.

One can check the relations:

$$[\hat{P}_0,\hat{Q}_1] = i[P_0,Q_1]_S = i\widehat{\{P_0,Q_1\}}, \tag{3.5}$$

$$[\hat{P}_0,\hat{Q}_2] = -\tfrac{1}{2}(\nabla_j \circ [P_0,Q_2]_S^j + [P_0,Q_2]_S^j \circ \nabla_j) = i\widehat{\{P_0,Q_2\}}, \tag{3.6}$$

$$[\hat{P}_1,\hat{Q}_1] = -\tfrac{1}{2}(\nabla_j \circ [P_1,Q_1]_S^j + [P_1,Q_1]_S^j \circ \nabla_j) = i\widehat{\{P_1,Q_1\}}. \tag{3.7}$$

Quantum corrections appear explicitly whenever $k+\ell>2$, as can be seen from the next commutators:

$$[\hat{P}_1,\hat{Q}_2] = i\widehat{\{P_1,Q_2\}} + i\hat{A}_{P_1,Q_2} \tag{3.8}$$

where

$$A_{P_1,Q_2} = \tfrac{1}{2}\nabla_j \circ Q_2^{jk} \circ \nabla_k(\nabla_\ell P_1^\ell) \tag{3.9}$$

is a scalar quantum correction that may vanish in some special instances, e.g., if the vector-field P_1 is divergence-free (in particular if it is a Killing vector-field).

The previous formulas can be found, in a different guise, in Ref. 11. Here, we will go one step further and compute the commutators $[\hat{P}_2,\hat{Q}_2]$ which involve third-order differential operators. To that end, we propose to quantize homogeneous cubic polynomials according to

$$\hat{P}_3 = -\frac{i}{2}(\nabla_j \circ P_3^{jk\ell} \circ \nabla_k \circ \nabla_l + \nabla_j \circ \nabla_k \circ P_3^{jk\ell} \circ \nabla_\ell) \tag{3.10}$$

as a "minimal" choice to ensure the symmetry of the resulting operator.

Remark 3.3: The formula (3.10) precisely coincides with the projectively equivariant quantization[7] $\mathcal{Q}_{0,1}(P):\mathcal{F}_0(M)\to\mathcal{F}_1(M)$ restricted to cubic polynomials.

The previously mentioned commutator is actually given by

$$[\hat{P}_2,\hat{Q}_2] = [P_2,Q_2]_S^{jk\ell}\nabla_j \circ \nabla_k \circ \nabla_\ell + \tfrac{3}{2}(\nabla_j[P_2,Q_2]_S^{jk\ell})\nabla_k \circ \nabla_\ell + \left[\tfrac{1}{2}(\nabla_j\nabla_k[P_2,Q_2]_S^{jk\ell}) + \tfrac{2}{3}(\nabla_k B_{P_2,Q_2}^{k\ell})\right]\nabla_\ell, \tag{3.11}$$

where the skew-symmetric tensor

$$B^{jk}_{P,Q} = P^{\ell[j}\,\nabla_\ell\nabla_m Q^{\,k]m} + P^{\ell[j}\,R^{\,k]}_{m,n\ell}Q^{mn} - (P \leftrightarrow Q) - \nabla_\ell P^{m[j}\,\nabla_m Q^{\,k]\ell} - P^{\ell[j}\,R_{\ell m}Q^{\,k]m} \tag{3.12}$$

satisfies, in addition, $B_{P,Q}=-B_{Q,P}$. We have used the following convention for the Riemann and Ricci tensors, viz. $R^{\ell}_{\ i,jk}=\partial_j\Gamma^{\ell}_{ik}-(j\leftrightarrow k)+\ldots$, and $R_{ij}=R^{k}_{\ i,kj}$.

We can rewrite the commutator (3.11) with the help of the quantization prescription (3.4) and (3.10) as

$$[\hat{P}_2,\hat{Q}_2] = i\widehat{\{P_2,Q_2\}} + i\hat{A}_{P_2,Q_2} \tag{3.13}$$

where

$$A_{P_2,Q_2} = -\tfrac{2}{3}(\nabla_k B^{k\ell}_{P_2,Q_2})\xi_\ell \tag{3.14}$$

is a divergence-free vector-field associated with the tensor (3.12) and providing the potential quantum correction for quadratic polynomials; recall that, according to (3.4), one has $\hat{A}_{P_2,Q_2}=(i/2)(A^{\ell}_{P2,Q2}\circ\nabla_\ell+\nabla_{\ell}\circ A^{\ell}_{P_2,Q_2})$.

We thus have

Proposition 3.4: The commutator of the quantum operators $\hat{P}$ and $\hat{Q}$ associated with two general quadratic polynomials $P=P_2+P_1+P_0$ and $Q=Q_2+Q_1+Q_0$ reads

$$\frac{1}{i}[\hat{P},\hat{Q}] = \widehat{\{P,Q\}} + \hat{A}_{P_2,Q_2} + \hat{A}_{P_1,Q_2} - \hat{A}_{Q_1,P_2} \tag{3.15}$$

where the third-order differential operator $\widehat{\{P,Q\}}$ is given by (3.10).

Proof: The formula (3.15) results trivially from the previously computed commutators and from collecting the anomalous terms appearing in (3.8) and (3.13) only. □

Remark 3.5: In the special case where $Q_2=H$ as given by (2.3), the anomalous tensor (3.12) takes the form

$$B^{jk}_{P,H} = -\tfrac{1}{2}\nabla^{[j}\,\nabla_\ell P^{\,k]\ell} - P^{\ell[j}\,R^{\,k]}_{\ell}$$

and reduces to

$$B^{jk}_{P,H} = -\,P^{\ell[j}\,R^{\,k]}_{\ell} \tag{3.16}$$

if P is a Killing tensor.[11]

Remark 3.6. In the particular case where $H=\frac{1}{2}g^{jk}(\xi_j-eA_j)(\xi_k-eA_k)$ is the Hamiltonian of the electromagnetic coupling, our quantum commutator (3.15) reduces to Carter's formula (6.16) in Ref. 11.

The purpose of our paper is, indeed, to study, using explicit examples, how classical integrability behaves under the "minimal" quantization rules proposed in Ref. 11 and somewhat extended here. The next section will be devoted to the computation of the quantum corrections in (3.8) and (3.13) for all the examples that have been previously introduced.

B. The equivariance Lie algebra

So far, the transformation property of the quantization rules (3.4) and (3.10) under a change of coordinates has been put aside. It is mandatory to investigate if these rules are consistent with the map $\mathcal{Q}:P\mapsto\hat{P}$ (which has been defined for cubic polynomials, $P=\Sigma_{k=0}^{3}P^{i_1\cdots i_k}\xi_{i_1}\ldots\xi_{i_k}$, only) being equivariant with respect to some Lie subgroup of the group of diffeomorphisms of configuration space, M.

Restricting considerations to the infinitesimal version of the sought equivariance, we will therefore look for the set $\mathfrak{g}$ of all vector fields X with respect to which our quantization is

equivariant, namely $L_X\mathcal{Q}=0$. From its very definition, $\mathfrak{g}$ is a Lie subalgebra of the Lie algebra, Vect(M), of vector fields of M. The previous condition means that, for each polynomial P, the following holds:

$$L_X(\mathcal{Q}(P)\phi) - \mathcal{Q}(L_XP)\phi - \mathcal{Q}(P)L_X\phi = 0, \tag{3.17}$$

where $L_X\phi$ denotes the Lie derivative of the half-density ϕ of M with respect to the vector field $X \in \mathfrak{g}$ and $L_XP=\{X,P\}$ is the Poisson bracket of $X=X^i\xi_i$ and P.

Let us recall that, putting locally $\phi=f|\mathrm{vol}|^{1/2} \in \mathcal{F}_{1/2}$ with $f \in C^\infty(M)$, we get the following expression for the Lie derivative: $L_X\phi=(Xf+1/2\mathrm{div}(X)f)|\mathrm{vol}|^{1/2}$, or with a slight abuse of notation, $L_X\phi=X^j\nabla_j\phi+\frac{1}{2}(\nabla_jX^j)\phi=\frac{1}{2}(X_j\circ\nabla_j+\nabla_j\circ X^j)\phi$, that is

$$L_X\phi = \frac{1}{i}\hat{X}\phi \tag{3.18}$$

for any $X \in \mathrm{Vect}(M)$.

The equivariance condition (3.17) must hold for any $\phi \in \mathcal{F}_{1/2}$ and thus translates into

$$[\hat{X},\hat{P}] = i\widehat{\{X,P\}} \tag{3.19}$$

for any $X \in \mathfrak{g}$ and any cubic polynomial P. The condition (3.19) characterizes the Lie algebra $\mathfrak{g}$ we are looking for. We will consider successively the case of polynomials of increasing degree:

(i) Returning to the previous relations (3.5) and (3.7) together with $X=P_1$ and $P=Q_0+Q_1$, we readily find that the Lie algebra $\mathfrak{g}_1$ spanned by the solutions of (3.19) restricted to polynomials P of degree one is $\mathfrak{g}_1=\mathrm{Vect}(M)$.

(ii) Let us now proceed to the case of quadratic polynomials $P=P^{jk}\xi_j\xi_k$. The relations (3.7) and (3.9) give, in that case, the following equivariance defect:

$$[\hat{X},\hat{P}] - i\widehat{\{X,P\}} = \frac{i}{2}\nabla_j\circ P^{jk}\circ\nabla_k(\nabla_\ell X^\ell)\mathbf{1}. \tag{3.20}$$

This defect vanishes for any such P iff $\nabla_k(\nabla_\ell X^\ell)=0$, i.e.,

$$d(\mathrm{div}(X)) = 0. \tag{3.21}$$

The vector fields X with constant divergence now span a subspace $\mathfrak{g}_2 \subset \mathfrak{g}_1$ which is, indeed, an infinite dimensional Lie subalgebra of Vect(M). The "minimal" quantization restricted to quadratic polynomials is therefore equivariant with respect to the group of all diffeomorphisms which preserve the volume up to a multiplicative nonzero constant.

(iii) Let us finally consider homogeneous cubic polynomials $P=P^{jk\ell}\xi_j\xi_k\xi_\ell$ and compute the equivariance defect in this case. A tedious calculation leads to

$$[\hat{X},\hat{P}] - i\widehat{\{X,P\}} = i\hat{Z}, \quad Z = Z^j\xi_j, \tag{3.22}$$

with

$$Z^j = \nabla_k[P^{jk\ell}\nabla_\ell\,\mathrm{div}(X) - P^{\ell m[j}\,L_X\Gamma^{\,k]}_{\ell m}] \tag{3.23}$$

where

$$L_X\Gamma^k_{\ell m} = \nabla_\ell\nabla_m X^k - R^k{}_{m,n\ell}X^n \tag{3.24}$$

is the Lie derivative of the symmetric linear connection ∇ with respect to the vector field X.

Proposition 3.7: The Lie algebra $\mathfrak{g} \subset \mathrm{Vect}(M)$ *with respect to which the "minimal" quantization* (3.4) and (3.10) *is equivariant is* $\mathrm{aff}(M,\nabla)$, *the Lie algebra of affine vector fields of* (M,∇).

Proof: The equivariance condition (3.19), defining the Lie algebra $\mathfrak{g}_3$ we are looking for, is

equivalent to $Z=0$ in (3.22) for all symmetric tensor fields $P^{jk\ell}$, i.e., thanks to (3.23) to

$$T_k^{jk\ell}\nabla_\ell \operatorname{div}(X) - T_k^{\ell m[j} L_X \Gamma^{k]}_{\ell m} = 0$$

for all tensor fields $T_k^{\ell mj} = T_k^{(\ell mj)}$. This readily implies that

$$2\delta^j_{(i}\,\delta^k_\ell \nabla_{m)} \operatorname{div}(X) + \delta^j_{(i} L_X \Gamma^k{}_{\ell m)} - \delta^k_{(i} L_X \Gamma^j{}_{\ell m)} = 0.$$

Summing over $i=j$, one gets

$$2n\delta^k_m \nabla_\ell \operatorname{div}(X) + 4\delta^k_\ell \nabla_m \operatorname{div}(X) + (n+1) L_X \Gamma^k_{\ell m} - \delta^k_m L_X \Gamma^i_{\ell i} - \delta^k_\ell L_X \Gamma^i_{mi} = 0,$$

where $n=\dim(M)$, hence $\nabla_i \operatorname{div}(X)=0$ and $L_X\Gamma^k_{ij} = \delta^k_i \varphi_j + \delta^k_j \varphi_i$ for some one-form φ depending upon the (projective) vector field X. The expression (3.24) of the Lie derivative of the symmetric connection ∇ then yields $L_X\Gamma^j_{ij} = (n+1)\varphi_i = 0$ since we have found that $\nabla_i \nabla_j X^j = 0$. This entails $L_X \Gamma^k_{ij} = 0$, proving that $\mathfrak{g} = \mathfrak{g}_3$ is nothing but the Lie algebra $\mathrm{aff}(M, \nabla)$ of affine vector fields. □

We thus obtain the nested equivariance Lie algebras

$$\mathfrak{g} = \mathrm{aff}(M, \nabla) \subset \mathfrak{g}_2 \subset \mathfrak{g}_1 = \mathrm{Vect}(M),$$

where $\mathfrak{g}_2$ is the Lie algebra of vector fields with constant divergence. (Note that if M is compact without boundary, $\mathfrak{g}_2$ reduces to the Lie algebra of divergence-free vector fields.)

Conspicuously, our quantization scheme turns out to be equivariant with respect to a rather small Lie subgroup of $\mathrm{Diff}(M)$, namely of the affine group of (M, ∇). It would be interesting to investigate to what extent the equivariance under the sole affine group, $\mathrm{GL}(n, \mathbf{R}) \ltimes \mathbf{R}^n$, of a flat affine structure (M, ∇) allows one to uniquely extend to the whole algebra of polynomials the quantization scheme we have devised for cubic polynomials.

C. The quantum Stäckel system

The quantization of the general Stäckel system (see Sec. II D) has first been undertaken by Benenti, Chanu, and Rastelli in Refs. 4 and 5. We will derive here the covariant expression of the quantum correction associated to the "minimal" quantization, with the help of the results obtained in Sec. III A.

Denote by $I_i = I_{2,i} + I_{0,i}$ the ith Stäckel conserved quantity, $i=1,\ldots,n$, in (2.11) where the indices 0 and 2 refer to the degree of homogeneity with respect to the coordinates ξ. Applying (3.15) with $P_1 = Q_1 = 0$, $P_2 = I_{2,i}$, and $Q_2 = I_{2,j}$ one gets

$$[\hat{I}_i, \hat{I}_j] = [\hat{I}_{2,i}, \hat{I}_{2,j}] = i\hat{A}_{I_{2,i}, I_{2,j}} = \tfrac{2}{3}\left(\nabla_k B^{k\ell}_{I_{2,i}, I_{2,j}}\right)\nabla_\ell.$$

Remark 3.8: This result shows that there are no quantum corrections produced by the potential term. More generally, start with a system defined by independent, homogeneous, quadratic observables $H_1, \ldots, H_n$ which is integrable at the classical and quantum levels. Consider a new set of observables $H_1 + U_1, \ldots, H_n + U_n$ obtained by adding potential terms $U_1, \ldots, U_n$; if the new system is classically integrable, it will remain integrable at the quantum level.

We are now in position to prove the following

Proposition 3.9: The quantum correction (3.12) *of a general Stäckel system, with commuting conserved quantities* $I_1, \ldots, I_n$ *defined by* (2.11), *retains the form*

$$B^{k\ell}_{I_{2,i}, I_{2,j}} = -2 I^{s[k}_{2,i} R_{st} I^{\ell]t}_{2,j} \tag{3.25}$$

for $i, j = 1, \ldots, n$, *where* R_{st} *denotes the components of the Ricci tensor of the metric associated with the Hamiltonian* I_1.

Proof: As a preliminary remark, let us observe that the Stäckel metric, given by (2.10), needs not be Riemannian. So we will write it

$$g = \sum_{i=1}^{n} \frac{(dx^i)^2}{A_1^i(x)} = \sum_{a=1}^{n} \eta_a (\theta^a)^2, \tag{3.26}$$

where $(\theta^a = \mathrm{d}x^a / \sqrt{|A_1^a|})_{a=1,\ldots,n}$ is the orthonormal moving coframe and the signature of g is given by $\eta_a = \mathrm{sign}(A_1^a)$. We will denote by $(e_a = \sqrt{|A_1^a|}\partial_a)_{a=1,\ldots,n}$ the associated orthonormal frame with respect to the metric $\eta_{ab} = \eta_a \delta_{ab}$ used to raise and lower frame indices.

Let us recall, in order to fix the notation, that the connection form ω satisfies the structure equation $\mathrm{d}\theta^a + \omega^a{}_b \wedge \theta^b = 0$ and the associated curvature form, Ω, given by $\Omega^a{}_b = \mathrm{d}\omega^a{}_b + \omega^a{}_c \wedge \omega^c{}_b$, is expressed in terms of the Riemann tensor by $\Omega^a{}_b = \frac{1}{2} R^a{}_{b,cd} \theta^c \wedge \theta^d$. The indices $a, \ldots, d$ run from 1 to n and the Einstein summation convention is used when no ambiguity arises. Denoting by $R^\ell{}_{i,jk}$ the local components of the Riemann tensor, we have $R^a{}_{b,cd} = \theta^a_\ell R^\ell{}_{i,jk} e^i_b e^j_c e^k_d$.

We start off with the calculation of the connection form, ω, and of some components of the curvature form, Ω. Straightforward computation, using relation (2.13), then yields for the nonvanishing components of the connection

$$\omega_{ab,a} = \tfrac{1}{2} \eta_b C_b^a \frac{|A_1^b|^{3/2}}{|A_1^a|}, \quad a \neq b, \quad \omega_{ab,c} = \omega_{ab}(e_c),$$

the other nontrivial components $\omega_{ab,b}$ are obtained accordingly. For the curvature, a lengthy computation gives the special components

$$R_{ac,cb} = 3(-\eta_a \omega_{ca,c} \omega_{ab,a} - \eta_b \omega_{cb,c} \omega_{ba,b} + \eta_c \omega_{ca,c} \omega_{cb,c}), \quad a \neq b, \tag{3.27}$$

which will be needed in the sequel.

Two last ingredients are the introduction of the frame components of various objects. We will denote the Killing tensor $I_{2,i}$ (respectively, $I_{2,j}$) as P (respectively, Q). Their frame components $P = P^{bc} e_b \otimes e_c$, and similarly for Q, will be

$$P^{bc} = p_b \delta_{bc}, \quad p_b = \frac{A_i^b}{2|A_1^b|}, \quad Q^{bc} = q_b \delta_{bc}, \quad q_b = \frac{A_j^b}{2|A_1^b|}. \tag{3.28}$$

The covariant derivative will have the frame components

$$\mathcal{D}_c P_{ab} = e_c(P_{ab}) - \omega^s{}_{a,c} P_{sb} - \omega^s{}_{b,c} P_{as}.$$

The equations which express that P^{ab} is a Killing tensor are now

$$\begin{aligned} e_b(p_a) &= 2\omega_{ab,a}(\eta_a p_a - \eta_b p_b), \quad a \neq b, \\ e_a(p_a) &= 0, \end{aligned} \tag{3.29}$$

where the repeated indices are not summed over. One can check that they hold true using the explicit form of p_a given in (3.28) and the identity (2.13).

Using all of the previous information one can compute the frame components of the various pieces appearing in the tensor $B^{ij}_{P,Q}$. We have successively

$$\begin{aligned} P^{s[i} \nabla_s \nabla_t Q^{j]t} - (P \leftrightarrow Q) = \sum_{l \neq i,j} & (4\omega_{li,l}\omega_{lj,l} - 3\eta_l \eta_i \omega_{li,l}\omega_{ij,i} - 3\eta_l \eta_j \omega_{lj,l}\omega_{ji,j}) \\ & \times [p_i q_j - \eta_l p_l \eta_i q_j + \eta_i q_l \eta_i p_j - (i \leftrightarrow j)] \end{aligned}$$

and

$$\nabla_s P^{t[i} \nabla_t Q^{j]s} = \tfrac{1}{2} \sum_l \omega_{li,l}\omega_{lj,l} [p_i q_j - \eta_l p_l \eta_i q_j + \eta_l q_l \eta_i p_j - (i \leftrightarrow j)].$$

Combining these relations, and using (3.27), we get

$$P^{s[i}\nabla_s\nabla_t Q^{j]t} - (P \leftrightarrow Q) - \nabla_s P^{t[i}\nabla_t Q^{j]s} = \tfrac{1}{2}\sum_l \eta_l R_{il,lj}[p_i q_j - \eta_l p_l \eta_i q_j + \eta_l q_l \eta_i p_j - (i \leftrightarrow j)].$$

Let us then compute

$$P^{s[i}R^{j]}{}_{u,vs}Q^{uv} - (P \leftrightarrow Q) = \tfrac{1}{2}\sum_l \eta_l R_{il,lj}[\eta_l p_l \eta_i q_j - \eta_l q_l \eta_i p_j - (i \leftrightarrow j)].$$

Collecting all the pieces leaves us with

$$P^{s[i}\nabla_s\nabla_t Q^{j]t} + P^{s[i}R^{j]}{}_{u,vs}Q^{uv} - (P \leftrightarrow Q) - \nabla_s P^{t[i}\nabla_t Q^{j]s} = \tfrac{1}{2}\sum_l \eta_l R_{il,lj}(p_i q_j - p_j q_i). \tag{3.30}$$

The last sum is nothing but the frame components of the tensor $-P^{s[i}R_{st}Q^{j]t}$, so that we have obtained the tensorial relation

$$P^{s[i}\nabla_s\nabla_t Q^{j]t} + P^{s[i}R^{j]}{}_{u,vs}Q^{uv} - (P \leftrightarrow Q) - \nabla_s P^{t[i}\nabla_t Q^{j]s} = -P^{s[i}R_{st}Q^{j]t}, \tag{3.31}$$

which implies

$$B^{ij}{}_{P,Q} = -2P^{s[i}R_{st}Q^{j]t}, \tag{3.32}$$

in agreement with Ref. 5. This ends the proof of Proposition 3.9. □

Now we can come to the central point of our analysis: is a Stäckel system integrable at the quantum level? The answer is given by the following

Corollary 3.10: (Refs. 4 and 5) *A Stäckel system is integrable at the quantum level iff*

$$R_{ij} = 0 \quad \text{for } i \neq j, \quad \text{where } i,j = 1,\ldots,n, \tag{3.33}$$

in the special coordinates which are constituent to this system.

Proof: The Killing tensors $I_{2,i}$ are diagonal, for $i=1,\ldots,n$, in the Stäckel coordinate system, and the proof follows from (3.25). □

The conditions (3.33) are known as the Robertson conditions,[31] as interpreted by Eisenhart.[18] Quite recently, Benenti *et al.*[4] have refined the definition of the separability of the Schrödinger equation and shown that, for Stäckel systems, the Robertson conditions are necessary and sufficient for the separability of the Schrödinger equation. As mentioned in Remark 2.1, the classical integrability is equivalent to the separability of the Hamilton–Jacobi equation; the situation for these systems can therefore be summarized by the following diagram:

$$\begin{array}{ccccc} \text{Classical integrability} & \Leftrightarrow & \text{separable Hamilton-Jacobi} \\ \Downarrow & \text{provided} & R_{ij}=0\ (i\neq j) \\ \text{Quantum integrability} & \Leftrightarrow & \text{separable Schrödinger.} \end{array}$$

D. The quantum ellipsoid and Neumann systems

It is now easy to prove that the ellipsoid geodesic flow (see Sec. II E), including the potential given in (2.16), is integrable at the quantum level. Using the coordinates (x^i) and the (Riemannian) metric given by (2.22), one can check that the Ricci tensor has components

$$R_{ij} = \frac{\mathcal{N}}{x^i}\sum_{s\neq i}\frac{1}{x^s}g_{ij}, \quad \mathcal{N} = \frac{a_0 a_1 \cdots a_n}{x^1 \cdots x^n},$$

and therefore satisfies the Robertson conditions. As already emphasized, the occurrence of an additional potential is irrelevant for the quantum analysis since the potential terms do not generate quantum corrections (see Remark 3.8).

Similarly we get the quantum integrability for the Neumann system (see Sec. II F) using the metric on S^n given by (2.38). The Ricci tensor being given by

$$R_{ij} = (n-1)g_{ij},$$

the Robertson conditions are again satisfied.

E. The quantum generalized Kerr–Newman system

The quantization of the four commuting observables (2.47) and (2.48) is straightforward.

In view of the relations given in Sec. III all quantum commutators vanish except for $[\hat{\tilde{H}}, \hat{\tilde{P}}]$; this is due to the fact that the conserved quantities $\tilde{S}$ and $\tilde{T}$ [see (2.48)] are Killing–Maxwell vector fields.

The anomalous terms in the previous commutator are A_{P_2,H_2}, A_{P_1,H_2}, and A_{P_2,H_1} where $P_2 = P^{ij}\xi_i\xi_j$, $H_2 = \frac{1}{2}g^{ij}\xi_i\xi_j$, $P_1 = -2P^{ij}\xi_i A_j$, and $H_1 = -g^{ij}\xi_i A_j$.

The vector field A_{P_2,H_2} given by (3.14) actually vanishes because, cf. (3.16), $B^{jk}_{P_2,H_2} = -P^{\ell[j}R_\ell^{\ k]} = 0$ as a consequence of (2.7); indeed the tensor P anti-commutes with the electromagnetic field strength F, implying that it commutes with the stress-energy electromagnetic tensor, hence with the Ricci tensor in view of the Einstein–Maxwell equations.[11]

The two other anomalous terms (3.9) also vanish as it turns out that $\nabla_j A^j = 0$ [see (2.44)] and $\nabla_j(P^{jk}A_k) = 0$.

This derivation reproduces and extends Carter's results to the generalized Kerr–Newman solution, in a somewhat shorter manner.

Remark 3.11: Our analysis of quantum integrability for the generalized Kerr-Newman solution in four dimensions can be carried over into recent work[19,23,32] dealing with five-dimensional black holes. In these cases, classical integrability follows from the existence of three Killing vectors and one quadratic Killing tensor, besides the Hamiltonian. These metrics being Einstein, the above arguments given for the generalized Kerr–Newman case apply just as well, ensuring quantum integrability. This fact is in agreement with the separability of the Laplace operator.

F. The quantum multi-center system

For this example too, the quantization is straightforward. The single point to be checked for quantum integrability is just the commutator $[\hat{H}, \hat{P}]$, with the possible quantum correction (3.16) given by $-P^{\ell[j}R_\ell^{\ k]}$. Here it vanishes trivially since these metrics are Ricci-flat.

G. The quantum Di Pirro system

As seen in Sec. II I, the classical integrability of this system is provided by three commuting observables: on the one hand H, P, respectively, given by (2.51) and (2.52), and $T = \xi_3$ if $c(x^3) = \text{const.}$, and on the other hand H, P and $J = \xi_1 x^2 - \xi_2 x^1$ if $a = b$, γ depend on r only.

At the quantum level, the Killing vectors $\hat{T}$ and $\hat{J}$ do commute with $\hat{H}$ according to (3.8) and (3.9). As for the commutator $[\hat{P}, \hat{H}]$ of the quantized Killing tensors, it is given by (3.16), namely $B_{P,H} = -\frac{1}{2}P^{\ell[j}R_\ell^{\ k]}\partial_j \wedge \partial_k$, and one finds

$$B_{P,H} = -\frac{3}{16}\frac{c'(x^3)}{(\gamma(x^1,x^2) + c(x^3))^3}(a(x^1,x^2)\partial_1\gamma(x^1,x^2)\partial_1 \wedge \partial_3 + b(x^1,x^2)\partial_2\gamma(x^1,x^2)\partial_2 \wedge \partial_3).$$

For the system (H,P,T), this quantum correction vanishes since $c'(x^3) = 0$, implying quantum integrability. However, for the system (H,P,J), in the generic case $\gamma \neq \text{const.}$, we get $B_{P,H} \neq 0$, showing that the minimal quantization rules may produce quantum corrections.

IV. DISCUSSION AND OUTLOOK

It would be worthwhile to get insight into the status of our "minimal" quantization rules and to their relationship with other bona fide quantization procedures. Among the latter, let us mention those obtained by geometric means, and more specifically by imposing equivariance of the quantization mapping, $\mathcal{Q}$, with respect to some symmetry group, G, e.g., a group of automorphisms of a certain geometric structure on configuration space, M. We refer to Refs. 24, 15–17, and 6 for a detailed account on equivariant quantization. The two main examples are, respectively, the projectively, $G=SL(n+1,\mathbf{R})$, and conformally, $G=O(p+1,q+1)$, equivariant quantizations which have been shown to be uniquely determined.[24,15–17] For instance, the conformally equivariant quantization $\mathcal{Q}_{1/2}:\mathcal{F}_{1/2}(M)\to\mathcal{F}_{1/2}(M)$ has been explicitly computed for quadratic[16] and cubic[25] observables; for example, if $P=P^{ij}\xi_i\xi_j$ we then have

$$\mathcal{Q}_{1/2}(P)=\hat{P}+\beta_3\nabla_i\nabla_j(P^{ij})+\beta_4 g^{ij}g_{k\ell}\nabla_i\nabla_j(P^{k\ell})+\beta_5 R_{ij}P^{ij}+\beta_6 R g_{ij}P^{ij} \tag{4.1}$$

where the "minimal" quantum operator

$$\hat{P}=-\nabla_i\circ P^{ij}\circ\nabla_j \tag{4.2}$$

is given by (3.4), together with $\beta_3=-n/(4(n+1))$, $\beta_4=-n/(4(n+1)(n+2))$, $\beta_5=n^2/(4(n-2)(n+1))$, $\beta_6=-n^2/(2(n^2-4)(n^2-1))$, assuming $n=\dim(M)>2$. In (4.1) we denote by R_{ij} the components of the Ricci tensor and by R the scalar curvature. The formula (4.1) provides a justification of the term "minimal" for the mapping $P\mapsto\hat{P}$ given by (3.4) and (3.10).

We have checked that, in the special instance of the geodesic flow of the ellipsoid discussed in Sec. II E, the quantum commutators of the observables I_i defined in (2.30), namely $[\mathcal{Q}_{1/2}(I_i),\mathcal{Q}_{1/2}(I_j)]$, fail to vanish for $i\neq j=1,\ldots,n$. Had we started from the expression (4.1) with adjustable coefficients $\beta_3,\ldots,\beta_6$, the requirement that the latter commutator be vanishing imposes $\beta_3=\ldots=\beta_6=0$, leading us back to the minimal quantization rule (4.2).

Despite their nice property of preserving, to a large extent, integrability (from classical to quantum), the "minimal" quantization rules still remain an ad hoc procedure, defined for observables at most cubic in momenta, and do not follow from any sound constructive principle, be it of a geometric or an algebraic nature. The quest for a construct leading unambiguously to a genuine "minimal" quantization procedure remains an interesting challenge. As discussed in Sec. III B, the equivariance assumption with respect to the affine group might be helpful for determining the sought "minimal" quantization of polynomials of higher degree. This analysis is required for the quantization of, e.g., the newly discovered integrable systems[14] which involve cubic Killing tensors.

Another field of applications of the present work could be the search for quantum integrability of the geodesic flow on the higher dimensional generalizations of the Kerr metric which have been under intense study lately.[19,12,36]

Still another perspective for future work would be to generalize the previous computation of quantum corrections to the case of classical integrability in the presence of an electromagnetic field in a purely gauge invariant manner. In particular the approach presented in Sec. II B should be further extended at the quantum level via the quantization of the Schouten–Maxwell brackets.

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Noether's second theorem for BRST symmetries

D. Bashkirov[a)]
Department of Theoretical Physics, Moscow State University, 117234 Moscow, Russia

G. Giachetta[b)] and L. Mangiarotti[c)]
Department of Mathematics and Informatics, University of Camerino, 62032 Camerino (MC), Italy

G. Sardanashvily[d)]
Department of Theoretical Physics, Moscow State University, 117234 Moscow, Russia

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We present Noether's second theorem for graded Lagrangian systems of even and odd variables on an arbitrary body manifold X in a general case of BRST symmetries depending on derivatives of dynamic variables and ghosts of any finite order. As a preliminary step, Noether's second theorem for Lagrangian systems on fiber bundles $Y \to X$ possessing gauge symmetries depending on derivatives of dynamic variables and parameters of arbitrary order is proved. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1899988]

I. INTRODUCTION

Different variants of Noether's second theorem state that, if a Lagrangian admits symmetries depending on parameters, its variational derivatives obey certain relations, called the Noether identities. We present Noether's second theorem in the case of BRST transformations depending on derivatives (jets) of dynamic variables and ghosts of arbitrary order. In particular, this is the case of the field-antifield BRST theory and BV quantization.[1,2] Special attention is paid to global aspects of Noether's second theorem as a preliminary step of the global analysis of BV quantization.[3,4]

We start with a classical Lagrangian system on a fiber bundle $Y \to X$ subject to even gauge transformations depending on even dynamic variables, even parameters, and their derivatives of any order. For this purpose, we consider Lagrangian formalism on the composite fiber bundle $E \to Y \to X$, where $E \to Y$ is a vector bundle of gauge parameters. Accordingly, gauge transformations are represented by a linear differential operator υ on E taking its values in the vertical tangent bundle VY of $Y \to X$ (Sec. II). The Noether identity for a Lagrangian L is defined as a differential operator Δ on the fiber bundle (13) which takes its values in the density-dual

$$E^* \underset{Y}{\otimes} \overset{n}{\wedge} T^*X, \quad n = \dim X, \tag{1}$$

of E and whose kernel contains the image of the Euler–Lagrange operator δL of L, i.e., $\Delta \circ \delta L = 0$ (Definition 4). Expressed in these terms, Noether's second theorem (Sec. III, Theorem 5) follows at once from the properties of differential operators on dual fiber bundles (Appendix A, Theorem 16). Namely, there exists the intertwining operator $\eta(\upsilon) = \Delta$, $\eta(\Delta) = \upsilon$ such that

$$\eta(\eta(\upsilon)) = \upsilon, \quad \eta(\eta(\Delta)) = \Delta, \tag{2}$$

[a)]Electronic mail: bashkir@phys.msu.ru
[b)]Electronic mail: giovanni.giachetta@unicam.it
[c)]Electronic mail: luigi.mangiarotti@unicam.it
[d)]Electronic mail: sard@grav.phys.msu.su

$$\eta(v \circ v') = \eta(v') \circ \eta(v), \quad \eta(\Delta' \circ \Delta) = \eta(\Delta) \circ \eta(\Delta'). \tag{3}$$

The appropriate notions of reducible Noether identities and gauge symmetries are formulated, and their equivalence with respect to the intertwining operator η is proved (Sec. IV).

This formulation of Noether's second theorem is generalized to the case of graded Lagrangian systems of even and odd variables and BRST symmetries (Sec. VII, Theorem 15). We describe odd variables and their jets on an arbitrary smooth manifold X as generating elements of the structure ring of a graded manifold whose body is X.[4,5] This definition differs from that of jets of a graded fiber bundle,[6] but reproduces the heuristic notion of jets of ghosts in the above-mentioned field–antifield BRST theory.[1,7]

We consider BRST symmetries of a graded Lagrangian, i.e., its nilpotent odd symmetries depending on ghosts as parameters (Sec. VI). In particular, BRST symmetries come from the above-mentioned gauge symmetries by replacement of even parameters with odd ghosts (Example 5). In this case, the nilpotency condition implies that original gauge symmetries form an algebra.

The key point is that, in order to define the Noether identity associated to BRST symmetries, one should introduce antifields and the Koszul–Tate differential. If a Noether identity is reducible, $(0 \leqslant k)$-stage ghosts and antighosts are called into play (Sec. VIII), and we come to the complete tuple of fields, ghosts, and antifields in the field–antifield BRST theory.[1] We, however, leave this theory outside the scope of the present work, and keep an original graded Lagrangian independent of ghosts and antifields.

II. GAUGE SYSTEMS ON FIBER BUNDLES

Recall that an r-order Lagrangian on a fiber bundle $Y \to X$ is defined as a density

$$L = \mathcal{L}\omega : J^r Y \to \overset{n}{\wedge} T^* X, \quad \omega = dx^1 \wedge \cdots \wedge dx^n, \tag{4}$$

on the r-order jet manifold $J^r Y$ of sections of $Y \to X$. Jet manifolds of $Y \to X$ make up the inverse system

$$X \overset{\pi}{\leftarrow} Y \overset{\pi_0^1}{\leftarrow} J^1 Y \leftarrow \cdots J^{r-1} Y \overset{\pi_{r-1}^r}{\leftarrow} J^r Y \leftarrow \cdots. \tag{5}$$

In the sequel, the index $r=0$ stands for Y. Accordingly, we have the direct system

$$\mathcal{O}^* X \overset{\pi^*}{\to} \mathcal{O}^* Y \overset{\pi_0^{1*}}{\to} \mathcal{O}_1^* Y \to \cdots \mathcal{O}_{r-1}^* Y \overset{\pi_{r-1}^{r*}}{\to} \mathcal{O}_r^* Y \to \cdots \tag{6}$$

of graded differential algebras (henceforth GDAs) $\mathcal{O}_r^* Y$ of exterior forms on jet manifolds $J^r Y$ with respect to the pull-back monomorphisms π_{r-1}^{r*}. Its direct limit $\mathcal{O}_\infty^* Y$ is a GDA consisting of all exterior forms on finite order jet manifolds modulo the pull-back identification.

The projective limit $(J^\infty Y, \pi_r^\infty : J^\infty Y \to J^r Y)$ of the inverse system (5) is a Fréchet manifold.[8] A bundle atlas $\{(U_Y; x^\lambda, y^i)\}$ of $Y \to X$ yields the coordinate atlas

$$\{((\pi_0^\infty)^{-1}(U_Y); x^\lambda, y^i_\Lambda)\}, \quad y'^i_{\lambda+\Lambda} = \frac{\partial x^\mu}{\partial x'^\lambda} d_\mu y'^i_\Lambda, \quad 0 \leqslant |\Lambda|, \tag{7}$$

of $J^\infty Y$, where $\Lambda = (\lambda_k \ldots \lambda_1)$ is a symmetric multi-index, $\lambda + \Lambda = (\lambda \lambda_k \ldots \lambda_1)$, and

$$d_\lambda = \partial_\lambda + \sum_{0 \leqslant |\Lambda|} y^i_{\lambda+\Lambda} \partial_i^\Lambda, \quad d_\Lambda = d_{\lambda_r} \circ \cdots \circ d_{\lambda_1} \tag{8}$$

are the total derivatives. There is the restriction epimorphism $\mathcal{O}_\infty^* Y \to \mathcal{O}_\infty^* U_Y$. Therefore, $\mathcal{O}_\infty^* Y$ can be written in a coordinate form where the horizontal one-forms $\{dx^\lambda\}$ and the contact one-forms $\{\theta^i_\Lambda = dy^i_\Lambda - y^i_{\lambda+\Lambda} dx^\lambda\}$ are generating elements of the $\mathcal{O}_\infty^0 U_Y$-algebra $\mathcal{O}_\infty^* U_Y$. Though $J^\infty Y$ is not a smooth manifold, elements of $\mathcal{O}_\infty^* Y$ are exterior forms on finite order jet manifolds and, therefore, their coordinate transformations are smooth.

There is the canonical decomposition $\mathcal{O}^*_\infty Y = \oplus \mathcal{O}^{k,m}_\infty Y$ of $\mathcal{O}^*_\infty Y$ into $\mathcal{O}^0_\infty Y$-modules $\mathcal{O}^{k,m}_\infty Y$ of k-contact and m-horizontal forms together with the corresponding projectors $h_k: \mathcal{O}^*_\infty Y \to \mathcal{O}^{k,*}_\infty Y$ and $h^m: \mathcal{O}^*_\infty Y \to \mathcal{O}^{*,m}_\infty Y$. Accordingly, the exterior differential on $\mathcal{O}^*_\infty Y$ is split into the sum $d = d_H + d_V$ of the nilpotent total and vertical differentials

$$d_H(\phi) = dx^\lambda \wedge d_\lambda \phi, \quad d_V(\phi) = \theta^i_\Lambda \wedge \partial^\Lambda_i \phi, \quad \phi \in \mathcal{O}^*_\infty Y.$$

One also introduces the $\mathbb{R}$-module projector

$$\varrho = \sum_{0<k} \frac{1}{k} \overline{\varrho} \circ h_k \circ h^n, \quad \overline{\varrho}(\phi) = \sum_{0 \leqslant |\Lambda|} (-1)^{|\Lambda|} \theta^i \wedge [d_\Lambda(\partial^\Lambda_i \rfloor \phi)], \quad \phi \in \mathcal{O}^{>0,n}_\infty Y, \tag{9}$$

of $\mathcal{O}^*_\infty Y$ such that $\varrho \circ d_H = 0$, and the nilpotent variational operator $\delta = \varrho \circ d$ on $\mathcal{O}^{*n}_\infty Y$. Let us put $\mathbf{E}_k = \varrho(\mathcal{O}^{k,n}_\infty Y)$. Then the GDA $\mathcal{O}^*_\infty Y$ is split into the well-known variational bicomplex.[4,8–10] Here, we are concerned with its variational subcomplex

$$0 \to \mathbb{R} \to \mathcal{O}^0_\infty Y \xrightarrow{d_H} \mathcal{O}^{0,1}_\infty Y \cdots \xrightarrow{d_H} \mathcal{O}^{0,n}_\infty Y \xrightarrow{\delta} \mathbf{E}_1 \xrightarrow{\delta} \mathbf{E}_2 \to \cdots \tag{10}$$

and the subcomplex of one-contact forms

$$0 \to \mathcal{O}^{1,0}_\infty Y \xrightarrow{d_H} \mathcal{O}^{1,1}_\infty Y \cdots \xrightarrow{d_H} \mathcal{O}^{1,n}_\infty Y \xrightarrow{\varrho} \mathbf{E}_1 \to 0. \tag{11}$$

They possess the following cohomology.[3,4,11]

Theorem 1: The cohomology of the variational complex (10) equals the de Rham cohomology of Y.

Theorem 2: The complex (11) is exact.

Any finite order Lagrangian L (4) is an element of $\mathcal{O}^{0,n}_\infty Y$, while

$$\delta L = \mathcal{E}_i \theta^i \wedge \omega = \sum_{0 \leqslant |\Lambda|} (-1)^{|\Lambda|} d_\Lambda(\partial^\Lambda_i \mathcal{L}) \theta^i \wedge \omega \in \mathbf{E}_1 \tag{12}$$

is its Euler–Lagrange operator taking the values in the vector bundle

$$T^*Y \underset{Y}{\wedge} (\overset{n}{\wedge} T^*X) = V^*Y \underset{Y}{\otimes} \overset{n}{\wedge} T^*X. \tag{13}$$

The components $\mathcal{E}_i$ of δL are called the variational derivatives. We further abbreviate $A \approx 0$ with an equality which holds on-shell. This means that A is an element of a module over the ideal I_L of the ring $\mathcal{O}^0_\infty Y$ which is locally generated by the variational derivatives $\mathcal{E}_i$ (12) and their total derivatives $d_\Lambda \mathcal{E}_i$. Thus, I_L is a differential ideal.

By virtue of Theorem 1, every δ-closed Lagrangian $L \in \mathcal{O}^{0,n}_\infty Y$ is the sum

$$L = h_0 \psi + d_H \sigma, \quad \sigma \in \mathcal{O}^{0,n-1}_\infty Y, \tag{14}$$

where ψ is a closed n-form on Y. Theorem 2 provides the $\mathbb{R}$-module decomposition

$$\mathcal{O}^{1,n}_\infty Y = \mathbf{E}_1 \oplus d_H(\mathcal{O}^{1,n-1}_\infty Y).$$

Given a Lagrangian $L \in \mathcal{O}^{0,n}_\infty Y$, we have the corresponding decomposition

$$dL = \delta L - d_H \Xi \tag{15}$$

where $\Xi_L = \Xi + L$ is a Lepagean equivalent of L.

Let $\mathfrak{d}\mathcal{O}^0_\infty Y$ be the $\mathcal{O}^0_\infty Y$-module of derivations of the $\mathbb{R}$-ring $\mathcal{O}^0_\infty Y$. Any $\vartheta \in \mathfrak{d}\mathcal{O}^0_\infty Y$ yields the graded derivation (the interior product) $\vartheta \rfloor \phi$ of the GDA $\mathcal{O}^*_\infty Y$ given by the relations

$$\vartheta \rfloor df = \vartheta(f), \quad f \in \mathcal{O}^0_\infty Y,$$

$$\vartheta(\phi\wedge\sigma)=(\vartheta\rfloor\phi)\wedge\sigma+(-1)^{|\phi|}\phi\wedge(\vartheta\rfloor\sigma),\quad \phi,\sigma\in\mathcal{O}^*_\infty Y,$$

and its derivation (the Lie derivative)

$$\begin{aligned}&\mathbf{L}_\vartheta\phi=\vartheta\rfloor d\phi+d(\vartheta\rfloor\phi),\quad \phi\in\mathcal{O}^*_\infty Y,\\ &\mathbf{L}_\vartheta(\phi\wedge\phi')=\mathbf{L}_\vartheta(\phi)\wedge\phi'+\phi\wedge\mathbf{L}_\vartheta(\phi').\end{aligned}\tag{16}$$

Relative to an atlas (7), a derivation $\vartheta\in\mathfrak{d}\mathcal{O}^0_\infty Y$ reads[4]

$$\vartheta=\vartheta^\lambda\partial_\lambda+\vartheta^i\partial_i+\sum_{|\Lambda|>0}\vartheta^i_\Lambda\partial^\Lambda_i,\tag{17}$$

where the tuple of derivations $\{\partial_\lambda,\partial^\Lambda_i\}$ is defined as the dual of the set $\{dx^\lambda,dy^i_\Lambda\}$ of generating elements for the $\mathcal{O}^0_\infty Y$-algebra $\mathcal{O}^*_\infty Y$ with respect to the interior product $\rfloor$, and local functions ϑ^λ, ϑ^i, $\vartheta^i_\Lambda\in\mathcal{O}^0_\infty Y$ obey the transformation law

$$\vartheta'^\lambda=\frac{\partial x'^\lambda}{\partial x^\mu}\vartheta^\mu,\quad \vartheta'^i_\Lambda=\sum_{|\Sigma|\leqslant|\Lambda|}\frac{\partial y'^i_\Lambda}{\partial y^j_\Sigma}\vartheta^j_\Sigma+\frac{\partial y'^i_\Lambda}{\partial x^\mu}\upsilon^\mu.\tag{18}$$

Note that the tuple of derivations $\{\partial^\Lambda_i\}$ is the dual of the basis $\{\theta^i_\Lambda\}$ of contact forms.

A derivation ϑ is called contact if the Lie derivative $\mathbf{L}_\vartheta$ (16) preserves the contact ideal of the GDA $\mathcal{O}^*_\infty Y$ generated by contact forms. A derivation ϑ (17) is contact iff

$$\vartheta^i_\Lambda=d_\Lambda(\vartheta^i-y^i_\mu\vartheta^\mu)+y^i_{\mu+\Lambda}\vartheta^\mu,\quad 0<|\Lambda|.\tag{19}$$

Any contact derivation admits the horizontal splitting

$$\vartheta=\vartheta_H+\vartheta_V=\vartheta^\lambda d_\lambda+\left(\upsilon^i\partial_i+\sum_{0<|\Lambda|}d_\Lambda\upsilon^i\partial^\Lambda_i\right),\quad \upsilon^i=\vartheta^i-y^i_\mu\vartheta^\mu,\tag{20}$$

relative to the canonical connection $\nabla=dx^\lambda\otimes d_\lambda$ on the $C^\infty(X)$-ring $\mathcal{O}^0_\infty Y$.[5,12] Its vertical part ϑ_V is completely determined by the first summand

$$\upsilon=\upsilon^i(x^\lambda,y^i_\Lambda)\partial_i,\quad 0\leqslant|\Lambda|\leqslant k.\tag{21}$$

This is a section of the pull-back $VY\underset{Y}{\times}J^kY\to J^kY$ of the vertical tangent bundle $VY\to Y$ onto J^kY,[13] i.e., υ (21) is a k-order VY-valued differential operator on Y (see Appendix A). One calls this differential operator the *generalized vector field* on Y.

Proposition 3: It follows from the splitting (15) that the Lie derivative of a Lagrangian L (4) along a contact derivation ϑ (20) fulfills the first variational formula

$$\mathbf{L}_\vartheta L=\upsilon\rfloor\delta L+d_H(h_0(\vartheta\rfloor\Xi_L))+\mathcal{L}d_V(\vartheta_H\rfloor\omega),\tag{22}$$

where Ξ_L is a Lepagean equivalent of L.[4]

A contact derivation ϑ (20) is called variational if the Lie derivative (22) is d_H-exact, i.e., $\mathbf{L}_\vartheta L=d_H\sigma$, $\sigma\in\mathcal{O}^{0,n-1}_\infty$. A glance at the expression (22) shows that: (i) a contact derivation ϑ is variational only if it is projected onto X (i.e., its components ϑ^λ depend only on coordinates on X), (ii) ϑ is variational iff its vertical part ϑ_V is variational, (iii) it is variational if $\upsilon\rfloor\delta L$ is d_H-exact.

By virtue of item (ii), we can restrict our consideration to vertical contact derivations $\vartheta=\vartheta_V$. A generalized vector field υ (21) is called a *variational symmetry* of a Lagrangian L if it generates a variational vertical contact derivation.

One can also consider locally variational contact derivations when the Lie derivative (22) is δ-closed, but any locally variational gauge symmetry is always variational (see Remark 1 in the following).

Turn now to the notion of a gauge symmetry. A Lagrangian system on a fiber bundle $Y \to X$ is said to be a gauge theory if its Lagrangian L admits a family of variational symmetries parametrized by elements of a vector bundle $E \to Y$ as follows.

Let $E \to Y$ be a vector bundle coordinated by (x^λ, y^i, ξ^r). Given a Lagrangian L on Y, let us consider its pull-back, say again L, onto E. Let ϑ_E be a vertical contact derivation of the $\mathbb{R}$-ring $\mathcal{O}^0_\infty E$ whose restriction

$$\vartheta = \vartheta_E|_{\mathcal{O}^0_\infty Y} = \sum_{0 \leqslant |\Lambda|} d_\Lambda v^i \partial^\Lambda_i \tag{23}$$

to $\mathcal{O}^0_\infty Y \subset \mathcal{O}^0_\infty E$ is linear in coordinates ξ^r_Ξ. It is determined by a generalized vector field (i.e., a VE-valued differential operator) v_E on E whose canonical projection

$$v: J^k E \overset{v_E}{\to} VE \to E \underset{Y}{\times} VY$$

[see the exact sequence (35) below] is a linear VY-valued differential operator

$$v = \sum_{0 \leqslant |\Xi| \leqslant m} v^{i,\Xi}_r(x^\lambda, y^i_\Sigma) \xi^r_\Xi \partial_i \tag{24}$$

on E. Let ϑ_E be a variational symmetry of a Lagrangian L on E, i.e.,

$$v_E \rfloor \delta L = v \rfloor \delta L = d_H \sigma. \tag{25}$$

Then one says that v (24) is a *gauge symmetry* of a Lagrangian L on Y.

Remark 1: As was mentioned above, any locally variational gauge symmetry ϑ_E, when the Lie derivative $\mathbf{L}_{\vartheta_E} L$ is δ-closed, is variational. By virtue of Theorem 1, $\mathbf{L}_{\vartheta_E} L$ takes the form (14) where ψ is a closed form on E. Since $E \to Y$ is a vector bundle, Y is a strong deformation retract of E and, consequently, the de Rham cohomology of E equals that of Y. Then any closed form on E is the sum of the pull-back of a closed form on Y and an exact form on E. The former is independent of fiber coordinates ξ^r on $E \to Y$. Since the Lie derivative $\mathbf{L}_\vartheta L$ is linear in ξ^r_Λ, it is always d_H-exact, i.e., ϑ_E is variational.

III. NOETHER'S SECOND THEOREM I

Let us start with the notion of the Noether identity.

Definition 4: Given a Lagrangian L (4) and its Euler–Lagrange operator δL (12), let $E \to Y$ be a vector bundle and Δ a linear differential operator of order $0 \leqslant m$ on the vector bundle (13) with the values in the density-dual $\overline{E}^*$ (1) of E such that

$$\Delta \circ \delta L = 0. \tag{26}$$

This condition is called the *Noether identity*, and Δ is the *Noether operator*.

Given bundle coordinates $(x^\lambda, y^i, \overline{y_i})$ on the fiber bundle (13) and (x^λ, y^i, ξ^r) on E, a Noether operator Δ in Definition 4 is represented by the density

$$\Delta = \Delta_r \xi^r \omega = \sum_{0 \leqslant |\Lambda| \leqslant m} \Delta^{i,\Lambda}_r(x^\lambda, y^j_\Sigma) \overline{y}_{\Lambda i} \xi^r \omega \in \mathcal{O}^{0,n}_\infty [E \underset{Y}{\times} V^* Y], \quad 0 \leqslant |\Sigma| \leqslant m, \tag{27}$$

(see Appendix A). Then the Noether identity (26) takes the coordinate form

$$\left[\sum_{0 \leqslant |\Lambda| \leqslant m} \Delta^{i,\Lambda}_r d_\Lambda \mathcal{E}_i \right] \xi^r \omega = 0, \tag{28}$$

where $\mathcal{E}_i$ are variational derivatives (12).

Remark 2: We further use the relations

$$\sum_{0\leqslant|\Lambda|\leqslant k} B^\Lambda d_\Lambda A' = \sum_{0\leqslant|\Lambda|\leqslant k} (-1)^{|\Lambda|} d_\Lambda(B^\Lambda) A' + d_H\sigma, \tag{29}$$

$$\sum_{0\leqslant|\Lambda|\leqslant k} (-1)^{|\Lambda|} d_\Lambda(B^\Lambda A) = \sum_{0\leqslant|\Lambda|\leqslant k} \eta(B)^\Lambda d_\Lambda A, \tag{30}$$

$$\eta(B)^\Lambda = \sum_{0\leqslant|\Sigma|\leqslant k-|\Lambda|} (-1)^{|\Sigma+\Lambda|} C^{|\Sigma|}_{|\Sigma+\Lambda|} d_\Sigma B^{\Sigma+\Lambda}, \quad C^a_b = \frac{b!}{a!(b-a)!}, \tag{31}$$

$$(\eta\circ\eta)(B)^\Lambda = B^\Lambda, \tag{32}$$

for any exterior forms $A'\in\mathcal{O}^{*,n}_\infty Z$, $A\in\mathcal{O}^*_\infty z$ and any local function $B^\Lambda\in\mathcal{O}^0_\infty Z$ on jet manifolds of a fiber bundle $Z\to X$.

Theorem 5: If a Lagrangian L (4) admits a gauge symmetry υ (24), its Euler–Lagrange operator obeys the Noether identity (28) where

$$\Delta^{i,\Lambda}_r = \eta(\upsilon)^{i,\Lambda}_r = \sum_{0\leqslant|\Sigma|\leqslant m-|\Lambda|} (-1)^{|\Sigma+\Lambda|} C^{|\Sigma|}_{|\Sigma+\Lambda|} d_\Sigma \upsilon^{i,\Sigma+\Lambda}_r. \tag{33}$$

Conversely, if the Euler–Lagrange operator of a Lagrangian L obeys the Noether identity (28), this Lagrangian admits a gauge symmetry υ (24) where

$$\upsilon^{i,\Lambda}_r = \eta(\Delta)^{i,\Lambda}_r = \sum_{0\leqslant|\Sigma|\leqslant m-|\Lambda|} (-1)^{|\Sigma+\Lambda|} C^{|\Sigma|}_{|\Sigma+\Lambda|} d_\Sigma \Delta^{i,\Sigma+\Lambda}_r. \tag{34}$$

The relations (2) hold.

Proof: Given a differential operator υ (24), the operator $\Delta=\eta(\upsilon)$ expressed in the coordinate form (33) is defined in accordance with Theorem 16. Since the density

$$\upsilon \rfloor \delta L = \upsilon^i \mathcal{E}_i\omega = \sum_{0\leqslant|\Xi|\leqslant m} \upsilon^{i,\Xi}_r \xi^r_\Xi \mathcal{E}_i\omega$$

is d_H-exact, the Noether identity

$$\delta(\upsilon \rfloor \delta L) = \eta(\upsilon)\circ\delta L = 0$$

holds. Conversely, any Noether operator Δ (27) defines the VY-valued differential operator $\upsilon=\eta(\Delta)$ on E expressed in the coordinate form (34). This differential operator gives rise to a VE-valued differential operator (i.e., a generalized vector field) υ_E on E and, thus, defines a contact derivation ϑ_E of $\mathcal{O}^0_\infty E$. Indeed, let us consider the exact sequence of vector bundles

$$0\to V_Y E\to VE\to E\underset{Y}{\times} VY\to 0, \tag{35}$$

where $V_Y E$ is the vertical tangent bundle of $E\to Y$. Any splitting Γ of this exact sequence lifts υ to the generalized vector field $\upsilon_E=\Gamma\circ\upsilon$ on E, but the Lie derivative $\mathbf{L}_{\vartheta_E}L$ is independent of the choice of a splitting Γ. Due to the Noether identity (28), we obtain

$$\begin{aligned} 0 &= \sum_{0\leqslant|\Lambda|\leqslant m} \xi^r \Delta^{i,\Lambda}_r d_\Lambda \mathcal{E}_i\omega = \sum_{0\leqslant|\Lambda|\leqslant m} (-1)^{|\Lambda|} d_\Lambda(\xi^r\Delta^{i,\Lambda}_r)\mathcal{E}_i\omega + d_H\sigma \\ &= \sum_{0\leqslant|\Xi|\leqslant m} \upsilon^{i,\Xi}_r \xi^r_\Xi \mathcal{E}_i\omega + d_H\sigma = \upsilon\rfloor\delta L + d_H\sigma, \end{aligned}$$

i.e., υ is a gauge symmetry of L. Due to the equality (32), the relations (2) hold.

Example 3: If a gauge symmetry

$$v = (v_r^i \xi^r + v_r^{i,\mu} \xi_\mu^r)\partial_i \tag{36}$$

is of first jet order in parameters, the corresponding Noether operator and Noether identity read

$$\Delta_r^i = v_r^i - d_\mu v_r^{i,\mu}, \quad \Delta_r^{i,\mu} = -v_r^{i,\mu}, \tag{37}$$

$$[v_r^i \mathcal{E}_i - d_\mu (v_r^{i,\mu} \mathcal{E}_i)]\xi^r \omega = 0. \tag{38}$$

Any Lagrangian L has gauge symmetries. In particular, there always exist trivial gauge symmetries

$$v = \sum_\Lambda \eta(M)_r^{i,\Lambda} \xi_\Lambda^r, \quad M_r^{i,\Lambda} = \sum_\Sigma T^{i,j,\Lambda,\Sigma} d_\Sigma \mathcal{E}_j, \quad T_r^{j,i,\Lambda,\Sigma} = -T_r^{i,j,\Sigma,\Lambda},$$

corresponding to the trivial Noether identity

$$\sum_{\Sigma,\Lambda} T_r^{j,i,\Lambda,\Sigma} d_\Sigma \mathcal{E}_j d_\Lambda \mathcal{E}_i = 0.$$

Furthermore, given a gauge symmetry v (24), let h be a linear differential operator on some vector bundle $E' \to Y$, coordinated by (x^λ, y^i, ξ'^s), with values in the vector bundle E. Then the composition

$$v_0' = v \circ h = v_s'^{i,\Lambda} \xi_\Lambda'^s \partial_i, \quad v_s'^{i,\Lambda} = \sum_{\Xi+\Xi'=\Lambda} \sum_{0 \leqslant |\Sigma| \leqslant m-|\Xi|} v_r^{i,\Xi+\Sigma} d_\Sigma h_s^{r,\Xi'},$$

is a variational symmetry of the pull-back onto E' of a Lagrangian L on Y, i.e., a gauge symmetry of L. In view of this ambiguity, we agree to say that a gauge symmetry v (24) of a Lagrangian L is complete if a different gauge symmetry v_0' of L factors through v as

$$v_0' = v \circ h + T, \quad T \approx 0.$$

A complete gauge symmetry always exists, but the vector bundle of its parameters need not be finite-dimensional.

Accordingly, given the Noether operator (27), let H be a linear differential operator on $\overline{E}^*$ with values in the density-dual $\overline{E'}^*$ (1) of some vector bundle $E' \to Y$. Then the composition $\Delta' = H \circ \Delta$ is also a Noether operator. We agree to call the Noether operator (27) complete if a different Noether operator Δ' factors through Δ as

$$\Delta' = H \circ \Delta + F, \quad F \approx 0.$$

Proposition 6: A gauge symmetry v of a Lagrangian L is complete iff so is the associated Noether operator.

Proof: The proof follows at once from Proposition 17 in Appendix A. Given a gauge symmetry v of L, let v_0' be a different gauge symmetry. If $\eta(v)$ is a complete Noether operator, then

$$\eta(v_0') = H \circ \eta(v) + F, \quad F \approx 0,$$

and, by virtue of the relations (3), we have

$$v_0' = v \circ \eta(H) + \eta(F),$$

where $\eta(F) \approx 0$ because I_L is a differential ideal. The converse is similarly proved.

Example 4: Let us consider the gauge theory of principal connections on a principal bundle $P \to X$ with a structure Lie group G.[12] These connections are represented by sections of the quotient

$$C = J^1P/G \to X, \tag{39}$$

called the bundle of principal connections. This is an affine bundle coordinated by (x^λ, a^r_λ) such that, given a section A of $C \to X$, its components $A^r_\lambda = a^r_\lambda \circ A$ are coefficients of the familiar local connection form (i.e., gauge potentials). Let $J^\infty C$ be the infinite order jet manifold of $C \to X$ coordinated by $(x^\lambda, a^r_{\Lambda\lambda})$, $0 \leqslant |\Lambda|$. We consider the GDA $\mathcal{O}^*_\infty C$. Infinitesimal generators of local one-parameter groups of automorphisms of a principal bundle P are G-invariant projectable vector fields on $P \to X$. They are associated to sections of the vector bundle $T_G P = TP/G \to X$. This bundle is endowed with the coordinates $(x^\lambda, \tau^\lambda = \dot{x}^\lambda, \xi^r)$ with respect to the fiber bases $\{\partial_\lambda, e_r\}$ for $T_G P$, where $\{e_r\}$ is the basis for the right Lie algebra $\mathfrak{g}$ of G such that $[e_p, e_q] = c^r_{pq} e_r$. If

$$u = u^\lambda \partial_\lambda + u^r e_r, \quad v = v^\lambda \partial_\lambda + v^r e_r, \tag{40}$$

are sections of $T_G P \to X$, their bracket reads

$$[u,v] = (u^\mu \partial_\mu v^\lambda - v^\mu \partial_\mu u^\lambda)\partial_\lambda + (u^\lambda \partial_\lambda v^r - v^\lambda \partial_\lambda u^r + c^r_{pq} u^p v^q) e_r. \tag{41}$$

Any section u of the vector bundle $T_G P \to X$ yields the vector field

$$u_C = u^\lambda \partial_\lambda + (c^r_{pq} a^p_\lambda u^q + \partial_\lambda u^r - a^r_\mu \partial_\lambda u^\mu)\partial^\lambda_r \tag{42}$$

on the bundle of principal connections C (39). It is an infinitesimal generator of a one-parameter group of automorphisms of C.[12] Let us consider the bundle product

$$E = C \underset{X}{\times} T_G P, \tag{43}$$

coordinated by $(x^\lambda, \tau^\lambda, \xi^r, a^r_\lambda)$. It can be provided with the generalized vector field

$$v_E = v = (c^r_{pq} a^p_\lambda \xi^q + \xi^r_\lambda - a^r_\mu \tau^\mu_\lambda - \tau^\mu a^r_{\mu\lambda})\partial^\lambda_r. \tag{44}$$

For instance, this is a gauge symmetry of the global Chern–Simons Lagrangian.[14] Let us consider a subbundle $V_G P = VP/G \to X$ of the vector bundle $T_G X$ coordinated by (x^λ, ξ^r). Its sections $u = u^r e_r$ are infinitesimal generators of vertical automorphisms of P. Let us restrict the bundle product (43) to

$$E = C \underset{X}{\times} V_G P. \tag{45}$$

It is provided with the generalized vector field

$$v_E = v = (c^r_{pq} a^p_\lambda \xi^q + \xi^r_\lambda)\partial^\lambda_r. \tag{46}$$

This is a gauge symmetry of the Yang–Mills Lagrangians,[14] and yields the well-known Noether identity

$$[c^r_{pq} a^p_\lambda \mathcal{E}^\lambda_r - d_\lambda(\mathcal{E}^\lambda_q)]\xi^q \omega = 0.$$

IV. REDUCIBLE GAUGE THEORIES

Recall that the notion of a reducible Noether identity has come from that of a reducible constraint,[15] but it involves differential relations.

Definition 7: A complete Noether operator $\Delta \neq 0$ (27) and the corresponding Noether identity (26) are said to be *N-stage reducible* ($N = 0, 1, \ldots$) if there exist vector bundles $E_k \to Y$ and differential operators Δ_k, $k = 0, \ldots, N$, such that:

(i) Δ_k is a linear differential operator on the density-dual $\overline{E^*_{k-1}}$ of E_{k-1} with values in the density-dual $\overline{E^*_k}$ of E_k, where $E_{-1} = E$;
(ii) $\Delta_k \neq 0$ for all $k = 0, \ldots, N$;

(iii) $\Delta_k \circ \Delta_{k-1} \approx 0$ for all $k=0,\ldots,N$, where $\Delta_{-1}=\Delta$;
(iv) if Δ'_k is another differential operator possessing these properties, then it factors through Δ_k on-shell.

In particular, a zero-stage reducible Noether operator is called reducible. In this case, given bundle coordinates $(x^\lambda, y^i, \overline{\xi_r})$ on $\overline{E^*}$ and $(x^\lambda, y^i, \xi^{r_0})$ on E_0, a differential operator Δ_0 reads

$$\Delta_0 = \sum_{0\leqslant|\Xi|\leqslant m_0} \Delta^{r,\Xi}_{r_0} \overline{\xi_{\Xi r}} \xi^{r_0}\omega. \tag{47}$$

Then the reduction condition $\Delta_0 \circ \Delta \approx 0$ takes the coordinate form

$$\sum_{0\leqslant|\Xi|\leqslant m_0} \Delta^{r,\Xi}_{r_0} d_\Xi \left(\sum_{0\leqslant|\Lambda|\leqslant m} \Delta^{i,\Lambda}_r \overline{y_{\Lambda i}} \right) \xi^{r_0}\omega \approx 0, \tag{48}$$

i.e., the left-hand side of this expression takes the form

$$\sum_{0\leqslant|\Sigma|\leqslant m_0+m} M^{i,\Sigma}_{r_0} \overline{y_{\Sigma i}} \xi^{r_0} \otimes \omega,$$

where all the coefficients $M^{i,\Sigma}_{r_0}$ belong to the ideal I_L.

Definition 8: A complete gauge symmetry $v \not\approx 0$ (24) is said to be N-stage reducible if there exist vector bundles E_k and differential operators v^k, $k=0,\ldots,N$, such that:

(i) v^k is a linear differential operator on the vector bundle E_k with values in the vector bundle E_{k-1};
(ii) $v_k \not\approx 0$ for all $k=0,\ldots,N$;
(iii) $v^{k-1} \circ v^k \approx 0$ for all $k=0,\ldots,N$, where v^k, $k=-1$, stands for v;
(iv) if v'^k is another differential operator possessing these properties, then v^k factors through v'^k on-shell.

Theorem 9: A gauge symmetry v is N-stage reducible iff so is the associated Noether identity.

Proof: The proof follows at once from Theorem 16 and Proposition 17. Let us put $\Delta_k = \eta(v^k)$, $k=0,\ldots,N$. If $v^k \approx 0$, then $\eta(v^k) \approx 0$ because I_L is a differential ideal. By the same reason, if v^{k-1} and v^k obey the reduction condition $v^{k-1} \circ v^k \approx 0$, then

$$\eta(v^{k-1} \circ v^k) = \eta(v^k) \circ \eta(v^{k-1}) \approx 0.$$

The converse is justified in the same way. The equivalence of the conditions in items (iv) of Definitions 7 and 8 is proved similarly to that in Proposition 6.

V. GRADED LAGRANGIAN SYSTEMS

Recall that, by virtue of Batchelor's theorem,[16] any graded manifold $(\mathcal{U}, X)$ with a body X is isomorphic to the one whose structure sheaf $\mathcal{U}_Q$ is formed by germs of sections of the exterior product

$$\wedge Q^* = \mathbb{R} \underset{X}{\oplus} Q^* \underset{X}{\oplus} \overset{2}{\wedge} Q^* \underset{X}{\oplus} \cdots, \tag{49}$$

where Q^* is the dual of some real vector bundle $Q \to X$ of fiber dimension m. In field models, a vector bundle Q is usually given from the beginning. Therefore, we consider graded manifolds $(X, \mathcal{U}_Q)$ where Batchelor's isomorphism is fixed, and call $(X, \mathcal{U}_Q)$ the simple graded manifold constructed from Q. The structure ring $\mathcal{A}_Q$ of sections of $\mathcal{U}_Q$ consists of sections of the exterior bundle (49) called graded functions. Given bundle coordinates (x^λ, q^a) on Q with transition functions $q'^a = \rho^a_b q^b$, let $\{c^a\}$ be the corresponding fiber bases for $Q^* \to X$, together with transition functions $c'^a = \rho^a_b c^b$. Then (x^λ, c^a) is called the local basis for the graded manifold $(X, \mathcal{U}_Q)$. With respect to this basis, graded functions read

$$f = \sum_{k=0}^{m} \frac{1}{k!} f_{a_1 \cdots a_k} c^{a_1} \cdots c^{a_k},$$

where $f_{a_1 \cdots a_k}$ are local smooth real functions on X, and we omit the symbol of the exterior product of elements c^a.

Given a graded manifold $(X, \mathcal{U}_Q)$, let $\mathfrak{d}\mathcal{A}_Q$ be the $\mathcal{A}_Q$-module of $\mathbb{Z}_2$-graded derivations of the $\mathbb{Z}_2$-graded ring of $\mathcal{A}_Q$, i.e.,

$$u(ff') = u(f)f' + (-1)^{[u][f]} f u(f'), \quad u \in \mathfrak{d}\mathcal{A}_Q, \quad f, f' \in \mathcal{A}_Q,$$

where $[.]$ denotes the Grassmann parity. Its elements are called $\mathbb{Z}_2$-graded (or, simply, graded) vector fields on $(X, \mathcal{U}_Q)$. Due to the canonical splitting $VQ = Q \times Q$, the vertical tangent bundle $VQ \to Q$ of $Q \to X$ can be provided with the fiber bases $\{\partial_a\}$ which is the dual of $\{c^a\}$. Then a graded vector field takes the local form $u = u^\lambda \partial_\lambda + u^a \partial_a$, where u^λ, u^a are local graded functions. It acts on $\mathcal{A}_Q$ by the rule

$$u(f_{a \ldots b} c^a \cdots c^b) = u^\lambda \partial_\lambda (f_{a \ldots b}) c^a \cdots c^b + u^d f_{a \ldots b} \partial_d \rfloor (c^a \cdots c^b). \tag{50}$$

This rule implies the corresponding transformation law

$$u'^\lambda = u^\lambda, \quad u'^a = \rho^a_j u^j + u^\lambda \partial_\lambda (\rho^a_j) c^j.$$

Then one can show[5,12] that graded vector fields on a simple graded manifold can be represented by sections of the vector bundle $\mathcal{V}_Q \to X$ which is locally isomorphic to the vector bundle $\wedge Q^* \otimes_X (Q \oplus_X TX)$.

Using this fact, we can introduce graded exterior forms on the simple graded manifold $(X, \mathcal{U}_Q)$ as sections of the exterior bundle $\wedge \mathcal{V}^*_Q$, where $\mathcal{V}^*_Q \to X$ is the $\wedge Q^*$-dual of $\mathcal{V}_Q$. They are characterized both by the Grassmann parity and the familiar form degree. Relative to the dual local bases $\{dx^\lambda\}$ for T^*X and $\{dc^b\}$ for Q^*, graded one-forms read

$$\phi = \phi_\lambda dx^\lambda + \phi_a dc^a, \quad \phi'_a = \rho^{-1b}_a \phi_b, \quad \phi'_\lambda = \phi_\lambda + \rho^{-1b}_a \partial_\lambda (\rho^a_j) \phi_b c^j,$$

where dx^λ are even and dc^b are odd. The duality morphism is given by the interior product

$$u \rfloor \phi = u^\lambda \phi_\lambda + (-1)^{[\phi_a]} u^a \phi_a.$$

Graded exterior forms constitute the bigraded differential algebra (henceforth BGDA) $\mathcal{C}^*_Q$ with respect to the bigraded exterior product

$$\phi \wedge \phi' = (-1)^{|\phi||\phi'| + [\phi][\phi']} \phi' \wedge \phi, \quad \phi, \phi' \in \mathcal{C}^*_Q,$$

and the exterior differential

$$d(\phi \wedge \phi') = d\phi \wedge \phi' + (-1)^{|\phi|} \phi \wedge d\phi', \quad \phi, \phi' \in \mathcal{C}^*_Q.$$

Since the jet bundle $J^r Q \to X$ of a vector bundle $Q \to X$ is a vector bundle, let us consider the simple graded manifold $(X, \mathcal{U}_{J^r Q})$ constructed from $J^r Q \to X$. Its local basis is $\{x^\lambda, c^a_\Lambda\}$, $0 \leq |\Lambda| \leq r$, together with the transition functions

$$c'^a_{\lambda+\Lambda} = d_\lambda (\rho^a_j c^j_\Lambda), \quad d_\lambda = \partial_\lambda + \sum_{|\Lambda| < r} c^a_{\lambda+\Lambda} \partial^\Lambda_a, \tag{51}$$

where the graded derivations ∂^Λ_a are the duals of c^a_Λ. Let $\mathcal{C}^*_{J^r Q}$ be the BGDA of graded exterior forms on the graded manifold $(X, \mathcal{U}_{J^r Q})$. A linear bundle morphism $\pi^r_{r-1} : J^r Q \to J^{r-1} Q$ yields the corresponding monomorphism of BGDAs $\mathcal{C}^*_{J^{r-1} Q} \to \mathcal{C}^*_{J^r Q}$. Hence, there is the direct system of BGDAs

$$\mathcal{C}^*_Q \xrightarrow{\pi_0^{1*}} \mathcal{C}^*_{J^1Q} \cdots \xrightarrow{\pi_{r-1}^{r*}} \mathcal{C}^*_{J^rQ} \to \cdots. \tag{52}$$

Its direct limit $\mathcal{C}^*_\infty Q$ consists of graded exterior forms on graded manifolds $(X, \mathcal{U}_{J^rQ})$, $r \in \mathbb{N}$, modulo the pull-back identification, and it inherits the BGDA operations intertwined by the monomorphisms π^{r*}_{r-1}. It is locally a free $C^\infty(X)$-algebra locally generated by the elements $(1, c^a_\Lambda, dx^\lambda, \theta^a_\Lambda = dc^a_\Lambda - c^a_{\lambda+\Lambda} dx^\lambda)$, $0 \leqslant |\Lambda|$, where c^a_Λ and θ^a_Λ are odd.

In order to regard even and odd dynamic variables on the same footing, let $Y \to X$ hereafter be an affine bundle, and let $\mathcal{P}^*_\infty Y \subset \mathcal{O}^*_\infty Y$ be the $C^\infty(X)$-subalgebra of exterior forms whose coefficients are polynomial in the fiber coordinates on jet bundles $J^rY \to X$. This notion is intrinsic since any element of $\mathcal{O}^*_\infty Y$ is an exterior form on some finite order jet manifold and all jet bundles $J^rY \to X$ are affine. One can think of the GDA $\mathcal{P}^*_\infty Y$ as being the BGDA whose elements are even. Let us consider the product

$$\mathcal{S}^*_\infty[Q;Y] = \mathcal{C}^*_\infty Q \wedge \mathcal{P}^*_\infty Y \tag{53}$$

of bigraded algebras $\mathcal{C}^*_\infty Q$ and $\mathcal{P}^*_\infty Y$ over their common graded subalgebra $\mathcal{O}^*X$ of exterior forms on X.[4] It consists of the elements

$$\sum_i \psi_i \otimes \phi_i, \quad \sum_i \phi_i \otimes \psi_i, \quad \psi \in \mathcal{C}^*_\infty Q, \quad \phi \in \mathcal{P}^*_\infty Y,$$

modulo the commutation relations

$$\begin{gathered} \psi \otimes \phi = (-1)^{|\psi||\phi|} \phi \otimes \psi, \quad \psi \in \mathcal{C}^*_\infty Q, \quad \phi \in \mathcal{P}^*_\infty Y, \\ (\psi \wedge \sigma) \otimes \phi = \psi \otimes (\sigma \wedge \phi), \quad \sigma \in \mathcal{O}^*X. \end{gathered} \tag{54}$$

These elements are endowed with the total form degree $|\psi \otimes \phi| = |\psi| + |\phi|$ and the total Grassmann parity $[\psi \otimes \phi] = [\psi]$. Their multiplication

$$(\psi \otimes \phi) \wedge (\psi' \otimes \phi') := (-1)^{|\psi'||\phi|} (\psi \wedge \psi') \otimes (\phi \wedge \phi') \tag{55}$$

obeys the relation

$$\varphi \wedge \varphi' = (-1)^{|\varphi||\varphi'| + [\varphi][\varphi']} \varphi' \wedge \varphi, \quad \varphi, \varphi' \in \mathcal{S}^*_\infty[Q;Y],$$

and makes $\mathcal{S}^*_\infty[Q;Y]$ (53) into a bigraded $C^\infty(X)$-algebra. For instance, elements of the ring $\mathcal{S}^0_\infty[Q;Y]$ are polynomials of odd c^a_Λ and even y^i_Λ with coefficients in $C^\infty(X)$.

The algebra $\mathcal{S}^*_\infty[Q;Y]$ is provided with the exterior differential

$$d(\psi \otimes \phi) := (d_{\mathcal{C}} \psi) \otimes \phi + (-1)^{|\psi|} \psi \otimes (d_{\mathcal{P}} \phi), \quad \psi \in \mathcal{C}^*_\infty Q, \quad \phi \in \mathcal{P}^*_\infty Y, \tag{56}$$

where $d_{\mathcal{C}}$ and $d_{\mathcal{P}}$ are exterior differentials on the differential algebras $\mathcal{C}^*_\infty Q$ and $\mathcal{P}^*_\infty Y$, respectively. It obeys the relations

$$d(\varphi \wedge \varphi') = d\varphi \wedge \varphi' + (-1)^{|\varphi|} \varphi \wedge d\varphi', \quad \varphi, \varphi' \in \mathcal{S}^*_\infty[Q;Y],$$

and makes $\mathcal{S}^*_\infty[Q;Y]$ into a BGDA, which is locally generated by the elements

$$(1, c^a_\Lambda, y^i_\Lambda, dx^\lambda, \theta^a_\Lambda = dc^a_\Lambda - c^a_{\lambda+\Lambda} dx^\lambda, \theta^i_\Lambda = dy^i_\Lambda - y^i_{\lambda+\Lambda} dx^\lambda), \quad 0 \leqslant |\Lambda|,$$

where c^a_Λ, θ^a_Λ are odd and y^i_Λ, dx^λ, θ^i_Λ are even. The cohomology of its de Rham complex

$$0 \to \mathbb{R} \to \mathcal{S}^0_\infty[Q;Y] \xrightarrow{d} \mathcal{S}^1_\infty[Q;Y] \cdots \xrightarrow{d} \mathcal{S}^k_\infty[Q;Y] \to \cdots \tag{57}$$

equals the de Rham cohomology $H^*(X)$ of X.[4] We agree to call elements of $\mathcal{S}^*_\infty[Q;Y]$ the *graded exterior forms* on X.

Hereafter, let the collective symbols s^A_Λ and θ^A_Λ stand for both even and odd generating elements c^a_Λ, y^i_Λ, θ^a_Λ, θ^i_Λ of the $C^\infty(X)$-algebra $\mathcal{S}^*_\infty[Q;Y]$ which, thus, is locally generated by $(1, s^A_\Lambda, dx^\lambda, \theta^A_\Lambda)$, $|\Lambda| \geqslant 0$. Since $s^A_\Lambda = d_\Lambda s^A$ and $\theta^A_\Lambda = ds^A_\Lambda + s^A_{\lambda+\Lambda} dx^\lambda$, the BGDA $\mathcal{S}^*_\infty[Q;Y]$ is completely specified by the elements s^A together with their transition functions. Therefore, we agree to call $\{s^A\}$ the *local basis* for $\mathcal{S}^*_\infty[Q;Y]$.

Similarly to $\mathcal{O}^*_\infty Y$, the BGDA $\mathcal{S}^*_\infty[Q;Y]$ is decomposed into $\mathcal{S}^0_\infty[Q;Y]$-modules $\mathcal{S}^{k,r}_\infty[Q;Y]$ of k-contact and r-horizontal graded forms together with the corresponding projections h_k and h^r. Accordingly, the exterior differential d (56) on $\mathcal{S}^*_\infty[Q;Y]$ is split into the sum $d = d_H + d_V$ of the total and vertical differentials

$$d_H(\phi) = dx^\lambda \wedge d_\lambda(\phi), \quad d_V(\phi) = \theta^A_\Lambda \wedge \partial^\Lambda_A \phi, \quad \phi \in \mathcal{S}^*_\infty[Q;Y].$$

The projection endomorphism ϱ of $\mathcal{S}^*_\infty[Q;Y]$ is given by

$$\varrho = \sum_{k>0} \frac{1}{k} \overline{\varrho} \circ h_k \circ h^n, \quad \overline{\varrho}(\phi) \sum_{0 \leqslant |\Lambda|} (-1)^{|\Lambda|} \theta^A \wedge [d_\Lambda(\partial^\Lambda_A \rfloor \phi)], \quad \phi \in \mathcal{S}^{>0,n}_\infty[Q;Y],$$

similar to (9). The graded variational operator $\delta = \varrho \circ d$ is introduced. Then the BGDA $\mathcal{S}^*_\infty[Q;Y]$ is split into the $\mathbb{Z}_2$-graded variational bicomplex analogous to the above-mentioned variational bicomplex of $\mathcal{O}^*_\infty Y$.

We restrict our consideration to the short variational subcomplex

$$0 \to \mathbb{R} \to \mathcal{S}^0_\infty[Q;Y] \overset{d_H}{\to} \mathcal{S}^{0,1}_\infty[Q;Y] \cdots \overset{d_H}{\to} \mathcal{S}^{0,n}_\infty[Q;Y] \overset{\delta}{\to} \mathbf{E}_1 \tag{58}$$

and the subcomplex of one-contact graded forms

$$0 \to \mathcal{S}^{1,0}_\infty[Q;Y] \overset{d_H}{\to} \mathcal{S}^{1,1}_\infty[Q;Y] \cdots \overset{d_H}{\to} \mathcal{S}^{1,n}_\infty[Q;Y] \overset{\varrho}{\to} \mathbf{E}_1 \to 0, \tag{59}$$

of the BGDA $\mathcal{S}^*_\infty[Q;Y]$. They possess the following cohomology.[4]

Theorem 10: The cohomology of the complex (58) equals the de Rham cohomology $H^*(X)$ of X.

Theorem 11: The complex (59) is exact.

One can think of the elements

$$L = \mathcal{L}\omega \in \mathcal{S}^{0,n}_\infty[Q;Y], \quad \delta L = \theta^A \wedge \mathcal{E}_A \omega = \sum_{0 \leqslant |\Lambda|} (-1)^{|\Lambda|} \theta^A \wedge d_\Lambda(\partial^\Lambda_A L)\omega \in \mathbf{E}_1 \tag{60}$$

of the complexes (58)–(59) as being a *graded Lagrangian* and its Euler–Lagrange operator, respectively. The components $\mathcal{E}_A$ of δL are graded variational derivatives.

By virtue of Theorem 10, every δ-closed graded Lagrangian L (60) is the sum

$$\phi = \psi + d_H \xi, \quad \xi \in \mathcal{S}^{0,n-1}_\infty[Q;Y], \tag{61}$$

where ψ is a nonexact n-form on X.

The global exactness of the complex (59) at the term $\mathcal{S}^{1,n}_\infty[Q;Y]$ results in the following.[4]

Proposition 12: Given a graded Lagrangian $L = \mathcal{L}\omega$, there is the decomposition

$$dL = \delta L - d_H \Xi, \quad \Xi \in \mathcal{S}^{1,n-1}_\infty[Q;Y], \tag{62}$$

$$\Xi = \sum_{s=0} \theta^A_{\nu_s \cdots \nu_1} \wedge F^{\lambda \nu_s \cdots \nu_1}_A \omega_\lambda, \quad F^{\nu_k \cdots \nu_1}_A = \partial^{\nu_k \cdots \nu_1}_A \mathcal{L} - d_\lambda F^{\lambda \nu_k \cdots \nu_1}_A + h^{\nu_k \cdots \nu_1}_A, \tag{63}$$

where local graded functions h obey the relations $h^\upsilon_a = 0$, $h^{(\nu_k \nu_{k-1}) \cdots \nu_1}_a = 0$.

Proposition 12 states the existence of a global finite order Lepagean equivalent $\Xi_L = \Xi + L$ of any graded Lagrangian L. Locally, one can always choose Ξ (63) where all functions h vanish.

VI. BRST SYMMETRIES

A graded derivation $\vartheta \in \mathfrak{d}\mathcal{S}^0_\infty[Q;Y]$ of the $\mathbb{R}$-ring $\mathcal{S}^0_\infty[Q;Y]$ is said to be contact if the Lie derivative $\mathbf{L}_\vartheta$ preserves the ideal of contact graded forms of the BGDA $\mathcal{S}^*_\infty[Q;Y]$. With respect to the local basis $\{s^A\}$ for the BGDA $\mathcal{S}^*_\infty[Q;Y]$, any contact graded derivation takes the form

$$\vartheta = \vartheta_H + \vartheta_V = \vartheta^\lambda d_\lambda + \left(\vartheta^A \partial_A + \sum_{|\Lambda|>0} d_\Lambda \vartheta^A \partial^\Lambda_A\right), \tag{64}$$

where tuple of graded derivations $\{\partial_\lambda, \partial^\Lambda_A\}$ is defined as the dual of the tuple $\{dx^\lambda, ds^A_\Lambda\}$ of generating elements of the $\mathcal{S}^0_\infty[Q;Y]$-algebra $\mathcal{S}^*_\infty[Q;Y]$, and ϑ^λ, ϑ^A are local graded functions.[4] The interior product $\vartheta \rfloor \phi$ and the Lie derivative $\mathbf{L}_\vartheta \phi$, $\phi \in \mathcal{S}^*_\infty[Q;Y]$, are defined by the same formulas

$$\vartheta \rfloor \phi = \vartheta^\lambda \phi_\lambda + (-1)^{[\phi_A]} \vartheta^A \phi_A, \quad \phi \in \mathcal{S}^1_\infty[Q;Y],$$

$$\vartheta \rfloor (\phi \wedge \sigma) = (\vartheta \rfloor \phi) \wedge \sigma + (-1)^{|\phi|+[\phi][\vartheta]} \phi \wedge (\vartheta \rfloor \sigma), \quad \phi, \sigma \in \mathcal{S}^*_\infty[Q;Y],$$

$$\mathbf{L}_\vartheta \phi = \vartheta \rfloor d\phi + d(\vartheta \rfloor \phi), \quad \mathbf{L}_\vartheta(\phi \wedge \sigma) = \mathbf{L}_\vartheta(\phi) \wedge \sigma + (-1)^{[\vartheta][\phi]} \phi \wedge \mathbf{L}_\vartheta(\sigma),$$

as those on a graded manifold. One can justify that any vertical contact graded derivation ϑ (64) satisfies the relations

$$\vartheta \rfloor d_H \phi = -d_H(\vartheta \rfloor \phi), \quad \mathbf{L}_\vartheta(d_H \phi) = d_H(\mathbf{L}_\vartheta \phi), \quad \phi \in \mathcal{S}^*_\infty[Q;Y]. \tag{65}$$

Proposition 13: It follows from the splitting (12) that the Lie derivative $\mathbf{L}_\vartheta L$ of a Lagrangian L along a contact graded derivation ϑ (64) fulfills the first variational formula

$$\mathbf{L}_\vartheta L = \vartheta_V \rfloor \delta L + d_H(h_0(\vartheta \rfloor \Xi_L)) + d_V(\vartheta_H \rfloor \omega)\mathcal{L}, \tag{66}$$

where $\Xi_L = \Xi + L$ is a Lepagean equivalent of L given by the coordinate expression (63).[4]

A contact graded derivation ϑ is said to be variational if the Lie derivative (66) is d_H-exact. A glance at the expression (66) shows that: (i) a contact graded derivation ϑ is variational only if it is projected onto X, (ii) ϑ is variational iff its vertical part ϑ_V is variational.

Therefore, we restrict our consideration to vertical contact graded derivations

$$\vartheta = \sum_{0 \leqslant |\Lambda|} d_\Lambda v^A \partial^\Lambda_A, \tag{67}$$

where the tuple of graded derivations $\{\partial^\Lambda_A\}$ is defined as the dual of the tuple $\{\theta^\Lambda_A\}$ of contact graded forms. Such a derivation is completely determined by its first summand

$$v = v^A(x^\lambda, s^A_\Lambda)\partial_A, \quad 0 \leqslant |\Lambda| \leqslant k, \tag{68}$$

which is also a graded derivation of $\mathcal{S}^0_\infty[Q;Y]$. It is called the *generalized graded vector field.* A glance at the first variational formula (66) shows that ϑ (67) is variational iff $v \rfloor \delta L$ is d_H-exact.

A vertical contact graded derivation ϑ (67) is said to be nilpotent if

$$\mathbf{L}_v(\mathbf{L}_v \phi) = \sum_{|\Sigma| \geqslant 0, |\Lambda| \geqslant 0} \left(v^B_\Sigma \partial^\Sigma_B(v^A_\Lambda)\partial^\Lambda_A + (-1)^{[s^B][v^A]} v^B_\Sigma v^A_\Lambda \partial^\Sigma_B \partial^\Lambda_A\right)\phi = 0 \tag{69}$$

for any horizontal graded form $\phi \in \mathcal{S}^{0,*}_\infty[Q;Y]$. One can show[4] that ϑ is nilpotent only if it is odd and iff the equality

$$\mathbf{L}_\vartheta(v^A) = \sum_{|\Sigma| \geqslant 0} v^B_\Sigma \partial^\Sigma_B(v^A) = 0 \tag{70}$$

holds for all v^A.

Example 5: Let $Y \to X$ be an affine bundle, L (4) a Lagrangian of a gauge theory on Y and υ (24) its gauge symmetry where

$$E = Y \underset{X}{\times} V$$

is the pull-back onto Y of a vector bundle $V \to X$ coordinated by (x^λ, ξ^r). Let us consider the BGDA $\mathcal{S}^*_\infty[V;Y] = \mathcal{C}^*_\infty V \wedge \mathcal{P}^*_\infty Y$ possessing a local basis $\{c^r, y^i\}$. Let $L \in \mathcal{O}^{0,n}_\infty Y$ be a polynomial in y^i_Λ, $0 \leqslant |L|$. Then it is a graded Lagrangian $L \in \mathcal{P}^{0,n}_\infty Y \subset \mathcal{S}^{0,n}_\infty[V;Y]$ in $\mathcal{S}^*_\infty[V;Y]$. Since $E \to Y$ is the pull-back bundle, a gauge symmetry υ (24) gives rise to the generalized vector field $\upsilon_E = \upsilon$ on E, and the latter defines the generalized graded vector field υ (68) by the formula

$$\upsilon = \sum_{0 \leqslant |\Xi| \leqslant m} \upsilon^{i,\Xi}_r(x^\lambda, y^i_\Sigma) c^r_\Xi \partial_i. \tag{71}$$

It is easily justified that the vertical contact graded derivation ϑ (67) generated by υ (71) is variational for the graded Lagrangian L. It is odd, but need not be nilpotent. However, one can try to find a nilpotent contact graded derivation generated by some generalized graded vector field

$$\upsilon = \sum_{0 \leqslant |\Lambda| \leqslant m} \upsilon^{i,\Lambda}_r c^r_\Lambda \partial_i + u^r \partial_r \tag{72}$$

which coincides with ϑ on $\mathcal{P}^*_\infty Y$. In this case, the nilpotency conditions (70) read

$$\sum_\Sigma d_\Sigma \left(\sum_\Xi \upsilon^{i,\Xi}_r c^r_\Xi \right) \sum_\Lambda \partial^\Sigma_i (\upsilon^{j,\Lambda}_s) c^s_\Lambda + \sum_\Lambda d_\Lambda(u^r) \upsilon^{j,\Lambda}_r = 0, \tag{73}$$

$$\sum_\Lambda \left(\sum_\Xi d_\Lambda(\upsilon^{i,\Xi}_r c^r_\Xi) \partial^\Lambda_i + d_\Lambda(u^r) \partial^\Lambda_r \right) u^q = 0 \tag{74}$$

for all indices j and q. They are equations for graded functions $u^r \in \mathcal{S}^0_\infty[V;Y]$. Since these functions are polynomials

$$u^r = u^r_{(0)} + \sum_\Gamma u^{r,\Gamma}_{(1)p} c^p_\Gamma + \sum_{\Gamma_1,\Gamma_2} u^{r,\Gamma_1\Gamma_2}_{(2)p_1p_2} c^{p_1}_{\Gamma_1} c^{p_2}_{\Gamma_2} + \cdots \tag{75}$$

in c^s_Λ, Eqs. (73) and (74) take the form

$$\sum_\Sigma d_\Sigma \left(\sum_\Xi \upsilon^{i,\Xi}_r c^r_\Xi \right) \sum_\Lambda \partial^\Sigma_i (\upsilon^{j,\Lambda}_s) c^s_\Lambda + \sum_\Lambda d_\Lambda(u^r_{(2)}) \upsilon^{j,\Lambda}_r = 0, \tag{76}$$

$$\sum_\Lambda d_\Lambda(u^r_{(k\neq 2)}) \upsilon^{j,\Lambda}_r = 0, \tag{77}$$

$$\sum_\Lambda \sum_\Xi d_\Lambda(\upsilon^{i,\Xi}_r c^r_\Xi) \partial^\Lambda_i u^q_{(k-1)} + \sum_{m+n-1=k} d_\Lambda(u^r_{(m)}) \partial^\Lambda_r u^q_{(n)} = 0. \tag{78}$$

One can think of equalities (76) and (78) [and, consequently, the nilpotency conditions (73) and (74)] as being the generalized commutation relations and generalized Jacobi identities of gauge transformations, respectively.[17] For instance, let us consider a gauge system on a principal bundle and the generalized vector field υ (44) in Example 4. Following the procedure above, we replace parameters ξ^r and τ^λ with the odd ghosts C^r and C^λ, respectively, and obtain the generalized graded vector field

$$v = (c^r_{pq} a^p_\lambda C^q + C^r_\lambda - a^r_\mu C^\mu_\lambda - C^\mu a^r_{\mu\lambda})\partial^\lambda_r + \left(-\tfrac{1}{2} c^r_{pq} C^p C^q - C^\mu C^r_\mu\right)\partial_r + C^\lambda_\mu C^\mu \partial_\lambda \tag{79}$$

such that the vertical contact graded derivation (67) generated by v (79) is nilpotent. In the case of the vertical gauge symmetry (46), we obtain the familiar BRST transformation

$$v = (c^r_{pq} a^p_\lambda C^q + C^r_\lambda)\partial^\lambda_r - \tfrac{1}{2} c^r_{pq} C^p C^q \partial_r \tag{80}$$

of Yang–Mills theory.

Generalizing Example 5, we describe BRST symmetries in a general setting as follows.

Let $\mathcal{S}^*_\infty[Q;Y]$ be the BGDA (53) and $L \in \mathcal{S}^{0,n}_\infty[Q;Y]$ a graded Lagrangian. We agree to call generating elements s^A of $\mathcal{S}^*_\infty[Q;Y]$ the fields. Let $V \to X$ be a vector bundle coordinated by (x^λ, ξ^r). By analogy with $\mathcal{S}^*_\infty[Q;Y]$, we consider the BGDA,

$$\mathcal{S}^*_\infty[QV;Y] = \mathcal{C}^*_\infty[Q \underset{X}{\times} V] \wedge \mathcal{P}^*_\infty Y, \tag{81}$$

whose local basis is $\{s^A, c^r\}$. Obviously, L is also a graded Lagrangian in $\mathcal{S}^*_\infty[QV;Y]$. Let

$$\vartheta = \sum_{0 \leqslant |\Lambda|} (d_\Lambda v^A \partial^\Lambda_A + d_\Lambda v^r \partial^\Lambda_r) \tag{82}$$

be a graded contact derivation of the $\mathbb{R}$-ring $\mathcal{S}^0_\infty[QV;Y]$ generated by an odd generalized graded vector field

$$v = v^A \partial_A + v^r \partial_r \tag{83}$$

whose restriction to $\mathcal{S}^*_\infty[Q;Y]$ is linear in c^r_Λ, i.e.,

$$v = \sum_{0 \leqslant |\Xi| \leqslant m} c^r_\Xi v^{A,\Xi}_r(x^\lambda, s^B_\Sigma)\partial_A + v^r \partial_r. \tag{84}$$

If ϑ (82) is variational for L and nilpotent, we say that v (84) is a *BRST symmetry* of L. Following the terminology of BRST theory, we agree to call generating elements c^r of $\mathcal{S}^*[QV;Y]$ the *ghosts.*

VII. NOETHER'S SECOND THEOREM II

In order to introduce Noether identities in the case of BRST symmetries, let us extend the BGDA $\mathcal{S}^*[QV;Y]$ (81) to the BGDA

$$S^*_\infty[Q\overline{Y^*}V; Y\overline{Q^*}] = \mathcal{C}^*_\infty[Q \underset{X}{\times} \overline{Y^*} \underset{X}{\times} V] \wedge \mathcal{P}^*_\infty[Y \underset{X}{\times} \overline{Q^*}], \tag{85}$$

where $\overline{Q^*}$ is the density-dual of Q and $\overline{Y^*}$ is the density dual of the vector bundle $\widetilde{Y} \to X$ which the affine bundle Y is modeled on (e.g., $\widetilde{Y} = Y$ if Y is a vector bundle). The local basis for the BGDA $\mathcal{S}^*_\infty[Q\overline{Y^*}V; Y\overline{Q^*}]$ is $\{s^A, c^r, \overline{s_A}\}$. Following the terminology of the field–antifield BRST theory, we call generating elements $\overline{s_A}$ of $\mathcal{S}^*_\infty[Q\overline{Y^*}V; Y\overline{Q^*}]$ the *antifields*. Their Grassmann parity is $[\overline{s_A}] = ([s^A]+1) \bmod 2$.

The BGDA $\mathcal{S}^*_\infty[Q\overline{Y^*}V; Y\overline{Q^*}]$ (85) is provided with the *Koszul–Tate differential* defined as the nilpotent contact graded derivation

$$\overline{\delta} = \sum_{0 \leqslant |\Lambda|} \overleftarrow{\partial}^{\Lambda A} d_\Lambda \mathcal{E}_A, \tag{86}$$

where $\mathcal{E}_A$ are the graded variational derivatives (60) and the tuple of graded right derivations $\overleftarrow{\partial}^{\Lambda A}$ is the dual of the tuple of contact graded forms $\{\theta_{\Lambda A}\}$, i.e.,

$$\theta_{\Lambda A}\rfloor\overleftarrow{\partial}^{\Sigma B} = \delta^{\Sigma}_{\Lambda}\delta^{A}_{B},$$

where multi-indices Σ and Λ are regard modulo permutations. Because of the expression (60) for δL, it is convenient to describe the Koszul–Tate differential as a graded derivation acting on graded functions and forms ϕ on the right by the rule

$$\overline{\delta}(\phi) = \mathrm{d}\phi\rfloor\overline{\delta} + \mathrm{d}(\phi\rfloor\overline{\delta}), \quad \overline{\delta}(\phi\wedge\phi') = (-1)^{[\phi']}\overline{\delta}(\phi)\wedge\phi' + \phi\wedge\overline{\delta}(f').$$

Definition 14: Given a graded Lagrangian $L\in\mathcal{S}^{*}_{\infty}[Q;Y]\subset\mathcal{S}^{*}_{\infty}[Q\overline{Y^{*}}V;Y\overline{Q^{*}}]$ (60), we say that its Euler–Lagrange operator δL (60) obeys a Noether identity if there exists a $\overline{\delta}$-closed even graded density

$$\Delta = c^{r}\Delta_{r}\omega = \sum_{0\leqslant|\Lambda|\leqslant m} c^{r}\Delta^{A,\Lambda}_{r}(x^{\lambda},s^{B}_{\Sigma})\overline{s_{\Lambda A}}\omega \in \mathcal{S}^{0,n}_{\infty}[Q\overline{Y^{*}}V;Y\overline{Q^{*}}], \tag{87}$$

which is linear both in ghosts c^{r} and antifields $\overline{s_{A}}$ and their jets $\overline{s_{\Lambda A}}$. The above-mentioned *Noether identity* reads

$$\overline{\delta}(\Delta) = c^{r}\left[\sum_{0\leqslant|\Lambda|\leqslant m}\Delta^{A,\Lambda}_{r}d_{\Lambda}\mathcal{E}_{A}\right]\omega = 0. \tag{88}$$

Then Noether's second theorem for BRST symmetries is formulated as follows.

Theorem 15: If v (84) is a BRST symmetry of a graded Lagrangian L, then

$$\begin{aligned}\Delta = \eta(v) &= \sum_{0\leqslant|\Lambda|\leqslant m} c^{r}\eta(v)^{A,\Lambda}_{r}\overline{s_{\Lambda A}}\omega,\\ \eta(v)^{A,\Lambda}_{r} &= \sum_{0\leqslant|\Sigma|\leqslant m-|\Lambda|}(-1)^{|\Sigma+\Lambda|}\mathcal{C}^{|\Sigma|}_{|\Sigma+\Lambda|}d_{\Sigma}v^{A,\Sigma+\Lambda}_{r},\end{aligned} \tag{89}$$

is a $\overline{\delta}$-closed graded density (87). Conversely, if a $\overline{\delta}$-closed graded density Δ (87) exists, the generalized graded vector field

$$\begin{aligned}v = \eta(\Delta) &= \sum_{0\leqslant|\Xi|\leqslant m} c^{r}_{\Xi}\eta(\Delta)^{A,\Xi}_{r}\partial_{A},\\ \eta(\Delta)^{A,\Lambda}_{r} &= \sum_{0\leqslant|\Sigma|\leqslant m-|\Lambda|}(-1)^{|\Sigma+\Lambda|}\mathcal{C}^{|\Sigma|}_{|\Sigma+\Lambda|}d_{\Sigma}\Delta^{A,\Sigma+\Lambda}_{r},\end{aligned} \tag{90}$$

generates a contact graded derivation (82) which is variational for the graded Lagrangian L, but it need not be nilpotent. The relations (2) hold.

Proof: The first summand of the generalized vector field (84) defines the graded function

$$v = \sum_{0\leqslant|\Xi|\leqslant m} c^{r}_{\Xi}v^{A,\Xi}_{r}(x^{\lambda},s^{B}_{\Sigma})s_{A} \in \mathcal{S}^{*}_{\infty}[QQ^{*}V;Y\widetilde{Y}^{*}], \tag{91}$$

and *vice versa*. Then the proof follows from Theorem 18 in Appendix B. By virtue of this theorem, the graded function (91) yields the graded density (89). Since the graded density $v\rfloor\delta L$ is d_{H}-exact, we obtain the equality

$$\delta(v\rfloor\delta L) = \overline{\delta}(\eta(v)) = 0.$$

Conversely, the graded density (87) yields the graded function (91) where $v^{A,\Xi}_{r} = \eta(\Delta)^{A,\Xi}_{r}$. Since Δ (87) is $\overline{\delta}$-closed, we have

$$0 = \sum_{0\leqslant|\Lambda|\leqslant m} c^r\Delta_r^{A,\Lambda} d_\Lambda \mathcal{E}_A\omega = \sum_{0\leqslant|\Lambda|\leqslant m} (-1)^{|\Lambda|} d_\Lambda(c^r\Delta_r^{A,\Lambda})\mathcal{E}_A\omega + d_H\sigma$$
$$= \sum_{0\leqslant|\Xi|\leqslant m} c^r_\Xi v_r^{A,\Xi}\mathcal{E}_A\omega + d_H\sigma = v \rfloor \delta L + d_H\sigma,$$

i.e., the graded contact derivation generated by v (90) is variational for L. Due to the equality (32), the relations (2) hold.

Bearing in mind the field–antifield BRST theory and BV quantization, the Noether identity (88) can be rewritten as follows. Let us consider the BGDA $\mathcal{S}^*_\infty[Q\overline{Y}^*V; Y\overline{Q}^*\overline{V}^*]$ possessing the local basis $\{s^A, c^r, \overline{s_A}, \overline{c_r}\}$, where even elements $\overline{c_r}$ are called *antighosts* of the ghosts c^r. Clearly, the graded density Δ (87) is an element of $\mathcal{S}^*_\infty[Q\overline{Y}^*V; V\overline{Q}^*\overline{V}^*]$. Then this BGDA is provided with the contact graded right derivation

$$\overline{\delta_c} = \sum_{0\leqslant|\Lambda|} \left(\overleftarrow{\partial}^{\Lambda A} d_\Lambda \mathcal{E}_A + \overleftarrow{\partial}^{\Lambda r} d_\Lambda \Delta_r\right), \tag{92}$$

where the tuple of graded right derivations $\overleftarrow{\partial}^{\Lambda r}$ is the dual of $\theta_{\Lambda r}$. It is easily justified that the graded density Δ (87) obeys the Noether identity (88) iff the graded right derivation $\overline{\delta_c}$ (92) is nilpotent. It is the extension of the Koszul–Tate differential (86) to antighosts. For instance, the graded density Δ is always $\overline{\delta_c}$-exact.

VIII. REDUCIBLE BRST SYMMETRIES

The notion of a reducible Noether identity in Sec. IV is straightforwardly generalized to BRST symmetries, but we formulate it in terms of the Koszul–Tate differential. We say that the Noether identity (88) is N-stage reducible if the following conditions hold.

(a) There exists a set of vector bundles $V_{-1}=V, V_0, \ldots, V_N$ over X, and we consider the BGDA

$$\overline{\mathcal{S}}^*_\infty\{N\} = \mathcal{S}^*_\infty[Q\overline{Y}^*VV_1\ldots V_{2k-1}\ldots\overline{V}^*_0\ldots\overline{V}^*_{2k}\ldots; Y\overline{Q}^*V_0\ldots V_{2k}\ldots\overline{V}^*\overline{V}^*_1\ldots\overline{V}^*_{2k-1}\ldots]. \tag{93}$$

It possesses a local basis

$$\{s^A, \overline{s_A}, c^r, c^{r_0}, \ldots, c^{r_N}, \overline{c_r}, \overline{c_{r_0}}, \ldots, \overline{c_{r_N}}\}, \quad [c^{r_k}] = k \bmod 2, \tag{94}$$

where c^{r_k} and $\overline{c_{r_k}}$ are called the k-stage ghosts and antighosts, respectively..

(b) The BGDA (93) contains the graded density Δ (87) and a set of even graded densities

$$\Delta_{(k)} = c^{r_k}\Delta_{r_k}\omega = \sum_\Lambda c^{r_k}\Delta_{r_k}^{r_{k-1},\Lambda}(x^\lambda, s^B_\Sigma)\overline{c}_{\Lambda r_{k-1}}\omega, \quad k=0,\ldots,N, \tag{95}$$

such that the contact graded derivation

$$\overline{\delta_N} = \sum_{0\leqslant|\Lambda|} (\overleftarrow{\partial}^{\Lambda A} d_\Lambda \mathcal{E}_A + \overleftarrow{\partial}^{\Lambda r} d_\Lambda \Delta_r + \overleftarrow{\partial}^{\Lambda r_0} d_\Lambda \Delta_{r_0} + \cdots + \overleftarrow{\partial}^{\Lambda r_N} d_\Lambda \Delta_{r_N}) \tag{96}$$

is weakly nilpotent, i.e., $\overline{\delta_N}(\overline{\delta_N}(f))$ is $\overline{\delta}$-exact for any graded function $f\in\overline{\mathcal{S}}^0_\infty\{N\}$. This nilpotency condition is equivalent to the requirement that all the compositions

$$\sum_\Xi c^{r_k}\Delta_{r_k}^{r_{k-1},\Xi} d_\Xi\left(\sum_\Lambda \Delta_{r_{k-1}}^{r_{k-2},\Lambda}\overline{c}_{\Lambda r_{k-2}}\right), \quad k=1,\ldots,N, \tag{97}$$

are $\overline{\delta}$-exact. The graded derivation $\overline{\delta_N}$ (96) is called the *N-stage Koszul–Tate differential.*

(c) No graded density Δ, $\Delta_{(k)}$, $k=0,\ldots,N$, is $\overline{\delta}$-exact. Let $V'_0,\ldots,V'_{N'}$, be another set of vector bundles such that $V'_{k\leqslant N}$ contains V_k as a direct summand. Then the corresponding BGDA $\overline{\mathcal{S}}^*_\infty\{N'\}$ (93) contains the graded densities Δ (87), $\Delta_{(k)}$ (95), $k=0,\ldots,N$, and it is provided with the contact

graded derivation $\overline{\delta}_N$ (96). If there exists another set $\Delta'_{(k)}$, $k=0,\ldots,N'$, of graded densities obeying the conditions in item (b), then any graded density $\Delta'_{(k)}$ of this set is $\overline{\delta}_N$-exact.

Note, that following the arguments in Sec. III, one can say that the Noether identity (88) is complete if it obeys the condition (c).

If the Noether identity (88) is reducible, the associated BRST symmetry (90) is reducible as follows.

Let us consider the BGDA

$$\mathcal{S}^*_\infty\{N\} = \mathcal{S}^*_\infty[QQ^*VV^*V_1V_1^*\ldots V_{2k-1}V_{2k-1}^*\ldots;Y\tilde{Y}^*V_0V_0^*\ldots V_{2k}V_{2k}^*\ldots], \tag{98}$$

possessing the local basis $\{s^A, s_A, c^r, c^{r_0}, \ldots, c^{r_N}, c_r, c_{r_0}, \ldots, c_{r_N}\}$. By virtue of Theorem 18, each graded density $\Delta_{(k)}$ (95), $k=0,\ldots,N$, defines the graded function

$$v_{(k)} = \sum_\Xi c^{r_k}_\Xi \eta(\Delta_{(k)})^{r_{k-1},\Xi}_{r_k} c_{r_{k-1}} \in \mathcal{S}^0_\infty(\{N\}$$

and, consequently, the generalized graded vector field

$$v_{(k)} = \sum_\Xi c^{r_k}_\Xi \eta(\Delta_{(k)})^{r_{k-1},\Xi}_{r_k} \partial_{r_{k-1}} \in \mathcal{S}^0_\infty\{N\}, \tag{99}$$

which yields a contact graded derivation of the BGDA $\overline{\mathcal{S}}^*_\infty\{N\}$. Similar to the proof of Theorem 9, one can show that they possess the following properties.

(a′) Contact graded derivations ϑ and $\vartheta_{(k)}$ generated by the generalized graded vector fields v (90) and $v_{(k)}$ (99) are not weakly $\overline{\delta}$-exact, i.e., $\vartheta(f)$ and $\vartheta_{(k)}(f)$ are not $\overline{\delta}$-exact for some graded function $f \in \overline{\mathcal{S}}^*_\infty\{N\}$.

(b′) Contact graded derivations generated by the generalized graded vector fields

$$\sum_\Lambda d_\Lambda\left(\sum_\Xi c^{r_0}_\Xi \eta(\Delta_{(0)})^{r,\Xi}_{r_0}\right)\eta(\Delta)^{A,\Lambda}_r \partial_A, \tag{100}$$

$$\sum_\Lambda d_\Lambda\left(\sum_\Xi c^{r_k}_\Xi \eta(\Delta_{(k)})^{r_{k-1},\Xi}_{r_k}\right)\eta(\Delta_{(k-1)})^{r_{k-2},\Lambda}_{r_{k-1}} \partial_{r_{k-2}}, \quad k=1,\ldots,N, \tag{101}$$

are weakly $\overline{\delta}$-exact. This condition can be reformulated as follows. Let us consider the BGDA

$$\mathcal{S}^*_\infty[QQ\overline{Y}^*VV_1\ldots V_{2k-1}\ldots\overline{V}_0^*\ldots\overline{V}_{2k}^*\ldots;Y\tilde{Y}\overline{Q}^*V_0\ldots V_{2k}\ldots\overline{V}^*\overline{V}_1^*\ldots\overline{V}_{2k-1}^*\ldots]$$

whose basis consists of elements (94) and the elements s'^A associated to the additional bundles Q and $\tilde{Y}$. Let us replace the generalized graded vector field v (90) with

$$v' = \sum_{0\leq|\Xi|\leq m} c^r_\Xi \eta(\Delta)^{A,\Xi}_r(x^\lambda, s^B_\Sigma)\partial'_A, \tag{102}$$

where the graded derivations ∂'_A are dual of the basis elements s'^A. Then the contact graded derivation generated by the generalized graded vector field

$$v_N = v' + v_{(0)} + \cdots + v_{(N)} \tag{103}$$

is weakly nilpotent.

(c′) Let $v_{N'}$ be the generalized graded vector field (103) defined by the graded densities $\Delta'_{(k)}$ in item (c) above. Then there exists some generalized graded vector field u such that $v_{N'} - [u, v_N]$ is weakly $\overline{\delta}$-exact.

Conversely, one can show the following. Let v (90) be a BRST symmetry of a graded Lagrangian L. Let us assume that there exists a set of generalized graded vector fields

$$v_{(k)} = \sum_{\Xi} c^{r_k}_{\Xi} v^{r_{k-1},\Xi}_{r_k} \partial_{r_{k-1}} \in \mathcal{S}^0_\infty\{N\}, \tag{104}$$

which obey the conditions in items (a′)–(c′). Then the graded density (15) defines a complete reducible Noether identity where the graded densities

$$\Delta_{(k)} = \sum_{\Lambda} c^{r_k} \eta(v_{(k)})^{r_{k-1},\Lambda}_{r_k}(x^\lambda, s^B_\Sigma)\overline{c}_{\Lambda r_{k-1}}$$

obey the conditions in items (a)–(c).

In contrast with the generalized graded vector field v_N (103), the contact graded derivation generated by the generalized graded vector field $v + v_{(0)} + \cdots + v_{(N)}$ need not be weakly nilpotent. Its extension to the nilpotent one provides a BRST symmetry of the field–antifield BRST theory whose Lagrangian depends on ghosts and antifields.

APPENDIX A

A k-order differential operator on a fiber bundle $Y \to X$ with values in a fiber bundle $Z \to X$ is defined as a section Δ of the fiber bundle

$$J^k Y \underset{X}{\times} Z \to J^k Y.$$

It admits an m-order jet prolongation $\Delta^{(m)}$ as a section of the fiber bundle

$$J^{m+k} Y \underset{X}{\times} J^m Z \to J^{m+k} Y.$$

By a differential operator throughout is meant its appropriate finite order jet prolongation. Given bundle coordinates (x^λ, y^i) on Y and (x^λ, z^A) on Z, a differential operator Δ reads

$$z^A \circ \Delta = \Delta^A(x^\lambda, y^i_\Lambda), \quad z^A_\Sigma \circ \Delta^{(m)} = d_\Sigma \Delta^A, \quad 0 \leqslant |\Lambda| \leqslant k, \quad 0 \leqslant |\Sigma| \leqslant m.$$

If Z is a composite fiber bundle $\pi \circ \pi_{ZY}: Z \to Y \to X$ and the relation $\pi_{ZY} \circ \Delta = \pi^k_0$ holds, a differential operator Δ is identified to a section of the fiber bundle

$$J^k Y \underset{Y}{\times} Z \to J^k Y$$

or, equivalently, a bundle morphism

$$J^k Y \underset{Y}{\to} Z.$$

Let $E \to Y$ and $Q \to Y$ be vector bundles. A k-order Q-valued differential operator v on $E \to X$ is called linear on $E \to Y$ (or, simply, linear) if $v: J^k E \to Q$ is a morphism of the vector bundle $J^k E \to J^k Y$ to the vector bundle $Q \to Y$ over $\pi^k_0: J^k Y \to Y$. Given bundle coordinates (x^λ, y^i, ξ^r) on E and (x^λ, y^i, q^a) on Q, such an operator is represented by the function

$$v = v^a q_a = \sum_{0 \leqslant |\Lambda| \leqslant m} v^{a,\Lambda}_r(x^\lambda, y^i_\Sigma)\xi^r_\Lambda q_a \in \mathcal{O}^0_\infty[E \underset{Y}{\times} Q^*], \quad 0 \leqslant |\Sigma| \leqslant m. \tag{A1}$$

Let us consider the density-dual $\overline{E^*}$ (1) of a vector bundle $E \to Y$ and that $\overline{Q^*}$ of $Q \to Y$ coordinated by $(x^\lambda, y^i, \overline{q_a})$. Let Δ be a linear $\overline{E^*}$-valued differential operator on $\overline{Q^*}$. It is represented by the density

$$\Delta = \Delta_r \xi^r \omega = \sum_{0 \leqslant |\Lambda| \leqslant m} \Delta^{a,\Lambda}_r(x^\lambda, y^i_\Sigma)\overline{q}_{\Lambda a}\xi^r \omega \in \mathcal{O}^{0,n}_\infty[E \underset{Y}{\times} Q^*], \quad 0 \leqslant |\Sigma| \leqslant m. \tag{A2}$$

Theorem 16: Any linear Q-valued differential operator v (A1) on E yields the linear $\overline{E}^*$-valued differential operator

$$\eta(v) = \sum_{0\leqslant|\Lambda|\leqslant m} \eta(v)_r^{a,\Lambda}\overline{q}_{\Lambda a}\xi^r\omega,$$
$$\eta(v)_r^{a,\Lambda} = \sum_{0\leqslant|\Sigma|\leqslant m-|\Lambda|} (-1)^{|\Sigma+\Lambda|}C_{|\Sigma+\Lambda|}^{|\Sigma|}d_\Sigma(v_r^{a,\Sigma+\Lambda}), \tag{A3}$$

on $\overline{Q}^*$. Conversely, any linear $\overline{E}^*$-valued differential operator Δ (A2) on $\overline{Q}^*$ defines the linear Q-valued differential operator

$$\eta(\Delta) = \sum_{0\leqslant|\Lambda|\leqslant m} \eta(\Delta)_r^{a,\Lambda}\xi_\Lambda^r q_a,$$
$$\eta(\Delta)_r^{a,\Lambda} = \sum_{0\leqslant|\Sigma|\leqslant m-|\Lambda|} (-1)^{|\Sigma+\Lambda|}C_{|\Sigma+\Lambda|}^{|\Sigma|}d_\Sigma(\Delta_r^{a,\Sigma+\Lambda}), \tag{A4}$$

on E. The relations (2) hold.

Proof: The function v (A1) defines the density

$$\overline{v} = \sum_{0\leqslant|\Lambda|\leqslant m} v_r^{a,\Lambda}\xi_\Lambda^r\overline{q}_a\omega \in \mathcal{O}_\infty^{0,n}[\underset{Y}{E\times}Q^*]. \tag{A5}$$

Its Euler–Lagrange operator

$$\delta(\overline{v}) = \mathcal{E}_i dy^i\wedge\omega + \mathcal{E}_r d\xi^r\wedge\omega + \mathcal{E}^a d\overline{q}_a\wedge\omega$$

takes its values in the fiber bundle

$$V^*(\underset{Y}{E\times}Q^*)\underset{\underset{Y}{E\times}Q^*}{\otimes}\overset{n}{\wedge}T^*X, \tag{A6}$$

where

$$V^*(\underset{Y}{E\times}Q^*)$$

is the vertical cotangent bundle of the fiber bundle

$$\underset{Y}{E\times}Q^*\to X.$$

Let

$$\alpha_E: V^*(\underset{Y}{E\times}Q^*)\to V_Y^*(\underset{Y}{E\times}Q^*)\to V_Y^*E \tag{A7}$$

be the canonical projection of

$$V^*(\underset{Y}{E\times}Q^*)$$

onto the vertical cotangent bundle

$$V_Y^*(\underset{Y}{E\times}Q^*)$$

of the fiber bundle

$$E\underset{Y}{\times}Q^* \to Y$$

and, afterwards, onto the vertical cotangent bundle V_Y^*E of $E \to Y$. Then we obtain a differential operator $(\alpha_E \circ \delta)(\overline{v})$ on

$$E\underset{Y}{\times}Q^*$$

with values in the fiber bundle

$$V_Y^*E \underset{E}{\otimes} \overset{n}{\wedge} T^*X.$$

It reads

$$(\alpha_E \circ \delta)(\overline{v}) = \mathcal{E}_r \overline{\mathrm{d}\xi^r} \otimes \omega = \sum_{0 \leq |\Lambda| \leq m} (-1)^{|\Lambda|} d_\Lambda (v_r^{a,\Lambda} \overline{q_a}) \overline{\mathrm{d}\xi^r} \otimes \omega,$$

where $\{\overline{\mathrm{d}\xi^r}\}$ is the fiber basis for $V_Y^*E \to E$. Due to the canonical isomorphism

$$V_Y^*E = E^*\underset{Y}{\times}E,$$

this operator defines the density

$$\sum_{0 \leq |\Lambda| \leq m} (-1)^{|\Lambda|} d_\Lambda (v_r^{a,\Lambda} \overline{q_a}) \xi^r \omega \in \mathcal{O}_\infty^{0,n}[E\underset{Y}{\times}Q^*]$$

and, by virtue of the formula (30), the desired differential operator (A3). Conversely, the Euler–Lagrange operator of the density (A2) takes its values in the fiber bundle (A6) and reads

$$\delta(\overline{v}) = \mathcal{E}_i dy^i \wedge \omega + \mathcal{E}_r d\xi^r \wedge \omega + \mathcal{E}^a d\overline{q_a} \wedge \omega. \tag{A8}$$

In order to repeat the above-mentioned procedure, let us consider a volume form $J\omega$ on X and substitute $\mathrm{d}\overline{q_a} \wedge \omega = J\mathrm{d}q_a \wedge \omega$ into expression (A8). Using the projection

$$\alpha_Q : V^*(E\underset{Y}{\times}Q^*) \to V_Y^*Q^*$$

similar to α_E (A7) and the canonical isomorphism

$$V_Y^*Q^* = Q\underset{Y}{\times}Q^*,$$

we come to the density

$$\sum_{0 \leq |\Lambda| \leq m} (-1)^{|\Lambda|} d_\Lambda (\Delta_r^{a,\Lambda} \xi^r) q_a J\omega \in \mathcal{O}_\infty^{0,n}[E\underset{Y}{\times}Q^*]$$

and, hence, the function

$$\sum_{0 \leq |\Lambda| \leq m} (-1)^{|\Lambda|} d_\Lambda (\Delta_r^{a,\Lambda} \xi^r) q_a \in \mathcal{O}_\infty^{0,n}[E\underset{Y}{\times}Q^*],$$

defining the desired operator (A4). The relations (2) result from the relation (32).

Relations (2) show that the intertwining operator η (A3) and (A4) provides a bijection between the sets $\mathrm{Diff}(E,Q)$ and $\mathrm{Diff}(\overline{Q^*},\overline{E^*})$ of differential operators (A1) and (A2).

Proposition 17: Compositions of operators $v \circ v'$ and $\Delta' \circ \Delta$ obey the relations (3).

Proof: It suffices to prove the first relation. Let $v \circ v' \in \mathrm{Diff}(E',Q)$ be a composition of differ-

ential operators $v \in \mathrm{Diff}(E,Q)$ and $v' \in \mathrm{Diff}(E',E)$. Given fiber coordinates (ξ^r) on $E \to Y$, (ϵ^p) on $E' \to Y$ and $(\overline{q_a})$ on $\overline{Q}^* \to Y$, this composition defines the density (A5)

$$\overline{v \circ v'} = \sum_{\Lambda} v_r^{a,\Lambda} d_\Lambda \left(\sum_{\Sigma} v_p'^{r,\Sigma} \epsilon_\Sigma^p \right) \overline{q_a} \omega.$$

Following the relation (29), one can bring this density into the form

$$\sum_{\Sigma} v_p'^{r,\Sigma} \epsilon_\Sigma^p \sum_{\Lambda} (-1)^{|\Lambda|} d_\Lambda (v_r^{a,\Lambda} \overline{q_a}) \omega + d_H \sigma = \sum_{\Sigma} v_p'^{r,\Sigma} \epsilon_\Sigma^p \sum_{\Lambda} \eta(v)_r^{a,\Lambda} \overline{q}_{\Lambda a} \omega + d_H \sigma.$$

Its Euler–Lagrange operator projected to $V_Y^* E' \underset{E'}{\otimes} T^* X$ is

$$\sum_{\Sigma} (-1)^{|\Sigma|} d_\Sigma \left(v_p'^{r,\Sigma} \sum_{\Lambda} \eta(v)_r^{a,\Lambda} \overline{q}_{\Lambda a} \right) \overline{d\epsilon}^p \otimes \omega = \sum_{\Sigma} \eta(v')_p^{r,\Sigma} d_\Sigma \left(\sum_{\Lambda} \eta(v)_r^{a,\Lambda} \overline{q}_{\Lambda a} \right) \overline{d\epsilon}^p \otimes \omega,$$

which leads to the desired composition $\eta(v') \circ \eta(v)$.

APPENDIX B

The following is a graded counterpart of Theorem 16.

Let $T \to X$ and $W \to X$ be vector bundles, W^* the dual of W, and $\overline{W}^*$ the density-dual (1) of W. Given the BGDA $\mathcal{S}_\infty^*[Q;Y]$ (53), let us consider its extensions to a BGDA $\mathcal{S}_\infty^*[T,W^*]$ with the local basis $\{s^A, t^r, w_a\}$, where elements t^r and w_a are either even or odd, and to a BGDA $\mathcal{S}_\infty^*[T,\overline{W}^*]$ possessing the local basis $\{s^A, t^r, \overline{w}_a\}$, where $[\overline{w}_a] = ([w_a]+1) \bmod 2$.

Theorem 18: Given a graded function

$$v = \sum_{0 \leq |\Lambda| \leq m} t_\Lambda^r v_r^{a,\Lambda}(x^\lambda, s_\Sigma^A) w_a \in \mathcal{S}_\infty^0[T,W^*], \tag{B1}$$

linear in t_Λ^r and w_a, there exists a graded density

$$\begin{aligned} \eta(v) &= \sum_{0 \leq |\Lambda| \leq m} t^r \eta(v)_r^{a,\Lambda} \overline{w}_{\Lambda a} \omega \in \mathcal{S}_\infty^{0,n}[T,\overline{W}^*], \\ \eta(v)_r^{a,\Lambda} &= \sum_{0 \leq |\Sigma| \leq m-|\Lambda|} (-1)^{|\Sigma+\Lambda|} C_{|\Sigma+\Lambda|}^{|\Sigma|} d_\Sigma (v_r^{a,\Sigma+\Lambda}), \end{aligned} \tag{B2}$$

linear in t^r and $\overline{w}_{\Lambda_a}$. Conversely, such a density

$$\Delta = \sum_{0 \leq |\Lambda| \leq m} t^r \Delta_r^{a,\Lambda} \overline{w}_{\Lambda a} \omega \tag{B3}$$

defines the graded function

$$\begin{aligned} \eta(\Delta) &= \sum_{0 \leq |\Lambda| \leq m} t_\Lambda^r \eta(\Delta)_r^{a,\Lambda} w_a \in \mathcal{S}_\infty^0[T,W^*], \\ \eta(\Delta)_r^{a,\Lambda} &= \sum_{0 \leq |\Sigma| \leq m-|\Lambda|} (-1)^{|\Sigma+\Lambda|} C_{|\Sigma+\Lambda|}^{|\Sigma|} d_\Sigma (\Delta_r^{a,\Sigma+\Lambda}), \end{aligned} \tag{B4}$$

linear in t_Λ^r and w_a.

Proof: The graded function v (B1) defines the graded density

$$\overline{v} = \sum_{0\leqslant|\Lambda|\leqslant m} t^r_\Lambda v^{a,\Lambda}_r(x^\lambda, s^A_\Sigma)\overline{w}_a\omega \in \mathcal{S}^0_\infty[T, \overline{W}^*].$$

Its Euler–Lagrange operator $\delta(\overline{v})$ (60) contains the summand

$$\mathcal{E}_r\theta^r \wedge \omega = \sum_{0\leqslant|\Lambda|\leqslant m} (-1)^{|\Lambda|}\theta^r \wedge d_\Lambda(v^{a,\Lambda}_r\overline{w}_a)\omega,$$

which defines the graded density

$$\sum_{0\leqslant|\Lambda|\leqslant m} (-1)^{|\Lambda|}t^r d_\Lambda(v^{a,\Lambda}_r\overline{w}_a)\omega$$

owing to the canonical isomorphism $V^*T = T^* \times T$. Using the relation (30), we come to the formula (B2). The converse is proved similarly to the proof of Theorem 16.

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Some physical appearances of vector coherent states and coherent states related to degenerate Hamiltonians

S. Twareque Ali[a)]
Department of Mathematics and Statistics, Concordia University, Montréal, Québec, Canada H4B 1R6

F. Bagarello[b)]
Dipartimento di Metodi e Modelli Matematici, Facoltà di Ingegneria, Università di Palermo, I-90128 Palermo, Italy

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In the spirit of some earlier work on the construction of vector coherent states (VCS) over matrix domains, we compute here such states associated to some physical Hamiltonians. In particular, we construct vector coherent states of the Gazeau–Klauder type. As a related problem, we also suggest a way to handle degeneracies in the Hamiltonian for building coherent states. Specific physical Hamiltonians studied include a single photon mode interacting with a pair of fermions, a Hamiltonian involving a single boson and a single fermion, a charged particle in a three-dimensional harmonic force field and the case of a two-dimensional electron placed in a constant magnetic field, orthogonal to the plane which contains the electron. In this last example, which is related to the fractional quantum Hall effect, an interesting modular structure emerges for two underlying von Neumann algebras, related to opposite directions of the magnetic field. This leads to the existence of coherent states built out of Kubo-Martin-Schwinger (KMS) states for the system. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1901343]

I. INTRODUCTION

In some earlier work,[4,20] a fairly systematic method has been introduced for constructing vector coherent states (VCS) over various types of matrix domains. The construction included earlier types of vector coherent states, arising mainly in nuclear physical problems, under the additional assumption of the existence of a resolution of the identity. (A detailed discussion of this point, as well as an exhaustive reference to the earlier literature is given in Ref. 4.) In the present paper we apply the method developed in Refs. 4 and 20 to construct vector coherent states arising from various physical Hamiltonians. The kind of coherent states we generate are thus vectorial generalizations of the Gazeau–Klauder type[10] of coherent states. Some of the Hamiltonians we consider have degenerate spectra and in order to deal with this situation, we attempt a second generalization of the Gazeau–Klauder formalism. There have been earlier attempts in the literature for handling degeneracies when constructing coherent states associated to Hamiltonians.[8,15] The method we suggest here is somewhat different from the one suggested in Ref. 15 and radically different from that suggested in Ref. 8. However, we feel that the present method is more economical in the introduction of additional parameters defining the coherent states—we only need one additional parameter. We also look at situations where the degeneracy is countably infinite. In this context, in the case of a two-dimensional electron placed in a constant magnetic field, orthogonal to the plane which contains the electron, we encounter a highly interesting modular

[a)]Electronic mail: stali@mathstat.concordia.ca
[b)]Electronic mail: bagarell@unipa.it; www.unipa.it/~bagarell

algebraic structure generated by the observables of the problem, leading to the rather unexpected appearance of equilibrium statistical mechanical states of the well-known Kubo-Martin-Schwinger (KMS) type.[14] It is worth recalling that this model, while well known even from textbooks on quantum mechanics, is of additional interest in that it is the building block for writing down the many-body Hamiltonian for the fractional quantum Hall effect, see Ref. 7 and references therein. It is well known that the eigenspectrum of the single electron Hamiltonian can be found explicitly, and that there exists an infinite degeneracy for each eigenvalue (the so-called *Landau levels*).[5]

The rest of this paper is organized as follows: In Sec. II we review the Gazeau–Klauder construction within the framework of reproducing kernel Hilbert spaces. This general framework is then used in Sec. III to construct vector coherent states of the Gazeau–Klauder type. We illustrate the method with a couple of physical examples. Section generalizes the treatment to Hamiltonians with degeneracies. We treat the cases of finite and infinite degeneracies separately and illustrate the finite situation with a number of physical examples. In Section V we work out, in detail, a physical example in which infinite degeneracies occur. In this example we also observe the existence of a modular algebraic structure and the appearance of KMS states, familiar from equilibrium statistical mechanics. Finally, in the Appendix we collect together explicit computations of some of the more unfamiliar formulas in Secs. IV A and V.

II. THE GAZEAU–KLAUDER SCHEME REVISITED

The Gazeau–Klauder scheme[10] is a method for constructing coherent states $|J,\gamma\rangle$, where $J \geqslant 0$ and $\gamma \in \mathbb{R}$, associated to physical Hamiltonians H, which have discrete nondegenerate spectra. The states must satisfy the following properties:

(i) *Continuity*, the mapping $(J,\gamma) \to |J,\gamma\rangle$ is continuous in some appropriate topology.
(ii) *Resolution of the identity*, $\int |J,\gamma\rangle\langle J,\gamma| \mathrm{d}m(J,\gamma) = I$, where I is the identity in the Hilbert space and dm is some appropriate measure.
(iii) *Temporal stability*, $e^{-iHt}|J,\gamma\rangle = |J,\gamma+\omega t\rangle$, for some constant ω.
(iv) *Action identity*, $\langle J,\gamma|H|J,\gamma\rangle = \omega J$.

Their construction, which we shall review below, works if H has no degenerate eigenstates and, furthermore, if the lowest eigenvalue is exactly zero. This second requirement can always be imposed for reasonable physical systems, since all physically relevant Hamiltonians H must be bounded from below, in order to admit a ground state. This means that there exists a lowest eigenvalue $E_{\min} > -\infty$, so that we can define a new Hamiltonian, $\widetilde{H} = H - E_{\min} I$, whose lowest eigenvalue is clearly zero. Furthermore H and $\widetilde{H}$ have *exactly* the same dynamical content, since they obey the same commutation relations with all the observables of the system. For such a Hamiltonian, in the Gazeau–Klauder scheme, one writes the eigenvalues as $E_n = \omega\epsilon_n$ by introducing a sequence of dimensionless quantities $\{\epsilon_n\}$ ordered as $0 = \epsilon_0 < \epsilon_1 < \epsilon_2 < \cdots$. Then, the Gazeau–Klauder coherent states are defined as

$$|J,\gamma\rangle := \mathcal{N}(J)^{-1/2} \sum_{k=0}^{\infty} \frac{J^{n/2} e^{-i\varepsilon_n \gamma}}{\sqrt{\rho_n}} |n\rangle, \tag{2.1}$$

where $\mathcal{N}$ is a normalization factor, which turns out to be dependent on J only, the $|n\rangle$ are the eigenstates of H and the ρ_n are positive numbers, which are fixed by the requirement of the action identity to be $\rho_n = \epsilon_1 \epsilon_2 \cdots \epsilon_n$.

In the rest of this section we recapitulate the Gazeau–Klauder construction, with the aim of putting the discussion in a somewhat more general context, which will also enable us to extend the construction to include vector coherent states and to cases where each energy level is (a) finitely degenerate and (b) infinitely degenerate. The essential mathematical ingredient in the construction is a reproducing kernel Hilbert space. Although this concept is a familiar one, both in the physical and the mathematical literature, we summarize below some essential features, putting them in the context of the present discussion.

A. Some generalities

Recall that a reproducing kernel Hilbert space (see, for example, Refs. 2, 6, and 16 for detailed discussions) $\mathfrak{H}_{\text{ker}}$, consists of functions $f: X \to \mathbb{C}$ on some topological space X, with the property that, for all $x \in X$, the evaluation map E_x: $\mathfrak{H}_{\text{ker}} \to \mathbb{C}$, $E_x(f) = f(x)$, is continuous. Such a space may or may not be an L^2-space or a subspace of an L^2-space and its scalar product, which we denote by $\langle \cdot | \cdot \rangle_{\text{ker}}$, may be given in more general ways. (Although the space $\mathfrak{H}_{\text{ker}}$ could be finite or infinite dimensional, we shall only be interested in the infinite dimensional case here.) The continuity of the evaluation map implies that for each $x \in X$, there exists a vector $\xi_x \in \mathfrak{H}_{\text{ker}}$ such that

$$f(x) = \langle \xi_x | f \rangle_{\text{ker}}, \quad \text{for any } f \in \mathfrak{H}_{\text{ker}}. \tag{2.2}$$

The vectors ξ_x, $x \in X$, are total in $\mathfrak{H}_{\text{ker}}$ (i.e., their linear span is dense in the space), as can be easily seen. Furthermore, they can be used to define the reproducing kernel, $K: X \times X \to \mathbb{C}$, for this space,

$$K(y,x) := \langle \xi_y | \xi_x \rangle_{\text{ker}} = \xi_x(y), \tag{2.3}$$

the second equality following from (2.2). If now $\{\Psi_n\}_{n=0}^{\infty}$ is an orthonormal basis of $\mathfrak{H}_{\text{ker}}$, then writing

$$\xi_x = \sum_{n=0}^{\infty} \lambda_n(x) \Psi_n, \quad \lambda_n(x) = \langle \Psi_n | \xi_x \rangle_{\text{ker}} = \overline{\Psi_n(x)},$$

and taking account of (2.3), we get

$$K(x,y) = \sum_{n=0}^{\infty} \Psi_n(x) \overline{\Psi_n(y)}. \tag{2.4}$$

It should be noted that the above equation is true for any orthonormal basis, so that the kernel $K(x,y)$ is independent of the basis chosen to express it. An equivalent condition for the existence of a reproducing kernel is that there be an orthonormal basis for which,

$$\sum_{n=0}^{\infty} |\Psi_n(x)|^2 < \infty, \quad \text{for all } x \in X. \tag{2.5}$$

If we *symbolically* write the scalar product of $\mathfrak{H}_{\text{ker}}$ as

$$\langle f | g \rangle_{\text{ker}} = \int_X \overline{f(x)} g(x) \mathrm{d}\mu(x),$$

then using (2.2) and (2.3) we may also write

$$\langle \xi_x | \xi_y \rangle_{\text{ker}} = \int_X \overline{\xi_x(z)} \xi_y(z) \mathrm{d}\mu(z) = \int_X \langle \xi_x | \xi_z \rangle_{\text{ker}} \langle \xi_z | \xi_y \rangle_{\text{ker}} \, \mathrm{d}\mu(z).$$

Referring again to (2.3) and noting that the vectors ξ_x are total in $\mathfrak{H}_{\text{ker}}$, the above equation may be re-expressed either as

$$K(x,y) = \int_X K(x,y) K(z,y) \mathrm{d}\mu(z), \tag{2.6}$$

or as

$$\int_X |\xi_x\rangle\langle\xi_z| \mathrm{d}\mu(z) = I_{\text{ker}}, \tag{2.7}$$

where $I_{\ker}$ is the identity operator on $\mathfrak{H}_{\ker}$. Thus, these equations appear now as the well-known *reproducing property* for the kernel $K(x,y)$ and the *resolution of the identity* generated by the vectors ξ_x, respectively. Once more we emphasize that in general, Eqs. (2.6) and (2.7) only have symbolic meaning. However, if in fact $\mathfrak{H}_{\ker}$ is an L^2 space with respect to some real measure $\mathrm{d}\mu$ on X (or a subspace of such a space), then the above equations do make literal sense. In view of equations (2.6) and (2.7), we may call the vectors ξ_x the *coherent states* defined by the kernel $K(x,y)$ and they in fact characterize the reproducing kernel Hilbert space $\mathfrak{H}_{\ker}$. However, since $\|\xi_x\|^2 = K(x,x)$, these states are generally not normalized. If $K(x,x) \neq 0$, we may define the normalized vectors $\zeta_x = [K(x,x)]^{-1/2}\xi_x$, for which we would have the "resolution of the identity"

$$\int_X |\zeta_z\rangle\langle\zeta_z| K(z,z)\mathrm{d}\mu(z) = I_{\ker}.$$

Coherent states, of all types appearing in the physical literature, can be built by simply transporting the above structure to some other appropriate Hilbert space by a basis change. To see this, let $\mathfrak{H}$ be an abstract (separable, complex) Hilbert space and $\{\phi_n\}_{n=0}^{\infty}$ an orthonormal basis of it. Define the unitary map, $V: \mathfrak{H}_{\ker} \to \mathfrak{H}$ by $V|\Psi_n\rangle = |\phi_n\rangle$, $n = 0, 1, 2, \ldots$. Then the vectors

$$|\eta_x\rangle := V|\xi_x\rangle = \sum_{n=0}^{\infty} \overline{\Psi_n(x)}|\phi_n\rangle, \tag{2.8}$$

define (non-normalized) coherent states on $\mathfrak{H}$. They are associated to the same reproducing kernel as the ξ_x since,

$$K(x,y) = \langle \eta_x | \eta_y \rangle_{\mathfrak{H}} = \langle \xi_x | \xi_y \rangle_{\ker}$$

and satisfy a "resolution of the identify" similar to (2.7):

$$\int_X |\eta_z\rangle\langle\eta_z| \mathrm{d}\mu(z) = I_{\mathfrak{H}},$$

where again, this equation is to be generally interpreted in the sense of (2.6). Furthermore, for arbitrary $\phi \in \mathfrak{H}$, the function $f(x) = \langle \eta_x | \phi \rangle_{\mathfrak{H}}$ defines a vector in $\mathfrak{H}_{\ker}$ and it is easy to see that the inverse of the isometry V is given by this relation, i.e., $(V^{-1}\phi)(x) = \langle \eta_x | \phi \rangle_{\mathfrak{H}}$. Usually, in the physical literature one works with the normalized vectors

$$|x\rangle = [K(x,x)]^{-1/2}|\eta_x\rangle = [K(x,x)]^{-1/2} \sum_{n=0}^{\infty} \overline{\Psi_n(x)}|\phi_n\rangle. \tag{2.9}$$

It will later become apparent that the above coherent states coincide with $|J,\gamma\rangle$ in (2.1) upon identifying $\Psi_n(x)$ with $J^{n/2}e^{i\epsilon_n\gamma}/\sqrt{\rho_n}$, ρ_n with $\epsilon_1\epsilon_2\cdots\epsilon_n = \epsilon_n!$ and $\mathcal{N}(J)$ with $K(x,x)$.

To summarize the preceding discussion, coherent states are linear superpositions of the elements of a basis in a Hilbert space, the components in the expansion being the values taken at a point by a set of vectors forming a basis in a reproducing kernel Hilbert space. Alternatively, referring to (2.5), we may identify the reproducing kernel Hilbert space $\mathfrak{H}_{\ker}$ with a subspace of ℓ^2 generated by the infinite sequences, $\{\Psi_0(x), \Psi_1(x), \Psi_2(x), \ldots, \Psi_n(x), \ldots\}$, $x \in X$. An associated family of coherent states is then simply given by the vectors, $\{\overline{\Psi_0(x)}, \overline{\Psi_1(x)}, \overline{\Psi_2(x)}, \ldots, \overline{\Psi_n(x)}, \ldots\}$, $x \in X$, in this subspace. To see that this way of looking at coherent states does indeed include all the standard types of coherent states, let us assume that we are given a family of coherent states, $|\lambda\rangle$, $\lambda \in \Lambda$, on some Hilbert space $\mathfrak{R}$. The parameter space Λ is assumed to be a topological space. Being coherent states means that the vectors either satisfy a resolution of the identity,

$$\int_{\Lambda} |\lambda\rangle\langle\lambda| \mathrm{d}w(\lambda) = I_{\mathfrak{R}},$$

with respect to some measure dw defined on Λ, or else that the mapping $\phi \to f$, with $f(\lambda) = \langle\lambda|\phi\rangle$, where ϕ runs through $\mathfrak{R}$, is an isometry between $\mathfrak{R}$ and a reproducing kernel Hilbert space $\mathfrak{R}_{\mathrm{ker}}$ of functions on Λ. (In fact the first case implies the second.) In either case, if we choose an orthonormal basis $\{\phi_n\}_{n=0}^{\infty}$ in $\mathfrak{R}$ and expand the coherent states in this basis,

$$|\lambda\rangle = \sum_{n=0}^{\infty} \overline{f_n(\lambda)}|\phi_n\rangle, \quad f_n(\lambda) = \langle\lambda|\phi_n\rangle,$$

then the functions f_n are easily seen to form a basis for the Hilbert space $\mathfrak{R}_{\mathrm{ker}}$ with reproducing kernel $K(\lambda,\lambda') = \langle\lambda|\lambda'\rangle$.

The above considerations can also be generalized to the case where $\mathfrak{H}_{\mathrm{ker}}$ is a space of vector valued functions and the kernel $K(x,y)$ is matrix valued, yielding vector coherent states (see Refs. 4 and 20).

B. The Gazeau–Klauder situation

In the light of the preceding discussion, in order to develop a systematic method for generating coherent states and vector coherent states of the Gazeau–Klauder type, we begin by defining a Hilbert space, $\mathfrak{H}_{\mathrm{ns}}$, of functions $f: \mathbb{R} \to \mathbb{C}$, which is complete with respect to the scalar product

$$\langle f|g\rangle_{\mathrm{ns}} = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \overline{f(\gamma)} g(\gamma) \mathrm{d}\gamma. \tag{2.10}$$

The vectors f_x, $x \in \mathbb{R}$,

$$f_x(\gamma) = e^{ix\gamma}, \tag{2.11}$$

are of unit norm and for any two distinct numbers x, x', the corresponding vectors f_x and $f_{x'}$ are orthogonal. This also means that the space $\mathfrak{H}_{\mathrm{ns}}$ is nonseparable. Although this space is not an L^2 space, by abuse of notation we shall still symbolically write the scalar product as

$$\langle f|g\rangle_{\mathrm{ns}} = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \overline{f(\gamma)} g(\gamma) \mathrm{d}\gamma := \int_{\mathbb{R}} \overline{f(\gamma)} g(\gamma) \mathrm{d}\mu_{\mathcal{B}}(\gamma), \tag{2.12}$$

(d$\mu_{\mathcal{B}}$ is usually referred to as the *Bohr measure*). If $\{\epsilon_n\}_{n=0}^{\infty}$ is a sequence of numbers in $\mathbb{R}$ (we assume that $\epsilon_n \neq \epsilon_m$ if $n \neq m$), then the set of vectors

$$f_n(\gamma) = e^{i\epsilon_n\gamma}, \quad n = 0,1,2,\ldots, \tag{2.13}$$

forms a countable orthonormal set and hence the closure of their linear span is a separable subspace of $\mathfrak{H}_{\mathrm{ns}}$. We denote this subspace by $\mathfrak{H}_{\mathrm{ang}}$ and it is such subspaces of $\mathfrak{H}_{\mathrm{ns}}$ that we shall use for constructing coherent states. The reason for the subscript will become clear presently. Suppose next, that the sequence $\{\epsilon_n\}_{n=0}^{\infty}$ is so chosen that the following conditions are satisfied:

(1) $\epsilon_0=0$ and the series

$$\sum_{n=0}^{\infty}\frac{J^n}{\epsilon_n!},\quad J\in\mathbb{R}^+,\quad \epsilon_n!=\epsilon_1\epsilon_2\epsilon_3\cdots\epsilon_n,\quad \epsilon_0!=1,$$

has a radius of convergence $L>0$.

(2) There exists a measure $\mathrm{d}\nu$ on $\mathbb{R}^+$ which solves the moment problem

$$\int_0^L J^n\,\mathrm{d}\nu(J)=\epsilon_n!,\quad \int_0^L \mathrm{d}\nu(J)=1.$$

Then the vectors r_n, $n=0,1,2,\ldots$, in $L^2((0,L),\mathrm{d}\nu)$ defined by

$$r_n(J)=\frac{J^{n/2}}{\sqrt{\epsilon_n!}},\tag{2.14}$$

are of unit norm and span the space. Thus the vectors

$$\Psi_n=r_n\otimes f_n,\quad \Psi_n(J,\gamma)=\frac{J^{n/2}e^{i\epsilon_n\gamma}}{\sqrt{\epsilon_n!}},\quad n=0,1,2,3,\ldots,\tag{2.15}$$

form an *orthonormal basis* in the Hilbert space $\mathfrak{H}_{\text{ac-ang}}=L^2((0,L),\mathrm{d}\nu)\otimes\mathfrak{H}_{\text{ang}}$. Since the vectors Ψ_n satisfy the condition [analogous to (2.5)],

$$\sum_{n=0}^{\infty}|\Psi_n(J,\gamma)|^2=\sum_{n=0}^{\infty}\frac{J^n}{\epsilon_n!}:=\mathcal{N}(J)<\infty,\tag{2.16}$$

for all $(J,\gamma)\in(0,L)\times\mathbb{R}^+$, the space $\mathfrak{H}_{\text{ac-ang}}$ is a reproducing kernel Hilbert space with kernel

$$K(J,\gamma;J',\gamma')=\sum_{n=0}^{\infty}\Psi_n(J,\gamma)\overline{\Psi_n(J',\gamma')}=\sum_{n=0}^{\infty}\frac{(JJ')^{n/2}e^{i\epsilon_n(\gamma-\gamma')}}{\epsilon_n!}.\tag{2.17}$$

By (2.3), the (non-normalized) coherent states, $\xi_{J,\gamma}$, defined on $\mathfrak{H}_{\text{ac-ang}}$ and associated to this kernel are then

$$\xi_{J,\gamma}(J'\gamma')=K(J',\gamma';J,\gamma)=\langle\xi_{J',\gamma'}|\xi_{J,\gamma}\rangle_{\text{ac-ang}},\tag{2.18}$$

while for any $\Psi\in\mathfrak{H}_{\text{ac-ang}}$, we have the relation,

$$\langle\xi_{J,\gamma}|\Psi\rangle_{\text{ac-ang}}=\Psi(J,\gamma).$$

Adopting the notation of (2.12), we may also symbolically write a resolution of the identity as

$$\int_0^L\left[\int_{-\infty}^{\infty}|\xi_{J,\gamma}\rangle\langle\xi_{J,\gamma}|\mathrm{d}\mu_{\mathcal{B}}(\gamma)\right]\mathrm{d}\nu(J)=I_{\text{ac-ang}},\tag{2.19}$$

where $I_{\text{ac-ang}}$ denotes the identity in $\mathfrak{H}_{\text{ac-ang}}$. The above equation is to be understood in the sense that for arbitrary Φ, $\Psi\in\mathfrak{H}_{\text{ac-ang}}$,

$$\int_0^L\left[\int_{-\infty}^{\infty}\langle\Psi|\xi_{J,\gamma}\rangle\langle\xi_{J,\gamma}|\Phi\rangle\mathrm{d}\mu_{\mathcal{B}}(\gamma)\right]\mathrm{d}\nu(J)=\int_0^L\left[\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}\overline{\Psi(J,\gamma)}\Phi(J,\gamma)\mathrm{d}\gamma\right]\mathrm{d}\nu(J)=\langle\Psi|\Phi\rangle.$$

In the Gazeau–Klauder construction of coherent states, related to Hamiltonians with discrete spectra, one assumes that the Hamiltonian is given on some abstract Hilbert space $\mathfrak{H}$ in the orthonormal basis $\{\phi_n\}_{n=0}^{\infty}$ by

$$H = \omega \sum_{n=0}^{\infty} \epsilon_n |\phi_n\rangle\langle\phi_n|, \quad \epsilon_0 = 0, \tag{2.20}$$

where ω is a constant with the dimensions of energy (we take $\hbar = 1$). The variable J is then generally identified with the classical action and γ with the conjugate angle. It is this identification that prompted our choice of the subscripts for the Hilbert spaces $\mathfrak{H}_{\text{ang}}$ and $\mathfrak{H}_{\text{ac-ang}}$.

Following (2.8) we can now construct the *non-normalized* Gazeau–Klauder-type coherent states in $\mathfrak{H}$ using the vectors (2.15),

$$|\eta_{J,\gamma}\rangle = \sum_{n=0}^{\infty} \overline{\Psi_n(J,\gamma)} |\phi_n\rangle = \sum_{n=0}^{\infty} \frac{J^{n/2} e^{-i\epsilon_n \gamma}}{\sqrt{\epsilon_n!}} |\phi_n\rangle. \tag{2.21}$$

Once again, the map

$$W: \mathfrak{H} \to \mathfrak{H}_{\text{ac-ang}}, \quad (W\phi)(J,\gamma) = \langle \eta_{J,\gamma}|\phi\rangle_{\mathfrak{H}},$$

is unitary. If instead, we use the normalized vectors,

$$|J,\gamma\rangle = \mathcal{N}(J)^{-1/2} |\eta_{J,\gamma}\rangle, \tag{2.22}$$

with $\mathcal{N}$ as in (2.16), the resolution of the identity becomes

$$\int_0^L \left[\int_{\mathbb{R}} |J,\gamma\rangle\langle J,\gamma| \mathcal{N}(J) \mathrm{d}\mu_{\mathcal{B}}(\gamma) \right] \mathrm{d}\nu(J) = I_{\mathfrak{H}}. \tag{2.23}$$

We also have the formal reconstruction formula,

$$|\phi\rangle = \int_0^L \left[\int_{\mathbb{R}} \Phi(J,\gamma) |J,\gamma\rangle \mathcal{N}(J) \mathrm{d}\mu_{\mathcal{B}}(\gamma) \right] \mathrm{d}\nu(J), \quad \Phi(J,\gamma) = \langle J,\gamma|\phi\rangle_{\mathfrak{H}}, \tag{2.24}$$

which easily follows from (2.23).

The Gazeau–Klauder coherent states are characterized by the *temporal stability* property,

$$e^{-iHt}|J,\gamma\rangle = |J,\gamma+\omega t\rangle, \tag{2.25}$$

and the *action identity*,

$$\langle J,\gamma|H|J,\gamma\rangle_{\mathfrak{H}} = \omega J. \tag{2.26}$$

If for a given Hamiltonian, $\epsilon_0 \neq 0$, then as discussed in Sec. II, we work with the shifted Hamiltonian $H' = H - \omega\epsilon_0 I_{\mathfrak{H}}$, and use $\varepsilon_n = \epsilon_n - \epsilon_0$ to construct coherent states. In this case,

$$\begin{aligned} e^{-iHt}|J,\gamma\rangle &= e^{-iH't} e^{-i\omega\epsilon_0 t}|J,\gamma\rangle = e^{-i\omega\epsilon_0 t}|J,\gamma+\omega t\rangle, \\ \langle J,\gamma|H|J,\gamma\rangle_{\mathfrak{H}} &= \langle J,\gamma|H' + \omega\epsilon_0|J,\gamma\rangle_{\mathfrak{H}} = \omega J + \omega\epsilon_0. \end{aligned} \tag{2.27}$$

One final comment about coherent states of the type (2.21), there are two probability densities naturally associated with them. The first is the one associated with the measure $\mathrm{d}\nu$ (over the interval $[0,J]$). The second is the discrete density associated with the "event" $\{\phi_n\}$, given by

$$|\langle \phi_n|J,\gamma\rangle|^2 = \frac{J^n}{\epsilon_n! \mathcal{N}(J)}.$$

The physical meaning of these and their inter-relation are discussed in detail in Ref. 11.

III. VECTOR COHERENT STATES OF THE GAZEAU–KLAUDER TYPE

Suppose now that the Hamiltonian H (acting on the Hilbert space $\mathfrak{H}$) has a discrete positive spectrum and that the eigenvectors ϕ_{jk}, $j=1,2,3,\ldots,N<\infty$, $k=0,1,2,3,\ldots,\infty$, can be grouped into N families, each containing an infinite number of vectors. (Such a situation could arise, for example, through the lifting of an N-fold degeneracy in the energy spectrum, by an interaction. Therefore k labels the *main* energy levels while j labels the *sublevels* generated by, e.g., a small perturbation.) Furthermore, assume that the corresponding eigenvalues $E_{jk}=\omega\epsilon_{jk}$ satisfy $\epsilon_{j0}=0$, $j=1,2,3,\ldots,N$, and $\epsilon_{jk}\neq\epsilon_{j'\ell}$ if $k\neq\ell$ and $\forall j,j'$. Denote by $\mathfrak{H}_j$ the subspace of $\mathfrak{H}$ spanned by the vectors ϕ_{jk}, $k=0,1,2,\ldots,\infty$, and by $\mathbb{P}_j$ the projection operator onto this subspace. Then $H=\oplus_{j=1}^{N}H_j$, with $H_j=\omega\Sigma_{k=0}^{\infty}\epsilon_{jk}|\phi_{jk}\rangle\langle\phi_{jk}|$, which leaves $\mathfrak{H}_j$ stable. We will give an example of such a decomposition in the first application below. In $\mathfrak{H}_j$ we define the coherent states,

$$|J_j,\gamma_j\rangle=\mathcal{N}(J_j)^{-1/2}\sum_{k=0}^{\infty}\frac{J_j^{k/2}e^{-i\epsilon_{jk}\gamma_j}}{\sqrt{\epsilon_{j1}\epsilon_{j2}\ldots\epsilon_{jk}}}|\phi_{jk}\rangle. \tag{3.1}$$

Here $-\infty<\gamma_j<\infty$ and $0\leqslant J_j<L_j=\lim_{k\to\infty}\epsilon_{jk}$, and we assume that $L_j>0$. The normalization factor $\mathcal{N}(J_j)$ is chosen so that

$$\langle J_j,\gamma_j|J_k,\gamma_k\rangle=\delta_{jk}. \tag{3.2}$$

These states also satisfy

$$e^{-iH_jt}|J_j,\gamma_j\rangle=|J_j,\gamma_j+\omega t\rangle,\quad \langle J_j,\gamma_j|H_k|J_k,\gamma_k\rangle=\omega J_j\delta_{jk}, \tag{3.3}$$

and the "partial resolution of the identity"

$$\int_0^{L_j}\left[\int_{\mathbb{R}}|J_j,\gamma_j\rangle\langle J_j,\gamma_j|\mathcal{N}(J_j)\mathrm{d}\mu_{\mathcal{B}}(\gamma_j)\right]\mathrm{d}\nu_j(J_j)=\mathbb{P}_j, \tag{3.4}$$

where $\mathrm{d}\mu_{\mathcal{B}}$ is as in (2.12) and the measure $\mathrm{d}\nu_j(J_j)$ is defined through the moment problem

$$\int_0^{L_j}J^n\,\mathrm{d}\nu_j(J)=\epsilon_{j1}\epsilon_{j2}\cdots\epsilon_{jn},\quad \int_0^{L_j}\mathrm{d}\nu_j(J)=1. \tag{3.5}$$

Next, introducing the diagonal matrices,

$$\begin{gathered}\mathbf{J}=\mathrm{diag}(J_1,J_2,\ldots,J_N),\quad \boldsymbol{\epsilon}_k=\mathrm{diag}(\epsilon_{1k},\epsilon_{2k},\ldots,\epsilon_{Nk}),\\ \boldsymbol{\gamma}=\mathrm{diag}(\gamma_1,\gamma_2,\ldots,\gamma_N),\quad \boldsymbol{\epsilon}_k!=\boldsymbol{\epsilon}_1,\boldsymbol{\epsilon}_2\cdots\boldsymbol{\epsilon}_k,\end{gathered} \tag{3.6}$$

and the vectors

$$|\boldsymbol{\Phi}_k;j\rangle=\begin{pmatrix}0\\ \vdots\\ |\phi_{jk}\rangle\\ \vdots\\ 0\end{pmatrix},\quad j=1,2,\ldots,N,\quad k=0,1,2,\ldots, \tag{3.7}$$

we may rewrite the vectors (3.1) as

$$|\mathbf{J},\boldsymbol{\gamma};j\rangle := \mathcal{N}(J_j)^{-1/2}\sum_{n=0}^{\infty}[\boldsymbol{\varepsilon}_k!]^{-1/2}\mathbf{J}^{k/2}\exp[-i\boldsymbol{\varepsilon}_k\gamma]|\boldsymbol{\Phi}_k;j\rangle = \begin{pmatrix} 0 \\ \vdots \\ |J_j,\gamma_j\rangle \\ \vdots \\ 0 \end{pmatrix}. \tag{3.8}$$

We call these states *vector coherent states* for the Hamiltonian H. Note that, in this representation, H is a diagonal operator, $H=\mathrm{diag}\,(H_1,H_2,\ldots,H_N)$, each H_j being an infinite diagonal matrix with eigenvalues $\omega\boldsymbol{\epsilon}_{jk}$, $k=0,1,2,\ldots$.

$$e^{-iHt}|\mathbf{J},\boldsymbol{\gamma};j\rangle = |\mathbf{J},\boldsymbol{\gamma}+\omega t\mathbf{d}_j;j\rangle, \quad \langle\mathbf{J},\boldsymbol{\gamma};j|H|\mathbf{J},\boldsymbol{\gamma};j\rangle = \omega J_j, \tag{3.9}$$

where $\mathbf{d}_j$ is the diagonal matrix with one in the jj position and zeroes elsewhere. Furthermore, we have the resolution of the identity on $\mathfrak{H}$,

$$\sum_{j=0}^{N}\int_0^{L_N}\cdots\int_0^{L_1}\left[\int_{\mathbb{R}^N}|\mathbf{J},\boldsymbol{\gamma};j\rangle\langle\mathbf{J},\boldsymbol{\gamma};j|\mathcal{N}(J_j)\mathrm{d}\mu_{\mathcal{B}}(\gamma)\right]\mathrm{d}\nu(\mathbf{J}) = I_{\mathfrak{H}}, \tag{3.10}$$

with

$$\mathrm{d}\nu(\mathbf{J}) = \mathrm{d}\nu(J_1)\mathrm{d}\nu(J_2)\cdots\mathrm{d}\nu(J_N), \quad \mathrm{d}\mu_{\mathcal{B}}(\boldsymbol{\gamma}) = \mathrm{d}\mu_{\mathcal{B}}(\gamma_1)\mathrm{d}\mu_{\mathcal{B}}(\gamma_2)\cdots\mathrm{d}\mu_{\mathcal{B}}(\gamma_N).$$

In view of the fact that [see also (3.2)]

$$\langle\mathbf{J},\boldsymbol{\gamma};j|\mathbf{J},\boldsymbol{\gamma};\ell\rangle = \delta_{j\ell}, \tag{3.11}$$

a general vector coherent state for such a system may be written as a linear combination,

$$|\mathbf{J},\boldsymbol{\gamma}\rangle = \sum_{j=0}^{N} c_j|\mathbf{J},\boldsymbol{\gamma};j\rangle.$$

However, such a state would, in general, not be of the Gazeau–Klauder type, unless the levels $\boldsymbol{\epsilon}_{jk}$, $j=1,2,\ldots,N$, are degenerate for all k. Associated to the vector coherent states (3.8) is the *matrix-valued* reproducing kernel, $\mathbf{K}(\mathbf{J},\boldsymbol{\gamma},\mathbf{J}',\boldsymbol{\gamma}')$, with matrix elements

$$\mathbf{K}(\mathbf{J},\boldsymbol{\gamma};\mathbf{J}',\boldsymbol{\gamma}')_{j\ell} = \langle\mathbf{J},\boldsymbol{\gamma};\mathbf{j}|\mathbf{J}',\boldsymbol{\gamma};\ell\rangle. \tag{3.12}$$

This kernel has the properties,

$$\mathbf{K}(\mathbf{J},\boldsymbol{\gamma};\mathbf{J},\boldsymbol{\gamma})_{jj} = \||\mathbf{J},\boldsymbol{\gamma};j\rangle\|^2 > 0, \quad \mathbf{K}(\mathbf{J},\boldsymbol{\gamma};\mathbf{J}',\boldsymbol{\gamma}')_{j\ell} = \overline{\mathbf{K}(\mathbf{J}',\boldsymbol{\gamma}';\mathbf{J},\boldsymbol{\gamma})_{\ell j}},$$

$$\sum_{j'=0}^{N}\int_0^{L_N}\cdots\int_0^{L_1}\left[\int_{\mathbb{R}^N}\mathbf{K}(\mathbf{J},\boldsymbol{\gamma};\mathbf{J}'',\boldsymbol{\gamma}'')_{jj'}\mathbf{K}(\mathbf{J}'',\boldsymbol{\gamma}'';\mathbf{J}',\boldsymbol{\gamma}')_{j'\ell}\mathcal{N}(J_\ell)\mathrm{d}\mu_{\mathcal{B}}(\boldsymbol{\gamma}'')\right]\mathrm{d}\nu(\mathbf{J}'') = \mathbf{K}(\mathbf{J},\boldsymbol{\gamma};\mathbf{J}',\boldsymbol{\gamma}')_{j\ell}. \tag{3.13}$$

Some examples: Let us consider a model described by the Hamiltonian

$$H = \omega a^\dagger a + \boldsymbol{\epsilon}_1 c_1^\dagger c_1 + \boldsymbol{\epsilon}_2 c_2^\dagger c_2 + (g_1 c_1^\dagger c_1 + g_2 c_2^\dagger c_2)(a + a^\dagger), \tag{3.14}$$

where the following commutation rules hold:

$$[a,a^\dagger] = \{c_1,c_1^\dagger\} = \{c_2,c_2^\dagger\} = I \tag{3.15}$$

and

$$[a^{\sharp}, a_i^{\sharp}] = \{c_1, c_1\} = \{c_2, c_2\} = 0, \tag{3.16}$$

where $a^{\#}$ stands for a or $a^{\dagger}$, $[A,B]=AB-BA$ and $\{A,B\}=AB+BA$. This model, which describes an interaction between a single mode, $(a,a^{\dagger})$, of the radiation field with two Fermi-type modes, has been analyzed quite recently in Ref. 17.

A convenient feature of the above Hamiltonian is that its spectrum can be obtained explicitly, as well as its eigenvectors. In fact, considering the *fermionic* part, it is clear that all the eigenstates of H must be of the following form:

$$\Phi = \varphi \otimes \Psi_{kl}, \quad \text{where } \Psi_{kl} = (c_1^{\dagger})^k (c_2^{\dagger})^l \Psi_{00}, \tag{3.17}$$

with $k,l=0,1$, and where $\Psi_{0,0}$ is the fermionic vacuum, $c_j\Psi_{00}=0$, for $j=1,2$. The vector φ must still be determined, but it is clear that it cannot, in general, be proportional to $(a^{\dagger})^n\cdot\varphi_0$, where $a\varphi_0=0$, since the interaction part of H is not diagonal on these vectors. However it is a rather simple exercise to check that

$$H(\varphi \otimes \Psi_{00}) = \omega a^{\dagger} a (\varphi \otimes \Psi_{00}),$$

$$\begin{aligned} H(\varphi \otimes \Psi_{10}) &= (\omega a^{\dagger} a + \epsilon_1 + g_1(a + a^{\dagger}))(\varphi \otimes \Psi_{10}), \\ H(\varphi \otimes \Psi_{01}) &= (\omega a^{\dagger} a + \epsilon_2 + g_2(a + a^{\dagger}))(\varphi \otimes \Psi_{01}), \end{aligned} \tag{3.18}$$

$$H(\varphi \otimes \Psi_{11}) = (\omega a^{\dagger} a + \epsilon_1 + \epsilon_2 + (g_1 + g_2)(a + a^{\dagger}))(\varphi \otimes \Psi_{11}).$$

To proceed further, we observe that in each of the four cases above, φ is an eigenvector of a self-adjoint operator of the type,

$$B_{kl} = \omega A_{kl}^{\dagger} A_{kl} + \left(\varepsilon_{kl} - \frac{g_{kl}^2}{\omega}\right) I, \quad A_{kl} = a + \frac{g_{kl}}{\omega}, \quad [A_{kl}, A_{kl}^{\dagger}] = 1, \quad k,l = 0,1, \tag{3.19}$$

where,

$$\varepsilon_{kl} = l\varepsilon_1 + k\varepsilon_2, \quad g_{kl} = lg_1 + kg_2, \quad l,k = 0,1.$$

We know, however, that

$$A_{kl} = \exp\left[i\sqrt{2}\frac{g_{kl}}{\omega} P \right] a \exp\left[-i\sqrt{2}\frac{g_{kl}}{\omega} P \right], \quad \text{where } P = \frac{a - a^{\dagger}}{i\sqrt{2}}.$$

Thus, the eigenvectors of B_{kl} are,

$$|\Phi_n^{kl}\rangle = \exp\left[i\sqrt{2}\frac{g_{kl}}{\omega} P \right] |n\rangle = \frac{(A_{kl}^{\dagger})^n}{\sqrt{n!}} |\Phi_0^{kl}\rangle, \tag{3.20}$$

where $|n\rangle = a^n/\sqrt{n!}|0\rangle$ are the eigenvectors of the usual number operator $N=a^{\dagger}a$.

The diagonalization of H is now complete. Our results can be summarized as follows:
eigenstates of H, $\{\varphi_n^{kl} := \Phi_n^{kl} \otimes \Psi_{kl}$, where $n=0,1,2,\ldots$, and $k,l=0,1\}$,
eigenvalues of H, $\{E_n^{kl}$, with $n=0,1,2,\ldots$, and $k,l=0,1\}$,

where the relevant quantities are shown in the following table.

k, l	$E_n^{kl}=$	$\Psi_{kl}=$	$\Phi_n^{kl}=$	where	and
0, 0	ωn	Ψ_{00}	$\frac{(a^\dagger)^n}{\sqrt{n!}}\Phi_0^{00}$	$a\Phi_0^{00}=0$	
1, 0	$\omega n+\epsilon_1-\frac{g_1^2}{\omega}$	$c_1^\dagger\Psi_{00}$	$\frac{(A_{10}^\dagger)^n}{\sqrt{n!}}\Phi_0^{10}$	$A_{10}\Phi_0^{10}=0$	$A_{10}=a+\frac{g_1}{\omega}$
0, 1	$\omega n+\epsilon_2-\frac{g_2^2}{\omega}$	$c_2^\dagger\Psi_{00}$	$\frac{(A_{01}^\dagger)^n}{\sqrt{n!}}\Phi_0^{01}$	$A_{01}\Phi_0^{01}=0$	$A_{01}=a+\frac{g_2}{\omega}$
1, 1	$\omega n+\epsilon_1+\epsilon_2-\frac{(g_1+g_2)^2}{\omega}$	$c_1^\dagger c_2^\dagger\Psi_{00}$	$\frac{(A_{11}^\dagger)^n}{\sqrt{n!}}\Phi_0^{11}$	$A_{11}\Phi_0^{11}=0$	$A_{11}=a+\frac{g_1+g_2}{\omega}$

From (3.20) it is also clear that the vectors Φ_0^{kl} are just the well-known canonical coherent states $|z\rangle$, with $z=-g_{kl}/\omega$. Thus, in the position space representation these vectors are shifted Gaussians,

$$\Phi_0^{kl}(x)\simeq e^{-1/2(x+\sqrt{2}g_{kl})^2},\quad k=0,1.$$

In order to build Gazeau–Klauder type of coherent states for this Hamiltonian, we see now that it breaks up into four orthogonal parts,

$$H=\oplus_{k,l=0,1}H_{kl},\quad \text{where } H_{kl}=\sum_{n=0}^{\infty}E_n^{kl}|\varphi_n^{kl}\rangle\langle\varphi_n^{kl}|. \tag{3.21}$$

Since the lowest eigenvalue E_0^{kl}, for the component Hamiltonian H_{kl}, is zero only for $k=l=0$, we work with $H'=\oplus_{k,l=0,1}H'_{kl}$, where $H'_{kl}=\Sigma_{n=0}^{\infty}(E_n^{kl}-E_0^{kl})|\varphi_n^{kl}\rangle\langle\varphi_n^{kl}|$. But $E_n^{kl}-E_0^{kl}=\omega n$. (Note that H and H' commute.) Thus, the vector coherent states of the present model are 4-component vectors, involving the standard canonical coherent states, $|z_{kl}\rangle$, $k,l=0,1$, $z_{kl}\in\mathbb{C}$, built on the bosonic vacuum state Φ_0^{kl}. Thus, introducing the diagonal matrix $\mathfrak{Z}=\mathrm{diag}(z_{00},z_{10},z_{01},z_{11})$, we can write the vectors (3.8) for the present case as

$$|\mathfrak{Z};kl\rangle=|z_{kl}\rangle|\Psi_{kl}\rangle=e^{-|z_{kl}|^2/2}\sum_{n=0}^{\infty}\frac{\mathfrak{Z}^n}{\sqrt{n!}}|\Psi_{kl}\rangle|\Phi_n^{kl}\rangle,\quad j,k=1,2, \tag{3.22}$$

where in the present representation, the vectors Ψ_{kl} form the canonical basis of $\mathbb{C}^4$,

$$\Psi_{00}=\begin{pmatrix}1\\0\\0\\0\end{pmatrix},\quad \Psi_{10}=\begin{pmatrix}0\\1\\0\\0\end{pmatrix},\quad \Psi_{01}=\begin{pmatrix}0\\0\\1\\0\end{pmatrix},\quad \Psi_{11}=\begin{pmatrix}0\\0\\0\\1\end{pmatrix}.$$

These then are the Gazeau–Klauder-type vector coherent states for the Hamiltonian (3.14). Equations (3.9) and (3.10) have obvious transcriptions for these states.

One could also consider the following variant of the Hamiltonian (3.14):

$$H = \omega a^\dagger a + \epsilon_1 c_1^\dagger c_1 + \epsilon_2 c_2^\dagger c_2 + \sum_{i,j=1}^{2} g_{ij} c_i^\dagger c_j (a + a^\dagger), \tag{3.23}$$

where the same commutation rules (3.15) and (3.16) are assumed and

$$g = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}$$

is a 2×2 Hermitian matrix, $g=\overline{g}^T$. Let V be the unitary matrix which diagonalizes g,

$$VgV^{-1} = g_d := \begin{pmatrix} g_1 & 0 \\ 0 & g_2 \end{pmatrix},$$

so that, defining

$$d = \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = Vc = V\begin{pmatrix} c_1 \\ c_2 \end{pmatrix},$$

and $d^\dagger = c^\dagger V^\dagger = (d_1^\dagger, d_2^\dagger)$, the operators d_j again obey the same anticommutation relations as the c_j. Also, $\Sigma_{i,j=1}^2 g_{ij} c_i^\dagger c_j = g_1 d_1^\dagger d_1 + g_2 d_2^\dagger d_2$. However, if $\epsilon_1 \neq \epsilon_2$, this change of variables would make the free fermionic Hamiltonian $\epsilon_1 c_1^\dagger c_1 + \epsilon_2 c_2^\dagger c_2$ no longer diagonal, while if $\epsilon_1 = \epsilon_2 = \epsilon$ we get

$$H = \omega a^\dagger a + \epsilon d_1^\dagger d_1 + \epsilon d_2^\dagger d_2 + (g_1 d_1^\dagger d_1 + g_2 d_2^\dagger d_2)(a + a^\dagger),$$

for which the entire analysis performed above can be repeated.

Remark: A possible method for describing a nondegenerate two-level atom (i.e., $\epsilon_1 \neq \epsilon_2$), which is the one considered in Ref. 17, can be obtained by adapting the previous procedure as follows: we consider a fictitious three-level atom interacting with the radiation field in the following way:

$$H = \omega a^\dagger a + \epsilon (c_1^\dagger c_1 + c_2^\dagger c_2 + c_3^\dagger c_3) + \sum_{i,j=1}^{3} g_{ij} c_i^\dagger c_j (a + a^\dagger),$$

where now $\{g_{ij}\}$ is a 3×3 Hermitian matrix. We recover a two-level system by considering a subspace of the complete Hilbert space spanned by the vectors $\Psi_{kl} \otimes \Phi_n^{kl}$, where the Φ_n^{kl} are constructed by trivially extending the foregoing procedure. Next we take $\Psi_0^{00} = \Psi_0$ to be the ground state of c_j, $j=1,2,3$ and set $\Psi_{10} = c_1^\dagger \Psi_0$, $\Psi_{01} = c_2^\dagger c_3^\dagger \Psi_0$, and $\Psi_{11} = c_1^\dagger c_2^\dagger c_3^\dagger \Psi_0$. (The interpretation is clear, Ψ_0 corresponds to both levels of our atom being empty, while Ψ_{10}, Ψ_{01}, and Ψ_{11} correspond, respectively, to the first, second, and both levels being occupied.)

If it is now possible to ensure that the resulting energy spectrum E_n^{kl}, $n=0,1,2,\ldots$, $k,l=0,1$, has no degeneracies, we could build Grazeau–Klauder-type coherent states for this system. On the other hand, it is easily verified that degeneracy will be avoided if the physical constants of the model satisfy the following inequalities:

$$0 < \epsilon_1 - \frac{g_1^2}{\omega} < \epsilon_2 - \frac{g_2^2}{\omega} < \epsilon_1 + \epsilon_2 - \frac{(g_1^2 + g_2^2)}{\omega} < \omega.$$

In this case we set $E_0 = E_0^{00} = 0$, $E_1 = E_0^{10} = \epsilon_1 - g_1^2/\omega$, $E_2 = E_0^{01} = \epsilon_2 - g_2^2/\omega$, $E_3 = E_0^{11} = \epsilon_1 + \epsilon_2 - [(g_1^2 + g_2^2)/\omega]$, $E_4 = E_1^{00} = \omega$, and so on and write, for the corresponding eigenstates $\varphi_0 = \varphi_0^{00}$, $\varphi_1 = \varphi_0^{10}$, $\varphi_2 = \varphi_0^{01}$, $\varphi_3 = \varphi_0^{11}$, $\varphi_4 = \varphi_1^{00}$, and so on. Finally, defining $\epsilon_n = E_n/\omega$, we recover a sequence of quantities satisfying the inequalities $0 = \epsilon_0 < \epsilon_1 < \epsilon_2 < \cdots$, as required in Ref. 10. Thus we obtain the coherent states $|J, \gamma\rangle = N(J)^{-1/2} \Sigma_{n=0}^{\infty} [(J^{n/2} e^{-i\gamma\epsilon_n})/\sqrt{\epsilon_n!}] \varphi_n$, with all the required properties.

IV. HAMILTONIANS WITH DEGENERACIES

Here we extend the preceding construction to the situation in which some (or perhaps all) of the eigenvalues of the given Hamiltonian have degeneracies. We will consider two situations, first, where all the degeneracies are finite and second, where they are all countably infinite. In the first case, we will show that a natural way to recover all the required properties of the Gazeau–Klauder-type coherent states, such as the resolution of the identity, temporal stability, and the action identity, among others, is to introduce a third parameter into the definition of the coherent states, replacing $|J,\gamma\rangle$ by $|J,\gamma,\theta\rangle$. The extension we are proposing is somewhat different from that suggested in Refs. 8 and 15, since it only involves one extra parameter. Moreover, as we will demonstrate, our method can also be adapted to the case of infinite degeneracies.

A. Finite degeneracies

Let us now consider a Hamiltonian H, the eigenvalues of which are all discrete with the lowest eigenvalue being again zero. Assume that the nth level, $E_n=\omega\epsilon_n$, has a degeneracy $d(n)$, in general different from 1. We assume $d(n)<\infty$, for all n. Denote by $|n,j\rangle$, $n=0,1,2,\ldots$, $j=1,2,\ldots,d(n)$, the eigenvectors of the Hamiltonian H so that $H|n,j\rangle=E_n|n,j\rangle$, with n labeling the level and j counting the degeneracy. As usual we introduce the dimensionless quantity ϵ_n and again, without loss of generality, arrange them in the sequence $0=\epsilon_0<\epsilon_1<\epsilon_2<\cdots$. This means that the Hamiltonian is $H=\omega\Sigma_{n=0}^{\infty}\Sigma_{j=1}^{d(n)}\epsilon_n|n,j\rangle\langle n,j|$. We next introduce the parameter $\theta\in[0,2\pi)$ and define

$$|J,\gamma,\theta\rangle := \mathcal{N}(J)^{-1/2}\sum_{n=0}^{\infty}\sum_{j=1}^{d(n)}\frac{J^{n/2}e^{-i\epsilon_n\gamma}e^{-ij\theta}}{\sqrt{\rho_n}}|n,j\rangle, \tag{4.1}$$

with J and γ as before. We now prove that, for appropriate choice of ρ_n, these states satisfy the following properties, which naturally generalize the analogous ones stated at the beginning of Sec. II:

(i) *Continuity*, if $(J,\gamma,\theta)\to(J',\gamma',\theta')$ then $|J,\gamma,\mu\rangle\to|J',\gamma',\mu'\rangle$.
(ii) *Resolution of the identity*, $\int|J,\gamma,\theta\rangle\langle J,\gamma,\theta|\mathrm{d}m(J,\gamma,\theta)=I$, for some appropriately chosen measure dm.
(iii) *Temporal stability*, $e^{-iHt}|J,\gamma,\theta\rangle=|J,\gamma+\omega t,\theta\rangle$, for some constant ω.
(iv) *Action identity*, $\langle J,\gamma,\theta|H|J,\gamma,\theta\rangle=\omega J$.

Indeed, continuity follows automatically from the definition itself. As for normalization, we observe that

$$\langle J,\gamma,\theta|J,\gamma,\theta\rangle=\mathcal{N}(J)^{-1}\sum_{n,m=0}^{\infty}\sum_{j=1}^{d(n)}\sum_{l=0}^{d(m)}\frac{J^{n/2+m/2}e^{-i(\epsilon_n-\epsilon_m)\gamma}e^{-i(j-l)\theta}}{\sqrt{\rho_n\rho_m}}\langle m,l|n,j\rangle=\mathcal{N}(J)^{-1}\sum_{n=0}^{\infty}\sum_{j=1}^{d(n)}\frac{J^n}{\rho_n}$$
$$=\mathcal{N}(J)^{-1}\sum_{n=0}^{\infty}\frac{J^n d(n)}{\rho_n},$$

from which we conclude that $\langle J,\gamma,\theta|J,\gamma,\theta\rangle=1$ if and only if

$$\mathcal{N}(J)=\sum_{n=0}^{\infty}\frac{J^n d(n)}{\rho_n}. \tag{4.2}$$

Of course, this is a power series in J and we assume that it has a radius of convergence $L>0$.

The proof of temporal stability is easy,

$$e^{-iHt}|J,\gamma,\theta\rangle = e^{-iHt}\mathcal{N}(J)^{-1/2}\sum_{n=0}^{\infty}\sum_{j=1}^{d(n)}\frac{J^{n/2}e^{-i\epsilon_n\gamma}e^{-ij\theta}}{\sqrt{\rho_n}}|n,j\rangle = \mathcal{N}(J)^{-1/2}\sum_{n=0}^{\infty}\sum_{j=1}^{d(n)}\frac{J^{n/2}e^{-i\epsilon_n\gamma}e^{-ij\theta}}{\sqrt{\rho_n}}e^{-i\omega\epsilon_n t}|n,j\rangle$$
$$= |J,\gamma+\omega t,\theta\rangle.$$

In order for the action identity to be satisfied, we need a condition on the ρ_n. Since $\epsilon_0=0$, we get

$$\langle J,\gamma,\theta|H|J,\gamma,\theta\rangle = \omega J\left[\mathcal{N}(J)^{-1}\sum_{n=1}^{\infty}\frac{\epsilon_n J^{n-1}d(n)}{\rho_n}\right].$$

Thus, in order for the action identity to hold the expression within the square brackets must equal one. This can be achieved if we require that

$$\frac{\epsilon_n d(n)}{\rho_n} = \frac{d(n-1)}{\rho_{n-1}}, \quad n=1,2,3,\ldots,$$

for then

$$\rho_n = \epsilon_n\frac{d(n)}{d(n-1)}\rho_{n-1} = \cdots = \epsilon_n!\frac{d(n)}{d(0)}\rho_0, \quad \text{by iteration.}$$

We choose $\rho_0=d(0)$ so that

$$\rho_n = \epsilon_n! d(n), \quad n=0,1,2,\ldots, \quad \text{and} \quad \mathcal{N}(J)=\sum_{n=0}^{\infty}\frac{J^n}{\epsilon_n!}. \tag{4.3}$$

Thus the coherent states (4.1) become

$$|J,\gamma,\theta\rangle := \mathcal{N}(J)^{-1/2}\sum_{n=0}^{\infty}\sum_{j=1}^{d(n)}\frac{J^{n/2}e^{-i\epsilon_n\gamma}e^{-ij\theta}}{\sqrt{\epsilon_n! d(n)}}|n,j\rangle. \tag{4.4}$$

It remains only to determine the measure dm in order for the resolution of the identity to be satisfied. Proceeding as in Sec. II, and assuming that the measure dν solves the moment problem

$$\int_0^L J^n\,\mathrm{d}\nu(J) = \epsilon_n! d(n), \quad n=0,1,2,\ldots, \tag{4.5}$$

we take

$$\mathrm{d}m(J,\gamma,\theta) = \frac{\mathcal{N}(J)}{2\pi}\mathrm{d}\nu(J)\mathrm{d}\mu_{\mathcal{B}}(\gamma)\mathrm{d}\theta, \tag{4.6}$$

where d$\mu_{\mathcal{B}}$ is the symbolic measure defined in (2.12). Then, we prove exactly as in Sec. II, the identity [see (2.23)]

$$\frac{1}{2\pi}\int_0^L\left\{\int_2^{2\pi}\left[\int_{\mathbb{R}}|J,\gamma,\theta\rangle\langle J,\gamma,\theta|\mathcal{N}(J)\mathrm{d}\mu_{\mathcal{B}}(\gamma)\right]\mathrm{d}\theta\right\}\mathrm{d}\nu(J) = I_{\mathfrak{H}}. \tag{4.7}$$

Remark: If $d(n)=1$ for all n, the above coherent states coincide, apart from an inessential overall phase $e^{-i\theta}$, with the usual Gazeau–Klauder coherent states (2.1). However, when the Hamiltonian H has a nontrivial degeneracy, it is interesting to notice the presence of $d(n)$ in the denominator of the expression for the coherent states in (4.4), which implies that the radius of convergence L depends not only on the eigenvalues of the Hamiltonian but also on their degen-

eracies. Similarly, the measure $d\nu$, solving the moment problem (4.5) and appearing in the resolution of the identity, depends on the degeneracy.

Example 1: Consider the following simple example, consisting of a single boson and a single fermion: $H=\omega(a^\dagger a+c^\dagger c)$, where $[a,a^\dagger]=\{c,c^\dagger\}=I$ and $[a^\#,c^\#]=0$, $x^\#$ being x or $x^\dagger$. Introducing the vacuum Φ_0 of a, and Ψ_0 of c and taking, as usual $\Phi_n=[(a^\dagger)^n/\sqrt{n!}]\Phi_0$, $n=0,1,2,\ldots$, and $\Psi_j=(c^\dagger)^j\Psi_0$, $j=0,1$, we can write the eigenvectors of H as $\varphi_{n,j}=\Phi_0\otimes\Psi_0$ if $n=j=0$, and $\varphi_{n,j}=\Phi_{n-j}\otimes\Psi_j$, if $n=1,2,3,\ldots$, and $j=0,1$. The corresponding eigenvalues are $E_{n,j}=n\omega$, so that they turn out to be degenerate in j. In particular we have $d(0)=1$ and $d(n)=2$ for all $n\geqslant 1$. The normalization can be computed using (4.2), and we get

$$\mathcal{N}(J)=\sum_{n=0}^{\infty}\frac{J^n d(n)}{\rho_n}=1+2\sum_{n=1}^{\infty}\frac{J^n}{\rho_n}=1+\sum_{n=1}^{\infty}\frac{J^n}{n!}=e^J.$$

Definition (4.1) yields therefore,

$$|J,\gamma,\theta\rangle\coloneqq e^{-J/2}\left[e^{-i\theta}|\varphi_{00}\rangle+\sum_{n=1}^{\infty}\sum_{j=1}^{2}\frac{J^{n/2}e^{-in\gamma}e^{-ij\theta}}{\sqrt{2n!}}|\varphi_{nj}\rangle\right]. \tag{4.8}$$

Actually, this time we can restrict the variable γ to the interval $[0,2\pi)$ and use the measure $d\mu_{\mathcal{B}}(\gamma)=(1/2\pi)d\gamma$ in (4.6) instead of the one in (2.12). Furthermore, $0\leqslant J<\infty$ and the measure $d\nu(J)$ must solve the moment problem

$$\int_0^{\infty}J^n\,d\nu(J)=\begin{cases}1, & \text{if } n=0,\\ 2n!, & \text{if } n\geqslant 1.\end{cases}$$

It is then easily seen that $d\nu(J)=[2e^{-J}-\delta(J)]dJ$. Thus, writing

$$dm(J,\gamma,\theta)=\frac{e^J}{4\pi^2}[2e^{-J}-\delta(J)]dJ\,d\gamma\,d\theta,$$

we can prove the resolution of the identity,

$$\int|J,\gamma,\theta\rangle\langle J,\gamma,\theta|dm(J,\gamma,\theta)=I.$$

Finally, introducing the complex variable $z=re^{-i\gamma}=J^{1/2}e^{-i\gamma}$, $z\in\mathbb{C}$, we can rewrite (4.8) as

$$|z,\theta\rangle=e^{-|z|^2/2}\left[e^{-i\theta}|\varphi_{00}\rangle+\sum_{n=1}^{\infty}\sum_{j=1}^{2}\frac{z^n e^{-ij\theta}}{\sqrt{2n!}}|\varphi_{nj}\rangle\right]. \tag{4.9}$$

Example 2: As a second example consider a particle of mass m constrained to move on the xy plane and subject to the force $\vec{F}=(-kx-by,-ky-bx,0)$, derivable from the potential $V(x,y)=\frac{1}{2}k(x^2+y^2)+bxy$. In the rotated coordinates $\xi_\pm=(1/\sqrt{2})(x\pm y)$, this potential assumes the form $V(\xi_+,\xi_-)=\frac{1}{2}m(\omega_+^2\xi_+^2+\omega_-^2\xi_-^2)$, where $\omega_\pm^2=(1/m)(k\pm b)$. The Hamiltonian looks like a two-dimensional harmonic oscillator since, in an obvious notation, we also have $p_x^2+p_y^2=p_+^2+p_-^2$. Introducing finally the creation and annihilation operators for the $\pm$ modes and adding an inessential constant we get $H=\omega_+a_+^\dagger a_++\omega_-a_-^\dagger a_-$. The eigenvalues are therefore $E_{n_+,n_-}=\omega_+n_++\omega_-n_-$ and the corresponding eigenstates are $\varphi_{n_+,n_-}=[(a_+^\dagger)^{n_+}(a_-^\dagger)^{n_-}/\sqrt{n_+!n_-!}]\varphi_{00}$, where $a_-\varphi_{00}=a_+\varphi_{00}=0$. Let us now take, as a concrete example, $b=3k/5$. Then the eigenvalues can be written as $E_{n_+,n_-}=\omega_-(2n_++n_-)$ and the degeneracy can be simply deduced, we notice that the spectrum is ω_-n, $n=2n_++n_-=0,1,2,\ldots$, and $d(2n)=d(2n+1)=n+1$. Therefore, since $\rho_{2n}=(2n)!(n+1)$ and $\rho_{2n+1}=(2n+1)!(n+1)$, we may write

$$|J,\gamma,\theta\rangle = e^{-J/2}\sum_{l=0}^{\infty}\sum_{j=1}^{l+1}\frac{J^l e^{-2i\gamma l}e^{-i\theta j}}{\sqrt{(2l)!(l+1)}}\left[|\Psi_{2l,j}\rangle + \frac{\sqrt{J}e^{-i\gamma}}{\sqrt{2l+1}}|\Psi_{2l+1,j}\rangle\right], \tag{4.10}$$

where we have introduced the states $\Psi_{n,j}$, $n=0,1,2,\ldots$, and $j=1,2,\ldots,d(n)$, in order to keep track of the degeneracy of H. It is trivial to check that these states display temporal stability and the action identity, while it does not seem to be an easy task to find an explicit expression for a measure with respect to which a resolution of the identity would be satisfied. However, as we will discuss in the Appendix, it is possible to find weight functions, which are not necessarily everywhere positive, with respect to which a resolution of the identity could be defined in a *weak* sense.

Example 3: Let us consider now a particle of mass m and electric charge e, subject to a three-dimensional harmonic force $\vec{F}=-k(x,y,z)$ and placed in a uniform magnetic field, oriented along the z axis and given by the vector potential $\vec{A}=(B/2)(-y,x,0)$. The Hamiltonian

$$H = \frac{1}{2m}\left(p_x + \frac{eB}{2}y\right)^2 + \frac{1}{2m}\left(p_y - \frac{eB}{2}x\right)^2 + \frac{1}{2m}p_z^2 + \frac{1}{2}k(x^2+y^2+z^2),$$

can be rewritten as

$$H = N_+(\tilde{\omega}+\Omega) + N_-(\tilde{\omega}-\Omega) + N_z\omega,$$

where we have introduced

$$\Omega = \frac{eB}{2m}, \quad \omega^2 = \frac{k}{m}, \quad \tilde{\omega}^2 = \Omega^2+\omega^2,$$

$$a_u = \frac{1}{\sqrt{2}}\left(\sqrt{m\tilde{\omega}}u + \frac{i}{\sqrt{m\tilde{\omega}}}p_u\right), \quad u=x,y, \quad a_z = \frac{1}{\sqrt{2}}\left(\sqrt{m\omega}z + \frac{i}{\sqrt{m\omega}}p_z\right),$$

$$a_\pm = \frac{a_x \pm i a_y}{\sqrt{2}}, \quad N_\pm = a_\pm^\dagger a_\pm, \quad N_z = a_z^\dagger a_z.$$

The eigenvalues and the eigenstates of H are easily found to be

$$E_{n_+,n_-,n_z} = n_+(\tilde{\omega}+\Omega) + n_-(\tilde{\omega}-\Omega) + n_z\omega,$$

$$\varphi_{n_+,n_-,n_z} = \frac{(a_+^\dagger)^{n_+}(a_-^\dagger)^{n_-}(a_z^\dagger)^{n_z}}{\sqrt{n_+!n_-!n_z!}}\varphi_{000},$$

where $a_-\varphi_{000}=a_+\varphi_{000}=a_z\varphi_{000}=0$. In order to simplify the computation of the degeneracy of this Hamiltonian we assume that $\Omega \ll \omega$. In this approximation H can be written as $H \simeq \omega(N_+ + N_- + N_z)$, which means that the eigenvalues really depend only on $n=n_+ + n_- + n_z$. As in the previous examples we can introduce the eigenvalues $E_n=\omega n$ while the degeneracy of the nth energy level is $d(n)=\Sigma_{k=1}^{n+1}k=\frac{1}{2}(n+1)(n+2)$. If we denote the corresponding eigenstates by Ψ_{nj}, $n=0,1,2,\ldots$, $j=1,2,\ldots,d(n)$, we find

$$|J,\gamma,\theta\rangle := \sqrt{2}e^{-J/2}\sum_{n=0}^{\infty}\sum_{j=1}^{d(n)}\frac{J^{n/2}e^{-in\gamma}e^{-ij\theta}}{\sqrt{(n+2)!}}|\Psi_{nj}\rangle. \tag{4.11}$$

Once again, in this case we may introduce the complex variable $z=re^{-i\gamma}=J^{1/2}e^{-i\gamma}$, $z\in\mathbb{C}$, and write these coherent states as

$$|z,\theta\rangle = \sqrt{2}e^{-|z|^2/2}\sum_{n=0}^{\infty}\sum_{j=1}^{d(n)}\frac{z^n e^{-ij\theta}}{\sqrt{(n+2)!}}|\Psi_{nj}\rangle. \tag{4.12}$$

In this case the resolution of the identity takes the form,

$$\frac{1}{4\pi^2}\int_0^{\infty}\int_0^{2\pi}\int_0^{2\pi}|z,\theta\rangle\langle z,\theta|r^5\,\mathrm{d}\gamma\,\mathrm{d}\theta\,\mathrm{d}r = I. \tag{4.13}$$

It is trivial to check that all the other stated properties are satisfied as well. We should mention here that coherent states for this Hamiltonian have been constructed before (see Refs. 9 and 12). However the treatment there is somewhat different, in that the authors obtain multidimensional coherent states which allow them to study the Berezin–Lieb inequalities for the associated thermodynamic potential.

B. Infinite degeneracies

We are now in a position to construct coherent states for Hamiltonians with infinite degeneracies. Let $\tilde{\mathfrak{H}}$ be an abstract Hilbert space and $\{\phi_{k\ell}\}_{k,\ell=0}^{\infty}$ an orthonormal basis in it,

$$\langle\phi_{k\ell}|\phi_{k'\ell'}\rangle = \delta_{kk'}\delta_{\ell\ell'}.$$

Using these and the basis vectors Ψ_n [see (2.15)] of $\mathfrak{H}_{\text{ac-ang}}$ we now build several families of coherent states on $\tilde{\mathfrak{H}}$

(1) Vector coherent states, VCS1.
These are infinite component vector coherent states,

$$|J,\gamma;\ J'\gamma';\ \ell\rangle^1 = \frac{\Psi_\ell(J',\gamma')}{[\mathcal{N}(J)\mathcal{N}(J')]^{1/2}}\sum_{n=0}^{\infty}\overline{\Psi_n(J,\gamma)}|\phi_{n\ell}\rangle = \frac{J'^{\ell/2}e^{i\epsilon_\ell\gamma'}}{[\mathcal{N}(J)\mathcal{N}(J')]^{1/2}}\sum_{n=0}^{\infty}\frac{J^{n/2}e^{-i\epsilon_n\gamma}}{[\epsilon_\ell!\,\epsilon_n!]^{1/2}}|\phi_{n\ell}\rangle, \tag{4.14}$$

with components $\ell=0,1,2,\ldots$, where $\mathcal{N}(J)=\Sigma_{n=0}^{\infty}(J^n/\epsilon_n!)$. These vectors satisfy the normalization

$$\sum_{\ell=0}^{\infty}{}^1\langle J,\gamma;\ J',\gamma';\ \ell|J,\gamma;\ J',\gamma';\ \ell\rangle^1 = 1$$

(note that according to our present convention, the individual vectors are not normalized) and the resolution of identity condition,

$$\sum_{\ell=0}^{\infty}\int_{\mathbb{R}}\int_{\mathbb{R}}\left[\int_0^L\int_0^L|J,\gamma;\ J',\gamma';\ \ell\rangle^{11}\langle J,\gamma;\ J',\gamma';\ \ell|\right.$$
$$\left.\times\,\mathrm{d}\mu_{\mathcal{B}}(\gamma)\mathrm{d}\mu_{\mathcal{B}}(\gamma')\right]\mathcal{N}(J)\mathcal{N}(J')\mathrm{d}\nu(J)\mathrm{d}\nu(J') = I_{\tilde{\mathfrak{H}}}. \tag{4.15}$$

Notice that $\Psi_\ell(J',\gamma')\overline{\Psi_n(J,\gamma)}$ in (4.14) could be replaced by $\overline{\Psi_\ell(J',\gamma')}\Psi_n(J,\gamma)$ without affecting any of the results stated here, this would simply amount to replacing γ and γ' by $-\gamma$ and $-\gamma'$. The same remark also holds for formulas (4.22) and (4.25) below. However, a deeper significance of this interplay between the two options will emerge when we discuss modular structures in Sec. V below.
Consider now the Hamiltonian

$$H_1 = \sum_{n,\ell=0}^{\infty} \omega\epsilon_n |\phi_{n\ell}\rangle\langle\phi_{n\ell}| = \omega A_1^\dagger A_1, \tag{4.16}$$

where A_1, $A_1^\dagger$ are the operators

$$A_1\phi_{n\ell} = \sqrt{\epsilon_n}\phi_{n-1\ell}, \quad A_1^\dagger\phi_{n\ell} = \sqrt{\epsilon_{n+1}}\phi_{n+1\ell}. \tag{4.17}$$

Each level $\omega\epsilon_n$ of this Hamiltonian is infinitely degenerate, with ℓ counting the degeneracy. Thus the states (4.14) are Gazeau–Klauder-type vector coherent states for this Hamiltonian. Indeed, they satisfy the time stability condition,

$$e^{-iH_1 t}|J,\gamma;\ J'\gamma';\ \ell\rangle^1 = |J,\gamma+\omega t;\ J'\gamma';\ \ell\rangle^1, \tag{4.18}$$

and an action identity, which we could write either as

$$\frac{{}^1\langle J,\gamma;\ J'\gamma';\ \ell|H_1|J,\gamma;\ J'\gamma';\ \ell\rangle^1}{\|\|J,\gamma;\ J'\gamma';\ \ell\rangle^1\|^2} = \omega J, \tag{4.19}$$

or as

$$\sum_{\ell=0}^{\infty} {}^1\langle J,\gamma;\ J',\gamma';\ \ell|H_1|J,\gamma;\ J',\gamma';\ \ell\rangle^1 = \omega J, \tag{4.20}$$

where we have summed over the degenerate levels.

Note that we could just as well have constructed vector coherent states in this example, using an orthonormal basis $\{\Psi_n\}_{n=0}^{\infty}$ in an arbitrary reproducing kernel Hilbert space $\mathfrak{H}_{\rm ker}$,

$$|J,\gamma;\ x;\ \ell\rangle = \frac{\Psi_\ell(x)}{[K(x,x)\mathcal{N}(J')]^{1/2}}\sum_{n=0}^{\infty}\frac{J^{n/2}e^{-i\epsilon_n\gamma}}{[\epsilon_\ell!\,\epsilon_n!]^{1/2}}|\phi_{n\ell}\rangle, \tag{4.21}$$

with $K(x,x)$ as in (2.5) and the degeneracies would again be handled as before. However, the special choice made in (4.14) enables us to write down the related family of vector coherent states, appearing in (4.22) below, which are the coherent states of a second Hamiltonian, acting on the degeneracy levels.

(2) Vector coherent states, VCS2.

These are a second set of similar vector coherent states

$$|J,\gamma;\ J'\gamma';\ n\rangle^2 = \frac{\overline{\Psi_n(J,\gamma)}}{[\mathcal{N}(J)\mathcal{N}(J')]^{1/2}}\sum_{\ell=0}^{\infty}\Psi_\ell(J',\gamma')|\phi_{n\ell}\rangle = \frac{J^{n/2}e^{-i\epsilon_n\gamma}}{[\mathcal{N}(J)\mathcal{N}(J')]^{1/2}}\sum_{\ell=0}^{\infty}\frac{J'^{\ell/2}e^{i\epsilon_\ell\gamma'}}{[\epsilon_\ell!\,\epsilon_n!]^{1/2}}|\phi_{n\ell}\rangle, \tag{4.22}$$

with components $n=0,1,2,\ldots$. Defining a second Hamiltonian,

$$H_2 = \sum_{n,\ell=0}^{\infty} \omega\epsilon_\ell |\phi_{n\ell}\rangle\langle\phi_{n\ell}| = \omega A_2^\dagger A_2, \tag{4.23}$$

where A_2, $A_2^\dagger$ are the operators

$$A_2\phi_{n\ell} = \sqrt{\epsilon_\ell}\phi_{n\ell-1}, \quad A_2^\dagger\phi_{n\ell} = \sqrt{\epsilon_{\ell+1}}\phi_{n\ell+1}, \tag{4.24}$$

we see that the states (4.22) are Kazeau–Klauder-type coherent states for this Hamiltonian. The two Hamiltonians H_1 and H_2 commute and, in fact, H_2 lifts the degeneracy of H_1 and vice versa.

Finally, we can define a third set of coherent states as below.

(3) Bicoherent states, BCS.

These are basically the summed-over versions of the previous two

$$|J,\gamma;\ J',\gamma'\rangle^{\mathrm{BCS}} = \frac{1}{[\mathcal{N}(J)\mathcal{N}(J')]^{1/2}} \sum_{n,\ell=0}^{\infty} \overline{\Psi_n(J,\gamma)}\Psi_\ell(J',\gamma')|\phi_{n\ell}\rangle$$

$$= \frac{1}{[\mathcal{N}(J)\mathcal{N}(J')]^{1/2}} \sum_{n,\ell=0}^{\infty} \frac{J^{n/2}J'^{\ell/2}e^{-i(\epsilon_n\gamma-\epsilon_\ell\gamma')}}{[\epsilon_n!\epsilon_\ell!]^{1/2}}|\phi_{n\ell}\rangle, \tag{4.25}$$

which can be considered as being the multidimensional coherent states (see Ref. 12) of the Hamiltonian,

$$H = H_1 - H_2 = \sum_{n,\ell=0}^{\infty} \omega(\epsilon_n - \epsilon_\ell)|\phi_{n\ell}\rangle\langle\phi_{n\ell}| = \omega[A_1^\dagger A_1 - A_2^\dagger A_2]. \tag{4.26}$$

These coherent states are normalized to unity; they satisfy the resolution of the identity,

$$\int_{\mathbb{R}}\int_{\mathbb{R}}\left[\int_0^L\int_0^L |J,\gamma;\ J',\gamma'\rangle^{\mathrm{BCS}\ \mathrm{BCS}}\langle J,\gamma;\ J',\gamma'|\mathrm{d}\mu_{\mathcal{B}}(\gamma)\mathrm{d}\mu_{\mathcal{B}}(\gamma')\right]\mathcal{N}(J)\mathcal{N}(J')\mathrm{d}\nu(J)\mathrm{d}\nu(J') = I_{\tilde{\mathfrak{H}}}, \tag{4.27}$$

temporal stability condition,

$$e^{-iHt}|J,\gamma;\ J',\gamma'\rangle^{\mathrm{BCS}} = |J,\gamma+\omega t;\ J',\gamma'+\omega t\rangle^{\mathrm{BCS}}, \tag{4.28}$$

and the action identity,

$${}^{\mathrm{BCS}}\langle J,\gamma;\ J',\gamma'|H|J,\gamma;\ J',\gamma'\rangle^{\mathrm{BCS}} = \omega(J-J'). \tag{4.29}$$

A physical example of a Hamiltonian admitting such infinite degeneracies is worked out in the following section.

V. ELECTRON IN A MAGNETIC FIELD

A single electron of unit charge, placed in the *xy* plane and subjected to a constant magnetic field, pointing along the negative *z* direction, has the classical Hamiltonian,

$$H_{\mathrm{elec}} = \frac{1}{2}(\vec{p}+\vec{A})^2 = \frac{1}{2}\left(p_x + \frac{y}{2}\right)^2 + \frac{1}{2}\left(p_y - \frac{x}{2}\right)^2, \tag{5.1}$$

where we have chosen the magnetic vector potential to be $\vec{A}=\frac{1}{2}(y,-x,0)$, using the convenient units introduced in Ref. 7. In this reference it is shown that H_{elec} is the single-electron free Hamiltonian related to the so-called *fractional quantum Hall effect*, FQHE, whose static and dynamical behaviors are yet to be fully understood.[13] In particular, different copies of H_{elec} are used to build up the free Hamiltonian for the *N*-electron system as follows: $H_0^{(N)}=\Sigma_{i=1}^N H_{\mathrm{elec}}(i)$. The many-body model of the FQHE consists, then, of a two-dimensional electron gas, 2DEG (that is a gas of electrons constrained to a two-dimensional layer) in a positive uniform background and subjected to a uniform magnetic field along *z*, whose Hamiltonian (for *N* electrons) is (Ref. 7) $H^{(N)}=H_0^{(N)}+\lambda(H_C^{(N)}+H_B^{(N)})$, with $H_0^{(N)}$ as above, $H_C^{(N)}$ is the canonical Coulomb interaction between charged particles, $H_C^{(N)}=\frac{1}{2}\Sigma_{i\neq j}^N(1/|r_i-r_j|)$, and $H_B^{(N)}$ is the interaction of the charges with the positive background.

One usually considers $\lambda(H_C^{(N)}+H_B^{(N)})$ as a perturbation on the free Hamiltonian $H_0^{(N)}$, and looks for the eigenstates of $H_0^{(N)}$ in the form of a Slater determinant built up with single electron wave functions, the eigenstates of H_{elec}. Already, the solution of this static problem is very hard and many proposals exist in literature. Moreover, a completely satisfactory explanation of the plateau observed for the resistivity tensor is still far from being at hand. For these reasons all possibilities for getting a deeper understanding of this phenomenon would appear relevant. With this in mind we study below a modular structure associated with the single electron model and construct vector

coherent states for the associated Hamiltonians. In a later publication we intend to report on results, using these coherent states, which shed light on the FQHE. We might add, however, that the appearance of this rather sophisticated mathematical structure in this context, is in itself interesting.

On $\tilde{\mathfrak{H}}=L^2(\mathbb{R}^2,\mathrm{d}x\,\mathrm{d}y)$ we introduce the quantized observables,

$$p_x+\frac{y}{2}\to Q_1=-i\frac{\partial}{\partial x}+\frac{y}{2};\quad p_y-\frac{x}{2}\to P_1=-i\frac{\partial}{\partial y}-\frac{x}{2}, \tag{5.2}$$

which satisfy $[Q_1,P_1]=iI_{\tilde{\mathfrak{H}}}$ and in terms of which the quantum Hamiltonian, corresponding to H_{elec} becomes

$$H_1=\tfrac{1}{2}(P_1^2+Q_1^2). \tag{5.3}$$

This is just the oscillator Hamiltonian in one dimension, with eigenvalues $E_n=\omega\left(n+\frac{1}{2}\right)$, $n=0,1,2,\ldots,\infty$. Each level is infinitely degenerate, and we will denote the corresponding normalized eigenvectors by $\Psi_{n\ell}$, $\ell=0,1,2,\ldots,\infty$. If the magnetic field were aligned along the positive z axis [with $\vec{A}=\frac{1}{2}(-y,x,0)$], the corresponding quantum Hamiltonian would have been

$$H_2=\tfrac{1}{2}(P_2^2+Q_2^2). \tag{5.4}$$

with

$$Q_2=-i\frac{\partial}{\partial y}+\frac{x}{2},\quad P_2=-i\frac{\partial}{\partial x}-\frac{y}{2}, \tag{5.5}$$

and $[Q_2,P_2]=iI_{\bar{\mathfrak{H}}}$. The two sets of operators $\{Q_i,P_i\}$, $i=1,2$, mutually commute,

$$[Q_1,Q_2]=[Q_1,P_2]=[P_1,Q_2]=[P_1,P_2]=0. \tag{5.6}$$

(Note that at the classical level, the transformation $(x,y,p_x,p_y)\to[x'=p_x+(y/2),y'=p_y+(x/2),p_{x'}=p_y-(x/2),p_{y'}=p_y-(y/2)]$ is canonical, i.e., $\mathrm{d}x\wedge\mathrm{d}p_x+\mathrm{d}y\wedge\mathrm{d}p_y=\mathrm{d}x'\wedge\mathrm{d}p_{x'}+\mathrm{d}y'\wedge\mathrm{d}p_{y'}$.**)** Thus, $[H_1,H_2]=0$ and the eigenvectors $\Psi_{n\ell}$ of H_1 can be so chosen that they are also the eigenvectors of H_2 in the manner

$$H_1\Psi_{n\ell}=\omega\left(n+\tfrac{1}{2}\right)\Psi_{n\ell},\quad H_2\Psi_{n\ell}=\omega\left(\ell+\tfrac{1}{2}\right)\Psi_{n\ell}, \tag{5.7}$$

so that H_2 lifts the degeneracy of H_1 and vice versa. We shall assume that this has been done.

While we shall follow the technique outlined in the preceding section to construct vector coherent states for the above two Hamiltonians, we shall first analyze the algebraic structures generated by these operators, to get a deeper insight into the nature of the resulting coherent states. In the process we shall display some von Neumann algebraic properties, the appearance of KMS states and, as stated earlier, a certain *modular structure* carried by the above model. The appearance of KMS states in the present context is interesting since, as is well known, KMS states are equilibrium states for infinite-dimensional quantum systems and the associated modular structures, being linked to the (effective) Hamiltonian of the system, are closely related to their dynamical behavior Both these aspects may therefore shed additional light on some still unclear aspects of the FQHE. Details of the mathematical theory underlying modular these structures may be found in Refs. 2, 3, 14, 18, and 19.

On $\mathfrak{H}=L^2(\mathbb{R})$ let Q and P be the usual position and momentum operators in the Schrödinger representation. Denote by $\mathcal{B}_2(\mathfrak{H})\simeq\mathfrak{H}\otimes\bar{\mathfrak{H}}$ the space of Hilbert–Schmidt operators on $\mathfrak{H}$. This is again a Hilbert space, with the scalar product $\langle X|Y\rangle_2=\mathrm{Tr}[X^*Y]$. Let $\{\phi_n\}_{n=0}^{\infty}$ be the orthonormal basis of $\mathfrak{H}$ consisting of the eigenvectors of the oscillator Hamiltonian $H_{\mathrm{osc}}=\frac{1}{2}(P^2+Q^2)$, i.e., $H_{\mathrm{osc}}\phi_n=\omega\left(n+\frac{1}{2}\right)\phi_n$, $n=0,1,2,\ldots$. Then,

$$\phi_{n\ell} := |\phi_n\rangle\langle\phi_\ell|, \quad n,\ell = 0,1,2,\ldots,\infty, \tag{5.8}$$

is an orthonormal basis for $\mathcal{B}_2(\mathfrak{H})$. On $\mathfrak{H}$ define the unitary operators,

$$U(x,y) = e^{-i(xQ+yP)}, \quad (U(x,y)\phi)(\xi) = e^{-ix[\xi-(y/2)]}\phi(\xi - y), \quad (x,y) \in \mathbb{R}^2, \quad \phi \in \mathfrak{H}. \tag{5.9}$$

Then, it is well known (see, for example, Ref. 2) that the map,

$$\mathcal{W}:\mathcal{B}_2(\mathfrak{H}) \to L^2(\mathbb{R}^2, \mathrm{d}x\mathrm{d}y) = \tilde{\mathfrak{H}}, \quad (\mathcal{W}X)(x,y) = \frac{1}{(2\pi)^{1/2}}\mathrm{Tr}[U(x,y)^* X], \tag{5.10}$$

is unitary. Next, if A and B are two operators on $\mathfrak{H}$, we define by $A \vee B$ the operator

$$A \vee B(X) = AXB^*, \quad X \in \mathcal{B}_2(\mathfrak{H}).$$

For a large class of operators A, B (in particular when A and B are both bounded operators), $A \vee B$ defines a linear operator on $\mathcal{B}_2(\mathfrak{H})$. Then straightforward computations (as shown in the Appendix) yield,

$$\mathcal{W}\begin{pmatrix} Q \vee I_{\mathfrak{H}} \\ P \vee I_{\mathfrak{H}} \end{pmatrix}\mathcal{W}^{-1} = \begin{pmatrix} Q_1 \\ P_1 \end{pmatrix}, \quad \mathcal{W}\begin{pmatrix} I_{\mathfrak{H}} \vee Q \\ I_{\mathfrak{H}} \vee P \end{pmatrix}\mathcal{W}^{-1} = \begin{pmatrix} P_2 \\ Q_2 \end{pmatrix}, \tag{5.11}$$

and

$$\mathcal{W}\begin{pmatrix} H_{\mathrm{osc}} \vee I_{\mathfrak{H}} \\ I_{\mathfrak{H}} \vee H_{\mathrm{osc}} \end{pmatrix}\mathcal{W}^{-1} = \begin{pmatrix} H_1 \\ H_2 \end{pmatrix}, \quad \mathcal{W}\phi_{n\ell} = \Psi_{n\ell}, \tag{5.12}$$

where the $\phi_{n\ell}$ are the basis vectors defined in (5.8) and the $\Psi_{n\ell}$ are the normalized eigenvectors defined in (5.7). This also means that these latter vectors form a basis of $\tilde{\mathfrak{H}} = L^2(\mathbb{R}^2, \mathrm{d}x\,\mathrm{d}y)$.

In the sequel we shall also need the thermal equilibrium state, at inverse temperature β, corresponding to the Hamiltonian H_{osc}. This is the density matrix,

$$\rho_\beta = \frac{e^{-\beta H_{\mathrm{osc}}}}{\mathrm{Tr}[e^{-\beta H_{\mathrm{osc}}}]} = (1 - e^{-\omega\beta})\sum_{n=0}^{\infty} e^{-n\omega\beta}|\phi_n\rangle\langle\phi_n|. \tag{5.13}$$

On $\tilde{\mathfrak{H}}$, for each $(x,y) \in \mathbb{R}^2$, define the operators

$$U_1(x,y) = \mathcal{W}[U(x,y) \vee I_{\mathfrak{H}}]\mathcal{W}^{-1}, \quad U_2(x,y) = \mathcal{W}[I_{\mathfrak{H}} \vee U(x,y)^*]\mathcal{W}^{-1}, \tag{5.14}$$

and let $\mathfrak{A}_i$ $i=1,2$, be the von-Neumann algebra (see, e.g., Ref. 19) generated by the unitary operators $\{U_i(x,y)\,|\,(x,y) \in \mathbb{R}^2\}$. Then using the unitary map $\mathcal{W}$, the following modular structure can easily be inferred for the pair of von Neumann algebras $\mathfrak{A}_1$ and $\mathfrak{A}_2$ (for details on modular structures see Ref. 18 and for the particular type of algebras appearing here, see Refs. 2 and 3).

(1) The algebra $\mathfrak{A}_1$ is the commutant of the algebra $\mathfrak{A}_2$ and vice versa and $\mathfrak{A}_1 \cap \mathfrak{A}_2 = \mathbb{C}I_{\tilde{\mathfrak{H}}}$.
(2) If $\{\lambda_n\}_{n=0}^{\infty}$ is a sequence of nonzero positive numbers such that $\Sigma_{n=0}^{\infty}\lambda_n = 1$, then the vector $\Phi = \Sigma_{n=0}^{\infty}\lambda_n^{1/2}\Psi_{nn}$ is cyclic and separating for $\mathfrak{A}_1$. In particular, we shall work with the vector $\Phi = \Phi_\beta$, for which the λ_n correspond to the thermal state ρ_β in (5.13):

$$\Phi_\beta = [1 - e^{-\omega\beta}]^{1/2}\sum_{n=0}^{\infty} e^{-n\omega\beta/2}\Psi_{nn}, \quad \text{i.e., } \lambda_n = (1 - e^{-i\omega\beta})e^{-n\omega\beta}. \tag{5.15}$$

(3) The map

$$S_\beta:\tilde{\mathfrak{H}} \to \tilde{\mathfrak{H}}, \quad S_\beta[U_1(x,y)\Phi_\beta] = U_1(x,y)^*\Phi_\beta, \tag{5.16}$$

is closable and has the polar decomposition,

$$S_\beta = J_\beta \Delta_\beta^{1/2}, \tag{5.17}$$

where J_β is the *antiunitary* operator:

$$J_\beta \Psi_{n\ell} = \Psi_{\ell n}, \quad J_\beta^2 = I_{\tilde{\mathfrak{H}}}, \quad J_\beta \Phi_\beta = \Phi_\beta, \tag{5.18}$$

so that $J_\beta \mathfrak{A}_1 J_\beta = \mathfrak{A}_2$, and Δ_β is the self-adjoint operator,

$$\Delta_\beta = \sum_{n,\ell=0}^{\infty} \frac{\lambda_n}{\lambda_\ell} |\Psi_{n\ell}\rangle\langle\Psi_{n\ell}| = e^{-\beta H} \quad \text{where } H = H_1 - H_2, \tag{5.19}$$

the Hamiltonians H_1 and H_2 being as in (5.7). [We reproduce the derivation of (5.17)–(5.19) in the Appendix.] The operator Δ_β defines a one parameter group of evolution, $t \to \alpha_\beta(t)$ on the algebra $\mathfrak{A}_1$,

$$\alpha_\beta(t)[A] = \Delta_\beta^{-it/\beta} A \Delta_\beta^{it/\beta} = e^{itH} A e^{-itH} = e^{itH_1} A e^{-itH_1}, \quad A \in \mathfrak{A}_1. \tag{5.20}$$

(4) The state φ_β, defined on the algebra $\mathfrak{A}_1$ by the vector Φ_β,

$$\langle \varphi_\beta; A\rangle = \langle \Phi_\beta | A\Phi_\beta\rangle_{\tilde{\mathfrak{H}}}, \quad A \in \mathfrak{A}_1, \tag{5.21}$$

is a faithful normal vector state which is invariant under the evolution α_β,

$$\langle \varphi_\beta; \alpha_\beta(t)[A]\rangle = \langle \varphi_\beta; A\rangle. \tag{5.22}$$

Furthermore, φ_β is a KMS state[14,18] in the following sense: for $A, B \in \mathfrak{A}_1$, define the function $F_{A,B}$ of the real variable t,

$$F_{A,B}(t) = \langle \varphi_\beta; A\alpha_\beta(t)[B]\rangle. \tag{5.23}$$

Then this function has an analytic extension to the open strip $\{z = t + iv \,|\, 0 < v < \beta\}$ and furthermore,

$$F_{A,B}(t + i\beta) = \langle \varphi_\beta; \alpha_\beta(t)[B]A\rangle. \tag{5.24}$$

Going back now to the problem of constructing coherent states for this system we can immediately write down three types of states, in analogy with (4.14), (4.22), and (4.25).

(1) Vector coherent states of the Hamiltonian $H_1 - (\omega/2) I_{\tilde{\mathfrak{H}}}$.
These are the states on $\tilde{\mathfrak{H}} = L^2(\mathbb{R}^2, \mathrm{d}x\, \mathrm{d}y)$,

$$|z, \overline{z'}; \ell\rangle^1 = e^{-(|z|^2 + |z'|^2)/2} \overline{z'}^{\ell} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!\ell!}} |\Psi_{n\ell}\rangle, \quad \ell = 0, 1, 2, \ldots, \infty. \tag{5.25}$$

They are obtained by replacing $J^{n/2} e^{-i\epsilon_n \gamma}$ by $z^n = r^n e^{in\theta}$ and $J'^{\ell/2} e^{-i\epsilon_\ell \gamma'}$ by $z'^{\ell} = r'^{\ell} e^{i\ell\theta'}$ in (4.14), with $z, z' \in \mathbb{C}$. The resolution of the identity now takes the form

$$\frac{1}{(2\pi)^2} \sum_{\ell=0}^{\infty} \int_{\mathbb{C}\times\mathbb{C}} |z, \overline{z'}; \ell\rangle^{11} \langle z, \overline{z'}; \ell| \mathrm{d}x\, \mathrm{d}x'\, \mathrm{d}y\, \mathrm{d}y' = I_{\tilde{\mathfrak{H}}}, \tag{5.26}$$

where $z = (1/\sqrt{2})(y - ix)$ and $z' = (1/\sqrt{2})(y' - ix')$. Let us introduce the operators,

$$A_\ell = \frac{1}{\sqrt{2}}(Q_\ell + iP_\ell), \quad A_\ell^\dagger = \frac{1}{\sqrt{2}}(Q_\ell - iP_\ell), \quad H_\ell = A_\ell^\dagger A_\ell + \frac{\omega}{2}, \quad \ell = 1, 2. \tag{5.27}$$

Then, it is not hard to see that,

$$U_1(z) := U_1(x,y) = e^{zA_1^\dagger - \overline{z}A_1} = e^{-\frac{1}{2}|z|^2} e^{zA_1^\dagger} e^{-\overline{z}A_1}. \tag{5.28}$$

Also, since

$$A_1|\Psi_{n\ell}\rangle = \sqrt{n}|\Psi_{n-1\ell}\rangle, \quad A_1^\dagger|\Psi_{n\ell}\rangle = \sqrt{n+1}|\Psi_{n+1\ell}\rangle,$$

it easily follows that,

$$|z,\overline{z}';\ell\rangle^1 = e^{-|z'|^2/2}\frac{\overline{z}'^\ell}{\sqrt{\ell!}}U_1(z)|\Psi_{0\ell}\rangle. \tag{5.29}$$

(2) Vector coherent states of the Hamiltonian $H_2-(\omega/2)I_{\tilde{\mathfrak{H}}}$.
Following (4.22), we have the analogous set of vector coherent states

$$|z,\overline{z}';n\rangle^2 = e^{-(|z|^2+|z'|^2)/2}z^n\sum_{\ell=0}^{\infty}\frac{\overline{z}'^\ell}{\sqrt{n!\ell!}}|\Psi_{n\ell}\rangle = e^{-|z|^2/2}\frac{z^n}{\sqrt{n!}}U_2(z')|\Psi_{n0}\rangle, \quad n=0,1,2,\ldots,\infty, \tag{5.30}$$

with $U_2(z')=\mathcal{W}[I_{\mathfrak{H}}\vee U(z')^*]\mathcal{W}^{-1}$ [see (5.14)], which satisfy a resolution of the identity similar to (5.26).

(3) Coherent states of the Hamiltonian $H=H_1-H_2$.
These are the "bicoherent states," analogous to (4.25),

$$|z,\overline{z}'\rangle^{\mathrm{BCS}} = e^{-(|z|^2+|z'|^2)/2}\sum_{n,\ell=0}^{\infty}\frac{z^n\overline{z}'^\ell}{\sqrt{n!\ell!}}|\Psi_{n\ell}\rangle = U_1(z)U_2(z')|\Psi_{00}\rangle. \tag{5.31}$$

(4) Coherent states built from the thermal equilibrium state.
As yet another example related to this system, we build coherent states, starting with the thermal state Φ_β [see (5.15) and (5.21)]. We define these states as

$$|z,\overline{z},\beta\rangle^{\mathrm{KMS}} = U_1(z)|\Phi_\beta\rangle = e^{zA_1^\dagger-\overline{z}A_1}|\Phi_\beta\rangle. \tag{5.32}$$

In view of the fact that for any normalized vector $\phi\in\mathfrak{H}$, the vectors $U(z)\phi$, $z\in\mathbb{C}$, where $U(z):=U(x,y)$ [see (5.9)], satisfy

$$\frac{1}{2\pi}\int_{\mathbb{C}}|U(z)\phi\rangle\langle U(z)\phi|\mathrm{d}x\,\mathrm{d}y = I_{\mathfrak{H}},$$

we deduce, using the isometry $\mathcal{W}$ in (5.10) that the coherent states (5.32) satisfy the resolution of the identity condition

$$\frac{1}{2\pi}\int_{\mathbb{C}}|z,\overline{z},\beta\rangle^{\mathrm{KMS\ KMS}}\langle z,\overline{z},\beta|\mathrm{d}x\,\mathrm{d}y = I_{\tilde{\mathfrak{H}}}. \tag{5.33}$$

Also, since

$$U_1(z)|\Psi_{nn}\rangle = \frac{1}{\sqrt{n!}}(A_1^\dagger-\overline{z}I_{\tilde{\mathfrak{H}}})^nU_1(z)|\Psi_{0n}\rangle = \frac{1}{\sqrt{n!}}\left(\frac{\partial}{\partial z}-\frac{\overline{z}}{z}I_{\tilde{\mathfrak{H}}}\right)^nU_1(z)|\Psi_{0n}\rangle, \tag{5.34}$$

which follows from the fact that

$$(A_1^\dagger)^n|\Psi_{0n}\rangle = \sqrt{n!}|\Psi_{nn}\rangle \quad \text{and } U_1(z)|\Psi_{0n}\rangle = e^{-|z|^2/2}\sum_{k=0}^{\infty}\frac{(zA_1)^k}{k!}|\Psi_{0n}\rangle,$$

we may rewrite (5.32) as

$$|z,\overline{z},\beta\rangle^{\mathrm{KMS}} = [1-e^{-\omega\beta}]^{1/2}\sum_{n=0}^{\infty}\sqrt{n!}e^{-n\omega\beta/2}\left(\frac{\partial}{\partial z}-\frac{\overrightarrow{\overline{z}}}{2}\right)^n|z;n\rangle, \tag{5.35}$$

where we have set

$$|z;n\rangle = U_1(z)|\Psi_{0n}\rangle.$$

Furthermore, using the fact that

$$(A_2^\dagger)^n|\Psi_{n0}\rangle = \sqrt{n!}|\Psi_{nn}\rangle,$$

we may also write

$$|z,\overline{z},\beta\rangle^{\mathrm{KMS}} = [1-e^{-\omega\beta}]^{1/2}\sum_{n=0}^{\infty}e^{-n\omega\beta/2}\left(\frac{\partial}{\partial z}-\frac{\overrightarrow{\overline{z}}}{2}\right)^n A_2^n|z;0\rangle. \tag{5.36}$$

It should be pointed out that the coherent states (5.32) are not of the Gazeau–Klauder type. States of the type

$$\left(\frac{\partial}{\partial z}-\frac{\overrightarrow{\overline{z}}}{2}\right)^n|z;n\rangle = (A_1^\dagger-\overline{z}\tilde{I_{\mathfrak{H}}})^n|z;n\rangle,$$

are finite linear combinations of *photon-added coherent states* (see Ref. 1), which have been studied extensively in the optical literature. Note that

$$\langle z;n|z';m\rangle = e^{-(|z|^2+|z'|^2)/2}e^{\overline{z}z'}\delta_{nm}. \tag{5.37}$$

Finally, note that since $U_1(x,y)^* = U_1(-x,-y)$, using (5.16) we can get another family of coherent states built on the thermal state Φ_β:

$$S_\beta|z,\overline{z},\beta\rangle^{\mathrm{KMS}} = |-z,-\overline{z},\beta\rangle^{\mathrm{KMS}}.$$

Obviously, these also satisfy the same resolution of the identity as (5.33).

We shall consider in more detail the relationship between the above algebraic structure and the different kinds of coherent states discussed here, as well as their use in the analysis of the quantum Hall effect, in a subsequent paper.

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APPENDIX

We work out here some of the results quoted in the preceding two sections.

The measure in Example 2 of Sec. IV A

The proof of the existence of the measure in Example 2 of Sec. IV A will be considered as a particular case of a more general situation.

We are looking for a "density" $f(x)$ such that, given a sequence of numbers ρ_n, the following equation holds:

$$\int_0^\infty f(x)x^n\,\mathrm{d}x = \rho_n, \quad n = 0,1,2,\ldots .$$

It is convenient to introduce a new function $\tilde{f}(x)$ as $f(x)=e^{-x}\tilde{f}(x)$ and restate the problem as follows: we are looking for a function $\tilde{f}(x)$ such that

$$\int_0^\infty \tilde{f}(x)x^n(e^{-x}\,\mathrm{d}x) = \rho_n, \quad n = 0,1,2,\ldots . \tag{A1}$$

As is well known, the orthonormalization procedure in $L^2(\mathbb{R}^+, e^{-x}\,\mathrm{d}x)$ for x^n produces the Laguerre polynomials,

$$x^n \to L_n(x) = \sum_{k=0}^{n} \binom{n}{n-k} \frac{(-1)^k}{k!} x^k, \tag{A2}$$

and $\langle L_n | L_l \rangle = \delta_{nl}$, where the scalar product is, of course, the one in $L^2(\mathbb{R}^+, e^{-x}\,\mathrm{d}x)$. If we consider the linear combination of (A1) with the coefficients given in (A2) we get

$$\int_0^\infty \tilde{f}(x)L_n(x)(e^{-x}\,\mathrm{d}x) = \sum_{k=0}^{n} \binom{n}{n-k} \frac{(-1)^k}{k!}\rho_k =: d_n. \tag{A3}$$

It is clear then that we must take $\tilde{f}(x)=\Sigma_{n=0}^{\infty} d_n L_n(x)$, provided this sum converges and consequently, the required "density" is $f(x)=e^{-x}[\Sigma_{n=0}^{\infty} d_n L_n(x)]$. Note however, that this function is not everywhere positive.

We can say more on the coefficients d_n by recalling that $\rho_{2n}=(2n)!(n+1)$ and $\rho_{2n+1}=(2n+1)!(n+1)$. It is an easy exercise to check that

$$d_n = \sum_{l=0}^{[n/2]} \binom{n}{n-2l}(l+1) - \sum_{l=0}^{[(n-1)/2]} \binom{n}{n-(2l+1)}(l+1),$$

where $[r]$ stands for the integer part of the rational number r. This implies that $d_1=0$ and $d_n = 2^{n-2}$ for all $n \geqslant 2$, so that $\tilde{f}(x)$ cannot be a square-integrable function. However, if we consider the sequence $\{\tilde{f}_N | N \in \mathbb{N}\}$, where $\tilde{f}_N(x)=\Sigma_{n=0}^{N} d_n L_n(x)$, it is possible to show that it converges with respect to a certain family of test functions. For that we define

$$\mathcal{D}_b = \left\{ f \in \mathcal{D}([0,1]) \,\middle|\, \int_0^1 \left| \frac{d^k}{\mathrm{d}x^k} f(x) \right| \mathrm{d}x \leqslant 1, \ \forall\, k = 0,1,2,\ldots \right\}. \tag{A4}$$

This is a nonempty subset of $\mathcal{D}([0,1])$. We can check that

$$I_{NM} := \int_0^\infty (\tilde{f}_N(x) - \tilde{f}_M(x))\varphi(x)\mathrm{d}x \to 0, \tag{A5}$$

as $N, M \to \infty$ for all $\varphi \in \mathcal{D}_b$. This follows from the fact that

$$L_n(x) = \frac{1}{n!} e^x \frac{d^n}{\mathrm{d}x^n}(e^{-x}x^n)$$

and from the properties of $\mathcal{D}_b$. Thus, using integration by parts

$$|I_{NM}| \leqslant \sum_{n=M+1}^{N} \frac{|d_n|}{n!} \int_0^1 \left| x^n \left(1 + \frac{d}{dx}\right)^n \varphi(x) \right| dx \leqslant \sum_{n=M+1}^{N} \frac{2^{n-2} \cdot 2^n}{n!} \to 0,$$

as $N, M \to \infty$.

It may be worth remarking that the set $\mathcal{D}_b$ could be replaced by some larger set without affecting the final result. However, the estimates above would have been harder to obtain. Thus, since such a stronger result would not be very relevant in the present context, we will not consider this generalization here.

Proof of (5.11)

We only demonstrate the first two relations in (5.11), since the other two follow in an entirely analogous manner. Moreover, (5.12) is a direct consequence of (5.11). Consider $X \in \mathcal{B}_2(\mathfrak{H})$ of the type $X = |\phi\rangle\langle\psi|$, such that both ϕ and ψ are in the domains of the operators Q and P, are differentiable and vanish at infinity. Then,

$$(\mathcal{W}X)(x,y) = \frac{1}{(2\pi)^{1/2}} \mathrm{Tr}[U(x,y)^* X] = \frac{1}{(2\pi)^{1/2}} \langle U(x,y)\psi | \phi \rangle_{\mathfrak{H}} = \frac{1}{(2\pi)^{1/2}} \int_{\mathbb{R}} e^{ix[\xi - (y/2)]} \overline{\psi(\xi - y)} \phi(\xi) d\xi.$$

Thus,

$$\begin{aligned}(\mathcal{W}Q \vee I_{\mathfrak{H}}(X))(x,y) &= \frac{1}{(2\pi)^{1/2}} \langle U(x,y)\psi | Q\phi \rangle_{\mathfrak{H}} = \frac{1}{(2\pi)^{1/2}} \int_{\mathbb{R}} e^{ix[\xi - (y/2)]} \overline{\psi(\xi - y)} \xi \phi(\xi) d\xi \\ &= \left(-i \frac{\partial}{\partial x} + \frac{y}{2} \right) \\ &\quad \times \left[\frac{1}{(2\pi)^{1/2}} \int_{\mathbb{R}} e^{ix[\xi - (y/2)]} \overline{\psi(\xi - y)} \phi(\xi) d\xi \right],\end{aligned}$$

implying

$$(\mathcal{W}Q \vee I_{\mathfrak{H}}(X))(x,y) = \left(-i \frac{\partial}{\partial x} + \frac{y}{2} \right) (\mathcal{W}X)(x,y).$$

Extending by linearity on appropriate domains, we get

$$\mathcal{W}Q \vee I_{\mathfrak{H}} \mathcal{W}^{-1} = -i \frac{\partial}{\partial x} + \frac{y}{2} = Q_1.$$

Next,

$$(\mathcal{W}P \vee I_{\mathfrak{H}}(X))(x,y) = \frac{1}{(2\pi)^{1/2}} \langle U(x,y)\psi | P\phi \rangle_{\mathfrak{H}} = \frac{1}{(2\pi)^{1/2}} \int_{\mathbb{R}} e^{ix[\xi - (y/2)]} \overline{\psi(\xi - y)} \left(-i \frac{\partial}{\partial \xi} \right) \phi(\xi) d\xi.$$

Now,

$$\begin{aligned}-i \frac{\partial}{\partial \xi} [e^{ix[\xi - (y/2)]} \overline{\psi(\xi - y)} \phi(\xi)] &= x e^{ix[\xi - (y/2)]} \overline{\psi(\xi - y)} \phi(\xi) + e^{ix[\xi - (y/2)]} \left(-i \frac{\partial}{\partial \xi} \right) \overline{\psi(\xi - y)} \phi(\xi) \\ &\quad + e^{ix[\xi - (y/2)]} \overline{\psi(\xi - y)} \left(-i \frac{\partial}{\partial \xi} \right) \phi(\xi).\end{aligned}$$

Integrating both sides of this equation with respect to ξ from $-\infty$ to ∞ and noting that $\psi(\xi)$, $\phi(\xi) \to 0$ as $\xi \to \pm\infty$, and $(\partial/\partial\xi)\psi(\xi - y) = -(\partial/\partial y)\psi(\xi - y)$, we get

$$0 = \frac{x}{(2\pi)^{1/2}} \int_{\mathbb{R}} e^{ix[\xi-(y/2)]} \overline{\psi(\xi-y)}\, \phi(\xi) + \frac{1}{(2\pi)^{1/2}} \int_{\mathbb{R}} e^{ix[\xi-(y/2)]} \left(i \frac{\partial}{\partial y} \right) \overline{\psi(\xi-y)}\, \phi(\xi)$$
$$+ \frac{1}{(2\pi)^{1/2}} \int_{\mathbb{R}} e^{ix[\xi-(y/2)]} \overline{\psi(\xi-y)} \left(- i \frac{\partial}{\partial \xi} \right) \phi(\xi).$$

Thus,

$$(\mathcal{W}P \vee I_{\mathfrak{H}}(X))(x,y) = \left(- i \frac{\partial}{\partial y} - \frac{x}{2} \right) (\mathcal{W}X)(x,y),$$

and again, extending by linearity on appropriate domains we get

$$\mathcal{W}P \vee I_{\mathfrak{H}} \mathcal{W}^{-1} = - i \frac{\partial}{\partial y} - \frac{x}{2} = P_1.$$

Proof of (5.17)–(5.19)

Since the vectors Ψ_{jk}, $j,k=0,1,2,\ldots,\infty$, form a basis of $\tilde{\mathfrak{H}}[=L^2(\mathbb{R}^2, \mathrm{d}x\, \mathrm{d}y)]$, we may write

$$U_1(x,y)\Phi_\beta = \sum_{i=0}^{\infty} \lambda_i^{1/2} U_1(x,y)\Psi_{ii} = \sum_{i,j,k=0}^{\infty} \lambda_i^{1/2} \langle \Psi_{jk} | U_1(x,y)\Psi_{ii} \rangle_{\tilde{\mathfrak{H}}} \Psi_{jk}.$$

Now, using the isometry $\mathcal{W}\phi_{jk} = \mathcal{W}(|\phi_j\rangle\langle\phi_k|) = \Psi_{jk}$ [see (5.8) and (5.12)], the first relation in (5.14) and the fact that the vectors ϕ_i, $i=0,1,2,\ldots,\infty$, form an orthonormal basis of $\mathfrak{H}$, we obtain

$$\langle \Psi_{jk} | U_1(x,y)\Psi_{ii} \rangle_{\tilde{\mathfrak{H}}} = \mathrm{Tr}[|\phi_k\rangle\langle\phi_j| U(x,y) |\phi_i\rangle\langle\phi_i|] = \langle \phi_j | U(x,y)\phi_i \rangle \delta_{ik} = (2\pi)^{1/2} \overline{\Psi_{ji}(x,y)}\, \delta_{ik},$$

the second equality following from (5.10). Thus,

$$U_1(x,y)\Phi_\beta = (2\pi)^{1/2} \sum_{i,j=0}^{\infty} \lambda_i^{1/2} \overline{\Psi_{ji}(x,y)} \Psi_{ji}. \tag{A6}$$

Similarly,

$$U_1(x,y)^* \Phi_\beta = (2\pi)^{1/2} \sum_{i,j=0}^{\infty} \lambda_j^{1/2} \Psi_{ij}(x,y)\Psi_{ji} = (2\pi)^{1/2} \sum_{i,j=0}^{\infty} \lambda_j^{1/2} \Psi_{ji}(x,y)\Psi_{ij}. \tag{A7}$$

Next, applying the operator S_β to both sides of (A6) and taking account of the fact that this operator is antilinear, we get

$$S_\beta[U_1(x,y)\Phi_\beta] = U_1(x,y)^* \Phi_\beta = (2\pi)^{1/2} \sum_{i,j=0}^{\infty} \lambda_i^{1/2} \Psi_{ji}(x,y) S_\beta \Psi_{ji}.$$

Comparing this equation with (A7) we immediately see that

$$S_\beta \Psi_{ji} = \left[\frac{\lambda_j}{\lambda_i} \right]^{1/2} \psi_{ij},$$

from which (5.17)–(5.19) follow directly.

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Reconstruction of universal Drinfeld twists from representations

Christian Blohmann
Department of Mathematics, University of California, Berkeley, California 94720-3840
International University Bremen, School of Engineering and Science, Campus Ring 1, 28759 Bremen, Germany

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Universal Drinfeld twists are inner automorphisms which relate the coproduct of a quantum enveloping algebra to the coproduct of the undeformed enveloping algebra. Even though they govern the deformation theory of classical symmetries and have appeared in numerous applications, no twist for a semisimple quantum enveloping algebra has ever been computed. It is argued that universal twists can be reconstructed from their well-known representations. A method to reconstruct an arbitrary element of the enveloping algebra from its irreducible representations is developed. For the twist this yields an algebra valued generating function to all orders in the deformation parameter, expressed by a combination of basic and ordinary hypergeometric functions. It is shown how the generating function can be expanded to the formal power series of the twist. An explicit expression for the universal twist of su(2) is given up to third order. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1901344]

I. INTRODUCTION

Quantum enveloping algebras are formal deformations of the enveloping Hopf algebras of Lie algebras.[1] While the notion of quantum enveloping algebras is very general, comprising arbitrary deformations, the most famous examples are the Drinfeld–Jimbo deformations[2,3] which act as natural symmetry structures on quantum spaces.[4–6] Drinfeld observed that every quantum enveloping algebra is related to the corresponding undeformed enveloping algebra by an inner automorphism which he called universal twist[7] and which now bears his name. Given the universal Drinfeld twist one can reconstruct the corresponding quantum enveloping algebra up to isomorphism. In this sense, the twist contains all information on the quantum deformation of a classical symmetry.[8]

Due to their pivotal role for the deformation theory of symmetries, universal Drinfeld twists have found numerous important applications beyond the structure theory of quantum enveloping algebras, such as to quantum statistics on quantum spaces,[9] quantum spin chains,[10,11] noncommutative quantum field theory,[12] or to algebraic geometry,[13] just to name a few recent examples. Our original motivation was the observation that certain twists yield a covariant realization of quantum spaces by a star product[14,15] within the framework of deformation quantization.[16] Such a description of noncommutative spaces by formal deformations of algebras[17] has appeared naturally in the context of string theory,[18] the construction of gauge theories on noncommutative spaces,[19,20] and the subsequent development of noncommutatvie quantum field theories. (For reviews of noncommutative field theories see Refs. 21 and 22.)

The noncommutative geometry on which so far most noncommutative quantum field theories have been constructed is defined by constant commutators of the space–time observables. Such a noncommutativity breaks Lorentz symmetry, which had to be expected because the constant commutator can be viewed as due to a constant background field, in string theory a constant *B*-field on a D-brane. It was hoped that a small noncommutativity would lead to an equally small violation of Lorentz symmetry. However, on the level of regularization of loop diagrams an

interdependence of ultraviolet and infrared cutoff scales appears[23,24] which seems to put even large scale Lorentz symmetry and weakened notions of locality of noncommutative quantum field theory into doubt,[25] indicating that the breaking of symmetries is not under good control—at least for the case of constant noncommutativity. These serious deficiencies seem to be reason enough to reconsider such deformations, for which the symmetry structure can be deformed together with the space, so that covariance is preserved. That is, quantum spaces[4–6] which carry a covariant representation of the Drinfeld–Jimbo deformation[2,3] of the enveloping symmetry algebra. Three particularly important quantum spaces, the quantum plane, quantum Euclidean 4-space, and quantum Minkowski space, have been shown to be realizable as deformation quantization[8,14] by universal Drinfeld twists.[15] (For more information on the relation between quantum groups and deformation quantization we refer the reader to Ref. 26.)

While the quantum enveloping algebra can be reconstructed rather easily given the universal Drinfeld twist, there is no general soution for the inverse problem of calculating the Drinfeld twist for a given quantum deformation. The existence of twists is proved by homological methods which are inherently nonconstructive. To our best knowledge, no universal Drinfeld twist for the Drinfeld–Jimbo deformation of a semisimple Lie algebra has ever been computed successfully, not even for the simplest possible case of su_2. (In Refs. 27 and 28 the nonsemisimple case of the Heisenberg algebra was studied.) It could be argued that the universal twist is more or less the square root of the universal $\mathcal{R}$-matrix, so that Drinfeld's ingenious but simple construction of the $\mathcal{R}$-matrix by the dual pairing of the Borel–Hopf subalgebras might be used. For the case of triangular deformations this reasoning appears to lead, indeed, to a method to construct the twist.[29] For the nontriangular Drinfeld–Jimbo deformations, however, this argument falls short, as is confirmed by the complexity of the expressions derived in Ref. 30. But even though there are no closed form expressions or simple constructions for the twist, one might expect that a brute force calculation by means of a computer algebra system should be possible up to an order of the perturbation parameter high enough for all reasonable applications. However, it turns out that the naive attempt of an algebraic order by order calculation quickly runs into overwhelming combinatorial problems, as it was described in Ref. 30 where the authors did not go beyond the second order.

A closer inspection of the brute force approach reveals, first, that the number of operations which must be carried out increases at least exponentially with the order of the perturbation parameter, so the algorithm is certainly nonpolynomial. Second, the results expressed in terms of the Poincaré–Birkhoff–Witt basis of the enveloping algebra are extremely lengthy and do not appear to provide any structural insight. Third, it is unclear how to implement the algorithm such that it yields the particular twist which realizes the star product of quantum spaces. In conclusion, it is fair to say that the calculation of universal Drinfeld twists turns out to be a computational problem in any respect.

While little is known about the calculation of universal twists in the enveloping algebra, their representations are well understood and have been computed explicitly. They are essentially given by a contraction of deformed and undeformed Clebsch–Gordan coefficients as it was first observed in Ref. 31. For the Drinfeld–Jimbo q-deformation the Clebsch–Gordan coefficients are known explicitly, so we obtain the representations of the twist in a closed form, expressed by basic and ordinary hypergeometric functions. The approach to the calculation of universal twists presented here is to reconstruct the twists from their representations. The obvious advantage of this approach is that, rather than starting with algebraic calculations from scratch, it builds on the computational effort which has gone into the calculation of q-Clebsch–Gordan coefficients. The explicit calculations in this paper are carried out for $\mathcal{U}_q(\mathrm{su}_2)$ although the methods will be seen to be generic.

We will proceed as follows: In order to make this paper reasonably self-contained we will start in Sec. II with a short introduction to universal Drinfeld twists, giving some basic results which will be referred to in the following. Moreover, we briefly explain why universal twists appear naturally in the context of star products. In Sec. III we will develop a method to reconstruct an element in the enveloping algebra from its irreducible representations. From Lie theory it is clear that in the semisimple case the representations determine the algebra element uniquely. But how

do we actually compute it? The key to developing a constructive method is the choice of a suitable basis of $\mathcal{U}_q(\mathrm{su}_2)$. We will choose the basis of tensor operators because the matrix elements satisfy useful orthogonality relations, which then lead to the desired reconstruction method. The results are given in Proposition 2 and Eq. (27). In Sec. IV we apply the reconstruction method to the representations of the universal Drinfeld twist. This leads to the main result presented here, a formula for the the universal Drinfeld twist, given in Eq. (46) by an algebra-valued generating function in $q=e^{\hbar}$. In order to obtain the twist to each order in the perturbation parameter $\hbar$, we yet need to expand the generating function in powers of $\hbar$. Surprisingly, the problem of perturbative expansion of basic hypergeometric functions has recieved little attention in the literature. In particular, no closed formulas for such expansions have been derived as yet. While a thorough study of this problem is beyond the scope of this paper, we present the first few steps in this direction which suffice to make the order of order expansion of the generating function of the twist accessible to efficient computer algebra calculations. This is exemplified in Eq. (59) where the universal twist of $\mathcal{U}_\hbar(\mathrm{su}_2)$ was computed up to third order. In Sec. V we concludingly assess the computational value of the generating function of the twist and indicate how the approach presented here will be naturally continued.

II. BRIEF INTRODUCTION TO DRINFELD TWISTS

For the reader's convenience we briefly review how Drinfeld twists appear naturally in the study of formal deformations of algebras and Hopf algebras. The approach and the results described here are essentially due to Gerstenhaber[17] and Drinfeld.[1,7] The formal perturbation parameter is $\hbar$, the completion of a complex vector space or algebra A with respect to the $\hbar$-adic topology by formal power series is denoted as usual by $A[[\hbar]]$.

An $\hbar$-adic algebra A' is called a deformation of an algebra A if $A'/\hbar A'$ and A are isomorphic as algebras. Analogously, an $\hbar$-adic Hopf algebra H' is called a deformation of a Hopf algebra H if $H'/\hbar H'$ and H are isomorphic as Hopf algebras. Recall, that $\mathcal{U}(\mathfrak{g})$ is a Hopf algebra with the canonical Lie–Hopf structure defined on the generators $g\in\mathfrak{g}$ by the coproduct $\Delta(g)=g\otimes 1+1\otimes g$, counit $\varepsilon(g)=0$, and antipode $S(g)=-g$. The Drinfeld–Jimbo algebra $\mathcal{U}_\hbar(\mathfrak{g})$ is a deformation of this Hopf algebra $\mathcal{U}(\mathfrak{g})$. This can be seen by developing the commutation relations and the Hopf structure of $\mathcal{U}_\hbar(\mathfrak{g})$ as formal power series in $\hbar$ and keeping only the zeroth order terms, which yields the commutation relations and the Lie–Hopf structure of $\mathcal{U}(\mathfrak{g})$.

Gerstenhaber has shown[17] that whenever the second Hochschild cohomology of A with coefficients in A is zero, $H^2(A,A)=0$, then all deformations of A are trivial up to isomorphism. That is, any deformation A' of A is isomorphic to the $\hbar$-adic completion of the undeformed algebra, $A'\cong A[[\hbar]]$. Algebras with this property are called rigid. The second Whitehead lemma states that the second Lie algebra cohomology of a semisimple Lie algebra $\mathfrak{g}$ and, hence, the second Hochschild cohomology of its enveloping algebra is zero. Therefore, the enveloping algebra $\mathcal{U}(\mathfrak{g})$ of a semisimple Lie algebra $\mathfrak{g}$ is rigid. In particular, there is an isomorphism of algebras $\alpha:\mathcal{U}_\hbar(\mathfrak{g})\to\mathcal{U}(\mathfrak{g})[[\hbar]]$, by which the the Hopf structure Δ', ε', S' of $\mathcal{U}_\hbar(\mathfrak{g})$ can be transfered to $\mathcal{U}(\mathfrak{g})[[\hbar]]$,

$$\Delta_\hbar := (\alpha\otimes\alpha)\circ\Delta'\circ\alpha^{-1},\quad \varepsilon_\hbar := \varepsilon'\circ\alpha^{-1},\quad S_\hbar := \alpha\circ S'\circ\alpha^{-1}, \tag{1}$$

such that α becomes an isomorphism of Hopf algebras from $\mathcal{U}_\hbar(\mathfrak{g})$ to $\mathcal{U}(\mathfrak{g})[[\hbar]]$ with this deformed Hopf structure. Let α' be another such isomorphism and $\Delta'_\hbar$, $\varepsilon'_\hbar$, $S'_\hbar$ be defined as in Eq. (1) with α' instead of α. Then α' is an isomorphism of Hopf algebras from $\mathcal{U}_\hbar(\mathfrak{g})$ to $\mathcal{U}(\mathfrak{g})[[\hbar]]$ with the primed Hopf structure,

$$(\mathcal{U}(\mathfrak{g})[[\hbar]],\Delta_\hbar,\varepsilon_\hbar,S_\hbar)\xleftarrow{\alpha}\mathcal{U}_\hbar(\mathfrak{g})\xrightarrow{\alpha'}(\mathcal{U}(\mathfrak{g})[[\hbar]],\Delta'_\hbar,\varepsilon'_\hbar,S'_\hbar), \tag{2}$$

hence, $\alpha'\circ\alpha^{-1}$ is an isomorphism of Hopf algebras. We conclude that, while the Hopf structure (1) may depend on the isomorphism α, it is unique up to an isomorphism of Hopf algebras.

As a consequence of the first Whitehead lemma, the first Hochschild cohomology of the enveloping algebra $\mathcal{U}(\mathfrak{g})$ of a semisimple Lie algebra is zero. This implies, that the two homomorphisms Δ and $\Delta_\hbar$ from $\mathcal{U}(\mathfrak{g})[[\hbar]]$ to $(\mathcal{U}(\mathfrak{g})\otimes\mathcal{U}(\mathfrak{g}))[[\hbar]]$ with $\Delta_\hbar=\Delta+\mathcal{O}(\hbar)$ are related by an inner automorphism, as it was observed by Drinfeld.[1,7]

Theorem 1 (Drinfeld): *Let $\mathfrak{g}$ be a semisimple Lie algebra, and let $\Delta_\hbar$ be defined as in Eq. (1). Then there is an invertible element $\mathcal{F}\in(\mathcal{U}(\mathfrak{g})\otimes\mathcal{U}(\mathfrak{g}))[[\hbar]]$ such that $\Delta_\hbar(g)=\mathcal{F}\Delta(g)\mathcal{F}^{-1}$, which is called a Drinfeld twist from Δ to $\Delta_\hbar$.*

It can be shown that such a Drinfeld twist not only relates the deformed and undeformed coproducts but also the counits and antipodes. Hence, a universal Drinfeld twist uniquely determines the corresponding quantum enveloping algebra. In that sense the twist contains the entire structural information on a quantum deformation of an enveloping algebra. The twist of Theorem 1 is not unique. For a given quantum enveloping algebra any two twists are related by a noncommutative 2-coboundary in the sense of Ref. 32.

Drinfeld has shown, that the isomorphism of $\mathcal{U}(\mathfrak{g})[[\hbar]]$ and $\mathcal{U}_\hbar(\mathfrak{g})$ can be chosen to leave a given Cartan subalgebra invariant.

Theorem 2 (Drinfeld,[1] Proposition 4.3): *Let $\mathfrak{g}$ be a semisimple Lie algebra and $\mathfrak{h}\subset\mathfrak{g}$ a Cartan subalgebra. Then there exists an isomorphism of $\hbar$-adic algebras $\alpha:\mathcal{U}_\hbar(\mathfrak{g})\to\mathcal{U}(\mathfrak{g})[[\hbar]]$ such that $\alpha=\mathrm{id}+\mathcal{O}(\hbar)$ and $\alpha|_\mathfrak{h}=\mathrm{id}_\mathfrak{h}$.*

The important consequence of this theorem for representation theory is that weight vectors and weight spaces of representations of the deformed and underformed algebras can be identified. While in this sense, the irreducible representations of quantum alebras are equivalent to the usual representations, the nonequivalent coproducts on the enveloping algebra and its quantum deformation lead to different tensor representation in the deformed and undeformed case. For Drinfeld–Jimbo deformations $\mathcal{U}_\hbar(\mathrm{su}_2)$, which are the Hopf duals of quantum groups, the reduction of tensor representations are given by q-deformed Clebsch–Gordan coefficients. As the deformed and undeformed coproducts are related by a Drinfeld twist, it was quickly realized[31] that the representations of Drinfeld twists ought to be given by a combination of deformed and undeformed Clebsch–Gordan coefficients. Indeed, one can rigorously prove the following proposition.[15]

Proposition 1: *There is a universal Drinfeld twist $\mathcal{F}$ from $\mathcal{U}(\mathrm{su}_2)$ to $\mathcal{U}_\hbar(\mathrm{su}_2)$, the inverse of which has the matrix elements*

$$\langle j_1,m_1';j_2,m_2'|\mathcal{F}^{-1}|j_1,m_1;j_2,m_2\rangle=\sum_{j,m}\left(\begin{array}{cc|c} j_1 & j_2 & j\\ m_1' & m_2' & m\end{array}\right)_q\left(\begin{array}{cc|c} j_1 & j_2 & j\\ m_1 & m_2 & m\end{array}\right) \tag{3}$$

in an irreducible representation of $\mathcal{U}(\mathrm{su}_2)\otimes\mathcal{U}(\mathrm{su}_2)$ with weights j_1, j_2 and basis $|j_1,m_1;j_2,m_2\rangle := |j_1,m_1\rangle\otimes|j_2,m_2\rangle$, where the expressions in parentheses denote the q-deformed and undeformed Clebsch–Gordan coefficients.

Here, we gave the formula for the representations of the inverse of the twist, because the inverse realizes the covariant star product of the corresponding quantum space: Recall that the action of an enveloping algebra $\mathcal{U}(\mathfrak{g})$ on an algebra $\mathcal{X}$ is called covariant if for all x, $y\in\mathcal{X}$ and $g\in\mathcal{U}(\mathfrak{g})$,

$$g\triangleright(xy)=(g_{(1)}\triangleright x)(g_{(2)}\triangleright y), \tag{4}$$

using the Sweedler notation $g_{(1)}\otimes g_{(2)}\equiv\Delta_\hbar(g)$ for the coproduct. In mathematical terminology $\mathcal{X}$ is called a module algebra. For the undeformed coproduct Eq. (4) simply means that the elements of the Lie algebra $\mathfrak{g}\subset\mathcal{U}(\mathfrak{g})$ act as derivations on $\mathcal{X}$. A quantum space, which is by definition a module algebra of the quantum deformation $\mathcal{U}_\hbar(\mathfrak{g})$, is realized by a star product on a function algebra in a covariant manner only if the analogous condition

$$g\triangleright(x\star y)=(g_{(1_\hbar)}\triangleright x)\star(g_{(2_\hbar)}\triangleright y) \tag{5}$$

holds, where $g_{(1_\hbar)}\otimes g_{(2_\hbar)}\equiv\Delta_\hbar(g)$ is the Sweedler notation for the deformed coproduct. If we define the star product map by

$$x \star y := (\mathcal{F}^{-1}_{[1]} \triangleright x)(\mathcal{F}^{-1}_{[2]} \triangleright y), \tag{6}$$

where we use the Sweedler-type notation $\mathcal{F}^{-1}_{[1]} \otimes \mathcal{F}^{-1}_{[2]} \equiv \mathcal{F}^{-1}$, covariance condition (5) is satisfied because $\Delta_\hbar(g) = \mathcal{F}\Delta(g)\mathcal{F}^{-1}$. But are there twists for which Eq. (6) also defines an associative product, thus realizing the algebra of a quantum space? It turns out that the twist of Proposition 1 realizes the quantum plane and, essentially, also quantum Euclidean 4-space, and quantum Minkowski space.[15]

III. THE RECONSTRUCTION METHOD

A. The tensor operator basis

We want to find a method to reconstruct elements of the enveloping algebra $\mathcal{U}(\mathrm{su}_2)$ from their irreducible representations. Consider the Cartan–Weyl basis $\{E, H, F\}$ of su_2 with commutation relations

$$[H,E] = 2E, \quad [H,F] = -2F, \quad [E,F] = H, \tag{7}$$

the compact real form being given by the $*$-structure $E^* = F$, $H^* = H$, $F^* = E$. For our purposes the usual Poincare–Birkhoff–Witt basis of ordered monomials of the generators

$$\mathcal{B}_{\mathrm{PBW}} = \{E^i H^j F^k | i,j,k \in \mathbb{N}_0\} \tag{8}$$

turns out to be not particularly convenient. The irreducible representations of the ordered monomials do not satisfy any obvious orthogonality relations which would allow us to draw immediate conclusions from the representations of a given algebra element to its coefficients with respect to this basis. Recall that for each half-integer weight $j \in \frac{1}{2}\mathbb{N}_0$ there is one irreducible unitary representation of $\mathcal{U}(\mathrm{su}_2)$ defined on the orthonormal weight-j (or spin-j) basis $\{|j,m\rangle, m = -j, -j+1, \ldots, j\}$ by

$$E|j,m\rangle = \sqrt{(j+m+1)(j-m)}\,|j,m+1\rangle,$$

$$F|j,m\rangle = \sqrt{(j+m)(j-m+1)}\,|j,m-1\rangle,$$

$$H|j,m\rangle = 2m|j,m\rangle. \tag{9}$$

The structure homomorphism $\rho^j : \mathcal{U}(\mathrm{su}_2) \to \mathrm{End}(\mathbb{C}^{2j+1})$ is given by the matrix elements, $\rho^j(g)^{m'}{}_m := \langle j,m'|g|j,m\rangle$. Since the Lie algebra su_2 is simple, any representation of $\mathcal{U}(\mathrm{su}_2)$ can be decomposed into a direct sum of irreducible subrepresentations, each of which is isomorphic to a representation given by (9). This is in particular true for the adjoint action of $\mathcal{U}(\mathrm{su}_2)$ on itself which is defined on the generators as

$$\mathrm{ad}\, g \triangleright u := [g,u], \quad g \in \mathrm{su}_2 \subset \mathcal{U}(\mathrm{su}_2), \quad u \in \mathcal{U}(\mathrm{su}_2). \tag{10}$$

Let $\{T^j_m \in \mathcal{U}(\mathrm{su}_2) \,|\, m = -j, \ldots, j\}$ be a weight basis of a weight-j subrepresentation of the adjoint representation, that is,

$$[g, T^j_m] = \sum_{m'} T^j_{m'} \rho^j(g)^{m'}{}_m \equiv \sum_{m'} T^j_{m'} \langle j,m'|g|j,m\rangle \tag{11}$$

for all $g \in \mathrm{su}_2$. Such a basis $\{T^j_m\}$ is called a weight-j tensor operator of su_2. The set of all weight-0 operators is the center of $\mathcal{U}(\mathrm{su}_2)$. As commutative algebra, the center is generated by the canonical quadratic Casimir element $C := 2\Sigma_{ij} g_i g_j K^{ij}$, where $\{g_i\}$ is a basis of the Lie algebra, K^{ij} is the inverse of the Killing metric $K_{ij} := \mathrm{tr}(\mathrm{ad}\, g_i\, \mathrm{ad}\, g_j)$, and where the factor 2 was insterted for convenience. In the Cartan–Weyl basis we obtain

$$C = \tfrac{1}{2}EF + \tfrac{1}{2}FE + \tfrac{1}{4}H^2 = EF + \tfrac{1}{4}H(H-2), \tag{12}$$

such that the polynomial algebra $\mathbb{C}[C]$ is the center of $\mathcal{U}(\mathrm{su}_2)$. The representations of the Casimir element,

$$C|j,m\rangle = j(j+1)|j,m\rangle, \tag{13}$$

show that C is the ususal square of angular momentum.

By definition, T^j_j is the highest weight vector of a weight-j subrepresentation of the adjoint representation, so $(\mathrm{ad}\,E)\triangleright T^j_j \equiv [E,T^j_j]=0$ and $(\mathrm{ad}\,C)\triangleright T^j_j = j(j+1)T^j_j$. From these two equalities it follows, that $T^j_j = zE^j$, where z is some element of the center. If we pick z from the number field we get the tensor operators

$$T^J_J := \alpha E^J, \quad \alpha \in \mathbb{C}, \tag{14}$$

from which all other tensor operators can be obtained by multiplication by a central element. Here α is a normalization constant, which will later be chosen for convenience. From now on we denote by T^J_M always the tensor operator which is generated by αE^J. We use capital letters for the indices in order to allow in the formulas which we will derive below for a clear disctinction of the weights pertaining to the adjoint action from those pertaining to matrix representations. The fact that, as module with respect to the adjoint action, $\mathcal{U}(\mathrm{su}_2)$ can be completely decomposed into irreducible submodules implies that

$$\mathcal{B}_{\mathrm{tensor}} = \{C^k T^J_M | k,J \in \mathbb{N}_0, M = -J, -J+1, \ldots, J\} \tag{15}$$

is a basis of $\mathcal{U}(\mathrm{su}_2)$, which we will call the tensor basis. The fact that (15) is a basis of $\mathcal{U}(\mathrm{su}_2)$ means that the tensor operators are a basis of $\mathcal{U}(\mathrm{su}_2)$ as free module over its center. Thus, every element $a \in \mathcal{U}(\mathrm{su}_2)$ can be written uniquely as

$$a = \sum_{J,M} a^J_M T^J_M, \quad a^J_M \in \mathbb{C}[C], \tag{16}$$

where the sum runs over a finite subset of all allowed integer values of J and M. Reconstructing the element a from its representations now amounts to finding the polynomials a^J_M.

B. The reconstruction method

Let us compute the irreducible representations of Eq. (16). First, we consider the central coefficients a^J_M. Since a^J_M is a polynomial in the Casimir, the matrix element is a polynomial of the weight j of the representation,

$$\langle j,m|a^J_M|j,m\rangle =: a^J_M(j) \in \mathbb{C}[j]. \tag{17}$$

Due to Eq. (13) this polynomial satisfies

$$a^J_M = a^J_M(-j-1), \tag{18}$$

since it is actually a polynomial in $j(j+1)$ or, equivalently, a quadratic polynomial in $j+\frac{1}{2}$. Conversely, given a polynomial $p(j) \in \mathbb{C}[j]$ which satisfies $p(j)=p(-j-1)$ there exists a unique polynomial in the Casimir which has $p(j)$ as its matrix elements. For an intuitive notation we will denote this polynomial by $p(\hat{j}) \in \mathbb{C}[C]$, such that its defining equation takes the suggestive form

$$\langle j,m|p(\hat{j})|j,m\rangle = p(j). \tag{19}$$

The map $p(j) \mapsto p(\hat{j})$ could be viewed as substitution

$$j \mapsto \hat{j} = \tfrac{1}{2}(\sqrt{4C+1} - 1), \tag{20}$$

where the relation $p(j)=p(-j-1)$ guarantees that the square roots drop out such that $p(\hat{j})$ is a polynomial in C only. We emphasize that we do not add such a square root of the Casimir to the algebra, though. We view $p(\hat{j})$ merely as a suggestive notation for the element of the center which is uniquely defined by Eq. (19).

The matrix elements of the tensor operators are given by the Wigner–Eckhart theorem,

$$\langle j,m'|T^J_M|j,m\rangle = \langle j\|T^J\|j\rangle \left(\begin{array}{cc|c} J & j & j \\ M & m & m' \end{array} \right), \tag{21}$$

where the reduced matrix element $\langle j\|T^J\|j\rangle$ does not depend on m, m', or M, and where the expression in parentheses denotes the Clebsch–Gordan coeffient. The explicit form and some properties of Clebsch–Gordan coefficients and their q-deformations can be found for example in Ref. 33. The reduced matrix elements will be computed below.

The irreducible representations of Eq. (16) now take the form

$$\langle j,m'|a|j,m\rangle = \sum_{J,M} a^J_M(j)\langle j\|T^J\|j\rangle \left(\begin{array}{cc|c} J & j & j \\ M & m & m' \end{array} \right). \tag{22}$$

The main advantage of using the tensor basis (15) instead of the Poincaré–Birkhoff–Witt basis (8) is the fact, that the Clebsch–Gordan coefficients satisfy orthogonality relations which can be used in order to solve Eq. (22) for $a^J_M(j)$. Using the well-known orthogonality relation

$$\sum_{m,m'} \left(\begin{array}{cc|c} J & j & j \\ M & m & m' \end{array} \right) \left(\begin{array}{cc|c} J' & j & j \\ M' & m & m' \end{array} \right) = \frac{2j+1}{2J+1} \delta_{JJ'} \delta_{MM'} \tag{23}$$

we thus arrive at the following.

Proposition 2: *Let $a \in \mathcal{U}(\mathrm{su}_2)$ be an element of the enveloping algebra with matrix elements $\langle j,m'|a|j,m\rangle$ with respect to the irreducible representations defined in Eqs. (9). Let $T^J_M \in \mathcal{U}(\mathrm{su}_2)$ be the minimal degree tensor operators generated by $T^J_J \sim E^J$ and $\langle j\|T^J\|j\rangle$ their reduced matrix elements. Then we have the following*:

(i) *For all integers $J \geqslant 0$ and $M, |M| \leqslant J$ the expression*

$$a^J_M(j) := \frac{(2J+1)}{(2j+1)\langle j\|T^J\|j\rangle} \sum_{m,m'} \left(\begin{array}{cc|c} J & j & j \\ M & m & m' \end{array} \right) \langle j,m'|a|j,m\rangle \tag{24}$$

defines a polynomial in j which is nonzero for only a finite number of values of J and M.

(ii) *The polynomials $a^J_M(j)$ are quadratic in $j+\frac{1}{2}$, the substitution*

$$(j_1 + \tfrac{1}{2})^2 \mapsto C + \tfrac{1}{4} \tag{25}$$

yielding polynomials in the Casimir element C which are denoted by $a^J_M(\hat{j})$.

(iii) *The element a can be written as*

$$a = \sum_{J,M} a^J_M(\hat{j}) T^J_M. \tag{26}$$

This reconstruction method can be readily generalized to the tensor product $\mathcal{U}(\mathrm{su}_2) \otimes \mathcal{U}(\mathrm{su}_2)$. Let $a \in \mathcal{U}(\mathrm{su}_2) \otimes \mathcal{U}(\mathrm{su}_2)$ be an element of the tensor product, let $\langle j_1, m_1'; j_2, m_2'|a|j_1, m_1; j_2, m_2\rangle$ denote its matrix elements with respect to irreducibles representation of each tensor factor. First we need to calculate

$$a^{J_1J_2}_{M_1M_2}(j_1,j_2) := \frac{(2J_1+1)(2J_2+1)}{(2j_1+1)(2j_2+1)\langle j_1\|T^{J_1}\|j_1\rangle\langle j_2\|T^{J_2}\|j_2\rangle}\sum_{\substack{m_1,m_1'\\ m_2,m_2'}}\left(\begin{array}{cc|c} J_1 & j_1 & j_1\\ M_1 & m_1 & m_1'\end{array}\right)\left(\begin{array}{cc|c} J_2 & j_2 & j_2\\ M_2 & m_2 & m_2'\end{array}\right)$$

$$\times\langle j_1,m_1';j_2,m_2'|a|j_1,m_1;j_2,m_2\rangle, \tag{27}$$

which defines polynomials, which are quadratic in $\left(j_1+\frac{1}{2}\right)$ and $\left(j_2+\frac{1}{2}\right)$. Then we substitute

$$(j_1+\tfrac{1}{2})^2\mapsto(C+\tfrac{1}{4})\otimes 1,\quad (j_2+\tfrac{1}{2})^2\mapsto 1\otimes(C+\tfrac{1}{4}) \tag{28}$$

in order to obtain the unique central elements

$$a^{J_1J_2}_{M_1M_2}(\hat{j}_1,\hat{j}_2)\in\mathbb{C}[C\otimes 1,1\otimes C], \tag{29}$$

the representations of which are given by the polynomials (27). Finally, reconstruct the element of the tensor algebra by

$$a=\sum_{\substack{J_1,M_1\\ J_2,M_2}} a^{J_1J_2}_{M_1M_2}(\hat{j}_1,\hat{j}_2)T^{J_1}_{M_1}\otimes T^{J_2}_{M_2}. \tag{30}$$

We will now apply this reconstruction method to the Drinfeld twist (3).

IV. RECONSTRUCTION OF THE UNIVERSAL DRINFELD TWIST

A. Calculation of the tensor basis

In order to obtain explicit formulas from the reconstruction method of Proposition 2 we need to calculate the tensor operators T^J_M in terms of the Poincaré–Birkhoff–Witt basis as well as the reduced matrix elements $\langle j\|T^J\|j\rangle$. We start with the reduced matrix elements.

From Eq. (9) we can derive the representation of powers of the generators

$$E^J|j,m\rangle=\sqrt{(-1)^J(j+m+1)_J(m-j)_J}|j,m+J\rangle,$$

$$F^J|j,m\rangle=\sqrt{(-1)^J(j-m+1)_J(-m-j)_J}|j,m-J\rangle, \tag{31}$$

where

$$(x)_J := (x)(x+1)\cdots(x+J-1) \tag{32}$$

denotes the Pochhammer symbol. From Eqs. (31) we obtain for the irreducible representations of the tensor operator (14) on the one hand,

$$\langle j,j|T^J_J|j,j-J\rangle=\langle j,j|\alpha E^J|j,j-J\rangle=\alpha\sqrt{\frac{(2j)!J!}{(2j-J)!}} \tag{33}$$

for $J\leqslant 2j$. On the other hand, we have due to the Wigner–Eckhart theorem (21),

$$\langle j,j|T^J_J|j,j-J\rangle=\langle j\|T^J\|j\rangle\left(\begin{array}{cc|c} J & j & j\\ J & j-J & j\end{array}\right)=\langle j\|T^J\|j\rangle\sqrt{\frac{(2j+1)!(2J)!}{(2j+J+1)!J!}}, \tag{34}$$

where we have inserted the explicit expression for the Clebsch–Gordan coefficient. We conclude that

$$\langle j\|T^J\|j\rangle=\alpha\sqrt{\frac{(2j+J+1)!J!J!}{(2j+1)(2j-J)!(2J)!}}. \tag{35}$$

For our purposes, it is convenient to choose the normalization constant α such that

$$\langle J \| T^J \| J \rangle = 1, \tag{36}$$

for which we must set

$$\alpha := \sqrt{\frac{(2J+1)!}{(3J+1)!J!}}. \tag{37}$$

From now on we will assume this choice of α, for which the value of the reduced matrix element (35) becomes

$$\langle j \| T^J \| j \rangle = \sqrt{\frac{(2J+1)(2j+J+1)!J!}{(2j+1)(3J+1)!(2j-J)!}}. \tag{38}$$

From the heighest weight vector T^J_J we obtain the weight basis by repeated action of the lowering operator $\mathrm{ad}\, F$. More precisely, from Eq. (31) we conclude that

$$T^J_M = [(-1)^{J-M}(J-M)!(-2J)_{J-M}]^{-1/2} (\mathrm{ad}\, F)^{J-M} \triangleright T^J_J = \sqrt{\frac{(2J+1)(J+M)!}{(3J+1)!J!(J-M)!}} (\mathrm{ad}\, F)^{J-M} \triangleright E^J \tag{39}$$

for $|M| \leqslant J$. The remaining computational problem for an explicit expression of T^j_m in terms of the Poincaré–Birkhoff–Witt basis is the lexicographic reordering of $(\mathrm{ad}\, F)^{J-M} \triangleright E^J$. Details of the computation are provided in Appendix A. As result we obtain

$$T^J_M = (-1)^{J+M} \sqrt{\frac{(2J+1)J!(J-M)!(J+M)!}{(3J+1)!}} \times \sum_{p=0}^{p \leqslant (J-M)/2} \frac{(-1)^p}{p!(p+M)!} E^{p+M} \binom{J+H-1}{J-M-2p} F^p \quad \text{for } M \geqslant 0, \tag{40a}$$

$$T^J_M = (-1)^{J-M} \sqrt{\frac{(2J+1)J!(J-M)!(J+M)!}{(3J+1)!}} \times \sum_{p=0}^{p \leqslant (J+M)/2} \frac{(-1)^p}{p!(p-M)!} E^{p} \binom{J+H-1}{J+M-2p} F^{p-M} \quad \text{for } M < 0, \tag{40b}$$

where the algebra valued binomial coefficient is defined by

$$\binom{X}{k} := \frac{(-1)^k (-X)_k}{k!}, \tag{41}$$

denoting a polynomial in X. For a complete expansion in terms of ordered monomials we yet must expand the binomials in powers of H,

$$\binom{J+H-1}{J \pm M - 2p} = \sum_{n=0}^{J \pm M - 2p} H^n \sum_{k=n}^{J-M \pm 2p} \frac{1}{k!} \binom{J-1}{J \pm M - 2p - k} s(k,n), \tag{42}$$

where $s(k,n)$ are Stirling numbers of the first kind.

B. The generating function for the Drinfeld twist

We will now apply the reconstruction method of Sec. III to the inverse of the universal Drinfeld twist $\mathcal{F}^{-1}$ of Proposition 1. Inserting the representations (3) of the twist into Eq. (27) the inverse twist can be expressed according to Eq. (30) as

$$\mathcal{F}^{-1}=\sum_{\substack{J_1,M_1\\J_2,M_2}}\frac{(2J_1+1)(2J_2+1)}{(2\hat{j}_1+1)(2\hat{j}_2+1)\langle\hat{j}_1\|T^{J_1}\|\hat{j}_1\rangle\langle\hat{j}_2\|T^{J_2}\|\hat{j}_2\rangle}\sum_{\substack{m_1,m_1'\\m_2,m_2'}}\begin{pmatrix}J_1 & \hat{j}_1 & \hat{j}_1\\ M_1 & m_1 & m_1'\end{pmatrix}\begin{pmatrix}J_2 & \hat{j}_2 & \hat{j}_2\\ M_2 & m_2 & m_2'\end{pmatrix}$$
$$\times\sum_{j,m}m_2\,m_2\begin{pmatrix}\hat{j}_1 & \hat{j}_2 & j\\ m_1' & m_2' & m\end{pmatrix}\begin{pmatrix}\hat{j}_1 & \hat{j}_2 & j\\ m_1 & m_2 & m\end{pmatrix}_q T^{J_1}_{M_1}\otimes T^{J_2}_{M_2}, \tag{43}$$

where we recall that the hats on $\hat{j}_1$ and $\hat{j}_2$ indicate that the coefficients of the tensor operators are polynomials in $C\otimes 1$ and $1\otimes C$ which we obtain after substitution (28). Equation (43) does in general not yield an element of $\mathcal{U}(\mathrm{su}_2)\otimes\mathcal{U}(\mathrm{su}_2)$ for any fixed value of q. It must be understood as algebra valued generating function in $q=\mathrm{e}^{\hbar}$ which produces in each order of $\hbar$ an element of $\mathcal{U}(\mathrm{su}_2)\otimes\mathcal{U}(\mathrm{su}_2)$ proper. An explicit expansion up to third order in $\hbar$ will be given in the next section.

Note that while the entire dependence on $\hbar$ is contained in the q-deformed Clebsch–Gordan coefficient, the arguments of the latter are contracted with the arguments of undeformed Clebsch–Gordan coefficients. We can confine the $\hbar$-dependence further by using the following identity for the Clebsch–Gordan coefficients which is derived in Appendix B:

$$\begin{pmatrix}J_1 & j_1 & j_1\\ M_1 & m_1 & m_1'\end{pmatrix}\begin{pmatrix}J_2 & j_2 & j_2\\ M_2 & m_2 & m_2'\end{pmatrix}\begin{pmatrix}j_1 & j_2 & j\\ m_1' & m_2' & m\end{pmatrix}$$
$$=\sum_{J,j'}\beta\begin{Bmatrix}J_1 & j_1 & j_1\\ J_2 & j_2 & j_2\\ J & j' & j\end{Bmatrix}\begin{pmatrix}J_1 & J_2 & J\\ M_1 & M_2 & M\end{pmatrix}\begin{pmatrix}j_1 & j_2 & j'\\ m_1 & m_2 & m'\end{pmatrix}\begin{pmatrix}J & j' & j\\ M & m' & m\end{pmatrix}, \tag{44}$$

where the expression in braces denotes the $9j$ symbol, the factor β is defined as

$$\beta:=\sqrt{(2J+1)(2j'+1)(2j_1+1)(2j_2+1)}, \tag{45}$$

and $m_1'=M_1+m_1$, $m_2'=M_2+m_1$, $M=M_1+M_2$, $m'=m_1+m_2$. Inserting Eq. (44) into Eq. (43) we obtain

$$\mathcal{F}^{-1}=\sum_{J_1,J_2,J}\sum_{j,j'}\frac{(2J_1+1)(2J_2+1)}{\langle\hat{j}_1\|T^{J_1}\|\hat{j}_1\rangle\langle\hat{j}_2\|T^{J_2}\|\hat{j}_2\rangle}\sqrt{\frac{(2J+1)(2j'+1)}{(2\hat{j}_1+1)(2\hat{j}_2+1)}}\begin{Bmatrix}J_1 & \hat{j}_1 & \hat{j}_1\\ J_2 & \hat{j}_2 & \hat{j}_2\\ J & j' & j\end{Bmatrix}$$
$$\times\sum_m\begin{pmatrix}J & j'\\ 0 & m\end{pmatrix}\begin{pmatrix}j\\ m\end{pmatrix}\sum_{m_1,m_2}\begin{pmatrix}\hat{j}_1 & \hat{j}_2 & j'\\ m_1 & m_2 & m\end{pmatrix}\begin{pmatrix}\hat{j}_1 & \hat{j}_2 & j\\ m_1 & m_2 & m\end{pmatrix}_q\sum_M\begin{pmatrix}J_1 & J_2 & J\\ M & -M & 0\end{pmatrix}T^{J_1}_M\otimes T^{J_2}_{-M}, \tag{46}$$

where we have used that from condition $m_1'+m_2'=m=m_1+m_2$ in Eq. (43) it follows that $M=0$ and $m'=m$.

In the form of Eq. (46) the generating function gives us some insight into the structure of the the twist. The first line of Eq. (46) and the first Clebsch–Gordan coefficient on the second line do not depend on the deformation parameter $\hbar$ and contain only well-known functions, the $9j$ symbol and the Clebsch–Gordan coefficient essentially being given by hypergeometric functions.

The summation over M in the last line eliminates the dependence on the magnetic quantum numbers M_1 and M_2 of the tenor operator basis. The fact that the magnetic quantum number of the tensor operators $T^{J_1}_{M_1}\otimes T^{J_2}_{M_2}$ which appear in the Drinfeld twist add up to zero, $M_1+M_2=M=0$, can also be understood on a more abstract level. Up to isomorphism, the quantum deformation of an enveloping algebra does not affect the Cartan subalgebra as it was stated in Theorem 2. For the Drinfeld–Jimbo deformation $\mathcal{U}_\hbar(\mathrm{su}_2)$ which we consider here this means that

$$\Delta(H) = \Delta_\hbar(H) = H \otimes 1 + 1 \otimes H, \tag{47}$$

which implies that the Drinfeld twist $\mathcal{F}$ must commute with $\Delta(H)$. From

$$[\Delta(H), T^{J_1}_{M_1} \otimes T^{J_2}_{M_2}] = 2(M_1 + M_2)(T^{J_1}_{M_1} \otimes T^{J_2}_{M_2}) \tag{48}$$

we conclude that only those products of tensor operators can appear in $\mathcal{F}$ and $\mathcal{F}^{-1}$ for which $M_1 + M_2 = 0$.

The dependence of Eq. (46) on the deformation parameter is contained in the contraction of the deformed and undeformed Clebsch–Gordan coefficient over m_1 and m_2 in the second line. The representation theoretic interpretation of this term is the following: We can use both, the undeformed and the deformed coproduct, to define a tensor product representation of two irreducible representations with weights j_1 and j_2, defining the undeformed and deformed structure maps as

$$\rho^{j_1 \otimes j_2} := (\rho^{j_1} \otimes \rho^{j_2}) \circ \Delta \quad \text{and} \quad \rho^{j_1 \otimes j_2}_\hbar := (\rho^{j_1} \otimes \rho^{j_2}) \circ \Delta_\hbar. \tag{49}$$

Both representations can be reduced into irreducible components. Denoting the basis vectors of the irreducible weight-j subrepresentation of the undeformed and deformed tensor representation by $|j_1, j_2 \to j, m\rangle$ and $|j_1, j_2 \to j, m\rangle_\hbar$, respectively, we obtain

$$\langle j_1, j_2 \to j', m | j_1, j_2 \to j, m \rangle_\hbar = \sum_{m_1, m_2} \left(\begin{matrix} j_1 & j_2 \\ m_1 & m_2 \end{matrix} \middle| \begin{matrix} j' \\ m \end{matrix} \right) \left(\begin{matrix} j_1 & j_2 \\ m_1 & m_2 \end{matrix} \middle| \begin{matrix} j \\ m \end{matrix} \right)_q. \tag{50}$$

In other words the deformation is now expressed as the change of basis from the irreducible components of tensor representations with respespect to the undeformed coproduct Δ to those with respect to the deformed coproduct $\Delta_\hbar$. Again, the expression on the right-hand side of Eq. (50) is to be understood as generating function. While the q-Clebsch–Gordan coefficient are well-known functions for a given value of q, little is known about its perturbative expansion in powers of $\hbar$.

C. Perturbative expansion

Ideally, we would like to find a closed form expression for the Drinfeld twist in each order of $\hbar$. This would require a closed form expansion of Eq. (50), which is essentially given by a sum of the product of the ordinary hypergeometric function ${}_3F_2$ and its basic (q-deformed) counterpart ${}_3\varphi_2$. To our best knowledge such hybrid combinations of ordinary and basic hypergeometric functions have not been studied in the literature yet and little is known about the perturbative expansion of basic hypergeometric functions in powers of $\hbar = \ln q$ or other possible perturbation parameters such as $q - q^{-1}$ and $q - 1$. Studying the general problem of perturbative expansion of basic hypergeometric functions is beyond the scope of this paper. This is ongoing research and will be presented elsewhere. Here we will only expand the q-deformed Pochhammer symbol, which is the building block of basic hypergeometric functions. This will enable us to carry out the explicit calculation of each order of the Drinfeld twist by a Taylor series expansion of the generating functions (43) and (46).

For our purposes it is convenient to consider the q-Pochhammer symbol $[x]_n$ which is defined by symmetric quantum numbers $[x]$,

$$[x]_n := [x] \cdot [x+1] \cdots [x+n-1], \quad [x] = \frac{e^{x\hbar} - e^{-x\hbar}}{e^{\hbar} - e^{-\hbar}} = \frac{\sinh x\hbar}{\sinh \hbar}. \tag{51}$$

Considering the logarithm of the Pochhammer symbols will turn the product of the q-numbers into the sum of their logarithms. Using the well-known formula

$$\ln\frac{\sinh x}{x}=\sum_{k=1}^{\infty}\frac{2^{2k-1}B_{2k}}{k(2k)!}x^{2k}, \tag{52}$$

where B_{2k} are Bernoulli numbers, we obtain for the expansion of the logarithm of a quantum number

$$\ln\frac{[x]}{x}=\sum_{k=1}^{\infty}\frac{2^{2k-1}B_{2k}}{k(2k)!}(x^{2k}-1)\hbar^{2k}. \tag{53}$$

The Pochhammer symbol can then be expressed as exponential of the sum of this power series,

$$\frac{[x]_n}{(x)_n}=\exp\left(\sum_{k=1}^{\infty}\frac{2^{2k-1}B_{2k}}{k(2k)!}\sum_{j=0}^{n-1}\{(x+j)^{2k}-1\}\hbar^{2k}\right). \tag{54}$$

The sum is carried out using

$$\sum_{j=0}^{n-1}(x+j)^{2k}=\frac{B_{2k+1}(x+n)-B_{2k+1}(x)}{2k+1}, \tag{55}$$

where $B_k(x)$ denotes Bernoulli polynomials. We thus get

$$\frac{[x]_n}{(x)_n}=\exp\left(\sum_{k=1}^{\infty}\frac{2^{2k-1}B_{2k}}{k(2k)!}\left\{\frac{B_{2k+1}(x+n)-B_{2k+1}(x)}{2k+1}-n\right\}\hbar^{2k}\right). \tag{56}$$

This formula could serve as starting point for a perturbative expansion of general q-hypergeometric functions. Here it suffices to deduce from Eq. (56) the expansion of the Pochhammer symbol in $\hbar$. Up to third order we obtain

$$\begin{aligned}\frac{[x]_n}{(x)_n}&=1+\frac{1}{3}B_2\{B_3(x+n)-B_3(x)-3n\}\hbar^2+\mathcal{O}(\hbar^4)\\&=1+\frac{1}{36}(-5n-3n^2+2n^3-6nx+6n^2x+6nx^2)\hbar^2+\mathcal{O}(\hbar^4).\end{aligned} \tag{57}$$

This expression is polynomial in n and x to each order of $\hbar$. Inserting it into Eq. (27) yields the searched-for polynomials in $C\otimes 1$ and $1\otimes C$. From the generating functions (43) or (46) we then obtain the universal Drinfeld twist up to third order in $\hbar$.

Each order $\mathcal{F}_k^{-1}$ of the expansion $\mathcal{F}^{-1}=\Sigma_k\mathcal{F}_k^{-1}\hbar^k$ is alternatingly symmetric or antisymmetric with respect to the exchange of tensor factors by the transpose $\tau(a\otimes b)=b\otimes a$ according to

$$\tau(\mathcal{F}_k^{-1})=(-1)^k\mathcal{F}_k^{-1}. \tag{58}$$

This property can be derived from the fact that the transpose of the deformed coproduct amounts to a change of sign of the perturbation parameter, from which it follows that $\tau(\mathcal{F}^{-1}(\hbar))=\mathcal{F}^{-1}(-\hbar)$. Alternatively, it can be derived from the symmetry properties of the q-Clebsch–Gordan coefficients with respect to the transformation $q\mapsto q^{-1}$. The explicit expressions for the first three orders of the twist we finally obtain are

$$\mathcal{F}_1^{-1}=2(T_{-1}^1\otimes T_1^1-T_{-1}^1\otimes T_1^1)=2T_{-1}^1\otimes T_1^1-\text{transpose}, \tag{59a}$$

$$\mathcal{F}_2^{-1}=-\frac{1}{18}C\otimes C+\frac{\sqrt{14}}{6}T_0^2\otimes C+\frac{\sqrt{21}}{6}(T_1^1\otimes T_{-1}^2-T_{-1}^1\otimes T_1^2)+\frac{21}{2}T_{-2}^2\otimes T_2^2-\frac{7}{4}T_0^2\otimes T_0^2+\text{transpose}, \tag{59b}$$

$$\mathcal{F}_3^{-1} = \frac{\sqrt{2}}{180}(3-4C)T_0^1 \otimes C + \frac{\sqrt{7}}{30}T_0^2 \otimes (9-2C)T_0^1 + \frac{1}{75}[7-21(C\otimes 1 + 1\otimes C) - 12C\otimes C]T_{-1}^1 \otimes T_1^1$$
$$+ \frac{7}{2}T_{-2}^2 \otimes T_2^2 + \frac{\sqrt{6}}{3}T_0^3 \otimes C + \frac{2\sqrt{2}}{5}[T_1^3 \otimes (1-3C)T_{-1}^1 - T_{-1}^3 \otimes (1-3C)T_1^1] + \sqrt{21}T_0^2 \otimes T_0^3$$
$$+ \sqrt{105}(T_{-2}^3 \otimes T_2^2 + T_2^3 \otimes T_{-2}^2) + 18(5T_{-3}^3 \otimes T_2^3 + T_{-1}^3 \otimes T_1^3) - \text{transpose}, \tag{59c}$$

where "transpose" is shorthand for the tensor transpose of all preceding terms such that each expression becomes symmetric or antisymmetric, respectively. One can use Eqs. (40) in order to express the result in terms of the Poincaré–Birkhoff–Witt basis. However, this yields expressions which are much longer than those of Eqs. (59), indicating that the tensor operator basis seems to be the better choice within the context of Drinfeld twists.

The calculations leading to Eqs. (59) are elementary but lengthy and are best carried out using computer algebra. With the expansion (56) of the q-Pochhammer symbol at hand the Taylor series expansion of the generating function (43) is reduced to addition and multiplication of polynomials, operations which are implemented efficiently by all common computer algebra systems. Hence, the explicit calculation of the Drinfeld twist to third order is not significantly limited by computing resources in any way. In any case, by the method presented here it is possible to compute the twist explicitly to orders which are high enough for the applications of Drinfeld twists to mathematical physics which we had in mind.

V. CONCLUSION

Although the existence of universal Drinfeld twists can be proved rather easily, their calculation is a notoriously difficult and long standing problem. While we still did not derive a closed form for each order in the perturbation parameter of the universal twist of $\mathcal{U}_\hbar(\mathrm{su}_2)$, significant progress towards this goal was presented here. In Eq. (46) we have given a generating function for the twist to all orders which can be easily expanded in powers of $\hbar$, as demonstrated in Eq. (59). Moreover, the generating function, which is expressed in terms of basic and ordinary hypergeometric functions, gives new insight into the general structure of the twist.

It is not difficult to understand why the proof of existence of the twist is so easy but the computation is so hard. The existence proof relies mainly on the fact that the first Hochschild cohomolgy of the enveloping algebra is zero. This means that every 1-cocycle is the coboundary of a 0-cocycle or, in other words, every derivation is inner. But we do not know how to compute this 0-cocycle. If in analogy to differential forms we view the inversion of the coboundary operator as a sort of integration, then the nonconstructive existence proof uses integrability but does not tell us how to actually integrate. Just as in differential calculus, this cohomological type of integration turns out to be a difficult problem. In contrast, the series expansion of the generating function (46) in powers of $\hbar$ is a problem of differentiation. While integration is an art, differentiation is a simple technique which can be left to a computer algebra system. This is the reason why we consider the availability of a generating function as significant progress.

The computer algebra expansion of the generating function is computationally cheap and produces expansions of the twist which will suffice for many applications. However, it is not completely satisfactory as it produces expansion formulas like Eq. (59) containing a lot of "magical" combinatorial numbers which cannot be explained any further. In Eq. (46) the dependence of the twist on the perturbation parameter is entirely confined to the q-Clebsch–Gordon coefficient, that is, essentially to the basic hypergeometric function ${}_3\varphi_2$ with basis $q=e^\hbar$. Hence, the remaining problem which still separates us from a truly closed form expression for the universal twist is the perturbative expansion of this basic hypergeometric function in powers of $\hbar$. To our best knowledge, the question of perturbative expansion of basic hypergeometric functions, which seems so obvious in the context of quantum groups, has so far not recieved any systematic treatment in the special functions literature. Therefore, we had to make in Sec. IV C our own first step in this direction, computing a closed form expression for the q-deformed Pochhammer symbol in Eq.

(56). We believe that, further pursuing this approach, a closed form expansion of basic hypergeometric functions and, hence, a closed form of the universal Drinfeld twist of $\mathcal{U}_\hbar(\mathrm{su}_2)$ can be achieved.

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APPENDIX A: CALCULATION OF THE TENSOR OPERATOR BASIS

Expressing the tensor operator basis in terms of the Poincaré–Birkhoff–Witt basis amounts to the normal ordering of Eq. (39). While it is possible to carry out the normal ordering using the commutation relations of $\mathcal{U}(\mathrm{su}_2)$, this turns out to be surpisingly cumbersome. Therefore, we present an alternative approach which is much more in the spirit of this paper: We deduce the normal ordered expression from the representations of the tensor operators.

Let us assume that $M \geqslant 0$. Starting from the Wigner–Eckart theorem (21), using (38) for the reduced matrix elements and the well-known explicit formula

$$\begin{aligned}\left(\begin{array}{cc|c} j_1 & j_2 & j \\ m_1 & m_2 & m \end{array}\right) &= (-1)^{m_1-j_1}\sqrt{\frac{(2j+1)(j_1+j_2-j)!}{(j_1+j_2+j+1)!(j_1-j_2+j)!(j_2-j_1+j)!}} \\ &\times \frac{(j_2+j-m_1)!}{(j_2-j+m_1)!}\sqrt{\frac{(j_1+m_1)!(j_2-m_2)!(j+m)!}{(j_1-m_1)!(j_2+m_2)!(j-m)!}} \\ &\times {}_3F_2\left(\begin{matrix} m_1-j_1, j_1+m_1+1, m-j \\ j_2-j+m_1+1, -j-j_2+m_1 \end{matrix}\right)\end{aligned} \tag{A1}$$

for the Clebsch–Gordan coefficients,[33] we derive for the matrix elements of the tensor operators

$$\begin{aligned}\langle j,m'|T^J_M|j,m\rangle &= (-1)^{J+M}\sqrt{\frac{(2J+1)(J-M)!}{(3J+1)!(J)!\,(J+M)!}}\,\delta_{m',m+M}\sqrt{(-1)^M(j+m+1)_M(-j+m)_M} \\ &\times \sum_k (-1)^k\binom{J+M}{k}(-j-m-k)_J(j+1-m-k)_J.\end{aligned} \tag{A2}$$

We want to deduce the element of the algebra in the Poincaré–Birkhoff–Witt basis from these representations. Towards this end we will compare Eq. (A2) with the matrix elements of monomials

$$\begin{aligned}\langle j,m'|E^pF^p|j,m\rangle &= \delta_{m'm}(-1)^p(-j-m)_p(j-m+1)_p, \\ \langle j,m'|E^M|j,m\rangle &= \delta_{m',m+M}\sqrt{(-1)^M(j+m+1)_M(-j+m)_M}.\end{aligned} \tag{A3}$$

We immediately see that the second line of Eq. (A2) is the matrix element of E^M. The last line has yet to be written in a different form. For this, we need a variant of the Pfaff–Saalschütz summation formula

$$(a-c)_n(b-c)_n = \sum_{p=0}^{n}\binom{n}{p}(-c)_{n-p}(a+b-c+p)_{n-p}(a)_p(b)_p, \tag{A4}$$

from which we get for $a=-j-m$, $b=j-m+1$, $c=k$, $n=J$,

$$(-j-m-k)_J(j-m+1-k)_J=\sum_{p=0}^{J}\binom{J}{p}(-k)_{J-p}(-2m+1-k+p)_{J-p}(-j-m)_p(j-m+1)_p, \tag{A5}$$

and a variant of the Vandermonde summation formula

$$\sum_{k=0}^{n}(-1)^k\binom{n}{k}(-k)_q(-k-x)_q=(-1)^n n!\binom{q}{n-q}(-x-q)_{2q-n}. \tag{A6}$$

Inserting first Eq. (A5) and then Eq. (A6) into the last line of Eq. (A2) we obtain

$$\sum_{k=0}^{J+M}(-1)^k\binom{J+M}{k}(-j-m-k)_J(j+1-m-k)_J=\sum_{p=0}^{p\leqslant J-M/2}\frac{J!(J+M)!}{p!(M+p)!}\binom{2m-2p+J-1}{J-M-2p}\times(-j-m)_p(j-m+1)_p, \tag{A7}$$

Comparing this with the matrix element (A3), we obtain the equality of matrix elements,

$$\langle j,m'|T^J_M|j,m\rangle=(-1)^{J+M}\sqrt{\frac{(2J+1)J!\,(J-M)!\,(J+M)!}{(3J+1)!}}\sum_{p=0}^{p\leqslant J-M/2}\frac{(-1)^p}{p!(M+p)!}\langle j,m'|E^{p+M}\binom{J+H-1}{J-M-2p}F^p|j,m\rangle, \tag{A8}$$

from which we can deduce Eq. (40a). The analogous calculations for $M\leqslant 0$ lead to Eq. (40b).

APPENDIX B: DERIVATION OF EQ. (44)

In order to derive Eq. (44) we recall that, while the Clebsch–Gordan coefficients reduce tensor representations, this reduction is neither commutative nor associative. Let us denote by D^j the irreducible weight-j representation. The isomorphism which corresponds to the exchange of the order in a product representation, $D^{j_1}\otimes D^{j_2}\to D^{j_1}\otimes D^{j_2}$, is given by a change of sign

$$\left(\begin{array}{cc|c} j_1 & j_2 & j\\ m_1 & m_2 & m\end{array}\right)=(-1)^{j-j_1-j_2}\left(\begin{array}{cc|c} j_2 & j_1 & j\\ m_2 & m_1 & m\end{array}\right), \tag{B1}$$

where j_1+j_2-j is always an integer. The associator which corresponds to changing the order of reduction of a product of three irreducible representations, $D^{j_1}\otimes(D^{j_2}\otimes D^{j_3})_{j_{23}}\to(D^{j_1}\otimes D^{j_2})_{j_{12}}\otimes D^{j_2}$ is by definition given by the Racah coefficients,

$$\left(\begin{array}{cc|c} j_2 & j_3 & j_{23}\\ m_2 & m_3 & m_{23}\end{array}\right)\left(\begin{array}{cc|c} j_1 & j_{23} & j\\ m_1 & m_{23} & m\end{array}\right)=\sum_{j_{12}}\left(\begin{array}{cc|c} j_1 & j_2 & j_{12}\\ m_1 & m_2 & m_{12}\end{array}\right)\left(\begin{array}{cc|c} j_{12} & j_3 & j\\ m_{12} & m_3 & m\end{array}\right)\mathbf{R}^{j_1j_2j_3}_{j_{12}j_{23}j}, \tag{B2}$$

where $m_{12}=m_1+m_2$, $m_{23}=m_2+m_3$. Using Eqs. (B1) and (B2) the change of the reduction of a tensor product of four representations according to

$$(D^{j_1}\otimes D^{j_2})_{j_{12}}\otimes(D^{j_1}\otimes D^{j_1})_{j_{34}}\to((D^{j_1}\otimes D^{j_2})_{j_{12}}\otimes D^{j_3})_{j'}\otimes D^{j_4}\to(D^{j_3}\otimes(D^{j_1}\otimes D^{j_2})_{j_{12}})_{j'}\otimes D^{j_4}\to((D^{j_3}\otimes D^{j_1})_{j_{13}}\otimes D^{j_2})_{j'}\otimes D^{j_4}\to(D^{j_1}\otimes D^{j_3})_{j_{13}}\otimes(D^{j_2}\otimes D^{j_4})_{j_{24}} \tag{B3}$$

is then expressed as

$$
\begin{aligned}
&\left(\begin{array}{cc|c} j_1 & j_2 & j_{12} \\ m_1 & m_2 & m_{12} \end{array}\right)\left(\begin{array}{cc|c} j_3 & j_4 & j_{34} \\ m_3 & m_4 & m_{34} \end{array}\right)\left(\begin{array}{cc|c} j_{12} & j_{34} & j \\ m_{12} & m_{34} & m \end{array}\right) \\
&\quad=\sum_{j'}\left(\begin{array}{cc|c} j_1 & j_2 & j_{12} \\ m_1 & m_2 & m_{12} \end{array}\right)\left(\begin{array}{cc|c} j_{12} & j_3 & j' \\ m_{12} & m_3 & m' \end{array}\right)\left(\begin{array}{cc|c} j' & j_4 & j \\ m' & m_4 & m \end{array}\right)\mathbf{R}^{j_{12}j_3j_4}_{j'j_{34}j} \\
&\quad=\sum_{j'}\left(\begin{array}{cc|c} j_1 & j_2 & j_{12} \\ m_1 & m_2 & m_{12} \end{array}\right)\left(\begin{array}{cc|c} j_3 & j_{12} & j' \\ m_3 & m_{12} & m' \end{array}\right)\left(\begin{array}{cc|c} j' & j_4 & j \\ m' & m_4 & m \end{array}\right)\mathbf{R}^{j_{12}j_3j_4}_{j'j_{34}j}(-1)^{j'-j_{12}-j_3} \\
&\quad=\sum_{j_{13},j'}\left(\begin{array}{cc|c} j_3 & j_1 & j_{13} \\ m_3 & m_1 & m_{13} \end{array}\right)\left(\begin{array}{cc|c} j_{13} & j_2 & j' \\ m_{13} & m_2 & m' \end{array}\right)\left(\begin{array}{cc|c} j' & j_4 & j \\ m' & m_4 & m \end{array}\right)\mathbf{R}^{j_3j_1j_2}_{j_{13}j_{12}j'}\mathbf{R}^{j_{12}j_3j_4}_{j'j_{34}j}(-1)^{j'-j_{12}-j_3} \\
&\quad=\sum_{j_{13},j_{24}}\left(\begin{array}{cc|c} j_1 & j_3 & j_{13} \\ m_1 & m_3 & m_{13} \end{array}\right)\left(\begin{array}{cc|c} j_2 & j_4 & j_{24} \\ m_2 & m_4 & m_{24} \end{array}\right)\left(\begin{array}{cc|c} j_{13} & j_{24} & j \\ m_{13} & m_{24} & m \end{array}\right) \\
&\qquad\times\sum_{j'}\mathbf{R}^{j_{13}j_2j_4}_{j'j_{24}j}\mathbf{R}^{j_3j_1j_2}_{j_{13}j_{12}j'}\mathbf{R}^{j_{12}j_3j_4}_{j'j_{34}j}(-1)^{j'-j_{12}+j_{13}-j_1-2j_3},
\end{aligned}
\tag{B4}
$$

where $m_{ij}=m_i+m_j$ for $i,j\in\{1,2,3,4\}$, $i<j$. Next we express the Racah coefficients in terms of $6j$ symbols,

$$
\mathbf{R}^{j_1j_2j_3}_{j_{12}j_{13}j}=(-1)^{j_1+j_2+j_3+j}\sqrt{(2j_{12}+1)(2j_{13}+1)}\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{13} \end{Bmatrix}. \tag{B5}
$$

Using the symmetries of the $6j$ symbol and the definition of the $9j$ symbol we can rewrite the last line of Eq. (B4) as

$$
\begin{aligned}
&\sum_{j'}\mathbf{R}^{j_{13}j_2j_4}_{j'j_{24}j}\mathbf{R}^{j_3j_1j_2}_{j_{13}j_{12}j'}\mathbf{R}^{j_{12}j_3j_4}_{j'j_{34}j}(-1)^{j'-j_{12}+j_{13}-j_1-2j_3} \\
&\qquad=\alpha\sum_{j'}(-1)^{2j'}(2j'+1)\begin{Bmatrix} j_{13} & j_2 & j' \\ j_4 & j & j_{24} \end{Bmatrix}\begin{Bmatrix} j_3 & j_1 & j_{13} \\ j_2 & j' & j_{12} \end{Bmatrix} \\
&\qquad\quad\times\begin{Bmatrix} j_{12} & j_3 & j' \\ j_4 & j & j_{34} \end{Bmatrix}=\alpha\sum_{j'}(-1)^{2j'}(2j'+1) \\
&\qquad\quad\times\begin{Bmatrix} j_3 & j_{13} & j_1 \\ j_2 & j_{12} & j' \end{Bmatrix}\begin{Bmatrix} j_4 & j_{24} & j_2 \\ j_{13} & j' & j \end{Bmatrix}\begin{Bmatrix} j_{34} & j & j_{12} \\ j' & j_3 & j_4 \end{Bmatrix} \\
&\qquad=\alpha\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix},
\end{aligned}
\tag{B6}
$$

where the factor α is defined as

$$
\alpha:=(-1)^{2j}\sqrt{(2j_{12}+1)(2j_{34}+1)(2j_{13}+1)(2j_{24}+1)}. \tag{B7}
$$

From Eqs. (B4) and (B6) we finally obtain

$$
\begin{aligned}
&\left(\begin{array}{cc|c} j_1 & j_2 & j_{12} \\ m_1 & m_2 & m_{12} \end{array}\right)\left(\begin{array}{cc|c} j_3 & j_4 & j_{34} \\ m_3 & m_4 & m_{34} \end{array}\right)\left(\begin{array}{cc|c} j_{12} & j_{34} & j \\ m_{12} & m_{34} & m \end{array}\right) \\
&\quad=\sum_{j_{13},j_{24}}\alpha\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix}\left(\begin{array}{cc|c} j_1 & j_3 & j_{13} \\ m_1 & m_3 & m_{13} \end{array}\right)\left(\begin{array}{cc|c} j_2 & j_4 & j_{24} \\ m_2 & m_4 & m_{24} \end{array}\right)\left(\begin{array}{cc|c} j_{13} & j_{24} & j \\ m_{13} & m_{24} & m \end{array}\right).
\end{aligned}
\tag{B8}
$$

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Bifurcations from the endpoints of the essential spectrum in the linearized nonlinear Schrödinger problem

Scipio Cuccagna
DISMI, University of Modena and Reggio Emilia, 42100 Italy

Dmitry Pelinovsky
Department of Mathematics, McMaster University, Hamilton, Ontario, Canada L8S 4K1

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We study bifurcations of eigenvalues from the endpoints of the essential spectrum in the linearized nonlinear Schrödinger problem in three dimensions. We show that a resonance and an eigenvalue of positive energy at the endpoint may bifurcate only to a real eigenvalue of positive energy, while an eigenvalue of negative energy at the endpoint may also bifurcate to complex eigenvalues. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1901345]

I. INTRODUCTION

We consider the nonlinear Schrödinger (NLS) equation in three dimensions,

$$i\psi_t = -\Delta\psi + U(x)\psi + F(|\psi|^2)\psi, \tag{1.1}$$

where $(x,t) \in \mathbb{R}^3 \times \mathbb{R}$ and $\psi \in \mathbb{C}$. For suitable functions $U(x)$ and $F(|\psi|^2)$, the NLS equation (1.1) possesses special solutions,

$$\psi = \phi(x)e^{i\omega t}, \quad \omega > 0, \tag{1.2}$$

where $\phi(x)$ is an exponentially decreasing solution of the elliptic problem,

$$-\Delta\phi + \omega\phi + U(x)\phi + F(\phi^2)\phi = 0, \tag{1.3}$$

such that $\phi: \mathbb{R}^3 \to \mathbb{R}$ and $\phi \in C^\infty$. Linearization of the nonlinear Schrödinger equation (1.1) with the ansatz,

$$\psi = (\phi(x) + \varphi(x)e^{iz t} + \overline{\theta}(x)e^{-i\overline{z}t})e^{i\omega t}, \tag{1.4}$$

leads to the spectral problem,

$$\mathcal{L}\boldsymbol{\psi} = z\boldsymbol{\psi}, \tag{1.5}$$

where $\boldsymbol{\psi} = (\varphi, \theta)^T$ and the linear operator $\mathcal{L}$ on $L^2(\mathbb{R}^3 \mapsto \mathbb{C}^2)$ takes the form $\mathcal{L} = \sigma_3\mathcal{H}$, where

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathcal{H} = \begin{pmatrix} -\Delta + \omega + f(x) & g(x) \\ g(x) & -\Delta + \omega + f(x) \end{pmatrix}, \tag{1.6}$$

and

$$f(x) = U(x) + F(\phi^2) + F'(\phi^2)\phi^2, \quad g(x) = F'(\phi^2)\phi^2.$$

We assume that $U(x) \in C^\infty$ is exponentially decreasing and $F \in C^\infty, F(0) = 0$, such that $f, g: \mathbb{R}^3 \to \mathbb{R}$ are exponentially decaying C^∞-functions.

We denote the point spectrum of $\mathcal{L}$ as $\sigma_p(\mathcal{L})$ and the essential spectrum of $\mathcal{L}$ as $\sigma_e(\mathcal{L})$. We have shown in Cuccagna *et al.* (2005) that the spectrum of $\mathcal{L}$ is associated to the sign of the energy functional defined in $H^1(\mathbb{R}^3 \mapsto \mathbb{C}^2)$,

$$h = \langle \psi, \mathcal{H}\psi \rangle. \tag{1.7}$$

In particular, an eigenvalue is of positive (respectively, negative) energy if $h>0$ (respectively, $h<0$). We showed in Cuccagna *et al.* (2005) that the nonsingular part of $\sigma_e(\mathcal{L})$ has always positive energy. We also proved that an embedded eigenvalue z of positive energy $h>0$ disappears under a generic perturbation in the context of operator $\mathcal{L}$, while one of negative energy $h<0$ bifurcates into isolated complex eigenvalues of $\sigma_p(\mathcal{L})$. The latter result generalizes an older work by Grillakis (1990), while the former one is new and consistent with the theory of embedded eigenvalues for standard Schrödinger operators.

In this paper we apply a generic perturbation to $\mathcal{L}$ in the case when the points $z=\pm\omega$, that are thresholds of $\sigma_e(\mathcal{L})$, are either eigenvalues or resonances of rank one. We show how the resonance or eigenvalue can either disappear in a different sheet of the Riemann surface associated to the resolvent of $\mathcal{L}$ or move away from the essential spectrum becoming an isolated real eigenvalue, or a pair of isolated complex eigenvalues. Furthermore we study the dependence of this singularity on the perturbation, obtaining an analogue of the similar work by Klaus and Simon (1980) on standard Schrödinger operators. We note that the resonance and eigenvalues at the endpoints are typically eliminated by hypothesis in the analysis of the NLS equation (1.1) and the linearized NLS problem (1.5) [Cuccagna (2001), Perelman (2004), Schlag (2004)]

One application of our result is the analysis of the NLS equation (1.1) in the case when operator $H_0=-\Delta+U(x)$ supports $-\mu_1<\cdots<-\mu_N$ negative eigenvalues and when the threshold 0 is either a resonance or an eigenvalue. It is well known [Tsai and Yau (2002)] that the NLS equation (1.1) admits then nonlinear standing wave solutions of form (1.2) with ω close to μ_n for any preassigned n and these standing wave solutions are small. Their stability properties depend crucially on the spectral properties of the related $\mathcal{L}$ which turns out to be a small perturbation of $\sigma_3(H_0+\omega)$ by the smallness of the standing wave. In the case of $n=1$, the discrete spectrum of $\mathcal{L}$ is close to that of $\sigma_3(H_0+\omega)$, in particular has at least $2N$ elements with the point 0 of multiplicity 2. Our paper can be used to track the threshold singularity of operator $\mathcal{L}$ under perturbation.

Another possible application occurs when we add a small nonlinear perturbation $\epsilon\delta F(|\psi|^2)\psi$ to the main equation (1.1). Under appropriate conditions, the ground state can be shown to depend smoothly on ϵ. Now, if for $\epsilon=0$ and a given value of ω operator $\mathcal{L}$ has resonances or eigenvalues at the thresholds, one can ask what happens to these singularities for nearby $\epsilon\neq 0$. The present paper gives a tool for analysis, avoiding details of specific applications.

For earlier work on "edge bifurcations," which is the name for bifurcations of resonances from the endpoints, see Kapitula and Sandstede [(2002), (2004)] where the main tool is the Evans function. Since the Evans function seems better suited to one-dimensional (1D) problems, our present work is based on theory by Jensen and Kato (1979) for scalar Schrödinger operators, applied here to the linearized NLS problem (1.5). Notice that our work is more general than Kapitula and Sandstede [(2002), (2004)] since it allows also eigenvalues at the endpoints and it does not depend on whether the solution $\phi(x)$ is a ground state. Furthermore we answer to a specific question [see Corollary 5.4 in Kapitula *et al.* (2004)] by showing that it is impossible for a resonant pole to become an unstable (complex) eigenvalue.

Our paper is structured as follows. The formalism of operator resolvent near the endpoints is exposed in Sec. II. Bifurcations of a simple resonance and a simple eigenvalue from the endpoint are described in Secs. III and IV, respectively. Section V gives the proof of Lemma 4.7.

II. OPERATOR RESOLVENT NEAR THE ENDPOINTS

Using standard Pauli matrices σ_2 and σ_3, we write $\mathcal{L}$ explicitly as

$$\mathcal{L} = (-\Delta + \omega + f(x))\sigma_3 + ig(x)\sigma_2, \tag{2.1}$$

such that $\sigma_3\mathcal{L}\sigma_3=\mathcal{L}^*$. We also decompose the operator $\mathcal{L}$ into the unbounded differential part $\mathcal{L}_0$ and bounded potential part $V(x)$ as $\mathcal{L}=\mathcal{L}_0+V(x)$, where $\mathcal{L}_0=(-\Delta+\omega)\sigma_3$ and $V(x)=f(x)\sigma_3$

$+ig(x)\sigma_2$. We assume that $V(x)$ is continuous, exponentially decaying matrix-valued function, such that

$$|V_{i,j}(x)| \leqslant Ce^{-\alpha|x|}, \quad \forall\, x \in \mathbb{R}^3, \quad 1 \leqslant i,j \leqslant 2, \tag{2.2}$$

for some $\alpha > 0, C > 0$. In these notations, the spectral problem (1.5) is rewritten as

$$(\mathcal{L}_0 - z)\boldsymbol{\psi} = -V(x)\boldsymbol{\psi}. \tag{2.3}$$

We use the weighted H^τ_s and L^2_s spaces defined as

$$H^\tau_s = \left\{f:(\omega - \Delta)^{r/2} f \in L^2_s\right\}, \tag{2.4}$$

$$L^2_s = \left\{f:(1 + |x|^2)^{s/2} f \in L^2\right\}. \tag{2.5}$$

We also use the standard Fourier transform in L^2,

$$f(p) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} f(x) e^{ipx}\, dx, \quad f(x) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} f(p) e^{-ipx}\, dp. \tag{2.6}$$

We denote the operator resolvent as $\mathcal{R}(z) = (\mathcal{L} - z)^{-1}$ and $\mathcal{R}_0(z) = (\mathcal{L}_0 - z)^{-1}$, such that

$$\mathcal{R}(z) = (I + \mathcal{R}_0(z)V)^{-1}\mathcal{R}_0(z). \tag{2.7}$$

The domain of the essential spectrum $\sigma_e(\mathcal{L})$ is located at $\mathcal{D}_e = (-\infty, -\omega] \cup [\omega, \infty)$, such that the points $z = \pm\omega$ are endpoints of $\sigma_e(\mathcal{L})$.

Let us consider bifurcations from the endpoint $z = \omega$, since bifurcations from the other endpoint $z = -\omega$ are obtained from the symmetry of the problem (2.3). When $z \notin \mathcal{D}_e$ but $|z - \omega|$ is small, we introduce the parametrization,

$$z = \omega - \zeta^2, \quad \operatorname{Re} \zeta > 0, \tag{2.8}$$

and consider the kernel of $R_0(\zeta) \equiv \mathcal{R}_0(\omega - \zeta^2), \operatorname{Re} \zeta > 0$ in the explicit form

$$R_0(\zeta) = \frac{\sigma_3}{4\pi|x-y|} \begin{bmatrix} e^{-\zeta|x-y|} & 0 \\ 0 & e^{-\sqrt{2\omega - \zeta^2}|x-y|} \end{bmatrix}. \tag{2.9}$$

When $\zeta \to 0$, the resolvent $R_0(\zeta)$ has the Taylor series expansion in $\mathcal{B}(H^{-1}_s, H^1_{-s}), s > \frac{3}{2}$,

$$R_0(\zeta) = R_0 - \zeta R_1 + \zeta^2 R_2 - \zeta^3 R_3 + \mathrm{O}(\zeta^4), \quad \operatorname{Re} \zeta > 0, \tag{2.10}$$

where

$$R_0 = \frac{\sigma_3}{4\pi|x-y|} \begin{bmatrix} 1 & 0 \\ 0 & e^{-\sqrt{2\omega}|x-y|} \end{bmatrix}, \quad R_1 = \frac{1}{4\pi} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \tag{2.11}$$

$$R_2 = \frac{\sigma_3}{8\pi} \begin{bmatrix} |x-y| & 0 \\ 0 & \dfrac{e^{-\sqrt{2\omega}|x-y|}}{\sqrt{2\omega}} \end{bmatrix}, \quad R_3 = \frac{1}{24\pi} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} |x-y|^2. \tag{2.12}$$

If the function $\boldsymbol{\psi}(x)$ solves the problem (2.3) for $z = \omega$, the components $\psi_1(x)$ and $\psi_2(x)$ satisfy the equations

$$\Delta\psi_1 = f\psi_1 + g\psi_2, \tag{2.13}$$

$$(\Delta - 2\omega)\psi_2 = g\psi_1 + f\psi_2. \tag{2.14}$$

Define

$$C_0 = \int_{\mathbb{R}^3} (f\psi_1 + g\psi_2)\mathrm{d}x. \tag{2.15}$$

The bounded linear operator $(I+R_0V)$ is defined in $L^2_{-s}, s>\frac{1}{2}$. When it has a kernel, then $|C_0|<\infty$ for the function $\boldsymbol{\psi}(x)$. The following two cases are different: (i) $C_0\neq 0$ and (ii) $C_0=0$. The first case is referred to as the resonance and the second case is referred to as the eigenvalue of the linearized NLS problem (2.3).

Since $(f\psi_1+g\psi_2)\in H^2_s, s>0$ and $f(x), g(x)$ decay exponentially, it follows from (2.14) that $\psi_2(x)$ decays exponentially too, such that $\psi_2\in H^2_s, s>0$. When $C_0\neq 0, \psi_1(x)$ decays algebraically as $1/|x|$, such that $\psi_1\in H_{-s}, s>\frac{1}{2}$. When $C_0=0, \psi_1(x)$ decays more rapidly as $1/|x|^2$, such that $\psi_1\in H_{-s}, s>-\frac{1}{2}$, including the energy space $H^1_0\subset L^2$. We summarize that

$$C_0 \neq 0, \quad \mathrm{Ker}(I+R_0V)\in H^1_{-s}, \quad s>\tfrac{1}{2}, \tag{2.16}$$

$$C_0 = 0, \quad \mathrm{Ker}(I+R_0V)\in H^1_{-s}, \quad s>\tfrac{1}{2}. \tag{2.17}$$

In either case, we study the kernel of the adjoint operator $\mathrm{Ker}(I+V^*R_0)$ and the generalized kernel $N_g(I+R_0V)=\cup_{n=1}^{\infty}\mathrm{Ker}(I+R_0V)^n$ in the following two lemmas.

Lemma 2.1: Let $\boldsymbol{\psi}\in\mathrm{Ker}(I+R_0V), \boldsymbol{\psi}\in H^1_{-s}, s>\frac{1}{2}$. *Then,* $\boldsymbol{\phi}=V^*\sigma_3\boldsymbol{\psi}\in\mathrm{Ker}(I+V^*R_0), \boldsymbol{\phi}\in H^{-1}_s, s>\frac{1}{2}$, *such that* $V^*\sigma_3$ *is an injection of* $\mathrm{Ker}(I+R_0V)$ *to* $\mathrm{Ker}(I+V^*R_0)$.

Proof: It follows from direct computations for $\boldsymbol{\psi}\neq\mathbf{0}$ that

$$(I+V^*R_0)V^*\sigma_3\boldsymbol{\psi} = V^*(I+R_0V^*)\sigma_3\boldsymbol{\psi} = V^*\sigma_3(I+R_0V)\boldsymbol{\psi} = \mathbf{0},$$

such that $\boldsymbol{\phi}=V^*\sigma_3\boldsymbol{\psi}\in\mathrm{Ker}(I+V^*R_0)$ and $\boldsymbol{\phi}\in H^{-1}_s, s>\frac{1}{2}$. We show that $\boldsymbol{\phi}\neq\mathbf{0}$. Since $V^*\sigma_3=\sigma_3V$, then $\boldsymbol{\phi}=\sigma_3V\boldsymbol{\psi}=\mathbf{0}$ implies that $V\boldsymbol{\psi}=\mathbf{0}$ and $(\mathcal{L}_0-\omega)\boldsymbol{\psi}=\mathbf{0}$, or equivalently, $\Delta\psi_1=0$ and $(\Delta-2\omega)\psi_2=0$. However, if $\boldsymbol{\psi}\in H^1_{-s}, s>\frac{1}{2}$, then the latter equations imply that $\boldsymbol{\psi}=\mathbf{0}$, which is impossible. ■

Lemma 2.2: The generalized kernel $N_g(I+R_0V)$ *in* $H^1_{-s}, s>\frac{1}{2}$, *coincides with* $\mathrm{Ker}(I+R_0V)$.

Proof: Let $\boldsymbol{\psi}\in\mathrm{Ker}(I+R_0V)$. The generalized kernel $N_g(I+R_0V)$ is bigger than the kernel $\mathrm{Ker}(I+R_0V)$ iff there exists a solution of the derivative equation,

$$(I+R_0V)\boldsymbol{\psi}_1 = \boldsymbol{\psi}, \quad \boldsymbol{\psi}_1\in H^1_{-s}, \quad s>\tfrac{1}{2}. \tag{2.18}$$

Then,

$$\langle\boldsymbol{\psi}, V^*\sigma_3\boldsymbol{\psi}\rangle = \langle(I+R_0V)\boldsymbol{\psi}_1, V^*\sigma_3\boldsymbol{\psi}\rangle = \langle\boldsymbol{\psi}_1, V^*(I+R_0V^*)\sigma_3\boldsymbol{\psi}\rangle = \langle\boldsymbol{\psi}_1, V^*\sigma_3(I+R_0V)\boldsymbol{\psi}\rangle = 0,$$

such that $\langle\boldsymbol{\psi}, \sigma_3V\boldsymbol{\psi}\rangle = -\langle\boldsymbol{\psi}, \sigma_3(\mathcal{L}_0-\omega)\boldsymbol{\psi}\rangle = 0$. Since $\sigma_3(\mathcal{L}_0-\omega) = -\Delta+\omega-\omega\sigma_3$ and $\boldsymbol{\psi}\neq\mathbf{0}$, the quadratic form $\langle\boldsymbol{\psi}, \sigma_3V\boldsymbol{\psi}\rangle$ is nonzero for $\boldsymbol{\psi}\in H^1_{-s}, s>\frac{1}{2}$, such that no solution $\boldsymbol{\psi}_1(x)$ exists in the problem (2.18). ■

Since geometric and algebraic dimensions of the kernel of $(I+R_0V)$ coincide in $H^1_{-s}, s>\frac{1}{2}$, we introduce a natural splitting,

$$H^1_{-s} = \mathrm{Ker}(I+R_0V)\oplus[\mathrm{Ker}(I+V^*R_0)]^{\perp}, \tag{2.19}$$

$$H^{-1}_s = [\mathrm{Ker}(I+R_0V)]^{\perp}\oplus\mathrm{Ker}(I+V^*R_0), \tag{2.20}$$

where $\perp$ is defined in terms of the pairing of H^1_{-s} and H^{-1}_s. We denote $\mathcal{S}_0$ as the projection of H^1_{-s} to $\mathrm{Ker}(I+R_0V)$, associated to the splitting (2.19), and $\mathcal{S}_0^*$ as the dual projection in the dual space

H_s^{-1}, associated to the splitting (2.20). In what follows, we assume that the dimension of $\mathrm{Ker}(I+R_0V)$ is one. The two cases in (2.16) and (2.17) are considered separately in Secs. III and IV.

III. BIFURCATION OF A SIMPLE RESONANCE

Here we assume that $\mathrm{Ker}(I+R_0V)\subsetneq H_0^1$, such that $z=\omega$ is a resonance of $\sigma_e(\mathcal{L})$ but not an eigenvalue. It is clear from (2.13) in the case of $C_0\neq 0$ that there is only one eigenvector $\boldsymbol{\psi}(x)$ which decays as $1/|x|$ and belongs to $H^1_{-s}, s>\frac{1}{2}$. Therefore, the resonance at $z=\omega$ is always simple, such that the dimension of $\mathrm{Ker}(I+R_0V)$ in $H^1_{-s}, s>\frac{1}{2}$ is one. Since $C_0\neq 0$, we normalize the eigenvector $\boldsymbol{\psi}\in\mathrm{Ker}(I+R_0V)$ by the condition

$$\int_{\mathbb{R}^3}(f\psi_1+g\psi_2)\mathrm{d}x=\sqrt{4\pi}, \tag{3.1}$$

such that

$$R_1V\boldsymbol{\psi}=\frac{1}{\sqrt{4\pi}}\mathbf{e}_1, \quad \mathbf{e}_1=\begin{bmatrix}1\\0\end{bmatrix}.$$

By Lemma 2.2, we have $\langle\boldsymbol{\psi},V^*\sigma_3\boldsymbol{\psi}\rangle\neq 0$, such that the spectral projection, associated with the splitting (2.19), is

$$\mathcal{S}_0=\boldsymbol{\psi}\frac{\langle\cdot,V^*\sigma_3\boldsymbol{\psi}\rangle}{\langle\boldsymbol{\psi},V^*\sigma_3\boldsymbol{\psi}\rangle}. \tag{3.2}$$

Following the analysis of Jensen and Kato (1979), we study the Taylor series expansions of $(I+R_0(\zeta)V)$ near $z=\omega$, or equivalently $\zeta=0$.

Lemma 3.1: Let $\mathcal{S}=\mathcal{I}-\mathcal{S}_0$. The following statements are true:

(i) *Operator $\mathcal{S}(I+R_0V)\mathcal{S}$ is invertible in $\mathcal{B}(\mathcal{S}H^1_{-s},\mathcal{S}H^1_{-s})$ with the inverse denoted by $\mathcal{K}$.*
(ii) *Operator $\mathcal{S}_0^*V^*\sigma_3R_1V\mathcal{S}_0=\mathcal{S}_0^*V^*R_1V\mathcal{S}_0$ is invertible in $\mathcal{B}(\mathcal{S}_0H^1_{-s},\mathcal{S}_0^*H_s^{-1})$ with the inverse $\boldsymbol{\psi}\langle\cdot,\boldsymbol{\psi}\rangle$.*

Proof: To prove (i), we notice that the splitting in (2.19) and (2.20) is invariant for $(I+R_0V)$, such that $\mathcal{S}(I+R_0V)\mathcal{S}$ is the restriction of $(I+R_0V)$ on $[\mathrm{Ker}(I+V^*R_0)]^\perp$. Since it has an empty kernel and R_0V is compact, the statement (i) follows from the Fredholm alternative theorem.

To prove (ii), we denote the dual of $\boldsymbol{\psi}$ as $\boldsymbol{\phi}\in\mathcal{S}_0^*H_s^{-1}\subseteq\mathrm{Ker}(I+V^*R_0)$, such that $\langle\boldsymbol{\psi},\boldsymbol{\phi}\rangle=1$. Then $\mathcal{S}_0^*=\boldsymbol{\phi}\langle\cdot,\boldsymbol{\psi}\rangle$ and

$$\mathcal{S}_0^*V^*R_1V\mathcal{S}_0\boldsymbol{\psi}=\frac{1}{\sqrt{4\pi}}\mathcal{S}_0^*V^*\mathbf{e}_1=\frac{1}{\sqrt{4\pi}}\boldsymbol{\phi}\langle\mathbf{e}_1,V\boldsymbol{\psi}\rangle=\boldsymbol{\phi},$$

where the last equality is due to normalization (3.1). Therefore, $\mathcal{S}_0^*V^*R_1V\mathcal{S}_0=\boldsymbol{\phi}\langle\cdot,\boldsymbol{\phi}\rangle$, which has the inverse $\boldsymbol{\psi}\langle\cdot,\boldsymbol{\psi}\rangle$. ■

Lemma 3.2: The following expansion is valid in $\mathcal{B}(H^1_{-s},H^1_{-s})$ for $s>\frac{5}{2}$ near $\zeta=0$:

$$(I+R_0(\zeta)V)^{-1}=-\zeta^{-1}\boldsymbol{\psi}\langle\cdot,V^*\sigma_3\boldsymbol{\psi}\rangle+\mathcal{K}+\mathrm{O}(\zeta), \quad \mathrm{Re}\,\zeta>0. \tag{3.3}$$

Proof: Let

$$\mathcal{X}=\mathcal{S}H^1_{-s}\oplus\mathcal{S}_0H^1_{-s}=H^1_{-s}, \quad \mathcal{Y}=\mathcal{S}H^1_{-s}\oplus\mathcal{S}_0^*H_s^{-1}$$

and

$$\mathcal{B} = \begin{bmatrix} \mathcal{S} & 0 \\ 0 & \zeta^{-\frac{1}{2}}\mathcal{S}_0 \end{bmatrix}, \quad \mathcal{C} = \begin{bmatrix} \mathcal{S} & 0 \\ 0 & \zeta^{-\frac{1}{2}}\mathcal{S}_0^* V^* \sigma_3 \end{bmatrix}.$$

If $\mathcal{S}\mathbf{u}=\mathbf{0}$, then $\mathbf{u}\in\mathcal{S}_0 H^1_{-s}$ and $\mathcal{S}_0^* V^* \sigma_3$ is injective by Lemma 2.1 and definition of $\mathcal{S}_0^*$. As a result, $\mathcal{B}:\mathcal{X}\mapsto H^1_{-s}$ is an isomorphism, while $\mathcal{C}:H^1_{-s}\mapsto\mathcal{Y}$ is injective. Let $\mathcal{A}\equiv\mathcal{C}(I+R_0(\zeta)V)\mathcal{B}$. Then,

$$\mathcal{A} = \mathcal{C}(I+R_0V)\mathcal{B} - \zeta\mathcal{C}R_1V\mathcal{B} + \mathrm{O}(\zeta^2) = \begin{bmatrix} \mathcal{S}(I+R_0V)\mathcal{S} & 0 \\ 0 & -\mathcal{S}_0^* V^* \sigma_3 R_1 V \mathcal{S}_0 \end{bmatrix} + \mathrm{O}(\zeta).$$

If $\mathcal{A}$ is invertible, $\mathcal{B}$ is surjective, and $\mathcal{C}$ is injective, then, by Lemma 3.12 of Jensen and Kato (1979), we have

$$(I+R_0(\zeta)V)^{-1} = \mathcal{B}\mathcal{A}^{-1}\mathcal{C},$$

such that the expansion (3.3) holds by the Neumann expansion argument. ■

Using (2.7), (2.10), and (3.3), we have the following result.

Corollary 3.3: The following expansion is valid in $\mathcal{B}(H^{-1}_s, H^1_{-s})$ for $s>\frac{5}{2}$ near $\zeta=0$:

$$R(\zeta) = \zeta^{-1}\langle\cdot,\sigma_3\boldsymbol{\psi}\rangle\boldsymbol{\psi} + \mathrm{O}(1), \quad \mathrm{Re}\,\zeta>0. \tag{3.4}$$

In order to work in L^2 rather than in a weighted space $L^2_{-s}, s>\frac{1}{2}$, we use the Birman–Schwinger formulation of the spectral problem (2.3) for $V=B^*A$ [Cuccagna *et al.* (2005)];

$$(I+\mathcal{Q}_0(z))\boldsymbol{\Psi} = \mathbf{0}, \quad \mathcal{Q}_0(z) = A\mathcal{R}_0(z)B^*, \quad z\in\mathbb{C}\setminus\mathcal{D}_e, \tag{3.5}$$

where

$$\boldsymbol{\Psi} = -A\boldsymbol{\psi}, \quad \boldsymbol{\psi} = \mathcal{R}_0(z)B^*\boldsymbol{\Psi}. \tag{3.6}$$

It is clear from (2.9) that $Q_0(\zeta)\equiv\mathcal{Q}_0(\omega-\zeta^2)$, initially defined for $\mathrm{Re}\,\zeta>0$, admits an analytical extension in an open set around $\zeta=0$ with values in $\mathcal{B}(L^2,H^2)$, such that $Q_0=Q(0)$ is well defined. Moreover, for any positive integer n, the map $\boldsymbol{\psi}\mapsto -A\boldsymbol{\psi}$ is an isomorphism,

$$\mathrm{Ker}(I+R_0V)^n \subset L^2_{-s} \mapsto \mathrm{Ker}(I+Q_0)^n \subset L^2, \quad s>\tfrac{1}{2}, \tag{3.7}$$

such that the inverse map is $\boldsymbol{\Psi}\mapsto R_0B^*\boldsymbol{\Psi}$. By Lemma 2.2, there exists an $(I+Q_0)$-invariant splitting,

$$L^2 = \mathrm{Ker}(I+Q_0)\oplus[\mathrm{Ker}(I+Q_0^*)]^\perp. \tag{3.8}$$

We denote $\mathcal{P}_0$ by the projection of L^2 on $\mathrm{Ker}(I+Q_0)$ and $\mathcal{P}_0^*$ by the dual projection.

With the use of Corollary 3.3, we consider the family of operators $\mathcal{L}_1=\mathcal{L}+\epsilon V_1$, where the perturbation potential $V_1(x)$ satisfies the same assumption as the potential $V(x)$, while the unperturbed operator $\mathcal{L}$ has a simple resonance. Let $\mathcal{R}_1(z)=(\mathcal{L}_1-z)^{-1}$ and define $\mathcal{Q}(z)=A_1\mathcal{R}(z)B_1^*$ and $\mathcal{Q}_1(z)=A_1\mathcal{R}_1(z)B_1^*=(I+\epsilon\mathcal{Q}(z))^{-1}\mathcal{Q}(z)$, where $V_1=B_1^*A_1$. We can always factorize V_1 so that $A_1=A$. It follows from (2.7) with $A_1=A$ that

$$\mathcal{Q}(z) = (I+A\mathcal{R}_0(z)B_1^*)^{-1}A\mathcal{R}_0(z)B_1^* = (I+\mathcal{Q}_0(z))^{-1}A\mathcal{R}_0(z)B_1^*.$$

We again use parametrization (2.8) and denote $Q(\zeta)\equiv\mathcal{Q}(\omega-\zeta^2), \mathrm{Re}\,\zeta>0$. Since $(I+Q_0(\zeta))^{-1}$ can be extended meromorphically from $\mathrm{Re}\,\zeta>0$ to $\mathrm{Re}\,\zeta\leqslant 0$, then $Q(\zeta)$ is a meromorphic function of $\zeta\in\mathbb{C}$. Similarly, $Q_1(\zeta)$ is also a meromorphic function of $\zeta\in\mathbb{C}$.

The main results of this section are formulated in the following two propositions.

Proposition 3.4: Let ϵ be a small positive parameter. If $\langle\psi,V_1^*\sigma_3\psi\rangle<0$, then $\sigma_p(\mathcal{L}_1)$ includes a real eigenvalue $z(\epsilon), z(\epsilon)<\omega$, such that

$$z(\epsilon) = \omega - \epsilon^2\langle\boldsymbol{\psi},V_1^*\sigma_3\boldsymbol{\psi}\rangle^2 + \mathrm{o}(\epsilon^2). \tag{3.9}$$

If $\langle \psi, V_1^* \sigma_3 \psi \rangle > 0$, *then* $\sigma_p(\mathcal{L}_1)$ *does not include an eigenvalue in the neighborhood of* $z=\omega$. *In both cases, resonance at* $z=\omega$ *disappears at* $\epsilon \neq 0$.

Proof: It follows from Corollary 3.3 that

$$Q(\zeta) = \zeta^{-1} A\psi \langle \cdot, B_1 \sigma_3 \psi \rangle + Q_c(\zeta),$$

where $Q_c(\zeta)$ is bounded for small $|\zeta|$. Then for Re $\zeta > 0$, we have

$$Q_1(\zeta) = [I + \epsilon \zeta^{-1}(I + \epsilon Q_c(\zeta))^{-1} A\psi \langle \cdot, B_1 \sigma_3 \psi \rangle]^{-1} (I + \epsilon Q_c(\zeta))^{-1} Q(\zeta), \tag{3.10}$$

which can be extended meromorphically from Re $\zeta > 0$ to Re $\zeta \leqslant 0$. By Fredholm theorem, the first factor on the right-hand side of (3.10) has singularities at $\zeta = \zeta(\epsilon)$, where $\zeta(\epsilon)$ is the solution of the linear equation,

$$\zeta + \epsilon \langle \psi, V_1^* \sigma_3 \psi \rangle - \epsilon^2 \langle Q_c(0) A\psi, B_1 \sigma_3 \psi \rangle + \mathrm{O}(\epsilon^3) = 0. \tag{3.11}$$

By implicit function theorem, there is a unique solution $\zeta = \zeta(\epsilon)$ for small ϵ, such that

$$\zeta(\epsilon) = -\epsilon \langle \psi, V_1^* \sigma_3 \psi \rangle + 0(\epsilon^2). \tag{3.12}$$

The map $\zeta = \sqrt{\omega - z}$ transforms the domain $\mathcal{D} = \{z \in \mathbb{C} : z \notin [\omega, \infty)\}$ into the first sheet of the Riemann surface $\mathcal{D}_1 = \{\zeta \in \mathbb{C} : \mathrm{Re}\, \zeta > 0\}$, which is connected with the second sheet $\mathcal{D}_2 = \{\zeta \in \mathbb{C} : \mathrm{Re}\, \zeta < 0\}$. When the root of (3.11) belongs to $\mathcal{D}_1$, the corresponding point $z \in \mathcal{D}$ is the eigenvalue of $\mathcal{L}_1$, at least for small ϵ, since the singularities of $\mathcal{Q}_1(z) = A\mathcal{R}_1(z)B_1^*$ coincide with the singularities of $\mathcal{R}_1(z)$. When the root of (3.11) belongs to $\mathcal{D}_2$, the corresponding point z belongs to the compliment of the closure of $\mathcal{D}$ in the Riemann surface, which continues $\mathcal{D}$ across $z \in [\omega, \infty)$. As a result, it does not belong to the closure of $\mathcal{D}$, such that it is not an eigenvalue. ■

Proposition 3.5: If $\epsilon > 0$ *and* $\langle \psi, V_1^* \sigma_3 \psi \rangle < 0$, *the new eigenvalue* $z(\epsilon)$ *with the corresponding eigenvector* $\psi_\epsilon(x)$ *has the positive energy norm* (1.7), *such that*

$$\langle \psi_\epsilon, \mathcal{H} \psi_\epsilon \rangle > 0, \quad \forall\ \epsilon > 0. \tag{3.13}$$

Proof: Using (3.5), we look for a solution of the problem:

$$(I + AR_0(\zeta(\epsilon))(B^* + \epsilon B_1^*))(\Psi + \tilde{\Psi}_\epsilon) = 0,$$

where $\Psi = -A\psi$ and $\tilde{\Psi}_\epsilon \in [\mathrm{Ker}(I + Q_0^*)]^\perp$. Projecting the equation on $[\mathrm{Ker}(I + Q_0^*)]^\perp$ with operator $\mathcal{P}_0^*$, we have the problem,

$$F(\tilde{\Psi}_\epsilon, \epsilon) = \mathcal{P}_0^*(I + AR_0(\zeta(\epsilon))(B^* + \epsilon B_1^*))\tilde{\Psi}_\epsilon + \epsilon \mathcal{P}_0^* A R_0(\zeta(\epsilon)) B_1^* \Psi + \mathcal{P}_0^* A[R_0(\zeta(\epsilon)) - R_0] B^* \Psi = 0,$$

where $F(0,0) = 0$ and

$$\frac{\partial F}{\partial \tilde{\Psi}_\epsilon}(0,0) = \mathcal{P}_0^*(I + Q_0^*).$$

Since $\mathcal{P}_0^*(I + Q_0^*)$ is an isomorphism in $[\mathrm{Ker}(I + Q_0^*)]^\perp$, the function $\tilde{\Psi}_\epsilon$ is a smooth function of ϵ, by implicit function theorem. Therefore, we define

$$\psi_\epsilon = R_0(\zeta(\epsilon))(B^* + \epsilon B_1^*)(\Psi + \tilde{\Psi}_\epsilon).$$

Since $R_0(\zeta(\epsilon)) \in B(L_s^2, H_{-s}^2)$ and $(B^* + \epsilon B_1^*)(\Psi + \tilde{\Psi}_\epsilon) \in L_s^2, s > \frac{1}{2}$ are continuous in ϵ at $\epsilon = 0$, we conclude that

$$\lim_{\epsilon\to 0^+} \boldsymbol{\psi}_\epsilon(x) = \boldsymbol{\psi}(x), \quad \boldsymbol{\psi}_\epsilon \in L^2_{-s}, \quad s > \tfrac{1}{2}.$$

It follows from the system (2.13) and (2.14) in the case (2.16) that $\psi_1 \notin L^2(\mathbb{R})$ and $\psi_2 \in L^2(\mathbb{R})$. By Fatou lemma, we have the limit

$$\lim_{\epsilon\to 0} \langle \boldsymbol{\psi}_\epsilon, \mathcal{H}\boldsymbol{\psi}_\epsilon\rangle = \omega\|\psi_1\|^2_{L^2} - \omega\|\psi_2\|^2_{L^2} = +\infty.$$

By continuity, the inequality (3.13) holds for $\epsilon > 0$. ■

IV. BIFURCATION OF A SIMPLE EIGENVALUE

Here we assume that $\mathrm{Ker}(I+R_0V) \subseteq H^1_0$, such that $z=\omega$ is an eigenvalue of $\sigma_p(\mathcal{L})$. Let $\psi \in \mathrm{Ker}(\mathcal{L}-\omega) \subset L^2$ and we assume that $\dim \mathrm{Ker}(\mathcal{L}-\omega) = 1$. Let $\mathcal{P}_0$ be the spectral projection in L^2 onto $\mathrm{Ker}(\mathcal{L}-\omega)$, such that

$$\mathcal{P}_0 = \boldsymbol{\psi}\frac{\langle \cdot, \sigma_3\boldsymbol{\psi}\rangle}{\langle \boldsymbol{\psi}, \sigma_3\boldsymbol{\psi}\rangle}. \tag{4.1}$$

It is proved in Cuccagna *et al.* (2005), Sec. III that a simple eigenvalue has non zero energy (1.7) such that $\langle \boldsymbol{\psi}, \sigma_3\boldsymbol{\psi}\rangle \neq 0$. Since $C_0=0$ in (2.15), it is clear that $R_1V\boldsymbol{\psi}=\mathbf{0}$. Furthermore, we have the following result.

Lemma 4.1: Let $\mathbf{u},\mathbf{v}$ *be two functions in* $H^{-1}_s, s>\frac{5}{2}$, *such that* $R_1\mathbf{u}=R_1\mathbf{v}=0$ *and* $\langle \mathbf{e}_1,\mathbf{u}\rangle = \langle \mathbf{e}_1,\mathbf{v}\rangle = 0$, *where* $\mathbf{e}_1=(1,0)^T$. *Then,*

$$\langle R_2\mathbf{u},\mathbf{v}\rangle = -\langle R_0\mathbf{u}, R_0\mathbf{v}\rangle. \tag{4.2}$$

Proof: The proof is given with a direct computation

$$\langle R_2\mathbf{u},\mathbf{v}\rangle = \lim_{\zeta\to 0} \zeta^{-2}\langle [R_0(\zeta)-R_0]\mathbf{u},\mathbf{v}\rangle = \lim_{\zeta\to 0} \zeta^{-2}\left\langle \sigma_3 \begin{bmatrix} \frac{1}{p^2+\zeta^2} - \frac{1}{p^2} & 0 \\ 0 & \frac{1}{p^2+2\omega-\zeta^2} - \frac{1}{p^2+2\omega} \end{bmatrix} \hat{\mathbf{u}}, \hat{\mathbf{v}} \right\rangle$$

$$= -\left\langle \begin{bmatrix} \frac{1}{p^4} & 0 \\ 0 & \frac{1}{(p^2+2\omega)^2} \end{bmatrix} \hat{\mathbf{u}}, \hat{\mathbf{v}} \right\rangle = -\langle R_0\mathbf{u}, R_0\mathbf{v}\rangle,$$

where $\hat{\mathbf{u}}(p)$ is the Fourier transform of $\mathbf{u}(x)$, defined by (2.6). ■

We apply the splitting of $H^1_{-s}, s>-\frac{1}{2}$, defined by (2.19), with projection $\mathcal{S}_0$ to $\mathrm{Ker}(I+R_0V)$, such that $\mathcal{S}=\mathcal{I}-\mathcal{S}_0$.

Lemma 4.2: The following statements are true:

(i) $\mathcal{P}_0^*V^*R_2\sigma_3V\mathcal{P}_0 = -\mathcal{P}_0^*\sigma_3\mathcal{P}_0$ *and* $\mathcal{S}_0^*V^*\sigma_3R_2V\mathcal{S}_0 = -\mathcal{S}_0^*\sigma_3\mathcal{S}_0$.
(ii) *Operator* $\mathcal{S}_0^*\sigma_3\mathcal{S}_0$ *is invertible in* $\mathcal{B}(\mathcal{S}_0H^1_{-s}, \mathcal{S}_0^*H^{-1}_s)$, *with the inverse* $\mathcal{P}_0\sigma_3$.

Proof: To prove (i), we note that $\sigma_3V\mathcal{P}_0\mathbf{u}$ and $V\mathcal{P}_0\mathbf{v}$ for any $\mathbf{u},\mathbf{v} \in H^1_{-s}, s>-\frac{1}{2}$ satisfy assumptions of Lemma 4.1 and, therefore,

$$\langle R_2\sigma_3 V\mathcal{P}_0\mathbf{u}, V\mathcal{P}_0\mathbf{v}\rangle = -\langle R_0\sigma_3 V\mathcal{P}_0\mathbf{u}, R_0 V\mathcal{P}_0\mathbf{v}\rangle = -\langle \sigma_3\mathcal{P}_0\mathbf{u}, \mathcal{P}_0\mathbf{v}\rangle = -\langle \mathcal{P}_0^*\sigma_3\mathcal{P}_0\mathbf{u}, \mathbf{v}\rangle.$$

The second part of (i) follows from the relations $\mathcal{P}_0\mathcal{S}_0=\mathcal{S}_0$ and $\mathcal{S}_0^*\mathcal{P}_0^*=\mathcal{S}_0^*$.

To prove (ii), let $\boldsymbol{\phi}\in\mathcal{S}_0^*H_s^{-1}\subseteq\mathrm{Ker}(I+V^*R_0)$ be the dual of $\boldsymbol{\psi}$, such that $\langle\boldsymbol{\psi},\boldsymbol{\phi}\rangle=1$. Therefore,

$$\mathcal{S}_0=\boldsymbol{\psi}\langle\cdot,\boldsymbol{\phi}\rangle,\quad \mathcal{S}_0^*=\boldsymbol{\phi}\langle\cdot,\boldsymbol{\psi}\rangle,\quad \mathcal{S}_0^*\sigma_3\mathcal{S}_0=\boldsymbol{\phi}\langle\cdot,\boldsymbol{\phi}\rangle\langle\boldsymbol{\psi},\sigma_3\boldsymbol{\psi}\rangle,$$

such that

$$(\mathcal{S}_0^*\sigma_3\mathcal{S}_0)^{-1}=\boldsymbol{\psi}\frac{\langle\cdot,\boldsymbol{\psi}\rangle}{\langle\boldsymbol{\psi},\sigma_3\boldsymbol{\psi}\rangle}=\mathcal{P}_0\sigma_3.$$

■

Lemma 4.3: The following expansion is valid in $\mathcal{B}(H^1_{-s},H^1_{-s})$ for $s>\frac{5}{2}$ near $\zeta=0$:

$$(I+R_0(\zeta)V)^{-1}=-\zeta^{-2}\mathcal{P}_0V+\zeta^{-1}\mathcal{P}_0VR_3V\mathcal{P}_0V+\mathrm{O}(1),\quad \mathrm{Re}\,\zeta>0. \tag{4.3}$$

Proof: The proof is similar to that of Lemma 3.2. Let

$$\mathcal{X}=\mathcal{S}H^1_{-s}\oplus\mathcal{S}_0H^1_{-s}=H^1_{-s},\quad \mathcal{Y}=\mathcal{S}H^1_{-s}\oplus\mathcal{S}_0^*H_s^{-1}$$

and

$$\mathcal{B}=\begin{bmatrix}\mathcal{S} & 0\\ 0 & \zeta^{-1}\mathcal{S}_0\end{bmatrix},\quad \mathcal{C}=\begin{bmatrix}\mathcal{S} & 0\\ 0 & \zeta^{-1}\mathcal{S}_0^*V^*\sigma_3\end{bmatrix}.$$

If $\mathcal{S}\mathbf{u}=\mathbf{0}$, then $\mathbf{u}\in\mathrm{Ker}(I+R_0V)$ and $V^*\sigma_3$ is injective in $\mathrm{Ker}(I+V^*R_0)$ by Lemma 2.1. As a result, $\mathcal{B}:\mathcal{X}\mapsto\mathcal{X}$ is surjective, while $\mathcal{C}:\mathcal{X}\mapsto\mathcal{Y}$ is injective. Let $\mathcal{A}\equiv\mathcal{C}(I+R_0(\zeta)V)\mathcal{B}$. Using the Taylor series expansion (2.10), we have

$$\mathcal{A}=\mathcal{A}_0-\zeta\mathcal{A}_1+\mathrm{O}(\zeta^2),$$

where

$$\mathcal{A}_0=\begin{bmatrix}\mathcal{S}(I+R_0V)\mathcal{S} & 0\\ 0 & \mathcal{S}_0^*V^*\sigma_3R_2V\mathcal{S}_0\end{bmatrix},\quad \mathcal{A}_1=\begin{bmatrix}\mathcal{S}R_1V\mathcal{S} & 0\\ 0 & \mathcal{S}_0^*V^*\sigma_3R_3V\mathcal{S}_0\end{bmatrix}.$$

By Neumann expansions, we have $\mathcal{A}^{-1}=\mathcal{A}_0^{-1}+\zeta\mathcal{A}_0^{-1}\mathcal{A}_1\mathcal{A}_0^{-1}+\mathrm{O}(\zeta^2)$, such that

$$\mathcal{A}^{-1}=\begin{bmatrix}\mathcal{K}_0 & 0\\ 0 & -(\mathcal{S}_0^*\sigma_3\mathcal{S}_0)^{-1}\end{bmatrix}+\zeta\begin{bmatrix}\mathcal{K}_0\mathcal{S}R_1V\mathcal{S}\mathcal{K}_0 & 0\\ 0 & (\mathcal{S}_0^*\sigma_3\mathcal{S}_0)^{-1}\mathcal{S}_0^*V^*\sigma_3R_3V\mathcal{S}_0(\mathcal{S}_0^*\sigma_3\mathcal{S}_0)^{-1}\end{bmatrix}+\mathrm{O}(\zeta^2),$$

where $\mathcal{K}_0=(\mathcal{S}(I+R_0V)\mathcal{S})^{-1}$. Since $(I+R_0(\zeta)V)^{-1}=\mathcal{B}\mathcal{A}^{-1}\mathcal{C}$, the expansion (4.3) holds. ■

Using (2.7), (2.10), and (4.3), as well as $\mathcal{P}_0VR_0=-\mathcal{P}_0$ and $\mathcal{P}VR_1=0$, we have the following result.

Corollary 4.4: The following expansion is valid in $\mathcal{B}(H_s^{-1},H^1_{-s})$ for $s>\frac{5}{2}$ near $\zeta=0$:

$$R(\zeta)=\zeta^{-2}\mathcal{P}_0-\zeta^{-1}\mathcal{P}_0VR_3V\mathcal{P}_0+\mathrm{O}(1),\quad \mathrm{Re}\,\zeta>0. \tag{4.4}$$

Similar to Sec. III, we use Corollary 4.4 and consider the family of operators $\mathcal{L}_1=\mathcal{L}+\epsilon V_1(x)$, where the perturbation potential $V_1(x)$ satisfies the same assumption as the potential $V(x)$, while the unperturbed operator $\mathcal{L}$ has a simple eigenvalue. Let $\mathcal{R}_1(z)=(\mathcal{L}_1-z)^{-1}$ and define $\mathcal{Q}(z)=A\mathcal{R}(z)B_1^*$ and $\mathcal{Q}_1(z)=A\mathcal{R}_1(z)B_1^*=(I+\epsilon\mathcal{Q}(z))^{-1}\mathcal{Q}(z)$, where $V_1=B_1^*A$. As in Sec. III, functions $Q(\zeta)$ and $Q_1(\zeta)$ can be meromorphically extended from $\mathrm{Re}\,\zeta>0$ to $\mathrm{Re}\,\zeta\leqslant 0$. The main result of this section is formulated in the following proposition.

Proposition 4.5: Let ϵ be a small positive parameter and let $\langle R_3V\boldsymbol{\psi},V^*\sigma_3\boldsymbol{\psi}\rangle\neq 0$. Then,

(i) *eigenvalue at $z=\omega$ disappears as $\epsilon\neq 0$.*

(ii) *Let* $\langle \psi, \sigma_3 \psi \rangle < 0$. *Then* $\sigma_p(\mathcal{L}_1)$ *near* $z=\omega$ *includes one real eigenvalue* $z(\epsilon) < \omega$ *if* $\langle \psi, V_1^* \sigma_3 \psi \rangle > 0$ *and two complex eigenvalues* $z_{1,2}(\epsilon)$ *if* $\langle \psi, V_1^* \sigma_3 \psi \rangle < 0$. *Asymptotic approximations of the eigenvalues* $z(\epsilon)$ *and* $z_{1,2}(\epsilon)$ *are given by*

$$z(\epsilon) = \omega + \epsilon \frac{\langle \psi, V_1^* \sigma_3 \psi \rangle}{\langle \psi, \sigma_3 \psi \rangle} + \mathrm{O}(\epsilon^{3/2}) \tag{4.5}$$

and

$$\mathrm{Re}(z_{1,2}(\epsilon)) = \omega + \epsilon \frac{\langle \psi, V_1^* \sigma_3 \psi \rangle}{\langle \psi, \sigma_3 \psi \rangle} + \mathrm{O}(\epsilon^2), \tag{4.6}$$

$$\mathrm{Im}(z_{1,2}(\epsilon)) = \pm \epsilon^{3/2} \sqrt{\frac{\langle \psi, V_1^* \sigma_3 \psi \rangle}{\langle \psi, \sigma_3 \psi \rangle}} \frac{\langle R_3 V \psi, V^* \sigma_3 \psi \rangle \langle \psi, V_1^* \sigma_3 \psi \rangle}{\langle \psi, \sigma_3 \psi \rangle^2} + \mathrm{O}(\epsilon^2). \tag{4.7}$$

(iii) *Let* $\langle \psi, \sigma_3 \psi \rangle > 0$. *Then* $\sigma_p(\mathcal{L}_1)$ *near* $z=\omega$ *includes one real eigenvalue* $z(\epsilon) < \omega$, *given by* (4.5), *if* $\langle \psi, V_1^* \sigma_3 \psi \rangle < 0$ *and no eigenvalues if* $\langle \psi, V_1^* \sigma_3 \psi \rangle > 0$.

The proof of Proposition is based on the following elementary result.

Lemma 4.6: Consider a quadratic equation,

$$\zeta^2 - \epsilon \zeta F(\epsilon, \zeta) + \epsilon G(\epsilon, \zeta) = 0, \tag{4.8}$$

where $F(\epsilon, \zeta)$ *and* $G(\epsilon, \zeta)$ *are analytic in* ϵ *and* ζ *at the point* (0, 0), *such that* $G(0,0) \neq 0$ *and*

$$\left. \frac{\partial F(0,\zeta)}{\partial \zeta} \right|_{\zeta=0} = \left. \frac{\partial G(0,\zeta)}{\partial \zeta} \right|_{\zeta=0} = 0. \tag{4.9}$$

Then, for small ϵ, *the quadratic equation* (4.8) *has exactly two solutions* $\zeta_{1,2}(\epsilon)$, *such that* $|\zeta_j(\epsilon) - \zeta_{j0}(\epsilon)| = \mathrm{O}(\epsilon^{3/2})$, *where* $\zeta_{j0}(\epsilon), j=1, 2$, *are solutions of the quadratic equation*

$$\zeta^2 - \epsilon \zeta F(0,0) + \epsilon G(0,0) = 0. \tag{4.10}$$

Proof: Let $\mu = \epsilon^{1/2}$ and substitute $\zeta = \mu \xi$. Introducing another parameter λ, we rewrite the quadratic equation (4.8) in the form,

$$\xi^2 - \mu \xi F(\lambda \mu^2, \lambda \mu \xi) + G(\lambda \mu^2, \lambda \mu \xi) = 0. \tag{4.11}$$

The case $\lambda = 1$ gives (4.8), while the case $\lambda = 0$ gives (4.10). Since $G(0,0) \neq 0$ by assumption, there exist two analytical solutions of (4.11), by the implicit function theorem, which are defined for small $\mu > 0$ and $\lambda \in [0,1]$. Since

$$\xi(1,\mu) - \xi(0,\mu) = \int_0^1 \partial_\lambda \xi(\lambda, \mu) \mathrm{d}\lambda,$$

we apply implicit differentiation of (4.11) and find that

$$\begin{aligned} &[2\xi - \mu F(\lambda \mu^2, \lambda \mu \xi) - \lambda \mu^2 \xi \partial_2 F(\lambda \mu^2, \lambda \mu \xi) + \lambda \mu \partial_2 G(\lambda \mu^2, \lambda \mu \xi)] \partial_\lambda \xi - \mu^3 \xi \partial_1 F(\lambda \mu^2, \lambda \mu \xi) \\ &\quad - \mu^2 \xi^2 \partial_2 F(\lambda \mu^2, \lambda \mu \xi) + \mu^2 \partial_1 G(\lambda \mu^2, \lambda \mu \xi) + \mu \xi \partial_2 G(\lambda \mu^2, \lambda \mu \xi) = 0, \end{aligned}$$

where ∂_1 and ∂_2 are derivatives in the first and second arguments. Under constraints (4.9), we have $\partial_\lambda \xi = \mathrm{O}(\mu^2)$, such that $|\zeta(1,\mu) - \zeta(0,\mu)| = \mathrm{O}(\mu^3)$. ■

Proof of Proposition 4.5: It follows from Corollary 4.4 that

$$Q(\zeta) = \zeta^{-2} A \mathcal{P}_0 B_1^* - \zeta^{-1} A \mathcal{P}_0 V R_3 V \mathcal{P}_0 B_1^* + Q_c(\zeta), \tag{4.12}$$

where $Q_c(\zeta)$ is bounded for small ζ. As a result, for $\mathrm{Re}\, \zeta > 0$, we have

$$Q_1(\zeta) = [I + \epsilon(I + \epsilon Q_c(\zeta))^{-1}[\zeta^{-2}A\mathcal{P}_0B_1^* - \zeta^{-1}A\mathcal{P}_0VR_3V\mathcal{P}_0B_1^*]]^{-1}(I + \epsilon Q_c(\zeta))^{-1}Q(\zeta),$$

which can be extended meromorphically for Re $\zeta \leqslant 0$. Singularities of $Q_1(\zeta)$ near $\zeta = 0$ correspond to zeros of

$$\det\left[\zeta^2 + \epsilon(I + \epsilon Q_c(\zeta))^{-1}\left(A\psi\frac{\langle B_1^*\cdot, \sigma_3\psi\rangle}{\langle\psi, \sigma_3\psi\rangle} - \zeta A\psi\frac{\langle R_3V\mathcal{P}_0B_1^*\cdot, V^*\sigma_3\psi\rangle}{\langle\psi, \sigma_3\psi\rangle}\right)\right].$$

The determinant equation can be written as the quadratic equation (4.8), where $F(\epsilon, \zeta)$ and $G(\epsilon, \zeta)$ are defined for Re $\zeta > 0$ as

$$F(\epsilon, \zeta) = \frac{\langle R_3V\psi, V^*\sigma_3\psi\rangle}{\langle\psi, \sigma_3\psi\rangle^2}\langle B_1^*(I + \epsilon Q_c(\zeta))^{-1}A\psi, \sigma_3\psi\rangle, \tag{4.13}$$

$$G(\epsilon, \zeta) = \frac{1}{\langle\psi, \sigma_3\psi\rangle}\langle B_1^*(I + \epsilon Q_c(\zeta))^{-1}A\psi, \sigma_3\psi\rangle, \tag{4.14}$$

and they can be analytically continued to Re $\zeta \leqslant 0$. It is clear from (4.13) and (4.14) that

$$F(0, \zeta) = \frac{\langle R_3V\psi, V^*\sigma_3\psi\rangle\langle\psi, V_1^*\sigma_3\psi\rangle}{\langle\psi, \sigma_3\psi\rangle^2}, \quad G(0, \zeta) = \frac{\langle\psi, V_1^*\sigma_3\psi\rangle}{\langle\psi, \sigma_3\psi\rangle},$$

such that the condition (4.9) is satisfied. By Lemma 4.6, there exist two solutions of (4.8) in the $O(\epsilon^{3/2})$-neighborhood of solutions of (4.10), when $\langle\psi, V_1^*\sigma_3\psi\rangle \neq 0$. Solutions of (4.10) are expanded as

$$\zeta_{\pm 0}(\epsilon) = \pm\epsilon^{1/2}\sqrt{-\frac{\langle\psi, V_1^*\sigma_3\psi\rangle}{\langle\psi, \sigma_3\psi\rangle}} + \frac{\epsilon}{2}\frac{\langle R_3V\psi, V^*\sigma_3\psi\rangle\langle\psi, V^*\sigma_3\psi\rangle}{\langle\psi, \sigma_3\psi\rangle^2} + O(\epsilon^{3/2}). \tag{4.15}$$

When $\langle\psi, V_1^*\sigma_3\psi\rangle/\langle\psi, \sigma_3\psi\rangle < 0$, there is a unique real eigenvalue of operator $\mathcal{L}_1$ in the neighborhood of $z = \omega$, such that $z = \omega - \zeta_{+0}^2 + O(\epsilon^{3/2})$, which results in (4.5). The other solution $\zeta_{-0}(\epsilon)$ corresponds to Re $\zeta < 0$ and, by arguments in the proof of Proposition 3.4, it does not correspond to an eigenvalue of operator $\mathcal{L}_1$.

When $\langle\psi, V_1^*\sigma_3\psi\rangle/\langle\psi, \sigma_3\psi\rangle > 0$, we have to consider the $O(\epsilon)$ term of the asymptotic expansion (4.15). Due to the constraint $C_0 = 0$ in (2.15), we have

$$\langle R_3V\psi, V^*\sigma_3\psi\rangle = -\frac{1}{12\pi}\sum_{j=1}^{3}|(x_j, f\psi_1 + g\psi_2)|^2 \leqslant 0. \tag{4.16}$$

Since $\langle R_3V\psi, V^*\sigma_3\psi\rangle \neq 0$, then $\langle R_3V\psi, V^*\sigma_3\psi\rangle < 0$. Therefore, it follows from (4.15) that

$$\text{Im } \zeta_{\pm 0}(\epsilon) = \pm\epsilon^{1/2}\sqrt{\frac{\langle\psi, V_1^*\sigma_3\psi\rangle}{\langle\psi, \sigma_3\psi\rangle}} + O(\epsilon^{3/2}),$$

$$\text{Re } \zeta_{\pm 0}(\epsilon) = \frac{\epsilon}{2}\frac{\langle R_3V\psi, V^*\sigma_3\psi\rangle\langle\psi, V_1^*\sigma_3\psi\rangle}{\langle\psi, \sigma_3\psi\rangle^2} + O(\epsilon^{3/2}).$$

In the case $\langle\psi, \sigma_3\psi\rangle > 0$ and $\langle\psi, \mathbf{V}_1^*\sigma_3\psi\rangle > 0$, we have Re $\zeta_{\pm 0} < 0$, such that no eigenvalues of $\mathcal{L}_1$ exist in the neighborhood of $z = \omega$. In the case $\langle\psi, \sigma_3\psi\rangle < 0$ and $\langle\psi, V_1^*\sigma_3\psi\rangle < 0$, we have Re $\zeta_{\pm 0} > 0$, such that two complex eigenvalues of $\mathcal{L}_1$ exist in the neighborhood of $z = \omega$, with the asymptotic approximations (4.6) and (4.7). ■

A more special result occurs in the case when $\langle R_3V\psi, V^*\sigma_3\psi\rangle = 0$, which includes spherically

symmetric potential $V(x)$ with spherically symmetric eigenvector $\boldsymbol{\psi}(x)$, see (4.16). In order to study this special case, we need to extend the theory of wave operators from Kato (1966) and Cuccagna *et al.* (2005). Following Cuccagna *et al.* (2005), we consider a decomposition of L^2 into the $\mathcal{L}$-invariant Jordan blocks:

$$L^2 = \sum_{z \in \sigma_p(\mathcal{L})} N_g(\mathcal{L} - z) \oplus X_c(\mathcal{L}), \quad X_c(\mathcal{L}) = \left[\sum_{z \in \sigma_p(\mathcal{L})} N_g(\mathcal{L}^* - z) \right]^{\perp}, \tag{4.17}$$

and, equivalently,

$$L^2 = \sum_{z \in \sigma_p(\mathcal{L})} N_g(\mathcal{L}^* - z) \oplus X_c(\mathcal{L}^*), \quad X_c(\mathcal{L}^*) = \left[\sum_{z \in \sigma_p(\mathcal{L})} N_g(\mathcal{L} - z) \right]^{\perp}, \tag{4.18}$$

where $\sigma_p(\mathcal{L}) = \sigma_p(\mathcal{L}^*)$ and $N_g(\mathcal{L} - z) = \cup_{n=1}^{+\infty} \mathrm{Ker}(\mathcal{L} - z)^n$. The invariant splittings (4.17) and (4.18) hold in the assumption that $\sigma_p(\mathcal{L}) \cap \sigma_e(\mathcal{L})$ is a union of simple eigenvalues, such that $N_g(\mathcal{L} - z) = \mathrm{Ker}(\mathcal{L} - z)$ for $z \in \mathcal{D}_e$. The action of $\mathcal{L}$ in $X_c(\mathcal{L})$ is given by the scattering theory of wave operators Kato (1966), which is based on the following existence result.

Lemma 4.7: Let $A(x)$ and $B(x)$ be exponentially decaying potentials and $\sigma_p(\mathcal{L}) \cap \sigma_e(\mathcal{L})$ be a union of simple eigenvalues, which includes the endpoints $z = \pm\omega$ without resonance. Let $\langle R_3 V \boldsymbol{\psi}, V^* \sigma_3 \boldsymbol{\psi} \rangle = 0$. There exist isomorphisms $W: L^2 \mapsto X_c(\mathcal{L})$ and $Z: X_c(\mathcal{L}) \mapsto L^2$, which are inverse of each other, defined as follows:

$$\forall u \in L^2, \forall v \in X_c(\mathcal{L}^*), \langle Wu, v \rangle = \langle u, v \rangle + \lim_{\epsilon \to 0^+} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \langle A(\mathcal{L}_0 - \lambda - i\epsilon)^{-1} u, B(\mathcal{L}^* - \lambda + i\epsilon)^{-1} v \rangle \mathrm{d}\lambda, \tag{4.19}$$

and

$$\forall u \in X_c(\mathcal{L}), \forall v \in L^2, \langle Zu, v \rangle = \langle u, v \rangle + \lim_{\epsilon \to 0^+} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \langle A(\mathcal{L} - \lambda - i\epsilon)^{-1} u, B(\mathcal{L}_0 - \lambda + i\epsilon)^{-1} v \rangle \mathrm{d}\lambda. \tag{4.20}$$

We prove this result in Sec. V. Using Lemma 4.7, we consider bifurcation of the simple eigenvalue in the special case when $\langle R_3 V \boldsymbol{\psi}, V^* \sigma_3 \boldsymbol{\psi} \rangle = 0$.

Proposition 4.8: Let ϵ be a small positive parameter and $\langle R_3 V \boldsymbol{\psi}, V^* \sigma_3 \boldsymbol{\psi} \rangle = 0$. Then, Proposition 4.5 holds, but the asymptotic expansion (4.7) *is modified as follows*:

$$\mathrm{Im}(z_{1,2}(\epsilon)) = \pm \epsilon^{5/2} \frac{2\pi^2 |\hat{\psi}_1(0)|^2}{\langle \boldsymbol{\psi}, \sigma_3 \boldsymbol{\psi} \rangle} \sqrt{\frac{\langle \boldsymbol{\psi}, V_1^* \sigma_3 \boldsymbol{\psi} \rangle}{\langle \boldsymbol{\psi}, \sigma_3 \boldsymbol{\psi} \rangle}} + \mathrm{O}(\epsilon^3), \tag{4.21}$$

where $\tilde{\boldsymbol{\psi}} = Z \mathcal{P}_c V_1 \boldsymbol{\psi}$ and $\hat{\boldsymbol{\psi}}(p)$ is the Fourier transform of $\tilde{\boldsymbol{\psi}}(x)$.

Proof: We use the splittings (4.17) and (4.18) and define operator $\mathcal{P}_c$ as the projection of L^2 on $X_c(\mathcal{L})$. It is clear from (4.12) that

$$Q_c(\zeta) = A(\mathcal{I} - \mathcal{P}_0) R(\zeta) B_1^* = \sum_{z \in \sigma_p(\mathcal{L}) \setminus \{\omega\}} A \mathcal{P}_z R(\zeta) B_1^* + A P_c \mathcal{R}(\zeta) B_1^*.$$

In the special case $\langle R_3 V \boldsymbol{\psi}, V^* \sigma_3 \boldsymbol{\psi} \rangle = 0$, the quadratic equation (4.8) has $F(\epsilon, \zeta) = 0$ and

$$G(\epsilon, \zeta) = G(0, \zeta) + \epsilon \partial_1 G(0, \zeta) + \mathrm{O}(\epsilon^2),$$

where

$$G(0,\zeta) = \frac{\langle \psi, V_1^* \sigma_3 \psi \rangle}{\langle \psi, \sigma_3 \psi \rangle},$$

and

$$\partial_1 G(0,\zeta) = -\frac{\langle B_1^* Q_c(\zeta) A\psi, \sigma_3 \psi \rangle}{\langle \psi, \sigma_3 \psi \rangle} = -\frac{\langle (\mathcal{I} - \mathcal{P}_0) R(\zeta) V_1 \psi, V_1^* \sigma_3 \psi \rangle}{\langle \psi, \sigma_3 \psi \rangle}.$$

The term $\partial_1 G(0,\zeta)$ consists of the contribution from all eigenvalues of $\sigma_p(\mathcal{L})$ different from $z = \omega$ and from the contribution from $X_c(\mathcal{L})$. The first contribution can be estimated as follows:

$$\mathrm{Im} \sum_{z \in \sigma_p(\mathcal{L}) \setminus \{\omega\}} \langle \mathcal{P}_z R(\zeta) V_1 \psi, V_1^* \sigma_3 \psi \rangle = \mathrm{O}(\zeta^2).$$

This estimate is based on the expansion for real-valued $V_1(x)$ and $\psi(x)$ [see Cuccagna *et al.* (2005)],

$$\sum_{z \in \sigma_p(\mathcal{L}) \setminus \{\omega\}} \langle \mathcal{P}_z \mathcal{R}(z) V_1 \psi, V_1^* \sigma_3 \psi \rangle = \sum_{z_j \in \mathbb{R}} (z - z_j)^{-1} \langle P_{z_j} V_1 \psi, V^* \sigma_3 \psi \rangle + \sum_{z_j \in \mathbb{C}} [(z - z_j)^{-1} \langle P_{z_j} V_1 \psi, V^* \sigma_3 \psi \rangle + (z - \overline{z_j})^{-1} \langle P_{\overline{z_j}} V_1 \psi, V^* \sigma_3 \psi \rangle]. \tag{4.22}$$

Since $\mathcal{P}_{z_j} \sigma_3$ is self-adjoint for $z_j \in \mathbb{R}$, the factor $\langle P_{z_j} V_1 \psi, V^* \sigma_3 \psi \rangle$ is real. Then, the first term in (4.22) has the imaginary part of order $\mathrm{O}(\mathrm{Im}\, z)$ or $\mathrm{O}(\zeta^2)$ for $z = \omega - \zeta^2$. Similarly, the operator $(\mathrm{Re}\, z - z_j)^{-1} \mathcal{P}_{z_j} \sigma_3 + (\mathrm{Re}\, z - \overline{z_j})^{-1} \mathcal{P}_{\overline{z_j}} \sigma_3$ is self-adjoint for $z_j \in \mathbb{C}$, such that the second term in (4.22) has the imaginary part of order $\mathrm{O}(\mathrm{Im}\, z)$ or $\mathrm{O}(\zeta^2)$. The second contribution in $\partial_1 G(0,\zeta)$ can be estimated by using wave operators, which satisfy the following identities [Cuccagna *et al.* (2005)]:

$$P_c^* \sigma_3 = \sigma_3 P_c, \quad W^* \sigma_3 = \sigma_3 Z, \quad Z^* \sigma_3 = \sigma_3 W, \quad Z\mathcal{L} = \mathcal{L}_0 Z. \tag{4.23}$$

Since $\mathcal{P}_c V_1 \psi \in X_c(\mathcal{L})$, there exists $\tilde{\psi} \in L^2$, such that $\mathcal{P}_c V_1 \psi = W \tilde{\psi}$. As a result, we have

$$\langle \mathcal{P}_c R(\zeta) V_1 \psi, V_1^* \sigma_3 \psi \rangle = \langle R(\zeta) V_1 \psi, \sigma_3 W \tilde{\psi} \rangle = \langle Z R(\zeta) V_1 \psi, \sigma_3 \tilde{\psi} \rangle = \langle R_0(\zeta) \tilde{\psi}, \sigma_3 \tilde{\psi} \rangle.$$

Since $\langle R_0 \tilde{\psi}, \sigma_3 \tilde{\psi} \rangle$ and $\langle R_1 \tilde{\psi}, \sigma_3 \tilde{\psi} \rangle$ are real valued, we finally have

$$\mathrm{Im}\, \partial_1 G(0,\zeta) = \frac{\langle R_1 \tilde{\psi}, \sigma_3 \tilde{\psi} \rangle}{\langle \psi, \sigma_3 \psi \rangle} \mathrm{Im}\, \zeta + \mathrm{O}(\zeta^2). \tag{4.24}$$

The quadratic equation (4.8) is now read as follows

$$\zeta^2 + \epsilon G(\epsilon, \zeta) = 0. \tag{4.25}$$

In the case $G(0,0) > 0$, we have from Lemma 4.6 that

$$\mathrm{Im}\, \zeta_{1,2}(\epsilon) = \pm \epsilon^{1/2} \sqrt{\frac{\langle \psi, V_1^* \sigma_3 \psi \rangle}{\langle \psi, \sigma_3 \psi \rangle}} + \mathrm{O}(\epsilon^{3/2}),$$

in addition, by expansion (4.24), we have from (4.25) that $2\, \mathrm{Re}\, \zeta\, \mathrm{Im}\, \zeta = -\epsilon^2\, \mathrm{Im}\, \zeta \partial_1 \partial_2 G(0,0) + \mathrm{O}(\epsilon^3, \epsilon^2 \zeta^2)$, such that

$$\mathrm{Re}\, \zeta_{1,2}(\epsilon) = -\frac{\epsilon^2}{2} \frac{\langle R_1 \tilde{\psi}, \sigma_3 \tilde{\psi} \rangle}{\langle \psi, \sigma_3 \psi \rangle} + \mathrm{O}(\epsilon^{5/2}).$$

Direct computations from (2.11) show that

$$\langle R_1\tilde{\boldsymbol{\psi}}, \sigma_3\tilde{\boldsymbol{\psi}}\rangle = \frac{1}{4\pi}\left(\int_{\mathbb{R}^3}\tilde{\psi}_1\,dx\right)\left(\int_{\mathbb{R}^3}\tilde{\psi}_1^*\,dx\right) = 2\pi^2|\hat{\psi}_1(0)|^2 \geqslant 0,$$

where $\hat{\psi}_1(p)$ is the Fourier transform of $\psi_1(x)$, defined by (2.6). Again, we have $\mathrm{Re}\,\zeta_{1,2}(\epsilon) > 0$ in the case $\langle \boldsymbol{\psi}, \sigma_3\boldsymbol{\psi}\rangle < 0$ and $\hat{\psi}_1(0) \neq 0$, such that two complex eigenvalues of $\mathcal{L}_1$ exist in the neighborhood of $z = \omega$, with the asymptotic approximations (4.6) and (4.21). ■

V. PROOF OF LEMMA 4.7

According to Kato (1966), Lemma 4.7 is valid if we can prove that there exists $c > 0$ such that $\forall \epsilon \neq 0$, the following bounds are true:

$$\int_{-\infty}^{\infty} \|A(\mathcal{L}_0 - i\epsilon - \lambda)^{-1}\mathbf{u}\|^2\,d\lambda \leqslant c\|\mathbf{u}\|^2, \quad \mathbf{u} \in L^2, \tag{5.1}$$

$$\int_{-\infty}^{\infty} \|B(\mathcal{L}_0 - i\epsilon - \lambda)^{-1}\mathbf{u}\|^2\,d\lambda \leqslant c\|\mathbf{u}\|^2, \quad \mathbf{u} \in L^2, \tag{5.2}$$

$$\int_{-\infty}^{\infty} \|B(\mathcal{L}^* - i\epsilon - \lambda)^{-1}\mathbf{u}\|^2\,d\lambda \leqslant c\|\mathbf{u}\|^2, \quad \forall\, \mathbf{u} \in X_c(\mathcal{L}^*), \tag{5.3}$$

$$\int_{-\infty}^{\infty} \|A(\mathcal{L} - i\epsilon - \lambda)^{-1}\mathbf{u}\|^2\,d\lambda \leqslant c\|\mathbf{u}\|^2, \quad \forall\, \mathbf{u} \in X_c(\mathcal{L}). \tag{5.4}$$

The bounds (5.1) and (5.2) are proved in Corollary to Theorem XIII.25 in Reed and Simon (1978). We prove the bound (5.4), while the bound (5.3) can be proved similarly. Following Cuccagna *et al.* (2005), we write

$$A(\mathcal{L} - z)^{-1}\mathbf{v} = (I + \mathcal{Q}_0^+(z))^{-1}A(\mathcal{L}_0 - z)^{-1}\mathbf{v}, \quad \mathbf{v} \in X_c(\mathcal{L}), \tag{5.5}$$

where $\mathcal{Q}_0^+(z)$ is continuation of $Q_0(z)$ from $\mathrm{Im}\,z > 0$ to $\mathrm{Im}\,z \geqslant 0$. The operator $(I + \mathcal{Q}_0^+(z))^{-1}$ is uniformly bounded in z away from the eigenvalues of $\sigma_p(\mathcal{L})$. It has pole singularities at the eigenvalues of $\sigma_p(\mathcal{L})$, which were considered in Cuccagna *et al.* (2005), Lemma 4.3. The endpoint eigenvalues $z = \pm\omega$ were excluded from Cuccagna *et al.* (2005). Here we shall consider the eigenvalue $z = \omega$. We need to show that $A(\mathcal{L} - z)^{-1}\mathbf{v}$ has L^2-norm which is uniformly bounded in $\epsilon > 0$, for $\mathrm{Im}\,z = \epsilon$ and $\mathrm{Re}\,z \approx \omega$. Near $z = \omega$, we have the following expansion in the space of operators $L^2 \to L^2$:

$$(I + \mathcal{Q}_0^+(z))^{-1} = \frac{1}{\omega - z}A\mathcal{P}_0B^* + \mathrm{O}(1).$$

Due to the bounds (5.1) and (5.2), we only need to study $(\omega - z)^{-1}A\mathcal{P}_0V\mathcal{R}_0(z)\mathbf{v}$, for $\mathbf{v} \in X_c(\mathcal{L})$ near $z = \omega$. We use the relation

$$\langle VR_0\mathbf{v}, \sigma_3\boldsymbol{\psi}\rangle = -\langle \mathbf{v}, \sigma_3\boldsymbol{\psi}\rangle = 0, \quad \forall\, \mathbf{v} \in X_c(\mathcal{L}).$$

As a result,

$$\frac{1}{\omega - z}\mathcal{P}_0V\mathcal{R}_0(z)\mathbf{v} = \frac{\boldsymbol{\psi}}{\omega - z}\frac{\langle V\mathcal{R}_0(z)\mathbf{v}, \sigma_3\boldsymbol{\psi}\rangle}{\langle \boldsymbol{\psi}, \sigma_3\boldsymbol{\psi}\rangle} = \frac{\boldsymbol{\psi}}{\omega - z}\frac{\langle V|\mathcal{R}_0(z) - R_0|\mathbf{v}, \sigma_3\boldsymbol{\psi}\rangle}{\langle \boldsymbol{\psi}, \sigma_3\boldsymbol{\psi}\rangle} = -\boldsymbol{\psi}\frac{\langle VR_0\mathcal{R}_0(z)\mathbf{v}, \sigma_3\boldsymbol{\psi}\rangle}{\langle \boldsymbol{\psi}, \sigma_3\boldsymbol{\psi}\rangle}$$

$$= \boldsymbol{\psi}\frac{\langle \mathcal{R}_0(z)\mathbf{v}, \sigma_3\boldsymbol{\psi}\rangle}{\langle \boldsymbol{\psi}, \sigma_3\boldsymbol{\psi}\rangle}.$$

We need to show that $\langle \mathcal{R}_0(z)\mathbf{v}, \sigma_3 \boldsymbol{\psi} \rangle$ is in Hardy space H^2 for $\mathrm{Im}\, z > 0$, which is true if $\boldsymbol{\psi}(x)$ belong to the space of Rollnick potentials,

$$\int_{\mathbb{R}} \int_{\mathbb{R}} \frac{|\boldsymbol{\psi}(x)||\boldsymbol{\psi}(x)|}{|x-y|^2} \mathrm{d}x\mathrm{d}y < \infty. \tag{5.6}$$

It is clear from (2.14) that $\psi_2(x)$ decays exponentially as $|x| \to \infty$. Since $C_0 = 0$ in (2.15) and $(x_j, f\psi_1 + g\psi_2) = 0, j = 1, 2, 3$ in (4.16), it follows from (2.13) that $\psi_1(x)$ decays algebraically as $|x|^{-3}$. As a result, the eigenvector $\boldsymbol{\psi}(x)$ satisfies the condition (5.6).

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Erratum: Coherent states on spheres [J. Math. Phys. 43, 1211 (2002)]

Brian C. Hall
University of Notre Dame, Department of Mathematics, Notre Dame, Indiana 46556

Jeffrey J. Mitchell
Department of Mathematics, Baylor University, Waco, Texas 76798

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We have identified three minor errors in our paper, none of which affects the overall logical structure.

First, the differential equation for $\nu(s,R)$ in Theorem 2 contains a sign error. The correct equation is

$$\frac{d\nu(s,R)}{ds} = \frac{1}{2}\left[\frac{\partial^2 \nu}{\partial R^2} + (d-1)\frac{\cosh R}{\sinh R}\frac{\partial \nu}{\partial R}\right].$$

The above equation is the one used in the proof of Theorem 2; compare Lemma 4.

Second, on page 1227, in the proof of Theorem 2, we assert that the operators J_{a}^2 and $J_{\overline{\mathrm{a}}}^2$ are self-adjoint. This is not correct. However, $J_{\mathrm{a}}^2 + J_{\overline{\mathrm{a}}}^2$ *is* self-adjoint, and this is all that is needed in the proof.

Third, in Sec. IX, we assert that the action of the little group is trivial if and only if Eq. (57) holds. This assertion is not correct in the case $d=1$. What we actually prove is that (for all $d \geqslant 1$) the action of the Lie algebra of the little group is trivial if and only if Eq. (57) holds. When $d \geqslant 2$, the little group is connected and so the triviality of the action of the Lie algebra implies the triviality of the action of the little group itself. When $d=1$, however, the little group is disconnected and its action may be nontrivial even when the action of the Lie algebra is trivial.

In the case $d=1$, our results hold under the stronger assumption that the action of the little group is trivial. This assumption implies (but is not implied by) Eq. (57).

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Vittorio Giovannetti
NEST-INFM and Scuola Normale Superiore, Piazza dei Cavalieri 7, I-56126, Pisa, Italy

Seth Lloyd
Massachusetts Institute of Technology, Department of Mechanical Engineering and Research Laboratory of Electronics, Cambridge, Massachusetts 02139

Mary Beth Ruskai
Department of Mathematics, Tufts University, Medford, Massachusetts 02155

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This article was originally published online on 22 March 2005 without some of the authors' proof corrections. These corrections involved (i) Corollary 2, (ii) the matrix in the first complete sentence after Eq. (25), (iii) the phrase preceding Eq. (35), and (iv) horizontal rules in Table I. AIP apologizes for these errors. All online versions of the article have been corrected. The article as it appeared in the printed version of the journal contained all corrections, with the exception of the addition of parentheses around $(1-c)$ in the line preceding Eq. (35).

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Scattering kernel for polyatomic molecules

J. Gilbert Méolans[a] and S. Kokou Dadzie[b]
Université de Provence, UMR CNRS 6595, Département de Mécanique Energétique, 5 rue Enrico Fermi 13453, Marseille Cedex 13, France

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A polyatomic scattering kernel phenomenologically presented in a previous paper is derived from an integral operator formulation. The five parameters involved in the scattering kernel expression are shown to be equal to the accommodation coefficients of various fluxes at the wall, namely, the fluxes of the three components of the momentum and the fluxes of the rotational and vibrational energies of molecules. Under its present form the model is especially convenient for the diatomic molecules. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1904703]

I. INTRODUCTION

During the last 20 years a need of new knowledge appeared concerning the interaction of gases with solid surfaces in order to formulate realistic boundary conditions in rarefied gas dynamics.[1–4] In spatial research the challenge was especially to predict correct heat fluxes and drag forces on engines reentering in planetary atmospheres. With the recent developments of the gaseous microflows, where the flow fields are characterized by moderately high Knudsen numbers, this topic acquired still more interest. This paper is devoted to the derivation of realistic laws linking the distribution functions of the reflected and the incoming particles at the wall. As it is well known such laws may be used as boundary conditions in order to resolve the Boltzmann equation. Moreover, in the slip regime, these laws also allow us to obtain more accurate velocity slip and temperature jumps at the wall, so the validity domain of the continuum equations is extended up to higher Knudsen numbers when these equations are associated to the correct boundary conditions.

In a previous paper[5] we developed a model of a scattering kernel for unstructured molecules using an integral operator formulation as illustrated by Cercignani.[6,7] At the end of this previous work the proposed scattering kernel was extended to the case of molecules with internal structure on the basis of brief phenomenological arguments. In the present paper, the integral operator formulation is generalized to a polyatomic gas, then the polyatomic scattering kernel is methodologically derived from the study of an eigenvalue equation and the meaning of the five parameters introduced in the kernel is clarified.

In Sec. II we deduced the polyatomic scattering kernel, investigating the associated integral operator. In its fully developed form the scattering kernel appears as a linear combination of 32 partial kernels declining all the possible associations of, respectively, diffusive and specular processes (according to three directions) and elastic or inelastic processes (for the internal modes). The 32 coefficients of this combination are the weight of the various accommodation processes and they depend on five basic parameters. These five parameters are shown to be, respectively, equal to the accommodation coefficients of the momentum components and of the internal energies. In Sec. III, we present a general comment on this method of integral operator in the framework of scattering kernel derivation.

[a]Electronic mail: gilbert.meolans@polytech.univ-mrs.fr
[b]Electronic mail: kokou.dadzie@polytech.univ-mrs.fr; URL: http://www.polytech.univ-mrs.fr

II. POLYATOMIC SCATTERING KERNEL DERIVATION

We consider the problem of finding the scattering kernel,

$$B(V',E_{ir'},E_{iv'},g_{ir'},V,E_{ir},E_{iv},g_{ir}),$$

governing the reflection of polyatomic molecules at the wall. V' is the velocity of the impinging gas particle referred to the wall, $V'=(V'_x,V'_y,V'_z)\in\{\Omega'=\Omega'_x\times\Omega'_y\times\Omega'_z=\mathbb{R}_-\times\mathbb{R}\times\mathbb{R}\}$ and V the velocity of the reflected one referred to the wall, $V=(V_x,V_y,V_z)\in\{\Omega=\Omega_x\times\Omega_y\times\Omega_z=\mathbb{R}_+\times\mathbb{R}\times\mathbb{R}\}$. These velocities reduce to the peculiar velocities when the slip velocity at the wall is neglected. V_R is defined as $V_R=(-V_x,V_y,V_z)$, and (x,y,z) are the three spatial coordinates with x the normal axis to the wall oriented from the wall towards the gas. $E_{ir'}$ and $E_{iv'}$ are, respectively, the rotational energy and the vibrational energy of an incident particle at the wall. Similarly E_{ir} and E_{iv} are, respectively, the rotational energy and the vibrational energy of a reflected particle at the wall. Then the subscripts ir and iv are the quantum numbers related to the internal energy of a particle, hence they are integers; g_{ir} is the weight of the rotational degeneracy and will be taken here equal to $(2ir+1)$. The kernel B, which is the density of probability that a molecule in a state $(V',E_{ir'},E_{iv'})$ hitting the wall at any point X of the wall is reflected at the same point in a state (V,E_{ir},E_{iv}), must satisfy the following conditions detailed in Ref. 5:[1–3] the non-negativity,

$$B(V',E_{ir'},E_{iv'},g_{ir'},V,E_{ir},E_{iv},g_{ir})\geqslant 0, \tag{1}$$

the normalization,

$$\sum_{ir,iv}\int_{\Omega}B(V',E_{ir'},E_{iv'},g_{ir'},V,E_{ir},E_{iv},g_{ir})d_V=1, \tag{2}$$

and the reciprocity relation,

$$\begin{aligned}&|V'_x|e^{-\|V'\|^2/C_w^2}e^{-\varepsilon_{ir'}}e^{-\varepsilon_{iv'}}g_{ir'}B(V',E_{ir'},E_{iv'},V,E_{ir},E_{iv})\\&\quad=V_xe^{-\|V\|^2/C_w^2}e^{-\varepsilon_{ir}}e^{-\varepsilon_{iv}}g_{ir}B(-V,E_{ir},E_{iv},-V',E_{ir'},E_{iv'}),\end{aligned} \tag{3}$$

where

$$\varepsilon_{ir}=\frac{E_{ir}}{kT_w},\quad \varepsilon_{iv}=\frac{E_{iv}}{kT_w} \tag{4}$$

with k the Boltzmann constant and T_w the wall temperature.

A. Analytical derivation from integral operator

Let us write the transformation

$$\begin{aligned}K(V,E_{ir},E_{iv},g_{ir},V',E_{ir'},E_{iv'},g_{ir'})&=[|V'_x|f_0(V',E_{ir'},E_{iv'})]^{1/2}[|V_x|f_0(V,E_{ir},E_{iv})]^{-1/2}\\&\quad\times B(V'_R,E_{ir'},E_{iv'},g_{ir'},V,E_{ir},E_{iv},g_{ir}),\end{aligned} \tag{5}$$

where $f_0(V,E_{ir},E_{iv})$ is the local equilibrium distribution function at the temperature T_w of the wall, defined by

$$f_0(V,E_{ir},E_{iv})=\frac{n}{(C_w\sqrt{\pi})^3}e^{-\|V\|^2/C_w^2}\frac{g_{ir}e^{-\varepsilon_{ir}}e^{-\varepsilon_{iv}}}{Q_rQ_v} \tag{6}$$

with

$$Q_r = \sum_{ir} g_{ir} e^{-\varepsilon_{ir}}, \quad Q_v = \sum_{iv} e^{-\varepsilon_{iv}}, \quad C_w^2 = \frac{2kT_w}{m}. \tag{7}$$

Since f_0 is a known function the problem of finding B is equivalent to finding K. The normalization condition and the non-negativity conditions on B imply obviously the same conditions on K.

Note F_r the set of the rotational energy states E_{ir}, and F_v the set of the vibrational energy states E_{iv}. Consider the five elementary Hilbert spaces of states $L^2(\Omega_\kappa)_{\kappa=x,y,z}$, $L^2(F_r)$, and $L^2(F_v)$ of square summable functions with their corresponding usual scalar product

$$\langle \varphi_{\kappa 1}, \varphi_{\kappa 2} \rangle_\kappa = \int_{\Omega_\kappa} \varphi_{\kappa 1}(V) \varphi_{\kappa 2}(V) d_V \quad \text{for all } \varphi_{\kappa 1}, \varphi_{\kappa 2} \in L^2(\Omega_\kappa), \quad \kappa = x,y,z,$$

$$\langle \varphi_{r1}, \varphi_{r2} \rangle_r = \sum_{ir} \varphi_{r1}(E_{ir}) \varphi_{r2}(E_{ir}) \quad \text{for all } \varphi_{r1}, \varphi_{r2} \in L^2(F_r),$$

$$\langle \varphi_{v1}, \varphi_{v2} \rangle_v = \sum_{iv} \varphi_{v1}(E_{iv}) \varphi_{v2}(E_{iv}) \quad \text{for all } \varphi_{v1}, \varphi_{v2} \in L^2(F_v).$$

Consider the tensor product $\mathcal{L} = L^2(\Omega_x) \otimes L^2(\Omega_y) \otimes L^2(\Omega_z) \otimes L^2(F_r) \otimes L^2(F_v)$ of the five Hilbert spaces of states. Let us remark that this tensor product of Hilbert space $\mathcal{L}$ is dense in the Hilbert space $\mathcal{H} = L^2(\Omega) \otimes L^2(F_r) \otimes L^2(F_v)$ where the scalar product is defined by

$$\langle \varphi_1, \varphi_2 \rangle = \sum_{ir,iv} \int_\Omega \varphi_1(V, E_{ir}, E_{iv}) \varphi_2(V, E_{ir}, E_{iv}) d_V \text{ for all } \varphi_1, \varphi_2 \in \mathcal{H}. \tag{8}$$

Instead of studying the problem of the kernel K, we study the linear integral associated operator A defined on $\mathcal{H}$ by

$$A(\psi) = \sum_{ir',iv'} \int_{\Omega'} K(V, E_{ir}, E_{iv}, g_{ir}, V', E_{ir'}, E_{iv'}, g_{ir'}) \psi(V', E_{ir'}, E_{iv'}, g_{ir'}) d_{V'}. \tag{9}$$

Assume that the operator A has a purely discrete spectrum, and assume that its eigenfunctions are all in the Hilbert space $\mathcal{L}$. The kernel K can be written in the form

$$\begin{aligned} K = \sum_{j_x,j_y,j_z,j_r,j_v=0}^{\infty} & \lambda_{j_x,j_y,j_z,j_r,j_v} \psi_{j_x}(V_x) \psi_{j_y}(V_y) \psi_{j_z}(V_z) \psi_{j_r}(E_{ir}) \psi_{j_v}(E_{iv}) \\ & \times \psi_{j_x}(V_x') \psi_{j_y}(V_y') \psi_{j_z}(V_z') \psi_{j_r}(E_{ir'}) \psi_{j_v}(E_{iv'}), \end{aligned} \tag{10}$$

where the functions $\psi_{j_x}(V_x) \psi_{j_y}(V_y) \psi_{j_z}(V_z) \psi_{j_r}(E_{ir}) \psi_{j_v}(E_{iv})$ are the eigenfunctions of A with their corresponding eigenvalues $\lambda_{j_x,j_y,j_z,j_r,j_v}$. According to the non-negativity and the normalization conditions, the eigenvalues must satisfy $\lambda_{j_x,j_y,j_z,j_r,j_v} \in [0,1]$ for all $j_x, j_y, j_z, j_r, j_v \in \mathbb{N}$. Moreover, one can see that, in the tensor product space $\mathcal{L}$, the scalar product (8) equals the scalar product defined in this tensor product space $\mathcal{L}$ by the product of the five elementary scalar products (8). So, we can suppose that the eigenvalues have the form $\lambda_{j_x} \lambda_{j_y} \lambda_{j_z} \lambda_{j_r} \lambda_{j_v}$ and that the set of functions $\psi_{j_\chi}(M_\chi), j_\chi \in \mathbb{N}$, is a function basis of the χ corresponding Hilbert space $\chi = x,y,z,r,v$. Therefore, the expression (10) can be written as a product of five infinite sums,

$$K = \prod_{\chi \in \{x,y,z,r,v\}} \sum_{j=0}^{\infty} \lambda_{j_\chi} \psi_{j_\chi}(M_\chi) \psi_{j_\chi}(M_\chi'), \quad M_\chi = V_x, V_y, V_z, E_{ir}, E_{iv}. \tag{11}$$

Define $\psi_0 = \psi_{0_x} \psi_{0_y} \psi_{0_z} \psi_{0_r} \psi_{0_v}$ by

$$\psi_{0_x}(V_x) = \frac{\sqrt{2}}{C_w}|V_x|^{1/2}e^{-V_x^2/2C_w^2}, \quad \psi_{0_y}(V_y) = (C_w\sqrt{\pi})^{-1/2}e^{-V_y^2/2C_w^2},$$

$$\psi_{0_z}(V_z) = (C_w\sqrt{\pi})^{-1/2}e^{-V_z^2/2C_w^2}, \quad \psi_{0_r}(E_{ir}) = \sqrt{\frac{g_{ir}}{Q_r}}e^{-1/2\epsilon_{ir}}, \quad \psi_{0_v}(E_{iv}) = \frac{e^{-1/2\epsilon_{iv}}}{\sqrt{Q_v}}.$$

Let us prove that ψ_0 is an eigenfunction of A. Mathematically, the normalization condition can be also written

$$\sum_{ir',iv'} \int_{\Omega'} B(-V,E_{ir},E_{iv},g_{ir},-V'_R,E_{ir'},E_{iv'},g_{ir'})d_{V'} = 1, \tag{12}$$

from this relation (12), the reciprocity relation (3) leads to

$$\sum_{ir',iv'} \int_{\Omega'} |V'_x|f_0(V',E_{ir'},E_{iv'})B(V'_R,E_{ir'},E_{iv'},g_{ir'},V,E_{ir},E_{iv},g_{ir})d_{V'} = |V_x|f_0(-V,E_{ir},E_{iv}). \tag{13}$$

Using the relation (13), the calculation of $A(\psi_0)$ gives $A(\psi_0)=\psi_0$. Consequently $\psi_0=\psi_{0_x}\psi_{0_y}\psi_{0_z}\psi_{0_r}\psi_{0_v}$ is an eigenfunction of the operator A associated to the eigenvalue 1.

Now, following the five state parameters, let us introduce five parameters related to the eigenvalues as follows: $\lambda_{0_\chi}=1$, and for $j\neq 0, \lambda_{j_\chi}=(1-\alpha_\chi)$ for all $\chi=x,y,z,r,v$. The relation (11) becomes

$$K = \prod_{\chi\in\{x,y,z,r,v\}} \left[\psi_{0_\chi}(M_\chi)\psi_{0_\chi}(M'_\chi) + (1-\alpha_\chi)\sum_{j=1}^{\infty} \psi_{j_\chi}(M_\chi)\psi_{j_\chi}(M'_\chi) \right]$$

which may be written

$$K = \prod_{\chi\in\{x,y,z,r,v\}} \left[\alpha_\chi\psi_{0_\chi}(M_\chi)\psi_{0_\chi}(M'_\chi) + (1-\alpha_\chi)\sum_{j=1}^{\infty} \psi_{j_\chi}(M_\chi)\psi_{j_\chi}(M'_\chi) \right].$$

Finally, using the following property,

$$\sum_{j=0}^{\infty} \psi_{j_\chi}(M_\chi)\psi_{j_\chi}(M'_\chi) = \delta(M_\chi - M'_\chi),$$

where δ is the dirac function, it is obtained

$$\begin{aligned} K = {} & \{\alpha_x\psi_{0_x}(V_x)\psi_{0_x}(V'_x) + (1-\alpha_x)\delta(V_x-V'_x)\}\{\alpha_y\psi_{0_y}(V_y)\psi_{0_y}(V'_y) + (1-\alpha_y)\delta(V_y-V'_y)\} \\ & \times\{\alpha_z\psi_{0_z}(V_z)\psi_{0_z}(V'_z) + (1-\alpha_z)\delta(V_z-V'_z)\}\{\alpha_r\psi_{0_r}(V_r)\psi_{0_r}(V'_r) + (1-\alpha_r)\delta(V_r-V'_r)\} \\ & \times\{\alpha_v\psi_{0_v}(V_v)\psi_{0_v}(V'_v) + (1-\alpha_v)\delta(V_v-V'_v)\}. \end{aligned} \tag{14}$$

Applying inversely the transformation (5), the operator B corresponding to the kernel K above [relationship (14)] is

$$B(V',E_{ir'},E_{iv'},g_{ir'},V,E_{ir},E_{iv},g_{ir}) = \left\{(1-\alpha_x)\,\delta(V_x'+V_x)+\alpha_x\frac{2V_x}{C_w^2}e^{-V_x^2/C_w^2}\right\}$$
$$\times\left\{(1-\alpha_y)\,\delta(V_y'-V_y)+\alpha_y\frac{1}{C_w\sqrt{\pi}}e^{-V_y^2/C_w^2}\right\}$$
$$\times\left\{(1-\alpha_y)\,\delta(V_z'-V_z)+\alpha_z\frac{1}{C_w\sqrt{\pi}}e^{-V_z^2/C_w^2}\right\}$$
$$\times\left\{(1-\alpha_r)\,\delta(E_{ir'}-E_{ir})+\alpha_r\frac{g_{ir}}{Q_r}e^{-\epsilon_{ir}}\right\}$$
$$\times\left\{(1-\alpha_v)\,\delta(E_{iv'}-E_{iv})+\alpha_v\frac{1}{Q_v}e^{-\epsilon_{iv}}\right\}. \tag{15}$$

In the further calculations, we will note the scattering kernel (15) simply as

$$B = P_x P_y P_z P_r P_v,$$

where P_x, P_y, P_z, P_r, P_v correspond, respectively, to the five factors of the expression (15). It would be seen that these five factors satisfy

$$\int_0^{+\infty} P_x d_{V_x} = \int_{-\infty}^{+\infty} P_y d_{V_y} = \int_{-\infty}^{+\infty} P_z d_{V_z} = \sum_{ir} P_r = \sum_{iv} P_v = 1. \tag{16}$$

On the other hand when developing the expression (15) one obtains the kernel B as combination of 32 elementary scattering kernels where the coefficients are functions of the α_χ.

B. On the coefficient α_χ

In this section we prove that the five coefficients α_χ involved in the scattering kernel equal, respectively, the accommodation coefficients of the various fluxes of the five microscopic state parameters ($M_\chi = V_x, V_y, V_z, E_{ir}, E_{iv}$).

The accommodation coefficient β_χ of a physical property M_χ at the wall is defined through the relation[3,4,8]

$$\beta_\chi = \frac{\Phi_\chi^- - \Phi_\chi^+}{\Phi_\chi^- - \Phi_\chi^e}, \tag{17}$$

where Φ_χ^- is the incoming flux at the wall of the property M_χ, Φ_χ^+ is the corresponding reflected flux, and Φ_χ^e is the reflected flux in the hypothetical situation of perfect accommodation to the wall. These various fluxes are written

$$\Phi_\chi^- = \sum_{ir',iv'} \int_{\Omega'} m|V_x'|M_\chi' f^-(V',E_{ir'},E_{iv'},g_{ir'})\,d_{V'}, \tag{18}$$

$$\Phi_\chi^+ = \sum_{ir,iv} \int_{\Omega} m|V_x|M_\chi f^+(V,E_{ir},E_{iv},g_{ir})\,d_V, \tag{19}$$

where f^- and f^+ are, respectively, the incident and the reflected distribution functions linked by the relation

$$|V_x| f_i^+(V,E_{ir},g_{ir},E_{iv}) = \sum_{ir',iv'} \int_{\Omega'} |V_x'| f^-(V',E_{ir'},g_{ir'},E_{iv'}) B(V',E_{ir'},g_{ir'},E_{iv'},V,E_{ir},g_{ir},E_{iv}) d_{V'}. \tag{20}$$

Accounting for (20), the reflected flux Φ_χ^+ [expression (19)] may be rewritten as

$$\Phi_\chi^+ = \sum_{ir',iv'} \int_{\Omega'} m|V_x'| f^-(V',E_{ir'},g_{ir'},E_{iv'}) \left[\sum_{ir,iv} \int_{\Omega} M_\chi P_x P_y P_z P_r P_v d_V \right] d_{V'} \tag{21}$$

and the reflected flux in the case of perfect accommodation is written as

$$\Phi_\chi^e = \sum_{ir',iv'} \int_{\Omega'} m|V_x'| f^-(V',E_{ir'},g_{ir'},E_{iv'}) \left[\sum_{ir,iv} \int_{\Omega} M_\chi B_e d_V \right] d_{V'}, \tag{22}$$

where B_e, the perfect accommodation scattering kernel, is defined by

$$B_e = \frac{2g_{ir}}{Q_r Q_v C_w^4 \pi} V_x e^{-\|V\|^2/C_w^2} e^{-\epsilon_{ir}} e^{-\epsilon_{iv}}. \tag{23}$$

1. Calculation of β_y and β_z

The tangential accommodation coefficient, β_y is obtained by substituting $M_\chi = V_y$ in the definition relation (17). In this case it is easily seen that $\Phi_y^e = 0$. Then accounting for the property (16) the expression (21) leads to

$$\Phi_y^+ = (1-\alpha_y) \sum_{ir',iv'} \int_{\Omega'} m V_y' |V_x'| f^-(V',E_{ir'},g_{ir'},E_{iv'}) d_{V'}.$$

It results immediately from expression (17)

$$\beta_y = 1 - \frac{\Phi_y^+}{\Phi_y^-} = \alpha_y.$$

Similarly it is found,

$$\beta_z = 1 - \frac{\Phi_z^+}{\Phi_z^-} = \alpha_z.$$

2. Calculation of β_x

The normal accommodation coefficient is obtained by substituting $M_\chi = |V_x|$ in the definition (17). In this case, accounting for the property (16) and the expressio of the partial operator P_x, it is obtained

$$\sum_{ir,iv} \int_{\Omega} |V_x| P_x P_y P_z P_r P_v d_V = -(1-\alpha_x) V_x' + \alpha_x \frac{C_w \sqrt{\pi}}{2}$$

then the expression (21) yields.

$$\Phi_x^+ - \Phi_x^- = \alpha_x \sum_{ir',iv'} \int_{\Omega'} m|V_x'| f^-(V',E_{ir'},E_{iv'},g_{ir'}) \left(V_x' + \frac{C_w \sqrt{\pi}}{2} \right) d_{V'}.$$

The calculation of Φ^e leads easily to

$$\Phi_x^e - \Phi_x^- = \sum_{ir',iv'} \int_{\Omega'} m|V_x'| f^-(V', E_{ir'}, E_{iv'}, g_{ir'}) \left(V_x' + \frac{C_w\sqrt{\pi}}{2} \right) d_{V'}.$$

Consequently we obtained from the relation (17),

$$\beta_x = \alpha_x.$$

3. Calculation of β_r and β_v

Now substitute $M_\chi = g_{ir}E_{ir}$ in the relation (17). Accounting for the property (16) it is obtained

$$\sum_{ir,iv} \int_{\Omega} g_{ir}E_{ir}P_xP_yP_zP_rP_v d_V = \sum_{ir} g_{ir}E_{ir}P_r = (1-\alpha_r) g_{ir'}E_{ir'} + \alpha_r \frac{Q_r^*}{Q_r},$$

where we have noted

$$Q_r^* = \sum_{ir} g_{ir}^2 E_{ir} e^{-\varepsilon_{ir}}.$$

Then the expression of Φ^+ leads to

$$\Phi_{E_{ir}}^- - \Phi_{E_{ir}}^e = \alpha_r \sum_{ir',iv'} \int_{\Omega'} m|V_x'| f^-(V', E_{ir'}, E_{iv'}, g_{ir'}) \left(g_{ir'}E_{ir'} - \frac{Q_r^*}{Q_r} \right) d_{V'}.$$

Using the expression (23) of B_e, we obtain

$$\sum_{ir,iv} \int_{\Omega} g_{ir}E_{ir}B_e d_V = \frac{Q_r^*}{Q_r}$$

and then

$$\Phi_{E_{ir}}^- - \Phi_{E_{ir}}^e = \sum_{ir',iv'} \int_{\Omega'} m|V_x'| f^-(V', E_{ir'}, E_{iv'}, g_{ir'}) \left(g_{ir'}E_{ir'} - \frac{Q_r^*}{Q_r} \right) d_{V'}$$

consequently,

$$\beta_r = \alpha_r.$$

In the same way, substituting $M_\chi = E_{iv}$, it is found

$$\beta_v = \alpha_v.$$

In conclusion, the five parameters α_χ involved in the scattering kernel (15) are the accommodation coefficients corresponding to the five state parameters, namely the three momentum components and the two internal energy degrees.

III. COMMENT ON THE METHOD USED IN SCATTERING KERNEL DERIVATION

The $\mathcal{H}$ Hilbert space corresponds generally to the Hilbert space used in the framework of the modelling of the Boltzmann equation in polyatomic gases. Following the quantum mechanic concept, the wall and then the boundary conditions can be represented by an operator defined on this $\mathcal{H}$ Hilbert space.[4,6,8,9] Therefore the problem of boundary condition for the Boltzmann equation can be basically formulated through the integral operator (9), so this formulation is convenient for solving the linearized Boltzmann equation. The reciprocity relation assumption globally means that the local equilibrium distribution function must be invariant by the kernel B.[8,9] This last condition, which contains thermodynamic properties is the most important condition. In addition, it is the only one condition containing physical meaning. This condition leads to the first eigen-

function representation ψ_0. The other eigenfunctions remain unknown. At this step of the scattering kernel construction, one should suggest to choose the set of the other eigenfunctions[10] or a finite number of them. But, such a way would be a purely mathematical construction without real physical justifications.[4,7]

Then, another way consists to analyze physically the accommodation process. Let us consider the couple gas/surface characterized by its macroscopic properties. It seems convenient to assume that for each microscopic property p of the molecules, the solid surface behaves in a way perfectly defined in the accommodation process. In other worlds, in a gas/surface configuration, physically and geometrically given, for each microscopic property there is a linear relation between the amount of the p flux accommodated by the wall and the amount of the p incoming flux. So the accommodation at the wall of any physical microscopic property provides a physical information through a corresponding accommodation coefficient. Thus, five elementary accommodation coefficients associated to the five basic parameters defining the molecule states (the three momentum components, rotational energy, vibrational energy) are naturally introduced completely describing the molecules behavior in the reflection process. In this way, the present construction of the polyatomic scattering kernel is based on five accommodation coefficients, and corresponds to an integral operator partially degenerated involving 32 different eigenvalues in its expansion: from our point of view, this construction appears physically founded and completely describing the reflection process.

IV. CONCLUDING REMARKS

We have established a scattering kernel for structured molecules involving one rotational and one vibrational energy mode. A convenient integral operator formulation is used assuming a purely discrete spectrum and assuming eigenvalues depending on five basic parameters in respect to the five state parameters of the molecules (and then assuming a partial degeneracy of the integral operator). These five basic parameters are shown to be the accommodation coefficients of, respectively, the three momentum accommodation coefficients and the accommodation coefficients of the two internal energy modes.

Under its factorized form (15), the proposed scattering kernel is easy to use in analytical calculations or to be implemented in numerical modelling. In order to show its physical meaning, the expression (15) may be developed. Under its developed form, the scattering kernel appears as a linear combination of 32 elementary scattering kernels (listed in the Appendix). All these elementary kernels correspond to various situations of accommodation at the wall which have been described in Ref. 5. The linear combination coefficients, which represent the weight of the various types of accommodation in the reflection process, are combinations of the factors α_χ and $(1-\alpha_\chi)$ (see the Appendix). In each elementary kernel each molecule state accommodates independently from the others. So the new kernel allows us to take into account the interplay between the molecule freedom degrees when interacting at the wall.[11] Up to now, the data available concerning the whole set of accommodation coefficients involved in the proposed scattering kernel are rare; that makes a complete validation of the model difficult.

Finally, let us add that, in the form presented here, the scattering kernel accounts for a single rotational and a single vibrational mode. This description is sufficient in any condition for diatoms. In the case of more complex polyatomic structures, involving various vibrational (or rotational) modes, the present form of scattering kernel remains directly usable, as long as the various vibrational (or rotational) modes remain in the same thermodynamics state (i.e., in local equilibrium the ones with the others). In a contrary situation (for example, in strong vibrational nonequilibrium conditions) it may be pertinent—depending on the considered time scale—to distinguish various vibrational (or rotational) accommodation coefficients to describe the reflection process. In such a case, the scattering kernel should be written in the same way as previously, but it should involve more than five state parameters, and thus more than five accommodation coefficients.

APPENDIX: DIFFERENT WRITING OF THE SCATTERING KERNEL *B* OF RELATION (15)

Let

$$\tilde{P}_0 = \delta(E_{ir'} - E_{ir})\,\delta(E_{iv'} - E_{iv}), \quad \tilde{P}_{rv} = \frac{e^{-\varepsilon_{ir}}}{Q_r} g_{ir} \frac{e^{-\varepsilon_{iv}}}{Q_v},$$

$$\tilde{P}_v = \delta(E_{ir'} - E_{ir}) \frac{e^{-\varepsilon_{iv}}}{Q_v}, \quad \tilde{P}_r = \frac{e^{-\varepsilon_{ir}}}{Q_r} g_{ir}\,\delta(E_{iv'} - E_{iv}). \tag{A1}$$

Develop partially the expression (15). The scattering kernel can be written in the form presented in Ref. 5, as follows:

$$B = \left(\sum_{\kappa} \mu_\kappa B_\kappa(V', V) \right) (1 - \alpha_r)(1 - \alpha_v)\tilde{P}_0 + \alpha_v(1 - \alpha_r)\tilde{P}_v + \alpha_r(1 - \alpha_v)\tilde{P}_r + \alpha_v\alpha_r\tilde{P}_{rv}, \tag{A2}$$

where B_κ the elementary scattering kernels, and μ_κ their corresponding coefficients in the case of unstructured molecule given in Ref. 5, are recalled below,

$$B_0(V', V) = \delta(V_x + V'_x)\,\delta(V_y - V'_y)\,\delta(V_z - V'_z),$$

$$B_{yz}(V', V) = \frac{1}{\pi C_w^2}\,\delta(V_x + V'_x) e^{-V_y^2/C_w^2} e^{-V_z^2/C_w^2},$$

$$B_{xz}(V', V) = \frac{2}{C_w^3\sqrt{\pi}} V_x\,\delta(V_y - V'_y) e^{-V_x^2/C_w^2} e^{-V_z^2/C_w^2},$$

$$B_{xy}(V', V) = \frac{2}{C_w^3\sqrt{\pi}} V_x\,\delta(V_z - V'_z) e^{-V_x^2/C_w^2} e^{-V_y^2/C_w^2},$$

$$B_{xyz}(V', V) = \frac{2}{\pi C_w^4} V_x e^{-V_x^2/C_w^2} e^{-V_y^2/C_w^2} e^{-V_z^2/C_w^2},$$

$$B_z(V', V) = \frac{1}{C_w\sqrt{\pi}}\,\delta(V_x + V'_x)\,\delta(V_y - V'_y) e^{-V_z^2/C_w^2},$$

$$B_y(V', V) = \frac{1}{C_w\sqrt{\pi}}\,\delta(V_x + V'_x)\,\delta(V_z - V'_z) e^{-V_y^2/C_w^2},$$

$$B_x(V', V) = \frac{2}{C_w^2} V_x\,\delta(V_y - V'_y)\,\delta(V_z - V'_z) e^{-V_x^2/C_w^2},$$

and

$$\mu_{xz} = \alpha_x\alpha_z(1 - \alpha_y), \quad \mu_{xy} = \alpha_x\alpha_y(1 - \alpha_z), \quad \mu_{yz} = \alpha_y\alpha_z(1 - \alpha_x), \quad \mu_x = \alpha_x(1 - \alpha_y)(1 - \alpha_z), \quad \mu_{xyz} = \alpha_x\alpha_y\alpha_z, \quad \mu_0 = (1 - \alpha_x)(1 - \alpha_y)(1 - \alpha_z), \quad \mu_y = \alpha_y(1 - \alpha_x)(1 - \alpha_z), \quad \mu_z = \alpha_z(1 - \alpha_x)(1 - \alpha_y).$$

A complete development of expression (15) yields the scattering kernel written as a sum of 32 elementary polyatomic scattering kernels $B_\kappa\tilde{P}_{in}$ as follows:

$$B = \sum_{\kappa,in} \mu_\kappa \mu_{in} B_\kappa \tilde{P}_{in},$$

where $\tilde{P}_{in}$ refers to the four partial operators $\tilde{P}_0, \tilde{P}_v, \tilde{P}_r, \tilde{P}_{rv}$ defined in the relationship (A1) and μ_{in} to their respective coefficients in the formula (A2). In this developed form it is clear that this scattering kernel describes various types of accommodation processes at the wall. Each of the partial scattering kernels $B_\kappa \tilde{P}_{in}$ corresponds to a particular type of accommodation. There are exactly 32 types.

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On the infimum of quantum effects

Aurelian Gheondea[a)]
Department of Mathematics, Bilkent University, 06800 Bilkent, Ankara, Turkey and Institutul de Matematică al Academiei Române, C.P. 1-764, 014700 Bucureşti, România

Stanley Gudder[b)]
Department of Mathematics, University of Denver, Denver, Colorado 80208

Peter Jonas[c)]
Institut für Mathematik, Technische Universität Berlin, 10623 Berlin, Germany

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The quantum effects for a physical system can be described by the set $\mathcal{E}(\mathcal{H})$ of positive operators on a complex Hilbert space $\mathcal{H}$ that are bounded above by the identity operator. While a general effect may be unsharp, the collection of sharp effects is described by the set of orthogonal projections $\mathcal{P}(\mathcal{H})\subseteq\mathcal{E}(\mathcal{H})$. Under the natural order, $\mathcal{E}(\mathcal{H})$ becomes a partially ordered set that is not a lattice if $\dim\mathcal{H}\geqslant 2$. A physically significant and useful characterization of the pairs $A,B\in\mathcal{E}(\mathcal{H})$ such that the infimum $A\wedge B$ exists is called the infimum problem. We show that $A\wedge P$ exists for all $A\in\mathcal{E}(\mathcal{H})$, $P\in\mathcal{P}(\mathcal{H})$ and give an explicit expression for $A\wedge P$. We also give a characterization of when $A\wedge(I-A)$ exists in terms of the location of the spectrum of A. We present a counterexample which shows that a recent conjecture concerning the infimum problem is false. Finally, we compare our results with the work of Ando on the infimum problem. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1904704]

I. INTRODUCTION

A quantum mechanical measurement with just two values 1 and 0 (or yes and no) is called a *quantum effect*. These elementary measurements play an important role in the foundations of quantum mechanics and quantum measurement theory.[3–5,7,14,16,18] We shall follow the Hilbert space model for quantum mechanics in which effects are represented by positive operators on a complex Hilbert space $\mathcal{H}$ that are bounded above by the identity operator I. In this way the set of effects $\mathcal{E}(\mathcal{H})$ becomes

$$\mathcal{E}(\mathcal{H})=\{A\in\mathcal{B}(\mathcal{H}):0\leqslant A\leqslant I\}.$$

The set of orthogonal projections $\mathcal{P}(\mathcal{H})\subseteq\mathcal{E}(\mathcal{H})$ corresponds to sharp effects while a general $A\in\mathcal{E}(\mathcal{H})$ may be unsharp (fuzzy, imprecise). Employing the usual order $A\leqslant B$ for the set of bounded self-adjoint operators $\mathcal{S}(\mathcal{H})$ on $\mathcal{H}$, we see that $(\mathcal{E}(\mathcal{H}),\leqslant)$ is a partially ordered set. It is well known that $(\mathcal{E}(\mathcal{H}),\leqslant)$ is not a lattice if $\dim\mathcal{H}\geqslant 2$. However, if the infimum $A\wedge B$ of $A,B\in\mathcal{E}(\mathcal{H})$ exists then $A\wedge B$ has the important property of being the largest effect that physically implies both A and B. It would thus be of interest to give a physically significant and useful characterization of when $A\wedge B$ exists. This so-called infimum problem has been considered for at least 10 years.[2,10–12,17,19]

Before discussing the progress that has been made toward solving the infimum problem, let us compare the situation with that of the partially ordered set $(\mathcal{S}(\mathcal{H}),\leqslant)$. Of course, if A,B

[a)]Electronic mail: aurelian@fen.bilkent.edu.tr and gheondea@imar.ro
[b)]Electronic mail: sgudder@math.du.edu
[c)]Electronic mail: jonas@math.tu-berlin.de

$\in \mathcal{S}(\mathcal{H})$ are comparable, that is, $A \leqslant B$ or $B \leqslant A$, then $A \wedge B$ exists and is the smaller of the two. A surprising result of Kadison[15] states that the converse holds. Thus, for $A, B \in \mathcal{S}(\mathcal{H})$, $A \wedge B$ exists in $\mathcal{S}(\mathcal{H})$ if and only if A and B are comparable. We conclude that $(\mathcal{S}(\mathcal{H}), \leqslant)$ is an antilattice which is as far from being a lattice as possible. The situation is quite different in $(\mathcal{E}(\mathcal{H}), \leqslant)$. In fact it is well known that $P \wedge Q$ exists in $\mathcal{E}(\mathcal{H})$ for all $P, Q \in \mathcal{P}(\mathcal{H})$. More generally, we shall show that $A \wedge P$ exists in $\mathcal{E}(\mathcal{H})$ for all $A \in \mathcal{E}(\mathcal{H})$, $P \in \mathcal{P}(\mathcal{H})$ and give an explicit expression for $A \wedge P$. The existence of $A \wedge P$ has already been proved in Ref. 18 but we present a different proof here.

For $A, B \in \mathcal{E}(\mathcal{H})$ let $P_{A,B}$ be the orthogonal projection onto the closure of $\mathrm{Ran}(A^{1/2}) \cap \mathrm{Ran}(B^{1/2})$. It is shown in Ref. 19 that if $\dim \mathcal{H} < \infty$ then $A \wedge B$ exists in $\mathcal{E}(\mathcal{H})$ if and only if $A \wedge P_{A,B}$ and $B \wedge P_{A,B}$ are comparable and in this case $A \wedge B$ is the smaller of the two. This was considered to be a solution to the infimum problem for the case $\dim \mathcal{H} < \infty$ and it was conjectured in Ref. 19 that this result also holds in general. One of our main results is that this conjecture is false. We shall present an example of a pair $A, B \in \mathcal{E}(\mathcal{H})$ with $\dim \mathcal{H} = \infty$ for which $A \wedge B$ exists in $\mathcal{E}(\mathcal{H})$ but $A \wedge P_{A,B}$ and $B \wedge P_{A,B}$ are not comparable. In addition, we prove that, assuming $A \wedge B$ exists, $P_{A,B}$ is the smallest of all orthogonal projections P having the property that $(A \wedge P) \wedge (B \wedge P)$ exists and $(A \wedge P) \wedge (B \wedge P) = A \wedge B$. Combined with the counter-example as described before, this means that, in the infinite dimensional case, there is no orthogonal projection to replace $P_{A,B}$ and have a positive solution to the infimum problem.

The *negation* A' of an effect A is defined to be the effect $A' = I - A$. Physically, A' is the effect A with its values 1 and 0 reversed. We also present a simple spectral characterization of when $A \wedge A'$ exists in $\mathcal{E}(\mathcal{H})$. The result is essentially the same as Theorem 2 in Ref. 2, with the difference that we express the condition in terms of the location of the spectrum of A and the proof is based on the matrix representations obtained in the preceding section.

Ando has given a solution to the infimum problem in terms of a generalized shorted operator.[2] However, in our opinion, these shorted operators do not have a physical significance in contrast to the operationally defined operators $A \wedge P_{A,B}$ and $B \wedge P_{A,B}$. Finally, we discuss the relationship between our work and that of Ando. First, we show that the shorted operator of A by B is always smaller than $A \wedge P_{A,B}$. Actually, it is the fact, that in the infinite dimensional case, the shorted operator of A by B can be strictly smaller than $A \wedge P_{A,B}$, that is responsible for the failure of a solution of the infimum problem similar to the finite dimensional case. This can be viewed from the counter-example as before, but we record also a simpler one that illustrates this situation.

We now briefly discuss connections between the infimum problem and physics. Quantum effects have been studied by mathematicians and physicists for over 40 years.[5,16,17] Besides the applications of effect-valued measures in quantum measurement theory, many researchers consider effects to be the basic elements of important quantum structures. In recent times quantum effects have been organized into a structure called an effect algebra[7,10] and their order properties have been studied.[11,12,17] Among other things, the effect algebra $\mathcal{E}(\mathcal{H})$ is a partially ordered set and if $A \wedge B$ exists for $A, B, \in \mathcal{E}(\mathcal{H})$, then this effect has important physical properties. In particular, among all the effects that have a smaller probability of occurring than both A and B, $A \wedge B$ has the largest probability. Thus if $A \wedge B$ exists, then $A \wedge B$ has a crucial physical significance. In the case where A and B are sharp, A and B are projections, $A \wedge B$ always exists and is the projection onto the intersection of their ranges. But if A and B are not sharp, the situation is much more complicated. An interesting special case is when $A \in \mathcal{E}(\mathcal{H})$ and $P \in \mathcal{P}(\mathcal{H})$. In this case $A \wedge P$ always exists and if A and P commute (are compatible) then $A \wedge P = AP$. However, if A and P do not commute an explicit closed form expression for $A \wedge P$ has been difficult to obtain and is now presented in Theorem 2.2. We can now define conditional probabilities

$$\mathrm{prob}(A|P) = \mathrm{prob}(A \wedge P)/\mathrm{prob}(P)$$

and conditional measurements and these may have useful physical applications. Finally, our Example 4.2 gives a surprising phenomenon that does not occur in finite dimensional Hilbert spaces. The existence of effects such as those in this example may have interesting physical significance.

II. INFIMUM OF A QUANTUM EFFECT AND A SHARP EFFECT

We first record a parametrization of bounded positive 2×2 matrices with operator entries, in terms of operator balls.

In the following we make use of the *Frobenius-Schur factorization*: for T, X, Y, Z bounded operators on appropriate spaces and T boundedly invertible, we have

$$\begin{bmatrix} T & X \\ Y & Z \end{bmatrix} = \begin{bmatrix} I & 0 \\ YT^{-1} & I \end{bmatrix} \begin{bmatrix} T & 0 \\ 0 & Z - YT^{-1}X \end{bmatrix} \begin{bmatrix} I & T^{-1}X \\ 0 & I \end{bmatrix}. \tag{2.1}$$

For instance, by using Frobenius–Schur factorizations and a perturbation argument one can obtain the following classical result of Shmulyan.[21]

Theorem 2.1: *Let $A \in \mathcal{B}(\mathcal{H})$ be self-adjoint and $\mathcal{H}=\mathcal{H}_1 \oplus \mathcal{H}_2$ an orthogonal decomposition of $\mathcal{H}$. Then $A \geqslant 0$ if and only if it has a matrix representation of the following form:*

$$A = \begin{bmatrix} A_1 & A_1^{1/2}\Gamma A_2^{1/2} \\ A_2^{1/2}\Gamma^* A_1^{1/2} & A_2 \end{bmatrix} \quad \text{with respect to } \mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2, \tag{2.2}$$

where $A_1 \in \mathcal{B}(\mathcal{H}_1)^+$, $A_2 \in \mathcal{B}(\mathcal{H}_2)^+$, and $\Gamma \in \mathcal{B}(\mathcal{H}_2, \mathcal{H}_1)$ is contractive.

In addition, the operator Γ can be chosen in such a way that $\mathrm{Ker}(\Gamma) \supseteq \mathrm{Ker}(A_2)$ *and* $\mathrm{Ker}(\Gamma^*) \supseteq \mathrm{Ker}(A_1)$, *and in this case it is unique.*

For two effects $A, B \in \mathcal{E}(\mathcal{H})$ we denote by $A \wedge B$, the *infimum*, equivalently, the *greatest lower bound*, of A and B over the partially ordered set $(\mathcal{E}(\mathcal{H}), \leqslant)$, if it exists. To be more precise, $A \wedge B$ is an operator in $\mathcal{E}(\mathcal{H})$ uniquely determined by the following properties: $A \wedge B \leqslant A$, $A \wedge B \leqslant B$, and an arbitrary operator $D \in \mathcal{E}(\mathcal{H})$ satisfies both $D \leqslant A$ and $D \leqslant B$ if and only if $D \leqslant A \wedge B$. Characterizations of the existence of infimum for positive operators have been obtained for the finite-dimensional case in Ref. 19, and in general in Ref. 2.

In Theorem 4.4 of Ref. 19 it is proved that the infimum $A \wedge P$ exists for any $A \in \mathcal{E}(\mathcal{H})$ and $P \in \mathcal{P}(\mathcal{H})$. As a consequence of Theorem 2.1 we can obtain an explicit description of $A \wedge P$, together with another proof of the existence.

Theorem 2.2: *For any $A \in \mathcal{E}(\mathcal{H})$ and $P \in \mathcal{P}(\mathcal{H})$ the infimum $A \wedge P$ exists, more precisely, if A has the matrix representation as in* (2.2) *with respect to the orthogonal decomposition $\mathcal{H}$* $=\mathrm{Ran}(P) \oplus \mathrm{Ker}(P)$, *where* $A_1 \in \mathcal{E}(\mathrm{Ran}(P))$, $A_2 \in \mathcal{E}(\mathrm{Ker}(P))$, *and* $\Gamma \in \mathcal{B}(\mathrm{Ker}(P), \mathrm{Ran}(P))$, *with* $\|\Gamma\| \leqslant 1$, $\mathrm{Ker}(\Gamma) \supseteq \mathrm{Ker}(A_2)$ *and* $\mathrm{Ker}(\Gamma^*) \supseteq \mathrm{Ker}(A_1)$, *then*

$$A \wedge P = \begin{bmatrix} A_1^{1/2}(I - \Gamma\Gamma^*)A_1^{1/2} & 0 \\ 0 & 0 \end{bmatrix} \quad \text{with respect to } \mathcal{H} = \mathrm{Ran}(P) \oplus \mathrm{Ker}(P). \tag{2.3}$$

Proof: Let $A \in \mathcal{E}(\mathcal{H})$ and $P \in \mathcal{P}(\mathcal{H})$. In the following we consider the orthogonal decomposition $\mathcal{H}=\mathrm{Ran}(P) \oplus \mathrm{Ker}(P)$. By Theorem 2.1 A has a matrix representation as in (2.2), with $A_1 \in \mathcal{B}(\mathrm{Ran}(P))^+$, $A_2 \in \mathcal{B}(\mathrm{Ker}(P))^+$, and $\Gamma \in \mathcal{B}(\mathrm{Ker}(P), \mathrm{Ran}(P))$, with $\|\Gamma\| \leqslant 1$, $\mathrm{Ker}(\Gamma) \supseteq \mathrm{Ker}(A_2)$ and $\mathrm{Ker}(\Gamma^*) \supseteq \mathrm{Ker}(A_1)$. Since $A \leqslant I$ it follows that $A_1 \leqslant I_{\mathrm{Ran}(P)}$ and $A_2 \leqslant I_{\mathrm{Ker}(P)}$. Consider the operator $D \in \mathcal{B}(\mathcal{H})$, defined by the matrix in (2.3). Clearly $0 \leqslant D \leqslant P$, in particular $D \in \mathcal{E}(\mathcal{H})$. In addition,

$$A - D = \begin{bmatrix} A_1^{1/2}\Gamma\Gamma^* A_1^{1/2} & A_1^{1/2}\Gamma A_2^{1/2} \\ A_2^{1/2}\Gamma^* A_1^{1/2} & A_2 \end{bmatrix} = [\Gamma^* A_1^{1/2} A_2^{1/2}]^* [\Gamma^* A_1^{1/2} A_2^{1/2}] \geqslant 0,$$

hence $A \geqslant D$.

Let $C \in \mathcal{E}(\mathcal{H})$ be such that $C \leqslant A, P$. From $C \leqslant P$ it follows that $CP=PC=C$ and hence

$$C = \begin{bmatrix} C_1 & 0 \\ 0 & 0 \end{bmatrix} \quad \text{with respect to } \mathcal{H} = \mathrm{Ran}(P) \oplus \mathrm{Ker}(P).$$

Then

$$0 \leqslant A - C = \begin{bmatrix} A_1 - C_1 & A_1^{1/2}\Gamma A_2^{1/2} \\ A_2^{1/2}\Gamma^* A_1^{1/2} & A_2 \end{bmatrix}. \tag{2.4}$$

The matrix with operator entries in (2.4) can be factored as

$$\begin{bmatrix} I_{\mathrm{Ran}(P)} & 0 \\ 0 & A_2^{1/2} \end{bmatrix} \begin{bmatrix} A_1 - C_1 & A_1^{1/2}\Gamma \\ \Gamma^* A_1^{1/2} & I_{\mathrm{Ker}(P)} \end{bmatrix} \begin{bmatrix} I_{\mathrm{Ran}(P)} & 0 \\ 0 & A_2^{1/2} \end{bmatrix}. \tag{2.5}$$

Note that by $\mathrm{Ker}(\Gamma) \supseteq \mathrm{Ker}(A_2)$ or, equivalently, $\overline{\mathrm{Ran}(\Gamma^*)} \subseteq \overline{\mathrm{Ran}(A_2)}$, $A - C$ and each of the factors of (2.5) map the subspace $\mathcal{H}' = \mathrm{Ran}(P) \oplus \overline{\mathrm{Ran}(A_2)}$ into itself. Since $\mathrm{diag}(I_{\mathrm{Ran}(P)} A_2^{1/2})$ regarded as an operator on $\mathcal{H}'$, is symmetric and has dense range, $A - C \geqslant 0$ implies that the middle term in (2.5) regarded as an operator in $\mathcal{H}'$ is non-negative. By performing a Frobenius–Schur factorization of this middle term, we find $A_1^{1/2}\Gamma\Gamma^* A_1^{1/2} \leqslant A_1 - C_1$, that is, $C_1 \leqslant A_1^{1/2}(I_{\mathrm{Ran}(P)} - \Gamma\Gamma^*)A_1^{1/2}$, or, equivalently, $C \leqslant D$.

We thus proved that $A \wedge P$ exists and has the matrix representation as in (2.3). □

Remark 2.3: If $A \in \mathcal{E}(\mathcal{H})$, E_A is the spectral function of A and Δ is a Borel subset of $[0, 1]$, then $A \wedge E_A(\Delta) = AE_A(\Delta)$. This is an immediate consequence of Theorem 2.2. The second to last sentence in the proof of Theorem 2.2 can also be demonstrated by using the well-known fact that any operator matrix of the form

$$\begin{bmatrix} A & B \\ B^* & I \end{bmatrix} \tag{2.6}$$

is positive if and only if $A \geqslant 0$ and $BB^* \leqslant A$.

Let $A, B \in \mathcal{E}(\mathcal{H})$. By $P_{A,B}$ we denote the orthogonal projection onto the closure of $\mathrm{Ran}(A^{1/2}) \cap \mathrm{Ran}(B^{1/2})$. As mentioned in the introduction, the infimum problem for a finite dimensional space $\mathcal{H}$ was solved in Ref. 19 by showing that $A \wedge B$ exists if and only if $A \wedge P_{A,B}$ and $B \wedge P_{A,B}$ are comparable, and that $A \wedge B$ is the smaller of $A \wedge P_{A,B}$ and $B \wedge P_{A,B}$. The following proposition shows that for $\dim \mathcal{H} = \infty$ the infimum problem for A and B can be reduced to the same problem for the "smaller" operators $A \wedge P_{A,B}$ and $B \wedge P_{A,B}$. In Sec. IV we will see that in this case the infimum problem cannot be solved in the same fashion, as conjectured in Ref. 19.

Proposition 2.4: Let $A, B \in \mathcal{E}(\mathcal{H})$. Then $A \wedge B$ exists if and only if $(A \wedge P_{A,B}) \wedge (B \wedge P_{A,B})$ exists. In this case $A \wedge B = (A \wedge P_{A,B}) \wedge (B \wedge P_{A,B})$.

Proof: Note first that the operators $A \wedge P_{A,B}$ and $B \wedge P_{A,B}$ exist, e.g., by Theorem 2.2.

Let us assume that $(A \wedge P_{A,B}) \wedge (B \wedge P_{A,B})$ exists and let $C \in \mathcal{E}(\mathcal{H})$ be such that $C \leqslant A, B$, thus we have $\mathrm{Ran}(C^{1/2}) \subseteq \mathrm{Ran}(A^{1/2}) \cap \mathrm{Ran}(B^{1/2}) \subseteq \mathrm{Ran}(P_{A,B})$ and hence $C \leqslant P_{A,B}$. Therefore, $C \leqslant A \wedge P_{A,B}$ and $C \leqslant B \wedge P_{A,B}$ and hence, by the majorization theorem as in Ref. 6, $C \leqslant (A \wedge P_{A,B}) \wedge (B \wedge P_{A,B})$. Taking into account that $(A \wedge P_{A,B}) \wedge (B \wedge P_{A,B}) \leqslant A, B$ it follows that $A \wedge B$ exists and equals $(A \wedge P_{A,B}) \wedge (B \wedge P_{A,B})$.

Conversely, let us assume that $A \wedge B$ exist. Then, $A \wedge B \leqslant P_{A,B}$. This relation and $A \wedge B \leqslant A, B$ give $A \wedge B \leqslant A \wedge P_{A,B}$, $A \wedge B \leqslant B \wedge P_{A,B}$. Let $C \in \mathcal{E}(\mathcal{H})$ be such that $C \leqslant A \wedge P_{A,B}$, $B \wedge P_{A,B}$. Then $C \leqslant A$, B, $P_{A,B}$ and, in particular, $C \leqslant A \wedge B$. □

One may ask for which orthogonal projections P except $P_{A,B}$ the statement of Proposition 2.4 is true. It turns out that $P_{A,B}$ is the infimum of the set of those projections P.

Theorem 2.5: *Let $A, B \in \mathcal{E}(\mathcal{H})$ such that $A \wedge B$ exists. Let $\Pi_{A,B}$ be the set of all orthogonal projections subject to the properties that $(A \wedge P) \wedge (B \wedge P)$ exists and $(A \wedge P) \wedge (B \wedge P) = A \wedge B$. Then*

$$\Pi_{A,B} = \{P \in \mathcal{P}(\mathcal{H}) | P_{A,B} \leqslant P\}.$$

In order to prove the above stated proposition, we first consider the connection of parallel sum with the infimum of quantum effects (see also Ref. 2). To see this, instead of giving the original definition as in Ref. 8, we prefer to introduce the parallel sum of two quantum effects by means of the characterization of Pekarev–Shmulyan,[20]

$$\langle (A:B)h,h\rangle = \inf\{\langle Aa,a\rangle + \langle Bb,b\rangle | h = a + b\}, \text{for all } h \in \mathcal{H}. \tag{2.7}$$

Theorem 2.6: (Refs. 8 and 20) *Let* $A,B \in \mathcal{B}(\mathcal{H})^+$. *Then*

(i) $0 \leqslant A: B \leqslant A, B$,
(ii) $A:B = B:A$,
(iii) $\mathrm{Ran}((A:B)^{1/2}) = \mathrm{Ran}(A^{1/2}) \cap \mathrm{Ran}(B^{1/2})$,
(iv) *if* $A_1, B_1 \in \mathcal{B}(\mathcal{H})^+$ *are such that* $A \leqslant A_1$ *and* $B \leqslant B_1$, *then* $A:B \leqslant A_1:B_1$,
(v) *if* $A+B$ *is boundedly invertible, then* $\|A:B\| = A(A+B)^{-1}B$,
(vi) *If* $A_n \searrow A$ *and* $B_n \searrow B$ *strongly, then* $A_n:B_n \searrow A:B$ *strongly*.

In view of the properties of the parallel sum listed above, a moment of thought shows that if $P,Q \in \mathcal{P}(\mathcal{H})$, that is, P and Q are orthogonal projections in $\mathcal{H}$, then $P \wedge Q$ over $\mathcal{E}(\mathcal{H})$ always exists and coincides with the orthogonal projection onto $\mathrm{Ran}(P) \cap \mathrm{Ran}(Q)$. By Theorem 4.3 in Ref. 8 we also have $P \wedge Q = 2(P:Q)$.

Lemma 2.7: Let $A,B \in \mathcal{E}(\mathcal{H})$ *be such that* $A \wedge B$ *exists. Then*

(i) $\mathrm{Ran}((A \wedge B)^{1/2}) = \mathrm{Ran}((A:B)^{1/2})$,
(ii) $(A \wedge B)^{1/2} = (A:B)^{1/2}V$ *for some boundedly invertible operator* $V \in \mathcal{B}(\mathcal{H})$,
(iii) $A:B \leqslant A \wedge B \leqslant \gamma(A:B)$, *for some* $\gamma > 0$.

Proof: Since $A \wedge B \leqslant A$ it follows that $\mathrm{Ran}((A \wedge B)^{1/2}) \subseteq \mathrm{Ran}(A^{1/2})$. Similarly we have $\mathrm{Ran}((A \wedge B)^{1/2}) \subseteq \mathrm{Ran}(B^{1/2})$, hence $\mathrm{Ran}((A \wedge B)^{1/2}) \subseteq \mathrm{Ran}(A^{1/2}) \cap \mathrm{Ran}(B^{1/2}) = \mathrm{Ran}((A:B)^{1/2})$.

For the converse inclusion, note that $A:B \leqslant A$ and $A:B \leqslant B$; since $A:B \leqslant A:I = A(A+I)^{-1} \leqslant A$. Thus, by the definition of $A \wedge B$, it follows that $A:B \leqslant A \wedge B$. In particular, this proves that $\mathrm{Ran}((A \wedge B)^{1/2}) \supseteq \mathrm{Ran}((A:B)^{1/2})$, and hence (i) is proved.

The assertions (ii) and (iii) are consequences of (i) and the majorization theorem as in Ref. 6. □

Lemma 2.8: If $A,B \in \mathcal{E}(\mathcal{H})$ *and* $A \wedge B$ *exists, then* $A \wedge B \leqslant P_{A,B}$ *and* $\mathrm{Ran}(A \wedge B)$ *is dense in* $\mathrm{Ran}(P_{A,B})$.

Proof: This is a consequence of Theorem 2.6 and Lemma 2.7. □

We now come back to Theorem 2.5.

Proof of Theorem 2.5: Let $P \in \Pi_{A,B}$. Then $A \wedge B \leqslant P$ and hence $\overline{\mathrm{Ran}(A \wedge B)} \subseteq \mathrm{Ran}(P)$. Therefore, by Lemma 2.8 $\mathrm{Ran}(P_{A,B}) \subseteq \mathrm{Ran}(P)$, that is, $P_{A,B} \leqslant P$.

Assume that $P \geqslant P_{A,B}$. We claim that then $(A \wedge P) \wedge (B \wedge P)$ exists and it coincides with $(A \wedge P_{A,B}) \wedge (B \wedge P_{A,B})$. Evidently, $(A \wedge P_{A,B}) \wedge (B \wedge P_{A,B}) \leqslant A \wedge P, B \wedge P$. Let $C \in \mathcal{E}(\mathcal{H})$ with $C \leqslant A \wedge P$, $B \wedge P$. Then $C \leqslant A \wedge B \leqslant P_{A,B}$ and hence,

$$C \leqslant (A \wedge P_{A,B}) \wedge (B \wedge P_{A,B}).$$

Therefore, $(A \wedge P) \wedge (B \wedge P)$ exists and, by Proposition 2.4 it coincides with $A \wedge B$. □

III. INFIMUM OF A QUANTUM EFFECT AND ITS NEGATION

The *negation* A' of an effect A is defined to be the effect $A' = I - A$. Physically, A' is the effect A with its values 1 and 0 reversed. In the following we present a characterization of when $A \wedge A'$ exists in $\mathcal{E}(\mathcal{H})$ in terms of the location of the spectrum of A. The theorem essentially coincides with the result of Ando (Ref. 2, Theorem 2), the difference consists on that we express the condition with the help of the spectrum of A and the proof is based on the matrix representations as in Sec. II. There is also a similar characterization in Ref. 13.

Theorem 3.1: *Let* A *be a quantum effect on the Hilbert space* $\mathcal{H}$. *Then the following assertions are equivalent:*

(i) $A \wedge (I - A)$ *exists*,
(ii) $\sigma(A)$, *the spectrum of* A, *is contained either in* $\{0\} \cup \left[\frac{1}{2}, 1\right]$ *or in* $\left[0, \frac{1}{2}\right] \cup \{1\}$,
(iii) $A \wedge P_{A,I-A}$ *and* $(I-A) \wedge P_{A,I-A}$ *are comparable, that is, either* $A \wedge P_{A,I-A} \leqslant (I-A) \wedge P_{A,I-A}$ *or* $(I-A) \wedge P_{A,I-A} \leqslant A \wedge P_{A,I-A}$.

In addition, if either of the above holds, letting $g \in C([0,1])$ *be the function*

$$g(t) = \min(t, 1-t) = \begin{cases} t, & 0 \leqslant t \leqslant \frac{1}{2}, \\ 1-t, & \frac{1}{2} \leqslant t \leqslant 1, \end{cases} \tag{3.1}$$

we have, by continuous functional calculus, $A \wedge (I-A) = g(A)$.

Proof: Let E_A denote the spectral function of A. In view of Proposition 2.4, $A \wedge (I-A)$ exists if and only if $(A \wedge P_{A,I-A}) \wedge ((I-A) \wedge P_{A,I-A})$ exists. A moment of thought shows that $P_{A,I-A} = E_A((0,1))$ and hence, by Remark 2.3, we have that $A \wedge P_{A,I-A} = AE_A((0,1))$ and $(I-A) \wedge P_{A,I-A} = (I-A)E_A((0,1))$. Thus, without restricting the generality, we can and will assume in the following that 0 and 1 are not eigenvalues of A. Now, the equivalence of (ii) with (iii) is a matter of elementary spectral theory for selfadjoint operators, hence we will prove only the equivalence of (i) and (ii).

To prove that (ii) implies (i), let us assume that $\sigma(A)$ is contained either in $\{0\} \cup [\frac{1}{2}, 1]$ or in $[0, \frac{1}{2}] \cup \{1\}$. To make a choice, let us assume that $\sigma(A) \subseteq \{0\} \cup [\frac{1}{2}, 1]$. Since, by assumption, 0 is not an eigenvalue of A, it follows that $\sigma(A) \subseteq [\frac{1}{2}, 1]$. Then $A \geqslant I-A$ and clearly $A \wedge (I-A) = I-A = g(A)$, where the function g is defined as in (3.1). A similar argument holds in case we assume $\sigma(A) \subseteq [0, \frac{1}{2}] \cup \{1\}$; in this case $A \wedge (I-A) = A = g(A)$.

Conversely, let us assume that $A \wedge (I-A) = D$, the infimum of A and $I-A$ over $\mathcal{E}(\mathcal{H})$, exists. Using the spectral measure E_A of A, let $E_1 = E_A([0,1/2])$, $A_1 = A|E_1\mathcal{H}$, $E_2 = E_A((1/2,1])$, $A_2 = A|E_2\mathcal{H}$. We write D as an operator matrix with respect to the decomposition $\mathcal{H} = E_1\mathcal{H} \oplus E_2\mathcal{H}$,

$$D = \begin{bmatrix} D_1 & D_1^{1/2}\Gamma D_2^{1/2} \\ D_2^{1/2}\Gamma^* D_1^{1/2} & D_2 \end{bmatrix},$$

with contractive $\Gamma \in \mathcal{B}(E_2\mathcal{H}, E_1\mathcal{H})$, cf. Theorem 2.1. Since $g(A) \leqslant A, I-A$, by the definition of D we have

$$0 \leqslant D - g(A) = \begin{bmatrix} D_1 - A_1 & D_1^{1/2}\Gamma D_2^{1/2} \\ D_2^{1/2}\Gamma^* D_1^{1/2} & D_2 - (I_2 - A_2) \end{bmatrix}. \tag{3.2}$$

Therefore, $0 \leqslant D_1 - A_1$ while taking into account that $D \leqslant A$ it follows that $D_1 \leqslant A_1$, hence $D_1 = A_1$. Similarly, $0 \leqslant D_2 - (I_2 - A_2)$ and, since $D \leqslant I-A$ it follows $D_2 \leqslant I_2 - A_2$, hence $D_2 = I_2 - A_2$. Thus, the main diagonal of the matrix in (3.2) is null, hence (e.g., by Theorem 2.1) it follows that $D = g(A)$.

Further, let $\varepsilon \in (0, 1/4)$, and consider the operators

$$E_{\varepsilon,1} = E_A((\varepsilon, -\varepsilon + 1/2)), \quad E_{\varepsilon,2} = E_A((\varepsilon + 1/2, 1 - \varepsilon)). \tag{3.3}$$

Denote $E_\varepsilon = E_{\varepsilon,1} + E_{\varepsilon,2}$ and $A_\varepsilon = A|E_\varepsilon\mathcal{H}$. We show that $A_\varepsilon \wedge (I - A_\varepsilon)$ exists. To see this, we remark that, as proven before, $g(A) = A \wedge (I-A)$, so we actually show that $D_\varepsilon = D|E_\varepsilon\mathcal{H} = g(A_\varepsilon)$ coincides with $A_\varepsilon \wedge (I - A_\varepsilon)$. Indeed, assume that for some $C_\varepsilon \in \mathcal{E}(E_\varepsilon\mathcal{H})$ we have $C_\varepsilon \leqslant A_\varepsilon, I - A_\varepsilon$. Then, letting $C = C_\varepsilon E_\varepsilon \in \mathcal{E}(\mathcal{H})$ it follows that $C \leqslant A, I-A$. Since $D = A \wedge (I-A)$ this implies $C \leqslant D$ and hence $C_\varepsilon \leqslant D_\varepsilon$. Therefore, D_ε coincides with $A_\varepsilon \wedge (I - A_\varepsilon)$.

We finally prove that (i) implies (ii). Assume that (i) holds and (ii) is not true. Then there exists $\varepsilon \in (0, 1/4)$ such that $E_{\varepsilon,1} \neq 0$ and $E_{\varepsilon,2} \neq 0$, where we use the notation as in (3.3). Letting

$$A_{\varepsilon,1} = A|E_{\varepsilon,1}\mathcal{H}, \quad A_{\varepsilon,2} = A|E_{\varepsilon,2}\mathcal{H},$$

and $d = \varepsilon(1 + \sqrt{3})^{-1}$, consider an arbitrary contraction $T \in \mathcal{B}(E_{\varepsilon,2}\mathcal{H}, E_{\varepsilon,1}\mathcal{H})$. In the following all operator matrices are understood with respect to the decomposition $E_{\varepsilon,1}\mathcal{H} \oplus E_{\varepsilon,2}\mathcal{H}$. Then, letting

$$C = \begin{bmatrix} A_{\varepsilon,1} - \mathrm{d}I_{\varepsilon,1} & \sqrt{3}\,\mathrm{d}T \\ \sqrt{3}\,\mathrm{d}T^* & I_{\varepsilon,2} - A_{\varepsilon,2} - \mathrm{d}I_{\varepsilon,2} \end{bmatrix} = \begin{bmatrix} A_{\varepsilon,1} - \varepsilon I_{\varepsilon,1} + \sqrt{3}\,\mathrm{d}I_{\varepsilon,1} & \sqrt{3}\mathrm{d}T \\ \sqrt{3}\,\mathrm{d}T^* & I_{\varepsilon,2} - A_{\varepsilon,2} - \varepsilon I_{\varepsilon,2} + \sqrt{3}\,\mathrm{d}I_{\varepsilon,2} \end{bmatrix}$$
$$= \begin{bmatrix} A_{\varepsilon,1} - \varepsilon I_{\varepsilon,1} & 0 \\ 0 & I_{\varepsilon,2} - A_{\varepsilon,2} - \varepsilon I_{\varepsilon,2} \end{bmatrix} + \sqrt{3}d \begin{bmatrix} I_{\varepsilon,1} & T \\ T^* & I_{\varepsilon,2} \end{bmatrix} \geqslant 0,$$

we have

$$A_\varepsilon - C = \begin{bmatrix} \mathrm{d}I_{\varepsilon,1} & -\sqrt{3}\,\mathrm{d}T \\ -\sqrt{3}\,\mathrm{d}T^* & 2A_{\varepsilon,2} - I_{\varepsilon,2} + \mathrm{d}I_{\varepsilon,2} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 2A_{\varepsilon,2} - I_{\varepsilon,2} - 2\,\mathrm{d}I_{\varepsilon,2} \end{bmatrix} + d \begin{bmatrix} I_{\varepsilon,1} & -\sqrt{3}T \\ -\sqrt{3}T^* & 3I_{\varepsilon,2} \end{bmatrix} \geqslant 0$$

and

$$I - A_\varepsilon - C = \begin{bmatrix} I_{\varepsilon,1} - 2A_{\varepsilon,1} + \mathrm{d}I_{\varepsilon,1} & -\sqrt{3}T \\ -\sqrt{3}\,\mathrm{d}T^* & \mathrm{d}I_{\varepsilon,2} \end{bmatrix} = \begin{bmatrix} I_{\varepsilon,1} - 2A_{\varepsilon,1} - 2\,\mathrm{d}I_{\varepsilon,1} & 0 \\ 0 & 0 \end{bmatrix} + d \begin{bmatrix} 3I_{\varepsilon,1} & -\sqrt{3}T \\ -\sqrt{3}\,\mathrm{d}T^* & I_{\varepsilon,2} \end{bmatrix}$$
$$\geqslant 0.$$

But, the operator

$$(A_\varepsilon \wedge (I_\varepsilon - A_\varepsilon)) - C = g(A_\varepsilon) - C = d \begin{bmatrix} I_{\varepsilon,1} & -\sqrt{3}T \\ -\sqrt{3}T^* & I_{\varepsilon,2} \end{bmatrix}$$

is not non-negative for some choices of T, unless at least one of the spectral projections $E_{\varepsilon,1}$ and $E_{\varepsilon,2}$ is trivial. Since ε is arbitrarily small, it follows that A cannot simultaneously have spectral points in $(0,1/2)$ and $(1/2,1)$. Therefore, (i) implies (ii). □

IV. TWO EXAMPLES

In this section we answer in the negative a question raised in Ref. 19. First we recall how the problem of the existence of the infimum of A and B in $\mathcal{E}(\mathcal{H})$ can be reduced to the infimum problem for some quantum effects and their negations. Assume, in addition, that $\mathrm{Ker}(A+B)=0$. Let f_{A+B} be the affine (that is, linear on convex combinations) mapping defined as in Ref. 9 by

$$f_{A+B}:\{C|0 \leqslant C \leqslant A+B\} \to \{D|0 \leqslant D \leqslant P_{A+B}\}, \tag{4.1}$$

with $C=(A+B)^{1/2}f_{A+B}(C)(A+B)^{1/2}$. By Theorem 2.2 in Ref. 9, f_{A+B} is well defined. Since f_{A+B} is an affine isomorphism, $A\wedge B$ exists if and only if $f_{A+B}(A)\wedge f_{A+B}(B)$ exists. As

$$f_{A+B}(A) + f_{A+B}(B) = f_{A+B}(A+B) = I$$

we are in the situation of Theorem 3.1.

Actually, the following more general fact holds.

Lemma 4.1: Let $A \in \mathcal{E}(\mathcal{H})$, $0 \leqslant C$, $D \leqslant A$, and consider the mapping f_A as defined in (4.1). *Then $C\wedge D$ exists if and only if $f_A(C)\wedge f_A(D)$ exists and, in this case, we have*

$$f_A(C \wedge D) = f_A(C) \wedge f_A(D).$$

Proof: This is a consequence of Theorem 2.5 in Ref. 9. □

By Proposition 2.4, the infimum of A and B exists if and only if the infimum of $A\wedge P_{A,B}$ and $B\wedge P_{A,B}$ exists or, equivalently, the infimum of the restrictions $\widetilde{A} := A\wedge P_{A,B}|P_{A,B}\mathcal{H}$ and $\widetilde{B} := B\wedge P_{A,B}|P_{A,B}\mathcal{H}$ exists. Since $\mathrm{Ker}(\widetilde{A}+\widetilde{B})=\{0\}$, $\widetilde{A}\wedge\widetilde{B}$ exists if and only if $f_{\widetilde{A}+\widetilde{B}}(\widetilde{A})\wedge f_{\widetilde{A}+\widetilde{B}}(\widetilde{B})$ exists, and for the pair $f_{\widetilde{A}+\widetilde{B}}(\widetilde{A}), f_{\widetilde{A}+\widetilde{B}}(\widetilde{B})$ we observe that Theorem 3.1 applies. Therefore, under the additional assumptions that 0 and 1 are not eigenvalues of $f_{\widetilde{A}+\widetilde{B}}(\widetilde{A})$ and $f_{\widetilde{A}+\widetilde{B}}(\widetilde{B})$, $\widetilde{A}\wedge\widetilde{B}$ exists if and only if $A\wedge P_{A,B}$ and $B\wedge P_{A,B}$ are comparable; in this case, $A\wedge B$ coincides with the smaller of the

$A \wedge P_{A,B}$ and $B \wedge P_{A,B}$. For a finite dimensional Hilbert space it was proven in Ref. 19 that the infimum of the operators $A \wedge P_{A,B}$ and $B \wedge P_{A,B}$ exists if and only if they are comparable.

The next example shows that, contrary to the finite dimensional case, we may have two quantum effects B_1 and B_2 for which $B_1 \wedge B_2$ exists, but $(B_1 \wedge P_{B_1,B_2})$ and $(B_2 \wedge P_{B_1,B_2})$ are not comparable.

Example 4.2: Let $\mathcal{H}=L^2[-1,1]$ and A be the operator of multiplication with the square of the independent variable on $\mathcal{H}$, $(Ax)(t)=t^2x(t)$, for all $x \in L^2[-1,1]$. Then A is a non-negative contraction on $\mathcal{H}$, that is, a quantum effect, and the same is its square root $A^{1/2}$, that is, $(A^{1/2}x)(t) = |t|x(t)$, $x \in L^2[-1,1]$. Note that A, and hence $A^{1/2}$, are injective.

Let $\mathbf{1}$ be the constant function equal to 1 on $[-1,1]$, $\theta(t) := \operatorname{sgn}(t)$, and $\chi_\pm := \frac{1}{2}(\mathbf{1} \pm \theta)$, the characteristic functions of $[0, 1]$ and, respectively, $[-1,0]$. All these functions are in $L^2[-1,1]$. Note that $\mathbf{1}$ and θ span the same two dimensional space as $\chi_\pm$. Denote

$$\mathcal{H}_0 = \mathcal{H} \ominus \operatorname{span}\{\mathbf{1}, \theta\} = \mathcal{H} \ominus \operatorname{span}\{\chi_+, \chi_-\}.$$

With respect to the decomposition

$$\mathcal{H} = \mathbb{C}\mathbf{1} \oplus \mathbb{C}\ \theta \oplus \mathcal{H}_0$$

consider two quantum effects C_1 and C_2 on $\mathcal{H}$ defined by

$$C_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{1}{2}I_0 \end{bmatrix}, \quad C_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2}I_0 \end{bmatrix},$$

where I_0 is the identity operator on $\mathcal{H}_0$. Clearly we have $C_1 + C_2 = I$ and letting

$$B_1 = A^{1/2}C_1A^{1/2}, \quad B_2 = A^{1/2}C_2A^{1/2},$$

we have

$$B_1 + B_2 = A.$$

Comparing the spectra of C_1 and C_2 and using Theorem 3.1, it follows that $C_1 \wedge C_2$ exists, but C_1 and C_2 are not comparable. Therefore, using Lemma 4.1, it follows that $B_1 \wedge B_2$ exists, but B_1 and B_2 are not comparable. In the following we will prove that $P_{B_1,B_2} = I$, that is, $\operatorname{Ran}(B_1^{1/2}) \cap \operatorname{Ran}(B_2^{1/2})$ is dense in $\mathcal{H}$. We divide the proof in several steps.

Step 1: $A^{1/2}\mathcal{H}_0$ is dense in $\mathcal{H}$.

Indeed, let $f \in \mathcal{H} = L^2[-1,1]$ be a function such that for all $h_0 \in \mathcal{H}_0$ we have

$$0 = \langle A^{1/2}h_0, f\rangle = \langle h_0, A^{1/2}f\rangle.$$

Then $A^{1/2}f$ is a linear combination of the functions $\mathbf{1}$ and θ, that is, there exist scalars α and β such that

$$|t|f(t) = \alpha + \beta \operatorname{sgn}(t), \quad t \in [-1,1]$$

and hence

$$f(t) = \frac{\alpha + \beta \operatorname{sgn}(t)}{|t|} = \begin{cases} \dfrac{\alpha+\beta}{t}, & 0 < t \leqslant 1, \\ \dfrac{\beta-\alpha}{t}, & -1 \leqslant t < 0. \end{cases}$$

Since $f \in L^2[-1,1]$ this shows that $f=0$ and the claim is proven.

Let us consider the following linear manifolds in $\mathcal{H}$:

$$\mathcal{F} := \{f \in L^2[-1,1] | f \text{ piecewise constant}\},$$

$$\mathcal{F}_0 := \{f \in \mathcal{F} | \exists\ \varepsilon > 0 \text{ s.t. } f|(-\varepsilon,\varepsilon) = 0, \langle f, \chi_- \rangle = \langle f, \chi_+ \rangle = 0\}.$$

Step 2: $\mathcal{F}_0$ is dense in $\mathcal{H}_0$.

Indeed, to see this, let us first note that $\mathcal{F}_0 \subset \mathcal{H}_0$. If h_0 is an arbitrary vector in $\mathcal{H}_0$ and $\varepsilon > 0$, there exists $f_1 \in \mathcal{F}$ such that

$$\|h_0 - f_1\| \leqslant \frac{\varepsilon}{8} \text{ hence } |\langle h_0 - f_1, \chi_\pm \rangle| \leqslant \frac{\varepsilon}{8}. \tag{4.2}$$

Moreover, there exists $f_2 \in \mathcal{F}$ such that it is zero in a neighbourhood of zero and

$$\|f_1 - f_2\| \leqslant \frac{\varepsilon}{8}. \tag{4.3}$$

Consequently,

$$\|h_0 - f_2\| \leqslant \frac{\varepsilon}{4} \quad \text{and hence } |\langle h_0 - f_2, \chi_\pm \rangle| \leqslant \frac{\varepsilon}{4}. \tag{4.4}$$

Let

$$f_3 = f_2 + 2\chi_{[1/2,1]}\langle h_0 - f_2, \chi_+ \rangle + 2\chi_{[-1,-1/2]}\langle h_0 - f_2, \chi_- \rangle.$$

Then, from the choice of f_2 it follows

$$\langle f_3, \chi_+ \rangle = \langle f_2, \chi_+ \rangle + \langle h_0 - f_2, \chi_+ \rangle = \langle h_0, \chi_+ \rangle = 0$$

and

$$\langle f_3, \chi_- \rangle = \langle f_2, \chi_- \rangle + \langle h_0 - f_2, \chi_- \rangle = \langle h_0, \chi_- \rangle = 0,$$

hence $f_3 \in \mathcal{F}_0$. Finally, from (4.2), (4.3), and (4.4) we get

$$\|h_0 - f_3\| \leqslant \|h_0 - f_1\| + \|f_1 - f_2\| + \|f_2 - f_3\| \leqslant \varepsilon,$$

and the claim is proven.

Finally, we prove the following.

Step 3: $P_{B_1,B_2} = I$, that is, $\mathrm{Ran}(B_1^{1/2}) \cap \mathrm{Ran}(B_2^{1/2})$ is dense in $\mathcal{H}$.

In the following we are using the inverse operator $A^{-1/2}$ on its range. By the preceding claim, $A^{1/2}(A^{-1/2}\mathcal{F}_0)$ is a linear submanifold in $\mathcal{H}_0$ and dense in it. Since the restrictions of C_1 and C_2 to $\mathcal{H}_0$ coincide with $\frac{1}{2}I_0$, it follows that the linear manifolds $C_1A^{1/2}(A^{-1}\mathcal{F}_0)$ and $C_2A^{1/2}(A^{-1}\mathcal{F}_0)$ coincide and are dense in $\mathcal{H}_0$. Consequently, the linear manifolds $A^{1/2}C_1A^{1/2}(A^{-1}\mathcal{F}_0)$ and $A^{1/2}C_2A^{1/2}(A^{-1}\mathcal{F}_0)$ coincide and, by Step 1 and Step 2, they are dense in $\mathcal{H}$. Thus, the linear manifold,

$$\mathcal{L} = B_1(A^{-1/2}\mathcal{F}_0) = B_2(A^{-1/2}\mathcal{F}_0) \subseteq \mathrm{Ran}(B_1) \cap \mathrm{Ran}(B_2) \subseteq \mathrm{Ran}(B_1^{1/2}) \cap \mathrm{Ran}(B_2^{1/2}),$$

is dense in $\mathcal{H}$. This concludes the proof of the last step, and the example.

In order to explain the connection with the characterization of the existence of infimum obtained by Ando in Ref. 2 we consider the comparison of $A \wedge P_{A,B}$ with the *generalized shorted* operator, as considered in Ref. 2.

Lemma 4.3: Let $A, B \in \mathcal{E}(\mathcal{H})$. Then, for any sequence α_n of positive numbers that converge increasingly to infinity, we have

$$\text{SO-}\lim_{n\to\infty}(A:\alpha_n B) \leqslant A \wedge P_{A,B}, \tag{4.5}$$

and the limit does not depend on the sequence (α_n).

Proof: First note that the sequence of positive operators $A:\alpha_n B$ is nondecreasing and bounded by A, cf. Ref. 8. Consequently, the strong operator limit exists and does not depend on the sequence α_n increasing to infinity. We thus can take $\alpha_n=n$. Since the parallel sum is strongly continuous in the second variable with respect to nondecreasing sequences, cf. Theorem 2.6, we have $A:nB\leqslant A$ and, since $\mathrm{Ran}((A:nB)^{1/2})=\mathrm{Ran}(A^{1/2})\cap\mathrm{Ran}(B^{1/2})$ it follows $A:nB\leqslant P_{A,B}$ and hence (4.5) holds. □

Given two positive operators A and B, the *generalized shorted operator* $[B]A$ is defined (see Ref. 1) by

$$[B]A=\lim_{n\to\infty} A:(nB).$$

The main result in Ref. 2 states that the infimum $A\wedge B$ exists if and only $[B]A$ and $[A]B$ are comparable and, in this case, $A\wedge B$ is the smaller of $[A]B$ and $[B]A$. In view of this result and our Example 4.2, it follows that, in general, (4.5) cannot be improved to equality. Here we have a simpler example emphasizing this fact.

Example 4.4: Let $\mathcal{H}=L^2[0,1]$ and A the operator of multiplication with the function t^2. Then A is bounded, contractive, and positive. In addition, $A^{1/2}$ is the operator of multiplication with the independent variable t. Note that both A and $A^{1/2}$ are injective.

Further, let **1** be the function constant 1 in $L^2[0,1]$ and note that it does not belong to the range of either A or $A^{1/2}$. Let C be a non-negative contraction in $\mathcal{H}$ with kernel $\mathbb{C}1$ and define $B=A^{1/2}CA^{1/2}$. Then the operator B is injective and hence its range is dense in $\mathcal{H}$. Since $\mathrm{Ran}(B)\subseteq\mathrm{Ran}(B^{1/2})$ and, by construction, $\mathrm{Ran}(B)\subseteq\mathrm{Ran}(A^{1/2})$ as well, it follows that $\mathrm{Ran}(A^{1/2})\cap\mathrm{Ran}(B^{1/2})$ is dense in $\mathcal{H}$, hence $P_{A,B}=I$.

For each $n\geqslant 1$ consider the function $v_n\in L^2[0,1]$ defined by

$$v_n(t)=\begin{cases}0, & 0\leqslant t\leqslant 1/n,\\ 1/t & 1/n<t\leqslant 1.\end{cases}$$

Note that $A^{1/2}v_n=\chi_{(1/n,1]}$, the characteristic function of the interval $(1/n,t]$. Taking into account that the sequence of functions $\chi_{(1/n,1]}$ converges in norm to the function **1**, it follows that

$$\langle Bv_n,v_n\rangle=\langle CA^{1/2}v_n,A^{1/2}v_n\rangle=\langle C\chi_{(1/n,1]},\chi_{(1/n,1]}\rangle\to\langle C\mathbf{1},\mathbf{1}\rangle=0.$$

Let α_n be a sequence of positive numbers increasing to $+\infty$ and such that $\alpha_n\langle Bv_n,Bv_n\rangle$ converges to 0. It is easy to see that this is always possible. Then using the characterization of the parallel sum as in Theorem 2.6.(vi), for arbitrary $n\geqslant m>2$ we have

$$\begin{aligned}\langle(A:\alpha_nB)v_mv_m\rangle&=\inf\{\langle Au,u\rangle+\alpha_n\langle Bv,v\rangle|v_m=u+v\}=\inf\{\langle A(v_m-v),v_m-v\rangle+\alpha_n\langle Bv,v\rangle|v\in\mathcal{H}\}\\&=\inf\{\langle Av_m,v_m\rangle-2\,\mathrm{Re}\langle Av_m,v\rangle+\langle Av,v\rangle+\alpha_n\langle Bv,v\rangle|v\in\mathcal{H}\}\leqslant\langle Av_m,v_m\rangle\\&\quad-2\,\mathrm{Re}\langle Av_m,v_n\rangle+\langle Av_n,v_n\rangle+\alpha_n\langle Bv_n,v_n\rangle=1-\frac{1}{m}-2+\frac{2}{m}+1-\frac{1}{n}+\alpha_n\langle Bv_n,v_n\rangle\\&=\frac{1}{m}-\frac{1}{n}+\alpha_n\langle Bv_n,v_n\rangle\to\frac{1}{m}<\frac{1}{2}\ \text{as}\ n\to\infty.\end{aligned}$$

On the other hand,

$$\langle Av_m,Av_m\rangle=1-\frac{1}{m}\geqslant\frac{1}{2}.$$

Hence, we have strict inequality in (4.5).

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Distinguishing bipartitite orthogonal states using LOCC: Best and worst cases

Michael Nathanson[a)]
Department of Mathematics, Northeastern University, Boston Massachusetts 02115

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Two types of results are presented for distinguishing pure bipartite quantum states using local operations and classical communications. We examine sets of states that can be perfectly distinguished, in particular showing that any three orthogonal maximally entangled states in $C^3 \otimes C^3$ form such a set. In cases where orthogonal states cannot be distinguished, we obtain upper bounds for the probability of error using LOCC taken over all sets of k orthogonal states in $C^n \otimes C^m$. In the process of proving these bounds, we identify some sets of orthogonal states for which perfect distinguishability is not possible. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1914731]

I. INTRODUCTION

There is much interest in understanding what can and cannot be achieved using local operations and classical communications (LOCC) on a composite quantum system, pursued with an eye towards applications in communication and cryptography. One of the first and most basic problems in LOCC is that of distinguishing orthogonal quantum states. While some direct applications of this problem do exist (for instance, data hiding[13] and corrected channels[8,9]), these are limited by the usual assumption that no additional entanglement exists between the two parties. However, the problem of LOCC discrimination has proved a fertile area for attempts to better understand the relationship between entanglement and locality, the mysterious interplay that underlies virtually all quantum communication and cryptography protocols. It is in this spirit that the current work is undertaken.

The setup for bipartite LOCC is quite simple: Two parties (by convention Alice and Bob) are physically separate but share a quantum state. Each may perform local quantum operations on his/her piece of the system, but the two may only communicate through a classical channel. In this paper, we will suppose that Alice and Bob share one of a known set of orthogonal states; their task is to determine the identity of this state (even if it is destroyed in the process). Since the possible states are orthogonal, they clearly could be distinguished and preserved were global operations permitted.

The most fundamental and surprising results in this area are those of Walgate *et al.*,[15] that *any* two orthogonal states can be locally distinguished; and of Bennett *et al.*,[2] that there exists a basis of product states that cannot be distinguished with LOCC. These two facts demonstrate that there is no simple relationship between entanglement and locality, which has led to further exploration, e.g., Refs. 10 and 14.

Following the definitive result for two states,[15] work has been done to identify larger sets of orthogonal states that can and cannot be perfectly distinguished with LOCC. Both Refs. 5 and 6 looked at generalized Bell bases in $C^n \otimes C^n$. Fan[5] showed that any k such states can be perfectly distinguished if n is prime and $k(k-1) \leqslant 2n$, in particular, in the case $k=n=3$. The question was posed in Ref. 6 whether *any* three maximally entangled states could be distinguished; we answer this question in the affirmative. We also also give a sufficient condition for perfect distinguish-

[a)]Electronic mail: nathanson.m@neu.edu

ability among maximally entangled states in $C^n \otimes C^n$ using unbiased bases, thus providing an alternative proof of the result in Ref. 5.

It not always possible to perfectly distinguish k orthogonal vectors when $k>2$. For instance, Ghosh *et al.* showed that k generalized Bell states in $C^n \otimes C^n$ cannot be distinguished with LOCC if $k>n$.[6,7] In the second part of this paper we establish lower bounds on the effectiveness of probabilistic LOCC discrimination of orthogonal vectors. If Alice and Bob share one of k arbitrary orthogonal vectors in $C^n \otimes C^n$, what is their guaranteed minimal probability of correctly identifying it? And which sets of states achieve this minimum? These questions have an immediate application to a data hiding setup, as described in Ref. 13 in which a "Boss" can clear prior entanglement between Alice and Bob before giving them pieces of a secret quantum state to work on.

It is shown that for $2 \leqslant k \leqslant 4$, k arbitrary orthogonal vectors in $C^m \otimes C^n$ can be correctly identified with probability at least $2/k$, and this bound is tight. An interesting fact is that this does not depend on the dimension of the overall space—the worst case occurs when the states are embedded in a $C^2 \otimes C^2$ subspace. Our final result translates these ideas into the more familiar language of mutual information and recovers a bound implied by Ref. 1.

The bounds from these propositions identify sets of vectors for which perfect distinguishability is impossible. In particular, we generalize Ref. 6 to show that no k maximally entangled states can be perfectly distinguished if $k>n$. The bounds also lead to the well-known result of Horodecki *et al.*[10] that a complete basis of perfectly distinguishable vectors must be a product basis.

As a final comment, we note the distinction made in Ref. 4 between LOCC protocols that have so-called infinite resources and those that use a finite number of rounds of communication and remain in finite-dimensional ancillary spaces. The results in this paper are established under the assumption that all protocols terminate with probability one and that each ancillary system is finite dimensional.

The paper is organized as follows: In Sec. II we state the results and give the necessary background, and in Secs. III and IV we provide the proofs.

II. STATEMENT OF RESULTS

Following the result in Ref. 15, we would like to identify sets of k orthogonal vectors that can be perfectly distinguished with LOCC for $k>2$. For instance, it is immediate that any three orthogonal states can be perfectly distinguished if two of them are product states. Also, from Ref. 5, any 3 states of a generalized Bell basis of $C^n \otimes C^n$ can be distinguished if $n \geqslant 3$; the question for general maximally entangled vectors in $C^3 \otimes C^3$ is noted but not answered in Ref. 6.

Proposition 1: Any three orthogonal maximally entangled states in $C^3 \otimes C^3$ can be perfectly distinguished using LOCC.

It is not clear whether any 3 orthogonal maximally entangled states are distinguishable in $C^n \otimes C^n$. However, the following proposition gives a sufficient condition for distinguishing maximally entangled states using the idea of mutually unbiased bases, which arise in several areas of quantum information (see, for instance Refs. 11 and 16). The more general notion of a common unbiased basis is not well studied but is defined here for convenience.

Definition 2: Let $\mathcal{A}=\{\mathcal{A}_i : i \in \mathcal{I}\}$ be a family of orthonormal bases of C^n, with $\mathcal{A}_i = \{|a_{i1}\rangle, |a_{i2}\rangle, \ldots, |a_{in}\rangle\}$ and $\mathcal{I}$ some indexing set.

A basis $\mathcal{B}$ of C^n is a common unbiased basis for $\mathcal{A}$ if, for all $|b\rangle \in \mathcal{B}$ and for all $i \in \mathcal{I}$, $1 \leqslant j \leqslant n$:

$$|\langle b|a_{ij}\rangle|^2 = \frac{1}{n}. \tag{1}$$

So, a set of bases $\mathcal{A}$ is mutually unbiased if and only if for all $i \in \mathcal{I}$, $\mathcal{A}_i$ is a common unbiased basis for $\mathcal{A}-\{\mathcal{A}_i\}$.

In the following proposition, we write our states in terms of a (noncanonical) standard maximally entangled state of $C^n \otimes C^n$:

$$|ME_n\rangle := \frac{1}{\sqrt{n}}\sum_{j=0}^{n-1}|j\rangle|j\rangle. \tag{2}$$

Proposition 3: Let $|\Psi_1\rangle, |\Psi_2\rangle, \ldots, |\Psi_k\rangle$ *be orthogonal, maximally entangled vectors in* $C^n \otimes C^n$, *with* $|\Psi_i\rangle = (I \otimes B_i)|ME_n\rangle$.

For each pair (i,j), *let* $\mathcal{A}_{ij}$ *be a basis of eigenvectors of* $B_i^\dagger B_j$, *and let*

$$\mathcal{A} = \{\mathcal{A}_{ij}: 1 \leqslant i < j \leqslant k\}.$$

If the family $\mathcal{A}$ *has a common unbiased basis, then the k states can be perfectly distinguished by LOCC.*

The result is actually more general—we do not require that the states be maximally entangled, only that the matrices $B_i^\dagger B_j$ be diagonalizable. For instance, we could use the same proof to show that any simultaneously diagonalizable orthogonal states can be locally distinguished. These are sets of the form

$$\left\{ |\varphi_i\rangle = \sum_{j=0}^{n-1} u_{ij}|jj\rangle, 1 \leqslant i \leqslant n \right\}, \tag{3}$$

where u is an $n \times n$ unitary matrix.

The main result of Ref. 5 follows from Proposition 3. It involves the generalized Pauli matrices $Z = \Sigma_j e^{2\pi i j/n}|j\rangle\langle j|$ and $X = \Sigma_j |j\rangle\langle j+1|$ and the generalized Bell basis,

$$\mathrm{BB}_n := \{(I \otimes X^m Z^l)|ME_n\rangle : 0 \leqslant m,l \leqslant n-1\} \subset C^n \otimes C^n. \tag{4}$$

Corollary 4 (H. Fan): Let $|\Psi_1\rangle, |\Psi_2\rangle, \ldots, |\Psi_k\rangle$ *be orthogonal, maximally entangled vectors in* $C^n \otimes C^n$, *with n prime and* $|\Psi_i\rangle \in \mathrm{BB}_n$.

Then if $k(k-1)/2 \leqslant n$, *the k vectors can be perfectly distinguished by LOCC.*

Proof: This follows from the fact that for n prime, the eigenbases of $\{X^m Z^l : 0 \leqslant l,m < n\}$ form a maximum set of $(n+1)$ mutually unbiased bases in C^n.[11] Up to a global phase,

$$(X^{m_i}Z^{l_i})^\dagger (X^{m_j}Z^{l_j}) \equiv X^{m_j - m_i} Z^{l_j - l_i}, \tag{5}$$

so the eigenbases of the pairwise products also belong to the set of mutually unbiased bases. As long as the number of pairs (i,j) is less than the number of mutually unbiased bases, then there exists a common unbiased basis and the proposition can be applied. But this is the condition that $k(k-1)/2 < n+1$.

It is not always possible to distinguish maximally entangled states (Ref. 7), which raises the question of how bad it can be (or conversely, what minimal level of success is guaranteed). When perfect discrimination is not possible, one possible strategy is unambiguous discrimination, in which either the correct identity of the state is discovered or else a generic error message is returned. Another strategy is minimum error discrimination, in which the protocol always produces one of the possible states, but this identification might be incorrect. The challenge in this case is to find a protocol that minimizes the probability of error. It is this problem of minimum error discrimination that we will consider throughout the rest of the paper.

Suppose Alice and Bob share one of the orthogonal vectors $\{|\Psi_i\rangle\}$ with *a priori* probabilities $\{p_i\}$. They apply a LOCC protocol, which produces a best guess as to the identity of their state. Define $P(\{|\Psi_i\rangle\}, \{p_i\})$ as the probability that Alice and Bob correctly identify which vector they share, assuming an optimal strategy is used. We are interested in the worst case scenario–what ensembles of k orthogonal vectors are hardest to distinguish using LOCC? Initially, we restrict ourselves to maximally entangled states and define

$$f_{\mathrm{me}}(k,n) := \min_{\{|\Psi_i\rangle\},\{p_i\}} P(\{|\Psi_i\rangle\},\{p_i\}), \tag{6}$$

where the minimum is taken over probability distributions p_i and sets of orthogonal maximally entangled states $\{|\Psi_1\rangle,\ldots,|\Psi_k\rangle\}\subset C^n\otimes C^n$.

We immediately observe that f_{me} is a nonincreasing function in both k and n; as k and n increase, the minimum is taken over larger nested sets. We note that for all n, $f_{\mathrm{me}}(2,n)=1$, since two orthogonal states can always be distinguished by LOCC.[15] Proposition 1 is equivalent to the fact that $f_{\mathrm{me}}(3,3)=1$.

But there are limitations to what can be done if the number of vectors is bigger than the dimension.

Proposition 5: For all $2\leqslant n\leqslant k\leqslant n^2$,

$$\frac{2}{k}\leqslant f_{\mathrm{me}}(k,n)\leqslant\frac{n}{k}. \tag{7}$$

In the case $n=3\leqslant k\leqslant 9$,

$$f_{\mathrm{me}}(k,3)=\frac{3}{k}. \tag{8}$$

.

We can also define a more general function in which we remove the assumption that the states are maximally entangled,

$$f(k,n) := \min_{\{|\Psi_i\rangle\},\{p_i\}} P(\{|\Psi_i\rangle\},\{p_i\}), \tag{9}$$

where the minimum is taken over probability distributions p_i and *all* sets of orthogonal states $\{|\Psi_1\rangle,\ldots,|\Psi_k\rangle\}\subset C^n\otimes C^n$.

Again, f is nonincreasing with respect to n and k and $f(2,n)=1$. Also, for $k\leqslant m^2\leqslant n^2$, k maximally entangled vectors in $C^m\otimes C^m$ can be embedded in $C^n\otimes C^n$, so $f(k,n)\leqslant f_{\mathrm{me}}(k,m)$. The previous results for f_{me} imply bounds on f.

Proposition 6: For $2\leqslant n\leqslant k\leqslant n^2$,

$$\frac{2}{k}\leqslant f(k,n)\leqslant\frac{\lceil\sqrt{k}\rceil}{k}. \tag{10}$$

In particular,

$$f(3,n)=\frac{2}{3},\quad f(4,n)=\frac{1}{2}. \tag{11}$$

.

The function $f(k,n)$ is defined only when the two spaces have the same dimension. We could just as easily have defined $f(k,m,n)$ for k vectors in $C^m\otimes C^n$ and applied Lemma 8 to that. However, we have discovered no bounds on this that do not follow from inclusion; that is, for $m\leqslant n$, the best we can say is

$$f(k,n)\leqslant f(k,m,n)\leqslant f(k,m),\quad k\leqslant m^2, \tag{12}$$

$$f(k,n)\leqslant f(k,m,n)\leqslant\frac{n}{k},\quad m^2<k\leqslant mn. \tag{13}$$

.

We note that for $k \leqslant 4$, $f(k,n)$ is independent of n; the k vectors are most difficult to distinguish when they are squeezed into the smallest possible space. It seems entirely possible that $f(k,n)$ will remain independent of n, even for higher values of k.

Propositions 5 and 6 are proved using the following lemmas. In fact, most of the work goes into the proof of Lemma 8, as it requires us to analyze Alice and Bob's protocol in detail.

Lemma 7: For all $2 \leqslant j \leqslant k \leqslant n^2$,

$$\frac{j}{k} f_{\mathrm{me}}(j,n) \leqslant f_{\mathrm{me}}(k,n), \tag{14}$$

$$\frac{j}{k} f(j,n) \leqslant f(k,n). \tag{15}$$

Lemma 8: Given k equally probable vectors $\{|\Psi_1\rangle, \ldots, |\Psi_k\rangle\} \subset C^m \otimes C^n$, $n \leqslant k \leqslant mn$, *with the property that for each i,* $|\Psi_i\rangle = (I \otimes U_i)|\Psi_1\rangle$ *for* U_i *unitary. Then the k vectors can be distinguished using LOCC with probability that is at most* n/k.

The assumption in Lemma 8 is equivalent to the fact that the C^n party can unilaterally transform $|\Psi_i\rangle$ into $|\Psi_j\rangle$ for any i,j. The lemma includes the special case in which all the states are maximally entangled. Also, note that there is no assumption here that the states are orthogonal, though this is clearly the most interesting case.

Examples: Given a basis of four orthogonal maximally entangled states in $C^2 \otimes C^2$, one naive notion is to ignore two of the possible states and perfectly distinguish the remaining two, thus achieving the lower bound in Lemma 7. Lemma 8 states that this, in fact, is an optimal strategy for identifying the given state. Proposition 6 combines the lemmas to say that this is the worst case for trying to distinguish four orthogonal states.

Likewise, given $k > 3$ orthogonal maximally entangled states in $C^3 \otimes C^3$, one can discard all but three of them and then perfectly distinguish those that remain using Proposition 1. Again, the lemma states that this is optimal. However, for $k=4$ or $k=5$, this succeeds with probability greater than $\frac{1}{2}$ and so is no longer the worst case in $C^3 \otimes C^3$. A worse case would be four equally probable maximally entangled states in a $C^2 \otimes C^2$ subspace.

Finally, we look at an example using the generalized Bell basis BB_n defined in (4). Suppose we wish to distinguish the states in a set $T \subset \mathrm{BB}_n$ with $|T| = k$. If n is prime, then the argument in Ref. 5 implies that Alice and Bob can correctly identify their vectors with probability n/k; Lemma 8 shows that this is in fact optimal.

The following modification of Lemma 8 establishes a necessary condition to distinguish a set of states.

Proposition 9: Given k equally probable vectors $\{|\Psi_1\rangle, \ldots, |\Psi_k\rangle\} \subset C^m \otimes C^n$ *and let* λ_M *be the largest Schmidt coefficient in any of the* $|\Psi_i\rangle$. *Then the k vectors can be distinguished using LOCC with probability that is at most* $\lambda_M mn/k$.

In particular, if k vectors can be perfectly distinguished with LOCC, then $\lambda_M \geqslant k/mn$.

It is interesting to note that in the case of perfect distinguishability, this proposition gives a lower bound on the maximal Schmidt coefficient, while the result of Chen and Li[3] gives an upper bound on the number of nonzero Schmidt coefficients.

The following generalizes the work of Ref. 6 by setting $\lambda_M = 1/n$ above.

Corollary 10: No k maximally entangled states in $C^n \otimes C^n$ *can be perfectly distinguished with LOCC if* $k > n$.

Both Proposition 9 and the result in Ref. 3 imply the fundamental result of Horodecki *et al.*, that a distinguishable basis must be a product basis.[10]

Corollary 11 (Horodecki et al): Let $\{|\Psi_1\rangle, \ldots, |\Psi_{mn}\rangle\}$ *be an orthonormal basis of* $C^m \otimes C^n$, *and suppose these vectors can be perfectly distinguished using LOCC. Then each of the vectors is a product vector*.

To see this as a consequence of Proposition 9, suppose we have have one of the $|\Psi_i\rangle$ with equal probability. Then clearly $\lambda_M = k/mn = 1$. Examining the proof of Proposition 9 reveals that if $|\Psi_i\rangle$ has maximal Schmidt coefficient $\lambda_i < \lambda_M$, then either $P(Z=i)=0$ or else the inequality on $P(Z=V)$ is strict. Neither of these is possible with perfect distinguishability, which means $\lambda_i = \lambda_M = 1$ and $|\Psi_i\rangle$ is a product state for all i.

These types of results are useful in that they allow us to identify classes of sets of k vectors in $C^m \otimes C^n$ that cannot be perfectly distinguished. Also, they provide an upper bound on the probabilities and allow us to deduce optimal strategies for correct identification.

The function $f(k,n)$ is one way of assessing how much information Alice and Bob can gain from LOCC measurements on their vectors. Another approach would be to use the classical mutual information between the identity V of the vector sent and the outcomes of Alice and Bob's measurements. (This idea was explored, for instance, with reference to the specific nine-state ensemble in Ref. 2.) Let Y represent the outcomes of the first $r-1$ measurements and Z indicate the final measurement, i.e., the conclusion as to the value of V, and write

$$I(V;YZ) = H(V) - H(V|YZ), \tag{16}$$

where H is the Shannon entropy.

As we defined $f(k,n)$, we define a function $g(k,n)$ based on mutual information. Assuming that Alice and Bob use optimal measurements, we can consider $I(V;YZ)$ to be the optimal mutual information between the input vector V and the measurement results:

$$g(k,n) \coloneqq \min_{\{|\Psi_i\rangle\}} I(V;YZ). \tag{17}$$

Note that we now assume that all the k vectors are equally likely; there is no sensible lower bound if the entropy of the *a priori* probability distribution is allowed to approach zero.

Proposition 12: The function $g(k,n)$ defined above for $1 < k \leqslant n^2$ satisfies the following bounds:

$$\frac{2}{k}\log 2 \leqslant g(k,n) \leqslant \log\lceil\sqrt{k}\rceil. \tag{18}$$

This proposition is proved as a consequence of Lemma 8. The same upper bound can be seen as a consequence of the following inequality given in Ref. 1:

$$I_{acc}^{\mathrm{LOCC}} \leqslant S(\rho_A) + S(\rho_B) - \sum_i p_i S(\rho_A^i), \tag{19}$$

where I_{acc}^{LOCC} is the classical mutual accessible information using LOCC, S is the von Neumann entropy, $\rho = \Sigma p_i |\Psi_i\rangle\langle\Psi_i|$, and ρ_A and ρ_B are the partial traces.

Let the $|\Psi_i\rangle$ be maximally entangled states in $C^n \otimes C^n$. Then

$$\rho_A^i = \rho_A = \rho_B = \frac{1}{n} I_n, \quad \forall\, i, \tag{20}$$

$$I_{acc}^{\mathrm{LOCC}} \leqslant S(\rho_A) + S(\rho_B) - \sum_i p_i S(\mathrm{Tr}_A(|\Psi_i\rangle\langle\Psi_i|)), \tag{21}$$

$$\leqslant \log n + \log n - \sum_i p_i S(\mathrm{Tr}_A(|\Psi_i\rangle\langle\Psi_i|)) = \log n. \tag{22}$$

This gives another way to see that k maximally entangled states in $C^n \otimes C^n$ cannot be distinguished if $k > n$.

Example: Recall the set BB_n defined in (4); it is a generalized Bell basis for $C^n \otimes C^n$. Suppose Alice and Bob share a state $|\Psi\rangle = (I \otimes X^m Z^l)|\mathrm{ME}_n\rangle$, uniformly chosen from BB_n. Each measures in the standard basis, allowing them to perfectly determine the value of m but giving no information about l.

If at this point they make a guess as to the value of l, they will be correct with probabilty $1/n$, which saturates the inequality in Lemma 8, and hence is optimal for $P(Z=V)$.

Perhaps more surprising, this protocol is also optimal with respect to classical mutual information, as $I(V;YZ) = \log n$ and the proof of the upper bound in Proposition 12 shows that this is maximal.

III. PROOFS OF PROPOSITIONS FOR DISTINGUISHING MAXIMALLY ENTANGLED STATES

A. Preliminaries

As has been previously noted (for instance in Ref. 12), there is one-to-one correspondence between states $|\Psi\rangle \in C^n \otimes C^m$ and $m \times n$ complex matrices B given by $|\Psi\rangle = (I \otimes B)|\mathrm{ME}_n\rangle$, where $|\mathrm{ME}_n\rangle$ is the standard maximally entangled $C^n \otimes C^n$ state defined in (2). Throughout the paper, we will use the following property, which was noted in Ref. 12 and implicitly used in Ref. 15.

Lemma 13: For any $m \times n$ matrix A written in the standard basis,

$$\sqrt{n}(I \otimes A)|\mathrm{ME}_n\rangle = \sqrt{m}(A^T \otimes I)|\mathrm{ME}_m\rangle. \tag{23}$$

In particular, setting $m=1$,

$$\sqrt{n}(I \otimes \langle v|)|\mathrm{ME}_n\rangle = |\overline{v}\rangle \otimes I, \tag{24}$$

where $|\overline{v}\rangle$ denotes the entrywise complex conjugate of $|v\rangle$ in the standard basis.

We adopt the convention of associating states $|\Psi\rangle$ with $\langle\Psi|\Psi\rangle = 1$ and $m \times n$ matrices B with $\mathrm{Tr}\, B^\dagger B = n$. This correspondence has the following immediate properties:

(1) If $|\Psi_i\rangle = (I \otimes B_i)|\mathrm{ME}_n\rangle$ for $i=1,2$, then $\langle\Psi_1|\Psi_2\rangle = 1/n\ \mathrm{Tr}\, B_1^\dagger B_2$.
(2) $\|B^\dagger B\|_\infty = n\lambda_M$, where λ_M is the largest Schmidt coefficient of $|\Psi\rangle$.
(3) $|\Psi\rangle = (I \otimes B)|\mathrm{ME}_n\rangle \in C^n \otimes C^n$ is maximally entangled if and only if B is unitary.

We will use this correspondence throughout what follows.

B. Proof of proposition 1

For $i=1,2,3$, write $|\Psi_i\rangle = (I \otimes B_i)|\mathrm{ME}_3\rangle$ with B_i unitary and $\mathrm{Tr}\, B_i^\dagger B_j = 3\delta_{ij}$. The matrix $B_2^\dagger B_1$ is a traceless 3×3 unitary matrix, so its eigenvalues are $\{1, \omega, \omega^2\}$, with $\omega = e^{i2\pi/3}$. The same is also true for $B_3^\dagger B_2$. We write these matrices in terms of their eigenvectors:

$$B_2^\dagger B_1 = \sum_{i=0}^{2} \omega^i |e_i\rangle\langle e_i|, \quad B_3^\dagger B_2 = \sum_{i=0}^{2} \omega^i |f_i\rangle\langle f_i|. \tag{25}$$

Given $|\Psi_i\rangle$, for i unknown, choose a unitary U and measure the first system in the basis $\{\overline{U}|j\rangle : j = 0,1,2\}$, where $\overline{U}$ indicates the entrywise complex conjugate of U. If the outcome of the measurement is $x \in \{0,1,2\}$, then Lemma 13 implies the state now looks like

$$(\overline{U}|x\rangle\langle x|U^T \otimes I)|\Psi_i\rangle = (\overline{U}|x\rangle\langle x|U^T \otimes B_i)|\mathrm{ME}_n\rangle, \tag{26}$$

$$= (\overline{U}|x\rangle \otimes B_i)(\langle x|U^T \otimes I)|\mathrm{ME}_n\rangle, \tag{27}$$

$$= \frac{1}{\sqrt{n}}(\overline{U}|x\rangle \otimes B_i)(I \otimes U|x\rangle), \tag{28}$$

$$= \frac{1}{\sqrt{n}}\overline{U}|x\rangle \otimes B_i U|x\rangle. \tag{29}$$

In particular, after normalization, the second system is in the state

$$B_i U|x\rangle. \tag{30}$$

We want to show that for an appropriate choice of U, the vectors $\{B_1U|x\rangle, B_2U|x\rangle, B_3U|x\rangle\}$ are orthogonal for all x. The proof is constructive and is achieved in three steps:

(1) Observe that the quantity $|\langle e_i|f_j\rangle|^2$ depends only on $(j-i) \bmod 3$.
(2) Show that we can adjust the phases of the $|e_i\rangle$ and $|f_j\rangle$ so that we may assume that $\langle e_i|f_j\rangle$ depends only on $(j-i) \bmod 3$.
(3) Let our unitary U be the Fourier matrix in the basis $\{|e_i\rangle\}$ and show that the vectors $\{B_1U|x\rangle, B_2U|x\rangle, B_3U|x\rangle\}$ are orthogonal for all x.

The proof of each step is given below. Note that all operations on indices are assumed to be taken modulo 3.

(1) Since $\mathrm{Tr}\, B_3^\dagger B_1 = 0$:

$$0 = \mathrm{Tr}\, B_3^\dagger B_2 B_2^\dagger B_1 = \sum_{i,j} \omega^{i+j}|\langle e_i|f_j\rangle|^2 = \sum_{i,k} \omega^k|\langle e_i|f_{k-i}\rangle|^2. \tag{31}$$

For any $a_k \geqslant 0$, $\Sigma_{k=0}^2 \omega^k a_k = 0$ implies that all the a_k are the same. Therefore,

$$\sum_i |\langle e_i|f_{-i}\rangle|^2 = \sum_i |\langle e_i|f_{1-i}\rangle|^2 = \sum_i |\langle e_i|f_{2-i}\rangle|^2. \tag{32}$$

Combining with the normalization conditions for any i, j,

$$\sum_k |\langle e_k|f_j\rangle|^2 = \sum_k |\langle e_i|f_k\rangle|^2 = 1 \tag{33}$$

gives a linear system of seven independent equations in the nine unknowns $|\langle e_i|f_j\rangle|^2$ whose solutions look like this:

$$(|\langle e_i|f_j\rangle|^2)_{ij} = \begin{pmatrix} |a|^2 & |c|^2 & |b|^2 \\ |b|^2 & |a|^2 & |c|^2 \\ |c|^2 & |b|^2 & |a|^2 \end{pmatrix}. \tag{34}$$

That is, the quantity $|\langle e_i|f_j\rangle|^2$ depends only on $(j-i) \bmod 3$.

(2) Let V be the unitary matrix whose (i,j) entry is given by $\langle e_i|f_j\rangle$. From above, $|V_{i,j}|$ depends only on $(j-i) \bmod 3$. We would like to have $V_{i,j}$ itself depend only on $(j-i) \bmod 3$. We accomplish this by adjusting the phases of $|e_i\rangle$ and $|f_j\rangle$, which is equivalent to finding diagonal unitaries U_1 and U_2 such that

$$V' = U_1 V U_2^\dagger = \begin{pmatrix} a & c & b \\ b & a & c \\ c & b & a \end{pmatrix}, \tag{35}$$

for some $a, b, c \in C$. Write $m_{ij} = \arg(\langle e_i | f_j \rangle)$ and

$$U_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\alpha} & 0 \\ 0 & 0 & e^{i\beta} \end{pmatrix}, \quad U_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\gamma} & 0 \\ 0 & 0 & e^{i\delta} \end{pmatrix}.$$

Solving a system of three linear equations in the phases of the first two columns of V allows us to set

$$\gamma = \frac{1}{3} \sum_{j=0}^{2} (m_{1j} - m_{0j}), \tag{36}$$

$$\alpha = m_{00} - m_{11} + \gamma, \tag{37}$$

$$\beta = m_{01} - m_{20} - \gamma. \tag{38}$$

Put these values into U_1 and U_2 and choose δ to adjust the top right corner, which gets our matrix into the form

$$V' = \begin{pmatrix} a & c & b \\ b & a & ce^{i\delta_1} \\ c & b & ae^{i\delta_2} \end{pmatrix}. \tag{39}$$

The fact that V' is unitary implies its columns are orthogonal, yielding the three equations:

$$\begin{pmatrix} 1 & 1 & 1 \\ e^{i\delta_1} & 1 & e^{i\delta_2} \\ e^{-i\delta_2} & e^{-i\delta_1} & 1 \end{pmatrix} \begin{pmatrix} \overline{ac} \\ \overline{cb} \\ \overline{ba} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \tag{40}$$

The determinant of the above matrix cannot be zero unless $e^{i\delta_1} = e^{i\delta_2} = 1$, which means that in fact V' is already in the desired form (35).

Adjusting our matrix V was equivalent to adjusting the phases of the vectors $|e_i\rangle$ and $|f_j\rangle$. Therefore, without loss of generality, we assume that $\langle e_i | f_j \rangle$ depends only on $(j-i) \bmod 3$ and define

$$A_k := \langle e_i | f_{k+i} \rangle, \tag{41}$$

which is independent of i.

(3) For $x \in \{0, 1, 2\}$ define

$$U|x\rangle = \frac{1}{\sqrt{3}} \sum_{i=0}^{2} \omega^{ix} |e_i\rangle. \tag{42}$$

Explicit calculation shows that for all x, the vectors $B_1 U|x\rangle$, $B_2 U|x\rangle$, $B_3 U|x\rangle$ are pairwise orthogonal:

$$3\langle x|U^\dagger B_2^\dagger B_1 U|x\rangle = \sum_k \omega^{-kx}\omega^k\omega^{kx} = 0, \tag{43}$$

$$3\langle x|U^\dagger B_3^\dagger B_2 U|x\rangle = \sum_{k,i,l} \omega^{-kx}\omega^i\omega^{lx}\langle e_k|f_i\rangle\langle f_i|e_l\rangle, \tag{44}$$

$$= \sum_{k,i,l} \omega^{(l-k)x}\omega^i A_{i-k}\overline{A_{i-l}}, \tag{45}$$

$$= \sum_{k',l'} (\omega^{(k'-l')x}A_{k'}\overline{A_{l'}})\sum_i \omega^i = 0, \tag{46}$$

$$3\langle x|U^\dagger B_3^\dagger B_1 U|x\rangle = \langle x|U^\dagger B_3^\dagger B_2 B_2^\dagger B_1 U|x\rangle, \tag{47}$$

$$= \sum_{k,i,l} \omega^{(l-k)x}\omega^{i+l}A_{i-k}\overline{A_{i-l}}, \tag{48}$$

$$= \sum_{k',l'} (\omega^{(k'-l')x}\omega^{-l'}A_{k'}\overline{A_{l'}})\sum_i \omega^{2i} = 0. \tag{49}$$

This proves that, for all x, the vectors $B_1U|x\rangle$, $B_2U|x\rangle$, $B_3U|x\rangle$ are orthogonal and hence can be perfectly distinguished.

C. Proof of proposition 3

Let $\mathcal{B}=\{|b_1\rangle,\ldots|b_n\rangle\}$ be the common unbiased basis. We need to show that for any $i\neq j$ and any k, the vectors $B_i|b_k\rangle$ and $B_j|b_k\rangle$ are orthogonal. Using the eigenbasis $\mathcal{A}_{ij}$, write

$$B_i^\dagger B_j = \sum_s \lambda_s|e_s\rangle\langle e_s|. \tag{50}$$

Then for all k,

$$\langle b_k|B_i^\dagger B_j|b_k\rangle = \sum_s \lambda_s|\langle b_k|e_s\rangle|^2, \tag{51}$$

$$= \frac{1}{n}\sum_s \lambda_s, \tag{52}$$

$$= \frac{1}{n}\mathrm{Tr}\, B_i^\dagger B_j = 0. \tag{53}$$

IV. PROOFS ON THE WORST CASES FOR DISTINGUISHING ORTHOGONAL STATES

Throughout what follows, let V be the true identity of the vector $|\Psi_i\rangle$, and let Z be Alice and Bob's best guess of the value of V, which we assume is also the outcome of the final measurement. Their goal, then, is to maximize $P(Z=V)$.

A. Proof of propositions 5 and 6 using the lemmas

Setting $j=2$ in Lemma 7 gives us the desired lower bounds, since $f_{\mathrm{me}}(2,n)=f(2,n)=1$. As long as $k\leqslant n^2$, there exist k orthogonal maximally entangled vectors in $C^n\otimes C^n$, so Lemma 8 implies that $f_{\mathrm{me}}(k,n)\leqslant n/k$. In the case $k\leqslant 9$, we know $f_{\mathrm{me}}(3,3)=1$ so

$$\frac{3}{k}=\frac{3}{k}f_{\mathrm{me}}(3,3)\leqslant f_{\mathrm{me}}(k,3)\leqslant\frac{3}{k}, \tag{54}$$

so $f_{\mathrm{me}}(k,3)=3/k$. Similarly, if $k\leqslant m^2\leqslant n^2$, then $f(k,n)\leqslant f_{\mathrm{me}}(k,m)$, since we can embed maximally entangled $C^m\otimes C^m$ vectors into $C^n\otimes C^n$. The minimum value of m for which we can do this is $\lceil\sqrt{k}\rceil$, which implies

$$f(k,n)\leqslant\frac{\lceil\sqrt{k}\rceil}{k}. \tag{55}$$

In the case $2\leqslant k\leqslant 4$, $\lceil\sqrt{k}\rceil=2$ and

$$\frac{2}{k}=\frac{2}{k}f(2,n)\leqslant f(k,n)\leqslant\frac{2}{k}, \tag{56}$$

which implies

$$f(k,n)=\frac{2}{k}. \tag{57}$$

B. Proof of lemma 7

We prove the lemma for the function $f(k,n)$; the proof for f_{me} is identical. Given any orthogonal vectors $|\Psi_i\rangle\in\{|\Psi_1\rangle,\ldots,|\Psi_k\rangle\}$ with probabilities $p_1\geqslant p_2\geqslant\cdots\geqslant p_k$. There exists an algorithm that can distinguish the first j of these vectors with probability that is at least $f(j,n)$. Applying this algorithm to the received vector $|\Psi_i\rangle$ cannot succeed if $i>j$, but clearly

$$P(Z=V)\geqslant P(Z=V,i\leqslant j), \tag{58}$$

$$=P(i\leqslant j)P(Z=V|i\leqslant j), \tag{59}$$

$$\geqslant\frac{j}{k}f(j,n), \tag{60}$$

which gives the desired lower bound on $f(k,n)$.

C. Proof of lemma 8

For this proof, we will need to examine the measurement process more closely. As mentioned earlier, we will assume that the protocol terminates with probability 1. In fact, through the calculation, we will assume there exists an r such that the protocol terminates after at most r rounds of communication. Completing the argument for arbitrary r is sufficient. Let R be the actual number of rounds needed to complete to protocol and let p_r be the probability that more than r rounds are needed. Then

$$P(Z=V) = (1-p_r)P(Z=V|R \leqslant r) + p_r P(Z=V|R > r), \tag{61}$$

$$\leqslant P(Z=V|R \leqslant r) + p_r. \tag{62}$$

Our proof will show that for any r, $P(Z=V|R \leqslant r) \leqslant n/k$. Taking the limit as $r \to \infty$, p_r gets arbitrarily small and we can bound $P(Z=V)$ by n/k.

The actions of Alice and Bob will consist of adding ancilla systems, performing unitary operations, and performing measurements. All of these can be encoded into a POVM. Alice measures first; we write her POVM as $\mathcal{X}^T = \{X_1^T, X_2^T, \ldots, X_{k_1}^T\}$. (Because we will eventually apply Lemma 13 to show the effect of Alice's POVM on Bob's system, we write it in terms of the transpose.) Suppose Alice gets the result j_1; then Bob uses a POVM that depends on j_1: $\mathcal{E}_{j_1} = \{E(j_1)_1, E(j_1)_2, \ldots, E(j_1)_{k_2}\}$. Alice then measures in a POVM that depends on j_1 and j_2, and so on. After r rounds of measurement, Alice and Bob have effectively measured, using the POVM,

$$\{(\mathcal{X}^T_{j_1,j_2,\ldots j_{r-1}} \otimes \mathcal{E}_{j_1,j_2,\ldots j_r}) : j_1, j_2, \ldots, j_r \geqslant 0\}, \tag{63}$$

which are defined recursively as in Ref. 2:

$$\begin{aligned} \mathcal{X}^T_{j_1,j_2,\ldots j_{r-1}} &= X^T(j_1, j_2, \ldots, j_{r-2})_{j_{r-1}} \mathcal{X}^T_{j_1,j_2,\ldots j_{r-3}}, \\ \mathcal{E}_{j_1,j_2,\ldots j_r} &= E(j_1, j_2, \ldots, j_{r-1})_{j_r} \mathcal{E}_{j_1,j_2,\ldots j_{r-2}}. \end{aligned} \tag{64}$$

The subscripts show that each measurement depends on the previous outcomes. Here each $X^T(m_0)$ and $E(m_1)$ is a POVM, where m_0 is a vector encoding an even number of previous outcomes and m_1 encodes an odd number. This corresponds to the fact that Alice and Bob alternate measurements, so Alice's action will always depend on an even number of previous results while's Bob's will always depend on an odd number. As usual, we have the normalization

$$\sum_i (X(m_0)_i^T)^\dagger X(m_0)_i^T = I_{d_A(m_0)} = \sum_i X(m_0)_i X(m_0)_i^\dagger, \tag{65}$$

$$\sum_i E(m_1)_i^\dagger E(m_1)_i = I_{d_B(m_1)}, \tag{66}$$

where $d_A(m_0)$ and $d_B(m_1)$ are sufficiently large dimensions to include any ancilla spaces.

Alice and Bob start with the state $|\Psi_i\rangle = (I \otimes B_i)|\mathrm{ME}_n\rangle$ and then apply the POVM above, getting results $m = (j_1, j_2, \ldots, j_{r-1})$ and j_r, for r an even number. Then, using Lemma 13, their state now looks like

$$(\mathcal{X}_m^T \otimes \mathcal{E}_{m,j_r})(I \otimes B_i)|\mathrm{ME}_n\rangle = I \otimes (\mathcal{E}_{m,j_r} B_i \mathcal{X}_m)|\mathrm{ME}_n\rangle. \tag{67}$$

This state is not normalized—its magnitude indicates the probability of this outcome. Without loss of generality, we assume that the final measurement identifies the best guess of the value of V. This gives us a more formal definition of our optimal measurement, where we sum over all outcomes with the final output equal to the correct state identity:

$$P(\{|\Psi_i\rangle\}, \{p_i\}) \coloneqq \sup_{\mathcal{X},\mathcal{E}} P(Z=V), \tag{68}$$

$$P(Z=V)=\sum_i P(Z=V=i), \tag{69}$$

$$=\sum_{i,m} p_i\langle\Psi_i|(\overline{\mathcal{X}}_m\mathcal{X}_m^T\otimes\mathcal{E}_{m,i}^\dagger\mathcal{E}_{m,i}\ |\Psi_i\rangle, \tag{70}$$

$$=\sum_{i,m} p_i\langle \mathrm{ME}_n|(I\otimes\mathcal{X}_m^\dagger B_i^\dagger\mathcal{E}_{m,i}^\dagger\mathcal{E}_{m,i}B_i\mathcal{X}_m\ |\mathrm{ME}_n\rangle \tag{71}$$

$$=\frac{1}{n}\sum_{i,m} p_i\ \mathrm{Tr}(X_m^\dagger B_i^\dagger\mathcal{E}_{m,i}^\dagger\mathcal{E}_{m,i}B_iX_m). \tag{72}$$

The measurements might make use of ancilla systems, so we write P_A and P_B as the projections back onto our original Alice and Bob spaces; since each B_i maps Alice's space to Bob's, we see that $P_BB_i=B_iP_A=B_i$. Recall also that $\mathrm{Tr}\,B_i^\dagger B_i=n$ by assumption.

We may now turn to the lemma, which assumes that $|\Psi_i\rangle=(I\otimes U_iB)|\mathrm{ME}_n\rangle$ with U_i unitary and B fixed. Suppose Alice and Bob make r measurements with the POVMs described in (64). We assume that r is even so Bob measures last—we can always append a trivial measurement to make this so. Suppose that the first $r-2$ measurement outcomes are contained in the vector $m=(j_1,j_2,\ldots,j_{r-2})$. For simplicity we write j_{r-1} as j and assume that $Z=V$ if and only if Bob's final measurement $j_r=i$. Plugging this into (72) and setting $p_i=1/k$ yields

$$P(Z=V)=\frac{1}{kn}\sum_{m,j,i}\mathrm{Tr}(X_m^\dagger B_i^\dagger\mathcal{E}_{m,i}^\dagger\mathcal{E}_{m,i}B_iX_m), \tag{73}$$

$$=\frac{1}{kn}\sum_{m,j,i}\mathrm{Tr}(X_m^\dagger B_i^\dagger P_B\mathcal{E}_{m,i}^\dagger\mathcal{E}_{m,i}P_BB_iX_m), \tag{74}$$

$$\leqslant\frac{1}{kn}\sum_{m,j,i}(\mathrm{Tr}\,P_B\mathcal{E}_{m,j,i}^\dagger\mathcal{E}_{m,j,i}P_B)(\mathrm{Tr}\,B_i\mathcal{X}_{m,j}\mathcal{X}_{m,j}^\dagger B_i^\dagger), \tag{75}$$

$$=\frac{1}{kn}\sum_{m,j,i}(\mathrm{Tr}\,P_B\mathcal{E}_{m,j,i}^\dagger\mathcal{E}_{m,j,i})(\mathrm{Tr}\,B^\dagger B\mathcal{X}_{m,j}\mathcal{X}_{m,j}^\dagger). \tag{76}$$

In (75), we use the fact that for matrices $A,B\geqslant 0$, $\mathrm{Tr}\,AB\leqslant(\mathrm{Tr}\,A)(\mathrm{Tr}\,B)$, and in (76) we use the assumption of the lemma that $B_i=U_iB$. The key observation now is that there is no i in the second term of (76); rewriting the first term as in (64) shows that summing the first term over i yields the identity matrix on the inside, allowing us to drop two subscripts, not just one:

$$\mathrm{Tr}\left(\sum_i P_B\mathcal{E}_{m,j,i}^\dagger\mathcal{E}_{m,j,i}\right)=\mathrm{Tr}\left(\sum_i P_B\mathcal{E}_m^\dagger E(m,j)_i^\dagger E(m,j)_i\mathcal{E}_m\right), \tag{77}$$

$$=\mathrm{Tr}(P_B\mathcal{E}_m^\dagger\mathcal{E}_m). \tag{78}$$

This corresponds to the fact that Alice does nothing during Bob's measurement phase. We now have

$$P(Z=V) \leqslant \frac{1}{kn}\sum_{m,j} (\mathrm{Tr}\, P_B \mathcal{E}_m^\dagger \mathcal{E}_m)(\mathrm{Tr}\, B^\dagger B \mathcal{X}_{m,j} \mathcal{X}_{m,j}^\dagger). \tag{79}$$

Now, there is no j in the first term, only in the second, so we can likewise sum to get the identity on the inner term. Alternating in this way, we can count back through the measurements until they all sum to the identity and we are left with

$$P(Z=V) \leqslant \frac{1}{kn}\mathrm{Tr}(P_B)\mathrm{Tr}(B^\dagger B) = \frac{1}{kn}(n)(n) = \frac{n}{k}. \tag{80}$$

This shows that even if Alice and Bob add ancilla systems to do their measurements, the relevant bound comes from the dimension of Bob's system. This proves the lemma.

D. Proof of proposition 9

In Eq. (75), we insert the projection onto Alice's space P_A and use Hölder's inequality to note that

$$\mathrm{Tr}\, B_i \mathcal{X}_{m,j} \mathcal{X}_{m,j}^\dagger B_i^\dagger = \mathrm{Tr}\, B_i P_A \mathcal{X}_{m,j} \mathcal{X}_{m,j}^\dagger P_A B_i^\dagger, \tag{81}$$

$$\leqslant \|B_i^\dagger B_i\|_\infty \,\mathrm{Tr}\, P_A \mathcal{X}_{m,j} \mathcal{X}_{m,j}^\dagger P_A, \tag{82}$$

$$\leqslant n\lambda_M \,\mathrm{Tr}\, P_A \mathcal{X}_{m,j} \mathcal{X}_{m,j}^\dagger P_A, \tag{83}$$

since $\|B_i^\dagger B_i\|_\infty \leqslant \max_i \|B_i^\dagger B_i\|_\infty = n\lambda_M$. Aside from the new factor of $n\lambda_M$, the rest of the calculation from Lemma 8 remains unchanged, inserting P_A for B so that (80) becomes

$$P(Z=V) \leqslant \frac{1}{kn}(n\lambda_M)\mathrm{Tr}(P_B)\mathrm{Tr}(P_A) = \frac{\lambda_M}{k}(n)(m) = \frac{\lambda_M mn}{k}. \tag{84}$$

E. Proof of proposition 12

The lower bound comes from the idea of tossing out all but two of the vectors and distinguishing them perfectly. At worst, this process gives you $(2/k)\log 2$ bits of information. The upper bound arises in the case of k states to which Lemma 8 applies. The joint probability distribution on (V,Y,Z) must have two properties. First, that the marginal distribution on V is uniform, since the states are equally likely. Second, by relabeling in Lemma 8, we see that for any permutation $\sigma \in S_k$, $P(Z=\sigma(V)) \leqslant n/k$. The set of distributions with these properties is a convex set on which the mutual information is convex. The extreme points of this set are distributions for which Z takes on only n values and Y is a function of Z. Hence the maximum happens at an extreme point and

$$I(V;YZ) \leqslant H(YZ) = H(Z) \leqslant \log n. \tag{85}$$

This implies that the maximum mutual information in this case is $\log n$. Making n as small as possible, we see that

$$g(k,n) \leqslant \log\lceil \sqrt{k} \rceil. \tag{86}$$

V. CONCLUSION

In summary, we have demonstrated that several classes of maximally entangled states that can be distinguished using LOCC. By examining the measurement process itself, we have explored bounds on both the success probability and the mutual information and shown that the well-understood $C^2 \otimes C^2$ Bell basis provides the worst case of three or four vectors with respect to either of these measures. In the process, we have identified some sets of states that cannot be

perfectly distinguished. It is hoped that through better understanding best and worst cases of the distinguishing problem, we can further our understanding of the interplay between locality and entanglement.

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Time reversal and *n*-qubit canonical decompositions

Stephen S. Bullock[a)]
Mathematical and Computational Sciences Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899

Gavin K. Brennen[b)]
Atomic Physics Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899

Dianne P. O'Leary[c)]
MCSD, National Institute of Standards and Technology, and Department of Computer Science, University of Maryland, College Park, Maryland 20742

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On pure states of n quantum bits, the *concurrence entanglement monotone* returns the norm of the inner product of a pure state with its spin-flip. The monotone vanishes for n odd, but for n even there is an explicit formula for its value on mixed states, i.e., a closed-form expression computes the minimum over all ensemble decompositions of a given density. For n even a matrix decomposition $\nu=k_1ak_2$ of the unitary group is explicitly computable and allows for study of the monotone's dynamics. The side factors k_1 and k_2 of this concurrence canonical decomposition (CCD) are concurrence symmetries, so the dynamics reduce to consideration of the a factor. This unitary a phases a basis of entangled states, and the concurrence dynamics of u are determined by these relative phases. In this work, we provide an explicit numerical algorithm computing $\nu=k_1ak_2$ for n odd. Further, in the odd case we lift the monotone to a two-argument function. The *concurrence capacity* of ν according to the double argument lift may be nontrivial for n odd and reduces to the usual concurrence capacity in the literature for n even. The generalization may also be studied using the CCD, leading again to maximal capacity for most unitaries. The capacity of $\nu\otimes I_2$ is at least that of ν, so odd-qubit capacities have implications for even-qubit entanglement. The generalizations require considering the spin-flip as a time reversal symmetry operator in Wigner's axiomatization, and the original Lie algebra homomorphism defining the CCD may be restated entirely in terms of this time reversal. The polar decomposition related to the CCD then writes any unitary evolution as the product of a time-symmetric and time-antisymmetric evolution with respect to the spin-flip. En route we observe a Kramers' nondegeneracy: the existence of a nondegenerate eigenstate of any *time reversal symmetric* n-qubit Hamiltonian demands (i) n even and (ii) maximal concurrence of said eigenstate. We provide examples of how to apply this work to study the kinematics and dynamics of entanglement in spin chain Hamiltonians. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1900293]

I. INTRODUCTION

The entanglement theory of two quantum bits is now well understood. Let ρ be a mixed two-qubit quantum state, described by a 4×4 Hermitian density matrix. Hill and Wootters[22] describe all classes of ρ up to evolution by unitaries in terms of the concurrence. This concurrence

[a)]Electronic mail: stephen.bullock@nist.gov
[b)]Electronic mail: gavin.brennen@nist.gov
[c)]Electronic mail: oleary@cs.umd.edu

is explicitly a function of the eigenvalues of $\rho(\sigma^y)^{\otimes 2}\overline{\rho}(\sigma^y)^{\otimes 2}$, where the factor $\tilde{\rho}=(\sigma^y)^{\otimes 2}\overline{\rho}(\sigma^y)^{\otimes 2}$ may be interpreted as the spin-flip of ρ. Further, for pure states the entropy of the partial trace to either one-qubit subsystem is a one-to-one function of the concurrence, so that both measures agree as to which two-qubit states are more or less entangled. Local states (tensors) are unentangled, while states locally equivalent to Bell states have maximal entropy and concurrence.

For other systems, entanglement theory is more complicated. Even for two *d*-level systems (qudits) it is not typical to use a single function to quantify entanglement,[45] and research into generalized concurrences continues.[20] Instead we focus on the multi-partite qubit case. The key point is that it is not sensible in *n*-qubits to speak of a *unique* maximally entangled state. More precisely, suppose now ρ is a $2^n\times 2^n$ Hermitian density matrix describing a mixed *n*-qubit state. A unitary evolution is given by a $2^n\times 2^n$ unitary matrix, say ν, with the evolution being $\rho\mapsto\nu\rho\nu^\dagger$. A partial ordering of such ρ as more or less entangled follows by stipulating that (i) for $\nu=\otimes_{j=1}^n\nu_j$ local unitary, ρ and $\nu\rho\nu^\dagger$ are equally entangled, while (ii) the ρ becomes no more entangled on average after applying any sequence of local measurements and local unitaries, i.e., after applying local completely positive maps.[23] More entangled is a partial order which has distinct maximal elements for $n\geqslant 3$. For example, in three qubits, two states which are maximally entangled yet locally inequivalent are given as follows:[16]

$$|GHZ\rangle=(1/\sqrt{2})[|000\rangle+|111\rangle],\quad |W\rangle=(1/\sqrt{3})[|001\rangle+|010\rangle+|100\rangle]. \tag{1}$$

There are nine distinct maxima of the partial order in four qubits,[44] and strong theoretical evidence suggests that the number of such *entanglement types* grows quite rapidly with *n* (e.g., Ref. 33).

To quantify multi-partite entanglement, one often uses functions known as entanglement monotones.[3,45] All such monotones must vanish on any local state. A monotone might also vanish on certain entangled states but definitively reports that a state is not local should its value be nonzero. The value on a mixed state ρ is defined to be the minimum over all ensemble decompositions of ρ of the ensemble weighted-average. A monotone is convex on density matrices, since entanglement does not increase under mixing of states. Monotones are also nonincreasing *on average* under local quantum operations and classical communication. Among popular monotones are Meyer's *Q*-measure,[6,32] the Schmidt measure,[18] and certain polynomial invariants[3] of eigenvalues of density matrices representing stochastic mixtures of pure data states.

The *n*-qubit concurrence is an entanglement monotone. To define the monotone, we first note that *throughout* υ refers to the spin-flip of the *n*-qubit state space. Concurrence for a pure state[48] is the component on a pure state of its spin-flip:

$$C_n(|\psi\rangle)=|\langle\psi|\upsilon|\psi\rangle|/\langle\psi|\psi\rangle,$$

where

$$\upsilon|\psi\rangle=\overline{(-i\sigma^y)^{\otimes n}|\psi\rangle}=(-i\sigma^y)^{\otimes n}\overline{|\psi\rangle}. \tag{2}$$

The concurrence of an *n* qubit state with *n* odd vanishes identically. This monotone is noteworthy for two reasons. First, there is an explicit, computable closed-form expression for the minimum $C_n(\rho)$ which is again defined in terms of the eigenvalues of $\rho\tilde{\rho}=\rho(\sigma^y)^{\otimes n}\overline{\rho}(\sigma^y)^{\otimes n}$.[7,42] Second, in the context of concurrence dynamics we may study entanglement dynamics. This paper concerns itself with the latter topic, and we henceforth consider only pure states and unitary maps.

The primary mathematical tool used in this paper is the concurrence canonical decomposition (CCD). This is discussed in detail in Sec. II. Briefly, it is a way to decompose a unitary on *n* qubits into a factor that changes concurrence and factors that do not. Let $\nu:\mathcal{H}_n\rightarrow\mathcal{H}_n$ be a unitary evolution. Consider the CCD $\nu=k_1ak_2$.[8] Now k_1 and k_2 are symmetries of the concurrence, reducing concurrence dynamics to the second factor. This *a* factor applies relative phases to a basis of *GHZ*-like states. Such phases are not unique due to choices of diagonalization while computing the CCD, but the spectrum spec(a^2) is uniquely determined by ν. Moreover, the two-qubit test for maximal entanglement capacity[49] generalizes to *n* qubit concurrence capacities if *n* is even:

Let $\nu = k_1 a k_2$ be a CCD of ν. Consider spec(a^2) as a subset of the unit circle. Then for $n = 2p$, there is a $|\psi\rangle \in \mathcal{H}_n$ with $C_n(|\psi\rangle) = 0$ and $C_n(\nu|\psi\rangle) = 1$ if and only if 0 is within the convex hull of spec(a^2).[8,49]

Also, for even n there is an explicit numerical algorithm for computing the CCD and hence spec(a^2).[8]

This work presents three new results. The first is an extension of concurrence capacities to the case n odd. For n even, the concurrence symmetry group K to which k_1, k_2 belong is up to a similarity transform an orthogonal group. For n odd, K is not orthogonal but symplectic, a has repeat eigenvalues, and $C_{2p-1}(|\psi\rangle) = 0$ for all $|\psi\rangle$. Nonetheless, we define a two-argument lift of the usual concurrence, say $\mathcal{C}(|\phi\rangle, |\psi\rangle)$. [See Eq. (7).] Suppose we define the amount of concurrence an odd-qubit unitary ν creates to be

$$\kappa(\nu) = \max\{\mathcal{C}(\nu|\phi\rangle, \nu|\psi\rangle); \mathcal{C}(|\phi\rangle, |\psi\rangle) = 0\}. \tag{3}$$

This generalized capacity has the following properties:

- For n even, the one-argument concurrence capacity and the two-argument capacity of ν coincide.
- For n odd, often $\kappa_n(\nu) \neq 0$ for the pairwise capacity despite $C_n(|\psi\rangle) \equiv 0$. Further, $\kappa_n(\nu) = 1$ if and only if 0 lies within the convex hull of spec(a^2) for any CCD by $\nu = k_1 a k_2$.
- *Concurrence capacity monotonicity:* Using double argument capacities, the capacity of $\nu \otimes I_2$ is always at least that of ν.

Hence there exists a theory of odd-qubit concurrence dynamics, even though concurrence vanishes identically (on the diagonal) in odd qubits.

Second, we present an explicit numerical algorithm for computing the odd-qubit CCD. Various matrix logarithms must be computed, after which one invokes work in the numerical analysis literature[15] to diagonalize a time reversal symmetric Hamiltonian using symplectic matrices.

We close with the third observation, which we will refer to as *Kramers' nondegeneracy:*

On the n-quantum bit state space, suppose that a υ-time reversal symmetric Hamiltonian H has a nondegenerate eigenstate $|\lambda\rangle$. Then (i) n is even and (ii) $C_n(|\lambda\rangle) = 1$. In particular, $|\lambda\rangle$ is entangled, i.e. $|\lambda\rangle \neq \otimes_{j=1}^{n} |\psi_j\rangle$.

The proof follows from viewing υ as a time reversal symmetry operator in Wigner's axiomatization, a point of view which also simplifies the derivation of the CCD. Kramers' nondegeneracy leads one to wonder whether useful entangled states may be produced by cooling the system of qubits coupled to a υ-time reversal symmetric Hamiltonian. We consider the perturbative stability of this entanglement while breaking the time reversal symmetry here, while the thermal stability of the Kramers' nondegeneracy for the quantum XY model is considered elsewhere.[7]

II. BACKGROUND AND PRIOR WORK

Since our key tool is a generalized canonical decomposition,[8] we review the canonical decomposition literature. The two-qubit canonical decomposition (CD) states that any two-quantum bit unitary evolution ν, i.e., any 4×4 unitary matrix ν, may be written:

$$\nu = e^{i\varphi}(u_1 \otimes u_2) a (u_3 \otimes u_4). \tag{4}$$

Here u_1, u_2, u_3, u_4 are one-qubit (2×2) unitary matrices, which may be chosen to have determinant one. The unitary a is diagonal in the Bell basis and may be thought of as applying relative phases to this basis. However, it is better computationally to think of a as phasing the *magic basis*[4,29] instead:

$$|\mathrm{m}0\rangle = (|00\rangle + |11\rangle)/\sqrt{2}, \quad |\mathrm{m}1\rangle = (|01\rangle - |10\rangle)/\sqrt{2},$$

$$|\mathrm{m}2\rangle = (i|00\rangle - i|11\rangle)/\sqrt{2}, \quad |\mathrm{m}3\rangle = (i|01\rangle + i|10\rangle)/\sqrt{2}. \tag{5}$$

Let E be defined by $E|j\rangle = |\mathrm{m}j\rangle$, and let $\mathrm{SU}(2^n)$ denote the Lie group of determinant one $2^n \times 2^n$ unitary matrices, $\mathrm{SO}(2^n)$ denotes determinant one orthogonal matrices, and $\mathrm{D}(2^n)$ denotes the diagonal $2^n \times 2^n$ unitary matrices. A diagonalization argument shows $\mathrm{SU}(4) = \mathrm{SO}(4)\mathrm{D}(4)\mathrm{SO}(4)$. Moreover, the magic basis has the property that $E^\dagger \mathrm{SU}(2) \otimes \mathrm{SU}(2) E = \mathrm{SO}(4)$, i.e., *determinant one* tensors have real matrix coefficients in the basis. Thus the canonical decomposition may be computed by transforming the diagonalization through E:

$$\mathrm{SU}(4) = [E\mathrm{SO}(4)E^\dagger][E\mathrm{D}(4)E^\dagger][E\mathrm{SO}(4)E^\dagger] = \mathrm{SU}(2) \otimes \mathrm{SU}(2)(E\mathrm{D}(4)E^\dagger)\mathrm{SU}(2) \otimes \mathrm{SU}(2). \tag{6}$$

We next provide a brief account and references for the best known applications and generalizations of the CD.

Makhlin[31] anticipates the canonical decomposition by directly computing that the double cosets $[\mathrm{SU}(2) \otimes \mathrm{SU}(2)] \backslash \mathrm{SU}(4) / [\mathrm{SU}(2) \otimes \mathrm{SU}(2)]$ are parametrized by three real parameters, the number of parameters in a given $\det(a) = 1$. The CD appears explicitly in Kraus and Cirac.[28] In an important paper, Khaneja, Brockett, and Glaser point out that one may view the CD as an example of the $G = KAK$ decomposition theorem for $G = \mathrm{SU}(4)$, $K = \mathrm{SU}(2) \otimes \mathrm{SU}(2)$, and $A = \Delta$ the commutative Lie group that phases the magic (or Bell) basis.[24] They also consider the matrix factorization from the point of view of control theory in order to compute minimum times for applying a given two-qubit unitary evolution. Zhang, Vala, Sastry, and Whaley made use of this observation to describe which 4×4 unitaries ν are equivalent up to tensors of one-qubit rotations. The factor $a \in \Delta$ is not unique but depends on choices of diagonalization, and these are described geometrically using Weyl chambers. Specifically, the Weyl group orbit of any a produces all possible a, and each orbit intersects the Weyl chamber once. For $G = \mathrm{SU}(4)$, the Weyl chamber is a tetrahedron.[49] The terms canonical decomposition and magic basis are by now standard, and there are published surveys (e.g., Ref. 13, Sec. II.B). Moreover, explicit control sequences for two-qubit unitary evolution have been mapped using the CD [Ref. 37, Eq. (B2)].[14] The timing arguments of Khaneja *et al.*[24] have been recently verified in liquid-state NMR.[35]

There are many applications of the two-qubit CD. In addition to timing as above, they include (i) studying the entanglement capacity of two-qubit operations,[49] (ii) building efficient (small) quantum circuits in two qubits,[10,41,43,46] and (iii) classifying which two-qubit computations require fewer than average multiqubit interactions.[41,46]

Besides the CCD,[8] there is another n-qubit generalization of the canonical decomposition due to Khaneja and Glaser.[25] It is also defined in terms of a $G = KAK$ decomposition. Label $N = 2^n$ for the remainder. The type of a $G = KAK$ decomposition follows from a classification theorem of Cartan involutions and determines the groups K and A up to Lie isomorphism. [The classification appears in Helgason (Ref. 21, p. 518, see the same for details).] Given $G = \mathrm{SU}(N)$, the three possible types demand $K \cong \mathrm{SO}(N)$ (type **AI**), $K \cong \mathrm{Sp}(N/2)$ a symplectic group (type **AII**), or $K \cong \mathrm{S}[\mathrm{U}(p) \oplus \mathrm{U}(q)]$ for $p+q=N$ a block unitary (type **AIII**). In the **AII** case, the structure of the A group also demands any $a \in A$ has even-degenerate eigenvalues. The two-qubit canonical decomposition is type **AI**, and indeed the similarity transform by E shows $\mathrm{SU}(2) \otimes \mathrm{SU}(2) \cong \mathrm{SO}(4)$. The CCD alternates **AI** and **AII** as n is even or odd. The KGD of Khaneja and Glaser technically contains two $G = KAK$ decompositions, the first of which is type **AIII** for $n > 2$. In fact, the KGD is similar to the cosine sine decomposition (CSD) of numerical linear algebra[11] and so may be computed numerically. Physically, the $K \cong \mathrm{S}[\mathrm{U}(N/2) \oplus \mathrm{U}(N/2)]$ group of the KGD may be viewed as those unitaries commuting with measurements in the z basis of the least significant qubit, i.e., commuting with $I_{N/2} \otimes \sigma^z$.

We next recall notation from quantum computing. The one-qubit state space is $\mathcal{H}_1 = \mathbb{C}\{|0\rangle\} \oplus \mathbb{C}\{|1\rangle\}$. For n quantum bits, $\mathcal{H}_n = (\mathcal{H}_1)^{\otimes n} = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_1$. (See Ref. 36.) A local state $|\psi\rangle$ is any state which may be written as $\otimes_{j=1}^n |\psi_j\rangle$ for $|\psi_j\rangle \in \mathcal{H}_1$, while an *entangled* state is any state which is not local. Notations such as, e.g., $|7\rangle$ refer not to the state of a qudit but rather to a multiqubit

state, e.g., $|7\rangle = |1\rangle \otimes |1\rangle \otimes |1\rangle$. The *n*-concurrence of Eq. (2) is an entanglement monotone.[8] Besides the well-known two-qubit concurrence,[22] even qubit concurrences *n*-qubits [Ref. 48, Ref. 40—Eq. (62), Ref. 8] have also been studied. Since the single-argument concurrence vanishes for *n* odd, we introduce a two-argument generalization.

For υ per Eq. (2), the *concurrence bilinear form*[8] is the map $\mathcal{C}_n: \mathcal{H}_n \times \mathcal{H}_n \to \mathbb{C}$ given by

$$\mathcal{C}_n(|\phi\rangle, |\psi\rangle) = \overline{\langle \phi | \upsilon | \psi \rangle}. \tag{7}$$

The complex conjugate forces the two-argument function to be complex bilinear rather than complex bi-antilinear, and the concurrence monotone is the norm of the form on the diagonal: $\mathcal{C}_n(|\phi\rangle) = |\mathcal{C}_n(|\phi\rangle, |\phi\rangle)|$. The bilinear form $\mathcal{C}_n$ is symmetric for *n* even and antisymmetric for *n* odd, which causes vanishing of the monotone *but not the form* in the odd-qubit case.

The CD is an example of the $G = KAK$ decomposition theorem (Ref. 21, Theorem 8.6, Sec. VII.8) for $G = \mathrm{SU}(N)$. This theorem produces a decomposition of a reductive Lie group *G* for any θ, $\mathfrak{a}$ as follows:

- The map $\theta: \mathfrak{g} \to \mathfrak{g}$ for $\mathfrak{g} = \mathrm{Lie}(G)$ is a Cartan involution (Ref. 21, Sec. X.6.3, p. 518). By definition,[50] (i) $\theta^2 = \mathbf{1}_{\mathfrak{g}}$ and (ii) $\theta[X, Y] = [\theta X, \theta Y]$ for all $X, Y \in \mathfrak{g}$. As is standard, we write $\mathfrak{g} = \mathfrak{p} \oplus \mathfrak{k}$ for the decomposition of $\mathfrak{g}$ into the -1 and $+1$ eigenspace of θ.
- Given θ, $\mathfrak{a} \subset \mathfrak{p}$ is a commutative subalgebra which is maximal commutative in $\mathfrak{p}$.

Note that $\mathfrak{k}$ is closed under the Lie bracket, while this is trivially true for $\mathfrak{a}$. Thus the exponential of each is a group. Label $K = \exp \mathfrak{k}$, $A = \exp \mathfrak{a}$, where for linear $G \subset GL(n, \mathbb{C})$ the exponential may be interpreted as a matrix exponential. The theorem then asserts that $G = KAK = \{k_1 a k_2; k_1, k_2 \in K, a \in A\}$.

The CD is seen to be an example as follows, cf. Ref. 24. Take $\theta: \mathfrak{su}(4) \to \mathfrak{su}(4)$ by $\theta(X) = (-i\sigma^y)^{\otimes 2} \overline{X} (-i\sigma^y)^{\otimes 2}$ and $\mathfrak{a} = \mathrm{span}_{\mathbb{R}}\{i|0\rangle\langle 0| - i|1\rangle\langle 1| - i|2\rangle\langle 2| + i|3\rangle\langle 3|, i|0\rangle\langle 3| + i|3\rangle\langle 0|, i|1\rangle\langle 2| + i|2\rangle\langle 1|\}$. Extending these choices to *n* qubits produces the CCD:

Definition II.1: [CCD, Ref. 8] Define $\theta: \mathfrak{su}(N) \to \mathfrak{su}(N)$ by $\theta(X) = [(-i\sigma^y)^{\otimes n}]^\dagger \overline{X} (-i\sigma^y)^{\otimes n}$. Then $\mathfrak{k}$ denotes the $+1$-eigenspace of θ while $\mathfrak{p}$ denotes the -1-eigenspace. Finally, in case *n* is even we define

$$\begin{aligned}\mathfrak{a} = \mathrm{span}_{\mathbb{R}}(&\{i|j\rangle\langle j| + i|N-j-1\rangle\langle N-j-1| - i|j+1\rangle\langle j+1| - i|N-j-2\rangle\langle N-j-2|; \quad 0 \leqslant j \leqslant 2^{n-1} \\ &- 2\} \sqcup \{i|j\rangle\langle N-j-1| + i|N-j-1\rangle\langle j|; 0 \leqslant j \leqslant 2^{n-1} - 1\},)\end{aligned} \tag{8}$$

with $A = \exp \mathfrak{a}$. In case *n* odd, we drop the second set:

$$\begin{aligned}\mathfrak{a} = \mathrm{span}_{\mathbb{R}}(&\{i|j\rangle\langle j| + i|N-j-1\rangle\langle N-j-1| - i|j+1\rangle\langle j+1| - i|N-j-2\rangle\langle N-j-2|; \\ &0 \leqslant j \leqslant 2^{n-1} - 2\}).\end{aligned} \tag{9}$$

The *concurrence canonical decomposition (CCD)* in *n*-qubits is the resulting matrix decomposition $\mathrm{SU}(N) = KAK$. Note that *n* may be even or odd.

In an earlier work,[8] computations in Dirac (bra-ket) notation show that $\theta(X)$ is a Cartan involution and $\mathfrak{a}$ is maximal-commutative in $\mathfrak{p}$. The $G = KAK$ theorem (Ref. 21, Theorem 8.6, Sec. VII.8) then shows that the CCD exists. Further, the CCD may be computed numerically in the even qubit case.[8]

The CCD is a useful tool for studying concurrence capacities since $K = \exp(\mathfrak{k})$ consists of symmetries of the concurrence form of Eq. (7), where $\mathfrak{k}$ is given per Definition II.1,[8]

$$(\nu \in K) \Leftrightarrow [\mathcal{C}_n(\nu|\phi\rangle, \nu|\psi\rangle) = \mathcal{C}_n(|\phi\rangle, |\psi\rangle) \text{ for all } |\phi\rangle, |\psi\rangle \in \mathcal{H}_n]. \tag{10}$$

In particular, the above may be used to verify that $\mathrm{SU}(2)^{\otimes n} \subseteq K$ as a subgroup of large codimension. One explanation for the fact that *K* alternates between orthogonal and symplectic groups is to note that the form $\mathcal{C}_n$ is symmetric or antisymmetric as *n* is even or odd.[8] Another outlook,

illustrated in Sec. V, is that the spin-flip υ is a bosonic or fermionic time reversal symmetry operator as n is even or odd, i.e., $\upsilon^{-1}=(-1)^n\upsilon$.

III. ODD-QUBIT CONCURRENCE CAPACITIES

The main results of this section are summarized in Theorem III.11. Each is proven in turn.

A. Double-argument capacities generalize single-argument capacities

To begin, we introduce a pairwise concurrence capacity $\kappa_n(\nu)$ and denote earlier concurrence capacities[8] with a tilde,

$$\begin{aligned}\tilde{\kappa}_n(\nu) &= \max\{\mathcal{C}_n(\nu|\psi\rangle);\langle\psi|\psi\rangle = 1,\mathcal{C}_n(|\psi\rangle) = 0\},\\ \kappa_n(\nu) &= \max\{|\mathcal{C}_n(\nu|\phi\rangle,\nu|\psi\rangle)|;\langle\phi|\phi\rangle = \langle\psi|\psi\rangle = 1,\mathcal{C}_n(|\phi\rangle,|\psi\rangle) = 0\}.\end{aligned} \tag{11}$$

Due to Eq. (10), any CCD of a unitary $\nu=k_1ak_2$ implies $\tilde{\kappa}_n(\nu)=\tilde{\kappa}_n(a)$[8] and $\kappa_n(\nu)=\kappa_n(a)$.

Proposition III.1: Suppose $n=2p$ is an even number of qubits. Then $\kappa_n(\nu)=\tilde{\kappa}_n(\nu)$.

The proof requires certain results from the literature.[8,49]

- There is an $n=2p$ qubit entangler E_0 so that for any $k\in K$, $E_0kE_0^\dagger$ is a real unitary matrix, i.e., orthogonal. The columns of E_0 resemble $|GHZ\rangle$ states.
- For this E_0, any CCD $\nu=k_1ak_2$ moreover has $d=E^\dagger aE$ for $d=\Sigma_{j=0}^{N-1}d_j|j\rangle\langle j|$ diagonal. As d is unitary diagonal, each d_j is on the unit circle within $\mathbb{C}$.
- The concurrence spectrum becomes $\lambda_c(\nu)=\{d_j^2\}_{j=0}^{N-1}$. Then $\tilde{\kappa}_{2n}(\nu)=1$ if and only if $0\in\mathbb{C}$ lies within the convex hull of $\lambda_c(\nu)$, a subset of the unit circle (Ref. 8, Lemma III.2).
- A corollary (Ref. 8, Scho. 2.18) of the symmetry group theorem shows that E_0 also translates between $\mathcal{C}_n(-,-)$ and a simpler bilinear form: $\mathcal{C}_n(E_0z_1,E_0z_2)=z_1^Tz_2$.

Example III.2: We use the CD to compute a two-qubit concurrence capacity. Consider a family of controlled-phase gates, e.g., $\nu(t)=e^{-it}|0\rangle\langle 0|+e^{-it}|1\rangle\langle 1|+e^{-it}|2\rangle\langle 2|+e^{3it}|3\rangle\langle 3|$ with $\det[\nu(t)]=1$. A possible CD is:

$$\nu(t) = (e^{-it\sigma^z}\otimes I_2)e^{it\sigma^z\otimes\sigma^z}(I_2\otimes e^{-it\sigma^z}). \tag{12}$$

The central factor is a valid choice for a in $\nu(t)=k_1ak_2$, since $e^{it\sigma^z\otimes\sigma^z}$ is also diagonal in the magic basis. Thus $\lambda_c[\nu(t)]=\mathrm{spec}(e^{2it\sigma^z\otimes\sigma^z})=\{e^{2it},e^{2it},e^{-2it},e^{-2it}\}$. Only for $t\in\pi/4\mathbb{Z}$ do we have 0 within the convex hull of $\lambda_c[\nu(t)]$, and the convex hull theorem asserts $\tilde{\kappa}_2[\nu(\pi/4)]=1$. Indeed, up to phase $\nu(\pi/4)=|0\rangle\langle 0|+|1\rangle\langle 1|+|2\rangle\langle 2|-|3\rangle\langle 3|$. Moreover, if

$$H=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$

is the Hadamard gate,[36] a standard identity converts $\nu(\pi/4)$ into the quantum controlled-not:

$$\mathrm{CNOT} = |00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 11| + |11\rangle\langle 10| = (I_2\otimes H)\,\nu(\pi/4)(I_2\otimes H). \tag{13}$$

Thus $\nu(\pi/4)$ carries an unentangled state to a maximally entangled state, since $\mathrm{CNOT}(H\otimes I_2)|00\rangle=\mathrm{CNOT}(1/\sqrt{2})(|00\rangle+|10\rangle)=(1/\sqrt{2})(|00\rangle+|11\rangle)$. More intricate examples in two-qubits[41,49] and an even number of qubits[9] are available in the literature.

Lemma III.3: Suppose the number of qubits is even. Let $z_1=\Sigma_{j=0}^{N-1}a_j|j\rangle$, $z_2=\Sigma_{j=0}^{N-1}b_j|j\rangle$, and $z_3=\Sigma_{j=0}^{N-1}c_j|j\rangle$ throughout, and let $\lambda_c(\nu)=\{\lambda_j\}_{j=0}^{N-1}$. Then we have the following:

$$\tilde{\kappa}_n(\nu) = \max\left\{\left|\sum_{j=0}^{N-1}c_j^2\lambda_j\right|;z_3^\dagger z_3 = 1, z_3^Tz_3 = 0\right\},$$

$$\kappa_n(\nu) = \max\left\{ \left| \sum_{j=0}^{N-1} a_j b_j \lambda_j \right| ; z_1^\dagger z_1 = z_2^\dagger z_2 = 1, z_1^T z_2 = 0 \right\}. \tag{14}$$

Proof of Lemma III.3: The first equation appears in Ref. 8; cf. Ref. 49. For the second, take vectors z_1, z_2 and label $x=E_0z_1$, $y=E_0z_2$. Then

$$[\mathcal{C}_n(x,y)=0] \Leftrightarrow [\mathcal{C}_n(E_0z_1,E_0z_2)=0] \Leftrightarrow [z_1^T z_2 = 0]. \tag{15}$$

Moreover, without loss of generality by choice of z_1, z_2, and symmetry we may suppose $\nu = E_0 d E_0^\dagger$ for $d^2=\Sigma_{j=0}^{N-1}\lambda_j|j\rangle\langle j|$. Then $\mathcal{C}_n(E_0dE_0^\dagger x, E_0dE_0^\dagger y)=\mathcal{C}_n(E_0dz_1, E_0dz_2)=(z_1^T d^T)dz_2=\Sigma_{j=0}^{N-1}a_jb_j\lambda_j$.

Proof of Proposition III.1: Let a_j, b_j be chosen so as to maximize the expression for $\kappa_n(\nu)$ per Lemma III.3, i.e., $\kappa_n(\nu)=|\Sigma_{j=0}^{N-1}a_jb_j\lambda_j|$. Now choose complex numbers c_j so that $c_j^2=a_jb_j$, and put $z_3=\Sigma_{j=0}^{N-1}c_j|j\rangle$. We note that $z_3^Tz_3=0$. Moreover, $z_3^\dagger z_3 \leqslant 1$, for

$$\sum_{j=0}^{N-1}|c_j|^2 = \sum_{j=0}^{N-1}|c_j^2| = \sum_{j=0}^{N-1}|a_jb_j| \leqslant \sum_{j=0}^{N-1}\frac{1}{2}|a_j|^2 + \frac{1}{2}|b_j|^2 = 1. \tag{16}$$

Label $t^2=z_3^\dagger z_3$, noting $t^2\leqslant 1$. Then $(t^{-1}z_3)^\dagger(t^{-1}z_3)=1$, so by definition of $\tilde{\kappa}_{2p}(\nu)$ we have

$$\kappa_n(\nu) \geqslant \tilde{\kappa}_n(\nu) \geqslant \left| \sum_{j=0}^{N-1} t^{-2}c_j^2\lambda_j \right| = t^{-2}\left| \sum_{j=0}^{N-1} a_jb_j\lambda_j \right| = t^{-2}\kappa_n(\nu). \tag{17}$$

Thus $t=1$ and hence $\kappa_n(\nu)=\tilde{\kappa}_n(\nu)$. □

B. Monotonicity

We next demonstrate concurrence capacity monotonicity, i.e., that $j\mapsto\kappa_{n+j}(\nu\otimes I_2^{\otimes j})$ is monotonic. It provides another justification for odd-qubit concurrence capacities, despite $\mathcal{C}_{2p-1}\equiv 0$. For if $\kappa_{2p-1}(\nu)>0$, then there is a $2p$-qubit state $|\psi\rangle$ with $C_{2p}(|\psi\rangle)=0$ while $C_{2p}[(\nu\otimes I_2)|\psi\rangle] \geqslant \kappa_{2p-1}(\nu)$.

Proposition III.4: Let n be either even or odd, $\nu\in \mathrm{SU}(N)$ an n-qubit computation, and let I_2 denote the trivial one-qubit computation. Then $\kappa_{n+1}(\nu\otimes I_2)\geqslant\kappa_n(\nu)$.

Proof: Choose $|\phi\rangle$, $|\psi\rangle$ such that $\kappa_n(\nu)=\mathcal{C}_n(\nu|\phi\rangle,\nu|\psi\rangle)$ while $\mathcal{C}_n(|\phi\rangle,|\psi\rangle)=0$. Then $|\phi\rangle\otimes|0\rangle$ and $|\psi\rangle\otimes|1\rangle$ are a null-concurrent pair of $(n+1)$-qubit states:

$$\mathcal{C}_{n+1}(|\phi\rangle\otimes|0\rangle,|\psi\rangle\otimes|1\rangle) = \overline{(\langle\phi|\otimes\langle 0|)}(-i\sigma^y)^{\otimes n+1}(|\psi\rangle\otimes|1\rangle) = [\mathcal{C}_n(|\phi\rangle,|\psi\rangle)](\overline{\langle 0|}(-i\sigma^y)|1\rangle). \tag{18}$$

Now $\overline{\langle 0|}(-i\sigma^y)|1\rangle=1$, so the above expression is $[0](1)=0$. A similar argument demonstrates that

$$\mathcal{C}_{n+1}[(\nu\otimes I_2)(|\phi\rangle\otimes|0\rangle),(\nu\otimes I_2)(|\psi\rangle\otimes|1\rangle)] = [\mathcal{C}_n(\nu|\phi\rangle,\nu|\psi\rangle)][\mathcal{C}_1(|0\rangle,|1\rangle)]. \tag{19}$$

The second term of the product is one, while the first is $\kappa_n(\nu)$. Thus we have exhibited a pair for which $\nu\otimes I_2$ raises the pairwise concurrence by at least $\kappa_n(\nu)$. Since $\kappa_{n+1}(\nu\otimes I_2)$ is the maximum over all null-concurrent pairs, while $|\phi\rangle\otimes|0\rangle$, $|\psi\rangle\otimes|1\rangle$ is such, we see $\kappa_{n+1}(\nu\otimes I_2)\geqslant\kappa_n(\nu)$. □

C. Parity-independent concurrence spectra

We extend the maximal concurrence capacity condition of Zhang *et al.* and Bullock, Brennen[8] to odd-qubit systems. The first step is a definition valid in either parity.

Definition III.5: Let $\nu\in\mathrm{SU}(N)$, $N=2^n$. For n of either parity, the concurrence spectrum $\lambda_c(\nu)$ is the set $\lambda_c(\nu)=\mathrm{spec}([(-i\sigma^y)^{\otimes n}]^\dagger\nu(-i\sigma^y)^{\otimes n}\nu^T)$. Viewing ν as an $\mathbb{R}$-linear map, equivalently $\lambda_c(\nu)=\mathrm{spec}(\nu\upsilon\nu^\dagger\upsilon^{-1})$.

We briefly show this coincides with the definition of the even-qubit concurrence spectrum of the literature.[8] The definition ibid. states that the concurrence spectrum is the spectrum of $(E_0^\dagger \nu E_0)(E_0^\dagger \nu E_0)^T$. Indeed, given $E_0 E_0^T = (-i\sigma^y)^{\otimes n}$ per the classification of E with $E\mathrm{SO}(N)E^\dagger = K$ ibid.,

$$\mathrm{spec}(E_0^\dagger \nu E_0)(E_0^\dagger \nu E_0)^T = \mathrm{spec}(E_0^\dagger \nu E_0 E_0^T \overline{E_0}) = \mathrm{spec}[(E_0 E_0^T)^\dagger \nu E_0 E_0^T \nu^T] = \mathrm{spec}[(-i\sigma^y)^{\otimes n} \nu (-i\sigma^y)^{\otimes n} \nu^T]. \tag{20}$$

In fact, the same argument shows that $\lambda_c(\nu)$ is the spectrum $(E^\dagger \nu E)(E^\dagger \nu E)^T$ for any E as above, cf. Ref. 31.

The odd-qubit case requires different similarity matrices, say F,[8] which translate K not into an orthogonal group but rather a symplectic group per Eq. (22). For the concurrence form $\mathcal{C}_n(-,-)$ n-odd is antisymmetric, and symplectic rather than orthogonal groups are the appropriate symmetries of antisymmetric bilinear forms (i.e., two-forms). For a standard similarity matrix, we take

$$F_0 = \sum_{j=0}^{N/2-1} |j\rangle\langle j| + |N-j-1\rangle\langle j| + \iota_j(|j\rangle\langle N/2+j| - |N-j-1\rangle\langle N/2+j|),$$

where

$$\{\iota_j\}_{j=0}^{N/2-1} \subset \{\pm 1\} \text{ by } (-i\sigma^y)^{\otimes n} = \sum_{j=0}^{N/2-1} \iota_j(|N-j-1\rangle\langle j| - |j\rangle\langle N-j-1|). \tag{21}$$

Also, label throughout $J_N = (-i\sigma^y) \otimes I_{N/2}$. Before showing that F_0 translates K into the standard symplectic group, we show that F_0 carries $\mathcal{C}(-,-)$ to the standard two-form $\mathcal{A}(-,-)$.

Lemma III.6: For $\mathcal{A}(|\phi\rangle, |\psi\rangle) = \overline{\langle\phi|}\, J_N |\psi\rangle$, $\mathcal{C}_n(F_0|\phi\rangle, F_0|\psi\rangle) = \mathcal{A}(|\phi\rangle, |\psi\rangle)$ *for all* $|\phi\rangle, |\psi\rangle \in \mathcal{H}_n$.

Proof: $\mathcal{C}_n(F_0|\phi\rangle, F_0|\psi\rangle) = \overline{\langle\phi|} F_0^T (-i\sigma^y)^{\otimes n} F_0 |\psi\rangle$. Now $F_0 J_N F_0^T = (-i\sigma^y)^{\otimes n}$ [Ref. 8, Proposition II.14], whence $F_0^T (-i\sigma^y)^{\otimes n} F_0 = J_N$. □

Now $\mathrm{Sp}(N/2)$ is that copy of the symplectic group which embeds within $\mathrm{SU}(N)$ as the symmetries of $\mathcal{A}(-,-)$, i.e., satisfying $\mathcal{A}(\nu|\phi\rangle, \nu|\psi\rangle) = \mathcal{A}(|\phi\rangle, |\psi\rangle)$ for all $|\phi\rangle, |\psi\rangle \in \mathcal{H}_n$. In block form:

$$\begin{aligned} \mathrm{Sp}(N/2) &= \{\nu \in \mathrm{SU}(N); \nu^T J_N \nu = J_N\} \\ &= \left\{ \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in \mathrm{SU}(N); \begin{matrix} A^T C \text{ is symmetric}, B^T D \text{ is symmetric}, \\ A^T D - C^T B = I \end{matrix} \right\} \end{aligned} \tag{22}$$

As $E_0 \mathrm{SO}(N)\ E_0^\dagger = K_{2p}$, so too $F_0 \mathrm{Sp}(N/2)\ F_0^T = K_{2p-1}$.

We next associate $\lambda_c(\nu)$ to $\mathrm{spec}(a^2)$ for $\nu = k_1 a k_2$ in the odd-qubit case. Suppose we label D to be the following diagonal subalgebra of $\mathrm{SU}(N)$:

$$D = \left\{ \sum_{j=0}^{N/2-1} d_j(|j\rangle\langle j| + |N/2+j\rangle\langle N/2+j|);\ \prod_{j=0}^{N/2-1} d_j = \pm 1 \right\}. \tag{23}$$

Now there is a standard $\mathrm{SU}(N) = KAK$ decomposition which follows from $\theta_{\mathbf{AII}}(iH) = J_N(-iH^T)J_N^\dagger$ (Ref. 21, Sec. X.2, p. 452) and $\mathfrak{a} = \log D$ as above. Given a $\nu \in \mathrm{SU}(2^{2p-1})$, it writes $\nu = \omega_1 d \omega_2$, with $\omega_j \in \mathrm{Sp}(N/2)$, $j = 1,2$ and $d \in D$.

Suppose given $\nu \in \mathrm{SU}(2^{2p-1})$, we then write $F_0^T \nu F_0 = \omega_1 d \omega_2$, with $\omega_j \in \mathrm{Sp}(N/2)$, $j = 1,2$ and $d \in D$. The odd-qubit CCD again follows by a similarity transform: $\nu = (F_0 \omega_1 F_0^T)(F_0 d F_0^T) \times (F_0 \omega_2 F_0^T)$ with $a = F_0 d F_0^T \in A$, $k_j = F_0 \omega_j F_0^T \in K$, $j = 1,2$ is a CCD. Note that a is diagonal on the *GHZ*-like basis states $\{F_0|j\rangle\}$.

Lemma III.7: Let $n = 2p-1$. *Then for* $\nu = (F_0 \omega_1 F_0^T)(F_0 d F_0^T)(F_0 \omega_2 F_0^T)$ *the CCD as above with* $d = \sum_{j=0}^{N/2-1} d_j(|j\rangle\langle j| + |N/2+j\rangle\langle N/2+j|)$ *diagonal and determinant one, we have* $\lambda_c(\nu) = \{d_j^2\}_{j=0}^{N/2-1} \sqcup \{d_j^2\}_{j=0}^{N/2-1}$ (*counted with multiplicity*.)

Proof: Given A, B, invertible, $\mathrm{spec}(AB)=\mathrm{spec}(BA)$. Also, Eq. (10) is equivalent to a matrix equation $k^T(-i\sigma^y)^{\otimes n}k=(-i\sigma^y)^{\otimes n}$ for all $k\in K$. Recall $F_0J_NF_0^T=(-i\sigma^y)^{\otimes n}$. Then

$$\begin{aligned}\lambda_c(\nu) &= \mathrm{spec}([(-i\sigma^y)^{\otimes n}]^\dagger \nu(-i\sigma^y)^{\otimes n}\nu^T) = \mathrm{spec}([(-i\sigma^y)^{\otimes n}]^\dagger k_1 a k_2(-i\sigma^y)^{\otimes n}k_2^T a^T k_1^T)\\ &= \mathrm{spec}(k_1^T[(-i\sigma^y)^{\otimes n}]k_1 a k_2[(-i\sigma^y)^{\otimes n}]^T k_2^T a^T) = \mathrm{spec}(k_1^T[(-i\sigma^y)^{\otimes n}]k_1 a[k_2^T(-i\sigma^y)^{\otimes n}k_2]^T a^T)\\ &= \mathrm{spec}([(-i\sigma^y)^{\otimes n}]a[(-i\sigma^y)^{\otimes n}]^T a^T) = \mathrm{spec}(-[F_0J_NF_0^T]F_0 d F_0^T[F_0J_NF_0^T]F_0 d^T F_0^T)\\ &= \mathrm{spec}(-F_0J_N d J_N d^T F_0^T) = \mathrm{spec}(-J_N d J_N d) = \mathrm{spec}(d^2). \end{aligned} \tag{24}$$

The last equality makes use of $d\in D$ repeat diagonal. □

D. A convex hull argument in odd qubits

Definition III.8: Suppose $n=2p-1$. The *reduced concurrence spectrum* $\tilde{\lambda}_c(\nu)$ of $\nu\in \mathrm{SU}(N)$ is the set $\{\lambda_j\}_{j=0}^{N/2-1}$ for $\nu=k_1(F_0dF_0^T)k_2$ a canonical decomposition of ν and $d=\Sigma_{j=0}^{N/2-1}\sqrt{\lambda_j}(|j\rangle\langle j|+|N/2+j\rangle\langle N/2+j|)$. The *convex hull* $\mathrm{CH}[\tilde{\lambda}_c(\nu)]$ of $\tilde{\lambda}_c(\nu)$ is the set of convex linear combinations of the points of $\tilde{\lambda}_c(\nu)$, i.e.,

$$\mathrm{CH}[\tilde{\lambda}_c(\nu)] = \left\{ \sum_{j=0}^{N/2-1} t_j\lambda_j; 0\leqslant t_j\leqslant 1,\ \sum_{j=0}^{N/2-1} t_j = 1, \lambda_j\in\tilde{\lambda}_c(\nu)\right\}. \tag{25}$$

Proposition III.9: Suppose $n=2p-1$ is an odd number of qubits. Throughout, label $z_1=\Sigma_{j=0}^{N-1}a_j|j\rangle$, $z_2=\Sigma_{j=0}^{N-1}b_j|j\rangle$, and $\tilde{\lambda}_c(\nu)=\{\lambda_j\}_{j=0}^{N/2-1}$. Then the following hold:

- $\kappa_n(\nu)=\max\{|\Sigma_{j=0}^{N/2-1}\lambda_j(a_{N/2+j}b_j-a_jb_{N/2+j})|; z_1^TJ_Nz_2=0, z_1^\dagger z_1=z_2^\dagger z_2=1\}$,
- $(\kappa_n(\nu)=1)\Leftrightarrow(0\in\mathrm{CH}[\tilde{\lambda}_c(\nu)])$.

Proof: The first item follows from Lemma III.6, substituting $x=F_0z_1$, $y=F_0z_2$. We continue to the next item.

For the second item, we first prove $\Rightarrow$. If $\kappa_n(\nu)=1$, then we may choose z_1, z_2 so that

$$\begin{aligned} 1 &= \left|\sum_{j=0}^{N/2-1}\lambda_j(a_{N/2+j}b_j-a_jb_{N/2+j})\right| \leqslant \sum_{j=0}^{N/2-1}|a_{N/2+j}b_j-a_jb_{N/2+j}|\\ &\leqslant \sum_{j=0}^{N/2-1}\sqrt{|a_j|^2+|a_{N/2+j}|^2}\sqrt{|b_j|^2+|b_{N/2+j}|^2}\leqslant 1. \end{aligned} \tag{26}$$

Here, note that the second inequality is an iterate of $\mathcal{C}_1(|\phi\rangle,|\psi\rangle)\leqslant\sqrt{\langle\phi|\phi\rangle\langle\psi|\psi\rangle}$, for all $|\phi\rangle,|\psi\rangle\in\mathcal{H}_1$. The last inequality in Eq. (26) is the Schwarz inequality.

Now label $\alpha_j=a_{N/2+j}b_j-a_jb_{N/2+j}$, for $0\leqslant j\leqslant N/2-1$. Then by Eq. (26),

$$1 = \left|\sum_{j=0}^{N/2-1}\lambda_j\alpha_j\right| = \sum_{j=0}^{N/2-1}|\lambda_j\alpha_j| = \sum_{j=0}^{N/2-1}|\alpha_j|. \tag{27}$$

Thus there must exist some $z\in\mathbb{C}$, $z\bar{z}=1$, so that $\lambda_j\alpha_j=z|\alpha_j|$, and moreover $\Sigma_{j=0}^{N/2-1}|\alpha_j|=1$. On the other hand, $z_1^TJ_Nz_2=0$ demands that $0=\Sigma_{j=0}^{N/2-1}\alpha_j=z\Sigma_{j=0}^{N/2-1}|\alpha_j|\bar{\lambda}_j$. Multiplying by $\bar{z}$ and taking the complex conjugate, $0=\Sigma_{j=0}^{N/2-1}|\alpha_j|\lambda_j$ which given $\Sigma_{j=0}^{N/2-1}|\alpha_j|=1$ by Eq. (27) demands $0\in\mathrm{CH}[\tilde{\lambda}_c(\nu)]$.

Consider now the converse case, i.e., $0\in\mathrm{CH}[\tilde{\lambda}_c(\nu)]$. Then there exist t_j real, non-negative so that $0=\Sigma_{j=0}^{N/2-1}t_j\lambda_j$. For $0\leqslant j\leqslant N/2-1$, label complex numbers $\alpha_j=t_j\bar{\lambda}_j$, so that we have $1=\Sigma_{j=0}^{N/2-1}|\alpha_j|$ and moreover $0=\bar{0}=\Sigma_{j=0}^{N/2-1}t_j\bar{\lambda}_j=\Sigma_{j=0}^{N/2-1}\alpha_j$. We are reduced to the following question: May we choose $\{a_j\}_{j=0}^{N-1}$, $\{b_j\}_{j=0}^{N-1}$ so that

$$\alpha_j = a_{N/2+j}b_j - a_j b_{N/2+j}, \quad \sum_{j=0}^{N-1} |a_j|^2 = \sum_{j=0}^{N/2-1} |b_j|^2 = 1. \tag{28}$$

To do this, write $\alpha_j = |\alpha_j| e^{i \arg \alpha_j}$, and take $a_j = \sqrt{|\alpha_j|}$, $a_{N/2+j} = 0$, $b_j = 0$, and $b_{N/2+j} = -e^{i \arg \alpha_j}\sqrt{|\alpha_j|}$. Then we see that $a_{N/2+j}b_j - a_j b_{N/2+j} = \alpha_j$. Moreover,

$$|a_j|^2 + |a_{N/2+j}|^2 = |\alpha_j|, \quad |b_j|^2 + |b_{N/2+j}|^2 = |\alpha_j|, \quad \sum_{j=0}^{N/2-1} |\alpha_j| = 1. \tag{29}$$

Thus the vectors z_1, z_2 per the statement of the proposition are normalized to be norm one. □

Hence, as in the even-qubit case, a convex hull criterion on the middle factor of the CCD determines which odd-qubit unitaries ν have concurrence capacity equal to the maximal possible capacity, i.e., one. The new feature, doubly degenerate eigenvalues in $\lambda_c(\nu)$ arising from the D above required for type **AII** will *a posteriori* be an instance of Kramers' degeneracy; see Sec. V.

Corollary III.10: For $n = 2p-1$, $\lim_{p\mapsto\infty} da(\{a \in A; \kappa_n(a) = 1\}) = 1$.

The proof of the Corollary follows by considering probability density functions on the unit circle,[8] given that the number of concurrence eigenvalues grows exponentially with n. Thus most unitary evolutions for large n (of either parity) are maximally entangling as measured by concurrence. It would be interesting but technically challenging to restate this in terms of Haar measure du on SU(N). The difficulty is that the pullback measure from the $K \times A \times K$ to SU(N) is singular, namely singular near the set where the A factor is an identity. For future reference, we summarize the concurrence capacity results of this section.

Theorem III.11: *Let* $\kappa_n(\nu)$, $\tilde{\kappa}_n(\nu)$ *be the pairwise concurrence capacity and concurrence capacity, respectively*.

1. *The pairwise capacity and the capacity are equal in any even number of qubits. Thus,*

$$\tilde{\kappa}_n(\nu) = \begin{cases} \kappa_n(\nu), & n = 2p \text{ even} \\ 0, & n = 2p-1 \text{ odd}. \end{cases} \tag{30}$$

2. *For n either even or odd, any CCD by* $\nu = k_1 a k_2$ *satisfies* $\kappa_n(\nu = k_1 a k_2) = \kappa_n(a)$.
3. *For any n, we must have* $\kappa_{n+1}(\nu \otimes I_2) \geqslant \kappa_n(\nu)$.
4. *Suppose* $n = 2p-1$ *is odd. Then for da the Haar measure on A,*

$$\lim_{p\mapsto\infty} \mathrm{Prob}(\kappa_n(a) = 1) = \lim_{p\mapsto\infty} da(\{a \in A; \kappa_n(a) = 1\}) = 1. \tag{31}$$

IV. AN ALGORITHM COMPUTING THE ODD-QUBIT CCD

In this section, we close a gap in the literature. Specifically, we present an algorithm for computing the CCD when the number of qubits is odd. We make use of an algorithm[15] by Dongarra, Gabriel, Koelling, and Wilkinson cited in a survey[12] of diagonalization arguments. The algorithm,[15] which appears in the numerical matrix analysis literature, improves the numerical stability and computational efficiency of the earlier work on time reversal by Dyson.[17]

Recall from Sec. III C that it suffices to compute the standard type **AII** *KAK* decomposition given by SU(N) = Sp($N/2$)DSp($N/2$) with D the repeat diagonal subgroup of SU(N). For given $\nu \in \mathrm{SU}(2^{2p-1})$ for which we wish to compute the CCD, suppose we obtain $F_0^T \nu F_0 = \omega_1 d \omega_2$, with $\omega_j \in \mathrm{Sp}(N/2)$, $j = 1, 2$ and $d \in D$. Then ν will have CCD $\nu = k_1 a k_2 = (F_0 \omega_1 F_0^T)(F_0 d F_0^T)(F_0 \omega_2 F_0^T)$. Before computing SU($N$) = Sp($N/2$)$D$Sp($N/2$), we make one new definition.

Definition IV.1: Let $H \in \mathbb{C}^{N\times N}$ be Hermitian. Recall $J_N = (-i\sigma^y) \otimes I_{N/2}$. We say that the Hamiltonian H is J_N*-skew symmetric* iff $HJ_N - J_N H^T = 0$.

Remark IV.2: In Ref. 15, the above is the definition of "H has a time reversal symmetry." Indeed, time reversal symmetry follows for the operator $\Theta = J_N \tau$, (τ complex conjugation) per the upcoming Definition V.1. Moreover, for the standard type **AII** Cartan involution (Ref. 21, p. 452)

$\theta_{\mathbf{AII}}(X)=J_N\overline{X}J_N^T$, let $\mathfrak{su}(N)=\mathfrak{p}_{\mathbf{AII}}\oplus\mathfrak{k}_{\mathbf{AII}}$ for the corresponding Cartan decomposition into -1 and $+1$ eigenspaces. Then H is J_N skew-symmetric if and only if $iH\in\mathfrak{p}_{\mathbf{AII}}$. Indeed on $\mathfrak{su}(N)$, $\overline{X}=-X^T$. Hence $-iH=J_N\overline{iH}J_N^T=-J_NiH^TJ_N^T$ if and only if $HJ_N=J_NH^T$.

A. Algorithm for the standard AII *KAK* decomposition, SU(*N*)=Sp(*N*/2)*D*Sp(*N*/2)

The outline below for computing the standard $\mathrm{SU}(N)=KAK$ decomposition of type **AII** (see Sec. III C) is similar to the **AI** case used in Ref. 8 to compute the even-qubit CCD. The added difficulties are (i) a more complicated formula for p^2 and (ii) a more delicate diagonalization argument for p^2 once computed. In fact, the latter requires the symplectic diagonalization argument referenced above.

Lemma IV.3: Suppose $\nu\in\mathrm{SU}(N)$ *with* $\nu=pk$ *for* $p=\exp(iH)$ *with H a* J_N *skew-symmetric Hamiltonian and* $k\in\mathrm{Sp}(N/2)$. *Then* $p^2=-\nu J_N\nu^TJ_N$.

Proof: We have $H^T=-J_NHJ_N$, given $J_N^\dagger=J_N^T=-J_N$. Thus for any $t\in\mathbb{R}$, $[\exp(iHt)]^T=J_N^\dagger\exp(iHt)J_N=-J_N\exp(iHt)J_N$. This holds in particular for p. Now put $w=\nu^\dagger$, so that $w=\tilde{k}\tilde{p}$ for $\tilde{k}=k^\dagger$, $\tilde{p}=p^\dagger$. Thus $\tilde{p}^T=J_N^\dagger\tilde{p}J_N$. Moreover, $k\in\mathrm{Sp}(N/2)$ demands $\tilde{k}^TJ_N\tilde{k}=J_N$, as $\mathrm{Sp}(N/2)$ is a group. Thus $-J_Nw^TJ_Nw=\tilde{p}^2$. Taking the adjoint of each side produces the result. □

With this lemma, we now present the algorithm for computing the standard type **AII** decomposition.

1. Suppose $\nu=pk$ per Lemma IV.3. Compute $p^2=-\nu J_N\nu^TJ_N$.
2. We may write $p=\exp(iH)$ for some J_N skew-symmetric Hamiltonian H. Compute a logarithm of $p^2=\exp(2iH)$. The diagonalizing matrix implicit in computing the matrix log need not be symplectic, and generic logarithms will take the form $2iH$ for some $(2)H$ which is J_N skew-symmetric.
3. Compute a symplectic matrix $\omega_1\in\mathrm{Sp}(N/2)$ so that $iH_2=\omega_1^\dagger(iH)\omega_1$ is repeat diagonal, per Sec. IV B.
4. Label $p=\omega_1\exp(iH_2)\omega_1^\dagger$ and $d=\exp(iH_2)$. Compute $\omega_3=p^\dagger\nu$. Then $\omega_3\in\mathrm{Sp}(N/2)$.
5. Put $\omega_2=\omega_1^\dagger\omega_3\in\mathrm{Sp}(N/2)$. Note that $\omega_1d\omega_1^\dagger=p$. Thus the type **AII** decomposition is $\nu=[\omega_1]\times[d][\omega_1^\dagger\omega_3]=\omega_1d\omega_2$.

This concludes the overview of computing $\mathrm{SU}(N)=\mathrm{Sp}(N/2)D\mathrm{Sp}(N/2)$. The next section details step 3.

B. Symplectic diagonalization

In this section we address the problem of finding the eigendecomposition of a matrix H which is J_N skew-symmetric. Generically, these techniques work on any square matrix with an even number of rows and columns, and there are no simplifications when the size is a power of two. Thus we describe the generic case where

$$J_{2\ell}=\begin{pmatrix}\mathbf{0} & -I_\ell\\ I_\ell & \mathbf{0}\end{pmatrix}$$

and $H=H^\dagger$ is also $J_{2\ell}$ skew symmetric.

Explicitly, $J_{2\ell}$-skew symmetric means

$$H=\begin{pmatrix}A & B\\ -\overline{B} & \overline{A}\end{pmatrix},$$

where $A=A^\dagger$ and $B=-B^T$ are $\ell\times\ell$ matrices. We will construct a unitary skew-symmetric Hamiltonian matrix ω of the form

$$\omega = \begin{pmatrix} U & V \\ -\overline{V} & \overline{U} \end{pmatrix},$$

so that the columns of ω are the (right) eigenvectors of H. Each eigenvalue λ_k for $k=1,\ldots,\ell$ of H is real and of multiplicity 2. In particular, both the kth and the $(\ell+k)$th columns of ω are eigenvectors of H corresponding to λ_k. Also, given the block form, $\omega \in \mathrm{Sp}(N/2)$ up to global phase.

The algorithm of Dongarra *et al.*[15] proceeds in two major steps. First we reduce H to block diagonal form using a similarity transformation, and then we use the QR algorithm to find the eigenvalues of the blocks. We consider each of these phases in turn.

First, we construct a skew-symmetric Hamiltonian unitary matrix Q of the form

$$Q = \begin{pmatrix} Q_1 & Q_2 \\ -\overline{Q_2} & \overline{Q_1} \end{pmatrix}$$

so that

$$QHQ^\dagger = \begin{pmatrix} T & 0 \\ 0 & T \end{pmatrix}$$

where T is real, symmetric, and tridiagonal. We initialize Q to be the $2\ell \times 2\ell$ identity matrix. In order to preserve the structure, we construct Q as the product of two simple types of matrices:

- The product of 2×2 skew-symmetric Hamiltonian matrices is also skew-symmetric Hamiltonian, and if we let $r^2=|a|^2+|b|^2$, then a matrix of the form

$$\begin{pmatrix} \overline{a}/r & -b/r \\ \overline{b}/r & a/r \end{pmatrix}$$

  is unitary. In addition,

$$\begin{pmatrix} \overline{a}/r & -b/r \\ \overline{b}/r & a/r \end{pmatrix}\begin{pmatrix} a & b \\ -\overline{b} & \overline{a} \end{pmatrix} = \begin{pmatrix} r & 0 \\ 0 & r \end{pmatrix}$$

  so the unitary matrix can be used to introduce zeros. Choose j between 1 and ℓ and construct a matrix R as the $2\ell\times 2\ell$ identity matrix except that entries $R_{\ell+j,\ell+j}=\overline{R_{j,j}}=a/r$ and $R_{j,\ell+j}=-\overline{R_{\ell+j,\ell+j}}=-b/r$. Then the product RH is equal to H except that the entries in rows j and $\ell+j$ become

$$\begin{pmatrix} (RH)_{j,k} & (RH)_{j,\ell+k} \\ (RH)_{\ell+j,k} & (RH)_{\ell+j,\ell+k} \end{pmatrix} = \begin{pmatrix} \overline{a}/r & -b/r \\ \overline{b}/r & a/r \end{pmatrix}\begin{pmatrix} A_{j,k} & B_{j,k} \\ -\overline{B_{j,k}} & \overline{A_{j,k}} \end{pmatrix}, \tag{32}$$

  $k=1,\ldots,\ell$. Since this product is skew-symmetric Hamiltonian, so is RH, and it can be shown in a similar way that $(RH)R^\dagger$ is skew-symmetric Hamiltonian. Thus we can use R as a similarity transformation that preserves the structure.
- Let S be a real orthogonal matrix of dimension $\ell\times\ell$. Then

$$\begin{pmatrix} S & 0 \\ 0 & S \end{pmatrix}\begin{pmatrix} A & B \\ -\overline{B} & \overline{A} \end{pmatrix}\begin{pmatrix} S^\dagger & 0 \\ 0 & S^\dagger \end{pmatrix} = \begin{pmatrix} SAS^\dagger & SBS^\dagger \\ -\overline{SBS^\dagger} & \overline{SAS^\dagger} \end{pmatrix} \tag{33}$$

  is skew-symmetric Hamiltonian.

Using these matrices, our construction takes $\ell-1$ steps. We describe the first step in detail.

The first step places zeros in the first column of the matrix in rows 3 through 2ℓ. To put a zero in position $(\ell+j,1)$ $(j=1,\ldots,n)$, we construct an R matrix involving rows j and $\ell+j$. If $r_j^2=|A_{j,1}|^2+|B_{j,1}|^2$, then this matrix R_j is the identity matrix except that entries $R_{\ell+j,\ell+j}=\overline{R_{j,j}}=A_{j,1}/r_j$ and $R_{j,\ell+j}=-R_{\ell+j,\ell+j}=-B_{j,1}/r_j$. We replace H by $(RH)R^\dagger$ and update Q by premultiplying by R_j, repeating this for $j=1,\ldots,\ell$.

We complete the first step by putting zeros in rows 3 through ℓ of column 1. Note that these elements are now real, since elements 2 through ℓ are just the values r_j. Thus we can construct a real orthogonal reflection (Householder) matrix of the form $S=I-2ss^T$ where $\hat{s}=[0,r_2+\|r\|,r_3,\ldots,r_n]^T$ and $s=\hat{s}/\|\hat{s}\|$. A similarity transformation of H by

$$\begin{pmatrix} S & 0 \\ 0 & S \end{pmatrix}$$

produces the required zeros, and Q is updated by premultiplying by this matrix.

Steps 2 through $\ell-1$ are similar; in step k we first put zeros in the B portion of column k using R matrices and then zero elements $k+2$ through ℓ of the A portion using a reflection matrix. The final result is that the transformed H has a real tridiagonal matrix T in place of A and $\overline{A}$ and zeros elsewhere.

The QR algorithm is considered to be the algorithm of choice for determining all of the eigenvalues and eigenvectors of a real symmetric tridiagonal matrix. We use the algorithm to form X, the matrix of eigenvectors of T. Implementation of the algorithm requires care, and high quality implementations are available, for example, in LAPACK.[2] Other codes are available at http://www.netlib.org.

We construct the eigenvector matrices U and V as $U=Q_1^\dagger X$ and $V=Q_2{}^T X$. Note that most implementations of the QR algorithm do not guarantee that the eigenvalues are ordered, so a final sort of the eigenvalues and the columns of U and V should be done at the end if desired.

V. TIME REVERSAL, THE CCD, AND KRAMERS' NONDEGENERACY

The section presents three topics, all following from an interpretation of υ from Eq. (2) as a time reversal symmetry operator. First, the Cartan involution defining the CCD may be rewritten entirely in terms of the spin-flip, and the eigenspaces of $\theta(iH)$ are associated to time symmetric and antisymmetric Hamiltonians H in a natural way. Second, a well-known procedure exists to convert any $G=KAK$ decomposition into a polar decomposition, and the polar decomposition associated to the CCD writes a unitary $\nu\in \mathrm{SU}(N)$ as a product of two factors, one evolution by a time symmetric Hamiltonian and one evolution by a time anti-symmetric Hamiltonian. Third, we demonstrate the entangled eigenstates of Kramers' nondegeneracy as described in the introduction and consider the perturbative stability of this entanglement under time reversal symmetry breaking.

A. Spin-flips as time reversal symmetry operators

Recall the *Bloch sphere* (e.g., Ref. 36), which provides a picture of the data space of one qubit. As a remark, the Bloch sphere may be thought of as a parametrization of the complex projective line $\mathbb{CP}^1$ (e.g., Ref. 34, Sec. 40). Briefly, $\mathbb{CP}^1$ is the set of all equivalence classes of vectors in $\mathbb{C}^2$ up to multiple by a nonzero complex scalar. To associate such a class with a Bloch vector, normalize $|\psi\rangle$ as above so as to write $|\psi\rangle=re^{it}[\cos(\theta/2)|0\rangle+e^{i\varphi}\sin(\theta/2)|1\rangle]$. The Bloch sphere vector of $|\psi\rangle$, say $[|\psi\rangle]$, is given in spherical coordinates by $(1,\theta,\varphi)$ (Ref. 36, p. 15). Recall also that the north pole is $[|0\rangle]$ and $[|1\rangle]$ is the south pole.

Now let $\vec{b}\in(\mathbb{F}_2)^n$ be an n-bit string. The typical procedure when quantizing a classical computation is to extend the classical outputs linearly without phases. Thus, a reasonable interpretation of quantum bit-flip would be $(\sigma^x)^{\otimes n}$. This is the common interpretation, but note that in one qubit

σ^x is not reflection on the Bloch sphere and indeed has a fixed state, $(1/\sqrt{2})(|0\rangle+|1\rangle)$. Rather, the odd reflection of a single qubit under the Bloch parametrization of $\mathbb{CP}^1$ is the spin-flip $|\psi\rangle\mapsto\overline{(-i\sigma^y)|\psi\rangle}=(-i\sigma^y)\overline{|\psi\rangle}$.

The appropriate physical interpretation of the spin-flip is as a time reversal symmetry operator (Ref. 47, Chap. 26, Ref. 19, pp. 314–322, Refs. 27 and 39). Wigner defined a generic time reversal symmetry operator Θ as any $\mathbb{R}$-linear involutive map of the quantum Hilbert space which is antiunitary, i.e., complex anti-linear $(\Theta(\alpha|\psi_1\rangle+\beta|\psi_2\rangle)=\overline{\alpha}\Theta|\psi_1\rangle+\overline{\beta}\Theta|\psi_2\rangle)$, and orthogonal in the induced real inner-product on $\mathbb{R}^{2p}\cong\mathbb{C}^p$. Generic time reversal symmetry operators are usually denoted by a capital Θ; we ask the reader's forebearance in distinguishing this from the lower-case θ describing a Cartan involution.

Such a time reversal symmetry operator Θ maps the state of a system to its motion-reversed state, so that momentum eigenstates transform as $\Theta|\mathbf{p}\rangle=|-\mathbf{p}\rangle$. In particular, if our qubit is a spin $\frac{1}{2}$ particle, e.g., with $|0\rangle=|\uparrow\rangle$ and $|1\rangle=|\downarrow\rangle$, then υ per Eq. (2) reverses the one-qubit spin vector on the Bloch sphere and so is the natural quantum angular momentum reversal in n-qubits. Indeed, the total spin angular momentum, $\vec{S}=\Sigma_{j=1}^n\vec{\sigma}_j$, is inverted under time reversal: $\upsilon\vec{S}\upsilon^{-1}=-\vec{S}$. Spin-flip operators may be defined for d-level systems (qudits) but may not both preserve pure states and commute with local unitaries.[38]

We note in passing that the spin-flip picture also allows one to quickly rederive one of the monotone properties. Namely, antipodal points in the Bloch sphere parametrization of the complex projective line $\mathbb{CP}^1$ correspond to Hermitian-orthogonal states of $\mathcal{H}_1$. Hence, $C_n(|\psi\rangle)=|\langle\psi|\upsilon|\psi\rangle|=0$ if $|\psi\rangle=\otimes_{j=1}^n|\psi_j\rangle$ (the monotone property,) since in this event $\langle\psi|\upsilon|\psi\rangle$ has a factor $\langle\psi_j|\upsilon|\psi_j\rangle=0$. More generally $C_n(|\psi\rangle)=0$ whenever $|\psi\rangle=|\psi_1\rangle\otimes|\psi_2\rangle$ for $|\psi_1\rangle\in\mathcal{H}_{n-1}$ and $[|\psi_2\rangle]$ a point on the Bloch sphere. However, the latter is not an equivalence for n even. Consider $|\mathrm{W}_4\rangle=(1/2)\times(|0001\rangle+|0010\rangle+|0100\rangle+|1000\rangle)$.

B. Time reversal and the CCD Cartan involution

We next show that physically, the eigenspaces of the Cartan involution producing the CCD correspond to υ-time symmetric and υ-time antisymmetric Hamiltonians. They are then explicitly described in the Pauli-tensor basis of $\mathfrak{su}(N)$ in much more compact form than in Dirac notation.[8]

Definition V.1: Consider H a Hamiltonian on a finite dimensional Hilbert space $\mathcal{H}$, i.e., H is self-adjoint within $\mathrm{End}_{\mathbb{C}}(\mathcal{H})\subset\mathrm{End}_{\mathbb{R}}(\mathcal{H})$. Then H is time reversal symmetric with respect to Θ iff $H=\Theta H\Theta^{-1}$ as elements of $\mathrm{End}_{\mathbb{R}}(\mathcal{H})$. A Hamiltonian is time reversal anti-symmetric with respect to Θ iff $H=-\Theta H\Theta^{-1}$.

Proposition V.2: Let $\theta(X)$ per Definition II.1. Label $\mathfrak{su}(N)=\mathfrak{p}\oplus\mathfrak{k}$ as the -1 and $+1$-eigenspaces of θ. Let υ be the spin-flip. Then (i) for H a traceless Hamiltonian, so that $iH\in\mathfrak{su}(N)$, $\theta(iH)=\upsilon(iH)\upsilon^{-1}$, with the right-hand side viewed as a composition of $\mathbb{R}$-linear maps. Also (ii) (H has time reversal symmetry with respect to υ) $\Leftrightarrow(iH\in\mathfrak{p})$, and (iii) ($H$ has time reversal anti-symmetry with respect to υ) $\Leftrightarrow(iH\in\mathfrak{k})$.

Proof: Let τ denote the complex conjugation operator $|\psi\rangle\mapsto\overline{|\psi\rangle}$. Then $\upsilon=(-i\sigma^y)^{\otimes n}\tau=\tau(-i\sigma^y)^{\otimes n}$, given $-i\sigma^y$ real. So $\upsilon^{-1}=\tau[(-i\sigma^y)^{\otimes n}]^\dagger$. Moreover, $[(-i\sigma^y)^{\otimes n}]^\dagger=(-I_N)^n(-i\sigma^y)^{\otimes n}$. Finally, $\tau(iH)\tau=\overline{iH}$. Thus,

$$\upsilon(iH)\upsilon^{-1}=(-i\sigma^y)^{\otimes n}\tau(iH)\tau[(-i\sigma^y)^{\otimes n}]^\dagger=(-I_N)^n(-i\sigma^y)^{\otimes n}\overline{(iH)}[(-i\sigma^y)^{\otimes n}]=\theta(iH). \quad (34)$$

The latter two items follow at once. □

With the above proposition, we may describe the infinitesimal Cartan decomposition $\mathfrak{su}(n)=\mathfrak{p}\oplus\mathfrak{k}$ directly in terms of tensors of Pauli operators. Let j denote either 0, x, y, or z, with $\sigma^j=I_2$ in case $j=0$ and Pauli matrices σ^x, σ^y, or σ^z as appropriate otherwise. A multi-index $J=j_1j_2\cdots j_k\cdots j_n$ denotes a string of length n, and J will be said to be nonzero if some $j_k\neq 0$. Finally, let $i\sigma^{\otimes J}$ denote $i\otimes_{k=1}^n(\sigma^{j_k})$. Then $\mathfrak{su}(N)=\oplus_{\text{all nonzero }J}\mathbb{R}\{i\sigma^{\otimes J}\}$. We have the following corollary, discovered independently by Bremner *et al.* (Ref. 5, Theorem 5) which has recently reappeared in a different context (Ref. 1, p. 243).

Corollary V.3: Continue the convention of the previous paragraph, and write

$$\mathfrak{su}(N) = \left(\bigoplus_{\#J=0 \bmod 2} \mathbb{R}\{i\sigma^{\otimes J}\} \right) \oplus \left(\bigoplus_{\#J=1 \bmod 2} \mathbb{R}\{i\sigma^{\otimes J}\} \right). \tag{35}$$

The above is the infinitesimal Cartan decomposition of $\theta(iH)$, *i.e.,* $\mathfrak{p} = \oplus_{\#J=0 \bmod 2} \mathbb{R}\{i\sigma^{\otimes J}\}$, and $\mathfrak{k} = \oplus_{\#J=1 \bmod 2} \mathbb{R}\{i\sigma^{\otimes J}\}$. *In particular, K is the Lie group of those unitaries which are exponentials of Hamiltonians with time reversal anti-symmetry with respect to* υ.

Proof: Distinct Pauli matrices anti-commute, each has $(\sigma^j)^2 = I_2$, and σ^y is purely imaginary while σ^x, σ^z, and I_2 are real. Considering the tensors case by case completes the proof. □

C. A time reversal polar decomposition

We next consider the polar decomposition which may be derived from the CCD. In most treatments, the polar decomposition of a general Cartan involution is proven and then a $G = KAK$ theorem is derived from it. We next use the CCD to produce a polar decomposition for time reversal symmetry. This practical decision avoids rearguing the $G = KAK$ theorem for compact groups (Ref. 21, Theorem 8.6, Sec. VII.8).

Corollary V.4: Suppose $\nu \in \mathrm{SU}(N)$ *is a phase normalized quantum computation in n qubits. Then we may write* $\nu = \exp(iH_\mathfrak{p})\exp(iH_\mathfrak{k})$ *for some Hamiltonians* $H_\mathfrak{p}$, $H_\mathfrak{k}$ *such that* $H_\mathfrak{p}$ *has time reversal symmetry and* $H_\mathfrak{k}$ *has time reversal anti-symmetry with respect to the spin-flip* υ.

Proof: Let $\nu = k_1 a k_2$ be the CCD of $\nu \in \mathrm{SU}(N)$. Then in particular $\nu = (k_1 a k_1^\dagger)(k_1 k_2)$. Since K is a group, $k_1 k_2$ is a time antisymmetric evolution by Proposition V.2. Moreover, let $a = \exp iH$ for $iH \in \mathfrak{a} \subset \mathfrak{p}$ a time symmetric Hamiltonian. As $iH \in \mathfrak{p}$, we have $\theta(iH) = [(-i\sigma^y)^{\otimes n}]^\dagger \overline{(iH)}(-i\sigma^y)^{\otimes n} = -iH$. Moreover, $k \in K$ is a symmetry of the concurrence form [Eq. (10)] which as a matrix equation demands $k^T(-i\sigma^y)^{\otimes n}k = (-i\sigma^y)^{\otimes n}$. Hence $k_1^T(-i\sigma^y)^{\otimes n} = (-i\sigma^y)^{\otimes n}k_1^\dagger$, and for $k_1 iHk_1^\dagger \in \mathfrak{p}$:

$$\theta(k_1 iHk_1^\dagger) = [(-i\sigma^y)^{\otimes n}]^\dagger \overline{k_1}\,\overline{(iH)}k_1^T(-i\sigma^y)^{\otimes n} = k_1[(-i\sigma^y)^{\otimes n}]^\dagger \overline{(iH)}(-i\sigma^y)^{\otimes n}k_1^\dagger = -k_1(iH)k_1^\dagger. \tag{36}$$

Thus $k_1(iH)k_1^\dagger$ has time reversal symmetry, and the usual matrix exponential formula [valid since $\mathrm{SU}(N)$ is linear] shows $k_1 a k_1^\dagger = \exp[k_1(iH)k_1^\dagger]$. □

Remark V.5: Note that the vector space decomposition $\mathfrak{su}(N) = \mathfrak{p} \oplus \mathfrak{k}$ makes clear any such ν may be approximated by rapid pulsing of the time symmetric and anti-symmetric factors, by applying the Trotter formula (e.g., Ref. 36, Sec. 4.7.2). However, the decomposition above requires no such pulsing of the time-symmetric and time-antisymmetric Hamiltonians.

D. Kramers' nondegeneracy

Finally, we rederive Kramers' degeneracy in the case of υ and note a further, υ-specific nondegeneracy property. Recall Kramers' degeneracy[26,27] proves that the eigenstates of a collection of an odd number of spin $\frac{1}{2}$ electrons become doubly degenerate in the exclusive presence of a time-reversal-symmetric interaction, such as an electric field. The degeneracy is broken with the introduction of a magnetic field. In terms of an energy Hamiltonian H of the system, the degeneracy corresponds to 2 or greater dimensional eigenspace for energy eigenstates.

Lemma V.6: Suppose that $|\psi\rangle \in \mathcal{H}_n$ *is an eigenstate of some traceless Hamiltonian H which has time reversal symmetry, with eigenvalue* $\lambda \in \mathbb{R}$. *Then the spin-flip* $\upsilon|\psi\rangle$ *is also an eigenstate of eigenvalue* λ.

Proof: Since iH has time reversal symmetry, $\theta(iH) = -iH$. Thus $(-i\sigma^y)^{\otimes n}(iH) + \overline{(iH)}(-i\sigma^y)^{\otimes n} = 0$, and taking a complex conjugate produces $(-i\sigma^y)^{\otimes n}\overline{(iH)} + (iH)(-i\sigma^y)^{\otimes n} = 0$. Now $(iH)|\psi\rangle = \lambda|\psi\rangle$, so that

$$(iH)\upsilon|\psi\rangle = (iH)(-i\sigma^y)^{\otimes n}\overline{|\psi\rangle} = -(-i\sigma^y)^{\otimes n}\overline{(iH)|\psi\rangle} = -(-i\sigma^y)^{\otimes n}\overline{i\lambda|\psi\rangle} = i\lambda\upsilon|\psi\rangle. \tag{37}$$

This concludes the proof. □

Theorem V.7 [cf. Kramers' degeneracy—Refs. 26, 27, and 39 (p. 281)]. *Let H be a traceless Hamiltonian on some number n of quantum-bits. Suppose H has time reversal symmetry with respect to* υ. *Let* λ *be a fixed eigenvalue of H. Then either (i)* λ *is degenerate with even multiplicity*

or (ii) the normalized eigenstate $|\lambda\rangle$ *has* $C_n(|\lambda\rangle)=1$. *For n odd, case (i) holds: all* λ *are degenerate with even multiplicity*.

Proof: Let λ_j be some eigenvalue of H. By Lemma V.6, both $|\lambda_j\rangle$ and $\upsilon|\lambda_j\rangle$ are energy eigenstates. Should these two states be linearly independent, then λ_j is degenerate. If any eigenvalue is nondegenerate, say λ_k, then by antiunitarity of υ, we must have $\upsilon|\lambda_k\rangle=e^{i\varphi}|\lambda_k\rangle$ for some global phase φ. Using $C_n(|\lambda_k\rangle)=|\langle\lambda_k|\upsilon|\lambda_k\rangle|$ we see that this eigenstate must have concurrence one.

Suppose in particular $n=2p-1$. Then $\mathcal{C}_n(-,-)$ is antisymmetric and vanishes on the diagonal, implying $\langle\lambda_j|\upsilon|\lambda_j\rangle=0$ for all j. Consequently, $|\lambda_j\rangle$ and $\upsilon|\lambda_j\rangle$ are Hermitian orthogonal and may not be dependent, implying case (i). □

Thus, for the spin-flip υ there is in addition to the Kramers' degeneracy a Kramers' nondegeneracy. As always, if n is odd so that the total n-qubit system is a fermion, then a time reversal symmetric Hamiltonian implies that all energy eigenstates are degenerate. Yet moreover in the specific case of υ and *n even*, a nondegenerate eigenstate must also have maximal concurrence and hence be entangled.

We provide some illustrative examples. First note that there are many systems endowed with time reversal symmetric Hamiltonians. In particular, any system with (exclusively) pairwise nearest neighbor coupling between qubits has $iH\in\mathfrak{p}$, by Corollary V.3. An example of an interaction that occurs in many solid state systems is the quantum XYZ model:

$$H_{\mathrm{XYZ}}=\sum_{\langle j,k\rangle}J_x\sigma_j^x\sigma_k^x+J_y\sigma_j^y\sigma_k^y+J_z\sigma_j^z\sigma_k^z \tag{38}$$

with $J_{x,y,z}\in\mathbb{R}$ where the sum is taken over all nearest neighbor pairs and the boundaries may be fixed or periodic. In one dimension, these nearest neighbor coupled systems are known as spin chains. Spin chain Hamiltonians are of great theoretical interest, for under the appropriate parameter regime they exhibit long range classical correlations near a quantum phase transition.[30] We can characterize the dynamics of entanglement in spin chains using the concurrence capacity. With this goal in mind we observe the following useful fact:

Proposition V.8: Let $\mathfrak{p}$, $\mathfrak{k}$ *be as in Corollary V.3. If* $iH\in\mathfrak{p}$ *and* $H\in\mathbb{R}^{N\times N}$, *then* $\lambda_c(u=e^{-iHt})=\{e^{-2i\lambda_j t}\}$ *where* $t\in\mathbb{R}$ *parameterizes time and* $\lambda_j\in\mathbb{R}$ *are the eigenvalues of H*.

Proof: By Definition III.5 the concurrence spectrum of the unitary generated by iH, $u=e^{-iHt}$ is

$$\begin{aligned}\lambda_c(u)&=\mathrm{spec}[(-i\sigma^y)^{\otimes n\dagger}e^{iHt}(-i\sigma^y)^{\otimes n}(e^{-iHt})^T]=\mathrm{spec}(e^{-iHt}e^{-iH^Tt})\\&=\mathrm{spec}(e^{-2iHt})\qquad\qquad=\{e^{-2i\lambda_j t};\lambda_j\in\mathrm{spec}(H)\}.\end{aligned} \tag{39}$$

We have used $(-i\sigma^y)^{\otimes n\dagger}\overline{iH}(-i\sigma^y)^{\otimes n}=-iH$ and therefore $(-i\sigma^y)^{\otimes n\dagger}H(-i\sigma^y)^{\otimes n}=H$ because H is real. The third line is a consequence of H being Hermitian. □

The quantum XYZ Hamiltonian has time reversal symmetry with respect to the spin-flip υ. We next demonstrate how to build up entanglement with such a system. Consider a collection of n qubits laid out in a cyclic array interacting under the Ising class of Hamiltonians given by H_{XYZ} with $J_x=J_y=0$: $H_{Is}=\Sigma_{j=1}^n J_z\sigma_j^z\sigma_{j+1}^z$, where we identify $\sigma_{n+1}^z=\sigma_1^z$.

The eigenvalues are given by $\{\lambda_j\}=\{J_z(n-2\Sigma_k j_k\oplus j_{k+1});j=j_1j_2\ldots j_n\}$,[30] where the addition is done modulo 2 over the components j_k of the binary expansion of j. For n even, each eigenvalue λ_j is paired with another of opposite sign and in particular, $\lambda_0=-\lambda_{N-1}$ with $|\lambda_0|=n|J_z|=\lambda^{\max}$. The concurrence spectrum of $u=e^{-iH_{Is}t}$ is composed of complex conjugate pairs and the concurrence capacity $\tilde{\kappa}_n(u)$ may be computed explicitly. Then $\tilde{\kappa}_n(u)=\max\{|\Sigma_{j=0}^{N-1}a_j^2e^{-2i\lambda_j t}|;z^\dagger z=1,z^Tz=0\}$ where $z=\Sigma_{j=0}^{N-1}a_j|j\rangle$, per Eq. (14). Maximum capacity is obtained when the convex hull condition is satisfied which occurs precisely when the concurrence spectrum extends outside the right half of the complex plane. The minimum time at which this occurs is given by $e^{-2i\lambda^{\max}t_{\min}}=i$ or $t_{\min}=\pi/4|\lambda_0|=\pi/4n|J_z|$.

The existence of a time reversal symmetry in the interaction between qubits gives us important information about the nature of quantum correlations in the energy eigenstates. Applying Theorem V.7, we immediately find that the ground state of a Hamiltonian H with time reversal symmetry has maximum n-concurrence if it is unique. Examples of interactions satisfying these

conditions are the XYZ Hamiltonian with $(J_x=J_y=J_z=J>0)$, denoted the XXX Hamiltonian, and the XY Hamiltonian $(J_x=J_y, J_z=0)$.[30] In particular, the XXX Hamiltonian with $J>0$ has been shown to have nondegenerate ground states in any number of dimensions, with or without periodic boundary conditions, provided the underlying lattice has a reflection symmetry about some plane (ibid.).

To illustrate this phenomenon we consider what happens when the time reversal symmetry is broken by adding a time-antisymmetric term to the XY Hamiltonian:

$$H=\sum_{j=1}^{n} J\left(\frac{1+g}{4}\sigma_j^x\sigma_{j+1}^x+\frac{1-g}{4}\sigma_j^y\sigma_{j+1}^y\right)+\frac{h_z}{2}\sigma_j^z, \tag{40}$$

where $\sigma_{n+1}^{\alpha}\equiv\sigma_1^{\alpha}$. The presence of the linear term proportional to the total spin projection operator $S_z=\Sigma_{j=1}^{n}\sigma_j^z$, breaks the time reversal symmetry so that $iH\notin\mathfrak{p}$ when $h_z\neq 0$. For zero magnetic field and $0\leqslant g<1$, the Hamiltonian is time reversal symmetric and the ground state is nondegenerate meaning the concurrence is maximal. In the isotropic case $(g=0)$, the Hamiltonian commutes with S_z and eigenstates are independent of h_z. For magnetic field strengths below some critical value, $|h|<h_{\text{crit}}$ the ground state corresponds to an eigenstate with eigenvalue $s_z=0$ of the operator S_z. This ground state has maximal concurrence. For $|h_z|>h_{\text{crit}}$, the ground state corresponds to an eigenvalue $s_z\neq 0$ and the concurrence is zero.[7]

VI. CONCLUSIONS

We show that the odd-qubit concurrence canonical decomposition admits generalizations of all constructions studied on the even qubit CCD. In particular, a generalized pairwise concurrence capacity may be defined, and the operators for which this is maximal are characterized by a convex hull condition on the concurrence spectrum. Again for an odd number of qubits, we find that for large odd *n* most unitaries have maximal concurrence capacities. Moreover, we provide an explicit algorithm for computing the odd-qubit CCD.

These advances are complemented by new interpretation of the original inputs to the $G=KAK$ theorem which define the CCD. Specifically, they may be rewritten in terms of time reversal symmetry υ which is the spin-flip in *n* quantum bits, and the CCD is best understood in terms of such symmetries. For example, the odd-qubit CCD is a type **AII** *KAK* decomposition, and as such must have degenerate eigenvalues. In fact, this recaptures Kramers' degeneracy for the odd-qubit spin-flip, and a more careful study of the arguments reveals a Kramers' nondegeneracy: Nondegenerate eigenstates of υ time reversal symmetric Hamiltonians only exist when the number of quantum bits is even and *moreover* must be highly entangled. Specifically, such $|\lambda\rangle$ are highly entangled in the sense that the concurrence $C_n(|\lambda\rangle)=|\langle\lambda|\upsilon|\lambda\rangle|=1$. Finally, the polar decomposition extracted from the CCD in the usual way accomplishes the following: any unitary *n*-qubit evolution is a product of precisely one time reversal symmetric and one time reversal antisymmetric evolution.

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An isoperimetric problem for leaky loops and related mean-chord inequalities

Pavel Exner[a)]
Department of Theoretical Physics, Nuclear Physics Institute, Academy of Sciences, 25068 Řež near Prague, Czechia, and Doppler Institute, Czech Technical University, Břehová 7, 11519 Prague, Czechia

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We consider a class of Hamiltonians in $L^2(\mathbb{R}^2)$ with attractive interaction supported by piecewise C^2 smooth loops Γ of a fixed length L, formally given by $-\Delta - \alpha\delta(x-\Gamma)$ with $\alpha>0$. It is shown that the ground state of this operator is locally maximized by a circular Γ. We also conjecture that this property holds globally and show that the problem is related to an interesting family of geometric inequalities concerning mean values of chords of Γ. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1914728]

I. INTRODUCTION

There is a small number of topics which can be regarded as a trademark for mathematical physics. One of them without any doubt concerns relations between geometric properties of constraints and/or interaction and extremal values of a spectral quantity; classical examples are the Faber–Krahn inequality[12,14] or the PPW conjecture proved by Ashbaugh and Benguria.[3]

A common feature of these and analogous problems is that the extremum is reached by shapes having a rotational symmetry. At the same time, the nature of the extremum may be different. While a ball *minimizes* the principal eigenvalue of the Dirichlet Laplacian among regions of a fixed volume, for nonsimply connected regions like annular strips or layers considered in Refs. 8 and 13, built over a curve (surface) of a fixed length (area), the circular shape is on the contrary a *maximizer*. A natural topological way to understand this difference becomes smeared, however, when the particle is not localized by boundary conditions but by a potential, a regular or a singular one.

In this paper we consider such a problem associated with a class of operators in $L^2(\mathbb{R}^2)$ which are given formally by the expression

$$H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x-\Gamma), \tag{1.1}$$

where $\alpha>0$ and Γ is a C^2 loop in the plane (see below for exact assumptions) having a fixed length $L>0$. A motivation to study these operators comes from the theory of *leaky quantum graphs*—see Refs. 5 and 9 and related papers, a bibliography can be found in Ref. 1—aiming at a more realistic model of quantum wire structures which would take quantum tunneling into account.

Our aim is to show that the ground-state energy of $H_{\alpha,\Gamma}$ is (sharply) maximized when Γ is a circle. We will be able to prove that this property holds *locally* conjecturing its global validity. There are several reasons why one may expect this result to be valid. On one hand, we know from Ref. 11 that in the limit of strong coupling, $\alpha\to\infty$, the ground-state dependence on Γ is given in the leading order by the lowest eigenvalue of the operator $-\mathrm{d}^2/\mathrm{d}s^2-\frac{1}{4}\gamma(s)^2$ on $L^2([0,L])$ with periodic boundary conditions where γ is the curvature of Γ, and the latter is easily seen to be globally sharply maximized when γ is constant along Γ. On the other hand, by Ref. 10 the

a)Electronic mail: exner@ujf.cas.cz

operator $H_{\alpha,\Gamma}$ can be approximated in the strong resolvent sense by point interaction Hamiltonians with the point interactions equidistantly spaced along Γ and properly chosen coupling constants, and from Ref. 7 we know that the ground state of such an operator is locally maximized by a regular polygon.

Needless to say, neither of the above observations proves the desired result. The first one is global, but it holds only asymptotically and we do not know whether the error term will not spoil the inequality. The second argument holds for any $\alpha>0$, suggesting the local validity, but the polygons approximating the circle do not have exactly the same lengths.

Our main tools in this paper are the generalized Birman–Schwinger principle in combination with the convexity of the Green's function. They allow us to reformulate the problem in a purely geometric way, in terms of *mean value of chords* of arc segments of Γ. Since such geometric inequalities are of an independent interest, we discuss them in Sec. IV separately in a broader context, including the discrete version which arose in connection with the polygon problem treated in Ref. 7. Before doing that, we will formulate in the next section the problem and state our main result, Theorem 2.1, and provide the mentioned reformulation in Sec. III. After the discussion of the inequalities we will finish the proof of Theorem 2.1 and present some concluding remarks.

II. FORMULATION AND THE MAIN RESULT

We will assume throughout that $\Gamma:[0,L]\to\mathbb{R}^2$ is *a closed curve*, $\Gamma(0)=\Gamma(L)$, *parametrized by its arclength, which is* C^1*-smooth, piecewise* C^2*, and has no cusps.* (There are, of course, no local cusps under the C^1 assumption, but we have not excluded self-intersections, so the last requirement means that the curve meets itself at such a point at a nonzero angle. In fact, our main result can be pushed through under a slightly weaker regularity assumption, namely that $\dot{\Gamma}$ is absolutely continuous.) Unless stated otherwise, we will mean by the curve Γ for simplicity both the above-mentioned function and its image in the plane. Furthermore, we introduce the equivalence relation: Γ and Γ' belong to the same equivalence class if one can be obtained from the other by a Euclidean transformation of the plane. Spectral properties of the corresponding $H_{\alpha,\Gamma}$ and $H_{\alpha,\Gamma'}$ are obviously the same, and we will usually speak about a curve Γ having in mind the corresponding equivalence class. It is clear that the stated regularity assumptions are satisfied, in particular, by the circle, say $\mathcal{C}:=\{((L/2\pi)\cos s,(L/2\pi)\sin s):s\in[0,L]\}$, and its equivalence class.

First of all we have to give a rigorous meaning to the operator (1.1). Following Refs. 4 and 5, we can do that in two ways. The more general one is to consider a positive Radon measure m on $\mathbb{R}^2$ and $\alpha>0$ such that

$$(1+\alpha)\int_{\mathbb{R}^2}|\psi(x)|^2\,\mathrm{d}m(x)\leqslant a\int_{\mathbb{R}^2}|\nabla\psi(x)|^2\,\mathrm{d}x+b\int_{\mathbb{R}^2}|\psi(x)|^2\,\mathrm{d}x, \tag{2.1}$$

holds for all ψ from the Schwartz space $\mathcal{S}(\mathbb{R}^2)$ and some $a<1$ and b. The map I_m defined on $\mathcal{S}(\mathbb{R}^2)$ by $I_m\psi=\psi$ extends by density uniquely to

$$I_m:W^{1,2}(\mathbb{R}^2)\to L^2(m):=L^2(\mathbb{R}^2,\mathrm{d}m); \tag{2.2}$$

abusing notation we employ the same symbol for a continuous function and the corresponding equivalence classes in both $L^2(\mathbb{R}^2)$ and $L^2(m)$. The inequality (2.1) extends to $W^{1,2}(\mathbb{R}^2)$ with ψ replaced by $I_m\psi$ at the left-hand side. This makes it possible to introduce the following quadratic form:

$$\mathcal{E}_{-\alpha m}(\psi,\phi):=\int_{\mathbb{R}^2}\overline{\nabla\psi(x)}\,\nabla\phi(x)\mathrm{d}x-\alpha\int_{\mathbb{R}^2}(I_m\overline{\psi})(x)(I_m\phi)(x)\mathrm{d}m(x), \tag{2.3}$$

with the domain $W^{1,2}(\mathbb{R}^2)$; it is straightforward to see that under the condition (2.1) it is closed and below bounded, with $C_0^\infty(\mathbb{R}^2)$ as a core, and thus associated with a unique self-adjoint operator. Furthermore, (2.1) is satisfied with any $a>0$ provided m belongs to the generalized Kato class,

$$\lim_{\epsilon\to 0}\sup_{x\in\mathbb{R}^2}\int_{B(x,\epsilon)}|\ln|x-y||\mathrm{d}m(y)=0, \tag{2.4}$$

where $B(x,\epsilon)$ is the ball of radius ϵ and center x. Choosing now for m the Dirac measure supported by the curve one can check easily that the condition (2.4) is satisfied under our assumptions about Γ, hence we may identify the above mentioned self-adjoint operator with the formal one given by (1.1).

The described definition applies naturally to a much wider class of perturbations than we need here. Since Γ is supposed to be smooth, with the normal defined everywhere, we can define $H_{\alpha,\Gamma}$ alternatively through boundary conditions. Specifically, it acts as $-\Delta\psi$ on any ψ from the domain consisting of functions which belong to $W^{2,2}(\mathbb{R}^2\setminus\Gamma)$, they are continuous at the curve Γ and their normal derivatives have a jump there,

$$\frac{\partial\psi(x)}{\partial n_+}-\frac{\partial\psi(x)}{\partial n_-}=-\alpha\psi(x),\quad \text{for } x=\Gamma(s),\quad \forall\, s\in[0,L].$$

It is straightforward to check that such an operator is e.s.a. and its closure can be identified with (1.1) defined in the above described way.[4] The advantage of the second definition is that it has an illustrative meaning which corresponds well to the concept of a δ interaction in the cross cut of the curve.

Since the curve is finite, by Refs. 4 and 5 we have $\sigma_{\mathrm{ess}}(H_{\alpha,\Gamma})=[0,\infty)$ while the discrete spectrum is nonempty and finite, so that

$$\epsilon_1\equiv\epsilon_1(\alpha,\Gamma):=\inf\sigma(-\Delta_{\alpha,\Gamma})<0;$$

we ask for which Γ the principal eigenvalue is maximal. The main result of this paper is a partial answer to this question, namely, the following.

Theorem 1: *Within the specified class of curves, $\epsilon_1(\alpha,\Gamma)$ is for any fixed $\alpha>0$ and $L>0$ locally sharply maximized by a circle.*

While we do not give a general answer here, we suggest what it should be.

Conjecture 2.2: The circle is a sharp global maximizer, even under weaker regularity assumptions.

III. BIRMAN–SCHWINGER REFORMULATION

For operators associated with the quadratic form (2.3), one can establish a generalized Birman–Schwinger principle—we refer to Ref. 4 for a detailed discussion. In particular, if k^2 belongs to the resolvent set of $H_{\alpha,\Gamma}$ we put $R^k_{\alpha,\Gamma}:=(H_{\alpha,\Gamma}-k^2)^{-1}$. The free resolvent R^k_0 is defined for $\mathrm{Im}\,k>0$ as an integral operator in $L^2(\mathbb{R}^2)$ with the kernel

$$G_k(x-y)=\frac{i}{4}H_0^{(1)}(k|x-y|).$$

Next we have to introduce embedding operators associated with R^k_0. Let μ,ν be arbitrary positive Radon measures on $\mathbb{R}^2$ with $\mu(x)=\nu(x)=0$ for any $x\in\mathbb{R}^2$. By $R^k_{\nu,\mu}$ we denote the integral operator from $L^2(\mu):=L^2(\mathbb{R}^2,\mathrm{d}\mu)$ to $L^2(\nu)$ with the kernel G_k, in other words, we suppose that

$$R^k_{\nu,\mu}\phi=G_k*\phi\mu,$$

holds ν—a.e. for all $\phi\in D(R^k_{\nu,\mu})\subset L^2(\mu)$. In our case the two measures will be the Dirac measure supported by Γ, denoted by m if necessary, and the Lebesgue measure $\mathrm{d}x$ on $\mathbb{R}^2$, in different combinations. With this notation one can express the generalized BS principle as follows.

Proposition 3.1: (i) There is a $\kappa_0>0$ such that the operator $I-\alpha R^{i\kappa}_{m,m}$ on $L^2(m)$ has a bounded inverse for any $\kappa\geqslant\kappa_0$.

(ii) Let $\mathrm{Im}\, k>0$. *Suppose that* $I-\alpha R^k_{m,m}$ *is invertible and the operator*

$$R^k := R^k_0 + \alpha R^k_{\mathrm{d}x,m}[I-\alpha R^k_{m,m}]^{-1}R^k_{m,\mathrm{d}x}$$

from $L^2(\mathbb{R}^2)$ *to* $L^2(\mathbb{R}^2)$ *is everywhere defined. Then* k^2 *belongs to* $\rho(H_{\alpha,\Gamma})$ *and* $(H_{\alpha,\Gamma}-k^2)^{-1}=R^k$.

(iii) $\dim\ker(H_{\alpha,\Gamma}-k^2)=\dim\ker(I-\alpha R^k_{m,m})$ *for any* k *with* $\mathrm{Im}\, k>0$.

(iv) An eigenfunction of $H_{\alpha,\Gamma}$ *associated with such an eigenvalue* k^2 *can be written as*

$$\psi(x)=\int_0^L R^k_{\mathrm{d}x,m}(x,s)\,\phi(s)\mathrm{d}s,$$

where ϕ *is the corresponding eigenfunction of* $\alpha R^k_{m,m}$ *with the eigenvalue one.*

Proof of (i)–(iii) is given in Ref. 4, for (iv) see Ref. 15. ■

Denoting conventionally $k=i\kappa$ with $\kappa>0$ as corresponding to the bound-state energy $-\kappa^2$, we can thus rephrase our problem as a search for solutions to the integral-operator equation,

$$\mathcal{R}^\kappa_{\alpha,\Gamma}\phi=\phi,\quad \mathcal{R}^\kappa_{\alpha,\Gamma}(s,s') := \frac{\alpha}{2\pi}K_0(\kappa|\Gamma(s)-\Gamma(s')|), \tag{3.1}$$

on $L^2([0,L])$, where K_0 is the Macdonald function. Referring again to Refs. 4 and 15 we find that the operator-valued function $\kappa\mapsto\mathcal{R}^\kappa_{\alpha,\Gamma}$ is strictly decreasing in $(0,\infty)$ and $\|\mathcal{R}^\kappa_{\alpha,\Gamma}\|\to 0$ as $\kappa\to\infty$. In fact, the two properties can be checked also directly. The first one follows from the one-to-one correspondence of the eigenvalue branches (as functions of κ) to those of $H_{\alpha,\Gamma}$ which are obviously strictly monotonous as functions of α; the second one in turn comes from the explicit form of the kernel together with the dominated convergence theorem.

Next we use the fact that the maximum eigenvalue of $\mathcal{R}^\kappa_{\alpha,\Gamma}$ is simple. This conclusion results from the following considerations: the kernel of the operator is by (3.1) strictly positive, so $\mathcal{R}^\kappa_{\alpha,\Gamma}$ is positivity improving. It further means that for any nonzero $\phi,\chi\geqslant 0$ the functions $\mathcal{R}^\kappa_{\alpha,\Gamma}\phi$, $\mathcal{R}^\kappa_{\alpha,\Gamma}\chi$ are also strictly positive. Hence $(\phi,(\mathcal{R}^\kappa_{\alpha,\Gamma})^2\chi)\neq 0$, and as a consequence, $\mathcal{R}^\kappa_{\alpha,\Gamma}$ is ergodic; then the claim follows from Theorem XIII.43 of Ref. 16. In view of Proposition 3.1(iii) the ground state of $H_{\alpha,\Gamma}$ is, of course, also simple.

If Γ is a circle the operator $H_{\alpha,\mathcal{C}}$ has a full rotational symmetry, so the corresponding eigenspace supports a one-dimensional representation of the group $O(2)$. Let us denote the ground-state eigenfunction of $H_{\alpha,\mathcal{C}}$ as $-\tilde\kappa_1^2$ (we will use an overtilde to distinguish quantities referring to the circle). The correspondence between the eigenfunctions given by Proposition 3.1(iv) then requires that the respective eigenfunction of $\mathcal{R}^{\tilde\kappa_1}_{\alpha,\mathcal{C}}$ corresponding to the unit eigenvalue is constant; we can choose it as $\tilde\phi_1(s)=L^{-1/2}$. Then we have

$$\max\sigma(\mathcal{R}^{\tilde\kappa_1}_{\alpha,\mathcal{C}})=(\tilde\phi_1,\mathcal{R}^{\tilde\kappa_1}_{\alpha,\mathcal{C}}\tilde\phi_1)=\frac{1}{L}\int_0^L\int_0^L\mathcal{R}^{\tilde\kappa_1}_{\alpha,\mathcal{C}}(s,s')\mathrm{d}s\,\mathrm{d}s',$$

and, on the other hand, for the same quantity referring to a general Γ a simple variational estimate gives

$$\max\sigma(\mathcal{R}^{\tilde\kappa_1}_{\alpha,\Gamma})\geqslant(\tilde\phi_1,\mathcal{R}^{\tilde\kappa_1}_{\alpha,\Gamma}\tilde\phi_1)=\frac{1}{L}\int_0^L\int_0^L\mathcal{R}^{\tilde\kappa_1}_{\alpha,\Gamma}(s,s')\mathrm{d}s\,\mathrm{d}s'.$$

Hence to check that the circle is a maximizer it sufficient to show that

$$\int_0^L\int_0^L K_0(\kappa|\Gamma(s)-\Gamma(s')|)\mathrm{d}s\,\mathrm{d}s'\geqslant\int_0^L\int_0^L K_0(\kappa|\mathcal{C}(s)-\mathcal{C}(s')|)\mathrm{d}s\,\mathrm{d}s', \tag{3.2}$$

holds *for all* $\kappa>0$ and Γ of the considered class, or at least for Γ in the vicinity of $\mathcal{C}$ to prove the local result in Theorem 2.1. Since the kernel is symmetric with respect to the two variables, we

can replace the double integral by $2\int_0^L \mathrm{d}s \int_0^s \mathrm{d}s'$. By another simple change of variables we find that the above claim is equivalent to positivity of the functional

$$F_\kappa(\Gamma) := \int_0^{L/2} \mathrm{d}u \int_0^L \mathrm{d}s [K_0(\kappa|\Gamma(s+u)-\Gamma(s)|) - K_0(\kappa|\mathcal{C}(s+u)-\mathcal{C}(s)|)],$$

where the second term in the integrand is, of course, independent of s being equal to $K_0((\kappa L/\pi)\sin(\pi u/L))$. Now we employ the (strict) convexity of K_0 which yields by means of the Jensen inequality the following estimate:

$$\frac{1}{L}F_\kappa(\Gamma) \geqslant \int_0^{L/2} \left[K_0\left(\frac{\kappa}{L}\int_0^L |\Gamma(s+u)-\Gamma(s)|\mathrm{d}s \right) - K_0\left(\frac{\kappa L}{\pi}\sin\frac{\pi u}{L} \right) \right] \mathrm{d}u,$$

where the inequality is sharp unless $\int_0^L |\Gamma(s+u)-\Gamma(s)|\mathrm{d}s$ is independent of s. Finally, we observe that K_0 is decreasing in $(0,\infty)$; hence it is sufficient to check the inequality

$$\int_0^L |\Gamma(s+u)-\Gamma(s)|\mathrm{d}s \leqslant \frac{L^2}{\pi}\sin\frac{\pi u}{L}, \tag{3.3}$$

for all $u \in (0, \frac{1}{2}L]$ and to show that is sharp unless Γ is a circle.

IV. MEAN-CHORD INEQUALITIES

The inequality (3.3) to which we have reduced our problem can be regarded as an element of a wider family which we are now going to describe. Let $\Gamma\colon [0,L] \to \mathbb{R}^2$ be again a loop in the plane; for the moment we do not specify its regularity properties. Let us consider all the arcs of Γ having length $u \in (0, \frac{1}{2}L]$. The mentioned inequalities are the following:

$$C_L^p(u)\colon \int_0^L |\Gamma(s+u)-\Gamma(s)|^p \,\mathrm{d}s \leqslant \frac{L^{1+p}}{\pi^p}\sin^p\frac{\pi u}{L}, \quad p>0, \tag{4.1}$$

$$C_L^{-p}(u)\colon \int_0^L |\Gamma(s+u)-\Gamma(s)|^{-p} \,\mathrm{d}s \geqslant \frac{\pi^p L^{1-p}}{\sin^p\frac{\pi u}{L}}, \quad p>0. \tag{4.2}$$

They have also a discrete counterpart for an equilateral polygon $\mathcal{P}_N$ of N vertices and side length $l>0$. Let $\{y_n\}$ be the family of its vertices, where the index values are identified modulo N; then we introduce

$$D_{N,l}^p(m)\colon \sum_{n=1}^N |y_{n+m}-y_n|^p \leqslant \frac{Nl^p \sin^p\frac{\pi m}{N}}{\sin^p\frac{\pi}{N}}, \quad p>0, \tag{4.3}$$

$$D_{N,l}^{-p}(m)\colon \sum_{n=1}^N |y_{n+m}-y_n|^{-p} \geqslant \frac{N\sin^p\frac{\pi}{N}}{l^p \sin^p\frac{\pi m}{N}}, \quad p>0, \tag{4.4}$$

for any $m=1,\ldots,\lfloor \frac{1}{2}N \rfloor$, where $[\cdot]$ denotes as usual the entire part.

In all the cases the right-hand side corresponds, of course, to the case with maximal symmetry, i.e., to the circle and regular polygon $\widetilde{\mathcal{P}}_N$, respectively. *We conjecture* that without regularity

restrictions $C_L^{\pm p}(u)$ *holds for any* $p \leq 2$ *and the same is true for* $D_{N,l}^{\pm p}(m)$, and furthermore, we expect the inequalities *to be sharp unless* $\Gamma = \mathcal{C}$ *or* $\mathcal{P}_N = \widetilde{\mathcal{P}}_N$, *respectively*. In the polygon case it is clear that the claim may not be true for $p > 2$ as the example of a rhomboid shows: $D_{4,l}^p(2)$ is equivalent to $\sin^p \phi + \cos^p \phi \leq 2^{1-p/2}$ for $0 < \phi < \pi$. We are unable at this moment to demonstrate the inequalities (4.1)–(4.4) in full generality; below we will present a few particular cases.

It is obvious that the inequalities have a scaling property, so without loss of generality one can assume, e.g., $L = 1$ and $l = 1$; in such a case we drop the corresponding symbol from the label. If necessary we can include also the case $p = 0$ when the inequalities turn into trivial identities.

Proposition 4.1: $C_L^p(u) \Rightarrow C_L^{p'}(u)$ *and* $D_{N,l}^p(m) \Rightarrow D_{N,l}^{p'}(m)$ *if* $p > p' > 0$.

Proof: The claim follows from the convexity of $x \mapsto x^\alpha$ in $(0, \infty)$ for $\alpha > 1$,

$$\frac{L^{1+p}}{\pi^p} \sin^p \frac{\pi u}{L} \geq \int_0^L (|\Gamma(s+u) - \Gamma(s)|^{p'})^{p/p'} \, \mathrm{d}s \geq L \left(\frac{1}{L} \int_0^L |\Gamma(s+u) - \Gamma(s)|^{p'} \, \mathrm{d}s \right)^{p/p'}.$$

It is now sufficient to take both sides to the power p'/p; in the same way one checks the second implication. ∎

Proposition 4.2: $C_L^p(u) \Rightarrow C_L^{-p}(u)$ *and* $D_{N,l}^p(m) \Rightarrow D_{N,l}^{-p}(m)$ *for any* $p > 0$.

Proof: The Schwarz inequality implies

$$\int_0^L |\Gamma(s+u) - \Gamma(s)|^{-p} \, \mathrm{d}s \geq \frac{L^2}{\int_0^L |\Gamma(s+u) - \Gamma(s)|^p \, \mathrm{d}s} \geq \frac{L^2 \pi^p}{L^{1+p} \sin^p \frac{\pi u}{L}},$$

and similarly for the polygon case. ∎

These simple relations mean that to check the above stated conjecture one needs only to verify $C^2(u)$ and $D_N^2(m)$. We will address the continuous case in the next section; here we notice that the results of Ref. 7 in combination with the last two propositions leads to the following conclusions.

Theorem 4.3: *(a)* $D_{N,l}^1(m)$ *holds locally for any* N *and* $m = 1, \ldots, \lceil \frac{1}{2} N \rceil$, *i.e., in a vicinity of the regular polygon, and, consequently,* $D_{N,l}^{\pm p}(m)$ *holds locally for any* $p \in (0, 1]$.

(b) $D_{N,l}^1(2)$ *holds globally for any* N, *and so does* $D_{N,l}^{\pm p}(2)$ *for each* $p \in (0, 1]$.

V. PROOF OF THEOREM 2.1

After this interlude let us return to our main problem. Notice first that our regularity hypothesis allows us to characterize Γ by its (signed) curvature $\gamma := \dot{\Gamma}_2 \ddot{\Gamma}_1 - \dot{\Gamma}_1 \ddot{\Gamma}_2$ which is by assumption a piecewise continuous function in $[0, L]$. The advantage is that γ specifies uniquely the equivalence class related by Euclidean transformations which can be represented by

$$\Gamma(s) = \left(\int_0^s \cos \beta(s') \mathrm{d}s', \int_0^s \sin \beta(s') \mathrm{d}s' \right), \tag{5.1}$$

where $\beta(s) := \int_0^s \gamma(s') \mathrm{d}s'$ is the bending angle relative to the tangent at the chosen initial point, $s = 0$. To ensure that the curve is closed, the conditions

$$\int_0^L \cos \beta(s') \mathrm{d}s' = \int_0^L \sin \beta(s') \mathrm{d}s' = 0, \tag{5.2}$$

must be satisfied. Using this parametrization we can rewrite the left-hand side of the inequality (4.1) in the form

$$\int_0^L \left[\left(\int_s^{s+u} \cos \beta(s') \mathrm{d}s' \right)^2 + \left(\int_s^{s+u} \sin \beta(s') \mathrm{d}s' \right)^2 \right]^{p/2} \mathrm{d}s := c_\Gamma^p(u),$$

or, equivalently,

$$c_\Gamma^p(u) = \int_0^L \mathrm{d}s \left[\int_s^{s+u} \mathrm{d}s' \int_s^{s+u} \mathrm{d}s'' \cos(\beta(s') - \beta(s'')) \right]^{p/2}.$$

By Proposition (4.1) it is sufficient to check that the quantity $c_\Gamma^2(u)$ is maximized by the circle, i.e., by $\beta(s) = 2\pi s/L$. Rearranging the integrals we get

$$\begin{aligned} c_\Gamma^2(u) &= \int_0^L \mathrm{d}s' \int_{s'-u}^{s'+u} \mathrm{d}s'' \int_{\max\{s'-u, s''-u\}}^{\min\{s', s''\}} \mathrm{d}s \cos(\beta(s') - \beta(s'')) \\ &= \int_0^L \mathrm{d}s' \int_{s'-u}^{s'+u} \mathrm{d}s''[\min\{s', s''\} - \max\{s' - u, s'' - u\}]\cos(\beta(s') - \beta(s'')), \end{aligned}$$

or

$$c_\Gamma^2(u) = \int_0^L \mathrm{d}s' \int_{s'-u}^{s'+u} \mathrm{d}s''[u - |s' - s''|]\cos(\beta(s') - \beta(s'')).$$

Next, we change the integration variables to $x := s' - s''$ and $z := \frac{1}{2}(s' + s'')$,

$$c_\Gamma^2(u) = \int_{-u}^{u} \mathrm{d}x(u - |x|) \int_0^L \mathrm{d}z \cos\left(\beta\left(z + \frac{1}{2}x \right) - \beta\left(z - \frac{1}{2}x \right) \right),$$

and since the functions involved are even w.r.t. x we finally get

$$c_\Gamma^2(u) = 2\int_0^u \mathrm{d}x(u - x) \int_0^L \mathrm{d}z \cos\left(\int_{z-1/2x}^{z+1/2x} \gamma(s)\mathrm{d}s \right). \tag{5.3}$$

As a certain analogy to Theorem 4.3b we can prove the sought global inequality in the case when the curve arcs in question are sufficiently short and/or the tangent vector direction does change too fast.

Proposition 5.1: Suppose that Γ *has no self-intersections and the inequality* $\beta(z + \frac{1}{2}u) - \beta(z - \frac{1}{2}u) \leqslant \frac{1}{2}\pi$ *is valid for all* $z \in [0, L]$, *then* $C_L^2(u)$ *holds.*

Proof: We employ concavity of cosine in $(0, \frac{1}{2}\pi)$ obtaining

$$\begin{aligned} c_\Gamma^2(u) &\leqslant 2L \int_0^u \mathrm{d}x(u - x)\cos\left(\frac{1}{L}\int_0^L \mathrm{d}z \int_{z-(1/2)x}^{z+(1/2)x} \gamma(s)\mathrm{d}s \right) \\ &= 2L \int_0^u \mathrm{d}x(u - x)\cos\left(\frac{1}{L}\int_0^L \mathrm{d}s\gamma(s) \int_{s-(1/2)x}^{s+(1/2)x} \mathrm{d}z \right) \\ &= 2L \int_0^u \mathrm{d}x(u - x)\cos\frac{2\pi x}{L} = \frac{L^3}{\pi^2}\sin^2\frac{\pi u}{L}, \end{aligned}$$

since $\int_0^L \gamma(s)\mathrm{d}s = \pm 2\pi$ for a curve without self-intersections. Moreover, the function $z \mapsto \int_{z-(1/2)x}^{z+(1/2)x} \gamma(s)\mathrm{d}s$ is constant for $x \in (0, u)$ *iff* $\gamma(\cdot)$ is constant; hence the circle corresponds to a sharp maximum. ■

This result, however, does not help us with our main problem, because we need the inequality to be valid for all arclengths. As indicated before, we can prove a local result which will imply Theorem 2.1.

Theorem 5.2: *Under the regularity assumptions of Sec. III, the inequality* $C_L^2(u)$ *holds locally for any* $L > 0$ *and* $u \in (0, \frac{1}{2}L]$, *and, consequently,* $C_L^{\pm p}(u)$ *holds locally for any* $p \in (0, 2]$.

Proof: Gentle deformations of a circle can be characterized by the curvature

$$\gamma(s) = \frac{2\pi}{L} + g(s),$$

where g is a piecewise continuous functions which is small in the sense that $\|g\|_\infty \ll L^{-1}$ and satisfies the condition $\int_0^L g(s)\mathrm{d}s = 0$. The function in the last integral of (5.3) can be then expanded as

$$\cos\frac{2\pi x}{L} - \sin\frac{2\pi x}{L}\int_{z-(1/2)x}^{z+(1/2)x} g(s)\mathrm{d}s - \frac{1}{2}\cos\frac{2\pi x}{L}\left(\int_{z-(1/2)x}^{z+(1/2)x} g(s)\mathrm{d}s\right)^2 + \mathcal{O}(g^3),$$

where the error term is a shorthand for $\mathcal{O}(\|Lg\|_\infty^3)$. Substituting this expansion into (5.3) we find that the term linear in g vanishes, because

$$\int_0^L \mathrm{d}z \int_{z-(1/2)x}^{z+(1/2)x} g(s)\mathrm{d}s = \int_0^L \mathrm{d}s\, g(s)\int_{s-(1/2)x}^{s+(1/2)x} \mathrm{d}z = 0,$$

and thus

$$c_\Gamma^2(u) = \frac{L^3}{\pi^2}\sin^2\frac{\pi u}{L} - I_g(u) + \mathcal{O}(g^3), \tag{5.4}$$

where

$$I_g(u) := \int_0^u \mathrm{d}x(u-x)\cos\frac{2\pi x}{L}\int_0^L \mathrm{d}z\left(\int_{z-(1/2)x}^{z+(1/2)x} g(s)\mathrm{d}s\right)^2.$$

We need to show that $I_g(u) > 0$ unless $g = 0$ identically. Notice that for $u \leqslant \frac{1}{4}L$ this property holds trivially. For $u \in (\frac{1}{4}L, \frac{1}{2}L]$ we use the fact that g is periodic and piecewise continuous, so we can write it through its Fourier series,

$$g(s) = \sum_{n=1}^{\infty}\left(a_n \sin\frac{2\pi n s}{L} + b_n\cos\frac{2\pi n s}{L}\right),$$

with the zero term missing, where $\Sigma_n(a_n^2 + b_n^2)$ is finite (and small). Using

$$\int_{z-(1/2)x}^{z+(1/2)x} g(s)\mathrm{d}s = \frac{L}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\left(a_n\sin\frac{2\pi n z}{L} + b_n\cos\frac{2\pi n z}{L}\right)\sin\frac{\pi n x}{L},$$

together with the orthogonality of the Fourier basis we find

$$I_g(u) = \int_0^u \mathrm{d}x(u-x)\cos\frac{2\pi x}{L}\sum_{n=1}^{\infty}\frac{L^3}{2\pi^2}\frac{a_n^2+b_n^2}{n^2}\sin\frac{\pi n x}{L}.$$

Since the summation and integration can be obviously interchanged, we have

$$I_g(u) = \frac{L^5}{2\pi^4}\sum_{n=1}^{\infty}\frac{a_n^2+b_n^2}{n^2}F_n\left(\frac{\pi u}{L}\right), \tag{5.5}$$

where

$$F_n(v) := \int_0^v (v-y)\cos 2y \sin ny\,\mathrm{d}y.$$

These integrals are equal to

$$F_1(v) = \frac{1}{18}(9\sin v - \sin 3v - 6v),$$

$$F_2(v) = \frac{1}{32}(4v - \sin 4v),$$

$$F_n(v) = \frac{nv}{n^2-4} - \frac{\sin(n-2)v}{2(n-2)^2} - \frac{\sin(n+2)v}{2(n+2)^2}, \quad n \geqslant 3.$$

Using the fact that $\sin x < x$ for $x > 0$ we see immediately that $F_n(v) > 0$ for $v > 0$ and $n \geqslant 2$. On the other hand, $F_1(v)$ has in the interval $(0, \pi/2)$ a single positive maximum, at some $v > \pi/4$, from which it decreases to the value $F_1(\pi/2) = \frac{1}{18}(10-3\pi) > 0$. Summing up this argument, we have found that the quantity (5.5) is positive unless all the coefficients a_n, b_n are zero. ■

Remark 5.3: One may wonder what happened with the closedness requirement (5.2). As the argument shows we were able to demonstrate the claim using only the weaker property that $\beta(0) = \beta(L)$. This is possible, of course, for small deformations only! As an illustration, consider Γ in the form of an "overgrown paperclip" which satisfies the condition $\beta(0) = \beta(L)$ but not (5.2), i.e., a line segment with two U turns at the ends. Making the latter short one can get $c_\Gamma^2(\frac{1}{2}L)$ arbitrarily close to $\frac{1}{3}L^3$ which is larger than L^3/π^2.

VI. EXTENSIONS AND CONCLUSIONS

To support our expectations that the result given in Theorem 2.1 holds globally and under weaker regularity assumptions, consider a simple example.

Example 6.1: Let Γ be a curve consisting of two circular segments of radius $R > L/4\pi$, i.e., it is given by the equations

$$\left(x \pm R\cos\frac{L}{2R}\right)^2 + y^2 = R^2, \quad \text{for } \pm x \geqslant 0. \tag{6.1}$$

For $R > L/2\pi$ it is "lens shaped," for $L/4\pi < R < L/2\pi$ "apple shaped;" it is not smooth except in the trivial case of a circle, $R = L/2\pi$. The curvature of this Γ equals

$$\gamma(s) = \frac{1}{R} + \left(\pi - \frac{L}{2R}\right)(\delta(s) + \delta(s - L/2));$$

hence

$$c_\Gamma^2(u) = 2\int_0^u \mathrm{d}x(u-x)\left[(L-2x)\cos\frac{x}{R} - 2x\cos\frac{L-2x}{2R}\right]\mathrm{d}x,$$

and evaluating the integral, we arrive at

$$c_\Gamma^2(u) = 8R^3\left\{\frac{L}{2R}\sin^2\frac{u}{2R} + 4\left(\frac{u}{2R}\cos\frac{u}{2R} - \sin\frac{u}{2R}\right)\cos\frac{L}{4R}\cos\frac{L-2u}{4R}\right\}.$$

This function has for each $u \in (0, \frac{1}{2}L]$ a maximum at $R = L/2\pi$ and one can check directly that its value is smaller for any other R. In particular, in the limit $R \to \infty$ we have $c_\Gamma^2(u) \to Lu^2 - \frac{4}{3}u^3$ as one can find also directly with the "lens" degenerate into a double line segment; this value is less than $(L^3/\pi^2)\sin^2(\pi u/L)$ because $\sin^2 x > x^2 - (4/3\pi)x^3$ holds in $(0, \pi/2)$.

To summarize our discussion, to prove Conjecture 2.2 it is sufficient to verify the inequality $C_L^p(u)$ for some $p \geqslant 1$ under appropriate regularity hypothesis. Naturally, one can ask also about the ground-state maximizer in smaller families of curves Γ which do not contain the circle; examples could be polygonal loops with a fixed or limited number of vertices, or various pre-

scribed compositions of arcs belonging to specific classes, circular, elliptic, parabolic, etc. Obviously a reasonable strategy is to look first for curves as close to the circle as possible within the given class. Sometimes one expects that the answer will be the curve with maximum symmetry as in the polygon case, in other situations it may not be true.

Another, and maybe more important extension of the present problem concerns a maximizer for the generalized Schrödinger operator in $\mathbb{R}^3$ with an attractive δ interaction supported by a closed surface of a fixed area A, and its generalization to closed hypersurfaces of codimension one in $\mathbb{R}^d$, $d>3$. In the case of $d=3$ we have a heuristic argument relying on Refs. 6 and 8 similar to that used in the Introduction, which suggests that the problem is solved by the sphere, provided the discrete spectrum is not empty, of course, which is a nontrivial assumption in this case—for properties of the corresponding operators, see Ref. 2. The Birman–Schwinger reduction of the problem similar to that of Sec. III can be performed again and the task is thus reduced to verification of a geometric inequality analogous to (4.1) which we can label as $C_A^{d,p}(u)$. We will discuss this problem in a following paper.

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Operational distance and fidelity for quantum channels

Viacheslav P. Belavkin[a)]
Department of Mathematics, University of Nottingham, NG7 2RD Nottingham, United Kingdom

Giacomo Mauro D'Ariano[b)]
QUIT Group, INFM Unità di Pavia, Università di Pavia, Dipartimento di Fisica "A. Volta," via Bassi 6, I-27100 Pavia, Italy and Center for Photonic Communication and Computing, Department of Electrical and Computer Engineering, Northwestern University, Evanston, Illinois 60208-3118

Maxim Raginsky[c)]
Center for Photonic Communication and Computing, Department of Electrical and Computer Engineering, Northwestern University, Evanston, Illinois 60208-3118

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We define and study a fidelity criterion for quantum channels, which we term the *minimax fidelity*, through a noncommutative generalization of maximal Hellinger distance between two positive kernels in classical probability theory. Like other known fidelities for quantum channels, the minimax fidelity is well defined for channels between finite-dimensional algebras, but it also applies to a certain class of channels between infinite-dimensional algebras (explicitly, those channels that possess an operator-valued Radon-Nikodym density with respect to the trace in the sense of Belavkin-Staszewski) and induces a metric on the set of quantum channels that is topologically equivalent to the CB-norm distance between channels, precisely in the same way as the Bures metric on the density operators associated with statistical states of quantum-mechanical systems, derived from the well-known fidelity ("generalized transition probability") of Uhlmann, is topologically equivalent to the trace-norm distance. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Many problems in quantum information science,[1,2] both in theory and in experiment, involve finding a set of quantum-mechanical states or channels that solve some sort of an optimization problem, typically formulated in terms of a numerical criterion that measures how close a given pair of states or operations are to each other. (Many such criteria have been proposed to date, each defined with specific theoretical or experimental considerations in mind; see Ref. 3 for a recent comprehensive survey.)

Let us first consider the case of quantum states, i.e., density operators. Let $\mathfrak{h}$ be a complex separable Hilbert space associated to a quantum-mechanical system. Given a pair of density operators ρ,σ, i.e., positive trace-class operators with unit trace, one can use either the *fidelity*[4–7]

$$F(\rho,\sigma) := \mathrm{Tr}[(\rho^{1/2}\sigma\rho^{1/2})^{1/2}] \tag{1}$$

or the *trace-norm (half-) distance*

[a)]E-mail address: vpb@maths.nott.ac.uk
[b)]Author to whom correspondence should be addressed. E-mail address: dariano@unipv.it
[c)]E-mail address: maxim@ece.northwestern.edu

$$D(\rho,\sigma) := \tfrac{1}{2}\|\rho-\sigma\|_{\mathrm{T}}, \tag{2}$$

where $\|\rho\|_{\mathrm{T}} := \mathrm{Tr}|\rho|$ and $|\rho| := (\rho^{\dagger}\rho)^{1/2}$.[8,9] Loosely speaking, two states ρ and σ are close to each other if $F(\rho,\sigma)$ is large, or if $D(\rho,\sigma)$ is small. In fact, as follows from the key inequality[5,10]

$$1-F(\rho,\sigma) \leqslant D(\rho,\sigma) \leqslant \sqrt{1-F^2(\rho,\sigma)}, \tag{3}$$

the fidelity and the trace-norm distance are equivalent in the sense that any two density operators that are close to one another in the sense of (1) are also close in the sense of (2), and vice versa.

As for *quantum channels*, i.e., normal completely positive unital mappings from an operator algebra $\mathcal{B}=\mathcal{B}(\mathfrak{h})$ into another algebra $\mathcal{A}=\mathcal{B}(\mathfrak{g})$, where $\mathfrak{g}$ and $\mathfrak{h}$ are complex separable Hilbert spaces, things get somewhat complicated. Consider, for instance, the case when $\mathfrak{g}$ is finite-dimensional, and let $m := \dim \mathfrak{g}$. Fix an orthonormal basis $\{|j\rangle\}_{j=1}^{m}$ of $\mathfrak{g}$, and let $|\psi\rangle := m^{-1/2}\Sigma_{j=1}^{m}|j\rangle \otimes |j\rangle$ be the normalized maximally entangled vector in the product space $\mathfrak{g}\otimes\mathfrak{g}$. Given two quantum channels $\Phi,\Psi:\mathcal{B}\to\mathcal{A}$, one can measure their closeness in terms of the fidelity of the states on $\mathcal{B}\otimes\mathcal{A}$, obtained from the maximally entangled state $\pi=|\psi\rangle\langle\psi|$ by applying the predual channels Φ_{T} and Ψ_{T} (cf. Sec. II for precise definitions) to the first factor in the tensor product:

$$\Phi_{\mathrm{T}}\otimes\mathrm{id}(\pi) = \frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{m}\Phi_{\mathrm{T}}(|i\rangle\langle k|)\otimes|i\rangle\langle k| \equiv \rho,$$

$$\Psi_{\mathrm{T}}\otimes\mathrm{id}(\pi) = \frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{m}\Psi_{\mathrm{T}}(|i\rangle\langle k|)\otimes|i\rangle\langle k| \equiv \sigma.$$

The fidelity $F(\rho,\sigma)$, taken as the *channel fidelity*

$$\mathcal{F}(\Phi,\Psi) := F(\Phi_{\mathrm{T}}\otimes\mathrm{id}(\pi),\quad \Psi_{\mathrm{T}}\otimes\mathrm{id}(\pi)), \tag{4}$$

by Raginsky in Ref. 11, enjoys many properties parallel to those of the fidelity (1) for quantum states. Alternatively, one can adopt the (half-) distance[1,12,13]

$$\mathcal{D}(\Phi,\Psi) := \tfrac{1}{2}\|\Phi-\Psi\|_{\mathrm{CB}}, \tag{5}$$

where $\|\cdot\|_{\mathrm{CB}}$ denotes the so-called *norm of complete boundedness* (or CB-norm for short; cf. Sec. II C for details). We note that the CB-norm half-distance (5) can be given in terms of the trace-norm distance (2) between density operators by means of the variational expression[1,12,13]

$$\mathcal{D}(\Phi,\Psi) = \sup_{\pi} D(\Phi_{\mathrm{T}}\otimes\mathrm{id}(\pi),\quad \Psi_{\mathrm{T}}\otimes\mathrm{id}(\pi)), \tag{6}$$

where the supremum is taken over all density operators π on the tensor product space $\mathfrak{g}\otimes\mathfrak{g}$. By analogy with density operators of the states, we are tempted to say that two quantum channels, Φ and Ψ, are close either if $\mathcal{F}(\Phi,\Psi)$ is large or if $\mathcal{D}(\Phi,\Psi)$ is small. However, in addition to the finite-dimension restriction $\dim\mathfrak{g}<\infty$ [the only case under which the definition (4) of the channel fidelity makes sense], we encounter the following difficulty. It turns out[11] that, as a criterion of closeness, the CB-norm distance (5) is strictly stronger than the fidelity measure (4) in the sense that even when $\mathcal{D}(\Phi,\Psi)$ is large, $\mathcal{F}(\Phi,\Psi)$ may be quite large as well, and may even become equal to one in the limit $\dim\mathfrak{g}\to\infty$. Consider, for instance, the case $\Psi=\mathrm{id}$. Then one can show[11] that

$$1-\mathcal{D}(\Phi,\mathrm{id}) \leqslant \mathcal{F}(\Phi,\mathrm{id}) \leqslant \sqrt{1-(1/4)\mathcal{D}^2(\Phi,\mathrm{id})}, \tag{7}$$

and we immediately see that when Φ is such that $\mathcal{D}(\Phi,\mathrm{id})$ attains its maximum value of unity, the fidelity $\mathcal{F}(\Phi,\mathrm{id})$ is still bounded between 0 and $\sqrt{3}/2$. To make matters worse, the only bound on (5) in terms of (4) known so far is

$$1 \geqslant \mathcal{D}(\Phi,\Psi) \geqslant 1 - \mathcal{F}(\Phi,\Psi), \tag{8}$$

as follows readily from Eqs. (3) and (6). Furthermore, one can easily find sequences $\{\Phi_m\}$, $\{\Psi_m\}$ of channels $\Phi_m,\Psi_m:\mathcal{B}(\mathbb{C}^m)\to\mathcal{B}(\mathbb{C}^m)$, such that $\mathcal{D}(\Phi_m,\Psi_m)\neq 0$ for all m, while

$$\lim_{m\to\infty} \mathcal{F}(\Phi_m,\Psi_m) = 1.$$

Indeed, consider the unitarily implemented channels

$$\Phi_m(B) = U_m^\dagger B U_m, \quad \Psi(B) = V_m^\dagger B V_m$$

with the unitaries U_m, V_m chosen in such a way that $U_m \neq V_m$ but

$$\lim_{m\to\infty} \frac{1}{m} \mathrm{Tr}(U_m^\dagger V_m) = 1.$$

Thus, the channel fidelity (4), apart from being applicable only in finite-dimensional settings, has the distinct disadvantage of not being equivalent to the CB-norm distance, in contrast to the case of the Uhlmann fidelity (1) and the trace-norm distance (2) on the state space of a quantum-mechanical system.

The goal of this paper is to define and study a new fidelity criterion for quantum channels, which we term the *minimax fidelity* and which is a noncommutative generalization of maximal Hellinger distance between two positive kernels in classical probability theory. Unlike the channel fidelity (4) of Ref. 11, the minimax fidelity is not only well defined for channels between finite-dimensional algebras, but also applies to a certain class of channels between infinite-dimensional algebras (explicitly, those channels that possess an operator-valued Radon-Nikodym density with respect to the trace in the sense of Belavkin-Staszewski[14]) and is equivalent to the CB-norm distance, echoing the way the Uhlmann fidelity (1) for density operators is equivalent to the trace-norm distance (2).

Apart from these technical features, the minimax fidelity $f(\Phi,\Psi)$ between two quantum channels Φ,Ψ has a direct *operational* meaning: intuitively, it is defined as the minimum overlap of output states (density operators) of the predual channels $\Phi_\mathsf{T},\Psi_\mathsf{T}$, when the operator-sum decompositions[2] of the latter are chosen to be maximally overlapping; this is spelled out in precise terms in Sec. IV E. Our central result (Theorem 1) demonstrates that the minimax fidelity is independent of the order of these two optimizations. Furthermore, the equivalence of our minimax fidelity to the CB-norm distance, which is stated precisely in Sec. V in terms of *dimension-free* bounds, is a promising avenue for the study and characterization of dimension-free bounds (whenever they exist) on other operationally meaningful distance measures for quantum operations[3] in terms of the CB-norm distance. As pointed out in Ref. 15, such bounds are crucial for a successful generalization of the usual quantum capacity of a channel[1,2] (i.e., with respect to the identity channel) to the case of comparing quantum channels to an arbitrary reference channel. We plan to pursue these matters further in a future publication.

The paper is organized as follows. In Sec. II we fix the definitions and notation used throughout the paper. The minimax fidelity is then introduced in Sec. III. Section IV is devoted to the evaluation of the minimax fidelities in the various mathematical settings that arise in quantum information theory. Next, in Sec. V, we list key properties of the minimax fidelity. Finally, in Sec. VI we sketch some example applications of the minimax fidelity to several problems of quantum information theory.

II. PRELIMINARIES, DEFINITIONS, NOTATION

A. Pairings, states, operations

Let $\mathfrak{h}$ be a complex separable Hilbert space; let $\mathcal{B}$ denote the Banach algebra $\mathcal{B}(\mathfrak{h})$ of all bounded linear operators on $\mathfrak{h}$ with the usual operator norm $\|\cdot\|$; and let $\mathcal{B}_\mathsf{T}$ denote the Banach space $\mathcal{B}_\mathsf{T}(\mathfrak{h})$ of trace-class operators on $\mathfrak{h}$ with the trace norm $\|\cdot\|_\mathsf{T}$. The set of normal states on $\mathcal{B}$,

i.e., ultraweakly continuous positive unital linear functionals on $\mathcal{B}$, will be denoted by $\mathcal{S}(\mathcal{B})$ or, whenever we need to exhibit the underlying Hilbert space explicitly, by $\mathcal{S}(\mathfrak{h})$. Generic elements of $\mathcal{S}(\mathcal{B})$ will be denoted by the stylized Greek letters $\varpi, \varrho, \varsigma$. Note that the operator norm on $\mathcal{B}$ can be written as $\|B\| = \sup\{\varrho(|B|) : \varrho \in \mathcal{S}(\mathcal{B})\}$.

We equip $\mathfrak{h}$ (and shall equip all Hilbert spaces introduced in the sequel) with an isometric involution $J = J^\dagger$, $J^2 = \mathbb{1}_\mathfrak{h}$, having the properties of complex conjugation,

$$J\sum_j \lambda_j \eta_j = \sum_j \overline{\lambda_j} J\eta_j, \quad \forall\, \lambda_j \in \mathbb{C},\ \eta_j \in \mathfrak{h}.$$

We can thus define the *transpose* of any $B \in \mathcal{B}$ as $\widetilde{B} := JB^\dagger J$, as well as introduce the trace pairing[16]

$$(B, \rho) := \mathrm{Tr}(B\widetilde{\rho}) = \mathrm{Tr}(\widetilde{B}\rho), \quad \forall\, B \in \mathcal{B},\ \rho \in \mathcal{B}_\mathsf{T} \tag{9}$$

of $\mathcal{B}$ and $\mathcal{B}_\mathsf{T}$. Under this pairing, which differs from the usual one in that $B \in \mathcal{B}$ is paired with the transpose of $\rho \in \mathcal{B}_\mathsf{T}$ rather than directly with ρ, normal linear functionals on $\mathcal{B}$ are in a one-to-one correspondence with the elements of $\mathcal{B}_\mathsf{T}$. Thus to each normal state ϱ we associate a unique positive trace-class operator with unit trace, denoted by the standard Greek letter ρ and referred to as the *density operator* corresponding to ϱ, via $\varrho(B) = (B, \rho)$ for all $B \in \mathcal{B}$. Similarly, density operators corresponding to states denoted by ϖ and ς will be denoted by π and σ, respectively.

Apart from natural arguments from standard representation theory of operator algebras, one reason why we chose to pair B with the transposed operator $\widetilde{\rho} = J\rho^\dagger J$, rather than with ρ, is to be able to keep all notations conveniently parallel to the classical (commutative) case, as will be amply demonstrated throughout the paper. Note also that we can fix a complete orthonormal basis $\{|j\rangle\}$ of $\mathfrak{h}$ and express the pairing (9) in terms of the matrix elements of B and ρ as

$$(B, \rho) = \sum_{j,k} \langle j|B|k\rangle \cdot \langle j|\rho|k\rangle \equiv \sum_{j,k} B_{jk}\rho^{jk},$$

where we have used the covariant indices for the matrix elements of bounded operators in $\mathcal{B}$ and the contravariant indices for the matrix elements of trace-class operators in $\mathcal{B}_\mathsf{T}$, when the latter are identified via the pairing (9) with normal linear functionals on $\mathcal{B}$. Yet another reason to opt for the pairing of B with the transposed operator $\widetilde{\rho}$, further elaborated upon in Sec. II B, is that then the density operator ρ of a normal state ϱ will coincide with the operational density of ϱ, understood as a quantum operation from $\mathcal{B}$ into the Abelian algebra $\mathbb{C}$.

Introducing another Hilbert space $\mathfrak{g}$, the algebra $\mathcal{A} := \mathcal{B}(\mathfrak{g})$, and the trace class $\mathcal{A}_\mathsf{T} := \mathcal{B}_\mathsf{T}(\mathfrak{g})$, let us consider *quantum operations*, i.e., the completely positive normal linear mappings $\Phi : \mathcal{B} \to \mathcal{A}$ such that $\Phi(\mathbb{1}_\mathfrak{h}) \leqslant \mathbb{1}_\mathfrak{g}$; if $\Phi(\mathbb{1}_\mathfrak{h}) = \mathbb{1}_\mathfrak{g}$, then Φ is referred to as a *quantum channel*. Any quantum operation Φ possesses a unique *predual* $\Phi_\mathsf{T} : \mathcal{A}_\mathsf{T} \to \mathcal{B}_\mathsf{T}$, defined as the transpose of Φ with respect to the trace pairing (9), i.e.,

$$(\Phi(B), \rho) = (B, \Phi_\mathsf{T}(\rho)), \quad \forall\, B \in \mathcal{B},\ \rho \in \mathcal{A}_\mathsf{T}. \tag{10}$$

Conversely, given a normal completely positive linear map $\Phi : \mathcal{A}_\mathsf{T} \to \mathcal{B}_\mathsf{T}$ such that $\mathrm{Tr}_\mathfrak{h}\Phi(\rho) \leqslant \mathrm{Tr}_\mathfrak{g}\rho$ for all $\rho \in \mathcal{A}_\mathsf{T}$, we define its *dual* with respect to the trace pairing (9) as the unique mapping $\Phi^\mathsf{T} : \mathcal{B} \to \mathcal{A}$ for which

$$(B, \Phi(\rho)) = (\Phi^\mathsf{T}(B),\ \rho), \quad \forall\, B \in \mathcal{B}, \rho \in \mathcal{A}_\mathsf{T}. \tag{11}$$

Using these definitions, one readily obtains that $\Phi_\mathsf{T}^\mathsf{T} = \Phi$ for any normal completely positive map $\Phi : \mathcal{B} \to \mathcal{A}$. Alternatively, one may define the predual of a normal completely positive map $\Phi : \mathcal{B} \to \mathcal{A}$ as the unique normal completely positive map $\Phi_\mathsf{T} : \mathcal{A}_\mathsf{T} \to \mathcal{B}_\mathsf{T}$ such that $\Phi_\mathsf{T}^\mathsf{T} = \Phi$.

If Φ is given in the Kraus form[17] $\Phi(B) = \Sigma F_j^\dagger B F_j$, or more generally as an integral

$$\Phi(B) = \int_Z F(z)^\dagger B F(z) \mathrm{d}\mu(z), \tag{12}$$

with respect to a positive measure μ on a measurable space $(Z, \mathcal{B}_Z)$, where the integration is understood in the sense of Bochner,[18] then the predual map Φ_T has the transposed integral form

$$\Phi_\mathsf{T}(\rho) = \int_Z F_\mathsf{T}(z)^\dagger \rho F_\mathsf{T}(z) \mathrm{d}\mu(z),$$

where $\mathfrak{g} \ni \xi \mapsto \langle \xi | F_\mathsf{T}(z)$ are Hilbert-transposed to the operators $\mathfrak{h} \ni \eta \mapsto \langle \eta | F(z)$, that is $F_\mathsf{T}(z) = \widetilde{F(z)}$ for all $z \in Z$.

Any normal state $\varrho \in \mathcal{S}(\mathcal{B})$ is automatically a quantum channel from $\mathcal{B}$ into the Abelian algebra $\mathbb{C}$, and it is readily seen that the density operator ρ of ϱ, understood as acting on $\lambda \in \mathbb{C}$ on the right, $\mathbb{C} \ni \lambda \mapsto \lambda\rho$, is precisely the predual $\varrho_\mathsf{T}: \mathbb{C} \to \mathcal{B}_\mathsf{T}$. Indeed, given $B \in \mathcal{B}$ and $\lambda \in \mathbb{C}$, we have

$$(\varrho(B), \lambda) = (B, \lambda\rho) = (B, \varrho_\mathsf{T}(\lambda)),$$

which proves our claim that $\rho = \varrho_\mathsf{T}$. Thus we also have that $\varrho = \varrho_\mathsf{T}^\mathsf{T} = \rho^\mathsf{T}$.

B. Operational densities

In order to avoid technicalities involving unbounded operators, we shall henceforth assume that all quantum operations we deal with are *completely majorized* by the trace, considered as the map $\tau(\sigma) = \mathbb{1}_\mathfrak{g} \mathrm{Tr}\, \sigma$ of $\mathcal{B}_\mathsf{T}$ into $\mathcal{A} = \mathcal{B}(\mathfrak{g})$, in the sense[14] that there exists a constant $\lambda > 0$ such that the difference $\lambda\tau - \Phi$ is a completely positive map $\mathcal{B}_\mathsf{T} \to \mathcal{A}$. For example, this condition is satisfied by all quantum operations between finite-dimensional algebras.[19] As was proven in Ref. 14, in this case there exists a unique positive operator Φ_τ on the Hilbert space $\mathcal{H} := \mathfrak{g} \otimes \mathfrak{h}$, called the *density* of Φ with respect to the trace τ, such that

$$\Phi(B) = \mathrm{Tr}_\mathfrak{h}[(\mathbb{1}_\mathfrak{g} \otimes \widetilde{B})\Phi_\tau], \tag{13}$$

where $\mathrm{Tr}_\mathfrak{h}\, Y$, $Y \in \mathcal{B}(\mathcal{H})$, denotes the partial trace of Y with respect to $\mathfrak{h}$,

$$(\mathrm{Tr}_\mathfrak{h} Y, \rho) = (Y, \rho \otimes \mathbb{1}_\mathfrak{h}), \quad \forall\, \rho \in \mathcal{B}_\mathsf{T}(\mathfrak{g}).$$

Moreover, Φ_τ as a linear operator on $\mathcal{H}$ is bounded and majorized by $\lambda: 0 \leqslant \Phi_\tau \leqslant \lambda \mathbb{1}_\mathcal{H}$, and the operation is unital, $\Phi(\mathbb{1}_\mathfrak{h}) = \mathbb{1}_\mathfrak{g}$ [contractive, $\Phi(\mathbb{1}_\mathfrak{h}) \leqslant \mathbb{1}_\mathfrak{g}$] if and only if $\mathrm{Tr}_\mathfrak{h}\, \Phi_\tau = \mathbb{1}_\mathfrak{g}$ ($\mathrm{Tr}_\mathfrak{h}\, \Phi_\tau \leqslant \mathbb{1}_\mathfrak{g}$). This is equivalent to saying that the predual map $\Phi_\mathsf{T}: \mathcal{A}_\mathsf{T} \to \mathcal{B}_\mathsf{T}$, which, using Eqs. (10) and (13), can be written as

$$\Phi_\mathsf{T}(\rho) = \mathrm{Tr}_\mathfrak{g}[\Phi_\tau(\widetilde{\rho} \otimes \mathbb{1}_\mathfrak{h})], \tag{14}$$

is trace preserving (trace decreasing).

As an example, consider a normal state ϱ on $\mathcal{B}$, which, being a quantum channel into $\mathbb{C}$, satisfies the complete majorization condition with $\lambda = \|\rho\|$, where ρ is the density operator of ϱ. Furthermore, it is easy to see that $\varrho_\tau = \rho$. Indeed, we can write

$$\varrho(B) = (B, \rho) = \mathrm{Tr}(B\widetilde{\rho}) = \mathrm{Tr}(\widetilde{B}\rho) = \mathrm{Tr}_\mathfrak{h}[(\mathbb{1}_\mathbb{C} \otimes \widetilde{B})\rho],$$

and the desired result follows upon comparing this with Eq. (13). This provides additional justification for our definition of the trace pairing in Eq. (9), since we then have that $\varrho_\mathsf{T} = \rho = \varrho_\tau$ for any normal state ϱ.

If the operation $\Phi: \mathcal{B} \to \mathcal{A}$ is given in the generalized Kraus form (12), we can write down its operational density Φ_τ explicitly. To this end, suppose that all operators $F(z)$ are determined by generalized bra-vectors $\Gamma(z) = (F(z)|$, densely defined as the linear functionals

$$\Gamma(z)|\xi\otimes\eta\rangle = \langle\xi|F(z)|\eta\rangle \equiv (F(z)||\xi\otimes\eta\rangle)$$

on the linear span of the ket-vectors $|\xi\otimes\eta\rangle \equiv \widetilde{\xi\otimes\eta}$ in $\mathcal{H}=\mathfrak{g}\otimes\mathfrak{h}$, where $\xi\in\mathfrak{g}$ is also treated as a bra-vector such that $J\xi=\langle\xi|$ and $|\xi\rangle=\tilde{\xi}$. Then the operational density Φ_τ of Φ is given by the corresponding decomposition

$$\Phi_\tau = \int \Gamma(z)^\dagger\Gamma(z)\mathrm{d}\mu(z) \equiv \Gamma^\dagger\Gamma, \tag{15}$$

where the integral is, again, understood in the sense of Bochner.

C. Completely bounded maps

Completely positive linear maps between operator algebras are a special case of *completely bounded* maps.[20] Consider, as before, the algebras $\mathcal{B}=\mathcal{B}(\mathfrak{h})$ and $\mathcal{A}=\mathcal{B}(\mathfrak{g})$. For each $n\in\mathbb{N}$ define the *n*th *matrix level* $\mathcal{M}_n(\mathcal{B})\simeq\mathcal{B}\otimes\mathcal{M}_n$, where $\mathcal{M}_n$ denotes the algebra of $n\times n$ matrices with complex entries. That is, $\mathcal{M}_n(\mathcal{B})$ is the space of $n\times n$ matrices with $\mathcal{B}$-valued entries,

$$\mathcal{M}_n(\mathcal{B}) := \{[B_{ij}]: B_{ij}\in\mathcal{B}, 1\leqslant i,j\leqslant n\}.$$

Analogous construction can also be applied to $\mathcal{A}$ to yield the matrix levels $\mathcal{M}_n(\mathcal{A})$. Each matrix level $\mathcal{M}_n(\mathcal{B})$ inherits a *-algebra structure from $\mathcal{B}$ through

$$[B_{ij}][C_{ij}] := \left[\sum_{k=1}^{n} B_{ik}C_{kj}\right], \quad [B_{ij}]^\dagger := [B_{ij}^\dagger].$$

In fact, by identifying $\mathcal{M}_n(\mathcal{B})$ via a natural *-isomorphism with the algebra $\mathcal{B}(\mathfrak{h}^{(n)})$ of bounded linear operators on $\mathfrak{h}^{(n)}$, the direct sum of *n* copies of $\mathfrak{h}$, one can make $\mathcal{M}_n(\mathcal{B})$ into a C^*-algebra. Thus, each matrix level of $\mathcal{B}$ possesses a unique C^*-norm.

Now, for any $n\in\mathbb{N}$ a linear map $\Lambda:\mathcal{B}\to\mathrm{A}$ induces the map $\Lambda^{(n)}:=\Lambda\otimes\mathrm{id}_n$ from $\mathcal{M}_n(\mathcal{B})$ into $\mathcal{M}_n(\mathcal{A})$, defined by $\Lambda^{(n)}:[B_{ij}]\mapsto[\Lambda(B_{ij})]$. Let us define the *norm of complete boundedness* (or CB-norm) by $\|\Lambda\|_{\mathrm{CB}}:=\sup\{\|\Lambda^{(n)}\|:n\in\mathbb{N}\}$, where

$$\|\Lambda^{(n)}\| := \sup_{B\in\mathcal{M}_n(\mathcal{B}),\|B\|\leqslant 1}\|\Lambda^{(n)}(B)\|$$

is the usual operator norm of $\Lambda^{(n)}$. A linear map $\Lambda:\mathcal{B}\to\mathcal{A}$ is called *completely bounded* if $\|\Lambda\|_{\mathrm{CB}}<\infty$. Every completely positive map $\Phi:\mathcal{B}\to\mathcal{A}$ is automatically completely bounded, with $\|\Phi\|_{\mathrm{CB}}=\|\Phi(1_\mathfrak{h})\|$. For a general completely bounded map Λ, one has, by definition, $\|\Lambda(1_\mathfrak{h})\|\leqslant\|\Lambda\|\leqslant\|\Lambda\|_{\mathrm{CB}}$.

Passing to the predual map $\Lambda_\mathsf{T}:\mathcal{A}_\mathsf{T}\to\mathcal{B}_\mathsf{T}$, we can similarly define induced maps $\Lambda_\mathsf{T}^{(n)}:\mathcal{M}_n(\mathcal{A}_\mathsf{T})\to\mathcal{M}_n(\mathcal{B}_\mathsf{T})$, $n\in\mathbb{N}$, and the predual CB-norm

$$\|\Lambda\|_{\mathrm{CB}}^{\mathsf{T}} := \sup_{n\in\mathbb{N}}\|\Lambda^{(n)}\|_\mathsf{T},$$

where

$$\|\Lambda^{(n)}\|_\mathsf{T} := = \sup_{\rho\in\mathcal{M}_n(\mathcal{A}_\mathsf{T}):\|\rho\|_\mathsf{T}\leqslant 1}\|\Lambda^{(n)}(\rho)\|_\mathsf{T}.$$

It is easy to see that $\|\Lambda^{(n)}\|=\|\Lambda_\mathsf{T}^{(n)}\|_\mathsf{T}$ for all $n\in\mathbb{N}$, so that $\|\Lambda\|_{\mathrm{CB}}=\|\Lambda_\mathsf{T}\|_{\mathrm{CB}}^{\mathsf{T}}$. It is also straightforward to see that the "unstabilized" norms $\|\cdot\|$ and $\|\cdot\|_\mathsf{T}$ are tensor supermultiplicative (i.e., $\|\Lambda_1\otimes\Lambda_2\|\geqslant\|\Lambda_1\|\,\|\Lambda_2\|$), whereas the corresponding CB-norms are tensor multiplicative (i.e., $\|\Lambda_1\otimes\Lambda_2\|_{\mathrm{CB}}=\|\Lambda_1\|_{\mathrm{CB}}\|\Lambda_2\|_{\mathrm{CB}}$).

There is also a useful nonvariational formula for the CB-norm of a map $\Lambda:\mathcal{B}\to\mathcal{A}$. Namely, let ℓ^2 denote the Hilbert space of square-summable infinite sequences of complex numbers, and let $\mathcal{K}(\ell^2)$ denote the space of compact operators on ℓ^2. Then $\|\Lambda\|_{\mathrm{CB}}=\|\Lambda\otimes\mathrm{id}_{\mathcal{K}(\ell^2)}\|$. Since we have

assumed that $\mathcal{B}=\mathcal{B}(\mathfrak{h})$ with $\mathfrak{h}$ a complex separable Hilbert space, and since all complex separable Hilbert spaces are canonically isomorphic to ℓ^2, we may also write $\|\Lambda\|_{\mathrm{CB}}=\|\Lambda\otimes \mathrm{id}_{\mathcal{K}(\mathfrak{h})}\|$.

D. Miscellany

Any positive operator $B\in\mathcal{B}(\mathfrak{h})$ has a unique positive square root, denoted by $B^{1/2}$ and defined as the positive operator $X\in\mathcal{B}(\mathfrak{h})$ such that $B=X^2$. This definition can be extended to any operator A that is similar to a positive operator $\Delta\in\mathcal{B}(\mathfrak{h})$, in the sense that there exists an operator $S\in\mathcal{B}(\mathfrak{h})$ such that $A=S\Delta S^+$, where S^+ is the pseudoinverse of S, equal to S^{-1} on ran S and to 0 on ker S. In that case, we may *define* $\sqrt{A}:=S\Delta^{1/2}S^+$. From now on, in order to distinguish this extended definition of the square root from the usual one, we shall always use the square root symbol $\sqrt{\cdot}$ for this extended definition, and reserve the exponent notation $\cdot^{1/2}$ for the usual definition.

Consider now two positive operators $A,B\in\mathcal{B}(\mathfrak{h})$. It is easy to see that their product AB is similar to $A^{1/2}BA^{1/2}$ with $S=A^{1/2}$. Note that the operator AB is positive when restricted to the closure of ran A, when the latter is equipped with the weighted inner product $\langle v|\chi\rangle_A:=\langle A^{-1/2}v|A^{-1/2}\chi\rangle$:

$$\langle v|ABv\rangle_A=\langle A^{-1/2}v|A^{-1/2}ABv\rangle=\langle v|Bv\rangle\geqslant 0,\qquad \forall\, v\in\overline{\mathrm{ran}A}.$$

Thus we may define $\sqrt{AB}:=S(A^{1/2}BA^{1/2})S^+$ with $S=A^{1/2}$.

This notation, again, allows for a convenient parallelism between the classical (commutative) formalism and the quantum (noncommutative) one. Indeed, consider two mutually commuting positive trace-class operators ρ, σ, let $\{|x\rangle\}$ denote the set of their common eigenvectors, and let $\rho_x\equiv\langle x|\rho|x\rangle$, $\sigma_x\equiv\langle x|\sigma|x\rangle$ denote the corresponding eigenvalues. Then $\sqrt{\rho\sigma}$ is also trace-class, and

$$\mathrm{Tr}\sqrt{\rho\sigma}=\sum_x\sqrt{\rho_x\sigma_x}.$$

If $\mathrm{Tr}\,\rho=1=\mathrm{Tr}\,\sigma$, then $P:=\{\rho_x\}$ and $Q:=\{\sigma_x\}$ are probability distributions, and $\mathrm{Tr}\,\sqrt{\rho\sigma}$ then gives the classical fidelity (also known as the *Bhattacharyya coefficient*)[10] $F(P,Q)$ between P and Q.

Our main technical tool in this paper is given by the following:

Lemma 1: Let $\mathcal{H}$ be a complex separable Hilbert space, and let R, $S\in\mathcal{B}(\mathcal{H})$ be positive operators such that $R^{1/2}SR^{1/2}$ is trace class. Then the supremum

$$\sup_{X,Y\in\mathcal{B}(\mathcal{H})}\{\mathrm{Tr}(X^\dagger Y+Y^\dagger X):X^\dagger X=R,Y^\dagger Y=S\}=2\,\mathrm{Tr}\sqrt{RS}\tag{16}$$

is achieved on any $X\in\mathcal{B}(\mathcal{H})$ satisfying the condition $X^\dagger X=R$, say $X=R^{1/2}$, and $Y=Y_o$ satisfying the equation

$$Y_oX^\dagger=(XSX^\dagger)^{1/2}=XY_o^\dagger.\tag{17}$$

Proof: To prove the lemma one can use either the polar decomposition or the method of Lagrange multipliers. We shall use the latter. Fixing an X satisfying $X^\dagger X=R$, we can write the Lagrange function as

$$\mathsf{L}=\mathrm{Tr}(X^\dagger Y+Y^\dagger X-Y^\dagger YL),$$

where $L=L^\dagger\in\mathcal{B}(\mathcal{H})$ is the operator-valued Lagrange multiplier corresponding to the hermiticity condition $S=Y^\dagger Y=S^\dagger$. At the stationary point

$$\delta\mathsf{L}=\mathrm{Tr}(X^\dagger-LY^\dagger)\,\delta Y+(X-YL)\,\delta Y^\dagger=0,$$

so $Y=Y_o$ must satisfy the equation $YL=X$ (the other equation, $LY^\dagger=X^\dagger$, corresponding to $Y^\dagger=Y_o^\dagger$, is obtained by taking the Hermitian adjoint). Thus $Y_o=XL^{-1}$, where L^{-1} should be determined from $L^{-1}X^\dagger XL^{-1}=S$. Multiplying this on the left by X and on the right by $X^\dagger$ yields $(XL^{-1}X^\dagger)^2=XSX^\dagger$, or

$XL^{-1}X^\dagger=(XSX^\dagger)^{1/2}$. Thus, we indeed have that $Y_oX^\dagger=(XSX^\dagger)^{1/2}=XY_o^\dagger$, and therefore that

$$\mathrm{Tr}(Y_oX^\dagger + XY_o^\dagger) = 2\,\mathrm{Tr}((XSX^\dagger)^{1/2}). \tag{18}$$

This extremal value is precisely the maximal value due to convexity of the function being maximized in Eq. (16). Note that, since $(U^\dagger XSX^\dagger U)^{1/2}=U^\dagger(XSX^\dagger)^{1/2}U$ for any unitary U, the value of the supremum in Eq. (16), which coincides with Eq. (18), does not depend on the choice of X satisfying $X^\dagger X=R$. Indeed, by virtue of the polar decomposition $X=UR^{1/2}$,

$$2\,\mathrm{Tr}(XSX^\dagger)^{1/2} = 2\,\mathrm{Tr}(U^\dagger(XSX^\dagger)^{1/2}U) = 2\,\mathrm{Tr}((R^{1/2}SR^{1/2})^{1/2}).$$

Rewriting this trace in the equivalent form $2\,\mathrm{Tr}(X^\dagger Y_o)$ with

$$X^\dagger Y_o = R^{1/2}(R^{1/2}SR^{1/2})^{1/2}R^{-1/2} \equiv \sqrt{RS}$$

corresponding to $X=R^{1/2}$, we obtain the extremal value in Eq. (16). □

We shall also need the following simple, but useful, result:

Lemma 2: Let S be a compact subset of a complex Banach space V, such that $x\in S$ implies $\lambda x\in S$ for all $\lambda\in\mathbb{C}$ with $|\lambda|=1$. Let $f:V\to\mathbb{C}$ be a continuous function which is homogeneous of order 1, i.e., $f(\lambda x)=\lambda f(x)$ for all $\lambda\in\mathbb{C}$ and all $x\in V$. Then

$$\sup_{x\in S}|f(x)| = \sup_{x\in S}\mathrm{Re}\, f(x). \tag{19}$$

Proof: Let $x^*\in S$ be such that $|f(x^*)|=\sup_{x\in S}|f(x)|$, with $f(x^*)=|f(x^*)|e^{i\arg f(x^*)}$. Let $x^{**}:=e^{-i\arg f(x^*)}x^*$. By the homogeneity of f,

$$f(x^{**}) = e^{-i\arg f(x^*)}f(x^*) = |f(x^*)|.$$

But then $|f(x^{**})|=f(x^{**})=\mathrm{Re}\, f(x^{**})$. Since $\mathrm{Re}\,\lambda\leqslant|\lambda|$ for all $\lambda\in\mathbb{C}$, the lemma is proved. □

III. OPERATIONAL FIDELITIES AND DISTANCES

A. Classical kernel fidelity

The fidelity distinguishing different quantum operations without the restriction on the Hilbert space dimensionality was suggested by Belavkin in Ref. 21 on the basis of a noncommutative generalization of the maximal Hellinger distance between two positive kernels. Namely, given a locally compact space X and a measure space $(Y,\mathcal{B}_Y,\mu)$, where μ is a positive measure, let us denote by $\mathcal{A}$ the algebra $\mathcal{C}(X)$ of bounded continuous functions on X, and by $\mathcal{B}_\mathsf{T}\equiv\mathcal{C}_\mathsf{T}(Y)$ the space of absolutely μ-integrable complex functions on Y. A *positive kernel* $\mathbf{P}$ is then given in terms of a function $p(\cdot|\cdot):Y\times X\to\mathbb{R}^+$, such that $P_x:=p(\cdot|x)\in\mathcal{B}_\mathsf{T}$ for all $x\in X$, while $P:=\int_Y p(y|\cdot)\mathrm{d}\mu(y)\in\mathcal{A}$. Given two positive kernels $\mathbf{P}$ and $\mathbf{Q}$, the squared pointwise Hellinger distance

$$d_H^2(P_x,Q_x) := \frac{1}{2}\int(\sqrt{p(y|x)}-\sqrt{q(y|x)})^2\mathrm{d}\mu(y) = \int\left[\frac{1}{2}(p(y|x)+q(y|x)) - \sqrt{p(y|x)q(y|x)}\right]\mathrm{d}\mu(y) \tag{20}$$

is well defined and finite for each $x\in X$, so that we can define

$$d_H^2(\mathbf{P},\mathbf{Q}) := \frac{1}{2}\sup_{x\in X}\int(\sqrt{p(y|x)}-\sqrt{q(y|x)})^2\mathrm{d}\mu(y) \equiv \|d_H^2(P_x,Q_x)\|, \tag{21}$$

the last expression indicating the fact that $d_H^2(\mathbf{P},\mathbf{Q})$ is given by the supremum of the squared pointwise Hellinger distance (20) over all $x\in X$. Note that the squared Hellinger distance $d_H^2(P,Q)$ between two positive distributions $P=p(\cdot)$ and $Q=q(\cdot)$ is the minimal mean quadratic distance

$$d_H^2(P,Q) = \frac{1}{2}\inf_{\chi,\psi\in C(Y)}\left\{\int |\chi(y)-\psi(y)|^2 \mathrm{d}\mu(y) : |\chi(\cdot)|^2 = p(\cdot), |\psi(\cdot)|^2 = q(\cdot)\right\}$$

$$= \left(1, \tfrac{1}{2}(P+Q)\right) - \sup_{\psi:|\psi(\cdot)|^2=q(\cdot)} \int \sqrt{p(y)}\,\mathrm{Re}\,\psi(y)\mathrm{d}\mu(y), \tag{22}$$

where $(f,P)=\int f(y)p(y)d\mu(y)$ denotes the integral pairing of $f\in\mathcal{C}(Y)$ with $P\in\mathcal{C}_{\mathrm{T}}(Y)$. The *relative fidelity*

$$f(P,Q) = \frac{1}{\sqrt{(1,P)(1,Q)}} \sup_{\psi:|\psi(\cdot)|^2=q(\cdot)} \int \sqrt{p(y)}\,\mathrm{Re}\,\psi(y)\mathrm{d}\mu(y) = \frac{(1,\sqrt{PQ})}{\sqrt{(1,P)(1,Q)}} \tag{23}$$

of the distributions P and Q is obviously related to the distance (22) by

$$d_H^2(P,Q) + \sqrt{(1,P)(1,Q)}f(P,Q) = \left(1, \tfrac{1}{2}(P+Q)\right). \tag{24}$$

If $P_x := p(\cdot|x)$ and $Q_x := q(\cdot|x)$ are conditional distributions with constant integrals $(1,P_x)$ and $(1,Q_x)$, e.g., normalized to unity, this relation also remains valid for the minimal fidelity

$$f(\mathbf{P},\mathbf{Q}) = \inf_{x\in X} f(P_x,Q_x),$$

which can alternatively be defined by the minimax formula

$$f(\mathbf{P},\mathbf{Q}) = \inf_{x\in X} \sup_{\psi:|\psi(\cdot|x)|^2=Q_x(\cdot)} \frac{(1,\sqrt{P_x}\,\mathrm{Re}\,\psi(\cdot|x))}{\sqrt{(1,P_x)(1,Q_x)}}, \tag{25}$$

where the supremum is achieved on $\psi(\cdot|x)\equiv\psi_\circ(\cdot|x)$ satisfying $\psi(y|x)=\sqrt{q(y|x)}$. In particular, if $\mathbf{P}$ and $\mathbf{Q}$ are probability kernels, $(1,P_x)=1=(1,Q_x)$ for all $x\in X$, then

$$d_H^2(\mathbf{P},\mathbf{Q}) = 1 - \inf_{x\in X}\int \sqrt{p(y|x)q(y|x)}\mathrm{d}\mu(y) \equiv 1 - f(\mathbf{P},\mathbf{Q}),$$

where

$$f(\mathbf{P},\mathbf{Q}) = \inf_{x\in X}\int \sqrt{p(y|x)q(y|x)}\mathrm{d}\mu(y) \equiv \inf_{x\in X}(1,\sqrt{P_xQ_x}) \tag{26}$$

is the minimax fidelity of the classical channels described by these kernels.

B. Quantum operational fidelity

Generalizing Eq. (21), one can define the squared Hellinger distance between quantum operations Φ and Ψ with the respective operational densities $\Phi_\tau,\Psi_\tau\in\mathcal{B}(\mathcal{H})$, $\mathcal{H}=\mathfrak{g}\otimes\mathfrak{h}$, as

$$d_H^2(\Phi,\Psi) = \tfrac{1}{2}\inf_{\Gamma,\Upsilon\in\mathcal{B}(\mathcal{H})}\{\|\mathrm{Tr}_{\mathfrak{h}}(\Gamma-\Upsilon)^\dagger(\Gamma-\Upsilon)\| : \Gamma^\dagger\Gamma=\Phi_\tau, \Upsilon^\dagger\Upsilon=\Psi_\tau\}. \tag{27}$$

The operators $\Gamma,\Upsilon\in\mathcal{B}(\mathcal{H})$, such that $\Gamma^\dagger\Gamma=\Phi_\tau$ and $\Upsilon^\dagger\Upsilon=\Psi_\tau$, are naturally thought of as the *purifications* of Φ_τ and Ψ_τ, respectively. This means that we can fix an orthonormal basis $\{|j\rangle\}$ of $\mathcal{H}$, say the product basis $|j\rangle=|i\rangle\otimes|k\rangle\equiv|i,k\rangle$, where $\{|i\rangle\}$ and $\{|k\rangle\}$ are some fixed orthonormal bases of $\mathfrak{g}$ and $\mathfrak{h}$, respectively, and represent any such Γ and Υ as strongly convergent sums

$$\Gamma = \sum_j |j\rangle\langle j|\Gamma \equiv \sum_j |j\rangle(F_j|, \quad \Upsilon = \sum_j |j\rangle\langle j|\Upsilon \equiv \sum_j |j\rangle(V_j|, \tag{28}$$

where the generalized bra-vectors $(F_j|$ define the bounded operators $F_j,V_j:\mathfrak{g}\to\mathfrak{h}$ through

$$\langle k|F_j|i\rangle = (F_j|(|i\rangle \otimes |k\rangle) = \langle j\|\Gamma|i,k\rangle, \quad \langle k|V_j|i\rangle = (V_j|(|i\rangle \otimes |k\rangle) = \langle j\|\Upsilon|i,k\rangle.$$

As seen directly from this definition, the mapping $(F|\mapsto F$ is linear: $(aF+bG|\mapsto aF+bG$. Using Eq. (28), we may write

$$\Phi_\tau = \sum_j |F_j)(F_j| \equiv \Gamma^\dagger\Gamma, \quad \Psi_\tau = \sum_j |V_j)(V_j| \equiv \Upsilon^\dagger\Upsilon, \tag{29}$$

where the sums converge in the strong operator topology. This determines the Kraus decompositions[17] $\Phi(B)=\Sigma_j F_j^\dagger B F_j$, $\Psi(B)=\Sigma_j V_j^\dagger B V_j$ of the maps $\Phi,\Psi:\mathcal{B}\to\mathcal{A}$. Analogously, upon defining the mappings $F,V:\mathfrak{g}\to\mathfrak{h}\otimes\mathcal{H}$ by

$$F\upsilon := \sum_j F_j\upsilon \otimes |j\rangle, \quad V\upsilon := \sum_j V_j\upsilon \otimes |j\rangle,$$

we can write the maps Φ,Ψ in the Stinespring form[22] as $\Phi(B)=F^\dagger(B\otimes\mathbb{1}_\mathcal{H})F$ and $\Psi(B)=V^\dagger(B\otimes\mathbb{1}_\mathcal{H})V$.

Taking into account the fact that $\|A^\dagger A\|=\sup_{\varrho\in\mathcal{S}(\mathfrak{g})}\varrho(A^\dagger A)$ and defining the positive function

$$c(\cdot;\cdot):\mathcal{B}(\mathcal{H})\times\mathcal{B}_\mathsf{T}(\mathfrak{g})\to\mathbb{R},$$

$$c(A;\rho) := \tfrac{1}{2}\mathrm{Tr}(A(\rho\otimes\mathbb{1}_\mathfrak{h})A^\dagger),$$

we can rewrite the fidelity distance (27) in the following minimax form:

$$d_H^2(\Phi,\Psi) = \inf_{\Gamma,\Upsilon\in\mathcal{B}(\mathcal{H})}\left\{\sup_{\varrho\in\mathcal{S}(\mathfrak{g})} c(\Gamma-\Upsilon;\rho):\Gamma^\dagger\Gamma=\Phi_\tau,\Upsilon^\dagger\Upsilon=\Psi_\tau\right\}. \tag{30}$$

On the other hand, generalizing Eq. (20) to quantum operations, we can define the squared pointwise distance

$$d_H^2(\Phi,\Psi)(\varrho) := \inf_{\Gamma,\Upsilon\in\mathcal{B}(\mathcal{H})}\{c(\Gamma-\Upsilon;\rho):\Gamma^\dagger\Gamma=\Phi_\tau,\Upsilon^\dagger\Upsilon=\Psi_\tau\} \tag{31}$$

between Φ and Ψ on the set $\mathcal{S}(\mathfrak{g})$ of all normal states on $\mathcal{A}=\mathcal{B}(\mathfrak{g})$. Just as with the probability kernels in the commutative setting described in the preceding section, $d_H^2(\Phi,\Psi)$ coincides with the supremum of $d_H^2(\Phi,\Psi)(\varrho)$ over all normal states $\varrho\in\mathcal{S}(\mathfrak{g})$ whenever Φ and Ψ are (proportional to) quantum channels:

Theorem 1: *Let $\Phi,\Psi:\mathcal{B}\to\mathcal{A}$ be quantum operations with the respective operational densities $\Phi_\tau,\Psi_\tau\in\mathcal{B}(\mathcal{H})$. Suppose that for all $\varrho\in\mathcal{S}(\mathfrak{g})$ the pairings*

$$(\Phi_\tau,\rho\otimes\mathbb{1}_\mathfrak{h}) \equiv \varrho[\Phi(\mathbb{1}_\mathfrak{h})], \quad (\Psi_\tau,\rho\otimes\mathbb{1}_\mathfrak{h}) \equiv \varrho[\Psi(\mathbb{1}_\mathfrak{h})] \tag{32}$$

are constant. Then

$$d_H^2(\Phi,\Psi) = \sup_{\varrho\in\mathcal{S}(\mathfrak{g})} d_H^2(\Phi,\Psi)(\varrho). \tag{33}$$

Furthermore, then we have that

$$d_H^2(\Phi,\Psi) + \sqrt{\|\Phi\|\,\|\Psi\|}f(\Phi,\Psi) = \tfrac{1}{2}(\|\Phi\|+\|\Psi\|), \tag{34}$$

where

$$f(\Phi,\Psi) = \inf_{\varrho\in\mathcal{S}(\mathfrak{g})}\sup_{\Upsilon\in\mathcal{B}(\mathcal{H}):\Upsilon^\dagger\Upsilon=\Psi_\tau}\frac{\mathrm{Re}\,\mathrm{Tr}[\Phi_\tau^{1/2}\Upsilon(\rho\otimes\mathbb{1}_\mathfrak{h})]}{\sqrt{\varrho[\Phi(\mathbb{1}_\mathfrak{h})]}\sqrt{\varrho[\Psi(\mathbb{1}_\mathfrak{h})]}} \tag{35}$$

is the minimax fidelity *between Φ and Ψ.*

Proof: Fix an arbitrary $\varrho\in\mathcal{S}(\mathfrak{g})$. From Eq. (32) it follows that

$$\|\Phi\| = \sup_{\varrho \in \mathcal{S}(\mathfrak{g})} \varrho[\Phi(\mathbb{1}_{\mathfrak{h}})] = \varrho[\Phi(\mathbb{1}_{\mathfrak{h}})],$$

and the same goes for Ψ. Therefore, given any pair $\Gamma, \Upsilon \in \mathcal{B}(\mathcal{H})$ such that $\Gamma^\dagger\Gamma = \Phi_\tau$ and $\Upsilon^\dagger\Upsilon = \Psi_\tau$, we can write

$$\begin{aligned} c(\Gamma - \Upsilon; \rho) &= \tfrac{1}{2}\mathrm{Tr}((\Gamma - \Upsilon)^\dagger(\Gamma - \Upsilon)(\rho \otimes \mathbb{1}_{\mathfrak{h}})) = \tfrac{1}{2}\mathrm{Tr}((\Phi_\tau + \Psi_\tau)(\rho \otimes \mathbb{1}_{\mathfrak{h}}) - (\Gamma^\dagger\Upsilon + \Gamma\Upsilon^\dagger)(\rho \otimes \mathbb{1}_{\mathfrak{h}})) \\ &= \tfrac{1}{2}(\|\Phi\| + \|\Psi\| - \mathrm{Tr}[(\Gamma^\dagger\Upsilon + \Gamma\Upsilon^\dagger)(\rho \otimes \mathbb{1}_{\mathfrak{h}})]), \end{aligned}$$

whence it follows that

$$d_H^2(\Phi, \Psi)(\varrho) = \inf_{\substack{\Gamma:\Gamma^\dagger\Gamma = \Phi_\tau \\ \Upsilon:\Upsilon^\dagger\Upsilon = \Psi_\tau}} c(\Gamma - \Upsilon; \rho) = \tfrac{1}{2}\left(\|\Phi\| + \|\Psi\| - \sup_{\substack{\Gamma:\Gamma^\dagger\Gamma = \Phi_\tau \\ \Upsilon:\Upsilon^\dagger\Upsilon = \Psi_\tau}} \mathrm{Tr}[(\Gamma^\dagger\Upsilon + \Gamma\Upsilon^\dagger)(\rho \otimes \mathbb{1}_{\mathfrak{h}})]\right).$$

Taking the supremum of both sides over all $\varrho \in \mathcal{S}(\mathfrak{g})$, we obtain

$$\sup_{\varrho \in \mathcal{S}(\mathfrak{g})} d_H^2(\Phi, \Psi)(\varrho) = \tfrac{1}{2}\left(\|\Phi\| + \|\Psi\| - \inf_{\varrho \in \mathcal{S}(\mathfrak{g})} \sup_{\substack{\Gamma:\Gamma^\dagger\Gamma = \Phi_\tau \\ \Upsilon:\Upsilon^\dagger\Upsilon = \Psi_\tau}} \mathrm{Tr}[(\Gamma^\dagger\Upsilon + \Gamma\Upsilon^\dagger)(\rho \otimes \mathbb{1}_{\mathfrak{h}})]\right). \tag{36}$$

On the other hand,

$$d_H^2(\Phi, \Psi) = \inf_{\substack{\Gamma:\Gamma^\dagger\Gamma = \Phi_\tau \\ \Upsilon:\Upsilon^\dagger\Upsilon = \Psi_\tau}} \sup_{\varrho \in \mathcal{S}(\mathfrak{g})} c(\Gamma - \Upsilon; \rho) = \tfrac{1}{2} \inf_{\substack{\Gamma:\Gamma^\dagger\Gamma = \Phi_\tau \\ \Upsilon:\Upsilon^\dagger\Upsilon = \Psi_\tau}} \sup_{\varrho \in \mathcal{S}(\mathfrak{g})} (\|\Phi\| + \|\Psi\| - \mathrm{Tr}[(\Gamma^\dagger\Upsilon + \Gamma\Upsilon^\dagger)(\rho \otimes \mathbb{1}_{\mathfrak{h}})]),$$

which yields

$$d_H^2(\Phi, \Psi) = \tfrac{1}{2}\left(\|\Phi\| + \|\Psi\| - \sup_{\substack{\Gamma:\Gamma^\dagger\Gamma = \Phi_\tau \\ \Upsilon:\Upsilon^\dagger\Upsilon = \Psi_\tau}} \inf_{\varrho \in \mathcal{S}(\mathfrak{g})} \mathrm{Tr}[(\Gamma^\dagger\Upsilon + \Gamma\Upsilon^\dagger)(\rho \otimes \mathbb{1}_{\mathfrak{h}})]\right). \tag{37}$$

Note that the right-hand sides of Eqs. (36) and (37) differ only in the order of the extrema. Thus, establishing the validity of Eq. (33) amounts to justifying the interchange of the extrema.

According to Lemma 1, the supremum over Γ and Υ in Eq. (36) can be evaluated by fixing $\Gamma = \Phi_\tau^{1/2}$ first and then varying only over all $\Upsilon \in \mathcal{B}(\mathcal{H})$ such that $\Upsilon^\dagger\Upsilon = \Psi_\tau$. By the polar decomposition, any such Υ has the form $U\Psi_\tau^{1/2}$ for some partial isometry U. Thus we have

$$\begin{aligned} \sup_{\substack{\Gamma:\Gamma^\dagger\Gamma = \Phi_\tau \\ \Upsilon:\Upsilon^\dagger\Upsilon = \Psi_\tau}} \mathrm{Tr}[(\Gamma^\dagger\Upsilon + \Gamma\Upsilon^\dagger)(\rho \otimes \mathbb{1}_{\mathfrak{h}})] &= 2 \sup_{\Upsilon:\Upsilon^\dagger\Upsilon = \Psi_\tau} \mathrm{Re}\,\mathrm{Tr}[\Phi_\tau^{1/2}\Upsilon(\rho \otimes \mathbb{1}_{\mathfrak{h}})] \\ &= 2 \sup_U \mathrm{Re}\,\mathrm{Tr}[\Phi_\tau^{1/2}U\Psi_\tau^{1/2}(\rho \otimes \mathbb{1}_{\mathfrak{h}})], \end{aligned} \tag{38}$$

where the supremum in Eq. (38) is taken over all partial isometries U such that

$$\Psi_\tau^{1/2}U^\dagger U\Psi_\tau^{1/2} = \Psi_\tau.$$

Since the expression being minimized is linear in U and the isometries are the extreme points of the unit ball $\mathsf{B}_1(\mathcal{H}) := \{X \in \mathcal{B}(\mathcal{H}) : \|X\| \leqslant 1\}$ of all bounded operators,[23] we may instead take the supremum over the entire unit ball:

$$\sup_{\Upsilon:\Upsilon^\dagger\Upsilon = \Psi_\tau} \mathrm{Re}\,\mathrm{Tr}[\Phi_\tau^{1/2}\Upsilon(\rho \otimes \mathbb{1}_{\mathfrak{h}})] = \sup_{X \in \mathsf{B}_1(\mathcal{H})} \mathrm{Re}\,\mathrm{Tr}[\Phi_\tau^{1/2}X\Psi_\tau^{1/2}(\rho \otimes \mathbb{1}_{\mathfrak{h}})]. \tag{39}$$

Since the expression being maximized in the right-hand side of Eq. (39) is affine in both X and ρ, and since $\mathsf{B}_1(\mathcal{H})$ and $\mathcal{S}(\mathfrak{g})$ are closed convex subsets of $\mathcal{B}(\mathcal{H})$ and $\mathcal{B}_\mathsf{T}(\mathfrak{g})$, respectively, it follows from standard minimax arguments[24] that we can indeed interchange the extrema to obtain $f_-(\Phi, \Psi) = f_+(\Phi, \Psi)$, where

$$f_-(\Phi,\Psi) := \inf_{\varrho\in\mathcal{S}(\mathfrak{g})} \sup_{X\in\mathsf{B}_1(\mathcal{H})} \mathrm{Re}\,\mathrm{Tr}[\Phi_\tau^{1/2} X \Psi_\tau^{1/2}(\rho\otimes\mathbb{1}_\mathfrak{h})]$$

$$f_+(\Phi,\Psi) := \sup_{X\in\mathsf{B}_1(\mathcal{H})} \inf_{\varrho\in\mathcal{S}(\mathfrak{g})} \mathrm{Re}\,\mathrm{Tr}[\Phi_\tau^{1/2} X \Psi_\tau^{1/2}(\rho\otimes\mathbb{1}_\mathfrak{h})],$$

which proves the claim of Eq. (33). The rest is straightforward. □

As seen immediately from Theorem 1, when Φ and Ψ are quantum channels, then

$$d_H^2(\Phi,\Psi) + f(\Phi,\Psi) = 1,$$

with the minimax fidelity given by

$$f(\Phi,\Psi) = \inf_{\varrho\in\mathcal{S}(\mathfrak{g})} \sup_{Y:Y^\dagger Y=\Psi_\tau} \mathrm{Re}\,\mathrm{Tr}[\Phi_\tau^{1/2} Y(\rho\otimes\mathbb{1}_\mathfrak{h})]. \tag{40}$$

IV. EVALUATING THE FIDELITY DISTANCES

A. Fidelities for quantum states and quantum effects

Consider two normal states ϱ,ς on $\mathcal{B}=\mathcal{B}(\mathfrak{h})$ as quantum channels from $\mathcal{B}$ into the Abelian algebra $\mathcal{A}=\mathcal{B}(\mathfrak{g})$ with $\mathfrak{g}\simeq\mathbb{C}$. In this case, the operational densities $\varrho_\tau,\varsigma_\tau$ of ϱ,ς coincide with the corresponding density operators ρ,σ: $\varrho_\tau=\rho$ and $\varsigma_\tau=\sigma$. The predual maps $\varrho_\mathsf{T},\varsigma_\mathsf{T}:\mathcal{A}_\mathsf{T}\simeq\mathbb{C}\to\mathcal{B}_\mathsf{T}$ can then be thought of as the *state creation operations*, $\varrho_\mathsf{T}(\lambda)=\lambda\rho$ and $\varsigma_\mathsf{T}(\lambda)=\lambda\sigma$ for $\lambda\in\mathbb{C}$.

In order to compute the minimax fidelity $f(\varrho,\varsigma)$, we have to consider all $\chi,\psi\in\mathcal{B}$ that give the decompositions $\rho=\chi^\dagger\chi$ and $\sigma=\psi^\dagger\psi$. Note that we can always write these decompositions as purifications

$$\rho=\sum_j |\chi_j\rangle\langle\chi_j|, \quad \sigma=\sum_j |\psi_j\rangle\langle\psi_j|,$$

where $|\chi_j\rangle := \chi|j\rangle, |\psi_j\rangle := \psi|j\rangle$ with respect to a fixed orthonormal basis $\{|j\rangle\}$ of $\mathfrak{h}$. We then have the minimum quadratic distance

$$d_H^2(\varrho,\varsigma) = \tfrac{1}{2} \inf_{\substack{\chi\in\mathcal{B}:\chi^\dagger\chi=\rho\\ \psi\in\mathcal{B}:\psi^\dagger\psi=\sigma}} \sup_{\varpi\in\mathcal{S}(\mathfrak{g})} \varpi[(\chi-\psi)^\dagger(\chi-\psi)] \equiv \tfrac{1}{2} \inf_{\substack{\chi\in\mathcal{B}:\chi^\dagger\chi=\rho\\ \psi\in\mathcal{B}:\psi^\dagger\psi=\sigma}} \mathrm{Tr}[(\chi-\psi)^\dagger(\chi-\psi)],$$

where the last equality is due to the fact that $\dim\mathfrak{g}=1$. Expanding the product under the trace, we can write

$$d_H^2(\varrho,\varsigma) = \tfrac{1}{2}\Big[\mathrm{Tr}(\rho+\sigma) - \sup_{\chi,\psi\in\mathcal{B}} \{\mathrm{Re}\,\mathrm{Tr}(\chi^\dagger\psi): \chi^\dagger\chi=\rho, \psi^\dagger\psi=\sigma\}\Big] \tag{41}$$

$$= 1 - \sup_{\substack{\chi\in\mathcal{B}:\chi^\dagger\chi=\rho\\ \psi\in\mathcal{B}:\psi^\dagger\psi=\sigma}} \mathrm{Re}\,\mathrm{Tr}(\chi^\dagger\psi) \tag{42}$$

$$\equiv 1 - f(\varrho,\varsigma). \tag{43}$$

According to Lemma 1, the supremum in Eq. (42) is attained at any $\chi\in\mathcal{B}$ satisfying the condition $\chi^\dagger\chi=\rho$, say $\chi=\rho^{1/2}$, and $\psi=\psi_\circ$ satisfying the equation $\psi_\circ\chi^\dagger=(\chi\sigma\chi^\dagger)^{1/2}=\chi\psi_\circ^\dagger$:

$$f(\varrho,\varsigma) = \sup_{\substack{\chi\in\mathcal{B}:\chi^\dagger\chi=\rho\\ \psi\in\mathcal{B}:\psi^\dagger\psi=\sigma}} \mathrm{Re}\,\mathrm{Tr}(\chi^\dagger\psi) = \sup_{\psi\in\mathcal{B}(\mathfrak{h})} \{\mathrm{Re}\mathrm{Tr}(\rho^{1/2}\psi): \psi^\dagger\psi=\sigma\} = \mathrm{Tr}\,\sqrt{\rho\sigma}.$$

Observe that the standard Uhlmann fidelity between the density operators ρ and σ, $F(\rho,\sigma)$ in Eq. (1), can be written as $F(\rho,\sigma)=\|\rho^{1/2}\sigma^{1/2}\|_\mathsf{T}=\mathrm{Tr}\,\sqrt{\rho\sigma}$. Thus the minimax fidelity between two normal

states ϱ and ς on $\mathcal{B}$, or, equivalently, between the state creation operations $\varrho_{\mathsf{T}}, \varsigma_{\mathsf{T}}: \mathbb{C} \to \mathcal{B}_{\mathsf{T}}(\mathfrak{h})$, agrees with the Uhlmann fidelity between the respective density operators ρ and σ of ϱ and ς.

Next we turn to the other extreme case, namely that of the *state annihilation operations* Φ, Ψ with the preduals $\Phi_{\mathsf{T}}(\rho) = (\Phi_\tau, \rho), \Psi_{\mathsf{T}}(\rho) = (\Psi_\tau, \rho)$, corresponding to $\dim \mathfrak{h} = 1$. They are completely specified by the *effects*, i.e., the positive operators $\Phi_\tau, \Psi_\tau \in \mathcal{B}(\mathfrak{g})$ satisfying $0 \leqslant \Phi_\tau, \Psi_\tau \leqslant \mathbb{1}_{\mathfrak{g}}$, which can be purified as in (29), where $\Gamma_j = \langle j|\Gamma, \Upsilon_j = \langle j|\Upsilon$ are the bra-vectors corresponding to an orthonormal basis $\{|j\rangle\}$ in $\mathfrak{g}$. The squared pointwise minimax distance between the state annihilation operations Φ, Ψ, or, equivalently between the effects Φ_τ, Ψ_τ, on the set $\mathcal{S}(\mathfrak{g})$ of normal states $\varrho = \rho^{\mathsf{T}}$ on $\mathcal{B}(\mathfrak{g})$ is given by the minimum

$$d_H^2(\Phi, \Psi)(\varrho) = \tfrac{1}{2} \inf_{\Gamma, \Upsilon \in \mathcal{B}(\mathfrak{g})} \{\mathrm{Tr}[(\Gamma - \Upsilon)^\dagger (\Gamma - \Upsilon)\rho] : \Gamma^\dagger \Gamma = \Phi_\tau, \Upsilon^\tau \Upsilon = \Psi_\tau\}$$

of the quadratic distance between their purifications $\Gamma, \Upsilon \in \mathcal{B}(\mathfrak{g})$. The solution of this problem is likewise given by Lemma 1 with $R = \Phi_\tau$ and $S = \rho \Psi_\pi \rho$. Thus the optimum

$$d_H^2(\Phi, \Psi)(\varrho) = \tfrac{1}{2} \mathrm{Tr}[(\Phi_\tau + \Psi_\tau)\rho] - \mathrm{Tr} \sqrt{\Phi_\tau (\rho \Psi_\pi \rho)}$$

is attained at any $\Gamma \in \mathcal{B}$ satisfying the condition $\Gamma^\dagger \Gamma = \Phi_\tau$, say $\Gamma = \Phi_\tau^{1/2}$, and the corresponding $\Upsilon = \Upsilon_\circ$ satisfying the equation $\Upsilon_\circ \rho \Gamma^\dagger = \sqrt{\Gamma \rho \Psi_\pi \rho \Gamma^\dagger} = \Gamma \rho \Upsilon_\circ^\dagger$. The maximum of this distance over all states,

$$\begin{aligned} d_H^2(\Phi, \Psi) &= \sup_{\varrho \in \mathcal{S}(\mathfrak{g})} d_H^2(\Phi, \Psi)(\varrho) \\ &\equiv \sup_{\varrho \in \mathcal{S}(\mathfrak{g})} \left(\tfrac{1}{2} \mathrm{Tr}[(\Phi_\tau + \Psi_\tau)\rho] - \mathrm{Tr} \sqrt{\Phi_\tau (\rho \Psi_\pi \rho)} \right) \\ &= \sup_{\varrho \in \mathcal{S}(\mathfrak{g})} \inf_{\Gamma, \Upsilon \in \mathcal{B}(\mathfrak{g})} \{Tr[(\Gamma - \Upsilon)^\dagger (\Gamma - \Upsilon)\rho] : \Gamma^\dagger \Gamma = \Phi_\tau, \Upsilon^\dagger \Upsilon = \Psi_\tau\}, \end{aligned}$$

is given by the minimax quadratic distance

$$d_H^2(\Phi, \Psi) = \tfrac{1}{2} \inf_{\Gamma, \Upsilon \in \mathcal{B}(\mathfrak{g})} \{\|\Gamma - \Upsilon\|^2 : \Gamma^\dagger \Gamma = \Phi_\tau, \Upsilon^\dagger \Upsilon = \Psi_\tau\},$$

interchange of the extrema following from standard minimax arguments,[24] and the fact that all Γ, Υ satisfying, respectively, $\Gamma^\dagger \Gamma = \Phi_\tau$ and $\Upsilon^\dagger \Upsilon = \Psi_\tau$ are contained in the unit ball of $\mathcal{B}(\mathfrak{g})$.

B. Semiclassical fidelity

It is straightforward to extend the formalism of Sec. III A involving the commutative Hellinger distance between two positive kernels to the case of mappings from a set X into positive trace-class operators on the Hilbert space $\mathfrak{h}$, i.e., $\boldsymbol{\rho}: x \in X \mapsto \rho(x) \in \mathcal{B}_{\mathsf{T}}(\mathfrak{h})$ and $\boldsymbol{\sigma}: x \in X \mapsto \sigma(x) \in \mathcal{B}_{\mathsf{T}}(\mathfrak{h})$ with $\rho(x), \sigma(x) \geqslant 0$ for all $x \in X$. We thus have the pointwise Hellinger distance

$$d_H^2(\rho(x), \sigma(x)) = \left(\mathbb{1}, \tfrac{1}{2}[\rho(x) + \sigma(x)]\right) - \sqrt{(\mathbb{1}, \rho(x))(\mathbb{1}, \sigma(x))} f(\rho(x), \sigma(x))$$

in terms of the trace pairing $(B, \rho) = \mathrm{Tr}(B\widetilde{\rho})$ of $B \in \mathcal{B} = \mathcal{B}(\mathfrak{h})$ and $\rho \in \mathcal{B}_{\mathsf{T}} = \mathcal{B}_{\mathsf{T}}(\mathfrak{h})$, where

$$f(\rho(x), \sigma(x)) = \frac{(\mathbb{1}, \sqrt{\rho(x)\sigma(x)})}{\sqrt{(\mathbb{1}, \rho(x))(\mathbb{1}, \sigma(x))}} = \frac{\mathrm{Tr} \sqrt{\rho(x)\sigma(x)}}{\sqrt{\mathrm{Tr}\, \rho(x) \mathrm{Tr}\, \sigma(x)}}.$$

The semi-classical operational distance between $\boldsymbol{\rho} = \rho(\cdot)$ and $\boldsymbol{\sigma} = \sigma(\cdot)$ can then be defined as

$$d_H^2(\boldsymbol{\rho}, \boldsymbol{\sigma}) = \sup_{x \in X} d_H^2(\rho(x), \sigma(x)) \equiv \|d_H^2(\rho(\cdot), \sigma(\cdot))\|. \tag{44}$$

When $\mathrm{Tr}\, \rho(x) = 1 = \mathrm{Tr}\, \sigma(x)$ for all $x \in X$, i.e., when $\boldsymbol{\rho}$ and $\boldsymbol{\sigma}$ are *classical-to-quantum*, c-q (or *semiclassical*), channels, Eq. (44) can be written as $d_H^2(\boldsymbol{\rho}, \boldsymbol{\sigma}) = 1 - f(\boldsymbol{\rho}, \boldsymbol{\sigma})$, where

$$f(\boldsymbol{\rho},\boldsymbol{\sigma}) = \inf_{x\in X} \mathrm{Tr}[\rho(x)^{1/2}\sigma(x)\rho(x)^{1/2}]^{1/2} = \inf_{x\in X} \mathrm{Tr}\sqrt{\rho(x)\sigma(x)} \equiv \inf_{x\in X} F(\rho(x),\sigma(x))$$

is the minimax fidelity of $\boldsymbol{\sigma}$ relative to $\boldsymbol{\rho}$.

C. Semiquantum fidelity

Next we consider the opposite of semiclassical operations—namely, the *semiquantum operations* which correspond to quantum measurements as quantum-to-classical (q-c) channels. Such operations are given as

$$\Phi(b) = \int_Y b(y)\Phi_\tau(y)\mathrm{d}\mu(y) \equiv (b,\Phi_\tau)$$

on the algebra $\mathcal{B}=\mathcal{C}(Y)$ of continuous bounded functions $b: Y\to\mathbb{C}$, where $(Y,\mathcal{B}_Y,\mu)$ is a measure space, by specifying the positive operator-valued Bochner μ-integrable functions $\Phi_\tau: Y\to\mathcal{A}=\mathcal{B}(\mathfrak{g})$. If

$$\Phi(1) = (1,\Phi_\tau) = \mathbb{1}_\mathfrak{g},$$

the predual maps $\mathcal{A}\ni\rho\mapsto\Phi_\mathsf{T}(\rho)(\cdot)\in\mathcal{C}_\mathsf{T}(Y)$,

$$\Phi_\mathsf{T}(\rho)(y) := (\Phi_\tau(y),\rho) \equiv \varrho[\Phi_\tau(y)],$$

define for each input quantum state $\varrho\in\mathcal{S}(\mathfrak{g})$ a classical probability density on $(Y,\mathcal{B}_Y,\mu)$, that is, they describe quantum measurements by the positive operator-valued measures (POVMs) $M(\mathrm{d}y)=\Phi_\tau(y)\mathrm{d}\mu(y)$.

In order to avoid technicalities in defining the semi-quantum fidelity distance between two q-c channels $\Phi,\Psi:\mathcal{B}\to\mathcal{A}$, we shall assume that $\Phi_\tau(y),\Psi_\tau(y)$ are weakly continuous bounded functions on Y. Then the squared distance $d_H^2(\Phi,\Psi)$ can be written as

$$\mathrm{d}_H^2(\Phi,\Psi) = \inf_{\Gamma,\Upsilon:\Gamma^\dagger\Gamma=\Phi_\tau,\Upsilon^\dagger\Upsilon=\Psi_\tau} \left\| \int (\Gamma(y)-\Upsilon(y))^\dagger(\Gamma(y)-\Upsilon(y))\mathrm{d}\mu(y) \right\|, \tag{45}$$

where the decompositions $\Gamma^\dagger\Gamma=\Phi_\tau$ and $\Upsilon^\dagger\Upsilon=\Psi_\tau$ are understood in the pointwise sense as

$$\Phi_\tau(y) = \Gamma(y)^\dagger\Gamma(y), \quad \Psi_\tau(y) = \Upsilon(y)^\dagger\Upsilon(y), \quad \forall\, y\in Y.$$

The infimum in Eq. (45) is achieved at any $\Gamma\in\mathcal{A}\otimes\mathcal{C}_\mathsf{T}(Y)$ satisfying the condition $\Gamma^\dagger\Gamma=\Phi_\tau$, say $\Gamma(y)=\Phi_\tau(y)^{1/2}$, and the corresponding $\Upsilon=\Upsilon_\mathrm{o}$ satisfying the equation

$$\Upsilon_\mathrm{o}(y)\rho\Gamma(y)^\dagger = [\Gamma(y)\rho\Psi_\tau(y)\rho\Gamma(y)^\dagger]^{1/2} = \Gamma(y)\rho\Upsilon_\mathrm{o}(y)^\dagger.$$

The maximum of this minimal distance over all states,

$$\mathrm{d}_H^2(\Phi,\Psi) = \sup_{\varrho\in\mathcal{S}(g)} \int \left(\frac{1}{2}\mathrm{Tr}[(\Phi_\tau(y)+\Psi_\tau(y))\rho] - \mathrm{Tr}\sqrt{\Phi_\tau(y)(\rho\Psi_\tau(y)\rho)}\right)\mathrm{d}\mu(y),$$

is equal to $d_H^2(\Phi,\Psi)=1-f(\Phi,\Psi)$ in the measurement operation case $\Phi(1)=\mathbb{1}_\mathfrak{g}=\Psi(1)$, where

$$f(\Phi,\Psi) = \inf_{\varrho\in\mathcal{S}(\mathfrak{g})} \int \mathrm{Tr}\sqrt{\Phi_\tau(y)(\rho\Psi_\tau(y)\rho)}\mathrm{d}\mu(y). \tag{46}$$

D. Operational fidelity formula

Now we can easily evaluate the minimax formula (30) for the fidelity of two general quantum operations $\Phi,\Psi:\mathcal{B}\to\mathcal{A}$, $\mathcal{B}=\mathcal{B}(\mathfrak{h})$, $\mathcal{A}=\mathcal{B}(\mathfrak{g})$. The solution of this problem is also given by Lemma 1 with $R=\Phi_\tau$ and $S=(\rho\otimes\mathbb{1}_\mathfrak{h})\Psi_\tau(\rho\otimes\mathbb{1}_\mathfrak{h})$. For a given $\varrho\in\mathcal{S}(\mathfrak{g})$, the supremum in

$$d_H^2(\Phi,\Psi)(\varrho)=\tfrac{1}{2}(\mathrm{Tr}[(\Phi_\tau+\Psi_\tau)(\rho\otimes\mathbb{1}_\mathfrak{h})]-2\sup_{\Gamma,\Upsilon\in\mathcal{B}(\mathcal{H})}\{\mathrm{Re}\,\mathrm{Tr}[\Gamma^\dagger\Upsilon(\rho\otimes\mathbb{1}_\mathfrak{h})]:\Gamma^\dagger\Gamma=\Phi_\tau,\Upsilon^\dagger\Upsilon=\Psi_\tau\})$$

is equal to $\mathrm{Tr}\sqrt{\Phi_\tau[(\rho\otimes\mathbb{1}_\mathfrak{h})\Psi_\tau(\rho\otimes\mathbb{1}_\mathfrak{h})]}$, and is achieved at any $\Gamma\in\mathcal{B}(\mathcal{H})$ satisfying the condition $\Gamma^\dagger\Gamma=\Phi_\tau$, say $\Gamma=\Phi_\tau^{1/2}$, and the corresponding $\Upsilon=\Upsilon_\mathrm{o}$ satisfying the equation

$$\Upsilon_\mathrm{o}(\rho\otimes\mathbb{1}_\mathfrak{h})\Gamma^\dagger=[\Gamma(\rho\otimes\mathbb{1}_\mathfrak{h})\Psi_\tau(\rho\otimes\mathbb{1}_\mathfrak{h})\Gamma^\dagger]^{1/2}=\Gamma(\rho\otimes\mathbb{1}_\mathfrak{h})\Upsilon_\mathrm{o}^\dagger.$$

When Φ,Ψ are quantum channels, or, equivalently, when the preduals $\Phi_\mathsf{T},\Psi_\mathsf{T}$ are trace preserving, Theorem 1 says that the maximum of this distance over all states,

$$d_H^2(\Phi,\Psi)=\sup_{\varrho\in\mathcal{S}(\mathfrak{g})}\mathrm{Tr}\Big(\tfrac{1}{2}(\Phi_\tau+\Psi_\tau)(\rho\otimes\mathbb{1}_\mathfrak{h})-\sqrt{\Phi_\tau[(\rho\otimes\mathbb{1}_\mathfrak{h})\Psi_\tau(\rho\otimes\mathbb{1}_\mathfrak{h})]}\Big),\tag{47}$$

can be written as $d_H^2(\Phi,\Psi)=1-f(\Phi,\Psi)$, where

$$f(\Phi,\Psi)=\inf_{\varrho\in\mathcal{S}(\mathfrak{g})}\mathrm{Tr}\sqrt{\Phi_\tau[(\rho\otimes\mathbb{1}_\mathfrak{h})\Psi_\tau(\rho\otimes\mathbb{1}_\mathfrak{h})]}\tag{48}$$

is the minimax fidelity between Φ and Ψ.

E. Operational fidelity in terms of Kraus and Stinespring decompositions

Consider, as before, two quantum channels $\Phi,\Psi:\mathcal{B}\to\mathcal{A}$, where $\mathcal{B}=\mathcal{B}(\mathfrak{h})$ and $\mathcal{A}=\mathcal{B}(\mathfrak{g})$. Given the minimax fidelity

$$f(\Phi,\Psi)=\inf_{\varrho\in\mathcal{S}(\mathfrak{g})}\sup_{\substack{\Gamma:\Gamma^\dagger\Gamma=\Phi_\tau\\ \Upsilon:\Upsilon^\dagger\Upsilon=\Psi_\tau}}\mathrm{Re}\,\mathrm{Tr}[\Gamma^\dagger\Upsilon(\rho\otimes\mathbb{1}_\mathfrak{h})]=\inf_{\varrho\in\mathcal{S}(\mathfrak{g})}\sup_{\substack{\Gamma:\Gamma^\dagger\Gamma=\Phi_\tau\\ \Upsilon:\Upsilon^\dagger\Upsilon=\Psi_\tau}}|\mathrm{Tr}[\Gamma^\dagger\Upsilon(\rho\otimes\mathbb{1}_\mathfrak{h})]|$$

between Φ and Ψ, where the second equality follows from Lemma 2, the supremum over all Γ and Υ satisfying, respectively, $\Gamma^\dagger\Gamma=\Phi_\tau$ and $\Upsilon^\dagger\Upsilon=\Psi_\tau$ can be replaced with the supremum over all Kraus decompositions of Φ and Ψ, i.e., over all collections $\{F_j\}$, $\{V_j\}$ of bounded operators $\mathfrak{g}\to\mathfrak{h}$, determined from Φ_τ,Ψ_τ via Eqs. (29) and (28):

$$f(\Phi,\Psi)=\inf_{\varrho\in\mathcal{S}(\mathfrak{g})}\sup_{\{F_j\},\{V_j\}}\left|\sum_j\varrho(F_j^\dagger V_j)\right|.\tag{49}$$

Just as in the proof of Theorem 1, we may restrict ourselves only to those Γ,Υ that can be written as $\Gamma=U\Phi_\tau^{1/2},\Upsilon=V\Psi_\tau^{1/2}$ for some isometries U,V. Thus, if we write $\Phi_\tau^{1/2}$ and $\Psi_\tau^{1/2}$ in the form of Eq. (28) as

$$\Phi_\tau^{1/2}=\sum_j|j\rangle\langle\hat{F}_j|,\quad\Psi_\tau^{1/2}=\sum_j|j\rangle\langle\hat{V}_j|,$$

then it follows that, given isometries U, we can write

$$\Gamma=U\Phi_\tau^{1/2}=\sum_j|j\rangle\left(\sum_\ell U_{j\ell}\hat{F}_\ell\right|\equiv\sum_j|j\rangle\langle\hat{F}_j(U)|,$$

and similarly for $\Upsilon=V\Psi_\tau^{1/2}$. Thus

$$f(\Phi,\Psi)=\inf_{\varrho\in\mathcal{S}(\mathfrak{g})}\sup_{U,V}\left|\sum_j\varrho[\hat{F}_j(U)^\dagger\hat{V}_j(V)]\right|=\inf_{\varrho\in\mathcal{S}(\mathfrak{g})}\sup_U\left|\sum_j\varrho[\hat{F}_j(U)^\dagger\hat{V}_j]\right|.$$

Turning now to the infimum over all normal states ϱ on $\mathcal{A}\equiv\mathcal{B}(\mathfrak{g})$, we may equivalently consider all pairs $\{\varphi,\mathcal{K}\}$, where φ is a normal $*$-representation of $\mathcal{A}$ on a Hilbert space $\mathcal{K}$:

$$f(\Phi,\Psi) := \inf_{\{\varphi,\mathcal{K}\};\upsilon\in\mathcal{K},\|\upsilon\|=1} \sup_{U} \left| \sum_j \langle \upsilon|\varphi[\hat{F}_j(U)^\dagger \hat{V}_j]|\upsilon\rangle \right|.$$

Since all normal $*$-representations of the full operator algebra $\mathcal{B}(\mathfrak{g})$ are unitarily equivalent to an amplification $B\mapsto B\otimes 1_{\mathfrak{k}}$ for some Hilbert space $\mathfrak{k}$, we can write

$$f(\Phi,\Psi) := \inf_{\upsilon\in\mathfrak{g}\otimes\mathfrak{k};\|\upsilon\|=1} \sup_{U} \left| \sum_j \langle \upsilon|\hat{F}_j(U)^\dagger \hat{V}_j \otimes 1_{\mathfrak{k}}|\upsilon\rangle \right|. \tag{50}$$

Introducing the vectors $|\upsilon,\Phi\rangle, |\upsilon,\Psi\rangle \in \mathfrak{g}\otimes\mathfrak{k}\otimes\mathcal{H}$, defined by

$$|\upsilon,\Phi\rangle := \sum_j (\hat{F}_j \otimes 1_{\mathfrak{k}})\upsilon \otimes |j\rangle, \quad |\upsilon,\Psi\rangle := \sum_j (\hat{V}_j \otimes 1_{\mathfrak{k}})\upsilon \otimes |j\rangle,$$

we obtain yet another form of the minimax fidelity:

$$f(\Phi,\Psi) = \inf_{\upsilon\in\mathfrak{g}\otimes\mathfrak{k}} \sup_{U} |\langle \upsilon,\Phi|1_{\mathfrak{g}\otimes\mathfrak{k}} \otimes U|\upsilon,\Psi\rangle|. \tag{51}$$

For a fixed $\upsilon\in\mathfrak{g}\otimes\mathfrak{k}$, taking the supremum over U is tantamount to taking the supremum of $|\langle\chi|\xi\rangle|$ over all pairs of unit vectors $\chi,\xi\in\mathfrak{g}\otimes\mathfrak{k}\otimes\mathcal{H}$ such that

$$\mathrm{Tr}_{\mathcal{H}}|\chi\rangle\langle\chi| = \sum_j (\widetilde{F_j}\otimes 1_{\mathfrak{k}})|\upsilon\rangle\langle\upsilon|(\widetilde{F_j}\otimes 1_{\mathfrak{k}})^\dagger \equiv \Phi_{\mathsf{T}} \otimes \mathrm{id}(|\upsilon\rangle\langle\upsilon|),$$

$$\mathrm{Tr}_{\mathcal{H}}|\xi\rangle\langle\xi| = \sum_j (\widetilde{V_j}\otimes 1_{\mathfrak{k}})|\upsilon\rangle\langle\upsilon|(\widetilde{V_j}\otimes 1_{\mathfrak{k}})^\dagger \equiv \Psi_{\mathsf{T}} \otimes \mathrm{id}(|\upsilon\rangle\langle\upsilon|),$$

which, in conjunction with the standard results on the Uhlmann fidelity (1) between density operators,[6,7] finally yields

$$f(\Phi,\Psi) = \inf_{\upsilon\in\mathfrak{g}\otimes\mathfrak{k}:\|\upsilon\|=1} F(\Phi_{\mathsf{T}} \otimes \mathrm{id}(|\upsilon\rangle\langle\upsilon|), \Psi_{\mathsf{T}} \otimes \mathrm{id}(|\upsilon\rangle\langle\upsilon|)) = \inf_{\varrho\in\mathcal{S}(\mathfrak{g}\otimes\mathfrak{k})} F(\Phi_{\mathsf{T}} \otimes \mathrm{id}(\rho), \Psi_{\mathsf{T}} \otimes \mathrm{id}(\rho)).$$

Note that we may always take $\mathfrak{k}$ isomorphic to $\mathfrak{g}$:

$$f(\Phi,\Psi) = \inf_{\upsilon\in\mathfrak{g}\otimes\mathfrak{g},\|\upsilon\|=1} F(\Phi_{\mathsf{T}} \otimes \mathrm{id}(|\upsilon\rangle\langle\upsilon|), \Psi_{\mathsf{T}} \otimes \mathrm{id}(|\upsilon\rangle\langle\upsilon|)). \tag{52}$$

Given some Kraus decompositions $\{F_j\}$, $\{V_j\}$ of Φ and Ψ, respectively, we may define the operators

$$F\xi := \sum_j F_j\xi \otimes |j\rangle, \quad V\xi := \sum_j V_j\xi \otimes |j\rangle$$

from $\mathfrak{g}$ into $\mathfrak{h}\otimes\mathcal{H}$ and express Φ and Ψ in the Stinespring form $\Phi(B)=F^\dagger(B\otimes 1_{\mathcal{H}})F$, $\Psi(B)=V^\dagger(B\otimes 1_{\mathcal{H}})V$ (cf. Sec. III B). Then we may rewrite Eq. (49) as

$$f(\Phi,\Psi) = \inf_{\varrho\in\mathcal{S}(\mathfrak{g})} \sup_{F,V} |\mathrm{Tr}(F\rho V^\dagger)|,$$

where the supremum is over all $F,V:\mathfrak{g}\to\mathfrak{h}\otimes\mathcal{H}$ giving the Stinespring decompositions of Φ and Ψ, respectively. We may, as before, fix F and V, say, by considering the "canonical" Kraus decompositions $\{\hat{F}_j\}$, $\{\hat{V}_j\}$, and instead take the supremum over all unitaries $U\in\mathsf{U}(\mathcal{H})$:

$$f(\Phi,\Psi) = \inf_{\varrho\in\mathcal{S}(\mathfrak{g})} \sup_{U} |\mathrm{Tr}[(1_{\mathfrak{h}}\otimes U)F\rho V^\dagger]| = \inf_{\varrho\in\mathcal{S}(\mathfrak{g})} \sup_{U} |\mathrm{Tr}[U\,\mathrm{Tr}_{\mathfrak{h}}(F\rho V^\dagger)]|,$$

which yields another useful formula

$$f(\Phi,\Psi) = \inf_{\varrho\in\mathcal{S}(\mathfrak{g})} \|\mathrm{Tr}_{\mathfrak{h}}(F\rho V^{\dagger})\|_{\mathsf{T}} \tag{53}$$

for the minimax fidelity between the channels Φ,Ψ. It is, in fact, not hard to show that the right-hand side of Eq. (53) does not depend on the particular choice of the Stinespring operators F,V, as long as we agree to dilate the input Hilbert space $\mathfrak{h}$ by the "canonical" auxiliary Hilbert space $\mathcal{H}=\mathfrak{g}\otimes\mathfrak{h}$.

We note that the constructions of this section are valid more generally for channels given in terms of the continual Kraus decompositions

$$\Phi(B) = \int_Z F(z)^{\dagger}BF(z)\mathrm{d}\mu(z), \quad \Psi(B) = \int_Z V(z)^{\dagger}BV(z)\mathrm{d}\nu(z),$$

provided that the measures μ and ν are equivalent, i.e., absolutely continuous with respect to each other. Then Eq. (49) is a special instance of the more general expression

$$f(\Phi,\Psi) = \inf_{\varrho\in\mathcal{S}(\mathfrak{g})} \sup_{\{F(z)\},\{V(z)\}} \left| \varrho\left(\int_Z \sqrt{\mathrm{d}\nu/\mathrm{d}\mu}F(z)^{\dagger}V(z)\mathrm{d}\mu(z) \right) \right|,$$

where $\mathrm{d}\nu/\mathrm{d}\mu$ is the Radon-Nikodym derivative of ν with respect to μ, for the case when both μ and ν are counting measures, $\mathrm{d}\mu=\mathrm{d}\nu=1$, on a finite or countably infinite set.

V. PROPERTIES OF THE OPERATIONAL FIDELITY

In this section we establish several key properties of the minimax fidelity between quantum operations. These properties follow almost immediately from the corresponding properties enjoyed by the fidelity (1) on density operators:

(F.1) F is symmetric, $F(\rho,\sigma)=F(\sigma,\rho)$, bounded between 0 and 1, and $F(\rho,\sigma)=1$ if and only if $\rho=\sigma$.

(F.2) F is jointly concave over all pairs of density operators.

(F.3) F is unitarily invariant, i.e., $F(\rho,\sigma)=F(U\rho U^{\dagger},U\sigma U^{\dagger})$ for any unitary U.

(F.4) F is monotone with respect to quantum channels: $F(\Phi_{\mathsf{T}}(\rho),\Phi_{\mathsf{T}}(\sigma))\geqslant F(\rho,\sigma)$ for every quantum channel Φ.

(F.5) The *Bures distance* $d_B(\cdot,\cdot):=\sqrt{1-F(\cdot,\cdot)}$ is topologically equivalent to the trace-norm half-distance $D(\cdot,\cdot)$:

$$2^{-1/2}D(\rho,\sigma) \leqslant d_B(\rho,\sigma) \leqslant \sqrt{D(\rho,\sigma)}$$

[cf. Eq. (3)]. Property (F.2), in fact, follows from *strong concavity* of F,[2] i.e.,

$$F\left(\sum_i p_i\rho_i, \sum_i q_i\sigma_i\right) \geqslant \sum_i \sqrt{p_iq_i}F(\rho_i,\sigma_i) \tag{54}$$

for all $0\leqslant p_i,q_i\leqslant 1$ such that $\Sigma_i p_i=1=\Sigma_i q_i$.

Using Eq. (52), we can immediately obtain for the minimax fidelity $f(\cdot,\cdot)$ on pairs of quantum channels the following analogs of properties (F.1)–(F.4) of the fidelity $F(\cdot,\cdot)$ on pairs of density operators:

(f.1) f is symmetric, bounded between 0 and 1, and $f(\Phi,\Psi)=1$ if and only if $\Phi=\Psi$.

(f.2) f is jointly concave over all pairs of channels.

(f.3) f is invariant under both left and right composition with unitarily implemented channels, i.e.,

$$f(\Theta_U\circ\Phi,\Theta_U\circ\Psi) = f(\Phi,\Psi)$$

and

$$f(\Phi \circ \Theta_V, \Psi \circ \Theta_V) = f(\Phi, \Psi)$$

for any two channels $\Phi, \Psi : \mathcal{B}(\mathfrak{h}) \to \mathcal{B}(\mathfrak{g})$ and any two unitaries $U \in \mathsf{U}(\mathfrak{g})$, $V \in \mathsf{U}(\mathfrak{h})$, where $\Theta_U(B) := U^\dagger B U$, and Θ_V is defined analogously.

(f.4) f is monotone with respect to both left and right composition with quantum channels, i.e., $f(\Phi \circ \Phi_1, \Psi \circ \Phi_1) \geqslant f(\Phi, \Psi)$ and $f(\Phi_2 \circ \Phi, \Phi_2 \circ \Psi) \geqslant f(\Phi, \Psi)$ for any two channels $\Phi, \Psi : \mathcal{B} \to \mathcal{A}$, all channels Φ_1 into $\mathcal{B}$, and all channels Φ_2 on $\mathcal{A}$. Just as in the case of the fidelity between density operators, the minimax fidelity f possesses the strong concavity property

$$f\left(\sum_i p_i \Phi_i, \sum_i q_i \Psi_i\right) \geqslant \sum_i \sqrt{p_i q_i} f(\Phi_i, \Psi_i). \tag{55}$$

On the other hand, deriving for the minimax fidelity f an analog of property (F.5) of the Uhlmann fidelity F requires a bit more work. To this end, let us consider two channels $\Phi, \Psi : \mathcal{B} \to \mathcal{A}, \mathcal{B} = \mathcal{B}(\mathfrak{h}), \mathcal{A} = \mathcal{B}(\mathfrak{g})$. Suppose first that $\mathfrak{g}$ is infinite dimensional and separable. Then $\mathfrak{g} \simeq \ell^2$, and we can rewrite Eq. (55) as

$$f(\Phi, \Psi) = \inf_{v \in \mathfrak{g} \otimes \ell^2 : \|v\| = 1} F(\Phi_\mathsf{T} \otimes \mathrm{id}(|v\rangle\langle v|), \Psi_\mathsf{T} \otimes \mathrm{id}(|v\rangle\langle v|)).$$

The space ℓ^2 contains, as a dense subset, the pre-Hilbert space ℓ_0^2 of all infinite sequences of complex numbers with all but finitely many components equal to zero. Using this fact and the continuity property (F.5) of the fidelity F, we obtain

$$f(\Phi, \Psi) = \inf_{v \in \mathfrak{g} \otimes \ell_0^2 : \|v\| = 1} F(\Phi_\mathsf{T} \otimes \mathrm{id}(|v\rangle\langle v|), \Psi_\mathsf{T} \otimes \mathrm{id}(|v\rangle\langle v|)).$$

Using this expression in conjunction with Eq. (3), we get the bounds

$$f(\Phi, \Psi) \geqslant 1 - \sup_{v \in \mathfrak{g} \otimes \ell_0^2 : \|v\| = 1} D(\Phi_\mathsf{T} \otimes \mathrm{id}(|v\rangle\langle v|), \Psi_\mathsf{T} \otimes \mathrm{id}(|v\rangle\langle v|)), \tag{56}$$

$$f^2(\Phi, \Psi) \leqslant 1 - \sup_{v \in \mathfrak{g} \otimes \ell_0^2 : \|v\| = 1} D^2(\Phi_\mathsf{T} \otimes \mathrm{id}(|v\rangle\langle v|) - \Psi_\mathsf{T} \otimes \mathrm{id}(|v\rangle\langle v|)). \tag{57}$$

Now, for any completely bounded map $\Lambda : \mathcal{B}(\mathfrak{h}) \to \mathcal{B}(\mathfrak{g})$, the image of the set $\{|v\rangle\langle v| : v \in \mathfrak{g} \otimes \ell_0^2, \|v\| = 1\}$ under the predual map $\Lambda_\mathsf{T} \otimes \mathrm{id} : \mathcal{B}_\mathsf{T}(\mathfrak{g} \otimes \ell_0^2) \to \mathcal{B}_\mathsf{T}(\mathfrak{h} \otimes \ell_0^2)$ is contained in the trace-norm closure of the linear span of $\{|\xi\rangle\langle\xi| : \xi \in \mathfrak{h} \otimes \ell_0^2, \|\xi\| = 1\}$, which is dual to the tensor product $\mathcal{B}(\mathfrak{h}) \otimes \mathcal{K}(\ell^2)$, where $\mathcal{K}(\ell^2)$ is the space of compact operators on ℓ^2. Thus, by duality we have

$$\sup_{v \in \mathfrak{g} \otimes \ell_0^2 : \|v\| = 1} D(\Phi_\mathsf{T} \otimes \mathrm{id}(|v\rangle\langle v|), \Psi_\mathsf{T} \otimes \mathrm{id}(|v\rangle\langle v|)) = \tfrac{1}{2} \|(\Phi - \Psi) \otimes \mathrm{id}_{\mathcal{K}(\ell^2)}\| \equiv \mathcal{D}(\Phi, \Psi),$$

where $\mathcal{D}(\Phi, \Psi)$ denotes the CB-norm half-distance $\frac{1}{2}\|\Phi - \Psi\|_{\mathrm{CB}}$, and the last equality follows from the formula $\|\Lambda\|_{\mathrm{CB}} = \|\Lambda \otimes \mathrm{id}_{\mathcal{K}(\ell^2)}\|$ for any completely bounded map Λ.

On the other hand, when $\dim \mathfrak{g} = m < \infty$, we can use the fact[20] that, for any completely bounded map Λ into $\mathcal{B}(\mathfrak{g})$,

$$\|\Lambda\|_{\mathrm{CB}} = \|\Lambda \otimes \mathrm{id}_{\mathcal{M}_m}\| = \|\Lambda_\mathsf{T} \otimes \mathrm{id}_{\mathcal{M}_m}\|_\mathsf{T},$$

where $\mathcal{M}_m$ denotes the algebra of $m \times m$ complex matrices, it follows that

$$\sup_{v \in \mathfrak{g} \otimes \mathfrak{g} : \|v\| = 1} D(\Phi_\mathsf{T} \otimes \mathbb{1}(|v\rangle\langle v|), \Psi_\mathsf{T} \otimes \mathbb{1}(|v\rangle\langle v|)) = \mathcal{D}(\Phi, \Psi).$$

In either case, we immediately derive the inequality

$$1 - \mathcal{D}(\Phi,\Psi) \leqslant f(\Phi,\Psi) \leqslant \sqrt{1 - \mathcal{D}^2(\Phi,\Psi)}, \tag{58}$$

which, when expressed in terms of the Hellinger distance $d_H(\cdot,\cdot) := \sqrt{1-f(\cdot,\cdot)}$ as

$$2^{-1/2}\mathcal{D}(\Phi,\Psi) \leqslant d_H(\Phi,\Psi) \leqslant \sqrt{\mathcal{D}(\Phi,\Psi)}, \tag{59}$$

yields the desired property

(f.5) the Hellinger distance $d_H(\cdot,\cdot) := \sqrt{1-f(\cdot,\cdot)}$ is topologically equivalent to the CB-norm distance [cf. Eq. (59)].

This completes our survey of the basic properties of the minimax fidelity f.

VI. SOME EXAMPLES AND APPLICATIONS

The expressions for the minimax fidelity, derived in Sec. IV for different kinds of quantum operations encountered in quantum information theory, share the common feature of being set up as variational problems, namely, as minimizations of a concave functional over a convex set. This feature of the minimax fidelity renders the problem of computing it amenable to robust numerical methods (see Ref. 3 for detailed discussion of numerical optimization methods for the calculation of fidelitylike measures in quantum information theory). However, there are instances in which the minimax fidelity between two quantum channels can be written down in a more explicit form. In this section we sketch some examples of such instances.

Before we proceed, we would like to remind the reader of the assumption we made in Sec. II B, namely that all the channels we deal with are completely majorized by the trace in the sense of Ref. 14. This assumption, while allowing us to circumvent certain technicalities involving unbounded operators, is somewhat restrictive, as one can easily find examples of quantum channels between infinite-dimensional algebras (e.g., unitarily or isometrically implemented channels; see Ref. 21 for details) that do not satisfy this condition of complete majorization. However, owing to the CB-continuity of the minimax fidelity (cf. Sec. V), we may always regard such channels as CB-limits of sequences of channels with finite-dimensional output algebras. Thus, given a channel $\Phi:\mathcal{B}\to\mathcal{A}, \mathcal{B}=\mathcal{B}(\mathfrak{h}), \mathcal{A}=\mathcal{B}(\mathfrak{g})$ with $\dim\mathfrak{g}=\infty$, we consider a sequence $\{P_n\}$ of finite-dimensional projections such that $P_n\to\mathbb{1}_g$ strongly, and the corresponding sequence $\{\Phi_n\}$ of quantum operations $\Phi_n(B) := P_n\Phi(B)P_n$, so that $\Phi_n(B)\to\Phi(B)$ uniformly as $n\to\infty$ for each $B \in \mathcal{B}$, and each Φ_n is a channel from $\mathcal{B}$ into $P_n\mathcal{A}P_n$, with $\lim_{n\to\infty}\|\Phi-\Phi_n\|_{\mathrm{CB}}=0$.

With this in mind, in the examples below we shall not worry about the issue of bounded versus unbounded operational densities.

A. Unitary maps

In the case of channels Θ_U,Θ_V implemented by the unitaries $U,V:\mathfrak{h}\to\mathfrak{h}$, i.e., $\Theta_U(B) = U^\dagger BU$ and $\Theta_V(B)=V^\dagger BV$, the minimax fidelity $f(\Phi,\Psi)$ is easily evaluated using Eq. (49):

$$f(\Theta_U,\Theta_V) = \inf_{\varrho\in\mathcal{S}(\mathfrak{g})} |\varrho(W)|,$$

where we have defined $W := U^\dagger V$. Let $\mathrm{Sp}(W)$ denote the spectrum of W, which is a closed compact subset of the unit circle $\mathbb{T}$ in the complex plane, and let $E^W(\mathrm{d}z)$ denote the corresponding spectral measure of W. Then we can write

$$f(\Theta_U,\Theta_V) = \inf_{\varrho\in\mathcal{S}(\mathfrak{g})} \left| \int_{\mathrm{Sp}(W)} z M^{W,\varrho}(\mathrm{d}z) \right|,$$

where $M^{W,\varrho}(\mathrm{d}z)$ is the probability measure $\varrho[E^W(\mathrm{d}z)] \equiv (E^W(\mathrm{d}z),\rho)$. Thus

$$f(\Theta_U,\Theta_V) = \mathrm{dist}(0,\overline{\mathrm{co}\,\mathrm{Sp}(W)}), \tag{60}$$

where $\overline{\mathrm{co}\,\mathrm{Sp}(W)}$ denotes the closed convex hull of $\mathrm{Sp}(W)$, and $\mathrm{dist}(z,S) := \inf\{|z-z'| : z' \in S\}$ for any $z \in \mathbb{C}$ and $S \subset \mathbb{C}$. Clearly, $f(\Theta_U,\Theta_V)=1$ if and only if $\overline{\mathrm{co}\,\mathrm{Sp}\,W} \subset \mathbb{T}$, i.e., if and only if $W = \lambda \mathbb{1}_{\mathfrak{h}}$ with $|\lambda|=1$, which is equivalent to $\Theta_U=\Theta_V$.

When $\dim \mathfrak{h} < \infty$, $\mathrm{Sp}(W)$ is a finite subset of $\mathbb{T}$, so that $\overline{\mathrm{co}\,\mathrm{Sp}(W)}$ is a polygon in the complex plane, and Eq. (60) shows that $f(\Theta_U,\Theta_V)$ is simply the distance d from this polygon to the origin. On the other hand, recalling the formula[12] $\mathcal{D}(\Theta_U,\Theta_V)=\sqrt{1-d^2}$, we see that the upper bound in Eq. (58) is saturated by the unitarily implemented channels.

B. Random unitary channels

Continuing with the setup from the preceding example, let us consider channels of the form

$$\Phi(B) = \sum_i p_i \Theta_{U_i}(B), \quad \Psi(B) = \sum_i q_i \Theta_{U_i}(B), \tag{61}$$

where Θ_{U_i} are unitarily implemented channels and $\mathbf{p} \equiv \{p_i\}$, $\mathbf{q} \equiv \{q_i\}$ are probability distributions. It then follows immediately from the strong concavity property (55) of the minimax fidelity that

$$f(\Phi,\Psi) \geqslant \sum_i \sqrt{p_i q_i} \equiv F(\mathbf{p},\mathbf{q}). \tag{62}$$

When $\dim \mathfrak{h} < \infty$, the inequality in (62) becomes equality when the unitaries U_i are orthogonal in the Hilbert-Schmidt sense, $\mathrm{Tr}\, U_i^\dagger U_k = \dim \mathfrak{h} \cdot \delta_{ik}$. On the other hand, when $\mathfrak{h}$ is infinite dimensional, this orthogonality condition does not make sense unless we consider channels given in terms of continual Kraus decompositions, so that the sums in Eq. (62) are replaced with integrals with respect to some positive measure μ, and agree to understand orthogonality in the sense of operator-valued Schwartz distributions. As an example, consider the following.

Let $\mathfrak{h}=\mathcal{F}$, the boson Fock space, let a and $a^\dagger$ be the field annihilation and creation operators, and let $D(z) := \exp(za^\dagger - \overline{z}a)$, $z \in \mathbb{C}$, be the unitary displacement operators obeying the Weyl relation $D(z)D(z') = \mathrm{e}^{\mathrm{i}\,\mathrm{Im}\, zz'} D(z+z')$. Given a function $f \in L^2(\mathbb{C}, \mathrm{d}z)$, where $\mathrm{d}z := \mathrm{d}(\mathrm{Re}\, z)\mathrm{d}(\mathrm{Im}\, z)$, we define its *Weyl-Fourier transform* as $D(f) := \pi^{-1/2}\int_{\mathbb{C}} f(z)D(z)\mathrm{d}z$. Since f is square integrable, $D(f)$ is a Hilbert-Schmidt operator, and it can be easily shown that

$$\mathrm{Tr}[D(f)^\dagger D(g)] = \int_{\mathbb{C}} \overline{f(z)} g(z)\mathrm{d}z \equiv \langle f,g\rangle_{L^2(\mathbb{C})}, \quad \forall\, f,g \in L^2(\mathbb{C})$$

so that $\mathrm{Tr}[D(z)^\dagger D(z')] = \pi\delta^{(2)}(z-z')$, $z,z' \in \mathbb{C}$, where $\delta^{(2)}(\lambda) := \delta(\mathrm{Re}\,\lambda)\delta(\mathrm{Im}\,\lambda)$ is the Dirac δ-function in the complex plane.

With this in mind, consider the family of channels $\Gamma^{(\mu)} : \mathcal{B}(\mathcal{F}) \to \mathcal{B}(\mathcal{F})$, $\mu \in \mathbb{R}^+$, with the preduals given by

$$\Gamma_*^{(\mu)}(\rho) := \frac{1}{\pi\mu}\int_{\mathbb{C}} D(z)\rho D(z)^\dagger \exp(-|z|^2/\mu)\mathrm{d}z$$

(in quantum optics these channels model the so-called *Gaussian displacement noise*[25]). Then the minimax fidelity between $\Gamma^{(\mu)}$ and $\Gamma^{(\nu)}$ is given by

$$f(\Gamma^{(\mu)},\Gamma^{(\nu)}) = \frac{(\mu\nu)^{1/2}}{\frac{1}{2}(\mu+\nu)}. \tag{63}$$

Owing to the inequality between the geometric and the arithmetic means, the right-hand side of Eq. (63) is always bounded between 0 and 1, and the maximum value of 1 is attained if and only

if $\mu=\nu$, i.e., $\Gamma^{(\mu)}=\Gamma^{(\nu)}$. This, of course, agrees with the properties of the minimax fidelity (cf. Sec. V).

C. Master equation

Consider a strongly continuous semigroup of channels $\{\Phi^{(t)}:\mathcal{B}(\mathfrak{h})\to\mathcal{B}(\mathfrak{h})\}_{t\in\mathbb{R}^+}$, with the preduals $\Phi_{\mathrm{T}}^{(t)}$ satisfying the Lindblad master equation[26]

$$\frac{\mathrm{d}\Phi_{\mathrm{T}}^{(t)}(\rho)}{\mathrm{d}t}=X\rho X^\dagger-\frac{1}{2}(X^\dagger X\rho+\rho X^\dagger X) \tag{64}$$

for some $X\in\mathcal{B}(\mathfrak{h})$. Introducing the dilating Hilbert space $\mathcal{H}=\mathfrak{h}\otimes\mathfrak{h}$ with the basis $\{|0\rangle,|1\rangle,\ldots\}$, we can, for an infinitesimal time $t=\varepsilon$, write the predual of the channel $\Phi^{(\varepsilon)}$ in the Stinespring form

$$\Phi_{\mathrm{T}}^{(\varepsilon)}(\rho)=\mathrm{Tr}_{\mathcal{H}}A_\varepsilon\rho A_\varepsilon^\dagger, \tag{65}$$

where the map $A_\varepsilon:\mathfrak{h}\to\mathfrak{h}\otimes\mathcal{H}$ is given by

$$A_\varepsilon\upsilon:=\left(\mathbb{1}_{\mathfrak{h}}-\tfrac{1}{2}\varepsilon X^\dagger X\right)\upsilon\otimes|0\rangle+\sqrt{\varepsilon}X\upsilon\otimes|1\rangle+O(\varepsilon^2), \tag{66}$$

$O(\varepsilon^2)$ indicating terms with norm bounded from above by $M\varepsilon^2$ for some constant $M\geqslant 0$. Note that $A_0\upsilon=\upsilon\otimes|0\rangle$, so that $T^{(0)}=\mathrm{id}$. We can then evaluate the partial trace

$$\mathrm{Tr}_{\mathfrak{h}}[A_\varepsilon\rho A_0^\dagger]=\left(1-\tfrac{1}{2}\varepsilon\langle X^\dagger X\rangle_\rho\right)|0\rangle\langle 0|+\sqrt{\varepsilon}\langle X\rangle_\rho|1\rangle\langle 0|+O(\varepsilon^2), \tag{67}$$

where $\langle B\rangle_\rho:=\mathrm{Tr}(B\rho)$ for $B\in\mathcal{B}(\mathfrak{h})$. Then, again up to an additive term of operator norm $O(\varepsilon^2)$,

$$\mathrm{Tr}_{\mathfrak{h}}[A_\varepsilon\rho A_0^\dagger]^\dagger\mathrm{Tr}_{\mathfrak{h}}[A_\varepsilon\rho A_0^\dagger]\approx\left[\left(1-\tfrac{1}{2}\varepsilon\langle X^\dagger X\rangle_\rho\right)^2+\varepsilon|\langle X\rangle_\rho|^2\right]|0\rangle\langle 0|, \tag{68}$$

which allows us to compute, up to $O(\varepsilon^2)$, the minimax fidelity between the channel $T^{(\varepsilon)}$ after an infinitesimal time ε and the identity map. Using Eq. (53), we obtain

$$f(T^{(\epsilon)},\mathrm{id})=\inf_{\varrho\in\mathcal{S}(\mathfrak{g})}\|\mathrm{Tr}_{\mathfrak{h}}[A_\varepsilon\rho A_0^\dagger]\|_{\mathrm{T}}\approx\sqrt{1-\varepsilon C}, \tag{69}$$

where

$$C=\inf_{\varrho\in\mathcal{S}(\mathfrak{g})}(\langle X^\dagger X\rangle_\rho-|\langle X\rangle_\rho|^2). \tag{70}$$

D. Impossibility of quantum bit commitment

The statement of topological equivalence of the noncommutative Hellinger distance and the CB-norm distance between a pair of quantum channels, i.e., Eq. (59), is essentially the "continuity argument" at the heart of a proof of "impossibility of quantum bit commitment (QBC)."[27] Quantum bit commitment is a cryptographic objective in which one party, Alice, commits a bit to another party, Bob, in such a way that the corresponding protocol is *concealing* (i.e., Bob is not able to retrieve the bit before the opening) and *binding* (i.e., Alice cannot change the bit after the commitment). The impossibility proof asserts that if the protocol is perfectly concealing, then it is necessarily not binding, and invokes a continuity argument for "asymptotically" concealing protocols, stating that Alice's probability of successful cheating approaches unity, while Bob's cheating probability becomes close to the value $\frac{1}{2}$ (pure guessing). (The reader should be aware that the impossibility proof in Ref. 27 is valid for a restricted class of protocols, i.e., those that are nonaborting and have a single commitment step. For wider classes of protocols, it is still a matter of debate whether a secure QBC protocol exists.[28]) In this example we derive the continuity argument from the expression of Alice's and Bob's respective cheating probabilities as a consequence of the topological equivalence between the Hellinger distance and the CB-norm distance in Eq. (59).

From the point of view of Bob, Alice's action of committing the bit is equivalent to a channel $\Phi_{\mathbf{A}^{(b)}}$ on an algebra $\mathcal{B}(\mathfrak{h})$, $\dim \mathfrak{h} < \infty$, for each value of the committed bit $b=0,1$, where $\mathbf{A}^{(b)} \equiv \{A_j^{(b)}\}_{j=1}^k$ is a collection of operators satisfying the Kraus condition $\Sigma_{j=1}^k A_j^{(b)\dagger} A_j^{(b)} = \mathbb{1}$, and $\Phi_{\mathbf{A}^{(b)}}$ denotes the channel induced by this Kraus decomposition. At the opening, Alice informs Bob about which element of the Kraus decomposition $\mathbf{A}^{(b)}$ she actually used in the commitment. However, prior to unveiling the label j, Alice can perform an *EPR attack* with the purpose of changing the Kraus decomposition to another equivalent decomposition $\mathbf{A}^{(b)}(V) \equiv \{A_j^{(b)}(V)\}$, where $A_j^{(b)}(V) := \Sigma_\ell A_l^{(b)} V_{j\ell}$ for some $V \in \mathsf{U}(\mathbb{C}^k)$. The EPR attack is achieved by Alice via the unitary transformation V on an ancillary k-dimensional space $\mathcal{H}$. The conditional probability that Alice can cheat successfully by convincing Bob that she has committed, say, $b=1$, while having successfully committed $b=0$ instead, is given by

$$P_c^A(V,\upsilon) = \sum_j \frac{|\langle \upsilon | A_j^{(0)\dagger}(V) A_j^{(1)} \otimes \mathbb{1}_{\mathcal{H}} | \upsilon \rangle|^2}{\|(A_j^{(1)} \otimes \mathbb{1}_{\mathcal{H}})\upsilon\|^2}, \tag{71}$$

where $\|(A_j^{(0)} \otimes \mathbb{1}_{\mathcal{H}})\upsilon\|^2$ is the probability that the jth Kraus element is unveiled. Which V should Alice use? Without any knowledge of $|\upsilon\rangle$, the best she can do is to adopt a conservative strategy of choosing the V that will maximize her cheating probability in the worst-case scenario, namely for the anonymous state $|\upsilon\rangle$ chosen by Bob to minimize $P_c^A(V,\upsilon)$. This is the *minimax* choice of V, corresponding to the cheating probability

$$\overline{P_c^A} := \sup_{V \in \mathsf{U}(\mathbb{C}^k)} \inf_{\upsilon \in \mathfrak{h} \otimes \mathcal{H}; \|\upsilon\|=1} P_c^A(V,\upsilon). \tag{72}$$

On the other hand, for equiprobable bit values $b \in \{0,1\}$ Bob's optimal probability of cheating is given by the probability of error in discriminating between the corresponding output states, more precisely

$$\overline{P_c^B} = \tfrac{1}{2} + \tfrac{1}{4} \sup_{\upsilon \in \mathfrak{h} \otimes \mathcal{H}; \|\upsilon\|=1} \left\| \rho_{\mathbf{A}^{(0)}}^{\upsilon} - \rho_{\mathbf{A}^{(1)}}^{\upsilon} \right\|_1 = \tfrac{1}{2}[1 + \mathcal{D}(\Phi_{\mathbf{A}^{(0)}}, \Phi_{\mathbf{A}^{(1)}})], \tag{73}$$

where we have defined $\rho_{\mathbf{A}}^{\upsilon} := \Phi_{\mathbf{A}} \otimes \mathrm{id}(|\upsilon\rangle\langle\upsilon|)$. Using Jensen's inequality, we can bound Alice's cheating probability $P_c^A(V,\upsilon)$ from below as

$$P_c^A(V,\upsilon) \geqslant \left| \sum_j |\langle \upsilon | A_j^{(0)}(V)^\dagger A_j^{(1)} \otimes \mathbb{1}_{\mathcal{H}} | \upsilon \rangle| \right|^2. \tag{74}$$

Note that the value of the max-min in Eq. (72) will not change if we perform the maximization over the closed convex hull of $\mathsf{U}(\mathbb{C}^k)$, i.e., the set $\mathsf{K}(\mathbb{C}^k)$ of all linear contractions on $\mathbb{C}^k$, and the minimization over the closed convex hull of the pure states on $\mathfrak{h} \otimes \mathcal{H}$, i.e., the set $\mathcal{S}(\mathfrak{h} \otimes \mathcal{H})$ of states on $\mathcal{B}(\mathfrak{h} \otimes \mathcal{H})$, thus completing the domain of the max-min to the product $\mathsf{K}(\mathbb{C}^k) \times \mathcal{S}(\mathfrak{h} \otimes \mathcal{H})$ of compact convex sets. Now, the functional

$$F(V,\rho) := \sum_j \mathrm{Re}\, \mathrm{Tr}\{\rho [A_j^{(0)}(V)^\dagger A_j^{(1)} \otimes \mathbb{1}_{\mathcal{H}}]\} \tag{75}$$

is affine in both $V \in \mathsf{K}(\mathbb{C}^k)$ and $\rho \in \mathcal{S}(\mathfrak{h} \otimes \mathcal{H})$, so that we can use standard minimax arguments[24] to justify the interchange of extrema in Eq. (72), and then apply Lemma 2 to obtain

$$\sup_{V \in \mathsf{U}(\mathbb{C}^k)} \inf_{\upsilon \in \mathfrak{h} \otimes \mathcal{H}} |F(V, |\upsilon\rangle\langle\upsilon|)| = \sup_{V \in \mathsf{K}(\mathbb{C}^k)} \inf_{\varrho \in \mathcal{S}(\mathfrak{h} \otimes \mathcal{H})} |F(V,\rho)| \tag{76}$$

$$= \inf_{\varrho \in \mathcal{S}(\mathfrak{h} \otimes \mathcal{H})} \sup_{V \in \mathsf{K}(\mathbb{C}^k)} |F(V,\rho)| \tag{77}$$

$$= \inf_{v \in \mathfrak{h} \otimes \mathcal{H}; \|v\|=1} \sup_{V \in \mathrm{U}(k)} |F(V, |v\rangle\langle v|)|. \tag{78}$$

Now, since a monotone function does not affect the saddle point, we can use Eqs. (50), (72), (74), and (78) to obtain

$$\overline{P}_c^A \geqslant f^2(\Phi_{\mathbf{A}^{(0)}}, \Phi_{\mathbf{A}^{(1)}}).$$

Using Eq. (59) and then Eq. (73), we finally obtain the chain of estimates

$$\overline{P}_c^A \geqslant f^2(\Phi_{\mathbf{A}^{(0)}}, \Phi_{\mathbf{A}^{(1)}}) \geqslant [1 - \mathcal{D}(\Phi_{\mathbf{A}^{(0)}}, \Phi_{\mathbf{A}^{(1)}})]^2 \geqslant [1 - 2(\overline{P}_c^B - 1/2)]^2,$$

where it follows that, for "asymptotically" concealing protocols, i.e., those for which $\overline{P}_c^B \to \frac{1}{2}$, Alice's probability of cheating will approach unity, and the protocol will not be binding.

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Generalized density functional theories using the *k*-electron densities: Development of kinetic energy functionals

Paul W. Ayers[a)]
Department of Chemistry, McMaster University, Hamilton, Ontario, L8S 4M1, Canada

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Several explicit formulas for the kinetic energy of a many-electron system as a functional of the *k*-electron density are derived, with emphasis on the electron pair density. The emphasis is on general techniques for deriving approximate kinetic energy functionals and features generalized Weisacker bounds and methods using density-matrix reconstruction. Adapting results from statistical mechanics, a hierarchy of equations is derived that links electron pairs, triplets, quadruplets, etc.; this may be used to derive more accurate approximations. Several methods for defining the exact kinetic energy functional are presented, including the generalizations of the Levy and Lieb formulations of density-functional theory. Together with *N*-representability constraints on the *k*-density, this paper provides the basis for "generalized density functional theories" based on the electron pair density. There are also implications for conventional density-functional theory, notably regarding the development of more accurate density functionals for the kinetic energy. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1922071]

I. INTRODUCTION

Due to the prohibitive cost associated with accurate solutions to the many-electron Schrödinger equation, most computational modeling of many-electron systems does not use the many-electron wave function. Instead, one typically considers some simpler descriptor of the system, typically a few-electron Green's function, density-matrix, or electron density.[1–3] For systems with more than a hundred electrons, these approaches provide the basis for almost every study of many-electron phenomenon. While some of these techniques are exact in principle, practical applications always use approximations, commonly neglecting or approximating certain aspects of electron correlation. One particularly popular method, especially for systems containing hundreds (or even thousands!) of electrons, is density-functional theory.[4,5] In density-functional theory, the electron density is the fundamental descriptor of the system. While there exists an exact formulation of density-functional theory,[6–8] all practical calculations use approximations to the kinetic energy of and the electron–electron repulsion energy between the electrons. Finding accurate approximate functionals is very important, but also very difficult.

Partly motivated by the difficulties one encounters when approximating the kinetic energy and electron–electron repulsion energy in terms of the electron density, there has been recent interest in "higher-order" density-functional theories,[4,5] in which either the first-order reduced density matrix[7,9–31] or the electron pair density[28,32–40] (hereafter called the 2-density) is used as the fundamental variable. In the first case, the kinetic energy functional is known exactly, leaving only the electron–electron repulsion energy to be approximated. When the 2-density

[a)]Electronic mail: ayers@mcmaster.ca

$$\rho_2(\boldsymbol{x}_1,\boldsymbol{x}_2) \equiv \left\langle \Psi \left| \sum_{i=1}^{N} \sum_{j\neq i}^{N} \delta(\boldsymbol{r}_i - \boldsymbol{x}_1)\,\delta(\boldsymbol{r}_j - \boldsymbol{x}_2) \right| \Psi \right\rangle \tag{1}$$

is used as the fundamental variable, the electron–nuclear attraction and electron–electron repulsion energies are known exactly,

$$V_{ne}[\rho_2,v] = \int\int \rho_2(\boldsymbol{x}_1,\boldsymbol{x}_2)\frac{[v(\boldsymbol{x}_1)+v(\boldsymbol{x}_2)]}{2(N-1)}\mathrm{d}\boldsymbol{x}_1\mathrm{d}\boldsymbol{x}_2, \tag{2}$$

$$V_{ee}[\rho_2] = \frac{1}{2}\int\int \frac{\rho_2(\boldsymbol{x}_1,\boldsymbol{x}_2)}{|\boldsymbol{x}_1-\boldsymbol{x}_2|}\mathrm{d}\boldsymbol{x}_1\mathrm{d}\boldsymbol{x}_2, \tag{3}$$

but no explicit expression for the kinetic energy functional is known. However, because the electron–electron repulsion energy is known exactly, there is no need for an adiabatic connection formalism in 2-density functional theory (2-DFT), and the kinetic energy functional of the pair density is homogeneous of degree two with respect to coordinate scaling:[28]

$$T[\rho_2(\boldsymbol{x}_1,\boldsymbol{x}_2)] = \gamma^2 T[\rho_2(\gamma\boldsymbol{x}_1,\gamma\boldsymbol{x}_2)]. \tag{4}$$

Equation (4) is to be contrasted with the much more complicated scaling behavior of the exchange-correlation energy with respect to the electron density.[41]

The kinetic energy component of the exchange-correlation energy, $T_c[\rho]$, also has a very complicated scaling with respect to the electron density.[41] This implies that it may be much easier to develop accurate and robust kinetic energy functionals for the 2-density than it is to develop kinetic energy functionals of the 1-density.[42] (The 1-density is the usual electron density used in density-functional theory.)

There is another obstacle, however, in developing computational methods based on the electron pair density, and that is the N-representability problem: given a kinetic energy functional, the energy and ground state 2-density may be obtained using the variational principle

$$\begin{aligned} E_u^{\mathrm{gs}} &= \min_{\rho_2\in\mathcal{N}}[T[\rho_2] + V_{ee}[\rho_2] + V_{ne}[\rho_2,v]], \\ \rho_2^{\mathrm{gs}}(\boldsymbol{x},\boldsymbol{x}') &= \arg\min_{\rho_2\in\mathcal{N}}[T[\rho_2] + V_{ee}[\rho_2] + V_{ne}[\rho_2,v]], \end{aligned} \tag{5}$$

but the search is restricted to 2-densities that are N-representable. The studies of Davidson,[43] Samveylan,[34] and Pistol[38] demonstrate that forcing the N-representability constraints is not a trivial matter. (Note, in particular, that the explicit constructions of Samveylan and Pistol scale exponentially with the number of electrons.[34,38])

There has been some recent progress in characterizing the ensemble-N-representability constraints for the k-electron spin-densities (hereafter referred to as the k-density), $\rho_k^{\sigma_1\cdots\sigma_k}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k)$. $\rho_k^{\sigma_1\cdots\sigma_k}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_k)$ denotes the probability that there is a σ_1-spin electron at $\boldsymbol{x}_1$, a σ_2-spin electron at $\boldsymbol{x}_2,\ldots$, and a σ_k-spin electron at $\boldsymbol{x}_N$. Thus,

$$\rho_k^{\sigma_1\sigma_2\cdots\sigma_k}(\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_k) \equiv \left\langle \Psi \left| \sum_{i_k\neq i_1,i_2,\ldots,i_{k-1}}^{N} \cdots \sum_{i_2\neq i_1}^{N}\sum_{i_1=1}^{N}\prod_{j=1}^{k} \delta_{s_{i_j},\sigma_j}\delta(\boldsymbol{r}_{i_j}-\boldsymbol{x}_j) \right| \Psi \right\rangle. \tag{6}$$

If $\rho_k^{\sigma_1\cdots\sigma_k}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_k)$ is ensemble-N-representable, then there is an "ensemble average" of electronic states,

$$\Gamma_N^{(N)}(\boldsymbol{z}_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_N;\boldsymbol{z}_1',\boldsymbol{z}_2',\ldots,\boldsymbol{z}_N') \equiv \sum_\nu w_\nu \Psi_\nu(\boldsymbol{z}_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_N)\Psi_\nu^*(\boldsymbol{z}_1',\boldsymbol{z}_2',\ldots,\boldsymbol{z}_N') \tag{7}$$

$(0 \leqslant w_\nu \leqslant 1;\ \Sigma_\nu w_\nu = 1)$, such that

$$\rho_k^{\sigma_1\ldots\sigma_k}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_k) = \sum_\nu w_\nu \left\langle \Psi_\nu \left| \sum_{i_k\neq i_1,i_2,\ldots,i_{k-1}}^{N} \cdots \sum_{i_2\neq i_1}^{N} \sum_{i_1=1}^{N} \prod_{j=1}^{k} \delta_{s_{i_j},\sigma_j}\delta(\boldsymbol{r}_{i_j}-\boldsymbol{x}_j) \right| \Psi_\nu \right\rangle. \tag{8}$$

In Eq. (7) and in the following, $\boldsymbol{z}$ is often used as a shorthand for the spatial and spin coordinates of an electron, $\boldsymbol{z}_i=(\boldsymbol{r}_i,\sigma_i)$.

Even if the N-representability problem for the k-density was solved, the problem of constructing the kinetic energy as a functional of the k-density, however, still remains. This paper addresses this issue by presenting approximate functionals, developing general techniques for deriving new functionals, deriving useful bounds for the kinetic energy, and revealing the links between this problem and other, more conventional, approaches to many-body quantum mechanics. To this end, in Sec. II we prove that exact kinetic energy functionals exist. The construction is explicit (albeit computationally intractable), and is modeled after Levy's and Lieb's constructions of exact functionals in density-functional theory.[7,8] The Levy-constrained search approach has been presented before,[38] but the approach using Lieb's search is new. Section III is concerned with approximate functionals and proving bounds for the kinetic energy. Specificially, two different approaches to the kinetic energy functional are developed, one of which generalizes the Weisacker bounds from density-functional theory[39,40,44] and the other of which is based on density-matrix reconstruction, recovering in a special case the results of March and Santamaria.[45] Section IV points out connections between this approach and other methods in the literature, with emphasis on how extensions to the Lee–Jackson–Feenberg hierarchy of equations can be used to systematically obtain more accurate functionals. Implications for practical computational approaches, including density-functional theory, are discussed in Sec. V.

II. EXACT FUNCTIONALS FROM THE CONSTRAINED-SEARCH AND LEGENDRE-TRANSFORM PROCEDURES

Perhaps the simplest approaches to the kinetic energy functional of the k-density are obtained by extending the methods used to define density-functionals in density-functional theory. For instance, adapting Valone's[17] constrained search[7,46] over ensemble-N-representable density matrices, we have[37]

$$T[\rho_k^{\sigma_1\ldots\sigma_k}] \equiv \underbrace{\min}_{\Gamma_N^{(N)}\to\rho_k^{\sigma_1\ldots\sigma_k}} \mathrm{Tr}(\hat{T}\Gamma_N^{(N)}), \tag{9}$$

where $\Gamma_N^{(N)}$ is a convex sum or "ensemble" of antisymmetric N-electron wave functions [cf. Eq. (7)] and the notation indicates that the search includes only the density matrices that satisfy Eq. (8). This approach to the kinetic energy functional was presented, over a decade ago, in a prescient paper by Ziesche.[39,40]

Note that the electron–nuclear and electron–electron energies are explicit functionals of the k-density, and do not depend on the particular N-electron state with which the k-density is associated; Eq. (9) is then derived directly from the variational principle for the energy, Eq. (5). Note that we can only write Eq. (9) for k-densities that are ensemble-N-representable, as otherwise there will be no $\Gamma_N^{(N)}$ consistent with the k-density in question.

Equivalent to Eq. (9) is the generalization of Lieb's Legendre transform spin-density functional,[8,47] which we state only for the 2-density

$$T[\rho_2] \equiv \underbrace{\sup_{v^\sigma(\boldsymbol{r}),V_r^{\sigma\sigma'}(\boldsymbol{r}_1,\boldsymbol{r}_2)}}\left[E[\{v^\sigma,V_r^{\sigma\sigma'}\};N_\alpha,N_\beta] - \sum_{\sigma,\sigma'=\alpha,\beta}\left(\begin{array}{l}\frac{1}{2}\int\int \rho_2^{\sigma\sigma'}(\boldsymbol{x}_1,\boldsymbol{x}_2)V_r^{\sigma\sigma'}(\boldsymbol{x}_1,\boldsymbol{x}_2)\mathrm{d}\boldsymbol{x}_1\mathrm{d}\boldsymbol{x}_2 \\ -\int\int \rho_2^{\sigma\sigma'}(\boldsymbol{x}_1,\boldsymbol{x}_2)\frac{[v^\sigma(\boldsymbol{x}_1)+v^{\sigma'}(\boldsymbol{x}_2)]}{2(N-1)}\mathrm{d}\boldsymbol{x}_1\mathrm{d}\boldsymbol{x}_2\end{array}\right)\right] \tag{10}$$

where $E[\{v^\sigma,V_r^{\sigma\sigma'}\};N]$ is the energy of an N-electron system with spin-dependent external potentials $\{v^\sigma(\boldsymbol{r})\}_{\sigma=\alpha,\beta}$ and interelectronic interaction potentials $\{V_r^{\sigma\sigma'}(\boldsymbol{r}_1,\boldsymbol{r}_2)\}_{\sigma,\sigma'=\alpha,\beta}$,

$$E[\{v^\sigma,V_r^{\sigma\sigma'}\};N_\alpha,N_\beta] \equiv \underbrace{\min_{\Psi}}\frac{\left\langle \Psi \left| \sum_{\sigma,\sigma'}\sum_{i=1}^{N}\left(\begin{array}{l}-\frac{\nabla_i^2}{2}+|\sigma_i\rangle\frac{v^\sigma(\boldsymbol{r}_i)}{2}\langle\sigma_i|+|\sigma_i'\rangle\frac{v^{\sigma'}(\boldsymbol{r}_i)}{2}\langle\sigma_i'| \\ +\sum_{j>i}^{N}|\sigma_i\rangle|\sigma_j'\rangle V_r(\boldsymbol{r}_i,\boldsymbol{r}_j)\langle\sigma_j'|\langle\sigma_i|\end{array}\right)\right| \Psi \right\rangle}{\langle\Psi|\Psi\rangle}. \tag{11}$$

The Legendre-transform approach to the k-density with $k>2$ is similar, but complicated by the fact that the supremum must include k-body potentials. For this reason we will only derive Eq. (10) in the present work. The spin-free analogues of Eqs. (9) and (10) are perhaps more useful for formal theory: such functionals depend on the components of the spin-resolved 2-density only through

$$\rho_2(\boldsymbol{x},\boldsymbol{x}') = \sum_{\sigma,\sigma'}\rho_2^{\sigma\sigma'}(\boldsymbol{x},\boldsymbol{x}'). \tag{12}$$

The derivation of Eq. (10) will be familiar to density-functional aficionados but, for the sake of completeness, the proof follows. Suppose we are given two systems, with external potentials $v(\boldsymbol{z})\neq\tilde{v}(\boldsymbol{z})$ and interelectron potentials $V_r(\boldsymbol{z},\boldsymbol{z}')\neq\tilde{V}_r(\boldsymbol{z},\boldsymbol{z}')$, where it is understood that external potentials and/or the interelectronic potentials differ by more than just an additive constant. Given the 2-density, $\rho_2^{\sigma\sigma'}(\boldsymbol{z},\boldsymbol{z}')$ of the former system, it follows from the variational principle that

$$T[\rho_2^{\sigma\sigma'}] + \int\int \rho_2(\boldsymbol{z}_1,\boldsymbol{z}_2)\frac{[v(\boldsymbol{z}_1)+v(\boldsymbol{z}_2)]}{2(N-1)}\mathrm{d}\boldsymbol{z}_1\mathrm{d}\boldsymbol{z}_2 + \frac{1}{2}\int\int \rho_2(\boldsymbol{z}_1,\boldsymbol{z}_2)V_r(\boldsymbol{z}_1,\boldsymbol{z}_2)\mathrm{d}\boldsymbol{z}_1\mathrm{d}\boldsymbol{z}_2 > E[\tilde{v},\tilde{V}_r;N_\sigma]. \tag{13}$$

Clearly, then, the maximum value in Eq. (10) is obtained when the search over potentials finds the potentials appropriate to $\rho_2(\boldsymbol{z},\boldsymbol{z}')$, namely $v(\boldsymbol{z})$ and $V_r(\boldsymbol{z},\boldsymbol{z}')$. At the maximum, then, Eq. (10) is an identity,

$$T[\rho_2] \equiv E[v,V_r;N_\sigma] - \int\int \rho_2(\mathbf{z}_1,\mathbf{z}_2)\frac{[v(\mathbf{z}_1)+v(\mathbf{z}_2)]}{2(N-1)}d\mathbf{z}_1 d\mathbf{z}_2 - \frac{1}{2}\int\int \rho_2(\mathbf{z}_1,\mathbf{z}_2)V_2(\mathbf{z}_1,\mathbf{z}_2)d\mathbf{z}_1 d\mathbf{z}_2, \tag{14}$$

which established the exactness of the generalized Lieb functional, Eq. (10).

Just as some N-representable electron densities are not ensemble-v-representable,[8,48] some ensemble-N-representable 2-pair densities will not be ensemble-(v,V_r)-representable. [A 2-density is not ensemble-(v,V_r)-representable if there are no potentials, $(v(\mathbf{z}),V_r(\mathbf{z},\mathbf{z}'))$ for which the 2-density can be expressed as a convex sum of degenerate N-electron ground state(s).] For such states, the maximum in Eq. (10) does not exist, and is replaced by a supremum. (The supremum exists because the kinetic energy of any ensemble-N-representable density-matrices is finite.) Because a supermum is never achieved, if $\tilde{\rho}_2(\mathbf{z},\mathbf{z}')$ is not ensemble-(v,V_r)-representable, then

$$E_{v,V_r}[\tilde{\rho}_2^{nv}] > E[v,V_r;N]. \tag{15}$$

Because 2-densities that are not ensemble-(v,V_r)-representable do not minimize the energy for any choice of potentials, the generalized Lieb functional is consistent with the variational principle. Just as with their density-functional analogues, the constrained search functional, Eq. (9), and the Legendre-transform functional, Eq. (10), are equivalent.[8] The proof, however, is rather more involved than the preceding analysis.

III. APPROXIMATE KINETIC ENERGY FUNCTIONALS

A. Kinetic energy from the *N*-electron distribution function

For real-valued wave functions and pure states, the kinetic energy of the N-electron distribution function,

$$n_N^{(N)}(\mathbf{z}_1,\ldots,\mathbf{z}_N) = (\Psi(\mathbf{z}_1,\ldots,\mathbf{z}_N))^2 \tag{16}$$

is given by[49,50]

$$\begin{aligned} T[n_N^{(N)}] &= \sum_{i=1}^{N}\left\langle \frac{\nabla_i n_N^{(N)}(\mathbf{z}_1,\ldots,\mathbf{z}_N)\cdot\nabla_i n_N^{(N)}(\mathbf{z}_1,\ldots,\mathbf{z}_N)}{8n_N^{(N)}(\mathbf{z}_1,\ldots,\mathbf{z}_N)}\right\rangle_{1\ldots N} \\ &= -\sum_{i=1}^{N}\left\langle \frac{n_N^{(N)}(\mathbf{z}_1,\ldots,\mathbf{z}_N)\nabla_i^2[\ln n_N^{(N)}(\mathbf{z}_1,\ldots,\mathbf{z}_N)]}{8}\right\rangle_{1\ldots N}, \end{aligned} \tag{17}$$

where $\langle\ \rangle_{1\ldots N}$ is a convenient shorthand for the integration over the coordinates of electrons $1,2,\ldots,N$. For $n_N^{(N)}$ that do not correspond to pure states, the kinetic energy functional is significantly more complicated, requiring a constrained search over ensemble-N-representable density matrices, $\Gamma_N^{(N)}$,

$$T[n_N^{(N)}] \equiv \min_{\Gamma_N^{(N)}\to n_N^{(N)}} \mathrm{Tr}[\hat{T}\Gamma_N^{(N)}]. \tag{18}$$

If one naively applies Eq. (17) to an $n_N^{(N)}$ that is ensemble-N-representable, one obtains a lower bound to the true answer,

$$T[n_N^{(N)}] \equiv \min_{\Gamma_N^{(N)}\to n_N^{(N)}} \mathrm{Tr}[\hat{T}\Gamma_N^{(N)}] \geqslant \sum_{i=1}^{N}\left\langle \frac{\nabla_i n_N^{(N)}(\mathbf{z}_1,\ldots,\mathbf{z}_N)\cdot\nabla_i n_N^{(N)}(\mathbf{z}_1,\ldots,\mathbf{z}_N)}{8n_N^{(N)}(\mathbf{z}_1,\ldots,\mathbf{z}_N)}\right\rangle_{1\ldots N}. \tag{19}$$

Equation (19) follows directly from the triangle inequality for the Sobolev ($\mathbb{H}^1$) norm. For completeness, however, an elementary proof of this inequality is provided in the Appendix.

The importance of Eq. (17) [and even Eq. (18)] is that one can *reconstruct* the N-electron density from the 2-density by a variety of methods: cluster expansion techniques, hierarchies of

equations, etc. Though such methods are not practical computational techniques for large numbers of electrons, their mere existence is important, suggesting ways to construct systematically improvable families of approximations to the exact kinetic-energy functional. In particular, methods originally developed for statistical-mechanical simulations of fermions[51] may be profitably applied to computing the kinetic energy of molecular systems.

It is frequently convenient to consider an alternative k-electron density, $n_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k)$, which is normalized to one,

$$n_k^{(N)}(\boldsymbol{z}_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k) \equiv \int\int\int \cdots \int\int\int \Gamma_N^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N;\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)\mathrm{d}\boldsymbol{z}_{k+1}\ldots\mathrm{d}\boldsymbol{z}_N. \tag{20}$$

To obtain the k-density from $n_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)$, one simply multiplies by the appropriate normalization factor, obtaining

$$\rho_k^{\sigma_1\ldots\sigma_k}(\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_k) = \left(\frac{N_\alpha!N_\beta!}{(N_\alpha-m_\alpha)!(N_\beta-m_\beta)!}\right) n_k^{(N)}(\sigma_1,\boldsymbol{x}_1;\ldots;\sigma_k,\boldsymbol{x}_k), \tag{21}$$

where N_α and N_β are the number of α-spin and β-spin electrons and m_α and m_β are the number of α-spin and β-spin indices in $\rho_k^{\sigma_1\ldots\sigma_k}(\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_k)$,

$$m_\sigma \equiv \sum_{i=1}^{k} \delta_{\sigma\sigma_i}. \tag{22}$$

B. Generalized-Weisacker bounds for the kinetic energy

Using Eq. (17), one expects approximations to the kinetic energy may be obtained from the k-density. To this end, we write $n_N^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)$ in terms of $n_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k)$ using Bayes' theorem,

$$f_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N) \equiv \frac{n_N^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)}{n_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k)}. \tag{23}$$

Because $f_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots\boldsymbol{z}_N)$ represents the probability of observing electrons at $(\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N)$ given that there are electrons at $(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k)$,

$$\int\int\ldots\int f_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N)\mathrm{d}\boldsymbol{z}_{k+1}\ldots\mathrm{d}\boldsymbol{z}_N = 1: \tag{24}$$

that is, the probability of observing electrons $k+1,k+2,\ldots,N$ *somewhere* is unity. [Alternatively, Eq. (24) follows directly from the definitions, Eqs. (20) and (23).] With this background we can prove the following theorem:

Theorem 1: *(Lower bounds on the kinetic energy of pure states.)* If $\{\rho_k^{\sigma_1\ldots\sigma_k}\}_{k=1}^N$ are N-representable, the Weisacker-type bounds,

$$T_w^{(k)}[\rho] \equiv \sum_{\sigma_1=\alpha,\beta}\left[N_{\sigma_1}\left(\frac{(N_\alpha-m_\alpha)!(N_\beta-m_\beta)!}{N_\alpha!N_\beta!}\right)\times\max_{\sigma_2,\sigma_3,\ldots,\sigma_k}\int\int\cdots\int\frac{\nabla_1\rho_k^{\sigma_1\ldots\sigma_N}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k)\nabla_1\rho_k^{\sigma_1\ldots\sigma_N}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k)}{8\rho_k^{\sigma_1\ldots\sigma_N}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k)}\mathrm{d}\boldsymbol{r}_1,\ldots,\mathrm{d}\boldsymbol{r}_k\right] \tag{25}$$

provide a nondecreasing set of bounds on the true kinetic energy of the system,

$$T_w^{(1)}[\rho_1^{\sigma_1}] \leqslant T_w^{(2)}[\rho_2^{\sigma_1\sigma_2}] \leqslant \cdots \leqslant T_w^{(N)}[\rho_N^{\sigma_1\ldots\sigma_N}] \leqslant T_{\text{exact}}. \tag{26}$$

The inequalities are strict unless $f_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots\boldsymbol{z}_N)$ is constant for all $\boldsymbol{z}_1$ for some $k<N$, in which case $T_w^{(k)}=T_w^{(k+1)}=\cdots=T_w^{(N)}$. [In Eq. (25), it is understood that the variation over spin states

is restricted by the multiplicity of the system. That is, the number of σ-spin electrons, m_σ, in Eq. (25) cannot exceed the total number of electrons with this spin, N_σ.]

Proof: The Weisacker functional can be shown to be a lower bound to the true kinetic energy using the Cauchy–Schwarz inequality,[52] and Eq. (26) follows from a straightforward generalization of that argument. A more elementary method of proof will suffice here, however. Substituting the definition of $f_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N)$ into Eq. (17), we can write[49,53]

$$
\begin{aligned}
T[n_N^{(N)}] &= \sum_{\sigma_1=\alpha,\beta} N_{\sigma_1} \int \left\langle \frac{|\nabla_1 (n_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k) f_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N))|^2}{8 n_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k) f_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N)} \right\rangle_{2\ldots N} \mathrm{d}\boldsymbol{r}_1 \\
&= \sum_{\sigma_1=\alpha,\beta} N_{\sigma_1} \int \left\langle \frac{|\nabla_1 n_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k)|^2}{8 n_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k)} f_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N) \right\rangle_{2\ldots N} \mathrm{d}\boldsymbol{r}_1 \\
&\quad + \sum_{\sigma_1=\alpha,\beta} N_{\sigma_1} \int \frac{1}{4} \langle \nabla_1 n_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k) \cdot \nabla_1 f_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N) \rangle_{2\ldots N} \mathrm{d}\boldsymbol{r}_1 \\
&\quad + \sum_{\sigma_1=\alpha,\beta} N_{\sigma_1} \int \left\langle \frac{n_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k)}{8 f_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N)} \cdot \right. \\
&\qquad \left. \times |\nabla_1 f_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N)|^2 \right\rangle_{2\ldots N} \mathrm{d}\boldsymbol{r}_1 \\
&= \sum_{\sigma_1=\alpha,\beta} N_{\sigma_1} \int \left\langle \frac{|\nabla_1 n_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k)|^2}{8 n_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k)} \right\rangle_{2\ldots k} \mathrm{d}\boldsymbol{r}_1 \\
&\quad + \sum_{\sigma_1=\alpha,\beta} N_{\sigma_1} \int \frac{1}{4} \langle \nabla_1 n_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k) \cdot \nabla(1) \rangle_{2\ldots k} \mathrm{d}\boldsymbol{r}_1 \\
&\quad + \sum_{\sigma_1=\alpha,\beta} N_{\sigma_1} \int \left\langle n_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k) \frac{|\nabla_1 f_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N)|^2}{8 f_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N)} \right\rangle_{2\ldots N} \mathrm{d}\boldsymbol{r}_1 .
\end{aligned}
\tag{27}
$$

The normalization of $f_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N)$ [Eq. (24)] is used to make the second simplification in Eq. (27). Note that the last term in Eq. (27), as a product of two non-negative functions, will be positive unless $f_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N)$ is a constant, independent with respect to changes in $\boldsymbol{z}_1$, so that $\nabla_1 f_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k|\boldsymbol{z}_{k+1},\ldots,\boldsymbol{z}_N)=0$. For this reason,

$$
T[n_N^{(N)}] \geqslant \sum_{\sigma_1=\alpha,\beta} N_{\sigma_1} \int \left\langle \frac{|\nabla_1 n_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k)|^2}{8 n_k^{(N)}(\boldsymbol{r}_1,\sigma_1,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_k)} \right\rangle_{2\ldots k} \mathrm{d}\boldsymbol{r}_1 . \tag{28}
$$

Next, note that the result is independent of the spins of electrons $2\ldots N$, provided the total number of α-spin electrons and β-spin electrons in Eq. (27) are N_α and N_β, respectively. That is, due to the symmetry of $n_N^{(N)}$ with respect to interchange of electronic coordinates (both space and spin), we need not sum over spin in evaluating the angular brackets in Eqs. (17), (27), and (28) (provided we renormalize $n_k^{(N)}$ so that $\langle n_k^{(N)} \rangle_{1\ldots k}=1$). It follows from the derivation, then, that Eq. (28) holds regardless how we choose the spins of electrons $2\ldots N$. Choosing the spins to make the bound as tight as possible gives

$$T[n_N^{(N)}] \geqslant \sum_{\sigma_1=\alpha,\beta} N_{\sigma_1} \underbrace{\max}_{\sigma_2,\sigma_3,\ldots,\sigma_k} \left\langle \frac{|\nabla_1 n_k^{(N)}(\boldsymbol{r}_1,\sigma_1;\boldsymbol{r}_2,\sigma_2,\ldots,\boldsymbol{r}_k,\sigma_k)|^2}{8n_k^{(N)}(\boldsymbol{r}_1,\sigma_1;\boldsymbol{r}_2,\sigma_2,\ldots,\boldsymbol{r}_k,\sigma_k)} \right\rangle_{1\ldots k}. \tag{29}$$

Equation (25) follows from the relation between n_k^N and $\rho_k^{\sigma_1\cdots\sigma_k}$,. Noting that $T_w^{(1)}[\rho_1^{\sigma_1}]$ is the Weisacker bound on the kinetic energy,[44] we call $T_w^{(k)}[\rho_k^{\sigma_1\cdots\sigma_k}]$ the *k*th-Weisacker bound.[44] Since $T_w^{(N)}[\rho_N^{\sigma_1\cdots\sigma_N}]$ is given by Eq. (17), the *N*th-Weisacker bound is a lower bound for ensemble-*N* representable $\rho_k^{\sigma_1\cdots\sigma_k}$, and exact for pure-state-*N*-representable $\rho_k^{\sigma_1\cdots\sigma_k}$.

It remains to show that the Weisacker bounds, $T_w^k[\rho_k^{\sigma_1\cdots\sigma_k}]$, are an increasing sequence of approximations to the true kinetic energy. Defining

$$b_{k-1}^{(k)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_{k-1}|\boldsymbol{z}_k) \equiv \frac{n_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k)}{n_{k-1}^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_{k-1})} \tag{30}$$

and repeating the argument in Eq. (27), we find that

$$T_w^{(k-1)}[\rho_{k-1}^{\sigma_1,\ldots\sigma_{k-1}}] \leqslant T_w^{(k)}[\rho_k^{\sigma_1\cdots\sigma_k}] \tag{31}$$

with the equality holding only if

$$\sum_{\sigma_1=\alpha,\beta} N_{\sigma_1} \left\langle n_{k-1}^{(N)}(\boldsymbol{r}_1,\sigma_1,\ldots,\boldsymbol{r}_{k-1},\sigma_{k-1}) \frac{|\nabla_1 b_{k-1}^{(k)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_{k-1}|\boldsymbol{z}_k)|^2}{8b_{k-1}^{(k)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_{k-1}|\boldsymbol{z}_k)} \right\rangle_{1\ldots k} = 0 \tag{32}$$

for some choice of the electron spins, $\{\sigma_i\}_{i=2}^k$. But this would indicate that

$$b_{k-1}^{(k)} = \frac{f_{k-1}^{(N)}}{f_k^{(N)}}$$

is constant with respect to changes in any of the first $k-1$ electronic coordinates. Because $f_{k-1}^{(N)}$ has the coordinate of the $(k-1)$st electron as a variable, while $f_k^{(N)}$ does not, this implies that $f_{k-1}^{(N)}$ (and hence $f_k^{(N)}$) is also constant with respect to changes in any of the first $k-1$ electronic coordinates. That the Weisacker bounds form an increasing sequence immediately follows. □

We conclude this section by discussing the accuracy of the Weisacker bounds. Clearly, the Weisacker bound from the 2-density will be tighter than that from the usual electron density. That is, just because the Weisacker kinetic energy functional is not suitable for density-functional theory does not mean that $T_w^{(k)}[\rho_k^{\sigma_1\cdots\sigma_k}]$ is similarly poor. In particular, the derivation of Eq. (27) shows that the error in $T_w^{(k)}[\rho_k^{\sigma_1\cdots\sigma_k}]$ is caused by neglecting the correlated motions between groupings containing more than *k* electrons. While assuming that electrons act totally independently is a poor assumption, we might expect that except for those rare instances where more than two electrons are close together, the effect of correlations between three (or more) electrons can be safely neglected. It is reasonable to hope that $T_w^{(2)}[\rho_2^{\sigma_1\sigma_2}]$ is already a good approximation to the kinetic energy and, by the same argument, that the quality of the Weisacker bounds rapidly improves with increasing *k*.

Another perspective on the Weisacker bounds is obtained by considering the *N*-representability of the underlying density matrices. $T_w^{(k)}[\rho_k^{\sigma_1\cdots\sigma_k}]$ can be derived by assuming that the *k*th order reduced density matrix,

$$\Gamma_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k;\boldsymbol{z}_1',\ldots,\boldsymbol{z}_k') = \sum_{i=1}^{\infty} \omega_i^{(k,N)} \psi_i^{(k,N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k) \psi_i^{(k,N)}(\boldsymbol{z}_1',\ldots,\boldsymbol{z}_k') \tag{33}$$

has only one occupied "natural" *k*-electron function, $\psi_i^{(k,N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k) \equiv \sqrt{n_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k)}$. That is,

$$\Gamma_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k;\boldsymbol{z}_1',\ldots,\boldsymbol{z}_k') \approx \sqrt{n_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k)}\sqrt{n_k^{(N)}(\boldsymbol{z}_1',\ldots,\boldsymbol{z}_k')}. \tag{34}$$

Note that the maximum (in this case, only) occupation number of $\Gamma_k^{(N)}$ is 1, which violates an N-representability condition on the occupation numbers, $\{\omega_i^{(k,N)}\}_{i=1}^{\infty}$ of the kth-order reduced density matrix,[54–57]

$$\max_i \omega_i^{(k,N)} \leqslant \frac{1}{N-k+1}, \tag{35}$$

unless $k=N$. That is, the Pauli exclusion principle prevents all the electrons in an N-electron system for being described by the same k-electron state.

We may profitably construct approximate kinetic energy functionals based on the analysis in Eq. (27). For instance, one may consider

$$T[\rho_k^{\sigma_1\cdots\sigma_k}] \approx T_w^{(k)}[\rho_k^{\sigma_1\cdots\sigma_k}] + \sum_{\sigma_1=\alpha,\beta} N_{\sigma_1}\left(\frac{(N_\alpha-m_\alpha)!(N_\beta-m_\beta)!}{N_\alpha!N_\beta!}\right) \times\left\langle \rho_k^{\sigma_1\cdots\sigma_k}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k)\frac{|\nabla_1\tilde{f}_k^{(N)}(\boldsymbol{r}_1,\sigma_1;,\ldots;\boldsymbol{r}_k,\sigma_k|\boldsymbol{r}_{k+1},\sigma_{k+1};,\ldots;\boldsymbol{r}_N\sigma_N)|^2}{8\tilde{f}_k^{(N)}(\boldsymbol{r}_1,\sigma_1;,\ldots;\boldsymbol{r}_k,\sigma_k|\boldsymbol{r}_{k+1},\sigma_{k+1};,\ldots;\boldsymbol{r}_N\sigma_N)}\right\rangle_{1\ldots N}, \tag{36}$$

where $\tilde{f}_k^{(N)}$ denotes an approximation to the exact conditional probability distribution function defined by Eq. (23). Since Eq. (36) requires performing a $3N$-dimensional integration, it will probably be more practical to settle for approximations of a high-order Weisacker approximation. For example, a functional of the form

$$T_w^{(n)}[\rho_n^{\sigma_1\cdots\sigma_n}] \approx T_w^{(k)}[\rho_k^{\sigma_1\cdots\sigma_k}] + \sum_{\sigma_1=\alpha,\beta} N_{\sigma_1}\left(\frac{(N_\alpha-m_\alpha)!(N_\beta-m_\beta)!}{N_\alpha!N_\beta!}\right) \times\left\langle \rho_k^{\sigma_1\cdots\sigma_k}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k)\frac{|\nabla_1\tilde{b}_k^{(n)}(\boldsymbol{r}_1,\sigma_1;,\ldots;\boldsymbol{r}_k,\sigma_k|\boldsymbol{r}_{k+1},\sigma_{k+1};,\ldots;\boldsymbol{r}_n\sigma_n)|^2}{8\tilde{b}_k^{(n)}(\boldsymbol{r}_1,\sigma_1;,\ldots;\boldsymbol{r}_k,\sigma_k|\boldsymbol{r}_{k+1},\sigma_{k+1};,\ldots;\boldsymbol{r}_n\sigma_n)}\right\rangle_{1\ldots n}, \tag{37}$$

where $\tilde{b}_k^{(n)}$ approximates the conditional distribution function defined by Eq. (30), could be significantly more accurate than the kth-order Weisacker approximation. Based on the preceding arguments, one expects functionals like Eq. (37) will typically underestimate the kinetic energy of a system.

C. Weisacker functionals for the kinetic energy of the 2-density

The form of the Weisacker functional for the 2-density is of special interest in the present work, as the 2-density is the simplest quantity for which the electron–electron repulsion energy can be evaluated exactly. Define the pair correlation function,

$$g_2^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2) \equiv \frac{\rho_2^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)}{\rho_1^{\sigma_1}(\boldsymbol{r}_1)\rho_1^{\sigma_2}(\boldsymbol{r}_2)}, \tag{38}$$

and the hole correlation function,

$$h_2^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2) \equiv g_2^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2) - 1. \tag{39}$$

Recalling the normalization of the exchange-correlation hole,

$$\int \rho_1^{\sigma_2}(\boldsymbol{r}_2) h^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)\mathrm{d}\boldsymbol{r}_2 = -\,\delta_{\sigma_1\sigma_2}, \tag{40}$$

$T_w^2[\rho_2^{\sigma_1\sigma_2}]$ can be simplified to

$$T_w^{(2)}[\rho] \equiv \sum_{\sigma_1=\alpha,\beta} N_{\sigma_1} \cdot \underbrace{\max_{\sigma_2=\alpha,\beta}}\left[\left(\frac{(N_\alpha-\delta_{\alpha\sigma_1}-\delta_{\alpha\sigma_2})!(N_\beta-\delta_{\beta\sigma_1}-\delta_{\beta\sigma_2})!}{N_\sigma!N_\beta!}\right)\right.$$
$$\left.\times\int\int \frac{\nabla_1\rho_2^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)\cdot\nabla_1\rho_2^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)}{8\rho_2^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)}\mathrm{d}\boldsymbol{r}_1\mathrm{d}\boldsymbol{r}_2\right]$$
$$=\sum_{\sigma_1=\alpha,\beta}\left[T_w^{(1)}[\rho_1^{\sigma_1}]+\underbrace{\max_{\sigma_2=\alpha,\beta}}\left[\left(\frac{N_{\sigma_1}(N_\alpha-\delta_{\alpha\sigma_1}-\delta_{\alpha\sigma_2})!(N_\beta-\delta_{\beta\sigma_1}-\delta_{\beta\sigma_2})!}{N_\alpha!N_\beta!}\right)\right.\right.$$
$$\left.\left.\times\int\int\rho_1^{\sigma_1}(\boldsymbol{r}_1)\rho_1^{\sigma_2}(\boldsymbol{r}_2)\frac{\nabla_1 h_2^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)\cdot\nabla_1 h_2^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)}{8(1+h_2^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2))}\mathrm{d}\boldsymbol{r}_1\mathrm{d}\boldsymbol{r}_2\right]\right]$$
$$\leqslant T_{\mathrm{exact}}[\rho_2]. \tag{41}$$

Corrections to the second-order Weisacker functional can be constructed using Eq. (37). Since relatively simple methods for constructing the 3-density and 4-density from the 2-density are known (see, for example, Secs. III G and III H), approximations to $T_w^{(3)}$ and $T_w^{(4)}$ should be feasible.

After this paper was submitted, results equivalent to those of this section were published by Furche.[40] There is also a strong connection between this model for the kinetic-energy of the 2-density and the equations for $\sqrt{\rho_2(\boldsymbol{r}_1,\boldsymbol{r}_2)}$ proposed by Nagy[32,39] (and later by Furche[40]); the "uncorrected" kinetic energy computed in such theories is implicitly identical to Eq. (41) (albeit without the maximization over the choice of spins). The derivations and explanation in these references offer an instructive perspective that is often complementary to that presented here.

D. Kinetic energy from reduced density matrices

To this point we have focused on the idea that the kinetic energy can be computed (either approximately or exactly) from the k-density. A more common approach, however, is to use the kth-order reduced density matrix, $\Gamma_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k;\boldsymbol{z}_1',\ldots,\boldsymbol{z}_k')$ [cf. Eq. (34)].[54,55] From the definition of the reduced density matrix,

$$T[\Gamma_k^{(N)}] \equiv \sum_{\sigma_1=\alpha,\beta} N_{\sigma_1}\int\int\int\left(\begin{array}{l}\delta(\boldsymbol{r}_1-\boldsymbol{r}_1')\\ \times-\dfrac{\nabla_1^2}{2}\Gamma_k^{(N)}(\boldsymbol{r}_1,\sigma_1;\ldots;\boldsymbol{r}_k,\sigma_k;\boldsymbol{r}_1',\sigma_1;\boldsymbol{r}_2,\sigma_2;\ldots;\boldsymbol{r}_k,\sigma_k)\end{array}\right)\mathrm{d}\boldsymbol{r}_1\ldots\mathrm{d}\boldsymbol{r}_k\mathrm{d}\boldsymbol{r}_1'. \tag{42}$$

That is, we need only evaluate the kinetic energy of a single electron (all electrons are identical), with the kinetic energy appropriately weighted by the number of electrons of each spin. From Eq. (42), just the first-order density matrix is sufficient to compute the kinetic energy,

$$T[\Gamma_1^{(N)}] \equiv \sum_{\sigma=\alpha,\beta} N_\sigma\int\int\delta(\boldsymbol{x}-\boldsymbol{x}')\left(-\frac{\nabla_x^2}{2}\right)\Gamma_1^{(N)}(\boldsymbol{x},\sigma;\boldsymbol{x}',\sigma)\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{x}'. \tag{43}$$

The importance of Eq. (43) arises from the existence of methods for constructing the reduced density matrices and Green's functions (of which the reduced density matrices can be regarded as initial values) from k-densities. The first-order reduced density matrix is of special interest: not only is Eq. (43) an especially simple functional, but also because the known ensemble-N-representability conditions for $\Gamma_1^{(N)}$ constrain the derivation of methods for constructing approximate first-order density matrices from 2-densities.

Even though exact reconstruction is probably computationally impracticable, approximate reconstructions may be useful insofar as the reduced density matrices so constructed should be "close to" ensemble-*N*-representable," in the sense that the (unknown and/or unenforced) *N*-representability constraints will be only "slightly" violated. (Similar considerations presumably underlie the computational utility of the contracted Schrödinger equation, whereby the interrelations between the density matrices seems to help solve the *N*-representability problem by severely restricting the number of permissible density matrices.)[58–63]

The significance of the preceding abstract discussion is bolstered by the existence of a general method for constructing the $(k-1)$-order reduced density matrix from the k-density. To this end, write the cumulant expansion for $\Gamma_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k;\boldsymbol{z}_1',\ldots,\boldsymbol{z}_k')$ in terms of reduced density matrices of lower order plus a "connected piece," $\Delta_k^{(N)}(\boldsymbol{z}_1,\ldots\boldsymbol{z}_k;\boldsymbol{z}_1',\ldots,\boldsymbol{z}_k')$, correcting this form.[64–66] The sequential relation between the density matrices,

$$\Gamma_j^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_j;\boldsymbol{z}_1',\ldots,\boldsymbol{z}_j') = \int\int\int \Gamma_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k;\boldsymbol{z}_1',\ldots,\boldsymbol{z}_k')\mathrm{d}\boldsymbol{z}_{j+1}\ldots\mathrm{d}\boldsymbol{z}_k, \tag{44}$$

allows us to write the lower-order density matrices in the cumulant expansion in terms of $\Gamma_{k-1}^{(N)}$, so that the cumulant expansion equation can be written in the form

$$\Gamma_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k;\boldsymbol{z}_1',\ldots,\boldsymbol{z}_k') = f(\Gamma_{k-1}^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_{k-1};\boldsymbol{z}_1',\ldots,\boldsymbol{z}_{k-1}')) + \Delta_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k;\boldsymbol{z}_1',\ldots,\boldsymbol{z}_k'). \tag{45}$$

The connected piece, $\Delta_k^{(N)}$, is either neglected or approximated using the k-density and/or the $(k-1)$-order density matrix. Setting the primed variables equal to the unprimed variables in Eq. (45) gives a nonlinear equation for $\Gamma_{k-1}^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_{k-1};\boldsymbol{z}_k,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_{k-1})$ in terms of the k-density. $\Gamma_{k-1}^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_{k-1};\boldsymbol{z}_k,\boldsymbol{z}_2,\ldots,\boldsymbol{z}_{k-1})$ can then be used to approximate the kinetic energy,

$$\begin{aligned} T_{\mathrm{DM}}^{(k)}[\rho_k^{\sigma_1\cdots\sigma_k}] &\equiv \sum_{s=\alpha,\beta} N_s \int\int\int \left(\begin{array}{l} \delta(\boldsymbol{r}_1-\boldsymbol{r}_k) \\ \times\left(-\frac{\nabla_1^2}{2}\right)\Gamma_{k-1}^{(N)}(\boldsymbol{r}_1,s;\boldsymbol{r}_2,\sigma_2;\ldots,\boldsymbol{r}_{k-1},\sigma_{k-1};\boldsymbol{r}_k,s;\boldsymbol{r}_2,\sigma_2;\ldots,\boldsymbol{r}_{k-1},\sigma_{k-1}) \end{array} \right) \mathrm{d}\boldsymbol{r}_1\cdots\mathrm{d}\boldsymbol{r}_k \\ &\approx T_{\mathrm{exact}}[\rho_k^{\sigma_1\cdots\sigma_k}]. \end{aligned} \tag{46}$$

For $k>2$, the kinetic energy constructed using this procedure, $T_{\mathrm{DM}}^{(k)}[\rho_k]$, is an upper bound on the true kinetic energy if

- the k-density and the $(k-1)$-order density matrix constructed therefrom have the same 2-density and $\Gamma_{k-1}^{(N)}$ is ensemble-*N*-representable
  or
- there exists an ensemble-*N*-representable $(k-1)$-order density matrix with the correct 2-density and a lower kinetic energy than the $\Gamma_{k-1}^{(N)}$ determined from Eq. (45).

The second condition is sufficient to ensure that the kinetic energy functional using the first-order density matrix, $T_{\mathrm{DM}}^{(1)}[\rho_2]$, will be an upper bound to the true kinetic energy.

E. Density-matrix functionals for the kinetic energy of the 2-density

In general, there is no explicit solution to Eq. (45), which must then be solved numerically. However, when the 2-density is used, the cumulant expansion takes a simple form, namely

$$\gamma_2^{\sigma_1\sigma_1'\sigma_2\sigma_2'}(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{r}_1',\boldsymbol{r}_2') = \gamma_1^{\sigma_1\sigma_1'}(\boldsymbol{r}_1;\boldsymbol{r}_1')\gamma_1^{\sigma_2\sigma_2'}(\boldsymbol{r}_2;\boldsymbol{r}_2') - \gamma_1^{\sigma_1\sigma_2}(\boldsymbol{r}_1;\boldsymbol{r}_2')\gamma_1^{\sigma_1'\sigma_2'}(\boldsymbol{r}_1';\boldsymbol{r}_2) + \mathcal{D}_2^{\sigma_1\sigma_1'\sigma_2\sigma_2'}(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{r}_1',\boldsymbol{r}_2'), \tag{47}$$

where, for convenience, we have used density matrices,

$$\gamma_k^{\sigma_1\ldots\sigma_k\sigma_1'\ldots\sigma_k'}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k;\boldsymbol{r}_1',\ldots,\boldsymbol{r}_k') \equiv \left(\frac{N_\alpha! N_\beta!}{(N_\alpha - m_\alpha)!(N_\beta - m_\beta)!}\right)\Gamma_k^{(N)}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k;\boldsymbol{z}_1',\ldots,\boldsymbol{z}_k'), \tag{48}$$

with the same normalization as the k-densities. [The relationship between $\Gamma_k^{(N)}$ and $\gamma_k^{\sigma_1\ldots\sigma_k'}$ is directly analogous to that between $n_k^N(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_k)$ and $\rho_k^{\sigma_1\ldots\sigma_k}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k)$, cf. Eq. (21).]

Setting the primed and unprimed variables equal in Eq. (47), and using the definition of the hole correlation function [Eq. (39)], one finds

$$\rho_1^{\sigma_1}(\boldsymbol{r}_1)\rho_1^{\sigma_2}(\boldsymbol{r}_2)h^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2) = -\left|\gamma_1^{\sigma_1\sigma_2}(\boldsymbol{r}_1;\boldsymbol{r}_2)\right|^2 + \mathcal{D}_2^{\sigma_1\sigma_2\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{r}_1,\boldsymbol{r}_2). \tag{49}$$

Renewed interest in natural orbital functional theories has seen the proliferation of a variety of expressions for $\mathcal{D}_2^{\sigma_1\sigma_2\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{r}_1,\boldsymbol{r}_2)$ in terms of the natural orbitals of the first-order density matrix,[13,15,20,21,26]

$$\gamma_1^{\sigma}(\boldsymbol{r}_1;\boldsymbol{r}_1') \equiv \sum_{i=1}^{\infty} \pi_{i,\sigma}^{(1)}\chi_{i,\sigma}^{(1)}(\boldsymbol{r})(\chi_{i,\sigma}^{(1)}(\boldsymbol{r}'))^*. \tag{50}$$

[Comparing Eq. (50) to Eq. (34), we see that

$$\begin{aligned}\chi_{i,\sigma}^{(1)}(\boldsymbol{r}) &\equiv \psi_i^{(1)}(\boldsymbol{z}),\\ \pi_{i,\sigma}^{(1)} &\equiv N_\sigma \cdot \omega_{i,\sigma}^{(1)},\end{aligned} \tag{51}$$

so the ensemble-N-representability constraints on the natural orbital populations is simply $0 \leqslant \pi_{i,\sigma}^{(1)} \leqslant 1$.[12,29,55–57,67]] While these approximations seem to have severe shortcomings when they are used to approximate the hole-correlation function (and thereby the electron–electron repulsion energy),[14,22,25,27,31,68] the approximation might provide adequate accuracy for the kinetic energy when the procedure is inverted, with a given 2-density used to compute the natural orbitals and their occupation numbers or, equivalently, the first-order density matrix.

Equation (49) can be solved exactly when the connected piece is ignored, recovering the independent particle result,

$$\rho_1^{\sigma_1}(\boldsymbol{r}_1)\rho_1^{\sigma_2}(\boldsymbol{r}_2)h^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2) \equiv -\left|\gamma_1^{\sigma_1\sigma_2}(\boldsymbol{r}_1;\boldsymbol{r}_2)\right|^2. \tag{52}$$

It follows that

$$h^{\alpha\beta}(\boldsymbol{r},\boldsymbol{r}') \equiv 0 \tag{53}$$

and

$$h^{\sigma\sigma}(\boldsymbol{r},\boldsymbol{r}') \leqslant 0, \quad \sigma = \alpha,\beta. \tag{54}$$

Unless Eqs. (53) and (54) are satisfied, Eq. (52) does not have a solution. If Eq. (52) does have a solution and the resulting density matrix is ensemble-N-representable, then the kinetic energy from $\gamma_1^{\sigma\sigma}(\boldsymbol{r},\boldsymbol{r}')$ is an upper bound to the exact kinetic functional defined by Eqs. (9) and (10).

Because Eq. (52) gives an expression for the squared magnitude of the density matrix, rather than the density matrix itself, it is useful to derive a kinetic energy functional for $\left|\gamma_1^{\sigma_1\sigma_2}(\boldsymbol{r}_1;\boldsymbol{r}_2)\right|^2$. Selecting the phase of the natural orbitals so that the first-order density matrix is real, one obtains[45]

$$T_{\mathrm{MS}}[\gamma_1] \equiv \sum_{\sigma=\alpha,\beta} \int\int \frac{\nabla_{\boldsymbol{r}}(\gamma_1^{\sigma\sigma}(\boldsymbol{r}_1,\boldsymbol{r}_2))^2 \cdot \nabla_{\boldsymbol{r}}(\gamma_1^{\sigma\sigma}(\boldsymbol{r}_1,\boldsymbol{r}_2))^2}{8(\gamma_1^{\sigma\sigma}(\boldsymbol{r}_1,\boldsymbol{r}_2))^2} \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2$$

$$= \sum_{\sigma=\alpha,\beta} \sum_{i=1}^{\infty} (\pi_{i,\sigma}^{(1)})^2 \int \nabla \psi_{i,\sigma}^{(1)}(\boldsymbol{r}) \cdot \nabla \psi_{i,\sigma}^{(1)}(\boldsymbol{r}) \mathrm{d}\boldsymbol{r}$$

$$\leqslant \sum_{\sigma=\alpha,\beta} \sum_{i=1}^{\infty} (\pi_{i,\sigma}^{(1)}) \int \nabla \psi_{i,\sigma}^{(1)}(\boldsymbol{r}) \cdot \nabla \psi_{i,\sigma}^{(1)}(\boldsymbol{r}) \mathrm{d}\boldsymbol{r} \equiv T_{\mathrm{exact}}[\gamma_1], \tag{55}$$

where the equality holds only in the independent particle model, where all the natural orbital occupations are zero or one. Substituting Eq. (52) into Eq. (55), one obtains the result of March and Santamaria,[45]

$$T_{\mathrm{MS}}[\rho_2^{\sigma\sigma}] \equiv \sum_{\sigma=\alpha,\beta} \left(-\frac{1}{8}\right) \int\int \frac{\nabla_1 \rho_1^{\sigma}(\boldsymbol{r}_1)\rho_1^{\sigma}(\boldsymbol{r}_2)h^{\sigma\sigma}(\boldsymbol{r}_1,\boldsymbol{r}_2) \cdot \nabla_1 \rho_1^{\sigma}(\boldsymbol{r}_1)\rho_1^{\sigma}(\boldsymbol{r}_2)h^{\sigma\sigma}(\boldsymbol{r}_1,\boldsymbol{r}_2)}{8\rho_1^{\sigma}(\boldsymbol{r}_1)\rho_1^{\sigma}(\boldsymbol{r}_2)h^{\sigma\sigma}(\boldsymbol{r}_1,\boldsymbol{r}_2)} \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2$$

$$= \sum_{\sigma=\alpha,\beta} \left[T_w^{(1)}[\rho_1^{\sigma}] - \frac{1}{8} \int\int \rho_1^{\sigma}(\boldsymbol{r}_1)\rho_1^{\sigma}(\boldsymbol{r}_2) \frac{\nabla_1 h^{\sigma\sigma}(\boldsymbol{r}_1,\boldsymbol{r}_2) \cdot \nabla_1 h^{\sigma\sigma}(\boldsymbol{r}_1,\boldsymbol{r}_2)}{h^{\sigma\sigma}(\boldsymbol{r}_1,\boldsymbol{r}_2)} \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \right]. \tag{56}$$

Equation (56) is similar to the second Weisacker approximation, Eq. (41), and recalls the form of many previous "full Weisacker plus correction" results in density-functional theory.[49,53,69–72] Equation (56) can be applied even when Eq. (54) does not hold. However, the March–Santamaria functional is not generally a rigorous upper bound to the true kinetic energy. Because Eq. (56) is an exact expression for the noninteracting kinetic energy if the exchange-hole is used instead of the exchange-correlation hole in Eq. (56), and because the noninteracting kinetic energy is only slightly less than the true kinetic energy,[73–75] Eq. (56) should provide the basis for quantitative approximations to the true kinetic energy.

F. A tool for checking the accuracy of approximate functionals

Suppose one has, using the variational principle or some other means, arrived at an approximate 2-density for the electronic system with external potential $v(\boldsymbol{r})$. Were the 2-density exact, the virial theorem would imply that

$$2T[\rho] + V_{ee}[\rho_2] = \int \rho(\boldsymbol{r}) \boldsymbol{r} \cdot \nabla v(\boldsymbol{r}) \mathrm{d}\boldsymbol{r}, \tag{57}$$

where $V_{ee}[\rho_2]$ is given by Eq. (3) and the electron density is given by

$$\rho(\boldsymbol{r}) \equiv \rho_1^{\alpha}(\boldsymbol{r}) + \rho_1^{\beta}(\boldsymbol{r}). \tag{58}$$

For an approximate 2-density and/or an approximate kinetic energy functional, Eq. (57) will usually not be exactly satisfied, and so can be used to estimate the error in the approximation. [Equation (57) will, however, be satisfied if the kinetic energy functional has the appropriate scaling; cf. Eq. (4). The author thanks Mel Levy for making this important observation.] It should be noted that the same approach could be used to assess the accuracy of electron–electron repulsion functionals in theories based on the first-order reduced density matrix. In all cases, however, Eq. (57) is not a practical functional, since it requires knowledge of the external potential for which the given 2-density is the ground state. This is impossible to find for non-v-representable densities and, even when a density is v-representable, it is difficult to construct the external potential computationally.[76]

IV. FROM THE 2-DENSITY TO THE KINETIC ENERGY

A. Survey of the literature

Accurately calculating the kinetic energy of a given 2-density, $\rho_2^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)$, seems to require expressions relating the 2-density to the many-electron distributions of higher order (Sec. II B) and/or expressions for the cumulants of the reduced density-matrices. Both problems have been explored in many different contexts over a long period of time, and so a concise and selective survey of the literature is appropriate.

The first methods for constructing the *k*-density from the 2-density were in classical statistical mechanics, where both exact expressions[77–80] and accurate approximate representations[50,80–87] have been extensively explored. The possibility of extending the classical results to quantum mechanical systems was recognized by Abe in his 1959 paper,[78] with early published results from De Dominiciis and Martin.[88–92] Concurrently, researchers were developing sequential relations between the Green's functions in quantum physics and statistical mechanics.[93–95] Insofar as the density matrices can be regarded as initial values of the Green's functions, we recognize relationships between the first-order Green's function and the higher-order Green's functions have implications for constructing kinetic energy functionals using the approach of Secs. III D and III E [cf. Eqs. (45) and (47)]. The early work of Martin and Schwinger is directly relevant.[95] Bridging the gap between these two lines of research is the work of Lee and Yang, who showed how a system of fermions can be modeled as a collection of classical particles subject to additional one-body, two-body, …, and *N*-body potentials.[96] Motivated by the success of hierarchies of equations and diagrammatic expansion techniques for the closures thereof in simulations of classical systems, analogues to these results were derived for quantum systems. One may cite the work on the family of Fermi-hypernetted chain approximations[97–103] and the Chakravarty–Woo equations[104–107] as representative examples.

Foreshadowing the Hohenberg–Kohn theorem,[6] the preceding results are typically derived by using a Legendre transformation to change the variables of the system from the one- and two-body potentials to the one- and two-body distribution functions, density matrices, or Green's functions. Then, known expressions for the properties of a system in terms of the potentials were converted to expressions in terms of the appropriate distribution functions. Later researchers derived exact expressions for higher-order Green's functions in terms of the lower order Green's functions, proved the Legendre transform existed, and proved that the theoretical results can be derived without making unwarranted assumptions about the convergence of various perturbation series.[108–114]

These threads of research continue at present. For example, recent studies where electronic systems are treated as classical systems with an effective "Pauli repulsion potential"[51,103,115] and "classical temperature"[116,117] can be viewed as approximations to the Lee–Yang quantum-classical mapping. The contracted Schrödinger equation and the methods employed for constructing higher-order density matrices from their lower-order counterparts[64,118,119] recall the equation-of-motion method[95] and the similar closures used therein.

The relevance of this prior work to constructing approximations for the kinetic energy from the 2-density places computational techniques based on the 2-density into context, and allow us to draw on these related results in further development of this theory. In particular, developing accurate kinetic energy functionals of the *k*-density using the general techniques in Secs. III B and III D should be a relatively straightforward theoretical exercise. Finding functionals that are both accurate and computationally efficient, so that the resulting theory compares favorably to traditional ways of addressing electron correlation, is expected to be more difficult, and some suggestions along these lines follow.

B. The Hierarchy of Lee, Jackson, and Feenberg

Given a 2-density, $\rho_2^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)$, constructing an accurate kinetic energy functional using either the Weisacker-based functionals or the density-matrix based approach will often rely on expressing the *k*-density (with $k>2$) as a functional of the 2-density, so that higher-order kinetic energy

functionals like Eq. (25) or (46) can be used. This problem is similar to the problem of constructing closures in statistical mechanics. For example, one might employ the convolution approximation for the 3-density,

$$\rho_{3,\mathrm{conv}}^{\sigma_1\sigma_2\sigma_3}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3) \equiv \rho_1^{\sigma_1}(\boldsymbol{r}_1)\rho_1^{\sigma_2}(\boldsymbol{r}_2)\rho_1^{\sigma_3}(\boldsymbol{r}_3)\left(\begin{array}{l} 1 + h^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2) + h^{\sigma_1\sigma_3}(\boldsymbol{r}_1,\boldsymbol{r}_3) + h^{\sigma_2\sigma_3}(\boldsymbol{r}_2,\boldsymbol{r}_3) \\ + h^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)h^{\sigma_2\sigma_3}(\boldsymbol{r}_2,\boldsymbol{r}_3) + h^{\sigma_1\sigma_3}(\boldsymbol{r}_1,\boldsymbol{r}_3)h^{\sigma_3\sigma_2}(\boldsymbol{r}_3,\boldsymbol{r}_2) \\ + h^{\sigma_3\sigma_1}(\boldsymbol{r}_3,\boldsymbol{r}_1)h^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2) \\ + \int \rho^{\sigma'}(\boldsymbol{x}')h^{\sigma_1\sigma'}(\boldsymbol{r}_1,\boldsymbol{x}')h^{\sigma_2\sigma'}(\boldsymbol{r}_2,\boldsymbol{x}')h^{\sigma_3\sigma'}(\boldsymbol{r}_3,\boldsymbol{x}')\mathrm{d}\boldsymbol{x}' \end{array}\right) \tag{59}$$

or the superposition approximation,

$$\rho_{3,\mathrm{sup}}^{\sigma_1\sigma_2\sigma_3}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3) \equiv \rho_1^{\sigma_1}(\boldsymbol{r}_1)\rho_1^{\sigma_2}(\boldsymbol{r}_2)\rho_1^{\sigma_3}(\boldsymbol{r}_3)\left(\begin{array}{l} 1 + h^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2) + h^{\sigma_1\sigma_3}(\boldsymbol{r}_1,\boldsymbol{r}_3) + h^{\sigma_2\sigma_3}(\boldsymbol{r}_2,\boldsymbol{r}_3) \\ + h^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)h^{\sigma_2\sigma_3}(\boldsymbol{r}_2,\boldsymbol{r}_3) + h^{\sigma_1\sigma_3}(\boldsymbol{r}_1,\boldsymbol{r}_3)h^{\sigma_3\sigma_2}(\boldsymbol{r}_3,\boldsymbol{r}_2) \\ + h^{\sigma_3\sigma_1}(\boldsymbol{r}_3,\boldsymbol{r}_1)h^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2) \\ + h^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)h^{\sigma_2\sigma_3}(\boldsymbol{r}_2,\boldsymbol{r}_3)h^{\sigma_3\sigma_1}(\boldsymbol{r}_3,\boldsymbol{r}_1) \end{array}\right). \tag{60}$$

As noted by Lee, Jackson, and Feenberg,[50] however, neither of these approximations is entirely satisfactory. In particular, the convolution approximation does not always satisfy the electron coalescence N-representability condition,

$$\rho_3^{\sigma_1,\sigma_2,\sigma_3}(\boldsymbol{r},\boldsymbol{r},\boldsymbol{r}) = 0. \tag{61}$$

The superposition approximation satisfies Eq. (61), but it does not generally satisfy the sequential relations,

$$\rho_{k-1}^{\sigma_1\sigma_2\cdots\sigma_{k-1}}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_{k-1}) = \left(\frac{1}{N_{\sigma_k} - m_{\sigma_k}}\right)\int \rho_k^{\sigma_1\sigma_2\cdots\sigma_k}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_k)\mathrm{d}\boldsymbol{x}_k \tag{62}$$

[m_{σ_k} was defined in Eq. (22)]. (The convolution approximation does satisfy the sequential relations.)[50] Unfortunately, the author knows of no closed form (series solutions are available[50,77,78,120]) that satisfies both the sequential relations and the electron coalescence criterion. Still, one might hope that the 3-densities constructed using the convolution approximation [Eq. (59)] or the superposition approximation [Eq. (60)] "inherit" near-N-representability from their underlying 2-density, so that kinetic energy formulas employing Eqs. (59) and (60) might, at least, provide some improvement over forms in which the 3-density was never constructed. It should be noted that higher-order convolution approximations[50] and superposition approximations[81] are available.

Without an acceptable closed form for the closure, one might explore the possibility of using a hierarchy of equations to determine $\rho_{k>2}^{\sigma_1\cdots\sigma_k}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k)$ from $\rho_2^{\sigma_1\sigma_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)$. The following analysis adapts one hierarchy of this type, derived by Lee, Jackson, and Feenberg for quantum fluids in the absence of an external electrostatic potential,[50] to the electronic structure problem. From the Schrödinger equation for the ground state wave function, $\Psi(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)$,

$$0 = \Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)\left(\sum_{i=1}^{N} -\frac{\nabla_i^2}{2} + \sum_{i=1}^{N}\left(v(\boldsymbol{r}_i) + \sum_{j=i+1}^{N}\frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}\right) - E_0\right)\Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N), \tag{63}$$

where E_0 is the ground state energy. To express the ground state energy and the ground state wave function in terms of the k-densities, we start by writing Eq. (63) in terms of $|\Psi_0|^2$, using the identity [cf. Eq. (17)]

$$\Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)\frac{\nabla_i^2}{2}\Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N) \equiv \frac{\nabla_i^2}{8}(\Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N))^2 + (\Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N))^2\frac{\nabla_i^2}{8}\ln(\Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N))^2, \tag{64}$$

where it is assumed that the wave function is real. Substituting Eq. (64) into Eq. (63), one obtains

$$\sum_{i=1}^{N}\frac{\nabla_i^2}{8}(\Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N))^2 = (\Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N))^2 \times\sum_{i=1}^{N}\left(-\frac{\nabla_i^2}{8}\ln(\Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N))^2 + v(\boldsymbol{r}_i) + \sum_{j=i+1}^{N}\frac{1}{|\boldsymbol{r}_i-\boldsymbol{r}_j|} - E_0\right). \tag{65}$$

In order to eliminate the dependence on the energy and obtain a hierarchy reminiscent of those from the classical theory of fluids, we introduce a function reminiscent of the partition function,

$$Q(\beta) \equiv \langle\Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)|e^{-\beta\mathcal{W}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)}|\Psi(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)\rangle, \tag{66}$$

where

$$\mathcal{W}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_n) \equiv \sum_{i=1}^{N}\left(-\frac{\nabla_i^2}{8}\ln(\Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N))^2 + v(\boldsymbol{r}_i) + \sum_{j=i+1}^{N}\frac{1}{|\boldsymbol{r}_i-\boldsymbol{r}_j|}\right). \tag{67}$$

Equation (65) can then be rewritten as

$$\sum_{i=1}^{N}\frac{\nabla_i^2}{8}(\Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N))^2 = \left.\frac{\partial}{\partial\beta}\left(\frac{(\Psi_0(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N))^2 e^{-\beta\mathcal{W}(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)}}{Q(\beta)}\right)\right|_{\beta=0}. \tag{68}$$

The kth order in the hierarchy is obtained by defining, in analogy to Eq. (8),

$$\rho_k^{\sigma_1\sigma_2\ldots\sigma_k}(\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_k,\beta) = \frac{\left\langle\Psi\left|\left(\sum_{i_k\neq i_1,i_2,\ldots,i_{k-1}}^{N}\cdots\sum_{i_2\neq i_1}^{N}\sum_{i_1=1}^{N}\prod_{j=1}^{k}\delta_{s_{i_j},\sigma_j}\delta(\boldsymbol{r}_{i_j}-\boldsymbol{x}_j)\right)e^{-\beta\mathcal{W}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N)}\right|\Psi\right\rangle}{Q(\beta)}. \tag{69}$$

Then, from Eq. (68)

$$\sum_{i=1}^{k}\frac{\nabla_i^2}{8}\rho_k^{\sigma_1\ldots\sigma_k}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k,0) = \left.\frac{\partial\rho_k^{\sigma_1\ldots\sigma_k}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_k,\beta)}{\partial\beta}\right|_{\beta=0}, \tag{70}$$

where $\rho_k^{\sigma_1\ldots\sigma_k}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k,0)$ is just the usual k-density, $\rho_k^{\sigma_1\ldots\sigma_k}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k)$. In deriving Eq. (70) it is helpful to remember that

$$0 = \int\frac{\nabla_i^2}{2}|\Psi(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)|^2\mathrm{d}\boldsymbol{r}_i = \lim_{r_i\to\infty}\int_0^{2\pi}\int_0^{\pi}(\nabla_i|\Psi(\boldsymbol{z}_1,\ldots,\boldsymbol{z}_N)|^2\cdot\hat{\boldsymbol{r}}_i)r_i^2\sin\theta_i\mathrm{d}\theta_i\mathrm{d}\phi_i; \tag{71}$$

the surface of integration is a sphere whose radius, r_i, tends to infinity.

The reason Eq. (70) constitutes a hierarchy of equations is because it is difficult to evaluate

$$\left.\frac{\partial \rho_k^{\sigma_1 \ldots \sigma_k}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_k, \beta)}{\partial \beta}\right|_{\beta=0}$$

directly from the definition Eq. (69). However, suppose one is given an expression for the k-density, $\rho_k^{\sigma_1 \ldots \sigma_k}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_k, \beta)$, in terms of the l-densities ($l<k$). Using the chain rule for functional derivatives, Eq. (70) yields

$$\begin{aligned}\sum_{i=1}^{k} \nabla_i^2 \rho_k^{\sigma_1 \ldots \sigma_k}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_k, 0) &= 8 \sum_{l=1}^{k-1} \int \int \int \left(\frac{\delta \rho_k^{\sigma_1 \ldots \sigma_k}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_k, \beta)}{\delta \rho_l^{s_1 \ldots s_l}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_l, \beta)} \times \left. \frac{\partial \rho_l^{s_1 \ldots s_l}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_l, \beta)}{\partial \beta} \right|_{\beta=0} \right) \mathrm{d}\boldsymbol{x}_1 \ldots \mathrm{d}\boldsymbol{x}_l \\ &= \sum_{l=1}^{k-1} \int \int \int \frac{\delta \rho_k^{\sigma_1 \ldots \sigma_k}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_k, \beta)}{\delta \rho_l^{s_1 \ldots s_l}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_l, \beta)} \left(\sum_{i=1}^{l} \nabla_i^2 \rho_l^{s_1 \ldots s_l}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_l, 0) \right) \mathrm{d}\boldsymbol{x}_1 \ldots \mathrm{d}\boldsymbol{x}_l. \end{aligned} \tag{72}$$

Equation (72) will not be satisfied by an inexact closure. However, if one proposes a general form of the closure, wherein the weight or functional form of various terms depends on some parameters, one may regard Eq. (72) as a nonlinear equation for those parameters, with the "optimal" choice of parameters being that which minimizes the residual error in Eq. (72).

The most important cases of Eq. (72) are probably the case where $k=2$,

$$(\nabla_1^2 + \nabla_2^2) \rho_2^{\sigma_1 \sigma_2}(\boldsymbol{r}_1, \boldsymbol{r}_2, 0) = \int \frac{\delta \rho_2^{\sigma_1 \sigma_2}(\boldsymbol{r}_1, \boldsymbol{r}_2, \beta)}{\delta \rho_1^{s}(\boldsymbol{x})} (\nabla_{\boldsymbol{x}}^2 \rho_1^{s}(\boldsymbol{x})) \mathrm{d}\boldsymbol{x} \tag{73}$$

(which might be useful for deriving hole-correlation functionals for use in density-functional theory) and $k=3$,

$$(\nabla_1^2 + \nabla_2^2 + \nabla_3^2) \rho_3^{\sigma_1 \sigma_2 \sigma_3}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, 0) = \int \frac{\delta \rho_3^{\sigma_1 \sigma_2 \sigma_3}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \beta)}{\delta \rho_2^{s_1 s_2}(\boldsymbol{x}_1, \boldsymbol{x}_2, \beta)} [(\nabla_{\boldsymbol{x}_1}^2 + \nabla_{\boldsymbol{x}_2}^2) \rho_2^{s_1 s_2}(\boldsymbol{x}_1, \boldsymbol{x}_2)] \mathrm{d}\boldsymbol{x}_1 \mathrm{d}\boldsymbol{x}_2, \tag{74}$$

which is useful for approximating the 3-density in terms of the 2-density. One might, for example, seek to find the linear combination of the convolution and superposition approximations, Eqs. (59) and (60), which minimizes the residual error in Eq. (74).

V. DISCUSSION

A. Implications for computational methods based on the *k*-density

In combination with N-representability conditions on the k-density, the path to accurate kinetic energy functionals developed in this paper provides the basis for computational approaches to quantum chemistry using the k-density ($k \geqslant 2$). This approach, based on the minimization of the energy as a functional of the k-density subject to the constraints imposed by ensemble-N-representability, is sketched in Sec. I, with Eq. (5) encapsulating the essence of the approach for the case that is probably most important, with $k=2$. Such methods may be termed k-density-functional theory, and constitute a hierarchy of methods bridging the gap between the usual density-functional theory ($k=1$) and direct approaches to the Schrödinger equation ($k=N$). Just as Sham, Görling, Levy, Bartlett, and others have shown how the exact exchange-correlation density-functional can be constructed by adapting standard approaches to the quantum many-body problem,[113,114,121–124] the techniques in Secs. III and IV show how existing approaches to the quantum many-body problem can inform the construction of an accurate kinetic energy functional. The computational demands and accuracy of such approaches will necessarily resemble the many-body methods on which they are based, limiting the utility of such approaches. However, insights gleaned from these well-understood techniques can guide the development of more practical and efficient methods. In particular, just as a combination of physical insight and parameter-fitting has

rendered density-functional theory the method of choice for quantum mechanical simulations of large systems, one may expect physical insights from exact and systematic formulations of the kinetic-energy functionals, possibly coupled with limited fitting of parameters, to produce accurate kinetic-energy functionals of the *k*-density.

When one restricts oneself to the 2-density, there is the prospect of using one of the simpler kinetic-energy functionals presented in Secs. III C and III E. In this case, the resulting theory will be approximate, but as argued in those sections, there are reasons to believe the errors may be small. In addition, because the 2-density is a function of only two spatial coordinates, such methods should be competitive with methods based on the first-order density matrix and, implicitly, not much more expensive than Kohn–Sham density-functional theory,[125] which can also be considered a first-order density matrix method.

B. Implications for density-functional theory

One of the most important outstanding problems in density-functional theory is the lack of a satisfactory kinetic-energy density functional for atoms and molecules.[42] Present functionals give poor results when used for variational all-electron calculations on atoms and molecules, presumably because the *N*-representability constraints on the first-order density matrix implicit in such functionals are insufficient.[126,127] In addition, as first pointed out by Levy, Perdew, Parr, and Balduz, if the total energy functional employed in a calculation can be functionally differentiated, then the dissociation of molecules into fragments will be described incorrectly (since the number of electrons in the fragments will be noninteger).[128–131] The Kohn–Sham kinetic energy is similarly nondifferentiable,[132] but present orbital-free approximations to the Kohn–Sham kinetic-energy violate this constraint.

All these issues are surmounted in the Kohn–Sham implementation of density-functional theory: by using the kinetic energy of the Kohn–Sham reference system of noninteracting fermions, $T_s[\rho]$, the *N*-representability constraints and derivative discontinuity are largely accounted for, with residual errors confined to the small correlation-kinetic energy correction, $T_c[\rho] \equiv T[\rho] - T_s[\rho]$.[125] The computational cost of this ansatz is the self-consistent determination of the first-order density matrix for the Kohn–Sham reference system, which renders Kohn–Sham calculations much more costly than calculations based on orbital-free functionals for the kinetic energy. From this perspective, one can consider the Kohn–Sham kinetic energy to be a composite functional of the electron density: the Kohn–Sham kinetic energy is an explicit functional of the Kohn–Sham orbitals (or Kohn–Sham density matrix), which is determined implicitly from the electron density via the Kohn–Sham equations.

The development in Sec. III shows that the kinetic energy is readily approximated from the 2-density. Hence, by formulating an approach whereby the 2-density is generated from the electron density, one could construct kinetic energy functionals using the 2-density as an "auxiliary functional" of the electron density. An added benefit of this approach is that the unknown, but less problematic, electron–electron repulsion energy density functional is supplanted by the exact expression, Eq. (3). That is, by using the 2-density as an intermediary between the electron density and the kinetic-energy and electron–electron repulsion energy, one can avoid the ubiquitous Kohn–Sham reference system, leading to an entirely new perspective on practical methods for density-functional theory computation. Insofar as the March–Santamaria form for the kinetic energy, Eq. (56), is exact for the noninteracting reference system, even the simplest kinetic-energy functionals of the 2-density may be expected to give accuracy approaching that of conventional Kohn–Sham DFT.

The outstanding problem is that the 2-density must be expressed as functional of the 1-density. Such a pursuit can be guided by the Lee–Jackson–Feenberg hierarchy, cf. Eq. (73). The author's work along these lines will be communicated separately.

C. Summary

In constructing an approach to quantum chemistry based on the k-density, there are two main requirements. First of all, one must know the ensemble-N-representability constraints on the k-density, $\rho_k^{\sigma_1\cdots\sigma_k}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k)$. With these constraints either known or effectively approximated, one can minimize an energy functional of the k density over the set of ensemble-representable k-densities, and obtain

$$E_v^{\mathrm{gs}} = \min_{\rho_k^{\sigma_1\cdots\sigma_k}\in\mathcal{N}} [T[\rho_k^{\sigma_1\cdots\sigma_k}] + V_{ee}[\rho_k^{\sigma_1\cdots\sigma_k}] + V_{ne}[\rho_k^{\sigma_1\cdots\sigma_k},v]],$$
$$\rho_k^{\sigma_1\cdots\sigma_k}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_k) = \arg\min_{\rho_k^{\sigma_1\cdots\sigma_k}\in\mathcal{N}}[T[\rho_k^{\sigma_1\cdots\sigma_k}] + V_{ee}[\rho_k^{\sigma_1\cdots\sigma_k}] + V_{ne}[\rho_k^{\sigma_1\cdots\sigma_k},v]], \tag{75}$$

where the notation has the same meaning as that in Eq. (5). In order to use Eq. (75), one has to express the kinetic energy as a functional of the k-density. In Sec. II, exact approaches based on the Levy–Valone constrained search [Eq. (9)] and Lieb's generalized Legendre transform [Eq. (10)] are presented. While these do not represent practical approaches to the kinetic energy functional, they do set the standard by which all approximate functionals must be judged, and can be used to establish analytic constraints on the properties of the exact functional.

Unlike exact approaches based on the constrained-search or Legendre-transform, the emphasis in Sec. III is on controlled and systematic approximations to the kinetic energy functionals. Section III B develops a series of lower bounds on the kinetic energy of pure states; these are essentially generalizations of the Weisacker functional for density-functional theory. Section III C applies this analysis to the 2-density, deriving the simple working formula, Eq. (41), which is a lower bound to the true kinetic energy. The leading order correction to Eq. (41), involves three-electron correlations; these terms could be considered analogous to triple-excitations in conventional multi-configuration approaches to the electron correlation problem, and might be suspected to be negligible except when three or more electrons are close together. For this reason, we may hope that Eq. (41) is a reasonably tight lower bound to the true kinetic energy.

Section III D uses the technique of density-matrix reconstruction to construct a different kinetic energy functional—one that is often an upper bound. Section III E uses this technique to derive a simple kinetic energy functional of the 2-density, Eq. (56). Equation (56) is exact for a system of noninteracting electrons. Because the correction to the noninteracting kinetic energy (often called the correlation-kinetic energy and denoted $T_c[\rho]$) is small and readily approximated using density-functionals, we suspect that Eq. (56) can be used as the basis for practical computational methods based on the 2-density.

The easiest way to improve these functionals for the kinetic energy in terms of the k-density is to introduce information about l-electron correlations, which can be done by constructing $\rho_{l>k}^{\sigma_1\cdots\sigma_l}(\boldsymbol{x}_1\ldots\boldsymbol{x}_l)$ as a functional of $\rho_k^{\sigma_1\cdots\sigma_k}(\boldsymbol{x}_1\ldots\boldsymbol{x}_k)$. Techniques for this reconstruction are analogous to methods used in wave-function-based quantum chemistry and statistical mechanics, and are reviewed in Sec. IV A. Section IV B discusses the possibility of constructing the l-density using approximate closures and hierarchies of equations. Together with the results from Secs. III B and III D, this leads to families of systematically improvable kinetic energy functionals, so that one can construct a kinetic energy functional of any desired accuracy. At present, it is unclear whether the reconstruction of higher-order electron densities is preferable to a direct treatment using the higher-order densities; this, as well as computational implementation of the ideas contained herein, is a topic for further research.

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APPENDIX: DERIVATION OF EQ. (19)

Suppose that $n_N^{(N)}$ is not pure-state N-representable, but can be represented in terms of an ensemble with only two components,

$$n_N^{(N)}(\mathbf{z}_1, \ldots, \mathbf{z}_N) \equiv w_1(\Psi_1(\mathbf{z}_1, \ldots, \mathbf{z}_N))^2 + w_2(\Psi_2(\mathbf{z}_1, \ldots, \mathbf{z}_N))^2. \tag{A1}$$

(For ensembles with more than two components, the argument proceeds by induction from the two-component case.) In this case, the exact kinetic energy can be written as

$$\begin{aligned} T_{\text{exact}}[n_N^{(N)}] &\equiv \frac{1}{2}\langle \nabla \sqrt{w_1(\Psi_1)^2} \cdot \nabla \sqrt{w_1(\Psi_1)^2} \rangle + \frac{1}{2}\langle \nabla \sqrt{w_2(\Psi_2)^2} \cdot \nabla \sqrt{w_2(\Psi_2)^2} \rangle \\ &\geqslant T_w^{(N)}[\rho_N^{\sigma_1 \ldots \sigma_N}] \equiv \frac{1}{2}\langle \nabla \sqrt{n_N^{(N)}} \cdot \nabla \sqrt{n_N^{(N)}} \rangle. \end{aligned} \tag{A2}$$

In Eq. (A2), the gradient is evaluated in $3N$-dimensions. The inequality on the second line of Eq. (A2) is the statement we wish to prove.

To derive Eq. (A2), merely note that

$$\begin{aligned} &\frac{1}{2}\langle \nabla \sqrt{f} \cdot \nabla \sqrt{f} \rangle + \frac{1}{2}\langle \nabla \sqrt{g} \cdot \nabla \sqrt{g} \rangle - \frac{1}{2}\langle \nabla \sqrt{f+g} \cdot \nabla \sqrt{f+g} \rangle \\ &= \left\langle \frac{\nabla f \cdot \nabla f}{8f} \right\rangle + \left\langle \frac{\nabla g \cdot \nabla g}{8g} \right\rangle - \left\langle \frac{\nabla (f+g) \cdot \nabla (f+g)}{8(f+g)} \right\rangle \\ &= \left\langle g^2 \frac{\nabla f \cdot \nabla f}{8fg(f+g)} \right\rangle + \left\langle f^2 \frac{\nabla g \cdot \nabla g}{8fg(f+g)} \right\rangle - 2\left\langle fg \frac{\nabla (f+g) \cdot \nabla (f+g)}{8fg(f+g)} \right\rangle \\ &= \left\langle \frac{g^4}{8fg(f+g)} \nabla \left(\frac{f}{g}\right) \cdot \nabla \left(\frac{f}{g}\right) \right\rangle \geqslant 0 \end{aligned} \tag{A3}$$

Identifying $f = w_1(\Psi_1)^2$ and $g = w_2(\Psi_2)^2$, Eq. (A2) immediately follows. Excepting the trivial cases where (a) w_1 or w_2 is zero or (b) $(\Psi_1)^2 = (\Psi_2)^2$, the inequality is strict—the kinetic energy is strictly larger than the N-electron Weisacker approximation, $T_w^{(N)}[\rho_N^{\sigma_1 \ldots \sigma_N}]$.

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Analytic solution of the Schrödinger equation for the Coulomb-plus-linear potential. I. The wave functions

Guillaume Plante
Physics Department, Columbia University, New York, New York 10027

Adel F. Antippa
Département de Physique, Université du Québec à Trois-Rivières, Trois-Rivières, Québec, Canada G9A 5H7

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We solve the Schrödinger equation for a quark–antiquark system interacting via a Coulomb-plus-linear potential, and obtain the wave functions as power series, with their coefficients given in terms of the combinatorics functions. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1931041]

I. INTRODUCTION

The Coulomb-plus-linear potential, $V(r)=-a/r+br$, also known as the Cornell potential, has received a great deal of attention both in particle physics, more precisely in the context of meson spectroscopy where it is used to describe systems of quark and antiquark bound states, and in atomic and molecular physics where it represents a radial Stark effect in hydrogen.

The Coulomb-plus-linear potential was used with considerable success in models describing systems of bound heavy quarks.[1–5] It was introduced as a mathematically simple potential incorporating characteristics of interquark interactions and accounting for the features of the spectrum of charmed quark–antiquark bound states. The potential includes the short distance Coulombic interaction of quarks, known from perturbative quantum chromodynamics (QCD), and the large distance quark confinement, known from lattice QCD, via the linear term in a simple form. It is also in good agreement with the central part of the static heavy quark potential derived from dual QCD (Ref. 6) and from lattice QCD.[7,8]

Solutions of the Schrödinger equation for the Coulomb-plus-linear potential have been investigated with a large number of techniques and also as a special case of the generalized Killingbeck potential, $V(r)=-a/r+br+cr^2$.

In the context of perturbation theory, Mehta and Patil[9] showed that the eigenvalues of the Coulomb-plus-linear potential have an asymptotic perturbation series in the linear coupling parameter b. Killingbeck[10] showed how the hypervirial theorem could be used to calculate the perturbation series for the energy of spherically symmetric ($l=0$) states without calculation of the perturbed wave functions. Padé approximants to the divergent energy series were used to obtain the eigenvalues. Austin[11] extended the calculation of the perturbation series to higher order and to a broader range of values of the perturbation parameter. Using the same technique, Lai and Lin[12] obtained the eigenvalues for different values of the orbital angular momentum quantum number.

In the framework of the WKB approximation, Seetharaman *et al.*[13] obtained a nonperturbative approximate analytic expression for the energy in terms of complete elliptic integrals. Thidé and Linnaeus[14] and Brau[15] also obtained approximate analytical results for the eigenvalues using, respectively, higher-order phase integral quantization and Bohr–Sommerfeld quantization.

Chhajlany and Letov[16] obtained exact results for the Coulomb-plus-linear potential for specific values of the coupling parameters following a technique used by Saxena and Varma[17] to find exact solutions for the problem of a Coulomb potential with a polynomial radial perturbation $2\lambda r+2\lambda^2 r^2$. The technique works by searching a solution in the form of a product of an interpolating function and two functions with the correct endpoint behavior. If the coefficients of the power series of the interpolating function are related by a Nth order recursion relation, then the

eigenvalues are obtained by requiring that the interpolating function be a polynomial of degree n, i.e., by explicitly setting N successive coefficients of its power series to zero. This arbitrary condition also results in the quantization of some of the coupling parameters of the potential. The eigenvalues found converge to the true eigenvalues as the degree of the polynomial goes to infinity.

In Ref. 16, this technique is applied to the case of a Coulomb potential with a radial perturbation $\mu r+\alpha^2 r^2$. The requirement that the solution be polynomial leads to the quantization of the quadratic coupling α which now depends on the linear coupling μ and on the orbital angular momentum quantum number. The eigenvalues of the Coulomb-plus-linear potential are recovered because α goes to zero as the degree of the polynomial goes to infinity, letting the generalized Killingbeck potential go to the desired potential.

Solutions for the Coulomb-plus-linear potential have also been investigated using the Hill determinant method by Chaudhuri *et al.*[18] where the eigenvalues are obtained as the zeros of an infinite dimensional determinant associated with the infinite system of linear equations relating the coefficients of the power series of the solution.

Fulcher *et al.*[19] showed that analytic expressions for the eigenvalues of the low-lying states can be obtained by expanding the radial part of the wave function in a basis of functions given by the product of a centrifugal barrier, an exponential function, and a Laguerre polynomial. Their approach transforms the problem of the Schrödinger equation for the Coulomb-plus-linear potential to a matrix diagonalization problem where the matrix elements are given by analytic expressions. The eigenvalues of the matrix converge to the true eigenvalues when the size of the basis becomes sufficiently large.

The solutions of the Schrödinger equation for a central polynomial type potential $V(r)=\Sigma_{i=1}^{I} a_i r^{\nu_i}$ with $\nu_i \geqslant -1$ can be written as the product of a spherical harmonic, a centrifugal barrier r^l, a decreasing exponential function and an unknown function $\eta(r)$ that admits a power series expansion. The factor r^l dominates near the origin, the exponential factor is the function with the correct asymptotic behavior and $\eta(r)$ is the solution that dominates at intermediate distances. Explicit solutions in terms of special functions exist in only two special cases of the potential, $\nu_1=-1$ and $\nu_1=2$ both with $I=1$. This is due to the fact that, only in these two cases, are the expansion coefficients of the function $\eta(r)$ related by a two-term recursion relation. In all other cases they are related by a three- or more-term recursion relation.

The usual method used to solve multiterm linear recursion relations with nonconstant coefficients is to compute the first terms of the series, guess the general solution and prove it by mathematical induction. While this is easily achieved for two term recursion relations, it is almost impossible for recursion relations with three or more terms. Antippa and Phares developed a general formalism for solving linear multiterm recursion relations with nonconstant coefficients[20] in terms of algebraic combinatorial expressions called combinatorics functions. The first application of this formalism to the solution of the Schrödinger equation with polynomial type central potentials was to the case of the linear potential.[21,22] The wave functions were obtained as power series expansions with their coefficients given in terms of functionals called structure functions, a special kind of combinatorics function. The energy eigenvalue equation was obtained by requiring that the asymptotic behavior of the wave function be that of the asymptotic solution of the Schrödinger equation for the linear potential. The eigenvalues were given by the roots of an infinite order polynomial.

The series solution of the Schrödinger equation for the Coulomb-plus-linear potential leads to a four-term recursion relation with nonconstant coefficients. The same method used to solve the Schrödinger equation for the linear potential can be used to obtain a solution for the Coulomb-plus-linear potential. The purpose of this paper is to obtain an analytic expression for the nonrelativistic Schrödinger wave functions of the Coulomb-plus-linear potential.

The organization of the paper is as follows: in Sec. II we set up the problem and obtain the coefficients of the power series expansion of the wave functions in terms of structure functions, in

Sec. III we derive recursion relations for the structure functions and in Sec. IV we present the general expression for the wave functions of the Coulomb-plus-linear potential and give explicit expressions for the first six coefficients of the power series.

II. RADIAL EQUATION

A. Dimensionless radial equation

Consider a quark-antiquark system interacting via a Coulomb-plus-linear potential,

$$V(r) = V_0 + \kappa r - \frac{\alpha}{r}. \tag{1}$$

Since the potential has spherical symmetry, then the solutions of the time-independent Schrödinger equation are of the form

$$\psi_{nlm}(\vec{r}) = R_{nl}(r)Y_l^m(\theta,\phi), \tag{2}$$

where $R_{nl}(r)=u_{nl}(r)/r$, and $u_{nl}(r)$ is a solution of the radial Schrödinger equation,

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{\mathrm{d}r^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)\right]u_{nl}(r) = E_{nl}u_{nl}(r). \tag{3}$$

Inserting the expression for the potential as given by Eq. (1), into Eq. (3), leads to

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{\mathrm{d}r^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V_0 + \kappa r - \frac{\alpha}{r}\right]u_{nl}(r) = E_{nl}u_{nl}(r). \tag{4}$$

Applying the scale transformation $x=ar$ to the above equation, and dividing through by $-\hbar^2a^2/2\mu$, leads further to

$$\left[\frac{d^2}{\mathrm{d}x^2} - \frac{l(l+1)}{x^2} - \frac{2\mu\kappa x}{\hbar^2a^3} + \frac{2\mu\alpha}{\hbar^2 ax} + \frac{2\mu}{\hbar^2a^2}(E_{nl}-V_0)\right]u_{nl}(x) = 0. \tag{5}$$

Setting the parameter a to

$$a = \left(\frac{2\mu\kappa}{\hbar^2}\right)^{1/3} \tag{6}$$

gives it the dimensions of inverse length, and consequently x becomes dimensionless. Substituting the above expression for a, into Eq. (5) reduces this latter to

$$\left[\frac{d^2}{\mathrm{d}x^2} - \frac{l(l+1)}{x^2} - x + \frac{1}{x}\left(\frac{4\mu^2\alpha^3}{\hbar^4\kappa}\right)^{1/3} + \left(\frac{\sqrt{2\mu}}{\hbar\kappa}\right)^{2/3}(E_{nl}-V_0)\right]u_{nl}(x) = 0. \tag{7}$$

By defining the dimensionless coupling constant ρ and the dimensionless energy parameter t_{nl}, respectively, by

$$\rho = \left(\frac{4\mu^2}{\hbar^4\kappa}\right)^{1/3}\alpha \tag{8}$$

and

$$t_{nl} = \left(\frac{2\mu}{\hbar^2\kappa^2}\right)^{1/3}(E_{nl}-V_0) \tag{9}$$

we finally obtain the radial Schrödinger equation in terms of dimensionless parameters, as

$$\left[\frac{d^2}{dx^2} - \frac{l(l+1)}{x^2} - x + \frac{\rho}{x} + t_{nl}\right] u_{nl}(x) = 0. \tag{10}$$

Solving the Schrödinger Eq. (1), for the Coulomb-plus-linear potential, has thus been reduced to solving the radial equation (10), for the functions $u_{nl}(x)$.

B. Series solutions for $u_{nl}(x)$

Equation (10) has the generic form

$$\frac{d^2u_{nl}}{dx^2} + p(x)\frac{du_{nl}}{dx} + q(x)u_{nl} = 0 \tag{11}$$

with

$$p(x) = 0, \tag{12}$$

$$q(x) = -\frac{l(l+1)}{x^2} - x + \frac{\rho}{x} + t_{nl}. \tag{13}$$

Since $xp(x)$ and $x^2q(x)$ are entire functions, then Eq. (10) has a series solution with an infinite radius of convergence, of the form[23]

$$v_{nl}(x,s) = \sum_{i=0}^{\infty} a_i(s)x^{i+s} \tag{14}$$

with the coefficients $a_i(s)$ given by the recursion relation

$$F(s+i)a_i(s) + \sum_{j=0}^{i-1}[(j+s)p_{i-j} + q_{i-j}]a_j(s) = 0, \tag{15}$$

where $F(s)$ is defined by

$$F(s) = s(s-1) + p_0 s + q_0 \tag{16}$$

and p_k and q_k are the coefficients of the power series expansions of $xp(x)$ and $x^2q(x)$, respectively. That is

$$p_k = \frac{1}{k!}\left.\frac{d^k(xp(x))}{dx^k}\right|_{x=0}, \tag{17}$$

$$q_k = \frac{1}{k!}\left.\frac{d^k(x^2q(x))}{dx^k}\right|_{x=0}. \tag{18}$$

Independent solutions of Eq. (11) are obtained, via Eq. (14), by setting the value of s equal to the roots

$$s_{\pm} = \frac{(1-p_0) \pm \sqrt{(1-p_0)^2 - 4q_0}}{2} \tag{19}$$

of the indicial equation

$$F(s) = 0. \tag{20}$$

From Eqs. (12) and (13) we see that in the case of the second order differential equation (11), $p_k=0$ for $k=0,1,2,\ldots,\infty$ and $q_k=0$ for $k=4,5,6,\ldots,\infty$, while the nonzero values of q_k are

$$q_0 = -l(l+1), \quad q_1 = \rho, \quad q_2 = t_{nl}, \quad q_3 = -1. \tag{21}$$

Consequently, the recursion relation (15) reduces to

$$F(s+i)a_i(s) + \rho a_{i-1}(s) + t_{nl}a_{i-2}(s) - a_{i-3}(s) = 0 \tag{22}$$

with $a_i = 0$ for $i < 0$. The function $F(s)$ as given by Eq. (16) takes the special form

$$F(s) = s(s-1) - l(l+1). \tag{23}$$

The roots, as given by Eq. (19), of the indicial equation (20), reduce to the simple form

$$s_+ = l+1 \quad \text{and } s_- = -l. \tag{24}$$

When the above values for the indices are used with Eq. (23), they lead, respectively, to

$$F(s_+ + i) = i(i+2l+1) \tag{25}$$

and

$$F(s_- + i) = i(i-2l-1). \tag{26}$$

Since the roots of the indicial equation differ by an integer then the general solution of Eq. (11) is given by[23]

$$h_{nl}(x) = Au_{nl}(x) + Bw_{nl}(x), \tag{27}$$

where

$$u_{nl}(x) = v_{nl}(x, s_+) = x^{l+1}\sum_{m=0}^{\infty} b_m x^m, \quad b_m = a_m(s)\big|_{s=l+1} \tag{28}$$

and

$$w_{nl}(x) = u_{nl}(x)\ln x + v_{nl}(x, s_-) = x^{l+1}\ln x \sum_{m=0}^{\infty} b_m x^m + x^{-l}\sum_{m=0}^{\infty} c_m x^m, \quad c_m = a_m(s)\big|_{s=-l}. \tag{29}$$

For $R_{nl}(r)$ to be regular at the origin, $h_{nl}(x)/x$ must be regular at the origin. At threshold $u_{nl}(x)/x \sim_{x\to 0} x^l$ and is regular for all non-negative values of l. On the other hand, the first term in $w_{nl}(x)/x$ has a threshold behavior $[w_{nl}(x)]_1/x \sim_{x\to 0} x^l \ln x$ and has a logarithmic singularity at the origin, while the second term of $w_{nl}(x)/x$ has a threshold behavior $[w_{nl}(x)]_2/x \sim_{x\to 0} x^{-l-1}$, and has an $l+1$ order pole at the origin for all non-negative values of l. Consequently, the regularity of $R_{nl}(r)$ at the origin requires setting $B=0$, and the solution of Eq. (11) with the boundary conditions imposed is $Au_{nl}(x)$. Since the recursion relation does not determine b_0, then the coefficient A can be absorbed in b_0. Hence the solution of Eq. (11) which is regular at the origin is given by

$$u_{nl}(x) = x^{l+1}\sum_{m=0}^{\infty} b_m x^m \tag{30}$$

with the coefficients $b_m = a_m(s_+)$ determined by the recursion relation (22) with $s = s_+$. Combining Eqs. (22) and (25) we obtain the recursion relation for b_m as

$$m(m+2l+1)b_m + \rho b_{m-1} + t_{nl}b_{m-2} - b_{m-3} = 0 \quad m = 0,1,2,\ldots,\infty \tag{31}$$

subject to the boundary conditions $b_m = \lambda_0 \delta_{m0}$ for $m \leqslant 0$. Hence, the solution of the radial equation (10) for the function $u_{nl}(x)$ has been reduced to the solution of the recursion relation (31) for the coefficients b_m.

C. Solution of the recursion relation

We define the function $f(m,l)$ by

$$f(m,l) = \frac{1}{F(s_+ + m)} = \frac{1}{m(m+2l+1)} \tag{32}$$

so that the above recursion relation can be rewritten as

$$b_m = -\rho f(m,l) b_{m-1} - t_{nl} f(m,l) b_{m-2} + f(m,l) b_{m-3}. \tag{33}$$

Furthermore, we define

$$f_1(m) = -\rho f(m,l), \quad f_2(m) = -t_{nl} f(m,l), \quad f_3(m) = f(m,l) \tag{34}$$

to obtain

$$b_m = f_1(m) b_{m-1} + f_2(m) b_{m-2} + f_3(m) b_{m-3}, \quad m = 0,1,2,\ldots,\infty \tag{35}$$

subject to the boundary conditions

$$b_m = \lambda_0 \delta_{m0} \quad \text{for } m \leqslant 0. \tag{36}$$

The recursion relation (35), subject to boundary conditions (36), is cast in standard form.[20]

Equation (35) is a four-term linear recursion relation with variable coefficients. A solution of this equation in terms of the special combinatorics functions can be obtained using the method introduced by Antippa *et al.*[20] The solution of a linear recursion relation of the form

$$b_m = \sum_{k=1}^{N} f_{a_k}(m) b_{m-a_k} \quad \text{for } m > j_0 \tag{37}$$

with boundary conditions

$$b_{j_0 - i} = \lambda_i \quad \text{for } i = 0,1,2,\ldots,a_N - 1, \tag{38}$$

is[20]

$$b_m = \sum_{i=0}^{a_N - 1} \lambda_i \overline{C}_2(j_0 - i, m, i), \tag{39}$$

where $\overline{C}_2(m_1,m_2,d)$ is a constrained combinatorics function of the second kind. The solution of the recursion relation (35) has thus been reduced to the evaluation of the combinatorics function $\overline{C}_2(j_0 - i, m, i)$.

D. The combinatorics functions

The constrained combinatorics function of the second kind $\overline{C}_2(m_1,m_2,d)$ is a discrete functional defined over the ordered partitions of the interval $[m_1,m_2]$ with the first part of the ordered partition constrained to be of length greater than d. The parts a_i available for partitioning, are the elements of a set $\mathcal{A}$,

$$\mathcal{A} = \{a_1, a_2, \ldots, a_N\}, \quad 0 < a_1 < a_2 < \cdots < a_N. \tag{40}$$

The subintervals of an ordered partition are denoted by δ_j, and a possible ordered partition is represented by $(\delta_1, \delta_2, \ldots, \delta_n)$, where $\delta_j \in \mathcal{A}$. The points at which subintervals end are denoted by s_j,

$$s_0 = m_1, \quad s_j = m_1 + \sum_{i=1}^{j} \delta_i, \quad s_n = m_2. \tag{41}$$

The building blocks from which the combinatorics functions are constructed are the functionals $F_n^q(m_1, m_2)$ defined over the qth ordered partition of the interval $[m_1, m_2]$ into n parts belonging to the set $\mathcal{A}$, according to[20]

$$F_n^q(m_1, m_2) = \prod_{j=1}^{n} f_{\delta_j}(s_j). \tag{42}$$

The special combinatorics functions of the first kind, $C_1(m_1, m_2, n)$, are obtained by summing the $F_n^q(m_1, m_2)$ over the ordered partitions of the interval $[m_1, m_2]$ into n parts,

$$C_1(m_1, m_2, n) = \sum_{q=1}^{q_{\max}(m_1, m_2, n)} F_n^q(m_1, m_2). \tag{43}$$

The special combinatorics functions of the second kind are obtained by summing the special combinatorics functions of the first kind over the possible values of n,

$$C_2(m_1, m_2) = \sum_{n \in \mathcal{N}(m_2 - m_1)} C_1(m_1, m_2, n), \tag{44}$$

where the set $\mathcal{N}(m_2 - m_1)$ is the set of all the number of parts n into which an interval of length $m_2 - m_1$ can be partitioned. The special combinatorics functions of the second kind can thus be expressed as the sum of the $F_n^r(m_1, m_2)$ over all ordered partitions of the interval $[m_1, m_2]$,

$$C_2(m_1, m_2) = \sum_{r=1}^{r_{\max}(m_1, m_2)} F_{n(r)}^r(m_1, m_2), \tag{45}$$

where the number of parts $n(r)$ is now a function of the partition number r. The constrained combinatorics functions of the second kind are related to the special combinatorics functions of the second kind by[24]

$$\overline{C_2}(m_1, m_2, d) = \sum_{\substack{a_k \in \mathcal{A} \\ a_k > d}} f_{a_k}(m_1 + a_k) C_2(m_1 + a_k, m_2). \tag{46}$$

In the special case of $d = 0$, the above equation reduces to

$$\overline{C_2}(m_1, m_2, 0) = \sum_{a_k \in \mathcal{A}} f_{a_k}(m_1 + a_k) C_2(m_1 + a_k, m_2) \tag{47}$$

but the special combinatorics functions obey the recursion relation[25]

$$C_2(m_1, m_2) = \sum_{a_k \in \mathcal{A}} f_{a_k}(m_1 + a_k) C_2(m_1 + a_k, m_2). \tag{48}$$

Hence combining (47) and (48),

$$\overline{C_2}(m_1, m_2, 0) = C_2(m_1, m_2). \tag{49}$$

Note that Eq. (49) is also a coherence condition which can be derived directly from the respective definitions of the special and constrained combinatorics functions of the second kind.

E. Reduction of the combinatorics functions

In the case of Eq. (35), the set $\mathcal{A}$ of allowed parts is given by (see Ref. 20)

$$\mathcal{A} = \{1,2,3\}. \tag{50}$$

Thus $N=3$, $a_1=1$, $a_2=2$, and $a_3=3$. Furthermore, the boundary conditions are given by

$$b_m = \lambda_0 \delta_{m0} \quad \text{for } m \leqslant 0 \tag{51}$$

thus $j_0=0$. Hence, in the case of Eq. (35) subject to boundary conditions (36), the solution for b_m as given by Eq. (39) reduces to

$$b_m = \sum_{i=0}^{2} b_{-i}\overline{C}_2(-i,m,i) = \sum_{i=0}^{2} \lambda_0 \delta_{-i0}\overline{C}_2(-i,m,i) = \lambda_0 \overline{C}_2(0,m,0) \tag{52}$$

and using Eq. (49),

$$b_m = \lambda_0 C_2(0,m). \tag{53}$$

The special combinatorics functions of the second kind $C_2(0,m)$ are given, via Eq. (45), in terms of the functionals $F^r_{n(r)}(m_1,m_2)$. So we need to evaluate these latter functionals.

We define the triplet (p_1,p_2,p_3) representing the number of parts of lengths (1, 2, 3) for a possible ordered partition r of an interval $[0,m]$ into n parts, where p_i is the number of parts of length i. Examining Eq. (34) we notice that the $f_{\delta_j}(s_j)$ are equal to a constant times $f(m,l)$. The number of times these constants will appear in expression (42) as multiplicative factors is related to the number of parts of length 1 for $-\rho$, the number of parts of length 2 for $-t_{nl}$ and the number of parts of length 3 for 1. In order to simplify the notation, we will, from now on, drop the subscripts n and l on t. The $F^r_{n(r)}(0,m)$ can therefore be expressed as

$$F^r_{n(r)}(0,m) = (-\rho)^{p_1}(-t)^{p_2}\prod_{j=1}^{n(r)} f(s_j,l), \tag{54}$$

while the special combinatorics functions of the second kind become[26]

$$C_2(0,m) = \sum_{r=1}^{r_{\max}(0,m)} (-\rho)^{p_1}(-t)^{p_2}\prod_{j=1}^{n(r)} f(s_j,l) \tag{55}$$

leading, via Eq. (53), to the following expression for b_m:

$$b_m = \lambda_0 \sum_{r=1}^{r_{\max}(0,m)} (-\rho)^{p_1}(-t)^{p_2}\prod_{j=1}^{n(r)} f(s_j,l), \tag{56}$$

where s_j is given by Eq. (41), and $f(s_j,l)$ is given, via Eq. (32) as

$$f(s_j,l) = \frac{1}{s_j(s_j+2l+1)}. \tag{57}$$

Evaluating the product over $f(s_j,l)$ in Eq. (56) is an algebraic combinatorial ordered partitioning problem, and so is the sum over r.

F. Partitions

A partition $p(m,n)=1^{p_1}2^{p_2}3^{p_3}$ of an interval of length m into n parts belonging to the set {1, 2, 3} is subject to the constraints

$$p_1 + p_2 + p_3 = n, \tag{58a}$$

TABLE I. Relations between m, n, p_1, p_2, and p_3.

λ	1	2	3
$\Sigma_{i=1}^{3}(\lambda-i)p_i=\lambda n-m$	$p_2+2p_3=m-n$	$p_3-p_1=m-2n$	$2p_1+p_2=3n-m$
$n=\lambda^{-1}(m+\Sigma_{i=1}^{3}(\lambda-i)p_i)$	$n=m-p_2-2p_3$	$n=\lfloor(m+p_1-p_3)/2\rfloor$	$n=\lfloor(m+2p_1+p_2)/3\rfloor$
$m=\lambda n-\Sigma_{i=1}^{3}(\lambda-i)p_i$	$m=n+p_2+2p_3$	$m=2n+p_3-p_1$	$m=3n-2p_1-p_2$
$(\lambda-j)\,p_j\vert_{j=(\lambda+1)\bmod 3}=\lambda n-m-(\lambda-j)\,p_j\vert_{j=(\lambda+2)\bmod 3}$	$p_2=m-n-2p_3$	$p_3=m-2n+p_1$	$p_1=\lfloor(3n-m-p_2)/2\rfloor$
$(\lambda-j)\,p_j\vert_{j=(\lambda+2)\bmod 3}=\lambda n-m-(\lambda-j)\,p_j\vert_{j=(\lambda+1)\bmod 3}$	$p_3=\lfloor(m-n-p_2)/2\rfloor$	$p_1=2n-m+p_3$	$p_2=3n-m-2p_1$

$$p_1 + 2p_2 + 3p_3 = m. \tag{58b}$$

Subtracting (58b) from λ times (58a) we obtain

$$\sum_{i=1}^{3} (\lambda - i)p_i = \lambda n - m. \tag{59}$$

By setting λ successively equal to 1, 2, and 3 we eliminate p_i, for $i=1,2,3$, respectively, from the equations, leading to

$$(\lambda - j)p_j|_{j=(\lambda+1)\bmod 3} + (\lambda - j)p_j|_{j=(\lambda+2)\bmod 3} = \lambda n - m \tag{60}$$

from which we obtain the results presented in Table I. The results of Table I will be used throughout. For example, from the fourth row of the table we see that an interval $[0,m]$ can be partitioned into n parts belonging to {1, 2} if and only if $m=n+p_2$ or $m=2n-p_1$. Similarly it can be partitioned into n parts belonging to {2, 3} if and only if $m=2n+p_3$ or $m=3n-p_2$. Finally it can be partitioned into n parts belonging to {1, 3} if and only if $m=n+2p_3$ or $m=3n-2p_1$.

Equation (58) imposes two linear constraints on the five parameters m, n, p_1, p_2, and p_3, and hence only three of them are independent. Thus, given m, knowledge of any two other parameters, uniquely determines the partition $p(m,n)=1^{p_1}2^{p_2}3^{p_3}$. This result is also explicitly evident from Table I. Specifically, given m, p_2 and p_3 uniquely determine the partition $p(m,n)=1^{p_1}2^{p_2}3^{p_3}$. From Table I, the number of parts n is then given by

$$n(m,p_2,p_3) = m - p_2 - 2p_3 \tag{61}$$

while the number of parts of length 1 is given by

$$p_1(m,p_2,p_3) = m - 2p_2 - 3p_3. \tag{62}$$

G. The sum over *r*

The results obtained in Sec. II F allow us to evaluate the sum over ordered partitions (sum over r) appearing in Eqs. (55) and (56) of Sec. II E.

Let $\mathcal{O}(m_1,m_2)$ designate the set of *ordered partitions* of an interval $[m_1,m_2]$ into parts belonging to {1, 2, 3}, and let $\mathcal{O}_{p_3}(m_1,m_2)$ designate a subset of $\mathcal{O}(m_1,m_2)$, all of whose elements have exactly p_3 parts of length 3. Since the minimum number of parts of length 3 is 0 and the maximum is $\lfloor(m_2-m_1)/3\rfloor$ then the set $\mathcal{O}(m_1,m_2)$ can be expanded as

$$\mathcal{O}(m_1,m_2) = \bigcup_{p_3=0}^{\lfloor(m_2-m_1)/3\rfloor} \mathcal{O}_{p_3}(m_1,m_2). \tag{63}$$

Furthermore, let $\mathcal{O}_{p_3,p_2}(m_1,m_2)$ designate a subset of $\mathcal{O}_{p_3}(m_1,m_2)$, all of whose elements have exactly p_3 parts of length 3 and p_2 parts of length 2. The minimum number of parts of length 2 is

0 and since the partitions contain p_3 parts of length 3 then the maximum is $\lfloor (m_2-m_1-3p_3)/2 \rfloor$. Hence the set of ordered partitions of the interval $[m_1,m_2]$ containing exactly p_3 parts of length 3 can be expanded as

$$\mathcal{O}_{p_3}(m_1,m_2) = \bigcup_{p_2=0}^{\lfloor (m_2-m_1-3p_3)/2 \rfloor} \mathcal{O}_{p_3,p_2}(m_1,m_2) \tag{64}$$

leading, via Eq. (63), to

$$\mathcal{O}(m_1,m_2) = \bigcup_{p_3=0}^{\lfloor (m_2-m_1)/3 \rfloor} \bigcup_{p_2=0}^{\lfloor (m_2-m_1-3p_3)/2 \rfloor} \mathcal{O}_{p_3,p_2}(m_1,m_2). \tag{65}$$

The ordered partitions of the set $\mathcal{O}_{p_3,p_2}(m_1,m_2)$ all correspond to the same partition $p(m,n) = 1^{p_1}2^{p_2}3^{p_3}$ since knowledge of the length of the interval and of p_2 and p_3 completely specifies it. Furthermore the different subsets $\mathcal{O}_{p_3,p_2}(m_1,m_2)$ are disjoint

$$\mathcal{O}_{p_3,p_2}(m_1,m_2) \cap \mathcal{O}_{p_3',p_2'}(m_1,m_2) = \emptyset \quad \text{for } p_3 \neq p_3' \text{ or } p_2 \neq p_2'. \tag{66}$$

Hence

$$\sum_{o \in \mathcal{O}(m_1,m_2)} = \sum_{p_3=0}^{\lfloor (m_2-m_1)/3 \rfloor} \sum_{p_2=0}^{\lfloor (m_2-m_1-3p_3)/2 \rfloor} \sum_{o \in \mathcal{O}_{p_3,p_2}(m_1,m_2)}. \tag{67}$$

The sum over r (the sum over ordered partitions) appearing in Eqs. (55) and (56) of Sec. II E can thus be evaluated as follows:

$$\sum_{r=1}^{r_{\max}(0,m)} = \sum_{p_3=0}^{\lfloor m/3 \rfloor} \sum_{p_2=0}^{\lfloor (m-3p_3)/2 \rfloor} \sum_{o \in \mathcal{O}_{p_3,p_2}(m_1,m_2)}. \tag{68}$$

Let $o_{\max}(p)$, be the number of ordered partitions corresponding to a given partition $p(m,n) = 1^{p_1}2^{p_2}3^{p_3}$ [the cardinality of $\mathcal{O}_{p_3,p_2}(m_1,m_2)$], then[27]

$$o_{\max}(p) = \frac{n!}{p_1!p_2!p_3!}, \quad n = p_1 + p_2 + p_3. \tag{69}$$

Furthermore, let $\mathcal{O}_{p_2}(m_1,m_2,n)$ be the set of ordered partitions of the interval $[m_1,m_2]$ into n parts corresponding to the partition $1^{p_1}2^{p_2}3^{p_3}$. Note that since any three parameters of Eqs. (58) uniquely determines the partition $p(m,n) = 1^{p_1}2^{p_2}3^{p_3}$, then

$$\mathcal{O}_{p_3,p_2}(m_1,m_2) = \mathcal{O}_{p_2}(m_1,m_2,n)\big|_{n=m_2-m_1-p_2-2p_3}. \tag{70}$$

Making use of Eqs. (68) and (70), the combinatorics function given by Eq. (55) can be rewritten as

$$C_2(0,m) = \sum_{p_3=0}^{\lfloor m/3 \rfloor} \sum_{p_2=0}^{\lfloor (m-3p_3)/2 \rfloor} \left(\sum_{o \in \mathcal{O}_{p_2}(0,m,n)} (-\rho)^{p_1}(-t)^{p_2} \prod_{j=1}^{n} f(s_j,l) \right), \tag{71}$$

where n and p_1 are, respectively, given by Eqs. (61) and (62). Since p_1 and p_2 do not depend on ordering (on o), then they can be taken outside the second summation to obtain

$$C_2(0,m) = \sum_{p_3=0}^{\lfloor m/3 \rfloor} \sum_{p_2=0}^{\lfloor (m-3p_3)/2 \rfloor} (-\rho)^{p_1}(-t)^{p_2} \left(\sum_{o \in \mathcal{O}_{p_2}(0,m,n)} \prod_{j=1}^{n} f(s_j,l) \right). \tag{72}$$

In analogy with the structure functions introduced in Ref. 21, we introduce the structure functions $\beta_l(m_1,m_2;n,p_2)$ defined over the ordered partitions of the interval $[m_1,m_2]$ into n parts, p_2 of which are of length 2, as

$$\beta_l(m_1,m_2;n,p_2)=\sum_{o\in\mathcal{O}_{p_2}(m_1,m_2,n)}\prod_{j=1}^{n}f(s_j,l) \tag{73}$$

so that Eq. (72) may be expressed as, replacing p_1 and n by their respective expressions in terms of m, p_2 and p_3 [Eqs. (61) and (62)],

$$C_2(0,m)=\sum_{p_3=0}^{\lfloor m/3\rfloor}\sum_{p_2=0}^{\lfloor (m-3p_3)/2\rfloor}(-\rho)^{m-2p_2-3p_3}(-t)^{p_2}\beta_l(0,m;m-p_2-2p_3,p_2). \tag{74}$$

Inserting the above expression for the combinatorics function of the second kind in Eq. (53) and rearranging we finally find that the coefficients b_m are given by

$$b_m=\lambda_0(-1)^m\sum_{j=0}^{\lfloor m/3\rfloor}(-1)^j\sum_{i=0}^{\lfloor (m-3j)/2\rfloor}(-1)^i\beta_l(0,m;m-2j-i,i)\rho^{m-3j-2i}t^i. \tag{75}$$

The coefficients b_m are polynomials in t of order $m/2$ if m is even or $(m-1)/2$ if m is odd.

III. STRUCTURE FUNCTIONS

A. Fundamental cases

The $\beta_l(m_1,m_2;n,p_2)$ are, in general, complicated expressions. However, in three particular cases, they can be expressed compactly. These cases are $\beta_l(m_1,m_1+n;n,0)$, $\beta_l(m_1,m_1+2n;n,n)$, and $\beta_l(m_1,m_1+3n;n,0)$. They all have in common the fact that $o_{\max}(p)=1$, that is, there is only one possible ordered partition for each partition p. The three structure functions $\beta_l(m_1,m_1+n;n,0)$, $\beta_l(m_1,m_1+2n;n,n)$, and $\beta_l(m_1,m_1+3n;n,0)$ correspond to the values $p_1=n$, $p_2=n$, and $p_3=n$, respectively.

1. Segments of length 1 ($m=n$ and $p_1=n$)

In the case of $\beta_l(m_1,m_1+n;n,0)$, the length of the interval to be partitioned is $m=n$, and $p_2=0$. Hence from Table I, we have $p_1=n$ and $p_3=0$, and that is the interval is partitioned exclusively into segments of unite length. Thus $o_{\max}(p)=1$ and $s_j=m_1+j$ leading to

$$\beta_l(m_1,m_1+n;n,0)=\sum_{o\in\mathcal{O}_{p_2=0}(m_1,m_1+n,n)}\prod_{j=1}^{n}f(s_j,l)=\prod_{j=1}^{n}f(m_1+j,l) \tag{76}$$

and using Eq. (32), we have

$$\beta_l(m_1,m_1+n;n,0)=\prod_{j=1}^{n}\frac{1}{(m_1+j)}\prod_{j=1}^{n}\frac{1}{(m_1+2l+1+j)}. \tag{77}$$

Making use of the Pochhammer notation (see Appendix A), the above equation can be rewritten as

$$\beta_l(m_1,m_1+n;n,0)=\{(m_1+1)^{[n]}(m_1+2l+2)^{[n]}\}^{-1}. \tag{78}$$

2. Segments of length 2 ($m=2n$ and $p_2=n$)

In the case of $\beta_l(m_1,m_1+2n;n,n)$, the length of the interval to be partitioned is $m=2n$, and $p_2=n$. Hence from Table I, we have $p_1=0$ and $p_3=0$, that is the interval is partitioned exclusively into segments of length 2. Thus $o_{\max}(p)=1$ and $s_j=m_1+2j$ leading to

$$\beta_l(m_1,m_1+2n;n,n) = \sum_{o\in\mathcal{O}_{p_2=n}(m_1,m_1+2n,n)} \prod_{j=1}^{n} f(s_j,l) = \prod_{j=1}^{n} f(m_1+2j,l)$$
$$= \prod_{j=1}^{n} \frac{1}{(m_1+2j)} \prod_{j=1}^{n} \frac{1}{(m_1+2j+2l+1)}$$
$$= \frac{1}{2^{2n}} \prod_{j=1}^{n} \frac{1}{(m_1/2+j)} \prod_{j=1}^{n} \frac{1}{((m_1+1)/2+l+j)}. \tag{79}$$

The above equation can be rewritten as

$$\beta_l(m_1,m_1+2n;n,n) = \{2^{2n}[(m_1+2)/2]^{[n]}[(m_1+2l+3)/2]^{[n]}\}^{-1}. \tag{80}$$

3. Segments of length 3 ($m=3n$ and $p_3=n$)

In the case of $\beta_l(m_1,m_1+3n;n,0)$, the length of the interval to be partitioned is $m=3n$, and $p_2=0$. Hence from Table I, we have $p_3=n$ and $p_1=0$, in other words the interval is partitioned exclusively into segments of length 3. Thus $o_{\max}(p)=1$ and $s_j=m_1+3j$ leading to

$$\beta_l(m_1,m_1+3n;n,0) = \{3^{2n}[(m_1+3)/3]^{[n]}[(m_1+2l+4)/3]^{[n]}\}^{-1}. \tag{81}$$

B. Recursion relations for the structure functions

To determine the structure functions, we proceed in two steps. First, using the results of the preceding section as initial conditions, we establish a recursive procedure for determining $\beta_l(m_1,m_2;n,0)$. Next, we use these values of $\beta_l(m_1,m_2;n,0)$ as initial conditions, and determine a recursive expression for $\beta_l(m_1,m_2;n,p_2)$ in the case $p_2\neq 0$.

1. Structure functions of the form $\beta_l(m_1,m_2;n,0)$

Following the procedure of Ref. 21, the structure functions of the form $\beta_l(m_1,m_2;n,0)$ will be determined recursively by establishing a relation between the structure functions $\beta_l(m_1,m_2;n,0)$ corresponding to partitions with p_3 parts of length 3, and the structure functions $\beta_l(m_1,m_2';n',0)$ corresponding to partitions with a smaller number of parts of length 3.

Let $\mathcal{T}(m_1,m_2,n)$ be the set of all *ordered partitions*, of $[m_1,m_2]$ into n parts, corresponding to the *partition* $1^{p_1}2^0 3^{p_3}$. Since, given m_1, m_2, and n, the value of p_2 uniquely determines the partition $p(m_2-m_1,n)=1^{p_1}2^{p_2}3^{p_3}$, then

$$\mathcal{T}(m_1,m_2,n) = \mathcal{O}_{p_2=0}(m_1,m_2,n) \tag{82}$$

and

$$\sum_{o\in\mathcal{O}_{p_2=0}(m_1,m_2,n)} = \sum_{\pi\in\mathcal{T}(m_1,m_2,n)}. \tag{83}$$

Let $\mathcal{T}_i(m_1,m_2,n)$, $i=0,1,2,\ldots,p_3$, be a subset of $\mathcal{T}(m_1,m_2,n)$ whose elements satisfy two additional constraints: (i) the last i parts of the ordered partition are of length 3 and (ii) the $(n-i)$th part of the ordered partition is of length 1 (see Fig. 1). Note that

$$\mathcal{T}(m_1,m_2,n) = \bigcup_{i=0}^{p_3} \mathcal{T}_i(m_1,m_2,n) \tag{84}$$

and that the subsets $\mathcal{T}_i(m_1,m_2,n)$ are disjoint,

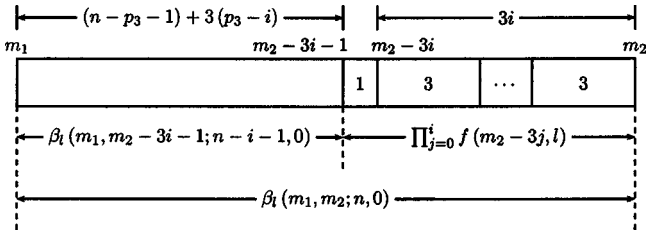

FIG. 1. Graphical representation of the partitions which are elements of the set $\mathcal{T}_i(m_1,m_2,n)$ and their corresponding structure functions.

$$\mathcal{T}_i(m_1,m_2,n) \cap \mathcal{T}_j(m_1,m_2,n) = \emptyset \quad \text{for } i \neq j, \tag{85}$$

hence

$$\sum_{\pi \in \mathcal{T}(m_1,m_2,n)} = \sum_{i=0}^{p_3} \sum_{\pi \in \mathcal{T}_i(m_1,m_2,n)} . \tag{86}$$

Combining Eqs. (83) and (86) we have the summation equation,

$$\sum_{o \in \mathcal{O}_{p_2=0}(m_1,m_2,n)} = \sum_{i=0}^{p_3} \sum_{\pi \in \mathcal{T}_i(m_1,m_2,n)} . \tag{87}$$

Note also (see Fig. 1), that there is a one-to-one correspondence between the elements of $\mathcal{T}_i(m_1,m_2,n)$ and the elements of $\mathcal{O}_{p_2=0}(m_1,m_2-3i-1,n-i-1)$,

$$\mathcal{T}_i(m_1,m_2,n) \leftrightarrow \mathcal{O}_{p_2=0}(m_1,m_2-3i-1,n-i-1), \tag{88}$$

hence

$$\sum_{\pi \in \mathcal{T}_i(m_1,m_2,n)} = \sum_{o \in \mathcal{O}_{p_2=0}(m_1,m_2-3i-1,n-i-1)} . \tag{89}$$

The structure function $\beta_l(m_1,m_2;n,0)$ is given via Eq. (73) as

$$\beta_l(m_1,m_2;n,0) = \sum_{o \in \mathcal{O}_{p_2}(m_1,m_2,n)} \prod_{j=1}^{n} f(s_j,l) \tag{90}$$

and due to Eq. (87), it can be rewritten as

$$\beta_l(m_1,m_2;n,0) = \sum_{i=0}^{p_3} \left(\sum_{\pi \in \mathcal{T}_i(m_1,m_2,n)} \prod_{j=1}^{n} f(s_j,l) \right). \tag{91}$$

Now

$$\prod_{j=1}^{n} f(s_j,l) = \left(\prod_{j=1}^{n-i-1} f(s_j,l) \right) \left(\prod_{j=n-i}^{n} f(s_j,l) \right) \tag{92}$$

and since all partitions belonging to the set $\mathcal{T}_i(m_1,m_2,n)$ have their last i parts of length 3, then from Eq. (41), with $\delta_j=3$ for $n-i+1 \leqslant j \leqslant n$, and $s_{n-i}=m_2-3i$ we have

$$s_{n-i+j'} = s_{n-i} + 3j' = m_2 - 3(i-j') \quad \text{for } j' = 1,2,\ldots,i \tag{93}$$

and consequently

$$\prod_{j=n-i}^{n} f(s_j,l) = \prod_{j'=0}^{i} f(s_{n-i+j'},l) = \prod_{j'=0}^{i} f(m_2 - 3(i-j'),l) = \prod_{j=0}^{i} f(m_2 - 3j,l). \tag{94}$$

Combining Eqs. (89), (92), and (94), Eq. (91) can be rewritten as

$$\beta_l(m_1,m_2;n,0) = \sum_{i=0}^{p_3} \left(\prod_{j=0}^{i} f(m_2 - 3j,l) \sum_{o \in \mathcal{O}_{p_2=0}(m_1,m_2-3i-1,n-i-1)} \prod_{j=1}^{n-i-1} f(s_j,l) \right). \tag{95}$$

But

$$\sum_{o \in \mathcal{O}_{p_2=0}(m_1,m_2-3i-1,n-i-1)} \prod_{j=1}^{n-i-1} f(s_j,l) = \beta_l(m_1,m_2-3i-1;n-i-1,0). \tag{96}$$

Hence Eq. (95) becomes

$$\beta_l(m_1,m_2;n,0) = \sum_{i=0}^{p_3} \beta_l(m_1,m_2-3i-1;n-i-1,0) \prod_{j=0}^{i} f(m_2-3j,l). \tag{97}$$

The fourth cell of the fourth row of Table I gives an expression for the length of an interval in terms of n, p_2, and p_3. Setting $p_2=0$, we obtain the length of intervals that can be partitioned into n parts belonging to $\{1, 3\}$ as $m_2-m_1=n+2p_3$. Inserting this results in Eq. (97), we obtain

$$\beta_l(m_1,m_1+n+2p_3;n,0) = \sum_{i=0}^{p_3} \beta_l(m_1,m_1+n+2p_3-3i-1;n-i-1,0) \prod_{j=0}^{i} f(m_1+n+2p_3-3j,l). \tag{98}$$

The product can be expressed as

$$\begin{aligned} \prod_{j=0}^{i} f(m_1+n+2p_3-3j,l) &= \prod_{j=0}^{i} \frac{1}{(m_1+n+2p_3-3j)} \prod_{j=0}^{i} \frac{1}{(m_1+n+2p_3-3j+2l+1)} \\ &= \frac{1}{3^{2(i+1)}} \prod_{j=0}^{i} \frac{1}{((m_1+n+2p_3)/3-j)} \prod_{j=0}^{i} \frac{1}{((m_1+n+2p_3+2l+1)/3-j)} \end{aligned} \tag{99}$$

or in Pochhammer notation

$$\prod_{j=0}^{i} f(m_1+n+2p_3-3j,l) = \frac{3^{-2(i+1)}}{[(m_1+n+2p_3)/3]^{(i+1)}[(m_1+n+2p_3+2l+1)/3]^{(i+1)}}. \tag{100}$$

Substituting this result in Eq. (98), we finally obtain

$$\beta_l(m_1,m_1+n+2p_3;n,0) = \sum_{i=0}^{p_3} \frac{3^{-2(i+1)} \beta_l(m_1,m_1+n+2p_3-3i-1;n-i-1,0)}{[(m_1+n+2p_3)/3]^{(i+1)}[(m_1+n+2p_3+2l+1)/3]^{(i+1)}}. \tag{101}$$

The recursion equation (101), can alternatively be written as a recursion relation in p_1, by making use of the relation $p_3=n-p_1$ to obtain

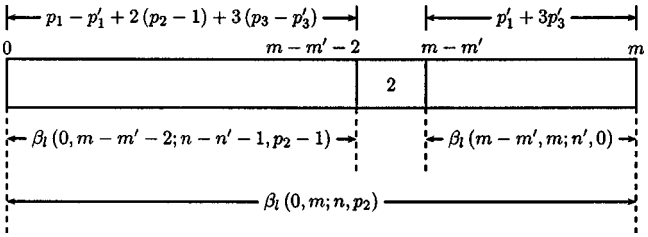

FIG. 2. Graphical representation of the relation between the partitions which are elements of the set $\mathcal{O}_{p_2-1}(0,m-m'-2,n-n'-1)$ and the partitions which are elements of the sets $\mathcal{O}_{p_2=0}(m-m',m,n')$ and $\mathcal{S}_{p_2}^{n',m'}(0,m,n)$, as well as their corresponding structure functions.

$$\beta_l(m_1,m_1+3n-2p_1;n,0)=\sum_{i=0}^{n-p_1}\frac{3^{-2(i+1)}\beta_l(m_1,m_1+3n-2p_1-3i-1;n-i-1,0)}{[(m_1+3n-2p_1)/3]^{(i+1)}[(m_1+3n-2p_1+2l+1)/3]^{(i+1)}}. \tag{102}$$

In the appendix we evaluate the above Eq. (102) for $p_1=n$ and reproduce Eq. (78).

2. Structure functions of the form $\beta_l(0,m;n,p_2)$

In this section, we derive a recursion relation for the structure functions $\beta_l(0,m;n,p_2)$, evaluated over the ordered partitions of the interval $[0,m]$ into n parts belonging to {1, 2, 3}, and corresponding to the partition $1^{p_1}2^{p_2}3^{p_3}$.

To this end we note that the structure functions $\beta_l(m_1,m_2;n,p_2)$ are combinatorics functions (see Secs. II C and II D) evaluated over the set of ordered partitions $\mathcal{O}_{p_2}(m_1,m_2,n)$, with the set of parts $\mathcal{A}=\{a_1,a_2,\ldots,a_N\}$ given by $\mathcal{A}=\{1,2,3\}$, and the corresponding variable coefficients, $f_{a_i}(m)$ for $a_i=1,2,3$, given by

$$f_1(m)=f_2(m)=f_3(m)=f(m,l), \tag{103}$$

where $f(m,l)$ is given by Eq. (32). Hence, $\beta_l(m_1,m_2;n,p_2)$ is obtained from $\mathcal{O}_{p_2}(m_1,m_2,n)$ by a homomorphism H from $(\mathcal{O}^*,\cup,\otimes)$ to $(R,+,\times)$, where the $*$ indicates the power set (see Ref. 25 Sec. II C, or Ref. 28 Sec. III A, or Ref. 29 Sec. 2.2.1):

$$(\mathcal{O}^*,\cup,\otimes)\overset{H}{\rightarrow}(R,+,\times) \tag{104}$$

and Eq. (90) can be rewritten as

$$\beta_l(m_1,m_2;n,p_2)=H(\mathcal{O}_{p_2}(m_1,m_2,n)). \tag{105}$$

Let $\mathcal{S}_{p_2}^{n',m'}(0,m,n)$ be the set of ordered partitions of the interval $[0,m]$ into n parts (p_1,p_2,p_3) (with $p_2\geqslant 1$ and $m\geqslant 2$), subject to the following constraints (i) the last n' parts are not of length 2, (ii) the $(n-n')$th part is of length 2, and (iii) the total length of the last n' parts is m'. Thus

$$n'=p_1'+p_3', \tag{106}$$

$$m'=p_1'+3p_3', \tag{107}$$

where p_1' and p_3' are the number of parts of lengths 1 and 3, respectively, to the right of the $(n-n')$th part of length 2. Their ranges are $0\leqslant p_1'\leqslant p_1$ and $0\leqslant p_3'\leqslant p_3$. The ordered partitions of the set $\mathcal{S}_{p_2}^{n',m'}(0,m,n)$ are presented in Fig. 2.

The set $\mathcal{S}_{p_2}^{n',m'}(0,m,n)$ can be expressed as follows (see Fig. 2):

$$\mathcal{S}_{p_2}^{n',m'}(0,m,n) = \mathcal{O}_{p_2-1}(0,m-m'-2,n-n'-1) \otimes \{m-m'-2,m-m'\} \otimes \mathcal{O}_{p_2=0}(m-m',m,n'). \tag{108}$$

Furthermore, the set of all ordered partitions of the interval $[0,m]$ into n parts (p_1,p_2,p_3) (with $p_2 \geqslant 1$ and $m \geqslant 2$) is given by the union of the sets $\mathcal{S}_{p_2}^{n',m'}(0,m,n)$ over all possible values of n' and m', that is,

$$\mathcal{O}_{p_2}(0,m,n) = \cup_{n'}\left(\cup_{m'} \mathcal{S}_{p_2}^{n',m'}(0,m,n)\right). \tag{109}$$

Combining Eqs. (108) and (109) we have

$$\mathcal{O}_{p_2}(0,m,n) = \cup_{n'}\cup_{m'} \mathcal{O}_{p_2-1}(0,m-m'-2,n-n'-1) \otimes \{m-m'-2,m-m'\} \otimes \mathcal{O}_{p_2=0}(m-m',m,n'). \tag{110}$$

Applying the homomorphism H to Eq. (110) leads to

$$H(\mathcal{O}_{p_2\geqslant 1}(0,m,n)) = \sum_{n'}\sum_{m'} H(\mathcal{O}_{p_2-1}(0,m-m'-2,n-n'-1)) \times H(\{m-m'-2,m-m'\})H(\mathcal{O}_{p_2=0}(m-m',m,n')) \tag{111}$$

which evaluates to

$$\beta_l(0,m;n,p_2) = \sum_{n'}\sum_{m'} \beta_l(0,m-m'-2;n-n'-1,p_2-1) f_2(m-m') \beta_l(m-m',m;n',0) \tag{112}$$

and due to Eq. (103) becomes

$$\beta_l(0,m;n,p_2) = \sum_{n'}\sum_{m'} \frac{\beta_l(0,m-m'-2;n-n'-1,p_2-1)\beta_l(m-m',m;n',0)}{(m-m')(m-m'+2l+1)}. \tag{113}$$

Making use of Eqs. (106) and (107), the double sum over the values of m' and n' can be converted into a double sum over p_1' and p_3', ranging, respectively, from 0 to p_1 and from 0 to p_3, and we finally obtain

$$\beta_l(0,m;n,p_2) = \sum_{p_1'=0}^{p_1}\sum_{p_3'=0}^{p_3} \frac{\beta_l(m-p_1'-3p_3',m;p_1'+p_3',0)}{(m-p_1'-3p_3')(m-p_1'-3p_3'+2l+1)} \times \beta_l(0,m-p_1'-3p_3'-2;n-p_1'-p_3'-1,p_2-1). \tag{114}$$

IV. THE WAVE FUNCTIONS

In this section we use the results of the preceding sections to obtain the wave functions of the Coulomb-plus-linear potential and then proceed to calculate the first six coefficients of the power series expansion of the wave functions.

A. General expression for the wave functions

The wave functions for the Coulomb-plus-linear potential are given by Eq. (2) as

$$\psi_{nlm}(\vec{r}) = r^{-1}u_{nl}(r)Y_l^m(\theta,\phi). \tag{115}$$

The functions $u_{nl}(r)$ are given by Eq. (30), with $x=(2\mu\kappa/\hbar^2)^{1/3}r$, leading to

$$u_{nl}(r) = r^{l+1}\sum_{k=0}^{\infty} b_k \left(\frac{2\mu\kappa}{\hbar^2}\right)^{(k+l+1)/3} r^k. \tag{116}$$

Substituting the above expression for $u_{nl}(r)$ in Eq. (115), inserting the expression for the coefficients b_k [Eq. (75)] and replacing ρ and t by Eqs. (8) and (9), respectively, we finally find that the wave functions for the Coulomb-plus-linear potential are given by

$$\psi_{nlm}(\vec{r}) = \lambda_0 Y_l^m(\theta,\phi) r^l \left(\frac{2\mu\kappa}{\hbar^2}\right)^{(l+1)/3} \sum_{k=0}^{\infty} (-1)^k \sum_{j=0}^{\lfloor k/3 \rfloor} (-1)^j \sum_{i=0}^{\lfloor (k-3j)/2 \rfloor} (-1)^i \times \left(\frac{2\mu}{\hbar^2}\right)^{k-2j-i} \beta_l(0,k;k-2j-i,i)\kappa^j \alpha^{k-3j-2i} (E_{nl}-V_0)^i r^k. \tag{117}$$

B. Explicit expressions for the power series coefficients

We now give expressions for the first six coefficients b_m, $m=1,2,3,4,5,6$ of the power series. The computation of a coefficient proceeds in the following way: (i) Eq. (75) is used to obtain an expression for the coefficient b_m in terms of structure functions. (ii) Recursion relations (102) and (114), obtained in Sec. III B, are used to bring the expression for the coefficient to a form containing only fundamental structure functions, that is, structure functions of the form $\beta_l(m_1,m_1+n;n,0)$ or $\beta_l(m_1,m_1+2n;n,n)$ or $\beta_l(m_1,m_1+3n;n,0)$. The upper summation limits of Eq. (114) are obtained using Table I. (iii) The fundamental structure functions can then be evaluated using Eqs. (78), (80), and (81).

The coefficient b_0 was arbitrarily chosen as λ_0 and we can verify that Eq. (75) with $m=0$ leads to

$$b_0 = \lambda_0 \beta_l(0,0;0,0) = \lambda_0. \tag{118}$$

The coefficients b_1 to b_6 are given by

$$b_1 = -\lambda_0 \beta_l(0,1;1,0)\rho, \tag{119}$$

$$b_2 = \lambda_0[\beta_l(0,2;2,0)\rho^2 - \beta_l(0,2;1,1)t], \tag{120}$$

$$b_3 = \lambda_0[-\beta_l(0,3;3,0)\rho^3 + \beta_l(0,3;2,1)\rho t + \beta_l(0,3;1,0)], \tag{121}$$

$$b_4 = \lambda_0[\beta_l(0,4;4,0)\rho^4 - \beta_l(0,4;3,1)\rho^2 t + \beta_l(0,4;2,2)t^2 - \beta_l(0,4;2,0)\rho], \tag{122}$$

$$b_5 = -\lambda_0[\beta_l(0,5;5,0)\rho^5 - \beta_l(0,5;4,1)\rho^3 t + \beta_l(0,5;3,2)\rho t^2 - \beta_l(0,5;3,0)\rho^2 + \beta_l(0,5;2,1)t], \tag{123}$$

$$b_6 = \lambda_0[\beta_l(0,6;6,0)\rho^6 - \beta_l(0,6;5,1)\rho^4 t + \beta_l(0,6;4,2)\rho^2 t^2 - \beta_l(0,6;3,3)t^3 - \beta_l(0,6;4,0)\rho^3 + \beta_l(0,6;3,1)\rho t + \beta_l(0,6;2,0)]. \tag{124}$$

Evaluating the structure functions we find that

$$b_1 = -\lambda_0 \frac{\rho}{(2l+2)^{[1]}}, \tag{125}$$

$$b_2 = \frac{\lambda_0}{2!(2l+2)^{[2]}}[\rho^2 - (2l+2)t], \tag{126}$$

$$b_3 = \frac{\lambda_0}{3!(2l+2)^{[3]}}\{-\rho^3 + [2(2l+3) + (2l+2)]\rho t + 2(2l+2)^{[2]}\}, \tag{127}$$

$$b_4 = \frac{\lambda_0}{4!(2l+2)^{[4]}}\{\rho^4 - [3(2l+4) + 2(2l+3) + (2l+2)]\rho^2 t + 3(2l+2)(2l+4)t^2 - [2(2l+2)^{[2]} + 6(2l+3)^{[2]}]\rho\}, \tag{128}$$

$$b_5 = \frac{-\lambda_0}{5!(2l+2)^{[5]}}\{\rho^5 - [4(2l+5) + 3(2l+4) + 2(2l+3) + (2l+2)]\rho^3 t + [8(2l+3)(2l+5) + 4(2l+2)(2l+5) + 3(2l+2)(2l+4)]\rho t^2 - [2(2l+2)^{[2]} + 6(2l+3)^{[2]} + 12(2l+4)^{[2]}]\rho^2 + [8(2l+2)^{[2]}(2l+5) + 12(2l+2)(2l+4)^{[2]}]t\}, \tag{129}$$

$$b_6 = \frac{\lambda_0}{6!(2l+2)^{[6]}}\{\rho^6 - [5(2l+6) + 4(2l+5) + 3(2l+4) + 2(2l+3) + (2l+2)]\rho^4 t + \{5(2l+6)[3(2l+4) + 2(2l+3) + (2l+2)] + 4(2l+5)[2(2l+3) + (2l+2)] + 3(2l+4)(2l+2)\}\rho^2 t^2 - 15(2l+2)(2l+4)(2l+6)t^3 - [2(2l+2)^{[2]} + 6(2l+3)^{[2]} + 12(2l+4)^{[2]} + 20(2l+5)^{[2]}]\rho^3 + \{5(2l+6) \times [2(2l+2)^{[2]} + 6(2l+3)^{[2]}] + 8(2l+2)^{[2]}(2l+5) + 12(2l+2)(2l+4)^{[2]} + 20[(2l+2) + 2(2l+3)](2l+5)^{[2]}\}\rho t + 40(2l+2)^{[2]}(2l+5)^{[2]}\}. \tag{130}$$

In the $\alpha \to 0$ limit, the Coulomb-plus-linear potential, parametrized as in (1), reduces to the linear potential. A consistency check would be to reproduce, in this limit, the coefficients obtained in the case of the linear potential. Setting $\alpha = 0$ in the potential corresponds, via Eq. (8), to setting $\rho = 0$ in the expressions for the coefficients. In the case $\rho = 0$, Eqs. (119)–(124) reduce to

$$b_1|_{\rho=0} = 0, \tag{131}$$

$$b_2|_{\rho=0} = -\lambda_0 \beta_l(0,2;1,1)t, \tag{132}$$

$$b_3|_{\rho=0} = \lambda_0 \beta_l(0,3;1,0), \tag{133}$$

$$b_4|_{\rho=0} = \lambda_0 \beta_l(0,4;2,2)t^2, \tag{134}$$

$$b_5|_{\rho=0} = -\lambda_0 \beta_l(0,5;2,1)t, \tag{135}$$

$$b_6|_{\rho=0} = \lambda_0[-\beta_l(0,6;3,3)t^3 + \beta_l(0,6;2,0)]. \tag{136}$$

Note that the structure functions appearing in these expressions are all of the form $\beta_l(0,m;n,3n-m)$, that is, they are defined over partitions containing only parts of length 2 or 3 (see Table I). Since the structure functions $\beta_l(0,m;n,p_2)$ and the structure functions $\beta_l(0,m;n)$ of Ref. 21 are defined in an analogous manner [see Eq. (73) of this paper and (3.14a) of Ref. 21] and since the $f(m,l)$ function [Eq. (57) of this paper and Eq. (3.3b) of Ref. 21] is the same in both cases, then the structure functions $\beta_l(0,m;n,3n-m)$ are equal to the structure functions $\beta_l(0,m;n)$ of Ref. 21. With this in mind, it can easily be checked that the above expressions reproduce the coefficients given by Eqs. (3.17a) and (3.17b) of Ref. 21, repeated here for convenience

$$b_{2k}^{\mathrm{lin}} = \lambda_0 \sum_{j=0}^{\lfloor k/3 \rfloor} \beta_l(0,2k;k-j)(-t)^{k-3j} \quad (k \geqslant 1), \tag{137}$$

$$b_{2k+1}^{\mathrm{lin}} = \lambda_0 \sum_{j=0}^{\lfloor (k-1)/3 \rfloor} \beta_l(0,2k+1;k-j)(-t)^{k-1-3j} \quad (k \geqslant 1). \tag{138}$$

V. CONCLUSION

We solved the Schrödinger equation for a quark–antiquark system interacting via a Coulomb-plus-linear potential. The series solution of the Schrödinger equation involved a four-term recursion relation relating the coefficients of the power series expansion of the wave function. This recursion relation was solved in terms of *combinatorics functions* which were then reduced to *structure functions*. Finally, recursion relations were derived to explicitly calculate these *structure functions*. The present work on the wave functions of the Schrödinger equation for the Coulomb-plus-linear potential lays the mathematical framework necessary to formulate and solve the corresponding eigenvalue equation.

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APPENDIX A: POCHHAMMER SYMBOLS

The following notation is used for the Pochammer symbols:[30]

$$x^{(n)} = x(x-1)\cdots(x-n+1) = \prod_{i=1}^{n}(x+1-i) = \frac{\Gamma(x+1)}{\Gamma(x-n+1)}, \tag{A1}$$

$$x^{[n]} = x(x+1)\cdots(x+n-1) = \prod_{i=1}^{n}(x-1+i) = \frac{\Gamma(x+n)}{\Gamma(x)}, \tag{A2}$$

where $x^{(n)}$ is the descending Pochhammer symbol (or falling factorial) and $x^{[n]}$ is the ascending Pochammer symbol (or rising factorial). An ascending Pochammer can be converted to a descending Pochhammer, and vice versa, via

$$x^{(n)} = (x-n+1)^{[n]}, \quad x^{[n]} = (x+n-1)^{(n)}. \tag{A3}$$

Furthermore, the Pochhammer symbols can be factorized using the following properties:

$$x^{(n)} = x^{(i)}(x-i)^{(n-i)}, \quad x^{[n]} = x^{[i]}(x+i)^{[n-i]}. \tag{A4}$$

APPENDIX B: THE RECURSIVE RELATION FOR $\beta_l(m_1,m_2;n,0)$

In this appendix we demonstrate that the recursive relation for the structure function $\beta_l(m_1,m_2;n,0)$, as given by Eq. (102), in the special case of $p_1=n$, reduces to the expression of the fundamental structure function in which all parts are of unit length [Eq. (78)]. Setting $p_1=n$ in Eq. (102), we obtain

$$\beta_l(m_1,m_1+n;n,0) = \frac{\beta_l(m_1,m_1+n-1;n-1,0)}{3^2[(m_1+n)/3]^{(1)}[(m_1+n+2l+1)/3]^{(1)}} \tag{B1}$$

$$= \frac{\beta_l(m_1, m_1 + n - 1; n - 1, 0)}{(m_1 + n)(m_1 + n + 2l + 1)} \tag{B2}$$

but

$$\beta_l(m_1, m_1 + n - 1; n - 1, 0) = \{(m_1 + 1)^{[n-1]}(m_1 + 2l + 2)^{[n-1]}\}^{-1}. \tag{B3}$$

Hence

$$\beta_l(m_1, m_1 + n; n, 0) = \{(m_1 + n)(m_1 + 1)^{[n-1]}(m_1 + n + 2l + 1)(m_1 + 2l + 2)^{[n-1]}\}^{-1} \tag{B4}$$

leading to

$$\beta_l(m_1, m_1 + n; n, 0) = \{(m_1 + 1)^{[n]}(m_1 + 2l + 2)^{[n]}\}^{-1} \tag{B5}$$

which is identical to Eq. (78).

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Solvable $\mathcal{PT}$-symmetric model with a tunable interspersion of nonmerging levels

Miloslav Znojil[a)]
Nuclear Physics Institute, Academy of Sciences of the Czech Republic, 250 68 Řež, Czech Republic

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We study the spectrum in such a $\mathcal{PT}$-symmetric square well (of a diameter $L \leqslant \infty$) where the "strength of the non-Hermiticity" is controlled by the two parameters, viz., by an imaginary coupling ig and by the distance $\ell < L$ of its onset from the origin. We solve this problem and confirm that the spectrum is discrete and real in a nonempty interval of $g \leqslant g_0(\ell, L)$. Surprisingly, a specific distinction between the bound states is found in their asymptotic stability/instability with respect to an unlimited growth of g beyond $g_0(\ell, L)$. In our model, *all* of the low-lying levels remain asymptotically unstable at the small $\ell \ll L$ and finite L while only the stable levels survive near $\ell \approx L < \infty$ *or* in the purely imaginary force limit with $0 < \ell < L = \infty$. In between these two extremes, an unusual and tunable, variable pattern of the interspersed "robust" and "fragile" subspectra of the real levels is obtained. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1925249]

I. INTRODUCTION

Around 1992, Bessis succeeded in attracting attention of a few people to a certain toy Hamiltonian (with some relevance in quantum field theory) which appeared to produce the real and discrete spectrum of energies in spite of being manifestly non-Hermitian.[1] A few years later, Bender and Boettcher returned to his mind-boggling problem and published a numerical study[2] of the whole class of the perceivably more general one-dimensional Schrödinger equations

$$\left[-\frac{d^2}{dx^2} + V(x) + iW(x) \right] \psi(x) = E\psi(x), \tag{1}$$

where, in our present perspective, the real component of the potential was assumed spatially symmetric while its Hermiticity-violating partner was chosen as spatially antisymmetric,

$$\mathcal{P}V(x)\mathcal{P} = V(-x) = +V(x), \quad \mathcal{P}W(x)\mathcal{P} = W(-x) = -W(x).$$

The latter study confirmed that the similar models [exhibiting, obviously, the parity ($\mathcal{P}$) times time-reversal ($\mathcal{T}$) symmetry] may possess *both* the purely real and partially (or, perhaps, completely) complex spectra. The Bender's and Boettcher's Fig. 1 (*loc. cit.*) illustrated the existence of the spectrum which proved "robustly real," i.e., real in a wide range of parameters of their "massless" $\mathcal{PT}$-symmetric model. In contrast, a merely slightly modified "massive" $\mathcal{PT}$-symmetric model of their Fig. 3 (*loc. cit.*) behaved quite differently. The values of many of its energy levels proved extremely sensitive to the very small variations of the parameters and, moreover, even the very reality of some energies proved "fragile" in the sense that after a very small change of a parameter of the model, certain energy pairs merged and disappeared forming, presumably, the complex conjugate pairs. At present, many more similar and more or less purely numerical examples exists (cf., e.g., the recent paper[3] for a sample of references).

a)Electronic mail; znojil@ujf.cas.cz

The recent progress in our understanding of the various $\mathcal{PT}$-symmetric quantum Hamiltonians H may be briefly summarized as an observation that their symmetry is important. First, it was established that the time-reversal-type antilinear operator factor $\mathcal{T}$ merely mediates the Hermitian conjugation $A \to A^{\dagger}$.[4,5] The role of parity $\mathcal{P}$ is more subtle and seems to offer the main mathematical key to the study of the $\mathcal{PT}$-symmetric quantum Hamiltonians H within the so-called Krein-space theory (cf., e.g., Ref. 6 for a nice as well as concise introduction to this language).

On the background of these *mathematical* observations, the formalism lost its originally highly enigmatic features in the context of *physics*. During the last two or three years, the use of the $\mathcal{PT}$-symmetric quantum models has in fact been accepted as just opening new horizons within the standard quantum mechanics. At present, virtually all the people active in the field would agree that it is only necessary to make the resulting physical picture complete by a revitalization of its probabilistic contents and tractability. This is being achieved via an introduction of the "missing" (and, in fact, quite nontrivial) metric $\eta \neq I$ in the Hilbert space of states.[6–8]

The temporary doubts and puzzles related, typically, to the applicability of the formalism look, at least roughly, clarified. One feels urged to return to many recently neglected and apparently evasive and mathematically more subtle questions like the problems of the robustness/fragility of the individual energies or of a global typology of the spectra. We believe that it is time for their deeper and more technical study via, say, simplified and, first of all, *non-numerically tractable* models. A new one, with rather surprising properties and descriptive features of the spectrum, is to be proposed and analyzed in what follows.

A. Non-Hermitian square-well-type models

Within $\mathcal{PT}$-symmetric quantum mechanics a one-parametric non-Hermitian square well (NSW) model has been described in Ref. 9. A key merit of the NSW model lies in a combination of its straightforward mathematical solvability with an exceptional transparency of its applications. In this way, the NSW model was able to offer an insight into the mechanism of the spontaneous $\mathcal{PT}$-symmetry breaking.[10] Next, due to its elementary character, the NSW model has been selected by Bagchi *et al.*[11] as a starting point of a systematic supersymmetric generation of solvable non-Hermitian Hamiltonians with $\mathcal{PT}$-symmetry and real spectra. Last but not least, Mostafazadeh and Batal[7] choose the NSW model in their very recent illustrative application of the $\mathcal{PT}$-symmetric quantum mechanics in its present, mathematically as well as physically more or less consistent updated form (readers may consult some of the available reviews for more details.[12])

In our recent paper[13] we revealed that a certain "hidden" shortcoming of the NSW model may be seen in its "fragility," i.e., in an instability of all the higher energy levels with respect to a certain highly speculative form of a complex-coordinate perturbation. Although such an observation does not have any *immediate* impact on the applications of the NSW model in Refs. 7, 10, and 11, certain doubts survive concerning the possible manifestations of some more serious instabilities in some of the generalized, NSW-type (NSWT) models.

For our present purposes let us vaguely characterize the latter NSWT potentials as piecewise constant. Then we may immediately recollect the existence of several "user-friendly" NSWT examples incorporating square-well models on a compact domain[14] or systems based on the use of point interactions.[15] Unfortunately, even within this class, the expectations concerning the stability of the spectrum are not always fulfilled. One may recollect, e.g., a spontaneous complexification of the high-lying part of many NSWT spectra as detected in very early numerical studies of certain particular potentials in Ref. 16. The phenomenon looks puzzling and makes all the NSWT models worth a more detailed non-numerical study.

B. The choice of a specific example

In applied quantum mechanics the construction of the majority of phenomenological models relies quite heavily on the correspondence principle which tries to connect each quantum model with its classical predecessor. $\mathcal{PT}$-symmetric quantum mechanics offers a weakening of this connection.[17] The operator of parity $\mathcal{P}$ is indefinite so that, as we already mentioned, the formal-

ism requires an explicit *additional* construction of a Hamiltonian-dependent positively definite metric $\eta>0$ in Hilbert space. Equivalently, this may be mediated by the construction of a quasiparity $\mathcal{Q}$ (Ref. 18) or charge $\mathcal{C}$,[19] both defined as a product $\eta\mathcal{P}$. In practical calculations this means that the metric is often being introduced in a suitably factorized form.[20]

It is worth adding that the quasiparity in $\eta=\mathcal{QP}$ is easily defined in some exactly solvable examples[18] while the charge in $\eta=\mathcal{CP}$ has immediate connotations in field theory.[19] In between these two extremes the authors of Ref. 7 revealed that the application of the formalism to the particular NSW model proves facilitated by a perturbative connection between the NSW model and a Hermitian square well. Their construction of $\eta^{(\mathrm{NSW})}$ profited from the existence of a finite-dimensional matrix approximation of the non-Hermitian part of the NSW Hamiltonian. A transition to the extended NSWT class of models looks promising and comotivates also our present project.

Within such a framework we intend to pay attention to the family of Schrödinger equations (1) where the interaction is non-Hermitian but manifestly $\mathcal{PT}$-symmetric. For the sake of definiteness we shall contemplate the less interesting real part of the potential just in the most elementary infinitely deep square-well form,

$$V(x)=\begin{cases}+\infty\\ 0\\ +\infty\end{cases}\quad\text{for}\quad\begin{cases}x>L,\\ -L<x<L,\\ x<-L.\end{cases}\tag{2}$$

This means that all our wave functions must vanish at its walls,

$$\psi(-L)=\psi(L)=0.\tag{3}$$

By adding any imaginary interaction we break the Hermiticity of the Hamiltonian. By doing so in the $\mathcal{PT}$-symmetric manner we preserve a chance and good hope of having the energies real.[2]

For the sake of definiteness and in a way generalizing the NSW model of Ref. 9 we shall assume that the Hermiticity-breaking term W is composed of two purely imaginary steps which both vanish inside a subinterval $(-\ell,\ell)$ of the interval $(-L,L)$,

$$W(x)=\begin{cases}+ig,\\ 0\\ -ig\end{cases}\quad\text{for}\quad\begin{cases}\mathrm{Re}\,x>\ell>0,\\ \mathrm{Re}\,x\in(-\ell,\ell),\\ \mathrm{Re}\,x<-\ell.\end{cases}\tag{4}$$

A priori, the strength of the Hermiticity-violating imaginary force may be expected proportional to the coupling $g>0$ and inversely proportional to $\ell<L$.

Our interest in the particular two-parametric model (4) results from the obvious need of an enhancement of flexibility of its one-parametric NSW predecessor and also from the lasting possibility of its rigorous mathematical description by means of the efficient moving-lattice method of Ref. 13 (reviewed also briefly in Appendix A below). Among additional purposes of the study of the similar NSWT models one may list a search for reliable comparisons between different potentials revealing, hopefully, some new, unnoticed characteristic features of their spectra. One would like to understand, e.g., how the details of the shape of $W(x)$ could influence the stability of the spectrum, or how one could control the domain of parameters where all the energies remain real.

Some of the NSWT studies have been motivated by their potential capacity of mimicking the properties of unsolvable models and, in particular, of one of the most popular $\mathcal{PT}$-symmetric toy interactions $W(x)=ix^3$.[21] Some parallels are definitely there since in the latter unsolvable case the spectrum was proved real, non-negative and discrete.[22] Of course, there are always good reasons for an introduction of more parameters in NSW. Thus, the new freedom of a weakening of the non-Hermiticity by the choice of $\ell>0$ might simulate analogies with the Bender's and Boettcher's

generalized $\mathcal{PT}$-symmetric family $W(x)=-(ix)^{3-\mu}$ characterized by an abrupt change of its spectral properties at $\mu=1$ and by the spontaneous complexification of all the sufficiently high-lying energies inside the interval $\mu\in(1,2)$ of the shape parameter.[2]

The possibility of the latter correspondence passes an easy test at $\ell=0$ and $L=\infty$ when the general solutions of our Schrödinger Eq. (1) are mere exponentials at any real $g>0$. Once we demand that they vanish in infinity we have

$$\psi(x)=\begin{cases} B_+\exp(-\sigma x), & \sigma^2=ig-E, \qquad \mathcal{R}e\,\sigma>0, \quad x\in(0,\infty), \\ B_-\exp(\sigma' x), & \sigma'^2=-ig-E, \quad \mathcal{R}e\,\sigma'>0, \quad x\in(-\infty,0). \end{cases} \tag{5}$$

When $x\to 0^{\pm}$ the coincidence of the right and left limit of $\psi(x)$ itself specifies the normalization, $B_+=B_-$, while the second matching rule $\psi'(0^+)=\psi'(0^-)$ implies that $\sigma=-\sigma'$, i.e., Eq. (5) has no solutions at $g>0$. It is of no avail to admit that $\mathcal{R}e\,\sigma\to 0$ and $\mathcal{R}e\,\sigma'\to 0$ and to employ the scattering boundary conditions since, unless $g=0$, the matching-compatible states remain always incompatible with our differential Schrödinger equation on a half-line.

We may conclude that both the discrete and continuous spectra are empty at $\ell=0$ for $g>0$ and $L=\infty$. This reconfirms our above expectations since the emptiness of the spectrum also characterizes the Bender's and Boettcher's toy interaction $W(x)=-(ix)^{3-\mu}$ at the Herbst's extreme shape parameter $\mu=2$.[23] At the same time, the spectrum abruptly ceases to be empty at $\mu<2$ (Ref. 2) as well as at $\ell>0$ while $L=\infty$ (cf. the proof of this assertion as given in Appendix B below).

II. THE METHOD

A. Wave functions and their matching

As long as our potential is piecewise constant at $0<\ell<L<\infty$ we may postulate

$$\psi(x)=\begin{cases} \psi_-(x)=B_-\sinh\kappa^*(L+x), & x\in(-L,-\ell), \\ \psi_0(x)=C\cos kx+iD\sin kx, & x\in(-\ell,\ell), \\ \psi_+(x)=B_+\sinh\kappa(L-x), & x\in(\ell,L), \end{cases} \tag{6}$$

where $\kappa=s+it$, $E=k^2=t^2-s^2$, $g=2st>0$ and where s, t, and k are assumed real and, for the sake of definiteness, positive. In other words, we assume that within a not yet specified nonempty domain of parameters g and ℓ the $\mathcal{PT}$-symmetry of the wave functions remains unbroken. In the way proposed in Ref. 9 we prescribe the phase,

$$\psi(x)=\text{real symmetric}+\text{imaginary antisymmetric}$$

and deduce that C and D are real. Next, we differentiate

$$\psi'(x)=\begin{cases} \psi'_-(x)=\kappa^*B_-\cosh\kappa^*(L+x), & x\in(-L,-\ell), \\ \psi'_0(x)=-kC\sin kx+ikD\cos kx, & x\in(-\ell,\ell), \\ \psi'_+(x)=-\kappa B_+\cosh\kappa(L-x), & x\in(\ell,L), \end{cases}$$

and write down the following four matching conditions:

$$\psi_-(-\ell)=\psi_0(-\ell), \quad \text{i.e., } B_-\sinh\kappa^*(L-\ell)=C\cos k\ell-iD\sin k\ell,$$

$$\psi'_-(-\ell)=\psi'_0(-\ell), \quad \text{i.e., } \kappa^*B_-\cosh\kappa^*(L-\ell)=kC\sin k\ell+ikD\cos k\ell,$$

$$\psi_+(\ell)=\psi_0(\ell), \quad \text{i.e., } B_+\sinh\kappa(L-\ell)=C\cos k\ell+iD\sin k\ell,$$

$$\psi_+'(\ell) = \psi_0'(\ell), \quad \text{i.e.,} \quad -\kappa B_+ \cosh \kappa(L-\ell) = -kC \sin k\ell + ikD \cos k\ell .$$

Two of them define the (complex) values of $B_\pm$ so that we are left with the pair of the matching constraints,

$$(kC \sin k\ell + ikD \cos k\ell)\sinh \kappa^*(L-\ell) = (C \cos k\ell - iD \sin k\ell)\kappa^* \cosh \kappa^*(L-\ell),$$

$$(kC \sin k\ell - ikD \cos k\ell)\sinh \kappa(L-\ell) = (C \cos k\ell + iD \sin k\ell)\kappa \cosh \kappa(L-\ell).$$

These two relations are complex conjugate of each other so that we must consider just one of them, say,

$$(kC \sin k\ell - ikD \cos k\ell)\sinh(s+it)(L-\ell) = (C \cos k\ell + iD \sin k\ell)\kappa \cosh(s+it)(L-\ell) \quad (7)$$

with $k \geqslant 0$.

B. Matching equations in the $\sigma-\tau-\varrho$ space

After we abbreviate $\sigma = s(L-\ell)$, $\tau = t(L-\ell)$, and $\varrho = k\ell$, Eq. (7) reads

$$\varrho(L-\ell)(C \sin \varrho - iD \cos \varrho)[\sinh \sigma \cos \tau + i \cosh \sigma \sin \tau] = \ell(\sigma + i\tau)(C \cos \varrho + iD \sin \varrho) \times [\cosh \sigma \cos \tau + i \sinh \sigma \sin \tau]. \quad (8)$$

We must keep in mind that

$$\tau^2 = \sigma^2 + \frac{(L-\ell)^2}{\ell^2}\varrho^2$$

while the respective real and imaginary parts of Eq. (8) must be treated as independent equations

$$\begin{aligned} &\varrho(L-\ell)(C \sin \varrho \sinh \sigma \cos \tau + D \cos \varrho \cosh \sigma \sin \tau) \\ &\quad = \ell[\sigma(C \cos \varrho \cosh \sigma \cos \tau - D \sin \varrho \sinh \sigma \sin \tau) \\ &\qquad - \tau(C \cos \varrho \sinh \sigma \sin \tau + D \sin \varrho \cosh \sigma \cos \tau)] \end{aligned} \quad (9)$$

and

$$\begin{aligned} &\varrho(L-\ell)(C \sin \varrho \cosh \sigma \sin \tau - D \cos \varrho \sinh \sigma \cos \tau) \\ &\quad = \ell[\sigma(C \cos \varrho \sinh \sigma \sin \tau + D \sin \varrho \cosh \sigma \cos \tau) \\ &\qquad + \tau(C \cos \varrho \cosh \sigma \cos \tau - D \sin \varrho \sinh \sigma \sin \tau)]. \end{aligned} \quad (10)$$

In the next step we notice that the latter equations form a linear algebraic homogeneous set for the two coefficients C and D. They possess a nontrivial solution if and only if the secular determinant $\mathcal{D}$ vanishes. After we abbreviate $\Omega = \tan \varrho$ (= a quickly oscillating function of ϱ), $T = \tan \tau$ (= a quickly oscillating function of τ) and $\Sigma = \tanh \sigma$ (= a monotonous and bounded function of σ) we can evaluate $\mathcal{D}$. After a lengthy calculation the secular condition $\mathcal{D} = 0$ acquires the following compact form:

$$X(\sigma) + Y(\tau) + F(R)[x(\sigma) + y(\tau)] = 0, \quad (11)$$

where

$$X(\sigma) = \frac{1+\Sigma^2}{1-\Sigma^2}\sigma^2 = \sigma^2 \cosh 2\sigma,$$

$$Y(\tau)=\frac{1-T^2}{1+T^2}\tau^2=\tau^2\cos 2\tau,$$

$$x(\sigma)=\frac{\Sigma}{1-\Sigma^2}\sigma=\frac{1}{2}\sigma\sinh 2\sigma,$$

$$y(\tau)=\frac{T}{1+T^2}\tau=\frac{1}{2}\tau\sin 2\tau,$$

$$F(R)=\frac{1-\Omega^2}{\Omega}R=\frac{2R}{\tan 2\varrho},\quad \varrho=\varrho(R)=\frac{\ell}{L-\ell}R.$$

We may rescale our coupling $g=2Z/(L-\ell)^2$ and conclude that our Z-independent secular equation (11),

$$\sin 2\varrho(R)[\sigma^2\cosh 2\sigma+\tau^2\cos 2\tau]+R\cos 2\varrho(R)[\sigma\sinh 2\sigma+\tau\sin 2\tau]=0 \tag{12}$$

only must be complemented by the two trivial constraints,

$$\sigma\tau=Z,\quad \tau^2-\sigma^2=R^2. \tag{13}$$

The triplets of roots R_n, σ_n, and τ_n of this triplet of equations with $n=0,1,\ldots$ define all the bound-state energies E_n by the elementary formula

$$E_n=\frac{1}{(L-\ell)^2}R_n^2\equiv\frac{1}{(L-\ell)^2}(\tau_n^2-\sigma_n^2). \tag{14}$$

In an indirect check of the recipe we may recollect its $\ell\to 0$ (i.e., $\varrho\to 0$) limit and conclude that our present Eq. (12) degenerates smoothly and correctly back to the known secular $\ell=0$ equation [cf. Eq. (9) in Ref. 9].

C. Matching in the moving-lattice representation

The basic tool for a rigorous analysis of the form of the solutions of our matching constraints is the moving-lattice method of Ref. 13 as reviewed in Appendix A below. Skipping the majority of details let us only note that for an analysis of this type, one of the recommended techniques seems to be the reduction of the problem to $\sigma-\tau$ plane. Preserving the definition of $\tau=\tau(N,t)$ of Appendix A and replacing the definition of $\sigma=\sigma(N,t)$ by another formula,

$$\sigma=\sigma(N,t,K,r)=\pi\times\sqrt{[N+t]^2+\left[\frac{L-\ell}{2\ell}(K+r)\right]^2},$$

we eliminate the coordinate R. A shortcoming of this approach is that our matching condition (12) transferred into the $\sigma-\tau$ plane must be understood as the following quadratic equation for τ:

$$\Phi_t\tau^2+\omega_{K,r,t}\tau+\Omega_{K,r,t}(\sigma)=0, \tag{15}$$

where we abbreviated

$$\omega_{K,r,t}=\frac{(L-\ell)\pi\Psi_t}{2\ell\Xi_r}(K+r),\quad \Omega_{K,r,t}(\sigma)=\Xi_r\left[\sigma^2\cosh 2\sigma+\frac{\omega_{K,r,t}}{\Psi_t}\sigma\sinh 2\sigma\right].$$

This defines $\tau=\tau_{K,r,t}(N)$ on the lattice, the "motion" of which will be controlled not only by t and r but also, not so strongly, by K. Technically, the price to be paid is still reasonable—we get the closed form of the matching-compatible function $\tau=\tau(\sigma)$ as the two well-known root formulas

from Eq. (15). Nevertheless, significant simplifications of the resulting picture may be mediated by the direct inspection of the equations in question.

III. SOLUTIONS

A. Matching equations in the $\sigma-\tau$ plane

Building far-reaching analogies with the $\ell=0$ special case would be misleading because the form of our matching constraint (12) is discontinuous in the limit $\ell\to 0$. Thus, let us assume that $\ell\neq 0$ and study Eq. (12) in its full-fledged form. First, we abbreviate $\mathcal{M}(\sigma,\tau)=\sigma\sinh 2\sigma+\tau\sin 2\tau$ and $\mathcal{N}(\sigma,\tau)=\sigma^2\cosh 2\sigma+\tau^2\cos 2\tau$ and rewrite our matching constraint (12) as the secular equation

$$\mathcal{D}(\sigma,\tau,R)=Q(\sigma,\tau)+\frac{\tan 2\varrho(R)}{R}=0,\quad Q(\sigma,\tau)=\frac{\mathcal{M}(\sigma,\tau)}{\mathcal{N}(\sigma,\tau)}. \tag{16}$$

This enables us to formulate several obvious observations.

[O1] The shape of both the functions $\mathcal{M}(\sigma,\tau)$ and $\mathcal{N}(\sigma,\tau)$ of two variables is easily deduced using their separability, $\mathcal{X}(\sigma,\tau)=\mathcal{X}(\sigma,0)+\mathcal{X}(0,\tau)$, $\mathcal{X}=\mathcal{M},\mathcal{N}$.

[O2] The smoothness of the σ and τ dependence of the denominator $\mathcal{N}(\sigma,\tau)$ facilitates also the determination of the shape of $\mathcal{F}(\sigma,\tau)=1/\mathcal{N}(\sigma,\tau)$.

[O3] In $\sigma-\tau$ plane we may visualize the shape of the second fraction in (16) as a function which is constant along hyperbolas $R(\sigma,\tau)=\sqrt{\tau^2-\sigma^2}=\text{fixed}$.

All these innocent-looking observations have several far-reaching though not always obvious consequences and form in fact a background for a rigorous analysis of the spectrum.

B. A rigorous graphical interpretation of $Q(\sigma,\tau)$

In more detail, observation [O1] means that the surfaces defined by the two non-negative function(s) $\mathcal{X}(\sigma,0)\geqslant 0$ have the form of the two only slightly different parabolic valleys with the same degenerate minimum (=zero) which coincides with the axis $\sigma=0$. The pertaining second components $\mathcal{X}(0,\tau)$ differ more from each other but both are adding a structurally similar perpendicular set of infinitely many parallel hills and valleys possessing a steadily increasing (though always finite) amplitude. As an obvious result of the superposition, both the resulting surfaces $\mathcal{X}(\sigma,\tau)$ cross the zero plane merely along certain ovals $O_n^{\mathcal{X}}$, and both of them only get negative in their interior.

The precise shape of these ovals (numbered by $n=0,1,\ldots$) may fully rigorously be determined using the moving-lattice method (cf. Appendix A) but even without any use of the moving lattices the qualitative character of their shape is obvious and we may conclude that the zero lines of $\mathcal{M}(\sigma,\tau)$ and $\mathcal{N}(\sigma,\tau)$ form the families of ovals $O_n^{\mathcal{M}}$ and $O_n^{\mathcal{N}}$ located within the stripes of $\tau\in[(n+1/2)\pi,(n+1)\pi]$ and $\tau\in[(n+1/4)\pi,(n+3/4)\pi]$, respectively. All of them are symmetric with respect to the reflection $\sigma\to-\sigma$ and their size in the σ direction increases with τ.

Examples of these structures may be found in both Refs. 9 and 13 and another illustration appears in Fig. 1 here. In fact, the figure displays another surface $Q(\sigma,\tau)=\mathcal{M}(\sigma,\tau)/\mathcal{N}(\sigma,\tau)$ (within a narrow window of $0\leqslant Q\leqslant 0.05$) but the shape of the curve where $\mathcal{M}$ vanishes ($O_1^{\mathcal{M}}\equiv V_1$) appears there clearly since the denominator $\mathcal{F}(\sigma,\tau)=1/\mathcal{N}(\sigma,\tau)$ has its zeros, generically, elsewhere (cf. observation [O2]). Besides the oval V_1 (and a part of $O_0^{\mathcal{M}}\equiv V_0$) the picture displays another oval $O_1^{\mathcal{N}}\equiv D_1$ of the zeros of the denominator $\mathcal{N}$. Incidentally it lies within the chosen interval of $\tau\in(3,7)$ and remains visible due to a numerical artifact of a spurious projection of an infinite discontinuity of the function $\mathcal{F}(\sigma,\tau)$.

Although the visibility of the discontinuities reflects just an imperfection of the graphical representation of the surface, it will prove useful in what follows.

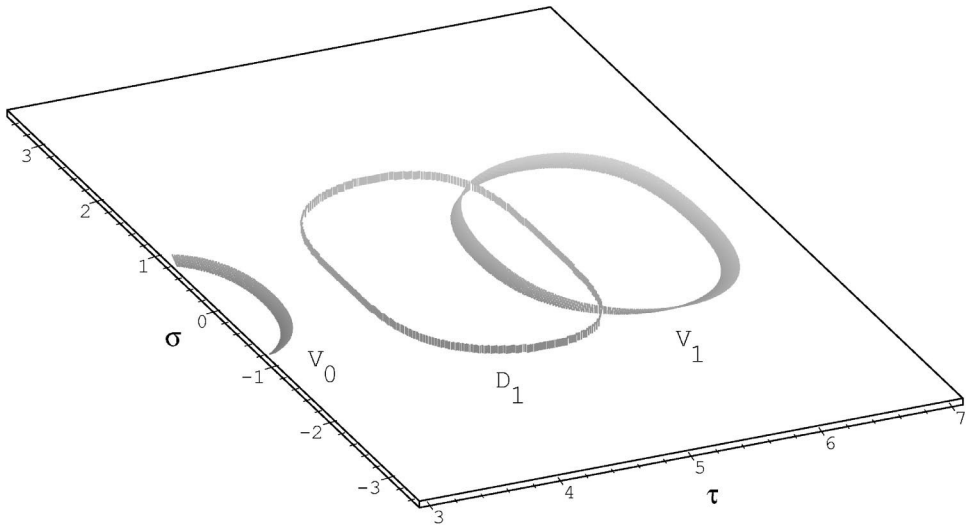

FIG. 1. A thin slice through the surface $Q(\sigma,\tau)=\mathcal{M}/\mathcal{N}$.

C. The role of the second component of $\mathcal{D}[\sigma,\tau,R(\sigma,\tau)]$

The presence of the subsurface generated by the second, R-dependent component $\mathcal{D}_{(R)}[R(\sigma,\tau)]$ in Eq. (16) does not violate the separation between σ and τ too much (cf. observation [O3]). At the smallest absolute values of σ we may safely return to the approximation of $\mathcal{D}_{(R)}[R(\sigma,\tau)]$ by a function of a single variable, $[\tan 2\varrho(R)]/R\approx[\tan 2\ell\tau/(L-\ell)]/\tau$. This picture only becomes deformed, at the larger σ, by being bent to the right, i.e., along hyperbolas $R(\sigma,\tau)=$constant.

A clear understanding of the τ-dependence of the whole surface $\mathcal{D}[\sigma,\tau,R(\sigma,\tau)]$ will be obtained when we distinguish between the domain of the "small τ" **(**where $[\tan 2\ell\tau/(L-\ell)]/\tau\approx 2\ell/(L-\ell)$ is positive and virtually constant**)**, "medium τ" **(**with the repeated quick growth of the curve $[\tan 2\ell\tau/(L-\ell)]/\tau$ from minus infinity up to plus infinity within each interval of the constant length $\Delta\tau=\pi(L-\ell)/2\ell$**)** and "large τ" **(**where the values of $\mathcal{D}_{(R)}[R(\sigma,\tau)]\approx 1/\tau$ become very small up to the very thin layers near the singularity hyperbolas H_n**)**. Due to the local dominance of the latter singularities H_n at any $n=0,1,\ldots$ it is easy to imagine that the sign of the whole function $\mathcal{D}[\sigma,\tau,R(\sigma,\tau)]$ is positive and negative in their left and right vicinity, respectively. This "rule of thumb" enables us to deduce the sign of the whole function $\mathcal{D}[\sigma,\tau,R(\sigma,\tau)]$ in all our figures.

D. The left-moving hyperbolic discontinuities H_n

In the domain of the small shifts $\ell\ll 1$ the numerical values of the R-dependent component $\mathcal{D}_{(R)}[R(\sigma,\tau)]$ of Eq. (16) remain almost constant and small. In this regime the above-mentioned "small-τ" constraint $\tau\ll(L-\ell)/\ell$ is not particularly restrictive so that the matching-compatible roots of equation $\mathcal{D}=0$ remain very similar to their $\ell=0$ predecessors in quite a large leftmost portion of the $\sigma-\tau$ plane. In our notation, the first few ovals $O_n^{\mathcal{D}}\equiv V_n$ of the zeros of the secular determinant stay only perturbatively shifted and deformed by an increase of $\ell\ll 1$.

With the growth of ℓ or $\lambda=\ell/(L-\ell)$ the leftmost discontinuity-hyperbola H_0 of the surface $\mathcal{D}[\sigma,\tau,R(\sigma,\tau)]$ moves to the left and emerges in the right half of Fig. 2 where we choose the scale-independent parameter $\lambda=11/40$ which corresponds to $\ell=11L/51$. This means that we are just leaving the domain of the small shifts $\ell\ll 1$ so that the deformation of the nodal oval $O_1^{\mathcal{D}}\equiv V_1$ becomes perceivable, caused by the closeness of H_0 to the ℓ-independent discontinuity oval $D_1\equiv O_1^{\mathcal{N}}$ inherited from the never-vanishing factor $\mathcal{F}(\sigma,\tau)=1/\mathcal{N}(\sigma,\tau)$.

In a way which generalizes the illustrative Fig. 2, each hyperbolic singularity H_k [defined by the equation $R(\sigma,\tau)=(L-\ell)(k+1/2)\pi/\ell$ with $k=0,1,\ldots$] moves to the left with the growth of ℓ

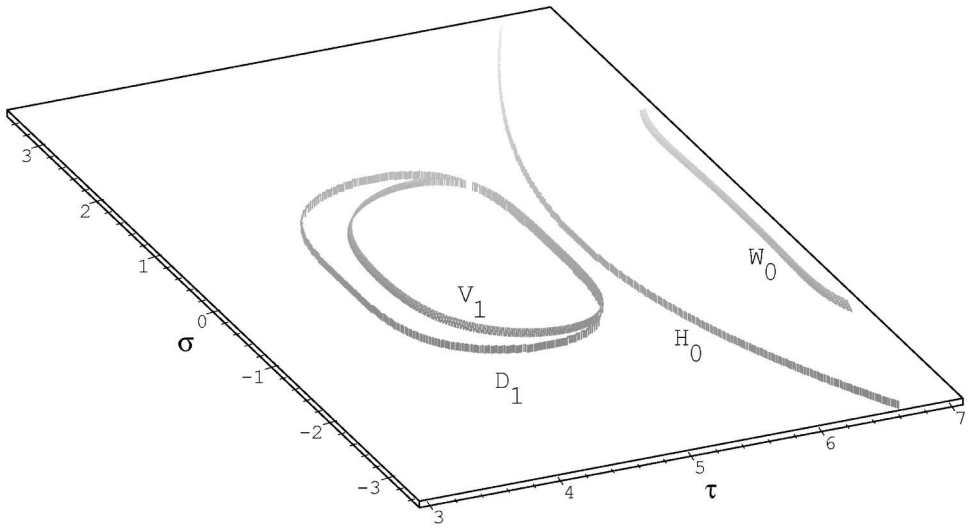

FIG. 2. A thin slice through the surface of the secular determinant $\mathcal{D}(\sigma,\tau)$ at $\lambda=\ell/(L-\ell)=0.275$.

and λ. Once it gets close to the Nth singularity oval D_{N-1}, it touches it at a point with the coordinates $\sigma_{(\mathrm{in})}^{(N,k)}=0$ and $\tau_{(\mathrm{in})}^{(N,k)}=(N-1/4)\pi$ at the critical value $\lambda=2\ell/(L-\ell)=(4k+2)/(4N-1)\equiv\lambda_{(\mathrm{in})}^{(N,k)}$ of the shift.

With the further growth of λ the intersection of the hyperbola with the standing oval moves to the left and disappears, curiously enough, at a certain pair of points with the "last-contact" $|\sigma|=|\sigma_{(\mathrm{out})}^{(N,k)}|>0$ and $\tau=\tau_{(\mathrm{out})}^{(N,k)}<(N-3/4)\pi$. The latter value lies slightly below the oval's end. Let us skip here the proof of this subtlety as not too relevant.

E. A completion of the list of the nodal lines

We are now prepared to detect *all* the nodal curves of $\mathcal{D}[\sigma,\tau,R(\sigma,\tau)]$ and to determine their qualitative ℓ-dependence in all the interval of $\ell\in(0,L)$ and/or of $\lambda=\lambda(\ell)\in(0,\infty)$. For the first inspiration we return to Fig. 2 where the oval of zeros $O_1^{\mathcal{D}}\equiv V_1$ cannot be interpreted as a mere small perturbation of $O_1^{\mathcal{M}}$ in spite of the fact that the singularity hyperbola H_0 still did not touch the singularity oval $O_1^{\mathcal{N}}\equiv D_1$ since $\lambda=0.275<\lambda_{(\mathrm{in})}^{(2,1)}=2/7\approx0.286$.

Still, the much more important observation made in Fig. 2 concerns the emergence of the new curve W_0 of the new zeros of the function $\mathcal{D}$. At the chosen λ this curve just entered Fig. 2 at its right side. Our next Fig. 3 confirms that the new nodal curve W_0 moves to the left and gets deformed in a way reflecting the presence of a steep oval dip in $Q(\sigma,\tau)$ below $\tau=2\pi$. We choose $\lambda=0.355$ which is still safely smaller than the lower estimate $(4k-2)/(4N-3)=0.4$ of the singularity hyperbola's "jumped-over" parameter $\lambda_{(\mathrm{out})}^{(2,1)}\approx0.403$.

The "next-step snapshot" of Fig. 4 at $\lambda=0.395$ shows how the same dip deforms the shape of the oval $O_1^{\mathcal{D}}\equiv V_1$ in the domain where the function of R is small. In the subsequent Fig. 5 we finally see how the two curves of the zeros merge while a topologically new situation is created and sampled at $\lambda=0.415>\lambda_{(\mathrm{out})}^{(2,1)}$.

We may summarize that for the growing λ the motion of the singular component $\tan 2\varrho(R)/R$ of our secular determinant $\mathcal{D}(\sigma,\tau)$ to the left gives a clear guide how to keep the ℓ dependence of its zero lines under full control. The emergence and the asymptotically hyperbolic shape of the new (and, in fact, not quite expected) nonoval curves W_m of zeros follows immediately from the asymptotic smallness of the positive component $Q(\sigma,\tau)\sim1/\sigma^2$ of $\mathcal{D}(\sigma,\tau)$ at the larger $|\sigma|\gg1$.

Due to the reasonably elementary character of the function $\mathcal{D}(\sigma,\tau)$ we are able to understand

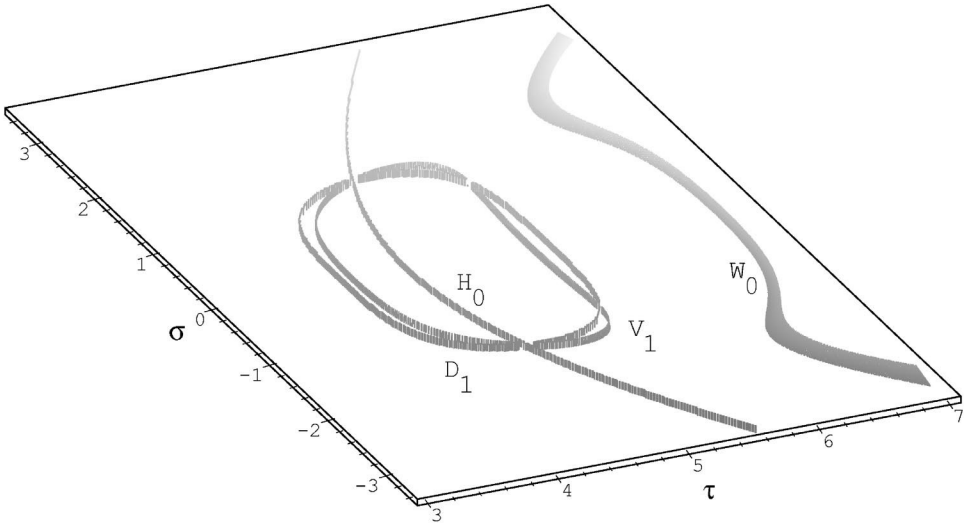

FIG. 3. Same as Fig. 2, $\lambda = 0.355$.

that the pattern sampled by Figs. 2–5 is entirely universal. Always, step by step, the nodal ovals V_n as well as their asymptotically hyperbolic nodal-line partners W_m become deformed by the existence of the dip in the numerator function $\mathcal{M}(\sigma, \tau)$.

Of course, after the hyperbola of singularities H_k as well as its strongly deformed trailing nodal curve W_k "creep" over the fixed singularity oval D_j (as well as over its attached and strongly deformed zero curve V_j), the smoother shapes of both the nodal curves W_k and V_j are more or less recovered, and only their ordering remains permanently reversed. In spite of the apparent nonlinearity of the "creeping-over" effects, their details might again be analyzed algebraically, using an adapted version of the moving-lattice method of Sec. II C.

The most important reward compensating an increase in complexity of the latter recipe is that one becomes able to treat one of the two roots of Eq. (15), say, as a "nonperturbative" solution at the small ℓ. The most important example of its role are the hyperbolic nodal curves W_m which move to the right in τ with the decrease of ℓ and which disappear in infinity in the NSW limit of $\ell \to 0$.

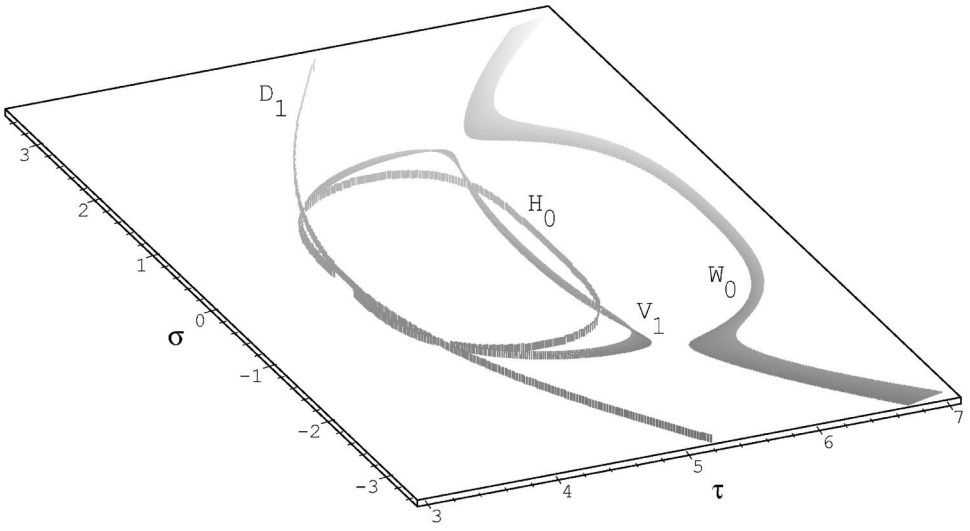

FIG. 4. Same as Fig. 2, $\lambda = 0.395$.

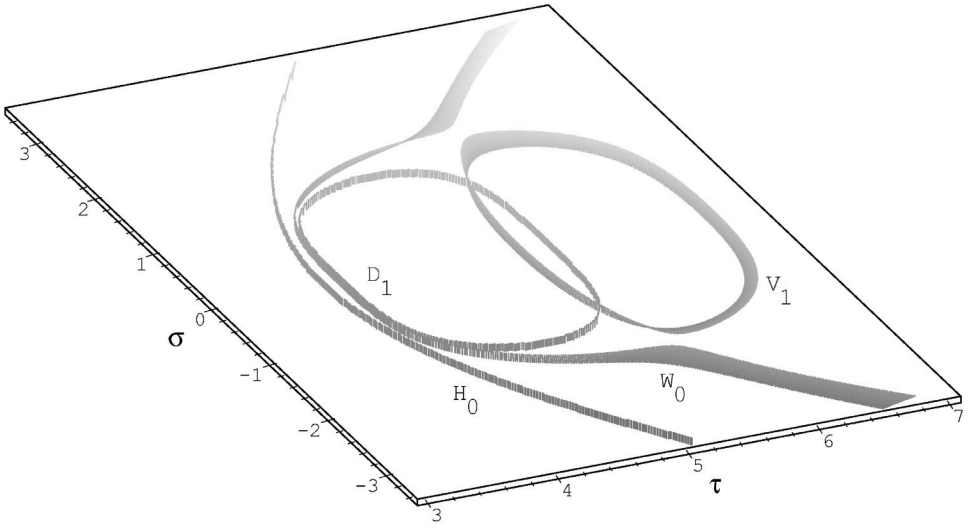

FIG. 5. Same as Fig. 2, $\lambda = 0.415$.

IV. ENERGIES

A. Graphical representation and classification

On the background of the preceding material, what remains for us to do is a combination of the above-described knowledge of the nodal lines of $\mathcal{D}[\sigma, \tau, R(\sigma, \tau)]$ with the coupling-dependence constraint $\sigma \times \tau = Z = (L-\ell)^2 g/2$. A sample of the intersections of this type (i.e., of a typical final solution) is offered in Fig. 6 where $\lambda = 2.40$ is neither small nor large and where we choose $Z = Z^{(a)} = 1.00$ and $Z = Z^{(b)} = 2.24$ (= the critical "exceptional-point" value of Ref. 9) for illustration. The conclusions which are illustrated by this graph have a general validity:

(i) We always have $\tau > \sigma > 0$ which means that all the real bound-state energies E_n remain positive at $Z > 0$.

(ii) Some of the energies remain real at *any* value of $Z > 0$. They correspond to the intersections of the hyperbola $\sigma = Z/\tau$ with the hyperbolic nodal lines W_m and may be called "stable," $E = E_m^{(s)}$.

(iii) All the other energies $E = E_n^{(u)}$ correspond to the intersections of the hyperbola $\sigma = Z/\tau$ with the nodal ovals V_k. At a sufficiently small Z the latter intersections remain real [see the line (a) with $Z = 1$ in Fig. 6].

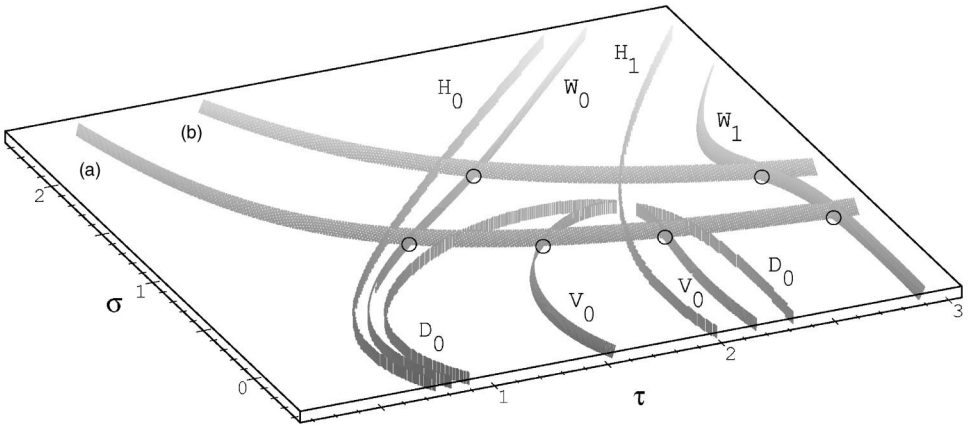

FIG. 6. Solutions at $Z^{(a)} = 1.00$ and $Z^{(b)} = 2.24$, intersections marked by circles, $\lambda = 2.4$.

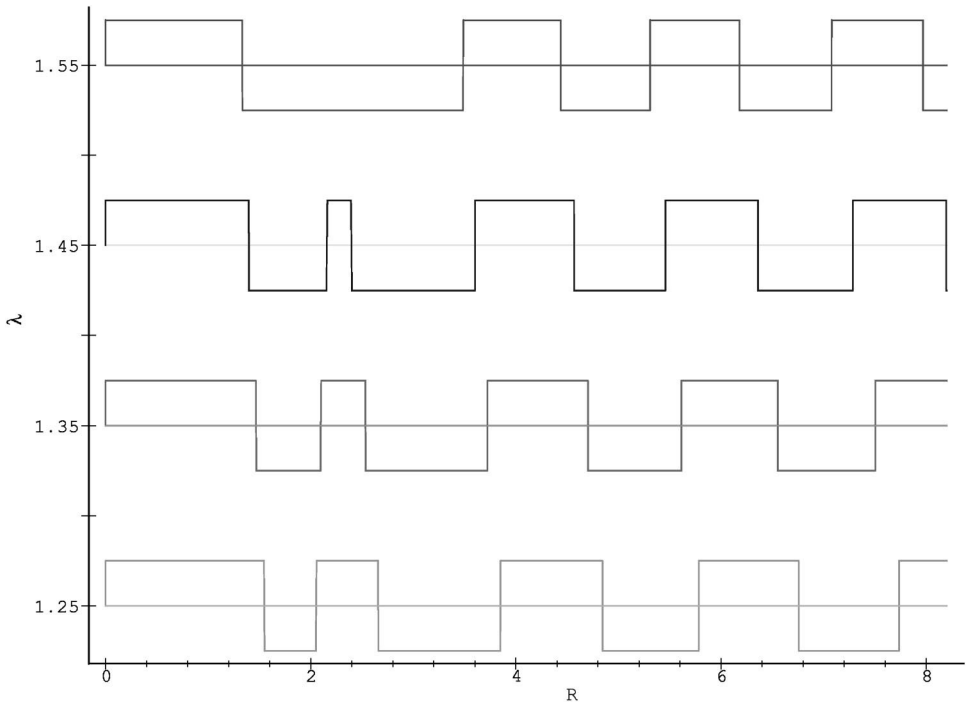

FIG. 7. Four rescaled graphs of the function $\hat{\mathcal{D}}(R)$.

(iv) We may call the latter energies "unstable" as they merge in pairs and form complex conjugate doublets[4] beyond certain "exceptional-point"[24] values of ℓ and Z [illustration, the line (b) in Fig. 6].

The decomposition of the spectrum into its stable and unstable parts varies with ℓ or $\lambda = \ell/(L-\ell)$ in an obvious manner. Hence, the stability pattern in the spectrum will be entirely different at the small and large λ since in the former case the hyperbolic curves W_n only generate the high-lying energies and *vice versa*.

B. Numerical construction

After all our previous detailed analysis of the qualitative features of the spectrum the numerical determination of energies becomes fully routine. Indeed, as long as we know $\tau = Z/\sigma$, the rule $\tau^2 - \sigma^2 = R^2$ leads immediately to the definition of

$$\sigma = \sigma(R) = \sqrt{\frac{2Z^2}{R^2 + \sqrt{R^4 + 4Z^2}}}. \tag{17}$$

In parallel to such an introduction of the closed function $\sigma = \sigma(R)$ of R we may return once more to the recipe $\tau = Z/\sigma(R)$ and re-read it as another explicit definition of the second auxiliary function $\tau(R) = Z/\sigma(R)$ of R.

In such a setting, the purely numerical determination of the bound-state energies is reduced to the search for the roots R_n of Eq. (12), i.e., of the zeros of the secular determinant,

$$\hat{\mathcal{D}}(R) = [\sigma^2(R)\cosh 2\sigma(R) + \tau^2(R)\cos 2\tau(R)]\sin 2\lambda R + R[\sigma(R)\sinh 2\sigma(R) + \tau(R)\sin 2\tau(R)]\cos 2\lambda R \tag{18}$$

converted now in the function of the single variable $R \sim \sqrt{E}$. An illustration of such a search is given in Fig. 7 at a fixed choice of $Z = 2$. The quadruplet of the graphs of the secular determinant

$\hat{\mathcal{D}}(R)=\mathcal{D}[\sigma(R),\tau(R),R]$ is presented there at the four different values 1.25, 1.35, 1.45, and 1.55 of λ (indicated along the vertical axis). In each of these graphs we magnified the vertical units near $\hat{\mathcal{D}}(R)\approx 0$ and compressed them to a single point representing all the bigger values of $|\hat{\mathcal{D}}(R)|\geqslant\varepsilon$. In this way the picture samples the left-hand side of Eq. (18) solely near its zeros. Our magnification of the vertical dimension marks these zeros by the virtually straight parts of the curve which are seen as practically perpendicular to the horizontal axis.

The set of graphs in Fig. 7 illustrates the λ dependence of the bound-state roots R_n. We see that a pair of the unstable energies may merge and cease to be real after a fine-tuned growth of λ. This illustrates the complexification of the unstable energies which is *not* caused by the growth of Z but rather by the growth of λ. At the first sight this phenomenon looks like a paradox because we are now *weakening* the non-Hermiticity in fact. Fortunately, this paradox is still easily understood once we imagine (and check, say, in the spirit of Figs. 2 and 3) that the growth of λ "pushes" *all* the zeros (including of course also the nodal oval in question) to the left. Of course, this oval cannot get prolonged in the σ direction because the function $\mathcal{M}(\sigma,\tau)$ itself grows too quickly with σ. This implies that the two real intersections of the oval with the hyperbola $\sigma=Z/\tau$ disappear because the latter curve grows to the left.

In the light of an additional scaling in Eq. (14) one may only admire the subtlety of the phenomenon, the verification of which very much profits from the exact solvability of the model. An independent confirmation of the absence of any contradictions may be also offered via a further simplification of mathematics. This inspires us to pay particular attention to the "most counterintuitive" limiting case where $L\to\infty$. Such an analysis may be of an independent interest as it simulates, very roughly, the shape of the most popular antisymmetric and purely imaginary potential $V(x)\sim ix^3$ with real spectrum.[22] As long as this discussion already lies somewhat beyond the scope of the present text, it is moved to Appendix B.

V. CONCLUSIONS

After more than 10 years of an intensive research many people now seem to believe that we now better understand the key problems related to the so-called $\mathcal{PT}$-symmetric as well as to many other similar non-Hermitian models or, in the more rigorous terminology, to all the models where the metric remains nontrivial, $\eta\neq I$.[25] By the way, not all the related results are new. For example, Scholz *et al.*[26] (inspired, presumably, by a few earlier mathematical as well as physical publications) studied the similar $\eta\neq I$ models more than 10 years ago and coined the name "quasi-Hermitian" for them.

Still, one cannot deny that during the last 7 years, a new and intensive excitement has been caused by the discoveries of the reality of the spectra in many $\mathcal{PT}$-symmetric models. The emphasis of the research has been shifted, typically, to the explicit constructions of the charge $\mathcal{C}$ (Ref. 20) or to the more detailed analysis of what happens at the "exceptional" points where the reality of the spectrum is being lost.[24,27] A few unusual features exhibited by our present model seem to offer another welcome and clear intuitive guidance in this area.

We found our results interesting since the merger and subsequent spontaneous complexification of some "twin" pairs $E^{(\pm\text{twin})}$ of the energies cannot be easily described within the usual textbook models where the metric is "trivial," $\eta_{(\text{trivial})}=I$. It is also in this context where considerations based on our present model could lead to a deeper insight in the underlying mechanisms and mathematics, not only because our model is solvable but also because it proves able to provide different "twin-merging" patterns in the spectrum. Indeed, by the choice of the shape parameter ℓ we may, up to a large extent, prescribe *which* particular excitations (say, in the low-lying spectrum) should remain robustly stable and which ones should form the unstable, fragile "twins" merging at some sufficiently large couplings $g_{(\text{critical})}$.

In the similar constructions and studies, one might feel hesitant whether his/her models should be simpler or more realistic. We believe that one should transfer the insight gained in the solvable models (like in the present one) to all the more realistic applications where just some approximate

methods can be used. In this sense we already mentioned a parallelism between the role of the shift ℓ in our solvable model and of the exponent μ in the power-law potentials with $\mathcal{PT}$-symmetry.

It is encouraging to see that a certain nontrivial enrichment of the merging pattern has been detected, more or less in parallel, within the class of the power-law forces.[27] In this comparison, our present model's merit lies in its exact solvability. Definitely, it proves able to offer a comparably rich pattern of the mergers of the levels.

This being said, the *key* phenomenological and "model-building" specific merit of our present new version of the $\mathcal{PT}$-symmetric square-well model is still to be seen in the "global" structure of its spectrum. There, one observes that the "fragile" and the "robust" levels seem to form the two sets which may be moved with respect to each other as a whole. Thus, the *whole* spectrum becomes "almost completely robust" in one extreme (which is "almost Hermitian") and "almost all fragile" in another extreme which is, near $\ell \approx 0$, "maximally non-Hermitian."

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APPENDIX A: THE METHOD OF MOVING LATTICE

Secular Eq. (12) and its descendants contain quickly oscillating trigonometric functions of arguments 2τ and 2ϱ. In the spirit of Ref. 13 it makes sense to reparametrize both these variables according to the rules

$$\tau = \tau(N,t) = \pi N + \pi t, \quad N = 0,1,\ldots, \quad t \in (0,1),$$

$$\varrho = \pi K + \pi r, \quad K = 0,1,\ldots, \quad r \in (0,1)$$

which separate their "large" change (by an integer multiple of the period 2π so that the trigonometric function itself remains unchanged) from a "small" change [within one period $(0,2\pi)$]. Thus, once we define

$$\Psi = \sin 2\tau = \sin 2\pi t, \quad \Phi = \cos 2\tau = \cos 2\pi t,$$

$$\Xi = -\tan 2\varrho = -\tan \pi r,$$

all our trigonometric functions in question become independent of both the integer variables. Thus, once we decide to work, say, in the $\sigma - R$ plane, we simply introduce a lattice $\mathcal{L}_{t,r}$ of points with coordinates

$$\sigma = \sigma(N,t) = \frac{Z}{\tau(\sigma)} = \frac{Z}{\pi N + \pi t}$$

and

$$R = \frac{L-\ell}{\ell}\varrho(R) = \frac{\pi(L-\ell)}{2\ell}(K+r),$$

where $t \in (0,1)$ and $r \in (0,1)$ are fixed while $N = 0,1,\ldots$ and $K = 0,1,\ldots$ remain variable. Our secular equation (12) then becomes more easily analyzed at the fixed $t \in (0,1)$ and $r \in (0,1)$ when it may be re-read as a simplified mapping $\sigma \to R$ with

$$R = R_{t,r}(\sigma) = \Xi_r \times \frac{\sigma^4 \cosh 2\sigma + Z^2 \Phi_t}{\sigma^3 \sinh 2\sigma + \sigma Z \Psi_t}, \tag{A1}$$

i.e., $R_{t,r} \approx \Xi_r |\sigma|$ at $|\sigma| \gg 1$ while

$$R_{t,r} \approx \frac{Z}{\sigma} \times \frac{\Phi_t \Xi_r}{\Psi_t}$$

at $|\sigma| \ll 1$, etc. In the subsequent step, remembering that the latter formulas hold on the lattice $\mathcal{L}(t,r)$ only, we must let this lattice move with the variation of t and/or r. Within each box numbered by the pair (N,K) of non-negative integers we would be able to rederive all the qualitative geometric considerations of Sec. III in an alternative, quantitative manner.

APPENDIX B: SHALLOW WELL

In the infinite-size limit $L \to \infty$ our model degenerates to a purely imaginary square well with asymptotic boundary conditions

$$\psi(\pm\infty) = 0 \tag{B1}$$

and with the $\mathcal{PT}$-symmetric matching conditions in the origin,

$$\psi(0) = 1, \quad \partial_x \psi(0) = iG. \tag{B2}$$

This means that we have the general solution

$$\psi(x) = \begin{cases} \cos kx + B \sin kx, & x \in (0,\ell), \quad k^2 = E, \\ (L + iN)\exp(-\sigma x), & x \in (\ell,\infty), \quad \sigma^2 = iT^2 - k^2, \end{cases} \tag{B3}$$

with $T = \sqrt{g}$ and with the the purely imaginary constant $B = iG/k$.

1. Matching conditions at $x = \ell$

Let us split $\sigma = p + iq$ in its real and imaginary part with $p, q \geqslant 0$. This gives the rules $p^2 + k^2 = q^2$ and $2pq = T^2$, easily reparametrized in terms of a single variable α,

$$p = q \cos \alpha, \quad k = q \sin \alpha, \quad q = \frac{T}{\sqrt{2 \cos \alpha}}, \quad \alpha \in (0, \ell/2). \tag{B4}$$

The standard matching at the point of discontinuity is immediate,

$$\cos k\ell + B \sin k\ell = (L + iN)\exp(-\sigma\ell),$$

$$-\sin k\ell + B \cos k\ell = -\frac{\sigma}{k}(L + iN)\exp(-\sigma\ell).$$

After we abbreviate $\sigma/k = -\tan \Omega\ell$, we get an elementary complex condition of the matching of logarithmic derivatives at $x = \ell$,

$$G = -ik \tan(k + \Omega)\ell. \tag{B5}$$

Its real part defines our first unknown parameter, $G = G(\alpha)$. Due to our normalization conventions, the imaginary part of the right-hand-side expression must vanish, $\mathrm{Re}[\tan(k+\Omega)\ell] = 0$. An elementary rearrangement of such an equation acquires the form of an elementary quadratic algebraic equation for $X = \tan k\ell$. Its two explicit solutions read

$$X_1 = \frac{p + q}{k}, \quad X_2 = \frac{p - q}{k} \tag{B6}$$

or, after all the insertions,

$$\tan\left[\frac{\ell T \sin \alpha^{(+)}}{\sqrt{2 \cos \alpha^{(+)}}}\right] = \tan\left[\frac{\ell - \alpha^{(+)}}{2}\right], \tag{B7}$$

$$\tan\left[\frac{\ell T \sin\alpha^{(-)}}{\sqrt{2\cos\alpha^{(-)}}}\right] = \tan\left[-\frac{\alpha^{(-)}}{2}\right]. \tag{B8}$$

These equations specify, in implicit manner, the two respective infinite series of the appropriately bounded real roots $\alpha=\alpha_n^{(\pm)}\in(0,\ell/2)$.

2. Energies

For $\alpha\in(0,\ell/2)$ the left-hand-side arguments in Eqs. (B7) and (B8) run from zero to infinity and the functions oscillate infinitely many times from minus infinity to plus infinity. In contrast, the limited variation of the argument α makes both the right-hand side functions monotonic, very smooth and bounded, $\tan[(\ell-\alpha^{(+)})/2]\in(1,\infty)$ and $\tan[\alpha^{(-)}/2]\in(0,1)$. This indicates that our roots $k=k(\alpha_n^{(\pm)})$ will all lie within well determined intervals,

$$k_n^{(+)}\in\left(n+\frac{1}{4},n+\frac{1}{2}\right),\quad n=0,1,\ldots,$$

$$k_m^{(-)}\in\left(m+\frac{3}{4},m+1\right),\quad m=0,1,\ldots.$$

An additional merit of parametrization (B4) lies in an unambiguous removal of the tangens operators from both Eqs. (B7) and (B8). This gives

$$k_n^{(+)}=n+\frac{1}{2}-\frac{\omega_n^{(+)}}{4},\quad k_m^{(-)}=m+1-\frac{\omega_m^{(-)}}{4},\quad \omega_n^{(\pm)}=\frac{2\alpha_n^{(\pm)}}{\ell}\in(0,1).$$

After a change of notation with $\omega_n^{(+)}=\omega_{2n}$ and $\omega_n^{(-)}=\omega_{2n+1}$, we may finally combine the latter two rules in the single secular equation

$$\sin\left(\frac{\ell}{2}\omega_N\right)=\frac{2N+2-\omega_N}{4T}\cdot\sqrt{2\cos\left(\frac{\ell}{2}\omega_N\right)},\quad N=0,1,\ldots. \tag{B9}$$

In a graphical interpretation this equation represents an intersection of a tangenslike curve with the infinite family of parallel lines. This is illustrated in Fig. 8. The equation generates, therefore, an infinite number of real roots $\omega_N\in(0,1)$ at all the non-negative integers $N=0,1,\ldots$. The discrete spectrum is unbounded from above and remains constrained by the inequalities

$$\frac{(N+1/2)^2}{4}\leqslant E_N\leqslant\frac{(N+1)^2}{4} \tag{B10}$$

independently of the coupling T.

3. Wave functions

Equation (B5) in combination with Eqs. (B7) and (B8) determines the real parameter

$$G=G^{(\pm)}=-\frac{k^2}{q\pm p} \tag{B11}$$

responsible for the behavior of the wave functions near the origin [remember that $B=iG/k$ in Eq. (B3)]. For its deeper analysis let us first introduce an auxiliary linear function of ω and N,

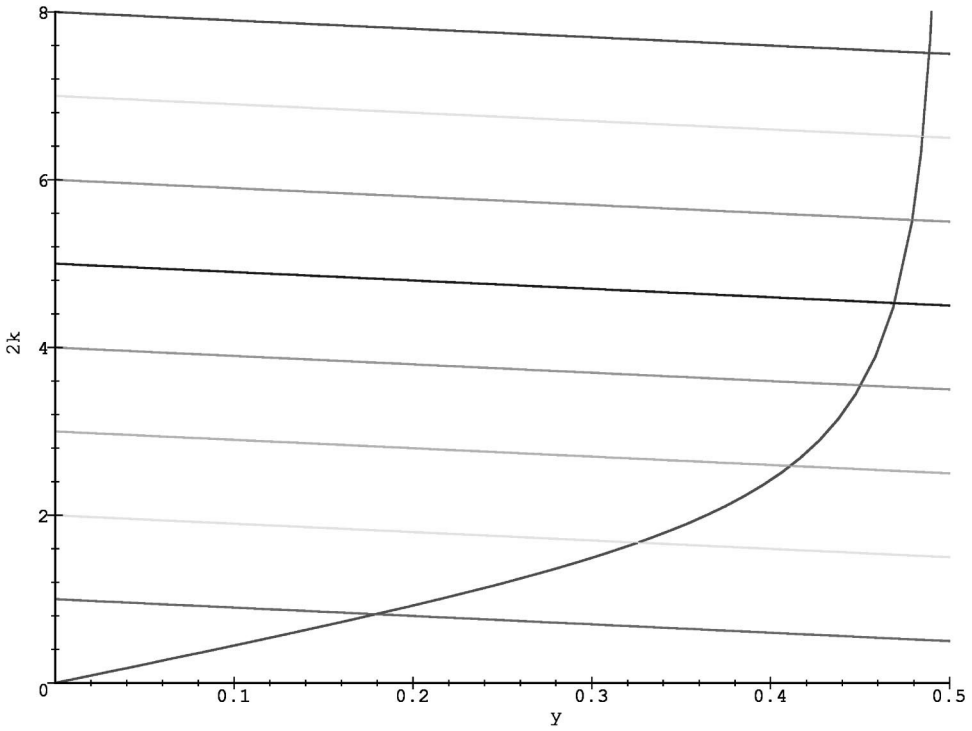

FIG. 8. Graphical solution of Eq. (B9) ($y=\omega_N/2, T=1$)

$$\sqrt{R(\omega_N,N)} = \frac{2N+2-\omega_N}{4T} \in \left(\frac{N+1/2}{2T}, \frac{N+1}{2T}\right)$$

and reinterpret our secular Eq. (B9) as an algebraic quadratic equation with the unique positive solution,

$$\cos\left(\frac{\ell}{2}\omega_N\right) = \frac{1}{R(\omega_N,N)+\sqrt{R^2(\omega_N,N)+1}}. \tag{B12}$$

This is an amended implicit definition of the sequence ω_N. As long as the right-hand side expression is very smooth and never exceeds one, the latter formula reverifies that the root ω_N is always real and bounded as required.

In the weak coupling regime (i.e., in the domain of the large and almost constant $R \gg 1$ with the small square-well height T or at the higher excitations), our new secular equation (B12) gives a better picture of our bound-state parameters $\omega_N = 1-\eta_N$ which all lie very close to one. The estimate

$$\frac{\ell}{2}\eta_N = \arcsin\frac{1}{R+\sqrt{R^2+1}} \approx \frac{1}{2R} - \frac{5}{48R^3} + \cdots$$

represents also a quickly convergent iterative algorithm for the efficient numerical evaluation of the roots ω_N. One can conclude that in a way compatible with our *a priori* expectations, the value of $p=p_N=\mathrm{Re}\,\sigma \approx q/2R$ is very close to zero and, as a consequence, the asymptotic decrease of our wave functions remains slow. We have $q=q_N=\mathrm{Im}\,\sigma \approx k$ so that, asymptotically, our wave functions very much resemble free waves $\exp(-ikx)$. In the light of Eq. (B11) we have also $\psi(x) \approx \exp(-ikx)$ near the origin.

In the strong coupling regime (i.e., for very small R representing, say, the low-lying excitations in a deep well with $T \gg 1$) we get an alternative estimate

$$\frac{\ell}{4}\omega_N = \arcsin\sqrt{\frac{1}{2}[R-(\sqrt{1+R^2}-1)]} \approx \frac{1}{2}R - \frac{1}{4}R^2 + \cdots \ll \frac{\ell}{4}.$$

In the extreme of $R \to 0$ the present spectrum of energies moves towards (and precisely coincides with) the well-known levels of the infinitely deep Hermitian square well of the same width $I=(-\ell,\ell)$. In this sense, the "complex-rotation" transition from the Hermitian well to its present non-Hermitian $\mathcal{PT}$-symmetric alternative proves amazingly smooth.

The wave functions exhibit the similar tendency. In the outer region, they are proportional to $\exp(-px)$ and decay very quickly since $p=\mathcal{O}(R^{-1/2})$. The parameter $G^{(\pm)}$ becomes strongly superscript dependent,

$$G^{(+)} = -\frac{k^2}{q+p} = \mathcal{O}(R^{3/2}), \quad G^{(-)} = -(q+p) = \mathcal{O}(R^{-1/2}).$$

This means that in the interior domain of $x \in (-\ell,\ell)$, the wave functions with the superscript $^{(+)}$ and $^{(-)}$ become dominated by their spatially even and odd components $\cos kx$ and $\sin kx$, respectively. In this sense, the superscript mimics (or at least keeps the trace of) the quantum number of the slightly broken spatial parity $\mathcal{P}$.

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Superconductivity by means of the subquantum medium coherence

M. Agop[a)]
Department of Physics, University of Athens, Athens 15771, Greece
and Department of Physics, Technical "Gh. Asachi" University, Iasi 6600, Romania

P. D. Ioannou
Department of Physics, University of Athens, Athens 15771, Greece

P. Nica
Department of Physics, University of Athens, Athens 15771, Greece
and Department of Physics, Technical "Gh. Asachi University, Iasi 6600, Romania

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In the hydrodynamic formulation of the scale relativity theory one shows that a stable vortices distribution of bipolaron type induces superconducting pairs by means of the quantum potential. Then, usual mechanisms (as, for example, the exchange interaction used in the bipolaron theory) are reduced to the coherence on the subquantum medium, the superconducting pairs resulting as a one-dimensional projection of a fractal. The temperature dependences of the superconducting parameters (coherence length, critical speed, pair breaking time, carriers concentration, penetration depth, critical field, critical current) and the concordance with the experimental data and other theories are analyzed. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1904163]

I. INTRODUCTION

One of the modern theories which deals with high-temperature superconductivity is the bipolaron theory.[1,2] The bipolarons are pairs of spin polarons with zero total spin like the Cooper pairs from the Bardeen–Cooper–Schrieffer (BCS) theory,[3] but unlike the Cooper pairs, the spin polarons form pairs in the real space and not only close to the energy interval Δ centered on the Fermi level. The bonding forces acting between the spin-polarons constituting the boson (bipolaron) are exchange-type forces. Under these circumstances Δ corresponds to the superconducting gap, and T_C is the temperature for Bose–Einstein gas to become degenerate. As an example, between the Cu–O planes spin polarons are formed, and they consist of holes and electrons; the holes originate from O–2*p* and the electrons from the Cu–3*d* orbitals. They become ordered as in Fig. 1(a).[1,2] The exchange mechanism between the spin-polarons leads to a stable distribution—the bipolarons [Fig. 1(b)] which endow the material with superconducting properties.

More recently, some superconducting properties have been explained by considering the charge carriers (electrons and holes) are quantized vortexlike objects, ordered in two vortex streets having antiparallel vortices.[4] The interaction between these vortexlike objects is mediated by a subquantum level with superfluid properties. For superconducting matter the status of such a medium is imposed by the hydrodynamic formulation of the scale relativity (SR) theory,[5] a unique mechanism inducing superconductivity, by means of a fractal string (a string in a fractal space–time).

Having in view these results, in the present paper we suggest new mechanisms for approaching superconductivity. Accordingly, once given the distribution from Fig. 1(a) we substitute the

[a)]Author to whom correspondence should be addressed: Stradela Florilor, nr. 2, Iasi - 700514, Romania. Electronic mail: magop@phys.tuiasi.ro

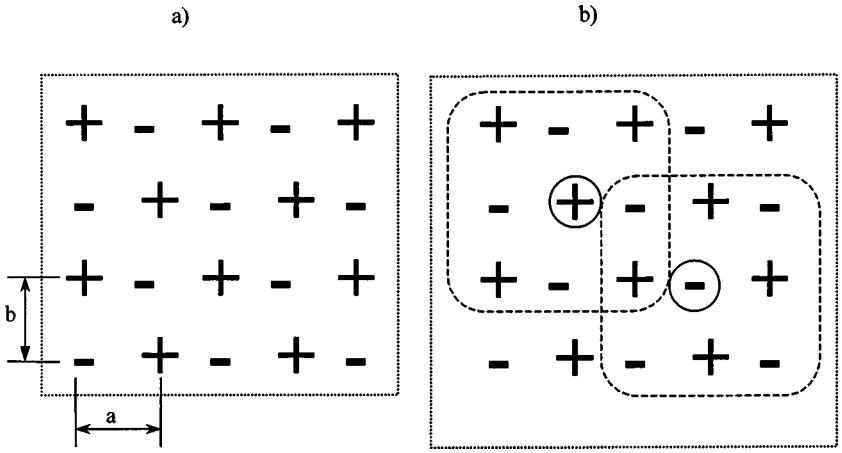

FIG. 1. (a) The holes and electrons distribution between the Cu–O planes associated to the distribution of zeros and poles of the potential (63). (b) The bipolarons distribution induced by means of the exchange mechanism.

exchange interaction (used in the bipolaron theory) by the sub quantum medium interaction. Superconducting pairs result, as being a one-dimensional (1D) projections of a fractal and the temperature dependences of the superconducting parameters.

II. SCALE RELATIVITY HYDRODYNAMIC EQUATIONS, QUANTUM POTENTIAL, DYNAMIC AND STATIC STATES

The SR theory extends Einstein's principle of relativity to scale transformation of resolution. It is based on the giving up of the axiom of differentiability of the space–time continuum. Three consequences arise from this withdrawal[5] (for details see Appendix A): (i) The geodesics of a nondifferentiable space–time are fractal and in infinite number, this leads one to use a fluidlike description $v=v[x(t),t]$ and implies adding new terms in the differential equations of the mean motion; (ii) the geometry of space–time become fractal, i.e., explicitly resolution dependent; this allows one to describe a nondifferentiable physics in terms of differential equation acting in the scale space. The requirement that these equations satisfy the principle of SR leads to introduce scale laws having a Galilean form (constant fractal dimension), then a log-Lorentzian form. In this framework, the Planck length-time scale becomes minimal impassable scale, invariant under dilatations, and the cosmic length scale (related to the cosmological constant) a maximal one. Recent measurements of the cosmological constant have confirmed the theoretical predicted value.[6] Then we attempt to construct a generalized SR, which includes nonlinear scale transformations and scale-motion coupling. In this last framework, one can interpret gauge invariance as scale invariance on the internal resolutions. This approach allowed us to make theoretical predictions concerning coupling constants and elementary particle masses (electron, Higgs boson, vacuum energy of Higgs field). These predictions are successfully checked using recently improved experimental values. Each elementary displacement is then described in terms of the sum, $dX=dx+d\xi$, of a mean classical displacement $dx=v\,dt$ and of a fractal fluctuation $d\xi$, whose behavior satisfies the principle of SR. It is such that $\langle d\xi\rangle=0$ and $\langle d\xi^2\rangle=2D\,dt$. The existence of this fluctuation implies introducing new second order terms in the differential equation of motion; (iii) time reversibility is broken at the infinitesimal level, this can be described in terms of a two-valuedness of the velocity vector, for which we use a complex representation, $\mathbf{V}=(v_+ + v_-)/2 - i(v_+ - v_-)/2$.

These three effects can be combined to construct a complex time-derivative operator

$$\delta/dt = \partial_t + \mathbf{V}\cdot\nabla - iD\Delta, \tag{1}$$

where the mean velocity $\mathbf{V}=dx/dt$ is now complex, and D is a parameter characterizing the fractal behavior of trajectories (for details of this problem see Appendix A).

Let us consider the covariant derivative (1) and the **V** complex velocity[5]

$$\mathbf{V} = -2iD\nabla \ln \psi \tag{2}$$

Applying the $\delta/\mathrm{d}t$ covariant derivative to the **V** complex velocity, we obtain

$$(\delta/\mathrm{d}t)\mathbf{V} = -2iD[\partial_t(\nabla \ln \psi) - 2iD(\nabla \ln \psi \cdot \nabla)(\nabla \ln \psi) - iD\Delta(\nabla \ln \psi)] \tag{3}$$

or still, considering the identity[5]

$$\begin{gathered}\nabla(\Delta\psi/\psi) = \Delta(\nabla \ln \psi) + 2(\nabla \ln \psi \cdot \nabla)(\nabla \ln \psi), \\ (\delta/\mathrm{d}t)\mathbf{V} = -2D\nabla[i(\partial_t\psi/\psi) + D(\Delta\psi/\psi)].\end{gathered} \tag{4}$$

For a fractal space–time, Newton's second principle takes the form

$$m(\delta/\mathrm{d}t)\mathbf{V} = -\nabla U \tag{5}$$

or explicitly

$$\nabla U = [2imD(\partial_t\psi/\psi) + 2mD^2(\Delta\psi/\psi)] \tag{6}$$

with U the potential.

Integrating this equation yields

$$D^2\Delta\psi + iD\partial_t\psi = \frac{U}{2m}\psi \tag{7}$$

up to an arbitrary phase factor $\alpha(t)$ which may be set to zero by a suitable choice of the phase of ψ. If there is no external fied, $U=0$, the convariance is explicit, since Newton's equation of inertial motion

$$(\delta/\mathrm{d}t)\mathbf{V} = 0.$$

The hydrodynamic model in the nondifferentiable space–time is built, replacing the complex velocity $\mathbf{V} = -2iD\nabla \ln(Ae^{iS})$ (A the amplitude and S the phase), i.e.,

$$\mathbf{V} = \mathbf{v} + i\mathbf{u}, \tag{8a}$$

$$\mathbf{v} = 2D\nabla S, \tag{8b}$$

$$\mathbf{u} = -iD\nabla \ln \rho, \tag{8c}$$

$$\rho = A^2 \tag{8d}$$

in (3) and replacing it in (5). It first follows that

$$-m^{-1}\nabla \cdot U = \{\partial_t(\mathbf{v} - iD\nabla \ln \rho) + [(\mathbf{v} - iD\nabla \ln \rho)\cdot\nabla](\mathbf{v} - iD\nabla \ln \rho) - iD\Delta(\mathbf{v} - iD\nabla \ln \rho)\}. \tag{9}$$

Using the identities

$$\Delta\nabla = \nabla\Delta, \tag{10a}$$

$$(\nabla f \cdot \nabla)(\nabla f) = 2^{-1}\nabla(\nabla f)^2, \tag{10b}$$

$$f^{-1}\Delta f = \Delta \ln f + (\nabla \ln f)^2, \tag{10c}$$

and separating in (9) the real and the imaginary parts [up to an arbitrary phase factor $\beta(t)$ which may be set to zero by a suitable choice of the phase of ψ] we obtain

$$m(\partial_t \mathbf{v} + (\mathbf{v}\cdot\nabla)\mathbf{v}) = -\nabla(U-Q), \tag{11a}$$

$$\partial_t \rho + \nabla\cdot(\rho\mathbf{v}) = 0, \tag{11b}$$

where Q is the quantum potential and has the expression[7]

$$Q = -2mD^2\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}. \tag{12}$$

Another form of (12), i.e.,

$$Q = -mD\nabla\cdot\mathbf{u} - \tfrac{1}{2}m\mathbf{u}^2 \tag{13}$$

is obtained combining the imaginary part **u**, (8c) of the complex velocity (8a), with the relation (12) using the identity (10c). Thus, the quantum potential depends only on the imaginary part of the complex velocity. Since **u** arises of nondifferertiability according to the nondifferentiable space model of quantum mechanics, it might be stressed that the quantum potential comes from the nondifferentiability of the quantum space–time (subquantum medium).

The wave function of $\Psi(\mathbf{r},t)$ is invariant when its phase changes by an integer multiple of 2π. Indeed, Eq. (8b) gives

$$\oint m\mathbf{v}\,\mathrm{d}r = 2mD\oint \mathrm{d}S = 4\pi nmD, \quad n = 0, \pm 1, \pm 2, \ldots \tag{14}$$

a condition of compatibility between the SR hydrodynamic model and the wave mechanics.[8]

For $D=\hbar/2m^*$ with $m^*=2m_e$ the mass of the Cooper pair the relation (14) becomes $\oint \mathbf{p}\cdot\mathrm{d}\mathbf{r} = nh$. This result can be identified with the quantification law of the gravitomagnetic flux $\phi_g = n\phi_{0g}$ with $\phi_{0g}=h/2m_e$ the gravitational fluxoid. Indeed, the generalized momentum of the Cooper pair in the gravitomagnetic field $\mathbf{B}_g=\nabla\times\mathbf{A_g}$ with $\mathbf{A_g}$ the potential vector of the gravitomagnetic field, $\mathbf{P}_g=2m_e\mathbf{v}+2m_e\mathbf{A}_g=\hbar\nabla S+2m_e\mathbf{A}_g$ is null, i.e., $\mathbf{P}_g\equiv 0$.[9]

Through integration we obtain

$$\hbar\oint \nabla S = \pm 2\pi n\hbar = 2m_e\oint \mathbf{A}_g\cdot\mathrm{d}\mathbf{r} = 2m_e\int\int_{\partial\Sigma}\mathbf{B}_g\cdot\mathrm{d}\mathbf{O} = 2m_e\phi_g,$$

i.e.,[9]

$$\phi_g = n\phi_{0g}, \quad \phi_{0g} = h/2m_e.$$

In the magnetic field $\mathbf{B}=\nabla\times\mathbf{A}$ with **A** the potential vector of the electromagnetic field, the generalized momentum of the Cooper pair $\mathbf{P}=\hbar\nabla S+2e\mathbf{A}$ is null, i.e., $\mathbf{P}=0$.[2] From here, by means of integration follows that

$$\hbar\oint \nabla S = \pm 2\pi n\hbar = 2e\oint \mathbf{A}\,\mathrm{d}\mathbf{r} = 2e\int\int_{\partial\Sigma}\mathbf{B}\cdot\mathrm{d}\mathbf{O} = 2e\phi_e.$$

the quantization law of the magnetic flux,[2]

$$\phi_e = n\phi_{0e}, \quad \phi_{0e} = h/2e,$$

with ϕ_{0e} the magnetic fluxoid.

The set of Eqs. (11a) and (11b) represents a complete system of differential equations for the fields $\rho(\mathbf{r},t)$ and $\mathbf{v}(r,t)$; relation (14) relates each solution $(\rho,\mathbf{v})_n$ with the wave solution Ψ in a unique way.

The field $\rho(\mathbf{r},t)$ is a probability distribution, namely the probability of finding the particle in the vicinity d$\mathbf{r}$ of the point $\mathbf{r}$ at time t,

$$d\mathbf{P} = \rho\, dr, \tag{15a}$$

$$\iiint \rho\, dr = 1, \tag{15b}$$

the space integral being extended over the entire area of the system. Any time variation of the probability density $\rho(\mathbf{r},t)$ is accompanied by a probability current $\rho\mathbf{v}$ pointing towards or outward from the corresponding field point $\mathbf{r}$ [Eq. (11b)].

The position probability of the real velocity field $\mathbf{v}(r,t)$ [Eq. (11a)], varies with space and time similar to a hydrodynamic fluid placed in the force field of an external potential $U(\mathbf{r},t)$ and a quantum potential (12). The fluid (in the sense of a statistical particles ensemble) exhibits, however, an essential difference compared to an ordinary fluid, in a rotation motion $\mathbf{v}(r,t)$ increases (decreases) with the decreasing (increasing) distance $\mathbf{r}$ from the center [Eq. (14)].

The expectation values for the real velocity field and the velocity operator $\hat{\mathbf{v}} = -2iD\nabla$ (Ref. 5) of wave mechanics are equal,

$$\langle \mathbf{v} \rangle = \iiint \rho \mathbf{v}\, dr = \iiint \Psi^* \hat{\mathbf{v}} \Psi\, dr = \langle \hat{\mathbf{v}} \rangle_{WM}, \tag{16}$$

but in the higher order, $|n| > 2$, similar identities are invalid, namely $\langle \mathbf{v}^n \rangle \neq \langle \mathbf{v}^n \rangle_{WM}$. The expectation for the quantum force vanishes at all times (theorem of Ehrenfest[8]), i.e.,

$$\langle -\nabla Q \rangle = \iiint \rho(-\nabla Q) d\mathbf{r} = 0 \tag{17}$$

or explicitly

$$2mD^2 \iiint \rho \nabla \left(\frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} \right) d\mathbf{r} = mD^2 \oint (\rho \nabla \nabla \ln \rho) \cdot d\mathbf{\acute{o}} = 0. \tag{18}$$

Two types of fractal stationary states are to be distinguished. (i) Dynamic states. For $\partial/\partial t = 0$ and $\mathbf{v} \neq 0$, Eqs. (11a) and (11b) give

$$\nabla \left(\frac{1}{2} m\mathbf{v}^2 + U - 2mD^2 \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} \right) = 0, \tag{19a}$$

$$\nabla(\rho \mathbf{v}) = 0, \tag{19b}$$

namely

$$\frac{1}{2} m\mathbf{v}^2 + U - 2mD^2 \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} = E, \tag{20a}$$

$$\rho \mathbf{v} = \nabla \times \mathrm{F}. \tag{20b}$$

Consequently, inertia $m\mathbf{v} \cdot \nabla \mathbf{v}$, exterior forces $(-\nabla U)$, and quantum forces $(-\nabla Q)$ are in balance at every field point [Eq. (19a)]. The sum of the kinetic energy $m\mathbf{v}^2/2$, external (U), and quantum potential energy (Q) is invariant, i.e., equal to the integration constant $E \neq E(\mathbf{r})$ [Eq. (20a)]. $E \equiv \langle E \rangle$ represents the total energy of the dynamic system. The probability flow density $\rho\mathbf{v}$ has no sources [Eq. (19b)], i.e., its streamlines are closed [Eq. (20b)]. (ii) Static states. For $\partial/\partial t = 0$ and $\mathbf{v} = 0$, Eqs. (11a) and (11b) give

$$\nabla\left(U-2mD^2\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}\right)=0, \tag{21}$$

i.e.,

$$U-2mD^2\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}=E. \tag{22}$$

The exterior force $(-\nabla U)$ is balanced by the quantum force $(-\nabla Q)$ at any field point [Eq. (21)]. The sum of the exterior (U) and interior (Q) potential energy is invariant, i.e., equal to the integration constant $E\neq E(\mathbf{r})$ [Eq. (22)]. $E\equiv<E>$ represents the total energy of the fractal static system.

In the general case, making $U=0$ in Eq. (11a), multiplying it by ρ and taking into account (11b), it becomes[10]

$$\partial_t(m\rho v_k)+\partial_{x_i}(m\rho v_i v_k)=-\rho\partial_{x_k}[2mD^2\rho^{-1/2}\partial_{x_l}\partial_{x_l}\rho^{1/2}]. \tag{23}$$

Using the notation[10]

$$\pi_{ik}=m\rho\mathbf{v}_i\mathbf{v}_k-\sigma_{ik}, \tag{24a}$$

$$\sigma_{ik}=m\rho D^2\partial_{x_l}\partial_{x_k}(\ln\rho), \tag{24b}$$

Eq. (23) takes the simple form[10]

$$\partial_t(m\rho\mathbf{v}_k)=-\partial_{x_l}\pi_{ik}. \tag{25}$$

The analogy with classical fluid mechanics works will if one introduces the cinematic[10]

$$\nu=D/2 \tag{26}$$

and dynamic

$$\eta=\tfrac{1}{2}mD\rho \tag{27}$$

viscosities. Under these circumstances π_{ik} defines the momentum flux density tensor and σ_{ik} the internal stress tensor

$$\sigma_{ik}=\eta(\partial_{x_k}u_i+\partial_{x_l}u_k). \tag{28}$$

Since from (24a) and (24b) one can see that the internal stress tensor is built using the quantum potential, the equations of hydrodynamic model in the nondifferentiable space–time are nothing but a system of equations of the Navier–Stokes type where the quantum potential plays the role of an internal stress tensor. Then the dynamical regime implies the system of equations of Navier–Stokes type, a system which is generally difficult to be solved.

III. STATIC STATES AND KINK TYPE SOLUTIONS

Assimilating the coherent quantum fluid particle (of superfluid or superconducting type) with the vortex type objects, one finds that $U=A\rho$ with $A=A(\Gamma,\hat{\sigma})=\text{const}$—see Appendix B (for details on this problem see also Ref. 8). First, from (22) it results

$$\Delta(\rho)^{1/2}+\frac{E}{2mD^2}\rho^{1/2}-\frac{A}{2mD^2}\rho^{3/2}=0 \tag{29}$$

and with the substitutions

$$\xi = (E/2mD^2)^{-1/2}, \tag{30a}$$

$$f = (A\rho/E)^{1/2}, \tag{30b}$$

$$x_r = (x/\xi), \tag{30c}$$

$$y_r = (y/\xi), \tag{30d}$$

$$z_r = (z/\xi), \tag{30e}$$

it results in the non linear differential equation

$$\Delta f + f(1 - f^2) = 0. \tag{31}$$

We will restrict to the (1D) case, this is

$$\frac{d^2 f}{dx_r^2} = f^3 - f, \tag{32}$$

Multiplying both sides of Eq. (32) by (df/dx_r), and performing integration over x_r we obtain

$$\frac{df}{dx_r} = \sqrt{\frac{1}{2}f^4 - f^2 + C}, \tag{33}$$

where

$$C = \left[\left(\frac{df}{dx_r}\right)^2 - \frac{1}{2}f^4 + f^2\right]_{x=x_r^0}. \tag{34}$$

Equation (34) is obviously a restriction imposed on the order parameter, f, showing the boundary conditions. A further integration of Eq. (33) leads to

$$\frac{x_r - x_r^0}{\sqrt{2}} = \int_0^f \frac{df}{\sqrt{(f_1^2 - f^2)(f_2^2 - f^2)}}, \tag{35}$$

where

$$f_{1,2}^2 = 1 \mp \sqrt{1 - 2C}. \tag{36}$$

By the change of variable $\varphi = f/f_1$, Eq. (35) becomes

$$f_2 \frac{x_r - x_r^0}{\sqrt{2}} = \int_0^{f/f_1} \frac{d\varphi}{\sqrt{(1 - \varphi^2)(1 - k^2\varphi^2)}}, \tag{37}$$

where we made the notation

$$k \equiv f_1/f_2. \tag{38}$$

Writing f_1 and f_2 in terms of k, $f_1^2 = (2k^2/1+k^2)$, $f_2^2 = (2/1+k^2)$, Eq. (37) becomes

$$\frac{x_r - x_r^0}{\sqrt{1 + k^2}} = \int_0^{\varphi_1} \frac{d\varphi}{\sqrt{(1 - \varphi^2)(1 - k^2\varphi^2)}}, \tag{39}$$

where the superior limit is

$$\varphi_1 = f\sqrt{\frac{1+k^2}{2k^2}}.$$

We distinguish two cases, (i) $k \leqslant 1$ and (ii) $k \geqslant 1$. In both cases, Eq. (39) can be solved in the terms of the Jacobian elliptic functions, $\mathrm{sn}(u|k)$, of argument u and modulus k.[11]

(i) For $k \leqslant 1$, the class of solutions of Eq. (39) becomes

$$f = \sqrt{\frac{2k^2}{1+k^2}}\mathrm{sn}\left(\left.\frac{x_r - x_r^0}{\sqrt{1+k^2}}\right| k\right). \tag{40}$$

In the limit $k \to 0$, Eq. (40) can be approximated as

$$f = \sqrt{\frac{2k^2}{1+k^2}}\sin\left(\frac{x_r - x_r^0}{\sqrt{1+k^2}}\right) \to 0 \tag{41}$$

and for $k \to 1$ one obtains the kink solution

$$f = \sqrt{\frac{2k^2}{1+k^2}}\mathrm{th}\left(\frac{x_r - x_r^0}{\sqrt{1+k^2}}\right). \tag{42}$$

It is well known that the Ginzburg–Landau model (GLM) also supports two solutions, zero and hyperbolic tangent which correspond to the Cooper pair.[2]

(ii) If $k > 1$, by the substitution $\eta = f\varphi$, Eq. (39) becomes

$$k\frac{x_r - x_r^0}{\sqrt{1+k^2}} = \int_0^{\eta_1} \frac{\mathrm{d}\eta}{\sqrt{(1-\eta^2/k^2)(1-\eta^2)}} \tag{43}$$

with

$$\eta_1 = f\sqrt{\frac{1+k^2}{2}}$$

which gives the class of solutions

$$f = \sqrt{\frac{2}{1+k^2}}\mathrm{sn}\left(\left.\frac{x_r - x_r^0}{\sqrt{1+k^2}}k\right| \frac{1}{k}\right). \tag{44}$$

We are able now to get the expressions of some superconducting parameters. Thus, from Eqs. (39) and (43), by integration and using the relation which defines the relative coherence length,[2] it results in

$$\xi_r = \begin{cases} (1+k^2)^{1/2}K(k), & k \leqslant 1, \quad (45a) \\ k^{-1}(1+k^2)^{1/2}K(1/k), & k > 1, \quad (45b) \end{cases}$$

where $K(k)$ is the complete elliptic integral of the first kind,[11] $K(k) = \int_0^{\pi/2}(1-k^2\sin^2\varphi)^{-1/2}\,\mathrm{d}\varphi$.

The relative critical speed

$$v_r = \begin{cases} (1+k^2)^{-1/2}K^{-1}(k), & k \leqslant 1, \quad (46a) \\ k(1+k^2)^{-1/2}K^{-1}(1/k), & k > 1, \quad (46b) \end{cases}$$

and the relative pair breaking time

$$\tau_r = \begin{cases} (1+k^2)K^2(k), & k \leqslant 1, \quad (47a) \\ k^{-2}(1+k^2)K^2(1/k), & k > 1 \quad (47b) \end{cases}$$

are deduced from (45a) and (45b) and the relations which define these parameters.[2]

In the 1D case, we can express the relative superconducting carrier concentration as

$$n_r = |f|^2 = \begin{cases} \dfrac{2k^2}{1+k^2}\mathrm{sn}^2\left(\dfrac{x_r - x_r^0}{\sqrt{1+k^2}}\middle| k\right), & k \leqslant 1, \quad (48a) \\ \dfrac{2}{1+k^2}\mathrm{sn}^2\left(\dfrac{k(x_r - x_r^0)}{\sqrt{1+k^2}}\middle| \dfrac{1}{k}\right), & k > 1. \quad (48b) \end{cases}$$

In order to establish a direct connection with experimental observations in the physical systems, the acquired spatial dependence of n_r can be cancelled by averaging $|f|^2$ on a period, $2K$,

$$n_r = \begin{cases} \dfrac{2}{1+k^2}\left(1 - \dfrac{E(k)}{K(k)}\right), & k \leqslant 1, \quad (49a) \\ \dfrac{2}{k(1+k^2)}\left(1 - \dfrac{E(1/k)}{K(1/k)}\right), & k > 1, \quad (49b) \end{cases}$$

where $E(k)$ is the complete elliptic integral of the second kind of modulus k (Ref. 11) $E(k) = \int_0^{\pi/2}(1-k^2\sin^2\varphi)^{1/2}\,\mathrm{d}\varphi$.

By using Eqs. (49a) and (49b) and the London definition of the penetration depth,[2] we obtain the relative penetration depth in the case of spatial gradients

$$\lambda_r = \begin{cases} \left[\dfrac{2}{1+k^2}\left(1 - \dfrac{E(k)}{K(k)}\right)\right]^{-1/2}, & k \leqslant 1, \quad (50a) \\ \left[\dfrac{2}{k(1+k^2)}\left(1 - \dfrac{E(1/k)}{K(1/k)}\right)\right]^{-1/2}, & k > 1. \quad (50b) \end{cases}$$

For the relative critical field, we derive the expression

$$B_r = \begin{cases} \dfrac{2}{1+k^2}\sqrt{2\left(1 - \dfrac{E(k)}{K(k)}\right)}, & k \leqslant 1, \quad (51a) \\ \dfrac{2}{k(1+k^2)}\sqrt{2\left(1 - \dfrac{E(1/k)}{K(1/k)}\right)}, & k > 1. \quad (51b) \end{cases}$$

The relative critical current density

$$j_r = \begin{cases} \dfrac{2}{(1+k^2)^{3/2}}\left(\dfrac{1}{K(k)} - \dfrac{E(k)}{K^2(k)}\right), & k \leqslant 1, \quad (52a) \\ \dfrac{2}{(1+k^2)^{3/2}}\left(\dfrac{1}{K(1/k)} - \dfrac{E(1/k)}{K^2(1/k)}\right), & k > 1 \quad (52b) \end{cases}$$

is obtained from (46a), (46b), (49a), and (49b) and the expression which defines j_r.

The important characteristics of the material versus k are illustrated in Figs. 2(a)–2(g). One can notice a clear discontinuity at $k=1$ for all superconducting parameters. This leads to the idea that the point $k=1$, could be associated with the transition from superconducting into normal state.

IV. TEMPERATURE DEPENDENCES OF THE SUPERCONDUCTING PARAMETERS

Probably the most important physical consideration which concerns our results, from the applicative point of view, is that we need to introduce the temperature dependences of the superconducting parameters. Taking into account that all the superconducting parameters suffer a discontinuity for $k=1$ [as can been seen in Figs. 2(a)–2(g)], one can admit the following functional dependence of the modulus of the elliptic function on the reduced temperature:

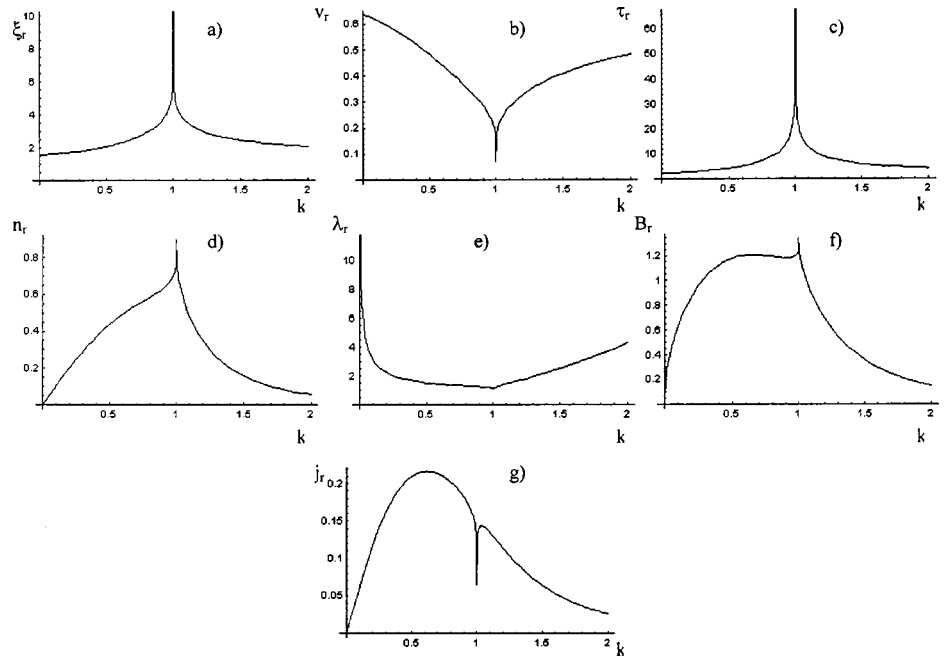

FIG. 2. (a) The k dependence of the relative coherence length. (b) The k dependence of the relative critical speed. (c) The k dependences of the relative pair breaking time. (d) The k dependences of the average relative concentration. (e) The k dependences of the relative penetration depth. (f) The k dependences of the relative critical field. (g) The k dependences of the relative critical current density.

$$k = t = T/T_C. \tag{53}$$

To avoid the confusion and to obtain the exact temperature dependences of the superconducting parameters, we will admit adequate normalizations of these parameters and the restriction $k<1$. Thus, the dependence on t of the coherence length is

$$(\xi(t)/\xi(0)) = (2/\pi)(1+t^2)^{1/2}K(t). \tag{54}$$

Figure 3(a) shows the relation (54) in comparison with the one given by the BCS theory,[2] i.e., $(\xi(t)/\xi(0))=(1-t^2)^{-1/2}$ (dashed line). In the relation (54) $K(t)=\int_0^{\pi/2}(1-t^2\sin^2\varphi)^{-1/2}\,d\varphi$.

The dependence on t of the critical speed is

$$(v_C(t)/v_C(0)) = (\pi/2)(1+t^2)^{-1/2}K^{-1}(t). \tag{55}$$

In Fig. 3(b) one can see the comparison between the (55) dependence and the one given by the BCS theory,[2] i.e., $(v_C(t)/v_C(0))=(1-t^2)^{1/2}$ (dashed line).

The dependence on t of the pair breaking time is

$$(\tau(t)/\tau(0)) = (4/\pi^2)(1+t^2)K^2(t). \tag{56}$$

Figure 3(c) presents together the dependence (56) and the one given by BCS theory,[2] i.e., $(\tau(t)/\tau(0))=(1-t^2)^{-1}$ (dashed line).

Comparing with the BCS theory,[2] similar behaviors of the coherence length [Fig. 3(a)], critical speed [Fig. 3(b)] and pair breaking time [Fig. 3(c)] can be observed.

In order to get the dependence of the concentration on t one admits first that

$$(n(t)/n(0)) = \rho = (E/A)f^2 \approx (\xi(0)/\xi(t))^2 f^2 = 3.7\cdot(1+t^2)^{-1}K^{-2}(t)f^2 \tag{57}$$

with

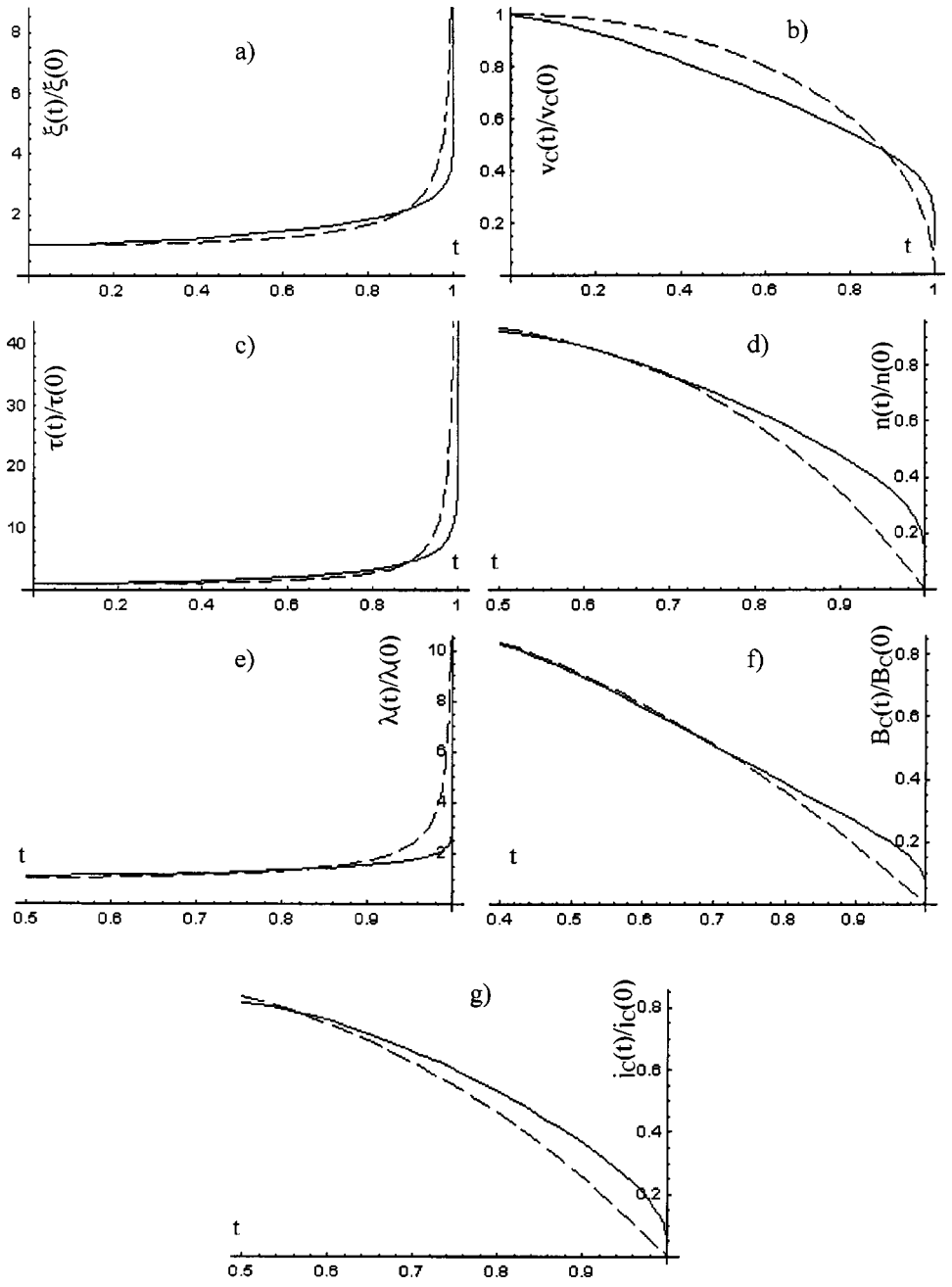

FIG. 3. (a) The t dependence of the relative coherence length in comparison with the one given by BCS theory. (b) The t dependences of the relative critical speed in comparison with the one given by BCS theory. (c) The t dependence of the relative pair breaking time in comparison with the one given by BCS theory. (d) The t dependence of the average relative concentration in comparison with the experimental one. (e) The t dependence of the relative penetration depth in comparison with the one given by bifluid model. (f) The t dependences of the relative critical field in comparison with the one given by BCS theory. (g) The t dependence of the relative critical current density in comparison with the one given by BCS theory.

$$(2mD^2/A) = \xi^2(0), \tag{58a}$$

$$(2mD^2/E) = \xi^2(t). \tag{58b}$$

By inserting Eq. (49a) in Eq. (57) one finds

$$(n(t)/n(0)) = 3.7 \cdot (1+t^2)^{-2}K^{-2}(t)[1-(E(t)/K(t))]. \tag{59}$$

The concordance with the experimental data described by $(n(t)/n(0))=(1-t^4)$ (Ref. 2) (dashed line) is good in the limits $0.5<t<1$, as can be seen in Fig. 3(d). As temperature decreases, the superconducting concentration is recovered. Consequently, our equation can describe the superconducting behavior starting from temperatures equal to $0.5T_c$ until the critical temperature.

The reduced temperature dependence of the penetration depth

$$(\lambda(t)/\lambda(0)) = 0.55 \cdot (1+t^2)K(t)[1-(E(t)/K(t))]^{-1/2} \tag{60}$$

is in agreement with the data of the bifluid model $(\lambda(t)/\lambda(0))=(1-t^4)^{-1/2}$ [2] [dashed line, Fig. 3(e)], for $0.5<t<1$.

In the case of the critical field,

$$(B_C(t)/B_C(0)) = 7.67 \cdot (1+t^2)^{-2}K^{-2}(t)[1-(E(t)/K(t))]^{1/2} \tag{61}$$

the concordance with the experimental data, which is well described by $(B_C(t)/B_C(0))=(1-t^2)^2$ (dashed line), can be seen in Fig. 3(f), where Eq. (61) fits data for $0.4<t<1$.

The dependence on t of the critical current density is

$$(j_C(t)/j_C(0)) = 26.7 \cdot (1+t^2)^{-3/2}K^{-3}(t)[1-(E(t)/K(t))]. \tag{62}$$

In Fig. 3(g) one can see the comparison between the (62) dependence and the one given by the BCS theory,[2] i.e., $(j_C(t)/j_C(0))=(1-t^2)^{1/2}(1-t^4)^{1/2}$ (dashed line). The concordance is good in the limits $0.5<t<1$.

Summarizing this section, we would emphasize that the derived expressions of the superconducting parameters $(n(t),\lambda(t),B_C(t),j_C(t))$ are amendable to experimental verifications in the range about $0.5<t<1$. At the same time, $\xi(t),v_C(t),\tau(t)$ have similar behaviors for $0<t<1$.

V. NONDIFFERENTIABILITY AND SUPERCONDUCTIVITY

The choice $U=A\rho$—see Sec. III, induces nondifferentiability through the imaginary speed **u**. In particular, for $k\to 0$, $x^0/\xi \equiv K(k)$ and an adequate normalization, from (40), (44), and (8c) it results $u=D\partial_x \ln(\mathrm{cn}(x_r))=(D/\xi)(\mathrm{sn}(x_r)\mathrm{dn}(x_r)/\mathrm{cn}(x_r))$. From here, the two-dimensional (2D) generalization of the real speed field, $\Omega=\ln(u\xi/D)$, i.e.,

$$\Omega = \Gamma \ln\left[\frac{\mathrm{sn}(\underline{u})\mathrm{dn}(\underline{u})}{\mathrm{cn}(\underline{u})}\right] \tag{63}$$

with

$$\underline{u} = \frac{K}{a}\underline{z}, \tag{64a}$$

$$\underline{z} = x + iy, \tag{64b}$$

$$K/K' = b/a, \tag{64c}$$

$$K = \int_0^{\pi/2} (1-k^2\sin^2\varphi)^{-1/2}\,\mathrm{d}\varphi, \tag{64d}$$

$$K' = \int_0^{\pi/2} (1-k'^2\sin^2\varphi)^{-1/2}\,\mathrm{d}\varphi, \tag{64e}$$

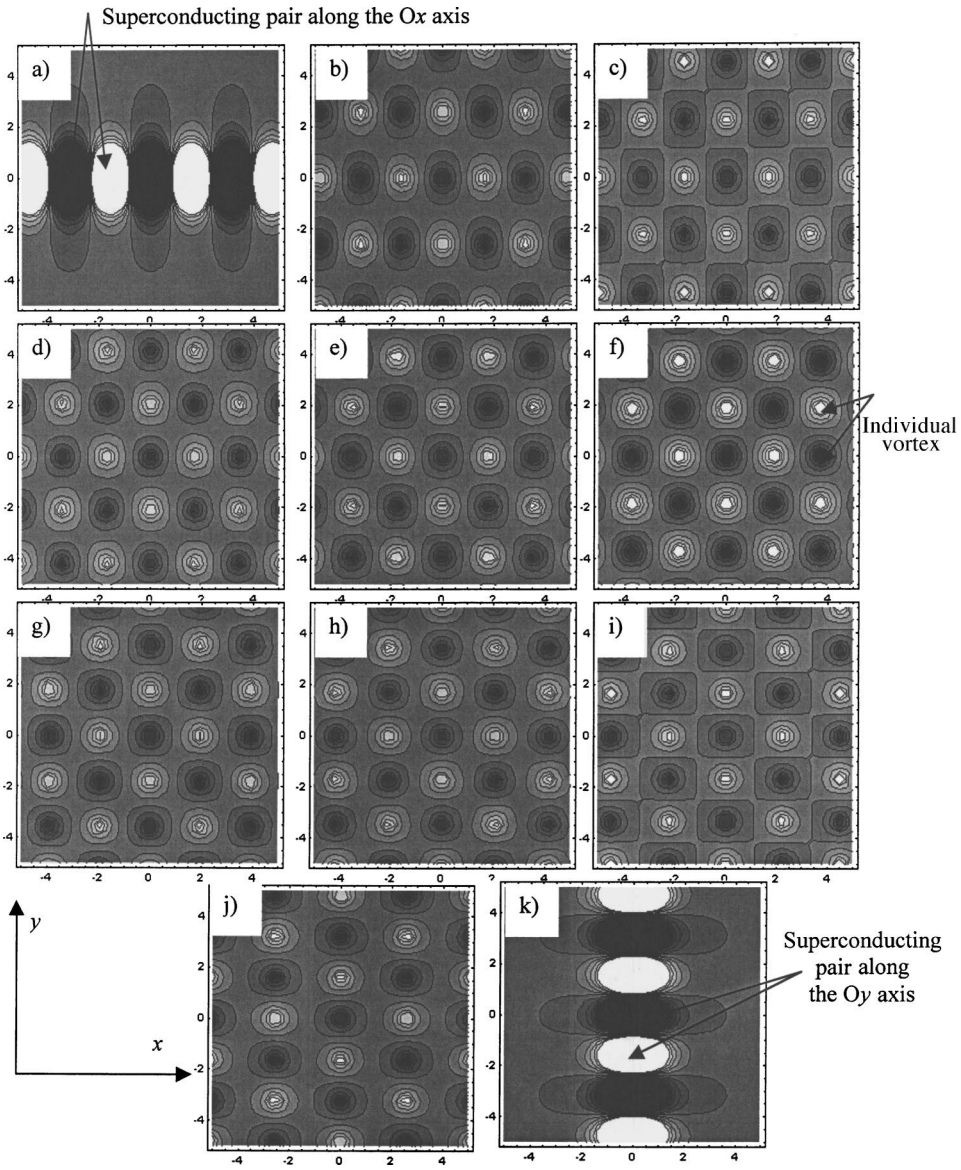

FIG. 4. (a)–(k) The k dependences, of the equipotential lines corresponding to the real part of the complex potential (63). Superconducting pairs along the Ox and Oy axes.

$$k^2 + k'^2 = 1 \tag{64f}$$

describes the stable distribution—the bipolarons[1,2,12] from Fig. 1(b).

In relations (63) and (64a)–(64d) cn, dn are the Jacobi elliptic functions,[11] K, K' the complete elliptic integrals of first kind of k modulus,[11] a, b the lattice constants along Ox and Oy axis, respectively, and Γ the vortex constant.[13] In Figs. 4(a)–4(k) one shows the equipotential curves $\mathrm{Re}\,\Omega = 0$ for $k = 0$–1 and in Fig. 5 the corresponding fractal dimension $\mathbf{D}$ (Ref. 14) dependence with k, i.e., $\mathbf{D} = \mathbf{D}(k)$. The following aspects result.

(i) The parameter k gives the vortices coherence in the lattice (the phase and amplitude correlation of the vortices[13,15]). For $k = 0$ and $k = 1$ the coherence is maximum through vortex pairs forming, along Ox axis [Fig. 4(a)] or Oy axis [Fig. 4(k)], respectively. For $k = 0.5$ the coherence is minimum through vortex individualizing [Fig. 4(f)].

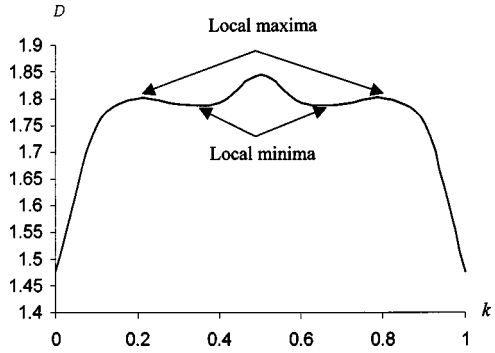

FIG. 5. The k dependence of the fractal dimension. It results that through k the fractal dimension is a measure of the coherence degree.

Mathematically, the vortices coherence implies $\Omega(u)=\Omega(u')$. Such a relation occurs if, and only if, between u and u' it exists the homography

$$u=\frac{au'+b}{cu'+d},$$

where $a, b, c, d \in \mathrm{N}$, $ad-bc\equiv 1$, $u=\omega_2/\omega_1$, $u'=\omega_2'/\omega_1'$, (ω_2/ω_1) and (ω_2'/ω_1') being the fundamental period pairs of a two equivalent elliptic function $(\mathrm{sn}\cdot\mathrm{dn}/\mathrm{cn})$—the equivalence theorem of elliptic functions.[11] In particular, for $c=1$ and $d=0$, the vortices coherence is generated by the $\varepsilon^{(\infty)}$ space–time[16]—see Appendix C. Therefore, the vortices amplitude and phase correlations in the lattice are of Cantorian type [for example, in the vortices synchronization by frequency looking, the frequency ratio is $v=1/(2n+1)$ (Ref. 2)]. Such result implies the fractionar statistics, i.e., the anyonic mechanism.[2]

(ii) The $\mathbf{D}=\mathbf{D}(k)$ curve symmetry shows the simultaneous coherence extension along this two axis, i.e., in plane. Besides, for the high temperature superconductivity, the coherence in the superconducting pairs form is achieved only in Cu–O planes.[2,17]

(iii) The fractal dimension varies from the minimum $\mathbf{D}\approx 1.445$, and local minima $\mathbf{D}\approx 1.755$, to maxima $\mathbf{D}\approx 1.850$ and local maxima $\mathbf{D}\approx 1.80$, respectively. Moreover, the observations superconducting pair–superconducting pair correlations can be associated with a (limited) fractal with dimension of $\mathbf{D}\approx 1.80$.[2,14] This fractal dimension represents a manifestation of the fact that the observed fractal should have emerged from two-dimensional sheetlike objects (superconductivity is a property characterizing 2D objects[2,17]).

(iv) Figures 4(a) and 4(k) correspond to the final structures developed in the coherence process and Figs. 4(e)–4(g) to the initial ones. Furthermore, the time evolution of the coherence process given by the iterated map of the $(\mathrm{sn}\,\mathrm{dn}/\mathrm{cn})$ function shows that this is generated by means of a fractal (superconducting fractal) (Fig. 6) [its fractal dimension (or Hausdorff–Besicovich dimension[14]), $\mathbf{D}\approx 2.4$ is greater than the topological one $\mathbf{D}\approx 2$] In such a context, the structures described by Figs. 4(a)–4(k), i.e., the coherence sequences, are projections of the superconducting fractal.

VI. ONE-DIMENSIONAL PROJECTION OF A SUPERCONDUCTING FRACTAL: COOPER PAIRS

Let us demonstrate that the superconducting pairs are 1D projections of the superconducting fractal from Fig. 6. Having this aim in view, let us consider the potential projection along Ox axis, i.e.,

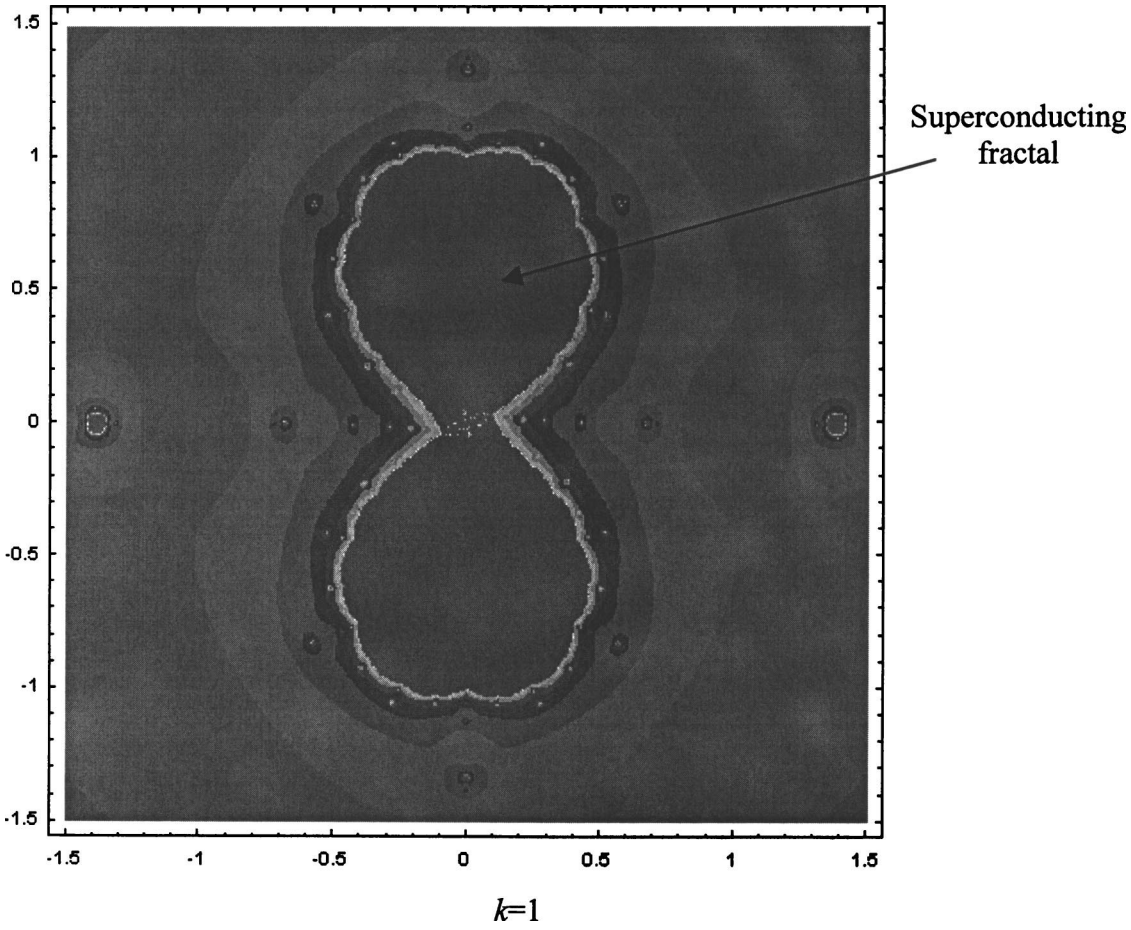

FIG. 6. The superconducting fractal given by an iterated map of the (sn dn/cn) function.

$$\Omega(x;k) = \Gamma \ln\left[\frac{\mathrm{sn}\left(\frac{K}{a}x;k\right)\mathrm{dn}\left(\frac{K}{a}x;k\right)}{\mathrm{cn}\left(\frac{K}{a}x;k\right)}\right]. \tag{65}$$

The quantum states, being stationary and with $E=0$ (for details see Refs. 8 and 17), Eq. (22), with $U=\Omega(x;k)$ and substitutions

$$\sqrt{\rho} = f, \tag{66a}$$

$$(Kx/a) = u \tag{66b}$$

takes the form

$$\frac{d^2f}{dx^2} - \left(\frac{\Gamma}{2mD}\right)\ln\left(\frac{\mathrm{sn}(u)\mathrm{dn}(u)}{\mathrm{cn}(u)}\right)f = 0, \tag{67}$$

The nonlinear Helmholtz like Eq. (67) can be solved only approximately. Using the WKBJ method[8,12] we get

$$f \sim \frac{A}{\sqrt{p}} e^{\mp \int p \, dx}, \tag{68a}$$

$$A = \text{const} \tag{68b}$$

with

$$p^2 = \frac{1}{\Lambda^2} \ln\left(\frac{\text{sn}(u)\text{dn}(u)}{\text{cn}(u)}\right) \tag{69a}$$

$$\frac{1}{\Lambda^2} \equiv \frac{\Gamma}{2mD^2}, \tag{69b}$$

Λ being a dissipation characteristic length (Kolmogorov model),[14] i.e., the minimal dimension of a vortexlike particle. Then, the density of probability ρ becomes

$$\tilde{n} \approx \frac{A^2 \ddot{E}^2}{\ln\left(\frac{\text{sn}(u)\text{dn}(u)}{\text{cn}(u)}\right)} \exp\left[\mp \frac{2a}{\ddot{E}K(k)} \int \sqrt{\ln\left(\frac{\text{sn}(u)\text{dn}(u)}{\text{cn}(u)}\right)} du \right]. \tag{70}$$

The integral from Eq. (70) can be rewritten in the form

$$\Im = \int \sqrt{\ln\left(\frac{\text{sn}(u)\text{dn}(u)}{\text{cn}(u)}\right)} du = \mp \frac{1}{2} \int \frac{\sqrt{\mu}\, d\mu}{\sqrt{\cosh^2 \mu - k^2}}, \tag{71}$$

for

$$\mu = \ln\left(\frac{\text{sn}(u)\text{dn}(u)}{\text{cn}(u)}\right). \tag{72}$$

In the general case this integral cannot be evaluated. However, for $k=0$ the integral (71) takes the form

$$\Im = \mp \frac{1}{2} \sum_{n=0}^{\infty} \frac{E_{2n}}{(2n)\left(2n+\frac{3}{2}\right)} \mu^{(2n+3/2)} \quad \left(|\mu| < \frac{\partial}{2}\right) \tag{73}$$

with E_{2n} the Euler constants ($E_0=1, E_1=0, E_2=-1, E_3=0$). Finally, substituting in the integral (71)

$$\text{sn}(u,0) = \sin u, \quad \text{cn}(u,0) = \cos u, \quad \text{dn}(u,0) = 1, \quad K(0) = \partial/2, \tag{74}$$

the density ρ becomes

$$\tilde{n} \approx \frac{A\ddot{E}^2}{\ln\left[\text{tg}\left(\frac{\partial x}{2a}\right)\right]} \exp\left\{ \mp \frac{2a}{\partial x} \sum_{n=0}^{\infty} \frac{E_{2n}}{(2n)\left(2n+\frac{3}{2}\right)} \left[ln\left(\text{tg}\frac{\partial x}{2a}\right)\right]^{(2n+3/2)} \right\}. \tag{75}$$

The relation (75) works only with the restriction

$$\frac{1}{p}\frac{d}{dx}(\ln p) \ll 1 \tag{76}$$

that is true for domains closed to the zeros of the same sign of the potential (63) (for details see Ref. 15). In the relation (75) we can consider only the first four series terms because the others are negligible—Fig. 7. In Fig. 8 the density ρ is plotted as a function of x and a/Λ. One notices that for a/Λ ratio values greater than 10^3, the density splits into two parts, signifying the formation of

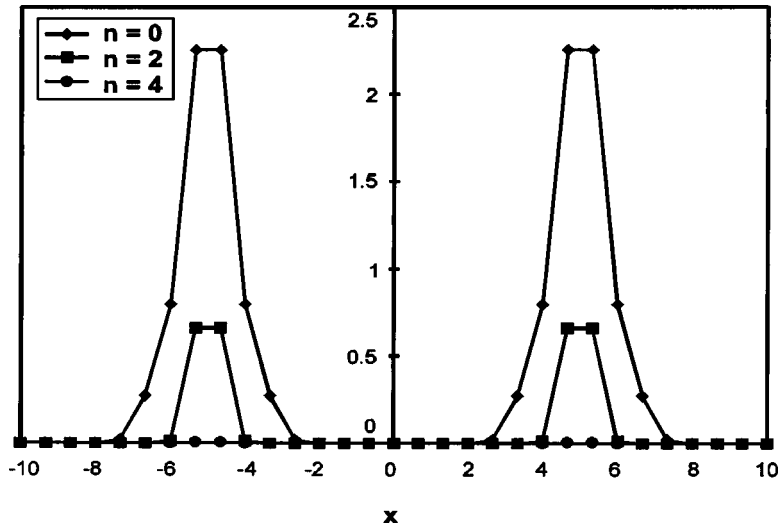

FIG. 7. The representation of the first four series terms of (75).

the superconducting pairs. In such a context, if $\Lambda \approx \Lambda_C \approx 3.8 \times 10^{-13}$ m (the minimal dimension of the vortexlike particle is the electron wavelength[2,17]) than $a > 3.8 \times 10^{-10}$ m. Such a value corresponds to the minimum distance between two vortices to form a pair (coherence length—for details see Refs. 2 and 17).

The case $k=1$ is presented in Figs. 9(a) and 9(b). It also results the superconducting pair (Cooper pair) forming—the states density is symmetric on $x=0$ and increases toward $k=1$.

VII. CONCLUSIONS

The main conclusions of the present paper are as follows.

(i) In the hydrodynamic formulation of the SR theory one obtains the conservation equations of momentum and probability density.

(ii) Through momentum conservation law one introduces the quantum potential as a measure of nondifferentiability of the quantum space–time. In such a frame, the quantum space–time is identified with a subquantum medium of superfluid properties.

(iii) One finds the compatibility relation between the SR hydrodynamic model and the wave mechanics and one defines the dynamic and static states.

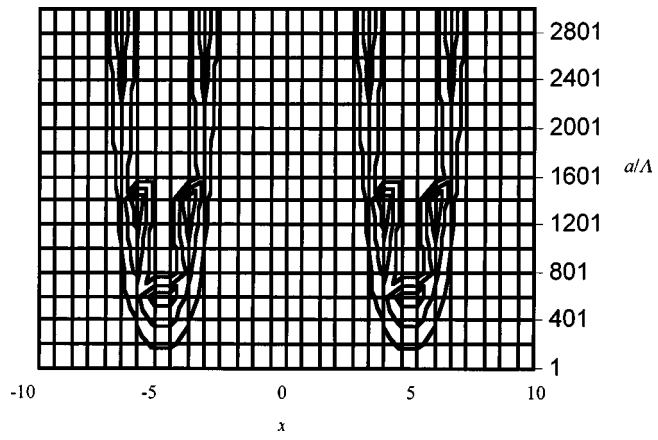

FIG. 8. 2D dependence of the density (75) on x and a/Λ.

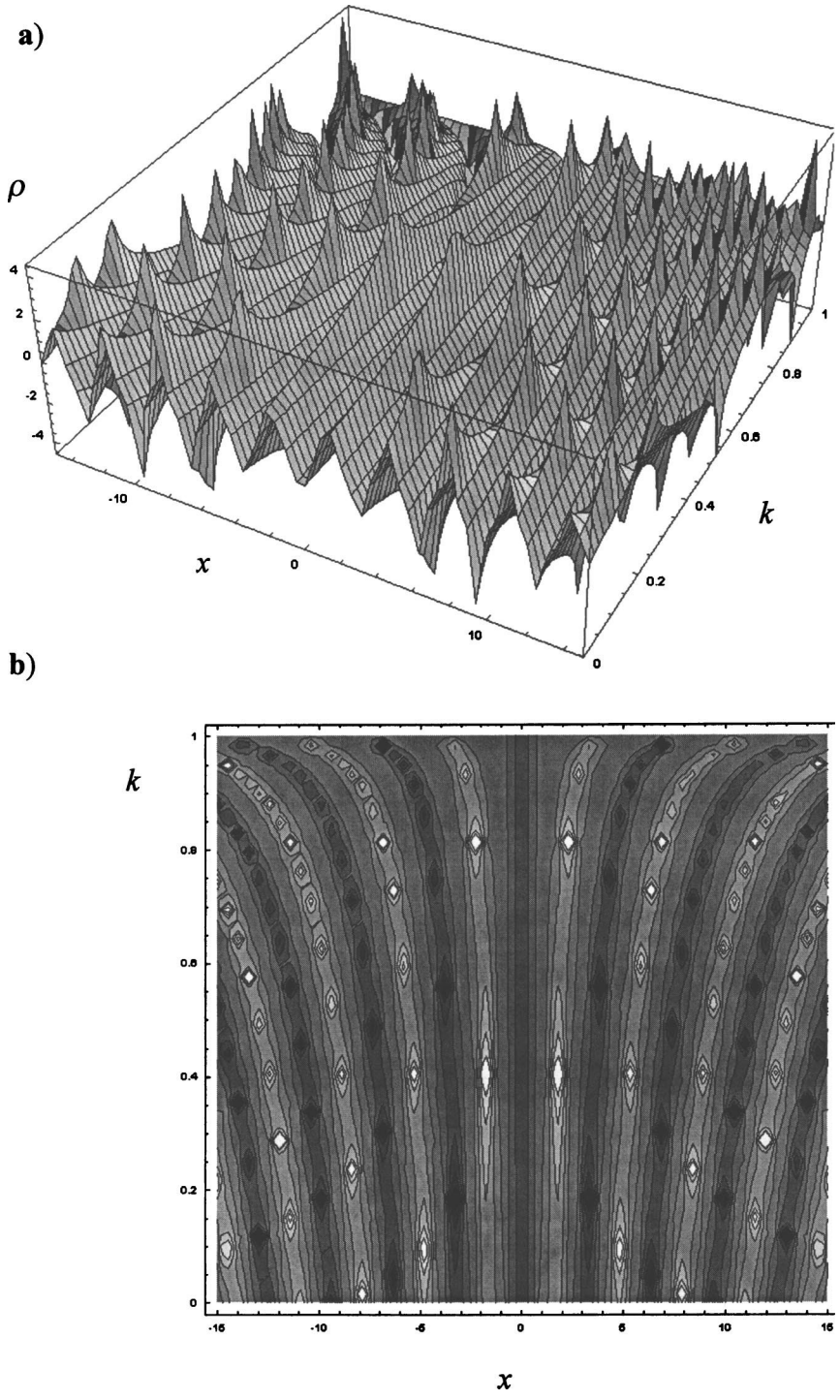

FIG. 9. (a) 3D dependence of the density (75) on x and k. (b) 2D dependence of the density (75) on x and k.

(iv) One defines a stable vortex lattice of bipolaron type by means of the potential (63) and one specifies some of its properties (the equipotential curves, the fractal dimensions variation, etc). In such a context, by an iterated map, one builds the superconducting fractal.

(v) One demonstrates that the superconducting pairs are 1D projections of this fractal. Mathematically, the problem resumes to the determination of the probability field obtained by identi-

fying the quantum potential (12) with the projection on Ox axis of complex potential (63). It results the splitting of the probability field that in our opinion corresponds to a superconducting pair (Cooper pair). In such a context, one gives an evaluation of the coherence length.

(vi) The superconductivity in such structures is achieved through the coherence on the subquantum medium.

(vii) The temperature dependences of the superconducting parameters are given and the concordances with experimental data and other theories are analyzed.

(viii) If $S=\text{const}$ and $\nabla\cdot\mathbf{u}=\Delta\ln\rho=0$ (the quantum fluid is incompressible), the 1D Eq. (22) admits for $E=A=\text{const}$ the speed fields

$$u_x = i[(2A/m)(1-\rho)]^{1/2}.$$

Then, the quantum potential takes a very simple expression which is proportional to the density of states of the Cooper pairs, i.e.,

$$Q = -(mu_x^2/2) = A(1-\rho).$$

When the density of states of the Cooper pairs becomes zero (i.e., the material is normal) the quantum potential takes a finite value, A, and when it becomes 1 (i.e., the entire material becomes superconducting), the quantum potential turns to zero—the entire quantity of energy from the subquantic medium transfers to the superconducting pairs. Consequently, one can assume the energy from the background subquantic medium can be stoked by transforming all the particles from the environment into Cooper pairs and then "freezing" them. The superconductor acts like a subquantic medium energy accumulator.

(ix) In the SR theory the space–time of quantum mechanics is continuous and nondifferentiable. Nondifferentiability is induced by means of the fractal, a global mechanism when explaining superconductivity, the 2D projection of the fractal generates the mechanism responsible of the type II superconductivity (the anyonic mechanism[2]) and the 1D projection the mechanism responsible of the type I superconductivity (the Cooper pairs). In such a context, by means of the generalized coherence of the quantum fluid the superconducting parameters occur as intrinsic properties of this fluid.

ACKNOWLEDGMENTS

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APPENDIX A

Strictly, the nondifferentiability of the coordinates means that the velocity $V=\mathrm{d}X/\mathrm{d}t$ is no longer defined. However, continuity and nondifferentiability implies scale divergence.[5,14] Therefore, the basis of the method consists in replacing the classical velocity by a function that explicitly depends on the resolution, $V=V(\varepsilon)$. Only $V(\varepsilon)$ is undefined, while $V(\varepsilon)$ is now defined for any nonzero ε. The scale dependence of the velocity forces one to complete the standard equations of physics by differential equations of scale. The simplest possible equation that one can write for V is a first order, renormalization-group-like differential equation, written in terms of the dilatation operator $d/d\ln\varepsilon$,[5] in which the infinitesimal scale dependence of V is determined by the field V itself, namely,

$$\frac{\mathrm{d}V}{d\ln\varepsilon} = \Gamma(V). \tag{A1}$$

The -function here is *a priori* unknown, but we can use the fact that $V<1$ (in motion-relativistic units) to expand it in terms of a Taylor expansion. One obtains

$$\frac{dV}{d\ln\varepsilon} = a + bV + O(V^2), \tag{A2}$$

where a and b are constants (independent of ε, but possibly dependent on the space–time coordinates). Setting $b=-\delta$ and $a=r\delta$, we obtain the solution of this equation under the form

$$V = v + k\varepsilon^{-\delta}, \tag{A3}$$

where k is an integration constant (independent of ε). From the dimensional analysis, we can write it under the form $k=\zeta\lambda^{\delta}$, with $\_=\_(t)$ dimensionless, $\langle\zeta^2\rangle=1$ and $\_$ a constant length scale. We get

$$V = v + \zeta\left(\frac{\lambda}{\varepsilon}\right)^{\delta}. \tag{A4}$$

We recognize here a typical fractal behavior with fractal dimension $\mathbf{D}=\mathbf{D}_{\tau}+\delta$, where $\mathbf{D}_{\tau}$ is the topological dimension (=1 here, since the description concerns displacements along geodesical curves). However, at large scales $\varepsilon \gg \lambda$, the velocity shows a classical (i.e., scale independent) behavior, $V\approx v$, while at small scales $\varepsilon ll \lambda$, it shows a power law, scale divergent behavior $V \approx \zeta(\lambda\varepsilon^{-1})^{\delta}$. The transition scale $\_$ (that will be interpreted in what follows as the Compton scale) thus stands out as a fractal–nonfractal transition scale (that takes place not in space, but in the new resolution dimension).

The resolution ε in the above formula is a space resolution, $\varepsilon=\delta X$. We can relate it to time resolution by writing (A4) in the asymptotic domain $\varepsilon<\lambda$ under the form

$$\frac{\delta X}{c\,\delta t} \approx \left(\frac{\lambda}{\delta X}\right)^{\mathbf{D}-1}. \tag{A5}$$

This provides us with a fundamental, well-known formula on fractals,

$$\delta X^{\mathbf{D}} = \lambda^{\mathbf{D}-1} c\,\delta t. \tag{A6}$$

By reinserting this result in (A4), we obtain the following expression (where we have reinserted the indices) for the elementary displacement in terms of time-resolution:[5]

$$dX^i = v\,dt + \lambda^{l-1/\mathbf{D}}\zeta^i (c\,dt)^{1/\mathbf{D}}, \tag{A7}$$

where we have identified the time resolution with the time differential element.

As we shall see in what follows, the first terms yields classical physics while the second is one of the sources of quantum behavior. They are both present whatever the scale, but the classical term is dominant at large scales while the quantum term is dominant at small scales. Then, the quantum and classical laws are irreducible to each other, but they both find their origin in a single, more profound, scale-dependent description whose equations take the form given by (A1) in the simplest case. In the special case of fractal dimension $\mathbf{D}=2$, the time transition is easily identified with the de Broglie time scale $\tau\approx c\lambda/v^2=\hbar/mv^2$, by writing (A7) under the form

$$dX = v\,dt\left[-\zeta(c\lambda/v^2\,dt)^{1/2}\right], \tag{A8}$$

The nondifferentiable nature of space–time implies an even more dramatic consequence, namely, a breaking of differential time reflection invariance. Let us consider indeed the usual definition of the derivative of a given function with respect to time

$$\left(\frac{df}{dt}\right) = \lim_{dt\to 0}\frac{f(t+dt)-f(t)}{dt} = \lim_{dt\to 0}\frac{f(t)-f(t-dt)}{dt}. \tag{A9}$$

The two definitions are equivalent in the differentiable case. One passes from one to the other by the transformation $dt\to -dt$ (time reflection invariance at the infinitesimal level). In the nondiffer-

entiable situation considered here, both definitions fail, since the limits are no longer defined. The scale-relativistic method solves this problem in the following way.

We attribute to the differential element dt the new meaning of a variable, identified with a time resolution, $dt=\delta t$ (substitution principle). The passage to the limit $dt\to 0$ is actually devoid of physical meaning (an infinite energy would be needed to really perform a measurement at zero time resolution interval). The physics is now in the behavior of the function during the zoom operation on dt. The two functions f'_+ and f'_- are now defined as explicit functions of t and of dt,

$$f'_+(t,dt)=\frac{f(t+dt)-f(t)}{dt},$$
$$f'_-(t,dt)=\frac{f(t)-f(t-dt)}{dt}. \tag{A10}$$

When applied to the space variable, we get for each geodesic two velocities that are fractal functions of resolution, $v_+(t,dt)$ and $v_-(t,dt)$. In order to go back to the classical microscopic domain, we smooth out each geodesic with balls of radius larger than _ (the fractal/nonfractal transition), then we take the average on the whole set of geodesics. We get two mean velocities $v_+(t)=\langle v_+(t,dt\gg\tau)\rangle$ and $v_-(t)=\langle v_-(t,dt\gg\tau)\rangle$, but after this double averaging process, there is no reason for these two velocities to be equal, contrarily to what happens in the classical, differentiable case.[5]

In summary, while the concept of velocity was classically a single concept, we must introduce, if space–time is nondifferentiable, two velocities instead of one even when going back to the classical domain. Such a two valuedness of the velocity vector is a specific consequence of nondifferentiability that has no standard counterpart (in the sense of differential physics), since it finds its origin in a breaking of the symmetry ($dt\to -dt$). Such a symmetry was considered self-evident up to now in physics (since the differential element dt disappears when passing to the limit), so that it has not been analyzed on the same footing as the other well-known symmetries. Note that it is actually different from the time reflection symmetry T, even though infinitesimal irreversibility implies global irreversibility.

Now, at the level of our description, we have no way to favor v_+ rather than v_-. Both choices are equally qualified for the description of the laws on nature. The only solution to this problem is to consider both the forward ($dt>0$) and backward ($dt<0$) processes together. The number of degrees of freedom is doubled with respect to the classical, differentiable description (six velocity components instead of three).

A simple and natural way to account for this doubling of the needed information consists in complex number and the complex product. As we shall recall hereafter, this is the origin of the complex nature of the wave function in quantum mechanics, since the probability amplitude is defined in terms of the complex action that is naturally introduced in such a theory. But one can demonstrate that the complex calculus is nothing but a particular choice of representation that achieves the simplest description. Namely, using a different product would introduce additional terms in the Schrödinger equation.[5] Note also that the new complex process, as a whole, recovers the fundamental property of microscopic reversibility.

We then can write

$$dX^i_\pm = dx^i_\pm + d\xi^i_\pm, \tag{A11}$$

respectively, for the forward process (+) and backward process (−). From our above discussion, the fluctuation $d\zeta_\pm$ is written

$$\left\langle \frac{\mathrm{d}\xi_{\pm}^{i}}{\mathrm{d}t}\frac{\mathrm{d}\xi_{\pm}^{j}}{\mathrm{d}t}\right\rangle = \pm\,\delta^{ij}c^{2}\left(\frac{\lambda}{c\,\mathrm{d}t}\right)^{2-2/\mathbf{D}}. \tag{A12}$$

This relation is invariant under translations and rotations in space between Cartesian coordinate systems. In the special, Galilean scale-relativistic case that we consider here, the scale invariant is the fractal dimension itself. The fractal dimension of typical quantum mechanical paths is $\mathbf{D}=2$. We shall reduce our discussion in what follows to this particular case. When $\mathbf{D}=2$, (A12) becomes

$$\left\langle \mathrm{d}\xi_{\pm}^{i}\mathrm{d}\xi_{\pm}^{j}\right\rangle = \pm\,\lambda\delta^{ij}c\,\mathrm{d}t. \tag{A13}$$

We can now jump to the second step of the fractal-space description, by constructing the covariant derivative that describes the combined effects of the new displacement laws and scale laws. We define mean forward (+) and backward (−) derivatives, which, once applied to x', yield the above forward and backward mean velocities

$$\frac{d_{+}x^{i}(t)}{\mathrm{d}t} = v_{+}^{i}, \tag{A14a}$$

$$\frac{d_{-}x^{i}(t)}{\mathrm{d}t} = v_{-}^{i}. \tag{A14b}$$

The averaging is here taken on the family of geodesics. As a consequence, the Born statistical interpretation of quantum mechanics will be ensured from the very beginning of our construction, since the particle can be identified with one random geodesic among their infinite set (more generally, with the subset of the geodesics that share the geometric properties that correspond to a given measurement result). The forward and backward derivatives of (A14a) and (A14b) can be combined in terms of a complex derivative operator,[5]

$$\frac{\delta}{\mathrm{d}t} = \frac{(d_{+}+d_{-})-i(d_{+}-d_{-})}{2\,\mathrm{d}t} \tag{A15}$$

which, when applied to the position vector, yields a complex velocity

$$\mathbf{V}^{i} = \frac{\delta}{\mathrm{d}t}x^{i} = \mathbf{V}^{i} - iU^{i} = \frac{v_{+}^{i}+v_{-}^{i}}{2} - i\frac{v_{+}^{i}-v_{-}^{i}}{2}. \tag{A16}$$

Consider a function $f(X,t)$, and expand its total differential to second order. We get

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \nabla f\cdot\frac{\mathrm{d}X}{\mathrm{d}t} + \frac{1}{2}\sum_{i,j}\frac{\partial^{2}f}{\partial x_{i}\,\partial x_{j}}\frac{\partial X_{i}\,\partial X_{j}}{\mathrm{d}t}. \tag{A17}$$

We may now compute the forward and backward derivatives of f. In this averaging procedure, the mean value of $\mathrm{d}X_{i}/\mathrm{d}t$ amount to $d_{\pm}x_{i}/\mathrm{d}t = v_{\pm i}$, while $\langle \mathrm{d}X_{i}\,\mathrm{d}X_{j}\rangle$ reduces to $\langle \mathrm{d}\xi_{\pm i}\,\mathrm{d}\xi_{\pm j}\rangle$, so that the last term of (A17) amounts to a Laplacian thanks to (A13). We obtain

$$d_{\pm}f/\mathrm{d}t = \partial/\partial t + v_{\pm}\tfrac{1}{2}\lambda c\Delta. \tag{A18}$$

By combining them we get our final expression for the complex scale-covariant derivative,

$$\frac{\delta}{\mathrm{d}t} = \frac{\partial}{\partial t} + \mathbf{V}\cdot\nabla - i\frac{1}{2}\lambda c\Delta. \tag{A19}$$

We now apply the principle of scale covariance, and postulate that the passage from classical (differentiable) mechanics to the new nondifferentiable mechanics that is considered here can be implemented by replacing the standard time derivative $d/\mathrm{d}t$ by the complex operator $\delta/\mathrm{d}t$. As a

consequence, we are now able to write the equation of geodesics of the fractal space under its covariant form,

$$\frac{\delta^2}{dt^2}x^i = 0. \tag{A20}$$

In the present paper between λ and D measures,

$$D = \tfrac{1}{2}\lambda c. \tag{A21}$$

APPENDIX B

Let us consider a quantum fluid of identical particles. To each particle of fluid one can associate by means of its spin the vector potential $\mathbf{A}$ and the vortex field $\mathbf{\Omega}$,

$$\mathbf{A} = \mathrm{curl}(\Gamma\hat{\sigma}/r), \tag{B1a}$$

$$\mathbf{U} = \mathrm{curl}\,\mathbf{A}, \tag{B1b}$$

and by self-interaction the potential

$$W = -\Gamma\hat{\sigma}\cdot\grave{\mathbf{U}} = \Gamma^2[\hat{\sigma}\,\mathrm{curl}\,\mathrm{curl}(\hat{\sigma}/r)] = \Gamma^2[(\hat{\sigma}\cdot\nabla)(\hat{\sigma}\cdot\nabla)(1/r) - (\hat{\sigma}\cdot\hat{\sigma})\nabla^2(1/r)]. \tag{B2}$$

Since

$$(\hat{\sigma}\cdot\nabla)(\hat{\sigma}\cdot\nabla) = (1/3)(\hat{\sigma}\cdot\hat{\sigma})\nabla^2, \tag{B3a}$$

$$\nabla^2(1/r) = -4\pi\delta(r), \tag{B3b}$$

one gets

$$W = (8\pi/3)\Gamma^2(\hat{\sigma}\cdot\hat{\sigma})\delta(r). \tag{B4}$$

Then, the mean value of the potential is

$$U = \langle W\rangle = \frac{8\pi}{3}\Gamma^2(\hat{\sigma}\cdot\hat{\sigma})\int \psi^*\delta(r)\psi d^3x = A(\Gamma,\hat{\sigma})|\psi(0)|^2. \tag{B5}$$

In the previous relations, $\mathbf{i}=\Gamma\hat{\sigma}$ is the vortex momentum, Γ is the vortex constant, and $A(\Gamma,\hat{\sigma})$ is a constant. Consequently, assimilating the quantum fluid particles with vortex type objects, the potential U will be proportional with the concentration of the particles.

APPENDIX C

$\underline{\Omega}(u)=\underline{\Omega}(u')$ if and only if between u and u' it exists the transformation $u=(au'+b)/(cu'+d), a,b,c,d\in N, ad-bc=1$, with $u=(\omega_2/\omega_1), u'=(\omega'_2/\omega'_1)$, and $(\omega_1,\omega_2)(\omega'_1,\omega'_2)$ the fundamental periods pairs of a two equivalent elliptic function (sn dn/cn) (the equivalence theorem of elliptic functions[7]).

Let us consider a transformation element in the matrix form

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

Under the special conditions $c=1, d=0$ we can calculate the eigenvalues as follows: The characteristic equation of this matrix is

$$\begin{pmatrix} a-\lambda & b \\ 1 & -\lambda \end{pmatrix} = 0,$$

$$\lambda^2 - a\lambda - b = 0, \quad \lambda_{1,2} = \tfrac{1}{2}[a \pm (a^2 + 4b)^{1/2}].$$

For different values of a and b we obtain members which are irrational numbers. Let us begin with the quadratic equations and $b=1$ or $b=-1$. In this case, the quadratic equations are of the following type: $x^2-a_nx-1=0, x^2-a_nx+1=0$ or $x^2-a_nx+(-1)^n=0$. For $a_1=1, a_2=3, a_3=4, a_4=7$ one finds

$$a_1 = 1, \quad x^2 - 1x - 1 = 0, \quad x_1^{(1)} = -\phi, \quad x_2^{(1)} = 1/\phi = (1 + \phi),$$

$$a_2 = 3, \quad x^2 - 3x + 1 = 0, \quad x_1^{(2)} = \phi^2, \quad x_2^{(2)} = 1/\phi^2 = (3 - \phi^2),$$

$$a_3 = 4, \quad x^2 - 4x - 1 = 0, \quad x_1^{(3)} = -\phi^3, \quad x_2^{(3)} = 1/\phi^3 = (4 + \phi^3),$$

$$a_2 = 7, \quad x^2 - 7x + 1 = 0, \quad x_1^{(4)} = \phi^4, \quad x_2^{(4)} = 1/\phi^4 = (7 - \phi^4).$$

Consequently, one can write that for $a_n=a_{n-2}+a_{n-1}, a_1=1, a_2=3, n>2$, one finds $x^2-a_nx+(-1)^n=0, x_1^{(n)}=(-\phi)^n, x_2^{(n)}=1/\phi^n=(a_{n-2}+a_{n-1})+(-1)^{n-1}\phi^n$.

Under these special conditions we obtain the irrational roots, $x_1^{(n)}=(-\phi)^n, x_2^{(n)}=(1/\phi)^n$ which are contained in the limit set. This clearly shows the connection between the geometry induced by the previous transformation, KAM theorem, the VAK and El Naschie's $\varepsilon^{(\infty)}$ theory for determining the mass spectrum of high elementary particles as a function of the golden mean $\phi=(\sqrt{5}-1)/2$.[16] Consequently, the vortex coherence in the lattice implies the $\varepsilon^{(\infty)}$ space.

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Representation of the contextual statistical model by hyperbolic amplitudes

Andrei Khrennikov[a)]
MSI, University of Växjö, S-35195, Sweden

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We continue the development of a so-called contextual statistical model (here context has the meaning of a complex of physical conditions). It is shown that, besides contexts producing the conventional trigonometric cos-interference, there exist contexts producing the hyperbolic cos-interference. Starting with the corresponding interference formula of total probability we represent such contexts by hyperbolic probabilistic amplitudes or in the abstract formalism by normalized vectors of a hyperbolic analogue of the Hilbert space. There is obtained a hyperbolic Born's rule. Incompatible observables are represented by noncommutative operators. This paper can be considered as the first step towards hyperbolic quantum probability. We also discuss possibilities of experimental verification of hyperbolic quantum mechanics: in physics of elementary particles, string theory as well as in experiments with nonphysical systems, e.g., in psychology, cognitive sciences, and economy. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1931042]

I. INTRODUCTION

In Ref. 1 there was presented a so-called contextual viewpoint of the origin of quantum (conditional) probabilities (here a *context* has the meaning of a complex of physical conditions). Such an approach gives the possibility to unify classical Kolmogorov (measure theoretical) and quantum (Hilbert space) probability theories by constructing a natural representation of the Kolmogorov model in a complex Hilbert space. Thus in the contextual approach quantum probabilistic behavior (in particular, *interference of probabilities*) is simply a consequence of a very special representation of Kolmogorov probabilities—by complex amplitudes (vectors in a complex Hilbert space). Each representation is based on a fixed pair of observables (Kolmogorov random variables) *a* and *b—reference observables*—which produce the contextual image of a Kolmogorov probability space in a complex Hilbert space. The crucial point is that all Kolmogorov probabilities should be considered as conditional (or better to say contextual) probabilities, cf. Accardi,[2–4] Ballentine,[5,6] W. De Muynck,[7,8] S. Gudder,[9,10] A. Lande,[11] G. Mackey.[12]

In Ref. 1 we introduced a class $\mathcal{C}^{\mathrm{tr}}$ of contexts ("trigonometric contexts") which can be represented by complex probabilistic amplitudes inducing the representation in the complex Hilbert space. The $\mathcal{C}^{\mathrm{tr}}$ consists of context producing the conventional trigonometric cos-interference. However, in general the set of contexts is not reduced to the class of trigonometric contexts $\mathcal{C}^{\mathrm{tr}}$. There exist contexts producing the hyperbolic cosh-interference. The set of hyperbolic contexts is denoted by the symbol $\mathcal{C}^{\mathrm{hyp}}$.

In this paper we show that it is possible to represent contexts belonging to $\mathcal{C}^{\mathrm{hyp}}$ by so-called *hyperbolic amplitudes*. Such amplitudes take values in the set of "hyperbolic numbers" (two-dimensional Clifford algebra). It will be demonstrated that in the hyperbolic framework we can proceed quite far in the same directions as in the trigonometric framework. We obtain hyperbolic analogues of the interference of probabilities, probability amplitudes, Born's rule, representation

[a)]International Center for Mathematical Modeling in Physics and Cognitive Sciences. Electronic mail: andrei.khrennikov@msi.vxu.se; supported by EU-Network QP and Applications.

of incompatible observables by noncommuting operators. The crucial difference between two representations is that in the hyperbolic case the principle of superposition is violated.

II. CONTEXTUAL VIEWPOINT TO THE KOLMOGOROV MODEL AND INTERFERENCE OF PROBABILITIES

In this section we repeat the main points of contextual measure-theoretical approach to interference of probabilities, see Ref. 1 for details.

Let $(\Omega,\mathcal{F},\mathbf{P})$ be a Kolmogorov probability space: Ω is an arbitrary set, $\mathcal{F}$ is a σ-field of subsets of Ω and $\mathbf{P}$ is a countably additive measure on $\mathcal{F}$ taking values in $[0, 1]$ and normalized by one (Kolmogorov probability). By the standard Kolmogorov axiomatics sets $A\in\mathcal{F}$ represent *events*. In our simplest model of *contextual probability* (which can be called the Kolmogorov contextual space) the same system of sets, $\mathcal{F}$, is used to represent complexes of experimental physical conditions—*contexts*.

Thus depending on circumstances a set $O\in\mathcal{F}$ will be interpreted either as event or as context. We shall sharply distinguish events and contexts on phemenological level, but we shall use the same mathematical object $\mathcal{F}$ to represent both events and contexts in a mathematical model. In principle, in a mathematical model events and contexts can be represented by different families of sets, e.g., in Renye's model. We will not do this from the beginning. But later we will fix families of contexts, e.g., $\mathcal{C}^{\text{tr}}$ or $\mathcal{C}^{\text{hyp}}$, which are proper subfamilies of $\mathcal{F}$.

The conditional probability is mathematically defined by the Bayes' formula: $\mathbf{P}(A/C)=\mathbf{P}(AC)/\mathbf{P}(C)$, $P(C)\neq 0$. In our contextual model this probability has the meaning of the probability of occurrence of the event A under the complex of physical conditions C. Thus it would be more natural to call $\mathbf{P}(A/C)$ a *contextual probability* and not *conditional probability*. Roughly speaking to find $\mathbf{P}(A/C)$ we should find parameters ω^A favoring for the occurrence of the event A among parameters ω^C describing the complex of physical conditions C.

Let $\mathcal{A}=\{A_n\}$ be finite or countable *complete group of disjoint contexts* (or in the event-terminology—complete group of disjoint events),

$$A_iA_j=\emptyset,\quad i\neq j,\quad \cup_i A_i=\Omega.$$

Let $B\in\mathcal{F}$ be an event and $C\in\mathcal{F}$ be a context and let $\mathbf{P}(C)>0$. We have the standard *formula of total probability:* $\mathbf{P}(B/C)=\Sigma_n\mathbf{P}(A_n/C)\mathbf{P}(B/A_nC)$. Let $a=a_1,\ldots,a_n$ and $b=b_1,\ldots,b_n$ be discrete random variables. Then

$$\mathbf{P}(b=b_i/C)=\sum_n \mathbf{P}(a=a_n/C)\mathbf{P}(b=b_i/a=a_n,C). \tag{1}$$

We remark that sets

$$B_x=\{\omega\in\Omega: b(\omega)=x\}\quad \text{and } A_y=\{\omega\in\Omega: a(\omega)=y\} \tag{2}$$

have two different interpretations. On the one hand, these sets represent events corresponding to occurrence of the values $b=x$ and $a=y$, respectively. On the other hand, they represent contexts (complexes of physical conditions) corresponding to selections of physical systems with respect to values $b=x$ and $a=y$, respectively. The main problem with the formula of total probability is that in general it is impossible to construct a context "A_yC" corresponding to a selection with respect to the value $a=y$ which would not disturb systems prepared by the context C. But only in the absence of disturbance we can use the set theoretical operation of intersection. This paper would like to modify the formula of total probability by eliminating sets "A_yC" which in general do not represent physically realizable contexts.

A set C belonging to $\mathcal{F}$ is said to be a *nondegenerate context* with respect to $\mathcal{A}=\{A_n\}$ if $\mathbf{P}(A_nC)\neq 0$ for all n. We denote the set of such contexts by the symbol $\mathcal{C}_{\mathcal{A},\text{nd}}$.

Let $\mathcal{A}=\{A_n\}$ and $\mathcal{B}=\{B_n\}$ be two complete groups of disjoint contexts. They are said to be *incompatible* if $\mathbf{P}(B_nA_k)\neq 0$ for all n and k. Thus $\mathcal{B}$ and $\mathcal{A}$ are incompatible iff every B_n is a nondegenerate context with respect to $\mathcal{A}$ and vice versa. Random variables a and b inducing, see

(2), incompatible complete groups $\mathcal{A}=\{A_n\}$ and $\mathcal{B}=\{B_n\}$ of disjoint contexts are said to be *incompatible random variables.*

Theorem 2.1: (Interference formula of total probability) *Let* $\mathcal{A}=\{A_1,A_2=\Omega\backslash A_1\}$ *and* $\mathcal{B}=\{B_1,B_2=\Omega\backslash B_1\}$ *be incompatible and let a context* $C\in\mathcal{C}_{\mathcal{A},\mathrm{nd}}$. *Then, for any* $B\in\mathcal{B}$,

$$\mathbf{P}(B/C)=\sum_{j=1}^{2}\mathbf{P}(A_j/C)\mathbf{P}(B/A_j)+2\lambda(B/\mathcal{A},C)\sqrt{\prod_{j=1}^{2}\mathbf{P}(A_j/C)\mathbf{P}(B/A_j)},$$

where

$$\lambda(B/\mathcal{A},C)=\frac{\mathbf{P}(B/C)-\sum_{j=1}^{2}\mathbf{P}(B/A_j)\mathbf{P}(A_j/C)}{2\sqrt{\mathbf{P}(A_1/C)\mathbf{P}(B/A_1)\mathbf{P}(A_2/C)\mathbf{P}(B/A_2)}}.$$

To prove the theorem, we set the expression for λ into the sum and obtain identity. In fact, this formula is just a representation of the probability $\mathbf{P}(A/C)$ in a special way. The $\lambda(B/\mathcal{A},C)$ are called *coefficients of statistical disturbance.* We shall use at few occasions the following result:

Lemma 2.1: *Let conditions of Theorem 2.1 hold true. Then*

$$\sum_{k}\lambda(B_k/\mathcal{A},C)\sqrt{\mathbf{P}(A_1/C)\mathbf{P}(A_2/C)\mathbf{P}(B_k/A_1)\mathbf{P}(B_k/A_2)}=0. \tag{3}$$

Proof: We have

$$1=\sum_{k}\mathbf{P}(B_k/C)=\sum_{k}\sum_{n}\mathbf{P}(A_n/C)\mathbf{P}(B_k/A_n)+\sum_{k}\lambda(B_k/\mathcal{A},C)\sqrt{\mathbf{P}(A_1/C)\mathbf{P}(A_2/C)\mathbf{P}(B_k/A_1)\mathbf{P}(B_k/A_2)}.$$

But $\Sigma_n(\Sigma_k\mathbf{P}(B_k/A_n))\mathbf{P}(A_n/C)=1$.

(1) Suppose that for every $B\in\mathcal{B}$, $|\lambda(B/\mathcal{A},C)|\leqslant 1$. In this case we can introduce statistical parameters $\theta(B/\mathcal{A},C)\in[0,2\pi]$ and represent the coefficients of statistical disturbance in the trigonometric form, $\lambda(B/\mathcal{A},C)=\cos\theta(B/\mathcal{A},C)$. Parameters $\theta(B/\mathcal{A},C)$ are said to be *relative phases* of an event B with respect to $\mathcal{A}$ (in the context C). We have the following interference formula of total probability,

$$\mathbf{P}(B/C)=\sum_{j=1}^{2}\mathbf{P}(A_j/C)\mathbf{P}(B/A_j)+2\cos\theta(B/\mathcal{A},C)\sqrt{\prod_{j=1}^{2}\mathbf{P}(A_j/C)\mathbf{P}(B/A_j)}.$$

This is nothing other than the famous *formula of interference of probabilities.*

In Ref. 1 there was shown that by starting with this formula we can construct the representation of the set of trigonometric contexts

$$\mathcal{C}^{\mathrm{tr}}=\{C\in\mathcal{C}_{a,\mathrm{nd}}:|\lambda(B_j/a,c)|\leqslant 1,j=1,2\}$$

in the complex Hilbert space, obtain Born's rule and represent incompatible variables a and b by (noncommutative) operators.

(2) Suppose that for every $B\in\mathcal{B}$, $|\lambda(B/\mathcal{A},C)|\geqslant 1$. In this case we can introduce statistical parameters $\theta(B/\mathcal{A},C)\in(-\infty,+\infty)$ and represent the coefficients of statistical disturbance in the trigonometric form, $\lambda(B/\mathcal{A},C)=\pm\cosh\theta(B/\mathcal{A},C)$. Parameters $\theta(B/\mathcal{A},C)$ are said to be hyperbolic *relative phases.* In this case we obtain the formula of total probability with hyperbolic cosh-interference,

$$\mathbf{P}(B/C)=\sum_{j=1}^{2}\mathbf{P}(A_j/C)\mathbf{P}(B/A_j)\pm 2\cosh\theta(B/\mathcal{A},C)\sqrt{\prod_{j=1}^{2}\mathbf{P}(A_j/C)\mathbf{P}(B/A_j)}. \tag{4}$$

The aim of this paper is to show that by starting with this formula we can construct the representation of the set of hyperbolic contexts,

$$\mathcal{C}^{\text{hyp}} = \{C \in \mathcal{C}_{a,\text{nd}} : |\lambda(B_j/a,c)| \geqslant 1, j = 1,2\}$$

in the hyperbolic Hilbert space, obtain an analogue of Born's rule and represent incompatible variables a and b by (noncommutative) operators.

We can also consider the case of mixed hypertrigonometric behavior, one of the coefficients is larger than 1 and one is smaller than 1. However, in this paper we shall discuss only the case of the hyperbolic interference.

In our further considerations the complete groups of disjoint contexts $\mathcal{A}$ and $\mathcal{B}$ will correspond to some incompatible random variables a and b. We shall use the symbols $\lambda(b=x/a,C)$ instead of $\lambda(b=x/\mathcal{A},C)$.

III. REPRESENTATION OF CONTEXTS BY HYPERBOLIC AMPLITUDES, HYPERBOLIC HILBERT SPACE REPRESENTATION

Everywhere below we study contexts producing the hyperbolic interference for incompatible dichotomous random variables $a=a_1$, a_2, $b=b_1$, b_2. This pair of variables will be fixed. We call such variables reference variables. For each pair a, b of reference variables we construct a representation of the set of contexts $\mathcal{C}^{\text{hyp}}$ in hyperbolic Hilbert space ("quantumlike representation").

A. Hyperbolic algebra

Instead of the field complex numbers **C**, we shall use so-called hyperbolic numbers, namely the two-dimensional Clifford algebra, **G**. We call this algebra *hyperbolic algebra*.

Remark 3.1: Of course, it is rather dangerous to invent an own name for a notion established almost as firm as complex numbers. We use a new name, hyperbolic algebra, for the well-known algebraic object, the two-dimensional Clifford algebra, by the following reasons. First we explain why we dislike to use the standard notion Clifford algebra in this particular case. The standard Clifford machinery was developed around noncommutative features of general Clifford algebras. The two-dimensional Clifford algebra, hyperbolic algebra in our terminology, is commutative. Commutativity of **G** is very important in our considerations. We now explain why we propose the name hyperbolic algebra. Hyperbolic functions are naturally related to the algebraic structure of **G** through a hyperbolic generalization of Euler's formula for the complex numbers. This is the crucial point of our considerations—the possibility to use this algebraic structure to represent some special transformations for hyperbolic functions.

Denote by the symbol j the generator of the algebra **G** of hyperbolic numbers,

$$j^2 = 1.$$

The algebra **G** is the two-dimensional real algebra with basis $e_0=1$ and $e_1=j$. Elements of **G** have the form $z=x+jy$, $x, y \in \mathbf{R}$. We have $z_1+z_2=(x_1+x_2)+j(y_1+y_2)$ and $z_1z_2=(x_1x_2+y_1y_2)+j(x_1y_2+x_2y_1)$. This algebra is commutative. It is not a field—not every element has the inverse one.

We introduce an involution in **G** by setting $\overline{z}=x-jy$ and set $|z|^2=z\overline{z}=x^2-y^2$. We remark that $|z|=\sqrt{x^2-y^2}$ is not well defined for an arbitrary $z \in \mathbf{G}$. We set $\mathbf{G}_+=\{z \in \mathbf{G}: |z|^2 \geqslant 0\}$. We remark that $\mathbf{G}_+$ is a multiplicative semigroup as follows from the equality

$$|z_1z_2|^2 = |z_1|^2|z_2|^2.$$

Thus, for $z_1, z_2 \in \mathbf{G}_+$, we have that $|z_1z_2|$ is well defined and $|z_1z_2|=|z_1||z_2|$. We define a hyperbolic exponential function by using a hyperbolic analogue of the Euler's formula,

$$e^{j\theta} = \cosh\theta + j\sinh\theta, \theta \in \mathbf{R}.$$

We remark that

$$e^{j\theta_1}e^{j\theta_2} = e^{j(\theta_1+\theta_2)}, \quad \overline{e^{j\theta}} = e^{-j\theta}, \quad |e^{j\theta}|^2 = \cosh^2\theta - \sinh^2\theta = 1.$$

Hence, $z = \pm e^{j\theta}$, always belongs to $\mathbf{G}_+$. We also have

$$\cosh\theta = \frac{e^{j\theta}+e^{-j\theta}}{2}, \quad \sinh\theta = \frac{e^{j\theta}-e^{-j\theta}}{2j}.$$

We set $\mathbf{G}_+^* = \{z \in \mathbf{G}_+ : |z|^2 > 0\}$. Let $z \in \mathbf{G}_+^*$. We have

$$z = |z|(x/|z|) + j(y/|z|) = \operatorname{sign} x|z|\left(\frac{x \operatorname{sign} x}{|z|} + j\frac{y \operatorname{sign} x}{|z|}\right).$$

As $(x^2/|z|^2) - (y^2/|z|^2) = 1$, we can represent $x \operatorname{sign} x = \cosh\theta$ and $y \operatorname{sign} x = \sinh\theta$, where the phase θ is unequally defined. We can represent each $z \in \mathbf{G}_+^*$ as

$$z = \operatorname{sign} x|z|e^{j\theta}.$$

By using this representation we can easily prove that $\mathbf{G}_+^*$ is a multiplicative group. Here $1/z = -(\operatorname{sign} x/|z|)e^{-j\theta}$. The unit circle in $\mathbf{G}$ is defined as $S_1 = \{z \in \mathbf{G} : |z|^2 = 1\} = \{z = \pm e^{j\theta}, \theta \in (-\infty, +\infty)\}$. It is a multiplicative subgroup of $\mathbf{G}_+^*$.

To construct a $\mathbf{G}$-linear representation of the set $\mathcal{C}^{\mathrm{hyp}}$ of hyperbolic contexts, we shall use the following elementary formula:

$$D = A + B \pm 2AB\cosh\theta = |\sqrt{A} \pm e^{j\theta}\sqrt{B}|^2, \tag{5}$$

for real coefficients $A, B > 0$.

B. Hyperbolic probability amplitude, hyperbolic Born's rule

We set $Y = \{a_1, a_2\}$, $X = \{b_1, b_2\}$ ("spectra" of random variables a and b). Let $C \in \mathcal{C}^{\mathrm{hyp}}$. We set

$$p_C^a(y) = \mathbf{P}(a = y/C), \quad p_C^b(x) = \mathbf{P}(b = x/C), \quad p(x/y) = \mathbf{P}(b = x/a = y),$$

$x \in X$, $y \in Y$. The interference formula of total probability (4) can be written in the following form:

$$p_C^b(x) = \sum_{y \in Y} p_C^a(y)p(x/y) \pm 2\cosh\theta_C(x)\sqrt{\Pi_{y\in Y}p_C^a(y)p(x/y)}, \tag{6}$$

where $\theta_C(x) = \theta(b = x/a, C) = \pm\operatorname{arccosh}|\lambda(b = x/a, C)|$, $x \in X$, $C \in \mathcal{C}^{\mathrm{hyp}}$. Here the coefficient λ is defined by

$$\lambda(b = x/a, C) = \frac{p_C^b(x) - \sum_{y\in Y} p_C^a(y)p(x/y)}{2\sqrt{\Pi_{y\in Y}p_C^a(y)p(x/y)}}. \tag{7}$$

By using (5) we can represent the probability $p_C^b(x)$ as the square of the hyperbolic amplitude,

$$p_C^b(x) = |\varphi_C(x)|^2, \tag{8}$$

where

$$\varphi(x) \equiv \varphi_C(x) = \sqrt{p_C^a(a_1)p(x/a_1)} + \epsilon_C(x)e^{j\theta_C(x)}\sqrt{p_C^a(a_2)p(x/a_2)}. \tag{9}$$

Here $\epsilon_C(x) = \operatorname{sign}\lambda(x/a, C)$. We remark that by Lemma 2.1,

$$\sum_{x\in X} \epsilon_C(x) = 0. \tag{10}$$

Thus we have a *hyperbolic generalization of Born's rule* for the b variable, see (8).

C. Hyperbolic Hilbert space

Hyperbolic Hilbert space is **G**-linear space (module) **E** with a **G**-linear scalar product, a map $(\cdot,\cdot) : \mathbf{E}\times\mathbf{E}\to\mathbf{G}$ that is

(1) linear with respect to the first argument, $(az+bw,u)=a(z,u)+b(w,u)$, $a, b\in\mathbf{G}$, $z, w, u\in\mathbf{E}$;
(2) symmetric, $(z,u)=\overline{(u,z)}$;
(3) nondegenerate, $(z,u)=0$ for all $u\in\mathbf{E}$ iff $z=0$.

Remark 3.2: If we consider **E** as just a **R**-linear space, then $(\cdot,\cdot)$ is a bilinear form which is not positive defined. In particular, in the two-dimensional case we have the signature $(+,-,+,-)$.

D. Hyperbolic Hilbert space representation

We introduce the space $\Phi(X,\mathbf{G})$ of functions, $\varphi: X\to\mathbf{G}$. Since $X=\{b_1,b_2\}$, the $\Phi(X,\mathbf{G})$ is the two-dimensional **G** module. We define the **G**-scalar product by

$$(\varphi,\psi)=\sum_{x\in X}\varphi(x)\overline{\psi}(x) \tag{11}$$

with conjugation in the algebra **G**. The system of Dirac δ-functions $\{e_x^b\equiv\delta_x\}_{x\in X}$ is an orthonormal basis in the hyperbolic Hilbert space $H^{\mathrm{hyp}}=(\Phi(X,\mathbf{G}),(\cdot,\cdot))$. Thus we have the hyperbolic analogue of the Born's rule in H^{hyp},

$$p_C^b(x)=|(\varphi_C,e_x^b)|^2. \tag{12}$$

Let $X\subset R$. By using the hyperbolic Hilbert space representation (12) of the Born's rule we obtain the hyperbolic Hilbert space representation of the expectation of the (Kolmogorovian) random variable b,

$$E(b/C)=\sum_{x\in X}xp_C^b(x)=\sum_{x\in X}x|\varphi_C(x)|^2=\sum_{x\in X}x(\varphi_C,e_x^b)\overline{(\varphi_C,e_x^b)}=(\hat{b}\varphi_C,\varphi_C), \tag{13}$$

where the (self-adjoint) operator $\hat{b}: H^{\mathrm{hyp}}\to H^{\mathrm{hyp}}$ is determined by its eigenvectors, $\hat{b}e_x^b=xe_x^b$, $x\in X$. This is the multiplication operator in the space of **G**-valued functions $\Phi(X,\mathbf{G})$,

$$\hat{b}\varphi(x)=x\varphi(x).$$

By (13) the conditional expectation of the Kolmogorovian random variable b is represented with the aid of the self-adjoint operator $\hat{b}$.

Thus we constructed a **G**-linear representation of the contextual Kolmogorov model,

$$J^{b/a}:\mathcal{C}^{\mathrm{hyp}}\to H^{\mathrm{hyp}}.$$

We set $S_{\mathcal{C}^{\mathrm{hyp}}}=J^{b/a}(\mathcal{C}^{\mathrm{hyp}})$. This is a subset of the unit sphere S of the Hilbert space H^{hyp}. We introduce the coefficients

$$u_j^a=\sqrt{p_C^a(a_j)},\quad u_j^b=\sqrt{p_C^b(b_j)},\quad p_{ij}=p(b_j/a_i),\quad u_{ij}=\sqrt{p_{ij}},\quad \theta_j=\theta_C(b_j), \tag{14}$$

and $\epsilon_i=\epsilon(b_i)$. We remark that the coefficients u_j^a, u_j^b depend on a context C; so $u_j^a=u_j^a(C)$, $u_j^b=u_j^b(C)$. We also consider the *matrix of transition probabilities* $\mathbf{P}^{b/a}=(p_{ij})$. It is always a *stochastic matrix*, $p_{i1}+p_{i2}=1$, $i=1,2$. In further considerations we shall also consider *double stochastic matrices*, $p_{1j}+p_{2j}=1$, $j=1,2$.

We represent a state φ_C by $\varphi_C=v_1^be_1^b+v_2^be_2^b$, where $v_i^b=u_1^au_{1i}+\epsilon_iu_2^au_{2i}e^{j\theta_i}$. So

$$p_C^b(b_i) = |v_i^b|^2 = |u_1^a u_{1i} + \epsilon_i u_2^a u_{2i} e^{j\theta_i}|^2.$$

This is the **G**-linear representation of the hyperbolic interference of probabilities. This formula can also be derived in the formalism of the hyperbolic Hilbert space, see Sec. IV. We remark that here the **G**-linear combination $u_1^a u_{1i} + \epsilon_i u_2^a u_{2i} e^{j\theta_i}$ belongs to $\mathbf{G}_+^*$.

Thus for any context $C_0 \in \mathcal{C}^{\text{hyp}}$ we can represent φ_{C_0} in the form

$$\varphi_{C_0} = u_1^a e_1^a + u_2^a e_2^a,$$

where

$$e_1^a = (u_{11}, u_{12}), \quad e_2^a = (\epsilon_1 e^{j\theta_1} u_{21}, \epsilon_2 e^{j\theta_2} u_{22}).$$

As in the **C** case,[1] we introduce the matrix V with coefficients $v_{11} = u_{11}$, $v_{21} = u_{21}$, and $v_{12} = \epsilon_1 e^{j\theta_1} u_{21}$, $v_{22} = \epsilon_2 e^{j\theta_2} u_{22}$. We remark that here coefficients $v_{ij} \in \mathbf{G}_+^*$. In the same way as in the complex case the Born's rule

$$p_{C_0}^a(a_i) = |(\varphi_{C_0}, e_i^a)|^2 \tag{15}$$

holds true in the a-basis iff $\{e_i^a\}$ is an orthonormal basis in H^{hyp}. The latter is equivalent to the **G** unitary of the matrix V (corresponding to the transition from $\{e_i^b\}$ to $\{e_i^a\}$): $\overline{V^*} V = I$, or

$$\overline{v}_{11} v_{11} + \overline{v}_{21} v_{21} = 1, \quad \overline{v}_{12} v_{12} + \overline{v}_{22} v_{22} = 1, \tag{16}$$

$$\overline{v}_{11} v_{12} + \overline{v}_{21} v_{22} = 0. \tag{17}$$

Thus $1 = u_{11}^2 + u_{21}^2 = p(b_1/a_1) + p(b_1/a_2)$ and $1 = u_{12}^2 + u_{22}^2 = p(b_2/a_1) + p(b_2/a_2)$. Thus the first two equations of the **G** unitary are equivalent to the double stochasticity of $\mathbf{P}^{b/a}$ (as in the **C** case[1]). We remark that the equations (16) can be written as

$$|v_{11}|^2 + |v_{21}|^2 = 1, \quad |v_{12}|^2 + |v_{22}|^2 = 1, \tag{18}$$

cf. Sec. IV. The third unitarity equation (17) can be written as

$$u_{11} u_{12} \epsilon_1 e^{-j\theta_2} + u_{21} \epsilon_2 e^{-j\theta_2} u_{22} = 0. \tag{19}$$

By using double stochasticity of $\mathbf{P}^{a/b}$ we obtain $e^{j\theta_1} = e^{j\theta_2}$. Thus

$$\theta_1 = \theta_2. \tag{20}$$

Lemma 3.1: *Let a and b be incompatible random variables and let* $\mathbf{P}^{b/a}$ *be double stochastic. Then*

$$\cosh \theta_C(b_2) = \cosh \theta_C(b_1) \tag{21}$$

for any context $C \in \mathcal{C}^{\text{hyp}}$.

Proof: By Lemma 2.1 we have

$$\sum_x \epsilon(x) \cosh \theta_C(x) \sqrt{\Pi_y p_C^a(y) p(x/y)} = 0.$$

Double stochasticity of $\mathbf{P}^{b/a}$ implies (21).

The constraint (21) induced by double stochasticity can be written as the constraint to phases

$$\theta_C(b_2) = \pm \theta_C(b_1). \tag{22}$$

To obtain unitary of the matrix V of transition $\{e_i^b\} \to \{e_i^a\}$ we should choose phases according to (20). And by (22) we can always do this for a double stochastic matrix of transition probabilities.

By choosing such a representation we obtain the hyperbolic generalization of the Born's rule for the a variable,

$$p_C^a(a_j) = |(\varphi, e_j^a)|^2. \tag{23}$$

We now investigate the possibility to use one fixed basis $\{e_j^a \equiv e_j^a(C_0)\}$, $C_0 \in \mathcal{C}^{\text{hyp}}$, for all states φ_C, $C \in \mathcal{C}^{\text{hyp}}$. For any $C \in \mathcal{C}^{\text{hyp}}$ we would like to have the representation

$$\phi_C = v_1^a(C)e_1^a(C_0) + v_2^a(C)e_2^a(C_0), \quad \text{where } |v_j^a(C)|^2 = p_C^a(a_j). \tag{24}$$

We have

$$\phi_C(b_1) = u_1^a(C)v_{11}(C_0) + \epsilon_C(b_1)\epsilon_{C_0}(b_1)e^{j[\theta_C(b_1)-\theta_{C_0}(b_1)]}u_2^a(C)v_{12}(C_0),$$

$$\phi_C(b_2) = u_1^a(C)v_{21}(C_0) + \epsilon_C(b_2)\epsilon_{C_0}(b_2)e^{j[\theta_C(b_2)-\theta_{C_0}(b_2)]}u_2^a(C)v_{22}(C_0).$$

Thus to obtain (24) we should have

$$\epsilon_C(b_1)\epsilon_{C_0}(b_1)e^{j[\theta_C(b_1)-\theta_{C_0}(b_1)]} = \epsilon_C(b_2)\epsilon_{C_0}(b_2)e^{j[\theta_C(b_2)-\theta_{C_0}(b_2)]}.$$

Thus

$$\theta_C(b_1) - \theta_{C_0}(b_1) = \theta_C(b_2) - \theta_{C_0}(b_2), \text{ or } \theta_C(b_1) - \theta_C(b_2) = \theta_{C_0}(b_1) - \theta_{C_0}(b_2).$$

By choosing the representation with (20) we satisfy the above condition.

Theorem 3.1: *We can construct the quantumlike (Hilbert space) representation of a contextual Kolmogorov space such that the hyperbolic Born's rule holds true for both reference variables a and b iff the matrix of transition probabilities* $\mathbf{P}^{b/a}$ *is double stochastic.*

We remark that basic contexts $B_x = \{\omega \in \Omega : b(\omega) = x\}$, $x \in X$, always belong to $\mathcal{C}^{\text{hyp}}$, so $\varphi_{B_x} \in H^{\text{hyp}}$; and $B_x \in \mathcal{C}^{\text{tr}} \cap \mathcal{C}^{\text{hyp}}$ iff a and b are uniformly distributed ($\mathbf{P}^{a/b}$ and $\mathbf{P}^{b/a}$ are double stochastic).

IV. HYPERBOLIC QUANTUM MECHANICS

As in the ordinary quantum formalism, we represent physical states by normalized vectors of a hyperbolic Hilbert space $\mathbf{E} : \varphi \in \mathbf{E}$ and $(\varphi, \varphi) = 1$. We shall consider only dichotomous physical variables and quantum states belonging to the two-dimensional Hilbert space. Thus everywhere below $\mathbf{E}$ denotes the two-dimensional space. Let $a = a_1$, a_2 and $b = b_1$, b_2 be two physical variables. We represent them by $\mathbf{G}$-linear operators, $\hat{a} = a_1|a_1\rangle\langle a_1| + a_2|a_2\rangle\langle a_2|$ and $\hat{b} = b_1|b_1\rangle\langle b_1| + b_2|b_2\rangle\langle b_2|$, where $\{|a_i\rangle\}_{i=1,2}$ and $\{|b_i\rangle\}_{i=1,2}$ are two orthonormal bases in $\mathbf{E}$. The latter condition plays the fundamental role in hyperbolic quantum mechanics. This is an analogue of the representation of physical observables by self-adjoint operators in the conventional quantum mechanics (in the complex Hilbert space).

Let φ be a state (normalized vector belonging to $\mathbf{E}$). We can perform the following operation (which is well defined from the mathematical point of view). We expend the vector φ with respect to the basis $\{|b_i\rangle\}_{i=1,2}$,

$$\varphi = v_1^b|b_1\rangle + v_2^b|b_2\rangle, \tag{25}$$

where the coefficients (coordinates) v_i^b belong to $\mathbf{G}$. We remark that we consider the two-dimensional $\mathbf{G}$-Hilbert space. There exists (by definition) a basis consisting of two vectors. As the basis $\{|b_i\rangle\}_{i=1,2}$ is orthonormal, we have (as in the complex case) that

$$|v_1^b|^2 + |v_2^b|^2 = 1. \tag{26}$$

However, we could not automatically use Born's probabilistic interpretation for normalized vectors in the hyperbolic Hilbert space, it may be that $v_i^b \notin \mathbf{G}_+$ and hence $|v_i^b|^2 < 0$ (in fact, in the

complex case we have $\mathbf{C}=\mathbf{C}_+$; thus there is no problem with positivity). Since we do not want to consider negative probabilities, in such a case we cannot use the hyperbolic version of Born's probability interpretation.

Definition 4.1: *A state φ is decomposable with respect to the system of states $\{|b_i\rangle\}_{i=1,2}$ (b-decomposable) if*

$$v_i^b \in \mathbf{G}_+. \tag{27}$$

In such a case we can use generalization of Born's probabilistic interpretation for a hyperbolic Hilbert space. Numbers

$$p_\varphi^b(b_i) = |v_i^b|^2, \quad i = 1,2,$$

are interpreted as probabilities for values $b=b_i$ for the **G**-quantum state φ.

We remark that in this framework (here we started with a hyperbolic Hilbert space and not with a contextual statistical model, cf. Sec. III) a hyperbolic generalization of Born's rule is a postulate.

Thus decomposability is not a mathematical notion. This is not just linear algebraic decomposition of a vector with respect to a basis. This is a physical notion describing the possibility of probability interpretation of a measurement over a state. As it was already mentioned, in hyperbolic quantum mechanics a state $\varphi\in\mathbf{E}$ is not always decomposable. Thus for an observable b there can exist a state φ such that the probabilities $p_\varphi^b(b_i)$ are not well defined. One of the reasons for this can be the impossibility to perform the b-measurement for systems in the state φ. Such a situation is quite natural from the experimental viewpoint. Moreover, it looks surprising that in ordinary quantum (as well as classical) theory we can measure any observable in any state. I think that this is just a consequence of the fact that there was fixed the set of states corresponding to a rather special class of physical observables. Thus in the hyperbolic quantum formalism for each state $\varphi\in\mathbf{E}$ there exists its own set of observables $\mathcal{O}(\varphi)$. And in general $\mathcal{O}(\varphi)\neq\mathcal{O}(\psi)$. We cannot exclude another possibility. The set of observables $\mathcal{O}$ does not depend on a state φ. And the result of an individual measurement of any $b\in\mathcal{O}$ is well defined for any state φ. But relative frequencies of realizations of the value $b=b_k$ do not converge to any limit. Therefore probabilities are not well defined. Thus the principle of the statistical stabilization should be violated, cf. Ref. 13.

Let $\mathcal{K}$ be a Kolmogorov probability model and let $\varphi\in S_{\mathcal{C}^{\text{hyp}}}$. Thus $\varphi=\varphi_C$ for some context $C\in\mathcal{C}^{\text{hyp}}$. Let the matrix of transition probabilities $\mathbf{P}^{b/a}$ be double stochastic. Then φ is decomposable with respect to both reference variables b and a. Moreover, basis vectors $e_i^b=|b_i\rangle$ are a decomposable and vice versa.

We now start the derivation of the hyperbolic probabilistic rule by using the hyperbolic Hilbert space formalism. Suppose that a state $\varphi\in\mathbf{E}$ is a decomposable,

$$\varphi = v_1^a|a_1\rangle + v_2^a|a_2\rangle$$

and the coefficients $v_i^a\in\mathbf{G}_+$.

We also suppose that each state $|a_i\rangle$ is decomposable with respect to the system of states $\{|b_i\rangle\}_{i=1,2}$. We have

$$|a_1\rangle = v_{11}|b_1\rangle + v_{12}|b_2\rangle, \quad |a_2\rangle = v_{21}|b_1\rangle + v_{22}|b_2\rangle, \tag{28}$$

where the coefficients v_{ik} belong to $\mathbf{G}_+$. We have (since both bases are orthonormal)

$$|v_{11}|^2 + |v_{12}|^2 = 1, \quad |v_{21}|^2 + |v_{22}|^2 = 1, \tag{29}$$

cf. (18). We can use the probabilistic interpretation of numbers $p_{ik}=|v_{ik}|^2$, namely $p_{ik}=p_{|a_i\rangle}(b_k)$ is the probability for $b=b_k$ in the state $|a_i\rangle$.

Let us consider matrix $V=(v_{ik})$. As in the complex case, the matrix V is unitary, since vectors $|a_1\rangle=(v_{11},v_{12})$ and $|a_2\rangle=(v_{21},v_{22})$ are orthonormal. Hence we have normalization conditions (29) and the orthogonality condition,

$$v_{11}\overline{v_{21}} + v_{12}\overline{v_{22}} = 0, \tag{30}$$

cf. (17). It must be noticed that in general unitarity does not imply that $v_{ik} \in \mathbf{G}_+$. The latter condition is the additional constraint on the unitary matrix V. Let us consider the matrix $\mathbf{P}^{b/a} = (p_{ik})$. This matrix is double stochastic (since V is unitary).

By using the **G**-linear space calculation (the change of the basis) we get $\varphi = v_1^b|b_1\rangle + v_2^b|b_2\rangle$, where $v_1^b = v_1^a v_{11} + v_2^a v_{21}$ and $v_2^b = v_1^a v_{12} + v_2^a v_{22}$.

We remark that decomposability is not transitive. In principle φ may not be decomposable with respect to $\{|b_i\rangle\}_{i=1,2}$, despite the decomposability of φ with respect to $\{|a_i\rangle\}_{i=1,2}$ and the decomposability of the latter system with respect to $\{|b_i\rangle\}_{i=1,2}$.

The possibility of decomposability is based on two (totally different) conditions, (26), normalization, and (27), positivity. Any **G**-unitary transformation preserves the normalization condition. Thus we get automatically that $|v_1^b|^2 + |v_2^b|^2 = 1$. However, the condition of positivity in general is not preserved, it can be that $v_i^b \notin \mathbf{G}_+$ even if we have $v_i^a \in \mathbf{G}_+$ and the matrix V is **G** unitary.

Finally, suppose that φ is decomposable with respect to $\{|b_i\rangle\}_{i=1,2}$. Thus $v_k^b \in \mathbf{G}_+$. Therefore coefficients $p_\varphi^b(b_i) = |v_i^b|^2$ can be interpreted as probabilities for $b = b_k$ for the **G**-quantum state φ.

Let us consider states such that coefficients v_i^a, v_{ik} belong to $\mathbf{G}_+^*$. We can uniquely represent them as

$$v_i^a = \pm\sqrt{p_\varphi^a(a_i)}e^{j\xi_i}, \quad v_{ik} = \pm\sqrt{p_{ik}}e^{j\gamma_{ik}}, \quad i,k, = 1,2.$$

We find that

$$p_\varphi^b(b_1) = p_\varphi^a(a_1)p_{11} + p_\varphi^a(a_2)p_{21} + 2\epsilon_1 \cosh\,\theta_1\sqrt{p_\varphi^a(a_1)p_{11}p_\varphi^a(a_2)p_{21}}, \tag{31}$$

$$p_\varphi^b(b_2) = p_\varphi^a(a_1)p_{12} + p_\varphi^a(a_2)p_{22} + 2\epsilon_2 \cosh\,\theta_2\sqrt{p_\varphi^a(a_1)p_{12}p_\varphi^a(a_2)p_{22}}, \tag{32}$$

where $\theta_i = \eta + \gamma_i$ and $\eta = \xi_1 - \xi_2$, $\gamma_1 = \gamma_{11} - \gamma_{21}$, $\gamma_1 = \gamma_{12} - \gamma_{22}$, and $\epsilon_i = \pm$. To find the right relation between signs of the last terms in equations (31) and (32), we use the normalization condition

$$|v_2^b|^2 + |v_2^b|^2 = 1 \tag{33}$$

(which is a consequence of the normalization of φ and orthonormality of the system $\{|b_i\rangle\}_{i=1,2}$).

We remark that the normalization condition (33) can be reduced to relations between coefficients of the transition matrix V. So it does not depend on the original a-decomposition of φ, namely coefficients v_i^a. Condition of positivity, $|v_i^b|^2 \geqslant 0$, could not be written by using only coefficients of V. We also need to use coefficients v_i^a. Therefore it seems to be impossible to find such a class of linear transformations V that would preserve condition of positivity, "decomposition group" of operators.

Equation (33) is equivalent to the equation

$$\sqrt{p_{12}p_{22}}\cosh\,\theta_2 \pm \sqrt{p_{11}p_{21}}\cosh\,\theta_2 = 0. \tag{34}$$

Thus we must choose opposite signs in Eqs. (31) and (32). Unitarity of V also implies that $\theta_1 - \theta_2 = 0$, so $\gamma_1 = \gamma_2$. We recall that in the ordinary quantum mechanics we have similar conditions, but trigonometric functions are used instead of hyperbolic and phases γ_1 and γ_2 are such that $\gamma_1 - \gamma_2 = \pi$.

Finally, we get that unitary linear transformations in the **G**-Hilbert space (in the domain of decomposable states) represent the following transformation of probabilities:

$$p_{\varphi}^{b}(b_1) = p_{\varphi}^{a}(a_1)p_{11} + p_{\varphi}^{a}(a_2)p_{21} \pm 2\epsilon_1 \cos\theta_1 \sqrt{p_{\varphi}^{a}(a_1)p_{11}p_{\varphi}^{a}(a_2)p_{21}}, \tag{35}$$

$$p_{\varphi}^{b}(b_2) = p_{\varphi}^{a}(a_1)p_{12} + p_{\varphi}^{a}(a_2)p_{22} \mp 2\epsilon_2 \cosh\theta_2 \sqrt{p_{\varphi}^{a}(a_1)p_{12}p_{\varphi}^{a}(a_2)p_{22}}. \tag{36}$$

This is hyperbolic interference. In Sec. II it was derived from the contextual statistical model and then in Sec. III by using interference formulas we obtained the hyperbolic Hilbert space representation for contexts. In this section we started directly from the hyperbolic Hilbert space representation and derived interference of probabilities.

V. EXPERIMENTAL VERIFICATION OF HYPERBOLIC QUANTUM MECHANICS

This paper contains an important experimental prediction.

In statistical experiments with physical (micro as well as macro) systems there could be produced not only the ordinary trigonometric, but also the hyperbolic interference picture.

We start with the general description of interference experiments for discrete observables. There are considered two dichotomous observables, a, "slit number;" and b, "position of a particle on the registration screen." The observable a is measured in the following way. Particle detectors are placed behind the screen having two open slits. The observable $a=j$ if the detector behind the jth slit clicks. To define another observable, we choose some domain D on the registration screen and we set $b=1$ if a particle is registered inside D and $b=0$ if outside. The complex of physical conditions under consideration (context) C is screen with two open slits and the registration screen. We find frequency probabilities $p_C^b(1)$ and $p_C^b(0)$ by counting the number of particles inside and outside the domain D on the registration screen. Then we perform the measurement of the a variable by placing detectors behind the first screen. We find frequency probabilities $p_C^a(1)$ and $p_C^a(2)$ by counting the numbers of particles passing through the first screen and the second screen, respectively [if the source is located symmetrically with respect to screens, then $p_C^a(a=1)=p_C^a(a=2)=1/2$]. We also find transition probability $p^{b/a}(i/j)$ by closing the jth slit and performing the b measurement under this complex of physical conditions. For systems described by classical (noncontextual) probability theory we get the well-known formula of total probability,

$$p_C^b(x) = p_C^a(1)p^{b/a}(x/1) + p_C^a(2)p^{b/a}(x/2).$$

Here the coefficient of statistical disturbance $\lambda(b=x/a,C)=0$. For systems described by quantum probability, we get the interference formula,

$$p_C^b(x) = p_C^a(1)p^{b/a}(x/1) + p_C^a(2)p^{b/a}(x/2) + 2\cos\theta\sqrt{p_C^a(1)p^{b/a}(x/1)p_C^a(2)p^{b/a}(x/2)}.$$

This formula is usually derived in the Hilbert space formalism. In the book of Feynman and Hibs[14] violation of the formula of total probability was considered as the most important exhibition of difference between probabilistic laws for classical and quantum systems. However, in papers of some authors, e.g., Refs. 2, 5–8, and 13 there was pointed out that violation of the formula of total probability is just an exhibition of contextuality of quantum probabilities.

In this paper we predict that contextual statistics produced by experiments of two slit type is not reduced to classical and quantum. Besides the absence of interference and the quantum trigonometric interference, we predict a type of interference—the hyperbolic interference. In our approach it is very easy to find the type of interference of probabilities. In a statistical test for some context C we calculate the coefficient

$$\lambda(a=x/b,C) = \frac{p_C^b(x) - p_C^a(1)p^{b/a}(x/1) - p_C^a(2)p^{b/a}(x/2)}{2\sqrt{p_C^a(1)p^{b/a}(x/1)p_C^a(2)p^{b/a}(x/2)}}.$$

An empirical situation with $\lambda(a=x/b,C)>1$ would yield evidence for quantumlike hyperbolic behavior. The coefficient $\lambda(a=x/b,C)$ can be easily calculated on the basis of statistical data.

Thus our hyperbolic quantum mechanics predicts a testable result, namely the hyperbolic interference, that ordinary quantum mechanics does not.

We wrote about experiments of "two slit type." They need not be precisely experiments with space variables. The a and b can be any pair of incompatible observables. Incompatibility is understood as the impossibility to escape mutual disturbances in the process of measurement. The coefficient $\lambda(a=x/b,C)$ gives the measure of statistical disturbance. Classical measurements are characterized by (statistically) negligibly small mutual disturbances, so here $\lambda(b=x/a,C)=0$ (and we have the conventional formula of total probability). Quantum measurements are characterized by mutual disturbances which are not negligible (statistically). Here $\lambda(b=x/a,C)\in(0,1]$. The conventional formula of total probability is violated and we have the conventional trigonometric interference. However, the quantum case, i.e., $\lambda(b=x/a,C)\in(0,1]$, does not describe all nonclassical measurements. There can exist incompatible observables which produce mutual disturbances which are (statistically) essentially larger than the conventional quantum disturbances. In such a case $\lambda(a=x/b,C)>1$. As in the quantum case, the conventional formula of total probability is violated, but we have nonconventional hyperbolic interference.

Thus hyperbolic interference might be found in experiments with systems which are essentially more sensitive to disturbance effects of measurement devices than quantum systems. So to find such an interference we should go to scales of space, time, and energy, distances and time intervals which are essentially smaller than approached in the conventional quantum experiments. One may speculate that there can be some connections with string theory and cosmology. It may be that quantum mechanics for string theory and cosmology is hyperbolic quantum mechanics.

Another possibility to find hyperbolic interference (which looks more realizable at the present technological level) is to look for observables on ordinary quantum or classical systems which would produce very strong statistical disturbances.

Since we derived the hyperbolic (as well as the conventional trigonometric) interference in the general contextual probabilistic approach, our formalism can be applied to any kind of system, for example, cognitive systems. Experiments of the two slit type can be done for cognitive systems, e.g., human beings. Here observables a and b are given in the form of questions. It might be that cognitive systems can produce hyperbolic interference and should be described by hyperbolic quantum mechanics.

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Lifting Bell inequalities

Stefano Pironio[a)]
Institute for Quantum Information, California Institute of Technology, Pasadena, California 91125

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A Bell inequality defined for a specific experimental configuration can always be extended to a situation involving more observers, measurement settings, or measurement outcomes. In this article, such "liftings" of Bell inequalities are studied. It is shown that if the original inequality defines a facet of the polytope of local joint outcome probabilities then the lifted one also defines a facet of the more complex polytope. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1928727]

I. INTRODUCTION

In a typical Bell experiment, two or more entangled particles are distributed to separate observers. Each observer measures on his particle one from a set of possible observables and obtains some outcome. One of the most striking features of quantum mechanics is that the resulting joint outcome probabilities can violate a Bell inequality,[1] indicating that quantum mechanics is not, in Bell's terminology, locally causal. This prediction has been confirmed, up to some loopholes, in numerous laboratory experiments.[2,3] The implications of nonlocality for our fundamental description of nature[4,5] have long been discussed; more recently, nonlocality has also acquired a significance in quantum information science.[6–12] From this perspective, being able to decide whether a joint probability distribution can be reproduced with classical randomness only, or whether entanglement is necessary, is an important issue.

For a given number of observers, measurement settings, and measurement outcomes, the set of joint probabilities accessible to locally causal theories is a convex polytope.[13] It is therefore completely characterized by a finite number of linear inequalities that these probabilities must satisfy—that is, by a finite number of Bell inequalities. Each of these inequalities corresponds to a *facet* of the local polytope. Note, however, that not every Bell inequality represents a facet. Facet inequalities are the ones which characterize precisely the border between the local and the nonlocal region. They form a minimal and complete set of Bell inequalities.

In the simple situation where they are only two observers, two measurement choices, and two outcomes per measurement, all the facet inequalities are known:[14,15] up to permutation of the outcomes, they correspond to the Clauser–Horne–Shimony–Holt (CHSH) inequality.[16] Beyond this, little is known. It is in principle possible to obtain all the facet inequalities of an arbitrary Bell polytope using specific algorithms. In practice this only allows one to extend the range of solved cases to a few more observers, measurements, or outcomes,[17,18] as these algorithms are excessively time-consuming. The problem of listing all facet inequalities has in fact been demonstrated to be NP-complete;[19] it is therefore unlikely that it could be solved in full generality. Discouraging as this result may seem, it nevertheless leaves open several possibilities. First, complete sets of facet inequalities may be obtained for particular classes of Bell polytopes or for simplified versions of them. For instance, in the case where "full correlation functions" are considered instead of complete joint probability distributions, all facet inequalities are known for Bell scenarios consisting of an arbitrary number of parties with two measurement choices and two outcomes.[20,21]

[a)]Electronic mail: spironio@caltech.edu

Second, in more complicated situations it may still be possible to obtain partial lists of facets. For instance, families of facet inequalities are known for arbitrary number of measurements[19] or outcomes.[22]

Further progress in the derivation of Bell inequalities would certainly benefit from a better characterization of the general properties of Bell polytopes. This is the motivation behind the present article. The question that we will investigate is how, and to what extent, the facial structure of a Bell polytope determines the facial structure of more complex polytopes. More specifically consider a bipartite Bell experiment characterized by the probability $p_{k_1k_2|j_1j_2}$ for the first observer to obtain outcome k_1 and for the second one to obtain outcome k_2, given that the first observer measures j_1 and the second one j_2. Suppose that each observer chooses one from two dichotomic observables, that is, $k_1, k_2 \in \{1,2\}$ and $j_1, j_2 \in \{1,2\}$. A necessary condition for this experiment to be reproducible by a local model is that the joint probabilities satisfy the CHSH inequality

$$p_{11|11} + p_{11|12} + p_{11|21} - p_{11|22} + p_{22|11} + p_{22|12} + p_{22|21} - p_{22|22} \geqslant 0. \tag{1}$$

Although this inequality is defined for the specific Bell scenario that we have just described, it also constrains the set of local joint probabilities involving more observers, measurements, and outcomes. Indeed, as was noted by Peres[23] there are obvious ways to extend Bell inequalities to more complex situations, or to *lift* them following the terminology of polytope theory. As an illustration, let us consider the following three possible extensions of our CHSH scenario.

(i) *More observers*. Consider a tripartite Bell experiment with joint probability distribution $p_{k_1k_2k_3|j_1j_2j_3}$, where $k_1, k_2, k_3 \in \{1,2\}$ and $j_1, j_2, j_3 \in \{1,2\}$. A necessary condition for this tripartite distribution to be local is that the probabilities $\tilde{p}_{k_1k_2|j_1j_2}$ for the first two observers to measure j_1 and j_2 and to obtain outcomes k_1 and k_2 *conditional* on the third observer measuring $j_3=1$ and obtaining $k_3=1$ satisfy the CHSH inequality. These conditional probabilities are given by $\tilde{p}_{k_1k_2|j_1j_2}=p_{k_1k_21|j_1j_21}/p_{1_3|1_3}$, where the marginal $p_{1_3|1_3}=\sum_{k_1,k_2}p_{k_1k_21|j_1j_21}$ is independent of j_1 and j_2 by no signaling (see Sec. III A). Inserting these probabilities in (1) and multiplying both sides by $p_{1_3|1_3}$ leads to

$$p_{111|111} + p_{111|121} + p_{111|211} - p_{111|221} + p_{221|111} + p_{221|121} + p_{221|211} - p_{221|221} \geqslant 0, \tag{2}$$

a natural extension of the CHSH inequality to three parties.

(ii) *More measurements*. Consider our original bipartite Bell scenario, but assume that the second observer may choose between three different measurement settings $j_2 \in \{1,2,3\}$. Clearly, a necessary condition for the corresponding joint distribution to be reproducible by a local model is that, when restricted to the probabilities involving $j_2 \in \{1,2\}$, it satisfies the CHSH inequality. Therefore, inequality (1) is, as such, a valid Bell inequality for this three-measurement scenario.

(iii) *More outcomes*. Suppose now that the measurement apparatus of the second observer may output one out of three distinct values $k_2 \in \{1,2,3\}$. Merging the outcomes $k_2=2$ and $k_2=3$, we obtain an effective two-outcomes distribution with probabilities $\tilde{p}_{k_11|j_1j_2}=p_{k_11|j_1j_2}$ and $\tilde{p}_{k_12|j_1j_2}=p_{k_12|j_1j_2}+p_{k_13|j_1j_2}$. The existence of a local model for the original distribution obviously implies a model for the coarse-grained one. Expressing the fact that the $\tilde{p}_{k_1k_2|j_1j_2}$ should satisfy (1), we thus deduce the following lifting

$$p_{11|11} + p_{11|12} + p_{11|21} - p_{11|22} + p_{22|11} + p_{22|12} + p_{22|21} - p_{22|22} + p_{23|11} + p_{23|12} + p_{23|21} - p_{23|22} \geqslant 0 \tag{3}$$

of the CHSH inequality to three outcomes.

These three examples can be combined and used sequentially to lift the CHSH inequality to an arbitrary number of observers, measurements, and outcomes. It is also straightforward to generalize them to other Bell inequalities than the CHSH one. How strong are the constraints on the joint probabilities obtained in this way? We will show that if the original inequality describes a facet of the original polytope, then the lifted one is also a facet of the more complex polytope. This implies, for instance, that the CHSH inequality is a facet of every Bell polytope since it is a facet of the simplest one.

This article is organized as follows. Section II introduces the concepts and notations that will be used in the remainder of the paper. In particular, we briefly review the definition of Bell polytopes and elementary notions of polytope theory. In Sec. III, we derive some basic properties of Bell polytopes that are necessary to prove our main results concerning the lifting of facet inequalities. These results are presented in Sec. IV. We conclude with a discussion and some open questions in Sec. V.

II. DEFINITIONS

A. Bell scenario

Consider n systems and assume that on each system i a measurement $j \in \{1,\ldots,m_i\}$ is made, yielding an outcome $k \in \{1,\ldots,v_{ij}\}$. Note that the number of possible measurements m_i may be different for each system i, and that the number of possible outcomes v_{ij} may be different for each measurement j on system i. Such a Bell scenario is thus characterized by the triple (n,m,v) where $m=(m_1,\ldots,m_n)$ specifies the number of possible measurements per system, and where the table $v=[(v_{11},\ldots,v_{1m_1});\ldots;(v_{n1},\ldots,v_{nm_n})]$ specifies the number of possible outcomes per measurement on each system. When notations such as $(n,2,v)$ are used, it should be understood that $m_i=2$ for all i.

The joint probability of obtaining the outcomes $(k_1,\ldots,k_n)$ given the measurement settings $(j_1,\ldots,j_n)$ will be denoted $p_{k_1\ldots k_n|j_1\ldots j_n}$. We will view these $t=\Pi_{i=1}^{n}(\Sigma_{j=1}^{m_i}v_{ij})$ probabilities as forming the components of a vector p in $\mathbb{R}^t$. For a given observer $i \in \{1,\ldots,n\}$, measurement $j \in \{1,\ldots,m_i\}$ and outcome $k \in \{1,\ldots,v_{ij}\}$, we will often be interested in the subset of the components of p that have the indices k_i and j_i corresponding to observer i fixed, and equal, respectively, to k and j. In other words, we will be interested in the variables $p_{k_1\ldots k_{i-1}k\,k_{i+1}\ldots k_n|j_1\ldots j_{i-1}j\,j_{i+1}\ldots j_n}$. The restriction of p to these components will be denoted $p(i,j,k)$.

B. Bell polytopes

The set $\mathcal{B}\subseteq\mathbb{R}^t$ of correlations reproducible within a locally causal model is the set of correlations p satisfying

$$p_{k_1\ldots k_n|j_1\ldots j_n}=\int \mathrm{d}\mu q(\mu)P(k_1|j_1,\mu)\ldots P(k_n|j_n,\mu),$$

where $q(\mu)\geqslant 0$, $\int \mathrm{d}\mu\, q(\mu)=1$, and $P(k_i|j_i,\mu)$ is the probability of obtaining the measurement outcome k_i given the setting j_i and the hidden-variable μ.[1,4] From this definition it is easily deduced (see Ref. 13 for instance) that p is generated by specifying probabilities for every assignment of one of the possible outcomes to each of the measurement settings. More precisely, let the table $\lambda=[(\lambda_{11},\ldots,\lambda_{1m_1});\ldots;(\lambda_{n1},\ldots,\lambda_{nm_n})]$ assign to each measurement j on system i the outcome λ_{ij}. The (finite) set of all such possible assigmenents will be denoted Λ. Let

$$p^{\lambda}_{k_1\ldots k_n|j_1\ldots j_n}=\begin{cases}1 & \text{if } \lambda_{1j_1}=k_1,\ldots,\lambda_{nj_n}=k_n\\ 0 & \text{otherwise}\end{cases} \tag{4}$$

be the deterministic vector corresponding to the assignment λ. Then

$$\mathcal{B}=\left\{p\in\mathbb{R}^t \middle| p=\sum_{\lambda\in\Lambda} q_\lambda p^\lambda, q_\lambda\geqslant 0, \sum_{\lambda\in\Lambda} q_\lambda = 1\right\}. \tag{5}$$

The set $\mathcal{B}$ of local correlations is thus the convex hull of a finite number of points, i.e., it is a polytope. The deterministic vectors $\{p^\lambda|\lambda\in\Lambda\}$ form the extreme points of this polytope.

C. Notions of polytope theory

We review in this section some elementary notions of polytope theory. For more detailed introductions, see Refs. 24–26.

The points $p_1,\ldots,p_n$ in $\mathbb{R}^t$ are said to be affinely independent if the unique solution to $\Sigma_i\mu_i p_i=0$, $\Sigma_i\mu_i=0$ is $\mu_i=0$ for all i, or equivalently, if the points $p_2-p_1,\ldots,p_n-p_1$ are linearly independent. They are affinely dependent otherwise. The affine hull of a set of points is the set of all their affine combinations. An affine set has dimension D, if the maximum number of affinely independent points it contains is $D+1$.

Let $\mathcal{B}\subseteq\mathbb{R}^t$ be a polytope defined as in (5). Let $(b,b_0)\in\mathbb{R}^{t+1}$ define the inequality $b\cdot p\geqslant b_0$. If this inequality is satisfied for all $p\in\mathcal{B}$, it is called a valid inequality for the polytope $\mathcal{B}$, or a Bell inequality in the context of Bell polytopes. Note that to check whether an inequality is a valid inequality, it is sufficient, by convexity, to check whether it is satisfied by the extreme points $\{p^\lambda|\lambda\in\Lambda\}$. Given the valid inequality $b\cdot p\geqslant b_0$, the set $F=\{p\in\mathcal{B}|b\cdot p=b_0\}$ is called a face of $\mathcal{B}$ and the inequality is said to support F. If $F\neq\emptyset$ and $F\neq\mathcal{B}$, it is a proper face. The dimension of F is the dimension of its affine hull. Proper faces clearly satisfy $\dim F\leqslant\dim\mathcal{B}-1$. Proper faces of maximal dimension are called facets. An inequality $b\cdot p\geqslant b_0$ thus supports a facet of $\mathcal{B}$ if and only if $\dim\mathcal{B}$ affinely independent of $\mathcal{B}$ satisfy it with equality.

A fundamental result in polyhedral theory, known as Minkowski–Weyl's theorem, states that a polytope represented as the convex hull of a finite number of points, as in (5), can equivalently be represented as the intersection of finitely many half-spaces:

$$\mathcal{B}=\{p\in\mathbb{R}^t|b^i\cdot p\geqslant b_0^i,\ \text{for all } i\in I\}, \tag{6}$$

where $\{b^i\cdot p\geqslant b_0^i, i\in I\}$ is a finite set of inequalities. The inequalities supporting facets of $\mathcal{B}$ provide a minimal set of such inequalities.[27] In particular, any valid inequality for $\mathcal{B}$ can be derived from the facet inequalities.

Given a Bell scenario (n,m,v), the task of finding all the Bell inequalities is thus the problem of finding all the facets of the convex polytope $\mathcal{B}(n,m,v)$ defined by (4) and (5). This connection between the search for optimal Bell inequalities and polyhedral geometry was observed by different authors.[14,23,28,29] For discussions on the complexity of this facet enumeration task see Refs. 19 and 30. For the instances for which this problem has been partially or completely solved, see Refs. 14, 15, 17–22, 31, and 32.

III. BASIC PROPERTIES OF BELL POLYTOPES

A. Affine hull

Local correlations $p\in\mathcal{B}$ satisfy the following equality constraints: *the normalization conditions*

$$\sum_{k_1\ldots k_n} p_{k_1\ldots k_n|j_1\ldots j_n}=1 \tag{7}$$

for all $j_1,\ldots,j_n$; *and the no signaling conditions*

$$\sum_{k_i} p_{k_1\ldots k_i\ldots k_n|j_1\ldots j_i\ldots j_n}=\sum_{k_i} p_{k_1\ldots k_i\ldots k_n|j_1\ldots j_i'\ldots j_n} \tag{8}$$

for all i, $k_1,\ldots k_{i-1}$, $k_{i+1},\ldots,k_n$ and $j_1,\ldots j_{i-1}$, j_i,j_i', $j_{i+1},\ldots,j_n$.

The no signaling conditions imply that for each subset $\{i_1,\ldots,i_q\}$ of size q of the observers, the q-marginals $p_{k_{i_1}\ldots k_{i_q}|j_{i_1}\ldots j_{i_q}}=\Sigma_{k_{i_{q+1}}}\ldots\Sigma_{k_{i_n}}p_{k_1\ldots k_n|j_1\ldots j_n}$ are well-defined, that is, are independent of the precise value of the measurement settings $j_{i_{q+1}}\ldots j_{i_n}$.

The two conditions (7) and (8) also imply that the polytope $\mathcal{B}$ is not full dimensional in $\mathbb{R}^t$, i.e., it is contained in an affine subspace. The following theorem generalizes results given in Refs. 22 and 19.

Theorem 1: *The constraints* (7) and (8) *fully determine the affine hull of* $\mathcal{B}$ *and*

$$\dim \mathcal{B}=\prod_{i=1}^{n}\left(\sum_{j=1}^{m_i}(v_{ij}-1)+1\right)-1. \tag{9}$$

Proof: Consider the marginals $p_{k_{i_1}\ldots k_{i_q}|j_{i_1}\ldots j_{i_q}}$ as defined above for all possible subsets $\{i_1,\ldots,i_q\}$ of size q, and for all $q=1,\ldots,n$. Of these marginals retain only the ones such that $k_i\neq 1$ for all $i\in\{i_1,\ldots,i_q\}$. These probabilities define in total $D=\Pi_{i=1}^{n}(\Sigma_{j=1}^{m_i}(v_{ij}-1)+1)-1$ numbers. It is straightforward to check that their knowledge is sufficient to reconstruct, using the normalization and no signaling conditions, the original $p_{k_1\ldots k_n|j_1\ldots j_n}$. This implies that the affine subspace defined by (7) and (8) is of dimension $\leqslant D$.

Let us now show that $\dim\mathcal{B}\geqslant D$, or equivalently that $\mathcal{B}$ contains $D+1$ affinely independent points. For this, note that the definition (4) implies that an extreme point p^{λ} can be written as the product $p^{\lambda}_{k_1\ldots k_n|j_1\ldots j_n}=p^{\lambda}_{k_1|j_1}\ldots p^{\lambda}_{k_n|j_n}$, where $p^{\lambda}_{k_i|j_i}$ is a vector of length $\Sigma_{j=1}^{m_i}v_{ij}$ such that

$$p^{\lambda}_{k_i|j_i}=\begin{cases}1 & \text{if } \lambda_{ij_i}=k_i\\ 0 & \text{otherwise.}\end{cases} \tag{10}$$

For fixed i, consider, for each $j_i'\in\{1,\ldots,m_i\}$ and for each $k_i'\in\{2,\ldots,v_{ij_i'}\}$, the points $p^{\lambda}_{k_i|j_i}$ defined by $\lambda_{ij_i}=1$ for all $j_i\neq j_i'$ and $\lambda_{ij_i'}=k_i'$. In addition, consider the vector $p^{\lambda}_{k_i|j_i}$ defined by $\lambda_{ij_i}=1$ for all j_i. These $\Sigma_{j=1}^{m_i}(v_{ij}-1)+1$ points are linearly independent. The products $p^{\lambda}_{k_1\ldots k_n|j_1\ldots j_n}=p^{\lambda}_{k_1|j_1}\ldots p^{\lambda}_{k_n|j_n}$ of all these points thus define $\Pi_{i=1}^{n}(\Sigma_{j=1}^{m_i}(v_{ij}-1)+1)=D+1$ linearly independent extreme points of $\mathcal{B}$, which are therefore also affinely independent. □

Since $\mathcal{B}$ is not full dimensional, it follows that there is no unique way to write down a valid inequality for $\mathcal{B}$. More specifically, the inequalities $b\cdot p\geqslant b_0$ and $(b+\mu c)\cdot p\geqslant(b+\mu c_0)$, where $\mu\in\mathbb{R}$ and where $c\cdot p=c_0$ is a linear combination of the equalities (7) and (8), impose the same constraints on $\mathcal{B}$. In particular, it is always possible to use the normalization conditions to rewrite an inequality such that its lower bound is 0, that is, in the form $b\cdot p\geqslant 0$. This fact will be used later on.

B. Trivial facets and nontrivial polytopes

In addition to the normalization and no signaling conditions, $\mathcal{B}$ also satisfy the following *positivity conditions*:

$$p_{k_1\ldots k_n|j_1\ldots j_n}\geqslant 0 \tag{11}$$

for all $k_1,\ldots,k_n$ and $j_1,\ldots,j_n$.

Theorem 2: *The positivity conditions support facets of* $\mathcal{B}$.

Proof: Without loss of generality, suppose that $p_{k_1\ldots k_n|j_1\ldots j_n}\geqslant 0$ is such that the $k_1,\ldots,k_n$ are all different than 1. Then, in the proof of Theorem 1, we enumerated $\dim\mathcal{B}+1$ affinely independent points, $\dim\mathcal{B}$ of which satisfy $p_{k_1\ldots k_n|j_1\ldots j_n}=0$. □

The normalization, no signaling, and positivity conditions are obviously not only satisfied by local probabilities, but also by all no signaling nonlocal ones, and in particular by quantum ones. The only useful constraints that separate the local region from the nonlocal thus correspond to the facets of $\mathcal{B}$ that are not of the form (11).

Let us also note that when determining the facets of a Bell polytope, we can always assume that n, m_i and v_{ij} are all $\geqslant 2$ because otherwise all the corresponding facets are trivial or belong to simpler polytopes. Indeed,

(i) the only facet inequalities of one-partite polytopes are the positivity constraints,
(ii) all the facet inequalities of a polytope where $m_i=1$ for some party i are equivalent to the facet inequalities of the polytope obtained by discarding that party,
(iii) a polytope with $v_{ij}=1$ for some measurement j of party i is equivalent to the polytope obtained by discarding that measurement choice.

Point (i) is easily established. To show (ii), assume that $\mathcal{B}$ is a polytope such that for party i the only measurement choice is $j \in \{1\}$. A valid inequality for $\mathcal{B}$ can thus be written as

$$\sum_k b_k \cdot p(i,j,k) \geqslant 0, \tag{12}$$

where, without loss of generality, the right-hand side is equal to zero. It then follows that for all $k \in \{1,\ldots,v_{ij}\}$ the following inequalities

$$b_k \cdot p(i,j,k) \geqslant 0 \tag{13}$$

are also valid for $\mathcal{B}$. Indeed, for each extreme point p^λ, either the assignment λ is such that $\lambda_{ij}=k$ and (12) and (13) impose the same constraints on p^λ, or $\lambda_{ij} \neq k$ and (13) gives the trivial inequality $0 \geqslant 0$. Every extreme point satisfying (12) thus also satisfies (13). Note further that every extreme point satisfying (12) with equality also satisfies (13) with equality. This implies that the face supported by (12) cannot be—unless (12) is itself equivalent to one of the inequalities (13)—a facet of $\mathcal{B}$, because it lies in the intersection of the faces supported by (13) and is therefore of dimension $<\dim \mathcal{B}-1$. We can thus assume that all facet inequalities of $\mathcal{B}$ are of the form (13). It will be shown in Sec. IV A that all these facet inequalities are equivalent to facet inequalities of the polytope obtained by discarding party i. Finally, point (iii) follows immediately when we notice that a polytope with $v_{ij}=1$ for some measurement j of party i and the polytope obtained by discarding that measurement have the same dimension and have their extreme points in one-to-one correspondence.

C. A useful lemma

As we have reminded earlier an inequality defines a facet of a polytope $\mathcal{B}$ if and only if it is satisfied by $\dim B$ affinely independent points of $\mathcal{B}$. To prove the results of the next section concerning the lifting of facet inequalities, we will then need to count the number of affine points that a facet contains. The following lemma will be our main tool to achieve this task.

Lemma 3: *Let the inequality $b \cdot p \geqslant b_0$ support a facet of $\mathcal{B}(n,m,v)$. Let $i' \in \{1,\ldots,n\}$, $j' \in \{1,\ldots,m_{i'}\}$ and $k' \in \{1,\ldots,v_{i'j'}\}$. Then there are at exactly r extreme points p^λ of $\mathcal{B}$ such that $b \cdot p^\lambda = b_0$, $\lambda_{i'j'}=k'$, and such that the r restrictions $p^\lambda(i',j',k')$ are affinely independent, where*

(i) $r=\Pi_{i\neq i'}(\Sigma_{j=1}^{m_i}(v_{ij}-1)+1)-1$, *if $b \cdot p \geqslant b_0$ is equivalent to an inequality of the form $c \cdot p(i',j',k') \geqslant 0$;*
(ii) $r=\Pi_{i\neq i'}(\Sigma_{j=1}^{m_i}(v_{ij}-1)+1)$, *otherwise.*

Proof: Let $\{p^\delta \mid \delta \in \Delta \subseteq \Lambda\}$ be $\dim \mathcal{B}$ affinely independent extreme points which belong to the facet supported by $b \cdot p \geqslant b_0$. Among these, let $\{p^\gamma \mid \gamma \in \Gamma \subseteq \Delta\}$ be the extreme points satisfying $\gamma_{i'j'}=k'$ and such that their restrictions $\{p^\gamma(i',j',k') \mid \gamma \in \Gamma\}$ are affinely independent.

Consider the polytope $\mathcal{B}^{n-1}$ obtained from $\mathcal{B}$ by discarding party i'. The components of $p \in \mathcal{B}^{n-1}$ are thus of the form $p_{k_1\ldots k_{i'-1}k_{i'+1}\ldots k_n|j_1\ldots j_{i'-1}j_{i'+1}\ldots j_n}$. Given that $p^\gamma(i',j',k')$ corresponds to the components of p^γ where the indices associated to the i'th party are fixed and satisfy $k_{i'}=k'$, $j_{i'}=j'$, given that $\gamma_{i'j'}=k'$, and given definition (4), it follows that each $p^\gamma(i',j',k')$ can be identified with an extreme point of the $(n-1)$-partite polytope $\mathcal{B}^{n-1}$ [and conversely, each extreme point of $\mathcal{B}^{n-1}$ can be identified with the restriction $p^\gamma(i',j',k')$ of some extreme point $p^\gamma \in \mathcal{B}$

satisfying $\gamma_{i'j'}=k']$. Thus no more than dim $\mathcal{B}^{n-1}$ of the $p^{\gamma}(i',j',k')$ can be affinely independent, and $r \leqslant \dim \mathcal{B}^{n-1}+1=\Pi_{i\neq i'}(\Sigma_{i=1}^{m_i}(v_{ij}-1)+1)$. Alternatively, one could have deduced the same result starting from the fact that the p^{γ} satisfy the implicit equalities (7) and (8), and counting the number of constraints that these equalities impose on the $p^{\gamma}(i',j',k')$.

Suppose that $r<\dim \mathcal{B}^{n-1}+1$. Then the $\{p^{\gamma}|\,\gamma\in\Gamma\}$ satisfy at least one constraint

$$c\cdot p(i',j',k')=0 \tag{14}$$

linearly independent from the implicit equalities of $\mathcal{B}$. Following the remark at the end of Sec. III A, we have not lost generality by taking the right-hand side of (14) equal to zero. Note that the constraint (14) is in fact satisfied by all $\{p^{\delta}|\,\delta\in\Delta\}$. Indeed, either $\delta_{i'j'}\neq k'$ and (14) gives the trivial equation $0=0$, or $p^{\delta}(i',j',k')$ is affinely dependent from the $p^{\gamma}(i',j',k')$, which satisfy (14).

As the $\{p^{\delta}|\,\delta\in\Delta\}$ form a set of dim $\mathcal{B}$ independent extreme points, they can satisfy at most one constraint linearly independent from the implicit equalities of $\mathcal{B}$, i.e., there can only be one constraint of the form (14). Thus at most $r=\dim \mathcal{B}^{n-1}=\Pi_{i\neq i'}(\Sigma_{i=1}^{m_i}(v_{ij}-1)+1)-1$. Furthermore, as the $\{p^{\delta}|\,\delta\in\Delta\}$ already satisfy the equality $b\cdot p=b_0$, this can only be the case if (14) is equivalent to $b\cdot p=b_0$, that is if $b\cdot p\geqslant b_0$ is equivalent either to $c\cdot p(i',j',k')\geqslant 0$ or $(-c)\cdot p(i',j',k')\geqslant 0$. □

IV. LIFTING BELL INEQUALITIES

We now move on to study the liftings of Bell inequalities that we have presented in Sec. I and their natural generalizations. We will prove that these liftings are facet-preserving. It was already shown in Ref. 19 that a Bell inequality that supports a facet of $\mathcal{B}(2,m,2)$ also supports a facet of $\mathcal{B}(2,m',2)$ for all $m'\geqslant m$. Furthermore, in Ref. 33 liftings of "partial constraint satisfaction polytopes" (polytopes encountered in certain optimization problems) were considered. Although such liftings were studied independently from any potential relation to Bell inequalities, it turns out that partial constraint satisfaction polytopes over a complete bipartite graph are bipartite Bell polytopes (in particular, the "4-cycle inequality" introduced in Ref. 33 corresponds to the CHSH inequality). The results presented in Ref. 33 then imply that an inequality that supports a facet of $\mathcal{B}(2,m,v)$ also supports a facet of $\mathcal{B}(2,m',v')$ for all $m'\geqslant m$, $v'\geqslant v$. It is in fact these results that inspired the ones that are presented here.

In Secs. IV A–IV C, we will see that the lifting of an arbitrary inequality to a situation involving, respectively, one more observer, one more measurement outcome, and one more measurement setting are facet-preserving. Combined together these results imply that a Bell inequality that supports a facet of a Bell polytope $\mathcal{B}(n,m,v)$, also supports, when lifted in the appropriate way, a facet of any higher dimensional polytope $\mathcal{B}(n',m',v')$ with $n'\geqslant n$, $m'\geqslant m$, $v'\geqslant v$.

A. One more observer

Consider a polytope $\mathcal{B}\equiv\mathcal{B}(n,m,v)$, where the n parties are labeled $\{1,\ldots,i'-1,i'+1\ldots,n+1\}$ for some value i'. Let the inequality

$$b\cdot p\geqslant 0 \tag{15}$$

be valid for $\mathcal{B}$. Note that we have taken, without loss of generality, the right-hand side of (15) to be equal to 0. Let us extend the polytope $\mathcal{B}$ by inserting an additional observer in position i'. The resulting $(n+1)$-partite polytope will be denoted $\mathcal{B}^{n+1}$.

Given a point $p\in\mathcal{B}^{n+1}$, remember that $p(i',j',k')$ represents the probabilities of p for which the indices corresponding to the measurement setting and the outcome of party i' are fixed, and are equal, respectively, to j' and k'. Therefore $p(i',j',k')/p_{k'_{i'}|j'_{i'}}$, where $p_{k'_{i'}|j'_{i'}}$ denotes the marginal probability for observer i' to measure j' and obtain k', is the joint outcome probability distribution for the n observers $\{1,\ldots,i'-1,i'+1,\ldots n+1\}$ conditional on party i' measuring j' and obtaining k'. Either this conditional probability is equal to zero, or it corresponds to a point of $\mathcal{B}$. In both cases, it satisfies (15). It thus follows immediately that the following inequality

$$b \cdot p(i',j',k') \geqslant 0 \tag{16}$$

is valid for $\mathcal{B}^{n+1}$. Further, this lifting is facet-preserving.

Theorem 4: *The inequality* (15) *supports a facet of* $\mathcal{B}$ *if and only if* (16) *supports a facet of* $\mathcal{B}^{n+1}$.

Proof: As we have noted in the proof of Lemma 3, the restriction $p^{\lambda}(i',j',k')$ of an extreme point p^{λ} of $\mathcal{B}^{n+1}$ satisfying $\lambda_{i'j'}=k'$ can be identified with an extreme point of $\mathcal{B}$, and conversely. Moreover, it is clear that if $p^{\lambda}(i',j',k')$ satisfy (16) with equality the corresponding extreme point of $\mathcal{B}$ satisfy (15) with equality, and the other way around.

Assume that (16) supports a facet of $\mathcal{B}^{n+1}$. Then it follows from Lemma 3 that they are $\Pi_{i\neq i'}(\Sigma_{j=1}^{m_i}(v_{ij}-1)+1)-1=\dim \mathcal{B}$ extreme points of $\mathcal{B}^{n+1}$ that satisfy (16) with equality, such that $\lambda_{i'j'}=k'$ and for which the restrictions $p^{\lambda}(i',j',k')$ are affinely independent. By the above remark, these extreme points define $\dim \mathcal{B}$ affinely independent extreme points of $\mathcal{B}$ that satisfy (15) with equality, hence this inequality supports a facet of $\mathcal{B}$.

To prove the converse statement, suppose now that (15) defines a facet of $\mathcal{B}$, that is, there exist $\dim \mathcal{B}$ affinely independent extreme points of $\mathcal{B}$ that satisfy it with equality. By the above remark, there thus exist $\dim \mathcal{B}$ extreme points of $\mathcal{B}^{n+1}$ that satisfy (16) with equality, such that $\lambda_{i'j'}=k'$ and for which the restrictions $p^{\lambda}(i',j',k')$ are affinely independent. To show that (16) defines a facet of $\mathcal{B}^{n+1}$, it thus remains to find $\dim \mathcal{B}^{n+1}-\dim \mathcal{B}$ affinely independent points satisfying it with equality. For this, consider[34] the extreme points of $\mathcal{B}^{n+1}$ with $\lambda_{i'j'}\neq k'$. They form an affine subspace of dimension $\dim \mathcal{B}^{n+1}-\Pi_{i\neq i'}(\Sigma_{j=1}^{m_i}(v_{ij}-1)+1)=\dim \mathcal{B}^{n+1}-\dim \mathcal{B}-1$ since they can be identified with the extreme points of the polytope involving one outcome less than $\mathcal{B}^{n+1}$ for the measurement j'. Moreover, because they verify $p^{\lambda}(i',j',k')=0$, they satisfy (16) with equality, and are affinely independent from the extreme points for which $\lambda_{i'j'}=k'$. □

We thus have just shown that any facet inequality of an n-partite polytope can be extended to a facet inequality for a situation involving $n+1$ parties. This result can be used sequentially so that facets of n-party polytopes are lifted to $(n+k)$-partite polytopes. For instance, the positivity conditions (11) can be viewed as the successive lifting of 1-party inequalities.

The result holds in the other direction as well, since any facet inequality of the form (16) is the lifting of an n-partite inequality. When studying Bell polytopes, it is thus in general sufficient to consider *genuinely n-partite inequalities*, that is, inequalities that cannot be written in a form that involves only probabilities associated with one specific measurement setting j' and one specific outcome k' for some party i'. Note that we can extend this definition to also exclude all inequalities such as (12) that involve only probabilities associated to one measurement setting (but possibly several outcomes corresponding to this measurement). Indeed, we have noted at the end of Sec. III B that such inequalities cannot be stronger than inequalities of the form (16).

B. One more measurement outcome

Consider a polytope $\mathcal{B}\equiv\mathcal{B}(n,m,v)$, where for measurement j' of party i' the $v_{i'j'}$ outcomes are labeled $\{1,\ldots,k'-1,k'+1,\ldots,v_{i'j'}+1\}$ for some k'. Let

$$b \cdot p \geqslant b_0 \tag{17}$$

be a genuinely n-partite inequality valid for $\mathcal{B}$. Let us consider the polytope $\mathcal{B}^{v+1}$ obtained from $\mathcal{B}$ by allowing an extra outcome k' for the measurement j' of party i'. To lift the inequality $b\cdot p \geqslant b_0$ to the polytope $\mathcal{B}^{v+1}$, we can merge the additional outcome k' with some other outcome $k^* \in\{1,\ldots,k'-1,k'+1,\ldots,v_{i'j'}+1\}$, and insert the resulting probability distribution in (15). This results in the inequality

$$b \cdot p + b(i',j',k^*) \cdot p(i',j',k') \geqslant b_0. \tag{18}$$

Theorem 5: *If the genuinely n-partite inequality* (15) *supports a facet of* $\mathcal{B}$, *then* (18) *supports a facet of* $\mathcal{B}^{v+1}$.

Proof: The dimension of $\mathcal{B}^{v+1}$ equals $\dim \mathcal{B}+\Pi_{i\neq i'}(\Sigma_{j=1}^{m_i}(v_{ij}-1)+1)$. The extreme points of $\mathcal{B}$

that belong to the facet $b\cdot p\geqslant b_0$ provide $\dim \mathcal{B}$ affinely independent points satisfying (18) with equality. By Lemma 3, there exist $\Pi_{i\neq i'}(\Sigma_{j=1}^{m_i}(v_{ij}-1)+1)$ extreme points p^{λ} with $\lambda_{i'j'}=k^*$ that saturate (15), and thus (18), and for which the $p^{\lambda}(i',j',k^*)$ are affinely independent. Replace k^* by k' in these extreme points. These new extreme points still satisfy (18) with equality and are affinely independent with all the previous ones, since they are the unique extreme points with $p^{\lambda}(i',j',k')\neq 0$. In total, we thus enumerated $\dim \mathcal{B}^{v+1}=\dim \mathcal{B}+\Pi_{i\neq i'}(\Sigma_{j=1}^{m_i}(v_{ij}-1)+1)$ affinely independent point satisfying (18) with equality. □

C. One more measurement setting

Consider a polytope $\mathcal{B}\equiv\mathcal{B}(n,m,v)$, where for party i' the $m_{i'}$ measurements are labeled $\{1,\ldots,j'-1,j'+1,\ldots,m_{i'}+1\}$ for some j'. Let the polytope $\mathcal{B}^{m+1}$ be the polytope obtained from $\mathcal{B}$ by allowing the additional measurement setting j' for party i'. An inequality $b\cdot p\geqslant b_0$ valid for $\mathcal{B}$ is also clearly valid for $\mathcal{B}^{m+1}$. Moreover, the following stronger result holds.

Theorem 6: *Let $b\cdot p\geqslant b_0$ be a genuinely n-partite inequality supporting a facet of $\mathcal{B}$. Then it is also support a facet of $\mathcal{B}^{m+1}$.*

Proof: Consider the polytope $\tilde{\mathcal{B}}^{m+1}$ defined as $\mathcal{B}^{m+1}$ but such that for the measurement j' of party i' is associated a single possible outcome, i.e., $v_{i'j'}=1$. The inequality $b\cdot p\geqslant b_0$ is a valid genuinely n-partite inequality for $\tilde{\mathcal{B}}^{m+1}$. Further, since $\tilde{\mathcal{B}}^{m+1}$ and $\mathcal{B}$ have the same dimension, it is also facet defining for $\tilde{\mathcal{B}}^{m+1}$. Following the procedure to lift an inequality to more outcomes delineated in Sec. IV B, this inequality can be lifted from $\tilde{\mathcal{B}}^{m+1}$ to $\mathcal{B}^{m+1}$. Since $b\cdot p\geqslant b_0$ does not involve components associated with the measurement j' of party i', this results in the inequality $b\cdot p\geqslant b_0$ itself. By Theorem 5, this inequality is facet defining for $\mathcal{B}^{m+1}$. □

V. CONCLUSION

We have shown that the facial structure of Bell polytopes is organized in a hierarchical way, with all the facets of a given polytope inducing, through their respective liftings, facets of more complex polytopes. Instead of considering the entire set of facets of a Bell polytope, it is thus in general sufficient to characterize the ones that do not belong to simpler polytopes. It would be interesting to investigate whether this fact could be exploited to improve the efficiency of the algorithms used to list facet inequalities or to simplify analytical derivations of Bell inequalities.

Note that for certain polytopes, the complete set of facet inequalities is constituted entirely by inequalities lifted from more elementary polytopes. For instance for Bell scenarios involving two observers, the first having a choice between two dichotomic measurements and the second one between an arbitrary number of them, all the facet-defining inequalities correspond to liftings of the CHSH inequality.[18,31] A natural extension of the results reported in this article would then be to investigate more generally when inequalities lifted from simpler polytopes describe complete sets of facets. Progress along this line would allow one to narrow down the class of Bell scenarios that have to be considered to find new Bell inequalities. Following this approach, all the polytopes for which the only facets correspond to liftings of the CHSH inequality have recently been characterized.[35]

Finally, let us note that while the facet-preserving liftings that we have considered are interesting because they throw light on the structure of Bell polytopes, the inequalities obtained in this way are not essentially different from the original ones, they are merely re-expressions of these inequalities adapted to more general scenarios. However, it is also in principle possible to consider more complicated generalizations of Bell inequalities that alter significantly their intrinsic structure. For instance, the family of Bell inequalities introduced in Ref. 36 can be understood as being generated by successive nontrivial liftings of the CHSH inequality. Studying such liftings, as well as the other possible extensions of our results, seems a promising path toward a more accurate characterization of the constraints that separate the set of local joint probabilities from the set of nonlocal ones.

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Neveu–Schwarz fivebrane and tachyon condensation

Debashis Ghoshal[a] and Dileep P. Jatkar[b]
Harish-Chandra Research Institute, Chhatnag Road, Jhusi, Allahabad 211019, India

Maximilian Kreuzer[c]
Institut für Theoretische Physik, Technische Universität Wien, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria

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We argue that a semi-infinite D6-brane ending on an NS5-brane can be obtained from the condensation of the tachyon on the unstable D9-brane of type IIA theory. The construction uses a combination of the descriptions of these branes as solitons of the worldvolume theory of the D9-brane. The NS5-brane, in particular, involves a gauge bundle which is operator valued, and hence is better thought of as a gerbe. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1922069]

I. INTRODUCTION

In type IIA string theory a D6-brane can end on a Neveu–Schwarz (NS) fivebrane in a supersymmetric configuration.[1] The simplest way to see this is to start from a fundamental string ending on a D5-brane in type IIB theory. Indeed this defines a *Dirichlet* fivebrane. Now by S-duality followed by T-dualities along all the spatial directions of the worldvolume of the resulting NS5-brane we reach the desired configuration. Recall that this system (and its T-dual cousins) are essential ingredients in "brane engineering" of gauge theory dynamics following Ref. 2.

Naively a semi-infinite brane in a flat space cannot exist by charge conservation. There is a quantized charge of a D6-brane through a two-sphere enclosing it. However, in case of a semi-infinite brane this S^2 can just be "slipped off" the end and collapsed, leading to an apparent contradiction. This argument fails because we are in a situation with a nontrivial Neveu–Schwarz B-field provided by the fivebrane. The gauge-invariant field strength is not simply the curvature of the RR one-form gauge field.[3] The NS B-field also couples to the Chan–Paton gauge field modifying the Bianchi identity[4] to $dF \sim H$.

We would like to obtain the semi-infinite D6-brane ending on a NS5-brane via tachyon condensation on the unstable D9-brane. According to Sen,[5] all D-branes in type IIA string theory arise as solitons of the worldvolume theory on the D9-branes. (For early work on tachyon condensation in string theory, see Ref. 6.) In particular, the stable D6-brane is an 't Hooft-Polyakov monopole of the gauge field-tachyon system on at least two D9-branes.[7] The situation is more complicated in the presence of the nontrivial B-field due to the fivebrane (see Ref. 8 where many configurations involving D-branes and the NS5-brane were discussed). Any configuration must satisfy the modified Bianchi identity. In our case, the relation $dF \sim H$ must hold for both the final D6-NS5-brane configuration *after* the tachyon condensation, as well as *before* it, for the D9-NS5-brane system. The problem of tachyon condensation in the presence of an H field whose quantized charges are $\mathbf{Z}_n$ valued was analyzed in Ref. 4. This was generalized to the usual integrally quantized case in Ref. 9, which argues that in this situation one needs to consider the group of unitary operators in a Hilbert space as the gauge group on the D9-brane. Operator valued gauge fields appear in a natural way in the solitons of noncommutative gauge theory.[10,11] Indeed, Harvey and Moore[12] have suggested a configuration to describe a NS5-brane as a noncommutative soliton

[a]Electronic mail: ghoshal@mri.ernet.in
[b]Electronic mail: dileep@mri.ernet.in
[c]Electronic mail: kreuzer@hep.itp.tuwien.ac.at

of open string theory (see also Ref. 13). We present our arguments in this setup.

It turns out that our construction is related to one version of what is called a *gerbe*,[14] one in which it is described by operator valued gauge fields. (Let us note parenthetically that in their study of the antisymmetric tensor gauge fields, Freund and Nepomechie[15] discovered gerbes in string theory. Some recent applications to string theory may be found in Refs. 16 and 17.) As a matter of fact, the NS5-D6-brane configuration has been obtained as a stable solution of massive type IIA supergravity,[16] in the language of gerbes. However, a different description of gerbes in terms of local U(1) bundles was used in Ref. 16, which did not discuss tachyon condensation either.

II. FIELD THEORY ANALOG

It is instructive to look at a simpler field theory model, in four space–time dimension, which share the essential features of the brane configuration we wish to obtain after tachyon condensation. This model consists of a semi-infinite Nielsen–Olesen vortex of the Abelian Higgs model ending on a Dirac monopole. We can think of this monopole as a singular limit of the 't Hooft-Polyakov monopole in the SO(3) Georgi–Glashaw model. With the Higgs field pointed radially outwards in the field space, this is a nonsingular solution to the equations of motion with mass proportional to M_W/g_{YM}^2. The Nielsen–Olesen vortex, on the other hand, has constant finite energy per unit length. A semi-infinite vortex ending on a monopole is then an infinite energy configuration. To minimize its energy, the vortex will reduce its length thereby pulling the monopole along all the way to infinity. Hence the semi-infinite vortex string ending on a monopole is unstable.

There exists a remarkable way to stabilize this configuration by putting the monopole inside an accelerating black hole.[18] Here we begin with the Abelian Higgs model coupled to gravity. This model has cosmic string, i.e., Nielsen–Olesen vortex solution as well as, say, a Schwarzschild black hole solution. Let us consider a configuration in which the vortex ends on a black hole. In this case one finds an axisymmetric metric with a conical singularity on the accelerating Schwarzschild black hole, whose metric up to a conformal factor is (see the third reference in Ref. 19),

$$\mathrm{d}s^2 = f(r)\mathrm{d}t^2 - f^{-1}(r)\mathrm{d}r^2 - r^2\mathrm{d}\theta^2 - r^2(1-\alpha)^2\sin^2\theta\,\mathrm{d}\phi^2, \tag{1}$$

where

$$f(r) = \left(1 - \frac{2M}{r} - A^2r^2\right)$$

and A is the acceleration of the black hole. The deficit angle of the conical singularity is proportional to α. This is a reflection of the fact that the vortex is piercing the black hole horizon. The Schwarzschild black hole horizon has the topology of a two sphere. Suppose in the frame of an asymptotic observer the vortex ends on the south pole of the horizon, then we can take a loop on the horizon around the south pole and measure the magnetic flux of the vortex. For one vortex configuration, the *angle valued* Higgs field Φ winds once around this loop. Now, by deforming this loop we can shrink it at the north pole. Since the vortex pierces the horizon only once, the shrinking of the loop at the north pole seems to lead to a contradiction. However, this result is misleading as the value of Φ is gauge dependent. The vortex is also accompanied by a topologically nontrivial gauge field configuration. A consistent solution corresponds to defining the Hopf fibration over S^2. This can be achieved by defining two charts on S^2,

$$\mathcal{U}_N = \{\theta, \phi: \theta < \pi\}, \quad \mathcal{U}_S = \{\theta, \phi: \theta > 0\}. \tag{2}$$

On the overlap, the fields are related by the transition function $g_{\mathrm{NS}} = \exp(-i\phi)$ as

$$\exp(i\Phi_N) = g_{NS}\exp(i\Phi_S), \quad A_{N\mu} = A_{S\mu} + ig_{NS}^{-1}\partial_\mu g_{NS}. \tag{3}$$

Since the vortex is on the lower hemisphere, we can take $\Phi_N=0$ and $A_N=0$ on the northern hemisphere and connect it to the vortex configuration on the southern hemisphere via the topologically nontrivial transition function. This configuration makes sense as long as the S^2 horizon does not shrink to zero size. This is ensured by the fact that the extended Schwarzschild geometry in the Kruskal coordinates is a wormhole with topology $S^2\times\mathbf{R}$, the minimum radius of the sphere being $2GM$. In the extended geometry, absence of the vortex in the northern hemisphere can be explained in the following manner. As the vortex approached the south pole of the horizon it goes down the throat of the wormhole and reappears through the horizon in the other asymptotic region.

Let us now get back to the winding number of Φ. This quantity is not gauge invariant in the presence of a nontrivial gauge field configuration. The field Φ is also not single valued everywhere on the sphere. We can, however, define a quantity

$$\mathcal{A} = d\Phi - A, \tag{4}$$

which is both gauge invariant and single valued. In the northern hemisphere we have chosen $\Phi_N=0$ and $A_N=0$, which implies even in the southern hemisphere the net winding charge should vanish. Clearly $\mathcal{A}$ being single valued has zero winding charge. On the other hand, we saw that a vortex solution near the south pole has $d\Phi$ winding number one. Hence we conclude that the integral of A around the loop near the south pole also has unit winding charge.

III. NEVEU–SCHWARZ FIVEBRANE IN OPEN STRING THEORY

The NS5-brane is a soliton of the closed string theory. Therefore one does not expect to see detailed features of it in open string theory. Nevertheless, it turns out that some topological aspect of the NS5-brane can be captured in terms of open strings. Harvey and Moore[12] have a configuration with the right H-flux. In fact they have argued that the NS5-brane may be thought of as a particular soliton in the noncommutative gauge theory of the unstable D9-brane in type IIA theory. This is inspired by the idea of a noncommutative tachyon.[11]

We will now review this construction. In Ref. 12, the space–time topology is chosen to be $\mathbf{R}^{1,4}\times\mathbf{R}^2_{NC}\times S^2\times S^1$ and the H-flux is through the 3-cycle $S^2\times S^1$. This is based on an example in Ref. 20. We will work, however, with $\mathbf{R}^{1,4}\times\mathbf{R}^2_{NC}\times S^3$, which is the space–time topology, at least in the near horizon limit, of the NS5-brane.[21] There is a *constant* NS B-field along $\mathbf{R}^2_{NC}$. It should be emphasized that this is not the B-field that contributes to the H-flux, but has the effect of making the (the $\mathbf{R}^2_{NC}$ part of) space–time noncommutative. Therefore we may treat the tachyon, gauge, and other fields as operator valued on $\mathbf{R}^{1,4}\times S^3$. Henceforth we will concentrate only on the S^3 part.

In Refs. 9 and 22, it was argued that the gauge group in noncommutative gauge theory is $\mathrm{U}_{\mathrm{cpt}}(\mathcal{H})$, a subgroup of unitary operators in a Hilbert space $\mathcal{H}$ of the form $u=\mathbf{1}+K$, where $K\in\mathcal{K}(\mathcal{H})$ is a compact operator. Conjugation by elements of the group $\mathrm{U}(\mathcal{H})$ are automorphisms of the corresponding Lie algebra $\mathcal{K}(\mathcal{H})$ of compact operators. However, since the U(1) center of $\mathrm{U}(\mathcal{H})$ acts trivially, the automorphism of $\mathcal{K}(\mathcal{H})$, [and hence of $\mathrm{U}_{\mathrm{cpt}}(\mathcal{H})$], is really $\mathrm{PU}(\mathcal{H})=\mathrm{U}(\mathcal{H})/\mathrm{U}(1)$. The Lie algebra valued gauge field and the tachyon which transform in the adjoint representation are therefore valued in $\mathcal{K}(\mathcal{H})$. A nontrivial gauge bundle may be constructed with a twist by an element of $\mathrm{Aut}(\mathcal{K}(\mathcal{H}))=\mathrm{PU}(\mathcal{H})$. The proposal of Ref. 12 is that an appropriate nontrivial $\mathrm{PU}(\mathcal{H})$ bundle on S^3, with the tachyon field at the maximum of the potential, represents a D9-brane and a NS5-brane. Moreover, when the tachyon condenses to a minimum of the potential, there is only a NS5-brane as the D9-brane ought to have disappeared according to Sen's conjecture.[5]

The key to the construction of this $\mathrm{PU}(\mathcal{H})$ bundle is the fact that $\pi_2(\mathrm{PU}(\mathcal{H}))=\mathbf{Z}$. It is then possible to patch together trivial bundles on local coordinate charts of S^3 along their overlaps. This is a one higher dimensional generalization of the construction of a monopole on S^2, which used the fact that $\pi_1(\mathrm{U}(1))=\mathbf{Z}$. As we have mentioned before, the base space in Ref. 12 is $S^2\times S^1$. The Hopf fibration $S^3\to S^2$ and the covering space of the fiber $\mathbf{R}\to S^1$ defines a natural $S^1\times\mathbf{Z}$ bundle

on it. This is embedded in PU($\mathcal{H}$) by lifting the circle coordinate to an angle valued position operator $\hat{\Omega}$ and its (integrally quantized) conjugate momentum $\hat{L}$ satisfying a Heisenberg algebra

$$[\hat{\Omega},\hat{L}] = i\hat{1}. \tag{5}$$

Let us review some details of this construction following Ref. 20. One starts with a principle U(1) bundle $P(\mathrm{U}(1))$ over a base manifold X and the universal covering space $\mathbf{R}$ of S^1. This defines a principle $P(\mathrm{U}(1)\times\mathbf{Z})$ bundle over the base space $X\times S^1$. In the following we will consider the specific example of the Hopf bundle $X=S^2$ and $P(\mathrm{U}(1))=S^3$. Given a (vector) space V on which the group G acts, it is possible to define a fiber bundle $E_V\to X\times S^1$ associated to the principle G bundle by the quotient $(P(G)\times V)/G$. The fiber of this bundle [recall that in the associated bundle the sections coming from a quotient action of G on $G\times V$ are identified as $(s,v)\sim(sg,g^{-1}v)$ providing a twist] is isomorphic to V. The frame bundle and the tangent bundle to a manifold is an example of such a pair. Another natural association is one in which V is the Lie algebra $\hat{g}$ of G or any of its representations. The G action on V, in turn, induces an adjoint action on the space of linear operators $\mathcal{L}(V)$ on V. One can, therefore, construct an associated "bundle" whose fiber is $\mathcal{L}(V)$ and the transition functions g_{ij} act by adjoint action (with the center acting trivially). In particular, our objective will be to construct a bundle whose fiber consists of operators in the Hilbert space $\mathcal{H}$ of square integrable functions $L^2(S^1)$ of a projective representation of the Heisenberg group H, which is a central extension of the group $S^1\times\mathbf{Z}$.

In order to specify the bundle, it will be sufficient to give a local trivialization over open sets $\mathcal{U}_i$, in which we specify the Hilbert space of functions and provide the transition functions. Let $(x=(\psi,\theta),\phi)$ be points in $S^2\times S^1$ and

$$p{:}S^3\times\mathbf{R}\to S^2\times S^1$$

be the projection map of the smaller bundle with which the construction proceeds. The fiber $p^{-1}(x)$ is a circle S^1_x without any fixed base point. The universal cover $\tilde{S}^1_x\sim\mathbf{R}_x$ is ambiguous up to the cyclic group generated by T which shifts the coordinate of $\mathbf{R}_x$ by (2π times) an integer. Consider the Hilbert space of functions

$$\mathcal{H}_{(x,\phi)} = \{f{:}\mathbf{R}_x\to\mathbf{R}_x | f(T(\xi)) = e^{i\phi}\cdot f(\xi), \tilde{\xi}\in\mathbf{R}_x\}. \tag{6}$$

Of course, the space depends on the choice of coordinates on the universal cover, but the ambiguity is up to an action of T, which acts as multiplication by a scalar leading to a unique projective Hilbert space. Let S^1 be a circle which we can identify with the fiber S^1_x. With an abuse of notation we will use the same angular coordinate ξ on both these circles. Consider the square integrable functions $f(\xi)$ on the circle satisfying the following property under the isomorphism $\lambda_{(x,\phi)}{:}L^2(S^1)\sim\mathcal{H}_{(x,\phi)}$:

$$\lambda_{(x,\phi)}(f(\xi)) = \exp\left(\frac{i}{2\pi}\xi\phi\right)f(\xi).$$

This specifies the local trivialization. It is easy to check that the above satisfies the property required of $\mathcal{H}_{(x,\phi)}$ defined above.

The Lie algebra $\hat{\mathfrak{h}}$ of the group H has generators

$$(\hat{L},\hat{1}) = \left(-i\frac{\mathrm{d}}{\mathrm{d}\xi},\hat{1}\right).$$

Since the spectrum of the angular momentum $\hat{L}$ is discrete, there is no Lie algebra associated with the generator $\hat{\Omega}$ of the Heisenberg algebra (5). Rather $\exp(2\pi i\hat{\Omega})\sim T$ is the generator of the automorphism discussed earlier. The group H acts by adjoint action on $\hat{\mathfrak{h}}$. While the action of the center and the shift in S^1 generated by $\hat{L}$ is trivial, the $\mathbf{Z}$ acts nontrivially as follows:

$$e^{2\pi i\ell\hat{\Omega}}\hat{L}e^{-2\pi i\ell\hat{\Omega}} = \hat{L} - 2\pi\ell\hat{1}. \tag{7}$$

The sections of the associated PU($\mathcal{H}$) bundle are vectors $v(x,\phi)$ in $\hat{\mathsf{h}}$ satisfying

$$v(x,\phi + 2\pi\ell) = e^{2\pi i\ell\hat{\Omega}}v(x,\phi)e^{-2\pi i\ell\hat{\Omega}}.$$

Writing v in terms of the basis elements as $v=v_1(x,\phi)\hat{1}+v_2(x,\phi)\hat{L}$, we get: $v_1(x,\phi+2\pi\ell) = v_1(x,\phi)-2\pi\ell v_2(x,\phi)$ and $v_2(x,\phi+2\pi\ell)=v_2(x,\phi)$.

The final ingredient is a linear function from the PU($\mathcal{H}$) bundle to $\mathbf{R}$. In order to motivate this, let us start with the exact sequence of vector spaces V_C (generated by $\hat{1}$), $\hat{\mathsf{h}}$ and $V_{\hat{L}}$ (generated by $\hat{L}$). The exact sequence of bundles

$$E_{\mathbf{R}} \to E_{\hat{\mathsf{h}}} \to E_{V_{\hat{L}}}$$

follows from it, moreover, $E_{\mathbf{R}} \sim \mathbf{R}\times(S^2\times S^1)$ is a trivial bundle. However, while in the former sequence $\hat{\mathsf{h}}$ cannot be written as a direct sum of V_C and $V_{\hat{L}}$, it is possible to do so in the latter (although the Lie algebra will not be respected in the process). The linear function, which we will call "tr,"

$$\mathrm{tr}: E_{\hat{\mathsf{h}}} \to \mathbf{R},$$

provides this decomposition. For a vector $v\in\hat{\mathsf{h}}$, which can be written in terms of the basis elements as $v=v_1(x,\phi)\hat{1}+v_2(x,\phi)\hat{L}$, we define

$$\mathrm{tr}(v) = (v_1(x,\phi) - \phi v_2(x,\phi)). \tag{8}$$

It is clear from (7) that the function tr is well defined on the PU($\mathcal{H}$) bundle. In particular, when $v_1=0$, $v_2=1$, we have

$$\mathrm{tr}(\hat{L}) = \phi.$$

We will use this in a moment.

In order to specify a connection on this bundle, we start with a connection on the priciple U(1) bundle $p:S^3\to S^2$, which is the familiar monopole gauge field configuration $A^{(M)}$. The gauge field of this bundle is a one-form on S^2 valued in the Lie algebra generated by $-i(\mathrm{d}/\mathrm{d}\xi)$. The gauge connection of the PU($\mathcal{H}$) bundle is a one-form valued in $\hat{\mathsf{h}}$ and is taken to be $A^{(M)}$. Since $\hat{\mathsf{h}}$ is Abelian, the curvature of this connection is a two-form,

$$F^{(M)} = dA^{(M)}\hat{L},$$

where we have displayed the $\hat{\mathsf{h}}$ dependent part explicitly (this is the same as writing $F=F^aT^a$ in YM theories). Acting with the linear function tr, we obtain $\mathrm{tr}\,F^{(M)}=\mathrm{d}A^{(M)}\phi$. This is called the "scalar curvature" in Ref. 20. It is a two-form which is not closed, rather $\mathrm{d}\,\mathrm{tr}\,F^{(M)}\sim\mathrm{vol}(S^2\times S^1)$.

In case of the S^3 base, once again we use the Hopf fibration, however, this time, following Ref. 23 the U(1) action along the fiber is lifted to a U(1) action in PU($\mathcal{H}$) with the help of a cocycle. Let us consider S^3 as the unit sphere defined by $x_1^2+x_2^2+x_3^2+x_4^2=1$, which may be written as

$$|z_0|^2 + |z_1|^2 = 1,$$

in terms of complex coordinates of $\mathbf{C}^2[x_1+ix_2, x_3+ix_4]$. Let us cover S^3 by charts

$$\mathcal{U}_0 = \{(z_0, z_1) \in S^3 : |z_0| \geqslant |z_1|\},$$
$$\mathcal{U}_1 = \{(z_0, z_1) \in S^3 : |z_0| \leqslant |z_1|\}. \tag{9}$$

Each $\mathcal{U}_i$ is topologically a disc times S^1 and they overlap on a two-torus

$$\mathcal{U}_0 \cap \mathcal{U}_1 = T^2 = \{(z_0, z_1) \in S^3 : |z_0| = |z_1| = 1/\sqrt{2}\}. \tag{10}$$

The simplest way to see that S^3 has this topological structure is to think $S^3 = \mathbf{R}^3 \cup \{\infty\}$. Now, if we remove a solid torus from $\mathbf{R}^3$, what remains, together with the point at infinity, is also a solid torus. Introduce coordinates (ψ, θ, ϕ) on S^3 such that $z_0 = \cos(\psi/2) e^{i(\phi+\theta)/2}$ and $z_1 = \sin(\psi/2) e^{i(\phi-\theta)/2}$. The bundle structure of Hopf fibration is given by the local trivializations

$$\mathcal{U}_0 \sim \left(\frac{z_1}{z_0}, \frac{z_0}{|z_0|}\right), \quad \mathcal{U}_1 \sim \left(\frac{z_0}{z_1}, \frac{z_1}{|z_1|}\right), \tag{11}$$

along with the transition function z_0/z_1 on the overlap. The U(1) action

$$(z_0, z_1) \to (e^{-i\omega} z_0, e^{-i\omega} z_1) \tag{12}$$

along the fiber is an isometry of S^3. [The metric in these coordinates is $ds^2 = \frac{1}{4}(d\psi^2 + \sin^2\psi\, d\theta^2 + (d\phi + \cos\psi\, d\theta)^2)$.]

The PU($\mathcal{H}$) bundle on S^3 is specified by a map

$$g_{01} : \mathcal{U}_0 \cap \mathcal{U}_1 = T^2 \to \mathrm{PU}(\mathcal{H}). \tag{13}$$

Local trivializations

$$f_0 : \mathcal{U}_0 \to \mathcal{K}(\mathcal{H}), \quad f_1 : \mathcal{U}_1 \to \mathcal{K}(\mathcal{H})$$

are related by $f_0 = g_{01}(f_1) = g_{01} f_1 g_{01}^{-1}$ on the overlap. The topological properties of the bundle are characterized by the homotopy class of g_{01}, an element of maps from T^2 to PU($\mathcal{H}$). Now since $\pi_n(\mathrm{U}(\mathcal{H})) = 0$ for all n,[24] we have $\pi_{n-1}(\mathrm{U}(1)) = \pi_n(\mathrm{PU}(\mathcal{H}))$, hence the only nonvanishing homotopy group of PU($\mathcal{H}$) is π_2 and this is $\mathbf{Z}$. The homotopy classes of maps g_{01} of interest is therefore isomorphic to $H^2(T^2, \mathbf{Z})$ (see, for example, Ref. 25 Chap. 1). Now, using the relation[26] between the differential complexes on $\mathcal{U}_0$, $\mathcal{U}_1$, $\mathcal{U}_0 \cup \mathcal{U}_1 = S^3$ and $\mathcal{U}_0 \cap \mathcal{U}_1 = T^2$, we have $H^2(T^2, \mathbf{Z}) = H^3(S^3, \mathbf{Z}) = \mathbf{Z}$.

Let us define the U(1) action (12) on the PU($\mathcal{H}$) bundle as

$$\Omega_\omega : (f_0, f_1) \to (f_0^\omega, f_1^\omega),$$
$$\text{where,} \quad f_0^\omega(z_0, z_1) = f_0(e^{-i\omega} z_0, e^{-i\omega} z_1), \tag{14}$$
$$f_1^\omega(z_0, z_1) = h(\omega, z_0, z_1)(f_1(e^{-i\omega} z_0, e^{-i\omega} z_1)),$$

for a function $h(\omega, z_0, z_1) : S^1 \times \mathcal{U}_1 \to \mathrm{PU}(\mathcal{H})$ which satisfy

$$h(\omega, z_0, z_1) = g_{01}^{-1}(z_0, z_1) g_{01}(e^{-i\omega} z_0, e^{-i\omega} z_1) \quad \text{for } (z_0, z_1) \in \mathcal{U}_0 \cap \mathcal{U}_1,$$
$$h(\omega_1 + \omega_2, z_0, z_1) = h(\omega_1, z_0, z_1) h(\omega_2, e^{-i\omega_1} z_0, e^{-i\omega_1} z_1) \quad \text{for } (z_0, z_1) \in \mathcal{U}_1. \tag{15}$$

The first of the conditions (15) ensures that the patching condition given by (13) is respected. In other words, Ω_ω is an automorphism of the triple $(f_0, f_1; g_{01})$ used to define the PU($\mathcal{H}$) bundle. The second condition is a group homomorphism that identifies an S^1 in PU($\mathcal{H}$). The existence of Ω_ω with the required properties is proven in Ref. 23. [The PU($\mathcal{H}$) bundle on S^3 has also been defined through local trivializations $S^3 = D_+^3 \cup D_-^3$, $D_+^3 \cap D_-^3 = S^2$ at the equator.[27] The topological

properties of the bundle are characterized by maps from S^2 to PU($\mathcal{H}$). This, however, does not seem suitable for our purpose as there is no natural U(1) action.]

We will use the above to propose a construction along the lines of Ref. 12, with Ω_ω playing the role of $\hat{\Omega}$ in (5). We cannot identify $\hat{L}$ explicitly in PU($\mathcal{H}$), but proceed with the assumption that there is one such $\hat{L}$ such that (5) is true. This assumption is not untenable since the size of the fiber in Hopf fibration is fixed, namely 4π, therefore the spectrum of $\hat{L}$ is discrete. Motivated by the construction in $S^2 \times S^1$ and the Hopf bundle description of S^3 outlined above, we propose the following expression for the gauge fields using the two charts (11) of $S^{2'}$.

$$A_0 = +\frac{i}{2}(1-\cos\psi)\mathrm{d}\theta\cdot\hat{L},$$
$$A_1 = -\frac{i}{2}(1+\cos\psi)\mathrm{d}\theta\cdot\hat{L}, \tag{16}$$

where we have displayed the algebra generator explicitly. Recall the charts overlap for $\psi=\pi/2$, where the transition functions $(\psi,\theta)\to(\pi-\psi,-\theta)$ of the Hopf bundle ensures that A_0 and A_1 differ by a gauge transformation.

The "scalar curvature" of the gauge field (16) is obtained by taking the tr:

$$\mathrm{tr}\,F = \frac{i}{2}\sin\psi\,\mathrm{d}\psi\wedge\mathrm{d}\theta(\phi+\theta),$$

where, in analogy with (8), we have used $\mathrm{tr}\,\hat{L}=\phi+\theta$, the value of the coordinate of the Hopf fiber of the base space. Notice that this is a well-defined two-form. Finally,

$$\mathrm{d}\,\mathrm{tr}\,F = \frac{i}{2}\sin\psi\,\mathrm{d}\psi\wedge\mathrm{d}\theta\wedge\mathrm{d}\phi \tag{17}$$

is the volume form on S^3 yielding a unit three-form flux through it. It is assumed here that the tachyon is trivial, it is zero corresponding to the maximum of the potential. In other words, this gauge field configuration describes the unstable D9-brane in presence of the NS5-brane.

The NS5-brane so constructed has its worldvolume along $\mathbf{R}^{1,4}$ as well as along one of the noncommutative dimensions in $\mathbf{R}^2_{NC}$. We refer to Ref. 12 for some subtleties with this description.

Finally, although we have been talking about a PU($\mathcal{H}$) bundle, the above construction is not a bundle in the usual sense. In the Appendix, we show how it satisfies the conditions required of a gerbe.

IV. SEMI-INFINITE D6-BRANE AND NS FIVEBRANE

In Sec. III we have constructed a configuration of the operator valued gauge fields in the noncommutative worldvolume theory of the unstable D9-brane of type IIA theory. This configuration carries a unit H-flux through S^3, and satisfies the modified Bianchi $\mathrm{d}\,\mathrm{tr}\,F=H$. It is argued[12] that for the tachyon at the maximum of the potential, this configuration describes the D9-NS5-brane system, while at a minimum there is only a NS5-brane. One expects that, when the tachyon is nontrivial, we should have a configuration of the NS5-brane together with a D-brane of appropriate codimension.

Recall, that in the absence of any H-flux (no NS5-brane), all the stable Dp-branes may be obtained as odd codimension soliton solutions of the tachyon and gauge field theory. In particular the D6-brane is the 't Hooft-Polyakov monopole of the U(2) theory on two D9-branes.[7] Let (x_1,x_2,x_3) be the space transverse to the would be D6-brane. Identifying $\mathrm{SU}(2)\subset\mathrm{U}(2)$ with the (covering space) of the SO(3) group of rotations, the configuration is

$$T \sim x_i \sigma^j,$$
$$A_i \sim \epsilon_{ijk} x^j \sigma^k, \tag{18}$$

where σ^i are the Pauli matrices. There should also be some convergence factors on the right-hand side. One important feature of this construction is that it is local, i.e., it relies only on coordinates in a small neighborhood of the origin where the D6-brane is located.

The configuration we would like to obtain is that of a semi-infinite D6-brane that ends on the NS5-brane. The fivebrane shares all its worldvolume dimensions with the D6-brane, whose additional dimension has a boundary on which the NS5-brane lies. Let us put the NS-brane at the origin of its transverse $\mathbf{R}^4$ directions. This space is foliated by S^3 of varying radii, with the size finally saturating to give the "throat" geometry.[21] The D6-brane appears to be a string which pierces the S^3's at, say, the south pole. Although, to an observer far away from the origin, it would seem that the D6-brane ends on the NS5-brane at the origin, it would be more correct to say that it goes down the "throat." Actually for our case, where there are two noncommutative dimensions and the D6-brane worldvolume extends along both, this picture is an extrapolation from the commutative limit. In particular, the radial direction in $\mathbf{R}^4$, i.e., the direction transverse to S^3 is one of the noncommutative directions.

We would like to argue that the situation is different *after* tachyon condensation. The operator $\hat{\Omega}$ is a shift along the Hopf fiber of S^3. The process of tachyon condensation selects a special point, which we may choose to be the south pole. The fields are localized around this point, in particular, also along the Hopf fiber through it. This in turn, determines the value of the operator $\hat{\Omega}$ to be, say, zero, to an accuracy $\Delta\Omega \sim \varepsilon$. As a result, there is a large uncertainty in the value of the conjugate variable $\hat{L}$: $\Delta L \sim 1/\varepsilon$. This, in effect, makes the spectrum of $\hat{L}$ continuous for sufficiently small ε. Therefore, after the tachyon has condensed, it should be possible to shift $\hat{L}$ by an arbitrary amount. This is in contrast to the previous section in which the fields are not localized in S^3.

We can follow the field theory example in Sec. II and use continuous gauge transformation of the form $\exp(ix\hat{\Omega})$ (for any real x) available now to propose the following gauge field configurations:

$$A_0 = +\frac{i}{2}(1-\cos\psi)\mathrm{d}\theta \cdot \hat{L},$$
$$A_1 = -\frac{i}{2}(1+\cos\psi)\mathrm{d}\theta \cdot (\hat{L} + (\phi-\theta)\hat{1}). \tag{19}$$

At the overlap, an operator valued U(1) gauge transformation,

$$A_1 = e^{-i(\phi-\theta)\hat{\Omega}} A_0 e^{i(\phi-\theta)\hat{\Omega}}, \tag{20}$$

relates the gauge configurations from the chart $\mathcal{U}_0$ to $\mathcal{U}_1$.

An operator valued U(1) gauge transformation is in fact equivalent to the gauge transformation of the B field (see the Appendix and Ref. 17). The field configuration (19) has the property that in the chart $\mathcal{U}_0$, $\mathrm{d}\,\mathrm{tr}\,F_0 \sim \mathrm{vol}(S^3)$ as before, but in $\mathcal{U}_1$, $\mathrm{tr}\,F_1$ and hence $\mathrm{d}\,\mathrm{tr}\,F_1$ vanish. Hence there is a NS H-flux through $\mathcal{U}_0$ but none through $\mathcal{U}_1$.

Continuing to follow the field theory example, we now need to show that the operator valued U(1) gauge field configuration (19) arises from a configuration of the tachyon and gauge fields (in the S^3 part of the worldvolume of the non-BPS D9-brane). This ought to localize the energy around the south pole of S^3, which we assume is at the origin of $\mathcal{U}_0$. Unfortunately, we are not able to write this explicitly. However, the operator corresponding to the tachyon field is expected to be of the form

$$T \sim \int \mathrm{d}\varphi |\varphi\rangle\langle\varphi| e^{-\varphi^2/\varepsilon^2}, \tag{21}$$

which is a projection operator. Interestingly, in Ref. 7, it is shown that the configuration (18) can also be thought of as a two step process of a vortex and a kink. This seems more natural in the present situation as the local symmetry group around the south pole is $\mathrm{SO}(2)\times\mathbf{R}$, since $\mathcal{U}_0$ has the topology of a cylinder $D_0^2\times S^1$, which naturally accommodates this break up.

V. BIANCHI IDENTITIES AND CHARGE CONSERVATION

In Ref. 16 the NS5-D6-brane configuration described in Sec. IV was shown, following a construction in Ref. 14, to be a solution of type IIA supergravity using a description of gerbes as local line bundles. There the various charge conservation conditions are discussed in detail. Briefly, consider an S^2 surrounding the D6-brane. There is a flux of the RR one-form gauge field $C^{(1)}_{\mathrm{RR}}$ through it. In the absence of any H-flux, this measures the quantized RR charge of the D6-brane. This arises from the Chern–Simons couplings, ($\mathrm{d}T\wedge F_{CP}\wedge C^{(7)}$, $\mathrm{d}T\wedge\mathrm{d}T\wedge\mathrm{d}T\wedge C^{(7)}$, etc.), on the D9-brane. When a NS B-field is present, the correct gauge invariant field strength for this field is[3]

$$G^{(2)}_{\mathrm{RR}} = \mathrm{d}C^{(1)}_{\mathrm{RR}} + mB, \tag{22}$$

where B is the NS two-form and m is the mass parameter. Similarly,

$$\mathcal{F} = dA_{CP} - B \tag{23}$$

is a gauge invariant combination of the field strength involving the Chan–Paton gauge field.

In our description, the flux is through a two-cycle T^2 at the overlap of $\mathcal{U}_0$ and $\mathcal{U}_1$. This is assumed to enclose D6-brane at the south pole of S^3. Since the D6-brane is semi-infinite, there is no Chan–Paton gauge field flux through the chart $\mathcal{U}_1$. We can also choose to set $B=0$ here. This means $\mathcal{F}=0$ in $\mathcal{U}_1$, and in particular, there is no $\mathcal{F}$-flux through it. Notice that $\mathcal{F}$ is gauge invariant and therefore $\mathcal{F}$-flux must vanish everywhere. The overlap T^2 is the boundary of a three-space $\mathcal{U}_0$, which is that part of the S^3 through which there is a nontrivial H-flux. The anomalous Bianchi identity[3] from (22) ensures that there is no net six-brane charge. By drawing analogy with the field theory example, it now follows that the net monopole charge through a T^2 (at the overlap of $\mathcal{U}_0$ and $\mathcal{U}_1$ or any deformation of it in $\mathcal{U}_0$), enclosing the south pole of S^3 should also vanish. Since $\mathcal{F}$-flux through T^2 vanishes and the flux of $\mathrm{d}A_{CP}$ does not, we conclude that the monopole charge evaluated by integrating $\mathrm{d}A_{CP}$ over a T^2 enclosing the south pole is equal to the boundary value of the H-flux through the three-space $D_0^2\times S^1$ enclosed by T^2, i.e.,

$$\oint_{T^2} \mathrm{d}A_{CP} = \int_{D_0^2\times S^1} H = \oint_{T^2} B. \tag{24}$$

This in effect implies a modified Bianchi identity

$$\mathrm{d}F_{CP} = H \tag{25}$$

for the NS5-D6-brane configuration.

VI. DISCUSSION

We have argued how to realize a configuration in which a semi-infinite D6-brane ends on a NS5-brane via condensation of the tachyon field on the worldvolume of unstable D9-branes. Both the five- as well as the six-brane are solitonic configurations in the noncommutative field theory on the D9-brane. Let us emphasize that although the six-brane by itself is a solution of this field theory, the NS5-brane is only a configuration. In the framework of open string theory, it is as yet unclear in what sense a solitonic object of closed string theory can be realized as a solution. Some

topological aspect of the NS5-brane can, however, be reproduced. Our intersecting brane configuration, in which we have combined features of Refs. 7 and 12, is also not a solution of the open string equations of motion.

The geometrical description we have used is strictly valid for large values of NS5-brane charge, or far away from the core of the fivebrane. Moreover, two of the longitudinal directions of our D6-brane carry a constant B field. This is the B field introduced to have a noncommutative worldvolume theory. The Chern–Simons coupling $B\wedge C^{(5)}_{\mathrm{RR}}$ therefore results in an induced D4-brane charge in the configuration.

Let us end by some speculative remarks on D3-branes in SU(2) WZW model. In this case, it is well-known that the symmetries allow only D2-branes and D0-branes along conjugacy classes of the group manifold.[28] These are S^2's at some fixed "latitudes" of S^3. On the other hand, Ref. 29 argued in favor of D3-branes which wrap almost all of S^3 except for a set of points. More recently, based on consistency with T-duality, Ref. 30 showed that there should be D3-branes which are "fat" D-strings. These have the topology of a cylinder reminiscent of the coordinate charts we have used in our construction of the NS5-D9-brane configuration. While a single fat string cannot cover the entire group manifold without having a singularity, it seems possible for a configuration of two fat D-strings "linked" together to do so. A nontrivial linking should capture the fact that this configuration is a gerbe. This may be possible with operator valued gauge fields on the fat strings.

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APPENDIX: GERBES

Gerbes are generalization of U(1) bundles (more generally line bundles) on a manifold. This appendix contains a quick description of gerbes. Further details and references can be found in the expository article by Hitchin.[14] Reference 17 is an incomplete list of their applications in string theory.

Consider a manifold $\mathcal{M}$ and a set of open charts $\{\mathcal{U}_i\}$ that covers it: $\mathcal{M}=\cup_i\mathcal{U}_i$. We will assume, for simplicity, that each $\mathcal{U}_i$ is contractible. A *1-gerbe* $\mathcal{G}$ on $\mathcal{M}$ is defined by a set of U(1) bundles $\mathcal{L}_{ij}$ on each (ordered) overlap $\mathcal{U}_i\cap\mathcal{U}_j$, satisfying the following conditions

(i) $\mathcal{L}_{ji}=\mathcal{L}_{ij}^*$, (where $\mathcal{L}^*$ is the bundle dual to $\mathcal{L}$),
(ii) on triple overlaps $\mathcal{U}_i\cap\mathcal{U}_j\cap\mathcal{U}_k$, the tensor product bundle $\mathcal{L}_{ij}\otimes\mathcal{L}_{jk}\otimes\mathcal{L}_{ki}$ has a nowhere vanishing section s_{ijk},
(iii) on quadruple overlaps $\mathcal{U}_i\cap\mathcal{U}_j\cap\mathcal{U}_k\cap\mathcal{U}_l$, the section $s_{ijk}\otimes s^*_{ijl}\otimes s_{ikl}\otimes s^*_{jkl}=1$.

Notice that in the last condition, the tensor product of the sections is that of a trivial bundle $\mathcal{M}\times\mathrm{U}(1)$, as follows from the other two conditions. Let us also note that if we take $\mathcal{L}_{ij}=\mathcal{L}_i\otimes\mathcal{L}_j^*$, where $\mathcal{L}_i$ are U(1) bundles on $\mathcal{U}_i$, then all the conditions are trivially satisfied. Therefore this is called a trivial gerbe.

The above may be generalized to k-gerbes by defining line bundles on $(k+1)$-fold overlaps with appropriate conditions. An ordinary line bundle is a 0-gerbe from this point of view. It should be noted that (except for $k=0$) the "total space" of a gerbe is not a manifold, as the definition involves conditions on more than two overlaps.

A *connection* on a 1-gerbe is specified by connections A_{ij} for each $\mathcal{L}_{ij}$ and a two-form B_i on each chart $\mathcal{U}_i$, such that

(i) $A_{ij}=-A_{ji}$,
(ii) s_{ijk} is flat with respect to the induced connection,
(iii) on $\mathcal{U}_i\cap\mathcal{U}_j$, we have $B_i-B_j=dA_{ij}$.

The "curvature" $H=dB$ of this connection is independent of the chart and hence makes sense globally. The cohomology of H is characterized by $H^3(\mathcal{M},\mathbf{Z})$. The quantization is analogous to the case of usual U(1) gauge fields.[31]

As an example, let us describe the "NS5-brane." Consider space–time of the form $\mathbf{R}^{1,5}\times\mathbf{R}\times S^3$, the geometry of the NS5-brane. The only relevant part of it is S^3, on which we will construct a gerbe such that it carries an H-flux. This example is due to Hitchin[14] (and has been used in Ref. 16). First, we cover S^3 with two open 3-discs $D^3_{\pm}$, which overlap around a region around the equatorial S^2. The overlap $D^3_+\cap D^3_-$ has the topology of a "cylinder" $S^2\times\mathbf{R}$. For the U(1) bundle on the overlap, we take the monopole bundle on S^2 (more precisely, the pull-back of this bundle). Let A_{+-} be the gauge field and $F=dA_{+-}$ be its curvature. In order to give their concrete forms, let us introduce coordinates (α,β,γ) on S^3, such that the metric is

$$ds^2 = d\alpha^2 + \sin^2\alpha(d\beta^2 + \sin^2\beta\, d\gamma^2).$$

The overlap region is $\pi/2-\epsilon<\alpha<\pi/2+\epsilon$, and $F_{+-}\sim\sin\beta\, d\beta\wedge d\gamma$. We need to specify the gerbe connections $B_{\pm}$. To this end, consider a partition of unity $\varphi_{\pm}$. Recall that these are functions with supports, respectively, in $D^3_{\pm}$, such that $0\leqslant\varphi_{\pm}\leqslant 1$ and $\varphi_+ + \varphi_- = 1$ at each point. We write,

$$B_{\pm} = \pm\,\varphi_{\pm}F_{+-},$$

which satisfy the condition $B_+ - B_- = F_{+-}$. It is easy to check that the curvature $H=dB$ is independent of the chart. In fact it equals $F_{+-}\wedge d\varphi_+$, which is supported on the overlap. Therefore, using the quantization of the monopole field F_{+-}, we see that the H-flux through S^3 is integrally quantized. It is curious that the gerbe defining an NS5-brane is roughly like a monopole (F part) times a kink (φ part), quite similar to, say, the soliton description of D6-brane in Ref. 7. Reference 16 describes the NS5- and semi-infinite D6-brane configuration in this language.

Finally, let us show how the $\mathcal{K}(\mathcal{H})$ valued gauge fields patched together by $\mathrm{Aut}(\mathcal{K}(\mathcal{H}))=\mathrm{PU}(\mathcal{H})$ satisfy the axioms of a gerbe. In the construction of Sec. III, we have only two coordinate charts, so there is not much to check. Consider, instead, a general setup where we have local trivializations given by maps

$$f_i:\mathcal{U}_i\to\mathcal{K}(\mathcal{H}),$$

which satisfy $f_i=g_{ij}(f_j)=g_{ij}f_jg_{ij}^{-1}$, for $g_{ij}\in\mathrm{PU}(\mathcal{H})$, on twofold overlaps. Hence, on triple overlaps $h_{ijk}=g_{ij}g_{jk}g_{ki}$ must be an element of U(1), [since action of the U(1) center of U($\mathcal{H}$) is trivial]. These h_{ijk}'s may be taken as the sections s_{ijk}'s of (trivial) U(1) bundles on threefold overlaps. It is also easy to check that the conditions on fourfold overlaps is satisfied.

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Normal ordering and boundary conditions in open bosonic strings

Nelson R. F. Braga[a] and Hector L. Carrion[b]
Instituto de Física, Universidade Federal do Rio de Janeiro, Caixa Postal 68528, 21941-972 Rio de Janeiro, Brazil

Cresus F. L. Godinho[c]
Centro Brasileiro de Pesquisas Físicas, Rua Dr Xavier Sigaud 150, 22290-180, Rio de Janeiro, Rio de Janeiro, Brazil

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Boundary conditions play a nontrivial role in string theory. For instance, the rich structure of D-branes is generated by choosing appropriate combinations of Dirichlet and Neumann boundary conditions. Furthermore, when an antisymmetric background is present at the string end points (corresponding to mixed boundary conditions) space time becomes noncommutative there. We show here how to build up normal ordered products for bosonic string position operators that satisfy both equations of motion and open string boundary conditions at the quantum level. We also calculate the equal time commutator of these normal ordered products in the presence of an antisymmetric tensor background. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1914727]

I. INTRODUCTION

Recent progress in string theory[1] indicates a scenario where our four-dimensional space-time should correspond to a D-brane[2] representing the boundary of a larger manifold. This idea also proved useful indicating a possible explanation for the hierarchy problem.[3,4] One important consequence of such a model is the noncommutativity of space-time coordinates in our four-dimensional world.[5–7] The reason is that D-branes correspond to the space where open string end points are located and where the corresponding string boundary conditions must be satisfied. In the presence of an antisymmetric tensor background these conditions are incompatible with commuting coordinates.

Since antisymmetric fields show up in the massless spectrum of closed strings living on the D-branes it is reasonable to suspect that our physical world could be noncommutative at very small length scales. This is one of the reasons for the increasing interest in studying many aspects of noncommutative quantum field theories as can be seen, for example, in Refs. 7,8. Furthermore, this fact illustrates the nontrivial role of boundary conditions in string theory and the importance of taking them into account when considering the quantization of open strings.

In quantum field theory, products of quantum fields at the same space-time points are, in general, singular objects. The same thing happens in string theory if one multiplies position operators, that can be taken as conformal fields on the world sheet. This situation is well known and one can remove the singular part of the operator products by defining normal ordered well-behaved objects.[9] This is important, for example, when one builds up the generators of conformal transformations and investigate the realization, at the quantum level, of the classical symmetries.

[a]Electronic mail: braga@if.ufrj.br
[b]Electronic mail: mlm@if.ufrj.br
[c]Electronic mail: godinho@cbpf.br

Normal ordered products of operators are usually defined so as to satisfy the classical equations of motion at quantum level. Our purpose in this article is to define normal ordered products for open string position operators that additionally satisfy the boundary conditions. This way we will define a normal ordering that will be valid also at string end points. We will also investigate the relation between this new definition for normal ordering and the noncommutativity of space-time coordinates.

II. STRING POSITION OPERATOR PRODUCTS

The classical action for a bosonic string in the presence of a constant antisymmetric background taking a world sheet with a Euclidean signature is

$$S = \frac{1}{4\pi\alpha'}\int_{\Sigma} d^2\sigma(g^{ab}\eta_{\mu\nu}\partial_a X^\mu\,\partial_b X^\nu - i\epsilon^{ab}B_{\mu\nu}\,\partial_a X^\mu\,\partial_b X^\nu), \tag{1}$$

where X^μ are the space-time string coordinates and $B_{\mu\nu}$ is the antisymmetric field. The string world sheet Σ is represented by the parameters $\sigma_1 \equiv \tau, \sigma_2 \equiv \sigma$ with, as usual, the boundary (string end points) at $\sigma = 0, \pi$. The Euclidean world sheet metric is $g^{\tau\tau} = g^{\sigma\sigma} = 1$ and the antisymmetric tensor is chosen by $\epsilon^{\tau\sigma} = 1$.

The variation of the action gives us a volume term that vanishes imposing the equations of motion,

$$(\partial_\tau^2 + \partial_\sigma^2)X^\mu = 0, \tag{2}$$

plus a boundary term that vanishes if we additionally impose that the string coordinates satisfy the boundary conditions

$$(\eta_{\mu\nu}\,\partial_\sigma X^\nu + iB_{\mu\nu}\,\partial_\tau X^\nu)\big|_{\sigma=0} = 0,$$

$$(\eta_{\mu\nu}\,\partial_\sigma X^\nu + iB_{\mu\nu}\,\partial_\tau X^\nu)\big|_{\sigma=\pi} = 0. \tag{3}$$

These boundary conditions, when imposed at the quantum level, are responsible for the noncommutativity of the position operators.[5,7] We can infer this result by realizing that these conditions represent constraints in phase space relating position and conjugate momenta.

It is convenient, for studying the quantum operators, to introduce complex world sheet coordinates: $z = \tau + \imath\sigma$, $\bar{z} = \tau - \imath\sigma$; $\partial_z = 1/2(\partial_\tau - \imath\partial_\sigma)$, $\partial_{\bar{z}} = 1/2(\partial_\tau + \imath\partial_\sigma)$.

The action takes the form

$$S = \frac{1}{2\pi\alpha}\int dz^2[\,\eta_{\mu\nu}\,\partial_z X^\mu\,\partial_{\bar{z}} X^\nu - B_{\mu\nu}\,\partial_z X^\mu\,\partial_{\bar{z}} X^\nu], \tag{4}$$

while classical equations of motion and boundary conditions take the form

$$\partial_{\bar{z}}\partial_z X^i = 0, \tag{5}$$

$$(\eta_{\mu\nu}(\partial_z - \partial_{\bar{z}}) + B_{\mu\nu}(\partial_z + \partial_{\bar{z}}))X^\nu\big|_{z=\bar{z}} = 0,$$

$$(\eta_{\mu\nu}(\partial_z - \partial_{\bar{z}}) + B_{\mu\nu}(\partial_z + \partial_{\bar{z}}))X^\nu\big|_{z=\bar{z}+2\pi i} = 0. \tag{6}$$

We can study the properties of quantum operators by considering the expectation values of the corresponding classical objects. Defining the expectation value of an operators $\mathcal{F}$ as[9]

$$\langle \mathcal{F}[X] \rangle = \int [dX] \exp(-S[X]) \mathcal{F}[X], \tag{7}$$

and using the fact that the path integral of a total derivative vanishes one finds that the equations of motion and boundary conditions are realized for the expectation values of string coordinates X^ν,

$$0 = \int [dX] \frac{\delta}{\delta X^\nu(z',\bar{z}')} \exp(-S[X]) = \left\langle \frac{1}{\pi\alpha'} \partial_{\bar{z}'} \partial_{z'} X_\nu(z',\bar{z}') \right\rangle + \frac{1}{2\pi\alpha'} \oint_{\partial\Sigma} \delta^2(z-z') \langle (\eta_{\nu\mu}(\partial_z - \partial_{\bar{z}}) + B_{\nu\mu}(\partial_z + \partial_{\bar{z}})) X^\mu(z,\bar{z}) dz \rangle = 0. \tag{8}$$

The last (singular) term is integrated over the boundary, where $dz = d\bar{z}$. This equation implies that both string equations of motion and the boundary condition hold as expectation values. So the corresponding quantum position operators satisfy the equivalent conditions (as long as they are not multiplied by other operators located at the same world sheet point)

$$\partial_{\bar{z}} \partial_z \hat{X}^\nu(z,\bar{z}) = 0, \tag{9}$$

$$(\eta_{\nu\mu}(\partial_z - \partial_{\bar{z}}) + B_{\nu\mu}(\partial_z + \partial_{\bar{z}})) \hat{X}^\mu \Big|_{z=\bar{z}} = 0,$$

$$(\eta_{\nu\mu}(\partial_z - \partial_{\bar{z}}) + B_{\nu\mu}(\partial_z + \partial_{\bar{z}})) \hat{X}^\mu \Big|_{z=\bar{z}+2\pi i} = 0. \tag{10}$$

Products of operators at the same point will have a singular behavior. We can see this by calculating

$$0 = \int [dX] \frac{\delta}{\delta X^\nu(z',\bar{z}')} \exp(-S[X]) X^\rho(z'',\bar{z}'') = \left\langle \delta^2(z'-z'') \delta^\rho_\nu + \left(\frac{1}{\pi\alpha'} \partial_{\bar{z}'} \partial_{z'} X_\nu(z',\bar{z}') X^\rho(z'',\bar{z}'') + \frac{1}{2\pi\alpha'} \oint_{\partial\Sigma} \delta^2(z-z') (\eta_{\nu\mu}(\partial_z - \partial_{\bar{z}}) + B_{\nu\mu}(\partial_z + \partial_{\bar{z}})) X^\mu(z,\bar{z}) X^\rho(z'',\bar{z}'') dz \right\rangle = 0. \tag{11}$$

The volume term gives an extra singular term to the equation of motion for a product of two fields,

$$\frac{1}{\pi\alpha'} \langle \partial_{z'} \partial_{\bar{z}'} X^\mu(z',\bar{z}') X^\nu(z'',\bar{z}'') \rangle = -\eta^{\mu\nu} \langle \delta^2(z'-z'',\bar{z}'-\bar{z}'') \rangle, \tag{12}$$

while the boundary terms vanishes if this product of two fields satisfies the same boundary condition as the single field

$$\langle (\eta_{\nu\mu}(\partial_{z'} - \partial_{\bar{z}'}) + B_{\nu\mu}(\partial_{z'} + \partial_{\bar{z}'})) X^\mu(z',\bar{z}') X^\rho(z'',\bar{z}'') \Big|_{\text{Bound.}} \rangle = 0, \tag{13}$$

where Bound. means that we are taking this condition both at $z = \bar{z}$ and at $z = \bar{z} + 2\pi i$. Thus the products of operators will satisfy

$$\partial_{\bar{z}'} \partial_{z'} \hat{X}^\mu(z',\bar{z}') \hat{X}^\nu(z'',\bar{z}'') = -\pi\alpha' \eta^{\mu\nu} \delta^2(z'-z'',\bar{z}'-\bar{z}''), \tag{14}$$

$$(\eta_{\nu\mu}(\partial_{z'} - \partial_{\bar{z}'}) + B_{\nu\mu}(\partial_{z'} + \partial_{\bar{z}'})) \hat{X}^\mu(z',\bar{z}') \hat{X}^\rho(z'',\bar{z}'') \Big|_{\text{Bound.}} = 0. \tag{15}$$

If we define a normal ordered product of two position operators in the standard way,[9]

$$:\hat{X}^\mu(z,\bar{z}) \hat{X}^\nu(z',\bar{z}'): = \hat{X}^\mu(z,\bar{z}) \hat{X}^\nu(z',\bar{z}') + \frac{\alpha'}{2} \eta^{\mu\nu} \ln|z-z'|^2, \tag{16}$$

it satisfies the equation of motion at the quantum level:

$$\partial_{\bar{z}}\partial_z:\hat{X}^\mu(z,\bar{z})\hat{X}^\nu(z',\bar{z}'):=0, \tag{17}$$

but fails to satisfy the boundary conditions. So we will introduce a different kind of normal ordered product satisfying both the equation of motion and boundary conditions.

The mathematical problem posed by defining the normal ordering is related to that of calculating the Green's functions.[10–13] The normal ordered product is defined by subtracting out the corresponding Green's functions. So we can find normal ordered products satisfying open string boundary condition using the solutions to open the string Green's functions.

At this point it is more convenient to choose world sheet coordinates that simplify the representation of the boundary. In the present coordinates the boundary $\sigma=0$ corresponds to $z=\bar{z}$, and $\sigma=\pi$ to $z=\bar{z}+2\pi i$. Introducing

$$w=e^{\tau+i\sigma}; \quad \bar{w}=e^{\tau-i\sigma},$$

the complete boundary corresponds just to the region $w=\bar{w}$. On the other hand, the factor $w\bar{w}$ in $\partial_z\partial_{\bar{z}}=w\bar{w}\partial_w\partial_{\bar{w}}$ cancel out precisely the Jacobian of the coordinate transformation in such a way that the action in terms of $w,\bar{w}$ has still the same form as in Eq. (4). The boundary conditions take the form

$$(\eta_{\mu\nu}(w\partial_w-\bar{w}\partial_{\bar{w}})+B_{\mu\nu}(w\partial_w+\bar{w}\partial_{\bar{w}}))\hat{X}^\nu\big|_{w=\bar{w}}=(\eta_{\mu\nu}(\partial_w-\partial_{\bar{w}})+B_{\mu\nu}(\partial_w+\partial_{\bar{w}}))\hat{X}^\nu\big|_{w=\bar{w}}=0. \tag{18}$$

This implies that starting with a solution in coordinates $z,\bar{z}$ that satisfies the boundary conditions just at $\sigma=0$ and replacing everywhere $z,\bar{z}$ by $w,\bar{w}$ we get a new solution that satisfies the boundary conditions both at $\sigma=0$ and $\sigma=\pi$.

So our new normal ordering is defined as

$$:\hat{X}^\mu(w,\bar{w})\hat{X}^\nu(w',\bar{w}'):=\hat{X}^\mu(w,\bar{w})\hat{X}^\nu(w',\bar{w}')+\frac{\alpha'}{2}\eta^{\mu\nu}\ln|w-w'|^2+\frac{\alpha'}{2}([\eta+B]^{-1}[\eta-B])^{\mu\nu}\ln(w-\bar{w}')+\frac{\alpha'}{2}([\eta+B][\eta-B]^{-1})^{\mu\nu}\ln(\bar{w}-w')+\alpha' D^{\mu\nu}, \tag{19}$$

where $D^{\mu\nu}$ is a constant that may depend on B but not on the coordinates.

It is important to note that even when the antisymmetric tensor background is not present ($B_{\mu\nu}=0$) the normal ordering of expression (19) does not reduce to the standard normal ordering of Eq. (16), discussed in the literature. This is a new result: for open strings one must always use the normal ordering (19) rather than (16) otherwise the boundary conditions will not be satisfied.

III. EQUAL TIME COMMUTATORS

It is important to investigate the effect of this normal ordering on the commutators of position operators to check if the noncommutativity of space-time coordinates in the presence of the antisymmetric tensor background is changed. We can rewrite Eq. (19) in a more convenient form for calculating the commutators:

$$:\hat{X}^\mu(w,\bar{w})\hat{X}^\nu(w',\bar{w}'):=\hat{X}^\mu(w,\bar{w})\hat{X}^\nu(w',\bar{w}')+\frac{\alpha'}{2}\eta^{\mu\nu}\ln|w-w'|^2-\alpha'\eta^{\mu\nu}\ln|w-\bar{w}'|+\alpha' G^{\mu\nu}\ln|w-\bar{w}'|^2+\frac{1}{2\pi}\Theta^{\mu\nu}\ln\left(\frac{w-\bar{w}'}{\bar{w}-w'}\right)+\alpha' D^{\mu\nu}, \tag{20}$$

where we introduced

$$G^{\mu\nu} = ([\eta + B]^{-1}\eta[\eta - B]^{-1})^{\mu\nu},$$

$$\Theta^{\mu\nu} = -2\pi\alpha'([\eta + B]^{-1}B[\eta - B]^{-1})^{\mu\nu}. \tag{21}$$

Now we calculate the normal ordered commutator at boundary points $w = \overline{w} = \tau, w' = \overline{w'} = \tau'$ using the same choice for the constant $D^{\mu\nu}$ and the same procedure as in Ref. 7,

$$:[\hat{X}^{\mu}(\tau),\hat{X}^{\nu}(\tau')]: \equiv :\hat{X}^{\mu}(\tau)\hat{X}^{\nu}(\tau'):- :\hat{X}^{\nu}(\tau')\hat{X}^{\mu}(\tau): = [\hat{X}^{\mu}(\tau),\hat{X}^{\nu}(\tau')] + \alpha' G^{\mu\nu}\ln((\tau-\tau')^2)$$
$$-\frac{i}{2}\Theta^{\mu\nu}\epsilon(\tau-\tau') - \alpha' G^{\nu\mu}\ln((\tau'-\tau)^2) + \frac{i}{2}\Theta^{\nu\mu}\epsilon(\tau'-\tau) = [\hat{X}^{\mu}(\tau),\hat{X}^{\nu}(\tau')]. \tag{22}$$

So the commutator does not get any extra contribution from the new normal ordering prescription. The equal time commutator thus keeps the same form calculated in Ref. 7 (see also Refs. 14,15):

$$:[\hat{X}^{\mu}(\tau),\hat{X}^{\nu}(\tau)]: = i\Theta^{\mu\nu}. \tag{23}$$

This is a nontrivial result. The commutator of position operators was calculated by Seiberg and Witten[7] using the open string Green's function. Here we have defined a normal ordering by subtracting precisely this Green's function from the product of position operators. So one could think that the commutator of two normal ordered products would be zero. However, we have shown that this is not the case because the extra terms cancel and the commutator is unchanged.

Concluding, the new normal ordering for position operators that is consistent with both equations of motion and boundary conditions at the quantum level does not spoil the previous results related to the noncommutativity of space-time coordinates.

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Bose–Einstein condensate and spontaneous breaking of conformal symmetry on Killing horizons

Valter Moretti[a] and Nicola Pinamonti[b]
Department of Mathematics, Faculty of Science, University of Trento, via Sommarive 14, I-38050 Povo (TN), Italy

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Local scalar quantum field theory (in Weyl algebraic approach) is constructed on degenerate semi-Riemannian manifolds corresponding to Killing horizons in spacetime. Covariance properties of the C^*-algebra of observables with respect to the conformal group $\mathrm{PSL}(2,\mathbb{R})$ are studied. It is shown that, in addition to the state studied by Guido, Longo, Roberts, and Verch for bifurcated Killing horizons, which is conformally invariant and KMS at Hawking temperature with respect to the Killing flow and defines a conformal net of von Neumann algebras, there is a further wide class of algebraic (coherent) states representing spontaneous breaking of $\mathrm{PSL}(2,\mathbb{R})$ symmetry. This class is labeled by functions in a suitable Hilbert space and their GNS representations enjoy remarkable properties. The states are nonequivalent extremal KMS states at Hawking temperature with respect to the residual one-parameter subgroup of $\mathrm{PSL}(2,\mathbb{R})$ associated with the Killing flow. The KMS property is valid for the two local subalgebras of observables uniquely determined by covariance and invariance under the residual symmetry unitarily represented. These algebras rely on the physical region of the manifold corresponding to a Killing horizon cleaned up by removing the unphysical points at infinity [necessary to describe the whole $\mathrm{PSL}(2,\mathbb{R})$ action]. Each of the found states can be interpreted as a different thermodynamic phase, containing Bose–Einstein condensate, for the considered quantum field. It is finally suggested that the found states could describe different black holes. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1917310]

I. INTRODUCTION

In a remarkable paper,[11] among other results, Guido, Longo, Roberts, and Verch show that, in a globally hyperbolic spacetime containing a bifurcate Killing horizon,[17] the local algebra of observables (realized as bounded operators associated to bounded space–time regions in a suitable Hilbert space) may induce a local algebra of observables localized at the horizon itself with interesting properties. In fact, the induced local algebra turns out to be covariant with respect to a unitary representation of Möbius group of the circle $\mathrm{PSL}(2,\mathbb{R}) := \mathrm{SL}(2,\mathbb{R})/\{\pm I\}$ defined in the Hilbert space of the system. The covariance property is referred to the geometric action of the Möbius group of the circle on the horizon as explained below. The work, on one hand, uses general theorems due to Wiesbrock[39,40] establishing the existence of $\mathrm{SL}(2,\mathbb{R})$ representations related to modular operators of von Neumann algebras. On the other hand, it enjoys some interplay with several "holographic" ideas (including LightFront Holography) in quantum field theory (QFT).[34,25–27]

The central mathematical object employed in Ref. 11 is a net of von Neumann algebras built upon a certain state which is assumed to exist and satisfy the following requirement. Its restriction

[a]Istituto Nazionale di Alta Matematica "F.Severi," unità locale di Trento. Electronic mail: moretti@science.unitn.it
[b]Istituto Nazionale di Fisica Nucleare, Gruppo Collegato di Trento. Electronic mail: pinamont@science.unitn.it

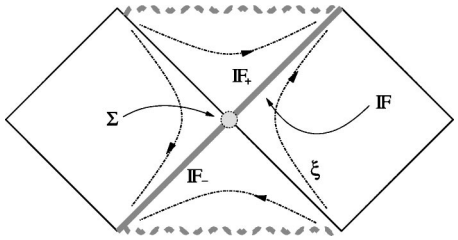

FIG. 1. Carter–Penrose conformal diagram of Kruskal space–time.

to the subnet of observables which are localized at the horizon, must be KMS at Hawking temperature for the Killing flow. In that case, the net of observables localized at the future horizon $\mathbb{F}$ (see Fig. 1) is shown to support a unitary representation of $\mathrm{PSL}(2,\mathbb{R})$ giving rise to a *conformal net* (see for instance Refs. 4, 8, 10, and 5, and references therein).

It is worth noticing that the full $\mathrm{PSL}(2,\mathbb{R})$-covariance of the observables of the conformal net is apparent when one extends the future Killing horizon $\mathbb{F}$ by adding points at infinity obtaining a manifold $\mathbb{S}^1\times\Sigma$, Σ being the transverse manifold at the bifurcation of horizons. $\mathbb{S}^1$ represents nothing but the history $\mathbb{R}$ of a particle of light living on the future horizon compactified into a circle by means of the addition of a point at infinity. The addition of points at infinity is necessary because $\mathrm{PSL}(2,\mathbb{R})$ acts properly as a subgroup of the diffeomorphisms of the circle $\mathbb{S}^1$ and not the line $\mathbb{R}$. In particular the action of $\mathrm{PSL}(2,\mathbb{R})$ on $\mathbb{S}^1$ includes arbitrary rotations of the circle itself which shift the point at infinity in the physical region $\mathbb{R}$.

From a physical point of view these transformations have no meaning. So it seems that the found covariance of the observables localized at the horizon under the full group $\mathrm{PSL}(2,\mathbb{R})$ is actually too large. The problem could be traced back to the state used to construct the von Neumann net of observables.

In spite of this drawback, the results proved in Ref. 11 show the existence of a nice interplay of Killing horizons, thermal states at the correct physical temperature, and conformal symmetry. This result is strongly remarkable in its own right.

In the first part of this paper we give an explicit procedure to build up a local algebra of observables localized on a degenerate semi-Riemannian manifold $\mathbb{M}:=\mathbb{S}^1\times\Sigma$ (obtained from future or past Killing horizons in particular) based on Weyl quantization procedure. This is done without referring to external (bulk) algebras and states and restriction procedures. We find, in fact, a conformal net of observables relying on a $\mathrm{PSL}(2,\mathbb{R})$-invariant vacuum λ. At algebraic level there is a representation α of $\mathrm{PSL}(2,\mathbb{R})$ made of $*$-automorphisms of the Weyl algebra $\mathcal{W}(\mathbb{M})$ and there is a state λ on $\mathcal{W}(\mathbb{M})$ which is invariant under α. In the GNS representation of λ,α is implemented covariantly by a unitary representation U of $\mathrm{PSL}(2,\mathbb{R})$. Moreover it is shown that λ is KMS at Hawking temperature, with respect to the generator of conformal dilatations, in suitable regions $\mathbb{F}_\pm$ of $\mathbb{M}$ (see Fig. 1). $\mathbb{F}_\pm$ do not include points at infinity and are the two disjoint regions in $\mathbb{F}$, respectively, in the past and in the future of the bifurcation surface.

In the second part we try to solve the problem focused above concerning the physical inappropriateness of the full $\mathrm{PSL}(2,\mathbb{R})$ covariance whenever $\mathbb{M}$ is realized by adding (unphysical) points at infinity to a future Killing horizon $\mathbb{F}$.

To this end, it is proven that it is possible to get rid of the unphysical action of $\mathrm{PSL}(2,\mathbb{R})$ and single out the physical part of the horizon at *quantum level, i.e., in Hilbert space*, through a sort of *spontaneous breaking of* $\mathrm{PSL}(2,\mathbb{R})$ *symmetry*. In fact, we establish the existence of other, unitarily inequivalent, GNS representations of $\mathcal{W}(\mathbb{M})$ based on new coherent KMS states λ_ζ at Hawking temperature. Here ζ denotes any functions in $L^2(\Sigma)$. Those states are no longer invariant under the whole representation α and in particular they are not invariant under the unphysical transformations of $\mathrm{PSL}(2,\mathbb{R})$. However the residual symmetry still is covariantly and unitarily implementable and singles out the algebras $\mathcal{A}(\mathbb{F}_+)$ and $\mathcal{A}(\mathbb{F}_-)$ as unique invariant subalgebras. The states λ_ζ represent different *thermodynamical phases* with respect to λ (this is because the states

λ_ζ are extremal KMS states) at Hawking temperature. Those states have different properties in relation with the appearance of a Bose–Einstein condensate localized at the horizon. Finally we suggest that these states could, in fact, denote different black holes. In this view the bosonic field ϕ generating the Weyl representations could represent a noncommutative coordinate in the physical regions $\mathbb{F}_\pm$, whereas its mean value represents the classical coordinate describing the parameter of integral curves of the Killing vector restricted to the horizon.

Several comments concerning the representation of the whole group $\mathrm{Diff}^+(\mathbb{S}^1)$ and in particular its Lie algebra in the presence of the transverse manifold Σ, are spread throughout the work.

II. SCALAR FREE QFT ON DEGENERATE SEMI-RIEMANNIAN MANIFOLDS

A. Basic definitions and notation

In this paper we deal with metric-degenerate semi-Riemannian manifolds of the product form $\mathbb{S}^1\times\Sigma$, where Σ is a connected oriented d-dimensional manifold equipped with a positive metric. $\mathbb{S}^1$ is assumed to be oriented and endowed with the null metric. $\mathbb{S}^1\times\Sigma$ itself is oriented by the orientation induced from those of $\mathbb{S}^1$ and Σ. $\mathbb{S}^1\times\Sigma$ will be called degenerate manifold in the following and it will be denoted by $\mathbb{M}$ throughout. A standard frame θ on the factor $\mathbb{S}^1$ of $\mathbb{M}$ is a positive-oriented local coordinate patch on $\mathbb{S}^1$ which maps $\mathbb{S}^1\backslash\{\infty\}$ bijectively to the segment $-\pi<\theta<\pi$, ∞ being a point of $\mathbb{S}^1$. Throughout $C_c^\infty(\mathbb{M};\mathbb{R})$ and $C_c^\infty(\mathbb{M};\mathbb{C})$ denote the space of compactly supported real-valued, respectively, complex-valued, smooth functions on $\mathbb{M}$ and ω_Σ is the volume form on Σ induced by the metric of Σ. $C_c^\infty(\mathbb{M};\mathbb{C})$ is endowed with a natural symplectic (i.e., bilinear and antisymmetric) form given by, if ψ, $\psi'\in C_c^\infty(\mathbb{M};\mathbb{C})$,

$$\Omega(\psi,\psi') := \int_{\mathbb{M}} \psi'\epsilon_\psi - \psi\epsilon_{\psi'}, \quad \text{where } \epsilon_\psi := \mathrm{d}\psi\wedge\omega_\Sigma. \tag{1}$$

Concerning KMS states we adopt the Definition 5.3.1 in Ref. 2 (see also Chap. V of Ref. 13 where the σ-weak topology used in the definition above in the case of a von Neumann algebra is called *weak $*$-topology*, also known as *ultraweak topology*).

The symbol $\mathbb{N}$ denotes the set of natural numbers $\{0,1,2,\ldots\}$, whereas $\mathbb{N}'$ means $\mathbb{N}\backslash\{0\}$.

B. Bifurcate Killing horizon and Kruskal cases

A simple example of three-dimensional degenerate manifold can be obtained from a submanifold of Kruskal manifold. However, everything that follows is valid, more generally, for any $(d+2)$-dimensional globally hyperbolic space–time containing a bifurcate Killing horizon[17] if replacing $\mathbb{S}^2$ with a generic d-dimensional spacelike submanifold Σ. A basis of Killing vector fields of Kruskal space–time is made of three fields: two generating the $\mathbb{S}^2$ symmetry and ξ generating the time evolution in the two static open wedges where ξ is timelike. The region where $(\xi,\xi)=0$ is made of the union of two three-dimensional submanifolds, $\mathbb{P}$ and $\mathbb{F}$, which we call, respectively, the past and the future Killing horizon of the manifold in reference to Fig. 1. $\mathbb{P}\cap\mathbb{F}$ is the *bifurcation surface*, i.e., a spacelike two-dimensional oriented submanifold where $\xi=0$, given by $\mathbb{S}^2$ equipped with the Euclidean standard metric of a two-sphere with radius given by a Schwarzschild one r_s. That metric is induced from the space–time metric. $\mathbb{F}$ is isometric to the degenerate manifold $\mathbb{R}\times\mathbb{S}^2$. $\mathbb{R}$ is made of the orbits of the null Killing vector ξ restricted to $\mathbb{F}$. We assume that the origin of $\mathbb{R}$ is arranged to belong to the bifurcation manifold $\mathbb{S}^2$. The metric induced on $\mathbb{F}$ is degenerate along $\mathbb{R}$ and invariant under $\mathbb{R}$ displacements. A degenerate manifold $\mathbb{M}=\mathbb{S}^1\times\Sigma$ can, obviously, be obtained from $\mathbb{F}$ by adding a point at infinity ∞ to $\mathbb{R}$ producing $\mathbb{S}^1$. In this case $\mathbb{M}=\mathbb{S}^1\times\mathbb{S}^2$. Orientation of $\mathbb{S}^1$ is that induced by $\mathbb{R}$. Then $\theta(V)=2\tan^{-1}V$, with $V\in\mathbb{R}$, is a standard frame on $\mathbb{S}^1$.

Other examples of degenerate manifold arise from the event horizon of topological black-holes,[36,21] where Σ is replaced by a compact two-dimensional manifold of arbitrary nonnegative genus.

C. Weyl/symplectic approach

In Refs. 25–27 we have considered the limit case of a degenerate manifold $\mathbb{M}=\mathbb{S}^1$ where $\mathbb{M}\backslash\{\infty\}$ is as part of its boundary made of a bifurcate Killing horizon in two-dimensional (2D) Minkowski space–time. In that case local QFT can be induced on $\mathbb{M}$, by means of a suitable restriction procedure of standard linear QFT in the bulk space–time. This restriction actually enjoys some holographic properties because it preserves information about bulk quantum field theory. Here we construct QFT on a general degenerate manifold $\mathbb{M}=\mathbb{S}^1\times\Sigma$ without referring to any restriction procedure. The restriction procedure with holographic properties could be generalized to more complicated manifolds (Kruskal manifold in particular) and this issue will be investigated elsewhere. The formulation of real scalar QFT on a degenerate manifold $\mathbb{M}$ we present here is an adaptation of the theory of fields obeying linear field equations in globally hyperbolic space–times.[2,17,37,38] (In this paper, barring few differences, we make use of conventions and notation of Ref. 38.) The starting point of QFT is the real vector space of wave functions $\mathcal{S}(\mathbb{M}) \coloneqq C_c^\infty(\mathbb{M};\mathbb{R})/\sim$, where $\psi\sim\psi'$ iff $\epsilon_\psi=\epsilon_{\psi'}$. Ω induces a symplectic form on $\mathcal{S}(\mathbb{M})$ still indicated by Ω and defined by, if $[\psi]$, $[\psi']\in\mathcal{S}(\mathbb{M})$,

$$\Omega([\psi],[\psi']) \coloneqq \Omega(\psi,\psi'). \tag{2}$$

Remarks:

(1) Two facts hold, (a) $\psi\sim\psi'$ iff $\partial(\psi-\psi')/\partial\rho=0$ everywhere, and (b) $\epsilon_\psi=(\partial\psi/\partial\rho)\mathrm{d}\rho\wedge\omega_\Sigma$, ρ being any (local) coordinate on $\mathbb{S}^1$. Using (a) and (b) one proves straightforwardly that $\Omega([\psi],[\psi'])$ is well defined, that is it does not depend on the representatives ψ, ψ' chosen in the classes $[\psi]$, $[\psi']$.

(2) Ω is *nondegenerate* on $\mathcal{S}(\mathbb{M};\mathbb{R})$, that is $\Omega([\psi],[\psi'])=0$ for all $[\psi']\in\mathcal{S}(\mathbb{M})$ implies $[\psi]=0$. The definition $\mathcal{S}(\mathbb{M}) \coloneqq C_c^\infty(\mathbb{M};\mathbb{R})/\sim$ gets rid of the degenerateness of Ω on $C_c^\infty(\mathbb{M};\mathbb{R})$ due to functions constant in $\mathbb{S}^1$. Nondegenerateness allows the use of standard procedure to build up QFT within the Weyl formalism as explained below. Another possibility to remove degenerateness is to define $\mathcal{S}(\mathbb{M})$ as the space of $C_c^\infty(\mathbb{M};\mathbb{R})$ functions with vanishing integral with respect to some measure $\mathrm{d}\rho$ induced by a coordinate ρ on $\mathbb{S}^1$. Such a definition, different to that given above, would break invariance under orientation-preserving diffeomorphisms of $\mathbb{S}^1$, which is a natural physical requirement due to the absence of a metric on $\mathbb{S}^1$. Breaking diffeomorphism invariance will enter the theory through the choice of a reference quantum state.

(3) *Henceforth we indicate a wave function* $[\psi]$ *by* ψ *if the notation is not misunderstandable.*

"Wave function" is quite an improper term, due to the absence of any equation of motion on $\mathbb{M}$, nevertheless the "wave functions" introduced here play a role similar to that of the smooth solutions of Klein–Gordon equation in a globally hyperbolic space–time. As $\mathcal{S}(\mathbb{M})$ is a real vector space equipped with a *nondegenerate* symplectic form Ω, there exist a complex C^*-algebra (Theorem 5.2.8 in Ref. 2) generated by elements, $W(\psi)$ with $\psi\in\mathcal{S}(\mathbb{M})$ satisfying, for all ψ, $\psi'\in\mathcal{S}(\mathbb{M})$,

$$\text{(W1)}\quad W(-\psi)=W(\psi)^*,\quad \text{(W2)}\quad W(\psi)W(\psi')=e^{i\Omega(\psi,\psi')/2}W(\psi+\psi').$$

That C^*-algebra, indicated by $\mathcal{W}(\mathbb{M})$, is unique up to (isometric) $*$-isomorphisms (Theorem 5.2.8 in Ref. 2). As consequences of (W1) and (W2), $\mathcal{W}(\mathbb{M})$ admits unit $I=W(0)$, each $W(\psi)$ is unitary and, from the nondegenerateness of Ω, $W(\psi)=W(\psi')$ if and only if $\psi=\psi'$. $\mathcal{W}(\mathbb{M})$ is called Weyl algebra associated with $\mathcal{S}(\mathbb{M})$ and Ω whereas the $W(\psi)$ are called symplectically smeared (abstract) Weyl operators. The formal interpretation of elements $W(\psi)$ is $W(\psi)\equiv e^{i\Omega(\psi,\hat{\phi})}$ where $\Omega(\psi,\hat{\phi})$ are symplectically smeared scalar fields as we shall see shortly.

D. Implementing locality: Fields smeared with forms

In a globally hyperbolic space–time X the *local* smearing is obtained employing real compactly supported functions f instead of solutions of field equations[38] to smear field operator. In particular one gives a rigorous meaning to

$$\hat{\phi}(f) = \int_X \hat{\phi}(x) f(x) \mathrm{d}\mu(x), \tag{3}$$

μ being the measure induced by the metric of X. The support of the smearing function f gives a suitable notion of support of the associated observable $\hat{\phi}(f)$. In this way locality can be implemented by stating that observables with causally disjoint supports commute. In our case it is impossible to assign a unique support to a class of equivalence $[\psi]$ and thus implementation of locality is not very straightforward in the symplectic approach. Furthermore, there is no natural measure μ on $\mathbb{M}$ as that present in (3) because $\mathbb{S}^1$ is metrically degenerate. Both problems can be solved by using compactly supported forms instead of compactly supported functions. Let us indicate by $\mathcal{D}(\mathbb{M})$ the space of real forms ϵ_ψ [see (1)] with $\psi \in C_c^\infty(\mathbb{M};\mathbb{R})$. In a globally hyperbolic space–time[38] the relation between wave functions and smooth compactly supported functions [now elements of $\mathcal{D}(\mathbb{M})$] used in (3), is implemented by the *causal propagator*, $E:\mathcal{D}(\mathbb{M}) \to \mathcal{S}(\mathbb{M})$.[38] It is a $\mathbb{R}$-linear surjective map which associates a smooth function with wave functions (supported in the causal set generated by the support of the smooth function) and satisfies several properties. The crucial property describing the interplay of E and Ω reads, if $E(\omega,\omega') := \int_{\mathbb{M}} E(\omega)\omega'$,

$$\Omega(E\omega, E\omega') = E(\omega,\omega') \quad \text{for all } \omega,\omega' \in \mathcal{D}(\mathbb{M}). \tag{4}$$

In our case (4) and surjectivity determine E uniquely on $\mathbb{M}$.

Proposition 2.1: *On a degenerate manifold $\mathbb{M} := \mathbb{S}^1 \times \Sigma$ there is a unique surjective $\mathbb{R}$-linear map $E:\mathcal{D}(\mathbb{M}) \to \mathcal{S}(\mathbb{M})$ satisfying (4). Moreover the following facts hold.*

(a) *If θ is a standard frame on $\mathbb{S}^1$ and $\omega \in \mathcal{D}(\mathbb{M})$ is realized as a 2π-periodic form in θ viewed as positive-oriented coordinate $\mathbb{R}$ and $s \in \Sigma$, E admits the representation*

$$(E(\omega))(\theta,s) = \left[\frac{1}{4} \int_{\theta' \in [-\pi,\pi] s' \in \Sigma} \left(\mathrm{sign}(\theta') - \frac{\theta'}{\pi} \right) \delta(s,s') \omega(\theta - \theta', s') \right]. \tag{5}$$

(b) *E is* bijective *and in particular, for $\psi \in \mathcal{S}(\mathbb{M})$, $\omega \in \mathcal{D}(\mathbb{M})$, one has*

$$E(\epsilon_\psi) = \tfrac{1}{2}\psi \quad \textit{and} \quad \epsilon_{E(\omega)} = \tfrac{1}{2}\omega. \tag{6}$$

Thus $(\omega,\omega') \mapsto E(\omega,\omega')$ is a nondegenerate symplectic form on $\mathcal{D}(\mathbb{M})$.

Proof: The fact that E defined in (5) satisfies (4) can be proved straightforwardly by direct computation. Direct computation shows also the validity of (6) proving injectivity and surjectivity. Any linear surjective map E satisfying (4) fulfills also $\Omega(\psi, E\omega') = \int_{\mathbb{M}} \psi\omega'$ for every $\psi \in \mathcal{S}(\mathbb{M})$ and $\omega' \in \mathcal{D}(\mathbb{M})$. If E, E' are surjective linear maps satisfying (4), one has $\Omega(\psi, E\omega - E'\omega) = \int_{\mathbb{M}} \psi(\omega - \omega) = 0$ for every $\psi \in \mathcal{S}(\mathbb{M})$. Ω is nondegenerate and thus $E\omega - E'\omega = 0$ for every $\omega \in \mathcal{D}(\mathbb{M})$. Hence $E = E'$. The final statement is now obvious. □

We shall call the bijective map E in (5) causal propagator, regardless of the partial inappropriateness of the name due to the lack of field equations. In space–times, existence of field equations is responsible for the failure of the injectivity of the causal propagator. $\delta(s,s')$ in (5) has an evident physical meaning if $(\mathbb{S}^1 \setminus \{\infty\}) \times \Sigma$ is thought as the future Kruskal Killing horizon and E is interpreted as the limit case of a properly defined causal propagator. As the boundary of a causal set $J(S)$, for $S \subset \Sigma$, is made of portions of the factor $\mathbb{S}^1$, causal separation of sets S, $S' \subset \Sigma$ assigned at different "times" of $\mathbb{S}^1 \setminus \{\infty\}$, is equivalent to $S \cap S' = \emptyset$.

As in space–times, if $\omega \in \mathcal{D}(\mathbb{M})$, the form-smeared (abstract) Weyl field is defined as

$$V(\omega) := W(E\omega). \tag{7}$$

With this definition one immediately gets Weyl relations once again. For all $\omega,\ \eta \in \mathcal{D}(\mathbb{M})$,

$$\text{(V1)} \quad V(-\omega) = V(\omega)^*, \quad \text{(V2)} \quad V(\omega)V(\eta) = e^{iE(\omega,\eta)/2}V(\omega+\eta).$$

Since E is injective, differently from the extent in a space–time, $V(\omega)=V(\omega')$ if and only if $\omega=\omega'$. A notion of *locality* on $\mathbb{M}$ (in a straightforward extension of an original idea due to Sewell[35]) can be introduced at this point by the following proposition (the proof is in the Appendix).

Proposition 2.2: $[V(\omega),V(\omega')]=0$ *for* $\omega,\ \omega' \in \mathcal{D}(\mathbb{M})$ *if one of the conditions is fulfilled:*

(a) *there are two open disjoint segments* $I,\ I' \subset \mathbb{S}^1$ *with supp* $\omega \subset I\times\Sigma$ *and supp* $\omega' \subset I'\times\Sigma$,
(b) *there are two open disjoint sets* $S,\ S' \subset \Sigma$ *with supp* $\omega \subset \mathbb{S}^1\times S$ *and supp* $\omega' \subset \mathbb{S}^1\times S'$.

The $*$-algebra $\mathcal{W}(\mathbb{M})$ is *local* in the sense stated in the thesis of Proposition 2.2. Notice that supp $\omega \cap$ supp $\omega' = \varnothing$ does not imply commutativity of $V(\omega)$ and $V(\omega')$ in general.

E. Fock representations

Breaking invariance under orientation-preserving $\mathbb{S}^1$-diffeomorphisms, Fock representations of $\mathcal{W}(\mathbb{M})$ can be introduced as follows generalizing part of the construction presented in 2.4 of Ref. 12 and in Ref. 27. From a physical point of view, the procedure resembles quantization with respect to Killing time in a static space–time. Fix a standard frame θ on $\mathbb{S}^1$. Any representative ψ of $[\psi] \in \mathcal{S}(\mathbb{M})$ can be expanded in Fourier series in the parameter θ, where $\mathbb{N}' := \mathbb{N}\backslash\{0\}$,

$$\psi(\theta,s) \sim \sum_{n\in\mathbb{N}'} \frac{e^{-in\theta}\widetilde{\psi(s,n)_+}}{\sqrt{4\pi n}} + \sum_{n\in\mathbb{N}'} \frac{e^{in\theta}\overline{\widetilde{\psi(s,n)_+}}}{\sqrt{4\pi n}} = \psi_+(\theta,s) + \overline{\psi_+(\theta,s)}. \tag{8}$$

ψ_+ is the θ-positive frequency part of ψ. The term with $n=0$ was discarded due to the equivalence relation used defining $\mathbb{S}(\mathbb{M})$, the remaining terms depend on $[\psi]$ only. $\Sigma \ni s \mapsto \widetilde{\psi(s,n)_+}$ is smooth, supported in a compact set of Σ independent from n and, using integration by parts, for any $\gamma>0$, there is $C_\gamma \geqslant 0$ with $\|\widetilde{\psi(\cdot,n)_+}\|_\infty \leqslant C_\gamma n^{-\gamma}$ for $n \in \mathbb{N}'$ so that the series in (8) converges uniformly and θ-derivative operators can be interchanged with the symbol of summation. The found estimation and Fubini's theorem entail that the sesquilinear form

$$\langle \psi'_+, \psi_+ \rangle := -i\Omega(\overline{\psi'_+}, \psi_+) \tag{9}$$

on the space of complex linear combinations of θ-positive frequency parts satisfies

$$\langle \psi'_+, \psi_+ \rangle = \sum_{n=1}^{\infty} \int_\Sigma \overline{\widetilde{\psi'(s,n)_+}}\widetilde{\psi(s,n)_+}\omega_\Sigma(s) = \int_\Sigma \sum_{n=1}^{\infty} \overline{\widetilde{\psi'(s,n)_+}}\widetilde{\psi(s,n)_+}\omega_\Sigma(s). \tag{10}$$

Thus it is positive and defines a Hermitian scalar product. The one-particle space $\mathcal{H}$ is now defined as the completion with respect to $\langle\cdot,\cdot\rangle$ of the space of positive θ-frequency parts ψ_+ of wave functions. Due to (10), $\mathcal{H}$ is isomorphic to $\ell^2(\mathbb{N})\otimes L^2(\Sigma,\omega_\Sigma)$. [The construction of $\mathcal{H}$ is equivalent to that performed in the approach of Ref. 38 (see also Ref. 17) using the real scalar product on $\mathcal{S}(\mathbb{M})$, $\mu(\psi,\psi') := -\mathrm{Im}\,\Omega(\psi_+,\psi'_+)$ and the map $K:\mathcal{S}(\mathbb{M}) \ni \psi \mapsto \psi_+ \in \mathcal{H}$.] $\mathfrak{F}_+(\mathcal{H})$ is the symmetrized Fock space with vacuum state Ψ and one-particle space $\mathcal{H}$. The field operator symplectically smeared with $\psi \in \mathcal{S}(\mathbb{M})$ and the field operator smeared with the form $\omega \in \mathcal{D}(\mathbb{M})$ are, respectively, the operators

$$\Omega(\psi,\hat{\phi}) := ia(\overline{\psi_+}) - ia^\dagger(\psi_+) \quad \text{and} \quad \hat{\phi}(\omega) := \Omega(E\omega,\hat{\phi}), \tag{11}$$

where the operators $a^\dagger(\psi_+)$ and $a(\overline{\psi_+})$ ($\mathbb{C}$-linear in $\overline{\psi_+}$), respectively, create and annihilate the state ψ_+. The common invariant domain of all the involved operators is the dense linear manifold $F(\mathcal{H})$ spanned by the vectors with finite number of particle. $\Omega(\psi,\hat{\phi})$ and $\hat{\phi}(\omega)$ are essentially self-

adjoint on $F(\mathcal{H})$ [they are symmetric and $F(\mathcal{H})$ is dense and made of analytic vectors] and satisfy bosonic commutation relations (CCR),

$$[\Omega(\psi,\hat{\phi}),\Omega(\psi',\hat{\phi})] = -i\Omega(\psi,\psi')I \quad \text{and} \quad [\hat{\phi}(\omega),\hat{\phi}(\omega')] = -iE(\omega,\omega')I.$$

The definition $\hat{\phi}(\omega) := \Omega(E\omega,\hat{\phi})$ is here nothing but a rigorous interpretation of the formula $\hat{\phi}(\omega) = \int_{\mathbb{M}} \hat{\phi}(x)\omega(x)$. Finally the unitary operators

$$\hat{W}(\psi) := e^{i\overline{\Omega(\psi,\hat{\phi})}} \quad \text{and, equivalently,} \quad \hat{V}(\omega) := \hat{W}(E\omega) = e^{i\overline{\hat{\phi}(\omega)}} \tag{12}$$

enjoy properties (W1), (W2) and, respectively (V1), (V2), so that they define a unitary representation $\hat{\mathcal{W}}(\mathbb{M})$ of $\mathcal{W}(\mathbb{M})$ which is also irreducible. The proof of these properties follows from Propositions 5.2.3 and 5.2.4 in Ref. 2. [There the symplectic form is $\sigma = -2\Omega$ and the field operator $\Phi(\underline{\psi_+})$ of Proposition 5.2.3 of Ref. 2 is $\Phi(\psi_+) = 2^{-1/2}\Omega(J\psi,\hat{\phi})$ where $J\psi = -i\psi_+ + i\overline{\psi_+}$ if $\psi = \psi_+ + \underline{\psi_+}$. Notice that $J(\mathcal{S}(\mathbb{M})) \subset \mathcal{S}(\mathbb{M})$, that is false in general with other definitions of $\mathcal{S}(\mathbb{M})$!]

If $\Pi : \mathcal{W}(\mathbb{M}) \to \hat{\mathcal{W}}(\mathbb{M})$ denotes the unique (Ω being nondegenerate) C^*-algebra isomorphism between those two Weyl representations, $(\mathfrak{F}_+(\mathcal{H}),\Pi,\Psi)$ coincides, up to unitary transformations, with the GNS triple associated with the algebraic pure state λ on $\mathcal{W}(\mathbb{M})$ uniquely defined by the requirement (see the Appendix)

$$\lambda(W(\psi)) := e^{-\langle\psi_+,\psi_+\rangle/2}. \tag{13}$$

III. CONFORMAL NETS ON DEGENERATE MANIFOLDS

A. Diff$^+$($\mathbb{S}^1$), PSL(2,$\mathbb{R}$) and associated $*$-automorphisms on $\mathbb{M}$

We recall here some basic notions of conformal representations on $\mathbb{S}^1$. Let Vect($\mathbb{S}^1$) be the infinite-dimensional Lie algebra of the infinite-dimensional Lie group (see Milnor[23]) of orientation-preserving smooth diffeomorphisms of the circle Diff$^+$($\mathbb{S}^1$). Vect($\mathbb{S}^1$) is the real linear space of smooth vector fields on $\mathbb{S}^1$ whose associated one-parameter diffeomorphisms preserve the orientation of $\mathbb{S}^1$. Vect$^{\mathbb{C}}$($\mathbb{S}^1$) denotes the complex Lie algebra Vect($\mathbb{S}^1$) $\oplus\, i$ Vect($\mathbb{S}^1$) with usual Lie brackets $\{\cdot,\cdot\}$ and involution $\imath : X \mapsto -\overline{X}$ for $X \in$ Vect$^{\mathbb{C}}$($\mathbb{S}^1$), so that $\imath(\{X,Y\}) = \{\imath(Y),\imath(X)\}$. Vect($\mathbb{S}^1$) is the (real) sub-Lie-algebra of Vect$^{\mathbb{C}}$($\mathbb{S}^1$) of anti-Hermitian elements with respect to $\imath$. $\mathfrak{a}$ denotes the Lie subalgebra of Vect$^{\mathbb{C}}$($\mathbb{S}^1$) whose elements have a finite number of Fourier component with respect to a standard frame θ which is supposed to be fixed from now on. A basis for $\mathfrak{a}$ is made of fields

$$\mathfrak{L}_n := ie^{in\theta}\partial_\theta \quad \text{with } n \in \mathbb{Z}. \tag{14}$$

They enjoy the so-called *Hermiticity condition*, $\imath(\mathfrak{L}_n) = \mathfrak{L}_{-n}$ and the well-known *Virasoro commutation rules* with vanishing central charge, $[\mathfrak{L}_n,\mathfrak{L}_m] = (n-m)\mathfrak{L}_{n+m}$.

We remind that SL(2,$\mathbb{R}$) and SU(1,1) are isomorphic through the map SL(2,$\mathbb{R}$) $\ni h \mapsto g \in$ SU(1,1) where

$$g := \begin{pmatrix} \zeta & \overline{\eta} \\ \eta & \overline{\zeta} \end{pmatrix}, \quad h = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}, \quad \text{and} \quad \zeta := \frac{\alpha+\delta+i(\beta-\gamma)}{2}, \quad \eta := \frac{\delta-\alpha-i(\beta+\gamma)}{2}.$$

Diff$^+$($\mathbb{S}^1$) includes the Möbius group of the circle PSL(2,$\mathbb{R}$) := SU(1,1)/$\{\pm I\}$ as a finite-dimensional subgroup: Thinking $\mathbb{S}^1$ as the unit complex circle parametrized by θ, an element $g \in$ PSL(2,$\mathbb{R}$) is injectively associated with the diffeomorphism $g \in$ Diff$^+$($\mathbb{S}$),

$$g{:}e^{i\theta}\mapsto \frac{\zeta e^{i\theta}+\overline{\eta}}{\eta e^{i\theta}+\overline{\zeta}} \quad \text{with } \theta\in[-\pi,\pi]. \tag{15}$$

The corresponding inclusion of Lie algebras is illustrated by the fact that the three $\imath$-anti-Hermitian linearly independent elements of $\mathfrak{a}$,

$$\mathcal{K}:=i\mathfrak{L}_0=-\partial_\theta,\quad \mathcal{S}:=i\frac{\mathfrak{L}_1+\mathfrak{L}_{-1}}{2}=-\cos\theta\partial_\theta,\quad \mathcal{D}:=i\frac{\mathfrak{L}_1-\mathfrak{L}_{-1}}{2}=-\sin\theta\partial_\theta \tag{16}$$

enjoy the commutation rules of the elements k, s, d of the basis of the Lie algebra $\mathrm{sl}(2,\mathbb{R})$ with

$$k=\frac{1}{2}\begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix},\quad s=\frac{1}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},\quad d=\frac{1}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}. \tag{17}$$

In particular k is the generator of the subgroup of rotations $\mathrm{SO}(2)/\pm I\subset\mathrm{PSL}(2,\mathbb{R})$ given by dispacements in θ. $\mathrm{Diff}^+(\mathbb{S}^1)$ acts naturally as a group of *isometries* on the semi-Riemannian manifold $\mathbb{M}=\mathbb{S}^1\times\Sigma$. If $g\in\mathrm{Diff}^+(\mathbb{S}^1)$, we shall use the same symbol to indicate the associated diffeomorphism of $\mathbb{M}$.

B. Invariance with respect to PSL(2,$\mathbb{R}$)

From now on we use the following notation. If $g\in\mathrm{Diff}^+(\mathbb{S}^1)$ and $\psi\in C_c^\infty(\mathbb{M};\mathbb{C})$, $\psi^{(g)}:=\psi\circ g$. If $[\psi]\in\mathcal{S}(\mathbb{M})$, the element $[\psi]^{(g)}:=[\psi^{(g)}]$ is well defined and it will be indicated by $\psi^{(g)}$ simply if the meaning is clear from the context. The usual pull-back action on forms $\omega\in\mathcal{D}(\mathbb{M})$ will be denoted similarly, $\omega^{(g)}:=g^*\omega$. Notice that g^* leaves $\mathcal{D}(\mathbb{M})$ fixed. Using (6), it results that if $\psi=E\omega$ with $\omega\in\mathcal{D}(\mathbb{M})$ then $\omega^{(g)}=2\epsilon_{\psi^{(g)}}\in\mathcal{D}(\mathbb{M})$. Ω and E are *invariant* under $\mathrm{Diff}^+(\mathbb{S}^1)$. That is, for all ψ, $\phi\in C_c^\infty(\mathbb{M};\mathbb{C})$, $g\in\mathrm{Diff}^+(\mathbb{S}^1)$ and ω, $\eta\in\mathcal{D}(\mathbb{M})$,

$$\Omega(\psi,\phi)=\Omega(\psi^{(g)},\phi^{(g)}),\quad \text{and}\quad E(\omega,\eta)=E(\omega^{(g)},\eta^{(g)}). \tag{18}$$

Therefore, as a consequence of general results [(4) in Theorem 5.2.8 of Ref. 2], $\mathrm{Diff}^+(\mathbb{M})$ admits a representation $\alpha{:}g\mapsto\alpha_g$ made of $*$-automorphisms of the algebra $\mathcal{W}(\mathbb{M})$ induced by

$$\alpha_g(V(\omega)):=V(\omega^{(g^{-1})}). \tag{19}$$

In the following we employ only *the restriction* of the representation α to the Möbius group of the circle $\mathrm{PSL}(2,\mathbb{R})\ni g\mapsto\alpha_g$ in terms of $*$-automorphisms of $\mathcal{W}(\mathbb{M})$.

The definition of the state λ (13) is not $\mathrm{Diff}^+(\mathbb{S}^1)$ invariant since it relies upon the choice of a preferred standard frame θ. Let us show that actually a different standard frame θ' produces the same λ provided the coordinate transformation $\theta'=\theta'(\theta)$ belongs to $\mathrm{PSL}(2,\mathbb{R})$.

Theorem 3.1: *Let θ be a standard frame on $\mathbb{S}^1$ of $\mathbb{M}:=\mathbb{S}^1\times\Sigma$, consider the state on $\mathcal{W}(\mathbb{M})$, λ (13) and the representation α of PSL$(2,\mathbb{R})$ defined above. The following hold.*

(a) *λ is invariant under α, that is $\lambda(\alpha_g(w))=\lambda(w)$ for all $g\in PSL(2,\mathbb{R})$ and $w\in\mathcal{W}(\mathbb{M})$.*
(b) *If θ' is another standard frame $\mathbb{S}^1$ such that the coordinate transformation $\theta'=\theta'(\theta)$ belongs to PSL$(2,\mathbb{R})$, then $\lambda'=\lambda$ where λ' is the analog of λ referred to θ'.*

The proof arises from (13) using the invariance of Ω under $\mathrm{Diff}^+(\mathbb{S}^1)$ and the following lemma.

Lemma 3.1: *Let θ be a standard frame on $\mathbb{S}^1$ of $\mathbb{M}:=\mathbb{S}^1\times\Sigma$. The action of PSL$(2,\mathbb{R})\subset\mathrm{Diff}^+(\mathbb{S}^1)$ preserves positive frequency parts. That is, if $g\in PSL(2,\mathbb{R})$, $\psi\in\mathcal{S}(\mathbb{M})$, $\omega\in\mathcal{D}(\mathbb{M})$,*

$$(\psi^{(g)})_+=(\psi_+\circ g)\quad\text{and}\quad(\omega^{(g)})_+=g^*\omega_+, \tag{20}$$

*where $\omega_+:=\epsilon_{\phi_+}$ is called the θ-*positive-frequency part *of any form $\omega:=\epsilon_\phi$ in $\mathcal{D}(\mathbb{M})$.*

Proof: From *Remark* on p. 271 of Ref. 27 one finds that $(\psi^{(g)})_+=(\psi_+\circ g)$ for all $g\in \mathrm{PSL}(2,\mathbb{R})$ and $\psi\in\mathcal{S}(\mathbb{M})$. The result straightforwardly extends to $\omega\in\mathcal{D}(\mathbb{M})$ using the definition of $\mathcal{D}(\mathbb{M})$. □.

We stress that (20) does *not* hold for generic diffeomorphisms $g\in \mathrm{Diff}^+(\mathbb{S}^1)$.

C. Virasoro representations and conformal nets

Let us investigate on the existence of operator representations of Virasoro algebra and the real subalgebra $\mathrm{sl}(2,\mathbb{R})$ in the Fock space $\mathfrak{F}_+(\mathcal{H})$ introduced above focusing, in particular, on the relationship with the algebra $\hat{\mathcal{W}}(\mathbb{M})$. Fix a standard frame θ on $\mathbb{S}^1$ and build up the associated Fock space and the Weyl representation. It is possible to introduce in $\mathfrak{F}_+(\mathcal{H})$ a new class of operators which generalizes chiral currents straightforwardly. If $\mathbb{N}':=\{1,2,3,\ldots\}$ and $\{u_j\}_{j\in\mathbb{N}'}$ is a Hilbert basis of $L^2(\Sigma,\omega_\Sigma)$ the vectors

$$Z_{jn}(\theta,s):=\frac{u_j(s)e^{-in\theta}}{\sqrt{4\pi n}}$$

define a Hilbert basis of the one-particle space $\mathcal{H}$. We can always reduce to the case of *real* vectors u_j and we assume that henceforth. [$L^2(\Sigma,\omega_\Sigma)$ is separable since the Borel measure induced by ω_Σ is σ-finite and the Borel σ-algebra of Σ is countably generated (the topology of Σ being second countable by definition of manifold). If $\{u_j\}$ is a Hilbert basis $\{\overline{u_j}\}$ is such. Orthonormalization procedure of a maximal set of linearly independent generators in the set of all $u_j+\overline{u_j}, i(u_j-\overline{u_j})$ yields a real Hilbert basis.] The functions $\mathcal{D}(\mathbb{M})\ni\omega\mapsto a(E\omega)$ and $\mathcal{D}(\mathbb{M})\ni\omega\mapsto a^\dagger(E\omega)$, where the operators work on the domain $F(\mathcal{H})$, can be proved to be distributions using the strong-operator topology [to show it essentially use (1) in Proposition 5.2.3 in Ref. 2] and the usual test-function topology on $\mathcal{D}(\mathbb{M})$ induced by families of seminorms referred to derivatives (of any order) in coordinates of components of forms ω (see 2.8 in Ref. 7). $\mathcal{D}(\mathbb{M})\ni\omega\mapsto\hat{\phi}(\omega)$ admits the distributional kernel

$$\hat{\phi}(\theta,s)=\frac{1}{i\sqrt{4\pi}}\sum_{(n,j)\in\mathbb{Z}\times\mathbb{N}'}\frac{u_j(s)e^{-in\theta}}{n}J_n^{(j)}, \tag{21}$$

where the (generalized) chiral currents $J_n^{(j)}:F(\mathcal{H})\to F(\mathcal{H})$ are defined as follows:

$$J_0^{(j)}=0,\quad J_n^{(j)}=i\sqrt{n}a(\overline{Z_{jn}})\quad\text{if } n>0\quad\text{and}\quad J_n^{(j)}=-i\sqrt{-n}a^\dagger(Z_{j,-n})\quad\text{if } n<0.$$

They satisfy on $F(\mathcal{H})$ both the Hermiticity condition $J_n^{(j)\dagger}\restriction_{F(\mathcal{H})}=J_{-n}^{(j)}$ and the oscillator commutation relations $[J_n^{(j)},J_m^{(i)}]=n\delta^{ij}\delta_{n,-m}I$. Introducing the usual normal order prescription $:\cdots:$ "operators $J_p^{(j)}$ with negative index p must precede those with positive index p," one can try to define the linearly independent operators, with $c\in\mathbb{N}'\cup\{\infty\}$,

$$L_k^{(c)}:=\frac{1}{2}\sum_{n\in\mathbb{Z},j\leqslant c}:J_n^{(j)}J_{k-n}^{(j)}:,\quad L_k:=L_k^{(\infty)} \tag{22}$$

on some domain in $\mathfrak{F}_+(\mathcal{H})$. We shall denote the complex infinite-dimensional algebra spanned by $L_k^{(c)}$ by $\hat{d}_c$. One can formally show that L_k have two equivalent geometric expressions

$$L_k=\frac{1}{2i}:\Omega(\hat{\phi},\mathfrak{L}_k(\hat{\phi})):, \tag{23}$$

$$L_k = \int_{\mathbb{M}} :\partial_\theta \hat{\phi} \partial_\theta \hat{\phi}: (\theta, s) e^{ik\theta} \, \mathrm{d}\theta \wedge \omega_\Sigma, \tag{24}$$

$\mathfrak{L}_k(\hat{\phi})$ is the "scalar field" obtained by the action of the differential operator $\mathfrak{L}_k$ (naturally extended from $\mathbb{S}^1$ to the product $\mathbb{M}=\mathbb{S}^1\times\Sigma$) on the "scalar field" ϕ. The same formulas hold if replacing $L_k^{(c)}$ for L_k and replacing $\hat{\phi}$ with $\hat{\phi}^{(c)}$ given by the right-hand side of (21) with the sum over j restricted to the set $\{1,2,\ldots, c\}$. If c is finite the following proposition can be proved by direct inspection.

Proposition 3.1: *Fix a standard frame θ on $\mathbb{S}^1$ of $\mathbb{M}=\mathbb{S}^1\times\Sigma$, take $c\in\mathbb{N}'$ and consider the real vector space $\hat{\mathfrak{a}}_c$ generated by the operators $L_n^{(c)}$ in* (22) *equipped with the commutator $[\cdot,\cdot]$ and the involution $\hat{\mathfrak{a}}_c \ni a \mapsto a^\dagger{\restriction}_{F(\mathcal{H})}$). The following holds.*

(a) *The elements of $\hat{\mathfrak{a}}_c$ are well defined on $F(\mathcal{H})$ which is a dense invariant space of common analytic vectors.*

(b) *$(\hat{\mathfrak{a}}_c, [\cdot,\cdot], \cdot^\dagger{\restriction}_{F(\mathcal{H})})$ is a central representation, with central charge c, of the algebra $(\mathfrak{a}, \{\cdot,\cdot\}, \imath)$ (that is a unitarizable Virasoro representation) since the following relations hold:*

$$L_{-n}^{(c)} = L_n^{(c)\dagger}{\restriction}_{F(\mathcal{H})}, \tag{25}$$

$$[L_n^{(c)}, L_m^{(c)}] = (n-m)L_{n+m}^{(c)} + \frac{(n^3-n)c}{12}\delta_{n+m,0} I. \tag{26}$$

(c) *The representation is* positive energy, *i.e., the generators of rotations $L_0^{(j)}$ is non-negative.*

(d) *Each operator $L_n^{(c)}$ does not depend on the choice for the real base $\{u_j\}_{j\leq c}$ (but depends on the finite dimensional subspace spanned by those vectors).*

Notice that the found Virasoro representations are strongly reducible.[15] Once they are decomposed into unitarizable irreducible highest-weight representations,[15] they can be exponentiated (Refs. 9, 18, and 5) obtaining unitary strongly continuous representations of $\mathrm{Diff}^+(\mathbb{S}^1)$.

In general there is no physical reason to single out a Hilbert basis $\{u_j\}$ or equivalently a sequence $\cdots\mathcal{H}_k\subset\mathcal{H}_{k+1}\cdots$ of finite dimensional subspace of$L^2(\Sigma, \omega_\Sigma)$. In the presence of particular symmetries for Σ a class of finite dimensional subspaces can be picked out referring to the invariant subspaces with respect to a unitary representation on $L^2(\Sigma, \omega_\Sigma)$ of the symmetry group. For instance, think of $\Sigma=\mathbb{S}^2$, in that case one may decompose $\psi\in L^2(\mathbb{S}^2)$ using (real and imaginary parts of) spherical harmonics Y_m^l. Hence a suitable class of finite dimensional subspaces are those with fixed angular momentum $l=0, 1, 2, \ldots$. The sphere $\mathbb{S}^2$ is reconstructed as a sequence of *fuzzy spheres* (Ref. 20) with greater and greater angular momentum l. The associated Virasoro representations have central charges $c_l=2l+1$.

In the absence of symmetries only the case $c=\infty$ seems to be physically interesting. Let us turn attention on this case. Serious problems arise when trying to give a rigorous meaning to all the operators L_n. First of all (26) becomes meaningless due to $c=\infty$ in the right-hand side. Furthermore, by direct inspection one finds that, if $n<-1$, the domain of L_n cannot include any vector of $F(\mathcal{H})$ due to an evident divergence (this drawback would arise also for $|n|=1$ if $J_0^{(j)}=0$ were false). However, by direct inspection, one finds that L_n with $n\geqslant -1$ are well defined on $F(\mathcal{H})$ which is, in fact, a common invariant dense domain made of analytic vectors, moreover $L_n\Psi=0$. The central charge does not appear considering commutators of those operators. The complex space (finitely) spanned by those vectors is closed with respect to the commutator but, unfortunately, it is *not* with respect to the Hermitian conjugation so that they cannot represent a Lie algebra of observables. However, restricting to the case $|n|\leqslant 1$ everything goes right and one gets a Lie algebra closed with respect to the Hermitian conjugation. Anti-Hermitian linearly independent operators generating that Lie algebra are

$$iK := iL_0, \quad iS := i\frac{L_1 + L_{-1}}{2}, \quad iD := \frac{L_1 - L_{-1}}{2}. \tag{27}$$

They enjoy the commutation rules of the elements k,s,d of the basis of the Lie algebra $\mathrm{sl}(2,\mathbb{R})$ (17). As a consequence a representation $R:\mathrm{sl}(2,\mathbb{R}) \to \mathfrak{L}(F(\mathcal{H}))$ can be realized by assuming $iK = R(k), iS = R(s), iD = R(d)$ and $R:\alpha k + \beta s + \gamma d \mapsto \alpha iK + \beta iS + \gamma iD$ for all $\alpha,\beta,\gamma \in \mathbb{R}$. One expects that this representation is associated, via exponentiation, with a strongly continuous (projective) unitary representation of the universal covering of $\mathrm{SL}(2,\mathbb{R})$, $\widetilde{\mathrm{SL}(2,\mathbb{R})}$. Let us prove that such a representation does exist and enjoys remarkable properties.

Theorem 3.2: *Fix a standard frame θ on $\mathbb{S}^1$ of $\mathbb{M} = \mathbb{S}^1 \times \Sigma$ and construct the GNS (Fock) realization of $\mathcal{W}(\mathbb{M})$ associated with the state λ in* (13) *and the representation R. It turns out that the Hermitian operators $iR(x)$, with $x \in sl(2,\mathbb{R})$, are essentially self-adjoint on $F(\mathcal{H})$ and there is a unique strongly continuous representation $PSL(2,\mathbb{R}) \ni g \mapsto U(g):\mathfrak{F}_+(\mathcal{H}) \to \mathfrak{F}_+(\mathcal{H})$ with*

$$U(\exp(tx)) = e^{t\overline{iR(x)}} \quad \textit{for all } x \in sl(2,\mathbb{R}) \textit{ and } t \in \mathbb{R}. \tag{28}$$

The following further facts hold.

(a) *U is a positive-energy representation of $PSL(2,\mathbb{R})$—that is the self-adjoint generator $\overline{K}$ of the subgroup of rotations, has non-negative spectrum—and furthermore $\sigma(\overline{K}) = \{0,1,2,\ldots\}$.*
(b) *U and its generators do not depend on the choice of the basis $\{u_j\}_{j\in\mathbb{Z}} \subset L^2(\Sigma,\omega_\Sigma)$. In particular, U is the tensorialization of $U\restriction_{\mathcal{H}}$. Referring to the factorization of the one-particle space $\mathcal{H} = \ell^2(\mathbb{C}) \otimes L^2(\Sigma,\omega_\Sigma)$, it holds $U\restriction_{\mathcal{H}} = V \otimes I$, where V is the restriction to the one-particle space of the representation U in the simplest case $\mathbb{M} = \mathbb{S}^1$.*
(c) *Each subspace of $\mathfrak{F}_+(\mathcal{H})$ with finite number of particles is invariant under U.*
(d) *The GNS representative of λ, Ψ, is invariant under U and it is the only unit vector of $\mathfrak{F}_+(\mathcal{H})$ invariant under $\{e^{it\overline{D}}\}_{t\in\mathbb{R}}$ up to phases.*

The proof of the theorem is given in the Appendix. The following further theorem states that $\hat{\mathcal{W}}(\mathbb{M})$ transform covariantly under this representation with respect to the action of the diffeomorphisms of $\mathrm{PSL}(2,\mathbb{R}) \subset \mathrm{Diff}^+(\mathbb{S}^1)$ seen in Sec. II B.

Theorem 3.3: *With hypotheses and notation of Theorem 3.2, the following holds.*

(a) *U is $PSL(2,\mathbb{R})$ covariant. In other words it implements unitarily the representation α of* $\mathrm{PSL}(2,\mathbb{R})$ *defined in Theorem 3.2: For all $g \in PSL(2,\mathbb{R})$,*

$$U(g) w U(g)^\dagger = \alpha_g(w) \quad \textit{for all } w \in \hat{\mathcal{W}}(\mathbb{M}). \tag{29}$$

(b) *The one-parameter group of $*$-automorphisms associated with the one-parameter group of diffeomorphisms, respectively, generated by vector fields $\mathcal{K}$, $\mathcal{S}$, $\mathcal{D}$ correspond, through (29), to the one-parameter unitary subgroups of U, respectively, generated by iK, iS, iD.* [Sign conventions should be clear, anyway to fix them notice that formally $[iK, \hat{\phi}(\theta,s)] = -\partial_\theta \hat{\phi}(\theta,s)$.]

The proof of the theorem is given in the Appendix. Theorems 3.2 and 3.3 have a remarkable consequence concerning the existence of a so-called *conformal net on* $\mathbb{S}^1$ associated with the algebra $\hat{\mathcal{W}}(\mathbb{M})$. This fact has a wide spectrum of relevant consequences in physics and in mathematics, see for instance Refs. 4, 8, 10, and 5, and references therein. We remind the reader that any weakly closed $*$-subalgebra of the unital C^*-algebra of all bounded operators on a Hilbert space is called *von Neuman algebra* if it contains the unit operator. For several theoretical reasons (see Ref. 13) the largest set of bounded observables of a quantum system represented in a Hilbert space may be assumed to be made of the self-adjoint elements of a suitable von Neumann algebra. If X is a $*$-algebra of bounded operators over a Hilbert space, X' denotes the algebra of the bounded operators which commute with each element of X and it results that[13] X is a von

Neumann algebra if and only if $X=(X')'$. In any case, $X'':=(X')'$ is the minimal von Neumann algebra which contains X. It is called the *von Neumann algebra generated by X*.

Definition 3.1: *Let $\mathcal{I}$ be the set of nonempty, nondense, open intervals of $\mathbb{S}^1$. Assume that $\mathbb{S}^1$ is equipped with a standard coordinate frame θ. A* conformal net on $\mathbb{S}^1$ *is any triple $(\mathcal{A},\Psi,U)$ where $\mathcal{A}$ is any family $\{\mathcal{A}(I)|I\in\mathcal{I}\}$ of von Neumann algebras on an infinite-dimensional separable complex Hilbert space $\mathcal{H}_{\mathcal{A}}$, and the following properties hold.*

(C1) ***Isotony:*** *$\mathcal{A}(I)\subset\mathcal{A}(J)$, if $I\subset J$ with $I,J\in\mathcal{I}$.*
(C2) ***Locality:*** *$\mathcal{A}(I)\subset\mathcal{A}(J)'$, if $I\cap J=\emptyset$ with $I,J\in\mathcal{I}$.*
(C3) ***Möbius covariance:*** *$U(g)\mathcal{A}(I)U(g)^\dagger=\mathcal{A}(gI)$, $I\in\mathcal{I}$, $g\in PSL(2,\mathbb{R})$, where U is a strongly continuous unitary representation of $PSL(2,\mathbb{R})$ in $\mathcal{H}_{\mathcal{A}}$ and g denotes the Möbius transformation (15) associated with θ.*
(C4) ***Positivity of the energy:*** *The representation U is a positive-energy representation.*
(C5) ***U-invariance and uniqueness of the vacuum:*** *$\Psi\in\mathcal{H}_{\mathcal{A}}$ is the unique (up to phases) unit vector invariant under U.*
(C6) ***Cyclicity of the vacuum:*** *Ψ is cyclic for the algebra $\mathcal{A}(\mathbb{S}^1):=\vee_{I\in\mathcal{I}}\mathcal{A}(I)$.*

We have the following theorem.

Theorem 3.4: *Fix a standard frame θ on $\mathbb{S}^1$ of $\mathbb{M}=\mathbb{S}^1\times\Sigma$ and define the associated Weyl algebra $\hat{\mathcal{W}}(\mathbb{M})$ in the Fock space $\mathfrak{F}_+(\mathcal{H})$ with vacuum state Ψ and the representation of $PSL(2,\mathbb{R})$, U of Theorems 3.2 and 3.3. With those hypotheses the family*

$$\mathcal{A}=\{\mathcal{A}(I)|I\in\mathcal{I}\}\quad \text{with } \mathcal{A}(I)=\{\hat{V}(\omega)|\text{supp }\omega\subset I\times\Sigma\}'', \tag{30}$$

together with Ψ and U form a conformal net on $\mathbb{S}^1$ such that $\hat{\mathcal{W}}(\mathbb{M})\subset\mathcal{A}(\mathbb{S}^1)$.

Proof: (C1), (C2), and (C3) are straightforward consequences of the definition (30) using the fact that (von Neumann's density theorem) $\mathcal{A}(K)$ is the closure with respect to the strong operator topology of the $*$-algebra generated by the elements in $\{\hat{W}(\omega)|\text{supp }\omega\subset K\times\Sigma\}$, employing Proposition 2.2 concerning (C2) and Theorem 3.3 concerning (C3). (C4) and (C5) are part of Theorem 3.2. (C6) is a consequence of the fact that Ψ is cyclic with respect to $\hat{\mathcal{W}}(\mathbb{M})$ (see the Appendix) and $\hat{\mathcal{W}}(\mathbb{M})\subset\mathcal{A}(\mathbb{S}^1)$. This inclusion is a consequence of the fact that, if I, $J\in\mathcal{I}$ and $\mathbb{S}^1=I\cup J$, then, due to (W2), each element of $\hat{\mathcal{W}}(\mathbb{M})$ has the form $c\hat{W}(\omega)\hat{W}(\omega')$ where supp $\omega\subset I\times\Sigma$, supp $\omega'\subset J\times\Sigma$ and $|c|=1$, so that $\hat{\mathcal{W}}(\mathbb{M})\subset\mathcal{A}(I)\vee\mathcal{A}(J)\subset\mathcal{A}(\mathbb{S}^1)$. □

Remarks:

(1) Our construction of a conformal net for, in particular, a bifurcate Killing horizon in a globally hyperbolic space–time, is explicit in giving the effective form of the unitary representation of $\mathrm{PSL}(2,\mathbb{R})$ and the relationship with the whole Virasoro algebra. It does not require any assumption on the existence of any algebra of observables in the space–time where $(\mathbb{S}^1\setminus\{\infty\})\times\Sigma$ can be viewed to be embedded, or any KMS state on that algebra. A different approach was presented in Ref. 11 where it is shown that, in a globally hyperbolic space–time containing a bifurcate Killing horizon, a conformal net can be obtained by restriction to the horizon of a local algebra in the space–time realized using a GNS representation with cyclic vector which satisfies the KMS condition with respect to the Killing time flow. The unitary representation of $\mathrm{PSL}(2,\mathbb{R})$ was obtained there making use of relevant results by Weisbrock *et al.*[40,39,12] on the interplay of modular theory and conformal theory. It seems plausible that our construction can be recovered also using the approach of Ref. 11 defining a bulk algebra of observables and a KMS state appropriately. This topic will be investigated elsewhere.
(2) Conformal nets enjoy relevant properties.[4,8,10,5]
Reeh–Schlieder property: Ψ is cyclic and separating for every $\mathcal{A}(I)$.
Bisognano–Wichmann property: The modular operator Δ_I associated with every $\mathcal{A}(I)$ satisfies $\Delta_I^{it}=U(\exp(2\pi\mathcal{D}_I))$ for every $t\in\mathbb{R}$, $\{\exp(t\mathcal{D}_I)\}_{t\in\mathbb{R}}\subset\mathrm{PSL}(2,\mathbb{R})$ being the one-parameter subgroup which leaves I invariant [with $\mathcal{D}_I$ defined as in remark (2) after Theorem 4.1

below] so that Ψ is a KMS state for $\mathcal{A}(I)$ at inverse temperature 2π with respect to $-\mathcal{D}_I$ for $\mathcal{A}((0,\pi))$.
Haag duality: $\mathcal{A}(I)' = \mathcal{A}(\mathrm{Int}(\mathbb{S}^1 \backslash I))$ for every $\mathcal{A}(I)$.
Irreducibility: $\mathcal{A}(\mathbb{S}^1)$ includes all of bounded operators on $\mathcal{H}_{\mathcal{A}}$.
Factoriality: Each $\mathcal{A}(I)$ is a type III_1 factor.
Additivity: For every $\mathcal{A}(I)$, it holds $\mathcal{A}(I) \subset \vee_{J\in S}\mathcal{A}(J)$ if $\cup_{J\in S} J \supset I$.

(3) With obvious changes, Theorems 3.2, 3.3, and 3.4 are still valid if one considers operators $L_n^{(c)}$ with $c<\infty$, $|n|\leqslant 1$ and the real basis u_j is made of smooth functions with $j \leqslant c$.

IV. SPONTANEOUS BREAKING OF SL(2,$\mathbb{R}$) SYMMETRY AND THERMAL STATES

A. Back to physics

Consider the degenerate manifold $\mathbb{M} = \mathbb{S}^1 \times \mathbb{S}^2$ obtained by the future Killing horizon $\mathbb{F} \equiv \mathbb{R} \times \mathbb{S}^2$ of the Kruskal manifold as discussed in Sec. II A. (However what we say can be generalized to globally hyperbolic space–times with a bifurcate Killing horizon.) In particular the orientation of $\mathbb{S}^1 = \mathbb{R} \cup \{\infty\}$ is that induced on $\mathbb{R}$ from time orientation of the space–time. Let θ be a standard frame on $\mathbb{S}^1$ such that, with $\mathcal{D}$ given in (16),

$$\xi\restriction_{\mathbb{F}} = -\kappa\mathcal{D}, \tag{31}$$

ξ being the global Killing field defining Schwarzschild time in both static wedges and κ being the *surface gravity* which is constant on the Killing horizon $\mathbb{F}$, $\kappa = (4GM)^{-1}$, M being the mass of the black hole.[37,38] *Equation (31) does not fix a standard frame uniquely. However the remaining freedom does not affect the construction we present as a consequence of Theorem 4.3 below*. The requirement (31) implies that the *adimensional* parameter $v \in \mathbb{R}$ of the integral curves of $-\mathcal{D}$ on $\mathbb{F}$ coincides, up the factor κ^{-1} and the choice for the origin, with the usual light-coordinate [this fact is evident using well-known global Kruskal null coordinates U, V (Ref. 37)]: $v = \kappa(t + r_*)$. There r_* is the usual *Regge–Wheeler tortoise coordinate* and t the Schwarzschild time, that is the parameter of the integral curves of ξ in any Schwarzschild wedge. In our picture the point ∞ of $\mathbb{S}^1 = \mathbb{R} \cup \{\infty\}$ corresponds to $\theta = \pi$ whereas $\theta = 0$ corresponds to the bifurcation surface of $\mathbb{F}$ (see Sec. II A).

Let us illustrate the physical consequences of the choice (31) for bosonic QFT built up on the future Horizon together with a Möbius-covariant representation of PSL(2,$\mathbb{R}$) everything associated with the preferred choice for the coordinate θ on $\mathbb{S}^1$.

A celebrated result by Kay and Wald[17] states that any globally defined quasifree state on a globally hyperbolic space–time with a bifurcate Killing horizon (Kruskal manifold in particular) which is invariant under ξ and satisfies some further requirement (*Hadamard condition* imposed on the two-point function of the quasifree state in particular)[17] must be unique and KMS with respect to ξ with the *Hawking inverse temperature* $\beta_H = 2\pi/\kappa$. From a physical point of view, one expects that the system of the field defined on the horizon be in thermal equilibrium with the state in the bulk. More precisely, since $\partial_{\kappa t}$ reduces to $-\mathcal{D}$ on the future horizon due to (31), one might assume that the natural state on the Killing horizon is a KMS state with respect to $-\mathcal{D}$ at the inverse temperature 2π: That coincides with Hawking inverse temperature referred to the adimensional "time" v on $\mathbb{F}$. A first-glance candidate for such a state is just the restriction to λ to the algebra of observables supported in the future Killing horizon (omitting the unphysical points $\{\infty\} \times \mathbb{S}^2$). This is because λ enjoys the very inverse temperature 2π referred to as $-\mathcal{D}$. On the other hand, there are physical reasons to reject that candidate. Indeed, the circle $\mathbb{S}^1 = \mathbb{R} \cup \{\infty\}$ admits two physically distinguishable points: The point at infinity, which cannot be reached physically because it corresponds to a surface which does not belong to the Kruskal manifold. The other point corresponds to the bifurcation manifold where ξ vanishes. (In the general case $\mathbb{M} := \mathbb{S}^1 \times \Sigma$ considered in this work, $\mathbb{M}$ itself cannot represent a portion of space–time due to the presence of closed causal curves lying in $\mathbb{S}^1$ and thus one point of $\mathbb{S}^1$ at least must be removed to make contact with physics.) The remaining points of $\mathbb{S}^1$ are physically equivalent barring the fact that they are

either in the past or in the future of $\theta=0$. This determines two regions $\mathbb{F}_- \equiv (-\pi,0)\times\mathbb{S}^2$ and $\mathbb{F}_+ \equiv (0,\pi)\times\mathbb{S}^2$ in the physical part $\mathbb{R}\times\mathbb{S}^1$, of the manifold $\mathbb{S}^1\times\mathbb{S}^2$, corresponding to, respectively, the future and past part—with respect to the bifurcation manifold—of the future Killing horizon of Kruskal space–time. Conversely, the whole $\mathrm{PSL}(2,\mathbb{R})$ unitary representation, referred to the Fock space $\mathfrak{F}_+(\mathcal{H})$ built upon λ, which, in turn, is invariant under the whole representation U, cannot select those physical regions. In particular $\mathrm{PSL}(2,\mathbb{R})$ includes arbitrary displacements of the coordinate θ. Those transformations connect the physical regions with the points at infinity. For these reasons λ seems not to be completely satisfactory from the point of view of physics in spite of its relevant thermal properties.

Once a reference state μ is fixed on $\mathcal{W}(\mathbb{M})$, the physical regions $\mathbb{F}_\pm$ correspond to von Neumann algebras $\mathcal{A}(\mathbb{F}_+)$ and $\mathcal{A}(\mathbb{F}_-)$ (based upon the GNS representation of μ) representing the observables in those regions.

In the following we show that it is possible to single out those physical regions at *quantum, i.e., Hilbert space, level* through a sort of *spontaneous breaking of* $\mathrm{SL}(2,\mathbb{R})$ *symmetry* referring to a new state $\lambda_\zeta \neq \lambda$ which *preserves* the relevant thermal properties. We mean that the following facts, actually valid for any manifold $\mathbb{M}=\mathbb{S}^1\times\Sigma$, hold true. At algebraic level there is a representation α of Möbius group of the circle $\mathrm{PSL}(2,\mathbb{R})$ made of $*$-automorphisms of the Weyl algebra $\mathcal{W}(\mathbb{M})$. Moreover, we have seen in Theorems 3.2 and 3.3 that there is a state λ on $\mathcal{W}(\mathbb{M})$ which is invariant under α and, in the GNS representation of λ, α is implemented unitarily and covariantly by a representation U of $\mathrm{PSL}(2,\mathbb{R})$. We show below that there are other, unitarily inequivalent, GNS representations of $\mathcal{W}(\mathbb{M})$ based on new states λ_ζ which are no longer invariant under the whole α, but such that, the residual symmetry is still covariantly and unitarily implementable and singles out the algebras $\mathcal{A}(\mathbb{F}_+)$ and $\mathcal{A}(\mathbb{F}_-)$ as unique invariant algebras. We show also that every λ_ζ enjoys the same thermal (KMS) properties as λ and it represents a different thermodynamical phase with respect to λ.

B. Symmetry breaking

We need some definitions to go on. Coming back to the general case $\mathbb{M}=\mathbb{S}^1\times\Sigma$ where Σ is any Riemannian manifold, fix a standard frame $\theta\in(-\pi,+\pi)$ on $\mathbb{S}^1$. The regions $\mathbb{F}_\pm$ are defined as those containing the points $(0,\pi)\times\Sigma$ and $(-\pi,0)\times\Sigma$, respectively. Consider the one-parameter subgroup of Möbius transformations $\mathbb{R}\ni t\to\exp(t\mathcal{D})$ where $\mathcal{D}:=-\sin\theta(\partial/\partial\theta)$ in $\mathbb{M}$. It admits 0 and π as unique fixed points. On the other hand, it is simply proven that (up to nonvanishing factors) $\mathcal{D}$ is the unique nonzero vector field in the representation of $\mathrm{sl}(2,\mathbb{R})$ which vanishes at 0 and π. As a consequence that subgroup is the unique (up to rescaling of the parameter) nontrivial one-parameter subgroup of $\mathrm{PSL}(2,\mathbb{R})$ which admits $(0,\pi)$ and $(-\pi,0)$ as invariant segments. The origin of the parameter v of the integral curves of $-\mathcal{D}$ can be arranged in order that

$$v=\Gamma(\theta):=\ln\left|\tan\frac{\theta}{2}\right|, \tag{32}$$

where v ranges monotonically in $\mathbb{R}$ with $\mathrm{d}v/\mathrm{d}\theta>0$ for $\theta\in(0,\pi)$, whereas it ranges monotonically in $\mathbb{R}$ with $\mathrm{d}v/\mathrm{d}\theta<0$ for $\theta\in(-\pi,0)$. In spite of its singularity at $\theta=0$, the function Γ in (32) is locally integrable. Thus for any fixed function $\zeta\in L^2(\Sigma,\omega_\Sigma)$, $\Lambda_\zeta(V(\omega)):=\lambda(V(\omega))e^{i\int_{\mathbb{M}}\Gamma(\zeta\omega_+ +\overline{\zeta\omega_+})}$ is well defined if $\omega\in\mathcal{D}(\mathbb{M})$. Let us show that Λ_ζ extends to a state on $\mathcal{W}(\mathbb{M})$. It holds $\Lambda_\zeta(V(0))=1$. Using (V1), (V2) and imposing linearity, Λ_ζ defines a linear functional on the $*$-algebra generated by all objects of $V(\omega)$. As λ is positive, Λ_ζ turns out to be positive too, finally $\mathbb{R}\ni t\mapsto\Lambda_\zeta(V(\omega))$ is continuous. For known theorems[19] there is a unique extension λ_ζ of Λ_ζ to a state on $\mathcal{W}(\mathbb{M})$: If the real function $\zeta\in L^1_{\mathrm{loc}}(\Sigma,\omega_\Sigma)$ is fixed, it is the unique state satisfying,

$$\lambda_\zeta(V(\omega))=\lambda(V(\omega))e^{i\int_{\mathbb{M}}\Gamma(\zeta\omega_+ +\overline{\zeta\omega_+})} \tag{33}$$

for all $\omega\in\mathcal{D}(\mathbb{M})$. Similar states, obtained by linear deformation of the vacuum state of a Fock representation of Weyl algebra, are known in the literature as *coherent states*. They were studied in Ref. 33 for photons in flat space–time and in Ref. 22 (see also Ref. 32). Several propositions

presented in those works could be readapted to our case with some effort. We think anyway that the shortest way consists of giving independent proofs based on more modern general results of local quantum physics[13] as the proofs of our propositions are not very complicated. Similar states for free QFT defined in globally hyperbolic spacetimes containing a bifurcate Killing horizon give rise to the failure of the uniqueness property proven in Ref. 17 (see the first footnote on p. 70 in Ref. 17).

λ_ζ and its GNS triple $(\mathfrak{H}_\zeta, \Pi_\zeta, \Psi_\zeta)$ enjoy the remarkable properties stated in the theorems below.

Theorem 4.1: *Fix a standard frame θ on $\mathbb{S}^1$ of $\mathbb{M}=\mathbb{S}^1\times\Sigma$, define $\mathcal{D}$ as in (16) and the group of $*$-automorphisms α representing PSL$(2,\mathbb{R})$ as in Theorem 3.1, $\{\alpha_t^{(\mathcal{X})}\}_{t\in\mathbb{R}}$ being any one-parameter subgroup associated with the vector field $\mathcal{X}$. If $\zeta\in L^2(\Sigma,\omega_\Sigma)$ and λ_ζ is the state defined in (33) with GNS triple $(\mathfrak{H}_\zeta,\Pi_\zeta,\Psi_\zeta)$, the following holds:*

(a) *The map $V(\omega)\mapsto V(\omega)e^{i\int_{\mathbb{M}}\Gamma(\zeta\omega_+ + \overline{\zeta\omega_+})}$, $\omega\in\mathcal{D}(\mathbb{M})$, uniquely extends to a $*$-automorphism γ_ζ on $\mathcal{W}(\mathbb{M})$ and*

$$\lambda_\zeta(w)=\lambda(\gamma_\zeta w), \quad \text{for all } w\in\mathcal{W}(\mathbb{M}), \tag{34}$$

$$\gamma_\zeta\circ\alpha_t^{(\mathcal{D})}=\alpha_t^{(\mathcal{D})}\circ\gamma_\zeta, \quad \text{for all } t\in\mathbb{R}. \tag{35}$$

(b) (i) *λ_ζ is pure,* (ii) *if $\zeta\neq\zeta'$ i.e., λ_ζ and $\lambda_{\zeta'}$ are not quasiequivalent,* (iii) *λ_ζ is invariant under $\{\alpha_t^{(\mathcal{D})}\}_{t\in\mathbb{R}}$, but it is not under any other one-parameter subgroup of α (barring those associated with $c\mathcal{D}$ for $c\in\mathbb{R}$ constant) when $\zeta\neq 0$ almost everywhere.*

(c) *$\mathfrak{H}_\zeta$ identifies with a Fock space $\mathfrak{F}_+(\mathcal{H}_\zeta)$ with vacuum vector Ψ_ζ and, for all $\omega\in\mathcal{D}(\mathbb{M})$,*

$$\Pi_\zeta: V(\omega)\mapsto\hat{V}_\zeta(\omega):=e^{i\overline{\hat{\phi}_\zeta(\omega)}}, \quad \text{where } \hat{\phi}_\zeta(\omega):=\hat{\phi}_0(\omega)+\left\{\int_{\mathbb{M}}\Gamma\left(\zeta\omega_+ + \overline{\zeta\omega_+}\right)\right\}I, \tag{36}$$

$\hat{\phi}_0(\omega)$ being here the standard field operator in the Fock space $\mathfrak{F}_+(\mathcal{H}_\zeta)$ as in Sec. II E.

(d) *There is a strongly continuous one-parameter group of unitary operators $\{U_\zeta^{(\mathcal{D})}(t)\}_{t\in\mathbb{R}}$ with*

$$\alpha_t^{(\mathcal{D})}(w)=U_\zeta^{(\mathcal{D})}(t)wU_\zeta^{(\mathcal{D})\dagger}(t) \quad \text{for all } t\in\mathbb{R} \quad \text{and } w\in\hat{\mathcal{W}}_\zeta(\mathbb{M}):=\Pi_\zeta(\mathcal{W}_\zeta(\mathbb{M})). \tag{37}$$

Moreover (the derivative is performed in the strong sense where it exists)

$$\left.\frac{d}{dt}\right|_{t=0}U_\zeta^{(\mathcal{D})}(t)=\frac{-i}{2}\overline{:\Omega(\hat{\phi}_0,\mathcal{D}\hat{\phi}_0):}\,. \tag{38}$$

The proof is in the Appendix.

Theorem 4.2: *In the hypotheses of Theorem 4.1 the following holds for net of von Neumann algebras,*

$$\mathcal{A}_\zeta=\{\mathcal{A}_\zeta(I)|I\in\mathcal{I}\}, \quad \text{with } \mathcal{A}_\zeta(I)=\{\hat{V}_\zeta(\omega)|\text{supp }\omega\subset I\times\Sigma\}''. \tag{39}$$

(a) *$\mathcal{A}_\zeta\supset\hat{\mathcal{W}}_\zeta(\mathbb{M})$ and it enjoys the following properties:* (i) *isotony,* (ii) *locality,* (iii) *$\{\exp(t\mathcal{D})\}_{t\in\mathbb{R}}$-covariance,* (iv) *$U_\zeta^{(\mathcal{D})}$-invariance and uniqueness of the vacuum Ψ_ζ,* (v) *cyclicity of the vacuum Ψ_ζ,* (vi) *Reeh–Schlieder,* (vii) *Haag duality,* (viii) *factoriality,* (ix) *irreducibility,* (x) *additivity.*

(b) *If $\zeta\neq 0$ i.e., $\mathcal{A}_\zeta(\mathbb{F}_+):=\mathcal{A}_\zeta((0,\pi))$ and $\mathcal{A}_\zeta(\mathbb{F}_-):=\mathcal{A}_\zeta((-\pi,0))$ are the unique $\{U_t^{(\mathcal{D})}\}_{t\in\mathbb{R}}$-invariant algebras in $\mathcal{A}_\zeta$.*

(c) *If Δ is the modular operator associated with $\mathcal{A}_\zeta(\mathbb{F}_+)$ then*

$$\Delta^{it}=U_\zeta^{(\mathcal{D})}(2\pi t), \quad \text{for all } t\in\mathbb{R}. \tag{40}$$

Thus λ_ζ is a KMS state on $\mathcal{A}_\zeta(\mathbb{F}_+)$ with temperature $T=1/2\pi$, with respect to $\{\alpha_t^{(-\mathcal{D})}\}_{t\in\mathbb{R}}$ [extended to σ-weak one-parameter group of $*$-automorphisms of $\mathcal{A}_\zeta(\mathbb{F}_+)$ through (37)].

Proof: (a) and (c) Since the difference between $\hat{V}_\zeta(\omega)$ and $e^{i\overline{\hat{\phi}_0(\omega)}}$ amounts to a phase only, each algebra $\mathcal{A}_\zeta(I)$ of $\mathcal{A}_\zeta$ coincides with the analog constructed starting from operators $e^{i\overline{\hat{\phi}_0(\omega)}}$ and using the same $I\in\mathcal{I}$. Hence Theorem 3.4 and subsequent Remark (2) hold using the field $\hat{\phi}_0$, replacing Ψ with Ψ_ζ and employing the representation U of $\mathrm{PSL}(2,\mathbb{R})$ which leaves Ψ_ζ unchanged. Notice that U does not implement α! In this way all the properties cited in the thesis turn out to be automatically proved with the exception of (iii) and (iv). However using (35) and (38) and (d) of Theorem 3.2 also those properties can be immediately proved. The proof of (c) is straightforward. $\mathcal{A}_\zeta((0,\pi))$ coincides with the analog constructed starting from operators $e^{i\overline{\hat{\phi}_0(\omega)}}$. In that case the thesis holds with respect to the subgroup of U, $e^{t:\Omega(\hat{\phi}_0,\mathcal{D}(\hat{\phi}_0)):/2}$ [Remark (2) after Theorem 3.4]. Now (38) implies the validity of the thesis in our case.

(b) Since $\mathcal{D}$ admits the only zeros at $\theta=0$ and $\theta=\pi\equiv-\pi$, the only open nonempty and nondense intervals of $\mathbb{S}^1$ which are invariant under the one-parameter group $\{g_t^{(\mathcal{D})}\}_{t\in\mathbb{R}}$ generated by $\mathcal{D}$ are $(0,\pi)$ and $(-\pi,0)$. $\mathcal{D}$-covariance reads $U_\zeta^{(\mathcal{D})}(t)\mathcal{A}_\zeta(I)U_\zeta^{(\mathcal{D})\dagger}(t)=\mathcal{A}_\zeta(g_t^{(\mathcal{D})}(I))$ and thus $\mathcal{A}_\zeta((0,\pi))$ and $\mathcal{A}_\zeta((-\pi,0))$ are invariant under $\{U_\zeta^{(\mathcal{D})}(t)\}_{t\in\mathbb{R}}$. Let us prove their uniqueness. Consider the case of $I=(a,b)$ with $0\leqslant a<b<\pi$. There are $t'>0$ and $a'>0$, with $a'<b$ and such that $g_{t'}^{(\mathcal{D})}(a',b)\cap(a,b)=\varnothing$. Therefore, by locality it holds $[U_\zeta^{(\mathcal{D})}(t')\mathcal{A}_\zeta((a',b))U_\zeta^{(\mathcal{D})\dagger}(t'),\mathcal{A}_\zeta((a,b))]=0$, i.e. $[\mathcal{A}_\zeta((a',b)),U_\zeta^{(\mathcal{D})}(-t')\mathcal{A}_\zeta((a,b))U_\zeta^{(\mathcal{D})\dagger}(-t')]=0$. If $\mathcal{A}_\zeta((a,b))$ were invariant under $\{U_\zeta^{(\mathcal{D})}(t)\}_{t\in\mathbb{R}}$, the latter identity above would imply that $[\mathcal{A}_\zeta((a',b)),\mathcal{A}_\zeta((a,b))]=0$, and thus in particular $\mathcal{A}_\zeta((a',b))\subset\mathcal{A}_\zeta((a',b))'$ which is trivially false because elements $\hat{V}_\zeta(\omega)\in\mathcal{A}_\zeta((a',b))$ generally do not commute. All the remaining cases can be reduced to that studied above with obvious adaptations. □

Remarks:

(1) (c) in the last theorem is valid also replacing $\mathbb{F}_-$ for $\mathbb{F}_+$ and $\mathcal{D}$ for $-\mathcal{D}$ as well. Theorems 4.1 and 4.2 hold in particular for $\Sigma=\mathbb{S}^2$ and $\mathbb{M}=\mathbb{S}^1\times\mathbb{S}^2$. In that case one finds easily that λ_ζ *is invariant under the group of $*$-automorphisms induced by the action of SO*(3) *as isometry group on $\mathbb{S}^2$ if and only if ζ is constant i.e. on $\mathbb{S}^2$.*
Generic Σ do not admit SO(3) as a group of isometries, in that case λ_ζ is invariant under the relevant isometry group of Σ provided ζ is so. Finally we notice that the hypotheses $\zeta\in L^2(\Sigma,\omega_\Sigma)$ can be relaxed in $\zeta\in L^1_{\mathrm{loc}}(\Sigma,\omega_\Sigma)$ (the space of locally integrable functions on Σ with respect to ω_Σ) both in Theorems 4.1 and 4.2, the only result that could fail to hold is (ii) in (b) of Theorem 4.1.

(2) Theorems 4.1 and 4.2 refer to the pair of segments $(0,\pi)$ and $(-\pi,0)$ in the circle realized as the segment $[-\pi,\pi]$ with $-\pi\equiv\pi$. From a physical point of view there is no way to distinguish between the pair of regions $(0,\pi)$, $(-\pi,0)$ and any other pair of open nonempty segments I, $J\subset\mathbb{S}^1$ such that $J=\mathrm{int}(\mathbb{S}^1\setminus I)$. This is because there is no way to measure segments on $\mathbb{S}^1$ as the metric is degenerate therein. In fact the theorem can be stated for any pair of such segments. To prove it we notice that there exists a Möbius diffeomorphism $g:\mathbb{S}^1\to\mathbb{S}^1$ with $I=g((0,\pi))$ and $J=g((-\pi,0))$. [Assume that, in coordinates θ, I has length equal or shorter than J. The diffeomorphism g^{-1} is the composition of a rigid rotation generated by $\mathcal{K}$ which maps the center of I in 0, a dilatation generated by $\mathcal{D}$ which enlarges the transformed I up to $(-\pi/2,\pi/2)$ and another anticlockwise rigid rotation of $\pi/2$.] Hence, Theorems 4.1 and 4.2 can be restated replacing $(0,\pi)$ and $(-\pi,0)$ with, respectively, I and J, replacing the state (33) with the state and assuming to have fixed some $\zeta\in L^2(\Sigma,\omega_\Sigma)$,

$$\lambda_I(V(\omega)):=\lambda(V(\omega))e^{i\Gamma_I(\omega)},\quad\text{with }\Gamma_I(\omega):=\int_{\mathbb{M}}\Gamma(\zeta g^*\omega_+ + \overline{\zeta g^*\omega_+})$$

and replacing $\mathcal{D}$ with the generator $\mathcal{D}_I$ of the one-parameter subgroup of $\mathrm{PSL}(2,\mathbb{R})$ $\mathbb{R}\ni t\mapsto\exp(t\mathcal{D}_I):=g\circ\exp(t\mathcal{D})\circ g^{-1}$ which leaves invariant I and J ($\mathcal{D}_I$ does not depend on

the choice of g).

Notice also that if I, J is a pair of segments as said above and h is any Möbius transformation, $h(I)$, $h(J)$ still is a pair of open nonempty segments with $h(J)=\mathrm{int}(\mathbb{S}^1\backslash h(I))$ and it holds (using also Lemma 3.1)

$$\lambda_{h(I)}(V(\omega)) = \lambda_I(V(h^*\omega)).$$

This fact means that the PSL(2,$\mathbb{R}$) symmetry, broken at Hilbert-space level, is restored at an algebraic level by considering the whole class of states λ_I. The residual Virasoro representation after breaking PSL(2,$\mathbb{R}$) symmetry is analyzed in the Appendix.

(3) Considering again the particular case of the Kruskal manifold, the requirement (31), that is $-\sin\theta\partial_\theta = -\kappa^{-1}\xi|_{\mathbb{F}}$, fixes the standard frame only up to a coordinate transformation $\theta' = \theta'(\theta)$, where θ' being any other positive oriented coordinate frame on $\mathbb{S}^1$ satisfying $\sin\theta'\partial_{\theta'} = \sin\theta\partial_\theta$. Since our construction of quantum field theory on $\mathbb{M}$ relies upon the choice of a standard frame on $\mathbb{S}^1$, a natural question is the following: *Are quantum field theories based on* λ_ζ *and its analog* λ'_ζ *with obvious notation, unitarily equivalent?* (Notice that ζ is the same for both states). The answer is strongly positive because of the following general result.

Theorem 4.3: *With the same hypotheses as in Theorem 4.1, let* θ' *be another standard frame on* $\mathbb{S}^1$. *Referring to the coordinate frame* θ', *let* $\mathcal{D}'$ *be the vector field analog of* $\mathcal{D}$ *and let* λ'_ζ *be the state analog of* λ_ζ [*both states defined on* $\mathcal{W}(\mathbb{M})$]. *If* $\mathcal{D}'=\mathcal{D}$ *then, for any* $\zeta \in L^2(\Sigma, \omega_\Sigma)$,

$$\lambda'_\zeta = \lambda_\zeta. \tag{41}$$

Proof: In our hypotheses $\theta'(\theta) = 2\tan^{-1}(e^c \tan(\theta/2))$ for some $c \in \mathbb{R}$. The transformation $\theta \to \theta'(\theta)$ *interpreted as an active diffeomorphism* is nothing but the action of the element $\alpha^{(\mathcal{D})}_{-c}$ of the one-parameter group generated by $\mathcal{D}$. Since λ_ζ is invariant under that group [(b) in Theorem 4.1] the thesis is true. □

V. TOWARDS PHYSICAL INTERPRETATIONS

Consider the case of $\mathbb{M}$ constructed by the future Killing horizon of Kruskal manifold (however Theorem 5.1 below holds true for a generic degenerate manifold $\mathbb{M}=\mathbb{S}^1\times\Sigma$). As is well known the complete maximal Kruskal solution of Einstein equation describes a space–time with an eternal pair of black hole–white hole. However, some features (e.g., Hawking radiation) of real black holes produced by collapse can be modelled by using the right Schwarzschild wedge and the region containing the future singularity in Kruskal manifold, the region about $\mathbb{F}_+$ (see Refs. 37 and 38) in particular. $\mathbb{F}_+$ itself can be considered as (an extension of the) actual event horizon of a physical black hole. The space–time of a physical black hole obtained by stellar collapse has no white hole neither Killing bifurcate horizon. Nevertheless, in the sense stated below a physical black hole will asymptotically approach such a space–time (at least a space–time including a bifurcate Killing horizon). Indeed, in Ref. 31 Racz and Wald considered a globally hyperbolic, stationary space–time containing a black hole but no white hole, assuming, further, that the event horizon $\mathbb{E}$ of the black hole is a Killing horizon with compact cross sections. With those hypotheses they proved that if surface gravity is nonzero and constant throughout the horizon, one can globally extend the initial space–time so that the image of $\mathbb{E}$ is a proper subset of a regular bifurcate Killing horizon in the enlarged space–time. In that paper they also provided necessary and sufficient conditions for the extendibility of matter fields to the enlarged space–time. These results support the view that any space–time representing the asymptotic final state of a black hole formed by gravitational collapse may be assumed to possess a bifurcate Killing horizon (see Ref. 31 for details). Therefore, from a physical point of view, it is worth investigating the physical meaning for the theory referred to as the GNS representation of λ_ζ when restricting to the region $\mathbb{F}_+$.

A. Extremal KMS states: Existence of different thermodynamical phases

By construction λ_ζ are KMS states on the C^*-algebra $\mathcal{W}(\mathbb{F}_+)$, the Weyl algebra generated by Weyl operators $V(\omega)$ with supp $\omega \subset \mathbb{F}_+$ which is contained in $\mathcal{A}_\zeta(\mathbb{F}_+)$. As states on $\mathcal{W}(\mathbb{F}_+)$, λ_ζ and $\lambda_{\zeta'}$ can be compared also if $\zeta \neq \zeta'$ [they do not belong to a common folium if (ii) in (b) of Theorem 4.1 holds, so they cannot be compared on a common von Neumann algebra of observables in that case]. The next theorem, valid for the general case $\mathbb{M}=\mathbb{S}^1\times\Sigma$, shows that $\{\lambda_\zeta\}_{\zeta\in L^2(\Sigma,\omega_\Sigma)}$ is a family of extremal states in the convex space of KMS states over $\mathcal{W}(\mathbb{F}_+)$ at inverse temperature 2π with respect to $-\mathcal{D}$.

Theorem 5.1: *With the same hypotheses as in Theorem 4.1 the following holds*.

(a) *Any state* λ_ζ [*with* $\zeta \in L^2(\Sigma, \omega_\Sigma)$] *defines an extremal state in the convex set of KMS states on the* C^**-algebra* $\mathcal{W}(\mathbb{F}_+)$ *at inverse temperature* 2π *with respect to* $\{\alpha_t^{(-\mathcal{D})}\}_{t\in\mathbb{R}}$.

(b) *Different choices of* ζ *individuate different states on* $\mathcal{W}(\mathbb{F}_+)$ *which are not unitarily equivalent as well*.

Proof: Let $(\mathfrak{H}_\zeta, \Pi_\zeta, \Psi_\zeta)$ be the GNS representations of λ_ζ. The GNS representations of $\lambda_\zeta\restriction_{\mathcal{W}(\mathbb{F}_+)}$ must be (up to unitary equivalences) $(\mathfrak{H}_\zeta, \Pi_\zeta\restriction_{\mathcal{W}(\mathbb{F}_+)}, \Psi_\zeta)$ due to Reeh–Schlieder property [(a) in Theorem 4.2] of $\mathcal{A}_\zeta(\mathbb{F}_+)$. Since $\mathcal{A}_\zeta(\mathbb{F}_+) = \Pi_\zeta\restriction''_{\mathcal{W}(\mathbb{F}_+)}$ is a (type III_1) factor, the state $\lambda_\zeta\restriction_{\mathcal{W}(\mathbb{F}_+)}$—namely $\Pi_\zeta\restriction_{\mathcal{W}(\mathbb{F}_+)}$—is primary (see Sec. III.2.2 in Ref. 13). As a consequence, by Theorem 1.5.1 in Ref. 13, the KMS state $\lambda_\zeta\restriction_{\mathcal{W}(\mathbb{F}_+)}$ is extremal in the space of KMS states on $\mathcal{W}(\mathbb{F}_+)$ with respect to $\alpha_t^{(-\mathcal{D})}$ at the temperature of $\lambda_\zeta\restriction_{\mathcal{W}(\mathbb{F}_+)}$ itself. Obviously $\lambda_\zeta\restriction_{\mathcal{W}(\mathbb{F}_+)} \neq \lambda_{\zeta'}\restriction_{\mathcal{W}(\mathbb{F}_+)}$ because, if $\zeta-\zeta'$ is not zero almost everywhere, the integrals in the exponentials defining λ_ζ and $\lambda_{\zeta'}$ produce different results when applied to $V(\omega)$ with supp $\omega \subset \mathbb{F}_+$ with a suitable choice of ω. The proof of nonequivalence is the same as done (see the Appendix) for the states defined in the whole von Neumann algebras. □

The natural interpretation of this fact is that the states λ_ζ, restricted to the observables in the physical region $\mathbb{F}_+$, are nothing but *different thermodynamical phases* of the same system at the Hawking temperature (see Sec. V.1.5 in Ref. 13).

B. Bose–Einstein condensate and states λ_ζ with ζ real

In the following we assume that ζ is real. Let us examine some features of the generators $\hat{\phi}_\zeta$ of the Weyl representation associated with λ_ζ when restricted to the physical region $\mathbb{F}_+$. Consider $\omega \in \mathcal{D}(\mathbb{M})$ such that supp $\omega \subset \mathbb{F}_+$ and such that $\omega(v,s)$ can be rewritten as $[\partial\psi(v,s)/\partial v]\mathrm{d}v\wedge\omega_\Sigma$ where ψ is smooth and compactly supported in $\mathbb{F}_+$. Similar "wave functions" ψ have been considered in Ref. 26 building up scalar QFT on a Killing horizon ($\mathbb{F}_+$ in our case). Using (32) we can write the formal expansion

$$\hat{\phi}_\zeta(\omega) = \int_{\mathbb{F}_+} \hat{\phi}_0(\theta_+(v))\omega(v,s) + \int_{\mathbb{F}_+} \zeta(s) v\, \omega(v,s). \tag{42}$$

In terms of wave functions, if $\Omega_{\mathbb{F}_+}$ is the restriction of the right-hand side of the definition of Ω given in (1) to real smooth functions compactly supported in $\mathbb{F}_+$, it holds

$$\Omega(\psi, \hat{\phi}_\zeta) = \Omega_{\mathbb{F}_+}(\psi, \hat{\phi}_0) - \int_\Sigma \left(\int_{-\infty}^{+\infty} \psi(v,s)\mathrm{d}v \right) \zeta(s)\omega_\Sigma(s). \tag{43}$$

The group of elements $e^{itH_\zeta} := U_\zeta^{(-\mathcal{D})}(t), t\in\mathbb{R}$ generates displacements $v \mapsto v-t$ in the variable v in the argument of the wave functions ψ, since v is just the parameter of the integral curves of $-\mathcal{D}$ which takes the form $\partial/\partial v$ in $\mathbb{F}_+$. Using Fourier transformation with respect to v we can write down

$$\psi(v,s) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}_+} \mathrm{d}E\, \widetilde{\psi_+(E,s)} e^{-iEv} + \overline{\widetilde{\psi_+(E,s)}} e^{iEv}. \tag{44}$$

In heuristic sense H_ζ acts on the wave functions ψ as the multiplicative operator $\widetilde{\psi_+(E,s)} \mapsto E\widetilde{\psi_+(E,s)}$. Physically speaking, thermal properties of λ_ζ are referred just to the energy notion associated with that Hamiltonian. Actually, as is well known, this interpretation must be handled with great care, the interpretation of $\widetilde{\psi_+}$ as a representative of a one-particle quantum state can be done in a Fock space whose vacuum state does not coincide with the KMS state λ_ζ (see Sec. V.1.4 and the discussion on p. 219 of Ref. 13.) Using (44) and (43) can be rewritten as

$$\Omega(\psi, \hat{\phi}_\zeta) = \Omega_{\mathbb{F}_+}(\psi, \hat{\phi}_0) - \sqrt{2\pi} \int_\Sigma \zeta(s) \widetilde{\psi(0,s)}_+ \omega_\Sigma(s). \tag{45}$$

From (45) it is apparent that $\hat{\phi}_\zeta$ gets contributions from *zero-energy modes* ($E=0$) as it happens in *Bose–Einstein condensate*. To this end see Chap. 6 of Ref. 30 and 5.2.5 of Ref. 2, especially p. 72, where in the decomposition of the KMS state ω (after the thermodynamical limit) in $\mathbb{R}^\nu$-ergodic states, the mathematical structure of the latter states resemble that of the states λ_ζ. The decomposition of the field operator (42) into a "quantum" (with vanishing expectation value) and a "classical" (i.e., commuting with all the elements of the algebra) part is typical of the theoretical description of a boson system containing a Bose–Einstein condensate; the classical part plays the role of an *order parameter*.[6,30]

Let us focus attention on the generator of $U_\zeta^{(-\mathcal{D})}(t) = e^{itH_\zeta}$ in the representation of a state λ_ζ. Using Theorem 4.1 we find [both sides are supposed to be restricted to the core $F(\mathcal{H}_\zeta)$]

$$H_\zeta = \int_{\mathbb{M}} \sin(\theta) : \frac{\partial \hat{\phi}_\zeta}{\partial \theta} \frac{\partial \hat{\phi}_\zeta}{\partial \theta} : (\theta, s) \mathrm{d}\theta \wedge \omega_\Sigma(s).$$

Indeed, if $\theta_\pm(v) = \pm 2 \tan^{-1}(e^v)$ are the inverse functions of $v = \Gamma(\theta)$ in $\mathbb{F}_+$ and $\mathbb{F}_-$, respectively, passing from coordinates (θ, s) to coordinates (v, s) and employing the field $\hat{\phi}_0$ the right-hand side of the formula above can be rearranged as

$$\begin{aligned} H_\zeta = \lim_{N \to +\infty} \Bigg\{ & \int_{\mathbb{F}_+} \chi_N(v) : \frac{\partial \hat{\phi}_0}{\partial v} \frac{\partial \hat{\phi}_0}{\partial v} : (\theta_+(v), s) \mathrm{d}v \wedge \omega_\Sigma(s) + \|\zeta\|^2 \int_{\mathbb{R}} \chi_N(v) \mathrm{d}v \\ & - \int_{\mathbb{F}_-} \chi_N(v) : \frac{\partial \hat{\phi}_0}{\partial v} \frac{\partial \hat{\phi}_0}{\partial v} : (\theta_-(v), s) \mathrm{d}v \wedge \omega_\Sigma(s) - \|\zeta\|^2 \int_{\mathbb{R}} \chi_N(v) \mathrm{d}v \Bigg\}, \end{aligned}$$

where the function χ_N is smooth with compact support in $[-N, N]$ and becomes the constant function 1 for $N \to +\infty$. The two constant terms in brackets cancel out each other, they have the opposite sign, and the final form of H_ζ is just that in (d) of Theorem 4.1. The normal ordering prescription used in the integrals is defined by subtracting $(\Psi, \hat{\phi}_0(\theta', s') \hat{\phi}_0(\theta, s) \Psi)$ before applying derivatives and then smoothing with a product of delta in θ, θ' and s, s'. We do not enter into mathematical details here which are quite standard procedures of applied microlocal analysis similar to that used in Hadamard regularization.[3,14,24]

From the decomposition of H_ζ written above, we see that it is made of two contributions $H_\zeta^{(-)}$, $H_\zeta^{(+)}$, respectively, localized at the two disjoint regions of $\mathbb{F}$, $\mathbb{F}_-$, and $\mathbb{F}_+$. The two terms have the same value with opposite sign as one expects from the indefiniteness of the self-adjoint generator D (corresponding to the fact that the Killing vector $-\mathcal{D}$ changes orientation passing from $\mathbb{F}_+$ to $\mathbb{F}_-$). Let us concentrate on the second term in the contribution $H_\zeta^{(+)}$ to H_ζ due to $\mathbb{F}_+$. It is a volume divergence

$$E_\zeta := \|\zeta\|^2 \int_{\mathbb{R}} \mathrm{d}v\,.$$

This can be interpreted as the energy of the BE condensate localized at $\mathbb{F}_+$ whose density is *finite* and amounts to $\|\zeta\|^2$.

C. Conclusions: Can the condensate describe physical properties of a black hole?

Here, to conclude, we try to give some hints to relate the properties of the condensate with space–time, i.e., Schwarzschild black hole, properties. To do it we start from a deeper point of view. The only difference between two different Schwarzschild black holes concerns their masses, that is their Schwarzschild radii. Since we want to ascribe this difference to a feature of a state, the background and the system supporting the state must be independent from the black-hole radius. In this way the states λ_ζ must be referred to as a quantum field theory on an abstract manifold $\mathbb{M}=\mathbb{S}^1\times\mathbb{S}^2$ with a metric on $\mathbb{S}^2$ which does not coincide with the actual metric of a particular black hole. We assume the hypothesis of spherical symmetry so that the metric on $\mathbb{S}^2$ is determined by fixing the value of an adimensional parameter only (the radius rate for instance). In this view a state λ_ζ on the scalar field $\hat{\phi}$ must fix the geometry of the black hole under the constraints of the presence of a Killing horizon and spherical symmetry. Since we are in fact dealing with quantum gravity we adopt natural Planck units ($\hbar=c=G=1$) so that we can employ pure numbers in the following. In particular, the pure number defining the radius of $\mathbb{S}^2$ will be denoted by r_0.

The idea that the assignment of a (classical) scalar field fixes the metric of a space–time (solution of Einstein equations) when other constraints are given on the metric is not new, the so-called dimensional-reduction theory for gravitation leads to such a scenario (e.g., see Ref. 29 with cited references) where the scalar field is related to the dilation field. Now we adopt a similar point of view but, in addition, we assume also that the assignment of the configuration of the scalar field is due to the assignment of a quantum state of that field. Let us see how this idea can be implemented from the following remark.

Spherical symmetry implies that ζ must be constant on $\mathbb{S}^2$ [see Remark (1) after Theorem 4.2]. Since the considered states are coherent the field admits a nonvanishing averaged value. Formally it holds

$$\lambda_\zeta(\hat{\phi}_\zeta(\theta,s)) = v_\zeta(\theta)\,. \tag{46}$$

(See remarks below.) Hence the mean value of $\hat{\phi}_\zeta$ with respect to λ_ζ picks out a preferred coordinate frame along the light lines of $\mathbb{F}_+$. So, up to the choice of the origin, the mean value of the field $\hat{\phi}_\zeta$ defines a preferred coordinate v_ζ in the physical region $\mathbb{F}_+$. Now the natural hypotheses is that v_ζ is the parameter of the Killing field $\xi\restriction_{\mathbb{F}_+}$ of the considered black hole as in Sec. IV A. In other words we are saying that ζ determines a black hole in the class of Schwarzschild ones by determining its surface gravity through the identity (both sides are pure numbers since we are employing natural Planck units),

$$\zeta = \kappa^{-1}. \tag{47}$$

Such a black hole must have horizon surface $S_\zeta = \pi\zeta^2$. As a consequence we find that

$$\|\zeta\|^2 = 4\pi\zeta^2 r_0^2 \tag{48}$$

scales as the actual surface of the black hole horizon (and it is exactly the measure of the surface provided $r_0=1/2$). This provides some clues for an interpretation of $\|\zeta\|^2$ that is, equivalently, the *density of energy* of the condensate $E_\zeta/\int_{\mathbb{R}}\mathrm{d}v$.

Remarks: A pair of mathematical remarks are necessary to interpret (46).

(1) $\lambda_\zeta(\hat{\phi}_\zeta(\theta,s))$ is not well defined and it could be thought of as the weak limit of a sequence $\lambda_\zeta(\hat{\phi}_\zeta(\omega_n))$ where the forms ω_n regularize Dirac' s delta centered in $(\theta,s)\in\mathbb{F}$.

(2) Furthermore, one must take into account that the allowable forms have the shape $\omega_n(\theta,s)=[\partial f_n(\theta,s)/\partial\theta]\mathrm{d}\theta\wedge\omega_\Sigma$ where f_n is *periodic* in θ. It is not possible to produce a regularization sequence for $\delta(s,s')[\partial\delta(\theta'-\theta)/\partial\theta]\mathrm{d}\theta\wedge\omega_\Sigma$ in this way due to the periodic constraint. The drawback can easily be skipped by fixing an origin $v_{\zeta 0}$ for v_ζ (corresponding to some θ_0) for the coordinate x. In other words one considers a sequence of forms $\omega_n^{(\theta,s)}$ induced by smooth θ-periodic functions $f_n^{(\theta,s)}(\theta')=\delta_n(s'-s)[\Theta_n(\theta-\theta')+\Theta_n(\theta'-\theta_0)]$, where $\{\delta_n(s')\}$ regularize $\delta(s')$ and $\{\Theta_n(\theta')\}$ regularize the step distribution whose derivative is just $\delta(\theta')$. In this sense

$$\lim_{n\to+\infty}\lambda_\zeta(\hat{\phi}_\zeta(\omega_n^{(\theta,s)}))=v_\zeta(\theta)-v_{\zeta 0}.$$

The presented results could lead to an interesting scenario which deserves future investigation. The Kruskal space–time could be a classical object arising by spontaneous breaking of SL(2,$\mathbb{R}$) symmetry as well as Bose–Einstein condensation due to a state of a local QFT defined on a certain conformal net. In particular the abstract field operator ϕ can be seen as a noncommutative coordinate on $\mathbb{F}_+$. [Obviously noncommutativity arises from canonical commutation relations $[\phi(\theta,s),\phi(\theta',s')]=iE(\theta,s,\theta',s')$.] Commutativity is restored under the choice of an appropriate coherent state on that $*$-algebra considering the averaged values of the field. This state also fixes the actual black hole. (A recent remarkable application of some ideas of noncommutative geometry to conformal net theory and black holes appears in Ref. 16.) With a pair of fields ϕ defined on $\mathbb{F}$ and the other defined on the past Killing horizon $\mathbb{P}$ we may define, through the outlined way, global null coordinates in the complete r, t section of right Schwarzschild wedge. A subject deserving future investigation concerns the issue if, in addition to the null coordinates in the plane r, t, it is possible to give a quantum interpretation to the transverse coordinate and the whole metric of the Kruskal manifold.

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APPENDIX

A.1. Fock representation and GNS theorem: The interplay of the Fock representation presented in Sec. III and GNS theorem[13,1] is simply sketched. Using notation introduced therein, if $\Pi:\mathcal{W}(\mathbb{M})\to\hat{\mathcal{W}}(\mathbb{M})$ denotes the unique (Ω being nondegenerate) C^*-algebra isomorphism between those two Weyl representations, it turns out that $(\mathfrak{F}_+(\mathcal{H}),\Pi,\Psi)$ is the GNS triple associated with a particular pure algebraic state λ (quasifree[1,17] and invariant under the automorphism group associated with ∂_θ) on $\mathcal{W}(\mathbb{M})$ we go to introduce. Define

$$\lambda(W(\psi)):=e^{-\langle\psi_+,\psi_+\rangle/2}$$

then extend λ to the $*$-algebra finitely generated by all the elements $W(\psi)$ with $\psi\in\mathcal{S}(\mathbb{M})$, by linearity and using (W1), (W2). It is simply proven that, $\lambda(\mathbb{I})=1$ and $\lambda(a^*a)\geqslant 0$ for every element a of that $*$-algebra so that λ is a state. As the map $\mathbb{R}\ni t\mapsto\lambda(W(t\psi))$ is continuous, known theorems[19] imply that λ extends uniquely to a state λ on the complete Weyl algebra $\mathcal{W}(\mathbb{M})$. On the other hand, by direct computation, one finds that $\lambda(W(\psi))=\langle\Psi,\hat{W}(\psi)\Psi\rangle$. Since a state on a C^* algebra is continuous, this relation can be extended to the whole algebras by linearity and continuity and using (W1), (W2) so that a general GNS relation is verified,

$$\lambda(a)=\langle\Psi,\Pi(a)\Psi\rangle\quad\text{for all } a\in\mathcal{W}(\mathbb{M}).\tag{A1}$$

To conclude, it is sufficient to show that Ψ is cyclic with respect to Π. Let us show it. If $\hat{\mathcal{F}}(\mathbb{M})$ denotes the $*$-algebra generated by field operators $\Omega(\psi,\hat{\phi})$, $\psi\in\mathcal{S}(\mathbb{M})$, defined on $F(\mathcal{H})$, $\hat{\mathcal{F}}(\mathbb{M})\Psi$

is dense in the Fock space (see Proposition 5.2.3 in Ref. 2). Let $\Phi \in \mathfrak{F}_+(\mathcal{H})$ be a vector orthogonal to both Ψ and to all the vectors $\hat{W}(t_1\psi_1)\cdots\hat{W}(t_n\psi_n)\Psi$ for $n=1,2,\ldots$ and $t_i \in \mathbb{R}$ and $\psi_i \in \mathcal{S}(\mathbb{M})$. Using Stone theorem to differentiate in t_i for $t_i=0$, starting from $i=n$ and proceeding backwards up to $i=1$, one finds that Φ must also be orthogonal to all of the vectors $\Omega(\psi_1,\hat{\phi})\cdots\Omega(\psi_n,\hat{\phi})\Psi$ and thus vanishes because $\hat{\mathcal{F}}(\mathbb{M})\Psi$ is dense. This result means that $\Pi(\mathcal{W}(\mathbb{M}))\Psi$ is dense in the Fock space too, i.e., Ψ is cyclic with respect to Π. Since Ψ satisfies also (A1), the uniqueness of the GNS triple proves that the triple $(\mathfrak{F}_+(\mathcal{H}), \Pi, \Psi)$ is just (up to unitary transformations) the GNS triple associated with λ. Since the Fock representation is irreducible, λ is pure.

A.2. Residual Virasoro representation after breaking PSL$(2,\mathbb{R})$ *symmetry:* The complex Lie algebra $(\mathfrak{a},\{\cdot,\cdot\},\imath)$ of vector field on $\mathbb{S}^1$ (see discussion in Sec. III A) is made of vector fields on $\mathbb{S}^1$ whose diffeomorphism groups, generated by their real and imaginary parts, do not admit (in general) $\mathbb{F}_\pm$ as invariant regions, when extended to $\mathbb{M}=\mathbb{S}^1\times\Sigma$. This happens in particular for generators $\mathcal{L}_n=ie^{in\theta}\partial_\theta$. However, it is possible to rearrange that basis in order to partially overcome the problem. Consider the equivalent basis of $\mathfrak{a}$ made of the following real vector fields $-i\mathcal{L}_0$, $\mathcal{E}_n := (1-\cos((2n)\theta))\partial_\theta$, $\mathcal{O}_n := (1+\cos((2n+1)\theta))\partial_\theta$, $\mathcal{G}_n := -\sin(n\theta)\partial_\theta$ with $n=1,2,\ldots$. Barring $-i\mathcal{L}_0$ and $\mathcal{O}_n$, the other fields admit $\mathbb{F}_\pm$ as invariant regions. Moreover the fields $\mathcal{G}_n$ define a Lie algebra with respect to the usual Lie bracket whereas $\mathcal{E}_n$, or $\mathcal{E}_n$ together $\mathcal{G}_n$, do not. However allowing infinite linear combinations of vector fields—using for instance L^2-convergence for the components of vector fields with respect to ∂_θ (the same result holds anyway using stronger notions of convergence as uniform convergence of functions and their derivatives up to some order)—one sees that each $\mathcal{E}_n$ can be expanded as an infinite linear combination of $\mathcal{G}_n$. From these considerations one might expect, at least, that fields $\mathcal{E}_n$, but *not the vectors* $\mathcal{L}_n$ *and* $\mathcal{O}_n$, admit some operator representation in $\mathfrak{H}_\zeta$ in terms of the field operator $\hat{\phi}_\zeta$. In fact this is the case if ζ is a real function in $L^2(\Sigma,\mathrm{d}\Sigma)$. If one tries to define operators $L^{(c)}_{\zeta n}$ as in (23) with $\hat{\phi}^{(c)}$ replaced with $\hat{\phi}^{(c)}_\zeta := \hat{\phi}^{(c)}+\zeta\Gamma$, one immediately faces ill-definiteness of those operators due to infinite additive terms and the same problem arises for formal operators $O^{(c)}_n := L^{(c)}_{\zeta 0}+(L^{(c)}_{\zeta 2n+1}+L^{(c)}_{\zeta -2n-1})/2$ and also for $E^{(c)}_n := L^{(c)}_{\zeta 0}-(L^{(c)}_{\zeta 2n}+L^{(c)}_{\zeta -2n})/2$. However these terms cancel out if considering the operators $G^{(c)}_n := (L^{(c)}_{\zeta -n}-L^{(c)}_{\zeta n})/(2i)$ with $n=1,2,\ldots$, which are well defined and essentially self-adjoint on $F(\mathcal{H}_\zeta)$. Moreover, the operators $G^{(c)}_n$ define a Lie algebra with respect to the commutator. [Direct inspection shows that if $c=\infty$ none of the considered operators is well defined on $F(H_\zeta)$.] It is plausible that operators $\overline{G^{(c)}_n}$ define one-parameter groups which implement covariance with respect to analogous groups of diffeomorphisms generated by associated vector fields $\mathcal{G}_n$, and that the exponentiation of the algebra of $G^{(c)}_n$ produces a unitary representation of a (perhaps the) subgroup of $\mathrm{Diff}^+(\mathbb{S}^1)$ of the diffeomorphisms which leaves $\mathbb{F}_\pm$ invariant. However, it is worth stressing that, barring the case $\overline{G^{(c)}_1}$ which generates just $U^{(\mathcal{D})}_\zeta(t)$, Ψ_ζ is not invariant under the remaining unitary groups.

A.3. Proofs of some theorems:

Proof of Proposition 2.2: Let θ be a standard frame on $\mathbb{S}^1$. Assume the condition (a) holds. We can write $\omega=\epsilon_f$ and $\omega'=\epsilon_{f'}$ for some functions f, $f' \in \mathbb{C}^\infty(\mathbb{S}^1\times\Sigma;\mathbb{C})$. To use these facts we notice that, in the general case, it holds $E(\epsilon_f,\epsilon_{f'})=\Omega(f,f')/4$ by Proposition 2.1. Therefore, by (V2), to conclude the proof it is sufficient to show that $\Omega(f,f')=0$. Let us prove it. In our hypotheses f' is constant in the variable θ in $I\times\Sigma$ since $\partial f'(\theta,s)/\partial\theta=0$ therein and $I\times\Sigma$ is connected by paths with s constant. Moreover, if t, t' are the endpoints of I, it must hold $f(t,s)=f(t',s)$ for every $s \in \Sigma$. Indeed $\partial f(\theta,s)/\partial\theta=0$ vanishes outside $I\times\Sigma$—and thus f is constant in θ in that set as before—and f is periodic in θ at s fixed by hypotheses. Integrating by parts in the right-hand side of the definition of Ω given in (1) with f and f' in place of ψ and ψ',

$$\Omega(f,f') = 2\int_\Sigma \omega_\Sigma(s)\int_{\mathbb{S}^1} f'(\theta,s)\frac{\partial f}{\partial\theta}(\theta,s)\mathrm{d}\theta = 2\int_\Sigma \omega_\Sigma(s)\int_I f'(\theta,s)\frac{\partial f}{\partial\theta}(\theta,s)\mathrm{d}\theta.$$

f' is constant in θ in $I\times\Sigma$ and $f(t',s)=f(t,s)$, t, t' being the extreme points of I, so that

$$\frac{1}{2}\Omega(f,f') = \int_I f'(\theta,s)\frac{\partial f}{\partial\theta}(\theta,s)\mathrm{d}\theta = f'(s)\int_I \frac{\partial f}{\partial\theta}(\theta,s)\mathrm{d}\theta = f'(s)(f(t',s) - f(t,s)) = 0.$$

Now suppose that (b) holds true. In this case one has

$$i\Omega(f,f') = 2\int_\Sigma \omega_\Sigma(s)\int_{\mathbb{S}^1} f'(\theta,s)\frac{\partial f}{\partial\theta}(\theta,s)\mathrm{d}\theta = 2\int_S \omega_\Sigma(s)\int_{\mathbb{S}^1} f'(\theta,s)\frac{\partial f}{\partial\theta}(\theta,s)\mathrm{d}\theta.$$

Since $\partial f'(\theta,s)/\partial\theta = 0$ in the set $\mathbb{S}^1\times S$ which is connected by paths with s constant, f' does not depend on θ in that set and thus

$$\frac{1}{2}\Omega(f,f') = 2\int_S \omega_\Sigma(s)f'(s)\int_{\mathbb{S}^1}\frac{\partial f}{\partial\theta}(\theta,s)\mathrm{d}\theta = 2\int_S \omega_\Sigma(s)f'(s) = 0.$$

Finally (W2) or equivalently (V2) entails the thesis. □

Proof of Theorem 3.2: The operator $L := K^2+S^2+D^2$ is essentially self–adjoint on $F(\mathcal{H})$ since the dense invariant space $F(\mathcal{H})$ is made of analytic vectors. The proof is straightforward by direct estimation of $\|L^n\Psi\|$ with $\Psi\in F(\mathcal{H})$ (there is a constant $C_\Psi\geqslant 0$ with $\|L^n\Psi\|\leqslant C_\Psi^n$). As a consequence of some results by Nelson (Theoem 5.2, Corellary 9.1, Lemma 9.1, and Lemma 5.1 in Ref. 28) the Hermitean operators $iR(x)$ with $x\in \mathrm{sl}(2,\mathbb{R})$ are essentially self-adjoint on $F(\mathcal{H})$ and there is a unique strongly continuous representation $\mathrm{SL}(2,\mathbb{R})\ni g\mapsto \mathrm{U}(g):\mathfrak{F}_+(\mathcal{H})\to\mathfrak{F}_+(\mathcal{H})$ such that (28) holds true.

(a) k generates the one-parameter subgroup $\mathbb{S}^1$ in $\mathrm{SL}(2,\mathbb{R})$—that is $\mathbb{R}\ni t\mapsto\exp(tk)$ with period 4π—as well as the one-parameter subgroup $\mathbb{R}\ni t\mapsto l(t)$ isomorphic to $\mathbb{R}$ in $\mathrm{SL}(2,\mathbb{R})$. From the general theory of $\mathrm{SL}(2,\mathbb{R})$ representations, a representation $\mathrm{SL}(2,\mathbb{R})\ni g\mapsto V(g)$ is in fact a representation of $\mathrm{SL}(2,\mathbb{R})$ if $t\mapsto V(l(t))$ has period $4\pi/k$ for some integer $k\neq 0$. It is simply proved that the operator K is the tensorialization of the operator defined on $\ell^2(\mathbb{C})\otimes L^2(\Sigma,\omega_\Sigma)$ by extending

$$\{C_n\}_{n=1,2,\ldots}\otimes u_j \mapsto \{nC_n\}_{n=1,2,\ldots}\otimes u_j$$

by linearity. As a consequence the spectrum of $\overline{K}$ is the set $\sigma(\overline{K})=\{0,1,2,\ldots\}$ where the eigenspace with eigenvalue 0 is one dimensional and it is generated by the vacuum state Ψ. This implies that $\mathbb{R}\ni t\mapsto e^{it\overline{K}}=\mathrm{U}(l(t))$ has period 2π. As a first consequence U is a proper representation of $\mathrm{SL}(2,\mathbb{R})$. Furthermore, since $\sigma(\overline{K})$ is non-negative, the representation is a positive-energy representation. Finally, notice that $-I=e^{2\pi k}$ and thus $\mathrm{U}(-I)=e^{i2\pi\overline{K}}=I$ and so U is a representation of $\mathrm{PSL}(2,\mathbb{R}) := \mathrm{SL}(2,\mathbb{R})/\pm I$.

(b) and (c). From direct inspection one sees that the operators K, S, D are tensorializations of the respective operators $K\restriction_{\mathcal{H}}$, $S\restriction_{\mathcal{H}}$, $D\restriction_{\mathcal{H}}$, in particular their restriction to the space generated by the vacuum vector coincide with the operator 0. Moreover, decomposing $\mathcal{H}=\ell^2(\mathbb{C})\otimes L^2(\Sigma,\omega_\Sigma)$, one finds

$$K\restriction_{\mathcal{H}} = K_0\otimes 0, \quad S\restriction_{\mathcal{H}} = S_0\otimes 0, \quad D\restriction_{\mathcal{H}} = D_0\otimes 0,$$

where K_0, S_0, and D_0 are obtained by restricting to the one-particle space the operators K, S, and D defined in the case $\mathbb{M}=\mathbb{S}^1$ (without transverse manifold). Using again Nelson results these operators give rise to a representation $\mathrm{SL}(2,\mathbb{R})\ni g\mapsto V(g)\otimes I$ in $\mathcal{H}$. (This representation is, in fact, an irreducible representation of $\mathrm{SL}(2,\mathbb{R})$, see Ref. 27.) By tensorialization this representation extends to a representation U′ in the whole Fock space. By construction, the generators iK', iS', iD' of this representation ad associated with k, s, d, respectively, coincides with iK, iS, iD, on $F(\mathcal{H})$, respectively. Nelson's uniqueness property implies that $\mathrm{U}'=\mathrm{U}$. By construction U (=U′) admits every space with finite number of particles as invariant space, including the space with zero particles spanned by the vacuum state.

(d) First of all, as said above, U leaves invariant the space generated by the vacuum vector Ψ so that it is an invariant vector up to a phase. Let us show that this is the only unit vector with this property. By (b), the operator $\overline{D}$ is the tensorialization of $\overline{D_0 \oplus I} = \overline{D_0 \oplus I}$ where the generator of V, $\overline{D_0}$, is defined on the one-particle space in the case of the absence of Σ, $\ell^2(\mathbb{C})$, and I acts on $L^2(\Sigma, \omega_\Sigma)$. In Refs. 26 and 27 the representation V has been studied, realized, under a suitable Hilbert space isomorphism, in the space $L^2(\mathbb{R}^+, \mathrm{d}E)$. In that space $\overline{D_0}$ is the closure of the essentially self-adjoint operator $-i(Ed/\mathrm{d}E + 1/2)$. The original dense, invariant domain of $-i(Ed/\mathrm{d}E + 1/2)$ is a core for D_0 made of smooth functions on $(0, +\infty)$ (see Ref. 26 for details) of the form $\sqrt{E}e^{-\beta E}P(E)$ with $\beta > 0$ a constant not depending on the considered function and P any polynomial. Under the unitary transformation U, which takes the form $(\mathrm{U}\psi)(x) := (2\pi)^{-1/2}\int_0^{+\infty} e^{-ix \ln E}\psi(E)/\sqrt{E}\,\mathrm{d}E$ on the domain of $-i(Ed/\mathrm{d}E + 1/2)$, this operator becomes the operator position X [i.e., $(X\psi)(x) = x\psi(x)$] on $L^2(\mathbb{R}, \mathrm{d}x)$ restricted to a core contained in the Schwartz space. As a consequence $\sigma(\overline{D_0}) = \sigma_c(\overline{D_0}) = \sigma(X) = \mathbb{R}$ and, similarly, $\sigma(\overline{D_0 \oplus I}) = \sigma_c(\overline{D_0 \oplus I}) = \mathbb{R}$. Therefore, passing to the tensorialization, $\sigma(\overline{D}) = \mathbb{R}$ and $\sigma_p(\overline{D}) = \{0\}$ with, up to phases, unique eigenvector given by the vacuum vector Ψ. If Φ is a unit vector which is up-to-phases invariant under U, it must be in particular $e^{itX}\Phi = u_X(t)\Phi$ where X is any real linear combination of K, S, D and $|u_X| = 1$. As the domain of X is dense, it contains a vector Φ' with $\langle \Phi', \Phi\rangle \neq 0$ and thus $u_X(t) = \langle e^{-itX}\Phi', \Phi\rangle / \langle \Phi', \Phi\rangle$ is differentiable at $t = 0$ by Stones' theorem. As a consequence, the left-hand side $e^{itX}\Phi = u_X(t)\Phi$ must be differentiable at $t = 0$. By Stone theorem Φ belongs to the domain of $\overline{X}$ and it holds $\overline{X}\Phi = \lambda_X\Phi$ where $\lambda_X = -i\,\mathrm{d}u_X/\mathrm{d}t|_{t=0}$. Specializing the identity to $X = D$, from the spectral structure of $\overline{D}$, one concludes that it must be $\lambda_D = 0$ and, up to phases, $\Phi = \Psi$. □

Proof of Theorem 3.3: (a) and (b) To establish (29) it is sufficient to prove those identities for $w = \hat{V}(\omega)$ with $\omega \in \mathcal{D}(\mathbb{M})$ and $g \in PSL(2, \mathbb{R})$. Actually, with the said choices for w,

$$\mathrm{U}(g)a\mathrm{U}^\dagger(g) = \alpha'_g(a) \quad \text{for all } a \in \hat{\mathcal{F}}(\mathbb{M}). \tag{A2}$$

implies (29). For if (A2) holds, taking the adjoint twice for both sides one gets the relations for self-adjoint field operators $U(g)\hat{\phi}(\omega)U^\dagger(g) = \hat{\phi}(\omega^{(g^{-1})})$. Then (12) implies (29) for $w = \hat{V}(\omega)$ via standard spectral theory. To conclude the proof of (a) it is now sufficient to show the validity of (A2) with $a = \hat{\phi}(\omega)$ or of the equivalent statement

$$\mathrm{U}(g)\Omega(\psi, \hat{\phi})\mathrm{U}^\dagger(g) = \Omega(\psi^{(g^{-1})}, \hat{\phi}) \quad \text{for all } \psi \in \mathcal{S}(\mathbb{M}) \quad \text{and} \quad g \in \mathrm{PSL}(2, \mathbb{R}). \tag{A3}$$

In turn, using the fact that U preserves the vacuum vector and is the tensorialization of $\mathrm{U}\restriction_{\mathcal{H}}$ (Theorem 3.2) as well as (11) one sees that (A3) is equivalent to

$$\psi^{(g)} = \mathrm{U}(g^{-1})\restriction_{\mathcal{H}}\psi_+ + \overline{\mathrm{U}(g^{-1})\restriction_{\mathcal{H}}\psi_+} \quad \text{for all } \psi \in \mathcal{S}(\mathbb{M}) \quad \text{and} \quad g \in \mathrm{PSL}(2, \mathbb{R}). \tag{A4}$$

Let us prove (A4). If $\psi \in \mathcal{S}(\mathbb{M})$ and $g \in \mathrm{Diff}^+(\mathbb{S}^1)$ the map $\psi \mapsto \psi^{(g)}$ induces a $\mathbb{R}$-linear map from the space of θ-positive frequency parts ψ_+ to the same space given by

$$\psi_+ \mapsto S(g)\psi_+ := ((\psi_+ + \overline{\psi_+})^{(g^{-1})})_+.$$

In this way the action of g on the wave function ψ is equivalent to the action of $S(g)$ on its positive frequency part ψ_+:

$$\psi^{(g^{-1})} = S(g)\psi_+ + \overline{S(g)\psi_+}. \tag{A5}$$

However, in general, $S(g)$ is not $\mathbb{C}$-linear (and thus it cannot be seen as a map $\mathcal{H} \to \mathcal{H}$) since, using $\chi_+ := i\psi_+$ above, one gets $S(g)(i\psi_+) = ((i\psi_+ - i\overline{\psi_+})^{(g^{-1})})_+ = i((\psi_+ - \overline{\psi_+})^{(g^{-1})})_+ \neq i((\psi_+ + \overline{\psi_+})^{(g^{-1})})_+ = iS(g)\psi_+$. Actually, if $g \in \mathrm{PSL}(2, \mathbb{R})$, it turns out that $(\overline{\psi_+} \circ g^{-1})_+ = 0$ so that $S(g)\psi_+ = (\psi_+ \circ g^{-1})_+$ and S is $\mathbb{C}$-linear. This nontrivial result was proven in Lemma (i) 3.1. To conclude the proof it is

sufficient to show that $S(g)=\mathrm{U}(g)\restriction_{\mathcal{H}}$ for all $g\in \mathrm{PSL}(2,\mathbb{R})$. To establish such an identity we first notice that $S(g):\mathcal{H}\to\mathcal{H}$ is a unitary representation of $\mathrm{PSL}(2,\mathbb{R})$. The only fact non-self-evident is that $S(g)$ preserve the scalar product. It is however true because, if $\chi:=i\psi_+-i\overline{\psi_+}$, it holds

$$\langle\psi_+,\psi'_+\rangle=-i\Omega(\overline{\psi_+},\psi'_+)=\frac{-i}{2}(\Omega(\psi,\psi')+i\Omega(\chi,\psi'))$$

now, due to (A5) we can replace the arguments ψ_+,ψ'_+ by, respectively, $S(g)\psi_+$, $S(g)\psi'_+$ and the arguments ψ, ψ', χ, by $\psi^{(g^{-1})}$, $\psi'^{(g^{-1})}$, $\chi^{(g^{-1})}$, respectively, obtaining a similar identity; finally, since the action of positive-oriented diffeomorphisms of $\mathbb{S}^1$ preserves the symplectic form, one has $\Omega(\psi^{(g^{-1})},\psi'^{(g^{-1})})+i\Omega(\chi^{(g^{-1})},\ \psi'^{(g^{-1})})=\Omega(\psi,\psi')+i\Omega(\chi,\psi')$ and thus $\langle S(g)\psi_+,S(g)\psi'_+\rangle=\langle\psi_+,\psi'_+\rangle$. To conclude the proof it is sufficient to notice that, by direct inspection making use of Stone theorem one finds (details are very similar to those in the corresponding part of Theorem 2.4 in Ref. 27) that, if $\psi_{nj}=\{\delta_{np}\}_{p=1,2,\ldots}\otimes u_j\in\ell^2(\mathbb{C})\otimes L^2(\Sigma,\omega_\Sigma)=\mathcal{H}$,

$$iX\psi_{nj}=\frac{d}{\mathrm{d}t}S(\exp(tx))\psi_{nj},$$

where $X=K$, S, D, and, respectively, $x=k$, s, d [k, d, s being the basis of $\mathrm{sl}(2,\mathbb{R})$ introduced above]. On the other hand, the same result holds, by construction, for the representation $\mathrm{U}\restriction_{\mathcal{H}}$

$$iX\psi_{nj}=\frac{d}{\mathrm{d}t}\mathrm{U}(\exp(tx))\psi_{nj}.$$

Since the elements ψ_{nj} span a dense space of analytic vectors for $K\restriction^2_{\mathcal{H}}+S\restriction^2_{\mathcal{H}}+D\restriction^2_{\mathcal{H}}$, by the results by Nelson cited in the proof of Theorem 3.2, $S=\mathrm{U}\restriction_{\mathcal{H}}$. Now (A5) implies (A4) and this concludes the proof. □

Proof of Theorem 4.1: (a) Consider the closure $\mathcal{W}_\zeta(\mathbb{M})$ of the $*$-algebra in $\mathcal{W}(\mathbb{M})$ spanned elements $V_\zeta(\omega):=V(\omega)e^{i\int_{\mathbb{M}}\Gamma(\zeta\omega_++\overline{\zeta\omega_+})}$ with $\omega\in\mathcal{D}(\mathbb{M})$. Obviously the obtained C^*-algebra coincides with $\mathcal{W}(\mathbb{M})$ itself. On the other hand, its generators $V_\zeta(\omega)$ satisfy (V1) and (V2) and thus, by Theorem 5.8.8 in Ref. 2 there is a unique $*$-isomorphism $\gamma_\zeta:\mathcal{W}(\mathbb{M})\to\mathcal{W}_\zeta(\mathbb{M})=\mathcal{W}(\mathbb{M})$ with $\gamma_\zeta(V(\omega))=V(\omega)e^{i\int_{\mathbb{M}}\Gamma(\zeta\omega_++\overline{\zeta\omega_+})}$. Finally, by construction $\lambda(\gamma_\zeta(V(\omega)))=\lambda_\zeta(V(\omega))$ and thus, linearity and continuity imply (33). Let us proof (35). Due to linearity and continuity, it is sufficient to show the validity of the relation when restricting to elements $V_\zeta(\omega)$. In turn, since $V(\omega)$ is invariant under $g_t:=\exp(t\mathcal{D})$ and using Lemma 3.1, the validity of (35) for those elements is a consequence of the invariance of the integral $\int_{\mathbb{M}}\zeta\Gamma\omega_+$ under the action of g_t^* on the argument ω_+ which we go to prove. If $\mathcal{D}(\mathbb{M})\ni\omega=[\partial f(\theta,s)/\partial\theta]\mathrm{d}\theta\wedge\omega_\Sigma(s)$ and defining $\theta_\pm(v)=\pm2\tan^{-1}(e^v)$, direct computation yields

$$\int_{\mathbb{M}}\zeta\Gamma\omega_+=-\lim_{N\to+\infty}\int_{-N}^{N}\mathrm{d}v\int_\Sigma\omega_\Sigma(s)\zeta(s)[f_+(\theta_+(v),s)-f_+(\theta_-(v),s)]+\text{boundary terms}.$$

Using periodicity of f_+ in θ, boundary terms can be rearranged into a term

$$\lim_{\Theta\nearrow\pi}\left[(\Theta-\pi)\ln\left(\left|\tan\frac{\Theta}{2}\right|\right)\int_\Sigma\zeta(s)\frac{f_+(\Theta,s)-f_+(\pi,s)}{\Theta-\pi}\omega_\Sigma\right]$$

and three other similar terms where $-\pi$ or 0 replaces π. The last integral can be bounded uniformly in Θ using Lagrange theorem since $\partial f_+/\partial\theta$ is continuous and compactly supported. As a consequence the limit vanishes and the boundary terms can be dropped. Finally, using the fact that v is the parameter of the integral curves of $\mathcal{D}$ one has,

$$\int_{\mathbb{M}} \zeta\Gamma g_t^* \omega_+ = -\lim_{N\to+\infty}\int_{-N}^{N} \mathrm{d}v \int_\Sigma \omega_\Sigma(s)\zeta(s)[f_+(\theta_+(v-t),s) - f_+(\theta_-(v-t),s)]$$

$$= -\lim_{N\to+\infty}\int_{-N+t}^{N+t} \mathrm{d}v \int_\Sigma \omega_\Sigma(s)\zeta(s)[f_+(\theta_+(v),s) - f_+(\theta_-(v),s)] = \int_{\mathbb{M}} \zeta\Gamma\omega_+,$$

so that the invariance of the integral functional under $\exp(t\mathcal{D})$ is evident.

(b) Let us start from the bottom. Since λ is invariant under the whole $\mathrm{PSL}(2,\mathbb{R})$ group, invariance (noninvariance) of λ_ζ is equivalent to invariance (noninvariance) of the integral functional in the right-hand side of (33). Let us study that integral. Take $\omega(\theta,s) = [\partial f(\theta)/\partial v]h(s)\mathrm{d}\theta\wedge\omega_\Sigma(s)$ where s are coordinates on Σ and the real functions f and h are smooth with the latter compactly supported as well. Assume $\zeta\neq 0$ almost everywhere. We can fix h such that $\int_\Sigma \zeta h = e^{i\alpha}$. In this case

$$\int_{\mathbb{M}} \Gamma(\zeta\omega_+ + \overline{\zeta\omega_+}) = \int_{\mathrm{S}^1} \Gamma(\theta)\left(e^{i\alpha}\frac{\partial f_+}{\partial\theta}\mathrm{d}\theta + \mathrm{c.c.}\right).$$

As a consequence, if $\{g_t\}_{t\in\mathbb{R}}$ denotes the one-parameter subgroup of $\mathrm{PSL}(2,\mathbb{R})$ generated by $X = (a+b\cos\theta + c\sin\theta)\partial_\theta$, with $a,b,c\in\mathbb{R}$, one has

$$\left.\frac{d}{\mathrm{d}t}\right|_{t=0}\int_{\mathbb{M}} \Gamma(\zeta g_t^*\omega_+ + \overline{\zeta g_t^*\omega_+}) = \int_{\mathrm{S}^1}\Gamma(\theta)\left(e^{i\alpha}\frac{\partial}{\partial\theta}\left((a+b\cos\theta+c\sin\theta)\frac{\partial f_+}{\partial\theta}\right)\mathrm{d}\theta + \mathrm{c.c.}\right).$$

The invariance of the integral implies that the left-hand must vanish no matter the choice of f

$$\int_{\mathrm{S}^1}\Gamma(\theta)\frac{\partial}{\partial\theta}\left((a+b\cos\theta+c\sin\theta)\frac{\partial e^{i\alpha}f_+}{\partial\theta}\right)\mathrm{d}\theta + \mathrm{c.c.} = 0.$$

Using $f(\theta) := \cos(\theta-\alpha)$ one finds that it must be $a=0$ as a consequence of the identity above. Then using $f(\theta) := \cos(2\theta-\alpha)$ one finds that it must also be $b=0$. We conclude that the integral functional is invariant at most under the group generated by $c\sin\theta\partial/\partial\theta = -c\mathcal{D}$. On the other hand, the proof of such an invariance arises directly from (34) and (35) using the fact that λ is invariant under $\alpha_t^{(\mathcal{D})}$ as stated in (c) in Theorem 3.4.

The fact that λ_ζ is pure (that is extremal) is an immediate consequence of (33) using the fact that γ_ζ is bijective and λ is pure. As the λ_ζ are pure their GNS representations are irreducible. Therefore the proof of the fact that λ_ζ and $\lambda_{\zeta'}$ are not quasiequivalent if $\zeta\neq\zeta'$, almost everywhere, reduces to the proof that, if $\zeta\neq\zeta'$ almost everywhere, there is no unitary transformation $\mathrm{U}:\mathfrak{F}_+(\mathcal{H}_\zeta)\to\mathfrak{F}_+(\mathcal{H}_{\zeta'})$ such that $\mathrm{U}\hat{V}_\zeta(\omega)U^{-1} = \hat{V}_{\zeta'}(\omega)$ for all $\omega\in\mathcal{D}(\mathbb{M})$. We shall make use of the first statement in (c) which will be proved independently from the following. Suppose that there is such a unitary transformation for some choice of $\zeta\neq\zeta'$. As a consequence one also gets the identity $\mathrm{U}\hat{V}_\zeta(\omega)e^{-i(\int_{\mathbb{M}}\zeta\Gamma\omega_+ + \mathrm{c.c.})}\mathrm{U}^{-1} = \hat{V}_{\zeta'}(\omega)e^{-i(\int_{\mathbb{M}}\zeta\Gamma\omega_+ + \mathrm{c.c.})}$. That is, redefining $\zeta'-\zeta\to\zeta\neq 0$, one has $\mathrm{U}e^{i\hat{\phi}_\zeta(\omega)}\mathrm{U}^\dagger = e^{i\hat{\phi}_0(\omega)}$ where we have also identified the one-particle Hilbert spaces $\mathcal{H}_0$ and $\mathcal{H}_\zeta$ with the one-particle space $\mathcal{H}$ of the GNS representation of λ (and thus the Fock spaces). Via Stone theorem (using above $\omega = t\omega$ and $t\in\mathbb{R}$) one gets $\mathrm{U}\hat{\phi}_\zeta(\omega) = \hat{\phi}_0(\omega)\mathrm{U}$, that is $i\mathrm{U}a(\overline{\psi_+}) - a^\dagger(\psi_+) + (\int_{\mathbb{M}}\zeta\Gamma\epsilon_{\psi_+} + \mathrm{c.c.})\mathrm{U} = ia(\overline{\psi_+}) - a^\dagger(\psi_+)\mathrm{U}$ where $\psi_+ = E\omega_+$ according with (b) in Proposition 2.1. Using the analogous relation for $\psi' := i\psi_+ - i\overline{\psi_+}$ one gets in the end

$$\mathrm{U}[\overline{a(\overline{\psi_+}) - a^\dagger(\psi_+)} + \overline{a(\overline{\psi_+}) + a^\dagger(\psi_+)}] - \left(4i\int_{\mathbb{M}}\overline{\zeta\Gamma\epsilon_{\overline{\psi_+}}}\right)\mathrm{U} = [\overline{a(\overline{\psi_+}) - a^\dagger(\psi_+)} + \overline{a(\overline{\psi_+}) + a^\dagger(\psi_+)}]\mathrm{U}.$$

Applying both sides to the vacuum state Ψ_ζ and computing the scalar product of the resulting vectors with Ψ_ζ itself, the identity above implies that

$$-\left(2i\int_{\mathbb{M}}\overline{\zeta\Gamma\epsilon_{\overline{\psi_+}}}\right)\langle\Psi_\zeta, U\Psi_\zeta\rangle = \langle a^\dagger(\psi_+)\Psi_\zeta, U\Psi_\zeta\rangle.$$

If $\{\psi_{+m}\}_{m\in\mathbb{N}'}$ is a Hilbert base of $\mathcal{H}_\zeta$, iteration of the procedure sketched above produces

$$\langle\Psi_\zeta, U\Psi_\zeta\rangle\prod_n \frac{\lambda_m^{N_m}}{\sqrt{N_m!}} = \langle N_1, N_2, \ldots, N_m, \ldots|U\Psi_\zeta\rangle \tag{A6}$$

for any vector with finite number of particles $|N_1, N_2, \ldots, N_m, \ldots\rangle$, N_m being the occupation number of the state ψ_{+m} and where $\lambda_m := -2i\int_{\mathbb{M}}\overline{\zeta\Gamma\epsilon_{\overline{\psi_{+m}}}}$. It must be $\langle\Psi_\zeta, \mathrm{U}\Psi_\zeta\rangle \neq 0$, otherwise all components of $U\Psi_\zeta$ would vanish producing $\mathrm{U}\Psi_\zeta = 0$ which is impossible since U is unitary. Conversely, as $\|\Psi_\zeta\|^2 = 1$, it must hold $\|\mathrm{U}\Psi_\zeta\|^2 = 1$. This identity can be expanded with the basis of states $|N_1, N_2, \ldots, N_m, \ldots\rangle$ and a straightforward computation which employs (A6) produces

$$\|\mathrm{U}\Psi_\zeta\|^2 = |\langle\Psi_\zeta, U\Psi_\zeta\rangle|^2 \exp\left(\sum_{m=1}^{+\infty}|\lambda_m|^2\right). \tag{A7}$$

The series can explicitly be computed using a basis $\psi_{(n,j)}(\theta, s) = u_j(s)(e^{-in\theta}/\sqrt{4\pi n})$, where u_j is any basis of $L^2(\Sigma, \omega_\Sigma)$ made of compactly supported real smooth functions. [The space $\mathcal{C}$ of smooth compactly supported functions on Σ is dense in $L^2(\Sigma, \omega_\Sigma)$. As the latter is separable $\mathcal{C}$ contains a countable subset $\mathcal{C}'$ still dense in $L^2(\Sigma, \omega_\Sigma)$. In turn one may extract from $\mathcal{C}'$ a subset $\mathcal{C}''$ of linearly independent elements which span the same dense space as $\mathcal{C}'$. Usual orthonormalization procedure applied to $\mathcal{C}''$ gives a Hilbert basis for $L^2(\Sigma, \omega_\Sigma)$ made of smooth compactly supported functions. One obtains the wanted basis of u_j.] In that case $\int_\Sigma\overline{\zeta u_j}\omega_\Sigma \neq 0$ for some $j = j_0$ [otherwise the function ζ on Σ would have $L^2(\Sigma, \omega_\Sigma)$-norm zero]. One finds $|\lambda_{2n+1,j_0}|^2 = C|\int_\Sigma\zeta u_{j_0}\omega_\Sigma|^2(2n+1)^{-1}$ with $C > 0$ so that the series in (A7) diverges and the found contradiction shows that U cannot exist.

(c) By direct inspection one finds that the operators $V_\zeta(\omega)$ enjoy (V1) and (V2). Therefore, (Theorem 5.2.8, in Ref. 2) the C^*-algebra $\hat{\mathcal{W}}_\zeta(\mathbb{M})$ given by the closure of the $*$-algebra generated by $V_\zeta(\omega)$ is a representation of Weyl algebra and there is a $*$-algebra isomorphism of C^* algebras, $\Pi_\zeta : \mathcal{W}(\mathbb{M}) \to \hat{\mathcal{W}}_\zeta(\mathbb{M})$ which satisfies (36). The vacuum vector of $\mathfrak{H}_\zeta = \mathfrak{F}_+(\mathcal{H}_\zeta)$ is cyclic with respect to Π_ζ because $\hat{\mathcal{W}}_\zeta(\mathbb{M})\Psi_\zeta$ is the same space as the dense space (see part A.1 of this Appendix) spanned by vectors $e^{i\overline{\hat{\phi}(\omega_1)}}\ldots e^{i\overline{\hat{\phi}(\omega_n)}}\Psi_\zeta$, $n = ,1,2,\ldots$. Finally it holds

$$\begin{aligned}\lambda_\zeta(V(\omega)) &= \lambda(V(\omega))e^{i(\int_{\mathbb{M}}\zeta\Gamma\omega_+ + \mathrm{c.c.})} = \langle\Psi_\zeta, e^{i\overline{\hat{\phi}(\omega)}}\Psi_\zeta\rangle e^{i(\int_{\mathbb{M}}\zeta\Gamma\omega_+ + \mathrm{c.c.})} = \langle\Psi_\zeta, e^{\overline{i(\hat{\phi}(\omega) + \int_{\mathbb{M}}\zeta\Gamma\omega_+ + \mathrm{c.c.})}}\Psi_\zeta\rangle \\ &= \langle\Psi_\zeta, \hat{V}_\zeta(\omega)\Psi_\zeta\rangle,\end{aligned}$$

that is $\lambda_\zeta(V(\omega)) = \langle\Psi_\zeta, \Pi_\zeta(V(\omega))\Psi_\zeta\rangle$. By linearity and continuity this relation extends to the whole algebras, $\lambda_\zeta(w) = \langle\Psi_\zeta, \Pi_\zeta(w)\Psi_\zeta\rangle$, $w \in \mathcal{W}(\mathbb{M})$. We conclude that $(\mathfrak{F}_+(\mathcal{H}_\zeta), \Pi_\zeta, \Psi_\zeta)$ is the (unique, up to unitary transformations) GNS triple for λ_ζ.

(d) Let us denote by $\{g_t\}_{t\in\mathbb{R}}$ the one-parameter group of Möbius transformations generated by $\mathcal{D}$. The statements (a) and (b) in Theorem 3.3 imply that if D is defined as $(1/2i) : \Omega(\hat{\phi}_0, \mathcal{D}(\hat{\phi}_0))$: then $e^{itD}e^{i\overline{\hat{\phi}_0(\omega)}}e^{-itD} = e^{i\overline{\hat{\phi}_0(g_t^{-1^*}\omega)}}$. Since $\int_{\mathbb{M}}\zeta\Gamma\omega_+ + \mathrm{c.c.}$ is invariant under the action of g_t on ω as seen in the proof of (a), we have also

$$e^{itD}e^{i\overline{\hat{\phi}_0(\omega)}}e^{i(\int_{\mathbb{M}}\zeta\Gamma\omega_+ + \text{c.c.})}e^{-itD} = e^{i\overline{\hat{\phi}_0(g_t^{-1*}\omega)}}e^{i\left(\int_{\mathbb{M}}\zeta\Gamma g_t^{-1*}\omega + \text{c.c.}\right)}$$

that can be rewritten as $e^{itD}\hat{V}_\zeta(\omega)e^{-itD} = \hat{V}_\zeta(\omega^{(g_t^{-1})})$ and thus extends to the whole Weyl algebra proving (37). □

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The Epstein–Glaser approach to perturbative quantum field theory: graphs and Hopf algebras

Alexander Lange[a)]
Max-Planck-Institut für Mathematik in den Naturwissenschaften, Inselstrasse 22-26, 04103 Leipzig, Germany

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The paper aims at investigating perturbative quantum field theory in the approach of Epstein and Glaser (EG) and, in particular, its formulation in the language of graphs and Hopf algebras (HAs). Various HAs are encountered, each one associated with a special combination of physical concepts such as normalization, localization, pseudounitarity, causal regularization, and renormalization. The algebraic structures, representing the perturbative expansion of the *S*-matrix, are imposed on operator-valued distributions equipped with appropriate graph indices. Translation invariance ensures the algebras to be analytically well defined and graded total symmetry allows to formulate bialgebras. The algebraic results are given embedded in the corresponding physical framework, covering the two EG versions by Fredenhagen and Scharf that differ with respect to the concrete recursive implementation of causality. Besides, the ultraviolet divergences occurring in Feynman's representation are mathematically reasoned. As a final result, the change of the renormalization scheme in the context of EG is modeled via a HA and interpreted as the EG analog of Kreimer's HA. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1893215]

I. INTRODUCTION

In perturbative quantum field theory (pQFT) interaction of elementary particles is modeled to describe the outcomes of scattering experiments. In the approach of Epstein and Glaser (EG) the scattering matrix is investigated as a formal power series,

$$S(a\tau)=\sum_{n=0}^{\infty}\frac{a^n}{n!}T_n(\tau^{\otimes n}),\qquad \begin{cases} a & \text{coupling (constant)},\\ \tau & \text{infrared regularization (test function)}, \end{cases} \tag{1}$$

representing an operator-valued distribution acting on the Fock space of free quantum fields, where in the adiabatic limit, $\tau\to 1$, the square of the corresponding scalar product, $|\langle final|S(a\tau)|initial\rangle|^2$, is supposed to yield the scattering probability. Based on the interaction term T_1, which is assumed to be local, the higer order terms T_n, $n>1$, of the perturbative expansion can be deduced by "only" applying causality. In general the series does not converge in any norm, but in a few cases it is at least Borel summable (cf. Ref. 1, Sec. 41.4). Despite this fact, conceptually, the theory is determined only up to the so-called renormalization freedom. However, renormalization in the usual sense, as a subtraction of counterterms, does not have to be performed. This actually reflects the original motivation of EG,[2] namely, to give a proof of locality (i.e., renormalizability by local counterterms) just by proceeding the sketched way which can be seen as a parallel road to the well-known BPHZ approach[3–5] although, referring to the abstract intial setting (1), coming from the same junction.

[a)]Electronic mail: alange@mis.mpg.de

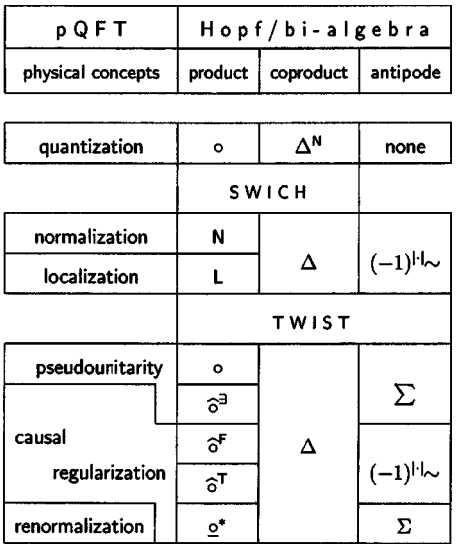

FIG. 1. Hopf algebras modeling pQFT in the EG approach.

The specified title of this paper refers to terminology which so far has not properly been implemented into the considered approach. Graphs do not appear in the EG framework and its recent versions,[6,7] and Hopf algebras (HAs), from the perspective of physics, constitute a well-developed concept only in the subject of quantum groups, having decent applications in statistical physics (cf. Ref. 8, Secs. 3.7, 7.6, 8.7). Here, graphs serve as indices for the n-point distributions T_n, and the inductive method to obtain the latter is modeled by various HAs.

In 1997, Kreimer[9] discovered that the counterterms in Zimmermann's forest formula,[5] which underlies renormalization in the Feyman graph approach, can be interpreted as an antipode condition of a HA. By then one has obviously overcome the mathematical lack which had been associated with renormalization before. But the finding of the mathematical structure alone could not fully eliminate the mysticism involved—the occurance of a combinatorial HA in this context requires further explanation. The method developed by EG would give a closer look at the physics involved. From a similar point of view (cf. Ref. 10, p. 689), in 2000, Kreimer[11] formulated the research problem of investigating the EG approach under the aspect of HAs; the content of Ref. 12 was not considered as the solution.

The brief history of contributions to the topic of EG-relevant HAs in pQFT starts in 2000 when Fauser[13] describes a HA that combines normal and time ordering. In the same year, based on the work of Fredenhagen and co-workers,[7,14–16] Pinter[17] discusses the question of uniqueness of EG's n-point distributions to establish a link to Kreimer's HA. In 2002, Brouder *et al.*[18,19] have taken up the previous two results again; they revive the work of Rota and Stein[20,21] about combinatorial HAs and present a link to quantum groups. Recent publications along this line are Refs. 22 and 23.

In the present paper, which uses a very general formulation of pQFT, Kreimer's HA is reconstructed in the EG approach via a scheme of HAs associated with different physical concepts such as normalization (referring to the normal product construction), localization, pseudounitarity, causality and an associated regularization, and eventually renormalization, cf. Fig. 1. The overall strategy has been to represent iterated solutions (e.g., of the pertubative expansion) in terms of antipode conditions. At the beginning of this project, which was the topic of the author's thesis,[24] it was not clear what the involved physical instances would be and neither whether one would be able to realize the aimed correspondence at all.

According to recent results, the starting point for the construction of the sketched HAs can be fixed by a bialgebra which most naturally models the quantum character of the considered physical objects. The algebra formalizes products of free quantum fields and the coalgebra normal products

of the latter. By switching the coalgebra into an algebra and adding a shuffling coalgebra which respects graded total symmetry (GTS) one can easily construct a HA which encodes normal ordering. Going over to a ring of scalars containing delta distributions, one can as well include the concept of localization. Extending this ring by propagators that satisfy the spectral condition and by translation invariant (TI) distributions, one obtains an algebra which formalizes the Wick expansion. The product is again the composition, i.e., the circle product, which defines a so-called twist with respect to the localized normal product. With the shuffling coproduct and an antipode given by Schmitt's formula, which implements pseudounitarity, the resulting Laplace[25] HA models the perturbative expansion. This structure must be extended again to explicitly implement causality. In accordance with the well-known ultraviolet problems of pQFT, causality requires an adequate regularization. For the three considered approches, i.e., the two recent EG versions of Fredenhagen (EGF) and Scharf (EGS) as well as the Feynman approach of Bogoliubov–Shirkov (BS), which vary with respect to the concrete product and antipode, this is realized by localization on causally determined space–time regions. In order to finally reestablish the concept of renormalization in the language of HAs one must consider graded commutative versions of the causally regularizing HAs. Then one can, in analogy to Kreimer's achievements, via some kind of deformation, describe the change of the renormalization scheme in terms of HAs.

The content has been arranged according to the items just given. This organizes the paper as follows. Free quantum fields and their algebraic structures with respect to normalization and localization are introduced in Sec. II. Including interaction, Sec. III continues with the formal expansion of the *S*-matrix and the construction of associated (Hopf) algebras. In Sec. IV, causality and renormalization get explicitly implemented into pQFT, leading to various HAs. More detailed explanation is given at the beginning of the sections.

Some technical remarks: Independent of its mathematical importance, only propositions which immediately refer to the table of Fig. 1 are called theorems. To keep the number of pages in reasonable bounds, most of the proofs are only sketched, especially when they can be found in Ref. 24 or in some other reference. The remaining calculations are provided in Appendix A. Furthermore, one finds appended examples illustrating the text and a list of symbols and abbreviations that are less standard.

II. LOCAL INTERACTION OF FREE QUANTIZED FIELDS

A. Free quantized fields

The basic physical objects in pQFT, the free quantized fields, are given here in a rather abstract way, emphasizing on physical aspects such as the causal and the spectral condition but also on mathematical ones. For instance, free fields are shown to form a bialgebra where the normal product serves as a coproduct.

1. The physical setup

The inner product of the one particle Hilbert space $\mathcal{H}_p$,

$$\frac{1}{i\hbar}(f,g)_p^+ \propto \Delta_p^+(f,g) := (\Delta_p^+ * g)(f^*), \quad f,g \in \mathcal{D}_p, \tag{2}$$

is induced by the fundamental solutions of a wave (i.e., a TI and relativistically covariant linear hyperbolic) operator, where Δ_p^+, given via Fourier transformation $(F\Delta_p^+)(k) = \theta(k^0)(F\Delta_p)(k)$, is the positive frequency part of the difference $\Delta_p = \Delta_p^R - \Delta_p^A$ between the retarded and advanced Green's functions [fulfilling $\operatorname{supp} \Delta_p^{R|A}(\cdot - y) \subseteq y + \overline{V}_{+|-}$, $\forall y \in \mathbb{R}^{1+d}$, where $\overline{V}_{+|-}$ is the closed forward|backward lightcone, i.e., $\overline{V}_+ = \{x \in \mathbb{R}^{1+d} \,|\, \sqrt{x_1^2 + \cdots + x_d^2} \leqslant x_0\} = -\overline{V}_-$]. The appropriate test function space, of Schwartz class say, is denoted by $\mathcal{D}_p$. In addition to the adjoint f^* of a test function $f \in \mathcal{D}_p$, one will also have to apply the transposed of the former, $\tilde{f} := f^{*t}$. Notice, Planck's constant $\hbar$ has been implemented and the velocity of light $c := 1$.

Following a notation similar to Ref. 26 (e.g., covariance is not simulated here), general indices ν (and μ, respectively) are supposed to determine derived (anti)particles, $p=[\![\nu]\!]$ (and $\tilde{p}=[\![\mu]\!]$, respectively), representing propagators including derivatives in terms of the Pauli Jordan function, i.e.,

$$\Delta_p = (\Delta^{\nu\mu})_{[\![\nu]\!]=p,[\![\mu]\!]=\tilde{p}}, \quad \text{where } \Delta^{\nu\mu} \overset{\partial\cdots}{\sim} D_{m_\nu} = D^+_{m_\nu} + D^-_{m_\nu} \tag{3}$$

and $D^\pm_{m_\nu}(x) = \pm[i/(2\pi)^{1+\mathrm{d}}]\int \mathrm{d}\vec{k}[e^{\mp ikx}/2\omega_\nu(\vec{k})]$ where $\omega_\nu(\vec{k}) = \sqrt{\vec{k}^2 + (m_\nu^2/\hbar^2)}$. *Antiparticles* $\tilde{p}=[\![\tilde{\nu}]\!]$ are always assumed to exist, at least formally, defined by

$$\Delta^+_{\tilde{p}}(x) = -s_p \Delta^-_p(-x)^t, \quad \text{where } s_p := (-1)^{2\,\mathrm{spin}(p)} \tag{4}$$

and where Δ^-_p symbolizes the negative frequency part.

Quantum fields φ_p associated with particles p are defined as operators on (the dense subspace of) Fock space $\mathcal{D}^{\mathrm{F}}_p = \oplus_{n\geqslant 0} S^{\sigma_p}_n \mathcal{D}^{\otimes n}_p \subset \mathcal{H}^{\mathrm{F}}_p$, i.e., in terms of annihilation and creation operators,

$$\begin{pmatrix} \varphi_p(f) \\ \varphi_{\tilde{p}}(\tilde{f}) \end{pmatrix} = A^-_p \begin{pmatrix} a_p(f) \\ a_{\tilde{p}}(\tilde{f}) \end{pmatrix} + A^+_p \begin{pmatrix} a^*_p(f) \\ a^*_{\tilde{p}}(\tilde{f}) \end{pmatrix}, \quad f \in \mathcal{D}_p, \tag{5}$$

where for the considered theories

$$A^-_p = \begin{pmatrix} 1 & 0 \\ 0 & \gamma_p \end{pmatrix} \quad \text{and } A^+_p = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{6}$$

so that by the choice of $\gamma_p = -1 \in \{\pm 1\}$ one can also model ghost fields. As usual, on $\mathcal{D}^{\mathrm{F}}_p \ni |h\rangle = (h_0, h_1(\cdot), h_2(\cdot,\cdot), \ldots)$,

$$(a_p(f)|h\rangle)_n = \sqrt{n+1}(f, h_{n+1}(\cdot,\ldots))^+_p, \tag{7}$$

$$(a^*_p(f)|h\rangle)_n = \sqrt{n} S^{\sigma_p}_n (f \otimes h_{n-1}), \tag{8}$$

where (anti)symmetrization characterizes bosons (fermions, respectively),

$$S^{\sigma_p}_n h_n = \frac{1}{n!} \sum_{\pi \in S_n} \sigma_p(\pi) h_n \circ \pi, \tag{9}$$

and $\sigma_p(\cdot)$ defines the *grading* with respect to the statistics σ_p,

$$\sigma_p(\pi) = \begin{cases} 1 \\ (\mathrm{sgn}\ \pi) \end{cases} \quad \text{if } \sigma_p = \begin{cases} +1 \\ (-1, \text{ respectively}). \end{cases} \tag{10}$$

Derived fields $\varphi_{p'} = \partial\cdots\varphi_p$ are as well, in order to be treated as free, considered to be given by *derived particles* $p' \in A'(p)$,

$$\left(\bigcirc_{\mu\in I} \partial^\mu\right)\varphi^\nu(f) := \varphi_\nu\left((-1)^{|I|}\left(\bigcirc_{\mu\in I}\partial^\mu\right)f\right), \quad I \text{ depends on } (\nu, p'). \tag{11}$$

The graded commutators of free fields have been defined to fulfill the *causal property*, i.e., $\gamma_p = 1/s_p\sigma_p \equiv s_p\sigma_p$, which imposes them,

$$[\varphi^\nu(f), \varphi^\mu(\tilde{g})]^\circ_{\sigma_p} := \varphi^\nu(f) \circ \varphi^\mu(\tilde{g}) - \sigma_p \varphi^\mu(\tilde{g}) \circ \varphi^\nu(f) \tag{12}$$

$$= i\hbar\gamma_p \Delta^{\nu\mu}(f,g)\mathrm{id}_{\mathcal{F}} =: i\hbar\Delta^{\nu\mu}_\gamma(f,g), \tag{13}$$

to have a causal support, i.e.,

$$[\varphi^{\nu}(f),\varphi^{\mu}(\tilde{g})]^{\circ}_{\sigma_p}=0 \quad \text{if supp } f\subseteq\mathbb{R}^{1+\mathrm{d}}\setminus(\text{supp } g+(\overline{V_+}\cup\overline{V_-})), \tag{14}$$

where $[\![\nu]\!]=p$ and $[\![\mu]\!]=\tilde{p}'$. Whenever spin and statistics do not coincide the particle is a ghost, cf. Ref. 27. The annihilation and creation part commutators read (i.e., in density notation, with $x,y\in\mathbb{R}^{1+\mathrm{d}}$)

$$[\varphi^{\nu}_{\mp}(x),\varphi^{\mu}_{\pm}(y)]^{\circ}_{\sigma_p}=i\hbar\Delta^{\nu\mu}_{\pm\gamma}(x-y). \tag{15}$$

The upper case, representing the positive frequency part, reflects the *spectral condition* which, applied by Wick's theorem later in the text, ensures the propagators' multiplication as distributions to be well defined. Namely, as $F\Delta^{+}_{i}\in\mathcal{S}'(\overline{V_+})$, i.e.,

$$\text{supp } F\Delta^{+}_{i}\subseteq\overline{V_+},\quad \forall\, i\leqslant n, \tag{16}$$

the so-called Fourier product[28]

$$\prod_{i\leqslant n}\Delta^{+}_{i}(x):=F^{-1}(F(\Delta^{+}_{1}(x))*\ldots*F(\Delta^{+}_{n}(x)))\in\mathcal{S}'(\mathbb{R}^{1+\mathrm{d}}). \tag{17}$$

Moreover, as the associative and commutative convolution lies in $\mathcal{S}'(\overline{V_+})$ again,[29] the resulting product satisfies the spectral condition as well.

The relevant counter example is *Feynman's (time-ordered) propagator*

$$\Delta^{\mathrm{F}}:=\mathsf{T}\Delta^{+}. \tag{18}$$

Applying the causality condition, this leads to the well-known representation,

$$\Delta^{\mathrm{F}\gamma}_{p}(x)=\mathsf{T}\Delta^{+\gamma}_{p}(x):=\theta(x^0)\Delta^{+\gamma}_{p}(x)+\sigma_p\theta(-x^0)\Delta^{+\gamma}_{\tilde{p}}(-x) \tag{19}$$

$$=\theta(x^0)\Delta^{+\gamma}_{p}(x)-\theta(-x^0)\Delta^{-\gamma}_{p}(x), \tag{20}$$

which shows that the spectral condition does not hold true.

2. The initial bialgebra

Starting the algebraic considerations for an arbitrarily chosen pQFT, let P denote the finite set of particles and $A'(p)$ the class of derived particles associated with $p\in\mathrm{P}$. Then the common Fock space is formed by a symmetrized tensor product, $\mathcal{H}^{\mathrm{F}}_{\mathrm{P}}:=(S_{|\mathrm{P}|}\otimes_{p\in\mathrm{P}})(\otimes_{q\in A'(p)}\mathcal{H}^{\mathrm{F}}_{q})$. Compatible with this definition, the composition of field operators $\mathcal{F}_{\mathrm{p}}:=\{\phi^{i}\equiv\varphi_{\mathrm{p}_i}(x_i)\,|\,i\in\mathbb{N}\}$, that are fixed by a given surjective map $\mathrm{p}:\mathbb{N}\ni i\mapsto\mathrm{p}_i\in\mathrm{P}$ which models the whole scattering scenario, is commutative only, cf. (13), if the associated particles do not belong to the same class of derived particles, i.e., $[\varphi_{\mathrm{p}_1}(x_1),\varphi_{\mathrm{p}_2}(x_2)]^{\circ}=0$ if $\mathrm{p}_2\notin A'(\mathrm{p}_1)$.

The admissible compositions $\mathcal{F}=\mathbb{C}\langle\mathcal{F}_{\mathrm{p}},+,\circ\rangle/(\cdots\circ\phi\circ\cdots\circ\phi\circ\cdots)$ of field operators $\mathcal{F}_{\mathrm{p}}$, where multiple occurances are excluded, generate an algebra $(\mathcal{F},\mathbb{C},+,\circ,\eta)$ with unity (map $\eta:=\cdot\,\mathrm{id}_{\mathcal{H}^{\mathrm{F}}_{\mathrm{p}}}$). In accordance with the following rule of resolving brackets, "$\bigcirc_{i\leqslant n}\phi^{i}$ with brackets" $=\phi^{1}\circ(\cdots\circ(\phi^{n-1}\circ\phi^{n})\cdots)$, the composition is always assumed to be associative. In a similar spirit, as these field operators act linearly on their domain, which is a dense subspace of the Fock space $\mathcal{H}^{\mathrm{F}}_{\mathrm{p}}$, distributivity is implemented. However, repeating the statement above, the composition algebra of free fields is not graded commutative.

To model local interaction, as the following example shows, the composition is not a good product. In the limit of coinciding space–time points the vacuum expectation is not defined,

$$\langle 0|\varphi^{\nu}(x)\circ\varphi^{\mu}(y)|0\rangle=\underbrace{\langle 0|\varphi^{\nu}(x)\,\mathsf{N}\,\varphi^{\mu}(y)|0\rangle}_{=0,\ \forall x,y}+i\hbar\underbrace{\Delta^{\nu\mu}_{+\gamma}(x-y)}_{\to_{x\to y}(?)}\equiv 0+(?). \tag{21}$$

The vanishing expectation, i.e., the first expression on the right-hand side (rhs) is induced by the so-called normal product,

$$\varphi^{\nu}(x) \,\mathsf{N}\, \varphi^{\mu}(y) = \varphi^{\nu}_{+}(x) \circ \varphi^{\mu}_{-}(y) + \sigma_p \varphi^{\mu} + (y) \circ \varphi^{\nu}_{-}(x). \tag{22}$$

As already applied in (15), left-hand side (lhs), the subscript sign $+|-$ denotes the projection $\mathrm{pr}_{\pm}: \phi \mapsto \phi_{\pm}$ onto the creation|annihilation part, cf. (5). For more than two factors the normal product is defined by

$$\mathsf{N}\phi^{\otimes J} := \sum_{J_+ \in \mathcal{P}_2^0(J)} \sigma_J(J_{\pm}) \bigcirc \phi_+^{\otimes J+} \circ \bigcirc \phi_-^{\otimes J-}, \tag{23}$$

where σ_J denotes the grading sign formulated on tuples $\otimes J \equiv (J_1, \ldots, J_n) \in \mathbb{N}_{\neq}^n$ of $n \in \mathbb{N}$ distinct numbers (i.e., $J_i \neq J_j$ if $i \neq j$, $\forall i,j \leqslant n$) that represent (indices of) particles p_{Ji}, where $J_{\pm} = (J_+, J_-) \in \mathcal{P}_2^{(0)}(J)$ denotes a 2-partition of J (respectively, including empty parts), and where $\phi^{\otimes J} := \bigotimes_{j \in J} \phi^j$. The grading $\sigma: S_n \to \mathbb{Z}_2$, $(J \mapsto K) = \pi \mapsto \sigma(\pi) = \sigma_J(K)$ is a representation of the permutation group $(S_n, \circ)$ on $(\mathbb{Z}_2, \cdot)$. In accordance with the definition of the common Fock space $\mathcal{H}_{\mathrm{P}}^{\mathrm{F}}$ it can be given in terms of the statistical coefficients σ_p, i.e.,

$$\sigma(\pi) := \prod_{p \in \mathrm{P}} \sigma_p(\pi|_p) = \prod_{\substack{p \in \mathrm{P} \\ \mathrm{sgn}(x|_p) = \sigma_p = -1}} \sigma_p(\pi|_p) \quad \text{and } \sigma_p(\varnothing) := 1, \tag{24}$$

where $\pi|_p: J|_p \mapsto \pi(J|_p)$ denotes a subpermutation of π which exclusively applies to derived particles $A'(p)$ with respect to p, defined on the subtuple $J|_p := (J_i)_{(\exists i \leqslant n) p_{J_i} \in A'(p)}$.

Important for the (Hopf/bi-) algebraic scenario going to be presented is the fact that the normal product can be denoted with the help of a coproduct,

$$\Delta^{\mathsf{N}} := (\mathrm{pr}_+ \otimes \mathrm{pr}_-) \circ \Delta, \tag{25}$$

which is based on the graded shuffling coproduct,

$$\Delta(\phi^{\bigcirc J}) = \sum_{J_{\pm} \in P_2^0(J)} \sigma_J(J_{\pm}) \phi^{\bigcirc J+} \otimes \phi^{\bigcirc J-}. \tag{26}$$

Immediately one observes that

$$\mathsf{N} = \bigcirc \circ \Delta^{\mathsf{N}} \circ \bigcirc, \tag{27}$$

and Lemma A.2 in the appendix verifies the implicit claim about Δ and Δ^{N} being coproducts. Therefore, as one easily verifies, $(\mathcal{F}, \mathbb{C}, +, \Delta^{(\mathsf{N})})$ forms a (non)cocommutative coalgebra (respectively) where only Δ comes with a counit,

$$\varepsilon(\phi) = \begin{cases} c & \text{if } \phi = c1, \\ 0 & \text{otherwise}. \end{cases} \tag{28}$$

Moreover, $\Delta^{(\mathsf{N})}$ as well as ε, can be shown to define homomorphisms with respect to the composition product. This leads to the main result of this section.

Theorem 2.1: $(\mathcal{F}, \mathbb{C}, +, \circ, \eta, \Delta^{(\mathsf{N})}, \varepsilon)$ *forms a bialgebra (without counit, respectively).*

Proof: All that is left to show is an immediate consequence of Lemma A.3. □

Remark 2.2: Because of (21), only the structure in parentheses is relevant for local pQFT.

Furthermore, one observes that the latterly introduced objects are equipped with the very quantum theoretic property of GTS, which models indistinguishable particles governed by particular statistics.

Proposition 2.3: *The normal product* N, *as well as the associated (and, respectively, the shuffling) coproduct* $\Delta^{(\mathsf{N})}$, *and the Feynman propagator* Δ^{F} *are all GTS.*

Proof: GTS of $\Delta^{(\mathsf{N})}$, which holds true because of Lemma A.1, immediately implies GTS of N. Applying (19), one gets

$$\Delta_p^{\mathsf{F}\gamma}(x) = \sigma_p \Delta_{\tilde{p}}^{\mathsf{F}\gamma}(-x) \tag{29}$$

which, due to the propagator's TI, just expresses GTS. □

B. Normalization and localization

The composition algebra of free fields does not provide an adequate algebraic structure for modeling local interaction. As only the normal product is suitable for such a purpose, indicated by (21), the bialgebraic structure must be modified again.

1. An appropriate weakening of structure

In fact, one drops the "co" again and *switches* the previously constructed coalgebra into an algebra. As Δ^{N} is coassociative the normal product N is associative, and therefore, the normal $\mathbb{C}$-compositions $\mathcal{N} := \{\bigcirc \circ \Delta^{\mathsf{N}}(\phi) \,|\, \phi \in \mathcal{F}\}$ constitute a graded commutative algebra with unity, i.e., $(\mathcal{N}, \mathbb{C}, +, \mathsf{N}, \eta)$. Notice, graded cocommutativity has switched to graded commutativity. Because of its shared GTS property, the right candidate for an additional coalgebra is the one with the shuffling coproduct, i.e., $(\mathcal{N}, \mathbb{C}, +, \Delta, \epsilon)$. Together with an appropriate antipode the structure of normally ordered free field operators $\mathcal{N}$ turns out to be a HA.

Theorem 2.4: *$(\mathcal{N}, \mathsf{N}, \eta, \Delta, \varepsilon)$ forms [both] a graded [co]commutative bialgebra which moreover, with the antipode $\mathsf{S} := (-1)^{|\cdot|}\sim$, i.e.,*

$$\mathsf{S}(\phi^{\mathsf{N}J}) = (-1)^n \phi^{\mathsf{N}\tilde{J}}, \quad \forall\, J \in \mathbb{N}^n_{\neq}, \quad \forall\, n \in \mathbb{N} \tag{30}$$

[where $\tilde{J} := (J_n, \ldots, J_1)$], defines a HA.

Proof: The bialgebra part follows from Lemma A.3. Notice that graded [co]commutativity is nothing else than GTS, thus realized for N (and Δ^{N}, respectively). It remains to prove the *antipode condition*, i.e., $\mathsf{N} \circ (\mathsf{S} \otimes \mathrm{id}) \circ \Delta = \eta \circ \varepsilon = \mathsf{N} \circ (\mathrm{id} \otimes \mathsf{S}) \circ \Delta$. For the nontrivial case, i.e., $n > 0$, where $\eta \circ \varepsilon = 0$, one can write the rhs (and similarly the lhs) as a sum over vanishing pairs,

$$\begin{aligned} \mathsf{N} \circ (\mathrm{id} \otimes \mathsf{S}) \circ \Delta(\phi^{\bigcirc J}) &= \sum_{\substack{J_\pm \in \mathcal{P}_2^0(J) \\ |J_-| \text{ odd}}} (\sigma_J(J_\pm)\phi^{\bigcirc J_+} \mathsf{N}(-1)\phi^{\bigcirc \tilde{J}_-} + \underbrace{\sigma_J(K_\pm)\phi^{\bigcirc K_+} \mathsf{N}\phi^{\bigcirc \tilde{K}_-}}) \\ &= \ldots + \underbrace{\sigma_J(K_\pm)\sigma_{J_\pm}(K_\pm)}_{=\sigma_J(J_\pm)} \phi^{\bigcirc J_+} \mathsf{N}\, \phi^{\bigcirc \tilde{J}_-} = 0, \end{aligned}$$

where $K_+ := J'_+ \otimes (j) \otimes J''_+$ and $K_- := J'_- \otimes J''_-$ provided $J_+ = J'_+ \otimes J''_+$ and $J_- = J'_- \otimes (j) \otimes J''_-$. The first brace results from GTS of N and the second from the composition laws of the grading σ being a group representation. □

Going over from the bialgebra of free field operators to the bialgebra of normally ordered field operators, i.e., $\mathcal{F} \to \mathcal{N}$,

$$\phi^{\bigcirc J} \mapsto \phi^{\mathsf{N}J}, \quad \bigcirc \mapsto \mathsf{N} \quad \text{and } \Delta^{\mathsf{N}} \mapsto \Delta \tag{31}$$

(as well as $\eta \mapsto \eta$), referred to as *normalization* here, this defines a functor that switching from a non[co]commutative to a graded [co]commutative bialgebra weakens the considered algebraic structure.

2. Another ring of scalars

In order to model local interaction one must describe different free particles localized at the same space–time point. In the chosen mathematical context of distributions this is done by applying Dirac's delta distributions. The implementation of the latter within the (Hopf) algebraic formalism can be realized by changing to another ring of scalars.

With tuples $J\in\mathbb{N}^n$ of $n\in\mathbb{N}$ numbers representing particles one associates the following products of delta distributions:

$$\delta^{\Pi J}\equiv\prod\delta^{\otimes J}:=\begin{cases}\prod_{i<n}\delta(x_{J_{i+1}}-x_{J_i}) & \text{if } J\in\mathbb{N}^n_{\neq},\\ 0, & \text{otherwise.}\end{cases}\tag{32}$$

Generated by these distributions and its derivatives, one obtains an algebra of localizing scalars,

$$\mathbb{L}:=\mathbb{C}\oplus\mathbb{C}\langle\{\partial^\beta\delta^K|\beta\in\mathbb{N}^2,K\in\mathbb{N}^2_{\neq}\},+,\cdot\rangle/(\delta^K\cdot\partial^\beta\delta^K,\delta^K-\delta^{\tilde{K}}),\tag{33}$$

i.e., having excluded multiple occurances of $\delta^{\Pi J}$, even with respect to permuations of its indices, and added the unity. The localized quantum field operators $\phi^{\mathsf{L}J}:=\delta^{\Pi J}\phi^{\mathsf{N}J}$ are introduced as a $\mathbb{C}$-submodule,

$$\mathcal{L}:=\bigoplus_{J\in\mathbb{N}^n_{\neq},n\geqslant 0}\mathbb{C}\{\phi^{\mathsf{L}J}|\phi^j\in\mathcal{F}_{\mathrm{p}},\forall j\in J\},\tag{34}$$

of $\mathbb{L}\otimes\mathcal{N}=:\mathcal{N}_{\mathbb{L}}$ equipped with an (associative and distributive) product, $\mathsf{L}:\phi^{\mathsf{L}J}\otimes\phi^{\mathsf{L}K}\mapsto\phi^{\mathsf{L}(J\otimes K)}$, which varies from the one that is naturally given on $\mathcal{N}_{\mathbb{L}}$ i.e., $\Pi\otimes\mathsf{N}\circ(\mathrm{id}\otimes\tau\otimes\mathrm{id})=:\mathsf{N}$, where $\tau:J\otimes K\mapsto K\otimes J$ denotes the flip operation. The latter two spaces as well carry the all over announced stucture.

Theorem 2.5: $(\mathcal{N}_{\mathbb{L}},\mathbb{L},+,\mathsf{N},\eta,\Delta,\varepsilon,\mathrm{S})$ *and its substructure* $(\mathcal{L},\mathbb{C},+,\mathsf{L},\eta,\Delta,\varepsilon,\mathrm{S})$ *form graded [co]commutative HAs over the ring* $\mathbb{L}$ *and, respectively, the field* $\mathbb{C}$.

Proof: Except for the explained modifications, this is again the content of Theorem 2.4. □

C. Interaction

Utilizing EG's language of distributions, interaction of quantum fields naturally implements the concept of classical background fields. The Hamiltonian modeling local interaction is formed by the adiabatic limit of coupled localized field operators. The presentation concludes this preliminary section. Throughout the paper, only polynomial interaction is considered, leading to the well-known identification of graphs as applied to the EG approach in the two subsequent sections.

1. Monomial couplings and the adiabatic limit

In the considered physical setup the coupling Σ_b is given by a monomial in $\mathcal{L}$. Let $M\in\mathbb{N}^m_{\neq}$ symbolize a tuple of $m\in\mathbb{N}$ particles. Then

$$\Sigma_b(\phi^{\mathsf{L}M})=\sum_{\bar{\mu}\in M}\sum_{|\alpha|\leqslant\omega_b}b^{\alpha,\bar{\mu}}(\partial^\alpha\delta^{\Pi\bar{\mu}})\phi^{\mathsf{N}\bar{\mu}}\tag{35}$$

formalizes a coupling monomial, b labels the associated coupling coefficients $b^{\alpha,\bar{\mu}}\in\mathbb{C}$ where α serves as a suitable multi-index, and $\omega_b\geqslant 0$ denotes the order of singularity. Spelled out explicitly, $\Sigma_b\phi^{\mathsf{L}M}\equiv\Sigma_b\varphi^{\mathsf{L}M}(x)$ formally depends on m space–time variables $x\equiv(x_1,\ldots,x_m)\in\mathbb{R}^{(1+\mathrm{d})\times m}$, even though (because of the localization which uses delta distributions) only one of them is independent.

The adiabatic limit replaces those m variables by a single one, i.e.,

$$\mathsf{A}_{x_i}\Sigma_b\phi^{\mathsf{L}M}:=\lim_{\tau\to 1}\langle\Sigma_b\varphi^{\mathsf{L}M}(x),\tau(x_1,\ldots,x_{i-1},x_{i+1},\ldots,x_m)\rangle_{m-1}\tag{36}$$

$$=\langle \Sigma_b \varphi^{\mathsf{L}M}(\ldots,x_i,\ldots),1(x_1,\ldots,x_{i-1},x_{i+1},\ldots,x_m)\rangle_{m-1}, \tag{37}$$

where, as well as in general, $\langle t(x),\tau(x)\rangle_m := \int_{\mathbb{R}^{(1+\mathrm{d})\times m}} t(x)\tau(x)\mathrm{d}x_1\cdots\mathrm{d}x_m$ denotes the distributions' dual bracket and $1(x)$ symbolizes an arbitrary test function in $\mathcal{D}^{\otimes}_{\mathrm{p}_M} := \bigotimes_{i\leqslant m}\mathcal{D}_{\mathrm{p}_{M_i}}$ with value "1" in a neighborhood of the origin $x=0\in\mathbb{R}^{(1+\mathrm{d})\times m}$. Of course, one may introduce another variable $x_\bullet\in\mathbb{R}^{1+\mathrm{d}}$. Then

$$\mathsf{A}_{x_\bullet}\Sigma_b\phi^{\mathsf{L}M} = \delta(x_\bullet) * \mathsf{A}_{x_1}\Sigma_b\phi^{\mathsf{L}M} = \langle \delta(x_\bullet - x_1)\Sigma_b\varphi^{\mathsf{L}M}(x), 1^{\Pi M}(x)\rangle_m, \tag{38}$$

which yields the prototype of a so-called interaction Hamiltonian.

In the algebraic context of normalization and localization the composition of monomial couplings and adiabatic limits is quite straightforward. For any $i\leqslant n$, let $\overline{M_i}\in\mathbb{N}^{m_i}_{\neq}$ denote an $m_i\in\mathbb{N}$ tuple of particles and b_i the associated coupling of order $\overline{\omega_{b_i}}$. Furthermore, form tuples of the latter objects and let $y\in\mathbb{R}^{(1+\mathrm{d})\times n}$. Then

$$\mathsf{N}_{i\leqslant n}\mathsf{A}_{y_i}\Sigma_{b_i}\phi^{\mathsf{L}\overline{M_i}} = \mathsf{A}_y^{\otimes\overline{M}}\Sigma_{\Pi b}\phi^{\mathsf{N}\circ\mathsf{L}\overline{M}}, \tag{39}$$

where $\mathsf{A}_y^{\otimes\overline{M}} = \mathsf{A}_{y_1}^{\overline{M_1}}\cdots\mathsf{A}_{y_n}^{\overline{M_n}}$ specifies the application of the adiabatic limit (in the obvious way) and

$$\Sigma_{\Pi b}\phi^{\mathsf{N}\circ\mathsf{L}\overline{M}} = \sum_{\hat{\mu}\in\overline{M}}\sum_{|\overline{\alpha}|\leqslant\overline{\omega}_b}\prod_{i\leqslant n} b_i^{\overline{\alpha}_i,\hat{\mu}_i}(\partial^{\Pi\overline{\alpha}}\delta^{\Pi^2\hat{\mu}})\phi^{\mathsf{N}^{\circ 2}\hat{\mu}}. \tag{40}$$

2. Physical supplements

To make a coupling monomial a physical magnitude it might be supplemented by another coupling constant, and to get a reasonable physical theory some of those prototype Hamiltonians with vanishing order of singularity might be additively combined.

Moreover, the concrete physical model, fixed by the interaction Hamiltonian, contains classical background fields that are given by scalar (e.g., real or Grassmann) valued test functions $\tau_p\in\mathcal{D}_p$, supposed to smear the operator valued distributions. Those are nonquantized fields that, in order to be equipped with the required indices, are as well labeled by particles $p\in\mathrm{C}\equiv\mathrm{P}\setminus\mathrm{Q}$, referred to as virtual ones. The particles considered so far are renamed $\mathrm{Q}\subseteq\mathrm{P}$. Notice that virtual particles $p\neq(\emptyset)\in\mathrm{C}$, if not just representing a nonindexed real valued test function $\tau_{(\emptyset)}$, may also have to follow nontrivial statistics.

Let the disjoint union $\mathcal{I}=\mathcal{C}\dot{\cup}\mathcal{Q}\subset\mathcal{P}(\mathbb{N})$ denote a system of subsets of basic indices, i.e., $\{c_j\}\in\mathcal{C}$ and $\mathcal{Q}_j\in\mathcal{Q}$ where $j\leqslant m\in\mathbb{N}$, which is supposed to specify virtual particles $p_j=\mathrm{p}_{c_j}\in\mathrm{C}$, that label associated couplings a_{p_j}, b_{p_j}, as well as tuples of particles $Q_j=(\mathrm{p}_i)_{i\in\mathcal{Q}_j}\subset\mathrm{Q}$ and their coordinates, x_{c_j} and $x_{Q_j}=(x_i)_{i\in\mathcal{Q}_j}$. Then the smeared abstract interaction Hamiltonian reads

$$H_{\mathcal{I}}(\tau^{\oplus\mathcal{C}}) = \sum_{j\leqslant m} a_{p_j}\left\langle \mathsf{A}_{x_{c_j}}\left(\Sigma_{b_{p_j}}\varphi^{\mathsf{L}Q_j}(x_{Q_j})\right),\tau_{c_j}(x_{c_j})\right\rangle_1. \tag{41}$$

Example 2.6: Quantum electrodynamics (QED) in an external electromagnetic field is, using the conventional notions (e.g., $\overline{\psi}$, ψ for the spinorial positron and electron, A^{cl}, A for the classical and quantized electromagnetic field, all equipped with localized space–time indices, and colons for the normal product), described by the interaction Hamiltonian, $(e/i\hbar)\,{:}\overline{\psi}(x)\gamma^\mu\psi(x){:}\,(A_\mu(x)+A^{\mathrm{cl}}_\mu(x))$. Therefore, one must identify $a=e/i\hbar$, $c=\gamma$, and $\varphi\in\{\overline{\psi},\psi,A\}$. The two sorts of test functions are real and Grassmann valued, i.e., $\tau\in\{\tau_{(\emptyset)},A^{\mathrm{cl}}\}$.

III. PERTURBATIVE EXPANSION

Underlying the expansion of the *S*-matrix, there is a HA whose antipode condition represents the property of pseudounitarity, cf. Fig. 1. This result will be achieved at the end of the section

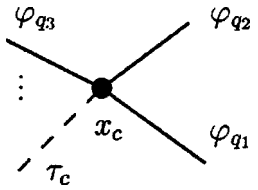

FIG. 2. A vertex.

having constructed an algebra of operator-valued distributions modeling Wick-expansion without explicit implementation of causality enriched by a graded shuffling coalgebra and an antipode given by Schmitt's formula.

A. The concept of graphs

In addition to vertex tuples and rather unusual for the EG approach, graphs and their GTS versions are chosen as indices for the *n*-point distributions, constructed to provide a direct correspondence with the configuration space variables that determine the support of the latter.

1. Vertices and graphs

The elements of the index set $\mathcal{I}$ in Sec. II C 2, and correspondingly the prototype interaction Hamiltonians, are interpreted as vertices, cf. Fig. 2.

Starting from an initial set U of vertices, the perturbative expansion leads to objects that can be interpreted as graphs $\mathrm{G_U}=\mathcal{G}(\mathrm{U})$ formed by these vertices. Renormalization then allows, by forgetting about the inner graph structure, to reinterpret graphs as vertices, i.e., $\Omega:\mathrm{G_U}\to\mathrm{W}$, which produces new vertices in $\mathrm{W}\backslash\mathrm{U}$. With all these vertices one as well forms graphs in $\mathrm{G_W}=\mathcal{G}(\mathrm{W})$ that can again be *shrunken* to vertices via the map $\Omega:\mathrm{G_W}\to\mathrm{W}$. This rough description of the vertex-generating induction, illustrated in Fig. 3, must be supplemented by the remark that physical conditions such as symmetries, discussed in Sec. IV B 2, restrict the number of physically relevant vertices, to $\mathrm{V}\subseteq\mathrm{W}$ say.

Formally, the pairs $v\equiv(P,b)\in Q^n\times\mathbb{C}^{|\mathcal{P}_n(\omega_b)|\times\Pi|P|}$ of particle tuples $P=\mathrm{P}(v)$ and coupling coefficients $b=\mathrm{b}(v)$, where $\mathcal{P}_n(\omega_b)=\{\alpha\in\mathbb{N}^n\,|\,\Sigma_{i\leqslant n}\alpha_i\equiv|\alpha|\leqslant\omega_b\}$ and $n\equiv|P|$, are supposed to define vertices $v\in\{\mathrm{U},\mathrm{V},\mathrm{W}\}$. Graphs are defined as pairs $\Gamma\equiv(\overline{v},l)$ of a vertex tuple $\overline{v}=\mathrm{V}(\Gamma)$ and a $|\overline{v}|\times|\overline{v}|$ matrix $l=\mathrm{l}(\Gamma)$ of (sets of internal) lines $l_{rs}\subseteq\{(i,j)\in\mathbb{N}_{|\overline{p}|}\times\mathbb{N}_{|\overline{q}|}\,|\,\gamma_{\overline{p_iq_j}}\neq0,\overline{p}\equiv\overline{v_r},\overline{q}\equiv\overline{v_s}\}$ that form a collection of index pairs representing two matching particles where so-called tadpoles are excluded, i.e., $l_{rr}=\emptyset$.

Keeping the notations, the iterated tuple $\mathrm{I}(\Gamma)\equiv(I_r)_{r\leqslant|\overline{v}|}$ of particles that support the internal lines of a graph Γ, referred to as representing the internal half-lines, can be reobtained by $I_r=(\mathrm{P}_i(\overline{v_r}))_{i\in\mathrm{l}_r}$ where $\mathrm{l}_r=\{\mathrm{pr}_1\,\lambda\,|\,\lambda\in l_{rs},s\leqslant|\overline{v}|\}$. Hence, the tuple $\mathrm{E}(\Gamma)\equiv(E_r)_{r\leqslant|\overline{v}|}$ representing the external half-lines is given by $E_r=(\mathrm{P}_i(\overline{v_r}))_{i\in\overline{\mathrm{l}_r}}$, where $\overline{\mathrm{l}_r}=\mathbb{N}_{|\mathrm{P}(\overline{v_r})|}\backslash\mathrm{l}_r$.

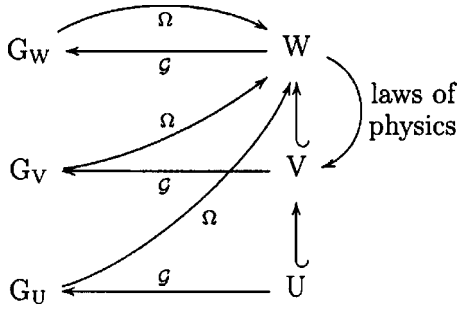

FIG. 3. Generation of graphs and of (new) vertices.

In order to introduce graph related cardinalities Euler's formula is stated, i.e.,

$$|\Gamma| = \#\Gamma - |l| + |\overline{v}|, \quad \text{where} \quad \begin{cases} |\Gamma| \\ \#\Gamma \text{ denotes the} \\ |l| \text{ number of} \\ |\overline{v}| \end{cases} \quad \begin{cases} \text{connected components,} \\ \text{independent loops,} \\ \text{(internal) lines,} \\ \text{vertices.} \end{cases} \tag{42}$$

The number of lines can be obtained by $|l| = \Sigma_{r<s\leqslant|\overline{v}|}|l_{rs}|$.

The map p which identifies particles p_i via basic indices $i \in I \subset \mathbb{N}$ and thus provides a correspondence with space–time variables $x_i \in \mathbb{R}^{1+\mathrm{d}}$ can consistently be extended to identify vertex tuples and associated classes of graphs as well. One must only consider a bigger system $\mathcal{J} := \mathcal{C} \dot{\cup} \mathcal{Q} \subseteq \mathcal{P}(\mathbb{N})$ of subsets of indices than $\mathcal{I}$ in Sec. II C 2, i.e., $c_J := \dot{\cup}_{j\in J}\{c_j\}$ and $Q_J := \dot{\cup}_{j\in J} Q_j$ satisfying $c_J \cap c_K = \emptyset$ and $Q_J \cap Q_K = \emptyset$, for $J, K \in \mathcal{P}(\mathbb{N})$.

Lemma 3.1: *There are a system* $\mathcal{J}$ *and a surjective map* $\mathrm{p}: \mathbb{N} \to \mathrm{P}$,

$$n \mapsto \begin{cases} \mathrm{p}^{\mathrm{C}}_n \in \mathrm{C} \\ \mathrm{p}^{\mathrm{Q}}_n \in \mathrm{Q} \end{cases} \quad \textit{if } n \in \begin{cases} \mathbb{N}_{\mathrm{C}}, \\ \mathbb{N}_{\mathrm{Q}}, \end{cases} \quad \textit{where } \mathbb{N}_{\mathrm{C}} \cap \mathbb{N}_{\mathrm{Q}} = \emptyset, \quad \textit{such that}$$

$(\forall \overline{v} \in \cup_{n\geqslant 0} W^n)(\exists J \in \mathbb{N}^n_{\neq})(\forall j \in J)(\mathrm{b}(\overline{v_j}) = b_{\mathrm{p}^{\mathrm{C}}(c_j)} \wedge \mathrm{P}(\overline{v_j}) = (\mathrm{p}^{\mathrm{Q}}(i))_{i\in Q_j})$.

Proof: Decompose the operation of forming graphs, i.e., $\mathcal{G} = \cup_{n\leqslant 0}\mathcal{G}_n$, so that $\mathcal{G}_n : \mathcal{P}(W) \to \mathcal{P}(\mathrm{G_W})$, $\mathrm{W}_k \mapsto \mathcal{G}_n(\mathrm{W}_k)$ yields graphs Γ with $n = |\mathrm{V}(\Gamma)|$ vertices, $\mathrm{V}(\Gamma) \in \mathrm{W}_k^{\times n}$. Then the existence of $\mathcal{J}$ and p is guaranteed by the inductive construction of $\mathrm{W} = \cup_{k>1}\mathrm{W}_k$, and thus $\mathrm{G_W} = \cup_{\mathrm{n}\geqslant 1}\mathcal{G}_{\mathrm{n}}(\mathrm{W_n})$, from finite sets $\mathrm{W}_{k+1} = \{\Omega(\Gamma) \in \mathrm{W} \,|\, \Gamma \in \mathcal{G}_k(\mathrm{W}_k)\}$ starting with $\mathrm{W}_1 = \mathrm{U}$. □

Consequently, p^{C} realizes the announced correspondence. As vertices of tuples $\overline{v}$ or of graphs $\Gamma \equiv (\overline{v}, l)$ are now associated with virtual particles, $\overline{v_j} = \Gamma_j \sim \mathrm{p}^{\mathrm{C}}_i$, the former are associated with space–time variables x_i as well, i.e.,

$$x_\cdot : \overline{v_j} \mapsto x_{v_j} := x_i \quad \text{and} \quad \Gamma_j \mapsto x_{\Gamma_j} := x_i, \text{ respectively.} \tag{43}$$

This will be essential to incorporate causality, cf. Sec. IV.

2. Algebras of graphs

For the algebraic considerations graphs are always assumed to form a complex vector space which respects the $\mathbb{N}$-grading corresponding to the number of vertices, i.e., $(\mathrm{G_V}, \mathbb{C}, +)$ where $\mathrm{G_V} = \oplus_{n\geqslant 0}\mathbb{C}\mathcal{G}_n(\mathrm{V})$.

Let $\Gamma^i \equiv (\overline{v^i}, l^i)$, for $i \leqslant 2$, denote two graphs. Then there are $|\overline{v^1}| \times |\overline{v^2}|$ matrices $l^{12} \in \mathbb{M}_{|\overline{v^1}|\times|\overline{v^2}|}(\mathcal{P}(\mathbb{N}^{\times 2}))$ yielding a new graph by combining the former (cf. Example B.1), i.e.,

$$\Gamma^1 \sqcup_{l^{12}} \Gamma^2 := \left(\overline{v^1} \otimes \overline{v^2}, \begin{pmatrix} l^1 & l^{12} \\ \widetilde{l}^{\,12} & l^2 \end{pmatrix} \right), \tag{44}$$

so that the required symmetry, $l_{rs} = \widetilde{l}_{sr} := \{(\mathrm{pr}_2\lambda, \mathrm{pr}_1\lambda) \,|\, \lambda \in l_{sr}\}$, is realized. The admissible ones, i.e., $l^{12} \in 1(\Gamma^1, \Gamma^2)$, are called concatenation matrices. In contrast to the matrices of lines, $l^{12} = \Sigma_{r\leqslant|\overline{v^1}|, s\leqslant|\overline{v^2}|}|l^{12}_{rs}|$.

The previous composition defines the Wick product of graphs, i.e., $\sqcup_\Sigma = \Sigma_{l^{12}\in 1(\cdot,\cdot)} \circ \sqcup_{l^{12}}$. Respectively, by linear extension one considers GTS versions of graphs, $\sqcup\Gamma := (1/n!)\Sigma_{\pi\in S_n}\sigma(\pi)\pi(\Gamma) \in \oplus_{n\geqslant 0} S^\sigma_n \mathbb{C}\mathcal{G}_n(\mathrm{V}) =: \mathrm{G}^\sigma_{\mathrm{V}}$, where the permutation $\pi(\Gamma) := (\pi(\overline{v}), \pi(l))$ acts on the vertex tuple as well as on the matrix of lines, i.e., $\pi(\overline{v}) := (\overline{v}_{\pi(r)})_{r\leqslant n}$ and $\pi(l) := (l_{\pi(r)\pi(s)})_{r,s\leqslant n}$, and the grading is reduced to the graph's vertex tuple, i.e., $\sigma_\Gamma(\pi(\Gamma)) := \sigma_{\mathrm{V}(\Gamma)}(V \circ \pi(\Gamma))$, discussed right below in Sec. III B 1.

Lemma 3.2: $(\mathrm{G}^{[\sigma]}_{\mathrm{V}}, \mathbb{C}, +, \sqcup_\Sigma, \emptyset)$ *forms an algebra [in both cases] where the empty graph serves as unity.*

Proof: Compare Sec. 3.2.2 in Ref. 24, pp. 75ff. □

Associativity can be illustrated introducing the inverse concept of concatenation, i.e., separation into subgraphs that, with respect to the reference graph, are completely determined by their vertices. Let $(\Gamma^1,\ldots,\Gamma^k)\in\mathcal{P}_k^{(0)}(\Gamma)$ denote a k-partition (with possibly empty subgraphs, respectively) of the graph $\Gamma\in \mathrm{G}_{\mathrm{V}}^{[\sigma]}$ iff there are a permutation $\pi\in S_k$ and appropriate concatenation matrices, $l^1,\ldots,l^{k-1}$, such that $\pi(\Gamma)=\Gamma^1\sqcup_{l^1}(\cdots\sqcup_{l^{k-1}}\Gamma^k)\cdots)$ [appropriately extended, respectively].

Let $\Gamma\in \mathrm{G}_{\mathrm{V}}^{(\sigma)}$. Then $\mathrm{G}_{\Gamma}^{[\sigma]}:=\mathcal{P}(\Gamma)=\{\Gamma'\,|\,(\Gamma',\ldots)\in\mathcal{P}_2^0(\Gamma)\}\subset \mathrm{G}_{\mathrm{V}}^{[\sigma]}$ denotes the power set which contains all subgraphs of Γ. Graphs in $\mathrm{G}_{\mathrm{V}}^{[\sigma]}$ can be composed as Γ-restricted graphs, i.e., via $\sqcup_\Gamma=(\sigma_\Gamma^0\circ\sqcup_\Sigma)\sqcup_\Sigma$, where

$$\sigma_\Gamma^0:\mathrm{G}_{\mathrm{V}}^{[\sigma]}\to\{-1,0,1\},\quad \Gamma'\mapsto\begin{cases}\sigma_\Gamma(\Gamma') & \text{if } \Gamma'\in G_\Gamma^{[\sigma]},\\ 0 & \text{otherwise,}\end{cases}\tag{45}$$

and $\sigma_\Gamma(\Gamma')=\sigma_{\Gamma'}(\Gamma)\equiv\sigma(\pi)$, regarding $\pi:\Gamma'\mapsto\Gamma$ as a permutation in $S_{|\mathrm{V}(\Gamma')|}$.

Proposition 3.3: $(\mathrm{G}_{\mathrm{V}}^{[\sigma]},\mathbb{C},+,\sqcup_\Gamma,\emptyset)$ *forms an algebra, and* $(\mathrm{G}_\Gamma^{[\sigma]},\ldots)$ *identifies its largest zero divisor free subalgebra* $(\mathrm{G}_{\Gamma'}^{\sigma},\ldots)$, $\Gamma'\in\mathrm{G}_{\mathrm{V}}^{[\sigma]}$.

Proof: Associativity of $\sqcup_\Sigma$ implies associativity of $\sqcup_\Gamma$. The other statements required are rather obvious, cf. Ref. 24, Sec. 3.2.2. □

B. The expansion of the *S*-matrix

In the EG approach the S-matrix is expanded in terms of operator-valued GTS n-point distributions. In contrast to the conventional approach, Wick and time ordering are not mixed. This allows to construct analytically well-defined algebras (relevant for the distribution's scalar parts) ensured alone by the presumed physical properties, i.e., TI and the spectral condition.

1. Infrared regularization, the ansatz, and GTS

The S-matrix is supposed to depend on coupling constants a_p and normalized test functions $\tau_p\in\mathcal{D}_p$ [i.e., $\tau_p(0)=1$] that, representing external classical fields $p\in\mathrm{C}$, serve as an infrared regularization. To obtain concrete physical quantities, the following adiabatic limit must be taken:

$$S\big((a\tau)_C^{\oplus}\big)=\lim_{\epsilon\to0}S\big((a\tau_\epsilon)_C^{\oplus}\big),\quad \forall\,\tau:\tau\circ\epsilon\equiv\tau_\epsilon\xrightarrow{L^\infty(K)}{}_{\epsilon\to0}1,\quad \forall\,K\Subset\mathbb{R}^{1+\mathrm{d}}.\tag{46}$$

This task, however, will not be regarded in this paper. Notice, as the vertices in V correspond to the set $\mathcal{C}$ in Sec. II C 2, which specifies the virtual particles $\mathrm{C}=\{\mathrm{p}_i\,|\,i\in\mathcal{C}\}$, the former are used as indices as well.

The expansion of the S-matrix is given with respect to a renormalization scheme $\mathcal{R}$ (only discussed in Sec. IV B) and the (somehow related) set V of vertices. The ansatz, chosen in accordance with the original ones of Bogoliubov and Shirkov (BS),[30] EG, and Scharf,[31] reflects the Dyson series (cf. Example B.2), i.e.,

$$S_{\mathrm{V}}^{\mathcal{R}}\big((a\tau)^{\oplus\mathrm{V}}\big)=\sum_{n\geqslant0}\frac{1}{n!}\sum_{\overline{v}\in\mathrm{V}^n}a^{\Pi\overline{v}}\Big\langle T_{\overline{v}}^{\mathcal{R}}(y),\tau^{\sqcap\overline{v}}(y)\Big\rangle_n,\tag{47}$$

where $T_{\overline{v}}\in C(S'_{|\overline{v}|}\mathcal{D}_{\overline{v}}^{\otimes},\mathcal{H}_{\mathrm{P}}^{\mathrm{F}})$ are operator-valued n-point distributions, i.e., strongly continuous mappings, indexed by vertices. The interaction Hamiltonian prototypes can be reidentified as $H_p=i\hbar a_pT_{(p)}$.

The vertex distributions are assumed to be GTS, i.e., $T_{\overline{v}}=\sigma(\pi)T_{\pi(\overline{v})}\circ\pi$, $\forall\pi\in S_n$. Here, σ symbolizes the grading on vertex tuples, given again by (24), but $\pi|_p:\overline{v}|_p\mapsto\pi(\overline{v}|_p)$ denotes a subpermutation of π defined on $\overline{v}|_p=(\overline{v_k})_{k'\mathrm{odd}}$, where $k'=\Sigma_{q\in A'(p)}1_{q=v_i\wedge v=\overline{v_k}}$ (cf. Ref. 24, p. 45). This is again a representation of $\mathcal{S}_n$ on $\mathbb{Z}_2$; and one also writes $\sigma_U(V):=\sigma(U\mapsto V)$, for vertex tuples $U,V\in\mathbb{N}_{\neq}^n$.

Lemma 3.4: *The two definitions of* σ *are consistent, i.e.,* $\sigma_U(V)=\sigma_{[U]}([V])$ *where, only here,*

$[\cdot]$ *symbolizes the formal transfer from a vertex tuple into a particle tuple by simply omitting brackets and couplings.*

Proof: Compare Lemma 2.1.7 in Ref. 24, p. 45. □

Of course, the test functions associated with vertex tuples are GTS as well, $\tau^{\sqcap\overline{v}} \equiv \tau^{\sqcap\overline{c}} := S_n^\sigma \tau^{\otimes\overline{c}} \in S_n^\sigma \mathcal{D}_{\overline{c}}^{\otimes} \equiv S_n^\sigma \mathcal{D}_{\overline{v}}^{\otimes}$, where $\overline{c} \in \mathrm{C}_{\neq}^n$ denotes the corresponding tuple of virtual particles. Again, the definitions are consistent.

Lemma 3.5: $\sigma_{\overline{v}}(\pi(\overline{v})) = \sigma_{\overline{c}}(\pi(\overline{c}))$, $\forall \pi \in \mathcal{S}_n$.

Proof: Applying the permutation π to both sides of the dual brackets in (47), this results in $\sigma_{\overline{v}}(\pi(\overline{v}))\sigma_{\overline{c}}(\pi(\overline{c})) = 1$. Therefore, the statement is due to the fact that $\sigma(\pi) \in \{\pm 1\}$. □

2. Algebras of n-point distributions

Founded on Wick's theorem, referring to the expansion rule of normal products with respect to the composition product (also regarded as twist or Cliffordization), one constructs an algebra of graph distributions over a carefully chosen ring of TI scalar distributions. Those TI distributions $t^J \in \mathcal{S}'(\mathbb{R}^{(1+\mathrm{d})\times n})$, $J \in \mathbb{N}_{\neq}^n$, i.e.,

$$t^J \equiv t_J(\tau) = t_J(\tau(\cdot - z^{\times n})), \quad \forall\, \tau \in \mathcal{S}(\mathbb{R}^{(1+\mathrm{d})\times n}), \quad \forall\, z \in \mathbb{R}^{1+\mathrm{d}}, \tag{48}$$

are supposed to form an $\mathbb{N}$-graded algebra with respect to the direct product,

$$\mathbb{T} := \mathbb{C} \oplus \mathbb{C}\langle\{t^K | K \in \mathbb{N}_{\neq}^n, n \in \mathbb{N}\}, +, \cdot\rangle / (t^{(\ldots,k,\ldots)} \cdot t^{(\ldots,k,\ldots)}), \tag{49}$$

covering the (algebra of) localizing scalars $\mathbb{L}$ as well as the positive frequency part propagators with derivatives $\Delta_+^J \equiv \Delta_{\mathrm{p}_{J_1}}^{+\gamma}(x_{J_1} - x_{J_2})$, i.e.,

$$\mathbb{P} := \mathbb{C} \oplus \mathbb{C}\langle\{\partial^\beta \Delta_+^K | \beta \in \mathbb{N}^2, K \in \mathbb{N}_{\neq}^2, \gamma_K \neq 0\}, +, \cdot\rangle / (\tilde{\Delta_+^K} \cdot \partial^\beta \Delta_+^K), \tag{50}$$

that, with respect to the Fourier product and in accordance with the spectral condition (cf. end of Sec. II A 1), form an algebra as well. Notice, $\mathbb{L}$ and $\mathbb{P}$ are ideals in $\mathbb{T}$. Combining the two previously defined algebras, one gets another commutative algebra,

$$\mathbb{T}_{\mathrm{P}} := \mathbb{T} \otimes \mathbb{P} / (t \otimes p - p \otimes t, \cdots \underbrace{t^{(\ldots,K_{1|2},\ldots,K_{2|1},\ldots)}}_{\neq t^{(\ldots,K_{1|2},\ldots)} t^{(\ldots,K_{1|2},\ldots)}} \otimes \cdots \Delta_+^K) \tag{51}$$

which, on the level of distributions, encodes the Fourier and the direct product, and additionally, the well-defined product of distributions with continuous functions. Including localization, the related commutative algebra $(\mathbb{T}_{\mathrm{PL}}, \mathbb{C}, +, \cdot, 1)$ is given by

$$\mathbb{T}_{\mathrm{PL}} := \mathbb{T}_{\mathrm{P}} \otimes \mathbb{L} / (t \otimes l - l \otimes t, \cdots \underbrace{t^{(\ldots,K_{1|2},\ldots,K_{2|1},\ldots)}}_{\text{irreducible in } \mathbb{T}_{\mathrm{P}}} \otimes \cdots \delta^K - \cdots \otimes \cdots \delta^K). \tag{52}$$

Again, the substructures are ideals, i.e., $\mathbb{T}_{\mathrm{PL}} \subset \mathbb{T}_{\mathrm{P}} \subset \mathbb{T}$. Similar to Sec. II B 2, those algebras will mainly be applied as rings.

Turning to the operator side, let $\mathcal{T}_{\mathrm{V}} := \oplus_{n\geqslant 0} \cup \{\mathcal{T}_\Gamma | \Gamma \in \mathrm{G}_{\mathrm{V}}, |\mathrm{V}(\Gamma)| = n\}$ be the $\mathbb{N}$-graded space of graph-indexed n-point distributions

$$\mathcal{T}_\Gamma = \{\Sigma_{\mathrm{b}(\Omega\Gamma)} t_{\mathrm{I}(\Gamma)}(\bullet) \mathsf{A}_\bullet^{\otimes \mathrm{V}(\Gamma)} \phi^{\mathrm{N}\circ\mathrm{LE}(\Gamma)} \in \mathcal{C}(S_n^\sigma \mathcal{D}_{\mathrm{V}(\Gamma)}^{\otimes}, \mathcal{H}_{\mathrm{P}}^{\mathrm{F}}) | t_{\mathrm{I}(\Gamma)} \in \mathbb{T}\}, \tag{53}$$

where, in terms of the couplings at the vertices of $\mathrm{V}(\Gamma)$, the coupling at the vertex $\Omega\Gamma$ reads

$$\mathrm{b}(\Omega\Gamma) = \prod_{r<s\leqslant n} \prod_{(i,j)\in \mathrm{l}_{rs}(\Gamma)} \sum_{\substack{\mu \\ [\![\mu]\!]\in P_{ri}}} \sum_{\substack{\nu \\ [\![\nu]\!]\in P_{sj}}} \prod_{k\leqslant n} b_{\mathrm{V}_k(\Gamma)}^{\alpha_k, P_k}. \tag{54}$$

Then $\mathcal{T}_{\mathrm{V}}$ is obviously a submodule of $\mathbb{T}_{\mathrm{PL}} \otimes \mathcal{N}$, and it is algebraically closed with respect to the composition product.

Proposition 3.6: $(\mathcal{T}_{\mathrm{V}}, \mathbb{T}_{\mathrm{PL}}, +, \circ, \eta)$ *forms an algebra*.

Proof: This is the content of Proposition 3.3.2 in Ref. 24, p. 85, which in the presented approach serves as the alternative to EG's Theorem 0 in Ref. 2, p. 229. In order to illustrate the crucial points, let $T^i \in \mathcal{T}_{\Gamma^i}$ with scalars $t^i \equiv t_{\mathrm{I}(\Gamma^i)} \in \mathbb{T}$, for $\Gamma^i \in \mathrm{G}_{\mathrm{V}}$ and $i \leqslant 2$, and use the abbreviation $N(\bullet) := \mathsf{A}^{\otimes \mathrm{V}(\bullet)}_{\chi^{\otimes}_{\mathrm{V}(\bullet)}} \phi^{\mathsf{N} \circ \mathrm{LE}(\bullet)}$. Then

$$T^1 \circ T^2 = \sum_{l \in 1(\Gamma^1, \Gamma^2)} (i\hbar)^{|l|} \Sigma_{\mathrm{b}(\Omega(\Gamma^1 \sqcup_l \Gamma^2))} t^l N(\Gamma^1 \sqcup_l \Gamma^2) \in \mathcal{T}_{\mathrm{V}}, \tag{55}$$

having a well-defined associated scalar distribution that is again TI, i.e.,

$$t^l(y^1 \otimes y^2) = t^1(y^1) t^2(y^2) \amalg^l_{(\Gamma^1, \Gamma^2)}(y^1, y^2) \in \mathbb{T}_{\mathrm{P}}. \tag{56}$$

The most rhs expression abbreviates a certain product of positive frequency propagators (also referred to as Wick contractions, cf. below),

$$\amalg^l_{(\Gamma^1, \Gamma^2)}(y^1, y^2) := \prod_{r \leqslant |P^1|, s \leqslant |P^2|} \prod_{(i,j) \in l_{rs}} \Delta^{P^1_{ri} P^2_{sj}}_{+\gamma}(y^1_r - y^2_s) \in \mathbb{P}, \tag{57}$$

which is well defined due to the spectral condition (16). Besides TI, for the analytical part, the proof of the algebraic part rests upon the following. □

Lemma 3.7: (Wick's theorem.) *Keeping the notations, then*

$$N(\Gamma^1) \circ N(\Gamma^2) = \sum_{l \in 1(\Gamma^1, \Gamma^2)} (i\hbar)^{|l|} \amalg^l_{(\Gamma^1, \Gamma^2)} N(\Gamma^1 \sqcup_l \Gamma^2). \tag{58}$$

Proof: On the level of free field operators, and provided $[\cdot, \cdot]^{\otimes}_{\sigma} \propto \mathrm{id}_{\mathcal{H}^{\mathrm{F}}_{\mathrm{P}}}$, the expansion reads

$$\phi^{\mathsf{N}I} \otimes \phi^{\mathsf{N}J} = \sum_{\Lambda \subseteq \mathbb{N}_{|I|} \times \mathbb{N}_{|J|}} \left(\prod_{\lambda \in \Lambda} [\phi^{I_{\lambda_1}}_-, \phi^{J_{\lambda_2}}_+]^{\otimes}_{\sigma} \right) \phi^{\mathsf{N}(I \otimes_\Lambda J)}, \tag{59}$$

where $I \otimes_\Lambda J = (I_i)_{i \in \mathbb{N}_{|I|} \setminus \{\lambda_1 | \lambda \in \Lambda\}} \otimes (J_i)_{i \in \mathbb{N}_{|J|} \setminus \{\lambda_2 | \lambda \in \Lambda\}}$, for tuples I, J. This is proven by successive insertion of Wick contractions,

$$\phi^i_- \otimes \phi^j_+ = [\phi^i_-, \phi^j_+]^{\otimes}_{\sigma} + \sigma_{(i,j)}((j,i)) \phi^j_+ \otimes \phi^i_-,$$

moving the ϕ^j_+'s to the left and the ϕ^i_-'s to the right. Due to (15), the brackets in (59) can be replaced by propagators. In accordance with the definition of $\mathbb{T}_{\mathrm{PL}}$, the localizing delta distribution's are supposed to dominate (i.e., erase) the propagators, which reduces (58) and (59). □

Remark 3.8: Associativity of the algebra, i.e., $N(\Gamma^1) \circ (N(\Gamma^2) \circ N(\Gamma^3)) = (N(\Gamma^1) \circ N(\Gamma^2)) \circ N(\Gamma^3)$, is equivalent to the 2-cocycle condition for $\amalg$, i.e., $\amalg_{(\Gamma^1, \Gamma^2 \sqcup_\Gamma \Gamma^3)} \amalg_{(\Gamma^2, \Gamma^3)} = \amalg_{(\Gamma^1, \Gamma^2)} \amalg_{(\Gamma^1 \sqcup_\Gamma \Gamma^2, \Gamma^3)}$, $\forall \Gamma^i \in \mathrm{G}_\Gamma$, $i \leqslant 3$, which is obviously fulfilled. In the context of Refs. 20 and 21, $\amalg_{(\cdot,\cdot)}$ is called a *Laplace pair* and the relation (58), regarded as a so-called *twist* (cf. Ref. 22), is understood as *Cliffordization*.

3. Graph and vertex distributions

In the present context the physically relevant solution of the perturbation expansion is assumed to be given—formally, without having introduced the essential concepts of their derivation yet, cf. Sec. IV.

Graph distributions $\mathcal{R}^{\mathsf{T}}_{\mathrm{G_V}} := \oplus_{n \geqslant 0} \mathbb{C}\{T^{\mathcal{R}}_\Gamma \,|\, \Gamma \in \mathrm{G_V}, |\mathrm{V}(\Gamma)| = n\}$, supposed to solve the perturbative expansion by respecting causality, are introduced via a vector space homomorphism,

$$T^{\mathcal{R}}_{\bullet}:\mathrm{G_V}\to T_\Gamma,\quad \Gamma\mapsto T^{\mathcal{R}}_\Gamma:=(i\hbar)^{\#\Gamma-|\Gamma|}\Sigma_{\mathrm{b}(\Omega\Gamma)}t^{\mathcal{R}}_{\mathrm{I}(\Gamma)}N(\Gamma), \tag{60}$$

fixing the associated scalar valued n-point distributions $t^{\mathcal{R}}_{\mathrm{I}(\Gamma)}\in S^{\sigma}_n\mathcal{D}^{\otimes}_{\mathrm{V}(\Gamma)}\subset\mathbb{T}$, that are supposed to be given with respect to a renormalization scheme $\mathcal{R}$, and via a GTS requirement,

$$T^{\mathcal{R}}_{\pi(\Gamma)}=\sigma(\pi)T^{\mathcal{R}}_\Gamma,\quad \forall\ \pi\in\mathcal{S}_{|\mathrm{V}(\Gamma)|} \tag{61}$$

(which can only be motivated in Sec. IV cf. Remark 4.17).

Remark 3.9: According to GTS, one may alternatively have introduced $T^{\mathcal{R}}_{\bullet}$ as a vector space isomorphism, $\mathrm{G}^{\sigma}_{\mathrm{V}}\to T_\Gamma$.

Lemma 3.10: *Let* Γ^1, Γ^2 *be independent, i.e.,* $\nexists c\in\mathbb{C}$ *s.t.* $\sqcap\Gamma^1=c\sqcap\Gamma^2$. *Then* $c_1T_{\Gamma^1}+c_2T_{\Gamma^2}=0$, $\forall c_1, c_2\in\mathbb{C}$, *implies that* $T^{\mathcal{R}}_{\Gamma^1}=T^{\mathcal{R}}_{\Gamma^2}=0$.

Proof: This is an immediate consequence of the previous remark. □

Defining the homomorphism $T^{\mathcal{R}}_{\bullet}$ only for graphs $\mathrm{G}_\Gamma\subset\mathrm{G_V}$, this leads to the vector space $\mathcal{R}^{\mathsf{T}}_{\mathrm{G}_\Gamma}$ of Γ-restricted graph distributions with a finite grading. On this space, a product is given by

$$\circ^{\mathsf{T}}_\Gamma:T^{\mathcal{R}}_{\Gamma^1}\otimes T^{\mathcal{R}}_{\Gamma^2}\mapsto T^{\mathcal{R}}_{\Gamma^1\sqcup_\Gamma\Gamma^2}. \tag{62}$$

Lemma 3.11: *Let* $\Gamma,\Gamma'\in\mathrm{G_V}$ *and* $*\in\{\mathrm{V},\Gamma'\}$. *Then* $(\mathcal{R}^{\mathsf{T}}_{\mathrm{G}_*},\mathbb{C},+,\circ^{\mathsf{T}}_\Gamma,\eta)$ *forms an algebra (which is free of zero divisors only if* $*\subseteq\Gamma$*).*

Proof: Obviously, $T^{\mathcal{R}}_{\bullet}:\mathrm{G}_*\to\mathcal{R}^{\mathsf{T}}_{\mathrm{G}_*}$ defines an algebra homomorphism. [Compare (45), if $\Gamma^1\not\subseteq\Gamma$ or $\Gamma^2\not\subseteq\Gamma$ then $T_{\Gamma^1}\circ^{\mathsf{T}}_\Gamma T_{\Gamma^2}\equiv T_{\Gamma^1\sqcup_\Gamma\Gamma^2}=T_0\equiv 0$.] □

Consider the following restrictions of the composition product obtained by redefining the right-hand side of (55):

$$T^1\circ T^2=:\sum_{l\in 1(\Gamma^1,\Gamma^2)}T^1\circ_l T^2=:\sum_{\Upsilon\in\mathrm{G_V},(\Gamma^1,\Gamma^2)\in\mathcal{P}^0_2(\Upsilon)}T^1\circ_\Upsilon T^2, \tag{63}$$

where $T^1\circ_l T^2=T^1\circ_\Upsilon T^2$ iff $\exists\pi\in\mathcal{S}_{|\Upsilon|}$ s.t. $l=(\mathbb{I}\ \emptyset)\cdot 1(\pi\circ\Upsilon)\cdot(\emptyset\ \mathbb{I})^t$. For any fixed graph $\Gamma\in\mathrm{G_V}$, this induces a Γ-restricted product on the TI distributions $\mathcal{T}_\mathrm{V}$, i.e., $\circ_\Gamma:\mathcal{T}_{\Gamma^1}\otimes\mathcal{T}_{\Gamma^2}\to\mathcal{T}_{\Gamma^1\sqcup_\Gamma\Gamma^2}$,

$$T^1\circ_\Gamma T^2:=\begin{cases}\sigma_\Upsilon(\Gamma)T^1\circ_\Upsilon T^2 & \text{if } \exists!\Upsilon\in\mathcal{P}(\Gamma)\text{s.t.}(\Gamma^1,\Gamma^2)\in\mathcal{P}^0_2(\Upsilon),\\ 0, & \text{otherwise}.\end{cases} \tag{64}$$

Then $\mathcal{R}_{\mathrm{G}_\Gamma}:=\oplus_{n\geqslant 0}\mathbb{C}\{\bigcirc_\Gamma\oplus_{i\leqslant r}T^{\mathcal{R}}_{\Gamma^i}|\Gamma^i\in\mathrm{G}_\Gamma,\Sigma_{i\leqslant r}|\mathrm{V}(\Gamma^i)|=n\}$ denotes the corresponding space of distributions defining a $\mathbb{C}$-submodule of $\mathcal{T}_\mathrm{V}$ and thus a $\mathbb{C}$-algebra, $(\mathcal{R}_{\mathrm{G}_\Gamma},\mathbb{C},+,\circ_\Gamma,\eta)$.

Remark 3.12: The consistency of the choice of the scalar $(i\hbar)^{\#\Gamma-|\Gamma|}$ in (60) can be checked with the help of Euler's formula (42), cf. Corollary 3.3.8 in Ref. 24, p. 90.

Now, the vertex distributions used in Ansatz (47) reappear as a sum over graph distributions,

$$T^{\mathcal{R}}_{\overline{v}}=\sum_{\Gamma\in\mathrm{G_V},\mathrm{V}(\Gamma)=\overline{v}}T^{\mathcal{R}}_\Gamma,\quad \forall\,\overline{v}\in\mathrm{V}, \tag{65}$$

so that the space of vertex distributions, $\mathcal{R}^{\mathsf{T}}_\mathrm{V}:=\oplus_{n\geqslant 0}\mathbb{C}\{T^{\mathcal{R}}_{\overline{v}}|\overline{v}\in\mathrm{V},|\overline{v}|=n\}$, can be introduced by restricting the homomorphism $T^{\mathcal{R}}_{\bullet}$ to be defined on the vector space of vertex tuples, i.e., $\oplus_{n\geqslant 0}\mathbb{C}\{\overline{v}\,||\overline{v}|=n\}\equiv\mathrm{V}\to\mathcal{T}_\mathrm{V}$, $\overline{v}\mapsto T^{\mathcal{R}}_{\overline{v}}$.

Lemma 3.13: *Let* $\circ^{\mathsf{T}}:T^{\mathcal{R}}_{\overline{v}^1}\otimes T^{\mathcal{R}}_{\overline{v}^2}\to T^{\mathcal{R}}_{\overline{v}^1\otimes\overline{v}^2}$. *Then* $(\mathcal{R}^{\mathsf{T}}_\mathrm{V},\mathbb{C},+,\circ^{\mathsf{T}},\eta)$ *forms an algebra.*

Proof: Obviously, $T^{\mathcal{R}}_{\bullet}:\mathrm{V}\to\mathcal{T}_\mathrm{V}$ defines an algebra homomorphism. □

Furthermore, $\mathcal{R}_\mathrm{V}:=\oplus_{n\geqslant 0}\mathbb{C}\{\bigcirc_{i\leqslant r}T^{\mathcal{R}}_{\overline{v}^i}|\overline{v^i}\in\mathrm{V},\Sigma_{i\leqslant r}|\overline{v^i}|=n\}$ denotes the space of vertex distributions which defines a $\mathbb{C}$-submodule of $\mathcal{T}_\mathrm{V}$ and thus a $\mathbb{C}$-algebra, $(\mathcal{R}_\mathrm{V},\mathbb{C},+,\circ,\eta)$.

4. HAs underlying pseudounitarity

The perturbative expansion can now be modeled by a HA. In accordance with the power series ansatz (47), let

$$\sum_{n\geqslant 0}\frac{1}{n!}\sum_{\overline{v}\in \mathrm{V}^n} a^{\Pi\overline{v}}\left\langle \widetilde{T}^{\mathcal{R}}_{\overline{v}}(y),\tau^{\sqcap\overline{v}}(y)\right\rangle_n := S^{\mathcal{R}}_{\mathrm{V}}\left((a\tau)^{\oplus \mathrm{V}}\right)^{-1}, \tag{66}$$

where the inverse n-point distributions $\widetilde{T}_{\overline{v}}\in C(S^{\sigma}_{|\overline{v}|}\mathcal{D}^{\otimes}_{\overline{v}},\mathcal{H}^{\mathrm{F}}_{\mathrm{p}})$, supposed to be GTS as well, are denoted by a tilde. Formally, the inverse of the S-matrix is characterized by the *relation of pseudounitarity*, i.e.,

$$S^{\mathcal{R}}_{\mathrm{V}}(\xi)^{-1}\circ S^{\mathcal{R}}_{\mathrm{V}}(\xi)=\mathrm{id}_{\mathcal{H}^{\mathrm{F}}_{\mathrm{p}}}=S^{\mathcal{R}}_{\mathrm{V}}(\xi)\circ S^{\mathcal{R}}_{\mathrm{V}}(\xi)^{-1},\quad \forall\ \xi\in\mathcal{D}^{\oplus}_{\mathrm{V}}(\mathbb{R}^{1+\mathrm{d}}). \tag{67}$$

Remark 3.14: The probabilistic interpretation of quantum theory is ensured by requiring unitarity. But, for gauge theories and their unphysical states, unitarity can only be pseudo (i.e., true on a subspace of the Fock space $\mathcal{H}^{\mathrm{F}}_{\mathrm{p}}$), i.e., $S(\xi)^{-1}=S(\xi)^{K}$, where K is a pseudoadjoint (i.e., adjoint for a subdomain). Questions of that kind were investigated extensively by Scharf and collaborators in the 1990s, cf. Refs. 32–34.

In terms of n-point distributions the relation of pseudounitarity reads as follows.

Lemma 3.15: *Let T_Y, $T_Z\in\mathcal{R}_{\mathrm{V}}$, where Y, $Z\in\mathrm{V}$, and let $\emptyset\neq X\in\mathrm{V}$. Then*

$$\sum_{(Y,Z)\in\mathcal{P}^0_2(X)}\sigma_X(Y\otimes Z)\widetilde{T}_Y\circ T_Z=0=\sum_{(Y,Z)\in\mathcal{P}^0_2(X)}\sigma_X(Y\otimes Z)T_Y\circ\widetilde{T}_Z. \tag{68}$$

Moreover, $\widetilde{T}_Y$, $\widetilde{T}_Z\in\mathcal{R}_{\mathrm{V}}$ and therefore the inverse distributions are GTS.

Proof: To obtain (68), perform the power expansion (cf. Lemma 3.3.15 in Ref. 24, p. 94). The other claim is a side result. □

This statement can be rewritten assuming the tilde to be linear, i.e., assigning the tilde to graph distributions in the following straightforward manner:

$$\sum_{\Gamma\in\mathrm{G}_{\mathrm{V}},\mathrm{V}(\Gamma)=\overline{v}}\widetilde{T}^{\mathcal{R}}_{\Gamma}:=\widetilde{T}^{\mathcal{R}}_{\overline{v}}. \tag{69}$$

Corollary 3.16: *Let $\emptyset\neq\Gamma'\in\mathrm{G}_{\Gamma}$ and $\Gamma\in\mathrm{G}_{\mathrm{V}}$. Then*

$$\sum_{(\Gamma^1,\Gamma^2)\in\mathcal{P}^0_2(\mathrm{Y})}\sigma_{\Gamma}(\Gamma^1\sqcup_{\Gamma}\Gamma^2)\widetilde{T}^{\mathcal{R}}_{\Gamma^1}\circ_{\Gamma}T^{\mathcal{R}}_{\Gamma^2}=0=\sum_{(\Gamma^1,\Gamma^2)\in\mathcal{P}^0_2(\mathrm{Y})}\sigma_{\Gamma}(\Gamma^1\sqcup_{\Gamma}\Gamma^2)T^{\mathcal{R}}_{\Gamma^1}\circ_{\Gamma}\widetilde{T}^{\mathcal{R}}_{\Gamma^2}. \tag{70}$$

Proof: Insert the expansions (65) and (69) into (68) and apply Lemma 3.10 (cf. Corollary 3.3.17 in Ref. 24, p. 97).

The previous two equations, if interpreted as antipode conditions, motivate to consider $\mathcal{R}_{\mathrm{V}}$ and $\mathcal{R}_{\mathrm{G}_{\Gamma}}$, respectively, as HAs.

Theorem 3.17: $(\mathcal{R}_*,\mathbb{C},+,\circ_{(\Gamma)},\eta,\Delta,\varepsilon,\mathrm{S}_{(\circ_{\Gamma})})$, *where $*=\mathrm{V}$ (respectively, $=\mathrm{G}_{\Gamma}$, for any $\Gamma\in\mathrm{G}_{\mathrm{V}}$), forms a HA. The tilde serves as antipode, i.e., $\mathrm{S}_{(\circ_{\Gamma})}T:=\widetilde{T}$, which, e.g., in $\mathcal{R}_{\mathrm{G}_{\Gamma}}$, is explicitely given by*

$$\mathrm{S}_{\circ_{\Gamma}}T^{\mathcal{R}}_{\Gamma'}=\sum_{r=1}^{|\mathrm{V}(\Gamma')|}(-1)^r\sum_{(\Gamma^1,\ldots,\Gamma^r)\in\mathcal{P}_r(\Gamma')}\sigma_{\Gamma}(\Gamma^1\sqcup_{\Gamma}\cdots\sqcup_{\Gamma}\Gamma^r)T^{\mathcal{R}}_{\Gamma^1}\circ_{\Gamma}\cdots\circ_{\Gamma}T^{\mathcal{R}}_{\Gamma^r}. \tag{71}$$

Proof: It only remains to show the representation of the antipode. This will be done by induction over the number of vertices. Assume (71) is fulfilled for $|\mathrm{V}(\Gamma')|=n$, which is true for $n=1$. Then, starting with the antipode condition, one reproduces (71),

$$
\begin{aligned}
S_{\circ_\Gamma} T^{\mathcal{R}}_{\Upsilon} &= -T^{\mathcal{R}}_{\Upsilon} - \sum_{(\Gamma',\Gamma'')\in\mathcal{P}_2(\Upsilon)} \sigma_\Gamma(\Gamma' \sqcup_\Gamma \Gamma'') S_{\circ_\Gamma} T^{\mathcal{R}}_{\Gamma'} \circ_\Gamma T^{\mathcal{R}}_{\Gamma''} \\
&= -T^{\mathcal{R}}_{\Upsilon} - \sum_{r=1}^{n} (-1)^r \sum_{(\Gamma',\Gamma'')\in\mathcal{P}_2(\Upsilon)} \sum_{(\Gamma^1,\ldots,\Gamma^r)\in\mathcal{P}_r(\Gamma')} \\
&\quad \times \sigma_\Gamma(\Gamma' \sqcup_\Gamma \Gamma'') \sigma_\Gamma(\Gamma^1 \sqcup_\Gamma \cdots \sqcup_\Gamma \Gamma^r) T^{\mathcal{R}}_{\Gamma^1} \circ_\Gamma \cdots \circ_\Gamma T^{\mathcal{R}}_{\Gamma^r} \circ_\Gamma T^{\mathcal{R}}_{\Gamma''} \\
&= -\sum_{r=0}^{n} (-1)^r \sum_{(\Gamma',\ldots,\Gamma^r,\Gamma'')\in\mathcal{P}_{r+1}(\Upsilon)} \sigma_\Gamma(\Gamma^1 \sqcup_\Gamma \cdots \sqcup_\Gamma \Gamma^r \sqcup_\Gamma \Gamma'') \cdots = \sum_{r=1}^{n+1} (-1)^r \sum_{(\Gamma^1,\ldots,\Gamma^r,\Gamma'')\in\mathcal{P}_r(\Upsilon)} \cdots,
\end{aligned}
$$

for the graph Υ with $|V(\Upsilon)| = n+1$ and hence for any such graph. □

Remark 3.18: Rota and Stein[20,21] have obtained this kind of antipode for their *plethystic HAs* and refer to the general version of (71) as *Schmitt formula* (indicated by "Σ" in Fig. 1).

IV. RENORMALIZED CAUSAL pQFT

This section provides an algebraic formalism for the main qualities determining the *S*-matrix in the considered framework of pQFT, i.e., causality and renormalization. As the EG approach is a recursive method it is free of subdivergences. A change of the renormalization scheme, however, indicates all the structure contained in Kreimer's HA. In contrast to most of the existing work on EG and following the preceding section, the presentation here is given in terms of graph instead of vertex distributions.

A. Causal regularization

Causality defines the graph distributions only outside the so-called diagonals. The required regularization, performed as a localization on the corresponding causally determined space–time region in configuration space, allows a characterization in terms of HAs. In addition to two EG versions, that vary with respect to the concrete but recursive implementation of causality, Feynman's approach to pQFT is recalled, which due to the mixing of Wick with time ordering yields an explicit representation of graph distributions. However, the unavoidable coarse localization reasons the occurrence of subdivergences.

1. Causality

Preparing the two EG versions, two relations of causality are formulated for sets of space–time points, $X, Y \subseteq \mathbb{R}^{1+d}$, i.e., *causal ordering* $\precsim$, given by

$$
X \cap (Y + \overline{V_+}) = \emptyset \Leftrightarrow : X \precsim Y \Leftrightarrow Y \succsim X, \tag{72}
$$

and *weak causal ordering* $\precsim^{\exists} (\supseteq \precsim)$, given by

$$
\exists (x,y) \in X \times Y \text{ s.t. } \{x\} \precsim \{y\} \Leftrightarrow : X \precsim^{\exists} Y \Leftrightarrow Y \succsim^{\exists} X. \tag{73}
$$

Both these relations are not reflexive, i.e., $\exists X \not\precsim^{(\exists)} X$. Coinciding space–time points cannot be compared with respect to causality. This fact reasons the necessity of renormalization and makes it look acceptable from the physics' point of view.

Accordingly, one distinguishes two sorts of configuration space regions. For the one sort, the *causal cones*, the space–time points are causally related, whereas for the other, the *diagonals*, that model coinciding space–time points, they are not. Let $P \in \mathcal{P}_r(\Gamma)$ where $\Gamma \in G_V$ and $r \leqslant n \equiv |V(\Gamma)|$. Then

$$\mathrm{cone}_P^{(\exists)} := \{y \in \mathbb{R}^{(1+d)\times n} | \{y_{P_1}^{\otimes}\} \gtrsim^{(\exists)} \cdots \gtrsim^{(\exists)} \{y_{P_r}^{\otimes}\}\} \tag{74}$$

define (respectively, two) TI open cones on the configuration space $\mathbb{R}^{(1+d)\times n} := \times_{i\leqslant n}\mathbb{R}^{1+d}$. Furthermore, the sets of r coinciding points,

$$\mathrm{diag}_P := \{y \in \mathbb{R}^{(1+d)\times n} | y_i = y_j,\ \forall\, i,j \in P_s,\ \forall\, s \leqslant r\}, \tag{75}$$

are called the (sub)diagonals with respect to P [if $P \neq (\Gamma)$, respectively]. Subtracting

$$\mathrm{diag}_r^n := \bigcup_{s<r} \bigcup_{P\in\mathcal{P}_s(I)} \mathrm{diag}_P \tag{76}$$

from the configuration space, one obtains the *causally determined region* which contains at least r noncoinciding space–time points, i.e.,

$$\mathbb{R}_{r\neq}^{(1+d)\times n} := \mathbb{R}^{(1+d)\times n} \setminus \mathrm{diag}_r^n. \tag{77}$$

One uses the following abbreviations, $\mathbb{R}_{\times}^{(1+d)\times n} := \mathbb{R}_{2\neq}^{(1+d)\times n}$ and $\mathbb{R}_{\neq}^{(1+d)\times n} := \mathbb{R}_{n\neq}^{(1+d)\times n}$.

Lemma 4.1: *Let* $\Gamma \in \mathrm{G_V}$ *and* $r \leqslant n \equiv |\mathrm{V}(\Gamma)|$. *Then*

$$\bigcup_{P\in\mathcal{P}_r(\Gamma)} \mathrm{cone}_P = \mathbb{R}_{r\neq}^{(1+d)\times n}. \tag{78}$$

Let Γ, Γ_1, $\Gamma'' \in \mathrm{G_V}$ *where* $(\Gamma_1, \Gamma'') \in \mathcal{P}_2(\Gamma)$ *and* $|V(\Gamma_1)| = 1$. *Then*

$$\mathrm{cone}_{(\Gamma_1,\Gamma'')}^{\exists} \cup \mathrm{cone}_{(\Gamma'',\Gamma_1)}^{\exists} = \mathbb{R}_{\times}^{(1+d)\times n}, \tag{79}$$

where the two cones are represented by

$$\mathrm{cone}^{\exists}_{\begin{cases}(\Gamma_1,\Gamma'')\\(\Gamma'',\Gamma_1)\end{cases}} = \bigcup_{(\Gamma_Q,\Gamma_P)\in\mathcal{P}_2(\Gamma),\Gamma_1\subseteq\begin{cases}\Gamma_Q\\\Gamma_P\end{cases}} \mathrm{cone}_{(\Gamma_Q,\Gamma_P)}. \tag{80}$$

Proof: These (four) relations follow immediately from the definitions above. □

Utilizing only the causal relation, the S-matrix is called causal iff,

$$\mathrm{supp}\ \xi^1 \gtrsim \mathrm{supp}\ \xi^2 \Rightarrow S_{\mathrm{V}}^{\mathcal{R}}(\xi^1 + \xi^2) = S_{\mathrm{V}}^{\mathcal{R}}(\xi^1) \circ S_{\mathrm{V}}^{\mathcal{R}}(\xi^2), \tag{81}$$

$\forall\, \xi^i \in \mathcal{D}_{\mathrm{V}}^{\oplus}(\mathbb{R}^{1+d})$, $i \leqslant 2$. There is an equivalent characterization in terms of graph distributions.

Proposition 4.2: *The S-matrix is causal iff* $\mathrm{supp}\ \xi^1 \gtrsim \mathrm{supp}\ \xi^2$ *implies*

$$T_{\Gamma'}^{\mathcal{R}}(\xi^1 \sqcap \xi^2) = \sigma_{\Gamma'}(\Gamma^1 \sqcup_{\Gamma} \Gamma^2) T_{\Gamma^1}^{\mathcal{R}}(\xi^1) \circ_{\Gamma} T_{\Gamma^2}^{\mathcal{R}}(\xi^2), \tag{82}$$

$\forall (\Gamma^1, \Gamma^2) \in \mathcal{P}_2(\Gamma')$, $\forall \Gamma' \subseteq \Gamma \in \mathrm{G_V}$, *and* $\forall\, \xi^i \in \mathcal{D}_{\mathrm{V}(\Gamma^i)}^{\otimes}$, $i \leqslant 2$.

Proof: This is due to power expansion (cf. Lemma 4.1.4 in Ref. 24, p. 103). □

In the EG approach, i.e., in the sequel, the S-matrix is assumed to be causal.

2. Regularization of two EG versions

EG's method is an implicit induction over subgraphs where the implementation of causality leads to localized n-point distributions (being GTS and having TI scalar parts) of the form $T_{\Gamma'}^{r\neq} := T_{\Gamma'}^{\mathcal{R}}|_{\mathbb{R}_{r\neq}^{(1+d)\times n}} \in \mathcal{R}_{\mathrm{G}_\Gamma}^{\mathsf{T}}(\mathbb{R}_{r\neq}^{(1+d)\times n})$, for $r \leqslant n \equiv |\mathrm{V}(\Gamma')|$, $\Gamma' \in \mathcal{P}(\Gamma)$, and $\Gamma \in \mathrm{G_V}$.

EG à la Fredenhagen (EGF): For each graph Γ and each $r \leqslant n$ one chooses a partition of unity $(\chi_P)_{P\in\mathcal{P}_r(\Gamma)}$ of class C^{∞} subordinate to the finite open covering $(\mathrm{cone}_P)_{P\in\mathcal{P}_r(\Gamma)}$ of the metric space $\mathbb{R}_{r\neq}^{(1+d)\times n}$, i.e.,

$$\sum_{P\in\mathcal{P}_r(\Gamma)} \chi_P(x) = 1, \quad \forall\, x \in \mathbb{R}_{r\neq}^{(1+d)\times n}, \tag{83}$$

$$\text{where} \quad 0 \leqslant \chi_P \in C^\infty(\mathbb{R}^{(1+d)\times n}_{r\neq}) \tag{84}$$

$$\text{and} \quad \operatorname{supp}\chi_P \subset \operatorname{cone}_P. \tag{85}$$

It is well known that partitions of this kind exist (e.g., cf. Ref. 35, p. 214).

Proposition 4.3: *The graph distributions are (uniquely) determined by*

$$T^\chi_{\Gamma'} := \sum_{(\Gamma^1,\ldots,\Gamma^r)\in\mathcal{P}_r(\Gamma')} \chi_{(\Gamma^1,\ldots,\Gamma^r)}\sigma_\Gamma(\Gamma^1\sqcup_\Gamma\ldots\sqcup_\Gamma\Gamma^r)T^{\mathcal{R}}_{\Gamma^1}\circ_\Gamma\ldots\circ_\Gamma T^{\mathcal{R}}_{\Gamma^r} \tag{86}$$

(independently of χ), i.e., $T^{r\neq}_{\Gamma'} = T^\chi_{\Gamma'}|_{\mathbb{R}^{(1+d)\times n}_{r\neq}} \in \mathcal{R}^{\mathsf{T}}_{G_\Gamma}(\mathbb{R}^{(1+d)\times n}_{r\neq})$.

Proof: By applying (78) one can straightforwardly generalize Ref. 7 where only the case of $r=2$ is considered (cf. Proposition 4.2.6 in Ref. 24, p. 110). □

EG à la Scharf (EGS): The genuine approach is based on two expressions,

$$\text{the} \quad \begin{cases}\text{retarded}\\ \text{advanced}\end{cases} \quad \text{distribution} \quad \begin{cases} R_{(\Gamma_1,\Gamma'')} := T_{\Gamma'} + R'_{(\Gamma_1,\Gamma'')},\\ A_{(\Gamma_1,\Gamma'')} := T_{\Gamma'} + A'_{(\Gamma_1,\Gamma'')},\end{cases} \tag{87}$$

where, applying Scharf's notation,

$$R'_{(\Gamma_1,\Gamma'')} := \sum_{(\Gamma^1,\Gamma^2)\in\mathcal{P}_2(\Gamma'),\Gamma_1\subseteq\Gamma^1} \sigma_\Gamma(\Gamma^1\sqcup\Gamma^2)T^{\mathcal{R}}_{\Gamma^1}\circ_\Gamma\tilde{T}^{\mathcal{R}}_{\Gamma^2}, \tag{88}$$

$$A'_{(\Gamma_1,\Gamma'')} := \sum_{(\Gamma^1,\Gamma^2)\in\mathcal{P}_2(\Gamma'),\Gamma_1\subseteq\Gamma^2} \sigma_\Gamma(\Gamma^1\sqcup\Gamma^2)\tilde{T}^{\mathcal{R}}_{\Gamma^1}\circ_\Gamma T^{\mathcal{R}}_{\Gamma^2}. \tag{89}$$

These expressions vanish when restricted to appropriate cones.

Lemma 4.4: *Let* Γ, Γ_1, $\Gamma''\in G_V$ *where* $(\Gamma_1,\Gamma'')\in\mathcal{P}_2(\Gamma)$ *and* $|V(\Gamma_1)|=1$. *Then*

$$A_{(\Gamma_1,\Gamma'')}|_{\operatorname{cone}^\exists_{(\Gamma'',\Gamma_1)}} = 0 = \mathcal{R}_{(\Gamma_1,\Gamma'')}|_{\operatorname{cone}^\exists_{(\Gamma_1,\Gamma'')}}. \tag{90}$$

Proof: One must apply the property (80) of cones of weak causality, cf. Lemma 4.2.12 in Ref. 24, pp. 113ff. □

Again, but formally varying from the named version (cf. Remark 4.7 below), one considers a partition of unity. For each triple of graphs Γ, Γ_1, $\Gamma''\in G_V$ where $(\Gamma_1,\Gamma'')\subset\mathcal{P}_2(\Gamma)$ and $|V(\Gamma_1)|=1$ one chooses a partition of unity $(\chi^\exists_s)$, $s\leqslant 2$ of class C^∞ subordinate to the finite open covering $\operatorname{cone}^\exists := (\operatorname{cone}^\exists_{(\Gamma_1,\Gamma'')}, \operatorname{cone}^\exists_{(\Gamma'',\Gamma_1)})$ of the metric space $\mathbb{R}^{(1+d)\times n}_\times$, i.e.,

$$\chi^\exists_1(x) + \chi^\exists_2(x) = 1, \quad \forall\, x\in\mathbb{R}^{(1+d)\times n}_\times, \tag{91}$$

$$\text{where} \quad 0\leqslant\chi^\exists_s\in C^\infty(\mathbb{R}^{(1+d)\times n}_\times) \tag{92}$$

$$\text{and} \quad \operatorname{supp}\chi^\exists_s\subset\operatorname{cone}^\exists_s, \quad s\leqslant 2. \tag{93}$$

Example 4.5: One may use the partitions of unity χ introduced for the EGF approach to define such a $\chi^\exists$, i.e., $\chi^\exists_s := \Sigma_{P\in\mathcal{P}_2(\Gamma'),\Gamma_1\subseteq P_s}\chi_P$, $s\leqslant 2$.

Proposition 4.6: *The graph distributions are (uniquely) determined by*

$$T^\exists_{\Gamma'} := -\chi^\exists_1 R'_{(\Gamma_1,\Gamma'')} - \chi^\exists_2 A'_{(\Gamma_1,\Gamma'')} \tag{94}$$

(independently of $\chi^\exists$), i.e., $T^\times_{\Gamma'} = T^\exists_{\Gamma'}|_{\mathbb{R}^{(1+d)\times n}_\times} \in \mathcal{R}^{\mathsf{T}}_{G_\Gamma}(\mathbb{R}^{(1+d)\times n}_\times)$.

Proof: This is a consequence of (80) and Lemma 4.4 (cf. Prop. 4.2.15 in Ref. 24, p. 116). □

Remark 4.7: In the original EGS version the *n*-point distribution is obtained actually via a

so-called *splitting* of the *causal distribution* $D:=R'-A'=R-A$. Here, the mapping $D\mapsto\chi_2^{\exists}D$ defines a regularized splitting, i.e.,

$$T^{\times}_{\Gamma'} = \chi_2^{\exists}D_{(\Gamma_1,\Gamma'')}\big|_{\mathbb{R}^{(1+d)\times n}_{\times}} - R'_{(\Gamma_1,\Gamma'')}\big|_{\mathbb{R}^{(1+d)\times n}_{\times}}. \tag{95}$$

3. Regularizing HAs

As causal regularization is understood to be a localization of distributions on subregions of noncoinciding space–time points in configuration space it can be modeled algebraically via A^0-modules $\overline{A}=A^0\overline{1}\oplus\bigoplus_{n\geqslant 0}\overline{A^n}$ that are extensions of $\mathbb{N}$-graded (configuration space depending) modules $A=\bigoplus_{n\geqslant 0}A^n$, where $\overline{A^n}=\bigoplus_{r\leqslant n}A^n(\mathbb{R}^{(1+d)\times n}_{r\neq})$ and $\overline{1}$ denotes the formally defined unity. In concrete cases they will be used as algebras. The instances of those modules (respectively, algebras) are the (algebra of) n-point distributions $\mathcal{R}_{G_\Gamma}$ as well as the tensor product structure $C^\infty\otimes\mathcal{R}_{G_\Gamma}$, with C^∞ functions multiplied pointwise.

The regularization for the EGF (respectively, EGS) version is given as a subalgebra of $\overline{C^\infty\otimes\mathcal{R}_{G_\Gamma}}$ which is isomorphic to $\overline{\mathcal{R}}_{G_\Gamma}$ as an algebra, i.e., $\big(\hat{\mathcal{R}}^{(\exists)}_{G_\Gamma},\mathbb{C},+,\hat{\circ}^{(\exists)}_{\Gamma},\overline{1}\big)$, where

$$\overline{\mathcal{R}}_{G_\Gamma}\overset{\iota}{\cong}\hat{\mathcal{R}}^{(\exists)}_{G_\Gamma}\overset{\vartheta^{(\exists)}}{\hookrightarrow}\overline{C^\infty\otimes\mathcal{R}_{G_\Gamma}} \tag{96}$$

and, for at least $r\in\mathbb{N}$ noncoinciding space–time points, the embedding algebra homomorphism

$$\vartheta^{(\exists)}:\hat{\bigcirc}^{(\exists)}_{\Gamma}\iota\big(T^{\otimes}_P|_{\mathbb{R}^{(1+d)\times n}_{r\neq}}\big)=:\hat{\bigcirc}^{(\exists)}_{\Gamma}\hat{T}^{\otimes}_P\mapsto\vartheta^{(\exists)}_P\otimes\bigcirc_\Gamma T^{\otimes}_P|_{\mathbb{R}^{(1+d)\times n}_{r\neq}} \tag{97}$$

is realized via functions $\vartheta^{(\exists)}_P\in C^\infty(\mathbb{R}^{(1+d)\times n}_{r\neq})$ indexed with r-partitions $P\in\mathcal{P}^0_r(\Gamma')$ of graphs $\Gamma'\in G_\Gamma$, where $r\leqslant n\equiv|V(\Gamma')|$. Those *causally ordering functions* will be used to model the considered regularizing algebra. One of their general properties is according to the defining isomorphism, i.e., $\vartheta^{(\exists)}_{(\Gamma')}=1$, $\forall\Gamma'\in G_\Gamma$. The costructure is introduced by the graded shuffling coproduct, where $\Delta(\overline{1})=\overline{1}\otimes\overline{1}$ and $\varepsilon(\overline{1})=1$. Moreover, the (respectively, two) algebras above define bialgebras $\big(\hat{\mathcal{R}}^{(\exists)}_{G_\Gamma},\mathbb{C},+,\hat{\circ}^{(\exists)}_{\Gamma},\eta,\Delta,\varepsilon\big)$.

Notice, one always applies the following abbreviation, $T_{\Gamma'}=\hat{T}_{(\Gamma')}\in\hat{\mathcal{R}}^{(\exists)}_{G_\Gamma}$.

Modeling EGF: The causally ordering functions are given in terms of the partition of unity,

$$\vartheta_p:=\tfrac{1}{2}\chi_{\check{P}},\quad\forall P\in\mathcal{P}^0_r(\Gamma'),\quad\forall\Gamma'\in G_\Gamma,\quad\forall r\leqslant|V(\Gamma')|, \tag{98}$$

where $\check{P}\in\mathcal{P}_s(\Gamma')$, for $s\leqslant r$, denotes the tuple P reduced by empty graph entries. This motivates a further general property of ϑ, i.e.,

$$\vartheta_P=\vartheta_Q\quad\text{if}\quad\check{P}=\check{Q}\quad\text{and}\quad|P|=|Q|. \tag{99}$$

Theorem 4.8: $(\hat{\mathcal{R}}_{G_\Gamma},\mathbb{C},+,\hat{\circ}_\Gamma,\eta,\Delta,\varepsilon,S^{\hat{\circ}_\Gamma})$ *forms a HA where*

$$S^{\hat{\circ}_\Gamma}T_{\Gamma'}=\begin{cases}T_\varnothing & \text{if }\Gamma'=\varnothing,\\ -T_{\Gamma'}, & \text{otherwise.}\end{cases} \tag{100}$$

Proof: It remains to check the antipode condition. This can be done by rewriting EGF's induction (Proposition 4.3), i.e., $0=\frac{1}{2}T^{\times}_{\Gamma'}-T^{\chi/2}_{\Gamma'}$. Let $L:=\mathbb{R}^{(1+d)\times n}_{\times}$, then

$$
\begin{aligned}
0 = & \left(1-\frac{1}{2}\right)\chi_{(\Gamma')}T_{\Gamma'}\Big|_L - \frac{1}{2}\sum_{(\Gamma^1,\Gamma^2)\in\mathcal{P}_2(\Gamma')}\chi_{(\Gamma^1,\Gamma^2)}\sigma_{\Gamma'}(\Gamma^1\sqcup_\Gamma\Gamma^2)T_{\Gamma^1}\circ_\Gamma T_{\Gamma^2}\Big|_L \\
= & \ \vartheta_{(\Gamma',\varnothing)}\otimes T_{\Gamma'}|_L - \vartheta_{(\varnothing,\Gamma')}\otimes T_{\Gamma'}|_L - \sum_{(\Gamma^1,\Gamma^2)\in\mathcal{P}_2(\Gamma')}\vartheta_{(\Gamma^1,\Gamma^2)}\otimes\sigma_{\Gamma'}(\cdots)\cdots\Big|_L \\
= & \ T_{\Gamma'}\hat{\circ}_\Gamma T_\varnothing + T_\varnothing\hat{\circ}_\Gamma(-T_{\Gamma'}) + \sum_{(\Gamma^1,\Gamma^2)\in P_2(\Gamma')}\sigma_{\Gamma'}(\Gamma^1\sqcup_\Gamma\Gamma^2)T_{\Gamma^1}\hat{\circ}_\Gamma(-T_{\Gamma^2}) \\
= & \ \hat{\bigcirc}_\Gamma\circ(\mathrm{id}\otimes \mathrm{S}_{\hat{\circ}_\Gamma})\circ\Delta T_{\Gamma'}.
\end{aligned}
$$

The other side of the antipode condition follows similarly. □

Modeling EGS: There are two extra properties of $\vartheta^\exists$, i.e.,

$$
\vartheta^\exists_P = \begin{cases} \vartheta^\exists_{(\cdots\sqcup_\Gamma P_{i-1},P_i,P_{i+1}\sqcup_\Gamma\cdots)} & \text{if } \exists\,\Gamma_1\subseteq P_i \text{ s.t. } y_1 = x_{\Gamma_1}, \\ \vartheta^\exists_{\sqcup_\Gamma P}, & \text{otherwise,} \end{cases} \tag{101}
$$

and

$$
\vartheta^\exists_p = \begin{cases} \vartheta^\exists_{(\Gamma_1,\Gamma'')} \\ \vartheta^\exists_{(\Gamma'',\Gamma_1)} \end{cases} \quad \text{if} \quad \exists\,\Gamma_1\subseteq\begin{cases} P_1 \\ P_r \end{cases} \text{s.t. } y_1 = x_{\Gamma_1}, \tag{102}
$$

so that the causally ordering functions can also be given in terms of the partition of unity,

$$
\vartheta^\exists_P := \begin{cases} \chi^\exists_s & \text{if } \exists\,\Gamma_1\subseteq P_s \text{ s.t. } y_1 = x_{\Gamma_1} \text{ and } P\in\mathcal{P}_2(\Gamma'), \\ 0, & \text{otherwise,} \end{cases}
$$

$\forall P\in\mathcal{P}^0_r(\Gamma')$, $\Gamma'\in\mathrm{G}_\Gamma$, $r\leqslant|\mathrm{V}(\Gamma')|$.

Theorem 4.9: $(\hat{\mathcal{R}}^\exists_{\mathrm{G}_\Gamma},\mathbb{C},+,\hat{\circ}^\exists_\Gamma,\eta,\Delta,\varepsilon,\mathrm{S}_{\hat{\circ}^\exists_\Gamma})$ *forms a HA where*

$$
\mathrm{S}_{\hat{\circ}^\exists_\Gamma}T_{\Gamma'} = \begin{cases} 0 & \text{if } \exists\,\Gamma_1\subseteq\Gamma' \text{ s.t. } y_1 = x_{\Gamma_1}, \\ \mathrm{S}_{\circ_\Gamma}T_{\Gamma'}, & \text{otherwise.} \end{cases} \tag{103}
$$

Proof: Again, it remains to check the antipode condition. By rewriting the *R*-part of EGS' induction (cf. Lemma 4.4), i.e., $0=\chi^\exists_1 R_{(\Gamma_1,\Gamma'')}|_L = \chi^\exists_1 T^\exists_{\Gamma'} + \chi^\exists_1 R'_{(\Gamma_1,\Gamma'')}|_L$, where $L:=\mathbb{R}^{(1+d)\times n}_\times$, one obtains

$$
\begin{aligned}
0 = & \ \chi^\exists_1 T_{\Gamma'}|_L + \chi^\exists_1\sum_{(\Gamma^1,\Gamma^2)\in\mathcal{P}_2(\Gamma'),\Gamma_1\subseteq\Gamma^1}\sigma_\Gamma(\Gamma^1\sqcup_\Gamma\Gamma^2)T_{\Gamma^1}\circ_\Gamma\mathrm{S}_{\circ_\Gamma}T_{\Gamma^2}\Big|_L \\
= & \ \vartheta^\exists_{(\Gamma',\theta)}\otimes T_{\Gamma'}|_L + \sum_{(\Gamma^1,\Gamma^2)\in\mathcal{P}_2(\Gamma'),\Gamma_1\subseteq\Gamma^1}\vartheta^\exists_{(\Gamma^1,\Gamma^2)}\otimes\sigma_{\Gamma'}(\Gamma^1\sqcup_\Gamma\Gamma^2)T_{\Gamma^1}\circ_\Gamma\mathrm{S}_{\circ_\Gamma}T_{\Gamma^2}\Big|_L \\
= & \sum_{(\Gamma^1,\Gamma^2)\in\mathcal{P}^0_2(\Gamma'),\Gamma_1\subseteq\Gamma^1}\vartheta^\exists_{(\Gamma^1,\Gamma^2)}\otimes\sigma_{\Gamma'}(\Gamma^1\sqcup_\Gamma\Gamma^2)T_{\Gamma^1}\circ_\Gamma\mathrm{S}_{\circ_\Gamma}T_{\Gamma^2}\Big|_L \\
= & \sum_{(\Gamma^1,\Gamma^2)\in\mathcal{P}^0_2(\Gamma')}\sigma_{\Gamma'}(\Gamma^1\sqcup_\Gamma\Gamma^2)T_{\Gamma'}\hat{\circ}^\exists_\Gamma\,\mathrm{S}_{\hat{\circ}^\exists_\Gamma}T_{\Gamma^2} \equiv \hat{\bigcirc}^\exists_\Gamma\circ(\mathrm{id}\otimes\mathrm{S}_{\hat{\circ}^\exists_\Gamma})\circ\Delta T_{\Gamma'}.
\end{aligned}
$$

Similarly, the other side of the antipode condition follows from the *A*-part.

4. BS' Feynman approach

The conventional approach to pQFT is written in terms of Feynman propagators. This leads to an explicit representation of graph distributions in momentum space which, without iterated renormalization as indicated below, suffers from so-called ultraviolet subdivergences. When going over

to configuration space this means that the distributions are determined only on $L:=\mathbb{R}^{(1+d)\times n}_{\neq}$. Even if the aspect of causality has already been investigated by BS[30] only the work of BPHZ[3–5] could verify the correctness of the common method of curing subdivergences via renormalization over so-called forests of subgraphs (which is the main application of Kreimer's HA[9]).

Lemma 4.10: *Let $\Gamma'=\Gamma^1\sqcup_l\Gamma^2$ be a graph and $P'\equiv P^1\otimes P^2=(P\circ \mathrm{V}_i(\Gamma'))_{i\leqslant n}$, $n\equiv|V(\Gamma')|$, the associated tuples of particles. Localized on L, time-ordered [cf. (B2) in the Appendix B] Wick contractions can be represented by Feynman contractions, i.e.,*

$$(\mathrm{T}\amalg)^l_{(\Gamma^1,\Gamma^2)}\Big|_L=\prod\nolimits^l_{(\Gamma^1,\Gamma^2)}\Big|_L,\quad \textit{where}\ \prod\nolimits^l_{(\Gamma^1,\Gamma^2)}:=\prod_{\substack{(i,j)\in l_{rs}\\ r\leqslant|P^1|,s\leqslant|P^2|}}\Delta_{F\gamma}^{P^1_{ri}P^2_{sj}}. \tag{104}$$

Proof: As chronological cycles $C\subset M$ can be excluded by localization on L, one confirms

$$\begin{aligned}\prod\nolimits^l_{(\Gamma^1,\Gamma^2)}\Big|_L&=\prod_{\substack{(i,j)\in l_{rs}\\ r\leqslant|P^1|,s\leqslant|P^2|}}(\theta_{(r,s)}\Delta_{+\gamma}^{P^1_{ri}P^2_{sj}}+\sigma\theta_{(s,r)}\Delta_{+\gamma}^{P^2_{sj}P^1_{ri}})\Big|_L=\sum_{\substack{M\subseteq M^{12}\cup M^{21}\\ (u,v)\in M\Leftrightarrow(v,u)\notin M}}\prod_{\substack{(i,j)\in\overline{l}_{uv}\\ (u,v)\in M}}\theta_{(u,v)}\sigma_{\mathrm{I}(\Gamma')}\\ &\times(P'_u,P'_v)\Delta_{+\gamma}^{P'_{ui}P'_{vj}}\Big|_L=\sum_{\substack{M\subseteq M^{12}\cup M^{21}\\ \nexists C\subset M\text{cycle}}}\prod_{(u,v)\in M}\theta_{(u,v)}\sigma_{I(\Gamma')}(\Gamma'_u\sqcup_\varnothing\Gamma'_v)\amalg^{\overline{l}_{uv}}_{(\Gamma'_u,\Gamma'_v)}\Big|_L\\ &=\sum_{\pi\in S_n}\theta_{\pi(\Gamma')}\sigma_{\mathrm{I}(\Gamma^1\sqcup_l\Gamma^2)}(\pi(\Gamma'))\prod_{i<j\leqslant n}\prod\nolimits^{\overline{\pi\circ l_{ij}}}_{(\pi\circ\Gamma'_i,\pi\circ\Gamma'_j)}\Big|_L=(\mathrm{T}\amalg)^l_{(\Gamma^1,\Gamma^2)}\Big|_L,\end{aligned}$$

where the omitted variables in $\Delta^{**}_{+\gamma}(y_{**})$ are related as follows:

$$y_{uv}:=y'_u-y'_v=\begin{cases}y_r-y_s=:y_{rs}\\ y_s-y_r=:y_{sr}\end{cases}\quad\text{if }(u,v)=\begin{cases}(\tau,s+|\nu^1|),\\ (s+|\nu^1|,r).\end{cases}$$

The sets $\left\{\begin{smallmatrix}M^{12}\\ M^{21}\end{smallmatrix}\right.$ collect the corresponding pairs $(u,v)\in\mathbb{N}_n\times\mathbb{N}_n$ of indices, and the bar over the concatenation matrix $l\in\mathrm{l}(\Gamma^1,\Gamma^2)$ denotes its conversion into a matrix of lines, $\overline{l}:=\left(\begin{smallmatrix}\varnothing & l\\ \tilde{l} & \varnothing\end{smallmatrix}\right)$. □

Remark 4.11: Restricted to $x_{uv}\in\mathbb{R}^{1\times n}_{\neq}\times\mathbb{R}^{d\times n}\subset L$, the products of step functions vanish whenever their variables form a chronological cycle C, i.e.,

$$\prod_{(u,v)\in C}\theta_{(u,v)}(x_{uv})\equiv\prod_{(u,v)\in C}\theta(x^0_{uv})=0\ \text{if}\ \sum_{(u,v)\in C}x^0_{uv}=0.$$

The localization on L is sufficient, namely $\operatorname{supp}\Delta^{**}_{+\gamma}\subseteq\overline{V}_+\cup\overline{V}_-=:\overline{V}$, yielding $\operatorname{supp}\theta_{(*,*)}\Delta^{**}_{+\gamma}\subseteq L\cap\overline{V}\subset\mathbb{R}^{1\times n}_{\neq}\times\mathbb{R}^{d\times n}$.

Without localization, a simple consideration about the role of cycles, that correspond to so-called loops in Feyman diagrams, motivates the phenomenon of renormalization freedom.

Example 4.12: Let (r,s,t) be a cycle, i.e., $\theta(x^0_{rs})\theta(x^0_{st})\theta(x^0_{tr})|_{\mathbb{R}^{1\times3}_{\neq}\times\mathbb{R}^{d\times3}}=0$, and apply TI. Then, on the subspace generated by $x_r=x_t$,

$$\theta(x^0)\theta(-x^0)\big|_{(\mathbb{R}\setminus\{0\})\times\mathbb{R}^d}=0,\quad\text{where } x:=x_{rs}=-x_{st}.$$

The restriction cannot be dropped, as one realizes by applying the 1hs to certain distributions t. For example, let $t=\delta$ be the Dirac distribution, and let the product be defined via a regularization of θ, e.g., $\theta_n(x^0):=\frac{1}{2}(1+\tanh(nx^0))$. Then, induced by this particular regularization,

$$\theta(x^0)\theta(-x^0)t(x):=\lim_{n\to\infty}\theta_n(x^0)\theta_n(-x^0)t(x)=\tfrac{1}{4}\delta(x^0),$$

which obviously spoils associativity (i.e., the algebraic structure),

$$\tfrac{1}{4}\delta(x)=\theta(x^0)\theta(-x^0)\delta(x)\neq(\theta(x^0)\theta(-x^0))\delta(x)=0\,\delta(x).$$

This is consistent with the no-go theorem of Schwartz.[36]

Proposition 4.13: *Localized on L, graph distributions can be represented by time-ordered products* $T^{\neq}_{\Gamma'}=T^{\mathcal{R}}_{\Gamma^1}\circ^{\mathsf{T}}_{\Gamma}\cdots\circ^{\mathsf{T}}_{\Gamma}T^{\mathcal{R}}_{\Gamma^r}\big|_L\in\mathcal{R}^{\mathsf{T}}_{\mathrm{G}_\Gamma}(L)$, *where*

$$T^{\neq}_{\Gamma'}=(i\hbar)^{\#\Gamma'-|\Gamma'|}\Sigma_{b(\Omega\Gamma')}t^{\mathcal{R}}_{\mathrm{I}(\Gamma^1)}t^{\mathcal{R}}_{\mathrm{I}(\Gamma^2)}\prod_{(\Gamma^1,\Gamma^2)}^{l}N(\Gamma^l)\Bigg|_L, \tag{105}$$

for $r:=2$ *and* $\Gamma'\equiv\Gamma^1\sqcup_l\Gamma^2$.

Proof: The scalar part rests upon Lemma 4.10 and the structural part upon the following. □

Lemma 4.14: (Wick's theorem of time ordering.) *Keeping the notations*,

$$N(\Gamma^1)\circ^{\mathsf{T}}_{\Gamma}N(\Gamma^2)_L=\sum_{\substack{l\in\mathrm{l}(\Gamma^1,\Gamma^2)\\ \Gamma^1\sqcup_l\Gamma^2=\Gamma^1\sqcup_\Gamma\Gamma^2}}(i\hbar)^{|l|}\prod_{(\Gamma^1,\Gamma^2)}^{l}N(\Gamma^1\sqcup_l\Gamma^2)\Bigg|_L. \tag{106}$$

Proof: This follows from (58) and (104) (cf. Lemma 4.2.25 in Ref. 24, p. 122). □

Remark 4.15: Associativity of $\circ^{\mathsf{T}}_{\Gamma}$ corresponds with $\Pi_{(\cdot,\cdot)}$ being a 2-cocyle. In addition to $\amalg$, also Π can be considered as a Laplace pairing.

Explicitly, the graph distributions (60) can be characterized by the following.

Proposition 4.16: (Feynman diagrams) *Localized on L, graph distributions are (uniquely) determined by their scalar parts*,

$$t^{\mathcal{R}}_{\mathrm{I}(\Gamma')}\big|_L=\Pi^{\Gamma}_{\Gamma'}\big|_L,\quad \textit{where}\ \Pi^{\Gamma}_{\Gamma'}=\prod_{r<s\leqslant n}\prod_{\Gamma'_r\sqcup_\Gamma\Gamma'_s\in\mathcal{P}(\Gamma')}\Pi^{\mathrm{l}(\Gamma')_{rs}}_{(\Gamma'_r,\Gamma'_s)} \tag{107}$$

(independent of the renormalization scheme $\mathcal{R}$*).*

Proof: This is a consequence of Proposition 4.13. The calculation of (107) is similar to the one in the proof of Lemma 4.10 [cf. (4.139) in Ref. 24, p. 127].

Remark 4.17: Immediately, (29), (104), and (107) imply GTS of $t_{\mathrm{I}(\Gamma')}|_L$.

For completion, one can as well present an algebraic formulation of the BS regularization in the sense of Sec. IV A 3. The corresponding causally ordering functions read

$$\vartheta^{\mathsf{T}}:\hat{\bigcirc}^{\mathsf{T}}_{\Gamma}\hat{T}^{\otimes}_P\mapsto\vartheta^{\mathsf{T}}_P\otimes\bigcirc^{\mathsf{T}}_{\Gamma}T^{\otimes}_P|_L,\quad\text{where}\ \ \vartheta^{\mathsf{T}}_P:=1|_L, \tag{108}$$

$\forall P\in\mathcal{P}^0_r(\Gamma')$, $\forall\Gamma'\in\mathrm{G}_\Gamma$, $\forall r\leqslant|\mathrm{V}(\Gamma')|$.

Theorem 4.18: $\big(\hat{\mathcal{R}}^{\mathsf{T}}_{\mathrm{G}_\Gamma},\mathbb{C},+,\hat{\circ}^{\mathsf{T}}_{\Gamma},\eta,\Delta,\varepsilon,\mathrm{S}_{\hat{\circ}^{\mathsf{T}}_{\Gamma}}\big)$ *forms a HA where*

$$\mathrm{S}_{\hat{\circ}^{\mathsf{T}}_{\Gamma}}T_{\Gamma'}=(-1)^{|\mathrm{V}(\Gamma')|}T_{\tilde{\Gamma}'}. \tag{109}$$

Proof: It remains to check the antipode condition. Due to the claimed form of the antipode, the calculation is analogous to the one that proves Theorem 2.4. Formally, one would only have to substitute $\mathsf{N}:=\mathsf{T}$ and $\phi^{\bigcirc_J}:=T_{\Gamma'}$. □

B. Renormalization

For both EG versions the concept of renormalization can be implemented using EGF's method[7] of extending localized distributions to the smallest diagonal. For the remaining text, let $*\in\{\mathsf{F},\exists,\mathsf{T}\}$ symbolize the reference to one of the three causal regularizations where, to include EGF, $\hat{\mathcal{R}}^{\mathsf{F}}_{\mathrm{G}_\Gamma}:=\hat{\mathcal{R}}_{\mathrm{G}_\Gamma}$ and $\hat{\circ}^{\mathsf{F}}_{\Gamma}:=\hat{\circ}_{\Gamma}$.

1. Implementation via an extension of distributions

Renormalization can be understood as a method to (re)obtain elements of $\hat{\mathcal{R}}^{*}_{G_\Gamma}$ which are not determined by causality, introduced here without reference to the concrete regularization via a projective map,

$$\hat{\text{ren}} \equiv \hat{} \circ \text{ren}: \hat{\mathcal{R}}^{*n}_{G_\Gamma}(\mathbb{R}^{(1+d)\times n}_{r\neq}) \to \mathcal{R}^{*n}_{G_\Gamma} \hookrightarrow \hat{\mathcal{R}}^{*n}_{G_\Gamma}, \quad \hat{\text{ren}}|_{\hat{\mathcal{R}}^{*n}_{G_\Gamma}(\mathbb{R}^{(1+d)\times n})} = \text{id}. \tag{110}$$

In particular, when performing the causally regularizing induction step, this map is supposed to implement the renormalization scheme $\mathcal{R}$ depending on the underlying graph Γ',

$$\text{ren}^{\mathcal{R}}_{\Gamma'}: T^{r\neq}_{\Gamma'} \mapsto T^{\mathcal{R}}_{\Gamma'}, \quad \forall\, r \leqslant n. \tag{111}$$

For both EG versions, renormalization is performed as an extension of the considered graph distribution [i.e., (86) and (94), where $r:=2$] to the diagonal diag^n_2, performed on its scalar part [cf. (60)], i.e.,

$$T^{\mathcal{R}}_{\Gamma'} := \text{ren}^{\mathcal{R}}_{\Gamma'} T^{\times}_{\Gamma'} \equiv (i\hbar)^{\#\Gamma' - |\Gamma'|} \Sigma_{b(\Omega\Gamma')} \text{ext}^{\varrho,k}_{\Gamma'}(t^{\times}_{I(\Gamma)}) N(\Gamma'), \tag{112}$$

where reflecting the involved renormalization freedom (i.e., ambiguity), the extension $\text{ext}^{\varrho,k}_{\Gamma'}: \mathcal{D}'^{\otimes}_{I(\Gamma')}(\mathbb{R}^{(1+d)\times n}_{\times}) \to \mathcal{D}'^{\otimes}_{I(\Gamma')}$ is indexed by an auxiliary function $\varrho \in \mathcal{S}(\mathbb{R}^{(1+d)\times n})$ and a set (abbreviated by k) of complex constants $k^{\alpha, I(\Gamma')}_{\Gamma'}$, for $|\alpha| \leqslant \omega_{\Gamma'}$. Depending on the associated graph Γ', the instances for ϱ and k can up to a few restrictions be chosen arbitrarily. The concrete choice of $(\varrho_{\Gamma'}, k_{\Gamma'})$ fixes a particular renormalization scheme, i.e., $\mathcal{R} = \{(\varrho_{\Gamma'}, k_{\Gamma'}) | \Gamma' \text{ divergent}\}$. According to the assumed property of TI, the relevant dimension reduces to $\dim = (1+d)(n-1)$, and hence, the diagonal $\text{diag}^n_2 \subset \mathbb{R}^{(1+d)\times n}$ goes over into the origin $\{0\} \subset \mathbb{R}^{\dim}$.

For the BS approach, renormalization can only be given formally due to its coarse regularization, i.e., $T^{\mathcal{R}}_{\Gamma'} := \text{ren}^{\mathcal{R}}(T^{\mathcal{R}}_{\Gamma^1} \hat{\circ}_\Gamma T^{\mathcal{R}}_{\Gamma^2}) \equiv \mathcal{T}^{\mathcal{R}}_{\Gamma^1} \circ^{\mathsf{T}}_\Gamma T^{\mathcal{R}}_{\Gamma^2}$ where $\Gamma' \equiv \Gamma^1 \sqcup_\Gamma \Gamma^2$. For a concrete realization one must apply EG.

In the EG framework renormalization is as well based on power counting. This can be realized, as in the EGF version, via the so-called scaling degree,

$$\text{sd}(t) := \inf\left\{\rho \middle| \lim_{\lambda\to 0} \lambda^{\rho-\dim} t(\tau(\lambda^{-1}\cdot)) = 0,\ \forall\ \tau \in \mathcal{D}(\mathbb{R}^{\dim})\right\}, \tag{113}$$

which counts the inverse power of distributions $t \in \mathcal{D}'(\mathbb{R}^{\dim})$ at the origin of $\mathbb{R}^{\dim}$, i.e., $t(x) = O(|x|^{\text{sd}})$ as $|x| \to 0$. Then the extension of distributions is characterized as follows.

Proposition 4.19: *Let $t^{\times} \in \mathcal{S}(\mathbb{R}^{\dim}\backslash\{0\})$ with scaling degree $\rho := \text{sd}(t^{\times}) < \infty$. Then there exist extensions $t^{\varrho,k} \equiv \text{ext}^{\varrho,k}(t^{\times}) \in \mathcal{S}(\mathbb{R}^{\dim})$ with the same finite scaling degree* $\text{sd}(t^{\varrho,k}) = \rho$, *i.e., $t^{\varrho,k}(\tau^{\times}) = t^{\times}(\tau^{\times})$, $\forall \tau^{\times} \in \mathcal{S}(\mathbb{R}^{\dim}\backslash\{0\})$. Two cases have to be distinguished. If the distribution $t^{\times}$ is not singular, i.e., if its singular order ω is negative, then the extended distribution $t^{\varrho,k}$ is uniquely determined. Otherwise, if the* singular order $\omega := \rho - \dim \geqslant 0$, *uniqueness is violated. Then the extension depends, first, on an arbitrarily chosen tempered function $\varrho \in \mathcal{S}(\mathbb{R}^{\dim})$ which satisfies $\varrho(0) = 1$ and $\partial^\alpha \varrho(0) = 0$, and second, on an arbitrary set of constants $k^\alpha \in \mathbb{C}$ which defines the extended distribution on a set of test functions, $x \mapsto x^\alpha \varrho(x)$, i.e., $t^{\varrho,k}(\cdot^\alpha \varrho(\cdot)) = k^\alpha$, $\forall \alpha$, $|\alpha| \leqslant \omega$.*

Proof: Compare Theorems 5.2 and 5.3 in Ref. 7, pp. 645ff. □

Remark 4.20: More precisely, the extended distribution reads

$$t^{\varrho,k}(\tau) = t^{\times}(W_{\omega,\varrho}\tau) + \sum_{|\alpha|\leqslant\omega} \frac{k^\alpha}{\alpha!} \partial^\alpha \tau(0), \tag{114}$$

so that in the *second case*, where an associated graph would be called *divergent*, the following projection cannot be the identity, $W_{\omega,\varrho}: \mathcal{S}(\mathbb{R}^{\dim}) \to \mathcal{S}_\omega(\mathbb{R}^{\dim})$, $\tau \mapsto W_{\omega,\varrho}\tau$ where $(W_{\omega,\varrho}\tau)(x) = \tau(x) - \Sigma_{|\alpha|\leqslant\omega}(\partial^\alpha \tau(0)/\alpha!) x^\alpha \varrho(x)$, and where $\mathcal{S}_\omega = \{\xi \in \mathcal{S} | \partial^\alpha \xi(0) = 0, |\alpha| \leqslant \omega\}$ denotes test function space appropriate for the unique extension t in the *first case*, i.e., $t(\tau^{\times}_\omega) = t^{\times}(\tau^{\times}_\omega)$, $\forall \tau^{\times}_\omega \in \mathcal{S}_\omega(\mathbb{R}^{\dim}\backslash\{0\})$.

As the singular order is supposed to be preserved by the extension, (114) and the following lemma allow to describe the difference of the scalar distributions $t^{\mathcal{R}_i}_{\mathrm{I}(\Gamma)} := t^{\varrho,k_i}_{\mathrm{I}(\Gamma)}$ with respect to renormalization schemes $\mathcal{R}_i$, $i \leqslant 2$, by a polynomial in derivatives of the delta distribution, i.e.,

$$t^{\mathcal{R}_2}_{\mathrm{I}(\Gamma)} - t^{\mathcal{R}_1}_{\mathrm{I}(\Gamma)} = \sum_{|\alpha| \leqslant \omega_\Gamma} k_\Gamma^{\alpha,\mathrm{I}(\Gamma)} \partial^\alpha \delta^{\Pi \mathrm{V}(\Gamma)}, \tag{115}$$

with coefficients $k^\alpha = k_2^\alpha - k_1^\alpha$ formed by the difference of the renormalization constants in $\mathcal{R}_2$ and $\mathcal{R}_1$, provided that ϱ has been fixed.

Lemma 4.21: *Let* $t \in \mathcal{S}'(\mathbb{R}^{\dim})$ *and* $\operatorname{supp} t = \{0\}$. *Then* $\exists ! \{k^\alpha \in \mathbb{C} \,|\, |\alpha| \leqslant \omega \equiv [\mathrm{sd}(t)]\}$ *s.t.* $t(x) = \Sigma_{|\alpha| \leqslant \omega} k^\alpha \Pi_{i \leqslant \dim} \partial^{\alpha_i} \delta(x_i)$.

Proof: Compare a textbook on distributions, e.g., Ref. 37, Sec. 8.4. □

2. On the physical meaning

The diagram in Fig. 3, especially the "laws of physics" arrow, will now be supplemented with more detail.

Classification of theories: By applying the scaling degree's additive properties that, based on the scaling degree $2\rho_{p'} := \mathrm{sd}(\Delta^{+\gamma}_{p'}) \leqslant 2|p'| + \mathrm{sd}(\Delta^{+\gamma}_{p})$ of the propagator $\Delta^{+\gamma}_{p'} \equiv (-1)^{|p'|} \partial_{p'} \partial_{\tilde{p}'} \Delta^{+\gamma}_{p}$, lead to

$$\rho_v = \sum_{i \leqslant |P(v)|} \rho_{P_i(v)} \quad \text{and} \quad \rho_\Gamma = \sum_{k \leqslant |\mathrm{I}(\Gamma)|} \rho_{\mathrm{I}_k(\Gamma)}, \tag{116}$$

one determines the singular order $\omega_\Gamma = \rho_\Gamma - \dim$ of the graph Γ, i.e.,

$$\omega_\Gamma = \sum_{k \leqslant |\mathrm{V}(\Gamma)|} \omega_{\mathrm{V}_k(\Gamma)} - \omega_{\Omega(\Gamma)}, \quad \text{where } \omega_v := \rho_v - (1 + \mathrm{d}). \tag{117}$$

Power counting therefore reproduces the well-known classes, called

$$\begin{cases} \text{nonrenormalizable} \\ \text{renormalizable} \\ \text{super-renormalizable} \end{cases} \text{if} \quad \begin{cases} (\exists v \in \mathrm{U})\, \omega_v > 0, \\ (\forall v \in \mathrm{U})\, \omega_v \leqslant 0, (\exists v \in \mathrm{U})\, \omega_v = 0, \\ (\forall v \in \mathrm{U})\, \omega_v < 0, \end{cases} \tag{118}$$

or as usual, in numbers of divergent graphs $\mathrm{G}_{\mathrm{div}}$ and vertices $\mathrm{V}_{\mathrm{div}}$,

$$\text{if} \begin{cases} |\mathrm{V}_{\mathrm{div}}| \begin{cases} = \infty, \\ < \infty, \end{cases} & \text{where} \quad \mathrm{V}_{\mathrm{div}} = \{v \in \mathrm{W} | (\exists \Gamma \in \mathrm{G}_{\mathrm{div}}) v = \Omega\Gamma\}, \\ |\mathrm{G}_{\mathrm{div}}| < \infty, & \mathrm{G}_{\mathrm{div}} = \{\Gamma \in \mathrm{G}_{\mathrm{W}} | \omega_\Gamma \geqslant 0\}. \end{cases} \tag{119}$$

This is illustrated for a "toy pQFT" with $|\mathrm{U}| = 1$ initial vertex which couples m scalar fields ϕ.

Example 4.22: Let $H_{\mathcal{I}} \propto :\phi^m:$. Since $\Delta^+_\phi(x) = O(|x|^{-2})$ as $x \to 0$, $\rho_\phi = 1$, and $\rho_{\phi^m} = m$. Then, for a graph Γ consisting (exclusively) of ϕ^m vertices,

$$\omega_\Gamma = |\mathrm{V}(\Gamma)|(m - (1 + \mathrm{d})) - |\mathrm{E}(\Gamma)| + (1 + \mathrm{d}). \tag{120}$$

Depending on the considered space–time dimension $1 + \mathrm{d}$, i.e.,

$$\begin{cases} < m, \\ = m, \\ > m, \end{cases} \quad \text{so that} \quad \begin{cases} \mathrm{V}_{\mathrm{div}} = \mathrm{W}, \\ \mathrm{V}_{\mathrm{div}} = \{v \in \mathrm{W} |\, |\mathrm{P}(v)| \leqslant m\}, \\ \mathrm{G}_{\mathrm{div}} \subseteq \left\{\Gamma \in \mathrm{G}_{\mathrm{W}} |\, |\mathrm{V}(\Gamma)| \leqslant \frac{1+\mathrm{d}}{1+\mathrm{d}-m}\right\}, \end{cases} \tag{121}$$

one reproduces the above classes of renormalizable theories.

Renormalization freedom: Besides TI, which was implemented explicitly, k_Γ must satisfy other symmetries. For instance, GTS is ensured by the condition $k_\Gamma^{\alpha,\mathrm{I}(\Gamma)} = \sigma_\Gamma(\mathrm{I}(\pi \circ \Gamma)) k_{\pi(\Gamma)}^{\pi(\alpha),\mathrm{I}(\pi\circ\Gamma)}$,

$\forall \alpha$, $|\alpha| \leqslant \omega_\Gamma$. The requirements for Lorentz invariance are investigated in Ref. 38. Moreover, the physicists' strategy of selecting new vertices produced by renormalization is to implement further (physical) symmetries, e.g., C,P,T, invariance, pseudounitarity, and gauge invariance; Scharf[6] calls this *the principle of perturbative gauge invariance.*

Example 4.23: (Scalar QED) Let $H_{\mathcal{I}} = e : \phi^*(\partial^\mu \phi) A_\mu : - e : (\partial^\mu \phi^*) \phi A_\mu :$. Then there are two initial vertices,

$u_1 =$ 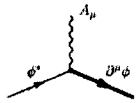 , $u_2 =$ 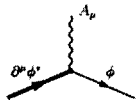 .

Consider d=3. Then $\omega_\Gamma = -\omega_{\Omega(\Gamma)} \equiv 1 + d - \rho_{\Omega(\Gamma)}$, i.e., a graph Γ is divergent only if $E(\Gamma) \leqslant 4$ and "$\partial\phi$" $\notin E(\Gamma)$. Therefore, three candidates $V \backslash U \subseteq V_{\text{div}}$ of new physical vertices are generated by renormalization,

$v_1 =$ 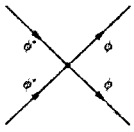 , $v_2 =$ 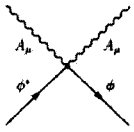 , $w_1 =$ 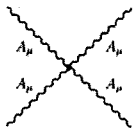 .

However, only v_1 and v_2 are relevant (cf. Ref. 31, pp. 335ff). In accordance with pseudounitarity, $T_{(v_1)}(x) = : \phi^{*2}(x) \phi^2(x) :$, where $a_{v_1} = \lambda \in i\mathbb{R}$, and in accordance with gauge and C invariance, $T_{(v_2)}(x) = (1/i\hbar) g^{\mu\nu} : \phi^*(x) \phi(x) A_\mu(x) A_\nu(x) :$ where $a_{v_2} = e^2/i\hbar$. In the conventional approach, one would then rewrite the interaction Hamiltonian by summing over V, i.e., $H_{\mathcal{I}} = i\hbar \Sigma_{v \in V} a_v T_v$.

3. EG counterparts of Kreimer's HA

The goal is to model the change of the renormalization scheme via a HA similar to Kreimer's.[9] Formally, this is in contrast with the literature[12,17] where it has been claimed having extracted Kreimer's HA of renormalization in the EG approach (which should be impossible). In fact, similar to Kreimer's approach in Ref. 11, one can deform graded commutative versions of (the three) causally regularizing HAs in order to construct the aimed HA. However, the resulting HAs are still coassociative. This is in contrast with Kreimer's structure, which is noncoassociative and precisely referred to as a quasi-HA.

Graded commutative versions of the causally regularizing HAs are given as quotient algebras, $\underline{\mathcal{R}}^*_{G_\Gamma} = \hat{\mathcal{R}}^*_{G_\Gamma} / {}^*_\Gamma[\cdot,\cdot]^\otimes_\sigma$, divided by the ideal which is generated by the graded commutator, i.e., $(\underline{\mathcal{R}}^*_{G_\Gamma}, \mathbb{C}, +, \underline{\circ}^*_\Gamma, \eta, \Delta, \varepsilon, S_{\underline{\circ}^*_\Gamma})$ where the product reads

$$\underline{T}_{\Gamma^1} \underline{\circ}^*_\Gamma \underline{T}_{\Gamma^2} = \tfrac{1}{2} [\hat{T}_{\Gamma^1}, \hat{T}_{\Gamma^2}]^{\hat{\circ}^*_\Gamma}_{-\sigma}, \quad \forall\, T_{\Gamma^1}, T_{\Gamma^2} \in \mathcal{R}^{\mathsf{T}}_{G_\Gamma}. \tag{122}$$

Again, one abbreviates the new representatives by the former notation, $T_{\Gamma'} = \underline{T}_{(\Gamma')} \in \underline{\mathcal{R}}^*_{G_\Gamma}$. Notice, due to graded commutativity, $\underline{\mathcal{R}}^{\mathsf{T}}_{G_\Gamma} = \hat{\mathcal{R}}^{\mathsf{T}}_{G_\Gamma}$ and $\underline{\circ}^{\mathsf{T}}_\Gamma = \hat{\circ}^{\mathsf{T}}_\Gamma$.

As another prerequisite one introduces the algebra of tuples of strongly decreasing graphs, $(\mathcal{G}^{\supset}_\Gamma, \mathbb{C}, +, \cdot, \varnothing)$, which is defined as the quotient of the tensor algebra of graphs divided by an ideal of nondecreasing graphs,

$$\mathcal{G}^{\supset}_\Gamma = \bigoplus_{n \geqslant 0} G^{\otimes n}_\Gamma \Big/ \big((\ldots, \Gamma^2) \otimes (\Gamma^1, \ldots),\ \sqcap \Gamma^2 \not\supseteq \sqcap \Gamma^1, \tag{123}$$

$$(\ldots, \Gamma^2, \Gamma^1, \ldots) - (\ldots, \Gamma^1, \ldots),\ \sqcap \Gamma^2 = \sqcap \Gamma^1 \big). \tag{124}$$

The EG counterpart of Kreimer's HA, providing the transition $(\mathcal{R} \to \mathcal{R}') =: \mathcal{K}$ of renormalization schemes, is a HA $\underline{\mathcal{K}}^*_{G_\Gamma}$ which defines an extension of $\underline{\mathcal{R}}^*_{G_\Gamma}$. This HA can be constructed in complete analogy to the latter, starting with the counterpart of $\mathcal{R}^{\mathsf{T}}_{G_\Gamma}$, i.e., $\mathcal{K}^{\mathsf{T}}_{G_\Gamma}$

$:=\oplus_{n\geqslant 0}\mathbb{C}\{k_{\overline{\Gamma'}}T^{\mathcal{R}}_{\Gamma'}\,|\,\overline{\Gamma'}\in\mathcal{G}^{\supset}_{\Gamma},\overline{\Gamma'}_{|\overline{\Gamma'}|}=\Gamma',|\mathrm{V}(\Gamma')|=n\}$ where, analogous to (60),

$$k_{\overline{\Gamma'}}T^{\mathcal{R}}_{\Gamma'}:=(i\hbar)^{\#\Gamma'-|\Gamma'|}\Sigma_{\mathrm{b}(\Omega\Gamma')}k_{\overline{\Gamma'}}t^{\mathcal{R}}_{\mathrm{I}(\Gamma')}N(\Gamma') \tag{125}$$

which, chosen in accordance with (115), is determined by its scalar part,

$$\mathbb{T}\ni k_{\overline{\Gamma'}}t^{\mathcal{R}}_{\mathrm{I}(\Gamma')}:=\begin{cases} t^{\mathcal{R}}_{\mathrm{I}(\Gamma')} & \text{if } \overline{\Gamma'}=\emptyset,\\ \displaystyle\sum_{|\alpha|\leqslant\omega_{\Gamma'}} k^{\alpha,\mathrm{I}(\Gamma')}_{\overline{\Gamma'}\cdot(\Gamma')}\partial^{\alpha}\delta^{\mathrm{IV}(\Gamma')}, & \text{otherwise}. \end{cases} \tag{126}$$

The complex constants $k^{\alpha,\mathrm{I}(\Gamma')}_{\overline{\Gamma'}\cdot(\Gamma')}$ with multi-index α and particle indices $\mathrm{I}(\Gamma')$, depending on the product of the graph Γ' with an appropriate tuple of decreasing graphs $\overline{\Gamma'}$, fix the transition $\mathcal{K}$. As an empty sums is zero, $k_{\overline{\Gamma'}}T^{\mathcal{R}}_{\Gamma'}$ vanishes for nondivergent graphs Γ', i.e., if $\omega_{\Gamma'}<0$.

The additional structure in $\mathcal{K}_{\mathrm{G}_\Gamma}$ (i.e., the HA analogous to $\mathcal{R}_{\mathrm{G}_\Gamma}$) can be introduced as an action of an algebra, $k_\bullet:\mathcal{G}^{\supset}_{\Gamma}\to\mathrm{End}(\mathcal{K}_{\mathrm{G}_\Gamma})$ ($k_{\overline{\Gamma'}}T^{\mathcal{R}}_{\Gamma'}=0$ if $\sqcup\overline{\Gamma'}_{|\overline{\Gamma'}|}\not\supseteq\sqcap\Gamma'$), i.e., $k_{\overline{\Gamma^2}}\circ k_{\overline{\Gamma^1}}=k_{\overline{\Gamma^1}\cdot\overline{\Gamma^2}}$, $\forall\overline{\Gamma^1},\overline{\Gamma^2}\in\mathcal{G}^{\supset}_{\Gamma}$, so that, $\forall\overline{\Gamma'}\in\mathcal{G}^{\supset}_{\Gamma}$, $k_{\overline{\Gamma'}}$ defines a HA homomorphism, i.e., $k_{\overline{\Gamma'}}\circ\bigcirc_\Gamma=\bigcirc_\Gamma\circ(k_{\overline{\Gamma'}}\otimes k_{\overline{\Gamma'}})$, $\Delta\circ k_{\overline{\Gamma'}}=(k_{\overline{\Gamma'}}\otimes k_{\overline{\Gamma'}})\circ\Delta$, and $\mathrm{S}_{\circ_\Gamma}\circ k_{\overline{\Gamma'}}=k_{\overline{\Gamma'}}\circ\mathrm{S}_{\circ_\Gamma}$. Along this line, starting with Sec. III B 3, one repeats all the algebraic constructions for $\mathcal{K}$. As far as renormalization is involved, the scheme is still $\mathcal{R}$. One must only require that transition and renormalization exchange, i.e., $k_{\overline{\Gamma'}}\circ\mathrm{ren}^{\mathcal{R}}_{\Gamma'}:=\mathrm{ren}^{\mathcal{R}}_{\Gamma'}\circ k_{\overline{\Gamma'}}$, whenever $\overline{\Gamma'}_{|\overline{\Gamma'}|}\supset\sqcup\Gamma'$.

Theorem 4.24: *$(\underline{\mathcal{K}}^*_{\mathrm{G}_\Gamma},\mathbb{C},+,\underline{\circ}^*_{\Gamma'},\eta,\Delta,\epsilon,\mathrm{S}_{\underline{\circ}^*_\Gamma})$ forms a HA which extends $\mathcal{R}^*_{\mathrm{G}_\Gamma}$, and $k_\bullet:\mathcal{G}^{\supset}_{\Gamma}\to\mathrm{End}(\mathcal{K}^*_{\mathrm{G}_\Gamma})$ defines an action of an algebra where, $\forall\overline{\Gamma'}\in\mathcal{G}^{\supset}_{\Gamma}$, $k_{\overline{\Gamma'}}$ is a HA homomorphism. More precisely, $(\forall T'\in\underline{\mathcal{K}}^*_{\mathrm{G}_\Gamma})$ $(\exists!T\in\underline{\mathcal{R}}^*_{\mathrm{G}_\Gamma})$ $(\exists!\overline{\Gamma'}\in\mathcal{G}^{\supset}_{\Gamma})$ s.t. $k_{\overline{\Gamma'}}T=T'$, i.e., $k_\bullet:\mathcal{G}^{\supset}_{\Gamma}\to\mathrm{Hom}(\underline{\mathcal{R}}^*_{\mathrm{G}_\Gamma},\underline{\mathcal{K}}^*_{\mathrm{G}_\Gamma})$ where $T'\in\underline{\mathcal{R}}^*_{\mathrm{G}_\Gamma}\subset\underline{\mathcal{K}}^*_{\mathrm{G}_\Gamma}$ requires $T=T'\equiv k_\emptyset T$.*

Proof: This is the result of the constructions in the preceding sections, but in the context of $\mathcal{K}$ instead of $\mathcal{R}$. □

The theorem gets meaning when claiming the concrete embedding of the new scheme $\mathcal{R}'$, i.e., $\underline{\mathcal{R}}^*_{\mathrm{G}_\Gamma}\overset{\iota}{\cong}\underline{\mathcal{R}}'^*_{\mathrm{G}_\Gamma}\subset\underline{\mathcal{K}}^*_{\mathrm{G}_\Gamma}$,

$$\iota:T^{\mathcal{R}}_{\Gamma'}\mapsto T^{\mathcal{R}'}_{\Gamma'}:=T^{\mathcal{R}}_{\Gamma'}+\mathrm{S}^{k\geqslant 1}_{\underline{\circ}^*_\Gamma}T^{\mathcal{R}}_{\Gamma'}\quad\forall\,\Gamma'\in\mathrm{G}_\Gamma, \tag{127}$$

where $\mathrm{S}^{k}_{\underline{\circ}^*_\Gamma}T^{\mathcal{R}}_{\Gamma'}\equiv k_\bullet\circ\mathrm{S}_{\underline{\circ}^*_\Gamma}T^{\mathcal{R}}_{\Gamma'}:=\mathrm{S}_{\underline{\circ}^*_\Gamma}(k_{(\Gamma')}T^{\mathcal{R}}_{\Gamma'})$, $n\equiv|\mathrm{V}(\Gamma')|$, and $\mathrm{S}^{k\geqslant 1}_{\underline{\circ}^*_\Gamma}T^{\mathcal{R}}_{\Gamma'}=\mathrm{S}^{k}_{\underline{\circ}^*_\Gamma}T^{\mathcal{R}}_{\Gamma'}$, except for $n=1$, where $\mathrm{S}^{k\geqslant 1}_{\underline{\circ}^*_\Gamma}T^{\mathcal{R}}_{\Gamma'}=0$. The correctness of this setting rests upon the requirement that $\mathrm{supp}(T^{\mathcal{R}'}_{\Gamma'}-T^{\mathcal{R}}_{\Gamma'})\subseteq\mathrm{diag}^n_n$, which is guaranteed by the following fact.

Lemma 4.25: $\mathrm{supp}(\mathrm{S}^{k\geqslant 1}_{\underline{\circ}^*_\Gamma}T^{\mathcal{R}}_{\Gamma'})\subseteq\mathrm{diag}^n_n$.

Proof: This can be shown by expansion of the antipode, i.e.,

$$\mathrm{S}^{k}_{\underline{\circ}^*_\Gamma}T^{\mathcal{R}}_{\Gamma'}=\mathrm{ren}^{\mathcal{R}}_{(\Gamma')}\circ k_{(\Gamma')}\Bigg(-T^{\mathcal{R}}_{\Gamma'}-\sum_{(\Gamma^1,\Gamma^2)\in\mathcal{P}_2(\Gamma')}\sigma_\Gamma(\Gamma^1\sqcup_\Gamma\Gamma^2)\mathrm{S}^{k}_{\underline{\circ}^*_\Gamma}T^{\mathcal{R}}_{\Gamma'}\,\underline{\circ}^*_\Gamma\,T^{\mathcal{R}}_{\Gamma^2}\Bigg), \tag{128}$$

and applying an adequate induction argument. For example, if $\underline{\mathcal{K}}^*_{\mathrm{G}_\Gamma}$ and $\mathrm{supp}\,K^i\subseteq\mathrm{diag}^{n_i}_{n_i}$, $i\leqslant 2$, where $n=n_1+n_2$, then $\mathrm{supp}(K^1\underline{\circ}^*_\Gamma K^2)\subseteq\mathrm{diag}^n_n$. □

For the case, $*=\mathsf{T}$, one can state the transition between the schemes explicitly.

Example 4.26: Let $P\in\mathcal{P}_r(\Gamma')$, $r\leqslant n$. Then R is called a P-tree iff $R\in\mathcal{G}^{\supset\times r}_{\Gamma}$, $(\forall j<r)$ $(R_{ij})_{i\leqslant j}\in\mathcal{P}_j(\Gamma')$ and $\exists!\,i_j\in\{i_{j-1},i_{j-1}+1\}$s.t.$(R_{i_jj+1},R_{i_j+1j+1})\in\mathcal{P}_2(R_{i_jj})$ where $i_1=1$, and $(R_{ir})_{i\leqslant r}=P$. Applying this notation, one obtains

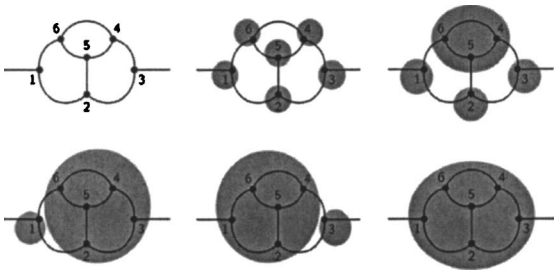

FIG. 4. A sample graph of ϕ^3 theory and its (five) partitions P of divergent subgraphs.

$$T^{\mathcal{R}'}_{\Gamma'} = T^{\mathcal{R}}_{\Gamma'} + \sum_{r<n} \sum_{P\in\mathcal{P}_r(\Gamma')} \sigma_{\Gamma'}(P) \sum_{R\ P-\text{tree}} \bigcirc^{\mathsf{T}}_{i\leqslant r} k_{R_i} T^{\mathcal{R}}_{P_i}. \tag{129}$$

For the (most) trivial transition (in this context), i.e., $k_{\overline{\Gamma'}} := k_{(\Gamma)}$, $\forall \overline{\Gamma'} \in \mathcal{G}^{\supset}_{\Gamma}$, this reduces to

$$T^{\mathcal{R}'}_{\Gamma'} = T^{\mathcal{R}}_{\Gamma'} + \sum_{r<n} \sum_{P\in\mathcal{P}_r(\Gamma')} \sigma_{\Gamma'}(P) \bigcirc^{\mathsf{T}}_{i\leqslant r} k_{P_i} T^{\mathcal{R}}_{P_i}, \tag{130}$$

corresponding to Pinter's result, cf. Eq. (14) in Ref. 17, p. 6.

Starting the comparison with the conventional approach, the following two examples illustrate how overlapping divergences are treated in the EG framework.

Example 4.27: Consider $H_{\mathcal{I}} \propto \phi^3$ for $\mathrm{d}=2$ and, especially, the graph in Fig. 4. Then the singular order of the divergent subgraphs $\Upsilon = P_i$ is given by $\omega_\Upsilon = 3 - |\mathrm{E}(\Upsilon)|$, i.e.,

$$\omega_\Upsilon = \begin{cases} 1 & \text{if } \mathrm{V}(\Upsilon) \in \{(4,5,6),(1,\ldots,6)\}, \\ 0, & \text{otherwise}. \end{cases}$$

Notice, the two subgraphs with loops, i.e., $((1,2,5,6),\ldots)$ and $((2,3,4,5),\ldots)$, which because of their 4 (>3) external lines are not divergent, do not contribute to the so-called forest formula (129).

Here, loops obviously do not play the distinguished role they play in the conventional approach (cf. Example 4.12). That holds true for tree graphs as well.

Example 4.28: Consider scalar QED for $\mathrm{d}=3$ and, especially, the graph in Fig. 5. Then the singular order of the divergent subgraphs $\Upsilon = P_i$ is given by $\omega_\Upsilon = 4 - |\mathrm{E}(\Upsilon)| = 0$. Notice, also tree graphs, i.e., $((1,2),\ldots)$ and $((3,4),\ldots)$, do represent divergent subgraphs.

Even if the structure of graphs presented here varies from Kreimer's (which is only pre-Lie), one can identify the following connection.

Remark 4.29: Let R be Kreimer's map which is supposed to leave the short distance singularities unaltered, e.g., if $\mathrm{reg}(\varepsilon) = \sum_{n=-p}^{\infty} c_n \varepsilon^n, p>0$, denotes a regularization for $\varepsilon \to 0$ then

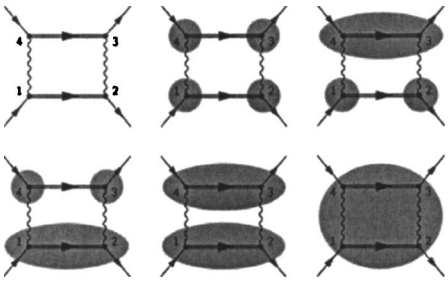

FIG. 5. A sample graph of scalar QED and its (five) partitions P of divergent subgraphs.

$R:\mathrm{reg}(\varepsilon)\mapsto\mathrm{reg}(\varepsilon)-\Sigma_{n\leqslant 0}c'_n\varepsilon^n$. Then one observes the following correspondence between the presented and Kreimer's HA:

$$k_\bullet \leftrightarrow R \text{ (i.e., } S^{k_\bullet}_{\circ^*_\Gamma} \leftrightarrow S_R) \quad \text{and} \quad \mathrm{ren}^{\mathcal{R}} \leftrightarrow \mathrm{id}-R, \tag{131}$$

reflecting the algebraic structure and, respectively, the function of renormalization.

In order to ensure that the deformed antipode S_R defines a homomorphism (which, for $S_{\circ^*_\Gamma}$, is fulfilled for free) the map R, and thus $\mathrm{id}-R$, have to satisfy a multiplicativity constraint, i.e.,

$$R(XY)+R(X)R(Y)=R(XR(Y))+R(R(X)Y), \tag{132}$$

the so-called Rota–Baxter relation, cf. Ref. 39.

Moreover, one can motivate the quasiness of Kreimer's deformed HA.

Remark 4.30: In the spirit of Kreimer's presentation, e.g., in Ref. 11, one may interpret the functor $\mathrm{Hom}(\underline{\mathcal{R}}^*_{G_\Gamma},\underline{\mathcal{K}}^*_{G_\Gamma})$ as a deformation of HAs induced by deforming,

$$\text{either the antipode,} \quad S_{\circ^*_\Gamma} \mapsto S^{k_\bullet}_{\circ^*_\Gamma} \equiv k_\bullet \circ S_{\circ^*_\Gamma}, \tag{133}$$

$$\text{or the coproduct,} \quad \Delta \mapsto \Delta^k \equiv (k_\bullet \otimes k_\bullet)\circ\Delta, \tag{134}$$

while keeping the coproduct or antipode, respectively, fixed. Then it is obvious why the deformed HA in Kreimer's original approach is only quasi (i.e., noncoassociative). Namely, $(\mathrm{id}\otimes\Delta^k)\circ\Delta^k T^{\mathcal{R}}_{\Gamma'}=(\Delta^k\circ\mathrm{id})\circ\Delta^k T^{\mathcal{R}}_{\Gamma'}$ is true only if the transition $k_\bullet$ is trivial.

A more detailed presentation of the content of this section will be given elsewhere.[40]

V. CONCLUSIONS AND OUTLOOK

About 10 years ago HAs entered the framework of pQFT. At that time Wick and Feynman contractions (i.e., $\sqcup\!\!\sqcup$ and $\sqcap$) have been identified, by Rota and Stein,[20,21] as examples for Laplace pairs in the context of combinatorial HAs. Since then, the formal perturbative expansion could have been considered as given by a Laplace HA. However, only recently has this been done, cf. Refs. 13 and 22. The knowledge about it did not get that popular among physicists as Kreimer's Hopf algebraic description of renormalization[9] in the late 1990s.

In this paper, both these HA approaches to pQFT (i.e., Entries 4 and 7 and, respectively, Entry 8 in the table of Fig. 1) get represented in the EG framework. The causally regularizing HAs (Entries 5–7) can therefore be regarded as a bridge between them. Furthermore, as an EG only feature, the HAs modeling normalization and localization of free fields (Entries 2–3) appear as the stucture that Cliffordization twists into the Laplace HA representing the perturbative expansion.

Topics for further research supplementing and extending the presented scenario of HAs, which apparently underlies the EG approach to pQFT, could read as follows (enumerated from the physical to the mathematical one):

i In the spirit of Kreimer's more recent work,[41,42] one might also think about implementing Scharf's principle[6] of perturbative gauge invariance into the HA context.

ii As Laplace pairs can be interpreted as objects in the theory of quantum groups (cf. Refs. 18, 19, and 22), namely as so-called R-forms (cf. Ref. 43, Sec. VIII.5), investigations in this direction, e.g., incorporating broader algebraic concepts as done in Ref. 23, still seem to be fruitful.

iii Following an idea of Kontsevich,[44] one might try to understand renormalization as a dual procedure to the compactification of the configuration space;[45] see also Ref. 46.

ACKNOWLEDGMENTS

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APPENDIX A: CALCULATIONS

Lemma A.1: $\Delta^{(\mathsf{N})}$, *i.e.,* Δ *and* Δ^{N}, *are GTS.*

Proof: The two claims can be proven at once, where the possible empty alternative is symbolized by brackets. Let $X\subseteq \mathrm{P}^n$, $n\in\mathbb{N}$, and let $\pi\in S_n$ be a permutation on X. Then

$$\Delta^{(\mathsf{N})}(\varphi^{\bigcirc\pi(X)}) = \sum_{P_\pm\in\mathcal{P}_2^0(\pi(X))} \sigma_{\pi(X)}(P_\pm)\cdots$$

$$= \sum_{P_\pm\in\mathcal{P}_2^0(X)} \sigma_{\pi(X)}(X)\sigma_X(P_\pm)\cdots = \sigma(\pi)\Delta^{(\mathsf{N})}(\varphi^{\bigcirc X}),$$

where the following identity for sets of partitions, i.e., $\mathcal{P}_2^0=\mathcal{P}_2^0\circ\pi$, $\forall\pi\in S_n$, and following the group representation rule for the grading sign, $\sigma_Y(Z)=\sigma_Y(X)\sigma_X(Z)$, $\forall X, Y, Z\in\mathrm{P}^n$, were used. □

Lemma A.2: Δ *and* Δ^{N} *are coassociative where, for the first coproduct,* ε *also satisfies the counit property.*

Proof: The three calculations below verify the claims. Let $X\in\mathrm{P}^n$, $n\in\mathbb{N}$. First,

$$(\mathrm{id}\otimes\Delta)\circ\Delta(\varphi^{\bigcirc X}) = \sum_{P\in\mathcal{P}_2^0(X)} \sigma_X(P)\varphi^{\bigcirc P_1}\otimes\Delta(\varphi^{\bigcirc P_2})$$

$$= \sum_{P\in\mathcal{P}_2^0(X)} \sigma_X(P)\varphi^{\bigcirc P_1}\otimes \sum_{Q\in\mathcal{P}_2^0(P_2)} \sigma_{P_2}(Q)\varphi^{\bigcirc Q_1}\otimes\varphi^{\bigcirc Q_2}$$

$$= \sum_{(P_1,Q_1,Q_2)\in\mathcal{P}_3^0(X)} \sigma_X(P_1,Q_1,Q_2)\varphi^{\bigcirc P_1}\otimes\varphi^{\bigcirc Q_1}\otimes\varphi^{\bigcirc Q_2}$$

$$\cdots$$

$$=(\Delta\otimes\mathrm{id})\circ\Delta(\varphi^{\bigcirc X}),$$

second

$$(\mathrm{id}\otimes\varepsilon)\circ\Delta(\varphi^{\bigcirc X}) = \sum_{P\in\mathcal{P}_2^0(X)} \sigma_X(P)\varphi^{\bigcirc P_1}\otimes\varepsilon(\varphi^{\bigcirc P_2})$$

$$=\sigma_X(X\otimes\emptyset)\varphi^{\bigcirc X}\otimes 1=\varphi^{\bigcirc X}$$

$$\cdots$$

$$=(\varepsilon\otimes\mathrm{id})\circ\Delta(\varphi^{\bigcirc X}),$$

which have been rather standard, and third,

$$(\mathrm{id}\otimes\Delta^{\mathsf{N}})\circ\Delta^{\mathsf{N}}(\varphi^{\bigcirc X}) = \sum_{P\in\mathcal{P}_2^0(X)} \sigma_X(P)\mathrm{pr}_+\circ\varphi^{\bigcirc P_1}\otimes\mathrm{pr}_-\circ\Delta^{\mathsf{N}}(\varphi^{\bigcirc P_2})$$

$$= \sum_{P\in\mathcal{P}_2^0(X)} \sigma_X(P)\varphi_+^{\bigcirc P_1} \otimes \sum_{Q\in\mathcal{P}_2^0(P_2)} \sigma_{P_2}(Q)\mathrm{pr}_- \circ \varphi_+^{\bigcirc Q_1} \otimes \mathrm{pr}_- \circ \varphi_-^{\bigcirc Q_2}$$

$$= \sum_{P\in\mathcal{P}_2^0(X)} \sigma_X(P)\varphi_+^{\bigcirc P_1} \otimes \sigma_{P_2}(\varnothing \otimes P_2)1 \otimes \varphi_-^{\bigcirc P_2}$$

$$= \sum_{P\in\mathcal{P}_2^0(X)} \sigma_X(P)\varphi_+^{\bigcirc P_1} \otimes 1 \otimes \varphi_-^{\bigcirc P_2}$$

$$\cdots$$

$$= (\Delta^{\mathsf{N}} \otimes \mathrm{id}) \circ \Delta^{\mathsf{N}}(\varphi^{\bigcirc X}),$$

where the projection properties, $\mathrm{pr}_\pm^2 = \mathrm{pr}_\pm$ and $\mathrm{pr}_\mp \circ \mathrm{pr}_\pm = 0$, were applied. □

Lemma A.3: *$\Delta^{(\mathsf{N})}$ and ε define homomorphisms with respect to the products $\square \in \{\circ, \mathsf{N}\}$.*

Proof: Let X^1, $X^2 \subset \mathrm{P}^n$, $n \in \mathbb{N}$. Then

$$\varepsilon(\varphi^{\square X^1} \square \varphi^{\square X^2}) \equiv \varepsilon(\varphi^{\square X^1})\varepsilon(\varphi^{\square X^2}) = \begin{cases} 1 & \text{if } X^1 = X^2 = \varnothing, \\ 0, & \text{otherwise,} \end{cases} \tag{A1}$$

and

$$\Delta^{(\mathsf{N})}(\varphi^{\square X^1} \square \varphi^{\square X^2}) = \sum_{P\in P_2^0(X^1\otimes X^2)} \sigma_{X^1\otimes X^2}(P)\varphi_{(+)}^{\square P_1} \otimes \varphi_{(-)}^{\square P_2}$$

$$= \sum_{\substack{P\in P_2^0(X^1\otimes X^2) \\ P_i = P_i^1 \otimes P_i^2, i\leqslant 2 \\ P_i^j \in P_2^0(X^j), j\leqslant 2}} \sigma_{X^1}(P^1)\sigma_{X^2}(P^2) \underbrace{\varphi_{(+)}^{\square P_1^1} \circ \varphi_{(+)}^{\square P_1^2} \otimes \varphi_{(-)}^{\square P_2^1} \circ \varphi_{(-)}^{\square P_2^2}}_{=\left(\varphi_{(+)}^{\square P_1^1} \otimes \varphi_{(-)}^{\square P_2^1}\right) \square \left(\varphi_{(+)}^{\square P_1^2} \otimes \varphi_{(-)}^{\square P_2^2}\right)}$$

$$= \Delta^{(\mathsf{N})}(\varphi^{\square X^1}) \square \Delta^{(\mathsf{N})}(\varphi^{\square X^2}),$$

where a decomposition of the grading sign based on the group representation were applied. □

APPENDIX B: ILLUSTRATIONS

Example B.1: Illustrated for two graphs of QED (cf. Example 2.6), e.g., for

$\Gamma^1 \equiv (X^1, \Lambda^1) =$ 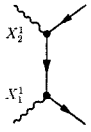 , $\Gamma^2 \equiv (X^2, \Lambda^2) =$ 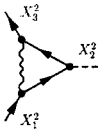

with vertices $(\overline{\psi}, \psi, A)$, except of $X_2^2 = (\overline{\psi}, \psi, A^{\mathrm{cl}})$, and matrices of lines

$$\Lambda^1 = \begin{pmatrix} \varnothing & \{(1,2)\} \\ \{(2,1)\} & \varnothing \end{pmatrix}, \quad \Lambda^2 = \begin{pmatrix} \varnothing & \{(2,1)\} & \{(3,3)\} \\ \{(1,2)\} & \varnothing & \{(2,1)\} \\ \{(3,3)\} & \{(1,2)\} & \varnothing \end{pmatrix},$$

the concatenation with the matrix

$$\Lambda^{12} = \begin{pmatrix} \{(2,1)\} & \varnothing & \varnothing \\ \varnothing & \varnothing & \{(1,2)\} \end{pmatrix},$$

yields the graph

$$\Gamma^1 \sqcup_{\Lambda^{12}} \Gamma^2 \equiv \left(X, \begin{pmatrix} \Lambda^1 & \Lambda^{12} \\ \tilde{\Lambda}^{12} & \Lambda^2 \end{pmatrix} \right) =$$

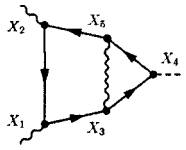

Example B.2: Consider the following quantum model, where the time evolution is determined by the Schrödinger equation, $i\hbar\partial_t\varphi(t,\vec{x}) = H(t)\varphi(t,\vec{x})$, and an interaction Hamiltonian, $H(t) = \int_{\mathbb{R}^d} dx\, H(t,\vec{x})$. The S-matrix $S = \lim_{t_\pm \to \pm\infty} U(t_+,t_-)$ is the limit of an unitary operator U which describes the time evolution of an incoming free field. By repeatedly applying the integrated Schrödinger equation, $\varphi(t,\vec{x}) = \varphi(s,\vec{x}) - (i/\hbar)\int_s^t dt_1\, H(t_1)\varphi(t_1,\vec{x})$, one obtains the so-called *Dyson series*,

$$U(t,s) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{\hbar^n} \int_s^t dt_1 \cdots \int_s^{t_{n-1}} dt_n H(t_1)\cdots H(t_n).$$

By inserting the time-ordering operation, i.e.,

$$\mathsf{T}(h(t_1,\ldots,t_n)) = \sum_{\pi\in S_n} \theta_{(t_{\pi_1},\ldots,t_{\pi_n})}\sigma(\pi)h(t_{\pi_1},\ldots,t_{\pi_n}), \tag{B1}$$

where

$$\theta_{(t_1,\ldots,t_n)} := \theta(t_1 - t_2)\cdots\theta(t_{n-1} - t_n) = \begin{cases} 1 & \text{if } t_1 > \cdots > t_n, \\ 0, & \text{otherwise} \end{cases} \tag{B2}$$

denotes a product of step functions, the limit can be performed,

$$S = 1 + \sum_{n=1}^{\infty} \frac{1}{n!(i\hbar)^n} \int_{\mathbb{R}^{1+d}} dt_1\, dx_1 \cdots \int_{\mathbb{R}^{1+d}} dt_n\, dx_n\, \mathsf{T}(H(t_1,\vec{x}_1)\cdots H(t_n,\vec{x}_n)).$$

APPENDIX C: SYMBOLS AND ABBREVIATIONS

GTS	graded total symmetry (symmetric, respectively)
TI	translation invariance (invariant, respectively)
$\phi^{\square_J}$, $\phi_J^{\square}$	$\phi^{\square_J} := \square_{j\in J}\phi^j$ and $\phi_J^{\square} := \square_{j\in J}\phi_j$, for any kind of product "$\square$"
$[\cdot,\cdot]_\sigma^{\otimes}$	graded commutator, cf. (12)
N	normal product, cf. (27) and (39)
L	localization, cf. (34)
$\Sigma_{\ldots}$	coupling monomial, cf. (35), (41), and (54)
$\Omega: G_V \to V$	shrinking of graphs G_v to vertices V, cf. Sec. III A 1
$\sqcup_\Gamma$	composition of graphs with Γ being a reference graph, cf. (44)
U	Wick contractions, cf. (57); in accordance with BS' notation: $\mathsf{U}_{(i,j)} := \mathsf{N}(\ldots\otimes\phi^i\otimes\cdots\otimes\phi^j\otimes\ldots) = [\phi_-^i,\phi_+^j]_\sigma^{\otimes}\mathsf{N}(\ldots\otimes\cdots\otimes\ldots)$
$\circ_\Gamma^*$	product of distributions with Γ being a reference graph, cf. (62) and (64)
$\mathrm{cone}_P^{(\exists)}$	(weak) causal cone with respect to a partition P, cf. (74)
$\mathbb{R}^{\dim}_{\neq r}$	causally determined spacetime region, cf. (77)
$\hat{\circ}_\Gamma^*$	product of causally regularized distributions, cf. (97)

Π Feynman contractions, cf. (104); in accordance with BS' notation:
$\Pi_{(i,j)} := \mathsf{N}(\cdots \otimes \phi^i \otimes \cdots \otimes \phi^j \otimes \cdots) = \mathsf{T}[\phi^i_-, \phi^j_+]^{\otimes}_{\sigma} \mathsf{N}(\cdots \otimes \cdots \otimes \cdots)$
$\circ^*_\Gamma$ graded commutative product of regularized distributions, cf. (122)
$* = \exists, \mathsf{F}, \mathsf{T}$ referring to the method of EGS, EGF, BS, respectively

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Derivation of particle, string, and membrane motions from the Born–Infeld electromagnetism

Yann Brenier[a)]
INLN, U.M.R., C.N.R.S. 6618, Université de Nice Sophia-Antipolis, Parc Valrose, 06108 Nice Cedex 2, France

Wen-An Yong[b)]
IWR, Universität Heidelberg, Im Neuenheimer Feld 294, 69120 Heidelberg, Germany

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We derive classical particle, string, and membrane motion equations from a rigorous asymptotic analysis of the Born–Infeld nonlinear electromagnetic theory. We first add to the Born–Infeld equations the corresponding energy-momentum conservation laws and write the resulting system as a nonconservative symmetric 10×10 system of first-order PDEs. Then we show that four rescaled versions of the system have smooth solutions existing in the (finite) time interval where the corresponding limit problems have smooth solutions. Our analysis is based on a continuation principle previously formulated by Yong for (singular) limit problems. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1925248]

I. INTRODUCTION

The Born–Infeld (BI) equations were originally introduced in Ref. 1 as a nonlinear correction to the standard linear Maxwell equations for electromagnetism. They form a 6×6 system of conservation laws, together with two solenoidal constraints on the magnetic field and electric displacement. This system has many remarkable physical and mathematical features. Introduced in 1934, the BI model was designed to cure the classical divergence of the electrostatic field generated by point charges, by introducing an absolute limit to it (just like the speed of light is an absolute limit for the particle velocity in special relativity). The value of the absolute field was fixed by Born and Infeld according to physical considerations. As a result, for moderate electromagnetic fields, the discrepancy between the BI model and the classical Maxwell equations is noticable only at subatomic scales (10^{-15} meters). However, for very large values of the field, the BI model gets very different from the Maxwell model and, as will be rigorously established in this paper, rather describes the evolution of point particles along straight lines, or vibrating strings or vibrating membranes, depending on the considered scales.

Although the BI model was rapidly given up due to the emergence of quantum electrodynamics (QED) in the 1940s, there has been a lot of recent interest in it. In high energy physics, D-branes can be modelled according to a generalization of the BI model.[14,5] In differential geometry, the BI equations are closely related to the study of extremal surfaces in the Minkowski space. From the partial differential equations (PDEs) viewpoint, the initial value problem (IVP) has been recently investigated by Lindblad (in the "scalar case" of extremal surfaces[12]) and by Chae and Huh.[3] They show the existence of global smooth solutions, for small initial data (in a regime sufficiently close to the Maxwell limit), using Klainerman's null forms and energy estimates. In mathematical physics, QED has recently been revisited by Kiessling who used a quantization technique well suited to nonlinear PDEs, involving a relativistic version of the Fisher information.[9]

a)Electronic mail: brenier@math.unice.fr
b)Electronic mail: yong.wen-an@iwr.uni-heidelberg.de

In Ref. 2, Brenier exploited the fact that the energy density and the Poynting vector satisfy certain additional conservation laws and lifted the Born–Infeld model to a 10×10 system of conservation laws, by using the energy density and the Poynting vector as new unknown variables. The resulting ABI (augmented Born–Infeld) system provides a set of equations coupling the electromagnetic field and a virtual fluid having the electromagnetic energy as mass and the Poynting vector as momentum. It was pointed out that the ABI system has some remarkable structural properties like existence of a strictly convex entropy, Galilean invariance of fluid mechanics, and full linear degeneracy.

Moreover, three asymptotic regimes of the ABI system are studied in Ref. 2, using Dafermos' relative entropy method[4] to analyze the resulting (singular) limit problems. With such analysis, the linear Maxwell equations are derived for low fields, some pressureless MHD equations, describing vibrating strings, for high fields, and pressureless gas equations for very high fields. Unfortunately, these results postulate the existence of global weak solutions for the ABI system (although they do not require *a priori* bounds on them). This is a major weakness, since the global existence of weak solutions to the IVP remains an outstanding open problem for essentially all multidimensional system of nonlinear hyperbolic conservation laws.

The goal of this paper is to use the framework of smooth solutions and energy estimates to get definite asymptotic results, using a nonconservative form of the ABI system. It will be shown that IVPs of the rescaled ABI systems have smooth solutions existing in the (finite) time interval where the corresponding reduced problems have smooth solutions. The analysis is based on a continuation principle previously formulated in Ref. 17 for (singular) limit problems, and combines formal asymptotic expansions with error estimates of energy type for symmetrizable hyperbolic systems. We also consider a high field regime, involving vibrating membranes, which was disregarded in Ref. 2.

The use of the continuation principle makes our analysis quite different from the classical one due to Klainerman and Majda.[10,11,13] With the latter, one shows the existence in a scaling-independent time interval, which may be properly contained in the time interval where the corresponding reduced problems have smooth solutions. The difference of the two approaches makes significant sense when the reduced problems have global smooth solutions. Such an example is given in Sec. VI D for low fields. See also Sec. III.

As a by-product and first step of our analysis, we observe that the nonconservation form of the ABI equations constitutes a *symmetric* (not only *symmetrizable*) hyperbolic system. Thus, the local well-posedness of the ABI system becomes obvious. Note that the symmetry does not follow directly from the existence of a strictly convex entropy proved in Ref. 2, since the latter involves the solenoidal constraints and thus the entropy is not that in the usual sense. About this point see also Serre.[15] Moreover, we show that the solenoidal constraints are compatible with the symmetric hyperbolic systems and point out a few possibly important structural properties thereof. In addition, the nonconservative ABI system, remarkably enough, is well defined for all states in $\mathbb{R}^{10}$, in sharp contrast with the conservative version, which requires the density field h to be non-negative. Indeed, the nonconservative system involves the inverse density field τ, which substitutes for h^{-1} and can take any real values, negative, positive, or null. As a consequence, the previously mentioned asymptotic results trivially follow from the symmetry of the nonconservative ABI system, at least for short time intervals. So an important technical issue of this paper is to extend these time intervals according to the existence time interval of the solutions to the limit equations, by using the method discussed above.

The paper is organized as follows. In Sec. II, we introduce the nonconservative augmented Born–Infeld equations and point out some of its structural properties. In Sec. III, we introduce three high field limits of the ABI equations and show that they, respectively, describe particle, string, and membrane motions. In Sec. IV, a crude asymptotic analysis is performed just by using the symmetric structure of the nonconservative ABI system. In Sec. V, an abstract theorem is established for the rescaled ABI systems. This theorem is applied to four concrete asymptotic regimes in Sec. VI to get sharper results. The paper ends with an appendix, which contains the continuation principle for (singular) limit problems of symmetrizable hyperbolic systems.

Notation: Let $\Omega=\mathbb{R}^d$ or $\mathbb{T}^d$ (the d-dimensional torus). L^2 is the space of square integrable (vector- or matrix-valued) functions on Ω and its norm is denoted by $\|\cdot\|$. In case A depends on another variable t as well as on $x\in\Omega$, we write $\|A(t)\|$ or $\|A(\cdot,t)\|$ to recall that the norm is taken with respect to x while t is viewed as a parameter. Similar notation will be adopted for the function spaces introduced below. For a non-negative integer k, the Sobolev space $H^k=H^k(\Omega)$ is defined as the space of functions whose distributional derivatives of order $\leqslant k$ are all in L^2. We use $\|\cdot\|_k$ to denote the norm of H^k. Furthermore, $C(J,H^k)$ denotes the space of continuous functions on the interval J with values in H^k. Finally, partial time derivatives will be frequently denoted by u_t, instead of $\partial_t u$.

II. THE BORN–INFELD SYSTEM AND ITS NONCONSERVATIVE AUGMENTED VERSION

Let B and D be time-dependent vector fields in $\mathbb{R}^3$. The Born–Infeld (BI) equations read (see, e.g., Ref. 2)

$$B_t+\nabla\times\left(\frac{B\times V+D}{h}\right)=0,\quad D_t+\nabla\times\left(\frac{D\times V-B}{h}\right)=0,\quad \operatorname{div}B=\operatorname{div}D=0, \tag{2.1}$$

where

$$h=\sqrt{1+|B|^2+|D|^2+|D\times B|^2},\quad V=D\times B, \tag{2.2}$$

and $|\cdot|$ stands for the Euclidean norm. Immediately notice that the classical (homogeneous) Maxwell equations

$$B_t+\nabla\times D=0,\quad D_t-\nabla\times B=0,\quad \operatorname{div}B=\operatorname{div}D=0 \tag{2.3}$$

can be seen as the limit of the BI equations for weak fields $B,D\ll 1$.

In Ref. 2, Brenier exploited the fact that, for smooth solutions of the BI system, the energy density h and the Poynting vector V satisfy additional conservation laws—the first two lines in (2.4) below, and used h and V as unknown variables to augment the BI model as a 10×10 system of conservation laws. Set

$$v=V/h,\quad b=B/h,\quad d=D/h.$$

The ABI (augmented Born–Infeld) system can be written as

$$\begin{aligned}
&h_t+\operatorname{div}(hv)=0,\\
&(hv)_t+\operatorname{div}(hv\otimes v-hb\otimes b-hd\otimes d)=\nabla h^{-1},\\
&(hb)_t+\operatorname{div}(hb\otimes v-hv\otimes b)+\nabla\times d=0,\\
&(hd)_t+\operatorname{div}(hd\otimes v-hv\otimes d)-\nabla\times b=0
\end{aligned} \tag{2.4}$$

along with

$$\operatorname{div}(hb)=\operatorname{div}(hd)=0. \tag{2.5}$$

See Ref. 2 for further discussions about this ABI system.

Here we only consider smooth solutions to the ABI system. Therefore, we may focus on the nonconservative form of (2.4) with (2.5). Set $\tau=h^{-1}$. By using the identity

$$\operatorname{div}(d\otimes b)=(b\cdot\nabla+\operatorname{div}b)d,$$

we can easily verify that smooth solutions to (2.4) with (2.5) satisfy

$$\begin{aligned} &\tau_t + v \cdot \nabla \tau - \tau \operatorname{div} v = 0, \\ &v_t + v \cdot \nabla v - b \cdot \nabla b - d \cdot \nabla d - \tau \nabla \tau = 0, \\ &b_t + v \cdot \nabla b - b \cdot \nabla v + \tau \nabla \times d = 0, \\ &d_t + v \cdot \nabla d - d \cdot \nabla v - \tau \nabla \times b = 0. \end{aligned} \tag{2.6}$$

This is a symmetric hyperbolic system,

$$W_t + \sum_{j=1}^{3} A_j(W) W_{x_j} = 0 \tag{2.7}$$

for $W=(\tau, v^T, b^T, d^T)^T$, with homogeneous quadratic nonlinearities. Here the superscript "T" denotes the transpose operation and the coefficient matrix is

$$A_j(W) = v_j I_{10} + \begin{pmatrix} 0 & -\tau e_j^T & 0_3^T & 0_3^T \\ -\tau e_j & 0_{3\times 3} & -b_j I_3 & -d_j I_3 \\ 0_3 & -b_j I_3 & 0_{3\times 3} & \tau e_j \times \\ 0_3 & -d_j I_3 & -\tau e_j \times & 0_{3\times 3} \end{pmatrix} \tag{2.8}$$

with v_j the jth component of v, I_k the unit matrix of order k, e_j the jth column of I_3, 0_3 the origin of $\mathbb{R}^3$, and $0_{3\times 3}$ the origin of $\mathbb{R}^{3\times 3}$. Notice that (2.7) makes sense for all states

$$W = (\tau, v^T, b^T, d^T)^T \in \mathbb{R}^{10}, \tag{2.9}$$

not only for $\tau > 0$ and even if the solenoidal constraints (2.5) do not hold.

It is remarkable that the coefficient matrix $A_j(W)$ *linearly* depends on W and the symmetry is independent of the solenoidal constraints, which are needed in Ref. 2 to show the existence of a strictly convex entropy function.

Also notice that, in the original BI equations, B, D, h, and V are linked together by the algebraic relations (2.2). This means that the original BI equations exactly correspond to the nonconservative formulation (2.6), with the further restriction that $W=(\tau, v^T, b^T, d^T)^T$ must be valued in the "BI manifold" defined by

$$\tau > 0, \quad \tau^2 + b^2 + d^2 + v^2 = 1, \quad \tau v = d \times b. \tag{2.10}$$

Of course, as for the original ABI system, the BI manifold is an invariant set for system (2.6).

The equivalence of (2.6) and (2.4) with (2.5) is illustrated here.

Proposition 2.1: If initial data for (2.6) satisfy the constraints in (2.5), then the corresponding smooth solutions to (2.6) satisfy (2.4) as well as (2.5).

Proof: It suffices to verify (2.5). To do this, we notice that the smooth solutions to (2.6) satisfy $h_t + \operatorname{div}(hv) = 0$ and

$$(hb)_t + \nabla \times (hb \times v) + \nabla \times d + \operatorname{div}(hb) v = 0,$$

where $h = \tau^{-1}$. Thus, we have

$$(\operatorname{div}(hb))_t + v \cdot \nabla (\operatorname{div}(hb)) + \operatorname{div}(hb) \operatorname{div} v = 0.$$

Since $\operatorname{div}(hb) = 0$ initially, we have $\operatorname{div}(hb) = 0$ for all t. Similarly, we can show $\operatorname{div}(hd) = 0$. This completes the proof. □

Furthermore, we point out the following important property of the symmetric hyperbolic system (2.6) or (2.7) with (2.8).

Proposition 2.2: Let $W=(\tau, v^T, b^T, d^T)^T$ be a smooth solution to (2.6) with $\tau > 0$. Then

$$\partial_t(hI_{10}) + \sum_j \partial_{x_j}(hA_j(W)) = \mathrm{div}(hb)C_1 + \mathrm{div}(hd)C_2$$

holds with C_1 and C_2 constant symmetric matrices and $h=\tau^{-1}$. In particular, if intial data for (2.6) satisfy the solenoidal constraints in (2.5), then

$$\partial_t(hI_{10}) + \sum_j \partial_{x_j}(hA_j(W)) = 0.$$

Proof: From the explicit expression of the coefficient matrix given in (2.8) it follows that

$$\partial_t(hI_{10}) + \sum_j \partial_{x_j}(hA_j(W)) = (h_t + \mathrm{div}(hv))I_{10} + \sum_j \partial_{x_j}\begin{pmatrix} 0 & -e_j^T & 0_3^T & 0_3^T \\ -e_j & 0_{3\times 3} & -hb_jI_3 & -hd_jI_3 \\ 0_3 & -hb_jI_3 & 0_{3\times 3} & e_j\times \\ 0_3 & -hd_jI_3 & -e_j\times & 0_{3\times 3} \end{pmatrix}$$

$$= -\begin{pmatrix} 0 & 0_3^T & 0_3^T & 0_3^T \\ 0_3 & 0_{3\times 3} & \mathrm{div}(hb)I_3 & \mathrm{div}(hd)I_3 \\ 0_3 & \mathrm{div}(hb)I_3 & 0_{3\times 3} & 0_{3\times 3} \\ 0_3 & \mathrm{div}(hd)I_3 & 0_{3\times 3} & 0_{3\times 3} \end{pmatrix}.$$

This completes the proof. □

III. HIGH FIELD LIMITS: PARTICLE, STRING, AND MEMBRANE MOTIONS

Observe that, for the nonconservative system (2.6), the states $W=(0,v^T,b^T,d^T)^T$, for which $\tau=0$, are not singular, while, for the conservative ABI system (2.4), they correspond to fields (B,D) of infinite intensity. (Indeed $\tau=h^{-1}$.) (Let us recall that, for classical gas dynamics equations, the state $\tau=0$ is always singular.)

Due to the special structure of (2.6), the corresponding "reduced" states $(v^T,b^T,d^T)^T$ solve the following "reduced" system

$$\begin{aligned} &v_t + v\cdot\nabla v - b\cdot\nabla b - d\cdot\nabla d = 0, \\ &b_t + v\cdot\nabla b - b\cdot\nabla v = 0, \\ &d_t + v\cdot\nabla d - d\cdot\nabla v = 0. \end{aligned} \tag{3.1}$$

A further reduction is obtained as $d=0$, which leads to

$$\begin{aligned} &v_t + v\cdot\nabla v - b\cdot\nabla b = 0, \\ &b_t + v\cdot\nabla b - b\cdot\nabla v = 0. \end{aligned} \tag{3.2}$$

Finally, $\tau=0$ and $b=d=0$ reduce (2.6) to a single equation

$$v_t + v\cdot\nabla v = 0. \tag{3.3}$$

Notice the parallel reduction of the BI manifold (2.10) to the following reduced manifolds

$$b^2 + d^2 + v^2 = 1, \quad d\times b = 0, \quad v\cdot b = v\cdot d = 0, \tag{3.4}$$

$$b^2 + v^2 = 1, \quad v\cdot b = 0, \tag{3.5}$$

$$v^2 = 1, \tag{3.6}$$

respectively, associated to (3.1)–(3.3).

These three sets of "high field" equations have a simple physical and geometrical interpretation. Indeed, system (3.3) describes a continuum of particles moving along straight lines with constant speed, as well known. If, in addition, (3.6) holds true, these particles can be interpreted as massless particles with unit velocities. System (3.2) is more subtle and describes collections of vibrating strings, as will be shown below. Condition (3.5) guarantees that these strings are genuine relativistic strings. Notice that (3.2) can also be interpreted as a shallow water MHD equation (without gravity terms), following Ref. 6. Similarly, system (3.1) describes vibrating membranes. These statements follow from the following observation.

Proposition 3.1: Let $(s,r,u) \in \mathbb{R}^3 \to X(t,s,r,u)$ *be a smooth family of diffeomorphisms of* $\mathbb{R}^3$, *depending on* $t \in [-T,T]$. *Let* λ, μ *be two non-negative real constants. Assume that*

$$\partial_{tt} X = \lambda \partial_{ss} X + \mu \partial_{rr} X \tag{3.7}$$

holds true. Implicitly define

$$b(t,X(t,s,r,u)) = \partial_s X(t,s,r,u), \tag{3.8}$$

$$d(t,X(t,s,r,u)) = \partial_r X(t,s,r,u), \tag{3.9}$$

$$v(t,X(t,s,r,u)) = \partial_t X(t,s,r,u). \tag{3.10}$$

Then (b,d,v), *respectively, is a smooth solution to system (3.1) if* $\lambda = \mu = 1$, *system (3.2) if* $\lambda = 1$ and $\mu = 0$, *and equation (3.3) if* $\lambda = \mu = 0$.

Proof: The proof is a straightforward application of the chain rule: differentiate (3.8)–(3.10) with respect to t, use Eq. (3.7) and get the desired equations (3.1)–(3.3).

Geometrical interpretation: According to (3.7), in the case $\lambda = \mu = 0$, each trajectory $t \to X(t,r,s,u)$ is a straight line, as (r,s,u) varies in $\mathbb{R}^3$. In the case $\lambda = 1$ and $\mu = 0$, each surface $(t,s) \to X(t,r,s,u)$ solves the wave equation

$$\partial_{tt} X = \partial_{ss} X,$$

and describes a vibrating string, as (r,u) varies in $\mathbb{R}^2$. Notice that the algebraic constraint (3.5) reads

$$\partial_t X^2 + \partial_s X^2 = 1, \quad \partial_t X \cdot \partial_s X = 0,$$

which, together with the wave equation, means that these strings are genuinely relativistic (i.e., they are extremal surfaces in the Minkowski space). Similarly, in the case $\lambda = \mu = 1$, each $(t,s,r) \to X(t,r,s,u)$ describes a vibrating membrane as u varies along the real line.

Global smooth solutions to the string system (3.2). From Proposition 3.1, we see that the high field equation (3.2) has nontrivial global smooth solutions for smooth initial conditions sufficiently close to suitable trivial solutions. Any constant vector $B_0 \neq 0$ provides a trivial solution $b = B_0$, $v = 0$ and a corresponding family of diffeomorphisms is $X(t,s,r,u) = sB_0 + rD_0 + uB_0 \times D_0$, where $D_0 \neq 0$ is arbitrarily chosen such that $B_0 \cdot D_0 = 0$. Then, for any initial condition (b,v) chosen sufficiently close to the trivial solution, Eq. (3.2) has a global smooth solution. Indeed, it is enough to (i) introduce an initial diffeomorphism $X(0,s,r,u)$ implicitly defined by

$$\partial_s X(0,s,r,u) = b(0,X(0,s,r,u)),$$

(ii) for each fixed (s,u) solve the wave equation (3.7) with $\mu = 0$ and

$$\partial_t X(0,s,r,u) = v(0,X(0,s,r,u)),$$

(iii) ensure that, for all t, $(s,r,u)\to X(t,s,r,u)$ still is a diffeomorphism of $\mathbb{R}^3$, by choosing initial data $(b,v)(0,x)$ sufficiently close to $(B_0,0)$, (iv) globally define a solution (b,v) to (3.2) by

$$\partial_s X(t,s,r,u) = b(t,X(t,s,r,u)), \quad \partial_t X(t,s,r,u) = v(t,X(t,s,r,u)).$$

So, we see that the high field limit equations formally derived from the ABI system do have global smooth solutions in the neighborhood of some trivial solutions. This is also true for the original BI equations, as shown by Chae and Huh.[3] We conjecture the same property for the ABI system. (Concerning the existence of global classical solutions for the gas dynamics equations, we refer to Ref. 7.)

IV. A CRUDE ASYMPTOTIC ANALYSIS

According to well-known results on symmetric system of first-order PDEs,[13] there is a positive continuous function θ attached to system (2.6) such that, for all initial conditions W_0 belonging to the (homogeneous) Sobolev space H^s, where $s>3/2+1$ is fixed (say $s=3$), there is a unique strong solution $t\to W(t)$ to (2.6) such that $W(0)=W_0$, defined at least in the time interval $[-T,T]$ where $T=\theta(\|W_0\|_s)$. In addition, this solution depends continuously on W_0 in the space $C^0([-T,T],H^{s'})$ for all $s'<s$. Thus, we get without effort the following asymptotic result.

Theorem 4.1: *Let $\epsilon\in]0,1]$. Let $W_{0\epsilon}=(\tau_{0\epsilon},v_{0\epsilon},b_{0\epsilon},d_{0\epsilon})$ be a smooth initial condition, depending on ϵ, uniformly bounded in H^s for some $s>3/2+1$, distant from $W_0=(0,v_0,b_0,d_0)$ by ϵ in $H^{s'}$ norm for some $s'<s$. Then, there is a time interval $[-T,T]$, where $T>0$ does not depend on ϵ, such that systems (2.6) and (3.1) both have a unique strong solution $W^\epsilon=(\tau^\epsilon,v^\epsilon,b^\epsilon,d^\epsilon)$ and (v,b,d), with respective initial condition $W_{0\epsilon}$ and (v_0,b_0,d_0) on $[-T,T]$. Moreover, their distance in $C^0([-T,T],H^s)$ norm is of order ϵ.*

Of course, in the special case when $d_0=0$, the limit equation (3.1) reduces to the "string equation" (3.2). Similarly, as $b_0=d_0$, (3.1) reduces to (3.3). Let us point out that this result is obtained without effort, because of the remarkable structure of the nonconservative augmented version of the BI equations. A direct asymptotic analysis of the *original* BI equations (2.1) would have been considerably more difficult.

Need for refined asymptotic results: The main weakness of Theorem 4.1 is that the uniform existence time T is not at all optimal. Indeed, T depends on the H^s norm of the initial conditions, which is very far from being sharp. As a matter of fact, in many situations the optimal existence times T^* for the limit systems (3.1)–(3.3) can be explicitly computed. Therefore, we want a sharper existence time of form $T=T^*+O(\epsilon)$. This goal will be achieved in the next section through more refined arguments.

V. REFINED ASYMPTOTIC ANALYSIS

Consider IVPs of the ABI system (2.6) [or (2.7) with (2.8)] with initial data $W_{0\epsilon}$, which depends on ϵ in a certain topological space. Suppose an approximate smooth solution $W_\epsilon=W_\epsilon(x,t)$ has been constructed (see the next section) and is well defined for $(x,t)\in\Omega\times[0,T_*]$ with a certain $T_*>0$. Here Ω stands for the three-dimensional torus (for simplicity, we consider periodic initial data only). Define *the residual* of W_ϵ as

$$R=R(W_\epsilon) := W_{\epsilon t}+\sum_{j=1}^{3} A_j(W_\epsilon)W_{\epsilon x_j}. \tag{5.1}$$

This section is devoted to the proof of the following general result.

Theorem 5.1: *Let $s\geqslant 3$ be an integer. Suppose $W_{0\epsilon}\in H^s$ for each ϵ different from a certain singular point* (*say* 0), *$W_\epsilon(\cdot,t)\in H^{s+1}$, and*

$$\delta := \|W_{0\epsilon} - W_\epsilon(\cdot,0)\|_s^2 + \int_0^{T_*} \|R(\cdot,t)\|_s^2 \, dt \to 0$$

as ϵ approaches to the singular point 0. *Moreover, suppose there is a* 10×10*-matrix* L_ϵ*, which is bounded and invertible for* $\epsilon \neq 0$*, such that* $|L_\epsilon^{-1}|\sqrt{\delta} \to 0$ *as* $\epsilon \to 0$, $\sup_\epsilon \|L_\epsilon^{-1} W_{0\epsilon}\|_s < \infty$, *and* $\sup_{t,\epsilon} \|L_\epsilon^{-1} W_\epsilon(\cdot,t)\|_{s+1} < \infty$.

Then there is a neighborhood of $\epsilon = 0$ *such that, for all* ϵ *in the neighborhood, the ABI system (2.6) with initial data* $W_{0\epsilon}$ *has a unique classical solution*

$$W^\epsilon \in C([0,T_*], H^s).$$

Moreover, the error estimate

$$\|W^\epsilon(\cdot,t) - W_\epsilon(\cdot,t)\|_s \leqslant K\sqrt{\delta}, \quad \forall\, t \in [0,T_*], \tag{5.2}$$

holds with K a constant independent of ϵ.

Proof: Set $U_\epsilon = L_\epsilon^{-1} W_\epsilon$ for $\epsilon \neq 0$. Then (5.1) becomes

$$U_{\epsilon t} + \sum_{j=1}^{3} A_j(U_\epsilon, \epsilon) U_{\epsilon x_j} = L_\epsilon^{-1} R \tag{5.3}$$

with

$$A_j(U,\epsilon) = L_\epsilon^{-1} A_j(L_\epsilon U) L_\epsilon.$$

Accordingly, we consider the following IVP

$$U_t + \sum_j A_j(U,\epsilon) U_{x_j} = 0,$$

$$U(x,0) = \overline{U}(x,\epsilon) := L_\epsilon^{-1} W_{0\epsilon}. \tag{5.4}$$

This is a symmetrizable hyperbolic system with $A_0(U,\epsilon) := L_\epsilon^T L_\epsilon$ as its symmetrizer.

Since $\sup_\epsilon \|\overline{U}(\cdot,\epsilon)\|_s < \infty$ and $\sup_{t,\epsilon} \|U_\epsilon(\cdot,t)\|_{s+1} < \infty$ with $s \geqslant 3$, we deduce from the Sobolev embedding theorem that both $\overline{U}$ and U_ϵ take values in a bounded subset of the state space $\mathbb{R}^{10}$. Namely, there is an open set G such that

$$\bigcup_{x,t,\epsilon} \{\overline{U}(x,\epsilon), U_\epsilon(x,t)\} \subset G \subset\subset \mathbb{R}^{10}.$$

Thus, we can choose G_1 so that

$$G \subset\subset G_1 \subset\subset \mathbb{R}^{10}.$$

For each fixed $\epsilon (\neq 0)$, since $\overline{U}(x,\epsilon) \in G \subset\subset G_1$ for all $x \in \Omega$ and $\overline{U}(\cdot,\epsilon) \in H^s$ with $s \geqslant 3$, it follows from the local-in-time existence theory[13] for IVPs of symmetrizable hyperbolic systems that there is a maximal time $T_\epsilon = T_\epsilon(G_1) > 0$ so that the rescaled problem (5.4) has a unique classical solution

$$U^\epsilon \in C([0,T_\epsilon), H^s) \quad \text{and } U^\epsilon(x,t) \in G_1 \ \ \forall\, (x,t) \in \Omega \times [0,T_\epsilon).$$

Thus we only need to show $T_\epsilon > T_*$ and the error estimate in (5.2). Moreover, it suffices to prove the estimate (5.2) for $t \in [0, \min\{T_*, T_\epsilon\})$, thanks to the continuation principle (Lemma 9.1 in Ref. 17, see also the Appendix of this paper) and $|L_\epsilon^{-1}|\sqrt{\delta} \to 0$ as $\epsilon \to 0$.

Now we turn to derive the error estimate (5.2) for $t \in [0, \min\{T_*, T_\epsilon\})$. Notice that, in that time interval, both U^ϵ and U_ϵ are regular. We compute from (5.3) and (5.4) that $E = W_\epsilon - W^\epsilon = L_\epsilon(U_\epsilon - U^\epsilon)$ satisfies

$$E_t + \sum_j A_j(W^\epsilon)E_{x_j} = R - \sum_j A_j(E)W_{\epsilon x_j}.$$

Here we have used the linearity of $A_j = A_j(W)$ with respect to W. Differentiating this equation with ∂^α for a multi-index α satisfying $|\alpha| \leqslant s$ and setting $E_\alpha = \partial^\alpha E$, we get

$$E_{\alpha t} + \sum_j A_j(W^\epsilon)E_{\alpha x_j} = R_\alpha + F^\alpha. \tag{5.5}$$

Here

$$F^\alpha = \sum_j [A_j(W^\epsilon), \partial^\alpha]E_{x_j} - \left\{ \sum_j A_j(E)W_{\epsilon x_j} \right\}_\alpha .$$

Recall that $A_j(W^\epsilon)(j=1,2,\ldots,d)$ are all symmetric. Multiplying the equation (5.5) with E_α^T from the left, we get

$$(|E_\alpha|^2)_t + \sum_j \{E_\alpha^T A_j(W^\epsilon)E_\alpha\}_{x_j} = 2\,\mathrm{Re}\,E_\alpha^T(R_\alpha + F^\alpha) + E_\alpha^T\left\{ \sum_j \frac{\partial A_j(W^\epsilon)}{\partial x_j} \right\}E_\alpha. \tag{5.6}$$

The right-hand side of (5.6) is treated as follows:

$$\begin{aligned} &2\,\mathrm{Re}\,E_\alpha^T(R_\alpha + F^\alpha) \leqslant 2|E_\alpha|^2 + |R_\alpha|^2 + |F^\alpha|^2, \\ &\sum_j \frac{\partial A_j(W^\epsilon)}{\partial x_j} \leqslant C\sum_j |W^\epsilon_{x_j}| \leqslant C\|W^\epsilon\|_s, \end{aligned} \tag{5.7}$$

where C is a generic constant and the well-known Sobolev inequality has been used. Moreover, we apply the Moser-type calculus inequalities in Sobolev spaces[13] to F^α and obtain

$$\begin{aligned} \|F^\alpha\| &\leqslant C\|W_{\epsilon x_j}\|_s\|E\|_{|\alpha|} + C\|W^\epsilon\|_s\|E_{x_j}\|_{|\alpha|-1} \\ &\leqslant C\|W_\epsilon\|_{s+1}\|E\|_{|\alpha|} + C(\|W_\epsilon\|_s + \|E\|_s)\|E\|_{|\alpha|} \leqslant C(1 + \|E\|_s)\|E\|_{|\alpha|}. \end{aligned} \tag{5.8}$$

Here the boundedness of $\|W_\epsilon\|_{s+1}$ is used. Integrating (5.6) over $(x,t) \in \Omega \times [0,T]$ with $T < \min\{T_\epsilon, T_*\}$ and using (5.7) and (5.8) yields

$$\|E_\alpha(T)\|^2 \leqslant \|E_\alpha(0)\|^2 + \int_0^T \|R_\alpha(t)\|^2\,\mathrm{d}t + C\int_0^T (1 + \|E(t)\|_s^2)\|E(t)\|_{|\alpha|}^2\,\mathrm{d}t. \tag{5.9}$$

Summing up (5.9) for all multi-indices α with $|\alpha| \leqslant s$, we get

$$\|E(T)\|_s^2 \leqslant \|E(0)\|_s^2 + \int_0^T \|R(t)\|_s^2\,\mathrm{d}t + C\int_0^T (1 + \|E(t)\|_s^2)\|E(t)\|_s^2\,\mathrm{d}t \leqslant \delta + C\int_0^T (1 + \|E(t)\|_s^2)\|E(t)\|_s^2\,\mathrm{d}t.$$

Applying the Gronwall lemma to the last inequality yields

$$\|E(T)\|_s^2 \leqslant \delta \exp\left[C\int_0^T (1 + \|E(t)\|_s^2)\mathrm{d}t \right] \equiv \Phi(T). \tag{5.10}$$

Thus, we have

$$\Phi'(t) = C(1 + \|E(t)\|_s^2)\Phi(t) \leqslant C\Phi(t) + C\Phi^2(t).$$

Applying the nonlinear Gronwall-type inequality in Ref. 16 to the last inequality yields

$$\|E(t)\|_s^2 \leqslant \Phi(t) \leqslant \exp(CT_*) \tag{5.11}$$

for $t \in [0, \min\{T_\epsilon, T_*\})$ if $\Phi(0) = \delta < \exp(-CT_*)$. From (5.10) and (5.11) it follows that

$$\|E(t)\|_s \leqslant K\sqrt{\delta}$$

for all $t \in [0, \min\{T_\epsilon, T_*\})$. This completes the proof. □

We conclude this section with a remark.

Remark 5.1: In case $W_\epsilon(x,t)$ is defined globally in time and the conditions of Theorem 5.1 hold for $T_* = \infty$, we actually prove the following existence result for the ABI system (2.6): For any $T < \infty$, there is a neigborhood of $\epsilon = 0$ such that, for all ϵ in the neighborhood, the ABI system (2.6) with initial data $W_{0\epsilon}$ has a unique classical solution

$$W^\epsilon \in C([0,T], H^s).$$

Moreover, the error estimate in (5.2) holds for $t \leqslant T$ and the constant K depends on T.

VI. ASYMPTOTIC REGIMES

In this section, we apply Theorem 5.1 to four concrete asymptotic regimes. For simplicity, we will always take

$$W_{0\epsilon}(x) = W_\epsilon(x,0).$$

In addition, we do not make remarks parallel to Remark 5.1.

A. Membrane motion equations

Let ϵ be a small parameter. If the ABI system (2.6) is solved with initial data of the form

$$\tau(x,0) = O(\epsilon), \quad v(x,0) = O(1), \quad b(x,0) = O(1), \quad d(x,0) = O(1),$$

it is natural to take

$$L_\epsilon = \mathrm{diag}(\epsilon, I_3, I_3, I_3)$$

in Theorem 5.1. This L_ϵ is bounded for $\epsilon \leqslant 1$, invertible for $\epsilon \neq 0$ and $|L_\epsilon^{-1}| = \epsilon^{-1}$. This is a high field regime disregarded in Ref. 2. It might be incompatible with the BI regime (2.10), contrary to the other ones to be discussed in the following subsections. The rescaled system (5.4) reads

$$\begin{aligned}
&\tilde{\tau}_t + \tilde{v} \cdot \nabla \tilde{\tau} - \tilde{\tau} \,\mathrm{div}\, \tilde{v} = 0, \\
&\tilde{v}_t + \tilde{v} \cdot \nabla \tilde{v} - \tilde{b} \cdot \nabla \tilde{b} - \tilde{d} \cdot \nabla \tilde{d} - \epsilon^2 \tilde{\tau} \nabla \tilde{\tau} = 0, \\
&\tilde{b}_t + \tilde{v} \cdot \nabla \tilde{b} - \tilde{b} \cdot \nabla \tilde{v} + \epsilon \tilde{\tau} \nabla \times \tilde{d} = 0, \\
&\tilde{d}_t + \tilde{v} \cdot \nabla \tilde{d} - \tilde{d} \cdot \nabla \tilde{v} - \epsilon \tilde{\tau} \nabla \times \tilde{b} = 0.
\end{aligned} \tag{6.1}$$

Here $\tilde{\tau}$, $\tilde{v}$, $\tilde{b}$, and $\tilde{d}$ denote the components of the scaled variable $U = L_\epsilon^{-1} W = (\tilde{\tau}, \tilde{v}^T, \tilde{b}^T, \tilde{d}^T)^T$.

In order to apply Theorem 5.1 to this regime, we drop the tildes in (6.1) and seek an approximate solution W_ϵ of the form

$$W_\epsilon = L_\epsilon U_\epsilon, \quad U_\epsilon = U_0(x,t) + \epsilon U_1(x,t)$$

with the first component of U_1 being 0. Plugging this ansatz into (6.1), we see that $U_0 = (\tau_0, v_0, b_0, d_0)$ solves

$$\tau_t + v \cdot \nabla \tau - \tau \operatorname{div} v = 0,$$

$$v_t + v \cdot \nabla v - b \cdot \nabla b - d \cdot \nabla d = 0,$$

$$b_t + v \cdot \nabla b - b \cdot \nabla v = 0, \tag{6.2}$$

$$d_t + v \cdot \nabla d - d \cdot \nabla v = 0$$

and $U_1 = (0, v_1, b_1, d_1)$ satisfies

$$v_t + v_0 \cdot \nabla v - b_0 \cdot \nabla b - d_0 \cdot \nabla d = - v \cdot \nabla v_0 + b \cdot \nabla b_0 + d \cdot \nabla d_0,$$

$$b_t + v_0 \cdot \nabla b - b_0 \cdot \nabla v = b \cdot \nabla v_0 - v \cdot \nabla b_0 - \tau_0 \nabla \times d_0, \tag{6.3}$$

$$d_t + v_0 \cdot \nabla d - d_0 \cdot \nabla v = d \cdot \nabla v_0 - v \cdot \nabla d_0 + \tau_0 \nabla \times b_0.$$

Notice that the last three equations in (6.2) are just (3.1).

Now we solve (6.2) and (6.3) to obtain U_0 and U_1. Note that the last three equations in (6.2) form a symmetric hyperbolic system of nonlinear equations. By the local existence theory[8,13] for IVPs of symmetrizable hyperbolic systems, if $(v_0, b_0, d_0)(\cdot, 0) \in H^s$ with $s \geqslant 3$, then there is $T_* > 0$ such that the corresponding IVP has a unique classical solution $(v_0, b_0, d_0) \in C([0, T_*], H^s)$. With v_0 thus obtained, we obtain $\tau_0 \in C([0, T_*], H^{s-1})$ by solving the first equation in (6.2):

$$\tau_t + v_0 \cdot \nabla \tau - \tau \operatorname{div} v_0 = 0,$$

which is a linear equation, with $\tau(\cdot, 0) \in H^{s-1}$. Similarly, by using the existence theory[8] for IVPs of linear symmetrizable hyperbolic systems, we obtain $U_1 = (0, v_1, b_1, d_1) \in C([0, T_*], H^{s-1})$ by solving (6.3) with appropriate initial data.

With $U_\epsilon = U_0 + \epsilon U_1 \in C([0, T_*], H^{s-1})$ thus obtained, it is easy to see that the residual R, defined in (5.1), satisfies

$$R = \epsilon^2 O(1) \in C([0, T_*], H^{s-2}).$$

Thus, we deduce the following conclusion from Theorem 5.1, together with Corollary 1 of Theorem 2.2 in Ref. 13—a continuation principle.

Corollary 6.1: Let $s \geqslant 3$ be an integer. Assume $W_{0\epsilon}(x) = W_\epsilon(x, 0) \in H^{s+2}$. Then there exists $T_* > 0$ and $\epsilon_0 > 0$ such that, for each $\epsilon \in (0, \epsilon_0]$, the ABI system (2.6) with initial data $W_{0\epsilon}$ has a unique classical solution

$$W^\epsilon = (\tau^\epsilon, v^\epsilon, b^\epsilon, d^\epsilon) \in C([0, T_*], H^{s+2}).$$

Moreover, the error estimates

$$\| (\tau^\epsilon - \epsilon\tau_0, v^\epsilon - v_0 - \epsilon v_1, b^\epsilon - b_0 - \epsilon b_1, d^\epsilon - d_0 - \epsilon d_1)(\cdot, t) \|_s \leqslant K\epsilon^2,$$

for $t \in [0, T_*]$, hold with K a constant independent of ϵ. In particular, we have

$$\| (\tau^\epsilon, v^\epsilon - v_0, b^\epsilon - b_0, d^\epsilon - d_0)(\cdot, t) \|_s = \epsilon O(1).$$

Remark 6.1: Theorem 5.1 claims that $W^\epsilon \in C([0, T_*], H^s)$. Since $W_{0\epsilon} = W_\epsilon(\cdot, 0) \in H^{s+2}$, it follows from Corollary 1 of Theorem 2.2 in Ref. 13 that this solution W^ϵ has better regularity, that is,

$$W^\epsilon \in C([0, T_*], H^{s+2}).$$

This argument applies to Corollaries 6.2–6.4 in the following subsections.

B. String motion equations

Consider the ABI system (2.6) with initial data of the form

$$\tau(x,0)=O(\epsilon),\quad v(x,0)=O(1),\quad b(x,0)=O(1),\quad d(x,0)=O(\epsilon)$$

with $\epsilon \ll 1$. This is the high field regime considered in Ref. 2. As in the preceding subsection, we take

$$L_\epsilon = \mathrm{diag}(\epsilon, I_3, I_3, \epsilon I_3)$$

in Theorem 5.1. This L_ϵ is bounded for $\epsilon \ll 1$, invertible for $\epsilon \neq 0$ and $|L_\epsilon^{-1}| = \epsilon^{-1}$. Then the rescaled system (5.4) reads

$$\begin{aligned}
&\tau_t + v\cdot\nabla\tau - \tau\,\mathrm{div}\, v = 0,\\
&v_t + v\cdot\nabla v - b\cdot\nabla b - \epsilon^2 d\cdot\nabla d - \epsilon^2\tau\nabla\tau = 0,\\
&b_t + v\cdot\nabla b - b\cdot\nabla v + \epsilon^2\tau\nabla\times d = 0,\\
&d_t + v\cdot\nabla d - d\cdot\nabla v - \tau\nabla\times b = 0.
\end{aligned} \tag{6.4}$$

Dropping the ϵ^2 terms, we obtain

$$\begin{aligned}
&\tau_t + v\cdot\nabla\tau - \tau\,\mathrm{div}\, v = 0,\\
&v_t + v\cdot\nabla v - b\cdot\nabla b = 0,\\
&b_t + v\cdot\nabla b - b\cdot\nabla v = 0,\\
&d_t + v\cdot\nabla d - d\cdot\nabla v - \tau\nabla\times b = 0.
\end{aligned} \tag{6.5}$$

Notice that the second and third equations in (6.5) are just (3.2).

To solve (6.5), we note that the second and third equations in (6.5) form a symmetric hyperbolic system of nonlinear equations. Thus, if $(v,b)(\cdot,0)\in H^s$ with $s\geqslant 3$, then there is $T_*>0$ such that the corresponding IVP has a unique classical solution $(v_0,b_0)\in C([0,T_*],H^s)$. With v_0 and b_0 thus obtained, we see from the existence theory[8] for linear problems that the decoupled hyperbolic system of linear equations,

$$\begin{aligned}
&\tau_t + v_0\cdot\nabla\tau - \tau\,\mathrm{div}\, v_0 = 0,\\
&d_t + v_0\cdot\nabla d - d\cdot\nabla v_0 - \tau\nabla\times b_0 = 0,
\end{aligned}$$

with appropriate initial data, has a unique classical solution $(\tau_0,d_0)\in C([0,T_*],H^{s-1})$.

Now we take $W_\epsilon = L_\epsilon U_\epsilon$ in Theorem 5.1 with U_ϵ obtained above. It is clear that the residual R, defined in (5.1), satisfies

$$\sup_t \|\epsilon^{-2}R(\cdot,t)\|_{s-2} < \infty.$$

Thus we deduce the following conclusion from Theorem 5.1, together with Corollary 1 of Theorem 2.2 in Ref. 13.

Corollary 6.2: Let $s\geqslant 3$ be an integer. Assume $W_{0\epsilon}=W_\epsilon(\cdot,0)\in H^{s+2}$. Then there is $\epsilon_0>0$ such that, for all $\epsilon\in(0,\epsilon_0]$, the ABI system (2.6) with initial data $W_{0\epsilon}$ has a unique classical solution

$$W^\epsilon = (\tau^\epsilon, v^\epsilon, b^\epsilon, d^\epsilon) \in C([0,T_*],H^{s+2}).$$

Moreover, the error estimates

$$\|(\tau^\epsilon - \epsilon\tau_0, v^\epsilon - v_0, b^\epsilon - b_0, d^\epsilon - \epsilon d_0)(\cdot,t)\|_s \leqslant K\epsilon^2, \quad \forall\, t \in [0,T_*],$$

hold with K a constant independent of ϵ.

The interested reader can derive Corollary 6.2 directly from Corollary 6.1 with initial data satisfying $(v_1, b_1, d_0)(x,0) = 0$.

C. Particle motion equations

Now we consider the ABI system (2.6) with initial data of the form

$$\tau(x,0) = O(\epsilon^2), \quad v(x,0) = O(1), \quad b(x,0) = O(\epsilon), \quad d(x,0) = O(\epsilon)$$

with $\epsilon \ll 1$. This is the very high field regime considered in Ref. 2. As in the preceding subsections, we take

$$L_\epsilon = \mathrm{diag}(\epsilon^2, I_3, \epsilon I_3, \epsilon I_3)$$

in Theorem 5.1. This L_ϵ is bounded for $\epsilon \ll 1$, invertible for $\epsilon \neq 0$ and $|L_\epsilon^{-1}| = \epsilon^{-2}$. Then the rescaled system (5.4) reads

$$\begin{gathered}
\tau_t + v \cdot \nabla\, \tau - \tau\, \mathrm{div}\, v = 0, \\
v_t + v \cdot \nabla\, v - \epsilon^2 b \cdot \nabla\, b - \epsilon^2 d \cdot \nabla\, d - \epsilon^4 \tau \nabla\, \tau = 0, \\
b_t + v \cdot \nabla\, b - b \cdot \nabla\, v + \epsilon^2 \tau \nabla \times d = 0, \\
d_t + v \cdot \nabla\, d - d \cdot \nabla\, v - \epsilon^2 \tau \nabla \times b = 0.
\end{gathered} \tag{6.6}$$

In order to see what Theorem 5.1 means for this rescaled system, we look for an approximate solution W_ϵ of the form

$$W_\epsilon = L_\epsilon U_\epsilon, \quad U_\epsilon = (\tau_0, v_0 + \epsilon^2 v_1, b_0, d_0)(x,t).$$

Plugging this ansatz into (6.6), we see that (τ_0, v_0, b_0, d_0) should solve

$$\begin{gathered}
\tau_t + v \cdot \nabla\, \tau - \tau\, \mathrm{div}\, v = 0, \\
v_t + v \cdot \nabla\, v = 0, \\
b_t + v \cdot \nabla\, b - b \cdot \nabla\, v = 0, \\
d_t + v \cdot \nabla\, d - d \cdot \nabla\, v = 0
\end{gathered} \tag{6.7}$$

and v_1 should satisfy

$$v_t + v_0 \cdot \nabla\, v + v \cdot \nabla\, v_0 = b_0 \cdot \nabla\, b_0 + d_0 \cdot \nabla\, d_0. \tag{6.8}$$

Notice that the second equation in (6.7) is just (3.3).

As in the preceding subsections, Eqs. (6.7) and (6.8) can be solved by using the local-in-time existence theorey[8,13] for IVPs of quasilinear and linear symmetrizable hyperbolic systems. In particular, if initial data for (6.7) satisfy $v_0(\cdot,0) \in H^{s+3}$ and $(\tau_0, b_0, d_0)(\cdot,0) \in H^{s+2}$, then there exists $T_* > 0$ so that the corresponding IVP has a unique classical solution (τ_0, v_0, b_0, d_0) satisfying

$$v_0 \in C([0,T_*], H^{s+3}), \quad (\tau_0, b_0, d_0) \in C([0,T_*], H^{s+2}).$$

Moreover, if $v_1(\cdot,0) \in H^{s+1}$, then the IVP of (6.8) has a unique classical solution

$$v_1 \in C([0,T_*],H^{s+1}).$$

With W_ϵ thus obtained, it is easy to see that the residual R, defined in (5.1), satisfies

$$R = \epsilon^3 \operatorname{diag}(\epsilon, \epsilon I_3, I_3, I_3) O(1) \in C([0,T_*],H^s).$$

Thus we have $\|R(\cdot,t)\|_s = \epsilon^3 O(1)$ and the following corollary from Theorem 5.1 together with Corollary 1 of Theorem 2.2 in Ref. 13.

Corollary 6.3: Let $s \geqslant 3$ be an integer. Assume $W_{0\epsilon} = W_\epsilon(\cdot,0) \in H^{s+3}$. Then there is $\epsilon_0 > 0$ such that, for all $\epsilon \in (0,\epsilon_0]$, the ABI system (2.6) with initial data $W_{0\epsilon}$ has a unique classical solution

$$W^\epsilon = (\tau^\epsilon, v^\epsilon, b^\epsilon, d^\epsilon) \in C([0,T_*],H^{s+3}).$$

Moreover, the error estimates

$$\|(\tau^\epsilon - \epsilon^2\tau_0, v^\epsilon - v_0 - \epsilon^2 v_1, b^\epsilon - \epsilon b_0, d^\epsilon - \epsilon d_0)(\cdot,t)\|_s \leqslant K\epsilon^3,$$

for $t \in [0,T_*]$, hold with K a constant independent of ϵ.

D. The Maxwell equations

Finally, we consider the ABI system (2.6) with initial data of the form

$$\tau(x,0) = 1 + O(\epsilon^2), \quad v(x,0) = O(\epsilon^2), \quad b(x,0) = O(\epsilon), \quad d(x,0) = O(\epsilon)$$

with $\epsilon \ll 1$. This is the low field regime considered in Ref. 2. As in the preceding subsections, we take

$$L_\epsilon = \operatorname{diag}(1, \epsilon^2 I_3, \epsilon I_3, \epsilon I_3)$$

in Theorem 5.1. This L_ϵ is bounded for $\epsilon \ll 1$, invertible for $\epsilon \neq 0$ and $|L_\epsilon^{-1}| = \epsilon^{-2}$. Then the rescaled system (5.4) reads

$$\begin{aligned}
&\tau_t + \epsilon^2 v \cdot \nabla \tau - \epsilon^2 \tau \operatorname{div} v = 0,\\
&v_t + \epsilon^2 v \cdot \nabla v - b \cdot \nabla b - d \cdot \nabla d - \epsilon^{-2}\tau \nabla \tau = 0,\\
&b_t + \epsilon^2 v \cdot \nabla b - \epsilon^2 b \cdot \nabla v + \tau \nabla \times d = 0,\\
&d_t + \epsilon^2 v \cdot \nabla d - \epsilon^2 d \cdot \nabla v - \tau \nabla \times b = 0.
\end{aligned} \tag{6.9}$$

In order to apply Theorem 5.1 to this case, we seek an approximate solution W_ϵ of the form

$$W_\epsilon = L_\epsilon U_\epsilon, \quad U_\epsilon = (1 + \epsilon^2 \tau_1, v_0, b_0, d_0).$$

Plugging this ansatz into (6.9), we see that (v_0, b_0, d_0) solves

$$\begin{aligned}
&v_t - b \cdot \nabla b - d \cdot \nabla d - \nabla \tau_1 = 0,\\
&b_t + \nabla \times d = 0,\\
&d_t - \nabla \times b = 0
\end{aligned} \tag{6.10}$$

and τ_1 satisfies

$$\tau_t - \operatorname{div} v_0 = 0. \tag{6.11}$$

Having (6.10) and (6.11), we determine U_ϵ as follows. By solving the last two lines in (6.10) (the standard linear Maxwell equations), we obtain b_0 and d_0. Then v_0 and τ_1 solve the inhomogeneous linear hyperbolic system

$$v_t - \nabla \tau = b_0 \cdot \nabla b_0 + d_0 \cdot \nabla d_0,$$

$$\tau_t - \operatorname{div} v = 0.$$

Note that here solved are only hyperbolic systems of linear equations with constant coefficients.

Assume $(b_0, d_0, v_0, \tau_1)(\cdot, 0) \in H^s$. It is easy to see that $W_\epsilon \in C([0,\infty), H^{s-1})$ and the residual R satisfies

$$R = \epsilon^3 \operatorname{diag}(\epsilon, \epsilon I_3, I_3, I_3) O(1) \in C([0,\infty), H^{s-2}).$$

Thus $\|R(\cdot,t)\|_{s-2} = \epsilon^3 O(1)$. In conclusion, from Theorem 5.1 and Corollary 1 of Theorem 2.2 in Ref. 13 we have the following.

Corollary 6.4: Let $s \geqslant 3$ be an integer. Assume $W_{0\epsilon} = W_\epsilon(\cdot, 0) \in H^{s+2}$. Then for any $T > 0$ there is $\epsilon_0 > 0$ such that, for each $\epsilon \in (0, \epsilon_0]$, the ABI system (2.6) with initial data $W_{0\epsilon}$ has a unique classical solution

$$W^\epsilon = (\tau^\epsilon, v^\epsilon, b^\epsilon, d^\epsilon) \in C([0,T], H^{s+2}).$$

Moreover, the error estimates

$$\|(\tau^\epsilon - 1 - \epsilon^2 \tau_1, v^\epsilon - \epsilon^2 v_0, b^\epsilon - \epsilon b_0, d^\epsilon - \epsilon d_0)(\cdot, t)\|_s \leqslant K \epsilon^3,$$

for $t \in [0,T]$, hold with K a constant independent of ϵ but dependent on T.

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APPENDIX: A CONTINUATION PRINCIPLE FOR SINGULAR LIMIT PROBLEMS

For the convenience of the reader, we present in this appendix the convergence-stability lemma previously formulated (Yong thanks Heinrich Freistühler and Denis Serre for pointing out two errors in an earlier version of this formulation. Thanks also go to Ya-Guang Wang for valuable discussions which improve the presentation) by Yong in Ref. 17 for IVPs of quasilinear symmetrizable hyperbolic systems depending (singularly) on parameters

$$U_t + \sum_{j=1}^{d} A_j(U, \epsilon) U_{x_j} = Q(U, \epsilon) \tag{A.1}$$

for $x \in \Omega = \mathbb{R}^d$ or $\mathbb{T}^d$ (the d-dimensional torus). Here ϵ represents a parameter in a *topological space*, $A_j(U,\epsilon)(j = 1, 2, \ldots, d)$ and $Q(U,\epsilon)$ are (matrix- or vector-valued) smooth functions of $U \in G \subset \mathbb{R}^n$ (state space) for each ϵ (possible) different from a certain singular point, say 0.

For each fixed $\epsilon (\neq 0)$, consider the IVP of (A.1) with initial data $\bar{U}(x,\epsilon)$. Assume $\bar{U}(x,\epsilon) \in G_0 \subset\subset G$ for all $x \in \Omega$ and $\bar{U}(\cdot,\epsilon) \in H^s$ with $s > d/2 + 1$ an integer. Let G_1 be a subset of the state space and satisfy $G_0 \subset\subset G_1$ [see (A.3) below]. According to the local-in-time existence theory for IVPs of symmetrizable hyperbolic systems (see Theorem 2.1 in Ref. 13), there exists $T > 0$ so that (A.1) with initial data $\bar{U}(x,\epsilon)$ has a unique classical solution,

$$U^\epsilon \in C([0,T], H^s) \quad \text{and } U^\epsilon(x,t) \in G_1 \ \ \forall\, (x,t) \in \Omega \times [0,T].$$

Define

$$T_\epsilon = \sup\{T > 0 : U^\epsilon \in C([0,T], H^s) \quad \text{and } U^\epsilon(x,t) \in G_1 \ \ \forall\, (x,t) \in \Omega \times [0,T]\}. \tag{A.2}$$

Namely, $[0, T_\epsilon)$ is the maximal time interval for the existence of H^s-solutions with values in G_1. Note that $T_\epsilon = T_\epsilon(G_1)$ depends on G_1 and may tend to zero as ϵ approaches to the singular point 0.

In order to show that $\underline{\lim}_{\epsilon \to 0} T_\epsilon > 0$, we make the following assumption.

Convergence assumption: there exists $T_* > 0$ and $U_\epsilon = U_\epsilon(x,t)$ defined for $(x,t) \in \Omega \times [0, T_*]$ and $\epsilon (\neq 0)$, satisfying

$$\bigcup_{x,t,\epsilon} \{U_\epsilon(x,t)\} \subset\subset G, \quad U_\epsilon(\cdot,t) \in H^s, \quad \text{and } \sup_{t,\epsilon} \|U_\epsilon(\cdot,t)\|_s < \infty,$$

such that for $t \in [0, \min\{T_*, T_\epsilon\})$,

$$\sup_{x,t} |U^\epsilon(x,t) - U_\epsilon(x,t)| = o(1),$$

$$\sup_{t} \|U^\epsilon(\cdot,t) - U_\epsilon(\cdot,t)\|_s = O(1),$$

as ϵ goes to the singular point.

Under this assumption, we slightly modify the argument in Ref. 16 to prove the following.

Lemma 6.5: Suppose $\overline{U}(x,\epsilon) \in G_0 \subset\subset G$ *for all* $x \in \Omega$ *and* $\epsilon (\neq 0)$, $\overline{U}(\cdot,\epsilon) \in H^s$ *with* $s > d/2 + 1$ *an integer, and the convergence assumption holds. Then, for each* G_1 *satisfying*

$$G_0 \cup \bigcup_{x,t,\epsilon} \{U_\epsilon(x,t)\} \subset\subset G_1 \subset G, \tag{A.3}$$

there is a neighborhood of the singular point such that

$$T_\epsilon(G_1) > T_*$$

for all ϵ *in the neighborhood.*

Proof: Otherwise, there is a G_1 satisfying (A.3) and a sequence $\{\epsilon_k\}_{k \geq 1}$ such that $\lim_{k \to \infty} \epsilon_k = 0$ and $T_{\epsilon_k} = T_{\epsilon_k}(G_1) \leq T_*$. Thanks to (A.3) and the convergence assumption, there exists $\widetilde{G}$, satisfying $\cup_{x,t,\epsilon} \{U_\epsilon(x,t)\} \subset\subset \widetilde{G} \subset\subset G_1$, and a certain k such that $U^{\epsilon_k}(x,t) \in \widetilde{G}$ for all $(x,t) \in \Omega \times [0, T_{\epsilon_k})$. On the other hand, we deduce from

$$\|U^\epsilon(\cdot,t)\|_s \leq \|U^\epsilon(\cdot,t) - U_\epsilon(\cdot,t)\|_s + \|U_\epsilon(\cdot,t)\|_s$$

and the convergence assumption that $\|U^{\epsilon_k}(\cdot,t)\|_s$ is bounded uniformly with respect to $t \in [0, T_{\epsilon_k})$. Now we could apply Theorem 2.1 in Ref. 13, beginning at a time t less than T_{ϵ_k} (k is fixed here), to continue the solution beyond $T_{\epsilon_k}(G_1)$. This contradicts the definition of $T_{\epsilon_k}(G_1)$ in (A.2) and, hence, the proof is complete. □

To our knowledge, such a sharp continuation principle has not appeared explicitly in the published literature other than Ref. 17. Thanks to this lemma, the study of the singular limit problems is reduced to find a $U_\epsilon(x,t)$ such that the convergence assumption holds. In verifying the two error estimates in the convergence assumption, we often take G_1 satisfying $G_1 \subset\subset G$ and being convex. Furthermore, we notice that, in the time interval $[0, \min\{T_*, T_\epsilon\})$, both U^ϵ and U_ϵ are regular and take values in the precompact subset G_1.

Remark: Similar lemmas can be easily formulated for other evolution differential equations. In fact, such a lemma can be regarded as a part of the local-in-time existence theory of any evolution equations.

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Asymptotics of regulated field commutators for Einstein-Rosen waves

J. Fernando Barbero G.[a] and Guillermo A. Mena Marugán[b]
Instituto de Estructura de la Materia, Centro de Física Miguel A. Catalán, C.S.I.C., Serrano 121, 28006 Madrid, Spain

Eduardo J. S. Villaseñor[c]
Departamento de Matemáticas, Escuela Politécnica Superior, Universidad Carlos III de Madrid, Avda. de la Universidad 30, 28911 Leganés, Spain

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We discuss the asymptotic behavior of regulated field commutators for linearly polarized, cylindrically symmetric gravitational waves and the mathematical techniques needed for this analysis. We concentrate our attention on the effects brought about by the introduction of a physical cutoff in the study of the microcausality of the model and describe how the different physically relevant regimes are affected by its presence. Specifically we discuss how genuine quantum gravity effects can be disentangled from those originating in the introduction of a regulator. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1864251]

I. INTRODUCTION

Linearly polarized cylindrical waves, also known as Einstein-Rosen waves,[1,2] provide a symmetry reduction of general relativity that can be used as a test bed for the quantization of the theory. This system displays several interesting features that contribute to its relevance. On one hand, it has an infinite number of local degrees of freedom and, hence, it is a genuine quantum field theory (in contradistinction to other symmetry reductions, such as Bianchi models, that have a finite number of global degrees of freedom). On the other, the system is tractable both classically and quantum mechanically, thus allowing us to derive exact consequences independent of any approximation scheme.[3–8] The main reason behind this success and tractability is the fact that the gravitational degrees of freedom of the model are encoded in a free, massless, axially symmetric, scalar field that evolves in an auxiliary Minkowskian background.

In previous papers we have analyzed the issue of microcausality in this system; in particular, we have studied in detail the smearing of light cones owing to the quantization of the gravitational field.[7,8] The main tool for this type of analysis is the study *in vacuo* of the field commutator evaluated at different space–time points. As is well known, the commutator of quantum fields reflects the causal structure of space–time (Minkowskian space–time in ordinary perturbative quantum field theory) in the sense that the quantum fields in spatially separated space–time points commute. This is true for all standard types of quantum fields, i.e., scalar, fermion, or vector fields, though issues related to gauge invariance must be carefully considered in this last case. In the specific model that we are interested in, gauge invariance has been discussed in Ref. 9. The authors of that paper conclude that it is correct to use the Ashtekar-Pierri gauge fixed action, written in terms of the axially symmetric scalar field, to derive gauge invariant information about the model.

[a]Electronic mail: fbarbero@iem.cfmac.csic.es
[b]Electronic mail: mena@iem.cfmac.csic.es
[c]Electronic mail: ejsanche@math.uc3m.es

In a recent work[8] we discussed the situation when no cutoff is introduced in the system, studying the unregulated commutator. The main results reached were the following. First, one can clearly see that light cones are smeared by quantum gravity effects; in fact it is possible to obtain a quantitative measure of this smearing and show how sharp light cones are recovered in the limit of large distances as compared to the natural length scale of the model, the Planck length. It is also interesting to point out that the asymptotic behavior of the commutator in the different physically relevant regimes strongly depends on the causal relationship between the different space–time points involved. Second, one finds a singularity structure in the commutator that differs from that of the free theory; in particular, the field commutator for equal values of the radial coordinate R is singular. Finally, one observes that, in the case when one of the space–time points that appear in the commutator corresponds to the symmetry axis, there are quantum effects that persist for large values of the difference of the time coordinates. This effect is reminiscent of the large quantum gravity effects first discussed by Ashtekar.[4,6,10,11]

The purpose of this paper is to study how the conclusions of Ref. 8 are changed by the introduction of a cutoff. As is well known, regulators are generally necessary in order to have well-defined quantum field theories. One can justify its use, for example, by noticing that the action of the field operator on the vacuum in a Fock space is not a vector in the Hilbert space because it has infinite norm. In order to have a well-defined action of the field operator one regulates it by introducing smearing functions that render the norms of these states finite. The problem then consists in removing these regulators (or rather showing that the physical results are independent of them).

In principle, it is possible to argue that the results derived in the absence of regulators somehow approximate those derived after their introduction; this is straightforward to see in the case of cutoffs. In the presence of a cutoff Λ, the improper integrals that define the field commutator become proper because the integration region is a closed interval $[0,\Lambda]$. For a given value of the parameters that appear in the integral (involving the values of the space–time coordinates of the quantum fields and the gravitational constant) it is always possible to choose a value for Λ such that the integral with the cutoff is well approximated by the integral extended to $[0,\infty)$.

Of course it is conceivable that the cutoff is not just a mathematical device but rather a physical scale defining a fundamental limit for the resolution of our measurements. If space–time becomes discrete at short distances (such as the Planck length), the continuum space–time picture breaks down and, certainly, it would be difficult to justify the extension of the integrals involved in the definition of field commutators (or S matrix elements, for that matter) to infinite intervals in momenta (inverse length). Our point of view here is that the introduction of a cutoff can mimic some of the effects appearing after a successful quantization of gravity (for example, in the loop quantum gravity approach), and hence we plan to study its effect within the consistent framework provided by the Einstein-Rosen waves. It is also interesting to point out here that the cutoff by itself can produce some of the effects expected from quantum gravity. In particular, it is possible to show that light cones are also smeared by cutoffs.[12] In our opinion this makes it necessary to study in detail how the effects of the cutoff and quantum gravity can be disentangled.

The paper is organized as follows. After this introduction, we briefly review the main results about microcausality in quantum cylindrical gravitational waves and introduce the commutators that we will discuss in the rest of the paper. We will then study the field commutators in the presence of a cutoff with the help of the asymptotic techniques already employed in Ref. 8. Here the situation is simpler because we will only have to consider integrals over closed intervals. We will discuss one by one the asymptotic behaviors in the different parameters involved. In Sec. VI we will derive a power series expansion in the gravitational constant for the commutator in the presence of a cutoff in the spirit of ordinary perturbative quantum field theory, and discuss the uniform convergence of this series under appropriate conditions on the cutoff in Sec. VII. We end the paper with a discussion of our results and our conclusions.

II. THE FIELD COMMUTATOR

Einstein-Rosen waves describe topologically trivial space–times with two linearly independent, commuting, spacelike, and hypersurface orthogonal Killing vector fields[1,2,13] endowed with a metric that can be written as

$$ds^2 = e^{\gamma-\psi}(-dT^2 + dR^2) + e^{-\psi}R^2 d\theta^2 + e^{\psi}dZ^2. \tag{1}$$

Here we use the coordinates (T,R,θ,Z), $T\in\mathbb{R}$, $R\in[0,\infty)$, $\theta\in[0,2\pi)$, $Z\in\mathbb{R}$, and ψ and γ are functions only of R and T. The Einstein field equations are very simple. The scalar field ψ satisfies the wave equation for a massless, axially symmetric scalar field in three dimensions,

$$\partial_T^2\psi - \partial_R^2\psi - \frac{1}{R}\partial_R\psi = 0,$$

and the function γ can be expressed in terms of this field[3,6] as

$$\gamma(R) = \frac{1}{2}\int_0^R d\overline{RR}[(\partial_T\psi)^2 + (\partial_{\overline{R}}\psi)^2].$$

We will use in the following a system of units such that $c=\hbar=1$ and define $G\equiv\hbar G_3$, where G_3 denotes the gravitational constant per unit length in the direction of the symmetry axis.[14] The function $\gamma(R)$ (apart from a factor of $8G$) has a simple physical interpretation: it is the energy of the scalar field in a ball of radius R whereas γ_∞ denotes $\lim_{R\to\infty}\gamma(R)$ (the energy of the whole two-dimensional flat space). It is also possible to show[3,7] that $\gamma_\infty/(8G)$ coincides with the Hamiltonian H_0 of the system obtained by a linearization of the metric (1).

In order to have a unit asymptotic timelike Killing vector and a physical notion of energy (per unit length) we introduce the coordinates (t,R,θ,Z) defined by $T=e^{-\gamma_\infty/2}t$. In these coordinates the metric takes the form[2,13]

$$ds^2 = e^{\gamma-\psi}(-e^{-\gamma_\infty}dt^2 + dR^2) + e^{-\psi}R^2 d\theta^2 + e^{\psi}dZ^2.$$

By taking a sufficiently fast fall-off for ψ as $R\to\infty$, this metric describes asymptotically flat cylindrical space–times such that ∂_t is a unit timelike Killing vector in the asymptotic region. In the $2+1$-dimensional framework these space–times are asymptotically flat at spacelike and null infinities[15,16] (the appropriate introduction of null infinity will be needed in order to study the S matrix of the model). It is also worthwhile noting that these space–times have a nonzero deficit angle.

The Einstein field equations can be obtained from a Hamiltonian action principle.[13,17,18] A remarkable (and useful) feature of the physical Hamiltonian H (associated with the physical time t) is the fact that it is a function of the Hamiltonian corresponding to the free scalar field, H_0:

$$H = E(H_0) = \frac{1}{4G}(1 - e^{-4GH_0}).$$

In terms of the T-time and imposing regularity at the axis $R=0$[3], the classical solutions for the field ψ can be written as

$$\psi(R,T) = \sqrt{4G}\int_0^\infty dk J_0(Rk)[A(k)e^{-ikT} + A^\dagger(k)e^{ikT}],$$

where $A(k)$ and its complex conjugate $A^\dagger(k)$ are fixed by the initial conditions. The free Hamiltonian H_0 can be written now as

$$\frac{\gamma_\infty}{8G} = H_0 = \int_0^\infty dk k A^\dagger(k) A(k).$$

Using this expression, we obtain the t-evolution of the field

$$\psi_E(R,t) = \sqrt{4G}\int_0^\infty dk J_0(Rk)[A(k)e^{-ikte^{-\gamma_\infty/2}} + A^\dagger(k)e^{ikte^{-\gamma_\infty/2}}].$$

The quantization can be carried out in the usual way by introducing a Fock space where $\hat{\psi}(R,0)$, the quantum counterpart of $\psi(R,0)$, is the operator-valued distribution[19] given by[20]

$$\hat{\psi}(R,0;\Lambda=\infty) = \hat{\psi}_E(R,0;\Lambda=\infty) = \sqrt{4G}\int_0^\infty dk J_0(Rk)[\hat{A}(k) + \hat{A}^\dagger(k)]. \tag{2}$$

Its action on Fock space is determined by those of $\hat{A}(k)$ and $\hat{A}^\dagger(k)$, the annihilation and creation operators, with nonvanishing commutators given by $[\hat{A}(k_1),\hat{A}^\dagger(k_2)] = \delta(k_1,k_2)$.

We can regulate the field by introducing suitable functions $g(k)$ that render finite the norms of the states obtained by acting with the quantum field on Fock space vectors. In the following we will make the simplest choice $g(k) = \chi_{[0,\Lambda_k]}(k)$ (here $\chi_{[a,b]}$ denotes the characteristic function of the interval $[a,b]$). By doing this the integration region in (2) becomes compact and we have

$$\hat{\psi}(R,0) = \hat{\psi}_E(R,0) = \sqrt{4G}\int_0^{\Lambda_k} dk J_0(Rk)[\hat{A}(k) + \hat{A}^\dagger(k)]. \tag{3}$$

Evolution in T is given by the unitary operator $\hat{U}_0(T) = \exp(-iT\hat{H}_0)$, where

$$\hat{H}_0 = \int_0^\infty dk k \hat{A}^\dagger(k)\hat{A}(k)$$

is the quantum Hamiltonian operator of a three-dimensional, axially symmetric scalar field. The cutoff-regulated quantum scalar field in the Heisenberg picture is hence given by

$$\hat{\psi}(R,T) = \hat{U}_0^\dagger(T)\hat{\psi}(R,0)\hat{U}_0(T) = \sqrt{4G}\int_0^{\Lambda_k} dk J_0(Rk)[\hat{A}(k)e^{-ikT} + \hat{A}^\dagger(k)e^{ikT}].$$

If we describe the evolution in our model in terms of the physical time t, the quantum Hamiltonian is $\hat{H} = E(\hat{H}_0) = (1-e^{-4G\hat{H}_0})/(4G)$ and unitary evolution is given by $\hat{U}(t) = \exp(-it\hat{H})$. With this time evolution the annihilation and creation operators in the Heisenberg picture are

$$\hat{A}_E(k,t) \equiv \hat{U}^\dagger(t)\hat{A}(k)\hat{U}(t) = \exp[-itE(k)e^{-4G\hat{H}_0}]\hat{A}(k),$$

$$\hat{A}_E^\dagger(k,t) = \hat{A}^\dagger(k)\exp[itE(k)e^{-4G\hat{H}_0}],$$

where $E(k) = (1-e^{-4Gk})/(4G)$, and the regulated field operator evolved with the physical Hamiltonian [that we denote as $\hat{\psi}_E(R,t)$] is given by

$$\hat{\psi}_E(R,t) = \sqrt{4G}\int_0^{\Lambda_k} dk J_0(Rk)[\hat{A}_E(k,t) + \hat{A}_E^\dagger(k,t)].$$

The field commutator $[\hat{\psi}_E(R_1,t_1),\hat{\psi}_E(R_2,t_2)]$ can be computed from these expressions.[7] Since we are dealing with an effectively interacting theory this operator is not proportional to the identity in the Fock space basis that we are using and, hence, we have to consider its matrix elements. As in

previous work we will concentrate on the vacuum expectation value. If a cutoff Λ_k is introduced, this is given by

$$\frac{1}{8iG}\langle 0|[\hat{\psi}_E(R_1,t_1),\hat{\psi}_E(R_2,t_2)]|0\rangle = \int_0^{\Lambda_k} dk J_0(R_1k)J_0(R_2k)\sin\left[\frac{t_2-t_1}{4G}(1-e^{-4Gk})\right], \tag{4}$$

which can be seen to depend on the time coordinates only through their difference t_2-t_1, which we will assume in the following to be positive. Notice that it depends symmetrically on R_1 and R_2. The functional dependence in G is less trivial, a fact that requires special attention when studying the limit in which the relevant lengths and time differences are much larger than the Planck length.[8]

It is convenient to refer the dimensional parameters of these integrals to another length scale, which we choose as R_1. We hence introduce $R_2=\rho R_1$, $t_2-t_1=R_1\tau$, and $\lambda=R_1/4G$ and rewrite (4) as

$$\frac{1}{8iG}\langle 0|[\hat{\psi}_E(R_1,t_1),\hat{\psi}_E(R_2,t_2)]|0\rangle = \frac{\lambda}{R_1}\Im\left\{\int_0^{\Lambda_q} dq J_0(\lambda q)J_0(\rho\lambda q)e^{i\tau\lambda(1-e^{-q})}\right\} \tag{5}$$

after introducing the new variable $k=q/(4G)$. Here $\Im$ denotes the imaginary part and $\Lambda_q=4G\Lambda_k$.

Physically, the cutoff Λ_k (which in principle has the dimensionality of an inverse length) could be interpreted as having its origin in the existence of a minimum length. This comes out naturally in loop quantum gravity where space is discrete and the area and volume operators have minimum eigenvalues of the order of the Planck area and volume, respectively. In fact, the existence of a minimum length (of the size of the Planck scale) can be considered a generic feature of essentially every quantum theory.[21] The interpretation of the adimensional cutoff Λ_q would follow from that of Λ_k, so it may be reasonable to expect that it be a number of order unity; nevertheless we will treat it as a free parameter in the following.

III. ASYMPTOTIC BEHAVIOR IN ρ

Let us start by considering the behavior of (5) when the parameter ρ grows to infinite or approaches $\rho=0$. This integral can be written as a standard h-transform[22] by the change of variables $t=q\lambda$. The most convenient way to get its asymptotic behavior in $\rho\to\infty$ is by rewriting it in the form

$$\frac{1}{R_1}\Im\left[\int_0^{\infty} dt J_0(\rho t)J_0(t)e^{i\tau\lambda(1-e^{-t/\lambda})} - \int_{R_1\Lambda_k}^{\infty} dt J_0(\rho t)J_0(t)e^{i\tau\lambda(1-e^{-t/\lambda})}\right]. \tag{6}$$

One can then use the asymptotic behavior obtained for the first integral in Ref. 8, and find the asymptotics of the second integral by standard integration by parts [employing the fact that[23] $J_0(k)=-J_0'(k)/k-J_0''(k)$]. By doing this one gets the following two contributions:

$$\frac{1}{R_1}\left[\frac{\tau}{2\lambda\rho^3}+\frac{1}{\rho^5}\left(\frac{9\tau}{8\lambda}-\frac{3\tau}{8\lambda^3}+\frac{9\tau^2}{2\lambda}\right)\right]+O\left(\frac{1}{\rho^7}\right),$$

$$\frac{1}{\rho R_1}\Im[J_1(\Lambda_k R_1\rho)J_0(\Lambda_k R_1)e^{i\tau\lambda(1-e^{-\Lambda_k R_1/\lambda})}]+O\left(\frac{1}{\rho^{5/2}}\right).$$

The first one is cutoff independent but subdominant with respect to the second, hence we see that the presence of a cutoff changes the asymptotic behavior in ρ. This is the kind of behavior that one would expect even in a Lorentz covariant theory after the introduction of a cutoff because of the breaking of the Lorentz symmetry. The novel feature here is the presence of cutoff independent terms. Although the cutoff-dependent one dominates in the asymptotic limit, there may be a transient regime, whose onset will be controlled by the value of Λ_k, in which the asymptotic behavior is given by the first term. This will be most evident when $\Lambda_k\to\infty$.

In the $\rho \to 0$ limit we get

$$\frac{1}{R_1}\Im\int_0^{R_1\Lambda_k} dt J_0(t) e^{i\tau\lambda(1-e^{-t/\lambda})} + O(\rho) = \frac{\lambda}{R_1}\Im\int_0^{\Lambda_q} dq J_0(\lambda q) e^{i\tau\lambda(1-e^{-q})} + O(\rho), \tag{7}$$

as a result of the continuity at $\rho=0$ of the integral defining the commutator (5).

IV. ASYMPTOTIC BEHAVIOR IN τ

The integral in (5) has the convenient form of an *h*-transform and, hence, it can be studied by standard Mellin transform methods[22] if the asymptotic parameter is chosen to be ρ; however, this is no longer true if the asymptotic parameter is taken to be τ (which corresponds to considering large separations in the time coordinates). This fact introduces some mathematical difficulties in the asymptotic analysis. In this case one has to consider the cases $\rho=0$ and $\rho\neq 0$ separately.

If $\rho=0$, one finds that the asymptotic behavior when $\tau\to\infty$ without the cutoff is given by[8]

$$\frac{1}{R_1}\sqrt{\frac{\lambda}{2\pi\log\tau}}\Im\{e^{i[(\pi/4)+\tau\lambda-\lambda\log(\tau\lambda)]}e^{(\pi/2)\lambda}\Gamma(i\lambda) + e^{-i[(\pi/4)-\tau\lambda-\lambda\log(\tau\lambda)]}e^{-(\pi/2)\lambda}\Gamma(-i\lambda)\} + O\left(\frac{1}{\log\tau}\right), \tag{8}$$

whereas for $\rho\neq 0$ we get

$$\begin{aligned}
&\frac{1}{2\pi R_1\sqrt{\rho}\log\tau}\Im\{e^{i[(\pi/2)+\tau\lambda-\lambda(1+\rho)\log(\tau\lambda)]}e^{(\pi/2)\lambda(1+\rho)}\Gamma[i\lambda(1+\rho)]\\
&+ e^{-i[(\pi/2)-\tau\lambda-\lambda(1+\rho)\log(\tau\lambda)]}e^{-(\pi/2)\lambda(1+\rho)}\Gamma[-i\lambda(1+\rho)]\\
&+ e^{i[\tau\lambda-\lambda(1-\rho)\log(\tau\lambda)]}e^{(\pi/2)\lambda(1-\rho)}\Gamma[i\lambda(1-\rho)]\\
&+ e^{i[\tau\lambda-\lambda(\rho-1)\log(\tau\lambda)]}e^{(\pi/2)\lambda(\rho-1)}\Gamma[i\lambda(\rho-1)]\} + O\left(\frac{1}{(\log\tau)^2}\right).
\end{aligned} \tag{9}$$

The most interesting feature of these expressions is their unusual dependence on the asymptotic parameter τ; in fact, the dependence on inverse powers of logarithms (especially on the inverse square root of $\log\tau$) cannot be obtained by direct application of the usual asymptotic expressions derived by Mellin transform techniques.[8] It is also remarkable how slowly the commutator decays in τ, in particular in the axis $\rho=0$, a fact that is suggestive of the large quantum gravity effects discussed by Ashtekar.[4] Outside the axis the decay is faster but still quite slow. A consequence of the different asymptotic behaviors in τ for $\rho=0$ and $\rho\neq 0$ is the impossibility to recover (8) as the limit when $\rho\to 0$ of (9). As we can see, the frequency of the oscillations of the commutator in τ is controlled by λ (proportional to the inverse of G) in such a way that although the amplitude of the oscillations decays very slowly, they will average to zero on scales larger than the Planck length.

When we introduce a cutoff Λ_k, the above asymptotic expressions change to

$$\frac{1}{R_1}\Im\left\{\frac{i}{\tau}[1-e^{i\tau\lambda(1-e^{-\Lambda_k R_1/\lambda})}e^{\Lambda_k R_1/\lambda}J_0(\Lambda_k R_1)J_0(\rho\Lambda_k R_1)]\right\} + O\left(\frac{1}{\tau^2}\right), \tag{10}$$

valid both for $\rho=0$ and $\rho\neq 0$. This can be obtained by straightforward integration by parts. An interesting situation develops at this point because the asymptotic behavior of the integral in τ behaves in a discontinuous way in the cutoff. In the analysis carried out to study the asymptotic behavior in ρ we found out that the cutoff-dependent term, in spite of being dominant, goes to zero in the limit $\Lambda_k\to\infty$. Here the situation is different: taking now $\Lambda_k\to\infty$ in (10) does not lead to the asymptotic expressions corresponding to $\Lambda_k=\infty$. That is, the asymptotic behavior of the improper integral in (4) is not the limit when $\Lambda_k\to\infty$ of (5). As in the case of the asymptotics in ρ, one expects that there must be a transient regime in which the behavior in τ of (5) is given by (8) and

(9). We will not consider here a precise characterization of this transient behavior for arbitrary values of the relevant parameters because its main properties can be conveniently discussed, at least for large λ, by looking at the $\lambda\to\infty$ asymptotics of the commutator in the (ρ,τ) plane.

The $\tau\to 0$ limit is easy to analyze. In fact what we find, both with and without the cutoff, is that the series obtained by expanding $e^{i\pi\lambda(1-e^{-t/\lambda})}$ in powers of $e^{-t/\lambda}$, exchanging integration and infinite sum, and computing the resulting integrals gives a series that converges to the value of the commutator.

V. ASYMPTOTIC BEHAVIOR IN λ

The asymptotic behavior in λ is studied by following the procedure described in Ref. 8. It is worth remarking that the limit $\lambda\to\infty$ of the regulated field commutator cannot be identified with that in which the gravitational constant G vanishes if one admits that the dimensionful cutoff $\Lambda_k<\infty$ is kept constant in principle. On the contrary, the two limits could be considered equivalent only under the assumption that Λ_k increases as the inverse of G for small gravitational constant, so that its dimensionless counterpart $\Lambda_q=4G\Lambda_k$ may remain fixed.

The analysis of the asymptotics in λ when the cutoff is present is simultaneously simpler in some respects and more complicated in others compared with the case when no cutoff is introduced. It is simpler because the lengthy analysis needed to discuss the asymptotics of the improper integral is not necessary now. It is more complicated in the sense that the final asymptotic expressions contain additional terms and also because the number of regions with different λ-asymptotic regimes in the (ρ,τ) plane increases.

We have to consider now the cases $\rho=0$ and $\rho\neq 0$ separately. Let us consider first $\rho=0$ and write the rhs of (5) as[8]

$$\Im\left\{-\frac{i\lambda e^{i\tau\lambda}}{2\pi R_1}\int_0^{\Lambda_q}dq\oint_\gamma dt\frac{1}{t}e^{\lambda[(q/2)(t-1/t)-i\tau e^{-q}]}\right\},\tag{11}$$

after using the usual integral representation for the Bessel functions J_n $(n=0,1,\ldots)$,

$$J_n(z)=\frac{1}{2\pi i}\oint_\gamma\frac{dt}{t^{n+1}}e^{(z/2)(t-1/t)},$$

where γ is a closed, positively oriented, simple path in the complex plane surrounding the origin. Notice that we are integrating an integrable function in a compact region, so we can write the integrals in any order we want. The asymptotic analysis of (11) can be carried out by following the same steps as in Ref. 8. As we did there, it is useful to introduce neutralizers to split the integral in three pieces I_j, $j=1,2,3$, and choose appropriate contours for each of them. These integrals are

$$I_j\equiv\Im\left\{-\frac{i\lambda e^{i\tau\lambda}}{2\pi R_1}\int_0^{\Lambda_q}dq\oint_\gamma dt\nu_j(q)\frac{1}{t}e^{\lambda[(q/2)(t-1/t)-i\tau e^{-q}]}\right\},$$

where we have introduced the neutralizer functions $\nu_j(q)$, $j=1,2,3$, satisfying $\nu_1+\nu_2+\nu_3=1$ in $[0,\Lambda_q]$ and

$$\nu_1(q)=1 \text{ if } q\in[0,\alpha_1],$$

$$\nu_1(q)=0 \text{ if } q\in[\alpha_2,\Lambda_q],$$

$$\nu_2(q)=0 \text{ if } q\in[0,\alpha_1]\cup[\beta_2,\Lambda_q],$$

$$\nu_2(q)=1 \text{ if } q\in[\alpha_2,\beta_1],$$

$$\nu_3(q) = 0 \text{ if } q \in [0, \beta_1],$$

$$\nu_3(q) = 1 \text{ if } q \in [\beta_2, \Lambda_q],$$

with $0 < \alpha_1 < \alpha_2 < \beta_1 < \beta_2 < \Lambda_q$ (these parameters are chosen as in Ref. 8). By doing this the effective integration regions in q are $[0, \alpha_2]$, $[\alpha_1, \beta_2]$, and $[\beta_1, \Lambda_q]$ and the boundary $q=0$ appears only in the first.

The asymptotics in λ of the integral I_1 is best obtained by choosing an integration contour satisfying $\Re(t - 1/t) \leqslant 0$ (that passes necessarily through $t=i$ and $t=-i$). By using the same method of Ref. 8 we see that the first two relevant terms are given by the contour integrals

$$\frac{1}{\pi R_1} \Im \left\{ i \oint_\gamma \frac{dt}{t^2 + 2i\pi t - 1} \right\},$$

$$- \frac{1}{2\pi R_1} \Im \left\{ \frac{i}{\lambda} \oint_\gamma dt \frac{8i\pi t^2}{(t^2 + 2i\pi t - 1)^3} \right\},$$

whose sum gives

$$\frac{1}{R_1 \sqrt{\tau^2 - 1}} \text{ for } \tau > 1$$

and

$$\frac{\pi(1 + 2\tau^2)}{2R_1 \lambda (1 - \tau^2)^{5/2}} \text{ for } \tau < 1.$$

Although the second term will be subdominant with respect to some of the contributions coming from I_2 and I_3, it improves the approximation of the full commutator obtained from the asymptotics in λ in the region $\tau < 1$.

The contribution of I_3 to the asymptotics in λ is obtained from the contour integral (corresponding to the boundary at $q = \Lambda_q$)

$$\Im \left\{ \frac{ie^{i\tau\lambda}}{2\pi R_1} \oint_\gamma dt \frac{2}{t} \frac{(t - 1/t + 2i\tau e^{-\Lambda_q}) e^{(\lambda\Lambda_q/2)(t-1/t) - i\tau e^{-\Lambda_q}}}{\Lambda_q^2 (t + 1/t)^2 - (t - 1/t + 2i\tau e^{-\Lambda_q})^2} \right\}.$$

The asymptotics in λ of this integral can be easily studied by using the method of steepest descents. This gives

$$\Im \left\{ \frac{2ie^{i\tau\lambda(1 - e^{-\Lambda_q})}}{R_1 (\tau^2 e^{-2\Lambda_q} - 1) \sqrt{2\pi\lambda\Lambda_q}} \left[i\tau e^{-\Lambda_q} \sin\left(\lambda\Lambda_q - \frac{\pi}{4} \right) - \cos\left(\lambda\Lambda_q - \frac{\pi}{4} \right) \right] \right\}.$$

Finally, the integral I_2 (for which we choose for γ the curve $|t| = 1$) only contributes when the stationary points of the exponent are in the integration region. This happens only when $1 < \tau < e^{\Lambda_q}$. The contribution to the first relevant order in λ is[8]

$$\Im \left\{ \frac{1}{R_1} \frac{e^{i\lambda(\tau - \log \tau - 1)}}{\sqrt{\log \tau}} \right\}.$$

Adding up the different terms we get

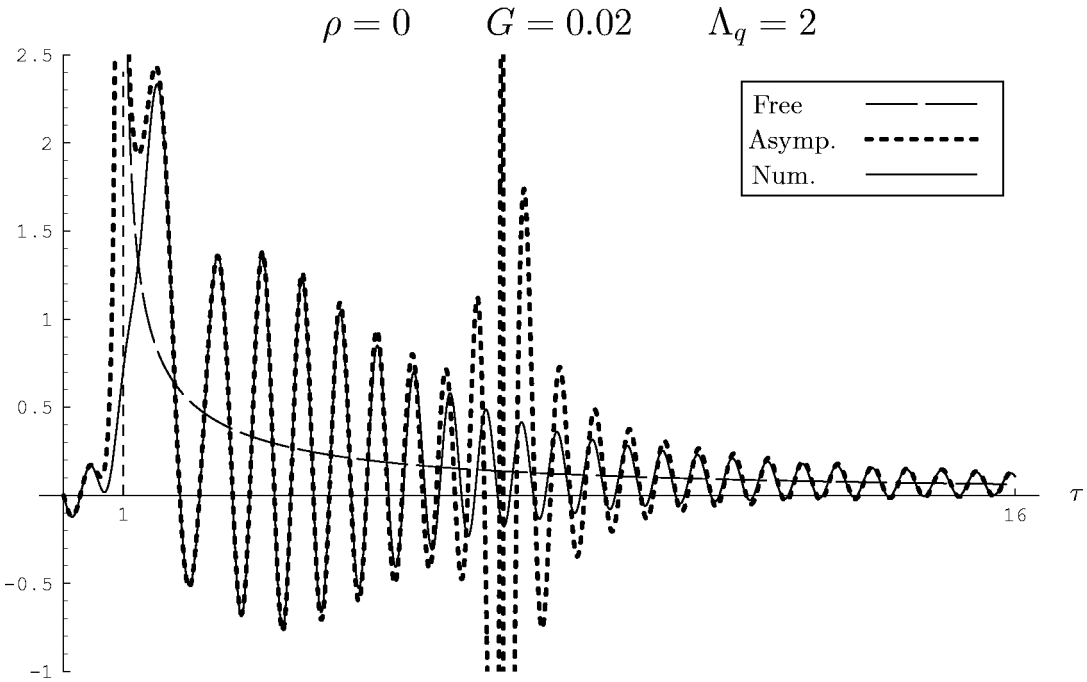

FIG. 1. Asymptotic approximation in λ for the field commutator over $8iG$ as a function of τ for $\rho=0$, $G=0.02$, and $\Lambda_q=2$. We compare it both with a numerical computation of the integral that defines it and with the unregulated free commutator. As we can see, the approximation is good except at the points where the asymptotic behavior changes ($\tau=1$ and $\tau=e^{\Lambda_q}$). Notice the difference in the amplitude of the oscillations for $\tau<e^{\Lambda_q}$ and $\tau>e^{\Lambda_q}$.

$$\theta(1-\tau)\frac{\tau(1+2\tau^2)}{2R_1\lambda(1-\tau^2)^{5/2}}+\theta(\tau-1)\frac{1}{R_1\sqrt{\tau^2-1}}+\theta(\tau-1)\,\theta(e^{\Lambda_q}-\tau)\Im\left\{\frac{1}{R_1}\frac{e^{i\lambda(\tau-\log\,\tau-1)}}{\sqrt{\log\,\tau}}\right\}$$
$$+\Im\left\{\frac{2ie^{i\tau\lambda(1-e^{-\Lambda_q})}}{R_1(\tau^2e^{-2\Lambda_q}-1)\sqrt{2\pi\lambda\Lambda_q}}\left[i\tau e^{-\Lambda_q}\sin\left(\lambda\Lambda_q-\frac{\pi}{4}\right)-\cos\left(\lambda\Lambda_q-\frac{\pi}{4}\right)\right]\right\}, \tag{12}$$

where θ denotes the step function.

We see that the final result consists of several contributions: the free commutator for an infinite cutoff, a $1/\lambda$ correction for $\tau<1$, the term with the $1/\sqrt{\log\,\tau}$ dependence for $1<\tau<e^{\Lambda_q}$, and a cutoff-dependent contribution for all values of τ that fall off to zero when $\Lambda_q\to\infty$. If the cutoff goes to infinity, the commutator can be approximated by the one obtained in Ref. 8; however, if it is of order one (as would be the case if it is defined by the Planck length), then that approximation is no longer valid. Notice that the values of $\tau\in(1,e^{\Lambda_q})$ are those for which the asymptotics provided by the unregulated commutator are a correct approximation. This is roughly the transient region in the τ parameter mentioned in the previous subsection.

Figures 1–3 show the behavior of the field commutator (over $8iG$) when $\rho=0$ as a function of τ for several values of Λ_q. As we can see, the asymptotic approximation becomes singular between regions with different asymptotic regimes, but approximates well the exact value of the commutator (obtained by numerical methods) for the remaining values of τ. Notice that the singularity at $\tau=e^{\Lambda_q}$ of the asymptotic expansion lies outside the plotted region in Figs. 2 and 3.

In order to study the $\rho\neq0$ case we start by writing the rhs of (5) as

$$\Im\left\{-\frac{\lambda e^{i\tau\lambda}}{4\pi^2R_1}\int_0^{\Lambda_q}dq\oint_{\gamma_1}dt_1\oint_{\gamma_2}dt_2\frac{1}{t_1t_2}e^{\lambda[(q)(t_1-1/t_1)/2+\rho q(t_2-1/t_2)/2-i\tau e^{-q}]}\right\} \tag{13}$$

after employing the usual integral representation for the Bessel functions J_n ($n=0,1,\ldots$). Again it is helpful to introduce the same neutralizers as above to split the integral in three pieces I_j, $j=1,2,3$.

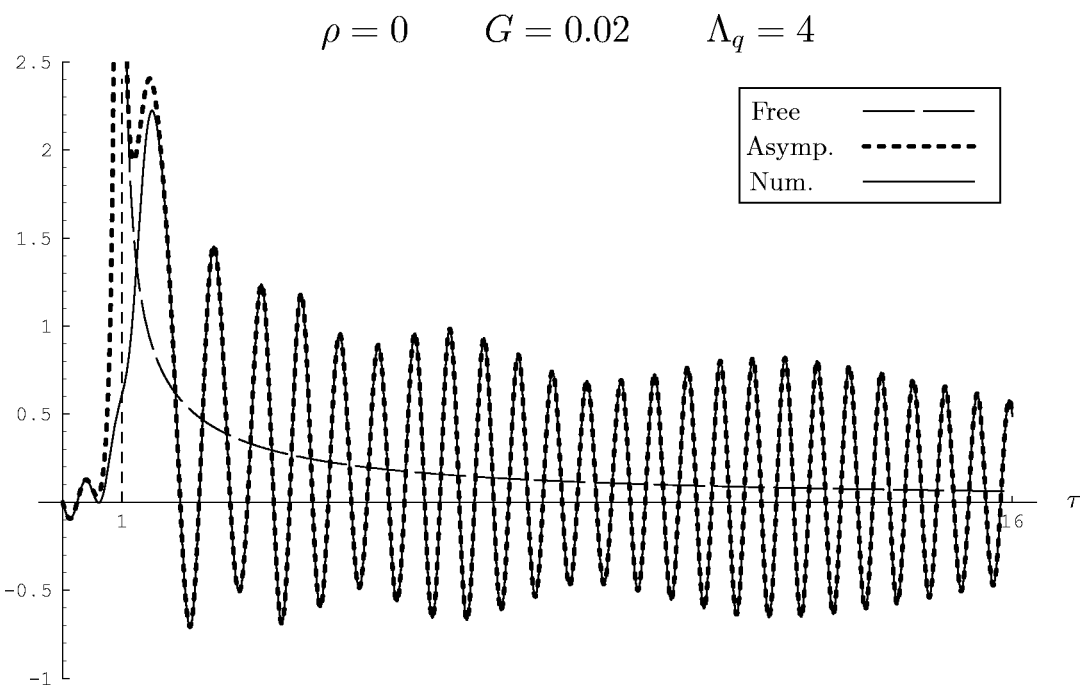

FIG. 2. Asymptotic approximation in λ for the field commutator over $8iG$ as a function of τ for $\rho=0$, $G=0.02$, and $\Lambda_q=4$ (compared both with a numerical computation of the integral that defines it and with the unregulated free commutator). As we can see, the asymptotic approximation is good except at $\tau=1$. Notice that the cutoff introduces a modulation of the amplitude in the region $1<\tau<e^{\Lambda_q}$. The singularity of the asymptotic approximation at $\tau=e^{\Lambda_q}$ lies outside the plotted region.

The integral I_1 gives the following two contributions:

$$\Im\left\{\frac{1}{2\pi^2 R_1}\oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2 \frac{1}{\rho t_1(t_2^2-1)+t_2(t_1^2+2i\pi t_1-1)}\right\} \tag{14}$$

and

$$\Im\left\{-\frac{2i\tau}{\pi^2 R_1 \lambda}\oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2 \frac{t_1^2 t_2^2}{[\rho t_1(t_2^2-1)+t_2(t_1^2+2i\pi t_1-1)]^3}\right\}. \tag{15}$$

Both integrals can be computed exactly[8] in terms of complete elliptic integrals of first and second kinds. The first one gives the contribution of the unregulated free commutator (i.e., with infinite cutoff).

In order to describe it we define regions I, II, and III by $0<\tau<|\rho-1|$, $|\rho-1|<\tau<\rho+1$, and $\rho+1<\tau$, respectively. They are shown in Fig. 4. In region I the free commutator is zero, whereas in regions II and III it is given by

region II,

$$\frac{1}{\pi R_1\sqrt{\rho}} K\left(\sqrt{\frac{\tau^2-(\rho-1)^2}{4\rho}}\right),$$

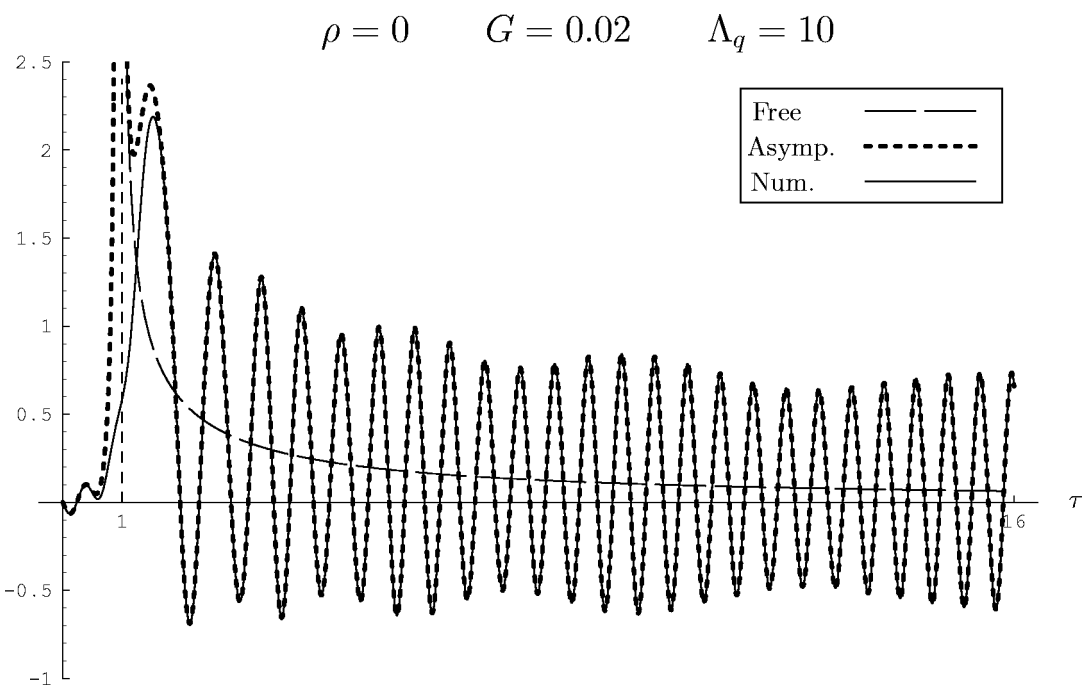

FIG. 3. Asymptotic approximation in λ for the field commutator over $8iG$ as a function of τ for $\rho=0$, $G=0.02$, and $\Lambda_q=10$ (compared both with a numerical computation of the integral that defines it and with the unregulated free commutator). As we can see, the asymptotic approximation is good except at $\tau=1$. The asymptotic approximation obtained in Ref. 8 is good in a large region in the τ axis. The singularity of the asymptotic approximation at $\tau=e^{\Lambda_q}$ lies outside the plotted region.

region III,

$$\frac{2}{\pi R_1}\frac{1}{\sqrt{\tau^2-(1-\rho)^2}}K\left(\sqrt{\frac{4\rho}{\tau^2-(1-\rho)^2}}\right).$$

The second contribution (15) can be computed by the method outlined in Appendix IV of Ref. 8, obtaining

region I,

$$\frac{\tau}{2\pi R_1\lambda}\left\{\frac{2[1+\rho^4+2\tau^2-3\tau^4+2\rho^2(\tau^2-1)]\sqrt{(1+\rho)^2-\tau^2}}{(1+\rho-\tau)^2(1-\rho+\tau)^2(-1+\rho+\tau)^2(1+\rho+\tau)^2}E\left(\sqrt{\frac{4\rho}{(1+\rho)^2-\tau^2}}\right)\right.$$
$$\left.-\frac{2\tau^2}{[\rho^4+(\tau^2-1)^2-2(1+\tau^2)\rho^2]\sqrt{(1+\rho)^2-\tau^2}}K\left(\sqrt{\frac{4\rho}{(1+\rho)^2-\tau^2}}\right)\right\}, \tag{16}$$

region II,

$$\frac{\tau}{2\pi R_1\lambda}\left\{\frac{1-2\rho^2+\rho^4+\tau^2-2\rho\tau^2+\rho^2\tau^2-2\tau^4}{\sqrt{\rho}[(1-\rho)^2-\tau^2][(1+\rho)^2-\tau^2]^2}K\left(\sqrt{\frac{(1+\rho)^2-\tau^2}{4\rho}}\right)\right.$$
$$\left.+\frac{4\sqrt{\rho}[1-2\rho^2+\rho^4+2\tau^2-3\tau^4+2\rho^2\tau^2]}{[\rho^4+(\tau^2-1)^2-2(1+\tau^2)\rho^2]^2}E\left(\sqrt{\frac{(1+\rho)^2-\tau^2}{4\rho}}\right)\right\}. \tag{17}$$

The value of (15) in region III is zero.

The integral I_3, on the other hand, can also be studied by the methods described in Ref. 8. The first relevant term to its asymptotic expansion in inverse powers of λ is derived from the double contour integral

$$\Im\left\{\frac{e^{i\tau\lambda}}{4\pi^2 R_1}\oint_{\gamma_1} dt_1 \oint_{\gamma_2} dt_2 \frac{2}{t_1 t_2}\frac{[t_1 - 1/t_1 + \rho(t_2 - 1/t_2) + 2i\tau e^{-\Lambda_q}]e^{\lambda[(\Lambda_q/2)(t_1-1/t_1)+\rho(\Lambda_q/2)(t_2-1/t_2)-i\tau e^{-\Lambda_q}]}}{\Lambda_q^2[(t_1+1/t_1)^2+\rho^2(t_2+1/t_2)^2]-[t_1-1/t_1+\rho(t_2-1/t_2)+2i\tau e^{-\Lambda_q}]^2}\right\}, \tag{18}$$

corresponding to $q=\Lambda_q$ and whose asymptotic behavior can be determined by employing standard techniques for multiple integrals.[22] In this way we obtain the following contribution:

$$\frac{1}{2\pi R_1 \Lambda_q \lambda\sqrt{\rho}}\left\{\frac{\sin[\lambda\Lambda_q(1+\rho)-\tau\lambda(1-e^{-\Lambda_q})]}{1+\rho-\tau e^{-\Lambda_q}} - \frac{\sin[\lambda\Lambda_q(1+\rho)+\tau\lambda(1-e^{-\Lambda_q})]}{1+\rho+\tau e^{-\Lambda_q}}\right.$$
$$\left. + \frac{\cos[\lambda\Lambda_q(1-\rho)-\tau\lambda(1-e^{-\Lambda_q})]}{1-\rho-\tau e^{-\Lambda_q}} - \frac{\cos[\lambda\Lambda_q(1-\rho)+\tau\lambda(1-e^{-\Lambda_q})]}{1-\rho+\tau e^{-\Lambda_q}}\right\}. \tag{19}$$

Finally, the integral I_2 is written in terms of a neutralizer that vanishes at $q=0$ and $q=\Lambda_q$. This integral is best studied by choosing the unit circumference centered in the origin of the complex plane as the integration contour γ. The contributions of this integral to the asymptotics of (13) come from the stationary points of the exponent in the integrand whenever they are within the integration region. This fact is controlled by the value of the cutoff Λ_q. The result is

$$\{\theta(\tau-\rho+1)\theta[(\rho-1)e^{\Lambda_q}-\tau]\theta(\rho-1)$$
$$+\theta(\tau+\rho-1)\theta[(1-\rho)e^{\Lambda_q}-\tau]\theta(1-\rho)\}\Im\left\{\frac{e^{-i\pi/4}e^{i\lambda[\tau+|\rho-1|(1+\log\tau/|\rho-1|)]}}{R_1\sqrt{2\pi\lambda\rho|1-\rho|}\log\tau/|1-\rho|}\right\}$$
$$+\theta(\tau-\rho-1)\theta[(\rho+1)e^{\Lambda_q}-\tau]\Im\left\{\frac{e^{i\pi/4}e^{i\lambda[\tau+(\rho+1)(\log 1+\rho/\tau-1)]}}{R_1\sqrt{2\pi\lambda\rho(1+\rho)}\log\tau/1+\rho}\right\},$$

where the step functions define the regions where the different stationary points contribute. As we can see and it is explained in Fig. 5, there are two contributions in some parts of the (ρ,τ) plane,

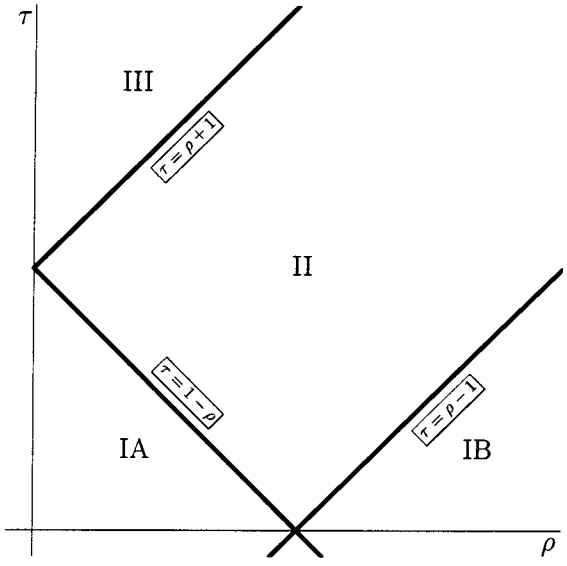

FIG. 4. Regions in the (ρ,τ) plane used in the discussion of the λ asymptotics and the free commutator. Region I is defined by $0<\tau<|\rho-1|$, region II by $|\rho-1|<\tau<\rho+1$, and region III by $\rho+1<\tau$.

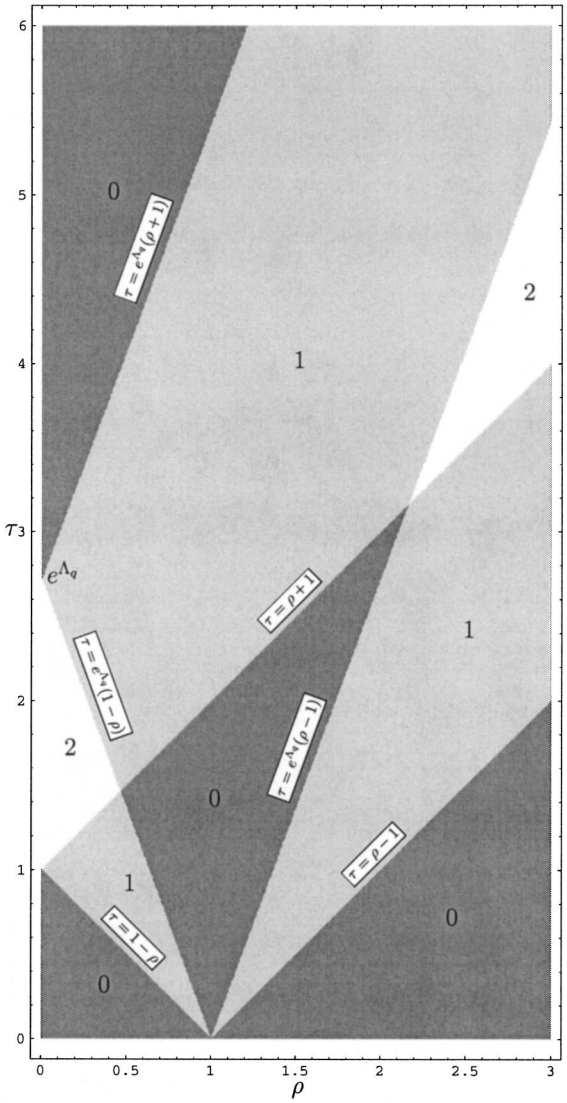

FIG. 5. Regions in the (ρ, τ) plane used in the discussion of the λ asymptotics in the presence of a cutoff $\Lambda_q = 1$. The label of each region indicates how many critical points contribute to the asymptotic expansion in λ.

only one in some other parts, and no contribution in the remaining ones. Notice that, whenever they differ from zero, these contributions are dominant with respect to those coming from the other integrals.

Several points are now in order. First it is interesting to realize that the singularity at $\rho = 1$ that exists when the cutoff is taken to be infinite (and is obviously absent now) shows up as the region defined by the lines $\tau = e^{\Lambda_q}(1-\rho)$, $\tau = e^{\Lambda_q}(\rho-1)$, and $\tau = e^{\Lambda_q}(\rho+1)$ shrinks with growing Λ_q. Another interesting feature of the commutator when the cutoff is present is the appearance of some regions where the leading asymptotic behavior is not given by the expressions obtained in Ref. 8 for infinite cutoff, namely the regions with $\tau > |1-\rho|$ labeled 0 in Fig. 5 and the region labeled 1 that connects them. On the contrary, there are two regions where two stationary points contribute to the asymptotics just as in the $\Lambda_q \to \infty$ case, showing the characteristic slow decay in the τ direction.[24] Of these two regions, the one closer to the axis is bounded, whereas the second one

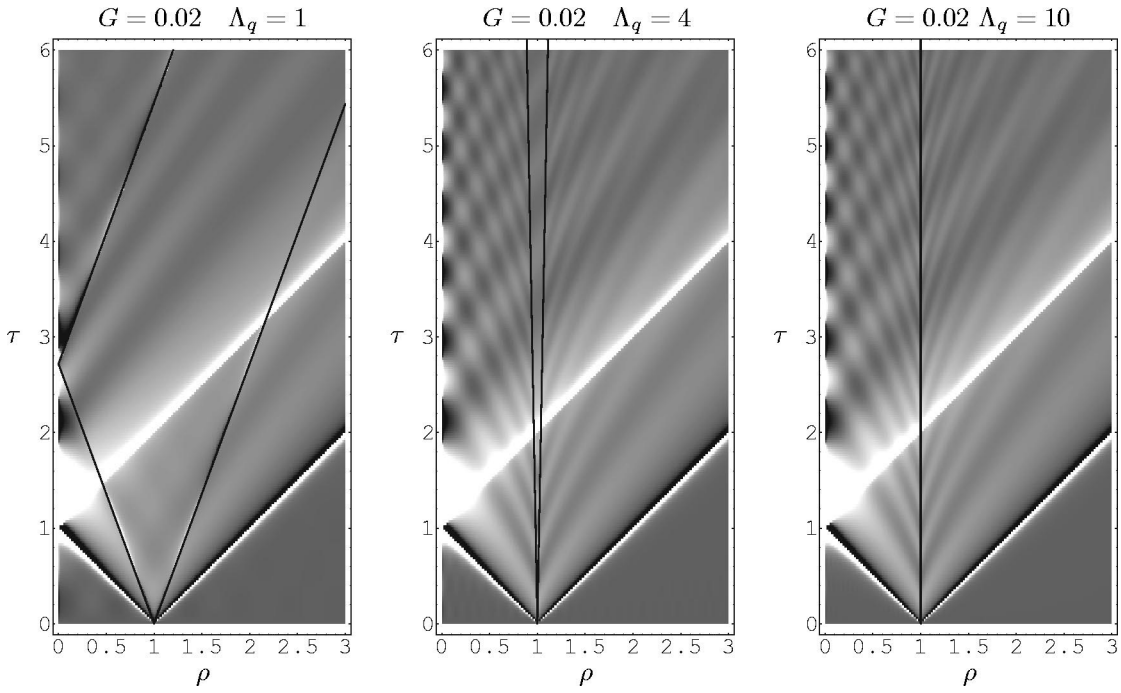

FIG. 6. Density plots of the commutator for $G=0.02$ and different values of Λ_q. Comparing the results with those of Ref. 8, we can see that the commutator in the regions labeled 2 in Fig. 4 is essentially equal to the one corresponding to an infinite cutoff. Notice also the process by which the singularity at R_1 appears.

[defined by the lines $\tau=e^{\Lambda_q}(\rho-1)$ and $\tau=\rho+1$] is not. The effect of the symmetry axis is evident in the sense that it is precisely there where one of the lines that limits the boundary of this region starts, namely $\tau=\rho+1$.

As we can see, the influence of the cutoff is important in some parts of the (ρ,τ) plane, but there are others where the asymptotic behavior is described at leading order(s) by the unregulated $\lambda\to\infty$ limit. The consideration of these different regions helps in describing the intermediate regimes where the infinite cutoff approximation is expected to work, at least for large values of λ. Finally, we want to point out that the most dramatic quantum effect observed when the cutoff is infinite, the very slow falloff of the commutator at the axis in the τ direction, is no longer present after introducing a regulator. This casts some doubts about the "observability" of large quantum gravitational fluctuations at the axis. These behaviors can be visually appreciated in Figs. 6–9.

VI. POWER EXPANSION IN *G*

In the above sections we have discussed the asymptotics of the regulated field commutator as a function of ρ, λ, and τ. These are dimensionless parameters obtained by using R_1 as a length scale. We want to discuss now the possibility of expanding this commutator as a power series in G. The main motivation to consider this issue is that one would expect to arrive at an expansion of this kind when adopting a standard perturbative approach for the treatment of the problem. As we will see, this can be done in a rather straightforward way if a cutoff is introduced in the system. However, our description breaks down when the cutoff is removed.

Let us analyze then the expansion of the vacuum expectation value of the commutator in powers of the quantum gravitational constant[25] $G=G_3\hbar$. To this end we rewrite (4) as

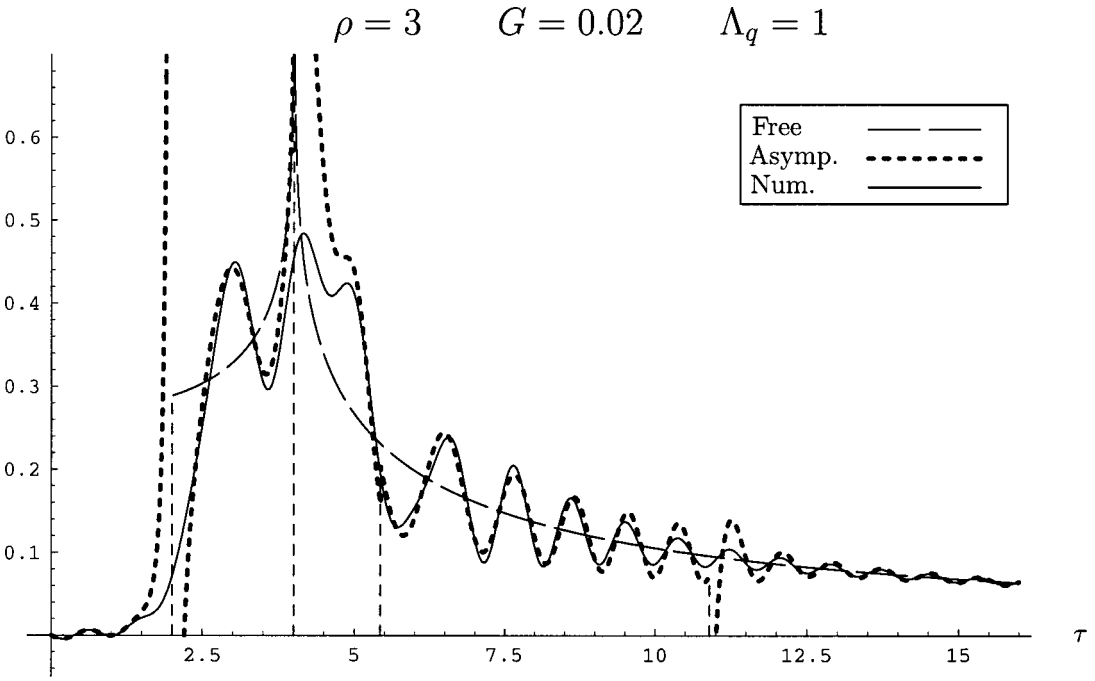

FIG. 7. Asymptotic approximation in λ for the field commutator over $8iG$ as a function of τ for $G=0.02$, $\rho=3$, and $\Lambda_q=1$ compared with a numerical approximation. The regions with different asymptotic regimes are shown. The asymptotic approximation is good except at the boundaries between these regions. The different types of behavior are also evident.

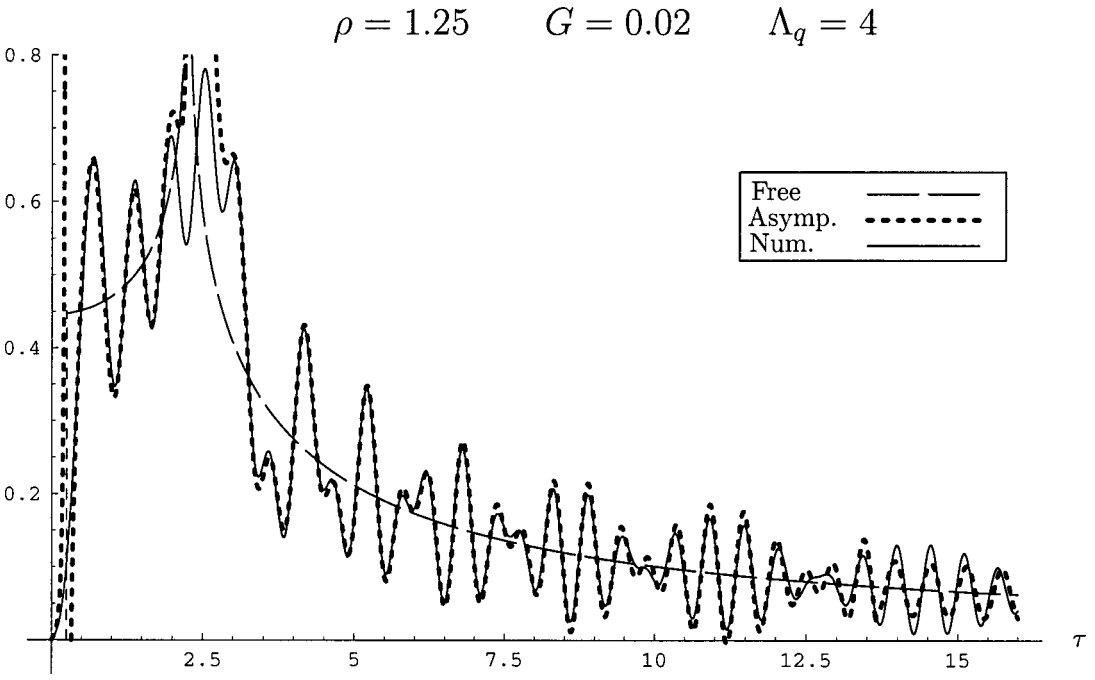

FIG. 8. Asymptotic approximation in λ for the field commutator over $8iG$ as a function of τ for $G=0.02$, $\rho=1.25$, and $\Lambda_q=4$ compared with a numerical approximation.

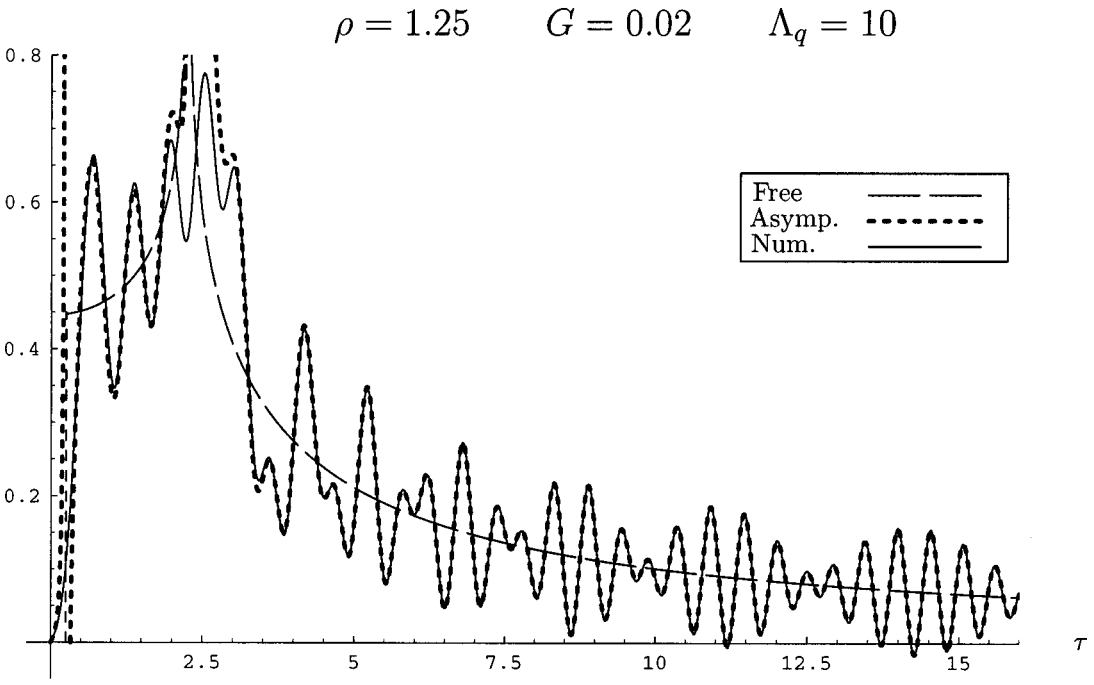

FIG. 9. Asymptotic approximation in λ for the field commutator over $8iG$ as a function of τ for $G=0.02$, $\rho=1.25$, and $\Lambda_q=10$ compared with a numerical approximation.

$$\frac{1}{8iG}\langle 0|[\hat{\psi}_E(R_1,t_1),\hat{\psi}_E(R_2,t_2)]|0\rangle = \int_0^{\Lambda_k} dk J_0(R_1k)J_0(R_2k)\sin\left[kR_1\tau\frac{(1-e^{-q})}{q}\right]. \tag{20}$$

With our conventions, both $kR_1\tau$ and $q=Gk$ are dimensionless, whereas k can be regarded to have dimensions of an inverse length. Note that all the dependence on G is contained in q, accepting that the cutoff Λ_k is fixed. Thus, in order to arrive at the desired series, we will expand the integrand in powers of the variable q. At this point, it is worth remarking that, had we described the regulated commutator by means of the dimensionless cutoff $\Lambda_q=4G\Lambda_k$ as in previous sections,[26] it would not have been possible to single out the dependence on the gravitational constant via that on q.

We will use the following formulas for the Taylor expansion of the functions involved in our expression (20) and the composition of the resulting series, assuming for the moment their convergence:

$$g(q) := \frac{1-q-e^{-q}}{q} = \sum_{n=1}^{\infty}\frac{(-q)^n}{(n+1)!}, \tag{21}$$

$$\sin(kR_1\tau+y) = \sin(kR_1\tau)\sum_{m=0}^{\infty}(-1)^m\frac{y^{2m}}{(2m)!} + \cos(kR_1\tau)\sum_{m=0}^{\infty}(-1)^m\frac{y^{2m+1}}{(2m+1)!}, \tag{22}$$

$$[g(q)]^m = \left[\sum_{n=1}^{\infty}\frac{(-q)^n}{(n+1)!}\right]^m = \sum_{p=m}^{\infty}a_p[m](-q)^p, \tag{23}$$

$$a_p[m] := \sum_{\sigma(p|m)} \prod_{i=1}^{m} \frac{1}{(n_i+1)!}, \tag{24}$$

where the range of the last sum extends to the sets of m integers n_i given by

$$\sigma(p|m) := \left\{ n_i \geqslant 1; \sum_{i=1}^{m} n_i = p \right\}. \tag{25}$$

Interchanging the sum and integration orders, one then obtains the formal series

$$\frac{1}{8iG}\langle 0|[\hat{\psi}_E(R_1,t_1),\hat{\psi}_E(R_2,t_2)]|0\rangle = \sum_{p=0}^{\infty} \int_0^{\Lambda_k} dk J_0(R_1k)J_0(R_2k)(-4Gk)^p F_p(kR_1\tau), \tag{26}$$

with

$$F_p(kR_1\tau) := \sin(kR_1\tau) \sum_{m=1}^{\mathrm{int}[p/2]} \frac{(-1)^m}{(2m)!} a_p[2m](kR_1\tau)^{2m} + \cos(kR_1\tau) \sum_{m=0}^{\mathrm{int}[(p-1)/2]} \frac{(-1)^m}{(2m+1)!} a_p[2m+1](kR_1\tau)^{2m+1}, \quad p \geqslant 1,$$

$$F_0(kR_1\tau) := \sin(kR_1\tau). \tag{27}$$

Here, the function int$[x]$ is the integer part of x, and the sum over m that multiplies the function $\sin(kR_1\tau)$ is understood to vanish when $p=1$. Note that, in the case of infinite cutoff, the first ($p=0$) term reproduces the commutator of the free-field theory. Moreover, then all the $p \geqslant 1$ additions to the free field contribution are integrals over $[0,\infty)$ of oscillating, nonbounded functions and, hence, at best conditionally convergent. So, in the unregulated theory ($\Lambda_k=\infty$), the above expansion should be taken only as a formal expression, and therefore we expect that the corresponding vacuum expectation value of the field commutator is not analytic in G.

Of course these problems disappear when we admit the existence of a finite cutoff $0<\Lambda_k<\infty$. Taking into account that all the functions $F_p(kR_1\tau)$ are analytic in k around the positive real axis, because F_p is a finite combination of products of analytic functions, and that so are the zeroth-order Bessel functions that appear in the integrals of (26), it is easy to conclude that all those integrals are well defined when they are restricted to a compact interval $[0,\Lambda_k]$. Thus, each term in the power series (26) is finite for any finite positive value of Λ_k.

In the rest of this section, we will discuss the formal manipulations that we have carried out with infinite sums in order to deduce the above expansion. First, notice that the Taylor series in (21), which is obtained from that of the exponential function, has an infinite convergence radius. When this series is substituted in (20), one obtains a trigonometric function similar to that on the lhs of (22), but with $y=kR_1\tau g(q)$ expanded in powers of q. On the other hand, relation (22) is just the formula for the sine of the sum of two angles, with the resulting functions $\sin y$ and $\cos y$ replaced with their Taylor expansion. The series compositions $\sin[kR_1\tau g(q)]$ and $\cos[kR_1\tau g(q)]$ can then be rearranged without problems employing for $[g(q)]^m$ the value given in (23) because $g(q)$ (which we recall that converges for all $q \in \mathbb{R}^+$) is always smaller than the convergence radii of the sine and cosine series, which are in fact infinite.

In this way, one arrives at an expectation value of the regulated commutator that is equal to an integral over the interval $k \in [0,\Lambda_k]$ of the series of functions $\Sigma_p f_p(k|R_1,R_2,\tau)$, with

$$f_p(k|R_1,R_2,\tau) := J_0(R_1k)J_0(R_2k)(-4Gk)^p F_p(kR_1\tau). \tag{28}$$

Since the functions $f_p(k)$ are clearly continuous in $k \in [0,\Lambda_k]$ (for all allowed values of R_1, R_2, and τ) and this interval is compact, they are all integrable in that region. As a consequence, it is

sufficient that the considered series of functions converges uniformly in $k \in [0, \Lambda_k]$ to guarantee that the integration can be interchanged with the infinite sum. We will postpone to the next section the proof of this uniform convergence, at least for a convenient choice of the cutoff.

In conclusion, we have seen that the field commutator *in vacuo*, regulated with a (dimensionful) fixed cutoff, can be expanded as a power series in the gravitational constant G, each term in the series being finite. Besides, all the manipulations performed to deduce this series are rigorously justified provided that the cutoff is chosen so that the series $\Sigma_p f_p(k|R_1, R_2, \tau)$ converges uniformly in $k \in [0, \Lambda_k]$. Furthermore, in fact, this requirement of uniform convergence automatically ensures that the corresponding integrated power series (26) converges, and that it does so to the actual value of the expectation value of the regulated commutator.

VII. UNIFORM CONVERGENCE

We want to demonstrate that there exists a nonzero value of the cutoff for which the series $\Sigma_p f_p(k|R_1, R_2, \tau)$ converges uniformly in $k \in [0, \Lambda_k]$ for any fixed non-negative value of R_1, R_2, and τ. Let us start by finding a convenient upper bound for the coefficients $a_p[m]$, with $m \geqslant 1$, defined in (24). First, note that $a_p[m] = 0$ unless $p \geqslant m$, because no set of the form $\sigma(p|m)$ exists with $n_i \geqslant 1$ if $\Sigma_{i=1}^m n_i = p < m$. In addition, since $(n_i + 1)! \geqslant 2$ for $n_i \geqslant 1$, we have that

$$a_p[m] \leqslant \frac{1}{2^m} \sum_{\sigma(p|m)} 1. \tag{29}$$

From our definition (25), the last sum equals the different ways to arrange $p - m$ nondistinguishable elements [namely, the excess about its minimum of the sum of m elements $n_i \geqslant 1$, which equals $p - m$ for $\sigma(p|m)$] between m different sets (which correspond to the m integers n_i). The result is given by the permutations of $(p - m) + m - 1$ elements (the latter $m - 1$ elements representing movable delimiters between the m sets) with possible repetition in $p - m$ (the genuine, nondistinguishable elements) and in $m - 1$ (the imaginary delimiters). Thus,

$$a_p[m] \leqslant \frac{1}{2^m} \frac{(p-1)!}{(p-m)!(m-1)!} \leqslant \frac{1}{2^m} \frac{p!}{(p-m)!}. \tag{30}$$

In the last inequality we have employed that $(m - 1)! p \geqslant 1$ for all $p \geqslant m \geqslant 1$.

Using that the absolute value of the sine and the cosine is never greater than the unity, it is not difficult then to deduce from (27) the following bound for $F_p(kR_1\tau)$, with $p \geqslant 1$:

$$|F_p(kR_1\tau)| \leqslant \sum_{m=1}^{p} \frac{k^m R_1 \tau^m}{m!} a_p[m] \leqslant \sum_{m=1}^{p} \left(\frac{kR_1\tau}{2}\right)^m \binom{p}{m} = \left(1 + \frac{kR_1\tau}{2}\right)^p - 1. \tag{31}$$

In the last step, we have employed the formula of the binomial expansion. Likewise, since the zeroth-order Bessel function is bounded by the unity in the positive real axis, we get that, for all non-negative values of R_1 and R_2,

$$|f_p(k|R_1, R_2, \tau)| \leqslant (4Gk)^p \left[\left(1 + \frac{kR_1\tau}{2}\right)^p - 1\right] \leqslant \left[4Gk\left(1 + \frac{kR_1\tau}{2}\right)\right]^p. \tag{32}$$

The last inequality is trivial, given that $4Gk \geqslant 0$. Note also that the bound on the rhs is valid even in the case $p = 0$, taking into account (28).

Finally, since $4Gk(1 + kR_1\tau/2)$ is a strictly increasing function of k in $[0, \Lambda_k]$, we obtain a bound independent of the variable k in the interval considered:

$$|f_p(k|R_1, R_2, \tau)| \leqslant \left[4G\Lambda_k\left(1 + \frac{\Lambda_k R_1\tau}{2}\right)\right]^p. \tag{33}$$

To obtain the desired convergence properties, it will suffice to require that

$$4G\Lambda_k\left(1+\frac{\Lambda_k R_1\tau}{2}\right)<1. \tag{34}$$

We then get that both $|f_p(k|R_1,R_2,\tau)|$ and its integral over $[0,\Lambda_k]$ are small corrections for large p, which tend to zero in the limit $p\to\infty$.

In order to prove the uniform convergence of the series $\Sigma_p f_p(k|R_1,R_2,\tau)$, we have to check that, for each $\epsilon>0$, there exists an integer P such that, for every $k\in[0,\Lambda_k]$,

$$\left|\sum_{p=P}^{\infty} f_p(k|R_1,R_2,\tau)\right|\leqslant\epsilon. \tag{35}$$

Taking into account inequality (34), it is clear that, given $\epsilon>0$, we can always find a sufficiently large integer P for which

$$\left[4G\Lambda_k\left(1+\frac{\Lambda_k R_1\tau}{2}\right)\right]^P<\epsilon\left[1-4G\Lambda_k\left(1+\frac{\Lambda_k R_1\tau}{2}\right)\right]. \tag{36}$$

Note that the choice of this P depends only on the values of ϵ, Λ_k, G, and $R_1\tau$. Using (33), we then have

$$\left|\sum_{p=P}^{\infty} f_p(k|R_1,R_2,\tau)\right|\leqslant\sum_{p=P}^{\infty}\left[4G\Lambda_k\left(1+\frac{\Lambda_k R_1\tau}{2}\right)\right]^p=\frac{[4G\Lambda_k(1+\Lambda_k R_1\tau/2)]^P}{1-4G\Lambda_k(1+\Lambda_k R_1\tau/2)}\leqslant\epsilon.$$

So, inequality (35) is valid for all k in the considered interval $[0,\Lambda_k]$, as we wanted to prove.

We have thus shown that, for a given τ, every choice of the cutoff $\Lambda_k>0$ that satisfies condition (34) leads to a convergent power series in the gravitational constant G for the expectation vacuum of the regulated commutator, regardless of the radial coordinates R_1 and R_2. Moreover, the power expansion converges indeed to the true value of this regulated commutator *in vacuo*.

VIII. CONCLUSIONS AND COMMENTS

We have studied in this paper the issue of microcausality for quantum Einstein-Rosen waves after a suitable cutoff is introduced to regulate the quantum fields. In more detail, we have considered the introduction of a momentum cutoff Λ_k (or its dimensionless counterpart Λ_q). We have discussed first the asymptotic expansions in terms of the dimensionless parameters ρ, τ, and λ along the lines of Ref. 8. Owing to the fact that these parameters are defined with the help of R_1, in principle one does not need to make explicit the dependence of the cutoff Λ_k on G in this case. On physical grounds, one could view this cutoff, for example, as the inverse of the Planck length.

We have seen that the introduction of a finite cutoff modifies some of the conclusions obtained in Ref. 8. In particular we have seen that some of the most dramatic effects present when the cutoff is infinite (in particular the behavior of the field commutators in the symmetry axis) are now somewhat mitigated. Nevertheless, we have been able to show that the approximation provided by the unregulated field commutator is a good one in some regions of the (ρ,τ) plane, and, in fact, there is an unbounded region where that approximation prevails. This indicates that, even though the influence of the cutoff is felt in some regions of the parameter space, it is irrelevant in others.

In Secs. VI and VII, on the other hand, we have considered the expansion of the field commutator in terms of the gravitational constant G. We notice, nonetheless, that condition (34) on the cutoff Λ_k, which guarantees the convergence of the series, depends on G. At this stage, one possibility would be to admit that the cutoff depends on the gravitational constant; however, the expansion obtained would then fail to provide a genuine power series in G, because this parameter would also enter the different terms in the series via the implicit dependence of Λ_k on it. Another possibility that indeed respects the interpretation of our expansion as a power series in G is the following. Employing that condition (34) is an inequality equation for Λ_k given in terms of a

function of G that is strictly increasing, it is easy to see that the inequality is satisfied for all values of G in a certain interval $[0,G_M]$ if and only if it is satisfied for G_M. Something similar happens with respect to the dependence on the value of $R_1\tau=|t_2-t_1|$, so that if we want to consider a whole time interval of the form $|t_2-t_1|\in[0,t_M]$, we only have to evaluate our condition at the maximum time lapse. In other words, to ensure the convergence of the series for $G\in[0,G_M]$ and any time difference in $[0,t_M]$, we only have to demand the requirement (34) at $G=G_M$ and $R_1\tau=t_M$, because then

$$4G\Lambda_k\left(1+\frac{\Lambda_k R_1\tau}{2}\right)<4G_M\Lambda_k\left(1+\frac{\Lambda_k t_M}{2}\right)<1. \tag{37}$$

In this way we arrive at a cutoff that is independent of the particular values considered for $|t_2-t_1|$ and the gravitational constant (in the commented intervals), and our expansion becomes a true power series in G. The above inequality leads to the following positive upper bound for Λ_k:

$$\Lambda_k\leqslant\frac{1}{t_M}\left(\sqrt{1+\frac{t_M}{2G_M}}-1\right). \tag{38}$$

Therefore, with a cutoff that satisfies this condition, the power series (26) converges in the interval $[0,G_M]$ for all radial positions R_1 and R_2 and $R_1\tau=|t_2-t_1|\in[0,t_M]$.

When t_M is small, the bound on Λ_k is approximately $1/(4G_M)$, whereas for large t_M it is nearly equal to $1/\sqrt{2G_Mt_M}$. In particular, with this bound the cutoff would have to be vanishingly small if we want a good convergent behavior in an infinitely large time interval ($t_M\to\infty$). An open question is whether it is possible or not to find a different, nonzero time-independent cutoff such that the expansion of the regulated commutator converges for any value of the time elapsed, i.e., for all $|t_2-t_1|\in\mathbb{R}^+$. We expect to encounter convergence problems when the time interval is unbounded; for instance, one can prove that the series (26) does not converge uniformly in $\tau\in\mathbb{R}^+$ with any choice of the cutoff Λ_k (for generic R_1 and R_2). Nonetheless, one can in fact consider a kind of semi-classical limit in which G_M tends to zero (and hence so does the value of the gravitational constant, which had been restricted to $[0,G_M]$), while the time interval where the convergence is granted reaches infinity.

In order to do this, one only needs to allow a dependence of t_M on G_M, so that the assumed maximum value of the time difference varies with that of the gravitational constant. Suppose, let us say, that $t_M(G_M)=G_M^{-\alpha}$ with $0<\alpha<1$. Then, the bound (38) on the cutoff becomes

$$\Lambda_k\leqslant G_M^{\alpha}\left(\sqrt{1+\frac{1}{2G_M^{(\alpha+1)}}}-1\right). \tag{39}$$

Thus, when G_M tends to zero, we get the asymptotic behavior $\Lambda_k\leqslant G_M^{(\alpha-1)/2}/\sqrt{2}$. Since $G_M^{(\alpha-1)/2}$ and $G_M^{-\alpha}$ diverge for vanishing G_M, because $0<\alpha<1$, we therefore conclude that the cutoff can be removed in the limit $G_M\to0$ while ensuring that the time interval $[0,t_M(G_M)]$, where the expansion is well defined, covers the positive real axis.

We finally discuss the physical interpretation of this type of cutoff. It turns out to be intimately related to the maximum resolution that can be reached for the physical time when a certain perturbative approach is adopted to describe the quantum dynamics.[27] In such an approach, one expands the evolution generator in powers of G and regards the free-field Hamiltonian as the dominant contribution, with the higher powers seen as corrections. The auxiliary time T, associated with the free-field Hamiltonian, then plays the role of evolution parameter in the quantum theory, whereas the physical time becomes an operator. It was shown in Ref. 27 that, under these circumstances, a resolution limit Δt emerges for the physical time,

$$[\Delta t]^2\geqslant 4G^2+4GT. \tag{40}$$

Employing the inequality $\sqrt{1+x}\leqslant x/(\sqrt{1+x}-1)$ for $x>0$, evaluated at $x=t_M/(2G)$, one can easily check from condition (38) that the inverse of the cutoff satisfies

$$\Lambda_k^{-1} \geqslant \sqrt{4G_M^2 + 2G_M t_M}. \tag{41}$$

Therefore, the bound on Λ_k^{-1} equals that on the time resolution Δt for a value $G=G_M$ of the gravitational constant and a time elapsed $T=2t_M$ (and thus of the same order as t_M). In this sense, one can assign to Λ_k^{-1} the interpretation of a genuine resolution limit in the physical time.

The future prospects for this line of work will focus on the issue of deriving and obtaining meaningful physical information from the S matrix of the model. We feel that the mathematical techniques employed here to study the asymptotics of field commutators, with and without a cutoff, will also be helpful in analyzing this issue. We plan to concentrate on this problem in the future.

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Covariant *q*-differential operators and unitary highest weight representations for $U_q\mathfrak{su}_{n,n}$

Dmitry Shklyarov[a)]
Department of Mathematics, Kansas State University, Manhattan, KS 66506

Genkai Zhang[b)]
Chalmers Tekniska Högskola/Göteborgs Universitet, Matematik 412 96, Göteborg, Sweden

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We investigate a one-parameter family of quantum Harish–Chandra modules of $U_q\mathfrak{sl}_{2n}$. This family is an analog of the holomorphic discrete series of representations of the group $\mathrm{SU}(n,n)$ for the quantum group $U_q\mathfrak{su}_{n,n}$. We introduce a *q*-analog of "the wave" operator (a determinant-type differential operator) and prove certain covariance property of its powers. This result is applied to the study of some quotients of the above-mentioned quantum Harish–Chandra modules. We also prove an analog of a known result by J. Faraut and A. Koranyi on the expansion of reproducing kernels which determines the analytic continuation of the holomorphic discrete series. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1927077]

I. INTRODUCTION

We start with recalling classical known results about analytic continuation of the weighted Bergman spaces in the unit disk and their explicit realization.

Recall that the group $\mathrm{SU}_{1,1}$ acts on the unit disk by fractional-linear transformations. Many important representations of the group are realized geometrically in various functional spaces on the disk and on the unit circle. In particular, representations of the discrete series admit a realization of that kind. Namely, consider the kernel $(1-z\overline{w})^{-\lambda}$ in the unit disk. For $\lambda>1$ it is the reproducing kernel for the so-called weighted Bergman space consisting of holomorphic functions that are square integrable with the weight $(1-|z|^2)^{\lambda-2}dm(z)$ [here $dm(z)$ is the normalized Lebesgue measure]. The group $\mathrm{SU}_{1,1}$ acts in the space via change of variable and a multiplier:

$$\pi_\lambda(g)(f(z)) = f(g^{-1}z)\cdot(cz+d)^{-\lambda}, \quad g^{-1}=\begin{pmatrix} a & b \\ c & d \end{pmatrix} \tag{1.1}$$

(for noninteger λ's one should consider the universal covering $\widetilde{\mathrm{SU}}_{1,1}$ instead of $\mathrm{SU}_{1,1}$). Thus obtained unitary representation belongs to the discrete series and is said to be a representation of the holomorphic discrete series for $\mathrm{SU}_{1,1}$ or $\widetilde{\mathrm{SU}}_{1,1}$.

The reproducing kernel $(1-z\overline{w})^{-\lambda}$ has analytic continuation in the parameter λ. This is obtained from the formula

$$(1-z\overline{w})^{-\lambda} = \sum_{m=0}^{\infty} (\lambda)_m \frac{(z\overline{w})^m}{m!}, \quad (\lambda)_m = \lambda\cdot(\lambda+1)\cdot\ \cdots\ \cdot(\lambda+m-1). \tag{1.2}$$

[a)]Electronic mail: shklyarov@math.ksu.edu
[b)]Electronic mail: genkai@math.chalmers.se

For $\lambda > 0$ the kernel is still positive definite, and the $SU_{1,1}$-action (1.1) in the associated Hilbert space is also unitary. For $\lambda = 1$, the Hilbert space is the Hardy space of holomorphic function on the closed disk whose boundary values are square integrable on the circle.

For further study of the previous representations, it is convenient to pass to the corresponding Harish–Chandra modules. Consider the space $\mathbb{C}[z]$ of polynomials on $\mathbb{C}$. The representation π_λ induces a representation of $\mathfrak{sl}_2(\mathbb{C}) = \mathfrak{su}_{1,1} \otimes \mathbb{C}$ on $\mathbb{C}[z]$ which may be defined for any $\lambda \in \mathbb{R}$ (and even for $\lambda \in \mathbb{C}$). Let us denote by $\mathcal{P}_\lambda$ the space $\mathbb{C}[z]$ endowed with the above-mentioned action of $\mathfrak{sl}_2(\mathbb{C})$. $\mathcal{P}_\lambda$ is irreducible for all positive λ's. However, if $\lambda = 1 - l$ for some positive integer l then $\mathcal{P}_\lambda = \mathcal{P}_{1-l}$ has the following composition series:

$$\{0\} \subset \mathcal{P}^{(0)}_{1-l} \subset \mathcal{P}_{1-l}, \tag{1.3}$$

where $\mathcal{P}^{(0)}_{1-l}$ is the submodule of polynomials of degree $\leqslant l-1$. The natural problem is to study the quotient $\mathcal{P}_{1-l}/\mathcal{P}^{(0)}_{1-l}$. This is the point where covariant differential operators appear on the scene. They play an important role in an explicit realization of the quotient. Namely, one checks that the differential operator $(\partial/\partial z)^l$ intertwines the actions π_{1-l} and π_{1+l}:

$$\left(\frac{\partial}{\partial z}\right)^l \cdot \pi_{1-l}(\xi) = \pi_{1+l}(\xi) \cdot \left(\frac{\partial}{\partial z}\right)^l, \quad \xi \in \mathfrak{sl}_2(\mathbb{C}). \tag{1.4}$$

Clearly, $(\partial/\partial z)^l$ induces an isomorphism from $\mathcal{P}_{1-l}/\mathcal{P}^{(0)}_{1-l}$ into $\mathcal{P}_{1+l}$, and this, in particular, proves unitarizability of the former module.

The unit disk is the simplest example of a bounded symmetric domain.[1] The above-mentioned results admit appropriate generalization for any such domain (of course, the group $SU_{1,1}$ is replaced by the group of biholomorphic automorphisms of the domain under consideration).

For the so-called tube domains, some generalizations of the covariance property (1.4) have been obtained by Shimura,[19] Arazy,[1] Jakobsen,[9] Jakobsen and Vergne,[13] and Jakobsen and Harris.[12] For example, in the case of the tube domain of type $I_{n,n}$ (the unit ball in the space of complex $n \times n$ matrices) the analog of (1.4) is a statement about an intertwining property of powers of the operator $\Box = \det(\partial/\partial z^\alpha_a)_{a,\alpha=1,\ldots,n}$ with respect to certain "twisted" action of the group $SU_{n,n}$ analogous to (1.1).

The generalized covariance property (1.4) has turned out to be useful beyond the problems we mentioned previously. It has been applied also to computing the Harish–Chandra homomorphism of invariant differential operators.[28]

Now for symmetric bounded domains the expansion (1.2) has been found by Ørsted[18] for type *I* matrix domains and in a general case by Faraut and Koranyi.[5] From this expansion one can read off the composition series analogous to (1.3); the covariant property of the intertwining operators is related to the classical Cayley–Capelli type formula. We note that the unitarity of the highest weight modules had been classified earlier by Jakobsen[8] using algebraic method; however the analytic approach as in Refs. 18 and 5 generated some other interesting analytic subjects and is related to many problems in special functions and orthogonal polynomials. For quantum groups the classification of unitary highest weight representations has also been done recently,[11] and we believe however that an analytic and concrete approach deserves pursuing.

In the present article we obtain analogs of (1.2), (1.3), and (1.4) for a quantum matrix ball, an analog of the tube domain of type $I_{n,n}$ which has been defined in framework of quantum group theory by Vaksman *et al.*[21]

In Ref. 22, the authors defined analogs of the weighted Bergman spaces on the quantum matrix ball. Also, they constructed analogs of the corresponding reproducing kernels and the twisted unitary action of the group $SU_{n,n}$. From the representation theoretic point of view, Ref. 22 presents a *q*-analog of the holomorphic discrete series of the group $SU_{n,n}$ (more precisely, analogs of the associated Harish–Chandra modules).

The natural problem now is to investigate those representations, particularly, to define their

"analytic continuation" and to study composition series of the resulting Harish–Chandra modules. In the case $n=2$, these problems were treated in Ref. 23. In the present paper, we deal with the case of arbitrary n.

The role of covariant differential operators in the classical theory of bounded symmetric domains and related Harish–Chandra modules is very well known.[9,12,13,19] Our intention is to bring covariant q-differential operators into the study of quantum Harish–Chandra modules and thus to demonstrate their importance in the quantum setting as well [note that similar questions have been already treated in the literature (see Ref. 3 and, especially, Ref. 10)]. We introduce a determinant-type q-differential operator similar to $\Box$ and prove a q-analog of the covariance property. In the last section, this result is applied to investigation of certain quotients of the above quantum Harish–Chandra modules.

Another goal of the paper is to obtain an analog of the aforementioned result by Faraut and Koranyi[5] which has allowed them to solve the problem of analytic continuation of the holomorphic discrete series in the classical setting.

As we already mentioned, there is a complete classification of unitarizable highest-weight modules over quantum groups (see Ref. 11). Thus, neither the holomorphic discrete series of the quantum group $\mathrm{SU}(n,n)$, constructed in Ref. 22, nor its analytic continuation, obtained in the present paper, give us a new family of unitary modules. The principal aim of the present paper, as well as other papers,[22,23] is to develop an "analytic and geometric" framework for studying quantum Harish–Chandra modules related to quantum Cartan domains, particularly, to show that there are substantial generalizations of known classical constructions and results connected with the holomorphic discrete series.

The paper is organized as follows. Sections II and III contain some preliminary material. In Sec. II, we recall some basic notions and results of quantum group theory (particularly, the notion of quantum space of matrices and of the quantized universal enveloping algebra $U_q\mathfrak{sl}_n$). This is done mainly for the purpose to set the notation we use further. Also, we recall certain hidden quantum $U_q\mathfrak{sl}_{2n}$ symmetry of the quantum matrix space discovered in Ref. 25. (This hidden symmetry was one of the first hints that there should be a substantial theory of q-bounded symmetric domains. These objects were invented a little later in Ref. 24). In the end of Sec. II we describe a twisted action (depending on a parameter λ) of $U_q\mathfrak{sl}_{2n}$ on the quantum matrix space. For λ large enough the corresponding Harish–Chandra modules are unitarizable representations of $U_q\mathfrak{su}_{n,n}$, which we call the holomorphic discrete series due to the previous motivation. Section III is devoted to q-differential operators. We recall there the notion of a q-differential operator with constant coefficients and describe certain properties of the algebra of such operators. Also, we introduce an analog of the operator $\Box$ and derive its "obvious" quantum symmetry which amounts to an intertwining property of the operator with an action of Hopf subalgebra $U_q\mathfrak{sl}_n \otimes U_q\mathfrak{sl}_n \subset U_q\mathfrak{sl}_{2n}$. This obvious symmetry is extended to a large hidden symmetry, namely, the intertwining property of the operator (and of its powers) with the twisted $U_q\mathfrak{sl}_{2n}$ actions. This covariance property is formulated and proved in Sec. IV. In the course of the proof, we use a number of results from the theory of quantum bounded symmetric domains, in particular, those obtained in Ref. 20 and, especially, results of Ref. 27. To keep the size of the paper reasonable, we have to be more sketchy in this part of the paper. We omit proofs of those results giving appropriate references instead. In the last section of the paper we investigate the holomorphic discrete series for $U_q\mathfrak{su}_{n,n}$. First of all, we use computations of Sec. IV to produce an analog of the result by Faraut and Koranyi[5] we mentioned earlier. Then we derive some applications of the covariance property.

II. QUANTUM SPACE OF MATRICES AND ITS SYMMETRIES

In this paper, the parameter q is supposed to be a number from the interval (0, 1).

A. Quantum space of matrices

Let us start with the definition of the algebra $\mathbb{C}[M_n]_q$ of polynomials on the quantum matrix space. It is the unital algebra given by its generators z_a^α (here, $a,\ \alpha=1,\ldots,n$, a is the column index and α is the row index) and the following relations:

$$z_a^\alpha z_b^\beta = \begin{cases} qz_b^\beta z_a^\alpha, & a=b \quad \text{and} \quad \alpha<\beta \quad \text{or} \quad a<b \quad \text{and} \quad \alpha=\beta \\ z_b^\beta z_a^\alpha, & a<b \quad \text{and} \quad \alpha>\beta \\ z_b^\beta z_a^\alpha + (q-q^{-1}) z_a^\beta z_b^\alpha, & a<b \quad \text{and} \quad \alpha<\beta. \end{cases} \tag{2.1}$$

These commutation relations, along with the relation

$$\det_q(\mathbf{z}) = \sum_{s\in S_n} (-q)^{l(s)} z_{a_1}^{\alpha_{s(1)}} z_{a_2}^{\alpha_{s(2)}} \cdots z_{a_n}^{\alpha_{s(n)}} = 1, \tag{2.2}$$

appeared for the first time in Ref. 4 as the relations between generators in the algebra $\mathbb{C}[SL_n]_q$ of regular functions on the quantum SL_n. It was suggested in Ref. 6 to discard (2.2) from the list of relations and to regard (2.1) as the defining relations of the algebra of polynomials on the quantum space of matrices. The algebra $\mathbb{C}[SL_n]_q$ is then the quotient of $\mathbb{C}[M_n]_q$ by the two-sided ideal generated by the element $\det_q(\mathbf{z})-1$ {note that the q-determinant $\det_q(\mathbf{z})$ belongs to the center of $\mathbb{C}[M_n]_q$ ([2, Sec. VII C 2])}. Also, the algebra $\mathbb{C}[M_n]_q$ is used to define the algebra of regular functions on the quantum GL_n. The latter is just the localization of the former with respect to the multiplicative system $\det_q(\mathbf{z})^m$, $m=1,2,\ldots$.

The crucial observation concerning the algebra $\mathbb{C}[M_n]_q$ was the discovery of the comultiplication

$$\mathbb{C}[M_n]_q \to \mathbb{C}[M_n]_q \otimes \mathbb{C}[M_n]_q, \quad z_a^\alpha \mapsto \sum_j z_a^j \otimes z_j^\alpha$$

which, along with the initial multiplication, makes $\mathbb{C}[M_n]_q$ into a bialgebra. The comultiplication maps the q-determinant $\det_q(\mathbf{z})$ to $\det_q(\mathbf{z})\otimes\det_q(\mathbf{z})$ and thus induces a comultiplication on the algebra $\mathbb{C}[SL_n]_q$. The latter, along with certain antipode and counit, makes $\mathbb{C}[SL_n]_q$ into a Hopf algebra.

All the above structures allow one to produce q-analogs of the left and right actions

$$L(g): f(\mathbf{z}) \mapsto f(g^{-1}\cdot\mathbf{z}), \quad R(g): f(\mathbf{z}) \mapsto f(\mathbf{z}\cdot g)$$

of SL_n in $\mathbb{C}[M_n]$. These q-analogs are usually described in terms of comodule algebras.[2] However, it is more convenient for us to use an "infinitesimal" version of those actions which is based on the notion of the quantum universal enveloping algebra $U_q\mathfrak{sl}_n$ due to Drinfeld[4] and Jimbo.[15]

First, we recall the definition of $U_q\mathfrak{sl}_n$ (we follow the notation of Ref. 14). The quantum universal enveloping algebra $U_q\mathfrak{sl}_n$ is the unital algebra generated by the elements E_i, F_i, $K_i^{\pm1}$, $i=1,\ldots,n$, which satisfy the relations

$$K_iK_j = K_jK_i, \quad K_iK_i^{-1} = K_i^{-1}K_i = 1,$$

$$K_iE_j = q^{a_{ij}}E_jK_i, \quad K_iF_j = q^{-a_{ij}}F_jK_i,$$

$$E_iF_j - F_jE_i = \delta_{ij}(K_i - K_i^{-1})/(q-q^{-1}),$$

$$E_i^2E_j - (q+q^{-1})E_iE_jE_i + E_jE_i^2 = 0, \quad |i-j|=1$$

$$F_i^2F_j - (q+q^{-1})F_iF_jF_i + F_jF_i^2 = 0, \quad |i-j|=1$$

$$[E_i,E_j]=[F_i,F_j]=0, \quad |i-j|\neq 1$$

with (a_{ij}) being the Cartan matrix of type A_{n-1}. Moreover, $U_q\mathfrak{sl}_n$ is a Hopf algebra. The comultiplication Δ, the antipode S, and the counit ε are determined by

$$\Delta(E_i)=E_i\otimes 1+K_i\otimes E_i, \quad \Delta(F_i)=F_i\otimes K_i^{-1}+1\otimes F_i, \quad \Delta(K_i)=K_i\otimes K_i, \tag{2.3}$$

$$S(E_i)=-K_i^{-1}E_i, \quad S(F_i)=-F_iK_i, \quad S(K_i)=K_i^{-1}, \tag{2.4}$$

$$\varepsilon(E_i)=\varepsilon(F_i)=0, \quad \varepsilon(K_i)=1. \tag{2.5}$$

It is observed in Ref. 4 that the Hopf algebras $U_q\mathfrak{sl}_n$ and $\mathbb{C}[SL_n]_q$ are dual to each other. This, in particular, allows one to use the language of $U_q\mathfrak{sl}_n$-module algebras instead of that of $\mathbb{C}[SL_n]_q$-comodule algebras mentioned previously. This is what we do in the present paper.

Let us recall now what the terminology "$U_q\mathfrak{sl}_n$-module algebra" means. Let A be a Hopf algebra. A unital algebra F is said to be an A-module algebra if F is an A-module, the unit of F is A-invariant [which means $\xi(1)=\varepsilon(\xi)\cdot 1$ for any $\xi\in A$], and, finally, the multiplication $F\otimes F\to F$ intertwines the A-actions (we recall that for any A-modules V_1, V_2 their tensor product is endowed with an A-module structure via the comultiplication $\Delta: A\to A\otimes A$).

Remark: In the sequel, we shall sometimes consider Hopf algebras with an additional structure, namely, Hopf $*$-algebras (a Hopf $*$-algebra is a pair $(A,*)$ where A is a Hopf algebra and $*$ is an involution in A with certain properties; see Ref. 2). In the case of Hopf $*$-algebras the above-mentioned definition includes an additional requirement. Namely, let $A_0=(A,*)$ be a Hopf $*$-algebra and F an algebra. Then F is said to be an A_0-module algebra if, first, F is an A-module algebra in the previous sense, and, second, F is involutive and the involutions in A and F agree as follows:

$$(\xi(f))^*=S(\xi)^*(f^*), \quad \xi\in A, f\in F. \tag{2.6}$$

[The notion of module algebras can be clarified in the classical setting of a Lie group G acting on a smooth G-space X. Denote by $\mathfrak{g}$ the Lie algebra of G. Then the universal enveloping algebra $U\mathfrak{g}$ acts on the space $C^\infty(X)$ via differential operators. The usual Leibnitz rule means that $C^\infty(X)$ is a $U\mathfrak{g}$-module algebra.]

Let us turn back to the quantum space of matrices. Now we are in position to describe the very well known "infinitesimal version" of the left and right actions of the quantum group SL_n in $\mathbb{C}[M_n]_q$. Note, however, that the left action we present below is not an analog of the classical one, mentioned earlier. It is more convenient for us to use an action that differs from the usual left one by a simple automorphism of $U_q\mathfrak{sl}_n$.

Proposition 2.1:

(i) *There exists a unique structure of $U_q\mathfrak{sl}_n$-module algebra in $\mathbb{C}[M_n]_q$ such that*

$$R(K_i)z_a^\alpha=\begin{cases} qz_a^\alpha, & a=i \\ q^{-1}z_a^\alpha, & a=i+1 \\ z_a^\alpha, & \text{otherwise}, \end{cases} \tag{2.7}$$

$$R(F_i)z_a^\alpha=\begin{cases} q^{1/2}z_{a+1}^\alpha, & a=i \\ 0, & \text{otherwise}, \end{cases} \qquad R(E_i)z_a^\alpha=\begin{cases} q^{-1/2}z_{a-1}^\alpha, & a=i+1 \\ 0, & \text{otherwise}. \end{cases} \tag{2.8}$$

(ii) *There exists a unique structure of $U_q\mathfrak{sl}_n$-module algebra in $\mathbb{C}[M_n]_q$ such that*

$$L(K_j)z_a^\alpha = \begin{cases} qz_a^\alpha, & \alpha = n-j \\ q^{-1}z_a^\alpha, & \alpha = n-j+1 \\ z_a^\alpha, & \text{otherwise}, \end{cases} \tag{2.9}$$

$$L(F_j)z_a^\alpha = \begin{cases} q^{1/2}z_a^{\alpha+1}, & \alpha = n-j \\ 0, & \text{otherwise}, \end{cases} \qquad L(E_j)z_a^\alpha = \begin{cases} q^{-1/2}z_a^{\alpha-1}, & \alpha = n-j+1 \\ 0, & \text{otherwise}. \end{cases} \tag{2.10}$$

(iii) *For any* $\xi, \eta \in U_q\mathfrak{sl}_n$ *the endomorphisms* $R(\xi)$, $L(\eta)$ *commute*

$$R(\xi)L(\eta)f = L(\eta)R(\xi)f, \quad f \in \mathbb{C}[M_n]_q.$$

Note that by statement (iii) in the above-mentioned proposition, the algebra $\mathbb{C}[M_n]_q$ is acted upon by the tensor product $U_q\mathfrak{sl}_n \otimes U_q\mathfrak{sl}_n$:

$$\xi \otimes \eta(f) = R(\xi)L(\eta)f.$$

One can check that the q-determinant $\det_q(\mathbf{z})$ (2.2) is invariant with respect to both left and right $U_q\mathfrak{sl}_n$-actions, i.e.,

$$R(\xi)\det_q(\mathbf{z}) = L(\xi)\det_q(\mathbf{z}) = \varepsilon(\xi)\cdot\det_q(\mathbf{z})$$

for any $\xi \in U_q\mathfrak{sl}_n$. Thus the formulas from Proposition 2.1 define left and right $U_q\mathfrak{sl}_n$-actions in $\mathbb{C}[SL_n]_q$. By analogy with the classical case, one has the following proposition (see Ref. 2).

Proposition 2.2: *The* $U_q\mathfrak{sl}_n \otimes U_q\mathfrak{sl}_n$*-module* $\mathbb{C}[SL_n]_q$ *splits into direct sum of simple pairwise nonisomorphic submodules whose lowest vectors are given via q-minors as follows:*

$$(z_n^n)^{a_1}(\mathbf{z}^{\wedge 2\{n-1,n\}}_{\{n-1,n\}})^{a_2}(\mathbf{z}^{\wedge 3\{n-2,n-1,n\}}_{\{n-2,n-1,n\}})^{a_3}\cdots(\mathbf{z}^{\wedge (n-1)\{2,\ldots,n\}}_{\{2,\ldots,n\}})^{a_{n-1}}.$$

We recall that the q-minors are defined by

$$(\mathbf{z}^{\wedge k})^{\{\alpha_1,\alpha_2,\ldots,\alpha_k\}}_{\{a_1,a_2,\ldots,a_k\}} \overset{\text{def}}{=} \sum_{s\in S_k}(-q)^{l(s)}z_{a_1}^{\alpha_{s(1)}}z_{a_2}^{\alpha_{s(2)}}\cdots z_{a_k}^{\alpha_{s(k)}} \tag{2.11}$$

with $\alpha_1 < \alpha_2 < \cdots < \alpha_k$, $a_1 < a_2 < \cdots < a_k$, and $l(s)$ being the length of $s \in S_k$. In particular, $\det_q(\mathbf{z}) = (\mathbf{z}^{\wedge n})^{\{1,2,\ldots,n\}}_{\{1,2,\ldots,n\}}$.

Let us denote the tensor product $U_q\mathfrak{sl}_n \otimes U_q\mathfrak{sl}_n$ with the canonical Hopf algebra structure by $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$. Thus, $\mathbb{C}[M_n]_q$ is a $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$-module algebra. It follows from the definition of the quantum universal enveloping algebra $U_q\mathfrak{sl}_n$ that there is an embedding of Hopf algebras $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n) \hookrightarrow U_q\mathfrak{sl}_{2n}$ determined by

$$1 \otimes E_i \mapsto E_i, \quad 1 \otimes F_i \mapsto F_i, \quad 1 \otimes K_i^{\pm 1} \mapsto K_i^{\pm 1}, \quad i = 1,\ldots,n-1,$$

$$E_i \otimes 1 \mapsto E_{n+i}, \quad F_i \otimes 1 \mapsto F_{n+i}, \quad K_i^{\pm 1} \otimes 1 \mapsto K_{n+i}^{\pm 1}, \quad i = 1,\ldots,n-1.$$

This is a q-analog of the embedding $SL_n \times SL_n \hookrightarrow SL_{2n}$ given, in the matrix realization, by

$$(A,B) \mapsto \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}.$$

In the next subsection we shall extend the above $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$-module algebra structure in $\mathbb{C}[M_n]_q$ to a structure of $U_q\mathfrak{sl}_{2n}$-module algebra.

B. A structure of $U_q\mathfrak{sl}_{2n}$-module algebra on $\mathbb{C}[M_n]_q$

In this subsection we describe a "hidden" $U_q\mathfrak{sl}_{2n}$-module algebra structure in $\mathbb{C}[M_n]_q$. It was discovered in Ref. 25. Its classical counterpart comes from an embedding of the matrix space M_n into the Grassmannian $\mathrm{Gr}_n(\mathbb{C}^{2n})$ as the affine cell $U\subset \mathrm{Gr}_n(\mathbb{C}^{2n})$ defined by the inequality $t\neq 0$ with t being a distinguished Plücker coordinate. A q-version of the embedding is described in Ref. 25, Proposition 0.7 (see also Proposition 5.4 from Ref. 21).

Let us turn to the quantum case. The following statement was proved in Ref. 21, Sec. 2.

***Proposition 2.3**: There exists a unique $U_q\mathfrak{sl}_{2n}$-module algebra structure in $\mathbb{C}[M_n]_q$ given on the Hopf subalgebra $U_q(\mathfrak{sl}_n\times\mathfrak{sl}_n)$ by the formulas from Proposition 2.1 and on the remaining generators $K_n^{\pm 1}$, F_n, E_n by*

$$K_n z_a^\alpha=\begin{cases} q^2 z_a^\alpha, & a=n \quad \text{and} \quad \alpha=n \\ q z_a^\alpha, & a=n \quad \text{and} \quad \alpha\neq n \quad \text{or} \quad a\neq n \quad \text{and} \quad \alpha=n \\ z_a^\alpha, & \text{otherwise,}\end{cases} \tag{2.12}$$

$$F_n z_a^\alpha=q^{1/2}\begin{cases}1, & a=n \quad \text{and} \quad \alpha=n\\ 0, & \text{otherwise,}\end{cases} \qquad E_n z_a^\alpha=-q^{1/2}\begin{cases} q^{-1} z_a^m z_n^\alpha, & a\neq n \quad \text{and} \quad \alpha\neq n\\ (z_n^m)^2, & a=n \quad \text{and} \quad \alpha=n\\ z_n^m z_a^\alpha, & \text{otherwise.}\end{cases} \tag{2.13}$$

Let us point out some straightforward but essential properties of this $U_q\mathfrak{sl}_{2n}$-action in $\mathbb{C}[M_n]_q$. Denote by $U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)$ the Hopf subalgebra in $U_q\mathfrak{sl}_{2n}$ derived from $U_q(\mathfrak{sl}_n\times\mathfrak{sl}_n)$ by adding the generators $K_n^{\pm 1}$. Clearly, elements of $U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)$ preserve the natural $\mathbb{Z}_+$-grading in $\mathbb{C}[M_n]_q$ given by powers of monomials. It is also obvious, that the generators F_n, E_n act in $\mathbb{C}[M_n]_q$ as endomorphisms of degrees -1 and 1, respectively. All this may be derived also from the following convenient description of the $\mathbb{Z}_+$-grading in $\mathbb{C}[M_n]_q$:

$$\deg f=N \Leftrightarrow \hat{K} f=q^{2N} f, \tag{2.14}$$

where $\hat{K}$ is the element of the center of $U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)$ given by

$$\hat{K}=(K_n)^n\cdot\prod_{j=1}^{n-1}(K_j K_{2n-j})^j. \tag{2.15}$$

For computational purposes, it is important to understand the structure of $\mathbb{C}[M_n]_q$ as a $U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)$-module in greater detail. The following statement is a straightforward consequence of Proposition 2.2.

***Proposition 2.4**: The $U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)$-module $\mathbb{C}[M_n]_q$ splits into direct sum of simple pairwise non-isomorphic submodules $\mathbb{C}[M_n]_q^{(k_1,k_2,\ldots,k_n)}$, $k_1\geqslant k_2\geqslant\cdots\geqslant k_n\geqslant 0$, whose lowest vectors are given by*

$$(z_n^n)^{k_1-k_2}\left(\mathbf{z}^{\wedge 2^{\{n-1,n\}}_{\{n-1,n\}}}\right)^{k_2-k_3}\left(\mathbf{z}^{\wedge 3^{\{n-2,n-1,n\}}_{\{n-2,n-1,n\}}}\right)^{k_3-k_4}\cdots(\det_q\mathbf{z})^{k_n}.$$

In what follows, the above $U_q\mathfrak{sl}_{2n}$-action in $\mathbb{C}[M_n]_q$ will be sometimes called "the initial" one, in contrast to a twisted action described in the next subsection.

Let us present another view on the above $U_q\mathfrak{sl}_{2n}$-action in $\mathbb{C}[M_n]_q$. The point is that the corresponding classical $U\mathfrak{sl}_{2n}$-action is well known in the theory of bounded symmetric domains (see, for instance, Ref. 1). In framework of this theory, it is constructed as follows. The vector space M_n contains the so-called matrix ball (the boundary symmetric domain of type $I_{n,n}$)

$$\mathcal{D} = \{\mathbf{z} \in M_n | \mathbf{z}\mathbf{z}^* < 1\}$$

(with $*$ being the hermitian conjugation and 1 the unit matrix). It is known that the real simple Lie group $\mathrm{SU}_{n,n}$ acts on $\mathcal{D}$ via biholomorphic automorphisms, and $S(U_n \times U_n) \subset \mathrm{SU}_{n,n}$ is the isotropy subgroup of the center $0 \in \mathcal{D}$. Thus elements of the universal enveloping algebra $U\mathfrak{su}_{n,n}$, and hence elements of its complexification $U\mathfrak{sl}_{2n}$, act on the space of holomorphic functions on $\mathcal{D}$ via differential operators. These differential operators have polynomial coefficients and, thus, preserve $\mathbb{C}[M_n]$. The resulting $U\mathfrak{sl}_{2n}$-action in $\mathbb{C}[M_n]$ is what we call the initial one. In framework of this approach, the result of Proposition 2.4 is just a q-analog of the famous Hua–Schmid decomposition[1] whereas the quantum enveloping algebra $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$ itself is an analog of the universal enveloping algebra of the complexified Lie algebra of the isotropy subgroup $S(U_n \times U_n)$.

C. A twisted $U_q\mathfrak{sl}_{2n}$-action on $\mathbb{C}[M_n]_q$

In this subsection we introduce a one-parameter family π_λ, $\lambda \in \mathbb{R}$, of $U_q\mathfrak{sl}_{2n}$-actions in $\mathbb{C}[M_n]_q$ such that the initial $U_q\mathfrak{sl}_{2n}$-action, defined in the previous subsection, corresponds to $\lambda = 0$. In the classical case the corresponding twisted $U\mathfrak{sl}_{2n}$-action π_λ for $\lambda \in \mathbb{Z}$ can be produced by trivializing the homogeneous line bundle $\mathcal{O}(-\lambda)$ on the Grassmannian $\mathrm{Gr}_n(\mathbb{C}^{2n})$ over the affine cell U. Namely, we identify the space of polynomials on M_n with the space of sections $\Gamma(U, \mathcal{O}(-\lambda))$ by $f(\mathbf{z}) \sim f(\mathbf{z}) \cdot t^{-\lambda}$ (here t is the distinguished Plücker coordinate mentioned at the beginning of the previous subsection) and define the $U\mathfrak{sl}_{2n}$-action π_λ as follows:

$$(\pi_\lambda(\xi)f) \cdot t^{-\lambda} = \xi(f \cdot t^{-\lambda}), \quad \xi \in U\mathfrak{sl}_{2n}. \tag{2.16}$$

Note that, among the actions π_λ, the initial action π_0 is the only one which makes $\mathbb{C}[M_n]$ into a $U\mathfrak{sl}_{2n}$-*module algebra*. This is true in the q-setting as well.

Let us define a quantum version of the $U\mathfrak{sl}_{2n}$-action (2.16)

Proposition 2.5: *For any* $\lambda \in \mathbb{R}$ *the formulas*

$$\pi_\lambda(K_j^{\pm 1})f = \begin{cases} K_j^{\pm 1} f, & j \neq n \\ q^{\pm\lambda} K_n^{\pm 1} f, & j = n, \end{cases}$$

$$\pi_\lambda(F_j)f = \begin{cases} F_j f, & j \neq n \\ q^{-\lambda} F_n f, & j = n, \end{cases} \qquad \pi_\lambda(E_j)f = \begin{cases} E_j f, & j \neq n \\ E_n f - q^{1/2}\dfrac{1-q^{2\lambda}}{1-q^2}(K_n f) z_n^n, & j = n \end{cases}$$

define a $U_q\mathfrak{sl}_{2n}$*-action in* $\mathbb{C}[M_n]_q$ (*in the right-hand sides the initial* $U_q\mathfrak{sl}_{2n}$*-action is used*).

This proposition was proved in Ref. 22 (Proposition 6.2). Note that π_0 coincides with the initial $U_q\mathfrak{sl}_{2n}$-action. For brevity, we shall denote the $U_q\mathfrak{sl}_{2n}$-module, corresponding to λ, by $\mathcal{P}_\lambda$, namely $\mathcal{P}_\lambda = (\mathbb{C}[M_n]_q, U_q\mathfrak{sl}_{2n}, \pi_\lambda)$.

The classical counterpart of the above twisted $U_q\mathfrak{sl}_{2n}$-action is also well known in the theory of bounded symmetric domains. The corresponding $\mathrm{SU}_{n,n}$-action (more precisely, the action of the universal covering $\widetilde{\mathrm{SU}}_{n,n}$) is defined by

$$\pi_\lambda(g): f(\mathbf{z}) \mapsto f(g^{-1}\mathbf{z}) \cdot J_{g^{-1}}(\mathbf{z})^{\lambda/2n} \tag{2.17}$$

with $J_{g^{-1}}(\mathbf{z})$ being the Jacobian of the biholomorphic map $\mathbf{z} \mapsto g^{-1}\mathbf{z}$ (see Ref. 1 for details). For $\lambda > 2n-1$ the action π_λ on a weighted Bergman space defines a holomorphic discrete scries representation of $\widetilde{SU}_{n,n}$. In the last section of the paper we will describe a unitary structure on $\mathcal{P}_\lambda$ which formally tends to the classical setting as $q \to 1$.

III. SOME q-DIFFERENTIAL OPERATORS

A. Basic definitions

One of our results is connected with a q-analog of the wave operator

$$\Box = \det\left(\frac{\partial}{\partial z_a^\alpha}\right).$$

We start with some general consideration of q-differential operators with constant coefficients.

To produce q-analogs of the partial derivatives, we use certain known first order differential calculus over $\mathbb{C}[M_n]_q$, see Ref. 2. Let $\Omega^1(M_n)_q$ be the $\mathbb{C}[M_n]_q$-bimodule given by its generators dz_a^α, $a,\alpha=1,\ldots,n$, and the relations

$$z_b^\beta dz_a^\alpha = \sum_{\alpha',\beta'=1}^{n} \sum_{a',b'=1}^{n} R_{\beta\alpha}^{\beta'\alpha'} R_{ba}^{b'a'} dz_{a'}^{\alpha'} \cdot z_{b'}^{\beta'},$$

with

$$R_{ba}^{b'a'} = \begin{cases} q^{-1}, & a=b=a'=b' \\ 1, & a\neq b \text{ and } a=a' \text{ and } b=b' \\ q^{-1}-q, & a<b \text{ and } a=b' \text{ and } b=a' \\ 0, & \text{otherwise}. \end{cases}$$

The map $d: z_a^\alpha \mapsto dz_a^\alpha$ can be extended to a linear operator $d:\mathbb{C}[M_n]_q \to \Omega^1(M_n)_q$ satisfying the Leibnitz rule $d(f_1f_2)=d(f_1)f_2+f_1d(f_2)$. The pair $(\Omega^1(M_n)_q, d)$ is the first order differential calculus over $\mathbb{C}[M_n]_q$ we need.

The calculus itself has been known for a long time.[2] However, its hidden $U_q\mathfrak{sl}_{2n}$-symmetry was observed much later in Ref. 25. To be more precise, it is proved in Ref. 27 that there exists a unique structure of a $U_q\mathfrak{sl}_{2n}$-module in $\Omega^1(M_n)_q$ such that, first, the map d is a morphism of $U_q\mathfrak{sl}_{2n}$-modules, and, second, the left and right multiplications

$$\mathbb{C}[M_n]_q \otimes \Omega^1(M_n)_q \to \Omega^1(M_n)_q, \quad \Omega^1(M_n)_q \otimes \mathbb{C}[M_n]_q \to \Omega^1(M_n)_q$$

are morphisms of $U_q\mathfrak{sl}_{2n}$-modules. This is usually expressed by saying that the first order differential calculus $(\Omega^1(M_n)_q, d)$ is $U_q\mathfrak{sl}_{2n}$-covariant. Before Ref. 25 appeared, only $U_q(\mathfrak{sl}_n\times\mathfrak{sl}_n)$-covariance of the calculus was known.

The first order differential calculus allows us to define the q-analogs of partial derivatives as follows: Set

$$\mathrm{d}f = \sum_{a=1}^{n} \sum_{\alpha=1}^{n} \frac{\partial f}{\partial z_a^\alpha} \cdot dz_a^\alpha, \quad f \in \mathbb{C}[M_n]_q.$$

Here the left-hand side defines the right-hand one.

It is quite reasonable to regard the unital subalgebra in $\mathrm{End}(\mathbb{C}[M_n]_q)$ generated by all the derivatives as an analog of the algebra of differential operators with constant coefficients. This algebra seems to be interesting in itself. First of all, it admits a very explicit description. Namely, it is observed in Ref. 20 (Section 2) that the map $z_a^\alpha \mapsto \partial/\partial z_a^\alpha$ may be extended to an algebra homomorphism $\Upsilon:\mathbb{C}[M_n]_q \to \mathrm{End}(\mathbb{C}[M_n]_q)$ which means that the operators $\partial/\partial z_a^\alpha$ satisfy the same commutation relations as the generators z_a^α of $\mathbb{C}[M_n]_q$ do. Further, the algebra is invariant with respect to a certain natural $U_q(\mathfrak{sl}_n\times\mathfrak{sl}_n)$-action in $\mathrm{End}(\mathbb{C}[M_n]_q)$ defined via a q-analog of the commutator. Let us describe this latter observation in full detail.

Endow the space $\mathrm{End}(\mathbb{C}[M_n]_q)$ with a structure of $U_q(\mathfrak{sl}_n\times\mathfrak{sl}_n)$-module as follows: For $\xi \in U_q(\mathfrak{sl}_n\times\mathfrak{sl}_n)$, $T\in\mathrm{End}(\mathbb{C}[M_n]_q)$ put

$$\xi(T) = \sum_j \xi_j'' \cdot T \cdot S^{-1}(\xi_j'),$$

where $\Sigma_j \xi_j' \otimes \xi_j'' = \Delta(\xi)$ [here Δ denotes the comultiplication in $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$], S is the antipode of $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$, and the elements in the right-hand side are multiplied within $\mathrm{End}(\mathbb{C}[M_n]_q)$. It is explained in Ref. 20 that the $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$-covariance of the first order differential calculus $(\Omega^1(M_n)_q, d)$ and the explicit formulas for the $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$-action in $\mathbb{C}[M_n]_q$, presented in Proposition 2.1, allow one to prove $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$-invariance of the linear span of all $\partial/\partial z_a^\alpha$ in $\mathrm{End}(\mathbb{C}[M_n]_q)$ and to describe the $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$-action on the partial derivatives explicitly. The explicit description is based on the following intertwining property of the homomorphism Υ

$$\Upsilon(\xi f) = \omega(\xi)\Upsilon(f), \quad \forall\, \xi \in U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n), \quad \forall\, f \in \mathbb{C}[M_n]_q$$

with ω being the automorphism of $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$ (the "Chevalley involution") given by

$$\omega(E_i) = -F_i, \quad \omega(F_i) = -E_i, \quad \omega(K_i^{\pm 1}) = K_i^{\mp 1}.$$

B. A *q*-wave operator

Here we apply the results from the previous subsection to study the q-wave operator given by

$$\Box_q = \sum_{s \in S_n} (-q)^{l(s)} \cdot \frac{\partial}{\partial z_1^{s(1)}} \cdot \frac{\partial}{\partial z_2^{s(2)}} \cdot \ \cdots \ \cdot \frac{\partial}{\partial z_n^{s(n)}}.$$

Clearly, the q-wave operator belongs to the center of the algebra of quantum differential operators with constant coefficients since $\Box_q = \Upsilon(\det_q(\mathbf{z}))$. The latter formula, together with $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$-invariance of the q-determinant and the above intertwining property of Υ, implies also that the operator $\Box_q$ commutes with the action of $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$ in $\mathbb{C}[M_n]_q$. Also, we can easily prove that

$$K_n \cdot \Box_q = q^{-2} \Box_q \cdot K_n. \tag{3.1}$$

Indeed, the degree of the operator $\Box_q$ in $\mathbb{C}[M_n]_q$ is equal to $-n$ which means $\hat{K} \cdot \Box_q = q^{-2n} \cdot \Box_q \cdot \hat{K}$ [see (2.14)]. The latter equality implies (3.1) since $\Box_q$ commutes with all the $K_i^{\pm 1}$'s for $i \neq n$.

IV. A COVARIANCE PROPERTY

A. Formulation

The intertwining properties of the q-wave operator derived above may be written in a unified way as follows:

$$\Box_q^l \cdot \pi_{n-l}(\xi) = \pi_{n+l}(\xi) \cdot \Box_q^l, \quad \xi \in U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n). \tag{4.1}$$

It turns out that this obvious symmetry of the operator $\Box_q^l$ is a part of a large hidden symmetry.

Theorem 4.1: *For any $l \in \mathbb{N}$ the linear operator $\Box_q^l : \mathbb{C}[M_n]_q \to \mathbb{C}[M_n]_q$ intertwines the $U_q\mathfrak{sl}_{2n}$-actions π_{n-l} and π_{n+l}:*

$$\Box_q^l \cdot \pi_{n-l}(\xi) = \pi_{n+l}(\xi) \cdot \Box_q^l, \quad \xi \in U_q\mathfrak{sl}_{2n}$$

(in other words, the map $\Box_q^l : \mathcal{P}_{n-1} \to \mathcal{P}_{n+1}$ is a morphism of $U_q\mathfrak{sl}_{2n}$-modules).

We will prove Theorem 4.1 in Sec. IV E. The proof uses some results from the theory of quantum bounded symmetric domains which we recall in the subsequent three subsections. Very briefly, the idea is as follows (compare with Ref. 1): We use the q-Cauchy-Szegö integral formula to rewrite the operator $\Box_q^l$ as a q-integral operator; then, using some standard technique, we prove that the q-integral operator intertwines the $U_q\mathfrak{sl}_{2n}$-actions π_{n-l} and π_{n+l}.

B. A q-analog of the Cauchy-Szegö integral representation

For any bounded symmetric domain there is a multivariable generalization of the famous Cauchy formula, the so-called Cauchy-Szegö integral representation.[1,7] This integral formula restores a holomorphic function on the domain from its boundary value on the Shilov boundary. In the case of the unit matrix ball the Cauchy-Szegö formula looks as follows:

$$f(\mathbf{z}) = \int_{S(\mathcal{D})} \frac{f(\boldsymbol{\zeta})}{\det(1-\mathbf{z}\boldsymbol{\zeta}^*)^n} \mathrm{d}\nu(\boldsymbol{\zeta}).$$

Here $S(\mathcal{D})$ is the Shilov boundary of the unit matrix ball $\mathcal{D} \in M_n$

$$S(\mathcal{D}) = \{\mathbf{z} \in M_n | \mathbf{z}\mathbf{z}^* = 1\},$$

and $\mathrm{d}\nu$ is the unique U_n-invariant normalized measure on $S(\mathcal{D})$ which, of course, coincides with the Haar measure under the identification $S(\mathcal{D}) = U_n$.

A q-analog of this formula was found in Ref. 27 in framework of quantum bounded symmetric domain theory. Particularly, in that paper q-analogs of the Shilov boundary $S(\mathcal{D})$, the measure $\mathrm{d}\nu$, and the kernel $\det(1-\mathbf{z}\boldsymbol{\zeta}^*)^{-n}$ were found. In this subsection we recall all these results. We omit proofs. An interested reader might want to look into Ref. 27 which is the main reference for this section.

The q-analog of the Shilov boundary is described by a (noncommutative) $*$-*algebra* of functions on it. It is also natural to require the quantum Shilov boundary to be a homogeneous space of the *quantum* group $\mathrm{SU}_{n,n}$. Here is an explicit construction.

The localization of $\mathbb{C}[M_n]_q$ with respect to the multiplicative system $\det_q(\mathbf{z})^{\mathbb{N}}$ is called the algebra of regular functions on the quantum GL_n and is denoted by $\mathbb{C}[GL_n]_q$ (see Sec. II A). It was observed in Ref. 27 (Lemma 2.1) that there exists a unique involution $*$ in $\mathbb{C}[GL_n]_q$ such that

$$(z_a^\alpha)^* = (-q)^{a+\alpha-2n} \det_q(\mathbf{z})^{-1} \cdot \mathbf{z}^{\wedge(n-1)J_\alpha}_{J_a}, \tag{4.2}$$

with $J_c \overset{\text{def}}{=} \{1,2,\ldots,n\}\backslash\{c\}$ [here we use the notation (2.11)]. The $*$-algebra $\mathrm{Pol}(S(\mathcal{D}))_q = (\mathbb{C}[GL_n]_q, *)$ is a q-analog of the polynomial algebra on the Shilov boundary of the matrix ball $\mathcal{D}$. Note that

$$\det_q(\mathbf{z})\det_q(\mathbf{z})^* = \det_q(\mathbf{z})^*\det_q(\mathbf{z}) = q^{-n(n-1)}. \tag{4.3}$$

Let's describe a structure of homogeneous space of the quantum group $\mathrm{SU}_{n,n}$ on the quantum Shilov boundary. Recall that the q-determinant $\det_q(\mathbf{z})$ belongs to the center of $\mathbb{C}[M_n]_q$ and is a "relative invariant" with respect to the $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-action:

$$\xi\det_q(\mathbf{z}) = \varepsilon(\xi) \cdot \det_q(\mathbf{z}), \quad \xi \in U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n), \quad K_n\det_q(\mathbf{z}) = q^2\det_q(\mathbf{z}). \tag{4.4}$$

Using (4.4), one can make $\mathrm{Pol}(S(\mathcal{D}))_q$ into a $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-module algebra. [More precisely, we can use the above formulas to define a $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-action on negative powers of $\det_q(\mathbf{z})$ which suffices to extend the $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-action from $\mathbb{C}[M_n]_q$ to $\mathrm{Pol}(S(\mathcal{D}))_q$.]

In fact [see Ref. 27 (Section 2)], the above $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-module algebra structure in $\mathrm{Pol}(S(\mathcal{D}))_q$ may be extended to a structure of $U_q\mathfrak{sl}_{2n}$-module algebra which coincides on the subspace $\mathbb{C}[M_n]_q \subset \mathrm{Pol}(S(\mathcal{D}))_q$ with the $U_q\mathfrak{sl}_{2n}$-module algebra structure described in Proposition 2.3.

Let us recall the definition of the "real form" $U_q\mathfrak{su}_{n,n}$ of the quantum universal enveloping algebra $U_q\mathfrak{sl}_{2n}$. $U_q\mathfrak{su}_{n,n}$ is simply the pair $(U_q\mathfrak{sl}_{2n}, *)$ with $*$ being an involution in $U_q\mathfrak{sl}_{2n}$ determined by

$$E_n^* = -K_nF_n, \quad F_n^* = -E_nK_n^{-1}, \quad (K_n^{\pm 1})^* = K_n^{\pm 1},$$

$$E_j^* = K_j F_j, \quad F_j^* = E_j K_j^{-1}, \quad (K_j^{\pm 1})^* = K_j^{\pm 1}, \quad \text{for } j \neq n.$$

It is not difficult to verify that $U_q\mathfrak{su}_{n,n} = (U_q\mathfrak{sl}_{2n}, *)$ is a Hopf $*$-algebra (see Ref. 2 for definitions). Evidently, the involution $*$ keeps the Hopf subalgebras $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$ and $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$ invariant, and we shall denote the corresponding Hopf $*$-subalgebras in $U_q\mathfrak{su}_{n,n}$ by $U_q(\mathfrak{su}_n \times \mathfrak{su}_n)$ and $U_q\mathfrak{s}(\mathfrak{u}_n \times \mathfrak{u}_n)$, respectively.

The crucial property of the involution (4.2) is the following observation: it makes $\mathrm{Pol}(S(\mathcal{D}))_q$ into a $U_q\mathfrak{su}_{n,n}$-module algebra (this is explained in Ref. 27 after Proposition 2.7). It is in this sense that the quantum Shilov boundary is a homogeneous space of the quantum group $\mathrm{SU}_{n,n}$.

To define a q-analog of the measure $\mathrm{d}\nu$ on $S(\mathcal{D})$, we note [see Ref. 27 (Section 3)] that the $*$-algebra $\mathrm{Pol}(S(\mathcal{D}))_q$ is closely related to the $*$-algebra $\mathbb{C}[U_n]_q = (\mathbb{C}[GL_n]_q, \star)$ of regular functions on the quantum group U_n where, we recall, the involution $\star$ is defined by $(z_a^\alpha)^\star = (-q)^{a-\alpha}(\det_q \mathbf{z})^{-1} \cdot \mathbf{z}^{\wedge(n-1)J_\alpha}_{J_a}$. (The quantum group U_n is one of the most well studied objects in quantum group theory. We refer to Ref. 16 for basic definitions and facts about this quantum group. Of course, there are many other good references.)

It is easy to check that $* = \theta^{-1} \cdot \star \cdot \theta$ where $\theta: \mathbb{C}[GL_n]_q \to \mathbb{C}[GL_n]_q$ is an automorphism given by $\theta: z_a^\alpha \mapsto q^{\alpha - n} z_a^\alpha$. It is known that the compact quantum group U_n possesses a unique normalized invariant integral, an analog of the Haar integral. The isomorphism θ of $*$-algebras $\mathrm{Pol}(S(\mathcal{D}))_q \to \mathbb{C}[U_n]_q$ allows us to "transfer" the invariant integral onto $\mathrm{Pol}(S(\mathcal{D}))_q$. In this way we get a positive $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-invariant linear functional $\mathrm{Pol}(S(\mathcal{D}))_q \to \mathbb{C}$, $f \mapsto \int_{S(\mathcal{D})_q} f \mathrm{d}\nu$ which is the analog of the integral with respect to $\mathrm{d}\nu$. The $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-invariance means

$$\int_{S(D)_q} \xi f \mathrm{d}\nu = \varepsilon(\xi) \cdot \int_{S(\mathcal{D})_q} f \mathrm{d}\nu, \quad \forall\, \xi \in U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n). \tag{4.5}$$

Finally let us describe the analog of the Cauchy-Szegö kernel $\det(1 - \mathbf{z}\boldsymbol{\zeta}^*)^{-n}$.

Consider the algebra $\mathrm{Pol}(M_n \times S(\mathcal{D}))_q = \mathbb{C}[M_n]_q^{\mathrm{op}} \otimes \mathrm{Pol}(S(\mathcal{D}))_q$ with "op" indicating the change of the multiplication to the opposite one. Equip it with a $\mathbb{Z}_+$-grading by setting $\deg(z_a^\alpha \otimes f) = 1$ for any $f \in \mathrm{Pol}(S(\mathcal{D}))_q$. Its completion with respect to this grading is denoted by $\mathrm{Fun}(M_n \times S(\mathcal{D}))_q$. The elements of $\mathrm{Fun}(M_n \times S(\mathcal{D}))_q$ are q-analogs of kernels of integral operators, while the elements of the subalgebra $\mathrm{Pol}(M_n \times S(\mathcal{D}))_q$ are q-analogs of polynomial kernels.

Let us comment on the replacement of the multiplication law in the first tensor multiplier in the definition of the algebra $\mathrm{Pol}(M_n \times S(\mathcal{D}))_q$. Given a Hopf algebra A and two A-module algebras F_1, F_2, A-invariant elements in $F_1 \otimes F_2$ *do not* form a subalgebra. However, they do form a subalgebra in $F_1^{\mathrm{op}} \otimes F_2$.[26] Almost all the kernels we encounter in the present paper are $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-invariant in $\mathrm{Pol}(M_n \times S(\mathcal{D}))_q$ or $\mathrm{Fun}(M_n \times S(\mathcal{D}))_q$ and so, as we have explained, form a subalgebra.

Let us explain now why we are interested in $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-invariant kernels. It is not difficult to prove that there is a one-to-one correspondence between $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-invariant elements in $\mathrm{Fun}(M_n \times S(\mathcal{D}))_q$ and endomorphisms of the $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-module $\mathbb{C}[M_n]_q$, explicitly given as follows: the element $K \in \mathrm{Fun}(M_n \times S(\mathcal{D}))_q$ defines the morphism $f \mapsto (1 \otimes \int_{S(\mathcal{D})_q})(K \cdot (1 \otimes f))$. In other words, a linear operator on $\mathbb{C}[M_n]_q$ intertwines the $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-action if and only if it is a q-integral operator with an invariant kernel.

It is convenient to choose some generators of $\mathrm{Pol}(M_n \times S(\mathcal{D}))_q$ and express all other invariant kernels from $\mathrm{Pol}(M_n \times S(\mathcal{D}))_q$ or $\mathrm{Fun}(M_n \times S(\mathcal{D}))_q$ as (finite or formal) series in those generators.

Consider the elements $\chi_k \in \mathrm{Pol}(M_n \times S(\mathcal{D}))_q$, $k = 1, \ldots, n$, given by

$$\chi_k = \sum \mathbf{z}^{\wedge k}_{J''}{}^{J'} \otimes (\mathbf{z}^{\wedge k}_{J''}{}^{J'})^* \tag{4.6}$$

where the sum is taken over the pairs of subsets $J', J'' \subset \{1, 2, \ldots, n\}$ of cardinality k. It turns out that the elements χ_k are pairwise commuting and $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-invariant [Ref. 22 (Section 10)].

Proposition 4.2: *The elements $\chi_1, \ldots, \chi_n$ generate the subalgebra of $U_q\mathfrak{s}(\mathfrak{gl}_n \times \mathfrak{gl}_n)$-invariant kernels in $\mathrm{Pol}(M_n \times S(\mathcal{D}))_q$ (which is therefore a commutative algebra).*

Sketch of a proof: Recall (see Proposition 2.4) that the $U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)$-module $\mathbb{C}[M_n]_q$ splits into direct sum of simple pairwise nonisomorphic submodules $\mathbb{C}[M_n]_q^{\mathbf{k}}$ with $\mathbf{k}=(k_1,k_2,\ldots,k_n)$, $k_1\geqslant k_2\geqslant\cdots\geqslant k_n\geqslant 0$. Thus, any endomorphism of the $U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)$-module $\mathbb{C}[M_n]_q$ is a (in general infinite) series of the form $\Sigma_{\mathbf{k}}c_{\mathbf{k}}\cdot\mathbf{P}^{\mathbf{k}}$ where $\mathbf{P}^{\mathbf{k}}$ stands for the projection in $\mathbb{C}[M_n]_q$ onto $\mathbb{C}[M_n]_q^{\mathbf{k}}$ parallel to the sum of other $U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)$-submodules and $c_{\mathbf{k}}$ are complex numbers. It is sufficient to show that each projection $\mathbf{P}^{\mathbf{k}}$ is a q-integral operator whose kernel is a function of $\chi_1,\ldots,\chi_n$. This may be done by using well known orthogonality relations for the quantum group U_n (see Ref. 16) and the precise relation between the quantum Shilov boundary and the quantum U_n described previously. ■

The projection $\mathbf{P}^{\mathbf{k}}$ can be written as a q-integral operator with a kernel $P^{\mathbf{k}}\in\mathrm{Pol}(M_n\times S(\mathcal{D}))_q$. Namely, let $u^{\mathbf{k}}$ be a polynomial such that $P^{\mathbf{k}}(\mathbf{z},\boldsymbol{\zeta}^*)=u^{\mathbf{k}}(\chi_1,\chi_2,\ldots,\chi_n)$. Consider the isomorphism

$$\mathrm{Fun}(M_n\times S(\mathcal{D}))_q^{U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)}\to\mathbb{C}[[x_1,x_2,\ldots,x_n]]^{S_n},\quad \chi_k\mapsto\sigma_k,\quad k=1,2,\ldots n \tag{4.7}$$

from the subalgebra $\mathrm{Fun}(M_n\times S(\mathcal{D}))_q^{U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)}$ of $U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)$-invariants in $\mathrm{Fun}(M_n\times S(\mathcal{D}))_q$ to the algebra of symmetric formal series of the variables $x_1,x_2,\ldots,x_n$, where σ_k is the ith elementary symmetric polynomial in $x_1,x_2,\ldots,x_n$. The image of $u^{\mathbf{k}}(\chi_1,\chi_2,\ldots,\chi_n)$ under the above isomorphism differs only by a constant from the so-called Schur polynomial $s_{\mathbf{k}}$ associated to the partition $\mathbf{k}$ (see Ref. 17) viz.

$$u^{\mathbf{k}}(\sigma_1,\sigma_2,\ldots,\sigma_n)=C(\mathbf{k})\cdot s_{\mathbf{k}}(x_1,x_2,\ldots,x_n). \tag{4.8}$$

We compute the coefficients $C(\mathbf{k})$ in the next subsection.

From now on, for a kernel $K\in\mathrm{Fun}(M_n\times S(\mathcal{D}))_q$ we shall sometimes write

$$K(\mathbf{z},\boldsymbol{\zeta}^*),\quad \int_{S(\mathcal{D})_q}K(\mathbf{z},\boldsymbol{\zeta}^*)\cdot f(\boldsymbol{\zeta})\mathrm{d}\nu(\boldsymbol{\zeta}),$$

instead of K and $(1\otimes\int_{S(\mathcal{D})_q})(K\cdot(1\otimes f))$, respectively.

Now we are ready to present the q-analog of the Cauchy-Szegö integral formula found in Ref. 27. In short, it represents the identity operator on $\mathbb{C}[M_n]_q$ in the form of a q-integral operator.

Theorem 4.3: [*Ref.* 27 (*Sec.* 5)] *For any element* $f\in\mathbb{C}[M_n]_q$ *one has*

$$f(\mathbf{z})=\int_{S(\mathcal{D})_q}C_q(\mathbf{z},\boldsymbol{\zeta}^*)f(\boldsymbol{\zeta})\mathrm{d}\nu(\boldsymbol{\zeta})$$

where $C_q=\Pi_{j=0}^{n-1}(1+\Sigma_{k=1}^{n}(-q^{2j})^k\chi_k)^{-1}$ (*a q-analog of the Cauchy-Szegö kernel*).

C. q-analogs of the kernels $\det(1-\mathbf{z}\boldsymbol{\zeta}^*)^{-N}$

Consider the family K_N, $N=1$, 2, …, of $U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)$-invariant kernels given by

$$K_N=\prod_{j=0}^{N-1}\left(1+\sum_{k=1}^{n}(-q^{2j})^k\chi_k\right)^{-1}. \tag{4.9}$$

Clearly, the q-Cauchy-Szegö kernel C_q defined in the previous subsection coincides with K_n. One also has

$$\lim_{q\to 1}K_N(\mathbf{z},\boldsymbol{\zeta}^*)=\det(1-\mathbf{z}\boldsymbol{\zeta}^*)^{-N}$$

(the limit should be understood formally). The aim of this subsection is to study these kernels and the associated q-integral operators in detail.

Let $\mathbf{K}_N$ be the $U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)$-intertwining q-integral operator corresponding to the kernel K_N:

$$\mathbf{K}_N f(\mathbf{z}) = \int_{S(\mathcal{D})_q} K_N(\mathbf{z}, \boldsymbol{\zeta}^*) \cdot f(\boldsymbol{\zeta}) \mathrm{d}\nu(\boldsymbol{\zeta}).$$

Then

$$\mathbf{K}_N = \sum_{\mathbf{k}} c_N^{\mathbf{k}} \cdot \mathbf{P}^{\mathbf{k}} \tag{4.10}$$

where $\mathbf{P}^{\mathbf{k}}$ stands for the projection defined in the previous subsection (see the proof of Proposition 4.2). We are interested in an explicit formula for the coefficients $c_N^{\mathbf{k}}$.

One may write (4.10) as an equality of kernels:

$$K_N(\mathbf{z}, \boldsymbol{\zeta}^*) = \sum_{\mathbf{k}} c_N^{\mathbf{k}} \cdot P^{\mathbf{k}}(\mathbf{z}, \boldsymbol{\zeta}^*). \tag{4.11}$$

This approach, along with formula (4.8), allows us to use some identities for the Schur functions[17] to compute $c_N^{\mathbf{k}}$.

Our first step toward computing the coefficients in (4.10) consists in computing the constants $C(\mathbf{k})$ in (4.8). For that purpose, we note that

$$K_n(\mathbf{z}, \boldsymbol{\zeta}^*) = \sum_{\mathbf{k}} P^{\mathbf{k}}(\mathbf{z}, \boldsymbol{\zeta}^*)$$

(this is just another way to formulate Theorem 4.3). In view of the explicit form of the q-Cauchy-Szegö kernel (Theorem 4.3) and the isomorphism (4.7), the latter can be written as follows:

$$\prod_{j=0}^{n-1} \left(1 + \sum_{k=1}^{n} (-q^{2j})^k \sigma_k \right)^{-1} = \sum_{\mathbf{k}} u^{\mathbf{k}}(\sigma_1, \sigma_2, \ldots, \sigma_n),$$

or, by taking into account (4.8)

$$\prod_{j=0}^{n-1} \left(1 + \sum_{k=1}^{n} (-q^{2j})^k \sigma_k \right)^{-1} = \sum_{\mathbf{k}} C(\mathbf{k}) \cdot s_{\mathbf{k}}(x_1, x_2, \ldots, x_n). \tag{4.12}$$

Recall, for any integer $N \geqslant 0$, the q-Pochhammer symbol $(x;q^2)_N = \Pi_{j=0}^{N-1}(1 - xq^{2j})$. We have then,

$$\prod_{j=0}^{N-1} \left(1 + \sum_{k=1}^{N} (-q^{2j})^k \sigma_k \right)^{-1} = \prod_{j=0}^{N-1} \left(\prod_{i=1}^{n} (1 - q^{2j} x_i) \right)^{-1} = \prod_{i=1}^{n} \frac{1}{(x_i; q^2)_N};$$

in particular for $N = n$ the equality (4.12) reads

$$\prod_{i=1}^{n} \frac{1}{(x_i; q^2)_n} = \sum_{\mathbf{k}} C(\mathbf{k}) \cdot s_{\mathbf{k}}(x_1, x_2, \ldots, x_n).$$

Now we are in position to make use of the following formula from:[17]

$$\prod_{i=1}^{n} \frac{(a x_i; q^2)_\infty}{(x_i; q^2)_\infty} = \sum_{\mathbf{k}} C(\mathbf{k}; a) \cdot s_{\mathbf{k}}(x_1, x_2, \ldots, x_n) \tag{4.13}$$

where

$$C(\mathbf{k};a)=\prod_{i=1}^{n}\frac{(aq^{2-2i};q^2)_{k_i}\cdot q^{2(i-1)k_i}}{(q^2;q^2)_{k_i+n-i}}\cdot\prod_{1\leqslant i<j\leqslant n}(1-q^{2k_i-2k_j-2i+2j}). \tag{4.14}$$

In our case $a=q^{2n}$ and thus the equality (4.8) acquires the form

$$u^{\mathbf{k}}(\sigma_1,\sigma_2,\ldots,\sigma_n)=C(\mathbf{k};q^{2n})\cdot s_{\mathbf{k}}(x_1,x_2,\ldots,x_n), \tag{4.15}$$

where

$$C(\mathbf{k};q^{2n})=\prod_{i=1}^{n}\frac{q^{2(i-1)k_i}}{(q^2;q^2)_{n-i}}\cdot\prod_{1\leqslant i<j\leqslant n}(1-q^{2k_i-2k_j-2i+2j}).$$

We turn back now to computing the coefficients in (4.10). Identifying K_N with its image under the isomorphism (4.7), we have, in view of (4.9),

$$K_N=\prod_{j=0}^{N-1}\left(1+\sum_{k=1}^{n}(-q^{2j})^k\sigma_k\right)^{-1}=\prod_{i=1}^{n}\frac{1}{(x_i;q^2)_N}.$$

By (4.13) and (4.15)

$$K_N=\sum_{\mathbf{k}}C(\mathbf{k};q^{2N})\cdot s_{\mathbf{k}}(x_1,x_2,\ldots,x_n)=\sum_{\mathbf{k}}\frac{C(\mathbf{k};q^{2N})}{C(\mathbf{k};q^{2n})}u^{\mathbf{k}}(\sigma_1,\sigma_2,\ldots,\sigma_n). \tag{4.16}$$

We have thus obtained the following proposition

Proposition 4.4: *The coefficients in* (4.10) *are given by*

$$c_N^{\mathbf{k}}=\frac{C(\mathbf{k};q^{2N})}{C(\mathbf{k};q^{2n})}=\prod_{i=1}^{n}\frac{(q^{2N+2-2i};q^2)_{k_i}}{(q^{2n+2-2i};q^2)_{k_i}}.$$

D. A *q*-analog of the Fock inner product

The aim of this subsection is to describe some results on a q-analog of the Fock inner product in $\mathbb{C}[M_n]$ obtained in Ref. 20. At the end of the subsection we shall prove a q-analog of one known result by Faraut and Koranyi[5] which compares the Fock inner product with the one in the Hilbert space of square-integrable functions on the Shilov boundary of the matrix ball.

Recall that the Fock inner product in the space $\mathbb{C}[M_n]$ is defined by

$$(f_1,f_2)_F=\int_{M_n}f_1(\mathbf{z})\overline{f_2(\mathbf{z})}e^{-\mathrm{tr}(\mathbf{z}\mathbf{z}^*)}\mathrm{d}\mathbf{z} \tag{4.17}$$

with $\mathrm{d}\mathbf{z}$ being the Lebesgue measure on M_n normalized so that $(1,1)_F=1$. The inner product possesses the following remarkable property:

$$\left(\frac{\partial f_1}{\partial z_a^\alpha},f_2\right)_F=(f_1,z_a^\alpha f_2)_F,\qquad\forall\, a,\alpha. \tag{4.18}$$

This property, along with $S(U_n\times U_n)$-invariance of the inner product, is quite useful in explicit computations of various norms.

Below we present a q-analog of the Fock inner product. But first we have to explain what is understood by an invariance of an inner product in the q-setting.

Let $A_0=(A,*)$ be a Hopf $*$-algebra. An inner product $(,)$ on an A-module V is said to be A_0-invariant if for all $v_1,v_2\in V$ and any $\xi\in A$

$$(\xi v_1,v_2)=(v_1,\xi^* v_2).$$

The following is one of the main results of Ref. 20.

Proposition 4.5: *There exists a (unique)* $U_q\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_n)$*-invariant inner product* $(\cdot,\cdot)_F$ *in* $\mathbb{C}[M_n]_q$ *satisfying the properties*

$$(1,1)_F=1,$$

$$\left(\frac{\partial f_1}{\partial z_a^\alpha},f_2\right)_F=(f_1,f_2\cdot z_a^\alpha)_F,\quad \forall\, a,\alpha.$$

Let $(\cdot,\cdot)_{S(\mathcal{D})}$ be the inner product in $\mathbb{C}[M_n]_q$ defined via the $U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)$-invariant integral on the quantum Shilov boundary

$$(f_1,f_2)_{S(\mathcal{D})}=\int_{S(\mathcal{D})_q} f_2(\boldsymbol{\zeta})^* f_1(\boldsymbol{\zeta})\mathrm{d}\nu(\boldsymbol{\zeta}).$$

Clearly, the inner product is $U_q\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_n)$-invariant. This is a consequence of (4.5) and the condition (2.6). Since $(\cdot,\cdot)_F$ and $(\cdot,\cdot)_{S(\mathcal{D})}$ are $U_q\mathfrak{s}(\mathfrak{u}_n\times\mathfrak{u}_n)$-invariant, the subspaces $\mathbb{C}[M_n]_q^{\mathbf{k}}$ are pairwise orthogonal with respect to both inner products, and the corresponding norms are proportional by the Schur lemma. The proportionality constant is computed in the classical setting by Faraut and Koranyi [Ref. 5 (Corollary 3.5)]. Here we present a q-analog of their result.

Proposition 4.6:

$$(f_1,f_2)_F=\frac{\prod_{i=1}^{n}(q^{2n+2-2i};q^2)_{k_i}}{(1-q^2)^{k_1+k_2+\ldots+k_n}}\cdot(f_1,f_2)_{S(\mathcal{D})},\quad f_1,f_2\in\mathbb{C}[M_n]_q^{\mathbf{k}}. \tag{4.19}$$

Proof: To prove the proposition, we need an explicit description of the inner product $(\cdot,\cdot)_F$.

Consider the algebra $\mathbb{C}[M_n\times M_n]_q=\mathbb{C}[M_n]_q\otimes\mathbb{C}[M_n]_q$. Equip it with the natural bigrading by setting $\deg(f_1\otimes f_2)=(\deg(f_1),\deg(f_2))$ for any $f_1,f_2\in\mathbb{C}[M_n]_q$. Its completion with respect to this bigrading is denoted by $\mathbb{C}[[M_n\times M_n]]_q$.

Let

$$\hat{\chi}_k=\sum_{\substack{J',J''\subset\{1,2,\ldots,n\}\\ \mathrm{card}(J')=\mathrm{card}(J'')=k}}\mathbf{z}^{\wedge k}{}_{J''}^{J'}\otimes\mathbf{z}^{\wedge k}{}_{J''}^{J'}\in\mathbb{C}[M_n\times M_n]_q,\quad k=1,\ldots,n.$$

Note that $\hat{\chi}_k$ are similar to the kernels χ_k defined in (4.6). Since the latter pairwise commute, the elements $\hat{\chi}_k$ pairwise commute as well. Put

$$\hat{K}_\infty=\prod_{j=0}^{\infty}\left(1+\sum_{k=1}^{n}(-q^{2j})^k\hat{\chi}_k\right)^{-1}\in\mathbb{C}[[M_n\times M_n]]_q.$$

Let $\langle\cdot,\cdot\rangle$ be the inner product in $\mathbb{C}[M_n]_q$ so that $\hat{K}_\infty$ is the reproducing kernel, namely, writing $\hat{K}_\infty=\Sigma_j k_j'\otimes k_j''$ we have then

$$f=\sum_j k_j'\cdot\langle f,k_j''\rangle$$

Lemma 4.7:

$$\left\langle\frac{\partial f_1}{\partial z_a^\alpha},f_2\right\rangle=\frac{1}{1-q^2}\cdot\langle f_1,f_2\cdot z_a^\alpha\rangle,\quad \forall\, a,\alpha.$$

Sketch of a proof: The inner product $\langle\cdot,\cdot\rangle$ is described in a slightly different way in Ref. 20

(Theorem 6.1). The equivalence of the two definitions may be deduced from Theorem 9.1 in Ref. 22 via the limit $\lambda \to \infty$. ■

The above lemma allows us to express the inner product $\langle \cdot, \cdot \rangle$ via the q-Fock one

$$\langle f_1, f_2 \rangle = (1 - q^2)^k \cdot (f_1, f_2)_F \tag{4.20}$$

for f_1, f_2 homogeneous of degree k. Thus, to prove the theorem it suffices to show that

$$\langle f_1, f_2 \rangle = \prod_{i=1}^{n} (q^{2n+2-2i}; q^2)_{k_i} \cdot (f_1, f_2)_{S(\mathcal{D})}, \quad f_1, f_2 \in \mathbb{C}[M_n]_q^{\mathbf{k}}.$$

It follows from the q-Cauchy-Szegö formula (Theorem 4.3) that the inner product $(\cdot, \cdot)_{S(\mathcal{D})}$ is the one associated to the kernel

$$\hat{K}_n = \prod_{j=0}^{n-1} \left(1 + \sum_{k=1}^{n} (-q^{2j})^k \hat{\chi}_k \right)^{-1} \in \mathbb{C}[[M_n \times M_n]]_q$$

in the same sense as described above for $\hat{K}_\infty$. It remains to use the same arguments as in the previous subsection and to compare the coefficients $C(\mathbf{k}; 0)$ and $C(\mathbf{k}; q^{2n})$ [see (4.14)]. ■

In the last section of the present paper we shall present a more general result which is due to Ørsted,[18] and Faraut and Koranyi[5] in the classical setting.

E. Proof of the covariance property

Now we are in position to prove Theorem 4.1.

In view of Theorem 4.3, $\Box_q^l$ is the integral operator with the kernel $\Box_q^l K_n(\mathbf{z}, \boldsymbol{\zeta}^*)$ (here and further we assume that the operator $\Box_q$ acts on a kernel in the first argument $\mathbf{z}$). We are going to compute the kernel explicitly.

Recall the notation $P^{\mathbf{k}}(\mathbf{z}, \boldsymbol{\zeta}^*)$ for the kernel of the q-integral operator $\mathbf{P}^{\mathbf{k}}: \mathbb{C}[M_n]_q \to \mathbb{C}[M_n]_q^{\mathbf{k}}$ (see Sec. IV C)

$$\mathbf{P}^{\mathbf{k}} f(\mathbf{z}) = \int_{S(\mathcal{D})_q} P^{\mathbf{k}}(\mathbf{z}, \boldsymbol{\zeta}^*) f(\boldsymbol{\zeta}) \mathrm{d}\nu(\boldsymbol{\zeta}).$$

By Theorem 4.3,

$$C_q(\mathbf{z}, \boldsymbol{\zeta}^*) = \sum_{\mathbf{k}} P^{\mathbf{k}}(\mathbf{z}, \boldsymbol{\zeta}^*).$$

Thus to compute the kernel $\Box_q^l C_q(\mathbf{z}, \boldsymbol{\zeta}^*)$ it suffices to compute $\Box_q^l P^{\mathbf{k}}(\mathbf{z}, \boldsymbol{\zeta}^*)$. We observe that

$$\Box_q(\mathbb{C}[M_n]_q^{\mathbf{k}}) = \begin{cases} \mathbb{C}[M_n]_q^{\mathbf{k}-1}, & k_n \geqslant 1 \\ \{0\}, & \text{otherwise}. \end{cases} \tag{4.21}$$

[We use the notation $\mathbf{k} - l = (k_1 - l, k_2 - l, \ldots, k_n - l)$.] Indeed, the operator $\Box_q$ is, in particular, a morphism of $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$-modules, and all $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$-modules, isomorphic to $\mathbb{C}[M_n]_q^{\mathbf{k}}$, have the form $\mathbb{C}[M_n]_q^{\mathbf{k}+m}$ for some (positive or negative) m. The left-hand side is then a subspace of right-hand side by (3.1). On the other hand, if $k_n \geqslant 1$ and $\Box_q(\mathbb{C}[M_n]_q^{\mathbf{k}}) \subsetneqq \mathbb{C}[M_n]_q^{\mathbf{k}-1}$ then $\Box_q(\mathbb{C}[M_n]_q^{\mathbf{k}}) = \{0\}$ since $\mathbb{C}[M_n]_q^{\mathbf{k}}$ and $\mathbb{C}[M_n]_q^{\mathbf{k}-1}$ are simple isomorphic $U_q(\mathfrak{sl}_n \times \mathfrak{sl}_n)$-modules. This, however, contradicts positive definiteness of the q-Fock inner product: we have $\Box_q(\det_q(\mathbf{z}) \cdot f) = 0$ for arbitrary element $f \in \mathbb{C}[M_n]_q^{\mathbf{k}-1}$ and so

$$0 = (\Box_q(\det_q(\mathbf{z}) \cdot f), f)_F = (\det_q(\mathbf{z}) \cdot f, \det_q(\mathbf{z}) \cdot f)_F.$$

The equality (4.21), together with (4.3) and (4.4), implies that for certain constant $c(\mathbf{k}, l)$

$$\square_q^l P^{\mathbf{k}}(\mathbf{z},\boldsymbol{\zeta}^*) = c(\mathbf{k},l) P^{\mathbf{k}-l}(\mathbf{z},\boldsymbol{\zeta}^*)\det_q(\boldsymbol{\zeta})^{*l}.$$

Indeed, the q-integral operators with the kernels $\square_q^l P^{\mathbf{k}}(\mathbf{z},\boldsymbol{\zeta}^*)$ and $P^{\mathbf{k}-l}(\mathbf{z},\boldsymbol{\zeta}^*)\det_q(\boldsymbol{\zeta})^{*l}$ belong to

$$\mathrm{Hom}_{U_q(\mathfrak{sl}_n\times\mathfrak{sl}_n)}(\mathbb{C}[M_n]_q^{\mathbf{k}},\mathbb{C}[M_n]_q^{\mathbf{k}-l}),$$

and thus differ by a constant (the latter space is one-dimensional since $\mathbb{C}[M_n]_q^{\mathbf{k}}$ and $\mathbb{C}[M_n]_q^{\mathbf{k}-l}$ are isomorphic irreducible $U_q(\mathfrak{sl}_n\times\mathfrak{sl}_n)$-modules). Our immediate aim is to compute $c(\mathbf{k},l)$.

Given an inner product $(\cdot,\cdot)$ in $\mathbb{C}[M_n]_q$ and a kernel $P(\mathbf{z},\boldsymbol{\zeta}^*)=\Sigma_j p_j'\otimes p_j''\in \mathrm{Pol}(M_n\times S(\mathcal{D}))_q$ we shall write $(f(\mathbf{z}),P(\mathbf{z},\boldsymbol{\zeta}^*))$ instead of $\Sigma_j(f,p_j')\cdot(p_j'')^*$.

Recall the notation $(\cdot,\cdot)_{S(\mathcal{D})}$ for the inner product defined in Sect. IV D via the invariant integral on the q-Shilov boundary. It is not difficult to observe that the reproducing property of the kernel $P^{\mathbf{k}}(\mathbf{z},\boldsymbol{\zeta}^*)$ is equivalent to

$$(f(\mathbf{z}),P^{\mathbf{k}}(\mathbf{z},\boldsymbol{\zeta}^*))_{S(\mathcal{D})} = f, \quad \forall\, f\in\mathbb{C}[M_n]_q^{\mathbf{k}}.$$

We have

$$\square_q^l P^{\mathbf{k}}(\mathbf{z},\boldsymbol{\zeta}^*) = c(\mathbf{k},l) P^{\mathbf{k}-l}(\mathbf{z},\boldsymbol{\zeta}^*)\det_q(\boldsymbol{\zeta})^{*l}$$

or

$$(f(\mathbf{z}),\square_q^l P^{\mathbf{k}}(\mathbf{z},\boldsymbol{\zeta}^*))_{S(\mathcal{D})} = c(\mathbf{k},l)\cdot(f(\mathbf{z}),P^{\mathbf{k}-l}(\mathbf{z},\boldsymbol{\zeta}^*)\det_q(\boldsymbol{\zeta})^{*l})_{S(\mathcal{D})},$$

for any $f\in\mathbb{C}[M_n]_q^{\mathbf{k}-l}$. By Theorem 4.6

$$\frac{(1-q^2)^{k_1+k_2+\ldots+k_n-2l_n}}{\prod_{i=1}^n (q^{2n+2-2i};q^2)_{k_i-l}}(f(\mathbf{z}),\square_q^l P^{\mathbf{k}}(\mathbf{z},\boldsymbol{\zeta}^*))_F = c(\mathbf{k},l)\cdot f(\boldsymbol{\zeta})\cdot\det_q(\boldsymbol{\zeta})^l,$$

and, due to the main property of the q-Fock product,

$$\frac{(1-q^2)^{k_1+k_2+\ldots+k_n-2l_n}}{\prod_{i=1}^n (q^{2n+2-2i};q^2)_{k_i-l}}(f(\mathbf{z})\det_q(\mathbf{z})^l,P^{\mathbf{k}}(\mathbf{z},\boldsymbol{\zeta}^*))_F = c(\mathbf{k},l)\cdot f(\boldsymbol{\zeta})\cdot\det_q(\boldsymbol{\zeta})^l.$$

Apply Theorem 4.6 once again:

$$\frac{\prod_{i=1}^n (q^{2n+2-2i};q^2)_{k_i}}{(1-q^2)^{2ln}\cdot\prod_{i=1}^n (q^{2n+2-2i};q^2)_{k_i-l}}(f(\mathbf{z})\det_q(\mathbf{z})^l,P^{\mathbf{k}}(\mathbf{z},\boldsymbol{\zeta}^*))_{S(\mathcal{D})} = c(\mathbf{k},l)\cdot f(\boldsymbol{\zeta})\cdot\det_q(\boldsymbol{\zeta})^l.$$

The reproducing property of the kernel $P^{\mathbf{k}}(\mathbf{z},\boldsymbol{\zeta}^*)$ implies that

$$\frac{\prod_{i=1}^n (q^{2n+2-2i};q^2)_{k_i}}{(1-q^2)^{2ln}\cdot\prod_{i=1}^n (q^{2n+2-2i};q^2)_{k_i-l}}\cdot f(\boldsymbol{\zeta})\cdot\det_q(\boldsymbol{\zeta})^l = c(\mathbf{k},l)\cdot f(\boldsymbol{\zeta})\cdot\det_q(\boldsymbol{\zeta})^l,$$

consequently,

$$c(\mathbf{k},l)=\frac{\prod_{i=1}^{n}(q^{2n+2-2i};q^2)_{k_i}}{(1-q^2)^{2ln}\cdot\prod_{i=1}^{n}(q^{2n+2-2i};q^2)_{k_i-l}}.$$

We then get

$$\Box_q^l K_n(\mathbf{z},\boldsymbol{\zeta}^*)=\sum_{\mathbf{k}:k_n\geqslant l}\frac{\prod_{i=1}^{n}(q^{2n+2-2i};q^2)_{k_i}}{(1-q^2)^{2ln}\cdot\prod_{i=1}^{n}(q^{2n+2-2i};q^2)_{k_i-l}}\cdot P^{\mathbf{k}-l}(\mathbf{z},\boldsymbol{\zeta}^*)\det_q(\boldsymbol{\zeta})^{*l}$$

$$=\sum_{\mathbf{k}}\frac{\prod_{i=1}^{n}(q^{2n+2-2i};q^2)_{k_{i+l}}}{(1-q^2)^{2ln}\cdot\prod_{i=1}^{n}(q^{2n+2-2i};q^2)_{k_i}}\cdot P^{\mathbf{k}}(\mathbf{z},\boldsymbol{\zeta}^*)\det_q(\boldsymbol{\zeta})^{*l}.$$

Finally, Proposition 4.4 implies

$$\Box_q^l K_n(\mathbf{z},\boldsymbol{\zeta}^*)=\frac{\prod_{i=1}^{n}(q^{2n+2--2i};q^2)_l}{(1-q^2)^{2ln}}\cdot K_{n+l}(\mathbf{z},\boldsymbol{\zeta}^*)\cdot\det_q(\boldsymbol{\zeta})^{*l}.$$

We have thus obtained

Proposition 4.8: *For any element $f\in\mathbb{C}[M_n]_q$ one has*

$$\Box_q^l f(\mathbf{z})=\frac{\prod_{i=1}^{n}(q^{2n+2-2i};q^2)_l}{(1-q^2)^{2ln}}\cdot\int_{S(\mathcal{D})_q}K_{n+l}(\mathbf{z},\boldsymbol{\zeta}^*)\det_q(\boldsymbol{\zeta})^{*l}f(\boldsymbol{\zeta})\mathrm{d}\nu(\boldsymbol{\zeta}).$$

Proposition 4.8 reduces the statement of Theorem 4.1 to the following proposition.

Proposition 4.9: *The integral operator*

$$f(\mathbf{z})\mapsto\int_{S(\mathcal{D})_q}K_{n+l}(\mathbf{z},\boldsymbol{\zeta}^*)\det_q(\boldsymbol{\zeta})^{*l}f(\boldsymbol{\zeta})d\nu(\boldsymbol{\zeta})$$

intertwines the $U_q\mathfrak{sl}_{2n}$-actions π_{n-l} and π_{n+l}.

Proof: We shall use a quantum version of the description (2.16) of the twisted action π_λ.

Let us extend the algebra $\mathbb{C}[M_n]_q$ by adding one more generator t [an analog of the distinguished Plücker coordinate t in (2.16)] such that

$$tz_a^\alpha=q^{-1}z_a^\alpha t,\quad a,\alpha=1,2,\ldots,n.$$

The localization of the resulting algebra with respect to the multiplicative system $t^{\mathbb{N}}$ will be denoted by $\mathbb{C}[M_n]_{q,t}$. It was noted in Ref. 21 that there exists a unique extension of the $U_q\mathfrak{sl}_{2n}$-module algebra structure in $\mathbb{C}[M_n]_q$ to the one in $\mathbb{C}[M_n]_{q,t}$ such that

$$E_jt=F_jt=(K_j^{\pm1}-1)t=0\quad(j\neq n),\quad F_nt=(K_n^{\pm1}-q^{\mp1})t=0,\quad E_nt=q^{-1/2}tz_n^n.\tag{4.22}$$

It is clear that the subspace $\mathbb{C}[M_n]_q\cdot t^{-\lambda}\subset\mathbb{C}[M_n]_{q,t}$ is $U_q\mathfrak{sl}_{2n}$-invariant for any $\lambda\in\mathbb{Z}$. The following is an equivalent definition of the $U_q\mathfrak{sl}_{2n}$-action π_λ:

$$(\pi_\lambda(\xi)f)\cdot t^{-\lambda}=\xi(f\cdot t^{-\lambda}),\quad \xi\in U_q\mathfrak{sl}_{2n},\quad f\in\mathbb{C}[M_n]_q.$$

In other words, the linear map

$$\mathbb{C}[M_n]_q\to\mathbb{C}[M_n]_q\cdot t^{-\lambda},\quad f\mapsto f\cdot t^{-\lambda}$$

intertwines the $U_q\mathfrak{sl}_{2n}$-action π_λ and the natural $U_q\mathfrak{sl}_{2n}$-action in $\mathbb{C}[M_n]_q\cdot t^{-\lambda}$.

We also need certain extension of the algebra $\mathrm{Pol}(S(\mathcal{D}))_q$. Let us add to $\mathrm{Pol}(S(\mathcal{D}))_q$ two generators t, t^* such that

$$tt^*=t^*t,\quad tz_a^\alpha=q^{-1}z_a^\alpha t,\quad t^*z_a^\alpha=q^{-1}z_a^\alpha t^*,\quad a,\alpha=1,2,\ldots,n.$$

Denote this new algebra by $\mathrm{Pol}(\hat{S}(\mathcal{D}))_q$ and its localization with respect to the multiplicative system $(tt^*)^{\mathbb{N}}$ by $\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}$. The involution in $\mathrm{Pol}(S(\mathcal{D}))_q$ can be extended to an involution in $\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}$ by setting $*:t\mapsto t^*$. It is proved in [Ref. 27 (Sec. 2)] that there exists a unique structure of $U_q\mathfrak{su}_{n,n}$-module algebra in $\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}$ which coincides with the original one on $\mathrm{Pol}(S(\mathcal{D}))_q\subset\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}$ and satisfies (4.22). Following [Ref. 27 (Sec. 3)], we equip $\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}$ with a bigrading:

$$\deg t=(0,1),\quad \deg t^*=(1,0),\quad \deg(z_a^\alpha)=\deg(z_a^\alpha)^*=(0,0),\quad a,\alpha=1,2,\ldots,n.$$

Obviously, the homogeneous components

$$\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}^{(i,j)}=\{f\in\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}|\deg f=(i,j)\}=t^{*i}\cdot\mathrm{Pol}(S(\mathcal{D}))_q\cdot t^j$$

are submodules of the $U_q\mathfrak{sl}_{2n}$-module $\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}$.

Proposition 4.9 is an immediate consequence of the following statement.

Lemma 4.10: *The linear operator from* $\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}^{(0,l-n)}$ *to* $\mathbb{C}[M_n]_q\cdot t^{-l-n}$ *given by*

$$f\cdot t^{l-n}\mapsto\left(\int_{S(\mathcal{D})_q}K_{n+l}(\mathbf{z},\boldsymbol{\zeta}^*)\det_q(\boldsymbol{\zeta})^{*l}f(\boldsymbol{\zeta})\mathrm{d}\nu(\boldsymbol{\zeta})\right)\cdot t^{-l-n}$$

is a morphism of $U_q\mathfrak{sl}_{2n}$*-modules*.

Proof of the lemma: The proof may be easily reduced to the following three statements:

(i) The linear map

$$\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}^{(0,l-n)}\to\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}^{(l,-n)},\quad f(\boldsymbol{\zeta})\cdot t^{l-n}\mapsto\det_q(\boldsymbol{\zeta})^{*l}f(\boldsymbol{\zeta})\cdot t^{*l}t^{-n}\qquad(4.23)$$

is a morphism of $U_q\mathfrak{sl}_{2n}$-modules. This statement follows from the results of Secs. II and III in Ref. 27.

(ii) Let $K_{n+l}(\mathbf{z},\boldsymbol{\zeta}^*)=\Sigma_j k_j'(\mathbf{z})\otimes k_j''(\boldsymbol{\zeta}^*)$. Then the element

$$\sum_j k_j'(\mathbf{z})\cdot t^{-l-n}\otimes t^{*(-l-n)}\cdot k_j''(\boldsymbol{\zeta}^*)\in(\mathbb{C}[M_n]_q\cdot t^{-l-n})\hat{\otimes}\,\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}^{(-l-n,0)}$$

is a $U_q\mathfrak{sl}_{2n}$-invariant (here the symbol $\hat{\otimes}$ has the same meaning as the one in the equality $\mathbb{C}[M_n]_q\hat{\otimes}\mathrm{Pol}(S(\mathcal{D}))_q=\mathrm{Fun}(M_n\times S(\mathcal{D}))_q$). The statement is a consequence of results of Sec. 8 in Ref. 22. This, together with statement (i), implies that the map

$$\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}^{(0,l-n)}\to(\mathbb{C}[M_n]_q\cdot t^{-l-n})\hat{\otimes}\,\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}^{(-n,-n)},$$

$$f(\boldsymbol{\zeta})\cdot t^{l-n}\mapsto\sum_j k_j'(\mathbf{z})\cdot t^{-l-n}\otimes t^{*(-l-n)}\cdot k_j''(\boldsymbol{\zeta}^*)\det_q(\boldsymbol{\zeta})^{*l}f(\boldsymbol{\zeta})\cdot t^{*l}t^{-n}\qquad(4.24)$$

is a morphism of $U_q\mathfrak{sl}_{2n}$-modules.

(iii) The linear functional

$$\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}^{(-n,-n)} \to \mathbb{C}, \quad t^{*(-n)} \cdot f \cdot t^{-n} \mapsto \int_{S(\mathcal{D})_q} f(\boldsymbol{\zeta}) \mathrm{d}\nu(\boldsymbol{\zeta})$$

is a $U_q\mathfrak{sl}_{2n}$-invariant integral. This is proved in Sec. III of Ref. 27. As a consequence of this statement and statements (i) and (ii) we get: the linear operator from $\mathrm{Pol}(\hat{S}(\mathcal{D}))_{q,x}^{(0,l-n)}$ to $\mathbb{C}[M_n]_q \cdot t^{-l-n}$ given by

$$f(\boldsymbol{\zeta}) \cdot t^{l-n} \mapsto \sum_j k_j'(\mathbf{z}) \cdot t^{-l-n} \cdot \int_{S(\mathcal{D})_q} \Theta_i(k_j''(\boldsymbol{\zeta}^*)\det{}_q(\boldsymbol{\zeta})^{*l} f(\boldsymbol{\zeta})) \mathrm{d}\nu(\boldsymbol{\zeta}) \tag{4.25}$$

is a morphism of $U_q\mathfrak{sl}_{2n}$-modules (here Θ_l means the automorphism of the algebra $\mathrm{Pol}(S(\mathcal{D}))_q$ given by $f \mapsto t^{*(-l)} \cdot f \cdot t^{*l}$).

Lemma 4.10 follows from the latter statement and the equality

$$\int_{S(\mathcal{D})_q} \Theta_l(f(\boldsymbol{\zeta})) \mathrm{d}\nu(\boldsymbol{\zeta}) = \int_{S(\mathcal{D})_q} f(\boldsymbol{\zeta}) \mathrm{d}\nu(\boldsymbol{\zeta}), \quad \forall\, f$$

which is due to the simple observation that the functional $\int_{S(\mathcal{D})_q} f(\boldsymbol{\zeta}) \mathrm{d}\nu(\boldsymbol{\zeta})$ "picks up" the constant term of f and the constant terms of $\Theta_l(f)$ and f are the same. ■

Proposition 4.9, consequently Theorem 4.1, is now proved. ■

V. HOLOMORPHIC DISCRETE SERIES FOR $U_q\mathfrak{su}_{n,n}$

In this last section we study the holomorphic discrete series representations for $U_q\mathfrak{su}_{n,n}$ and study their analytic continuation.

After giving a definition of the holomorphic discrete series for $U_q\mathfrak{su}_{n,n}$, we prove an analog of a classical known result by Faraut and Koranyi[5] which allows one to express the inner product in a module of the holomorphic discrete series via the Fock inner product. We use the result to prove unitarizability of the modules $\mathcal{P}_\lambda$ with $\lambda > n-1$; the discrete series parameters are $\lambda > 2n-1$. We apply then the covariance property, proved earlier, to studying certain quotients of the modules $\mathcal{P}_\lambda$.

A. Definition of the holomorphic discrete series

We start by recalling the definition of the holomorphic discrete series for $\mathrm{SU}_{n,n}$. Fix $\lambda > 2n-1$ and consider the Hilbert space of holomorphic functions on the unit matrix ball $\mathcal{D}$ which are square integrable with respect to the measure $\det(1-\mathbf{z}\mathbf{z}^*)^{\lambda-2n}\mathrm{d}\mathbf{z}$ (here $\mathrm{d}\mathbf{z}$ is the normalized Lebesgue measure: $\int_{\mathcal{D}} \mathrm{d}\mathbf{z} = 1$). It is known[1] that the operators (2.17) are unitary on that Hilbert space. The corresponding representation of $\widetilde{\mathrm{SU}}_{n,n}$ is said to be a representation of the holomorphic discrete series.

Now let us turn to the quantum setting. Suppose $A_0 = (A, *)$ is a Hopf $*$-algebra. An A-module V is said to be a unitarizable A_0-module if there exists an inner product $(,)$ on V such that for all $v_1, v_2 \in V$ and any $\xi \in A$

$$(\xi v_1, v_2) = (v_1, \xi^* v_2)$$

(that is, V possesses an A_0-invariant inner product, see Sec. IV D).

Unitarizable $U_q\mathfrak{su}_{n,n}$-modules substitute unitary representations of $\mathrm{SU}_{n,n}$ (or $\widetilde{\mathrm{SU}}_{n,n}$) in the quantum setting. The following statement was proved in Ref. 22 (Corollary 6.5).

Proposition 5.1: *For $\lambda > 2n-1$ there exists a unique inner product $(,)_\lambda$ in $\mathcal{P}_\lambda$ such that for all $f_1, f_2 \in \mathcal{P}_\lambda$ and $\xi \in U_q\mathfrak{sl}_{2n}$*

$$(\pi_\lambda(\xi)f_1,f_2)_\lambda=(f_1,\pi_\lambda(\xi^*)f_2)_\lambda,$$

with the normalization $(1,1)_\lambda=1$.

Clearly, the unitarizable $U_q\mathfrak{su}_{n,n}$-modules $\mathcal{P}_\lambda$, $\lambda>2n-1$, are q-analogs of unitary representation of the holomorphic discrete series for $\widetilde{\mathrm{SU}}_{n,n}$.

The inner product $(,)_\lambda$ may be described explicitly as follows. Let us use the notation from the proof of Proposition 4.6. Consider the element

$$\hat{K}_\lambda=\frac{\prod_{j=0}^{\infty}\left(1+\sum_{k=1}^{m}(-q^{2(\lambda+j)})^k\hat{\chi}_k\right)}{\prod_{j=0}^{\infty}\left(1+\sum_{k=1}^{m}(-q^{2j})^k\hat{\chi}_k\right)}\in\mathbb{C}[[M_n\times M_n]]_q. \tag{5.1}$$

Then the inner product $(,)_\lambda$ is the one associated with the previous element, i.e.,

$$f=\sum_j k_j'\cdot(f,k_j'')_\lambda \tag{5.2}$$

provided $\hat{K}_\lambda=\Sigma_j k_j'\otimes k_j''$ (see Theorem 9.1 in Ref. 22).

B. A *q*-analog of a result by Faraut and Koranyi (Ref. 5)

In this subsection, we present a q-analog of Corollary 3.7 in Ref. 5 where (in the classical setting) the Fock inner product and the inner products $(,)_\lambda$ are compared. We then apply the result to the problem of analytic continuation of the holomorphic discrete series for $U_q\mathfrak{su}_{n,n}$.

Using the arguments preceding Proposition 4.6 we deduce that the inner product $(,)_\lambda$ and the q-Fock inner product on a particular simple $U_q\mathfrak{s}(\mathfrak{gl}_n\times\mathfrak{gl}_n)$-submodule $\mathbb{C}[M_n]_q^{\mathbf{k}}\subset\mathbb{C}[M_n]_q$ are proportional. The proportionality constant is given by the following formula.

Proposition 5.2: *Let* $\lambda>2n-1$. *Then*

$$(f_1,f_2)_F=\frac{\prod_{i=1}^{n}(q^{2\lambda+2-2i};q^2)_{k_i}}{(1-q^2)^{k_1+k_2+\cdots+k_n}}\cdot(f_1,f_2)_\lambda,\quad f_1,f_2\in\mathbb{C}[M_n]_q^{\mathbf{k}}. \tag{5.3}$$

Proof: Consider the reproducing kernel

$$K_\lambda=\frac{\prod_{j=0}^{\infty}\left(1+\sum_{k=1}^{m}(-q^{2(\lambda+j)})^k\chi_k\right)}{\prod_{j=0}^{\infty}\left(1+\sum_{k=1}^{m}(-q^{2j})^k\chi_k\right)}$$

associated to the element (5.1). The image of this kernel under the isomorphism (4.7) is given by

$$\prod_{i=1}^{n}\frac{(q^{2\lambda}x_i;q^2)_\infty}{(x_i;q^2)_\infty}.$$

By repeating the computation from Sec. IV C, one gets

$$(f_1,f_2)_{S(\mathcal{D})}=\prod_{i=1}^{n}\frac{(q^{2\lambda+2-2i};q^2)_{k_i}}{(q^{2n+2-2i};q^2)_{k_i}}\cdot(f_1,f_2)_\lambda,\quad f_1,f_2\in\mathbb{C}[M_n]_q^{\mathbf{k}}.$$

What remains is to apply Proposition 4.6. ■

The result of the above proposition has an important application to the problem of analytic continuation of the holomorphic discrete series. The point is that (5.3) allows one to define the sesquilinear form $(,)_\lambda$ on $\mathbb{C}[M_n]_q$ for any $\lambda \in \mathbb{R}$ for which all the multipliers $\Pi_{i=1}^n (q^{2\lambda+2-2i};q^2)_{k_i}$ are nonzero. It is not difficult to prove that the resulting form is still $U_q\mathfrak{su}_{n,n}$-invariant with respect to the corresponding twisted action. Indeed, the invariance is equivalent to the infinitely many equalities of the form

$$(\pi_\lambda(\xi)f_1,f_2)_\lambda = (f_1,\pi_\lambda(\xi^*)f_2)_\lambda, \quad \xi \in U_q\mathfrak{sl}_{2n}, f_1,f_2 \in \mathbb{C}[M_n]_q.$$

After simple transformations, each equality becomes an equality of two Laurent polynomials in q^λ which is known to hold for $\lambda > 2n-1$ by Proposition 5.1, and, thus, for any λ. It is natural to pose the problem of finding those λ's for which the corresponding sesquilinear form is positive definite, i.e. the corresponding $U_q\mathfrak{su}_{n,n}$-modules are unitarizable. In the classical setting, such λ's are said to belong to the continuous part of the Wallach set.[1]

The above-mentioned proposition implies positive definiteness of the inner product $(f_1,f_2)_\lambda$ for any $\lambda > n-1$:

Corollary 5.3: *The $U_q\mathfrak{su}_{n,n}$-modules $\mathcal{P}_\lambda$ are unitarizable for $\lambda > n-1$.*

For $n=2$, this statement was obtained in Ref. 23 (see Proposition 6.1).

C. Some consequences of the covariance property

In the previous subsection, we were able to deduce some irreducibility and unitarity property of $U_q\mathfrak{sl}_{2n}$-modules $\mathcal{P}_\lambda$ for any λ from the results obtained earlier. We will not pursue all the details here. It is immediate that $\mathcal{P}_\lambda$ is reducible for $\lambda = n-1, n-2,\ldots$ for the following obvious reason: by the covariance property, $\mathcal{P}_{n-l}^{(0)} = \mathrm{Ker}\,\Box_q^l$ is a submodule in $\mathcal{P}_{n-l}$. A related application of the covariance property is the following.

Proposition 5.4: *For any $l \in \mathbb{N}$ $\mathcal{P}_{n-l}/\mathcal{P}_{n-l}^{(0)}$ is a unitarizable $U_q\mathfrak{su}_{n,n}$-module isomorphic to $\mathcal{P}_{n+l}$.*

Proof: Unitarizability follows from the covariance property, Corollary 5.3, and injectivity of the induced morphism $\mathcal{P}_{n-1}/\mathcal{P}_{n-1}^{(0)} \to \mathcal{P}_{n+l}$ of $U_q\mathfrak{sl}_{2n}$-modules. Actually, this latter morphism is an isomorphism. To prove this, it suffices to show that the operator

$$\Box_q^l : \mathbb{C}[M_n]_q \to \mathbb{C}[M_n]_q$$

is surjective. In turn, it suffices to prove the latter statement for $l=1$, i.e. to show that $\Box_q$ is surjective. But this follows from (4.21). ■

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Energy transport in the Vaidya system

J. P. Krisch and E. N. Glass
Department of Physics, University of Michigan, Ann Arbor, Michigan 48109

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Energy transport mechanisms can be generated by imposing relations between null tetrad Ricci components. Several kinds of mass and density transport generated by these relations are studied for the generalized Vaidya system. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1915290]

I. INTRODUCTION

The Vaidya[1] space–time generalized the Schwarzschild vacuum solution by allowing mass parameter m_0 to be a function of retarded time. The extension created a spherically symmetric null fluid atmosphere. Glass and Krisch[2] pointed out that allowing the mass function to also depend on the radial coordinate created a more complex atmosphere containing an anisotropic string fluid in addition to Vaidya radiation.

The fluid parameters for the Vaidya atmosphere $\{\rho, p_r, p_\perp\}$ all depend on time through their relationship to the time-dependent mass function $m(u,r)$; they control the motion of matter through the atmosphere. The Ricci tensor null tetrad components (i.e., Ricci spinor components), Φ_{11} and Φ_{22}, for the generalized Vaidya space–time also depend on both spatial and time derivatives of the mass function. If we impose relations between these components then those relations will, in turn, impose matter transport in the Vaidya system. Conversely, if a particular mode of matter transport were assumed for the mass or one of the fluid parameters, it would contain within it a Ricci relation. Relating Ricci components is a way of imposing and classifying a range of atmospheric matter transport mechanisms. In this paper we consider the generalized Vaidya metric,[2,3] and examine how functional relations between Φ_{11} and Φ_{22} lead to mass transport described by the diffusion equation, by the wave equation, and by a dissipative transport equation of Telegrapher type.

In studying fluid transport, the transport equations are often reducible to ordinary differential equations by introducing a similarity variable; a well-known example of this is the diffusion variable, $\eta \sim r/\sqrt{t}$, suggested by Boltzmann[4] in 1894. All the transport equations studied in this paper have similarity solutions. The physical similarity of matter fields has been discussed by many authors.[5–8] The matter transport considered here is in the atmosphere around a compact object or an already existing black hole. By examining the similarity structure of the mass solution to the transport equations, we are able to relate the function of proportionality between the Ricci components to the spatial part of a similarity variable.

The paper is structured as follows: In the next section we briefly review the generalized Vaidya space–time. Matter transport mechanisms and their similarity structure are discussed in Sec. III. Some explicit examples are given in Sec. IV. Metric and tetrad details are provided in the Appendix.

Our sign conventions are $2A_{\nu;[\alpha\beta]}=A_\mu R^\mu{}_{\nu\alpha\beta}$, $R_{\mu\nu}=R^\alpha{}_{\mu\nu\alpha}$, and metric signature $(+,-,-,-)$. Greek indices range over $(0,1,2,3)=(u,r,\vartheta,\varphi)$. $\dot{m}$ abbreviates $\partial m/\partial u$, m' abbreviates $\partial m/\partial r$, with another prime for each higher derivative. Overhead carets denote unit vectors. Field equations are $G_{\mu\nu}=-8\pi T_{\mu\nu}$.

II. GENERALIZED VAIDYA SPACE–TIME

The Vaidya metric generalizes vacuum Schwarzschild when $m_0 \to m(u)$,

$$g^{\mathrm{vad}}_{\alpha\beta}\,\mathrm{d}x^{\alpha}\,\mathrm{d}x^{\beta} = A^{\mathrm{vad}}\,\mathrm{d}u^2 + 2\,\mathrm{d}u\,\mathrm{d}r - r^2(\mathrm{d}\vartheta^2 + \sin^2\vartheta\,\mathrm{d}\varphi^2), \tag{1}$$

where $A^{\mathrm{vad}}=1-2m(u)/r$. The only nonzero Weyl null tetrad component is $\Psi_2=-m(u)/r^3$. The Ricci tensor, with $l_\alpha\,\mathrm{d}x^\alpha=\mathrm{d}u$, is

$$R^{\mathrm{vad}}_{\alpha\beta} = \frac{2\dot{m}}{r^2} l_\alpha l_\beta.$$

The Vaidya metric has been generalized so that $m(u)\to m(u,r)$ and $A^{\mathrm{vad}}\to A^{\mathrm{gv}}=1-2m(u,r)/r$,

$$g^{\mathrm{gv}}_{\alpha\beta}\,\mathrm{d}x^{\alpha}\,\mathrm{d}x^{\beta} = A^{\mathrm{gv}}\,\mathrm{d}\,u^2 + 2\,\mathrm{d}u\,\mathrm{d}r - r^2(\mathrm{d}\vartheta^2 + \sin^2\vartheta\,\mathrm{d}\varphi^2). \tag{2}$$

The metric is Petrov type **D** with l_μ and n_μ principal null vectors (details are in the Appendix),

$$l_\mu\,\mathrm{d}x^\mu = \mathrm{d}u, \tag{3a}$$

$$n_\mu\,\mathrm{d}x^\mu = (A^{\mathrm{gv}}/2)\mathrm{d}u + \mathrm{d}r, \tag{3b}$$

$$m_\mu\,\mathrm{d}x^\mu = -(r/\sqrt{2})(\mathrm{d}\vartheta + i\sin\vartheta\,\mathrm{d}\varphi). \tag{3c}$$

Basis vectors for the generalized Vaidya metric are the unit vector set $(\hat{v}_\mu,\hat{r}_\mu,\hat{\vartheta}_\mu,\hat{\varphi}_\mu)$ and the related null set $(l_\mu,n_\mu,m_\mu,\overline{m}_\mu)$ such that

$$g^{\mathrm{gv}}_{\mu\nu} = \hat{v}_\mu\hat{v}_\nu - \hat{r}_\mu\hat{r}_\nu - \hat{\vartheta}_\mu\hat{\vartheta}_\nu - \hat{\varphi}_\mu\hat{\varphi}_\nu = l_\mu n_\nu + n_\mu l_\nu - m_\mu\overline{m}_\nu - \overline{m}_\mu m_\nu. \tag{4}$$

In terms of the basis vectors, metric g^{gv} has energy-momentum[2]

$$-8\pi T^{\mathrm{gv}}_{\mu\nu} = \psi l_\mu l_\nu + \rho\hat{v}_\mu\hat{v}_\nu + p_r\hat{r}_\mu\hat{r}_\nu + p_\perp(\hat{\vartheta}_\mu\hat{\vartheta}_\nu + \hat{\varphi}_\mu\hat{\varphi}_\nu) \tag{5}$$

with components

$$4\pi\psi = -\dot{m}/r^2, \tag{6a}$$

$$4\pi\rho = -4\pi p_r = m'/r^2, \tag{6b}$$

$$8\pi p_\perp = -m''/r. \tag{6c}$$

The Einstein tensor is computed from g^{gv} and given by

$$G^{\mathrm{gv}}_{\mu\nu} = -2\Phi_{11}(l_\mu n_\nu + n_\mu l_\nu + m_\mu\overline{m}_\nu + \overline{m}_\mu m_\nu) - 2\Phi_{22} l_\mu l_\nu - (\mathcal{R}/4)g^{\mathrm{gv}}_{\mu\nu}, \tag{7}$$

with components

$$\Phi_{11} = (2m' - rm'')/(4r^2) = 2\pi(p_\perp - p_r), \tag{8a}$$

$$\Phi_{22} = -\dot{m}/r^2, \tag{8b}$$

$$\mathcal{R} = 2(rm'' + 2m')/r^2 = -16\pi(p_\perp + p_r). \tag{8c}$$

An inspection of Eq. (8) shows that a relation between Φ_{11} and Φ_{22} will generate matter transport.

$S_{\mu\nu}=\frac{1}{2}\left(R^{\mathrm{gv}}_{\mu\nu}-\frac{1}{4}\mathcal{R}^{\mathrm{gv}}g_{\mu\nu}\right)$ is the trace-free Ricci tensor. Its eigenspectrum determines the Segre type of metric $g^{\mathrm{gv}}_{\mu\nu}$. The characteristic equation, $\det[S-\lambda I]=0$, is

$$\lambda^4 - (\Phi_{22})\lambda^3 - 2(\Phi_{11}^2)\lambda^2 + (\Phi_{11}^2\Phi_{22})\lambda + \Phi_{11}^4 = 0, \tag{9}$$

with factors

$$(\lambda - \Phi_{11})(\lambda + \Phi_{11})(\lambda^2 - \Phi_{22}\lambda - \Phi_{11}^2). \tag{10}$$

This set corresponds to Segre type [2,(11)]. The Ricci relations established below will not change the Segre type.

III. GEOMETRY AND TRANSPORT OF MATTER

A. Mass diffusion from fluid relations

The fluid components of the energy-momentum in Eq. (6) depend on both time and spatial derivatives, so matter transport will occur. Implicit in these equations is the relation

$$4\pi r^2\dot{\rho} = \partial_r\dot{m}.$$

If one also assumes

$$\dot{m} = 4\pi D_0 r^2 \partial_r \rho$$

then both the mass and density obey diffusion equations, the mass diffusing in a space whose determinant is dual to Vaidya,[2]

$$\dot{\rho} = D_0\nabla^2\rho, \tag{11a}$$

$$\dot{m} = D_0\nabla^{-2}m \tag{11b}$$

with $\nabla^2 = r^{-2}(\partial/\partial r)r^2(\partial/\partial r)$, $\nabla^{-2} = r^2(\partial/\partial r)r^{-2}(\partial/\partial r)$, and D_0 the diffusion constant. Equating the nonzero Ricci components will also produce motion of the mass and density.

B. Mass diffusion from Ricci components

Consider the quantities $(4r\Phi_{11})$ and $(r^2\Phi_{22})$. Equations (8a) and (8b) (with no assumptions) allow the relation between these quantities to be written as

$$\partial_u(4r\Phi_{11}) = r^2\partial_r\left[\frac{\partial_r(r^2\Phi_{22})}{r^2}\right]. \tag{12}$$

If there is a general linear relation between Φ_{11} and Φ_{22} such as

$$\Phi_{22} = h_d(r)\Phi_{11}, \tag{13}$$

then both Ricci components will evolve diffusively. We will show in the next section that $h_d(r)$ is related to a spatial similarity variable for the diffusion equation. For exact solutions mass is a more physical quantity and, if we impose this relation and examine mass transport, Eqs. (8a) and (8b) imply

$$\Phi_{11} = -(r/4)\partial_r(m'/r^2), \tag{14a}$$

$$\Phi_{22} = -\dot{m}/r^2 = -(rh_d/4)\partial_r(m'/r^2). \tag{14b}$$

The linear relation (13) together with (14b) yields

$$\dot{m} = (r^3h_d/4)\partial_r(m'/r^2) \tag{15}$$

and so the mass will also move diffusively.

The homogeneous solution of Eq. (15) is

$$m = r^3 c_1(u) + c_2(u), \quad \dot{c}_2 + r^3 \dot{c}_1 = 0,$$

$$8\pi\rho = -8\pi p_r = 6c_1(u), \tag{16}$$

$$p_r = p_\perp.$$

Equation $\dot{c}_2 + r^3\dot{c}_1 = 0$ is satisfied only for c_1 and c_2 both constant.

C. Mass transport by wave motion

The basic relation between the Ricci components, Eq. (12), is

$$\partial_u(4r\Phi_{11}) = r^2\partial_r\left[\frac{\partial_r(r^2\Phi_{22})}{r^2}\right].$$

If one assumes the Ricci components are related by

$$\partial_u\Phi_{22} = h_w(r)\Phi_{11} \tag{17}$$

then $r^2\Phi_{22}$ will evolve as a wave equation solution. Focusing again on the mass behavior, Eq. (8a) for Φ_{11} and Eq. (8b) for Φ_{22} provide a wave equation for the mass,

$$\ddot{m} - (h_w/4)r^3 m = 0$$

or

$$\ddot{m} - (h_w/4)r^5\partial_r(r^{-2}\partial_r m) = 0. \tag{18}$$

Classical wave motion provides shape preserving traveling solutions to the wave equations for functions with argument $(kr - \omega t)$. Therefore, consider a variable of the form $\eta = R(r) - T(u)$. The wave equation becomes

$$[\dot{T}^2 - (h_w/4)r^3(R')^2]m_{\eta\eta} - [\ddot{T} + (h_w/4)(r^3R'' - 2r^2R')]m_\eta = 0. \tag{19}$$

The transport equation is

$$\alpha m_{\eta\eta} - \beta m_\eta = 0,$$

$$\dot{T}^2 - (h_w/4)r^3(R')^2 = \alpha,$$

$$\ddot{T} + (h_w/4)(r^3R'' - 2r^2R') = \beta.$$

The simplest solutions require α and β to be separately zero. These are

$$h_w = \frac{4c_1}{r^3(R')^2}, \quad R = c_2r^3 + c_3, \quad T = T_0u + T_1, \tag{20}$$

and, as in diffusive transport, the proportionality function between the Ricci components is related to the similarity variable. The mass is given by any function of argument η, $m = F(\eta)$.

D. Dissipative transport

It is clear that the mode of matter transport depends on the relation chosen between Φ_{22} and Φ_{11}. Dissipative waves obey a Telegrapher equation,[9] combining both wave and diffusive elements,

$$\ddot{\chi} - c_0^2 \nabla^2 \chi + c_1 \dot{\chi} = 0, \tag{21}$$

where $\nabla^2 \chi = (1/r^2)\partial_r (r^2 \partial_r \chi)$. The relationship

$$(\partial_u + \alpha_0)\Phi_{22} + h_t(r)\Phi_{11} = 0 \tag{22}$$

will generate an equation of Telegrapher form for mass,

$$\ddot{m} - (h_t/4) r \nabla^{-2} m + \alpha_0 \dot{m} = 0. \tag{23}$$

This form of causal dissipative transport provides a richer tool for modeling than a pure diffusion equation, since it avoids the infinite propagation speeds associated with parabolic diffusion equations.[10] Causal transport has recently been discussed by Herrera and Santos.[11] As before, the function of proportionality h_t is related to a similarity variable.

E. Similarity and h_d

To see the relation of the proportionality function to the similarity structure of the diffusion equation, assume a mass solution and similarity variable with forms

$$m - m_0 = T(u)F(\eta),$$

$$\eta = R(r)/L(u).$$

Rewriting the mass diffusion equation (15), with $F_\eta = \mathrm{d}F/\mathrm{d}\eta$ results in

$$F_{\eta\eta} + F_\eta \left[L \left\{ \frac{R''}{(R')^2} - \frac{2}{rR'} \right\} + \frac{4R}{h_d r (R')^2} \dot{L} \right] - \left[\frac{4}{h_d r (R')^2} L^2 \frac{\dot{T}}{T} \right] F = 0. \tag{24}$$

This diffusion equation should have similarity form[4]

$$F_{\eta\eta} + 2\alpha\eta F_\eta - \beta F = 0.$$

We look for solutions with the same similarity form, and so the coefficients impose constraints. The coefficient of F relates β and $h_d(r)$,

$$\beta = \frac{4}{h_d r (R')^2} L^2 \frac{\dot{T}}{T}. \tag{25}$$

Removing r-dependence provides the relation between $R(r)$ and $h_d(r)$,

$$h_d = \frac{4c_0}{r(R')^2}. \tag{26}$$

With this h_d constraint, the u-dependent part of the coefficient β implies

$$L^2 \frac{\dot{T}}{T} = \beta c_0. \tag{27}$$

This allows Eq. (24) to be written as

$$F_{\eta\eta} + F_\eta \left[L \left\{ \frac{R''}{(R')^2} - \frac{2}{rR'} \right\} + (R/c_0)\dot{L} \right] - \beta F = 0.$$

The coefficient of F_η requires

$$2\alpha\eta = 2\alpha(R/L) = L\left[\frac{R''}{(R')^2} - \frac{2}{rR'}\right] + (R/c_0)\dot{L}. \tag{28}$$

Solutions of this equation depend on the value of α. Some example solutions will be given in Sec. IV. We note here that the choice $R=R_0r^3+R_1$, which solves

$$R''/R' - 2/r = 0, \tag{29}$$

provides an analog of the Boltzman similarity variable. For this choice Eq. (28) yields

$$L^2 = 4c_0\alpha u + L_0^2$$

with similarity variable $R(r)/L(u)$

$$\eta = \frac{R_0r^3 + R_1}{\sqrt{4c_0\alpha u + L_0^2}}$$

and proportionality function

$$h_d = \frac{4c_0}{r^5R_0^2}.$$

If $c_0=D_0R_0^2$ then $h_d=4D_0/r^5$. This choice yields a simple diffusion equation for mass.

F. Similarity and h_t

Assuming a mass and similarity variable of the form

$$m - m_0 = T(u)F(\eta), \quad \eta = R(r)/L(u)$$

we find

$$\left[\frac{\dot{L}^2}{L^2}\frac{R^2}{T} - \left(\frac{h_t}{4}\right)r(R')^2\right]F_{\eta\eta} - \left[R\left(2\dot{L}\frac{\dot{T}}{T} + \ddot{L} - 2\frac{\dot{L}^2}{L} + \alpha_0\dot{L}\right) + \left(\frac{h_t}{4}\right)L(rR'' - 2R')\right]F_\eta + \left[L^2\left(\frac{\ddot{T}}{T} + \alpha_0\frac{\dot{T}}{T}\right)\right]F = 0.$$

The relationship of h_t to the scaling variable in this similarity equation depends on the form of the time scaling function. The example that we shall use in the next section has $L=L_0$, and for this choice the similarity equation becomes

$$-\frac{h_t}{4}r(R')^2F_{\eta\eta} + L_0\frac{h_t}{4}(2R' - rR'')F_\eta + L_0^2\left(\frac{\ddot{T}}{T} + \alpha_0\frac{\dot{T}}{T}\right)F = 0. \tag{30}$$

For this choice of L, we see the diffusive relation between the proportionality function and the spatial scaling function again emerges as

$$h_t = \frac{4c_0}{r(R')^2}. \tag{31}$$

Telegrapher transport could allow many other relations to be imposed, reflecting the richer solution structure of this transport mechanism. In the next section we give some examples.

IV. TRANSPORT EXAMPLES

A. Similarity solutions

As an example of the mass transport solutions based on similarity, we consider a single scenario to which we apply all three transport mechanisms. The physical setting considered is a compact object of mass $m(u,\eta)$ with an atmosphere in which transport is occurring. We use solutions where the scale variable R and proportionality function $h(r)$ are the same for all transports,

$$R=\frac{R_0}{3}r^3, \quad L=L_0, \quad h(r)=\frac{4c_0}{R_0^2 r^5}. \tag{32}$$

In simple diffusion problems, the choice $L=L_0$ is applied to bounded systems where L_0 can be identified with a natural physical scale. For the Vaidya black hole, the Schwarzschild radius provides a physical distance scale and we could identify L_0 with an associated distance.

1. Diffusive transport

For diffusive transport with the choices above, the equations describing the evolution of the mass function are

$$F_{\eta\eta}-\beta F=0, \quad \dot{T}/T=\beta c_0/L_0^2. \tag{33}$$

The mass function, with time parameter $\tau_0^{-1}=\beta D_0 R_0^2/L_0^2$, will be given by

$$\begin{gathered} m=m_0+T_0 e^{u/\tau_0}F(\eta), \\ F(\eta)=F_0\sin(\sqrt{|\beta|}\,\eta+\delta), \quad \beta<0=F_0\sinh(\sqrt{\beta}\,\eta+\delta), \quad \beta>0. \end{gathered} \tag{34}$$

For $\beta<0$, the atmosphere is decaying in time as the Vaidya photons carry energy out of the system, while for $\beta>0$, mass is accreting. From the field equations, the density of the atmosphere is described by

$$\rho=\rho_0 e^{-u/\tau_0}\cos(\sqrt{|\beta|}\,\eta+\delta)=\rho_0 e^{u/\tau_0}\cosh(\sqrt{\beta}\,\eta+\delta), \tag{35}$$

where we have identified the initial atmospheric density and a time constant for the accretion or decay

$$\rho_0=\frac{T_0 F_0\sqrt{|\beta|}}{2\pi L_0}. \tag{36}$$

The similarity variable in this example is simply a distance coordinate. The decaying solution could describe a bounded atmosphere whose density decreases with distance away from the surface. There is zero radial pressure outer boundary described by $\sqrt{|\beta|}\,\eta_B+\delta=\pi/2$. In the decaying solutions, the atmosphere will go asymptotically to zero leaving a compact object of mass m_0. Because of the outgoing Vaidya radiation, there is no vacuum match until the atmosphere is gone. For the accreting solution, there is no zero radial pressure boundary. Since the accreting mass is entering the atmosphere from the exterior, this is expected. The density profile depends strongly on the phase δ. For $\delta=0$, the density increases as one looks upward from the core surface. For nonzero δ, the density decreases going up from the surface, reaching a minimum value which might be identified with the boundary between the atmosphere and the source of the accreting mass.

2. Telegrapher transport

The equations for Telegrapher transport with the scaling functions chosen are

$$F_{\eta\eta} - \beta F = 0,$$

$$\frac{L_0^2}{c_0}\left(\frac{\ddot{T}}{T} + \alpha_0 \frac{\dot{T}}{T}\right) = \beta.$$

Telegrapher transport has a wider set of solutions for the scaling choice than pure diffusive transport. One solution, using $\beta = 0$, is

$$T = T_0 e^{-\alpha_0 u},$$

$$F = F_0 \eta, \tag{37}$$

$$m = m_0 + \rho_1 r^3 e^{-\alpha_0 u}, \quad \rho_1 = T_0 F_0 / L_0.$$

The atmospheric density is related to the mass through the field equations by $\rho = m'/(4\pi r^2)$. The density for this case does not vary with radial distance from the black hole but does reflect the atmospheric decay, approaching zero as the atmosphere vanishes and the mass becomes m_0,

$$\rho = \rho_0 e^{-\alpha_0 u}, \quad \rho_0 = 3R_0\rho_1/4\pi. \tag{38}$$

The $\beta \neq 0$ solutions are similar to the diffusive solutions,

$$T = T_0 e^{\gamma u}, \quad \beta = (L_0^2/c_1)(\gamma^2 + \alpha_0 \gamma),$$

$$F = F_0 \sin(\sqrt{|\beta|}\,\eta + \delta), \quad \beta < 0,$$
$$F = F_0 \sinh(\sqrt{\beta}\,\eta + \delta), \quad \beta > 0, \tag{39}$$

$$m = m_0 + T(u)F(\eta).$$

B. A diffusively evaporating atmosphere

(a) *The boundary behavior:* In this example, we consider a compact object whose atmosphere is diffusively evaporating. An exact mass solution, given in Ref. 2, is

$$m = m_0 + (4\pi/3)r^3\rho_0 - (4\pi/3)k_2(r^5/10 + \mathfrak{D}_0 u r^3). \tag{40}$$

For this example the proportionality function follows directly from the diffusion equation:

$$h_d = 4D_0/r.$$

The atmospheric density associated with this mass is

$$\rho = \rho_0 - k_2(r^2/6 + \mathfrak{D}_0 u). \tag{41}$$

A boundary can be defined by requiring the radial pressure (and density, from the equation of state) to be zero. Solving the density equation for a boundary radius gives the boundary as a function of retarded time,

$$R_b^2 = \frac{6}{k_2}(\rho_0 - k_2 \mathfrak{D}_0 u).$$

Let the boundary move inward as the atmosphere evaporates until the atmosphere is gone and the radius is at the compact object boundary, R_c. This happens in time u_0, thus

$$R_c^2 = \frac{6}{k_2}(\rho_0 - k_2 \mathfrak{D}_0 u_0). \tag{42}$$

It follows that

$$R_b^2(u) = R_c^2 + 6\mathfrak{D}_0(u_0 - u). \tag{43}$$

The bounding surface of the core is parametrized as $R_c = 2m_0\alpha$. Substituting into (43) provides

$$R_b^2(u) = 4m_0^2\alpha^2 + 6\mathfrak{D}_0(u_0 - u). \tag{44}$$

The mass function places a constraint on the parameters. From Eq. (42) at time u_0,

$$(\alpha - 1)m_0 = \frac{128}{45} k_2 \pi m_0^5 \alpha^5. \tag{45}$$

Using Eqs. (42) and (45), the time for the evaporation process to complete is

$$\mathfrak{D}_0 u_0 = \frac{2}{3}\alpha^2 m_0^2 \left[\frac{64\pi\rho_0 m_0^2 \alpha^3}{15(\alpha - 1)} - 1 \right]. \tag{46}$$

The density and mass evolve as

$$\rho = \frac{k_2}{6}(R_c^2 - R_b^2) + k_2 \mathfrak{D}_0(u_0 - u), \tag{47}$$

$$m = m_0 + \frac{4\pi k_2}{45} R_b^5 + \frac{4\pi}{3} k_2 R_b^3 \left[\frac{R_c^2 - R_b^2}{6} + \mathfrak{D}_0(u_0 - u) \right]. \tag{48}$$

(b) *Extremal case:* The time at which the evaporation of the atmosphere is complete has an extremal value. Extremising Eq. (46) one finds

$$\frac{2(\alpha - 1)^2}{\alpha^3(4\alpha - 5)} = \frac{64\pi\rho_0 m_0^2}{15}.$$

The extremal time for the evaporation is

$$\mathfrak{D}_0 u_0 = \frac{2}{3}\alpha^2 m_0^2 \left[\frac{3 - 2\alpha}{4\alpha - 5} \right]. \tag{49}$$

The second derivative shows this is a minimum. For positive times, we require

$$1.25 < \alpha < 1.5.$$

(c) *Time estimates:* Take m_0 to be a solar size, $m_0 \sim 1.5 \times 10^3$ m. The diffusivity constant $\mathfrak{D}_0$ is related to the constancy of the jump distance (L) and frequency (f).[4] $\mathfrak{D}_0$ can be estimated as

$$\mathfrak{D}_0 \sim L^2 f.$$

For example, if the Debye frequency in a solid is the same as the jump frequency, we would have $f \sim 10^{13}$ Hz and the jump distance could be of the order of an angstrom, so that an estimate for the diffusivity is

$$\mathfrak{D}_0 \sim 10^{-7}\ \mathrm{m}^2/\mathrm{s}.$$

Using these estimates, the time for the atmosphere to vanish by diffusion is roughly

$$u_0 = 10^7\left(\frac{2}{3}\right)\alpha^2 \times 2.25 \times 10^6\left[\frac{3-2\alpha}{4\alpha-5}\right] \sim 1.5 \times 10^{13}\left[\frac{3-2\alpha}{4\alpha-5}\right]\alpha^2.$$

For $\alpha=1.4$, the time is about $10^{13}\ \mathrm{s} \sim 10^5$ years. The diffusivity is much larger than is normally measured since not all atomic oscillations will have an associated jump. A smaller diffusivity would increase the time.

V. DISCUSSION

In this paper we have examined some of the atmospheric matter transport mechanisms introduced by imposing a relation between Ricci components of the generalized Vaidya space–time. We found that diffusive, wave, and general Telegrapher-type transport can all follow from such a relation. Imposing a Ricci relation is a way of unifying matter transport mechanisms; if one started with a particular transport mechanism then a Ricci relation would emerge.

Examples of the matter transport mechanisms were given. All of the exact solutions describe atmospheres that are either accreting or decaying. The first two examples had the same similarity function but the density profiles in each solution were very different. The first Telegrapher solution describes a core object with a decaying atmospheric density varying only with time, and whose tangential and radial stress are all spatially constant tensions. In the pure diffusive solution, the densities vary with both distance from the core surface and time. The decaying atmospheres could be bounded by an exterior fluid of Vaidya radiation. The accreting solutions were surrounded by the source of accreting matter and Vaidya radiation. The third example, with a different proportionality function, examined a diffusing atmosphere around a core object of radius R_c in the range $2.5m_0 < R_c < 3m_0$. For an $R_c = 2.8m_0$ object with a diffusivity based on a solid Debye frequency there was a minimum evaporation time of about 10^5 years. Jump frequencies based on the actual atmospheric fluid would increase this time. Apart from the actual size of the evaporation time for a specific object, the model predicts that atmospheres around smaller core objects, near the lower end of the range, will take very much longer to diffusively evaporate than the atmospheres of larger core objects. This can be understood by looking at the initial size of the atmosphere. Using Eq. (44) at $u=0$, Eq. (49), and the parametrized boundary surface $R_c = 2m_0\alpha$, the initial atmospheric radius is

$$R_b^2|_{u=0} = 2R_c^2\left[\frac{\alpha-1}{4\alpha-5}\right], \quad 1.25 < \alpha < 1.5.$$

The smaller core objects have larger atmospheric envelopes, taking longer to evaporate. The smaller core has an extended atmosphere because its gravitational field is not strong enough to hold the atmosphere compactly.

Some additional insights into the meaning of the proportionality function can be seen for diffusive and wave transport by writing the transport equations in terms of variable $w = r^3$. The diffusive and wave transport equations become

$$\dot{m} = \left(\frac{9r^5 h_d}{4}\right) m_{ww},$$

$$\ddot{m} = \left(\frac{9r^5 h_w}{4}\right) m_{ww}.$$

In each case we can find the functional form of $h(r)$ that will produce the simplest transport and can relate that value to the diffusion constant or the wave velocity. Our example solutions include this simple case and a case where the mass and density evolution are more complex.

The choice $h_d(r)=4D_0/r^5$ yields a simple (u,w) diffusion equation for mass. From the Ricci relations and the field equations we see that

$$\dot{m}/r^2 = 2\pi h_d(p_r - p_\perp)$$

indicating that, with the Ricci relations, mass transport is driven by the pressure anisotropy. This also illustrates a drawback of the mass transport ansatz. Φ_{11} is certainly zero for isotropic pressures with a string equation of state [Eq. (8a) with $p_\perp=p_r$]. The assumed relation, $\Phi_{22}=h_d(r)\Phi_{11}$, then says that there is no time variation in the mass for isotropic pressures. In general, when the two Ricci components are not related, the mass can vary with time, even in the case of isotropic pressures.

We list the assumptions that lead to matter transport. For diffusion the specific choice $h_d=4D_0/r^5$ is used.

Assumption	Transport
$\dot{m}=4\pi D_0 r^2\partial_r\rho$	$\dot{m}-D_0\nabla^{-2}m=0,\ \dot{\rho}-D_0\nabla^2\rho=0$
$\Phi_{22}=(4D_0/r^5)\Phi_{11}$	$\dot{m}-D_0\nabla^{-2}m=0$
$\partial_u\Phi_{22}=h_w(r)\Phi_{11}$	$\ddot{m}-(h_w/4)r^3\nabla^{-2}m=0$
$(\partial_u+\alpha_0)\Phi_{22}+h_t(r)\Phi_{11}=0$	$\ddot{m}-(h_t/4)r\nabla^{-2}m+\alpha_0\dot{m}=0$

We have seen that imposing a Ricci relation provides a broad arena to investigate a range of atmospheric transport processes in the generalized Vaidya space–time and is a rich source of new analytic mass solutions. The mass solutions that we presented focused on the growth or depletion of an atmosphere around a central object. They can be used to describe the behavior, for example, of isolated black hole atmospheres but also offer simple models of galaxies with a massive black hole at the center. The relationships we imposed on the Ricci components were investigated in terms of mass transport although the fundamental relationships described the evolution of the Ricci components themselves. The Ricci evolution is an interesting avenue for further investigation as they are input functions for the Riemann invariants. The evolution of the invariants and their syzigies will be discussed elsewhere.

APPENDIX: GENERALIZED VAIDYA PRINCIPAL NULL FRAME

The principal null frame Eq. (3) of the Petrov type **D** metric $g^{\rm gv}_{\mu\nu}$ obeys

$$l_{\mu;\nu} = (A'_{\rm gv}/2)l_\mu l_\nu - (1/r)(m_\mu\overline{m}_\nu + \overline{m}_\mu m_\nu), \tag{A1a}$$

$$n_{\mu;\nu} = -(A'_{\rm gv}/2)n_\mu l_\nu + (A^{\rm gv}/2r)(m_\mu\overline{m}_\nu + \overline{m}_\mu m_\nu), \tag{A1b}$$

$$m_{\mu;\nu} = (A^{\rm gv}/2r)l_\mu m_\nu - (1/r)n_\mu m_\nu + (\cot\vartheta/\sqrt{2}r)(m_\mu m_\nu - m_\mu\overline{m}_\nu). \tag{A1c}$$

with both principal null vectors l_μ and n_μ geodesic.

For tetrad $\{\hat{v},\hat{r},\hat{\vartheta},\hat{\varphi}\}$ and metric $g^{\rm gv}_{\mu\nu}=\hat{v}_\mu\hat{v}_\nu-\hat{r}_\mu\hat{r}_\nu-\hat{\vartheta}_\mu\hat{\vartheta}_\nu-\hat{\varphi}_\mu\hat{\varphi}_\nu$, the basis vectors are related by

$$\hat{v}_\mu\,{\rm d}x^\mu = A^{1/2}_{\rm gv}\,{\rm d}u + A^{-1/2}_{\rm gv}\,{\rm d}r = A^{-1/2}_{\rm gv}[n_\mu + (A_{\rm gv}/2)l_\mu]{\rm d}x^\mu, \tag{A2a}$$

$$\hat{r}_\mu\,{\rm d}x^\mu = A^{-1/2}_{\rm gv}\,{\rm d}r = A^{-1/2}_{\rm gv}[n_\mu - (A_{\rm gv}/2)l_\mu]{\rm d}x^\mu, \tag{A2b}$$

$$\hat{\vartheta}_\mu\,{\rm d}x^\mu = r\,{\rm d}\vartheta = (1/\sqrt{2})(m_\mu + \overline{m}_\mu){\rm d}x^\mu, \tag{A2c}$$

$$\hat{\varphi}_\mu \, \mathrm{d}x^\mu = r \sin\vartheta \, \mathrm{d}\varphi = -(i/\sqrt{2})(m_\mu - \overline{m}_\mu)\mathrm{d}x^\mu. \tag{A2d}$$

The kinematics of the $\hat{v}$ flow, acceleration, expansion, and shear, are described by

$$\hat{v}^\mu{}_{;\nu} = a^\mu \hat{v}_\nu + \sigma^\mu{}_\nu - (\Theta/3)(\hat{r}^\mu \hat{r}_\nu + \hat{\vartheta}^\mu \hat{\vartheta}_\nu + \hat{\varphi}^\mu \hat{\varphi}_\nu), \tag{A3}$$

where

$$a^\mu = [\dot{m}/r + A_{\mathrm{gv}} \partial_r (m/r)] A_{\mathrm{gv}}^{-3/2} \hat{r}^\mu, \tag{A4a}$$

$$\sigma^\mu{}_\nu = (\Theta/3)(-2\hat{r}^\mu \hat{r}_\nu + \hat{\vartheta}^\mu \hat{\vartheta}_\nu + \hat{\varphi}^\mu \hat{\varphi}_\nu), \tag{A4b}$$

$$\Theta = (\dot{m}/r) A_{\mathrm{gv}}^{-3/2}. \tag{A4c}$$

Spherical symmetry allows the function $m(u,r)$ to be identified as the mass within two surfaces of constant u and r, and invariantly defined from the sectional curvature of those surfaces,

$$-2m/r^3 = R_{\alpha\beta\mu\nu} \hat{\vartheta}^\alpha \hat{\varphi}^\beta \hat{\vartheta}^\mu \hat{\varphi}^\nu. \tag{A5}$$

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Random partial orders, posts, and the causal set approach to discrete quantum gravity

Avner Ash[a)]
Boston College, Chestnut Hill, Massachusetts 02467

Patrick McDonald[b)]
New College of Florida, Sarasota, Florida 34243

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We study a collection of Markov chains with values in the collection of partial orderings of the natural numbers. These systems arise naturally in the causal set approach to discrete quantum gravity and include the well-studied random partial orders of Alon, Bollobas, Brightwell, and Janson [Ann. Appl. Probab. **4**, 108–123 (1994)]. We prove that under the dynamics associated to Markov chains in our collection, posts occur infinitely often, almost surely. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1922070]

I. INTRODUCTION

The causal set approach to quantum gravity posits that the deep structure of space–time should be modeled on discrete structures admitting a causal order (cf. Bombelli *et al.*, 1987; Brightwell *et al.*, 2002a, 2002b; Dou and Sorkin, 2003; Martin *et al.*, 2002; Rideout and Sorkin, 2000; Sorkin, 2000, 1997, and references therein). Such discrete structures are called *causets*, and much work has been done to construct stochastic classical dynamics for causet evolution in hopes that this might serve as a guide to developing corresponding quantum dynamics. There is an attractive classification for possible stochastic dynamics for causets which satisfy a discrete version of covariance and relativistic causality: such dynamics are given by Markov chains which are defined by a sequence of coupling constants, t_n, $n \geqslant 0$, where $t_0 = 1$ and $t_n \geqslant 0$ for all $n > 0$ (cf. Rideout and Sorkin, 2000). Such dynamics are collectively referred to as "classical sequential growth models" (CSG).

In seeking to understand the possible role of CSG models in dealing with problems involving the unexplained "large numbers" in cosmology related to the size of the universe and its high degree of homogeneity and isotropy, Sorkin (2000) relates such problems to the number of cycles of contraction and re-expansion through which the universe has gone to date. He then notes that contraction followed by re-expansion has the effect of "renormalizing" the coupling constants of a CSG model in a definite manner [cf. (2.13) below], and argues that this observation provides a possible method for isolating a collection of dynamical laws which might play a distinguished physical role: those CSG models which are attractors under cycles of contraction and re-expansion. A study of such models was undertaken by Dou (1999) and further developed in Martin *et al.* (2002), where the authors note that the question of *which dynamical laws lead to cycles of contraction followed by re-expansion* is very much open.

The results of the above-mentioned studies suggest a natural avenue for further constraining the coupling constants defining the class of CSG models: consider those models which are stable "under cycles of contraction and re-expansion." A representation theorem for the corresponding class of Markov chains [which we call *GCD chains* (cf. Definition 2.4)] was established in Ash and McDonald (2003). This paper continues the study of GCD chains.

[a)]Electronic mail: avner.ash@bc.edu
[b)]Electronic mail: ptm@virtu.sar.usf.edu

The fixed points under renormalization play a fundamental role in understanding GCD chains and their relation to general CSG models. Every such fixed point is represented by the much-studied random graph process investigated by Barak and Erdós twenty years ago and known in the physics literature as *transitive percolation*.

Transitive percolation, the standard model for producing random partial orders on the natural numbers, is easy to describe inductively: Fix $0<p<1$ and suppose that we already have our randomly chosen partial order on n nodes labeled $0,1,\ldots,n-1$ (which is always assumed to be consistent with the natural ordering given by the node labelings). Introduce a new node (labeled n) and with probability p introduce an edge directed to the new node from each of the existing nodes, the addition of each edge being independent of all other edges. Finally, take the transitive closure of the partial order obtained once the random edges are determined (cf. Sec. II for examples).

A great deal is known about transitive percolation; the associated literature falls under a number of titles related to "random graphs" and there are many applications [cf. Bollobás and Brightwell (1997), and references therein]. Our interest is primarily directed toward the existence of *posts* which are defined to be nodes in a partial order of $\mathbb{N}$ which are ordered with respect to every other node in $\mathbb{N}$.

Posts were introduced by Alon, Bollobás, Brightwell, and Janson in (1994) where their properties with respect to transitive percolation were first studied. In particular, it was shown in Alon, Bollobás, Brightwell, and Janson (1994) that, under transitive percolation with any fixed p, an infinite number of posts occur, almost surely. Our main goal is to establish the same result for each of a certain dense family of GCD chains. Postponing the technicalities to Sec. II, we can give a statement of our main result:

Theorem 1.1: *Let M be a Markov chain taking values in the partial orderings on the natural numbers. Suppose that M exhibits general covariance, Bell causality and renormalizability (cf. Definition 2.1, Definition 2.3). Suppose further that the support of M (cf. Definition 2.6) is compact and that the supremum of the support is isolated. Then under the dynamics generated by M, an infinite number of posts occur, almost surely.*

In addition to providing new examples of dynamics which produce an infinite number of posts, almost surely, our result indicates that our notion of CSG models is consistent: If the dynamical laws are renormalizable (which follows from a hypothetical past with infinitely many cycles of contraction and re-expansion), then they will generate cycles of contraction and re-expansion infinitely often in the future. We expect our result to have a number of applications both in physics (discrete universes satisfying the hypotheses of our theorem will have an infinite number of cycles of expansion and contraction, almost surely) and in mathematics (various other properties of transitive percolation should also be inherited by random partial orders which satisfy the hypotheses of our theorem).

The paper is organized as follows: In Sec. II we provide the necessary background information and notation, including a mathematical introduction to causet dynamics and a discussion of the notion of "posts" in random partial orders. In Sec. III we provide a proof of our main result, Theorem 1.1.

In Sec. IV we prove a related theorem about the asymptotic behavior of GCD chains. Namely, in a sense made precise there, any GCD chain approaches a transitive percolation in the limit of large time. This result is illustrative of our viewpoint: We view transitive percolations as the building blocks of GCD chains and, in the limit of large time (again, in a sense made precise in Sec. IV), the behavior of any given GCD chain will be given by a transitive percolation associated to this chain. Unfortunately, this asymptotic property appears to be too weak in itself to imply the existence of infinitely many (or even just one) posts, almost surely.

Throughout the paper we usually work with *labeled* causets. In particular, references to "time" are usually references to a "gauge time" associated to a particular Markov chain and not to the physical time of space–time. Similarly, references to the "state of the system" involve references to the state of a particular Markov chain and not to the state of the physical universe at a particular time.

II. BACKGROUND

Let $[n]$ denote the set $\{0,1,2,\ldots,n\}$ with the natural partial order denoted by $<$. Let $\mathcal{C}_n$ be the collection of all subgraphs of the complete graph on the vertex set $[n]$. Suppose that $\mathcal{C} \in \mathcal{C}_n$ has an edge, ij, given by vertices i and j with $i<j$. We introduce a direction along edges by requiring that ij be directed from i to j. The graph C with edges so directed induces a partial order on $[n]$; we say $i<j$ if there is a directed edge in C from i to j. This provides an identification of a subset of the directed graphs on $[n]$ (those with edge directions consistent with the natural labeling of the vertices) with the collection of partial orders on $[n]$ which are extendible to the natural order on $[n]$. Allowing n to vary we define a set

$$\mathcal{C} = \bigcup_{n \in \mathbb{N}} \mathcal{C}_n. \tag{2.1}$$

We call elements of $\mathcal{C}$ *labeled causets*. We call any equivalence class of labeled causets under (order preserving) isomorphisms a *causet*. We will denote the equivalence classes by a tilde (for example, $\tilde{\mathcal{C}}$ is the set of all causets). In the calculations which follow, we usually work with labeled causets.

It is clear that for $m<n$, there is a natural inclusion $\mathcal{C}_m \subset \mathcal{C}_n$ which induces a partial order on $\mathcal{C}$. This partial order extends to causets, two causets being ordered if they admit representatives in $\mathcal{C}_n$, and $\mathcal{C}_m$ with $n<m$ and there exists an order preserving function $f: C \to D$ such that $f(C)$ is an initial segment of D. We will denote the partial order on both causets and labeled causets with the symbol $\prec\prec$.

Recall, a *link* in a partially ordered set is an irreducible relation (i.e., a relation that contains no other relation). A *path* in a partially ordered set is a sequence of elements of the set, each related to the next by a link.

Given $C \in \mathcal{C}$ and an element $x \in C$, we define the past of x by

$$\text{past}_C(x) = \{y \in C : y \prec x\}. \tag{2.2}$$

We will regard $\text{past}_c(x)$ as a poset with partial order given by the partial order of C. Similarly, the future of an element $x \in C$ is defined to be

$$\text{future}_C(x) = \{y \in C : x \prec y\}. \tag{2.3}$$

Given $C \in \mathcal{C}_n$, we will define the family of C, denoted $F(C)$, as those elements $D \in \mathcal{C}_{n+1}$ such that $C \prec\prec D$:

$$F(C) = \{D \in \mathcal{C}_{n+1} : C \prec\prec D\}. \tag{2.4}$$

Given $C \in \mathcal{C}_n$ and $D \in F(C)$, the *precursor set of the transition* $C \to D$, denoted $\text{Prec}(C,D)$, is the past of the element $x \in D \setminus C$:

$$\text{Prec}(C,D) = \text{past}_D(x) \subset C. \tag{2.5}$$

Note that $\text{Prec}(C,D)$ is a poset with partial order given by its description as the past of an element $x \in D$. The collection of *maximal elements associated to the transition* $C \to D$ is the collection of elements of C with links to the element x:

$$\max(C,D) = \{y \in D : y \text{ linked to } x,\ \{x\} = D \setminus C\}. \tag{2.6}$$

While the above-mentioned material is described in the context of labeled causets, a completely parallel development can be given for causets.

Before giving the formal definition of the Markov chains upon which our work will focus, we give an informal description of the processes with which we will deal.

Initially, the state of our system is given by the trivial poset consisting of a single point. At each increment of time, an element comes into existence as the "offspring" of elements already in existence. That is, at the beginning of the nth increment of time we have an element $C \in \mathcal{C}_n$ which

we evolve to an element $D \in \mathcal{C}_{n+1}$ by adding an element to C together with relations between the new element and a subset of elements of C (those elements in the past of the new element, i.e., those which bear some causal relationship to the new element). The new relations are determined randomly; the probability that any given collection of relations is added is given by a collection of transition probabilities which define the process.

We define a collection of Markov chains with state space $\mathcal{C}$ as follows:

Definition 2.1: We say that a Markov chain M with state space $\mathcal{C}$ belongs to the collection $\mathcal{M}$ if the transition probabilities of M satisfy:

(1) Given $C \in \mathcal{C}_n$, let $\mathrm{Prob}(C \to D)$ denote the transition probability corresponding to an evolution from causet C to causet D. Then $\mathrm{Prob}(C \to D) = 0$ if $D \notin F(C)$ and $\Sigma_{D \in F(C)} \mathrm{Prob}(C \to D) = 1$.

(2) (General Covariance) Let $\tilde{C} \in \tilde{\mathcal{C}}_n$. Suppose $\mathcal{P}_1$ and $\mathcal{P}_2$ are two paths from the trivial causet consisting of a single point to $\tilde{C}$ and write $\mathcal{P}_I = \{l_{i1}, \ldots, l_{in}\}$ where the l_{ij} are the links defining the path $\mathcal{P}_i$. Then

$$\prod_{k=1}^{n} \mathrm{Prob}(l_{1k}) = \prod_{k=1}^{n} \mathrm{Prob}(l_{2k}).$$

(3) (Causality) Suppose that $C \in \mathcal{C}_n$ and for $i = 1, 2$, suppose that $C_i \in F(C)$. Let $B \in \mathcal{C}_m$, $m \leqslant n$, be defined by

$$B = \mathrm{Prec}(C, C_1) \cup \mathrm{Prec}(C, C_2)$$

with poset structure induced by that of C. Let $B_i \in \mathcal{C}_{m+1}$ be B with an element added in the same manner as in the transitions $C \to C_i$. Then we require

$$\frac{\mathrm{Prob}(C \to C_1)}{\mathrm{Prob}(C \to C_2)} = \frac{\mathrm{Prob}(B \to B_1)}{\mathrm{Prob}(B \to B_2)}. \tag{2.7}$$

For a detailed discussion of these restrictions and results related to the corresponding dynamics, see Rideout and Sorkin (2000) and Dou (1999).

A special role in the theory will be played by those causets with no relations. We will denote the element of $\mathcal{C}_n$ with no relations by A_n. We note that there is a unique path in $\mathcal{C}$ of length n from A_0 to A_n.

Definition 2.2: Let $M \in \mathcal{M}$ and suppose that A_n is the causet on n nodes with no relations. Associate to M a sequence of positive constants $\{q_n\}_{n=0}^{\infty}$ defined by

$$q_0 = 1, \tag{2.8}$$

$$q_n = \mathrm{Prob}(A_n \to A_{n+1}), \tag{2.9}$$

where, as above, the expression appearing on the right-hand side of (2.9) denotes the probability of transition from A_n to A_{n+1}. We call the sequence $\{q_n\}$ *defining probabilities for the chain M*. If $q_n > 0$ for all n we say that the chain M is *generic*.

Rideout and Sorkin (2000) prove that for generic M, the sequence $\{q_n\}_{n=0}^{\infty}$ completely determines the theory associated to M. More precisely, given an element $C \in \mathcal{C}_n$, and $D \in F(C)$ [cf. (2.4)], let m be the number of maximal elements associated to the transition $C \to D$ [cf. (2.6)] and let ρ be the cardinality of the precursor set of the transition $C \to D$ [cf. (2.5)]. Then the transition probability for the evolution $C \to D$ is given by (cf. Rideout and Sorkin, 2000)

$$\mathrm{Prob}(C \to D) = q_n \sum_{k=0}^{m} (-1)^k \binom{m}{k} \frac{1}{q_{\rho-k}}. \tag{2.10}$$

Following Rideout and Sorkin (2000), we define a sequence t_n by

$$t_n = \sum_{k=0}^{n} (-1)^{n-k} \binom{n}{k} \frac{1}{q_k}. \tag{2.11}$$

Then we can recover the probabilities q_n from the sequence of t_n:

$$\frac{1}{q_n} = \sum_{k=0}^{n} \binom{n}{k} t_k. \tag{2.12}$$

We call the collection $\{t_n\}$ the *coupling constants* of the associated Markov chain. We note that if $\mathcal{S}_1$ is the collection of sequences of non-negative real numbers $T=\{t_n\}_{n=0}^{\infty}$ such that $t_0=1$, then there is a bijection between generic elements of $\mathcal{M}$ and elements of $\mathcal{S}_1$ given by associating to each element of $\mathcal{S}_1$ the associated collection of defining probabilities $\{q_n\}_{n=0}^{\infty}$ given by (2.12).

We constrain the class of Markov chains defined by Definition 2.1 further by requiring that they be *renormalizable under cycles of expansion and contraction*. We can state this requirement concisely in terms of a renormalization operator $\mathcal{R}:\mathcal{S}_1 \to \mathcal{S}_1$ defined by

$$(\mathcal{R}(T))_n = \frac{t_{n+1} + t_n}{t_0 + t_1}. \tag{2.13}$$

We define the stable set of the operator $\mathcal{R}$ by

$$\mathrm{Stab}(\mathcal{R}) = \left\{ T \in \mathcal{S}_1 : T \in \bigcap_{n \in \mathbb{N}} \mathcal{R}^n(\mathcal{S}_1) \right\}. \tag{2.14}$$

Definition 2.3: Let M be a Markov chain with coupling constants T satisfying $T \in \mathcal{S}_1$. We say that M is renormalizable if $T \in \mathrm{Stab}(\mathcal{R})$.

Using Definition 2.3 we define the Markov chains upon which we will focus:

Definition 2.4: Suppose that $M \in \mathcal{M}$ has coupling constants $T \in \mathcal{S}_1$. If M is renormalizable, we say that M defines a *generic causet dynamics* or *GCD chain*. We denote the collection of systems which are GCD chains by $\mathbb{M}$.

We denote by $\mathbb{S}$ the collection of coupling constants given by

$$\mathbb{S} = \mathcal{S}_1 \cap \mathrm{Stab}(\mathcal{R}). \tag{2.15}$$

From the relevant definitions it is clear that there is a bijection between elements of $\mathbb{M}$ and elements of $\mathbb{S}$ afforded by restricting the identification between $\mathcal{M}$ and $\mathcal{S}_1$.

The main result of Ash and McDonald (2003) is the following more subtle characterization of GCD chains:

Theorem 2.5: [*cf.* Ash and McDonald (2003)] *Suppose that $M \in \mathcal{M}$ has associated coupling constants $T=\{t_n\}$. Then $M \in \mathbb{M}$ if and only if there is a non-decreasing function $\alpha:\mathbb{R}^+ \to \mathbb{R}$ such that*

$$t_n = \int_0^{\infty} s^n d\alpha(s). \tag{2.16}$$

Definition 2.6: Let M be a GCD chain defined by coupling constants $\{t_n\}$. If $\alpha:\mathbb{R}^+ \to \mathbb{R}$ is a nondecreasing function satisfying (2.16) we say that α *represents* M. If $M \in \mathbb{M}$ is represented by α, we define the support of M to be the support of the measure $d\alpha$.

We can use Theorem 2.5 to give a second definition of transitive percolation:

Definition 2.7: Fix p, $0<p<1$. Transitive percolation is the GCD chain whose defining probabilities and coupling constants are given by

$$q_n = (1-p)^n \tag{2.17}$$

$$t_n = \left(\frac{p}{1-p}\right)^n.$$

Setting $d = p/(1-p) \in \mathbb{R}^+$, we see from (2.17) and (2.16) that transitive percolation corresponds to choosing α in Theorem 2.5 to be given by the appropriate Heaviside function:

$$\alpha(x) = \begin{cases} 0 & \text{if } x < d \\ 1 & \text{if } x \geqslant d. \end{cases} \tag{2.18}$$

It is a corollary of Theorem 2.5 [cf. Ash and McDonald (2003)] that for any GCD chain, we can write the transition probability for an arbitrary evolution using a representation. More precisely, given $C \in \mathcal{C}_n$ and $D \in F(C)$, evolution from C to D is effected by the addition of a new vertex, x_D, and a number of new edges. The transition probability for evolution from C to D under the GCD chain represented by α is given by [cf. Ash and McDonald (2003)]

$$\text{Prob}(C \to D) = \frac{\displaystyle\int_0^\infty s^m (1+s)^{\rho-m} d\alpha(s)}{\displaystyle\int_0^\infty (1+s)^n d\alpha(s)}, \tag{2.19}$$

where m is the number of maximal elements in the past of x_D [cf. (2.6)] and ρ is the number of elements in the past of x_D [cf. (2.5)]. In particular, for transitive percolation as given in Definition 2.7, the transition probabilities associated to the evolution $\mathcal{C}_n \ni C \to D \in F(C)$ given by (2.19) are given by

$$\text{Prob}(C \to D) = d^m (1+d)^{\rho-m-n}. \tag{2.20}$$

In the sequel we will have use for the measure space machinery associated to a Markov chain. To fix notation, we recall the standard constructions:

Let Ω be the collection of paths in $\mathcal{C}$. Thus, if $f \in \Omega$, then f is a function from $\mathbb{N}$ to $\mathcal{C}$ and for each $n \in \mathbb{N}$, $f(n)$ is linked to $f(n+1)$.

Given a finite collection of sets of causets, $\{A_1, A_2, \ldots, A_n\}$ with $A_j \subset \mathcal{C}_{i_j}$, we define a subset $A_{i_1,\ldots,i_n} \subset \Omega$ by

$$A_{i_1,\ldots,i_n} = \{S \in \Omega : S(i_j) \in A_j\}. \tag{2.21}$$

We call $A_{i_1,\ldots,i_n}$ the cylinder set defined by the sequence $A_1, A_2, \ldots, A_n$. We let Σ denote the sigma algebra generated by the collection of cylinder sets.

Let M be a GCD chain, $M(k)$ the state of the system at time k. Given a cylinder set $A = A_{i_1,\ldots,i_n}$, we can associate a probability to A:

$$\mathbb{P}_M(A) = \text{Prob}(M(j) \in A_j \text{ for } j = i_1, \ldots, i_n). \tag{2.22}$$

More generally, given $C \in \mathcal{C}_m$, we can regard C as an initial segment of a path generated by M (we call such an initial segment a *stem*). Given a cylinder set $A = A_{i_1,\ldots,i_n}$ we can consider starting the process at C and associate a probability to A,

$$\mathbb{P}_M^C(A) = \text{Prob}(M(j) \in A_j | M(m) = C \text{ for } j = i_1, \ldots, i_n). \tag{2.23}$$

By standard arguments, $\mathbb{P}_M^C$ extends to a probability measure on (Ω, Σ). When $D \in F(C)$ we can think of D as a cylinder set and the above convention gives

$$\mathbb{P}_M^C(D) = \text{Prob}(C \to D). \tag{2.24}$$

When $C = \{0\} \in \mathcal{C}_0$ we will, as above, drop the reference to C and write $\mathbb{P}_M^C = \mathbb{P}_M$ (*cf.* Brightwell *et*

al. (2002) for further study of this sigma algebra and measure and their invariance properties under relabeling the vertices of the causets).

Let

$$\mathcal{H} = \{f \in \Omega : f(0) \in \mathcal{C}_0, f(n+1) \in F(f(n))\}.$$

We call elements of $\mathcal{H}$ *histories* and we note that the measures constructed above charge the collection of histories. Given an element $H \in \mathcal{H}$, we can define a partial order on $\mathbb{N}$ by constructing a formal limit. More precisely, given $i, j \in \mathbb{N}$, we say that $i < j$ with respect to $\lim H$ if for all n sufficiently large, $i < j$ with respect to $H(n)$. This partial order facilitates discussion of posts:

Definition 2.8: The vertex i is a post in the history $H \in \mathcal{H}$ if every vertex $j \neq i$ satisfies $i < j$ with respect to $\lim H$ or $j < i$ with respect to $\lim H$.

Note that the sets

$$\mathcal{P}_i = \{H \in \mathcal{H} : i \text{ is a post in } H\} \tag{2.25}$$

are in the sigma algebra Σ generated by the cylinder sets. Let $\mathcal{P}_\infty$ be the event that an infinite number of posts occur. Then

$$\mathcal{P}_\infty = \cap_{n=1}^{\infty} \cup_{i=n}^{\infty} \mathcal{P}_i. \tag{2.26}$$

We note that it is a theorem of Alon, Bollobas, Brightwell, and Janson (1994) that for any transitive percolation M with associated parameter $d > 0$,

$$\mathbb{P}_M(\mathcal{P}_\infty) = 1.$$

Our goal is to extend this result to a large family of GCD chains.

III. PROOF OF THE MAIN RESULT

Suppose that $0 < x_1 < x_2 < \ldots < x_L < \infty$ and let δ_{x_i} be the delta mass concentrated at x_i. Let μ be a convex combination of the δ_{x_i}:

$$\mu = \sum_{i=1}^{L} \gamma_i \delta_{x_i}, \tag{3.1}$$

where $0 \leqslant \gamma_i \leqslant 1$ and $\Sigma_{i=1}^{L} \gamma_i = 1$. Then by Theorem 2.5 and Definition 2.7, μ represents a GCD chain.

Lemma 3.1: Let $\epsilon > 0$. Suppose that μ is as given in (3.1). Then there exists N such that for any $\overline{N} \geqslant N$, and any causet $C_{\overline{N}}$ on $\overline{N}$ elements, the probability that a post develops after time $\overline{N}$ under dynamics generated by μ, given stem $C_{\overline{N}}$, is greater than $1-\epsilon$.

Proof: Let $\epsilon > 0$ and suppose that μ is as given in (3.1). Let C_n be a causet on n elements. Let C_{n+1} be in the family of C_n and suppose that the transition $C_n \to C_{n+1}$ is characterized by m maximal elements and a precursor set of size ρ. By (2.19), under the dynamics generated by μ,

$$\mathbb{P}_\mu^{C_n}(C_{n+1}) = \frac{\sum_{i=1}^{L} \gamma_i x_i^m (1+x_i)^{\rho-m}}{\sum_{i=1}^{L} \gamma_i (1+x_i)^n}.$$

Let $\Gamma_i = (1+x_i)/(1+x_L)$. Then

$$\mathbb{P}_\mu^{C_n}(C_{n+1}) = \frac{\sum_{i=1}^{L-1} \gamma_i x_i^m (1+x_i)^{\rho-m}}{\sum_{i=1}^{L} \gamma_i (1+x_i)^n} + \frac{\mathbb{P}_{x_L}^{C_n}(C_{n+1})}{1 + \sum_{i=1}^{L-1} \frac{\gamma_i}{\gamma_L} \Gamma_i^n},$$

where $\mathbb{P}_{x_L}$ denotes probability with respect to transitive percolation with delta mass at x_L. Thus,

$$\mathbb{P}_{\mu}^{C_n}(C_{n+1}) \geqslant \mathbb{P}_{x_L}^{C_n}(C_{n+1}) \frac{1}{1+\sum_{i=1}^{L-1} \frac{\gamma_i}{\gamma_L} \Gamma_i^n}. \tag{3.2}$$

Given $C_N \in \mathcal{C}_N$, let S_{C_N} be the collection of histories with stem C_N which develop a post after time N. For $k > N$, let $S_{C_N}(k) \subset S_{C_N}$ be the collection of histories with stem C_N that develop their first post after time greater than N at vertex k. Given $N' > N$, let $S_{C_N}(k, N')$ be the cylinder set consisting of those histories which coincide with an element of $S_{C_N}(k)$ up to time N'. Thus, for $N' \geqslant k$, elements of $S_{C_N}(k, N')$ consist of histories of the form $C_N \to C_{N+1} \to \cdots \to C_{N'} \to \cdots$ where the node labeled k is ordered with respect to all other nodes in C_j, $j \leqslant k \leqslant N'$ and k is the least integer in $(N, N']$ with that property. It follows easily that

$$S_{C_N}(k) = \bigcap_{N' > N} S_{C_N}(k, N')$$

and for any GCD chain ν,

$$\mathbb{P}_{\nu}^{C_N}(S_{C_N}(k)) = \lim_{N' \to \infty} \mathbb{P}_{\nu}^{C_N}(S_{C_N}(k, N')). \tag{3.3}$$

We can write $\mathbb{P}_{\mu}^{C_N}(S_{C_N}(k, N'))$ as a sum of products:

$$\mathbb{P}_{\mu}^{C_N}(S_{C_N}(k, N')) = \sum_{S_{C_N}(k, N')} \prod_{n=N}^{N'-1} \mathbb{P}_{\mu}^{C_n}(C_{n+1}), \tag{3.4}$$

where the notation indicates that the sum is over all paths from C_N to $C_{N'}$ which develop a first post at node k, $N < k \leqslant N'$. We estimate each term in the product using (3.2). Thus,

$$\begin{aligned} \mathbb{P}_{\mu}^{C_N}(S_{C_N}(k)) &\geqslant \lim_{N' \to \infty} \sum_{S_{C_N}(k, N')} \prod_{n=N}^{N'-1} \mathbb{P}_{x_L}^{C_n}(C_{n+1}) \frac{1}{1+\sum_{i=1}^{L-1} \frac{\gamma_i}{\gamma_L} \Gamma_i^n} \\ &= \lim_{N' \to \infty} \sum_{S_{C_N}(k, N')} \left(\prod_{n=N}^{N'-1} \mathbb{P}_{x_L}^{C_n}(C_{n+1}) \right) \left(\prod_{n=N}^{N'-1} \frac{1}{1+\sum_{i=1}^{L-1} \frac{\gamma_i}{\gamma_L} \Gamma_i^n} \right). \end{aligned} \tag{3.5}$$

For $0 \leqslant z < 1$ and γ positive, the infinite product

$$\prod_{n=1}^{\infty} \frac{1}{1+\gamma z^n}$$

converges. Choose N so large that

$$\prod_{n=N}^{\infty} \frac{1}{1+\sum_{i=1}^{L-1} \frac{\gamma_i}{\gamma_L} \Gamma_i^n} \geqslant 1 - \epsilon. \tag{3.6}$$

From (3.4)–(3.6) we have for any $\overline{N} \geqslant N$, for $k > \overline{N}$ and for any causet $C_{\overline{N}}^{-} \in \mathcal{C}_{\overline{N}}^{-}$,

$$\mathbb{P}_{\mu}^{C_N}(S_{C_N^-}(k)) \geqslant (1-\epsilon) \lim_{N' \to \infty} \sum_{S_{C_N^-}(k,N')} \prod_{n=\overline{N}}^{N'-1} \mathbb{P}_{x_L}^{C_n}(C_{n+1}). \tag{3.7}$$

By (3.3) the limit on the right-hand side of (3.7) is the probability that a first post occurs at node k, given stem $C_{\overline{N}}^-$, under transitive percolation. Since identification of the first post after time $\overline{N}$ partitions $S_{C_N^-}$, we have

$$\begin{aligned}\mathbb{P}_{\mu}^{C_N}(S_{C_N^-}) &= \sum_{k \geqslant \overline{N}} \mathbb{P}_{\mu}^{C_N}(S_{C_N^-}(k)) \geqslant (1-\epsilon) \sum_{k \geqslant \overline{N}} \lim_{N' \to \infty} \sum_{S_{C_N^-}(k,N')} \prod_{n=\overline{N}}^{N'-1} \mathbb{P}_{x_L}^{C_n}(C_{n+1}) \\ &= (1-\epsilon) \sum_{k \geqslant \overline{N}} \lim_{N' \to \infty} \mathbb{P}_{x_L}^{C_N}(S_{C_N^-}(k,N')). \end{aligned} \tag{3.8}$$

It follows from the work of Alon, Bollobas, Brightwell, and Janson (1994) that the sum on the right-hand side of (3.8) is equal to one, which finishes the proof of the lemma. □

Lemma 3.2: Suppose that μ is as in (3.1) and let $\mathbb{P}_{\mu}$ be the associated probability measure. Let $\mathcal{P}_{\infty}$ be the event that an infinite number of posts occur [cf. (2.26)]. Then

$$\mathbb{P}_{\mu}(\mathcal{P}_{\infty}) = 1.$$

Proof: Let $\epsilon > 0$. As in (2.25), let $\mathcal{P}_i$ be the collection of histories which develop a post at node i. Given $C_N \in \mathcal{C}_N$, let S_{C_N} be as in the proof of Lemma 3.1. By Lemma 3.1, there exists N such that for all $\overline{N} \geqslant N$, for all histories H,

$$\mathbb{P}_{\mu}^{H(\overline{N})}(S_{H(\overline{N})}^-) \geqslant 1-\epsilon.$$

Since

$$\bigcup_{H \in \mathcal{H}} S_{H(\overline{N})}^- \subset \bigcup_{i=\overline{N}}^{\infty} \mathcal{P}_i \tag{3.9}$$

we conclude that

$$\mathbb{P}_{\mu}\left(\bigcup_{i=\overline{N}}^{\infty} \mathcal{P}_i \right) \geqslant 1-\epsilon. \tag{3.10}$$

Since ϵ was arbitrary, we conclude that for all n,

$$\mathbb{P}_{\mu}\left(\bigcup_{i=n}^{\infty} \mathcal{P}_i \right) = 1.$$

Noting that $\mathcal{P}_{\infty} = \liminf \mathcal{P}_i$ [cf. (2.26)], the proof is complete. □

The proof of Lemma 3.2 uses only the conclusion of Lemma 3.1. This being the case, we have:

Corollary 3.3: Suppose that ν is a GCD chain and let $\mathbb{P}_{\nu}$ be the associated probability measure. Suppose for every $\epsilon > 0$ there exists N such that for every $\overline{N} \geqslant N$ and every $C_{\overline{N}}^- \in \mathcal{C}_{\overline{N}}^-$, the probability that a post develops after time $\overline{N}$ under the dynamics associated to ν, given stem C_N, is greater than or equal to $(1-\epsilon)$. Let $\mathcal{P}_{\infty}$ be the event that an infinite number of posts occur. Then

$$\mathbb{P}_{\nu}(\mathcal{P}_{\infty}) = 1.$$

Proof of Theorem 1.1: Suppose that M is a compactly supported GCD chain represented by $\alpha: \mathbb{R}^+ \to \mathbb{R}$. Let $\epsilon > 0$ and write

$$c = \inf\{x : x \in \text{support}(d\alpha)\},$$

$$d = \sup\{x : x \in \text{support}(d\alpha)\}.$$

Choose a partition $I=\{x_i\}_{i=0}^{L}$, $c=x_0<x_1<\ldots,<x_L=d$ and set $\gamma_i=\alpha(x_i)-\alpha(x_{i-1})$. Then, since $d\alpha$ is a probability measure and α is nondecreasing, we have $0\leqslant\gamma_i\leqslant 1$ and $\Sigma_{i=1}^{L}\gamma_i=1$. With notation as in (3.1), let μ_I be defined by

$$\mu_I = \sum_{i=1}^{L} \gamma_i \delta_{x_i}. \tag{3.11}$$

Then μ_I is a GCD chain.

Given $C_n \in \mathcal{C}_n$ and $C_{n+1} \in F(C_n)$ we use (2.19) and we approximate

$$\mathbb{P}_M^{C_n}(C_{n+1}) = \frac{\int s^m (1+s)^{\rho-m} d\alpha}{\int (1+s)^n d\alpha} \tag{3.12}$$

by

$$\mathbb{P}_{\mu_I}^{C_n}(C_{n+1}) = \frac{\sum_{i=1}^{L} \gamma_i x_i^m (1+x_i)^{\rho-m}}{\sum_{i=1}^{L} \gamma_i (1+x_i)^n}. \tag{3.13}$$

As in the proof of Lemma 3.1, choose N so large that

$$\prod_{n=N}^{\infty} \frac{1}{1+\sum_{i=1}^{L-1} \frac{\gamma_i}{\gamma_L}\left(\frac{1+x_i}{1+d}\right)^n} \geqslant 1-\frac{\epsilon}{8}. \tag{3.14}$$

Let I' be a refinement of I, $I'=\{x_i'\}_{i=0}^{L'}$, with $x'_{L'-1}=x_{L-1}$. For $x_i' \in I'$, write $\gamma_i'=\alpha(x_i')-\alpha(x_{i-1}')$. Writing $x_{L-2}=x'_{L'-k}$, we note that for all j, $1<j\leqslant k$, $x'_{L'-j}<x'_{L'-1}$ and thus

$$\begin{aligned}
\sum_{i=L'-k+1}^{L'-1} \gamma_i' \left(\frac{1+x_i'}{1+d}\right)^n &\leqslant \sum_{i=L'-k+1}^{L'-1} \gamma_i' \left(\frac{1+x'_{L'-1}}{1+d}\right)^n \\
&= (\alpha(x'_{L'-1}) - \alpha(x'_{L'-k}))\left(\frac{1+x'_{L'-1}}{1+d}\right)^n \\
&= \gamma_{L-1}\left(\frac{1+x_{L-1}}{1+d}\right)^n.
\end{aligned}$$

Continuing inductively we conclude

$$\frac{1}{1+\sum_{i=1}^{L-1} \frac{\gamma_i}{\gamma_L}\left(\frac{1+x_i}{1+d}\right)^n} \leqslant \frac{1}{1+\sum_{i=1}^{L'-1} \frac{\gamma_i'}{\gamma_L}\left(\frac{1+x_i'}{1+d}\right)^n}. \tag{3.15}$$

Thus, the estimate (3.14) is uniform in N under refinements of the partition I which do not affect the last subinterval of the partition I. With S_{C_N}, $S_{C_N}(k)$, and $S_{C_N}(k,N')$ as defined in the proof of Lemma 3.1, we thus obtain that there exists N such that for all refinements I' of I which do not affect the last subinterval of I and all $k>N$, we have, for all $N'>k$,

$$\mathbb{P}_{\mu_{I'}}^{C_N}(S_{C_N}(k,N')) \geqslant \left(1-\frac{\epsilon}{6}\right) \sum_{S_{C_N}(k,N')} \prod_{n=N}^{N'-1} \mathbb{P}_d^{C_n}(C_{n+1}). \tag{3.16}$$

Because the sum on the right-hand side of (3.16) is $\mathbb{P}_d(S_{C_N}(k,N'))$, we have that there exists N such that for all refinements I' of I which do not affect the last subinterval of I,

$$\mathbb{P}_{\mu_{I'}}^{C_N}(S_{C_N}(k,N')) \geqslant \left(1-\frac{\epsilon}{6}\right)\mathbb{P}_d^{C_N}(S_{C_N}(k,N')) \tag{3.17}$$

for all $C_N \in \mathcal{C}_N$ and all $k>N$, all $N'>k$. Using the fact that the sets $S_{C_N}(k)$ partition S_{C_N} and that $\mathbb{P}_d^{C_N}(S_{C_N})=1$, we choose J so large that

$$\mathbb{P}_M^{C_N}(S_{C_N}) - \sum_{k=N}^{J} \mathbb{P}_M^{C_N}(S_{C_N}(k)) \leqslant \frac{\epsilon}{6}, \tag{3.18}$$

$$\sum_{k=N}^{J} \mathbb{P}_d^{C_N}(S_{C_N}(k)) \geqslant 1-\frac{\epsilon}{8}. \tag{3.19}$$

Having chosen J, choose N' so large that for all k, $N\leqslant k\leqslant J$, for all $N''\geqslant N'$,

$$\mathbb{P}_M^{C_N}(S_{C_N}(k)) - \mathbb{P}_M^{C_N}(S_{C_N}(k,N'')) \leqslant \frac{\epsilon}{6(J-N)}, \tag{3.20}$$

$$\sum_{k=N}^{J} \mathbb{P}_d^{C_N}(S_{C_N}(k,N'')) \geqslant 1-\frac{\epsilon}{6}. \tag{3.21}$$

Now suppose that d is an isolated point of support and choose an open interval $\mathcal{I}$ containing d such that $(\mathcal{I}\backslash\{d\})\cap \text{support}(d\alpha)$ is empty. Choose a partition I which includes a single point in $\mathcal{I}\backslash\{d\}$. Then, by the above, there exists N such that for all $C_N \in \mathcal{C}_N$, for all $k>N$, for all J and all N' large enough, and all partitions I' refining I, (3.17)–(3.21) hold.

Having chosen J and N' as above, note that under refinement (3.13) converges to (3.12). Choose a refinement I' such that for all k, $N\leqslant k\leqslant J$,

$$|\mathbb{P}_M^{C_N}(S_{C_N}(k,N')) - \mathbb{P}_{\mu_{I'}}^{C_N}(S_{C_N}(k,N'))| \leqslant \frac{\epsilon}{6(J-N)}. \tag{3.22}$$

Then

$$\begin{aligned}\mathbb{P}_M^{C_N}(S_{C_N}) &= \left(\mathbb{P}_M^{C_N}(S_{C_N}) - \sum_{k=N}^{J} \mathbb{P}_M^{C_N}(S_{C_N}(k))\right) + \left(\sum_{k=N}^{J} \mathbb{P}_M^{C_N}(S_{C_N}(k)) - \sum_{k=N}^{J} \mathbb{P}_M^{C_N}(S_{C_N}(k,N'))\right) \\ &\quad + \left(\sum_{k=N}^{J} \mathbb{P}_M^{C_N}(S_{C_N}(k,N')) - \sum_{k=N}^{J} \mathbb{P}_{\mu_{I'}}^{C_N}(S_{C_N}(k,N'))\right) + \sum_{k=N}^{J} \mathbb{P}_{\mu_{I'}}^{C_N}(S_{C_N}(k,N')) \\ &= T_1 + T_2 + T_3 + \sum_{k=N}^{J} \mathbb{P}_{\mu_{I'}}^{C_N}(S_{C_N}(k,N')).\end{aligned}$$

Using (3.18) we see that $|T_1|<\epsilon/6$. Using (3.20) we see that $|T_2|<\epsilon/6$. Using (3.22) we see that $|T_3|<\epsilon/6$. Thus,

$$\mathbb{P}_M^{C_N}(S_{C_N}) \geqslant \sum_{k=N}^{J} \mathbb{P}_{\mu_{I'}}^{C_N}(S_{C_N}(k,N')) - \frac{\epsilon}{2}.$$

Using (3.17) we conclude

$$\mathbb{P}_M^{C_N}(S_{C_N}) \geqslant \left(1 - \frac{\epsilon}{6}\right) \sum_{k=N}^{J} \mathbb{P}_d^{C_N}(S_{C_N}(k,N')) - \frac{\epsilon}{2}. \tag{3.23}$$

From (3.21) and (3.23), we conclude

$$\mathbb{P}_M^{C_N}(S_{C_N}) \geqslant \left(1 - \frac{\epsilon}{6}\right)\left(1 - \frac{\epsilon}{6}\right) - \frac{\epsilon}{2} \geqslant (1 - \epsilon).$$

Thus, we have proven that there exists N such that for all $C_N \in \mathcal{C}_N$, given stem C_N, a post develops after time N under the dynamics generated by M with probability one. From our proof it is clear that for any $\overline{N} \geqslant N$, for any $C_{\overline{N}} \in \mathcal{C}_{\overline{N}}$, the probability that a post develops after time $\overline{N}$ under the dynamics generated by M, given stem $C_{\overline{N}}$, is one. Given Corollary 3.3, this proves the theorem.

IV. RENORMALIZATION FLOW

In this section we study the behavior of sequences of coupling constants associated to systems described in Sec. II. In particular, we study the asymptotic behavior of such sequences under the repeated action of the operator $\mathcal{R}$ (the so-called renormalization flow). We show that in the limit of large time, the transition probabilities approach those of a transitive percolation.

Theorem 4.1: *Suppose that $T \in \mathcal{S}_1$ defines the coupling constants for a GCD chain. Let $\alpha: \mathbb{R}^+ \to \mathbb{R}$ be a nondecreasing function representing T as in (2.16). Suppose that $\{q_n\}_{n=0}^{\infty}$ are the defining probabilities given in (2.9). Then*

(1) *If the support of the measure $d\alpha$ is compact with*

$$t = \sup\{x : x \in \text{support}(d\alpha)\}, \tag{4.1}$$

then

$$\lim_{m\to\infty} \frac{q_{m+n}}{q_m} = \frac{1}{(1+t)^n}. \tag{4.2}$$

(2) *If the support of the measure $d\alpha$ is not compact, then*

$$\lim_{m\to\infty} \frac{q_{m+n}}{q_m} = \begin{cases} 1 & \text{if } n = 0 \\ 0 & \text{if } n \neq 0. \end{cases} \tag{4.3}$$

Proof: We denote by $L^q(\mathbb{R}^+, d\alpha)$ the Banach space with norm

$$\|f\|_q = \left(\int_0^{\infty} f^q d\alpha\right)^{1/q}.$$

Since $d\alpha$ is a probability measure, the function $g(x) = 1$ is in $L^q(\mathbb{R}^+, d\alpha)$ for all q. Let k be positive, $m > k$. Let q be defined by

$$\frac{1}{q} + \frac{k}{m} = 1.$$

By Hölder's inequality,

$$\|(1+s)\|_k \leqslant \|(1+s)\|_m. \tag{4.4}$$

Since α is nondecreasing and the function $(1+s)^k$ is continuous and strictly increasing on $\mathbb{R}^+$, there is a unique positive real number τ_k such that

$$\int_0^\infty (1+s)^k d\alpha = (1+\tau_k)^k. \tag{4.5}$$

From (4.4) and (4.5), the sequence $\{\tau_k\}$ is increasing.

Suppose that the support of the measure $d\alpha$ is compact with t as in (4.1). Suppose $\lim_{k\to\infty} \tau_k = \tau_*$ with $\tau_* < t$. Choose τ^* satisfying $\tau_* < \tau^* < t$. Then

$$\int_0^\infty (1+s)^k d\alpha = \int_0^{\tau^*} (1+s)^k d\alpha + \int_{\tau^*}^t (1+s)^k d\alpha.$$

As in (4.5) we can find unique $\mu_k \in [0, \tau^*)$ and $\nu_k \in [\tau^*, t]$ such that

$$\int_0^\infty (1+s)^k d\alpha = (1+\mu_k)^k \int_0^{\tau^*} d\alpha + (1+\nu_k)^k \int_{\tau^*}^t d\alpha.$$

By the argument used to establish that the τ_k are increasing, we have that the μ_k and the ν_k are increasing. By assumption, $d\alpha$ is supported near t and thus, $\int_{\tau^*}^t d\alpha \neq 0$ and, for k large enough and ϵ small enough, $\nu_k \geqslant \tau^* + \epsilon$. From this we conclude that $\int_0^\infty (1+s)^k d\alpha$ is, for large k, at least of the order of $(1+\tau^*+\epsilon)^k$, contradicting (4.5) and the choice of τ^*. We conclude that $\tau_* = t$, which proves the first claim of the theorem.

To prove the second claim of the theorem, note that either the sequence $\{\tau_k\}$ converges to a real number or it does not. If it does not converge to a real number, then it converges to ∞, and we are done. If we assume that it does converge to a real number, the construction of the sequences μ_k and ν_k lead to a contradiction. □

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Wyman's solution, self-similarity, and critical behavior

G. Oliveira-Neto[a] and F. I. Takakura[b]
Departamento de Física, Instituto de Ciencias Exatas, Universidade Federal de Juiz de Fora, CEP 36036-330, Juiz de Fora, Minas Gerais, Brazil

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The Wyman solution depends on two parameters, the mass M and the scalar charge Σ. If one fixes M to a positive value, say M_0, and lets Σ^2 take values along the real line, we show that this solution exhibits a type of critical behavior, in analogy with the nonstatic massless scalar field solutions. For $\Sigma^2>0$ the space-times have naked singularities, for $\Sigma^2=0$ one has a Schwarzschild black hole of mass M_0 and finally for $-M_0^2\leqslant\Sigma^2<0$ one has "wormhole-like" solutions. We also show that the Wyman solution is not self-similar, i.e., it does not admit a homothetic Killing vector. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1920308]

I. INTRODUCTION

The four-dimensional space-time generated by a minimally coupled, spherically symmetric, static, massless scalar field has been studied by many authors.[1–5] The general solution was found by Wyman in Ref. 2. From a particular case of the general Wyman's solution, Roberts showed how to construct a time-dependent solution.[3] The Roberts' solution has an important physical interest because it may represent the gravitational collapse of a scalar field. Later, Brady, and independently Oshiro *et al.*,[6] showed that Roberts' solution could be derived from the appropriated, time-dependent, Einstein-scalar equations by using a continuous self-similarity. They also showed that the Roberts' solution exhibits a critical behavior qualitatively identical to the one found numerically by Choptuik,[7] studying the same system of equations.

Using a discrete self-similarity of the system, Choptuik explicitly showed that the collapse results in two families of solutions depending on the value of a certain parameter p, which characterizes the scalar charge. In the first family, when $p<p_c$, the scalar field collapses up to a certain surface and then disperses. In the other family, when $p>p_c$, the scalar field collapses to form a black hole. The critical value p_c separates the two end states of the collapse. The critical solution ($p=p_c$) represents a naked singularity. Therefore, since it is given by a single value of the parameter, it has zero measure in the parameter space. In fact, the above results confirmed early studies of Christodoulou, who pioneered analytical studies of that model.[8]

The Wyman solution is not usually thought to be of great importance for the issue of gravitational collapse because it is static and the naked singularities derived from it are unstable against spherically symmetric linear perturbations of the system.[4,5] On the other hand, as we saw above, from a particular case of the Wyman solution one may derive the Roberts' one, which is of great importance for the issue of gravitational collapse. Also, it was shown that there are nakedly singular solutions to the static, massive scalar field equations which are stable against spherically symmetric linear perturbations.[5] Therefore, we think it is of great importance to gather as much information as we can about the Wyman solution for it may be helpful to better understand the scalar field collapse.

Self-similarity is an important symmetry that has been extensively used in order to study Einstein's equations describing the gravitational collapse. As was mentioned above, Roberts'

[a]Electronic mail: gilneto@fisica.ufjf.br
[b]Electronic mail: takakura@fisica.ufjf.br

solution admits a homothetic Killing vector; one may wonder if the Wyman solution also has this property. In the present work, we would like to show that the Wyman solution is not self-similar, i.e., it does not admit a homothetic Killing vector.

Wyman's solution depends on two parameters, the mass M and the scalar charge Σ. As we have seen above, Choptuik found a critical behavior in the solutions to the Einstein-scalar equations in terms of the parameter describing the scalar charge. Therefore, one may try to find critical behavior in Wyman's solution by fixing M and letting Σ vary. We would like to show that, if one fixes M to a positive value, say M_0, and let Σ^2 take values along the real line, this solution exhibits a type of critical behavior, in analogy with the nonstatic massless scalar field solutions.

In Sec. II, we demonstrate that the Wyman's solution is not self-similar, or, in other words, it does not admit a homothetic Killing vector.

In Sec. III, we show that Wyman's solution exhibits a type of critical behavior, in analogy with the nonstatic massless scalar field solutions.

Finally, in Sec. IV, we summarize the main points and results of the paper.

II. WYMAN'S SOLUTION AND CONTINUOUS SELF-SIMILARITY

In the present paper we work with the double-null coordinates (u,v); therefore, our starting point is Wyman's line element given in Eq. (14) of Ref. 3

$$ds^2 = -\left(1-\frac{2\eta}{r}\right)^{M/\eta} dv\, du + \left(1-\frac{2\eta}{r}\right)^{1-M/\eta} r^2 d\Omega^2, \tag{1}$$

where M is the mass parameter, $\eta^2 = M^2 + \Sigma^2$, and Σ is the scalar charge. The function $r(v,u)$ may be obtained if we integrate the following equation:

$$dv - du = 2\left(1-\frac{2\eta}{r}\right)^{-M/\eta} dr. \tag{2}$$

The above equation was derived by combining Eq. (10) of Ref. 3 with the analogous one for the coordinate u, for advanced null coordinates.

Let us now demonstrate that the Wyman solution is not self-similar, or, in other words, it does not admit a homothetic Killing vector. In order to do that, we start writing the most general form of a "radial" homothetic Killing vector for a spherically symmetric space-time in double null coordinates

$$\xi^a = \xi^v \delta^a_v + \xi^u \delta^a_u, \tag{3}$$

where ξ^v and ξ^u are both functions of v and u. Now, the condition for self-similarity is given by the equation $\mathcal{L}_\xi g = a_0 g$, where $\mathcal{L}_\xi$ denotes the Lie derivative with respect to ξ, g is the space-time metric, ξ is a vector field, and a_0 is a real constant. This last equation may, equivalently, be written in the following way:

$$\xi_{a;b} + \xi_{b;a} = a_0 g_{ab}, \tag{4}$$

where [;] means covariant differentiation.

With the aid of Eqs. (1)–(3), the condition (4) leads us to the following set of equations:

$$r_{,v}\xi^v + r_{,u}\xi^u = \frac{a_0}{2}\frac{r^2(1-2\eta/r)}{r-M-\eta}, \tag{5}$$

$$\xi^v{}_{,v} + \xi^u{}_{,u} + \frac{2M}{r^2(1-2\eta/r)}(r_{,v}\xi^v + r_{,u}\xi^u) = a_0, \tag{6}$$

$$\xi^u{}_{,v} = 0, \tag{7}$$

$$\xi^{v}{}_{,u} = 0. \tag{8}$$

The solutions to Eqs. (7) and (8) are, respectively

$$\xi^{v} = \xi^{v}(v) \text{ and } \xi^{u} = \xi^{u}(u), \tag{9}$$

where ξ^{v} depends only on v, and ξ^{u} depends only on u.

Now, introducing the right-hand side of Eq. (5) in Eq. (6), we may write

$$\xi^{v}{}_{,v} + \xi^{u}{}_{,u} = a_0 \frac{r - 2M - \eta}{r - M - \eta}. \tag{10}$$

We may obtain independently the expressions for $\xi^{v}{}_{,v}$ and $\xi^{u}{}_{,u}$ and introduce them in the left-hand side of Eq. (10). The resulting equation should be an identity, if the system of Eqs. (5)–(8) admits the solutions given in Eq. (9).

In order to obtain $\xi^{v}{}_{,v}$ and $\xi^{u}{}_{,u}$, we start using Eq. (2) to find

$$r_{,v} = \frac{1}{2}\left(1 - \frac{2\eta}{r}\right)^{M/\eta} = -r_{,u}. \tag{11}$$

Now, we introduce both values of $r_{,v}$ and $r_{,u}$ of Eq. (11) in Eq. (5) and write

$$\xi^{v} - \xi^{u} = a_0 \frac{r^2}{r - M - \eta}\left(1 - \frac{2\eta}{r}\right)^{1-(M/\eta)}. \tag{12}$$

Then, we may differentiate Eq. (12) with respect to v and, using the information from Eq. (9), we derive the following expression for $\xi^{v}{}_{,v}$:

$$\xi^{v}{}_{,v} = a_0 \frac{r_{,v}}{(r - M - \eta)^2} \frac{1}{(1 - 2\eta/r)^{M/\eta}} (r^2 - 4Mr - 2\eta r + 4M\eta + 2\eta^2 + 2M^2). \tag{13}$$

Proceeding in an analogous manner, we derive the following expression for $\xi^{u}{}_{,u}$:

$$\xi^{u}{}_{,u} = -a_0 \frac{r_{,u}}{(r - M - \eta)^2} \frac{1}{(1 - 2\eta/r)^{M/\eta}} (r^2 - 4Mr - 2\eta r + 4M\eta + 2\eta^2 + 2M^2). \tag{14}$$

Finally, introducing the values of $\xi^{v}{}_{,v}$ and $\xi^{u}{}_{,u}$ coming, respectively, from Eqs. (13) and (14) in the left-hand side of Eq. (10), we find

$$-Mr + M\eta + \eta^2 = 0. \tag{15}$$

This equation is not an identity; therefore, we may conclude that there are no self-similar solutions for the system (5)–(8). In fact, this result was expected since the case $\Sigma = 0$ is the Schwarzschild space-time,[3] which is not a self-similar solution.

III. WYMAN'S SOLUTION AND CRITICAL BEHAVIOR

Depending on the value of the parameters M and Σ, Wyman's solution may represent different static, asymptotically flat space-times.[1,3] When one sets $\Sigma = 0$, the scalar field (Φ) vanishes, as can be seen from Eq. (9) of Ref. 3

$$\Phi = \frac{\Sigma}{2\eta} \ln\left(1 - \frac{2\eta}{r}\right), \tag{16}$$

and one obtains the Schwarzschild solution with a mass M. Therefore, it is usual to consider M positive. It is important to introduce the function R

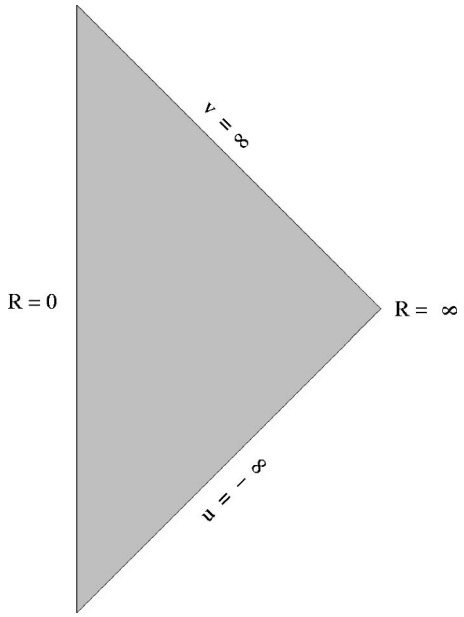

FIG. 1. Conformal diagram for a typical element of the set N. The time-like singularity lies at $R=0$ and spatial infinity at $R\to\infty$ $(v-u\to\infty)$.

$$R^2=\left(1-\frac{2\eta}{r}\right)^{1-M/\eta}r^2, \tag{17}$$

which is a function of r and, from Eq. (1), the quantity $4\pi R^2$ represents the proper area of each two-dimensional sphere obtained by fixing t and r. R can be written as a function of v and u with the aid of r, which is a function of v and u; $r(u,v)$ is obtained by the integration of Eq. (2).

For positive M one may let Σ^2 take values over the real line. For $\Sigma^2>0$, the solution represents space-times with a naked time-like singularity located at $R=0$ $(r=2\eta)$. This singularity is sometimes called a "central singularity" and is similar to that appearing in the "extreme" Reissner–Nordstrøm black hole and in the negative mass Schwarzschild space-time (see Fig. 1). From Eq. (16), the scalar field vanishes asymptotically, $R\to\infty$ (which is equivalent to $r\to\infty$ in the present case), and diverges at the singularity. For $\Sigma^2<0$, one considers the domain: $-M^2\leqslant\Sigma^2<0$, because if $\Sigma^2<-M^2$ from Eq. (1) the metric gets complex. The case $\Sigma^2=-M^2$ is well known in the literature as the Yilmaz–Rosen space-time.[9] In the space-times with $-M^2\leqslant\Sigma^2<0$, R is never zero. If one starts with a large value of R it diminishes, as we let it vary as a function of r, until it reaches a minimum value $\{R_{\min}=[(M-\eta)/(M+\eta)]^{1-M/\eta}(M+\eta)^2\}$. Then, it starts to increase again without limit, giving rise to a new asymptotically flat region. An important property of this space-time is that the scalar field equation (16) is imaginary. The imaginary scalar field also known as the ghost Klein–Gordon field[10] is an example of the type of matter called *exotic* by some authors.[11] It violates most of the energy conditions and is repulsive. This property helps explain why the collapsing scalar field never reaches $R=0$. Recently, the exotic matter has been in evidence due to the discovery that the universe is expanding at an accelerated rate.[12] This implies that the universe must be filled with matter which violates at least the strong energy condition.[12] This is the type of matter associated with the formation and stability of traversible wormholes.[11,13] In particular, the ghost Klein–Gordon field has been used as one of the first specific *exotic* matter models to explain the formation and stability of traversible wormholes.[10] Besides the above motivations for the use of *exotic* matter, which involve classical fields, one must not forget about the negative energy densities very common in quantum field theories.[14] We may interpret this case $-M^2\leqslant\Sigma^2<0$ as a "wormhole-like" solution.

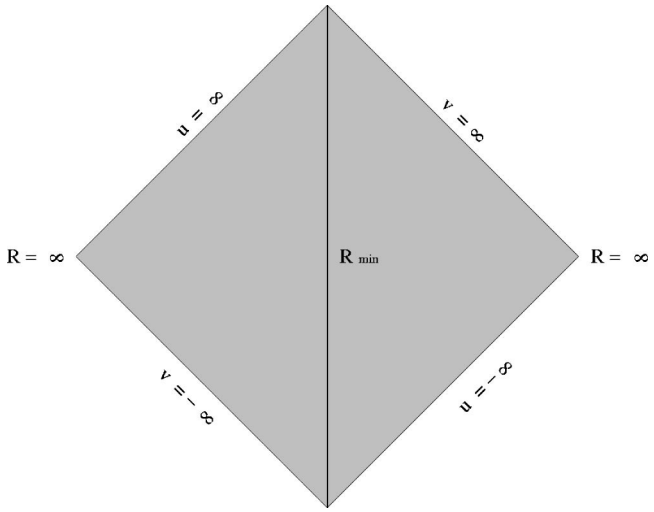

FIG. 2. Conformal diagram for a typical element of the set W. The $R_{\min}$, which may be identified as the wormhole throat, and the two spatial infinities $R\to\infty$ ($v-u\to\infty$ and $v-u\to-\infty$), one for each asymptotically flat region, are shown.

Based on the above properties of Wyman's solution, and taking in account the results of Refs. 6–8, on critical behavior in the spherical symmetric, massless, scalar field collapse, we conclude that Wyman's solution also shows a type of critical behavior, in analogy with the nonstatic massless scalar field solutions. Although the critical solution is of a different kind from the one discovered in the above-mentioned references, one may proceed here in the same way as the authors there, in order to show the critical behavior. One fixes the mass parameter M and considers the scalar charge Σ as the only free parameter. In the present case, as discussed above, we fix M to a positive value, say M_0. Σ^2 may take values in the domain, $(-M_0^2,\infty)$. For Σ^2 positive ($0<\Sigma^2<\infty$), we have a set (N) of solutions representing asymptotically flat, time-like, naked singularities. We show the conformal diagram of a typical element of the set N in Fig. 1. For Σ^2 negative ($-M_0^2<\Sigma^2<0$), we have a set (W) of solutions representing asymptotically flat, wormhole-like space-times. Figure 2 shows the conformal diagram of a typical element of the set W. Finally, for $\Sigma^2=0$, we obtain the critical solution. For fixed M this solution is a point in the parameter space of solutions and represents the Schwarzschild black hole with mass M_0.

IV. CONCLUSIONS

In the present work, we showed that the Wyman's solution is not self-similar or, in other words, it does not admit a homothetic Killing vector. We also showed that Wyman's solution exhibits a type of critical behavior in analogy with the dynamical massless scalar field case. We did that by fixing the mass M to a positive value, say M_0, and letting Σ^2 takes values along the real line. For $\Sigma^2>0$ the space-times have naked singularities; for $\Sigma^2=0$ one has a Schwarzschild black hole of mass M_0, and finally for $-M_0^2\leqslant\Sigma^2<0$ one has wormhole-like solutions. Here, the critical solution is a Schwarzschild black hole. Although this behavior is very different from the one discovered by Choptuik, one may have other kinds of critical solutions in the Einstein-scalar system, as demonstrated by Brady in Ref. 15.

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An exact solution of the five-dimensional Einstein equations with four-dimensional de Sitter-like expansion

Tomáš Liko[a] and Paul S. Wesson[b]
Department of Physics, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

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We present an exact solution to the Einstein field equations which is Ricci and Riemann flat in five dimensions, but in four dimensions is a good model for the early vacuum-dominated universe. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1926168]

I. INTRODUCTION

There has recently been an uprising in interest in finding exact solutions of the Kaluza–Klein field equations in five dimensions (5D) which reproduce and extend known solutions of the Einstein field equations in four dimensions (4D).[1–5] Particular interest revolves around solutions which are not only Ricci flat ($R_{AB}=0; A,B,\ldots\in\{0,1,2,3,4\}$ where R_{AB} is the 5D Ricci tensor), but also Riemann flat ($R_{ABCD}=0$, where the vanishing of the Riemann–Christoffel tensor means that we are considering the analog of the Minkowski metric in 5D).[6–11] This is because it is possible to have a flat 5D manifold which contains a curved 4D submanifold, as implied by Campbell's embedding theorem.[12–18] So, the universe may be "empty" and simple in 5D, but contain matter of complicated forms in 4D.[19,20] (This idea has been extended to higher-dimensional manifolds that are not Ricci flat, in particular manifolds with nonzero cosmological constant,[21,22] scalar field sources,[23] as well as manifolds with an arbitrary nondegenerate Ricci tensor.[24] In addition, the Campbell–Magaard theorem has been used to study the embedding of Randall–Sundrum-type branes in 5D manifolds,[25] suggesting that the curvature of any given brane is not necessarily determined by its stress-energy content.)

Despite the physical appeal of this idea, it is mathematically nontrivial to realize. This is because solutions of the flat and empty Einstein equations in 5D which correspond to solutions of $G_{\alpha\beta}=T_{\alpha\beta}(\alpha,\beta,\ldots\in\{0,1,2,3\})$ in 4D with acceptable physics, are rare. (Here $G_{\alpha\beta}$ is the 4D Einstein tensor and $T_{\alpha\beta}$ is the induced stress-energy tensor obtained via the standard reduction of the 5D equations to their 4D counterparts; see Ref. 20. We use units throughout which render the speed of light and Newton's gravitational constant invisible via $c=1, 8\pi G=1$.) In what follows, we present and derive the properties of an exact 5D solution which provides a good 4D model for the vacuum-dominated early universe.

II. A NEW SOLUTION AND ITS PROPERTIES

Consider the five-dimensional line element with coordinates t, r, θ, ϕ, ℓ such that

$$dS^2 = \frac{\ell^2}{L^2}dt^2 - \left[\ell \sinh\left(\frac{t}{L}\right)\right]^2 d\sigma_3^2 - d\ell^2$$

[a]Electronic mail: tliko@astro.uwaterloo.ca
[b]Tel: (519) 885-1211 ext. 2215; fax: (519) 746-8115; Webpage: http://astro.uwaterloo.ca/~wesson

$$\mathrm{d}\sigma_3^2 = \left(1 + \frac{kr^2}{4}\right)^{-2} (\mathrm{d}r^2 + r^2\,\mathrm{d}\theta^2 + r^2 \sin^2\theta\,\mathrm{d}\phi^2) \quad \text{and } k = -1. \tag{1}$$

In five dimensions this defines a manifold $(\mathcal{M}, g_{AB})$ that is indeed both Ricci flat and Riemann flat, thus giving Minkowski space $\mathbb{M}^5$ in a different coordinate system. That (1) satisfies the Ricci-flat equations $R_{AB}=0$ may be shown by tedious algebra (e.g., using the equations of Ref. 20), and confirmed by computer (e.g., using the program GRTensor of Ref. 26). The only humanly practical way to show that (1) also satisfies the Riemann-flat equations $R_{ABCD}=0$ is by computer, as may be verified.

The physical properties of the matter associated with (1) may, again, be derived either analytically or computationally. The basic procedure, in either approach, is to separate the purely 4D terms in $R_{AB}=0$ from the other ones, compare with $G_{\alpha\beta}=T_{\alpha\beta}$, and thereby obtain $T_{\alpha\beta} = T_{\alpha\beta}(x^4, \partial g_{AB}/\partial x^C)$. Since the Einstein equations $G_{AB}=0$ in empty 5D are equivalent to $R_{AB}=0$ by straight algebra, what we are doing here is simply solving in effect the 5D Einstein equations, comparing the results to the 4D Einstein equations, and thereby evaluating the stress-energy tensor $T_{\alpha\beta}$ necessary to balance the latter set of equations.

This procedure has in recent years been much used. A review of the algebraic technique and a list of applications is available.[20] Here we note that the procedure has been applied to cosmologies of the Friedmann–Robertson–Walker (FRW) type,[27] 3D spherically symmetric solutions,[28] solutions with off-diagonal metrics,[29] Gödel-type space–times,[30] and solutions containing a big bounce.[31–35] General theorems have also been proven, having to do with the field equations,[36] dynamics[37] and the algebraic classification of 5D solutions with their associated 4D stress-energy tensors.[38] However, there is the constraint that the $T_{\alpha\beta}$ given by algebra should correspond to the properties of matter indicated by observational cosmology. For the early universe, this means that the equation of state for the matter should be close to that of the "classical vacuum." Here, the sum of the density ρ and pressure p is zero, as in inflationary cosmology.[39] We now proceed to this and other consequences of metric (1), to investigate its physical acceptability.

The line element (1) can be written in the useful "canonical" form[40] such that

$$\mathrm{d}S^2 = \frac{\ell^2}{L^2}\left[\mathrm{d}t^2 - \left[L \sinh\left(\frac{t}{L}\right)\right]^2 \mathrm{d}\sigma_3^2\right] - \mathrm{d}\ell^2. \tag{2}$$

So with the 4D space–time metric

$$\begin{gathered} g_{\alpha\beta} = \mathrm{diag}[1, -\mathcal{F}_k(t,r), -r^2\mathcal{F}_k(t,r), -r^2\sin^2\theta\mathcal{F}_k(t,r)], \\ \mathcal{F}_k(t,r) = \left[L \sinh\left(\frac{t}{L}\right)\right]^2 \left(1 + \frac{kr^2}{4}\right)^{-2}, \end{gathered} \tag{3}$$

we find the components of the stress-energy tensor $T_{\alpha\beta}=G_{\alpha\beta}$ to be $T_0^0=3/L^2, T_1^1=T_2^2=T_3^3=3/L^2$. In comoving coordinates this defines an energy density $\rho=T_0^0=3/L^2$ and pressure $p=-(T_1^1+T_2^2+T_3^3)/3=-3/L^2$ for a vacuum with cosmological constant $\Lambda=3/L^2$ and equation of state $\rho+p=0$. The 4D Ricci scalar is $R=R_{\alpha\beta}g^{\alpha\beta}=12/L^2$, and the 4D curvature scalar is $K=R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta}=24/L^4$. This latter scalar implies that there are no singularities in the manifold because the constant $L \neq 0$.

Let us now look at (1), viewing its 4D part as describing an FRW model. The 4D hypersurfaces $\ell=$constant therefore describe cosmologies with scale factor given by $\mathcal{S}=\mathcal{S}(t)=L\sinh(t/L)$. Here the Hubble parameter $H \equiv \dot{\mathcal{S}}/\mathcal{S}$ and deceleration parameter $q \equiv -\mathcal{S}\ddot{\mathcal{S}}/\dot{\mathcal{S}}^2$ (with $\dot{\mathcal{S}}=\mathrm{d}\mathcal{S}/\mathrm{d}t$) are found to be

$$H = \frac{1}{L \tanh\left(\frac{t}{L}\right)} \quad \text{and} \quad q = -\tanh^2\left(\frac{t}{L}\right). \tag{4}$$

We note that H is infinite at $t=0$ and goes to $1/L=\sqrt{\Lambda/3}$ as $t\to\infty$, which is the Hubble parameter for de Sitter space–time. Also, q starts at zero when $t=0$ and goes to -1 for $t\to\infty$. This is in line with astrophysical data which currently constrain the deceleration parameter to $-1\leqslant q\leqslant 1$. Thus we conclude that our solution (1) describes an inflationary space–time on $\ell=$constant hypersurfaces, where the vacuum has repulsive properties.

The preceding paragraphs show that (1) has physical properties consistent with those of inflationary cosmology. However, the motivating factor for the latter approach to cosmology is that the (4D) horizon should grow fast enough to resolve certain problems of astrophysical nature, primarily to do with the 3 Kelvin microwave background.[41,42] First, we recall that the horizon distance at time t for any FRW model can be defined[43] such that

$$\int_r^0 \mathrm{d}r\left(1+\frac{kr^2}{4}\right)^{-1} = \int_0^t \frac{\mathrm{d}t'}{\mathcal{S}(t')}. \tag{5}$$

Multiplying both sides by the scale factor $\mathcal{S}(t)$ then gives

$$d_{PH} = \mathcal{S}(t)\int_r^0 \mathrm{d}r\left(1+\frac{kr^2}{4}\right)^{-1} = \mathcal{S}(t)\int_0^t \frac{\mathrm{d}t'}{\mathcal{S}(t')}, \tag{6}$$

which defines the proper distance to the particle horizon at time t. For the space–time (3) this is

$$d_{PH} = 2L\sinh\left(\frac{t}{L}\right)\left[\operatorname{arctanh}(1) - \operatorname{arctanh}\left(\exp\left(\frac{t}{L}\right)\right)\right]. \tag{7}$$

Here we see that d_{PH} is infinite because arctanh(1) is infinite. This means that during the inflationary period that the solution (1) describes on $\ell=$constant hypersurfaces, the entire universe is in causal contact. This is in line with the apparent isotropy of the microwave background.

Finally, we would like to point out an interesting coordinate transformation of the solution (1). Recall that $\sinh(t)=(\exp(t)-\exp(-t))/2$, which with the coordinate change $t\to tL$ in (1) gives

$$\mathrm{d}S^2 = \ell^2\,\mathrm{d}t^2 - \frac{1}{4}\ell^2(e^t+ke^{-t})^2\,\mathrm{d}\sigma_3^2 - \mathrm{d}\ell^2 \quad \text{with } k=-1. \tag{8}$$

This form of the metric resembles a solution noted by McManus.[9] For the solution (8), all 4D physical quantities are the same as those calculated for the solution (1), but with the replacement $L\to\ell$. The 4D space–time contained in (8) therefore still describes an inflationary vacuum with equation of state $\rho+p=0$. An important difference is that the 4D curvature scalar for (8) is $K=24/\ell^4$, which implies that the space–time in (8) has a singularity at the point where $\ell=0$. This is in contrast to the solution (1), for which all physical quantities of spacetime were calculated to be (finite) constants. Evidently the simple coordinate transformation $t\to tL$ casts (1) into a form where the vacuum evolves in accordance with how $x^4=\ell$ is determined by the extra component of the geodesic equation. This issue from the mathematical side has to do with whether we take the whole of the 4D part of the 5D manifold as defining the geometry of space–time, or whether we take the 4D part of the 5D manifold without its prefactor. This 5D issue resembles the 4D one in scalar-tensor theory, where it manifests itself as a choice between what are commonly called the Jordan and Einstein frames. From the physical side, the choice has to do with how we define space–time as a 4D slice of a 5D manifold; and we suggest that since the two choices only become differentiated over cosmological time scales, that it is essentially one of observation to decide.

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Multipolar expansions for closed and open systems of relativistic particles

David Alba[a)]
Dipartimento di Fisica, Universita' di Firenze, Polo Scientifico, via Sansone 1, 50019 Sesto Fiorentino, Italy

Luca Lusanna[b)]
Sezione INFN di Firenze Polo Scientifico, via Sansone 1, 50019 Sesto Fiorentino, Italy

Massimo Pauri[c)]
Dipartimento di Fisica, Universita' di Parma, Parco Area Scienze 7/A, 43100 Parma, Italy

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Dixon's multipoles for a system of N relativistic positive-energy scalar particles are evaluated in the rest-frame instant form of dynamics. The Wigner hyperplanes (intrinsic rest frame of the isolated system) turn out to be the natural framework for describing multipole kinematics. Classical concepts like the *barycentric tensor of inertia* turn out to be extensible to special relativity only by means of the quadrupole moments of the isolated system. Two new applications of the multipole technique are worked out for systems of interacting particles and fields. In the rest frame of the isolated system of either free or interacting positive energy particles it is possible to define a unique world line which embodies the properties of the most relevant centroids introduced in the literature as candidates for the collective motion of the system. This is no longer true, however, in the case of open subsystems of the isolated system. While effective mass, 3-momentum and angular momentum in the rest frame can be calculated from the definition of the *subsystem energy-momentum tensor*, the definitions of effective center of motion and effective intrinsic spin of the subsystem are not unique. Actually, each of the previously considered centroids corresponds to a different world line in the case of open systems. The pole–dipole description of open subsystems is compared to their description as effective extended objects. Hopefully, the technique developed here could be instrumental for the relativistic treatment of binary star systems in metric gravity. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1897841]

I. INTRODUCTION

An important area of research is nowadays the construction of templates for gravitational waves emitted by binary systems. Analytically, this can be done within the framework of post-Newtonian (PN) approximations by means of essentially nonrelativistic multipole expansions for compact bodies. On the other hand, since the main emission are supposed to take place in a region where the PN approximation fails, it would be desirable to have at disposal a relativistic treatment of multipolar expansions as a preliminary kinematical tool for dealing with open gravitating systems. This paper focuses just on the construction of a suitable relativistic kinematical background by exploiting an N-body system as a tool. A preliminary extension of the results of this paper to special relativistic perfect fluids is given in Ref. 1. Then using the framework of the

[a)]Electronic mail: alba@fi.infn.it
[b)]Electronic mail: lusanna@fi.infn.it
[c)]Electronic mail: pauri@pr.infn.it

rest-frame instant form of tetrad gravity developed in Refs. 2,3, the relativistic perfect fluids will be coupled to tetrad gravity and the relativistic multipolar expansion will be used in the weak field Hamiltonian linearization[3] leading to background-independent gravitational waves.[4]

The description of either extended or point-particle classical relativistic systems by means of multipolar expansions both in special and general relativity began at the end of the 1930s[5–10] and after many developments[11–19] was set in a final form by Dixon. His special[20] and general[21] relativistic formulation has been the reference standard for recent improvements.[22–24] Then, because of the difficulties in actual evaluations of general relativistic multipoles,[21] the studies of gravitational radiation in the PN regime led to the introduction of the more manageable irreducible symmetric trace-free Cartesian tensors (STF tensors).[25–28]

The multipolar expansion has been mainly used to make *pole–dipole* approximations of extended objects and to replace their equations of motion with the Papapetrou–Dixon–Souriau equations of motion[11,20–22,24] for the 4-momentum and the spin tensor of the objects. However, since in all these approaches the multipoles are defined as moments of the energy-momentum tensor of the system with respect to the world line of an arbitrary *centroid* (the *center of motion*), the intrinsic weakness of multipolar expansions lies in the absence of a *constitutive relation* connecting the 4-velocity of the centroid to the 4-momentum of the system. As a consequence, both from a practical and a theoretical point of view it is not known which is the most convenient choice for the definition of center of motion among, e.g., Pirani centroid,[14] Tulczyjew centroid,[15,18,23] Møller center of energy,[29] Corinaldesi–Papapetrou centroid,[12] Fokker–Pryce center of inertia (or of spin)[30–32] and many other possible centroids.

In this paper we will face these problems in the framework of special relativity from a viewpoint which can be generalized and adapted to the new canonical formulation of metric and tetrad gravity of Refs. 2 and 3. Our starting point are the results recently obtained[33] about a complete treatment of the kinematics of the relativistic *N*-body problem in the *rest-frame instant form of dynamics*.[34–37] This program required a reformulation of the theory of isolated relativistic systems and was essentially grounded upon Dirac's reformulation[38] of classical field theory (suitably extended to particles) on arbitrary spacelike hypersurfaces.[39,40] For each isolated system (containing any combination of particles, strings and fields) one obtains in this way a reformulation of the standard theory as a parametrized Minkowski theory.[34,37] This program contains the extra bonus of being naturally prepared for the coupling to gravity in its ADM formulation. The price to be paid is that the functions $z^\mu(\tau,\vec{\sigma})$ describing the embedding of the spacelike hypersurface in Minkowski space–time become configuration variables in the action principle. Since the action is invariant under separate τ-reparametrizations and space diffeomorphisms, first class constraints emerge ensuring the independence of the description of the choice of the $3+1$ splitting. The embedding configuration variables $z^\mu(\tau,\vec{\sigma})$ are thus the *gauge* variables associated with this particular kind of general covariance.[41]

In parametrized Minkowski theories in the case of particles, each particle must have *a well defined sign of the energy*, since the intersection of a timelike world line with a spacelike hypersurface corresponding to a value τ of the time parameter is identified by three numbers $\vec{\sigma}=\vec{\eta}(\tau)$ instead of four. Therefore, the two topologically disjoint branches of the mass hyperboloid cannot be simultaneously described as in the standard manifestly Lorentz-covariant theory, so that no mass-shell constraint appears. Each particle with a definite sign of the energy is described by the canonical coordinates $\vec{\eta}_i(\tau),\vec{\kappa}_i(\tau)$ while the 4-position of the particles are given by $x_i^\mu(\tau)=z^\mu(\tau,\vec{\eta}_i(\tau))$. The following 4-momenta $p_i^\mu(\tau)$ are $\vec{\kappa}_i$-dependent solutions of $p_i^2-m_i^2=0$ with the chosen sign of the energy.

In order to exploit the separate spatial and time reparametrization invariances of parametrized Minkowski theories, we can first of all restrict the foliation to spacelike *hyperplanes* as leaves. For each configuration of the isolated system with timelike 4-momentum, we further restrict to the special leaves defined by hyperplanes orthogonal to the conserved system 4-momentum (*Wigner hyperplanes*). This foliation is fully determined by the configuration of the isolated system. One gets in this way[34] the definition of the *Wigner-covariant rest-frame instant form of dynamics* for any isolated system whose configurations have well defined and finite Poincaré generators with

timelike total 4-momentum (see Ref. 42 for the traditional forms of dynamics). Finally, this formulation casts new light on the long standing problem of defining a relativistic center of mass. As well known, no definition of this concept can enjoy all the properties of its nonrelativistic counterpart. See Refs. 30–32, 43, and 44 for a partial bibliography of all the existing attempts.

We summarize here the main previous results necessary to understand all the subsequent technical developments (further details can be found in Appendix A of Ref. 33 and Sec. II):

(a) The Wigner hyperplanes are described by the embedding $z^\mu(\tau,\vec{\sigma}) = x_s^\mu(\tau) + \epsilon_r^\mu(u(p_s))\sigma^r$, where $x_s^\mu(\tau) = z^\mu(\tau,\vec{0})$ is an arbitrary centroid (origin of the 3-coordinates $\vec{\sigma}$) playing the role of the *center of motion* for multipolar expansions.

(b) The canonical variables describing the remaining freedom in the embedding are a *noncovariant canonical so-called external 4-center-of-mass* configurational variable $\tilde{x}_s^\mu(\tau) \neq x_s^\mu(\tau)$ and the conjugate 4-momentum p_s^μ, weakly equal to the total 4-momentum of the isolated system and orthogonal to the Wigner hyperplanes. The timelike unit vector $u^\mu(p_s) = p_s^\mu/\sqrt{p_s^2}$ $[p_{s\mu}\epsilon_r^\mu(u(p_s)) = 0]$ describes the orientation of Wigner hyperplanes in the chosen inertial system. These canonical variables describe a decoupled free point (*point particle clock*).

(c) The mathematical time τ is identified with the Lorentz scalar time $T_s = \tilde{x}_s \cdot p_s/\sqrt{p_s^2} = x_s \cdot p_s/\sqrt{p_s^2}$ of this decoupled point by means of the gauge fixing $T_s - \tau \approx 0$, which implies $\epsilon_s = \sqrt{p_s^2} = M_{\rm sys}, \dot{\tilde{x}}_s^\mu(\tau) = u^\mu(p_s)$ and $\dot{x}_s^\mu(\tau) = u^\mu(p_s) + \epsilon_r^\mu(u(p_s))\lambda_r(\tau)$ [$\lambda_r(\tau)$ are three arbitrary Dirac multipliers]. Here $M_{\rm sys}$ is the invariant mass of the isolated system. The decoupled point is now described by canonical 3-coordinates $\vec{z}_s = \epsilon_s[\vec{\tilde{x}}_s - (\vec{p}_s/p_s^o)\tilde{x}^o]$ (the *external 3-center of mass*) and $\vec{k}_s = \vec{p}_s/\epsilon_s$.[45]

(d) There is an *external* realization of the Poincaré group, whose Lorentz transformations (change of the inertial observer) induce a *Wigner rotation* of the 3-vectors inside each Wigner hyperplane. As shown in Ref. 33, the *external* Poincaré generators allow to define three concepts of the *external* collective variable, (i) the *external* noncovariant canonical *4-center of mass* (also named *4-center of spin*) $\tilde{x}_s^\mu$ (with 3-location $\vec{\tilde{\sigma}}$); (ii) the *external* noncovariant noncanonical Møller *4-center of energy* R_s^μ (with 3-location $\vec{\sigma}_R$); (iii) the *external* covariant noncanonical Fokker–Pryce *4-center of inertia* Y_s^μ (with 3-location $\vec{\sigma}_Y$). Only the canonical noncovariant center of mass $\tilde{x}_s^\mu(\tau)$ is relevant to the Hamiltonian treatment with Dirac constraints, while only the Fokker–Pryce Y_s^μ is a 4-vector by construction. See Ref. 33 for the construction of the *4-centers* starting from the corresponding *3-centers* (3-center of spin,[31] 3-center of energy,[29] 3-center of inertia[30,31]), which are group-theoretically defined in terms of generators of the external Poincaré group.

(e) Inside the Wigner hyperplanes the particles are described by Wigner spin-1 canonical 3-vectors $\vec{\eta}_i(\tau), \vec{\kappa}_i(\tau)$ restricted by the three first class constraints (the *rest-frame conditions*) $\vec{\kappa}_+ = \Sigma_{i=1}^N \vec{\kappa}_i \approx 0$, whose associated Dirac multipliers $\lambda_r(\tau)$ describe the freedom in the choice of the centroid $x_s^\mu(\tau)$. The rest-frame conditions imply that an *internal* 3-center-of-mass variable $\vec{\sigma}_{\rm c.m.}$ is a *gauge variable*, whose elimination through a gauge fixing[46] is equivalent to a definite choice of the world-line $x_s^\mu(\tau)$ of the centroid. Inside Wigner hyperplanes there is an unfaithful *internal* realization of the Poincaré algebra, the total *internal* 3-momentum of the isolated system vanishes due to the rest-frame conditions. The *internal* energy and angular momentum are the invariant mass $M_{\rm sys}$ and the spin [the angular momentum with respect to $\tilde{x}_s^\mu(\tau)$] of the isolated system, respectively. By means of the *internal* realization of the Poincaré algebra we can define three *internal* 3-centers of mass, the *internal* canonical 3-center of mass (or 3-center of spin) $\vec{q}_+$, the *internal* Møller 3-center of energy $\vec{R}_+$, and the *internal* Fokker–Pryce 3-center of inertia $\vec{y}_+$. However, because of the rest-frame condition $\vec{\kappa}_+ \approx 0$, *they all coincide*, $\vec{q}_+ \approx \vec{R}_+ \approx \vec{y}_+$. As a natural gauge fixing to the rest-frame conditions, we can add the vanishing of the *internal* Lorentz boosts $\vec{K}$ (recall that they are equal to $-\vec{R}_+/M_{\rm sys}$). This is equivalent to locate the internal canonical 3-center of mass $\vec{\sigma}_{\rm c.m.} = \vec{q}_+$ in $\vec{\sigma} = 0$, i.e., in the centroid $x_s^\mu(\tau) = z^\mu(\tau,\vec{0})$. Upon such gauge fixings, the world-line $x_s^\mu(\tau)$

becomes uniquely determined except for the arbitrariness in the choice of $x_s^\mu(0)$,

$$x_s^{(\vec{q}_+)\mu}(\tau) = x_s^\mu(0) + u^\mu(p_s)T_s, \tag{1.1}$$

and, modulo $x_s^\mu(0)$, it coincides with the *external* covariant noncanonical Fokker–Pryce 4-center of inertia, $x_s^\mu(\tau) = x_s^\mu(0) + Y_s^\mu$.[33]

In the gauge where $\epsilon_s \equiv M_{\rm sys}$, and $T_s \equiv \tau$, the canonical basis $\vec{z}_s, \vec{k}_s, \vec{\eta}_i, \vec{\kappa}_i$ is restricted by the three pairs of second class constraints $\vec{\kappa}_+ = \Sigma_{i=1}^N \vec{\kappa}_i \approx 0$, $\vec{q}_+ \approx 0$, so that $6N$ canonical variables describe the N particles as in the nonrelativistic case. We still need a canonical transformation $\vec{\eta}_i, \vec{\kappa}_i \mapsto \vec{q}_+[\approx 0], \vec{\kappa}_+[\approx 0], \vec{\rho}_a, \vec{\pi}_a$ $[a = 1, \ldots, N-1]$ identifying a set of relative canonical variables. The final $6N$-dimensional canonical basis is $\vec{z}_s, \vec{k}_s, \vec{\rho}_a, \vec{\pi}_a$. To get this result we need a highly nonlinear canonical transformation,[33] which can be obtained by exploiting the Gartenhaus–Schwartz singular transformation.[47]

At the end we obtain *the Hamiltonian for the relative motions as a sum of N square roots*, each one containing a squared mass and a quadratic form in the relative momenta, which goes into the nonrelativistic Hamiltonian for relative motions in the limit $c \to \infty$. This fact has the following implications.

(a) If one tries to make the inverse Legendre transformation to find the associated Lagrangian, it turns out that, due to the presence of square roots, the Lagrangian is a hyperelliptic function of $\dot{\vec{\rho}}_a$ already in the free case. A closed form exists only for $N=2$, $m_1 = m_2 = m$, $L = -m\sqrt{4 - \dot{\vec{\rho}}^2}$. This exceptional case already shows that the existence of the limiting velocity c forbids a linear relation between the spin (center-of-mass angular momentum) and the angular velocity.

(b) The N quadratic forms in the relative momenta appearing in the relative Hamiltonian *cannot be simultaneously diagonalized*. The Hamiltonian is anyway a sum of square roots, so that concepts like *reduced masses, Jacobi normal relative coordinates*, and *tensor of inertia* cannot be extended to special relativity. As a consequence, for example, a relativistic static orientation-shape SO(3) principal bundle approach[48,49] can be implemented only by using non-Jacobi relative coordinates.

(c) The best way of studying rotational kinematics, *viz.* the non-Abelian rotational symmetry associated with the conserved *internal* spin, is based on the concept of *canonical spin bases* with the associated concepts of *spin frames* and *dynamical body frames* introduced in Ref. 33. It is a remarkable fact that they can be built, just as in the nonrelativistic case,[50] starting from the canonical basis $\vec{\rho}_a, \vec{\pi}_a$.

As anticipated at the outset, our aim is to complete the study of relativistic kinematics for the N-body system by first evaluating the rest-frame Dixon multipoles[20] and then by analyzing the role of Dixon's multipoles for *open subsystems*. The basic technical tool will be the standard definition of the *energy momentum tensor* of the N positive-energy *free* particles on the Wigner hyperplane. It will be seen that, in order to get a sensible extension of this definition to open subsystems, a physically significant convention is required. On the whole, it turns out that the Wigner hyperplane is the natural framework for reorganizing a lot of kinematics connected with multipoles, but only when the gauge fixing $T_s - \tau \approx 0$ identifies the mathematical time τ with the rest-frame scalar time T_s. Only in this way, moreover, a concept like the *barycentric tensor of inertia* can be introduced in special relativity, specifically by means of the quadrupole moments.

A first application of the formalism is done for an isolated system of N positive-energy particles with *mutual action-at-a-distance interactions*. The formalism is then applied to the case of an *open* $n < N$ *particle subsystem* of an isolated system consisting of N charged positive-energy particles (with Grassmann-valued electric charges introduced to regularize the Coulomb self-energies) plus the electromagnetic field.[36] In the rest frame of the isolated system, a *suitable* definition of the energy-momentum tensor of the open subsystem allows to define its effective mass, 3-momentum, and angular momentum.

Then we evaluate the rest-frame Dixon multipoles of the energy-momentum tensor of the

open subsystem with respect to various centroids describing possible *collective centers of motion*. Unlike the case of isolated systems, each centroid generates a different world line and there are many candidates as effective centers of motion and effective intrinsic spin. Two centroids (namely the so-called *center of energy* and Tulczyjew centroid) show particularly interesting properties. The case $n=2$ is studied explicitly. It is also shown that the pole–dipole description of the two-particle cluster can be replaced by a description of the cluster as an extended system (its effective spin frame can be evaluated). This can be done, however, at the price of introducing an explicit dependence on the action of the external electromagnetic field upon the cluster. By comparing the effective parameters of an open cluster of n_1+n_2 particles to the effective parameters of the two clusters with n_1 and n_2 particles, it turns out in particular that only the effective *center of energy* appears to be a viable center of motion for studying the interactions of open subsystems.

For the sake of simplicity, we shall omit many explicit calculations. The interested reader may find them in an extended version of this paper given in Ref. 51.

A review of the rest-frame instant form of dynamics for N scalar free positive-energy particles and some new original results on the canonical transformation to the internal center of mass and relative variables are given in Sec. II.

In Sec. III we evaluate the energy momentum tensor in the Wigner hyperplanes.

Dixon's multipoles are introduced in Sec. IV. A special study of monopole, dipole, and quadrupole moments is given and the multipolar expansion is defined.

After the extension of the previous results to isolated systems with mutual action-at-a-distance interactions, in Sec. V we study the behavior of open subsystems of isolated systems, the centroids which are good candidates for the description the collective center of motion, and discuss the determination of the effective parameters (mass, spin, momentum, variables relative to the center of motion) for the open subsystem.

Some comments about standing problems are given in the Conclusions.

The Gartenhaus–Schwartz transformation is summarized in the Appendix.

II. REVIEW OF THE REST-FRAME INSTANT FORM

We briefly review the treatment of N free scalar positive-energy particles in the framework of parametrized Minkowski theory (see Appendixes A and B and Sec. II of Ref. 33).

The foliation associated to a $3+1$ splitting of Minkowski space–time is defined by an embedding $R\times\Sigma\to M^4$, $\sigma^A=(\tau,\vec{\sigma})\mapsto z^\mu(\tau,\vec{\sigma})$, with Σ an abstract 3-surface diffeomorphic to R^3. Σ_τ is the Cauchy surface of *equal time*. The 4-metric induced on Σ_τ is $g_{AB}[z]=z^\mu_A\eta_{\mu\nu}z^\nu_B$, a functional of z^μ, and the embedding coordinates $z^\mu(\tau,\vec{\sigma})$ are considered as independent fields. The $z^\mu_A(\sigma)=\partial z^\mu(\sigma)/\partial\sigma^A$ are flat cotetrad fields on Minkowski space–time with the z^μ_r's tangent to Σ_τ. The vectors $z^\mu_r(\tau,\vec{\sigma})$ are tangent to Σ_τ, whose unit normal field is $l^\mu(\tau,\vec{\sigma})=\epsilon^\mu{}_{\alpha\beta\gamma}[z^\alpha_1 z^\beta_2 z^\gamma_3]\times(\tau,\vec{\sigma})_1/\sqrt{\gamma(\tau,\vec{\sigma})}$. The dual tetrad fields are $z^A_\mu(\sigma)=\partial\sigma^A(z)/\partial z^\mu$, $z^A_\mu(\tau,\vec{\sigma})z^\mu_B(\tau,\vec{\sigma})=\delta^A_B$. The inverse of the 3-metric g_{rs} is denoted γ^{rs}, $\gamma^{ru}g_{us}=\delta^r_s$. While in Ref. 33 we used the metric convention $\eta_{\mu\nu}=\epsilon(+---)$ with $\epsilon=\pm$, in this paper we shall use $\epsilon=1$ like in Ref. 34.

Each particle is described by a configuration 3-vector $\vec{\eta}_i(\tau)$. The particle world line is $x^\mu_i(\tau)=z^\mu(\tau,\vec{\eta}_i(\tau))$, where $z^\mu(\tau,\vec{\sigma})$ are the embedding configuration variables describing the spacelike hypersurface Σ_τ.

The system of configuration variables $z^\mu(\tau,\vec{\sigma})$, $\vec{\eta}_i(\tau)$, is described by the action[34–36]

$$S=\int \mathrm{d}\tau\, d^3\sigma\, \mathcal{L}(\tau,\vec{\sigma})=\int \mathrm{d}\tau\, L(\tau),$$

$$\mathcal{L}(\tau,\vec{\sigma})=-\sum_{i=1}^{N}\delta^3(\vec{\sigma}-\vec{\eta}_i(\tau))m_i\sqrt{g_{\tau\tau}(\tau,\vec{\sigma})+2g_{\tau r}(\tau,\vec{\sigma})\dot{\eta}^r_i(\tau)+g_{rs}(\tau,\vec{\sigma})\dot{\eta}^r_i(\tau)\dot{\eta}^s_i(\tau)}. \tag{2.1}$$

The action is invariant under separate τ and $\vec{\sigma}$ reparametrizations. Therefore the canonical momenta $\rho_\mu(\tau,\vec{\sigma})=-\partial\mathcal{L}(\tau,\vec{\sigma})/\partial z^\mu_\tau(\tau,\vec{\sigma})$ and $\kappa_{ir}(\tau)=-\partial L(\tau)/\partial\dot{\eta}^r_i(\tau)$ satisfy the primary first class constraints

$$\mathcal{H}_\mu(\tau,\vec{\sigma}) = \rho_\mu(\tau,\vec{\sigma}) - l_\mu(\tau,\vec{\sigma})\sum_{i=1}^{N}\delta^3(\vec{\sigma}-\vec{\eta}_i(\tau))\sqrt{m_i^2-\gamma^{rs}(\tau,\vec{\sigma})\kappa_{ir}(\tau)\kappa_{is}(\tau)}$$

$$-z_{r\mu}(\tau,\vec{\sigma})\gamma^{rs}(\tau,\vec{\sigma})\sum_{i=1}^{N}\delta^3(\vec{\sigma}-\vec{\eta}_i(\tau))\kappa_{is}\approx 0, \tag{2.2}$$

so that the Dirac Hamiltonian is $H_D=\int d^3\sigma\,\lambda^\mu(\tau,\vec{\sigma})\mathcal{H}_\mu(\tau,\vec{\sigma})$, where $\lambda^\mu(\tau,\vec{\sigma})$ are Dirac multipliers. The standard particle 4-momentum is the following solution of $p_i^2-m_i^2=0$: $p_i^\mu(\tau)=l^\mu(\tau,\vec{\eta}_i(\tau))\sqrt{m_i^2-\gamma^{rs}(\tau,\vec{\eta}_i(\tau))\kappa_{ir}(\tau)\kappa_{is}(\tau)}+z^\mu(\tau,\vec{\eta}_i(\tau))\gamma^{rs}(\tau,\vec{\eta}_i(\tau))\kappa_{is}(\tau)$.

The conserved Poincaré generators are (the suffix "s" denotes the hypersurface Σ_τ)

$$p_s^\mu=\int d^3\sigma\,\rho^\mu(\tau,\vec{\sigma}),$$

$$J_s^{\mu\nu}=\int d^3\sigma[z^\mu(\tau,\vec{\sigma})\rho^\nu(\tau,\vec{\sigma})-z^\nu(\tau,\vec{\sigma})\rho^\mu(\tau,\vec{\sigma})]. \tag{2.3}$$

After the restriction to *Wigner hyperplane*,[52] $z^\mu(\tau,\vec{\sigma})=x_s^\mu(\tau)+\epsilon_r^\mu(u(p_s))\sigma^r$, the independent degrees of freedom of the embedding are reduced to the canonical coordinates x_s^μ, $p_s^\mu=\epsilon_s u^\mu(p_s)$ of a point particle and we have the following constraints and Dirac Hamiltonian[34,36] (the symbol $\overset{\circ}{=}$ means evaluated on the solutions of the equations of motion):

$$\tilde{\mathcal{H}}^\mu(\tau)=u^\mu(p_s)\left[\epsilon_s-\sum_{i=1}^{N}\sqrt{m_i^2+\vec{\kappa}_i^2}\right]+\epsilon_r^\mu(u(p_s))\sum_{i=1}^{N}\kappa_{ir}\approx 0,$$

or

$$\epsilon_s-M_{\rm sys}\approx 0,\quad M_{\rm sys}=\sum_{i=1}^{N}\sqrt{m_i^2+\vec{\kappa}_i^2},\quad \vec{p}_{\rm sys}=\vec{\kappa}_+=\sum_{i=1}^{N}\vec{\kappa}_i\approx 0,$$

$$H_D=\lambda^\mu(\tau)\tilde{\mathcal{H}}_\mu(\tau)=\lambda(\tau)[\epsilon_s-M_{\rm sys}]-\vec{\lambda}(\tau)\sum_{i=1}^{N}\vec{\kappa}_i,$$

$$\dot{x}_s^\mu(\tau)\overset{\circ}{=}\{x_s^\mu(\tau),H_D\}\approx -\lambda^\mu(\tau)=-\lambda(\tau)u^\mu(p_s)+\epsilon_r^\mu(u(p_s))\lambda_r(\tau),$$

$$\Rightarrow x_s^\mu(\tau)=x_s^\mu(0)-u^\mu(p_s)\int_0^\tau d\tau_1\lambda(\tau_1)+\epsilon_r^\mu(u(p_s))\int_0^\tau d\tau_1\lambda_r(\tau_1). \tag{2.4}$$

While the Dirac multiplier $\lambda(\tau)$ is determined by the gauge fixing $T_s-\tau\approx 0$, implying $\epsilon_s\equiv M_{\rm sys}$, and the value $\lambda(\tau)=-1$, the three Dirac's multipliers $\vec{\lambda}(\tau)$ describe the classical Zitterbewegung of the centroid $x_s^\mu(\tau)=z^\mu(\tau,\vec{0})$ which is the origin of the 3-coordinates on the Wigner hyperplane. Each gauge-fixing $\vec{\chi}(\tau)\approx 0$ to the three first class constraints $\vec{\kappa}_+\approx 0$ (defining the *internal rest-frame* 3-center of mass $\vec{\sigma}_{\rm c.m.}$) gives a different determination of the multipliers $\vec{\lambda}(\tau)$.[53] Therefore each gauge-fixing identifies a different world line for the covariant noncanonical centroid $x_s^{(\vec{\chi})\mu}(\tau)$. Of course, inside the Wigner hyperplane, three degrees of freedom of the isolated system become gauge variables. The natural gauge fixing for eliminating the first class constraints $\vec{\kappa}_+\approx 0$ is $\vec{\chi}(\tau)=\vec{\sigma}_{\rm c.m.}=\vec{q}_+\approx 0$ [vanishing of the location of the internal canonical 3-center of mass, see after Eq. (2.12)]. We have that $\vec{q}_+\approx 0$ implies $\lambda_r(\tau)=0$: in this way the *internal* 3-center of mass is located in a unique centroid $x_s^{(\vec{q}_+)\mu}(\tau)=z^\mu(\tau,\vec{\sigma}=0)$ $[\dot{x}_s^{(\vec{q}_+)\mu}=\dot{\tilde{x}}_s^\mu=u^\mu(p_s)]$.

Note that the constant $x_s^\mu(0)$ [and, therefore, also $\tilde{x}_s^\mu(0)$] is arbitrary, reflecting the arbitrariness

in the absolute location of the origin of the *internal* coordinates on each hyperplane in Minkowski space–time. The centroid $x_s^\mu(\tau)$ corresponds to the unique special relativistic center-of-mass-type world line for isolated systems of Refs. 54–56, which unifies previous proposals of Synge, Møller, and Pryce.

The only remaining canonical variables describing the Wigner hyperplane in the final Dirac brackets are a noncovariant canonical coordinate $\tilde{x}_s^\mu(\tau)$ (Ref. 57) and p_s^μ. The point with coordinates $\tilde{x}_s^\mu(\tau)$ is the decoupled canonical *external 4-center of mass* of the isolated system, which can be interpreted as a decoupled observer with his parametrized clock (*point particle clock*). Its velocity $\dot{\tilde{x}}_s^\mu(\tau)$ is parallel to p_s^μ, so that it has no classical Zitterbewegung.

The relation between $x_s^\mu(\tau)$ and $\tilde{x}_s^\mu(\tau)$ ($\vec{\tilde{\sigma}}$ is its 3-location on the Wigner hyperplane) is[33,34]

$$\tilde{x}_s^\mu(\tau) = (\tilde{x}_s^o(\tau); \vec{\tilde{x}}_s(\tau)) = z^\mu(\tau, \vec{\tilde{\sigma}}) = x_s^\mu(\tau) - \frac{1}{\epsilon_s(p_s^o + \epsilon_s)} \left[p_{s\nu} S_s^{\nu\mu} + \epsilon_s \left(S_s^{o\mu} - S_s^{o\nu} \frac{p_{s\nu} p_s^\mu}{\epsilon_s^2} \right) \right], \tag{2.5}$$

and we get $\dot{\tilde{x}}_s^\mu(\tau) = \{\tilde{x}_s^\mu(\tau), H_D\} = -\lambda(\tau) u^\mu(p_s)$ [$= u^\mu(p_s)$ when $\lambda(\tau) = -1$]. After the separation of the relativistic canonical noncovariant *external* 4-center of mass $\tilde{x}_s^\mu(\tau)$, the N particles are described on the Wigner hyperplane by the $6N$ Wigner spin-1 3-vectors $\vec{\eta}_i(\tau), \vec{\kappa}_i(\tau)$ restricted by the rest-frame condition $\vec{\kappa}_+ = \sum_{i=1}^N \vec{\kappa}_i \approx 0$.

The various spin tensors and vectors are[34]

$$J_s^{\mu\nu} = x_s^\mu p_s^\nu - x_s^\nu p_s^\mu + S_s^{\mu\nu} = \tilde{x}_s^\mu p_s^\nu - \tilde{x}_s^\nu p_s^\mu + \tilde{S}_s^{\mu\nu},$$

$$S_s^{\mu\nu} = [u^\mu(p_s)\epsilon_r^\nu(u(p_s)) - u^\nu(p_s)\epsilon_r^\mu(u(p_s))]\overline{S}_s^{\tau r} + \epsilon_r^\mu(u(p_s))\epsilon_s^\nu(u(p_s))\overline{S}_s^{rs} \equiv [\epsilon_r^\mu(u(p_s))u^\nu(p_s) - \epsilon_r^\nu(u(p_s))u^\mu(p_s)] \sum_{i=1}^N \eta_i^r \sqrt{m_i^2 c^2 + \vec{\kappa}_i^2} + [\epsilon_r^\mu(u(p_s))\epsilon_s^\nu(u(p_s)) - \epsilon_r^\nu(u(p_s))\epsilon_s^\mu(u(p_s))] \sum_{i=1}^N \eta_i^r \kappa_i^s,$$

$$\overline{S}_s^{AB} = \epsilon_\mu^A(u(p_s))\epsilon_\nu^B(u(p_s))S_s^{\mu\nu},$$

$$\overline{S}_s^{rs} \equiv \sum_{i=1}^N (\eta_i^r \kappa_i^s - \eta_i^s \kappa_i^r), \quad \overline{S}_s^{\tau r} \equiv -\sum_{i=1}^N \eta_i^r \sqrt{m_i^2 c^2 + \vec{\kappa}_i^2},$$

$$\tilde{S}_s^{\mu\nu} = S_s^{\mu\nu} + \frac{1}{\sqrt{p_s^2}(p_s^o + \sqrt{p_s^2})} [p_{s\beta}(S_s^{\beta\mu} p_s^\nu - S_s^{\beta\nu} p_s^\mu) + \sqrt{p_s^2}(S_s^{o\mu} p_s^\nu - S_s^{o\nu} p_s^\mu)],$$

$$\tilde{S}_s^{ij} = \delta^{ir}\delta^{js}\overline{S}_s^{rs}, \quad \tilde{S}_s^{oi} = -\frac{\delta^{ir}\overline{S}_s^{rs} p_s^s}{p_s^o + \sqrt{p_s^2}},$$

$$\vec{\overline{S}} = \sum_{i+1}^N \vec{\eta}_i \times \vec{\kappa}_i \approx \sum_{i=1}^N \vec{\eta}_i \times \vec{\kappa}_i - \vec{\eta}_+ \times \vec{\kappa}_+ = \sum_{a=1}^{N-1} \vec{\rho}_a \times \vec{\pi}_a. \tag{2.6}$$

Note that while $L_s^{\mu\nu} = x_s^\mu p_s^\nu - x_s^\nu p_s^\mu$ and $S_s^{\mu\nu}$ are not constants of the motion due to the classical Zitterbewegung [when $\vec{\lambda}(\tau) \neq 0$], both $\tilde{L}_s^{\mu\nu} = \tilde{x}_s^\mu p_s^\nu - \tilde{x}_s^\nu p_s^\mu$ and $\tilde{S}_s^{\mu\nu}$ are conserved.

The canonical variables $\tilde{x}_s^\mu, p_s^\mu$ for the *external* 4-center of mass, can be replaced by the canonical pairs[58]

$$T_s = \frac{p_s \cdot \tilde{x}_s}{\epsilon_s} = \frac{p_s \cdot x_s}{\epsilon_s}, \quad \epsilon_s = \pm\sqrt{p_s^2}, \quad \vec{z}_s = \epsilon_s\left(\vec{\tilde{x}}_s - \frac{\vec{p}_s}{p_s^o}\tilde{x}_s^o\right), \quad \vec{k}_s = \frac{\vec{p}_s}{\epsilon_s},$$

$$\tilde{x}_s^o = \sqrt{1+\vec{k}_s^2}\left(T_s + \frac{\vec{k}_s \cdot \vec{z}_s}{\epsilon_s}\right), \quad \vec{\tilde{x}}_s = \frac{\vec{z}_s}{\epsilon_s} + \left(T_s + \frac{\vec{k}_s \cdot \vec{z}_s}{\epsilon_s}\right)\vec{k}_s, \quad p_s^o = \epsilon_s\sqrt{1+\vec{k}_s^2},$$

$$\vec{p}_s = \epsilon_s \vec{k}_s, \tag{2.7}$$

which make explicit the interpretation of it as a *point particle clock*.

This nonpoint canonical transformation can be summarized as $[\epsilon_s - M_{\rm sys} \approx 0,\ \vec{\kappa}_+ = \Sigma_{i=1}^N \vec{\kappa}_i \approx 0]$

$$\begin{array}{|c|c|}\hline \tilde{x}_s^\mu & \vec{\eta}_i \\ \hline p_s^\mu & \vec{\kappa}_i \\ \hline \end{array} \longrightarrow \begin{array}{|c|c|c|}\hline \epsilon_s & \vec{z}_s & \vec{\eta}_i \\ \hline T_s & \vec{k}_s & \vec{\kappa}_i \\ \hline \end{array}. \tag{2.8}$$

After the addition of the gauge-fixing $T_s - \tau \approx 0$, the invariant mass $M_{\rm sys}$ of the system, which is also the *internal* energy of the isolated system, replaces the nonrelativistic Hamiltonian $H_{\rm rel}$ for the relative degrees of freedom: this reminds of the frozen Hamilton–Jacobi theory, in which the time evolution can be reintroduced by using the energy generator of the Poincaré group as Hamiltonian.

After the gauge fixings $T_s - \tau \approx 0$, the final Hamiltonian, the embedding of the Wigner hyperplane into Minkowski space–time and the Hamilton equations become

$$H_D = M_{\rm sys} - \vec{\lambda}(\tau) \cdot \vec{\kappa}_+,$$

$$z^\mu(\tau, \vec{\sigma}) = x_s^\mu(\tau) + \epsilon_r^\mu(u(p_s))\sigma^r = x_s^\mu(0) + u^\mu(p_s)\tau + \epsilon_r^\mu(u(p_s))\left(\sigma^r + \int_o^\tau d\tau_1 \lambda_r(\tau_1)\right),$$

$$\dot{\vec{\eta}}_i(\tau) \stackrel{\circ}{=} \frac{\vec{\kappa}_i(\tau)}{\sqrt{m_i^2 + \vec{\kappa}_i^2(\tau)}} - \vec{\lambda}(\tau), \quad \Rightarrow \vec{\kappa}_i(\tau) \stackrel{\circ}{=} m_i \frac{\dot{\vec{\eta}}_i(\tau) + \vec{\lambda}(\tau)}{\sqrt{1 - [\dot{\vec{\eta}}_i(\tau) + \vec{\lambda}(\tau)]^2}},$$

$$\dot{\vec{\kappa}}_i(\tau) \stackrel{\circ}{=} 0. \tag{2.9}$$

The particles' world lines in Minkowski space–time and the associated momenta are

$$x_i^\mu(\tau) = z^\mu(\tau, \vec{\eta}_i(\tau)) = x_s^\mu(\tau) + \epsilon_r^\mu(u(p_s))\,\eta_i^r(\tau),$$

$$p_i^\mu(\tau) = \sqrt{m_i^2 + \vec{\kappa}_i^2(\tau)}u^\mu(p_s) + \epsilon_r^\mu(u(p_s))\kappa_{ir}(\tau) \Rightarrow p_i^2 = m_i^2. \tag{2.10}$$

The *external* rest-frame instant form realization of the Poincaré generators[59] with nonfixed invariants $p_s^2 = \epsilon_s^2 \approx M_{\rm sys}^2$, $-p_s^2\vec{S}_s^2 \approx M_{\rm sys}^2\vec{S}^2$, is obtained from Eq. (2.6):

$$p_s^\mu = \sum_{i=1}^N p_i^\mu, \quad J_s^{\mu\nu} = \tilde{x}_s^\mu p_s^\nu - \tilde{x}_s^\nu p_s^\mu + \tilde{S}_s^{\mu\nu},$$

$$p_s^o = \sqrt{\epsilon_s^2 + \vec{p}_s^2} = \epsilon_s\sqrt{1+\vec{k}_s^2} \approx \sqrt{M_{\rm sys}^2 + \vec{p}_s^2} = M_{\rm sys}\sqrt{1+\vec{k}_s^2},$$

$$\vec{p}_s = \epsilon_s \vec{k}_s \approx M_{\rm sys}\vec{k}_s,$$

$$J_s^{ij} = \tilde{x}_s^i p_s^j - \tilde{x}_s^j p_s^i + \delta^{ir}\delta^{js}\sum_{i=1}^{N}(\eta_i^r \kappa_i^s - \eta_i^s \kappa_i^r) = z_s^i k_s^j - z_s^j k_s^i + \delta^{ir}\delta^{js}\epsilon^{rsu}\overline{S_s^u},$$

$$K_s^i = J_s^{oi} \approx \tilde{x}_s^o p_s^i - \tilde{x}_s^i \sqrt{M_{\rm sys}^2 + \vec{p}_s^{\,2}} - \frac{\delta^{ir} p_s^s \epsilon^{rsu}\overline{S_s^u}}{M_{\rm sys} + \sqrt{M_{\rm sys}^2 + \vec{p}_s^{\,2}}}. \tag{2.11}$$

On the other hand the *internal* realization of the Poincaré algebra is built inside the Wigner hyperplane by using the expression of $\overline{S_s^{AB}}$ given by Eq. (2.6) (II and W^2 are the two nonfixed invariants of this realization)

$$M_{\rm sys} = H_M = \sum_{i=1}^{N}\sqrt{m_i^2 + \vec{\kappa}_i^2}, \quad \vec{\kappa}_+ = \sum_{i=1}^{N}\vec{\kappa}_i \ (\approx 0),$$

$$\vec{J} = \sum_{i=1}^{N}\vec{\eta}_i \times \vec{\kappa}_i, \quad J^r = \overline{S^r} = \tfrac{1}{2}\epsilon^{ruv}\overline{S^{uv}} \equiv \overline{S_s^r},$$

$$\vec{K} = -\sum_{i=1}^{N}\sqrt{m_i^2 + \vec{\kappa}_i^2}\,\vec{\eta}_i = -M_{\rm sys}\vec{R}_+, \quad K^r = J^{or} = \overline{S_s^{\tau r}},$$

$$\Pi = M_{\rm sys}^2 - \vec{\kappa}_+^2 \approx M_{\rm sys}^2 > 0, \quad W^2 = -(M_{\rm sys}^2 - \vec{\kappa}_+^2)\vec{\overline{S_s^2}} \approx -M_{\rm sys}^2 \vec{\overline{S_s^2}}. \tag{2.12}$$

The constraints $\epsilon_s - M_{\rm sys} \approx 0, \vec{\kappa}_+ \approx 0$ have the following meaning.

(i) The constraint $\epsilon_s - M_{\rm sys} \approx 0$ is the bridge connecting the *external* and the *internal* realizations [the external spin coincides with the internal angular momentum due to Eq. (A11) of Ref. 33].

(ii) The constraints $\vec{\kappa}_+ \approx 0$, together with $\vec{K} \approx 0$ (i.e., $\vec{R}_+ \approx \vec{q}_+ \approx \vec{y}_+ \approx 0$), lead to an unfaithful *internal* realization, in which the only nonzero generators are the conserved energy and spin of an isolated system.

The determination of $\vec{q}_+$ for the N particle system has been carried out by the group theoretical methods of Ref. 60 in Sec. III of Ref. 33. As said in the Introduction there are three internal position variables $\vec{q}_+, \vec{R}_+, \vec{y}_+$, which can be defined in terms of the internal Poincaré generators (2.12). It can be shown[33] that, due to $\vec{\kappa}_+ \approx 0$, they all *coincide*, $\vec{q}_+ \approx \vec{R}_+ \approx \vec{y}_+$.

Therefore the gauge fixings $\vec{\chi}(\tau) = \vec{q}_+ \approx \vec{R}_+ \approx \vec{y}_+ \approx 0$ imply $\vec{\lambda}(\tau) \approx 0$ and identify the special centroid (1.1). As shown in Sec. IV, the addition of the gauge fixings $\vec{\chi}(\tau) = \vec{q}_+ \approx \vec{R}_+ \approx \vec{y}_+ \approx 0$ also implies that the Dixon center of mass of an extended object[20] and the Pirani[14] and Tulczyjew[15,18,23] centroids[61–63] all simultaneously coincide with the centroid $x_s^{(\vec{q}_+)\mu}(\tau)$.

The *external* realization (2.11) allows to build the analogous *external* 3-variables $\vec{q}_s, \vec{R}_s, \vec{Y}_s$. Equation (4.4) of Ref. 33 shows the construction of the associated *external* 4-variables $\tilde{x}_s^\mu, Y_s^\mu, R_s^\mu$ and their locations $\vec{\tilde{\sigma}}, \vec{\sigma}_Y, \vec{\sigma}_R$ on the Wigner hyperplane. The relevant point is that the *external* Fokker–Pryce noncanonical covariant 4-center of inertia Y_s^μ coincides with the centroid Eq. (1.1).

Finally, in Ref. 33 there is the definition of the following sequence of canonical transformations:

$$\boxed{\begin{array}{c}\vec{\eta}_i \\ \vec{\kappa}_i\end{array}} \longrightarrow \boxed{\begin{array}{cc}\vec{\eta}_+ & \vec{\rho}_a \\ \vec{\kappa}_+ & \vec{\pi}_a\end{array}} \longrightarrow \boxed{\begin{array}{cc}\vec{q}_+ & \vec{\rho}_{qa} \\ \vec{\kappa}_+ & \vec{\pi}_{qa}\end{array}}, \ a = 1,\ldots,N-1, \tag{2.13}$$

leading to the canonical separation of the internal 3-center of mass $(\vec{q}_+, \vec{\kappa}_+)$ from the internal relative variables $\vec{\rho}_{qa}, \vec{\pi}_{qa}$. Since the rest-frame condition $\vec{\kappa}_+ \approx 0$ implies[33] $\vec{\rho}_{qa} \approx \vec{\rho}_a$, $\vec{\pi}_{qa} \approx \vec{\pi}_a$, in the gauge $\vec{q}_+ \approx 0$ and in terms of the associated Dirac brackets we get an internal reduced phase space whose canonical basis is $\vec{\rho}_{qa} \equiv \vec{\rho}_a$, $\vec{\pi}_{qa} \equiv \vec{\pi}_a$, $a = 1, \ldots, N-1$.

The intermediate linear point canonical transformation in (2.13) is [actually this is a family of canonical transformations, since the γ_{ai}'s are any set of numbers satisfying $\Sigma_i \gamma_{ai} = 0$, $\Sigma_a \gamma_{ai} \gamma_{aj} = \delta_{ij} - (1/N)$, $\Sigma_i \gamma_{ai} \gamma_{bi} = \delta_{ab}$]

$$\vec{\eta}_i = \vec{\eta}_+ + \frac{1}{\sqrt{N}} \sum_a \gamma_{ai} \vec{\rho}_a,$$

$$\vec{\kappa}_i = \frac{1}{N} \vec{\kappa}_+ + \sqrt{N} \sum_a \gamma_{ai} \vec{\pi}_a,$$

$$\vec{\eta}_+ = \frac{1}{N} \sum_i \vec{\eta}_i, \quad \vec{\rho}_a = \sqrt{N} \sum_i \gamma_{ai} \vec{\eta}_i,$$

$$\vec{\kappa}_+ = \sum_i \vec{\kappa}_i, \quad \vec{\pi}_a = \frac{1}{\sqrt{N}} \sum_i \gamma_{ai} \vec{\kappa}_i. \tag{2.14}$$

The second canonical transformation has been defined in Sec. V of Ref. 33 by using a singular Gartenhaus–Schwartz transformation (see the Appendix), but there it was not written explicitly for $\vec{\kappa}_+ \neq 0$. For completeness its explicit form has been found and it is given at the end of the Appendix of this paper.

III. THE ENERGY-MOMENTUM TENSOR ON THE WIGNER HYPERPLANE

The Euler–Lagrange equations associated with the Lagrangian (2.1) are

$$\left(\frac{\partial \mathcal{L}}{\partial z^\mu} - \partial_A \frac{\partial \mathcal{L}}{\partial z^\mu_A} \right)(\tau, \vec{\sigma}) = \eta_{\mu\nu} \partial_A [\sqrt{g} T^{AB} z^\nu_B](\tau, \vec{\sigma}) \stackrel{\circ}{=} 0,$$

$$\frac{\partial L}{\partial \vec{\eta}_i} - \partial_\tau \frac{\partial L}{\partial \dot{\vec{\eta}}_i} = - \left[\frac{1}{2} \frac{T^{AB}}{\sqrt{g}} \right] \Bigg|_{\vec{\sigma} = \vec{\eta}_i} \frac{\partial g_{AB}}{\partial \vec{\eta}_i} - \partial_\tau \frac{g_{\tau r} + g_{rs} \dot{\eta}^s_i}{\sqrt{g_{\tau\tau} + 2 g_{\tau u} \dot{\eta}^u_i + g_{uv} \dot{\eta}^u_i \dot{\eta}^v_i}} \Bigg|_{\vec{\sigma} = \vec{\eta}_i} \stackrel{\circ}{=} \partial \dot{\vec{\eta}}_i$$

where we have introduced the energy-momentum tensor [here $\dot{\eta}^A_i(\tau) = (1; \dot{\vec{\eta}}_i(\tau))$],

$$T^{AB}(\tau, \vec{\sigma}) = - \left[\frac{2}{\sqrt{g}} \frac{\delta S}{\delta g_{AB}} \right](\tau, \vec{\sigma}) = - \sum_{i=1}^N \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) \frac{m_i \dot{\eta}^A_i(\tau) \dot{\eta}^B_i(\tau)}{\sqrt{g_{\tau\tau} + 2 g_{\tau u} \dot{\eta}^u_i + g_{uv} \dot{\eta}^u_i \dot{\eta}^v_i}}(\tau, \vec{\sigma}). \tag{3.2}$$

Because of the delta functions, the Euler–Lagrange equations for the fields $z^\mu(\tau, \vec{\sigma})$ are trivial $(0 \stackrel{\circ}{=} 0)$ everywhere except at the positions of the particles. They may be rewritten in a form valid for every isolated system as

$$\partial_A T^{AB} z^\mu_B \stackrel{\circ}{=} - \frac{1}{\sqrt{g}} \partial_A [\sqrt{g} z^\mu_B] T^{AB}. \tag{3.3}$$

When $\partial_A [\sqrt{g} z^\mu_B] = 0$, as it happens on the Wigner hyperplanes in the gauge $\vec{q}_+ \approx 0$ and $T_s - \tau \approx 0$, we get the conservation of the energy-momentum tensor T^{AB}, i.e., $\partial_A T^{AB} \stackrel{\circ}{=} 0$. Otherwise, there is a compensation coming from the dynamics of the surface.

On the Wigner hyperplane the energy-momentum tensor $T^{AB}(\tau, \vec{\sigma})$ takes the form

$$T^{\tau\tau}(\tau,\vec{\sigma}) = -\sum_{i=1}^{N} \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) \frac{m_i}{\sqrt{\dot{x}_s^2(\tau) + 2\dot{x}_{s\mu}(\tau)\epsilon_r^\mu(u(p_s)) - \dot{\vec{\eta}}_i^2(\tau)}},$$

$$T^{\tau r}(\tau,\vec{\sigma}) = -\sum_{i=1}^{N} \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) \frac{m_i \dot{\eta}_i^r(\tau)}{\sqrt{\dot{x}_s^2(\tau) + 2\dot{x}_{s\mu}(\tau)\epsilon_r^\mu(u(p_s)) - \dot{\vec{\eta}}_i^2(\tau)}},$$

$$T^{rs}(\tau,\vec{\sigma}) = -\sum_{i=1}^{N} \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) \frac{m_i \dot{\eta}_i^r(\tau)\dot{\eta}_i^s(\tau)}{\sqrt{\dot{x}_s^2(\tau) + 2\dot{x}_{s\mu}(\tau)\epsilon_r^\mu(u(p_s)) - \dot{\vec{\eta}}_i^2(\tau)}}. \tag{3.4}$$

With the position $x^\mu = z^\mu(\tau,\vec{\sigma})$, the same form is obtained from the energy momentum tensor of the standard manifestly Lorentz covariant theory with Lagrangian $S_S = \int d\tau L_S(\tau) = -\sum_{i=1}^N m_i \int d\tau \sqrt{\dot{x}_i^2(\tau)}$, restricted to positive energies[64]

$$T^{\mu\nu}(z(\tau,\vec{\sigma})) = -\left(\frac{2}{\sqrt{g}}\frac{\delta S_S}{\delta g_{\mu\nu}}\right)\Bigg|_{x=z(\tau,\vec{\sigma})} = \sum_{i=1}^{N} m_i \int d\tau_1 \frac{\dot{x}_i^\mu(\tau_1)\dot{x}_i^\nu(\tau_1)}{\sqrt{\dot{x}_i^2(\tau_1)}} \delta^4(x_i(\tau_1) - z(\tau,\vec{\sigma}))$$

$$= \sum_{i=1}^{N} \frac{1}{m_1} \int d\tau_1 \sqrt{\dot{x}_i^2(\tau_1)} p_i^\mu(\tau_1) p_i^\nu(\tau_1) \delta^4(x_i(\tau_1) - z(\tau,\vec{\sigma})) = \epsilon_A^\mu(u(p_s))\epsilon_B^\nu(u(p_s)) T^{AB}(\tau,\vec{\sigma}). \tag{3.5}$$

As shown explicitly in Ref. 51, on Wigner hyperplanes but only with $\tau \equiv T_s$ [so that $\dot{x}_s^\mu(\tau) = u^\mu(p_s) + \epsilon_r^\mu(u(p_s))\lambda_r(\tau)$ and $x_s^\mu(\tau) = x_s^\mu(0) + \tau u^\mu(p_s) + \epsilon_r^\mu(u(p_s))\int_0^\tau d\tau_1\, \lambda_r(\tau_1)$], we get for every value of the Dirac multiplier $\vec{\lambda}(\tau)$,

$$T^{\mu\nu}[x_s^\beta(T_s) + \epsilon_u^\beta(u(p_s))\sigma^\mu] = \epsilon_A^\mu(u(p_s))\epsilon_B^\nu(u(p_s)) T^{AB}(T_s,\vec{\sigma}) = \sum_{i=1}^{N} \delta^3(\vec{\sigma} - \vec{\eta}_i(T_s))$$

$$\times \Bigg[\sqrt{m_i^2 + \vec{\kappa}_i^2(T_s)} u^\mu(p_s) u^\nu(p_s) + k_i^r(T_s)(u^\mu(p_s)\epsilon_r^\nu(u(p_s))$$

$$+ u^\nu(p_s)\epsilon_r^\mu(u(p_s))) + \frac{\kappa_i^r(T_s)\kappa_i^s(T_s)}{\sqrt{m_i^2 + \vec{\kappa}_i^2(T_s)}} \epsilon_r^\mu(u(p_s))\epsilon_s^\nu(u(p_s)) \Bigg],$$

$$T^{\tau\tau}(T_s,\vec{\sigma}) = \sum_{i=1}^{N} \delta^3(\vec{\sigma} - \vec{\eta}_i(T_s)) \sqrt{m_i^2 + \vec{\kappa}_i^2(T_s)},$$

$$T^{\tau r}(T_s,\vec{\sigma}) = \sum_{i=1}^{N} \delta^3(\vec{\sigma} - \vec{\eta}_i(T_s)) \kappa_i^r(T_s),$$

$$T^{rs}(T_s,\vec{\sigma}) = \sum_{i=1}^{N} \delta^3(\vec{\sigma} - \vec{\eta}_i(T_s)) \frac{\kappa_i^r(T_s)\kappa_i^s(T_s)}{\sqrt{m_i^2 + \vec{\kappa}_i^2(T_s)}},$$

$$P_T^\mu = \int d^3\sigma\, T^{\mu\nu}[x_s^\beta(T_s) + \epsilon_u^\beta(u(p_s))\sigma^\mu] u_\nu(p_s) = p_s^\mu = M_{\rm sys} u^\mu(p_s) + \epsilon_r^\mu(u(p_s))\kappa_+^r \approx M_{\rm sys} u^\mu(p_s),$$

$$M_{\rm sys} = P_T^\mu u_\mu(p_s) = \sum_{i=1}^N \sqrt{m_i^2 c^2 + \vec{\kappa}_i^2(T_s)}, \tag{3.6}$$

where P_T^μ and $M_{\rm sys}$ are the total 4-momentum and the invariant mass of the isolated N-body system.

IV. DIXON'S MULTIPOLES FOR FREE PARTICLES ON THE WIGNER HYPERPLANE

In this section we will define the special relativistic Dixon multipoles on the Wigner hyperplane with $T_s - \tau \equiv 0$ for the N-body problem [see Eqs. (2.9) with $x_s^\mu(\tau) = x_o^\mu + u^\mu(p_s)T_s + \epsilon_r^\mu(u(p_s))$ $\int_o^\tau d\tau_1\, \lambda_r(\tau_1) = \vec{x}_s^{(q_+)\mu}(\tau) + \int_o^\tau d\tau_1\, \lambda_r(\tau_1)$]. By comparison, a list of the *nonrelativistic multipoles* for N free particles is given in Appendix A of Ref. 51.

Consider an arbitrary timelike world-line $w^\mu(\tau) = z^\mu(\tau, \vec{\eta}(\tau)) = x_s^\mu(\tau) + \epsilon_r^\mu(u(p_s))\,\eta^r(\tau)$ $= x_s^{(\vec{q}_+)\mu}(\tau) + \epsilon_r^\mu(u(p_s))\,\tilde{\eta}^r(\tau)$ [$\tilde{\eta}^r(\tau) = \eta^r(\tau) + \int_o^\tau d\tau_1\, \lambda_r(\tau_1)$] and evaluate the Dixon multipoles[20] on the Wigner hyperplanes in the natural gauge with respect to the given world line. A generic point will be parametrized by

$$\begin{aligned} z^\mu(\tau,\vec{\sigma}) &= x_s^\mu(\tau) + \epsilon_r^\mu(u(p_s))\sigma^r = x_s^{(\vec{q}_+)\mu}(\tau) + \epsilon_r^\mu(u(p_s))\left[\sigma^r + \int_0^\tau d\tau_1\, \lambda_r(\tau_1)\right] \\ &= w^\mu(\tau) + \epsilon_r^\mu(u(p_s))[\sigma^r - \eta^r(\tau)] \overset{\rm def}{=} w^\mu(\tau) + \delta z^\mu(\tau,\vec{\sigma}), \end{aligned} \tag{4.1}$$

so that $\delta z_\mu(\tau,\vec{\sigma})u^\mu(p_s) = 0$.

While for $\vec{\tilde{\eta}}(\tau) = 0$ [$\vec{\tilde{\eta}}(\tau) = \int_o^\tau d\tau_1\, \lambda_r(\tau_1)$] we get the multipoles relative to the centroid $x_s^\mu(\tau)$, for $\vec{\eta}(\tau) = 0$ we get those relative to the centroid $x_s^{(\vec{q}_+)\mu}(\tau)$. In the gauge $\vec{R}_+ \approx \vec{q}_+ \approx \vec{y}_+ \approx 0$, where $\vec{\lambda}(\tau) = 0$, it follows that $\vec{\eta}(\tau) = \vec{\tilde{\eta}}(\tau) = 0$ identifies the *barycentric* multipoles with respect to the centroid $x_s^{(\vec{q}_+)\mu}(\tau)$, which now carries the internal 3-center of mass.

A. Dixon's multipoles

Lorentz covariant *Dixon's multipoles* and their Wigner covariant counterparts on the Wigner hyperplanes are then defined as

$$\begin{aligned} t_T^{\mu_1\cdots\mu_n\mu\nu}(T_s,\vec{\eta}) &= t_T^{(\mu_1\cdots\mu_n)(\mu\nu)}(T_s,\vec{\eta}) = \epsilon_{r_1}^{\mu_1}(u(p_s))\cdots\epsilon_{r_n}^{\mu_n}(u(p_s))\epsilon_A^\mu(u(p_s))\epsilon_B^\nu(u(p_s))q_T^{r_1\cdots r_n AB}(T_s,\vec{\eta}) \\ &= \int d^3\sigma\, \delta z^{\mu_1}(T_s,\vec{\sigma})\cdots\delta z^{\mu_n}(T_s,\vec{\sigma})T^{\mu\nu}[x_s^{(\vec{q}_+)\beta}(T_s) + \epsilon_u^\beta(u(p_s))\sigma^\mu] \\ &= \epsilon_A^\mu(u(p_s))\epsilon_B^\nu(u(p_s)) \int d^3\sigma\, \delta z^{\mu_1}(T_s,\vec{\sigma})\cdots\delta z^{\mu_n}(T_s,\vec{\sigma})T^{AB}(T_s,\vec{\sigma}), \end{aligned}$$

$$\begin{aligned} q_T^{r_1\cdots r_n AB}(T_s,\vec{\eta}) = \int d^3\sigma[\sigma^{r_1} - \eta^{r_1}(T_s)]\cdots[\sigma^{r_n} - \eta^r(\tau_s)]T^{AB}(T_s,\vec{\sigma}) &= \delta_\tau^A\delta_\tau^B \sum_{i=1}^N [\eta_i^{r_1}(T_s) \\ - \eta^{r_1}(T_s)]\cdots[\eta_i^{r_n}(T_s) - \eta^{r_n}(T_s)]\sqrt{m_i^2 + \vec{k}_i^2(T_s)} &+ \delta_u^A\delta_v^B \sum_{i=1}^N [\eta_i^{r_1}(T_s) \\ - \eta^{r_1}(T_s)]\cdots[\eta_i^{r_n}(T_s) - \eta^{r_n}(T_s)]\frac{\kappa_i^u(T_s)\kappa_i^v(T_s)}{\sqrt{m_i^2 + \vec{\kappa}_i^2(T_s)}} &+ (\delta_\tau^A\delta_u^B + \delta_u^A\delta_\tau^B)\sum_{i=1}^N [\eta_i^{r_1}(T_s) \\ - \eta^{r_1}(T_s)]\cdots[\eta_i^{r_n}(T_s) - \eta^{r_n}(T_s)]\kappa_i^r(T_s), & \end{aligned}$$

$$u_{\mu_1}(p_s)t_T^{\mu_1\cdots\mu_n\mu\nu}(T_s,\vec{\eta})=0. \tag{4.2}$$

Related multipoles are

$$\begin{aligned}
p_T^{\mu_1\cdots\mu_n\mu}(T_s,\vec{\eta}) &= t_T^{\mu_1\cdots\mu_n\mu\nu}(T_s,\vec{\eta})u_\nu(p_s)=\epsilon_{r_1}^{\mu_1}(u(p_s))\cdots\epsilon_{r_n}^{\mu_n}(u(p_s))\epsilon_A^{\mu}(u(p_s))q_T^{r_1\cdots r_nA\tau}(T_s,\vec{\eta})\\
&=\epsilon_{r_1}^{\mu_1}(u(p_s))\cdots\epsilon_{r_n}^{\mu_n}(u(p_s))\sum_{i=1}^{N}[\eta_i^{r_1}(T_s)-\eta^{r_1}(T_s)]\cdots[\eta_i^{r_n}(T_s)-\eta^{r_n}(T_s)]\\
&\quad\times[\sqrt{m_i^2+\vec{\kappa}_i^2(\tau)}u^\mu(p_s)+k_i^r(T_s)\epsilon_r^\mu(u(p_s))],\ u_{\mu_1}(p_s)p_T^{\mu_1\cdots\mu_n\mu}(T_s,\vec{\eta})=0,\\
&\quad p_T^{\mu_1\cdots\mu_n\mu}(T_s,\vec{\eta})u_\mu(p_s)=\tilde{t}_T^{\mu_1\cdots\mu_n}(T_s,\vec{\eta}),
\end{aligned}$$

$$n=0\Rightarrow p_T^\mu(T_s,\vec{\eta})=\epsilon_A^\mu(u(p_s))q_T^{A\tau}(T_s)=P_T^\mu\approx p_s^\mu. \tag{4.3}$$

The inverse formulas, giving the *multipolar expansion*, are

$$\begin{aligned}
T^{\mu\nu}[w^\beta(T_s)+\delta z^\beta(T_s,\vec{\sigma})] &= T^{\mu\nu}[x_s^{(\vec{q}_+)\beta}(T_s)+\epsilon_r^\beta(u(p_s))\sigma^r]=\epsilon_A^\mu(u(p_s))\epsilon_B^\nu(u(p_s))T^{AB}(T_s,\vec{\sigma})\\
&=\epsilon_A^\mu(u(p_s))\epsilon_B^\nu(u(p_s))\sum_{n=0}^{\infty}(-1)^n\frac{q_T^{r_1\cdots r_nAB}(T_s,\vec{\eta})}{n!}\frac{\partial^n}{\partial\sigma^{r_1}\cdots\partial\sigma^{r_n}}\delta^3(\vec{\sigma}-\vec{\eta}(T_s))\\
&=\sum_{n=0}^{\infty}(-1)^n\frac{t_T^{\mu_1\cdots\mu_n\mu\nu}(T_s,\vec{\eta})}{n!}\epsilon_{r_1\mu_1}(u(p_s))\cdots\epsilon_{r_n\mu_n}(u(p_s))\frac{\partial^n}{\partial\sigma^{r_1}\cdots\partial\sigma^{r_n}}\\
&\quad\delta^3(\vec{\sigma}-\vec{\eta}(T_s)).
\end{aligned} \tag{4.4}$$

Note however that, as pointed out by Dixon,[20] the distributional equation (4.4) is valid only if analytic test functions are used, defined on the support of the energy-momentum tensor.

The quantities $q_T^{r_1\cdots r_n\tau\tau}(T_s,\vec{\eta})$, $q_T^{r_1\cdots r_nr\tau}(T_s,\vec{\eta})=q_T^{r_1\cdots r_n\tau r}(T_s,\vec{\eta})$, $q_T^{r_1\cdots r_nuv}(T_s,\vec{\eta})$ are the *mass density, momentum density, and stress tensor multipoles* with respect to the world-line $w^\mu(T_s)$ (barycentric for $\vec{\eta}=\tilde{\eta}=0$).

B. Monopoles

The *monopoles* correspond to $n=0$ and have the following expression[65] (see the Appendix for the definition of $\to_{\alpha\to\infty}$):

$$\begin{aligned}
q_T^{AB}(T_s,\vec{\eta}) &= \delta_\tau^A\delta_\tau^BM+\delta_u^A\delta_v^B\sum_{i=1}^{N}\frac{\kappa_i^u\kappa_i^v}{\sqrt{m_i^2+\vec{\kappa}_i^2}}+(\delta_\tau^A\delta_u^B+\delta_u^A\delta_\tau^B)\kappa_+^u\approx\\
&\to_{\alpha\to\infty}\delta_\tau^A\delta_\tau^B\sum_{i=1}^{N}\sqrt{m_i^2+N\sum_{de}\gamma_{di}\gamma_{ei}\vec{\pi}_{qd}\cdot\vec{\pi}_{qe}}+\delta_u^A\delta_v^BN\sum_{i=1}^{N}\frac{\sum_{ab}^{1\cdots N-1}\gamma_{ai}\gamma_{bi}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}}{\sqrt{m_i^2+N\sum_{de}\gamma_{di}\gamma_{ei}\vec{\pi}_{qd}\cdot\vec{\pi}_{qe}}}
\end{aligned}$$

$$q_T^{\tau\tau}(T_s,\vec{\eta})\to_{c\to\infty}\sum_{i=1}^{N}m_ic^2+\frac{1}{2}\sum_{ab}^{1\cdots N-1}\sum_{i=1}^{N}\frac{N\gamma_{ai}\gamma_{bi}}{m_i}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}+O(1/c)=\sum_{i=1}^{N}m_ic^2+H_{\mathrm{rel},nr}+O(1/c),$$

$$q_T^{r\tau}(T_s,\vec{\eta})=\kappa_+^r\approx 0,\ \textit{rest-frame condition(also at the non relativistic level)},$$

$$q_T^{uv}(T_s,\vec{\eta}) \to_{c\to\infty} \sum_{ab}^{1\cdots N-1} \sum_{i=1}^{N} \frac{N\gamma_{ai}\gamma_{bi}}{m_i} \pi_{qa}^u \pi_{qb}^v + O(1/c) = \sum_{ab}^{1\cdots N-1} k_{ab}^{-1} \pi_{qa}^u \pi_{qb}^v + O(1/c) = \sum_{ab}^{1\cdots N-1} k_{ab} \dot{\rho}_a^u \dot{\rho}_b^v + O(1/c) \tag{4.5}$$

where we have exploited Eqs. (5.10), (5.11) of Ref. 33 to obtain the expression in terms of the internal relative variables.

Therefore, independently of the choice of the world-line $w^\mu(\tau)$, in the rest-frame instant form the *mass monopole* $q_T^{\tau\tau}$ is the invariant mass $M_{\rm sys}=\Sigma_{i=1}^N \sqrt{m_i^2+\vec{\kappa}_i^2}$, while the *momentum monopole* $q_T^{r\tau}$ vanishes and q_T^{uv} is the *stress tensor monopole*.

C. Dipoles

The mass, momentum, and stress tensor *dipoles* correspond to $n=1$,

$$q_T^{rAB}(T_s,\vec{\eta}) = \delta_\tau^A \delta_\tau^B M_{\rm sys}[R_+^r(T_s) - \eta^r(T_s)] + \delta_u^A \delta_v^B \left[\sum_{i=1}^N \frac{\eta_i^r \kappa_i^u \kappa_i^v}{\sqrt{m_i^2+\vec{\kappa}_i^2}}(T_s) - \eta^r(T_s) q_T^{uv}(T_s,\vec{\eta}) \right] + (\delta_\tau^A \delta_u^B + \delta_u^A \delta_\tau^B) \left[\sum_{i=1}^N [\eta_i^r \kappa_i^u](T_s) - \eta^r(T_s)\kappa_+^u \right]. \tag{4.6}$$

The vanishing of the *mass dipole* $q_T^{r\tau\tau}$ implies $\vec{\eta}(\tau)=\vec{\tilde{\eta}}(\tau)-\int_0^\tau d\tau_1 \vec{\lambda}(\tau_1)=\vec{R}_+$ and identifies the world-line $w^\mu(\tau)=x_s^{(\vec{q}_+)\mu}(\tau)+\epsilon_r^\mu(u(p_s))$ $[R_+^r+\int_0^\tau d\tau_1 \lambda_r(\tau_1)]$. In the gauge $\vec{R}_+\approx\vec{q}_+\approx\vec{y}_+\approx 0$, where $\vec{\lambda}(\tau)=0$, this is the world-line $w^\mu(\tau)=x_s^{(\vec{q}_+)\mu}(\tau)$ of the centroid associated with the *internal Møller 3-center of energy* and, as a consequence of the rest-frame condition, also with the *rest-frame internal 3-center of mass* $\vec{q}_+$. Therefore we get the implications following from the vanishing of the barycentric [i.e., $\vec{\lambda}(\tau)=0$] mass dipole:

$$q_T^{r\tau\tau}(T_s,\vec{\eta}) = \epsilon_{\mu_1}^{r_1}(u(p_s))\tilde{t}_T^{\mu_1}(T_s,\vec{\eta}) = M_{\rm sys}[R_+^r(T_s) - \eta^r(T_s)] = 0, \text{ and } \vec{\lambda}(\tau)=0,$$

$$\Rightarrow \vec{\eta}(T_s) = \vec{\tilde{\eta}}(T_s) = \vec{R}_+ \approx \vec{q}_+ \approx \vec{y}_+. \tag{4.7}$$

In the gauge $\vec{R}_+\approx\vec{q}_+\approx\vec{y}_+\approx 0$, Eq. (4.7) with $\vec{\eta}=\vec{\tilde{\eta}}=0$ implies the vanishing of the time derivative of the barycentric mass dipole, this identifies the *center-of-mass momentum-velocity relation* (the so-called *constitutive equation*) for the system

$$\frac{dq_T^{r\tau\tau}(T_s,\vec{\eta})}{dT_s} \stackrel{\circ}{=} \kappa_+^r - M_{\rm sys}\dot{R}_+^r = 0. \tag{4.8}$$

The expression of the barycentric dipoles in terms of the internal relative variables, when $\vec{\eta}=\vec{\tilde{\eta}}=\vec{R}_+\approx\vec{q}_+\approx 0$ and $\vec{\kappa}_+\approx 0$, is obtained by using the results of the Appendix,

$$q_T^{r\tau\tau}(T_s,\vec{R}_+) = 0,$$

$$q_T^{ru\tau}(T_s,\vec{R}_+) = \sum_{i=1}^N \eta_i^r \kappa_i^u - R_+^r \kappa_+^u = \sum_{a=1}^{N-1} \rho_a^r \pi_a^u + (\eta_+^r - R_+^r)\kappa_+^u \to_{\alpha\to\infty} \sum_{a=1}^{N-1} \rho_{qa}^r \pi_{qa}^u \to_{c\to\infty} \sum_{a=1}^{N-1} \rho_a^r \pi_{qa}^u = \sum_{ab}^{1\cdots N-1} k_{ab} \rho_a^r \dot{\rho}_b^u,$$

$$q_T^{ruv}(T_s,\vec{R}_+)=\sum_{i=1}^{N}\eta_i^r\frac{\kappa_i^u\kappa_i^v}{H_i}-R_+^r\sum_{i=1}^{N}\frac{\kappa_i^u\kappa_i^v}{H_i}=\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\sum_{a=1}^{N-1}\gamma_{ai}\rho_a^r\frac{\kappa_i^u\kappa_i^v}{H_i}+(\eta_+^r-R_+^r)\sum_{i=1}^{N}\frac{\kappa_i^u\kappa_i^v}{H_i}$$

$$\rightarrow_{\alpha\rightarrow\infty}\sum_{a=1}^{N-1}\left(c\sqrt{N}\sum_{ij}^{1\cdots N}(\gamma_{ai}-\gamma_{aj})\frac{\sqrt{m_j^2+N\sum_{de}\gamma_{dj}\gamma_{ej}\vec{\pi}_{qd}\cdot\vec{\pi}_{qe}}}{\sqrt{m_i^2+N\sum_{de}\gamma_{di}\gamma_{ei}\vec{\pi}_{qd}\cdot\vec{\pi}_{qe}}}\right.$$

$$\left.\times\frac{\sum_{bc}^{1\cdots N-1}\gamma_{bi}\gamma_{ci}\pi_{qb}^u\pi_{qc}^v}{\sum_{k=1}^{N}\sqrt{m_k^2+N\sum_{de}\gamma_{dk}\gamma_{ek}\vec{\pi}_{qd}\cdot\vec{\pi}_{qe}}}\right)\rho_{qa}^r$$

$$=\rightarrow_{c\rightarrow\infty}\sum_{ij}^{1\cdots N}\sum_{a=1}^{N-1}\frac{\gamma_{ai}-\gamma_{aj}}{\sqrt{N}}\rho_a^r\frac{m_jN}{m_im}\sum_{bc}^{1\cdots N-1}\gamma_{bi}\gamma_{ci}\pi_{qb}^u\pi_{qc}^v+O(1/c)$$

$$=\frac{1}{\sqrt{N}}\sum_{abc}^{1\cdots N-1}\left[N\sum_{i=1}^{N}\frac{\gamma_{ai}\gamma_{bi}\gamma_{ci}}{m_i}-\frac{\sum_{j=1}^{N}m_j\gamma_{aj}}{m}\right]\rho_a^r\pi_{qb}^u\pi_{qc}^v+O(1/c).\tag{4.9}$$

The antisymmetric part of the related dipole $p_T^{\mu_1\mu}(T_s,\vec{\eta})$ identifies the *spin tensor*. Indeed, the *spin dipole* is

$$S_T^{\mu\nu}(T_s)[\vec{\eta}]=2p_T^{[\mu\nu]}(T_s,\vec{\eta})=2\epsilon_r^{[\mu}(u(p_s))\epsilon_A^{\nu]}(u(p_s))q_T^{rA\tau}(T_s,\vec{\eta})=M_{\rm sys}[R_+^r(T_s)-\eta^r(T_s)]$$

$$\times[\epsilon_r^\mu(u(p_s))u^\nu(p_s)-\epsilon_r^\nu(u(p_s))u^\mu(p_s)]+\sum_{i=1}^{N}[\eta_i^r(T_s)-\eta^r(T_s)]\kappa_i^s(T_s)[\epsilon_r^\mu(u(p_s))\epsilon_s^\nu(u(p_s))$$

$$-\epsilon_r^\nu(u(p_s))\epsilon_s^\mu(u(p_s))],$$

$$m_{u(p_s)}^\nu(T_s,\vec{\eta})=u_\mu(p_s)S_T^{\mu\nu}(T_s)[\vec{\eta}]=-\epsilon_r^\nu(u(p_s))[\overline{S_s^{\tau r}}-M_{\rm sys}\eta^r(T_s)]=-\epsilon_r^\nu(u(p_s))M_{\rm sys}[R_+^r(T_s)-\eta^r(T_s)]$$

$$=-\epsilon_r^\nu(u(p_s))q_T^{r\tau\tau}(T_s,\vec{\eta}),$$

$$\Rightarrow u_\mu(p_s)S_T^{\mu\nu}(T_s)[\vec{\eta}]=0,\quad\Rightarrow\vec{\eta}=\vec{R}_+,$$

$$\Downarrow barycentric\ spin\ for\ \vec{\eta}=\vec{\tilde{\eta}}=0,\ see\ Eq.\ (2.9),$$

$$S_T^{\mu\nu}(T_s)[\vec{\eta}=0]=S_s^{\mu\nu}\overset{\circ}{=}\sum_{i=1}^{N}\frac{m_i\eta_i^r(T_s)}{\sqrt{1-\dot{\vec{\eta}}_i^2(T_s)}}[\epsilon_r^\mu(u(p_s))u^\nu(p_s)-\epsilon_r^\nu(u(p_s))u^\mu(p_s)]$$

$$+\sum_{i=1}^{N}\frac{m_i\eta_i^r(T_s)\dot{\eta}_i^s(T_s)}{\sqrt{1-\dot{\vec{\eta}}_i^2(T_s)}}[\epsilon_r^\mu(u(p_s))\epsilon_s^\nu(u(p_s))-\epsilon_r^\nu(u(p_s))\epsilon_s^\mu(u(p_s))]$$

$$\overset{\circ}{=}\sum_i\eta_i^r(T_s)\sqrt{m_i^2+\vec{\kappa}_i^2}[\epsilon_r^\mu(u(p_s))u^\nu(p_s)-\epsilon_r^\nu(u(p_s))u^\mu(p_s)]+\epsilon^{rsu}\overline{S_s^u}\epsilon_r^\mu(u(p_s))\epsilon_s^\nu(u(p_s)).\tag{4.10}$$

This explains why $m_{u(p_s)}^\mu(T_s,\vec{\eta})$ is also called the *mass dipole moment*.

We find, therefore, that in the gauge $\vec{R}_+\approx\vec{q}_+\approx\vec{y}_+\approx0$ with $P_T^\mu=M_{\rm sys}\,u^\mu(p_s)=M_{\rm sys}\,\dot{x}_s^{(\vec{q}_+)\mu}(T_s)$ the Møller and barycentric centroid $x_s^{(\vec{q}_+)\mu}(T_s)$ is simultaneously the *Tulczyjew centroid*[15,18,23] [defined by $S_T^{\mu\nu}(T_s)[\vec{\eta}]P_{T_\nu}=0$, namely by $S_s^{or}=0$ in the momentum rest frame] and also the *Pirani centroid*[14]

[defined by $S_T^{\mu\nu}(T_s)[\vec{\eta}]\dot{x}_{s\nu}^{(\vec{q}_+)}=0$, namely by $S_s^{or}=0$ in the instantaneous-velocity rest frame]. In general, lacking a relation between 4-momentum and 4-velocity, they are different centroids.[66]

Note that noncovariant centroids could also be connected with the noncovariant external center of mass $\tilde{x}_s^\mu$ and the noncovariant external Møller center of energy.

D. Quadrupoles and the barycentric tensor of inertia

The *quadrupoles* correspond to $n=2$,

$$q_T^{r_1r_2AB}(T_s,\vec{\eta}) = \delta_\tau^A\delta_\tau^B\sum_{i=1}^N [\eta_i^{r_1}(T_s)-\eta^{r_1}(T_s)][\eta_i^{r_2}(T_s)-\eta^{r_2}(T_s)]\sqrt{m_i^2+\vec{\kappa}_i^2(T_s)} + \delta_u^A\delta_v^B\sum_{i=1}^N [\eta_i^{r_1}(T_s) - \eta^{r_1}(T_s)][\eta_i^{r_2}(T_s)-\eta^{r_2}(T_s)]\frac{\kappa_i^u\kappa_i^v}{\sqrt{m_i^2+\vec{\kappa}_i^2}}(T_s) + (\delta_\tau^A\delta_u^B+\delta_u^A\delta_\tau^B)\sum_{i=1}^N [\eta_i^{r_1}(T_s)-\eta^{r_1}(T_s)] \times[\eta_i^{r_2}(T_s)-\eta^{r_2}(T_s)]\kappa_i^u(T_s). \tag{4.11}$$

When the mass dipole vanishes, i.e., $\vec{\eta}=\vec{R}_+=\Sigma_i\vec{\eta}_i\sqrt{m_i^2+\vec{\kappa}_i^2}/M_{\rm sys}$, we get

$$q_T^{r_1r_2\tau\tau}(T_s,\vec{R}_+) = \sum_{i=1}^N (\eta_i^{r_1}-R_+^{r_1})(\eta_i^{r_2}-R_+^{r_2})\sqrt{m_i^2+\vec{\kappa}_i^2(T_s)},$$

$$q_T^{r_1r_2u\tau}(T_s,\vec{R}_+) = \sum_{i=1}^N (\eta_i^{r_1}-R_+^{r_1})(\eta_i^{r_2}-R_+^{r_2})\kappa_i^u,$$

$$q_T^{r_1r_2uv}(T_s,\vec{R}_+) = \sum_{i=1}^N (\eta_i^{r_1}-R_+^{r_1})(\eta_i^{r_2}-R_+^{r_2})\frac{\kappa_i^u\kappa_i^v}{\sqrt{m_i^2+\vec{\kappa}_i^2(T_s)}} = \frac{1}{N}\sum_{ijk}^{1\cdots N}\sum_{ab}^{1\cdots N-1}(\gamma_{ai}-\gamma_{aj}). \tag{4.12}$$

Following the nonrelativistic pattern, Dixon starts from the *mass quadrupole*,

$$q_T^{r_1r_2\tau\tau}(T_s,\vec{R}_+) = \sum_{i=1}^N [\eta_i^{r_1}\eta_i^{r_2}\sqrt{m_i^2+\vec{\kappa}_i^2}](T_s) - M_{\rm sys}\,R_+^{r_1}R_+^{r_2}, \tag{4.13}$$

and defines the following *barycentric tensor of inertia:*

$$I_{\rm Dixon}^{r_1r_2}(T_s) = \delta^{r_1r_2}\sum_u q_T^{uu\tau\tau}(T_s,\vec{R}_+) - q_T^{r_1r_2\tau\tau}(T_s,\vec{R}_+) = \sum_{i=1}^N [(\delta^{r_1r_2}(\vec{\eta}_i-\vec{R}_+)^2 - (\eta_i^{r_1}-R_+^{r_1})(\eta_i^{r_2} - R_+^{r_2}))\sqrt{m_i^2+\vec{\kappa}_i^2}](T_s) = \to_{\alpha\to\infty} \sum_{ab}^{1\cdots N-1}\left(\frac{1}{N}\sum_{ijk}^{1\cdots N}(\gamma_{ai}-\gamma_{aj})(\gamma_{bi}-\gamma_{bk}) \times \frac{\sqrt{m_i^2+N\sum_{de}\gamma_{di}\gamma_{ei}\vec{\pi}_{qd}\cdot\vec{\pi}_{qe}}}{\left(\sum_{h=1}^N\sqrt{m_h^2+N\sum_{de}\gamma_{dh}\gamma_{eh}\vec{\pi}_{qd}\cdot\vec{\pi}_{qe}}\right)^2}\right.$$

$$\times \sqrt{m_j^2 + N\sum_{de} \gamma_{dj}\gamma_{ej}\vec{\pi}_{qd}\cdot\vec{\pi}_{qe}}\sqrt{m_k^2 + N\sum_{de} \gamma_{dk}\gamma_{ek}\vec{\pi}_{qd}\cdot\vec{\pi}_{qe}}\Bigg)[\vec{\rho}_{qa}\cdot\vec{\rho}_{qb}\delta^{r_1r_2} - \rho_{qa}^{r_1}\rho_{qb}^{r_2}]$$

$$\to_{c\to\infty} \sum_{ab}^{1\cdots N-1}\sum_{ijk}^{1\cdots N}\frac{m_i m_j m_k}{Nm^2}(\gamma_{ai}-\gamma_{aj})(\gamma_{bi}-\gamma_{bk})\vec{\rho}_{qa}\cdot\vec{\rho}_{qb}\delta^{r_1r_2} - \rho_{qa}^{r_1}\rho_{qb}^{r_2}$$

$$\times\Bigg[1+\frac{1}{c}\Bigg(\frac{N\sum_{cd}^{1\cdots N-1}\gamma_{ci}\gamma_{di}\vec{\pi}_{qc}\cdot\vec{\pi}_{qd}}{2m_i^2}+\frac{N\sum_{cd}^{1\cdots N-1}\gamma_{cj}\gamma_{dj}\vec{\pi}_{qc}\cdot\vec{\pi}_{qd}}{2m_j^2}+\frac{N\sum_{cd}^{1\cdots N-1}\gamma_{ck}\gamma_{dk}\vec{\pi}_{qc}\cdot\vec{\pi}_{qd}}{2m_k^2}$$

$$-\frac{1}{m}\sum_{h=1}^{N}\frac{N\sum_{cd}^{1\cdots N-1}\gamma_{ch}\gamma_{dh}\vec{\pi}_{qc}\cdot\vec{\pi}_{qd}}{m_h}\Bigg)+O(1/c^2)\Bigg] = \sum_{ab}^{1\cdots N-1} k_{ab}[\vec{\rho}_{qa}\cdot\vec{\rho}_{qb}\delta^{r_1r_2} - \rho_{qa}^{r_1}\rho_{qb}^{r_2}]$$

$$+O(1/c) = I^{r_1r_2}[\vec{q}_{nr}] + O(1/c). \tag{4.14}$$

Note that in the nonrelativistic limit we recover the *tensor of inertia* of Eqs. (A11) of Appendix A of Ref. 51.

On the other hand, Thorne's definition of *barycentric tensor of inertia*[27] is

$$I^{r_1r_2}_{\text{Thorne}}(T_s) = \delta^{r_1r_2}\sum_u q_T^{uuA}{}_A(T_s,\vec{R}_+) - q_T^{r_1r_2A}{}_A(T_s,\vec{R}_+)$$

$$= \sum_{i=1}^{N}\frac{m_i^2(\delta^{r_1r_2}(\vec{\eta}_i-\vec{R}_+)^2-(\eta_i^{r_1}-R_+^{r_1})(\eta_i^{r_2}-R_+^{r_2}))}{\sqrt{m_i^2+\vec{\kappa}_i^2}}(T_s)\to_{\alpha\to\infty}\sum_{ab}^{1\cdots N-1}\Bigg(\frac{c}{N}\sum_{ijk}^{1\cdots N}(\gamma_{ai}-\gamma_{aj})$$

$$\times(\gamma_{bi}-\gamma_{bk})\frac{m_i^2\sqrt{m_j^2+N\sum_{de}\gamma_{dj}\gamma_{ej}\vec{\pi}_{qd}\cdot\vec{\pi}_{qe}}\sqrt{m_k^2+N\sum_{de}\gamma_{dk}\gamma_{ek}\vec{\pi}_{qd}\cdot\vec{\pi}_{qe}}}{\sqrt{m_i^2+N\sum_{de}\gamma_{di}\gamma_{ei}\vec{\pi}_{qd}\cdot\vec{\pi}_{qe}}\Big(\sum_{h=1}^{N}\sqrt{m_h^2+N\sum_{de}\gamma_{dh}\gamma_{eh}\vec{\pi}_{qd}\cdot\vec{\pi}_{qe}}\Big)^2}\Bigg)$$

$$\times[\vec{\rho}_{qa}\cdot\vec{\rho}_{qb}\delta^{r_1r_2} - \rho_{qa}^{r_1}\rho_{qb}^{r_2}] = \to_{c\to\infty}\sum_{ab}^{1\cdots N-1}\sum_{ijk}^{1\cdots N}\frac{m_i m_j m_k}{Nm^2}(\gamma_{ai}-\gamma_{aj})(\gamma_{bi}-\gamma_{bk})\vec{\rho}_{qa}\cdot\vec{\rho}_{qb}\delta^{r_1r_2}$$

$$-\rho_{qa}^{r_1}\rho_{qb}^{r_2}\times\Bigg[1+\frac{1}{c}\Bigg(-\frac{N\sum_{cd}^{1\cdots N-1}\gamma_{ci}\gamma_{di}\vec{\pi}_{qc}\cdot\vec{\pi}_{qd}}{2m_i^2}+\frac{N\sum_{cd}^{1\cdots N-1}\gamma_{cj}\gamma_{dj}\vec{\pi}_{qc}\cdot\vec{\pi}_{qd}}{2m_j^2}$$

$$+\frac{N\sum_{cd}^{1\cdots N-1}\gamma_{ck}\gamma_{dk}\vec{\pi}_{qc}\cdot\vec{\pi}_{qd}}{2m_k^2}-\frac{1}{m}\sum_{h=1}^{N}\frac{N\sum_{cd}^{1\cdots N-1}\gamma_{ch}\gamma_{dh}\vec{\pi}_{qc}\cdot\vec{\pi}_{qd}}{m_h}\Bigg)+O(1/c^2)\Bigg]$$

$$= \sum_{ab}^{1\cdots N-1} k_{ab}[\vec{\rho}_{qa}\cdot\vec{\rho}_{qb}\delta^{r_1r_2} - \rho_{qa}^{r_1}\rho_{qb}^{r_2}] + O(1/c) = I^{r_1r_2}[\vec{q}_{nr}] + O(1/c). \tag{4.15}$$

In this case too we recover the *tensor of inertia* of Eq. (A11) of Appendix A of Ref. 51.

Note that the Dixon and Thorne barycentric tensors of inertia differ at the post-Newtonian level

$$I^{r_1r_2}_{\rm Dixon}(T_s) - I^{r_1r_2}_{\rm Thorne}(T_s) = \frac{1}{c}\sum_{ab}^{1\cdots N-1}\sum_{ijk}^{1\cdots N}\frac{m_j m_k}{Nm^2}(\gamma_{ai}-\gamma_{aj})(\gamma_{bi}-\gamma_{bk})[\vec{\rho}_{qa}\cdot\vec{\rho}_{qb}\delta^{r_1r_2} - \rho^{r_1}_{qa}\rho^{r_2}_{qb}]\frac{N\sum_{cd}^{1\cdots N-1}\gamma_{ci}\gamma_{di}\vec{\pi}_{qc}\cdot\vec{\pi}_{qd}}{m_i} + O(1/c^2).$$

E. The multipolar expansion

By further exploiting the types of Dixon's multipoles analyzed in Appendix D of Ref. 51 (where there is also the proof of some basic formulas of Ref. 20 along the lines of this paper) as well as the consequences of Hamilton equations for an isolated system (equivalent to $\partial_\mu T^{\mu\nu}\overset{\circ}{=}0$), it turns out that the *multipolar expansion* (4.4) can be rearranged in the following form:

$$\begin{aligned}T^{\mu\nu}[x_s^{(\vec{q}_+)\beta}(T_s)+\epsilon^\beta_r(u(p_s))\sigma^r] &= T^{\mu\nu}[w^\beta(T_s)+\epsilon^\beta_r(u(p_s))(\sigma^r-\eta^r(T_s))] = u^{(\mu}(p_s)\epsilon_A^{\nu)}(u(p_s))[\delta^A_\tau M_{\rm sys}\\ &+\delta^A_u\kappa^u_+]\delta^3(\vec{\sigma}-\vec{\eta}(T_s))+\frac{1}{2}S_T^{\rho(\mu}(T_s)[\vec{\eta}]u^{\nu)}(p_s)\epsilon^r_\rho(u(p_s))\frac{\partial}{\partial\sigma^r}\\ &\delta^3(\vec{\sigma}-\vec{\eta}(T_s))\\ &+\sum_{n=2}^{\infty}\frac{(-1)^n}{n!}I_T^{\mu_1\cdots\mu_n\mu\nu}(T_s,\vec{\eta})\epsilon^{r_1}_{\mu_1}(u(p_s))\cdots\epsilon^{r_n}_{\mu_n}(u(p_s))\\ &\frac{\partial^n}{\partial\sigma^{r_1}\cdots\partial\sigma^{r_n}}\delta^3(\vec{\sigma}-\vec{\eta}(T_s)),\end{aligned}\tag{4.16}$$

where, for $n\geqslant 2$ and $\vec{\eta}=0$, $I_T^{\mu_1\cdots\mu_n\mu\nu}(T_s)=\frac{4(n-1)}{n+1}J_T^{(\mu_1\cdots\mu_{n-1}|\mu|\mu_n)\nu}(T_s)$, with $J_T^{\mu_1\cdots\mu_n\mu\nu\rho\sigma}(T_s)$ being the Dixon 2^{2+n}-*pole inertial moment tensors* given in Eqs. (D10) of Ref. 51. With this form of the multipolar expansion, the quadrupole term ($n=2$) takes the form [see Eq. (D11) of Ref. 51]

$$\begin{aligned}&\tfrac{1}{2}\Big(\tfrac{5}{3}u^\mu(p_s)u^\nu(p_s)q_F^{r_1r_2\tau\tau}(T_s,\vec{\eta})+\tfrac{1}{2}[u^\mu(p_s)\epsilon^\nu_u(u(p_s))+u^\nu(p_s)\epsilon^\mu_u(u(p_s))]q_T^{r_1r_2u\tau}(T_s,\vec{\eta})\\ &+\epsilon^\mu_{u_1}(u(p_s))\epsilon^\nu_{u_2}(u(p_s))\Big[q_T^{r_1r_2u_1u_2}(T_s,\vec{\eta})-\tfrac{3}{2}(q_T^{(r_1r_2u_1)u_2}(T_s,\vec{\eta})+q_T^{(r_1r_2u_2)u_1}(T_s,\vec{\eta}))+q_T^{(r_1r_2u_1u_2)}(T_s,\vec{\eta})\Big]\Big).\end{aligned}$$

Note that, as said in Appendix D of Ref. 51, Eq. (4.16) holds only if the multipoles are evaluated with respect to world-lines $w^\mu(\tau)=z^\mu(\tau,\vec{\eta}(\tau))$ with $\vec{\eta}(\tau)=\vec{\eta}=$const, namely with respect to one of the integral lines of the vector field $z^\mu_\tau(\tau,\vec{\sigma})\partial_\mu$.

On the Wigner hyperplane, the content of these 2^{n+2}-*pole inertial moment tensors* is replaced by the *Euclidean Cartesian tensors* $q_T^{r_1\cdots r_n\tau\tau}, q_T^{r_1\cdots r_n r\tau}, q_T^{r_1\cdots r_n rs}$. As shown in Appendix B of Ref. 51, we can decompose these Cartesian tensors in their irreducible STF (symmetric trace free) parts (the *STF tensors*).

For an isolated system described by the multipoles appearing in Eq. (4.16) [this is not true for those in Eq. (4.4)] the equations $\partial_\mu T^{\mu\nu}\overset{\circ}{=}0$ [see Eqs. (D4) and (D7) of Ref. 51] imply no more than the following *Papapetrou–Dixon–Souriau equations of motion*[11,21,22,24] for the total momentum $P^\mu_T(T_s)=\epsilon^\mu_A(u(p_s))q_T^{A\tau}(T_s)\approx p_s^\mu$ and the spin tensor $S_T^{\mu\nu}(T_s)[\vec{\eta}=0]$,

$$\frac{{\rm d}P^\mu_T(T_s)}{{\rm d}T_s}\overset{\circ}{=}0,$$

$$\frac{dS_T^{\mu\nu}(T_s)[\vec{\eta}=0]}{dT_s} \overset{\circ}{=} 2P_T^{[\mu}(T_s)u^{\nu]}(p_s) = 2\kappa_+^u \epsilon_u^{[\mu}(u(p_s))u^{\nu]}(p_s) \approx 0,$$

$$\text{or } \frac{dM_{\text{sys}}}{dT_s} \overset{\circ}{=} 0, \quad \frac{d\vec{\kappa}_+}{dT_s} \overset{\circ}{=} 0, \quad \frac{dS_s^{\mu\nu}}{dT_s} \overset{\circ}{=} 0. \tag{4.17}$$

For *open systems*, subsystems of an isolated system like in Sec. V, we have $\partial_\nu T^{\mu\nu} \overset{\circ}{=} F^\mu \neq 0$, with F^μ an external force. As shown in Ref. 20 for the case in which $F^\mu = -F^{\mu\nu}J_\nu (\partial_\mu J^\mu \overset{\circ}{=} 0)$ is the Lorentz force, the multipolar expansion (4.16) is still valid, while the equations of motion (4.17) become (P^μ and T_s are the conserved 4-momentum and the rest-frame time of the global isolated system)

$$\frac{dP_c^\mu(T_s)}{dT_s} \overset{\circ}{=} \int d^3\sigma\, F^\mu(T_s,\vec{\sigma}),$$

$$\frac{dS_c^{\mu\nu}(T_s)[\vec{\eta}=0]}{dT_s} \overset{\circ}{=} 2p_c^{[\mu}(T_s)u^{\nu]}(P) - \int d^3\sigma\, \sigma^r [\epsilon_r^\mu(u(P))F^\nu(T_s,\vec{\sigma}) - \epsilon_r^\nu(u(P))F^\mu(T_s,\vec{\sigma})]. \tag{4.18}$$

V. DIXON'S MULTIPOLES AND RELEVANT CENTROIDS FOR CLOSED AND OPEN SYSTEMS OF INTERACTING RELATIVISTIC PARTICLES

In this section we present new applications of the multipolar expansion to interacting systems of particles and fields. We first deal with the case of an isolated system of positive-energy relativistic particles with mutual action-at-a-distance interaction (see Sec. VIII of Ref. 33 and Sec. VI of Ref. 36); then we deal with the case of an *open particle subsystem* of an isolated system consisting of N charged positive-energy relativistic particles (with Grassmann-valued electric charges to regularize the Coulomb self-energies) plus the electromagnetic field.[36]

A. An isolated system of positive-energy particles with action-at-a-distance interactions

As mentioned in Sec. VIII of Ref. 33, the most general expression of the internal energy for an isolated system of N positive-energy particles with mutual action-at-a-distance interactions, in the rest-frame instant form, is

$$M = \sum_i \sqrt{m_i^2 + U_i + (\vec{\kappa}_i - \vec{V}_i)^2} + V, \tag{5.1}$$

where all the potentials $U_i, \vec{V}_i, V$ are functions of $\vec{\kappa}_i \cdot \vec{\kappa}_j, |\vec{\eta}_i - \vec{\eta}_j|, \vec{\kappa}_k \cdot (\vec{\eta}_i - \vec{\eta}_j)$. On the other hand, as shown at the end of Sec. II, in the free case we have

$$M_{(\text{free})} = \sum_i \sqrt{m_i^2 + \vec{\kappa}_i^2} = \sqrt{\mathcal{M}_{(\text{free})}^2 + \vec{\kappa}_+^2} \approx \mathcal{M}_{(\text{free})} = \sum_i \sqrt{m_i^2 + N\sum_{ab} \gamma_{ai}\gamma_{bi}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}}. \tag{5.2}$$

Since the 3-centers $\vec{R}_+$ and $\vec{q}_+$ become interaction dependent, in the interacting case we do not know the final canonical basis $\vec{q}_+, \vec{\kappa}_+, \vec{\rho}_{qa}, \vec{\pi}_{qa}$ explicitly. For an isolated system, however, we have $M = \sqrt{\mathcal{M}^2 + \vec{\kappa}_+^2} \approx \mathcal{M}$ with $\mathcal{M}$ independent of $\vec{q}_+$ ($\{M, \vec{\kappa}_+\} = 0$ in the internal Poincaré algebra). This suggests that also in the interacting case the same result should hold true. Indeed, by its very definition, the Gartenhaus–Schwartz transformation gives $\vec{\rho}_{qa} \approx \vec{\rho}_a, \vec{\pi}_{qa} \approx \vec{\pi}_a$ also in presence of interactions, so that we get

$$M|_{\vec{\kappa}_{+=0}} = \left(\sum_i \sqrt{m_i^2 + U_i + (\vec{\kappa}_i - \vec{V}_i)^2} + V \right) \Bigg|_{\vec{\kappa}_+=0} = \sqrt{\mathcal{M}^2 + \vec{\kappa}_+^2}|_{\vec{\kappa}_+} = \mathcal{M}|_{\vec{\kappa}_+=0}$$

$$= \sum_i \sqrt{m_i^2 + \tilde{U}_i + (\vec{\kappa}_i - \vec{\tilde{V}}_i)^2} + \tilde{V}, \tag{5.3}$$

where the potentials $\tilde{U}_i, \vec{\tilde{V}}_i, \tilde{V}$ are now functions of $\vec{\pi}_{qa} \cdot \vec{\pi}_{qb}, \vec{\pi}_{qa} \cdot \vec{\rho}_{qb}, \vec{\rho}_{qa} \cdot \vec{\rho}_{qb}$.

A relevant example of this type of isolated system has been studied in Ref. 36 starting from the isolated system of N charged positive-energy particles (with Grassmann-valued electric charges $Q_i = \theta^* \theta$, $Q_i^2 = 0$, $Q_i Q_j = Q_j Q_i \neq 0$ for $i \neq j$) plus the electromagnetic field. After a Shanmugadhasan canonical transformation, this system can be expressed only in terms of transverse Dirac observables corresponding to a radiation gauge for the electromagnetic field. The expression of the energy-momentum tensor in this gauge will be shown in the next section. In the semiclassical approximation of Ref. 36, the electromagnetic degrees of freedom are reexpressed in terms of the particle variables by means of the Lienard–Wiechert solution in the framework of the rest-frame instant form. In this way it has been possible to derive the exact semiclassical relativistic form of the action-at-a-distance Darwin potential in the reduced phase space of the particles. Note that this form is independent of the choice of the Green function in the Lienard–Wiechert solution. In Ref. 36 the associated energy-momentum tensor for the case $N=2$ [Eqs. (6.48)] is also given. The internal energy is $M = \sqrt{\mathcal{M}^2 + \vec{\kappa}_+^2} \approx \mathcal{M} = \Sigma_{i=1}^2 \sqrt{m_i^2 + \vec{\pi}^2} + (Q_1 Q_2 / 4\pi\rho)[1 + \tilde{V}(\vec{\pi}^2, \vec{\pi} \cdot (\vec{\rho}/\rho))]$ where $\tilde{V}$ is given in Eqs. (6.34), (6.35) [in Eqs. (6.36), (6.37) for $m_1 = m_2$]. The internal boost $\vec{\mathcal{K}}$ [Eq. (6.46)] allows the determination of the 3-center of energy $\vec{R}_+ = -\vec{\mathcal{K}}/M \approx \vec{q}_+ \approx \vec{y}_+$ in the present interacting case.

The knowledge of the energy-momentum tensor $T^{AB}(\tau, \vec{\sigma})$ and of $\vec{R}_+ \approx \vec{q}_+$ allows to apply our formalism to find the *barycentric multipoles of this interacting case*. It turns out that, in the gauge $\vec{R}_+ \approx \vec{q}_+ \approx \vec{y}_+ \approx 0$, all the formal properties studied in the preceding section (like the coincidence of all the relevant centroids) are reproduced in presence of mutual action-at-a-distance interactions.

B. Open subsystem of the isolated system of *N* positive-energy particles with Grassmann-valued electric charge plus the electromagnetic field

Let us now consider an open subsystem of the isolated system of N charged positive-energy particles plus the electromagnetic field in the radiation gauge. The energy-momentum tensor and the Hamilton equations on the Wigner hyperplane of the isolated system are ($\vec{\kappa}_+ = \Sigma_i \vec{\kappa}_i$; to avoid degenerations we assume that all the masses m_i are different)

$$T^{\tau\tau}(\tau, \vec{\sigma}) = \sum_{i=1}^N \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) \sqrt{m_i^2 + [\vec{\kappa}_i(\tau) - Q_i \vec{A}_\perp(\tau, \vec{\eta}_i(\tau))]^2} + \frac{1}{2} \Bigg[\left(\vec{\pi}_\perp + \sum_{i=1}^N Q_i \frac{\vec{\partial}}{\Delta} \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) \right)^2$$

$$+ \vec{B}^2 \Bigg](\tau, \vec{\sigma}) = \sum_{i=1}^N \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) \sqrt{m_i^2 + [\vec{\kappa}_i(\tau) - Q_i \vec{A}_\perp(\tau, \vec{\eta}_i(\tau))]^2} + \sum_{i=1}^N Q_i \vec{\pi}_\perp(\tau, \vec{\sigma})$$

$$\times \frac{\vec{\partial}}{\Delta} \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) + \frac{1}{2} [\vec{\pi}_\perp^2 + \vec{B}^2](\tau, \vec{\sigma}) + \frac{1}{2} \sum_{i,k,i \neq k}^{1 \cdots N} Q_i Q_k \frac{\vec{\partial}}{\Delta} \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) \cdot \frac{\vec{\partial}}{\Delta} \delta^3(\vec{\sigma} - \vec{\eta}_k(\tau)),$$

$$T^{\tau\tau}(\tau, \vec{\sigma}) = \sum_{i=1}^N \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) [\kappa_i^r(\tau) - Q_i A_\perp^r(\tau, \vec{\eta}_i(\tau))] + \left[\left(\vec{\pi}_\perp + \sum_{i=1}^N Q_i \frac{\vec{\partial}}{\Delta} \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) \right) \times \vec{B} \right]^r (\tau, \vec{\sigma}),$$

$$T^{rs}(\tau,\vec{\sigma}) = \sum_{i=1}^{N} \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) \frac{[\kappa_i^r(\tau) - Q_i A_\perp^r(\tau,\vec{\eta}_i(\tau))][\kappa_i^s(\tau) - Q_i A_\perp^s(\tau,\vec{\eta}_i(\tau))]}{\sqrt{m_i^2 + [\vec{\kappa}_i(\tau) - Q_i \vec{A}_\perp(\tau,\vec{\eta}_i(\tau))]^2}}$$
$$- \left[\frac{1}{2}\delta^{rs} \left[\left(\vec{\pi}_\perp + \sum_{i=1}^{N} Q_i \frac{\vec{\partial}}{\Delta} \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) \right)^2 + \vec{B}^2 \right] - \left[\left(\vec{\pi}_\perp + \sum_{i=1}^{N} Q_i \frac{\vec{\partial}}{\Delta} \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) \right)^r \right.$$
$$\left. \times \left(\vec{\pi}_\perp + \sum_{i=1}^{N} Q_i \frac{\vec{\partial}}{\Delta} \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)) \right)^s + B^r B^s \right] \Bigg] (\tau,\vec{\sigma}), \tag{5.4}$$

$$\dot{\vec{\eta}}_i(\tau) \stackrel{\circ}{=} \frac{\vec{\kappa}_i(\tau) - Q_i \vec{A}_\perp(\tau,\vec{\eta}_i(\tau))}{\sqrt{m_i^2 + (\vec{\kappa}_i(\tau) - Q_i \vec{A}_\perp(\tau,\vec{\eta}_i(\tau)))^2}},$$

$$\dot{\vec{\kappa}}_i(\tau) \stackrel{\circ}{=} \sum_{k\neq i} \frac{Q_i Q_k (\vec{\eta}_i(\tau) - \vec{\eta}_k(\tau))}{4\pi |\vec{\eta}_i(\tau) - \vec{\eta}_k(\tau)|^3} + Q_i \dot{\eta}_i^u(\tau) \frac{\partial}{\partial \vec{\eta}_i} A_\perp^u(\tau,\vec{\eta}_i(\tau)),$$

$$\dot{A}_{\perp r}(\tau,\vec{\sigma}) \stackrel{\circ}{=} -\pi_{\perp r}(\tau,\vec{\sigma}),$$

$$\dot{\pi}_\perp^r(\tau,\vec{\sigma}) \stackrel{\circ}{=} \Delta A_\perp^r(\tau,\vec{\sigma}) - \sum_i Q_i P_\perp^{rs}(\vec{\sigma}) \dot{\eta}_i^s(\tau) \delta^3(\vec{\sigma} - \vec{\eta}_i(\tau)),$$

$$\vec{\kappa}_+(\tau) + \int d^3\sigma [\vec{\pi}_\perp \times \vec{B}](\tau,\vec{\sigma}) \approx 0 \quad (\textit{rest-frame condition}). \tag{5.5}$$

Let us note that in this reduced phase space there are only either particle-field interactions or action-at-a-distance two-body interactions.

The particle world lines are $x_i^\mu(\tau) = x_o^\mu + u^\mu(p_s)\tau + \epsilon_r^\mu(u(p_s))\eta_i^r(\tau)$, while their 4-momenta are $p_i^\mu(\tau) = \sqrt{m_i^2 + [\vec{\kappa}_i - Q_i \vec{A}_\perp(\tau,\vec{\eta}_i)]^2} u^\mu(p_s) + \epsilon_r^\mu(u(p_s))[\kappa_i^r - Q_i A_\perp^r(\tau,\vec{\eta}_i)]$.

The generators of the internal Poincaré group are

$$\mathcal{P}^\tau_{(\mathrm{int})} = M = \sum_{i=1}^{N} \sqrt{m_i^2 + (\vec{\kappa}_i(\tau) - Q_i \vec{A}_\perp(\tau,\vec{\eta}_i(\tau)))^2} + \frac{1}{2} \sum_{i\neq j} \frac{Q_i Q_j}{4\pi |\vec{\eta}_i(\tau) - \vec{\eta}_j(\tau)|} + \int d^3\sigma \frac{1}{2} [\vec{\pi}_\perp^2 + \vec{B}^2](\tau,\vec{\sigma}),$$

$$\vec{\mathcal{P}}_{(\mathrm{int})} = \vec{\kappa}_+(\tau) + \int d^3\sigma [\vec{\pi}_\perp \times \vec{B}](\tau,\vec{\sigma}) \approx 0,$$

$$\mathcal{J}^r_{(\mathrm{int})} = \sum_{i=1}^{N} (\vec{\eta}_i(\tau) \times \vec{\kappa}_i(\tau))^r + \int d^3\sigma (\vec{\sigma} \times [\vec{\pi}_\perp \times \vec{B}]^r(\tau,\vec{\sigma}),$$

$$\mathcal{K}^r_{(\mathrm{int})} = -\sum_{i=1}^{N} \eta_i^r(\tau) \sqrt{m_i^2 + [\vec{\kappa}_i(\tau) - Q_i \vec{A}_\perp(\tau,\vec{\eta}_i(\tau))]^2} + \frac{1}{2} \left[Q_i \sum_{i=1}^{N} \sum_{j\neq i}^{1\cdots N} Q_j \int d^3\sigma\, \sigma^r \vec{c}(\vec{\sigma} - \eta_i^r(\tau)) \right.$$
$$\left. \cdot \vec{c}(\vec{\sigma} - \eta_j^r(\tau)) + Q_i \int d^3\sigma\, \pi_\perp^r(\tau,\vec{\sigma}) c(\vec{\sigma} - \eta_i^r(\tau)) \right] - \frac{1}{2} \int d^3\sigma\, \sigma^r (\vec{\pi}_\perp^2 + \vec{B}^2)(\tau,\vec{\sigma}), \tag{5.6}$$

with $c(\vec{\eta}_i - \vec{\eta}_j) = 1/(4\pi|\vec{\eta}_j - \vec{\eta}_i|)$ [$\Delta c(\vec{\sigma}) = \delta^3(\vec{\sigma})$, $\Delta = -\vec{\partial}^2$, $\vec{c}(\vec{\sigma}) = \vec{\partial}\, c(\vec{\sigma}) = \vec{\sigma}/(4\pi|\vec{\sigma}|^3)$].

Note that $\mathcal{P}^\tau_{(\mathrm{int})} = q^{\tau\tau}$ and $\mathcal{P}^r_{(\mathrm{int})} = q^{r\tau}$ are the mass and momentum monopoles, respectively.

For the sake of simplicity, consider the subsystem formed by the two particles of mass m_1 and m_2. Our considerations may be extended to any cluster of particles both in this case and in the case discussed in the preceding section. This subsystem is *open*, besides their mutual interaction, the two particles share Coulomb interaction with the other $N-2$ particles and are acted upon by the transverse electromagnetic fields.

By using the multipoles we select a set of *effective parameters* (mass, 3-center of motion, 3-momentum, spin) describing the two-particle cluster as a global entity subject to external forces in the global rest-frame instant form. This was the original motivation of the multipolar expansion in general relativity, replacing an extended object (an open system due to the presence of the gravitational field) with a set of multipoles concentrated on a center of motion. In the rest-frame instant form it is then possible to show that, unlike the case of isolated systems where, in the rest frame $\vec{\kappa}_+ \approx 0$, different conventions identify the same centroid, in the case of an open system different conventions lead to different centers of motion, although a preferred choice seems to stand out on the basis of some reasonable properties.

Given the energy-momentum tensor $T^{AB}(\tau,\vec{\sigma})$ (5.4) of the isolated system, it would seem natural to define *the energy-momentum tensor* $T^{AB}_{c(n)}(\tau,\vec{\sigma})$ *of an open subsystem composed by a cluster of* $n \leqslant N$ *particles* as the sum of all the terms in Eq. (5.4) containing a dependence on the variables $\vec{\eta}_i, \vec{\kappa}_i$, of the particles of the cluster. Besides kinetic terms, this tensor would contain internal mutual interactions as well as external interactions of the cluster particles with the environment composed by the other $N-n$ particles and by the transverse electromagnetic field. An ambiguity, however, appears, why should we attribute *all the external interactions with the other* $N-n$ *particles* to the cluster (note that no such ambiguity exists for the interaction with the electromagnetic field)? Since we have two-body interactions, it seems more reasonable to attribute only *half* of these external interactions to the cluster and consider the other half as a property of the remaining $N-n$ particles. In particular, according to the first choice if we consider two clusters composed by two nonoverlapping sets of n_1 and n_2 particles, respectively, we would get $T^{AB}_{c(n_1+n_2)} \neq T^{AB}_{c(n_1)} + T^{AB}_{c(n_2)}$, since the mutual Coulomb interactions between the two clusters are present in both $T^{AB}_{c(n_1)}$ and $T^{AB}_{c(n_2)}$. On the other hand according to the second choice we get $T^{AB}_{c(n_1+n_2)} = T^{AB}_{c(n_1)} + T^{AB}_{c(n_2)}$. Since this property is important for studying the mutual relative motion of two clusters in actual cases, we will adopt *the convention that the energy-momentum tensor of a n particle cluster contains only half of the external interaction with the other* $N-n$ *particles*.

Let us remark that, in the case of k-body forces, this convention should be replaced by the following rule: (i) for each particle m_i of the cluster and each k-body term in the energy-momentum tensor involving this particle, write $k = h_i + (k-h_i)$, where h_i is the number of particles of the cluster participating to this particular k-body interaction; (ii) only the fraction h_i/k of this particular k-body interaction term containing m_i must be attributed to the cluster.

Consider now the cluster composed by the two particles with mass m_1 and m_2. The knowledge of $T^{AB}_c \overset{\text{def}}{=} T^{AB}_{c(2)}$ on the Wigner hyperplane of the global rest-frame instant form allows to find the following 10 *nonconserved* charges [due to $Q_i^2 = 0$ we have $\sqrt{m_i^2 + [\vec{\kappa}_i - Q_i \vec{A}_\perp(\tau,\vec{\eta}_i)]^2} = \sqrt{m_i^2 + \vec{\kappa}_1^2} - Q_i[\vec{\kappa}_i \cdot \vec{A}_\perp(\tau,\vec{\eta}_i)/\sqrt{m_i^2+\vec{\kappa}_i^2}]$]:

$$M_c = \int d^3\sigma\, T_c^{\tau\tau}(\tau,\vec{\sigma}) = \sum_{i=1}^{2} \sqrt{m_i^2 + [\vec{\kappa}_i(\tau) - Q_i \vec{A}_\perp(\tau,\vec{\eta}_i(\tau))]^2} + \frac{Q_1 Q_2}{4\pi |\vec{\eta}_1(\tau) - \vec{\eta}_2(\tau)|^2}$$

$$+ \frac{1}{2} \sum_{i=1}^{2} \sum_{k \neq 1,2} \frac{Q_i Q_k}{4\pi |\vec{\eta}_i(\tau) - \vec{\eta}_k(\tau)|^2} = M_{c(\text{int})} + M_{c(\text{ext})},$$

$$M_{c(\text{int})} = \sum_{i=1}^{2} \sqrt{m_i^2 + \vec{\kappa}_i^2} - \frac{Q_1 Q_2}{4\pi |\vec{\eta}_1(\tau) - \vec{\eta}_2(\tau)|^2},$$

$$\vec{\mathcal{P}}_c = \left\{ \int d^3\sigma\, T_c^{r\tau}(\tau,\vec{\sigma}) \right\} = \vec{\kappa}_1(\tau) + \vec{\kappa}_2(\tau),$$

$$\vec{\mathcal{J}}_c = \left\{ \epsilon^{ruv} \int d^3\sigma [\sigma^u T_c^{v\tau} - \sigma^v T_c^{u\tau}](\tau,\vec{\sigma}) \right\} = \vec{\eta}_i(\tau) \times \vec{\kappa}_1(\tau) + \vec{\eta}_2(\tau) \times \vec{\kappa}_2(\tau),$$

$$\vec{\mathcal{K}}_c = -\int d^3\sigma\, \vec{\sigma} T_c^{\tau\tau}(\tau,\vec{\sigma}) = -\sum_{i=1}^{2} \vec{\eta}_i(\tau) \sqrt{m_i^2 + [\vec{\kappa}_i(\tau) - Q_i \vec{A}_\perp(\tau, \vec{\eta}_i(\tau))]^2} - \sum_{i=1}^{2} Q_i \int d^3\sigma\, \vec{\pi}_\perp(\tau,\vec{\sigma})$$
$$\times c(\vec{\sigma} - \vec{\eta}_i(\tau)) - Q_1 Q_2 \int d^3\sigma\, \vec{\sigma} \vec{c}(\vec{\sigma} - \vec{\eta}_1(\tau)) \cdot \vec{c}(\vec{\sigma} - \vec{\eta}_2(\tau)) - \frac{1}{2} \sum_{i=1}^{2} Q_i \sum_{k \neq 1,2} Q_k$$
$$\times \int d^3\sigma\, \vec{\sigma} \vec{c}(\vec{\sigma} - \vec{\eta}_i(\tau)) \cdot \vec{c}(\vec{\sigma} - \vec{\eta}_k(\tau)) = \vec{\mathcal{K}}_{c(\mathrm{int})} + \vec{\mathcal{K}}_{c(\mathrm{ext})},$$

$$\vec{\mathcal{K}}_{c(\mathrm{int})} = -\sum_{i=1}^{2} \vec{\eta}_i(\tau) \sqrt{m_i^2 + \vec{\kappa}_i^2} - Q_1 Q_2 \int d^3\sigma\, \vec{\sigma} \vec{c}(\vec{\sigma} - \vec{\eta}_1(\tau)) \cdot \vec{c}(\vec{\sigma} - \vec{\eta}_2(\tau)), \tag{5.7}$$

which do *not* satisfy the algebra of an internal Poincaré group because of the openess of the system. Since we are working in an instant form of dynamics, only the cluster internal energy and boosts depend on the (internal and external) interactions. Again $M_c = q_c^{\tau\tau}$ and $\mathcal{P}_c^r = q_c^{r\tau}$ are the mass and momentum monopoles of the cluster.

Another needed quantity is the momentum dipole

$$p_c^{ru} = \int d^3\sigma\, \sigma^r T_c^{u\tau}(\tau,\vec{\sigma}) = \sum_{i=1}^{2} \eta_i^r(\tau) \kappa_i^u(\tau) - \sum_{i=1}^{2} Q_i \int d^3\sigma\, c(\vec{\sigma} - \vec{\eta}_i(\tau)) [\partial^r A_\perp^s + \partial^s A_\perp^r](\tau,\vec{\sigma}),$$

$$p_c^{ru} + p_c^{ur} = \sum_{i=1}^{2} [\eta_i^r(\tau) \kappa_i^u(\tau) + \eta_i^u(\tau) \kappa_i^r(\tau)] - 2 \sum_{i=1}^{2} Q_i \int d^3\sigma\, c(\vec{\sigma} - \vec{\eta}_i(\tau)) [\partial^r A_\perp^s + \partial^s A_\perp^r](\tau,\vec{\sigma}),$$

$$p_c^{ru} - p_c^{ur} = \epsilon^{ruv} \mathcal{J}_c^v. \tag{5.8}$$

The time variation of the 10 charges (5.7) can be evaluated by using the equations of motion (5.5),

$$\frac{\mathrm{d}M_c}{\mathrm{d}\tau} = \sum_{i=1}^{2} Q_i \left(\frac{\vec{\kappa}_i(\tau) \cdot \vec{\pi}_\perp(\tau, \vec{\eta}_i(\tau))}{\sqrt{m_i^2 + \vec{\kappa}_i^2}} + \frac{1}{2} \sum_{k \neq 1,2} Q_k \left[\frac{\vec{\kappa}_i(\tau)}{\sqrt{m_i^2 + \vec{\kappa}_i^2}} + \frac{\vec{\kappa}_k(\tau)}{\sqrt{m_k^2 + \vec{\kappa}_k^2}} \right] \cdot \frac{\vec{\eta}_i(\tau) - \vec{\eta}_k(\tau)}{4\pi |\vec{\eta}_i(\tau) - \vec{\eta}_k(\tau)|^3} \right),$$

$$\frac{\mathrm{d}\mathcal{P}_c^r}{\mathrm{d}\tau} = \sum_{i=1}^{2} Q_i \left(\frac{\vec{\kappa}_i(\tau)}{\sqrt{m_i^2 + \vec{\kappa}_i^2}} \cdot \frac{\partial A_\perp^r(\tau, \vec{\eta}_i(\tau))}{\partial \vec{\eta}_i} + \sum_{k \neq 1,2} Q_k \frac{\eta_i^r(\tau) - \eta_k^r(\tau)}{4\pi |\vec{\eta}_i(\tau) - \vec{\eta}_k(\tau)|^3} \right),$$

$$\frac{\mathrm{d}\vec{\mathcal{J}}_c}{\mathrm{d}\tau} = \sum_{i=1}^{2} Q_i \left(\frac{\vec{\kappa}_i(\tau)}{\sqrt{m_i^2 + \vec{\kappa}_i^2}} \times \vec{A}_\perp(\tau, \vec{\eta}_i(\tau)) + \vec{\eta}_i(\tau) \times \left[\frac{\vec{\kappa}_i(\tau)}{\sqrt{m_i^2 + \vec{\kappa}_i^2}} \cdot \frac{\partial}{\partial \vec{\eta}_i} \right] \vec{A}_\perp(\tau, \vec{\eta}_i(\tau)) \right.$$
$$\left. - \sum_{k \neq i} Q_k \frac{\vec{\eta}_i(\tau) \times \vec{\eta}_k(\tau)}{4\pi |\vec{\eta}_i(\tau) - \vec{\eta}_k(\tau)|^3} \right),$$

$$
\begin{aligned}
\frac{d\mathcal{K}_c^r}{d\tau} &= -\mathcal{P}_c^r - \sum_{i=1}^{2} Q_i \eta_i^r(\tau) \frac{\vec{\kappa}_i(\tau)}{\sqrt{m_i^2+\vec{\kappa}_i^2(\tau)}} \cdot \left[\vec{\pi}_\perp(\tau,\eta_i^r(\tau)) + \sum_{k\neq i} Q_k \vec{c}(\eta_i^r(\tau)-\eta_k^r(\tau)) \right] \\
&+ \sum_{i=1}^{2} Q_i \left[\sum_{k\neq i} Q_k \frac{\vec{\kappa}_k(\tau)}{\sqrt{m_k^2+\vec{\kappa}_k^2(\tau)}} c(\eta_i^r(\tau)-\eta_k^r(\tau)) - \int d^3\sigma\, \vec{\pi}_\perp(\tau,\vec{\sigma}) \frac{\vec{\kappa}_i(\tau)\cdot\vec{c}(\vec{\sigma}-\eta_i^r(\tau))}{\sqrt{m_i^2+\vec{\kappa}_i^2(\tau)}} \right] \\
&+ \sum_{i=1}^{2} Q_i \sum_{k\neq 1} Q_k \int d^3\sigma\, c(\vec{\sigma}-\eta_i^r(\tau)) \left(\frac{\vec{\kappa}_k(\tau)}{\sqrt{m_k^2+\vec{\kappa}_k^2(\tau)}} \cdot \vec{\partial} \right) \vec{c}(\vec{\sigma}-\eta_k^r(\tau)) \\
&= Q_1 Q_2 \int d^3\sigma\, \vec{\sigma} \left(\left[\left(\frac{\vec{\kappa}_1(\tau)}{\sqrt{m_1^2+\vec{\kappa}_1^2(\tau)}} \cdot \vec{\partial} \right) \vec{c}(\vec{\sigma}-\eta_1^r(\tau)) \right] \cdot \vec{c}(\vec{\sigma}-\eta_2^r(\tau)) \right. \\
&+ \vec{c}(\vec{\sigma}-\vec{\eta}_1(\tau)) \cdot \left[\left(\frac{\vec{\kappa}_2(\tau)}{\sqrt{m_2^2+\vec{\kappa}_2^2(\tau)}} \cdot \vec{\partial} \right) \vec{c}(\vec{\sigma}-\eta_2^r(\tau)) \right] \\
&- \frac{1}{2} \sum_{i=1}^{2} Q_i \sum_{k\neq 1,2} Q_k \int d^3\sigma\, \vec{\sigma} \left(\left[\left(\frac{\vec{\kappa}_i(\tau)}{\sqrt{m_i^2+\vec{\kappa}_i^2(\tau)}} \cdot \vec{\partial} \right) \vec{c}(\vec{\sigma}-\eta_i^r(\tau)) \right] \cdot \vec{c}(\vec{\sigma}-\eta_k^r(\tau)) \right. \\
&+ \left. \vec{c}(\vec{\sigma}-\eta_i^r(\tau)) \cdot \left[\left(\frac{\vec{\kappa}_k(\tau)}{\sqrt{m_k^2+\vec{\kappa}_k^2(\tau)}} \cdot \vec{\partial} \right) \vec{c}(\vec{\sigma}-\eta_k^r(\tau)) \right] \right). \qquad (5.9)
\end{aligned}
$$

Let us remark that, if we have two clusters of n_1 and n_2 particles, respectively, our definition of cluster energy-momentum tensor implies

$$
\begin{aligned}
M_{c(n_1+n_2)} &= M_{c(n_1)} + M_{c(n_2)}, \\
\vec{\mathcal{P}}_{c(n_1+n_2)} &= \vec{\mathcal{P}}_{c(n_1)} + \vec{\mathcal{P}}_{c(n_2)}, \\
\vec{\mathcal{J}}_{c(n_1+n_2)} &= \vec{\mathcal{J}}_{c(n_1)} + \vec{\mathcal{J}}_{c(n_2)}, \\
\vec{\mathcal{K}}_{c(n_1+n_2)} &= \vec{\mathcal{K}}_{c(n_1)} + \vec{\mathcal{K}}_{c(n_2)}. \qquad (5.10)
\end{aligned}
$$

Then the main problem is the determination of an effective center of motion $\zeta_c^r(\tau)$ with world-line $w_c^\mu(\tau)=x_o^\mu+u^\mu(p_s)\tau+\epsilon_r^\mu(u(p_s))\zeta_c^r(\tau)$ in the gauge $T_s\equiv\tau$, $\vec{q}_+=\vec{R}_+=\vec{y}_+\equiv 0$ of the isolated system. The unit 4-velocity of this center of motion is $u_c^\mu(\tau)=\dot{w}_c^\mu(\tau)/\sqrt{1-\dot{\vec{\zeta}}_c^2(\tau)}$ with $\dot{w}_c^\mu(\tau)=u^\mu(p_s)+\epsilon_r^\mu(u(p_s))\dot{\zeta}_c^r(\tau)$. By using $\delta z^\mu(\tau,\vec{\sigma})=\epsilon_r^\mu(u(p_s))(\sigma^r-\zeta^r(\tau))$ we can define the multipoles of the cluster with respect to the world-line $w_c^\mu(\tau)$,

$$
q_c^{r_1\cdots r_n AB}(\tau) = \int d^3\sigma [\sigma^{r_1}-\zeta_c^{r_1}(\tau)]\cdots[\sigma^{r_n}-\zeta_c^{r_n}(\tau)] T_c^{AB}(\tau,\vec{\sigma}). \qquad (5.11)
$$

The mass and momentum monopoles and the mass, momentum, and spin dipoles are

$$
\begin{aligned}
q_c^{\tau\tau} &= M_c, \quad q_c^{r\tau} = \mathcal{P}_c^r, \\
q_c^{r\tau\tau} &= -\mathcal{K}_c^r - M_c\zeta_c^r(\tau) = M_c(R_c^r(\tau)-\zeta_c^r(\tau)), \\
q_c^{ru\tau} &= p_c^{ru}(\tau) - \zeta_c^r(\tau)\mathcal{P}_c^u,
\end{aligned}
$$

$$S_c^{\mu\nu} = [\epsilon_r^\mu(u(p_s))u^\nu(p_s) - \epsilon_r^\nu(u(p_s))u^\mu(p_s)]q_c^{r\tau\tau} + \epsilon_r^\mu(u(p_s))\epsilon_u^\nu(u(p_s))(q_c^{ru\tau} - q_c^{ur\tau}) = [\epsilon_r^\mu(u(p_s))u^\nu(p_s) - \epsilon_r^\nu(u(p_s))u^\mu(p_s)]M_c(R_c^r - \zeta_c^r) + \epsilon_r^\mu(u(p_s))\epsilon_u^\nu(u(p_s))[\epsilon^{ruv}\mathcal{J}_c^v - (\zeta_c^r\mathcal{P}_c^u - \zeta_c^u\mathcal{P}_c^r)],$$

$$\Rightarrow m_{c(p_s)}^\mu = -S_c^{\mu\nu}u_\nu(p_s) = -\epsilon_r^\mu(u(p_s))q_c^{r\tau\tau}. \tag{5.12}$$

Let us now consider the following possible definitions of effective centers of motion (many others are possible).

(1) *Center of energy*[29] *as center of motion*, $\vec{\zeta}_{c(E)}(\tau) = \vec{R}_c(\tau)$, where $\vec{R}_c(\tau)$ is *a 3-center of energy* for the cluster built by means of the standard definition

$$\vec{R}_c = -\frac{\vec{\mathcal{K}}_c}{M_c}. \tag{5.13}$$

It is determined by the requirement that either the mass dipole vanishes, $q_c^{r\tau\tau} = 0$ or the mass dipole moment with respect to $u^\mu(p_s)$ vanishes, $m_{c(p_s)}^\mu = 0$.

The center of energy seems to be the only center of motion enjoying the simple composition rule

$$\vec{R}_{c(n_1+n_2)} = \frac{M_{c(n_1)}\vec{R}_{c(n_1)} + M_{c(n_2)}\vec{R}_{c(n_2)}}{M_{c(n_1+n_2)}}. \tag{5.14}$$

The constitutive relation between $\vec{\mathcal{P}}_c$ and $\dot{\vec{R}}_c(\tau)$, see Eq. (4.8), is

$$0 = \frac{dq_c^{r\tau\tau}}{d\tau} = -\dot{\mathcal{K}}_c^r - \dot{M}_c R_c^r - M_c\dot{R}_c^r,$$

$$\Downarrow$$

$$\begin{aligned}
\vec{\mathcal{P}}_c = {} & M_c\dot{\vec{R}}_c + \dot{M}_c\vec{R}_c - \sum_{i=1}^2 Q_i\vec{\eta}_i(\tau)\frac{\vec{\kappa}_i(\tau)}{\sqrt{m_i^2 + \vec{\kappa}_i^2(\tau)}}\cdot\left[\vec{\pi}_\perp(\tau,\vec{\eta}_i(\tau)) + \sum_{k\neq i}Q_k\vec{c}(\vec{\eta}_i(\tau) - \vec{\eta}_k(\tau))\right] \\
& + \sum_{i=1}^2 Q_i\left[\sum_{k\neq i}Q_k\frac{\vec{\kappa}_k(\tau)}{\sqrt{m_k^2 + \vec{\kappa}_k^2(\tau)}}c(\vec{\eta}_i(\tau) - \vec{\eta}_k(\tau)) - \int d^3\sigma\,\vec{\pi}_\perp(\tau,\vec{\sigma})\frac{\vec{\kappa}_i(\tau)\cdot\vec{c}(\vec{\sigma} - \vec{\eta}_i(\tau))}{\sqrt{m_i^2 + \vec{\kappa}_i^2(\tau)}}\right] \\
& + \sum_{i=1}^2 Q_i\sum_{k\neq i}Q_k\int d^3\sigma\, c(\vec{\sigma} - \vec{\eta}_i(\tau))\left(\frac{\vec{\kappa}_k(\tau)}{\sqrt{m_k^2 + \vec{\kappa}_k^2(\tau)}}\cdot\vec{\partial}\right)\vec{c}(\vec{\sigma} - \vec{\eta}_k(\tau)) \\
= {} & Q_1Q_2\int d^3\sigma\,\vec{\sigma}\left(\left[\left(\frac{\vec{\kappa}_1(\tau)}{\sqrt{m_1^2 + \vec{\kappa}_1^2(\tau)}}\cdot\vec{\partial}\right)\vec{c}(\vec{\sigma} - \vec{\eta}_1(\tau))\right]\cdot\vec{c}(\vec{\sigma} - \vec{\eta}_2(\tau))\right. \\
& \left. + \vec{c}(\vec{\sigma} - \vec{\eta}_1(\tau))\cdot\left[\left(\frac{\vec{\kappa}_2(\tau)}{\sqrt{m_2^2 + \vec{\kappa}_2^2(\tau)}}\cdot\vec{\partial}\right)\vec{c}(\vec{\sigma} - \vec{\eta}_2(\tau))\right]\right) \\
& - \frac{1}{2}\sum_{i=1}^2 Q_i\sum_{k\neq 1,2}Q_k\int d^3\sigma\,\vec{\sigma}\left(\left[\left(\frac{\vec{\kappa}_i(\tau)}{\sqrt{m_i^2 + \vec{\kappa}_i^2(\tau)}}\cdot\vec{\partial}\right)\vec{c}(\vec{\sigma} - \vec{\eta}_i(\tau))\right]\cdot\vec{c}(\vec{\sigma} - \vec{\eta}_k(\tau))\right.
\end{aligned}$$

$$+\vec{c}(\vec{\sigma}-\vec{\eta}_i(\tau))\cdot\left[\left(\frac{\vec{\kappa}_k(\tau)}{\sqrt{m_k^2+\vec{\kappa}_k^2(\tau)}}\cdot\vec{\partial}\right)\vec{c}(\vec{\sigma}-\vec{\eta}_k(\tau))\right]\Bigg). \tag{5.15}$$

From Eq. (4.10) the associated cluster spin tensor is

$$S_c^{\mu\nu}=\epsilon_r^\mu(u(p_s))\epsilon_u^\nu(u(p_s))[q_c^{ru\tau}-q_c^{ur\tau}]=\epsilon_r^\mu(u(p_s))\epsilon_u^\nu(u(p_s))\epsilon^{ruv}[\mathcal{J}_c^v-(\vec{R}_c\times\vec{\mathcal{P}}_c)^v]. \tag{5.16}$$

(2) *Pirani centroid* $\vec{\zeta}_{c(P)}(\tau)$ (Ref. 14) *as center of motion*. It is determined by the requirement that the mass dipole moment with respect to 4-velocity $\dot{w}_c^\mu(\tau)$ vanishes (it involves the antisymmetric part of p_c^{ur})

$$m^\mu_{c(\dot{w}_c)}=-S_c^{\mu\nu}\dot{w}_{c\nu}=0,\quad \Rightarrow \dot{\vec{\zeta}}_{c(P)}\cdot\vec{\zeta}_{c(P)}=\dot{\vec{\zeta}}_{c(P)}\cdot\vec{R}_c,$$

$$\Downarrow$$

$$\vec{\zeta}_{c(P)}(\tau)=\frac{1}{M_c-\vec{\mathcal{P}}_c\cdot\dot{\vec{\zeta}}_{c(P)}(\tau)}[M_c\vec{R}_c-\vec{R}_c\cdot\dot{\vec{\zeta}}_{c(P)}(\tau)\vec{\mathcal{P}}_c-\dot{\vec{\zeta}}_{c(P)}(\tau)\times\vec{\mathcal{J}}_c]. \tag{5.17}$$

Therefore this centroid is implicitly defined as the solution of these three coupled first order ordinary differential equations.

(3) *Tulczyjew centroid* $\vec{\zeta}_{c(T)}(\tau)$ (Refs. 15,18, and 23) *as center of motion*. If we define the cluster 4-momentum $P_c^\mu=M_cu^\mu(p_s)+\mathcal{P}_c^s\epsilon_s^\mu(u(p_s))$ $[P_c^2=M_c^2-\vec{\mathcal{P}}_c^2\overset{\text{def}}{=}\mathcal{M}_c^2]$, its definition coincides with requiring the vanishing of the mass dipole moment with respect to P_c^μ (it involves the antisymmetric part of p_c^{ur})

$$m^\mu_{c(P_c)}=-S_c^{\mu\nu}P_{c\nu}=0,\quad \Rightarrow \vec{\mathcal{P}}_c\cdot\vec{\zeta}_{c(T)}=\vec{\mathcal{P}}_c\cdot\vec{R}_c,$$

$$\Downarrow$$

$$\vec{\zeta}_{c(T)}(\tau)=\frac{1}{M_c^2-\vec{\mathcal{P}}_c^2}[M_c^2\vec{R}_c-\vec{\mathcal{P}}_c\cdot\vec{R}_c\vec{\mathcal{P}}_c-\vec{\mathcal{P}}_c\times\vec{\mathcal{J}}_c]. \tag{5.18}$$

Let us show that this centroid satisfies the free particle relation as constitutive relation,

$$\vec{\mathcal{P}}_c=M_c\dot{\vec{\zeta}}_{c(T)},$$

$$\Downarrow$$

$$P_c^\mu=M_c[u^\mu(p_s)+\dot{\zeta}^s_{c(T)}\epsilon_s^\mu(u(p_s))],$$

$$q^{r\tau\tau}_{c(T)}=\frac{M_c}{M_c^2-\vec{\mathcal{P}}_c^2}[\vec{\mathcal{P}}_c^2\vec{R}_c+\vec{\mathcal{P}}_c\cdot\vec{R}_c\vec{\mathcal{P}}_c+\vec{\mathcal{P}}_c\times\vec{\mathcal{J}}_c],$$

$$S_c^{\mu\nu} = [\epsilon_r^\mu(u(p_s))u^\nu(p_s) - \epsilon_r^\nu(u(p_s))u^\mu(p_s)]q_{c(T)}^{r\tau\tau} + \epsilon_r^\mu(u(p_s))\epsilon_u^\nu(u(p_s))\epsilon^{ruv}[\mathcal{I}_c^v - (\vec{\zeta}_{c(T)} \times \vec{\mathcal{P}}_c)^v]. \tag{5.19}$$

If we use Eq. (5.17) to find a Pirani centroid such that $\dot{\vec{\zeta}}_c = \vec{\mathcal{P}}_c / M_c$, it turns out that the condition (5.17) becomes Eq. (5.18) and this implies Eq. (5.19).

The equations of motion,

$$M_c(\tau)\ddot{\vec{\zeta}}_{c(T)}(\tau) = \dot{\vec{\mathcal{P}}}_c(\tau) - \dot{M}_c(\tau)\dot{\vec{\zeta}}_{c(T)}(\tau), \tag{5.20}$$

contain both internal and external forces. In spite of the nice properties (5.19) and (5.20) of the Tulczyjew centroid, this effective center of motion suffers the drawback of lacking a simple composition property. The relation among the Tulczyjew centroids of clusters with n_1, n_2 and n_1+n_2 particles, respectively, is much more complicated of the composition (5.14) of the centers of energy.

All the previous centroids coincide for an isolated system in the rest-frame instant form with $\vec{\mathcal{P}}_c = \vec{\kappa}_+ \approx 0$ in the gauge $\vec{q}_+ \approx \vec{R}_+ \approx \vec{y}_+ \approx 0$.

(4) The *Corinaldesi–Papapetrou centroid*[12] *with respect to a timelike observer with, 4-velocity* $v^\mu(\tau), \zeta_{c(\mathrm{CP})}^{(v)}(\tau)$ *as center of motion.*

$$m_{c(v)}^\mu = -S_c^{\mu\nu} v_\nu = 0. \tag{5.21}$$

Clearly these centroids are unrelated to the previous ones being dependent on the choice of an arbitrary observer.

(5) The *Pryce center of spin*[30–32] *or classical canonical Newton–Wigner centroid* $\vec{\zeta}_{c(\mathrm{NW})}$. It defined as the solution of the differential equations implied by the requirement $\{\zeta_{c(\mathrm{NW})}^r, \zeta_{c(\mathrm{NW})}^s\} = 0$, $\{\zeta_{c(\mathrm{NW})}^r, \mathcal{P}_c^s\} = \delta^{rs}$. Note that, being in an instant form of dynamics, we have $\{\mathcal{P}_c^r, \mathcal{P}_c^s\} = 0$ also for an open system.

The two effective centers of motion which look more useful for applications seems to be the center of energy $\vec{\zeta}_{c(E)}(\tau)$ and Tulczyjew's centroid $\vec{\zeta}_{c(T)}(\tau)$, with $\vec{\zeta}_{c(E)}(\tau)$ preferred for the study of the mutual motion of clusters due to Eq. (5.14).

Therefore, in the spirit of the multipolar expansion, our two-body cluster may be described by an effective nonconserved internal energy (or mass) $M_c(\tau)$, by the world-line $w_c^\mu = x_o^\mu + u^\mu(p_s)\tau + \epsilon_r^\mu(u(p_s))\ \zeta_{c(E \text{ or } T)}^r(\tau)$ associated with the effective center of motion $\vec{\zeta}_{c(E \text{ or } T)}(\tau)$ and by the effective 3-momentum $\vec{\mathcal{P}}_c(\tau)$, with $\vec{\zeta}_{c(E \text{ or } T)}(\tau)$ and $\vec{\mathcal{P}}_c(\tau)$ forming a noncanonical basis for the collective variables of the cluster. A noncanonical effective spin for the cluster in the (1) and (3) cases is defined by the following:

(a) case of the center of energy,

$$\vec{\mathcal{S}}_{c(E)}(\tau) = \vec{\mathcal{J}}_c(\tau) - \vec{R}_c(\tau) \times \vec{\mathcal{P}}_c(\tau),$$

$$\frac{\mathrm{d}\vec{\zeta}_{c(E)}(\tau)}{\mathrm{d}\tau} = \frac{\mathrm{d}\vec{\mathcal{J}}_c(\tau)}{\mathrm{d}\tau} - \frac{\mathrm{d}\vec{R}_c(\tau)}{\mathrm{d}\tau} \times \vec{\mathcal{P}}_c(\tau) - \vec{R}_c(\tau) \times \frac{\mathrm{d}\vec{\mathcal{P}}_c(\tau)}{\mathrm{d}\tau},$$

(b) case of the Tulczyjew centroid,

$$\vec{\mathcal{S}}_{c(T)}(\tau) = \vec{\mathcal{J}}_c(\tau) - \vec{\zeta}_{c(T)}(\tau) \times \vec{\mathcal{P}}_c(\tau) = \frac{M_c^2(\tau)\vec{\mathcal{S}}_{c(E)}(\tau) - \vec{\mathcal{P}}_c(\tau) \cdot \vec{\mathcal{J}}_c(\tau)\vec{\mathcal{P}}_c(\tau)}{M_c^2(\tau) - \vec{\mathcal{P}}_c^2(\tau)},$$

$$\frac{\mathrm{d}\vec{\zeta}_{c(T)}(\tau)}{\mathrm{d}\tau} = \frac{\mathrm{d}\vec{\mathcal{J}}_c(\tau)}{\mathrm{d}\tau} - \vec{\zeta}_{c(T)}(\tau) \times \frac{\mathrm{d}\vec{\mathcal{P}}_c(\tau)}{\mathrm{d}\tau}. \tag{5.22}$$

Since our cluster contains only two particles, this pole–dipole description concentrated on the world-line $w_c^\mu(\tau)$ is equivalent to the original description in terms of the canonical variables $\vec{\eta}_i(\tau), \vec{\kappa}_i(\tau)$ (all higher multipoles are not independent quantities in this case).

Then, let us see whether it is possible to replace the description of the two-body system as an effective pole–dipole system, by a description of it as an effective extended two-body system obtained by introducing two noncanonical relative variables $\vec{\rho}_{c(E \text{ or } T)}(\tau)$, $\vec{\pi}_{c(E \text{ or } T)}(\tau)$ through the following definitions:

$$\vec{\eta}_1 \overset{\text{def}}{=} \vec{\zeta}_{c(E \text{ or } T)} + \tfrac{1}{2}\vec{\rho}_{c(E \text{ or } T)}, \quad \vec{\zeta}_{c(E \text{ or } T)} = \tfrac{1}{2}(\vec{\eta}_1 + \vec{\eta}_2),$$

$$\vec{\eta}_2 \overset{\text{def}}{=} \vec{\zeta}_{c(E \text{ or } T)} - \tfrac{1}{2}\vec{\rho}_{c(E \text{ or } T)}, \quad \vec{\rho}_{c(E \text{ or } T)} = \vec{\eta}_1 - \vec{\eta}_2,$$

$$\vec{\kappa}_1 \overset{\text{def}}{=} \tfrac{1}{2}\vec{\mathcal{P}}_c + \vec{\pi}_{c(E \text{ or } T)}, \quad \vec{\mathcal{P}}_c = \vec{\kappa}_1 + \vec{\kappa}_2,$$

$$\vec{\kappa}_2 \overset{\text{def}}{=} \tfrac{1}{2}\vec{\mathcal{P}}_c - \vec{\pi}_{c(E \text{ or } T)}, \quad \vec{\pi}_{c(E \text{ or } T)} = \tfrac{1}{2}(\vec{\kappa}_1 - \vec{\kappa}_2),$$

$$\vec{\mathcal{J}}_c = \vec{\eta}_1 \times \vec{\kappa}_1 + \vec{\eta}_2 \times \vec{\kappa}_2 = \vec{\zeta}_{c(E \text{ or } T)} \times \vec{\mathcal{P}}_c + \vec{\rho}_{c(E \text{ or } T)} \times \vec{\pi}_{c(E \text{ or } T)},$$

$$\Rightarrow \vec{\mathcal{S}}_{c(E \text{ or } T)} = \vec{\rho}_{c(E \text{ or } T)} \times \vec{\pi}_{c(E \text{ or } T)}. \tag{5.23}$$

Note that, even if it is suggested by a canonical transformation, the above transformation is in fact *not* a canonical transformation and it can only be defined since we are working in an instant form of dynamics, in which both $\vec{\mathcal{P}}_c$ and $\vec{\mathcal{J}}_c$ do not depend upon the interactions.

Note finally that we know everything about this new basis except for the unit vector $\vec{\rho}_{c(E \text{ or } T)}/|\vec{\rho}_{c(E \text{ or } T)}|$ and the momentum $\vec{\pi}_{c(E \text{ or } T)}$. However, this relevant lacking information can be extracted from the symmetrized momentum dipole $p_c^{ru} + p_c^{ur}$, which is a known effective quantity since Eq. (5.9) has the following expression in terms of the variables (5.23):

$$p_c^{ru} + p_c^{ur} + 2\sum_{i=1}^{2} Q_i \int d^3\sigma\, c(\vec{\sigma} - \vec{\eta}_i(\tau))[\partial^r A_\perp^s + \partial^s A_\perp^r](\tau, \vec{\sigma}) = \sum_{i=1}^{2} (\eta_i^r \kappa_i^u + \eta_i^u \kappa_i^r) = \zeta_{c(E \text{ or } T)}^r \mathcal{P}_c^u$$
$$+ \zeta_{c(E \text{ or } T)}^r \mathcal{P}_c^r + \rho_{c(E \text{ or } T)}^r \pi_{c(E \text{ or } T)}^u + \rho_{c(E \text{ or } T)}^u \pi_{c(E \text{ or } T)}^r. \tag{5.24}$$

A strategy for working out this information explicitly is provided by the construction of a *spin frame* which, following Ref. 33 for the $N-2$ case, is defined by $\hat{\mathcal{S}}_{c(E \text{ or } T)} = \vec{\mathcal{S}}_{c(E \text{ or } T)}/|\vec{\mathcal{S}}_{c(E \text{ or } T)}|$, $\hat{\mathcal{R}}_{c(E \text{ or } T)}$, $\hat{\mathcal{V}}_{c(E \text{ or } T)} = \hat{\mathcal{R}}_{c(E \text{ or } T)} \times \hat{\mathcal{S}}_{c(E \text{ or } T)}$, with $\hat{\mathcal{S}}_{c(E \text{ or } T)} \cdot \hat{\mathcal{R}}_{c(E \text{ or } T)} = 0$, $\hat{\mathcal{S}}_{c(E \text{ or } T)}^2 = \hat{\mathcal{R}}_{c(E \text{ or } T)}^2 = \hat{\mathcal{V}}_{c(E \text{ or } T)}^2 = 1$. Then we get the following decomposition ($\mathcal{S}_{c(E \text{ or } T)} = |\vec{\mathcal{S}}_{c(E \text{ or } T)}|$):

$$\vec{\rho}_{c(E \text{ or } T)} = \rho_{c(E \text{ or } T)} \hat{\mathcal{R}}_{c(E \text{ or } T)}, \quad \rho_{c(E \text{ or } T)} = |\vec{\eta}_1 - \vec{\eta}_2|,$$

$$\vec{\pi}_{c(E \text{ or } T)} = \tilde{\pi}_{c(E \text{ or } T)} \hat{\mathcal{R}}_{c(E \text{ or } T)} - \frac{\mathcal{S}_{c(E \text{ or } T)}}{\rho_{c(E \text{ or } T)}} \hat{\mathcal{V}}_{c(E \text{ or } T)}, \quad \tilde{\pi}_{c(E \text{ or } T)} = \vec{\pi}_{c(E \text{ or } T)} \cdot \frac{\vec{\rho}_{c(E \text{ or } T)}}{\rho_{c(E \text{ or } T)}}, \tag{5.25}$$

where $\rho_{c(E \text{ or } T)}$ is just the relative variable appearing in the Coulomb potential. Equations (5.25) show that only the three variables $\tilde{\pi}_{c(E \text{ or } T)}$ and $\hat{\mathcal{R}}_{c(E \text{ or } T)} = \vec{\rho}_{c(E \text{ or } T)} / \rho_{c(E \text{ or } T)}$ are still unknown. Then from Eqs. (5.23) and (5.24) we obtain

$$\begin{aligned} \rho^r_{c(E \text{ or } T)} \pi^u_{c(E \text{ or } T)} + \rho^u_{c(E \text{ or } T)} \pi^r_{c(E \text{ or } T)} &= 2\, \rho_{c(E \text{ or } T)} \tilde{\pi}_{c(E \text{ or } T)} \hat{\mathcal{R}}^r_{c(E \text{ or } T)} \hat{\mathcal{R}}^u_{c(E \text{ or } T)} - \mathcal{S}_{c(E \text{ or } T)} \\ &\times (\hat{\mathcal{R}}^r_{c(E \text{ or } T)} \hat{\mathcal{V}}^u_{c(E \text{ or } T)} + \hat{\mathcal{R}}^u_{c(E \text{ or } T)} \hat{\mathcal{V}}^r_{c(E \text{ or } T)}) = p^{ru}_c + p^{ur}_c \\ &- (\zeta^r_{c(E \text{ or } T)} \mathcal{P}^u_c + \zeta^u_{c(E \text{ or } T)} \mathcal{P}^r_c) + 2 \sum_{i=1}^{2} Q_i \int d^3\sigma\, c(\vec{\sigma} - \vec{\eta}_i(\tau)) \\ &\times [\partial^r A^u_\perp + \partial^u A^r_\perp](\tau, \vec{\sigma}) \overset{\text{def}}{=} F^{ru}_{c(E \text{ or } T)}, \end{aligned}$$

$$F^{ru}_{c(E \text{ or } T)} \mathcal{S}^u_{c(E \text{ or } T)} \equiv 0. \tag{5.26}$$

Now, these are three independent equations for $\tilde{\pi}_{c(E \text{ or } T)}$ and for the two degrees of freedom in the unit vector $\hat{\mathcal{R}}_{c(E \text{ or } T)}$ in terms of the known quantities $F^{ru}_{c(E \text{ or } T)}, \mathcal{S}_{c(E \text{ or } T)}$, $\rho_{c(E \text{ or } T)} = |\vec{\eta}_1 - \vec{\eta}_2|$. For instance we get $\tilde{\pi}_{c(E \text{ or } T)} = (\Sigma_r F^{rr}_{c(E \text{ or } T)})/2\, \rho_{c(E \text{ or } T)}$, which is independent of the vector potential because of the transversality of the latter. In conclusion, the external electromagnetic potential $\vec{A}_\perp$ enters only in the determination of the axis $\hat{\mathcal{R}}_{c(E \text{ or } T)}$ of the spin frame.

This completes the construction of the effective relative variables and of the effective spin frame using the extra input of the 3-momentum dipole. *In this way we get a description of the two-body cluster as an effective two-body system instead of a pole–dipole system.* The weak point of this description of the open system as an extended object is that, whatever definition of effective center of motion one exploits, the symmetrized momentum dipole $p^{ru}_c + p^{ur}_c$ *does not depend* on the cluster properties *only* but *also* on the external electromagnetic transverse vector potential at the particle positions, as shown by Eq. (5.8). As a consequence the spin frame, or equivalently the three Euler angles associated with the internal spin, depends upon the external fields.

If we accept this drawback, it is reasonable to expect that, taking into account higher multipoles, be possible to give a description of a cluster of $n \geqslant 3$ particles in terms of as many effective n-body systems as effective dynamical body frames following the scheme of Ref. 33.

This would open the possibility of obtaining effective descriptions of two clusters of n_1 and n_2 particles, respectively, and comparing it with the effective description of the cluster composed by the same $n_1 + n_2$ particles. Then it should be possible to find the relations among the three centers of motion of the $(n_1 + n_2)$, n_1, and n_2 clusters and the relative motion of the two n_1 and n_2 clusters. With this in view, adopting *the center of energy as center of motion* seems unavoidable because of the simple composition law (5.14). Whatever choice one adopts, however, it turns out that the relative motion of the two clusters depends on the external fields besides the effective parameters of the clusters.

These techniques can be extended to relativistic perfect fluids, if described in the rest-frame instant form as done in Ref. 1. Moreover, they are needed for the determination of the post-Minkowskian approximation to the quadrupole formula for the emission of gravitational waves (resummation of the post-Newtonian approximations) in the background-independent Hamiltonian linearization of tetrad gravity plus a perfect fluid.[4]

VI. CONCLUSIONS

A relativistic description of open systems like binary stars embedded in the gravitational field would be nowadays an important achievement in view of the construction of templates for the gravitational radiation. Even by approximating such description by means of a multipolar expansion in a way suitable for actually doing either analytical or numerical calculations, a big amount of kinematical technical preliminaries is needed anyway. With this in view, we had in mind to develop methods which could be useful in general relativity with relativistic perfect fluids as matter, where single or binary stars could be described by open fluid subsystems of the isolated system formed by the gravitational field plus the fluid in the rest-frame instant form of either metric or tetrad gravity.[2–4]

To pursue our program, in the present paper we have first of all completed the study of the relativistic kinematics of the system of N free scalar positive-energy particles in the rest-frame instant form of dynamics on Wigner hyperplanes, initiated in Ref. 33.

Then, we have evaluated the energy momentum tensor of the system on the Wigner hyperplane and then determined Dixon's multipoles for the N-body problem with respect to the *internal* 3-center of mass located at the origin of the Wigner hyperplane. For an isolated system most of the existing definitions of a collective centroid identify a unique world line, associated with the internal canonical 3-center of mass. In the rest-frame instant form these multipoles are *Cartesian (Wigner-covariant) Euclidean tensors*. While the study of the *monopole* and *dipole* moments in the rest frame gives information on the mass, the spin and the *internal* center of mass, the *quadrupole* moment provides the only (though not unique) way of introducing the concept of *barycentric tensor of inertia* for extended systems in special relativity.

By exploiting the *canonical spin bases* of Refs. 33 and 50 after the elimination of the internal 3-center of mass ($\vec{q}_+ = \vec{\kappa}_+ = 0$), the Cartesian multipoles $q_T^{r_1 \cdots r_n AB}$ can be expressed in terms of six *orientational* variables (the *spin vector* and the three *Euler angles* identifying the *dynamical body frame*) and of $6N-6$ (*rotational scalar*) *shape* variables, i.e., in terms of the canonical pairs of a canonical spin basis.

Having completed the discussion of the isolated system of N positive energy free scalar particles the formalism has been applied to an isolated system of N positive-energy particles with *mutual action-at-a-distance interactions*. Here again we find a unique world line describing the collective motion of the system.

On the other hand, in the case of an *open* $n < N$ *particle subsystem* of an isolated system consisting of N charged positive-energy particles plus the electromagnetic field a more complex description surfaces. In the rest frame of the isolated system a suitable definition of the energy-momentum tensor of the open subsystem allows to define its *effective mass, 3-momentum, and angular momentum*. However, unlike the case of isolated systems, each centroid putatively describing the *collective centers of motion*, gives rise to a different world line. Starting from the evaluation of the rest-frame Dixon multipoles of the energy-momentum tensor of the open subsystem with respect to various centroids, we get thereby *many candidates for the effective center of motion and the effective intrinsic spin*. Two centroids (viz. the center of energy and Tulczyjew's centroid) stand out because of their specific properties. In the case $n=2$ the pole–dipole description of the two-particle cluster can be replaced by a description of the cluster as an extended system (whose effective spin frame can be evaluated) at the price of introducing an explicit dependence on the cluster in the action of the external electromagnetic field.

Finally, by comparing the effective parameters of an open cluster of n_1+n_2 particles with the effective parameters of the two clusters with n_1 and n_2 particles, it is shown that only the effective *center of energy* can in fact play the role of a useful center of motion,

The kinematical concepts we have defined for closed and open N-body systems are sufficient for the treatment of relativistic continua like relativistic fluids. In Ref. 1 a preliminary extension to closed relativistic fluids is given.

APPENDIX: THE GARTENHAUS–SCHWARTZ TRANSFORMATION

In Ref. 33 we defined canonical internal relative variables with respect to the internal 3-center of mass $\vec{q}_+$ by exploiting a *Gartenhaus–Schwartz* canonical transformation. Let us stress that *while at the nonrelativistic level the transformation is a point-transformation both in the coordinates and the momenta, in the relativistic case we get a point-transformation only in the momenta*.

The canonical generator of the transformation is

$$G = \vec{q}_+ \cdot \vec{\kappa}_+, \tag{A1}$$

so that the finite transformation, depending on a parameter α, on a generic function F on the phase space is

$$F(\alpha) = F + \int_0^\infty d\overline{\alpha}\{F(\overline{\alpha}), G(\overline{\alpha})\}. \tag{A2}$$

In particular we have

$$\lim_{\alpha\to\infty} \vec{\kappa}_+(\alpha) = 0, \quad \lim_{\alpha\to\infty} \vec{q}_+(\alpha) = \infty. \tag{A3}$$

As mentioned in Sec. II, if we define the canonical transformation (2.14), then the quantities

$$\vec{\pi}_{qa} = \lim_{\alpha\to\infty} \vec{\pi}_a(\alpha), \quad \vec{\rho}_{qa} = \lim_{\alpha\to\infty} \vec{\rho}_a(\alpha), \tag{A4}$$

are well defined and the transformation

$$\vec{\eta}_i, \vec{\kappa}_i \to \vec{\kappa}_+, \vec{q}_+, \vec{\rho}_{qa}, \vec{\pi}_{qa}, \tag{A5}$$

is a canonical transformation

$$\{q_+^r, \kappa_+^s\} = \delta^{rs}, \quad \{\rho_{qa}^r, \pi_{qb}^s\} = \delta^{rs}\delta_{ab}, \tag{A6}$$

as said in Eq. (2.13).

The quantities $\vec{\rho}_{qa}, \vec{\pi}_{qa}$ are the searched internal relative variables, they describe the system after the gauge fixing $\vec{q}_+ \approx 0, \vec{\kappa}_+ \approx 0$. We have also

$$\vec{\kappa}_+ \approx 0 \Rightarrow \vec{\rho}_{qa} \approx \vec{\rho}_a, \quad \vec{\pi}_{qa} \approx \vec{\pi}_a. \tag{A7}$$

Thanks to these results, we can calculate a function F independent of $\vec{q}_+$ on the phase space, under the constraint $\vec{\kappa}_+ \approx 0$, by simply performing the limit

$$F|_{\vec{\kappa}_+\approx 0}(\vec{\rho}_{qa}, \vec{\pi}_{qa}) = \lim_{\alpha\to\infty} F(\alpha). \tag{A8}$$

This method is applied in Sec. IV for calculating the multipoles after the gauge fixing $\vec{q}_+ \approx 0, \vec{\kappa}_+ \approx 0$. These multipoles depend on $\vec{\kappa}_i$, so that (see Ref. 33)

$$\lim_{\alpha\to\infty} \vec{\kappa}_i(\alpha) = \sqrt{N} \sum_{a=1}^{N-1} \gamma_{ai} \vec{\pi}_{qa}, \tag{A9}$$

and on $(\vec{\eta}_i - \vec{R}_+)$, so that

$$\vec{\eta}_i - \vec{R}_+ = \sum_j (\vec{\eta}_i - \vec{\eta}_j) \frac{\sqrt{m_j^2 + \vec{\kappa}_j^2}}{\sum_k \sqrt{m_k^2 + \vec{\kappa}_k^2}} = \sum_j \sum_a \sqrt{N}(\gamma_{ai} - \gamma_{aj}) \vec{\rho}_a \frac{\sqrt{m_j^2 + \vec{\kappa}_j^2}}{\sum_k \sqrt{m_k^2 + \vec{\kappa}_k^2}}. \tag{A10}$$

Then using (A9) and (A4) we have

$$\lim_{\alpha\to\infty}(\vec{\eta}_i(\alpha)-\vec{R}_+(\alpha))=\sum_j\sum_a\sqrt{N}(\gamma_{ai}-\gamma_{aj})\vec{\rho}_{qa}\frac{\sqrt{m_j^2+N\Sigma_{ab}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}\gamma_{aj}\gamma_{bj}}}{\Sigma_k\sqrt{m_k^2+N\Sigma_{ab}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}\gamma_{ak}\gamma_{bk}}}. \tag{A11}$$

The following notation is used to denote the limits (A8):

$$F\to_{\alpha\to\infty}F|_{\vec{\kappa}_+\approx 0}(\vec{\rho}_{qa},\vec{\pi}_{qa}). \tag{A12}$$

For example, Eqs. (A9) and (A11) become

$$\vec{\kappa}_i\to_{\alpha\to\infty}\sqrt{N}\sum_{a=1}^{N-1}\gamma_{ai}\vec{\pi}_{qa},$$

$$\vec{\eta}_i-\vec{R}_+\to_{\alpha\to\infty}\sum_j\sum_a\sqrt{N}(\gamma_{ai}-\gamma_{aj})\vec{\rho}_{qa}\frac{\sqrt{m_j^2+N\Sigma_{ab}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}\gamma_{aj}\gamma_{bj}}}{\Sigma_k\sqrt{m_k^2+N\Sigma_{ab}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}\gamma_{ak}\gamma_{bk}}}. \tag{A13}$$

The closed form (A16)–(A18) of the canonical transformation (A5) was not given in Ref. 33, but it can derived from the following two equations of that paper [its Eq. (5.13) and (5.24)]:

$$\vec{\pi}_a(\alpha)=\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\gamma_{ai}\vec{\kappa}_i(\alpha),$$

$$\begin{aligned}\vec{\pi}_{qa}&\overset{\text{def}}{=}\vec{\pi}_a(\infty)=\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\vec{\kappa}_i(\infty)\\&=\vec{\pi}_a+\frac{\vec{n}_+}{\mathcal{M}}[(M_{\text{sys}}-\mathcal{M})\vec{n}_+\cdot\vec{\pi}_a-|\vec{\kappa}_+|H_a]\\&=\vec{\pi}_a-\frac{\vec{\kappa}_+}{\sqrt{M_{\text{sys}}^2-\vec{\kappa}_+^2}}\left[H_a-\frac{M_{\text{sys}}-\sqrt{M_{\text{sys}}^2-\vec{\kappa}_+^2}}{\vec{\kappa}_+^2}\vec{\kappa}_+\cdot\vec{\pi}_a\right]\approx\vec{\pi}_a,\end{aligned}$$

$$H_a=\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\gamma_{ai}H_i=\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\gamma_{ai}\sqrt{m_i^2+\vec{\kappa}_i^2},$$

$$\vec{\kappa}_i(\infty)=\sqrt{N}\sum_{a=1}^{N-1}\gamma_{ai}\vec{\pi}_{qa},$$

$$H_{(\text{rel})i}=H_i(\infty)=\sqrt{m_i^2+N\sum_{ab}^{1\ldots N-1}\gamma_{ai}\gamma_{bi}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}},$$

$$M_{\text{sys}}=\sum_{i=1}^{N}H_i=\sqrt{\mathcal{M}^2+\vec{\kappa}_+^2}\approx H_{(\text{rel})}=H_M(\infty)=\mathcal{M}=\sum_{i=1}^{N}H_i(\infty)=\sum_{i=1}^{N}\sqrt{m_i^2+N\sum_{ab}^{1\ldots N-1}\gamma_{ai}\gamma_{bi}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}}, \tag{A14}$$

$$\vec{\rho}_{qa} \overset{\text{def}}{=} \vec{\rho}_a(\infty) = \vec{\rho}_a - \sum_{i,j=1}^{N} \sum_{b=1}^{N-1} \gamma_{aj}(\gamma_{bi} - \gamma_{bj}) \frac{H_i}{M_{\text{sys}}} \left[\frac{|\vec{\kappa}_+| \vec{\kappa}_j(\infty)}{H_j(\infty)\sqrt{\Pi}} + \left(\frac{M_{\text{sys}}}{\sqrt{\Pi}} - 1 \right) \vec{n}_+ \right] \vec{n}_+ \cdot \vec{\rho}_b$$

$$= \vec{\rho}_a - \sum_{i,j=1}^{N} \sum_{b=1}^{N-1} \gamma_{aj}(\gamma_{bi} - \gamma_{bj}) \frac{H_i}{M_{\text{sys}}} \frac{\vec{\kappa}_j(\infty)}{H_j(\infty)\sqrt{\Pi}} \vec{\kappa}_+ \cdot \vec{\rho}_b \approx \vec{\rho}_a. \tag{A15}$$

Let us end by giving the explicit expression of the second canonical transformation (2.13). By using Eqs. (A14) and (A15) we get the following results.

(1) For $N=2(\gamma_{11}=-\gamma_{12}=1/\sqrt{2})$ we have

$$\vec{\eta}_1 = \vec{\eta}_+ + \tfrac{1}{2}\vec{\rho}, \quad \vec{\kappa}_1 = \tfrac{1}{2}\vec{\kappa}_+ + \vec{\pi},$$

$$\vec{\eta}_2 = \vec{\eta}_+ - \tfrac{1}{2}\vec{\rho}, \quad \vec{\kappa}_2 = \tfrac{1}{2}\vec{\kappa}_+ - \vec{\pi},$$

$$\vec{\eta}_+ = \tfrac{1}{2}(\vec{\eta}_1 + \vec{\eta}_2), \quad \vec{\kappa}_+ = \vec{\kappa}_1 + \vec{\kappa}_2,$$

$$\vec{\rho} = \vec{\eta}_1 - \vec{\eta}_2, \quad \vec{\pi} = \tfrac{1}{2}(\vec{\kappa}_1 - \vec{\kappa}_2),$$

$$\vec{J} = \vec{\eta}_1 \times \vec{\kappa}_1 + \vec{\eta}_2 \times \vec{\kappa}_2 = \vec{\eta}_+ \times \vec{\kappa}_+ + \vec{S} = \vec{q}_+ \times \vec{\kappa}_+ + \vec{S}_q, \quad \vec{S} = \vec{\rho} \times \vec{\pi}, \quad \vec{S}_q = \vec{\rho}_q \times \vec{\pi}_q,$$

$$\vec{R}_+ = \frac{\sqrt{m_1^2 + \vec{\kappa}_1^2}\,\vec{\eta}_1 + \sqrt{m_2^2 + \vec{\kappa}_2^2}\,\vec{\eta}_2}{\sqrt{m_1^2 + \vec{\kappa}_1^2} + \sqrt{m_2^2 + \vec{\kappa}_2^2}} = \vec{\eta}_+ + \frac{1}{2}\frac{\sqrt{m_1^2 + \vec{\kappa}_1^2} - \sqrt{m_2^2 + \vec{\kappa}_2^2}}{\sqrt{m_1^2 + \vec{\kappa}_1^2} + \sqrt{m_2^2 + \vec{\kappa}_2^2}}\vec{\rho},$$

$$\vec{q}_+ = \vec{R}_+ + \frac{\vec{S}_q \times \vec{\kappa}_+}{(\sqrt{m_1^2 + \vec{\kappa}_1^2} + \sqrt{m_2^2 + \vec{\kappa}_2^2})\left(\sqrt{m_1^2 + \vec{\kappa}_1^2} + \sqrt{m_2^2 + \vec{\kappa}_2^2} + \sqrt{(\sqrt{m_1^2 + \vec{\kappa}_1^2} + \sqrt{m_2^2 + \vec{\kappa}_2^2})^2 - \vec{\kappa}_+^2}\right)}. \tag{A16}$$

Then after some straightforward algebra we get (note that in Ref. 33 we used the notation $M_{(\text{free})}=M_{\text{sys}}$ and $\mathcal{M}^2_{(\text{free})}=\Pi$)

$$\sqrt{m_i^2 + \vec{\kappa}_i^2} = \frac{1}{2}\sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}_+^2}\left(1 + (-)^{i+1}\frac{m_1^2 - m_2^2}{\mathcal{M}^2_{(\text{free})}}\right) + (-)^{i+1}\frac{\vec{\pi}_q \cdot \vec{\kappa}_+}{\mathcal{M}_{(\text{free})}},$$

$$M_{(\text{free})} = \sqrt{m_1^2 + \vec{\kappa}_1^2} + \sqrt{m_2^2 + \vec{\kappa}_2^2} = \sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}_+^2} \approx \mathcal{M}_{(\text{free})} \overset{\text{def}}{=} \sqrt{m_1^2 + \vec{\pi}_q^2} + \sqrt{m_2^2 + \vec{\pi}_q^2},$$

$$\sqrt{m_1^2 + \vec{\kappa}_1^2} - \sqrt{m_2^2 + \vec{\kappa}_2^2} = \frac{2\vec{\pi}_q \cdot \vec{\kappa}_+}{\mathcal{M}_{(\text{free})}} + \frac{m_1^2 - m_2^2}{\mathcal{M}^2_{(\text{free})}}\sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}_+^2} \overset{\text{def}}{=} E,$$

$$\vec{\pi} = \vec{\pi}_q + \frac{\vec{\kappa}_+}{\mathcal{M}_{(\text{free})}\sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}_+^2}}\left[\vec{\pi}_q \cdot \vec{\kappa}_+\left(1 - (\sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}_+^2} - \mathcal{M}_{(\text{free})})\frac{\mathcal{M}_{(\text{free})}}{\vec{\kappa}_+^2}\right)\right.$$

$$\left. + (m_1^2 - m_2^2)\sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}_+^2}\right] \overset{\text{def}}{=} \vec{\pi}_q + F\vec{\kappa}_+,$$

$$\vec{\rho} = \vec{\rho}_q - \frac{A}{B}\frac{\vec{\kappa}_+ \cdot \vec{\rho}_q \vec{\pi}_q}{\mathcal{M}_{(\text{free})}\sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}^2_+}} \stackrel{\text{def}}{=} \vec{\rho}_q + C\vec{\pi}_q,$$

$$A = \frac{\sqrt{m_1^2 + \vec{\kappa}_1^2}}{\sqrt{m_2^2 + \vec{\pi}_q^2}} + \frac{\sqrt{m_2^2 + \vec{\kappa}_2^2}}{\sqrt{m_1^2 + \vec{\pi}_q^2}}, \quad B = 1 + \frac{A\vec{\pi}_q \cdot \vec{\kappa}_+}{\mathcal{M}_{(\text{free})}\sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}^2_+}},$$

$$\vec{\pi}_q = \vec{\pi} - \frac{\vec{\kappa}_+}{\sqrt{M^2_{(\text{free})} - \vec{\kappa}^2_+}}\left(\frac{1}{2}(\sqrt{m_1^2 + \vec{\kappa}_1^2} - \sqrt{m_2^2 + \vec{\kappa}_2^2}) - \frac{\vec{\kappa}_+ \cdot \vec{\pi}}{\vec{\kappa}^2_+}[M_{(\text{free})} - \sqrt{M^2_{(\text{free})} - \vec{\kappa}^2_+}]\right) \stackrel{\text{def}}{=} \vec{\pi} - D\vec{\kappa}_+,$$

$$\vec{\rho}_q = \vec{\rho} + \frac{A\vec{\kappa}_+ \cdot \vec{\rho}}{M_{(\text{free})}\sqrt{M^2_{(\text{free})} - \vec{\kappa}^2_+}}\vec{\pi}_q,$$

$$\vec{S}_q = \vec{S} - D\vec{\rho} \times \vec{\kappa}_+,$$

$$\vec{q}_+ = \vec{R}_+ + G\vec{S}_q \times \vec{\kappa}_+,$$

$$G = \frac{1}{M_{(\text{free})}(M_{(\text{free})} + \sqrt{M^2_{(\text{free})} - \vec{\kappa}^2_+})} = \frac{1}{\sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}^2_+}(\sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}^2_+} + \mathcal{M}_{(\text{free})})},$$

$$\vec{\eta}_+ = \vec{q}_+ - \frac{E}{2\sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}^2_+}}[\vec{\rho}_q + C\vec{\pi}_q] - G\vec{S}_q \times \vec{\kappa}_+,$$

$$\vec{\eta}_i = \vec{q}_+ + \frac{1}{2}\left((-)^{i+1} - \frac{E}{\sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}^2_+}}\right)(\vec{\rho}_q + C\vec{\pi}_q) - G\vec{S}_q \times \vec{\kappa}_+,$$

$$\vec{\kappa}_i = \left(\tfrac{1}{2} + (-)^{i+1}F\right)\vec{\kappa}_+ + (-)^{i+1}\vec{\pi}_q. \tag{A17}$$

(2) For $N > 2$ the results concerning the coordinates (and also $\vec{q}_+$) are much more involved due to the complexity of Eqs. (A15) so that we give only the following results for the momenta:

$$M(\text{free}) = \sum_i \sqrt{m_i^2 + \vec{\kappa}_i^2} = \sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}^2_+} \approx \mathcal{M}_{(\text{free})} = \sum_i \sqrt{m_i^2 + N\sum_{ab} \gamma_{ai}\gamma_{bi}\vec{\pi}_{qa} \cdot \vec{\pi}_{qb}},$$

$$\sqrt{m_i^2 + \vec{\kappa}_i^2} = \frac{1}{\mathcal{M}_{(\text{free})}}\left(\sqrt{N}\sum_a \gamma_{ai}\vec{\kappa}_+ \cdot \vec{\pi}_{qa} + \sqrt{m_i^2 + N\sum_{ab} \gamma_{ai}\gamma_{bi}\vec{\pi}_{qa} \cdot \vec{\pi}_{qb}}\sqrt{\mathcal{M}^2_{(\text{free})} + \vec{\kappa}^2_+}\right),$$

$$\vec{\kappa}_i = \frac{\vec{\kappa}_+}{N} + \sqrt{N}\sum_a \gamma_{ai}\left[\vec{\pi}_{qa} + \left(\frac{M_{(\text{free})}}{\mathcal{M}_{(\text{free})}} - 1\right)\frac{\vec{\kappa}_+ \cdot \vec{\pi}_{qa}}{\vec{\kappa}^2_+}\vec{\kappa}_+ + \frac{\vec{\kappa}_+}{\mathcal{M}_{(\text{free})}\sqrt{N}}\sum_i \gamma_{ai}\sqrt{m_i^2 + N\sum_{ab} \gamma_{ai}\gamma_{bi}\vec{\pi}_{qa} \cdot \vec{\pi}_{qb}}\right]. \tag{A18}$$

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On asymptotic Hopf invariant for Hamiltonian systems

Mikhail V. Deryabin
The Mads Clausen Institute, Syddansk Universitet, Sønderborg, DK 6400, Denmark and Department of Mechanics and Mathematics, Moscow State University, 119992 Moscow, Russia

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We give a definition and discuss main properties of the asymptotic Hopf invariant, or helicity, for Hamiltonian systems. The definition relies on a technical construction which is a definition of a relative Hopf invariant for divergence-free vector fields in multiconnected domains of the following type: (flat domain in $\mathbb{R}^2$) $\times$(circle). We prove correctness of the definitions, and discuss ergodic interpretation of the Hamiltonian Hopf invariant, together with its relation with the Calabi invariant. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1904511]

I. INTRODUCTION

The asymptotic Hopf invariant, or helicity of a divergence-free vector field (which, for example, can be a magnetic field) is an invariant, known in fluid dynamics and plasma physics. Being an invariant means that the helicity integral is preserved under an action on the vector field by an arbitrary volume-preserving diffeomorphism. Helicity was introduced in Refs. 14 and 15 and has been widely studied thereafter, see e.g., Ref. 3. One of the important applications of helicity is that it provides a lower bound for the magnetic energy, see, e.g., Ref. 5, and we also refer to Ref. 9 for explicit estimates for the lower bound for the energy, as well as a discussion of the geometry of the extremal vector fields.

We briefly remind the definition of helicity see, e.g., Ref. 3. Let M be a simply connected three-dimensional Riemannian manifold with boundary ∂M, let a 3-form μ be a volume form on M, and let ξ be a divergence-free vector field on M, tangent to the boundary ∂M. Consider a 2-form $\Omega_\xi = i_\xi \mu$. As M is simply connected, the form Ω_ξ is exact.

By definition, the *asymptotic Hopf invariant*, or *helicity* of the field ξ on M is an integral

$$\mathcal{H}(\xi) = \int_M \Omega_\xi \wedge d^{-1}\Omega_\xi. \tag{1}$$

Topological properties of helicity were discovered in Ref. 2, given a vector field on a three-dimensional simply connected domain, its helicity measures the average linking of the trajectories of this field. This property is also referred to as *ergodic*, as the proofs rely on Birkhoff's ergodic theorem. The topological description has also been generalized to higher dimensions, see, e.g., Refs. 16, 12, 13, and 6.

It is natural to try to extend the asymptotic Hopf invariant to Hamiltonian systems, indeed, one notices that in the extended phase space, a Hamiltonian vector field is a *curl* of a 1-form $p\,\mathrm{d}q - H\,\mathrm{d}t$, see, e.g., Ref. 1. Thus one can at least formally write down the same helicity integral as (1) (see Ref. 10). The problem is that Hamiltonian systems have no bounded simply connected invariant manifolds in the extended phase space (while multiconnected invariant manifolds certainly exist, for example, KAM-tori in Hamiltonian systems, close to integrable ones), while the asymptotic Hopf invariant does not exist for vector fields on multi-connected manifolds.[3]

First we define a *relative* Hopf invariant and a relative cross-helicity invariant for divergence-free vector fields in multiconnected domains of the type (flat domain in $\mathbb{R}^2$) $\times$(circle). Note that the simplest multiconnected manifold, invariant for a Hamiltonian system, is a solid torus, and it is clearly of the above type. The invariant we define describes the asymptotic linking of trajectories of these vector fields for some proper embedding of this domain into a sphere, assuming that

the domain itself is unlinked. We also discuss generalizations, when linking of the domain itself can be nontrivial. Then we consider Hamiltonian systems and discuss the relation of this invariant with the Calabi invariant.[8]

II. THE RELATIVE HOPF INVARIANT

As noted above, for vector fields in multiconnected manifolds (i.e., with nontrivial first homology group) there is no asymptotic Hopf invariant, the value of the integral (1) depends on a choice of a potential 1-form $d^{-1}\Omega_\xi$. We show that this choice can be made in some natural way for one case, important for applications.

Let a set V be a direct product of a circle (base) S^1 and a ring $R^2 \in \mathbb{R}^2$. Let μ be a volume 3-form, and let ξ be a divergence-free vector field, tangent to the boundary ∂V. Consider a 2-form $\Omega^2_\xi = i_\xi \mu$. This form is closed, since ξ is divergence-free (thus the Lie derivative $L_\xi \mu = d i_\xi \mu = 0$), and one can see that it is also exact (thus any divergence-free field tangent to the boundary ∂V is *null-homologious*). Indeed, the 2-cycle, on which the values of closed 2-forms are defined, is a two-torus, obtained by shrinking the ring R^2 to a circle. Integral of any closed 2-form over this torus equals the integral over any component of the boundary. But our 2-form Ω^2_ξ is identically zero on the boundary ∂V, as the field ξ is tangent to it.

We assume that in polar coordinates r, ϕ (mod 2π) the ring R^2 is given by $r \in [r_1, r_2]$. We take r, ϕ (mod 2π), t (mod 2π) as local coordinates on V.

Let γ_1 be a closed curve on the boundary ∂V, given by conditions $t = \text{const}$, $r = r_1$, and let a closed curve γ_2 be given by condition $\phi = \text{const}$, $r = r_2$.

We *choose* a 1-form $\omega^1_\xi = d^{-1}\Omega^2_\xi$ such that

$$\int_{\gamma_1} \omega^1_\xi = 0, \quad \int_{\gamma_2} \omega^1_\xi = 0. \tag{2}$$

Note that conditions (2) define a coset of 1-forms $[\omega^1_\xi]$, i.e., a 1-form modulo differential (as they define the values of a 1-form ω^1 on the fundamental group).

Definition 1: We call an integral

$$\mathcal{H}(\xi) = \int_V \Omega^2_\xi \wedge \omega^1_\xi,$$

a *relative Hopf invariant for the field ξ in V*.

Let another divergence-free vector field η be given on V, also being tangent to the boundary ∂V.

Definition 2: We call an integral

$$\mathcal{H}(\xi, \eta) = \int_V \Omega^2_\xi \wedge \omega^1_\eta,$$

where 1-form ω^1_η satisfies condition (2), a *relative cross-helicity of the fields ξ, η*. This choice of the potential 1-form is explained by the following crucial observation.

Assume that V is embedded into a sphere S^3, V is unlinked, and assume that the volume form $\mu = r\, \mathrm{d}r \wedge \mathrm{d}\phi \wedge \mathrm{d}t$. Let $r = r_1$, $\xi = (0,1,0)$ on the inner component of the boundary, and $r = r_2$, $\xi = (0,0,1)$ on the outer component.

Consider a set $\tilde{V} = \tilde{R}^2 \times S^1$, where the ring $\tilde{R}^2 \in \mathbb{R}^2$ is given by condition $r \in [\tilde{r}_1, \tilde{r}_2]$, where $r_1 > \tilde{r}_1$ and $r_2 < \tilde{r}_2$. We continue the volume form μ and the field ξ on $\tilde{V}$ (where the same local coordinates can be introduced as above) such, that μ remains the same, while $\xi \equiv (0,1,0)$ at $r < r_1$ and $\xi \equiv (0,0,1)$ at $r > r_2$.

As none of the trajectories of the field ξ in the domain $\tilde{V}\backslash V$ is linked with the trajectories of the field ξ in the domain $\tilde{V}$, we should expect that for a well-defined invariant, the relative helicities in domains V and $\tilde{V}$ are equal.

Proposition 1: Integrals

$$\int_V \Omega_\xi^2 \wedge \omega_\xi^1 = \int_{\tilde{V}} \Omega_\xi^2 \wedge \omega_\xi^1$$

for any $\tilde{r}_1$, $\tilde{r}_2$ *if and only if conditions* (2) *are satisfied.*

Proof: We consider the case when $\tilde{r}_1 = r_1$, $\tilde{r}_2 \neq r_2$, the general case is similar. In the domain $\tilde{V}\backslash V$, the 2-form $\Omega_\xi^2 = r\,\mathrm{d}r \wedge \mathrm{d}\phi$, thus $\omega_\xi^1 = (r^2/2 + f(\phi))\mathrm{d}\phi + g(t)\mathrm{d}t$ for some 2π-periodic functions f, g. Condition (2) means that $\int_0^{2\pi} g(t)\mathrm{d}t = 0$. However, this integral is zero if and only if

$$\int_{\tilde{V}\backslash V} \Omega_\xi^2 \wedge \omega_\xi^1 = \pi(\tilde{r}_2^2 - r_2^2) \int_0^{2\pi} g(t)\mathrm{d}t = 0.$$

□

Remarks: The condition for the ring R^2 being *flat* is of uttermost importance, if we drop this condition, then for different embeddings of the ring into $\mathbb{R}^2$ the same vector field may have different asymptotic linkings. A fiber can be more complicated, say, a disk with some number of holes, and the set V itself can be a nontrivial fibration over S^1. One can show that still any divergence-free vector field, tangent to the boundary, is null-homologious, as the corresponding 2-form is zero on every component of the boundary. As the fundamental group becomes more complicated, the number of conditions of the type (2) will grow.

It follows from Proposition 1 that condition (2) is *necessary* such that the relative Hopf invariant could be equal to asymptotic linking of the trajectories under an "appropriate" embedding of the set V into S^3, namely, the boundary torus should not be linked and the measure should be continued to the whole sphere. One can prove that this condition is also *sufficient*, say, by realizing this embedding. Instead, we demonstrate in an example that under our choice of a coset $[\omega_\xi^1]$ the relative Hopf invariant equals the asymptotic linking of the vector field ξ.

Let the field ξ be the Hopf vector field on a sphere S^3, in coordinates $x_1, x_2, x_3, x_4 \in \mathbb{R}^4$, where the sphere is given by relation $x_1^2 + x_2^2 + x_3^2 + x_4^2 = 1$, it is given by $\xi = (x_2, -x_1, x_4, -x_3)$.

Consider a solid torus V, $x_1^2 + x_2^2 \leqslant a^2$. We introduce local coordinates in the solid torus V [x_1, x_2, t (mod 2π)]. In these coordinates the Hopf field is $\xi = (x_2, -x_1, 1)$. As the volume form we take, as above, the 3-form $\mu = \mathrm{d}x_1 \wedge \mathrm{d}x_2 \wedge \mathrm{d}t$.

Proposition 2: Asymptotic linking of the Hopf field in the solid torus $x_1^2 + x_2^2 \leqslant a^2$, $a^2 < 1$ *equals the relative Hopf invariant* $\mathcal{H}(\xi)$.

Proof: The asymptotic linking of any two trajectories equals $1/4\pi^2$, see Ref. 3, example 4.5, the linking number for any two trajectories is 1, and all trajectories are periodic with the period 2π. Thus the asymptotic linking of the Hopf field in the solid torus V equals $\lambda_\xi = \mathrm{vol}(V)^2/4\pi^2 = \pi^2 a^4$. Now one can check by direct calculation that $\mathcal{H}(\xi) = \pi^2 a^4 = \lambda_\xi$. □

Remark: The asymptotic Hopf invariant for a vector field in a solid torus is usually calculated inserting the solid torus into a three-dimensional sphere, and setting the field being zero outside of the solid torus, see, e.g., Ref. 3 (as above the boundary torus should not be linked itself). However the *integral form* of such an invariant with condition (2) to the best of our knowledge has not been used before.

III. CORRECTNESS OF DEFINITIONS

Having justified the choice of the potential 1-forms, we now prove that the definitions above are consistent.

Lemma 1: The values of the relative Hopf invariant and the relative cross-helicity do not depend on a choice of 1-forms ω_ξ^1, ω_η^1, *that satisfy condition* (2).

Proof: Conditions (2) define a coset of 1-forms $[\omega^1]$, i.e., if $\omega^1+\alpha^1=d^{-1}\Omega^2$, then α^1 is exact. Now, the integral

$$\int_V \Omega^2 \wedge \alpha^1 = \int_V d(F\Omega^2) = \int_{\partial V} F\Omega^2 = 0.$$

□

From Lemma 1 we have the following.

Theorem 1: The relative Hopf invariant and the relative cross-helicity do not change under the action on the fields ξ, η of a volume-preserving diffeomorphism that maps the boundary ∂V on itself.

Proof: By Lemma 1, the definition of the integral $\mathcal{H}$ is invariant under coordinate transformations. □

Let now two divergence-free fields ξ_1, ξ_2 be given.

Theorem 2: Relative cross-helicities are symmetric, $\mathcal{H}(\xi_1,\xi_2)=\mathcal{H}(\xi_2,\xi_1)$.

Proof: We denote the 2-forms $\Omega_i^2=i_{\xi_i}\mu$, $\omega_i^1=d^{-1}\Omega_i^2$, $i=1,2$. Let, as above, r,ϕ,t be the coordinates in V, and let the volume form be $\mu=r\,\mathrm{d}r\wedge\mathrm{d}\phi\wedge\mathrm{d}t$ (note that this can be done by a variable change).

We first note that cross-helicities for an arbitrary field ξ and fields $\eta=(0,1,0)$ [and thus $\eta^*=(0,0,1)$] are symmetric. Proof relies on direct computation, one just has to check that

$$\int_V \Omega_\xi^2 \wedge \omega_\eta^1 - \int_V \Omega_\eta^2 \wedge \omega_\xi^1 = \int_{\partial V} \omega_\xi^1 \wedge \omega_\eta^1 = 0.$$

We next prove the following.

Lemma 2: Suppose that the integrals of the 2-forms Ω_1^2 and Ω_2^2 are equal over the surfaces $\Sigma_t=\{t=0\}$ and $\Sigma_\phi=\{\phi=0\}$. Then relative cross-helicities of the fields ξ_1 and ξ_2 are symmetric.

Proof of Lemma 2: Consider a 1-form $\omega_1^1-\omega_2^1$ on the boundary ∂V, which consists of two tori, $\partial V_1=\{r=r_1\}$ and $\partial V_2=\{r=r_2\}$. This form is closed, as each of the 2-forms Ω_1^2 and Ω_2^2 equal zero on both components of the boundary ∂V. Besides, the value of the 1-form $\omega_1^1-\omega_2^1$ on cycles γ_1, γ_2 is zero [by condition (2)], and on cycles $\sigma_1=\partial\Sigma_t\setminus\gamma_1$, $\sigma_2=\partial\Sigma_\phi\setminus\gamma_2$ is zero by the condition of the lemma. Thus the 1-form $\omega_1^1-\omega_2^1$ is *exact* both on ∂V_1 and ∂V_2. But the integral

$$\int_{\partial V} \omega_1^1 \wedge \mathrm{d}F = -\int_{\partial V} d(F\omega^1) = 0$$

for any function F. Thus,

$$\int_V \Omega_1^2 \wedge \omega_2^1 - \int_V \Omega_2^2 \wedge \omega_1^1 = 0.$$

To prove the theorem in the general case, it is sufficient to represent the field ξ_2 as a sum, $\xi_2=\xi_2^*+\eta_1+\eta_2$ where the fields $\eta_1=(0,0,c_1)$, $\eta_2=(0,c_2,0)$, $c_{1,2}=\mathrm{const}$ are such that the fields ξ_1 ξ_2^* satisfy condition of Lemma 2. □

Remark: The above results remain true if one replaces zero in the *second* condition (2) by an arbitrary constant,

$$\int_{\gamma_2} \omega^1 = k.$$

This can be done to relate the relative Hopf invariant with the asymptotic linking of the vector field, realizing nontrivial embeddings of the solid torus into the sphere S^3 (note that in Proposition 2 this embedding was trivial).

IV. THE HOPF INVARIANT FOR HAMILTONIAN SYSTEMS

Let M be a smooth $2n$-dimensional *exact* symplectic manifold (possibly unbounded). The condition for M to be exact means, that the symplectic 2-form Ω^2 is globally a differential of some 1-form. For example, one can consider cotangent bundles with a natural symplectic structure, see, e.g., Ref. 1.

Let p,q be local coordinates on M: $\Omega^2=\mathrm{d}p\wedge\mathrm{d}q$. Consider a Hamiltonian system that is given by a function $H(p,q,t)$, that is 2π-periodic in time t, on the extended phase space $M\times S^1$ $[t\ (\mathrm{mod}\ 2\pi)\in S^1]$. The corresponding Hamiltonian vector field in the extended phase space $\xi=(-\partial H/\partial q,\partial H/\partial p,1)$ annihilates the 2-form $\Omega_H=\Omega^2-\mathrm{d}H\wedge\mathrm{d}t$, $i_\xi\Omega_H=0$. Hamilton's equations are written in the standard form

$$\dot{p}=-\frac{\partial H}{\partial q},\quad \dot{q}=\frac{\partial H}{\partial p}. \tag{3}$$

Let a 1-form $\omega_H=d^{-1}\Omega_H$. In local coordinates p,q one can write it as $\omega_H=p\,\mathrm{d}q-H\,\mathrm{d}t$. The form ω_H is defined globally on $M\times S^1$, up to a closed 1-form. Note that having a Hamiltonian vector field, the corresponding Hamilton function cannot be uniquely reconstructed either, for example, add a constant to the function H, and the values of the 1-form ω_H 1-cycles will be changed.

Let, as above, $V\subset M\times S^1$ be a direct product of a ring and a circle, $V=R^2\times S^1$, $R^2\subset M$ is a 2-disk, $S^1=\{t\ (\mathrm{mod}\ 2\pi)\}$. Assume that V is an invariant set for the Hamiltonian system (3). Then on the boundary ∂V the 2-form $\Omega_H=0$. These invariant sets exist in Hamiltonian systems with one-and-a-half degrees of freedom, both integrable ones and close to integrable. We will assume that the restriction of the symplectic 2-form to R^2 is nondegenerate.

We define a coset of 1-forms $[\omega_H]$ by the following conditions:

$$\int_{\gamma_1}\omega_H=0,\quad \int_{\gamma_2}\omega_H=0, \tag{4}$$

where $\gamma_{1,2}\in\partial V$ are the cycles defined for conditions (2) in Sec. II.

Definition 3: We call an integral

$$\mathcal{H}(H)=\int_V\omega_H\wedge\Omega_H,$$

where ω_H satisfies condition (4), an *asymptotic Hopf invariant for the Hamiltonian vector field* with a Hamiltonian H.

Definition 4: An integral

$$\mathcal{H}(H,F)=\int_V\omega_H\wedge\Omega_F,$$

where ω_H, ω_F satisfies condition (4), will be referred to as a *cross-helicity of Hamiltonian vector fields* with Hamiltonians H, F.

Remarks: Instead of the volume form μ we use here the 3-form $\mu=\mathrm{d}p\wedge\mathrm{d}q\wedge\mathrm{d}t$. As in Sec. II, one can define the Hamiltonian Hopf invariants for fibrations over a circle with multiconnected fibers.

As a consequence of the corresponding results for the relative Hopf invariant (Sec. III), we get their symplectic versions.

Theorem 3: The values $\mathcal{H}(H)$, $\mathcal{H}(H,F)$ do not depend on a choice of the 1-form ω_H from the coset $[\omega_H]$, and they are invariant under symplectic diffeomorphisms, given by a single-valued generating function on V and sending the boundary to itself.

Proof: Take an invariant 3-form $\mu=\mathrm{d}p\wedge\mathrm{d}q\wedge\mathrm{d}t$, then $\Omega_H=i_\xi\mu$ and we can use Theorem 1. Note that since under symplectic coordinate transformation $p,q\to P=P(p,q,t)$, $Q=Q(p,q,t)$ with a generating function S the new Hamiltonian equals $H_1(P,Q,t)=H(p(P,Q,t),q(P,Q,t),t)$

$+\partial S/\partial t$, the 1-form ω_H will become $p\,\mathrm{d}q - H\,\mathrm{d}t = P\,\mathrm{d}Q - H_1\,\mathrm{d}t + dS(P,Q,t)$. Thus the form $P\,\mathrm{d}Q - H_1\,\mathrm{d}t$ belongs to the same coset $[\omega_H]$ and the value of the integral

$$\mathcal{H} = \int_V (P\,\mathrm{d}Q - H_1\,\mathrm{d}t) \wedge (\mathrm{d}P \wedge \mathrm{d}Q - \mathrm{d}H_1 \wedge \mathrm{d}t)$$

does not change. In a similar way, the integral $\mathcal{H}(H,F)$ can be treated. □

Corollary: The Hamiltonian Hopf invariant $\mathcal{H}(H)$ is a symplectic invariant of the Hamiltonian system with the Hamiltonian H.

The comparison of these two systems must be done in the following way. Let us compare two systems with invariant domains D_1^2 and D_2^2 (homotopically equivalent, i.e., disks with the same number of holes) in the phase space M, such that the areas of these domains coincide. Then, if the Hamiltonian Hopf invariants for these two systems are different, the systems are not symplectomorphic.

Remark: This invariant is finer than, say, the topological invariants of integrable Hamiltonian systems:[7] for example, it separates systems with proportional Hamiltonians, even if the relation of the Hamiltonians is a constant. This is clear from the invariant construction: as the Hamiltonian is multiplied by a constant, an asymptotic linking of the trajectories is changed.

An immediate corollary of Theorem 2 is the following.

Theorem 4: Hamiltonian cross-helicities are symmetric, $\mathcal{H}(H,F) = \mathcal{H}(F,H)$.

Note that both integrals of the 2-forms Ω_H, Ω_F upon the section $\Sigma = \{t=0\}$ are equal to the sum of the areas of the projection of Σ to 2-planes p_i, q_i.

V. THE HAMILTONIAN HOPF INVARIANT AND THE CALABI INVARIANT

The choice of condition (4) makes it possible to give a simple form for the relation of the asymptotic linking invariant in a solid torus with the Calabi invariant.[8]

We first remind the definition of the Calabi invariant. Let ϕ be a symplectic diffeomorphism of the 2-disk D^2, equipped with an area form μ, identical near the boundary ∂D. Take a 1-form α, such that $\mu = \mathrm{d}\alpha$. As the 1-form $\phi^*\alpha - \alpha$ is closed and vanishes near the boundary, there is a function $h(\phi): D^2 \to \mathbb{R}$, which vanishes near the boundary ∂D and satisfies

$$\mathrm{d}h(\phi) = \phi^*\alpha - \alpha.$$

By definition, the *Calabi invariant* of the area-preserving diffeomorphism ϕ is the integral,

$$\int_{D^2} h(\phi)\mu,$$

see Ref. 11. This definition also extends to higher dimensions, see, e.g., Ref. 3.

One can show[3] that, provided the symplectic diffeomorphism ϕ is defined by a Poincaré mapping of a period 2π for a Hamiltonian system (3), the Calabi invariant equals

$$2n \int_0^{2\pi} \int_{D^{2n}} H(p,q,t)(\Omega^2)^n\,\mathrm{d}t.$$

We will see that it is the latter definition that provides the relation of the Calabi invariant with the relative asymptotic Hopf invariant.

Let V be a solid torus.

Proposition 3: Let the differential dH be identically zero in a neighborhood of the boundary ∂V. Then under condition (4) the Hamiltonian Hopf invariant $\mathcal{H}$ equals (minus) the Calabi invariant of the symplectic diffeomorphism of the 2-disk $D^2 \subset M$, defined by a Poincaré mapping of a period 2π for the Hamiltonian system (3).

Proof: Assume first that the dimension $\dim M = 2$. Let the differential $\mathrm{d}H$ be identically zero in

a neighborhood of the boundary ∂V. Then $H=\text{const}$ on ∂V. Condition (4) means that this constant must be equal to zero. Consider now an integral

$$\mathcal{H} = \int_V \omega_H \wedge \Omega_H = -\int_V H\,\mathrm{d}p \wedge \mathrm{d}q \wedge \mathrm{d}t - \int_V p\,\mathrm{d}q \wedge \mathrm{d}H \wedge \mathrm{d}t = -2\int_V H\,\mathrm{d}p \wedge \mathrm{d}q \wedge \mathrm{d}t + \int_{\partial V} Hp\,\mathrm{d}q \wedge \mathrm{d}t.$$

The last integral equals zero, as $H=0$ on the boundary ∂V. The integral,

$$2\int_V H\,\mathrm{d}p \wedge \mathrm{d}q \wedge \mathrm{d}t,$$

is exactly the Calabi invariant.

Suppose now that the dimension $\dim M=2n>2$. As we assumed above, the restriction of the symplectic 2-form on the invariant set D^2 is nondegenerate. Then one can show that the restriction of the original Hamiltonian system to $V=D^2\times\{t \pmod{2\pi}\}$ is a Dirac constrained Hamiltonian system, cf. Ref. 4. Namely, the Hamiltonian vector field ξ in the solid torus V is given by the standard condition $i_\xi\omega^2=\mathrm{d}F$, where ω^2 is the restriction of the symplectic 2-form, and the function F is the restriction of the Hamiltonian on V. □

An important corollary of this observation is related to ergodic properties of the Calabi invariant, this invariant describes *relative asymptotic linking of the trajectories of the Hamiltonian vector field in the solid torus*, cf. Proposition 2.

In higher-dimensional cases, ergodic properties of the Calabi invariant can be deduced from general results on higher-dimensional analogues of the asymptotic Hopf invariant, see, e.g., Ref. 13.

Let α be an exact 2-form of rank 2 in a simply connected domain M (thus it defines a foliation of codimension 2). Let the vector field ξ be chosen by the condition $i_\xi\mu=\beta$, where μ is the volume form, and the form β is exact. Then an integral,

$$lk_\xi(\mathcal{F}) = \int_M d^{-1}\alpha \wedge \beta,$$

equals the average linking of the foliation $\mathcal{F}$, defined by the 2-form α, and the vector field ξ, see Refs. 3 and 13.

The forms α and β are easily defined for the Calabi invariant: the 2-form α is $\mathrm{d}H\wedge\mathrm{d}t$ (while the 1-form $d^{-1}\alpha=H\,\mathrm{d}t$), and $\beta=(\Omega^2)^n$. One can see that rank $\mathrm{d}H\wedge\mathrm{d}t=2$. Thus, as in the 3-dimensional case, the Calabi invariant equals *relative asymptotic linking of the foliation*, defined by the 2-form $\mathrm{d}H\wedge\mathrm{d}t$, *with the vector field* ξ, which in canonical coordinates $(p_1,q_1,\ldots,p_n,q_n,t)$ looks like $\xi=(0,\ldots,0,1)$. Note that instead of the vector field ξ one can take the Hamiltonian vector field with the Hamiltonian H, the form β certainly changes, but the value of the integral $lk_\xi(\mathcal{F})$ is preserved.

Remark: If the phase space is two dimensional, one can give another definition of the Calabi invariant in terms of the average orbit braiding, see, e.g., Ref. 11. Let $\{\phi_t\}$, $t\in[0,1]$ be a Hamiltonian isotopy of the two-disk D^2 to itself. Consider the map

$$\mathrm{Ang}_\phi: (D^2\times D^2)\setminus\Delta \to \mathbb{R}^2$$

(where Δ is the diagonal), that associates to any pair of points $x\neq y$ the angular variation of the vector from $\phi_t(x)$ to $\phi_t(y)$, when t goes from 0 to 1. Then the Calabi invariant is the integral of this function:

$$\mathcal{H}(\phi) = \int \int_{D^2 \times D^2} \mathrm{Ang}_{\phi}(x,y)\mu_x \mu_y,$$

where μ is the area 2-form on the disk D^2. Our construction shows that the average orbit braiding in this case equals the average linking of the trajectories. However, while a higher-dimensional analog of the angular definition of the Calabi invariant is unknown, its ergodic definition in terms of average linking of the field with the foliation is straightforward, as shown above.

VI. CONCLUSION AND ACKNOWLEDGMENTS

In this paper we considered a generalization of the asymptotic and cross-Hopf invariants for divergence-free vector fields in multiconnected domains of the type (flat domain) $\times S^1$. For a vector field in a solid torus one must choose a potential 1-form such that its integral along the torus meridian equals zero. Under this choice the value of the relative Hopf invariant becomes well-defined, and one can show that for the "correct" embedding of the solid torus into a 3-sphere it coincides with asymptotic linking of this field. For Hamiltonian vector fields the relative Hopf invariant is equal to the Calabi invariant, under the condition that the differential $\mathrm{d}H=0$ on the boundary of the domain. Ergodic properties of the Calabi invariant follow from this observation: the Calabi invariant describes relative asymptotic linking of the trajectories of the Hamiltonian vector field with the Hamiltonian H with the foliation, defined by the 2-form $\mathrm{d}H \wedge \mathrm{d}t$.

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Continuous limit of discrete sawtooth maps and its algebraic framework

Fabio Benatti[a)]
Dipartimento di Fisica Teorica, Università di Trieste, and Istituto Nazionale di Fisica Nucleare, Sezione di Trieste, Strada Costiera 11, 34014 Trieste, Italy

Valerio Cappellini[b)]
Dipartimento di Fisica Teorica, Università di Trieste, Strada Costiera 11, 34014 Trieste, Italy

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We study the presence of a logarithmic time scale in discrete approximations of sawtooth maps on the 2-torus. The techniques used are suggested by quantum mechanical similarities, and are based on a particular class of states on the torus, that fulfill dynamical localization properties typical of quantum coherent states. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1917283]

I. INTRODUCTION

Under the term of quantum chaos goes a rich phenomenology of behaviors[1–3] proper to quantum systems whose classical limit presents typical chaotic features as positive Lyapunov exponents (hyperbolic regime).[4–6]

The footprints of classical chaos are usually studied semiclassically when a suitable "$\hbar$"-like quantization parameter goes to zero; one then examines the differences between quantum and classical behaviors. In the hyperbolic case, quantum chaos reveals itself through the presence of a time scale, over which quantum and classical motions mimic each other, that increases as $-\log\hbar$.[1–3,7–9] This peculiar logarithmic time scale has to be compared with the scaling $\hbar^{-\alpha}$, $\alpha>0$, which is proper of quantum systems with regular classical limit.[1]

Heuristical explanations of the logarithmic time scale already indicate that the phenomenon is not exclusive of quantum systems, and thus of noncommutativity, but that it should also be present when the classical dynamics is looked at as the continuous limit of a family of discrete classical systems.[10]

Intrinsically discrete systems[11] and discretized classical continuous systems[12–14] have recently been objects of numerical analysis concerning the entropy production and the presence of a logarithmic time scale, whereas the ergodic properties of discretized discontinuous maps have been addressed in Ref. 15.

In the following, we shall rigorously show this fact to be true for sawtooth maps on the two-dimensional torus:[16–18] this will be done by forcing them to move on a square lattice and by retrieving the continuous dynamics when the lattice spacing goes to zero. Because of the analogies between quantization and discretization, we will make use of technologies strictly resembling the so-called *anti-Wick* quantization.[19]

We shall prove that a time-scale logarithmic in the lattice spacing appears; in comparison to previous results obtained studying numerically the entropy production,[14] a rigorous continuous limit is established that succeeds in controlling the discontinuities of sawtooth maps. Despite their classical nature, the entropy previously investigated was quantum mechanical; somewhat analo-

a)Electronic mail: fabio.benatti@ts.infn.it
b)Electronic mail: valerio.cappellini@ts.infn.it

gously, in this article, sawtooth maps will be studied by means of states, which play a role similar to quantum coherent states, whose choice is naturally provided by the lattice structure of discretized sawtooth maps. They will be shown to satisfy a *dynamical localization property* that makes them remain localized around the trajectories of the continuous dynamics, but only on a logarithmic time scale.

II. CLASSICAL DYNAMICAL SYSTEMS

Classical dynamics is usually described by means of a measure space χ, the phase space, endowed with the Borel σ algebra and a normalized measure μ, $\mu(\chi)=1$. The "volumes"

$$\mu(E)=\int_E \mu(\mathrm{d}\mathbf{x})$$

of measurable subsets $E\subseteq\chi$ represent the probabilities that a phase-point $\mathbf{x}\in\chi$ belong to them: the measure μ defines the statistical properties of the system and represents a possible state, which is taken to be an equilibrium state with respect to the given dynamics.

In such a scheme, a reversible discrete time dynamics amounts to an invertible measurable map $S:\chi\mapsto\chi$ such that $\mu\circ S=\mu$ and to its iterates $\{S^k|k\in\mathbb{Z}\}$: phase trajectories passing through $\mathbf{x}\in\chi$ at time 0 are then sequences $\{S^k\mathbf{x}\}_{k\in\mathbb{Z}}$.[6]

Classical dynamical systems are thus conveniently described by triplets (χ,μ,S); in the present work, we shall focus upon the following choices:

χ: the two-dimensional torus $\mathbb{T}^2=\mathbb{R}^2/\mathbb{Z}^2=\{\mathbf{x}=(x_1,x_2)\in\mathbb{R}^2 \pmod 1\}$;

μ: the Lebesgue measure, $\mu(\mathrm{d}\mathbf{x})=\mathrm{d}x_1\mathrm{d}x_2$, on $\mathbb{T}^2$;

S: an invertible measurable transformation on $\mathbb{T}^2$ that preserves the Lebesgue measure.

It is convenient to associate an algebraic triple $(\mathcal{M},\omega,\Theta)$ to the measure-theoretic triple $(\mathbb{T}^2,\mu,S)$, consisting of

$\mathcal{M}$: the (Abelian) Von Neumann $*$-algebra $L^\infty_\mu(\mathbb{T}^2)$ of essentially bounded functions on $\mathbb{T}^2$.[20,21]

ω_μ: the state (expectation) on $\mathcal{M}$, given by

$$\omega_\mu: L^\infty_\mu(\mathbb{T}^2)\ni f\mapsto \omega_\mu(f):=\int_{\mathbb{T}^2}\mu(\mathrm{d}\mathbf{x})f(x)\in\mathbb{R}^+. \tag{1}$$

Θ: the automorphism of $\mathcal{M}$ such that $\Theta(f)=f\circ S$, $\omega\circ\Theta=\omega$.

In the following, we shall consider a discretized version of $(\mathbb{T}^2,\mu,S)$ which arises by forcing the continuous classical system to live on a square lattice $L_N\subseteq\mathbb{T}^2$ of spacing $1/N$:

$$L_N:=\left\{\left.\frac{\mathbf{p}}{N}\right|\mathbf{p}\in(\mathbb{Z}/N\mathbb{Z})^2\right\}, \tag{2}$$

where $(\mathbb{Z}/N\mathbb{Z})$ denotes the residual class (mod N), that is $0\leqslant p_i\leqslant N-1$.

Taking the N^2 points as labels of the elements $\{|\ell\rangle\}_{\ell\in(\mathbb{Z}/N\mathbb{Z})^2}$ of an orthonormal basis (o.n.b.) of the $\mathcal{N}$-dimensional Hilbert space $\mathcal{H}_\mathcal{N}$, $\mathcal{N}:=N^2$, we will consider discrete algebraic triples $(\mathcal{D}_\mathcal{N},\tau_\mathcal{N},\Theta_\mathcal{N})$, consisting of

$\mathcal{D}_\mathcal{N}$: an $\mathcal{N}\times\mathcal{N}$ matrix algebra diagonal in the orthonormal basis introduced previously;

$\tau_\mathcal{N}$: the uniform state (expectation) on $D_\mathcal{N}$ defined by

$$\tau_\mathcal{N}:\mathcal{D}_\mathcal{N}\ni D\mapsto\tau_\mathcal{N}(D):=\frac{1}{\mathcal{N}}\mathrm{Tr}(D)\in\mathbb{R}^+; \tag{3}$$

$\Theta_\mathcal{N}$: an automorphism of $D_\mathcal{N}$ suitably reproducing Θ when $N\to\infty$ (see Sec. IV B).

Remark 2.1: As it will become evident in the following, up to a certain extent, discretization resembles quantization; in the latter case, instead of $\mathcal{D}_\mathcal{N}$, one deals with noncommutative matrix algebras, the typical instance being the finite dimensional quantization of the Arnold cat map.[22,23]

III. DISCRETIZATION OF PHASE SPACE

As sketched in the previous Remark, we proceed now to setup a discretization procedure close to the so-called anti-Wick quantization.[19]

Given the classical algebraic triple $(L^\infty_\mu(\mathbb{T}^2), \omega_\mu, \Theta)$, the aim of a discretization–dediscretization procedure (specifically an $\mathcal{N}$-dimensional discretization) is twofold:

- finding a pair of $*$-morphisms, $\mathcal{J}_{\mathcal{N},\infty}$ mapping $L^\infty_\mu(\mathbb{T}^2)$ into the abelian finite dimensional algebra $\mathcal{D}_\mathcal{N}$ and $\mathcal{J}_{\infty,\mathcal{N}}$ mapping backward $\mathcal{D}_\mathcal{N}$ into $L^\infty_\mu(\mathbb{T}^2)$;
- providing an automorphism $\Theta_\mathcal{N}$, the discrete dynamics, acting on $\mathcal{D}_\mathcal{N}$ such that it approximates the continuous one, Θ, on $L^\infty_\mu(\mathbb{T}^2)$ as follows:

$$\mathcal{J}_{\infty,\mathcal{N}} \circ \Theta^j_\mathcal{N} \circ \mathcal{J}_{\mathcal{N},\infty} \xrightarrow[N\to\infty]{} \Theta^j. \tag{4}$$

The latter requirement can be seen as a modification of the so-called Egorov's property (see Ref. 24). Intuitively, a discrete description of the measure-theoretic triple $(\mathbb{T}^2, \mu, S)$ becomes finer when we increase N, the number of points per linear dimension on the grid L_N in (2): this corresponds to enlarging the dimension of the Hilbert space $\mathcal{H}_\mathcal{N}$ associated to the corresponding algebraic triple $(\mathcal{D}_\mathcal{N}, \tau_\mathcal{N}, \Theta_\mathcal{N})$. In this sense, the lattice spacing $a := 1/N$ of the grid L_N is a natural "discretization parameter" playing an analogous role to the quantization parameter $\hbar$.

The difficulty is to find convenient $*$-morphisms $\mathcal{J}_{\mathcal{N},\infty}$ and $\mathcal{J}_{\infty,\mathcal{N}}$ that set up a rigorous asymptotic (in N) correspondence, of functions on $L^\infty_\mu(\mathbb{T}^2)$ and matrices in $\mathcal{D}_\mathcal{N}$ and, above all, between the discrete dynamics $\Theta_\mathcal{N}$ and the continuous one Θ.

Due to the similarities with quantization, we shall consider a discretization procedure based on states that we shall refer to as lattice states (LS for short) which mimic the use of coherent states in the study of the semiclassical limit. In the next section we will give a suitable definition of LS belonging to the Hilbert space $\mathcal{H}_\mathcal{N}$, that we shall use to discretize $(L^\infty_\mu(\mathbb{T}^2), \omega_\mu, \Theta)$.

A. Lattice states on $\mathbb{T}^2$

In analogy with the properties of quantum coherent states, we shall look for a class $\{|C_\mathcal{N}(\mathbf{x})\rangle \,|\, \mathbf{x} \in \mathbb{T}^2\} \in \mathcal{H}_\mathcal{N}$ of vectors, indexed by points $\mathbf{x} \in \mathbb{T}^2$, satisfying the following conditions which are borrowed from analogous quantum ones.[25]

Properties 3.1:

1. Measurability: $\mathbf{x} \mapsto |C_\mathcal{N}(\mathbf{x})\rangle$ is measurable on $\mathbb{T}^2$;
2. Normalization: $\|C_\mathcal{N}(\mathbf{x})\|^2 = 1$, $\mathbf{x} \in \mathbb{T}^2$;
3. Completeness: $\mathcal{N} \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{x}) |C_\mathcal{N}(\mathbf{x})\rangle\langle C_\mathcal{N}(\mathbf{x})| = \mathbb{1}$;
4. Localization: given $\epsilon > 0$ and $d_0 > 0$, there exists $N_0(\epsilon, d_0)$ such that for $N \geqslant N_0(\epsilon, d_0)$ and $d_{\mathbb{T}^2}(\mathbf{x}, \mathbf{y}) \geqslant d_0$ one has

$$\mathcal{N} |\langle C_\mathcal{N}(\mathbf{x}), C_\mathcal{N}(\mathbf{y})\rangle|^2 \leqslant \epsilon.$$

The symbol $d_{\mathbb{T}^2}(\mathbf{x}, \mathbf{y})$ used in the localization property stands for the length of the shorter segment connecting the two points $\mathbf{x}, \mathbf{y} \in \mathbb{T}^2$, namely

Definition 3.1: We shall denote by $d_{\mathbb{T}^2}(\mathbf{x}, \mathbf{y}) := \min_{\mathbf{n} \in \mathbb{Z}^2} \|\mathbf{x} - \mathbf{y} + \mathbf{n}\|_{\mathbb{R}^2}$ the distance on $\mathbb{T}^2$.

We shall now construct a family of $|C_\mathcal{N}(\mathbf{x})\rangle$. Let $\lfloor \cdot \rfloor$ denote the integer part of a real number, namely $x - 1 < \lfloor x \rfloor \leqslant x$ is the largest integer smaller than x; further, let $\langle \cdot \rangle$ denote the fractional parts, that is $\langle x \rangle := x - \lfloor x \rfloor$. Thus we will write

$$\mathbb{T}^2 \ni \mathbf{x} = \left(\frac{\lfloor N x_1 \rfloor}{N}, \frac{\lfloor N x_2 \rfloor}{N} \right) + \left(\frac{\langle N x_1 \rangle}{N}, \frac{\langle N x_2 \rangle}{N} \right),$$

or, more compactly,

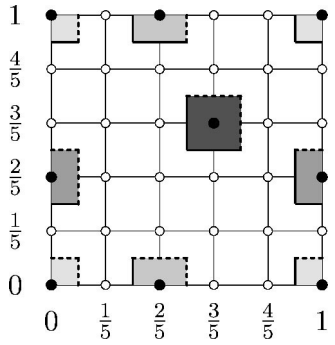

FIG. 1. All points in the shadowed square $I_{(3/5,3/5)} := \left[\frac{5}{10},\frac{7}{10}\right)\times\left[\frac{5}{10},\frac{7}{10}\right)\subset\mathbb{T}^2$ are associated with the grid point $\left(\frac{3}{5},\frac{3}{5}\right)$ (black dot). Thus, for all $\mathbf{x}\in I_{(3/5,3/5)}$, it turns out that $|C_{\mathcal{N}}(\mathbf{x})\rangle = |(3,3)\rangle \in \mathcal{H}_{\mathcal{N}}$.

$$\mathbf{x} = \frac{\lfloor N\mathbf{x}\rfloor}{N} + \frac{\langle N\mathbf{x}\rangle}{N}.$$

We proceed by associating to points of $\mathbb{T}^2$ specific lattice points.

Definition 3.2 (lattice states): Given $\mathbf{x}\in\mathbb{T}^2$, we shall denote by $\hat{\mathbf{x}}_N$ the element of $(\mathbb{Z}/N\mathbb{Z})^2$ given by

$$\hat{\mathbf{x}}_N = (\hat{x}_{N,1},\hat{x}_{N,2}) := \left(\left\lfloor Nx_1 + \tfrac{1}{2}\right\rfloor,\left\lfloor Nx_2 + \tfrac{1}{2}\right\rfloor\right), \tag{5}$$

and call lattice states on $\mathbb{T}2$ the vectors $|C_{\mathcal{N}}(\mathbf{x})\rangle$ defined by

$$\mathbb{T}^2 \ni \mathbf{x} \mapsto |C_{\mathcal{N}}(\mathbf{x})\rangle := |\hat{\mathbf{x}}_N\rangle \in \mathcal{H}_{\mathcal{N}}. \tag{6}$$

Remark 3.1: The family of states $|C_{\mathcal{N}}(\mathbf{x})\rangle$ is constructed by choosing, for each $\mathbf{x}\in\mathbb{T}^2$, that element of the basis of $\mathcal{H}_{\mathcal{N}}$ which is labeled by the closest element of L_N to $\mathbf{x}$.

Figure 1 represents a square lattice (L_5) of spacing $\frac{1}{5}$ by circles and connecting lines.

Proposition 3.1: The family of LS $\{|C_{\mathcal{N}}(\mathbf{x})\}$ *satisfies Properties 3.1.*

Proof: Measurability and normalization are straightforward. Completeness can be expressed as

$$\mathcal{N}\int_{\mathbb{T}^2}\mu(\mathrm{d}\mathbf{x})\langle\boldsymbol{\ell}|C_{\mathcal{N}}(\mathbf{x})\rangle\langle C_{\mathcal{N}}(\mathbf{x})|\mathbf{m}\rangle = \delta^{(N)}_{\boldsymbol{\ell},\mathbf{m}}, \quad \forall\,\boldsymbol{\ell},\mathbf{m}\in(\mathbb{Z}/N\mathbb{Z})^2,$$

where we have introduced the periodic Kronecker delta, that is $\delta^{(N)}_{\mathbf{n},\mathbf{0}}=1$ if and only if $\mathbf{n}\equiv\mathbf{0}$ (mod N). This is proved as follows:

$$\begin{aligned}
&\mathcal{N}\int_{\mathbb{T}^2}\mu(\mathrm{d}\mathbf{x})\langle\boldsymbol{\ell}|C_{\mathcal{N}}(\mathbf{x})\rangle\langle C_{\mathcal{N}}(\mathbf{x})|\mathbf{m}\rangle\\
&\quad= \mathcal{N}\int_0^1\mathrm{d}x_1\int_0^1\mathrm{d}x_2\langle\boldsymbol{\ell}|\hat{\mathbf{x}}_N\rangle\langle\hat{\mathbf{x}}_N|\mathbf{m}\rangle\\
&\quad= \mathcal{N}\delta^{(N)}_{\ell_1,m_1}\delta^{(N)}_{\ell_2,m_2}\left[\int_0^1\mathrm{d}x_1\,\delta^{(N)}_{\ell_1,\lfloor Nx_1+1/2\rfloor}\right]\left[\int_0^1\mathrm{d}x_2\,\delta^{(N)}_{\ell_2,\lfloor Nx_2+1/2\rfloor}\right]\\
&\quad= \mathcal{N}(\delta^{(N)}_{\ell_1,m_1}\delta^{(N)}_{\ell_2,m_2})\left[\int_{\ell_1-1/2/N}^{\ell_1+1/2/N}\mathrm{d}x_1\right]\left[\int_{\ell_2-1/2/N}^{\ell_2+1/2/N}\mathrm{d}x_2\right] = N^2\delta^{(N)}_{\boldsymbol{\ell},\mathbf{m}}\frac{1}{N^2} = \delta^{(N)}_{\boldsymbol{\ell},\mathbf{m}}.
\end{aligned}$$

Localization comes as follows: from Definition 3.2 (see Remark 3.1 and Fig 1), it turns out that $|C_{\mathcal{N}}(\mathbf{x})\rangle$ is orthogonal to every basis element labeled by a point of L_N whose toral distance $d_{\mathbb{T}^2}$ (see

Definition 3.1) from $\mathbf{x}$ is greater than $1/N\sqrt{2}$. As a consequence, the quantity $\langle C_{\mathcal{N}}(\mathbf{x}), C_{\mathcal{N}}(\mathbf{y})\rangle = 0$ if the distance on the torus between $\mathbf{x}$ and $\mathbf{y}$ is greater than $\sqrt{2}/N$. Thus, given $d_0 > 0$, it is sufficient to choose $N_0(\epsilon, d_0) > \sqrt{2}/d_0$, to have

$$N > N_0(\epsilon, d_0) \Rightarrow \mathcal{N}\langle C_{\mathcal{N}}(\mathbf{x}), C_{\mathcal{N}}(\mathbf{y})\rangle = 0.$$

■

Remarks 3.2:

(1) The last result in the previous proposition amounts to an even stronger localization property than Property 3.1.4; this is due to our particular choice of lattice states, which, as we shall see, is suited to the task of controlling sawtooth maps. In general, one can hardly hope to achieve orthogonality and must be content with the weaker localization condition 3.1.4.

(2) Although the set of LS of Definition 3.2 fulfill Properties 3.1, which are typical of coherent states, LS differ from them in that the context we are considering is commutative. In spite of this, it is convenient to adopt the formalism of quantum mechanics; in particular the set of LS is interpreted as a Hilbert orthonormal basis of Dirac kets, whose corresponding projectors form a partition of unit into indicator functions having support on small squares of the torus, as in Figure 1, whose side scales as $1/N$.

B. Anti-Wick discretization and its continuous limit on $\mathbb{T}^2$

In order to study the continuous limit and, more generally, the quasicontinuous behavior of $(\mathcal{D}_{\mathcal{N}}, \tau_{\mathcal{N}}, \Theta_{\mathcal{N}})$ when $N \to \infty$, we follow the semiclassical technique known as anti-Wick quantization. The other standard quantization technique, namely the Weyl procedure, despite being more straightforward and less technically heavy, is nevertheless more suited to smooth spaces of functions and was indeed instrumental in the study of discretized cat maps.[14] Instead, in our case, the anti-Wick procedure is a better choice due to the discontinuous character of the dynamics, as it will clearly appear in the next section.

We start choosing concrete discretization/de-discretization $*$-morphisms.

Definitions 3.3: Given the family $\{|C_{\mathcal{N}}(\mathbf{x})\rangle\}$ of lattice states in $\mathcal{H}_{\mathcal{N}}$, the anti-Wick-like discretization scheme (AW, for short) will be described by a one parameter family of (completely) positive unital map $\mathcal{J}_{\mathcal{N},\infty}: L^{\infty}_{\mu}(\mathbb{T}^2) \to \mathcal{D}_{\mathcal{N}}$

$$L^{\infty}_{\mu}(\mathbb{T}^2) \ni f \mapsto \mathcal{N}\int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{x}) f(\mathbf{x}) |C_{\mathcal{N}}(\mathbf{x})\rangle\langle C_{\mathcal{N}}(\mathbf{x})| =: \mathcal{J}_{\mathcal{N},\infty}(f) \in \mathcal{D}_{\mathcal{N}}.$$

The corresponding de-discretization operation will be described by the (completely) positive unital map $\mathcal{J}_{\infty,\mathcal{N}}: \mathcal{D}_{\mathcal{N}} \to L^{\infty}_{\mu}(\mathbb{T}^2)$

$$\mathcal{D}_{\mathcal{N}} \ni X \mapsto \langle C_{\mathcal{N}}(\mathbf{x}), X C_{\mathcal{N}}(\mathbf{x})\rangle =: \mathcal{J}_{\infty,\mathcal{N}}(X)(\mathbf{x}) \in L^{\infty}_{\mu}(\mathbb{T}^2).$$

Remarks 3.3: (i) Both maps are identity preserving (unital) because of the conditions satisfied by the family of lattice states and are completely positive, since both $L^{\infty}_{\mu}(\mathbb{T}^2)$ and $\mathcal{D}_{\mathcal{N}}$ are commutative algebras. One can also check that

$$\|\mathcal{J}_{\infty,\mathcal{N}} \circ \mathcal{J}_{\mathcal{N},\infty}(g)\|_{\infty} \leqslant \|g\|_{\infty}, \quad g \in L^{\infty}_{\mu}(\mathbb{T}^2).$$

(ii) Definition 3.3 yields $\tau_{\mathcal{N}} \circ \mathcal{J}_{\mathcal{N},\infty} = \omega_{\mu}$, with $\tau_{\mathcal{N}}$ given in (3).

In Appendix A, more operative details are presented, whereas in the following we prove some simple properties that incorporate minimal requests for rigorously defining the sense in which the discrete dynamical systems $(\mathcal{D}_{\mathcal{N}}, \tau_{\mathcal{N}}, \Theta_{\mathcal{N}})$ tends to $(L^{\infty}_{\mu}(\mathbb{T}^2), \omega_{\mu}, \Theta)$, when $1/N \to 0$.

Proposition 3.2:

(1) For all $f \in L^{\infty}_{\mu}(\mathbb{T}^2)$ and $X \in \mathcal{D}_{\mathcal{N}}$,

$$\omega_{\mu}(\overline{g}\mathcal{J}_{\infty,\mathcal{N}}(X)) = \tau_{\mathcal{N}}(\mathcal{J}_{\mathcal{N},\infty}(g)^* X);$$

(2) For all $f,g \in L^{\infty}_{\mu}(\mathbb{T}^2)$

$$\lim_{N\to\infty} \tau_{\mathcal{N}}(\mathcal{J}_{\mathcal{N},\infty}(f)^{*}\mathcal{J}_{\mathcal{N},\infty}(g)) = \omega_{\mu}(\overline{fg}) = \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{x})\overline{f(\mathbf{x})}g(\mathbf{x});$$

(3) For all $X \in \mathcal{D}_{\mathcal{N}}$, and for all $N \in \mathbb{N}^{+}$,

$$\mathcal{J}_{\mathcal{N},\infty} \circ \mathcal{J}_{\infty,\mathcal{N}}(X) = X;$$

(4) For all $f \in L^{\infty}_{\mu}(\mathbb{T}^2)$

$$\lim_{N\to\infty} \mathcal{J}_{\infty,\mathcal{N}} \circ \mathcal{J}_{\mathcal{N},\infty}(f) = f \ \mu - \text{a.e.}$$

Proof: The first two statements in the above proposition directly follow from Definitions 3.3 together with (6); the latter two are equivalent and their proof can be found in Ref. 25, the only difference being the dimension $\mathcal{N}$ of the Hilbert space $H_{\mathcal{N}}$, here $\mathcal{N}=N^2$, there $\mathcal{N}=N$. ■

Remark 3.4: Properties 1 and 2 in the previous proposition show how (GNS) scalar products in the discrete, respectively continuous limit, are related; Properties 3 and 4 concern instead the direct-inverse relations between the discretization and the de-discretization maps.

IV. DISCRETIZATION OF THE DYNAMICS

A. Classical description of sawtooth maps

We shall now focus on a special class of automorphisms of the torus, namely the sawtooth maps[16,17] (SM for short), that is on triples $(\mathbb{T}^2,\mu,S_{\alpha})$ where

$$S_{\alpha}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1+\alpha & 1 \\ \alpha & 1 \end{pmatrix}\begin{pmatrix} \langle x_1 \rangle \\ x_2 \end{pmatrix} \ (\mathrm{mod}\ 1), \quad \alpha \in \mathbb{R} = \begin{pmatrix} \langle (1+\alpha)\langle x_1\rangle + x_2 \rangle \\ \langle \alpha \langle x_1 \rangle + x_2 \rangle \end{pmatrix}. \tag{7}$$

Remarks 4.1

i. In the following, a point $\mathbf{x}$ of the torus, will correspond to an equivalence class of $\mathbb{R}^2$ points whose coordinates differ by integer values;

ii. without the fractional part, (7) is not well defined on $\mathbb{T}^2$ for noninteger α; indeed, the same point $\mathbf{x}=\mathbf{x}+\mathbf{n} \in \mathbb{T}^2, \mathbf{n} \in \mathbb{Z}^2$, would have (in general) $S_{\alpha}(\mathbf{x}) \neq S_{\alpha}(\mathbf{x}+\mathbf{n})$. Of course, $\langle\cdot\rangle$ is not necessary when $\alpha \in \mathbb{Z}$;

iii. the Lebesgue measure on $\mathbb{T}^2$ is *invariant* for all $\alpha \in \mathbb{R}$;

iv. if $\alpha \notin \mathbb{Z}$, the S_{α} are known as sawtooth maps;

v. when $\alpha \in \mathbb{Z}$, we shall write T_{α} instead of S_{α}. $T_1=\left(\begin{smallmatrix} 2 & 1 \\ 1 & 1 \end{smallmatrix}\right)$ is the Arnold cat map.[6] In general, $T_1 \in \{T_{\alpha}\}_{\alpha\in\mathbb{Z}} \subset \mathrm{SL}_2(\mathbb{Z}) \subset \mathrm{GL}_2(\mathbb{Z}) \subset \mathrm{M}_2(\mathbb{Z})$ where $\mathrm{M}_2(\mathbb{Z})$ is the subset of 2×2 matrices with integer entries, $\mathrm{GL}_2(\mathbb{Z})$ the subset of invertible matrices and $\mathrm{SL}_2(\mathbb{Z})$ the subset of matrices with determinant one: the dynamics generated by $T_{\alpha} \in \mathrm{SL}_2(\mathbb{Z})$ is called *Unimodular Group*[6] (UMG for short);

vi. after identifying $\mathbf{x}$ with canonical coordinates (q,p) and imposing the (mod 1) condition on both of them, the previous dynamics reads

$$\begin{aligned} q' &= q + p' \\ p' &= p + \alpha\langle q \rangle \end{aligned} \ (\mathrm{mod}\ 1). \tag{8}$$

This is nothing but the Chirikov standard map[3] in which $-(1/2\pi)\sin(2\pi q)$ is replaced by $\langle q\rangle$. The dynamics in (8) can also be thought of as generated by the (singular) Hamiltonian

$$H(q,p,t) = \frac{p^2}{2} - \alpha\frac{\langle q\rangle^2}{2}\delta_p(t),$$

where $\delta_p(t)$ is the periodic Dirac delta which makes the potential act through periodic kicks with period 1;[26]

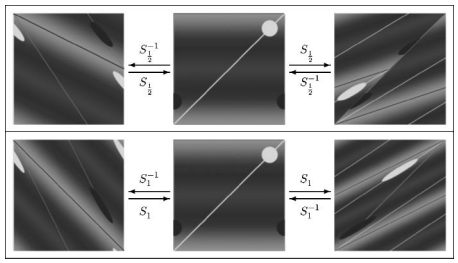

FIG. 2. In the upper row, we depict the effects of the discontinuities of a SM with $\alpha=\frac{1}{2}$; the picture in the middle shows the discontinuity lines γ_0 and γ_{-1}, whereas those on the right and left show how they evolve backward and forward in time. The different parallel bands help the reader to figure out the toral periodicity and the discontinuous character of the map, also highlighted by the aperiodic splits of two spots. Further, for sake of comparison, the lower row presents the same case of the upper one but for the continuous dynamics ($\alpha=1$).

vii. Sawtooth maps are invertible and the inverse is given by the expression

$$S_\alpha^{-1}\begin{pmatrix}x_1\\x_2\end{pmatrix}=\begin{pmatrix}1 & 0\\ -\alpha & 1\end{pmatrix}\left\langle\begin{pmatrix}1 & -1\\0 & 1\end{pmatrix}\begin{pmatrix}x_1\\x_2\end{pmatrix}\right\rangle \ (\mathrm{mod}\ 1)=\begin{pmatrix}\langle x_1-x_2\rangle\\ \langle\langle x_2\rangle-\alpha\langle x_1-x_2\rangle\rangle\end{pmatrix} \tag{9}$$

or, in other words,

$$\begin{aligned} q&=q'-p'\\ p&=-\alpha q+p' \end{aligned} \ (\mathrm{mod}\ 1).$$

It can indeed be checked that $S_\alpha(S_\alpha^{-1}(\mathbf{x}))=S_\alpha^{-1}(S_\alpha(\mathbf{x}))=\mathbf{x}$, $\forall\mathbf{x}\in\mathbb{T}^2$.

Further, S_α^{-1} preserves the Lebesgue measure on $\mathbb{T}^2$.

We now list a set of properties[16–18] of sawtooth maps that will be used in the following.

Properties 4.1 (of sawtooth maps)

(1) Sawtooth maps $\{S_\alpha\}$ are *discontinuous* on the subset $\gamma_0:=\{\mathbf{x}=(0,p),p\in\mathbb{T}\}\in\mathbb{T}^2$: two points close to γ_0, $A:=(\varepsilon,p)$ and $B:=(1-\varepsilon,p)$, have images that differ, in the $\varepsilon\to 0$ limit, by a vector $d^{(1)}_{S_\alpha}(A,B)=(\alpha,\alpha)$ (mod 1).

(2) Inverse sawtooth maps $\{S_\alpha^{-1}\}$ are *discontinuous* on the subset $\gamma_{-1}:=S_\alpha(\gamma_0)=\{\mathbf{x}=(p,p),p\in\mathbb{T}\}\in\mathbb{T}^2$: two points close to γ_{-1}, namely $A:=(p+\varepsilon,p-\varepsilon)$ and $B:=(p-\varepsilon,p+\varepsilon)$, have images that differ, in the $\varepsilon\to 0$ limit, by a vector $d^{(1)}_{S_\alpha^{-1}}(A,B)=(0,\alpha)$ (mod 1).

(3) The maps T_α and T_α^{-1} are *continuous*: $\alpha\in\mathbb{Z}\Rightarrow d^{(1)}_{T_\alpha}(A,B)=d^{(1)}_{T_\alpha^{-1}}(A,B)=(0,0)$ (mod 1).

(4) The eigenvalues of the matrix $S_\alpha=\left(\begin{smallmatrix}1+\alpha & 1\\ \alpha & 1\end{smallmatrix}\right)$ are $(\alpha+2\pm\sqrt{(\alpha+2)^2-4})/2$. They are conjugate complex numbers if $\alpha\in[-4,0]$, whereas one eigenvalue $\lambda>1$ if $\alpha\notin[-4,0]$. In this case, distances are stretched along the direction of the eigenvector $|\mathbf{e}_+\rangle$, $S_\alpha|\mathbf{e}_+\rangle=\lambda|\mathbf{e}_+\rangle$, contracted along that of $|\mathbf{e}_-\rangle$, $S_\alpha|\mathbf{e}_-\rangle=\lambda^{-1}|\mathbf{e}_-\rangle$: $\log\lambda$ is a (positive) *Lyapunov exponent*.

For such α's all periodic points are hyperbolic (see Fig. 2).[18]

Remarks 4.2: Because of the presence of the fractional part in (7) and (9), we have to distinguish the action of S_α and S_α^{-1} from a mere matrix action. We shall adopt the following notations.

i. With S_α the matrix $\left(\begin{smallmatrix}1+\alpha & 1\\ \alpha & 1\end{smallmatrix}\right)$ in Property 3.1.4, the expression $S_\alpha(\mathbf{x})$ will denote the action represented by (7), whereas $S_\alpha\cdot\mathbf{x}$ will denote the matrix action of S_α on the vector $\mathbf{x}$.

ii. When the dynamics arises from the action of the UMG (see Remark 4.1.v.), so, in particular, when $\{T_\alpha\}_{\alpha\in\mathbb{Z}}$ is the family of toral automorphisms, Eq. (7) assumes the simpler form $T_\alpha(\mathbf{x})=T_\alpha\cdot\mathbf{x}$ (mod 1).

iii. Analogously, expressions like $T_\alpha\cdot\mathbf{x}$, $T_\alpha^{\mathrm{tr}}\cdot\mathbf{x}$, $T_\alpha^{-1}\cdot\mathbf{x}$, and $(T_\alpha^{\mathrm{tr}})^{-1}\cdot\mathbf{x}$, will denote the actions by T_α itself, its transposed, its inverse, and the inverse of the transposed, respectively.

B. Algebraic description of continuous and discretized sawtooth maps

In this section we make use of the commutative (Von Neumann) algebra $L^\infty_\mu(\mathbb{T}^2)$ introduced in Sec. II and consider the algebraic description of sawtooth maps by triples $(L^\infty_\mu(\mathbb{T}^2), \omega_\mu, \Theta_\alpha)$, where ω_μ has been defined in (1) and $\Theta_\alpha: L^\infty_\mu(\mathbb{T}^2) \mapsto L^\infty_\mu(\mathbb{T}^2)$ is the discrete-time dynamics generated as follows:

$$\Theta_\alpha(f)(\mathbf{x}) := f(S_\alpha(\mathbf{x})), \quad \alpha \in \mathbb{R}.$$

The maps Θ^j_α, $j \in \mathbb{Z}$ are automorphisms of $L^\infty_\mu(\mathbb{T}^2)$ and leave the state ω_μ invariant.

Our aim is now to define a suitable discrete evolution $\Theta_{\mathcal{N},\alpha}$ on $\mathcal{D}_\mathcal{N}$, such that the discretized triplets $(\mathcal{D}_\mathcal{N}, \tau_\mathcal{N}, \Theta_{\mathcal{N},\alpha})$ converge to the continuous SM.

We start by introducing two different kinds of maps: the first ones, $U^{\pm j}_\alpha$, $j \in \mathbb{Z}$, are defined on the torus $\mathbb{T}^2([0,N)^2)$, namely $[0,N)\times[0,N)$ (mod N), and given by

$$\mathbb{T}^2([0,N)^2) \ni \mathbf{x} \mapsto U^0_\alpha(\mathbf{x}) := \mathbf{x} = NS^0_\alpha\left(\frac{\mathbf{x}}{N}\right) \in \mathbb{T}^2([0,N)^2), \tag{10a}$$

$$\mathbb{T}^2([0,N)^2) \ni \mathbf{x} \mapsto U^{\pm 1}_\alpha(\mathbf{x}) := NS^{\pm 1}_\alpha\left(\frac{\mathbf{x}}{N}\right) \in \mathbb{T}^2([0,N)^2), \tag{10b}$$

$$\mathbb{T}^2([0,N)^2) \ni \mathbf{x} \mapsto U^{\pm j}_\alpha(\mathbf{x}) := \underbrace{U^{\pm 1}_\alpha(U^{\pm 1}_\alpha(\cdots U^{\pm 1}_\alpha(U^{\pm 1}_\alpha}_{j \text{ times}}(\mathbf{x}))\cdots)), \quad j \in \mathbb{N}^+,$$

$$= NS^{\pm j}_\alpha\left(\frac{\mathbf{x}}{N}\right) \in \mathbb{T}^2([0,N)^2). \tag{10c}$$

The second class consists of maps $V^{\pm j}_\alpha$ from $\mathbb{T}^2([0,N)^2)$ onto its subset $(\mathbb{Z}/N\mathbb{Z})^2$, whose actions are as follows:

$$\mathbb{T}^2([0,N)^2) \ni \mathbf{x} \mapsto V^0_\alpha(\mathbf{x}) := \lfloor \mathbf{x} \rfloor = \pm\lfloor \pm U^0_\alpha(\lfloor \mathbf{x} \rfloor)\rfloor \in (\mathbb{Z}/N\mathbb{Z})^2, \tag{11a}$$

$$\mathbb{T}^2([0,N)^2) \ni \mathbf{x} \mapsto V^{\pm 1}_\alpha(\mathbf{x}) := \pm\lfloor \pm U^{\pm 1}_\alpha(\lfloor \mathbf{x} \rfloor)\rfloor \in (\mathbb{Z}/N\mathbb{Z})^2, \tag{11b}$$

$$\mathbb{T}^2([0,N)^2) \ni \mathbf{x} \mapsto V^{\pm j}_\alpha(\mathbf{x}) := \underbrace{V^{\pm 1}_\alpha(V^{\pm 1}_\alpha\ (\cdots V^{\pm 1}_\alpha\ (V^{\pm 1}_\alpha}_{j \text{ times}}\ (\lfloor \mathbf{x} \rfloor))\cdots)), \quad j \in \mathbb{N}^+,$$

$$= \underbrace{\pm\lfloor \pm U^{\pm 1}_\alpha\ (\pm\lfloor \pm U^{\pm 1}_\alpha(\cdots \pm\ \lfloor \pm U^{\pm 1}_\alpha\ (\pm\lfloor \pm U^{\pm 1}_\alpha}_{j \text{ times}}(\lfloor \mathbf{x} \rfloor)\rfloor)\rfloor\cdots)\rfloor)\rfloor \in (\mathbb{Z}/N\mathbb{Z})^2. \tag{11c}$$

Remark 4.3: The maps U^j_α are extensions of the S^j_α on the enlarged torus $\mathbb{T}^2([0,N)^2)$; however, they do not map the lattice L_N into itself, therefore we are forced to use the maps V^j_α to define a consistent discretized dynamics.

Definition 4.1: $\Theta_{\mathcal{N},\alpha}$ will denote the map:

$$\mathcal{D}_\mathcal{N} \ni X \mapsto \Theta_{\mathcal{N},\alpha}(X) := \sum_{\ell \in (\mathbb{Z}/N\mathbb{Z})^2} X_{V_\alpha(\ell),V_\alpha(\ell)} |\ell\rangle\langle\ell| \in \mathcal{D}_\mathcal{N}. \tag{12}$$

$\Theta_{\mathcal{N},\alpha}$ is a $*$-automorphism of $\mathcal{D}_\mathcal{N}$; indeed, the map

$$(\mathbb{Z}/N\mathbb{Z})^2 \ni \ell \mapsto V_\alpha(\ell) \in (\mathbb{Z}/N\mathbb{Z})^2$$

is a bijection, so that (12) can be rewritten in the more convenient form

$$\Theta_{\mathcal{N},\alpha}(X) = \sum_{\ell \in (\mathbb{Z}/N\mathbb{Z})^2} X_{V_\alpha(\ell),V_\alpha(\ell)} |\ell\rangle\langle\ell| = \sum_{V^{-1}_\alpha(\mathbf{s}) \in (\mathbb{Z}/N\mathbb{Z})^2} X_{\mathbf{s},\mathbf{s}} |V^{-1}_\alpha(\mathbf{s})\rangle\langle V^{-1}_\alpha(\mathbf{s})|$$

$$(\text{see Remark 4 . 4iii . }) = W_{\alpha N}\left(\sum_{\substack{\text{all equiv.}\\ \text{classes}}} X_{\mathbf{s},\mathbf{s}}|\mathbf{s}\rangle\langle\mathbf{s}|\right)W^*_{\alpha,N} = W_{\alpha,N}XW^*_{\alpha,N}, \tag{13}$$

where the operators $W_{\alpha,N}$, defined by linearly extending the maps

$$\mathcal{H}_{\mathcal{N}} \ni |\ell\rangle \mapsto W_{\alpha,N}|\ell\rangle := |V_\alpha^{-1}(\ell)\rangle \in \mathcal{H}_{\mathcal{N}}, \tag{14}$$

to $\mathcal{H}_{\mathcal{N}}$, are unitary: $W^*_{\alpha,N}|\ell\rangle := |V_\alpha(\ell)\rangle$.

For the same reason the state $\tau_{\mathcal{N}}$ is $\Theta_{\mathcal{N},\alpha}$-invariant and V_α is invertible too. Note that $\Theta^j_{\mathcal{N},\alpha} := \underbrace{\Theta_{\mathcal{N},\alpha}\circ\cdots\circ\Theta_{\mathcal{N},\alpha}}_{j \text{ times}}$ is implemented by $V^j_\alpha(\ell)$ given in (11c).

Remarks 4.4:

i. The double $\pm$ sign in front and within every floor function in equations (11) is needed in order to have $V^{\pm j}_\alpha(V^{\mp j}_\alpha(\mathbf{x})) = V^0_\alpha(\mathbf{x})$ (the identity when $\mathbf{x} \in (\mathbb{Z}/N\mathbb{Z})^2$); the reason is that, in general, $\lfloor -x\rfloor \neq -\lfloor x\rfloor$, for $x \notin \mathbb{Z}$ (see Ref. 27).

ii. When $\alpha \in \mathbb{Z}$, $(\mathbb{Z}/N\mathbb{Z})^2 \ni \ell \mapsto V_\alpha(\ell) = T_\alpha \cdot \ell \in (\mathbb{Z}/N\mathbb{Z})^2$, namely the action of the map V_α becomes that of a matrix (mod N). Moreover, in that case, U_α and V_α coincide.

iii. Since $\ell \mapsto V_\alpha(\ell)$ is a bijection, in (13) one can sum over the equivalence classes.

V. CONTINUOUS LIMIT OF THE DYNAMICS

One of the main issues in the semiclassical analysis is to compare if and how the quantum and classical time evolutions mimic each other when a suitable quantization parameter goes to zero.

In this article we are instead considering the possible agreement between the dynamics of continuous classical systems and that of a class of discrete approximants. In practice, in our case, we will study the difference

$$\Theta^j_\alpha - \mathcal{J}_{\infty,\mathcal{N}} \circ \Theta^j_{\mathcal{N},\alpha} \circ \mathcal{J}_{\mathcal{N},\infty} \tag{15}$$

which represents how much the discrete dynamics at timestep j differs from the continuous one at the same timestep.

For quantum systems, whose classical limit is chaotic, the situation is strikingly different from those with regular classical limit. In the former case, classical and quantum mechanics agree, that is a difference as in (15) is negligible, only over times j which scale logarithmically (and not as a power law) in the quantization parameter.

As we shall see, such a type of scaling is not exclusively related with noncommutativity; in fact, the quantization-like procedure developed so far, exhibits a similar behavior when $N \to \infty$ and we recover $(L^\infty_\mu(\mathbb{T}^2), \omega_\mu, \Theta_\alpha)$ as a continuous limit of $(\mathcal{D}_{\mathcal{N}}, \tau_{\mathcal{N}}, \Theta_{\mathcal{N},\alpha})$.

A. Continuous limit for sawtooth maps

Later on we shall show that the difference in (15) goes to zero in a suitable topology; for the moment we just note that the major difficulties in the proof are due to the discontinuous character of the fractional part that appears in (7).

It is therefore important to briefly discuss the discontinuities of the maps S_α.[16–18]

As already noted in Property 4.1.1, S_α is discontinuous on the circle γ_0; therefore S^n_α will be discontinuous on the preimages

$$\gamma_m := S^{-m}_\alpha(\gamma_0) \quad \text{for } 0 \leqslant m < n, \tag{16a}$$

whereas the discontinuities of S^{-n}_α lie on the sets

$$\gamma_{-m} := S^m_\alpha(\gamma_0) \quad \text{for } 0 < m \leqslant n. \tag{16b}$$

Apart from γ_{-1}, whose projection on the $[0,1)^2$ square is its diagonal (see Fig. 5), each set of the type γ_m (for γ_{-m} the argument is similar) is the (disjoint) union of segments parallel to each other

whose endpoints lie either on the same segment belonging to γ_p, $p<m$, or on two different segments belonging to γ_p and $\gamma_{p'}$, with $p' \leqslant p < m$.[17] It proves convenient to introduce the *discontinuity set* of S^n_α,

$$\mathbb{T}^2 \supset \Gamma_n := \bigcup_{p=0}^{n-1} \gamma_p, \tag{17}$$

and its complementary set, $G_n := \mathbb{T}^2 \backslash \Gamma_n$.

We now enlarge the previous definition from continuous sawtooth maps, to discretized ones.

Definitions 5.1: We shall call, "segment," denoted by (A,B), the shortest curve joining $A,B \in \mathbb{T}^2$, by $l(\gamma_p)$ the length of the curve γ_p and by

$$\overline{\gamma_p}(\varepsilon) := \{\mathbf{x} \in \mathbb{T}^2 | d_{\mathbb{T}^2}(\mathbf{x}, \gamma_p) \leqslant \varepsilon\} \tag{18}$$

the strip around γ_p of width ε, where the distance $d_{\mathbb{T}^2}(\cdot,\cdot)$ on the torus has been introduced in Definition 3.1.

Further, we shall denote by

$$\overline{\Gamma_n}(\varepsilon) := \bigcup_{p=0}^{n-1} \overline{\gamma_p}(\varepsilon) \tag{19}$$

the union of the strips up to $p=n-1$ and by $G^N_n(\varepsilon)$ the subset of points

$$G^N_n(\varepsilon) := \left\{ \mathbf{x} \in \mathbb{T}^2 \,\middle|\, \frac{\hat{\mathbf{x}}_N}{N} \notin \overline{\Gamma}_n(\varepsilon) \right\}, \tag{20}$$

where the lattice points $\hat{\mathbf{x}}_N$ have been introduced in Definition 3.2.

As already observed, in order to prove that the discretized SM tend to continuous SM when $N \to \infty$, the main problem is to control the discontinuities. It proves convenient to subdivide the lattice points into a *good* and *bad* set and show that, on the former, $V^q_\alpha \simeq U^q_\alpha$, at least on a certain time scale (see Remark 4.3). This will not turn out to be true for the bad set, however we shall show that the latter tends with N to a set of zero Lebesgue measure and thus becomes ineffective.

Following this strategy, we shall concretely show that the difference (15) goes to zero with $N \to \infty$ in the strong topology over the Hilbert space $L^2_\mu(\mathbb{T}^2)$. More precisely, we have the following theorem.

Theorem 1:

Let $(\mathcal{D}_\mathcal{N}, \tau_\mathcal{N}, \Theta_{\mathcal{N},\alpha})$ be a sequence of discretized SM as defined in Sect. IV: for all $\gamma > 3$,

$$\forall f \in L^\infty_\mu(\mathbb{T}^2), \qquad \underset{\substack{j,N \to \infty \\ j < 1/\gamma(\log N/\log \eta)}}{\text{s-lim}} (\Theta^j_\alpha - \mathcal{J}_{\infty,\mathcal{N}} \circ \Theta^j_{\mathcal{N},\alpha} \circ \mathcal{J}_{\mathcal{N},\infty})(f) = 0, \tag{21}$$

where the limit is in the strong topology over the Hilbert space $L^2_\mu(\mathbb{T}^2)$ and $\eta > \sqrt{2}$ is the largest eigenvalue of the matrix $|S_\alpha| := \sqrt{S^\dagger_\alpha S_\alpha}$, with S_α defined in Property 4.1.4.

The previous theorem indicates that the time limit and the continuous limit do not commute. In particular, the difference between the discretized dynamics and the continuous one can be made small by increasing N, while it becomes large beyond the time scale $j \simeq (1/\gamma)(\log N/\log \eta)$. This phenomenon is the same as in quantum chaos and points to discretization of phase space (in the traditional semi-classical treatment of quantum systems), rather than to noncommutativity, as the source of the so-called *logarithmic breaking time*. The constant γ is a *form factor*, which reflects the fine structure of the dynamics: for instance, in the case of quantum cat maps,[25] $\gamma = 2$.

Remark 5.1: The parameter $\gamma > 3$ in Theorem 1 may seem overestimated if compared with the case of the quantum cat map, where $\gamma = 2$. As we shall see (in particular in the next Proposition), the upper bound for γ is dictated by the discontinuities of the sawtooth maps, and not by commutativity. The corresponding exponent assumes the lower value $\gamma > 1$ in the case of discretized cat maps, that include sawtooth maps with integer α. This result will be presented in a forthcoming

paper,[28] in which we study the breaking time $\tau_B(N)$, here $(1/\gamma)(\log N/\log \eta)$, relative to the chaotic or nonchaotic properties of the dynamics. In particular, in the hyperbolic regime, the parameter $\log \eta$ of Theorem 1 is replaced by the Lyapunov exponent $\log \lambda$ whereas, in the elliptic regime, the two limits $j, N \to \infty$ do commute and in the parabolic one, the breaking time is given by $\tau_B(N) = N^{1/\gamma}$.

The proof of Theorem 1 consists of several steps, among which the most important is a property, satisfied by our choice of lattice states, which we shall call *dynamical localization.*

We give a full proof that our choice of lattice states satisfies such property, since it represents a natural request that should be fulfilled by any consistent discretization/de-discretization (quantization/de-quantization) scheme.

Remarks 5.2:

(1) In analogy to the quantum case, dynamical localization is what one expects from a good choice of states suited to the study of the continuous limit: in fact, it essentially amounts to asking that LS remain decently localized around the continuous trajectories while evolving with the corresponding discrete evolution. As we shall see this is the case only on logarithmic time scales. Informally, when $N \to \infty$, the quantities

$$K_j(\mathbf{x}, \mathbf{y}) := \langle C_{\mathcal{N}}(\mathbf{x}), W^j_{\alpha,N} C_{\mathcal{N}}(\mathbf{y}) \rangle$$

should behave as if $\mathcal{N}|K_j(\mathbf{x}, \mathbf{y})|^2 \simeq \delta(S^j_\alpha \mathbf{x} - \mathbf{y})$: this would make the discretization analogous to the notion of *regular quantization* described in Sec. V of Ref. 29. Actually, with our choice of LS, the quantity $K_j(\mathbf{x}, \mathbf{y})$ is a Kronecker delta.

(2) In quantum chaos, instead of seeking for the dynamical localization, one can study the *dynamical spreading* of coherent states. Consider for instance the classical function f over the phase space, its corresponding quantum observable $\mathrm{Op}_\hbar(f)$ and a coherent state $|C_\hbar(\mathbf{x})\rangle$ centered at the point $\mathbf{x}$. The time needed for the quantum mechanical expectation $\langle C_\hbar(\mathbf{x}), \mathrm{Op}_\hbar(f) C_\hbar(\mathbf{x}) \rangle$ to converge to the average of f over a suitable invariant measure can be explicitly analyzed. Recent work [7,9] shows also that this time scales logarithmically in $\hbar$, at least for the automorphisms on the 2-torus.

(3) The constraint $j \leqslant C \log \mathcal{N}$ is typical of *hyperbolic* behavior with Lyapunov exponent $\log \lambda$ and comes heuristically as follows: the expansion of an initial small distance δ can be exponential until the distance becomes the largest possible, namely $\delta \lambda^{T_B} \simeq 1$. After discretization, the minimal distance gives $\delta = 1/N$, therefore one estimates $T_B \simeq \log N / \log \lambda$, which is called *breaking time* and sets the time scale over which continuous and discretized dynamics mimic each other.

(4) In quantum chaos, the semiclassical analysis leads to an estimate of T_B exactly as above; further, the logarithmic dependence on $\hbar$ of T_B is a signature of the hyperbolic character of the classical limit. Conversely, if the classical limit is regular, then the time scale when quantum and classical behaviors are more or less indistinguishable goes as $\hbar^{-b}, b > 0$. Another interpretation of the breaking time is given in Ref. 8, where it is related to the shortest time needed for the system to transfer all scales $1 \geqslant \ell \geqslant \hbar$ down to the "quantum scale" $\hbar$. Indeed, this is the scale at which the differences among quantum and classical mechanics come up. Regarding the SM, the hyperbolic case corresponds to S_α with eigenvalue $\lambda > 1$, whereas the regular cases are the *elliptic* one (two complex eigenvalues) and the *parabolic* one (only one eigenvalue $= 1$).

(5) The dynamical localization property has fruitfully been used in several quantum contexts;[25] however, to our knowledge, this is the first instance, though not properly quantal, where dynamical localization is fully exposed.

Before proceeding with the proof of Theorem 1, it is important to notice that in its statement the Lyapunov exponent $\log \lambda$ does not appear but $\log \eta$, instead; of course λ and η are related for λ is eigenvalue of S_α, and η of $\sqrt{S^\dagger_\alpha S_\alpha}$ (see Remark 5.1).

As will become clear during the proof, the use of η and not of λ is required by the discontinuous character of SM. In fact, the discontinuities do not allow us to control the difference between the nth iterates of the discretized and the continuous dynamics, but instead force us to estimate that difference at each single time step up to n and to put all the estimates together. In the single time-step estimate, independently of whether the map is continuous or not, one must use η,

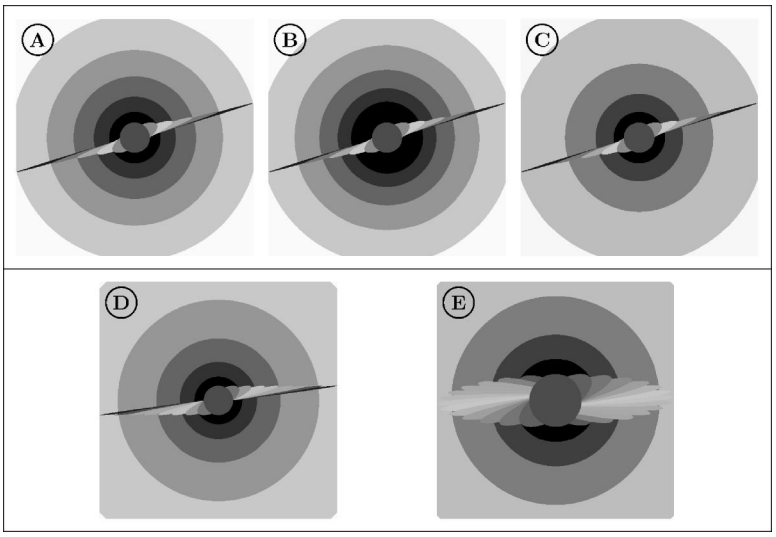

FIG. 3. In plots A, B, and C we compare the estimates of the (maximum) stretching given by the action of the SM $S_{1/10}$ and its temporal iterates $S^n_{1/10}$ ($n \leqslant 5$) given by λ, respectively η, on a small ball $B^0_{\mathbf{v}}$ of radius $\mathbf{v}$, centered in $(\frac{1}{2},\frac{1}{2}) \in \mathbb{T}^2$. The five evolved images of the ball, namely $\{B^n_{\mathbf{v}}, 1<n\leqslant 5\}$, are plotted together with $B^0_{\mathbf{v}}$, using different colors. In A we surround every evolved ball $B^n_{\mathbf{v}}$ with the smallest circle containing it. We compare that plot with B and C, in which the surrounding circles have radii proportional to $\lambda^n\mathbf{v}$, respectively, $\eta^n\mathbf{v}$; in both cases the correct radii of A are overestimated although, on the long run, circles in B provide a good approximation. The fake hyperbolicity given by η is clearly shown in D and E, where a parabolic SM S_0 and an elliptic one $S_{-1/20}$ are presented: in the first case the maximum spreading grows linearly, whereas in the second one it remains confined, and the estimate given by the surrounding circles of radii growing as powers of η is inappropriate. Note that in all examples C–E, the black circles of radii $\eta\mathbf{v}$ rightly surround $B^1_{\mathbf{v}}$.

which coincides with λ only when the dynamical matrix S_α is symmetric. Indeed, Fig. 3 shows that the eigenvalue η correctly describes how volumes behave under a single application of the dynamics, whereas λ underestimates it. On the contrary, it is λ^n which asymptotically controls the stretching, whereas η^n largely overestimates it. In the regular elliptic case, where $\lambda=0$ and $\eta \geqslant \sqrt{2}$, the use of η gives the impression of hyperbolic stretching, whereas the elliptic motion is confined: from the lower strip in Fig. 3 it is apparent that such hyperbolicity is spurious.

Theorem 2 (Dynamical localization with $\{|\mathbf{C}_{\mathcal{N}}(\mathbf{x})\rangle\}$ states):

For $\alpha \in \mathbb{R}$, $\beta \in \mathbb{R}^+\setminus(0,2]$ and $d_0>0$, there exists $N_0=N_0(\alpha,\beta,d_0) \in \mathbb{N}^+$ with the following property: if $N>N_0$ and $n<(1/\beta)(\log N/\log \eta)$, then

$$d_{\mathbb{T}^2}(S^n_\alpha(\mathbf{x}),\mathbf{y}) \geqslant d_0 \Rightarrow \langle C_{\mathcal{N}}(\mathbf{x}) \; | W^n_{\alpha,N} C_{\mathcal{N}}(\mathbf{y})\rangle = 0,$$

for all $\mathbf{y} \in \mathbb{T}^2$ and $\mathbf{x} \in G^N_n(\tilde{N}/2N)$, where $W^n_{\alpha,N}$ is the unitary operator defined in (14), *$\tilde{N} = 2\sqrt{2}(\sqrt{2}+1)\eta^{2n}$ and $G^N_n(\varepsilon)$ has been introduced in Definitions 5.1.*

In order to prove Theorem 2, we need the following result, whose proof can be found in Appendix B.

Proposition 5.1: With the notation of Definitions 3.1 and 5.1, and with $[E]^\circ$ denoting the complement of $E \subseteq \mathbb{T}^2$, $[E]^\circ := \mathbb{T}^2\setminus E$, the following inclusions hold:

$$\left[\overline{\Gamma}_n\left(\varepsilon + \frac{1}{\sqrt{2}N}\right)\right]^\circ \subseteq G^N_n(\varepsilon) \subseteq \left[\overline{\Gamma}_n\left(\varepsilon - \frac{1}{\sqrt{2}N}\right)\right]^\circ. \tag{22}$$

Further, for $\alpha \in \mathbb{R}$ and $n \in \mathbb{N}^+$, if

$$N > \tilde{N} = 2\sqrt{2}(\sqrt{2}+1)\eta^{2n}$$

and

$$\mathbf{x} \in G_n^N\left(\frac{\tilde{N}}{2N}\right)$$

then

$$d_{\mathbb{T}^2}\left(\frac{U_\alpha^p(N\mathbf{x})}{N}, \frac{V_\alpha^p(\hat{\mathbf{x}}_N)}{N}\right) \leqslant \frac{\sqrt{2}}{N}\left(\frac{\eta^{p+1}-1}{\eta-1}\right), \quad \forall\, p \leqslant n. \tag{23}$$

Proof of Theorem 2: Using the definition of $\{|C_{\mathcal{N}}(\mathbf{x})\rangle\}$ in (6), we easily compute

$$\langle C_{\mathcal{N}}(\mathbf{x}) \,|W_{\alpha,N}^n C_{\mathcal{N}}(\mathbf{y})\rangle = \langle \hat{\mathbf{x}}_N \,|V_\alpha^{-n}(\hat{\mathbf{y}}_N)\rangle = \delta^{(N)}_{V_\alpha^n(\hat{\mathbf{x}}_N),\hat{\mathbf{y}}_N}. \tag{24}$$

Using the triangular inequality, we get:

$$d_{\mathbb{T}^2}\left(\frac{U_\alpha^n(N\mathbf{x})}{N}, \mathbf{y}\right) \leqslant d_{\mathbb{T}^2}\left(\frac{U_\alpha^n(N\mathbf{x})}{N}, \frac{V_\alpha^n(\hat{\mathbf{x}}_N)}{N}\right) + d_{\mathbb{T}^2}\left(\frac{V_\alpha^n(\hat{\mathbf{x}}_N)}{N}, \frac{\hat{\mathbf{y}}_N}{N}\right) + d_{\mathbb{T}^2}\left(\frac{\hat{\mathbf{y}}_N}{N}, \mathbf{y}\right)$$

or equivalently, using the definitions (10),

$$d_{\mathbb{T}^2}\left(\frac{V_\alpha^n(\hat{\mathbf{x}}_N)}{N}, \frac{\hat{\mathbf{y}}_N}{N}\right) \geqslant d_{\mathbb{T}^2}(S_\alpha^n(\mathbf{x}), \mathbf{y}) - d_{\mathbb{T}^2}\left(\frac{U_\alpha^n(N\mathbf{x})}{N}, \frac{V_\alpha^n(\hat{\mathbf{x}}_N)}{N}\right) - d_{\mathbb{T}^2}\left(\frac{\hat{\mathbf{y}}_N}{N}, \mathbf{y}\right).$$

Now, since $d_{\mathbb{T}^2}(S_\alpha^n(\mathbf{x}), \mathbf{y}) \geqslant d_0$ by hypothesis, using (B1) in Appendix B and observing that $\mathbf{x} \in G_n^N(\tilde{N}/2N)$ permits us to use (23) in Proposition 5.1, namely that

$$N > \tilde{N} \Rightarrow d_{\mathbb{T}^2}\left(\frac{U_\alpha^n(N\mathbf{x})}{N}, \frac{V_\alpha^n(\hat{\mathbf{x}}_N)}{N}\right) \leqslant \frac{\sqrt{2}}{N}\left(\frac{\eta^{n+1}-1}{\eta-1}\right), \tag{25}$$

we can derive

$$d_{\mathbb{T}^2}\left(\frac{V_\alpha^n(\hat{\mathbf{x}}_N)}{N}, \frac{\hat{\mathbf{y}}_N}{N}\right) \geqslant d_0 - \frac{\sqrt{2}}{N}\left(\frac{\eta^{n+1}-1}{\eta-1}\right) - \frac{1}{\sqrt{2}N}.$$

The r.h.s. of the previous inequality can always be made strictly larger than $1/N$,

$$d_{\mathbb{T}^2}\left(\frac{V_\alpha^n(\hat{\mathbf{x}}_N)}{N}, \frac{\hat{\mathbf{y}}_N}{N}\right) > \frac{1}{N}, \tag{26}$$

by choosing an N larger than

$$N_{\mathsf{M}}(n) = \max\left\{\frac{1}{d_0}\left[1 + \sqrt{2}\left(\frac{\eta^{n+1}-1}{\eta-1}\right) + \frac{1}{\sqrt{2}}\right], \quad \tilde{N} = 2\sqrt{2}(\sqrt{2}+1)\,\eta^{2n}\right\}, \tag{27}$$

so that the condition on the l.h.s. of (25) is also satisfied. From (24) and (26), we have

$$N > N_{\mathsf{M}}(n) \Rightarrow \langle C_{\mathcal{N}}(\mathbf{x}) \,|W_{\alpha,N}^n C_{\mathcal{N}}(\mathbf{y})\rangle = 0. \tag{28}$$

Indeed, if the toral distance between two points $(\mathbf{z}, \mathbf{w})$ exceeds $1/N$, then the corresponding grid points $(\hat{\mathbf{z}}_N, \hat{\mathbf{w}}_N)$ are different and then the periodic Kronecker delta in (24) vanishes.

Since the (nondecreasing) function N_{M} in (27) is eventually bounded by $\eta^{\beta n}$ (β being strictly greater than two), we define $\overline{n}$ as the time when $N_{\mathsf{M}}(\overline{n}) = \eta^{\beta\overline{n}} =: N_0$, and choose $N > N_0$, $\mathbf{x} \in G_n^N(\tilde{N}/2N)$. Thus, if $0 < n < \overline{n}$, then $N > N_0 = N_{\mathsf{M}}(\overline{n}) > N_{\mathsf{M}}(n)$, whereas if $\overline{n} \leqslant n < (1/\beta)(\log N/\log \eta)$, then $N > \eta^{\beta n} > N_{\mathsf{M}}(n)$ and (28) holds for all $0 < n < (1/\beta)(\log N/\log \eta)$. ■

In order to proceed with the proof of Theorem 1, we need another auxiliary result which is proved in Appendix C.

Proposition 5.2: With the notation of Definition 5.1, the following relations hold for all $p \in \mathbb{N}$, $n \in \mathbb{N}^+$ and $\varepsilon \in \mathbb{R}^+$:

$$l(\gamma_p) \leqslant \eta^p, \tag{29a}$$

$$\mu(\overline{\gamma}_p(\varepsilon)) \leqslant 2\varepsilon\eta^p + \pi\varepsilon^2, \tag{29b}$$

$$\mu(\overline{\Gamma}_n(\varepsilon)) \leqslant 2(\sqrt{2}+1)\varepsilon\eta^n + \pi n\varepsilon^2. \tag{29c}$$

Moreover, if $N \in \mathbb{N}^+$ and $\widetilde{N} = 2\sqrt{2}(\sqrt{2}+1)\eta^{2n}$ [cfr. Eq. (23) in Proposition 5.1]:

$$N > \widetilde{N} \Rightarrow \mu\left(\left[G_n^N\left(\frac{\widetilde{N}}{2N}\right)\right]^\circ\right) \leqslant \frac{38\eta^{3n}}{N}. \tag{29d}$$

We are finally in position to conclude with

Proof of Theorem 1: We subdivide the proof in two steps: in the first we concentrate on continuous f, that is $f \in \mathcal{C}^0(\mathbb{T}^2)(\subset L^2_\mu(\mathbb{T}^2))$; in the second one we extend the result to essentially bounded function by applying the following corollary of Lusin's theorem:[21,30,31]

Given $f \in L^\infty_\mu(\chi)$, with χ compact, there exists a sequence $\{f_n\}$ of continuous functions on χ such that $|f_n| \leqslant \|f\|_\infty$ and converging to f μ—almost everywhere.

(1) Let $f \in \mathcal{C}^0(\mathbb{T}^2)$ and $\mathrm{Op}_{j,N}(f) := (\Theta^j_\alpha - \mathcal{J}_{\infty,\mathcal{N}} \circ \Theta^j_{\mathcal{N},\alpha} \circ \mathcal{J}_{\mathcal{N},\alpha})\,(f)$: notice that $\mathrm{Op}_{j,N}(f)$ is a multiplication operator on $L^2_\mu(\mathbb{T}^2)$, but also an $L^\infty_\mu(\mathbb{T}^2)$ (and thus also an $L^2_\mu(\mathbb{T}^2)$) function. According to (21), we must show that

$$\forall g \in L^2_\mu(\mathbb{T}^2), \qquad \lim_{\substack{j,N\to\infty \\ j<\frac{1}{\gamma}\frac{\log N}{\log \eta}}} \|\mathrm{Op}_{j,N}(f)g\|_2 = 0.$$

Using Schwartz's inequality first with g in the class of *simple functions* and then using their density in $L^2_\mu(\mathbb{T}^2)$, we have to show only that

$$\lim_{\substack{j,N\to\infty \\ j<\frac{1}{\gamma}\frac{\log N}{\log \eta}}} \|\mathrm{Op}_{j,N}(f)\|_2 = 0.$$

Explicitly, using (1), we write:

$$\begin{aligned}\|\mathrm{Op}_{j,N}(f)\|_2^2 = \omega_\mu(\mathrm{Op}_{j,N}(f)^*\mathrm{Op}_{j,N}(f)) &= \omega_\mu[(\Theta^j_\alpha f)^*(\Theta^j_\alpha f)] \\ &+ \omega_\mu[(\mathcal{J}_{\infty,\mathcal{N}} \circ \Theta^j_{\mathcal{N},\alpha} \circ \mathcal{J}_{\mathcal{N},\infty})(f)^*(\mathcal{J}_{\infty,\mathcal{N}} \circ \Theta^j_{\mathcal{N},\alpha} \circ \mathcal{J}_{\mathcal{N},\infty})(f)] \\ &- 2\,\mathrm{Re}\{\omega_\mu[(\Theta^j_\alpha f)^*(\mathcal{J}_{\infty,\mathcal{N}} \circ \Theta^j_{\mathcal{N},\alpha} \circ \mathcal{J}_{\mathcal{N},\infty})(f)]\},\end{aligned}$$

which via Proposition 3.2.1, becomes

$$\begin{aligned}\omega_\mu[\Theta^j_\alpha(\overline{f})\Theta^j_\alpha(f)] - 2\,\mathrm{Re}\{\tau_{\mathcal{M}}[\mathcal{J}_{\mathcal{N},\infty}(\Theta^j_\alpha f)^*(\Theta^j_{\mathcal{N},\alpha} \circ \mathcal{J}_{\mathcal{N},\infty})(f)]\} \\ + \tau_{\mathcal{M}}[(\mathcal{J}_{\mathcal{N},\infty} \circ \mathcal{J}_{\infty,\mathcal{N}} \circ \Theta^j_{\mathcal{N},\alpha} \circ \mathcal{J}_{\mathcal{N},\infty})(f)^*(\Theta^j_{\mathcal{N},\alpha} \circ \mathcal{J}_{\mathcal{N},\infty}) \\ \times(f)],\end{aligned}$$

that, using Proposition 3.2.3, can be recast as

$$
\begin{aligned}
&(\omega_\mu \circ \Theta_\alpha^j)(\overline{ff}) + \tau_{\mathcal{M}}[(\Theta_{\mathcal{N},\alpha}^j \circ \mathcal{J}_{\mathcal{N},\infty})(f)^*(\Theta_{\mathcal{N},\alpha}^j \circ \mathcal{J}_{\mathcal{N},\infty})(f)] \\
&\quad - 2\,\mathrm{Re}\{\tau_{\mathcal{M}}[(\mathcal{J}_{\mathcal{N},\infty} \circ \Theta_\alpha^j)(f)^*(\Theta_{\mathcal{N},\alpha}^j \circ \mathcal{J}_{\mathcal{N},\infty})(f)]\} \\
&\quad = \omega_\mu(|f|^2) + (\tau_{\mathcal{N}} \circ \Theta_{\mathcal{N},\alpha}^j)[\mathcal{J}_{\mathcal{N},\infty}(f)^* \mathcal{J}_{\mathcal{N},\infty}(f)] - 2\,\mathrm{Re}(I_{j,N}(f)),
\end{aligned}
$$

with

$$
\begin{aligned}
I_{j,N}(f) &:= \tau_{\mathcal{M}}[(\mathcal{J}_{\mathcal{N},\infty} \circ \Theta_\alpha^j)(f)^*(\Theta_{\mathcal{N},\alpha}^j \circ \mathcal{J}_{\mathcal{N},\infty})(f)] \\
&= \mathcal{N} \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{x}) \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{y}) \overline{f(\mathbf{y})} f(S_\alpha^j \mathbf{x}) |\langle C_{\mathcal{N}}(\mathbf{x}), W_{\alpha,N}^j C_{\mathcal{N}}(\mathbf{y})\rangle|^2.
\end{aligned}
$$

Now, Proposition 3.2.2 yields

$$
(\tau_{\mathcal{N}} \circ \Theta_{\mathcal{N},\alpha}^j)[\mathcal{J}_{\mathcal{N},\infty}(f)^* \mathcal{J}_{\mathcal{N},\infty}(f)] = \tau_{\mathcal{M}}[\mathcal{J}_{\mathcal{N},\infty}(f)^* \mathcal{J}_{\mathcal{N},\infty}(f)] \xrightarrow[N\to\infty]{} \omega_\mu(|f|^2),
$$

so that the strategy is to prove also that $I_{j,N}(f)$ goes to $\omega_\mu(|f|^2) = \int_{\mathbb{T}^2} \mu(d\mathbf{x}) |f(\mathbf{x})|^2$ when $j, N \to \infty$ with $j < (1/\gamma)(\log N / \log \eta)$.

Resorting to $G_n^N(\hat{N}/2N)$ in Definition 5.1, and to its complementary set $[G_n^N(\tilde{N}/2N)]^\circ = \mathbb{T}^2 \backslash G_n^N(\tilde{N}/2N)$, we can write

$$
\begin{aligned}
&\left| I_{j,N}(f) - \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{y}) |f(\mathbf{y})|^2 \right| \\
&\quad = \left| \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{x}) \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{y}) \overline{f(\mathbf{y})} (f(S_\alpha^j \mathbf{x}) - f(\mathbf{y})) \mathcal{N} |\langle C_{\mathcal{N}}(\mathbf{x}), W_{\alpha,N}^j C_{\mathcal{N}}(\mathbf{y})\rangle|^2 \right| \\
&\quad \leqslant \left| \int_{[G_n^N(\tilde{N}/2N)]^\circ} \mu(\mathrm{d}\mathbf{x}) \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{y}) \overline{f(\mathbf{y})} (f(S_\alpha^j \mathbf{x}) - f(\mathbf{y})) \mathcal{N} |\langle C_{\mathcal{N}}(\mathbf{x}), W_{\alpha,N}^j C_{\mathcal{N}}(\mathbf{y})\rangle|^2 \right| \\
&\quad + \left| \int_{G_n^N(\tilde{N}/2N)} \mu(\mathrm{d}\mathbf{x}) \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{y}) \overline{f(\mathbf{y})} (f(S_\alpha^j \mathbf{x}) - f(\mathbf{y})) \mathcal{N} |\langle C_{\mathcal{N}}(\mathbf{x}), W_{\alpha,N}^j C_{\mathcal{N}}(\mathbf{y})\rangle|^2 \right|. \qquad (30)
\end{aligned}
$$

For the first integral in the r.h.s. of the previous expression we have

$$
\begin{aligned}
&\left| \int_{[G_n^N(\tilde{N}/2N)]^\circ} \mu(\mathrm{d}\mathbf{x}) \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{y}) \overline{f(\mathbf{y})} (f(S_\alpha^j \mathbf{x}) - f(\mathbf{y})) \mathcal{N} |\langle C_{\mathcal{N}}(\mathbf{x}), W_{\alpha,N}^j C_{\mathcal{N}}(\mathbf{y})\rangle|^2 \right| \\
&\quad \leqslant 2(\|f\|_\infty)^2 \int_{[G_n^N(\tilde{N}/2N)]^\circ} \mu(\mathrm{d}\mathbf{x}) \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{y}) \mathcal{N} |\langle (W_{\alpha,N}^*)^j C_{\mathcal{N}}(\mathbf{x}), C_{\mathcal{N}}(\mathbf{y})\rangle|^2 \\
&\quad \leqslant 2(\|f\|_\infty)^2 \mu\left(\left[G_n^N\left(\frac{\tilde{N}}{2N} \right) \right]^\circ \right) \leqslant \frac{76\eta^{3j}}{N} (\|f\|_\infty)^2
\end{aligned}
$$

where we have used completeness and normalization Properties 3.1 and Eq. (29d) from Proposition 5.2; this term becomes negligible for large $N > \tilde{N}$ iff $j < (1/\gamma)(\log N / \log \eta)$, with $\gamma > 3$.

Now it remains to prove that the second term in (30) is also negligible for large N: selecting a ball $B(S_\alpha^j \mathbf{x}, d_0)$, one derives

$$\left|\int_{G_n^N(\tilde{N}/2N)}\mu(\mathrm{d}\mathbf{x})\int_{\mathbb{T}^2}\mu(\mathrm{d}\mathbf{y})\overline{f(\mathbf{y})}(f(S_\alpha^j\mathbf{x})-f(\mathbf{y}))\mathcal{N}|\langle C_\mathcal{N}(\mathbf{x}),W_{\alpha,N}^jC_\mathcal{N}(\mathbf{y})\rangle|^2\right|$$
$$\leqslant\left|\int_{G_n^N(\tilde{N}/2N)}\mu(\mathrm{d}\mathbf{x})\int_{B(S_\alpha^j\mathbf{x},d_0)}\mu(\mathrm{d}\mathbf{y})\overline{f(\mathbf{y})}(f(S_\alpha^j\mathbf{x})-f(\mathbf{y}))\mathcal{N}|\langle C_\mathcal{N}(\mathbf{x}),W_{\alpha,N}^jC_\mathcal{N}(\mathbf{y})\rangle|^2\right|$$
$$+\left|\int_{G_n^N(\tilde{N}/2N)}\mu(\mathrm{d}\mathbf{x})\int_{\mathbb{T}^2\setminus B(S_\alpha^j\mathbf{x},d_0)}\mu(\mathrm{d}\mathbf{y})\overline{f(\mathbf{y})}(f(S_\alpha^j\mathbf{x})-f(\mathbf{y}))\mathcal{N}|\langle C_\mathcal{N}(\mathbf{x}),W_{\alpha,N}^jC_\mathcal{N}(\mathbf{y})\rangle|^2\right|.$$

Applying the mean value theorem in the first double integral, we get that $\exists\mathbf{c}\in B(S_\alpha^j\mathbf{x},d_0)$ such that

$$\left|\int_{G_n^N(\tilde{N}/2N)}\mu(\mathrm{d}\mathbf{x})\int_{\mathbb{T}^2}\mu(\mathrm{d}\mathbf{y})\overline{f(\mathbf{y})}(f(S_\alpha^j\mathbf{x})-f(\mathbf{y}))\mathcal{N}|\langle C_\mathcal{N}(\mathbf{x}),W_{\alpha,N}^jC_\mathcal{N}(\mathbf{y})\rangle|^2\right|$$
$$\leqslant\int_{G_n^N(\tilde{N}/2N)}\mu(\mathrm{d}\mathbf{x})|\overline{f(\mathbf{c})}(f(S_\alpha^j\mathbf{x})-f(\mathbf{c}))|\int_{B(S_\alpha^j\mathbf{x},d_0)}\mu(\mathrm{d}\mathbf{y})\mathcal{N}|\langle(W_{\alpha,N}^*)^jC_\mathcal{N}(\mathbf{x}),C_\mathcal{N}(\mathbf{y})\rangle|^2$$
$$+2\|f\|_\infty^2\int_{G_n^N(\tilde{N}/2N)}\mu(\mathrm{d}\mathbf{x})\int_{\mathbb{T}^2\setminus B(S_\alpha^j\mathbf{x},d_0)}\mu(\mathrm{d}\mathbf{y})\mathcal{N}|\langle C_\mathcal{N}(\mathbf{x}),W_{\alpha,N}^jC_\mathcal{N}(\mathbf{y})\rangle|^2.$$

Finally, using completeness and normalization (Properties 3.1), we arrive at the upper bound

$$\leqslant\|f\|_\infty\sup_{\substack{\mathbf{z}\in\mathbb{T}^2\\ \mathbf{c}\in B(\mathbf{z},d_0)}}|(f(\mathbf{z})-f(\mathbf{c}))|+2\|f\|_\infty^2\,\mathcal{N}\sup_{\substack{\mathbf{x}\in G_n^N(\tilde{N}/2N)\\ \mathbf{y}\notin B(S_\alpha^j\mathbf{x},d_0)}}|\langle C_\mathcal{N}(\mathbf{x}),W_{\alpha,N}^jC_\mathcal{N}(\mathbf{y})\rangle|^2.$$

By uniform continuity, the first term can be made arbitrarily small, provided we choose d_0 small enough. For the second integral, we use Theorem 2, which provides us with $N_0=N_0(d_0)$ depending on the same d_0, such that the second term vanishes for all $N>N_0$ and for all $j<(1/\gamma)(\log N/\log\eta)$.

(2) In order to extend the result of point (1) to $f\in L_\mu^\infty(\mathbb{T}^2)$, we use the corollary of Lusin's theorem, choose a sequence $\{f_n\}_n$ as in its statement and estimate

$$\lim_{\substack{j,N\to\infty\\ j<(1/\gamma)(\log N/\log\eta)}}\|\mathrm{Op}_{j,N}(f)\|_2\leqslant\lim_{\substack{j,N\to\infty\\ j<(1/\gamma)(\log N/\log\eta)}}\|\mathrm{Op}_{j,N}(f-f_n)\|_2+\lim_{\substack{j,N\to\infty\\ j<(1/\gamma)(\log N/\log\eta)}}\|\mathrm{Op}_{j,N}(f_n)\|_2.$$

Using point (1), the second term in the r.h.s. of the previous equation can be bounded by arbitrarily small ε, indeed $f_n\in\mathcal{C}^0(\mathbb{T}^2)$.

For the first term we proceed as follows: using Definition 4.1 together with Eqs. (A5) and (A6) of Appendix A, we find

$$(\mathcal{J}_{\infty,\mathcal{N}}\circ\Theta_{\mathcal{N},\alpha}^j\circ\mathcal{J}_{\mathcal{N},\infty})(g)(\mathbf{x})=\sum_{\ell\in(\mathbb{Z}/N\mathbb{Z})^2}\Gamma_N(g)\left(\frac{V_\alpha(\ell)}{N}\right)\mathcal{X}_{Q_N(\ell/N)}(\mathbf{x}),\tag{31}$$

where g is any measurable function on $\mathbb{T}^2$. Then, because of how the running average operator (RAO) Γ_N is defined, for all $g\in L_\mu^1(\mathbb{T}^2)$ it follows that

$$\|(\mathcal{J}_{\infty,\mathcal{N}}\circ\Theta_{\mathcal{N},\alpha}^j\circ\mathcal{J}_{\mathcal{N},\infty})(g)\|_1\leqslant\|(\mathcal{J}_{\infty,\mathcal{N}}\circ\Theta_{\mathcal{N},\alpha}^j\circ\mathcal{J}_{\mathcal{N},\infty})(|g|)\|_1=\|g\|_1,$$

where $\|\cdot\|_1$ denotes the $L_\mu^1(\mathbb{T}^2)$-norm, and that

$$\|(\mathcal{J}_{\infty,\mathcal{N}}\circ\Theta^j_{\mathcal{N},\alpha}\circ\mathcal{J}_{\mathcal{N},\infty})(g)\|_\infty=\sup_{\ell\in(\mathbb{Z}/N\mathbb{Z})^2}\left\{\left|\Gamma_N(g)\left(\frac{\ell}{N}\right)\right|\right\}\leqslant\|\Gamma_N(g)\|_0\leqslant\|g\|_\infty.$$

Indeed, the first equality in the last formula comes from the definition of essential norm[21] (which in this case amounts to the greater absolute value assumed by the simple function $\mathcal{J}_{\infty,\mathcal{N}}\circ\Theta^j_{\mathcal{N},\alpha}\circ\mathcal{J}_{\mathcal{N},\infty}$), whereas the first inequality is a consequence of the continuity of Γ_N and the last one from Proposition A.1. Putting last two inequalities together, we obtain

$$\|(\mathcal{J}_{\infty,\mathcal{N}}\circ\Theta^j_{\mathcal{N},\alpha}\circ\mathcal{J}_{\mathcal{N},\infty})(g)\|_2\leqslant\|g\|_\infty\|g\|_1,$$

whence, setting $g=f-f_n$,

$$\begin{aligned}\|\mathrm{Op}_{j,N}(f-f_n)\|_2&=\|\Theta^j_\alpha(f-f_n)-\mathcal{J}_{\infty,\mathcal{N}}\circ\Theta^j_{\mathcal{N},\alpha}\circ\mathcal{J}_{\mathcal{N},\infty}(f-f_n)\|_2\\&\leqslant\|f-f_n\|_2+\|f-f_n\|_\infty\|f-f_n\|_1,\quad\forall\, j,N.\end{aligned}\tag{32}$$

Now convergence follows from Lusin's corollary. ■

VI. CONCLUSIONS

In this article we have considered discrete approximants of sawtooth maps on the torus and we have studied them in an algebraic framework modeled on the so-called anti-Wick quantization. In fact, finite-dimensional discretization and quantization can be seen as similar procedures in that they map an abelian Von Neumann algebra (of essentially bounded functions on phase space) into finite-dimensional matrix subalgebras, the only difference being whether the latter are diagonal (commutative) or not.

In the semiclassical analysis of classically chaotic quantum systems, the correspondence classical/quantum is usually observed only on time scales that are logarithmic in the quantization parameter $\hbar$. The motivation of our study was to show that the same phenomenon arises when a hyperbolic classical system is discretized, namely forced to move on a lattice, and afterwards the lattice spacing is set to zero.

Previous results[14] based on the numerical investigation of the entropy production indicate that it should indeed be so; however, these results were not supported by a solid framework where to analyze the continuous limit of the family of discrete approximants. This is the content of this article.

The major difficulty was represented by the need of controlling the discontinuous character of sawtooth maps, which was made possible by an appropriate choice of lattice states. In fact, similarly to the entropic approach which, despite the dynamics being classical, was based on a quantum dynamical entropy, the discretization/de-discretization procedure we set up is based on quantum tools.

The choice of lattice states was naturally pointed to by the lattice structure of the discrete phase-space and turned out to possess the right localization properties for mastering the discontinuities. The result is the appearance of a logarithmic time scale when the discrete hyperbolic SM tend to their continuous limit; namely, the continuous and discrete dynamics agree up to a *breaking time* which is proportional to the logarithm of the lattice spacing.

The proportionality constant does not involve the Lyapunov exponent, that is the eigenvalue $\lambda>1$ of the dynamical matrix S_α, rather the largest eigenvalue, η, of $\sqrt{S^\dagger_\alpha S_\alpha}$. In the case of elliptic SM, $|\lambda|=1$, $\eta>\sqrt{2}$; however the resulting breaking time is a spurious effect, while when $\lambda>1$, the presence of η in the breaking time seems to be an unavoidable consequence of the discontinuous dynamics.

APPENDIX A: ANTI-WICK DISCRETIZATION OF $L^\infty_\mu(\mathbb{T}^2)$

In this appendix we will apply Definitions 3.3 and discretize $L^\infty_\mu(\mathbb{T}^2)$ by means of the LS set $\{|C_\mathcal{N}(\mathbf{x})\rangle\,|\,\mathbf{x}\in\mathbb{T}^2\}\in\mathcal{H}_\mathcal{N}$ introduced in Sec. III A.

In this framework, the discretizing/de-discretizing operators of Definitions 3.3 read:

$$L^{\infty}_{\mu}(\mathbb{T}^2) \ni f \mapsto N^2 \int_{\mathbb{T}^2} \mu(d\mathbf{x}) f(\mathbf{x}) |\hat{\mathbf{x}}_N\rangle\langle\hat{\mathbf{x}}_N| =: \mathcal{J}_{\mathcal{N},\infty}(f) \in \mathcal{D}_{\mathcal{N}}, \tag{A1}$$

$$D_{\mathcal{N}} \ni \chi \mapsto \langle\hat{\mathbf{x}}_N|X|\hat{\mathbf{x}}_N\rangle =: \mathcal{J}_{\infty,\mathcal{N}}(X)(\mathbf{x}) \in \mathcal{S}(\mathbb{T}^2) \subset L^{\infty}_{\mu}(\mathbb{T}^2), \tag{A2}$$

where $\mathcal{S}(\mathbb{T}^2)$ denotes the set of *simple functions*[21] on the torus. The matrix elements of $\mathcal{J}_{\mathcal{N},\infty}(f)$ are as follows:

$$\begin{aligned} M^{(f)}_{\boldsymbol{\ell},\mathbf{m}} &:= \langle\boldsymbol{\ell}|\mathcal{J}_{\mathcal{N},\infty}(f)|\mathbf{m}\rangle = N^2 \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{x}) f(\mathbf{x}) \langle\boldsymbol{\ell}|\hat{\mathbf{x}}_N\rangle\langle\hat{\mathbf{x}}_N|\mathbf{m}\rangle \\ &= N^2 \int_0^1 \mathrm{d}x_1 \int_0^1 \mathrm{d}x_2 f(\mathbf{x}) \delta^{(N)}_{\ell_1,\hat{x}_{N,1}} \delta^{(N)}_{\ell_2,\hat{x}_{N,2}} \delta^{(N)}_{m_1,\hat{x}_{N,1}} \delta^{(N)}_{m_2,\hat{x}_{N,2}} \\ &= N^2 \delta^{(N)}_{\ell_1,m_1} \delta^{(N)}_{\ell_2,m_2} \int_0^1 \mathrm{d}x_1 \int_0^1 \mathrm{d}x_2 f(\mathbf{x}) \delta^{(N)}_{\ell_1,\lfloor Nx_1+1/2\rfloor} \delta^{(N)}_{\ell_2,\lfloor Nx_2+1/2\rfloor}. \end{aligned}$$

This implies

$$M^{(f)}_{\boldsymbol{\ell},\mathbf{m}} = N^2 \delta^{(N)}_{\boldsymbol{\ell},\mathbf{m}} \int_{\ell_1-1/2N}^{\ell_1+1/2N} \mathrm{d}x_1 \int_{\ell_2-1/2N}^{\ell_2+1/2N} \mathrm{d}x_2 f(\mathbf{x}), \tag{A3}$$

so that varying $f \in L^{\infty}_{\mu}(\mathbb{T}^2)$ yields Ran $(\mathcal{J}_{\mathcal{N},\infty}) = \mathcal{D}_{\mathcal{N}}$. In order to recast (A3) into a nicer expression, we introduce

Definition A.1 (Running Average Operator): Let $Q_N(\mathbf{x})$ denote the square of side $1/N$, oriented parallel to the axis of the torus and centered around $\mathbf{x}$; then, the running average operator $\Gamma_N : L^{\infty}_{\mu}(\chi) \mapsto \mathcal{C}^0(\mathbb{T}^2)$, is defined by

$$L^{\infty}_{\mu}(\mathbb{T}^2) \ni f(\mathbf{x}) \mapsto \Gamma_N(f)(\mathbf{x}) =: N^2 \int_{Q_N(\mathbf{x})} \mu(\mathrm{d}\mathbf{y}) f(\mathbf{y}) \in \mathcal{C}^0(\mathbb{T}^2).$$

Proposition A.1: Given $f \in L^{\infty}_{\mu}(\mathbb{T}^2)$, the function $f^{(Q)}_N := \Gamma_N(f)$ is uniformly continuous on $\mathbb{T}^2$; moreover, the running average operator has norm

$$\|\Gamma_N\|_{\mathcal{B}} := \sup_{f \in L^{\infty}_{\mu}(\mathbb{T}^2)} \frac{\|\Gamma_N(f)\|_0}{\|f\|_{\infty}} = 1. \tag{A4}$$

Proof: Let $\mathbf{x}_0 \in \mathbb{T}^2$, $\mathbf{x} \in Q_N(\mathbf{x}_0)$ and χ_E denote the characteristic function of $E \subset \mathbb{T}^2$. By Definition A.1:

$$\begin{aligned} |f^{(Q)}_N(\mathbf{x}_0) - f^{(Q)}_N(\mathbf{x})| &= N^2 \left| \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{y}) f(\mathbf{y}) (\chi_{Q_N(\mathbf{x}_0)}(\mathbf{y}) - \chi_{Q_N(\mathbf{x})}(\mathbf{y})) \right| \\ &\leqslant N^2 \|f\|_{\infty} \int_{\mathbb{T}^2} \mu(\mathrm{d}\mathbf{y}) |\chi_{Q_N(\mathbf{x}_0)}(\mathbf{y}) - \chi_{Q_N(\mathbf{x})}(\mathbf{y})| \\ &= N^2 \|f\|_{\infty} [\mu(Q_N(\mathbf{x}_0) \cup Q_N(\mathbf{x})) - \mu(Q_N(\mathbf{x}_0) \cap Q_N(\mathbf{x}))]. \end{aligned}$$

According to our hypothesis, $\mathbf{x} \in Q_N(\mathbf{x}_0)$, thus geometrical considerations lead to:

$$\mu(Q_N(\mathbf{x}_0) \cup Q_N(\mathbf{x})) \leqslant \left(\frac{1}{N} + |x_1 - x_{01}|\right)\left(\frac{1}{N} + |x_2 - x_{02}|\right)$$

$$\mu(Q_N(\mathbf{x}_0) \cap Q_N(\mathbf{x})) = \left(\frac{1}{N} - |x_1 - x_{01}|\right)\left(\frac{1}{N} - |x_2 - x_{02}|\right)$$

$$\mu(Q_N(\mathbf{x}_0) \cup Q_N(\mathbf{x})) - \mu(Q_N(\mathbf{x}_0) \cap Q_N(\mathbf{x})) \leqslant \frac{2}{N}(|x_1 - x_{01}| + |x_2 - x_{02}|) \leqslant \frac{2\sqrt{2}}{N}\|\mathbf{x}_0 - \mathbf{x}\|,$$

so that $|f_N^{(Q)}(\mathbf{x}_0) - f_N^{(Q)}(\mathbf{x})| \leqslant 2\sqrt{2}N\|f\|_\infty\|\mathbf{x}_0 - \mathbf{x}\|$, which proves the continuity of $f_N^{(Q)}$, while uniform continuity comes from $\mathbb{T}^2$ being compact.

Concerning the norm in (A4), the upper bound $\|\Gamma_N\|_{\mathcal{B}} \leqslant 1$ is clear and the maximum is reached by choosing f constant. ■

By means of the running average operator (RAO), the discretization operator in (A1) can be conveniently written as

$$\mathcal{J}_{\mathcal{N},\infty}(f) = \sum_{\boldsymbol{\ell} \in (\mathbb{Z}/N\mathbb{Z})^2} f_N^{(Q)}\left(\frac{\boldsymbol{\ell}}{N}\right)|\boldsymbol{\ell}\rangle\langle\boldsymbol{\ell}|. \tag{A5}$$

Analogously, the de-discretization operator in (A2) can be recast as

$$\mathcal{J}_{\infty,\mathcal{N}}(X)(\mathbf{x}) = \sum_{\boldsymbol{\ell} \in (\mathbb{Z}/N\mathbb{Z})^2} X_{\boldsymbol{\ell},\boldsymbol{\ell}}\delta^{(N)}_{\boldsymbol{\ell},\hat{\mathbf{x}}_N} = \sum_{\boldsymbol{\ell} \in (\mathbb{Z}/N\mathbb{Z})^2} X_{\boldsymbol{\ell},\boldsymbol{\ell}}\chi_{Q_N(\boldsymbol{\ell}/N)}(\mathbf{x}), \tag{A6}$$

thus proving that Ran $(\mathcal{J}_{\infty,\mathcal{N}}) = \mathcal{S}(\mathbb{T}^2)$.

Moreover, combining equations (A5) and (A6), we explicitly get the simple function arising from $f \in L^\infty_\mu(\mathbb{T}^2)$, via AW discretization/de-discretization:

$$(\mathcal{J}_{\infty,\mathcal{N}} \circ \mathcal{J}_{\mathcal{N},\infty})(f)(\mathbf{x}) = \sum_{\boldsymbol{\ell} \in (\mathbb{Z}/N\mathbb{Z})^2} \Gamma_N(f)\left(\frac{\boldsymbol{\ell}}{N}\right)\chi_{Q_N(\boldsymbol{\ell}/N)}(\mathbf{x}). \tag{A7}$$

The action of the operator $\mathcal{J}_{\infty,\mathcal{N}} \circ \mathcal{J}_{\mathcal{N},\infty}$ can be seen in Figs. 4 and 5.

APPENDIX B: PROOF OF PROPOSITION 4.1

We start by proving the inclusions (22).

For every real number t, we have $0 \leqslant \langle Nt + 1/2\rangle = Nt + 1/2 - \lfloor Nt + 1/2\rfloor < 1$, so that

$$\left| t - \frac{\left\lfloor Nt + \frac{1}{2}\right\rfloor}{N}\right| \leqslant \frac{1}{2N}, \quad \forall\, t \in \mathbb{R}.$$

From (5) in Definition 3.2, we derive

$$d_{\mathbb{T}^2}\left(\mathbf{x}, \frac{\hat{\mathbf{x}}_N}{N}\right) \leqslant \frac{1}{\sqrt{2}N}, \quad \forall\, \mathbf{x} \in \mathbb{T}^2. \tag{B1}$$

Then, let us consider the triangular inequality

$$d_{\mathbb{T}^2}(\mathbf{x},\mathbf{y}) \leqslant d_{\mathbb{T}^2}\left(\mathbf{x}, \frac{\hat{\mathbf{x}}_N}{N}\right) + d_{\mathbb{T}^2}\left(\frac{\hat{\mathbf{x}}_N}{N}, \mathbf{y}\right), \quad \forall\, \mathbf{y} \in \mathbb{T}^2, \tag{B2}$$

and let us take the infimum over the set $\mathbf{y} \in \Gamma_n$ defined in (17)

$$d_{\mathbb{T}^2}\left(\frac{\hat{\mathbf{x}}_N}{N}, \Gamma_n\right) \geqslant d_{\mathbb{T}^2}(\mathbf{x}, \Gamma_n) - d_{\mathbb{T}^2}\left(\mathbf{x}, \frac{\hat{\mathbf{x}}_N}{N}\right) \geqslant d_{\mathbb{T}^2}(\mathbf{x}, \Gamma_n) - \frac{1}{\sqrt{2}N},$$

where we used (B1). Therefore, considering the complement $[\overline{\Gamma}_n(\varepsilon)]^\circ$ of the union of strip of width ε, $\overline{\Gamma}_n(\varepsilon)$ defined in (19), we get that

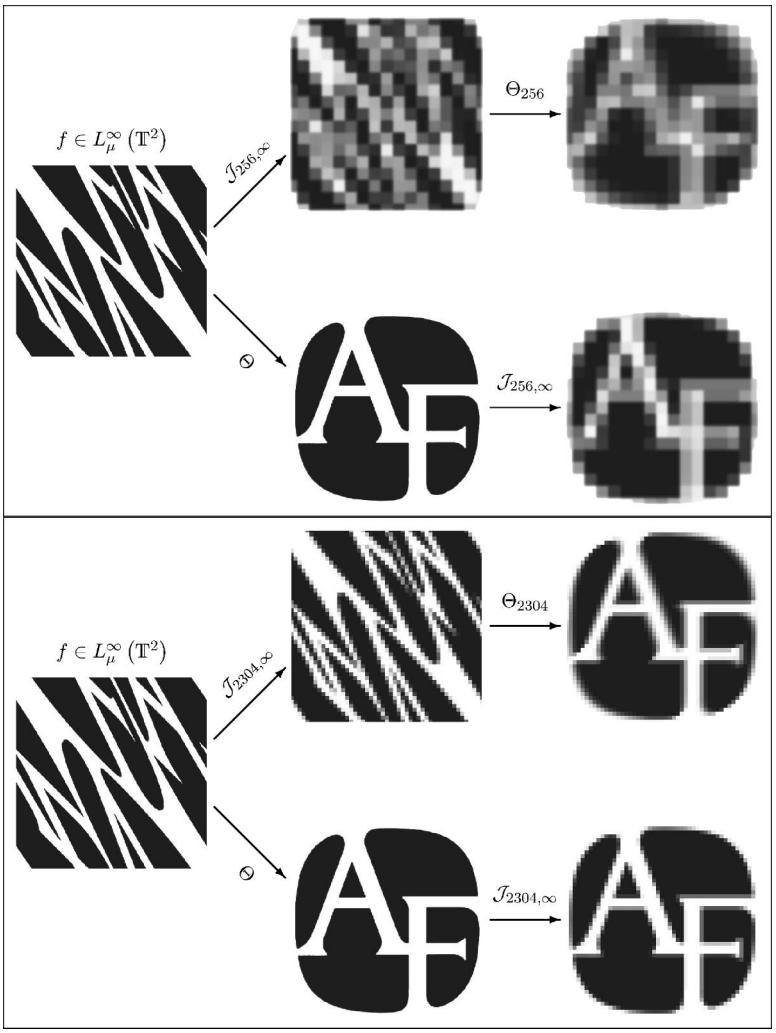

FIG. 4. These two plots show how the difference between $\mathcal{J}_{\mathcal{N},\infty}\circ\Theta_\alpha$ and $\Theta_{\mathcal{N},\alpha}\circ\mathcal{J}_{\mathcal{N},\infty}$ becomes smaller with N. For the continuous SM, Θ_1, the actions $\mathcal{J}_{\mathcal{N},\infty}\circ\Theta_1$ and $\Theta_{\mathcal{N},1}\circ\mathcal{J}_{\mathcal{N},\infty}$ on $f\in L^\infty_\mu(\mathbb{T}^2)$ (left part of both plots) are plotted for two different N: $N=16$ (top) and $N=48$ (bottom). The resulting matrices are mapped back, together with the function $\Theta_1(f)$, on the unfolded torus, by means of the de-discretization operator $\mathcal{J}_{\infty,\mathcal{N}}$.

$$\mathbf{x}\in[\overline{\Gamma}_n(\varepsilon)]^\circ \Rightarrow \frac{\hat{\mathbf{x}}_N}{N}\in\left[\overline{\Gamma}_n\left(\varepsilon-\frac{1}{\sqrt{2}N}\right)\right]^\circ.$$

Further, from (20), it follows that, if the lattice point $\hat{\mathbf{x}}_N/N$ does not belong to $\overline{\Gamma}_n(\varepsilon-1/\sqrt{2}N)$, then the corresponding point $\mathbf{x}\in\mathbb{T}^2$ must belong to $G_n^N(\varepsilon-1/\sqrt{2}N)$. Changing $\varepsilon-1/\sqrt{2}N\mapsto\varepsilon$ we obtain the first inclusion relation in Eq. (22); the second one follows by interchanging the role played by $\hat{\mathbf{x}}_N/N$ and $\mathbf{x}$ in (B2).

In order to prove (23), we start by considering the matrices $S_\alpha=\left(\begin{smallmatrix}1+\alpha & 1\\ \alpha & 1\end{smallmatrix}\right)$ and its inverse $S_\alpha^{-1}=\left(\begin{smallmatrix}1 & -1\\ -\alpha & 1+\alpha\end{smallmatrix}\right)$. Let η be the largest (positive) eigenvalue of $\sqrt{S_\alpha^\dagger S_\alpha}$; its characteristic polynomial for η is $\eta^4-(2\alpha^2+2\alpha+3)\eta^2+1=0$, where η attains its minimum $\eta_{\min}=\sqrt{2}$ at $\alpha=-\frac{1}{2}$. Then, we set $\widetilde{N}:=2\sqrt{2}(\sqrt{2}+1)\eta^{2n}$, $n\in\mathbb{N}$, choose $N>\widetilde{N}$ and proceed by induction.

$\boldsymbol{p}=\mathbf{0}$: from definitions (10) and (11), it follows

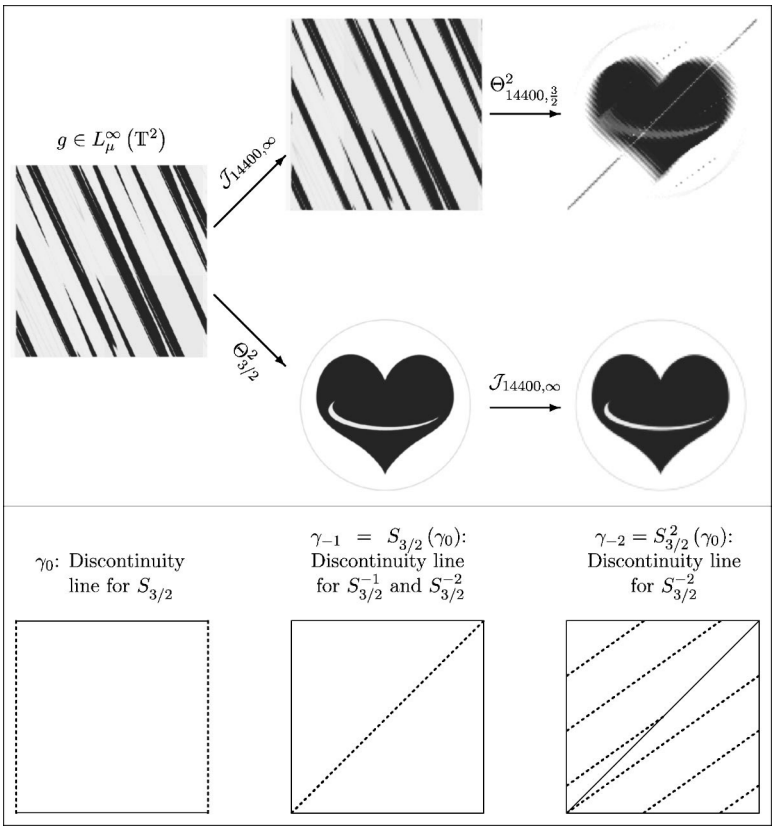

FIG. 5. Here, the same picture as in Fig. 4, is represented, with a finer discretization given by $N=120$ and a different function $g \in L^{\infty}_{\mu}(\mathbb{T}^2)$, for a discontinuous SM, $\Theta_{3/2}$, acting two times. Choosing a function g with sharp variation across γ_0, the preimage of γ_{-1}, the discontinuity of $\Theta_{3/2}$ makes it evident how the differences between $\mathcal{J}_{14\,400,\infty}\circ\Theta^2_{\alpha}$ and $\Theta^2_{14\,400,\alpha}\circ\mathcal{J}_{14\,400,\infty}$ are the greater the closer they are to the discontinuity line γ_{-1}. Of course, the longer the temporal evolution, the worse the correspondence, in the sense that several new discontinuity lines come to play a role. In the case at hand, the map acts twice, and γ_{-2} is felt by $\Theta^2_{14400,\alpha}\circ\mathcal{J}_{14400,\infty}$, as expected.

$$d_{\mathbb{T}^2}\left(\frac{U^0_{\alpha}(N\mathbf{x})}{N},\frac{V^0_{\alpha}(\hat{\mathbf{x}}_N)}{N}\right)=d_{\mathbb{T}^2}\left(\mathbf{x},\frac{\hat{\mathbf{x}}_N}{N}\right)<\frac{1}{\sqrt{2}N}<\frac{\sqrt{2}}{N},$$

where the first inequality follows from (B1), thus relation (23) holds for $p=0$.

$\boldsymbol{p=q-1}$, $\mathbf{1}\leqslant\boldsymbol{q}\leqslant\boldsymbol{n}$: since

$$d_{\mathbb{T}^2}\left(\frac{U^q_{\alpha}(N\mathbf{x})}{N},\frac{V^q_{\alpha}(\hat{\mathbf{x}}_N)}{N}\right)\leqslant d_{\mathbb{T}^2}\left(\frac{U_{\alpha}(U^{q-1}_{\alpha}(N\mathbf{x}))}{N},\frac{U_{\alpha}(V^{q-1}_{\alpha}(\hat{\mathbf{x}}_N))}{N}\right)+d_{\mathbb{T}^2}\left(\frac{U_{\alpha}(V^{q-1}_{\alpha}(\hat{\mathbf{x}}_N))}{N},\frac{V_{\alpha}(V^{q-1}_{\alpha}(\hat{\mathbf{x}}_N))}{N}\right),$$

using (10) in the first term and noting that, from definitions (10) and (11), the second term is less or equal to $\sqrt{2}/N$, we get

$$d_{\mathbb{T}^2}\left(\frac{U^q_{\alpha}(N\mathbf{x})}{N},\frac{V^q_{\alpha}(\hat{\mathbf{x}}_N)}{N}\right)\leqslant d_{\mathbb{T}^2}\left(S_{\alpha}\left(\frac{U^{q-1}_{\alpha}(N\mathbf{x})}{N}\right),S_{\alpha}\left(\frac{V^{q-1}_{\alpha}(\hat{\mathbf{x}}_N)}{N}\right)\right)+\frac{\sqrt{2}}{N}.$$

By the induction hypothesis we have

$$d_{\mathbb{T}^2}\left(\frac{U^{q-1}_{\alpha}(N\mathbf{x})}{N},\frac{V^{q-1}_{\alpha}(\hat{\mathbf{x}}_N)}{N}\right)\leqslant\frac{\sqrt{2}}{N}\left(\frac{\eta^q-1}{\eta-1}\right)\leqslant\frac{\sqrt{2}}{N}\frac{1}{\sqrt{2}-1}\eta^q \tag{B3}$$

$$(\eta > \sqrt{2}, 1 \leqslant q \leqslant n \Rightarrow) < \frac{1}{2}\eta^{q-2n} < \frac{1}{2}\eta^{-1}. \tag{B4}$$

Now we set $\varepsilon = \tilde{N}/2N$, taking into account that $n \geqslant \sqrt{2}$ and use the right inclusion in (22) to deduce that

$$\mathbf{x} \in G_n^N\left(\frac{\tilde{N}}{2N}\right) \Rightarrow \mathbf{x} \notin \overline{\Gamma}_n\left(\frac{\tilde{N}}{2N} - \frac{1}{\sqrt{2}N}\right).$$

At this point, we make use of the following result, which shall be proven in Lemma B.1.3: it states that if a point does not belong to $\overline{\Gamma}_n(\varepsilon)$, the union of the the strips of width $\varepsilon \leqslant \frac{1}{2}$ up to time n, then its orbit under S_α up to time $n-1$ is farther away than $\varepsilon\eta^{-q}$, $0 \leqslant q < n$ from the discontinuity line γ_0. Explicitly

$$\mathbf{x} \notin \overline{\Gamma}_n(\varepsilon) \Rightarrow d_{\mathbb{T}^2}(S_\alpha^q(\mathbf{x}), \gamma_0) > \varepsilon\eta^{-q}, \quad \forall\, 0 \leqslant q < n,$$

where

$$d_{\mathbb{T}^2}\left(\frac{U_\alpha^{q-1}(N\mathbf{x})}{N}, \gamma_0\right) > \left(\frac{\tilde{N}}{2N} - \frac{1}{\sqrt{2}N}\right)\eta^{1-q} > \frac{\sqrt{2}}{N}\left(\frac{\eta^{2n-1} - \eta^{q-1}}{\eta - 1}\right)\eta^{1-q} \geqslant \frac{\sqrt{2}}{N}\left(\frac{\eta^q - 1}{\eta - 1}\right), \tag{B5}$$

where the second inequality comes from $\eta \geqslant \sqrt{2}$, the relation $(\eta^n - 1)/(\eta - 1) \leqslant [1/(\sqrt{2} - 1)]\eta^n$ and the following estimates:

$$\left(\frac{\tilde{N}}{2N} - \frac{1}{\sqrt{2}N}\right) = \frac{\sqrt{2}}{N}\left((\sqrt{2}+1)\eta^{2n} - \frac{1}{2}\right) \geqslant \frac{\sqrt{2}}{N}\left[(\sqrt{2}+1)(\sqrt{2}-1)\frac{\eta^{2n} - \eta + \eta - 1}{\eta - 1} - \frac{1}{2}\right]$$
$$\geqslant \frac{\sqrt{2}}{N}\left[\eta\frac{\eta^{2n-1} - 1}{\eta - 1} + \frac{1}{2}\right] \geqslant \frac{\sqrt{2}}{N}\left(\frac{\eta^{2n-1} - \eta^{q-1}}{\eta - 1}\right).$$

Therefore, comparing (B5) with (B3)

$$d_{\mathbb{T}^2}\left(\frac{U_\alpha^{q-1}(N\mathbf{x})}{N}, \frac{V_\alpha^{q-1}(\hat{\mathbf{x}}_N)}{N}\right) < d_{\mathbb{T}^2}\left(\frac{U_\alpha^{q-1}(N\mathbf{x})}{N}, \gamma_0\right), \quad \forall\, q \leqslant n.$$

As a consequence, the segment $(U_\alpha^{q-1}(N\mathbf{x})/N, V_\alpha^{q-1}(\hat{\mathbf{x}}_N)/N)$ cannot cross the line γ_0. This condition, together with (B4), allows us to use another result proven in Lemma B.1.1b, which states that if a segment (A,B) on the torus does not cross the discontinuity line γ_0 then $d_{\mathbb{T}^2}(S_\alpha(A), S_\alpha(B)) \leqslant \eta d_{\mathbb{T}^2}(A,B)$. We can finally conclude with

$$d_{\mathbb{T}^2}\left(\frac{U_\alpha^q(N\mathbf{x})}{N}, \frac{V_\alpha^q(\hat{\mathbf{x}}_N)}{N}\right) \leqslant \eta\frac{\sqrt{2}}{N}\left(\frac{\eta^q - 1}{\eta - 1}\right) + \frac{\sqrt{2}}{N} = \frac{\sqrt{2}}{N}\left(\frac{\eta^{q+1} - 1}{\eta - 1}\right).$$

■

The following Lemma, which has been used in the proof of the previous proposition, deals with the geometrical properties of the sawtooth dynamics.

Lemma B.1: With η the largest (positive) eigenvalue of $\sqrt{S_\alpha^\dagger S_\alpha}$ and A, $B \in \mathbb{T}^2$ such that $d_{\mathbb{T}^2}(A,B) < \frac{1}{2}\eta^{-1}$, it follows:

(1a) If the segment (A,B) does not cross γ_{-1}, then

$$d_{\mathbb{T}^2}(S_\alpha^{-1}(A), S_\alpha^{-1}(B)) \leqslant \eta d_{\mathbb{T}^2}(A,B). \tag{B6a}$$

(1b) If (A,B) does not cross γ_0, then

$$d_{\mathbb{T}^2}(S_\alpha(A), S_\alpha(B)) \leqslant \eta d_{\mathbb{T}^2}(A,B). \tag{B6b}$$

(2) For any given $\alpha \in \mathbb{R}$, $p \in \mathbb{N}^+$ and $0 \leqslant \varepsilon \leqslant \frac{1}{2}\eta^{-1}$,

$$\mathbf{x} \in \overline{\gamma}_{p-1}(\varepsilon) \Rightarrow S_\alpha^{-1}(\mathbf{x}) \in (\overline{\gamma}_p(\eta\varepsilon) \cup \overline{\gamma}_0(\eta\varepsilon)).$$

(3) For any given $\alpha \in \mathbb{R}$, $n \in \mathbb{N}^+$ and $0 \leqslant \varepsilon \leqslant \frac{1}{2}$, with U_α^q as in (10),

$$\mathbf{x} \notin \overline{\Gamma}_n(\varepsilon) \Rightarrow d_{\mathbb{T}^2}\left(\frac{U_\alpha^q(N\mathbf{x})}{N}, \gamma_0\right) > \varepsilon\eta^{-q}, \quad \forall\, 0 \leqslant q < n.$$

Proof: In the course of the proof, we shall use that

$$\|S_\alpha^{\pm 1} \cdot \mathbf{v}\|_{\mathbb{R}^2} \leqslant \eta \|\mathbf{v}\|_{\mathbb{R}^2}, \tag{B7a}$$

$$\|S_\alpha^{\pm 1} \cdot \mathbf{v}\|_{\mathbb{R}^2} \geqslant \eta^{-1} \|\mathbf{v}\|_{\mathbb{R}^2}, \tag{B7b}$$

which directly follows from the definition of η, where $\mathbf{v}$ is any two-dimensional real vector.

In order to prove (B6), it is convenient to unfold $\mathbb{T}^2$ and the discontinuity of S_α on the plane $\mathbb{R}^2$. This is most easily done as follows. Points $A \in \mathbb{T}^2 = \mathbb{R}^2/\mathbb{Z}^2$ are represented by equivalence classes

$$[\mathbf{a}] := \{\mathbf{a} + \mathbf{n}, \mathbf{n} \in \mathbb{Z}^2\}, \quad \mathbf{a} \in [0,1)^2. \tag{B8}$$

Given A, $B \in \mathbb{T}^2$, let $A^b \in [\mathbf{a}]$ be such that

$$d_{\mathbb{T}^2}([\mathbf{a}],[\mathbf{b}]) = \|A^b - \mathbf{b}\|_{\mathbb{R}^2}.$$

Notice that

$$d_{\mathbb{T}^2}([\mathbf{a}],[\mathbf{b}]) = \|\mathbf{a} - \mathbf{b}\|_{\mathbb{R}^2} \text{ iff } \|\mathbf{a} - \mathbf{b}\|_{\mathbb{R}^2} \leqslant \frac{1}{2} \tag{B9}$$

(1a) (A,B) not crossing γ_{-1} means that the segment $(A^b,\mathbf{b})$ does not intersect γ_{-1}. Periodically covering the plane $\mathbb{R}^2$ by squares $[0,1)^2$, the γ_{-1} lines form a set of (parallel) straight lines $x_1 - x_2 = n \in \mathbb{Z}$; it follows that $(A^b,\mathbf{b})$ does not cross γ_{-1} iff

$$\lfloor A_1^b - A_2^b \rfloor = \lfloor b_1 - b_2 \rfloor, \tag{B10}$$

where the integral part on the r.h.s. takes values 0, −1, depending on which side of the diagonal γ_{-1} the point $\mathbf{b}$ lies within.

As $S_\alpha^\pm$ are not sensitive to the integer part of their arguments, their actions are the same on all elements of the equivalence classes (B8), that is

$$d_{\mathbb{T}^2}(S_\alpha^{-1}(A),S_\alpha^{-1}(B)) = d_{\mathbb{T}^2}(S_\alpha^{-1}([\mathbf{a}]),S_\alpha^{-1}([\mathbf{b}])) = d_{\mathbb{T}^2}(S_\alpha^{-1}(A^b),S_\alpha^{-1}(\mathbf{b})).$$

By expanding $\langle x \rangle = x - \lfloor x \rfloor$, using the definition of $S_\alpha^{-1}(\cdot)$ and putting together all integral contributions, condition (B10) yields

$$\begin{aligned} d_{\mathbb{T}^2}(S_\alpha^{-1}(A),S_\alpha^{-1}(B)) &= \min_{\mathbf{m} \in \mathbb{Z}^2} \|S_\alpha^{-1}(A) - S_\alpha^{-1}(B) + \mathbf{m}\|_{\mathbb{R}^2} \\ &= \min_{\mathbf{m}' \in \mathbb{Z}^2} \|S_\alpha^{-1} \cdot (A^b - \mathbf{b}) + \mathbf{m}'\|_{\mathbb{R}^2} = d_{\mathbb{T}^2}(S_\alpha^{-1} \cdot (A^b - \mathbf{b}),0). \end{aligned}$$

Applying (B7), since we assumed $d_{\mathbb{T}^2}(A,B) < \frac{1}{2}\eta^{-1}$, we estimate

$$\|S_\alpha^{-1} \cdot (A^b - \mathbf{b})\|_{\mathbb{R}^2} \leqslant \eta \|A^b - \mathbf{b}\|_{\mathbb{R}^2} = \eta d_{\mathbb{T}^2}(A,B) < \frac{1}{2}.$$

In particular, using (B9), the previous inequalities imply

$$d_{\mathbb{T}^2}(S_\alpha^{-1}\cdot(A^b-\mathbf{b}),0)=\|S_\alpha^{-1}\cdot(A^b-\mathbf{b})\|_{\mathbb{R}^2}\leqslant \eta d_{\mathbb{T}^2}(A,B).$$

(1b) Using the same argument as (1a), the union of γ_0 lines constitute a set of straight lines $x_1=n\in\mathbb{Z}$; therefore the segment $(A^b,\mathbf{b})$ does not cross γ_0 iff

$$\lfloor A_1^b\rfloor=\lfloor b_1\rfloor. \tag{B11}$$

As done before, by means of (B11), we arrive at

$$d_{\mathbb{T}^2}(S_\alpha(A),S_\alpha(B))=d_{\mathbb{T}^2}(S_\alpha(A^b),S_\alpha(\mathbf{b}))=d_{\mathbb{T}^2}(S_\alpha\cdot(A^b-\mathbf{b}),0).$$

The proof can now be completed exactly as for point (2a) before.

(2) We denote by $d_{\mathbb{T}^2}(\mathbf{x},\gamma)=\inf_{\mathbf{y}\in\gamma}d_{\mathbb{T}^2}(\mathbf{x},\mathbf{y})$ the distance of the point $\mathbf{x}\in\mathbb{T}^2$ from a curve $\gamma\in\mathbb{T}^2$. Then, from definition (18) we have:

$$\mathbf{x}\in\overline{\gamma}_{p-1}(\varepsilon)\Rightarrow\varepsilon\geqslant d_{\mathbb{T}^2}(\mathbf{x},\gamma_{p-1})=d_{\mathbb{T}^2}(\mathbf{x},\mathbf{y}^\star), \tag{B12}$$

where $\mathbf{y}^\star$ is the nearest point to $\mathbf{x}$ belonging to γ_{p-1}.

We distinguish two cases:

(2′) The segment $(\mathbf{x},\mathbf{y}^\star)$ does not cross (we stipulate that, if $\mathbf{y}^\star\in\gamma_{-1}$ or $\mathbf{x}\in\gamma_{-1}$, we are still in a noncrossing condition) γ_{-1}: From (B12) and point (1a), since $S_\alpha^{-1}(\mathbf{y}^\star)\in\gamma_p$ [see (16a)], we get

$$d_{\mathbb{T}^2}(S_\alpha^{-1}(\mathbf{x}),\gamma_p)\leqslant d_{\mathbb{T}^2}(S_\alpha^{-1}(\mathbf{x}),S_\alpha^{-1}(\mathbf{y}^\star))\leqslant\eta d_{\mathbb{T}^2}(\mathbf{x},\mathbf{y}^\star)\leqslant\eta\varepsilon.$$

Therefore $S_\alpha^{-1}(\mathbf{x})\in\overline{\gamma}_p(\eta\varepsilon)$.

(2″) The segment $(\mathbf{x},\mathbf{y}^\star)$ crosses γ_{-1}: In this case, there exists $\mathbf{z}\in\gamma_{-1}$ such that

$$d_{\mathbb{T}^2}(\mathbf{x},\mathbf{y}^\star)=d_{\mathbb{T}^2}(\mathbf{x},\mathbf{z})+d_{\mathbb{T}^2}(\mathbf{z},\mathbf{y}^\star). \tag{B13}$$

Then, from (B12) and (B13),

$$\varepsilon\geqslant d_{\mathbb{T}^2}(\mathbf{x},\mathbf{y}^\star)\geqslant d_{\mathbb{T}^2}(\mathbf{x},\mathbf{z}).$$

Since, according to (16), $S_\alpha^{-1}(\mathbf{z})\in\gamma_0$, from point (1a) we get

$$d_{\mathbb{T}^2}(S_\alpha^{-1}(\mathbf{x}),\gamma_0)\leqslant d_{\mathbb{T}^2}(S_\alpha^{-1}(\mathbf{x}),S_\alpha^{-1}(\mathbf{z}))\leqslant\eta\varepsilon,$$

that is $S_\alpha^{-1}(\mathbf{x})\in\overline{\gamma}_0(\eta\varepsilon)$.

(3) From point (2), it follows that when $0\leqslant\varepsilon\leqslant\frac{1}{2}$, for $p\in\mathbb{N}^+$,

$$\mathbf{x}\notin(\overline{\gamma}_p(\varepsilon)\cup\overline{\gamma}_0(\varepsilon))\Rightarrow S_\alpha(\mathbf{x})\notin\overline{\gamma}_{p-1}(\eta^{-1}\varepsilon). \tag{B14}$$

We prove by induction that when $0\leqslant\varepsilon\leqslant\frac{1}{2}$, for $m\in\mathbb{N}^+$,

$$\mathbf{x}\notin\bigcup_{p=0}^{m}\overline{\gamma}_p(\varepsilon)\Rightarrow S_\alpha(\mathbf{x})\notin\bigcup_{p=0}^{m-1}\overline{\gamma}_p(\eta^{-1}\varepsilon). \tag{B15}$$

For $m=1$, (B15) follows from (B14); if (B15) holds for $m=r$, then take

$$\mathbf{x}\notin\bigcup_{p=0}^{r+1}\overline{\gamma}_p(\varepsilon).$$

This means that

$$\mathbf{x}\notin\bigcup_{p=0}^{r}\overline{\gamma}_p(\varepsilon)$$

and $\mathbf{x}\notin(\overline{\gamma}_{r+1}(\varepsilon)\cup\overline{\gamma}_0(\varepsilon))$. Now, using the induction hypothesis and (B14), we get

$$\mathbf{x} \notin \bigcup_{p=0}^{r+1} \overline{\gamma_p}(\varepsilon) \Rightarrow S_\alpha(\mathbf{x}) \notin \bigcup_{p=0}^{r-1} \overline{\gamma_p}(\eta^{-1}\varepsilon)$$

$$S_\alpha(\mathbf{x}) \notin \overline{\gamma_r}(\eta^{-1}\varepsilon).$$

Setting $m=n-1$ and iterating q times the implication (B15) argument, we get

$$\mathbf{x} \notin \bigcup_{p=0}^{n-1} \overline{\gamma_p}(\varepsilon) \Rightarrow S_\alpha^q(\mathbf{x}) \notin \bigcup_{p=0}^{n-1-q} \overline{\gamma_p}(\eta^{-q}\varepsilon), \quad \forall\, 0 \leqslant q < n.$$

In particular $S_\alpha^q(\mathbf{x}) \notin \overline{\gamma_0}(\eta^{-q}\varepsilon)$, which leads to the lower bound

$$d_{\mathbb{T}^2}(S_\alpha^q(\mathbf{x}), \gamma_0) > \eta^{-q}\varepsilon, \quad \forall\, 0 \leqslant q < n,$$

where the result follows in view of definitions (10) and (19). ■

APPENDIX C. PROOF OF PROPOSITION 4.2

(a) In (16a), we have defined $\gamma_p = S_\alpha^{-p}(\gamma_0)$ where $S_\alpha^{-1}(\mathbf{x})$ (as well as $S_\alpha^{-p}(\mathbf{x})$) is a piecewise continuous mapping onto $\mathbb{T}^2$ with jump discontinuities across the γ_p lines due to the presence of the function $\langle\cdot\rangle$ in (9). Away from the discontinuities, $S_\alpha^{-p}(\mathbf{x})$ behaves as the matrix action $S_\alpha^{-p}\cdot\mathbf{x}$. We now want to estimate the length $l(\gamma_p)$; in order to do that, we unfold γ_p on the plane and calculate the length of the segment $\left\{\mathbf{x}\in\mathbb{R}^2 \middle| \mathbf{x} = S_\alpha^{-p}\cdot\binom{0}{y}, y\in[0,1)\right\}$, which, in its turn, is the image of γ_0 under the matrix action given by $S_\alpha^{-p}\cdot\mathbf{x}$. Therefore, using (B7), the result follows.

(b) Let $\overline{L}(\varepsilon)$ denote the set of points having distance from a segment of length L smaller or equal than ε: it has a volume (under the Lebesgue measure μ) given by

$$\mu(\overline{L}(\varepsilon)) = 2L\varepsilon + \pi\varepsilon^2,$$

where the last term on the r.h.s. takes into account rounding of the extremes of the strip by to semicircle of radius ε. Then (29b) follows from (29a).

(c) This follows from definition (19):

$$\mu(\overline{\Gamma}_n(\varepsilon)) = \mu\left(\bigcup_{p=0}^{n-1} \overline{\gamma_p}(\varepsilon)\right) \leqslant \sum_{p=0}^{n-1} \mu(\overline{\gamma_p}(\varepsilon)).$$

Using (29b), we can write:

$$\mu(\overline{\Gamma}_n(\varepsilon)) \leqslant 2\varepsilon \sum_{p=0}^{n-1} \eta^p + \sum_{p=0}^{n-1} \pi\varepsilon^2 = 2\varepsilon\frac{\eta^n - 1}{\eta - 1} + n\pi\varepsilon^2.$$

Finally the estimate $(x^p-1)/(x-1) \leqslant (\sqrt{2}+1)x^p$, valid for $x > \sqrt{2}$, yields

$$\mu(\overline{\Gamma}_n(\varepsilon)) \leqslant 2\varepsilon(\sqrt{2}+1)\eta^n + n\pi\varepsilon^2.$$

(d) By writing the left inclusion in (22) in terms of complementary sets, with $\varepsilon = \widetilde{N}/2N$, we get

$$\left[G_n^N\left(\frac{\widetilde{N}}{2N}\right)\right]^\circ \subseteq \overline{\Gamma}_n\left(\frac{\widetilde{N}}{2N} + \frac{1}{\sqrt{2}N}\right)$$

and so

$$\mu\left(\left[G_n^N\left(\frac{\tilde{N}}{2N}\right)\right]^\circ\right) \leqslant \mu\left(\overline{\Gamma}_n\left(\frac{\tilde{N}}{2N}+\frac{1}{\sqrt{2}N}\right)\right).$$

By substituting in (29c) $(\tilde{N}+\sqrt{2})/2N=\tilde{N}/2N+1/\sqrt{2}N$ in the place of ε, we get

$$\mu\left(\left[G_n^N\left(\frac{\tilde{N}}{2N}\right)\right]^\circ\right) \leqslant \frac{\tilde{N}+\sqrt{2}}{2N}(\sqrt{2}+1)\left(2\eta^n+\frac{n}{\sqrt{2}+1}\pi\frac{\tilde{N}+\sqrt{2}}{2N}\right). \tag{C1}$$

Finally, the r.h.s of (C1) can be estimated by the following upper bounds:

$$\pi\frac{\tilde{N}+\sqrt{2}}{2N}<2$$

$$\frac{n}{\sqrt{2}+1}<\eta^n$$

$$(\tilde{N}+\sqrt{2})(\sqrt{2}+1)<19\eta^{2n}$$

which hold for $\forall N>\tilde{N}$, $\eta\geqslant\sqrt{2}$, and $\forall n\in\mathbb{N}^+$. This ends the proof. ■

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Lagrangian formalism for nonlinear second-order Riccati systems: One-dimensional integrability and two-dimensional superintegrability

José F. Cariñena[a] and Manuel F. Rañada[b]
Departamento de Física Teórica, Facultad de Ciencias Universidad de Zaragoza, 50009 Zaragoza, Spain

Mariano Santander[c]
Departamento de Física Teórica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid, Spain

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The existence of a Lagrangian description for the second-order Riccati equation is analyzed and the results are applied to the study of two different nonlinear systems both related with the generalized Riccati equation. The Lagrangians are non-natural and the forces are not derivable from a potential. The constant value E of a preserved energy function can be used as an appropriate parameter for characterizing the behavior of the solutions of these two systems. In the second part the existence of two-dimensional versions endowed with superintegrability is proved. The explicit expressions of the additional integrals are obtained in both cases. Finally it is proved that the orbits of the second system, that represents a nonlinear oscillator, can be considered as nonlinear Lissajous figures © *2005 American Institute of Physics.* [DOI: 10.1063/1.1920287]

I. INTRODUCTION

Ince studied, in his well-known book of differential equations,[1] the following equation,

$$w'' + 3ww' + w^3 = q(z)$$

and proved that it has the general solution $w = u'/u$, where u is a general solution of the linear equation of the third order $u''' = q(z)u$. This equation was also studied by Davis in Ref. 2 as a particular case of the generalized Riccati equations (according to Davis the family of these nonlinear equations was first studied by E. Vessiot in 1895 and G. Vallenberg in 1899; see Refs. 3–5 for some more recent studies related with higher-order Riccati equations). Later on Leach *et al.*[6,7] considered the equation

$$\ddot{q} + q\dot{q} + \beta q^3 = 0 \tag{1}$$

and pointed out that "for $\beta = 1/9$ is linearizable, possesses eight symmetries and is completely integrable" and they add "consequently, we could expect that this remarkable mathematical property corresponds to an important physical one appearing (or disappearing) for this value which consequently would appear as a critical one." This particular $\beta = 1/9$ equation was also obtained in Ref. 8 in the study of nonlinear equations with the maximum number of symmetries (see Refs. 9–12, for the Lie symmetry approach to dynamical systems).

[a]Electronic mail: jfc@unizar.es
[b]Electronic mail: mfran@unizar.es
[c]Electronic mail: santander@fta.uva.es

Recently Chandrasekar *et al.*[13] have studied a generalization of this equation obtained as a particular case of the Lienard equation

$$\ddot{x} + f(x)\dot{x} + g(x) = 0$$

given by $f(x) = k\,x$ and $g(x) = (1/9)k\,x^3 + \lambda x$. Although this new equation also belongs to the generalized Riccati family studied by Davis and Leach *et al.*, they make use of a two step procedure to solve the problem: first they use the so-called Prelle-Singer method[14–17] for obtaining a set of time-dependent integrals of motion and secondly they use this time-dependent family in order to compute the solution. The result is interpreted, when $\lambda > 0$, as an "unusual Liénard type oscillator with properties of a linear harmonic oscillator." But we wish to call attention to one property discussed in the final part of the article (after finalizing with the Prelle-Singer method): the existence of a Lagrangian description.

The main objective of this article is to develop a deeper analysis of these nonlinear equations using the Lagrangian formalism as an approach. In fact, the starting point of our approach is the fact that the Riccati equation belongs to a family of nonlinear equations admitting a Lagrangian description. This has interesting consequences, the most important of them is that Riccati systems are systems endowed with a preserved energy function. We study the two nonlinear systems first in one dimension and then in two dimensions. Moreover we prove that the two-dimensional extensions are not only integrable but also superintegrable. We note that this situation has a certain similarity with the one-dimensional nonlinear oscillator studied by Mathews and Lakshmanan[18] that has been proved to admit a superintegrable two-dimensional version.[19]

The plan of this article is as follows: In Sec. II we present a Lagrangian approach to a family of nonlinear equations that includes the second-order Riccati equation as a particular case. Section III, devoted to the first nonlinear system ("dissipative"-looking system), is divided in three parts corresponding to the one-dimensional system, geometric formalism and symmetries, and two-dimensional system and super-integrability, respectively. Section. IV, that is devoted to the second nonlinear system ("nonlinear oscillator"), also first studies the $n=1$ system and then the two-dimensional system that, as we have pointed out, is also endowed with super-integrability. Finally in Sec. V we make some comments.

II. LAGRANGIAN FORMALISM AND SECOND-ORDER RICCATI EQUATIONS

In this article we shall consider the following nonlinear second-order equation

$$y'' + [b_0(t) + b_1(t)y]y' + a_0(t) + a_1(t)y + a_2(t)y^2 + a_3(t)y^3 = 0, \tag{2}$$

where we suppose that $a_3 > 0$ and the two functions b_0, b_1, are not independent but satisfy

$$b_0 = \frac{a_2}{\sqrt{a_3}} - \frac{a_3'}{2a_3}, \quad b_1 = 3\sqrt{a_3}.$$

The more important property of this equation is that it can be transformed into a third-order linear equation by the substitution

$$y(t) = \frac{1}{\sqrt{a_3(t)}}\frac{v'(t)}{v(t)}.$$

Thus Eq. (2), that is the natural second-order generalization of the wellknown Riccati equation, is therefore a nonlinear equation the solution of which can be expressed in terms of solutions of a linear equation of the third order. In fact, it can be considered as the particular $n=2$ case of a more general situation that can be approached by Lie theory or by the action of an operator R. From the Lie theory of symmetries of differential equations, the invariance of the n-order linear equation,

$$v^{(n)} + p_1(t)v^{(n-1)} + \cdots + p_n(t)v = 0,$$

under the vector field $X = v(\partial/\partial v)$, that represents the infinitesimal generator of dilations, means the existence of a change $v = e^u$ such that X becomes $X = \partial/\partial u$, and the transformed equation reduces to an equation of order $(n-1)$ for $y = u'$ that for the $n = 2$ reduces to the usual first-order Riccati equation. Alternatively if R denotes the following differential operator:

$$R = \frac{\mathrm{d}}{\mathrm{d}t} + y(t),$$

then the Riccati equation of order n is given by

$$(R^n + p_1 R^{n-1} + \cdots + p_{n+1}R + p_n)y + p_{n+1} = 0,$$

where $p_j = p_j(t)$, $j = 1, 2, \ldots, n+1$, are $n+1$ arbitrary functions. We note that these two methods lead to the subfamily of the nonlinear equations with the coefficient of the higher power equal to one; nevertheless the general Riccati equation is generated by the change $t = f(\tau)$ of the independent variable; for example for $n = 2$ we obtain

$$y'' + [p_1 + 3y]y' + p_3 + p_2 y + p_1 y^2 + y^3 = 0,$$

and after the time reparametrization we arrive at

$$\frac{\mathrm{d}^2 y}{\mathrm{d}\tau^2} + \left[\left(f' p_1 - \frac{f''}{f'}\right) + 3f' y\right]\frac{\mathrm{d}y}{\mathrm{d}\tau} + (f'^2 p_3) + (f'^2 p_2)y + (f'^2 p_1)y^2 + f'^2 y^3 = 0.$$

We are interested in the study of nonlinear systems given by (2) but first, in this section, we consider a more general family from which the second-order Riccati equation appears as a particular case.

At this point we recall that a Lagrangian function L is called 'natural' or 'of mechanical type' when it is of the form $L = T - V$, where T is a quadratic kinetic term and V is a potential function. Most of the known Lagrangian equations arise from Lagrangians of this particular type; nevertheless the Lagrangian formalism is well defined, not only for these specific functions but also for more general Lagrangian functions.

Proposition 1: The nonlinear second-order Riccati equation admits a Lagrangian description.

Proof: We first consider the following one degree of freedom Lagrangian:

$$L = \frac{1}{v_x + kU(x,t)}. \tag{3}$$

Then we arrive at the following second-order nonlinear equation:

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} + \left(\frac{3}{2}\right)kU_x'\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right) + \left(\frac{1}{2}\right)k^2 UU_x' + kU_t' = 0. \tag{4}$$

In the particular case of the function $U = U(x,t)$ being a quadratic function

$$U = c_0(t) + c_1(t)x + c_2(t)x^2,$$

Eq. (4) reduces to

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} + (b_0 + b_1 x)\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right) + a_0 + a_1 x + a_2 x^2 + a_3 x^3 = 0, \tag{5}$$

where the four functions a_0, a_1, a_2, a_3, are given by

$$a_0 = \tfrac{1}{2}c_0 c_1 + c_0', \quad a_1 = c_0 c_2 + \tfrac{1}{2}c_1^2 + c_1',$$

$$a_2 = \tfrac{3}{2}c_1c_2 + c_2', \quad a_3 = c_2^2,$$

and the two functions b_0 and b_1 satisfy the appropriate restrictions

$$b_0 = \tfrac{3}{2}c_1, \quad b_1 = 3c_2.$$

Thus, the second-order Riccati equation [Eq. (5)], that is a particular case of Eq. (4), is the Euler-Lagrange equation of the Lagrangian function (3) in the particular case of a quadratic function U.

As a corollary of this proposition we can state that, if the function U is time independent, then the nonlinear equation (4) has a first integral that can be interpreted as a preserved energy. The idea is as follows: if we restrict our study to the case of time-independent systems, that is, to nonlinear equations arising from a Lagrangian of the form

$$L = \frac{1}{v_x + kU(x)} \tag{6}$$

then we can define an associated Lagrangian energy E_L by the usual procedure

$$E_L = \Delta(L) - L, \quad \Delta = v_x \frac{\partial}{\partial v_x},$$

and we arrive to

$$E_L = \frac{-(2v_x + kU(x))}{(v_x + kU(x))^2}, \quad \frac{\mathrm{d}}{\mathrm{d}t}E_L = 0.$$

Note that L is non-natural and, as there is neither kinetic term T nor potential function V, the energy cannot be of the form $E_L = T + V$. Note also that a Lagrangian is defined up to certain ambiguities; that is, $\widetilde{L} = c_1L + \underset{\sim}{c_0}$ determines the same differential equation but it leads to an slightly different energy $\widetilde{E_L}$ given by $\widetilde{E_L} = c_1E_L - c_0$. In the natural case, c_1 is determined by the corresponding Riemannian metric (hence the classical one-half coefficient) and c_0 is absorbed in the potential; here we have just taken $c_1 = 1, c_0 = 0$. Concerning the negative sign, that could be considered as something inconvenient, it does not matter at all (it is only an aesthetic question); in fact it can be removed just by chosen $\widetilde{L} = -L$ as a new Lagrangian.

As for the natural case we can obtain the solution of the dynamics from the conservation law of the energy. If we assume that E_L takes the constant value $E_L = E$, then we arrive at

$$E\,v_x^2 + 2(1 + k\,E\,U(x))v_x + k(1 + k\,E\,U(x))U(x) = 0$$

and on solving for v_x and making separation of variables we arrive at

$$t - t_0 = -\int_{x_0}^{x} \frac{E\,\mathrm{d}x}{(1 + kEU(x)) \pm \sqrt{1 + kEU(x)}}. \tag{7}$$

The motion is confined to the region where $E \geqslant -1/(kU)$. To sum up, a time-independent system described by the nonlinear equation (4) is solvable and the solution of the dynamics is given (up to one integration) by (7).

A remarkable property is that the conservation of the energy E_L leads to a plus/minus sign in the expression for the velocity

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{-(1 + kEU(x)) \pm \sqrt{1 + kEU(x)}}{E}.$$

Thus, we obtain two different values for the velocity at the same point x. It is known that in the standard case of a particle in a potential $V(x)$ we also have two possibilities but both with the same

modulus (the positive value for the motion from left to right and the negative for the opposite motion from right to left). In this case the situation is different; we have a Lagrangian but not a potential and the two possible values differ, not just in the sign, but in the absolute value; thus the motions from left to right and from right to left take place at different velocities.

We close this section with the problem of the existence of alternative Lagrangians.

In differential geometric terms a time-independent Lagrangian function L determines an exact two-form ω_L defined as

$$\theta_L = \left(\frac{\partial L}{\partial v_x}\right) \mathrm{d}x, \quad \omega_L = -\,\mathrm{d}\,\theta_L,$$

in such a way that, when L is nonsingular, ω_L is symplectic and the dynamics is given by the vector field Γ_L solution of the equation

$$i(\Gamma_L)\omega_L = dE_L.$$

In this particular case ω_L and Γ_L are given by

$$\omega_L = \frac{2\mathrm{d}x \wedge \mathrm{d}v_x}{(v_x + kU(x))^3}, \quad \Gamma_L = v_x \frac{\partial}{\partial x} + F_x \frac{\partial}{\partial v_x}, \quad F_x = -\left(\frac{1}{2}\right) k(3v_x + kU(x))U_x'.$$

An important property of the Lagrangian formalism is that for one degree of freedom systems there exist many different equivalent Lagrangians.[20,21] A sketch of the proof is as follows: in a two-dimensional manifold all the symplectic forms must be proportional. Hence, for a one degree of freedom Lagrangian, any other symplectic form ω_2 must be proportional to ω_L, that is $\omega_2 = f\omega_L$. Then

$$i(\Gamma_L)\omega_2 = f\, i(\Gamma_L)\omega_L = f\mathrm{d}E_L.$$

The right-hand side is an exact one form if, and only if, $\mathrm{d}f \wedge \mathrm{d}E_L = 0$, which shows that f must be a function of E_L. In this case it can be proved that the new symplectic form ω_2 is derivable from an alternative Lagragian $L_2 \neq L$ for Γ_L.

In this particular case, starting with the Lagrangian (6) and assuming for the constant of motion f the particular expression $f = (-1/E_L)^{3/2}$, we have obtained the following function

$$L_2 = \sqrt{2v_x + kU(x)} \tag{8}$$

as a new alternative Lagrangian for the t-independent version of Eq. (4). This new Lagrangian, that is neither natural or of mechanical type, is equivalent to L in the sense that both determine the same dynamics. Nevertheless we must say that it is not clear whether L_2 will lead to simpler expressions for other dynamical properties; so, in the following, we only use the original Lagrangian (6).

III. LAGRANGIAN CONSERVATIVE APPROACH TO A "DISSIPATIVE"-LOOKING NONLINEAR SYSTEM

A. One-dimensional nonlinear system: Energy and integrability

We now apply the formalism introduced in Sec. II to the study of the following nonlinear equation:

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + 3kx\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right) + k^2x^3 = 0. \tag{9}$$

It is a special case of Eq. (2) and because of this is a Lagrangian equation. In fact, it is easy to verify that it can be obtained from the following Lagrangian function:

$$L = \frac{1}{v_x + kx^2}. \tag{10}$$

Two important properties are as follows.

(i) We note that the value $\beta = 1/9$, pointed out by Leach *et al.*[7] as the particular value introducing a high degree of regularity in the nonlinear problem (1), appears now as related with the Lagrangian origin of the equation. That is, only if $\beta = 1/9$, then Eq. (1) belongs to the Lagrangian family (9) arising from (10).

(ii) This equation looks like a dissipative equation with the damping term proportional to xv_x; nevertheless it is in fact a conservative system because of its Lagrangian origin. What happens is that the term conservative is usually considered in the Newtonian sense, that is, a particle moving in a one-dimensional potential and forces determined as the gradient of the potential. Here the force is a velocity-dependent force and conservative just means the existence of a preserved (non-Newtonian) energy function that is given by

$$E_L = \frac{-(2v_x + k\,x^2)}{(v_x + k\,x^2)^2}.$$

Next we turn to the solution of the dynamics. Instead of considering directly the nonlinear equation we can solve this problem by making use of the conservation law of the energy; if we assume $E_L = E$, then we arrive at

$$E\,v_x^2 + 2(1 + k\,Ex^2)v_x + k(1 + k\,Ex^2)x^2 = 0$$

and solving for v_x we obtain

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{-(1 + k\,Ex^2) \pm \sqrt{1 + k\,Ex^2}}{E}.$$

So, after integration, we arrive at

$$t = \frac{1}{kx}(1 \pm \sqrt{1 + k\,Ex^2})$$

which yields

$$x = \frac{2t}{kt^2 - E}$$

that represents the solution of the dynamics as a function of the constant value E of the Lagrangian energy (for ease of notation we give the solution for the particular initial conditions $(t_0 = 0, x_0 = 0)$). The system is well defined for $(k > 0, E < 0)$ and $(k < 0, E > 0)$, but for $(k < 0, E < 0)$ or $(k > 0, E > 0)$ it is singular at $t = \pm\sqrt{|E|/|k|}$. In fact the double change $(k, E) \to (-k, -E)$ is equivalent to a time-inversion (see Fig. 1).

Since $x(t)$ is the quotient of two polynomials in t, with the denominator of a higher degree than the numerator, the trajectories approach the origin when t increases. How can this behavior be compatible with the conservation of the energy? An analysis of the expression that E_L takes on the trajectories shows that it reduces to the quotient of two functions both going down as $t \to \infty$, but in such a way that the ratio remains constant. Moreover it can also be proved that the velocity v_x decreases as $t \to \infty$ in such a way that the particle approaches but never reaches the origin in the phase plane. The important point is that the dependence of E_L with respect to v_x is defined in such a way that even when $\mathrm{d}x/\mathrm{d}t$ decreases the value of E_L remains constant.

The phase space analysis shows that the origin is a nonelementary critical point for which the linear approximation is not valid. If we consider a small neighborhood of the point, then we find,

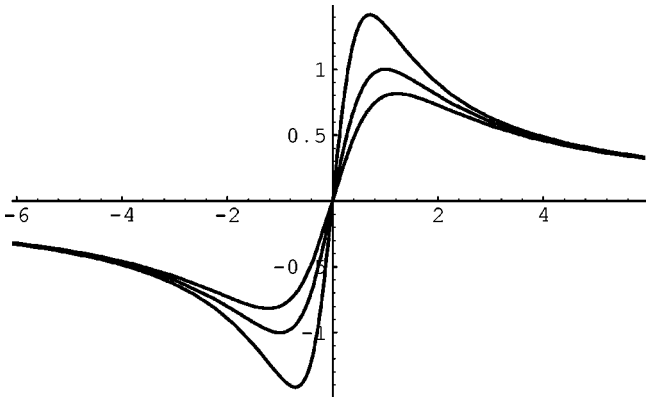

FIG. 1. Plot of x as a function of t, for $k=1$ and three different values of the energy: $E=-0.5$, $E=-1.0$, and $E=-1.5$.

when $k>0$, that it has four different sectors[22] (see Fig. 2): an elliptic sector (upper side), a hyperbolic sector (lower side) and two parabolic sectors (a source on the left and a sink on the right).

B. Symplectic formalism and master symmetries

It is known that the nonlinear equation (9) admits constants of motion depending explicitly on the time t.[13,16] Now we prove that this property is related with the fact that the Lagrangian (10) admits "master symmetries." This is in fact an important property, not only from the geometric point of view but also because it is directly related with the superintegrability of the two-dimensional version of this system.

A function T that satisfies the following property:

$$\frac{\mathrm{d}}{\mathrm{d}t}T\neq 0,\ldots,\quad \frac{\mathrm{d}^m}{\mathrm{d}t^m}T\neq 0,\quad \frac{\mathrm{d}^{m+1}}{\mathrm{d}t^{m+1}}T=0,$$

is called a generator of integrals of motion of degree m. Notice that this means that the function T is a nonconstant function generating a constant of motion by time derivation. If we denote by T_{x1} and T_{x2}, the functions

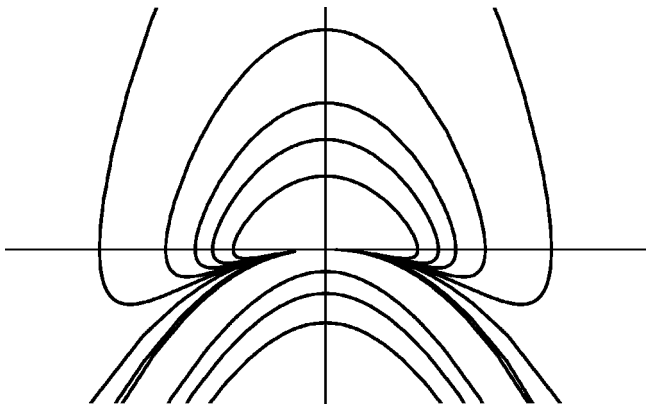

FIG. 2. Phase space trajectories, for $k=1$, in the neighborhood of the origin.

$$T_{x1} = \frac{1}{v_x + k\,x^2}, \quad T_{x2} = \frac{x}{v_x + k\,x^2},$$

then we have

$$\frac{\mathrm{d}}{\mathrm{d}t}T_{x2} = 1, \quad \frac{\mathrm{d}}{\mathrm{d}t}T_{x1} = k\,T_{x2}, \quad \frac{\mathrm{d}^2}{\mathrm{d}t^2}T_{x1} = k, \quad \frac{d^3}{dt^3}T_{x1} = 0.$$

Hence T_{x1} and T_{x2} are generators of integrals of motion for the Lagrangian (10).

In geometric terms this property is related with the existence of master symmetries.[23–27] If the dynamics is represented by a certain vector field Γ; then a vector field Z that satisfies the following two properties

$$[Z,\Gamma] = \widetilde{Z} \neq 0, \quad [\widetilde{Z},\Gamma] = 0,$$

is called a "master symmetry" of degree $m=1$ for Γ. If Z is such that

$$[Z,\Gamma] = \widetilde{Z} \neq 0, \quad [\widetilde{Z},\Gamma] \neq 0, \quad [[\widetilde{Z},\Gamma],\Gamma] = 0,$$

then it is called a master symmetry of degree $m=2$.

We focus our attention in the case of master symmetries given rise via $\widetilde{Z}$ to constants of motion. Let L be a time-independent Lagrangian, Z the Hamiltonian vector field of a certain function T, and suppose that Z is a (time-independent) master symmetry of Γ_L. Then the time-dependent vector field Y_Z determined by Z and defined as

$$Y_Z = Z + t[Z,\Gamma_L] + \tfrac{1}{2}t^2[[Z,\Gamma_L],\Gamma_L] + \ldots$$

is a time-dependent symmetry of Γ_L that, in the case $m=1$, satisfies

$$i(Y_Z)\Omega_E = \mathrm{d}[T - t\,\Gamma_L(T)]$$

where $\Omega_E = \omega_L + \mathrm{d}E_L \wedge \mathrm{d}t$. Hence the time-dependent function $J^t = T - t\,\Gamma_L(T)$ is a time-dependent constant of motion (for $m=2$ the corresponding constant J^t is quadratic in t).

We now return to the Lagrangian (10) and denote by Z_{x1} and Z_{x2}, the Hamiltonian vector fields of T_{x1} and T_{x2},

$$i(Z_{x1})\omega_L = \mathrm{d}T_{x1}, \quad i(Z_{x2})\omega_L = \mathrm{d}T_{x2},$$

which are given by

$$Z_{x1} = -\frac{1}{2}M_x\left(\frac{\partial}{\partial x} - 2kx\frac{\partial}{\partial v_x}\right),$$

$$Z_{x2} = -\frac{1}{2}M_x\left(x\frac{\partial}{\partial x} + (v_x - kx^2)\frac{\partial}{\partial v_x}\right),$$

where M_x denotes $M_x = v_x + k\,x^2$. Then we have

$$[Z_{x1},\Gamma_L] = -\,k\,Z_{x2}, \quad [[Z_{x1},\Gamma_L],\Gamma_L] = 0.$$

It is clear that Z_{x1} is a master symmetry. Concerning Z_{x2} it has some very interesting characteristics; it is a dynamical symmetry (i.e., $[Z_{x2},\Gamma_L]=0$) and it is a symplectic symmetry (that is, $\mathcal{L}_{Z_{x2}}\omega_L = 0$), but nevertheless it is not a Cartan symmetry of the Lagrangian system Γ_L because $Z_{x2}(E_L) \neq 0$. Recall that the two properties $\mathcal{L}_X\omega_L = 0$ and $[X,\Gamma_L]=0$ imply that $\mathcal{L}_X dE_L = 0$, but from this we only obtain that $X(E_L)$ must be a numerical constant.

As explained previously, the vector fields Z_{x1} and Z_{x2}, determine two new vector fields Y_1 and Y_2, given by

$$Y_1 = Z_{x2} + t[Z_{x2},\Gamma_L] = Z_{x2},$$

$$Y_2 = Z_{x1} + t[Z_{x1},\Gamma_L] + \tfrac{1}{2}t^2[[Z_{x1},\Gamma_L],\Gamma_L] = Z_{x1} - k\,t\,Z_{x2},$$

such that they satisfy

$$i(Y_1)\Omega_E = i(Z_{x2})\omega_L + Z_{x2}(E_L)dt = d[T_{x2} - t],$$

$$i(Y_2)\Omega_E = i(Z_{x1} - ktZ_{x2})\omega_L + Z_{x1}(E_L)\mathrm{d}t - ktZ_{x2}(E_L)\mathrm{d}t = \mathrm{d}\left[T_{x1} - ktT_{x2} + \tfrac{1}{2}kt^2\right].$$

Hence the two following functions:

$$J^t_{x1} = T_{x2} - t, \quad J^t_{x2} = T_{x1} - ktT_{x2} + \tfrac{1}{2}kt^2$$

are time-dependent integrals of motion determined by Z_{x1}, Z_{x2}, via Y_1, Y_2.

In the next subsection we see that these symmetries and these time-dependent integrals are the origin of the $n=2$ superintegrability.

C. Two-dimensional nonlinear system: Lagrangian formalism and superintegrability

We now want to study the nonlinear system

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + 3k_1x\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right) + k_1^2x^3 = 0,$$

$$\frac{\mathrm{d}^2y}{\mathrm{d}t^2} + 3k_2y\left(\frac{\mathrm{d}y}{\mathrm{d}t}\right) + k_2^2y^3 = 0, \tag{11}$$

representing the $n=2$ version of the nonlinear equation, [Eq. (9)]. It is clear, from the results of $n=1$, that these two equations can be considered as the Lagrange equations arising from the following two-dimensional Lagrangian

$$L = \frac{1}{v_x + k_1x^2} + \frac{1}{v_y + k_2y^2}. \tag{12}$$

Therefore the dynamics is characterized by preserving the following Lagrangian energy:

$$E_L = -\frac{(2v_x + k_1x^2)}{(v_x + k_1x^2)^2} - \frac{(2v_y + k_2y^2)}{(v_y + k_2y^2)^2}.$$

The first consequence of the Lagrangian character of the equations is that, as there is no coupling between the two degrees of freedom, the two one-dimensional energies are integrals of motion

$$I_1 = -\frac{(2v_x + k_1x^2)}{(v_x + k_1x^2)^2}, \quad I_2 = -\frac{(2v_y + k_2y^2)}{(v_y + k_2y^2)^2}, \quad \frac{\mathrm{d}}{\mathrm{d}t}I_i = 0, \quad i = 1,2.$$

Our main goal in the study of this nonlinear problem is to prove that this system possesses the rather unusual property of superintegrability. At this point we recall that a system is called superintegrable if it is integrable in the Liouville–Arnold sense and, in addition, possesses more independent first integrals than degrees of freedom (see Refs. 28–36 for some articles published in these last years and Ref. 37 for a recent workshop on superintegrability). It is clear that, for this particular $n=2$ system, superintegrability means the existence of a third independent integral I_3 coupling the two degrees of freedom in similar way as the angular momentum for the isotropic linear harmonic oscillator.

The four functions

$$J^t_{x1} = T_{x2} - t, \quad J^t_{x2} = T_{x1} - k_1 t\, T_{x2} + \tfrac{1}{2}k_1 t^2,$$

$$J^t_{y1} = T_{y2} - t, \quad J^t_{y2} = T_{y1} - k_2 t\, T_{y2} + \tfrac{1}{2}k_2 t^2,$$

are time-dependent constants of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}J^t_{xi} = 0, \quad \frac{\mathrm{d}}{\mathrm{d}t}J^t_{yi} = 0, \quad i = 1,2.$$

We can eliminate the time t by pairing these functions in two different ways and obtain the following two integrals of motion

$$I_3 = T_{x2} - T_{y2},$$

$$I_4 = k_2 T_{x1} + k_1 T_{y1} - k_1 k_2 T_{x2} T_{y2}$$

that take the form

$$I_3 = \frac{x}{v_x + k_1 x^2} - \frac{y}{v_y + k_2 y^2},$$

$$I_4 = \frac{k_2}{v_x + k_1 x^2} + \frac{k_1}{v_y + k_2 y^2} - \frac{k_1 k_2 xy}{(v_x + k_1 x^2)(v_y + k_2 y^2)}.$$

Hence, the nonlinear system given by the Eq. (11) and characterized by Lagrangian (12) is a superintegrable system.

In geometric terms the symplectic form ω_L and the dynamical vector field Γ_L are given by

$$\omega_L = \frac{2\,\mathrm{d}x \wedge \mathrm{d}v_x}{(v_x + kx^2)^3} + \frac{2\,\mathrm{d}y \wedge \mathrm{d}v_y}{(v_y + k_2 y^2)^3},$$

$$\Gamma_L = v_x \frac{\partial}{\partial x} + v_y \frac{\partial}{\partial y} + F_x \frac{\partial}{\partial v_x} + F_y \frac{\partial}{\partial v_y},$$

where $F_x = -k_1 x(3v_x + k_1 x^2)$ and $F_y = -k_2 y(3v_y + k_2 y^2)$. If we denote by Z_{xr} and Z_{yr}, the Hamiltonian vector fields of T_{xr} and T_{yr}, $r = 1,2$, then the vector field

$$X_3 = Z_{x2} - Z_{y2}$$

is a dynamical symmetry,

$$[X_3, \Gamma_L] = 0,$$

as well a Cartan symmetry,

$$X_3(E_L) = 0, \quad \mathcal{L}_{X_3}\omega_L = 0.$$

It determines the function I_3 as the corresponding Hamiltonian

$$i(X_3)\omega_L = \mathrm{d}I_3.$$

Similarly the vector field X_4 given by

$$X_4 = k_2 Z_{x1} + k_1 Z_{y1} - (k_1 k_2)(T_{y2} Z_{x2} + T_{x2} Z_{y2})$$

is also a dynamical symmetry as well a Cartan symmetry,

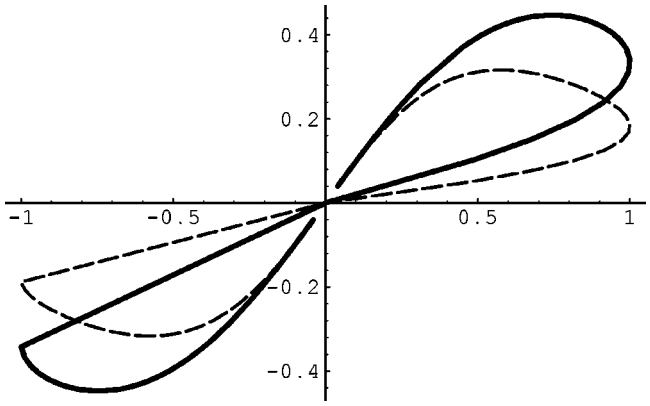

FIG. 3. "Figure eight" in the plane (x,y) corresponding to $k_1=k_2=1$ and energies $E_1=-1, E_2=-5$ (thick curve) and $E_1=-1, E_2=-10$ (dash curve).

$$[X_4,\Gamma_L]=0, \quad X_4(E_L)=0, \quad \mathcal{L}_{X_4}\omega_L=0$$

and determines the function I_4 as the corresponding Hamiltonian

$$i(X_4)\omega_L = \mathrm{d}I_4.$$

The main difference between these two symmetries is that X_3 is an exact symmetry of the Lagrangian, that is $X_3(L)=0$, and X_4 is a nonexact generalized Noether symmetry

$$X_4(L)=\frac{\mathrm{d}}{\mathrm{d}t}F_4, \quad F_4=-\frac{1}{2}\left(\frac{k_2}{M_x}+\frac{k_1}{M_y}\right),$$

so that I_4 is given by

$$i(X_4)\theta_L - F_4 = I_4.$$

An important property related with superintegrability is the existence of periodic orbits as, for example, in the Kepler problem or in the harmonic oscillator. This particular system is superintegrable but the motion, although bounded, is not periodic; instead, the trajectories are "almost closed." We have found that the trajectories in the plane (x,y) are in fact "figure eight" curves with the particle making a complete circuit as t goes from $-\infty$ to $+\infty$. The trajectory starts very close to the origin, passes through (0,0) only once and returns once more to the origin, but for $t\to-\infty$ and $t\to\infty$ only approaches (0,0) as a limit. Figure 3 shows two curves in the plane (x,y) corresponding to two different values of E_1 and E_2.

IV. LAGRANGIAN CONSERVATIVE APPROACH TO A NONLINEAR OSCILLATOR

A. One-dimensional system: Lagrangian formalism and integrability

We now consider the following non-natural Lagrangian

$$L=\frac{1}{kv_x+k^2x^2+w^2}, \tag{13}$$

where k and w are arbitrary constants; the notation w^2 for the new parameter clearly advances that it will be interpreted as a frequency. We arrive at the following nonlinear equation:

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2}+3kx\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)+k^2x^3+w^2x=0 \tag{14}$$

as well as to the following expression for the Lagrangian energy:

$$E_L = \frac{-(2kv_x + k^2x^2 + w^2)}{(kv_x + k^2x^2 + w^2)^2}.$$

We can solve this new nonlinear problem by using the same technique as in Eq. (9). Nevertheless we see that this new nonlinear equation is in fact a nonlinear oscillator and, because of this, we will use an approach that is as close as possible to the linear oscillator.

We denote by X and W_x the following two functions:

$$X = \frac{x}{(kv_x + k^2x^2 + w^2)}, \quad W_x = \frac{v_x + kx^2}{(kv_x + k^2x^2 + w^2)}.$$

Then we have the following two properties:

(i) The time evolution of X and W_x is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}X = W_x, \quad \frac{\mathrm{d}}{\mathrm{d}t}W_x = -w^2X.$$

(ii) X and W_x are related by

$$w^2X + kxW_x = x.$$

Next we see that property (i) is related to the conservation of energy and property (ii) to the solution of the dynamics. In fact, from (i) we conclude that the function I_{XW} defined as

$$I_{XW} = W_x^2 + w^2X^2,$$

is an integral of the motion. We remark that, as the system is one-dimensional, the two integrals, E_L and I_{XW}, cannot be independent; in fact I_{XW} turns out to be the energy associate to an equivalent Lagrangian $\widetilde{L}$ of the form $\widetilde{L}=c_1L+c_2$. A simple calculation gives

$$\widetilde{E_L} = \Delta(\widetilde{L}) - \widetilde{L} = I_{XW} \quad \text{with } \widetilde{L} = \left(\frac{w}{k}\right)^2 L - \frac{1}{k^2}.$$

Also from (i) we arrive at

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}X + w^2X = 0, \quad \frac{\mathrm{d}^2}{\mathrm{d}t^2}W_x + w^2W_x = 0$$

so that X and W_x are given by

$$X = \left(\frac{1}{w}\right)A\sin(wt + \phi), \quad W_x = A\cos(wt + \phi), \quad A = \sqrt{E},$$

where E is the constant value of the new energy function $\widetilde{E_L}=I_{XW}$. These two expressions, together with property (ii), lead to the following trigonometric function for the solution of the dynamics:

$$x = \frac{w\sqrt{E}\sin(wt + \phi)}{1 - k\sqrt{E}\cos(wt + \phi)}.$$

Figure 4 represents $x(t)$ as a function of t for several values of the energy E in the regular oscillatory region ($0<E<1/k^2$). It is clear that for small values of E the oscillations are rather similar to the oscillations of the linear system, but for other values of E (roughly speaking, for $E>0.3/k^2$) the nonlinearity introduces deformations in the oscillations. For higher values of E the nonlinearity drastically changes the aspect of the solution. Figure 5 shows the phase portrait; it clearly shows that the motions from left to right and from right to left take place at different velocities.

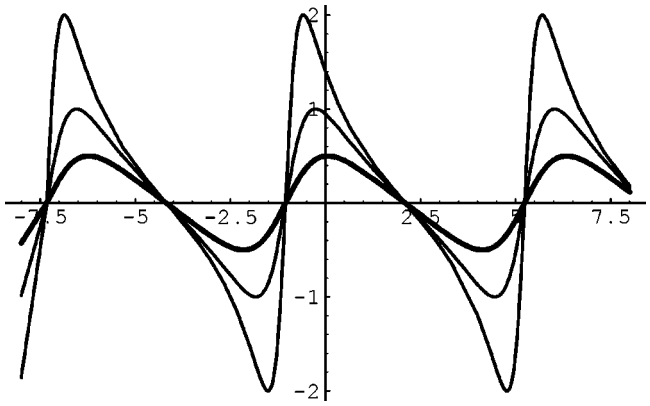

FIG. 4. Plot of x as a function of t, for $(k=1, w=1)$ and three different values of the energy: $E=0.2$ (small thick curve), $E=0.5$ (middle curve), and $E=0.8$ (curve with great oscillations). The $E=0.2$ curve is very similar to a pure sine or cosine curve but, for higher values of E, the plot shows clearly the effects of the nonlinearity.

B. Two-dimensional system: Superintegrability and nonlinear Lissajous figures

We now turn our attention to the two-dimensional version of this nonlinear oscillator. If we consider the following Lagrangian:

$$L = \frac{1}{k_1 v_x + k_1^2 x^2 + w_1^2} + \frac{1}{k_2 v_y + k_2^2 y^2 + w_2^2} \tag{15}$$

then we arrive at the following equations:

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} + 3\,k_1 x\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right) + k_1^2 x^3 + w_1^2 x = 0,$$

$$\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} + 3\,k_2 y\left(\frac{\mathrm{d}y}{\mathrm{d}t}\right) + k_2^2 y^3 + w_2^2 y = 0 \tag{16}$$

and to the following expression for the energy function:

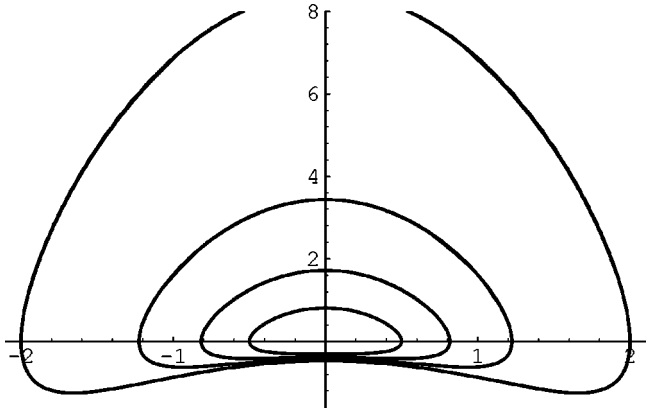

FIG. 5. Phase trajectories corresponding to four different values of the energy ($E=0.2$, 0.4, 0.6, and 0.8). The trajectories are closed curves representing periodic motions that for small values of E can be considered as rather similar to ellipses; for other values of E the curves modify their shape and they lengthen toward the upper side of the phase plane. The motion is asymmetric in the sense that the particle moves from right to left in a slowly way but returns, from left to right, with a much higher velocity that takes its maximum value at the center point $x=0$.

$$E_L = -\frac{(2\,k_1 v_x + k_1^2 x^2 + w_1^2)}{(k_1 v_x + k_1^2 x^2 + w_1^2)^2} - \frac{(2\,k_2 v_y + k_2^2 y^2 + w_2^2)}{(v_y + k_2 y^2 + w_2^2)^2}.$$

In this $n=2$ case we have two pairs of functions (X_j, W_j), $j=1,2$,

$$X_1 = \frac{x}{k_1 v_x + k_1^2 x^2 + w_1^2}, \quad W_1 = \frac{v_x + k_1 x^2}{k_1 v_x + k_1^2 x^2 + w_1^2},$$

$$X_2 = \frac{y}{k_2 v_y + k_2^2 y^2 + w_2^2}, \quad W_2 = \frac{v_y + k_2 y^2}{k_2 v_y + k_2^2 y^2 + w_2^2}$$

in such a way that we have

$$\frac{\mathrm{d}}{\mathrm{d}t} W_j = -w_j^2 X_j, \quad \frac{\mathrm{d}}{\mathrm{d}t} X_j = W_j$$

and

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} X_j + w_j^2 X_j = 0, \quad \frac{\mathrm{d}^2}{\mathrm{d}t^2} W_j + w_j^2 W_j = 0.$$

A similar calculation shows that

$$x = \frac{w_1^2 X_1}{1 - k_1 W_1}, \quad y = \frac{w_2^2 X_2}{1 - k_2 W_2},$$

from which we obtain solution of the dynamics

$$x = \frac{w_1 \sqrt{E_1} \sin(w_1 t + \phi_1)}{1 - k_1 \sqrt{E_1} \cos(w_1 t + \phi_1)}, \quad y = \frac{w_2 \sqrt{E_2} \sin(w_2 t + \phi_2)}{1 - k_2 \sqrt{E_2} \cos(w_2 t + \phi_2)}.$$

We now study the superintegrability of the rational case, that is, $w_1 = n_1 w_0$ and $w_2 = n_2 w_0$, with n_1 and n_2 positive integral numbers.

Proposition 2: Let $\mathbb{K}_1$ and $\mathbb{K}_2$ be the following two functions:

$$\mathbb{K}_j = W_j + \mathrm{i}\, n_j w_0 X_j, \quad j = 1,2.$$

Then the complex functions $\mathbb{K}_{ij}$ defined as

$$\mathbb{K}_{ij} = \mathbb{K}_i^{n_j} (\mathbb{K}_j^*)^{n_i}, \quad i,j = 1,2,$$

are constants of the motion.

Proof: The time evolution of the functions $\mathbb{K}_1$ and $\mathbb{K}_2$ is given by

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathbb{K}_j = \frac{\mathrm{d}}{\mathrm{d}t} W_j + \mathrm{i}\, n_j w_0 \frac{\mathrm{d}}{\mathrm{d}t} X_j = \mathrm{i}\, n_j w_0 \mathbb{K}_j, \quad j = 1,2.$$

On the other side we have

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathbb{K}_{ij} = \mathbb{K}_i^{n_j - 1} (\mathbb{K}_j^*)^{n_i - 1} \left(n_j \mathbb{K}_j^* \frac{\mathrm{d}}{\mathrm{d}t} \mathbb{K}_i + n_i \mathbb{K}_i \frac{\mathrm{d}}{\mathrm{d}t} \mathbb{K}_j^* \right)$$

and from here the property follows by direct calculus.

Thus the three functions

$$I_1 = |\mathbb{K}_1|^2, \quad I_2 = |\mathbb{K}_2|^2, \quad I_{12} = \mathbb{K}_1^{n_2}(\mathbb{K}_2^*)^{n_1},$$

are constants of the motion. The two first functions, I_1 and I_2, are the two one degree of freedom energies; concerning I_{12}, as it has complex value

$$I_{12} = I_4 + \mathrm{i}\, I_3,$$

it determines not just one but two real constants of motion. Of course, if we consider I_3 as the new additional constant, I_4 is a function of I_1, I_2, and I_3. We thus conclude that the existence of superintegrabilty and periodic trajectories (Lissajous figures) is preserved by the nonlinearity.

We particularize these results for the two first commensurable cases. In the isotropic case, $w_1 = w_2 = w_0$, the two functions, I_3 and I_4, are given by

$$I_3 = X_1 W_2 - X_2 W_1 = \frac{(xv_y - yv_x) + (k_2 y - k_1 x)xy}{(k_1 v_x + k_1^2 x^2 + w_0^2)(k_2 v_y + k_2^2 y^2 + w_0^2)},$$

$$I_4 = W_1 W_2 + w_0^2 X_1 X_2 = \frac{(v_x + k_1 x^2)(v_y + k_2 y^2) + w_0^2 xy}{(k_1 v_x + k_1^2 x^2 + w_0^2)(k_2 v_y + k_2^2 y^2 + w_0^2)},$$

representing the nonlinear versions of the angular momentum and the nondiagonal component of the Fradkin tensor respectively.[38,39] In fact, when $k_1, k_2 \to 0$, these two function reduce to the appropriate expressions

$$\lim_{k\to 0} I_3 = \left(\frac{1}{w_0^4}\right)(xv_y - yv_x),$$

$$\lim_{k\to 0} I_4 = \left(\frac{1}{w_0^4}\right)(v_x v_y + w_0^2 xy).$$

Of course, for $w_0 \to 0$, we recover the I_3 obtained in the previous section; I_4 just reduces to a trivial numerical constant.

$$\lim_{w\to 0} I_3 = \frac{(xv_y - yv_x) + (k_2 y - k_1 x)xy}{k_1 k_2 (v_x + k_1 x^2)(v_y + k_2 y^2)},$$

$$\lim_{w\to 0} I_4 = \frac{1}{k_1 k_2}.$$

Figure 6 represents some closed trajectories in the plane (x,y); it is clear that for small energies the curves look rather similar to the ellipses of the linear case, but for other (not so small) values of E the curves lose their elliptic shape and adopt other not so symmetric forms.

Now, we consider the anisotropic case $w_1 = w_0, w_2 = 2w_0$. Then I_3 and I_4 are given by

$$I_3 = (X_1 W_2 - X_2 W_1) W_1 + w_0^2 X_1^2 X_2 = \frac{(v_x + k_1 x^2)[(xv_y - yv_x) + (k_2 y - k_1 x)xy] + w_0^2 x^2 y}{(k_1 v_x + k_1^2 x^2 + w_0^2)^2 (k_2 v_y + k_2^2 y^2 + 4w_0^2)},$$

$$I_4 = W_1^2 W_2 + w_0^2 (4X_2 W_1 - X_1 W_2) X_1 = \frac{(v_x + k_1 x^2)^2 (v_y + k_2 y^2) + w_0^2 [4yv_x - xv_y + (4k_1 x - k_2 y)xy]x}{(k_1 v_x + k_1^2 x^2 + w_0^2)^2 (k_2 v_y + k_2^2 y^2 + 4w_0^2)}.$$

Figure 7 represents two nonlinear Lissajous figures in the plane (x,y). The situation is similar to that of Fig. 6; close resemblance with the linear figures for small values of the energies and rather strange figures for other values of E. We must say that, in this case, the form is strongly dependent on the phase difference $\phi_{12} = \phi_1 - \phi_2$.

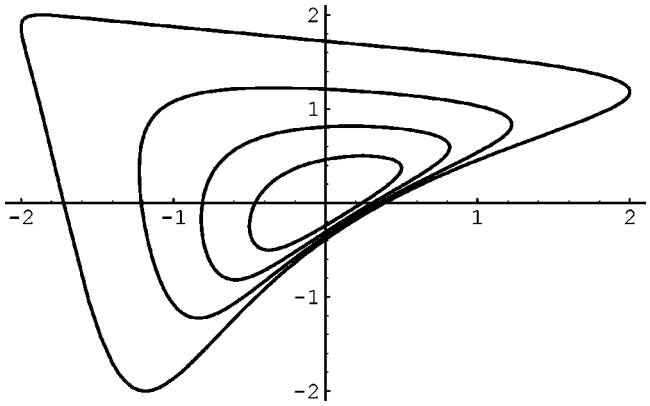

FIG. 6. Closed trajectories (ellipses in the linear case) in the plane (x,y) corresponding to $w_1=1, w_2=1$ and four different values of the energy ($E_1=E_2=0.2$, 0.4, 0.6 and 0.8).

V. FINAL COMMENTS

We have studied two nonlinear systems using, as starting point, the important property of the Lagrangian origin of the second-order Riccati equations. In this way we could use the constant value E of the energy as an appropriate parameter for characterizing the behavior of these two systems. Moreover we have proved the existence of two–dimensional versions endowed with superintegrability and we have obtained the explicit expressions of the additional integrals.

Concerning the superintegrability, we recall that most known superintegrable systems are superseparable systems, that is, systems that admit Hamilton–Jacobi separation of variables (Schrödinger in the quantum case) in more than one coordinate system. Nevertheless as all the systems studied in this paper are nonlinear systems with a nonstandard Lagrangian, the superintegrability has been proved by considering a different approach and without making use of the multiple separability. In spite of this the possible separation of variables in other coordinate systems than Cartesian ones must be studied.

We also mention that these two nonlinear systems can be generalized in several different ways by making use of the Lagrangian approach. First, we recall that we have proved in Sec. II the Lagrangian origin not only of the Riccati systems but also of the more general equation (4); this means that these more general equations could also be studied by making use of the conservation of the energy. Second, the Lagrangian (6) admits the following natural generalization

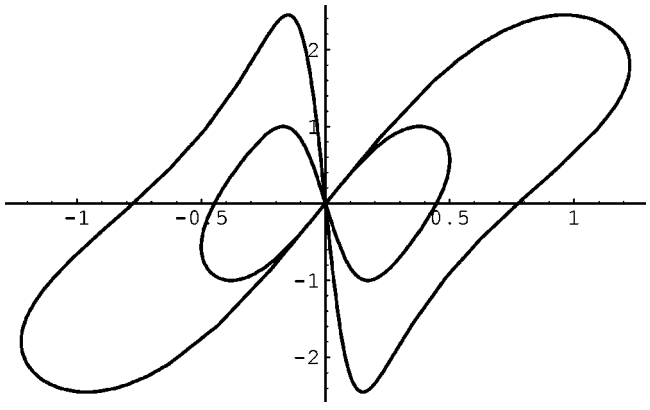

FIG. 7. Nonlinear Lissajous figures in the plane (x,y) corresponding to "figure eight" trajectories associated to $w_1=1, w_2=2$ and energies $E_1=E_2=0.2$ (small eight-looking curve) and $E_1=E_2=0.6$ (big butterfly-looking curve).

$$L = \frac{1}{m(x)v_x + k\,U(x)} \tag{17}$$

that leads to a nonlinear second-order equation with a position-dependent effective mass and an additional dissipative-looking term of the form $m'(x)v_x^2$. This new Lagrangian (17) seems interesting, not only because it generalizes (6) but also because it has a more direct geometrical interpretation since the linear function $m(x)v_x$ can be considered as associated to the one-form $\mu = m(x)dx$.

The Lagrangian (6) has, as associated Hamiltonian, the following function:

$$H = -2\sqrt{-p_x} - kU(x)p_x \tag{18}$$

that, in addition to its nonnatural character (as was to be expected), has the annoying presence of the momentum inside a root. In the particular case of the nonlinear oscillator the Hamiltonian is given as follows:

$$H = -\left[\frac{2w}{k^2}\sqrt{-kp_x} + \left(kx^2 + \frac{w^2}{k}\right)p_x\right] + \frac{1}{k^2}. \tag{19}$$

Nevertheless in this case we have an important property; in fact, if we make use of the canonical transformation $(x, p_x) \to (Q, P)$ given by

$$Q = \left(\frac{\sqrt{2}}{w}\right)x\sqrt{-kp_x}, \quad P = \left(\frac{\sqrt{2}}{k}\right)[1 - w\sqrt{-kp_x}],$$

then we arrive at

$$H = \tfrac{1}{2}(P^2 + w^2Q^2).$$

Hence the very peculiar Hamiltonian (19) and the standard linear oscillator are canonically related. Nevertheless note that this transformation has a nonpoint character and, because of this, it cannot be directly used in the Lagrangian approach. This brings up the question of the possible existence of similar nonpoint transformations for Hamiltonians obtained from other Riccati Lagrangians. We think that this possibility is an open question to be studied.

Finally, we mention the study of the quantized versions of all these nonlinear systems. We note that this question must be carried out only after the obtaining of the appropriate Hamiltonian versions (the direct quantum study of the Lagrangian equations appears as a difficult task). Nevertheless as the Lagrangians are nonstandard the Hamiltonians also appear with an unusual dependence of the momenta (see the previous expressions). In any case the possibility or impossibility of quantizing these systems is a matter that must be investigated.

ACKNOWLEDGMENTS

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Summation of divergent series and Borel summability for strongly dissipative differential equations with periodic or quasiperiodic forcing terms

Guido Gentile[a)]
Dipartimento di Matematica, Universitá di Roma Tre, Roma, I-00146, Italy

Michele V. Bartuccelli[b)] and Jonathan H. B. Deane[c)]
Department of Mathematics and Statistics, University of Surrey, Guildford, GU2 7XH, United Kingdom

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We consider a class of second order ordinary differential equations describing one-dimensional systems with a quasiperiodic analytic forcing term and in the presence of damping. As a physical application one can think of a resistor–inductor–varactor circuit with a periodic (or quasiperiodic) forcing function, even if the range of applicability of the theory is much wider. In the limit of large damping we look for quasiperiodic solutions which have the same frequency vector of the forcing term, and we study their analyticity properties in the inverse of the damping coefficient. We find that even the case of periodic forcing terms is nontrivial, as the solution is not analytic in a neighborhood of the origin: it turns out to be Borel summable. In the case of quasiperiodic forcing terms we need renormalization group techniques in order to control the small divisors arising in the perturbation series. We show the existence of a summation criterion of the series in this case also; however, this cannot be interpreted as Borel summability. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1926208]

I. INTRODUCTION

Consider the ordinary differential equation

$$\varepsilon\ddot{x} + \dot{x} + \varepsilon x^2 = \varepsilon f(\boldsymbol{\omega} t), \tag{1.1}$$

where $\boldsymbol{\omega} \in \mathbb{R}^d$ is the frequency vector, $f(\boldsymbol{\psi})$ is an analytic function,

$$f(\boldsymbol{\psi}) = \sum_{\boldsymbol{\nu} \in \mathbb{Z}^d} e^{i\boldsymbol{\nu}\cdot\boldsymbol{\psi}} f_{\boldsymbol{\nu}}, \tag{1.2}$$

with average $\alpha = a^2$, with $a > 0$ (hence $\langle f \rangle \equiv f_{\mathbf{0}} = \alpha$), and $\varepsilon > 0$ is a real parameter. Here and henceforth we denote with $\cdot$ the scalar product in $\mathbb{R}^d$. By the analyticity assumption of f there are two strictly positive constants F and ξ such that one has $|f_{\boldsymbol{\nu}}| \leqslant F e^{-\xi|\boldsymbol{\nu}|}$ for all $\boldsymbol{\nu} \in \mathbb{Z}^d$.

By writing $\gamma = 1/\varepsilon$ the equation becomes

$$\ddot{x} + \gamma\dot{x} + x^2 = f(\boldsymbol{\omega} t), \tag{1.3}$$

which describes a nonlinear electronic circuit, known as resistor–inductor–varactor circuit, subject to a quasiperiodic forcing function. Taking $d = 1$ and $f(\omega t) = \alpha + \beta \sin t$, this equation has been studied in Ref. 1, where, among other things, it has been found numerically that for γ large enough

[a)]Electronic mail: gentile@mat.uniroma3.it
[b)]Electronic mail: m.bartuccelli@surrey.ac.uk
[c)]Electronic mail: j.deane@surrey.ac.uk

there exists only one attracting periodic orbit and the corresponding period is $2\pi/\omega=2\pi$, the same as the forcing term. Furthermore one can prove analytically that such a periodic orbit is the only one in a neighborhood of radius $O(1/\gamma)$ around the point $(a,0)$.

Here we give some further analytical support to such numerical findings. In particular we show that, if we take as forcing term an analytic periodic function,

$$f(\psi)=\sum_{\nu\in\mathbb{Z}} e^{i\nu\psi}f_\nu, \quad f_0=\alpha>0, \tag{1.4}$$

then for ε small enough there is a $2\pi/\omega$-periodic solution, but this is not analytic in $\varepsilon=1/\gamma$ in a neighborhood the origin in the complex ε-plane. We find that such a solution is Borel summable.

We also show that by considering quasiperiodic forcing terms, as in (1.3), we still have a quasiperiodic solution with the same frequency vector $\boldsymbol{\omega}$ as the forcing term, but we can only say in general that such a solution is analytic in a domain with boundary crossing the origin.

Finally we shall see that considering more general nonlinearities introduces no further difficulties, and equations like

$$\ddot{x}+\gamma\dot{x}+g(x)=f(\boldsymbol{\omega}t), \quad \lim_{|x|\to\infty}\frac{|g(x)|}{|x|}=\infty, \tag{1.5}$$

with g and f both analytic in their arguments, can be dealt with essentially in the same way. Simply, we must impose a nondegeneracy condition on the function g, which reads as

$$\exists x_0 \text{ such that } g(x_0)=f_0 \quad \text{and } g'(x_0)\neq 0. \tag{1.6}$$

In the particular case of homogeneous $g(x)$, that is $g(x)=\sigma x^p$, with $p\geqslant 2$ an integer and $\sigma\in\mathbb{R}$, the condition is automatically satisfied if p is odd (for any value of σ), while it requires $\sigma f_0>0$ for p even, as assumed in (1.1).

The paper is organized as follows. For expository clearness we start with the case of periodic forcing terms. In Secs. II and III we show that a periodic solution with frequency ω in the form of a formal power series in ε (perturbation series) is well defined to all orders, and it admits a natural graphical representation. In Sec. IV we study further such a series, and we see that there is strong evidence to show that it diverges (even if we cannot exclude convergence definitely). The best bounds that we are able to provide for the coefficients grow as factorials. To obtain bounds which allow summability of the perturbation series we must perform a suitable summation in order to give the series a meaning. This is done in Sec. V, and the resummed series is found to represent a $2\pi/\omega$-periodic solution which is Borel summable in ε. To prove the latter property we rely on Nevanlinna's improvement of Watson's theorem.[12] In Sec. VI we consider the case of quasiperiodic forcing terms. We find that the perturbation series is well defined if the frequency vector of the forcing term satisfies a Diophantine condition, and, by using renormalization group techniques in order to deal with the small divisors problem, we find that the resummed series still converges to a quasiperiodic solution, and it defines a function analytic in a domain containing the origin in its boundary. We shall see that the bounds we find do not allow us any more to obtain Borel summability, unlike the case of periodic forcing terms. In Sec. VII we discuss how to extend the analysis to more general nonlinearities $g(x)$, by requiring the condition (1.6) to be satisfied.

The interest of the approach we propose is that it allows the use of perturbation theory which can be very natural in problems in which a small parameter appears. In fact analyticity in ε for ε close to 0 (that is in γ for γ large enough) could be proved very likely with other techniques (at least for periodic solutions in the case of periodic forcing terms), but a naive expansion in powers of ε is prevented by the lack of analyticity in a neighborhood of the origin. On the other hand, the perturbation series gives a very accurate description of the solution, hence it is important to know that such a series is an asymptotic series, and its use is fully justified. Finally we mention that the quasiperiodic solution we investigate is of physical relevance, hence it is useful to study its

properties. For instance in the case of the aforementioned resistor–inductor–varactor circuit in Ref. 1, for damping large enough, the $2\pi/\omega$-periodic solution is numerically found to attract any trajectory which remains bounded in phase space.

The techniques we use have been recently developed for problems of Hamiltonian stability, and are based on resummation methods that are familiar in quantum field theory (see Ref. 7 and references quoted therein). Here we show that they can be useful even in non-Hamiltonian problems with viscosity acting. We leave as an open problem to show whether the formal series of the periodic or quasiperiodic solutions are really divergent. We also note that we are not able to prove uniqueness of the quasiperiodic solutions we find by the resummation procedure, as in that case there is no uniqueness result as for analytic or Borel summable functions which one can rely upon. Furthermore, both for periodic and for quasiperiodic solutions, we cannot exclude existence of other solutions with the same rotation vector, which either are of a different form or even admit the same formal series, without being obtained through the same resummation procedure. Problems of the same kind were met in the study of hyperbolic lower-dimensional tori.[6]

II. FORMAL ANALYSIS

Consider first (1.1) for $d=1$, that is

$$\varepsilon\ddot{x} + \dot{x} + \varepsilon x^2 = \varepsilon f(\omega t), \tag{2.1}$$

with $f(\psi)$ given by (1.4). We look for bounded solutions (if any) which are analytic in ε, that is of the form

$$x(t) = \sum_{k=0}^{\infty} \varepsilon^k x^{(k)}(t). \tag{2.2}$$

Inserting (2.2) into (2.1) and equating terms of the same Taylor order we find the set of recursive equations

$$\dot{x}^{(0)} = 0,$$

$$\dot{x}^{(1)} = -\ddot{x}^{(0)} - x^{(0)2} + f, \tag{2.3}$$

$$\dot{x}^{(k)} = -\ddot{x}^{(k-1)} - \sum_{k_1+k_2=k-1} x^{(k_1)} x^{(k_2)}, \quad k \geqslant 2.$$

From the first equation (zeroth order) we obtain that $x^{(0)}$ must be constant, say $x^{(0)}=c_0$ with c_0 to be determined. The second equation (first order) can give a bounded solution only if $-c_0^2+\alpha=0$, which fixes $c_0=\sqrt{\alpha}=a$ and gives $x^{(1)}(t)$ as a periodic function with the same period of the forcing term,

$$x^{(1)}(t) = x^{(1)}(0) + \int_0^t \mathrm{d}t' (f(\omega t') - \alpha). \tag{2.4}$$

As each $x^{(k)}(t)$ depends on the functions $x^{(k')}(t)$ with $k' < k$, we expect that if there is any periodic solution then it must have the same period as the forcing term.

To continue the analysis to all orders it is more convenient to write the recursive equations (2.3) in Fourier space. The analysis to first order and the considerations above motivate us to write in (2.2),

$$x(t) = \sum_{k=0}^{\infty} \varepsilon^k x^{(k)}(t) = \sum_{k=0}^{\infty} \varepsilon^k \sum_{\nu\in\mathbb{Z}} e^{i\nu\omega t} x_\nu^{(k)}, \tag{2.5}$$

which inserted into (2.3) gives for $\nu \neq 0$,

$$x_\nu^{(0)} = 0,$$

$$x_\nu^{(1)} = \frac{f_\nu}{i\omega\nu}, \tag{2.6}$$

$$x_\nu^{(k)} = -(i\omega\nu)x_\nu^{(k-1)} - \frac{1}{i\omega\nu} \sum_{\substack{k_1+k_2=k-1 \\ k_1,k_2\geqslant 0}} \sum_{\nu_1+\nu_2=\nu} x_{\nu_1}^{(k_1)} x_{\nu_2}^{(k_2)}, \quad k \geqslant 2,$$

provided that one has for $\nu=0$,

$$\begin{aligned} 0 &= -x_0^{(0)2} + f_0, \\ 0 &= \sum_{\substack{k_1+k_2=k \\ k_1,k_2\geqslant 0}} \sum_{\nu_1+\nu_2=0} x_{\nu_1}^{(k_1)} x_{\nu_2}^{(k_2)}, \quad k \geqslant 1. \end{aligned} \tag{2.7}$$

If we set $x_0^{(k)}=c_k$ then the first of (2.7) fixes, as already noted,

$$c_0 = a = \sqrt{\alpha}, \tag{2.8}$$

because one has $f_0=\alpha>0$, while the second of (2.7) gives

$$\sum_{k'=0}^{k} \sum_{\nu_1\in\mathbb{Z}} x_{\nu_1}^{(k-k')} x_{-\nu_1}^{(k')} = 0. \tag{2.9}$$

The latter equation, by taking into account (2.8) and the first of (2.6), can be more conveniently written as

$$c_1 = 0, \quad c_k = -\frac{1}{2c_0} \sum_{k'=1}^{k-1} \sum_{\nu_1\in\mathbb{Z}} x_{\nu_1}^{(k-k')} x_{-\nu_1}^{(k')}, \quad k \geqslant 2, \tag{2.10}$$

which provides an iterative definition of the coefficients c_k as the right-hand side depends only on the coefficients $c_{k'}$ with $k'<k$. To deduce $c_1=0$ we used the first of (2.6), which, inserted into (2.9) for $k=1$, gives $2c_0c_1=0$, hence $c_1=0$ as $c_0\neq 0$.

The following result holds.

Lemma 2.1: *Consider (2.1) with f given by (1.4). Then there exists a formal power series solution (2.2) whose coefficients $x^{(k)}(t)$ are analytic in t. If f is a trigonometric polynomial, that is in (1.4) one has $|\nu|\leqslant N$ for some $N\in\mathbb{N}$, then for all $k\geqslant 0$ the functions $x^{(k)}(t)$ are trigonometric polynomials of order $[(k+1)/2]N$, where $[\cdot]$ denotes the integer part. This means that one has $x_\nu^{(2k)}=0$ and $x_\nu^{(2k-1)}=0$ for $|\nu|>kN$.*

Proof: The existence of a formal solution (2.2), with coefficients $x^{(k)}(t)$ analytic in t for all $k\geqslant 0$, follows from the analysis above. If f is a trigonometric polynomial of degree N, that the coefficients $x_\nu^{(k)}$ are trigonometric polynomials with the stated properties can be proved from (2.6) by induction on k. ■

Then the functions $x^{(k)}(t)$ are well defined to all orders. Before discussing the issue of convergence of the formal power series defining such functions we look for a graphical representation of the coefficients $x_\nu^{(k)}$.

III. GRAPHICAL REPRESENTATION AND TREE FORMALISM

We start by giving some abstract definitions.

Definition 3.1 (trees): *A tree θ is a graph, that is a connected set of points and lines, with no*

cycle, such that all the lines are oriented toward a unique point which has only one incident line. Such a point is called the root of the tree. All the points in a tree except the root are denoted nodes. The line entering the root is called the root line. The orientation of the lines in a tree induces a partial ordering relation between the nodes. We denote this relation by $\preccurlyeq$*, given two nodes* v *and* w*, we shall write* $w \preccurlyeq v$ *every time* v *is along the path (of lines) which connects* w *to the root.*

Given a tree θ, we can identify the following subsets in θ.

Definition 3.2 (endpoints): *We call* $E(\theta)$ *the set of endpoints in* θ*, that is the nodes which have no entering line. The endpoints can be represented either as* white bullets *or as* black bullets. *We call* $E_W(\theta)$ *the set of white bullets and* $E_B(\theta)$ *the set of black bullets. Of course* $E_W(\theta) \cup E_B(\theta) = E(\theta)$. *With each* $v \in E_W(\theta)$ *we associate a* mode *label* $\nu_v = 0$, *an* order *label* $k_v \in \mathbb{Z}_+$ *and a* node factor $F_v = c_{k_v}$. *With each* $v \in E_B(\theta)$ *we associate a* mode *label* $\nu_v \in \mathbb{Z}\setminus\{0\}$, *and a* node factor $F_v = f_{\nu_v}$.

Definition 3.3 (lines): *We denote with* $L(\theta)$ *the set of* lines *in* θ. *Each line* $\ell \in L(\theta)$ *leaves a point* v *and enters another one which we shall denote by* v'. *Since* ℓ *is uniquely identified with* v *(the point which* ℓ *leaves), we may write* $\ell = \ell_v$. *With each line* ℓ *we associate a* momentum *label* $\nu_\ell \in \mathbb{Z}$ *and a* propagator

$$g_\ell = \begin{cases} 1/(i\omega\nu_\ell), & \nu_\ell \neq 0, \\ 1, & \nu_\ell = 0, \end{cases} \tag{3.1}$$

and we say that the momentum ν_ℓ *flows through the line* ℓ. *The modes and the momenta are related as follows: if* $\ell = \ell_v$ *one has*

$$\nu_\ell = \sum_{i=1}^{s_v} \nu_{\ell_i} = \sum_{\substack{w \in E_B(\theta) \\ w \preccurlyeq v}} \nu_w, \tag{3.2}$$

where $\ell_1, \ldots, \ell_{s_v}$ *are the lines entering* v.

Definition 3.4 (vertices): *We denote by* $V(\theta)$ *the set of* vertices *in* θ, *that is the set of points which have at least one entering line. If* $V(\theta) \neq \emptyset$ *we call the vertex* v_0 *connected to the root the* last vertex *of the tree. If* s_v *denotes the number of lines entering* v *call* $\max_{v \in V(\theta)} s_v$ *the* branching number. *One can have either* $s_v = 1$ *or* $s_v = 2$. *We set* $V_s(\theta) = \{v \in V(\theta) : s_v = s\}$ *for* $s = 1, 2$; *of course* $V_1(\theta) \cup V_2(\theta) = V(\theta)$. *We define also* $V_0(\theta) = \{v \in V(\theta) : \nu_{\ell_v} = 0\}$; *one has* $V_0(\theta) \subset V_2(\theta)$. *We require that either* $V_0(\theta) = \emptyset$ *or* $V_0(\theta) = \{v_0\}$, *and that one can have* $v \in V_1(\theta)$ *only if* $\nu_{\ell_v} \neq 0$. *We associate with each vertex* $v \in V(\theta)$ *a* node factor

$$F_v = \begin{cases} -1, & s_v = 2 \quad \text{and } v \notin V_0(\theta), \\ -1/2c_0, & s_v = 2 \quad \text{and } v \in V_0(\theta), \\ -(i\omega\nu_{\ell_v})^2, & s_v = 1, \end{cases} \tag{3.3}$$

which is always well defined as $c_0 \neq 0$.

We call *equivalent* two trees which can be transformed into each other by continuously deforming the lines in such a way that they do not cross each other.

Let $\mathcal{T}_{k,\nu}$ be the set of inequivalent trees θ such that

(1) the number of vertices, the number of black bullets, and the order labels of the white bullets are such that we have

$$k_1 + k_2 + k_3 = k, \quad \text{if } \nu \neq 0,$$

$$k_1 + k_2 + k_3 = k + 1, \quad \text{if } \nu = 0, \tag{3.4}$$

if we set $k_1 = |V(\theta)|$, $k_2 = |E_B(\theta)|$, and $k_3 = \Sigma_{v \in E_W(\theta)} k_v$.

(2) The momentum flowing through the root line is ν.

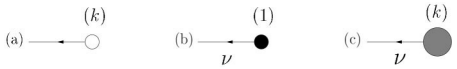

FIG. 1. Graphical representation of $x_0^{(k)}$, $x_\nu^{(1)}$, and $x_\nu^{(k)}$. For $\nu=0$ the latter reduces to the first graph, while for $k=1$ and $\nu \neq 0$ it reduces to the second graph. In the first graph the momentum is not shown as it is necessarily $\nu=0$.

We refer to $\mathcal{T}_{k,\nu}$ as the *set of trees of order k and total momentum* ν.

With the above definitions the following result holds.

Lemma 3.5: *For all* $k \geqslant 1$ *and all* $\nu \neq 0$ *one has*

$$x_\nu^{(k)} = \sum_{\theta \in \mathcal{T}_{k,\nu}} \mathrm{Val}(\theta), \quad \mathrm{Val}(\theta) = \left(\prod_{\ell \in L(\theta)} g_\ell \right) \left(\prod_{v \in E(\theta) \cup V(\theta)} F_v \right), \tag{3.5}$$

where $\mathrm{Val}: \mathcal{T}_{k,\nu} \to \mathbb{C}$ *is called the* value *of the tree. For* $k \geqslant 2$ *and* $\nu=0$ *one has*

$$x_0^{(k)} \equiv c_k = \sum_{\theta \in \mathcal{T}_{k,0}}{}^{*} \mathrm{Val}(\theta), \tag{3.6}$$

where $*$ *means that there are two lines entering the last vertex* v_0 *of* θ_0 *and neither one exits from an endpoint* v *with order label* $k_v=0$.

Proof: We can represent graphically $x_0^{(k)}=c_k$ as in Fig. 1(a), $x_\nu^{(1)}$, $\nu \neq 0$, as in Fig. 1(b), and, more generally, $x_\nu^{(k)}$ as in Fig. 1(c).

Then the third equation in (2.6) can be represented graphically as in Fig. 2, if we associate with the nodes and to the lines the node factors and the propagators, respectively, according to the definitions (3.1) and (3.3).

Analogously (2.10) is represented graphically as in Fig. 3, again if we use the graphical representations in Fig. 1 and associate with the lines and vertices the propagators (3.1) and the node factors (3.3), respectively.

Note that in this way we represent graphically each coefficient $x_\nu^{(k)}$ in terms of other coefficients $x_{\nu'}^{(k')}$, with $k' < k$, so that we can apply iteratively the graphical representation in Fig. 2 until only trees whose endpoints represent either $x_\nu^{(1)}$ with $\nu \neq 0$ (black bullets) or c_k are left (white bullets). This corresponds exactly to the expressions in (3.5) and (3.6). ■

To get familiar with the graphical representation (3.5) and (3.6) one should try to draw the trees which correspond to the first orders, and check that the sum of the values obtained with the graphical rules listed above gives exactly the same analytical expression which can be deduced directly from (2.6) and (2.10).

For instance for $k=2$ we obtain for $x_\nu^{(2)}$, $\nu \neq 0$, the graphical representation in Fig. 4 and for $c_2=x_0^{(2)}$ the graphical representation in Fig. 5.

For $k=3$ we obtain for $x_\nu^{(3)}$, $\nu \neq 0$, the graphical representation in Fig. 6 and for $c_3=x_0^{(3)}$ the graphical representation in Fig. 7, where we have explicitly used that $c_1=0$.

This can be continued to higher orders. In general a tree $\theta \in \mathcal{T}_{k,\nu}$ looks like in Fig. 8, where for simplicity no labels have been drawn other than the order labels of the white bullets. Note that each node can have only one or two entering lines, while the endpoints have no entering line at all. Moreover the momentum flowing through the line exiting a vertex v is equal to the sum of the

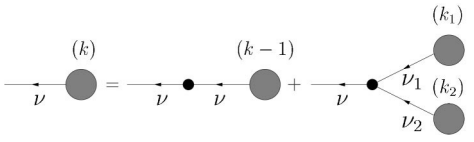

FIG. 2. Graphical representation of the third equation in (2.6) expressing the coefficient $x_\nu^{(k)}$ for $k \geqslant 2$ and $\nu \neq 0$ in terms of the coefficients $x_{\nu'}^{(k')}$ with $k' < k$. In the last graph one has the constraints $k_1+k_2=k-1$ and $\nu_1+\nu_2=\nu$.

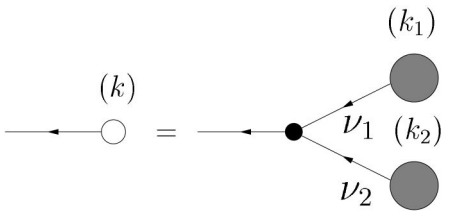

FIG. 3. Graphical representation of the equation (2.10) expressing the coefficient c_k for $k \geqslant 2$ in terms of the coefficients $x_{\nu'}^{(k')}$ with $k' < k$. Both k_1 and k_2 are strictly positive and $k_1 + k_2 = k$; moreover $\nu_1 + \nu_2 = 0$.

momenta flowing through the lines entering v, according to (3.2); this is a sort of conservation law. The order of the tree is given by the number of vertices and black bullets plus the sum of the order labels of the white bullets minus the number of vertices in $V_0(\theta)$. The latter is just $|V_0(\theta)| = 0$ if $\theta \in \mathcal{T}_{k,\nu}$, $\nu \neq 0$, and $|V_0(\theta)| = 1$ if $\theta \in \mathcal{T}_{k,0}$.

If a vertex v has $s_v = 1$, that is it has only one entering line ℓ, the latter cannot come out of a white bullet. Indeed if this occurs one should have $\nu_{\ell_v} = \nu_\ell = 0$, hence $F_v = 0$ by (3.3), so that the value of the tree containing such a vertex is zero.

Given a tree as in Fig. 8 we can represent each white bullet according to the graphical representation in Fig. 3, corresponding to the analytic formula (3.6), and expand again the two contributions $x_{\nu_1}^{(k_1)}$ and $x_{\nu_2}^{(k_2)}$ as sums of trees, and so on, iteratively, until the only white bullets which are left are the ones with order label $k = 0$. In this way we obtain a new graphical representation where the trees still look like those in Fig. 8, but now there are a few differences as follows:

(1) all the white bullets $v \in E_W(\theta)$ have order labels $k_v = 0$, and
(2) there can be lines $\ell \in L(\theta)$ with momentum $\nu_\ell = 0$ which come out of vertices, that is $V_0(\theta)$ can contain no element or more than one element.

Note that only lines coming out either from nodes in $V_0(\theta) \subset V_2(\theta)$ or from white bullets have vanishing momentum.

The order of the tree is then given by the number of elements of $V(\theta) \cup E_B(\theta)$ minus the number of elements of $V_0(\theta)$, that is $k = |V(\theta)| + |E_B(\theta)| - |V_0(\theta)|$. Of course $v_0 \in V_0(\theta)$ if and only if the momentum of the root line is vanishing, that is $\theta \in \mathcal{T}_{k,0}$ for some $k \geqslant 2$. It is important to stress that no line entering a vertex $v \in V_0(\theta)$ can come out of a white bullet (which now has necessarily an order label 0), because this would be against the constraint in the sum (3.6). This means that if two lines carrying zero momentum enter the same vertex v [so that $v \in V_0(\theta)$ according to (3.2)], then none of them can exit from a white bullet.

But up to these minor differences a tree representation like in (3.5) and (3.6) still holds. The advantage of these modified rules is that now the tree values are expressed no longer in terms of constants c_k to be determined, but only in terms of c_0 which is known. A tree drawn according these new rules is represented as in Fig. 8 with $k_1 = k_2 = k_3 = 0$ (and in particular a tree of this kind can contribute only to $x_\nu^{(k)}$ with $\nu \neq 0$). Note that we could avoid drawing the order labels associated with the endpoints, as they are uniquely determined as $k = 0$ for the white bullets and $k = 1$ for the black bullets. Of course, with respect to the caption of that figure, now the order k is given by the number of elements in $V(\theta)$ plus the number of elements in $E_B(\theta)$ minus the number of elements in $V_0(\theta)$.

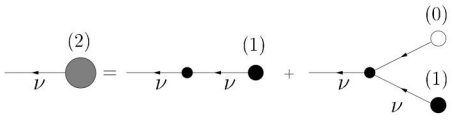

FIG. 4. Graphical representation of $x_\nu^{(2)}$ for $\nu \neq 0$. The second contribution must be counted twice, because there is also a tree with the white and black bullets exchanged; of course the latter has the same value.

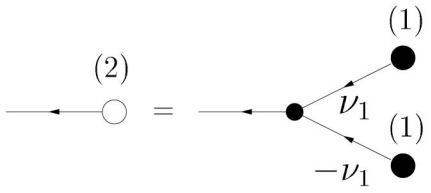

FIG. 5. Graphical representation of $c_2=x_0^{(2)}$. There is no contribution with any white bullet carrying order label $k=0$ and $k=1$ because of the restriction in the sum appearing in (3.6) and of the fact that $c_1=0$, respectively.

IV. FORMAL SOLUTIONS

The sum over the trees in (3.5) and (3.6), with the new definition of the set $\mathcal{T}_{k,\nu}$ given at the end of Sec. II, can be performed by summing over all possible "tree shapes" (that is trees without labels or *unlabeled trees*) and, for a fixed shape, over all possible assignments of mode labels. In the case of a trigonometric polynomial of degree N the latter can be bounded by $(2N)^{|E(\theta)|}$, because each endpoint v can have either a mode label $\nu_v \neq 0$, with $|\nu_v| \leqslant N$, or the mode label $\nu_v=0$, while the case of analytic functions (or even to obtain bounds which are uniform in N) must be discussed a little more carefully. The number of unlabeled trees with P nodes (vertices and endpoints) can be bounded by 2^{2P}.

Recall that $V_s(\theta)$ denotes the set of vertices v such that $s_v=s$; of course $V_1(\theta) \cup V_2(\theta)=V(\theta)$, and $V_0(\theta) \subset V_2(\theta)$. Analogously we can set

$$L_0(\theta)=\{\ell \in L(\theta):n_\ell=0,\},$$

$$L_1(\theta)=\{\ell \in L(\theta):\ell=\ell_v,v \in V_1(\theta)\}, \tag{4.1}$$

$$L_2(\theta)=L(\theta) \setminus (L_0(\theta) \cup L_1(\theta)),$$

with the splitting made in such a way that one has

$$\left|\prod_{v \in V_1(\theta)} F_v\right| \left|\prod_{\ell \in L_1(\theta)} g_\ell\right| \leqslant \prod_{\ell \in L_1(\theta)} |\omega \nu_\ell|, \quad \left|\prod_{\ell \in L_2(\theta)} g_\ell\right| \leqslant \prod_{\ell \in L_2(\theta)} \frac{1}{|\omega \nu_\ell|},$$

$$\left|\prod_{v \in V_0(\theta)} F_v\right| \leqslant \left(\frac{1}{2c_0}\right)^{|V_0(\theta)|}, \quad \left|\prod_{v \in E_W(\theta)} F_v\right| \leqslant c_0^{|E_W(\theta)|}, \tag{4.2}$$

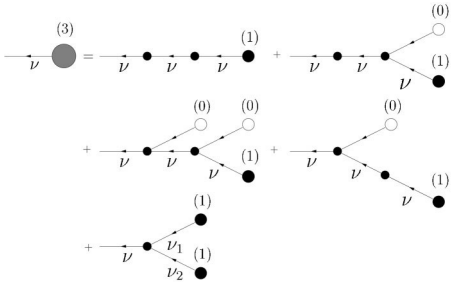

FIG. 6. Graphical representation of $x_\nu^{(3)}$ for $\nu \neq 0$. The second and fourth contributions must be counted twice, while the third one must be counted four times. There is no contribution with any white bullet carrying the order label $k=1$ as $c_1=0$.

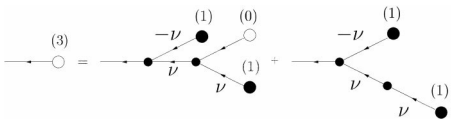

FIG. 7. Graphical representation of $c_3=x_0^{(3)}$. The second contribution must be counted twice, while the first one must be counted four times. There is no contribution with any white bullet carrying the order label $k=1$ as $c_1=0$.

$$\left|\prod_{v\in E_B(\theta)} F_v\right| \leqslant F^{|E_B(\theta)|} \prod_{v\in E_B(\theta)} e^{-\xi|\nu_v|},$$

where for each line ℓ one has $|\nu_\ell| \leqslant \Sigma_{v\in E_W(\theta)}|\nu_v|$.

The following result is useful when looking for bounds on the tree values.

Lemma 4.1: *Given a tree θ with branching number s one has $|E(\theta)| \leqslant (s-1)|V(\theta)|+1$. If k denotes the order of the tree θ, that is $|V(\theta)|-|V_0(\theta)|+|E_B(\theta)|=k$, one has the identity $|L_1(\theta)|+|L_2(\theta)|=k$, and the bounds $|V_1(\theta)| \leqslant k$, $|V_0(\theta)| \leqslant k-1$, $|E(\theta)| \leqslant k$ and $|E(\theta)|+|V(\theta)| \leqslant 2k-1$.*

Proof: It is a standard result on trees that one has $\Sigma_{v\in V(\theta)}(s_v-1)=|E(\theta)|-1$, so that the first bound follows. The bounds on $|V_1(\theta)|$, $|V_0(\theta)|$, $|E(\theta)|$ and $|E(\theta)|+|V(\theta)|$ can be easily proved by induction, while the identity $|L_1(\theta)|+|L_2(\theta)|=k$ follows from the observation that all lines in $L_1(\theta)$ and $L_2(\theta)$ come out either of vertices or of black bullets, and they have nonvanishing momentum. ■

Hence the number of lines in $L_1(\theta)$ is bounded by k, so that in (4.2) we can bound

$$\begin{aligned}\left(\prod_{\ell\in L_1(\theta)} |\omega\nu_\ell|\right)\left(\prod_{v\in E_B(\theta)} Fe^{-\xi|\nu_v|}\right) &\leqslant \left(\prod_{v\in E_B(\theta)} Fe^{-\xi|\nu_v|/2}\right)\left(\prod_{\ell\in L_1(\theta)} e^{-\xi|\nu_\ell|/2k}|\omega\nu_\ell|\right)\\ &\leqslant \left(\prod_{v\in E_B(\theta)} Fe^{-\xi|\nu_v|/2}\right)\left(\frac{2k|\omega|}{\xi}\right)^k, \qquad (4.3)\end{aligned}$$

and in the second line the product can be used to perform the sum over the Fourier labels—this gives a factor $F^kB_2^k$, with $B_2=2e^{-\xi/2}(1-\mathrm{e}^{-\xi/2})^{-1}$—while the last factor is bounded by $A_1B_1^k k!$, for some constants A_1 and B_1.

We can bound the value of a tree θ by using the bounds (4.2) and (4.3), and Lemma 4.1. If we define

$$\varepsilon_1^{-1} = \max\{B_1,|\omega|^{-1}\}\max\{c_0,FB_2\}\max\{1,(2c_0)^{-1}\}, \qquad (4.4)$$

with $c_0=\sqrt{\alpha}$, and take into account that the number of unlabeled trees in $\mathcal{T}_{k,\nu}$ is bounded by 2^{2k-1} (because each tree in $\mathcal{T}_{k,\nu}$ has at most $2k-1$ nodes), then

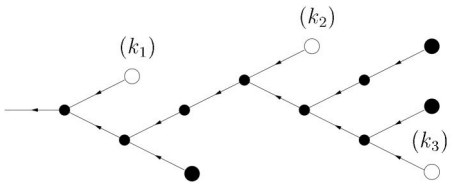

FIG. 8. Example of tree appearing in the graphical expansions (3.5) and (3.6). The number of lines entering any vertex v can be only either $s_v=1$ or $s_v=2$, while no line enters the endpoints. The order of the tree is given by the number of elements in $V(\theta)\setminus V_0(\theta)$ plus the number of elements in $E_B(\theta)$ plus the sum of the order labels of the white bullets. Then, if k_1, k_2, and k_3 are the order labels of the white bullets in the figure, the order of the tree is $k=k_1+k_2+k_3+10$ if $v_0 \in V_0(\theta)$ and $k=k_1+k_2+k_3+9$ if $v_0 \notin V_0(\theta)$. In the latter case one must have $k_1>0$ because of the constraint in the sum appearing in (3.6).

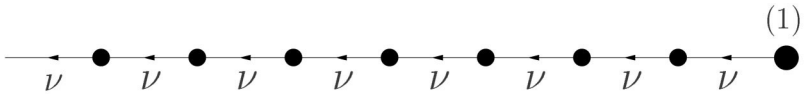

FIG. 9. Example of tree whose value grows as a factorial. If k is the order of the tree (hence there are $k-1$ vertices and 1 black bullet), then the value of the tree is given in (4.6).

$$|x_\nu^{(k)}| \leqslant A_1 \varepsilon_2^{-k} k\,!\,, \quad |x^{(k)}(t)| \leqslant A_1 \varepsilon_2^{-k} k\,!\,, \tag{4.5}$$

where we have set $\varepsilon_2 = \varepsilon_1 2^{-2}$.

A bound like (4.5) is obtained also in the case of forcing terms which are trigonometric polynomials, because in general we can bound the factors $|\omega\nu_\ell|$ in (4.2) only with kN (see Lemma 2.1), and this produces an overall bound proportional to $k!$ Note that in that case the bound B_2, arising from the sum over the Fourier labels, can be replaced with a factor $2N$, and B_1 can be replaced with $|\omega|N$.

Then we have proved the following result.

Proposition 4.2: *Given the equation (2.1) with f as in (1.4), there is only one periodic solution in the form of a formal power series, and the corresponding period is the same period $2\pi/\omega$ as the forcing term. The coefficients of such a formal power series satisfy the bounds (4.5).*

One could ask if the factorials arising in the bounds are only a technical problem, or whether they are a sign that the series really diverges. To order k one can easily provide examples of trees which grow like factorials; see for instance the tree represented in Fig. 9, where there are $k-1$ vertices with only one entering line. Then the corresponding value is

$$\mathrm{Val}(\theta) = (i\omega\nu)^{2(k-1)} \frac{1}{(i\omega\nu)^k} f_\nu = (i\omega\nu)^{k-2} f_\nu, \tag{4.6}$$

which behaves as $k!$ for large k. Furthermore it is unlikely that there are cancellations with the values of other trees because the value of any other tree $\theta \in \mathcal{T}_{k,\nu}$ can be proportional at most to $(i\omega\nu)^p$, with $p < k-2$ (strictly). Hence we expect that the coefficients $u_\nu^{(k)}$, even if well defined to all orders, grow like factorials, so preventing the convergence of the series.

The lack of analyticity is further supported by the following fact. If we consider (2.1) without the quadratic term and with $\alpha = 0$, that is

$$\varepsilon \ddot{x} + \dot{x} = f(\omega t), \quad f_0 = 0, \tag{4.7}$$

in Fourier space, we find $x_0 = 0$ and $i\omega\nu(1 + i\varepsilon\omega\nu)x_\nu = f_\nu$ for $\nu \neq 0$. Hence the equation is trivially solvable, and it gives

$$x(t) = \sum_{\nu \neq 0} \frac{f_\nu}{i\omega\nu(1 + i\varepsilon\omega\nu)} e^{i\omega\nu t}. \tag{4.8}$$

Of course the solution $x(t)$ of the linear equation is not analytic in ε (in a neighborhood of the origin) when f is an analytic function containing all the harmonics, as each point $\varepsilon = i/\omega\nu$ represents a singularity point for $x(t)$, and such points accumulate to the origin as $\nu \to \infty$. Then it is likely that also when the quadratic terms are taken into account the solution cannot be analytic. Therefore giving a meaning to the perturbation series requires some more work, and we discuss this next.

An important remark is that for any $k \geqslant 1$ there is no tree whose value can be bounded worse than proportionally to a factorial, as the estimates (4.5) show, indeed they have been obtained by bounding separately the value of each single tree. This observation will play an important role in the forthcoming analysis.

V. PERIODIC FORCING TERMS

To deal completely with the case of analytic functions and prove existence of the periodic solution, we must modify the graphical expansion envisaged in the preceding sections.

Let us come back to the equation (2.1), and write it in Fourier space. For $\nu \neq 0$ and denoting with x_ν the νth Fourier coefficient, we obtain

$$\varepsilon(i\omega\nu)^2 x_\nu + i\omega\nu\, x_\nu + \varepsilon \sum_{\nu_1+\nu_2=\nu} x_{\nu_1} x_{\nu_2} = \varepsilon f_\nu, \tag{5.1}$$

provided that for $\nu=0$ we have

$$\sum_{\nu_1+\nu_2=0} x_{\nu_1} x_{\nu_2} = 0. \tag{5.2}$$

Let us rewrite (5.1) as

$$\varepsilon(i\omega\nu)^2 x_\nu + i\omega\nu\, x_\nu + \mu\varepsilon \sum_{\nu_1+\nu_2=\nu} x_{\nu_1} x_{\nu_2} = \mu\varepsilon f_\nu, \tag{5.3}$$

and look for a solution $x(t)$ which is analytic in μ, which suggests us to write

$$x(t) = \sum_{k=0}^{\infty} \mu^k x^{[k]}(t). \tag{5.4}$$

Of course we want the value $\mu=1$ to be inside the analyticity domain. Note also that now $x^{[k]}$, the coefficient to order k, has a different meaning with respect to the previous expansion (1.4) in powers of ε, and for this reason with use a different symbol to denote it. We shall call the series (5.4) the *resummed series*, because the coefficients $x^{[k]}(t)$ depend on ε, and are given by the sum of infinitely many terms of the formal series (2.5).

Again for $k=0$ we must take $x_\nu^{[0]}=0$ for $\nu\neq 0$ and fix $c_0 \equiv x_0^{[0]} = \sqrt{\alpha}$, with $\alpha \equiv f_0$.

To order $k \geqslant 1$ (in μ) we obtain for $\nu \neq 0$,

$$i\omega\nu(1 + i\varepsilon\omega\nu) x_\nu^{[k]} = \varepsilon f_\nu \delta_{k,1} - \varepsilon \sum_{k_1+k_2=k-1} \sum_{\nu_1+\nu_2=\nu} x_{\nu_1}^{[k_1]} x_{\nu_2}^{[k_2]}, \tag{5.5}$$

while for $\nu=0$ we require

$$\sum_{k_1+k_2=k} \sum_{\nu_1+\nu_2=\nu} x_{\nu_1}^{[k_1]} x_{\nu_2}^{[k_2]} = 0. \tag{5.6}$$

By setting $c_k = x_0^{[k]}$ the latter equation can be written as [cf. (2.10)]

$$c_1 = 0, \quad c_k = -\frac{1}{2c_0} \sum_{k'=1}^{k-1} \sum_{\nu\in\mathbb{Z}} x_\nu^{[k-k']} x_{-\nu}^{[k']}, \quad k \geqslant 2. \tag{5.7}$$

Then we can proceed as in Sec. III, with some slight changes that we now explain. First of all note that (5.5) gives for $\nu \neq 0$,

$$x_\nu^{[0]} = 0,$$

$$x_\nu^{[1]} = \frac{\varepsilon f_\nu}{i\omega\nu(1 + i\varepsilon\omega\nu)},$$

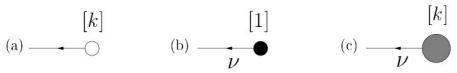

FIG. 10. Graphical representation of $x_0^{[k]}$, $x_\nu^{[1]}$, and $x_\nu^{[k]}$. For $\nu=0$ the latter reduces to the first graph, while for $k=1$ and $\nu\neq 0$ it reduces to the second graph. In the first graph the momentum is not shown as it is necessarily $\nu=0$.

$$x_\nu^{[k]} = -\frac{\varepsilon}{i\omega\nu(1+i\varepsilon\omega\nu)} \sum_{k_1+k_2=k-1} \sum_{\nu_1+\nu_2=\nu} x_{\nu_1}^{[k_1]} x_{\nu_2}^{[k_2]}, \quad k \geqslant 2. \tag{5.8}$$

Then the graphical representations of $x_0^{[k]}$, $x_\nu^{[1]}$, and $x_\nu^{[k]}$ are as in the previous case, with the only change in the representation of the order labels (because of the square brackets instead of the parentheses); see Fig. 10.

On the contrary the graphical representation of the third equation in (5.8) is as in Fig. 11.

At the end we obtain a tree expansion where the trees differ from the previous ones as they contain no vertex with only one entering line. With the previous notations this means that $L_1(\theta)=\emptyset$ and $V_1(\theta)=\emptyset$, hence $V(\theta)=V_2(\theta)$. Moreover also the propagators and the node factors of the vertices are different, as (3.1) and (3.2) must be replaced with

$$g_\ell = \begin{cases} 1/((i\omega\nu_\ell)(1+i\varepsilon\omega\nu_\ell)), & \nu_\ell \neq 0, \\ 1, & \nu_\ell = 0, \end{cases} \tag{5.9}$$

and, respectively,

$$F_v = \begin{cases} -\varepsilon, & v \notin V_0(\theta), \\ -1/2c_0, & v \in V_0(\theta), \end{cases} \tag{5.10}$$

and we recall once more that only vertices v with $s_v=2$ are allowed. Finally, the node factors associated with the endpoints are $F_v=c_{k_v}$ if v is a white bullet and $F_v=\varepsilon f_{\nu_v}$ if v is a black bullet.

As in Sec. III we can envisage an expansion in which all white bullets v have $k_v=0$ (simply by expanding iteratively in trees the white bullets of higher order). A tree appearing in this new expansion is represented in Fig. 12.

With the notations (4.1), we obtain the bounds

$$\left|\prod_{v\in V(\theta)\setminus V_0(\theta)} F_v\right| \leqslant |\varepsilon|^{|V(\theta)|}, \quad \left|\prod_{\ell\in L(\theta)} g_\ell\right| \leqslant \prod_{\ell\in L_2(\theta)} \frac{1}{|\omega\nu_\ell||1+i\varepsilon\omega\nu_\ell|},$$

$$\left|\prod_{v\in V_0(\theta)} F_v\right| \leqslant \left(\frac{1}{2c_0}\right)^{|V_0(\theta)|}, \quad \left|\prod_{v\in E_W(\theta)} F_v\right| \leqslant c_0^{|E_W(\theta)|}, \tag{5.11}$$

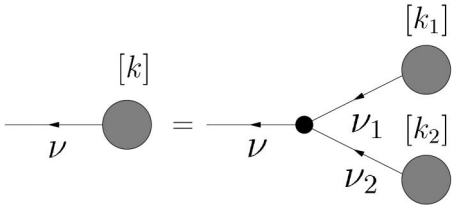

FIG. 11. Graphical representation of the second equation in (5.8) expressing the coefficient $x_\nu^{[k]}$ for $k\geqslant 2$ and $\nu\neq 0$ in terms of the coefficients $x_{\nu'}^{[k']}$ with $k'<k$. In the right-hand graph one has the constraints $k_1+k_2=k-1$ and $\nu_1+\nu_2=\nu$.

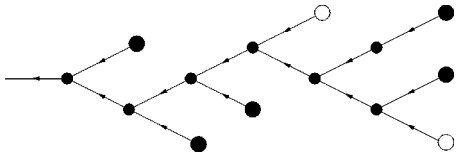

FIG. 12. Example of tree appearing in the new graphical expansion. The number of lines entering any vertex v can be only $s_v=2$. The order of the tree is given by $|B(\theta)|-|V_0(\theta)|$. All the white bullets have order labels (0), and additionally all the black bullets carry a label (1); hence we can avoid drawing explicitly such labels.

$$\left|\prod_{v\in E_B(\theta)} F_v\right| \leqslant F^{|E_B(\theta)|} \prod_{v\in E_B(\theta)} e^{-\xi|\nu_v|},$$

where we have again used the bound $|f_\nu|\leqslant Fe^{-\xi|\nu|}$, for suitable (strictly) positive constants F and ξ, which follows from the analyticity assumption on f.

For real ε we can bound each propagator by

$$|g_\ell| \leqslant \frac{1}{|\omega\nu_\ell|} \leqslant \frac{1}{|\omega|}, \tag{5.12}$$

so that the value of any tree $\theta\in\mathcal{T}_{k,\nu}$ can be bounded by

$$|\mathrm{Val}(\theta)| \leqslant |\varepsilon|^k|\omega|^{-k}(\max\{c_0,F\})^k(\max\{1,1/2c_0\})^k \prod_{v\in E_B(\theta)} e^{-\xi|\nu_v|}, \tag{5.13}$$

where we have again used Lemma 4.1. If we write

$$\prod_{v\in E_B(\theta)} e^{-\xi|\nu_v|} \leqslant e^{-\xi|\nu|/2}\left(\prod_{v\in E_B(\theta)} e^{-\xi|\nu_v|/2}\right), \tag{5.14}$$

we can proceed as in Sec. IV; we use the last product to perform the sum over the Fourier labels, which gives a factor B_2^k, whereas the sum over the unlabeled trees gives a factor 2^{2k-1}. At the end we obtain

$$|x_\nu^{(k)}| \leqslant \mu_2^{-k}, \quad |x^{(k)}(t)| \leqslant \mu_2^{-k}, \tag{5.15}$$

where we have set $\mu_2^{-1}=4|\omega|^{-1}\max\{1,1/2c_0\}\max\{FB_2,c_0\}|\varepsilon|$. Hence the radius of convergence μ_0 of the series expansion (5.4) is bounded as $\mu_0\geqslant\mu_2=O(1/|\varepsilon|)$, so that for ε small enough, say $|\varepsilon|<\varepsilon_3=(4|\omega|^{-1}\max\{1,1/2c_0\}\max\{FB_2,c_0\})^{-1}$, the value $\mu=1$ is inside the analyticity domain.

We can summarize the results found so far as follows.

Theorem 5.1: *Given the equation (2.1) with f analytic, there exists* $\varepsilon_0>0$ *such that for all real* ε *with* $|\varepsilon|<\varepsilon_0$ *there is only one periodic solution which admits a formal expansion in powers of* ε*, and the corresponding period is the same period* $2\pi/\omega$ *as the forcing term. An explicit bound is* $\varepsilon_0\geqslant\varepsilon_3=O(\omega)$.

Note that if ω is very large then very large values of ε are allowed.

We can investigate further the regularity properties in ε of the periodic solution found in Theorem 5.1, and see what happens for complex values of ε.

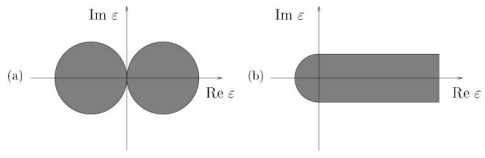

FIG. 13. (a) Region $\mathcal{C}_R$ in the complex ε-plane and (b) striplike region of analyticity $\mathcal{S}_B$ of the Borel transform. The region $\mathcal{C}_R$ is the union of two discs of radius $R/2$ and centers $(\pm R/2,0)$.

We need the following preliminary result [see Fig. 13(a) for the region $\mathcal{C}_R$].

Lemma 5.2: *Given* $\omega>0$ *and* $0<R<1/4\omega$ *let* $\mathcal{C}_R$ *be the pair of discs* $\mathcal{C}_R=\{\varepsilon:|\mathrm{Re}\,\varepsilon^{-1}|>R^{-1}\}$. *For all* $\varepsilon\in\mathcal{C}_R$ *and all* $\nu\in\mathbb{Z}\setminus\{0\}$ *one has* $|i\omega\nu(1+i\varepsilon\omega\nu)|\geqslant\omega/2$.

Proof: Write $\varepsilon=a+ib$ and $x=\omega\nu$, so that one has $|i\omega\nu(1+i\varepsilon\omega\nu)|=|x|\sqrt{(1-bx)^2+(ax)^2}\equiv F(x)$. If $\varepsilon\in\mathcal{C}_R$ one has $|a|\geqslant b^2/2R$. Fix $0<A<1$. If $|1-bx|\leqslant A$ then $\sqrt{(1-bx)^2+(ax)^2}\geqslant|ax|\geqslant b^2|x|/2R\geqslant|b|(1-A)/2R$, so that $F(x)\geqslant(1-A)^2/2R$. If $|1-bx|\geqslant A$ then $\sqrt{(1-bx)^2+(ax)^2}\geqslant A$, hence $F(x)\geqslant A|x|\geqslant\omega A$. Then choose $A=1-\sqrt{\omega R}\geqslant 1/2$; this gives $F(x)\geqslant\omega/2$. ■

Now fix $0<R<\bar{R}\equiv\varepsilon_3$ so small that $|\omega|R<1/4$, and consider the corresponding domain $\mathcal{C}_R$. We can apply Lemma 5.2 and deduce that any propagator g_ℓ is bounded by $|g_\ell|\leqslant 2/|\omega|$ for all $\varepsilon\in\mathcal{C}_R$.

This allows us to obtain the following result.

Proposition 5.3: *There exists* $R>0$ *small enough such that in the domain* $\mathcal{C}_R$ *one has the asymptotic expansion*

$$x(t)=\sum_{k=0}^{N-1}\varepsilon^k x^{(k)}(t)+\mathfrak{R}_N(\varepsilon),\quad |\mathfrak{R}_N(\varepsilon)|\leqslant AB^N N!\,|\varepsilon|^N, \tag{5.16}$$

where the constants A and B are uniform in N and in ε.

Proof: Write $x(t)$ as $x(t)=x_N(t)+\mathfrak{R}_N(t)$, where $x_N(t)$ is given by the sum of the first $N-1$ orders of the formal power series expansion of the solution $x(t)$ as in (5.16). For $\varepsilon\in\mathcal{C}_R$ the function (5.4) with $\mu=1$ is C^∞ in ε, hence we can estimate $\mathfrak{R}_N(\varepsilon)$ with a bound on the Nth derivative of $x(t)$ in $\mathcal{C}_R$, and this gives the bound in (5.16). ■

Of course the constants A and B in (5.16) are explicitly computable; in particular one finds $B=O(\varepsilon_3^{-1})$.

Then we are under the assumptions where Nevanlinna's theorem[11] (see also Ref. 12) can be applied, and hence the series for

$$\mathfrak{B}(t;\varepsilon)=\sum_{k=0}^{\infty}\frac{1}{k!}\varepsilon^k x^{(k)}(t) \tag{5.17}$$

converges for $|\varepsilon|<B$ [with B given in (5.16)] and has an analytic continuation to $\mathcal{S}_B=\{\varepsilon:\mathrm{dist}(\varepsilon,\mathbb{R}_+)<B\}$ [see Fig. 13(b)], satisfying for some constant K the bound $|\mathfrak{B}(t;\varepsilon)|\leqslant Ke^{|\varepsilon|/R}$ uniformly in every $\mathcal{S}_{B'}$ with $B'<B$. The function $x(t)$ can be represented as the absolutely convergent integral

$$x(t)=\frac{1}{\varepsilon}\int_0^\infty e^{-s/\varepsilon}\mathfrak{B}(t;s)\mathrm{d}s \tag{5.18}$$

for all $\varepsilon\in\mathcal{C}_R$, and this property can be stated by saying that $x(t)$ is Borel summable (in ε) and $\mathfrak{B}(t;\varepsilon)$ is its Borel transform.[9] This implies that the function given by the summation procedure described in Theorem 1 is unique. Therefore we have obtained the following result, which strengthens Theorem 1.

Theorem 5.4: *The solution given by Theorem 1 is Borel summable at the origin.*

Note that Watson's theorem cannot be invoked to obtain this result because the singularities are along the imaginary axis.

In particular if $f(\omega t)=\alpha+\beta\sin t$ then there is a periodic solution $x(t)=a+\varepsilon\beta\cos t+O(\varepsilon^2)$, with $a=\sqrt{\alpha}$, which has period 2π and moves around the fixed point $(x,\dot{x})=(a,0)$, and close to it within $O(\varepsilon)$. No other periodic solution analytic in ε can exist.

We conclude this section with two remarks. The summation criterion envisaged in this section is reminiscent of that used (in a more difficult situation) in Ref. 6 for hyperbolic lower-dimensional tori. However in that case we are not able to prove Borel summability because to order k the bounds were like $(k!)^\alpha$ for some $\alpha>1$. Neither extension to Watson's theorem[9]

analogous to the Nevanlinna–Sokal result (as those developed in Ref. 5) can be used because the exponent α is too large. We shall find a very similar situation in next section.

The lack of analyticity in ε in a neighborhood of the origin is due to the accumulation of singularity points along the imaginary axis in the complex ε-plane (where the quantity $1+i\varepsilon\omega\nu$ vanishes for $\nu\in\mathbb{Z}$). The analyticity domain is tangential to the imaginary axis, and this allows us to apply Nevanlinna's theorem. We find that this situation has some analogies with a different problem, the analyticity properties of rescaled versions of some dynamical systems, such as Siegel's problem[4] (and its linearization as considered in Ref. 10), the standard map[2] and generalized standard maps,[3] for complex rotation numbers tending to rational values in the complex plane. In those cases, however, only nontangential limits could be considered. Of course the situation is slightly more complicated there, because the set of accumulating singularity points is dense—and not only numerable as in the present case.

VI. QUASIPERIODIC FORCING TERMS

In the case of analytic quasiperiodic forcing terms, we shall assume a Diophantine condition on the rotation vector $\boldsymbol{\omega}$, that is

$$|\boldsymbol{\omega}\cdot\boldsymbol{\nu}| \geqslant C_0|\boldsymbol{\nu}|^{-\tau} \quad \forall\, \boldsymbol{\nu}\in\mathbb{Z}^d\setminus\{\mathbf{0}\}, \tag{6.1}$$

where $|\boldsymbol{\nu}|=|\boldsymbol{\nu}|_1\equiv|\nu_1|+\cdots+|\nu_d|$, and C_0 and τ are positive constants. We need $\tau\geqslant d-1$ in order to have a nonvoid set of vectors satisfying the condition (6.1), and $\tau>d-1$ in order to have a full measure set of such vectors. For simplicity (and without loss of generality) we can assume $C_0<\gamma/2$, with $\gamma=\min\{1,|c|\}$, where c is a suitable constant to be fixed as $c=-2c_0$, with $c_0=\sqrt{\alpha}$.

The equation of motion can be written in Fourier space as

$$i\boldsymbol{\omega}\cdot\boldsymbol{\nu}(1+i\varepsilon\boldsymbol{\omega}\cdot\boldsymbol{\nu})x_{\boldsymbol{\nu}}+\varepsilon\sum_{\boldsymbol{\nu}_1+\boldsymbol{\nu}_2=\boldsymbol{\nu}} x_{\boldsymbol{\nu}_1}x_{\boldsymbol{\nu}_2}=\varepsilon f_{\boldsymbol{\nu}}, \tag{6.2}$$

and the formal expansion for a quasiperiodic solution with frequency vector $\boldsymbol{\omega}$ reads as

$$x(t)=\sum_{k=0}^{\infty}\varepsilon^k x^{(k)}(t)=\sum_{k=0}^{\infty}\varepsilon^k\sum_{\boldsymbol{\nu}\in\mathbb{Z}^d} e^{i\boldsymbol{\nu}\cdot\boldsymbol{\omega}t}x_{\boldsymbol{\nu}}^{(k)}, \tag{6.3}$$

and to see that the coefficients $x_{\boldsymbol{\nu}}^{(k)}$ are well defined to all orders $k\geqslant 0$ one can proceed as in Sec. II, with no extra difficulty. In particular the Diophantine condition (6.1) is sufficient to assure analyticity in t of the coefficients $x^{(k)}(t)$.

Also the graphical representation can be worked out as in Sec. III. The only difference is that now the propagators of the lines with nonvanishing momentum $\boldsymbol{\nu}_\ell$, which is defined according to (3.2), with the vectors replacing the scalars, are given by $1/(i\boldsymbol{\omega}\cdot\boldsymbol{\nu}_\ell)$, the node factors associated with the vertices v with $s_v=1$ are given by $F_v=-(i\boldsymbol{\omega}\cdot\boldsymbol{\nu}_{\ell_v})^2$, and the node factors associated with the black bullets v are given by $F_v=f_{\boldsymbol{\nu}_v}$, with $\boldsymbol{\nu}_v\in\mathbb{Z}^d\setminus\{\mathbf{0}\}$. All the other notations remain unchanged.

This yields that the propagators and the node factors can be bounded as in (4.2) and (4.3), with just a few differences of notation. More precisely one has

$$\left|\prod_{v\in V_1(\theta)}F_v\right|\left|\prod_{\ell\in L_1(\theta)}g_\ell\right|\leqslant\prod_{\ell\in L_1(\theta)}|\boldsymbol{\omega}||\boldsymbol{\nu}_\ell|, \quad \left|\prod_{\ell\in L_1(\theta)}g_\ell\right|\leqslant\prod_{\ell\in L_1(\theta)}\frac{1}{|\boldsymbol{\omega}\cdot\boldsymbol{\nu}_\ell|}\leqslant C_0^{-1}|\boldsymbol{\nu}_\ell|^\tau,$$

$$\left|\prod_{v\in V_0(\theta)}F_v\right|\leqslant\left(\frac{1}{2c_0}\right)^{|V_0(\theta)|}, \quad \left|\prod_{v\in E_W(\theta)}F_v\right|\leqslant c_0^{|E_W(\theta)|}, \tag{6.4}$$

$$\left| \prod_{v \in E_B(\theta)} F_v \right| \leqslant F^{|E_B(\theta)|} \prod_{v \in E_B(\theta)} e^{-\xi|\boldsymbol{\nu}_v|},$$

where the only bound which introduces a real difficulty with respect to the case of periodic forcing terms is the second one in the first line. Indeed it is the source of a small divisors problem, which cannot be set only through the Diophantine condition (6.1).

To each order k we obtain for $x^{(k)}(t)$ a bound like $AB^k k!^{\max\{1,\tau\}}$, where the factor 1 arises from the propagators of the lines in $L_1(\theta)$ and the factor τ from those of the lines in $L_2(\theta)$ in (6.3). The last assertion is easily proved by reasoning as in (4.3), with $\max\{|\boldsymbol{\omega}||\boldsymbol{\nu}_\ell|, C_0^{-1}|\boldsymbol{\nu}_\ell|^\tau\} \leqslant \max\{C_0^{-1}, |\boldsymbol{\omega}|\}|\boldsymbol{\nu}_\ell|^{\max\{1,\tau\}}$ replacing ν_ℓ. In particular only for $d=2$ and $\tau=1$ we obtain the same bound proportional to $k!$ as in the case of periodic solution (of course with different constants A and B). Note that the vectors satisfying the Diophantine condition (6.1) with $\tau=1$ for $d=2$ is of zero measure but everywhere dense. An example of vector of this kind is $\boldsymbol{\omega}=(1,\gamma_0)$, where $\gamma_0 = (\sqrt{5}-1)/2$ is the golden section.

However, to deal with the problem of accumulation of small divisors and discuss the issue of convergence of the series, we need renormalization group techniques. The first step is just to introduce a multiscale decomposition of the propagators, and this leads naturally to the introduction of clusters and self-energy graphs into the trees. The discussion can be performed either as in Ref. 6 or as in Ref. 8 (and in Ref. 7). We choose to follow Ref. 8, which is more similar to the present problem because the propagators are scalar quantities and not matrices. In any case, with respect to the quoted reference, we shall use a multiscale decomposition involving only the quantities $|\boldsymbol{\omega}\cdot\boldsymbol{\nu}_\ell|$, that is without introducing any dependence on ε in the compact support functions. Indeed this is more suitable to investigate the analyticity properties in ε, and, as we shall see, we shall not need to exclude any real value of ε in order to give a meaning to the resummed series, a situation more reminiscent of Ref. 6 than of Ref. 8.

In the following we confine ourselves to outlining the main differences with respect to Ref. 8. Let us introduce the functions ψ_n and χ_n, for $n \geqslant 0$, as in Ref. 8, Sec. 5. In particular $\psi_n(|x|) \neq 0$ implies $|x| \geqslant 2^{-(n+1)}C_0$ and $\chi_n(|x|) \neq 0$ implies $|x| \leqslant 2^{-n}C_0$. We shall define recursively the *renormalized propagators* $g_\ell^{[n]} = g^{[n]}(\boldsymbol{\omega}\cdot\boldsymbol{\nu}_\ell;\varepsilon)$ and the *counterterms* $\mathcal{M}^{[n]}(\boldsymbol{\omega}\cdot\boldsymbol{\nu};\varepsilon)$ on scales n as

$$g^{[-1]}(x;\varepsilon) = 1, \quad M^{[-1]}(x;\varepsilon) = 0,$$

$$g^{[0]}(x;\varepsilon) = \frac{\psi_0(|x|)}{ix(1+i\varepsilon x)}, \quad M^{[0]}(x;\varepsilon) = \sum_{k=1}^{\infty} \sum_{T \in \mathcal{S}_{k,0}^{\mathcal{R}}} \mathcal{V}_T(x;\varepsilon),$$

$$g^{[n]}(x;\varepsilon) = \frac{\chi_0(|x|)\cdots\chi_{n-1}(|x|)\psi_n(|x|)}{ix(1+i\varepsilon x) + \mathcal{M}^{[n-1]}(x;\varepsilon)}, \tag{6.5}$$

$$\mathcal{M}^{[n]}(x;\varepsilon) = \mathcal{M}^{[n-1]}(x;\varepsilon) + \chi_0(|x|)\cdots\chi_{n-1}(|x|)\chi_n(|x|)M^{[n]}(x;\varepsilon),$$

$$M^{[n]}(x;\varepsilon) = \sum_{k=1}^{\infty} \sum_{T \in \mathcal{S}_{k,n}^{\mathcal{R}}} \mathcal{V}_T(x;\varepsilon),$$

where the set of renormalized self-energy graphs $\mathcal{S}_{k,n}^{\mathcal{R}}$ and the self-energy graphs $\mathcal{V}_T(x;\varepsilon)$ are defined as in Ref. 8, Sec. 6. We have explicitly used the fact that the first contribution to the self-energy graphs is of order $k=1$ (see Fig. 14). Note that one has $\chi_0(|x|)\cdots\chi_{n-1}(|x|)\chi_n(|x|) = \chi_n(|x|)$, so that if $g^{[n]}(x;\varepsilon) \neq 0$ then one has $2^{-(n+1)}C_0 \leqslant |x| \leqslant 2^{-(n-1)}C_0$.

Then one defines for $k \geqslant 1$

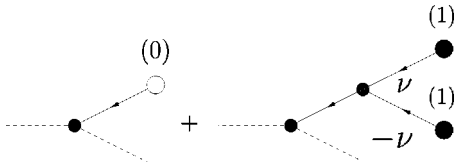

FIG. 14. Lower order contributions to the counterterm arising from self-energy graphs of order $k=1$ and $k=3$. The (dashed) external lines do not enter into the definition of self-energy graph, and they have been drawn only with the aim of helping to visualize the structure of the self-energy graph.

$$x_{\boldsymbol{\nu}}^{[k]} = \sum_{\theta \in \mathcal{T}_{k,\boldsymbol{\nu}}} \mathrm{Val}(\theta), \quad x_{\mathbf{0}}^{[k]} \equiv c_k = \sum_{\theta \in \mathcal{T}_{k,\mathbf{0}}}{}^{*}\mathrm{Val}(\theta), \tag{6.6}$$

where the tree value is defined as

$$\mathrm{Val}(\theta) = \left(\prod_{\ell \in L(\theta)} g_{\ell}^{[n_\ell]} \right) \left(\prod_{v \in E(\theta) \cup V(\theta)} F_v \right), \tag{6.7}$$

and, as before, $*$ means that there are two lines entering the last vertex v_0 of θ_0 and neither one exits from an endpoint v with order label $k_v=0$. For $k=1$ the second of (6.7) must be interpreted as $c_1=0$.

Furthermore one has

$$\begin{aligned} M^{[0]}(x;\varepsilon) &= M^{[0]}(0;\varepsilon) + O(\varepsilon^2 x), \\ M^{[0]}(0;\varepsilon) &= -2\varepsilon c_0 + M_2^{[0]}(0;\varepsilon), \quad M_2^{[0]}(0;\varepsilon) = O(\varepsilon^2), \end{aligned} \tag{6.8}$$

and an easy computation shows (cf. Fig. 14) that

$$M_2^{[0]}(0;\varepsilon) = \varepsilon^3 \frac{1}{c_0} \sum_{\boldsymbol{\nu} \neq \mathbf{0}} \psi_0^2(|\boldsymbol{\omega} \cdot \boldsymbol{\nu}|) \frac{|f_{\boldsymbol{\nu}}|^2}{(\boldsymbol{\omega} \cdot \boldsymbol{\nu})^2 (1 + (\varepsilon \boldsymbol{\omega} \cdot \boldsymbol{\nu})^2)} + O(\varepsilon^4), \tag{6.9}$$

so that in fact one has $M_2^{[0]}(0;\varepsilon)=O(\varepsilon^3)$.

Moreover to higher scales one has $M^{[n]}(x;\varepsilon)=M^{[n]}(0;\varepsilon)+O(\varepsilon^3 x)$, with

$$M^{[n]}(0;\varepsilon) = -\varepsilon^3 \frac{1}{c_0} \sum_{\boldsymbol{\nu} \neq \mathbf{0}} \sum_{n_1+n_2=n} \psi_{n_1}(|\boldsymbol{\omega} \cdot \boldsymbol{\nu}|) \psi_{n_2}(|\boldsymbol{\omega} \cdot \boldsymbol{\nu}|) \frac{|f_{\boldsymbol{\nu}}|^2}{(\boldsymbol{\omega} \cdot \boldsymbol{\nu})^2 (1 + (\boldsymbol{\omega} \cdot \boldsymbol{\nu})^2)} + O(\varepsilon^4), \tag{6.10}$$

so that each $M^{[n]}(0;\varepsilon)$ is a higher order correction to $M^{[0]}(0;\varepsilon)$ and it decays exponentially in n (because of the compact support functions).

The following result holds.

Lemma 6.1: *Assume that the renormalized propagators up to scale $n-1$ can be bounded as*

$$|g_{\ell}^{[n_\ell]}| \leq C_1^{-1} 2^{\beta n_\ell} \tag{6.11}$$

for some positive constants C_1 and β. Then for all $n' \leq n-1$ the number $N_{n'}(\theta)$ of lines on scale n' in θ is bounded by

$$N_{n'}(\theta) \leq K 2^{-n'/\tau} \sum_{v \in E_B(\theta)} |\boldsymbol{\nu}_v|, \tag{6.12}$$

for some positive constant K. If $|\varepsilon| < \varepsilon_0$, with ε_0 small enough, then for all $n' \leq n$ one has

$$|M^{[n']}(x;\varepsilon)| \leq D_1 |\varepsilon|^3 e^{-D_2 2^{n'/\tau}}, \quad |\partial_x M^{[n']}(x;\varepsilon)| \leq D_1 |\varepsilon|^3 e^{-D_2 2^{n'/\tau}}, \tag{6.13}$$

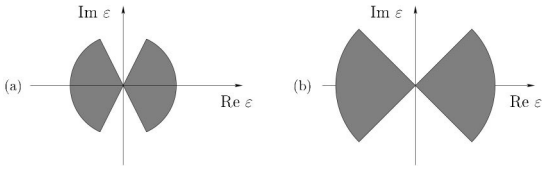

FIG. 15. Region $\mathcal{D}_{R,\lambda}$ in the complex ε-plane for $\lambda=\tan\pi/6$ (a) and for $\lambda=1$ (b). One can write $\lambda=\tan\varphi$, where φ is the angle between the imaginary axis and the line $a=\lambda b$.

for some C_1-independent positive constants D_1 and D_2. Only the constant D_1 depends on β. The constant ε_0 can be written as $\varepsilon_0=C_1C_2^{-\beta}C_3$, with C_2 and C_3 two positive constants independent of β and C_1.

Proof: The proof can be easily adapted from the proofs of Lemma 1 and Lemma 2 of Ref. 8.■

So we are left with the problem of proving that the renormalized propagators satisfy the bounds (6.11). To this end let us introduce the notation

$$F(x) = F_0(x) + c_1(\varepsilon)\varepsilon + c_2(\varepsilon,x)\varepsilon^2 x, \quad F_0(x) = ix(1+i\varepsilon x), \tag{6.14}$$

with $x=\boldsymbol{\omega}\cdot\boldsymbol{\nu}$ and the functions $c_1(\varepsilon)$ and $c_2(\varepsilon,x)$ such that $c_1(\varepsilon)=c+c_3(\varepsilon)\varepsilon$, with $c\neq 0$, and the functions $|c_2(\varepsilon,x)|$ and $|c_3(\varepsilon)|$ bounded by a constant c' uniformly (in ε and x). Recall that $\gamma=\min\{1,|c|\}$ and $C_0<\gamma/2$.

Fix $\lambda\in[0,1]$. Set $\mathcal{B}_R(0)=\{\varepsilon\in\mathbb{C}:|\varepsilon|<R\}$ and $\mathcal{D}_{R,\lambda}=\{\varepsilon=a+ib\in\mathcal{B}_{\lambda R}(0):|a|\geq\lambda|b|\}$ (see Fig. 15). The following result refines Lemma 5.2.

Lemma 6.2: *Given $0<R<1/4C_0$, let $\mathcal{C}_R$ be defined as in Lemma 5.2. For all $\varepsilon\in\mathcal{C}_R$ and all x one has $|F_0(x)|\geq\min\{C_0,|x|\}/2$, while for all $\varepsilon\in\mathcal{D}_{R,\lambda}$ one has $|F_0(x)|\geq\lambda|x|/2$.*

Proof: Write $\varepsilon=a+ib$, so that $|F_0(x)|=|x|\sqrt{(1-bx)^2+(ax)^2}$. For $\varepsilon\in\mathcal{C}_R$ set $A=1-\sqrt{C_0R}$. If $|x|\geq C_0$, for $|1-bx|\leq A$ one has $|F_0(x)|\geq|ax^2|\geq b^2x^2/2R\geq C_0/2$, while for $|1-bx|\geq A$ one has $|F_0(x)|\geq A|x|\geq|x|/2\geq C_0/2$. If $|x|\leq C_0$, for $|1-bx|\leq A$ one has $|F_0(x)|\geq|ax^2|\geq C_0/2\geq|x|/2$, while for $|1-bx|\geq A$ one has $|F_0(x)|\geq A|x|\geq|x|/2$. For $\varepsilon\in\mathcal{D}_{R,\lambda}$ set $A=1/2$, one finds $|F_0(x)|\geq\lambda|x|/2$. ■

Then the following result holds.

Lemma 6.3: *Set $x=\boldsymbol{\omega}\cdot\boldsymbol{\nu}$ and assume $|x|\leq C_0$. Then if R is small enough one has $|F(x)|\geq\lambda\gamma|x|/8$ for all $\varepsilon\in\mathcal{D}_{R,\lambda}$.*

Proof: Set $F_1(x)=F_0(x)+c\varepsilon$ and $\varepsilon=a+ib$. Then $F_1(x)=i(x+b(c-x^2))+a(c-x^2)$, and $|F(x)|\geq|F_1(x)|-c'|\varepsilon|^2(1+|x|)$. If $|x+b(c-x^2)|\geq|x|/2$ and $|bc|\geq 4|x|$ one has $|F_1(x)|\geq|c|\sqrt{b^2+a^2}/2\equiv|c\varepsilon|/2$, so that $|F(x)|\geq|c\varepsilon|/4\geq|cb|/4\geq|x|$. If $|x+b(c-x^2)|\geq|x|/2$ and $|bc|\leq 4|x|$ one has $|F_1(x)|\geq\gamma\max\{\sqrt{x^2+a^2},|\varepsilon|/4\}/2$, so that $|F(x)|\geq\gamma\sqrt{x^2+a^2}/4\geq\gamma|x|/4$. If $|x+b(c-x^2)|\leq|x|/2$ one has $|b(c-x^2)|\geq|x|/2$ and $|bc|\leq 3|x|$, which give $|\varepsilon|^2\leq 3|\varepsilon|\sqrt{a^2+x^2}/\gamma\leq 3\lambda R(|a|+|x|)/\gamma$, and $|F_1(x)|\geq|a(c-x^2)|\geq|a(c-x^2)|/2+(\lambda|x|/2)/2\geq\gamma\lambda(|a|+|x|)/4$, so that $|F(x)|\geq\gamma\lambda|x|/8$. ■

Then we can come back to the bounds of the renormalized propagators, and prove the following result.

Lemma 6.4: *If R is small enough for all $n\geq 0$ and all $\varepsilon\in\mathcal{D}_{R,\lambda}$ the renormalized propagators $g^{[n]}(x;\varepsilon)$ satisfy the bounds (6.11) with $\beta=1$ and $C_1=\lambda C_4$, with a λ-independent constant C_4.*

Proof: The proof can be done by induction on n. For $n=0$ the bound is trivially satisfied by Lemma 6.2. Assuming that the bounds hold for all $n'<n$ then we can apply Lemma 6.1 and deduce the bounds (6.13). In turn this implies that the renormalized propagators on scale n can be written as $g^{[n]}(x;\varepsilon)=1/F(x)$, with $F(x)$ written as in (6.14) for $c=-2c_0$ [cf. (6.8)], and for suitable functions $c_1(\varepsilon)$ and $c_2(\varepsilon,x)$, depending on n and satisfying the properties listed after (6.14) for some n-independent constant c'. Then by Lemma 6.3 the renormalized propagators $g^{[n]}(x;\varepsilon)$ satisfy the same bounds (6.11) with $C_1=O(\lambda)$ for $\varepsilon\in\mathcal{D}_{R,\lambda}$. ■

Of course for real ε the bound (6.11) is trivially satisfied, with $C_1=2^{-1}C_0$. This follows from Lemma 6.4 with $\lambda=1$, but it is obvious independently of that result because one has $c_1(\varepsilon)=c\varepsilon+O(\varepsilon^2)$, with $c=-2c_0\in\mathbb{R}$. If we want to take also complex values of ε, we have analyticity in a

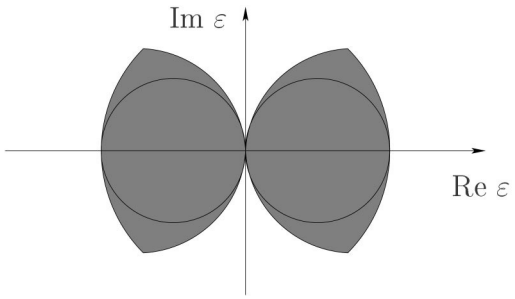

FIG. 16. Regions $\mathcal{D}_R$ and $\mathcal{C}_R$ in the complex ε-plane, $\mathcal{D}_R$ is the entire grey region, while $\mathcal{C}_R$ is the region contained inside the two circles.

domain D which can be written as $\mathcal{D}_R = \cup_{\lambda \in [0,1]} \mathcal{D}_{R,\lambda}$. One can easily realize that the region $\mathcal{C}_R$ is contained inside the domain $\mathcal{D}_R$ (cf. Fig. 16). Fix $\lambda = \tan \varphi$, with $\varphi \in [0, \pi/4]$ (see Fig. 15), for all such φ the line which forms an angle φ with the imaginary axis (see Fig. 15) and passes through the origin intersects the boundary of $\mathcal{D}_R$ at a distance $R \tan \varphi$ from the origin and the boundary of $\mathcal{C}_R$ at a distance $R \sin \varphi$. Hence we have an analyticity domain of the same form as in the case of periodic forcing terms. Nevertheless the results found so far do not allow us to obtain Borel summability, notwithstanding a circular analyticity domain $\mathcal{C}_R$ is found, as the bounds which are satisfied inside the region $\mathcal{C}_R$ are not uniform in ε (because of the dependence on λ).

Note that $\beta = 1$ in (6.11) is the same exponent appearing in the bounds of the propagators in the formal expansion. To obtain uniform bounds in a domain $\mathcal{C}_R$, for some value of R, we must allow larger values of β. The following result is obtained.

Lemma 6.5: *Set* $x = \boldsymbol{\omega} \cdot \boldsymbol{\nu}$ *and assume* $|x| < C_0$. *If* R *is small enough one has* $|F(x)| > \gamma |x|^2/2$ *for all* $\varepsilon \in \mathcal{C}_R$.

Proof: Set $F_1(x) = F_0(x) + c\varepsilon$ and $\varepsilon = a + ib$. If $|x + b(c - x^2)| \leq |x|/2$ one has $|b(c - x^2)| \geq |x|/2$ and $3|x| \geq |bc| \geq |x|/4$. Hence $|a(c - x^2)| \geq b^2 |c - x^2|/2R \geq |x|^2/16R|c|$, so that one has $|F_1(x)| \geq |a(c - x^2)| \geq |ac|/4 + |a(c - x^2)|/2 \geq \gamma(|a| + x^2/16Rc)/2$. On the other hand, one has $|\varepsilon|^2 = a^2 + b^2 \leq a^2 + 9x^2/c^2$, so that $|F(x)| \geq |F_1(x)| - 2c'|\varepsilon|^2 \geq |F_1(x)|/2 \geq \gamma x^2/2$. The case $|x + b(c - x^2)| \geq |x|/2$ can be discussed as in Lemma 6.3, and it gives $|F(x)| \geq \gamma |x|/4$. ■

Then we can prove the following result by proceeding exactly as in the proof of Lemma 8.

Lemma 6.6: *If* R *is small enough for all* $n \geq 0$ *and all* $\varepsilon \in \mathcal{C}_R$ *the renormalized propagators* $g^{[n]}(x; \varepsilon)$ *satisfy the bounds (6.11) with* $\beta = 2$ *and* C_1 *a suitable constant*.

The advantage of Lemma 6.4 with respect to Lemma 6.6 is that the bound of R is better, which means that the domain $\mathcal{C}_R$ contained inside $\mathcal{D}_R$ in the first case is larger than the domain $\mathcal{C}_R$ of the second case. The advantage of Lemma 6.6 is that it allows uniform bounds inside the corresponding domain $\mathcal{C}_R$ to be obtained. Nevertheless, because of the factor $\beta = 2$, a bound $AB^k k!^{2\tau}$ is obtained for the coefficients $x^{(k)}(t)$ of the formal solution, and a result analogous to Proposition 2 can be proved also for the present case, with $N!^{2\tau}$ replacing $N!$; we do not give the details as the proof is identical. Hence the bounds that we have are not good enough to obtain Borel summability in the case of quasiperiodic forcing terms, a situation strongly reminiscent of that encountered in Ref. 6. In fact at best one can set $\tau = 1$ for $d = 2$ (which, as noted above, corresponds to a set of Diophantine vectors of zero measure but everywhere dense), but this in turn implies a bound proportional to $N!^2$, which is not enough to apply Nevanlinna's theorem.

The conclusion is that the resummed series

$$x(t) = \sum_{k=0}^{\infty} \mu^k x^{[k]}(t), \tag{6.15}$$

where the coefficients $x^{[k]}(t)$ are given by

$$x^{[k]}(t) \sum_{\boldsymbol{\nu} \in \mathbb{Z}^d} e^{i\boldsymbol{\nu}\cdot\boldsymbol{\omega}t} x_{\boldsymbol{\nu}}^{[k]}, \tag{6.16}$$

with $x_{\boldsymbol{\nu}}^{[k]}$ defined by (6.6), is well defined and converges. In general it is not obvious—even if expected—that (6.15) solves the equation of motion (1.1). Indeed, unlike the case of periodic forcing terms, we have no result, such as Nevanlinna's theorem on Borel summability, which we can rely upon in order to link the resummed series to the formal series. Therefore we must check by hand that by expanding in powers of ε the resummed series we recover the formal power series (6.3). This means that the resummed series, which in principle could be unrelated to the equation of motion (because of the way it has been defined), in fact solves such an equation. Such a property can be proved by reasoning as in Ref. 8, Sec. 8. Again we omit the details, which can be easily worked out.

We can summarize our results in the following statement.

Theorem 6.7: *Given the equation (1.1) with f analytic in its argument and* $\boldsymbol{\omega}$ *satisfying the Diophantine condition (6.1), there exists* ε_0 *such that for all real* ε *with* $|\varepsilon| < \varepsilon_0$ *there is a quasi-periodic solution with the same frequency vector as the forcing term. Such a solution extends to a function analytic in the domain* $\mathcal{D}_R$ *shown in Fig. 16, with* $R = \varepsilon_0$.

The conclusion is that the summation criterion described here gives a well defined function, which is quasiperiodic and solves the equation of motion (1.1), but the criterion is not equivalent to Borel summability any more. In particular the issue of whether such quasiperiodic solutions are unique or not remains open, as in Ref. 6.

VII. EXTENSION TO MORE GENERAL NONLINEARITIES

When considering the equation (1.5) the formal analysis of Sec. II (and of Sec. VI in the case of quasiperiodic forcing terms) can be performed essentially in the same way. If we write

$$\begin{aligned} g(x) &= \sum_{p=0}^{\infty} \frac{1}{p!} g_p (x - c_0)^p, \quad g_p = \frac{\mathrm{d}^p g}{\mathrm{d}x^p}(c_0), \\ [g(x)]_{\boldsymbol{\nu}}^{(k)} &= \sum_{p=0}^{\infty} \frac{1}{p!} g_p \sum_{\substack{k_1 + \cdots + k_p = k \\ \nu_1 + \cdots + \nu_p = \nu}} x_{\boldsymbol{\nu}_1}^{(k_1)} \cdots x_{\boldsymbol{\nu}_p}^{(k_p)}, \quad k \geqslant 0, \end{aligned} \tag{7.1}$$

then the recursive equations for $\boldsymbol{\nu} \neq \mathbf{0}$ are

$$\begin{aligned} x_{\boldsymbol{\nu}}^{(0)} &= 0, \\ x_{\boldsymbol{\nu}}^{(1)} &= \frac{f_{\boldsymbol{\nu}}}{i\boldsymbol{\omega}\cdot\boldsymbol{\nu}}, \\ x_{\boldsymbol{\nu}}^{(k)} &= -(i\boldsymbol{\omega}\cdot\boldsymbol{\nu}) x_{\boldsymbol{\nu}}^{(k-1)} - \frac{1}{i\boldsymbol{\omega}\cdot\boldsymbol{\nu}} [g(x)]_{\boldsymbol{\nu}}^{(k-1)}, \quad k \geqslant 2, \end{aligned} \tag{7.2}$$

while the compatibility condition becomes $[g(x)]_{\mathbf{0}}^{(k)} = f_{\mathbf{0}} \delta_{k,0}$ for $k \geqslant 0$. The latter for $k = 0$ gives $g(c_0) = f_0$, while for $k \geqslant 1$ gives $g'(c_0) c_k + R(c_0, c_1, \ldots, c_{k-1}) = 0$, where the function $R(c_0, c_1, \ldots, c_{k-1})$ depends on the coefficients to all orders $k' < k$, hence, in particular, on the constants $c_0, \ldots, c_{k-1}$. Therefore the constants c_k can be fixed iteratively as

$$c_k = -\frac{1}{g'(c_0)} R(c_0, c_1, \ldots, c_{k-1}), \tag{7.3}$$

provided that one has $g'(c_0) \neq 0$, so that under the conditions (1.6) one has the formal solubility of the equations of motion (1.1). Note that the first condition in (1.6) requires $f_0 \in \mathrm{Ran}(g)$, and if such a condition is satisfied then the condition on the derivative is a genericity condition. Note also that the class of functions $g(x)$ which are not allowed depends on f (more precisely on its average f_0). For instance an explicit example of a function which does not satisfy (1.6) is $g(x) = 3x^2 - 2x^3$ if $f_0 = 1$.

The graphical representation differs from that of the preceding sections as now the number of lines entering a vertex v can assume any value $s_v \in \mathbb{N}$, and if $v \notin V_0(\theta)$ the corresponding node factor is

$$F_v = -\frac{\varepsilon}{s_v!} g_{s_v}, \tag{7.4}$$

which is bounded proportionally to some constant G to the power s_v. Since $\Sigma_{v \in V(\theta)}(s_v - 1) = |E(\theta)| - 1 \leqslant k - 1$ (by Lemma 4.1) this produces an overall constant G^{2k} in the tree value. Also the study of the convergence of both the formal series and the resummed series can then be performed as in the previous case, and no further difficulty arises. The constant c appearing after (6.14) becomes $-g'(c_0)$, instead of $-2c_0$, so that still one has $c \neq 0$ by the assumption (1.6).

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A super-integrable discretization of the Calogero model

Hideaki Ujino[a)]
Centre de Recherches Mathématiques, Université de Montréal, Montreal, Quebec, Canada H3C 3J7

Luc Vinet[b)]
Department of Mathematics and Statistics and Department of Physics, McGill University, Montreal, Quebec, Canada H3A 2J5

Haruo Yoshida[c)]
National Astronomical Observatory of Japan, Mitaka, Tokyo 181-8588, Japan

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A time discretization that preserves the super-integrability of the Calogero model is obtained by application of the integrable time discretization of the harmonic oscillator to the projection method for the Calogero model with continuous time. In particular, the difference equations of motion, which provide an explicit scheme for time integration, are explicitly presented for the two-body case. Numerical results exhibit that the scheme conserves all the (=3) conserved quantities of the (two-body) Calogero model with a precision of the machine epsilon times the number of iterations. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1931043]

I. INTRODUCTION

Numerical analysis of dynamical systems has great importance and a wide variety of applications in science and engineering. The elaboration of schemes for numerical analysis has a long and continuous history of studies as well as a rich accumulation of techniques. Whenever one applies numerical analysis to the equations of motion, one must discretize the time evolution of the dynamical system that is originally described by differential equations because of the lack of the notion of infinity in numerical analysis. This leads to difference equations, which do not usually describe the same dynamical system as the original one: time discretization is typically accompanied by modification of the original system, which may cause a significant difference in the behavior of the solution from that of the original system, particularly after integration over a long period. Understanding and controlling such modifications are thus important in the quest for more accurate long-time integration in numerical analysis.

The symplectic integration method (see, for instance, Refs. 1–3), or the symplectic integrator, is one of the time discretizations that was invented in such a quest. Given a Hamiltonian $H^{(0)}$, it is designed so that its one-step $(=\tau)$ time evolution gives the exact one-step time evolution of a modified Hamiltonian $\tilde{H} := H^{(0)} + \tau H^{(1)} + \tau^2 H^{(2)} + \cdots$. Since the modified Hamiltonian is conserved by the flow of the symplectic integrator, the fluctuation of the value of the original Hamiltonian $H^{(0)}$, i.e., the total energy of the system with continuous time, is bounded, which is far more favorable than unbounded increase or decrease of the total energy that one usually observes in other nonsymplectic discretizations. This is the reason why the symplectic integration method shows better accuracy even after long-time integration.

[a)]Present address: Gunma National College of Technology, Maebashi, Gunma 371-8530, Japan. Electronic mail: ujino@nat.gunma-ct.ac.jp
[b)]Electronic mail: luc.vinet@mcgill.ca
[c)]Electronic mail: h.yoshida@nao.ac.jp

However, even the symplectic integration method does not usually have modified constants of motion for all the constants of motion of a system, which often causes secular increase or decrease of the values of the constants of motion after long-time integration. For example, nonexistence of the modified constants of motion is proved for the two super-integrable models discretized by the symplectic integrator: the two-dimensional Harmonic oscillator with integer frequency ratio (except for the isotropic case) and the two-dimensional Kepler problem.[4,5] The orbits generated by the symplectic integrator are not closed, though those of the exact analytic solutions are closed, indeed.

Thus the following question naturally arises: are there any discretization schemes that preserve the (super-)integrability of (super-)integrable models? Actually, an extensive collection of the known integrable discretizations of integrable models is now available in the monograph[6] that was published in recent years. However, the super-integrable discretization of super-integrable models has not been studied that far yet. Quite recently, an affirmative answer to the question on the super-integrable discretization is shown for the Kepler problem for two- and three-dimensional cases,[7,8] where the integrable discretization of the harmonic oscillator[9] plays an essential role. The above super-integrable discretization conserves all the constants of motion, i.e., the Hamiltonian, the angular momentum and the Runge–Lenz vector, and generates a sequence of discrete points on the orbit of the exact analytic solution of the Kepler problem. And, of course, the orbit with the eccentricity less than unity is closed.

The purpose of this paper is to present a super-integrable discretization of the Calogero model,[10,11]

$$H := \frac{1}{2}\sum_{i=1}^{N}(p_i^2+\omega^2 x_i^2)+\frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\frac{a^2}{(x_i-x_j)^2}. \tag{1.1}$$

The real-valued quantities p_i, x_i, ω, and a in the Hamiltonian are the canonical momentum and coordinate of the ith particle, the strength of the external harmonic confinement and the interaction parameter, respectively. The Calogero model ($\omega \neq 0$) with N degrees of freedom (corresponding to the N-body case) is maximally super-integrable in the sense that it has $2N-1$ constants of motion which are independent of each other.[12] The super-integrable structure of the Calogero model is built up by the Lax formulation,[13,14] with which the eigenvalue problem of an oscillating Hermitian matrix[15] is intrinsically involved. We shall present a discretization that preserves the above super-integrable structure of the Calogero model for the general N-body case. It gives, in particular, the explicit form of the difference equations of motion of the Calogero model for the two-body case that conserves all the three constants of motion as

$$\begin{aligned}\Delta_+ x_{1,n} = {} & \frac{1}{1+\dfrac{\omega^2\Delta t^2}{4}}\left[p_{1,n}-\frac{\omega^2}{2}x_{1,n}\Delta t\right]+\frac{1}{1+\dfrac{\omega^2\Delta t^2}{4}}\frac{2a}{x_{1,n}-x_{2,n}}M_{i,n}\Delta t-2\left[\frac{1-\dfrac{\omega^2\Delta t^2}{4}}{1+\dfrac{\omega^2\Delta t^2}{4}}x_{1,n}\right.\\ & \left.+\frac{1}{1+\dfrac{\omega^2\Delta t^2}{4}}p_{1,n}\Delta t\right]M_{r,n}\Delta t+\left[\frac{1-\dfrac{\omega^2\Delta t^2}{4}}{1+\dfrac{\omega^2\Delta t^2}{4}}(x_{1,n}+x_{2,n})+\frac{1}{1+\dfrac{\omega^2\Delta t^2}{4}}(p_{1,n}+p_{2,n})\Delta t\right]\\ & \times(M_{i,n}^2+M_{r,n}^2\Delta t^2)\Delta t,\end{aligned}$$

$$\Delta_+ p_{1,n} = -\frac{\omega^2}{1+\frac{\omega^2\Delta t^2}{4}}\left[x_{1,n}+\frac{1}{2}p_{1,n}\Delta t\right]+\frac{1-\frac{\omega^2\Delta t^2}{4}}{1+\frac{\omega^2\Delta t^2}{4}}\frac{2a}{x_{1,n}-x_{2,n}}M_{i,n}-2\left[\frac{1-\frac{\omega^2\Delta t^2}{4}}{1+\frac{\omega^2\Delta t^2}{4}}p_{1,n}\right.$$
$$\left.-\frac{\omega^2}{1+\frac{\omega^2\Delta t^2}{4}}x_{1,n}\Delta t\right]M_{r,n}\Delta t+\left[\frac{1-\frac{\omega^2\Delta t^2}{4}}{1+\frac{\omega^2\Delta t^2}{4}}(p_{1,n}+p_{2,n})-\frac{\omega^2}{1+\frac{\omega^2\Delta t^2}{4}}(x_{1,n}+x_{2,n})\Delta t\right]$$
$$\times(M_{i,n}^2+M_{r,n}^2\Delta t^2)\Delta t,$$

$$\Delta_+ x_{2,n} = \Delta_+ x_{1,n}\big|_{1\leftrightarrow 2}, \quad \Delta_+ p_{2,n} = \Delta_+ p_{1,n}\big|_{1\leftrightarrow 2}, \tag{1.2}$$

with

$$M_{i,n} := \frac{a}{\sqrt{4a^2\Delta t^2+Y_n^2}}, \quad M_{r,n} := \frac{2a^2}{4a^2\Delta t^2+Y_n^2+Y_n\sqrt{4a^2\Delta t^2+Y_n^2}},$$

$$Y_n := \left[1-\frac{\omega^2\Delta t^2}{4}\right](x_{1,n}-x_{2,n})^2+(p_{1,n}-p_{2,n})(x_{1,n}-x_{2,n})\Delta t,$$

where $x_{i,n}$, $p_{i,n}$, $i=1,2$, are the coordinate and the momentum of the ith particle at the nth discrete time. The symbol Δ_+ denotes the advanced time difference defined by

$$\Delta_+ A_n := \frac{A_{n+1}-A_n}{\Delta t}, \tag{1.3}$$

for an arbitrary variable A_n (e.g., $A_n=x_{i,n}, p_{i,n}$) with the discrete time n.

The paper is organized as follows. In Sec. II, we present a brief summary of the projection method[15] (for review, see Refs. 16–18, for example), which gives a solution to the initial value problem of the Calogero model with continuous time. The Lax equations for the Calogero model provide a map from the Calogero model into the matrix-valued harmonic oscillator and also play an essential role in our discretization. Applying the integrable discretization for the harmonic oscillator,[9] we discretize the projection method in Sec. III. A discrete analogue of the Lax equations, which we call the dLax equations, is derived as a natural consequence of the discretization. In Sec. IV, we present the explicit forms of the dLax equations of the Calogero model for the two-body case, which are equivalent to the difference equations of motion (1.2). They provide an explicit scheme for the time integration of the model. Numerical results obtained by our integrable discretization as well as by two other discretization schemes, namely, the symplectic Euler and energy conservation methods, are also presented. Section V is dedicated to the summary and concluding remarks.

II. PROJECTION METHOD

In terms of the Lax pair for the Calogero–Moser model,[14]

$$L_{ij}(t) := p_i(t)\delta_{ij}+\frac{ia}{x_i(t)-x_j(t)}(1-\delta_{ij}),$$

$$M_{ij}(t) := \sum_{k(\neq i)} \frac{ia}{(x_i(t)-x_k(t))^2}\delta_{ij} - \frac{ia}{(x_i(t)-x_j(t))^2}(1-\delta_{ij}), \quad i,j=1,2,\ldots,N, \tag{2.1}$$

as well as a diagonal matrix

$$D(t) := \mathrm{diag}(x_1(t),x_2(t),\ldots,x_N(t)),$$

the canonical equation of motion for the Calogero model (1.1) can be cast into the Lax form,

$$\frac{\mathrm{d}L}{\mathrm{d}t} = [L,M] - \omega^2 D,$$

$$\frac{\mathrm{d}D}{\mathrm{d}t} = [D,M] + L,$$

where $[A,B] := AB - BA$, or equivalently,

$$\frac{\mathrm{d}L^{\pm}}{\mathrm{d}t} = [L^{\pm},M] \pm i\omega L^{\pm}, \tag{2.2}$$

where

$$L^{\pm}(t) := L(t) \pm i\omega D(t). \tag{2.3}$$

The Lax equations (2.2) allow the following relation between the products of L^+ and L^- and the Hamiltonian

$$\frac{\mathrm{d}}{\mathrm{d}t}((L^+)^{l_1}(L^-)^{m_1}\cdots) = [(L^+)^{l_1}(L^-)^{m_1}\cdots,M] + i\omega(l_1+\cdots-(m_1+\cdots))(L^+)^{l_1}(L^-)^{m_1}\cdots,$$

for any non-negative integers $l_1, m_1, \ldots$. Iterated use of the above formula yields

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\prod_i \mathrm{Tr}\left(\overrightarrow{\prod_j}(L^+)^{l_{i,j}}(L^-)^{m_{i,j}}\right)\right) &= \sum_i \prod_{i\neq k} \mathrm{Tr}\left(\overrightarrow{\prod_j}(L^+)^{l_{i,j}}(L^-)^{m_{i,j}}\right)\mathrm{Tr}\left[\overrightarrow{\prod_l}(L^+)^{l_{k,l}}(L^-)^{m_{k,l}},M\right] \\ &\quad + \sum_{k,l}(l_{k,l}-m_{k,l})\prod_i \mathrm{Tr}\left(\overrightarrow{\prod_j}(L^+)^{l_{i,j}}(L^-)^{m_{i,j}}\right) \\ &= \sum_{k,l}(l_{k,l}-m_{k,l})\prod_i \mathrm{Tr}\left(\overrightarrow{\prod_j}(L^+)^{l_{i,j}}(L^-)^{m_{i,j}}\right),\end{aligned}$$

where

$$\overrightarrow{\prod_j} A_j := A_1A_2\cdots.$$

Thus the constants of motion of the Calogero model can be constructed by taking the trace of any products of L^+ and L^- of the following form:

$$\prod_i \mathrm{Tr}\left(\overrightarrow{\prod_j}(L^+)^{l_{i,j}}(L^-)^{m_{i,j}}\right), \quad \text{if } \sum_{i,j} l_{i,j} = \sum_{i,j} m_{i,j}, \tag{2.4}$$

which includes the constants of motion given in Ref. 12. Considering the case $a=0$ where the matrices $L^{\pm}$ become diagonal, one can confirm the quantities given Eq. (2.4) above include at least

(and also at most) $2N-1$ constants of motion that are independent of each other. For example, one confirms

$$C_1 := \mathrm{Tr}\, L^+ \,\mathrm{Tr}\, L^- = \left(\sum_{i=1}^{N} p_i\right)^2 + \omega^2 \left(\sum_{i=1}^{N} x_i\right)^2,$$

$$I_1 := \mathrm{Tr}\, L^+ L^- = 2H, \quad I_2 = \mathrm{Tr}(L^+)^2 \mathrm{Tr}(L^-)^2, \tag{2.5}$$

are constants of motion of the Calogero model (1.1) that are independent of each other. Note that the relations satisfied by the Lax pairs[19,20]

$$[L^+, L^-] = -2i\omega[L, D] = -2\omega a(T - E), \quad T_{ij} := 1, \quad E_{ij} := \delta_{ij},$$

$$M^t[1, \ldots, 1] = 0, \quad [1, \ldots, 1]M = 0, \quad [\Leftrightarrow TM = MT = 0], \tag{2.6}$$

particularly the relations in the second line of Eq. (2.6) which we call the sum-to-zero property, have played a crucial role in the quantum analogue of the Lax formulation.

The initial value problem of the Calogero model can be solved by the projection method,[15] in which the Lax formulation presented above plays a crucial role. This method can be formulated in an analogous way to the Dirac picture in the time-dependent perturbation theory of quantum mechanics. Let us introduce $L_D^{\pm}$, the $L^{\pm}$ matrix in the "Dirac picture" by

$$L^{\pm}(t) =: e^{\pm i\omega t} L_D^{\pm}(t), \quad L^{\pm}(0) = L_D^{\pm}(0). \tag{2.7}$$

Then the Lax equation (2.2) is rewritten as

$$\frac{\mathrm{d}L_D^{\pm}}{\mathrm{d}t} = [L_D^{\pm}, M],$$

which has the same form as the Heisenberg equation in the Dirac picture with the time-dependent perturbation $M(t) := M(x_1(t), x_2(t), \ldots, x_N(t))$.

The above equation allows the formal solution as

$$L_D^{\pm}(t) = U^{\dagger}(0,t) L^{\pm}(0) U(0,t), \tag{2.8}$$

where the time-evolution unitary matrix $U(t',t)$ is given by the Dyson series of $M(t)$,

$$U(t',t) := \sum_{k=0}^{\infty} \int_{t'}^{t} \mathrm{d}t_k \int_{t'}^{t_k} \mathrm{d}t_{k-1} \cdots \int_{t'}^{t_2} \mathrm{d}t_1 M(t_1) \cdots M(t_{k-1}) M(t_k), \tag{2.9}$$

which has the semigroup property,

$$U(0,t) := U[\mathbf{x}(0), \mathbf{p}(0); a, \omega; t] = U[\mathbf{x}(0), \mathbf{p}(0); a, \omega; t'] U[\mathbf{x}(t'), \mathbf{p}(t'); a, \omega; t - t'] = U(0,t') U(t',t),$$

$$U^{\dagger}(0,t) = U(t,0). \tag{2.10}$$

Note that $U(t',t)$ has a constant eigenvector ${}^t[1, \ldots, 1]$ whose eigenvalue is unity,

$$U(t',t)\,{}^t[1, \ldots, 1] = {}^t[1, \ldots, 1], \quad [1, \ldots, 1] U(t',t) = [1, \ldots, 1] \Leftrightarrow U(t',t)T = TU(t',t) = T. \tag{2.11}$$

This property of $U(t',t)$ is a consequence of the sum-to-zero property of the matrix M in Eq. (2.6).

Substitution of the formal solution (2.8) into Eqs. (2.3) and (2.7) gives the following solution of the initial value problem of the Lax equation (2.2):

$$D(t) = U^{\dagger}(0,t)\frac{e^{i\omega t}L^{+}(0) - e^{-i\omega t}L^{-}(0)}{2i\omega}U(0,t),$$

$$L(t) = U^{\dagger}(0,t)\frac{e^{i\omega t}L^{+}(0) + e^{-i\omega t}L^{-}(0)}{2}U(0,t), \tag{2.12}$$

which means that the eigenvalues of the time-dependent Hermitian matrix $[e^{i\omega t}L^{+}(0) - e^{-i\omega t}L^{-}(0)]/2i\omega$ give the solution of the initial value problem of the Calogero model. The time-evolution unitary matrix $U(0,t)$, which has been formally introduced as the Dyson series of $M(t)$, is given here as the diagonalizing matrix.

The unitary matrix $U(0,t)$ provides a map of the Calogero model into the matrix-valued harmonic oscillator. Let us introduce the matrices

$$X^{\pm}(t) \coloneqq U(0,t)L^{\pm}(t)U^{\dagger}(0,t) = P(t) \pm i\omega Q(t),$$

$$P(t) \coloneqq U(0,t)L(t)U^{\dagger}(0,t), \quad Q(t) \coloneqq U(0,t)D(t)U^{\dagger}(0,t). \tag{2.13}$$

Substituting $X^{\pm}$ into the Lax equation (2.2), we have

$$\frac{\mathrm{d}X^{\pm}}{\mathrm{d}t} = \pm i\omega X^{\pm}, \tag{2.14}$$

which are equivalent to the equations of motion of the harmonic oscillator,

$$\frac{\mathrm{d}P}{\mathrm{d}t} = -\omega^2 Q, \quad \frac{\mathrm{d}Q}{\mathrm{d}t} = P. \tag{2.15}$$

Thus we confirm that the Lax equations of the Calogero model (2.2) can be mapped to the equations of motion of the matrix-valued harmonic oscillator, Eqs. (2.14) and (2.15). Though the Hermitian matrices $P(t)$ and $Q(t)$ can possess $2N^2$ parameters for their initial values, their definitions (2.13) introduce the restriction in the initial values,

$$P(0) = L(0), \quad Q(0) = D(0), \tag{2.16}$$

whose number $2N$ is the same as that of the Calogero model. The solution of the initial value problem of the above equations of motion is given by

$$Q(t) = D(0)\cos\omega t + \frac{L(0)}{\omega}\sin\omega t, \quad P(t) = L(0)\cos\omega t - \omega D(0)\sin\omega t [\Leftrightarrow X^{\pm}(t) = e^{\pm i\omega t}L^{\pm}(0)]. \tag{2.17}$$

Substitution of the above solution (2.17) into the definition of $P(t)$ and $Q(t)$ in Eq. (2.13) reproduces the solution of the initial value problem of the Calogero model (2.12). In particular, the coordinates of the Calogero model is given by the eigenvalues of the matrix-valued harmonic oscillator $Q(t)$ in Eq. (2.17). That is the essence of the projection method.

The restrictions on the initial values (2.16) can be explained in terms of the constraints on the variables $Q(t)$ and $P(t)$. From Eqs. (2.6) and (2.13), one can derive

$$[Q(t),P(t)] = U(0,t)[D(t),L(t)]U^{\dagger}(0,t) = iaU(0,t)(T-E)U^{\dagger}(0,t).$$

By use of the property of the time-evolution unitary matrix (2.11), one obtains

$$[Q,P] = ia(T-E), \tag{2.18}$$

which poses $N(N-1)$ constraints on the "unconstrained" variables $Q(t)$ and $P(t)$ given by two Hermitian matrices whose off-diagonal elements are pure imaginaries, i.e.,

$$Q_{ij}(t) := q_{ii}(t)\delta_{ij} + iq_{ij}(t), \quad P_{ij}(t) := p_{ii}(t)\delta_{ij} + ip_{ij}(t),$$

$$q_{ii}(t), \quad q_{ij}(t), \quad p_{ii}(t), \quad p_{ij}(t) \in \mathbb{R}, \quad q_{ij}(t) = -q_{ji}(t), \quad p_{ij}(t) = -p_{ji}(t). \tag{2.19}$$

The above restriction (2.19) is consistent with the solution of the initial value problem (2.17). The number of the independent variables in $Q(t)$ and $P(t)$ given by Eq. (2.19) is $N(N+1)$. One thus reproduces the number of the initial values $2N$ as the degrees of freedom of the constrained system, $N(N+1)-N(N-1)=2N$. The transformation (2.13) thus should be interpreted as a map of the Calogero model into the harmonic oscillator (2.15) of the Hermitian matrix given by Eq. (2.19) with the constraints (2.18).

III. INTEGRABLE DISCRETIZATION

As we have discussed in the preceding section, the equations of motion (the Lax equation) of the Calogero model can be mapped to those of the matrix-valued harmonic oscillator. We thus begin with the integrable discretization of the matrix-valued harmonic oscillator, whose difference equations of motion are given as

$$\Delta_+ Q_n = \tfrac{1}{2}(P_{n+1} + P_n),$$

$$\Delta_+ P_n = -\tfrac{1}{2}\omega^2(Q_{n+1} + Q_n), \tag{3.1}$$

where Q_n and P_n are Hermitian matrices whose initial values are fixed as $Q_0=D(0)$ and $P_0=L(0)$ so as to relate them with the difference analogue of the Calogero model. The difference equations given above have the same form as those for one-dimensional harmonic oscillator discretized by the energy conservation scheme,[9] which is nothing but the implicit midpoint rule giving a symplectic integration method of order 2 (see Theorem VI.3.4 in Ref. 1).

As in Eq. (2.13), we introduce the variables

$$X_n^{\pm} := P_n \pm i\omega Q_n.$$

This brings the difference equations of motion into

$$\Delta_+ X_n^{\pm} = \pm \tfrac{1}{2} i\omega (X_{n+1}^{\pm} + X_n^{\pm}),$$

which is equivalent to

$$\left(1 \mp \tfrac{1}{2} i\omega\Delta t\right) X_{n+1}^{\pm} = \left(1 \pm \tfrac{1}{2} i\omega\Delta t\right) X_n^{\pm}. \tag{3.2}$$

Defining the rescaled time step by

$$\Delta\tau := \frac{2}{\omega} \arctan \frac{\omega\Delta t}{2}, \tag{3.3}$$

the recursion relation (3.2) is rewritten as

$$X_{n+1}^{\pm} = \frac{1 \pm \dfrac{i\omega\Delta t}{2}}{1 \mp \dfrac{i\omega\Delta t}{2}} X_n^{\pm} = e^{\pm i\omega\Delta\tau} X_n^{\pm}.$$

Thus the solution of the initial value problem of the discrete harmonic oscillator is

$$X_n^{\pm} = e^{\pm in\omega\Delta\tau} X_0^{\pm},$$

or

$$Q_n = D(0)\cos n\omega\Delta\tau + \frac{1}{\omega}L(0)\sin n\omega\Delta\tau,$$

$$P_n = L(0)\cos n\omega\Delta\tau - \omega D(0)\sin n\omega\Delta\tau, \tag{3.4}$$

in terms of Q_n and P_n. The above solution (3.4) is exactly the same as that for the harmonic oscillator with the continuous time (2.17) up to time rescale (3.3).

The recursion relation (3.2) provides us with an efficient way to construct the constants of motion of the discrete harmonic oscillator. Consider an arbitrary product of X^+_{n+1} and X^-_{n+1} like $(X^+_{n+1})^{l_1}(X^-_{n+1})^{m_1}\cdots$, for $l_1, m_1 = 0,1,2,\ldots$, and reverse the time for one discrete time step using the recursion relation (3.2). Then one obtains

$$(X^+_{n+1})^{l_1}(X^-_{n+1})^{m_1}\cdots = e^{i\omega l_1\Delta\tau}(X^+_n)^{l_1}e^{-i\omega m_1\Delta\tau}(X^-_n)^{m_1}\cdots = e^{i\omega(l_1+\cdots-(m_1+\cdots))\Delta\tau}(X^+_n)^{l_1}(X^-_n)^{m_1}\cdots . \tag{3.5}$$

Taking the trace of the above relation, one obtains

$$\mathrm{Tr}\left(\prod_j^{\rightarrow}(X^+_{n+1})^{l_j}(X^-_{n+1})^{m_j}\right) = \exp\left(i\omega\Delta\tau\sum_k(l_k - m_k)\right)\mathrm{Tr}\left(\prod_j^{\rightarrow}(X^+_n)^{l_j}(X^-_n)^{m_j}\right).$$

Thus one can construct constants of motion of the discrete harmonic oscillator in a way parallel to what is done for the Calogero model (2.4) by

$$\prod_i \mathrm{Tr}\left(\prod_j^{\rightarrow}(X^+_n)^{l_{i,j}}(X^-_n)^{m_{i,j}}\right), \quad \text{when } \sum_{i,j} l_{i,j} = \sum_{i,j} m_{i,j}$$

as well as the matrix-valued constants of motion by

$$(X^+_{n+1})^{l_1}(X^-_{n+1})^{m_1}\cdots = (X^+_n)^{l_1}(X^-_n)^{m_1}\cdots ,$$

when $l_1+\cdots = m_1+\cdots$. In particular, the following quantity,

$$[X^+_n, X^-_n] = -2\omega a(T-E)[=[X^+_0, X^-_0]] \tag{3.6}$$

is conserved since it is a special case of the above matrix-valued constants of motion. Note that the constants of motion of the matrix-valued harmonic oscillator with continuous time can be given by the same formulas.

As we have confirmed, the solution of the harmonic oscillator with discrete time (3.4) and that with the continuous time (2.17) agree up to time rescale (3.3). Thus the eigenvalue of Q_n must trace the same trajectory of the Calogero model with continuous time. We shall discuss it more in detail.

Since the relations $Q_n = Q(n\Delta\tau)$ and $P_n = P(n\Delta\tau)$ hold as a consequence of Eqs. (2.17), (3.3), and (3.4), we also have analogous relations with (2.13) for Q_n and P_n,

$$D_n = U_n^\dagger Q_n U_n = D(n\Delta\tau), \quad L_n = U_n^\dagger P_n U_n = L(n\Delta\tau),$$

$$(D_n)_{ij} := x_{i,n}\delta_{ij}, \quad (L_n)_{ij} := p_{i,n}\delta_{ij} + \frac{ia}{x_{i,n}-x_{j,n}}(1-\delta_{ij}), \tag{3.7}$$

where the unitary matrix U_n is also given by the corresponding matrix in the theory for the model with continuous time

$$U_n = U(0, n\Delta\tau). \tag{3.8}$$

Introduce $L^\pm_n$ in analogy with $L^\pm$ in Eq. (2.3), i.e.,

$$L_n^{\pm} := L_n \pm i\omega D_n = U_n^{\dagger} X_n^{\pm} U_n \tag{3.9}$$

and substitute it into the recursion relation (3.2). Then one obtains

$$\left(1 \mp \tfrac{1}{2} i\omega\Delta t\right) U_{n+1} L_{n+1}^{\pm} U_{n+1}^{\dagger} = \left(1 \pm \tfrac{1}{2} i\omega\Delta t\right) U_n L_n^{\pm} U_n^{\dagger}.$$

By multiplying with $U_n^{\dagger}$ on the left and U_{n+1} on the right, one obtains a recursion relation of the matrices $L_n^{\pm}$,

$$\left(1 \mp \tfrac{1}{2} i\omega\Delta t\right) S_n L_{n+1}^{\pm} = \left(1 \pm \tfrac{1}{2} i\omega\Delta t\right) L_n^{\pm} S_n,$$

$$S_n := U_n^{\dagger} U_{n+1}, \tag{3.10}$$

which we shall call the discrete Lax equations, or in short, the dLax equations. They will play an essential role in the construction of the constants of motion for the discrete time model. From the definition of the unitary matrix S_n and using the semigroup property of the time-evolution unitary matrix $U(t',t)$ (2.10), one obtains

$$S_n := U_n^{\dagger} U_{n+1} = U(n\Delta\tau, (n+1)\Delta\tau) = S_n[\mathbf{x}_n, \mathbf{p}_n; a, \omega; \Delta t],$$

$$U_n = S_1 S_2 \cdots S_{n-1}, \quad U_0 = E. \tag{3.11}$$

This indicates that S_n is the one-step time-evolution matrix. We should note that *the discrete inhomogeneous Lax's equation* introduced for the Calogero–Moser model [the Hamiltonian (1.1) with $\omega=0$] in Ref. 21 inspired us with the above recursion equation (3.10). However, the explicit forms of the Lax pair and the derivation of the recursion relation of this paper are different from those in Ref. 21.

The recursion relation (3.10) can be interpreted as the discrete time analogue of the Lax equation of the Calogero model because of the following two reasons. The first reason is that the dLax equations (3.10) reduces to the Lax equations of the Calogero model (2.2) in the continuous time limit, $\Delta t \to 0$. The other reason is that the dLax equations also conserve the constants of motion of the Calogero model with continuous time. We shall discuss them more in detail.

From the Taylor expansions of $L_{n+1}=L((n+1)\Delta\tau)$ and $S_n=U(t'=n\Delta\tau, t=(n+1)\Delta\tau)$ together with the expression in the formal Dyson series (2.9) at $t=n\Delta\tau$, one obtains

$$L_{n+1}^{\pm} \sim L_n^{\pm} + \frac{\mathrm{d}L_n^{\pm}}{\mathrm{d}t}\Delta t + O(\Delta t^2),$$

$$S_n \sim E + M_n \Delta t + O(\Delta t^2), \quad M_n := M(n\Delta\tau). \tag{3.12}$$

Substitution of the above expressions into the dLax equations (3.10) yields

$$\left(1 \mp \frac{1}{2} i\omega\Delta t\right)(E + M_n\Delta t)\left(L_n^{\pm} + \frac{\mathrm{d}L_n^{\pm}}{\mathrm{d}t}\Delta t\right) = \left(1 \pm \frac{1}{2} i\omega\Delta t\right) L_n^{\pm}(E + M_n\Delta t).$$

Dividing the above relation by Δt and taking the limit $\Delta t \to 0$, one gets

$$\frac{\mathrm{d}L_n^{\pm}}{\mathrm{d}t} = [L_n^{\pm}, M_n] \pm i\omega L_n^{\pm},$$

which is nothing but the Lax equation of the Calogero model with continuous time.

In a way parallel to the construction of the constants of motion of the discrete harmonic oscillator, one can construct the constants of motion of the dLax equations (3.10). Using the definition (3.9) of $L_n^{\pm}$ in Eq. (3.5) and multiplying by $U_n^{\dagger}$ and U_{n+1}, respectively, from the left and the right, one gets

$$S_n(L_{n+1}^+)^{l_1}(L_{n+1}^-)^{m_1}\cdots = e^{i\omega l_1\Delta\tau}(L_n^+)^{l_1}e^{-i\omega m_1\Delta\tau}(L_n^-)^{m_1}\cdots S_n = e^{i\omega(l_1+\cdots-(m_1+\cdots))\Delta\tau}(L_n^+)^{l_1}(L_n^-)^{m_1}\cdots S_n.$$

Thus one has

$$(L_{n+1}^+)^{l_1}(L_{n+1}^-)^{m_1}\cdots = e^{i\omega(l_1+\cdots-(m_1+\cdots))\Delta\tau}S_n^\dagger(L_n^+)^{l_1}(L_n^-)^{m_1}\cdots S_n.$$

Since the trace of an arbitrary product of matrices is invariant under any cyclic change of the order of the matrices, one has

$$\mathrm{Tr}\left(\overrightarrow{\prod_j}(L_{n+1}^+)^{l_j}(L_{n+1}^-)^{m_j}\right) = \exp\left(i\omega\Delta\tau\sum_k(l_k-m_k)\right)\mathrm{Tr}\left(\overrightarrow{\prod_j}(L_n^+)^{l_j}(L_n^-)^{m_j}\right),$$

which leads to

$$\prod_i \mathrm{Tr}\left(\overrightarrow{\prod_j}(L_{n+1}^+)^{l_{i,j}}(L_{n+1}^-)^{m_{i,j}}\right) = \exp\left(i\omega\Delta\tau\sum_{k,l}(l_{k,l}-m_{k,l})\right)\prod_i \mathrm{Tr}\left(\overrightarrow{\prod_j}(L_n^+)^{l_{i,j}}(L_n^-)^{m_{i,j}}\right).$$

One thus concludes that

$$\prod_i \mathrm{Tr}\left(\overrightarrow{\prod_j}(L_n^+)^{l_{i,j}}(L_n^-)^{m_{i,j}}\right) \tag{3.13}$$

gives the constant of motion of the dLax equations (3.10) when

$$\sum_{i,j} l_{i,j} = \sum_{i,j} m_{i,j}.$$

This is in complete agreement with the situation for the Calogero model with continuous time (2.4).

Since $L_n^\pm$ should have the same form as $L^\pm$ for the continuous time model, the commutator between L_n^+ and L_n^- also should be a constant matrix as in Eq. (2.6). In the continuous time theory, this constant matrix is associated with the nontrivial constraints of the matrix-valued harmonic oscillator (2.18). One can observe the same situations in our discrete time model (3.10). Substitution of Eq. (3.9) into $[L_n^+,L_n^-]$ with the help of Eq. (3.6) yields

$$[L_n^+,L_n^-] = U_n^\dagger[X_n^+,X_n^-]U_n = U_n^\dagger(-2\omega a(T-E))U_n.$$

Since U_n and also S_n are made from the time-evolution unitary matrix $U(t',t)$ as in Eqs. (3.8) and (3.11), they also have a constant eigenvector ${}^t[1,\ldots,1]$ whose eigenvalues are unity,

$$U_n\,{}^t[1,\ldots,1] = {}^t[1,\ldots,1], \quad [1,\ldots,1]U_n = [1,\ldots,1] \Leftrightarrow U_nT = TU_n = T,$$

$$S_n\,{}^t[1,\ldots,1] = {}^t[1,\ldots,1], \quad [1,\ldots,1]S_n = [1,\ldots,1] \Leftrightarrow S_nT = TS_n = T. \tag{3.14}$$

Thus one immediately obtains

$$[L_n^+,L_n^-] = -2\omega a(T-E), \tag{3.15}$$

using the property (3.14) of U_n. The relation (3.15) is also equivalent to

$$[D_n,L_n] = ia(T-E).$$

Note that Eq. (3.7) provides the most general form of L_n that satisfies the above relation together with the diagonal matrix $(D_n)_{ij}=x_i\delta_{ij}$.

IV. DIFFERENCE EQUATIONS OF MOTION

Though we have developed an integrable discretization for the Calogero model in the preceding section, the difference equations of motion we have obtained is nevertheless a formal expression. An explicit expression for S_n is necessary in order to obtain the dLax equations for the Calogero model explicitly. To do this, we restrict the number of particles to two in the discussion of the explicit form of the S_n matrix.

From the dLax equations (3.10), one obtains

$$L_{n+1} \pm i\omega D_{n+1} := L_{n+1}^{\pm} = \frac{1 \pm \frac{1}{2}i\omega\Delta t}{1 \mp \frac{1}{2}i\omega\Delta t} S_n^{\dagger} L_n^{\pm} S_n.$$

Solution of the above equations with respect to D_{n+1} and L_{n+1} are given by

$$D_{n+1} = \frac{1}{2i\omega} S_n^{\dagger} \left[\frac{1 + \frac{1}{2}i\omega\Delta t}{1 - \frac{1}{2}i\omega\Delta t} L_n^{+} - \frac{1 - \frac{1}{2}i\omega\Delta t}{1 + \frac{1}{2}i\omega\Delta t} L_n^{-} \right] S_n,$$

$$L_{n+1} = \frac{1}{2} S_n^{\dagger} \left[\frac{1 + \frac{1}{2}i\omega\Delta t}{1 - \frac{1}{2}i\omega\Delta t} L_n^{+} + \frac{1 - \frac{1}{2}i\omega\Delta t}{1 + \frac{1}{2}i\omega\Delta t} L_n^{-} \right] S_n. \tag{4.1}$$

Since D_{n+1} is diagonal, S_n diagonalizes

$$\frac{1 + \frac{1}{2}i\omega\Delta t}{1 - \frac{1}{2}i\omega\Delta t} L_n^{+} - \frac{1 - \frac{1}{2}i\omega\Delta t}{1 + \frac{1}{2}i\omega\Delta t} L_n^{-}.$$

S_n thus can be constructed from the eigenvectors $\mathbf{v}_{i,n}$, $i=1,\ldots,N$ of the above matrix. Normalized eigenvectors $\mathbf{s}_{i,n}$ that constitute $S_n=[\mathbf{s}_{1,n}\cdots\mathbf{s}_{N,n}]$ should have the following form,

$$\mathbf{s}_{i,n} = \frac{\mathbf{v}_{i,n}}{\sum_{j=1}^{N} (\mathbf{v}_{i,n})_j} \Rightarrow \sum_{j=1}^{N} (\mathbf{s}_{i,n})_j = 1 \tag{4.2}$$

so as to satisfy the condition (3.14). Ordering of the eigenvectors $\mathbf{s}_{i,n}$ is uniquely determined by the Taylor expansion of S_n (3.12), or equivalently

$$\lim_{\Delta t \to 0} S_n = E. \tag{4.3}$$

Considering the Eqs. (4.1)–(4.3) all together, one confirms that

$$S_n = E + \frac{2ai\Delta t}{Y_n - 2ai\Delta t + \sqrt{4a^2\Delta t^2 + Y_n^2}} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} = E + (iM_{i,n}\Delta t - M_{r,n}\Delta t^2) \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$
$$\sim E + M_n \Delta t \quad (\Delta t \to 0) \tag{4.4}$$

gives the explicit form of the S_n matrix of the dLax equations for the Calogero model for the two-body case. It is straightforward to verify that the dLax equations (3.10) with the above S_n matrix (4.4) yields the difference equations of motion (1.2) shown in the introduction.

In order to confirm how well the dLax equations (3.10) with the S_n matrix (4.4) or the difference equations of motion (1.2) of the Calogero model with discrete time trace the behavior of that with continuous time, the explicit expression of the analytic solution for the continuous-time model is of great help, which is given by the eigenvalues of $Q(t)$ in Eq. (2.17). But there is another derivation. Since $U(t',t)$ is related to S_n according to Eq. (3.11) with $t' := n\Delta\tau$ and $t := (n+1)\Delta\tau$, one can obtain the explicit form of $U(t',t)$ for the two-body case from that of S_n (4.4),

$$U(t',t) = E + \frac{\dfrac{2ai\sin\omega(t-t')}{\omega}}{\mathcal{Y} - \dfrac{2ai\sin\omega(t-t')}{\omega} + \sqrt{\dfrac{4a^2\sin^2\omega(t-t')}{\omega^2} + \mathcal{Y}^2}} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix},$$

$$\mathcal{Y} := (x_1 - x_2)^2 \cos\omega(t-t') + (p_1 - p_2)(x_1 - x_2)\frac{\sin\omega(t-t')}{\omega}. \tag{4.5}$$

Substitution of the explicit forms of $U(0,t)$ (4.5) and $L^{\pm}(0)$ for the two-body case into Eq. (2.12), one obtains the explicit form of the analytic solution of the two-body Calogero model with continuous time,

$$\begin{aligned} x_1(t) &= \frac{1}{2}\left[(x_{1,0} + x_{2,0})\cos\omega t + \frac{1}{\omega}(p_{1,0} + p_{2,0})\sin\omega t \right] \\ &+ \frac{1}{2(x_{1,0} - x_{2,0})} \sqrt{\frac{4a^2\sin^2\omega t}{\omega^2} + \left[(x_{1,0} - x_{2,0})^2\cos\omega t + (p_{1,0} - p_{2,0})(x_{1,0} - x_{2,0})\frac{\sin\omega t}{\omega} \right]^2} \\ &=: x_1[\mathbf{x}_0, \mathbf{p}_0; a, \omega; t], \end{aligned}$$

$$\begin{aligned} p_1(t) &= \frac{1}{2}[(p_{1,0} + p_{2,0})\cos\omega t - \omega(x_{1,0} + x_{2,0})\sin\omega t] \\ &+ \frac{1}{2(x_{1,0} - x_{2,0})\sqrt{\dfrac{4a^2\sin^2\omega t}{\omega^2} + \left[(x_{1,0} - x_{2,0})^2\cos\omega t + (p_{1,0} - p_{2,0})(x_{1,0} - x_{2,0})\dfrac{\sin\omega t}{\omega} \right]^2}} \\ &\times \left[\frac{2a^2\sin 2\omega t}{\omega} + \left[(x_{1,0} - x_{2,0})^2\cos\omega t + (p_{1,0} - p_{2,0})(x_{1,0} - x_{2,0})\frac{\sin\omega t}{\omega} \right] \right. \\ &\left. \times [-\omega(x_{1,0} - x_{2,0})^2\sin\omega t + (p_{1,0} - p_{2,0})(x_{1,0} - x_{2,0})\cos\omega t] \right] =: p_1[\mathbf{x}_0, \mathbf{p}_0; a, \omega; t], \end{aligned}$$

$$x_2(t) = x_1(t)|_{1\leftrightarrow 2}, \quad p_2(t) = p_1(t)|_{1\leftrightarrow 2}. \tag{4.6}$$

The above expressions are used to numerically display the exact analytic results in the following figures. The initial values, the interaction parameter, the strength of the external harmonic well are set at $(x_1, p_1, x_2, p_2)|_{t=0} = (-4.00, 5.00, 2.00, 1.00)$, $a = 3.00$ and $\omega = 0.314$ throughout the numerical calculation in the following.

Figure 1 presents the time evolution of the coordinates and the momenta generated by the analytic solution and the difference equations of motion (1.2) that gives the super-integrable discretization. The time step in the super-integrable discretization is set at $\Delta t = 1.00$. The relation between the time t and the number of iterations n is given by $n = t/\Delta\tau$ where $\Delta\tau = 0.991\,903$. The time interval $240 \times (2\pi/\omega) = 4802 \leqslant t \leqslant 4842 = 242 \times (2\pi/\omega)$ corresponds to $4841 \leqslant n \leqslant 4881$ in terms of the number of iterations for the discrete case. As has been confirmed by the correspondence between the matrices L and D for the super-integrable discretization and those for the continuous time model (3.7), the solution of the discrete equations of motion (1.2) gives a sequence of canonical variables that are "sampled" from the orbit of the exact analytic solution, i.e.,

$$x_{i,n} = x_i(t = n\Delta\tau), \quad p_{i,n} = p_i(t = n\Delta\tau). \tag{4.7}$$

Even though the coordinates and the momenta generated by the difference equations of motion (1.2) are computed through sufficiently large numbers of iterations, they are in quite good agree-

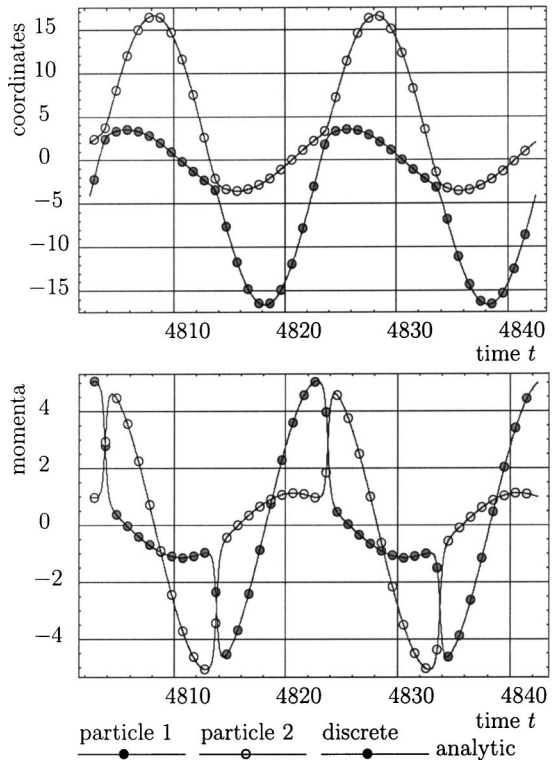

FIG. 1. The time evolution of the coordinates and the momenta generated by the analytic solution and the difference equations of motion (1.2).

ment with those of the exact analytic solution, which gives a good numerical confirmation of the correspondence (4.7).

One can confirm the precise agreement of the two solutions in a more reliable manner by observing the relative errors of the constants of motion. Using Eq. (2.4) [or Eq. (3.13)], we have already given three constants of motion of the Calogero model (2.5). Note that C_1 and I_1 correspond to the Hamiltonian for the center of mass and the Calogero Hamiltonian, respectively. Those three constants of motion give a set of independent conserved quantities. But just for convenience, we introduce a set of slightly modified constants of motion,

$$C_1 = (p_1 + p_2)^2 + \omega^2(x_1 + x_2)^2,$$

$$C_2 := 2I_1 - C_1 = (p_1 - p_2)^2 + \omega^2(x_1 - x_2)^2 + \frac{4a^2}{(x_1 - x_2)^2},$$

$$C_3 := \frac{I_1^2 - I_2}{4\omega^2} = (x_1 p_2 - x_2 p_1)^2 + \frac{2a^2(x_1^2 + x_2^2)}{(x_1 - x_2)^2}. \tag{4.8}$$

Note that C_2 is the Hamiltonian for the relative coordinates and C_3 can be interpreted as a "modified quadratic angular momentum." We use the above C_i's, $i=1,2,3$, for numerical calculation.

Figure 2 presents the relative errors of the constants of motion $C_i^{\mathrm{si}} := C_{i,n}/C_{i,0}$, $n=t/\Delta\tau$ of the discrete solutions given by the super-integrable discretization (1.2). The offsets $[=(i-1)\times 1.0]$ are added for convenience of presentation. Even though one sees the growth of errors caused by round-off errors that is inevitable in any numerical analysis, one confirms that all the constants of motion are conserved with a precision of the machine epsilon times the number of iterations. Thus

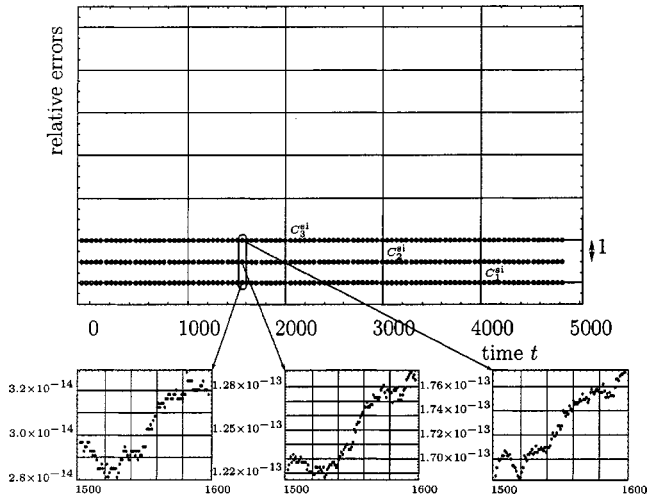

FIG. 2. The relative errors of the constants of motion $C_i^{\mathrm{si}} := C_{i,n}/C_{i,0}$, $n = t/\Delta\tau$, of the discrete solutions given by the super-integrable discretization (1.2).

one concludes that Fig. 2 presents a direct numerical verification of the fact that the difference equation of motion (1.2) preserves the super-integrability of the Calogero model.

Let us compare the above results with numerical demonstrations by two other discretizations. The first one is the energy conservation scheme (see pp. 159–161 in Ref. 1),

$$\Delta_+ x_{i,n} = \tfrac{1}{2}(p_{i,n+1} + p_{i,n}),$$

$$\Delta_+ p_{i,n} = -\frac{1}{2}\omega^2(x_{i,n+1} + x_{i,n}) + \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{a^2((x_{i,n+1} - x_{j,n+1}) + (x_{i,n} - x_{j,n}))}{(x_{i,n+1} - x_{j,n+1})^2 (x_{i,n} - x_{j,n})^2}, \tag{4.9}$$

which keeps two constants of motion C_1 and I_1 (consequently, C_2) exactly for arbitrary number of particles N. As one can see, the scheme (4.9) is an implicit scheme, which involves numerical solution of simultaneous algebraic equations. The other scheme is the symplectic Euler method (see Theorem VI.3.3 in Ref. 1),

$$\Delta_+ x_{i,n} = p_{i,n},$$

$$\Delta_+ p_{i,n} = -\omega^2 x_{i,n+1} + \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{2a^2}{(x_{i,n+1} - x_{j,n+1})^3}, \tag{4.10}$$

which is an explicit scheme. Note that Δ_+ denotes the advanced time difference (1.3).

Figures 3 and 4 present the relative errors $C_i^{\mathrm{ec,se}} := C_{i,n}/C_{i,0}$, $n = t/\Delta t$ of the discrete solution given by the energy conservation scheme (ec) and the symplectic Euler method (se) for the two body case ($N=2$). We should note that we do not present all the data of each relative errors to keep the size of the data file reasonable and that the offsets $[=(i-1)\times 1.0]$ are added for convenience of presentation. The initial condition, the coupling parameter and the strength of the harmonic confinement are the same as those given for the numerical calculation that gives Figs. 1 and 2. The discrete time step is set at $\Delta t = 0.200$ for these schemes.

One observes that the relative errors of the energies (C_1^{ec} and C_2^{ec}) calculated by the energy conservation scheme (4.9) remain within the order of the machine epsilon ($=10^{-16}$) times the number of iteration ($=t/\Delta t$), which gives a numerical confirmation that the energies are conserved

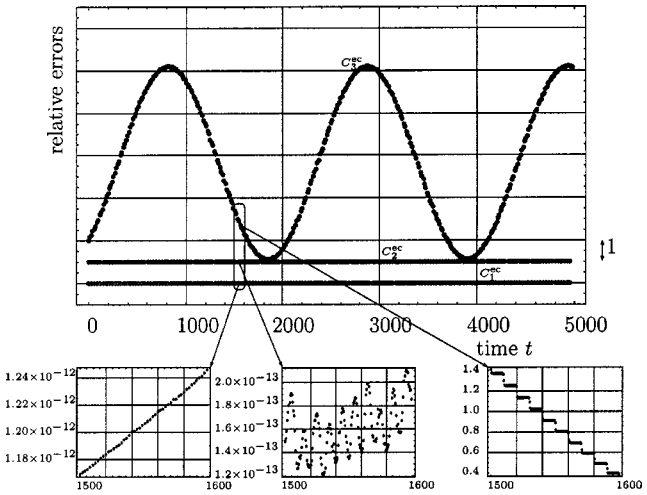

FIG. 3. The relative errors of the constants of motion, $C_i^{\mathrm{ec}} := C_{i,n}/C_{i,0}$, $n=t/\Delta t$, of the discrete solution given by the energy conservation scheme (4.9).

by the scheme. On the other hand, one also confirms that the relative errors (except for C_1^{ec} and C_2^{se}) are much larger than the order of machine epsilon times the number of iteration, even though one cannot observe growth of the relative errors in both two figures. These errors are not brought about by the round-off errors at the order of machine epsilon times the number of iteration, but by the schemes themselves. One perceives that there is a clear distinction between Fig. 2 or the super-integrable discretization (1.2) and Figs. 3 and 4 or the energy conservation scheme (4.9) and the symplectic Euler method (4.10).

One of the characteristics of the super-integrable system is that its bounded orbit is always closed in the phase space and, in particular, in the configuration space. As presented in Fig. 5, the orbit in the x_1–x_2 plane, or the "Lissajous plot" in other words, thus provides the distinctest way of comparing the three discretizations. The time interval of the Lissajous plots is $0 \leqslant t \leqslant 200$, which corresponds to 10 periods of motion. While the orbits generated by the energy conservation

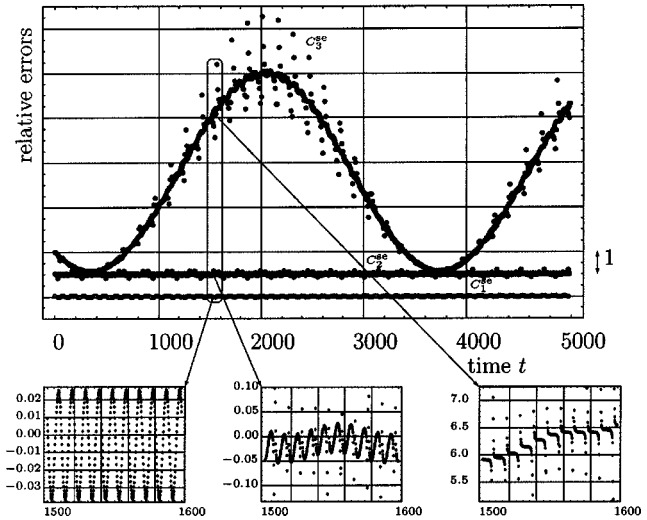

FIG. 4. The relative errors of the constants of motion, $C_i^{\mathrm{se}} := C_{i,n}/C_{i,0}$, $n=t/\Delta t$, of the discrete solution given by the symplectic Euler method (4.10).

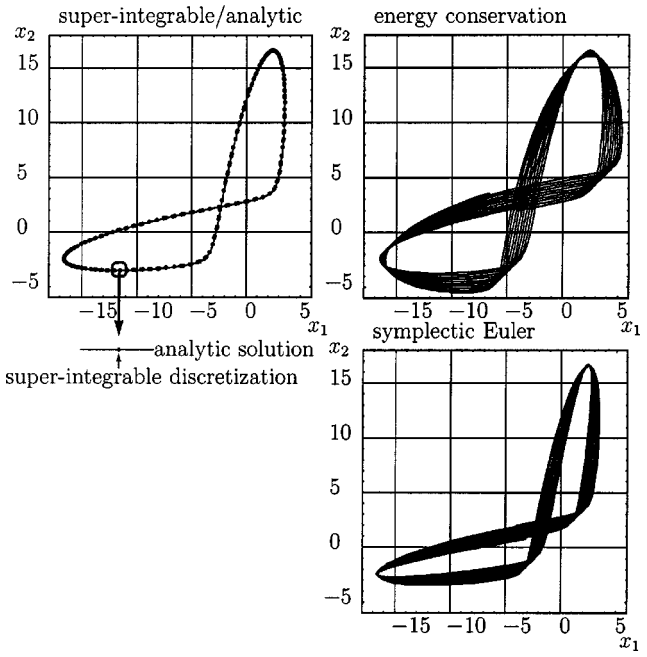

FIG. 5. The "Lissajous plots."

scheme and the symplectic Euler method are not closed, the orbit by the super-integrable discretization is always on that of the exact analytic solution, which is, of course, closed.

V. SUMMARY AND CONCLUDING REMARKS

The aim of the paper was to present a time discretization for the Calogero model that maintains its super-integrable structure. As discussed in Sec. II, the super-integrable structure of the original Calogero model is provided by the Lax formulation and the projection method, which are closely related to the equations of motion of the harmonic oscillator. With the help of the integrable discretization of the harmonic oscillator,[9] the Lax formulation and the projection method are discretized. As a consequence, a time discretization that preserves the super-integrability of the Calogero model is presented in Sec. III. In particular for the two-body case, an explicit form of the difference equations of motion (1.2) is obtained in Sec. IV. The difference equations give an explicit scheme for time integration. Numerical results by the super-integrable discretization (1.2) together with comparison with those by the energy conservation scheme (4.9) as well as the symplectic Euler method (4.10) are presented in five figures in Sec. IV, which give a intuitive numerical verification of the super-integrability of the scheme.

Last, we should give several remarks on previous studies that are relevant to the present work. In Refs. 21–23 (and also in Ref. 6), integrable discretizations of the rational Calogero–Moser model (the case $\omega=0$) and its trigonometric, elliptic and "relativistic" (a q-difference generalization with respect to space coordinates) generalizations were presented. The structure of the projection method also underlies these integrable discretizations, but the interaction parameter of the continuous-time models and the time step of the discrete-time models are related with each other in the integrable discretizations above. On the other hand, our discretization preserves not only the integrability but also the super-integrablity of the Calogero model and both the time-step Δt and the interaction parameter a independently appear in the discrete equations of motion. Thus our discretization is apparently different from that of the previous studies. The possibility of the mutual penetration of the particles in the time-discrete model was reported in Ref. 21, which is certainly unlike the continuous-time case. But the scheme given there is implicit and it could not provide a way to verify this possibility. In our super-integrable discretization of the present work,

however, we gave an explicit scheme of the Calogero model for the two-body case (1.2) and numerically observed in Fig. 1 that there was no penetration of the particles. And this observation should be the same for the Calogero–Moser case corresponding to the limit $\omega \to 0$ of the present work. The comparison of the two different discretizations together with additional consideration on the super-integrability of the rational Calogero–Moser model[24] will be presented in a separate paper. Further studies on the trigonometric, elliptic and relativistic Calogero–Moser model along the line of our super-integrable discretization of the Calogero model as well as to obtain explicit forms of the difference equations of motion for general *N*-body case (or at least three-body case) is worthy of interest.

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Periodic and homoclinic solutions of the modified 2+1 chiral model

Bo Dai[a)]
LMAM, School of Mathematical Sciences, Peking University, Beijing 100871, People's Republic of China

Chuu-Lian Terng[b)]
Department of Mathematics, University of California at Irvine, Irvine, California 92697-3875

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We use algebraic Bäcklund transformations (BTs) to construct explicit solutions of the modified 2+1 chiral model from $T^2\times\mathbb{R}$ to SU(n), where T^2 is a 2-torus. Algebraic BTs are parametrized by $z\in\mathbb{C}$ (poles) and holomorphic maps π from T^2 to $\mathrm{Gr}(k,\mathbb{C}^n)$. We apply Bäcklund transformations with carefully chosen poles and π's to construct infinitely many solutions of the 2+1 chiral model that are (i) doubly periodic in space variables and periodic in time, i.e., triply periodic, (ii) homoclinic in the sense that the solution u has the same stationary limit u_0 as $t\to\pm\infty$ and is tangent to a stable linear mode of u_0 as $t\to\infty$ and is tangent to an unstable mode of u_0 as $t\to-\infty$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1929688]

I. THE 2+1 CHIRAL MODEL

A *wave map* $J:\mathbb{R}^{2,1}\to\mathrm{SU}(n)$ is a critical point of the functional

$$\mathcal{E}(J)=\int_{\mathbb{R}^3}\|J^{-1}J_x\|^2+\|J^{-1}J_y\|^2-\|J^{-1}J_t\|^2\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t,$$

where $\|\xi\|^2=-\mathrm{tr}(\xi^2)$, and x, y, t are the standard space–time variables. The Euler–Lagrange equation of $\mathcal{E}$ is

$$(J^{-1}J_t)_t-(J^{-1}J_x)_x-(J^{-1}J_y)_y=0. \tag{1.1}$$

This equation is also called *the* 2+1 *chiral model*.

The *Ward equation* (or the *modified* 2+1 *chiral model*) is the following equation for $J:\mathbb{R}^{2,1}\to\mathrm{SU}(n)$:

$$(J^{-1}J_t)_t-(J^{-1}J_x)_x-(J^{-1}J_y)_y-[J^{-1}J_t,J^{-1}J_y]=0. \tag{1.2}$$

This equation is obtained by a dimension reduction and a gauge fixing of the self-dual Yang–Mills equation on $\mathbb{R}^{2,2}$ (cf. Ref. 11). We call a solution of the Ward equation a *Ward map*. The Ward equation is completely integrable and many techniques from integrable systems can be used to construct explicit solutions.[8,10,12]

We consider Ward maps satisfying the doubly periodic boundary condition in the space variables, i.e., Ward maps from $T^2\times\mathbb{R}$ to SU(n), where $T^2=S^1\times S^1$. Using the standard trick of writing a second order differential equation as a first order system on the tangent bundle of the

a)Electronic mail: daibo@math.pku.edu.cn
b)Electronic mail: cterng@math.uci.edu

phase space, we can view the Ward equation as a dynamical system on the tangent bundle $T(C^\infty(T^2,\mathrm{SU}(n)))$. The goal of this paper is to construct periodic and homoclinic orbits of this dynamical system.

A Ward map $J:T^2\times\mathbb{R}\to\mathrm{SU}(n)$ independent of t is a harmonic map from T^2 to $\mathrm{SU}(n)$. Equation for harmonic maps from T^2 to $\mathrm{SU}(n)$ is integrable. Techniques from integrable systems were used to construct harmonic maps from T^2 to SU(2) by Hitchin (Ref. 3), and from T^2 to $\mathrm{SU}(n)$ by Burstall, *et al.*[1]

A Ward map from $S^1\times S^1\times\mathbb{R}$ to $\mathrm{SU}(n)$ independent of the second variable is a wave map from $S^1\times\mathbb{R}$ to $\mathrm{SU}(n)$. Such wave maps were studied by Terng and Uhlenbeck in Ref. 9.

A solution u of an evolution PDE is *homoclinic* if u tends to the same stationary solution u_0 as $t\to\pm\infty$ and is tangent to a stable linear mode of u_0 as $t\to+\infty$ and is tangent to an unstable linear mode of u_0 as $t\to-\infty$. The existence of homoclinic orbits for a finite dimensional dynamical system indicates the chaotic behavior of the system (cf. Ref. 4). It is known that soliton equations in one space and one time variable (for example, sine-Gordon, KdV, and NLS), viewed as dynamical systems on certain function spaces, admit homoclinic orbits. Shatah and Strauss[6] proved that there are homoclinic wave maps from $S^1\times\mathbb{R}$ to S^2, and Terng and Uhlenbeck[9] proved the same result for wave maps from $S^1\times\mathbb{R}$ to any compact symmetric space. There have been many works concerning whether homoclinic orbits persist under small perturbation of these soliton equations in one space and one time variable (cf. Refs. 5 and 7, and references therein).

One result of this paper is the existence of infinitely many Ward maps from $T^2\times\mathbb{R}$ to $\mathrm{SU}(n)$ that are periodic in time. In other words, we prove that there are infinitely many triply periodic solutions of the Ward equation. Another result of this paper is to show that the Ward equation has infinitely many homoclinic orbits. We give an outline of our method next.

The 1-soliton Ward maps from $\mathbb{R}^{2,1}$ to $\mathrm{SU}(n)$ can be constructed as follows (cf. Ref. 11). Let $z\in\mathbb{C}\backslash\mathbb{R}$ be a constant, $V=(v_{ij})$ a meromorphic map from $\mathbb{C}$ to the space $\mathcal{M}^0_{n\times k}$ of rank k complex $n\times k$ matrices, $\pi(x,y,t)$ the Hermitian projection of $\mathbb{C}^n$ onto the subspace spanned by the k columns of $V(w)$, where

$$w=x+\frac{(z-z^{-1})y}{2}+\frac{(z+z^{-1})t}{2}.$$

Let $\pi^\perp=I-\pi$. Then

$$\hat{J}_{z,V}(x,y,t)=\pi^\perp(x,y,t)+\frac{\overline{z}}{z}\pi(x,y,t)$$

is a solution of the Ward equation. It has constant determinant, so we can normalize it to get a Ward map from $\mathbb{R}^{2,1}$ to $\mathrm{SU}(n)$,

$$J_{z,V}(x,y,t)=\left(\frac{z}{\overline{z}}\right)^{k/n}\left(\pi^\perp(x,y,t)+\frac{\overline{z}}{z}\pi(x,y,t)\right).$$

$J_{z,V}$ (or $\hat{J}_{z,V}$) will be called a *Ward* 1-*soliton*. If all entries of $V(w)$ are rational functions in w, then $J_{z,V}$ is a smooth Ward map and is asymptotically constant as $|(x,y)|\to\infty$. If all entries of V are elliptic functions of same periods, then $J_{z,V}$ is a smooth Ward map from $T^2\times\mathbb{R}$ to $\mathrm{SU}(n)$.

Algebraic Bäcklund transformations (BTs) for the Ward equation were constructed in Ref. 2. These are transformations that generate new Ward maps from a given Ward map and 1-solitons $J_{z,V}$ by a simple algebraic method.

We apply algebraic Bäcklund transformations repeatedly to 1-solitons associated to elliptic functions to construct infinitely many triply periodic Ward maps to $\mathrm{SU}(n)$.

Note that if the image of J lies in an Abelian subgroup of $\mathrm{SU}(n)$, then the Ward equation for J becomes the linear wave equation. For example, let m be an integer, and $a=\mathrm{diag}(im,-im)$. Then

$$J_0(x,y,t) = \exp(-(x+y)a)$$

is a doubly periodic, stationary Ward map, whose image lies in SO(2).

We apply algebraic BTs $2k$ times to J_0 with carefully chosen poles and projections to construct homoclinic Ward maps J_{2k} from $T^2\times\mathbb{R}$ to SU(n), and prove that J_{2k} tends to $(-1)^k J_0$ as $|t|\to\infty$ and J_{2k} are homoclinic.

This paper is organized as follows: We review the Lax pair and algebraic Bäcklund transformations for the Ward equation in Sec. II, and use elliptic functions to construct triply periodic Ward maps in Sec. III. In the last section, we construct (i) homoclinic Ward maps from $T^2\times\mathbb{R}$ to SU(n) that tend to stationary solutions, (ii) homoclinic Ward maps that tend to periodic solutions.

II. EXTENDED WARD MAPS AND BÄCKLUND TRANSFORMATIONS

The Ward equation is integrable in the sense that it can be written as the compatibility condition for a system of linear equations involving a spectral parameter $\lambda\in\mathbb{C}$. In fact, we have the following theorem (cf. Ref. 11):

Theorem 2.1: *Let* $J:\mathbb{R}^{2,1}\to\mathrm{SU}(n)$ *be a Ward map,* $\mathrm{d}x^2+\mathrm{d}y^2-\mathrm{d}t^2$ *be the Lorentzian metric on* $\mathbb{R}^{2,1}$,

$$u=\frac{t+y}{2},\quad v=\frac{t-y}{2}, \tag{2.1}$$

$A=J^{-1}J_u$, *and* $B=J^{-1}J_x$. *Then the following linear PDE system is solvable for* $\psi:\mathbb{R}^{2,1}\times\mathbb{C}\to\mathrm{GL}(n,\mathbb{C})$:

$$\begin{aligned}(\lambda\partial_x-\partial_u)\psi&=A\psi,\\ (\lambda\partial_v-\partial_x)\psi&=B\psi.\end{aligned} \tag{2.2}$$

Conversely, suppose $\mathcal{O}$ *is an open subset of* 0 *in* $\mathbb{C}$ *and* $\psi:\mathbb{R}^{2,1}\times\mathcal{O}\to\mathrm{GL}(n,\mathbb{C})$ *is a smooth map so that*

$$A:=(\lambda\psi_x-\psi_u)\psi^{-1},\quad B:=(\lambda\psi_v-\psi_x)\psi^{-1}$$

are independent of $\lambda\in\mathcal{O}$ *and* ψ *satisfies the* $U(n)$*-reality condition*

$$\psi(x,u,v,\overline{\lambda})^*\psi(x,u,v,\lambda)=I, \tag{2.3}$$

Then

$$J(x,y,t)=\psi(x,y,t,0)^{-1}$$

is a smooth solution of the Ward equation and $J^{-1}J_u=A$ *and* $J^{-1}J_x=B$.

A solution $\psi(x,y,t,\lambda)$ of (2.2) that satisfies the $U(n)$-reality condition (2.3) is called an *extended Ward map* and $J=\psi(\cdots,0)^{-1}$ the associated Ward map.

Given $z\in\mathbb{C}$ and a Hermitian projection π of $\mathbb{C}^n$, let

$$h_{z,\pi}(\lambda)=\pi^{\perp}+\frac{\lambda-z}{\lambda-\overline{z}}\pi=I+\frac{\overline{z}-z}{\lambda-\overline{z}}\pi,$$

where $\pi^{\perp}=I-\pi$. A direct computation implies that $h_{z,\pi}$ satisfies the $U(n)$-reality condition (2.3).

Let $V=(v_{ij}):\mathbb{C}\to\mathcal{M}^0_{n\times k}(\mathbb{C})$ be a meromorphic map, and $\pi(x,y,t)$ the Hermitian projection onto the subspace spanned by the columns of $V(w)$, where

$$w=x+zu+z^{-1}v,$$

and u, v are the light cone coordinates in the yt plane defined by (2.1). Since the entries of V are meromorphic functions, the projection π is smooth on $\mathbb{R}^{2,1}$. Set

$$\psi(x,y,t,\lambda) = h_{z,\pi(x,y,t)}(\lambda) = \pi^{\perp}(x,y,t) + \frac{\lambda - z}{\lambda - \bar{z}}\pi(x,y,t).$$

A direct computation implies that both $(\lambda\psi_x - \psi_u)\psi^{-1}$ and $(\lambda\psi_v - \psi_x)\psi^{-1}$ are independent of λ. By Theorem 2.1, ψ is an extended solution of the Ward equation and the associated Ward map is the 1-soliton,

$$J_{z,V}(x,y,t) = \left(\frac{z}{\bar{z}}\right)^{k/n}\psi(x,y,t,0)^{-1} = \left(\frac{z}{\bar{z}}\right)^{k/n}\left(\pi^{\perp}(x,y,t) + \frac{\bar{z}}{z}\pi(x,y,t)\right),$$

where $(z/\bar{z})^{k/n}$ is a normalizing constant to make $\det(J_{z,V}) = 1$.

The 1-soliton Ward map $J_{z,V}$ is a travelling wave because

$$w = x + zu + z^{-1}v = (x - v_1 t) + k_1(y - v_2 t) + ik_2(y - v_2 t),$$

where $z = re^{i\theta}$, $v_1 = -2r\cos\theta/(1+r^2)$, $v_2 = (1-r^2)/(1+r^2)$, and $k_1 + ik_2 = (z - z^{-1})/2$. Thus $J_{z,V}$ is a travelling wave with constant velocity $\vec{v} = [-2r\cos\theta/(1+r^2), (1-r^2)/(1+r^2)]$ on the xy plane. In particular, $J_{i,V}$ is a stationary Ward map, i.e., a harmonic map from $\mathbb{C}$ to SU(n).

The following theorem was proved in Ref. 2, which gives an algebraic method to produce new extended Ward maps from a given one.

Theorem 2.2 (Bäcklund transformation): *Let $\psi(x,y,t,\lambda)$ be an extended solution of the Ward equation and $J = \psi(\cdots,0)^{-1}$ the associated Ward map from $\mathbb{R}^{2,1}$ to* SU(n). *Choose $z \in \mathbb{C}\backslash\mathbb{R}$ such that $\psi(x,y,t,\lambda)$ is holomorphic and nondegenerate at $\lambda = z$. Let $h_{z,\pi(x,y,t)}(\lambda)$ be an extended* 1*-soliton solution, and $\tilde{\pi}(x,y,t)$ the Hermitian projection of $\mathbb{C}^n$ onto*

$$\psi(x,y,t,z)\mathrm{Im}(\pi(x,y,t)).$$

Then

$$\psi_1(x,y,t,\lambda) = h_{z,\tilde{\pi}(x,y,t)}(\lambda)\psi(x,,y,t,\lambda)$$

is a new extended solution to the linear system (2.2) with

$$(A,B) \to (A + (\bar{z} - z)\tilde{\pi}_x, B + (\bar{z} - z)\tilde{\pi}_v),$$

and the new Ward map is

$$J_1(x,y,t) = \left(\frac{z}{\bar{z}}\right)^{k/n} J(x,y,t)\left(\frac{\bar{z}}{z}\tilde{\pi}(x,y,t) + \tilde{\pi}^{\perp}(x,y,t)\right).$$

We will denote $\psi_1 = h_{z,\pi} * \psi$ and $J_1 = h_{z,\pi} * J$, the Bäcklund transformation generated by $h_{z,\pi}$.

III. PERIODIC WARD MAPS FROM $T^2 \times \mathbb{R}$ TO SU(n)

We use algebraic BTs to construct Ward maps into SU(n) that are either doubly periodic in space variables or triply periodic.

First we construct 1-soliton Ward maps that are doubly periodic. Let $z = re^{i\theta}$,

$$w(x,y,t) = x + zu + z^{-1}v = x + \frac{z - z^{-1}}{2}y + \frac{z + z^{-1}}{2}t,$$

and $\alpha = a + ib$. A direct computation shows that

$$w\left(x + a - \frac{k_1}{k_2}b, y + \frac{b}{k_2}, t\right) = w(x,y,t) + \alpha,$$

where $k_1 + ik_2 = (z - z^{-1})/2$. Let $f: \mathbb{C} \to \mathbb{C}$ be a meromorphic function such that $f(w + \alpha) = f(w)$ (i.e., periodic with period α), and

$$g(x,y,t) = f(w) = f(x + zu + z^{-1}v).$$

A direct computation shows that

$$g(x,y,t) = g\left(x + a - \frac{k_1}{k_2}b, y + \frac{b}{k_2}, t\right).$$

Hence

(1) if $\alpha = 2\pi$, then g is 2π-periodic in x;
(2) if $\alpha = 2\pi(k_1 + ik_2) = \pi(z - z^{-1})$, then g is 2π-periodic in y.

This shows that if each entry v_{ij} of the meromorphic map $V = (v_{ij}) : \mathbb{C} \to \mathcal{M}^0_{n\times k}(\mathbb{C})$ satisfies $v_{ij}(w + 2\pi) = v_{ij}(w + \pi(z - z^{-1})) = v_{ij}(w)$, i.e., an elliptic function with periods 2π and $\pi(z - z^{-1})$, then the 1-soliton $J_{z,V}$ is a doubly periodic Ward map with respect to the lattice $2\pi(\mathbb{Z}\times\mathbb{Z})$. An example of elliptic function is the well-known Weierstrass $\wp$-function

$$\wp(w) = \frac{1}{w^2} + \sum_{\gamma\in\Lambda\setminus\{0\}} \left(\frac{1}{(w-\gamma)^2} - \frac{1}{\gamma^2}\right),$$

where Λ is the lattice in $\mathbb{C}$ generated by 2π and $\pi(z - z^{-1})$. Other elliptic functions can be generated by Weierstrass $\wp$-functions and Jacobi elliptic functions. It is clear that $J_{z,V}$ is time periodic if and only if the ratio of the velocity, $v_1/v_2 = (-2r\cos\theta)/(1 - r^2)$, is rational.

Similar computation implies that given any rank 2 lattice Λ of $\mathbb{C}$ there are 1-soliton Ward maps from $\mathbb{C}/\Lambda\times\mathbb{R}$ to SU(n). Moreover, some of these 1-solitons are periodic in time, i.e., triply periodic. In particular, we get the following.

Theorem 1: *Let* $\tau = c_1 + ic_2$ *with* $c_2 \neq 0$, $\Lambda = \mathbb{Z}2\pi + \mathbb{Z}\tau$, $z = re^{i\theta}$ *a constant, and* $a + ib = c_1 + [(z - z^{-1})/2]c_2$. *If each entry* v_{ij} *of the meromorphic map* $V : \mathbb{C} \to \mathcal{M}^0_{n\times k}(\mathbb{C})$ *is an elliptic function with periods* 2π *and* $a + ib$, *then the extended* 1*-soliton solution* $h_{z,\pi}$ *is doubly periodic with periods* 2π *and* τ *and the associated* 1*-soliton,*

$$J_{z,V} = e^{i2k\theta/n} h_{z,\pi}(0)^{-1} = e^{i2k\theta/n}(\pi^{\perp} + e^{-2i\theta}\pi)$$

is a Ward map from $\mathbb{C}/\Lambda\times\mathbb{R}$ *to* SU(n), *where* $e^{i2k\theta/n}$ *is a normalizing constant, and* $\pi(x,y,t)$ *is the projection onto the subspace spanned by the columns of* $V(x + zu + z^{-1}v)$. *Moreover,*

(1) *if* $r \neq 1$ *and there exist integers* m_1, m_2 *such that*

$$\frac{2\cos\theta}{r - r^{-1}} = \frac{2\pi m_1 + m_2 c_1}{m_2 c_2},$$

then $J_{z,V}$ *is periodic in time with period* $T = [m_2 c_2 (r + r^{-1})/(r - r^{-1})]$,
(2) *if* $r = 1$ *and* $\cos\theta \neq 0$, *then* $J_{z,V}$ *is periodic in time with period* $T = 2\pi/\cos\theta$.

In the rest of the section we consider only the square torus. We will construct k-soliton Ward maps from $T^2\times\mathbb{R}$ to SU(n) that are also time periodic. To do this, we define

$$\mathcal{Z} = \{z = re^{i\theta} \in \mathbb{C}\setminus\mathbb{R} \,|\, z = e^{i\theta} \neq \pm i \text{ or } \cos\theta/(r - r^{-1}) \in \mathbb{Q}\},$$

where $\mathbb{Q}$ denotes the set of rational numbers. We have seen that for each $z \in \mathcal{Z}$, we can construct time periodic 1-solitons to the Ward equation. Moreover, the time period T depends on z only. In fact, the period function $T : \mathcal{Z} \to \mathbb{R}$ is defined as follows:

$$T(z)=\begin{cases}\dfrac{2\pi}{\cos\theta}, & \text{if } z=e^{i\theta}\neq\pm i,\\ \dfrac{2\pi m_2(r+r^{-1})}{r-r^{-1}}, & \text{if } z=re^{i\theta},\quad \dfrac{2\cos\theta}{r-r^{-1}}=\dfrac{m_1}{m_2}.\end{cases}\tag{3.1}$$

Apply Bäcklund transformations repeatedly with some rational conditions on the poles $z_1,\dots,z_m$ to get the following.

Theorem 3.2: *Let $\{z_1,\dots,z_m\}$ be a set of finite points in $\mathcal{Z}$ such that $z_i\neq z_j$, $\overline{z_j}$ for all $i\neq j$, and $h_{z_i,\pi_i}(\lambda)$ extended 1-soliton solutions leading to doubly periodic Ward maps, where $i,j=1,\dots,m$. Let $T_i=T(z_i)$ be the time period defined in* (3.1). *Let J_1 be the Ward map associated to h_{z_1,π_1}, i.e., $J_1=h_{z_1,\pi_1}(0)^{-1}$. Let J_m be the Ward map obtained by applying $m-1$ Bäcklund transformations to J_1,*

$$J_m=h_{z_m,\pi_m}*(\cdots*(h_{z_2,\pi_2}*J_1)\cdots).\tag{3.2}$$

If T_j/T_1 are rational numbers for all $2\leqslant j\leqslant m$, then J_m is a Ward map from $T^2\times\mathbb{R}$ to $SU(n)$ and is periodic in time. In other words, J_m is a triply periodic solution of the Ward equation.

Proof: We prove the two-soliton case. By Theorem 2, we have

$$h_{z_2,\pi_2}*h_{z_1,\pi_1}=h_{z_2,\tilde{\pi}_2}h_{z_1,\pi_1},$$

where $\operatorname{Im}\tilde{\pi}_2=h_{z_1,\pi_1}(z_2)\operatorname{Im}\pi_2=[I+(\overline{z_1}-z_1)/(z_2-\overline{z_1})\pi_1]\operatorname{Im}\pi_2$. Note that $\tilde{\pi}_2$ is periodic in time because π_1 and π_2 are time periodic and T_2/T_1 is rational. Thus we see that $h_{z_2,\pi_2}*h_{z_1,\pi_1}$ is time periodic, and so is the associated Ward map. The general case can be proved by induction. □

IV. HOMOCLINIC WARD MAPS

It is known that solutions of the sine-Gordon equation (SGE)

$$q_{tt}-q_{xx}=\sin q$$

give rise to wave maps from $\mathbb{R}^{1,1}$ to S^2. Breather solutions are 2-soliton solutions of the SGE that are periodic in the x variable. Shatah and Strauss proved in Ref. 6 that wave maps from $S^1\times\mathbb{R}$ to S^2 corresponding to breather solutions of the sine-Gordon equation are homoclinic wave maps. Applying Bäcklund transformation $2k$ times with carefully placed poles, Terng and Uhlenbeck constructed $2k$ soliton solutions for the sine-Gordon equation that are periodic in the space variable, and showed that the corresponding wave maps from $S^1\times\mathbb{R}$ to S^2 are also homoclinic. More generally they proved that there are homoclinic wave maps from $S^1\times\mathbb{R}$ into any compact symmetric space.[9]

In this section, we apply Bäcklund transformations with carefully chosen poles and Hermitian projections even times to certain stationary wave map into SO(2) to construct homoclinic Ward maps from $T^2\times\mathbb{R}$ to SU(n). To make the construction more illuminating, we will work on the SU(2) model. The SU(n) model is similar.

Let $m>0$ be an integer, and $a=\operatorname{diag}(im,-im)\in\mathrm{su}(2)$. It is easy to check that

$$\psi(\lambda)(x,y,t)=\psi(x,y,t,\lambda)=e^{((1-\lambda)x+(1+\lambda-\lambda^2)u-v)a}.\tag{4.1}$$

is an extended Ward map. So

$$J_0(x,y,t)=\psi(x,y,t,0)^{-1}=e^{-(x+u-v)a}=e^{-(x+y)a}$$

is a stationary Ward map, which is doubly periodic in the space variables. Note that J_0 is a harmonic map from T^2 to SO(2).

Next we compute the linearization of the Ward equation at the stationary solution $J_0 = e^{-(x+y)a}$, as well as its stable and unstable subspaces. Let $\mathcal{M} = C^\infty(T^2 \times \mathbb{R}, \mathrm{SU}(2))$. Then we can give a natural trivialization of the tangent bundle $T\mathcal{M}$ as follows. Given a curve $\gamma: (-\epsilon, \epsilon) \to \mathcal{M}$ with $\gamma(0) = J$, we identify the tangent vector $\gamma'(0)$ as

$$(\gamma(0), \gamma(0)^{-1}\gamma'(0)) = (J, J^{-1}\delta J).$$

This identifies $T\mathcal{M} = \mathcal{M} \times C^\infty(T^2 \times \mathbb{R}, \mathrm{su}(2))$.

Set $J^{-1}\delta J = \eta$. Compute directly to get

$$\begin{aligned}\delta(J^{-1}J_x) &= -(J^{-1}\delta J)J^{-1}J_x + J^{-1}(\delta J)_x \\ &= -\eta(J^{-1}J_x) + J^{-1}(J\eta)_x = -\eta(J^{-1}J_x) + J^{-1}(J_x\eta + J\eta_x) = \eta_x + [J^{-1}J_x, \eta].\end{aligned}$$

The computation for $\delta(J^{-1}J_y)$ and $\delta(J^{-1}J_t)$ is similar. So the linearization of the Ward equation at $J_0 = e^{-(x+y)a}$ is

$$\begin{aligned}&(\eta_t + [J^{-1}J_t, \eta])_t - (\eta_x + [J^{-1}J_x, \eta])_x - (\eta_y + [J^{-1}J_y, \eta])_y - [\eta_t + [J^{-1}J_t, \eta], J^{-1}J_y] \\ &\quad - [J^{-1}J_t, \eta_y + [J^{-1}J_y, \eta]] = \eta_{tt} - \eta_{xx} - \eta_{yy} + [a, \eta_x + \eta_y - \eta_t] = 0. \qquad (4.2)\end{aligned}$$

We note that the linearization at $J = -e^{-(x+y)a}$ is the same one. Write (4.2) in terms of entries $\eta = \begin{pmatrix} ir & \xi \\ -\bar{\xi} & -ir \end{pmatrix}$ to get

$$r_{tt} - r_{xx} - r_{yy} = 0, \qquad (4.3a)$$

$$\xi_{tt} - \xi_{xx} - \xi_{yy} + 2im(\xi_x + \xi_y - \xi_t) = 0. \qquad (4.3b)$$

This system is linear with constant coefficients, so it can be solved by Fourier series. Let

$$\xi = \sum_{j,l \in \mathbb{Z}} b_{jl}(t) e^{i(jx+ly)}$$

be the Fourier series expansion of ξ. Then by (4.3b), we have

$$b_{jl}'' - 2imb_{jl}' + (j^2 + l^2 - 2m(j+l))b_{jl} = 0,$$

where $'$ means differentiation with respect to t. Its auxiliary equation is

$$\gamma^2 - 2im\gamma + j^2 + l^2 - 2m(j+l) = 0.$$

It has roots

$$\gamma = im \pm \sqrt{m^2 - (j-m)^2 - (l-m)^2}.$$

Stable (unstable, respectively) modes come from $\mathrm{Re}(\gamma) < 0$ [$\mathrm{Re}(\gamma) > 0$, respectively]. So for $(j,l) \in \mathbb{Z}^2$ with $(j-m)^2 + (l-m)^2 < m^2$, there are stable and unstable modes corresponding to roots $im \mp \sqrt{m^2 - (j-m)^2 - (l-m)^2}$, respectively. Similar computation shows that the auxiliary equation for (4.3a) has only purely imaginary roots. So the above computation gives the following.

Proposition 4.1: Let $a = \mathrm{diag}(im, -im)$ *and* $J = \pm e^{-(x+y)a}$, *where* $m > 0$ *is an integer. Let*

$$B\mathbb{Z}_m = \{(j,l) \in \mathbb{Z}^2 | (j-m)^2 + (l-m)^2 < m^2\}.$$

Then

(1) *the unstable subspace of the linearization of the Ward equation at* J *is*

$$\oplus \{W_{jl}^+ | (j,l) \in B\mathbb{Z}_m\},$$

where W_{jl}^+ *is spanned by*

$$\eta_{jl}^{+}(c) = e^{\sqrt{m^2-(j-m)^2-(l-m)^2}t}\begin{pmatrix} 0 & ce^{i(jx+ly+mt)} \\ -\bar{c}e^{-i(jx+ly+mt)} & 0 \end{pmatrix}$$

with constant $c \in \mathbb{C}$.

(2) *The stable subspace at* J *is*

$$\oplus\{W_{jl}^{-} | (j,l) \in B\mathbb{Z}_m\},$$

where W_{jl}^{-} *is spanned by*

$$\eta_{jl}^{-}(c) = e^{-\sqrt{m^2-(j-m)^2-(l-m)^2}t}\begin{pmatrix} 0 & ce^{i(jx+ly+mt)} \\ -\bar{c}e^{-i(jx+ly+mt)} & 0 \end{pmatrix}$$

with $c \in \mathbb{C}$.

Let $z = re^{i\theta} \in \mathbb{C}\backslash\mathbb{R}$, $f(w)$ a meromorphic function on $\mathbb{C}$, $q(w) = \binom{1}{f(w)}$, $w = x + zu + z^{-1}v$, and $\pi(x,y,t)$ the Hermitian projection of $\mathbb{C}^2$ onto $\mathbb{C}q(w)$. Let ψ be the extended solution given by (4.1) and $J_0 = \psi^{-1}|_{\lambda=0} = e^{-a(x+y)}$ the associated Ward map. Consider the Bäcklund transformation $h_{z,\pi} * \psi$. We will find conditions on z and $f(w)$ so that $h_{z,\pi} * J_0$ is doubly periodic in space variables. By Theorem 2.2, we have

$$\psi_1 = h_{z,\pi} * \psi = h_{z,\tilde{\pi}}\psi, \tag{4.4}$$

where $\operatorname{Im}\tilde{\pi} = \mathbb{C}\tilde{q}$ and

$$\tilde{q}(x,y,t) = \psi(z)q(w) = e^{((1-z)x+(1+z-z^2)u-v)a}\begin{pmatrix} 1 \\ f(w) \end{pmatrix} \sim \begin{pmatrix} 1 \\ e^{2im((z-1)x+(z^2-z-1)u+v)}f(w) \end{pmatrix}.$$

Here "$q_1 \sim q_2$" means $\mathbb{C}q_1 = \mathbb{C}q_2$. From the formula

$$J_1 = h_{z,\pi} * J_0 = J_0\frac{1}{|z|}(\bar{z}\tilde{\pi} + z\tilde{\pi}^{\perp}),$$

we see that it is doubly periodic if and only if $\tilde{q}$ is. For this purpose, we try the following form of

$$f(w) = e^{2im(\alpha-z)w},$$

where $\alpha \in \mathbb{C}$ is a constant. Substitute this into $\tilde{q}(x,y,t)$ to get

$$e^{2im((z-1)x+(z^2-z-1)u+v)}f(w) = e^{2im((\alpha-1)x+((\alpha-1)z-1)u+\alpha z^{-1}v)} = e^{im(2(\alpha-1)x+((\alpha-1)z-\alpha z^{-1}-1)y+((\alpha-1)z+\alpha z^{-1}-1)t)}.$$

It is doubly periodic in x and y with period 2π if and only if

$$2m(\alpha-1) =: -j \in \mathbb{Z}, \tag{4.5a}$$

$$m((\alpha-1)z - \alpha z^{-1} - 1) =: -l \in \mathbb{Z}. \tag{4.5b}$$

From (4.5a), we have $\alpha = (2m-j)/2m$. Compute the imaginary part of (4.5b) to get

$$(\alpha-1)r\sin\theta + \alpha r^{-1}\sin\theta = 0.$$

Since $r > 0$, we see $0 < \alpha < 1$. This implies that $0 < j < 2m$, and $r = \sqrt{(2m-j)/j}$. By (4.5b) again, we have

$$m((\alpha-1)z - \alpha z^{-1} - 1) = -\sqrt{j(2m-j)}\cos\theta - m = -l.$$

It follows that

$$\sqrt{j(2m-j)}\cos\theta = l-m.$$

Hence l must satisfy

$$|l-m| < \sqrt{j(2m-j)}, \tag{4.6}$$

and $\cos\theta=[(l-m)/\sqrt{j(2m-j)}]$. It is easy to verify that the conditions for (j,l) are equivalent to $(j,l)\in\mathbb{Z}^2$, $(j-m)^2+(l-m)^2<m^2$, i.e., $(j,l)\in B\mathbb{Z}_m$. Therefore if we choose the following data: $(j,l)\in B\mathbb{Z}_m$, $z=re^{i\theta}$ with $r=\sqrt{(2m-j)/j}$, $\cos\theta=(l-m)/\sqrt{j(2m-j)}$, $\sin\theta>0$, $\alpha=(2m-j)/2m$, then $\mathrm{Im}\,\tilde{\pi}(x,y,t)=\mathbb{C}\tilde{q}(x,y,t)$, where

$$\tilde{q}(x,y,t)=\begin{pmatrix} 1 \\ e^{\sqrt{m^2-(j-m)^2-(l-m)^2}t}e^{-i(jx+ly+mt)} \end{pmatrix}$$

is doubly periodic in x and y. It follows that

$$\tilde{\pi}(x,y,t)=\frac{1}{1+e^{2A}}\begin{pmatrix} 1 & e^{A}e^{i(jx+ly+mt)} \\ e^{A}e^{-i(jx+ly+mt)} & e^{2A} \end{pmatrix},$$

where $A=\sqrt{m^2-(j-m)^2-(l-m)^2}t$. Therefore we obtain the following Ward map from $T^2\times\mathbb{R}$ to SU(2):

$$J_1=e^{-(x+y)a}\frac{1}{|z|}(\bar{z}\tilde{\pi}(x,y,t)+z\tilde{\pi}^{\perp}(x,y,t))=e^{-(x+y)a}(e^{-i\theta}\tilde{\pi}(x,y,t)+e^{i\theta}\tilde{\pi}^{\perp}(x,y,t)). \tag{4.7}$$

We now analyze the asymptotic behavior of J_1 as $t\to\pm\infty$. It is easy to see that

$$\tilde{\pi}\to\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{as } t\to+\infty,$$

and

$$\tilde{\pi}\to\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{as } t\to-\infty.$$

So

$$J_1\to e^{-(x+y)a}\begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix} \quad \text{as } t\to+\infty$$

and

$$J_1\to e^{-(x+y)a}\begin{pmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{pmatrix} \quad \text{as } t\to-\infty.$$

Thus $J_1: T^2\times\mathbb{R}\to\mathrm{SU}(2)$ is a heteroclinic Ward map. To construct homoclinic maps, we apply Bäcklund transformation again.

Choose $z_2=-\bar{z}$, and $\pi_2(x,y,t)$ Hermitian projection of $\mathbb{C}^2$ onto $\mathbb{C}q_2$, where $q_2=\binom{1}{f_2(w_2)}$, $f_2(w_2)=e^{2im(\alpha+\bar{z})w_2}$, $\alpha=(2m-j)/2m$, and $w_2=x-\bar{z}u-\bar{z}^{-1}v$. Now apply Bäcklund transformation to ψ_1 [defined by (4.4)] generated by $h_{-\bar{z},\pi_2(x,y,t)}$ to get

$$\psi_2=h_{-\bar{z},\pi_2(x,y,t)}*\psi_1=h_{-\bar{z},\tilde{\pi}_2(x,y,t)}\psi_1,$$

where $\mathrm{Im}\,\tilde{\pi}_2(x,y,t)=\mathbb{C}\tilde{q}_2(x,y,t)$ and

$$\tilde{q}_2 = \psi_1(-\overline{z})q_2 = h_{z,\tilde{\pi}(x,y,t)}(-\overline{z})\psi(-\overline{z})\begin{pmatrix} 1 \\ f_2(w_2) \end{pmatrix} \sim \left(I + \frac{\overline{z}-z}{-2\overline{z}}\tilde{\pi}(x,y,t)\right)\begin{pmatrix} 1 \\ e^A e^{-i(jx+(2m-l)y+mt)} \end{pmatrix}. \tag{4.8}$$

Here $A=\sqrt{m^2-(j-m)^2-(l-m)^2}t$. Note that $\tilde{q}(x,y,t)$ is doubly periodic in x and y. Therefore

$$J_2 = J_0\frac{1}{|z|}(z\tilde{\pi}+z\tilde{\pi}^{\perp})\frac{1}{|z_2|}(\overline{z_2}\tilde{\pi}_2+z_2\tilde{\pi}_2^{\perp}) = J_0(e^{-i\theta}\tilde{\pi}+e^{i\theta}\tilde{\pi}^{\perp})(-e^{i\theta}\tilde{\pi}_2-e^{-i\theta}\tilde{\pi}_2^{\perp})$$

is a Ward map from $T^2\times\mathbb{R}$ to SU(2), where $J_0=e^{-(x+y)a}$.

Next we study the asymptotic behavior of J_2. First look at the behavior of J_2 as $t\to-\infty$. Set

$$\xi = e^{\sqrt{m^2-(j-m)^2-(l-m)^2}t}, \quad f_1 = e^{-i(jx+ly+mt)}, \quad f_2 = e^{-i(jx+(2m-l)y+mt)}.$$

Then $\lim_{t\to-\infty}\xi=0$. Write

$$\tilde{q}_1 = \tilde{q} = \begin{pmatrix} 1 \\ \xi f_1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \xi f_1\begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

So the projection $\tilde{\pi}_1=\tilde{\pi}$ onto $\mathbb{C}\tilde{q}_1$ is

$$\tilde{\pi}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \xi\begin{pmatrix} 0 & \overline{f_1} \\ f_1 & 0 \end{pmatrix} + O(\xi^2).$$

Write $\alpha_1=(z-\overline{z})/2\overline{z}$. Then by (4.8) we have

$$\tilde{q}_2 = (I+\alpha_1\tilde{\pi}_1)\begin{pmatrix} 1 \\ \xi f_2 \end{pmatrix} = (I+\alpha_1\tilde{\pi}_1)\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \xi f_2\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right) = \begin{pmatrix} 1+\alpha_1 \\ 0 \end{pmatrix} + \alpha_1\xi f_1\begin{pmatrix} 0 \\ 1 \end{pmatrix} + \xi f_2\begin{pmatrix} 0 \\ 1 \end{pmatrix} + O(\xi^2)$$
$$\sim \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta_1\xi f_1\begin{pmatrix} 0 \\ 1 \end{pmatrix} + \beta_2\xi f_2\begin{pmatrix} 0 \\ 1 \end{pmatrix} + O(\xi^2),$$

where $\beta_1=\alpha_1/(1+\alpha_1)$, $\beta_2=1/(1+\alpha_1)$. So the projection $\tilde{\pi}_2$ onto $\mathbb{C}\tilde{q}_2$ is

$$\tilde{\pi}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \xi\begin{pmatrix} 0 & \overline{\beta_1 f_1} \\ \beta_1 f_1 & 0 \end{pmatrix} + \xi\begin{pmatrix} 0 & \overline{\beta_2 f_2} \\ \beta_2 f_2 & 0 \end{pmatrix} + O(\xi^2).$$

From the above computation, we see

$$\lim_{t\to-\infty}\tilde{\pi}_i = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad i=1,2.$$

Substitute $\tilde{\pi}_i$ into J_2 to get

$$J_2 = J_0(e^{-i\theta}\tilde{\pi}+e^{i\theta}\tilde{\pi}^{\perp})(-e^{i\theta}\tilde{\pi}_2-e^{-i\theta}\tilde{\pi}_2^{\perp})$$
$$= J_0\left(\begin{pmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{pmatrix} + \xi\begin{pmatrix} 0 & -2i\sin\theta\overline{f_1} \\ -2i\sin\theta f_1 & 0 \end{pmatrix} + O(\xi^2)\right)$$
$$\times\left(\begin{pmatrix} -e^{i\theta} & 0 \\ 0 & -e^{-i\theta} \end{pmatrix} + \xi\begin{pmatrix} 0 & -2i\sin\theta\overline{\beta_1 f_1} \\ -2i\sin\theta\beta_1 f_1 & 0 \end{pmatrix} + \xi\begin{pmatrix} 0 & -2i\sin\theta\overline{\beta_2 f_2} \\ -2i\sin\theta\beta_2 f_2 & 0 \end{pmatrix}\right.$$
$$\left. + O(\xi^2)\right) = J_0\left(-I + \xi\begin{pmatrix} 0 & c_1\overline{f_1} \\ -\overline{c_1}f_1 & 0 \end{pmatrix} + \xi\begin{pmatrix} 0 & c_2\overline{f_2} \\ -\overline{c_2}f_2 & 0 \end{pmatrix} + O(\xi^2)\right),$$

where c_1, $c_2\in\mathbb{C}$ are constants. It follows that $\lim_{t\to-\infty}J_2=-J_0$. Note that

$$\xi\begin{pmatrix} 0 & c_i\overline{f_i} \\ -\overline{c_i}f_i & 0 \end{pmatrix}, \quad i=1,2$$

is equal to the unstable mode $\eta^+_{j_i,l_i}(c_i)$ at $-J_0$ given in Proposition 4.1, where $(j_1,l_1)=(j,l)$ and $(j_2,l_2)=(j,2m-l)$. In other words, we have shown

$$\lim_{t\to-\infty}\left(J_2+J_0+J_0\sum_{i=1}^{2}\eta^+_{j_i,l_i}(c_i)\right)=0. \tag{4.9}$$

To analyze the asymptotic behavior of J_2 as $t\to+\infty$, we set

$$\rho=e^{-\sqrt{m^2-(j-m)^2-(l-m)^2}t}, \quad h_1=e^{i(jx+ly+mt)}, h_2=e^{i(jx+(2m-l)y+mt)}.$$

Then $\lim_{t\to+\infty}\rho=0$. A similar computation implies that

(1) $\tilde{q}_1$ is parallel to $\binom{\rho h_1}{1}$.

(2)

$$\tilde{\pi}_1=\begin{pmatrix}0&0\\0&1\end{pmatrix}+\rho\begin{pmatrix}0&h_1\\\overline{h_1}&0\end{pmatrix}+O(\rho^2),$$

and

$$\tilde{\pi}_2=\begin{pmatrix}0&0\\0&1\end{pmatrix}+\rho\begin{pmatrix}0&\gamma_1h_1\\\overline{\gamma_1}\overline{h_1}&0\end{pmatrix}+\rho\begin{pmatrix}0&\gamma_2h_2\\\overline{\gamma_2}\overline{h_2}&0\end{pmatrix}+O(\rho^2)$$

for some constants γ_1, γ_2.

(3)

$$J_2=J_0\left(-I+\rho\begin{pmatrix}0&d_1h_1\\-\overline{d_1}\overline{h_1}&0\end{pmatrix}+\rho\begin{pmatrix}0&d_2h_2\\-\overline{d_2}\overline{h_2}&0\end{pmatrix}+O(\rho^2)\right)$$

for some constants d_1, d_2. It follows that $\lim_{t\to+\infty}J_2=-J_0$.

(4)

$$\lim_{t\to+\infty}\left(J_2+J_0+J_0\sum_{i=1}^{2}\eta^-_{j_i,l_i}(d_i)\right)=0. \tag{4.10}$$

Formulas (4.9) and (4.10) imply that $J_2:T^2\times\mathbb{R}\to\mathrm{SU}(2)$ is a homoclinic Ward map.

Applying Bäcklund transformations even times, with pairs of poles and Hermitian projections chosen as above, we obtain more homoclinic Ward maps. The case for $m<0$ is similar. We summarize the above discussion to give the following.

Theorem 4.2: *Let m be a nonzero integer, $a=\mathrm{diag}(im,-im)$, and $J_0=e^{-(x+y)a}$. Choose $(j_{2k-1},l_{2k-1})\in\mathbb{Z}^2$ such that*

$$(j_{2k-1}-m)^2+(l_{2k-1}-m)^2<m^2, \quad m<l_{2k-1}$$

and $(j_{2k-1},l_{2k-1})\neq(j_{2h-1},l_{2h-1})$ for $1\leqslant k<h\leqslant N$. Let $(j_{2k},l_{2k})=(j_{2k-1},2m-l_{2k-1})$, $z_s=\sqrt{(2m-j_s)/[j_s]}e^{i\theta_s}$ with $\cos\theta_s=\mathrm{sgn}(m)[(l_s-m)/\sqrt{j_s(2m-j_s)}]$, and $\sin\theta_s=\mathrm{sgn}(m)\sqrt{1-\cos^2\theta_s}$, $s=1,\ldots,2N$. Let π_s be the Hermitian projection onto $\mathbb{C}\binom{1}{f_s(w_s)}$, where $f_s(w_s)=e^{i(2m-j_s-2mz_s)w_s}$ and $w_s=x+z_su+z_s^{-1}v$. Let

$$J_{2N}(x,y,t)=h_{z_{2N},\pi_{2N}}*(\cdots*(h_{z_1,\pi_1}*J_0(x,y,t))\cdots) \tag{4.11}$$

be the Ward map obtained by applying $2N$ Bäcklund transformations to J_0. Then $J_{2N}:T^2\times\mathbb{R}$

$\to SU(2)$ *is a homoclinic Ward map. Moreover,* $J_{2N} \to (-1)^N J_0$ *as* $t \to \pm\infty$.

Proof: We have shown the $N=1$ case. For general N, we use induction and the calculation is similar. □

The above construction can be generalized to SU(n) model easily.

Corollary 4.3: Let m, p be integers, $m \neq 0$, $1 \leqslant p \leqslant n-1$,

$$a = \begin{pmatrix} i(n-p)mI_p & 0 \\ 0 & -ipmI_{n-p} \end{pmatrix} \in \mathrm{su}(n),$$

$\psi = e^{((1-\lambda)x+(1+\lambda-\lambda^2)u-v)a}$ *the extended solution, and* $J_0 = e^{-(x+y)a}$ *the associated Ward map. Choose* $(j_{2k-1}, l_{2k-1}) \in \mathbb{Z}^2$ *such that*

$$\left(j_{2k-1} - \frac{nm}{2}\right)^2 + \left(l_{2k-1} - \frac{nm}{2}\right)^2 < \left(\frac{nm}{2}\right)^2, \quad \frac{nm}{2} < l_{2k-1}$$

and $(j_{2k-1}, l_{2k-1}) \neq (j_{2h-1}, l_{2h-1})$ *for* $1 \leqslant k < h \leqslant N$. *Let* $(j_{2k}, l_{2k}) = (j_{2k-1}, nm - l_{2k-1})$, $z_s = \sqrt{(nm-j_s)/[j_s]}e^{i\theta_s}$ *with* $\cos\theta_s = \mathrm{sgn}(m)[(l_s - nm/2)/\sqrt{j_s(nm-j_s)}]$, *and* $\sin\theta_s = \mathrm{sgn}(m)\sqrt{1-\cos^2\theta_s}$, $s = 1, \ldots, 2N$. *Let* $\pi_s(x,y,t)$ *be the Hermitian projection of* $\mathbb{C}^n$ *onto*

$$\mathbb{C}(1, \ldots, 1, f_s(w_s), \ldots f_s(w_s))^T,$$

where 1 *is repeated p times,* $f_s(w_s) = e^{i(nm-j_s-nmz_s)w_s}$ *is repeated* $(n-p)$ *times,* $w_s = x + z_s u + z_s^{-1} v$. *Let*

$$J_{2N}(x,y,t) = h_{z_{2N},\pi_{2N}} * (\cdots * (h_{z_1,\pi_1} * J_0(x,y,t)) \cdots) \tag{4.12}$$

be the Ward map obtained by applying $2N$ *Bäcklund transformations to* J_0. *Then* $J_{2N}: T^2 \times \mathbb{R} \to SU(n)$ *is a homoclinic Ward map. Moreover,* $J_{2N} \to (-1)^N J_0$ *as* $t \to \pm\infty$.

The method discussed above can also produce Ward maps, which are homoclinic to (time) periodic orbits. There are only some minor changes in the construction, so we just list the main steps for the SU(2) model.

(i) Let $m > 0$ be an integer, and $b = \mathrm{diag}(im, -im)$. Then

$$\psi = e^{(x+(\lambda+2)u)b}$$

is an extended solution, and the associated Ward map is

$$J_0 = \psi^{-1}|_{\lambda=0} = e^{-(x+2u)b} = e^{-(x+y+t)b},$$

which is triply periodic in the variables x, y, t.

(ii) Set $\eta = J^{-1}\delta J$. Then the linearization of the Ward equation at J_0 is

$$\eta_{tt} - \eta_{xx} - \eta_{yy} + [b, \eta_x + 2\eta_y - 2\eta_t] = 0.$$

The unstable subspace of the linearization of the Ward equation at J_0 is $\oplus W_{jl}^+$, where $(j,l) \in \mathbb{Z}^2$, $(j-m)^2 + (l-2m)^2 < m^2$, and W_{jl}^+ is spanned by

$$e^{\sqrt{m^2-(j-m)^2-(l-2m)^2}\,t}\begin{pmatrix} 0 & ce^{i(jx+ly+2mt)} \\ -\overline{c}e^{-i(jx+ly+2mt)} & 0 \end{pmatrix}$$

with constant $c \in \mathbb{C}$. The stable subspace at J_0 is $\oplus W_{jl}^-$, where (j,l) satisfies the same condition, and W_{jl}^- is spanned by

$$e^{-\sqrt{m^2-(j-m)^2-(l-2m)^2}\,t}\begin{pmatrix} 0 & ce^{i(jx+ly+2mt)} \\ -\overline{c}e^{-i(jx+ly+2mt)} & 0 \end{pmatrix}$$

with constant $c \in \mathbb{C}$.

(iii) Choose $(j,l)\in\mathbb{Z}^2$ with $(j-m)^2+(l-2m)^2<m^2$. Apply Bäcklund transformation $h_{z_1,\pi_1}*\psi$, where $z_1=re^{i\theta}$ with $r=\sqrt{(2m-j)/j}$, $\cos\theta=(l-2m)/\sqrt{j(2m-j)}$, $\sin\theta>0$, $\pi_1(x,y,t)$ is the Hermitian projection of $\mathbb{C}^2$ onto $\mathbb{C}\binom{1}{e^{2im\alpha_1 w_1}}$, $\alpha_1=(2m-j)/2m$, and $w_1=x+z_1u+z_1^{-1}v$. Then

$$\psi_1=h_{z_1,\pi_1}*\psi=h_{z_1,\tilde{\pi}_1}\psi,$$

where $\tilde{\pi}_1$ is the projection onto

$$\psi(z_1)\mathrm{Im}\,\pi_1=\mathbb{C}\begin{pmatrix}1\\ e^{\sqrt{m^2-(j-m)^2-(l-2m)^2}t}e^{-i(jx+ly+2mt)}\end{pmatrix}.$$

(iv) Choose $(j_2,l_2)=(j,4m-l)\in\mathbb{Z}^2$. Apply Bäcklund transformation again to get

$$\psi_2=h_{z_2,\pi_2}*\psi_1=h_{z_2,\tilde{\pi}_2}\psi_1.$$

Here $z_2=-\overline{z_1}$, and $\pi_2(x,y,t)$ is the Hermitian projection onto $\mathbb{C}q$, where $q=\binom{1}{e^{2im\alpha_2 w_2}}$, $\alpha_2=\alpha_1$, and $w_2=x-\overline{z_1}u-\overline{z_1}^{-1}v$. Then $\tilde{\pi}_2(x,y,t)$ is the projection onto

$$\mathbb{C}h_{z_1,\tilde{\pi}_1}(-\overline{z_1})\begin{pmatrix}1\\ e^{\sqrt{m^2-(j-m)^2-(l-2m)^2}t}e^{-i(jx+(4m-l)y+2mt)}\end{pmatrix}.$$

(v)

$$J_2=\psi_2^{-1}|_{\lambda=0}=J_0(e^{-i\theta}\tilde{\pi}_1+e^{i\theta}\tilde{\pi}_1^{\perp})(-e^{i\theta}\tilde{\pi}_2-e^{-i\theta}\tilde{\pi}_2^{\perp})$$

is a Ward map from $T^2\times\mathbb{R}$ to SU(2). Analyzing the asymptotic behavior of J_2 as $t\to\pm\infty$, we see that J_2 is transversal and homoclinic to the periodic orbit $-J_0$. Applying Bäcklund transformations even times with pairs of poles and Hermitian projections chosen similarly, we obtain more Ward maps which are homoclinic to $\pm J_0$.

The construction of homoclinic orbits to (time) periodic solutions for the SU(n) model is similar. Thus we have the following.

Theorem 4.4: *Let m, p be integers, $m\neq 0$, $1\leqslant p\leqslant n-1$,*

$$b=\begin{pmatrix}i(n-p)mI_p & 0\\ 0 & -ipmI_{n-p}\end{pmatrix}\in\mathrm{su}(n),$$

$\psi=e^{(x+(\lambda+2)u)b}$ the extended solution, and $J_0=e^{-(x+y+t)b}$ the associated Ward map. Choose $(j_{2k-1},l_{2k-1})\in\mathbb{Z}^2$ such that

$$\left(j_{2k-1}-\frac{nm}{2}\right)^2+(l_{2k-1}-nm)^2<\left(\frac{nm}{2}\right)^2,\quad nm<l_{2k-1}$$

and $(j_{2k-1},l_{2k-1})\neq(j_{2h-1},l_{2h-1})$ for $1\leqslant k<h\leqslant N$. Let $(j_{2k},l_{2k})=(j_{2k-1},2nm-l_{2k-1})$, $z_s=\sqrt{(nm-j_s)/[j_s]}e^{i\theta_s}$ with $\cos\theta_s=\mathrm{sgn}(m)[(l_s-nm)/\sqrt{j_s(nm-j_s)}]$, and $\sin\theta_s=\mathrm{sgn}(m)\sqrt{1-\cos^2\theta_s}$, $s=1,\ldots,2N$. Let $\pi_s(x,y,t)$ be the Hermitian projection of $\mathbb{C}^n$ onto

$$\mathbb{C}(1,\ldots,1,f_s(w_s),\ldots f_s(w_s))^T,$$

where 1 is repeated p times, $f_s(w_s)=e^{i(nm-j_s)w_s}$ is repeated $(n-p)$ times, and $w_s=x+z_su+z_s^{-1}v$. Let

$$J_{2N}(x,y,t)=h_{z_{2N},\pi_{2N}}*(\cdots*(h_{z_1,\pi_1}*J_0(x,y,t))\cdots)$$

be the Ward map obtained by applying $2N$ Bäcklund transformations to J_0. Then $J_{2N}:T^2\times\mathbb{R}\to SU(n)$ is a homoclinic Ward map. Moreover, $J_{2N}\to(-1)^NJ_0$ as $t\to\pm\infty$.

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Darboux points and integrability of Hamiltonian systems with homogeneous polynomial potential

Andrzej J. Maciejewski[a)]
Institute of Astronomy, University of Zielona Góra, Podgórna 50, PL-65-246 Zielona Góra, Poland

Maria Przybylska[b)]
Institut Fourier, UMR 5582 du CNRS, Université de Grenoble I, BP 74, 38402 Saint-Martin d'Hères, France and Toruń Centre for Astronomy, N. Copernicus University, Gagarina 11, PL-87-100 Toruń, Poland

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In this paper we study the integrability of natural Hamiltonian systems with a homogeneous polynomial potential. The strongest necessary conditions for their integrability in the Liouville sense have been obtained by a study of the differential Galois group of variational equations along straight line solutions. These particular solutions can be viewed as points of a projective space of dimension smaller by one than the number of degrees of freedom. We call them Darboux points. We analyze in detail the case of two degrees of freedom. We show that, except for a radial potential, the number of Darboux points is finite and it is not greater than the degree of the potential. Moreover, we analyze cases when the number of Darboux points is smaller than maximal. For two degrees of freedom the above-mentioned necessary condition for integrability can be expressed in terms of one nontrivial eigenvalue of the Hessian of potential calculated at a Darboux point. We prove that for a given potential these nontrivial eigenvalues calculated for all Darboux points cannot be arbitrary because they satisfy a certain relation which we give in an explicit form. We use this fact to strengthen maximally the necessary conditions for integrability and we show that in a generic case, for a given degree of the potential, there is only a finite number of potentials which satisfy these conditions. We also describe the nongeneric cases. As an example we give a full list of potentials of degree four satisfying these conditions. Then, investigating the differential Galois group of higher order variational equations, we prove that, except for one discrete family, among these potentials only those which are already known to be integrable are integrable. We check that a finite number of potentials from the exceptional discrete family are not integrable, and we conjecture that all of them are not integrable. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1917311]

I. INTRODUCTION

We consider $\mathbb{C}^{2n}$ as a symplectic linear space with canonical variables $\boldsymbol{q}=(q_1,\ldots,q_n)$, $\boldsymbol{p}=(p_1,\ldots,p_n)$. We are interested in Hamiltonian systems defined by Hamilton's function of the form

[a)]Electronic mail: maciejka@astro.ia.uz.zgora.pl
[b)]Electronic mail: maria.przybylska@astri.uni.torun.pl

$$H = \frac{1}{2}\sum_{i=1}^{n} p_i^2 + V(\boldsymbol{q}), \tag{1.1}$$

where $V=V(\boldsymbol{q}) \in \mathbb{C}[\boldsymbol{q}]$ is a homogeneous polynomial of degree $k>2$. The canonical Hamilton's equations have the well-known form

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{q} = \boldsymbol{p}, \quad \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{p} = -V'(\boldsymbol{q}), \tag{1.2}$$

where by $V'(\boldsymbol{q})$ we denote the gradient of $V(\boldsymbol{q})$. The classical problem concerns integrability of such systems.

To simplify our further exposition it is convenient to notice the following fact. It is easy to show that if Hamilton's equations (1.2) are integrable with potential $V(\boldsymbol{q})$, then they are integrable also with potential $V_A(\boldsymbol{q}) := V(A\boldsymbol{q})$, where $A \in \mathrm{PO}(n,\mathbb{C}) \subset \mathrm{GL}(n,\mathbb{C})$. Here by $\mathrm{PO}(n,\mathbb{C})$ we denote a group of $n \times n$ complex matrices A such that $AA^T = \alpha E$ where $\alpha \in \mathbb{C}^\star$. Thus, when we discuss integrability, we identify potentials V and V_A, for all $A \in \mathrm{PO}(n,\mathbb{C})$, and we say that they are equivalent. Later in this paper often a potential means a class of equivalent potentials and the phrase "potential V is integrable" means that the corresponding system (1.2) is integrable. By integrability we understand the integrability in the Liouville sense with first integrals which are complex meromorphic functions.

In spite of a very long history and numerous approaches little is known about the integrability of (1.2). In fact, an application of the direct method,[16,15] and the Painlevé test[9–12,20,39,40] gave only several examples of integrable systems for which additional first integrals are polynomials of low degrees. The most general result based on the direct method was obtained by Nakagawa and Yoshida.[37] These authors proved that if Hamiltonian system (1.2) with two degrees of freedom and a homogeneous potential of degree $k \geqslant 5$ admits an additional polynomial first integral F such that $\deg_p F \leqslant 4$, then it admits an additional polynomial first integral F such that $\deg_p F \leqslant 2$.

At the beginning of the 1980s Ziglin[43,44] developed an elegant theory which relates the integrability of Hamiltonian systems with properties of the monodromy group of variational equations along a particular solution. The Ziglin theory gives conditions necessary for integrability of a complex system with an arbitrary holomorphic Hamiltonian. Yoshida[42] used this theory to formulate a criterion for the integrability of system (1.2) with a homogeneous potential which is not necessarily a polynomial. The Yoshida criterion was formulated only for systems with two degrees of freedom and it has the form of inequalities. Thus, for systems depending on parameters, these values of parameters for which the system satisfies the necessary conditions for integrability form open sets in the space of parameters.

At the end of the previous century the Ziglin theory was considerably extended. Roughly speaking, the necessary conditions for integrability were expressed in terms of the differential Galois group[41] of variational equations. This approach was developed by Baider, Churchill, Morales, Ramis, Rod, Simó, and Singer, see Refs. 5 and 30, and references therein. It was shown that if the investigated system is integrable in the Liouville sense, then the identity component of the differential Galois group of the variational equations along a particular solution is Abelian, see Ref. 30 and Sec. I of Appendix A. For Hamiltonian systems (1.2) with homogeneous potential these conditions, as shown in Refs. 30 and 32, are much stronger than those given by Yoshida and they are applicable for systems with an arbitrary number of degrees of freedom. To describe them we have to introduce several definitions.

A nonzero point $\boldsymbol{d} \in \mathbb{C}^n$ is called a *Darboux point* of system (1.2) if it is a solution of

$$V'(\boldsymbol{d}) = \gamma \boldsymbol{d}, \tag{1.3}$$

where $\gamma \in \mathbb{C}^\star = \mathbb{C}\backslash\{0\}$. A Darboux point defines a two-dimensional plane in $\mathbb{C}^{2n}$ invariant with respect to the flow of the system (1.2). In fact, if $\boldsymbol{d}$ satisfies (1.3), then

$$\boldsymbol{q}(t) = \varphi(t)\boldsymbol{d}, \quad \boldsymbol{p}(t) = \dot{\varphi}(t)\boldsymbol{d} \tag{1.4}$$

is a solution of the system (1.2), provided that $\varphi(t)$ satisfies

$$\ddot{\varphi} = -\gamma\varphi^{k-1}.$$

From our definition of a Darboux point it follows that it is a point $[d_1:d_2:\cdots:d_n]$ of projective space $\mathbb{CP}^{n-1}$ for which its homogeneous coordinates satisfy (1.3).

The variational equations along solution (1.4) have the form

$$\dot{\boldsymbol{x}} = \boldsymbol{y}, \quad \dot{\boldsymbol{y}} = -\varphi(t)^{k-2}V''(\boldsymbol{d})\boldsymbol{x}. \tag{1.5}$$

Hessian $V''(\boldsymbol{d})$ of the potential V calculated at a Darboux point $\boldsymbol{d}$ is a symmetric matrix. Hence, in a generic case, there exists a complex orthogonal $n\times n$ matrix A such that the canonical transformation

$$\boldsymbol{x} = A\boldsymbol{\eta}, \quad \boldsymbol{y} = A\boldsymbol{\xi},$$

transforms system (1.5) to the form

$$\dot{\eta}_i = \xi_i, \quad \dot{\xi}_i = -\hat{\lambda}_i\varphi(t)^{k-2}\eta_i, \quad i = 1, \ldots, n,$$

or simply

$$\ddot{\eta}_i = -\hat{\lambda}_i\varphi(t)^{k-2}\eta_i, \quad i = 1, \ldots, n, \tag{1.6}$$

where $(\hat{\lambda}_1, \ldots, \hat{\lambda}_n)$ are eigenvalues of $V''(\boldsymbol{d})$. One of them, let us say $\hat{\lambda}_n$, is equal to $\gamma(k-1)$. For a given energy $e \in \mathbb{C}^\star$ the phase curve Γ_e associated with particular solution $\varphi(t)$ is, for $k \neq 0$, a hyperelliptic curve given by

$$\dot{\varphi}^2 = 2\frac{\gamma}{k}(\varepsilon - \varphi^k), \quad e = \frac{\gamma}{k}\varepsilon. \tag{1.7}$$

As was observed by Yoshida,[42] each of equations (1.6) can be transformed to the hypergeometric equation. It can be done by the following change of the independent variable:

$$t \to z := \frac{1}{\varepsilon}\varphi(t)^k. \tag{1.8}$$

As

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}x = \dot{z}^2x'' + \ddot{z}x', \quad {}' \equiv \frac{\mathrm{d}}{\mathrm{d}z},$$

after transformation (1.8) Eq. (1.6) reads

$$z(1-z)\eta_i'' + \left(\frac{k-1}{k} - \frac{3k-2}{2k}z\right)\eta_i' + \frac{\lambda_i}{2k}\eta_i = 0, \tag{1.9}$$

where $i=1,\ldots,n$, and $\lambda_i=\hat{\lambda}_i/\gamma$. Here we note that λ_i are eigenvalues of $\gamma^{-1}V''(\boldsymbol{d})$. Equation (1.9) is a hypergeometric differential equation for which the differences of exponents at $z=0$, $z=1$, and $z=\infty$ are

$$\frac{1}{k}, \quad \frac{1}{2}, \quad \frac{1}{2k}\sqrt{(k-2)^2 + 8k\lambda_i},$$

respectively.

Now, as variational equations have the form of a direct product of Eq. (1.9), their differential Galois group is also a direct product of the differential Galois groups of Eq. (1.9). All cases when the identity component of the differential Galois group of hypergeometric differential equation is solvable are known, see Ref. 17. This fact combined with Theorem A.1 was used by Morales-Ruiz and Ramis to formulate in Ref. 34 a general theorem concerning the integrability of Hamiltonian systems with a homogeneous potential. Here, we formulate this theorem for a polynomial homogeneous potential.

Theorem 1.1: *If Hamiltonian system (1.2) with polynomial homogeneous potential* $V(\boldsymbol{q})$ *of degree* $k>2$ *is meromorphically integrable in the Liouville sense, then for Darboux point values of* (k,λ_i) for $i=1,\ldots,n$ *belong to the following list*

$$1.\ \left(k,p+\frac{k}{2}p(p-1)\right),\quad 2.\ \left(k,\frac{1}{2}\left[\frac{k-1}{k}+p(p+1)k\right]\right),$$

$$3.\ \left(3,-\tfrac{1}{24}+\tfrac{1}{6}(1+3p)^2\right),\quad 4.\ \left(3,-\tfrac{1}{24}+\tfrac{3}{32}(1+4p)^2\right),$$

$$5.\ \left(3,-\tfrac{1}{24}+\tfrac{3}{50}(1+5p)^2\right),\quad 6.\ \left(3,-\tfrac{1}{24}+\tfrac{3}{50}(2+5p)^2\right),$$

$$7.\ \left(4,-\tfrac{1}{8}+\tfrac{2}{9}(1+3p)^2\right),\quad 8.\ \left(5,-\tfrac{9}{40}+\tfrac{5}{18}(1+3p)^2\right),$$

$$9.\ \left(5,-\tfrac{9}{40}+\tfrac{1}{10}(2+5p)^2\right),$$

where p is an integer.

Note that for a given k the eigenvalue $\lambda_n=k-1$ does not give a restriction for integrability. We called it the trivial eigenvalue. Here it is important to notice the following fact. Let $\boldsymbol{d}$ be a Darboux point of potential V. Then an equivalent potential V_A has a Darboux point $\tilde{\boldsymbol{d}}=A^T\boldsymbol{d}$ as we have

$$V_A'(\tilde{\boldsymbol{d}})=A^TV'(AA^T\boldsymbol{d})=A^TV'(\alpha\boldsymbol{d})=\alpha^{k-1}A^TV'(\boldsymbol{d})=\tilde{\gamma}\tilde{\boldsymbol{d}},$$

where $\tilde{\gamma}=\gamma\alpha^{k-1}$. Moreover, $\gamma^{-1}V''(\boldsymbol{d})$ and $\tilde{\gamma}^{-1}V_A''(\tilde{\boldsymbol{d}})$ have the same eigenvalues. Hence, these eigenvalues and the number of Darboux points characterize classes of equivalent potentials.

Theorem 1.1 gives the strongest known necessary conditions for the integrability of system (1.2). However, a problem appears again when the potential depends on parameters. Applying it we quickly distinguish *infinitely* many families of potentials for which these conditions are satisfied.

Although it seems that this problem is unavoidable, the aim of this paper is to show that at least for systems with two degrees of freedom it is not like that.

First of all, it is obvious that the more Darboux points of considered potential we know, the more conditions for its integrability we have. Hence, it is crucial to know how many Darboux points for a given potential exist, and how the number of Darboux points depends on parameters.

The second problem is more delicate and less obvious. Assume that for a given potential we found all Darboux points. Each of them gives us $n-1$ nontrivial eigenvalues which appear in the necessary conditions for integrability. The question is if all of these eigenvalues can be arbitrary. In other words, we ask if there exists a universal relation between all the eigenvalues calculated for all Darboux points.

In this paper we analyze the above-noted problems for the case of two degrees of freedom. In this case for a Darboux point $\boldsymbol{d}$ there is only one nontrivial eigenvalue

$$\lambda=\gamma^{-1}\mathrm{Tr}\,V''(\boldsymbol{d})-(k-1).$$

We show that for a generic homogeneous polynomial of degree k there exist k Darboux points. For each Darboux point we calculate the "shifted" nontrivial eigenvalue

$$\Lambda = \lambda - 1 = \gamma^{-1}\mathrm{Tr}\, V''(\boldsymbol{d}) - k.$$

Then, one of the main results of this paper is following.

Theorem 1.2: *Assume that a homogeneous polynomial potential $V(q_1, q_2)$ of degree $k>2$ has k different Darboux points. Then the shifted eigenvalues Λ_i calculated for these points satisfy the following relation*

$$\sum_{i=1}^{k} \frac{1}{\Lambda_i} = -1. \tag{1.10}$$

Our next result shows the importance of the above theorem. To formulate it let us denote by $\mathcal{V}_k$ the set of all homogeneous potentials V of degree k which have k different Darboux points. For each $V \in \mathcal{V}_k$ we have properly defined a collection $\mathbf{\Lambda}_V = \{\Lambda_1, \ldots, \Lambda_k\}$ of the shifted eigenvalues. Let $\mathcal{L}_k$ denote a set of all $\mathbf{\Lambda}_V$, for $V \in \mathcal{V}_k$, and $\mathcal{I}_k$ a set of those elements of $\mathcal{L}_k$ which correspond to the integrable potentials. Combining Theorem 1 with our Theorem 2 we prove the following.

Theorem 1.3: *For all $k>2$ set $\mathcal{I}_k$ is at most finite.*

As we will show, the assumption about the number of Darboux points in the above-mentioned theorems can be relaxed.

Having the above-noted results it is natural to ask for more. For example, it is natural to ask if we can give necessary and sufficient conditions for the integrability of system (1.2) for a polynomial potential of a fixed degree k. Obviously Theorem 1.1 and our above-mentioned results are not sufficient for this task—we need stronger necessary conditions for the integrability than those in Theorem 1.1. Hopefully, there exists a theorem by Morales-Ruiz, Ramis, and Simó[31] which gives the desired conditions. These conditions are expressed in terms of properties of the differential Galois group of higher order variational equations around a particular solution, see Sec. II of Appendix A.

In Ref. 23 we performed a detailed analysis of homogeneous potentials of degree three. Investigating this case we found a particular case of relation (1.10) and we noticed that without this relation it is hopeless to distinguish all integrable potentials. However, using the above-mentioned theorem of Morales-Ruiz, Ramis, and Simó we were able to give necessary and sufficient conditions for integrability of a homogeneous potential of degree three.

In this paper we investigate the case of a homogeneous potential of degree $k=4$. It appears that case $k=4$ is much more complicated than case $k=3$. Nevertheless, we performed our analysis almost up to the end, i.e., we give a full list of integrable potentials of degree four and we show that, except for one discrete but infinite family, the remaining potentials are not integrable. It seems that all potentials from the exceptional discrete family are not integrable but we are able to show this only for a finite number of potentials from this family.

The plan of this paper is the following. Section II contains general results concerning systems with two degrees of freedom. In Sec. III we analyze Hamiltonian system (1.2) with a homogeneous potential of degree 4. Section IV contains some general remarks and comments.

As to Sec. II, after showing some preliminary facts in Sec. II A, we analyze in Sec. II B the question about the number of Darboux points for a given homogeneous potential. The main results of this section are Lemma 2.2, which characterizes potentials without Darboux points, and Lemma 2.3 together with Corollary 2.2 which explain how the positions of Darboux points determine the potential. In Sec. II B we analyze the question about the number of Darboux points for a given potential. First we reduce the problem to counting the number of equilibria of an auxiliary system. Then the problem is reduced to an investigation of roots of two polynomials. Here, besides general facts about the finiteness of the number of Darboux points, in Lemma 2.2 we characterize cases when there are no Darboux points. In Sec. II C we introduce a meromorphic differential form such that the Darboux points are contained in its poles. The residue of this form at a simple Darboux point is the inverse of the shifted eigenvalue. Theorem 2.1 is a more general version of Theorem 1.2 formulated above. However, as we believe, the most important result in this section is Theo-

rem 2.3, which generalizes Theorem 1.2 "almost" maximally. We close this section with Theorem 2.4 showing that, generically, when the number of Darboux points is not maximal, then the potential is not integrable.

An analysis of integrability of homogeneous polynomial potentials of degree four given in Sec. III, starts from distinguishing cases when there are no Darboux points, when there is a multiple or exactly one Darboux point. In all these cases the potential depends on parameters and either Theorem 1.1 or our Theorem 1.2 is not applicable. In Sec. III B we give a list of all potentials satisfying the necessary conditions of Theorems 1.1 and 1.2. It contains only nine potentials. Three of them are known integrable potentials. The remaining ones are not integrable as we show in Sec. III C using the higher order variational equations. We also prove that potentials without Darboux points and those with a multiple Darboux point are not integrable. The only case when our investigation of the integrability is not performed until the end is a discrete but infinite family of potentials with one simple Darboux point. We were able to show only that a finite number of potentials from this family is not integrable.

In the Appendices, to make the paper self-contained, we give formulation of basic theoretical facts about differential Galois approach to the integrability.

II. TWO DEGREES OF FREEDOM

A. Preliminaries

As we already mentioned, a Darboux point can be considered as a point in a projective space. For $n=2$ it is $\mathbb{CP}^1$. This is why it is convenient to consider coordinates $(q_1,q_2)\in\mathbb{C}^2$ as the homogeneous coordinates $[q_1:q_2]$ on $\mathbb{CP}^1$. We identify the affine part of $\mathbb{CP}^1$ with points $[1:q_2]\in\mathbb{CP}^1$ and we parametrize it by coordinate $z=q_2/q_1$, $q_1\neq 0$. The other coordinate $\zeta=q_1/q_2$ is used to parametrize points in a neighborhood of infinity.

A linear transformation $\boldsymbol{q}\mapsto A\boldsymbol{q}$, $A\in\mathrm{PO}(2,\mathbb{C})$, induces an action of $\mathrm{PO}(2,\mathbb{C})$ on $\mathbb{CP}^1$ defined in the following way. For $A\in\mathrm{PO}(2,\mathbb{C})$ given by

$$A=\begin{bmatrix} a & b \\ -b & a \end{bmatrix}, \quad a^2+b^2\neq 0, \tag{2.1}$$

we have $\tau_A:\mathbb{CP}^1\to\mathbb{CP}^1$ given by

$$\tau_A([q_1:q_2])=[aq_1+bq_2:-bq_1+aq_2].$$

Thus, in the affine part of $\mathbb{CP}^1$ this action is

$$\tau_A(z)=\frac{az-b}{bz+a}, \tag{2.2}$$

and the image of the line at infinity $[0:q_2]$ is $\tau_A(\infty)=a/b$.

The group of matrices (2.1) forms a proper subgroup $\mathrm{PO}(2,\mathbb{C})^\circ$ of $\mathrm{PO}(2,\mathbb{C})$. It is the identity component of $\mathrm{PO}(2,\mathbb{C})$. Group $\mathrm{PO}(2,\mathbb{C})$ also contains a diagonal subgroup D_a which consists of matrices $A=\mathrm{diag}(a,-a)$, $a\in\mathbb{C}^\star$. For $A\in\mathrm{D}_a$ we have $\tau_A(z)=-z$, and $\tau_A(\infty)=\infty$. It is easy to check that $\tau_A\circ\tau_{A^T}=id$.

The following two propositions characterize the basic properties of the above-defined Möbius action. The easy proofs of them we left to the reader.

Proposition 2.1: If for $p\in\mathbb{CP}^1$ *we have* $\tau_A(p)=p$ *for all* $A\in\mathrm{PO}(2,\mathbb{C})^\circ$, *then* $p=[1:\pm i]$.

Proposition 2.2: For $p,\tilde{p}\in\mathbb{CP}^1\setminus\{[1:+i],[1:-i]\}$ *there exists* $A\in\mathrm{PO}(2,\mathbb{C})$ *such that* $\tilde{p}=\tau_A(p)$.

Let $V\in\mathbb{C}[q_1,q_2]$ be a homogeneous polynomial of degree $k>0$. We have

$$V(q_1,q_2)=q_1^kV(1,q_2/q_1)=q_2^kV(q_1/q_2,1),$$

and we define $v(z):=V(1,z)$ and $w(\zeta):=V(\zeta,1)$. Obviously v and w are nonzero polynomials of degree not greater than k. Moreover, we have

$$w(\zeta) = \zeta^k v(1/\zeta). \tag{2.3}$$

Hence if we write

$$v(z) = \sum_{i=0}^{k} v_{k-i} z^i, \tag{2.4}$$

then

$$w(\zeta) = \sum_{i=0}^{k} v_i \zeta^i. \tag{2.5}$$

If V_A is equivalent to V, i.e. $V_A(\boldsymbol{q}) = V(A\boldsymbol{q})$ for some $A \in \mathrm{PO}(2,\mathbb{C})^\circ$, then $v_A(z) := V_A(1,z)$ is given by

$$v_A(z) = (a + bz)^k v(\tau_A(z)), \tag{2.6}$$

and similarly, $w_A(\zeta) := V_A(\zeta, 1)$ has the form

$$w_A(\zeta) = (-b\zeta + a)^k w(\tau_{A^T}(\zeta)). \tag{2.7}$$

Simple calculations show the following.

Proposition 2.3: If $z_\star$ is a root of polynomial v, then $\tau_{A^T}(z_\star)$ is a root of polynomial v_A. If $\zeta_\star$ is a root of polynomial w, then $\tau_A(\zeta_\star)$ is a root of polynomial w_A.

By the above-mentioned property and Proposition 2.2 we can choose among all equivalent potentials such a representative V, for which polynomial v (or w) has one root in an arbitrary point of $\mathbb{CP}^1 \setminus \{[1:+i],[1:-i]\}$. This is always possible except for cases when all linear factors of V have the form $(q_2 \pm iq_1)$, i.e., when potential V has the following form:

$$V_{k,l} = \alpha(q_2 - iq_1)^l (q_2 + iq_1)^{k-l}, \quad l = 0, \ldots, k, \quad \alpha \in \mathbb{C}^\star. \tag{2.8}$$

We called the above potentials exceptional.

To prove some general statements it is convenient to assume that for a given potential V we can find an equivalent one V_A such that it contains monomial $q_1 q_2^{k-1}$ with a nonzero coefficient.

Lemma 2.1: Assume that $V \neq V_{l,l}$. If for all potentials V_A equivalent to V coefficient of monomial $q_1 q_2^{k-1}$ vanishes, then $V = 0$.

Proof: For a given V of degree k the coefficient of monomial $q_1 q_2^{k-1}$ is equal to v_1 in (2.4). From (2.5) it follows that $v_i = w'(0)$. Let us assume that for all $A \in \mathrm{PO}(2,\mathbb{C})^\circ$ we have $w_A'(0) = 0$. Then from (2.5) and (2.7) we obtain

$$w_A(\zeta) = a^k \sum_{i=0}^{k} v_i (\zeta + x)^i (1 - x\zeta)^{k-i}, \tag{2.9}$$

where $x = b/a$. Thus

$$w_A'(0) = a^k \sum_{i=0}^{k} v_i (i x^{i-1} - (k-i)x^{i+1}) = a^k \sum_{j=0}^{k} [(j+1)v_{j+1} - (k-j+1)v_{j-1}] x^j, \tag{2.10}$$

where we assumed that $v_{-1} = v_{k+1} = 0$. The above expression vanishes for all $x \neq \pm i$, hence it vanishes for all x. This implies that

$$(j+1)v_{j+1} - (k-j+1)v_{j-1} = 0 \quad \text{for } j = 0, \ldots, k.$$

Putting $\boldsymbol{v} = [v_0, \ldots, v_k]^T$, we rewrite the above-noted equation in the form

$$M\boldsymbol{v} = \boldsymbol{0}, \quad \boldsymbol{v} = [v_0, \ldots, v_k]^T, \tag{2.11}$$

where $(k+1)\times(k+1)$ matrix M has the form

$$M = \begin{bmatrix} 0 & -1 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 \\ k & 0 & -2 & 0 & 0 & \ldots & 0 & 0 & 0 \\ 0 & k-1 & 0 & -3 & 0 & \ldots & 0 & 0 & 0 \\ 0 & 0 & k-2 & 0 & -4 & \ldots & 0 & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & 0 & 0 & \ldots & -(k-2) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ldots & 0 & -(k-1) & 0 \\ 0 & 0 & 0 & 0 & 0 & \ldots & 2 & 0 & -k \\ 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 1 & 0 \end{bmatrix}. \tag{2.12}$$

Its determinant is given by

$$\det M = \begin{cases} (k!!)^2 & \text{for odd } k \\ 0 & \text{otherwise.} \end{cases}$$

The above finishes the proof for odd k. When $k=2l$ for some $l \in \mathbb{N}$, then, as it is easy to show, the rank of matrix M is k. Hence, it has a one-dimensional kernel. This kernel is spanned by vector $\boldsymbol{v}^r = [v_0^r, \ldots, v_{2l}^r]^T$, where

$$v_{2i+1}^r = 0, \quad v_{2i}^r = \binom{l}{i}, \quad \text{for } i = 0, \ldots, l.$$

To finish the proof it is enough to notice that

$$(1+z^2)^{2l} = \sum_{i=0}^{2l} v_i^r z^i.$$

□

As it is well known a homogeneous polynomial $V \in \mathbb{C}^2[q_1, q_2]$ of degree k can be written uniquely as a product of linear forms

$$V = \prod_{i=1}^{k} (\alpha_i q_1 + \beta_i q_2), \tag{2.13}$$

where

$$|\alpha_i| + |\beta_i| \neq 0 \quad \text{for } i = 1, \ldots, k.$$

Thus, for $A \in \mathrm{PO}(2, \mathbb{C})$ we have

$$V_A = \prod_{i=1}^{k} (\alpha_i' q_1 + \beta_i' q_2), \tag{2.14}$$

where

$$[\alpha_i', \beta_i'] = [\alpha_i, \beta_i]A \quad \text{for } i = 1, \ldots, k.$$

If $\alpha_i^2 + \beta_i^2 = 0$ for $i = 1, \ldots, k$, then $V = V_{k,l}$ for some $l \in \{0, \ldots, k\}$. Assume that $V \neq V_{k,l}$. Then for some $i_0 \in \{0, \ldots, k\}$, we have $\alpha_{i_0}^2 + \beta_{i_0}^2 \neq 0$, and we can find $A \in \mathrm{PO}(2, \mathbb{C})$ such that $\beta_{i_0}' = 0$ or $\alpha_{i_0}' = 0$.

Proposition 2.4: Assume that a homogeneous potential of degree k is not exceptional, then it is equivalent to $V = q_1 \widetilde{V}$, *where* $\widetilde{V}$ *is a homogeneous polynomial of degree* $k-1$.

The above observation was made by Hietarinta in Ref. 16. The above proposition shows that we can assume that $v_k = 0$ in (2.4) if the potential is not exceptional. Additionally, a nonzero coefficient of the potential can be normalized to one, so an equivalent class of potentials depends at most on $k-1$ parameters.

In the literature concerning searches for integrable potentials it is customary to assume that we can always normalize a homogeneous potential in such a way that the coefficient of monomial $q_1 q_2^{k-1}$ vanishes, see, e.g., Ref. 37. But, generally this claim is wrong even if we exclude the exceptional potentials, see Ref. 11.

Remark 2.1: As it was shown in Ref. 16, exceptional potentials $V_{k,0}$, $V_{0,k}$, $V_{k-1,1}$, $V_{1,k-1}$, *and* $V_{k,k}$ *are integrable for all k. Nothing is known about the integrability of the remaining exceptional potentials.*

B. Darboux points

It is convenient to introduce the following auxiliary system:

$$\dot{q}_1 = -\gamma q_1 + \frac{\partial V}{\partial q_1}, \quad \dot{q}_2 = -\gamma q_2 + \frac{\partial V}{\partial q_2}, \quad \gamma \in \mathbb{C}^\star. \tag{2.15}$$

The Jacobian matrix of the right-hand sides of the above-noted system is

$$J(\boldsymbol{q}) = V''(\boldsymbol{q}) - \gamma E. \tag{2.16}$$

A Darboux point of potential V is a nonzero equilibrium of system (2.15). Moreover, if $\boldsymbol{d}$ is an equilibrium of (2.15), then the matrix of linearizations of (2.15) at $\boldsymbol{d}$ is

$$J(\boldsymbol{d}) = V''(\boldsymbol{d}) - \gamma E.$$

Hence, if $(\lambda\gamma, \gamma(k-1))$ are the eigenvalues of $V''(\boldsymbol{d})$, then the eigenvalues of $J(\boldsymbol{d})$ are $(\gamma\Lambda, \gamma(k-2))$, where $\Lambda = \lambda - 1$. Notice that

$$\Lambda = \frac{1}{\gamma}\mathrm{Tr}\, V''(\boldsymbol{d}) - k = \frac{1}{\gamma}\mathrm{Tr}\, J(\boldsymbol{d}) - (k-2). \tag{2.17}$$

We show that this quantity does not depend on a representative of the Darboux point and hence it is a well-defined function of a Darboux point. In fact, let $\boldsymbol{d}$ and $\widetilde{\boldsymbol{d}}$ represent the same Darboux point, i.e., $\boldsymbol{d} = \alpha\widetilde{\boldsymbol{d}}$ for some $\alpha \in \mathbb{C}^\star$. Thus we have

$$V'(\boldsymbol{d}) = \gamma\boldsymbol{d}, \quad V'(\widetilde{\boldsymbol{d}}) = \widetilde{\gamma}\widetilde{\boldsymbol{d}}, \quad \text{where } \widetilde{\gamma} = \frac{\gamma}{\alpha^{k-2}}.$$

As a consequence

$$\Lambda = \frac{1}{\gamma}\mathrm{Tr}\, V''(\boldsymbol{d}) - k = \frac{\alpha^{k-2}}{\gamma}\mathrm{Tr}\, V''(\widetilde{\boldsymbol{d}}) - k = \frac{1}{\widetilde{\gamma}}\mathrm{Tr}\, V''(\widetilde{\boldsymbol{d}}) - k.$$

Let us introduce new coordinates $x = q_1$ and $z = q_2/q_1$. In new variables Eq. (2.15) has the form

$$\dot{x} = -\gamma x + x^{k-1}h(z), \quad \dot{z} = x^{k-2}g(z), \tag{2.18}$$

where

$$h(z) = kv(z) - zv'(z), \quad g(z) = (1+z^2)v'(z) - kzv(z), \tag{2.19}$$
$$v(z) = V(1,z) = \sum_{i=0}^{k} v_{k-i}z^i.$$

Notice that $\deg g \leqslant k$ and $\deg h \leqslant k-1$. To express the coefficients of polynomials h and g in terms of coefficients of v, let us write

$$g(z) = \sum_{i=0}^{k} g_{k-i}z^i, \quad h(z) = \sum_{i=0}^{k-1} h_{k-1-i}z^i. \tag{2.20}$$

Then, from the definition of polynomials g and h we obtain

$$g_j = -(j+1)v_{j+1} + (k-j+1)v_{j-1}, \quad j = 0, \ldots, k, \tag{2.21}$$

and

$$h_j = (j+1)v_{j+1}, \quad j = 0, \ldots, k-1, \tag{2.22}$$

where we assumed that $v_{-1} = v_{k+1} = 0$. From the above it follows that $g_0 = -v_1$, and $h_0 = v_1$.

A direct inspection of the highest order terms of the right-hand sides of the definitions of g and h shows the following.

Proposition 2.5: Let us denote $l = \deg v$. *If* $l < k$, *then* $\deg g = l+1$ *and* $\deg h = l$. *If* $l = k$, *then* $\deg g \leqslant k$ *and* $\deg h \leqslant k-1$. *Moreover, if* $v_1 \neq 0$, *then* $\deg g = k$ *and* $\deg h = k-1$.

Proposition 2.6: If V is a homogeneous potential of degree k and $V \neq V_{l,l}$ *when* $k = 2l$, *then the number of Darboux points is finite and it is at most k.*

Proof: Darboux points $[q_1 : q_2]$ with $q_1 \neq 0$ are given by solutions (x,z), $x \neq 0$ of the following system:

$$x^{k-2}h(z) = \gamma, \quad x^{k-2}g(z) = 0. \tag{2.23}$$

Hence, their z coordinates are roots of $g(z)$. Thus their number is finite provided that $g \neq 0$. If $g = 0$, then solving differential equation (2.19) we find that $v(z) = \alpha(1+z^2)^{k/2}$, i.e., $V = \alpha(q_1^2 + q_2^2)^{k/2}$.

Let us note that we can always assume that for all Darboux points $q_1 \neq 0$. In fact, if $[0 : d_2]$, $d_2 \neq 0$, is a Darboux point, then

$$\frac{\partial V}{\partial q_1}(0, d_2) = v_1 d_2^{k-1} = 0.$$

But from Lemma 2.1 it follows that we can always assume that $v_1 \neq 0$. Hence, $d_2 = 0$. We have a contradiction.

By Proposition 2.5 the highest possible degree of g is k, and this is why the number of Darboux points cannot be greater than k. □

Corollary 2.1: For a generic homogeneous potential of degree k there exist k Darboux points.

It is important to underline that not all roots of $g(z)$ are Darboux points. Note that it can happen that $g(z)$ and $h(z)$ have a common root $z_\star$, and then for this $z = z_\star$ system (2.23) has no solution.

Proposition 2.7: Polynomials $g(z)$ *and* $h(z)$ *have a common root* $z_\star$ *if and only if* $z_\star$ *is a multiple root of* $v(z)$.

Proof: If $z_\star$ is a multiple root of $v(z)$, then $v(z_\star) = v'(z_\star) = 0$, and from (2.19) it follows that $g(z_\star) = h(z_\star) = 0$.

From (2.19) we have $zh(z)+g(z)=v'(z)$. Thus if $g(z_\star)=h(z_\star)=0$, then $v'(z_\star)=0$, but this, together with $h(z_\star)=0$, implies that $v(z_\star)=0$. Hence, $z_\star$ is a multiple root of $v(z)$. □

Now we want to check if there exists at least one Darboux point for a given potential. To this end it is important to know a relation between the multiplicities of common roots of polynomials v and g.

For a polynomial $p\in\mathbb{C}[z]$ by $\mathrm{mult}(p,z_\star)$ we denote the multiplicity of $p(z)$ at $z=z_\star$.

Let us assume that $v(z)=(z-z_\star)^l\tilde{v}(z)$ where $l\geqslant 1$ and $\tilde{v}(z_\star)\neq 0$. Then from the definition of g we obtain

$$g(z)=(z-z_\star)^{l-1}\{(1+z^2)[l\tilde{v}(z)+(z-z_\star)\tilde{v}'(z)]-kz(z-z_\star)\tilde{v}(z)\}. \tag{2.24}$$

Thus, $g(z)$ is divisible by $(z-z_\star)^{l-1}$. We have $g(z)=(z-z_\star)^{l-1}\tilde{g}(z)$ where

$$\tilde{g}(z)=(1+z^2)[l\tilde{v}(z)+(z-z_\star)\tilde{v}'(z)]-kz(z-z_\star)\tilde{v}(z).$$

This implies that

$$\tilde{g}(z_\star)=l(1+z_\star^2)\tilde{v}(z_\star).$$

But $\tilde{v}(z_\star)\neq 0$, hence, if $z_\star\neq\pm i$ we have $\tilde{g}(z_\star)\neq 0$, and the multiplicity of $z_\star$ as a root of g is $l-1$. Hence, we conclude with the following.

Proposition 2.8: Assume that $z_\star\neq\pm i$ *and* $l=\mathrm{mult}(v,z_\star)\geqslant 1$, *then* $\mathrm{mult}(g,z_\star)=l-1$.

Let $z_\star=i$, then instead of (2.24) we obtain

$$g(z)=(z-i)^l[l(z+i)\tilde{v}(z)+(1+z^2)\tilde{v}'(z)-kz\tilde{v}(z)]. \tag{2.25}$$

Thus $g(z)$ is divisible by $(z-i)^l$, so $g(z)=(z-i)^l\tilde{g}(z)$ where

$$\tilde{g}(z)=l(z+i)\tilde{v}(z)+(1+z^2)\tilde{v}'(z)-kz\tilde{v}(z). \tag{2.26}$$

Hence we have

$$\tilde{g}(i)=(2l-k)i\tilde{v}(i). \tag{2.27}$$

As we obtain similar relations for $z_\star=-i$, we can formulate the following proposition.

Proposition 2.9: Assume that $l=\mathrm{mult}(v,z_\star)\geqslant 1$ *for* $z_\star=\pm i$. *If* $2l=k$, *then* $\mathrm{mult}(g,z_\star)>l$ *else* $\mathrm{mult}(g,z_\star)=l$.

Applying a similar reasoning it is easy to prove the following proposition.

Proposition 2.10: If $l=\mathrm{mult}(v,z_\star)\geqslant 1$, *then* $\mathrm{mult}(h,z_\star)=l-1$.

Now, we are ready to characterize potentials without Darboux points more precisely.

Lemma 2.2: If potential V *of degree* $k>2$ *does not have Darboux points, then all its linear factors are multiple. Moreover,* $V=V_{k,l}$ *for some* $l=2,\ldots,k-1$, *except for the case when* $k=2l$ *and* V *has a factor* $(q_2\pm iq_1)$ *with multiplicity* l.

Proof: By Proposition 2.7, if potential V has no Darboux points, then all roots of polynomial v are multiple and all of them are roots of polynomials g and h. Moreover, the only roots of g are those of v.

We have to prove only the second part of the proposition. By Lemma 2.1 we can assume that $v_1\neq 0$, and hence $\deg v=k-1$ or $\deg v=k$. Moreover, under this assumption $\deg g=k$, see Proposition 2.5. Polynomial v can be written in the form

$$v=\alpha\prod_{i=1}^{s}(z-z_i)^{l_i},\quad \sum_{i=1}^{s}l_i=m\in\{k-1,k\},$$

where integers $l_i>1$, for $i=1,\ldots,s$. By assumption, the only roots of g are z_i, so we can write it in the following form:

$$g = \beta \prod_{i=1}^{s} (z - z_i)^{n_i}, \quad \sum_{i=1}^{s} n_i = k,$$

where integers $n_i > 0$ for $i = 1, \ldots, s$. If $z_i \neq i$, then, by Proposition 2.8, $n_i = l_i - 1$, and we have

$$k = \sum_{i=1}^{s} n_i = \sum_{i=1}^{s} l_i - s = m - s,$$

and this is only possible when $s = 0$. Hence, among z_i we must have one or two equal to $\pm i$. Let us put $z_{s-1} = i$ and $z_s = -i$. For even k we assume that $l_{s-1} \neq k/2$ and $l_{s-1} \neq k/2$. Then, by Proposition 2.9, we have $n_{s-1} = l_{s-1}$ and $n_s = l_s$. Thus we obtain

$$k = \sum_{i=1}^{s} n_i = \sum_{i=1}^{s} l_i - (s - 2) = m + 2 - s.$$

So, $k - m = 2 - s \geqslant 0$, and hence there are at most two roots of v which are $\pm i$. □

In a case when $\pm i$ is a root of v with multiplicity $k/2$, as two examples in the following show, there exist potentials $V \neq V_{k,l}$ without a Darboux point.

Example 1:

$$V = (q_2 - iq_1)^2 (q_2 - aq_1)^2, \quad a \neq -i, \tag{2.28}$$

then

$$v(z) = (z - i)^2 (z - a)^2, \quad g(z) = 2(a + i)(z - a)(z - i)^3.$$

Thus, in fact, the above potential does not have any Darboux point for an arbitrary $a \neq \mp i$.

Example 2: Potential

$$V = (q_2 - iq_1)^4 (q_2 - aq_1)^2 (q_2 - bq_1)^2$$

has no Darboux points provided $ab = -1$ or $a = b$.

Thus, one parameter families of potentials without Darboux points can appear. This is not incidental—it can be proved that potentials of even degree k with factor $(q_2 \pm iq_1)^{k/2}$ and without Darboux points form at most one parameter families.

To determine the position of Darboux points for a given potential of degree $k > 2$ we have to solve a polynomial equation of degree k. Thus it seems that in a general case when $k > 4$ there are no analytical tools to study the integrability by means of Darboux points. We show that it is not like that.

Lemma 2.3: For odd $k > 2$, *the roots of polynomial* g *determine polynomial* v *uniquely up to a multiplicative constant*.

Proof: Without any loss of the generality we can assume that $\deg g = k$. Let z_i for $i = 1, \ldots, k$ be roots of g. To prove our lemma, we need to show that coefficients of polynomial v are uniquely determined by coefficients of polynomial g. For an arbitrary k we have relation (2.21) which can be rewritten as a system of linear equations

$$\boldsymbol{g} = M\boldsymbol{v}, \quad \boldsymbol{g}^T = [g_0, \ldots, g_k], \quad \boldsymbol{v}^T = [v_0, \ldots, v_k],$$

where matrix M is given by (2.12). As we know that for odd k $\det M \neq 0$, this finishes the proof.□

Corollary 2.2: For odd degree k, *the positions of* k *Darboux points of a potential determine this potential uniquely up to a multiplicative constant.*

For even k the rank of matrix M is k. Hence, for even k we have one parameter families of potentials having the same Darboux points. The reason for this fact is obvious if we notice that at a Darboux point the gradient of the potential is parallel to the radius vector. Hence, for even k potential V and $V + \alpha(q_1^2 + q_2^2)^{k/2}$ have the same Darboux points.

C. Necessary conditions for integrability

Now, we want to define a function $\Lambda:\mathbb{CP}^1\to\mathbb{C}$ which for a Darboux point with coordinate z gives $\Lambda(z)$—the eigenvalue defined by (2.17) for this point.

The Jacobian matrix of the right-hand sides of (2.18) has the form

$$J=\begin{bmatrix} -\gamma+(k-1)x^{k-2}h(z) & x^{k-1}h'(z) \\ (k-2)x^{k-3}g(z) & x^{k-2}g'(z) \end{bmatrix}, \tag{2.29}$$

hence

$$\frac{1}{\gamma}\mathrm{Tr}\,J-(k-2)=(1-k)\gamma+x^{k-2}[(k-1)h(z)+g'(z)].$$

The above quantity, when evaluated at a Darboux point, is equal to the eigenvalue defined by (2.17). To eliminate x from the above expression we notice that at a Darboux point we have

$$x^{k-2}=\frac{\gamma}{h(z)}.$$

The above considerations lead to the following definition of $\Lambda(z)$:

$$\Lambda(z)=\frac{g'(z)}{h(z)}. \tag{2.30}$$

Notice that if $z_\star$ is a multiple Darboux point, then $\Lambda(z_\star)=0$.

On the projective line $\mathbb{CP}^1$, where Darboux points are located, we define a meromorphic differential form ω which in coordinate z is given by

$$\omega=\frac{h(z)}{g(z)}\mathrm{d}z, \tag{2.31}$$

and in coordinate $\zeta=1/z$ by

$$\omega=-\frac{h(1/\zeta)}{g(1/\zeta)}\frac{\mathrm{d}\zeta}{\zeta^2}. \tag{2.32}$$

Let us denote by $\hat{\mathcal{V}}_{k,l}$ a set of homogeneous potentials of degree k which satisfy the following conditions:

C1: potential $V\in\hat{\mathcal{V}}_{k,l}$ has $0<l\leqslant k$ simple Darboux points, and

C2: if $(\pm iq_1+q_2)$ is a linear factor of V, then it has multiplicity 1.

We prove the following.

Theorem 2.1: *For $V\in\hat{\mathcal{V}}_{k,l}$ the following relation holds true:*

$$\sum_{i=1}^{l}\frac{1}{\Lambda_i}=-1. \tag{2.33}$$

Proof: For a given potential $V\in\hat{\mathcal{V}}_{k,l}$ we choose such a representative that $v_1\neq 0$. Then all its Darboux points are located in the affine part of $\mathbb{CP}^1$, and $\deg g=k$ and $\deg h=k-1$. Let z_i, for $i=1,\ldots,k$, denote roots of polynomial g. First we consider the case $l=k$. By assumption all roots of g are simple and, moreover, polynomials g and h are relatively prime. We put $\Lambda_i=\Lambda(z_i)$ for $i=1,\ldots,k$. The residue of ω at z_i for $i=1,\ldots,k$ is given by

$$\operatorname{res}(\omega, z_i) = \frac{h(z_i)}{g'(z_i)} = \frac{1}{\Lambda_i}. \tag{2.34}$$

Moreover, the residue of ω at infinity is

$$\operatorname{res}(\omega, \infty) = -\frac{h_0}{g_0} = 1. \tag{2.35}$$

Thus, by the Residue Theorem[28] we prove the theorem for $l=k$.

If $l<k$ we can assume that first l roots of g are simple and they are the Darboux points, and we put again $\Lambda_i=\Lambda(z_i)$ for $i=1,\ldots,l$. But now polynomials g and h are not relatively prime. Let p be a monic common factor of g and h. Then we can write $g=pg_1$ and $h=ph_1$ where g_1 and h_1 are relatively prime. We show that $\deg p=k-l$. In fact, $h(z_\star)=g(z_\star)=0$ if and only if $z_\star \in \{z_{l+1},\ldots,z_k\}$. By Proposition 2.7 $z_\star$ is also a multiple root of v. It is important to notice that $z_\star \neq \pm i$ by condition C2. So, from Propositions 2.8 and 2.9 we deduce that $\operatorname{mult}(g,z_\star) = \operatorname{mult}(h,z_\star)$. This proves our claim that $\deg p=k-l$.

Thus, we have

$$\omega = \frac{h(z)}{g(z)}\mathrm{d}z = \frac{h_1(z)}{g_1(z)}\mathrm{d}z, \tag{2.36}$$

and all finite poles of this form are Darboux points z_i, $i=1,\ldots,l$. Moreover

$$\frac{1}{\Lambda_i} = \frac{h(z_i)}{g'(z_i)} = \frac{p(z_i)h_1(z_i)}{p'(z_i)g_1(z_i)+p(z_i)g_1'(z_i)} = \frac{h_1(z_i)}{g_1'(z_i)} = \operatorname{res}(\omega, z_i), \tag{2.37}$$

for $i=1,\ldots,l$, and $\operatorname{res}(\omega,\infty)=1$. This finishes the proof. □

For each $V \in \hat{\mathcal{V}}_{k,l}$ we have properly defined a collection $\mathbf{\Lambda}_V=\{\Lambda_1,\ldots,\Lambda_l\}$. Let $\mathcal{L}_{k,l}$ denote a set of all $\mathbf{\Lambda}_V$, for $V \in \hat{\mathcal{V}}_{k,l}$, and $\mathcal{I}_{k,l}$ a set of those elements of $\mathcal{L}_{k,l}$ which correspond to the integrable potentials. Our main result in this section is formulated in the following theorem.

Theorem 2.2: *For all $k>2$ sets $\mathcal{I}_{k,l}$ for $l=1,\ldots,k$ are at most finite.*

Proof: For a potential $V \in \mathcal{V}_{k,l}$ its Darboux points are simple, hence $\Lambda_i \neq 0$ for $i=1,\ldots,l$. Thus, we can introduce quantities $X_i=1/\Lambda_i$. Using them we rewrite (2.33) in the form

$$\sum_{i=1}^{l} X_i = -1. \tag{2.38}$$

If the system is integrable, then, according to Theorem 1.1, each Λ_i belongs to a certain infinite set I_k for $i=1,\ldots,l$. From the list given in the thesis of Theorem 1.1 we deduce that sets I_k have the following properties:

1. $I_k=\{a_n^{(k)} \in \mathbb{Q}\setminus\{0\} \,|\, a_n^{(k)} > -1, n \in \mathbb{N}\}$,
2. for each k the sequence $\{a_n^{(k)}\}$ has only one accumulation point at infinity.

Hence X_i belong to a set $\mathcal{X}_k$ with the properties

1. $\mathcal{X}_k=\{x_n^{(k)} \in \mathbb{Q}\setminus\{0\} \,|\, x_n^{(k)} \in (-\infty,-1)\cup(0,\infty), n \in \mathbb{N}\}$.
2. For each k the sequence $\{x_n^{(k)}\}$ has only one accumulation point at 0. In particular, for each k only a finite number of $x_n^{(k)}$ take negative values not greater than -1.

From relation (2.38) it follows that at least one of X_i is negative. However, if X_i is negative, then it is not greater than -1. Hence, not all of X_i are negative. So assume that X_i for $i=m+1,\ldots,l$ are negative for some $0<m<l$. There is only finitely many choices for $X_{m+1},\ldots,X_l$. For each of them we can rewrite relation (2.38) in the form

$$\sum_{i=1}^{m} X_i = c > 0. \tag{2.39}$$

But by Lemma B.1, the above equation has at most a finite number of solutions $(X_1,\ldots,X_m) \in \mathcal{X}_k^m$. As we have finitely many possibilities for a choice of m, this finishes the proof. □

It is important to remark that these potentials $V \in \mathcal{V}_{k,l}$ for which $\mathbf{\Lambda}_V \in \mathcal{I}_{k,l}$ satisfy only the necessary conditions for integrability of Theorem 1.1 thus, not all of them are integrable.

A natural question appears: what happens when a potential V has a multiple Darboux point? To answer it let us rewrite (2.33) in the following form:

$$\sum_{i=1}^{l} \prod_{\substack{j=1 \\ j\neq i}}^{l} \Lambda_j = -\prod_{j=1}^{l} \Lambda_j. \tag{2.40}$$

Assume now that two Darboux points, let us say z_{l-1} and z_l, coincide, and $h(z_l)\neq 0$. Then, from (2.30), we have immediately that $\Lambda_{l-1}=\Lambda_l=0$. But when Λ_l and Λ_{l-1} tend to 0, then both sides of (2.40) vanish and hence, in such a case, Λ_i for $i=1,\ldots,l-2$ can be arbitrary. Hence, condition C1 imposed on potentials in Theorem 2.1 cannot be weakened.

The following example shows that condition C2 cannot be weakened either.

Example 3: Let

$$V = (q_2 - iq_1)^2(q_2 - aq_1), \quad a \neq \pm i.$$

For this potential we have

$$v = (z-i)^2(z-a), \quad g = (z-i)^2[(a+2i)z + 1 - 2ia], \quad h = -(z-i)[(a+2i)z - 3ia].$$

Thus, if $a\neq -2i$, then $z_\star=(2ia-1)/(a+2i)$ is the only simple Darboux point. It is easy to check that for this point we have $\Lambda(z_\star)=1$. Hence, for the considered potential, relation (2.33) is not valid, but, of course, it is not a counterexample for Theorem 2.1 as $V\notin \hat{\mathcal{V}}_{3,1}$. In fact, one can show that $\hat{\mathcal{V}}_{3,1}=\emptyset$.

The above example shows, among others, the need for a more careful investigation of condition C2.

Assume that potential V of degree k contains a linear factor (q_2-iq_1) with multiplicity $r>1$, $r\neq k/2$, but, if V has also a factor (q_2+iq_1), then its multiplicity is one. Moreover, we assume that V has the maximal number $l=k-r$ of simple Darboux points. For such potential we have

$$v = (z-i)^r \tilde{v}(z),$$

where $\tilde{v}(z)$ has only simple roots. By the results of Sec. II B, we also have

$$g = (z-i)^r \tilde{g}(z), \quad h = (z-i)^{r-1}\tilde{h}(z),$$

where

$$\tilde{g}(z) = [(r-k)z + ir]\tilde{v}(z) + (1+z^2)\tilde{v}'(z),$$

$$\tilde{h}(z) = [(k-r)z - ik]\tilde{v}(z) - z(z-i)\tilde{v}'(z),$$

and polynomials $\tilde{g}(z)$ and $\tilde{h}(z)$ are relatively prime and $h(i)\neq 0$. Hence, we have

$$\omega = \frac{h(z)}{g(z)}\mathrm{d}z = \frac{\widetilde{h}(z)}{g_1(z)}\mathrm{d}z, \quad g_1(z) = (z-i)\widetilde{g}(z).$$

Now, if z_i, for $i=1,\ldots,k-r$, denote the Darboux points, then, by the same arguments as in the proof of Theorem 2.1, we have

$$\mathrm{res}(\omega, z_i) = \frac{1}{\Lambda_i}.$$

But now, differential form ω has one additional simple pole at $z=i$. The residue of ω at this point is equal to

$$\mathrm{res}(\omega, i) = \frac{\widetilde{h}(i)}{g_1'(i)}.$$

But

$$g_1'(z) = \widetilde{g}(z) + (z-i)\widetilde{g}'(z),$$

so

$$g_1(i) = \widetilde{g}(i) = i(2r-k)\widetilde{v}(i).$$

As $\widetilde{h}(i) = -ir\widetilde{v}(i)$, we have

$$\mathrm{res}(\omega, i) = \frac{r}{k-2r}.$$

The residue of ω at infinity is 1, hence, invoking the Residue Theorem, we obtain the following relation:

$$\sum_{i=1}^{l} \frac{1}{\Lambda_i} = -1 - \frac{r}{k-2r}. \tag{2.41}$$

One can notice that in the above reasoning we can drop the assumption that the number of Darboux points is maximal, provided that if V has the factor (q_2+iq_1), then it has multiplicity one.

We can apply formula (2.41) to the potential from Example 3. For $k=3$, $l=1$ and $r=2$ from (2.41) we have $\Lambda_1=1$, i.e., exactly what we obtained by direct calculation.

The above considerations show that we can strengthen considerably our results modifying condition C2. Thus, instead of $\hat{\mathcal{V}}_{k,l}$, we define a bigger class of potentials $\mathcal{V}_{k,l}$. A homogeneous potential V belongs to $\mathcal{V}_{k,l}$ iff it satisfies two conditions:

V1: V has $0<l\leqslant k$ simple Darboux points, and

V2: if $(q_2\pm iq_1)$ is a linear factor of V, then its multiplicity is not $k/2$.

For $x,y\in\mathbb{R}$ we define

$$\theta_{x,y} := \begin{cases} 0 & \text{for } x<y, \\ 1 & \text{for } x\geqslant y. \end{cases}$$

The following theorem is a generalization of Theorem 2.1.

Theorem 2.3: *Let $V\in\mathcal{V}_{k,l}$, and $r_\pm$ be the respective multiplicities of linear factors $(q_2\pm iq_1)$ of V. Then*

$$\sum_{i=1}^{l} \frac{1}{\Lambda_i} = -1 - \theta_{r_+,2}\frac{r_+}{k-2r_+} - \theta_{r_-,2}\frac{r_-}{k-2r_-}. \tag{2.42}$$

Proof: We have already proved this theorem for a case when r_+ or r_- is smaller than 2. Thus

let us assume that $r_\pm \geqslant 2$. Under this assumption, for a potential V, we have

$$v = (z-i)^{r_+}(z+i)^{r_-}\tilde{v}(z),$$

where $\tilde{v}(z)$ is not divisible by $(z \pm i)$. Moreover, we also have

$$g = (z-i)^{r_+}(z+i)^{r_-}\tilde{g}(z), \quad h = (z-i)^{r_+-1}(z+i)^{r_--1}\tilde{h}(z),$$

where

$$\tilde{g}(z) = (z^2+1)\tilde{v}'(z) + [z(r_+ + r_- - k) + i(r_+ - r_-)]\tilde{v}'(z),$$

$$\tilde{h}(z) = [z^2(k - r_+ - r_-) + z(r_- - r_+) + k]\tilde{v}(z) - z(z^2+1)\tilde{v}'(z).$$

Let us assume for simplicity that the number of Darboux points is maximal, i.e., $l = k - r_+ - r_-$. Now, the differential form ω can be written as

$$\omega = \frac{h(z)}{g(z)}\mathrm{d}z = \frac{\tilde{h}(z)}{g_1(z)}\mathrm{d}z, \quad g_1(z) = (z^2+1)\tilde{g}(z),$$

where $\tilde{h}(z)$ and $g_1(z)$ are relatively prime. The only poles ω are all Darboux points z_i, the infinity and $\pm i$. Notice that

$$\tilde{h}(\pm i) = 2r_\pm \tilde{v}(\pm i),$$

and

$$g_1'(\pm i) = \pm 2i\tilde{g}(\pm i) = 2(k - 2r_\pm)v(\pm i).$$

Hence, we have

$$\mathrm{res}(\omega, \pm i) = \frac{r_\pm}{k - r_\pm}.$$

As the residue of ω at a Darboux point z_i is $1/\Lambda_i$, and at infinity it is 1, we have formula (2.42). We analyze a case when the number of Darboux points is smaller than maximal similarly as in the proof of Theorem 2.1. □

For $\mathcal{V}_{k,l}$, we keep the definitions of sets $\mathcal{L}_{k,l}$ and $\mathcal{I}_{k,l}$. An easy modification of the proof of Theorem 2.2 allows one to formulate the following.

Corollary 2.3: The thesis of Theorem 2.2 is valid for classes of potentials $\mathcal{V}_{k,l}$.

It is not difficult to write a general algorithm allowing one to find all elements of sets $\mathcal{I}_{k,l}$. Relation (2.33), or (2.42) gives a strong restriction, and sets $\mathcal{I}_{k,l}$ contain only a few elements. We analyzed case $k=3$ in detail in Ref. 23. As it was shown in that paper set $\mathcal{I}_{3,3}$ contains only four elements

$$\mathcal{I}_{3,3} = \{\{-1,-1,1\}\{-2/3,4,4\},\{-7/8,14,14\},\{-2/3,7/3,14\}\}.$$

For further usage, we determined set $\mathcal{I}_{4,4}$. It has five elements listed in Table I. Moreover, we find that $\mathcal{I}_{4,3} = \mathcal{I}_{4,2} = \emptyset$.

Remark 2.2: One can ask if there exists a relation of the form (2.42) *for a potential of degree $k=2l$ with a factor $(q_2 - iq_1)^l$. For such case we can try to calculate the residue of form ω at $z = i$, however, this residue depends on the coefficients of the potential.*

TABLE I. Elements of set $\mathcal{I}_{4,4}$.

Element	$\{\Lambda_1,\Lambda_2,\Lambda_3,\Lambda_4\}$
1	$\{-1,-1,2,2\}$
2	$\{-5/8,5,5,5\}$
3	$\{-5/8,2,20,20\}$
4	$\{-5/8,27/8,27/8,135\}$
5	$\{-5/8,2,14,35\}$

D. Reconstruction of the potential

When we try to apply the results obtained in Sec. II C for an investigation of potential of a given degree we meet the following problem: how to determine the coefficients of the potential knowing $\{\Lambda_1,\ldots,\Lambda_l,\}\in\mathcal{I}_{k,l}$.

A possible approach to this problem is the following. Let us assume a generic situation: potential V of degree k has the maximal number of simple Darboux points. Let z_i and Λ_i denote their coordinates and eigenvalues, for $i=1,\ldots,k$. Then, points (z_i,Λ_i) are contained in an algebraic subset $\mathcal{D}$ of $\mathbb{C}^2$ defined by zeros of two polynomials $g,f\in\mathbb{C}[z,\Lambda]$:

$$g(z)=0,\quad f(z,\Lambda):=h(z)\Lambda-g'(z)=0. \tag{2.43}$$

If by $I=\langle g,f\rangle$ we denote the ideal in $\mathbb{C}[z,\Lambda]$ generated by g and f, then $\mathcal{D}$ is just an algebraic variety associated with this ideal, i.e., in the algebraic geometry notation $\mathcal{D}=\mathbf{V}(I)$. Under our genericity assumption, the resultant $G=R(g,f,z)\in\mathbb{C}[\Lambda]$ of g and f with respect to z does not vanish, and $\deg G\leqslant k$. Moreover, by the extension theorem, see Ref. 8, Chap. 3, for each root $\Lambda_\star$ of G there exits $z_\star$ such that $(z_\star,\Lambda_\star)\in\mathcal{D}$. On the other hand, if $z_\star$ is a Darboux point and $\Lambda_\star$ the corresponding eigenvalue, then $\Lambda_\star$ is a root of the resultant G. Hence, $\{\Lambda_1,\ldots,\Lambda_k\}$ are roots of the resultant G.

The above observation allows one to investigate the general case when coefficients of polynomial V are unspecified. Again we make the assumption that there exists the maximal number of Darboux points, and without loss of generality we put $v_1=-1$. Then $g,f\in\mathbb{C}[z,\Lambda,v_0,v_2,\ldots,v_k]$, and $\mathcal{D}\subset\mathbb{C}^{k+2}$. The resultant $G=R(g,f,z)$ is an element of $\mathbb{C}[\Lambda,v_0,v_2,\ldots,v_k]$, and $\deg_\Lambda G\leqslant k$, but using the genericity arguments we can assume that $\deg_\Lambda G=k$. If we write

$$G=\sum_{m=0}^{k}G_{k-m}\Lambda^m,$$

where $G_m\in\mathbb{C}[v_0,v_2,\ldots,v_k]$ for $m=0,\ldots,k$, then the basic symmetric polynomials τ_m of $(\Lambda_1,\ldots,\Lambda_k)$ are given by the well-known formulas:

$$\tau_m=(-1)^m\frac{G_m}{G_0}\in\mathbb{C}(v_0,v_2\ldots,v_k),\quad m=1,\ldots,k. \tag{2.44}$$

When $(\Lambda_1,\ldots,\Lambda_k)$ is given, then we have to solve the above equations for unknown $(v_0,v_2,\ldots,v_k)$.

Notice that $(\Lambda_1,\ldots,\Lambda_k)$ is not an arbitrary point in $\mathbb{C}^n$. According to our assumptions, relation (2.33) is satisfied and this implies that $\tau_k=-\tau_{k-1}$, see (2.40). Hence, among all equations (2.44) only $k-1$ are independent. As we have k unknowns, the solutions of these equations generically form one parameter families. But we know that the equivalent potentials have the same eigenvalues. Thus we can choose a representative in each class of equivalent potentials. e.g., fixing the value of one coefficient. Then, solving (2.44) we obtain at most a finite number of solutions.

The above ideas need modifications when the number of Darboux points is smaller than maximal. We do not discuss this question here, but an example of such an analysis is given in the next section.

Theorems 2.1 and 2.3 cannot be applied in a case when the investigated potential has a non-simple Darboux point. Let us describe such potentials.

Proposition 2.11: If a homogeneous potential V has a multiple Darboux point $z_\star \in \mathbb{CP}^1$, then $z_\star \neq \pm i$.

Proof: If i is a Darboux point, then $v(i)=0$, see (2.19). Hence, $v(z)=(z-i)\tilde{v}(z)$, and, moreover, $\tilde{v}(i)\neq 0$, for otherwise i is not a Darboux point. Hence, $\mathrm{mult}(v,i)=1$, and, by Proposition 2.9, $\mathrm{mult}(g,i)=1$, so i is a simple Darboux point. □

By the above proposition, if V has a multiple Darboux point, we can assume that it is located in an arbitrary point of $\mathbb{CP}^1$, except points $\pm i$. If we locate it at $z=0$, then $g(z)$ has a root at this point with multiplicity greater than one and $h(0)\neq 0$. Thus,

$$g_k = v_{k-1} = 0, \quad g_{k-1} = -kv_k + 2v_{k-2} = 0, \quad h_{k-1} = kv_k \neq 0.$$

Hence we can formulate the following proposition.

Proposition 2.12: If a homogeneous potential of degree $k>2$ has a nonsimple Darboux point, then it is equivalent to the following one:

$$V = \sum_{i=1}^{k} v_{k-i} q_1^{k-i} q_2^i, \quad \textit{where} \quad v_{k-1}=0, \quad v_{k-2}=\frac{k}{2}v_k, \quad v_k \neq 0. \tag{2.45}$$

Thus, in the space of all homogeneous potentials of degree k those with a multiple Darboux point are contained in a hyperplane of codimension two.

E. A case when the number of Darboux points is not maximal

If a potential does not have the maximal number of Darboux points, then, as we showed, it has a linear factor $(\alpha q_1+\beta q_2)$ with multiplicity $l>1$. By a generic potential without the maximal number of Darboux points we understand a potential for which $l=2$, i.e., when we have the smallest possible degeneration, and additionally, $\alpha^2+\beta^2\neq 0$. The aim of this section is to show that such potentials are not integrable, or, more precisely, Hamiltonian system (1.2) does not admit an additional *rational* first integral.

If V is a generic potential without the maximal number of Darboux points, then we can assume that it has the form

$$V = q_2^2 \tilde{V}(q_1, q_2), \tag{2.46}$$

where $\deg \tilde{V}=k-2$ and $\tilde{V}(q_1,0)\neq 0$.

Theorem 2.4: *Hamiltonian system* (1.2) *with potential* (2.46) *does not admit an additional rational first integral.*

Proof: Equations of motion have the following form:

$$\begin{aligned} \dot{q}_1 &= p_1, \quad \dot{p}_1 = -q_2^2 \frac{\partial \tilde{V}}{\partial q_1}, \\ \dot{q}_2 &= p_2, \quad \dot{p}_2 = -q_2^2 \frac{\partial \tilde{V}}{\partial q_2} - 2q_2\tilde{V}. \end{aligned} \tag{2.47}$$

Hence, they admit the following particular solution:

$$q_1(t) = At + B, \quad p_1(t) = A, \quad q_2(t) = p_2(t) = 0, \tag{2.48}$$

where $A, B \in \mathbb{C}$. The variational equations for this solution have the form

$$\ddot{x}_1 = 0, \quad \ddot{x}_2 = -2\widetilde{V}(q_1(t),0)x_2, \tag{2.49}$$

and the second one is the normal variational equation. According to our assumption $\widetilde{V}(q_1,0) \neq 0$, we have

$$\widetilde{V}(q_1(t),0) = C(At+B)^{k-2}, \quad C \neq 0. \tag{2.50}$$

We fix $B=0$ and take A such that $2CA^{k-2}=-1$. Then the normal variational equation reads

$$\ddot{x} = t^m x, \quad m = k-2 > 0. \tag{2.51}$$

For this equation the infinity is the only singular point and it is an irregular singularity. We show that for an arbitrary $m>0$ this equation has no Liouvillian solutions, and, hence its differential Galois group is $\mathrm{SL}(2,\mathbb{C})$. To this end we apply the Kovacic algorithm[18] which is formulated for an equation $\ddot{x}=rx$ with an arbitrary rational $r=r(t)$. Three cases are distinguished in this algorithm. For Eq. (2.51) only Case 1 is possible. For an odd m the necessary conditions for the existence of a Liouvillian solution, given in Ref. 18 (Theorem, p. 8) are not satisfied. This proves our claim for odd m. When $m=2l$ is even we have to pass the first step of the algorithm for Case 1. According to it, we have to calculate the following numbers:

$$\alpha_\infty^\pm = \frac{1}{2}\left(\pm\frac{b}{a} - \nu\right), \tag{2.52}$$

where a, b, and ν are defined as follows. Let us expand $\sqrt{r}$ into the Laurent series at infinity, and let

$$[\sqrt{r}]_\infty = at^\nu + \cdots + d,$$

be the indicated part of this series. So, for our case $\nu=l$ and $a=1$. Number b is the coefficient of $t^{\nu-1}$ in $r-[\sqrt{r}]_\infty^2$. Hence in our case $b=0$, and thus $\alpha_\infty^\pm = -l/2 < 0$. But this, according to the next step of the algorithm, implies that the considered equation does not pass the algorithm for Case 1. As it is the only possible case, this proves our claim.

Thus the differential Galois group of the normal variational equation (2.51) is $\mathrm{SL}(2,\mathbb{C})$, so it is not Abelian. By Theorem 4.3 from Ref. 30 this shows that the considered Hamiltonian system does not admit an additional rational first integral. □

III. APPLICATION: INTEGRABLE POTENTIALS OF DEGREE FOUR

When $k=4$ all exceptional potentials are integrable with a polynomial additional first integral. Thus, we exclude them from our consideration. Moreover, according to Ref. 11, those potentials from which we cannot remove monomial $q_1q_2^3$ using a rotation are also integrable. Hence, we can assume that the potential has the form

$$V = \tfrac{1}{4}\widetilde{a}q_1^4 + \tfrac{1}{3}bq_1^3q_2 + \tfrac{1}{2}cq_1^2q_2^2 + \tfrac{1}{4}\widetilde{d}q_2^4 = \tfrac{1}{4}aq_1^4 + \tfrac{1}{3}bq_1^3q_2 + \tfrac{1}{4}dq_2^4 + \tfrac{1}{4}c(q_1^2+q_2^2)^2, \tag{3.1}$$

where

$$\widetilde{a} = a + c, \quad \widetilde{d} = d + c.$$

We put $z=q_2/q_1$. Then polynomial $v(z)=V(1,z)$ has the form

$$v(z) = \tfrac{1}{4}a + \tfrac{1}{3}bz + \tfrac{1}{4}dz^4 + \tfrac{1}{4}c(1+z^2)^2.$$

For this v, polynomials g and h, see (2.19), are the following:

$$g(z) = \tfrac{1}{3}b - az - bz^2 + dz^3, \quad h(z) = a + c + bz + cz^2. \tag{3.2}$$

Notice that if $c+d\neq 0$, then $q_1=0$, $q_2=1/\sqrt{c+d}$ is the only Darboux point with the first coordinate equal to zero. For this point its z coordinate is infinity. We denote $z_0=\infty$. Direct calculations show that for this point we have $\Lambda_0=-d/(c+d)$. Thus z_0 is a multiple Darboux point if $d=0$ and $c\neq 0$.

Our further analysis is divided into three steps. First, we distinguish those parameters' values for which V given by (3.1) does not have any Darboux points or has a multiple Darboux point. When a potential has no Darboux points Theorem 1.1 cannot be applied. When a potential has a multiple Darboux point, then neither Theorem 2.1 nor Theorem 2.3 can be used. It appears that the case when the potential has only one simple Darboux point is very peculiar. In the next step, we distinguish potentials with more than one simple Darboux point such that for them $\{\Lambda_1,\ldots,\Lambda_l\}\in\mathcal{I}_{4,l}$ for $l=2,3,4$. In this way we obtain a list of the distinguished potentials for which the necessary conditions of Theorem 1.1 for the integrability are satisfied. In the last step of our analysis, we apply the higher order variational equations for a study of the integrability of the distinguished potentials. Sections III A–III C correspond to the described steps.

A. Special cases

First, we distinguish potentials (3.1) which do not have Darboux points, as for them Theorem 1.1 is not applicable.

Proposition 3.1: Potential (3.1) *has no Darboux point if and only if it is equivalent to*

$$V_0 = \alpha(q_2 - iq_1)^2 q_2^2, \quad \alpha\in\mathbb{C}^\star. \tag{3.3}$$

Proof: Assume that potential (3.1) has no Darboux point. Then, in particular there is no Darboux point at infinity, so $c=-d$. Then we have

$$v(z) = \tfrac{1}{4}(a-d) + \tfrac{1}{3}bz - \tfrac{1}{2}dz^2.$$

By Lemma 2.2, $v(z)$ must have only multiple factors, so necessarily $d\neq 0$, and

$$2b^2 + 9(a-d)d = 0.$$

Then we can rewrite $v(z)$ in the following form:

$$v(z) = -\frac{1}{2}d(z-z_\star)^2, \quad z_\star = \frac{b}{2d},$$

and this gives

$$g(z) = d(z-z_\star)(z^2 - 2z_\star z - 1).$$

But the only root of g can be $z_\star$, and thus $z_\star=\pm i$. Both choices of $z_\star$ give a potential equivalent to (3.3). □

Our next attempt is to decide whether (3.1) has exactly one simple Darboux point.

Proposition 3.2: Potential (3.20) has exactly one simple Darboux point iff it is equivalent to

$$V_1 = \alpha q_2^4, \quad \alpha\in\mathbb{C}^\star, \tag{3.4}$$

or

$$V_2 = \tfrac{1}{2}\alpha q_1^2(q_1+iq_2)^2 + \tfrac{1}{4}(q_1^2+q_2^2)^2, \quad \alpha\in\mathbb{C}^\star. \tag{3.5}$$

Proof: If $z=\infty$ is the only simple Darboux point of potential (3.1), then $c+d\neq 0$. Moreover, we have $d\neq 0$, for otherwise the infinity is a double Darboux point. Thus $\deg g=3$, and $\deg h\leqslant 2$. None of the roots of g is a Darboux point, so h has at least one root. The only roots of g are those of polynomial h, hence we can write

$$g(z) = d(z - z_1)(z - z_2)^2. \tag{3.6}$$

A comparison with (3.2) gives the following identities:

$$b + 3dz_1z_2^2 = 0, \quad a + dz_2(2z_1 + z_2) = 0, \quad b - d(z_1 + 2z_2) = 0. \tag{3.7}$$

As z_1 and z_2 are roots of h, thus we have two more equations

$$a + c + bz_1 + cz_1^2 = 0, \quad a + c + bz_2 + cz_2^2 = 0. \tag{3.8}$$

Subtracting them we obtain

$$(z_1 - z_2)[b + c(z_1 + z_2)] = 0. \tag{3.9}$$

If $z_1 = z_2$, then from (3.7) we obtain $z_1^3 = z_1$. Thus either $z_1 = z_2 = 0$, or $z_1 = z_2 = \pm i$. In the first case $a = b = c = 0$, so the potential has the form (3.4). In the second case, when $z_1 = z_2 = i$, we have $a = 3d$ and $b = 3id$. As $c + d \neq 0$ we can put $c + d = 1$, and then we obtain potential (3.5). The choice $z_1 = z_2 = -i$ gives a potential equivalent to (3.5).

We show that case $z_1 \neq z_2$ is impossible. Let us assume that $z_1 \neq z_2$. Then, necessarily, $c \neq 0$, and from the fact that z_i are roots h we have

$$b = -c(z_1 + z_2), \quad a + c = cz_1z_2. \tag{3.10}$$

The above equations together with (3.7) form a system of linear homogeneous equations for unknown (a, b, c, d) with the following matrix of coefficients:

$$M = \begin{bmatrix} 0 & 1 & 0 & 3z_1z_2^2 \\ 1 & 0 & 0 & z_2(z_2 + 2z_1) \\ 0 & -1 & 0 & z_1 + 2z_2 \\ 0 & 1 & z_1 + z_2 & 0 \\ 1 & 0 & 1 - z_1z_2 & 0 \end{bmatrix}. \tag{3.11}$$

Let M_l denote lth 4×4 minor of the above matrix (obtained by scratching its l-row). We have

$$-M_1 = z_1 + z_2(2 + z_1^2 + z_1z_2 + z_2^2), \tag{3.12}$$

and

$$-M_3 = 2z_1^2z_2 + z_2^3 + 3z_1^2z_2^3. \tag{3.13}$$

But from Eq. (3.7) it follows that $3z_1z_2^2 = -z_1 - 2z_2$, hence we can rewrite M_3 in the following form:

$$-M_3 = z_2(z_1 - z_2)^2. \tag{3.14}$$

As all minors must vanish, we have immediately that $M_3 = M_1 = 0$ implies that $z_1 = z_2$, and this is a contradiction with our assumption that $z_1 \neq z_2$.

Now, we have to investigate the second possibility when infinity is not a Darboux point. Then we have $c = -d$, and polynomials v, g, and h have the forms

$$\begin{aligned} v(z) &= \tfrac{1}{4}(a - d) + \tfrac{1}{3}bz - \tfrac{1}{2}dz^2, \\ g(z) &= \tfrac{1}{3}b - az - bz^2 + dz^3, \\ h(z) &= (a - d) + bz - dz^2. \end{aligned} \tag{3.15}$$

First let us assume that $d \neq 0$. Then we can write

$$g = d(z - z_1)(z - z_2)(z - z_3).$$

We assume that z_3 is a Darboux point, so $z_2 \neq z_3$ and $z_1 \neq z_3$. Moreover, because z_1 and z_2 are not Darboux points they must be multiple roots of v. Hence, $z_1 = z_2$, and

$$2b^2 + 9(a - d)d = 0, \quad z_1 = \frac{b}{3d}.$$

But then

$$g(z) = d(z - z_1)(z^2 - 2zz_1 - 1), \quad h(z) = -d(z - z_1)(z - 2z_1).$$

However, z_1 must be a double root of g, but this is only possible when $z_1 = \pm i$. This implies that z_1 is the triple root of g and that there is no Darboux point. We have a contradiction, so $d = 0$.

Now, if $b \neq 0$, then deg $g = 2$ but g cannot have two distinct roots. In fact, only one of them can be a Darboux point and the second must be a multiple root of v. As now deg $v = 1$, it is impossible. Hence, g has one double root which is a Darboux point, so it is not a simple Darboux point. This implies that $b = 0$, and hence potential has the form (3.4). □

Let us notice here that potential V_2 does not belong to $\mathcal{V}_{4,1}$ as it has factor $(q_2 - iq_1)^2$.

Theorems 2.1 and 2.3 are not applicable when potential (3.1) has factor $(q_2 \pm iq_1)^2$. However, when $(z \pm i)^2$ is a factor of v, then, by Proposition 2.9, it is a factor of polynomial g with multiplicity at least 3, so the potential has at most one Darboux point. By similar arguments—when $(q_2 \pm iq_1)^3$ is a factor of potential (3.1), then it has at most one Darboux point. Hence, for a case when there exist two or three simple Darboux points we can apply Theorem 2.1.

What remains to be considered is a case when there exists a multiple Darboux point.

Proposition 3.3: Assume that potential (3.1) has a multiple Darboux point. Then it is equivalent to the following one:

$$V_3 = \tfrac{1}{4}aq_1^4 + \tfrac{1}{3}bq_1^3q_2 + \tfrac{1}{4}(q_1^2 + q_2^2)^2. \tag{3.16}$$

Proof: If the infinity is a multiple Darboux point, then, as we already mentioned, $d = 0$ and $c \neq 0$. Hence, in this case the potential is equivalent to (3.16). If a multiple Darboux point is not the infinity, then, by Proposition 2.11, it is different from $\pm i$. Thus, making a proper rotation, we can move it to infinity and then the obtained potential is equivalent to (3.16). □

B. Potentials with more than one simple Darboux point

Let us consider g and $f = h(z)\Lambda - g'(z)$ as polynomials in $\mathbb{C}[z, \Lambda, a, b, c, d]$. The resultant of g and f with respect to z is proportional to polynomial $G \in \mathbb{C}[\Lambda, a, b, c, d]$ which has the following form:

$$G = 3dG_0 - 3cG_0\Lambda + G_2\Lambda^2 + G_3\Lambda^3, \tag{3.17}$$

where

$$G_0 = 4b^4 + 3b^2(a^2 - 3d^2) + 6ad(2a^2 + 3b^2),$$

$$G_2 = -3[b^2 - ac + 3(a + c)d][3acd + 3a^2(c + d) + b^2(4c + 3d)], \tag{3.18}$$

$$G_3 = -3b^4(c + d) + 9(a + c)[cd + a(c + d)]^2 + 2b^2c[9a(c + d) + c(8c + 9d)].$$

It can be checked that G_3 up to a constant factor is the resultant of polynomials g and h with respect to z. Moreover, dG_0 is proportional to the discriminant of polynomial g. Polynomial g has at most three roots which we denote by z_1, z_2, and z_3. If z_i is a Darboux point, then we put $\Lambda_i = \Lambda(z_i)$. Of course Λ_i are roots of polynomial (3.17).

In the generic case, we have four Darboux points, thus necessarily $c+d\neq 0$ and $G_3\neq 0$. Without any loss of the generality we can assume $c+d=1$. All Darboux points are simple if to the above assumption we add $dG_0\neq 0$. As $\Lambda_0=-d$, $c=1-d$, and

$$\Lambda_1\Lambda_2\Lambda_3=-3d\frac{G_0}{G_3},$$

$$\Lambda_1\Lambda_2+\Lambda_2\Lambda_3+\Lambda_3\Lambda_1=-3c\frac{G_0}{G_3}, \tag{3.19}$$

$$\Lambda_1+\Lambda_2+\Lambda_3=-\frac{G_2}{G_3},$$

for given $\{\Lambda_0,\Lambda_1,\Lambda_2,\Lambda_3\}$ we have three equations for two unknowns a, b. Of course these equations are not independent. Solving them we find explicit values of coefficients a, b, c, and d. Note that having an element of $\mathcal{I}_{4,4}$, we have generally four different choices for Λ_0.

Elements of $\mathcal{I}_{4,4}$ are listed in Table I. Using them we solve the respective equations (3.19). Then, we select those solutions which give nonequivalent potentials listed in the following:

$$V_4=\tfrac{1}{4}aq_1^4+q_2^4, \tag{3.20}$$

$$V_5=4q_1^4+3q_1^2q_2^2+\tfrac{1}{4}q_2^4, \tag{3.21}$$

$$V_6=2q_1^4+\tfrac{3}{2}q_1^2q_2^2+\tfrac{1}{4}q_2^4, \tag{3.22}$$

$$V_7=\frac{151-880\sqrt{7}}{124}q_1^4+\frac{-20i}{31}(14+11\sqrt{7})q_1^3q_2+\frac{21}{2}q_1^2q_2^2+\frac{1}{4}q_2^4, \tag{3.23}$$

$$V_8=\tfrac{272}{3}q_1^4+68q_1^2q_2^2+\tfrac{1}{4}q_2^4, \tag{3.24}$$

$$V_9=-\frac{19\,472}{205}q_1^4+i\frac{4608}{41}\sqrt{\frac{446}{215}}q_1^3q_2+68q_1^2q_2^2+\frac{1}{4}q_2^4, \tag{3.25}$$

$$V_{10}=\frac{782\,329}{390\,720}q_1^4+\frac{-247i}{3256}\sqrt{\frac{3}{5}}q_1^3q_2+\frac{3}{2}q_1^2q_2^2+\frac{1}{4}q_2^4, \tag{3.26}$$

$$V_{11}=\frac{663-608\sqrt{86}}{428}q_1^4-\frac{2i}{107}(305+76\sqrt{86})q_1^3q_2+\frac{15}{2}q_1^2q_2^2+\frac{1}{4}q_2^4, \tag{3.27}$$

$$V_{12}=\frac{663+608\sqrt{86}}{428}q_1^4+\frac{2i}{107}(305-76\sqrt{86})q_1^3q_2+\frac{15}{2}q_1^2q_2^2+\frac{1}{4}q_2^4. \tag{3.28}$$

The first and second elements of Table I give potential V_4 and V_5, respectively. Potentials V_6 and V_7 correspond to the third element. The last two elements of Table I give the remaining five potentials. The first two of them correspond to the fourth element in Table I.

As $\mathcal{I}_{4,2}=\mathcal{I}_{4,3}=\emptyset$, the above gives the full list of the distinguished potentials.

C. Integrability of distinguished potentials

Among potentials V_i, $i=0,\ldots,12$ there are integrable ones. Namely, V_1, V_4, V_5, and V_6 are the known integrable potentials, see Refs. 15 and 16. Moreover, potential V_2 is integrable when $\alpha=-2$, see Ref. 11.

Now, our aim is to investigate the integrability of the remaining distinguished potentials. Our main tools are Theorem A.2 and Lemma A.1.

Let us consider potential (3.1) when $c+d\neq 0$. Without loss of the generality we can put $c+d=1$. Then Hamilton's equations of motion have a family of particular solutions associated with the Darboux point whose first coordinate vanishes. These solutions $\varphi(t,e)=(0,q_2(t),0,p_2(t))$ for given energy e are determined by

$$\dot{q}_2(t)^2+\tfrac{1}{2}q_2(t)^4=2e,\quad p_2(t)=\dot{q}_2(t). \tag{3.29}$$

If we put $q_2^2=-2v$, then the above equation transforms into

$$\dot{v}^2=4v^2-g_2v-g_3,\quad g_2=4e,\quad g_3=0. \tag{3.30}$$

Hence, $v=\wp(t)$ is the nondegenerated Weierstrass function with invariants g_2, g_3, provided $e\neq 0$. The variational equations along particular solutions have the following form:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix}\xi_1\\ \xi_2\\ \xi_3\\ \xi_4\end{bmatrix}=\begin{bmatrix}0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ 2c\wp(t) & 0 & 0 & 0\\ 0 & 6\wp(t) & 0 & 0\end{bmatrix}\begin{bmatrix}\xi_1\\ \xi_2\\ \xi_3\\ \xi_4\end{bmatrix}. \tag{3.31}$$

Notice that the above variational equations are equivalent to the direct product of two Lamé equations

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\xi_i=n_i(n_i+1)\wp(t)\xi_i,\quad i=1,2, \tag{3.32}$$

where $n_2=2$ and $n_1(n_1+1)=2c$. Now let us assume that $n_1\in\mathbb{Z}\setminus\{-1,0\}$. Under this assumption, for both equations we have the Lamé-Hermite case (see Appendix A 3). Hence, the differential Galois group of variational equations (3.31) is Abelian, and the necessary integrability conditions of Theorem 1 are fulfilled for arbitrary $a,b\in\mathbb{C}$. To prove the nonintegrability of the system for such cases we apply the higher order variational equations, see Appendix A 2. Because of the form of first-order variational equations investigation of the differential Galois group of higher order variational equations reduces to a local analysis, see Lemma A.1 in Appendix A 3.

Thus, for further calculations, we need the explicit form of nonhomogeneous terms in higher order variational equations (A4). The first of them is

$$\boldsymbol{f}_2=-q_2(t)[0,0,\xi_1^{(1)}(b\xi_1^{(1)}+2c\xi_2^{(1)}),c(\xi_1^{(1)})^2+3(\xi_2^{(1)})^2]^T, \tag{3.33}$$

where $\xi_i^{(1)}\equiv\xi_i$ for $i=1,\ldots,4$. The fundamental matrix $\boldsymbol{X}(t)$ of the homogeneous system (3.31) has the following form:

$$\boldsymbol{X}(t)=\begin{bmatrix}x_1(t) & x_2(t) & 0 & 0\\ 0 & 0 & y_1(t) & y_2(t)\\ \dot{x}_1(t) & \dot{x}_2(t) & 0 & 0\\ 0 & 0 & \dot{y}_1(t) & \dot{y}_2(t)\end{bmatrix}. \tag{3.34}$$

Here $x_1(t)$ and $x_2(t)$ are linearly independent solutions of Eq. (3.32) with $i=1$ chosen in such a way that $x_1(t)\dot{x}_2(t)-x_2(t)\dot{x}_1(t)=1$; similarly, $y_1(t)$ and $y_2(t)$ are linearly independent solutions of Eq. (3.32) with $i=2$ chosen in such a way that $y_1(t)\dot{y}_2(t)-y_2(t)\dot{y}_1(t)=1$. Thus, the inverse of $\mathbf{X}(t)$ is the following:

$$\boldsymbol{X}^{-1}(t)=\begin{bmatrix} \dot{x}_2(t) & 0 & -x_2(t) & 0 \\ -\dot{x}_1(t) & 0 & x_1(t) & 0 \\ 0 & -\dot{y}_2(t) & 0 & y_2(t) \\ 0 & \dot{y}_1(t) & 0 & -y_1(t) \end{bmatrix}. \tag{3.35}$$

In a neighborhood of $t=0$ solutions $x_1(t)$ and $x_2(t)$ have the following expansions:

$$\begin{aligned} x_1(t)&=t^{n_1+1}\left(1+\frac{n_1(n_1+1)g_2}{80(2n_1+5)}t^4+\cdots\right), \\ x_2(t)&=t^{-n_1}\left(-\frac{1}{2n_1+1}+\frac{n_1(n_1+1)g_2}{80(2n_1+1)(2n_1-3)}t^4+\cdots\right), \end{aligned} \tag{3.36}$$

where dots denote the higher order terms with respect to t. Expansions for $y_1(t)$ and $y_2(t)$ have form (3.36) with $n_1=2$. Furthermore, expansion of $q_2(t)$ is the following:

$$q_2(t)=\frac{i}{\sqrt{2}}\left(\frac{2}{t}+\frac{g_2}{20}t^3+\cdots\right). \tag{3.37}$$

According to Lemma A.1, to prove that the investigated potential is not integrable, we have to show that a logarithmic term in a local solution of the second variational equation appears. To this end, it is enough to show that at least one component of $\boldsymbol{\mu}^{(2)}=\mathbf{X}^{-1}(t)\boldsymbol{f}_2$ has a first-order pole at $t=0$, see formulas (A5) and (A6). In all further calculations we take

$$\boldsymbol{\xi}^{(1)}=[x_2(t),0,\dot{x}_2(t),0]^T.$$

Then, the first two components of $\boldsymbol{\mu}^{(2)}$ are

$$\mu_1^{(2)}=bq_2(t)x_2(t)^3, \quad \mu_2^{(2)}=-bq_2(t)x_1(t)x_2(t)^2. \tag{3.38}$$

Now, we are ready to prove the following.

Lemma 3.1: Potential (3.16) is integrable if and only if $a=b=0$.

Proof: For potential (3.16) $n_1=1$, so

$$x_1(t)=t^2+\cdots, \quad x_2(t)=-\tfrac{1}{3}t^{-1}+\cdots,$$

where dots denote the higher order terms with respect to t. Hence, from (3.38), we obtain

$$\mu_2^{(2)}=-ib\frac{\sqrt{2}}{9t}+\cdots.$$

Thus, by Lemma A.1 if $b\neq 0$, then potential (3.16) is not integrable.

Assume that $b=0$, and continue our calculations up to the third order. Solutions of the second-order variational equations have the form

$$\boldsymbol{\xi}^{(2)}=[0,z(t),0,\dot{z}(t)]^T, \quad z(t)=\frac{i\sqrt{2}}{36t}+\cdots.$$

Now, the second component of $\boldsymbol{\mu}^{(3)}=\mathbf{X}^{-1}(t)\boldsymbol{f}_3$ is

$$\mu_1^{(3)}=-x_1(t)x_2(t)((a+1)x_2(t)^2+2q_2(t)z(t))=\frac{a}{27t}+\cdots.$$

Thus, $\mu_2^{(3)}$ has a simple pole at $t=0$ with a nonzero residue for $a\neq 0$. Hence, again by Lemma A.1, if $b=0$ but $a\neq 0$, then potential (3.16) is not integrable. □

Lemma 3.2: Hamiltonian system (1.2) with potential $V=V_i$ for $i=7,\ldots,12$ does not admit an additional meromorphic first integral.

Proof: We proceed similarly as in the proof of the previous lemma. The only complication which appears is connected with the fact that, for the investigated potentials $n_1>1$, and an analysis of the leading terms of the Laurent series expansions is not sufficient. Moreover, to find a logarithmic term for some potentials we have to continue calculations up to the fifth-order variational equations. To perform this task we use the computer algebra, and conclusions are the following. For potentials V_7 and V_8 we have $n_1=6$ and $n_1=16$, respectively, and for them we find a logarithmic term in solutions of the fifth-order variational equations. For V_9 we have $n_1=16$ but a logarithmic term appears in solutions of the second-order variational equations. For potentials V_{10}, we have $n_1=2$, and a logarithmic term appears in solutions of the fifth-order variational equations. For the last two potentials, V_{11} and V_{12}, we have $n_1=5$, and a logarithmic term appears in solutions of the second-order variational equations. □

For potential V_0 Theorem 1.1 is not applicable. Nevertheless, we show the following.

Lemma 3.3: *Hamiltonian system (1.2) with potential $V=V_0$ does not admit an additional rational first integral.*

Proof: A proof follows from Theorem 2.4. □

The most difficult case is potential (3.5). Let us define three sets

$$J_1=\{p+2p(p-1)|p\in\mathbb{Z}\},\quad J_2=\left\{\frac{3}{8}+2p(p+1)|p\in\mathbb{Z}\right\},\tag{3.39}$$

$$J_3=\left\{-\frac{1}{8}+\frac{2}{9}(1+3p)^2|p\in\mathbb{Z}\right\}.\tag{3.40}$$

Then a direct application of Theorem 1.1 gives the following.

Proposition 3.4: *If Hamiltonian system (1.2) with potential $V=V_2$ given by (3.5) admits an additional meromorphic first integral, then*

$$c:=1-\alpha\in J_1\cup J_2\cup J_3.\tag{3.41}$$

Hence, we have three infinite families for investigation. When $c\in J_1$, then the variational equations along the particular solution corresponding to the only Darboux point have the form (3.31) with arbitrary $n_1\in\mathbb{Z}$. In this case, we can can apply Lemma A.1 for proving nonintegrability for small values of $|n_1|$. In this way we showed the following.

Proposition 3.5: If Hamiltonian system (1.2) with potential $V=V_2$ admits an additional meromorphic first integral, and $c\in J_1$, then either $c=3$, or $c=p+2p(p-1)$ for $|p|>12$, $p\in\mathbb{Z}$.

When $c\in J_2\cup J_3$, then we cannot apply Lemma A.1 because the Lamé equation corresponding to the normal variational equation is not in the Lamé–Hermite case. For these cases we applied the direct search for a polynomial first integral. Namely, for a given $p\in\mathbb{Z}$ we fixed $c=3/8+2p(p+1)$, and we looked for a polynomial first integral of degree not greater than 50. We checked that there is no such integral for $|p|\leqslant 6$. We checked similar cases when $c\in J_3$. Let us note that from Ref. 24 it follows that if the considered system possesses a rational additional first integral, then it possesses a polynomial one.

The above considerations justify our conjecture that potential V_2 given by (3.5) is integrable only when $\alpha=-2$.

IV. FINAL REMARKS

A natural question appears if it is possible to generalize the obtained results to higher dimensions. The answer to this question is positive and our paper on this subject is in preparation. However a generalization to higher dimensions is not so simple and new problems appear. We just remark that dimension two is distinguished for many reasons. The most important one is that in higher dimensions a homogeneous polynomial does not factor into linear forms.

Here it is worth mentioning that our approach is closely related with investigations of the integrability and uniformization properties of general homogeneous polynomial differential equations. For such a system a Darboux point is a point where the vector field is parallel to the radial direction. As is well known, see, e.g., Ref. 19, with each Darboux point we can associate the Kovalevskaya matrix. A necessary condition for the existence of polynomial first integrals can be expressed in a form of resonance relations among the eigenvalues of the Kovalevskaya matrix. Moreover, if all solutions of the investigated system are single-valued, then necessarily all the eigenvalues of the Kovalevskaya matrix are integers and the matrix is semi-simple (this is the statement of the Lapunov theorem). For quadratic three-dimensional systems Jean Moulin Ollagnier[36] showed that the eigenvalues of the Kovalevskaya matrix taken over all simple Darboux points cannot take arbitrary values. In other words there exist certain universal relations among them. A new geometrical interpretation of the Kovalevskaya–Lapunov analysis was done by Gulliot in his Ph.D. thesis.[13] From the point of view of extension of the results given in this paper into higher dimensions, the most important part of Refs. 13 and 14 concern an application of a Baum–Bott–like theorem for proving the above-mentioned relations among the eigenvalues of the Kovalevskaya matrix taken over all simple Darboux points.

We would like to mention that the results of this paper can be applied for an investigation of integrability of nonhomogeneous potentials. In fact, a polynomial potential $V(\boldsymbol{q})$ can be written in the form of the sum of homogeneous components

$$V(\boldsymbol{q}) = V_{\min}(\boldsymbol{q}) + \ \ldots \ + V_{\max}(\boldsymbol{q}),$$

where $V_{\min}(\boldsymbol{q})$ and $V_{\max}(\boldsymbol{q})$ are the homogeneous components of the lowest and the highest orders, respectively. It can be shown (see, e.g., Ref. 16) that if Hamiltonian system (1.2) with polynomial potential $V(\boldsymbol{q})$ is integrable, then potentials $V_{\min}(\boldsymbol{q})$ and $V_{\max}(\boldsymbol{q})$ are integrable.

Another question concerns an extension of the results of Sec. III to homogeneous potentials of degree higher than four. Here the main problem is connected with the fact that if $\deg V > k$, then the variational equations for a Darboux point are no longer a product of Lamé equations, and we have no tool as effective as Lemma A.1 for application of the higher order variational equations.

Our last observation is the following. In all integrable cases the differential Galois group of the normal variational equations is either contained in the triangular subgroup of $\mathrm{SL}(2,\mathbb{C})$, or it is an imprimitive of $\mathrm{SL}(2,\mathbb{C})$. We do not know an example of a natural Hamiltonian system when this group is a primitive finite group. The question is if it is a general property of natural Hamiltonian systems.

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APPENDIX A: DIFFERENTIAL GALOIS EXTENSION OF ZIGLIN THEORY

1. Basic theorem

Let M^n be a complex analytic manifold and $\boldsymbol{v}$ a holomorphic vector field on M^n. We consider the following differential equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{x} = \boldsymbol{v}(\boldsymbol{x}), \quad \boldsymbol{x} \in M^n, \quad t \in \mathbb{C}. \tag{A1}$$

Let $\boldsymbol{\varphi}(t)$ be a nonequilibrium solution of (A1). Its maximal analytic continuation defines a Riemann surface Γ with local coordinate t. Together with system (A1), we consider the variational equations (VEs) along Γ, i.e.,

$$\dot{\boldsymbol{\xi}} = T(\boldsymbol{v})\boldsymbol{\xi}, \quad T(\boldsymbol{v}) = \frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}}, \quad \boldsymbol{\xi} \in T_\Gamma M^n. \tag{A2}$$

The order of this system can be reduced by one. To do this we consider the induced system on the normal bundle $N := T_\Gamma M / T\Gamma$ of Γ,[19] i.e.,

$$\dot{\eta} = \pi_\star(T(\boldsymbol{v})\pi^{-1}\eta), \quad \eta \in N, \tag{A3}$$

where $\pi: T_\Gamma M \to N$ is the projection. The system of $s = n-1$ equations obtained in this way yields the so-called normal variational equations (NVEs).

Now, assume that M^n is symplectic, i.e., there exists a symplectic form ω on M^n and $n = 2m$. Moreover, let us assume also that vector field $\boldsymbol{v}$ is a Hamiltonian vector field, i.e., there exists a holomorphic function $H: M^n \to \mathbb{C}$ such that $\omega(\boldsymbol{v}, \boldsymbol{u}) = \mathrm{d}H \cdot \boldsymbol{u}$ for arbitrary vector field $\boldsymbol{u}$. For a given particular solution $\varphi(t)$ we fix the energy level $e = H(\varphi(t))$. Restricting (A1) to this level, we obtain a well-defined system on $(n-1)$ dimensional manifold with a known particular solution $\varphi(t)$. For this restricted system we perform the reduction of order of variational equations. Thus, the normal variational equations for a Hamiltonian system with $m = n/2$ degrees of freedom have dimension $s = 2(m-1)$.

In Ref. 43 Ziglin formulated a theorem which gives necessary conditions for the Hamiltonian system governed by a Hamilton's function H. These conditions are expressed in terms of the monodromy group of NVEs for a nonequilibrium particular solution. Later Ziglin investigations were developed by Baider, Churchill, Morales-Ruiz, Rod, Simó, and Singer by a differential Galois approach, see Refs. 7, 5, 35, 30, 32, 33, 1, and 2. The main theorem of this theory formulates necessary conditions for integrability of the investigated Hamiltonian system in terms of the differential Galois group on NVEs (or VEs), and can be formulated in the following way.

Theorem A.1: *Assume that a Hamiltonian system is meromorphically integrable in the Liouville sense in a neighborhood of the analytic phase curve* Γ, *and that NVEs (VEs) along* Γ *are Fuchsian. Then the identity component of the differential Galois group of NVEs (and of VEs) associated with* Γ *is Abelian*.

In a case when NVEs are not Fuchsian, then a necessary condition for the integrability is the same: the identity component of the differential Galois group of NVEs (and of VEs) must be Abelian. However, generally, we have to restrict the class of first integrals to the rational functions. For a discussion of this point, see Ref. 30, Chap. 4.

Applications of the above theorem can be found in the already cited papers and in Refs. 4, 3, 29, 22, 21, and 25–27.

2. Higher order variational equations

To explain in a simple way the idea of higher variational equations it is convenient to assume that $M^n = \mathbb{C}^n$, and to identify vector field $\boldsymbol{v}$ with a map $\boldsymbol{v}: \mathbb{C}^n \ni \boldsymbol{x} \mapsto \boldsymbol{v}(\boldsymbol{x}) \in T_x\mathbb{C}^n \simeq \mathbb{C}^n$. Now, if $\boldsymbol{\varphi}(t)$ is a particular solution of Eq. (A1), we put

$$\boldsymbol{x} = \boldsymbol{\varphi}(t) + \varepsilon\boldsymbol{\xi}^{(1)} + \varepsilon^2\boldsymbol{\xi}^{(2)} + \cdots + \varepsilon^k\boldsymbol{\xi}^{(k)} + \cdots,$$

where ε is a formal small parameter. Inserting the above-noted expansion into Eq. (A1) and comparing terms of the same order with respect to ε, we obtain the following chain of linear nonhomogeneous equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\xi}^{(k)} = \boldsymbol{A}(t)\boldsymbol{\xi}^{(k)} + \boldsymbol{f}_k(\boldsymbol{\xi}^{(1)}, \ldots, \boldsymbol{\xi}^{(k-1)}), \quad k = 1, 2, \ldots, \tag{A4}$$

where

$$\boldsymbol{A}(t) = \frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}}(\boldsymbol{\varphi}(t)),$$

and $\boldsymbol{f}_1 \equiv 0$. For a given k Eq. (A4) is called the kth order variational equation. We denote by $\boldsymbol{X}(t)$ the fundamental matrix of the homogeneous system, i.e., $n \times n$ matrix satisfying

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{X} = \boldsymbol{A}(t)\boldsymbol{X}, \quad \boldsymbol{X}(0) = \boldsymbol{E},$$

where $\boldsymbol{E}$ is the identity matrix. Then the solutions of kth order variational equations for $k > 1$ are given by

$$\boldsymbol{\xi}^{(k)}(t) = \boldsymbol{X}(t)\boldsymbol{c}(t), \tag{A5}$$

where $\boldsymbol{c}(t)$ is a solution of

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{c} = \boldsymbol{X}^{-1}(t)\boldsymbol{f}_k. \tag{A6}$$

There is an appropriate framework allowing to define the differential Galois group of the kth order variational equation, for details see Refs. 30 and 31. The following theorem was formulated in Ref. 31.

Theorem A.2: *Assume that a Hamiltonian system is meromorphically integrable in the Liouville sense in a neighborhood of the analytic curve* Γ. *Then the identity component of the differential Galois group of the kth order variational equations is Abelian for any* $k \in \mathbb{N}$.

Here we note that in Theorem A.1 the necessary conditions were obtained from an analysis of the first-order variational equations.

3. Lamé equation and higher order variational equations

The Lamé equation in the Weierstrass form reads

$$\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} = (A\wp(t) + B)y, \tag{A7}$$

where A and B are, in general, complex parameters and $\wp(t)$ is the elliptic Weierstrass function with invariants g_2, g_3. In other words, $\wp(t)$ is a solution of the differential equation

$$\dot{v}^2 = f(v), \quad f(v) = 4v^3 - g_2 v - g_3.$$

Parameters A, B, g_2, and g_3 are such that the discriminant $\Delta = g_2^3 - 27g_3^2 \neq 0$.

Classically, the Lamé equation (A7) is written with the parameter n instead of A related by the formula $A = n(n+1)$. It is possible to prove that the Lamé equation is solvable only in the following cases:

1. the Lamé and Hermite case (see, e.g., Ref. 38). Then $n \in \mathbb{Z}$ and the three other parameters are arbitrary,
2. the Brioschi–Halphen–Crowford case (see, e.g., Refs. 6 and 38). In this case $m := n + \frac{1}{2} \in \mathbb{N}$, and additionally B, g_2, g_3 should satisfy an appropriate algebraic condition,
3. the Baldassarri case.[6] Then $n + \frac{1}{2} \in \frac{1}{3}\mathbb{Z} \cup \frac{1}{4}\mathbb{Z} \cup \frac{1}{5}\mathbb{Z} \setminus \mathbb{Z}$, and there are additional algebraic conditions on B, g_2, g_3.

In the Lamé-Hermite case one solution is an elliptic function expressed in terms of $\wp$ and $\wp'$.

Let us assume that for a Hamiltonian system with two degrees of freedom the higher order variational equations have the form (A4) with

$$\boldsymbol{A}(t)=\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ A_1\wp(t)+B_1 & 0 & 0 & 0 \\ 0 & A_2\wp(t)+B_2 & 0 & 0 \end{bmatrix}. \tag{A8}$$

Thus, the first-order variational equations are equivalent to a product of two Lamé equations. Additionally, we assume that both copies of the Lamé equations belong to the Lamé–Hermite case, i.e., $A_i=n_i(n_i+1)$, $n_i\in\mathbb{Z}$ for $i=1,2$.

In the described situation we can check whether the differential Galois group of the higher order variational equations is Abelian investigating only the local monodromy around singularity $t=0$ of $\wp(t)$, for details see Refs. 30 and 31.

Lemma A.1: Under the assumption formulated above, the Galois group of higher order variational equations is Abelian if and only if their local monodromy around the singular point is the identity.

To apply the above lemma we just have to check if in the local solutions around $t=0$ of the second variational equations a logarithmic term appears. If it is so, then we have an obstacle for the integrability, if it is not so, we have to check if such term appears in a local solution of the third-order variational equations. This process can be continued up to an arbitrary high order.

For examples of application of the above lemma, see Refs. 27 and 33.

APPENDIX B: TECHNICAL LEMMA

We consider the following equation:

$$X_1+\cdots+X_m=c,\quad c>0. \tag{B1}$$

We look for its solutions $\boldsymbol{X}=(X_1,\ldots,X_m)\in\mathcal{X}^m$ where $\mathcal{X}$ is defined in the following way:

$$\mathcal{X}=\{x_n\in(0,\infty)|n\in\mathbb{N}\}, \tag{B2}$$

where $\lim_{n\to\infty}x_n=0$. We prove the following lemma.

Lemma B.1: For arbitrary $c>0$ Eq. (B1) *has at most a finite number of solutions in $\mathcal{X}^m$.*

Proof: We prove this lemma by induction with respect to m. For $m=1$ the statement of the lemma is evidently true. So, assume that it is true for $m-1$. We have to show that it is true for m. Let us assume the opposite: let $\boldsymbol{X}_p\in\boldsymbol{X}^m$, $p\in\mathbb{N}$ be an infinite sequence of different solutions of Eq. (B1). Points $\boldsymbol{X}_p$ belong to the compact set

$$T_c=\{(x_1,\ldots,x_m)\in\mathbb{R}^m|x_i\geqslant 0,\quad x_1+\cdots+x_m=c\}.$$

Thus, there exists a subsequence of $\boldsymbol{X}_p$ which tends to a certain $\tilde{\boldsymbol{X}}\in T_c$. Hence, we can assume that $\boldsymbol{X}_p=(X_{1,p},\ldots,X_{m,p})$ is chosen in such a way that $\lim_{p\to\infty}\boldsymbol{X}_p=\tilde{\boldsymbol{X}}$. Note that it cannot happen that all sequences $\{X_{i,p}\}$ for $i=1,\ldots,m$ contain infinitely many different numbers. In fact, if it is the case, then, for each $i=1,\ldots,m$ there exist a monotonically increasing series of integers $\{n_p\}$ such that $X_{i,p}=x_{n_p}$. But then each sequence $\{X_{i,p}\}$ converges to 0 which is impossible as their sum converges to a positive value. Hence, for at least one $i\in\{1,\ldots,m\}$, let us say $i=m$, sequence $\{X_{m,p}\}$ is constant for $p\geqslant p_0$. Note that $X_{m,p_0}<c$. As a result, we arrived to conclusion that there exist infinitely many solutions of equation

$$X_1+\cdots+X_{m-1}=c'$$

in $\mathcal{X}^{m-1}$ for certain $c'>0$. A contradiction with the inductive assumption finishes the proof. □

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Nonholonomic versus vakonomic dynamics on a Riemann–Cartan manifold

Yong-Xin Guo[a)]
Department of Physics, Liaoning University, Shenyang 110036, China

Yong Wang
Department of Physics, Guangdong Medical College, Zhanjiang 524023, China

G. Y. Chee
Department of Physics, Liaoning Normal University, Dalian 116029, China

Feng-Xiang Mei
Department of Applied Mechanics, Beijing Institute of Technology, Beijing 110081, China

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For the Chaplygin's nonholonomic constrained systems, the constraint manifold can be endowed with Riemann–Cartan geometric structure by nonholonomic mapping into a Riemann manifold. The two kinds of existing dynamics, nonholonomic dynamics and vakonomic dynamics, are compared in the framework of Riemann–Cartan geometry. It is proved that the equations of motion for nonholonomic and vakonomic dynamics are described by the equations of autoparallel and geodesic trajectories on the Riemann–Cartan constraint manifold, respectively. If the metricity condition of Riemann–Cartan connection is satisfied, the torsion (contorsion) of the Riemann–Cartan manifold characterizes the difference between the autoparallel and geodesic trajectories as well as the distinction between the nonholonomic and vakonomic equations. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Constrained systems are common dynamical systems in modern physics, mechanics and engineering,[1–13] which can be classified into holonomic and nonholonomic ones according to the Frobenius integrability condition of constraints the systems are subject to. Unlike a holonomic system, a nonholonomic system cannot be reduced to a free system with lower degrees of freedom in general. Furthermore, there exist two inequivalent dynamical theories on nonholonomic constrained systems. One is based on Hamilton's principle of lease action. Similar to treating holonomic constrained systems, the constraints are directly incorporated into Lagrangian $L \rightarrow L + \lambda^{\alpha} f_{\alpha}$ with λ^{α} being Lagrange multipliers treated as independent dynamical variables. The dynamical equations derived from the theory can be canonicalized since such a way to incorporate constraints into a dynamical description does not influence on the symplectic structure of phase space of the systems. This dynamics is usually referred to as vakonomic dynamics (variational axiomatic kind).[14,15] The other is based on d'Alembert–Lagrange principle (or Hölder's principle, Gauss's principle) satisfying the condition of ideal constraints. Chetaev's condition on variation of coordinates induced from the nonholonomic constraints is utilized to realize the ideal constraints. Such a theory is not canonically Lagrangian or Hamiltonian, and is called nonholonomic dynamics.[1,11] The above two dynamics are equivalent for holonomic systems.

The paradox that different dynamics can be derived from the same nonholonomic constrained system just because of beginning with different acknowledged principles makes nonholonomic

[a)]Electronic mail: guoyongxin@lnu.edu.cn

constrained systems and their relating theories become a focus of research and disputation.[16–19] Therefore, it has been an important work to compare the two dynamics of nonholonomic systems.

In this paper, nonholonomic dynamics of Chaplygin's linear constrained systems[20] is compared with the corresponding vakonomic dynamics in the framework of Riemann–Cartan geometry.[21,22] In Sec. II, we briefly review the method to construct a Riemann–Cartan manifold by using a nonholonomic mapping[23–28] from a Riemann manifold. In Sec. III, the calculus of nonholonomic variations is discussed on the manifold. The nonholonomic variations are classified into three kinds. In Sec. IV, the two kinds of equations of motion, nonholonomic and vakonomic, for linear nonholonomic constrained systems are proved to describe the autoparallel and geodesic trajectories on the manifold, respectively. Some simple examples are illustrated in Sec. V ended with a concluding remark. The Einstein's summation convention is used throughout this paper and $i, j=1,2,\ldots,n$; $\mu, \nu, \sigma, \rho, \lambda, \tau=1,2,\ldots,m$; $\alpha, \beta=m+1, m+2,\ldots,n$.

II. RIEMANN–CARTAN CONSTRAINT MANIFOLD

A general system is usually subject to two kinds of constraints, the holonomic and the nonholonomic. Suppose that the configuration space of the system is n-dimensional Riemann manifold Q with local coordinates $\{q^i\}$ after the holonomic constraints are reduced. The metric tensor field on manifold Q is defined by the Hessian of nondegenerate Lagrangian L. The configuration space can be further deformed into Riemann–Cartan manifold with both curvature and torsion by the nonholonomic constraints imposed.

Suppose the system is subject to $(n-m)$ linear nonholonomic constraints:

$$\dot{q}^\alpha = \varepsilon^\alpha_\mu(q^\nu)\dot{q}^\mu, \tag{1}$$

where $\{\dot{q}^\mu, \dot{q}^\alpha\}$ are generalized velocities of the system. These constraints are suitable to characterize most linear constrained systems. The systems subjected to such constraints are called Chaplygin's nonholonomic constrained systems.

A m-dimensional constraint manifold M with local coordinates $\{q^\mu\}$ can be constructed by the constraint equations (1). As a subspace of Riemann manifold Q, however, the constraint manifold M is not its invariant embedded submanifold since the vector fields on the constraint manifold M are not involutive due to anholonomy of the constraints (1). Nevertheless, the tangent space of the constraint manifold M can be embedded into the tangent space of Riemann manifold Q by a nonholonomic mapping $i_T: TM \to TQ$:

$$v^i = \varepsilon^i_\mu(q^\nu)v^\mu, \quad v^\mu \in T_qM, \tag{2}$$

induced by the constraints (1), where $\varepsilon^i_\mu = \varepsilon^\alpha_\mu$ if i takes $\alpha = m+1, m+2,\ldots,n$; $\varepsilon^i_\mu = \delta^\nu_\mu$ if i takes $\nu = 1,2,\ldots,m$. This mapping can induce a nonholonomic mapping i_q:

$$q^i(c_q) = \int_{c_q} \varepsilon^i_\mu(q)\mathrm{d}q^\mu \tag{3}$$

from the equivalence class $\langle q^\mu(t)\rangle$ of all paths on manifold M to that on manifold Q, where c_q denotes any path $q^\mu(t)$ on manifold M. The integrals can be classified according to the end points of paths $c_{q(t)}$ if the same initial point of the integrals is fixed, i.e., each point of $c_{q(t)}$ corresponds to an equivalence class of integrals $q^i(c_{q(t)})$. $\{q^i(c_{q(t)})\}$ can be recognized as pseudo-coordinates on manifold M. If the constraints are integrable, the above-noted integrals are independent of paths on M and $q^i(c_{q(t)})$ reduce to $q^i(t)$, the function of end point t of path $c_{q(t)}$. Then path $q^\mu(t) \in M$ corresponds to path $q^i(t) \in Q$ pointwise, i.e., $q^i = q^i(q^\mu)$.

It can be verified that the metric and connection on manifold M can be induced from the nonholonomic mappings (2) and (3) in the same way as in Ref. 23 by generalizing the Euclid space taken as auxiliary space to the Riemann manifold Q. First, the metric g_{ij} on Riemann

manifold Q induces the metric $g_{\mu\nu}$ on manifold M. According to the mapping (2), $u^i=\varepsilon^i_\mu u^\mu$, $v^j=\varepsilon^j_\nu v^\nu$, for $u^i,v^j\in T_{i_q(q)}Q$ and $u^\mu,v^\nu\in T_qM$. Then $(u,v)=g_{ij}u^iv^j=g_{ij}\varepsilon^i_\mu\varepsilon^j_\nu u^\mu v^\nu=(\varepsilon_\mu,\varepsilon_\nu)u^\mu v^\nu$. Therefore, the induced metric on manifold M is

$$g_{\mu\nu}=(\varepsilon_\mu,\varepsilon_\nu)=g_{ij}\varepsilon^i_\mu\varepsilon^j_\nu. \tag{4}$$

Second, the mappings (2) and (3) induce a connection on manifold M,

$$\Gamma^\sigma_{\mu\nu}=g^{\sigma\rho}(\varepsilon_\rho,\partial_\mu\varepsilon_\nu)=g^{\sigma\rho}g_{ij}\varepsilon^i_\rho\partial_\mu\varepsilon^j_\nu. \tag{5}$$

It is easy to verify the metricity condition of the connection, i.e., compatible condition of the connection with metric, $D_\mu g_{\nu\sigma}=0$, which makes the length of a vector invariant while parallel-transporting it along a path on manifold M. But the connection is asymmetric, i.e., $\Gamma^\sigma_{\nu\mu}\neq\Gamma^\sigma_{\mu\nu}$, whose antisymmetric part is named torsion of the connection:

$$S^\sigma_{\mu\nu}=\Gamma^\sigma_{[\mu\nu]}=\tfrac{1}{2}(\Gamma^\sigma_{\mu\nu}-\Gamma^\sigma_{\nu\mu})=\tfrac{1}{2}g^{\sigma\rho}g_{ij}\varepsilon^i_\rho(\partial_\mu\varepsilon^j_\nu-\partial_\nu\varepsilon^j_\mu). \tag{6}$$

Obviously, $S^\sigma_{\nu\mu}=0$ if the integrability condition of constraints, $\partial_\mu\varepsilon^j_\nu-\partial_\nu\varepsilon^j_\mu=0$, is satisfied.

Such an asymmetric connection compatible with metric is referred to as Riemann–Cartan connection. The constraint manifold M is then a Riemann–Cartan manifold with torsion $S^\sigma_{\mu\nu}$ and curvature

$$R^{\rho\tau}_{\mu\nu}=\tfrac{1}{2}g^{\rho\lambda}g^{\tau\sigma}g_{ij}(f^i_{\mu\lambda}f^j_{\nu\sigma}-f^i_{\nu\lambda}f^j_{\mu\sigma}), \tag{7}$$

where

$$f^i_{\mu\nu}=D_\mu\varepsilon^i_\nu=\partial_\mu\varepsilon^i_\nu-\Gamma^\sigma_{\mu\nu}\varepsilon^i_\sigma. \tag{8}$$

On the Riemann–Cartan constraint manifold M there exist two kinds of special curves, geodesic and autoparallel trajectories, as follows:

$$\ddot{q}^\mu+\overline{\Gamma}^\mu_{\nu\sigma}\dot{q}^\nu\dot{q}^\sigma=0, \tag{9a}$$

$$\ddot{q}^\mu+\Gamma^\mu_{\nu\sigma}\dot{q}^\nu\dot{q}^\sigma=0, \tag{9b}$$

where $\overline{\Gamma}^\mu_{\nu\sigma}=\frac{1}{2}g^{\mu\lambda}(\partial_\sigma g_{\nu\lambda}+\partial_\nu g_{\sigma\lambda}-\partial_\lambda g_{\nu\sigma})$ is Riemann–Christoffel connection. It can be proved in the following that the difference of shortness from straightness on Riemann–Cartan manifold can geometrically characterize the "inexplicable" deviation of vakonomic dynamics from nonholonomic dynamics.

III. NONHOLONOMIC VARIATIONS ON RIEMANN–CARTAN CONSTRAINT MANIFOLD

Let c_q and $\overline{c_q}$ be smooth curves connecting any two fixed points q^i_1 and q^i_2 on n-dimensional Riemann manifold Q. Consider a function $q^i(t,\alpha)\in C^2$ of two parameters, satisfying $q^i(t,0)=q^i(t)$, $q^i(t,1)=\overline{q^i}(t)$; $q^i(t_1,\alpha)=q^i_1$, $q^i(t_2,\alpha)=q^i_2$. Denote the differential along any path by $\mathrm{d}q^\mu=\partial_t q^i(t,\alpha)\mathrm{d}t\doteq v^i\mathrm{d}t$ while the variation of the path is denoted by $\delta q^i=\partial_\alpha q^i(t,\alpha)\mathrm{d}\alpha\doteq w^i\mathrm{d}\alpha$ with fixed ends condition

$$\delta q^i|_{t_{1,2}}=0,\qquad w^i|_{t_{1,2}}=0. \tag{10}$$

The vector field $w^i(q^j)\in T_qQ$ is called variation vector field on manifold Q. As in Ref. 23, denote d_v and d_w the derivative along vector fields v and w, respectively. The above-noted definition leads to the following commutation relation of differential and variational operations:

$$\mathrm{d}_w v^i-\mathrm{d}_v w^i=0, \tag{11}$$

which simply determine the variation of velocity. To define a variation it is necessary to specify the variation of velocity as well as the variation vector field.

A variation vector field $w^\mu(q^\nu) \in T_qM$ can also be defined on manifold M with torsion. The commutation relation (11) on Riemann manifold Q, however, cannot be simply transplanted to the constraint manifold M. Relation (11) leads to

$$\mathrm{d}_w(v^i - \varepsilon^i_\mu v^\mu) + (\partial_\mu \varepsilon^i_\rho - \partial_\rho \varepsilon^i_\mu) v^\rho w^\mu + \varepsilon^i_\mu (\mathrm{d}_w v^\mu - \mathrm{d}_v w^\mu) - \mathrm{d}_v (w^i - \varepsilon^i_\mu w^\mu) = 0. \tag{12}$$

Let $\varepsilon^\mu_i \doteq g^{\mu\nu} g_{ij} \varepsilon^j_\nu$ with $\varepsilon^\mu_i \varepsilon^i_\nu = \delta^\mu_\nu$; $\varepsilon^\mu_i \varepsilon^j_\mu = \delta^j_i$. Using this condition and the connection coefficients (5) obtained in last section, we are led to

$$\partial_\rho \varepsilon^i_\mu = \varepsilon^i_\sigma \Gamma^\sigma_{\rho\mu}, \quad \partial_\rho \varepsilon^\mu_i = -\varepsilon^\nu_i \Gamma^\mu_{\rho\nu}. \tag{13}$$

By the definition (6), it follows that

$$(\partial_\mu \varepsilon^i_\rho - \partial_\rho \varepsilon^i_\mu) = 2\varepsilon^i_\sigma S^\sigma_{\mu\rho}. \tag{14}$$

Therefore relation (12) can be transformed into

$$\mathrm{d}_w(v^i - \varepsilon^i_\mu v^\mu) + \varepsilon^i_\mu (\mathrm{d}_w v^\mu - \mathrm{d}_v w^\mu) - \mathrm{d}_v (w^i - \varepsilon^i_\mu w^\mu) = 2\varepsilon^i_\sigma S^\sigma_{\rho\mu} v^\rho w^\mu. \tag{15}$$

Because of the existence of torsion tensor $S^\sigma_{\rho\mu}$ the variation vector field on the constraint manifold M cannot satisfy the following conditions simultaneously:

$$d_v(w^i - \varepsilon^i_\mu w^\mu) = 0, \tag{16a}$$

$$d_w v^\mu - d_v w^\mu = 0, \tag{16b}$$

$$d_w(v^i - \varepsilon^i_\mu v^\mu) = 0, \tag{16c}$$

which means that unlike the case of holonomic systems, there does not exist a free variation on the manifold M. The unfree variation vector field w and the corresponding differential d_w are named nonholonomic variations. The first condition imposed on the variation of coordinates is induced from the constraints and is called Chetaev's condition. The second is the commutation relation of differential and variational operations which leads to the existence of smooth local coordinate net formed by the integral curves of vector fields v^μ and w^μ. The third condition is an invariance of constraint conditions with respect to the variation operation, making the variation of velocities be unfree.

According to relation (15), the nonholonomic variation can be classified into the following three kinds.

(1) Hölder's variation. Choose the first two relations from the last equations, i.e.,

$$\mathrm{d}_v(w^i_\mathrm{h} - \varepsilon^i_\mu w^\mu_\mathrm{h}) = 0, \quad \mathrm{d}_{w_\mathrm{h}} v^\mu - \mathrm{d}_v w^\mu_\mathrm{h} = 0. \tag{17}$$

It follows from (15) that

$$\mathrm{d}_{w_\mathrm{h}}(v^i - \varepsilon^i_\mu v^\mu) = 2\varepsilon^i_\sigma S^\sigma_{\rho\mu} v^\rho w^\mu_\mathrm{h}, \tag{18}$$

which indicates how the constraint conditions vary with respect to Hölder's variation due to the torsion of manifold M.

(2) Suslov's variation. Suppose that

$$\mathrm{d}_v(w^i_\mathrm{s} - \varepsilon^i_\mu w^\mu_\mathrm{s}) = 0, \quad \mathrm{d}_{w_\mathrm{s}}(v^i - \varepsilon^i_\mu v^\mu) = 0. \tag{19}$$

It leads from the relation (15) to

$$\mathrm{d}_{w_s} v^\sigma - \mathrm{d}_v w_s^\sigma = 2S^\sigma_{\rho\mu} v^\rho w_s^\mu, \tag{20}$$

which means that Suslov's variation does not commute with differentiation of coordinates. Making use of covariant differentiation,

$$D_v w_s^\sigma = \mathrm{d}_v w_s^\sigma + \Gamma^\sigma_{\rho\mu} v^\rho w_s^\mu, \quad D_{w_s} v^\sigma = \mathrm{d}_{w_s} v^\sigma + \Gamma^\sigma_{\rho\mu} w_s^\rho v^\mu. \tag{21}$$

The variation of velocity v^σ can be specified by

$$D_v w_s^\sigma - D_{w_s} v^\sigma = 0. \tag{22}$$

(3) Vakonomic variation. Let

$$\mathrm{d}_{w_v} v^\mu - \mathrm{d}_v w_v^\mu = 0, \quad \mathrm{d}_{w_v}(v^i - \varepsilon^i_\mu v^\mu) = 0. \tag{23}$$

Then it is referred from (15) that the Chetaev's conditions cannot be satisfied and are replaced with corresponding conditions

$$\mathrm{d}_v(w_v^i - \varepsilon^i_\mu w_v^\mu) = 2\varepsilon^i_\sigma S^\sigma_{\mu\rho} v^\rho w_v^\mu. \tag{24}$$

It should be pointed that all the three kinds of variations satisfy the fixed ends conditions

$$w^\mu|_{t_1} = w^\mu|_{t_2} = 0. \tag{25}$$

IV. NONHOLONOMIC VERSUS VAKONOMIC EQUATIONS ON CONSTRAINT MANIFOLD

We apply Suslov's variation and vakonomic variation to variational principle to get two kinds of dynamical equations for the Chaplygin's nonholonomic constrained systems.

First, we make use of Suslov's variation to check the recently discovered stationary action principle[25]

$$\mathrm{d}_{w_s} S = \mathrm{d}_{w_s} \int_{t_1}^{t_2} \mathcal{L}(q^\mu, v^\mu)\mathrm{d}t = 0. \tag{26}$$

Computing the variation directly and making use of the above variation condition (20) and fixed ends conditions (25), one can derive the equations of motion

$$\frac{\partial \mathcal{L}}{\partial q^\mu} - \mathrm{d}_v\left(\frac{\partial \mathcal{L}}{\partial v^\mu}\right) = 2S^\rho_{\mu\nu}\frac{\partial \mathcal{L}}{\partial v^\rho} v^\nu, \tag{27}$$

which describes nonholonomic dynamics on the constraint manifold M.

We concern the geometric property of nonholonomic equations (27). Substitute $\mathcal{L} = \frac{1}{2} g_{\mu\nu}(q) v^\mu v^\nu$ into Eq. (27), then

$$g_{\mu\nu}\dot{v}^\nu + (\overline{\Gamma}_{\mu\nu\rho} - 2S_{\rho\nu\mu}) v^\rho v^\nu = 0, \tag{28}$$

where $S_{\rho\nu\mu} = g_{\rho\lambda} S^\lambda_{\nu\mu}$, $\overline{\Gamma}_{\mu\nu\rho} = g_{\mu\lambda}\overline{\Gamma}^\lambda_{\nu\rho}$ and $\overline{\Gamma}^\lambda_{\nu\rho}$ is Christoffel symbols. Considering the geometric relation

$$\overline{\Gamma}_{\mu\nu\rho} - 2S_{\rho\nu\mu} = g_{\mu\lambda}\Gamma^\lambda_{\nu\rho} \tag{29}$$

and lift the index μ, then

$$D_v v^\lambda = \dot{v}^\lambda + \Gamma^\lambda_{\nu\rho} v^\rho v^\nu = 0. \tag{30}$$

Thus it can be seen that the equations of motion for nonholonomic dynamics describe the autoparallels of Riemann–Cartan constraint manifold M.

Second, apply the vakonomic variation to the action on the manifold M, the stationary action principle

$$\mathrm{d}_{w_v} S = \mathrm{d}_{w_v} \int_{t_1}^{t_2} \mathcal{L}(q^\mu, v^\mu)\mathrm{d}t = 0 \tag{31}$$

simply leads to vakonomic equations

$$\mathrm{d}_v \left(\frac{\partial \mathcal{L}}{\partial v^\mu} \right) - \frac{\partial \mathcal{L}}{\partial q^\mu} = 0. \tag{32}$$

In fact, it is Euler–Lagrange equations. Substitute $\mathcal{L} = \frac{1}{2} g_{\mu\nu}(q) v^\mu v^\nu$ into Eq. (32), then

$$\overline{D}_v v^\lambda = \dot{v}^\lambda + \overline{\Gamma}^\lambda_{\nu\rho} v^\rho v^\nu = 0, \tag{33}$$

which are the geodesic equations on Riemann–Cartan constraint manifold M. In the following we verify that the geodesic equations (33) are just a geometrical representation of vakonomic equations for Chaplygin's nonholonomic constrained systems in Riemann–Cartan constraint manifold.

Let L be a Lagrangian of a dynamical system on the Riemann manifold Q. Rewrite $(n-m)$ nonholonomic constraints (1) the system is subject to as follows:

$$f^\alpha = v^\alpha - \varepsilon^\alpha_\mu v^\mu = 0. \tag{34}$$

Based on Hamilton's principle of least action, the vakonomic equations

$$[L]_i = -\lambda_\alpha [f^\alpha]_i - \mathrm{d}_v(\lambda_\alpha) \frac{\partial f^\alpha}{\partial v^i} \tag{35}$$

can be derived by the method of Lagrange multipliers. Using the notations $\lambda_i = \delta^\alpha_i \lambda_\alpha$, $f^i = v^i - \varepsilon^i_\mu v^\mu = 0$ in order to map the equations onto the constraint manifold M conveniently, the vakonomic equations are then equivalent to

$$[L]_i = -\lambda_j [f^j]_i - \mathrm{d}_v \lambda_j \frac{\partial f^j}{\partial v^i}. \tag{36}$$

It can be derived by simple computation:

$$\frac{\partial f^j}{\partial v^i} = \delta^j_i - \delta^\mu_i \varepsilon^j_\mu, \quad \frac{\partial f^j}{\partial q^i} = -\delta^\nu_i \varepsilon^j_\sigma \Gamma^\sigma_{\nu\mu} v^\mu, \quad [f^j]_i = 2\delta^\nu_i \varepsilon^j_\sigma S^\sigma_{\mu\nu} v^\nu. \tag{37}$$

Substitute it into the vakonomic equations, then

$$[L]_i = -2\delta^\nu_i \lambda_j \varepsilon^j_\sigma S^\sigma_{\mu\nu} v^\nu + \mathrm{d}_v \lambda_i + \mathrm{d}_v \lambda_j \varepsilon^j_\mu \delta^\mu_i. \tag{38}$$

Supposing the Lagrangian L on Riemann manifold Q is independent of coordinates q^α and neglecting any integral constants, the Lagrange multipliers can be found out from the above equations

$$\lambda_i = -\varepsilon^\mu_i \frac{\partial L}{\partial v^\mu}, \quad \mathrm{d}_v \lambda_i = -\varepsilon^\mu_i D_v \left(\frac{\partial L}{\partial v^\mu} \right) \tag{39}$$

along with the reduction of vakonomic equations onto the constraint manifold M:

$$[L]_\mu = 2S^\sigma_{\mu\nu} v^\nu \frac{\partial L}{\partial v^\sigma} - D_v\left(\frac{\partial L}{\partial v^\mu}\right). \tag{40}$$

For a mechanical system, $L=\frac{1}{2}g_{\mu\nu}v^\mu v^\nu$, the above equations can be transformed into

$$g_{\mu\nu}\overline{D}_v v^\nu + g_{\mu\nu} D_v v^\nu = 2g_{\nu\sigma} S^\nu_{\mu\rho} v^\rho v^\sigma. \tag{41}$$

Expand further, then

$$2g_{\mu\nu}\overline{D}_v v^\nu + (K_{\mu\rho\sigma} - S_{\sigma\mu\rho}) v^\rho v^\sigma = 0, \tag{42}$$

where $K_{\mu\rho\sigma}=g_{\mu\nu}K^\nu_{\rho\sigma}=g_{\mu\nu}(\Gamma^\nu_{\rho\sigma}-\overline{\Gamma}^\nu_{\rho\sigma})$, $S_{\sigma\mu\rho}=g_{\nu\sigma}S^\nu_{\mu\rho}$. Substitute the geometric relation

$$K_{\mu\rho\sigma} - S_{\sigma\mu\rho} = K_{\rho\mu\sigma} = -K_{\sigma\mu\rho} \tag{43}$$

into the above equation, we finally obtain Eq. (33), a geodesic representation of vakonomic equations on the constraint manifold M.

Remark 1: We have not applied Hölder's variation to the action because the result is the same as that of the vakonomic variation if we did for the particular action, which does not imply that Hölder's variation cannot give any new result for general nonholonomic systems.

Remark 2: On the Riemann–Cartan manifold M satisfying the metricity of connection the autoparallel trajectories will coincide with the geodesic ones if the torsion vanishes. In this case the nonholonomic equations also coincide with the vakonomic ones. However, it does not mean that the constraints are integrable in the sense of Frobenius theorem although inverse proposition is certainly true. This fact will be illustrated by example 3 of Sec. V.

V. ILLUSTRATIVE EXAMPLES

Now we are going to show by the following simple examples how the interrelation between the nonholonomic and vakonomic equations can be geometrically characterized on a Riemann–Cartan manifold.

Example 1: We illustrate the above result by the following example of a nonholonomically constrained particle with the Lagrangian $L=\frac{1}{2}(\dot{x}^2+\dot{y}^2+\dot{z}^2)$ and the nonholonomic constraint $\dot{z}=y\dot{x}$.

By means of the usual method, the nonholonomic and vakonomic equations are given by

$$\ddot{x} + \frac{y\dot{x}\dot{y}}{1+y^2} = 0, \quad \ddot{y} = 0, \tag{44a}$$

$$\ddot{x} + \frac{2y\dot{x}\dot{y}}{1+y^2} = 0, \quad \ddot{y} - y\dot{x}^2 = 0, \tag{44b}$$

respectively. We will illustrate that they describe autoparallel and geodesic trajectories on a two-dimensional Riemann–Cartan constraint manifold M with local coordinates (x,y).

Let x,y; $\dot{x},\dot{y}$ play the role of the q^μ, $\dot{q}^\mu$ and $z,\dot{z}$ the role of the q^α, $\dot{q}^\alpha$ in our discussion of the general theory. Obviously, $i,j=1,2,3$; $\mu,\nu=1,2$; $\alpha=3$ and

$$\varepsilon^1_1 = 1, \varepsilon^1_2 = 0, \varepsilon^2_1 = 0, \varepsilon^2_2 = 1; \quad \varepsilon^3_1 = y, \varepsilon^3_2 = 0.$$

The metric $g_{\mu\nu}$ and $g^{\mu\nu}$ take the form

$$(g_{\mu\nu}) = \begin{pmatrix} 1+y^2 & 0 \\ 0 & 1 \end{pmatrix}, \quad (g^{\mu\nu}) = \begin{pmatrix} \frac{1}{1+y^2} & 0 \\ 0 & 1 \end{pmatrix}.$$

The nonvanishing coefficients of the corresponding Christoffel symbols are given by

$$\overline{\Gamma}^2_{11} = -y, \quad \overline{\Gamma}^1_{12} = \overline{\Gamma}^1_{21} = \frac{y}{1+y^2}.$$

Then the geodesic equations on the manifold M,

$$\ddot{q}^1 + 2\overline{\Gamma}^1_{12}\dot{q}^1\dot{q}^2 = 0, \quad \ddot{q}^2 + \overline{\Gamma}^2_{11}\dot{q}^1\dot{q}^1 = 0,$$

take the form of vakonomic equations (44b) after a replacement of q^1,q^2 with x,y.

It can be verified that the only one nonvanishing coefficient of Riemann–Cartan connection on the manifold M is

$$\Gamma^1_{21} = \frac{y}{1+y^2}.$$

Then the autoparallel equations

$$\ddot{q}^1 + \Gamma^1_{21}\dot{q}^2\dot{q}^1 = 0, \quad \ddot{q}^2 = 0$$

are simply the nonholonomic equations (44a) if the coordinates q^1,q^2 are replaced with x,y.

Example 2: A special Chaplygin sleigh. Let us consider the free motion of a sleigh on a horizontal plane in the case when the projection of the center of mass coincides with the point of contact of a sharp wheel and the plane. We suppose the simplified sleigh has unit mass and unit moment of inertia in $R^2 \times T^1$ with coordinates (x,y,φ), subjected to the nonholonomic constraint $\dot{y} = \dot{x}\tan\varphi$. Then the regular Lagrangian is given by $L = \frac{1}{2}(\dot{x}^2 + \dot{y}^2 + \dot{\varphi}^2)$.

We discuss the two kinds of differential equations on the Riemann–Cartan submanifold M of $R^2 \times T^1$ in the following. As is well known, the reduced nonholonomic and vakonomic equations for the system on M are given by

$$\ddot{x} + \dot{x}\dot{\varphi}\tan\varphi = 0, \quad \ddot{\varphi} = 0, \tag{45a}$$

$$\ddot{x} + 2\dot{x}\dot{\varphi}\tan\varphi = 0, \quad \ddot{\varphi} - \dot{x}^2\tan\varphi\sec^2\varphi = 0, \tag{45b}$$

respectively.

Take $i,j = 1,2,3$; $\mu,\nu = 1,2$; $\alpha = 3$. Denote $q^\mu,\dot{q}^\mu$ by x,φ; $\dot{x},\dot{\varphi}$ and $q^\alpha,\dot{q}^\alpha$ by $y,\dot{y}$. Obviously,

$$\varepsilon^1_1 = 1, \varepsilon^1_2 = 0, \varepsilon^2_1 = 0, \varepsilon^2_2 = 1; \quad \varepsilon^3_1 = \tan\varphi, \varepsilon^3_2 = 0.$$

The metric $g_{\mu\nu}$ and $g^{\mu\nu}$ take the form

$$(g_{\mu\nu}) = \begin{pmatrix} \sec^2\varphi & 0 \\ 0 & 1 \end{pmatrix}, \quad (g^{\mu\nu}) = \begin{pmatrix} \cos^2\varphi & 0 \\ 0 & 1 \end{pmatrix}.$$

Then the nonvanishing coefficients of the corresponding Christoffel symbols are given by

$$\overline{\Gamma}^2_{11} = -\tan\varphi\sec^2\varphi, \quad \overline{\Gamma}^1_{12} = \overline{\Gamma}^1_{21} = \tan\varphi.$$

The Riemann–Cartan connection is simple to compute with only one nonvanishing coefficient

$$\Gamma^1_{21} = \tan\varphi.$$

It is very easy to verify that the following autoparallel and geodesic equations,

$$\ddot{x} + \Gamma^1_{21}\dot{\varphi}\dot{x} = 0, \quad \ddot{\varphi} = 0,$$

$$\ddot{x} + 2\Gamma^1_{12}\dot{x}\dot{\varphi} = 0, \quad \ddot{\varphi} + \Gamma^2_{11}\dot{x}\dot{x} = 0,$$

are just the nonholonomic and vakonomic equations (45a) and (45b), respectively, by substituting the above nonvanishing connection coefficients into them.

Example 3: Consider the problem of a vertically rolling disk which is another paradigm of nonholonomic systems. Choose the following appropriate generalized coordinates: the coordinates (x,y) of the center of mass of the disk, the azimuthal angle ψ which determines the position of the disk, and angle ϕ describing its internal rotation.

Setting the mass of the disk equal to 1 for simplicity, the Lagrangian is given by $L=\frac{1}{2}(\dot{x}^2+\dot{y}^2)+\frac{1}{2}(I_1\dot{\phi}^2+I_2\dot{\psi}^2)$ where I_1 and I_2 are moments of inertia. This regular Lagrangian leads to Hessian metric g_{ij} with nonvanishing diagonal elements: $g_{11}=I_1$, $g_{22}=I_2$, $g_{33}=1$, $g_{44}=1$. The nonholonomic constraints are given by the condition of rolling without slipping

$$\dot{x} = (R\cos\psi)\dot{\phi}, \quad \dot{y} = (R\sin\psi)\dot{\phi},$$

where R is the radius of the disk. Following the usual procedure for setting up the nonholonomic and vakonomic equations, we can consider the two kinds of equations of motion as the same and simply read

$$(R^2 + I_1)\ddot{\phi} = 0, \quad I_2\ddot{\psi} = 0. \tag{46}$$

Making use of the following notational identifications: $(q^1,q^2,q^3,q^4)=(\phi,\psi;x,y)$, the above constraints leads to

$$\varepsilon^1_1 = 1, \varepsilon^1_2 = \varepsilon^2_1 = 0, \varepsilon^2_2 = 1; \quad \varepsilon^3_1 = R\cos\psi, \varepsilon^3_2 = 0, \varepsilon^4_1 = R\sin\psi, \varepsilon^4_2 = 0$$

from which the metrics are given by

$$(g_{\mu\nu}) = \begin{pmatrix} R^2 + I_1 & 0 \\ 0 & I_2 \end{pmatrix}, \quad (g^{\mu\nu}) = \begin{pmatrix} \frac{1}{R^2+I_1} & 0 \\ 0 & \frac{1}{I_2} \end{pmatrix}.$$

It is straightforward to compute in the same way as the above examples that all of the coefficients of Riemann–Christoffel and Riemann–Cartan connections vanish,

$$\overline{\Gamma}^{\mu}_{\nu\sigma} = 0, \quad \Gamma^{\mu}_{\nu\sigma} = 0 \quad (\mu,\nu,\sigma = 1,2),$$

which means that the autoparallel coincides with the geodesic and satisfies the same equations

$$\ddot{\phi} = 0, \quad \ddot{\psi} = 0.$$

They are equivalent to Eq. (46).

This example indicates that similar to the autoparallel and geodesic, the difference between nonholonomic and vakonomic dynamics for Chaplygin's nonholonomic constrained systems is determined by the torsion of the corresponding Riemann–Cartan constraint manifold. The integrability of the constraints is an efficient but not a necessary condition for the coincidence of the two dynamics.

Concluding remark. If a system is subject to Chaplygin's nonholonomic constraints, its configuration space is no longer a Riemann manifold but a Riemann–Cartan manifold with torsion, on which the free variation operation does not exist. The stationary action principles on the constraint manifold with respect to Suslov's variation and vakonomic variation lead to autoparallel equations and geodesic equations on the manifold, respectively. This result accords with principle of inertia and principle of control theory.

Similar to the geometrization of gravitational fields in general relativity and gravitational gauge theories, a system subject to Chaplygin's nonholonomic constraints in an Euclidean or a Riemann space is equivalent to a free system in a Riemann–Cartan space. By means of this

geometrization the seeming inconsistency between nonholonomic and vakonomic dynamics can be replaced by harmonious geometric relations: straightness and shortness on the same Riemann–Cartan manifold. The result are applicable to most autonomous nonholonomic constrained systems, which can be generalized to nonautonomous ones by means of the theory of connection on a contact manifold or a one-jet bundle in the forthcoming contribution.

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Complete analysis of phase transitions and ensemble equivalence for the Curie–Weiss–Potts model

Marius Costeniuc[a] and Richard S. Ellis[b]
Department of Mathematics and Statistics, University of Massachusetts, Amherst, Massachusetts 01003

Hugo Touchette[c]
School of Mathematical Sciences, Queen Mary, University of London, London, E1 4NS United Kingdom

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Using the theory of large deviations, we analyze the phase transition structure of the Curie–Weiss–Potts spin model, which is a mean-field approximation to the nearest-neighbor Potts model. It is equivalent to the Potts model on the complete graph on n vertices. The analysis is carried out both for the canonical ensemble and the microcanonical ensemble. Besides giving explicit formulas for the microcanonical entropy and for the equilibrium macrostates with respect to the two ensembles, we analyze ensemble equivalence and nonequivalence at the level of equilibrium macrostates, relating these to concavity and support properties of the microcanonical entropy. The Curie–Weiss–Potts model is the first statistical mechanical model for which such a detailed and rigorous analysis has been carried out. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1904507]

I. INTRODUCTION

The nearest-neighbor Potts model, introduced in Ref. 40, takes its place next to the Ising model as one of the most versatile models in equilibrium statistical mechanics.[49] Section I C of Ref. 49 presents a mean-field approximation to the Potts model, defined in terms of a mean interaction averaged over all the sites in the model. We refer to this approximation as the Curie–Weiss–Potts model. Both the nearest-neighbor Potts model and the Curie–Weiss–Potts model are defined by sequences of probability distributions of n spin random variables that may occupy one of q different states $\theta^1, \ldots, \theta^q$, where $q \geqslant 3$. For $q=2$ the Potts model reduces to the Ising model while the Curie–Weiss–Potts model reduces to the much simpler mean-field approximation to the Ising model known as the Curie–Weiss model.[14]

Two ways in which the Curie–Weiss–Potts model approximates the Potts model, and in fact gives rigorous bounds on quantities in the Potts model, are discussed in Refs. 31 and 39. Probabilistic limit theorems for the Curie–Weiss–Potts model are proved in Ref. 19, including the law of large numbers and its breakdown as well as various types of central limit theorems. The model is also studied in Ref. 20, which focuses on a statistical estimation problem for two parameters defining the model.

In order to carry out the analysis of the model in Refs. 19 and 20, detailed information about the structure of the set of canonical equilibrium macrostates is required, including the fact that it exhibits a discontinuous phase transition as the inverse temperature β increases through a critical value β_c. This information plays a central role in the present paper, in which we use the theory of large deviations to study the equivalence and nonequivalence of the sets of equilibrium mac-

[a]Electronic mail: costeniuc@math.umass.edu
[b]Electronic mail: rsellis@math.umass.edu
[c]Electronic mail: htouchet@alum.mit.edu

rostates for the microcanonical and canonical ensembles. An important consequence of the discontinuous phase transition exhibited by the canonical ensemble in the Curie–Weiss–Potts model is the implication that the nearest-neighbor Potts model on $\mathbb{Z}^d$ also undergoes a discontinuous phase transition whenever d is sufficiently large (Ref. 4, Theorem 2.1).

In Ref. 15 the problem of the equivalence of the microcanonical and canonical ensembles was completely solved for a general class of statistical mechanical models including short-range and long-range spin models and models of turbulence. This problem is fundamental in statistical mechanics because it focuses on the appropriate probabilistic description of statistical mechanical systems. While the theory developed in Ref. 15 is complete, our understanding is greatly enhanced by the insights obtained from studying specific models. In this regard the Curie–Weiss–Potts model is an excellent choice, lying at the boundary of the set of models for which a complete analysis involving explicit formulas is available.

For the Curie–Weiss–Potts model ensemble equivalence at the thermodynamic level is studied numerically in Ref. 29, Secs. 3–5. This level of ensemble equivalence focuses on whether the microcanonical entropy is concave on its domain; equivalently, whether the microcanonical entropy and the canonical free energy, the basic thermodynamic functions in the two ensembles, can each be expressed as the Legendre–Fenchel transform of the other (Ref. 15, pp. 1036–1037). Nonconcave anomalies in the microcanonical entropy partially correspond to regions of negative specific heat and thus thermodynamic instability.

The present paper significantly extends Ref. 29, Secs. 3–5 by analyzing rigorously ensemble equivalence at the thermodynamic level and by relating it to ensemble equivalence at the level of equilibrium macrostates via the results in Ref. 15. As prescribed by the theory of large deviations, the set $\mathcal{E}^u$ of microcanonical equilibrium macrostates and the set $\mathcal{E}_\beta$ of canonical equilibrium macrostates are defined in (2.4) and (2.3). These macrostates are, respectively, the solutions of a constrained minimization problem involving probability vectors on $\mathbb{R}^q$ and a related, unconstrained minimization problem. The equilibrium macrostates for the two ensembles are probability vectors describing equilibrium configurations of the model in each ensemble in the thermodynamic limit $n\to\infty$. For each $i=1,2,\ldots,q$, the ith component of an equilibrium macrostate gives the asymptotic relative frequency of spins taking the spin-value θ^i.

Defined via conditioning on the energy per particle, the microcanonical ensemble expresses the conservation of physical quantities such as the energy. Among other reasons, the mathematically more tractable canonical ensemble was introduced by Gibbs[22] in the hope that in the $n\to\infty$ limit the two ensembles are equivalent; i.e., all asymptotic properties of the model obtained via the microcanonical ensemble could be realized as asymptotic properties obtained via the canonical ensemble. Although most textbooks in statistical mechanics, including Refs. 1, 22, 28, 35, 41, and 44, claim that the two ensembles always give the same predictions, in general this is not the case.[48] There are many examples of statistical mechanical models for which nonequivalence of ensembles holds over a wide range of model parameters and for which physically interesting microcanonical equilibria are often omitted by the canonical ensemble. Besides the Curie–Weiss–Potts model, these models include the mean-field Blume–Emery–Griffiths model,[2,3,18] the Hamiltonian mean-field model,[12,36] the mean-field $X-Y$ model,[11] models of turbulence,[6,16,21,33,42] models of plasmas,[34,45] gravitational systems,[23–25,37,47] and a model of the Lennard-Jones gas.[5] It is hoped that our detailed analysis of ensemble nonequivalence in the Curie–Weiss–Potts model will contribute to an understanding of this fascinating and fundamental phenomenon in a wide range of other settings.

In the present paper, after summarizing the large deviation analysis of the Curie–Weiss–Potts model in Sec. II, we give explicit formulas for the elements of $\mathcal{E}_\beta$ and the elements of $\mathcal{E}^u$ in Secs. III and IV. This analysis shows that $\mathcal{E}_\beta$ exhibits a discontinuous phase transition at a critical inverse temperature β_c and that $\mathcal{E}^u$ exhibits a continuous phase transition at a critical energy u_c. The implications of these different phase transitions concerning ensemble nonequivalence are studied graphically in Sec. V and rigorously in Sec. VI, where we exhibit a range of values of the energy u for which the microcanonical equilibrium macrostates are not realized canonically; i.e., $\mathcal{E}^u$ is disjoint from $\mathcal{E}_\beta$ for all β. As described in the main theorem in Ref. 15 and summarized here

in Theorem 5.1, this range of values of the energy is precisely the set on which the microcanonical entropy is not concave. The analysis of this bridge between ensemble nonequivalence at the thermodynamic level and ensemble nonequivalence at the level of equilibrium macrostates is one of the main contributions of Ref. 15 for general models and of the present paper for the Curie–Weiss–Potts model. In a sequel to the present paper,[9] we will extend our analysis of the Curie–Weiss–Potts model to the so-called Gaussian ensemble[7,8,26,27,30,46] to show, among other results, that for each value of the energy for which the microcanonical and canonical ensembles are nonequivalent, we can find a Gaussian ensemble that is fully equivalent with the microcanonical ensemble.[10]

II. SETS OF EQUILIBRIUM MACROSTATES FOR THE TWO ENSEMBLES

Let $q \geqslant 3$ be a fixed integer and define $\Lambda = \{\theta^1, \theta^2, \ldots, \theta^q\}$, where the θ^i are any q distinct vectors in $\mathbb{R}^q$. In the definition of the Curie–Weiss–Potts model, the precise values of these vectors is immaterial. For each $n \in \mathbb{N}$ the model is defined by spin random variables $\omega_1, \omega_2, \ldots, \omega_n$ that take values in Λ. The canonical and microcanonical ensembles for the model are defined in terms of probability measures on the configuration spaces Λ^n, which consist of the microstates $\omega = (\omega_1, \ldots, \omega_n)$. We also introduce the n-fold product measure P_n on Λ^n with identical one-dimensional marginals

$$\overline{\rho} = \frac{1}{q}\sum_{i=1}^{q} \delta_{\theta^i}.$$

Thus for all $\omega \in \Lambda^n$, $P_n(\omega) = 1/q^n$. For $n \in \mathbb{N}$ and $\omega \in \Lambda^n$ the Hamiltonian for the q-state Curie–Weiss–Potts model is defined by

$$H_n(\omega) = -\frac{1}{2n}\sum_{j,k=1}^{n} \delta(\omega_j, \omega_k),$$

where $\delta(\omega_j, \omega_k)$ equals 1 if $\omega_j = \omega_k$ and equals 0 otherwise. The energy per particle is defined by

$$h_n(\omega) = \frac{1}{n} H_n(\omega).$$

For inverse temperature $\beta \in \mathbb{R}$ and subsets B of Λ^n the canonical ensemble is the probability measure $P_{n,\beta}$ defined by

$$P_{n,\beta}\{B\} = \frac{1}{\sum_{\omega \in \Lambda^n} \exp[-n\beta h_n(\omega)]} \cdot \sum_{\omega \in B} \exp[-n\beta h_n(\omega)].$$

For energy $u \in \mathbb{R}$ and $r > 0$ the microcanonical ensemble is the conditioned probability measure $P_n^{u,r}$ defined by

$$P_n^{u,r}\{B\} = P_n\{B | h_n \in [u - r, u + r]\}.$$

The key to our analysis of the Curie–Weiss–Potts model is to express both the canonical and the microcanonical ensembles in terms of the empirical vector

$$L_n = L_n(\omega) = (L_{n,1}(\omega), L_{n,2}(\omega), \ldots, L_{n,q}(\omega)),$$

the ith component of which is defined by

$$L_{n,i}(\omega) = \frac{1}{n}\sum_{j=1}^{n} \delta(\omega_j, \theta^i).$$

This quantity equals the relative frequency with which $\omega_j, j \in \{1, \ldots, n\}$, equals θ^i. L_n takes values in the set of probability vectors

$$\mathcal{P} = \left\{ \nu \in \mathbb{R}^q : \nu = (\nu_1, \nu_2, \ldots, \nu_q), \text{ each } \nu_i \geqslant 0, \sum_{i=1}^{q} \nu_i = 1 \right\}.$$

As we will see, each probability vector in $\mathcal{P}$ represents a possible equilibrium macrostate for the model.

There is a one-to-one correspondence between $\mathcal{P}$ and the set $\mathcal{P}(\Lambda)$ of probability measures on Λ, $\nu \in \mathcal{P}$ corresponding to the probability measure $\Sigma_{i=1}^{q} \nu_i \delta_{\theta^i}$. The element $\rho \in \mathcal{P}$ corresponding to the one-dimensional marginal $\overline{\rho}$ of the prior measures P_n is the uniform vector having equal components $1/q$.

We denote by $\langle \cdot, \cdot \rangle$ the inner product on $\mathbb{R}^q$. Since

$$\sum_{i=1}^{q} \sum_{j=1}^{n} \delta(\omega_j, \xi^i) \cdot \sum_{k=1}^{n} \delta(\omega_k, \xi^i) = \sum_{j,k=1}^{n} \delta(\omega_j, \omega_k),$$

it follows that the energy per particle can be rewritten as

$$h_n(\omega) = -\frac{1}{2n^2} \sum_{j,k=1}^{n} \delta(\omega_j, \omega_k) = -\frac{1}{2} \langle L_n(\omega), L_n(\omega) \rangle;$$

i.e.,

$$h_n(\omega) = \widetilde{H}(L_n(\omega)), \quad \text{where } \widetilde{H}(\nu) = -\tfrac{1}{2}\langle \nu, \nu \rangle \quad \text{for } \nu \in \mathcal{P}. \tag{2.1}$$

We call $\widetilde{H}$ the energy representation function.

We appeal to the theory of large deviations to define the sets of microcanonical equilibrium macrostates and canonical equilibrium macrostates. Sanov's theorem states that with respect to the product measures P_n, the empirical vectors L_n satisfy the large deviation principle (LDP) on $\mathcal{P}$ with rate function given by the relative entropy $R(\cdot|\rho)$ (Ref. 14, Theorem VIII.2.1). For $\nu \in \mathcal{P}$ this is defined by

$$R(\nu|\rho) = \sum_{i=1}^{q} \nu_i \log(q\nu_i).$$

We express this LDP by the formal notation $P_n\{L_n \in \mathrm{d}\nu\} \approx \exp[-nR(\nu|\rho)]$. The LDPs for L_n with respect to the two ensembles $P_{n,\beta}$ and $P_n^{u,r}$ in the thermodynamic limit $n \to \infty$, $r \to 0$ can be proved from the LDP for the P_n-distributions of L_n as in Theorems 2.4 and 3.2 in Ref. 15, in which minor notational changes have to be made. We express these LDPs by the formal notation

$$P_{n,\beta}\{L_n \in \mathrm{d}\nu\} \approx \exp[-nI_\beta(\nu)] \quad \text{and } P_n^{u,r}\{L_n \in \mathrm{d}\nu\} \approx \exp[-nI^u(\nu)], \tag{2.2}$$

where for $\nu \in \mathcal{P}$

$$I_\beta(\nu) = R(\nu|\rho) - \frac{\beta}{2}\langle \nu, \nu \rangle - \text{const}$$

and

$$I^u(\nu) = \begin{cases} R(\nu|\rho) - \text{const} & \text{if } -\frac{1}{2}\langle \nu, \nu \rangle = u, \\ \infty & \text{otherwise.} \end{cases}$$

The constants appearing in the definitions of I_β and I^u have the properties that $\inf_{\nu \in \mathcal{P}} I_\beta(\nu) = 0$ and $\inf_{\nu \in \mathcal{P}} I^u(\nu) = 0$. Thus I_β and I^u map $\mathcal{P}$ into $[0, \infty)$.

As the formulas in (2.2) suggest, if $I_\beta(\nu) > 0$ or $I^u(\nu) > 0$, then ν has an exponentially small probability of being observed in the corresponding ensemble in the thermodynamic limit. Hence it makes sense to define the corresponding sets of equilibrium macrostates to be

$$\mathcal{E}_\beta = \{\nu \in \mathcal{P} : I_\beta(\nu) = 0\} \quad \text{and} \quad \mathcal{E}^u = \{\nu \in \mathcal{P} : I^u(\nu) = 0\}.$$

A rigorous justification for this is given in Ref. 15, Theorem 2.4(d). Using the formulas for I_β and I^u, we see that

$$\mathcal{E}_\beta = \left\{ \nu \in \mathcal{P} : \nu \text{ minimizes } R(\nu|\rho) - \frac{\beta}{2}\langle \nu, \nu \rangle \right\} \tag{2.3}$$

and

$$\mathcal{E}^u = \left\{ \nu \in \mathcal{P} : \nu \text{ minimizes } R(\nu|\rho) \text{ subject to } -\tfrac{1}{2}\langle \nu, \nu \rangle = u \right\}. \tag{2.4}$$

Each element ν in $\mathcal{E}_\beta$ and $\mathcal{E}^u$ describes an equilibrium configuration of the model in the corresponding ensemble in the thermodynamic limit. The ith component ν_i gives the asymptotic relative frequency of spins taking the value θ^i.

The set $\mathcal{E}^u$ is defined for all u for which the constraint in the definition of I^u is satisfied for some $\nu \in \mathcal{P}$. Otherwise, $\mathcal{E}^u$ is not defined. If $\mathcal{E}^u$ is defined, then $\mathcal{E}^u$ is nonempty; if $\mathcal{E}^u$ is not defined, then we shall set $\mathcal{E}^u = \varnothing$.

The question of equivalence of ensembles at the level of equilibrium macrostates focuses on the relationships between $\mathcal{E}^u$, defined in terms of the constrained minimization problem in (2.4), and $\mathcal{E}_\beta$, defined in terms of the related, unconstrained minimization problem in (2.3). We will focus on this question in Secs. V and VI after we determine the structures of $\mathcal{E}_\beta$ and $\mathcal{E}^u$ in the next two sections.

III. FORM OF $\mathcal{E}_\beta$ AND ITS DISCONTINUOUS PHASE TRANSITION

In this section we derive the form of the set $\mathcal{E}_\beta$ of canonical equilibrium macrostates for all $\beta \in \mathbb{R}$. This form is given in Theorem 3.1, which shows that with respect to the canonical ensemble the Curie–Weiss–Potts model undergoes a discontinuous phase transition at the critical inverse temperature

$$\beta_c = \frac{2(q-1)}{q-2} \log(q-1). \tag{3.1}$$

In order to describe the form of $\mathcal{E}_\beta$, we introduce the function ψ that maps $[0, 1]$ into $\mathcal{P}$ and is defined by

$$\psi(w) = \left(\frac{1 + (q-1)w}{q}, \frac{1-w}{q}, \ldots, \frac{1-w}{q} \right); \tag{3.2}$$

the last $q-1$ components all equal $(1-w)/q$. Recalling that ρ is the uniform vector in $\mathcal{P}$ having equal components $1/q$, we see that $\rho = \psi(0)$.

Theorem 3.1: *For $\beta > 0$ let $w(\beta)$ be the largest solution of the equation*

$$w = \frac{1 - e^{-\beta w}}{1 + (q-1)e^{-\beta w}}. \tag{3.3}$$

The following conclusions hold.

(a) *The quantity* $w(\beta)$ *is well defined and lies in* $[0, 1]$. *It is positive, strictly increasing, and differentiable for* $\beta \in (\beta_c, \infty)$ *and satisfies* $w(\beta_c) = (q-2)/(q-1)$ *and* $\lim_{\beta \to \infty} w(\beta) = 1$.

(b) *For* $\beta \geqslant \beta_c$, *define* $\nu^1(\beta) = \psi(w(\beta))$ *and let* $\nu^i(\beta)$, $i = 2, \ldots, q$, *denote the points in* $\mathbb{R}^q$ *obtained by interchanging the first and ith components of* $\nu^1(\beta)$. *Then the set* $\mathcal{E}_\beta$ *defined in* (2.3) *has the form*

$$\mathcal{E}_\beta = \begin{cases} \{\rho\} & \text{for } \beta < \beta_c, \\ \{\rho, \nu^1(\beta_c), \nu^2(\beta_c), \ldots, \nu^q(\beta_c)\} & \text{for } \beta = \beta_c, \\ \{\nu^1(\beta), \nu^2(\beta), \ldots, \nu^q(\beta)\} & \text{for } \beta > \beta_c. \end{cases} \tag{3.4}$$

For $\beta \geqslant \beta_c$, *the vectors in* $\mathcal{E}_\beta$ *are all distinct and each* $\nu^i(\beta)$ *is continuous. The vector* $\nu^1(\beta_c)$ *is given by*

$$\nu^1(\beta_c) = \psi(w(\beta_c)) = \psi\left(\frac{q-2}{q-1}\right) = \left(1 - \frac{1}{q}, \frac{1}{q(q-1)}, \ldots, \frac{1}{q(q-1)}\right); \tag{3.5}$$

the last $q-1$ *components all equal* $1/q(q-1)$.

The form of $\mathcal{E}_\beta$ for $\beta > 0$ is proved in Appendix B from a new convex-duality theorem proved in Appendix A and from the complicated calculation of the global minimum points of a related function given in Theorem 2.1 in Ref. 19. The form of $\mathcal{E}_\beta$ for $\beta \leqslant 0$ is also determined in Appendix B. The other assertions in Theorem 3.1 are proved in Theorem 2.1 in Ref. 19.

For $\beta > 0$ the form of $\mathcal{E}_\beta$ reflects a competition between disorder, as represented by the relative entropy $R(\nu|\rho)$, and order, as represented by the energy representation function $-\frac{1}{2}\langle \nu, \nu \rangle$. For small $\beta > 0$, $R(\nu|\rho)$ predominates. Since $R(\nu|\rho)$ attains its minimum of 0 at the unique vector ρ, we expect that for small β, $\mathcal{E}_\beta$ should contain a single vector. On the other hand, for large $\beta > 0$, $-\frac{1}{2}\langle \nu, \nu \rangle$ predominates. This function attains its minimum at $\nu^1 = (1, 0, \ldots, 0)$ and at the vectors ν^i, $i = 1, \ldots, q$, obtained by interchanging the first and ith components of ν^1. Hence we expect that for large β, $\mathcal{E}_\beta$ should contain q distinct vectors $\nu^i(\beta)$ having the property that $\nu^i(\beta) \to \nu^i$ as $\beta \to \infty$. The major surprise of the theorem is that for $\beta = \beta_c$, $\mathcal{E}_\beta$ consists of the $q+1$ distinct vectors ρ and $\nu^i(\beta_c)$ for $i = 1, 2, \ldots, q$.

The discontinuous bifurcation in the composition of $\mathcal{E}_\beta$ from 1 vector for $\beta < \beta_c$ to $q+1$ vectors for $\beta = \beta_c$ to q vectors for $\beta > \beta_c$ corresponds to a discontinuous phase transition exhibited by the canonical ensemble. In Fig. 2 in Sec. V this phase transition is shown together with the continuous phase transition exhibited by the microcanonical ensemble. The latter phase transition and the form of the set of microcanonical equilibrium macrostates are the focus of the next section.

IV. FORM OF $\mathcal{E}^u$ AND ITS CONTINUOUS PHASE TRANSITION

We now turn to the form of the set $\mathcal{E}^u$ for all $u \in \left[-\frac{1}{2}, -1/2q\right]$, which is the set of u for which $\mathcal{E}^u$ is nonempty. In the specific case $q = 3$ part (c) of Theorem 4.2 gives the form of $\mathcal{E}^u$, the calculation of which is much simpler than the calculation of the form of $\mathcal{E}_\beta$. The proof is based on the method of Lagrange multipliers, which also works for general $q \geqslant 4$ provided the next conjecture on the form of the elements in $\mathcal{E}^u$ is valid. The validity of this conjecture has been confirmed numerically for all $q \in \{4, 5, \ldots, 10^4\}$ and all $u \in \left(-\frac{1}{2}, -1/2q\right)$ of the form $u = -\frac{1}{2} + 0.02k$, where k is a positive integer.

Conjecture 4.1: For any $q \geqslant 4$ *and all* $u \in \left(-\frac{1}{2}, -1/2q\right)$, *there exist* $a \neq b \in (0, 1)$ *such that modulo permutations, any* $\nu \in \mathcal{E}^u$ *has the form* $(a, b, \ldots, b)$, *the last* $q-1$ *components of which all equal* b.

Parts (a) and (b) of Theorem 4.2 are proved for general $q \geqslant 3$. Part (c) shows that modulo permutations, for $q = 3$, $\nu \in \mathcal{E}^u$ has the form $(a(u), b(u), b(u))$ and determines the precise formulas for $a(u)$ and $b(u)$. As specified in part (d), for $q \geqslant 4$ we can also determine the precise formula for $\nu \in \mathcal{E}^u$ provided Conjecture 4.1 is valid.

Theorem 4.2 shows that with respect to the microcanonical ensemble the Curie–Weiss–Potts model undergoes a continuous phase transition as u decreases from the critical energy value $u_c = -1/2q$. This contrast with the discontinuous phase transition exhibited by the canonical ensemble is closely related to the nonequivalence of the microcanonical and canonical ensembles for a range of u. Ensemble equivalence and nonequivalence will be explored in the next section, where we will see that it is reflected by support and concavity properties of the microcanonical entropy. An explicit formula for the microcanonical entropy is given in Theorem 4.3.

Theorem 4.2: *For $u \in \mathbb{R}$ we define $\mathcal{E}^u$ by* (2.4). *The following conclusions hold.*

(a) *For any $q \geqslant 3$, $\mathcal{E}^u$ is nonempty if and only if $u \in \left[-\frac{1}{2}, -1/2q\right]$. This interval coincides with the range of the energy representation function $\tilde{H}(\nu) = -\frac{1}{2}\langle \nu, \nu \rangle$ on $\mathcal{P}$.*

(b) *For any $q \geqslant 3$, $\mathcal{E}^{-1/2q} = \{\rho\} = \{(1/q, 1/q, \ldots, 1/q)\}$ and*

$$\mathcal{E}^{-1/2} = \{(1,0,\ldots,0),(0,1,\ldots,0),\ldots,(0,0,\ldots,1)\}.$$

(c) *Let $q=3$. For $u \in \left(-\frac{1}{2}, -1/2q\right)$, $\mathcal{E}^u$ consists of the three distinct vectors $\{\mu^1(u), \mu^2(u), \mu^3(u)\}$, where $\mu^1(u) = (a(u), b(u), b(u))$,*

$$a(u) = \frac{1 + \sqrt{2(-6u-1)}}{3} \quad \text{and } b(u) = \frac{2 - \sqrt{2(-6u-1)}}{6}. \tag{4.1}$$

The vectors $\mu^i(u)$, $i=2,3$, denote the points in $\mathbb{R}^3$ obtained by interchanging the first and the ith components of $\mu^1(u)$.

(d) *Let $q \geqslant 4$ and assume that Conjecture* 4.1 *is valid. Then for $u \in \left(-\frac{1}{2}, -1/2q\right)$, $\mathcal{E}^u$ consists of the q distinct vectors $\{\mu^1(u), \ldots, \mu^q(u)\}$, where $\mu^1(u) = (a(u), b(u), \ldots, b(u))$,*

$$a(u) = \frac{1 + \sqrt{(q-1)(-2qu-1)}}{q} \quad \text{and } b(u) = \frac{q - 1 - \sqrt{(q-1)(-2qu-1)}}{(q-1)q}.$$

The last $q-1$ components of $\mu^1(u)$ all equal $b(u)$, and the vectors $\mu^i(u)$, $i=2,\ldots,q$, denote the points in $\mathbb{R}^q$ obtained by interchanging the first and the ith components of $\mu^1(u)$.

We return to part (b) of Theorem 4.2 in order to discuss the nature of the phase transition exhibited by the microcanonical ensemble. The functions $a(u)$ and $b(u)$ given in (4.1) are both continuous for $u \in \left[-\frac{1}{2}, -1/2q\right]$ and satisfy

$$\lim_{u \to (-1/2q)^-} a(u) = \lim_{u \to (-1/2q)^-} b(u) = \frac{1}{q} = a\left(-\frac{1}{2q}\right) = b\left(-\frac{1}{2q}\right).$$

Therefore, for $i=1,\ldots,q$, $\lim_{u \to (-1/2q)^-} \mu^i(u) = \rho$. It follows that the microcanonical ensemble exhibits a continuous phase transition as u decreases from $u_c = -1/2q$, the unique equilibrium macrostate ρ for $u = u_c$ bifurcating continuously into the q distinct macrostates $\mu^i(u)$ as u decreases from its maximum value. This is rigorously true for $q=3$. Provided Conjecture 4.1 is true, it is also true for $q \geqslant 4$, as one easily checks using part (d) of Theorem 4.2.

Before proving Theorem 4.2, we introduce the microcanonical entropy

$$s(u) = -\inf\left\{R(\nu|\rho) : \nu \in \mathcal{P}, -\tfrac{1}{2}\langle \nu, \nu \rangle = u\right\}. \tag{4.2}$$

As we will see in the next section, this function plays a crucial role in the analysis of ensemble equivalence and nonequivalence for the Curie–Weiss–Potts model. The domain of s is the set $\operatorname{dom} s = \{u \in \mathbb{R} : s(u) > -\infty\}$; for $u \notin \operatorname{dom} s$, we set $s(u) = -\infty$. Since $R(\nu|\rho) < \infty$ for all $\nu \in \mathcal{P}$, $\operatorname{dom} s$ equals the range of $\tilde{H}(\nu) = -\frac{1}{2}\langle \nu, \nu \rangle$ on $\mathcal{P}$, which is the interval $\left[-\frac{1}{2}, -1/2q\right]$ [Theorem 4.2(a)].

Since $0 \leqslant R(\nu|\rho)$ for all $\nu \in \mathcal{P}$, $s(u) \in [-\infty, 0]$ for all u. The continuity of $R(\nu|\rho)$ on $\mathcal{P}$ and the compactness of the constraint set in (4.2) guarantee that for $u \in \operatorname{dom} s$ the infimum in the definition of $s(u)$ is attained for some $\nu \in \mathcal{P}$. Since $R(\nu|\rho) > R(\rho|\rho) = 0$ for all $\nu \neq \rho$, it follows that s attains its maximum of 0 at the unique value $-1/2q = -\frac{1}{2}\langle \rho, \rho \rangle$.

As we have just seen, $s(-1/2q)=0$. For $u\in\left(-\frac{1}{2},-1/2q\right)$, according to parts (c) and (d) of Theorem 4.2, $\mathcal{E}^u$ consists of the unique vector $\mu^1(u)$ modulo permutations. Since for $i=2,3,\ldots,q$, $R(\mu^i(u)|\rho)=R(\mu^1(u)|\rho)$, we conclude that

$$s(u)=-R(\mu^1(u)|\rho)=-a(u)\log(qa(u))-(q-1)b(u)\log(qb(u)).$$

Finally, for $u=-\frac{1}{2}$, modulo permutations $\mathcal{E}^u$ consists of the unique vector (1, 0,…,0) [see (4.7)], and so $s\left(-\frac{1}{2}\right)=-R((1,0,\ldots,0)|\rho)=-\log q$. The resulting formulas for $s(u)$ are recorded in the next theorem, where we distinguish between $q=3$ and $q\geqslant 4$.

Theorem 4.3: *We define the microcanonical entropy* $s(u)$ *in* (4.2). *The following conclusions hold.*

(a) $\operatorname{dom} s=\left[-\frac{1}{2},-1/2q\right]$; *for any* $u\in\operatorname{dom} s$, $u\neq -1/2q$, $s(u)<s(-1/2q)=0$; *and* $s\left(-\frac{1}{2}\right)=-\log q$.

(b) *Let* $q=3$. *Then for* $u\in\left(-\frac{1}{2},-1/2q\right)=\left(-\frac{1}{2},-\frac{1}{6}\right)$,

$$s(u)=-\frac{1+\sqrt{2(-6u-1)}}{3}\log(1+\sqrt{2(-6u-1)})-\frac{2-\sqrt{2(-6u-1)}}{3}\log\left(\frac{2-\sqrt{2(-6u-1)}}{2}\right). \tag{4.3}$$

(c) *Let* $q\geqslant 4$ *and assume that Conjecture* 4.1 *is valid. Then for* $u\in\left(-\frac{1}{2},-1/2q\right)$,

$$s(u)=-\frac{1+\sqrt{(q-1)(-2qu-1)}}{q}\log(1+\sqrt{(q-1)(-2qu-1)})-\frac{q-1-\sqrt{(q-1)(-2qu-1)}}{q}\log\left(\frac{q-1-\sqrt{(q-1)(-2qu-1)}}{q-1}\right). \tag{4.4}$$

We now turn to the proof of Theorem 4.2, which gives the form of $\mathcal{E}^u$. We start by proving part (a). The set $\mathcal{E}^u$ of microcanonical equilibrium macrostates consists of all $\nu\in\mathcal{P}$ that minimize the relative entropy $R(\nu|\rho)$ subject to the constraint that

$$\widetilde{H}(\nu)=-\tfrac{1}{2}\langle\nu,\nu\rangle=u.$$

Let $u=-\frac{1}{2}r^2$. Since $\mathcal{P}$ consists of all non-negative vectors in $\mathbb{R}^q$ satisfying $\nu_1+\cdots+\nu_q=1$, the constraint set in the minimization problem defining $\mathcal{E}^u$ is given by

$$C(u)=C\left(-\tfrac{1}{2}r^2\right)=\left\{\nu\in\mathbb{R}^q:\nu_1\geqslant 0,\ldots,\nu_q\geqslant 0,\sum_{j=1}^q\nu_j=1,\sum_{j=1}^q\nu_j^2=r^2\right\}. \tag{4.5}$$

Geometrically, $C\left(-\frac{1}{2}r^2\right)$ is the intersection of the non-negative orthant of $\mathbb{R}^q$, the hyperplane consisting of $\nu\in\mathbb{R}^\sigma$ that satisfy $\nu_1+\cdots+\nu_q=1$, and the hypersphere in $\mathbb{R}^q$ with center 0 and radius r. Clearly, $C(u)\neq\emptyset$ if and only if u lies in the range of the energy representation function $\widetilde{H}(\nu)=-\frac{1}{2}\langle\nu,\nu\rangle$ on $\mathcal{P}$. Because $0\leqslant R(\nu|\rho)<\infty$ for all $\nu\in C(u)$, the range of $\widetilde{H}$ on $\mathcal{P}$ also equals the set of u for which $\mathcal{E}^u\neq\emptyset$.

The geometric description of $C(u)$ makes it straightforward to determine those values of u for which this constraint set is nonempty. The smallest value of r for which $C\left(-\frac{1}{2}r^2\right)\neq\emptyset$ is obtained when the hypersphere of radius r is tangent to the hyperplane, the point of tangency being $\rho=(1/q,1/q,\ldots,1/q)$, the closest probability vector to the origin. The hypersphere and the hyperplane are tangent when $r=1/\sqrt{q}$, which coincides with the distance from the center of the hypersphere to the hyperplane. It follows that the largest value of u for which $C(u)\neq\emptyset$, and thus $\mathcal{E}^u\neq\emptyset$, is $u=-\frac{1}{2}r^2=-1/2q$. In this case

$$C\left(-\frac{1}{2q}\right)=\{\rho\}=\left\{\left(\frac{1}{q},\frac{1}{q},\ldots,\frac{1}{q}\right)\right\}=\mathcal{E}^{-1/2q}. \tag{4.6}$$

For all sufficiently large r, $C(-\frac{1}{2}r^2)$ is empty because the hypersphere of radius r has empty intersection with the intersection of the hyperplane and the non-negative orthant of $\mathbb{R}^q$. The largest value for r for which this does not occur is found by subtracting the two equations defining the hyperplane and the hypersphere. Since each $\nu_i \in [0,1]$, it follows that

$$0 \leqslant \sum_{i=1}^{q} \nu_i(1-\nu_i) = 1 - r^2,$$

and this in turn implies that $r^2 \leqslant 1$. Thus $r=1$ is the largest value for r for which $C(-\frac{1}{2}r^2) \neq \emptyset$. We conclude that the smallest value of u for which $C(u) \neq \emptyset$, and thus $\mathcal{E}^u \neq \emptyset$, is $u=-\frac{1}{2}r^2=-\frac{1}{2}$. The set $\mathcal{E}^{-\frac{1}{2}}$ consists of the points at which the hyperplane intersects each of the positive coordinate axes; i.e.,

$$\mathcal{E}^{-1/2} = \{(1,0,\ldots,0),(0,1,\ldots,0),\ldots,(0,0,\ldots,1)\}. \tag{4.7}$$

This completes the proof of part (a) of Theorem 4.2.

For $u \in [-\frac{1}{2}, -1/2q]$, we now determine the form $\mathcal{E}^u$ as specified in parts (b)–(d) of Theorem 4.2. Part (b) considers any $q \geqslant 3$ and the values $u=-1/2q$ and $u=-\frac{1}{2}$, part (c) $q=3$ and $u \in (-\frac{1}{2}, -1/2q)$, and part (d) $q \geqslant 4$ and $u \in (-\frac{1}{2}, -1/2q)$. Part (b) has already been proved; for $u=-1/2q$ and $u=-\frac{1}{2}$, the sets $\mathcal{E}^u$ are given in (4.6) and (4.7).

We now consider $q \geqslant 3$ and $u \in (-\frac{1}{2}, -1/2q)$. For $\nu \in \mathcal{P}$ define

$$K(\nu) = \sum_{j=1}^{q} \nu_j \quad \text{and } \tilde{H}(\nu) = -\tfrac{1}{2}\langle \nu, \nu \rangle.$$

By definition $\nu=(\nu_1,\ldots,\nu_q) \in \mathcal{E}^u$ if and only if ν minimizes $R(\nu|\rho)=\Sigma_{j=1}^q \nu_j \log(q\nu_j)$ subject to the constraints $K(\nu)=1$, $\tilde{H}(\nu)=u$, and $\nu_1 \geqslant 0,\ldots,\nu_q \geqslant 0$. For $u \in (-\frac{1}{2}, -1/2q)$ we divide into two parts the calculation of the form of $\nu \in \mathcal{E}^u$. First we use Lagrange multipliers to solve the constrained minimization problem when $\nu_1 > 0,\ldots,\nu_1 > 0$. Then we argue that the vectors ν found via Lagrange multipliers solve the original constrained minimization problem when $\nu_1 \geqslant 0,\ldots,\nu_q \geqslant 0$.

We introduce Lagrange multipliers γ and λ. Any critical point of $R(\nu|\rho)$ subject to the constraints $K(\nu)=1$, $\tilde{H}(\nu)=u$, and $\nu_1 > 0$, $\nu_2 > 0,\ldots,\nu_q > 0$ satisfies

$$\nabla R(\nu|\rho) = \gamma \nabla K(\nu) + \lambda \nabla \tilde{H}(\nu),$$

$$K(\nu) = 1,$$

$$\tilde{H}(\nu) = u,$$

$$\nu_j > 0 \quad \text{for } j = 1,2,\ldots,q.$$

This system of equations is equivalent to

$$1 + \log(q\nu_j) = \gamma - \lambda\nu_j \quad \text{for } j = 1,2,\ldots,q, \tag{4.8}$$

$$\sum_{j=1}^{q} \nu_j = 1,$$

$$-\frac{1}{2}\sum_{j=1}^{q} \nu_j^2 = u,$$

$$\nu_j > 0 \quad \text{for } j = 1,2,\ldots,q.$$

By the strict concavity of the logarithm, the first equation can have at most two solutions. Hence modulo permutations, there exists $n \in \{0,1,\ldots,q\}$ and distinct numbers $a,b \in (0,1)$ such that the first n components of any critical point ν all equal a and the last $q-n$ components of ν all equal b. The second and third equations in (4.8) take the form

$$na + (q-n)b = 1 \quad \text{and } na^2 + (q-n)b^2 = -2u. \tag{4.9}$$

If $n=0$, then $b=1/q$, while if $n=q$, then $a=1/q$. Both cases correspond to $\nu = (1/q,\ldots,1/q) = \rho$ and $u=-1/2q$, which does not lie in the open interval $\left(-\frac{1}{2},-1/2q\right)$ currently under consideration.

We now focus on $n \in \{1,\ldots,q-1\}$. In this case the two solutions of (4.9) are

$$a_1(n) = \frac{n - \sqrt{n(q-n)(-2qu-1)}}{nq}, \quad b_1(n) = \frac{q-n+\sqrt{n(q-n)(-2qu-1)}}{(q-n)q} \tag{4.10}$$

and

$$a_2(n) = \frac{n + \sqrt{n(q-n)(-2qu-1)}}{nq}, \quad b_2(n) = \frac{q-n-\sqrt{n(q-n)(-2qu-1)}}{(q-n)q}. \tag{4.11}$$

Since $u \in \left(-\frac{1}{2},-1/2q\right)$, these quantities are all well defined and $a_j(n) \neq b_j(n)$ for $j=1,2$. In addition,

$$a_1(q-n) = b_2(n) \quad \text{and } b_1(q-n) = a_2(n).$$

This means that the point having the first n components $a_2(n)$ and the last $q-n$ components $b_2(n)$ equals, modulo permutations, the point having the first $q-n$ components $a_1(q-n)$ and the last n components $b_1(q-n)$.

Thus, without loss of generality, we can seek solutions of the system (4.8) having the first n components $a_2(n)$ and the last $q-n$ components $b_2(n)$. While $a_2(1)$ and $b_2(1)$ are always positive for all $u \in \left(-\frac{1}{2},-1/2q\right)$, $b_2(n)$ might be negative for some $n \in \{2,\ldots,q-1\}$ and some $u \in \left(-\frac{1}{2},-1/2q\right)$. In this case the positivity constraint in the last line of (4.8) excludes such values of n and u.

We give full details when $q=3$, the case considered in part (c) of Theorem 4.2. When $q=3$, the interval $\left(-\frac{1}{2},-1/2q\right)$ equals $\left(-\frac{1}{2},-1/6\right)$ and we have $n \in \{1,2\}$. For $n=1$ and $n=2$ (4.11) takes the form

$$a_2(1) = \frac{1+\sqrt{2(-6u-1)}}{3}, \quad b_2(1) = \frac{2-\sqrt{2(-6u-1)}}{6}$$

and

$$a_2(2) = \frac{2+\sqrt{2(-6u-1)}}{6}, \quad b_2(2) = \frac{1-\sqrt{2(-6u-1)}}{3}.$$

For $u \in \left(-\frac{1}{2},-\frac{1}{4}\right)$, $b_2(2)$ is negative and hence a solution of (4.8) cannot have the form $(a_2(2),a_2(2),b_2(2))$. We conclude that when $u \in \left(-\frac{1}{2},-\frac{1}{4}\right)$, $\nu=(a_2(1),b_2(1),b_2(1))$ is, modulo permutations, the unique solution of (4.8) and thus the unique minimizer of $R(\nu|\rho)$ subject to the constraints in the last three lines of (4.8). For $u \in \left[-\frac{1}{4},-\frac{1}{6}\right)$, a straightforward calculation shows that

$$R((a_2(1),b_2(1),b_2(1))|\rho) < R((a_2(2),a_2(2),b_2(2))|\rho).$$

It follows again that $\nu=(a_2(1),b_2(1),b_2(1))$ is, modulo permutations, the unique minimizer of $R(\nu|\rho)$ subject to the constraints in the last three lines of (4.8). This completes the proof that for

$q=3$ and any $u \in \left(-\frac{1}{2}, -\frac{1}{6}\right)$, $\nu=(a_2(1), b_2(1), b_2(1))$ is, modulo permutations, the unique minimizer of $R(\mu|\rho)$ subject to the constraints $K(\nu)=1$, $\widetilde{H}(\nu)=u$, and $\nu_1>0$, $\nu_2>0$, $\nu_3>0$.

We now prove for $q=3$ that the minimizers found via Lagrange multipliers when $K(\nu)=1$, $\widetilde{H}(\nu)=u$, and $\nu_1>0$, $\nu_2>0$, $\nu_3>0$ also minimize $R(\nu|\rho)$ subject to the constraints $K(\nu)=1$, $\widetilde{H}(\nu)=u$, and $\nu_1 \geqslant 0$, $\nu_2 \geqslant 0$, $\nu_3 \geqslant 0$. If $\nu=(\nu_1, \nu_2, \nu_3)$ satisfies the latter constraints and has two components equal to zero, then modulo permutations $\nu=(1,0,0)$ and $\widetilde{H}(\nu)=u=-\frac{1}{2}$, which does not lie in the open interval $\left(-\frac{1}{2}, -\frac{1}{6}\right)$ currently under consideration. Thus we only have to consider the case where ν has one component equal to zero; i.e, $\nu=(0, a_0, b_0)$ with $a_0 \geqslant b_0$. In this case the second and third equations in (4.8) have the solution

$$a_0 = \frac{1+\sqrt{-4u-1}}{2}, \quad b_0 = \frac{1-\sqrt{-4u-1}}{2}.$$

We now claim that modulo permutations the unique minimizer of $R(\nu|\rho)$ subject to the constraints $K(\nu)=1$, $\widetilde{H}(\nu)=u$, and $\nu_1 \geqslant 0$, $\nu_2 \geqslant 0$, $\nu_3 \geqslant 0$ has the form $(a_2(1), b_2(1), b_2(1))$ found in the preceding paragraph. The claim follows from the calculation

$$R((a_2(1), b_2(1), b_2(1))|\rho) < R((0, a_0, b_0)|\rho),$$

which is valid for all $u \in \left(-\frac{1}{2}, -\frac{1}{6}\right)$. This completes the proof of part (c) of Theorem 4.2, which gives the form of $\nu \in \mathcal{E}^u$ for $q=3$ and $u \in \left(-\frac{1}{2}, -\frac{1}{6}\right)$.

We now turn to part (d) of Theorem 4.2, which gives the form of $\mathcal{E}^u$ for $q \geqslant 4$ and $u \in \left(-\frac{1}{2}, -1/2q\right)$. If, as in the case $q=3$, we knew that modulo permutations, the minimizers have the form $(a, b, \ldots, b)$ as specified in Conjecture 4.1, then as in the case $q=3$ we would be able to derive explicit formulas for these minimizers. If Conjecture 4.1 is true, then it is easily verified that modulo permutations, $\mathcal{E}^u$ consists of the unique point $\nu=(a_2(1), b_2(1), \ldots, b_2(1))$, where $a_2(1)$ and $b_2(1)$ are defined in (4.11) for $u \in \left(-\frac{1}{2}, -1/2q\right)$. This gives part (d) of Theorem 4.2. The proof of the theorem is complete.

At the end of Sec. VI we will see that there exists an explicit value of $u_0 \in \left(-\frac{1}{2}, -1/2q\right)$ such that Conjecture 4.1 is valid for any $q \geqslant 4$ and all $u \in \left(-\frac{1}{2}, u_0\right]$. Hence for these values of u the form of $\nu \in \mathcal{E}^u$ given in part (d) of Theorem 4.2 and the formula for $s(u)$ given in part (c) of Theorem 4.3 are both rigorously true.

V. EQUIVALENCE AND NONEQUIVALENCE OF ENSEMBLES

As we saw in Sec. III, the set $\mathcal{E}_\beta$ of canonical equilibrium macrostates undergoes a discontinuous phase transition as β increases through $\beta_c=[2(q-1)/(q-2)]\log(q-1)$, the unique macrostate ρ bifurcating discontinuously into the q distinct macrostates $\nu^{(i)}(\beta)$. By contrast, as we saw in Sec. IV, the set $\mathcal{E}^u$ of microcanonical equilibrium macrostates undergoes a continuous phase transition as u decreases from $u_c=-1/2q$, the unique macrostate ρ bifurcating continuously into the q distinct macrostates $\mu^i(u)$. The different continuity properties of these phase transitions shows already that the canonical and microcanonical ensembles are nonequivalent. In this section we study this nonequivalence in detail and relate the equivalence and nonequivalence of these two sets of equilibrium macrostates to concavity and support properties of the microcanonical entropy s defined in (4.2). This is done with the help of Fig. 2, which is based on the form of s in Fig. 1 and on the results on ensemble equivalence and nonequivalence in Theorem 5.1. In Figs. 3 and 4 at the end of the section we give, for $q=3$, a beautiful geometric representation of $\mathcal{E}_\beta$ and $\mathcal{E}^u$ that also shows the ensemble nonequivalence for a range of u.

We start by stating in Theorem 5.1 results on ensemble equivalence and nonequivalence for the Curie–Weiss–Potts model. Theorem 5.1 summarizes Theorems 4.4, 4.6, and 4.8 in Ref. 15, which apply to a wide range of statistical mechanical models. The Curie–Weiss–Potts model is a special case. In this special case, we will show that the values of u and β in part (a)(i) of the next theorem are related by the thermodynamic formula $s'(u)=\beta$ [Theorem 6.2(b)]. For $u \in \text{dom } s$ the

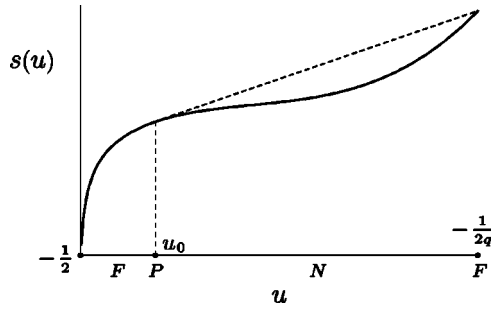

FIG. 1. Schematic graph of $s(u)$, showing the set $F=(-\frac{1}{2},u_0)\cup\{-1/2q\}$ of full ensemble equivalence, the singleton set $P=\{u_0\}$ of partial equivalence, and the set $N=(u_0,-1/2q)$ of nonequivalence. For $u\in F\cup P=(-\frac{1}{2},u_0]\cup\{-1/2q\}$, $s(u)=s^{**}(u)$; for $u\in N$, $s(u)<s^{**}(u)$ and the graph of s^{**} consists of the dotted line segment with slope β_c. The slope of s at $-\frac{1}{2}$ is ∞.

possible relationships between $\mathcal{E}^u$ and $\mathcal{E}_\beta$, given in part (a) of Theorem 5.1, are that either the ensembles are fully equivalent, partially equivalent, or nonequivalent. According to part (b) of the theorem, canonical equilibrium macrostates are always realized microcanonically—i.e., lie in $\mathcal{E}^u$ for some u—while according to part (a)(iii), microcanonical equilibrium macrostates are in general not realized canonically—i.e., do not lie in $\mathcal{E}_\beta$ for any β. It follows that the microcanonical ensemble is the richer of the two ensembles.

Theorem 5.1: *We define* s *by* (4.2) *and* $\mathcal{E}_\beta$ *and* $\mathcal{E}^u$ *by* (2.3) and (2.4). *The following conclusions hold.*

(a) *For fixed* $u\in\mathrm{dom}\,s$ *one of the following three possibilities occurs.*

(i) *Full equivalence: There exists* $\beta\in\mathbb{R}$ *such that* $\mathcal{E}^u=\mathcal{E}_\beta$. *This is the case if and only if* s *has a strictly supporting line at* u *with slope* β; *i.e.,*

$$s(v)<s(u)+\beta(v-u)\ \text{for all}\ v\neq u.$$

(ii) *Partial equivalence: There exists* $\beta\in\mathbb{R}$ *such that* $\mathcal{E}^u\subset\mathcal{E}_\beta$ *but* $\mathcal{E}^u\neq\mathcal{E}_\beta$. *This is the case if and only if* s *has a nonstrictly supporting line at* u *with slope* β; *i.e.,*

$$s(v)\leqslant s(u)+\beta(v-u)\ \textit{for all}\ v\in\mathbb{R}\ \textit{with equality for some}\ v\neq u.$$

(iii) *Nonequivalence: For all* $\beta\in\mathbb{R}$, $\mathcal{E}^u\cap\mathcal{E}_\beta=\emptyset$. *This is the case if and only if* s *has no supporting line at* u; *i.e., for any* $\beta\in\mathbb{R}$ *there exists* v *such that* $s(v)>s(u)+\beta(v-u)$.

(b) *Canonical is always realized microcanonically: For* $\nu\in\mathcal{P}$ *we define* $\widetilde{H}(\nu)=-\frac{1}{2}\langle\nu,\nu\rangle$. *Then for any* $\beta\in\mathbb{R}$,

$$\mathcal{E}_\beta=\bigcup_{u\in\widetilde{H}(\mathcal{E}_\beta)}\mathcal{E}^u.$$

We next relate ensemble equivalence and nonequivalence with concavity and support properties of s in the Curie–Weiss–Potts model. For $q=3$ an explicit formula for s is given in part (b) of Theorem 4.3. If Conjecture 4.1 is true, then the formula for s given in part (c) of Theorem 4.3 is also valid for $q\geqslant 4$. Figure 1 exhibits all the concavity and support features of s. However, Fig. 1 is not the actual graph of s but a schematic graph that accentuates the shape of s together with the intervals of strict concavity and nonconcavity of s. For arbitrary $q\geqslant 3$, as discussed in the second paragraph after Theorem 6.2, the concavity and support features of s exhibited in Fig. 1 follow from Theorems 5.1 and 6.2.

Concavity properties of s are defined in reference to the double-Legendre–Fenchel transform s^{**}, which can be characterized as the smallest concave, upper semicontinuous function that satisfies $s^{**}(u)\geqslant s(u)$ for all $u\in\mathbb{R}$ (Ref. 10, Proposition A.2). For $u\in\mathrm{dom}\,s$ we say that s is concave at u if $s(u)=s^{**}(u)$ and that s is not concave at u if $s(u)<s^{**}(u)$. Also, we say that s is

strictly concave at $u \in \operatorname{dom} s$ if s has a strictly supporting line at u and that s is strictly concave on a convex subset A of $\operatorname{dom} s$ if s is strictly concave at each $u \in A$. If s is strictly concave at u, then a straightforward argument shows that s is concave at u, as one expects [Ref. 10, Lemma 4.1(a)].

According to Fig. 1 and Theorem 5.1, there exists $u_0 \in \left(-\frac{1}{2}, -1/2q\right)$ with the following properties:

(i) s is strictly concave on the interval $\left(-\frac{1}{2}, u_0\right)$ and at the point $-1/2q$. Hence for $u \in F = \left(-\frac{1}{2}, u_0\right) \cup \{-1/2q\}$ the ensembles are fully equivalent [Theorem. 5.1(a)(i)]. In fact, for $u \in \operatorname{int} F = \left(-\frac{1}{2}, u_0\right)$, $\mathcal{E}^u = \mathcal{E}_\beta$ with β given by the thermodynamic formula $\beta = s'(u)$ [Theorem 6.2(b)].

(ii) s is concave but not strictly concave at u_0 and has a nonstrictly supporting line at u_0 that also touches the graph of s over the right-hand endpoint $-1/2q$. Hence for $u = u_0$ the ensembles are partially equivalent in the sense that there exists $\beta \in \mathbb{R}$ such that $\mathcal{E}^u \subset \mathcal{E}_\beta$ but $\mathcal{E}^u \neq \mathcal{E}_\beta$ [Theorem 5.1(a)(ii)]. In fact, β equals the critical inverse temperature β_c defined in (3.1).

(iii) s is not concave on the interval $N = (u_0, -1/2q)$ and has no supporting line at any $u \in N$ [Ref. 10, Theorem A.4(c)]. Hence for $u \in N$ the ensembles are nonequivalent in the sense that for all $\beta \in \mathbb{R}$, $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ [Theorem 5.1(a)(iii)].

As we have just seen, u_0 can be characterized in terms of concavity and support properties of s. The quantity u_0 can also be characterized in terms of mapping properties of $\widetilde{H}(\nu) = -\frac{1}{2}\langle \nu, \nu \rangle$. Using this characterization, we give an explicit formula for u_0 in (6.2).

We point out two additional features of Fig. 1. First, although $\mathcal{E}^u \neq \emptyset$ for u equal to the left-hand endpoint $-\frac{1}{2}$ of $\operatorname{dom} s$, we do not include this point in the set F of full ensemble equivalence. Indeed, s is not strictly concave at $-\frac{1}{2}$ because there is no strictly supporting line at $-\frac{1}{2}$; as one can see in (5.1), the slope of s at $-\frac{1}{2}$ is ∞. Nevertheless, by introducing the limiting set

$$\mathcal{E}_\infty = \{(1,0,\ldots,0),(0,1,\ldots,0),\ldots,(0,0,\ldots,1)\} = \lim_{\beta \to \infty} \mathcal{E}_\beta,$$

we can extend full ensemble equivalence to $u = -\frac{1}{2}$ since $\mathcal{E}^{-1/2} = \mathcal{E}_\infty$.

Second, for u in the interval N of ensemble nonequivalence, the graph of s^{**} is affine; this is depicted by the dotted line segment in Fig. 1. The slope of the affine portion of the graph of s^{**} equals the critical inverse temperature β_c defined in (3.1). This can be proved using concave-duality relationships involving s^{**} and the canonical free energy. The quantity β_c also satisfies an equal-area property, first observed by Maxwell (Ref. 28, p. 45) and explained in the context of another spin model in Ref. 18, p. 535.

The relationships stated in items (i), (ii), and (iii) above give valuable insight into equivalence and nonequivalence of ensembles in the Curie–Weiss–Potts model. These relationships are illustrated in Fig. 2. In this figure we exhibit the graph of s' and the sets $\mathcal{E}_\beta$ and $\mathcal{E}^u$ in order to compare the phase transitions in the two ensembles and to understand the implications for ensemble equivalence and nonequivalence. In order to accentuate properties of s', $\mathcal{E}_\beta$, and $\mathcal{E}^u$ that are related to ensemble equivalence and nonequivalence, we focus on $q = 8$. In presenting the graph of s' and the form of $\mathcal{E}^u$, we assume that for $q = 8$ Conjecture 4.1 is valid. We then appeal to part (c) of Theorem 4.3, which gives an explicit formula for s, and to part (d) of Theorem 4.2, which gives an explicit formula for the elements of $\mathcal{E}^u$. The derivative s', graphed in the top left plot in Fig. 2, is given by

$$s'(u) = \sqrt{\frac{q-1}{-2qu-1}}\left[\log\left(1+\sqrt{(q-1)(-2qu-1)}\right) - \log\left(1-\sqrt{\frac{-2qu-1}{q-1}}\right)\right]. \tag{5.1}$$

The canonical phase diagram, given in the top right plot in Fig. 2, summarizes the description of $\mathcal{E}_\beta$ given in Theorem 3.1 and shows the discontinuous phase transition exhibited by this ensemble at $\beta_c = [2(q-1)/(q-2)]\log(q-1) = \frac{7}{3}\log 7$. The solid line in this plot for $\beta < \beta_c$ represents the common value $\frac{1}{8}$ of each of the components of ρ, which is the unique phase for $\beta < \beta_c$. For $\beta > \beta_c$ there are eight phases given by $\nu^1(\beta)$ together with the vectors $\nu^i(\beta)$ obtained by inter-

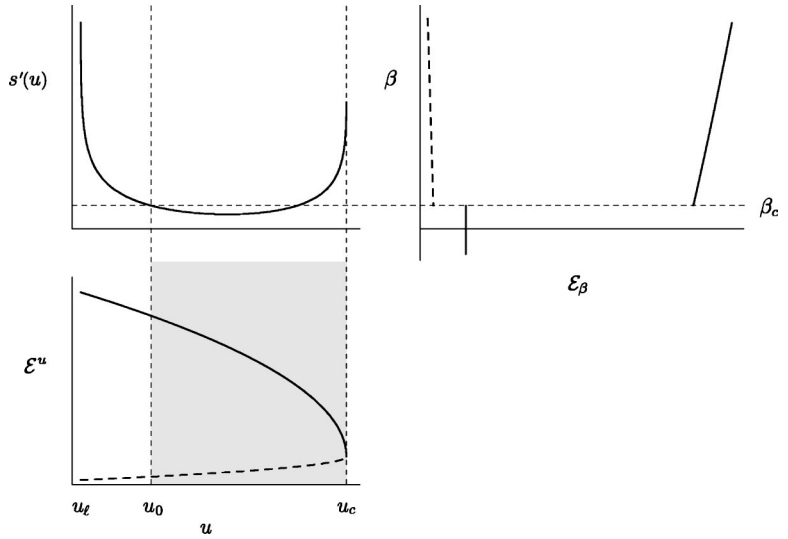

FIG. 2. For $q=8$ the top right plot shows $\mathcal{E}_\beta$, the top left plot the graph of $s'(u)$ for $u \in \operatorname{dom} s=[u_\ell,u_c]=\left[-\frac{1}{2},-1/2q\right]$, and the bottom left plot $\mathcal{E}^u$. The discontinuous phase transition at β_c in the top right plot and the continuous phase transition at u_c in the bottom left plot imply that the ensembles are nonequivalent for all $u \in N=(u_0,u_c)$. On this interval s is not concave and s^{**} is affine with slope β_c. The shaded area in the bottom left plot corresponds to the region of nonequivalence of ensembles delineated by $u \in N$.

changing the first and ith components of $\nu^1(\beta)$. Finally, for $\beta=\beta_c$ there are nine phases consisting of ρ and the vectors $\nu^i(\beta_c)$ for $i=1,2,\ldots,8$. The solid and dashed curves in the top right plot in Fig. 2 show the first component and the last seven, equal components of $\nu^1(\beta)$ for $\beta \in [\beta_c,\infty)$. The first component is a strictly increasing function equal to $\frac{7}{8}$ for $\beta=\beta_c$ and increasing to 1 as $\beta \to \infty$ while the last seven, equal components are strictly decreasing functions equal to $\frac{1}{56}$ for $\beta=\beta_c$ and decreasing to 0 as $\beta \to \infty$.

The microcanonical phase diagram, given in the bottom left plot in Fig. 2, summarizes the description of $\mathcal{E}^u$ given in Theorem 4.2 and shows the continuous phase transition exhibited by this ensemble as u decreases from the maximum value $u_c=-1/2q=-\frac{1}{16}$. The single phase ρ for $u=-\frac{1}{16}$ is represented by the point lying over this value of u. For $u \in \left[-\frac{1}{2},-\frac{1}{16}\right)$ there are eight phases given by $\mu^1(u)$ together with the vectors $\mu^i(u)$ obtained by interchanging the first and ith components of $\mu^1(u)$. The solid and dashed curves in the bottom left plot in Fig. 2 show the first component $a(u)$ and the last seven, equal components $b(u)$ of $\mu^1(u)$ for $u \in \left[-\frac{1}{2},-\frac{1}{16}\right)$. The first component is a strictly increasing function of $-u$ equal to $\frac{1}{8}$ for $u=-\frac{1}{16}$ and increasing to 1 as $u \to \left(-\frac{1}{2}\right)^+$, while the last seven, equal components are strictly decreasing functions of $-u$ equal to $\frac{1}{8}$ for $u=-\frac{1}{16}$ and decreasing to 0 as $u \to \left(-\frac{1}{2}\right)^+$.

The different nature of the two phase transitions—discontinuous in the canonical ensemble versus continuous in the microcanonical ensemble—implies that the two ensembles are not fully equivalent for all values of u. By necessity, the set $\mathcal{E}_\beta$ of canonical equilibrium macrostates must omit a set of microcanonical equilibrium macrostates. Further details concerning ensemble equivalence and nonequivalence can be seen by examining the graph of s', given in the top left plot of Fig. 2. This graph, which is the bridge between the canonical and microcanonical phase diagrams, shows that s' is strictly decreasing on the interval $\operatorname{int} F=\left(-\frac{1}{2},u_0\right)$, which is the interior of the set F of full ensemble equivalence. The critical value β_c equals the slope of the affine portion of the graph of s^{**} over the interval $N=(u_0,-1/2q)$ of ensemble nonequivalence. This affine portion is represented in the top left plot of Fig. 2 by the horizontal dashed line at β_c.

Figure 2 exhibits the full equivalence of ensembles that holds for $u \in \operatorname{int} F=\left(-\frac{1}{2},u_0\right)$ [Theorem 6.2(a)]. For u in this interval the solid and dashed curves representing the components of $\mu^1(u) \in \mathcal{E}^u$ can be put in one-to-one correspondence with the solid and dashed curves representing the

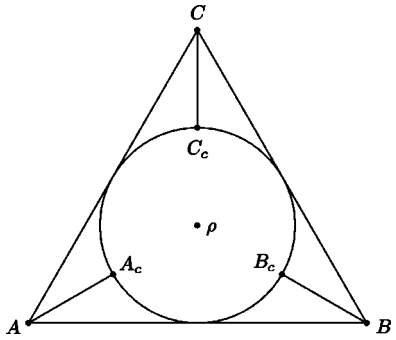

FIG. 3. Graphical representation of the set $\mathcal{E}_\beta$ of canonical equilibrium macrostates for $q=3$ showing the maximal circle of intersection corresponding to $u=u_0$; the vector ρ; the unit-coordinate vectors A, B, and C; and the macrostates $A_c=\nu^1(\beta_c)$, $B_c=\nu^2(\beta_c)$, and $C_c=\nu^3(\beta_c)$. The line segments $\overline{A_cA}$, $\overline{B_cB}$, and $\overline{C_cC}$ represent the elements of $\mathcal{E}_\beta$ for $\beta>\beta_c$.

same two components of $\nu^1(\beta)\in\mathcal{E}_\beta$ for $\beta\in(\beta_c,\infty)$. As we remarked earlier, the values of u and β are related by the thermodynamic formula $s'(u)=\beta$ [Theorem 6.2(b)]. Full equivalence of ensembles also holds for $u=-1/2q\in F$, the right-hand endpoint of the interval on which s is finite. The solid vertical line in the top right plot for $\beta<\beta_c$, which represents the unique canonical phase ρ, is collapsed in the bottom left plot to the single energy value $u=-1/2q$, which corresponds to the unique microcanonical phase ρ. This collapse shows that the canonical notion of temperature is somewhat ill-defined at $u=-1/2q$ since there are infinitely many values of β associated with this energy value. This feature of the Curie–Weiss–Potts model is not present, for example, in the mean-field Blume–Emery–Griffiths spin model, which also exhibits nonequivalence of ensembles.[18]

By comparing the top right and bottom left plots, we see that the elements of $\mathcal{E}^u$ cease to be related to those of $\mathcal{E}_\beta$ for $u\in N=(u_0,-1/2q)$, which is the interval on which s is not concave. For any energy value u in this interval no $\nu\in\mathcal{E}_\beta$ exists that can be put in correspondence with an equivalent equilibrium empirical vector contained in $\mathcal{E}^u$. Thus, although the equilibrium macrostates corresponding to $u\in N$ are characterized by a well-defined value of the energy, it is impossible to assign an inverse temperature β to those macrostates from the viewpoint of the canonical ensemble. In other words, the canonical ensemble is blind to all energy values u contained in the interval N of nonconcavity of s. This is closely related to the presence of the discontinuous phase transition seen in the canonical ensemble.

The quantity u_0 defined in (6.2) plays a central role in the analysis of phase transitions and ensemble equivalence in the Curie–Weiss–Potts model. First, as we saw in our discussion of Fig. 1, u_0 separates the interval $(-\frac{1}{2},u_0)$ of strict concavity of s and of full ensemble equivalence from the interval $(u_0,-1/2q)$ of nonconcavity of s and of ensemble nonequivalence. Second, part (a) of Lemma 6.1 shows that u_0 equals the limiting mean energy $\tilde{H}(\nu^1(\beta_c))$ in the canonical equilibrium macrostate $\nu^1(\beta)$ as $\beta\to(\beta_c)^+$. In Figs. 3 and 4 we present for $q=3$ a third, geometric interpretation of u_0 that is also related to ensemble nonequivalence.

Before explaining this third, geometric interpretation of u_0, we recall that according to part (a) of Theorem 4.2 specialized to $q=3$, $\mathcal{E}^u$ is nonempty, or equivalently the constraint set in (4.5) is nonempty, if and only if $u\in[-\frac{1}{2},-1/2q]=[-\frac{1}{2},-\frac{1}{6}]$. Geometrically, the energy constraint $\tilde{H}(\nu)=-\frac{1}{2}\langle\nu,\nu\rangle=u$ corresponds to the sphere in $\mathbb{R}^3$ with center 0 and radius $\sqrt{-2u}$. This sphere intersects the set $\mathcal{P}$ of probability vectors if and only if $u\in[-\frac{1}{2},-\frac{1}{6}]$. For $u=-\frac{1}{6}$, the sphere is tangent to $\mathcal{P}$ at the unique point ρ while for $u=-\frac{1}{2}$, the hypersphere intersects $\mathcal{P}$ at the q unit-coordinate vectors. The intersection of the sphere and $\mathcal{P}$ undergoes a phase transition at u_0 in the following sense. For $u\in[u_0,-\frac{1}{6})$ the sphere intersects $\mathcal{P}$ in a circle while for $u\in[-\frac{1}{2},u_0)$, the sphere intersects $\mathcal{P}$ in a proper subset of a circle; the complement of this subset lies outside the nonnegative octant of $\mathbb{R}^3$. For $u=u_0=-\frac{1}{4}$, the circle of intersection is maximal and is tangent to the boundary of $\mathcal{P}$.

The set $\mathcal{E}_\beta$ of canonical equilibrium macrostates for $q=3$ is represented in Fig. 3. In this figure

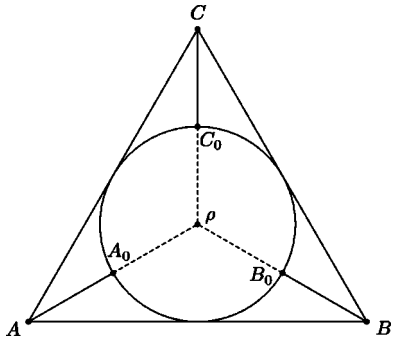

FIG. 4. Graphical representation of the set $\mathcal{E}^u$ of microcanonical equilibrium macrostates for $q=3$ showing the maximal circle of intersection corresponding to $u=u_0$; the vector ρ; the unit-coordinate vectors A, B, and C; and the macrostates $A_0=\mu^1(u_0)$, $B_0=\mu^2(u_0)$, and $C_0=\mu^3(u_0)$. The solid-line segments $\overline{A_0A}$, $\overline{B_0B}$, and $\overline{C_0C}$ represent the elements of $\mathcal{E}^u$ that are realized canonically. The dashed-line segments $\overline{\rho A_0}$, $\overline{\rho B_0}$, and $\overline{\rho C_0}$ represent the elements of $\mathcal{E}^u$ that are not realized canonically.

the maximal circle of intersection corresponding to $u=u_0=-\frac{1}{4}$ is shown together with the vector ρ at its center; the points A, B, and C representing the respective unit-coordinate vectors (1,0,0), (0,1,0), and (0,0,1); and the points A_c, B_c, and C_c representing the respective equilibrium macrostates $\nu^1(\beta_c)$, $\nu^2(\beta_c)$, and $\nu^3(\beta_c)$. These three macrostates lie on the maximal circle of intersection since $\widetilde{H}(\nu^1(\beta_c))=u_0$ [Lemma 6.1(b)]. For $\beta>\beta_c$ all $\nu\in\mathcal{E}_\beta$ have two equal components, and as $\beta\to\infty$ these vectors converge to the unit-coordinate vectors A, B, and C. Hence for $\beta>\beta_c$ the equilibrium macrostates $\nu^1(\beta)$, $\nu^2(\beta)$, and $\nu^3(\beta)$ are represented by the open line segments $\overline{A_cA}$, $\overline{B_cB}$, and $\overline{C_cC}$.

The set $\mathcal{E}^u$ of microcanonical equilibrium macrostates for $q=3$ is represented in Fig. 4. In this figure the maximal circle of intersection corresponding to $u=u_0=-\frac{1}{4}$ is shown together with the vector ρ at its center; the points A, B, and C representing the unit-coordinate vectors; and the points A_0, B_0, and C_0 representing the respective equilibrium macrostates $\mu^1(u_0)$, $\mu^2(u_0)$, and $\mu^3(u_0)$. For $u\in\left(-\frac{1}{2},-\frac{1}{6}\right)$ all $\nu\in\mathcal{E}^u$ have two equal components, and as $u\to\left(-\frac{1}{2}\right)^+$ they converge to the unit coordinate vectors A, B, and C. Hence for $u\in\left(-\frac{1}{2},-\frac{1}{6}\right)$ the equilibrium macrostates $\mu^1(u)$, $\mu^2(u)$, and $\mu^3(u)$ are represented by the open line segments $\overline{\rho A}$, $\overline{\rho B}$, and $\overline{\rho C}$. As we saw in the preceding section, for each $u\in\left(-\frac{1}{2},-\frac{1}{6}\right)$ the macrostates $\mu^1(u)$, $\mu^2(u)$, and $\mu^3(u)$ lie on the intersection of the sphere of radius $\sqrt{-2u}$ with $\mathcal{P}$. In particular, $A_0=\mu^1(u_0)$, $B_0=\mu^2(u_0)$, and $C_0=\mu^3(u_0)$ lie on the maximal circle of intersection.

The distinguishing feature of Fig. 4 is the three open dashed-line segments $\overline{\rho A_0}$, $\overline{\rho B_0}$, and $\overline{\rho C_0}$ representing the elements of $\mathcal{E}^u$ that are not realized canonically; namely, $\mu^1(u)$, $\mu^2(u)$, and $\mu^3(u)$ for $u\in\left(u_0,-\frac{1}{6}\right)$. The three half open solid-line segments $\overline{A_0A}$, $\overline{B_0B}$, and $\overline{C_0C}$ represent the elements of $\mathcal{E}^u$ that are realized canonically; namely, $\mu^1(u)$, $\mu^2(u)$, and $\mu^3(u)$ for $u\in\left(-\frac{1}{2},u_0\right]$. For each such u the value of β for which $\mathcal{E}^u=\mathcal{E}_\beta$ is determined by the equation $\widetilde{H}(\nu^1(\beta))=u$ [Theorem 6.2(a)]. Thus in Fig. 3 the corresponding elements of $\mathcal{E}_\beta$ lie on the intersection of the sphere of radius $\sqrt{-2u}$ and $\mathcal{P}$.

This completes our discussion of equivalence and nonequivalence of ensembles. In the next section we will prove a number of statements concerning ensemble equivalence and nonequivalence that have been determined graphically.

VI. PROOFS OF EQUIVALENCE AND NONEQUIVALENCE OF ENSEMBLES

Using the general results of Ref. 15, we stated in the preceding section the equivalence and nonequivalence relationships that exist between $\mathcal{E}^u$ and $\mathcal{E}_\beta$ and verified these relationships using the plots of these sets for $q=8$ given in Fig. 2. Our purpose in the present section is to prove these relationships using mapping properties of the mean energy function $u(\beta)$ defined for $\beta\neq\beta_c$ by

$$u(\beta) = \begin{cases} \widetilde{H}(\rho) = -\dfrac{1}{2q} & \text{for } \beta < \beta_c, \\ \widetilde{H}(\nu^1(\beta)) = -\frac{1}{2}\langle \nu^1(\beta), \nu^1(\beta)\rangle & \text{for } \beta > \beta_c. \end{cases} \tag{6.1}$$

Here $\nu^1(\beta)$ is the unique canonical equilibrium macrostate modulo permutations for $\beta > \beta_c$ [Theorem 3.1]. According to the next lemma, for $\beta > \beta_c$, $u(\beta)$ is continuous and strictly decreasing and $u(\beta) < -1/2q$, which equals the mean energy for $\beta < \beta_c$. It follows that as β increases through β_c, $u(\beta)$ is discontinuous, jumping down from $-1/2q$ to $\widetilde{H}(\nu^1(\beta))$. This discontinuity in $u(\beta)$ mirrors in a natural way the discontinuity in $\mathcal{E}_\beta$ as β increases through β_c.

We use the same notation u_0 for the quantity defined in (6.2) as for the quantity u_0 appearing in Fig. 1 in Sec. V because these two quantities coincide. Indeed, with u_0 defined in (6.2), we prove in Theorem 6.2 that the largest open interval on which full equivalence of ensembles holds is $\text{int } F = \left(-\frac{1}{2}, u_0\right)$. This coincides with the interior of the interval F shown in Fig. 1. As that figure exhibits, int F is the largest open interval on which s is strictly concave; by Theorem 5.1, that open interval coincides with the largest open interval on which full equivalence of ensembles holds.

Lemma 6.1: For $\beta \in [\beta_c, \infty)$ we define $\nu^1(\beta)$ as in part (b) *of Theorem 3.1 and we define*

$$u_0 = \frac{-q^2 + 3q - 3}{2q(q-1)}. \tag{6.2}$$

The following conclusions hold.

(a) $-\frac{1}{2} < u_0 < -1/2q$ *and* $\lim_{\beta \to (\beta_c)^+} u(\beta) = \widetilde{H}(\nu^1(\beta_c)) = u_0$.

(b) *The function mapping*

$$\beta \in (\beta_c, \infty) \mapsto u(\beta) = \widetilde{H}(\nu^1(\beta)) = -\tfrac{1}{2}\langle \nu^1(\beta), \nu^1(\beta)\rangle$$

is a strictly decreasing, differentiable bijection onto the interval $\left(-\frac{1}{2}, u_0\right)$.

Proof: (a) The inequalities involving u_0 follow immediately from the inequality $q \geqslant 3$. The relationship $\widetilde{H}(\nu^1(\beta_c)) = u_0$ is easily determined using the explicit form of $\nu^1(\beta_c)$ given in (3.5). That $\lim_{\beta \to (\beta_c)^+} u(\beta) = \widetilde{H}(\nu^1(\beta_c))$ follows from the definition of $u(\beta)$ and the continuity of $\nu^1(\beta)$ for $\beta \geqslant \beta_c$.

(b) For $w \in \mathbb{R}$ define

$$f(w) = -\frac{1}{2}\left(\frac{[1 + (q-1)w]^2}{q^2} + (q-1)\frac{[1-w]^2}{q^2} \right).$$

For $\beta \in (\beta_c, \infty)$ we use the formula for $\nu^1(\beta)$ given in part (b) of Theorem 3.1 to write $u(\beta) = -f(w(\beta))$. The quantity $w(\beta)$ is positive and strictly increasing, and for all $w > 0$,

$$f'(w) = \frac{(q-1)w}{q} > 0.$$

As the composition of two strictly increasing functions, for $\beta \in (\beta_c, \infty)$, $-u(\beta)$ is strictly increasing and thus $u(\beta)$ is strictly decreasing. In addition, since $\lim_{\beta \to \infty} w(\beta) = 1$ [Theorem 3.1(a)], we have $\lim_{\beta \to \infty} u(\beta) = -\frac{1}{2}$, and by part (a) of this lemma

$$\lim_{\beta \to (\beta_c)^+} u(\beta) = \widetilde{H}(\nu(\beta_c)) = u_0.$$

It follows that the function mapping $\beta \in (\beta_c, \infty) \mapsto u(\beta)$ is a strictly decreasing, differentiable bijection onto the interval $\left(-\frac{1}{2}, u_0\right)$. This completes the proof of part (b). ■

Mapping properties of $u(\beta)$ play an important role in the next theorem, in which we prove that the sets F, P, and N defined in (6.3) correspond to full equivalence, partial equivalence, and

nonequivalence of ensembles. For $u \in F$ we consider three subcases in order to indicate the value of β for which $\mathcal{E}^u = \mathcal{E}_\beta$; for $u \in \text{int } F = (-\frac{1}{2}, u_0)$, β and u are related by $\beta = s'(u)$ and $u = u(\beta)$. Part (c) shows an interesting degeneracy in the equivalence-of-ensemble picture, the set $\mathcal{E}^u$ for $u = -1/2q$ corresponding to all $\mathcal{E}_\beta$ for $\beta < \beta_c$. This is related to the fact that for all such values of β, $\mathcal{E}_\beta = \{\rho\}$ and thus the mean energy $u(\beta)$ equals $-1/2q$.

Theorem 6.2: *We define* $s(u)$ *in* (4.2), $u(\beta)$ *in* (6.1), $\mathcal{E}_\beta$ *in* (2.3), *and* $\mathcal{E}^u$ *in* (2.4). *We also define* β_c *in* (3.1) *and* u_0 *in* (6.2). *The sets*

$$F = \left(-\tfrac{1}{2}, u_0\right) \cup \left\{-\frac{1}{2q}\right\}, \quad P = \{u_0\}, \quad \text{and } N = \left(u_0, -\frac{1}{2q}\right) \tag{6.3}$$

have the following properties.

(a) *Full equivalence on* int F: *For* $u \in \text{int } F = (-\frac{1}{2}, u_0)$, *there exists a unique* $\beta \in (\beta_c, \infty)$ *such that* $\mathcal{E}^u = \mathcal{E}_\beta$; β *satisfies* $u(\beta) = \tilde{H}(\nu^1(\beta)) = u$.

(b) *For* $u \in \text{int } F = (-\frac{1}{2}, u_0)$, s *is differentiable. The values* u *and* β *for which* $\mathcal{E}^u = \mathcal{E}_\beta$ *in part* (a) *are also related by the thermodynamic formula* $s'(u) = \beta$.

(c) *Full equivalence at* $-1/2q$: *For* $u = -(1/2q) \in F$, $\mathcal{E}^{-1/2q} = \mathcal{E}_\beta$ *for any* $\beta < \beta_c$.

(d) *Partial equivalence on* P: *For* $u \in P = \{u_0\}$, $\mathcal{E}^{u_0} \subset \mathcal{E}_{\beta_c}$ *but* $\mathcal{E}^{u_0} \neq \mathcal{E}_{\beta_c}$. *In fact,* $\mathcal{E}_{\beta_c} = \mathcal{E}^{u_0} \cup \mathcal{E}^{-1/2q}$.

(e) *Nonequivalence on* N: *For any* $u \in N = (u_0, -1/2q)$, $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ *for all* $\beta \in \mathbb{R}$.

In reference to the properties of s given in part (b), one can show that the function mapping $u \in (-\frac{1}{2}, u_0) \mapsto s'(u)$ is a strictly decreasing, differentiable bijection onto the interval (β_c, ∞) and that this bijection is the inverse of the bijection mapping $\beta \in (\beta_c, \infty) \mapsto u(\beta)$.

Before we prove the theorem, it is instructive to compare its assertions with those in Theorem 5.1, which formulates ensemble equivalence and nonequivalence in terms of support properties of s. These support properties can be seen in the schematic plot of the the graph of s in Fig. 1. We start with part (a) of Theorem 6.2, which states that for any $u \in \text{int } F = (-\frac{1}{2}, u_0)$ there exists a unique $\beta \in (\beta_c, \infty)$ such that $\mathcal{E}^u = \mathcal{E}_\beta$. As promised in part (a)(i) of Theorem 5.1, this β is the slope of a strictly supporting line to the graph of s at u, and so s is strictly concave on int F. The situation that holds when $u = -1/2q$ [Theorem 6.2(c)] is also consistent with part (a)(i) of Theorem 5.1. For this value of u, which is the isolated point of the set F of full equivalence, there exist infinitely many strictly supporting lines to the graph of s, the possible slopes of which are all $\beta \in (-\infty, \beta_c)$. On the other hand, when $u = u_0$, which is the only value lying in the set P of partial equivalence, we have $\mathcal{E}^{u_0} \subset \mathcal{E}_{\beta_c}$ but $\mathcal{E}^{u_0} \neq \mathcal{E}_{\beta_c}$ [Theorem 6.2(d)]. In combination with part (a)(ii) of Theorem 5.1, it follows that there exists a nonstrictly supporting line at u_0 with slope β_c and that s is concave at u_0 but not strictly concave. Finally, for $u \in N = (u_0, -1/2q)$, we have $\mathcal{E}^u \cap \mathcal{E}_\beta = \emptyset$ for all $\beta \in \mathbb{R}$ [Theorem 6.2(e)]. In accordance with part (a)(iii) of Theorem 5.1, s has no supporting line at any $u \in N$, and by Theorem A.4 in Ref. 10 s is not concave at any $u \in N$.

Proof of Theorem 6.2: (a) For $\beta > \beta_c$ part (b) of Theorem 3.1 and part (b) of Theorem 5.1 imply that

$$\mathcal{E}_\beta = \{\nu^1(\beta), \ldots, \nu^q(\beta)\} = \bigcup_{u \in \tilde{H}(\mathcal{E}_\beta)} \mathcal{E}^u.$$

The symmetry of $\tilde{H}$ with respect to permutations implies that $\tilde{H}(\mathcal{E}_\beta) = \{\tilde{H}(\nu^1(\beta))\}$. Thus for any $\beta > \beta_c$

$$\mathcal{E}_\beta = \mathcal{E}^{\tilde{H}(\nu^1(\beta))}. \tag{6.4}$$

Since for any $u \in \text{int } F = (-\frac{1}{2}, u_0)$ there exists a unique $\beta \in (\beta_c, \infty)$ satisfying $u(\beta) = \tilde{H}(\nu^1(\beta)) = u$ [Lemma 6.1(b)], it follows that $\mathcal{E}^u = \mathcal{E}_\beta$.

(b) The differentiability of s on int F is proved in part (b) of Theorem 6.3, which depends only on part (a) of the present theorem. By part (a) of the present theorem and part (a) of Theorem 5.1, s has a strictly supporting line at each $u \in \text{int } F$. It follows that s is strictly concave on int F and

thus concave on int F [Ref. 10, Lemma 4.1(a)]; i.e., $s(u)=s^{**}(u)$ for all $u \in \text{int } F$. The differentiability of s on int F [Theorem 6.3(b)] combined with part (a) of Theorem A.3 in Ref. 10 implies that $s'(u)=\beta$.

(c) By (4.6) and part (b) of Theorem 3.1,

$$\mathcal{E}^{-1/2q}=\{\rho\}=\mathcal{E}_\beta \quad \text{for any } \beta<\beta_c. \tag{6.5}$$

(d) By part (b) of Theorem 3.1, symmetry, and part (a) of Lemma 6.1,

$$\tilde{H}(\mathcal{E}_{\beta_c})=\{\tilde{H}(\rho),\tilde{H}(\nu^1(\beta_c))\}=\left\{-\frac{1}{2q},u_0\right\}.$$

Hence by (6.4) and (6.5),

$$\mathcal{E}_{\beta_c}=\bigcup_{u\in\tilde{H}(\mathcal{E}_{\beta_c})}\mathcal{E}^u=\mathcal{E}^{-1/2q}\cup\mathcal{E}^{u_0}=\{\rho\}\cup\mathcal{E}^{u_0}.$$

However, $\rho\notin\mathcal{E}^{u_0}$ since ρ does not satisfy the constraint $\tilde{H}(\rho)=u_0$. It follows that $\mathcal{E}^{u_0}\subset\mathcal{E}_{\beta_c}$ but that $\mathcal{E}^{u_0}\neq\mathcal{E}_{\beta_c}$.

(e) If $u\in N$, then $u\notin\left(-\frac{1}{2},u_0\right)$, and so by part (b) of Lemma 6.1 $u\neq\tilde{H}(\nu^1(\beta))$ for any $\beta\in(\beta_c,\infty)$. Since by (6.4) $\mathcal{E}_\beta=\mathcal{E}^{\tilde{H}(\nu^1(\beta))}$ for all $\beta>\beta_c$, it follows that for all $\beta>\beta_c$,

$$\mathcal{E}^u\cap\mathcal{E}^{\tilde{H}(\nu^1(\beta))}=\emptyset$$

and thus that $\mathcal{E}^u\cap\mathcal{E}_\beta=\emptyset$. For any $\beta<\beta_c$ (6.5) states that $\mathcal{E}_\beta=\mathcal{E}^{-1/2q}=\{\rho\}$. Since $u\in N$, we have $u\neq -1/2q$ and thus $\mathcal{E}^{-1/2q}\cap\mathcal{E}^u=\emptyset$. It follows that $\mathcal{E}^u\cap\mathcal{E}_\beta=\emptyset$ for any $\beta<\beta_c$. Finally, for $\beta=\beta_c$ part (b) of Theorem 3.1 states that $\mathcal{E}_{\beta_c}=\{\rho,\nu^1(\beta_c),\ldots,\nu^q(\beta_c)\}$. However, since $\tilde{H}(\rho)=-(1/2q)\notin N$ and $\tilde{H}(\nu^i(\beta_c))=u_0\notin N$, none of the vectors in $\mathcal{E}_{\beta_c}$ satisfies the constraint $\tilde{H}(\nu)=u$. Thus $\mathcal{E}^u\cap\mathcal{E}_{\beta_c}=\emptyset$. We have proved $\mathcal{E}^u\cap\mathcal{E}_\beta=\emptyset$ for all $\beta\in\mathbb{R}$. The proof of the theorem is complete. ■

We end this section by showing that for arbitrary $q\geqslant 4$ and u in the equivalence sets $F\cup P=\left(-\frac{1}{2},u_0\right]\cup\{-1/2q\}$ the formulas for $\mathcal{E}^u$ and $s(u)$ given in part (d) of Theorem 4.2 and part (c) of Theorem 4.3 are rigorously true. Our strategy is to use the equivalence of the microcanonical and canonical ensembles for $u\in F\cup P$ and the fact that the form of $\mathcal{E}_\beta$ is known exactly for all β. Thus, we translate the form of $\nu\in\mathcal{E}_\beta$, as given in part (b) of Theorem 3.1, into the form of $\nu\in\mathcal{E}^u$ for $u\in F\cup P$. For $\beta\in[\beta_c,\infty)$, the last $q-1$ components of $\nu^1(\beta)\in\mathcal{E}_\beta$ are given by

$$\nu_j^1(\beta)=\frac{1-w(\beta)}{q}, \tag{6.6}$$

and these components are not equal to the first component. Since for each $u\in F\cup P$ there exists $\beta\in[\beta_c,\infty]$ such that either $\mathcal{E}^u=\mathcal{E}_\beta$ or $\mathcal{E}^u\subset\mathcal{E}_\beta$, it follows that modulo permutations all $\nu\in\mathcal{E}^u$ have their last $q-1$ components equal to each other. That is, modulo permutations there exist numbers a and b in $[0,1]$ such that $\nu=(a,b,\ldots,b)$. The possible values of a and b are easily determined by considering the constraints satisfied by $\nu\in\mathcal{E}^u$. These constraints are

$$a+(q-1)b=1 \quad \text{and } a^2+(q-1)b^2=-2u.$$

The two solutions of these equations are

$$a_1=\frac{1-\sqrt{(q-1)(-2qu-1)}}{q}, \quad b_1=\frac{q-1+\sqrt{(q-1)(-2qu-1)}}{(q-1)q}$$

and

$$a_2 = \frac{1 + \sqrt{(q-1)(-2qu-1)}}{q}, \quad b_2 = \frac{q - 1 - \sqrt{(q-1)(-2qu-1)}}{(q-1)q}.$$

Of the two values b_1 and b_2, only b_2 has the form given in (6.6) with

$$w(\beta) = \frac{\sqrt{(q-1)(-2qu-1)}}{q-1} \in [0,1].$$

We conclude that modulo permutations each $\nu \in \mathcal{E}^u$ has the form $(a_2, b_2, \ldots, b_2)$, in which the last $q-1$ components all equal b_2. This coincides with the formula for $\mu^1(u)$ given in part (d) of Theorem 4.2, which in turn gives the explicit formula for $s(u)$ in part (c) of Theorem 4.3. This information is summarized in part (a) of the next theorem. The differentiability of s on $\operatorname{int} F$, which is stated in part (b), is an immediate consequence of the explicit formula for $s(u)$.

Theorem 6.3: *We define* u_0 *in* (6.2). *The following conclusions hold.*

(a) *For arbitrary* $q \geqslant 4$ *and* u *in the equivalence sets* $F \cup P = (-\frac{1}{2}, u_0] \cup \{-1/2q\}$ *the formulas for* $\mathcal{E}^u$ *and* $s(u)$ *given in part* (d) *of Theorem* 4.2 *and part* (c) *of Theorem* 4.3 *are rigorously true.*

(b) *For arbitrary* $q \geqslant 4$, s *is differentiable on the interval* $\operatorname{int} F = (-\frac{1}{2}, u_0)$ *and* $s'(u)$ *is given by* (5.1).

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APPENDIX A: TWO RELATED MAXIMIZATION PROBLEMS

Theorem A.1 is a new result on the maximum points of certain functions related by convex duality. It is formulated for a finite, differentiable, convex function F on $\mathbb{R}^\sigma$ and its Legendre–Fenchel transform,

$$F^*(z) = \sup_{x \in \mathbb{R}^\sigma} \{\langle x, z\rangle - F(x)\}.$$

The domain of F^* is the set $\operatorname{dom} F^* = \{z \in \mathbb{R}^\sigma : F^*(z) < \infty\}$. With only minor changes in notation the theorem is also valid for a finite, Gateaux-differentiable, convex function on a Hilbert space.

Theorem A.1 will be applied in Appendix B to prove that for $\beta > 0$, $\mathcal{E}_\beta$ has the form given in part (b) of Theorem 3.1. Another application of Theorem A.1 is given in Proposition 3.4 in Ref. 17. It is used there to determine the form of the set of canonical equilibrium macrostates for another important spin system known as the mean-field Blume–Emery–Griffiths model.

Theorem A.1: *Let* σ *be a positive integer and* F *a finite, differentiable, convex function mapping* $\mathbb{R}^\sigma$ *into* $\mathbb{R}$. *Assume that* $\sup_{z \in \mathbb{R}^\sigma}\{F(z) - \frac{1}{2}\|z\|^2\} < \infty$ *and that* $F(z) - \frac{1}{2}\|z\|^2$ *attains its supremum. The following conclusions hold:*

(a) $\sup_{z \in \mathbb{R}^\sigma}\{F(z) - \frac{1}{2}\|z\|^2\} = \sup_{z \in \operatorname{dom} F^*}\{\frac{1}{2}\|z\|^2 - F^*(z)\}$.

(b) $\frac{1}{2}\|z\|^2 - F^*(z)$ *attains its supremum on* $\operatorname{dom} F^*$,

(c) *the global maximum points of* $F(z) - \frac{1}{2}\|z\|^2$ *coincide with the global maximum points of* $\frac{1}{2}\|z\|^2 - F^*(z)$.

Proof: We define the subdifferential of F^* at $z_0 \in \mathbb{R}^\sigma$ by

$$\partial F^*(z_0) = \{y \in \mathbb{R}^\sigma : F^*(z) \geqslant F^*(z_0) + \langle y, z - z_0\rangle \text{ for all } z \in \mathbb{R}^\sigma\}.$$

We also define the domain of ∂F^* to be the set of $z_0 \in \mathbb{R}^\sigma$ for which $\partial F^*(z_0) \neq \emptyset$. The proof of the theorem uses three properties of Legendre–Fenchel transforms (see Ref. 43 for background).

(1) F^* is a convex, lower semicontinuous function mapping $\mathbb{R}^\sigma$ into $\mathbb{R}\cup\{\infty\}$, and for all $z \in \mathbb{R}^\sigma$, $F^{**}(z)=(F^*)^*(z)$ equals $F(z)$ [Ref. 14, Theorem VI.5.3(a),(e)].
(2) If for some $z_0 \in \mathbb{R}^\sigma$ and $z \in \mathbb{R}^\sigma$ we have $z=\nabla F(z_0)$, then $F(z_0)+F^*(z)=\langle z_0,z\rangle$ [Ref. 14, Theorems VI.3.5(d) and VI.5.3(c)], and so $z \in \operatorname{dom} F^*$. In particular, if $z=z_0$, then $z_0 \in \operatorname{dom} F^*$ and $F(z_0)+F^*(z_0)=\|z_0\|^2$.
(3) For $z_0 \in \operatorname{dom} F^*$ and $y \in \partial F^*(z_0)$ we have $F(y)+F^*(z_0)=\langle y,z_0\rangle$ [Ref. 14, Theorem VI.5.3(c),(d)]. In particular, if $y=z_0$, then $F(z_0)+F^*(z_0)=\|z_0\|^2$.

We first prove part (a), which is a special case of Theorem C.1 in Ref. 13. Let $M=\sup_{z\in\mathbb{R}^\sigma}\{F(z)-\|z\|^2/2\}$. Since for any $z \in \operatorname{dom} F^*$ and x in $\mathbb{R}^\sigma$,

$$F^*(z) + M \geqslant \langle x,z\rangle - F(x) + M \geqslant \langle x,z\rangle - \|x\|^2/2,$$

we have

$$F^*(z) + M \geqslant \sup_{x\in\mathbb{R}^\sigma}\{\langle x,z\rangle - \|x\|^2/2\} = \|z\|^2/2.$$

It follows that $M \geqslant \|z\|^2/2 - F^*(z)$ and thus that $M \geqslant \sup_{z\in\operatorname{dom} F^*}\{\|z\|^2/2 - F^*(z)\}$. To prove the reverse inequality, let $N=\sup_{z\in\operatorname{dom} F^*}\{\|z\|^2/2-F^*(z)\}$. Then for any $z \in \mathbb{R}^\sigma$ and $x \in \operatorname{dom} F^*$

$$\|z\|^2/2 + N \geqslant \langle x,z\rangle - \|x\|^2/2 + N \geqslant \langle x,z\rangle - F^*(x).$$

Since $F^*(x)=\infty$ for $x \notin \operatorname{dom} F^*$, it follows from property 1 that

$$\|z\|^2/2 + N \geqslant \sup_{x\in\operatorname{dom} F^*}\{\langle x,z\rangle - F^*(x)\} = F(z)$$

and thus that $N \geqslant \sup_{z\in\mathbb{R}^\sigma}\{F(z)-\|z\|^2/2\}$.

In order to prove parts (b) and (c) of Theorem A.1, let z_0 be any point in $\mathbb{R}^\sigma$ at which $F(z) - \frac{1}{2}\|z\|^2$ attains its supremum. Then $z_0=\nabla F(z_0)$, and so by the last line of property (2), $z_0 \in \operatorname{dom} F^*$ and $F(z_0)+F^*(z_0)=\|z_0\|^2$. Part (a) now implies that

$$\sup_{z\in\mathbb{R}^\sigma}\left\{F(z) - \tfrac{1}{2}\|z\|^2\right\} = F(z_0) - \tfrac{1}{2}\|z_0\|^2 = \tfrac{1}{2}\|z_0\|^2 - F^*(z_0) = \sup_{z\in\operatorname{dom} F^*}\left\{\tfrac{1}{2}\|z\|^2 - F^*(z)\right\}.$$

We conclude that $\frac{1}{2}\|z\|^2 - F^*(z)$ attains its supremum on $\operatorname{dom} F^*$ at z_0. Not only have we proved part (b), but also we have proved half of part (c); namely, any global maximizer of $F(z)-\frac{1}{2}\|z\|^2$ is a global maximizer of $\frac{1}{2}\|z\|^2 - F^*(z)$.

Now let z_0 be any point at which $\frac{1}{2}\|z\|^2 - F^*(z)$ attains its supremum. Then for any $z \in \mathbb{R}^\sigma$

$$\tfrac{1}{2}\langle z_0,z_0\rangle - F^*(z_0) \geqslant \tfrac{1}{2}\langle z,z\rangle - F^*(z).$$

It follows that for any $z \in \mathbb{R}^\sigma$,

$$F^*(z) \geqslant F^*(z_0) + \tfrac{1}{2}(\langle z,z\rangle - \langle z_0,z_0\rangle) \geqslant F^*(z_0) + \langle z_0, z - z_0\rangle$$

and thus that $z_0 \in \partial F^*(z_0)$. By the last line of property (3) this implies that $F(z_0)+F^*(z_0)=\|z_0\|^2$. In conjunction with part (a) this in turn implies that

$$\sup_{z\in\operatorname{dom} F^*}\left\{\tfrac{1}{2}\|z\|^2 - F^*(z)\right\} = \tfrac{1}{2}\|z_0\|^2 - F^*(z_0) = F(z_0) - \tfrac{1}{2}\|z_0\|^2 = \sup_{z\in\mathbb{R}^\sigma}\left\{F(z) - \tfrac{1}{2}\|z\|^2\right\}.$$

We conclude that $F(z)-\frac{1}{2}\|z\|^2$ attains its supremum at z_0. This completes the proof of the theorem. ■

APPENDIX B: FORM OF $\mathcal{E}_\beta$

We first derive the form of $\mathcal{E}_\beta$ for $\beta>0$ as given in part (b) of Theorem 3.1. We then prove that $\mathcal{E}_\beta=\{\rho\}$ for all $\beta\leqslant 0$.

$\mathcal{E}_\beta$ is defined as the set of $\nu \in \mathcal{P}$ that minimize $R(\nu|\rho) - (\beta/2)\langle \nu, \nu\rangle$. Since $\beta > 0$, this is equivalent to

$$\mathcal{E}_\beta = \left\{ \nu \in \mathcal{P} : \nu \text{ maximizes } \frac{1}{2}\langle \nu, \nu\rangle - \frac{1}{\beta} R(\nu|\rho) \right\}. \tag{B1}$$

This maximization problem has the form of the right-hand side of part (a) of Theorem A.1; viz.,

$$\sup_{\nu \in \mathcal{P}} \left\{ \frac{1}{2}\langle \nu, \nu\rangle - \frac{1}{\beta} R(\nu|\rho) \right\} = \sup_{\nu \in \operatorname{dom} F^*} \left\{ \frac{1}{2}\|\nu\|^2 - F^*(\nu) \right\}$$

with $F^*(\nu) = (1/\beta) R(\nu|\rho)$.

In order to determine the function F having this Legendre–Fenchel transform, for $z \in \mathbb{R}^q$ we define the finite, differentiable, convex function

$$\Gamma(z) = \log\left(\sum_{i=1}^{q} e^{z_i} \frac{1}{q} \right) \tag{B2}$$

and set $\Gamma_\beta(z) = (1/\beta)\Gamma(\beta z)$. Since for $\nu \in \mathbb{R}^q$ (Ref. 14, Theorem VIII.2.2),

$$\Gamma^*(\nu) = \begin{cases} R(\nu|\rho) & \text{for } \nu \in \mathcal{P}, \\ \infty & \text{otherwise}, \end{cases}$$

it follows that for $\nu \in \mathbb{R}^q$,

$$(\Gamma_\beta)^*(\nu) = \sup_{z \in \mathbb{R}^q} \left\{ \langle z, \nu\rangle - \frac{1}{\beta}\Gamma(\beta z) \right\} = \frac{1}{\beta}\Gamma^*(\nu) = \begin{cases} \frac{1}{\beta} R(\nu|\rho) & \text{for } \nu \in \mathcal{P}, \\ \infty & \text{otherwise}. \end{cases}$$

Thus $F(z) = (1/\beta)\Gamma(\beta z)$. By part (a) of Theorem A.1,

$$\sup_{z \in \mathbb{R}^q} \left\{ \frac{1}{\beta}\Gamma(\beta z) - \frac{1}{2}\|z\|^2 \right\} = \sup_{\nu \in \mathcal{P}} \left\{ \frac{1}{2}\langle \nu, \nu\rangle - \frac{1}{\beta} R(\nu|\rho) \right\},$$

and by part (b) of the theorem the global maximum points of $\Gamma(\beta z) - \frac{1}{2}\|z\|^2$ and $\frac{1}{2}\langle \nu, \nu\rangle - (1/\beta) R(\nu|\rho)$ coincide.

Equation (B1) now implies that

$$\mathcal{E}_\beta = \left\{ z \in \mathbb{R}^q : z \text{ maximizes } \frac{1}{\beta}\Gamma(\beta z) - \frac{1}{2}\|z\|^2 \right\} = \left\{ z \in \mathbb{R}^q : z \text{ minimizes } \frac{\beta}{2}\|z\|^2 - \Gamma(\beta z) \right\}.$$

We summarize this discussion in the following corollary. Part (b) of the corollary is proved in part (b) of Theorem 2.1 in Ref. 19.

Corollary B.1: We define the finite, convex, continuous function Γ *in* (B2). *The following conclusions hold*.

(a) $\mathcal{E}_\beta$ *coincides with the set of global minimum points of*

$$G_\beta(z) = \frac{\beta}{2}\|z\|^2 - \log \sum_{i=1}^{q} e^{\beta z_i} = \frac{\beta}{2}\|z\|^2 - \Gamma(\beta z) - \log q.$$

(b) *For* $0 < \beta < \beta_c$, $\beta = \beta_c$, *and* $\beta > \beta_c$ *the set of global minimum points of* G_β *has the form given by the right-hand side of* (3.4) [*Theorem* 3.1(b)].

Corollary B.1 completes the proof of Theorem 3.1. Kiessling's proof of this corollary based on Lagrange multipliers is given in Appendix B of Ref. 20. Continuous analogues of the corollary are mentioned in Refs. 32, 33, and 38, but are not proved there.

We now show that for all $\beta \leqslant 0$, $\mathcal{E}_\beta = \{\rho\}$. This is obvious for $\beta = 0$ since $\nu = \rho$ is the unique vector in $\mathcal{P}$ that minimizes $R(\nu|\rho)$. Our goal is to prove that for $\beta < 0$, $\nu = \rho$ is also the unique vector in $\mathcal{P}$ that minimizes $R(\nu|\rho) - (\beta/2)\langle \nu, \nu \rangle$. Let $\overline{\nu}$ be a point in $\mathcal{P}$ at which $R(\nu|\rho) - (\beta/2) \times \langle \nu, \nu \rangle$ attains its infimum. For any $i = 1, 2, \ldots, q$,

$$\frac{\partial\left(R(\nu|\rho) - \dfrac{\beta}{2}\langle \nu, \nu \rangle\right)}{\partial \nu_i} = \log \nu_i + 1 - \beta \nu_i,$$

which is negative for all sufficiently small $\nu_i > 0$. It follows that $\overline{\nu}$ does not lie on the relative boundary of $\mathcal{P}$; i.e., $\overline{\nu_j} > 0$ for all $i = 1, 2, \ldots, q$. We complete the proof by showing that for any $1 \leqslant j < k \leqslant q$, $\overline{\nu_j} = \overline{\nu_k}$. Since ρ is the only point in $\mathcal{P}$ satisfying these equalities, we will be done.

Given $a \in (0, 1)$, we consider the reduced two-variable problem of minimizing $R(\nu|\rho) - (\beta/2)\langle \nu, \nu \rangle$ over $\nu_j > 0$ and $\nu_k > 0$ under the constraint $\nu_j + \nu_k = a$; all the other components ν_i are fixed and equal $\overline{\nu_i}$. Setting $\nu_k = a - \nu_j$, we define

$$F(\nu_j) = R(\nu|\rho) - \frac{\beta}{2}\langle \nu, \nu \rangle.$$

Differentiating with respect to ν_j shows that any global minimizer ν_j must satisfy

$$F'(\nu_j) = \log \nu_j - \log(a - \nu_j) - \beta(2\nu_j - a) = 0.$$

Since

$$F''(\nu_j) = \frac{1}{\nu_j} + \frac{1}{a - \nu_j} - 2\beta > 0,$$

$F'(\nu_j)$ is strictly increasing from negative values for all ν_j near 0 to positive values for all ν_j near a. It follows that the only root of $F'(\nu_j) = 0$ is $\nu_j = a/2$ and thus that $\nu_k = a/2 = \nu_j$. Being a global minimizer of $R(\nu|\rho) - (\beta/2)\langle \nu, \nu \rangle$ over $\mathcal{P}$, $\overline{\nu}$ is also a global minimizer of the reduced two-variable problem. Since $a \in (0, 1)$ is arbitrary, it follows that for any distinct pair of indices $\overline{\nu_j} = \overline{\nu_k}$. This completes the proof.

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Nondegenerate ultrametric diffusion

S. V. Kozyrev[a)]
Steklov Mathematical Institute, RAS, Gubkina 8, 119991 Moscow, Russia

V. Al. Osipov[b)] and V. A. Avetisov[c)]
The Semenov Institute of Chemical Physics, RAS, Kossygina 4, 119991 Moscow, Russia

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The general non-degenerate *p*-adic operators of ultrametric diffusion are introduced. Bases of eigenvectors for the introduced operators are constructed and the corresponding eigenvalues are computed. The long-time relaxation behavior of the ultrametric diffusion generated by the introduced operators are investigated. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1858447]

I. INTRODUCTION

Ultrametric diffusions (which are generated by ultrametric pseudodifferential operators) have important applications to models of complex systems. For example, in the papers of Refs. 1 and 2 it was shown that the Parisi matrix in the theory of spin glasses is related to a *p*-adic pseudodifferential operator. Ultrametric diffusion models were investigated in relation with models of relaxation in complex systems, see for instance.[3,4] In the recent works,[1,5,6] *p*-adic models of ultrametric diffusion has been discussed in connection with description of protein dynamics and characteristic types of relaxation in complex systems. In these papers the equivalence of the basin-to-basin kinetics approach, which describes relaxation in complex systems, and ultrametric diffusion models was mentioned. The mathematical theory of ultrametric diffusion was investigated in Refs. 7–9. Applications to biological models was discussed in Ref. 10. All of the above motivates the investigation of more general ultrametric pseudodifferential operators and more general models of ultrametric diffusion. In the paper of Ref. 11 a wide class of *p*-adic pseudodifferential operators was constructed and investigated with the help of basis of *p*-adic wavelets, constructed in Ref. 12. In the present paper we construct an even more general class of *p*-adic pseudodifferential operators.

The structure of the present paper is as follows.

In Sec. II we discuss the basin-to-basin kinetics models from the point of view of ultrametric diffusion theory.

In Sec. III we discuss different classes of *p*-adic models of ultrametric diffusion.

In Sec. IV we discuss the operators, investigated in Ref. 11 and give a new parametrization for kernels of such operators.

In Sec. V we introduce a new family of *p*-adic models of ultrametric diffusion, build the eigenbases for their generators, and compute the corresponding eigenvalues.

In Sec. VI we investigate the properties of ultrametric diffusion, generated by the constructed operators.

II. RELATION TO BASIN-TO-BASIN KINETICS

Ultrametric diffusion models are naturally related to the basin-to-basin kinetics approach proposed a rather long time ago. This relation was mentioned in the paper of Ref. 5 Here we

[a)]Electronic mail: kozyrev@mi.ras.ru
[b)]Electronic mail: vosipov@chph.ras.ru
[c)]Electronic mail: avetisov@chph.ras.ru

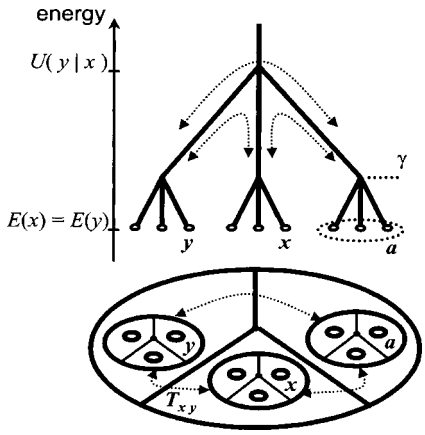

FIG. 1. A hierarchy of basins and activation barriers in the basin-to-basin kinetic approach. For an explanation of the notations see the text.

reproduce this discussion in more details in order to use it to introduce new classes of integration kernels for operators of ultrametric diffusion. The basin-to-basin kinetics approach was widely used in a computer study of the dynamics constrained by rough multidimensional energy landscapes.[13–16] In this approach, the kinetics of a complex system is approximated using separation of the space of states of the system into basins and separation of the corresponding time scales of transitions between the basins. The basin-to-basin kinetics approach can be outlined as follows. Let us consider a system that is described by a particle performing random walk in a rough energy landscape. The system is supposed to be arriving to the nearest quasiequilibrium state (the nearest local minimum on the energy landscape) from any initial state in the time, which is much smaller compared to the lifetime of this quasiequilibrium state. Therefore, we will reduce our consideration to the set of local minima of the energy landscape. Further, we assume that the set of local minima can be represented as a union of hierarchically nested subsets. These subsets we will call the basins of minima. Each of the basins is a union of the nonoverlapping basins of the smaller size (subbasins), each of these smaller basins is a union of the still smaller ones, etc. Moreover, we assume that the larger basins are separated by the higher activation barriers, and the smaller sub-basins are separated by the lower barriers, i.e., if the basin A is a sub-basin of the basin B, then the activation barriers between the maximal sub-basins of A is smaller than the activation barriers between the maximal sub-basins of B. The basin hierarchy corresponds to the hierarchy of the configuration rearrangements, and the hierarchy of the activation barriers corresponds to the hierarchy of characteristic times of these rearrangements.

More definitely, a basin-to-basin approximation of kinetics of a system with a rough energy landscape reduces to the following.

(I) In the basin-to-basin approximation, the space of states is divided into basins, each basin is divided into sub-basins in hierarchical way, and so on.
(II) The rate of transition probability between two states in the different basins depends only on the basins and does not depend on the states themselves.

Thus, the basin-to-basin kinetics can be understood as a diffusion (more definitely, as a jump process) in the ultrametric space.[1,5,6] In this language the property (I) corresponds to ultrametricity of the space of states, and the property (II) takes the form of local constancy of the rate of transition probability.

The multidimensional energy surface can be represented by a tree—a "skeleton" of a hierarchical landscape[14–17] (Fig. 1). This tree reflects the hierarchy of nestings and it is directed (i.e., it is a tree with a partial order). The vertices of the tree correspond to the basins, the partial order describes the ordering of the basins (i.e., the vertex A is larger than B if the corresponding basin A contains the basin B). The local minima of the landscapes correspond to minimal vertices with

respect to the introduced ordering. In the general case for a finite or an infinite tree, the set of local minima will be described by the absolute of the tree. The absolute of any tree has a natural structure of ultrametric space. Therefore a description of a rough energy landscape in terms of hierarchically nested basins is equivalent to the introduction of the ultrametric space of states.

The transition probability T_{xy} between the states y and x is determined by the position of the vertex $U(y|x)$ in which the tree branches into the paths going to the points x and y, and by the energies $E(x)$ and $E(y)$ of the states x and y (Fig. 1). In particular, if all the local minima have the same energy, then T_{xy} is determined only by the vertex $U(y|x)$, i.e., the transition probabilities has the property of permutation symmetry $T_{xy}=T_{yx}$.

III. *p*-ADIC MODELS OF ULTRAMETRIC DIFFUSION

The well-known example of an ultrametric space is the field of p-adic numbers $\mathbb{Q}_p$. In the works of Refs. 1, 5, and 6, p-adic description of ultrametric diffusion is introduced in the following way. The system states are parametrized by the p-adic coordinate x, a basin of states corresponds to the p-adic disk $B_\gamma(a)$ (Fig. 1). The p-adic disk $B_\gamma(a)$, is a set of all p-adic numbers $\{x:|x-a|_p \leqslant p^\gamma\}$, for which the p-adic distance from the disk center $a(a\in\mathbb{Q}_p)$ is less than or equal to the radius p^γ, where γ is an integer ($\gamma\in\mathbb{Z}$). The parameters γ and a distinguish the p-adic disks $B_\gamma(a)$.

To describe the system evolution we introduce the probability distribution function $f(x,t)$ that depends on the p-adic coordinate x and the real time t: the integral,

$$\int_B f(x,t)d\mu(x)$$

[$d\mu(x)$ is the Haar measure on $\mathbb{Q}_p$ (Ref. 7), is the probability of finding the system in the set B at time t.

The evolution of the function $f(x,t)$ is described by the equation

$$\frac{\partial f(x,t)}{\partial t} = -\int_{\mathbb{Q}_p} (T_{yx}f(x,t) - T_{xy}f(y,t))d\mu(y). \tag{1}$$

This is the master equation for ultrametric diffusion, and the linear integral operator on the rhs of (1);

$$Tf(x) = \int_{\mathbb{Q}_p} (T_{yx}f(x) - T_{xy}f(y))d\mu(y) \tag{2}$$

is called the operator of ultrametric diffusion.

The non-negative kernel T_{xy} is equal to the rate of transition from the state y to the state $x(T_{xy}:\mathbb{Q}_p\times\mathbb{Q}_p\mapsto\mathbb{R}_+)$. We consider the kernels T_{xy}, which are locally constant outside any vicinity of $x=y$. The complex-valued function $g(x)$, defined on $\mathbb{Q}_p$, is called locally constant, if

$$\forall x\in\mathbb{Q}_p,\quad \exists\,\gamma\in\mathbb{Z},\quad \forall\, z\in\mathbb{Q}_p:|z|_p\leqslant p^\gamma \Rightarrow g(x+z)=g(x).$$

In the simplest case the operators of ultrametric diffusion can be introduced by the kernels T^0_{xy} satisfying the following conditions:

(i)

$$\text{for fixed}\quad y,\quad \forall\, x,z\in\mathbb{Q}_p:|z|_p\leqslant|x-y|_p \Rightarrow T^0_{(x+z)y}=T^0_{xy},$$

$$\text{for fixed}\quad x,\quad \forall\, y,z\in\mathbb{Q}_p:|z|_p\leqslant|x-y|_p \Rightarrow T^0_{x(y+z)}=T^0_{xy}; \tag{3}$$

(ii)

$$T^0_{xy} = T^0_{yx},$$

i.e., the kernel T^0_{xy} is symmetric (and the corresponding operator is Hermitian, since T^0_{xy} is a real-valued function);

(iii)

$$\forall a \in \mathbb{Q}_p, \quad T^0_{xy} = T^0_{x-ay-a},$$

i.e., the kernel T^0_{xy} has the property of translation invariance.

In the following we will denote by T^0 the operator of ultrametric diffusion, and by T^0_{xy} the corresponding kernel. The general form of the kernels T^0_{xy} is given by the series

$$T^0_{xy} = \sum_{\gamma=-\infty}^{\infty} T^{(\gamma)} \delta_{p^\gamma, |x-y|_p}, \tag{4}$$

where δ is the Kronecker delta. The kernels T^0 can be equivalently described by the functions dependent only on p-adic norm of the difference of x and y: $T^0_{x,y} = \rho(|x-y|_p)$. The coefficients $T^{(\gamma)}$ of the series (4) and the function $\rho(|x-y|_p)$ are connected by the relation $T^{(\gamma)} = \rho(p^\gamma)$.

The properties (i)–(iii) allow us to use the p-adic Fourier transformation to compute the eigenvalues of the operator. If the series $\Sigma_{\gamma=0}^{\infty} p^\gamma T^{(\gamma)}$ converges, the eigenvalues of the operator T^0 are determined by the expression[7]

$$\lambda^0_\gamma = p^\gamma T^{(\gamma)} + (1 - p^{-1}) \sum_{\gamma' = \gamma+1} p^{\gamma'} T^{(\gamma')}.$$

Every eigenvalue λ^0_γ is infinitely degenerate.

The operators of the form T^0 were discussed in the context of p-adic mathematical physics. When the kernel has the form with

$$T_{xy} = \frac{p^\alpha - 1}{1 - p^{-1-\alpha}} |x-y|_p^{-(1+\alpha)}, \quad \alpha > 0,$$

the operator T^0 is the Vladimirov operator of p-adic fractional derivation.[7] Its eigenvalues are given by $\lambda_\gamma = p^{(1-\gamma)\alpha}$, $\gamma \in \mathbb{Z}$. Different examples of the operators T^0 have been recently investigated in Ref. 6.

In the context of basin-to-basin kinetics, the operator symmetry (hermiticity) property means that all the local minima of the energy landscape have equal energy. The translation invariance of the kernel means that the transition between x and y depends only on the ultrametric distance between x and y.

The translationally invariant operators T^0 are related to the Parisi matrices (see Refs. 1 and 2) that were used in the replica approach to spin glasses.[18] However, it is not very natural to assume that the energy landscapes of many other disordered systems (for instance, the energy landscapes of clusters, macromolecular structures, and biopolymers, discussed, for example, in Ref. 15) are described by the operators with translationally invariant kernels. Therefore, the ultrametric diffusion operators, more general than T^0, are of great importance.

Generally, the ultrametric diffusion operator T can be defined by (2), where the kernel satisfies some weaker conditions than conditions (i)–(iii). In the present paper we consider translationally *noninvariant* operators of ultrametric diffusion satisfying the hermiticity property. We will examine two types of such operators, T^{I} and T^{II}.

A family of operators of p-adic diffusion T^{I} has been recently investigated in the paper.[11] The local constancy conditions for these operators are given by (3), as well as for T^0, but T^{I} differs from T^0 by violating the condition (iii).

The kernel T^{I}_{xy} is described by the expression

$$T^{\mathrm{I}}_{xy} = \sum_{\gamma=-\infty}^{\infty} \sum_{n\in\mathbb{Q}_p/\mathbb{Z}_p} T^{(\gamma n)} \delta_{1,|p^{\gamma}x - p^{\gamma}y|_p} \Omega(p^{\gamma}x - n), \tag{5}$$

where the factor group $\mathbb{Q}_p/\mathbb{Z}_p$ is identified with a set of the fractions $\Sigma_{\gamma=1}^{k} n_{\gamma} p^{-\gamma}$, $n_{\gamma}=0,\ldots,p-1$, k is any natural number, and the coefficients $T^{(\gamma n)} \geqslant 0$. The function $\Omega(|x|_p)$ is an indicator of the p-adic disk,

$$\Omega(|x|_p) = \begin{cases} 1, & |x|_p \leqslant 1, \\ 0, & |x|_p > 1. \end{cases}$$

It was shown that if the series $\Sigma_{\gamma'=\gamma}^{\infty} p^{\gamma'} T^{(\gamma' n)}$ converges, the eigenvalues of the corresponding operator are given by

$$\lambda^{\mathrm{I}}_{\gamma n} = p^{\gamma} T^{(\gamma n)} + (1 - p^{-1}) \sum_{\gamma'=\gamma+1}^{\infty} p^{\gamma'} \sum_{n'\in\mathbb{Q}_p/\mathbb{Z}_p} T^{(\gamma' n')} \delta_{n', np^{\gamma'}}, \tag{6}$$

and, in general, are $p-1$ times degenerate. The eigenvalue $\lambda^{\mathrm{I}}_{\gamma n}$ corresponds to the eigenvectors

$$\varphi_{\gamma n j}(x) = p^{-\gamma/2} \chi_p(p^{\gamma-1} j x) \Omega(|p^{\gamma}x - n|_p), \tag{7}$$

where $j=1,\cdots,p-1$. Here the function $\chi_p(x)=\exp(2\pi i\{x\}_p)$ is an additive character on the field $\mathbb{Q}_p$, the symbol $\{x\}_p$ denotes a fractional part of the p-adic number. Recall that if the canonical decomposition of the p-adic number x is given by

$$x = p^{\gamma} \sum_{\mu=0}^{\infty} x_{\mu} p^{\mu}, \quad x_{\mu} = 0,\cdots,p-1, \quad x_0 \neq 0, \tag{8}$$

then the fractional part of the number x is determined by the following expression:

$$\{x\}_p = \begin{cases} 0, & \gamma \geqslant 0, \\ p^{\gamma}(x_0 + x_1 + \ldots + x_{|\gamma|-1} p^{|\gamma|-1}), & \gamma < 0. \end{cases}$$

As shown in Ref. 12, the set of vectors (7) forms an orthonormal basis in $L^2(\mathbb{Q}_p)$, which was called there the basis of p-adic wavelets.

In the present paper, in Sec. IV, we propose a new general expression for the kernel T^{I} and show the equivalence of this expression with (5).

In Sec. V we introduce the new type of transitionally noninvariant kernel, T^{II}, satisfying the weaker [compared with (3)] condition of local constancy:

$$\text{for fixed } y, \quad \forall x, \quad z\in\mathbb{Q}_p : |z|_p \leqslant p^{-1}|x-y|_p \Rightarrow T^{\mathrm{II}}_{(x+z)y} = T^{\mathrm{II}}_{xy}$$

$$\text{for fixed } x, \quad \forall y, \quad z\in\mathbb{Q}_p : |z|_p \leqslant p^{-1}|x-y|_p \Rightarrow T^{\mathrm{II}}_{x(y+z)} = T^{\mathrm{II}}_{xy} \tag{9}$$

Note that operator T^{II} is more general compared to T^{I}, but in some cases (see Sec. V) the operators T^{I} and T^{II} are identically equal, for instants when $p=2$.

We introduce the kernel T^{II} both in the functional form and in the form of a series, and we show the equivalence of these definitions. In this section, we find the eigenfunctions of the introduced operator, which form the basis in $L^2(\mathbb{Q}_p)$, compute the corresponding eigenvalues, and show that the eigenvalues, in general, are nondegenerate.

In Sec. VI, we investigate the properties of ultrametric diffusion, generated by the operators T^{I} and T^{II}. We consider the relaxation of the initially localized state. We show that the inhomogeneities of the landscape described by the translationally noninvariant kernels T^{I} and T^{II} are not

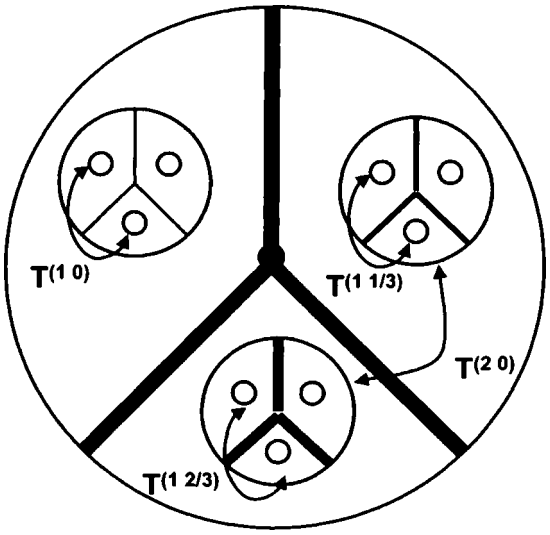

FIG. 2. The scheme of the transitions corresponding to the operator T^{I} with $p=3$. The lines of different thickness correspond to the different transition probabilities $T^{(\gamma n)}$ between the p-adic disks, which are marked by the circles.

essential for long-time relaxation, i.e., the asymptotics for the relaxation, correspondent to kernels T^{0}_{xy}, T^{I}_{xy}, T^{II}_{xy} will be the same for the cases when the corresponding kernels are naturally related in the way described in Sec. IV.

IV. TRANSLATIONALLY NONINVARIANT OPERATORS OF ULTRAMETRIC DIFFUSION T^{I}

In the present section we propose a new expression for the kernel T^{I} and show that this new expression is equivalent to the already known one. Expression (5) implies, that if $x\in B_{\gamma}(p^{-\gamma}n)$ and y satisfies the condition $|x-y|_p=p^{\gamma}$, then the kernel T^{I}_{xy} is equal to $T^{(\gamma n)}$. In this case, we can illustrate the basin-to-basin transitions with the help of the scheme in Fig. 2. The given transition scheme allows us to construct the expression of the operator T^{I}. To construct a new expression for the kernel T^{I}_{xy}, we use the following approach. The integration kernel T^{I}_{xy} of the operator should depend on the two arguments: (i) on the size of the minimal disk containing x and y, which is equal to the distance $|x-y|_p$; (ii) on the argument distinguishing the disk among the other disks of the same size. For the last purpose we fix the disk center. Since any point belonging to an ultrametric disk is its center, we will take as the center of the minimal disk, containing x and y the following:

$$\frac{\{x|x-y|_p\}_p}{|x-y|_p}=\begin{cases}\displaystyle\sum_{\mu=\log_p|x-y|_p+1}^{\log_p|x|_p} p^{-\mu}x_{\mu}, & |x|_p>|x-y|_p,\\ 0, & |x|_p\leqslant|x-y|_p,\end{cases} \tag{10}$$

where x_{μ} are the coefficients of the canonical decomposition (8) of the p-adic number x. Therefore, the kernel of the operator T^{I} can be represented by the function

$$\rho(|x-y|_p,\{x|x-y|_p\}_p). \tag{11}$$

The function (11) obviously do not have the translational invariance property. For this function the following proposition is satisfied.

Proposition 1: *The function (11) is symmetric with respect to the $x\mapsto y$, $y\mapsto x$ permutation. The function (11) satisfies the conditions (3) and (5). Moreover, any function satisfying the condition (5) can be represented in the form (11). Therefore the representations of the kernel T^{I} in the forms (11) and (5) are equivalent, and the equivalence is given by the relation*

$$T^{(\gamma n)} = \rho(p^{\gamma}, n), \quad \gamma \in \mathbb{Z}, \quad n \in \mathbb{Q}_p/\mathbb{Z}_p. \tag{12}$$

Proof: Let us prove the permutation symmetry: $\{y|x-y|_p\}_p = \{x|y-x|_p\}_p$. It follows that

$$\{x|x-y|_p\}_p - \{y|x-y|_p\}_p = \{(x-y)|x-y|_p\}_p = 0.$$

For proving the rest of the proposition, we will show at first that any function of the form (11) can be represented in the form (5). Actually, for any $x \in B_{\gamma}(p^{-\gamma}n)(n \in \mathbb{Q}_p/\mathbb{Z}_p)$ and any $y \in \mathbb{Q}_p$ satisfying the condition $|x-y|_p = p^{\gamma}$, we have $\{x|x-y|_p\}_p = \{n\}_p = n$. Hence,

$$\rho(|x-y|_p, \{x|x-y|_p\}_p) = \sum_{\gamma=-\infty}^{\infty} \sum_{n \in \mathbb{Q}_p/\mathbb{Z}_p} \rho(p^{\gamma}, n)\, \delta_{1,|p^{\gamma}x - p^{\gamma}y|_p}\, \Omega(p^{\gamma}x - n).$$

This means that the function (11) can be represented in the form of the series (5) with the coefficients $T^{(\gamma n)} = \rho(p^{\gamma}, n)$.

On the other hand, since no special restrictions are imposed on the function (11), then for all $\gamma \in \mathbb{Z}$ and $n \in \mathbb{Q}_p/\mathbb{Z}_p$ we can put $\rho(p^{\gamma}, n) = T^{(\gamma n)}$. Therefore the representations of the kernel T^{I} in the forms (11) and (5) are equivalent, and the equivalence is given by (12).

From the equivalence, it follows that the functions (11) and (5) have the same properties. In particular, the function (11) satisfies the condition (3). □

V. TRANSLATIONALLY NONINVARIANT OPERATORS OF ULTRAMETRIC DIFFUSION T^{II} AND THE BASIS OF GENERALIZED *p*-ADIC WAVELETS

Define the family of the operators of ultrametric diffusion T^{II}, with locally constant kernels of the most general form

$$T^{\mathrm{II}}_{xy} = \sum_{\gamma=-\infty}^{\infty} \sum_{n \in \mathbb{Q}_p/\mathbb{Z}_p} \sum_{\substack{j,k=0 \\ k \neq j}}^{p-1} T^{(\gamma njk)} \Omega(p|p^{\gamma}x - n - j|_p) \Omega(p|p^{\gamma}y - n - k|_p), \tag{13}$$

where $T^{(\gamma njk)} = T^{(\gamma nkj)} \geqslant 0$.

Theorem 2: *The function of the form (13) is symmetric with respect to permutation of the arguments, positive, and satisfies the condition (9).*

Moreover, an arbitrary positive symmetric function satisfying (9) can be represented in the form (13).

Proof: The positivity of T^{II}_{xy} is obvious. Permutation symmetry is obvious.

Prove that T^{II}_{xy} given by (13) satisfies (9). This property is easy to check for any product of two indicator functions in (13). By linearity, this proves that T^{II}_{xy} satisfy (9).

Vice versa, it is easy to see that the kernel (13) for x, y lying in the disks with the center in $p^{-\gamma}(n+j)$ and $p^{-\gamma}(n+k)$ correspondingly and the radius $p^{\gamma-1}$, takes the value $T^{(\gamma njk)}$.

Since all the space $x, y \in \mathbb{Q}_p \times \mathbb{Q}_p$ is the disjoint union of such subsets, therefore, taking an arbitrary positive and symmetric with respect to j, k coefficients $T^{(\gamma njk)}$, we are able to construct an arbitrary symmetric positive kernel satisfying (9). □

The kernel T^{II} can be equivalently described in the functional form.

Proposition 3: *The function,*

$$\rho(|x-y|_p, \{x|x-y|_p\}_p, \ \{xp^{-1}|x-y|_p\}_p, \ \{yp^{-1}|x-y|_p\}_p), \tag{14}$$

satisfies the condition (9). Moreover, any function satisfying the condition (9) can be represented in the form (14).

Under condition of symmetry of the function (14) with respect to permutation of x and y, the kernel T^{II} can be equivalently represented in the forms (14) and (13), and the equivalence is given by the relation

$$T^{(\gamma njk)} = \rho(p^{\gamma}, n, p^{-1}(n+j), p^{-1}(n+k)). \tag{15}$$

Proof: Let us show first that any function of the form (14) can be represented in the form (13). Actually, any x and y lying in the disks of the radius $p^{\gamma-1}$ with the centers in $p^{-\gamma}n+p^{-\gamma}j$ and $p^{-\gamma}n+p^{-\gamma}k$ ($n\in\mathbb{Q}_p/\mathbb{Z}_p$, j, $k=0,\ldots,p-1$ and $j\neq k$) can be represented in the form

$$x = p^{-\gamma}(n+j+pz_x), \quad |z_x|_p \leqslant 1,$$

$$y = p^{-\gamma}(n+k+pz_y), \quad |z_y|_p \leqslant 1.$$

When it follows that at $j\neq k$, $|x-y|_p = p^{\gamma}$, $\{x|x-y|_p\}_p = n$ and

$$\{xp^{-1}|x-y|_p\}_p = \{p^{-1}(n+j)+z_x\}_p = p^{-1}(n+j),$$

$$\{yp^{-1}|x-y|_p\}_p = \{p^{-1}(n+k)+z_y\}_p = p^{-1}(n+k).$$

Hence,

$$\rho(|x-y|_p, \{x|x-y|_p\}_p, \{xp^{-1}|x-y|_p\}_p, \{yp^{-1}|x-y|_p\}_p)$$
$$= \sum_{\gamma=-\infty}^{\infty} \sum_{n\in\mathbb{Q}_p/\mathbb{Z}_p} \rho(p^{\gamma}, n, p^{-1}(n+j), p^{-1}(n+k))\Omega(p|p^{\gamma}x-n-j|_p)\Omega(p|p^{\gamma}y-n-k|_p).$$

Thus, the function (14) can be represented in the form of the series (13), whose coefficients are determined by (15).

On the other hand, since no restrictions (except for permutation symmetry) are imposed on the function of the type (14), then for all $\gamma\in\mathbb{Z}$ and $n\in\mathbb{Q}_p/\mathbb{Z}_p$, j, $k=0,\ldots,p-1 (j\neq k)$ we can put $\rho(p^{\gamma}, n, p^{-1}(n+j), p^{-1}(n+k))$ to be equal to $T^{(\gamma njk)}$. Therefore the representations of the kernel in the forms (14) and (13) are equivalent.

Moreover, for the function (14) and the series (13), respectively, the condition of symmetry with respect to permutation of x and y in (14) and of the symmetry of the coefficients $T^{(\gamma njk)}$ with respect of permutation of j and k, are equivalent.

From this equivalence, it follows that the function (14) satisfies the condition (9), and any function satisfying the condition (9) can be represented in the form (14). □

Proposition 4: *If $T^{(\gamma njk)}$ in (13) does not depend on j and k, then the operator T^{II} reduces to T^{I}.*

Proof: Consider the kernel T^{II}_{xy} under the condition that $T^{(\gamma njk)}$ is independent on j and k:

$$T^{\mathrm{II}}_{xy} = \sum_{\gamma,n} T^{(\gamma n)} \sum_{j=0}^{p-1} \Omega(p|p^{\gamma}x-n-j|_p) \sum_{\substack{k=0 \\ k\neq j}}^{p-1} \Omega(p|p^{\gamma}y-n-k|_p). \tag{16}$$

Using the formula

$$\Omega(|p^{\gamma}x-n|_p) = \Omega(p^{-\gamma}|x-p^{-\gamma}n|_p) = \sum_{j=0}^{p-1} \Omega(p^{-\gamma+1}|x-p^{-\gamma}n-p^{-\gamma}j|_p) = \sum_{j=0}^{p-1} \Omega(p|p^{-\gamma}x-n-j|_p), \tag{17}$$

as well as the property of indicators of the disks

$$\Omega(|x-a|_p)\Omega(|y-a|_p) = \Omega(|x-a|_p)\Omega(|x-y|_p),$$

for the sum on j and k in (16) we have

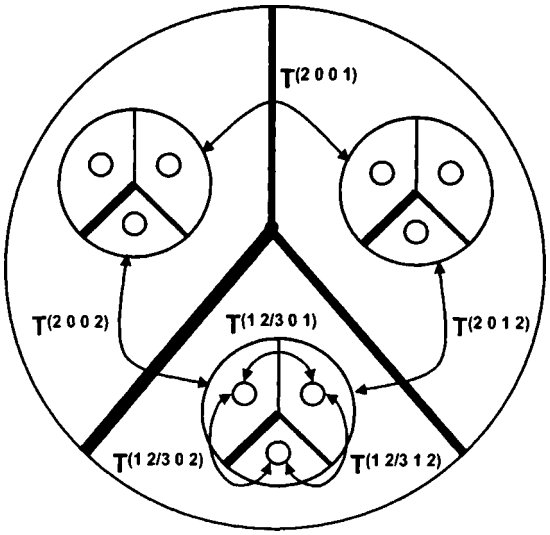

FIG. 3. The scheme of the transitions corresponding to the operator T^{II} with $p=3$.

$$\sum_{j=0}^{p-1}\Omega(p|p^{\gamma}x-n-j|_p)\sum_{\substack{k=0\\k\neq j}}^{p-1}\Omega(p|p^{\gamma}y-n-k|_p)$$

$$=\sum_{j=0}^{p-1}\Omega(p|p^{\gamma}x-n-j|_p)(\Omega(|p^{\gamma}y-n|_p)-\Omega(p|p^{\gamma}y-n-j|_p))$$

$$=\Omega(|p^{\gamma}x-n|_p)(\Omega(|p^{\gamma}y-n|_p)-\Omega(p|p^{\gamma}y-p^{\gamma}x|_p))$$

$$=\Omega(|p^{\gamma}x-n|_p)(\Omega(|p^{\gamma}y-p^{\gamma}x|_p)-\Omega(p|p^{\gamma}y-p^{\gamma}x|_p))$$

$$=\Omega(|p^{\gamma}x-n|_p)\,\delta_{1,|p^{\gamma}x-p^{\gamma}y|_p}.$$

□

Note that the operators T^{I} and T^{II} are identically equal for $p=2$. Actually, in this case the expression (13) contains only $T^{(\gamma n01)}$ and $T^{(\gamma n10)}$. Since $T^{(\gamma n01)}=T^{(\gamma n10)}$, from Proposition 4 it follows that $T^{\mathrm{I}}_{xy}=T^{\mathrm{II}}_{xy}$.

Unlike for the operator T^{I}, the kernel of the operator T^{II} formally depends on a couple of additional functions: $\{xp^{-1}|x-y|_p\}_p$ and $\{yp^{-1}|x-y|_p\}_p$. We will explain the meaning of these functions. Consider the transition between the states x and y (see Fig. 3). The probability for $x\mapsto y$ transition depends on a relative position of the basins between which the transition is carried out. Let x and y belong to the basin described by the p-adic disk $B_{\gamma}(a)$ of the radius $p^{\gamma}=|x-y|_p$ with the center in $a=\{xp^{\gamma}\}_p p^{-\gamma}$. Then the radii of the disks $B_{\gamma-1}(b)$ and $B_{\gamma-1}(c)$, between which the transition is carried out, are equal to $p^{-1}|x-y|_p$, and the disk centers are determined by the functions $b=\{xp^{\gamma-1}\}_p p^{-\gamma+1}$, $c=\{yp^{\gamma-1}\}_p p^{-\gamma+1}$.

Now we will construct the basis of eigenfunctions of the operator T^{II}.

Consider the $p\times p$ matrix $(\mathbf{W}^{(\gamma n)})_{ls}$ with matrix elements equal to $-T^{(\gamma njk)}$ for $j\neq k$ and equal to $\sum_{\substack{k=0\\k\neq l}}^{p-1}T^{(\gamma nkl)}$ for the diagonal elements:

$$\mathbf{W}^{(\gamma n)}_{ls}=\delta_{sl}\sum_{\substack{k=0\\k\neq l}}^{p-1}T^{(\gamma nlk)}-(1-\delta_{sl})T^{(\gamma nls)}. \tag{18}$$

It is easy to see that $\mathbf{W}^{(\gamma n)}$ is a real symmetric $p\times p$ matrix. Moreover, the matrix is positive.

Lemma 5: *The matrix* $\mathbf{W}^{(\gamma n)}$ *defined by (18) is positive.*

Proof: Compute the Hermitian form [we omit the (γn) index]

$$\langle z,\mathbf{W}z\rangle=\sum_{s=0}^{p-1}|z_s|^2\sum_{\substack{l=0\\ l\neq s}}^{p-1}W_{sl}-\sum_{s=0}^{p-1}\sum_{\substack{l=0\\ l\neq s}}^{p-1}z_s^*z_lW_{sl}=\sum_{s=0}^{p-1}\sum_{\substack{l=0\\ l\neq s}}^{p-1}W_{sl}(|z_s|^2-z_s^*z_l).$$

Combining the terms containing W_{sl} and W_{ls} and using the fact that $T^{(ls)}$ is a real symmetric matrix with non-negative entries, we obtain, for the combination of the terms

$$T_{sl}(|z_s|^2+|z_l|^2-z_s^*z_l-z_l^*z_s)\geqslant 0,$$

which proves the positivity and finishes the proof of the lemma. □

The matrix $\mathbf{W}^{(\gamma n)}$ has p non-negative eigenvalues. Let us assume that the jth $(j=1,\ldots,p-1)$ eigenvector has the coordinates $h^k_{\gamma nj}$, $k=0,\ldots,p-1$ and corresponds to the eigenvalue $\lambda_j^{(\gamma n)}$:

$$\sum_{k=0}^{p-1}W_{lk}^{(\gamma n)}h^k_{\gamma nj}=\lambda_j^{(\gamma n)}h^l_{\gamma nj}.$$

It is easy to see that the matrix $\mathbf{W}^{(\gamma n)}$ has the zero eigenvalue, which corresponds to the eigenvector with equal matrix elements: $h^k_{\gamma n0}=p^{-1/2}$ for all $k=0,\ldots,p-1$. Since eigenvectors are orthonormal we have

$$\sum_{k=0}^{p-1}h^{*k}_{\gamma nj}h^k_{\gamma nj'}=\delta_{jj'},\quad j,j'=0,\ldots,p-1. \tag{19}$$

Consider the function $\psi_{\gamma nj}(x)$ of the form

$$\psi_{\gamma nj}(x)=p^{(1-\gamma)/2}\sum_{k=0}^{p-1}h^k_{\gamma nj}\Omega(p|p^\gamma x-n-k|_p),$$

$$\gamma\in\mathbb{Z},\quad n\in\mathbb{Q}_p/\mathbb{Z}_p,\quad j=1,\ldots,p-1. \tag{20}$$

Note that $\psi_{\gamma nj}(x)$ is a locally constant function, constant on disks of the radius $p^{\gamma-1}$ and $\psi_{\gamma nj}(x)\in L^2(\mathbb{Q}_p)$. The functions $\psi_{\gamma nj}(x)$ we will call the generalized p-adic wavelets.

For further computations we use the following identity:

$$\Omega(p|p^\gamma x-n-k|_p)\Omega(p|p^{\gamma'}x-n'-l|_p)=\delta_{p^{\gamma'-\gamma(n+k),n'+l}}\theta(\gamma'-\gamma)\Omega(p|p^\gamma x-n-k|_p)+\delta_{n+k,p^{\gamma-\gamma'}(n'+l)}\times(1-\theta(\gamma'-\gamma))\Omega(p|p^{\gamma'}x-n'-l|_p), \tag{21}$$

where

$$\theta(\gamma)=\begin{cases}1, & \gamma>0,\\ 0, & \gamma\leqslant 0,\end{cases}$$

and $\delta_{p^{\gamma'-\gamma(n+k),n'+l}}$ is the Kronecker symbol on the group $\mathbb{Q}_p/p\mathbb{Z}_p$:

$$\Omega(|p^{\gamma'-\gamma}(n+k)-(n'+l)|_p)=\delta_{p^{\gamma'-\gamma(n+k),n'+l}},\quad \text{for } \gamma'\geqslant\gamma.$$

Theorem 6: *The set of functions* $\{\psi_{\gamma nj}(x)\}$, $\gamma\in\mathbb{Z}$, $n\in\mathbb{Q}_p/\mathbb{Z}_p$, $j=1,\ldots,p-1$ *is an orthonormal basis in* $L^2(\mathbb{Q}_p)$.

Proof: Consider the scalar product

$$p^{(\gamma-1)/2}p^{(\gamma'-1)/2}\langle\psi_{\gamma nj},\psi_{\gamma' n' j'}\rangle=\int_{Q_p}\sum_{s=0}^{p-1}h_{\gamma nj}^{*s}\Omega(p|p^{\gamma}x-n-s|_p)\sum_{l=0}^{p-1}h_{\gamma' n' j'}^{l}\Omega(p|p^{\gamma'}x-n'-l|_p)d\mu(x).$$

Using (21) we compute the following:

$$\begin{aligned}p^{(\gamma-1)/2}p^{(\gamma'-1)/2}\langle\psi_{\gamma nj},\psi_{\gamma' n' j'}\rangle&=\sum_{s=0}^{p-1}h_{\gamma nj}^{*s}\sum_{l=0}^{p-1}h_{\gamma' n' j'}^{l}\int_{Q_p}\Big(\delta_{p^{\gamma'-\gamma(n+s),n'+l}}\theta(\gamma'-\gamma)\Omega(p|p^{\gamma}x-n-s|_p)\\&\quad+\delta_{n+s,p^{\gamma-\gamma'(n'+l)}}(1-\theta(\gamma'-\gamma))\Omega(p|p^{\gamma'}x-n'-l|_p)\Big)d\mu(x)\\&=\sum_{s=0}^{p-1}h_{\gamma nj}^{*s}\sum_{l=0}^{p-1}h_{\gamma' n' j'}^{l}\Big(\delta_{p^{\gamma'-\gamma(n+s),n'+l}}\theta(\gamma'-\gamma)p^{\gamma-1}\\&\quad+\delta_{n+s,p^{\gamma-\gamma'(n'+l)}}(1-\theta(\gamma'-\gamma))p^{\gamma'-1}\Big).\end{aligned}$$

In this expression, if the first term is nonzero and $\gamma'>\gamma$, then $\delta_{p^{\gamma'-\gamma(n+s),n'+1}}$ does not depend on s, and we obtain the summation on s of the form $\Sigma_{s=0}^{p-1}h_{\gamma nj}^{*s}$ that is equal to zero for $j>0$.

In the same way, we prove that the second term does not vanish only for $\gamma'=\gamma$. This proves that

$$p^{(\gamma-1)/2}p^{(\gamma'-1)/2}\langle\psi_{\gamma nj},\psi_{\gamma' n' j'}\rangle=\delta_{\gamma\gamma'}\delta_{nn'}p^{\gamma-1}\sum_{s=0}^{p-1}h_{\gamma nj}^{*s}h_{\gamma nj'}^{s}=\delta_{\gamma\gamma'}\delta_{nn'}\delta_{\gamma\gamma'}p^{\gamma-1}\|h_{(\gamma n)j}\|^2,$$

which implies that $\{\psi_{\gamma nj}\}$ is an orthonormal system of functions.

To prove that the set of vectors $\{\psi_{\gamma nj}\}$ is an orthonormal basis [is total in $L^2(\mathbb{Q}_p)$] we use the Parseval identity. Since the set of indicators (characteristic functions) of p-adic disks is total in $L^2(\mathbb{Q}_p)$, it is enough to check the Parseval identity for the indicator $\Omega(p|p^{\gamma}x-n-s|_p)$. We have for the scalar product of the indicator and the wavelet,

$$\langle\Omega(p|p^{\gamma}x-n-s|_p),\psi_{\gamma' n' j'}\rangle=p^{(1-\gamma')/2}\sum_{l=0}^{p-1}h_{\gamma' n' j'}^{l}p^{\gamma-1}\Big(\delta_{p^{\gamma'-\gamma n,n'+l}}\theta(\gamma'-\gamma)+\delta_{\gamma\gamma'}\delta_{nn'}\delta_{sl}\Big).$$

Summing up the wavelets, we get

$$\begin{aligned}&\sum_{\gamma' n' j'}|\langle\Omega(p|p^{\gamma}x-n-s|_p),\psi_{\gamma' n' j'}(x)\rangle|^2\\&\quad=p^{\gamma-1}\left[\sum_{j'}|h_{\gamma nj'}^{s}|^2+p^{\gamma-1}\sum_{\gamma'>\gamma;n' j'}p^{1-\gamma'}\sum_{l=0}^{p-1}|h_{\gamma' n' j'}^{l}|^2\delta_{p^{\gamma'-\gamma_n,n'+l}}\right].\end{aligned}\tag{22}$$

Using the normalization condition we get

$$\sum_{j=1}^{p-1}h_{\gamma nj}^{*s}h_{\gamma nj}^{s}=1-p^{-1},\tag{23}$$

which implies for (22),

$$(1-p^{-1})p^{\gamma-1}\left[1+p^{\gamma-1}\sum_{\gamma'>\gamma}p^{1-\gamma'}\right]=(1-p^{-1})p^{\gamma-1}(1-p^{-1})^{-1}=p^{\gamma-1},$$

which proves the Parseval identity.

In the next theorem we prove that the constructed in the theorem above basis is an eigenbasis of the ultrametric diffusion operator T^{II} and compute the corresponding eigenvalues.

Theorem 7: *Let the kernel (13) satisfy the condition of convergence of the series*

$$\sum_{\gamma>0}\sum_{k=1}^{p-1} p^{\gamma}T^{(\gamma 0k0)}. \tag{24}$$

Then the operator (2) is a well defined operator in $L^2(\mathbb{Q}_p)$ *with the dense domain and the generalized p-adic wavelets* $\psi_{\gamma nj}$ *are eigenvectors for the operator* T^{II}:

$$T^{\mathrm{II}}\psi_{\gamma nj} = \lambda^{\mathrm{II}}_{\gamma nj}\psi_{\gamma nj},$$

with the eigenvalues

$$\lambda^{\mathrm{II}}_{\gamma nj} = p^{\gamma-1}\lambda_j^{(\gamma n)} + \sum_{\substack{\gamma' n' lk \\ l\neq k}} p^{\gamma'-1}T^{(\gamma' n' lk)}\delta_{p^{\gamma'-\gamma_{n,n'+l}}}\theta(\gamma'-\gamma). \tag{25}$$

Proof: Consider the action of the operator on the wavelet $\psi_{\gamma jn}$:

$$\begin{aligned} p^{(\gamma-1)/2}T^{\mathrm{II}}\psi_{\gamma nj}(x) &= p^{(\gamma-1)/2}\int T^{\mathrm{II}}_{xy}(\psi_{\gamma nj}(x)-\psi_{\gamma nj}(y))d\mu(y) \\ &= p^{\gamma'-1}\sum_{\substack{\gamma' n' lk \\ l\neq k}} T^{(\gamma' n' lk)}\Omega(p|p^{\gamma'}x-n'-l|_p)\sum_{s=0}^{p-1} h^s_{\gamma nj}\Omega(p|p^{\gamma}x-n-s|_p) \\ &\quad - \sum_{\substack{\gamma' n' lk \\ l\neq k}} T^{(\gamma' n' lk)}\Omega(p|p^{\gamma'}x-n'-l|_p)\sum_{s=0}^{p-1} h^s_{\gamma nj} \\ &\quad \times\int \Omega(p|p^{\gamma'}y-n'-k|_p)\Omega(p|p^{\gamma}y-n-s|_p)d\mu(y). \end{aligned}$$

Using (21) for $p^{(\gamma-1)/2}T^{\mathrm{II}}\psi_{\gamma nj}(x)$, we compute the following:

$$\begin{aligned} &\sum_{\substack{\gamma' n' lk \\ l\neq k}} T^{(\gamma' n' lk)}\sum_{s=0}^{p-1} h^s_{\gamma nj}\Big[\delta_{p^{\gamma'-\gamma(n+s),n'+l}}\theta(\gamma'-\gamma)p^{\gamma'-1}\Omega(p|p^{\gamma}x-n-s|_p) \\ &\quad + [\delta_{n+s,p^{\gamma-\gamma'}(n'+l)} - \delta_{n+s,p^{\gamma-\gamma'}(n'+k)}](1-\theta(\gamma'-\gamma))p^{\gamma'-1}\Omega(p|p^{\gamma'}x-n'-l|_p) \\ &\quad - \delta_{p^{\gamma'-\gamma(n+s),n'+k}}\theta(\gamma'-\gamma)p^{\gamma-1}\Omega(p|p^{\gamma'}x-n'-l|_p)\Big]. \end{aligned}$$

We prove that the term proportional to $1-\theta(\gamma'-\gamma)$ is equal to the following:

$$[\delta_{n+s,p^{\gamma-\gamma'}(n'+l)} - \delta_{n+s,p^{\gamma-\gamma'}(n'+k)}](1-\theta(\gamma'-\gamma)) = \delta_{\gamma\gamma'}\delta_{nn'}(\delta_{sl}-\delta_{sk})$$

and

$$\sum_{s=0}^{p-1} h^s_{\gamma nj}\delta_{p^{\gamma'-\gamma(n+s),n'+k}}\theta(\gamma'-\gamma) = \delta_{p^{\gamma'-\gamma_{n,n'+k}}}\theta(\gamma'-\gamma)\sum_{s=0}^{p-1} h^s_{\gamma nj} = 0,$$

since for $j=1,\ldots,p-1$, we have $\Sigma_{s=0}^{p-1}h^s_{\gamma nj}=0$.

This implies for $p^{(\gamma-1)/2}T^{\mathrm{II}}\psi_{\gamma nj}(x)$ the following:

$$p^{(\gamma-1)/2}T^{\mathrm{II}}\psi_{\gamma nj}(x)=\left[\sum_{\substack{\gamma' n' lk\\ l\neq k}} T^{(\gamma' n' lk)}\delta_{p^{\gamma'-\gamma_{n,n'+l}}}\theta(\gamma'-\gamma)p^{\gamma'-1}\right]\sum_{s=0}^{p-1}h^s_{\gamma nj}\Omega(p|p^{\gamma}x-n-s|_p)$$
$$+p^{\gamma-1}\sum_{s=0}^{p-1}h^s_{\gamma nj}\sum_{\substack{lk\\ l\neq k}}T^{(\gamma nlk)}(\delta_{sl}-\delta_{sk})\Omega(p|p^{\gamma}x-n-l|_p).$$

Consider

$$\sum_{s=0}^{p-1}h^s_{\gamma nj}\sum_{\substack{lk\\ l\neq k}}T^{(\gamma nlk)}(\delta_{sl}-\delta_{sk})\Omega(p|p^{\gamma}x-n-l|_p)$$

$$=\sum_{l=0}^{p-1}\Omega(p|p^{\gamma}x-n-l|_p)\sum_{s=0}^{p-1}\left(\delta_{sl}\sum_{\substack{lk\\ l\neq k}}T^{(\gamma nlk)}-(1-\delta_{sl})T^{(\gamma nls)}\right)h^s_{\gamma nj}$$
$$=\sum_{l=0}^{p-1}\Omega(p|p^{\gamma}x-n-l|_p)\lambda^{(\gamma n)}_j h^l_{\gamma nj}=p^{(\gamma-1)/2}\lambda^{(\gamma n)}_j\psi_{\gamma nj}(x).$$

Finally, we obtain

$$T^{\mathrm{II}}\psi_{\gamma nj}(x)=\left[p^{\gamma-1}\lambda^{(\gamma n)}_j+\sum_{\substack{\gamma' n' lk\\ l\neq k}}p^{\gamma'-1}T^{(\gamma' n' lk)}\delta_{p^{\gamma'-\gamma_{n,n'+l}}}\theta(\gamma'-\gamma)\right]\psi_{\gamma nj}(x).$$

Using the condition of convergence of the series (24) we obtain the proof of the theorem. □

VI. RELAXATION PROBLEM

Let us consider the relaxation problem formulated analogously to that in Refs. 1, 5, and 6 (see also the references therein). In these works, the evolution of probability distribution was described by the equation of the form (1) with the ultrametric diffusion operator of the type T^0. The initial distribution was taken homogeneous on $\mathbb{Z}_p$ [i.e., $f(x,0)=\Omega(|x|_p)$].

Consider the relaxation function of the system, $R(t)$, which describes the evolution of population of the system in the set where the initial distribution was concentrated. In the case when the initial distribution is the characteristic function of the unit ball with the center in zero, this reduces to

$$R(t)=\langle\Omega(|x|_p),e^{-Tt}\Omega(|x|_p)\rangle=\int_{\mathbb{Z}_p}f(x,t)d\mu(x).$$

It is known (see, in particular, Refs. 1, 3, 5, 6, and 19), for the case when the ultrametric diffusion is generated by T^0, the relaxation function $R(t)$ takes the form

$$R^0(t)=\langle\Omega(|x|_p),e^{-T^0t}\Omega(|x|_p)\rangle=(p-1)\sum_{\gamma=1}^{\infty}p^{-\gamma}\exp(-\lambda^0_{\gamma}t). \tag{26}$$

Let us investigate the relaxation behavior for the cases, when the ultrametric diffusion is generated by the operators T^{I} and T^{II}. The initial distribution we will take to be equal to the characteristic function of the disk:

$$f(x,0)=\Omega(|x-a|_p),\quad |a|_p=p^N,\quad N\geqslant 1 \tag{27}$$

and consider the relaxation function

$$R^{\mathrm{I}}(t) = \langle \Omega(|x-a|_p), e^{-T^{\mathrm{I}}t}\Omega(|x-a|_p)\rangle,$$

and R^{II}, defined analogously.

A. The operator T^{I}

Find the coefficients of the decomposition of the initial condition (27) in the basis of p-adic wavelets (7):

$$C_{\gamma nj} = \langle \Omega(|x-a|_p), \varphi_{\gamma nj}(x)\rangle = \varphi_{\gamma nj}(a)\,\theta(\gamma).$$

The solution of the Cauchy problem for the ultrametric diffusion equation (1) with the operator T^{I} and the initial condition (27) takes the form

$$f^{\mathrm{I}}(x,t) = \sum_{\gamma=1}^{\infty} \sum_{n\in \mathbb{Q}_p/\mathbb{Z}_p} \sum_{j=1}^{p-1} e^{-\lambda^{\mathrm{I}}_{\gamma n}t}\varphi_{\gamma nj}(a)\varphi^{*}_{\gamma nj}(x).$$

Then the relaxation function $R^{\mathrm{I}}(t)$ is given by the expression

$$R^{\mathrm{I}}(t) = \sum_{\gamma=1}^{\infty} \sum_{n\in \mathbb{Q}_p/\mathbb{Z}_p} \sum_{j=1}^{p-1} e^{-\lambda^{\mathrm{I}}_{\gamma n}t}|\varphi_{\gamma nj}(a)|^2 = (p-1)\sum_{\gamma=1}^{\infty} \sum_{n\in \mathbb{Q}_p/\mathbb{Z}_p} p^{-\gamma}e^{-\lambda^{\mathrm{I}}_{\gamma n}t}\Omega(|p^{\gamma}a-n|_p).$$

Taking into account that $|a|_p = p^N$ and $N \geqslant 1$, let us divide the series into the two parts: for $\gamma \leqslant N$ and for $\gamma > N$. For the second part the values of all the indicators are equal to one only if $n=0$; otherwise they are equal to zero. Hence, for the relaxation function $R^{\mathrm{I}}(t)$ we get

$$R^{\mathrm{I}}(t) = (p-1)\sum_{\gamma=1}^{N} p^{-\gamma}e^{-t\lambda^{\mathrm{I}}_{\gamma,p^{\gamma}a}} + (p-1)\sum_{\gamma=N+1}^{\infty} p^{-\gamma}e^{-t\lambda^{\mathrm{I}}_{\gamma 0}t}. \tag{28}$$

B. The operator T^{II}

The solution of the Cauchy problem for the ultrametric diffusion equation (1) with the operator T^{II} and the initial condition (27) takes the form

$$f^{\mathrm{II}}(x,t) = \sum_{\gamma=1}^{\infty} \sum_{n\in \mathbb{Q}_p/\mathbb{Z}_p} \sum_{j=1}^{p-1} e^{-\lambda^{\mathrm{II}}_{\gamma nj}t}\psi^{*}_{\gamma nj}(x)\psi_{\gamma nj}(a).$$

Then the relaxation function $R^{\mathrm{II}}(t)$ is given by the expression

$$R^{\mathrm{II}}(t) = \sum_{\gamma=1}^{\infty} \sum_{n\in \mathbb{Q}_p/\mathbb{Z}_p} \sum_{j=1}^{p-1} e^{-\lambda^{\mathrm{II}}_{\gamma nj}}|\psi_{\gamma nj}(a)|^2 = \sum_{\gamma=1}^{\infty} \sum_{n\in \mathbb{Q}_p/\mathbb{Z}_p} \sum_{j=1}^{p-1} e^{-\lambda^{\mathrm{II}}_{\gamma nj}}p^{1-\gamma}\sum_{k=0}^{p-1}|h^{k}_{\gamma nj}|^2\Omega(p|p^{\gamma}a-n-k|_p).$$

Taking into account that $|a|_p = p^N$ and $N \geqslant 1$, for the relaxation function $R^{\mathrm{II}}(t)$, we get

$$R^{\mathrm{II}}(t) = \sum_{\gamma=1}^{N} \sum_{j=1}^{p-1} \sum_{k=0}^{p-1} e^{-\lambda^{\mathrm{II}}_{\gamma nj}t}p^{1-\gamma}|h^{k}_{\gamma nj}|^2\delta_{p^{\gamma}a-k,n} + \sum_{\gamma=N+1}^{\infty} p^{-\gamma}\sum_{j=1}^{p-1} p|h^{0}_{\gamma 0j}|^2 e^{-\lambda^{\mathrm{II}}_{\gamma 0j}t}.$$

Comparing the formulas (26) and (28), we see that the long-time relaxation behavior for ultrametric diffusions generated by the operators T^0 and T^I coincide [i.e., the functions $R^0(t)$ and $R^{\mathrm{I}}(t)$ have the same asymptotic]. This shows that the particular properties of the energy landscape, such as local inhomogeneities, are not important for long-time behavior of the corresponding diffusion. Note that the given result generalizes the special case considered in the work[20] by Yoshino.

For the cases of the operators of the type T^{II}, the relaxation function behavior becomes more complicated. Note that if the landscape deviations from the regularity are small:

$$|\lambda^{\mathrm{II}}_{\gamma 0 j} - \langle \lambda^{\mathrm{II}}_{\gamma 0 j} \rangle_j| \ll \langle \lambda^{\mathrm{II}}_{\gamma 0 j} \rangle_j,$$

where $\langle \lambda^{\mathrm{II}}_{\gamma 0 j} \rangle_j = (p-1)^{-1} \Sigma_{j=1}^{p-1} \lambda^{\mathrm{II}}_{\gamma 0 j}$, then by (23) the long-time relaxation $R^{\mathrm{I}}(t)$ is a good approximation of the relaxation $R^{\mathrm{II}}(t)$.

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Planar (x,z) mixtures discrete Boltzmann equations with species either in odd or even |x|+|z| values

Henri Cornille
Service SPHT, CEA/Saclay 91191, Gif-sur-Yvette, France

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We present large size "physical" discrete Boltzmann equations or discrete velocity models results for binary mixtures of gas (light mass 1 and heavy mass M) in a half-plane (coordinates x,z, interface at $z=0$ without velocities except the rest-particle) where the sums $|\mathbf{x}|+|\mathbf{z}|$ are either odd or even for heavy or light species. The models fill all integer coordinates $z\neq 0$ of the plane with only a z spatial dependence [densities with $(\pm x, z)$ are equal]. Here, to previous results, we generalize with new mathematical tools, to any binary mixture with M ratio of any even to odd values, $M=2\mathbf{p}/(2\mathbf{q}+1)$ and ratio of odd to odd values $M=(2\mathbf{p}+1)/(2\mathbf{q}+1)$, $\mathbf{p},\mathbf{q}$ arbitrary integers. With only binary collisions, we construct large size "physical" discrete models (only mass, energy, and momentum along the z-axis invariants, without other invariants which are called spurious). We prove the existence of a "physical" square (diagonals along the x and z axes) grid where for the first component all $|x|+|z|\leqslant$ a sufficient value (function of $\mathbf{p}$ and $\mathbf{q}$) while for the other "physical" components we add 2, 4, etc., to the sufficient value. The numerical "physical" applications, with only binary collisions, could be done with this grid. The heavy species Hausdorff' dimension has the limit 2 when the number of velocities $\rightarrow\infty$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1868892]

I. INTRODUCTION

Contrary to many previous DBE (discrete BE) or DVMs (review papers in Ref. 1), in the continuous BE we only have binary collisions (no multiple), only physical invariants: mass, energy, momentum (no additional called spurious invariants) and not a finite number of velocities v_i. Now, there is an evolution in DBE: no multiple collisions, no spurious invariants and finite number of v_i which can be extended to an infinite number. Concerning finite DBE (versus continuous BE) velocities v_i, Cercignani,[2] in 1994, studying, at a homogeneous equilibrium state, the energy to the mass ratio for a single-gas (not mixtures), concluded that the associated rate (linked to the temperature) would be a drawback for DBE with a finite number of v_i. A partial answer to this criticism is to compare with the planar $d_H\simeq=2$ Hausdorff dimension of the DBE when the number of $v_i\rightarrow\infty$ and the intermediate models with a finite number of v_i. We can start with a finite "physical" v_i model and, with "physical tools," we enlarge the model in the whole plane and we must prove that each intermediate square-grid is "physical."

The first paper, trying to satisfy these criteria (except the planar extension) was for two $25v_i$ mixture models, discussed by Cercignani–Bobylev,[3] but with powerful computers spurious invariants were found.[4] With simple geometrical restrictions of these $25v_i$ (Cornille–Cercignani[3]) explained why only one was physical (new collisions eliminate the spurious invariant). "Physical" binary mixture models (light species, mass 1; heavy, $M>1$) tiling all the integers of the x,z plane were presented[5] with only binary collisions (particular M values), starting with "physical" models and extending, with physical tools, to new "physical." For the distribution of the heavy species different geometrical structures were found: squares, octagons, same number for the light and heavy species. In Refs. 3–5, the lack was missing constraints for the flows.

Half-space[6] (without velocities parallel to the interface) mixtures models were presented (Fig. 1). In particular models with $|\mathbf{x}|+|\mathbf{z}|$ either even (light species) or odd (heavy species) were found

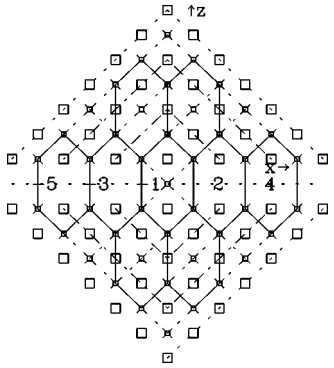

FIG. 1. $|x|+|z|$ odd (heavy), even (light). Here, $|x|+|z|\leqslant 7$.

for some M values and M even. The problem is whether this geometrical structure can exist for any rational fractional M values. Here we prove this same geometrical structure for 2 classes of ratios $M=2\mathbf{p}/(2\mathbf{q}+1)$ (even–odd) and $M=(2\mathbf{p}+1)/(2\mathbf{q}+1)$ (odd-odd). with $\mathbf{p}$ and $\mathbf{q}$ positive integers. The difficulty for the proofs, contrary to Refs. 2, 5, and 6, is the existence of two different arbitrary parameters. As in the continuum treatment of the problem and in DBE or DVMs[7,6,5] the spatial dependence of the gas is assumed to be one-dimensional depending upon the z variable. Associated physical properties for the boundaries of both the half-space and the two parallel interfaces problems were studied.[7] For single-gas Maxwellians at the interface, it was shown[6,7] how the impinging densities $z<0$ can be deduced from the emerging ones $z>0$. We recall recent interests in DBE, DVMs.[8] Here we only construct large size physical half-space models, filling all $z\neq 0$ coordinates. Like in Refs. 3–6, we require a restriction: the occupation of a site (x,z) without more than one particle.

Very often, in the literature, only numerical or geometrical regular grids are presented, but without the proof that the intermediate models are "physical" (no spurious). For the present models, it is clear that the components of the grid are squares (diagonals along the x,z axes) with $|x|+|z|$ either odd (heavy species) or even (light species). The important and nontrivial problem is to find the smallest $|x|+|z|$ value (or at least a sufficient value) such that the model is "physical" for all light and heavy densities with $|x|+|z|\leqslant$ that value. The tail of the first physical component grid (see Fig. 3 for $M=4/3$ and $|x|+|z|\leqslant 6$) depends on p,q while (tool 1.2) for the second, third, etc. (no spurious invariant) we add 2,4, etc., to that value. When p,q increase, the sufficient "physical" value increases too and it is the reason why we must reject the previous grid works without this research of the sufficient value for "physical" models.

The difficulties are binary collisions only physical invariants and half-space. For the two classes presented of M ratios mixtures, Secs. II and III the preliminary physical models have eight independent densities (six heavy, two light) and seven collisions (one with light and heavy). The previous tools, insufficient for the present study, (1, 2, etc., new densities), for the extensions of physical models are presented below 1.1–2 for one species in squares, rectangles or mixing collisions (three known).

Physical tools (Refs. 3–5) in order to enlarge "physical" models: Starting with a preliminary simple "physical" (no spurious invariants) model, we can for new "physical" add new momenta:

1.1: Four momenta of the same species of a physical mixture model being along rectangles or squares, to three (x_i,z_i) belonging to a previous physical DBE, DVMs we can include the last one (x_4,z_4).

For a mixing collision (light and heavy), if three belong to a physical model, we can add the last one,

$$f(a_1,b_1)F(x_1,z_1) - f(a_2,b_2)F(x_2,z_2) \to a_1 + x_1 = a_2 + x_2,$$
$$b_1 + z_1 = b_2 + z_2, x_1^2 + z_1^2 - x_2^2 - z_2^2 = M(a_2^2 + b_2^2 - a_1^2 - b_1^2). \tag{1}$$

We call the velocities, momenta, densities $\vec{v}_i=\vec{p}_i$, f_i (light species), $\vec{V}_j$, $\vec{P}_j=M\vec{V}_j$, F_j (heavy).

1.2: In mixture models with a light density for the rest-particle $f_0(0,0)$, if we prove that for $z\geqslant 0$ the light densities with $|x|+|z|=0,2,4$ are physical, then we can add (Refs. 5 and 6) all light densities with $|x|+|z|$ even. For the extension, if we start with half-space $|x|+|z|$ even $\leqslant 2c$, $\notin (\pm 2c,0)$, we can extend (with squares, rectangles three known) to $\leqslant 2c+2$, $2c+4$, etc. If the heavy densities with $|x|+|z|=1,3$ belong to a physical model, we can also add all heavy densities with $|x|+|z|$ odd. Similarly, the extension of the heavy is from $2c+1=3$ to $2c+1=5,7,\ldots$.

In Secs. II and III, we only have two light independent densities for the physical preliminary model, so that we cannot apply directly the two [1.2] results. However we show first that we can extend the heavy species in all odd values and second, with new collisions mixing heavy and light species we obtain other light values. The extensions for the light to $|x|+|z|=0,2,4$ and all even values are only found with the introductions of other tools which are explained below.

1.3: In some cases we can include 2,3, etc., new densities.[5,6] Starting with the old conservation laws of a previous "physical" model, with new densities we associate arbitrary constants to the evolution equations and we must have new collisions X_k including some previous densities with values fixed for each conservation law. For each new collision X_k the sum of these constants must be zero, and we must verify that the arbitrary constants are fixed, giving the right values of each conservation law: $[M_L],[M_l]$ for the macroscopic heavy and light masses and $[J],[2E]$ for the momentum along z and the energy. These starting mixture models are physical 2.1a, 3.1.

In 2.1b, 3.1, for the extension of the heavy species in the whole plane, we add new heavy squares, rectangles (three known) and with $|x|+|z|=1,3$ we extend to all odd values.

For the light species, in 2.2, 3.2–3.4, we have not this tool (three previous) but, from the extension of the heavy species, we have new collisions mixing heavy and light species and for instance in 2.1b, we can add four independent light physical but not for the Sec. III model. In both cases we do not have the light with $|x|+|z|=0,2,4$ and contrary to Ref. 6, we cannot use the 1.2 tool. The main problem remains to add the light in all the plane. We consider mainly collisions with light densities, including necessarily some old light. For the light mass conservation we have $M_l^{\text{old}}, M_l^{\text{new}}$ and we must only have $0=M_l^{\text{old}}+M_l^{\text{new}}$. For the old physical $f(x,z)$ the evolution equations $l(x,z)$ is multiplied by 1 for $x=0$ and 2 for $x\neq 0$. For the new $f(x,z)$, we associate arbitrary parameter $\mathbf{a}(\mathbf{x},\mathbf{z})$. In any collision, the sum of the old and new parameters must give zero. So we have a linear system of the number of collisions with these new $a(x,z)$ including the old values for the old densities. We try to find all $a(x,z)$ as linear combinations of arbitrary: a_0 (associated to the rest-particle f_0) and few other $a(x,z)$ called a_1,a_2, etc. Finally we try to find crucial relations, leading to $a_0=1$ and all the $a(x,z)$ having the physical value of a light mass conservation law. We must solve this linear system and the new model $M_l^{\text{old}}+M_l^{\text{new}}$ must only have $a(x,z)=1,2$ for $x=0,\neq 0$. We explicit the new necessary method used in Secs. II and III.

First, in Sec. II we have with very few collisions: $a(q-1,3q+1)$ only function of a_0 and $a(q,3q+2)=2$ Second Figs. 4(a)–4(c), we follow a path parallel to the $z=x$ axis,$(a(0,2q)=2-a_0)$ with $x=1,2$, etc., and get for $x=q-1$, q the previous $a(x,z)$ functions of both a_0, a_1 and $\mathbf{q}$. The compatibility with all $\mathbf{q}$ values leads to only $\mathbf{a}_0=\mathbf{1}$ and all $a(x,z)$ physical.

First, in Sec. III starting physical model, we have $a(x,x)=2$ for $x=2q-1$ and with few collisions $a(1,4q-3)$ function of only $\mathbf{a}_0$. Second, Fig. 5(b), we follow a path parallel to the $z=-x$ axis with $a(x,-x+4q-2)$ and x decreasing $2p-3$, $2p-5,\ldots,1$ giving another $a(1,4q-3)$ relation function of both $\mathbf{a}_0,\mathbf{q}$ and the compatibility still leads to $\mathbf{a}_0=\mathbf{1}$ and all $a(x,z)$ physical.

In 2.2, for the $2\mathbf{p}/(2\mathbf{q}+1)$, $\mathbf{q}\geqslant 1$ model, $(q=0$ in Ref. 6), we add new $f(x,z)$, $a(x,z)$ and for a set of these arbitrary parameters called a_k, $k=1,\ldots,q-1,q$ which are k or q dependent, we prove that they are linear combination of two, a_1,a_2. On the other hand $a_q=2$ and $a_{q-1}=10-8a_0$.

Comparing the two different explicit expressions (q-dependent or not), we deduce that $a_0=1$ and the arbitrary parameters a_k only have the physical values giving a "physical" model.

For $q=1,2,3$ and later for $2p/(2q+1)$, we give the sufficient values such that the model with all $|x|+|z|\leqslant$ that value be physical, giving the first $P=1$ component of the physical squares (diagonals along the x,z axes) grid, the second, third, etc., $P=2, 3, \ldots$ component being found adding 2,4, etc., to the sufficient value. The light and heavy densities having almost the same number of densities in large squares (extensions of Fig. 1), we study (in some examples), the Hausdorff's dimension of only the heavy species. We show that the large limit value is $d_H\to 2$ and notice that the P-square grid must be very large to approach this limit.

In 3.2–3.4, for the $(2\mathbf{p}+\mathbf{1})/(2\mathbf{q}+\mathbf{1})$ model, in order to extend the light species f, we still associate $a(x,z)$ and, for a pedagogical study, first we limit to $q=1,2$ with only the previous 1.1–2 tools and finally giving a general proof for q arbitrary with our generalized tool. We show two expressions for $a(1,4q-3)$, one with only a_0 and another with $\mathbf{q}$. The compatibility gives $a_0=1$ and all correct "physical" $a(x,z)$ values.

1.4: The presented models, filling all integer coordinates, have a regular grid (mesh-step 1). We can generalize[2–5] with a mesh-step h finite: $(\vec{v}\to h\vec{v},\vec{P}\to h\vec{P})$ and $\vec{v}^2\to(h\vec{v})^2,\vec{P}^2\to(h\vec{P})^2$ (collisions still valid). For the construction of physical models we present sets of P selected physical domains and we know (advantage to the standard numerical discretizations) that in all intermediate steps we have no spurious invariants. For brevity we write **Aj**,**Bk** for Appendix **Aj**,**Bk**. In the sequel, for a set y_s, we define $y_{i,j,\ldots,q}=\sum_{s=i}^{s=q}y_s$ and $y_{i,j}^{-}=y_i-y_j$.

For the heavy P^{th} squares grid with diagonals along the x,z axes, $|x|+|z|\leqslant\nu$, the Hausdorff dimension $d_H=\log N_\nu/\log L_\nu)$, we have $N_\nu=\nu(\nu+1)$ for the number of heavy densities and for the sizes $L_\nu=\sqrt{2}\nu$. We get $d_H\to 2$ when $\nu\to\infty$.

II. HEAVY MASS RATIO OF EVEN TO ODD: $M=2p/(2q+1)>1$ (Figs. 2–4)

2.1: Heavy species filling all $|x|+|z|$ odd, Fig. 2(a), only six light. First in 2.1a, we prove that a simple mixture model (six individual heavy and two light) is physical. We write the evolution equations as sums of collisions and eliminating successively these collisions we find three invariants IV, I, II for both the heavy and light masses conservations. For the momentum along z and the energy, we find the last invariant III. Second in 2.1b, with the simple tool of collisions in squares, rectangles (three known), we show that in the previous mixture physical model, the heavy species can be extended in the whole plane with $|x|+|z|$ odd and, with the new heavy, we can extend (four individual, four new light) a little bit the light species. However, with the Sec. I tools, we do not have sufficient light densities (only six), to extend in the plane.

2.1a: Starting physical model, Fig. 2(a) with six heavy $F_i(\pm x,z)$, two light $f_j(\pm x,z)$ densities [equal for $(\pm x, z)$]. We write both the mixing Γ and six heavy Ω_i collisions. We write the evolution equations $l_i=(\partial_t+z_i\partial_z)f_i$ [or $z_i\partial_z f(x_i,z_i)$] and L_j associated to f_i,F_j which are sums of collisions Γ,Ω_i where $f_i(F_j)$ are in the lost terms. We deduce the physical invariants.

Lemma 1, Fig. 2(a): With collisions, six Ω_i and one Γ mixing light and heavy densities, we show that the mixture (2.1) model with six heavy F, two light f is physical (no spurious invariants). We find four invariants I–II–III–IV equivalent to the four conservation laws, two for the heavy mass M_L, one for the light M_l, and only one new for both the momentum J and energy $2E$,

$$F_1(0,2p-3),\quad F_2(\pm1,2p-2),\quad F_3(\pm2,2p-1),\quad F_4(0,2p+1),\quad F_5(0,2p-1),\quad F_6(\pm1,2p),\tag{2.1}$$

$$f_q(\pm q,q),\quad f_{q+1}(\pm(q+1),q+1)\quad \text{densities equal for}(\pm x,z),$$

$$\Gamma=F_5(0,2p-1)f(q+1,q+1)-F_6(1,2p)f(q,q),\quad \Omega_1=F_5F_4-F_6^2,$$
$$\mathbf{i=0,1}\to\Omega_{2+i}=F_1F_{5-i}-F_{2+i}^2,\quad \Omega_{4+i}=F_{5-i}F_{3-i}-F_6F_{2+i},\quad \Omega_6=F_1F_6-F_3F_2,\tag{2.2}$$

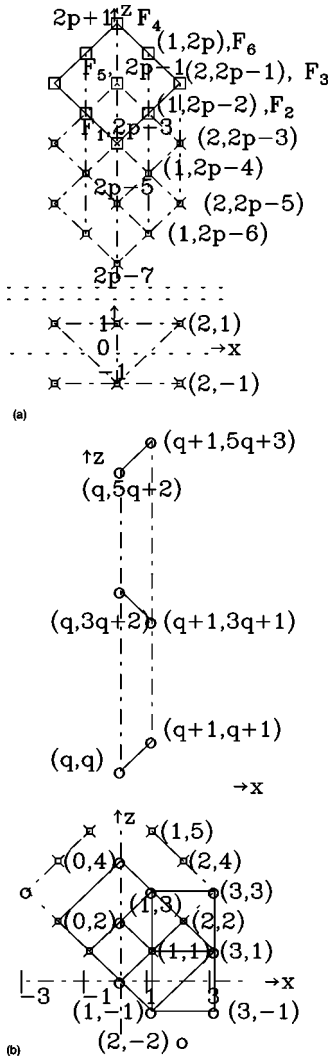

FIG. 2. $M=2_p/(2_q+1)$, $|x|+|z|$ odd.

$$\Gamma = l_q(q,q) = -\,l_{q+1}(q+1,q+1) \to M_l/2 = l(q,q) + l(q+1,q+1) = 0 \text{ IV},\ L_{1+3i} = -\,\Omega_{2-i,3} - 2\Omega_{6-i},$$

$$L_{2+i} = \Omega_{2+i,4+i,6} - \Omega_{5-i}, \quad L_5 = -\,2\Gamma - \Omega_{1,2} - 2\Omega_4, \quad L_6 = \Gamma + \Omega_{1,4,5} - \Omega_6. \tag{2.3}$$

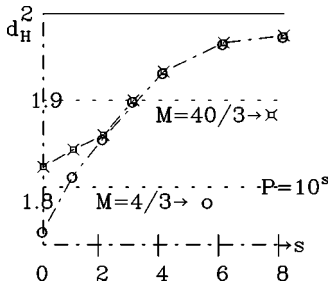

FIG. 3. $M=2_p/3f(x,z)$.

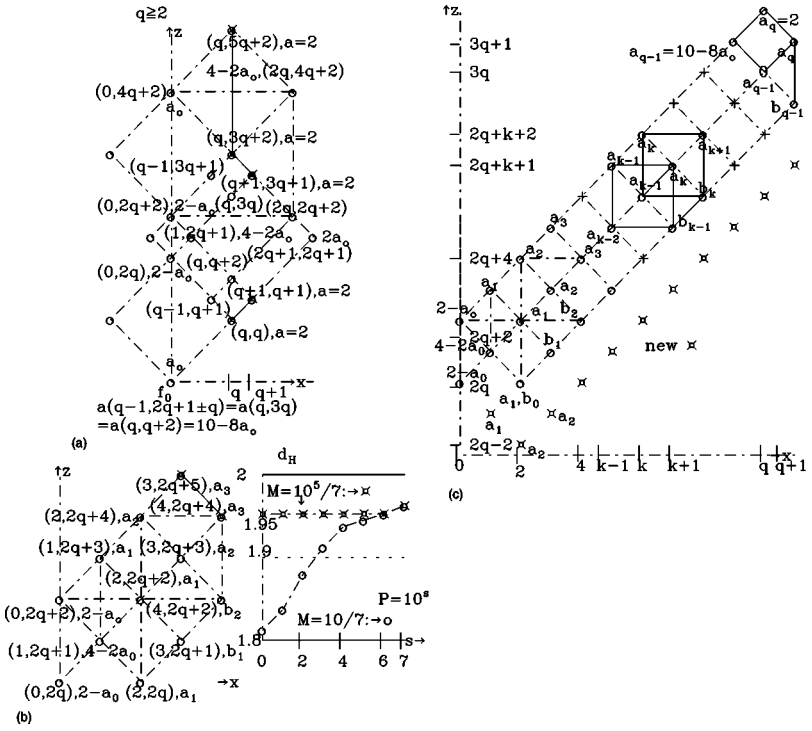

FIG. 4. $M=2_p/(2_q+1)$. (a) $q\geqslant 2$. (b) $(x,z)\to f(x,z)$. (c) $f(x,z)\to|x|+|z|$.

For the reader not familiarized with DBE, DVMs, we explain the coefficients 1 or 2 in the collisions. In Γ, we have one F_5 but two equal $F_6(\pm 1,2p)$ and consequently two collisions with Γ for L_6 and -2Γ for L_5. For the heavy mass we eliminate successively Γ,Ω_1 and get two invariants I, II. For the heavy mass conservation, we have a coefficient 1 for the L_i with $x_i=0$ (densities along the z axis), but two for $\pm x_i\neq 0$. For the momentum conservation J, we multiply the L_i,l_j by the z values of the associated densities and get for J and the energy $2E$, another invariant III. For the $2E$ conservation, we multiply with (x^2+z^2) for the heavy, still with M for the light,

$$L_5+2L_6=\Omega^-_{1,2}+2\Omega^-_{5,6}\to L_{4,5}+2L_6=-\Omega_{2,3}-2\Omega_6=L_1=-L_{2,3}\to \mathrm{I}{:}L_{2,3,4,5}+2L_6=0,$$
$$\mathrm{II}{:}L_{1,2,3}=0\to M_L=\mathrm{I}+\mathrm{II}=L_{1,4,5}+2L_{236}=0, \tag{2.4}$$

$$J=2ql_q+2(q+1)l_{q+1}+(2p-3)L_1+(2p-1)L_5+(2p+1)L_4+2(2p-2)L_2+2(2p-1)L_3+4pL_6$$
$$=2pM_L+[-2\mathrm{II}+\mathrm{III}]=0\to \mathrm{III}:=L_4-L_{1,5}-2L_2+2l_q=0, \tag{2.5}$$

$$2E=(2p-3)^2L_1+(2p-1)^2L_5+(2p+1)^2L_4+2(1+4p^2)L_6+2(4+(2p-1)^2)L_3+2(1+(2p-2)^2)$$
$$\times L_2+[q^2l_q+(q+1)^2l_{q+1}(q+1)2]8p/(2q+1)=(4p^2+1)M_L+2\mathrm{II}+4p(\mathrm{III}-2\mathrm{II}). \tag{2.6}$$

2.1b, Fig. 2(a) Lemma 2: Heavy $\mathbf{F}(\mathbf{x},\mathbf{z})$ filling all $|\mathbf{x}|+|\mathbf{z}|$ odd and only two light $\mathbf{f}(\mathbf{x},\mathbf{z})$. With heavy collisions in squares and rectangles and 3 $F\in$ (2.1), we add six new individual $F(x,z)$,

$$F(\pm x,z)\to(\pm x,z(p)\neq 0){:}\alpha=0,2{:}(2,2p-3-\alpha)(1,2p-4-\alpha),(0,2p-5-\alpha) \tag{2.7}$$

and $p\to p-1\to p-2$, etc. Physical F satisfy $|x|+|z|=1,3\to$ all odd but only two light f.

Proof of (2.7): With squares, rectangles (three known) Fig. 2(a), we add to (2.1), the last heavy $\overline{F}$,

$$F_3(2,2p-1)F_1(0,2p-3)-F_5(0,2p-1)\overline{F(2,2p-3)},$$
$$F_1(0,2p-3)F(2,2p-3)-F_2(1,2p-2)\overline{F(1,2p-4)},\quad p\neq 2,$$
$$F(1,2p-4)F(-1,2p-4)-F_1(0,2p-3)\overline{F(0,2p-5)}. \tag{2.8}$$

Similarly we get new heavy $F:\overline{(2,2p-5)}$, $\overline{(1,2p-6)}$, $\overline{(0,2p-7)}$ with $p\to p-1,\ldots,p-2,\ldots$.

Lemma 3: Physical DVMs with more light densities, six f, Fig. 2(b). With mixing collisions (three known), we now have six individual light $f(\pm x,z)$ [written (x,z)]

$$(\pm q,q),(\pm(q+1),q+1)\text{new}(\pm q,3q+2),(\pm q,5q+2),(\pm(q+1),3q+1),(\pm(q+1),5q+3). \tag{2.9}$$

Proof of (2.9), Fig. 2(b): To the (2.1) with two light $f(q,q)$, $f(q+1,q+1)$, we add successively four new $f\overline{(x,z)}$ with mixing collisions (F with $|x|+|z|$ odd) giving six physical $f(x,z)$,

$$f(q,q)F(x,2p+1+q)-\overline{f(q,3q+2)}F(x,2p-1-q)\ \text{either } x,q \text{ odd or even},$$

$$f(q,3q+2)F(x,4p+q)-\overline{f(q,5q+2)}F(x,4p-q),\quad |x|+q \text{ odd},$$

$$f(q+1,q+1)F(x,2p+q)-\overline{f(q+1,3q+1)}F(x,2p-q),\quad |x|+q \text{ odd},$$

$$f(q+1,3q+1)F(0,z+2(q+1))-\overline{f(q+1,5q+3)}F(0,z),\quad z \text{ odd}. \tag{2.10}$$

2.2: $M=2\mathbf{p}/(2\mathbf{q}+1)>1$, $\mathbf{q}\geqslant 1$. Light species filling all $|x|+|z|$ even, Figs. 3 and 4.

Our aim is to prove for the light species that for the sum of the $a(x,z)l(x,z)$ [l associated to $f(x,z)$ and $a(x,z)$ arbitrary], exists only one invariant, the light mass M_l and the only $a(x,z)$ possible values are (like for old physical densities $a=1,2$) 1, $x=0$ and 2, $x\neq 0$. For the old physical M_l^{old}, in (2.9) these six $a(\pm x\neq 0,z)=2$ values are satisfied but not for the new M_l^{new}. The $M_l=M_l^{\text{old}}+M_l^{\text{new}}=0$ is linear combination of the vanishing collisions and we must find constraints for the new $a(x,z)$ giving only the physical values. We obtain general physical results in 2.2a, b, c for arbitrary $\mathbf{q}$ and, in Lemma 4, Appendix A1, for a pedagogical reason, we give an independent $M=2p/3$, $q=1$ proof of a physical model.

Lemma 4, A1, Fig. 3: The $M=2\mathbf{p}/3$, $\mathbf{q}=1$ model is physical with a M_1 conservation law.

For $M=2\mathbf{p}/3$, A1, the physical $|x|+|z|$ are $\leqslant 2p+3$ for heavy and $\leqslant 6$ for the light species, With the 1.2 tool we can extend the physical light to 8,10, …,$2p+2$ or the heavy to $2p+5$, $2p+7$, $2p+9$, etc., giving $P=1,2$,etc., squares grid with diagonals along the x,z axes where all coordinates are filled for $|x|+|z|\leqslant \nu=2p+1+2P$ by heavy (odd) or light (even) physical species. In Fig. 3, we give the Hausdorff' dimension d_H for the heavy species with $M=4/3$, $40/3$, giving the same values for $P\geqslant 100$ and $\to d_H\sim 2$ for more and more P-squares-grid.

In 2.2a, for $\mathbf{q}$ arbitrary, we add new light $f(x,z)$ densities so that the associated arbitrary parameters $a(x,z)$ depend only on the arbitrary a_0 linked to the rest-particle f_0.

Adding light collisions, valid only for $q=1,2$, we find $a_0=1$, leading to a new physical mixture $M=2\mathbf{p}/5$, Appendix A2 model which can be extended to all light densities with $|x|+|z|$ even.

In 2.2b, $\mathbf{q}$ arbitrary, we add (light collisions) three associated $a(x,z)$ parameters. As application, the $M=2\mathbf{p}/7$, Appendix A model is physical in the whole plane.

In 2.2c, Appendix A, $\mathbf{q}$ arbitrary, the new $a(x,z)$ depend on more and more arbitrary parameters, but we prove that they only have the physical light species values.

2.2a, Fig. 4(a), general arbitrary $\mathbf{q}$ *results for the light species:* We add, to the physical light $f(x,z)$ with $a(x,z)=2$, (2.1)–(2.9), new light densities with collisions, but their associated (2.12) and (2.13) arbitrary $a(x,z)$ values, coming from vanishing collisions, depend on $a_0=a(0,0)$. So the light mass conservation law has two invariants, one spurious except $q=1$ with $a_0=1$, Appendix A.

For arbitrary $\mathbf{q}$, with collisions (three known), we get new $a(x,z)$ values which depend only on a_0,

$$\text{old, } \lambda = 0, 2q+2, \quad 2 = a(q, q+\lambda) = a(q+1, 3q+1+\lambda) = a(q, 5q+2) = a(q+1, q+1),$$

$$\begin{aligned}\text{new, } a(0,4q+2) &= a(2q+1,2q+1)/2 = a_0, \quad a(0,2q) = a(0,2q+2) = 2 - a_0 = a(2q,4q+2)/2 \\ &= a(1,2q+1)/2, \quad a(2q,2q+2) = 8 - 6a_0, \quad a(q,q+2) = a(q,3q) = 10 - 8a_0 \\ &= a(q-1 \neq 0, q+1) = a(q-1 \neq 0, 3q+1), \quad a(2q-1,2q+1) = 16 - 14a_0.\end{aligned} \tag{2.11}$$

[See Eqs. (2.12) and (2.13).]

Proof for (2.12) and (2.13) with one mixing Γ and 11 light different collisions,

$$\text{new, } \Gamma = f\overline{(2q+1,2q+1)}F(0,2p-2q-1) - f_0F(2q+1,2p) \to a(2q+1,2q+1) = 2a_0,$$

$$f_0f\overline{(0,4q+2)} - f^2(2q+1,2q+1) \to a(0,4q+2) = 2a_0 - a_0 = a_0, \quad f_0f\overline{(0,2q)} - f^2(q,q),$$

$$\begin{aligned}f_0f\overline{(0,2q+2)} - f^2(q+1,q+1) \to a(0,2q) &= a(0,2q+2) = 2 - a_0, \\ & f(q,3q+2)f(q,5q+2) - f(0,4q+2)f\overline{(2q,4q+2)}, \\ & f(0,2q+2)f(0,2q) - f^2\overline{(1,2q+1)}, \\ & f(2q,4q+2)f(0,2q+2) - \\ & f(0,4q+2)f\overline{(2q,2q+2)}, \to a(2q,4q+2) = a(1,2q+1) \\ = a(2q,2q+2)/2 + a_0 &= 4 - 2a_0,\end{aligned} \tag{2.12}$$

$$a(q,q+2) = a(q-1,q+1) = a(q-1,3q+1) = a(q,3q) = 10 - 8a_0, \quad a(2q-1,2q+1) = 16 - 14a_0,$$

$$\begin{aligned}& f(2q,2q+2)f(q+1,q+1) - f(2q+1,2q+1)f\overline{(q,q+2)}, \\ & f(2q,2q+2)f(q,q) - f(2q+1,2q+1) \\ & f\overline{(q-1,q+1)}, \quad f(q-1,q+1)f(q+1,3q+1) - f(q+1,q+1)f\overline{(q-1,3q+1)}, \\ & f(q-1,3q+1)f(q+1,3q+1) - f(q,3q+2)f\overline{(q,3q)}, f(q,3q)f(q,q+2) - f(1,2q \\ & +1)f\overline{(2q-1,2q+1)}\end{aligned} \tag{2.13}$$

Adding collisions valid for $q=1,2$ we get $a_0=1$ and $M=2\mathbf{p}/5$ in A2 is a physical model.

Lemma 5, Appendix A: With (2.12) and (2.13), the model $M=2\mathbf{p}/5$, $\mathbf{p}\geqslant 3$, $\mathbf{q}=2$ is physical.

In (2.12) and (2.13) for $\mathbf{q}=2$, $\mathbf{p}\geqslant 4$, the highest physical $|x|+|z|$ are $\leqslant \nu = 2p+5$ for heavy (12 for light) species with $P=1$. With the 1.2 tool we enlarge the light species $\leqslant 2p+6$, $2p+8$, $2p+10$, etc., and the heavy to $\nu = 2p+7$, $2p+9$, etc., giving the $P=2,3$, etc., squares grid.

2.2b: In Fig. 4(b) we add with squares (three known) to (2.12) and (2.13) new general $\mathbf{q}$, $\mathbf{a}(\mathbf{x},\mathbf{z})$ results,

$$\begin{aligned}\text{old, (2.12) and (2.13), } 2 - a_0 &= a(0,2q) = a(0,2q+2) = a(1,2q+1)/2, \\ & a(q+1,3q+1) = 2, \text{etc.}, \text{ new; } a_k, b_k,\end{aligned} \tag{2.14}$$

$$a_1 := a(1,2q+3) = a(2,2q+2) = a(2,2q), \quad a_2 = a(2,2q+4) = a(3,2q+3) = 3a_1 + 4(a_0 - 2),$$

$$b_1 := a(3,2q+1) = 2a_1 + 2(a_0 - 2) = a_2 - a_1 + 2(2 - a_0), \quad b_2 = a(4,2q+2) = 4a_1 + 6(a_0 - 2), \tag{2.15}$$

$$a_3 := a(4,2q+4) = a(3,2q+5) = 6a_1 + 10(a_0 - 2).$$

Fig. 4(b), Proof for (2.14) and (2.15): We define new a_k, b_k with collisions [three physical $f(x,z)$],

$$\begin{aligned}
&f(0,2q+2)\overline{f(2,2q+2)} - f(1,2q+1)\overline{f(1,2q+3)},\\
&\quad f(0,2q+2)\overline{f(2,2q)} - f(0,2q)\overline{f(2,2q+2)} \to a_1 := a(1,2q+3) = a(2,2q+2) = a(2,2q),\\
&\quad f(0,2q+2)\overline{f(3,2q+3)} - f(1,2q+1)\overline{f(2,2q+4)} \to a_2 = a(2,2q+4) = a(3,2q+3),\\
&\quad f(1,2q+3)f(2,2q) - f(0,2q+2)\overline{f(3,2q+1)},
\end{aligned} \tag{2.16}$$

$$f(1,2q+1)f(3,2q+3) - f(1,2q+3)f(3,2q+1) \to b_1 := a(3,2q+1) = 2a_1 + 2(a_0 - 2) = a_2 - a_1 + 2(2 - a_0), \quad a_2 := 3a_1 + 4(a_0 - 2),$$

$$f(2,2q+4)f(3,2q+1) - f(1,2q+3)\overline{f(4,2q+2)} \to b_2 := a(4,2q+2) = a_2 - a_1 + b_1 = 4a_1 + 6(a_0 - 2),$$

$$\begin{aligned}
&\overline{f(4,2q+4)}f(2,2q+2) - f(2,2q+4)f(4,2q+2)\\
&\qquad \to a_3 := a(4,2q+4) = a_2 - a_1 + b_2 = 6a_1 + 10(a_0 - 2), f(4,2q+4)f(2,2q+4)\\
&\qquad - \overline{f(3,2q+5)}f(3,2q+3) \to a(3,2q+5) = a_3.
\end{aligned} \tag{2.17}$$

Lemma 6, Appendix A3: The $M = 2\mathbf{p}/7$, $\mathbf{p} \geqslant 4$, $\mathbf{q} = 3$ model is physical with (2.12)–(2.15).

The highest $|x| + |z|$ value for the preliminary physical square grid being $2p+7$ (heavy $p \geqslant q+1 = 4$) and $6q+2 = 20$ (light), we enlarge heavy or light with the highest $\nu = 2p+12$, giving the first $P = 1$ component physical grid and $2p+10+2P$ for $P = 2$, etc. In Fig. 4(b), we present d_H for the heavy species, $M = 10/7$, $10^5/7$ with the same comment as previously for $M = 2p/3$.

2.2c, $M = 2\mathbf{p}/(2\mathbf{q}+1)$: General proof for light filling all $|x| + |z|$ even, Fig 4(c).

We could go on and study $2p/9$, $2p/11$, but with proofs more and more tedious, so in Appendix A, we give a proof for arbitrary $\mathbf{q}$ integer. In (2.14) and (2.15) we have given a_2, a_3 in terms of a_0, a_1 and we define in (2.16) and (2.17), a_k (function of k, a_0, a_1), that we apply to (2.11) and (2.13),

$$a_k = a(k+1,2q+k+1) = a(k,2q+k+2), \quad k = 1,2,\ldots,q \text{ and explicit } a_k \text{ in (3a5) and (3a6)},$$

$$(2\,.\,11) \to a_q = a(q,3q+2) = 2 \text{ (physical value)}, \quad (3a2) \to a_{q-1} = a(q-1,3q+1) = 10 - 8a_0.$$

We shall deduce (2.19), with Lemma 7, the physical values $a_0 = 1$, $a_k = 2$, $k = 1,\ldots,q$.

Lemma 7, Appendix A4:

$$a_k = a(k+1,2q+k+1) = k(k+1)a_1/2 + (k(k+1) - 2)(a_0 - 2). \tag{2.18}$$

With a collision Λ_k, we get (2.17) and with light collisions deduce (2.18) a relation between $a_{k-\lambda}$, $\lambda = 0,1,2,k-1$, k giving the new $a_4, a_5, \ldots, a_k$ of (2.16). For the crucial relations leading to $a_0 = 1$, giving two linear independent a_0, a_1 relations, we use the (2.16), a_k result (function of a_1, a_0) for $k = q$, $a_q = 2$ and $k = q-1$, $a_{q-1} = 10 - 8a_0$ and get the physical value $a_0 = 1$,

$$q(q+1)a_1/2 + (q(q+1) - 2)a_0 - 2(q(q+1) - 1) = 0,$$

$$q(q-1)a_1/2+(q(q-1)+6)a_0-2(q(q-1)+3)=0\rightarrow a_0=1,\quad a_1=2\rightarrow a_k=b_k=2. \tag{2.19}$$

With light collisions in squares and rectangles (three previous known) densities, we can include $|x|+|z|=0,2,4$ and all even values. In Fig. 4(c), from the physical model including integer coordinates of $z=2q+2+x$, $z=2q+x$, $2q-2+x$, we can add $z=2q-4+x$, $2q-6+x$, … .

Due to $a_q(x,z)$ in (2.17), we have for the light $|x|+|z|\leqslant 4q+2$ with $p\geqslant q+1$, but in (2.12), $\leqslant 6q+2$ for the light and $2p+2q+1$ for the heavy. For the first component (no spurious invariant) physical grid we enlarge either the light or the heavy with the highest $|x|+|z|\leqslant 2p+2q+2$ and $2p+2q+4$ for the second $P=2$ physical grid with all integer coordinates filled.

For the physical P-grid we consider, like in Fig. 1, squares with diagonals along the x and z axes with $|x|+|z|\leqslant\nu$ with $-\nu\leqslant z\leqslant\nu$. We have $\nu(\nu+1)$ heavy densities and for the Hausdorff's dimension d_H of the heavy species we have $d_H=\log(\nu(\nu+1))/\log(\nu\sqrt{2})\rightarrow 2$ when $\nu\rightarrow\infty$. For the examples given in Figs. 3, 4, and 4(b), we have $\nu=3M+2P+1$ and $\nu=7M+2P+5$.

III. $M=(2\mathbf{p}+1)/(2\mathbf{q}+1)$, FILLING EITHER $|x|+|z|$ ODD (HEAVY) OR EVEN (LIGHT)

In 3.1, we start with an eight individual F_i, f_j physical model and extend the heavy in the plane.

In 3.2, we add eight light $f(x,z)$ with associated $a(x,z)$ parameters which only depend on a_0.

In 3.3, Appendix B1, with $a_0=1$, the $M=(2\mathbf{p}+1)/3$, $\mathbf{q}=1$ planar model is physical.

In 3.4, B2–B3 the light f_i have associated arbitrary parameters a_0,a_1,a_2,a_3, etc. For $\mathbf{q}=2$, the model is physical and for q arbitrary, both $a_0=1$ and the other only have the physical values.

3.1 Lemma 8: With only two $f(x,z)$, the heavy species $F(x,z)$ fills all $|x|+|z|$ odd.

We start with the same six heavy (2.1), Fig. 2(a) model (with $\mathbf{p}\rightarrow\mathbf{p}+1$) but the two light are different. The heavy Ω_i collisions (2.2) are with the same F_i but not the mixture collision,

$$\text{heavy, } F_i(x,z)\text{:(2a1) but } p\rightarrow p+1;\quad \text{light, } f(x,2q+1\pm 2)\ x \text{ odd} \tag{3.1}$$

$$\Gamma=f(x,2q-1)F_4(0,2p+3)-f(x,2q+3)F_1(0,2p-1)\rightarrow\Gamma=l(x,2q+3)=-l(x,2q-1)\rightarrow M_l/2$$
$$=l(x,2q-1)+l(x,2q+3)=\mathrm{IV}=0,\quad L_4=-2\Gamma-\Omega_{1,3}-2\Omega_5,\quad L_1=2\Gamma-\Omega_{2,3}-2\Omega_6,$$

$$L_5=-\Omega_{1,2}-2\Omega_4,\quad L_6=\Omega_{1,4,5}-\Omega_6,\quad \mathbf{i}=\mathbf{0},\mathbf{1}\rightarrow L_{2+i}=\Omega_{2+i,4+i,6}-\Omega_{5-i}. \tag{3.2}$$

For the heavy mass M_L we eliminate successively Γ,Ω_3, get two invariants and $M_L=\mathrm{I}+\mathrm{II}$: For the momentum and the energy, we must only find another invariant III,

$$-\Omega_{1,2}-2\Omega_4=L_{1,4}+2L_3=L_5=-L_{2,6}\rightarrow\ \mathrm{I}:\ L_{1,2,4,6}+2L_3=0,\quad \mathrm{II}:\ L_{2,5,6}=0, \tag{3.3}$$

$$J=\sum c_i(p)L_i[(2\mathrm{a}5)\text{ with } p\rightarrow p+1]+2\sum_{\pm}(2q+1\pm 2)l(x,2q+1\pm 2)=2pM_L+2qM_l+\mathrm{III},$$

$$\mathrm{III}=L^{-}_{5,1}+3L_4+2L_3+4L_6+8l(x,2q+3),$$

$$2E=\sum d_i(p)L_i[(2\mathrm{a}6)\text{ with } p\rightarrow p+1]+2\sum_{\pm}[(x^2+(2p+1\pm 2)^2)l(x,2q+1\pm 2)=\text{const } M_l$$
$$+4p^2M_L+(4p+2)\mathrm{III}+3\mathrm{I}-\mathrm{II}]. \tag{3.4}$$

The mixture (3.1) model with two f is physical. Like in Lemma 2, with squares [$p\rightarrow p-1$, etc., in (2.7)], we extend the physical heavy species in $|x|+|z|=1,3$ and to all odd values of the plane.

3.2: General results for the light of $M=(2\mathbf{p}+1)/(2\mathbf{q}+1)$, $\mathbf{q}$ arbitrary Figs. 5(a)–5(c).

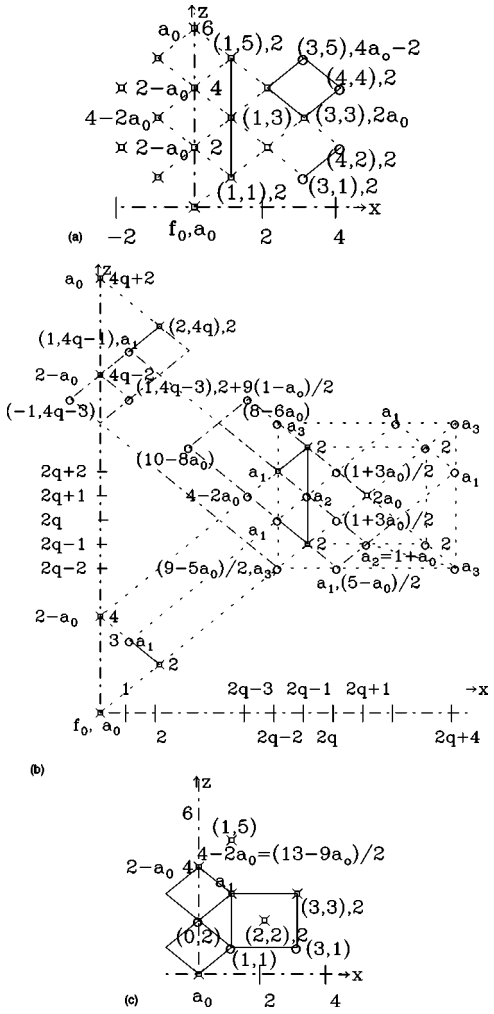

FIG. 5. (a) $M=(2_p+1)/3$. (b) $M=(2_p+1)/(2_q+1)$. (c) $M=(2_p+1)/5$.

Choosing $x=2q-1$ in (3.1), we start with the two light $f(x=2q-1,2q+1\pm2)$ [collision Γ in (3.1)], belonging to the previous physical mixture model. We add eight new $f(x,z)$ with associated arbitrary parameters $a(x,z)$ and show that they only depend on $a(0,0):=a_0$ (for f_0). At this stage the models do not satisfy $a(0,z)=1$, $a(x\neq0,z)=2$ and so are not "physical." In other sections, we prove that $a_0=1$, leading to "physical" models.

Lemma 9: With collisions, we add eight new light $f(\overline{x,z})$, $a(x,z)$ functions of $a_0=a(0,0)$,

$$\text{old, } 2=a(2q-1,2q+1\pm2);\quad \text{new, } 2=a(2,2)=a(2,4q)=2(\text{physical}), \tag{3.5}$$

$$a(0,4q+2)=a_0=a(2q+1,2q+1)/2,\quad a(0,4q-2)=a(0,4)=2-a_0=a(2q-3,2q+1)/2. \tag{3.6}$$

Proof of (3.5) and (3.6) with squares, rectangles (threeknown), old, $f(2q-1,2q-1)$, $F(x,2(p-q)),F(x,2(p+q+1))$; new, $f_0,f(2q+1,2q+1),f(0,4q\pm2),f(0,4),f(2,2),f(2,4q),f(2q-3,2q+1)$,

$$\Gamma_1=\overline{f(0,4q+2)}F(x,2(p-q))-f_0F(x,2(p+q+1))\rightarrow a(0,4q+2)=a_0,\quad x \text{ odd},$$

$$f_0 f(0,4q+2) - f^2\overline{(2q+1,2q+1)} \to a(2q+1,2q+1) = 2a_0, \quad f_0 f\overline{(0,4q-2)} - f^2(2q-1,2q-1),$$

$$f(0,4q+2)f\overline{(0,4)} - f^2(2q-1,2q+3) \to a(0,4) = a(0,4q-2) = 2 - a_0,$$

$$f(0,4)f(0,4q-2) - f^2\overline{(2q-3,2q+1)} \to a(2q-3,2q+1) = 4 - 2a_0,$$

$$f_0 f(0,4) - f^2\overline{(2,2)}, \quad f(0,4q+2)f(0,4q-2) - f^2(2,4q) \to a(2,2) = a(2,4q) = 2.$$

3.3: Lemma 10, Appendix B1: Fig. 5(a). The $M=(2\mathbf{p}+1)/3$, $\mathbf{q}=1$, $\mathbf{p}\geqslant 2$ model is physical.

For the first physical square grid, the highest $|x|+|z|$ are $2p+3$, 8 for heavy and light species. For $p>2$ we enlarge the light up to $2p+4$ for the first grid and $2p+6$, etc., for the second.

3.4: New general light results for $M=(2\mathbf{p}+1)/(2\mathbf{q}+1)$, filling $|x|+|z|$ even, Figs. 5(b) and 5(c).

Lemma 11: With the proof that $a_0=1$, the models $M=(2\mathbf{p}+1)/(2\mathbf{q}+1)$ are physical.

To the general old (3.5) and (3.6) results, we add new ones with new collisions. In addition to a_0, we add new arbitrary parameters a_1, a_2, etc., and we must prove that they only have the physical values. The method is simple, but tedious. In Appendix B2 with $a_1=a(1,4q-1)=(5-a_0)/2$, we get a physical $M=(2\mathbf{p}+1)/5$ model. In B 2–B 3, (3.11)–(3.13), we get a first $a(1,4q-3)$ function of a_0 and starting with $a(x,z)$ z and x of the order of $2q$, we obtain successively higher z and smaller x values and a second $a(1,4q-3)$ function of both a_0 and q. The compatibility requires $a_0=1$ and all $a(x,z)$ have the correct physical values 1 or 2 for the light mass conservation law. We start with $a(x,z)$ given in (3.5) and (3.6).

First Fig. 5(b), in B 2, with (3.5) and (3.6) and new collisions we define $a_1=\overline{a_1}$, a_2, a_3 and with (3.7)–(3.11), find $a_1=\overline{a_1}=(5-a_0)/2$ and a first $a(1,4q-3)$ function of a_0,

$$a_1 \coloneqq a(1,4q-1) = \overline{a_1} \coloneqq a(2q-2,2q) = a(1,3), \tag{3.7}$$

$$a_2 \coloneqq a(2q-1,2q+1) = 2a_1 - 4 + 2a_0, \tag{3.8}$$

$$2 = a(2q+c,2q+d), \quad c=-1,3, \quad d=-1,3, \quad a_3 \coloneqq a(2q+c,2q+d), \quad c=-2,4, \quad d=-2,4, \tag{3.9}$$

$$a_2 = 1 + a_0, \quad 2a_1 = 5 - a_0, \quad 2a(2q,2q) = 1 + 3a_0, \tag{3.10}$$

$$a_3 = (9-5a_0)/2, \quad a(1,4\mathbf{q}-3) = (13-9a_0)/2 = 2 + 9(1-a_0)/2. \tag{3.11}$$

Fig. 5(c), B2: $a_0=1$ with (3.5)–(3.11), the $M=(2\mathbf{p}+1)/5$, $\mathbf{q}=2$ model is physical.

$q=2$: For the first physical square grid, the highest $|x|+|z|$ are $2p+7$, 14 for heavy and light species. For $p>3$ we enlarge the light up to $2p+8$ for the first grid and $2p+10$, … for the second.

Second Fig. 5(b), in B 3, with collisions $\overline{\Lambda_i}(\beta)$ we deduce in (3.12) and (3.13) some general $a(x,z)$ which only depend on a_0, (x decreasing, z increasing, β odd). giving a second $a(1,4q-3)$ relation,

$$\beta = 3,5,\ldots, \quad a(2q-\beta,2q+\beta-2) = 2 + (1-a_0)(\beta-1)^2/2 \to a(1,4q-3), \tag{3.12}$$

$$\beta = 2q-1, \tag{3.13}$$

(3.11)–(3.13) $\to (1-a_0)[2(q-1)^2-9/2]=0 \to \mathbf{a}_0=1$ $\forall q\geqslant 1$ integer $\to a_1=a_2=a_3=2 \to a(0,z)=1$, $a(x\neq 0,z)=2 \to$ correct light mass values for physical mixture. With squares and rectangles (three f known), we can extend to all $|x|+|z|$ even values.

$q\geqslant 2$: For the first square grid, the highest $|x|+|z|$ are $2p+2q+3$ for the heavy species [$F(1,2(p+q+1))$ in (3.5)] and $4p+2q$ for the light [$f(2q+3.2q+3)$ in (4a9bis), B 3]. With the

heavy higher or smaller than the light if $p \gtrless q+3/2$, we enlarge the light or the heavy for the first square grid. For the second, third, etc., we add 2,4, etc., to both the heavy and light first square grid.

IV. CONCLUSION

If we recall the previous discussions, about "physical" or not 13 and 25 velocities models ($M=2,5$), the present physical models (filling all the half-plane without spurious invariants), with two arbitrary parameters, **p** and **q** represent some progress. In the previous works with only one arbitrary parameter or here for the explicit examples with p arbitrary but only $q=1,2,3$ we see that the proofs are more simple. However for planar models with 2 continuous coordinates, it seems clear for DVMs, DBE that we must extend the models with two arbitrary parameters and here we have presented a successful method for one species.

First in the starting physical model or adding few collisions, we retain two different $a(x,z)$ (with x,z coordinates differing of const **q**) with values depending on a_0, etc., but not on **q**. Second we seek a path linking the two $a(x,z)$, such that we can explicitly find the intermediate new $a(x,z)$ while the last depend not only on a_0, etc., but also on q. Then we have compatibilities depending on q and we must check whether or not the only possibility is $a_0=1$, etc., and physical $a(x,z)$ values.

Here we use mainly one general tool for $|x|+|z|$ odd (heavy) or even (light) and we have a similar number of heavy or light (also f_0) densities. Consequently, contrary to other distributions of the two species in the plane (octagons, dodecagons etc., for the heavy), only the heavy mass value M will be important for the physical studies. For any fractional rational M value with the same geometrical repartition of the light and heavy species, another task is for physical applications (previously for single gas[7,6]). Another problem is to see whether or not, a similar geometrical planar structure for heavy and light, could exist or not, for some irrational M values?

On the other hand we have proved the existence of "physical" (no spurious) square (diagonals along the x and z axes) grid with the first square component $|x|+|z| \leqslant$ a sufficient value which depends on the p and q parameters but which becomes very large when $\mathbf{p},\mathbf{q}$ increases while for the other larger squares of the grid, we add 2,4, etc., to that value. This means that for physical applications we cannot start with the same square grid first component for different p,q models and that the first square grid is very large when p,q increase. This constraint is not particular to the present models. For numerical regular grids filling the plane (without proof of no spurious invariants), similar problems can occur. Our main result is that the numerical calculations can be done in a "physical" square grid without spurious invariants but we must be careful for the tail of the starting first square which has been determined while for the additional squares of the grid, it is sufficient to add 2,4, etc.

Starting with a physical mixture model where the constants associated to the evolution equations for the light mass conservation law are either 1 or 2, we cannot apply directly the simple tools (except for q very small) of adding new light densities giving new physical models. So we are in the obligation to introduce arbitrary parameters $a(x,z)$ associated to the new $f(x,z)$, $l(x,z):a_0$ (rest-particle) and a_k, $k=1,2$, etc. Starting with a preliminary physical model with known old evolution equations, we add these new $a(x,z)$ and the vanishing new collisions are linear combinations of the new (unknown) and old (known) parameters. As explained above, the solution is to find for the same particular $a(x,z)$ two different values, but only one depending on **q** and the compatibilities $\forall q$, leading to all $a(x,z)$ having only the correct physical values.

We recall that for single-gas (only one species), the hexagons models give problems: one spurious relation or necessity of a multiple collision. However for the present mixture models filling either $|x|+|z|$ odd (heavy) or even (light), we present in Fig. 1, physical hexagons for the light species (sides $2,\sqrt{2}$) including the center (except along the x axis). However, for the missing centers, if we give up half-space, we can include successively physical centers $\underline{f(\pm(2q+2),0)}$, $q=0,1$, etc., integer, with the collisions: $f(\pm(2q+1),1)f(\pm(2q+1),-1)-f(\pm 2q,0)\underline{f(\pm(2q+2),0)}$.

Our proofs of physical models are done with all integers filling the plane, we recall 1.4 that, with scaling, they were generalized with a mesh-step finite, but as small as we want.

APPENDIX A: MODELS $M=2p/(2q+1)>1$ (APPENDIX A 1–A 4)

A 1 Lemma 4, Fig. 3: The $M=2\mathbf{p}/3$, $\mathbf{q}=1$ model is physical with a M_1 conservation law, old $f(x,z)$, $a(x,z)=2$: (1,1),(2,2), 2,4),(1,5)$\in$ Physical mixture (2.9) model, new $f(x,z)$, $a(x,z)$ arbitrary: (0,0),(3,3),(0,2),(1,3),(3,1),(3,±1), (2,−2), (A1).

Proof of A1: The new f satisfy eight collisions [three known, adding the last $f(\overline{x,z})$] with sums of $a(x,z)$ equal in lost and gain terms,

$$f(\overline{3,3})F(0,2p-3)-f_0F(3,2p)\rightarrow a(3,3)=2a_0,\quad f_0f(\overline{0,2})-f^2(1,1),f(0,2)f(2,2)-f(\overline{1,3})f(1,1) \tag{A1}$$

$$\rightarrow a(0,2)=a(1,3)/2=2-a_0,\quad f(1,3)f(\overline{3,1})-f(1,1)f(3,3),f_0f(3,1)-f(1,-1)f(2,2),f(1,1),$$

$$f(\overline{3,-1})-f(3,1)f(1,-1),\quad f_0f(3,-1)-f(1,1)f(\overline{2,-2})\rightarrow 4a_0-2=a(3,1)=a(1,-1)-2(a_0-1)$$

$$=a(3,-1)-6(a_0-1)=a(2,-2)-8(a_0-1),f(2,-2)F(0,2p+1)-f(1,-1)F(1,2p)\rightarrow a(2,-2)$$

$$=a(1,-1)\rightarrow a_0=1,f_0f(\overline{0,4})-f(2,2)^2a(0,4)=a(0,z)=1,a(x\neq 0,z)=2\rightarrow \text{A1}.$$

In (A1) we have three $(x,z)\rightarrow|x|+|z|=6$ and other $|x|+|z|=0,2,4\rightarrow$ all even values.

A 2, Lemma 5: *With* (2.12) and (2.13), the model $M=2\mathbf{p}/5$, $\mathbf{p}\geqslant 3$, $\mathbf{q}=2$ is physical.

Proof: (2.9), (2.12), and (2.13), $q=2\rightarrow a(2,2)=a(3,3)=a(3,7)=2$, $a(0,4)=2-a_0=a(1,5)/2$, $a(1,7)=a(1,3)=10-8a_0$, $a(3,5)=16-14a_0$. We add $f(3,7)f(1,5)-f(1,7)f(\overline{3,5})\rightarrow a(3,5)=6a_0-4=16-14a_0\rightarrow a_0=1\rightarrow a(0,4)=1,a(1,3)=a(1,7)=a(3,5)=2$,
$\rightarrow f(\overline{0,2})f(0,4)-f(1,3)^2\rightarrow a(0,2)=1,\quad f(0,2)f(2,2)-f(\overline{1,1})f(1,3)\rightarrow a(1,1)=2\rightarrow|x|+|z|=0,2,4\rightarrow$ all even values for light densities.

A 3, Lemma 6: The $M=2\mathbf{p}/7$, $\mathbf{p}\geqslant 4$, $\mathbf{q}=3$, Figs. 4(a) and 4(b) model is physical with (2.12)–(2.15).

Proof: (2.12)–(2.15) $\rightarrow a_3=a(4,10)=a(4,2q+4)=a(q+1,3q+1)=2=6a_1+10(a_0-2)$, (2.13) and (2.14) $\rightarrow a_2=a(3,9)=a(q,3q)=10-8a_0=a(3,2q+3)=3a_1+4(a_0-2)\rightarrow 3a_1=11-5a_0=18-12a_0\rightarrow a_0=1\rightarrow a_1=a_2=a_3=2$, etc.

The physical $a(0,z)=1$, $a(x\neq 0,z)=2$ for the light, have $z\geqslant q=3$ [Fig. 4(a)], but with squares, rectangles (three known) giving lower z values we get for the light, $|x|+|z|=0,2,4\rightarrow$ all even.

A 4, Proof for Lemma 7, light collisions $a_k=k(k+1)a_1/2+(k(k+1)-2)(a_0-2)$(2.16),

$$\Lambda_k=f(k,2q+k+2)f(1,2q+1)-f(k+1,2q+k+1)f(0,2q+2)\text{ with (3a1)}\rightarrow a_k:=a(k+1,2q+k+1)=a(k,2q+k+2),\quad\forall\, k=1,2,q,\quad b_k:=a(k+2,2q+k),\quad k=1,q-1,$$

$$(2\,.\,14)\rightarrow b_0=a(2,2q)=a(2,2q+2)=a_1\quad\text{and } b_1=a(3,2q+1)=2a_1+2(a_0-2)\text{(A2)}.$$

We have defined a_k,b_k and previous a_k, $k=1,2,3$ in (2.14) and (2.15) are generalized $\forall k>3$.

Collisions: $f(k+1,2q+k+1)f(k+1,2q+k-1)-f(k,2q+k)f(k+2,2q+k)$, $f(k+2,2q+k+2)f(k,2q+k)-f(k,2q+k+2)f(k+2,2q+k)$, $\rightarrow b_k=b_{k-1}+a_k-a_{k-1}=a_{k-1}+a_{k+1}-a_k$, $k\geqslant 2$.

Collisions: $f(k+2-k',2q+k-k')f(k,2q+k+2)-f(k-k',2q+k+2-k')f(k+2,2q+k)\rightarrow b_k=b_{k-2}+a_k-a_{k-2}..=b_{k-k'}+a_k-a_{k-k'}..=b_1+a_k-a_1=a_1+a_k+2(a_0-2)\rightarrow a_{k+1}=2a_k-a_{k-1}+a_1+2(a_0-2)\rightarrow a_k=2a_{k-1}+a_1-a_{k-2}+2(a_0-2)$, $k\geqslant 3$ (2.18). (2.16) for a_k was satisfied for a_2,a_3 in (2.14) and (2.15), now with the last (2.18), we verify also for a_4,a_5,

$$a_4=2a_3+a_1-a_2+2(a_0-2)=10a_1+18(a_0-2),a_5=2a_4+a_1-a_3+2(a_0-2)=15a_1+28(a_0-2).$$

For the (2.16) proof, we substitute a_{k-1}, a_{k-2} [written with (2.16)] into the last (2.18) and verify the (2.16) a_k. For b_k, with (2.18) we get $b_k=(k(k+1)+2)a_1/2+k(k+1)(a_0-2)$.

APPENDIX B: MODELS WITH $M=(2p+1)/(2q+1)>1$ (APPENDIX B 1–B 3)

B 1, Lemma 10, Fig. 5(a). With $a_0=1(f_0)$, the model $M=(2\mathbf{p}+1)/3$, $\mathbf{q}=1$ is physical. For a collision with the four $a(x,z)$ functions of a_0, the compatibility leads to $a_0=1$.

$$\text{old, } f\colon \to 2 = a(1,1) = a(1,5) = a(2,2) = a(2,4),$$
$$a(0,6) = a_0, \quad a(0,2) = a(0,4) = 2 - a_0 = a(1,3)/2, a(3,3) = 2a_0,$$

$$\text{new, } f\colon f(4,2), f(4,4), f(3,5), f(3,1) \to a(x, z \neq 0) = 1, 2(x = 0, \neq 0).$$

Proof: $\Gamma_2 = f\overline{(4,2)}F(2p,z) - f(2,2)F(2p+2,z) \to a(4,2) = 2$ (physical), odd $z=1,3$, etc.,

$$f(2,4)f(4,2) - f(2,2)f\overline{(4,4)} \to a(4,4) = 2(\text{physical}), \quad f(1,5)f(3,3) - f(1,3)f\overline{(3,5)} \to a(3,5)$$
$$= 4a_0 - 2, \quad f(2,4)f(4,4) - f(3,5)f(3,3) \to 6(1 - a_0) = 0, \to 1 = a_0$$
$$= a(0,i), i = 0,2,4, a(4,2) = a(2,2) = a(1,3) = 2, \quad f(2,2)f(4,2)$$
$$- f(3,3)f\overline{(3,1)} \to a(3,1) = 2, \to |x| + |z| = 0,2,4, \text{even}\ . \tag{B1}$$

B 2, Proof for (B2) and (B3): We introduce arbitrary $a_1(\overline{a_1}=a_1)$ and a_2 function of a_0, a_1,

$$f\overline{(1,4q-1)}f(2q-1,2q+3) - f\overline{(2q-2,2q+2)}f(2,4q) \to a_1 := a(1,4q-1) = a(2q-2,2q+2),$$

$$f\overline{(2q-2,2q)}f(2,2) - f(1,3)f(2q-1,2q-1) \to \overline{a_1} := a(2q-2,2q) = a(1,3), \tag{B2}$$

$$f(2q-2,2q)f(2q+1,2q+1) - f(2q-1,2q-1)f\overline{(2q,2q+2)} \to \overline{a_1} + 2a_0 - 2 = a(2q,2q+2),$$

$$f(2q-2,2q+2)f(2q+1,2q+1) - f(2q-1,2q+3)f\overline{(2q,2q)} \to a_1 + 2a_0 - 2 = a(2q,2q),$$

$$f(2q-2,2q+2)f(2q,2q) - f(2q-2,2q)f(2q,2q+2) \to a_1 = \overline{a_1}, \quad f(2q-2,2q+2)f(2q-2,2q)$$
$$- f(2q-3,2q+1)f\overline{(2q-1,2q+1)} \to a_2 := a(2q-1,2q+1) = 2a_1 - 4 + 2a_0. \tag{B3}$$

Fig. 5(b): Proof for (B4)–(B6) with (3.5), (3.6), (B2), and (B3). We get a_1, a_2, a_3, $a(1,4q-3)$ in terms of a_0,

$$\Gamma_2 = f(2q+3,2q-1)F(2p-1,z) - f(2q-1,2q-1)F(2p+3,z), f(2q-1,2q+3)f(2q+3,2q-1)$$
$$- f(2q-1,2q-1)f(2q+3,2q+3), \to 2 = a(2q+\lambda,2q+\mu), \lambda = -1,3, \quad \mu = -1,3\ , \tag{B4}$$

$$f(2q-2,2q)f(2q+3,2q+3) - f(2q-1,2q-1)f\overline{(2q+2,2q+4)} \to a_1 = a(2q+2,2q+4),$$

$$\Gamma_3 = f(2q+4,2q-2)F(2p-2,z) - f(2q-2,2q-2)F(2p+4,z), \quad \Gamma_4 = f(2q-2,2q+4)F(x,2p$$
$$- 2) - f(2q-2,2q-2)F(x,2p+4), \quad f(2q+4,2q+4)f(2q-2,2q-2) - f(2q-2,2q$$
$$+ 4)f(2q+4,2q-2) \to a_3 := a(2q+\lambda,2q+\mu), \quad \lambda = -2,4, \quad \mu = -2,4, \quad f(2q-2,2q$$
$$+ 2)f(2q+4,2q-2) - f(2q-2,2q-2)f\overline{(2q+4,2q+2)} \to a_1 = a(2q+4,2q$$
$$+ 2), \quad f\overline{(2q-1,2q+1)}f(2q+4,2q+2) - f(2q+2,2q+4)f(2q+1,2q-1), \quad f(2q-1,2q$$
$$+ 1)f(2q+1,2q-1) - f(2q-1,2q-1)f(2q+1,2q+1) \to a_2 = a(2q \mp 1,2q \pm 1) = 1 + a_0$$
$$= 2a_1 - 4 + 2a_0 \to 2a_1 = 5 - a_0, \quad 2a(2q,2q) = 1 + 3a\ , \tag{B5}$$

$$f(2q+4,2q+2)f(2q-2,2q)-f(2q+2,2q+4)\overline{f(2q,2q-2)}\to a_1=a(2q,2q-2),\quad f(2q-2,2q)f(2q,2q-2)-f(2q,2q)\overline{f(2q-2,2q-2)}\to a_3=a(2q-2,2q-2)=(9-5a_0)/2,\quad f(2q-2,2q-2)f(1,4q-1)-f(2q,2q)\overline{f(-1,4q-3)}\to \mathbf{a}(\pm 1,4\mathbf{q}-3)=(13-9\mathbf{a}_0)/2\ . \tag{B6}$$

Figure 5(c) with (3.5)–(3.11) $\to \mathbf{a}_0=1$ the $M=(2\mathbf{p}+1)/5$, $\mathbf{q}=2$ model is physical,

$$a(0,4)=2-a_0,\quad 2=a(2,2)=a(3,3),\quad a(1,5)=4-2a_0=(13-9a_0)/2\to a_0=1,\quad a(1,5)=2,\quad a_1=(5-a_0)/2=2=a(1,3).$$

For $|x|+|z|=0,2,4$ only $a(0,2)=1$, $a(1,1)=a(3,1)=2$ are missing but given with: $f(0,j+1)f(0,j-1)-f^2(1,j)$, $j=3,\ 1$, $f(1,1)f(3,3)-f(1,3)f(3,1)\to|x|+|z|$ all even values.

B 3, Fig.5(b): With (B4) $a(2q+\lambda,2q+\lambda)=2$, $\lambda=-1,\ 3$ and a collision $f(2q-\beta,2q+\beta-2)f(2q+3,2q+3)-f(2q-\beta+4,2q+\beta+2)f(2q-1,2q-1)$, we get

$$\mathbf{A}(\beta)=\mathbf{a}(2\mathbf{q}-\beta,2\mathbf{q}+\beta-2)=a(2q-\beta+4,2q+\beta+2)\ . \tag{B7}$$

With squares (three known) and collisions $\overline{\Lambda}_i(\beta)$, we successively get (B8) and (B9),

$$\overline{\Lambda}_1(\beta)=f(2q-\beta,2q+\beta+2)f(2q-\beta,2q+\beta-2)-f(2q-\beta+2,2q+\beta)f(2q-\beta-2,2q+\beta),$$

$$\overline{\Lambda}_2(\beta)=f(2q-\beta,2q+\beta-2)f(2q-\beta+4,2q+\beta+2)-f(2q-\beta+4,2q+\beta+2)f(2q-\beta,2q+\beta+2).$$

We start with $\overline{\Lambda}_1(1)$, successfully with (B7) and $\overline{\Lambda}_2(\beta)$, $\overline{\Lambda}_1(\beta)$, $\beta=3,5,7,\ldots$ we get

$$a(2q-3,2q+1)=4-2a_0,\quad a(2q-3,2q+5)=8-6a_0,\quad a(2q-5,2q+3)=10-8a_0,\quad a(2q-5,2q+7)=18-16a_0,\quad a(2q-7,2q+5)=20-18a_0,\quad a(2q-7,2q+9)=32-30a_0,\ldots\ . \tag{B8}$$

Going on, we deduce general $a(x,z)$ with x decreasing, z increasing, β odd,

$$\beta=1,3,5,\ldots,A(\beta)=a(2q-\beta,2q+\beta-2)=2+(1-a_0)(\beta-1)^2/2,$$

$$B(\beta)=a(2q-\beta,2q+\beta+2)=2+(1-a_0)(\beta-1)(\beta+3)/2 \tag{B9}$$

that we verify in $\overline{\Lambda}_i(\beta)$, $i=1,\ 2$ with $A(\beta)+B(\beta)=A(\beta+2)+B(\beta-2)=4+(1-a_0)(\beta^2-1)$, $2A(\beta)=B(\beta-4)+B(\beta)=4+(1-a_0)(\beta-1)^2$.

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Exponential convergence of coupled diffusion processes

Fuxi Zhang[a)]
LMAM, School of Mathematical Sciences, Peking University, Beijing 100871, China

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The coupled diffusion process, which describes Brownian motors, is an important model in the physics related to biophenomena. We address the exponential convergence of the Markov semigroup of a coupled diffusion process, and show the spectral gap inequality and Log-Sobolev inequality by comparing them with those of related diffusion processes. At the end of the paper, we provide sufficient conditions for a coupled diffusion process to converge exponentially. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1931040]

I. INTRODUCTION

Coupled diffusion processes (or CDP for short) model the systems of molecular motors, which attract much interest from physicists and biologists in recent years.[2,9,12,4,8,16] In the biological phenomena such as proteins in muscle fibers and eucariotic intracellular transport, macromolecules move along filaments called the track. It is crucial that there are several inner states of the macromolecules, and the chemical reaction causes transitions of the macromolecules among different inner states, while free energy of the chemical reaction can be converted to mechanical energy through ratchet effects.[7,3,17] The macromolecule thus becomes a motor, and is called a Brownian particle coupled with a chemical reaction. The motion of the motor along the filament is steplike, and the process is modelled as a Brownian motion at small scales in the level of nanometer and nanosecond. The impact of underlying chemical reaction can be considered as a particle source,[10,11] hence the Fokker–Planck equation of ρ_k, the probability density of the particles in the kth inner state, should be

$$\frac{\partial \rho_k(x,t)}{\partial t} + \frac{\partial \mathcal{J}_k(x,t)}{\partial x} = -q_{kk}(x)\rho_k(x,t) + \sum_{l;l\neq k} q_{lk}(x)\rho_l(x,t),$$

where q_{kl} describes the rate of the underlying chemical reaction,

$$\mathcal{J}_k = \mu_k^{-1}(-\kappa_B T\,\partial\,\rho_k/\partial x - \rho_k\,\partial\,W_k/\partial x + \rho_k f_{\text{ext}})$$

is the particle current, μ_k and κ_B are constants, T is the temperature, W_k is the potential along the filament, and f_{ext} is an external force field. In experimental situations, motors are observed moving long filaments towards their extremities. In other words, there is a net directional movement of the particle.[2,12,11,17] The potential of force along the filaments is generally periodic, and asymmetry within a period is indispensable for this phenomena.[8] Ratchet effect is related to the phenomena of stochastic resonance.[1,16,13] We refer to Ref. 16 as a comprehensive paper about the systems of molecular motors.

According to the ideas in Refs. 8 and 16, there are two components in describing the state of a particle at time t. One is the inner state of the motor, which is denoted by K_t, and the other is the space position of the motor, which is denoted by X_t. In this paper, we consider systems without external force fields, hence $\{(K_t,X_t): t\geqslant 0\}$ is a homogeneous Markov process with state space $\mathbb{X}=\{1,\ldots,N\}\times\mathbb{R}^d$, and obeys the following mechanism:

[a)]Electronic mail: zhangfxi@math.pku.edu.cn

$$\mathrm{d}X_t = \sqrt{\mathbf{A}}(K_t,X_t)d\mathbf{B}_t + \left(\mathbf{b} + \tfrac{1}{2}\nabla^T\mathbf{A}\right)(K_t,X_t)\mathrm{d}t,$$

$$\mathbf{P}(K_{t+\Delta t} = l | K_t = k, X_t) = q_{kl}(X_t)\Delta t + o(\Delta t), \quad l \neq k,$$

where $\mathbf{A}(k,x)$ is a $d\times d$ positive definite matrix, $\mathbf{b}(k,x)$ is a d-dimensional vector, $q_{kl}(x)\geqslant 0$, and $\{\mathbf{B}_t : t\geqslant 0\}$ is a Brownian motion on $\mathbb{R}^d$. Denote

$$\mathcal{L}_k = \tfrac{1}{2}\nabla\cdot(\mathbf{A}(k,\cdot)\nabla) + \mathbf{b}(k,\cdot)\cdot\nabla.$$

Then the generator of $\{(K_t,X_t) : t\geqslant 0\}$ has the following form:

$$\mathcal{L}f(k,x) = \mathcal{L}_k f(k,x) + \sum_{l:l\neq k} q_{kl}(x)(f(l,x) - f(k,x)).$$

Suppose the coefficients are smooth. In order that there is no explosion and that the process is not reducible, we suppose $q_{kl}(x)$ is bounded for all k, l, and for any k, l, there are $r\geqslant 0$, $k_1,\ldots,k_r$ and $x_1,\ldots,x_{r+1}\in\mathbb{R}^d$ such that

$$q_{kk_1}(x_1)q_{k_1k_2}(x_2)\cdots q_{k_{r-1}k_r}(x_r)q_{k_rl}(x_{r+1}) > 0.$$

In Ref. 14, we construct a CDP with generator $\mathcal{L}$ under the above assumptions.

In this paper, we address the exponential convergence of the CDP. Let $\{T(t) : t\geqslant 0\}$ be the semigroup of a Markov process, μ be its invariant distribution. We say that $T(t)$ converges exponentially if there exists $\delta>0$ such that for any $f\in L^2(\mathbb{X},\mu)$,

$$\|T(t)f - E_\mu f\| \leqslant C(f)e^{-\delta t}, \tag{1}$$

where $E_\mu f = \int f\,\mathrm{d}\mu$, $\|\cdot\|$ is the L^2 norm with respect to μ, and $C(f)$ is a constant relying on f. Let $\{\overline{T}(t) : t\geqslant 0\}$ be the symmetrization of $\{T(t) : t\geqslant 0\}$ with respect to μ. It is already known that

$$\|T(t)f - E_\mu f\| \leqslant \|\overline{T}(t)f - E_\mu f\|.$$

Hence we are only concerned with the case that $T(t)$ is symmetric. In this case, its generator $\mathcal{A}$ is self-adjoint in $L^2(\mu)$, and Eq. (1) is equivalent to that

$$\langle \mathcal{A}f, f\rangle \leqslant -\delta\|f - E_\mu f\|^2, \quad \forall\, f\in\mathcal{D}(\mathcal{A}), \tag{2}$$

where $\langle\cdot,\cdot\rangle$ is the inner product in $L^2(\mu)$, $\mathcal{D}(\mathcal{A})$ is the domain of $\mathcal{A}$. We say that $\mathcal{A}$ satisfies the spectral gap inequality, or $\mathcal{A}$ has a spectral gap if it satisfies (2). Another inequality, which ensures (1) is the log–Sobolev inequality. We call that $\mathcal{A}$ satisfies the log–Sobolev inequality with constant $c(>0)$ if

$$E_\mu f^2 \log f^2 - E_\mu f^2 \log E_\mu f^2 \leqslant -c\langle \mathcal{A}f, f\rangle, \quad \forall\, f\in\mathcal{D}(\mathcal{A}).$$

In this paper, when we mention the spectral gap (log–Sobolev) inequality about a generator, the probability measure is taken as its symmetric distribution.

The problem whether the generator satisfies the spectral gap inequality or the log–Sobolev inequality attracts much attention. For diffusion processes, there exist already considerable references, e.g., Refs. 5 and 6. The spectral gap inequality as well as the log–Sobolev inequality has a multiplying property, if two reversible Markov processes satisfy the spectral gap (log–Sobolev) inequality, then the independent coupling of them also does, whose generator is the sum of those of the two independent processes. Although the CDP is not an independent coupling of a Q process and a diffusion process, its generator is naturally separated into two parts explicitly. One is a diffusion generator caused by $\{X_t : t\geqslant 0\}$ and the other is a Q matrix caused by $\{K_t : t\geqslant 0\}$. We use the fact that the Q matrix is finite and negative in some sense to show that in the specific model of CDP, the spectral gap inequality can be simplified into those of diffusion processes. It is much better than the multiplying property. Let $q_{kk}(x) = -\Sigma_{l:l\neq k}q_{kl}(x)$ and $\mathbf{Q}(x) = (q_{kl}(x))$. Suppose

$\{(K_t, X_t): t \geqslant 0\}$ is a reversible CDP with initial distribution θ. Hence $\mathcal{L}$ is symmetric in $L^2(\mathbb{X}, \theta)$. In the beginning of Sec. II, we show that this implies the existence of symmetric densities of $\mathcal{L}_k$ and $\mathbf{Q}(x)$.

Theorem 1: *If $\mathcal{L}_k$ satisfies the spectral gap inequality for all k, then $\mathcal{L}$ also does.*

Theorem 2: *Suppose θ is a product measure. If $\mathcal{L}_k$ and $\mathbf{Q}(x)$ satisfy the log–Sobolev inequality with constant c for all k and x, then $\mathcal{L}$ also does.*

II. THE RELATIONSHIP BETWEEN $\mathcal{D}(\mathcal{L})$ AND $\mathcal{D}(\mathcal{L}_k)$

We begin this section with discussing the relationship of the symmetric measure of $\mathcal{L}$ with those of $\mathcal{L}_k$ and $\mathbf{Q}(x)$. Since $\{(K_t, X_t): t \geqslant 0\}$ is reversible, $V = \log \theta$ is a potential of $2\mathbf{A}^{-1}\mathbf{b}$, and $\{\theta(k,x): k = 1, \ldots, N\}$ is a reversible measure of the Q-matrix $\mathbf{Q}(x)$ for any $x \in \mathbb{R}^d$. Since the CDP is unexploded and $\mathbf{Q}$ is bounded, the diffusion process generated by $\mathcal{L}_k$ is unexploded. Therefore, the normalization of $\theta(k, \cdot)$ on $\{(k,x): \mathbb{R}^d\}$,

$$\rho_k(x) = \theta(k,x)/\pi_k, \quad \text{where } \pi_k = \int \theta(k,x)\mathrm{d}x,$$

is a reversible distribution density of $\mathcal{L}_k$.

For the sake of the reader, we recall the construction of the process in Ref. 14. Let

$$C(\mathbb{R}^d) = \text{the set of all bounded continuous functions on } \mathbb{R}^d;$$

$$C(\mathbb{X}) = \text{the set of all bounded continuous functions on } \mathbb{X};$$

$$C_0(\mathbb{X}) = \{f \in C(\mathbb{X}): \lim_{|x| \to +\infty} f(k,x) = 0, \forall\, k\};$$

$$C_0^\infty(\mathbb{X}) = \{f \in C(\mathbb{X}):\ f \text{ is smooth and has a compact support}\};$$

$$\mathbb{B}_n = \{(k,x): |x| < n\};$$

$$C_0(\mathbb{B}_n) = \{f \in C(\mathbb{X}): f|_{\mathbb{B}_n^c} = 0\};$$

$$C_0^\infty(\mathbb{B}_n) = \{f \in C_0^\infty(\mathbb{X}): \mathrm{supp}(f) \subset \mathbb{B}_n\}.$$

For any $\lambda > 0$ and $g \in C_0(\mathbb{B}_n)$, there is a unique solution of $(\lambda - \mathcal{L})f = g$ in $C_0(\mathbb{B}_n)$, which is denoted by $R_n(\lambda)g$. Choose h_n such that

$$h_n \in C_0^\infty(\mathbb{B}_n), \quad 0 \leqslant h_n \leqslant 1, \quad h_n|_{\mathbb{B}_{n-1}} = 1. \tag{3}$$

Then for any $\lambda > 0$ and nonnegative $g \in C(\mathbb{X})$, $R_n(\lambda)(h_n g)$ increases pointwise. Hence $R_n(\lambda)(h_n g)$ converges pointwise for any $g \in C(\mathbb{X})$. Denote the limit by $R(\lambda)g$. Then it belongs to $C(\mathbb{X})$ and is a global solution of $(\lambda - \mathcal{L})f = g$. $R(\lambda)$ is a positive continuous linear operator on $C(\mathbb{X})$, and $\|R(\lambda)g\|_\infty \leqslant \|g\|_\infty/\lambda$, where $\|\cdot\|_\infty$ is the supremum norm. Moreover, we show in Ref. 14 the following.

Lemma 2.1: *If $g_n \in C_0(\mathbb{B}_n)$ is non-negative and increases to $g \in C(\mathbb{X})$ as $n \to \infty$, then $R_n(\lambda)g_n$ increases to $R(\lambda)g$.*

Let $\hat{C}(\mathbb{X})$ be the minimal Banach space containing $C_0(\mathbb{X})$ and invariant under $\{R(\lambda): \lambda > 0\}$. Then $\{R(\lambda)|_{\hat{C}(X)}: \lambda > 0\}$ is a resolvent according to $\mathcal{L}$ with domain $\mathcal{D}(\mathcal{L}) = R(\lambda)\hat{C}(\mathbb{X})$. Hence it corresponds to a contraction semigroup $\{S(t): t \geqslant 0\}$ on $\hat{C}(\mathbb{X})$. Moreover, $C_0^\infty(\mathbb{X}) \subset \mathcal{D}(\mathcal{L})$.

Recall that θ is an invariant distribution. In order not to cause ambiguity, we denote by $\mathcal{D}(\mathcal{L}, L^2)$ the domain of $\mathcal{L}$ in the space $L^2(\mathbb{X}, \theta)$, by $\{\tilde{S}(t): t > 0\}$ and $\{\tilde{R}(\lambda): \lambda > 0\}$ the correspond-

ing Markov semigroup and resolvent. Then they are extensions of $\{S(t):t>0\}$ and $\{R(\lambda)|_{\hat{C}(X)}:\lambda>0\}$, respectively. The following proposition tells us $\{\tilde{R}(\lambda):\lambda>0\}$ is in fact an extension of $\{R(\lambda):\lambda>0\}$. As to $\mathcal{L}_k$, recall that ρ_k is its invariant distribution. Let $\mathcal{D}(\mathcal{L}_k,L^2)$, $\tilde{R}^{(k)}(\lambda)$, $R_n^{(k)}(\lambda)$, and $R^{(k)}(\lambda)$ be the corresponding notation.

Proposition 2.2: *For any* $\lambda>0$ *and any* $k\in\{1,\ldots,N\}$,

$$\tilde{R}(\lambda)|_{C(\mathbb{X})}=R(\lambda),\quad \tilde{R}^{(k)}(\lambda)|_{C(\mathbb{R}^d)}=R^{(k)}(\lambda).$$

Proof: For any non-negative function $f\in C(\mathbb{X})$, choose $f_n\in C_0^\infty(\mathbb{X})$ such that $0\leqslant f_n\leqslant f$ and f_n increases to f as $n\to\infty$. On the one hand, by Lemma 2.1, $R_n(\lambda)f_n$ increases to $R(\lambda)f$. This together with that $R_n(\lambda)f_n\leqslant R(\lambda)f_n\leqslant R(\lambda)f$ implies that $R(\lambda)f_n$ converges to $R(\lambda)f$. On the other hand, $R(\lambda)f_n=\tilde{R}(\lambda)f_n$ since $f_n\in C_0^\infty(\mathbb{X})\subset\mathcal{D}(\mathcal{L})$. Notice that f_n converges to f in L^2. $\tilde{R}(\lambda)f_n$ converges to $\tilde{R}(\lambda)f$ in L^2 since $\tilde{R}(\lambda)$ is continuous with respect to the L^2 norm. Therefore,

$$R(\lambda)f=\lim_{n\to+\infty}R(\lambda)f_n=\lim_{n\to+\infty}\tilde{R}(\lambda)f_n=\tilde{R}(\lambda)f,$$

i.e., $\tilde{R}(\lambda)|_{C(\mathbb{X})}=R(\lambda)$. As to $\mathcal{L}_k$, the result holds by the same deduction. □

Proposition 2.2 implies that

$$R(\lambda)C(\mathbb{X})=\tilde{R}(\lambda)C(\mathbb{X})\subset\tilde{R}(\lambda)L^2(\mathbb{X},\theta)=\mathcal{D}(\mathcal{L},L^2).$$

Proposition 2.3: $R(\lambda)C(\mathbb{X})$ *is a kernel of* $(\mathcal{L},\mathcal{D}(\mathcal{L},L^2))$, *i.e., it is a dense subset under the graph norm:* $\|f\|_{\mathcal{L}}=\|f\|+\|\mathcal{L}f\|$ *for any* $f\in\mathcal{D}(\mathcal{L},L^2)$.

Proof: For any $f\in\mathcal{D}(\mathcal{L},L^2)$, there exists $g\in L^2(\mathbb{X},e^V)$ such that $f=\tilde{R}(\lambda)g$. Since $C(\mathbb{X})$ is dense in $L^2(\mathbb{X},e^V)$, there exists $g_n\in C(\mathbb{X})$ such that $\lim_{n\to+\infty}\|g_n-g\|=0$. Hence $f_n=\tilde{R}(\lambda)g_n$ converges to f in L^2, which implies that $\mathcal{L}f_n=\lambda f_n-g_n$ converges to $\lambda f-g=\mathcal{L}f$ in L^2. In other words, f_n converges to f in $\|\cdot\|_{\mathcal{L}}$. This together with Proposition 2.2 yields the result. □

Proposition 2.4: *For any* $\lambda>0$,

$$R(\lambda)C(\mathbb{X})\subset\{f:f(k,\cdot)\in R^{(k)}(\lambda)C(\mathbb{R}^d),\ \forall\ k\}.$$

Proof: Suppose $f\in C(\mathbb{X})$. We assume that $f\geqslant 0$ first. Let $f_n=fh_n$, $g=R(\lambda)f$, $g_n=R_n(\lambda)f_n$, where h_n satisfies (3). Since $(\lambda-\mathcal{L})g_n=f_n$, $g_n(k,\cdot)$ is a solution of

$$(\lambda-\mathcal{L}_k)\varphi=f_n(k,\cdot)+\sum_{l=1}^N q_{kl}g_n(l,\cdot),$$

in $C_0(\mathbb{B}_n)$. Therefore,

$$\begin{aligned}g_n(k,\cdot)&=R_n^{(k)}(\lambda)\left(f_n(k,\cdot)+\sum_{l=1}^N q_{kl}g_n(l,\cdot)\right)\\&=R_n^{(k)}(\lambda)f_n(k,\cdot)+R_n^{(k)}(\lambda)\left(\sum_{l:l\neq k}q_{kl}g_n(l,\cdot)\right)-R_n^{(k)}(\lambda)(-q_{kk}g_n(k,\cdot)).\end{aligned}\tag{4}$$

By Lemma 2.1, since f_n increases to f, g_n increases to g. Hence as $n\to+\infty$, the non-negative functions $f_n(k,\cdot)$, $\Sigma_{l:l\neq k}q_{kl}g_n(l,\cdot)$, and $-q_{kk}g_n(k,\cdot)$ in $C_0(\mathbb{B}_n)$, respectively, increase to $f(k,\cdot)$, $\Sigma_{l:l\neq k}q_{kl}g(l,\cdot)$, and $-q_{kk}g(k,\cdot)$. Notice that $\mathbf{Q}$ is bounded, and f, $g\in C(\mathbb{X})$. The limit functions belong to $C(\mathbb{X})$. By Lemma 2.1, the right most functions in (4) converge as $n\to+\infty$, and

$$R(\lambda)f(k,\cdot) = \lim_{n\to+\infty} g_n(k,\cdot)$$
$$= R^{(k)}(\lambda)f(k,\cdot) + R^{(k)}(\lambda)\left(\sum_{l:l\neq k} q_{kl}g(l,\cdot)\right) - R^{(k)}(\lambda)(-q_{kk}g(k,\cdot)) \in R^{(k)}(\lambda)C(\mathbb{R}^d).$$

Then, for any $f\in C(\mathbb{X})$ and any k,

$$R(\lambda)f(k,\cdot) = R(\lambda)f^+(k,\cdot) - R(\lambda)f^-(k,\cdot) \in R^{(k)}(\lambda)C(\mathbb{R}^d),$$

which implies the result. □

Proposition 2.4 together with Proposition 2.3 yields that there exists a dense subset of $\mathcal{D}(\mathcal{L},L^2)$ contained in $\mathcal{D}(\mathcal{L}_1,L^2)\oplus\cdots\oplus\mathcal{D}(\mathcal{L}_N,L^2)$.

III. PROOFS OF THE MAIN RESULTS

Lemma 3.1 *(Ref. 15, Theorem XIII.1): Suppose $\mathcal{A}$ is self-adjoint on the Hilbert space $\mathcal{H}$, and is bounded above. Let*

$$\mu(\mathcal{A},g_1,\ldots,g_n) = \sup\{\langle \mathcal{A}g,g\rangle : g\in\mathcal{D}(\mathcal{A}),\|g\|=1,\langle g,g_i\rangle = 0, i=1,\ldots,n\},$$

$$\mu_n(\mathcal{A}) = \inf\{\mu(\mathcal{A},g_1,\ldots,g_n): g_1\ldots,g_n\in\mathcal{H}\}.$$

Then either $\mu_n(\mathcal{A}) = \sup\sigma_{\mathrm{ess}}(\mathcal{A})$, or $\sigma(\mathcal{A})\cap(\mu_n(\mathcal{A}),\infty)$ is a finite set.

Proof of Theorem 1: Recall that $\pi_k = \int\theta(k,x)\mathrm{d}x$, and $\rho_k(x) = \theta(k,x)/\pi_k$ is the symmetric distribution of $\mathcal{L}_k$. Given k, since $\mathcal{L}_k$ has a spectral gap, there exists $\delta_k>0$ such that for any $F\in\mathcal{D}(\mathcal{L}_k,L^2)$,

$$\langle \mathcal{L}_kF,F\rangle_{\rho_k} \leqslant -\delta_k\left(\int F^2(x)\rho_k(x)\mathrm{d}x - \left(\int F(x)\rho_k(x)\mathrm{d}x\right)^2\right),$$

where $\langle\cdot,\cdot\rangle_{\rho_k}$ is the inner product in $L^2(\mathbb{R}^d,\rho_k)$. By Proposition 2.4, for any $f\in R(\lambda)C(\mathbb{X})$, $f(k,\cdot)\in\mathcal{D}(\mathcal{L}_k,L^2)$ for any k, hence

$$\langle \mathcal{L}f,f\rangle = \sum_{k=1}^N \pi_k\langle \mathcal{L}_kf(k,\cdot),f(k,\cdot)\rangle_{\rho_k} + \sum_{k,l=1}^N\int\theta(k,x)q_{kl}(x)f(k,x)f(l,x)\mathrm{d}x \leqslant \sum_{k=1}^N \pi_k\langle \mathcal{L}_kf(k,\cdot),f(k,\cdot)\rangle_{\rho_k}$$
$$\leqslant -\sum_{k=1}^N \pi_k\delta_k\left(\int f^2(k,x)\rho_k(x)\mathrm{d}x - \left(\int f(k,x)\rho_k(x)\mathrm{d}x\right)^2\right)$$
$$\leqslant -\delta\|f\|^2 + M\sum_{k=1}^N \pi_k\left(\int f(k,x)\rho_k(x)\mathrm{d}x\right)^2, \tag{5}$$

where $\delta=\delta_1\wedge\cdots\wedge\delta_N$, $M=\delta_1\vee\cdots\vee\delta_N$, and the first inequality holds since $\mathbf{Q}(x)$ is a generator and hence negative. By Proposition 2.3, for any $f\in\mathcal{D}(\mathcal{L},L^2)$, there are $f_n\in R(\lambda)C(\mathbb{X})$, $n\geqslant 1$, such that

$$\lim_{n\to+\infty}\|f_n - f\|_{\mathcal{L}} = 0. \tag{6}$$

On the one hand, (5) holds for f_n since $f_n\in R(\lambda)C(\mathbb{X})$. On the other hand, $f_n(k,\cdot)$ converges to $f(k,\cdot)$ in $L^2(\mathbb{R}^d,\rho_k)$, hence also in L^1. It follows that

$$\lim_{n\to+\infty}\int f_n(k,x)\rho_k(x)\mathrm{d}x = \int f(k,x)\rho_k(x)\mathrm{d}x.$$

This together with (6) yields that (5) holds for f, since it holds for f_n. Let 1_k be the function which is 1 in the kth $\mathbb{R}^d$ and vanishes outside, i.e.,

$$1_k(l,x)=\begin{cases}1, & \text{if } l=k,\\ 0, & \text{otherwise.}\end{cases}$$

Then $\langle f,1_k\rangle=0$ if and only if $\int_{R^d} f(k,x)\rho_k(x)\mathrm{d}x=0$. Therefore, by (5), $\mu(\mathcal{L},1_1,\ldots,1_N)\leqslant-\delta$. Hence $\mu_N(\mathcal{L})\leqslant-\delta<0$. It follows that $\mathcal{L}$ has a spectral gap since $\mathcal{L}$ has only finite spectra in $(\mu_N(\mathcal{L}),0]$. □

Proof of Theorem 2: To simplify the notation, for any function f on $\mathbb{X}$, we denote $f_k(x)=f(k,x)$ and $\vec{f}(x)=(f_1(x),\ldots,f_N(x))$. Let $\varphi:(\mathbb{R}^+)^N\to\mathbb{R}$,

$$\varphi(\vec{g})=E_{\pi}\vec{g}\log\vec{g}-E_{\pi}\vec{g}\log E_{\pi}\vec{g}=\sum_{k=1}^{N}\pi_k g_k\log g_k-\left(\sum_{k=1}^{N}\pi_k g_k\right)\log\left(\sum_{k=1}^{N}\pi_k g_k\right).$$

Now we check that the Hessian matrix of φ is positive semidefinite, and hence φ is convex in $\vec{g}$. Notice that

$$\frac{\partial\varphi}{\partial g_k}(\vec{g})=\pi_k\left(\log g_k-\log\sum_{l=1}^{N}\pi_l g_l\right),$$

$$\frac{\partial^2\varphi}{\partial g_k\,\partial g_l}(\vec{g})=\begin{cases}\pi_k/g_k-\pi_k^2\left(\sum_{r=1}^{N}\pi_r g_r\right)^{-1}, & \text{if } k=l,\\ -\pi_k\pi_l\left(\sum_{r=1}^{N}\pi_r g_r\right)^{-1}, & \text{if } k\neq l.\end{cases}$$

For any vector $\vec{v}$ with dimension N,

$$\begin{aligned}\vec{v}^T\,\mathrm{Hess}(\varphi)(g)\vec{v}&=\sum_{k=1}^{N}\pi_k v_k^2/g_k-\left(\sum_{k,l=1}^{N}\pi_k\pi_l v_k v_l\right)\left(\sum_{r=1}^{N}\pi_r g_r\right)^{-1}\\&=\sum_{k=1}^{N}\pi_k v_k^2/g_k-\left(\sum_{k=1}^{N}\pi_k v_k\right)^2\left(\sum_{r=1}^{N}\pi_r g_r\right)^{-1}\end{aligned}$$

is non-negative since

$$\left(\sum_{k=1}^{N}\pi_k v_k\right)^2=\left(\sum_{k=1}^{N}(\pi_k g_k)^{1/2}((\pi_k/g_k)^{1/2}v_k)\right)^2\leqslant\left(\sum_{k=1}^{N}\pi_k g_k\right)\left(\sum_{k=1}^{N}\pi_k v_k^2/g_k\right).$$

Hence φ is convex. Thus for any non-negative function g on $\mathbb{X}$,

$$\varphi(E_{\rho}\vec{g})\leqslant E_{\rho}\varphi(\vec{g})=\int\varphi(\vec{g}(x))\rho(x)\mathrm{d}x.$$

For any $f\in R(\lambda)C(\mathbb{X})$, let $g=f^2$, and it follows that

$$\begin{aligned}E_{\theta}f^2\log f^2-E_{\theta}f^2\log E_{\theta}f^2&=E_{\pi}(E_{\rho}f^2\log f^2-E_{\rho}f^2\log E_{\rho}f^2)+(E_{\pi}(E_{\rho}f^2\log E_{\rho}f^2)\\&\quad-E_{\pi}E_{\rho}f^2\log E_{\pi}E_{\rho}f^2)=\sum_{k=1}^{N}\pi_k(E_{\rho}f^2(k,\cdot)\log f^2(k,\cdot)\\&\quad-E_{\rho}f^2(k,\cdot)\log E_{\rho}f^2(k,\cdot))+\varphi(E_{\rho}\vec{g})\leqslant-c\sum_{k=1}^{N}\pi_k E_{\rho}\langle\mathcal{L}_k f(k,\cdot),f(k,\cdot)\rangle_{\rho}\end{aligned}$$

$$+E_\rho\varphi(\vec{g}) \leqslant -c\sum_{k=1}^{N}\int (\mathcal{L}_k f(k,x))f(k,x)\pi_k\rho(x)\mathrm{d}x - c\int \sum_{k=1}^{N}\pi_k f(k,x)$$
$$\times\left(\sum_{k=1}^{N} q_{kl}(x)f(l,x)\right)\rho(x)\mathrm{d}x = -c\langle \mathcal{L}f,f\rangle,$$

where the first inequality holds since $f(k,\cdot)\in D(\mathcal{L}_k,L^2)$. For any $f\in\mathcal{D}(\mathcal{L},L^2)$, take $f_n\in R(\lambda)C(\mathbb{X})$ such that $\lim_{n\to+\infty}\|f_n-f\|_{\mathcal{L}}=0$. Choose a subsequence, which is still denoted by f_n, such that it converges almost surely. By the Fatou lemma,

$$E_\theta f^2\log f^2 1_{\{|f|\geqslant 1\}} \leqslant \lim_{n\to+\infty}\inf E_\theta f_n^2\log f_n^2 1_{\{|f_n|\geqslant 1\}}.$$

By the bounded convergence theorem,

$$E_\theta f^2\log f^2 1_{\{|f|<1\}} \leqslant \lim_{n\to+\infty} E_\theta f_n^2\log f_n^2 1_{\{|f_n|\geqslant 1\}}.$$

Hence

$$E_\theta f^2\log f^2 - E_\theta f^2\log E_\theta f^2 \leqslant \lim_{n\to+\infty}\inf(E_\theta f_n^2\log f_n^2 - E_\theta f_n^2\log E_\theta f_n^2)$$
$$\leqslant \lim_{n\to+\infty}\inf -c\langle \mathcal{L}f_n,f_n\rangle = -c\langle \mathcal{L}f,f\rangle,$$

which implies the result. □

At the end of this paper, we give a sufficient condition for the CDP to have a spectral gap. In fact, we show the following.

Lemma 3.2: *Let $\mathcal{L}=\frac{1}{2}\Delta+\frac{1}{2}\nabla V.\nabla$ be a generator of a diffusion process, and e^V be a reversible density. Suppose there is a multiplication operator $\widetilde{U}$, relative compact with respect to the Laplace operator Δ and having a lower bound, and $\delta>0$ such that*

$$U \triangleq \tfrac{1}{4}|\nabla V|^2+\tfrac{1}{2}\Delta V \geqslant \widetilde{U}+\delta. \tag{7}$$

Then $\mathcal{L}$ has a spectral gap.

This together with Theorem 1 yields the following.

Proposition 3.3: *Let*

$$\mathcal{L}f(k,x) = \tfrac{1}{2}\Delta f(k,x) + \tfrac{1}{2}\nabla V(k,x)\cdot\nabla f(k,x) + \sum_{l:l\neq k} q_{kl}(x)(f(l,x)-f(k,x)),$$

where q_{kl} is bounded. Let e^V be the reversible density. If for all k, $V(k,x)$ satisfies the condition in Lemma 3.2, then $\mathcal{L}$ has a spectral gap.

Remark 3.4: If $\liminf_{|x|\to+\infty}U(x)>0$, *then* (7) *holds. In this case, there exist $M,\delta,R>0$ such that $U\geqslant -M$ and $U(x)>\delta$ whenever $|x|>R$. Hence $U\geqslant\widetilde{U}+\delta$, where $\widetilde{U}:=-(M+\delta)1_{|x|<R}$ is relative compact with respect to Δ in $L^2(\mathbb{R}^d,\mathbf{m})$.*

Proof of Lemma 3.2: Let

$$\Phi: L^2(\mathbb{R}^d,e^V)\to L^2(\mathbb{R}^d,\mathbf{m}),\quad f\mapsto e^{V/2}f.$$

Then Φ is an isomorphism. Hence $\widetilde{\mathcal{L}}=\Phi\mathcal{L}\Phi^{-1}=\frac{1}{2}(\Delta-U)$ is self-adjoint on $L^2(\mathbb{R}^d,\mathbf{m})$ and has the same family of spectra as $\mathcal{L}$ in $L^2(\mathbb{R}^d,e^V)$. Now we check that $\widetilde{\mathcal{L}}$ has a spectral gap in $L^2(\mathbb{R}^d,\mathbf{m})$.

Since $\widetilde{U}$ is relative compact with respect to Δ, $\Delta-\widetilde{U}$ has the same essential spectra as Δ. Therefore,

$$\sigma_{\mathrm{ess}}(\Delta - \tilde{U}) = \sigma_{\mathrm{ess}}(\Delta) = (-\infty, 0].$$

It follows that $\sup \sigma_{\mathrm{ess}}(\Delta - \tilde{U}) = 0$. Notice that $\tilde{U}$ is bounded below, which implies that $\Delta - \tilde{U}$ is bounded above. By Lemma 3.1, $\mu_n(\Delta - \tilde{U}) < \delta/2$ for large n. Hence

$$\mu_n(\Delta - U) \leqslant \mu_n(\Delta - \tilde{U} - \delta) = \mu_n(\Delta - \tilde{U}) - \delta < -\delta/2. \tag{8}$$

It is concluded that the spectra of $\Delta - U$ in $[-\delta/2, 0]$ are discrete. Hence $\Delta - U$ has a spectral gap, which implies that $\tilde{\mathcal{L}} = (\Delta - U)/2$ does. Therefore, $\mathcal{L}$ has a spectral gap. □

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Observability of the scattering cross-section through phase decoherence

Timothy R. Field
Departments of Electrical and Computer Engineering and Mathematics, McMaster University, Hamilton, Ontario, Canada L8S 4L8

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We derive the stochastic dynamics for scattering of a wavelike field from a large population of scatterers whose dynamics is arbitrary. This leads to a result concerning the observability of the scattering cross section in terms of the resultant phase fluctuations that is independent of the population dynamics. An emergent concept is a certain notion of an ideal filter. The diffusion based model of *K*-scattering arises as a special case. The experimental implications of the results in a variety of contexts are discussed. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1926147]

I. INTRODUCTION

Motivated by the possible application of the recent results on electromagnetic scattering from random media to more general situations (e.g., medical imaging, wireless communications) than those encompassed by the *K*-distribution model (Field and Tough, 2003a, 2003b), the paper describes an interesting result in connection with inference of the scattering cross section or population, in local time. A special case of the result was reported previously in Field and Tough (2003b) [see paragraph above Eq. (2.35) therein], stating that the instantaneous values of the cross section are deducible through the phase fluctuations in the scattered field. This was demonstrated in the context of *K*-scattering. Intriguingly, the same result holds for an arbitrary population. More precisely, given the structure of a random walk model, component phase and step number fluctuations, the result holds for an arbitrary specification of population dynamics. In this sense, the result is a geometrical feature of (the dynamical extension of) Jakeman's random walk model with step number fluctuations (Jakeman, 1980), and as such should apply to a large number of experimental situations involving interference effects of wavelike fields arising from random populations. From a filtering point of view, the result represents an improvement on Kalman–particle filtering methods, since an *exact* expression for the hidden state (the population level) in terms of the additional phase degrees of freedom can be derived.

We adopt the consistent notation throughout for a continuous time stochastic processes q_t, with Ito differential $\mathrm{d}q_t$, and and squared volatility $\mathrm{d}q_t^2$.[1]

II. RANDOM WALK MODEL

It is well known that Rayleigh scattering can be described by a random walk model for the scattered field amplitude (cf. Jakeman, 1980; Tough, 1987; Jakeman and Tough, 1988) with a fixed number of steps. The pertinent expression for the resultant field amplitude according to this model is

[1]Thus the notation $\mathrm{d}q_t^2$, as occurs, e.g., for the phase process in Theorem 3.5, means that the differential is taken *before* the square.

$$\mathcal{E}_t^{(N)} = \sum_{j=1}^{N} \overbrace{a_j \exp[i\varphi_t^{(j)}]}^{s^{(j)}} \tag{2.1}$$

with (constant) population size N, random phasor step $s^{(j)}$, and form factors a_j.

In the aforementioned references all components of this expression are in effect considered at a given instant of time, thus not addressing the question of continuous time evolution properties or dynamics. This extra structure is supplied by a (phase) diffusion model (Field and Tough, 2003b) which takes the component phases $\{\varphi_t^{(j)}\}$ to be a collection of (displaced) Wiener processes evolving on a suitable time scale. Thus $\varphi_t^{(j)} = \Delta^{(j)} + \mathcal{B}^{\frac{1}{2}} W_t^{(j)}$, with component random initialization $\Delta^{(j)}$ uniformly distributed on the interval $[0, 2\pi)$. In situations where the component phasors $s^{(j)}$ are aligned initially (e.g., for the received $T2$ signal arising in magnetic resonance imaging, described, e.g., by Brown and Semelka, 2003 and discussed in Sec. IV) $\Delta^{(j)}$ are identical for all j, whereas in some cases [e.g., the statistical description of radar scattering from the sea surface, cf. Sec. 4(b) in Field and Tough, 2003a] it is more appropriate to draw $\Delta^{(j)}$ independently. In any case, these primitive assumptions enable us to derive the dynamics of Rayleigh scattering, essentially from first principles. The stochastic differential of (2.1), according to Ito's formula (e.g., Oksendal, 1998; Karatzas and Shreve, 1988), is given by

$$\mathrm{d}\mathcal{E}_t^{(N)} = \sum_{j=1}^{N} a_j \left(i\, \mathrm{d}\varphi_t^{(j)} - \frac{1}{2} \mathrm{d}\varphi_t^{(j)2} \right) \exp\left[i\varphi_t^{(j)} \right]. \tag{2.2}$$

If we write $\mathrm{d}\zeta_t$ for the first term on the right-hand side above, then for $t \geqslant T$, where T is the phase decoherence time such that $\{\varphi_t^{(j)} | t \geqslant T\}$ have negligible correlation, we have $|\mathrm{d}\zeta_t|^2 = (\Sigma_j a_j^2)\ \mathcal{B}\, \mathrm{d}t$, and therefore $\mathrm{d}\zeta_t = (\Sigma_j a_j^2)^{1/2} \mathcal{B}^{1/2}\, \mathrm{d}\xi_t$ where ξ_t is a complex-valued Wiener process (satisfying $|\mathrm{d}\xi_t|^2 = \mathrm{d}t$, $\mathrm{d}\xi_t^2 = 0$). Defining the (normalized) Rayleigh amplitude by $\gamma_t = \lim_{N\to\infty}[\mathcal{E}_t^{(N)} / N^{\frac{1}{2}}]$ leads to the resultant dynamics (cf. Field and Tough, 2003b).

Proposition 2.1: *For sufficiently large times $t \geqslant T$ the dynamics of Rayleigh scattering is given by the complex Ornstein–Uhlenbeck equation*

$$\mathrm{d}\gamma_t = -\tfrac{1}{2} \mathcal{B} \gamma_t\, \mathrm{d}t + \mathcal{B}^{\frac{1}{2}} \langle a^2 \rangle^{\frac{1}{2}}\, \mathrm{d}\xi_t. \tag{2.3}$$

If $\{\Delta^{(j)}\}$ are assumed independent then the result holds for arbitrarily small times.

If we rescale the (Rayleigh) amplitude according to $\gamma_t \mapsto \langle a^2 \rangle^{-1/2} \gamma_t$, then the rescaled field satisfies (2.3) with the form factors equal to unity. In what follows we shall therefore assume the field to be scaled in this way, i.e., $\langle a^2 \rangle = 1$. In the case of a fluctuating number of steps $N \mapsto N_t$ in (2.1), we define the (continuous-valued) cross section as $x_t = \lim_{N_t \to \infty}[N_t / \overline{N}]$. The resultant (normalized) amplitude $\psi_t = \lim_{N\to\infty}[\mathcal{E}^{(N_t)} / \overline{N}]$ therefore has the compound representation

$$\psi_t = x_t^{\frac{1}{2}} \gamma_t, \tag{2.4}$$

where $\gamma_t = \lim_{N\to\infty}[\mathcal{E}_t^{(N_t)} / N_t^{\frac{1}{2}}]$, and in which x_t and γ_t are independent processes. The intensity z_t has the compound representation $z_t = x_t u_t$, where $u_t = |\gamma_t|^2$ is the instantaneous intensity of the component (unit power) Rayleigh process (cf. the analysis of asymptotic behavior and propagators in Secs. III and IV of Field and Tough, 2003b).

It is perhaps worth clarifying at this point the precise meaning and definitions of the various amplitudes that have occurred in the exposition of the random walk model. We begin with $\mathcal{E}$, as the superposition of N random phasors, where N is fixed. For a large population, $N \to \infty$, and the root mean square (rms) of $\mathcal{E}$ tends to infinity. Thus, to obtain a finite resultant in the limit of an asymptotically large number of scatterers, we define a normalized Rayleigh amplitude γ, by dividing through by the rms value $N^{\frac{1}{2}}$. (Equivalently, we could absorb this normalization into the form factors a_j.) The term Rayleigh refers to the fact the the number of scatterers is fixed. In the general case that the scattering population fluctuates in time, we define the normalized amplitude

ψ as in the case of Rayleigh scattering, dividing $\mathcal{E}$ by the rms value $\overline{N^{\frac{1}{2}}}$, where now the number of terms N_t in the random walk fluctuates. Rearranging the resulting expression produces the compound representation of the resultant amplitude (2.4), for a general scattering process. The Rayleigh amplitude is then recovered if the cross section is unity.

The corresponding dynamical situation for weak scattering processes, i.e., where the field ψ_t lies in (weak) superposition with a coherent offset signal ϱ_t, is described in Field and Tough (2005).

III. GENERALIZED POPULATION DYNAMICS

In this section we propose a general scheme for describing scattering/interference of wavelike fields from random media, for which the statistical characteristics of the (scattering) population are taken to be arbitrary. With regard to the cross section and intensity variables, in Bayesian terms one may write $\mathbb{P}(x|z) \propto \mathbb{P}(z|x)\mathbb{P}(x)$ and interpret $\mathbb{P}(z|x)$ as the likelihood function L, $\mathbb{P}(x)$ as the prior P and $\mathbb{P}(x|z)$ as the posterior distribution. In K-scattering the constant (with respect to x) of proportionality is the reciprocal K-distribution for the intensity z. Our development shall entail the following, that we (1) preserve the likelihood L as the Rayleigh distribution, cf. the universality of arguments of central limit theorem type, (2) modify the prior P, i.e., consider general (endogenous) population dynamics appropriate to more complex population processes, under the assumption that x_t remains an Ito process (cf. Field and Tough, 2003a), and (3) preserve the mathematical structure of the random walk model (2.1) describing the resultant amplitude process.

Accordingly we specify that the underlying signal x_t is an Ito process that satisfies the generalized (in the sense of its relationship with the K-scattering model) stochastic differential equation (SDE)

$$\mathrm{d}x_t = \mathcal{A}b_t\,\mathrm{d}t + (2\mathcal{A}\Sigma_t)^{\frac{1}{2}}\,\mathrm{d}W_t^{(x)} \tag{3.1}$$

in which the drift and diffusion parameters b_t, Σ_t are, respectively, (real-valued) stochastic processes, not necessarily Ito processes, adapted to the filtration $\mathcal{F}_t^{(x)}$ corresponding to the Wiener process $W_t^{(x)}$. In other words, the continuous population dynamics is taken to lie within the general category of Ito processes. The special case of a diffusive population behavior arises when the SDE parameters are functions of state, i.e., $b_t = b(t,x_t)$ and $\Sigma_t = \Sigma(t,x_t)$ for given functions $b(\cdot,\cdot)$ and $\Sigma(\cdot,\cdot)$, in which case a corresponding Fokker–Planck description for the time evolution of the probability density is possible (e.g. Risken, 1989). The case of K-scattering (a special type of diffusion model) is obtained by setting $b(t,x) = (\alpha - x)$, $\Sigma(t,x) = x$, and arises as the continuous-valued (large N) limit of the birth–death–immigration (BDI) model (see Bartlett, 1966; Field and Tough, 2003b). We shall not require that x_t be a diffusion in what follows, however. The generalized dynamics of the resultant amplitude process can now be derived according to the scheme outlined at the end of Sec. II. For arbitrary γ_t, x_t an application of Ito's formula to (2.4) yields

$$\frac{\mathrm{d}\psi_t}{\psi_t} = \frac{\mathrm{d}\gamma_t}{\gamma_t} + \frac{\mathrm{d}x_t}{2x_t} - \frac{\mathrm{d}x_t^2}{8x_t^2}. \tag{3.2}$$

This enables the resultant amplitude dynamics to be calculated under the assumption that γ_t is a unit power Rayleigh process according to (2.3), with unit form factors.

Proposition 3.1: *The generalized resultant amplitude dynamics is given by*

$$\frac{\mathrm{d}\psi_t}{\psi_t} = \left[\mathcal{A}\left(\frac{b_t}{2x_t} - \frac{\Sigma_t}{4x_t^2}\right) - \frac{1}{2}\mathcal{B}\right]\mathrm{d}t + \left(\frac{\mathcal{A}\Sigma_t}{2x_t^2}\right)^{\frac{1}{2}}\mathrm{d}W_t^{(x)} + \left(\frac{\mathcal{B}^{\frac{1}{2}}}{\gamma_t}\right)\mathrm{d}\xi_t. \tag{3.3}$$

Observe that $\partial/\partial\mathcal{B}$ acting on the drift/volatility parameters in (3.3) yields expressions that are independent of b_t, Σ_t, as expected from the endogenous specification of population dynamics (3.1). Using the vanishing of the Ito products $\mathrm{d}\xi_t^2$, $\mathrm{d}\xi_t\,\mathrm{d}W_t^{(x)}$ and the property $|\mathrm{d}\xi_t|^2 = \mathrm{d}t$ the above result yields the squared amplitude fluctuations as follows.

Corollary 3.2:

$$\left(\frac{\mathrm{d}\psi_t}{\psi_t}\right)^2 = \frac{\mathcal{A}\Sigma_t}{2x_t^2}\mathrm{d}t, \tag{3.4}$$

$$|\mathrm{d}\psi_t|^2 = \left(\frac{\mathcal{A}\Sigma_t z_t}{2x_t^2} + \mathcal{B}x_t\right)\mathrm{d}t. \tag{3.5}$$

The generalized intensity dynamics can be computed from Proposition 3.1 and the identity $\mathrm{d}z_t \equiv \psi_t\,\mathrm{d}\psi_t^* + \psi_t^*\,\mathrm{d}\psi_t + \mathrm{d}\psi_t\,\mathrm{d}\psi_t^*$.

Proposition 3.3: *The generalized intensity SDE is given by*

$$\mathrm{d}z_t = \left[\mathcal{A}\left(\frac{b_t z_t}{x_t}\right) + \mathcal{B}(x_t - z_t)\right]\mathrm{d}t + (2\mathcal{A}\Sigma_t)^{\frac{1}{2}}\left(\frac{z_t}{x_t}\right)\mathrm{d}W_t^{(x)} + (2\mathcal{B}x_t z_t)^{\frac{1}{2}}\,\mathrm{d}W_t^{(r)}, \tag{3.6}$$

where

$$(\gamma_t^*\,\mathrm{d}\xi_t + \gamma_t\,\mathrm{d}\xi_t^*) \equiv \left(\frac{2z_t}{x_t}\right)^{\frac{1}{2}}\mathrm{d}W_t^{(r)}. \tag{3.7}$$

The intensity squared volatility is

$$\mathrm{d}z_t^2 = 2z_t\left(\frac{\mathcal{A}\Sigma_t z_t}{x_t^2} + \mathcal{B}x_t\right)\mathrm{d}t. \tag{3.8}$$

The propositions above reduce to the appropriate expressions in *K*-scattering (cf. Field and Tough, 2003a, 2003b) for appropriate choice of b, Σ. In respect of the generalized resultant phase dynamics, recall (Field and Tough, 2003b) the identity for the phase differential in terms of the amplitude

$$\mathrm{d}\theta_t \equiv \Im\left[\frac{\mathrm{d}\psi_t}{\psi_t} - \frac{1}{2}\left(\frac{\mathrm{d}\psi_t}{\psi_t}\right)^2\right], \tag{3.9}$$

where $\Im$ denotes the imaginary part. Since the right-hand side of (3.4) is *real* valued, only the first term on the right-hand side of (3.9) contributes to $\mathrm{d}\theta_t$, in respect of which

$$\Im\left[\frac{\mathrm{d}\psi_t}{\psi_t}\right] = \frac{\mathcal{B}^{\frac{1}{2}}}{2i}\left(\frac{\mathrm{d}\xi_t}{\gamma_t} - \frac{\mathrm{d}\xi_t^*}{\gamma_t^*}\right). \tag{3.10}$$

Thus we can deduce the phase behavior for a general population.

Proposition 3.4: *The generalized resultant phase dynamics is given by the SDE,*

$$\mathrm{d}\theta_t = \left(\frac{\mathcal{B}x_t}{2z_t}\right)^{\frac{1}{2}}\mathrm{d}W_t^{(\theta)}, \tag{3.11}$$

where $W_t^{(\theta)}$ *satisfies*

$$\frac{1}{i}(\gamma_t^*\,\mathrm{d}\xi_t - \gamma_t\,\mathrm{d}\xi_t^*) \equiv \left(\frac{2z_t}{x_t}\right)^{\frac{1}{2}}\mathrm{d}W_t^{(\theta)}. \tag{3.12}$$

Observe that, in contrast to the situation for the resultant amplitude and intensity SDEs (3.3) and (3.6), this is *functionally* identical to the corresponding result in *K*-scattering (i.e., independent of the population parameters b_t, Σ_t), the essential difference lying in the *evolutionary* structure of the processes x_t, z_t. Observe from (3.7) and (3.12) that the radial and angular fluctuations in the

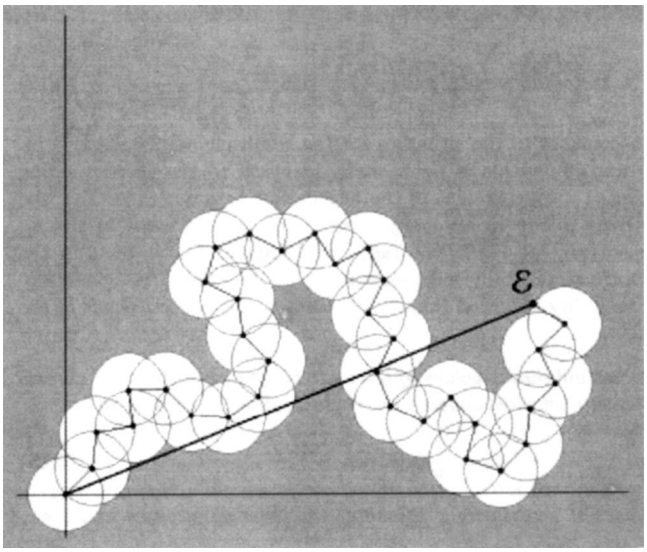

FIG. 1. Geometry of random walk for generalized scattering process—generically (almost everywhere) each component phasor point lies on two circles.

resultant amplitude are statistically independent in the general case. The squared phase volatility obtained from (3.11) leads to the central result of the paper.

Theorem 3.5: *The instantaneous values of the scattering cross section are observable through the intensity-weighted squared phase fluctuations according to*

$$x_t = \frac{2}{\mathcal{B}} z_t \, \mathrm{d}\theta_t^2 / \mathrm{d}t \tag{3.13}$$

if x_t is an Ito process, not necessarily a diffusion, and throughout space and time.

The (experimental) significance of this result is that the relation (3.13) is exact and moreover independent of the dynamics of x_t. The result resembles (but is distinct from) the minimal variance of the intensity-weighted phase derivative discussed in Jakeman *et al.*, (2001), for differentiable processes. In the present situation however, the processes considered are not differentiable, and instead the *squared* phase differential arises. Since the elements of the random walk model (2.1), preserved by the generalized framework given in the exposition of this section for dealing with general populations, are the only essential ingredients involved here, the result is geometrical in nature (cf. Fig. 1). With regard to this geometry, the derivations above show that the dynamics of the resultant field are not affected if the radii for each component phasor are drawn independently from an arbitrary probability distribution. (The result of the theorem was anticipated from a physical point of view previously in Field and Tough, 2003a; see discussion following Proposition 4.1. therein.)

A slight complication is posed in the computation of $\mathrm{d}\theta_t^2$ from experimental data, owing to the discontinuous-valued behavior of θ_t at coordinate intervals of 2π. This is resolved by instead using the (continuous-valued) phase-wrapped process $w_t = \exp(i\theta_t)$, whose stochastic differential is $\mathrm{d}w_t = \exp(i\theta_t)\left[i\,\mathrm{d}\theta_t - \frac{1}{2}\mathrm{d}\theta_t^2\right]$, which enables the squared phase fluctuations to be computed from the single-valued process w_t via $|\mathrm{d}w_t|^2 = \mathrm{d}\theta_t^2$. In respect of discrete-time implementation, we remark that if W_t is a Wiener process, then $\delta W_t = W_{t+h} - W_t$ is normally distributed as $\mathcal{N}(0,h)$, so that its square is a chi-squared $\chi^2(1)$ variable. The sum of n such variables is therefore distributed as $\chi^2(n)$, from which an estimate of $\mathrm{d}q_t^2$ from δq_t can be obtained (via the weak law of large numbers) by considering the interval from t to $t+\delta t$ divided into n pulse intervals each of length

h and letting $n\to\infty$ before taking the limit $\delta t\to \mathrm{d}t$ (Howison, private communication; see also Higham, 2004 and the exposition to Sec. 4 in Field and Tough, 2003a). In this respect we observe the following significant result.

Proposition 3.6: *In order to achieve an improved signal to noise ratio (SNR), it is sufficient merely to increase the pulse-rate n, without necessarily requiring a high amplitude signal* x_t.

The implications of this idea are discussed in Sec. IV in an experimental context, and illustrated with some synthetically generated data. The structure of (3.1) and (3.6) could be interpreted as an instance of the generalized Kalman filter (see Chap. 6 in Oksendal, 1998) in which the unknown state x_t is to be estimated from observations of z_t. It is significant that in this situation the dynamics of the filter stem from first principles and that the resulting statistics are non-Gaussian (notwithstanding the Gaussian nature of the Wiener process). The noise originates through two components, namely the intrinsic system noise $W_t^{(x)}$ which derives from fluctuations in the (endogenously specified) population model, and the measurement noise ξ_t arising from the particulars of the wavelike interference effects. The latter should be viewed as an exogenous device whose purpose is to probe the true underlying state of the system that is of primary interest, in this case the signal x_t.

Our development has demonstrated (an instance of) how, instead of attempting to filter the received signal to eliminate the noise (e.g., via a Kalman or particle filter), one can exploit the statistical fluctuation properties of the noise in order to infer the *exact* values of the underlying signal. This notion might appropriately be termed an *ideal filter* and constitutes a shift of viewpoint from the various conventional approaches to enhancement of signal to noise.

IV. EXPERIMENTAL IMPLICATIONS

A study of some synthetically generated data provides a clear illustration of the consequences of Theorem 3.5 in a variety of experimental contexts. The theoretical results are conveniently substantiated using synthetic data, as such enables direct verification of the accuracy of the state estimation from the observations, the precise value of the hidden state being known from the simulation. One can then compare the values of the state inferred from the observations alone, with the exact values of the underlying hidden state recorded in the simulation. The cross section was chosen to satisfy the SDE (3.1) with $b(t,x)=\alpha-x$, $\Sigma(t,x)=x$ so that x_t is a gamma variate and the process thus generated is appropriate to the types of scattering data found in radar applications (cf. Field and Tough, 2003a). Resultant amplitude data was simulated via integration of (3.3), which is achieved most effectively by a separate numerical integration of the (independent) component SDEs (2.3) and (3.1). We emphasize however, that the same types of numerical results as demonstrated below should hold for an arbitrary population, as shown theoretically in Theorem 3.5. For the purposes of the simulation, α was chosen to be large, to avoid numerical difficulties that can arise due to the singular behavior in the phase fluctuations at zeros of the intensity, implied by (3.11). The results of the simulation are provided in Fig. 2, which shows time series for the observed intensity, the exact cross section generated in the simulation (i.e., the unknown state one is trying to estimate), and the values of this state inferred from the observations of the scattered amplitude alone. The estimate of the state follows from Theorem 3.5 which, for discretely sampled data, implies

$$z_i\delta\theta_i^2 \propto x_i n_i^2, \tag{4.1}$$

where i is a discrete time index and $\{n_i\}$ are an independent collection of $\mathcal{N}(0,1)$ distributed random variables. Applying a smoothing average $\langle\cdot\rangle_\Delta$ to the left-hand side (the observations) of (4.1) with window $\mathbf{\Delta}=[t_0-\Delta,t_0+\Delta]$ yields an approximation to x_{t_0}, with an error that tends to zero as the number of pulses inside $\mathbf{\Delta}$ tends to infinity and $\Delta\to 0$ (see discussion of χ^2 statistic following Theorem 3.5).[2] On the other hand, smoothing the z_t time series, for any choice of parameter Δ, does not yield the desired close correlation with x_t; indeed any such attempt to

[2]We assume here that the sample paths of x_t are continuous, which is a consequence of (3.1).

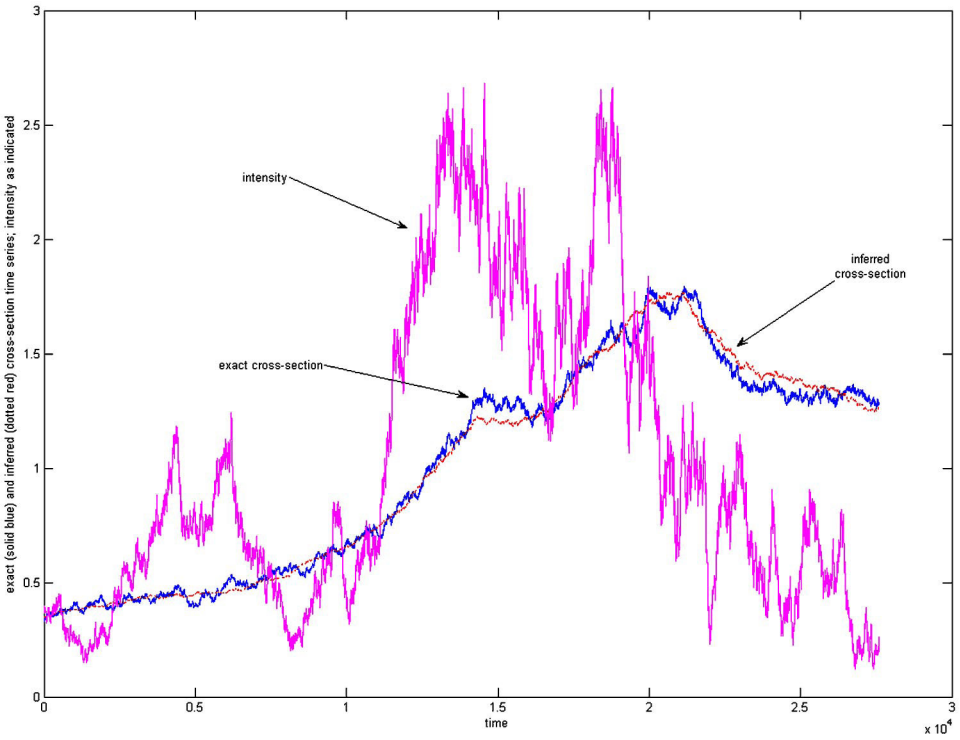

FIG. 2. (Color online) Estimation of the scattering cross section/population after relaxation time T through the effect of phase decoherence. (For parameter values $\alpha=10$, $\Delta=1200$ pulses, $\mathcal{A}=10^{-5}$, $\mathcal{B}=10^{-4}$ the figure shows a statistical correlation between the exact and inferred cross-section time series of 0.9954.)

decorrelate the speckle pattern merely produces an intensity profile with the same general shape as the original z_t, with oscillations on a time scale approximately equal to Δ.

The application of related earlier ideas in SDE theory to optical propagation and radar scattering has been reported in Sec. 4 of Field and Tough, (2003a). The current results should be of additional value in these types of experiments, through the ability to estimate the underlying scattering cross section for general scattering populations, in real time. When applied to experimental data, the results herein provide means for studying the behavior of random media based on statistical analysis of the inferred cross section alone, which has hitherto been regarded as the hidden state of the system. The electromagnetic scattering process should then appropriately be viewed as a secondary exogenous device, whose purpose is merely to extract the real time behavior of the underlying scattering cross section, where the latter is the object of primary interest.

Our results also suggest the application to the physics of magnetic resonance (MR) imaging and spectroscopy. The random medium (e.g., brain tissue) lies inside a background magnetic field B_0, with which the constituent (proton) spin vectors are aligned, in their minimum energy configuration. An applied RF pulse causes resonant absorption to occur, so that the spins realign, typically at a pulse flip angle of 90° to B_0. Radiation of this absorbed energy gives rise to the received MR signal (the free induction decay or FID), which is detected through the generation of electromotive force in a coil apparatus, due to the time varying local magnetic field.[3] The MR signal has the usual in-phase (I) and quadrature-phase (Q) components familiar from radio theory, and thus corresponds to the amplitude process $\Psi=I+iQ$ for each point in space. For a perfectly homogeneous (total) magnetic field throughout the medium, each spin vector precesses at the Larmor frequency ω_0 about the longitudinal axis, where ω_0 is given by the Larmor equation ω_0

[3]This effect is the result of Faraday's law, i.e., Maxwell's vector equation $\nabla\times\mathbf{E}=-\partial\mathbf{B}/\partial t$ integrated around a loop.

$= \gamma B_0$ and γ is the (local) gyromagnetic ratio (e.g., Brown and Semelka, 2003). (In the radar scattering situation described above, ω_0 corresponds to the Doppler frequency, arising from bulk wave motion in the scattering surface.) However, the local inhomogeneities in the net magnetic field, due to the local magnetic properties of the medium, give rise to a process known as spin–spin or $T2$ relaxation constituting the (random) exchange of energy between neighboring spins. These local perturbations in the total magnetic field can reasonably be considered as independent for each component spin, so that the dynamics of each spin vector can be modeled as a phase diffusion process with (transverse) resultant as in (2.1) and phase initializations $\{\Delta^{(j)}\}$ equal. After sufficient relaxation time $t \geqslant T$ has elapsed, phase decoherence occurs. In principle this enables the spin population to be tracked according to Theorem 3.5, and thus real time MR images to be generated. This application is explored in greater depth, and from a less detailed mathematical perspective, in Field, (2005).

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VSI$_j$ space–times and the ϵ-property

N. Pelavas, A. Coley, and R. Milson
Department of Mathematics and Statistics, Dalhousie University, Halifax, Nova Scotia

V. Pravda and A. Pravdová
Mathematical Institute, Academy of Sciences, Žitná 25, 115 67 Prague 1, Czech Republic

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We investigate Lorentzian space–times where all zeroth and first order curvature invariants vanish and discuss how this class differs from the one where all curvature invariants vanish (VSI). We show that for VSI space–times all components of the Riemann tensor and its derivatives up to some fixed order can be made arbitrarily small. We discuss this in more detail by way of examples. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1904707]

I. INTRODUCTION

Recently it was proven that in four-dimensional Lorentzian space–times all of the scalar invariants constructed from the Riemann tensor and its covariant derivatives are zero if and only if the space–time is of Petrov (P)-type III, N or O, all eigenvalues of the Ricci tensor are zero and hence of Plebański–Petrov (PP)-type N or O (Ref. 1) and the common multiple null eigenvector of the Weyl and Ricci tensors is geodesic, shear-free, expansion-free, and twist-free; let us refer to these space–times as vanishing scalar invariant (VSI) space–times. VSI space–times include the well-known *pp*-wave space–times.[2]

Since all of the scalar curvature invariants vanish, all VSI space–times are exact solutions of higher-order Lagrangian based theories (in which the action is given by higher order scalar corrections to the usual general relativistic action based on the Ricci scalar). It has subsequently been argued that, as in the case of *pp*-waves, VSI space–times are exact solutions in string theory,[3–5] when supported by appropriate bosonic massless fields of the string (such as, for example, a dilaton and an antisymmetric massless field). Solutions of classical field equations for which the counter terms required to regularize quantum fluctuations vanish (i.e., they suffer no quantum corrections to all loop orders) are also of importance because they offer insights into the behavior of the full quantum theory.[6]

In particular fundamental field theories only certain specific types of higher order corrections occur (cf. Refs. 7–9), and so for a space–time to be a solution of a particular field theory to all orders, with a specific effective action containing only certain higher order correction terms, it may not be necessary for *all* curvature invariants to vanish. Consequently it is also of interest to determine the set of spacetimes for which (only) the zeroth order curvature invariants vanish (i.e., algebraic scalar invariants constructed from the Riemann tensor), denoted VSI$_0$, those space–times for which (only) the zeroth *and* first order curvature invariants vanish (i.e., scalar invariants constructed from the Riemann tensor and its first covariant derivative), denoted VSI$_1$, and so on. In fact, it was proven in Ref. 1 that if all of the zeroth, first, and second order curvature invariants vanish, then necessarily all scalar curvature invariants vanish; so that VSI$_2$ is equivalent to the set of VSI space–times.

Let us first recall some properties of VSI space–times. Utilizing a complex null tetrad in the Newman–Penrose (NP) formalism it was shown that for P-types III and N the repeated null vector of the Weyl tensor ℓ^α is geodesic, shear-free, expansion-free, and twist-free (and the NP coefficients κ, σ, and ρ are consequently zero), and the Ricci tensor has the form

$$R_{\alpha\beta} = -2\Phi_{22}\ell_\alpha\ell_\beta + 4\Phi_{21}\ell_{(\alpha}m_{\beta)} + 4\Phi_{12}\ell_{(\alpha}\overline{m}_{\beta)}, \tag{1}$$

in terms of the nonzero Ricci components Φ_{ij}. For P-type O, the Weyl tensor vanishes and so it suffices that the Ricci tensor has the form (1). All of these space–times belong to Kundt's class,[10] and the metrics for all VSI space–times are displayed in Ref. 1. The generalized *pp*-wave solutions are of P-type N, PP-type O (so that the Ricci tensor has the form of null radiation) with $\tau=0$, and admit a covariantly constant null vector field.[2] The Ricci tensor (1) has four vanishing eigenvalues, and the PP-type is N for $\Phi_{12}\neq 0$ or O for $\Phi_{12}=0$. It is known that the energy conditions are violated in the PP-type N models[11] and hence attention is usually concentrated on the more physically interesting PP-type O case, which in the nonvacuum case corresponds to pure radiation.

It is well known that the necessary and sufficient conditions for space–times for which the zeroth order algebraic scalar curvature invariants vanish (VSI_0) are of P-type III, N or O and PP-type N or O. Moreover, the repeated principal null direction of Weyl must be aligned with an eigenvector of the Ricci tensor. The last condition follows from the vanishing of the mixed invariants (see Sec. 3.1 of Ref. 1). Next we determine the VSI_1 space–times.

II. VSI_1

We begin by assuming VSI_0 and determine the conditions which imply VSI_1. From the Bianchi identities it follows for VSI_0 that $\kappa=0$. The invariants used here are all constructed from spinors that are symmetrized before and after contractions. Since contractions are always performed with symmetrized spinors we need only give the number of indices contracted between any two spinors. In particular, we shall make use of the following invariant, $I_1\equiv(\nabla\Psi)^2(\nabla\overline{\Psi})^2$. Here $(\nabla\Psi)^2$ is used to indicate the contraction over four indices of two copies of $\nabla_{(AA'}\Psi_{BCDE)}$. The result is then symmetrized and contracted with its conjugate to give I_1.

A. Petrov-type III

Using $\Psi_3\neq 0$ with PP-type N or O, we have from the Bianchi identities that $\sigma\Psi_3=\rho\Phi_{12}$ and $\kappa=0$. Applying $\kappa=0$ throughout, we find that two of the Bianchi identities yield the following relation:

$$D\Psi_3 = \rho\Phi_{21} + \overline{\sigma}\Phi_{12} + 2(\rho-\varepsilon)\Psi_3. \tag{2}$$

Computing I_1 and using (2), we obtain

$$I_1 = \tfrac{576}{625}[81(\sigma\overline{\sigma}\Psi_3\overline{\Psi}_3)^2 + \sigma\overline{\sigma}\Psi_3\overline{\Psi}_3 X\overline{X} + (X\overline{X})^2], \tag{3}$$

where $X=\rho\Phi_{21}+\overline{\sigma}\Phi_{12}+5\rho\Psi_3$.

The vanishing of I_1 necessarily implies that $\sigma=0$, thus from the Bianchi identities $\rho\Phi_{12}=0$. If $\rho=0$ we get VSI. If $\Phi_{12}=0$ then (3) becomes $I_1=576(\rho\overline{\rho}\Psi_3\overline{\Psi}_3)^2$ which vanishes when $\rho=0$, giving VSI with PP-type O (null radiation).

B. Petrov-type N

Using $\kappa=0$ in the Bianchi identities we find that $\rho\Phi_{21}=-\overline{\sigma}\Phi_{12}$ and $\rho\Phi_{12}=0$. Therefore if $\Phi_{12}\neq 0$ then $\rho=0$ implies that $\sigma=0$, hence we recover VSI. If $\Phi_{12}=0$ then two of the Bianchi identities combine to yield $\sigma\Psi_4=\rho\Phi_{22}$. The conditions $\kappa=\Phi_{12}=0$ and $\sigma\Psi_4=\rho\Phi_{22}$ are necessary to characterize the VSI_1 PP-O null radiation models. Suppose that $\sigma=0$; then either $\rho=0$ and we have VSI, or $\rho\neq 0$ and $\Phi_{22}=0$ which necessarily characterizes the vacuum VSI_1 models. (See Ref. 12.)

To show sufficiency, we assume $\kappa=\Phi_{12}=0$ and then note that the remaining curvature components, Ψ_4 and Φ_{22}, both have boost weight -2. In the compacted (GHP) formalism[13] the relevant operators have boost weight 0 or 1 and the only spin coefficients with positive boost

weight are σ and ρ with weights 1; it follows that the covariant derivative of either Ψ_{ABCD} or $\Phi_{AB\dot{A}\dot{B}}$ will have components with only negative boost weight. Therefore, all zeroth and first order curvature invariants vanish, implying VSI_1.

C. Petrov-type O

The freedom in the frame can be used here to consider PP-type N and PP-type O null radiation separately, and it follows trivially from the Bianchi identities that $\kappa=\sigma=\rho=0$, so that we obtain VSI. Therefore all Petrov type O VSI_0 are VSI from the Bianchi identities.

In summary, the only space–times in the class VSI_1 that are not VSI are of P-type N and all have $\kappa=\Phi_{12}=0$. The first of these VSI_1 models have $\sigma\Psi_4=\rho\Phi_{22}$; exact solutions were found by Plebański.[11] The second of the VSI_1 models have $\sigma=\Phi_{22}=0$, and these are the vacuum Petrov-type N solutions with $\rho=\Theta+i\omega\neq 0$. If $\omega=0$ these solutions belong to the Robinson–Trautman class and all are known.[11] If $\omega\neq 0$ then the only twisting, vacuum, P-type N solution known is that of Hauser.[11]

There are other cases that may also be of interest. Notice the example in Ref. 14 in which there are scalar curvature invariants that are nonzero (constant, depending on a cosmological constant) while all higher order scalar curvature invariants are zero.

III. ε-PROPERTY

A scalar invariant for a matrix is a polynomial of the matrix entries that is invariant with respect to all changes of basis. It is easy to characterize all such invariants. Let M be an $n\times n$ matrix. The characteristic polynomial of M is given by

$$p_M(x)=\det(xI-M)=x^n+\sum_{j=1}^{n}(-1)^j\sigma_j(M)x^{n-j}.$$

The expressions $\sigma_j(M)$ are called the elementary symmetric polynomials of M and are the scalar invariants of M [$\sigma_1(M)$ is just the trace of M and $\sigma_n(M)$ is the determinant]. All other scalar invariants can be given as polynomials of $\sigma_1(M),\sigma_2(M),\ldots,\sigma_n(M)$. A matrix M for which the characteristic polynomial is just x^n is nilpotent. Now a matrix with the ε-property, i.e., the property that all entries can be made smaller than every given ε by a change of basis, must be nilpotent.[15] The converse is also true, that is, every nilpotent matrix necessarily possesses the ε-property. Therefore, a matrix is VSI_0 if and only if it is nilpotent. Hence we anticipate that VSI space–times will have the ε-property, and this is what we prove next.

Theorem: For and only for VSI space–times (in arbitrary dimension D and C^∞ metric) one can find, for arbitrarily large N and for arbitrarily small ε, a tetrad in which all components of the Riemann tensor and its derivatives up to order N are smaller than ε.

Proof: For non-VSI space–times there always exist a nonvanishing curvature invariant. Its value of course does not depend on the choice of the tetrad and thus there does not exist a tetrad with the desired property. It was proven in Ref. 1 that in four-dimensional VSI space–times the boost weight of all components of the Riemann tensor and its derivatives is negative. Thus with an appropriate boost we can make all components of the Riemann tensor and its derivatives up to a desired order N arbitrarily small.[16,17] □

It was pointed out by Penrose in Ref. 18 that P-types III and N have "the property that gravitational density can be made as small as we please by a suitable choice of time axis (following the wave)." It turns out that for VSI_0 space–times, not only the gravity density but the energy-momentum tensor can be made arbitrarily small by an appropriate boosting of the frame. In the case of VSI_1 space–times we can also make the first derivatives of the Riemann tensor essentially undetectable, and for VSI space–times it is possible to do this for arbitrarily large derivatives as well. Since experiments measure tetrad components of the Riemann tensor and as every experiment has some sensitivity limit, we can effectively, by an appropriate boost, "locally transform away" the Riemann tensor and its derivatives.

It is of interest to consider if any of the VSI space–times satisfy the following stronger ε-property. We shall say that the Riemann tensor has the uniform ε-property if, given an arbitrarily small ε, there exists a tetrad in which the components of the Riemann tensor and all of its derivatives are smaller than ε. Not all VSI space–times satisfy the uniform ε-property; this is shown by considering P-type N vacuum VSI space–times with $\tau \neq 0$. Let us denote

$$X_k = C_{abcd;e_1\cdots e_k} n^a \bar{m}^b n^c \bar{m}^d m^{e_1} \cdots m^{e_k}, \quad Y_k = C_{abcd;e_1\cdots e_k} \delta(n^a \bar{m}^b n^c \bar{m}^d m^{e_1} \cdots m^{e_k}). \tag{4}$$

By induction on k we shall show that the component $C_{2424;3\cdots 3} = X_k = -k!\,\tau^k \Psi_4$ for all orders k. From Ref. 1 we have the following relations:

$$\kappa = \sigma = \rho = \epsilon = 0, \quad \tau = \pi = 2\beta = 2\alpha, \quad \lambda = \mu = (2/3)\gamma, \tag{5}$$

where all of these spin coefficients are real, and ν is nonzero and complex as well. The Bianchi identities and NP equations then give

$$\delta\Psi_4 = -\tau\Psi_4, \quad D\Psi_4 = 0, \quad \delta\tau = \tau^2, \quad D\tau = 0. \tag{6}$$

It can be shown directly that $X_1 = C_{2424;3} = -\tau\Psi_4$, and using strong induction we assume that X_k has the required form. In general, the following recursive relation holds $X_k = \delta X_{k-1} - Y_{k-1}$, consequently this implies that $Y_{k-1} = 2(k-1)!\,\tau^k \Psi_4$. Similarly, $X_{k+1} = \delta X_k - Y_k$, and on expanding Y_k we observe that it is composed of terms with boost weight -2 and -1, but the boost weight -1 terms vanish as a result of a similar proof found in Ref. 1. To show this we note that in this case we have

$$\text{Þ}\Psi_4 = 0, \quad \text{Þ}\tau = 0, \quad \text{Þ}\rho' = -2\tau^2 = \text{Þ}\sigma', \quad \text{Þ}\kappa' = 6\tau\rho' \tag{7}$$

with commutators [19]

$$\text{Þ}\check{\partial} - \check{\partial}\text{Þ} = \tau\text{Þ}, \quad \text{Þ}\text{Þ}' - \text{Þ}'\text{Þ} = 2\tau(\check{\partial} + \check{\partial}') - (p+q)\tau^2.$$

Assuming that η is a tetrad component of the Weyl tensor of arbitrary order k with boost weight -2 such that $\text{Þ}\eta = 0$, it is straightforward to show that the following boost weight -1 scalars,

$$\text{Þ}^3(\kappa'\eta), \quad \text{Þ}^2(\sigma'\eta), \quad \text{Þ}^2(\rho'\eta), \quad \text{Þ}(\tau\eta), \quad \text{Þ}(\tau'\eta), \quad \text{Þ}\check{\partial}\eta, \quad \text{Þ}\check{\partial}'\eta, \quad \text{Þ}^2\text{Þ}'\eta$$

all vanish. Therefore Y_k consists of only the boost weight -2 term, hence we have that $Y_k = -2\tau X_k$ and thus $X_{k+1} = -(k+1)!\,\tau^{k+1}\Psi_4$. Since the component $C_{2424;3\cdots 3}$ can be made arbitrarily large by increasing the order, in this case the Riemann tensor cannot therefore satisfy the uniform ε-property.

A subclass of the VSI space–times for which the uniform ε-property is satisfied are those in which $\nabla^{(N)} R_{abcd} = 0$, where (N) denotes N covariant derivatives. Since only a finite set of components of the Riemann tensor and its derivatives are nonzero, then by an appropriate boost all components of the Riemann tensor and its derivatives can be made smaller than ε. In the case of $N=1$ we have the VSI symmetric spaces in which $\nabla_e R_{abcd} = 0$ (cases in which $N>1$ will be referred to as higher order symmetric spaces); we shall show that this class is nonempty. We consider the following line-element:

$$\mathrm{d}s^2 = 2h\,\mathrm{d}u^2 + 2\,\mathrm{d}u\,\mathrm{d}v - \mathrm{d}x^2 - \mathrm{d}y^2 \tag{8}$$

and solve $\nabla_e R_{abcd} = 0$, assuming that $h = h(u,x,y)$. After an appropriate coordinate transformation, which preserves the form of the metric, we find that $h = k(x^2+y^2) + c^2(x^2-y^2)$ where k and c are arbitrary constants. Using the NP tetrad $\ell^a = \delta^a_v, n^a = \delta^a_u - h\delta^a_v$ and $m^a = (i\delta^a_x - \delta^a_y)/\sqrt{2}$ it follows that the only nonvanishing spin coefficient is ν with Φ_{22} and Ψ_4 being constants. If $k=0$ and $c \neq 0$ we recover the P-type N vacuum symmetric space,[11] if $k \neq 0$ and $c=0$ we obtain the P-type O, PP-type O null radiation symmetric space.[11] These VSI symmetric spaces clearly satisfy the uniform ε-property. In P-type III it is known that no symmetric spaces exist;[11] however, the possibility

remains that P-type III VSI space–times satisfying the uniform ε-property may exist (for example, if $\nabla^{(N)}R_{abcd}=0$ for $N>1$).

To illustrate a higher order symmetric space, consider (8) with $h=g(u)(x^2-y^2)$, a subclass of the P-type N vacuum VSI space–times with $\tau=0$. Next, apply a boost so that $l'=Al$ and $n'=A^{-1}n$ where the boost parameter $A=Cg'(u)$ with C constant. Dropping the primes and working in the boosted frame we have the following nonvanishing scalars, $\nu=-\sqrt{2}g(y+ix)/A^2$, $\gamma=A'/(2A^2)$, and $\Psi_4=-2g/A^2$. It follows that the Weyl tensor has the form [20]

$$C_{abcd}=\tfrac{1}{2}C_{2i2j}\{\ell_a m_b^{(i)}\ell_c m_d^{(j)}\}, \tag{9}$$

where $i,j=3,4, m^{(3)}=\overline{m}$, and $m^{(4)}=m$, the only nonvanishing Weyl tetrad components are $C_{2i2i}=2g/A^2$. Let $X_0=C_{2i2i}$, then (9) is $C_{abcd}=\frac{1}{2}X_0\{\ell_a m_b^{(i)}\ell_c m_d^{(i)}\}$ and

$$\nabla_e C_{abcd}=\tfrac{1}{2}X_1\ell_e\{\ell_a m_b^{(i)}\ell_c m_d^{(i)}\}, \tag{10}$$

where $X_1=\Delta X_0+4\gamma X_0$. It can be shown that the nth order covariant derivative of the Weyl tensor has the following simple form:

$$\nabla_{e_n}\cdots\nabla_{e_1}C_{abcd}=\tfrac{1}{2}X_n\ell_{e_n}\cdots\ell_{e_1}\{\ell_a m_b^{(i)}\ell_c m_d^{(i)}\}. \tag{11}$$

Proceeding inductively, we obtain the following recurrence relation $X_n=\Delta X_{n-1}+2(n+1)\gamma X_{n-1}$. From (11) we have that the only nonvanishing nth order tetrad components of the Weyl tensor will be $C_{2i2i;2\cdots2}$. Again, by induction, one can show that $X_n=2A^{(n-1)}/(CA^{n+2})$ for all $n\geqslant 1$ (denoting the $n-1$ derivative of A as $A^{(n-1)}$ and $A^{(0)}=A$).

We now have an expression for the nth order derivatives of the tetrad components of the Weyl tensor

$$C_{2i2i;2\cdots2}=\frac{2g^{(n)}}{(Cg')^{n+2}}, \tag{12}$$

where it is assumed that $g'\neq 0$, otherwise the boost is degenerate. Therefore, for any $n\geqslant 2$ we can obtain an nth order symmetric space simply by setting $g(u)$ to be any polynomial in u of degree $n-1$. All of these VSI space–times will satisfy the uniform ε-property; more generally this is also satisfied if there exists a constant M such that $|g^{(n)}|\leqslant M$ for all n and $g'\neq 0$. On the other hand, we can use (12) to find examples of VSI space–times that do not satisfy the uniform ε-property. It is known [21] that every geodesic of (8) is either of type 1 or type 2, where type 1 refers to geodesics in the 2-surface u and ν constant and type 2 refers to geodesics in the 2-surface x and y constant. Let us consider type 2 geodesics, and set $x=x_0$, $y=y_0$. We find that the tangent vectors are given by $w^a=(a,b/(2a)-ag(u)(x_0^2-y_0^2),0,0)$ and parametrized by u. Here, $\dot{u}=a$ is a constant and $b=1$ or 0 for timelike or null geodesics, respectively. The NP tetrad defined above is parallel propagated along such geodesics, hence from (12) if the uniform ε-property is not satisfied at some order k then we obtain a parallel propagated curvature singularity of order k. That is, the curvature components of order k in a parallel propagated frame become unbounded along the geodesic; when $k=0$ we recover the definition[22] of a parallel propagated curvature singularity. In Ref. 23, geodesic motion in vacuum Kundt-type N solutions with $\tau\neq 0$ have revealed the existence of parallel propagated curvature singularities of order 0.

IV. CONCLUSION

We have determined the necessary and sufficient conditions that characterize VSI$_1$ space–times. Assuming VSI$_0$, we have shown that in P-type III, VSI$_1$ implies VSI and in P-type O, VSI$_0$ implies VSI. The only proper VSI$_1$ space–times occur in P-type N and PP-type O with $\kappa=\Phi_{12}=0$. In addition, the nonvacuum VSI$_1$ space–times are further characterized by $\sigma\Psi_4=\rho\Phi_{22}$, and the vacuum space–times have $\sigma=\Phi_{22}=0$. It has been shown that the ε-property offers an alternative characterization of the VSI space–times, in the sense that only for VSI space–times can a tetrad be found in which the Riemann tensor and its derivatives up to any fixed order can be made

arbitrarily small. A strengthening of the ε-property leads us to define the uniform ε-property; this condition determines a subclass of the VSI space–times where there exists a tetrad in which the components of the Riemann tensor and all of its derivatives can be made arbitrarily small. Some examples of VSI space–times satisfying the uniform ε-property have been presented.

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The Maurer–Cartan structure of BRST differentials

Jining Gao
Department of Mathematics, North Carolina State University, Raleigh, North Carolina 27695-8205

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In this paper, we construct a sequence of generators of the BRST complex and reformulate the BRST differential so that it acts on elements of the complex much like the Maurer–Cartan differential acts on left-invariant forms. Thus our BRST differential is formally analogous to the differential defined on the BRST formulation of the Chevalley–Eilenberg cochain complex of a Lie algebra. Moreover, for an important class of physical theories, we show that in fact the differential is a Chevalley–Eilenberg differential. As one of the applications of our formalism, we show that the BRST differential provides a mechanism which permits us to extend a nonintegrable system of vector fields on a manifold to an integrable system on an extended manifold. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1904708]

I. INTRODUCTION

Homological algebra has become an indispensable tool for the rigorous formulation of a wide variety of developments in theoretical physics. Applications of these techniques to physics has become so pervasive that they have gradually become identified as a new category of mathematical physics which has been called "cohomological physics" (Refs. 1, 3, and 9). One of the fruitful branches of this theory is the "cohomology" formulation of the BRST theory of constraints. Indeed the point of BRST theory is to replace the cohomology of the reduced space of a physical theory by the cohomology of a homological resolution of the space P being constrained.

In more detail, assume that P is a symplectic manifold and that one has a system of first class constraints on P. Let Σ denote the constraint surface defined as the set of zeros of the constraints. These constraints may or may not be independent. If they are independent they are called irreducible constraints and otherwise they are reducible. The Hamiltonian vector fields of the symplectic manifold P define a possibly singular foliation of Σ and the smooth functions on Σ which are constant on the leaves of this "foliation" are said to be gauge invariant and are called the observables of the theory. There is a differential d, called the longitudinal differential, defined on a certain (dual) Chevalley–Eilenberg complex with coefficients in the algebra $C^\infty(\Sigma)$ whose cohomology in degree zero in the irreducible case is the space of observables. It is clear in the literature that the zero degree cohomology of a certain complex is the space of observables but it is not clear that the complex is a Chevalley–Eilenberg complex and that the longitudinal differential is a Maurer–Cartan differential. These facts are established here in a rigorous manner.

BRST symmetry was developed in order to replace the original gauge symmetry on the constraint surface by a symmetry on the entire phase space P in such a manner that the longitudinal differential d could be extended to a differential S called the BRST differential to be defined on an enlarged complex in such a way that the BRST cohomology in degree zero is precisely the set of observables on Σ. The procedure is nontrivial even in the irreducible case but even more convoluted in the reducible case. An interesting question has to do with whether the BRST differential is a Maurer–Cartan differential (in the sense defined in Sec. II) and whether or not it is actually a Chevalley–Eilenberg differential defined on a (dual) Chevalley–Eilenberg complex as was the case for the longitudinal differential in the irreducible case.

Throughout the paper we almost always use the term BRST to refer to the version developed by Batalin, Fradkin, and Vilkovisky (Refs. 5 and 7) since our differentials are usually defined via an antibracket. This convention is in harmony with the usage of Henneaux and Teitelboim.[6]

The second section is devoted mainly to showing that in the case of irreducible constraints the BRST differential S is in fact a Maurer–Cartan differential and that it is a (dual) Chevalley–Eilenberg differential defined on a Chevalley–Eilenberg complex. Throughout the paper we restrict our attention to bosonic constraints for simplicity of exposition. It is shown that in the case one has a Hamiltonian system subject to bosonic irreducible constraints that the fact that $S^2=0$ implies the existence of a possibly singular "foliation" of the phase space P which agrees with the "foliation" of the constrained space defined by gauge symmetries. Generally, the BRST differential has an expansion

$$S = \delta + d + s_1 + \cdots + s_n + \cdots .$$

The Koszul–Tate differential δ and the longitudinal differential d are well understood but the other terms of the expansion are less well understood. We completely characterize s_1 in the irreducible case. Finally, in this chapter we also consider systems whose constraints are reducible. In particular we introduce a concept which we call an n-reducible complex. This is precisely the idea needed to formulate reducible physical theories rigorously. We show that every differential on such a complex is a mildly generalized Maurer–Cartan differential. In particular we show that the BRST differential is such a generalized Maurer–Cartan differential in the reducible case.

II. THE MAURER–CARTAN STRUCTURE OF BRST DIFFERENTIAL FOR THE IRREDUCIBLE CONSTRAINTS

Let (P,ω) be a n-dimensional symplectic manifold and let $\{,\}$ be the Poisson bracket defined by ω on the algebra of smooth functions $C^\infty(P)$. Assume that G_a, $a=1,\ldots,M$ are constraint functions which satisfy the condition:

$$\{G_a,G_b\} = C^c_{ab}G_c, \tag{2.1}$$

where C^c_{ab} are structure functions on P and let Σ be the constraint surface which is determined by the set of zeros of G_a. When (2.1) is satisfied we say that the constraints G_a are *first class constraints*. The Hamiltonian vector fields X_a corresponding to the functions G_a are defined by $X_a(f)=\{f,G_a\}$ for $f\in C^\infty(P)$. The fields X_a satisfy the condition $[X_a,X_b]\approx C^c_{ab}X_c$, i.e., the equation holds only on Σ, or as we say, they hold only "on shell." Under certain conditions the fields X_a define a foliation of Σ. Functions $f\in C^\infty(\Sigma)$ which are constant on the leaves of the foliation are said to be "gauge invariant" and are called classical observables.

In quantum field theory, it is difficult to utilize path integrals of functionals defined on the space of observables because they are only defined on the constraint surface. To overcome this difficulty the phase space P is extended and the gauge symmetry is replaced by BRST symmetries in a such way that the path integral can be utilized on functionals defined on arbitrary functions on the extended phase space. More precisely, to achieve this, one introduces an antighost variable P_a for every constraint function G_a and a differential δ called the Koszul–Tate differential which is defined on the complex $C[P_a]\otimes C^\infty(P)$ as follows:

$$\delta P_a = -G_a, \tag{2.2}$$

$$\delta f = 0, \tag{2.3}$$

where $f\in C^\infty(P)$. Additionally, new variables η^a are introduced which are in one-to-one correspondence with the space of independent gauge symmetries and another differential d called the longitudinal differential is defined on the complex $C^\infty(P)\otimes C[\eta^b]$ in a manner similar to the difinition of the Chevalley–Eilenberg differential. This differential is designed to implement the gauge symmetries. One extends δ and d to all of $C[P_a]\otimes C[\eta^b]$ by requiring that $\delta(\eta^a)=0$ and

$dP_a=0$. In some cases $\delta+d$ is a differential on the complex $C[P_a]\otimes C^\infty(P)\otimes C[\eta^b]$ whose square is zero and whose cohomology is precisely the space of classical observables. Often this fails to be true and $\delta+d$ must be extended by homological perturbation theory to obtain the (BFV version of the) BRST differential $S=\delta+d+s_1+\cdots$ in order to obtain the observables as zero degree cohomology classes. The differential S is clearly quite different from the longitudinal differential d, but we will show that S satisfies conditions totally analogous to those characterizing d in Henneaux and Teitelboim (Ref. 6, p. 117–119) in the case when the constraint functions are irreducible and bosonic.

Let $\Omega=C[P_a]\otimes C^\infty(P)\otimes C[\eta^b]$ and consider $\Omega^*=\oplus_{p=0}^\infty\Omega^p$, where Ω^p is the subset of Ω having ghost number p (defined below). For simplicity, we introduce the notation $\omega^I=\eta^{b_1}\cdots\eta^{b_{p+1}}P_{a_p}\cdots P_{a_1}$, and $\Omega^1=\{\alpha\in\Omega\,|\,\alpha=u_I\omega^I,u_I\in C^\infty(P)\}$ where I is the multi-index $(b_1,\ldots,b_{p+1},a_1,\ldots,a_p)$. Obviously the elements ω^I generate all Ω^p for $p\geqslant 1$. For completeness and clarity, we first describe our parity conventions as follows:

$$\epsilon(P_a)=\epsilon(G_a)+1=\epsilon(\eta^a),\quad \epsilon(AB)=\epsilon(A)+\epsilon(B). \tag{2.4}$$

Moreover the ghost number grading referred to above is defined as follows.

(1) The pure ghost number of each element of Ω is simply its degree as a polynomial in η^a.
(2) The antighost number of each element of Ω is its degree as a polynomial in P_a.
(3) The ghost number of each element x is the number puregh$(x)-$antigh(x). Notice that for A, $B\in\Omega$, gh$(AB)=$gh$(A)+$gh(B) and that $\epsilon(\omega^I)=1$ whenever $\epsilon(G_a)=0$. With these conventions, we will show that the BRST differential is essentially the Chevalley–Eilenberg differential when the constraints are bosonic and irreducible.

First, we recall how the Chevalley–Eilenberg differential is formulated in BRST notation. Let $\mathcal{G}$ be a Lie algebra spanned by a basis $\{e_i\}$ and $\mathcal{A}$ a commutative associative algebra. Let the mapping $\rho:\mathcal{G}\to\mathrm{End}(\mathcal{A})$ be a representation of $\mathcal{G}$ with representation space $\mathcal{A}$. Introduce a ghost variable η^i for every element e_i of the basis $\{e_i\}$. Let A denote the Z-graded algebra $\mathcal{A}\otimes C[\eta^1,\eta^2,\ldots]$ with the grading defined by the ghost number. The Chevalley–Eilenberg differential $d=d_{\mathrm{CE}}$ is defined on generators of the complex A as follows:

$$\mathrm{d}f=\rho(e_a)(f)\,\eta^a, \tag{2.5}$$

$$\mathrm{d}\eta^a=-\tfrac{1}{2}C^a_{cb}\eta^b\eta^c, \tag{2.6}$$

where f, $C^c_{ab}\in\mathcal{A}$. The mapping $d=d_{\mathrm{CE}}$ is extended to the entire graded algebra A by the Leibniz law

$$d(\alpha\beta)=(\mathrm{d}\alpha)\beta+(-1)^{\deg\alpha}\alpha(\mathrm{d}\beta). \tag{2.7}$$

Any differential which satisfies the conditions (2.5) and (2.6) will be called a Maurer–Cartan differential. Moreover we will say that d is a Chevalley–Eilenberg differential whenever there exists a Lie algebra $\mathcal{G}$ and a representation ρ into the endomorphisms of some commutative associative algebra $\mathcal{A}$ satisfying not only (2.6) but also (2.5) and (2.7). We do not require that our Lie algebra $\mathcal{G}$ be finite dimensional but our Lie algebras are finitely generated as modules over our algebra $\mathcal{A}$.

If we choose $\mathcal{A}=C^\infty(\Sigma)$ where Σ is the constraint surface defined above and if $e_a=X_a$, then the longitudinal differential is a Chevalley–Eilenberg differential of this type. In this case the vector fields X_a must be restricted to Σ and the Lie algebra is the subalgebra of vector fields on Σ spanned by the X_a over the algebra $C^\infty(\Sigma)$. The fact that this is a sub-Lie algebra follows from the identity $[X_a,X_b]=C^d_{ab}X_d+X_{C^d_{ab}}G_d$. The other properties follow immediately. We want to obtain an "off shell" version of this result.

Since $\epsilon(\omega^I)=1$ and $\mathrm{gh}(\omega^I)=1$ we call the set of monomials ω^I multighosts. Moreover, for the BRST differential S, it follows from $S\omega^I \in \Omega^2$, that

$$S\omega^K = -\tfrac{1}{2}C^K_{IJ}\omega^I\omega^J, \tag{2.8}$$

where $C^K_{IJ}=C^K_{JI}\in C^\infty(P)$. Similarly, for $f\in\Omega^0$, one has that $Sf=(\rho_I f)\omega^I$, since $Sf\in\Omega^1$. To summarize, we have following theorem.

Theorem 1: *If the constraint functions $\{G_a\}$ are irreducible and bosonic, the relevant BRST differential S defined on the complex $C[P_a]\otimes C^\infty(P)\otimes C[\eta^b]$ above is a Maurer–Cartan differential,*

$$Sf = (\rho_I f)\omega^I, \tag{2.9}$$

$$S\omega^K = -\tfrac{1}{2}C^K_{IJ}\omega^I\omega^J. \tag{2.10}$$

Notice that even though the longitudinal differential d is not nilpotent on the space $C[P_a]\otimes C^\infty(P)\otimes C[\eta^b]$, its BRST extension S is nilpotent and so is a differential. To determine how the BRST differential S and the longitudinal differential d are related, we compare the following formulas with the formulas (2.5) and (2.6):

$$Sf = (\rho_I f)\omega^I = (X_a f)\eta^a + s_1 f + \cdots + s_n f + \cdots, \tag{2.11}$$

$$S\eta^a = -\tfrac{1}{2}C^a_{cb}\eta^b\eta^c + s_1\eta^a + \cdots.$$

Note that the terms on the right-hand sides of (2.5) and (2.6) are summands of the right-hand side of these equations.

We claim that the BRST differential S is essentially a Chevalley–Eilenberg differential in the case that the constraints are bosonic and irreducible. The required Lie algebra is a sub-Lie algebra of the Lie algebra $\mathcal{X}(P)$ of all vector fields on P. Because of the way S has been extended to products, each of the mappings ρ_I defined by Eq. (2.9) above is a derivation of $C^\infty(P)$ and so is a vector field on P. We consider the submodule $\mathcal{G}(\rho)$ of $\mathcal{X}(P)$ spanned by the vector fields ρ_I over $C^\infty(P)$. We eventually show that it is a sub-Lie algebra of $\mathcal{X}(P)$. Each element of $\mathcal{G}(\rho)$ clearly acts as a derivation of the algebra $\mathcal{A}=C^\infty(P)$ and therefore is in $\mathrm{End}(\mathcal{A})$. Once we establish the fact that $\mathcal{G}(\rho)$ is a Lie algebra we will have the required data in order to show that S is a Chevalley–Eilenberg differential. First we need a lemma which is of interest in its own right.

Lemma 2: Assume that the constraints are bosonic and irreducible and consider the BRST differential S on the complex $C[P_a]\otimes C^\infty(P)\otimes C[\eta^b]$. Let $\rho=\rho_I$ denote the "representation" defined by the identities in Theorem 1. Then

$$S^2 f = \tfrac{1}{2}([\rho_J,\rho_I]f - C^K_{JI}(\rho_K)f)\omega^J\omega^I.$$

Moreover if $S^2 f=0$ for all $f\in C^\infty(P)$, then

$$S^2\omega^K = -\tfrac{1}{6}\{[\rho_I,[\rho_J,\rho_E]]^K + [\rho_J,[\rho_E,\rho_I]]^K + [\rho_E,[\rho_I,\rho_J]]^K\}.$$

Proof: We prove the first identity by noticing that since S is an odd derivation, we have

$$S^2 f = S((\rho_I f)\omega^I) = S(\rho_I f)\omega^I + (\rho_I f)S\omega^I. \tag{2.12}$$

It follows from the identities of Theorem 1 that

$$S^2 f = (\rho_J \rho_I)(f)\omega^J \omega^I + (\rho_I f)\left(-\tfrac{1}{2} C^I_{JK} \omega^J \omega^K\right) \tag{2.13}$$

$$= \tfrac{1}{2}[(\rho_J \rho_I) f - (\rho_I \rho_J) f]\omega^J \omega^I - \tfrac{1}{2} C^I_{JK} \omega^J \omega^K \rho_I f \tag{2.14}$$

$$= \tfrac{1}{2}[\rho_J, \rho_I] f \omega^J \omega^I - \tfrac{1}{2} C^K_{JI} \omega^J \omega^I (\rho_K) f \tag{2.15}$$

$$= \tfrac{1}{2}([\rho_J, \rho_I] f - C^K_{JI}(\rho_K) f)\omega^J \omega^I. \tag{2.16}$$

Thus the first of the two identities is true. We now prove the second identity. Since $S\omega^K = -\frac{1}{2} C^K_{IJ} \omega^I \omega^J$, where $I = (b_1, \ldots, b_{p+1}, a_1, \ldots, a_p)$ and $J = (\tilde{b}_1, \ldots, \tilde{b}_{p+1}, \tilde{a}_1, \ldots, \tilde{a}_p)$, we have

$$\begin{aligned}
S^2 \omega^K &= -\tfrac{1}{2}(S C^K_{IJ})\omega^I \omega^J - \tfrac{1}{2} C^K_{IJ} d\omega^I \omega^J + \tfrac{1}{2} C^K_{IJ} \omega^I d\omega^J \\
&= -\tfrac{1}{2}(\rho_E C^K_{IJ})\omega^E \omega^I \omega^J - \tfrac{1}{2} C^K_{IJ}\left(-\tfrac{1}{2} C^I_{\tilde{K}\tilde{L}} \omega^{\tilde{K}} \omega^L\right)\omega^J + \tfrac{1}{2} C^K_{IJ} \omega^I \left(-\tfrac{1}{2} C^J_{MN} \omega^M \omega^N\right) \\
&= -\tfrac{1}{2} \rho_E C^K_{IJ} \omega^E \omega^I \omega^J + \tfrac{1}{4} C^K_{IJ} C^I_{\tilde{K}\tilde{L}} \omega^{\tilde{K}} \omega^L \omega^J - \tfrac{1}{4} C^K_{IJ} C^J_{MN} \omega^I \omega^M \omega^N \\
&= -\tfrac{1}{2} \rho_E C^K_{IJ} \omega^E \omega^I \omega^J + \tfrac{1}{2} C^K_{IJ} C^I_{\tilde{K}\tilde{L}} \omega^{\tilde{K}} \omega^L \omega^J \\
&= -\tfrac{1}{6}(\rho_E C^K_{IJ} + \rho_I C^K_{JE} + \rho_J C^K_{EI})\omega^I \omega^J \omega^E + \tfrac{1}{6}(C^K_{MI} C^M_{JE} + C^K_{MJ} C^M_{EI} + C^K_{ME} C^M_{IJ})\omega^I \omega^J \omega^E \\
&\quad + \tfrac{1}{6}(\rho_E C^K_{IJ} + \rho_I C^K_{JE} + \rho_J C^K_{EI})\omega^I \omega^J \omega^E - \tfrac{1}{6}(C^K_{IM} C^M_{JE} + C^K_{JM} C^M_{EI} + C^K_{EM} C^M_{IJ})\omega^I \omega^J \omega^E.
\end{aligned} \tag{2.17}$$

Next notice that if we assume that $S^2 f = 0$ for all $f \in C^\infty(P)$, then $[\rho_J, \rho_E] = C^M_{JE} \rho_M$, $[\rho_E, \rho_I] = C^M_{EI} \rho_M$, $[\rho_I, \rho_J] = C^M_{IJ} \rho_M$, and we have

$$[\rho_I, [\rho_J, \rho_E]] = [\rho_I, C^M_{JE} \rho_M] = (\rho_I C^M_{JE})\rho_M + C^M_{JE}[\rho_I, \rho_M] \tag{2.18}$$

$$= (\rho_I C^M_{JE})\rho_M + C^M_{JE} C^K_{IM} \rho_K \tag{2.19}$$

$$= (\rho_I C^K_{JE} + C^M_{JE} C^K_{IM})\rho_K. \tag{2.20}$$

It follows that

$$[\rho_J, [\rho_E, \rho_I]] = (\rho_J C^M_{EI})\rho_M + C^M_{EI} C^K_{JM} \rho_K \tag{2.21}$$

$$= (\rho_J C^K_{EI} + C^M_{EI} C^K_{JM})\rho_K \tag{2.22}$$

and

$$[\rho_E, [\rho_I, \rho_J]] = (\rho_E C^M_{IJ})\rho_M + C^M_{IJ} C^K_{EM} \rho_K \tag{2.23}$$

$$= (\rho_E C^K_{IJ} + C^M_{IJ} C^K_{EM})\rho_K. \tag{2.24}$$

It follows from this last calculation that the negative of the sum of the Kth components of the right-hand sides of the last three equations is precisely six times the right-hand side of the identity for $S^2 \omega^K$ [see (2.17)]. The lemma follows.

Corollary 3: Assume that the constraints are bosonic and irreducible and consider the BRST differential S on the complex $C[P_a] \otimes C^\infty(P) \otimes C[\eta^b]$. *Since in fact* $S^2 = 0$ *we have that* $\mathcal{G}(\rho)$ *is a Lie subalgebra of* $\mathcal{X}(P)$ *with generators the set of vector fields* $\{\rho_I\}$ *on* $C^\infty(P)$.

Corollary 4: If the constraints of a Hamiltonian system are bosonic and irreducible, then the BRST differential is a Chevalley–Eilenberg differential on the complex $\mathcal{A} \otimes C[\omega^I]$ *where the alge-*

bra $\mathcal{A}$ is the algebra of smooth functions on P and where the ω^I are called multighosts instead of ghosts. Recall that the ω^I freely generate $\mathcal{A}\otimes C[\omega^I]$ as a module over $\mathcal{A}$.

Proof: The proof was outlined in the observations just prior to the lemma. The only gap in the argument was that we had not yet proved that $\mathcal{G}(\rho)$ is a Lie algebra which we now see is a corollary of the lemma.

Remark: The longitudinal differential d was initially defined "on shell," that is to say the underlying manifold was the constraint surface Σ. Formulated on this surface the square of d is zero and its cohomology in degree zero is the set of classical observables. The fact that d squares to zero "on shell" is related to the fact that the Hamiltonian vector fields X_a close under Lie brackets "on shell." They need not close "off shell."

In order to use the path integral formalism it is useful to extend the formalism "off shell." When the longitudinal differential d is extended "off shell" it no longer squares to zero and in fact the BRST differential was constructed to repair this defect.[6]

The fact that the BRST differential squares to zero "off shell" suggests that one should be able to supplement the vector fields X_a with other fields to obtain an integrable system which "foliates" P in such a manner that the possibly singular leaves provides the "foliation" of Σ provided by the Hamiltonian vector fields. We now show that this is true.

Recall that the generators ρ_I of the Lie algebra $\mathcal{G}(\rho)$ correspond to the multighosts $\omega^I = \eta^{b_1}\cdots\eta^{b_{p+1}}P_{a_p}\cdots P_{a_1}$ where I is the multi-index $(b_1,\ldots,b_{p+1},\ a_1,\ldots,a_p)$. In the case $p=0$ it is understood that ω^I is simply η^b for some index b. Thus the equation $S(f)=(\rho_I f)\omega^I$ of Theorem 1 has the terms $(\rho_a f)\eta^a$ as certain of its summands, where d is the exterior differential and s_k is a derivation which increases the antighost degree by k. Recall that these latter terms correspond to the longitudinal differential d in the expansion

$$S = \delta + d + s_1 + \cdots + s_n + \cdots . \tag{2.25}$$

of the BRST differential. Indeed for every $f\in C^\infty(P)$,

$$Sf = (\rho_a f)\eta^a + (\rho_I f)\omega^I + \cdots , \tag{2.26}$$

where antidegree $(\omega^I)\geqslant 1$, and we see that $\rho_a f$ is exactly the action of X_a on f. Consequently the ρ_a are simply the Hamiltonian vector fields X_a. The supplementary vector fields we require to obtain an integrable system are defined by $X_I=\rho_I$.

As an immediate consequence of these observations we have the following theorem.

Theorem 5: *The longitudinal differential d is defined in terms of the Hamiltonian vector fields X_i which form an open gauge algebra since $[X_i,X_j]\approx C_{ij}^k X_k$. Since $S^2=0$, there exists additional vector fields X_I on P such that $[X_i,X_j]=C_{ij}^k X_k + C_{ij}^I X_I$, and the fields X_i, X_I define an integrable system in the sense that they generate a subalgebra $\mathcal{G}(\rho)$ of the Lie algebra of all vector fields of P.*

We now determine further conditions imposed on the ρ_K by the fact that S is nilpotent.

Using (2.25) and the fact that $S^2=0$, the first three terms of the expansion of S^2 in terms of the antighost degree yields

$$\delta^2 = 0, \tag{2.27}$$

$$[\delta,d] = 0, \tag{2.28}$$

$$d^2 = -[\delta,s_1]. \tag{2.29}$$

By a calculation similar to the one in the proof of the lemma, and for arbitrary $f\in C^\infty(P)$ we have

$$d^2 f = \tfrac{1}{2}([\rho_i, \rho_j] f - C_{ij}^k \rho_k f)\, \eta^i \eta^j, \tag{2.30}$$

$$[\delta, s_1] f = (\delta s_1 f + s_1 \delta f) \tag{2.31}$$

$$= \delta s_1 f = \delta(\rho_{ab}^c f \eta^a \eta^b P_c), \tag{2.32}$$

where the ρ_{ab}^c are defined by the equation $s_1 f = \omega^I f = \rho_{ab}^c f \eta^a \eta^b P_c$ and the multi-index I is (abc). It follows that

$$[\delta, s_1] f = (\rho_{ab}^c f)\, \eta^a \eta^b P_c \tag{2.33}$$

$$= -(G_c)(\rho_{ab}^c f)\, \eta^a \eta^b. \tag{2.34}$$

Using the three identities above and comparing (2.30) with (2.34), we have

$$[X_j, X_i] = C_{ji}^k X_k + G_c \rho_{ij}^c. \tag{2.35}$$

Since ω^I is a derivation for each multi-index I we see that each ρ_{ij}^c is also a derivation on $C^\infty(P)$; we distinguish it from the derivation ρ_k by referring to it as a second order derivation.

We now show how these results may be applied to Hamiltonian systems having first-class constraints restricting our remarks to the case where P is R^n for some positive integer n. We adopt the same conventions as in Ref. 6 (pp. 52–53), in particular, let $G_a (a = 1, \ldots, M)$ denote the constraint functions of the system. Define vectors $X_a = X_a^\lambda \partial_\lambda$ via $X_a^\lambda = \omega^{\lambda\mu} \partial_\mu G_a$, where the matrix of components of the antisymmetric tensor $(\omega^{\lambda\mu})$ is the inverse of the matrix $\omega_{\mu\nu}$ of components of the symplectic structure ω on P. We observe that, for each $F \in C^\infty(P)$,

$$X_a F = X_a^\lambda \partial_\lambda F = \{F, G_a\}. \tag{2.36}$$

We know that if X_a^λ corresponds to G_a and X_b^λ corresponds to G_b then $[X_a, X_b]^\lambda$ corresponds to $[G_a, G_b]$. Moreover,

$$[X_a, X_b]^\lambda = \omega^{\lambda\mu} \partial_\mu (C_{ab}^c G_c) \tag{2.37}$$

$$= C_{ab}^c X_c^\lambda + G_c \omega^{\lambda\mu} \partial_\mu C_{ab}^c \approx C_{ab}^c X_c^\lambda. \tag{2.38}$$

Off the constraint surface, the second term on the right-hand side of (2.38) does not vanish unless $\partial_\mu C_{ab}^c = 0$. Thus $X_a^\lambda (a = 1, \ldots, M)$ form a closed distribution only on shell $G_a = 0$.

For the remainder of this section we provide a detailed calculation which determine consistency conditions for the summand s_1 (2.25).

First we determine the action of s_1 on the ghosts η^α. Since the vector fields $\{X_a\}$ satisfy the Jacobi identity it follows from a computation similar to the one of Lemma 2.2 that $d^2 \eta^a = 0$. Combined with the facts that $d^2 = -[\delta, s_1]$ and that $s_1 \eta^\alpha$ has antighost number one we have $s_1 \eta^\alpha = C_{abc}^{d\alpha} \eta^a \eta^b \eta^c P_d$. Then,

$$0 = -(\delta s_1 + s_1 \delta)\, \eta^\alpha = -\delta s_1 \eta^\alpha = C_{abc}^{d\alpha} \eta^a \eta^b \eta^c G_d. \tag{2.39}$$

Therefore $C_{abc}^{d\alpha} \eta^a \eta^b \eta^c G_d = 0$ and consequently we obtain the following consistency condition:

$$C_{abc}^{d\alpha} G_d = 0. \tag{2.40}$$

At this point we derive other consistency conditions which are required in order to compute $s_1 P_a$. Since d increases the ghost number by one we can write $dP_a = \eta^c C_{ca}^b P_b$ and

$$d^2P_a = d(dP_a) = d(\eta^c C^b_{ca} P_b) = (d\eta^c) C^b_{ca} P_b - \eta^c d(C^b_{ca} P_b)$$
$$= \left(-\tfrac{1}{2} C^c_{de} \eta^d \eta^e\right) P_b C^b_{ca} - \eta^c (\rho_d(C^b_{ca})\eta^d P_b + C^b_{ca} dP_b)$$
$$= -\tfrac{1}{2} C^c_{de} C^b_{ca} \eta^d \eta^e P_b - \rho_d(C^b_{ca})\eta^c \eta^d P_b - C^b_{ca} \eta^c (\eta^e C^d_{eb} P_d)$$
$$= \left(-\tfrac{1}{2} C^b_{ce} C^d_{ba} - C^b_{ca} C^d_{eb} - \rho_e(C^d_{ca})\right) \eta^c \eta^e P_d. \tag{2.41}$$

Since s_1 increases the antighost number by one we can write $s_1 P_a = C^{ef}_{cda} \eta^c \eta^d P_e P_f$. It follows that

$$\delta s_1 P_a = \delta(C^{ef}_{cda} \eta^c \eta^d P_e P_f) \tag{2.42}$$

$$= C^{ef}_{cda} \eta^c \eta^d ((\delta P_e) P_f - P_e \delta P_f) \tag{2.43}$$

$$= C^{ef}_{cda} \eta^c \eta^d (-G_e P_f + G_f P_e) \tag{2.44}$$

$$= -C^{ef}_{cda} G_e \eta^c \eta^d P_f + C^{ef}_{cda} G_f \eta^c \eta^d P_e \tag{2.45}$$

$$= 2C^{ef}_{cda} \eta^c \eta^d P_e G_f \tag{2.46}$$

and

$$s_1 \delta P_a = s_1(-G_a) = -s_1 G_a \tag{2.47}$$

$$= -(\rho^e_{cd} G_a) \eta^c \eta^d P_e. \tag{2.48}$$

Thus

$$(\delta s^1 + s^1 \delta) P_a = (2C^{ef}_{cda} G_f - \rho^e_{cd}(G_a)) \eta^c \eta^d P_e \tag{2.49}$$

$$= (2C^{df}_{cea} G_f - \rho^d_{ce}(G_a)) \eta^c \eta^e P_d. \tag{2.50}$$

Since $d^2 = -[\delta, s^1]$, by comparing (2.41) and (2.50) we have the following consistency conditions:

$$C^{df}_{cea} G_f = \tfrac{1}{2}\left(\rho^d_{ce}(G_a) + \rho_e(C^d_{ca}) + \tfrac{1}{2} C^b_{ce} C^d_{ba} + C^b_{ca} C^d_{eb}\right). \tag{2.51}$$

Notice that in case the constraint functions are irreducible this condition is equivalent to requiring that the left-hand side of (2.51) vanish "on shell."

In the last few paragraphs we have obtained consistency conditions (2.40) and (2.51) which are necessary in order to determine the action of s_1 on the generators. We have not attempted to determine the coefficients $C^{d\alpha}_{abc}$ and C^{df}_{cea} in the consistency equations since they can only guarantee the existence of perturbation terms of s_1.

III. THE MAURER–CARTAN STRUCTURE OF BRST DIFFERENTIAL UNDER THE REDUCIBLE CONSTRAINTS

In the preceding section we dealt only with irreducible constraints. In this section, we will generalize some of our results to include systems of reducible constraints. To achieve that, we introduce the concept of an *n*-reducible complex as follows.

Definition: Let $\Omega^* = \oplus_{n=0}^{\infty} \Omega^n$ be a graded algebra and assume that Ω^0 is an algebra such that Ω^* is a Ω^0-module. Let $A^p = \oplus_{n=0}^{p} \Omega^n$. If A^p is a finitely generated Ω^0-module and each component $\Omega^k (k > p)$ is generated by A^p, we call the complex Ω^* a *p*-reducible complex.

We are interested in investigating differentials on *p*-reducible complexes. First consider some examples of *p*-reducible complexes.

Example 1: Let R^n be *n*-dimensional Euclidean space and $\Omega^k(R^n)$ be the space of *k*-forms.

Since R^n has a global coordinate chart $(x^1,\ldots,x^n)$, every k-form can be written as

$$\omega = \omega_{i_1\cdots i_k} \mathrm{d}x^{i_1} \wedge \cdots \wedge \mathrm{d}x^{i_k}, \tag{3.1}$$

where $\omega_{i_1\cdots i_k}$ are smooth functions which belong to the space of 0-forms $\Omega^0(R^n)$, and where the 1-forms $\mathrm{d}x^1,\cdots,\mathrm{d}x^n$ generate all differential forms in $\Omega^k(R^n)$ over $\Omega^0(R^n)$ for $k\geqslant 1$. The complex $\Omega^*(R^n)=\oplus_{k=0}^n \Omega^k(R^n)$ is then a 1-reducible complex. The exterior differential d is defined as follows:

$$\mathrm{d}f = (\partial_i f)\mathrm{d}x^i, \tag{3.2}$$

$$d(\mathrm{d}x^i) = 0, \tag{3.3}$$

where $f\in\Omega^0(R^n)$, $\mathrm{d}x^i\in\Omega^1(R^n)$. One then extends the definition above to the entire space $\Omega^*(R^n)$ via the Leibniz formula.

Example 2 (Chevalley–Eilenberg cohomology): Let a pair (d,A) be a Chevalley–Eilenberg differential with its related complex $A=\mathcal{A}\otimes C[\eta^1,\eta^2,\ldots]$ discussed earlier. Obviously, the graded algebra A is generated by ghosts $\eta^1,\eta^2,\ldots$ over the underlying algebra $\mathcal{A}$ and consequently the complex A is a 1-reducible complex.

Example 3 (auxillary differential Δ): Typical kth reducible complexes arise from BRST operators in case the system is subject to $(k-1)$-reducible constraint conditions.

In BRST theory, a specific differential called the auxillary differential Δ is introduced to deal with longitudinal differentials defined on constraint surfaces subject to higher order reducibility conditions. Let Σ be a constraint surface and $\{\eta^{a_0}\}$ be the original ghosts (see Ref. 6 pp. 217–218).

Assume that Σ is defined by constraints which satisfy kth order reducibility conditions. In this case the reducibility of the constraints can be written as

$$Z^{a_{k-1}}_{a_k} Z^{a_{k-2}}_{a_{k-1}} = (-1)^{\epsilon_{a_{k-2}}} C^{a_{k-2},a_0}_{a_k} G_{a_0}, \tag{3.4}$$

$$k=1,\ldots,L, \quad a_k = 1,\ldots,m_k \tag{3.5}$$

for some m_k and appropriate functions $Z^{a_{k-1}}_{a_k}$ (see Ref. 6, p. 210).

Introduce higher order ghost variables η^{a_k} along with a differential Δ as follows:

$$\mathrm{puregh}(\eta^{a_k}) = k+1, \quad \epsilon(\eta^{a_k}) = \epsilon_{a_k} + k + 1, \tag{3.6}$$

$$\Delta F = 0, \quad \Delta\eta^{a_k} = \eta^{a_{k+1}} Z^{a_k}_{a_{k+1}} (-1)^{\epsilon_{a_k}+k+1}, \tag{3.7}$$

where F is an arbitary function on the constraint surface. To complete the definition of the auxillary differential Δ, one needs to introduce an auxillary grading as follows:

$$\mathrm{aux}(z^A) = 0 = \mathrm{aux}(\eta^{a_0}), \quad \mathrm{aux}(\eta^{a_k}) = k. \tag{3.8}$$

One then has that $\mathrm{aux}(\Delta)=1$ and that $\mathrm{puregh}(A)=\mathrm{aux}(A)+\deg(A)$. The complex $\Omega=C^\infty(\Sigma)\otimes C[\eta^{a_0},\eta^{a_1},\ldots,\eta^{a_k}]$ is then a $(k+1)$-reducible complex.

At this point, we characterize the differential on an arbitrary n-reducible complex and thereby generalize Theorem 1. We adopt the convention of the left action for d. Obviously, a differential d on a reducible complex Ω^* is uniquely and totally determined by its values on the space $A^p=\Omega^0\oplus\overline{A^p}$ and the Leibniz rule, where $\overline{A^p}=\oplus_{n=1}^p \Omega^n$. In order to see this in more detail we first assume that the finitely generated Ω^0 module A^p has a finite basis denoted by $(\omega^i_n)_{1\leqslant n\leqslant p}$ where the subindex means that $\omega^i_n\in\Omega^n$. Notice that the basis (ω^i_n) generates all the elements of every component Ω^k for $k>p$. With this notation, we define a differential d on the space A^p as follows:

$$\mathrm{d}f = (\rho^1_j f)\omega^j_1, \tag{3.9}$$

$$d\omega_m^i = -\tfrac{1}{2}\Sigma_{1\leqslant n\leqslant m} C_{jkn}^i \omega_{m-n+1}^j \omega_n^k, \tag{3.10}$$

where $f \in \Omega^0$ and the ρ_j^1 are derivations of Ω^0. If the complex Ω^* is a 1-reducible complex, the basis has only elements of the form ω_1^i and the formulas (3.9) and (3.10) reduce to

$$df = (\rho_j f)\omega_1^j \tag{3.11}$$

$$d\omega_1^i = -\tfrac{1}{2} C_{jk}^i \omega_1^j \omega_1^k \tag{3.12}$$

analogous to the formulas given by the Chevalley–Eilenberg differential.

The definition of the Koszul–Tate differential δ is then modified to reflect the reducibility conditions above. In the reducible case the longitudinal differential is not nilpotent on the space of $C^\infty(\Sigma)\otimes C[\eta^a]$, but is nilpotent on the subalgebra of longitudinal forms. In order to overcome this defect, an equivalent differential D (Ref. 6) is introduced such that $H^*(D)=H^*(d)$. At this point one has "differentials" δ and D on the extended space $\Omega^*=C[P_{a_0}, P_{a_1}, \ldots]\otimes C^\infty(\Sigma)\otimes C[\eta^{a_1}, \eta^{a_2}, \ldots]$ and it is possible to show that a BRST differential $S=\delta+D+s_1+\cdots$ defined on the complex Ω^* exists. It can be seen that the longitudinal complex $C^\infty(\Sigma)\otimes C[\eta^a]$ and the BRST complex Ω^* are both n-reducible complexes for appropriate n. Therefore we obtain the following generalization of Theorem 1. (See Refs. 2, 4, 8, and 10.)

Theorem 6: *If the constraints are bosonic and reducible the BRST differential has a structure similar to that of the longitudinal differential.*

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On the Casimir of the group ISL(n,R) and its algebraic decomposition

J. N. Pecina-Cruz[a)]
Bureau of Economic Geology, J.J. Pickle Research Campus, The University of Texas at Austin, University Station, Box X, Austin, Texas 78713-8294

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In this paper, an explicit expression for the Casimir operator (or the Casimir invariant) of the inhomogeneous group ISL(n,R) in its enveloping algebra is proposed, which using contractions of the tensorial indices of the generating operators P^{ρ} and E^{ν}_{μ} may be presented in the following [slightly more comprehensible as Eq. (1)] form. The Casimir is obtained by symmetrizing this expression. This tensor form is useful in the classification of particles in affine gravitational gauge theories; such as that based on ISL($4,R$). It is also proven that the Casimir of ISL(n,R) can be decomposed in terms of the Casimirs of its little groups, a key point in the posterior construction of its irreducible representations. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1915291]

I. INTRODUCTION

The special affine group ISL(n,R) is the semidirect product of the Abelian group of translations in n dimensions and the special linear, SL(n,R). The ISL($4,R$) group has been chosen as the gauge group in gauge theories of gravity;[1] therefore, the knowledge of its Casimirs will be necessary not only to investigate the irreducible representations of this group, but also to provide these theories with a wave equation.[2] It has been conjectured that a gauge theory for quantum gravity can be developed by enlarging the Poincare group to the group IGL($4,R$)[5]. However, the lack of invariants of this group,[3] prevents to classify the elementary particles of a theory based on that gauge group. Therefore, ISL($4,R$) is the best selection.[1,4] The group ISL(n,R) has a subgroup, the Poincare group, from which stems its importance in physics. The eigenvalues of the Casimir of the group ISL(n,R) provide quantum numbers to classify the particles of these theories in the same way that the eigenvalues of the Casimirs of the Poincare groups allow us to classify the particles according to their mass and spin. The eigenvalues of the Casimir of ISL(n,R) label the irreducible representations of the group. The invariants are also useful ingredients in the decomposition of reducible representations into irreducible ones. In the case of gauge theories of gravity based on ISL(n,R), it is important to decompose the unitary irreducible representations of the group ISL(n,R) into the unitary irreducible representations of the Poincare subgroup. This would bring a physical insight into the behavior of the elementary particles of these theories. In Sec. II, we construct the formula for the Casimir of ISL(n,R). In Sec. III, we discuss the induction proof used to guarantee the general validation of the formula for the Casimir of ISL(n,R). Finally in Sec. IV, the algebraic decomposition of ISL(n,R) is achieved.

II. CONSTRUCTION OF THE FORMULA FOR THE CASIMIR OF ISL(n,R)

In Ref. 3 it is proved that the group ISL(n,R) has one invariant. And in Ref. 6 it is proved that the order of this invariant is $\frac{1}{2}n(n+1)$. Based on this proof, the standard procedure for constructing

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[a)]Present address: Institute for Advanced Technology, The University of Texas at Austin, Ausin, Texas 78712.

invariants by contracting tensorial indices with the Levi–Civita antisymmetric pseudotensor and the generators of the Lie group,[7] we found a formula for the invariant of ISL(n,R). This expression is given by

$$\begin{aligned} \textit{Casimir ISL}(n,R) = \{ & \zeta^{\rho_1[(\theta_{11})\rho_2]\ldots,[(\theta_{n-2,1},\ldots,\theta_{n-2,n-2})\rho_{n-1}]}_{\xi_0\alpha_1,\ldots,\alpha_{n-1}\beta_1[\beta_2(\gamma_{11})],\ldots,[\beta_{n-1}(\gamma_{n-2,1},\ldots,\gamma_{n-2,n-2})]} \\ & \times P^{\xi_0}P^{\alpha_1}\cdots P^{\alpha_{n-1}}E^{\beta_1}_{\rho_1}E^{[\beta_2(\gamma_{11})]}_{[(\theta_{11})\rho_2]}\cdots E^{[\beta_{n-1}(\gamma_{n-2,1},\ldots,\gamma_{n-2,n-2})]}_{[(\theta_{n-2,1},\ldots,\theta_{n-2,n-2})\rho_{n-1}]}\}_{\textit{symmetrized}}, \end{aligned} \tag{1}$$

$$\xi_0,\theta_{ij},\gamma_{ij},\alpha_l,\rho_k,\beta_m = 0,1,\ldots,n-1, \quad i,j = 1,2,\ldots,n-2, \quad l,k,m = 1,2,\ldots,n-1,$$

where

$$E^{[\beta_2(\gamma_{11})]}_{[(\theta_{11})\rho_2]} = E^{\beta_2}_{\theta_{11}}E^{\gamma_{11}}_{\rho_2}$$

and

$$E^{[\beta_{n-1}(\gamma_{n-2,1},\ldots,\gamma_{n-2,n-2})]}_{[(\theta_{n-2,1},\ldots,\theta_{n-2,n-2})\rho_{n-1}]} = E^{\beta_{n-1}}_{\theta_{n-2,1}}E^{\gamma_{n-2,1}}_{\theta_{n-2,2}}\cdots E^{\gamma_{n-2,n-3}}_{\theta_{n-2,n-2}}E^{\gamma_{n-2,n-2}}_{\rho_{n-1}},$$

where $\zeta^{\cdots}_{\ldots\ldots}$ is given by the expression

$$\zeta^{\cdots}_{\ldots\ldots} = \epsilon_{\xi_0\beta_1\cdots\beta_{n-1}}(\delta_{\rho_1\alpha_1}\cdots\delta_{\rho_{n-1}\alpha_{n-1}})((\delta_{\theta_{11}\gamma_{11}})(\delta_{\theta_{21}\gamma_{21}}\delta_{\theta_{22}\gamma_{22}})\cdots(\delta_{\theta_{n-2,1}\gamma_{n-2,1}}\cdots\delta_{\theta_{n-2,n-2}\gamma_{n-2,n-2}})). \tag{2}$$

The E^{β}_{α} are the generators of the general linear group GL(n,R) in the Weyl basis[2] and the P^{α} are the generators of the Abelian subgroup of ISL(n,R). In formula (1), the following substitution must be carried out:

$$\mathbf{E}^{\alpha}_{\alpha} = E^{\alpha}_{\alpha} - E^{\alpha+1}_{\alpha+1}. \tag{3}$$

The commutation relations of ISL(n,R), are given then by

$$[P^{\rho},P^{\nu}] = 0, \quad [P^{\rho},E^{\nu}_{\mu}] = \delta_{\mu\rho}P^{\nu}, \quad [E^{\nu}_{\mu},E^{\tau}_{\lambda}] = \delta_{\nu\lambda}E^{\tau}_{\mu} - \delta_{\mu\tau}E^{\nu}_{\lambda}. \tag{4}$$

The E^{α}_{α}, the generators of the general linear group GL(n,R), are substituted by the traceless generators $\mathbf{E}^{\alpha}_{\alpha}$ of the special linear group SL(n,R). In Eq. (2), we define $\epsilon_{\xi_0}=1$.

III. THE INDUCTION PROOF

In Ref. 8, it is proved that the invariant of ISL(n,R) can be obtained by solving a system of linear first order partial differential equations (LFPDE). The system of LFPDE can trivially be solved for $n=1$. Thus, the first part of the induction is proven. In order to prove the second part of the induction method, we assume the formula is valid for $n=k$ and then prove that it is valid for $n=k+1$.

We can construct a scalar of the order required by Lemma 1, in Ref. 6, to be the invariant of ISL$(k+1,R)$. According to this lemma, the order of the invariant in the generators of this group should be $\frac{1}{2}(k+1)(k+2)$. In this same reference, it is proven that the invariant for this group would be of $k+1$ order in the generators of the translations. Therefore the invariant for ISL$(k+1,R)$ must be of $k+1$ order in the translations and of $\frac{1}{2}k(k+1)$ order in the nontranslations generators of the group ISL$(k+1,R)$. That is, the invariant of ISL$(k+1,R)$ must be different from the invariant for ISL(k,R) by a factor given by

$$P^{\alpha_k}E^{[\beta_k(\gamma_{k-1,1},\ldots,\gamma_{k-1,k-1})]}_{[(\theta_{k-1,1},\ldots,\theta_{k-1,k-1})\rho_k]}. \tag{5}$$

If we take into account the form of the invariants of ISL(n,R) for $n=1,2,3,4$ (Ref. 6) the formula we are assuming valid for $n=k$ and the factor given above, we can construct a scalar given by

$$\begin{aligned} \textit{Casimir ISL}(k+1,R) = \{ & \zeta^{\rho_1[(\theta_{11})\rho_2],\ldots,[(\theta_{k-2,1},\ldots,\theta_{k-2,k-2})\rho_{k-1}][(\theta_{k-1,1},\ldots,\theta_{k-1,k-1})\rho_k]}_{\xi_0\alpha_1,\ldots,\alpha_{k-1}\alpha_k\beta_1[\beta_2(\gamma_{11})],\ldots,[\beta_{k-1}(\gamma_{k-2,1},\ldots,\gamma_{k-2,k-2})][\beta_k(\gamma_{k-1,1},\ldots,\gamma_{k-1,k-1})]} \\ & \times P^{\xi_0}P^{\alpha_1}\cdots P^{\alpha_{k-1}}P^{\alpha_k}E^{\beta_1}_{\rho_1}E^{[\beta_2(\gamma_{11})]}_{[(\theta_{11})\rho_2]}\cdots E^{[\beta_{k-1}(\gamma_{k-2,1},\ldots,\gamma_{k-2,k-2})]}_{[(\theta_{k-2,1},\ldots,\theta_{k-2,k-2})\rho_{k-1}]} \\ & \times E^{[\beta_k(\gamma_{k-1,1},\ldots,\gamma_{k-1,k-1})]}_{[(\theta_{k-1,1},\ldots,\theta_{k-1,k-1})\rho_k]}\}_{\textit{symmetrized}}. \end{aligned} \tag{6}$$

This formula coincides with the Eq. (1) for $n=k+1$. However, the proof is not yet complete, since the scalar that we have constructed to be the invariant of ISL($k+1,R$) could be zero. Therefore, we must prove that the scalar given by Eq. (5) is not zero.

IV. THE ALGEBRAIC DECOMPOSITION OF ISL(N,R)

The proof that the scalar given by Eq. (5) does not vanish is based on an algebraic decomposition of the Casimir of ISL(n,R) in terms of the Casimirs of its little groups. This decomposition allows an immediate classification of the existent particles in a theory based on ISL(n_1,R), with n_1 any number.[5] Then making all the translations equal zero except P^0 in Eq. (5). That is,

$$\xi_0 = \alpha_1 = \cdots = \alpha_k = 0,$$

therefore

$$\rho_1 = \rho_2 = \cdots = \rho_k = 0.$$

Hence, the Casimir with all the translations zero except P^0 is given by

$$\begin{aligned} \textit{Casimir ISL}(k+1,R) = \{ & (P^0)^{k+1}\zeta^{0[(\theta_{11})0],\ldots,[(\theta_{k-1,1},\ldots,\theta_{k-1,k-1})0]}_{00,\ldots,0\beta_1[\beta_2(\gamma_{11})],\ldots,[\beta_k(\gamma_{k-1,1},\ldots,\gamma_{k-1,k-1})]}E^{\beta_1}_0E^{\gamma_{11}}_0\cdots E^{\gamma_{k-1,k-1}}_0 \\ & \times E^{\beta_2}_{\theta_{11}}E^{[\beta_3(\gamma_{21})]}_{[(\theta_{21})\theta_{22}]}\cdots E^{[\beta_k(\gamma_{k-1,1},\ldots,\gamma_{k-1,k-2})]}_{[(\theta_{k-1,1},\ldots,\theta_{k-1,k-2})\theta_{k-1,k-1}]}\}_{\textit{symmetrized}}, \end{aligned} \tag{7}$$

where

$$\begin{aligned} \zeta^{0[(\theta_{11})0],\ldots,[(\theta_{k-1,1},\ldots,\theta_{k-1,k-1})0]}_{00,\ldots,0\beta_1[\beta_2(\gamma_{11})],\ldots,[\beta_k(\gamma_{k-1,1},\ldots,\gamma_{k-1,k-1})]} = & \epsilon_{0\beta_1\cdots\beta_k}(\delta_{\theta_{11}\gamma_{11}}\delta_{\theta_{22}\gamma_{22}}\cdots\delta_{\theta_{k-1,k-1}\gamma_{k-1,k-1}})((\delta_{\theta_{21}\gamma_{21}}) \\ & \times(\delta_{\theta_{31}\gamma_{31}}\delta_{\theta_{32}\gamma_{32}})\cdots(\delta_{\theta_{k-1,1}\gamma_{k-1,1}}\cdots\delta_{\theta_{k-1,k-2}\gamma_{k-1,k-2}})). \end{aligned} \tag{8}$$

The terms of Eq. (6) with the $\theta=0$ generated by the contraction of the Levi–Civita pseudotensor cancel out by antisymmetry.

Therefore, the indices β,θ,γ can be shifted; instead of running from $0,1,\ldots,k$ they will run from $0,1,\ldots,k-1$. *This defines an isomorphism* between the subset of the generators, belonging to the factor which multiply P^{k+1} in Eq. (6), of the Lie algebra of ISL($k+1,R$) and the Lie algebra of ISL(k,R). Hence Eq. (7) can be given by

$$\begin{aligned} \zeta^{\theta_{11}[(\theta_{21})\theta_{22}],\ldots,[(\theta_{k-1,1},\ldots,\theta_{k-1,k-2})\theta_{k-1,k-1}]}_{\beta_1\gamma_{11}\gamma_{22},\ldots,\gamma_{k-1,k-1}\beta_2[\beta_3(\gamma_{21})],\ldots,[\beta_k(\gamma_{k-1,1},\ldots,\gamma_{k-1,k-2})]} = & \epsilon_{\beta_1\cdots\beta_k}(\delta_{\theta_{11}\gamma_{11}}\delta_{\theta_{22}\gamma_{22}}\cdots\delta_{\theta_{k-1,k-1}\gamma_{k-1,k-1}})((\delta_{\theta_{21}\gamma_{21}}) \\ & \times(\delta_{\theta_{31}\gamma_{31}}\delta_{\theta_{32}\gamma_{32}})\cdots(\delta_{\theta_{k-1,1}\gamma_{k-1,1}}\cdots\delta_{\theta_{k-1,k-2}\gamma_{k-1,k-2}})). \end{aligned} \tag{9}$$

The basis elements of the Lie algebra of the group ISL(n,R) can be represented by the $n+1$ by $n+1$ matrices given by

$$\begin{pmatrix} \mathrm{SL}(n,R) & P \\ 0 & 0 \end{pmatrix},$$

where P are the generators of the group of translations, and SL(n,R) are the generators of the special linear group in n dimensions. Therefore, the E^{α}_0 generators of the Eq. (6) can be considered as the translations P^{α} generators of the little group ISL(k,R) of $(p^0,0,0,\ldots,0_k)$.[9]

Using Eq. (8), Eq. (6) can be written in the following form:

$$\textit{Casimir ISL}(k+1,R) = \{(P^0)^{k+1}\zeta^{\theta_{11}[(\theta_{21})\theta_{22}],\ldots,[(\theta_{k-1,1},\ldots,\theta_{k-1,k-2})\theta_{k-1,k-1}]}_{\beta_1\gamma_{11}\gamma_{22},\ldots,\gamma_{k-1,k-1}\beta_2[\beta_3(\gamma_{21})],\ldots,[\beta_k(\gamma_{k-1,1},\ldots,\gamma_{k-1,k-2})]}E_0^{\beta 1}E_0^{\gamma_{11}}\cdots E_0^{\gamma_{k-1,k-1}} \times E_{\theta_{11}}^{\beta_2}E_{[(\theta_{21})\theta_{22}]}^{[\beta_3(\gamma_{21})]}\cdots E_{[(\theta_{k-1,1},\ldots,\theta_{k-1,k-2})\theta_{k-1,k-1}]}^{[\beta_k(\gamma_{k-1,1},\ldots,\gamma_{k-1,k-2})]}\}_{symmetrized}. \tag{10}$$

To take advantage of the isomorphism given above, we make the following substitution:

$$\beta_1 \to \xi_0, \beta_2 \to \beta_1, \beta_3 \to \beta_2, \ldots, \beta_k \to \beta_{k-1},$$

$$\theta_{11} \to \rho_1, \theta_{22} \to \rho_2, \ldots, \theta_{k-1,k-1} \to \rho_{k-1},$$

$$\gamma_{11} \to \alpha_1, \gamma_{22} \to \alpha_2, \ldots, \gamma_{k-1,k-1} \to \alpha_{k-1},$$

$$\theta_{21} \to \theta_{11}, (\theta_{31} \to \theta_{21}, \theta_{32} \to \theta_{22}), \ldots, (\theta_{k-1,1} \to \theta_{k-2,1}, \theta_{k-1,2} \to \theta_{k-2,2}, \ldots, \theta_{k-1,k-2} \to \theta_{k-2,k-2}),$$

$$\gamma_{21} \to \gamma_{11}, (\gamma_{31} \to \gamma_{21}, \gamma_{32} \to \gamma_{22}), \ldots, (\gamma_{k-1,1} \to \gamma_{k-2,1}, \gamma_{k-1,2} \to \gamma_{k-2,2}, \ldots, \gamma_{k-1,k-2} \to \gamma_{k-2,k-2}),$$

and by substituting into Eq. (9), we obtain

$$\textit{Casimir ISL}(k+1,R) = \{(P^0)^{k+1}(\textit{Casimir ISL}(k,R))\}_{symmetrized}. \tag{11}$$

We have obtained the Casimir of the little group ISL(k,R) from the Casimir of the group ISL$(k+1,R)$. We arrive at the same result if we take any of the other translations.

From the above discussion, it is clear that the Casimir of ISL$(k+1,R)$ given by Eq. (5) does not vanish, as claimed. This completes the induction proof. We conclude that the formula given by Eq. (1) is valid for any integer n.

V. CONCLUSION

Although the formula for the Casimir of ISL(n,R) has been written in the Weyl basis, this does not limit its application range. The advantage of our formula for ISL(n,R), over other possible formulation, is its immediate physical and mathematical application as shown above in the little group Casimir decomposition of ISL(n,R).

In gauge theories of gravity based on the group ISL$(4,R)$, it should be verified for the correct usage of the Casimir operator. The reason is that in these theories, the group ISO (1,3) must be a subgroup of the gauge group. This group has a different Lie algebra than that of the group ISO (4) which is a subgroup of ISL$(4,R)$. The applications of a deunitarizing inner automorphism,[4] which changes some of the generators of the group ISL(n,R) by a factor $\sqrt{-1}$, is necessary to extend the range of application of our formula. To avoid confusion we suggest using the notation ISL$(1,n-1,R)$ for the group that has as a subgroup ISO$(1,n-1)$.

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MHD α^2-dynamo, Squire equation and $\mathcal{PT}$-symmetric interpolation between square well and harmonic oscillator

Uwe Günther[a] and Frank Stefani[b]
Research Center Rossendorf, P.O. Box 510119, D-01314 Dresden, Germany

Miloslav Znojil[c]
Ústav Jaderné Fyziky AV ČR, 250 68 Řež, Czech Republic

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It is shown that the α^2-dynamo of magnetohydrodynamics, the hydrodynamic Squire equation as well as an interpolation model of $\mathcal{PT}$-symmetric quantum mechanics are closely related as spectral problems in Krein spaces. For the α^2-dynamo and the $\mathcal{PT}$-symmetric model the strong similarities are demonstrated with the help of a 2×2 operator matrix representation, whereas the Squire equation is reinterpreted as a rescaled and Wick-rotated $\mathcal{PT}$-symmetric problem. Based on recent results on the Squire equation the spectrum of the $\mathcal{PT}$-symmetric interpolation model is analyzed in detail and the Herbst limit is described as spectral singularity. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1915293]

I. INTRODUCTION

Non-Hermitian $\mathcal{PT}$-symmetric quantum mechanical systems[1–8] are known to possess spectral sectors with purely real eigenvalues as well as sectors with pairs of complex conjugate eigenvalues. Changes of certain system parameters can lead to spectral phase transitions from one sector to the other. The physics in the two sectors has been identified with phases of unbroken $\mathcal{PT}$-symmetry (real eigenvalues) and spontaneously broken $\mathcal{PT}$-symmetry (pairwise complex conjugate eigenvalues).[1,2] From a mathematical point of view, non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians are self-adjoint operators in Krein spaces[9–11]—Hilbert spaces with an additional indefinite metric structure—and the two spectral sectors correspond to Krein space states of positive or negative type (real eigenvalues) and neutral (isotropic) states (pairwise complex conjugate eigenvalues).

Apart from $\mathcal{PT}$-symmetric quantum mechanics (PTSQM), it is known that a certain class of spherically symmetric mean-field dynamo models[12] of magnetohydrodynamics (MHD) can be described by self-adjoint operators in Krein spaces as well.[13] These models show similar spectral phase transitions from real to pairwise complex conjugate eigenvalues[14]—and only the physical interpretation differs from that in PTSQM. For dynamos it simply consists in a transition from nonoscillatory states to oscillatory states.

In the present paper, we are going to briefly describe the underlying structural operator theoretic parallels between PTSQM models and the spherically symmetric MHD α^2-dynamo (Sec. II). The discussion will be illustrated with the help of a $\mathcal{PT}$-symmetric interpolation between a harmonic oscillator placed in a square well and an empty square well (Sec. III). This interpolation shows a rich structure of spectral phase transitions with a couple of unexpected features. Furthermore, we will show in Sec. IV that the eigenvalue problem of the $\mathcal{PT}$-symmetric (intermediate) interpolation model with linear complex potential (purely complex electrical field) within the square well is mathematically identical to the eigenvalue problem of the rescaled and Wick-rotated

[a]Electronic mail: u.guenther@fz-rossendorf.de
[b]Electronic mail: f.stefani@fz-rossendorf.de
[c]Electronic mail: znojil@ujf.cas.cz

Squire equation of hydrodynamics which describes the normal vorticity of a plane channel flow (Couette flow) with linear transversal velocity profile. Recent Airy function based results on the Squire equation allow us to analytically describe the spectral behavior of the PTSQM model in the limiting case when the width of the square well tends to infinity. In this limit we reproduce the Herbst model[15] with its empty spectrum. The limiting behavior occurs as a blowing-up of the spectrum to infinity along three directions on the complex plane—leaving behind a spectrally empty region at any fixed finite distance from the origin of the spectral plane. In Sec. V we briefly sketch some links of the obtained results to other physical setups and analytical techniques.

II. KREIN SPACE PROPERTIES OF $\mathcal{PT}$-SYMMETRIC QUANTUM MODELS AND OF THE SPHERICALLY SYMMETRIC MHD α^2-DYNAMO

A. $\mathcal{PT}$-symmetric quantum models

In their seminal letter[1] Bender and Boettcher identified $\mathcal{PT}$-symmetry as the essential property of the non-Hermitian quantum system,

$$H\psi(x) = E\psi(x), \quad H = -\frac{d^2}{dx^2} + gx^2(ix)^\nu, \tag{1}$$

which ensures the reality of its spectrum for exponents $\nu \in [0,2)$ and $\psi(x) \in \tilde{\mathcal{H}} = L_2(-\infty,\infty)$.[16] This allowed them not only to extend an earlier conjecture of Bessis and Zinn-Justin [whose numerical results indicated that quantum systems with complex potential $V(x) = ix^3$ might have a purely real spectrum], but also initiated the still lasting intensive study of generalized $\mathcal{PT}$-symmetric non-Hermitian systems.[17] Such systems are characterized by a $\mathcal{PT}$-symmetric Hamiltonian H,

$$[\mathcal{PT}, H] = 0, \tag{2}$$

where $\mathcal{P}$ denotes a reflection

$$\mathcal{P}x\mathcal{P} = -x, \quad \mathcal{P}\psi(x) = \psi(-x),$$

while the time-reversal operator $\mathcal{T}$ performs complex conjugation,

$$\mathcal{T}i\mathcal{T} = -i, \quad \mathcal{T}\psi(x) = \psi(x)^*. \tag{3}$$

Because both operators $\mathcal{P}$ and $\mathcal{T}$ are involution operators,

$$\mathcal{P}^2 = I, \quad \mathcal{T}^2 = I,$$

they induce natural $\mathbb{Z}_2$-gradings of the Hilbert space $\tilde{\mathcal{H}}$. For our subsequent analysis it suffices to consider the subclass of models which can be defined solely over the real line $x \in \mathbb{R}$. For such models the $\mathcal{T}$-induced $\mathbb{Z}_2$-grading corresponds to a splitting of the wave functions $\psi \in \tilde{\mathcal{H}}$ into real and imaginary components (what is of no direct physical interest in a quantum mechanical context; additionally one would have to work in a real Hilbert space with doubled dimension compared to the original complex one), whereas $\mathcal{P}$ induces a $\mathbb{Z}_2$-grading into parity even and parity odd components,

$$\psi(x) = \psi_+(x) + \psi_-(x), \quad \mathcal{P}\psi_\pm(x) = \psi_\pm(-x) = \pm\psi_\pm(x). \tag{4}$$

The corresponding $\mathbb{Z}_2$-graded Hilbert space splits as

$$\tilde{\mathcal{H}} = \mathcal{H}_+ \oplus \mathcal{H}_-, \quad \psi_\pm \in \mathcal{H}_\pm.$$

In the case of a simple $\mathcal{PT}$-symmetric one-particle system with Hamiltonian

$$H = -\partial_x^2 + V_+(x) + iV_-(x), \quad V_\pm(-x) = \pm V_\pm(x), \quad \Im V_\pm = 0 \tag{5}$$

it holds

$$H = \mathcal{P}H^\dagger\mathcal{P} \tag{6}$$

and $\mathcal{P}$ is a so called fundamental (canonical) operator symmetry[9,10] of H—i.e., H is $\mathcal{P}$-pseudo-Hermitian in the sense of Refs. 4 and 5. Operators with an involutive fundamental symmetry are known to be symmetric—and for appropriately chosen domain [boundary conditions for the functions $\psi(x)$] even self-adjoint—in a Krein space $\mathcal{K}$. For $\mathcal{P}$-pseudo-Hermitian operators over the real line this Krein space $\mathcal{K}_\mathcal{P}$ is given as[11,18,19]

$$(\mathcal{K}_\mathcal{P}, [.,.]_\mathcal{P}), \quad [\psi,\phi]_\mathcal{P} = (\psi, \mathcal{P}\phi) = \int_{C\subseteq\mathbb{R}} \psi^*(x)\mathcal{P}\phi(x)\mathrm{d}x = \int_{C\subseteq\mathbb{R}} \psi^*(x)\phi(-x)\mathrm{d}x. \tag{7}$$

Depending on the concrete problem, the integration in (7) is performed over a finite interval, $C=[-a,a]$, or over the complete real line, $C=(-\infty,\infty)\sim\mathbb{R}$. From (5) and (6) one immediately finds

$$[H\psi,\phi]_\mathcal{P} = [\psi, H\phi]_\mathcal{P}.$$

The Krein space inner (scalar) product $[\psi,\phi]_\mathcal{P}$ has the following properties:

(i) It coincides with the more general $\mathcal{PT}$ inner product of Bender *et al.*,[6,7]

$$(\psi,\phi)_{\mathcal{PT}} = \int_{C\subset\mathbb{C}} [\mathcal{PT}\psi(x)]\phi(x)\mathrm{d}x$$

when the integration path $C\subset\mathbb{C}$ of the latter integral is restricted to (an interval of) the real line, $C\subseteq\mathbb{R}$,

$$(\psi,\phi)_{\mathcal{PT}} = \int_{C\subseteq\mathbb{R}} [\mathcal{PT}\psi(x)]\phi(x)\mathrm{d}x = \int_{C\subseteq\mathbb{R}} [\mathcal{P}\psi(x)^*]\phi(x)\mathrm{d}x = \int_{C\subseteq\mathbb{R}} \psi(x)^*\mathcal{P}\phi(x) = [\psi,\phi]_\mathcal{P}.$$

(ii) In contrast to the "usual" positive definite metric structure of the Hilbert space $\tilde{\mathcal{H}} = \mathcal{H}_+ \oplus \mathcal{H}_-$,

$$(\tilde{\mathcal{H}}, (.,.)), \quad (\psi,\phi) = \int_{C\subseteq\mathbb{R}} \psi^*(x)\phi(x)\mathrm{d}x = \int_{C\subseteq\mathbb{R}} (\psi_+^*\phi_+ + \psi_-^*\phi_-)\mathrm{d}x,$$

with non-negative norm

$$\|\psi\|^2 = (\psi,\psi) = \|\psi_+\|^2 + \|\psi_-\|^2 \geqslant 0,$$

the scalar product $[\psi,\phi]_\mathcal{P}$ defines an indefinite metric structure in the Krein space $\mathcal{K}_\mathcal{P} = \mathcal{H}_+ \oplus \mathcal{H}_-$, what is easily seen from the decomposition (4)

$$[\psi,\phi]_\mathcal{P} = \int_{C\subseteq\mathbb{R}} (\psi_+^*\phi_+ - \psi_-^*\phi_-)\mathrm{d}x.$$

(iii) In rough analogy with timelike, spacelike, and lightlike (isotropic) vectors in Minkowski space, one distinguishes Krein space vectors of positive type, $[\psi_+,\psi_+]_\mathcal{P} = \|\psi_+\|^2 > 0$, of negative type, $[\psi_-,\psi_-]_\mathcal{P} = -\|\psi_-\|^2 < 0$, and neutral (isotropic) vectors,

$$[\psi,\psi]_\mathcal{P} = 0, \quad \psi = \psi_+ + \psi_-, \quad \|\psi_+\|^2 = \|\psi_-\|^2.$$

In order to make the structural Krein space analogies of PTSQM models and MHD dynamo setups maximally transparent, we rewrite the eigenvalue problem, $H\psi=E\psi$, for the $\mathcal{PT}$-symmetric Hamiltonian (5) in an equivalent 2×2 matrix operator representation. Introducing the projection operators

$$P_{\pm} := \tfrac{1}{2}(I \pm \mathcal{P})$$

we decompose wave function ψ and Hamiltonian H (see, e.g., Ref. 9) as

$$\psi = P_+\psi + P_-\psi = \psi_+ + \psi_-,$$

$$H = P_+HP_+ + P_-HP_+ + P_+HP_- + P_-HP_-.$$

In terms of the notation

$$H_{\pm\pm} := P_{\pm}HP_{\pm} = -\partial_x^2 + V_+(x), \quad H_{\pm\mp} := P_{\pm}HP_{\mp} = iV_-(x) \tag{8}$$

this gives

$$\begin{pmatrix} H_{++} & H_{+-} \\ H_{-+} & H_{--} \end{pmatrix}\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = E\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}, \quad \mathcal{P} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{9}$$

where

$$H_{\pm\pm} = H_{\pm\pm}^{\dagger}, \quad H_{+-} = -H_{-+}^{\dagger}. \tag{10}$$

If one replaces the matrix entries in (9) and (10) by appropriate constants one arrives at the schematic two-level model

$$H_H\begin{pmatrix} u \\ v \end{pmatrix} = E\begin{pmatrix} u \\ v \end{pmatrix}, \quad H_H = \begin{pmatrix} c+a & b \\ -b^* & c-a \end{pmatrix}, \quad a,c \in \mathbb{R}, \tag{11}$$

which may be read as an elementary exemplification of Heisenberg's linear-algebraic approach[20] to ($\mathcal{PT}$-symmetric) quantum mechanics and which was intensively studied in Refs. 6, 7, 18, and 21–23.

B. The spherically symmetric MHD α^2-dynamo

The magnetic fields of planets, stars, and galaxies are maintained by homogeneous dynamo effects, which can be successfully described within magnetohydrodynamics (MHD). One of the simplest dynamos is the spherically symmetric mean-field α^2-dynamo in its kinematic regime. This dynamo model is capable to play a similar paradigmatic role in MHD dynamo theory like the harmonic oscillator in quantum mechanics (QM). Its operator matrix has the form (see the Appendix for a few comments on the origin of this operator matrix and on the physics of α^2-dynamos)[13]

$$\hat{H}_l[\alpha] = \begin{pmatrix} -Q[1] & \alpha \\ Q[\alpha] & -Q[1] \end{pmatrix} \tag{12}$$

and consists of formally self-adjoint blocks

$$Q[\alpha] := p\alpha p + \alpha\frac{l(l+1)}{r^2},$$

where $p=-i(\partial_r+1/r)$ denotes the radial momentum operator. The operator $\hat{H}_l[\alpha]$ is defined over an interval $\Omega=[0,1]\ni r$ and acts on two-component vectors ϕ which describe the coupled

l-modes of the poloidal and toroidal magnetic field components of a mean-field dynamo model with helical turbulence function (α-profile) $\alpha(r)$.

Although the dynamo model is not $\mathcal{PT}$-symmetric, its operator $\hat{H}_l[\alpha]$ shares a basic underlying symmetry with PTSQM Hamiltonians—a $\mathbb{Z}_2$-graded pseudo-Hermiticity (J-pseudo-Hermiticity)[5,14] which is induced by the fundamental (canonical) symmetry,

$$\hat{H}_l[\alpha] = J\hat{H}_l^{\dagger}[\alpha]J, \quad J = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}.$$

Similar to the reflection operator $\mathcal{P}$ in (6), the operator J is unitary and involutive

$$J^{\dagger} = J^{-1}, \quad J^2 = I.$$

The boundary conditions on the vector function ϕ are set at $r=1$ (the rescaled surface radius of the star or planet whose fluid/plasma motion maintains the dynamo effect) and it is assumed that $\alpha(r>1)\equiv 0$. In the case of physically idealized boundary conditions at $r=1$ (see, e.g., Ref. 24), the domain $\mathcal{D}(\hat{H}_l[\alpha])$ of the operator $\hat{H}_l[\alpha]$ consists of functions ϕ such that

$$\mathcal{D}(\hat{H}_l[\alpha]) := \left\{ \phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} : \phi \in \tilde{\mathcal{H}} \equiv \mathcal{H} \oplus \mathcal{H}, \mathcal{H} = L_2(\Omega, r^2\,\mathrm{d}r), \Omega = [0,1], \phi(1) = 0, r\phi(r)|_{r\to 0} \to 0 \right\},$$

and $\hat{H}_l[\alpha]$ is self-adjoint in a Krein space

$$(\mathcal{K}_{\mathcal{J}}, [.,.]_{\mathcal{J}}), \quad [\psi,\phi]_J = \int_0^1 \psi^{\dagger} J \phi r^2\,\mathrm{d}r, \quad [\hat{H}_l\chi,\phi]_J = [\chi,\hat{H}_l\phi]_J.$$

It should be noted that for physically realistic boundary conditions

$$\hat{B}_l\phi|_{r=1} = 0, \quad \hat{B}_l = \mathrm{diag}[\partial_r + (l+1)/r, 1] \tag{13}$$

there exists no appropriate Krein space which could make the operator $\hat{H}_l[\alpha]$ J-self-adjoint.

The structures of PTSQM models and the α^2-dynamo can be compared most explicitly after passing from $\mathcal{K}_{\mathcal{J}}$ to an equivalent Krein space $\mathcal{K}_{\mu}$ with diagonal metric operator μ and redefined Hilbert spaces components, $L_2(\Omega, r^2\,\mathrm{d}r) \mapsto L_2(\Omega, \mathrm{d}r)$. The diagonalization yields

$$J \mapsto \mu := \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} = S^{-1}JS, \quad S = \frac{1}{\sqrt{2}}\begin{pmatrix} I & -I \\ I & I \end{pmatrix}, \tag{14}$$

$$\hat{H}_l[\alpha] \mapsto \check{H}_l[\alpha] = S^{-1}\hat{H}_l[\alpha]S = \frac{1}{2}\begin{pmatrix} Q[\alpha-2]+\alpha & -Q[\alpha]+\alpha \\ Q[\alpha]-\alpha & Q[-\alpha-2]-\alpha \end{pmatrix}, \tag{15}$$

$$\phi \mapsto \check{\phi} = \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \phi_2+\phi_1 \\ \phi_2-\phi_1 \end{pmatrix}, \tag{16}$$

whereas the unitary mapping $U: L_2(\Omega, r^2\,\mathrm{d}r) \mapsto L_2(\Omega, \mathrm{d}r)$ simplifies the structure of $Q[\alpha]$ and leads in (15) and (16) to the additional replacements

$$\phi_{1,2} \mapsto f_{1,2} := r\phi_{1,2}, \quad Q[\alpha] \mapsto q[\alpha] := rQ[\alpha]r^{-1} = -\partial_r\alpha(r)\partial_r + \alpha(r)\frac{l(l+1)}{r^2}. \tag{17}$$

By inspection of (8)–(10) and (14)–(17) we find that, in the chosen Krein space representations of the PTSQM model and the α^2-dynamo, the block structures of the metrics (involution operators) $\mathcal{P}$ and μ coincide, $\mathcal{P}=\mu$, but that the blocks of the $\mathcal{PT}$-symmetric Hamiltonian and the dynamo operator show significant structural differences [in a very rough analogy, the alpha profile $\alpha(r)$ has

some similarities to a position depending mass, as it was studied for QM models, e.g., in Ref. 25],

$$H_{\pm\pm} = -\partial_x^2 + V_+(x) \quad \leftrightarrow \quad -q[1] \pm \frac{q[\alpha]+\alpha}{2},$$

$$H_{\pm\mp} = iV_-(x) \quad \leftrightarrow \quad \mp\frac{q[\alpha]-\alpha}{2}.$$

It is clear that these differences in the differential expressions (as well as the different boundary conditions on the two-component eigenfunctions) will lead to different global behaviors of the corresponding operator spectra. Nevertheless, both types of systems share the same Krein-space induced features of level crossings, what will be briefly sketched in the next section.

C. Spectral phase transitions

Since the first PTSQM paper[1] of Bender and Boettcher it is known that $\mathcal{PT}$-symmetric Hamiltonians have a real spectrum when $\mathcal{PT}$-symmetry is an exact symmetry and not spontaneously broken (the corresponding eigenfunctions are invariant under a $\mathcal{PT}$-transformation), whereas spontaneously broken $\mathcal{PT}$-symmetry is connected with complex energies. [We recall that this follows from (2) and (3), the eigenvalue equation $H\psi=E\psi$ and its $\mathcal{PT}$-transformed, $H\mathcal{PT}\psi=E^*\mathcal{PT}\psi$. For real eigenvalues, $E=E^*$, it is natural to set $\psi=\mathcal{PT}\psi$, whereas $E\neq E^*$ necessarily implies $\psi \neq \mathcal{PT}\psi$.] A consistent PTSQM applicability and interpretation of the complex-energy states remains an open question up to now (cf., e.g., Ref. 26). For convenience, we shall call these states "unphysical" here.

The mathematically most interesting questions of PTSQM concern the transition between the physical and unphysical domains of their parameters. In the simple two-state model (11) it is easy to deduce that the quantized energies E are real ("physical") for $|a|>|b|$ while they form complex-conjugate pairs in the "unphysical" regime where $|a|<|b|$.[7,18] The boundary of its PTSQM applicability coincides with the double-cone hypersurface in parameter space where $|a|=|b|$. One easily verifies that whenever $|b|$ approaches $|a|$, the separate eigenenergies $E_\pm$ as well as the corresponding two independent bound-state eigenvectors coalesce and coincide. On the critical hypersurface the remaining (geometrical) eigenvector becomes supplemented by a so called associated vector (algebraic eigenvector)[14] and the Hamiltonian matrix H acquires a Jordan-block canonical structure.[14,27] The latter cannot be diagonalized and it only gives the doubly degenerate and real single "exceptional-point" eigenvalue $E=E_{(\mathrm{EP})}=c$ (cf., e.g., Ref. 28 for more details).

An exhaustive and consistent bound-state interpretation of the Schrödinger-type equation (1) is more difficult. For example, it requires the restriction of the range of exponents to a finite interval of $\nu\in(-1,2)$ for $\psi(x)\in L_2(-\infty,\infty)$ as usual defined on the real line.[1] A rigorous proof of the reality of the energies turned out unexpectedly difficult.[16,29] For larger exponents ν, the real line must be replaced by an appropriately deformed contour in the complex plane.[1,2]

A systematic analytical study of phase transition points is still lacking for PTSQM models; the same concerns efficient mathematical tools for deriving their location in parameter space. Similar to the double-cone hypersurfaces for the simple matrix model (11), one expects more complicated (and more interesting) global phase-transition hypersurfaces in case of the Schrödinger-type systems. Knowing the location of these phase transition hypersurfaces, one would know the boundaries of the "physical" regions of exact $\mathcal{PT}$-symmetry.

For the α^2-dynamo both types of eigenvalues—real ones as well as pairwise complex conjugate ones—have a clear physical meaning. They simply correspond to nonoscillatory and oscillatory dynamo states, respectively. But again it is of utmost interest to know the parameter configurations for which transitions between the two types of states (phases) occur. In the recent paper,[30] strong numerical indications were presented that magnetic field reversals (interchanges of North and South poles as they are evident from paleomagnetic data on the Earth magnetic field[31]) are induced by a special type of nonlinear dynamics in the vicinity of spectral phase transition points. [In the concrete case, the nonlinear transition mechanism between kinematic and saturated dy-

namo regime (a brief outline of the corresponding physics can be found in the Appendix) was simulated with the help of a so called α-quenching (see, e.g., Ref. 32) which simulates the nonlinear back-reaction of the induced magnetic fields on the α-profile $\alpha(r)$.]

The qualitative features of the real-to-complex phase transitions are essentially the same for PTSQM models and for the MHD α^2-dynamo. They correspond to transitions from Krein space states of positive and negative type to pairwise neutral (isotropic) states[11,14]—and a square-root branching of the spectral Riemann surface.[33,34] Such transitions are a generic feature of Krein-space setups and they are new compared with setups in Hilbert spaces with purely positive metric structures as in "usual" QM. The square-root branching behavior is easily seen by passing from the linear eigenvalue problems for the 2×2-operator matrices H and $\hat{H}_l[\alpha]$ of Eqs. (9) and (12),

$$(H-E)\psi=0, \quad (\hat{H}_l[\alpha]-\lambda)\phi=0,$$

via substitutions

$$\psi=\begin{pmatrix} \psi_+ \\ -\frac{1}{H_{+-}}[H_{++}-E]\psi_+ \end{pmatrix}, \quad \phi=\begin{pmatrix} \phi_1 \\ \frac{1}{\alpha}[Q(1)+\lambda]\phi_1 \end{pmatrix}$$

to the equivalent quadratic operator pencils

$$\left\{(H_{--}-E)\frac{1}{H_{+-}}(H_{++}-E)-H_{-+}\right\}\psi_+=0,$$

$$\left\{(Q[1]+\lambda)\frac{1}{\alpha}(Q[1]+\lambda)-Q[\alpha]\right\}\phi_1=0.$$

Both pencils are of the same generic operator type

$$L[\lambda]\psi=[A_2\lambda^2+A_1\lambda+A_0]\psi=0$$

with a scalar product

$$(\psi,L[\lambda]\psi)=a_2\lambda^2+a_1\lambda+a_0=0, \quad a_j:=(\psi,A_j\psi)$$

which can be used to deduce the local square-root branching behavior of the spectrum

$$\lambda_{1,2}=\frac{1}{2a_2}(-a_1\pm\sqrt{a_1^2-4a_0a_2}).$$

A typical α^2-dynamo spectrum with a large number of real-to-complex transitions is presented in Fig. 1 (see also Refs. 14 and 35). These crossings with real-to-complex transition occur at exceptional points (in the sense of Kato[36]) of (square root) branching type[37,38] and the corresponding eigenvalues have geometric multiplicity one and algebraic multiplicity two.[14] In contrast, crossings without real-to-complex transitions are of the same type as level crossings in Hermitian systems[11]–with geometric and algebraic multiplicity two.[39] Finally, we note that although locally crossings with real-to-complex transitions occur, in general, only between two spectral branches, globally much more branches are involved in mutual crossings (see Fig. 1). This reflects the fact that in general the spectrum forms a multisheet Riemann surface over the parameter space of the theory (see, e.g., Refs. 33, 34, and 40).

In the next section, we will analyze the spectral behavior of a $\mathcal{PT}$-symmetric interpolation model where we will find a similar rich structure of real-to-complex transitions as for the α^2-dynamo.

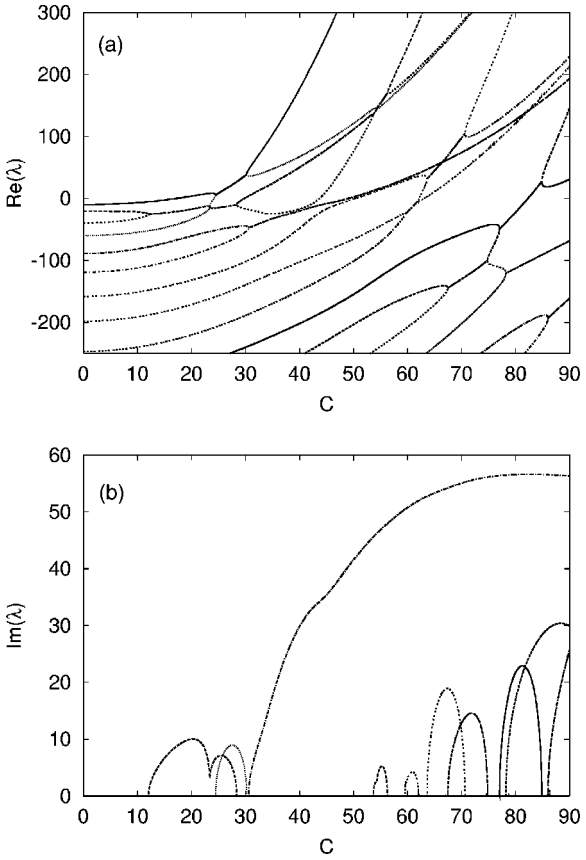

FIG. 1. Real and imaginary components of the α^2-dynamo spectrum as functions of the scale factor C of an α-profile $\alpha(r)=C\times(1-26.09\times r^2+53.64\times r^3-28.22\times r^4)$ in the case of angular mode number $l=1$ and physically realistic boundary conditions (13). The concrete coefficients in the quartic polynomial $\alpha(r)$ have their origin in numerical simulations of the field reversal dynamics (see Ref. 30). Only the imaginary components with $\Im\lambda\geqslant 0$ are shown. The complex conjugate ($\Im\lambda\leqslant 0$)-components are omitted for sake of brevity.

III. $\mathcal{PT}$-SYMMETRIC INTERPOLATION BETWEEN SQUARE WELL AND HARMONIC OSCILLATOR

In Schrödinger-type models (1) over the open real line $x\in(-\infty,\infty)$ a PTSQM-related separation of the "physical" and "unphysical" domains is, in general, a mathematically highly nontrivial problem. Its resolution requires a fairly subtle and rigorous mathematical argumentation.[16,29] A typical result of the WKB analysis of Ref. 1 was that in a half-open interval of $\nu\in[0,2)$ the energies remain real and that the $\mathcal{PT}$-symmetry of the wave functions remains unbroken. In parallel, a characteristic unphysical behavior of the system (1) has been found in the half-open interval of $\nu\in[-1,0)$, where at any $\nu<0$ all the sufficiently high-lying energies E_n with $n>n_0(\nu)$ "decay" in complex-conjugate pairs, $\Im E_n\neq 0$. Moreover, the spectrum becomes empty in the Herbst–Hamiltonian limit of the leftmost $\nu=-1$.[1]

A. Toy model $\mathcal{PT}$-symmetric differential equation

In the present section, we are going to extend the consideration of the Schrödinger-type system (1) to exponents from the interval $\nu\in[-2,0]$. The endpoints of this interval correspond to the purely real-valued Hermitian-system spectra of a freely moving particle with shifted off-set energy (for $\nu=-2$) and a harmonic oscillator (for $\nu=0$). For the exponents $\nu\in(-2,0)$ we expect a phase of spontaneously broken $\mathcal{PT}$-symmetry with an involved picture of real-to-complex spectral phase transitions.

In order to keep the numerical analysis sufficiently simple and robust, we assume the system located in a square well (box) of *finite* width $2b<\infty$ and Dirichlet boundary conditions imposed at the walls, $\psi(x=\pm b)=0$, i.e., we introduce an IR cutoff at the low-energy end of the spectrum (various aspects of square-well-related PTSQM setups have been earlier considered, e.g., in Refs. 11, 41, and 42). This enables us to rescale Eq. (1) to the equivalent equation

$$[-\partial_y^2 + G\, y^2 (iy)^\nu]\psi[x(y)] = \mu(E)\psi[x(y)] \tag{18}$$

with parameter-independent boundary conditions

$$\psi[x(\pm 1)] = 0, \tag{19}$$

but rescaled coupling constant and energy

$$G = g\, b^{4+\nu}, \quad \mu(E) = b^2 E.$$

In this notation, the original bound-state problem (1) with asymptotic Dirichlet boundary conditions at $x\to\pm\infty$ is replaced by the equivalent new problem defined within a fixed finite interval $[-1,1]$. In the limit of very small $b\approx 0$ the potential term becomes negligible, $G\approx 0$, and the interaction degenerates to an infinitely deep square well (box) at all ν. A completely similar situation occurs for systems with any nonvanishing finite b, but very small exponents, $\nu\approx -2$. In both extremal cases the problem remains exactly solvable. The original Bender–Boettcher problem corresponds to the strong-coupling limit, $G\to\infty$, $b\to\infty$, with g hold fixed, $g=G\, b^{-4-\nu}=\text{const}$.

For finite coupling constants $0<G<\infty$ one expects the energy spectrum to be divided into the following three sectors: into a low-energy sector with states which are involved in real-to-complex phase transitions, into an intermediate sector, where the ν-dependent energies still remain real, and into a high-energy sector with almost ν-independent purely real eigenvalues whose states experience only a small perturbations from the complex interaction term. The division into low energy and intermediate-and-high energy sectors has been qualitatively described in a recent paper[11] by Langer and Tretter who considered a square well model with an arbitrary $\mathcal{PT}$-symmetric potential V as perturbation. Starting from the energy spectrum of the empty square well, $\mu_k=k^2\pi^2/4$, $k=1, 2, \ldots$, they showed that there are no real-to-complex phase transitions for levels $k>k_s$ with k_s as the lowest level satisfying the supremum bound $\|V\|_\infty<(2k_s+1)\pi^2/8$. In case of our model with potential $V(y)=gb^{4+\delta}y^2(iy)^\nu$ the supremum norm (see, e.g., Ref. 43) reads (for $\nu\geqslant -2$)

$$\|V\|_\infty = \sup_{y\in[-1,1]} |V(y)| = |V(\pm 1)| = |g| b^{4+\nu}$$

so that it is ensured that there are no phase transitions for levels

$$k > k_s(b) > \frac{1}{2}\left[\frac{8}{\pi^2}|g| b^{4+\nu} - 1\right]. \tag{20}$$

According to Ref. 11 it holds for the corresponding real eigenvalues μ_k, $|\mu_k - k^2\pi^2/4| < |g| b^{4+\nu}$. The supremum bound is safe, but at the same time rather rough.[44] The subsequent exact numerical analysis shows that, depending on the concrete exponents ν, the real-to-complex phase transitions in the model (18) stop at much lower energy levels.

B. The emergence of $\Im E\neq 0$ on certain finite subintervals of $\nu\in(-2,0)$

In the generic case with $\nu\in(-2,0)$ and $b>0$, we have solved Eqs. (18) and (19) numerically by means of a shooting technique with a fifth-order Runge–Kutta method, utilizing and adapting standard routines from numerical recipes.[45] The corresponding code had been validated extensively in earlier work by comparison with known analytical results and other numerical results in dynamo theory and quantum mechanics.

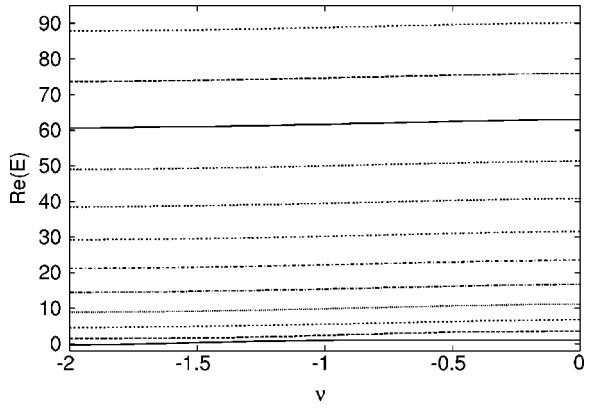

FIG. 2. Spectrum of the $\mathcal{PT}$-symmetric interpolation Hamiltonian $H=-\partial_x^2+x^2(ix)^\nu$ as function of the exponent ν for the cutoff length $b=2$. All eigenvalues are real and almost independent of ν. The spectrum is only slightly deviating from that of an empty square well.

A sample of the results of such a study is depicted in Figs. 2–6, where we have chosen $g=1$ and displayed the first few energy levels $E(\nu)$ over the entire interval $\nu \in (-2,0)$ for the sequence of values $b=2$, 4, 6, 7. The important results of this numerical experiment are the following:

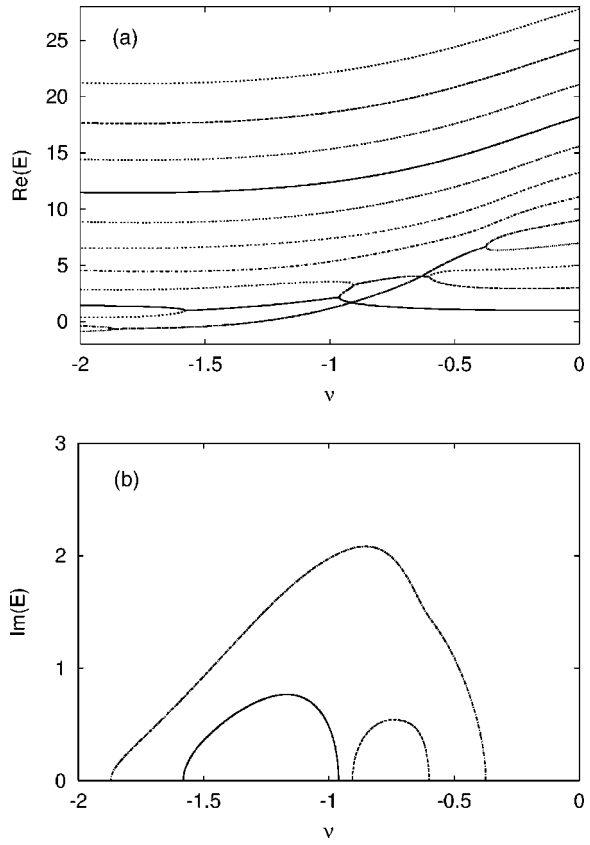

FIG. 3. Real and imaginary components of the spectrum in the case of a cutoff length $b=4$ [complex conjugate ($\Im\lambda \leqslant 0$) components omitted, as well as further higher lying levels without real-to-complex transitions]. The low-energy sector with its multiple real-to-complex transitions starts to form.

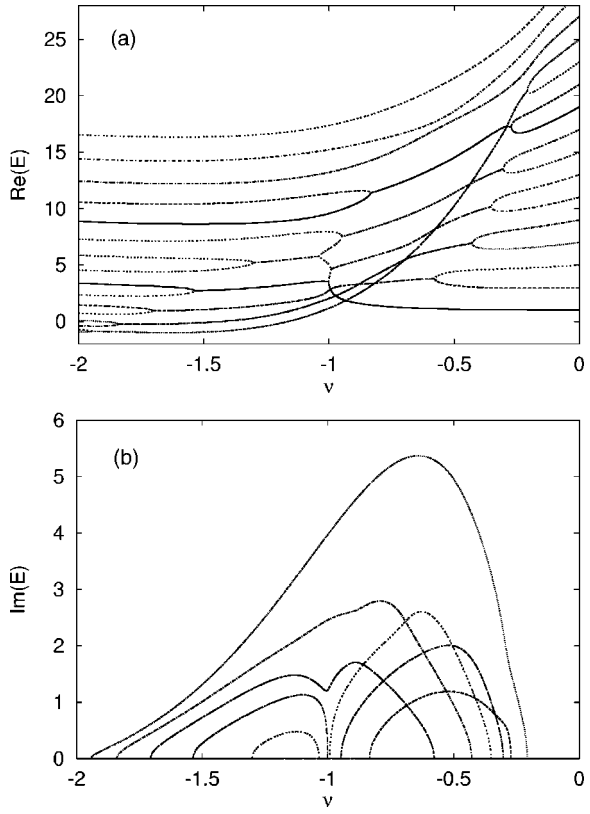

FIG. 4. Spectrum for a cutoff length $b=6$.

(i) At all sufficiently small b, as sampled in Fig. 2, the energy spectrum exhibits a more or less ν-independent square-well form.

(ii) At not too large b the spectrum, as sampled in Fig. 3, proves clearly separated into the high-lying part (where the energies still preserve their approximate ν independence), an intermediate perturbative part (where the perceivably ν-dependent energies still remain all real) and the low-lying part (where one encounters the first real-to-complex phase transitions).

(iii) The actual lowest level numbers $k_c(b)$ (critical level numbers) of the modes which are not involved in real-to-complex transitions lie much below the safe supremum bounds $k_s(b)$ of inequality (20). Choosing, for example, the exponents $\nu=-1/2$ and $\nu=-3/2$ we read off that

$$\nu=-1/2,\quad b=\begin{cases}2\\4\\6\\7\end{cases},\quad k_s(b)>\begin{cases}4.08\\51.4\\213\\367\end{cases},\quad k_c(b)=\begin{cases}1\\6\\14\\22\end{cases},$$

$$\nu=-3/2,\quad b=\begin{cases}2\\4\\6\\7\end{cases},\quad k_s(b)>\begin{cases}1.79\\12.5\\35.2\\52.1\end{cases},\quad k_c(b)=\begin{cases}1\\5\\9\\11\end{cases}.$$

(iv) Starting from the "intermediate width" region, sampled at $b=6$ in Fig. 4, we find that the *left-hand half* of the picture exhibits a clear transition from the slightly non-Hermitian

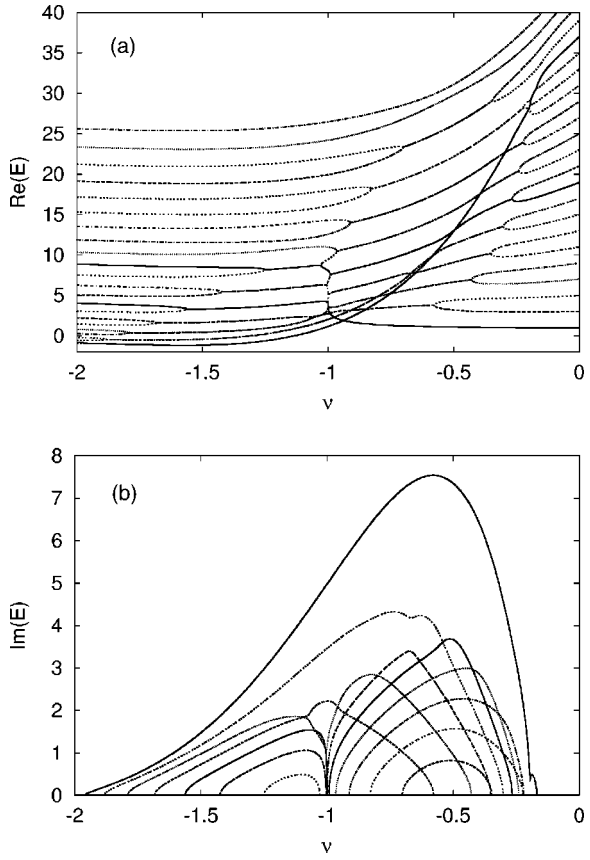

FIG. 5. At a cutoff length $b=7$ the generic structure of the spectrum is clearly visible. The weblike pattern of the real components (a) contains purely real branches in the vicinity of the left ($\nu=-2$) and right ($\nu=0$) endpoints of the considered interval as well as a chain of purely real intermediate segments in the vicinity of $\nu=-1$. (See Fig. 6 for a detailed view.) The increasing number of imaginary components (b) with high gradients $|\partial_\nu E(\nu\approx -1)| \gg 1$ which accumulate in the vicinity of $\nu=-1$ are first indications of the formation of a local spectral singularity at $\nu=-1$.

square well regime (with the higher energies all real) to its more strongly non-Hermitian extension where for all exponents ν not too distant from $\nu=-2$ the purely imaginary and finite component of the potential resembles the spatially antisymmetric part of the exactly solvable $\mathcal{PT}$-symmetric Heavyside step potential within a square well considered in Ref. 41. This explains why in Figs. 3–5 the continuing decrease of ν makes the respective two or three lowest pairs of the energies merge and complexify.

(v) At "sufficiently large" cutoffs b, all the *real* low-lying energies depicted in the *right-hand halves* of Figs. 4 and 5 obviously stabilize and approach the $b\to\infty$ limiting pattern as published in Refs. 1 and 16. In particular, we see that the ground-state energy remains real and that it starts growing more quickly only when the values of ν move down and closer to the Herbst limit of $\nu\to -1^+$. We observe that in a more appropriate way this growing real branch should be interpreted as a special type of ladder-shaped merger of intermediate real segments which actually correspond to level pairs with higher mode numbers. A zoomed view on this peculiarity is presented in Fig. 6, where it is clearly visible that a chain of exceptional points is located on this branch with alternating complex-valued segments branching off to the left and to the right. These segments fit, after further complex-to-real transitions, to the real eigenvalues of the $\nu\to 0$ and $\nu\to -2$ limit models.

(vi) When the cutoff b is increased the following simultaneous changes in the spectrum can be observed. In the upper low-energy region with $\nu>-1$ step by step more and more level pairs become twisted into the complex sector. With a "slight delay in b" and at $\nu<-1$ the lower of the twisted levels undergo a second pairwise real-to-complex transition with the

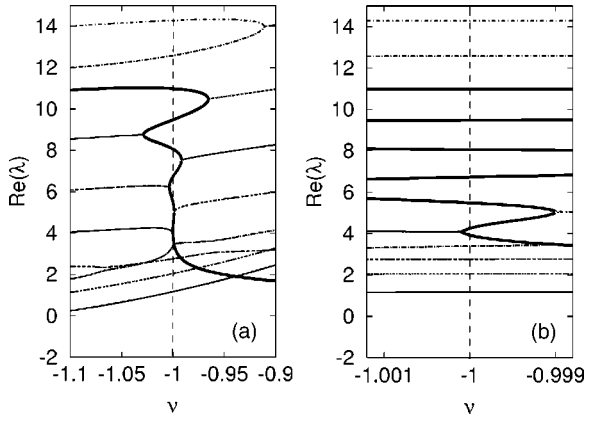

FIG. 6. The purely real curve (high-lighted fat) in the vicinity of $\nu=-1$ (cutoff length $b=7$) is formed by intermediate real segments between complex valued segments which branch off to the left and to the right. This leads to a ladderlike structure with exceptional points as nodes. The zoomed picture in (b) shows that the "oscillations" of the real curve about the line $\nu=-1$ persist also at its lower end, but with strongly reduced "amplitude." When the cutoff is slightly increased to $b\gtrsim 7$ the lowest exceptional (real-to-complex transition) point (b) will cross the line $\nu=-1$ and will in the region $\nu>-1$ coalesce with the other (nearest) exceptional point. As a result, one intermediate segment will be removed from the real curve and a purely complex-valued branch pair will smoothly tend from "far left" ($\nu<-1$) to "far right" ($\nu>-1$)—similar to the lower lying purely complex branches visible in the graphics.

levels below them. A sort of web structure is forming with a purely real branch remaining between the left ($\nu<-1$) and right ($\nu>-1$) purely complex (twisted) spectral regions. The complex-valued level pairs are branching off from the real branch forming a ladder-shaped structure. At the low-energy end of this ladder a second process occurs. The left ($\nu<-1$) complex level pairs are passing the line $\nu=-1$ and move to the right of it. There, at some $\nu>-1$ the corresponding exceptional point merges with an exceptional point of a right branch. As a result, one of the real segments between left and right off-branching levels disappears and a smooth complex-valued branch forms which extends over a large ν interval and whose imaginary components are increasing very fast when b is increased. It remains the real branch which becomes more and more vertical whereas the complex branch is not intersecting with it (the real component of the complex branch is coinciding at one point with the real branch but the imaginary components are not coinciding).

Analyzing the sequence of Figs. 2–6 we observe that, when the cutoff b is increased, a rather special (and seemingly inextricable) branch pattern of real and complex eigenvalues is forming in the vicinity of the exponent $\nu=-1$. [The phenomenon may be generic since in Ref. 46, the "wiggly upwards" spectral pattern has also been detected for a very different one-parametric family of asymptotically exponential $\mathcal{PT}$-symmetric potentials $V(x)=-(i\sinh x)^{\beta}$ near the Herbst-type exponent $\beta=1$.] The extreme steepness of an increasing number of imaginary branches and their accumulation at $\nu=-1$ (see Figs. 4 and 5) as well as the occurrence of the almost vertical real branch (Fig. 6) are indicating the formation of a local spectral singularity with $\partial_\nu E|_{\nu\to-1}\to\pm\infty$ at the (almost) vertical segments of the real-valued branch as well as on the imaginary branches close to the exceptional points of the "ladder" structure. From the figures it is not at all obvious how this pattern is compatible with the Herbst limit of an empty spectrum for $b\to\infty$ at $\nu=-1$. We will resolve this interesting puzzle in the next section.

IV. THE HERBST LIMIT AND ITS RELATION TO THE SQUIRE EQUATION OF HYDRODYNAMICS

In Ref. 15 it was shown by Herbst that the spectrum of a Hamiltonian with imaginary linear potential (imaginary homogeneous electric field) over the real line $x\in\mathbb{R}$ is empty. The differential expression of the corresponding operator coincides with that of the $\mathcal{PT}$-symmetric Schrödinger-type equation (18) with exponent $\nu=-1$,

$$[-\partial_y^2 - igb^3 y]\psi(y) = b^2 E\psi(y), \quad \psi(y = \pm 1) = 0. \tag{21}$$

The only difference of (21) compared to the Herbst model is in the Dirichlet boundary conditions at $y=\pm 1$ which restrict the system to a box (square well). Due to this analogy and for sake of brevity, we will call the model (21) a "Herbst box."

We start our consideration by noticing that Eq. (21) and the spectral function $\mu(b,E)=b^2E$ are invariant under the rescaling $b\mapsto g^{-1/3}b$, $E\mapsto g^{2/3}E$ so that henceforth we can set $g=1$, without loss of generality. The corresponding Herbst box Hamiltonian we denote as

$$H_{Hb}(b) \coloneqq -\partial_y^2 - ib^3 y. \tag{22}$$

Equation (21) itself is of Airy type and its solutions can be expressed as

$$\psi(y) = C_1 A_1[\xi(y)] + C_2 A_2[\xi(y)],$$

$$\xi(y) \coloneqq e^{i(\pi/3)}[-iby - E],$$

where $C_{1,2}=$const, and $A_1(\xi)$, $A_2(\xi)$ are any two of the Airy functions $\mathrm{Ai}(\xi)$, $\mathrm{Ai}(q\xi)$, $\mathrm{Ai}(q^2\xi)$ with $q \coloneqq e^{i2\pi/3}$. As usual, the boundary conditions lead to a characteristic determinant which defines the spectrum of the eigenvalue problem. In case of Eq. (21), it reads

$$\Delta(E) = A_1(\xi_+)A_2(\xi_-) - A_1(\xi_-)A_2(\xi_+) = 0, \quad \xi_\pm \coloneqq \xi(y = \pm 1). \tag{23}$$

Characteristic determinants of this type (built over Airy functions) have been intensively studied since 1995 in a paper series of Stepin[47,48] and Shkalikov *et al.*[49] (for related work see also Ref. 50) on the spectral properties of the Squire equation of hydrodynamics (the corresponding physical background can be found, e.g., in Refs. 51 and 52)

$$H_{\mathrm{Sq}}(\varepsilon) \coloneqq i\varepsilon\partial_y^2 + y, \quad (H_{\mathrm{Sq}} - \lambda)\chi = 0, \quad \chi(y = \pm 1) = 0, \quad \varepsilon \coloneqq (\tilde{\alpha}R)^{-1}. \tag{24}$$

Before we make the (obviously existing) relation of this model to the Herbst box model explicit, we briefly review a few of its properties.

The Squire equation (24) describes the normal vorticity of a plane Couette flow with linear velocity profile. The parameter $\tilde{\alpha}>0$ denotes a real-valued wave number which originates from the decomposition of a two-dimensional flow perturbation,

$$\Psi(x,y,t) = \chi(y)e^{i\tilde{\alpha}(x-\lambda t)},$$

$R>0$ is the Reynolds number and ε—the viscosity. The spectrum of H_{Sq} was found to have a Y-shaped form.[48,49,51] All the eigenvalues are located in a close vicinity of the three segments $(1,-i/\sqrt{3}]$, $(-1,-i/\sqrt{3}]$, $[-i/\sqrt{3},-i\infty)$. In the limit of large $R\to\infty$, $\tilde{\alpha}\geqslant 1$ and correspondingly small $\varepsilon\to 0^+$ the eigenvalue problem (24) turns into a singular perturbation problem and its eigenvalues show a remarkable limiting behavior. For $\varepsilon\to 0^+$, more and more eigenvalues "move in" from $-i\infty$ along the line $[-i/\sqrt{3},-i\infty)$, merge pairwise in the vicinity of the point $-i/\sqrt{3}$, and depart then (again pairwise) to move symmetrically along the segments $[1,-i/\sqrt{3}]$, $[-1,-i/\sqrt{3}]$ and to "fill" them step by step—leaving the Y-shape invariant. The process was described in Ref. 48 as a special type of transition from a discrete spectrum to a continuous one. Explicitly, the following asymptotic estimates were found in Refs. 48 and 49:

$$\lambda_n \sim -i\varepsilon\frac{\pi^2 n^2}{4} \in [-i/\sqrt{3},-i\infty), \quad n\to\infty, \tag{25}$$

$$\lambda_n^{\pm} \sim \pm 1 \pm \varepsilon^{1/3} s_n e^{\pm i\pi/6} \in (\pm 1,-i/\sqrt{3}], \quad \varepsilon\to 0^+, \tag{26}$$

where s_n are the zeros of the Airy function

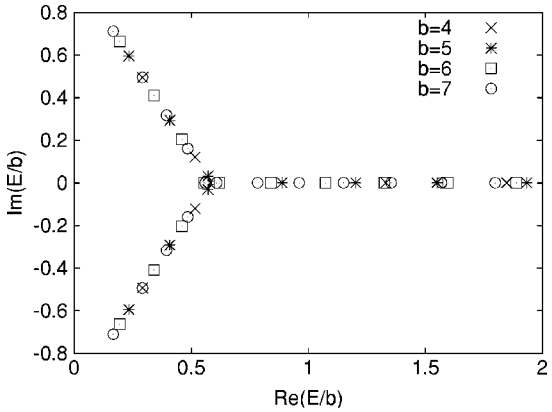

FIG. 7. The rescaled Herbst-box spectrum $E/b=i\lambda(\epsilon=b^{-3})$ coincides with the Wick-rotated Y-shaped spectrum of the Squire operator $H_{\mathrm{Sq}}(\varepsilon)$.

$$\mathrm{Ai}(s_n)=0, \quad s_n \in \mathbb{R}_-.$$

One clearly sees that the smaller ε is chosen the smaller the distances between the eigenvalues become—leading in the limit $\varepsilon \to 0$ to a quasicontinuous spectrum.

Noticing that the pairwise merging and splitting (level crossing) of the eigenvalues occurs at $\lambda^+ \sim \lambda^- \sim -i/\sqrt{3}$, it is easy to estimate that the value ε_n, for which this crossing is connected with the nth Airy function root s_n, is given by

$$\varepsilon_n^{1/3} \sim \frac{2}{|s_n|\sqrt{3}}. \tag{27}$$

Let us utilize the above results now for the Herbst-box model. A simple comparison of the eigenvalue problems (21) (for $g=1$) and (24) shows that these problems may be made coinciding if one sets

$$i\varepsilon^{-1}[H_{\mathrm{Sq}}(\varepsilon)-\lambda]\chi(y) \stackrel{!}{=} \mathcal{P}[H_{\mathrm{Hb}}(b)-b^2E]\mathcal{P}[\mathcal{P}\psi(y)]=0$$

and identifies

$$b^3=\varepsilon^{-1}, \quad E=ib\lambda, \quad \mathcal{P}H_{\mathrm{Hb}}(b)\mathcal{P}=i\varepsilon^{-1}H_{\mathrm{Sq}}(\varepsilon), \quad \mathcal{P}\psi(y)=\chi(y). \tag{28}$$

This means that the two models are related by the combined action of a rescaling, a Wick rotation and a coordinate reflection $\mathcal{P}$.

With the help of the estimates (25) and (26) it is now an easy task to explain the behavior of the Herbst-box spectrum $E(b)$.

(i) The rescaled spectrum $E(b)/b=i\lambda(\varepsilon=b^{-3})$ (shown in Fig. 7) is simply the Wick-rotated version of the original shape-invariant "Y" of the Squire operator $H_{\mathrm{Sq}}(\varepsilon)$. With increasing $b=\varepsilon^{-1/3}$ more and more eigenvalues "move in" from $+\infty$ and "fill" the two complex conjugate branches $(i,1/\sqrt{3}]$, $(-i,1/\sqrt{3}]$ of the "Y" as well as the half-line $[1/\sqrt{3},+\infty)$—in a similar way as in the original $\lambda(\varepsilon \to 0)$ limit. For $b \to \infty$ the spectrum becomes quasicontinuous on the rotated "Y."

(ii) Due to the shape invariance of $E(b)/b$, the spectrum $E(b)=ib\lambda(b^{-3})$ itself inflates when b increases. It is located in the close vicinity of the segments $(ib,b/\sqrt{3}]$, $(-ib,b/\sqrt{3}]$, $[b/\sqrt{3},+\infty)$ and moves with $b \to \infty$ to infinity—leaving (for sufficiently high b) an empty region at any fixed finite distance from the origin of the spectral E plane. Hence, we find (as required) that for $b \to \infty$ the Herbst-box spectrum turns into the empty spectrum of the original Herbst model over the real line $\mathbb{R}$.

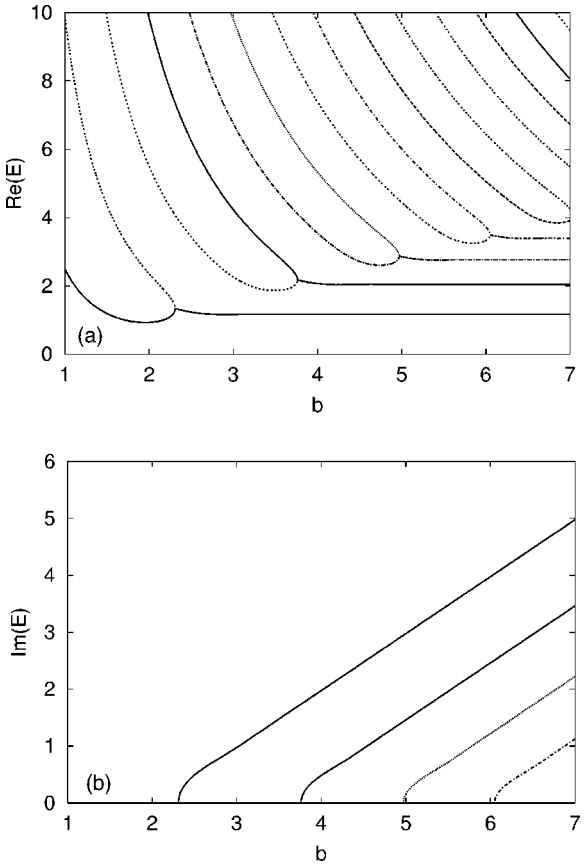

FIG. 8. Real and imaginary components of the Herbst-box spectrum as functions of the cutoff length b [complex conjugate ($\Im\lambda \leqslant 0$)-components omitted]. The asymptotical behavior of the complex-valued branches is clearly visible (constant real components and linear b dependence of the imaginary components).

(iii) For finite b, the asymptotic estimates (25) and (26) map into

$$E_k \sim \frac{\pi^2 k^2}{4b^2} \in b \times [1/\sqrt{3}, +\infty), \quad k \to \infty, \tag{29}$$

$$E_n^{\pm} \sim \pm ib \pm is_n e^{\pm i\pi/6} \in b \times (\pm i, 1/\sqrt{3}], \quad b \to \infty, \tag{30}$$

and we identify (29) as the pure square well spectrum

$$\mu(b, E_k) = b^2 E_k \sim \pi^2 k^2/4 \in b^3 \times [1/\sqrt{3}, +\infty) \tag{31}$$

of the high-energy sector which is almost not affected by the $\mathcal{PT}$-symmetric interaction. In contrast, the low-energy sector described by (30) shows a purely linear scaling behavior of the imaginary energy components $\Im E_n^{\pm}$, whereas the real components remain asymptotically fixed when b increases. This situation is also clearly visible from the numerical results presented in Fig. 8. The graphics of the equivalent spectrum $\mu(b, E)$, depicted in Fig. 9, provides a complementary description and shows how (for increasing b) the b-independent eigenvalues $\mu(b, E_k)$ of Eq. (31) leave the high-energy sector, obtain an explicit b dependence in the intermediate-energy sector and finally coalesce and split into complex conjugate pairs.

(iv) From the form of the spectral branches on the E plane (rotated "Y") it is clear that the level crossings in the vicinity of $E \sim b/\sqrt{3}$ correspond to the typical real-to-complex phase tran-

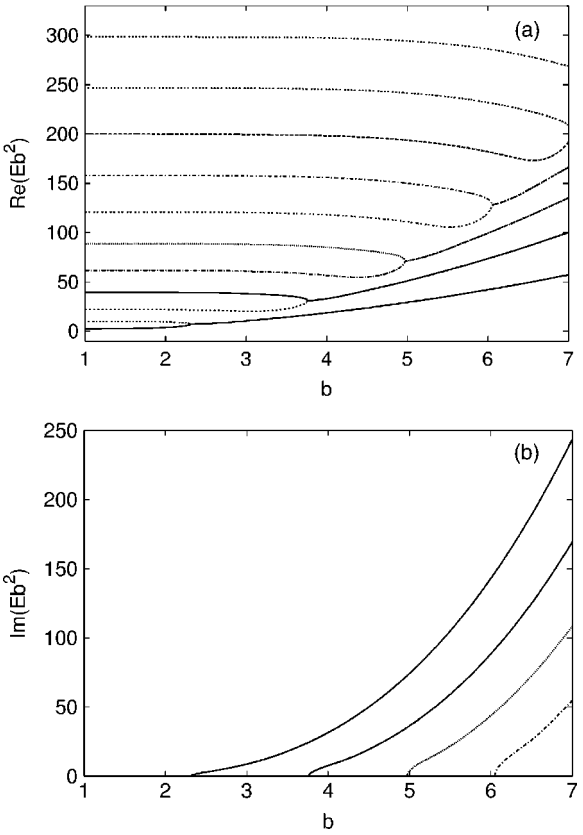

FIG. 9. The rescaled Herbst-box spectrum $\mu(b,E)=b^2E$ allows a complementary view on the transition from the high-energy sector to the intermediate and low-energy sector.

sitions of $\mathcal{PT}$-symmetric models in Krein spaces. With the help of relation (27) the cutoff-scales b_n and positions E_n of the level crossings can be roughly estimated as

$$b_n \sim |s_n|\sqrt{3}/2, \quad E_n \sim |s_n|/2. \tag{32}$$

One can use the explicit values of these b_n ($b_1 \approx 2.02$, $b_2 \approx 3.54$, $b_3 \approx 4.78$, $b_4 \approx 5.88$, $b_5 \approx 6.87$, $b_6 \approx 7.81$,…), to roughly derive the number of the lowest uncrossed modes in the cases $b=2,4,6,7$. For $b=2,4,6$ the result exactly coincides with the level crossing pattern shown (at $\nu=-1$) in Figs. 2–4, whereas the value b_5 is clearly smaller than the actual transition value $b_{5(c)}$ for which according to Figs. 6(b) and 8 holds $b_{5(c)} \gtrsim 7$. For completeness, we note that the asymptotic approximation[48] of the Airy function roots

$$|s_n| = \left[\frac{3\pi}{2}\left(n-\frac{1}{4}\right)\right]^{2/3} + O(n^{-4/3}), \quad n \to \infty$$

together with (32) yields the following rough estimate for the lowest purely real-valued mode:

$$k_a > \frac{4}{3\pi}\left(\frac{2}{\sqrt{3}}b\right)^{3/2} + \frac{1}{2}.$$

The scaling dimension $\kappa_a=3/2$ of this bound is only one-half of the scaling dimension $\kappa_s=4+\nu=3$ of the corresponding supremum bound (20). The exact positions of the level crossing points are given by the multiple roots of the characteristic determinant, $\Delta(E)$

$=0$, $\partial_E\Delta(E)=0$. This equation system can be simplified via Wronskian $W[A_1(.),A_2(.)]$ to yield the conditions

$$A_{1,2}(\xi_+) = \pm A_{1,2}(\xi_-)$$

(see Ref. 48 for the details). Plugging the numerical results from the eigenvalue solver into this equation with $A_{1,2}(\xi)$ chosen as in Ref. 48, $A_1(\xi) := \mathrm{Ai}(\xi)$, $A_2(\xi) := \mathrm{Ai}(q^2\xi)$, selects the condition $A_{1,2}(\xi_+)=A_{1,2}(\xi_-)$ and satisfies it within numerical working precision. For the same data holds $A_{1,2}(\xi_+) \neq -A_{1,2}(\xi_-)$.

(v) The spectral behavior $E(b)$ for increasing cutoff b can be summarized as follows. At the beginning, the real eigenvalues from the high-energy sector decrease as $E_k \sim \pi^2 k^2/(4b^2)$—moving into the intermediate energy region. When b approaches $b_n \sim |s_n|\sqrt{3}/2$ from below, the real eigenvalues $\{E_{2n-1}, E_{2n}\}$ (corresponding to a pair of positive and negative Krein space states[11]) coalesce at $E_{2n-1} \sim E_{2n} \sim |s_n|/2$ and a real-to-complex transition occurs $\{E_{2n-1}, E_{2n}\} \to \{E_n^+, E_n^-\}$. When b is further increased the real energy components remain fixed $\Re E_n^{\pm} \approx |s_n|/2$ [see Fig. 8(a)], whereas the imaginary components blow up linearly along the asymptotes $\Im E_n^{\pm} \sim \pm b \pm s_n\sqrt{3}/2$ [Fig. 8(b)].

Let us, for finite b, relate the obtained Herbst-box results to the spectral behavior of the $\mathcal{PT}$-symmetric interpolation model of the preceding section. Apart from the obvious one-to-one correspondence of the high-energy sectors [see (31)], a clear identification is immediately possible for those Herbst-box eigenvalues which are close to the imaginary axis and which have the largest imaginary components. These eigenvalues are located on the branches with the largest imaginary components in Figs. 3–5 (which stay complex when ν passes through the Herbst-box value $\nu=-1$). It is clearly visible from these figures that, for increasing b, the imaginary components are blowing up, whereas the real components remain asymptotically constant.

So far, we have found a clear correspondence for those regions on the Herbst-box "Y" which are located away from the center of the "Y" with its real-to-complex phase transitions. A more subtle situation occurs in the vicinity of this center. The corresponding Herbst box eigenvalues will map into points located close to (or on) the forming (almost) vertical segment of the purely real branch depicted in Fig. 6. From the zoomed graphics in Fig. 6(b) we observe that the purely real and almost vertical branch of the interpolation model "oscillates" around the Herbst-box line at $\nu=-1$ with strongly decreasing "amplitude" to its low-energy part. With increasing b this "decreasing amplitude" effect becomes stronger and the "oscillations" are only traceable with the help of an appropriately increased zooming scale. Nevertheless, it can be read off that the real-to-complex transition of the Herbst-box spectrum follows qualitatively the same scheme for any finite b. The real eigenvalues of the Herbst box are all located on the purely real branch of the interpolation model and the real-to-complex transition occurs when the lowest exceptional point on this branch moves from the left sector $\nu<-1$ through the Herbst-box value $\nu=-1$ into the right sector $\nu>-1$—to coalesce afterwards with the next higher exceptional point from the right sector. With this passing of the left-sector exceptional point through the line $\nu=-1$ the Herbst-box eigenvalues become pairwise complex conjugate with strongly increasing imaginary components [due to the asymptotically diverging gradient $\partial_\nu E(b\to\infty)|_{\nu\approx -1} \to \pm\infty$]. The real-to-complex transition with subsequently increasing imaginary components are illustrated in Fig. 10.

Finally, we note that in the limit $b\to\infty$, the lowest-lying intersection of the purely real branch with the Herbst-box line $\nu=-1$ moves away to infinity like $b/\sqrt{3}$ (the lower bound of the real segment $[b/\sqrt{3},\infty)$ of the Herbst-box "Y") so that the real branch itself remains for any finite energy in the right sector $\nu>-1$—approaching the Herbst-box line asymptotically. This reproduces the earlier observations of Refs. 1 and 16 for the spectrum of the Bender–Boettcher problem over the real line. Additionally, our Herbst-box results predict for this problem diverging imaginary components at $\nu=-1: |\Im E(b\to\infty, \nu\to -1)| \to \infty$. Taking these observations together we once more see that in the limit $b\to\infty$ a spectral singularity is forming at $\nu=-1$ with $|E(b\to\infty, \nu\to -1)| \to \infty$, $|\partial_\nu E(b\to\infty, \nu\to -1)| \to \infty$.

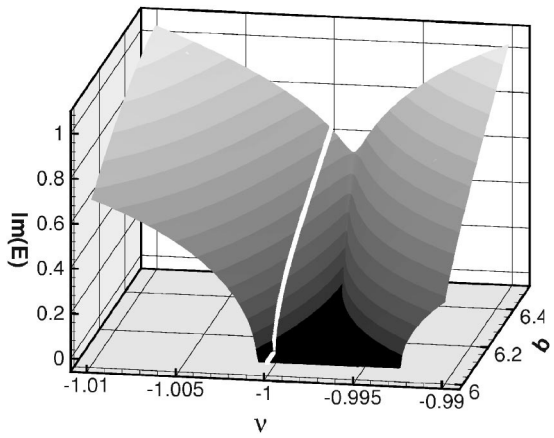

FIG. 10. Concrete example for the generic merging process of two complex-valued spectral branches (present here for $b<b_{\mathrm{coal}}\approx 6.36$) into a single complex-valued branch for $b>b_{\mathrm{coal}}$. The two exceptional (real-to-complex transition) points existing for $b<b_{\mathrm{coal}}$ are located on the plane $(\nu,b,\Im E=0)$ and coalesce at $b=b_{\mathrm{coal}}$. The corresponding point $(\nu_{\mathrm{coal}}\approx -0.9983>-1, b_{\mathrm{coal}}\approx 6.36, \Im E=0)$ is the starting (cusp) point of a sharp "valley" of the nonvanishing imaginary component which steeply grows and smooths when $b>b_{\mathrm{coal}}$ is further increased. The white curve marks the Herbst-box values. Before the two exceptional points coalesce, the left one of these points crosses the Herbst-box configuration at $(\nu=-1, b=b_c\approx 6.02, \Im E=0)$ and a real-to-complex transition occurs for the Herbst-box model.

V. CONLUSIONS

In the present paper we considered three models emerging in different physical setups, but which are closely related with each other by their underlying mathematical structure as spectral problems in Krein spaces. The models are a one-dimensional $\mathcal{PT}$-symmetric quantum mechanical interpolation setup defined over a square well of finite width $2b$, the spherically symmetric MHD α^2-dynamo as well as the Squire equation of hydrodynamics. For the PTSQM model and the α^2-dynamo we made their close relation transparent by transforming them into a 2×2 matrix operator representation with coinciding block structure of the Krein space metric (involution operator). In the case of the Squire equation we showed that the corresponding spectral problem is connected with a $\mathcal{PT}$-symmetric eigenvalue problem by a rescaling and Wick rotation. (It is clear that, apart from the Squire equation, there will exist other hydrodynamic equations which can be structurally identified as Wick-rotated $\mathcal{PT}$-symmetric systems in Krein spaces.)

Based on recent results on the spectrum of the Squire equation, we performed a qualitative analysis of the $\mathcal{PT}$-symmetric quantum mechanical interpolation model for arbitrary square well widths (cutoffs) $2b$. This allowed us to trace the emergence of the Herbst limit with its empty spectrum as a spectral singularity and to fit our results to those of the Bender–Boettcher equation over the real line. We obtained a rich structure of multiple spectral phase transitions from purely real eigenvalues to pairs of complex conjugate ones—as it was to expect for spectral problems in Krein spaces.

A deeper insight into the Herbst-box spectrum and a possible extension of the present results to $\mathcal{PT}$-symmetric Hamiltonians of the type $H_{M,N}=-\partial_x^2+x^{2M}(ix)^N$, $M,N=1,2,3,\ldots$ over square wells can probably be achieved by representing the characteristic determinant $\Delta(E)$ in (23) via Hadamar product representation of the Airy functions[53] as a spectral determinant of Bethe-ansatz type[16,29,54] and studying it by similar cocycle functional equations as in Ref. 55.

A question which was not touched in the present paper concerns the orthogonality of the Herbst-box eigenfunctions. For the Squire equation it is known that its eigenfunctions show a strong nonorthogonality[47,51] (due to the non-normality of the Squire operator) for eigenvalues in the vicinity of the branch point center of the "Y" (pseudospectral techniques[50,51,56] play an important role in this case). Our above considerations indicate on a link of this issue with the forming spectral singularity $|\partial_\nu E(\nu\approx -1, b\gg 1)|\gg 1$ in the vicinity of the almost vertical segments of the purely real branch in the spectrum of the $\mathcal{PT}$-symmetric interpolation model.

Finally, we would like to note two issues which seem of relevance for future considerations. The first one is in developing efficient mathematical tools to find the hypersurfaces in parameter space where spectral phase transitions of the real-to-complex type occur. [A two-step method similar in spirit was successfully used, e.g., in higher-dimensional gravitational models to obtain the stability regions in the moduli (parameter) space of these models (step one, find the critical hypersurfaces; step two, identify the stability/instability properties of the model aside from these hypersurfaces).[57]] Knowing these hypersurfaces, one would know the boundaries which separate the parameter space regions with unbroken $\mathcal{PT}$-symmetry from regions with spontaneously broken $\mathcal{PT}$-symmetry. In case of α^2-dynamos the corresponding knowledge would allow for a more precise prediction of configurations with tendency to magnetic field reversals. The second issue concerns methods for solving inverse spectral problems in Krein spaces. Such methods would be extremely helpful for the data analysis of the dynamo experiments which are planned for the near future at seven sites around the world.[58]

ACKNOWLEDGMENTS

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APPENDIX: A FEW COMMENTS ON THE PHYSICS OF MHD α^2-DYNAMOS

The dynamo operator $\hat{H}_l[\alpha]$ originates from the MHD mean-field induction equation (cf. Ref. 12)

$$\partial_t \mathbf{B} = \boldsymbol{\nabla} \times (\alpha \mathbf{B}) + \nu_m \Delta \mathbf{B} \tag{A1}$$

for the magnetic field **B**. This equation results from averaging over small scale turbulences in the velocity field of the electrically conducting fluid (or plasma) which drives the dynamo. The helical turbulence function $\alpha(x)$ [also called α-profile (in general setups, α is not a scalar function but a tensor[12])] encodes the net effect of the small scale physics on the large scale (mean) magnetic field **B**. For certain topologically nontrivial helical velocity and **B**-field configurations an inverse cascade effect occurs which induces an energy transfer from small-scale structures to large-scale structures (inverse to the energy transfer in usual turbulence cascades where the energy is pumped from large-scale structures into smaller structures until it finally dissipates and transforms into thermal energy). For sufficiently strong inverse cascade effects the advection term $\boldsymbol{\nabla} \times (\alpha \mathbf{B})$ starts to dominate over the diffusion term $\nu_m \Delta \mathbf{B}$ (ν_m is the magnetic diffusivity) and the magnetic field strength starts to grow exponentially. This kinematic dynamo effect (growing **B** field for a given velocity field of the fluid) is followed by a saturated dynamo regime where a balance between the dynamo effect and the back-reaction of the induced magnetic field on the velocity field (via Navier–Stokes equation) prevents a further growth of the field strength **B**. For completeness, we note that an MHD dynamo is an open system in which part of the kinetic energy of the conducting fluid (or plasma) transforms into magnetic field energy.

The dynamo eigenvalue problem

$$\hat{H}_l[\alpha]\phi_{l,n} = \lambda_{l,n}\phi_{l,n}, \quad \phi_{l,n}(t) \sim \exp \lambda_{l,n} t \tag{A2}$$

follows from the induction equation (A1) via a double decomposition: decomposing the **B** field into poloidal and toroidal components (what leads to the two-component vector structure of $\phi_{l,n}$) and expanding them further into spherical harmonics. In the simplest (toy model) case of a spherically symmetric dynamo configuration the corresponding modes decouple completely and one arrives at the spherical l-mode projection (12) and (A2) (the subscript n denotes the radial mode number).

Up to now only a single exactly solvable α^2-dynamo model is known—the model with constant α-profile.[12] Its spectrum is discrete, real,[59] bounded above and, depending on the value of

α, it is either completely negative (for α below a critical α_c: $\alpha < \alpha_c$) or it contains a finite number of positive eigenvalues $\lambda_{l,n} > 0$. The dynamo effect is dominated by these latter eigenmodes. In practice, it usually suffices to concentrate the analysis on the dominating upper most growing mode (or a few of the upper most modes) for dipole ($l=1$) and quadrupole ($l=2$) configurations. (There exist no "s-wave" α^2-dynamos with $l=0$.[12,13])

The spectral properties of the dynamo operator $\hat{H}_l[\alpha]$ are becoming much richer for inhomogeneous α-profiles $\alpha(r) \neq$ const, when real-to-complex transitions occur—as discussed in Sec. II C and shown in Fig. 1.

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Feynman integrals for nonsmooth and rapidly growing potentials

Margarida de Faria[a)]
CCM, University of Madeira, P-9000-390 Funchal, Portugal

Maria João Oliveira[b)]
Universidade of Aberta, P-1269-001 Lisbon, Portugal; CMAF, University of Lisbon, P-1649-003 Lisbon, Portugal; and BiBoS, University of Bielefeld, D-33501 Bielefeld, Germany

Ludwig Streit[c)]
BiBoS, University of Bielefeld, D-33501 Bielefeld, Germany and CCM, University of Madeira, P-9000-390 Funchal, Portugal

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The Feynman integral for the Schrödinger propagator is constructed as a generalized function of white noise, for a linear space of potentials spanned by finite (signed) measures of bounded support and Laplace transforms of such measures, i.e., locally singular as well as rapidly growing at infinity. Remarkably, all these propagators admit a perturbation expansion. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1904162]

I. INTRODUCTION

On a mathematical level of rigor, the construction of Feynman integrals for quantum mechanical propagators will have to be done for specific classes of potentials. In particular, the Feynman integrand has been identified as a well-defined generalized function in white noise space, e.g., for the following classes of potentials:

(i) (signed) finite measures which are "small" at infinity,[7,15]
(ii) Fourier transforms of measures,[18]
(iii) Laplace transforms of finite measures.[13]

Potentials in the third space are locally smooth but may grow rapidly at infinity, a prominent example is the Morse potential. On the other hand, the first of these classes includes locally singular potentials such as the Dirac delta function. It is also important for the construction of Feynman integrals with boundary conditions.[2] Hence it would be desirable to admit potentials which are linear combinations of elements from the first and third space. The present paper addresses this problem: we show the existence of Feynman integrals solving the propagator equation for such potentials.

II. WHITE NOISE ANALYSIS

In this section we briefly recall the concepts and results of white noise analysis used throughout this work (see, e.g., Refs. 1, 4, 5, 8, 11, 12, 14, and 16 for a detailed explanation).

The starting point of (one-dimensional) white noise analysis is the real Gelfand triple

[a)]Electronic mail: mfaria@uma.pt
[b)]Electronic mail: oliveira@cii.fc.ul.pt
[c)]Electronic mail: streit@physik.uni-bielefeld.de

$$S(\mathbb{R}) \subset L^2(\mathbb{R}) \subset S'(\mathbb{R}),$$

where $L^2 := L^2(\mathbb{R})$ is the real Hilbert space of all square integrable functions with respect to the Lebesgue measure, $\mathcal{S} := S(\mathbb{R})$ and $\mathcal{S}' := S'(\mathbb{R})$ are the real Schwartz spaces of test functions and tempered distributions, respectively. In the sequel we denote the norm on L^2 by $|\cdot|$, the corresponding inner product by $(\cdot,\cdot)$, and the dual pairing between $\mathcal{S}'$ and $\mathcal{S}$ by $\langle\cdot,\cdot\rangle$. The dual pairing $\langle\cdot,\cdot\rangle$ and the inner product $(\cdot,\cdot)$ are connected by

$$\langle f,\xi\rangle = (f,\xi), \quad f \in L^2, \quad \xi \in \mathcal{S}.$$

By $\{|\cdot|_p\}_{p\in\mathbb{N}}$ we denote a family of Hilbert norms topologizing the space $\mathcal{S}$.

Let $\mathcal{B}$ be the σ-algebra generated by the cylinder sets on $\mathcal{S}'$. Through the Minlos theorem one may define the white noise measure space $(\mathcal{S}',\mathcal{B},\mu)$ by giving the characteristic function

$$C(\xi) := \int_{\mathcal{S}'} e^{i\langle\omega,\xi\rangle}\, \mathrm{d}\mu(\omega) = e^{-1/2|\xi|^2}, \quad \xi \in \mathcal{S}.$$

Within this formalism a version of the (one-dimensional) Wiener Brownian motion is given by

$$B(t) := \langle\omega, \mathbb{1}_{[0,t)}\rangle, \quad \omega \in \mathcal{S}',$$

where $\mathbb{1}_A$ denotes the indicator function of a set A.

Now let us consider the complex Hilbert space $L^2(\mu) := L^2(\mathcal{S}',\mathcal{B},\mu)$. As this space quite often shows to be too small for applications, to proceed further we shall construct a Gelfand triple around the space $L^2(\mu)$. More precisely, first we shall choose a space of white noise test functions contained in $L^2(\mu)$ and then we work on its larger dual space of distributions. In our case we will use the space $(\mathcal{S})^{-1}$ of generalized white noise functionals or Kondratiev distributions and its well-known subspace $(\mathcal{S})'$ of Hida distributions (or generalized Brownian functionals) with corresponding Gelfand triples

$$(\mathcal{S})^1 \subset L^2(\mu) \subset (\mathcal{S})^{-1}$$

and

$$(\mathcal{S}) \subset L^2(\mu) \subset (\mathcal{S})'.$$

Instead of reproducing the explicit construction of $(\mathcal{S})^{-1}$ and $(\mathcal{S})'$ (see, e.g., Refs. 1 and 5), in Theorems 1 and 2 below we will define both spaces by their T-transforms. Given a $\Phi \in (\mathcal{S})^{-1}$, there exist $p,q \in \mathbb{N}_0$ such that we can define for every

$$\xi \in U_{p,q} := \{\xi \in \mathcal{S} : 2^q |\xi|_p^2 < 1\}$$

the T-transform of Φ by

$$T\Phi(\xi) := \langle\langle \Phi, \exp(i\langle\cdot,\xi\rangle)\rangle\rangle. \tag{1}$$

Here $\langle\langle\cdot,\cdot\rangle\rangle$ denotes the dual pairing between $(\mathcal{S})^{-1}$ and $(\mathcal{S})^1$ which is defined as the bilinear extension of the inner product on $L^2(\mu)$. In particular, for Hida distributions Φ, definition (1) extends to $\xi \in \mathcal{S}$. By analytic continuation, the definition of T-transform may be extended to the underlying complexified space $\mathcal{S}_{\mathbb{C}}$ of $\mathcal{S}$.

In order to define the spaces $(\mathcal{S})^{-1}$ and $(\mathcal{S})'$ through their T-transforms we need the following two definitions.

Definition 1: A function $F: U \to \mathbb{C}$ is holomorphic on an open set $U \subset \mathcal{S}_{\mathbb{C}}$ if

(1) *for all $\theta_0 \in U$ and any $\theta \in \mathcal{S}_{\mathbb{C}}$ the mapping $\mathbb{C} \ni \lambda \mapsto F(\lambda\theta + \theta_0)$ is holomorphic on some neighborhood of $0 \in \mathbb{C}$,*
(2) *F is locally bounded.*

Definition 2: A function $F:\mathcal{S}\to\mathbb{C}$ is called a U-functional whenever

(1) *for every $\xi_1,\xi_2\in\mathcal{S}$ the mapping $\mathbb{R}\ni\lambda\mapsto F(\lambda\xi_1+\xi_2)$ has an entire extension to $\lambda\in\mathbb{C}$,*
(2) *there exist constants $K_1,K_2>0$ such that*

$$|F(z\xi)|\leqslant K_1\exp(K_2|z|^2\|\xi\|^2),\quad \forall\, z\in\mathbb{C},\ \xi\in\mathcal{S}$$

for some continuous norm $\|\cdot\|$ on $\mathcal{S}$.

We are now ready to state the aforementioned characterization results.

Theorem 1: (Ref. 10) *Let $0\in U\subset\mathcal{S}_{\mathbb{C}}$ be an open set and $F:U\to\mathbb{C}$ be a holomorphic function on U. Then there is a unique $\Phi\in(\mathcal{S})^{-1}$ such that $T\Phi=F$. Conversely, given a $\Phi\in(\mathcal{S})^{-1}$ the function $T\Phi$ is holomorphic on some open set in $\mathcal{S}_{\mathbb{C}}$ containing 0. The correspondence between F and Φ is a bijection if one identifies holomorphic functions which coincide on some open neighborhood of 0 in $\mathcal{S}_{\mathbb{C}}$.*

Theorem 2: (Refs. 9 and 17) *The T-transform defines a bijection between the space $(\mathcal{S})'$ and the space of U-functionals.*

As a consequence of Theorem 1 one may derive the next two statements. The first one concerns the convergence of sequences of generalized white noise functionals and the second one the Bochner integration of families of the same type of generalized functionals. Similar results exist for Hida distributions (see, e.g., Ref. 5).

Theorem 3: *Let $(\Phi_n)_{n\in\mathbb{N}}$ be a sequence in $(\mathcal{S})^{-1}$ such that there are $p,q\in\mathbb{N}_0$ so that*

(1) *all $T\Phi_n$ are holomorphic on $U_{p,q}:=\{\theta\in\mathcal{S}_{\mathbb{C}}:2^q|\theta|_p^2<1\}$,*
(2) *there exists a $C>0$ such that $|T\Phi_n(\theta)|\leqslant C$ for all $\theta\in U_{p,q}$ and all $n\in\mathbb{N}$,*
(3) *$(T\Phi_n(\theta))_{n\in\mathbb{N}}$ is a Cauchy sequence in $\mathbb{C}$ for all $\theta\in U_{p,q}$.*

Then $(\Phi_n)_{n\in\mathbb{N}}$ converges strongly in $(\mathcal{S})^{-1}$.

Theorem 4: *Let $(\Lambda,\mathcal{F},\nu)$ be a measure space and $\lambda\mapsto\Phi_\lambda$ be a mapping from Λ to $(\mathcal{S})^{-1}$. We assume that there exists a $U_{p,q}\subset\mathcal{S}_{\mathbb{C}},p,q\in\mathbb{N}_0$, such that*

(1) *$T\Phi_\lambda$ is holomorphic on $U_{p,q}$ for every $\lambda\in\Lambda$,*
(2) *the mapping $\lambda\mapsto T\Phi_\lambda(\theta)$ is measurable for every $\theta\in U_{p,q}$,*
(3) *there is a $C\in L^1(\Lambda,\mathcal{F},\nu)$ such that*

$$|T\Phi_\lambda(\theta)|\leqslant C(\lambda),\quad \forall\,\theta\in U_{p,q},\quad \nu-a.a.\lambda\in\Lambda.$$

Then there exist $p',q'\in\mathbb{N}_0$, which only depend on p,q, such that Φ_λ is Bochner integrable. In particular,

$$\int_\Lambda \Phi_\lambda\,\mathrm{d}\nu(\lambda)\in(\mathcal{S})^{-1}$$

and $T(\int_\Lambda\Phi_\lambda\,\mathrm{d}\nu(\lambda))$ is holomorphic on $U_{p',q'}$. One has

$$\left\langle\!\left\langle\int_\Lambda\Phi_\lambda\,\mathrm{d}\nu(\lambda),\varphi\right\rangle\!\right\rangle=\int_\Lambda\langle\langle\Phi_\lambda,\varphi\rangle\rangle\mathrm{d}\nu(\lambda),\quad\forall\,\varphi\in(\mathcal{S})^1.$$

III. THE FREE FEYNMAN INTEGRAL

We follow Refs. 3 and 6 in viewing the Feynman integral as a weighted average over Brownian paths. We use a slight change in the definition of the paths, which are here modeled by

$$x(\tau) = x - \sqrt{\frac{\hbar}{m}}\int_\tau^t \omega(s)\mathrm{d}s := x - \sqrt{\frac{\hbar}{m}}\langle \omega, \mathbb{1}_{(\tau,t]}\rangle, \quad \omega \in \mathcal{S}'.$$

That is, instead of fixing the starting point of the paths, we fix the endpoint x at time t. In the sequel we set $\hbar = m = 1$. Correspondingly, the Feynman integrand for the free motion is defined by

$$I_0 := I_0(x,t|y,t_0) := N\exp\left(\frac{i+1}{2}\int_{\mathbb{R}} \omega^2(\tau)\mathrm{d}\tau\right)\delta(x(t_0)-y),$$

where, informally, N is a normalizing factor, more precisely, $N\exp(\cdot)$ is a Gauss kernel (see, e.g., Refs. 5 and 15). We recall that the Donsker delta function $\delta(x(t_0)-y)$ is used to fix the starting point of the paths at time $t_0 < t$. The T-transform of the free Feynman integrand

$$TI_0(\xi) = \frac{1}{\sqrt{2\pi i(t-t_0)}}\exp\left(-\frac{i}{2}\int_{\mathbb{R}} \xi^2(\tau)\mathrm{d}\tau\right)\exp\left(\frac{i}{2(t-t_0)}\left(\int_{t_0}^t \xi(\tau)\mathrm{d}\tau + x - y\right)^2\right) \tag{2}$$

is a U-functional and we use it to define I_0 as a Hida distribution (see Ref. 3).

From the physical point of view, equality (2) clearly shows that the Feynman integral $TI_0(0)$ is the free particle propagator

$$\frac{1}{\sqrt{2\pi i(t-t_0)}}\exp\left(\frac{i}{2(t-t_0)}(x-y)^2\right).$$

Besides this particular case, even for nonzero ξ the T-transform of I_0 has a physical interpretation. Integrating formally by parts we find

$$TI_0(\xi) = \int_{\mathcal{S}'} I_0(\omega)\exp\left(-i\int_{t_0}^t x(\tau)\dot{\xi}(\tau)\mathrm{d}\tau\right)\mathrm{d}\mu(\omega)\exp\left(-\frac{i}{2}\int_{[t_0,t]^c} \xi^2(\tau)\mathrm{d}\tau + ix\xi(t) - iy\xi(t_0)\right).$$

The term $\exp(-i\int_{t_0}^t x(\tau)\dot{\xi}(\tau)\mathrm{d}\tau)$ would thus correspond to a time-dependent potential $W(x,t) = \dot{\xi}(t)x$. In fact, it is straightforward to verify that

$$\Theta(t-t_0)\cdot TI_0(\xi) = K_0^{(\xi)}\exp\left(-\frac{i}{2}\int_{[t_0,t]^c} \xi^2(\tau)\mathrm{d}\tau + ix\xi(t) - iy\xi(t_0)\right),$$

where Θ is the Heaviside function and

$$K_0^{(\xi)} := K_0^{(\xi)}(x,t|y,t_0) := \frac{\Theta(t-t_0)}{\sqrt{2\pi i|t-t_0|}}\exp\left(-\frac{i}{2}\int_{t_0}^t \xi^2(\tau)\mathrm{d}\tau\right)\exp\left(\frac{i}{2|t-t_0|}\left(\int_{t_0}^t \xi(\tau)\mathrm{d}\tau + x - y\right)^2\right)$$
$$\times \exp(iy\xi(t_0) - ix\xi(t))$$

is the Green function corresponding to the potential W, i.e., $K_0^{(\xi)}$ obeys the Schrödinger equation

$$\left(i\partial_t + \frac{1}{2}\partial_x^2 - \dot{\xi}(t)x\right)K_0^{(\xi)}(x,t|y,t_0) = i\delta(t-t_0)\,\delta(x-y). \tag{3}$$

IV. INTERACTIONS

In the sequel $\mathcal{K}_1$ denotes the linear space of all potentials V on $\mathbb{R}$ of the form

$$V(x) = \int_{\mathbb{R}} e^{\alpha x}\,\mathrm{d}m(\alpha), \quad x \in \mathbb{R},$$

where m is a complex measure on the Borel sets on $\mathbb{R}$ fulfilling the condition

$$\int_{\mathbb{R}} e^{C|\alpha|} d|m|(\alpha) < \infty, \quad \forall\, C > 0 \tag{4}$$

(cf. Ref. 13), and $\mathcal{K}_2$ denotes the space of all potentials V on $\mathbb{R}$ which are generalized functions of the type

$$V(x) = \int_{\mathbb{R}} \delta(x-y)\mathrm{d}m(y), \quad x \in \mathbb{R},$$

where $\mathrm{d}m(y) := V(y)\mathrm{d}y$ is a finite signed Borel measure of bounded support (cf. Ref. 7).

Remark 5: *A Lebesgue dominated convergence argument shows that potentials in $\mathcal{K}_1$ are restrictions to the real line of entire functions.*[13] *In particular, they are locally bounded and smooth.*

Our aim is to define the Feynman integrand

$$I := I_0 \cdot \exp\left(-i\int_{t_0}^{t} V(x(\tau))\mathrm{d}\tau\right) \tag{5}$$

for a potential V of the form $V=V_1+V_2$, $V_i \in \mathcal{K}_i$,

$$V_1(x) = \int_{\mathbb{R}} e^{\alpha x}\, \mathrm{d}m_1(\alpha), \quad V_2(x) = \int_{\mathbb{R}} \delta(x-y)\mathrm{d}m_2(y), \tag{6}$$

where

$$x(\tau) = x - \int_{\tau}^{t} \omega(s)\mathrm{d}s, \quad \omega \in \mathcal{S}',$$

as before. In order to do this, first we must give a meaning to the heuristic expression (5). In Theorem 7 it will be shown that I is indeed a well-defined generalized white noise functional. Second, it has to be proven that the expectation of I solves the Schrödinger equation for the potential V.

As a first step we expand the exponential in (5) into a perturbation series. This leads to

$$\begin{aligned} I = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \sum_{k=0}^{n} \binom{n}{k} k! \int_{\Delta_k} d^k\tau \int_{t_0}^{t} d^{n-k}s \\ \times \int_{\mathbb{R}^k}\int_{\mathbb{R}^{n-k}} I_0 \exp\left(\sum_{l=1}^{n-k} \alpha_l x(s_l)\right) \prod_{j=1}^{k} \delta(x(\tau_j)-x_j) \prod_{l=1}^{n-k} \mathrm{d}m_1(\alpha_l) \prod_{j=1}^{k} \mathrm{d}m_2(x_j), \end{aligned} \tag{7}$$

where $\Delta_k := \{(\tau_1,\ldots,\tau_k) : t_0 < \tau_1 < \cdots < \tau_k < t\}$. In the above expression the integrals over $\Delta_k, \mathbb{R}^k$ and $[t_0,t]^{n-k}, \mathbb{R}^{n-k}$ disappear, respectively, for $k=0$ and $k=n$. Our aim is to apply Theorems 3 and 4 to show the existence of the above series and integrals. However, first we must establish the pointwise multiplication of generalized functionals

$$I_0 \exp\left(\sum_{l=1}^{n-k} \alpha_l x(s_l)\right) \prod_{j=1}^{k} \delta(x(\tau_j)-x_j)$$

as a well-defined generalized functional. Due to the characterization result Theorem 2 it is enough to define this product through its T-transform. Arguing informally, for $\xi \in \mathcal{S}$ we are led to

$$T\left(I_0 \exp\left(\sum_{l=1}^{n-k} \alpha_l x(s_l)\right)\prod_{j=1}^{k} \delta(x(\tau_j)-x_j)\right)(\xi)$$
$$= \int_{\mathcal{S}'} I_0 \exp\left(\sum_{l=1}^{n-k} \alpha_l x(s_l)\right)\prod_{j=1}^{k} \delta(x(\tau_j)-x_j)\exp(i\langle\omega,\xi\rangle)\mathrm{d}\mu(\omega)$$
$$= \exp\left(x\sum_{l=1}^{n-k}\alpha_l\right)\cdot T\left(I_0\prod_{j=1}^{k}\delta(x(\tau_j)-x_j)\right)\left(\xi+i\sum_{l=1}^{n-k}\alpha_l \mathbb{1}_{(s_l,t]}\right).$$

The product $I_0\Pi_{j=1}^{k}\delta(x(\tau_j)-x_j)$ is a slight generalization of the free Feynman integrand I_0, with more than just one delta function, and may be defined by its T-transform,

$$T\left(I_0\prod_{j=1}^{k}\delta(x(\tau_j)-x_j)\right)(\xi) = \exp\left(-\frac{i}{2}\int_{[t_0,t]^c}\xi^2(s)\mathrm{d}s + ix\xi(t)-iy\xi(t_0)\right)\prod_{j=1}^{k+1}K_0^{(\xi)}(x_j,\tau_j|x_{j-1},\tau_{j-1})$$
$$= \exp\left(-\frac{i}{2}\int_{\mathbb{R}}\xi^2(s)\mathrm{d}s\right)\prod_{j=1}^{k+1}\left\{\frac{1}{\sqrt{2\pi i(\tau_j-\tau_{j-1})}}\right.$$
$$\left.\times\exp\left(\frac{i}{2(\tau_j-\tau_{j-1})}\left(\int_{\tau_{j-1}}^{\tau_j}\xi(s)\mathrm{d}s + x_j - x_{j-1}\right)^2\right)\right\}. \tag{8}$$

Here $\tau_0 := t_0$, $x_0 := y$, $\tau_{k+1} := t$, and $x_{k+1} := x$. Clearly the explicit formula (8) is continuously extendable to all $\xi \in L^2$ which allows an extension of $T(I_0\Pi_{j=1}^{k}\delta(x(\tau_j)-x_j))$ to the argument $\xi + i\Sigma_{l=1}^{n-k}\alpha_l\mathbb{1}_{(s_l,t]}$.

Proposition 6: The product

$$\Phi_{n,k} := I_0 \exp\left(\sum_{l=1}^{n-k}\alpha_l x(s_l)\right)\prod_{j=1}^{k}\delta(x(\tau_j)-x_j)$$

defined by

$$T\Phi_{n,k}(\xi) = T\left(I_0\prod_{j=1}^{k}\delta(x(\tau_j)-x_j)\right)\left(\xi+i\sum_{l=1}^{n-k}\alpha_l\mathbb{1}_{(s_l,t]}\right)\exp\left(x\sum_{l=1}^{n-k}\alpha_l\right)$$
$$= \exp\left(-\frac{i}{2}\int_{\mathbb{R}}\left(\xi(s)+i\sum_{l=1}^{n-k}\alpha_l\mathbb{1}_{(s_l,t]}(s)\right)^2\mathrm{d}s\right)\prod_{j=1}^{k+1}\frac{1}{\sqrt{2\pi i(\tau_j-\tau_{j-1})}}$$
$$\times\exp\left(\sum_{j=1}^{k+1}\frac{i}{2(\tau_j-\tau_{j-1})}\left(\int_{\tau_{j-1}}^{\tau_j}\left(\xi(s)+i\sum_{l=1}^{n-k}\alpha_l\mathbb{1}_{(s_l,t]}(s)\right)\mathrm{d}s + x_j - x_{j-1}\right)^2\right)\exp\left(x\sum_{l=1}^{n-k}\alpha_l\right)$$

is a Hida distribution.

Proof: It is obvious that the latter explicit formula fulfills the first part of Definition 2, analyticity. In order to prove that $\Phi_{n,k}$ is a Hida distribution by application of Theorem 2, we must only show that $T\Phi_{n,k}$ also obeys a bound as in the second part of Definition 2. For every $\theta \in \mathcal{S}_{\mathbb{C}}$ we have

$$
\begin{aligned}
|T\Phi_{n,k}(\theta)| \leqslant \exp\left(|x|\sum_{l=1}^{n-k}|\alpha_l|\right)\prod_{j=1}^{k+1}\frac{1}{\sqrt{2\pi(\tau_j-\tau_{j-1})}}\left|\exp\left(-\frac{i}{2}\int_{\mathbb{R}}\theta^2(s)\mathrm{d}s\right.\right.\\
\left.\left.+\sum_{l=1}^{n-k}\alpha_l\int_{\mathbb{R}}\theta(s)\mathbb{1}_{(s_l,t]}(s)\mathrm{d}s\right)\right|\left|\exp\left(\sum_{j=1}^{k+1}\frac{i}{2(\tau_j-\tau_{j-1})}\left(\int_{\tau_{j-1}}^{\tau_j}\theta(s)\mathrm{d}s\right)^2\right)\right|\\
\times\left|\exp\left(\sum_{j=1}^{k+1}\frac{1}{\tau_{j-1}-\tau_j}\left(\int_{\tau_{j-1}}^{\tau_j}\theta(s)\mathrm{d}s\right)\sum_{l=1}^{n-k}\alpha_l\left(\int_{\tau_{j-1}}^{\tau_j}\mathbb{1}_{(s_l,t]}(s)\mathrm{d}s\right)\right)\right|\\
\times\left|\exp\left(\sum_{j=1}^{k+1}\frac{i(x_j-x_{j-1})}{\tau_j-\tau_{j-1}}\int_{\tau_{j-1}}^{\tau_j}\left(\theta(s)+i\sum_{l=1}^{n-k}\alpha_l\mathbb{1}_{(s_l,t]}(s)\right)\mathrm{d}s\right)\right|
\end{aligned}
$$

which is majorized by

$$
\begin{aligned}
|T\Phi_{n,k}(\theta)| &\leqslant \prod_{j=1}^{k+1}\frac{1}{\sqrt{2\pi(\tau_j-\tau_{j-1})}}\exp(2\|\theta\|^2)\exp\left((|x|+t-t_0+\|\theta\|^2)\sum_{l=1}^{n-k}|\alpha_l|\right)\\
&\quad\times\exp\left(4\max_{0\leqslant j\leqslant k+1}|x_j|\sum_{l=1}^{n-k}|\alpha_l|\right)\exp\left(\max_{0\leqslant j\leqslant k+1}(|x_j|^2)\right)\\
&=: C(\tau_1,\ldots,\tau_k;\alpha_1,\ldots,\alpha_{n-k};x_1,\ldots,x_k;\theta)\\
&=: C
\end{aligned}
\tag{9}
$$

independent of $s_1,\ldots,s_{n-k}$, where

$$
\|\theta\| := \sup_{s\in[t_0,t]}|\theta(s)|+\int_{t_0}^{t}|\dot{\theta}(s)|\mathrm{d}s+|\theta|
$$

is a continuous norm on $\mathcal{S}_{\mathbb{C}}$, cf. Appendix below. This estimate for $T\Phi_{n,k}$ is of the form required in Definition 2, which completes the proof. ■

According to Proposition 6, all $\Phi_{n,k}$ are Hida distributions and thus also generalized white noise functionals with $T\Phi_{n,k}$ entire on $\mathcal{S}_{\mathbb{C}}$. Moreover, each $T\Phi_{n,k}(\theta)$ is a measurable function of $\tau_1,\ldots,\tau_k;\ s_1,\ldots,s_{n-k};\ \alpha_1,\ldots,\alpha_{n-k};\ x_1,\ldots,x_k$ for every $\theta\in\mathcal{S}_{\mathbb{C}}$. Hence, in order to apply Theorem 4 to prove the existence of the integrals in I, we must only find a suitable integrable bound for $|T\Phi_{n,k}(\theta)|$. Since the measure m_1 fulfills the integrability condition (4) and the signed measure m_2 is finite and has support contained in some bounded interval $[-a,a]$, $a>0$, one may infer the integrability of C for every $\theta\in\mathcal{S}_{\mathbb{C}}$,

$$
\begin{aligned}
&\left|\int_{\Delta_k}d^k\tau\int_{t_0}^{t}d^{n-k}s\int_{\mathbb{R}^k}\prod_{j=1}^{k}\mathrm{d}m_2(x_j)\int_{\mathbb{R}^{n-k}}\prod_{l=1}^{n-k}d|m_1|(\alpha_l)C\right|\\
&\quad\leqslant\exp(2\|\theta\|^2+b^2)(t-t_0)^{n-k}\int_{\Delta_k}\prod_{j=1}^{k+1}\frac{1}{\sqrt{2\pi(\tau_j-\tau_{j-1})}}d^k\tau\left|\int_{\mathbb{R}}\mathrm{d}m_2(x)\right|^k\\
&\quad\times\left(\int_{\mathbb{R}}\exp((|x|+4b+t-t_0+\|\theta\|^2)|\alpha|)d|m_1|(\alpha)\right)^{n-k},
\end{aligned}
$$

where $b:=\max\{a,|y|,|x|\}$. Thus, according to Theorem 4, there exists an open set $U\subset\mathcal{S}_{\mathbb{C}}$ independent of n such that

$$I_{n,k} := \int_{\Delta_k} d^k\tau \int_{t_0}^{t} d^{n-k}s \int_{\mathbb{R}^k} \int_{\mathbb{R}^{n-k}} \Phi_{n,k} \prod_{l=1}^{n-k} \mathrm{d}m_1(\alpha_l) \prod_{j=1}^{k} \mathrm{d}m_2(x_j) \in (\mathcal{S})^{-1}$$

for each $k \leqslant n$ and every $n \in \mathbb{N}$, and all $TI_{n,k}$ are holomorphic on U. To conclude the existence of I we must only prove that the series in n converges in $(\mathcal{S})^{-1}$ in the strong sense. This follows from Theorem 3. In fact, due to (7), for every $\theta \in U$ one has

$$|TI(\theta)| \leqslant \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{k=0}^{n} \binom{n}{k} k! |TI_{n,k}(\theta)|,$$

where the right-hand side is upper bounded by the factor $\exp(2\|\theta\|^2 + b^2)$ times the Cauchy product of the convergent series

$$\left(\sum_{n=0}^{\infty} \frac{1}{n!} \left((t-t_0) \int_{\mathbb{R}} e^{(|x|+4b+t-t_0+\|\theta\|^2)|\alpha|} d|m_1|(\alpha) \right)^n \right) \left(\sum_{n=0}^{\infty} \left| \int_{\mathbb{R}} \mathrm{d}m_2(x) \right|^n \int_{\Delta_n} \prod_{j=1}^{n+1} \frac{1}{\sqrt{2\pi(\tau_j - \tau_{j-1})}} d^n\tau \right)$$

$$= \exp\left((t-t_0) \int_{\mathbb{R}} e^{(|x|+4b+t-t_0+\|\theta\|^2)|\alpha|} d|m_1|(\alpha) \right) \sum_{n=0}^{\infty} \left| \int_{\mathbb{R}} \mathrm{d}m_2(x) \right|^n \int_{\Delta_n} \prod_{j=1}^{n+1} \frac{1}{\sqrt{2\pi(\tau_j - \tau_{j-1})}} d^n\tau.$$

We note that the latter series converges because

$$\int_{\Delta_n} \prod_{j=1}^{n+1} \frac{1}{\sqrt{2\pi(\tau_j - \tau_{j-1})}} d^n\tau = \left(\frac{\Gamma(1/2)}{\sqrt{2\pi}} \right)^{n+1} \frac{(t-t_0)^{(n-1)/2}}{\Gamma\left(\frac{n+1}{2} \right)}$$

is rapidly decreasing in n.

In this way we have proved the following result.

Theorem 7: *For every $V_1 \in \mathcal{K}_1$ and $V_2 \in \mathcal{K}_2$ of the form (6), the*

$$I := \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \sum_{k=0}^{n} \binom{n}{k} k! \int_{\Delta_k} d^k\tau \int_{t_0}^{t} d^{n-k}s \int_{\mathbb{R}^k} \int_{\mathbb{R}^{n-k}} I_0 \exp\left(\sum_{l=1}^{n-k} \alpha_l x(s_l) \right)$$
$$\times \prod_{j=1}^{k} \delta(x(\tau_j) - x_j) \prod_{l=1}^{n-k} \mathrm{d}m_1(\alpha_l) \prod_{j=1}^{k} \mathrm{d}m_2(x_j)$$

exists as a generalized white noise functional. The series converges strongly in $(\mathcal{S})^{-1}$ and the integrals exist in the sense of Bochner integrals. Therefore we may express the T-transform of I by

$$TI(\theta) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \sum_{k=0}^{n} \binom{n}{k} k! \int_{\Delta_k} d^k\tau \int_{t_0}^{t} d^{n-k}s \int_{\mathbb{R}^k} \int_{\mathbb{R}^{n-k}} T\left(I_0 \exp\left(\sum_{l=1}^{n-k} \alpha_l x(s_l) \right) \prod_{j=1}^{k} \delta(x(\tau_j) - x_j) \right)(\theta)$$
$$\times \prod_{l=1}^{n-k} \mathrm{d}m_1(\alpha_l) \prod_{j=1}^{k} \mathrm{d}m_2(x_j)$$

for every θ in a neighborhood $\{\theta \in \mathcal{S}_{\mathbb{C}} : 2^q |\theta|_p^2 < 1\}$ of zero, for some p, $q \in \mathbb{N}_0$.

According to Theorem 7, I is a well-defined generalized white noise functional. In order to conclude that I defines a Feynman integrand it remains to show that the expectation $TI(0)$ of I solves the Schrödinger equation for a potential $V = V_1 + V_2$, $V_i \in \mathcal{K}_i$. As in the free motion case we consider, more generally,

$$K^{(\theta)}(x,t|y,t_0) := \Theta(t-t_0)TI(\theta)\exp\left(\frac{i}{2}\int_{[t_0,t]^c}\theta^2(\tau)\mathrm{d}\tau + iy\theta(t_0) - ix\theta(t)\right).$$

Insertion of $TI(\theta)$ as given in Theorem 7, with

$$T\left(I_0\exp\left(\sum_{l=1}^{n-k}\alpha_l x(s_l)\right)\prod_{j=1}^{k}\delta(x(\tau_j)-x_j)\right)$$

as in Proposition 6, yields

$$K^{(\theta)}(x,t|y,t_0) = \sum_{n=0}^{\infty} K_n^{(\theta)}(x,t|y,t_0),$$

with

$$\begin{aligned}K_n^{(\theta)}(x,t|y,t_0) := {}& \frac{(-i)^n}{n!}\int_{t_0}^{t} d^n s\int_{\mathbb{R}^n}\prod_{l=1}^{n}\mathrm{d}m_1(\alpha_l)K_0^{(\theta_n)}(x,t|y,t_0)\\ &+\sum_{k=1}^{n-1}\frac{(-i)^{n-k}}{(n-k)!}\int_{t_0}^{t} d^{n-k}s\int_{\mathbb{R}^{n-k}}\prod_{l=1}^{n-k}\mathrm{d}m_1(\alpha_l)G_k^{(\theta_{n-k})}(x,t|y,t_0)+G_n^{(\theta)}(x,t|y,t_0),\end{aligned} \tag{10}$$

where we have set $\theta_{n-k} := \theta_{n-k}(s_1,\ldots,s_{n-k},\alpha_1,\ldots,\alpha_{n-k}) := \theta + i\Sigma_{l=1}^{n-k}\alpha_l\mathbb{1}_{(s_l,t]}$ for $k=0,\ldots,n-1$, $\theta_0 := \theta$, and

$$G_k^{(\theta_{n-k})}(x,t|y,t_0) := (-i)^k\int_{\Delta_k} d^k\tau\int_{\mathbb{R}^k}\prod_{j=1}^{k}\mathrm{d}m_2(x_j)\prod_{j=1}^{k+1}K_0^{(\theta_{n-k})}(x_j,\tau_j|x_{j-1},\tau_{j-1})$$

for $k=1,\ldots,n$, $n>0$.

We expect $K^{(\theta)}$ to be the propagator corresponding to the potential $W(x,t)=V(x)+\dot{\theta}(t)x$.

Theorem 8: *$K^{(\theta)}(x,t|y,t_0)$ is a Green function for the Schrödinger equation*

$$(i\partial_t + \tfrac{1}{2}\partial_x^2 - \dot{\theta}(t)x - V(x))K^{(\theta)}(x,t|y,t_0) = i\delta(t-t_0)\delta(x-y). \tag{11}$$

In particular, $K(x,t|y,t_0) := TI(0)$ is a Feynman integral solving

$$i\partial_t K(x,t|y,t_0) = (-\tfrac{1}{2}\partial_x^2 + V(x))K(x,t|y,t_0) \quad \text{for } t > t_0. \tag{12}$$

Remark 3: K corresponds to a unitary evolution whenever $H=-\frac{1}{2}\partial_x^2+V$ has a unique self-adjoint extension.

Proof: Let us consider an interval $[T_0,T]$ such that $[t_0,t]\subset[T_0,T]$. Estimates similar to those done in the proof of Proposition 6 show that $K_n^{(\theta)}(\cdot,\cdot|y,t_0)$ is locally integrable on $\mathbb{R}\times[T_0,T]$ with respect to $\mathrm{d}m_2\times\mathrm{d}t$ and the Lebesgue measure. Therefore, we may regard $K_n^{(\theta)}$ as a distribution on $\mathcal{D}(\Omega) := \mathcal{D}(\mathbb{R}\times[T_0,T])$,

$$\langle K_n^{(\theta)}(\cdot,\cdot|y,t_0),\varphi\rangle = \int_{\mathbb{R}}\mathrm{d}x\int_{T_0}^{T}\mathrm{d}t\,K_n^{(\theta)}(x,t|y,t_0)\varphi(x,t), \quad \varphi\in\mathcal{D}(\Omega).$$

And we may also define a distribution $V_2K_n^{(\theta)}$ by setting

$$\langle V_2 K_n^{(\theta)}(\cdot,\cdot|y,t_0),\varphi\rangle = \int_{\mathbb{R}} \mathrm{d}m_2(x) \int_{T_0}^{T} \mathrm{d}t\, K_n^{(\theta)}(x,t|y,t_0)\varphi(x,t), \quad \varphi \in \mathcal{D}(\Omega).$$

To abbreviate we introduce the notation $\hat{L} := i\partial_t + \frac{1}{2}\partial_x^2 - \dot{\theta}(t)x$ and $\hat{L}^*$ for the dual operator. According to (10), observe that for any test function $\varphi \in \mathcal{D}(\Omega)$ one finds

$$\begin{aligned}\langle \hat{L} K_n^{(\theta)},\varphi\rangle = {} & \frac{(-i)^n}{n!}\left\langle \int_{t_0}^{\cdot} d^n s \int_{\mathbb{R}^n} \prod_{l=1}^{n} \mathrm{d}m_1(\alpha_l) K_0^{(\theta_n)}(\cdot,\cdot|y,t_0), \hat{L}^*\varphi \right\rangle \\ & + \sum_{k=1}^{n-1} \frac{(-i)^{n-k}}{(n-k)!}\left\langle \int_{t_0}^{\cdot} d^{n-k} s \int_{\mathbb{R}^{n-k}} \prod_{l=1}^{n-k} \mathrm{d}m_1(\alpha_l) G_k^{(\theta_{n-k})}(\cdot,\cdot|y,t_0), \hat{L}^*\varphi \right\rangle + \langle G_n^{(\theta)}(\cdot,\cdot|y,t_0), \hat{L}^*\varphi\rangle, \end{aligned} \tag{13}$$

where

$$\begin{aligned} & \frac{(-i)^n}{n!}\left\langle \int_{t_0}^{\cdot} d^n s \int_{\mathbb{R}^n} \prod_{l=1}^{n} \mathrm{d}m_1(\alpha_l) K_0^{(\theta_n)}(\cdot,\cdot|y,t_0), \hat{L}^*\varphi \right\rangle \\ & \quad = \frac{(-i)^{n-1}}{(n-1)!}\left\langle V_1 \int_{t_0}^{\cdot} d^{n-1} s \int_{\mathbb{R}^{n-1}} \prod_{l=1}^{n-1} \mathrm{d}m_1(\alpha_l) K_0^{(\theta_{n-1})}(\cdot,\cdot|y,t_0), \varphi \right\rangle, \end{aligned} \tag{14}$$

cf. Ref. 13, and

$$\langle G_n^{(\theta)}(\cdot,\cdot|y,t_0), \hat{L}^*\varphi\rangle = \langle V_2 G_{n-1}^{(\theta)}(\cdot,\cdot|y,t_0),\varphi\rangle, \tag{15}$$

cf. Refs. 15 and 7. The generic case (13) is intermediate between (14) and (15) and is dealt with by a combination of the corresponding techniques. This yields

$$\begin{aligned} & \left\langle \int_{t_0}^{\cdot} d^{n-k} s \int_{\mathbb{R}^{n-k}} \prod_{l=1}^{n-k} \mathrm{d}m_1(\alpha_l) G_k^{(\theta_{n-k})}(\cdot,\cdot|y,t_0), \hat{L}^*\varphi \right\rangle \\ & \quad = i(n-k)\left\langle V_1 \int_{t_0}^{\cdot} d^{n-k-1} s \int_{\mathbb{R}^{n-k-1}} \prod_{l=1}^{n-k-1} \mathrm{d}m_1(\alpha_l) G_k^{(\theta_{n-k-1})}(\cdot,\cdot|y,t_0), \varphi \right\rangle \\ & \qquad + \left\langle V_2 \int_{t_0}^{\cdot} d^{n-k} s \int_{\mathbb{R}^{n-k}} \prod_{l=1}^{n-k} \mathrm{d}m_1(\alpha_l) G_{k-1}^{(\theta_{n-k})}(\cdot,\cdot|y,t_0), \varphi \right\rangle, \end{aligned}$$

for any $k=2,\ldots,n-2$,

$$\begin{aligned} & \left\langle \int_{t_0}^{\cdot} d^{n-1} s \int_{\mathbb{R}^{n-1}} \prod_{l=1}^{n-1} \mathrm{d}m_1(\alpha_l) G_1^{(\theta_{n-1})}(\cdot,\cdot|y,t_0), \hat{L}^*\varphi \right\rangle \\ & \quad = i(n-1)\left\langle V_1 \int_{t_0}^{\cdot} d^{n-2} s \int_{\mathbb{R}^{n-2}} \prod_{l=1}^{n-2} \mathrm{d}m_1(\alpha_l) G_1^{(\theta_{n-2})}(\cdot,\cdot|y,t_0), \varphi \right\rangle \\ & \qquad + \left\langle V_2 \int_{t_0}^{\cdot} d^{n-1} s \int_{\mathbb{R}^{n-1}} \prod_{l=1}^{n-1} \mathrm{d}m_1(\alpha_l) K_0^{(\theta_{n-1})}(\cdot,\cdot|y,t_0), \varphi \right\rangle \end{aligned}$$

and

$$\left\langle \int_{t_0}^{\cdot} ds \int_{\mathbb{R}} \mathrm{d}m_1(\alpha_1) G_{n-1}^{(\theta_1)}(\cdot,\cdot|y,t_0), \hat{L}^*\varphi \right\rangle$$
$$= i\langle V_1 G_{n-1}^{(\theta)}(\cdot,\cdot|y,t_0),\varphi\rangle + \left\langle V_2 \int_{t_0}^{\cdot} ds \int_{\mathbb{R}} \mathrm{d}m_1(\alpha_1) G_{n-2}^{(\theta_1)}(\cdot,\cdot|y,t_0),\varphi \right\rangle.$$

As a result

$$\langle \hat{L} K_n^{(\theta)},\varphi\rangle = \frac{(-i)^{n-1}}{(n-1)!}\left\langle (V_1+V_2)\int_{t_0}^{\cdot} d^{n-1}s \int_{\mathbb{R}^{n-1}} \prod_{l=1}^{n-1} \mathrm{d}m_1(\alpha_l) K_0^{(\theta_{n-1})}(\cdot,\cdot|y,t_0),\varphi \right\rangle$$
$$+ \sum_{k=1}^{n-2} \frac{(-i)^{n-k-1}}{(n-k-1)!}\left\langle V_1 \int_{t_0}^{\cdot} d^{n-k-1}s \int_{\mathbb{R}^{n-k-1}} \prod_{l=1}^{n-k-1} \mathrm{d}m_1(\alpha_l) G_k^{(\theta_{n-k-1})}(\cdot,\cdot|y,t_0),\varphi \right\rangle$$
$$+ \sum_{k=2}^{n-1} \frac{(-i)^{n-k}}{(n-k)!}\left\langle V_2 \int_{t_0}^{\cdot} d^{n-k}s \int_{\mathbb{R}^{n-k}} \prod_{l=1}^{n-k} \mathrm{d}m_1(\alpha_l) G_{k-1}^{(\theta_{n-k})}(\cdot,\cdot|y,t_0),\varphi \right\rangle$$
$$+ \langle (V_1+V_2) G_{n-1}^{(\theta)}(\cdot,\cdot|y,t_0),\varphi\rangle,$$

which is equivalent to

$$\langle \hat{L} K_n^{(\theta)},\varphi\rangle = \langle (V_1+V_2) K_{n-1}^{(\theta)},\varphi\rangle, \quad \varphi \in \mathcal{D}(\Omega),$$

for any $n \geqslant 1$. Using (3) and summing over n, we obtain (11). ■

We conclude by an observation which is obvious from the above construction but somewhat unexpected given that the Hamiltonians with potentials in the class $\mathcal{K}_2$ will in general not admit a perturbative expansion (see, e.g., Ref. 13 for more on this).

Proposition 9: For any potential $V=g(V_1+V_2)$ with $V_i \in \mathcal{K}_i$, the solution K of the propagator equation (12) is analytic in the coupling constant g.

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APPENDIX: AN ESTIMATE

For the proof of Proposition 6, we need to estimate

$$|T\Phi_{n,k}(\theta)| \leqslant \exp\left(|x|\sum_{l=1}^{n-k}|\alpha_l|\right)\prod_{j=1}^{k+1}\frac{1}{\sqrt{2\pi(\tau_j-\tau_{j-1})}}\left|\exp\left(-\frac{i}{2}\int_{\mathbb{R}}\theta^2(s)\mathrm{d}s\right.\right.$$
$$\left.\left.+\sum_{l=1}^{n-k}\alpha_l\int_{\mathbb{R}}\theta(s)\mathbb{1}_{(s_l,t]}(s)\mathrm{d}s\right)\right|\left|\exp\left(\sum_{j=1}^{k+1}\frac{i}{2(\tau_j-\tau_{j-1})}\left(\int_{\tau_{j-1}}^{\tau_j}\theta(s)\mathrm{d}s\right)^2\right)\right|$$
$$\times\left|\exp\left(\sum_{j=1}^{k+1}\frac{1}{\tau_{j-1}-\tau_j}\left(\int_{\tau_{j-1}}^{\tau_j}\theta(s)\mathrm{d}s\right)\sum_{l=1}^{n-k}\alpha_l\left(\int_{\tau_{j-1}}^{\tau_j}\mathbb{1}_{(s_l,t]}(s)\mathrm{d}s\right)\right)\right|$$
$$\times\left|\exp\left(\sum_{j=1}^{k+1}\frac{i(x_j-x_{j-1})}{\tau_j-\tau_{j-1}}\int_{\tau_{j-1}}^{\tau_j}\left(\theta(s)+i\sum_{l=1}^{n-k}\alpha_l\mathbb{1}_{(s_l,t]}(s)\right)\mathrm{d}s\right)\right|.$$

We shall now estimate, consecutively, the exponents occuring in the above expression.

Using the Cauchy–Schwarz inequality we may approximate

$$\left|\exp\left(\sum_{l=1}^{n-k}\alpha_l\int_{\mathbb{R}}\theta(s)\mathbb{1}_{(s_l,t]}(s)\mathrm{d}s\right)\right| \leqslant \exp\left(\sum_{l=1}^{n-k}|\alpha_l|\left(\int_{\mathbb{R}}|\theta(s)|^2\,\mathrm{d}s\right)^{1/2}\sqrt{t-s_l}\right) \leqslant \exp\left(\sqrt{t-t_0}|\theta|\sum_{l=1}^{n-k}|\alpha_l|\right)$$

and, similarly,

$$\left|\sum_{j=1}^{k+1}\frac{i}{2(\tau_j-\tau_{j-1})}\left(\int_{\tau_{j-1}}^{\tau_j}\theta(s)\mathrm{d}s\right)^2\right| \leqslant \frac{1}{2}|\theta|^2,$$

as well as

$$\begin{aligned}
&\left|\sum_{j=1}^{k+1}\frac{1}{\tau_{j-1}-\tau_j}\left(\int_{\tau_{j-1}}^{\tau_j}\theta(s)\mathrm{d}s\right)\sum_{l=1}^{n-k}\alpha_l\left(\int_{\tau_{j-1}}^{\tau_j}\mathbb{1}_{(s_l,t]}(s)\mathrm{d}s\right)\right| \\
&\quad\leqslant \sum_{j=1}^{k+1}\frac{1}{\tau_j-\tau_{j-1}}\left(\int_{\tau_{j-1}}^{\tau_j}|\theta(s)|\mathrm{d}s\right)(\tau_j-\tau_{j-1})\sum_{l=1}^{n-k}|\alpha_l| \\
&\quad= \sum_{l=1}^{n-k}|\alpha_l|\int_{t_0}^{t}|\theta(s)|\mathrm{d}s \\
&\quad\leqslant \sqrt{t-t_0}|\theta|\sum_{l=1}^{n-k}|\alpha_l|.
\end{aligned}$$

In order to estimate the exponential of the function

$$\begin{aligned}
\sum_{j=1}^{k+1}\frac{i(x_j-x_{j-1})}{\tau_j-\tau_{j-1}}\int_{\tau_{j-1}}^{\tau_j}\left(\theta(s)+i\sum_{l=1}^{n-k}\alpha_l\mathbb{1}_{(s_l,t]}(s)\right)\mathrm{d}s &= \sum_{j=1}^{k+1}\frac{i(x_j-x_{j-1})}{\tau_j-\tau_{j-1}}\int_{\tau_{j-1}}^{\tau_j}\theta(s)\mathrm{d}s \\
&\quad+\sum_{l=1}^{n-k}\alpha_l\sum_{j=1}^{k+1}\frac{x_{j-1}-x_j}{\tau_j-\tau_{j-1}}\int_{\tau_{j-1}}^{\tau_j}\mathbb{1}_{(s_l,t]}(s)\mathrm{d}s,
\end{aligned}$$

first we proceed as in Ref. 18, i.e.,

$$\begin{aligned}
\sum_{j=1}^{k+1}\frac{x_j-x_{j-1}}{\tau_j-\tau_{j-1}}\int_{\tau_{j-1}}^{\tau_j}\theta(s)\mathrm{d}s &= \frac{x}{t-\tau_k}\int_{\tau_k}^{t}\theta(s)\mathrm{d}s-\frac{y}{\tau_1-t_0}\int_{t_0}^{\tau_1}\theta(s)\mathrm{d}s \\
&\quad+\sum_{j=1}^{k}x_j\left(\frac{\int_{\tau_{j-1}}^{\tau_j}\theta(s)\mathrm{d}s}{\tau_j-\tau_{j-1}}-\frac{\int_{\tau_j}^{\tau_{j+1}}\theta(s)\mathrm{d}s}{\tau_{j+1}-\tau_j}\right).
\end{aligned}$$

By the mean value theorem

$$\sum_{j=1}^{k}x_j\left(\frac{\int_{\tau_{j-1}}^{\tau_j}\theta(s)\mathrm{d}s}{\tau_j-\tau_{j-1}}-\frac{\int_{\tau_j}^{\tau_{j+1}}\theta(s)\mathrm{d}s}{\tau_{j+1}-\tau_j}\right)=\sum_{j=1}^{k}x_j(\theta(r_j)-\theta(r_{j+1})),$$

where $r_j\in(\tau_{j-1},\tau_j)$. Therefore

$$\begin{aligned}
\left|\sum_{j=1}^{k+1}\frac{i(x_j-x_{j-1})}{\tau_j-\tau_{j-1}}\int_{\tau_{j-1}}^{\tau_j}\theta(s)\mathrm{d}s\right| &\leqslant (|x|+|y|)\sup_{[t_0,t]}|\theta|+\max_{1\leqslant j\leqslant k}|x_j|\sum_{j=1}^{k}\left|\int_{r_j}^{r_{j+1}}\dot{\theta}(s)\mathrm{d}s\right| \\
&\leqslant 2\max_{0\leqslant j\leqslant k+1}|x_j|\left(\sup_{[t_0,t]}|\theta|+\int_{t_0}^{t}|\dot{\theta}(s)|\mathrm{d}s\right).
\end{aligned}$$

Now let us consider the sum

$$\sum_{l=1}^{n-k}\alpha_l\sum_{j=1}^{k+1}\frac{x_{j-1}-x_j}{\tau_j-\tau_{j-1}}\int_{\tau_{j-1}}^{\tau_j}\mathbb{1}_{(s_l,t]}(s)\mathrm{d}s.$$

Since $s_l\in[t_0,t]$, there is a $j_0\in\{0,1,\ldots,k\}$ such that $s_l\in[\tau_{j_0},\tau_{j_0+1}]$. This fact allows to rewrite the second sum in the latter expression as

$$x_{j_0+1}-x+(x_{j_0+1}-x_{j_0})\frac{s_l-\tau_{j_0+1}}{\tau_{j_0+1}-\tau_{j_0}}$$

leading to

$$\left|\sum_{l=1}^{n-k}\alpha_l\sum_{j=1}^{k+1}\frac{x_{j-1}-x_j}{\tau_j-\tau_{j-1}}\int_{\tau_{j-1}}^{\tau_j}\mathbb{1}_{(s_l,t]}(s)\mathrm{d}s\right|\leqslant 4\max_{0\leqslant j\leqslant k+1}|x_j|\sum_{l=1}^{n-k}|\alpha_l|.$$

Inserting these estimates we obtain

$$|T\Phi_{n,k}(\theta)|\leqslant\exp\left(|x|\sum_{l=1}^{n-k}|\alpha_l|\right)\prod_{j=1}^{k+1}\frac{1}{\sqrt{2\pi(\tau_j-\tau_{j-1})}}\exp(|\theta|^2)\exp\left(2\sqrt{t-t_0}|\theta|\sum_{l=1}^{n-k}|\alpha_l|\right)$$
$$\times\exp\left(2\max_{0\leqslant j\leqslant k+1}|x_j|\left(\sup_{[t_0,t]}|\theta|+\int_{t_0}^{t}|\dot{\theta}(s)|\mathrm{d}s\right)\right)\exp\left(4\max_{0\leqslant j\leqslant k+1}|x_j|\sum_{l=1}^{n-k}|\alpha_l|\right).$$

Now we introduce the norm

$$\|\theta\|:=\sup_{s\in[t_0,t]}|\theta(s)|+\int_{t_0}^{t}|\dot{\theta}(s)|\mathrm{d}s+|\theta|.$$

With respect to this norm one may bound the previous expression by

$$\exp\left(|x|\sum_{l=1}^{n-k}|\alpha_l|\right)\prod_{j=1}^{k+1}\frac{1}{\sqrt{2\pi(\tau_j-\tau_{j-1})}}\exp(\|\theta\|^2)\exp\left(2\sqrt{t-t_0}\|\theta\|\sum_{l=1}^{n-k}|\alpha_l|\right)$$
$$\times\exp\left(2\max_{0\leqslant j\leqslant k+1}|x_j|\|\theta\|\right)\exp\left(4\max_{0\leqslant j\leqslant k+1}|x_j|\sum_{l=1}^{n-k}|\alpha_l|\right).$$

Then we use

$$\sqrt{t-t_0}\|\theta\|\leqslant\tfrac{1}{2}(t-t_0+\|\theta\|^2)$$

and

$$2\max_{0\leqslant j\leqslant k+1}|x_j|\|\theta\|\leqslant\max_{0\leqslant j\leqslant k+1}(|x_j|^2)+\|\theta\|^2$$

to obtain the desired estimate (9).

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Multi-instantons in seven dimensions

E. K. Loginov[a)]
Physics Department, Ivanovo State University, Ermaka St. 39, Ivanovo, 153025, Russia

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We consider the self-dual Yang–Mills equations in seven dimensions. Modifying the t'Hooft construction of instantons in $d=4$, we find N-instanton $7d$ solutions which depend on $8N$ effective parameters and are E_6 invariant. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1920307]

I. INTRODUCTION

The pure Yang–Mills (YM) theory defined in the four-dimensional Euclidean space has a rich and interesting structure even at the classical level. The discovery of regular solutions to the YM field equations, which correspond to absolute minimum of the action (Belavin *et al.*),[1] has led to an intensive study of such a classical theory. One hopes that a deep understanding of the classical theory will be invaluable when one tries to quantize such a theory.

In the past few years, increased attention has been paid to gauge field equations in space-time of dimension greater than four, with a view to obtaining physically interesting theories via dimensional reduction.[2] Such equations appear in the many-dimensional theory of supergravity, in the low-energy effective theory of d-branes, and in M theory.[3] Using solutions of the YM equations in $d>4$ makes it possible to obtain soliton solutions in these theories.[4] It is known also that the YM theory in d dimensions may be reduced to the Yang-Mills-Higgs (YMH) theory in $k<d$ dimensions.[5] Hence, solutions of the YMH equations in $d=4$ may be obtained from solutions of the YM equations in $d>4$ dimensions.

In Ref. 6, the 4D self-dual Yang–Mills equations was generalized to the higher-dimensional linear relations (CDFN equations)

$$c_{mnps}F^{ps}=\lambda F_{mn}, \tag{1}$$

where the numerical tensor c_{mnps} is completely antisymmetric and $\lambda=\text{const}$ is a nonzero eigenvalue. It is obvious that these equations lead to the full YM equation, via the Bianchi identity. Several self-dual solutions of (1) were found in Ref. 7.

The paper is organized as follows. Sections II and III contain well-known facts about the Cayley–Dickson algebras and their derivations. In Sec. IV multi-instanton solutions of the G_2-invariant CDFN equations are found. In Sec. V the E_6 invariance of these solutions are proved.

II. CAYLEY–DICKSON ALGEBRAS

Let A be an algebra with an involution $x\to\overline{x}$ over a field F of characteristic $\neq 2$. Given a nonzero $\alpha\in F$, we define a multiplication on the vector space $(A,\alpha)=A\oplus A$ by

$$(x_1,y_1)(x_2,y_2)=(x_1x_2-\alpha\overline{y_2}y_1,y_2x_1+y_1\overline{x_2}).$$

This makes (A,α) an algebra over F. It is clear that A is isomorphically embedded into (A,α) and $\dim(A,\alpha)=2\dim A$. Let $e=(0,1)$. Then, $e^2=-\alpha$ and $(A,\alpha)=A\oplus Ae$. Given any $z=x+ye$ in (A,α) we suppose $\overline{z}=\overline{x}-ye$. Then, the mapping $z\to\overline{z}$ is an involution in (A,α).

a)Electronic mail: loginov@ivanovo.ac.ru

Starting with the base field F, the Cayley–Dickson construction leads to the following sequence of alternative algebras:

(1) F, the base field.
(2) $\mathbb{C}(\alpha)=(F,\alpha)$, a field if $x^2+\alpha$ is the irreducible polynomial over F; otherwise, $\mathbb{C}(\alpha)\simeq F\oplus F$.
(3) $\mathbb{H}(\alpha,\beta)=(\mathbb{C}(\alpha),\beta)$, a generalized quaternion algebra. This algebra is associative but not commutative.
(4) $\mathbb{O}(\alpha,\beta,\gamma)=(\mathbb{H}(\alpha,\beta),\gamma)$, a Cayley–Dickson algebra. It is easy to prove that this algebra is nonassociative.

The algebras in (1)–(4) are called composition. Any of them has the nondegenerate quadratic form (norm) $n(x)=x\overline{x}$, such that $n(xy)=n(x)n(y)$. The norm $n(x)$ defines the scalar product

$$(x,y)=\tfrac{1}{2}(\overline{x}y+\overline{y}x), \tag{2}$$

which is invariant with respect to all automorphisms of the composition algebra. It is known also that over the field $\mathbb{R}$ of real numbers, the above construction gives three split algebras (e.g., if $\alpha=\beta=\gamma=-1$) and four division algebras (if $\alpha=\beta=\gamma=1$): the fields of real $\mathbb{R}$ and complex $\mathbb{C}$ numbers, the algebras of quaternions $\mathbb{H}$ and octonions $\mathbb{O}$, taken with the Euclidean norm $n(x)$. Finally, note that any composition algebra is alternative, i.e., in any of them the associator

$$(x,y,z)=(xy)z-x(yz), \tag{3}$$

is skew symmetric over x,y,z. Note also that any simple nonassociative alternative algebra is isomorphic to the Cayley–Dickson algebra $\mathbb{O}(\alpha,\beta,\gamma)$.

As with any finite-dimensional algebra, the Cayley–Dickson algebra may be defined by "a multiplication table" in some fixed basis. For that we consider a real linear space A equipped with a nondenerate symmetric metric g of signature (8,0) or (4,4). Choose the basis $1,e_1,\ldots,e_7$ in A such that

$$g=\mathrm{diag}(1,\alpha,\beta,\alpha\beta,\gamma,\alpha\gamma,\beta\gamma,\alpha\beta\gamma), \tag{4}$$

where $\alpha,\beta,\gamma=\pm 1$. Define the multiplication

$$e_ie_j=-g_{ij}+c_{ij}{}^{k}e_k, \tag{5}$$

where the structural constants $c_{ijk}=g_{ks}c_{ij}{}^{s}$ are completely antisymmetric and different from 0 only if

$$c_{123}=c_{145}=c_{167}=c_{246}=c_{275}=c_{374}=c_{365}=1.$$

The multiplication (5) transforms A into a real linear algebra. It can easily be checked that A is isomorphic to $\mathbb{O}(\alpha,\beta,\gamma)$.

III. DERIVATIONS

Recall that a derivation of an algebra A is a linear transformation D of A, satisfying

$$(xy)D=(xD)y+x(yD),$$

for all $x,y\in A$. The derivations of Cayley–Dickson algebra may be described in intrinsic terms. Namely, let A be a Cayley–Dickson algebra. Then, for any $x,y\in A$ the mapping

$$D_{x,y}:z\to 2[z,[x,y]]+6(z,x,y), \tag{6}$$

is a derivation of A. Therefore, we have the linear mapping $\Lambda^2\to\mathrm{der}\,A$. Since any Cayley–Dickson algebra is simple, it follows that this mapping is surjective. In addition, the following relations:

$$D_{x,yz} = D_{y,xz} + D_{z,yx}, \tag{7}$$

$$[D_{x,y}, D_{z,t}] = D_{(xD_{z,t}),y} + D_{x,(yD_{z,t})}, \tag{8}$$

are true. Note also that the derivations algebra der A is a simple exceptional Lie algebra of type g_2.

Since the associator (3) of Cayley–Dickson algebra is skew symmetric over its arguments, it follows that we can define the completely antisymmetric tensor c_{ijkl} by

$$(e_i, e_j, e_k) = 2c_{ijk}{}^{l} e_l. \tag{9}$$

It is easy to prove that this tensor satisfies the following identities:

$$c_{ijs}c_{kl}{}^{s} = g_{ik}g_{jl} - g_{il}g_{jk} + c_{ijkl}, \tag{10}$$

$$c_{ijps}c_{kl}{}^{ps} = 4(g_{ik}g_{jl} - g_{il}g_{jk}) + 2c_{ijkl}, \tag{11}$$

and has the nonzero components

$$c_{4567} = c_{2367} = c_{2345} = c_{1357} = c_{1364} = c_{1265} = c_{1274} = 1.$$

Further, it follows from (2) and (9) that the tensor c_{ijkl} is invariant with respect to all automorphisms of algebra A. Noting that the group aut A is isomorphic to the Lie group of type G_2, we see that the tensor c_{ijkl} is G_2 invariant. Finally, rewriting the identity (7) in the form

$$c_i{}^{jk} D_{jk} = 0,$$

where the derivation $\frac{1}{8} D_{e_i,e_j}$ is denoted by the symbol D_{ij}, we get the following relations:

$$c_{ij}{}^{kl} D_{kl} = -2D_{ij}. \tag{12}$$

Since the algebra der A is a Lie algebra of type g_2 (or g_2' in the noncompact case), it follows that it may be considered as a subalgebra of the Lie algebra so(m,n) of type so(7) or so(3, 4). Hence, there exists the projector c^{+}_{ijkl} of one onto the subspace der A. Usually this projector is chosen in the form (see Ref. 7)

$$c^{+}_{ijkl} = \tfrac{1}{6}(2g_{ik}g_{lj} - 2g_{il}g_{jk} - c_{ijkl}). \tag{13}$$

In addition, it is easily shown that the derivations

$$D_{ij} = \tfrac{3}{2} c_{ij}^{+kl} E_{kl}, \tag{14}$$

where generators E_{kl} of the Lie algebra so(m,n) satisfy the switching relations

$$[E_{ij}, E_{kl}] = g_{k[i} E_{\ j]l} - g_{l[i} E_{\ j]k}.$$

Besides, it follows from (11) that

$$c_{ij}{}^{ps} c^{+}_{klps} = -2c^{+}_{ijkl}. \tag{15}$$

Comparing (14) and (15), we again obtain the identity (12).

IV. SOLUTIONS

Recall that the self-dual equations have been successfully tackled by the twister techniques, and in the case of finite action solutions by the algebraic ADHM construction.[8] A generalization of the ADHM construction for Eqs. (1) which break SO($4n$) up into $\mathrm{Sp}(1) \times \mathrm{Sp}(n)/Z_2$ was found in Ref. 9. However, in dimensions 7 and 8 there exists an exceptional G_2-covariant [respectively, Spin(7)-covariant] duality which is connected with the octonionic algebra. Therefore, the search of generalized ADHM construction in $d=7$ and 8 appears very attractive.

Such attempt was done in the recent paper.[10] In it the generalized ADHM construction in $d=8$ was built with the help of the algebra $L(\mathbb{O})$ of left multiplications of octonionic algebra $\mathbb{O}$. Unfortunately, calculating the field strength in that paper's Sec. V and proving its self-duality, the authors incorrectly use the equality $L[L(xy)z]=L(xyz)$, where $L(xyz)=x(yz)$ and $x,y,z\in\mathbb{O}$. By nonassociativity of the octonionic algebra, it would not be done (cp. Ref. 11).

Nevertheless, it is easy to get multi-instanton solutions (but not a generalized ADHM construction) of CDFN equations in seven dimensions. We choose the ansatz A_m in the form

$$A_m = \frac{\lambda^\dagger y^i}{1+y^\dagger y} D_{mi}, \tag{16}$$

where y is a column vector with the elements $y_1,\ldots,y_N$ of Cayley–Dickson algebra such that

$$y^\dagger = (y_1^k,\ldots,y_N^k)\overline{e_k}, \quad y_I^k \in \mathbb{R},$$

$$\lambda^\dagger = (\lambda_1,\ldots,\lambda_N), \quad \lambda_I \in \mathbb{R}^+,$$

$$y_I^k = (b_{IJ}^k + \delta_{IJ}x^k)\lambda_J, \quad b_{IJ}^k = b_{JI}^k.$$

Using the identities (8)–(10), we get the field strength

$$F_{mn} = -\frac{\lambda^\dagger\{(2+2y^\dagger y - y^i y_i^\dagger)D_{mn} + 3c^{+\ is}_{mn} D_{sj} y^j y_i^\dagger\}\lambda}{(1+y^\dagger y)^2},$$

where the tensor c^+_{ijkl} is defined by the equality (13). Now, it follows from (12) and (15) that the field strength F_{mn} satisfies the CDFN equations (1) for the Euclidean as for the pseudo-Euclidean metric of the form (4).

This construction of multi-instanton solutions of the CDFN equations may be easy to extend in eight dimensions. It is sufficient to take the projector f^+_{ijkl} of the algebra Lie of type so(8) or so(4,4) onto the subalgebra so(7) or so(3,4), respectively, in place of c^+_{ijkl}, to define the elements D'_{ij} of the form (14), and to prove an analog of the identity (15) (see Ref. 7). Then, choosing the ansatz A'_m in the form

$$A'_m = \frac{\lambda^\dagger y^i}{1+y^\dagger y} D'_{mi}, \tag{17}$$

where the indexes $m,i\in\{0,\ldots,7\}$, we can obtain the following expression for the field strength:

$$F'_{mn} = -\frac{1}{3}\frac{\lambda^\dagger\{(6+6y^\dagger y - 3y^i y_i^\dagger)D'_{mn} + 8f^{+\ is}_{mn} D'_{sj} y^j y_i^\dagger\}\lambda}{(1+y^\dagger y)^2}.$$

Obviously, the N-instanton solutions (16) and (17) depend on $8N$ and $9N$ effective parameters, respectively, and are a generalization of the t'Hooft solution in $d=4$ (see e.g., Ref. 12).

V. E_6 INVARIANCE

Let A be a real Cayley–Dickson algebra with the involution $x\to\overline{x}$, and let A_3 be the algebra of all 3×3 matrix with elements of A. Consider the set

$$J = \{(x_{ij}) \in A_3 | (\overline{x_{ij}}) = (x_{ji})\}.$$

The set J is a commutative nonassociative algebra with respect to the product

$$x\circ y = \tfrac{1}{2}(xy+yx).$$

The algebra J satisfies the identity

$$(x^2y)x = x^2(yx),$$

and is said to be an exceptional Jordan algebra.

Denote 3×3 matrix (x_{ij}) with the unique nonzero element $x_{ij}=1$ by the symbol ε_{ij} and choose in J the basis

$$E_1 = \varepsilon_{11}, \quad X_1(e_i) = e_i\varepsilon_{23} + \overline{e_i}\varepsilon_{32},$$

$$E_2 = \varepsilon_{22}, \quad X_2(e_j) = e_j\varepsilon_{31} + \overline{e_j}\varepsilon_{13},$$

$$E_3 = \varepsilon_{33}, \quad X_3(e_k) = e_k\varepsilon_{12} + \overline{e_k}\varepsilon_{21}, \tag{18}$$

where $e_0=1, e_1, \ldots, e_7$ is the standard basis of A. It can easily be checked that

$$E_\alpha \circ X_\beta(e_i) = \begin{cases} 0, & \text{if } \alpha = \beta, \\ \frac{1}{2}X_\beta(e_i), & \text{if } \alpha \neq \beta, \end{cases} \tag{19}$$

$$X_\alpha(e_i) \circ X_\beta(e_j) = \begin{cases} \delta_{ij}(E - E_\alpha), & \text{if } \alpha = \beta, \\ \frac{1}{2}X_\gamma(\overline{e_j e_i}), & \text{if } \alpha \neq \beta, \end{cases} \tag{20}$$

where E is the identity 3×3 matrix, and $(\alpha\beta\gamma)=(123),(231),(312)$.

It is well known (see, e.g., Ref. 13) that the derivations algebra der J is a simple exceptional Lie algebra of the type f_4. Since there is an isomorphic enclosure of the algebra g_2 into f_4, we can consider (16) as a field that takes its values in der J. To prove the F_4 invariance of these solutions, we find the trace of the matrix

$$X_\beta = \left\{[X_\alpha(e_i), X_\beta(e_j), X_\alpha(e_k)] - \tfrac{1}{2}[X_\alpha(e_i), X_\alpha(e_j), X_\alpha(e_k)]\right\} \circ X_\beta(e_l), \tag{21}$$

where $i,j,k \neq 0$, and we do not sum on the recurring indexes. Using (9), (19), and (20), we prove that

$$X_\beta = \tfrac{1}{2}c_{ijkl}(E - E_\beta),$$

and hence

$$\operatorname{tr} X_\beta = c_{ijkl}.$$

Since a trace of matrix in J is invariant with respect to all automorphisms of J, we prove the F_4 invariance of solutions of the corresponding CDFN equations.

Moreover, it can be proved that the tensor c_{ijkl} is E_6 invariant. Indeed, the group E_6 is a group of linear transformations of the space J that preserves the norm

$$n(X) = x_{11}x_{22}x_{33} + (x_{12}x_{23})x_{31} + x_{13}(x_{32}x_{21}) - x_{11}x_{23}x_{32} - x_{22}x_{31}x_{13} - x_{33}x_{12}x_{21},$$

where $X=(x_{ij}) \in J$. Choose an element X in the form

$$X = X_1 + X_2 - X_3 + E_1 + E_2,$$

where matrices E_α and X_β are defined by the relations (18) and (21), respectively. Then, it follows easily that the norm

$$n(X) = c_{ijkp}.$$

Since the group F_4 can be isomorphically enclosed into the group E_6, we prove the E_6 invariance of the found solutions.

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Inversible Max-Plus algebras and integrable systems

Tomoshiro Ochiai and Jose C. Nacher
Graduate School of Mathematical Sciences, The University of Tokyo, Tokyo 153-8914, Japan

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We present an extended version of max-plus algebra which includes the inverse operator of "max." This algebra enables us to ultradiscretize the system including subtractions and obtain new ultradiscrete equations. The known ultradiscrete equations can also be recovered by this construction. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1925247]

I. INTRODUCTION

An integrable system is one of the main subjects in mathematics and physics. Especially, soliton equations and integrable lattice models that have been studied as integrable systems in a variety of view points. Recently, because of the development of computer sciences, discrete and ultradiscrete versions of integral system have been attracting a great deal of attention. The ultradiscretization of soliton equations and other various important equations are intensively studied.[1–8] Moreover, it is known that the various ultradiscrete soliton equations are obtained from a solvable vertex model in statistical mechanics in a certain limiting procedure.[9,10] The key formula for the ultradiscretization is given by

$$\lim_{\epsilon \to +0} \epsilon \log(e^{X/\epsilon} + e^{Y/\epsilon}) = \max(X, Y) \tag{1.1}$$

for arbitrary real numbers X and Y. Using this formula, it is known that the field of real numbers can be transformed into the so-called "max-plus" algebra, which is well known in integrable systems. But the main difficulty for the usual ultradiscretization procedure is that there is no operator corresponding to the subtraction "$-$" (see Fig. 1). Therefore, so far, we cannot deal with the ultradiscretization of integral systems that include the subtraction.

In this paper, in order to solve this difficulty, we define an extended version of max-plus algebra called "inversible Max-Plus algebra," which includes the usual max-plus algebra and the operator corresponding to the subtraction:[1]

$$x \times y \to X + Y$$

$$x/y \to X - Y$$

$$x + y \to \max(X, Y)$$

$$x - y \to \ ?\ ?$$

FIG. 1. Ultra-discretization

[1]In this paper, we consider "Max" and "max" as different operators. We use "max" for the usual maximum operator, while we use "Max" for the inversible maximum operator, which is the new operator of our novel inversible algebra. The same holds for "Plus" ("plus") and "Minus" ("minus") operators.

Our construction is as follows. We shall define a Max-Plus algebra as $\mathbf{Z}$-module A with the operation $\mathrm{Max}: A \times A \to A$ satisfying

$$(\alpha + \beta) + \gamma = \alpha + (\beta + \gamma), \tag{1.2}$$

$$\mathrm{Max}(\mathrm{Max}(\alpha, \beta), \gamma) = \mathrm{Max}(\alpha, \mathrm{Max}(\beta, \gamma)), \tag{1.3}$$

$$\mathrm{Max}(\alpha + \beta, \alpha + \gamma) = \alpha + \mathrm{Max}(\beta, \gamma), \tag{1.4}$$

for $\alpha, \beta, \gamma \in A$. Max-Plus subalgebra and homomorphism are defined in the usual manner. The basic example is $\mathbf{Z}$ which is the ring of integer with $\mathrm{Max}(n,m) = \max(n,m)$, where $\max(n,m)$ stands for the maximum of the pair n and m.

In this paper, we explicitly construct Max-Plus algebra Ω and Ω_0 with $P: \Omega_0 \to \mathbf{Z}$ such that

(1) $\Omega \supset \Omega_0$ as Max-Plus algebra,
(2) $P: \Omega_0 \to \mathbf{Z}$ as Max-Plus homomorphism,
(3) There exists an element $\eta \in \Omega$ such that

$$\mathrm{Max}(\mathrm{Max}(\alpha, \beta), \beta + \eta) = \alpha \tag{1.5}$$

for arbitrary $\alpha, \beta \in \Omega$

We call Ω the inversible Max-Plus algebra, due to the inversible property of the Max operator (1.5).

It is known that we can construct ultradiscrete (UD) equation on $\mathbf{Z}$ from standard discrete partial differential equations (PDEs) satisfying certain conditions through the usual ultradiscretization procedure. But, using our constructions, we can construct UD equation on Ω from any discrete PDEs, even if they include the subtraction. If this UD equation and its solution on Ω belong to Ω_0, the projection P gives the UD equation and solutions on $\mathbf{Z}$ explained previously. As an application, we apply this inversible Max-Plus algebra Ω to a periodic recursive equation and obtain an UD periodic equation on Ω and $\mathbf{Z}$. Further, we apply this algebra to the ultradiscretization of the equation of motion for a free particle in physics.

Computational Biology: On the other hand, it is also worth noting the possible application of our new algebra in the emergent field of bioinformatics. Recently, the postsequence era has provided a huge wealth of biological data at the gene and molecular levels. Many mathematical and computational tools (e.g., boolean networks, hidden Markov model, and stochastic approach) are currently being used to study the relationships among thousands of basic building blocks of life as proteins, chemical compounds, and genes. However, the relationship and connection among these tools is unclear, and consequently, the research community usually considers them as separate and independent approaches. In contrast, we believe that the mentioned techniques are related to each other and even more, UD is the missing link between computational or discrete mathematics and the usual mathematics. More precisely, the computational mathematics and the usual matemathics are connected by the UD procedure given in this paper. Therefore, UD may shed light on the relation between two of the most used methods in molecular systems biology as boolean networks and stochastic processes. Consequently, we believe that further studies on this issue may contribute to improve the current techniques used in bioinformatics and enlighten the advances in the postgenomic era.

II. INVERSIBLE MAX-PLUS ALGEBRAS

A. Definition of $\tilde{\mathbf{Z}}$

Let $\mathbf{Z}_2 = \{0, \eta\}$ be the finite group of order two (i.e., $0+0=0$, $0+\eta=\eta$, $\eta+\eta=0$,) and set

$$\tilde{\mathbf{Z}} = \mathbf{Z} \oplus \mathbf{Z}_2 \cup \{-\infty\} = \{x + \xi | x \in \mathbf{Z}, \xi \in \mathbf{Z}_2\} \cup \{-\infty\}.$$

First, we shall define the "max" operator on $\tilde{\mathbf{Z}}$ (i.e., $\max: \tilde{\mathbf{Z}} \times \tilde{\mathbf{Z}} \to \tilde{\mathbf{Z}}$) as follows. For $a = x + \xi \in \mathbf{Z} \oplus \mathbf{Z}_2$, $a' = x' + \xi' \in \mathbf{Z} \oplus \mathbf{Z}_2$, set

$$\max(a, -\infty) = a,$$

$$\max(-\infty, -\infty) = -\infty,$$

and

$$\max(a, a') = \begin{cases} a & (x > x') \\ a & (x = x' \text{ and } \xi = \xi') \\ a' & (x < x') \\ -\infty & (x = x' \text{ and } \xi \neq \xi'). \end{cases}$$

Second, we shall define the "plus" operator on $\tilde{\mathbf{Z}}$ (i.e., $\text{plus}: \tilde{\mathbf{Z}} \times \tilde{\mathbf{Z}} \to \tilde{\mathbf{Z}}$) as follows. For $a = x + \xi \in \mathbf{Z} \oplus \mathbf{Z}_2$ and $a' = x' + \xi' \in \mathbf{Z} \oplus \mathbf{Z}_2$, set

$$\text{plus}(a, a') = (x + x') + (\xi + \xi'),$$

$$\text{plus}(a, -\infty) = -\infty,$$

$$\text{plus}(-\infty, -\infty) = -\infty.$$

In the sequel, we write $a + b$ for $\text{plus}(a, b)$ for the matter of convenience.

If $a \neq a' + \eta$, the order relations $a > a'$, $a < a'$ and $a = a'$ are defined by

$$a > a' \Leftrightarrow x > x',$$

$$a < a' \Leftrightarrow x < x',$$

$$a = a' \Leftrightarrow x = x' \text{ and } \xi = \xi'.$$

If $a \neq \eta$, define the absolute value $|a|$ by

$$|a| = \max(a, 0) + \max(-a, 0).$$

B. Definition of Ξ

Set

$$\tilde{\mathbf{Z}}^n = \{(a_1, \ldots, a_n) | a_1, \ldots, a_n \in \tilde{\mathbf{Z}}\}.$$

For a matter of convenience, an element $(a_1, \ldots, a_n)$ is denoted by $\mathbf{a}$ or $(a_i)_{i=1}^n$.

Set $\Xi = \cup_{n=1}^{\infty} \tilde{\mathbf{Z}}^n / \sim$, where the union is disjoint and the equivalence relation "$\sim$" is generated by

$$(\ldots, a_i, \ldots, a_j, \ldots) \sim (\ldots, a_j, \ldots, a_i, \ldots), \tag{2.1}$$

$$(a_1, \ldots, a_n, b, b + \eta) \sim (a_1, \ldots, a_n, -\infty), \tag{2.2}$$

$$(a_1, \ldots, a_n, -\infty) \sim (a_1, \ldots, a_n). \tag{2.3}$$

An element $(a_1,\ldots,a_n)$ is called irreducible, if n is minimum in its equivalence class. We remark that we can introduce the order relations into $a_1,\ldots,a_n$, if $(a_1,\ldots,a_n)$ is irreducible.

If there is no danger of confusion, the equivalence class defined by $(a_1,\ldots,a_n)$ is also denoted by $(a_1,\ldots,a_n)$.

Let us define "$\overline{\text{Max}}$" and "Plus" operators on $\Xi=\cup_{n=1}^{\infty}\tilde{\mathbf{Z}}^n/\sim$ (i.e., $\overline{\text{Max}}:\Xi\times\Xi\to\Xi$ and $\text{Plus}:\Xi\times\Xi\to\Xi$) as follows. For $\mathbf{a}=(a_i)_{i=1}^n=(a_1,\ldots,a_n)\in\Xi$ and $\mathbf{b}=(b_i)_{i=1}^m=(b_1,\ldots,b_m)\in\Xi$, set

$$\overline{\text{Max}}(\mathbf{a},\mathbf{b})=(a_1,\ldots,a_n,b_1,\ldots,b_m), \tag{2.4}$$

$$\begin{aligned}\text{Plus}(\mathbf{a},\mathbf{b})&=(a_i+b_j)_{i=1\ j=1}^{n\quad m}\\&=(a_1+b_j,\ldots,a_n+b_j)_{j=1}^m\\&=(a_1+b_1,a_2+b_1,\ldots,a_n+b_1,a_1+b_2,\ldots,a_n+b_m).\end{aligned} \tag{2.5}$$

In the sequel, we write $\mathbf{a}+\mathbf{b}$ for $\text{Plus}(\mathbf{a},\mathbf{b})$ for the matter of convenience.

Lemma 2.1: The previous definition is well defined.

Proof: It is enough to show that the definition is invariant under relations (2.1)–(2.3).

First, we will show the $\overline{\text{Max}}$ operator is invariant under relations (2.1)–(2.3). For $\mathbf{a}=(a_1,\ldots,a_i,\ldots,a_j,\ldots,a_n)$, $\mathbf{a}'=(a_1,\ldots,a_j,\ldots,a_i,\ldots,a_n)$, and $\mathbf{b}=(b_1,\ldots,b_m)$, we have

$$\begin{aligned}\overline{\text{Max}}(\mathbf{a},\mathbf{b})&=(a_1\ldots,a_i,\ldots,a_j,\ldots,a_n,b_1,\ldots,b_m)\\&=(a_1,\ldots,a_j,\ldots,a_i,\ldots,a_n,b_1,\ldots,b_m)=\overline{\text{Max}}(\mathbf{a}',\mathbf{b}),\end{aligned}$$

which shows the invariance under relation (2.1). For $\mathbf{a}=(a_1,\ldots,a_n,c,c+\eta)$, $\mathbf{a}'=(a_1,\ldots,a_n,-\infty)$, and $\mathbf{b}=(b_1,\ldots,b_m)$, we have

$$\overline{\text{Max}}(\mathbf{a},\mathbf{b})=(a_1\ldots,a_n,c,c+\eta,b_1,\ldots,b_m)=(a_1,\ldots,a_n,-\infty,b_1,\ldots,b_m)=\overline{\text{Max}}(\mathbf{a}',\mathbf{b}),$$

which shows the invariance under relation (2.2). For $\mathbf{a}=(a_1\ldots,a_n,-\infty)$, $\mathbf{a}'=(a_1,\ldots,a_n)$, and $\mathbf{b}=(b_1,\ldots,b_m)$, we have

$$\overline{\text{Max}}(\mathbf{a},\mathbf{b})=(a_1\ldots,a_n,-\infty,b_1,\ldots,b_m)=(a_1,\ldots,a_n,b_1,\ldots,b_m)=\overline{\text{Max}}(\mathbf{a}',\mathbf{b}),$$

which shows the invariance under relation (2.3).

Second, we will show the Plus operator is invariant under relation (2.1)–(2.3). For $\mathbf{a}=(a_1,\ldots,a_i,\ldots,a_j,\ldots,a_n)$, $\mathbf{a}'=(a_1,\ldots,a_j,\ldots,a_i,\ldots,a_n)$, and $\mathbf{b}=(b_1,\ldots,b_m)$, we have

$$\begin{aligned}\mathbf{a}+\mathbf{b}&=(a_1+b_k,\ldots,a_i+b_k,\ldots,a_j+b_k,\ldots,a_n+b_k)_{k=1}^m\\&=(a_1+b_k,\ldots,a_j+b_k,\ldots,a_i+b_k,\ldots,a_n+b_k)_{k=1}^m=\mathbf{a}'+\mathbf{b},\end{aligned}$$

which shows the invariance under relation (2.1). For $\mathbf{a}=(a_1\ldots,a_n,c,c+\eta)$, $\mathbf{a}'=(a_1,\ldots,a_n,-\infty)$, and $\mathbf{b}=(b_1,\ldots,b_m)$, we have

$$\mathbf{a}+\mathbf{b}=(a_1+b_k,\ldots,a_n+b_k,c+b_k,c+\eta+b_k)_{k=1}^m=(a_1+b_k,\ldots,a_n+b_k,-\infty+b_k)_{k=1}^m=\mathbf{a}'+\mathbf{b},$$

which shows the invariance under relation (2.2). For $\mathbf{a}=(a_1,\ldots,a_n,-\infty)$, $\mathbf{a}'=(a_1,\ldots,a_n)$, and $\mathbf{b}=(b_1,\ldots,b_m)$, we have

$$\mathbf{a}+\mathbf{b}=(a_1+b_k,\ldots,a_n+b_k,-\infty+b_k)_{k=1}^m=(a_1+b_k,\ldots,a_n+b_k)_{k=1}^m=\mathbf{a}'+\mathbf{b},$$

which shows the invariance under relation (2.3). □

Lemma 2.2: For $\mathbf{a},\mathbf{b},\mathbf{c}\in\Xi$, we have the following identities:

$$(\mathbf{a}+\mathbf{b})+\mathbf{c}=\mathbf{a}+(\mathbf{b}+\mathbf{c}), \tag{2.6}$$

$$\overline{\mathrm{Max}}(\overline{\mathrm{Max}}(\mathbf{a},\mathbf{b}),\mathbf{c})=\overline{\mathrm{Max}}(\mathbf{a},\overline{\mathrm{Max}}(\mathbf{b},\mathbf{c})), \tag{2.7}$$

$$\overline{\mathrm{Max}}(\mathbf{a}+\mathbf{b},\mathbf{a}+\mathbf{c})=\mathbf{a}+\overline{\mathrm{Max}}(\mathbf{b},\mathbf{c}), \tag{2.8}$$

$$\overline{\mathrm{Max}}(\overline{\mathrm{Max}}(\mathbf{a},\mathbf{b}),\mathbf{b}+\eta)=\mathbf{a}. \tag{2.9}$$

Proof: Suppose $\mathbf{a}=(a_1,\ldots,a_n)$, $\mathbf{b}=(b_1,\ldots,b_m)$, and $\mathbf{c}=(c_1,\ldots,c_l)$. The proof is straightforward from (2.4) and (2.5). First formula (2.6) is obtained by the following computation:

$$(\mathbf{a}+\mathbf{b})+\mathbf{c}=(a_i+b_j+c_k)_{i=1}^{n}{}_{j=1}^{m}{}_{k=1}^{l}=\mathbf{a}+(\mathbf{b}+\mathbf{c}).$$

Second formula (2.7) is obtained by the following computation:

$$\overline{\mathrm{Max}}(\overline{\mathrm{Max}}(\mathbf{a},\mathbf{b}),\mathbf{c})=(a_1\ldots,a_n,b_1,\ldots,b_m,c_1,\ldots,c_l)=\overline{\mathrm{Max}}(\mathbf{a},\overline{\mathrm{Max}}(\mathbf{b},\mathbf{c})).$$

Third formula (2.8) is obtained by the following computation:

$$\begin{aligned}\mathbf{a}+\overline{\mathrm{Max}}(\mathbf{b},\mathbf{c})&=\mathbf{a}+(b_1,\ldots,b_m,c_1,\ldots,c_l)\\&=(b_1+a_i,\ldots,b_m+a_i,c_1+a_i,\ldots,c_l+a_i)_{i=1}^{n}\\&=\overline{\mathrm{Max}}((b_1+a_i,\ldots,b_m+a_i)_{i=1}^{n},(c_1+a_i,\ldots,c_l+a_i)_{i=1}^{n})=\overline{\mathrm{Max}}(\mathbf{a}+\mathbf{b},\mathbf{a}+\mathbf{c}).\end{aligned}$$

Last formula (2.9) is obtained by the following computation:

$$\overline{\mathrm{Max}}(\overline{\mathrm{Max}}(\mathbf{a},\mathbf{b}),\mathbf{b}+\eta)=(a_1\ldots,a_n,b_1,\ldots,b_m,b_1+\eta,\ldots,b_m+\eta)=(a_1\ldots,a_n)=\mathbf{a}.$$

□

C. Definition of Φ

Set $\Phi=\Xi\times\Xi'/\sim$, where $\Xi'=\Xi\backslash\{(-\infty)\}$ and the equivalence relation is given by

$$(\mathbf{a},\mathbf{b})\sim(\mathbf{a}',\mathbf{b}')\Leftrightarrow\mathbf{a}+\mathbf{b}'=\mathbf{a}'+\mathbf{b}, \tag{2.10}$$

for $(\mathbf{a},\mathbf{b}),(\mathbf{a}',\mathbf{b}')\in\Xi\times\Xi'$. The equivalence class of $(\mathbf{a},\mathbf{b})$ is denoted by $\mathbf{a}-\mathbf{b}$. Then, we have

$$\Phi=\{\mathbf{a}-\mathbf{b}|\mathbf{a}\in\Xi,\mathbf{b}\in\Xi'\}.$$

Next, we will define Max, Plus, and "Minus" operators on Φ (i.e., Max: $\Phi\times\Phi\to\Phi$, Plus: $\Phi\times\Phi\to\Phi$ and Minus: $\Phi\times\Phi\to\Phi$) as follows. For $\alpha=\mathbf{a}-\mathbf{b}\in\Phi$ and $\alpha'=\mathbf{a}'-\mathbf{b}'\in\Phi$, set

$$\mathrm{Max}(\alpha,\alpha')=\overline{\mathrm{Max}}(\mathbf{a}+\mathbf{b}',\mathbf{a}'+\mathbf{b})-(\mathbf{b}+\mathbf{b}'), \tag{2.11}$$

$$\mathrm{Plus}(\alpha,\alpha')=(\mathbf{a}+\mathbf{a}')-(\mathbf{b}+\mathbf{b}'), \tag{2.12}$$

$$\mathrm{Minus}(\alpha,\alpha')=(\mathbf{a}+\mathbf{b}')-(\mathbf{b}+\mathbf{a}'). \tag{2.13}$$

In the sequel, for the matter of convenience, we write $\alpha+\alpha'$ and $\alpha-\alpha'$ for $\mathrm{Plus}(\alpha,\alpha')$ and $\mathrm{Minus}(\alpha,\alpha')$ respectively.

Lemma 2.3: The previous definition is well defined.

Proof: First, we will show the Max operator is invariant under relation (2.10). For $\mathbf{a}-\mathbf{b}=\mathbf{a}'-\mathbf{b}'\in\Phi$ and $\mathbf{c}-\mathbf{d}\in\Phi$, we have

$$\begin{aligned}\mathrm{Max}(\mathbf{a}-\mathbf{b},\mathbf{c}-\mathbf{d}) &= \overline{\mathrm{Max}}(\mathbf{a}+\mathbf{d},\mathbf{c}+\mathbf{b})-(\mathbf{b}+\mathbf{d})\\ &= \overline{\mathrm{Max}}(\mathbf{a}+\mathbf{b}'+\mathbf{d},\mathbf{c}+\mathbf{b}+\mathbf{b}')-(\mathbf{b}+\mathbf{b}'+\mathbf{d})\\ &= \overline{\mathrm{Max}}(\mathbf{a}'+\mathbf{b}+\mathbf{d},\mathbf{c}+\mathbf{b}+\mathbf{b}')-(\mathbf{b}+\mathbf{b}'+\mathbf{d})\\ &= \overline{\mathrm{Max}}(\mathbf{a}'+\mathbf{d},\mathbf{c}+\mathbf{b}')-(\mathbf{b}'+\mathbf{d})=\mathrm{Max}(\mathbf{a}'-\mathbf{b}',\mathbf{c}-\mathbf{d}),\end{aligned}$$

which shows the invariance under relation (2.10).

Second, we will show the Plus operator is invariant under relation (2.10). For $\mathbf{a}-\mathbf{b}=\mathbf{a}'-\mathbf{b}' \in \Phi$ and $\mathbf{c}-\mathbf{d}\in\Phi$, we have

$$\begin{aligned}(\mathbf{a}-\mathbf{b})+(\mathbf{c}-\mathbf{d}) &= (\mathbf{a}+\mathbf{c})-(\mathbf{b}+\mathbf{d})=(\mathbf{a}+\mathbf{b}'+\mathbf{c})-(\mathbf{b}+\mathbf{b}'+\mathbf{d})=(\mathbf{a}'+\mathbf{b}+\mathbf{c})-(\mathbf{b}+\mathbf{b}'+\mathbf{d})\\ &= (\mathbf{a}'+\mathbf{c})-(\mathbf{b}'+\mathbf{d})=(\mathbf{a}'-\mathbf{b}')+(\mathbf{c}-\mathbf{d}),\end{aligned}$$

which shows the invariance under relation (2.10).

Third, we will show the minus operator is invariant under relation (2.10). For $\mathbf{a}-\mathbf{b}=\mathbf{a}'-\mathbf{b}' \in \Phi$ and $\mathbf{c}-\mathbf{d}\in\Phi$, we have

$$\begin{aligned}(\mathbf{a}-\mathbf{b})-(\mathbf{c}-\mathbf{d}) &= (\mathbf{a}+\mathbf{d})-(\mathbf{b}+\mathbf{c})=(\mathbf{a}+\mathbf{b}'+\mathbf{d})-(\mathbf{b}+\mathbf{b}'+\mathbf{c})=(\mathbf{a}'+\mathbf{b}+\mathbf{d})-(\mathbf{b}+\mathbf{b}'+\mathbf{c})\\ &= (\mathbf{a}'+\mathbf{d})-(\mathbf{b}'+\mathbf{c})=(\mathbf{a}'-\mathbf{b}')-(\mathbf{c}-\mathbf{d}),\end{aligned}$$

which shows the invariance under relation (2.10). □

Next, we shall show that Φ has the Max-Plus algebra structures (1.2)–(1.4) and the inversible property (1.5). More precisely, we have the following lemma.

Lemma 2.4: For $\alpha,\beta,\gamma\in\Phi$, we have the following identities:

$$(\alpha+\beta)+\gamma=\alpha+(\beta+\gamma), \tag{2.14}$$

$$\mathrm{Max}(\mathrm{Max}(\alpha,\beta),\gamma)=\mathrm{Max}(\alpha,\mathrm{Max}(\beta,\gamma)), \tag{2.15}$$

$$\mathrm{Max}(\alpha+\beta,\alpha+\gamma)=\alpha+\mathrm{Max}(\beta,\gamma), \tag{2.16}$$

$$\mathrm{Max}(\mathrm{Max}(\alpha,\beta),\beta+\eta)=\alpha. \tag{2.17}$$

Proof: Suppose $\alpha=\mathbf{a}-\mathbf{b}$, $\beta=\mathbf{c}-\mathbf{d}$, and $\gamma=\mathbf{e}-\mathbf{f}$. First identity (2.14) is obtained by the following computation:

$$(\alpha+\beta)+\gamma=(\mathbf{a}+\mathbf{c}+\mathbf{e})-(\mathbf{b}+\mathbf{d}+\mathbf{f})=\alpha+(\beta+\gamma).$$

Second identity (2.15) is obtained by the following computation:

$$\begin{aligned}\mathrm{Max}(\mathrm{Max}(\alpha,\beta),\gamma &= \mathrm{Max}(\mathrm{Max}(\mathbf{a}-\mathbf{b},\mathbf{c}-\mathbf{d}),\mathbf{e}-\mathbf{f})\\ &= \mathrm{Max}(\overline{\mathrm{Max}}(\mathbf{a}+\mathbf{d},\mathbf{c}+\mathbf{b})-(\mathbf{b}+\mathbf{d}),\mathbf{e}-\mathbf{f})\\ &= \overline{\mathrm{Max}}(\overline{\mathrm{Max}}(\mathbf{a}+\mathbf{d},\mathbf{c}+\mathbf{b})+\mathbf{f},\mathbf{e}+\mathbf{b}+\mathbf{d})-(\mathbf{b}+\mathbf{d}+\mathbf{f})\\ &= \overline{\mathrm{Max}}(\overline{\mathrm{Max}}(\mathbf{a}+\mathbf{d}+\mathbf{f},\mathbf{c}+\mathbf{b}+\mathbf{f}),\mathbf{e}+\mathbf{b}+\mathbf{d})-(\mathbf{b}+\mathbf{d}+\mathbf{f})\\ &= \overline{\mathrm{Max}}(\mathbf{a}+\mathbf{d}+\mathbf{f},\overline{\mathrm{Max}}(\mathbf{c}+\mathbf{b}+\mathbf{f},\mathbf{e}+\mathbf{b}+\mathbf{d}))-(\mathbf{b}+\mathbf{d}+\mathbf{f})\\ &= \overline{\mathrm{Max}}(\mathbf{a}+\mathbf{d}+\mathbf{f},\overline{\mathrm{Max}}(\mathbf{c}+\mathbf{f},\mathbf{e}+\mathbf{d})+\mathbf{b})-(\mathbf{b}+\mathbf{d}+\mathbf{f})\\ &= \mathrm{Max}(\mathbf{a}-\mathbf{b},\overline{\mathrm{Max}}(\mathbf{c}+\mathbf{f},\mathbf{e}+\mathbf{d})-(\mathbf{d}+\mathbf{f}))\\ &= \mathrm{Max}(\mathbf{a}-\mathbf{b},\mathrm{Max}(\mathbf{c}-\mathbf{d},\mathbf{e}-\mathbf{f}))=\mathrm{Max}(\alpha,\mathrm{Max}(\beta,\gamma)).\end{aligned}$$

Third identity (2.16) is obtained by the following computation:

$$\begin{aligned}\mathrm{Max}(\alpha+\beta,\alpha+\gamma) &= \mathrm{Max}((\mathbf{a}-\mathbf{b})+(\mathbf{c}-\mathbf{d}),(\mathbf{a}-\mathbf{b})+(\mathbf{e}-\mathbf{f}))\\ &= \mathrm{Max}((\mathbf{a}+\mathbf{c})-(\mathbf{b}+\mathbf{d}),(\mathbf{a}+\mathbf{e})-(\mathbf{b}+\mathbf{f}))\\ &= \overline{\mathrm{Max}}((\mathbf{a}+\mathbf{c})+(\mathbf{b}+\mathbf{f}),(\mathbf{a}+\mathbf{e})+(\mathbf{b}+\mathbf{d}))-(\mathbf{b}+\mathbf{d}+\mathbf{b}+\mathbf{f})\\ &= \mathbf{a}-\mathbf{b}+\overline{\mathrm{Max}}(\mathbf{c}+\mathbf{f},\mathbf{e}+\mathbf{d}))-(\mathbf{d}+\mathbf{f})\\ &= \mathbf{a}-\mathbf{b}+\mathrm{Max}(\mathbf{c}-\mathbf{d},\mathbf{e}-\mathbf{f})=\alpha+\mathrm{Max}(\beta,\gamma).\end{aligned}$$

Final identity (2.17) is obtained by the following computation:

$$\begin{aligned}\mathrm{Max}(\mathrm{Max}(\alpha,\beta),\beta+\eta) &= \mathrm{Max}(\mathrm{Max}(\mathbf{a}-\mathbf{b},\mathbf{c}-\mathbf{d}),\mathbf{c}-\mathbf{d}+\eta)\\ &= \mathrm{Max}(\overline{\mathrm{Max}}(\mathbf{a}+\mathbf{d},\mathbf{c}+\mathbf{b})-(\mathbf{b}+\mathbf{d}),\mathbf{c}+\eta-\mathbf{d})\\ &= \overline{\mathrm{Max}}(\overline{\mathrm{Max}}(\mathbf{a}+\mathbf{d},\mathbf{c}+\mathbf{b})+\mathbf{d},\mathbf{c}+\eta+\mathbf{b}+\mathbf{d})-(\mathbf{b}+\mathbf{d}+\mathbf{d})\\ &= \overline{\mathrm{Max}}(\overline{\mathrm{Max}}(\mathbf{a}+\mathbf{d}+\mathbf{d},\mathbf{c}+\mathbf{b}+\mathbf{d}),\mathbf{c}+\mathbf{b}+\mathbf{d}+\eta)-(\mathbf{b}+\mathbf{d}+\mathbf{d})\\ &= \mathbf{a}+\mathbf{d}+\mathbf{d}-(\mathbf{b}+\mathbf{d}+\mathbf{d})=\mathbf{a}-\mathbf{b}=\alpha.\end{aligned}$$

□

D. Definition of inversible Max-Plus algebra Ω

For the matter of convenience, a one-component element $\mathbf{a}=(a)\in\Phi$ is denoted by a, and $\mathbf{b}=(0,-b_1,\ldots,-b_n)\in\Phi$ is denoted by $[b_1,\ldots,b_n]$, if there is no danger of confusion.

Lemma 2.5: We have

$$[a_1,\ldots,a_n]+[b_1,\ldots,b_n]=[\{a_i\}_{i=1}^n,\{b_i\}_{i=1}^m,\{a_i+b_j\}_{i=1\ j=1}^{n\ m}].$$

Proof: The computation is straightforward as follows:

$$\begin{aligned}[a_1,\ldots,a_n]+[b_1,\ldots,b_n] &= (0,-a_1,\ldots,-a_n)+(0,-b_1,\ldots,-b_n)\\ &= (0,\{-a_i\}_{i=1}^n,\{-b_i\}_{i=1}^m,\{-a_i-b_j\}_{i=1\ j=1}^{n\ m})\\ &= [\{a_i\}_{i=1}^n,\{b_i\}_{i=1}^m,\{a_i+b_j\}_{i=1\ j=1}^{n\ m}].\end{aligned}$$

□

Define a subset Ω of Φ by

$$\Omega=\{a+[b_1,\ldots,b_n]-[c_1,\ldots,c_m]\,|\,n,m\in\mathbf{N},a\in\tilde{\mathbf{Z}},b_i\in\tilde{\mathbf{Z}}_+,c_i\in\tilde{\mathbf{Z}}_+\},\tag{2.18}$$

where

$$\tilde{\mathbf{Z}}_+=\{x\in\mathbf{Z}\,|\,x\geqslant 0\}\cup\{x+\eta\in\mathbf{Z}\oplus\mathbf{Z}_2\,|\,x>0\}.$$

For $a+[b_1,\ldots,b_n]-[c_1,\ldots,c_m]\in\Omega$, we call "$a$" *a leading term* and "$[b_1,\ldots,b_n]-[c_1,\ldots,c_m]$" *a correction term*.

Lemma 2.6: We have

$$\Omega=\Phi.$$

Remark: Ω also has the Max-Plus algebra structures (1.2)–(1.4) and the inversible property (1.5), because of *Lemma 2.4*.

Proof: By definition, it is clear that $\Omega\subset\Phi$. Therefore, it is enough to show that $\Phi\subset\Omega$. For $\alpha=(a_1,\ldots,a_n)-(b_1,\ldots,b_m)\in\Phi$, we may assume that $(a_1,\ldots,a_n)$ and $(b_1,\ldots,b_m)$ are irreducible and $a_1\geqslant\ldots\geqslant a_n$ and $b_1\geqslant\ldots\geqslant b_n$, without loss of generality. Then, we have

$$(a_1,\ldots,a_n)-(b_1,\ldots,b_m)=a_1-b_1+(0,-(a_1-a_2),\ldots,-(a_1-a_n))-(0,-(b_1-b_2),\ldots,-(b_1-b_m))=a_1-b_1+[(a_1-a_2),\ldots,(a_1-a_n)]-[(b_1-b_2),\ldots,(b_1-b_m)]\in\Omega.$$

Here, we have used $(a_1-a_i)\in\tilde{\mathbf{Z}}_+(i=2,\ldots,n)$ and $(b_1-b_i)\in\tilde{\mathbf{Z}}_+(i=2,\ldots,m)$. □

Next, in the following two theorems, we shall express Plus, Minus and Max operators in Ω.

Theorem 2.7: *For* $\alpha=a+[b_1,\ldots,b_n]-[c_1,\ldots,c_m]\in\Omega$ *and* $\alpha'=a'+[b'_1,\ldots,b'_p]-[c'_1,\ldots,c'_q]\in\Omega$, *the result of the computation of Plus and Minus operators is given by*

$$\alpha+\alpha'=a+a'+C_+(\alpha,\alpha'),\tag{2.19}$$

$$\alpha-\alpha'=a-a'+C_-(\alpha,\alpha'),\tag{2.20}$$

where the correction terms C_+,C_- *are given by*

$$C_+(\alpha,\alpha')=[\{b_i\}_{i=1}^n,\{b'_i\}_{i=1}^p,\{b_i+b'_j\}_{i=1\ j=1}^{n\ p}]-[\{c_i\}_{i=1}^m,\{c'_i\}_{i=1}^q,\{c_i+c'_j\}_{i=1\ j=1}^{m\ q}],$$

$$C_-(\alpha,\alpha')=[\{b_i\}_{i=1}^n,\{c'_i\}_{i=1}^q,\{b_i+c'_j\}_{i=1\ j=1}^{n\ p}]-[\{c_i\}_{i=1}^m,\{b'_i\}_{i=1}^p,\{c_i+b'_j\}_{i=1\ j=1}^{m\ p}].$$

Proof: The computation is straightforward from Lemma 2.5 □.

Next, we express Max operator in Ω. For arbitrary $\alpha=a+[b_1,\ldots,b_n]\in\Omega$ and $\alpha'=a'+[b'_1,\ldots,b'_m]\in\Omega$ with irreducible expressions (i.e., $[b_1,\ldots,b_n]$ and $[b'_1,\ldots,b'_m]$ are irreducible), we may assume that $b_1\leqslant\cdots\leqslant b_n$ and $b'_1\leqslant\cdots\leqslant b'_m$, without loss of generality. Then, we have the following theorem.

Theorem 2.8: *(1) For* $\alpha=a+[b_1,\ldots,b_n]\in\Omega$ *and* $\alpha'=a'+[b'_1,\ldots,b'_m]\in\Omega$ *with* $b_1\leqslant\ldots\leqslant b_n$ *and* $b'_1\leqslant\cdots\leqslant b'_m$, *the expression of* $\mathrm{Max}(\alpha,\alpha')$ *is given as follows.*

If $a\neq a'+\eta$, we have

$$\mathrm{Max}(\alpha,\alpha')=\max(a,a')+C_m(\alpha,\alpha'),\tag{2.21}$$

where the correction term C_m is given by

$$C_m(\alpha,\alpha')=[|a-a'|,\{b_i+\max(a'-a,0)\}_{i=1}^n,\{b'_i+\max(a-a',0)\}_{i=1}^m].$$

If $a=a'+\eta$, we have

$$\mathrm{Max}(\alpha,\alpha')=\begin{cases}a-b_{k+1}+[\{b_i-b_{k+1}\}_{i=k+2}^n,\{b'_i-b_{k+1}+\eta\}_{i=k+1}^m]\\ \qquad\text{if } {}^{\exists}k<n,m \text{ s.t. } b_i=b'_i(1\leqslant i\leqslant k)\\ \qquad\qquad\text{and } ((b_{k+1}<b'_{k+1}) \text{ or } (b_{k+1}=b'_{k+1}+\eta))\\ a-b_{m+1}+[\{b_i-b_{m+1}\}_{i=m+2}^n]\\ \qquad\text{if } b_i=b'_i \text{ for } 1\leqslant i\leqslant m<n,\\ -\infty \quad \text{if } b_i=b'_i \text{ for } 1\leqslant i\leqslant m=n.\end{cases}\tag{2.22}$$

Remark 1: We will extend the above formula for general cases as follows. For

$$\alpha=a+[b_1,\ldots,b_n]-[c_1,\ldots,c_m]\in\Omega,$$

$$\alpha'=a'+[b'_1,\ldots,b'_p]-[c'_1,\ldots,c'_q]\in\Omega,$$

the expression of $\mathrm{Max}(\alpha,\alpha')$ can be computed by using (2.21) and (2.22) and the identity

$$\mathrm{Max}(\alpha,\alpha') = \mathrm{Max}(a+[b]+[c'],a'+[b']+[c]) - ([c]+[c']). \tag{2.23}$$

Here, notice that the first term on the right-hand side of (2.23) can be computed by (2.21) and (2.22).

Remark 2: In (2.22), for $[b_1,\ldots,b_n]$ and $[b'_1,\ldots,b'_m]$, we can assume that there are only the following three cases:

1. There exists $k\in\mathbf{N}$ and $k<n,m$ such that $b_i=b'_i$ $(i=1,\cdots,k)$ and $((b_{k+1}<b'_{k+1})$ or $(b_{k+1}=b'_{k+1}+\eta))$,
2. $m<n$ and $b_i=b'_i$ $(i=1,\cdots,m)$, and
3. $m=n$ and $b_i=b'_i$ $(i=1,\cdots,m)$,

without loss of generality. These three cases (1, 2 and 3) correspond to the first, second, and third cases in (2.22) respectively.

Proof of Theorem 2.8: Let us consider the case $a\neq a'+\eta$. Without loss of generality, we can assume that $a\geqslant a'$. Then, we have

$$\begin{aligned}\mathrm{Max}(\alpha,\alpha') &= \mathrm{Max}((a,a-b_1,\ldots,a-b_n),(a',a'-b'_1,\ldots,a'-b'_m))\\ &= (a,a-b_1,\ldots,a-b_n,a',a'-b'_1,\ldots,a'-b'_m)\\ &= a+(0,-b_1,\ldots,-b_n,-(a-a'),-(b'_1+a-a'),\ldots,-(b'_m+a-a'))\\ &= a+[a-a',b_1,\ldots,b_n,b'_1+a-a',\ldots,b'_m+a-a'],\end{aligned}$$

which shows that (2.21) holds for $a\geqslant a'$. We can prove (2.21) for the other case $a<a'$ in the same way.

Next, let us consider the case $a=a'+\eta$. First, we consider the first case in (2.22). (i.e., there exists $k\in\mathbf{N}$ and $k<n,m$ such that $b_i=b'_i$ $(i=1,\ldots,k)$ and $b_{k+1}<b'_{k+1}$.) In this case, we have

$$\begin{aligned}\mathrm{Max}(\alpha,\alpha') &= (a,a-b_1,\ldots,a-b_n,a',a'-b'_1,\ldots,a'-b'_m)\\ &= (a-b_{k+1},\ldots,a-b_n,a'-b'_{k+1},\ldots,a'-b'_m) = a-b_{k+1}+(0,-(b_{k+2}-b_{k+1}),\ldots,\\ &\quad -(b_n-b_{k+1}),-(b'_{k+1}-b_{k+1}+\eta),\ldots,-(b'_m-b_{k+1}+\eta))\\ &= a-b_{k+1}+[\{b_i-b_{k+1}\}_{i=k+2}^{n},\{b'_i-b_{k+1}+\eta\}_{i=k+1}^{m}],\end{aligned}$$

which shows the first case in (2.22). Second, we consider the second case in (2.22) (i.e., $m<n$ and $b_i=b'_i$ $(i=1,\ldots,m)$. In this case, we have

$$\begin{aligned}\mathrm{Max}(\alpha,\alpha') &= (a,a-b_1,\ldots,a-b_n,a',a'-b'_1,\ldots,a'-b'_m)\\ &= (a-b_{m+1},\ldots,a-b_n) = a-b_{m+1}+(0,-(b_{m+2}-b_{m+1}),\ldots,-(b_n-b_{m+1}))\\ &= a-b_{m+1}+[\{b_i-b_{m+1}\}_{i=m+2}^{n}],\end{aligned}$$

which shows the second case in (2.22). Third, we consider the third case in (2.22) (i.e., $m=n$ and $b_i=b'_i$ $(i=1,\ldots,m)$.) In this case, we have

$$\mathrm{Max}(\alpha,\alpha') = (a,a-b_1,\ldots,a-b_n,a',a'-b'_1,\ldots,a'-b'_n) = -\infty,$$

which shows the third case in (2.22). □

III. APPLICATIONS

A. Projection to the usual max-plus algebra Z

Let Ω_0 be a subset of Ω defined by $\Omega_0=\{a+[b_1,\ldots,b_n]-[c_1,\ldots.c_m]\in\Omega\,|\,a\in\mathbf{Z}\}\subset\Omega$. For $\alpha=a+[b_1,\ldots,b_n]-[c_1,\ldots.c_m]\in\Omega_0$, define a projection map P: $\Omega_0\to\mathbf{Z}$ by

$$\mathrm{P}(\alpha) = a. \tag{3.1}$$

Lemma 3.1: Ω_0 *is Max-Plus subalgebra.*

Proof: It is clear from (2.21), (2.19), and (2.20). Notice that $a, a' \in \mathbf{Z}$.

Theorem 3.2: *The map P:* $\Omega_0 \to \mathbf{Z}$ *is a homomorphism map with respect to Max, Plus, Minus operators. More precisely, for* $\alpha = a + [b_1, \ldots, b_n] - [c_1, \ldots . c_m] \in \Omega_0$ *and* $\alpha' = a' + [b'_1, \ldots, b'_p] - [c'_1, \ldots, c'_q] \in \Omega_0$, *we have*

$$\mathrm{P}(\mathrm{Max}(\alpha, \alpha')) = \max(a, a'),$$

$$\mathrm{P}(\alpha + \alpha') = a + a',$$

$$\mathrm{P}(\alpha - \alpha') = a - a'.$$

Proof: It is clear from (2.21), (2.19), and (2.20). Notice that $a, a' \in \mathbf{Z}$.

B. Faithful representation on Ω

For any positive real number ϵ and $a = x + \xi \in \tilde{\mathbf{Z}}$, set $\overline{a} = x + \overline{\xi} \in \mathbf{C}$, where

$$\overline{\xi} = \begin{cases} i\pi\epsilon & (\xi = \eta) \\ 0 & (\xi = 0). \end{cases}$$

For $\alpha = (a_i)_{i=1}^n - (b_i)_{i=1}^m = (a_1, \ldots, a_n) - (b_1, \ldots, b_m) \in \Phi$, define a map $\mathrm{R}_\epsilon : \Phi \to \mathbf{C}$ by

$$\mathrm{R}_\epsilon(\alpha) = \epsilon \log\left(\sum_i e^{\overline{a_i}/\epsilon}\right) - \epsilon \log\left(\sum_i e^{\overline{b_i}/\epsilon}\right) = \epsilon \log(e^{\overline{a_1}/\epsilon} + \ \ldots\ + e^{\overline{a_n}/\epsilon}) - \epsilon \log(e^{\overline{b_1}/\epsilon} + \ \ldots\ + e^{\overline{b_m}/\epsilon}).$$

Here we set $e^{\overline{a_i}/\epsilon}$ to be zero, if $a_i = -\infty$.

Lemma 3.3: The previous definition $\mathrm{R}_\epsilon : \Phi \to \mathbf{C}$ is well defined.

Proof: First, we shall show that the definition is invariant under relations (2.1)–(2.3). For $\mathbf{a} = (a_1, \ldots, a_i, \ldots, a_j, \ldots, a_n)$, $\mathbf{a}' = (a_1, \ldots, a_j, \ldots, a_i, \ldots, a_n)$, and $\mathbf{b} = (b_1, \ldots, b_m)$, we have

$$\begin{aligned} \mathrm{R}_\epsilon(\mathbf{a} - \mathbf{b}) &= \mathrm{R}_\epsilon((a_1, \ldots, a_i, \ldots, a_j, \ldots, a_n) - (b_1, \ldots, b_m)) \\ &= \epsilon \log(e^{\overline{a_1}/\epsilon} + \cdots + e^{\overline{a_i}/\epsilon} + \cdots + e^{\overline{a_j}/\epsilon} + \cdots + e^{\overline{a_n}/\epsilon}) - \epsilon \log(e^{\overline{b_1}/\epsilon} + \cdots + e^{\overline{b_m}/\epsilon}) \\ &= \epsilon \log(e^{\overline{a_1}/\epsilon} + \cdots + e^{\overline{a_j}/\epsilon} + \cdots + e^{\overline{a_i}/\epsilon} + \cdots + e^{\overline{a_n}/\epsilon}) - \epsilon \log(e^{\overline{b_1}/\epsilon} + \cdots + e^{\overline{b_m}/\epsilon}) \\ &= \mathrm{R}_\epsilon((a_1, \ldots, a_j, \ldots, a_i, \ldots, a_n) - (b_1, \ldots, b_m)) = \mathrm{R}_\epsilon(\mathbf{a}' - \mathbf{b}), \end{aligned}$$

which shows the invariance under relation (2.1). For $\mathbf{a} = (a_1 \ldots, a_n, c, c + \eta)$, $\mathbf{a}' = (a_1, \ldots, a_n, -\infty)$, and $\mathbf{b} = (b_1, \ldots, b_m)$, we have

$$\begin{aligned} \mathrm{R}_\epsilon(\mathbf{a} - \mathbf{b}) &= \mathrm{R}_\epsilon((a_1, \ldots, a_n, c, c + \eta) - (b_1, \ldots, b_m)) \\ &= \epsilon \log(e^{\overline{a_1}/\epsilon} + \cdots + e^{\overline{a_n}/\epsilon} + e^{\overline{c}/\epsilon} + e^{\overline{c + \eta}/\epsilon}) - \epsilon \log(e^{\overline{b_1}/\epsilon} + \cdots + e^{\overline{b_m}/\epsilon}) \\ &= \epsilon \log(e^{\overline{a_1}/\epsilon} + \cdots + e^{\overline{a_n}/\epsilon} + e^{\overline{c}/\epsilon} + e^{\overline{c}/\epsilon + i\pi}) - \epsilon \log(e^{\overline{b_1}/\epsilon} + \cdots + e^{\overline{b_m}/\epsilon}) \\ &= \epsilon \log(e^{\overline{a_1}/\epsilon} + \cdots + e^{\overline{a_n}/\epsilon} + e^{\overline{c}/\epsilon} - e^{\overline{c}/\epsilon}) - \epsilon \log(e^{\overline{b_1}/\epsilon} + \cdots + e^{\overline{b_m}/\epsilon}) \\ &= \epsilon \log(e^{\overline{a_1}/\epsilon} + \cdots + e^{\overline{a_n}/\epsilon}) - \epsilon \log(e^{\overline{b_1}/\epsilon} + \cdots + e^{\overline{b_m}/\epsilon}) = \mathrm{R}_\epsilon(\mathbf{a}' - \mathbf{b}), \end{aligned}$$

which shows the invariance under relation (2.2). For $\mathbf{a} = (a_1, \ldots, a_n, -\infty)$, $\mathbf{a}' = (a_1, \ldots, a_n)$, and $\mathbf{b} = (b_1, \ldots, b_m)$, we have

$$\mathrm{R}_\epsilon(\mathbf{a}-\mathbf{b}) = \mathrm{R}_\epsilon((a_1,\ldots,a_n,-\infty)-(b_1,\ldots,b_m))$$
$$= \epsilon\log(e^{\overline{a_1}/\epsilon}+\cdots+e^{\overline{a_n}/\epsilon}) - \epsilon\log(e^{\overline{b_1}/\epsilon}+\cdots+e^{\overline{b_m}/\epsilon}) = \mathrm{R}_\epsilon(\mathbf{a}'-\mathbf{b}),$$

which shows the invariance under relation (2.3).

Second, we shall show that the definition is invariant under relation (2.10). Suppose $(a_1,\ldots,a_n)-(b_1,\ldots,b_m)=(a_1',\ldots,a_p')-(b_1',\ldots,b_q')$. Then we have

$$(a_i+b_j')_{i=1\ j=1}^{n\ \ q} = (a_i'+b_j)_{i=1\ j=1}^{p\ \ m}.$$

Then, it follows that

$$\epsilon\log\left(\sum_{i=1}^{n}\sum_{j=1}^{q} e^{\overline{a_i+b_j'}/\epsilon}\right) = \epsilon\log\left(\sum_{i=1}^{p}\sum_{j=1}^{m} e^{\overline{a_i'+b_j}/\epsilon}\right). \tag{3.2}$$

Then, we have

$$\mathrm{R}_\epsilon((a_1,\ldots,a_n)-(b_1,\ldots,b_m)) = \epsilon\log\left(\sum_{i=1}^{n} e^{\overline{a_i}/\epsilon}\right) - \epsilon\log\left(\sum_{j=1}^{m} e^{\overline{b_j}/\epsilon}\right)$$
$$= \epsilon\log\left(\sum_{i=1}^{p} e^{\overline{a_i'}/\epsilon}\right) - \epsilon\log\left(\sum_{j=1}^{q} e^{\overline{b_j'}/\epsilon}\right) + \epsilon\log\left(\sum_{i=1}^{n}\sum_{j=1}^{q} e^{\overline{a_i+b_j'}/\epsilon}\right)$$
$$- \epsilon\log\left(\sum_{i=1}^{p}\sum_{j=1}^{m} e^{\overline{a_i'+b_j}/\epsilon}\right) = \epsilon\log\left(\sum_{i=1}^{p} e^{\overline{a_i'}/\epsilon}\right) - \epsilon\log\left(\sum_{j=1}^{q} e^{\overline{b_j'}/\epsilon}\right)$$
$$= \mathrm{R}_\epsilon((a_1',\ldots,a_p')-(b_1',\ldots,b_q')),$$

which shows the invariance under relation (2.10). Here, we have used (3.2) in the third line. □

For any positive real number ϵ, define a map $\mathrm{Max}_\epsilon:\mathbf{C}\times\mathbf{C}\to\mathbf{C}$ by

$$\mathrm{Max}_\epsilon(a,b) = \epsilon\log(e^{a/\epsilon}+e^{b/\epsilon}),$$

where $a,b\in\mathbf{C}$. Here, we remark that $\mathbf{C}$ with Max_ϵ has the Max-Plus algebra structures (1.2)–(1.4).

Theorem 3.4: *(1) The map* $\mathrm{R}_\epsilon:\Phi\to\mathbf{C}$ *is a representation of* Φ. *More precisely, for* $\alpha,\alpha'\in\Phi$, *we have*

$$\mathrm{R}_\epsilon(\mathrm{Max}(\alpha,\alpha')) = \mathrm{Max}_\epsilon(\mathrm{R}_\epsilon(\alpha),\mathrm{R}_\epsilon(\alpha')), \tag{3.3}$$

$$\mathrm{R}_\epsilon(\alpha+\alpha') = \mathrm{R}_\epsilon(\alpha)+\mathrm{R}_\epsilon(\alpha'), \tag{3.4}$$

$$\mathrm{R}_\epsilon(\alpha-\alpha') = \mathrm{R}_\epsilon(\alpha)-\mathrm{R}_\epsilon(\alpha'). \tag{3.5}$$

(2) If $\mathrm{R}_\epsilon(\alpha)=0$ *for any* ϵ, *then* $\alpha=0$.

Proof: (1) First, we will prove (3.3) as follows. For $\alpha=\mathbf{a}-\mathbf{b}=(a_1,\ldots,a_n)-(b_1,\ldots,b_m)\in\Phi$ and $\alpha=\mathbf{a}'-\mathbf{b}'=(a_1',\ldots,a_p')-(b_1',\ldots,b_q')\in\Phi$, we have

$$
\begin{aligned}
\mathrm{R}_\epsilon(\mathrm{Max}(\alpha,\alpha')) &= \mathrm{R}_\epsilon(\overline{\mathrm{Max}}(\mathbf{a}+\mathbf{b}',\mathbf{a}'+\mathbf{b})-(\mathbf{b}+\mathbf{b}')) \\
&= \mathrm{R}_\epsilon(((a_i+b_j')_{i=1}^{n\ q}{}_{j=1},(a_k'+b_l)_{k=1}^{p\ m}{}_{l=1})-(b_i+b_j')_{i=1}^{m\ q}{}_{j=1}) \\
&= \epsilon\log\left(\sum_{i,j} e^{\overline{a_i+b_j'}/\epsilon}+\sum_{i,j} e^{\overline{a_i'+b_j}/\epsilon}\right)-\epsilon\log\left(\sum_{i,j} e^{\overline{b_i+b_j'}/\epsilon}\right) \\
&= \epsilon\log\left(\frac{\sum_i e^{\overline{a_i}/\epsilon}}{\sum_i e^{\overline{b_i}/\epsilon}}+\frac{\sum_i e^{\overline{a_i'}/\epsilon}}{\sum_i e^{\overline{b_i'}/\epsilon}}\right)=\mathrm{Max}_\epsilon\left(\epsilon\log\left(\frac{\sum_i e^{\overline{a_i}/\epsilon}}{\sum_i e^{\overline{b_i}/\epsilon}}\right),\epsilon\log\left(\frac{\sum_i e^{\overline{a_i'}/\epsilon}}{\sum_i e^{\overline{b_i'}/\epsilon}}\right)\right) \\
&= \mathrm{Max}_\epsilon\left(\epsilon\log\left(\sum_i e^{\overline{a_i}/\epsilon}\right)-\epsilon\log\left(\sum_i e^{\overline{b_i}/\epsilon}\right),\epsilon\log\left(\sum_i e^{\overline{a_i'}/\epsilon}\right)-\epsilon\log\left(\sum_i e^{\overline{b_i'}/\epsilon}\right)\right) \\
&= \mathrm{Max}_\epsilon(\mathrm{R}_\epsilon(\alpha),\mathrm{R}_\epsilon(\alpha')),
\end{aligned}
$$

which shows (3.3). Second, we will prove (3.4) as follows:

$$
\begin{aligned}
\mathrm{R}_\epsilon(\mathrm{Max}(\alpha+\alpha')) &= \mathrm{R}_\epsilon((\mathbf{a}+\mathbf{a}')-(\mathbf{b}+\mathbf{b}')) \\
&= \mathrm{R}_\epsilon(((a_i+a_j')_{i=1}^{n\ p}{}_{j=1}-(b_i+b_j')_{i=1}^{m\ q}{}_{j=1}) \\
&= \epsilon\log\left(\sum_{i,j} e^{\overline{a_i+a_j'}/\epsilon}\right)-\epsilon\log\left(\sum_{i,j} e^{\overline{b_i+b_j'}/\epsilon}\right) \\
&= \epsilon\log\left(\sum_i e^{\overline{a_i}/\epsilon}\right)-\epsilon\log\left(\sum_i e^{\overline{b_i}/\epsilon}\right)+\epsilon\log\left(\sum_i e^{\overline{a_i'}/\epsilon}\right)-\epsilon\log\left(\sum_i e^{\overline{b_i'}/\epsilon}\right) \\
&= \mathrm{R}_\epsilon(((a_i)_{i=1}^n-(b_i)_{i=1}^m)+\mathrm{R}_\epsilon(((a_i')_{i=1}^n-(b_j')_{i=1}^q)=\mathrm{R}_\epsilon(\alpha)+\mathrm{R}_\epsilon(\alpha').
\end{aligned}
$$

This shows (3.4). We can obtain (3.5) in the same way.

(2) For $\alpha=(a_1,\ldots,a_n)-(b_1,\ldots,b_m)\in\Phi$, it is assumed that α is irreducible and $a_1\geqslant\cdots\geqslant a_n$ and $b_1\geqslant\cdots\geqslant b_n$. Then, we have

$$
\mathrm{R}_\epsilon(\alpha)=\epsilon\log(e^{\overline{a_1}/\epsilon}+\cdots+e^{\overline{a_n}/\epsilon})-\epsilon\log(e^{\overline{b_1}/\epsilon}+\cdots+e^{\overline{b_m}/\epsilon})=0.
$$

Hence, we have

$$
e^{\overline{a_1}/\epsilon}+\cdots+e^{\overline{a_n}/\epsilon}=e^{\overline{b_1}/\epsilon}+\cdots+e^{\overline{b_m}/\epsilon}.
$$

This equation is equal to

$$
e^{\overline{a_1}/\epsilon}(1+e^{-\overline{(a_1-a_2)}/\epsilon}+\cdots+e^{-\overline{(a_1-a_n)}/\epsilon})=e^{\overline{b_1}/\epsilon}(1+e^{-\overline{(b_1-b_2)}/\epsilon}+\cdots+e^{-\overline{(b_1-b_m)}/\epsilon}).
$$

Considering $\epsilon\to+0$, we have $a_1=b_1$. By using inductive argument, we obtain

$$
(a_1,\ldots,a_n)=(b_1,\ldots,b_m),
$$

which shows $\alpha=0$. □

C. Ultradiscrete recursive equation

Define $\mathrm{UD}:\mathbf{Z}\to\Omega$ by

$$
\mathrm{UD}(n)=\begin{cases}0+[\underbrace{0,\ldots,0}_{k-1}] & \text{if } n=k\\ -\infty & \text{if } n=0\\ \eta+[\underbrace{0,\ldots,0}_{k-1}] & \text{if } n=-k.\end{cases}
$$

Let $P:\mathbf{R}^n\to\mathbf{R}$ be a polynomial function of finite degree given by

$$P(x_1, \ldots, x_n) = \sum_{i_1,\ldots,i_n=1}^{N} a_{i_1\ldots i_n} x_1^{i_1} \ldots x_n^{i_n},$$

where $a_{i_1\cdots i_n} \in \mathbf{Z}$, $x_i \in \mathbf{R}$. For $P(x_1, \ldots, x_n)$, define its UD polynomial $P_{UD}: \Omega^n \to \Omega$ by

$$P_{UD}(X_1, \ldots, X_n) = \underset{i_1,\ldots,i_n=1}{\overset{N}{\mathrm{Max}}} (\mathrm{UD}(a_{i_1\ldots i_n}) + i_1 X_1 + \cdots + i_n X_n),$$

where $X_i \in \Omega$.

More generally, let $F: \mathbf{R}^n \to \mathbf{R}$ a rational function given by

$$F(x_1, \ldots, x_n) = \frac{P(x_n, \ldots, x_1)}{Q(x_n, \ldots, x_1)},$$

where P and Q are polynomial functions of finite degree. Then, we define its UD equation $F_{UD}: \Omega^n \to \Omega$ by

$$F_{UD}(X_1, \ldots, X_n) = P_{UD}(X_1, \ldots, X_n) - Q_{UD}(X_1, \ldots, X_n). \tag{3.6}$$

Remark: (3.6) is just obtained by the following transformations:

$$x_i \times y_j \to X_i + Y_j,$$

$$x_i / y_j \to X_i - Y_j,$$

$$x_i + y_j \to \mathrm{Max}(X_i, Y_j),$$

$$x_i - y_j \to \mathrm{Max}(X_i, Y_j + \eta),$$

$$a_{i_1\cdots i_n} \to \mathrm{UD}(a_{i_1\cdots i_n}). \tag{3.7}$$

This is the final mapping we want (i.e., the mapping from the usual algebra to the inversible Max-Plus algebra Ω). Here, we remark that the missing correspondence in Fig. 1 (i.e., $x - y \to ??$) is now clear, since this correspondence is given by $x_i - y_j \to \mathrm{Max}(X_i, Y_j + \eta)$ in the previous transformation.

Theorem 3.5: *Suppose a periodic recursive equation*

$$x_{n+1} = F(x_1, \ldots, x_n) = \frac{P(x_n, \ldots, x_1)}{Q(x_n, \ldots, x_1)} \tag{3.8}$$

on $\mathbf{R}$ *has period k (i.e.,* $x_{n+k} = x_n$*), then its UD periodic recursive equation*

$$X_{n+1} = F_{UD}(X_1, \ldots, X_n) = P_{UD}(X_1, \ldots, X_n) - Q_{UD}(X_1, \ldots, X_n)$$

on Ω *also has period k (i.e.,* $X_{n+k} = X_n$*).*

Proof: Substituting $x_n = e^{R_\epsilon(X_n)/\epsilon}$ into (3.8), we have

$$
\begin{aligned}
e^{R_\epsilon(X_{n+1})/\epsilon} &= \frac{P(e^{R_\epsilon(X_n)/\epsilon}, \ldots, e^{R_\epsilon(X_1)/\epsilon})}{Q(e^{R_\epsilon(X_n)/\epsilon}, \ldots, e^{R_\epsilon(X_1)/\epsilon})} \\
&= \frac{\sum_{i_1,\ldots,i_n=1}^{N} a_{i_1\cdots i_n} e^{(i_1 R_\epsilon(X_1)+\cdots+i_n R_\epsilon(X_n))/\epsilon}}{\sum_{i_1,\ldots,i_n=1}^{N} b_{i_1\cdots i_n} e^{(i_1 R_\epsilon(X_1)+\cdots+i_n R_\epsilon(X_n))/\epsilon}} \\
&= \frac{\sum_{i_1,\ldots,i_n=1}^{N} e^{(\epsilon \log a_{i_1\cdots i_n}+R_\epsilon(i_1X_1+\cdots+i_nX_n))/\epsilon}}{\sum_{i_1,\ldots,i_n=1}^{N} e^{(\epsilon \log b_{i_1\cdots i_n}+R_\epsilon(i_1X_1+\cdots+i_nX_n))/\epsilon}} \\
&= \frac{\sum_{i_1,\ldots,i_n=1}^{N} e^{R_\epsilon(U(a_{i_1\cdots i_n})+i_1X_1+\cdots+i_nX_n)/\epsilon}}{\sum_{i_1,\ldots,i_n=1}^{N} e^{R_\epsilon(U(b_{i_1\cdots i_n})+i_1X_1+\cdots+i_nX_n)/\epsilon}}.
\end{aligned}
$$

Here, in the last line, we have used

$$
\begin{aligned}
\epsilon \log a_{i_1\cdots i_n} &= \underbrace{\epsilon \log e^{0/\epsilon} + \cdots + e^{0/\epsilon}}_{a_{i_1\cdots i_n}} \\
&= R_\epsilon((\underbrace{0, \ldots, 0}_{a_{i_1\cdots i_n}})) \\
&= R_\epsilon(0 + [\underbrace{0, \ldots, 0}_{a_{i_1\cdots i_n}-1}]) \\
&= R_\epsilon(U(a_{i_1\cdots i_n})).
\end{aligned}
$$

Then, we have

$$
\begin{aligned}
R_\epsilon(X_{n+1}) &= \operatorname*{Max}_{i_1,\ldots,i_n=1}^{N}{}_\epsilon (R_\epsilon(U(a_{i_1\cdots i_n}) + i_1X_1 + \cdots + i_nX_n)) - \operatorname*{Max}_{i_1,\ldots,i_n=1}^{N}{}_\epsilon (R_\epsilon(U(b_{i_1\cdots i_n}) + i_1X_1 + \cdots + i_nX_n)) \\
&= R_\epsilon(\operatorname*{Max}_{i_1,\ldots,i_n=1}^{N} (U(a_{i_1\cdots i_n}) + i_1X_1 + \cdots + i_nX_n) - \operatorname*{Max}_{i_1,\ldots,i_n=1}^{N} (U(b_{i_1\cdots i_n}) + i_1X_1 + \cdots + i_nX_n)).
\end{aligned}
$$

Hence, we finally obtain

$$
\mathrm{R}_\epsilon(X_{n+1}) = \mathrm{R}_\epsilon(P_{UD}(X_1, \ldots, X_n) - Q_{UD}(X_1, \ldots, X_n)).
$$

On the other hand, we have $\mathrm{R}_\epsilon(X_{n+k}) = \mathrm{R}_\epsilon(X_n)$ from $x_{n+k} = x_n$. This implies $X_{n+k} = X_n$. □

IV. EXAMPLES

A. Simplest example with subtraction

Let us consider the most simple identity

$$
x + y - y = x. \tag{4.1}
$$

Although this identity is simple, we cannot ultradiscretize this identity by the usual UD procedure (1.1) due to the subtraction $(-y)$ in the left-hand side of this identitiy (4.1). However, by using our ultradiscretization mapping (3.6) [or (3.7)] to the inversible Max-Plus algebra Ω, we can ultradiscretize this identity (4.1) as follows:

$$
\mathrm{Max}(\mathrm{Max}(X, Y), Y + \eta) = X.
$$

For example, if we take $X = 1$ and $Y = 3$ in this equation, we have

$$\mathrm{Max}(\mathrm{Max}(1,3),3+\eta)=\mathrm{Max}(3+[2],3+\eta)=1.$$

This example clearly exhibits the inversible property (1.5) of the Max operator on Ω, which does not exist in usual max operator on $\mathbf{Z}$.

B. Periodic recursive equations

Next, we will give some examples of periodic recursive equations.

1. Example without subtraction

It is known that the periodic recursive equation

$$x_{n+1}=\frac{x_n+1}{x_{n-1}}$$

has period 5. Then, from Theorem 3.5, we find that its UD equation

$$X_{n+1}=\mathrm{Max}(X_n,0)-X_{n-1} \tag{4.2}$$

also has period 5. For example, we have

$$X_1=1,\quad X_2=5,\quad X_3=4+[5],\quad X_4=-1+[4,5],\quad X_5=-4+[1,5,6]-[5],\quad X_6=1,\quad X_7=5. \tag{4.3}$$

Remark: If $X_i\in\Omega_0$ for all i, then we can act the projection map $\mathrm{P}:\Omega_0\to\mathbf{Z}$ for both sides of Eq. (4.2). Then, we have

$$Y_{n+1}=\max(Y_n,0)-Y_{n-1}, \tag{4.4}$$

where $Y_i=P(X_i)$. For example, we have

$$Y_1=1,\quad Y_2=5,\quad Y_3=4,\quad Y_4=-1,\quad Y_5=-4,\quad Y_6=1,\quad Y_7=5,$$

which correspond to (4.3). This equation also has period 5.

Here we remark that this usual UD equation (4.4) on $\mathbf{Z}$ can also be obtained by the usual ultradiscretization procedure $\lim_{\epsilon\to+0}\epsilon\log(e^{X/\epsilon}+e^{Y/\epsilon})=\max(X,Y)$ given by (1.1).

In the following paragraph, we will give an example which cannot be ultradiscretized by the usual ultradiscretization procedure (1.1). Therefore, in the next example, our mapping to the inversible Max-Plus algebra (3.6) [or (3.7)] will be essentially necessary, instead of the usual ultradiscretization procedure (1.1).

2. Example with subtraction

The periodic recursive equation

$$x_{n+1}=\frac{x_n-1}{x_n+1}$$

has period 4. Then, from Theorem 3.5, we find that its UD equation

$$X_{n+1}=\mathrm{Max}(X_n,\eta)-\mathrm{Max}(X_n,0) \tag{4.5}$$

also has period 4. For example,

$$X_1 = 2, \quad X_2 = [2 + \eta] - [2], \quad X_3 = -2 + \eta, \quad X_4 = \eta + [2] - [2 + \eta], \quad X_5 = 2. \tag{4.6}$$

Remark: We cannot act the projection map $\mathrm{P}:\Omega_0 \to \mathbf{Z}$ for both sides of Eqs. (4.5) and (4.6), since all the variables X_i do not belong to Ω_0. Therefore, this is a new type of UD equations, which cannot be obtained by the usual ultradiscretization procedure (1.1).

C. Equation of motion for a free particle

1. Continuous equation

The equation of motion for a free particle is given by

$$\ddot{x} = 0. \tag{4.7}$$

The energy conservation law is given by

$$e = \tfrac{1}{2}(\dot{x})^2 = \text{constant}. \tag{4.8}$$

2. Discrete equation

It is known that the discrete version of the equation of motion (4.7) is given by

$$x_{n+2} = 2x_{n+1} - x_n, \tag{4.9}$$

and the discrete version of the energy conservation law (4.8) is given by

$$h_n = \sqrt{2e_n} = x_{n+1} - x_n = \text{constant}. \tag{4.10}$$

Here we remark that the discrete equations (4.9) and (4.10) cannot be ultradiscretized by the usual procedure (1.1), since there exists subtraction in (4.9) and (4.10). However, by using our ultradiscretization mapping (3.6) [or (3.7)] to the inversible Max-Plus algebra Ω, we can ultradiscretize both Eqs. (4.9) and (4.10), which will be explained in the following paragraph.

3. Ultradiscrete equation

Finally, by using our ultradiscretization mapping (3.6) [or (3.7)], the discrete equation (4.9) can be transformed into

$$X_{n+1} = \mathrm{Max}(X_n + [0], X_{n-1} + \eta), \tag{4.11}$$

which is the UD version of the equation of motion for a free particle.

In the same way, from (4.10), we obtain the UD version of the energy conservation for a free particle as follows:

$$H_n = \mathrm{Max}(X_{n+1}, X_n + \eta). \tag{4.12}$$

4. Trajectory of the UD equation of motion for a free particle

Repeatedly using (4.11) with the initial condition $X_1 = 0$ and $X_2 = 1$, we can obtain the trajectory of the free particle as follows:

$$X_1 = 0,$$

$$X_2 = 1,$$

$$X_3 = 1 + [0, 1 + \eta],$$

$$X_4 = 1 + [0, 0, 1 + \eta, 1 + \eta],$$

$$\vdots$$

$$X_n = 1 + [0^{n-2}, (1 + \eta)^{n-2}],$$

where 0^{n-2} [respectively, $(1+\eta)^{n-2}$] denotes the array of $n-2$ zeros [respectively, $(1+\eta)$]. For example, $[0^3, (1+\eta)^3]$ denotes $[0,0,0,1+\eta,1+\eta,1+\eta]$. Here we remark that the trajectory of the leading term of X_n $(n=1,2,\cdots)$ is suddenly stopped after $n \geqslant 2$, while the correction terms are still changing.

It is worth noticing that although the trajectory of the leading term of X_n is suddenly stopped in the UD world, the energy H_n is still conserved as follows:

$$H_1 = \mathrm{Max}(X_2, X_1 + \eta) = 1 + [1 + \eta],$$

$$H_2 = \mathrm{Max}(X_3, X_2 + \eta) = 1 + [1 + \eta],$$

$$\vdots$$

$$H_n = \mathrm{Max}(X_{n+1}, X_n + \eta) = 1 + [1 + \eta].$$

For the future work, it would be interesting to study the ultradiscretization of the well known theory (e.g., soliton theory, chaos theory, classical mechanics, etc.), using the inversible Max-Plus algebra Ω and its mapping (3.6) [or (3.7)].

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A nested sequence of projectors and corresponding braid matrices $\hat{R}(\theta)$. 1. Odd dimensions

A. Chakrabarti[a)]
Centre de Physique Théorique,[b)] *Ecole Polytechnique, 91128 Palaiseau Cedex, France*

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A basis of N^2 projectors, each an $N^2\times N^2$ matrix with constant elements, is implemented to construct a class of braid matrices $\hat{R}(\theta)$, θ being the spectral parameter. Only odd values of N are considered here. Our ansatz for the projectors P_α appearing in the spectral decomposition of $\hat{R}(\theta)$ leads to exponentials $\exp(m_\alpha\theta)$ as the coefficient of P_α. The sums and differences of such exponentials on the diagonal and the antidiagonal, respectively, provide the $(2N^2-1)$ nonzero elements of $\hat{R}(\theta)$. One element at the center is normalized to unity. A class of supplementary constraints imposed by the braid equation leaves $\frac{1}{2}(N+3)(N-1)$ free parameters m_α. The diagonalizer of $\hat{R}(\theta)$ is presented for all N. Transfer matrices $t(\theta)$ and $L(\theta)$ operators corresponding to our $\hat{R}(\theta)$ are studied. Our diagonalizer signals specific combinations of the components of the operators that lead to a quadratic algebra of N^2 constant $N\times N$ matrices. The θ dependence factors out for such combinations. $\hat{R}(\theta)$ is developed in a power series in θ. The basic difference arising for even dimensions is made explicit. Some special features of our $\hat{R}(\theta)$ are discussed in a concluding section. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1900291]

I. INTRODUCTION

In Sec. 8 of Ref. 1 a sequence of projectors with constant elements and particularly simple and convenient properties were introduced for arbitrary dimension N (i.e., $N^2\times N^2$ matrices). For the case $N=2$ they provide the spectral resolutions of the six-vertex and the eight-vertex models (Secs. 6 and 7 of Ref. 1, citing other sources). Along with N the set of projectors is enlarged in number and in dimension systematically at each step to give what we called a "nested sequence." The projectors were presented Ref. 1 for all N and their basic features were studied, including diagonalization, for arbitrary N. But no higher dimensional braid matrices were constructed on such bases. That was "beyond the scope" of that paper. Here we enlarge the scope and present explicit constructions for all *odd* N. Even dimensions will be studied separately elsewhere. Such a separation corresponds to strikingly different features arising in the respective cases.

After obtaining explicitly $\hat{R}(\theta)$ the corresponding transfer matrices $t(\theta)$ and $L(\theta)$ operators are studied. They are found to lead to a remarkable class of quadratic algebra (Sec. IV). Development of $\hat{R}(\theta)$ in powers of the spectral parameter θ is also studied (Sec. V). Basic differences arising for even dimensions are pointed out. (Sec. VI). The special features of our class of solutions are discussed in conclusion (Sec. VII). Construction of our solutions is presented in Appendix A and some basic results concerning $t(\theta)$ and $L(\theta)$ are collected together in Appendix B.

[a)]Electronic mail: chakra@cpht.polytechnique.fr
[b)]Laboratoire Propre du CNRS UPR A.0014.

II. BRAID MATRICES FOR ODD DIMENSIONS (ANSATZ AND SOLUTIONS)

We start by specifying our notations and conventions in detail since they turn out to be crucial in successful construction of the solutions. Thus, rather than using the simple and elegant notation of Sec. 8 of Ref. 1 for our projectors we introduce in the following a structure better suited to our present purpose.

Let

$$N = 2p - 1 \quad (p = 2,3, \dots)$$

and

$$\overline{i} = N - i + 1 \quad (i + \overline{i} = 2p,\ \overline{\overline{i}} = i)$$

so that for

$$i = 1,2, \dots ,(p-1),$$

respectively,

$$\overline{i} = (2p-1),(2p-2), \dots ,(p+1)$$

and

$$\overline{p} = p.$$

The $N^2 \times N^2$ braid matrix $\hat{R}(\theta)$, with the spectral parameter θ, is given in terms of its components as

$$\hat{R}(\theta) = (\hat{R}(\theta))_{ab,cd}(ab) \otimes (cd), \tag{2.1}$$

where (a,b,c,d) take values in the domain $(i,\overline{i},p)$ and (ab) is the $N \times N$ matrix with only one nonzero element, unity, at row a and column b.

The basis of projectors is given by (with $\epsilon = \pm$) the set

$$P_{pp} = (pp) \otimes (pp),$$

$$2P_{pi(\epsilon)} = (pp) \otimes (((ii) + (\overline{i}\overline{i})) + \epsilon((i\overline{i}) + (\overline{i}i))),$$

$$2P_{ip(\epsilon)} = (((ii) + (\overline{i}\overline{i})) + \epsilon((i\overline{i}) + (\overline{i}i))) \otimes (pp), \tag{2.2}$$

$$2P_{ij(\epsilon)} = (((ii) \otimes (jj) + (\overline{i}\overline{i}) \otimes (\overline{j}\overline{j})) + \epsilon((i\overline{i}) \otimes (j\overline{j}) + (\overline{i}i) \otimes (\overline{j}j))),$$

$$2P_{\overline{ij}(\epsilon)} = (((ii) \otimes (\overline{j}\overline{j}) + (\overline{i}\overline{i}) \otimes (jj)) + \epsilon((i\overline{i}) \otimes (\overline{j}j) + (\overline{i}i) \otimes (j\overline{j}))).$$

Condensing the triplets $(i,j,\epsilon),(i,p,\epsilon),\dots$ and also (pp) into $(\alpha,\beta,\dots)$ the basis (2.2) satisfies

$$P_\alpha P_\beta = \delta_{\alpha\beta} P_\alpha, \quad \sum_\alpha P_\alpha = I_{N^2 \times N^2}. \tag{2.3}$$

The total number of P_α is

$$1 + 4(p-1) + 4(p-1)^2 = (2p-1)^2 = N^2.$$

They have, apart from the overall factor $\frac{1}{2}$ for all projectors except P_{pp}, only the constant elements

$(\pm 1,0)$. There is, for example, no q in our formalism. The braid matrix is *postulated* in the spectrally resolved form

$$\hat{R}(\theta) = P_{pp} + \sum_{i,\epsilon} (f_{pi}^{(\epsilon)}(\theta) P_{pi(\epsilon)} + f_{ip}^{(\epsilon)}(\theta) P_{ip(\epsilon)}) + \sum_{i,j,\epsilon} (f_{ij}^{(\epsilon)}(\theta) P_{ij(\epsilon)} + f_{ij}^{(\epsilon)}(\theta) P_{\bar{ij}(\epsilon)}). \tag{2.4}$$

The coefficient of P_{pp} is normalized to unity. The (N^2-1) functions $f_{ab}^{(\epsilon)}$ are to be extracted from the constraints imposed by the braid equation

$$\hat{R}_{12}(\theta)\hat{R}_{23}(\theta+\theta')\hat{R}_{12}(\theta') = \hat{R}_{23}(\theta')\hat{R}_{12}(\theta+\theta')\hat{R}_{23}(\theta). \tag{2.5}$$

Here (suppressing θ)

$$\hat{R}_{12} = \hat{R} \otimes I_{N\times N}, \quad \hat{R}_{23} = I_{N\times N} \otimes \hat{R}.$$

In terms of the coefficients $(\hat{R}(\theta))_{ab,cd}$ defined in (2.1) one obtains [summing over the repeated indices (l,m,n)]

$$(\hat{R}(\theta))_{al,cm}(\hat{R}(\theta+\theta'))_{mn,ef}(\hat{R}(\theta'))_{lb,nd} = (\hat{R}(\theta'))_{cl,em}(\hat{R}(\theta+\theta'))_{ab,ln}(\hat{R}(\theta))_{nd,mf}. \tag{2.6}$$

This corresponds to the point $(ab)\otimes(cd)\otimes(ef)$ of the base space $V\otimes V\otimes V$. Our ansatz (2.4) along with (2.2) implies very strong constraints (typical of *odd* dimensions). The solutions are obtained in Appendix A. One has

$$f_{ab}^{(\epsilon)}(\theta) = \exp(m_{ab}^{(\epsilon)}\theta), \quad (ab) = (pi),(ip),(ij),(\bar{ij}), \tag{2.7}$$

where the parameters $m_{ab}^{(\epsilon)}$ are all independent *except* that for each i,

$$m_{ij}^{(\epsilon)} = m_{\bar{ij}}^{(\epsilon)}, \quad (\bar{j} = 2p - j). \tag{2.8}$$

The constraints (2.7) and (2.8) are *necessary and sufficient*. Thus for $N=3$ one has

$$\hat{R}(\theta) = \begin{pmatrix} a_+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_- \\ 0 & b_+ & 0 & 0 & 0 & 0 & 0 & b_- & 0 \\ 0 & 0 & a_+ & 0 & 0 & 0 & a_- & 0 & 0 \\ 0 & 0 & 0 & c_+ & 0 & c_- & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & c_- & 0 & c_+ & 0 & 0 & 0 \\ 0 & 0 & a_- & 0 & 0 & 0 & a_+ & 0 & 0 \\ 0 & b_- & 0 & 0 & 0 & 0 & 0 & b_+ & 0 \\ a_- & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_+ \end{pmatrix} \tag{2.9}$$

where

$$\begin{aligned} a_\pm &= \tfrac{1}{2}(e^{m_{11}^{(+)}\theta} \pm e^{m_{11}^{(-)}\theta}), \\ b_\pm &= \tfrac{1}{2}(e^{m_{12}^{(+)}\theta} \pm e^{m_{12}^{(-)}\theta}), \\ c_\pm &= \tfrac{1}{2}(e^{m_{21}^{(+)}\theta} \pm e^{m_{21}^{(-)}\theta}). \end{aligned} \tag{2.10}$$

The six parameters remaining after application of (2.8) (which imposes the repetation of $a_\pm$) are all *independent*. For $m_{ab}^{(-)} = m_{ab}^{(+)}$ one obtains hyperbolic functions as particular cases. For all N, the nonzero elements are confined to *the diagonal and the antidiagonal* as above with a common

element, unity, at the center. Apart from the normalized element, the coefficients of the projectors are simply exponentials. The total number of independent parameters $m_{ab}^{\pm}$ is

$$(2p-1)^2 - 1 - 2(p-1)^2 = 2(p^2-1) = \tfrac{1}{2}(N+3)(N-1). \tag{2.11}$$

Note that the coefficient of P_{pp} in (2.4) has to be nonzero for $\hat{R}(\theta)$ to be invertible and hence can safely be normalized to unity. Indeed, each coefficient in (2.4) has to be nonzero for $\hat{R}(\theta)$ to be invertible. This is more evident after diagonalization (Sec. III). For even N there is *no* index $p=\overline{p}$. In Appendix A the crucial role of the index p will be made more evident. The projectors $P_{pi(\epsilon)}$ and $P_{ip(\epsilon)}$ will be seen to impose the highly constrained solutions (2.7) with (2.8).

Implementing (2.8) one obtains from (2.4)

$$\hat{R}(\theta) = P_{pp} + \sum_{i,\epsilon} (f_{pi}^{(\epsilon)}(\theta) P_{pi(\epsilon)} + f_{ip}^{(\epsilon)}(\theta) P_{ip(\epsilon)}) + \sum_{i,j,\epsilon} f_{ij}^{(\epsilon)}(\theta)(P_{ij(\epsilon)} + P_{i\overline{j}(\epsilon)}). \tag{2.12}$$

Defining

$$\widetilde{P}_{ij(\epsilon)} = P_{ij(\epsilon)} + P_{i\overline{j}(\epsilon)} \tag{2.13}$$

and conserving all other projectors as before one obtains a basis of $(2p^2-1)$ projectors still satisfying (2.3) where now the indices summed over are (i,j,ϵ), (i,p,ϵ), (p,i,ϵ), (pp).

Now

$$\hat{R}(\theta) = P_{pp} + \sum_{i,\epsilon} (f_{pi}^{(\epsilon)}(\theta) P_{pi(\epsilon)} + f_{ip}^{(\epsilon)}(\theta) P_{ip(\epsilon)}) + \sum_{i,j,\epsilon} f_{ij}^{(\epsilon)}(\theta) \widetilde{P}_{ij(\epsilon)}. \tag{2.14}$$

In this basis *all* the $\frac{1}{2}(N+3)(N-1)$ parameters are independent. When they are all chosen to be distinct (and different from 1) the polynomial equation [of $\frac{1}{2}(N+3)(N-1)$ degree and with distinct roots] satisfied by $\hat{R}(\theta)$ and the projectors in terms of $\hat{R}(\theta)$ are obtained, respectively, as in (1.5) and (1.6) of Ref. 1. The initial basis, due to the symmetry and simplicity of the projectors, is most convenient for certain purposes. The second one has the virtue of eliminating constraints. Each should be implemented according to the context.

If two or more of the $\frac{1}{2}(N+3)(N-1)$ free parameters are allowed to coincide, then introducing the sum of the corresponding projectors [as in (2.13)] the basis can again be redefined [as in (2.14)]. The degree of the minimal polynomial equation satisfied by $\hat{R}(\theta)$ diminishes correspondingly.

Our matrices all satisfy

$$\hat{R}(-\theta)\hat{R}(\theta) = I, \quad \hat{R}(0) = I. \tag{2.15}$$

III. DIAGONALIZATION

Our general approach to diagonalization is presented step by step in Sec. 9 of Ref. 1.

The matrix M that diagonalizes each projector P_α of (2.3) [namely, P_{pp}, $P_{pi(\epsilon)}$, $P_{ip(\epsilon)}$, $P_{ij(\epsilon)}$, $P_{i\overline{j}(\epsilon)}$ of (2.2)] and hence $\hat{R}(\theta)$ of (2.4) is given below. As compared to the results of Sec. 8 of Ref. 1, M is presented here in our current notations. Set

$$\begin{aligned}\sqrt{2}M &= \sqrt{2}M^{-1} \\ &= \sqrt{2}(pp)\otimes(pp) + (pp)\otimes\left(\sum_i ((ii) - (i\overline{i}) + (\overline{i}i) + (\overline{i}\overline{i}))\right) + \left(\sum_i ((ii) - (i\overline{i}) + (\overline{i}i) + (\overline{i}\overline{i}))\right)\otimes(pp) \\ &\quad + \sum_{i,j}\Big(((ii) - (i\overline{i}))\otimes((jj) + (\overline{j}\overline{j})) + ((\overline{i}i) + (\overline{i}\overline{i}))\otimes((\overline{j}j) + (\overline{j}\overline{j}))\Big).\end{aligned} \tag{3.1}$$

One verifies in a straightforward fashion (with $\epsilon = \pm 1$ on the right) that

$$MP_{pp}M^{-1} = (pp) \otimes (pp),$$

$$2MP_{pk(\epsilon)}M^{-1} = (pp) \otimes ((1+\epsilon)(kk) + (1-\epsilon)(\overline{kk})),$$

$$2MP_{kp(\epsilon)}M^{-1} = ((1+\epsilon)(kk) + (1-\epsilon)(\overline{kk})) \otimes (pp), \tag{3.2}$$

$$2MP_{kl(\epsilon)}M^{-1} = (1+\epsilon)(kk) \otimes (ll) + (1-\epsilon)(\overline{kk}) \otimes (\overline{ll}),$$

$$2MP_{k\bar{l}(\epsilon)}M^{-1} = (1+\epsilon)(kk) \otimes (\overline{ll}) + (1-\epsilon)(\overline{kk}) \otimes (ll).$$

Hence taking account of (2.8) [i.e., $f_{ij}^{(\epsilon)}(\theta) = f_{\bar{i}\bar{j}}^{(\epsilon)}(\theta)$] one obtains

$$\begin{aligned} 2M\hat{R}(\theta)M^{-1} = {} & 2(pp) \otimes (pp) + \sum_{i,\epsilon} \Big(f_{pi}^{(\epsilon)}(\theta)((1+\epsilon)(pp) \otimes (ii) + (1-\epsilon)(pp) \otimes (\overline{ii})) + f_{ip}^{(\epsilon)}(\theta)((1+\epsilon) \\ & \times (ii) \otimes (pp) + (1-\epsilon)(\overline{ii}) \otimes (pp))\Big) \sum_{i,j,\epsilon} \Big(f_{ij}^{(\epsilon)}(\theta)((1+\epsilon)((ii) \otimes (jj) + (ii) \otimes (\overline{jj})) + (1 \\ & - \epsilon)((\overline{ii}) \otimes (jj) + (\overline{ii}) \otimes (\overline{jj})))\Big). \end{aligned} \tag{3.3}$$

For $N=3$ this gives

$$M\hat{R}(\theta)M^{-1} \equiv \hat{R}_d(\theta) = (e^{m_{11}^{(+)}\theta}, e^{m_{12}^{(+)}\theta}, e^{m_{11}^{(+)}\theta}, e^{m_{21}^{(+)}\theta}, 1, e^{m_{21}^{(-)}\theta}, e^{m_{11}^{(-)}\theta}, e^{m_{12}^{(-)}\theta}, e^{m_{11}^{(-)}\theta})_{(\mathrm{diag})}. \tag{3.4}$$

The diagonalizer is

$$\sqrt{2}M = \sqrt{2}M^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}. \tag{3.5}$$

The generalizations of (3.4) and (3.5) for all N are quite evident.

If an $\hat{R}(\theta)$ satisfying the braid equation (2.5) is diagonalized the corresponding $\hat{R}_d(\theta)$, in general, does *not* directly satisfy (2.5). This is evident from all the examples of Ref. 1. The general explanation is simple. Interpolated factors of the type $M_{12}M_{23}^{-1}$ will be lacking in the latter case as compared to the former. If $\hat{R}(\theta)$ is diagonal to *start with* (2.6) reduces to

$$(\hat{R}(\theta))_{aa,bb}(\hat{R}(\theta+\theta'))_{bb,cc}(\hat{R}(\theta'))_{aa,bb} = (\hat{R}(\theta'))_{bb,cc}(\hat{R}(\theta+\theta'))_{aa,bb}(\hat{R}(\theta))_{bb,cc}. \tag{3.6}$$

The braid equation is satisfied if, for each (a,b),

$$(\hat{R}(\theta))_{aa,bb}(\hat{R}(\theta'))_{aa,bb} = (\hat{R}(\theta+\theta'))_{aa,bb} \tag{3.7}$$

i.e., if

$$(\hat{R}(\theta))_{aa,bb} = e^{m_{ab}\theta}, \tag{3.8}$$

where the parameters m_{ab} are mutually *independent*. Now, conversely, if $\hat{R}(\theta)$ is conjugated as

$$\hat{R}'(\theta) = A\hat{R}(\theta)A^{-1} \tag{3.9}$$

in general, $\hat{R}'(\theta)$ will no longer satisfy the braid equation since such products as $A_{12}^{-1}A_{23}$ will depend on the structure of A. The structure of our M is such that for arbitrary odd N,

$$M^{-1}\hat{R}_d(\theta)M$$

continues to satisfy the braid equation *provided*

$$m_{ij}^{(\epsilon)} = m_{\bar{i}\bar{j}}^{(\epsilon)}.$$

Thus it is seen how the $2(p-1)^2$ crucial constraints (2.8), the structure of our nested sequence of projectors and that of our M are all linked.

The relevance of our M to the algebra of the L-operators is pointed out at the end of Sec. IV after displaying the crucial algebraic structure arising there.

IV. $L(\theta)$-OPERATORS AND TRANSFER MATRICES

A general discussion, citing relevant sources, is presented in Appendix B. Here the basic results concerning the $N\times N$ realizations of the N^2 blocks of the transfer matrix $t(\theta)$ and the operator $L^+(\theta)$ are used in the context of braid matrices constructed in Sec. II and Appendix A

In (B22) and (B23) we show in a transparent fashion why, unless (B16) is generalized, say, by implementing central operators in the argument of $\hat{R}(\theta-\theta')$, one cannot obtain an $L^-(\theta)\neq L^+(\theta)$. We do not study such general structures here and hence consider only the above-mentioned fundamental realizations of $L^+(\theta)$ with the standard prescription for coproduct. This will, in any case, provide a subalgebra in an appropriately generalized quasi-Hopf structure. This $L^+(\theta)$ and $t(\theta)$, as shown in (B28), are related (for the fundamental $N\times N$ representations of blocks) as

$$t(\theta) = PL^+(\theta)P, \quad (t_{ab}(\theta))_{cd} = (L_{cd}^+(\theta))_{ab}. \tag{4.1}$$

In studying multistate statistical models corresponding to our $\hat{R}(\theta)$ (see the comments and references in Sec. VII) the algebra of the blocks of $t(\theta)$ is particularly relevant. In our case this algebra is found (see the following) to be very simply related to the corresponding one for $L^+(\theta)$. So one can start either with $L^+(\theta)$ or $t(\theta)$ and then obtain the other easily. We choose to display the remarkable structure that emerges first in terms of $L^+(\theta)$. We start with (B14), i.e.,

$$L^+(\theta) = \hat{R}(\theta)P. \tag{4.2}$$

In terms of the matrices (ab) defined below (2.1), one obtains

$$L_{(pp)}^+ = (pp) \equiv X_{pp},$$

$$e^{-m_{ip}^{(\epsilon)}\theta}(L_{ip}^+(\theta) + \epsilon L_{\bar{i}\bar{p}}^+(\theta)) = (pi) + \epsilon(\bar{p}\bar{i}) \equiv X_{pi}^{(\epsilon)},$$

$$e^{-m_{pi}^{(\epsilon)}\theta}(L_{pi}^+(\theta) + \epsilon L_{\bar{p}\bar{i}}^+(\theta)) = (ip) + \epsilon(\bar{i}\bar{p}) \equiv X_{ip}^{(\epsilon)}, \tag{4.3}$$

$$e^{-m_{ij}^{(\epsilon)}\theta}(L_{ij}^+(\theta) + \epsilon L_{\bar{i}\bar{j}}^+(\theta)) = (ij) + \epsilon(\bar{i}\bar{j}) \equiv X_{ij}^{(\epsilon)},$$

$$e^{-m_{\bar{i}\bar{j}}^{(\epsilon)}\theta}(L_{\bar{i}\bar{j}}^+(\theta) + \epsilon L_{ij}^+(\theta)) = (\bar{j}\bar{i}) + \epsilon(ji) \equiv X_{ji}^{(\epsilon)}.$$

In the last equation (2.8) has been implemented, i.e.,

$$m_{\bar{ij}}^{(\epsilon)} = m_{ij}^{(\epsilon)}.$$

From these one obtains

$$\begin{aligned} 2L_{ij}^{+}(\theta) &= (e^{m_{ij}^{(+)}\theta}X_{ij}^{(+)} + e^{m_{ij}^{(-)}\theta}X_{ij}^{(-)}), \\ 2L_{\bar{ij}}^{+}(\theta) &= (e^{m_{ij}^{(+)}\theta}X_{ij}^{(+)} - e^{m_{ij}^{(-)}\theta}X_{ij}^{(-)}), \end{aligned} \tag{4.4}$$

and so on.

For $N=3$ one obtains (with $\epsilon=\pm 1$ in the matrices on the right)

$$L_{22}^{+}(\theta) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$L_{12}^{+}(\theta) + \epsilon L_{\bar{12}}^{+}(\theta) = e^{m_{12}^{(\epsilon)}\theta}\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & \epsilon \\ 0 & 0 & 0 \end{pmatrix},$$

$$L_{21}^{+}(\theta) + \epsilon L_{\bar{21}}^{+}(\theta) = e^{m_{21}^{(\epsilon)}\theta}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & \epsilon & 0 \end{pmatrix}, \tag{4.5}$$

$$L_{11}^{+}(\theta) + \epsilon L_{\bar{11}}^{+}(\theta) = e^{m_{11}^{(\epsilon)}\theta}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \epsilon \end{pmatrix},$$

$$L_{\bar{11}}^{+}(\theta) + \epsilon L_{11}^{+}(\theta) = e^{m_{11}^{(\epsilon)}\theta}\begin{pmatrix} 0 & 0 & \epsilon \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

The constant $N\times N$ matrices $X_{ab}^{(\epsilon)}$, where X_{pp} has only one nonzero element, unity, and all the others only two [(1, 1) or $(1,-1)$] specify a quadratic algebra. We give in the following only the *nonzero* bilinear products, all others vanishing. Further results, such as commutators, can be systematically obtained from those to follow:

$$\begin{aligned} &X_{pp}X_{pp} = X_{pp}, \quad X_{pp}X_{pi}^{(\epsilon)} = X_{pi}^{(\epsilon)}, \quad X_{ip}^{\epsilon}X_{pp} = X_{ip}^{\epsilon}, \\ &X_{pi}^{(\epsilon)}X_{ip}^{(\epsilon')} = (1+\epsilon\epsilon')X_{pp}, \quad X_{ip}^{(\epsilon)}X_{pj}^{(\epsilon')} = X_{ij}^{(\epsilon\epsilon')} + \epsilon X_{\bar{ij}}^{(\epsilon\epsilon')}, \\ &X_{pi}^{(\epsilon)}X_{ij}^{(\epsilon')} = X_{pj}^{(\epsilon\epsilon')}, \quad X_{ij}^{(\epsilon)}X_{jp}^{(\epsilon')} = X_{ip}^{(\epsilon\epsilon')}, \\ &X_{pi}^{(\epsilon)}X_{\bar{ij}}^{(\epsilon')} = \epsilon X_{pi}^{(\epsilon\epsilon')}, \quad X_{\bar{ji}}^{(\epsilon)}X_{ip}^{(\epsilon')} = \epsilon\epsilon' X_{jp}^{(\epsilon\epsilon')}, \\ &X_{ij}^{(\epsilon)}X_{jk}^{(\epsilon')} = X_{ik}^{(\epsilon\epsilon')}, \quad X_{ij}^{(\epsilon)}X_{\bar{jk}}^{(\epsilon')} = \epsilon X_{\bar{ik}}^{(\epsilon\epsilon')}, \end{aligned} \tag{4.6}$$

$$X_{ji}^{(\epsilon)} X_{ik}^{(\epsilon')} = X_{jk}^{(\epsilon\epsilon')}, \quad X_{ji}^{(\epsilon)} X_{ik}^{(\bar{\epsilon}')} = \epsilon X_{jk}^{(\epsilon\epsilon')}.$$

(No sum over repeated indices.)

Note that

$$C_1 \equiv \frac{1}{N}\left(X_{pp} + \sum_i X_{ii}^{(+)}\right) = \frac{1}{N} I_{N\times N}. \tag{4.7}$$

Hence $(X_{pp} - C_1)$ and $(X_{ii}^{(+)} - 2C_1)$, along with the others give an algebra of N^2 traceless matrices.

Higher dimensional realizations are given by the coproducts

$$\Delta L = L \dot{\otimes} L. \tag{4.8}$$

Here $\dot{\otimes}$ implies tensor product combined with matrix multiplication. The prescription can be implemented repeatedly in a straightforward fashion. But it leads, in general, to reducible structures. A systematic study of extraction of irreducible components is beyond the scope of this paper. Let us, however, take a closer look at the structure of the algebra (4.6) and the special role of the index p.

The generators without p (i.e., $X_{ij}^{(\epsilon)}$, $X_{\bar{i}\bar{k}}^{(\epsilon)}$) form a closed subalgebra. The generators with a single p (i.e., $X_{pi}^{(\epsilon)}$, $X_{ip}^{(\epsilon)}$) provide a semidirect product structure with the preceding set. But now to close it one has to extend the first set to a direct product structure by including X_{pp}.

From (4.1) and (4.3) it can be shown that $t(\theta)$ and $L^+(\theta)$ are essentially related through the interchange of the roles of $X_{pi}^{(\epsilon)}$ and $X_{ip}^{(\epsilon)}$. Thus for $N=3$ there is an interchange of $b_\pm$ and $c_\pm$. One obtains for this case

$$t(\theta) = \begin{pmatrix} a_+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_- \\ 0 & 0 & 0 & c_+ & 0 & c_- & 0 & 0 & 0 \\ 0 & 0 & a_- & 0 & 0 & 0 & a_+ & 0 & 0 \\ 0 & b_+ & 0 & 0 & 0 & 0 & 0 & b_- & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & b_- & 0 & 0 & 0 & 0 & 0 & b_+ & 0 \\ 0 & 0 & a_+ & 0 & 0 & 0 & a_- & 0 & 0 \\ 0 & 0 & 0 & c_- & 0 & c_+ & 0 & 0 & 0 \\ a_- & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_+ \end{pmatrix}, \tag{4.9}$$

$$L^+(\theta) = \begin{pmatrix} a_+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_- \\ 0 & 0 & 0 & b_+ & 0 & b_- & 0 & 0 & 0 \\ 0 & 0 & a_- & 0 & 0 & 0 & a_+ & 0 & 0 \\ 0 & c_+ & 0 & 0 & 0 & 0 & 0 & c_- & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & c_- & 0 & 0 & 0 & 0 & 0 & c_+ & 0 \\ 0 & 0 & a_+ & 0 & 0 & 0 & a_- & 0 & 0 \\ 0 & 0 & 0 & b_- & 0 & b_+ & 0 & 0 & 0 \\ a_- & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_+ \end{pmatrix}. \tag{4.10}$$

From these the 3×3 blocks can be read off.

We close this section by pointing out the relevance of our diagonalizer M of Sec. III to the structure of $L^+(\theta)$ [and hence of $t(\theta)$]. If one constructs

$$ML_+(\theta)M^{-1} \tag{4.11}$$

precisely the combinations on the left of the set (4.3) are seen to emerge. Thus our M leads directly to the remarkable structure (4.6).

V. θ EXPANSION

Let us start with the following notations and conventions

(1) The condensed notation $(\alpha,\beta,\ldots)$ of (2.3) implies for each index α either (pp) or a triplet (p,i,ϵ), $(i,j,\epsilon),\ldots$, and so on. We introduce sum over α' where in $\Sigma_{\alpha'}$ the index (pp) is *excluded*. As for the other projectors one may consider alternatively either the basis given by (2.12) or that by (2.14).

(2) We also define

$$H \equiv \sum_{\alpha'} m_{\alpha'} P_{\alpha'} \tag{5.1}$$

when, using (2.3),

$$H^n = \left(\sum_{\alpha'} m_{\alpha'} P_{\alpha'}\right)^n = \sum_{\alpha'} m_{\alpha'}^n P_{\alpha'}. \tag{5.2}$$

Now one can expand as follows (with $n \geqslant 1$):

$$\begin{aligned}\hat{R}(\theta) &= P_{pp} + \sum_{\alpha'} e^{m_{\alpha'}\theta} P_{\alpha'} = P_{pp} + \sum_{\alpha'}\left(1 + \sum_n \frac{(m_{\alpha'}\theta)^n}{n!}\right) P_{\alpha'} \\ &= I + \sum_n \frac{\theta^n}{n!}\left(\sum_{\alpha'} m_{\alpha'}^n P_{\alpha'}\right) = I + \sum_n \frac{\theta^n}{n!} H^n = e^{\theta H}\end{aligned} \tag{5.3}$$

Addition of $P_{pp}=(I-\Sigma_{\alpha'}P_{\alpha'})$ to H corresponds to a change of normalization of $\hat{R}(\theta)$ along with an evident redefinition $m_{\alpha'}\to(m_{\alpha'}-1)$. None of the considerations below are affected by such a redefinition $(\Sigma_{\alpha'}\to\Sigma_{\alpha})$ of H. More generally, say for q-deformed (A,B,C,D)-type algebras, if $\hat{R}(\theta)$ is spectrally resolved on a complete basis of projectors (Sec. II, Ref. 1), setting $l_i(\theta)=lnk_i(\theta)$ and normalizing suitably one obtains, following the steps leading to (5.3),

$$\hat{R}(\theta) = \sum_i k_i(\theta) P_i = \sum_i e^{l_i(\theta)} P_i = e^{(\Sigma_i l_i(\theta) P_i)} \tag{5.4}$$

Here, in general, upon expansion in powers of θ the exponents $l_i(\theta)$ lead to fairly involved structures. In our present case θ is simply a factor in the exponent. Hence the situation is much simpler. Using (5.3) the braid equation becomes (with $H_{12}=H\otimes I$, $H_{23}=I\otimes H$)

$$e^{\theta H_{12}} e^{(\theta+\theta')H_{23}} e^{\theta' H_{12}} = e^{\theta' H_{23}} e^{(\theta+\theta')H_{12}} e^{\theta H_{23}}. \tag{5.5}$$

Setting, with $(n,n',n'')\geqslant 1$,

$$S = \sum_n \frac{\theta^n}{n!} H_{12}^n, \quad S' = \sum_{n'} \frac{\theta'^{n'}}{n'!} H_{12}^{n'}, \quad S'' = \sum_{n''} \frac{(\theta+\theta')^{n''}}{n''!} H_{23}^{n''}. \tag{5.6}$$

The left-hand side of (5.5) is

$$(\text{L.H.S.}) = (I+S)(I+S'')(I+S') = I + (S+S'+S'') + (SS' + SS'' + S''S') + SS''S' \tag{5.7}$$

The (R.H.S.) is obtained from the (L.H.S.) via the following interchanges:

$$(12) \leftrightarrow (23), \quad \theta \leftrightarrow \theta'. \tag{5.8}$$

Now let us compare the coefficients of $\theta^r \theta'^s$ for different pairs (r,s) on both sides of (5.5).

The linear and the quadratic terms on both sides are found to be symmetric under (5.8) and hence cancel. Among the cubic terms only the coefficients of

$$\theta\theta'(\theta + \theta')$$

are found to lead to a nontrivial relation. One obtains, on regrouping terms,

$$[[H_{12},H_{23}],H_{12}] = [[H_{23},H_{12}],H_{23}]. \tag{5.9}$$

Compare this with (2.5). See also the remarks in Sec. VII.

But from (5.2) one obtains

$$H_{12}^2 = \sum_{\alpha'} m_{\alpha'}^2 (P_{\alpha'})_{12}, \quad H_{23}^2 = \sum_{\alpha'} m_{\alpha'}^2 (P_{\alpha'})_{23}. \tag{5.10}$$

Hence in terms of the projectors one obtains

$$\sum_{\alpha',\beta',\gamma'} m_{\alpha'} m_{\beta'} m_{\gamma'} ((P_{\alpha'})_{12}(P_{\beta'})_{23}(P_{\gamma'})_{12} - (P_{\alpha'})_{23}(P_{\beta'})_{12}(P_{\gamma'})_{23})$$

$$= \frac{1}{2} \sum_{\alpha',\beta'} m_{\alpha'} m_{\beta'} (m_{\alpha'} - m_{\beta'}) ((P_{\alpha'})_{12}(P_{\beta'})_{23} - (P_{\alpha'})_{23}(P_{\beta'})_{12}). \tag{5.11}$$

Since there are $\frac{1}{2}(N+3)(N-1)$ independent parameters m_α, comparing coefficients of distinct triplets on each side one obtains a series of results. We will not display them explicitly. In Sec. 3 of Ref. 2 we have studied analogous reductions (from trilinear to bilinear forms) for q-deformed unitary, orthogonal, and symplectic cases. There they were studied in the context of "modified braid equations" (Refs. 3 and 4) presented as a complementary facet of Baxterization (i.e., the introduction of a spectral parameter). Here we *started* from the θ-dependent form (2.5) and implemented our θ expansion leading to the hierarchy starting with (5.9) and (5.11). Without attempting to analyze how the higher order members of the hierarchy can be reduced in order, in successive steps, we just mention the following point concerning (5.11).

In (1.18) of Ref. 2, even for the orthogonal and the symplectic cases the modified braid equation could be expressed in terms of tensored $(\hat{R}(\theta))^{\pm 1}$ by expressing the projectors in their terms using the minimal (cubic) polynomial equation satisfied by $\hat{R}(\theta)$. For the unitary case (with a quadratic polynomial) the task was much more simple. In our present case, despite various particularly simple aspects, the order of the minimal polynomial increases as N^2 instead of remaining fixed as for the cases mentioned before. Hence relations of the type (5.11) are best considered in terms of projectors themselves.

Expansions in terms of the spectral parameter have been considered in the context of Yangian Double and central extensions.[5,6] We intend to study elsewhere analogous aspects generalizing our class of braid matrices.

VI. COMPARISON WITH EVEN DIMENSIONAL CASES

The sequence of projectors presented in Sec. 8 of Ref. 1 is a direct generalization of the basis arising in the spectral resolution of the six-vertex and the eight-vertex braid matrices. From the abundant literature on such models the most directly relevant sources are cited in Secs. 6 and 7 of Ref. 1. These 4×4 projectors are (with $\epsilon = \pm 1$ in the matrices)

$$2P_{1(\epsilon)} = \begin{pmatrix} 1 & 0 & 0 & \epsilon \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \epsilon & 0 & 0 & 1 \end{pmatrix}, \quad 2P_{2(\epsilon)} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & \epsilon & 0 \\ 0 & \epsilon & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{6.1}$$

But even for this simplest member ($N=2$) of the hierarchy the coefficients in

$$\hat{R}(\theta) = \sum_{\epsilon} (f_{1(\epsilon)}(\theta)P_{1(\epsilon)} + f_{2(\epsilon)}(\theta)P_{2(\epsilon)}) \tag{6.2}$$

are not constrained to simple exponentials as for $N=(2p-1)$. For the eight-vertex model (see sources cited in Sec. 7 of Ref. 1) one obtains

$$f_{1(\pm)}(\theta) = \frac{g_{(\pm)}(\theta)}{g_{(\pm)}(-\theta)}, \quad f_{2(\pm)}(\theta) = \frac{h_{(\pm)}(\theta)}{h_{(\pm)}(-\theta)}, \tag{6.3}$$

where with $z=e^{\theta}$, two parameters p and q and

$$(x;a)_{\infty} = \prod_{n \geqslant 0} (1 - xa^n), \tag{6.4}$$

$$g_{\pm}(z) = (\mp p^{1/2}q^{-1}z;p)_{\infty}(\mp p^{1/2}qz^{-1};p)_{\infty}, \tag{6.5}$$

$$h_{\pm}(z) = (q^{1/2}z^{-1/2} \pm q^{-1/2}z^{1/2})(\mp pq^{-1}z;p)_{\infty}(\mp pqz^{-1};p)_{\infty}. \tag{6.6}$$

The question of normalization is discussed in Sec. 7 of Ref. 1. In the trigonometric six-vertex limit one obtains (as in Sec. 6 of Ref. 1)

$$f_{1(\pm)}(\theta) = 1, \quad f_{2(+)}(\theta) = \frac{\cosh \frac{1}{2}(\gamma - \theta)}{\cosh \frac{1}{2}(\gamma + \theta)}, \quad f_{2(-)}(\theta) = \frac{\sinh \frac{1}{2}(\gamma - \theta)}{\sinh \frac{1}{2}(\gamma + \theta)}. \tag{6.7}$$

The reason for such a scope is that [unlike $p=\overline{p}$ for $N=(2p-1)$] for even N there is *no* index $i=\overline{i}$. The successive stages of the construction of solutions in Appendix A make it amply explicit how the presence of a $p(=\overline{p})$, along with the structure of the projectors in our nested sequence, constrains the coefficients to be simply exponentials. The generalization for $N=2n$ $(n>1)$ of the hyperbolic and elliptic solutions displayed above will be explored elsewhere implementing our basis of projectors.

VII. DISCUSSION

In Ref. 1 braid matrices were studied systematically via their spectral resolutions on appropriate bases of projectors. Such a study was already initiated in previous works (Refs. 2 and 7) and led to canonical factorization and diagonalization in Ref. 1. In Sec. 8 of Ref. 1 this approach was taken to its limit. In the other sections almost all *known* braid matrices of interest were studied via spectral resolutions. In Sec. 8 a basis of projectors (called a "nested sequence") with particularly simple, attractive properties was hopefully presented for constructing new classes of braid matrices in all dimensions. In such a basis, satisfying (2.3), one has N^2 matrices, each $N^2 \times N^2$ and with only constant elements [see (2.2) and (6.1)]. They can be considered as the most simple and symmetric generalizations of projectors appearing in the six-vertex and the eight-vertex models. But the central question was not addressed in Ref. 1. Can such a basis of projectors be dressed up with suitable coefficients to provide a braid matrix satisfying (2.5)? While the number of coefficients increases as N^2 the number of trilinear constraints on them corresponding to the products of $N^3 \times N^3$ matrices increases much faster. Hence the question. In this paper we present an affirmative answer and explicit solutions for all *odd N*. The even-N case will be studied elsewhere.

Let us note some basic features of our solutions in the context of the formulation in Ref. 1. The canonically factorizable form of the coefficients[1] give

$$\hat{R}(\theta) = \sum_i \frac{f_i(\theta)}{f_i(-\theta)} P_i. \tag{7.1}$$

This is evidently compatible with (2.7) since

$$e^{m\theta} = (e^{(1/2)m\theta})(e^{-(1/2)m\theta})^{-1}.$$

But in Ref. 1 we systematically extracted (see the relevant discussion in Ref. 1) the standard (non-Baxterized) braid matrices satisfying

$$\hat{R}_{12}\hat{R}_{23}\hat{R}_{12} = \hat{R}_{23}\hat{R}_{12}\hat{R}_{23} \tag{7.2}$$

as the limits

$$\lim_{\theta\to\pm\infty} \hat{R}(\theta) = (\hat{R})^{\pm 1}. \tag{7.3}$$

For our present class of solutions however each coefficient $e^{m_\alpha\theta}$ either diverges or vanishes in the above-mentioned limits. So rather than the Baxterization of a preexisting (7.2) to (2.5) this class can be considered (see Sec. V) to be an exponentiation of

$$[[H_{12},H_{23}],H_{12}] = [[H_{23},H_{12}],H_{23}] \tag{7.4}$$

to

$$\hat{R}_{12}(\theta)\hat{R}_{23}(\theta+\theta')\hat{R}_{12}(\theta') = \hat{R}_{23}(\theta')\hat{R}_{12}(\theta+\theta')\hat{R}_{23}(\theta) \tag{7.5}$$

since, as shown in Sec. V, the passage

$$H \equiv \sum_{\alpha'} m_{\alpha'} P_{\alpha'} \to \hat{R}(\theta) = e^{\theta H}$$

corresponds to one from (7.4) to (7.5).

One may compare this with the well-known so-called "classical" r-matrix equation obtained by expanding the q-dependent YB matrix $R(\theta)(=P\hat{R}(\theta))$ satisfying

$$R_{12}(\theta)R_{13}(\theta+\theta')R_{23}(\theta') = R_{23}(\theta')R_{13}(\theta+\theta')R_{12}(\theta) \tag{7.6}$$

in powers of $h(=\ln q)$. One obtains for

$$R_q(\theta) = I + 2hr(\theta) + O(h^2),$$

$$[r_{12}(\theta),(r_{13}(\theta+\theta') + r_{23}(\theta'))] + [r_{13}(\theta+\theta'),r_{23}(\theta')] = 0. \tag{7.7}$$

This has only single commutators. In our case there is no q. Expanding in powers of θ we obtain as the first nontrivial relation Eq. (7.4) with double commutators and with the two sides still directly related through the interchange $(12)\leftrightarrow(23)$. In the extensive literature concerning r-matrices one may note in particular a classification of solutions (Ref. 8). Our projectors lead to a solution of (7.4) with $\frac{1}{2}(N+3)(N-1)$ parameters for $N=(2p-1)$. A more general study, starting from (7.4) should be worthwhile.

We repeat a feature noted in Sec. V. Our class of solutions has many particularly simple aspects. But the number of projectors (P_α) and that of the parameters (m_α) increase as N^2 with the dimension. The degree of the minimal polynomial equation satisfied by $\hat{R}(\theta)$ increases with them. This is in sharp contrast with well-known cases corresponding to q-deformed unitary, orthogonal, and symplectic cases. There the structures of the projectors are much less simple. But their number

does not increase with the dimension. As noted below (2.14), the degree of the minimal polynomial can be lowered by allowing some of the free parameters to coincide, giving simpler subcases. But our solution is more general.

For $m^{+}_{ab} > m^{-}_{ab}$ all the nonzero elements of our $\hat{R}(\theta)$ are positive and hence can be consistently interpreted as Boltzmann weights of a multistate statistical model. In Sec. 11 of Ref. 1 the possibility of a class of multistate model was briefly indicated and compared with one proposed in Ref. 9. (See also Sec. 4 of Ref. 10.) In both cases $(2N^2-N)$ elements out of N^4 ones of $\hat{R}(\theta)$ are nonzero. Here we have $(2N^2-1)$ nonzero weights. Moreover the explicit solution of Ref. 9 (and Ref. 10) restricts the number of parameters as in the six-vertex model (Sec. VI). For our present class there is scope for more parameters, their possible number increasing with the dimension. More generally, since the distribution and the magnitudes of the weights are quite different, as compared to the references above, all the essential properties and features will be different (e.g., the partition function, the eigenvalues of the transfer matrix, the detailed content of the structure arising, say, from the Bethe ansatz, the algebra of the L-operators, the associated quantum Hamiltonian, possible knot invariants and also the associated noncommutative spaces). But an adequate exploration of such aspects will be a major enterprise which can only be attempted in future works. Here, we have presented the explicit braid matrix from which all will follow and briefly indicated the possibilities in certain directions (such as the L-operators).

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It is a pleasure to thank Daniel Arnaudon. Using a program, he verified for the first member of our hierarchy of solutions that the constraints obtained here are not only sufficient but also necessary. This was reassuring.

APPENDIX A: SOLVING THE BRAID EQUATION

In (2.6), namely,

$$(\hat{R}(\theta))_{al,cm}(\hat{R}(\theta+\theta'))_{mn,ef}(\hat{R}(\theta'))_{lb,nd} = (\hat{R}(\theta'))_{cl,em}(\hat{R}(\theta+\theta'))_{ab,ln}(\hat{R}(\theta))_{nd,mf} \tag{A1}$$

corresponding to the site $(ab)\otimes(cd)\otimes(ef)$ one has to implement the content of the ansatz (2.4). From (2.2) and (2.4) one obtains the following nonzero elements of $\hat{R}(\theta)$. The arguments θ are suppressed in (A2) to simplify the notation and the subscripts correspond to the sites $(ab)\otimes(cd)$,

$$\begin{aligned}
\hat{R}_{pp,pp} &= 1,\\
\hat{R}_{pp,ii} &= \tfrac{1}{2}(f^{(+)}_{pi} + f^{(-)}_{pi}) = \hat{R}_{pp,\bar{i}\bar{i}},\\
\hat{R}_{pp,,i\bar{i}} &= \tfrac{1}{2}(f^{(+)}_{pi} - f^{(-)}_{pi}) = \hat{R}_{pp,\bar{i}i},\\
\hat{R}_{ii,pp} &= \tfrac{1}{2}(f^{(+)}_{ip} + f^{(-)}_{ip}) = \hat{R}_{\bar{i}\bar{i},pp},\\
\hat{R}_{i\bar{i},pp} &= \tfrac{1}{2}(f^{(+)}_{ip} - f^{(-)}_{ip}) = \hat{R}_{\bar{i}i,pp},\\
\hat{R}_{ii,jj} &= \tfrac{1}{2}(f^{(+)}_{ij} + f^{(-)}_{ij}) = \hat{R}_{\bar{i}\bar{i},\bar{j}\bar{j}},\\
\hat{R}_{i\bar{i},j\bar{j}} &= \tfrac{1}{2}(f^{(+)}_{ij} - f^{(-)}_{ij}) = \hat{R}_{\bar{i}i,\bar{j}j},
\end{aligned} \tag{A2}$$

$$\hat{R}_{ii,jj\overline{\ }\overline{\ }} = \tfrac{1}{2}(f_{ij}^{(+)} + f_{ij}^{(-)}) = \hat{R}_{\overline{ii},jj},$$

$$\hat{R}_{\overline{ii},jj\overline{\ }\overline{\ }} = \tfrac{1}{2}(f_{ij}^{(+)} - f_{ij}^{(-)}) = \hat{R}_{ii,jj\overline{\ }\overline{\ }}.$$

These are the *only* nonzero elements, the total number being

$$1 + 8(p-1) + 8(p-1)^2 = 2(2p-1)^2 - 1 = 2N^2 - 1$$

Note the following points:

- The elements above all being situated on the diagonal and the antidiagonal there are none of the type $\hat{R}_{ii,jj\overline{\ }}$, $\hat{R}_{ii,jj\overline{\ }}$ and so on.
- In the product $(ab)\otimes(cd)\otimes(ef)$ for a given a, b can only be a or $\overline{a}$ for the coefficient to be nonzero. This holds also for the other pairs.
- Among (a,b,c,d,e,f) the number of with (or without) bar must be even for the coefficient to be nonzero. This is one consequence of (A2). However, in such countings one must keep in mind that $p=\overline{p}$.

The preceding considerations simplify considerably the computations as we analyze systematically the different classes of $(ab)\otimes(cd)\otimes(ef)$ with novanishing coefficients, lowering the multiplicity of (pp) in the triple product above by steps.

Case (1) The case $(pp)\otimes(pp)\otimes(pp)$ is trivial since (A1) reduces to

$$1 = 1.$$

Case (2) Next consider the classes (with $(ab)\neq(pp)$)

$$(1):\ (pp)\otimes(pp)\otimes(ab),$$

$$(2):\ (ab)\otimes(pp)\otimes(pp),$$

$$(3):\ (pp)\otimes(ab)\otimes(pp).$$

From our previous remarks it follows that it is sufficient to consider the possibilities

$$(ab) = (ii), (\overline{ii}).$$

Note also that in (A2) $\hat{R}_{pp,ii} = \hat{R}_{pp,\overline{ii}}$ and so on.

For (1), (A1) is easily seen to reduce to

$$\hat{R}(\theta+\theta'))_{pp,ab} = \hat{R}(\theta'))_{pp,ac}\ \hat{R}(\theta))_{pp,cb}. \tag{A3}$$

Analogous treatments of the subcases (1), (2), (3) lead, respectively (implementing (A2) with $\epsilon=\pm$ and also both possibilities for (ab) mentioned above) to the constraints

$$f_{pi}^{(\epsilon)}(\theta+\theta') = f_{pi}^{(\epsilon)}(\theta) f_{pi}^{(\epsilon)}(\theta'), \tag{A4}$$

$$f_{ip}^{(\epsilon)}(\theta+\theta') = f_{ip}^{(\epsilon)}(\theta) f_{ip}^{(\epsilon)}(\theta'), \tag{A5}$$

$$\begin{aligned} &f_{pi}^{(+)}(\theta) f_{pi}^{(+)}(\theta') f_{ip}^{(+)}(\theta+\theta') + f_{pi}^{(-)}(\theta) f_{pi}^{(-)}(\theta') f_{ip}^{(-)}(\theta+\theta') \\ &\quad = f_{pi}^{(+)}(\theta+\theta') f_{ip}^{(+)}(\theta) f_{ip}^{(+)}(\theta') + f_{pi}^{(-)}(\theta+\theta') f_{ip}^{(-)}(\theta) f_{ip}^{(-)}(\theta'). \end{aligned} \tag{A6}$$

On implementing (A4) and (A5) one reduces (A6) to an identity. Then from the first two one obtains the solutions

$$f_{pi}^{(\epsilon)}(\theta) = e^{m_{pi}^{(\epsilon)}\theta}, \tag{A7}$$

$$f_{ip}^{(\epsilon)}(\theta) = e^{m_{ip}^{(\epsilon)}\theta} \tag{A8}$$

the indeterminates $m_{pi}^{(\epsilon)}$, $m_{ip}^{(\epsilon)}$ being independent parameters.

Continuing to reduce the multiplicity of (pp) and remembering the restrictions implied by (A2) we start by considering successively the cases

$$(4)\text{: } (pp) \otimes (ii) \otimes (jj),$$

$$(5)\text{: } (pp) \otimes (\overline{ii}) \otimes (j\overline{j}),$$

$$(6)\text{: } (pp) \otimes (\overline{ii}) \otimes (jj).$$

The last one survives with nonzero coefficient since $p=\overline{p}$. We present directly the results, the derivations being straightforward.

Defining

$$A_{ab}(\theta) \equiv f_{ab}^{(+)}(\theta) + f_{ab}^{(-)}(\theta), \quad B_{ab}(\theta) \equiv f_{ab}^{(+)}(\theta) - f_{ab}^{(-)}(\theta)$$

one obtains, respectively, from the above-mentioned cases

$$A_{ij}(\theta+\theta') = f_{ij}^{(+)}(\theta) f_{ij}^{(+)}(\theta') + f_{ij}^{(-)}(\theta) f_{ij}^{(-)}(\theta'), \tag{A9}$$

$$A_{pi}(\theta)A_{pi}(\theta')B_{ij}(\theta+\theta') + B_{pi}(\theta)B_{pi}(\theta')B_{ij}(\theta+\theta') = A_{pi}(\theta+\theta')(B_{ij}(\theta)A_{ij}(\theta') + A_{ij}(\theta)B_{ij}(\theta')), \tag{A10}$$

$$A_{pi}(\theta)B_{pi}(\theta')A_{ij}(\theta+\theta') + B_{pi}(\theta)A_{pi}(\theta')A_{ij}(\theta+\theta') = B_{pi}(\theta+\theta')(A_{ij}(\theta')A_{ij}(\theta) + B_{ij}(\theta')B_{ij}(\theta)). \tag{A11}$$

Taking account of (A4) and (A5) [and hence of (A7) and (A8)] and noting that keeping $(\theta+\theta')$ fixed one can vary ψ in

$$\theta = \phi + \psi, \quad \theta' = \phi - \psi,$$

one finds that the last three equations are satisfied if

$$f_{ij}^{(\epsilon)}(\theta) = f_{ij}^{(\epsilon)}(\theta) \tag{A12}$$

and

$$f_{ij}^{(\epsilon)}(\theta) f_{ij}^{(\epsilon)}(\theta') = f_{ij}^{(\epsilon)}(\theta+\theta'). \tag{A13}$$

These are found to be *necessary* and *sufficient*. Hence

$$f_{ij}^{(\epsilon)}(\theta) = f_{ij}^{(\epsilon)}(\theta) = e^{m_{ij}^{(\epsilon)}\theta}. \tag{A14}$$

Permutation of the factors of the cases (4, 5, 6) above [such as $(ii)\otimes(pp)\otimes(jj)$ and so on] can be shown to lead to no supplementary constraints.

Finally one considers the cases

$$(ab) \otimes (cd) \otimes (ef),$$

where no factor is (pp). For each subcase the constraints implied by (A1) along with (A2) are

easily extracted. It is found that they are *all* satisfied by implementing (A12) and (A13). Since the subcases are treated quite similarly, it is sufficient to display two of them. We present again only the final steps. For

$$(ii) \otimes (jj) \otimes (kk)$$

with no barred index, (A13) reduces (A1), in terms of A_{ab} defined above, to

$$\text{L.H.S.} = \tfrac{1}{4} A_{ij}(\theta + \theta') A_{jk}(\theta + \theta') = \text{R.H.S.} \tag{A15}$$

Similarly, for

$$(\overline{ii}) \otimes (jj) \otimes (\overline{kk})$$

one obtains finally

$$\text{L.H.S.} = \tfrac{1}{4} B_{ij}(\theta + \theta') B_{jk}(\theta + \theta') = \text{R.H.S.} \tag{A16}$$

In both cases, apart from the exponential form for each f, (A14) is essential. Thus we have verified the solution announced in (2.7) and (2.8). It is instructive to compute explicitly the case (2.9) where one has only $(i, \overline{i}, p)$ with

$$i = 1, \quad p = 2.$$

One finds that (2.10) is sufficient. Moreover, if one sets

$$m_{11}^{(\epsilon)} \neq m_{11}^{(\epsilon)} \tag{A17}$$

so that $a_{\pm}$ is not repeated as in (2.9), the braid equation is *not* satisfied. This is an example of the necessity of (A14).

As a check, the solution for $N=3$ was also obtained [instead of directly using (A1) and (A2)] by computing the triple tensor products of the projectors in (2.5).

APPENDIX B: *L*-OPERATORS AND TRANSFER MATRICES (FUNDAMENTAL REPRESENTATIONS)

Here we collect together some known results (citing sources to follow) coherently with our notations and conventions and emphasize certain aspects arising in the presence of the spectral parameter θ.

For non-Baxterized braid matrices (without θ) satisfying

$$\hat{R}_{12}\hat{R}_{23}\hat{R}_{12} = \hat{R}_{23}\hat{R}_{12}\hat{R}_{23} \tag{B1}$$

the FRT equations for the L-operators [Eq. (2.3) of Ref. 11] can be expressed in our notations as

$$\hat{R} L_2^{\pm} L_1^{\pm} = L_2^{\pm} L_1^{\pm} \hat{R}, \tag{B2}$$

$$\hat{R} L_2^{+} L_1^{-} = L_2^{-} L_1^{+} \hat{R}. \tag{B3}$$

Here $\hat{R}$ is a $N^2 \times N^2$ matrix for any N and

$$L_1 = L \otimes I_{N\times N}, \quad L_2 = I_{N\times N} \otimes L.$$

Writing these in terms of components (as will be done in the following for the θ-dependent case) it can be shown that the lowest dimensional realizations of the N^2 blocks $L_{ab}^{\pm}$ (each $N \times N$) can be obtained in our notations, i.e., with

$$\hat{R} = \hat{R}_{ab,cd}(ab) \otimes (cd) \tag{B4}$$

as

$$(L^{+}_{ab})_{cd} = \hat{R}_{ad,cb}, \tag{B5}$$

$$(L^{-}_{ab})_{cd} = \hat{R}^{-1}_{ad,cb}, \tag{B6}$$

or

$$L^{+} = \hat{R}P = (PR)P = R_{21}, \tag{B7}$$

$$L^{-} = \hat{R}^{-1}P = (R^{-1}P)P = R^{-1}. \tag{B8}$$

Apart from differences of notations and conventions these correspond (to cite only one source) to Eq. (4.9) of Ref. 12. In the familiar $L^{\pm}$ of $Sl_q(2)$, implementing 2×2 realizations of $(q^{\pm H}, X_{\pm})$ one obtains (B7) and (B8), which however hold for *any* $\hat{R}$ satisfying (B1).

Now let us introduce θ. Corresponding to (B1) and (B2) one now has, respectively,

$$\hat{R}_{12}(\theta-\theta')\hat{R}_{23}(\theta)\hat{R}_{12}(\theta') = \hat{R}_{23}(\theta')\hat{R}_{12}(\theta)\hat{R}_{23}(\theta-\theta'), \tag{B9}$$

$$\hat{R}(\theta-\theta')L^{\pm}_{2}(\theta)L^{\pm}_{1}(\theta') = L^{\pm}_{2}(\theta')L^{\pm}_{1}(\theta)\hat{R}(\theta-\theta'). \tag{B10}$$

[The corresponding situation for (B3) will be discussed in the following.]

In terms of components one writes

$$(\hat{R}(\theta-\theta'))_{al,cm}(\hat{R}(\theta))_{mn,ef}(\hat{R}(\theta'))_{lb,nd} = (\hat{R}(\theta'))_{cl,em}(\hat{R}(\theta))_{ab,ln}(\hat{R}(\theta-\theta'))_{nd,mf}, \tag{B11}$$

$$(\hat{R}(\theta-\theta'))_{al,cm}(L^{\pm}(\theta)_{mf})_{en}(L^{\pm}(\theta')_{ld})_{nb} = (L^{\pm}(\theta')_{cm})_{el}(L^{\pm}(\theta)_{an})_{lb}(\hat{R}(\theta-\theta'))_{nd,mf}. \tag{B12}$$

One finds that [considering $L^{+}(\theta)$ to start with]

$$(L^{+}(\theta)_{ab})_{cd} = (\hat{R}(\theta))_{ad,cb} \tag{B13}$$

or

$$L^{+}(\theta) = \hat{R}(\theta)P = PR(\theta)P = R_{21}(\theta) \tag{B14}$$

is a solution. This is strictly analogous to (B7). The same solution evidently holds for $L^{-}(\theta)$. But if one wants to avoid the degeneracy

$$L^{-}(\theta) = L^{+}(\theta) \tag{B15}$$

can one obtain a different solution for $L^{-}(\theta)$ analogous to (B8)? We show below in a particularly transparent fashion that there is an obstruction if one directly generalizes (B3) as

$$\hat{R}(\theta-\theta')L^{+}_{2}(\theta)L^{-}_{1}(\theta') = L^{-}_{2}(\theta')L^{+}_{1}(\theta)\hat{R}(\theta-\theta'). \tag{B16}$$

When this is further generalized by introducing a central operator in the argument of $\hat{R}(\theta-\theta')$ on one side (or in a different fashion on each side) and thus distinguish the two arguments, there can be a way out. (Reference 13 is a review article citing numerous sources. Particularly relevant is Sec. 2.1.4.) But let us consider the consequences of (B16) combined with (B13) and (B14) and the basic properties (2.15), i.e.,

$$\hat{R}(-\theta) = \hat{R}^{-1}(\theta), \quad \hat{R}(0) = I. \tag{B17}$$

From (B14) and (B17),

$$L^{+}(0) = P, \quad L^{+}(0)_{ab} = (ba). \tag{B18}$$

[This has no counterpart for (B7).]

Hence setting $\theta=0$ in (B16), using (B16) and (B17) and then writing θ for θ' one obtains

$$\hat{R}^{-1}(\theta)P_2L_1^{-}(\theta) = L_2^{-}(\theta)P_1\hat{R}^{-1}(\theta). \tag{B19}$$

Writing (B19) in terms of components analogously to (B12) one obtains

$$(\hat{R}(-\theta))_{al,cm}(\delta_{mn}\delta_{fe})(L^{-}(\theta)_{ld})_{nb} = (L^{-}(\theta)_{cm})_{el}(\delta_{ab}\delta_{nl})(\hat{R}(-\theta))_{nd,mf} \tag{B20}$$

or

$$(\hat{R}^{-1}(\theta))_{al,cm}(L^{-}(\theta)_{ld})_{mb}\delta_{ef} = \delta_{ab}(L^{-}(\theta)_{cm})_{el}(\hat{R}^{-1}(\theta))_{ld,mf}. \tag{B21}$$

Hence, finally,

$$(\hat{R}^{-1}(\theta)L^{-}(\theta)P) \otimes I = I \otimes (L^{-}(\theta)P\hat{R}^{-1}(\theta)). \tag{B22}$$

For

$$L^{-}(\theta) = L^{+}(\theta) = \hat{R}(\theta)P, \quad L^{-}(\theta)P = \hat{R}(\theta) \tag{B23}$$

(B22) is trivially satisfied (furnishing a convincing check). But a distinct solution for $L^{-}(\theta)$ reducing (say, as $\theta\rightarrow\infty$) to (B8) is no longer available in the general case if (B16) is strictly maintained. One obtains (B8) easily from the symmetry of (B1) under inversion since, unlike for (B16), the orders of (θ,θ') on each side do not enter in that context. But even apart from that (B18) now imposes the constraint (B22), linear in $L^{-}(\theta)$. We do not consider in this paper generalizations of (B16) leading to quasi-Hopf structures for consistent coproducts.

We now consider transfer matrices and note how the lowest dimensional representations can be extracted from those of the L-operators. The transfer matrix $t(\theta)$ has to satisfy

$$\hat{R}(\theta-\theta')(t(\theta)\dot{\otimes}t(\theta')) = (t(\theta')\dot{\otimes}t(\theta))\hat{R}(\theta-\theta'), \tag{B24}$$

where $\dot{\otimes}$, combining tensor and matrix products, leads to

$$(t(\theta)\dot{\otimes}t(\theta')) = (t(\theta)\otimes I)(I\otimes t(\theta')) = t_1(\theta)\,.\,t_2(\theta'). \tag{B25}$$

Write (B24) as

$$(P\hat{R}(\theta-\theta')P)(P(t_1(\theta)P)(Pt_2(\theta')P) \;= (Pt_1(\theta')P)(Pt_2(\theta)P)(P\hat{R}(\theta-\theta')P) \tag{B26}$$

or

$$\hat{R}_{21}(\theta-\theta')t_2(\theta)t_1(\theta') = t_2(\theta')t_1(\theta)\hat{R}_{21}(\theta-\theta'). \tag{B27}$$

Now comparing (B27) with (B10) and (B14) one finds the solution

$$t(\theta) = (P\hat{R}(\theta)P)P = P\hat{R}(\theta) = R(\theta). \tag{B28}$$

In the absence of θ, i.e., for (B1), this corresponds (with some notational differences) to the realization ρ_{+} of Eq. (4.5) of Ref. 12. But corresponding to (B8), unavailable in our context, there is another realization ρ_{-} in Ref. 12. We are concerned only with (B28). Products analogous to (4.8)

of our Sec. IV lead to higher dimensional transfer matrices corresponding to longer chains as successive sites are added.

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Aspects of a new class of braid matrices: Roots of unity and hyperelliptic *q* for triangularity, *L*-algebra, link-invariants, noncommutative spaces

A. Chakrabarti[a)]
Centre de Physique Théorique, Ecole Polytechnique, 91128 Palaiseau Cedex, France

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Various properties of a class of braid matrices, presented before, are studied considering $N^2\times N^2 (N=3,4,\ldots)$ vector representations for two subclasses. For $q=1$ the matrices are nontrivial. Triangularity ($\hat{R}^2=I$) corresponds to polynomial equations for q, the solutions ranging from roots of unity to hyperelliptic functions. The algebras of L operators are studied. As a crucial feature one obtains $2N$ central, grouplike, homogenous quadratic functions of L_{ij} constrained to equality among themselves by the *RLL* equations. They are studied in detail for $N=3$ and are proportional to I for the fundamental 3×3 representation and hence for all iterated coproducts. The implications are analyzed through a detailed study of the 9×9 representation for $N=3$. The Turaev construction for link invariants is adapted to our class. A skein relation is obtained. Noncommutative spaces associated to our class of $\hat{R}$ are constructed. The transfer matrix map is implemented, with the $N=3$ case as example, for an iterated construction of noncommutative coordinates starting from an $(N-1)$ dimensional commutative base space. Further possibilities, such as multistate statistical models, are indicated. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1924701]

I. INTRODUCTION

A new class of braid matrices was presented in previous papers. The most convenient formulation can be found in Sec. 3 of Ref. 1. This is based on two previous works.[2,3] For ready reference we summarize below the essential features. In succeeding sections, the different properties of such braid matrices will be studied. Remarkable aspects will be encountered. We will *always* be concerned with $N^2\times N^2$ vector representations of braid matrices ($N=3, 4, \ldots$).

For proper appreciation one should start by noting explicitly the links *and* the crucial differences with the standard $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$ braid matrices. Our approach is consistently via spectral resolutions, i.e., in terms of projectors.

The Baxterized braid matrices (depending on a spectral parameter θ) satisfy

$$\hat{R}_{12}(\theta)\hat{R}_{23}(\theta+\theta')\hat{R}_{12}(\theta')=\hat{R}_{23}(\theta')\hat{R}_{12}(\theta+\theta')\hat{R}_{23}(\theta), \tag{1.1}$$

where

$$\hat{R}_{12}=\hat{R}\otimes I_N, \quad \hat{R}_{23}=I_N\otimes\hat{R},$$

and I_N is the $N\times N$ identity matrix.

For the standard $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$ cases (see sources cited in Sec. 2 of Ref. 1) one has

[a)]Laboratoire Propre du CNRS UPR A.0014. Electronic mail: chakra@cpht.polytechnique.fr

$$\hat{R}(\theta) = P_+ + v(\theta)P_- + w(\theta)P_0, \tag{1.2}$$

where the projectors satisfy

$$P_i P_j = \delta_{ij} P_i, \quad P_+ + P_- + P_0 = I_{N^2}. \tag{1.3}$$

All θ dependence is in $v(\theta)$ and $w(\theta)$. The projectors depend only on q.

The elegant canonical formulation (Sec. 2, Ref. 1) gives the following $v(\theta)$ and $w(\theta)$, where

$$q = \exp h.$$

One has for each case (independently of N)

$$v(\theta) = \frac{\sinh(h-\theta)}{\sinh(h+\theta)} \tag{1.4}$$

and two solutions for $w(\theta)$,

$$\mathrm{SO}_q(2n+1), \quad w(\theta) = \frac{\cosh\left(\left(n+\frac{1}{2}\right)h-\theta\right)}{\cosh\left(\left(n+\frac{1}{2}\right)h+\theta\right)}, \quad \frac{\sinh\left(\left(n-\frac{1}{2}\right)h-\theta\right)}{\sinh\left(\left(n-\frac{1}{2}\right)h+\theta\right)} v(\theta); \tag{1.5}$$

$$\mathrm{SO}_q(2n), \quad w(\theta) = \frac{\cosh(nh-\theta)}{\cosh(nh+\theta)}, \quad \frac{\sinh((n-1)h-\theta)}{\sinh((n-1)h+\theta)} v(\theta); \tag{1.6}$$

$$\mathrm{Sp}_q(2n), \quad w(\theta) = \frac{\sinh((n+1)h-\theta)}{\sinh((n+1)h+\theta)}, \quad \frac{\cosh(nh-\theta)}{\cosh(nh+\theta)} v(\theta). \tag{1.7}$$

In contrast, for our class (Sec. 3, Ref. 1), *conserving* the projectors but changing the coefficients, we have

$$v(\theta) = 1, \quad w(\theta) = \frac{\sinh(\eta-\theta)}{\sinh(\eta+\theta)}, \tag{1.8}$$

where

$$e^{\eta} + e^{-\eta} = ([N-\epsilon]+\epsilon) = \frac{q^{N-\epsilon} - q^{-N+\epsilon}}{q-q^{-1}} + \epsilon \tag{1.9}$$

and $\epsilon = \pm 1$ when the P_i are those for $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$, respectively. [An overall ambiguity of sign for the right-hand side of (1.9) has been fixed to assure real η for real q. This will be maintained throughout, though complex q will be considered later.]

We adopt the following notations for our $\hat{R}(\theta)$ when (1.8) is implemented:

(a) when P_i are those for SO_q our $\hat{R}(\theta)$ is of type $\hat{o}(N)$,

(b) when P_i are those for Sp_q our $\hat{R}(\theta)$ is of type $\hat{p}(N)$.

This is to signal the provenance of the projectors and also at the same time the fact that the coefficients (1.8) often lead to startlingly different properties as compared to the standard cases [from (1.4) to (1.7)].

For (1.8) we obtain

$$\hat{R}(\theta) = P_+ + P_- + \frac{\sinh(\eta-\theta)}{\sinh(\eta+\theta)} P_0 = I + \left(\frac{\sinh(\eta-\theta)}{\sinh(\eta+\theta)} - 1\right) P_0. \tag{1.10}$$

For completeness we give P_0 explicitly.[4,5] Let the n-tuple $(\rho_1, \rho_2, \ldots, \rho_N)$ be defined as follows for the respective cases indicated:

$$\mathrm{SO}_q(2n+1), \quad \left(n-\tfrac{1}{2}, n-\tfrac{3}{2}, \ldots, \tfrac{1}{2}, 0, -\tfrac{1}{2}, \ldots, -n+\tfrac{1}{2}\right), \tag{1.11}$$

$$\mathrm{SO}_q(2n), \quad (n-1, n-2, \ldots, 1, 0, 0, -1, \ldots, -n+1), \tag{1.12}$$

$$\mathrm{Sp}_q(2n), \quad (n, n-1, \ldots, 1, -1, \ldots, -n). \tag{1.13}$$

Define correspondingly for

$$\mathrm{SO}_q(N), \quad \epsilon = 1 \quad (i = 1, \ldots, N; \quad N = 2n, 2n+1), \tag{1.14}$$

$$\mathrm{Sp}_q(2n), \quad \epsilon = 1 \quad (i \leqslant n), \quad \epsilon = -1 \quad (i > n) \quad (i = 1, \ldots, 2n). \tag{1.15}$$

Set

$$i' = N + 1 - i. \tag{1.16}$$

Then corresponding to (1.11) and (1.12), in notations most suitable for us,

$$([N-1]+1)P_0 = \sum_{i,j=1}^{N} q^{(\rho_{i'} - \rho_j)} (ij) \otimes (i'j') \equiv P_0' \tag{1.17}$$

and corresponding to (1.13) and (1.15),

$$([N+1]-1)P_0 = \sum_{i,j=1}^{N} q^{(\rho_{i'} - \rho_j)} \epsilon_i \epsilon_j (ij) \otimes (i'j') \equiv P_0'. \tag{1.18}$$

Here (ij) denotes the $N \times N$ matrix with 1 at (row i, column j) and zero elsewhere.

These standard P_0 will be *carried over* to our $\hat{o}(2n+1)$, $\hat{o}(2n)$, $\hat{p}(2n)$. We do not indicate the q dependence explicitly [by denoting $\hat{o}_q(2n+1)$, for example] since for $q=1$ our constructions remain nontrivial. Our $\hat{R}$ matrices are *not* q deformations of a "classical" limit for a particular value of q such as 1. This is just one of the remarkable features to be studied below.

For $N=3$, the 9×9 projector P_0 is given by

$$(q+1+q^{-1})P_0 \equiv P_0' = \begin{vmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & q^{-1} & 0 & q^{-\frac{1}{2}} & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & q^{-\frac{1}{2}} & 0 & 1 & 0 & q^{\frac{1}{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & q^{\frac{1}{2}} & 0 & q & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix}. \tag{1.19}$$

This is the case that will be studied here extensively as the simplest example. For all N a basic feature is the proportionality of the rows with nonzero elements. This has important consequences. It remains here to display briefly the "pre-Baxterized" situation. Our canonical forms ensure, among various aspects studied in Ref. 1,

$$\hat{R}(-\theta) = (\hat{R}(\theta))^{-1}, \quad \hat{R}(0) = I_{N^2}. \tag{1.20}$$

The limits

$$\theta \to \pm\infty, \quad \hat{R}(\theta) \to \hat{R}^{\pm 1}$$

satisfy the (non-Baxterized, θ-independent) braid equation

$$\hat{R}_{12}\hat{R}_{23}\hat{R}_{12} = \hat{R}_{23}\hat{R}_{12}\hat{R}_{23}, \tag{1.21}$$

where one can substitute $\hat{R}^{-1}$ for $\hat{R}$.

For the standard cases,

$$(\mathrm{SO}_q(N)), \quad \hat{R}^{\pm 1} = P_+ - q^{\mp 2}P_- + q^{\mp N}P_0, \tag{1.22}$$

$$(\mathrm{Sp}_q(N)), \quad \hat{R}^{\pm 1} = P_+ - q^{\mp 2}P_- - q^{\mp (N+2)}P_0 \tag{1.23}$$

satisfy *cubic* equations. For our cases, with η given by (1.9), one has for all N the *quadratic* equation

$$(e^{\eta}\hat{R}) - (e^{\eta}\hat{R})^{-1} = (e^{\eta} - e^{-\eta})I \tag{1.24}$$

or

$$(\hat{R} - I)(\hat{R} + e^{-2\eta}I) = 0. \tag{1.25}$$

From (1.10), as $\theta \to \pm\infty$,

$$\hat{R}^{\pm 1} = I - (1 + e^{\mp 2\eta})P_0 = I - e^{\mp \eta}(e^{\eta} + e^{-\eta})P_0 = I - e^{\mp \eta}P_0'. \tag{1.26}$$

The last equation follows from (1.9), (1.17), and (1.18). Note that though P_0' is *not* a projector in (1.26), $\hat{R}$ is inverted by inverting the coefficient of P_0' due to the relation

$$P_0'^2 = (e^{\eta} + e^{-\eta})P_0'.$$

Other properties of $\hat{R}$ will be introduced later as they become directly relevant.

II. WHAT q FOR TRIANGULARITY?

A braid matrix for vector representation is called "triangular" if

$$\hat{R}^2 = I. \tag{2.1}$$

For the standard cases $(A, B, C, D)_q$ this is obtained trivially for $q = 1$. This is well known. But for comparison with our case let us briefly indicate how this happens for $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$.

For the projectors in (1.2) and (1.3) denote

$$(P_i)_{q=1} = \mathsf{P}_i \quad (i = +, -, 0) \tag{2.2}$$

and let

$$P = \sum_{i,j} (ij) \otimes (ji), \quad P^2 = I. \tag{2.3}$$

[Acting on the left P permutes specific rows and acting on the right the corresponding columns. This evident feature is mentioned since it plays a crucial role below (2.40).]

From (1.22) and (1.23) substituing the known explicit forms[4,5] of the projectors for $q = 1$, with upper and lower signs for the two cases, respectively,

$$\hat{R} = \mathsf{P}_+ - \mathsf{P}_- \pm \mathsf{P}_0 = \pm (I - 2\mathsf{P}_{\mp}) = P. \tag{2.4}$$

Hence

$$\hat{R}^2 = P^2 = I, \quad R = P\hat{R} = I \tag{2.5}$$

for both cases.

For $GL_q(N)$ one obtains the same result even more simply.

For our class $q=1$ gives a quite nontrivial situation, as emphasized already in Ref. 3. Denoting for all $N=(3,4,\ldots)$,

$$(\eta)_{q=1} = \hat{\eta}$$

from (1.9),

$$e^{\hat{\eta}} + e^{-\hat{\eta}} = N, \quad (1 + e^{\mp 2\hat{\eta}}) = \frac{2N}{N \pm (N^2-4)^{1/2}} \neq 2, \tag{2.6}$$

and from (1.26),

$$(\hat{R}^{\pm 1})_{q=1} = I - (1 + e^{\mp 2\hat{\eta}})\mathsf{P}_0, \quad \hat{R}^2 \neq 1. \tag{2.7}$$

The generalized Hecke condition is now

$$(e^{\hat{\eta}}\hat{R}) - (e^{\hat{\eta}}\hat{R})^{-1} = (e^{\hat{\eta}} - e^{-\hat{\eta}})I. \tag{2.8}$$

This cannot be conjugated to

$$(\hat{R} - I)(\hat{R} + I) = 0. \tag{2.9}$$

For (2.1) we need for our case

$$\eta = 0, \tag{2.10}$$

when

$$\hat{R} = I - 2P_0, \quad \hat{R}^2 = I + 4(P_0^2 - P_0) = I.$$

Hence from (1.9) for $\hat{o}(N)$ and $\hat{p}(N)$, respectively,

$$[N \mp 1] \pm 1 = e^{\eta} + e^{-\eta} = 2 \tag{2.11}$$

or, respectively,

$$\text{(A)} \quad q^{N-2} + q^{N-4} + \cdots + q^{-N+4} + q^{-N+2} = 1 \quad (N = 3,4,\ldots), \tag{2.12}$$

$$\text{(B)} \quad q^{N} + q^{N-2} + \cdots + q^{-N+2} + q^{-N} = 3 \quad (N = 4,6,\ldots). \tag{2.13}$$

The degrees of the polynomials can be lowered by changing variables as follows for the different cases. To start with (A) is divided into two subclasses,

$$(\text{A})_1, \quad N = 2n + 2 \quad (n = 1,2,\ldots).$$

Set

$$p = q^2, \quad Y = p + p^{-1} \tag{2.14}$$

when

$$q = \pm p^{\frac{1}{2}} = \pm \frac{1}{\sqrt{2}}(Y + \sqrt{Y^2 - 4})^{1/2}. \tag{2.15}$$

From (2.12),

$$S_n \equiv (p^n + p^{-n}) + (p^{n-1} + p^{-n+1}) + \cdots + (p^2 + p^{-2}) + (p + p^{-1}) = 0. \tag{2.16}$$

Note that for $(\mathrm{A})_1$ the right-hand side cancels with $p^0 = 1$. Now to express S_n in terms of Y implementing

$$S_{n+1} = YS_n - S_{n-1} + Y - 2 \tag{2.17}$$

one obtains finally

$$\begin{aligned} S_n = Y^n + Y^{n-1} - \binom{n-1}{1} Y^{n-2} - \binom{n-2}{1} Y^{n-3} + \binom{n-2}{2} Y^{n-4} \\ + \binom{n-3}{2} Y^{n-5} + \cdots + (-1)^r \left(\binom{n-r}{r} Y^{n-2r} + \binom{n-r-1}{r} Y^{n-2r-1} \right) + \cdots + c_1 Y + c_0, \end{aligned} \tag{2.18}$$

where

$$\begin{gathered} c_1 = (-1)^{s-1} s \quad (n = 2s, r = s-1), \quad c_1 = (-1)^s (s+1) \quad (n = 2s+1, r = s), \\ c_0 = -2 \quad (n = 2 + 4m, 3 + 4m;\ m = 0, 1, 2, \ldots), \quad c_0 = 0 \quad (n \neq 2 + 4m, 3 + 4m). \end{gathered} \tag{2.19}$$

Explicitly,

$$\begin{gathered} S_1 = Y, \\ S_2 = Y^2 + Y - 2 = (Y-1)(Y+2), \\ S_3 = Y^3 + Y^2 - 2Y - 2 = (Y+1)(Y^2 - 2), \\ S_4 = Y^4 + Y^3 - 3Y^2 - 2Y, \\ S_5 = Y^5 + Y^4 - 4Y^3 - 3Y^2 + 3Y, \\ S_6 = Y^6 + Y^5 - 5Y^4 - 4Y^3 + 6Y^2 + 3Y - 2, \\ S_7 = Y^7 + Y^6 - 6Y^5 - 5Y^4 + 10Y^3 + 6Y^2 - 4Y - 2, \\ S_8 = Y^8 + Y^7 - 7Y^6 - 6Y^5 + 15Y^4 + 10Y^3 - 10Y^2 - 4Y, \\ S_9 = Y^9 + Y^8 - 8Y^7 - 7Y^6 + 21Y^5 + 15Y^4 - 20Y^3 - 10Y^2 + 5Y, \end{gathered} \tag{2.20}$$

and so on.

$$(\mathrm{A})_2: \quad N = 2m + 1 \quad (m = 1, 2, \ldots).$$

Set

$$z = q + q^{-1}, \quad q^{\pm 1} = \tfrac{1}{2}(z \pm \sqrt{z^2 - 4}). \tag{2.21}$$

Retaining only the odd powers in (2.18) and (2.20) and adapting notations one obtains

$$\Sigma_{(2m-1)} = (q^{2m-1} + q^{-2m+1}) + (q^{2m-3} + q^{-2m+3}) + \cdots + (q + q^{-1})$$
$$= z^{2m-1} - \binom{2m-2}{1} z^{2m-3} + \binom{2m-3}{2} z^{2m-5} + \cdots$$
$$+ (-1)^r \binom{2m-r-1}{r} z^{2m-2r-1} + \cdots + (-1)^{m-1} mz. \tag{2.22}$$

Explicitly [noting that in contrast with (2.16) there is now 1 on the right-hand side below]

$$\Sigma_{N-2} = 1 \quad (N = 3,5,\ldots), \tag{2.23}$$

where

$$\Sigma_1 = z,$$

$$\Sigma_3 = z^3 - 2z,$$

$$\Sigma_5 = z^5 - 4z^3 + 3z, \tag{2.24}$$

$$\Sigma_7 = z^7 - 6z^5 + 10z^3 - 4z,$$

$$\Sigma_9 = z^9 - 8z^7 + 21z^5 - 20z^3 + 5z,$$

and so on.

Comparing (2.12) and (2.13) one sees that (B) is obtained from $(\mathrm{A})_1$, with now a nonzero right-hand side, as

$$\text{(B)} \quad S_n = 2 \quad \left(n = \frac{N}{2} = 2,3,\ldots\right). \tag{2.25}$$

Without trying to be exhaustive let us first point out some simple possibilities, particularly when (2.1) is obtained for q a *root of unity*. (See the relevant remarks in the concluding section.)

For $\hat{o}(3)$ one has from (2.23),

$$\Sigma_1 = q + q^{-1} = 1, \quad q = \frac{1}{2} + i\frac{\sqrt{3}}{2} = e^{i(\pi/3)}, \quad q^6 = 1. \tag{2.26}$$

For $\hat{o}(4)$ one has from (2.16) and (2.20),

$$Y = q^2 + q^{-2} = 0, \quad q = e^{i(\pi/4)}, \quad q^8 = 1. \tag{2.27}$$

Moreover, whenever $c_0 = 0$ from (2.19), i.e., for

$$\hat{o}(4), \hat{o}(10), \hat{o}(12), \ldots, \tag{2.28}$$

Y can be factorized and (2.27) is a solution.

For $\hat{o}(6)$ the two roots of

$$S_2 = (Y-1)(Y+2) = 0$$

correspond to

$$q^{12} = 1, \quad q^4 = 1. \tag{2.29}$$

For $\hat{o}(8)$ the roots of S_3 give

$$q^6 = 1, \quad q^{16} = 1. \tag{2.30}$$

For $\hat{o}(10)$ and $\hat{o}(12)$ [apart from (2.27)] one must solve *cubic* and *quartic* equations, respectively. We do not present this standard algebra here. For odd N one has again a cubic in z for $\hat{o}(5)$.

For $\hat{o}(14)$ onwards for $\hat{o}(2n)$ one has polynomials of sixth and higher degrees [already for Y before obtaining q from (2.15)]. Hence one needs *hyperelliptic* functions for Y.

For $\hat{o}(7)$ and $\hat{p}(10)$ one has quintics and *elliptic* solutions, respectively, for $z=(q+q^{-1})$ and $Y=(q^2+q^{-2})$. For higher dimensions one again encounters hyperelliptic functions here.

It is known[6,7] that the general case on a complex field

$$f(x) = a_0 x^n + a_1 x^{n-1} + \cdots + a_n = 0 \tag{2.31}$$

can be solved in terms of theta functions of zero arguments and the period matrix of the hyperelliptic curves

$$F^2 = x(x-1)f(x), \quad F^2 = x(x-1)(x-2)f(x) \tag{2.32}$$

for odd n and even n, respectively.

For quintics[7] one can, alternatively, implement further successive changes of variables (Tschirnhausen transformations) to obtain standard forms (the Bring–Jerrard quintic or the Brioschi quintic leading to the Jacobi sextic) which can be solved directly using elliptic functions. All this is however very complicated.

The coeffficients a_i of (2.31) are very special ones (binomial integers) for our case. What special (hopefully simplifying) features might they induce in the corresponding elliptic and hyperelliptic functions? An answer to this question is beyond the scope of this paper.

Let us contemplate the simplest case, that of $\hat{o}(3)$ with (2.26) giving

$$\hat{R} = I - \begin{vmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & q^{-1} & 0 & q^{-\frac{1}{2}} & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & q^{-\frac{1}{2}} & 0 & 1 & 0 & q^{\frac{1}{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & q^{\frac{1}{2}} & 0 & q & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix}, \tag{2.33}$$

where $q=e^{i(\pi/3)}$.

Remarkably this satisfies

$$\hat{R}_{12}\hat{R}_{23}\hat{R}_{12} = \hat{R}_{23}\hat{R}_{12}\hat{R}_{23}$$

along with

$$\hat{R}^2 = I.$$

A nonexistence theorem: For the standard cases [see (2.3), (2.4), and (2.5)],

$$(\hat{R})_{q=1} = P, \quad \hat{R}^2 = P^2 = I.$$

For the nonstandard Jordanian case (see Refs. 8 and 9 citing basic sources) considering again vector representations

$$\hat{R} = F^{-1}PF, \quad \hat{R}^2 = I, \tag{2.34}$$

where F is obtained through a "contraction".[8,9] Thus the Yang–Baxter matrix

$$R = P\hat{R} = (PF^{-1}P)F = F_{21}^{-1}F \tag{2.35}$$

is a "Drinfeld twist" of unity. This leads to various interesting features[8,9] making triangularity inherent without rendering $\hat{R}$ trivial. Can our constructions above (for $\eta=0$) be expressed as a conjugation of P as in (2.34)? *A priori* such a possibility cannot be discarded.

However, using our diagonalizers (see Appendix B of Ref. 1 for explicit constructions) one can prove quite simply and generally that *no* invertible F exists that can realize (2.34).

It is sufficient to consider $\hat{o}(3)$. Higher dimensions can be treated in a strictly parallel fashion. The essential result for us is that the diagonalizer M gives for (1.26),

$$M\hat{R}^{\pm 1}M^{-1} = (-e^{\mp 2\eta}, 1, 1, 1, 1, 1, 1, 1, 1)_{(\mathrm{diag})}. \tag{2.36}$$

For $\eta=0$, when $\hat{R}^2=I$, one thus obtains

$$M\hat{R}^{\pm 1}M^{-1} = (-1, 1, 1, 1, 1, 1, 1, 1, 1)_{(\mathrm{diag})} \equiv D. \tag{2.37}$$

Now assume that an F exists for our $\hat{R}$ satisfying (2.34). Then

$$MF^{-1}PFM^{-1} = D. \tag{2.38}$$

Defining

$$G = FM^{-1} \tag{2.39}$$

since $D^2=I$,

$$G = PGD. \tag{2.40}$$

The action of P here for the 9×9 case [see (2.3)] leaves the rows 1, 5, and 9 untouched and interchanges the pairs of rows

$$(2,4), (3,7), (6,8).$$

Now consider the action of D after parametrizing G in terms of parameters arbitrary to start with. In rows 1, 5, and 9 the first element is constrained to be zero the others being unrestricted. If row 2 is parametrized as

$$(a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_8, a_9) \tag{2.41}$$

then row 4 must be

$$(-a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_8, a_9). \tag{2.42}$$

Hence with arbitrary a_1, r_i denoting the row i,

$$(r_2 - r_4) = (2a_1, 0, 0, 0, 0, 0, 0, 0, 0). \tag{2.43}$$

Similarly, in evident notations,

$$(r_3 - r_5) = (2b_1, 0, 0, 0, 0, 0, 0, 0, 0), \tag{2.44}$$

$$(r_6 - r_8) = (2c_1, 0, 0, 0, 0, 0, 0, 0, 0). \tag{2.45}$$

This evidently implies that the determinant

$$\Delta G = 0. \tag{2.46}$$

Hence G is not invertible. Hence neither is $F=GM$.

This contradicts the assumption that an invertible F exists giving (2.34) for our $\hat{R}$.

III. *L*- ALGEBRA (GROUPLIKE CENTRAL ELEMENTS)

Before writing down the *RLL* equations and the implied constraints we signal the most remarkable features to emerge in Secs. III and IV. We will study them mostly in the context of the simplest case $\hat{o}(3)$, i.e., $N=3$.

(1) In the L^+ subalgebra one obtains $2N$ central, grouplike elements constrained to equality by the *RLL* equations. There are $2N$ corresponding ones for the L^- subalgebra.
(2) In standard cases grouplike elements are usually associated to "quantum determinants." But our above-mentioned sets have no determinantlike structure at all. Each one is the sum of N quadratic terms (no negetive signs).
(3) In the 3×3 fundamental representation of the L operators for $\hat{o}(3)$ these elements are proportional to I_3. Consistently with their grouplike property and centrality they are proportional to I_9 for the 9×9 coproduct representations. The explicit verification of this involves remarkable cancellations. Iterated coproducts of course lead to $I_{3^{2^p}}$ at the pth stage.
(4) In the standard cases, we are used to the coproducts being reducible. Thus the 9×9 coproducts $\Delta L^{\pm}_{ij}$ for $\mathrm{SO}_q(3)$ can be conjugated to block-diagonal forms corresponding to the familiar irreducible components $(9\times 9\rightarrow 5\times 5\oplus 3\times 3\oplus 1\times 1)$ or in terms of angular momenta $(1\times 1\rightarrow 2\oplus 1\oplus 0)$. But here one encounters obstructions in a systematic search for block diagonalizations. This is of course consistent with the central elements announced above being proportional to I. But since such a search reveals special features of the generators this aspect of the 9×9 coproduct mentioned above will be treated explicitly in the next section.

Let us now formulate the *RLL* constraints. The *FRT* equations[4] for the $L^{\pm}$ operators are, in our notations,

$$\hat{R}L^{\pm}_2L^{\pm}_1 = L^{\pm}_2L^{\pm}_1\hat{R}, \tag{3.1}$$

$$\hat{R}L^{+}_2L^{-}_1 = L^{-}_2L^{+}_1\hat{R} \quad (\hat{R}^{-1}L^{-}_2L^{+}_1 = L^{+}_2L^{-}_1\hat{R}^{-1}). \tag{3.2}$$

Here $\hat{R}$ is a $N^2\times N^2$ matrix satisfying (1.21) and $L^{\pm}$ have each N^2 components $L^{\pm}_{ij}(i,j=1,2,\ldots,N)$ arranged in a $N\times N$ matrix form with

$$L^{\pm}_2 = I_N\otimes L^{\pm}, \quad L^{\pm}_1 = L^{\pm}\otimes I_N. \tag{3.3}$$

From (1.26), with P'_0 given by (1.17) and (1.18),

$$\hat{R}^{\pm 1} = I + \lambda_{\pm}P'_0, \quad \lambda_{\pm} = -e^{\mp\eta}. \tag{3.4}$$

Here from (1.9), $\lambda_{\pm}$ are the roots of

$$\lambda + \lambda^{-1} + ([N\mp 1]\pm 1) = 0 \tag{3.5}$$

and, in particular, for $\hat{o}(3)$ of

$$\lambda + \lambda^{-1} + (q + 1 + q^{-1}) = 0. \tag{3.6}$$

This simple change of notation $(\eta\rightarrow\lambda)$ will permit below a compact, unified treatment of L^+ and L^- due to the symmetry,

$$(\lambda_+, L^+, L^-) \rightleftharpoons (\lambda_-, L^-, L^+). \tag{3.7}$$

This is a special feature of our class. We will often suppress below the superscripts and subscripts of L and λ, respectively, when dealing with (3.1) and write L_{ij} and λ.

From (3.1) and (3.4) one has

$$P'_0L^{\epsilon}_2L^{\epsilon}_1 = L^{\epsilon}_2L^{\epsilon}_1P'_0, \quad (\epsilon = \pm). \tag{3.8}$$

In these equations $\lambda_{\pm}$ do *not* appear explicitly. They do however appear for (3.2).

A. L^+ and L^- subalgebras

The grouplike elements belong to these subalgebras since the coproducts are defined separately for each. The *RLL* constraints lead to $(2N^2-1)$ equations for each subalgebra which separate into three subsets of $N(N-1)$, $N(N-1)$, $(2N-1)$, respectively. The total number is easily understood as follows.

The diagonalizer M (see Appendix B, Ref. 1) gives

$$MP_0'M^{-1} \approx (1,0,0,\ldots,0)_{(\mathrm{diag})}. \tag{3.9}$$

Conjugating the factors on both sides of (3.8) by M only the row 1 survives on the left and only the column 1 on the right. These have each N^2 elements and one element in common. Hence the result.

It is convenient to start by deriving some results in a form valid, more generally, for the whole algebra as follows. We consider $\hat{o}(N)$ for definiteness, the modifications for $\hat{p}(N)$ are evident.

Along with (1.17) and (3.3), for $N \geqslant 3$, we write

$$L_2L_1' = \sum_{i,j,k,l} L_{kl}L_{ij}'(ij) \otimes (kl), \tag{3.10}$$

where

$$L_2L_1' = L_2^{\epsilon}L_1^{\epsilon'}, \quad (\epsilon, \epsilon^1) = (+,+),(-,-),(+,-),(-,+).$$

One can show that (with $i' = N-i+1$).

$$P_0'L_2L_1' = \sum_{i,k,l} q^{-\rho_i} S_{lk}^{(1)}(ik) \otimes (i'l), \tag{3.11}$$

$$L_2'L_1P_0' = \sum_{i,k,l} q^{-\rho_i} S_{lk}^{(2)}(ki) \otimes (li'), \tag{3.12}$$

where

$$S_{lk}^{(1)} = \sum_j q^{-\rho_j} L_{j'l}L_{jk}', \tag{3.13}$$

$$S_{lk}^{(2)} = \sum_j q^{-\rho_j} L_{lj'}'L_{kj}. \tag{3.14}$$

We now go back to our subalgebras by setting $\epsilon = \epsilon'$, i.e., $L' = L$.

For $l \neq k'(l+k \neq N+1)$ one obtains from (3.8), due to the structure of P_0,

$$S_{lk}^{(1)} = \sum_j q^{-\rho_j} L_{j'l}L_{jk} = 0. \tag{3.15}$$

and

$$S_{lk}^{(2)} = \sum_i q^{-\rho_i} L_{li'}L_{ki} = 0. \tag{3.16}$$

Each set $(S^{(1)}, S^{(2)})$ corresponds to $N(N-1)$ equations and

$$S^{(1)} \to S^{(2)} \rightleftharpoons L_{ij} \to L_{ji}. \tag{3.17}$$

For

$$l + k = N + 1$$

one obtains (i and j assuming each value *independently* with $i+i'=j+j'=N+1$)

$$q^{-\rho_i} S^{(1)}_{ii'} = q^{-\rho_j} S^{(2)}_{jj'} \quad (i = 1,\ldots,N;\ j = 1,\ldots,N). \tag{3.18}$$

The equality of these $2N$ quadratic expressions give $(2N-1)$ equations. We will denote this set as $\hat{S}_3$. This provides the grouplike central elements. We will study this set in detail for $\hat{o}(3)$. For $N=3$ one obtains from (3.18),

$$q^{-\frac{1}{2}} S^{(1)}_{13} = S^{(1)}_{22} = q^{\frac{1}{2}} S^{(1)}_{31} = q^{-\frac{1}{2}} S^{(2)}_{13} = S^{(2)}_{22} = q^{\frac{1}{2}} S^{(2)}_{31}. \tag{3.19}$$

Or explicitly (with L all L^+ or all L^- below),

$$\begin{aligned}
(\hat{S}_3), \quad & L_{11}L_{33} + q^{-\frac{1}{2}} L_{21}L_{23} + q^{-1} L_{31}L_{13} \\
& = q^{\frac{1}{2}} L_{12}L_{32} + L_{22}L_{22} + q^{-\frac{1}{2}} L_{32}L_{12} \\
& = qL_{13}L_{31} + q^{\frac{1}{2}} L_{23}L_{21} + L_{33}L_{11} = L_{11}L_{33} + q^{-\frac{1}{2}} L_{12}L_{32} \\
& + q^{-1} L_{13}L_{31} = q^{\frac{1}{2}} L_{21}L_{23} + L_{22}L_{22} + q^{-\frac{1}{2}} L_{23}L_{21} \\
& = qL_{31}L_{13} + q^{\frac{1}{2}} L_{32}L_{12} + L_{33}L_{11}.
\end{aligned} \tag{3.20}$$

We denote the sets (3.15) and (3.16) by $\hat{S}_1$ and $\hat{S}_2$, respectively. For $N=3$ the first set is

$$\hat{S}_1,$$

$$\begin{aligned}
& q^{-\frac{1}{2}} L_{31}L_{11} + L_{21}L_{21} + q^{\frac{1}{2}} L_{11}L_{31} = 0, \\
& q^{-\frac{1}{2}} L_{32}L_{11} + L_{22}L_{21} + q^{\frac{1}{2}} L_{12}L_{31} = 0, \\
& q^{-\frac{1}{2}} L_{31}L_{12} + L_{21}L_{22} + q^{\frac{1}{2}} L_{11}L_{32} = 0, \\
& q^{-\frac{1}{2}} L_{33}L_{12} + L_{23}L_{22} + q^{\frac{1}{2}} L_{13}L_{32} = 0, \\
& q^{-\frac{1}{2}} L_{32}L_{13} + L_{22}L_{23} + q^{\frac{1}{2}} L_{12}L_{33} = 0, \\
& q^{-\frac{1}{2}} L_{33}L_{13} + L_{22}L_{23} + q^{\frac{1}{2}} L_{13}L_{33} = 0.
\end{aligned} \tag{3.21}$$

The set $\hat{S}_2$ is obtained immediately from $\hat{S}_1$ via (3.17).

We now show how the sets $(\hat{S}_1, \hat{S}_2, \hat{S}_3)$ imply the two basic properties of the members of $\hat{S}_3$, that they are (1) central and (2) grouplike.

(1) Exploiting systematically the sets $\hat{S}_i$ one can pass through different chains of intermediate steps. One possible sequence is as follows:

$$q^{\frac{1}{2}} L_{11}L_{23}L_{21} = q^{-\frac{1}{2}} L_{12}L_{32}L_{11} - q^{-\frac{1}{2}} L_{13}L_{21}L_{21} + q^{\frac{1}{2}} L_{12}L_{12}L_{31}, \tag{3.22}$$

$$qL_{11}L_{13}L_{31} = q^{-1} L_{13}L_{31}L_{11} - q^{-\frac{1}{2}} L_{13}L_{21}L_{21} - q^{\frac{1}{2}} L_{12}L_{12}L_{31}. \tag{3.23}$$

Summing these with $L_{11}L_{33}L_{11}$ one obtains [using again (3.20) in the last step]

$$L_{11}(qL_{13}L_{31}+q^{\frac{1}{2}}L_{23}L_{21}+L_{33}L_{11}) = (L_{11}L_{33}+q^{-\frac{1}{2}}L_{12}L_{32}+q^{-1}L_{13}L_{31})L_{11}$$
$$= (qL_{13}L_{31}+q^{\frac{1}{2}}L_{23}L_{21}+L_{33}L_{11})L_{11}. \tag{3.24}$$

Thus L_{11}, and similarly each L_{ij} can be shown to commute with the members of $\hat{S}_3$. Hence the latter are central.

(2) The rule for coproducts[4] (with L either L^+ or L^- throughout) is

$$\Delta L_{ij} = \sum_k L_{ik} \otimes L_{kj}. \tag{3.25}$$

Hence

$$\Delta L_{ab}\Delta L_{cd} = \sum_{i,j} L_{ai}L_{cj} \otimes L_{ib}L_{jd}. \tag{3.26}$$

Now let us start with the first member of $\hat{S}_3$ and compute the sum

$$\Sigma = \Delta L_{11}\Delta L_{33} + q^{-\frac{1}{2}}\Delta L_{21}\Delta L_{23} + q^{-1}\Delta L_{31}\Delta L_{13}. \tag{3.27}$$

Collecting terms and systematically implementing $\hat{S}_1$, $\hat{S}_2$ many terms cancel leaving

$$\Sigma = (L_{11}L_{33}+q^{-\frac{1}{2}}L_{21}L_{23}+q^{-1}L_{31}L_{13}) \otimes (L_{11}L_{33}+q^{-\frac{1}{2}}L_{21}L_{23}+q^{-1}L_{31}L_{13}). \tag{3.28}$$

Thus this and similarly the other members of $\hat{S}_3$ are grouplike.

For $\hat{o}(4)$ the eight members of $\hat{S}_3$ satisfy

$$q^{-1}S^{(1)}_{14} = S^{(1)}_{23} = S^{(1)}_{32} = qS^{(1)}_{41} = q^{-1}S^{(2)}_{14} = S^{(2)}_{23} = S^{(2)}_{32} = qS^{(2)}_{41}. \tag{3.29}$$

Their centrality and grouplike property can be established in strict analogy to the $\hat{o}(3)$ case. Moreover they indicate how the generalization for higher N can be carried out. Our presentation here will be limited to $\hat{o}(3)$.

B. Beyond the $L^{\pm}$ subalgebras

We now consider the "mixed" case (3.2). The major feature now is the explicit involvement of $\lambda_{\pm}$ [see (3.4) and (3.5)] in the constraints,

$$(I+\lambda_+P'_0)L^+_2L^-_1 = L^-_2L^+_1(I+\lambda_+P'_0), \tag{3.30}$$

$$(I+\lambda_-P'_0)L^-_2L^+_1 = L^+_2L^-_1(I+\lambda_-P'_0). \tag{3.31}$$

But even when P'_0 does not contribute, namely at

$$(ij)\otimes(kl), \quad (kl)\neq(i'j'),$$

one obtains simple but probing constraints. Retaining only such rows and columns one obtains a "reduced" matrix of $N(N-1)\times N(N-1)$ dimensions. For $N=3$ this corresponds to the suppression of rows and columns (3,5,7) leaving a 6×6 matrix. Using for this reduced case, for all N, the subscript r one extracts from (3.30) and (3.31),

$$(L^{\epsilon}_2L^{\epsilon'}_1)_{(r)} = (L^{\epsilon'}_2L^{\epsilon}_1)_{(r)}. \tag{3.32}$$

For $\epsilon=\epsilon'$ this is trivial, but not now, and one can go further as follows.

Since λ satisfies a quadratic equation one can linearize all polynomials in λ using λ_+ and $\lambda_-=(\lambda_+)^{-1}$. The symmetry of (3.30) and (3.31),

$$(\lambda_+ \to \lambda_-) \rightleftharpoons (L^+ \to L^-) \tag{3.33}$$

indicates the parametrization where the λ dependence is explicitly (and only) in the coefficient as

$$L^{\epsilon}_{ij} = A_{ij} + \lambda_{\epsilon} B_{ij}. \tag{3.34}$$

Now injecting (3.34) in (3.32) one obtains for each element of the *reduced matrix* ($L^{\pm}_{ab}$, $L^{\pm}_{cd}$, and so on)

$$(\lambda_+ - \lambda_-)(A_{ab}B_{cd} - B_{ab}A_{cd}) = 0, \quad (\lambda_+ \neq \lambda_-). \tag{3.35}$$

Thus the λ dependence is simply factored out for this reduced martix. Even when L^+ and L^- are considered in the context of the respective subalgebras they must satisfy (3.35). This will indeed be found to be the case in the explicit realizations of the following section.

We now come to parts where both I and P'_0 contribute and hence λ is directly involved. Instead of $\hat{S}_3$ of (3.20) one now has for $\hat{o}(3)$ nine relations of the type

$$\lambda_+(qL'_{31}L_{13} + q^{\frac{1}{2}}L'_{32}L_{12} + L'_{33}L_{11}) - (qL_{13}L'_{31} + q^{\frac{1}{2}}L_{23}L'_{21} + L_{33}L'_{11}) = q(L_{33}L'_{11} - L'_{33}L_{11}). \tag{3.36}$$

Instead of $\hat{S}_1$, $\hat{S}_2$ one now has equations of the type

$$\lambda_+(q^{-\frac{1}{2}}L_{31}L'_{11} + L'_{21}L_{21} + q^{\frac{1}{2}}L_{11}L'_{31}) = q^{\frac{1}{2}}(L'_{31}L_{11} - L_{31}L'_{11}) = (L'_{21}L_{21} - L_{21}L'_{21}) = q^{-\frac{1}{2}}(L'_{11}L_{31} - L_{11}L'_{31}). \tag{3.37}$$

For $\epsilon=\epsilon'$ one recovers the results for the subalgebras. We have obtained a systematic formulation of the full set of 81 constraints for $\hat{o}(3)$ exploiting certain symmetries. This will not be reproduced here. The generalizations of the results of this section for $N>3$ can be obtained fairly systematically.

C. From $L^{\pm}$ to $L(\theta)$

Since our $\hat{R}$ satisfies a quadratic equation (1.24) all the three FRT equations (3.1) and (3.2) can be condensed into a *single* one by defining in analogy to

$$\hat{R}(\theta) = \frac{e^{\eta+\theta}\hat{R} - e^{-\eta-\theta}\hat{R}^{-1}}{e^{\eta+\theta} - e^{-\eta-\theta}}, \tag{3.38}$$

$$L(\theta) = \frac{e^{\eta+\theta}L^+ - e^{-\eta-\theta}L^-}{e^{\eta+\theta} - e^{-\eta-\theta}}. \tag{3.39}$$

It can be shown that[10,11]

$$\hat{R}(\theta-\theta')L_2(\theta)L_1(\theta') = L_2(\theta')L_1(\theta)\hat{R}(\theta-\theta') \tag{3.40}$$

contains effectively all the three FRT equations. One can write (3.38), i.e., (1.10) as

$$\hat{R}(\theta) = 1 - \frac{\sinh\theta}{\sinh(\eta+\theta)}P'_0. \tag{3.41}$$

IV. FUNDAMENTAL AND COPRODUCT REPRESENTATIONS

Here we will study the $\hat{o}(3)$ fundamental (3×3) and the coproduct (9×9) representations. They illustrate the significance of the remarks (3) and (4) at the beginning of Sec. III. This will be commented upon at the end. Specific symmetries of the matrices obtained will be displayed. They might be helpful in a more systematic study of representations.

The general prescription for the fundamental representations ($N\times N$ blocks for all N) is as follows (see Appendix B of Ref. 11 for a systematic presentation citing basic sources):

$$L(\theta)=\hat{R}(\theta)P, \quad (L(\theta))_{q\to\pm\infty}=L^{\pm}=\hat{R}^{\pm 1}P. \tag{4.1}$$

A Hopf algebra can be defined[4,10] for L using

$$(L^{\pm})^{-1}=PL^{\mp}P=(L^{\mp})_{21}. \tag{4.2}$$

From (3.4), (3.6), and (4.1) one obtains (for the fundamental representations)

$$L=\begin{vmatrix} L_{11} & L_{12} & L_{13}\\ L_{21} & L_{22} & L_{23}\\ L_{31} & L_{32} & L_{33}\end{vmatrix},$$

$$\begin{aligned} L_{11}&=\begin{vmatrix}1&0&0\\0&0&0\\0&0&\lambda\end{vmatrix}, \quad L_{12}=\begin{vmatrix}0&0&0\\1&0&0\\0&q^{-\frac{1}{2}}\lambda&0\end{vmatrix}, \quad L_{13}=\begin{vmatrix}0&0&0\\0&0&0\\(1+q^{-1}\lambda)&0&0\end{vmatrix},\\ L_{21}&=\begin{vmatrix}0&1&0\\0&0&q^{\frac{1}{2}}\lambda\\0&0&0\end{vmatrix}, \quad L_{22}=\begin{vmatrix}0&0&0\\0&(1+\lambda)&0\\0&0&0\end{vmatrix}, \quad L_{23}=\begin{vmatrix}0&0&0\\q^{-\frac{1}{2}}\lambda&0&0\\0&1&0\end{vmatrix},\\ L_{31}&=\begin{vmatrix}0&0&(1+q\lambda)\\0&0&0\\0&0&0\end{vmatrix}, \quad L_{32}=\begin{vmatrix}0&q^{\frac{1}{2}}\lambda&0\\0&0&1\\0&0&0\end{vmatrix}, \quad L_{33}=\begin{vmatrix}\lambda&0&0\\0&0&0\\0&0&1\end{vmatrix}. \end{aligned} \tag{4.3}$$

One sets $\lambda=(\lambda_+,\lambda_-,\lambda(\theta))$ for $L=(L^+,L^-,L(\theta))$, respectively. One obtains $\lambda(\theta)$ directly from (3.39).

Note that (3.34) is evidently satisfied with

$$L_{11}^{\pm}=\begin{vmatrix}1&0&0\\0&0&0\\0&0&0\end{vmatrix}+\lambda_{\pm}\begin{vmatrix}0&0&0\\0&0&0\\0&0&1\end{vmatrix}\equiv A_{11}+\lambda_{\pm}B_{11},$$

and so on.

Now we consider the 9×9 coproducts of (4.3) given by

$$\Delta L_{ij}^{\pm}=\sum_k L_{ik}^{\pm}\otimes L_{kj}^{\pm}.$$

We will not present the easily obtained 9×9 matrices but the symmetries they exhibit for the reason mentioned before. Define the following (r_1,r_2): reflections about the diagonal and the antidiagonal, respectively,

$$f{:}(q\to q^{-1})(r_2r_1), \quad f(A)\equiv fA.$$

Then in terms of 3×3 blocks $A_{ij},\ldots,E_3$ (not exhibited here) one obtains with $(ij=11, 12, 13)$ and $(i'j'=33, 32, 31)$, respectively (and noting that λ is invariant for $q\to q^{-1}$)

$$\Delta L_{ij}=\begin{vmatrix} A_{ij} & 0 & 0 \\ B_{ij} & 0 & 0 \\ C_{ij} & q^{-\frac{1}{2}}\lambda B_{ij} & \lambda A_{ij} \end{vmatrix}, \quad f\Delta L_{ij}=\Delta L_{i'j'}=\begin{vmatrix} \lambda f A_{ij} & q^{\frac{1}{2}}\lambda f B_{ij} & f C_{ij} \\ 0 & 0 & f B_{ij} \\ 0 & 0 & f A_{ij} \end{vmatrix}, \tag{4.4}$$

$$\Delta L_{21}=\begin{vmatrix} 0 & D_1 & 0 \\ q^{-\frac{1}{2}}\lambda D_2 & D_3 & q^{\frac{1}{2}}\lambda D_1 \\ 0 & D_2 & 0 \end{vmatrix}, \quad f\Delta L_{21}=\Delta L_{23}=\begin{vmatrix} 0 & fD_2 & 0 \\ q^{-\frac{1}{2}}\lambda f D_1 & fD_3 & q^{\frac{1}{2}}\lambda f D_2 \\ 0 & fD_1 & 0 \end{vmatrix}, \tag{4.5}$$

$$\Delta L_{22}=f\Delta L_{22}=\begin{vmatrix} 0 & E_1 & 0 \\ q^{-\frac{1}{2}}\lambda f E_1 & E_3 & q^{\frac{1}{2}}\lambda E_1 \\ 0 & fE_1 & 0 \end{vmatrix}. \tag{4.6}$$

Having displayed the symmetries we now study in more detail the three generators ΔL_{ii}. For the standard cases the L_{ii} can be obtained directly in diagonal forms for irreducible representations[4] and through appropriate conjugations for reducible ones. For our 3×3 representation also they are diagonal with their sum proportional to I. But for the 9×9 coproducts above they are not diagonal. They do not commute mutually and hence cannot be diagonalized simultaneously. To better understand the structure encountered let us try to diagonalize the sum $(\Sigma_i \Delta L_{ii})$. Define

$$\mu=(q^{\frac{1}{2}}-q^{-\frac{1}{2}}), \quad z=(q^{\frac{1}{2}}+q^{-\frac{1}{2}}), \quad k=(q+4+q^{-1})^{-\frac{1}{2}}. \tag{4.7}$$

Set

$$\sqrt{2}N=\begin{vmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & zk & 0 & 2k & 0 & zk & 0 & 0 \\ 0 & 0 & \sqrt{2}k & 0 & -\sqrt{2}zk & 0 & \sqrt{2}k & 0 & 0 \\ \sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{2} \end{vmatrix}. \tag{4.8}$$

This is orthogonal, i.e.,

$$N^{-1}=N^T.$$

One obtains

$$N(\Delta L_{11}+\Delta L_{22}+\Delta L_{33})N^{-1}=\lambda(-y,y,y,-y,3,3,-y,-y,-y)_{(\mathrm{diag})}, \quad y=(q+1+q^{-1}). \tag{4.9}$$

The eigenvalues can be permuted through evident supplementary conjugations.

We have thus diagonalized the sum. Now let us look at the component terms. One has [denoting by (bd) a block diagonal structure]

$$N(\Delta L_{ii})N^{-1} = (\alpha_i, \beta_i, \gamma_i, \delta_i)_{(bd)} \quad (i = 1,2,3), \tag{4.10}$$

where

$$\alpha_1 = \frac{1}{2}\begin{vmatrix} 1 & 1 \\ -1 & -1 \end{vmatrix}, \quad \alpha_3 = \frac{\lambda^2}{2}\begin{vmatrix} 1 & -1 \\ 1 & -1 \end{vmatrix}, \quad \alpha_2 = \frac{1}{2}\begin{vmatrix} \lambda^2+1 & \lambda^2-1 \\ -\lambda^2+1 & -\lambda^2-1 \end{vmatrix}, \tag{4.11}$$

$$\beta_1 = \frac{\lambda^2}{2}\begin{vmatrix} -1 & -1 \\ 1 & 1 \end{vmatrix}, \quad \beta_3 = \frac{1}{2}\begin{vmatrix} -1 & 1 \\ -1 & 1 \end{vmatrix}, \quad \beta_2 = \frac{1}{2}\begin{vmatrix} -\lambda^2-1 & \lambda^2-1 \\ -\lambda^2+1 & \lambda^2+1 \end{vmatrix}, \tag{4.12}$$

$$\delta_1 = \begin{vmatrix} 1 & 0 \\ 0 & \lambda^2 \end{vmatrix}, \quad \delta_3 = \begin{vmatrix} \lambda^2 & 0 \\ 0 & 1 \end{vmatrix}, \quad \delta_2 = \begin{vmatrix} 0 & 0 \\ 0 & 0 \end{vmatrix}, \tag{4.13}$$

$$\gamma_1 = \frac{\lambda}{2}\begin{vmatrix} 3 & \mu k & \sqrt{2}(2+q^{-1})k \\ \mu k & 3z^2k^2 & \sqrt{2}(2+q^{-1})\mu k^2 \\ -\sqrt{2}(2+q)k & -\sqrt{2}(2+q)\mu k^2 & -2(z^2-1)k^2 \end{vmatrix}, \tag{4.14}$$

$$\gamma_3 = \frac{\lambda}{2}\begin{vmatrix} 3 & \mu k & -\sqrt{2}(2+q)k \\ \mu k & 3(1-2k^2) & -\sqrt{2}(2+q)\mu k^2 \\ \sqrt{2}(2+q^{-1})k & \sqrt{2}(2+q^{-1})\mu k^2 & -2(1-3k^2) \end{vmatrix}, \tag{4.15}$$

$$\gamma_2 = \frac{\lambda}{2}\begin{vmatrix} 0 & -2\mu k & \sqrt{2}\mu z k \\ -2\mu k & 12k^2 & \sqrt{2}\mu^2 z k^2 \\ \sqrt{2}\mu z k & \sqrt{2}\mu^2 z k^2 & -2(z^2-1)z^2k^2 \end{vmatrix}. \tag{4.16}$$

Note that

$$\alpha_1^2 = \alpha_3^2 = \beta_1^2 = \beta_3^2 = \begin{vmatrix} 0 & 0 \\ 0 & 0 \end{vmatrix}. \tag{4.17}$$

Such nilpotent matrices are *nondiagonalizable*.

It has been explicitly verified that not only $N(\Delta L_{ij})N^{-1}(i \neq j)$ are not correspondingly block diagonalized but *all* their nonzero elements lie systematically outside the blocks arising for $N(\Delta L_{ii})N^{-1}$. One can examine larger blocks, say, $(6 \otimes 6 \oplus 3 \otimes 3)$ after permuting the γ_i and δ_i blocks. But one finds that the whole 9×9 space is needed for $N(\Delta L_{ij})N^{-1}$. These results will not be displayed here though particularly for $q=1$ they aquire relatively simple forms. One can implement further conjugations and permutations but the essential features persist.

For the 3×3 representations all the members of $\hat{S}_3$ in (3.20) say, for example,

$$L_{11}L_{33} + q^{-\frac{1}{2}}L_{21}L_{23} + q^{-1}L_{31}L_{13} = \lambda I_3. \tag{4.18}$$

Also

$$L_{11} + L_{22} + L_{33} = (1+\lambda)I_3. \tag{4.19}$$

The members of $\hat{S}_3$ being grouplike (4.18) gives for the 9×9 coproducts $\lambda^2 I_9$. This has been verified explicitly. But $(\Sigma_i \Delta L_{ii})$ behaves quite differently as shown above.

The obstructions encountered in reduction of the 9×9 coproducts to smaller dimensional irreducible components [via block diagonalization in a fashion analogous, say, to the case of $SO_q(3)$] is consistent with the central $\hat{S}_3$ operators being proportional to I. But our study of ΔL_{ii}

reveals specific properties of these generators for higher dimensional representations (such as symmetries and nondiagonalizable blocks). This can be helpful in a more systematic study of representations. The symmetries displayed in (4.4), (4.5), and (4.6) stem from those of P_0 and hence should be significant more generally.

V. LINK INVARIANTS (TURAEV CONSTRUCTION)

A. Construction of "enhanced" operators

Given a matrix satisfying the braid equation the Turaev construction[12] of an enhanced Yang–Baxter operator (EY B) leads to explicit construction of invariants (invariant under Markov moves of first and second types) for oriented links. Such an enhanced system[12,13] consists of a $N^2\times N^2$ braid matrix $\hat{R}$, an $N\times N$ matrix f and elements (a,b), all invertible, satisfying the relations

$$\hat{R}^{\pm 1} f\otimes f = f\otimes f\hat{R}^{\pm 1}, \tag{5.1}$$

$$tr_2(\hat{R}^{\pm 1} f\otimes f) = a^{\pm 1} bf, \tag{5.2}$$

where one defines

$$tr_2\left(\sum_{ijkl} c_{ij,kl}(ij)\otimes(kl)\right) = \sum_{ij}\left(\sum_k c_{ij,kk}\right)(ij). \tag{5.3}$$

Let us first obtain (f,a,b) for our class of $\hat{R}$. Our spectral resolution and the properties of the projector P_0 [and hence of P_0' defined in (1.17) and (1.18)] render the constructions particularly transparent.

Define the *diagonal* $N\times N$ matrices f for the cases

(1) $\hat{o}(N),\ N=2n+1,\ n=1,2,\ldots,$

(2) $\hat{o}(N),\ N=2n,\ n=2,3,\ldots,$

(3) $\hat{p}(N),\ N=2n,\ n=2,3,\ldots,$

respectively, as follows:

(1) $$f=(q^{-(2n-1)},q^{-(2n-3)},\ldots,q^{-1},1,q,\ldots,q^{(2n-3)},q^{(2n-1)})(\text{diag}), \tag{5.4}$$

(2) $$f=(q^{-(2n-2)},q^{-(2n-4)},\ldots,q^{-2},1,1,q^2,\ldots,q^{(2n-4)},q^{(2n-2)})(\text{diag}), \tag{5.5}$$

(3) $$f=(q^{-2n},q^{-(2n-2)},\ldots,q^{-2},q^2,\ldots,q^{(2n-2)},q^{2n})(\text{diag}). \tag{5.6}$$

Note the following facts:

(1) The N diagonal elements of f, in each case, are the nonzero diagonal elements of the corresponding P_0' [related to the projector as $P_0=(trP_0')^{-1}P_0'$], the remaining $N(N-1)$ diagonal elements of P_0' being zero. Hence [with upper and lower signs for $\hat{o}(N)$ and $\hat{p}(N)$, respectively],

$$T\equiv trf = trP_0' = [N\mp 1]\pm 1 = -(\lambda_+ + \lambda_-) = e^{-\eta}+e^{\eta}, \tag{5.7}$$

where $e^{\pm\eta}$ are the roots of

$$e^{2\eta} - Te^{\eta} + 1 = 0. \tag{5.8}$$

(2) The $N^2\times N^2$ matrix $f\otimes f$, in each case, has 1 on rows *and* columns,

$$(N, 2N-1, 3N-2, \ldots, (N^2-N+1)).$$

These are precisely ones on which P_0' has nonzero elements. Hence directly (without further computations) we obtain

$$P_0' f \otimes f = f \otimes f P_0'. \tag{5.9}$$

(3) Using (1.17), (1.18), and (5.3) one obtains

$$tr_2(P_0' f \otimes f) = f. \tag{5.10}$$

Now from (5.9) and (5.10) it follows immediately,

$$\hat{R}^{\pm 1} f \otimes f = (I - e^{\mp \eta} P_0') f \otimes f = f \otimes f (I - e^{\mp \eta} P_0') = f \otimes f \hat{R}^{\pm 1} \tag{5.11}$$

and

$$tr_2(\hat{R}^{\pm 1} f \otimes f) = tr_2((I - e^{\mp \eta} P_0') f \otimes f) = (T - e^{\mp \eta}) f = e^{\pm \eta} f. \tag{5.12}$$

Hence

$$tr_2(\hat{R}^{\pm 1} f \otimes f) = a^{\pm 1} b f \quad (a = e^{\eta},\ b = 1). \tag{5.13}$$

Thus we have obtained for our $\hat{R}$, in terms of f introduced above, the enhanced operator

$$(\hat{R}, f, e^{\eta}, 1).$$

Our f is strictly analogous to those of Turaev for $\mathrm{SO}_q(2n+1)$, $\mathrm{SO}_q(2n)$, $\mathrm{Sp}_q(2n)$, respectively. But whereas for the standard cases a (α in the notation of Ref. 12) is also a simple power of q, for us it involves the square root of a Laurent polynomial in q. One obtains with $\delta = (1, 2, 0)$ for $\hat{o}(2n+1)$, $\hat{o}(2n)$, $\hat{p}(2n)$, respectively,

$$T = (q^{-2n+\delta} + q^{-2n-2+\delta} + \cdots + q^{2n+2-\delta} + q^{2n-\delta} + \delta) \tag{5.14}$$

and

$$a^{\pm 1} = e^{\pm \eta} = \tfrac{1}{2}(T \pm \sqrt{T^2 - 4}). \tag{5.15}$$

This is the crucial aspect for our class of $\hat{R}$. For the simplest case $\hat{o}(3)$ one obtains

$$a^{\pm 1} = \tfrac{1}{2}(q + 1 + q^{-1}) \pm \tfrac{1}{2}((q + 3 + q^{-1})(q - 1 + q^{-1}))^{\frac{1}{2}} \tag{5.16}$$

giving for $q = 1$,

$$a^{\pm 1} = \tfrac{3}{2} \pm \tfrac{1}{2}\sqrt{5}. \tag{5.17}$$

In general, for $q = 1$, as for the standard case f reduces to the $N \times N$ unit matrix but as emphasized before our $\hat{R}$ remains nontrivial and

$$a^{\pm 1} = \tfrac{1}{2}N \pm \tfrac{1}{2}\sqrt{N^2 - 4} \quad (N = 3, 4, \ldots). \tag{5.18}$$

The discussion of Sec. II shows that for solutions of (2.10),

$$\eta = 0, \quad a = 1, \tag{5.19}$$

implying a complex root of unity q for $N=3$ but finally elliptic and hyperelliptic ones as N increases. (Overcrossings and undercrossings degenerate for $\hat{R}=\hat{R}^{-1}$.)

[*Comparison of notations:* The present author is often confused by different significances of the same symbol (and vice versa) encountered elsewhere. The following points might be helpful in our context.

Turaev's R (Ref. 12) satisfying the braid equation (his Eq. 1),

$$R_1R_2R_1 = R_2R_1R_2,$$

is our $\hat{R}$. Our R is $P\hat{R}$, where

$$P(ij)\otimes(kl) = (kj)\otimes(il), \quad (ij)\otimes(kl)P = (il)\otimes(kj), \quad P(ij)\otimes(kl)P = (kl)\otimes(ij),$$

and R satisfies the Yang–Baxter equation,

$$R_{12}R_{13}R_{23} = R_{23}R_{13}R_{12}.$$

It must also be clearly noted that if σ (or τ) is defined as

$$\sigma(ij)\otimes(kl) = (kl)\otimes(ij) = P(ij)\otimes(kl)P,$$

then

$$\sigma R = PRP = R_{21} = \hat{R}P$$

does not satisfy the braid equation above (satisfied by $\hat{R}$). Moreover, since

$$P(f\otimes f)P = f\otimes f, \quad P^2 = I,$$

the condition (5.1) implies also (for the YB matrix R)

$$R^{\pm1}f\otimes f = f\otimes fR^{\pm1}.$$

This form is presented in Sec. 15.2.2 of Ref. 13. But $\hat{R}$ cannot be replaced by R in (5.2). The symbol I denotes σR in Sec. 15.2.2 of Ref. 13 and $-\sigma R$ at the end of Sec. 15.2.5.]

B. Link invariants and skein relation

We follow the presentation of Ref. 12 and Sec. 15 of Ref. 13 with some changes of notations. Let $\rho(\beta)$ be the representation of the braid β associated to $\hat{R}$ and let $\alpha(\beta)$ be the "augmentation homomorphism" changing by ±1 corresponding to the actions of $T^{\pm1}$, the generators of the braid group.

Define for our case (with $b=1$).

$$\mathsf{P}(\beta) = a^{-\alpha(\beta)}tr(\rho_m(\beta)\cdot f^{\otimes m}), \tag{5.20}$$

ρ_m being the endomorphism of $V^{\otimes m}$ associated to $\hat{R}$.

Using appropriately the properties (5.1) and (5.2) of f such a $\mathsf{P}(\beta)$ can be shown to be Markov invariant and provide an invariant of oriented links. Markov moves are defined, for example, in Sec. 15.1 of Ref. 13 and the proof of invariance of $\mathsf{P}(\beta)$ is given in Sec. 15.2 following Ref. 12.

For an "unknot" (no crossing) one has

$$\mathsf{P}(\circ) = tr\, f = T. \tag{5.21}$$

Using standard notations $(\overline{L_+},\overline{L_-},\overline{L_0})$ corresponding to one point of the projection of a braid differing by an overcrossing, undercrossing, and no crossing, respectively, one obtains in our case [following the steps below Eq. (6), Sec. 15.2 of Ref. 13]

$$x\mathsf{P}(\overline{L_+}) + y\mathsf{P}(\overline{L_-}) + z\mathsf{P}(\overline{L_0}) = a^{-\alpha(\beta)}tr((x\hat{R}^{-1} + y\hat{R} + zI) \otimes id^{\otimes 2} \otimes id^{\otimes(m-2)} \cdot \rho_m(\beta) \cdot f^{\otimes m}). \tag{5.22}$$

Now for our case,

$$e^{\eta}\hat{R} - e^{-\eta}\hat{R}^{-1} = (e^{\eta} - e^{-\eta})I. \tag{5.23}$$

Hence setting

$$x = -e^{-\eta}, \quad y = e^{\eta}, \quad z = -(e^{\eta} - e^{-\eta}) \tag{5.24}$$

one obtains the skein relation

$$e^{-\eta}\mathsf{P}(\overline{L_+}) - e^{\eta}\mathsf{P}(\overline{L_-}) = (e^{-\eta} - e^{\eta})\mathsf{P}(\overline{L_0}). \tag{5.25}$$

One can now exploit this relation along with (5.21) in well-known fashions to construct invariant polynomials. (See also Ref. 14 where a large number of sources are cited.) We will not present a full study of this aspect. Our aim has been to indicate the roles played by our coefficients $e^{\pm\eta}$ (an ingredient of our $\hat{R}$) in this context. This has been achieved in our brief treatment.

VI. FROM $\hat{R}$ TO NONCOMMUTATIVE SPACES

A. Coordinates, differentials, and mobile frames

We implement well-known prescriptions[15–17] in the context of our class of $\hat{R}$. For the $N^2 \times N^2$ matrix $\hat{R}$ satisfying

$$(\hat{R} - I)(\hat{R} + e^{-2\eta}I) = 0, \tag{6.1}$$

where for $\hat{o}(N)$, $\hat{p}(N)$, respectively,

$$e^{\eta} + e^{-\eta} = [N \mp 1] \pm 1,$$

let the coordinates $(x_1, x_2, \ldots, x_N)$ and the differentials $(\xi_1, \xi_2, \ldots, \xi_N)$ be ordered in N columns x and ξ, respectively.

The prescriptions for the associated covariant differential geometries satisfying the Leibnitz rule[15–17] are

$$(1) \qquad (\hat{R} - I)x \otimes x = 0, \quad x \otimes \xi = e^{2\eta}\hat{R}\xi \otimes x, \quad (\hat{R} + e^{-2\eta}I)\xi \otimes \xi = 0, \tag{6.2}$$

$$(2) \qquad (\hat{R} + e^{-2\eta}I)x \otimes x = 0, \quad x \otimes \xi = -\hat{R}\xi \otimes x, \quad (\hat{R} - I)\xi \otimes \xi = 0. \tag{6.3}$$

We concentrate below on (6.2). The set (6.3) can be treated analogously, essentially interchanging the roles of x and ξ [except for the (x, ξ) commutators].

From our previous definitions,

$$\hat{R} = I - e^{\mp\eta}P_0'.$$

Hence from (6.2),

$$P_0'x \otimes x = 0. \tag{6.4}$$

The set of constraints (6.4) reduces to a *single* one due to the proportionality of the nonzero rows of P_0'. This one is easy to write down for all N from (1.17) and (1.18). One obtains for

$$\hat{o}(3), \quad q^{-\frac{1}{2}}x_1x_3 + x_2x_2 + q^{\frac{1}{2}}x_3x_1 = 0, \tag{6.5}$$

$$\hat{o}(4), \quad q^{-1}x_1x_4 + x_2x_3 + x_3x_2 + qx_4x_1 = 0, \tag{6.6}$$

$$\hat{p}(4), \quad q^{-2}x_1x_4 + q^{-1}x_2x_3 - qx_3x_2 - q^2x_4x_1 = 0, \tag{6.7}$$

and so on. Consider now the constraints involving ξ with the $\hat{o}(3)$ case as example.

Define

$$\Pi = (q^{-\frac{1}{2}}\xi_1x_3 + \xi_2x_2 + q^{\frac{1}{2}}\xi_3x_1), \tag{6.8}$$

$$\Pi' = (q^{-\frac{1}{2}}\xi_1\xi_3 + \xi_2\xi_2 + q^{\frac{1}{2}}\xi_3\xi_1). \tag{6.9}$$

Now from (6.2) for $N=3$ with

$$e^{\eta} + e^{-\eta} = (q + 1 + q^{-1}),$$

one has

$$x_i\xi_j = e^{2\eta}\xi_ix_j \quad (i + j \neq 4), \tag{6.10}$$

$$x_1\xi_3 = e^{2\eta}\xi_1x_3 - e^{\eta}q^{-\frac{1}{2}}\Pi, \quad x_2\xi_2 = e^{2\eta}\xi_2x_2 - e^{\eta}\Pi, \quad x_3\xi_1 = e^{2\eta}\xi_3x_1 - e^{\eta}q^{\frac{1}{2}}\Pi, \tag{6.11}$$

$$\xi_i\xi_j = 0 \quad (i + j \neq 4), \tag{6.12}$$

$$q^{-\frac{1}{2}}\xi_1\xi_3 = y^{-1}q^{-1}\Pi', \quad \xi_2\xi_2 = y^{-1}\Pi', \quad q^{\frac{1}{2}}\xi_3\xi_1 = y^{-1}q\Pi', \quad y = (q + 1 + q^{-1}). \tag{6.13}$$

Note the consistency of the sum of the equations (6.13). For $N>3$,

$$\xi_i\xi_j = 0 \quad [i + j \neq (N + 1)]. \tag{6.14}$$

The coefficients of (Π, Π') are now obtained from (1.17) and (1.18), they are proportional to the nonzero elements in a row of P_0'. Also η will now be as below (6.1).

We now briefly consider the construction of mobile frames[17,18] (or "stehbeins" in the terminology of the authors cited). Let

$$\theta = \sum_i \theta_i\xi_i, \tag{6.15}$$

such that

$$[\theta, x_i] = 0. \tag{6.16}$$

From (6.2) and (6.16), remembering that in our conventions

$$\hat{R} = \hat{R}_{ij,kl}(ij) \otimes (kl)$$

and indicating all summations explicitly (and using the $L^{\pm}$ of Secs. III and IV),

$$\left(\sum_k \theta_k\xi_k\right)x_i = e^{-2\eta}\sum_{k,a,b} \theta_k\hat{R}^{-1}_{ka,ib}x_a\xi_b = e^{-2\eta}\sum_{k,a,b} \theta_k(\hat{R}^{-1}P)_{kb,ia}x_a\xi_b$$
$$= e^{-2\eta}\sum_{k,a,b} (\theta_kL^-_{kb,ia}x_a)\xi_b = x_i\left(\sum_b \theta_b\xi_b\right). \tag{6.17}$$

Hence

$$x_i\theta_j = e^{-2\eta}\sum_{k,l}\theta_k L^{-}_{kj,il}x_l. \tag{6.18}$$

Thus one obtains the commutators of (x_i,θ_j). For $N=3$, setting

$$\theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1 = \tau, \tag{6.19}$$

$$x_i\theta_i = e^{-2\eta}\tau - e^{-\eta}\theta_{i'}x_{i'} \quad (i=1,2,3),$$

$$x_1\theta_2 = -e^{-\eta}q^{\frac{1}{2}}\theta_3 x_2, \quad x_1\theta_3 = -e^{-\eta}\theta_3 x_1,$$

$$x_2\theta_1 = -e^{-\eta}q^{\frac{1}{2}}\theta_2 x_3, \quad x_2\theta_3 = -e^{-\eta}q^{-\frac{1}{2}}\theta_2 x_1,$$

$$x_3\theta_1 = -e^{-\eta}\theta_1 x_3, \quad x_3\theta_2 = -e^{-\eta}q^{-\frac{1}{2}}\theta_1 x_2. \tag{6.20}$$

Generalizations for $N>3$ are obtained analogously.

In Ref. 17 different solutions of θ [three solutions for $\mathrm{So}_q(3)$] are presented. They involve a dilatation operator and inverses of coordinates, a radius r being defined. We consider no extensions of our algebras or such solutions for θ in the present work.

B. Towers of noncommutative $(x_1,\ldots,x_N)$ on a commutative $(N-1)$-base space

In Eq. (1.3) of Ref. 4 it is pointed out that the mapping, implementing the transfer matrix t,

$$\delta(x_i) = \sum_k t_{ik}\otimes x_k \equiv (tx)_i \tag{6.21}$$

provides an iterative sequence of solutions. Since

$$\hat{R}(t\otimes I)(I\otimes t) = (t\otimes I)(I\otimes t)\hat{R} \tag{6.22}$$

for any polynomial of $f(\hat{R})$, if

$$f(\hat{R})(x\otimes x) = 0,$$

$$(t\otimes I)(I\otimes t)f(\hat{R})(x\otimes x) = f(\hat{R})(t\otimes I)(I\otimes t)(x\otimes x), \quad = f(\hat{R})(tx)\otimes(tx) = 0. \tag{6.23}$$

This is the mapping (6.21). It can evidently be iterated as

$$\delta((t^n x)\otimes(t^n x)) = (t^{n+1}x)\otimes(t^{n+1}x). \tag{6.24}$$

We denote this as

$$x^{(n)} \to x^{(n+1)}.$$

We note here a remarkable possibility, starting again with $\hat{o}(3)$ as an example.

Choose as the starting point a *commutative* solution of (6.5) as follows. With parameters $(a,b)\geqslant 0$ the following surface satisfies (6.5):

$$\begin{aligned} &x_1^{(0)} = a, \quad x_3^{(0)} = -b, \quad x_2^{(0)} = \pm\left((q^{\frac{1}{2}}+q^{-\frac{1}{2}})ab\right)^{\frac{1}{2}}, \\ &x_1^{(0)} = -a, \quad x_3^{(0)} = b, \quad x_2^{(0)} = \pm\left((q^{\frac{1}{2}}+q^{-\frac{1}{2}})ab\right)^{\frac{1}{2}}. \end{aligned} \tag{6.25}$$

As (a,b) varies through real, non-negative values one obtains a double cone whose projections on the (1,3) plane covers the second and the fourth quadrants. The vertices meet at the origin. The projections of the contours $x_2=$const on the (1,3) plane are parabolas. The origin is invariant under δ.

Now we implement δ as in (6.21) to obtain

$$x_i^{(1)} = (tx^{(0)})_i. \tag{6.26}$$

Consider for simplicity the 3×3 fundamental t-matrices. These are given by [compare (4.1) and see the reference cited above it]

$$t = t^+ = P\hat{R} = R = P(\hat{R}P)P = L_{21}^+ \tag{6.27}$$

and

$$t = t^- = P\hat{R}^{-1} = P(R^{-1}P) = (\hat{R}^{-1})_{21} = L_{21}^-. \tag{6.28}$$

We treat below $t^\pm$ together by setting correspondingly (for $N=3$)

$$\lambda = \lambda_\pm = \lambda^{\pm 1}, \quad (\lambda + \lambda^{-1} + y = 0). \tag{6.29}$$

For the fundamental representations of t our map gives

$$x_1^{(1)} = \begin{vmatrix} x_1^{(0)} & 0 & 0 \\ x_2^{(0)} & 0 & 0 \\ (1+q\lambda)x_3^{(0)} & q^{\frac{1}{2}}\lambda x_2^{(0)} & \lambda x_1^{(0)} \end{vmatrix}, \tag{6.30}$$

$$x_2^{(1)} = \begin{vmatrix} 0 & x_1^{(0)} & 0 \\ q^{\frac{1}{2}}\lambda x_3^{(0)} & (1+\lambda)x_2^{(0)} & q^{-\frac{1}{2}}\lambda x_1^{(0)} \\ 0 & x_3^{(0)} & 0 \end{vmatrix}, \tag{6.31}$$

$$x_3^{(1)} = \begin{vmatrix} \lambda x_3^{(0)} & q^{-\frac{1}{2}}\lambda x_2^{(0)} & (1+q^{-1}\lambda)x_1^{(0)} \\ 0 & 0 & x_2^{(0)} \\ 0 & 0 & x_3^{(0)} \end{vmatrix}. \tag{6.32}$$

The symmetries signalled above (4.4) reappear. Iteration now may proceed as

$$(x_i^{(0)}, x_i^{(1)}) \to (x_i^{(n)}, x_i^{(n+1)}).$$

At each stage, given *only* (6.5) for $x_i^{(n)}$ [and (6.29) for λ], $x_i^{(n+1)}$ also satisfies (6.5) and hence

$$(\hat{R} - I)x^{(n+1)} \otimes x^{(n+1)} = 0. \tag{6.33}$$

This has been verified explicitly. Moreover at each stage one can implement any chosen representation of t (say, the 9×9 rather than the 3×3). Thus one may obtain varied sequences in the iterations. The illustration above is sufficient for our purpose. Let us compare this construction with a parallel possibility for $SO_q(3)$. We refer to the results of Example 4.1.22 of Ref. 17. But for easier comparison with our results above we change the basis from the circular components to our type as

$$(x_-, y, x_+) \to (x_1, x_2, x_3).$$

Now (4.1.61) of Ref. 17 is

$$x_1x_2 = qx_2x_1, \quad x_3x_2 = q^{-1}x_2x_3, \quad (x_3x_1 - x_1x_3) = (q^{\frac{1}{2}} - q^{-\frac{1}{2}})x_2^2. \tag{6.34}$$

There are now three constraints as compared to a single one for (6.5). But one can choose the *commutative* (1, 3) plane (as compared to the double cone before) as the starting point by setting

$$x_2^{(0)} = 0, \quad x_1^{(0)}x_3^{(0)} = x_3^{(0)}x_1^{(0)}. \tag{6.35}$$

This satisfies all three constraints (6.34). Using the 3×3 t-matrix blocks for $SO_q(3)$ [and setting $\kappa=(q-q^{-1})$] one obtains

$$x_1^{(n+1)} = \begin{vmatrix} qx_1^{(n)} & 0 & 0 \\ 0 & x_1^{(n)} & 0 \\ 0 & 0 & q^{-1}x_1^{(n)} \end{vmatrix}, \tag{6.36}$$

$$x_2^{(n+1)} = \begin{vmatrix} x_2^{(n)} & \kappa x_1^n & 0 \\ 0 & x_2^{(n)} & q^{-\frac{1}{2}}\kappa x_1^n \\ 0 & 0 & x_2^{(n)} \end{vmatrix}, \tag{6.37}$$

$$x_3^{(n+1)} = \begin{vmatrix} q^{-1}x_3^{(n)} & q^{-\frac{1}{2}}\kappa x_2^n & \kappa(1-q^{-1})x_1^n \\ 0 & x_3^{(n)} & \kappa x_2^n \\ 0 & 0 & qx_3^{(n)} \end{vmatrix}. \tag{6.38}$$

Starting the iteration from (6.35) at each step x_i^n satisfies (6.34). As before one can use more general realizations of the t-matrix at any step. One may note that for this case

$$(q=1) \to x_i^{(n+1)} = I_3 \otimes x_i^{(n)}.$$

This is consistent with $\hat{R}=I$ for $q=1$ in the standard cases. But, as emphasized before, there is no such triviality for our class for any value of q (including 1). Note also that for our class the matrices $x_i^{(1)}$ and the iterated ones are noninvertible. This is a general feature for our class.

In the examples above one *starts* with a classical surface and iterating as above makes it more and more "fuzzy" in this specific sense. This should be compared with the "fuzzy sphere" of Ref. 17 (Sec. 7.2) where one starts fuzzy and a smooth surface is approached as a limit. One moves in opposite senses in the two formalisms.

So far we have studied the coordinate space (x_i) only. It must be noted carefully that one cannot obtain a consistent nontrivial set $\xi_i^{(0)}$ corresponding to $x_i^{(0)}$. This is evident from (6.10) to (6.13) where q is not restricted. So the whole covariant prescription can be introduced at a noncommutative stage only. This however does not alter the fact that one can build sequences of noncommutative (x_i) starting from a smooth surface.

For $N>3$, with (6.6) and (6.7) as simplest examples, one has evidently more flexibility in choosing $\xi_i^{(0)}$. Without going into details we indicate below for $\hat{o}(4)$ the stuctures (valid more generally) induced by our type of iterations,

$$\hat{o}(4), \quad \lambda + \lambda^{-1} + (q^2 + 2 + q^{-2}) = 0,$$

$$x_1^{(n+1)} = \begin{vmatrix} x_1^{(n)} & 0 & 0 & 0 \\ x_2^{(n)} & 0 & 0 & 0 \\ x_3^{(n)} & 0 & 0 & 0 \\ (1+\lambda)x_4^{(n)} & q^{-1}\lambda x_3^{(n)} & q^{-1}\lambda x_2^{(n)} & q^{-2}\lambda x_1^{(n)} \end{vmatrix}, \tag{6.39}$$

$$x_2^{(n+1)} = \begin{vmatrix} 0 & x_1^{(n)} & 0 & 0 \\ 0 & x_2^{(n)} & 0 & 0 \\ q\lambda x_4^{(n)} & (1+\lambda)x_3^{(n)} & \lambda x_2^{(n)} & q^{-1}\lambda x_1^{(n)} \\ 0 & x_4^{(n)} & 0 & 0 \end{vmatrix}, \tag{6.40}$$

$$x_3^{(n+1)} = \begin{vmatrix} 0 & 0 & x_1^{(n)} & 0 \\ q\lambda x_4^{(n)} & \lambda x_3^{(n)} & (1+\lambda)x_2^{(n)} & q^{-1}\lambda x_1^{(n)} \\ 0 & 0 & x_3^{(n)} & 0 \\ 0 & 0 & x_4^{(n)} & 0 \end{vmatrix}, \tag{6.41}$$

$$x_4^{(n+1)} = \begin{vmatrix} q^2\lambda x_4^{(n)} & q\lambda x_3^{(n)} & q\lambda x_2^{(n)} & (1+\lambda)x_1^{(n)} \\ 0 & 0 & 0 & x_2^{(n)} \\ 0 & 0 & 0 & x_3^{(n)} \\ 0 & 0 & 0 & x_4^{(n)} \end{vmatrix}. \tag{6.42}$$

The analogous structures for $\hat{p}(4)$ have also been obtained. The structures of the matrices are quite similar to those for $\hat{o}(4)$. The q dependence of the coefficients show typical differences along with sign changes. They will not be reproduced here. In each case, for all N, there is in each matrix one row and one column with nonzero elements. How they shift with i of $x_i^{(n)}$ should already be fairly apparent from the two preceding examples.

VII. REMARKS

We have started to explore the contents of a class of braid matrices presented previously. Unsurprisingly our study remains incomplete in all directions. We briefly indicate below perspectives of further developments.

For the standard cases (q-deformed unitary and orthogonal algebras) we have studied extensively elsewhere representations for q a root of unity.[19,20] (These two references cite many other sources.) We introduced "the method of fractional parts" for this purpose. Here we have noted (Sec. II) how certain roots of unity give triangularity ($\hat{R}^2 = I$) for different dimensions. A study of our L-algebras for such cases along similar lines can be of interest.

Our other solutions for triangularity involve elliptic aand hyperelliptic q with integer (binomial) coefficients in the defining equations. The roles of such functions deserve further explorations. Higher genus curves have appeared before[21,22] in the construction of statistical models as solutions of star–triangle (or Yang–Baxter) relations. There such curves are necessary ingredients of the solutions. In our case the situation is quite different. Our class of braid matrices have been obtained for *any* q. One can even set $q=1$ and still have interesting solutions. Our special values of q appear only when the additional constraint of triangularity is imposed and depend on the dimension N.

We have obtained some important general features of our L-algebras [see, for example, the equations from (3.11) to (3.18)]. But the explicit study of realizations is limited to 3×3 and 9×9 ones for $\hat{o}(3)$. This has already shown the crucial role of the central, grouplike elements we have constructed, thus achieving a principal goal. But a more general study of the L-algebras is desirable. Quadratic[23] and higher degree[24] homogenous algebras have been studied from a functional point of view yielding, for example, the Poincare series. (More sources are cited in Ref. 24.) The Poincare series for our algebra would show whether, and if so what, irreducible representations interpolate the $N^{2^p}\times N^{2^p}$ dimensional coproduct representations (corresponding, as pointed out in Sec. IV, to the central $\hat{S}_3$ elements proportional to $I_{N^{2^p}}$) obtained by iterating the coproduct prescription. We are unable to answer this question definitively at present, although attempts to

realize intermediate dimensional ones (between 3×3 and 9×9) exploiting the symmetries pointed out in Sec. IV seem to encounter obstructions. Our detailed study of the 9×9 case gives an idea of the features to be expected more generally.

The Turaev construction for link invariants turns out to be elegantly adaptable to our case. Systematic construction of invariant polynomials and possibility of generalizations to invariants of three-manifolds will be studied elsewhere.

Noncommutative geometries associated with our $\hat{R}$ have been presented indicating possible constructions of "noncommutative towers" on classical base spaces of dimensions $<N$. Here again a deeper study of the differential geometries remains to be done. Possible roles of our special values of q corresponding to triangularity should be interesting to explore in this context.

It follows from (1.10) or (3.41) along with (1.17) that for $\hat{o}(N)$, real positive q and

$$-\eta<\theta<0,$$

the elements of $\hat{R}(\theta)$ are all non-negetive (either zero or real positive). Hence such an $\hat{R}(\theta)$ along with the corresponding transfer matrix $t(\theta)$ [obtainable from $\hat{R}(\theta)$] can furnish the basis of a multistate statistical model. The elements of $\hat{R}(\theta)$ provide the Boltzmann weights. This class of model will be studied in a following paper.

The prescription (2.11) corresponds to real η. But the value $i\pi$ of η with -2 in (2.11) is also a solution with evident corresponding shifts for the right hand sides of two following equations. We will not discuss these cases separately here.

Our P_0 can easily be shown to lead to a Temperley-Lieb algebra. Constructions from this point of view citing numerous sources can be found in Ref. 25. Since in our case P_0 is already given (and well-known) we solve for the coefficient η in terms of the q appearing in P_0. Solving for the elements of P_0 in terms of the parameter of the coefficient (as is done in the approach of Ref. 25 and in the sources cited here) would have been impossibly complicated. Our excercise in Sec. II, for particularly simple case ($\eta=0$) gives an idea.

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Commutation relations for functions of operators

Mark K. Transtrum[a] and Jean-François S. Van Huele[b]
Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602

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We derive an expression for the commutator of functions of operators with constant commutations relations in terms of the partial derivatives of these functions. This result extends the well-known commutation relation between one operator and a function of another operator. We discuss the range of applicability of the formula with examples in quantum mechanics. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1924703]

I. INTRODUCTION

A characteristic feature of quantum theory is the appearance of noncommuting operators. It is perhaps most conspicuous in one-dimensional quantum mechanics where the position and momentum operators obey the canonical commutation relation

$$[x,p] \equiv xp - px = i\hbar. \tag{1}$$

In the coordinate representation of wave mechanics where the position operator x is realized by x multiplication and the momentum operator p by $\hbar/i$ times the derivation with respect to x, one can easily check that the canonical commutation relation Eq. (1) is identically satisfied by applying the commutation operator on a test wave function $\psi(x)$,

$$[x,p]\psi(x) = x\frac{\hbar}{i}\frac{\mathrm{d}\psi(x)}{\mathrm{d}x} - \frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}(x\psi(x)) = \frac{\hbar}{i}x\psi'(x) - \frac{\hbar}{i}\psi(x) - \frac{\hbar}{i}x\psi'(x) = i\hbar\psi(x). \tag{2}$$

For quantum mechanics in three-dimensional space the commutation relations are generalized to

$$[x_i,p_j] = i\hbar\delta_{i,j} \tag{3}$$

and augmented with new commutation relations

$$[x_i,x_j] = [p_i,p_j] = 0, \tag{4}$$

expressing the independence of the coordinates and of the momenta in the different dimensions.

When independent quantum mechanical systems are combined to form larger systems such as multiparticle systems, the commutation rules for the operators within the individual systems are preserved and augmented with vanishing commutation relations for operators acting on the different systems. Tensor products of the quantum mechanical spaces and of the operators that operate on them accommodate this extension naturally.

In the Heisenberg picture of quantum mechanics where the operators carry the time dependence of the system under consideration, the evolution of an individual operator A is determined by its commutator with the Hamiltonian operator H, the generator of the time evolution:

[a]Electronic mail: mktranstrum@hotmail.com
[b]Electronic mail: vanhuele@byu.edu

$$\frac{dA}{dt} = \frac{1}{i\hbar}[A,H] = 0. \tag{5}$$

Depending on the specific expression of the operators A and H in terms of the position and momentum operators, the evaluation of the commutators in a set of equations like Eq. (5) can become quite involved with implications on the integrability of the resulting differential equations.

The importance of evaluating commutators in quantum mechanics and the corresponding problem in quantum field theory is illustrated by the vast literature on the subject. Many sources and textbooks in quantum mechanics, starting with Dirac's seminal text [Dirac (1958)], state the canonical commutation relations either by postulating them, or by deriving them from their classical analogs, the canonical Poisson brackets, and then go on to show that they imply the following commutation between the position operator x and any reasonable function of the momentum operator $f(p)$:

$$[x, f(p)] = i\hbar f'(p) \tag{6}$$

and its symplectic twin

$$[p, f(x)] = -i\hbar f'(x), \tag{7}$$

where the ($'$) symbol denotes differentiation with respect to the variable. The derivation of Eqs. (6) and (7) is a typical and almost obligatory exercise in a modern text on quantum mechanics. The standard way of proceeding is to consider the commutator of x with increasing powers of p, to use induction, and to develop a Taylor expansion of the function f.

It may come as a surprise therefore that a further generalization of Eqs. (6) and (7) is never given. In fact we were not able to find an expression for the commutator of a function of x with a function of p in the literature. The present paper provides such an expression [Eq. (18) below when applied to $x_1 = x$ and $x_2 = p$] and goes a few steps further by giving the general commutator for functions of an arbitrary number of operators, with the restriction that all these operators have known commutation relations amongst themselves and that their commutators do not involve further operators (q-numbers) but only constants (c-numbers). To be specific, our formula does apply to functions of standard position and momentum operators in multiple dimensions and for multiple particles, as well as for functions of multiple raising and lowering (creation and annihilation) ladder operators, but it does not generally apply, for example, to functions of angular momentum operators. When dealing with angular momentum operators, one would need to reexpress them as functions of position and momentum, and then apply the formula to those operators directly. It does apply to functions of noncommuting position and momentum operators as considered in noncommutative space–time extensions of quantum theory [Snyder (1947), Jackiw (2001)] but only to the extent that the noncommutative operators obey constant, i.e., c-number, commutation relations.

In this paper, our approach to the problem is constructive. We state our general result first, consider simple cases, make use of the induction process, and proceed by generalization. Unless otherwise noted, we assume that the functions of the operators are well behaved in the sense that they can be expanded in Taylor series. In Sec. V we comment on the applicability of the formulas and give specific examples. In the Appendix we discuss correlations in the values of some summation indices that appear in our formulas and on the notation we developed to accommodate them.

II. ASSUMPTIONS

We begin by stating the definition of the commutator and list two properties that follow directly from this definition. The definition of the commutator, Eq. (8), linearity, Eq. (9), and Leibnitz's rule, Eq. (10), will all be used explicitly in our derivations

$$[A,B] = AB - BA, \tag{8}$$

$$[A,\alpha B + C] = \alpha[A,B] + [A,C], \tag{9}$$

$$[AB,C] = A[B,C] + [A,C]B. \tag{10}$$

In addition to the above-noted relations, we will use a third, well-known commutator relation between an operator and a function of another operator. Given two operators x_1 and x_2 with a constant commutation relation c, such that $[x_1,x_2]=c$, it can be shown that

$$[x_1, f(x_2)] = cf'(x_2), \tag{11}$$

where $f(x_2)$ is an analytic function with a Taylor expansion. We will accept this relation here and refer to our introductory section or to a text on quantum mechanics, e.g., Merzbacher (1998), for an outline of its derivation. For the canonical position and momentum in quantum mechanics, the constant c takes the value $i\hbar$.

III. GENERAL RESULT

The most general result that we present in this paper involves the commutator of two functions of an arbitrary number of operators. Given n operators $x_1,\ldots,x_n$ such that $[x_i,x_j]=c_{ij}$, where c_{ij} are c-numbers, we will show that

$$[f(x_1,\ldots,x_n),g(x_1,\ldots,x_n)] = \underbrace{\sum_{k_{1,2}}\sum_{k_{1,3}}\sum_{k_{2,3}}\cdots\sum_{k_{n-1,n}}}\left(\prod_{j=2}^{n}\prod_{i=1}^{j-1}\frac{(-c_{ij})^{k_{ij}}}{k_{ij}!}\right) \times (\partial_{x_1}^{k_1}\ldots\partial_{x_n}^{k_n}g\partial_{x_1}^{k_1'}\ldots\partial_{x_n}^{k_n'}f - \partial_{x_1}^{k_1}\ldots\partial_{x_n}^{k_n}f\partial_{x_1}^{k_1'}\ldots\partial_{x_n}^{k_n'}g), \tag{12}$$

where

$$k_i = \sum_{j=i+1}^{n} k_{ij} \tag{13}$$

and

$$k_i' = \sum_{j=1}^{i-1} k_{ji}. \tag{14}$$

The index of each summation ranges from zero to infinity ($i=0-\infty$) with the restriction that the indices within the underbrace ($\underbrace{\ }$) are not all simultaneously zero. We will use the underbrace throughout the paper to indicate this restriction. We refer to the Appendix for a further discussion of the summation indices and the underbrace. We notice that only dummy indices k_{ij} with $i<j$ appear in the summation.

If the restriction that the indices cannot be simultaneously zero did not apply, there would be a term with no partial derivatives on the right-hand side of Eq. (12). That term would be $gf-fg=[g,f]=-[f,g]$. Therefore, an equivalent statement of Eq. (12) reads

$$\sum_{k_{1,2}=0}^{\infty}\sum_{k_{1,3}=0}^{\infty}\sum_{k_{2,3}=0}^{\infty}\cdots\sum_{k_{n-1,n}=0}^{\infty}\left(\prod_{j=2}^{n}\prod_{i=1}^{j-1}\frac{(-c_{ij})^{k_{ij}}}{k_{ij}!}\right)(\partial_{x_1}^{k_1}\ldots\partial_{x_n}^{k_n}g\partial_{x_1}^{k_1'}\ldots\partial_{x_n}^{k_n'}f - \partial_{x_1}^{k_1}\ldots\partial_{x_n}^{k_n}f\partial_{x_1}^{k_1'}\ldots\partial_{x_n}^{k_n'}g) = 0. \tag{15}$$

We will derive the generalized commutation relation Eq. (12), and we note that Eq. (15) is an equivalent, more compact statement that does not contain commutators of functions explicitly.

All the results presented in this paper are special cases of this general result. We derive the result by constructing increasingly complex intermediate results in Sec. IV.

IV. DERIVATIONS

We start by looking at the effect of increasing the power of x_1 in Eq. (11),

$$[x_1^2, f(x_2)] = [x_1, f(x_2)]x_1 + x_1[x_1, f(x_2)]$$
$$= cf'(x_2)x_1 + x_1 cf'(x_2) = 2cx_1 f'(x_2) - c[x_1, f'(x_2)] = 2cx_1 f'(x_2) - c^2 f''(x_2). \quad (16)$$

We next show by induction that this result can be extended to an arbitrary power n,

$$[x_1^n, f(x_2)] = \sum_{k=1}^{n} (-1)^{k+1} \binom{n}{k} c^k x_1^{n-k} f^{(k)}(x_2). \quad (17)$$

Proof of Eq. (17): Equations (11) and (16) correspond to the cases $n=1$ and $n=2$ of the result to be derived. We consider a general n and expand the commutator using Leibnitz's rule applied to $x_1^n = x_1 x_1^{n-1}$:

$$[x_1^n, f(x_2)] = x_1[x_1^{n-1}, f(x_2)] + [x_1, f(x_2)]x_1^{n-1}$$
$$= \sum_{k=1}^{n-1} (-1)^{k+1} \binom{n-1}{k} c^k x_1^{n-k} f^{(k)}(x_2) + cf'(x_2)x_1^{n-1} = \sum_{k=1}^{n-1} (-1)^{k+1} \binom{n-1}{k} c^k x_1^{n-k} f^{(k)}(x_2)$$
$$+ cx_1^{n-1} f'(x_2) - \sum_{k=1}^{n-1} (-1)^{k+1} \binom{n-1}{k} c^{k+1} x_1^{n-1-k} f^{(k+1)}(x_2) = ncx_1^{n-1} f'(x_2)$$
$$+ \sum_{k=2}^{n-1} (-1)^{k+1} \binom{n-1}{k} c^k x_1^{n-k} f^{(k)}(x_2) + \sum_{k=2}^{n-1} (-1)^{k+1} \binom{n-1}{k-1} c^k x_1^{n-k} f^{(k)}(x_2)$$
$$+ (-1)^{n+1} c^n f^{(n)}(x_2) = \sum_{k=1}^{n} (-1)^{k+1} \binom{n}{k} c^k x_1^{n-k} f^{(k)}(x_2).$$

In the third line we used the identity $f'(x_2)x_1^{n-1} = x_1^{n-1} f'(x_2) - [x_1^{n-1}, f'(x_2)]$, and in the fourth line we have redefined the index of the second summation to range from two to $n-1$ and have written the nth term outside the summation. In the final line we have combined all terms under a single summation. This completes the proof of Eq. (17).

We now extend the left argument of the commutator to include an analytic function of x_1 and proceed by considering its Taylor expansion

$$[f(x_1), g(x_2)] = \left[\sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0) x_1^n, g(x_2) \right]$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0)[x_1^n, g(x_2)] = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0) \sum_{k=1}^{n} \binom{n}{k} (-1)^{(k+1)} c^k x_1^{n-k} g^{(k)}(x_2).$$

Interchanging the order of the summations, we find that we can write the result in terms of derivatives of the original function, $f(x_1)$. The result is

$$[f(x_1), g(x_2)] = -\sum_{k=1}^{\infty} \frac{(-c)^k}{k!} f^{(k)}(x_1) g^{(k)}(x_2). \quad (18)$$

We pause to comment on this new result. The double summation introduced by the Taylor expansions has been reduced to a single sum. Somehow in the expression for the commutator of

the two functions only the contributions from products of identical orders of derivatives survive. In a quantum mechanical context we see that the powers of position and momentum decrease simultaneously and make room for factors of $i\hbar$ factors as required by dimensional analysis.

We will now consider two analytic functions of two operators, $f(x_1,x_2)$ and $g(x_1,x_2)$. We want to write these as some expansion. We could use the one-dimensional Taylor expansion in x_1 and write

$$f(x_1,x_2) = \sum_{n=0}^{\infty} \phi_n(x_2) x_1^n,$$

where the coefficients are now functions of the operator x_2. Instead, we simply observe that expansions exist (either as Taylor series or otherwise) and write them generally as

$$f(x_1,x_2) = \sum_{n=0}^{\infty} \phi_n(x_2) f_n(x_1) \tag{19}$$

and

$$g(x_1,x_2) = \sum_{m=0}^{\infty} \gamma_m(x_2) g_m(x_1). \tag{20}$$

Since x_1 and x_2 do not commute we have made a choice in Eqs. (19) and (20) in writing all the x_2-dependence to the left of the x_1-dependence in every term in the sum. The ordering does affect the explicit expression for ϕ_n and γ_m but the final result can be obtained no matter what ordering is chosen. What matters is that one choice has been made and will be used consistently throughout the derivation. The final result will be formally independent of the specific choice of ϕ_n, f_n, γ_n, and g_n and will be expressed in terms of $f(x_1,x_2)$ and $g(x_1,x_2)$ only.

Now we can consider the commutator:

$$\begin{aligned}[f(x_1,x_2),g(x_1,x_2)] &= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} [\phi_n(x_2) f_n(x_1), \gamma_m(x_2) g_m(x_1)] \\ &= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} (\phi_n(x_2)\gamma_m(x_2)[f_n(x_1),g_m(x_1)] + \phi_n(x_2)[f_n(x_1),\gamma_m(x_2)]g_m(x_1) \\ &\quad + [\phi_n(x_2),\gamma_m(x_2)]g_m(x_1) f_n(x_1) + \gamma_m(x_2)[\phi_n(x_2),g_m(x_1)]f_n(x_1))\end{aligned}$$

and notice that simplification occurs because the commutators of two functions of the same operator vanish, resulting in

$$[f(x_1,x_2),g(x_1,x_2)] = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} (\phi_n(x_2)[f_n(x_1),\gamma_m(x_2)]g_m(x_1) + \gamma_m(x_2)[\phi_n(x_2),g_m(x_1)]f_n(x_1)).$$

Now we are in a position to apply Eq. (18) for two functions of a single operator each

$$\begin{aligned}[f(x_1,x_2),g(x_1,x_2)] = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} &\left(\phi_n(x_2)\left(-\sum_{k=1}^{\infty} \frac{(-c)^k}{k!} f_n^{(k)}(x_1)\gamma_m^{(k)}(x_2)\right) g_m(x_1) \right. \\ &\left. + \gamma_m(x_2)\left(\sum_{k=1}^{\infty} \frac{(-c)^k}{k!} g_m^{(k)}(x_1)\phi_n^{(k)}(x_2)\right) f_n(x_1)\right).\end{aligned}$$

Interchanging the order of the summations and factoring without commuting, we obtain

$$[f(x_1,x_2),g(x_1,x_2)] = -\sum_{k=1}^{\infty}\left(\frac{(-c)^k}{k!}\sum_{n=0}^{\infty}\phi_n(x_2)f_n^{(k)}(x_1)\sum_{m=0}^{\infty}\gamma_m^{(k)}(x_2)g_m(x_1)\right) + \sum_{k=1}^{\infty}\left(\frac{(-c)^k}{k!}\sum_{m=0}^{\infty}\gamma_m(x_2)g_m^{(k)}(x_1)\sum_{n=0}^{\infty}\phi_n^{(k)}(x_2)f_n(x_1)\right).$$

We now observe that the original function can be reassembled

$$\sum_{n=0}^{\infty}\phi_n(x_2)f_n^{(k)}(x_1) = \frac{\partial^k}{\partial x_1^k}\left(\sum_{n=0}^{\infty}\phi_n(x_2)f_n(x_1)\right) = \frac{\partial^k}{\partial x_1^k}f(x_1,x_2) \tag{21}$$

with similar formulas for partial derivatives of f with respect to x_2, and for g with respect to x_1 and x_2 and conclude that

$$[f(x_1,x_2),g(x_1,x_2)] = \sum_{k=1}^{\infty}\frac{(-c)^k}{k!}\left(\frac{\partial^k g}{\partial x_1^k}\frac{\partial^k f}{\partial x_2^k} - \frac{\partial^k f}{\partial x_1^k}\frac{\partial^k g}{\partial x_2^k}\right). \tag{22}$$

In Eq. (22) we have omitted the arguments of the functions from the expression for brevity. We will continue to do so wherever there is no ambiguity in the arguments of the functions.

Before we can derive our formula for two functions of an arbitrary number of operators, we must prove one more formula giving the commutator of a function of an arbitrary number of operators and a function of one operator.

Given $n-1$ operators x_i, $i=1\ldots(n-1)$ that each have a constant commutation relation with another given operator x_n, such that $[x_i,x_n]=c_{in}$ then

$$[f(x_1,\ldots,x_{n-1}),g(x_n)] = -\underbrace{\sum_{k_1}\cdots\sum_{k_{n-1}}}\left(\prod_{i=1}^{n-1}\frac{(-c_{in})^{k_i}}{k_i!}\right)(\partial_{x_1}^{k_1}\ldots\partial_{x_{n-1}}^{k_{n-1}}f\partial_{x_n}^{k}g), \tag{23}$$

where

$$k = \sum_{i=1}^{n-1}k_i.$$

We prove Eq. (23) by induction.

For $n=2$ Eq. (23) becomes

$$[f(x_1\ldots x_{n-1},g(x_n)] = -\underbrace{\sum_{k_1}}\left(\prod_{i=1}^{1}\frac{(-c_{1,2})^{k_i}}{k_i!}\right)\partial_{x_1}^{k_1}f\partial_{x_2}^{k}g = -\sum_{k=1}^{\infty}\frac{(-c_{1,2})^k}{k!}\partial_{x_1}^{k}f\partial_{x_2}^{k}g$$

which we recognize as equivalent to Eq. (18), derived earlier.

Now we consider an arbitrary n and, in analogy with Eq. (19), write

$$f(x_1,\ldots,x_{n-1}) = \sum_{m=0}^{\infty}\phi_m(x_{n-1})f_m(x_1,\ldots,x_{n-2}).$$

We expand the commutator using Leibnitz's rule to obtain

$$[f,g] = \sum_{m=0}^{\infty}(\phi_m[f_m,g] + [\phi_m,g]f_m).$$

We evaluate the first commutator using Eq. (23) since the left argument is now a function of $n-2$ operators. We evaluate the second commutator using Eq. (18). The result is

$$[f,g] = -\sum_{m=0}^{\infty}\left(\phi_m \underbrace{\sum_{k_1}\cdots\sum_{k_{n-2}}}\left(\prod_{i=1}^{n-2}\frac{(-c_{in})^{k_i}}{k_i!}\right)\partial_{x_1}^{k_1}\cdots\partial_{x_{n-2}}^{k_{n-2}} f_m \partial_{x_n}^{k} g\right) - \sum_{m=0}^{\infty}\sum_{k_{n-1}=1}^{\infty}\frac{(-c_{n-1,n})^{\kappa_{n-1}}}{k_{n-1}!}(\partial_{x_{n-1}}^{k_{n-1}}\phi_m)(\partial_{x_n}^{k_{n-1}} g) f_m \tag{24}$$

where

$$k = \sum_{i=1}^{n-1} k_i. \tag{25}$$

In the second term we apply the definition of the commutator Eq. (8) and Eq. (23) since again it involves a function of $n-2$ operators,

$$(\partial_{x_n}^{k_{n-1}} g) f_m = f_m(\partial_{x_n}^{k_{n-1}} g) + \underbrace{\sum_{k_1}\cdots\sum_{k_{n-2}}}\left(\prod_{i=1}^{n-2}\frac{(-c_{in})^{k_i}}{k_i!}\right)(\partial_{x_1}^{k_1}\cdots\partial_{x_{n-2}}^{k_{n-2}} f_m)(\partial_{x_n}^{k} g) \tag{26}$$

In the last term, we have used k defined in Eq. (25). Substituting this into Eq. (24) we have

$$\begin{aligned}[f,g] = &-\sum_{m=0}^{\infty}\left(\phi_m \underbrace{\sum_{k_1}\cdots\sum_{k_{n-2}}}\left(\prod_{i=1}^{n-2}\frac{(-c_{in})^{k_i}}{k_i!}\right)(\partial_{x_1}^{k_1}\cdots\partial_{x_{n-2}}^{k_{n-2}} f_m)(\partial_{x_n}^{k} g)\right) - \sum_{m=0}^{\infty}\left(\sum_{k_{n-1}=1}^{\infty}\left(\frac{(-c_{n-1,n})^{k_{n-1}}}{k_{n-1}!}\right)\right.\\ &\left.\times(\partial_{x_{n-1}}^{k_{n-1}}\phi_m) f_m(\partial_{x_n}^{k_{n-1}} g)\right) - \sum_{m=0}^{\infty}\underbrace{\sum_{k_1}\cdots\sum_{k_{n-2}}}\sum_{k_{n-1}=1}^{\infty}\left(\prod_{i=1}^{n-2}\frac{(-c_{in})^{k_i}}{k_i!}\right)\left(\frac{(-c_{n-1,n})^{k_{n-1}}}{k_{n-1}!}\right)\\ &\times(\partial_{x_{n-1}}^{k_{n-1}}\phi_m)\ (\partial_{x_1}^{k_1}\cdots\partial_{x_{n-2}}^{k_{n-2}} f_m)(\partial_{x_n}^{k} g).\end{aligned} \tag{27}$$

Since all terms contain derivatives of ϕ_m next to derivatives of f_m, we can eliminate the summation over m by using the observation made in Eq. (21) and write Eq. (27) in terms of the original function f. We also combine factors

$$\left(\prod_{i=1}^{n-2}\frac{(-c_{in})^{k_i}}{k_i!}\right)\left(\frac{(-c_{n-1,n})^{k_{n-1}}}{k_{n-1}!}\right) = \prod_{i=1}^{n-1}\frac{(-c_{in})^{k_i}}{k_i!}$$

to get

$$\begin{aligned}[f,g] = &-\underbrace{\sum_{k_1}\cdots\sum_{k_{n-2}}}\left(\prod_{i=1}^{n-2}\frac{(-c_{in})^{k_i}}{k_i!}\right)(\partial_{x_1}^{k_1}\cdots\partial_{x_{n-2}}^{k_{n-2}} f)(\partial_{x_n}^{k} g) - \sum_{k_{n-1}=1}^{\infty}\left(\frac{(-c_{n-1,n})^{k_{n-1}}}{k_{n-1}!}\right)(\partial_{x_{n-1}}^{k_{n-1}} f)(\partial_{x_n}^{k_{n-1}} g)\\ &-\underbrace{\sum_{k_1}\cdots\sum_{k_{n-2}}}\sum_{k_{n-1}=1}^{\infty}\left(\prod_{i=1}^{n-1}\frac{(-c_{in})^{k_i}}{k_i!}\right)(\partial_{x_1}^{k_1}\cdots\partial_{x_{n-2}}^{k_{n-2}}\partial_{x_{n-1}}^{k_{n-1}} f)(\partial_{x_n}^{k} g)\end{aligned} \tag{28}$$

We observe that in the first term, the indices of the summations are not simultaneously zero. In the last term, the first $n-2$ indices are not simultaneously zero. Thus, the first term corresponds to the case $k_{n-1}=0$. The second term is the case in which $k_1 \ldots k_{n-2}$ are simultaneously zero, and the third term is the case in which the indices of neither group are simultaneously zero. Therefore, these three terms can be collected into one term as we elaborate in the Appendix. This concludes the proof of Eq. (23).

We are now ready to prove our main result, Eq. (12). This proof will again proceed by induction.

First, we consider the case $n=2$:

$$[f(x_1,x_2),g(x_1,x_2)] = \sum_{\underbrace{k_{1,2}}} \left(\prod_{j=2}^{2} \prod_{i=1}^{j-1} \frac{(-c_{ij})^{k_{ij}}}{k_{ij}!} \right) ((\partial_{x_1}^{k_1}\partial_{x_2}^{k_2} g)(\partial_{x_1}^{k_1'}\partial_{x_2}^{k_2'} f) - (\partial_{x_1}^{k_1}\partial_{x_2}^{k_2} f)(\partial_{x_1}^{k_1'}\partial_{x_2}^{k_2'} g))$$

$$= \sum_{k=1}^{\infty} \frac{(-c_{1,2})^k}{k!} (\partial_{x_1}^{k} g \partial_{x_2}^{k} f - \partial_{x_1}^{k} f \partial_{x_2}^{k} g),$$

where we have used Eqs. (13) and (14) to find that $k_1=k_2'=k_{1,2}$ and $k_2=k_1'=0$. We recognize that this is just the result derived in Eq. (22).

We now consider an arbitrary value of n. We write the functions in analogy with Eqs. (19) and (20)

$$f(x_1, \ldots, x_n) = \sum_{m=0}^{\infty} \phi_m(x_n) f_m(x_1, \ldots, x_{n-1})$$

$$g(x_1, \ldots, x_n) = \sum_{p=0}^{\infty} \gamma_p(x_n) g_p(x_1, \ldots, x_{n-1}).$$

Applying Leibnitz's rule to $[f,g]$ we have

$$[f,g] = \sum_{m=0}^{\infty} \sum_{p=0}^{\infty} ([\phi_m, \gamma_p] g_p f_m + \gamma_p [\phi_m, g_p] f_m + \phi_m [f_m, \gamma_p] g_p + \phi_m \gamma_p [f_m, g_p]).$$

We observe that the first commutator vanishes since it involves the single operator x_n. We use Eq. (23) to evaluate the second and third terms. We use Eq. (12) to evaluate the last term, since both arguments are functions of $n-1$ operators. The result is

$$\begin{aligned}
[f,g] = & \sum_{m=0}^{\infty} \sum_{p=0}^{\infty} \gamma_p \left(\underbrace{\sum_{k_{1,n}} \cdots \sum_{k_{n-1,n}}} \left(\prod_{i=1}^{n-1} \frac{(-c_{in}^{k_{in}})}{k_{in}!} \right) (\partial_{x_1}^{k_{1,n}} \ldots \partial_{x_{n-1}}^{k_{n-1,n}} g_p)(\partial_{x_n}^{k_n} \phi_m) \right) f_m \\
& - \sum_{m=0}^{\infty} \sum_{p=0}^{\infty} \phi_m \left(\underbrace{\sum_{k_{1,n}} \cdots \sum_{k_{n-1,n}}} \left(\prod_{i=1}^{n-1} \frac{(-c_{in}^{k_{in}})}{k_{in}!} \right) (\partial_{x_1}^{k_{1,n}} \ldots \partial_{x_{n-1}}^{k_{n-1,n}} f_m)(\partial_{x_n}^{l_n} \gamma_p) \right) g_p \\
& + \sum_{m=0}^{\infty} \sum_{p=0}^{\infty} \phi_m \gamma_p \left(\underbrace{\sum_{k_{1,2}} \cdots \sum_{k_{n-2,n-1}}} \left(\prod_{j=2}^{n-1} \prod_{i=1}^{j-1} \frac{(-c_{ij})^{k_{ij}}}{k_{ij}!} \right) \right) (\partial_{x_1}^{\kappa_1} \ldots \partial_{x_{n-1}}^{\kappa_{n-1}} g_p)(\partial_{x_1}^{k_1'} \ldots \partial_{x_{n-1}}^{k_{n-1}'} f_m) \\
& - \sum_{m=0}^{\infty} \sum_{p=0}^{\infty} \phi_m \gamma_p \left(\underbrace{\sum_{k_{1,2}} \cdots \sum_{k_{n-2,n-1}}} \left(\prod_{j=2}^{n-1} \prod_{i=1}^{j-1} \frac{(-c_{ij})^{k_{ij}}}{k_{ij}!} \right) \right) (\partial_{x_1}^{\kappa_1} \ldots \partial_{x_{n-1}}^{\kappa_{n-1}} f_m)(\partial_{x_1}^{k_1'} \ldots \partial_{x_{n-1}}^{k_{n-1}'} g_p)
\end{aligned} \tag{29}$$

where we have used the abbreviation

$$\kappa_i = \sum_{j=i+1}^{n-1} k_{ij} \tag{30}$$

and k_i' is defined in Eq. (14).

First, we notice that the first two terms of Eq. (29) can be combined:

$$\underbrace{\sum \cdots \sum}_{k_{1n} \quad k_{n-1n}} \left(\prod_{j=2}^{n-1} \prod_{i=1}^{j-1} \frac{(-c_{ij})^{k_{ij}}}{k_{ij}!} \right) ((\partial_{x_1}^{k_{1n}} \ldots \partial_{x_{n-1}}^{k_{n-1n}} g) \partial_{x_n}^{k_n} f - (\partial_{x_1}^{k_{1n}} \ldots \partial_{x_{n-1}}^{k_{n-1n}} f) \partial_{x_n}^{k_n} g).$$

Next, we notice that ϕ_m and γ_p commute. Also, using the definition of the commutator we can change the order of $\phi_m(\partial_{x_1}^{k_1} \ldots \partial_{x_{n-1}}^{k_{n-1}} g_p)$ and $\gamma_p(\partial_{x_1}^{k_1} \ldots \partial_{x_{n-1}}^{k_{n-1}} f_m)$. We use Eq. (23) to evaluate these commutators. After substitution into Eq. (29), the result is:

$$\begin{aligned}
[f,g] = & \underbrace{\sum \cdots \sum}_{k_{1n} \quad k_{n-1n}} \left(\prod_{j=2}^{n-1} \prod_{i=1}^{j-1} \frac{(-c_{ij})^{k_{ij}}}{k_{ij}!} \right) (\partial_{x_1}^{k_{1,n}} \ldots \partial_{x_{n-1}}^{k_{n-1,n}} g \partial_{x_n}^{k_n} f - \partial_{x_1}^{k_{1,n}} \ldots \partial_{x_{n-1}}^{k_{n-1,n}} f \partial_{x_n}^{k_n} g) \\
& + \sum_{m=0}^{\infty} \sum_{p=0}^{\infty} \left(\underbrace{\sum \cdots \sum}_{k_{1,2} \quad k_{n-2,n-1}} \left(\prod_{j=2}^{n-1} \prod_{i=1}^{j-1} \frac{(-c_{ij})^{k_{ij}}}{k_{ij}!} \right) \right) \times \{ \gamma_p (\partial_{x_1}^{\kappa_1} \ldots \partial_{x_{n-1}}^{\kappa_{n-1}} g_p) \phi_m (\partial_{x_1}^{k_1'} \ldots \partial_{x_{n-1}}^{k_{n-1}'} f_m) \\
& - \phi_m (\partial_{x_1}^{\kappa_1} \ldots \partial_{x_{n-1}}^{\kappa_{n-1}} f_m) \gamma_p (\partial_{x_1}^{k_1'} \ldots \partial_{x_{n-1}}^{k_{n-1}'} g_p) \} \\
& + \sum_{m=0}^{\infty} \sum_{p=0}^{\infty} \left(\underbrace{\sum \cdots \sum}_{k_{1,2} \quad k_{n-2,n-1}} \underbrace{\sum \cdots \sum}_{k_{1,n} \quad k_{n-1,n}} \left(\prod_{j=2}^{n-1} \prod_{i=1}^{j-1} \frac{(-c_{ij})^{k_{ij}}}{k_{ij}!} \prod_{i=1}^{j-1} \frac{(-c_{ij})^{k_{ij}}}{k_{ij}!} \right) \right) \\
& \times \{ \gamma_p (\partial_{x_1}^{\kappa_1 + k_{1,n}} \ldots \partial_{x_{n-1}}^{\kappa_{n-1} + k_{n-1,n}} g_p) (\partial_{x_n}^{k_{1,n} + \ldots + k_{n-1,n}} \phi_m) (\partial_{x_1}^{k_1'} \ldots \partial_{x_{n-1}}^{k_{n-1}'} f_m) \\
& - \phi_m (\partial_{x_1}^{\kappa_1 + k_{1,n}} \ldots \partial_{x_{n-1}}^{\kappa_{n-1} + k_{n-1,n}} f_m) (\partial_{x_n}^{k_{1,n} + \ldots + k_{n-1,n}} \gamma_p) (\partial_{x_1}^{k_1'} \ldots \partial_{x_{n-1}}^{k_{n-1}'} g_p) \}.
\end{aligned}$$

Combining factors

$$\left(\prod_{j=2}^{n-1} \prod_{i=1}^{j-1} \frac{(-c_{ij})^{k_i j}}{k_{ij}!} \right) \left(\prod_{i=1}^{n-1} \frac{(-c_{in})^{k_{in}}}{k_{in}!} \right) = \prod_{j=2}^{n} \prod_{i=1}^{j-1} \frac{(-c_{ij})^{k_{ij}}}{k_{ij}!},$$

and rearranging the summations, we get

$$[f,g]=\underbrace{\sum_{k_{1,n}}\cdots\sum_{k_{n-1,n}}}\left(\prod_{j=2}^{n-1}\prod_{i=1}^{j-1}\frac{(-c_{ij})^{k_{ij}}}{k_{ij}!}\right)((\partial_{x_1}^{k_{1,n}}\cdots\partial_{x_{n-1}}^{k_{n-1,n}}g)(\partial_{x_n}^{k_n}f)-(\partial_{x_1}^{k_{1,n}}\cdots\partial_{x_{n-1}}^{k_{n-1,n}}f)(\partial_{x_n}^{k_n}g))$$

$$+\underbrace{\sum_{k_{1,2}}\cdots\sum_{k_{n-2,n-1}}}\left(\prod_{j=2}^{n-1}\prod_{i=1}^{j-1}\frac{(-c_{ij})^{k_{ij}}}{k_{ij}!}\right)((\partial_{x_1}^{\kappa_1}\cdots\partial_{x_{n-1}}^{\kappa_{n-1}}g)(\partial_{x_1}^{k'_1}\cdots\partial_{x_{n-1}}^{k'_{n-1}}f)-(\partial_{x_1}^{\kappa_1}\cdots\partial_{x_{n-1}}^{\kappa_{n-1}}f)$$

$$\times(\partial_{x_1}^{k'_1}\cdots\partial_{x_{n-1}}^{k'_{n-1}}g))+\underbrace{\sum_{k_{1,2}}\cdots\sum_{k_{n-2,n-1}}}\underbrace{\sum_{k_{1,n}}\cdots\sum_{k_{n-1,n}}}\left(\prod_{j=2}^{n}\prod_{i=1}^{j-1}\frac{(-c_{ij})^{k_{ij}}}{k_{ij}!}\right)\{(\partial_{x_1}^{\kappa_1+k_{1,n}}\cdots\partial_{x_{n-1}}^{\kappa_{n-1}+k_{n-1,n}}g)$$

$$\times(\partial_{x_1}^{k'_1}\cdots\partial_{x_{n-1}}^{k'_{n-1}}\partial_{x_n}^{k_{1,n}+\cdots+k_{n-1,n}}f)-(\partial_{x_1}^{\kappa_1+k_{1,n}}\cdots\partial_{x_{n-1}}^{\kappa_{n-1}+k_{n-1,n}}f)(\partial_{x_1}^{k'_1}\cdots\partial_{x_{n-1}}^{k'_{n-1}}\partial_{x_n}^{k_{1,n}+\cdots+k_{n-1,n}}g)\}.$$

Now we observe that

$$\kappa_i+k_{in}=\sum_{j=i+1}^{n-1}k_{ij}+k_{in}=k_i$$

and that

$$k_{1,n}+\ \ldots\ +k_{n-1,n}=k'_n$$

in accordance with Eqs. (13) and (14), which allows us to write

$$[f,g]=\underbrace{\sum_{k_{1,n}}\cdots\sum_{k_{n-1,n}}}\left(\prod_{j=2}^{n-1}\prod_{i=1}^{j-1}\frac{(-c_{ij})^{k_{ij}}}{k_{ij}!}\right)((\partial_{x_1}^{k_{1,n}}\cdots\partial_{x_{n-1}}^{k_{n-1,n}}g)(\partial_{x_n}^{k_n}f)-(\partial_{x_1}^{k_{1,n}}\cdots\partial_{x_{n-1}}^{k_{n-1,n}}f)(\partial_{x_n}^{k_n}g))$$

$$+\underbrace{\sum_{k_{1,2}}\cdots\sum_{k_{n-2,n-1}}}\left(\prod_{j=2}^{n-1}\prod_{i=1}^{j-1}\frac{(-c_{ij})^{k_{ij}}}{k_{ij}!}\right)((\partial_{x_1}^{k_1}\cdots\partial_{x_{n-1}}^{k_{n-1}}g)(\partial_{x_1}^{k'_1}\cdots\partial_{x_{n-1}}^{k'_{n-1}}f)-(\partial_{x_1}^{k_1}\cdots\partial_{x_{n-1}}^{k_{n-1}}f)$$

$$\times(\partial_{x_1}^{k'_1}\cdots\partial_{x_{n-1}}^{k'_{n-1}}g))+\underbrace{\sum_{k_{1,2}}\cdots\sum_{k_{n-2,n-1}}}\underbrace{\sum_{k_{1,n}}\cdots\sum_{k_{n-1,n}}}\left(\prod_{j=2}^{n}\prod_{i=1}^{j-1}\frac{(-c_{ij})^{k_{ij}}}{k_{ij}!}\right)((\partial_{x_1}^{k_1}\cdots\partial_{x_{n-1}}^{k_{n-1}}g)$$

$$\times(\partial_{x_n}^{k'_n}\partial_{x_1}^{k'_1}\cdots\partial_{x_{n-1}}^{k'_{n-1}}f)-(\partial_{x_1}^{k_1}\cdots\partial_{x_{n-1}}^{k_{n-1}}f)(\partial_{x_n}^{k'_n}\partial_{x_1}^{k'_1}\cdots\partial_{x_{n-1}}^{k'_{n-1}}g)).$$

Finally, we observe the ranges of the groups of indices. The first term does not contain the indices $k_{1,2},\ldots,k_{n-2,n-1}$ and, therefore, corresponds to the term in which they are simultaneously zero. Also, the indices $k_{1,n},\ldots,k_{n-1,n}$ do not appear in the second term, which then corresponds to the term in which they are simultaneously zero. The third term has both sets of indices. Thus the three terms can be combined (see the Appendix) noting that all the indices range from zero to infinity, but are not simultaneously zero. Upon doing so, the equation becomes (12), completing the proof.

V. DISCUSSION AND IMPLEMENTATION

The main result of this paper is Eq. (12). It gives a formula for the commutator of two functions of noncommuting operators. It can actually be written more compactly in the form of Eq. (15) in which both the left-hand side and the constraints on the summation indices have been removed. Equation (15) actually looks so simple that one wonders if it cannot be derived trivially from some general statement, instead of through the long and convoluted induction processes

presented in Sec. IV. We have not been able to do so. Equation (12) applies to reasonable functions f and g which have converging Taylor series. In the derivation, we interchanged the order of the summations, thereby replacing a series by another, a step that is valid when both series converge. We used the linearity of the derivative to derive term by term, a process that is again valid for converging series with converging derivatives. Of course all formulas apply also to all finite or truncated series such as those that appear when evaluating expressions to any finite order of perturbation theory for example. That is the spirit in which the formulas were derived and the area where they are most likely to find their domain of applicability. Since x_1 and x_2 in Eq. (22) and $x_1, x_2 \ldots, x_n$ in Eq. (12) are operators, the derivatives and partial derivatives need to be explained further. Already in Eq. (11) the derivative symbol refers to a derivative with respect to an operator. In the one-dimensional case Eq. (11) can easily be interpreted as the operator replacement of the derivative of a function with respect to a scalar variable. The prescription becomes: take the ordinary derivative of the function and replace in the resulting expression every occurrence of the variable x by an operator X. So for instance, denoting operators with capitals for now, the procedure to find the operator derivative in a particular case gives

$$(e^{3X})' \to (e^{3x})' = 3e^{3x} \to 3(e^{3X}).$$

When the function depends on two or more noncommuting operators however, an operational definition of the derivative needs to be supplied. We follow Louisell (1964) to define the derivative with respect to an operator in terms of the derivative with respect to a scalar parameter λ:

$$\partial_x f(x,p) = \lim_{\lambda \to 0} \frac{\partial}{\partial \lambda} f(x+\lambda, p). \tag{31}$$

and

$$\partial_{x_i} f(x_1, \ldots, x_i, \ldots, x_n) = \lim_{\lambda \to 0} \frac{\partial}{\partial \lambda} f(x_1, \ldots, x_i + \lambda, \ldots, x_n). \tag{32}$$

This definition reduces to the ordinary derivative shown above in the one-dimensional case:

$$\partial_x e^{3x} = \lim_{\lambda \to 0} \frac{\partial}{\partial \lambda} e^{3(x+\lambda)} = \lim_{\lambda \to 0} 3e^{3(x+\lambda)} = 3e^{3x}. \tag{33}$$

Let us now apply this definition for operator derivatives to a function of two operators x and p as an example of a situation that might arise in the evaluation of Eq. (12). It is clear that, as a result of the noncommutativity of x and p the ordinary composition or chain rule,

$$(f(g(x)))' = f'(g(x))g'(x) = g'(x)f'(g(x)) \tag{34}$$

cannot be applied without ambiguity since, for example,

$$\partial_x(\cos(xp)) \neq -\sin(xp)p \neq p(-\sin(xp) \quad \neq 1/2(-\sin(xp)\ p + p(-\sin(xp)). \tag{35}$$

For the exponential function however, we can follow Wilcox (1967) and adapt a result from Snider (1964) to obtain

$$\partial_x(e^{f(x,p)}) = \int_0^1 \mathrm{d}u e^{(1-u)f(x,p)}(\partial_x f(x,p))e^{uf(x,p)} \tag{36}$$

which can itself be used to get an explicit expression for the derivative operator in Eq. (35) above

$$\partial_x(\cos(xp)) = -\int_0^1 \mathrm{d}u \cos[(1-u)xp]p \sin(uxp) - \int_0^1 \mathrm{d}u \sin[(1-u)xp]p \cos(uxp). \tag{37}$$

This result is indeed quite different from that obtained from a naive application of the chain rule for derivatives with respect to commuting variables. Furthermore the result in Eq. (37) can be checked to any order of an expansion in powers of x or p. The derivative of a polynomial truncation of the cosine function yields the result obtained by truncation of the trigonometric functions in Eq. (37). We have developed algorithms for manipulating any polynomial expression of noncommuting operators [Transtrum and Van Huele (to be published)]. That linearity and Leibnitz's rule apply to the operational derivative follows from the fact that these properties are preserved in Eq. (31).

Finally we use Eq. (12) to derive the torque equation in the Heisenberg picture of quantum mechanics as an illustration of a commutator of two functions, one of which (only) can be expanded in a finite power series of its operators.

Consider the commutator of the nonrelativistic Hamiltonian,

$$H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(x,y,z),$$

with the z component of the angular momentum, $L_z = xp_y - yp_x$. Since the only nonvanishing commutators are $[x,p_x]=[y,p_y]=[z,p_z]=i\hbar$, the formula simplifies to

$$[L_z(x,y,p_x,p_y),H(x,y,z,p_x,p_y,p_z)] = \underbrace{\sum_k \sum_l \sum_m}_{} \frac{(-i\hbar)^{k+l+m}}{k!l!m!} \times ((\partial_x^k \partial_y^l \partial_z^m H)(\partial_{p_x}^k \partial_{p_y}^l \partial_{p_z}^m L_z) - (\partial_x^k \partial_y^l \partial_z^m L_z)(\partial_{p_x}^k \partial_{p_y}^l \partial_{p_z}^m H)) \tag{38}$$

By inspection, it is obvious that all mixed partial derivatives of L_z that occur in the above formula vanish. So, the above formula further simplifies to

$$\begin{aligned}[L_z,H] &= \sum_{k=1}^{\infty} \frac{(-i\hbar)^k}{k!}((\partial_x^k H)(\partial_{p_x}^k L_z) - (\partial_x^k L_z)(\partial_{p_x}^k H)) + \sum_{k=1}^{\infty} \frac{(-i\hbar)^k}{k!}((\partial_y^k H)(\partial_{p_y}^k L_z) - (\partial_y^k L_z)(\partial_{p_y}^k H)) \\ &\quad + \sum_{k=1}^{\infty} \frac{(-i\hbar)^k}{k!}((\partial_z^k H)(\partial_{p_z}^k L_z) - (\partial_z^k L_z)(\partial_{p_z}^k H)) \\ &= (-i\hbar)\left((\partial_x V)(-y) - p_y \frac{p_x}{m} + (\partial_y V)(x) - (-p_x)\frac{p_y}{m}\right) = (-i\hbar)((\partial_y V)x - (\partial_x V)y). \end{aligned} \tag{39}$$

Therefore

$$\frac{dL_z}{dt} = \frac{1}{i\hbar}[L_z,H] = xF_y - yF_x. \tag{40}$$

We recognize the torque about the z axis as expected.

In conclusion, we have presented an expression for the commutator of two functions of an arbitrary number of noncommuting operators whose commutators are constants. The formula is derived constructively using the induction process. The resulting expression involves partial derivatives of the functions with respect to the noncommuting operators. These partial derivatives can be evaluated directly in some simple cases or in general through series expansions and ordering algorithms to any order.

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APPENDIX: NOTATION FOR SUMMATION INDICES

In this appendix we comment on the use of our notation for the summation indices as they appear in Eqs. (12)–(14). First of all $k_1=k_n'=0$ for any n. We include these terms to see the symmetry in the formula.

Second, we note that when the summation indices have two subscripts, we separate the subscripts by commas when at least one of them involves a number. Thus we write $k_{1,2}$, $k_{1,i}$, and $k_{i-1,j}$, but k_{ij} instead of $k_{i,j}$. Similarly, we write $c_{1,2}$, $c_{1,i}$, and $c_{i-1,j}$, but c_{ij} instead of $c_{i,j}$. The simplification $c_{1,2}=c$ was made in the part of Sec. IV leading to Eq. (22).

Finally we discuss the correlation between the summation indices and the related underbrace notation in more depth. Throughout the paper, we frequently use notation of the form

$$\underbrace{\sum_{k_1}\cdots\sum_{k_n}} f(k_1,\ldots,k_n),$$

where the underbrace indicates that the summations range from zero to infinity but are not simultaneously zero. We will explain some of the properties associated with these expressions.

In the case that the underbrace includes only one index, that index cannot be zero, and the expression can be rewritten in more standard notation:

$$\underbrace{\sum_{k_1}} f(k_1)=\sum_{k_1=1}^{\infty} f(k_1).$$

Now, we consider the case that the underbrace contains two indices. Both cannot be zero simultaneously, but one can be zero as long as the other is nonzero. Thus, there are two summations which account for the cases in which one of the indices is zero. There is also the case that neither index is zero and a third term accounts for this:

$$\underbrace{\sum_{k_1}\sum_{k_2}} f(k_1,k_2)=\sum_{k_1=1}^{\infty} f(k_1,k_2=0)+\sum_{k_2=1}^{\infty} f(k_1=0,k_2)+\sum_{k_1=1}^{\infty}\sum_{k_2=1}^{\infty} f(k_1,k_2).$$

We observe here that this result implies that

$$\underbrace{\sum_{k_1}\sum_{k_2}} f(k_1,k_2)=\underbrace{\sum_{k_1}} f(k_1,k_2=0)+\underbrace{\sum_{k_2}} f(k_1=0,k_2)+\underbrace{\sum_{k_1}}\underbrace{\sum_{k_2}} f(k_1,k_2),$$

which we will generalize shortly.

It follows from the above argument, that, if there are n indices, $k_1,\ldots,k_n$, in an expression of the form

$$\underbrace{\sum_{k_1}\cdots\sum_{k_n}} f(k_1,\ldots,k_n),$$

there will be $\binom{n}{1}$ terms in which one index is nonzero, $\binom{n}{2}$ terms in which two indices are nonzero, and so forth. Thus, there will be

$$\sum_{k=1}^{n} \binom{n}{k} = 2^n - 1$$

terms altogether. For large numbers of indices, the underbrace notation is clearly more compact; however, for computational purposes, it will be necessary to expand the underbrace notation as we have done here for the cases $n=1$ and $n=2$.

Now we consider a situation that arises frequently in the derivations presented in this paper. This involves the case in which there are two groups of indices, $k_1,\ldots,k_n$ and $l_1,\ldots,l_m$ in an expression of the form

$$\underbrace{\sum_{k_1}\cdots\sum_{k_n}\sum_{l_1}\cdots\sum_{l_m} f},$$

where f depends on each of the indices. We show that the underbrace has the following property:

$$\underbrace{\sum_{k_1}\cdots\sum_{k_n}\sum_{l_1}\cdots\sum_{l_m} f} = \underbrace{\sum_{k_1}\cdots\sum_{k_n} f} + \underbrace{\sum_{l_1}\cdots\sum_{l_m} f} + \underbrace{\sum_{k_1}\cdots\sum_{k_n}} \underbrace{\sum_{l_1}\cdots\sum_{l_m} f}$$

which is an identity used often throughout the paper. Given a little thought, this expression seems reasonable, but we will present a slightly more rigorous proof.

The proof is not complicated; we simply count the number of terms on either side of the equation. The left-hand side of the equation has $2^{n+m}-1$ terms. The right-hand side has $2^n-1+2^m-1+(2^n-1)(2^m-1)=2^{n+m}-1$ terms. Since all of the terms on the the right involve summations in which some of the indices range from zero to infinity but are not simultaneously zero, we conclude that each term on the right-hand side of the equation also appears on the left with no repeated terms. Since both sides of the equation have equal numbers of terms, we conclude that the two expressions are equivalent.

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Stationary van Hove limit

Jan Dereziński[a] and Rafał Früboes[b]
Department of Mathematical Methods in Physics, Warsaw University, Hoża 74, 00-682, Warsaw, Poland

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The weak coupling (van Hove) limit of one parameter groups of contractions is studied by the stationary approach. We show that the resolvent of the properly renormalized and rescaled generator of a contractive semigroup has a limit as the coupling constant goes to zero. This limit is the resolvent of the generator of a certain contractive semigroup. Our results can be viewed as a stationary counterpart to the well known results about the weak coupling limit obtained by the time-dependent approach, due to Davies. We compare both approaches. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1904509]

I. INTRODUCTION

Let $\mathcal{X}$ be a Banach space with a distinguished bounded projection P. Suppose that U_t^λ is a one parameter strongly continuous group of isometries on $\mathcal{X}$ generated by $L_\lambda := L_0 + \lambda Q$. Assume that P commutes with the free dynamics $U_t^0 = \mathrm{e}^{tL_0}$ or equivalently P commutes with L_0. Our main object of interest is the reduced dynamics

$$\mathbb{R} \ni t \mapsto PU_t^\lambda P$$

as an operator on Ran P.

The reduced dynamics was studied in a series of papers[4,5] and in the book[6] by Davies. First he showed that the reduced dynamics after appropriately rescaling, i.e.,

$$t \mapsto PU_{t/\lambda^2}^\lambda P,$$

can be approximated, as the coupling constant λ goes to zero, by a certain one parameter semigroup on Ran P depending on λ. The generator of this semigroup is a quadratic polynomial in λ^{-1}. By the convergence we mean that for each fixed time t the norm of the difference between the resulting semigroup and the reduced rescaled dynamics tends to zero as $|\lambda|$ becomes smaller. We will call this result, for the reasons that soon become clear, the pointwise (in time) van Hove limit with the first order term.

The second result obtained by Davies describes the case with $PQP = 0$. He proved that the reduced dynamics with a rescaled time renormalized by the free evolution, i.e.,

$$t \mapsto U_{-t/\lambda^2}^0 PU_{t/\lambda^2}^\lambda P, \tag{1.1}$$

has a limit, for each fixed time t, as the coupling constant λ goes to zero. The limit is a one parameter semigroup, independent of λ. The generator of the resulting semigroup is often called the Davies generator. We will call this limit the pointwise (in time) van Hove limit without the first order term.

One can distinguish two approaches to semigroups, the time-dependent approach and the stationary approach. The former concentrates on the study of semigroups themselves. The latter

[a]Electronic mail: jan.derezinski@fuw.edu.pl
[b]Electronic mail: rafal.fruboes@fuw.edu.pl

focuses at the resolvent of their generators. Davies used the time-dependent approach, both in the choice of the assumptions for his results and in their statements. In our paper we use mostly the stationary approach.

Our main results are contained in three theorems. First in Theorem 3.1 we study, the stationary van Hove limit for the reduced dynamics as the coupling constant λ goes to zero. More precisely, we describe the asymptotics of the rescaled resolvent of L_λ reduced by P by the resolvent of a certain operator $A_{\lambda,0}$. This is the stationary counterpart to the first result of Davies.

Theorem 3.2 describes the case without the first order term ($PQP=0$). We additionally assume that the spectrum of PL_0P consist of isolated points. We obtain a simple asymptotics of the Laplace transform of (1.1) given by the resolvent of a certain operator Γ independent of λ commuting with PL_0P. We prove that the operator Γ is the generator of a contractive semigroup. This is the stationary counterpart to the second result of Davies.

The main results about the stationary van Hove limit involve resolvents. They have, however, easy time-dependent corollaries, which we call the smeared out weak coupling limit. By this we mean that the difference of the rescaled restricted dynamics and the approximating dynamics averaged over time with some continuous function of compact support tends to zero as the coupling constant goes to zero. This version of the result is also contained in Theorems 3.1 and 3.2.

In Theorem 3.3 we show how one can obtain pointwise (in time) van Hove limit without the first order term starting from the stationary van Hove limit.

Theorem 3.5 gives conditions when one can apply both the time-dependent method of Davies and our stationary results. We also find out that the semigroup obtained in the van Hove limit is generated by the so-called level shift operator, see Refs. 9–11 and 7.

In the physical literature one can trace back the weak coupling limit to works of Wigner–Weisskopf, Pauli and also van Hove.[18–20] First rigorous mathematical treatment of this issue comes from Davies,[4–6] who gave both its abstract theory and presented applications to open quantum systems (see also Ref. 14).

In his papers, Davies uses the time-dependent approach, i.e., he works with the restricted dynamics. The key step in this approach is the construction of the resulting semigroup by the integral formula (e.g., Theorem 3.1.33 in Ref. 3). The use of this formula induces technical assumptions which may be not easy to verify. For the convenience of the reader we describe the result of Davies in Theorem 3.4.

In our approach to the weak coupling limit, instead of working with the perturbed dynamics, we investigate the resolvent of the perturbed generator. We use some regularity assumptions for resolvents which seem easier to verify in some circumstances. In particular our regularity assumptions are closely related to the so-called limiting absorption principle which can be investigated with help of the so-called Mourre theory.[8]

We end this introduction with a description of the main physical motivation of our work—an application of the van Hove limit to open quantum systems. We essentially follow Ref. 14, see also Refs. 4 and 5. For more information, especially concerning the relationship of the van Hove limit to applications of the method of the level shift operator to the return to equilibrium, we refer the reader to Ref. 11. For related analysis of open quantum systems see also Refs. 15–17.

Let us consider a quantum mechanical system which consists of two parts—the small system $\mathcal{S}$ and the reservoir part $\mathcal{R}$. To describe $\mathcal{S}$ one chooses appropriate Hilbert space $\mathcal{H}_\mathcal{S}$. Then the states are given by density matrices (i.e., trace class normalized positive operators on $\mathcal{H}_\mathcal{S}$). The time evolution of the isolated small system $\mathcal{S}$ is implemented by the Hamiltonian $H_\mathcal{S}$. In a similar way we describe the reservoir part $\mathcal{R}$. We have Hilbert space $\mathcal{H}_\mathcal{R}$, the Liouvillean $L_\mathcal{R}$ (the generator of the time evolution) and density matrices on $\mathcal{H}_\mathcal{R}$. Let us additionally assume that there exists a stationary state, denoted $\omega_\mathcal{R}$, of $\mathcal{R}$ for the evolution implemented by $L_\mathcal{R}$.

The time evolution of whole system $\mathcal{S}+\mathcal{R}$ is given by self-adjoint operator

$$L_\lambda := H_\mathcal{S} \otimes \mathbf{1}_\mathcal{R} + \mathbf{1}_\mathcal{S} \otimes L_\mathcal{R} + \lambda V$$

acting on $\mathcal{H} := \mathcal{H}_\mathcal{S} \otimes \mathcal{H}_\mathcal{R}$ where V is some interaction operator and $\lambda \in \mathbb{R}$. Hence for any density matrix χ on $\mathcal{H}_\mathcal{S} \otimes \mathcal{H}_\mathcal{R}$ its evolution is given by

$$U_t^\lambda \chi := e^{-tiL_\lambda} \chi e^{tiL_\lambda}.$$

Assume that the initial state of $\mathcal{S}+\mathcal{R}$ is $\rho \otimes \omega_\mathcal{R}$ for some density matrix ρ on $\mathcal{H}_\mathcal{S}$. Then after time t the state of $\mathcal{S}+\mathcal{R}$ is given by $U_t^\lambda(\rho \otimes \omega_\mathcal{R})$. If we treat $\mathcal{R}$ just as a device which induces changes of $\mathcal{S}$ and we want only to know what happens to $\mathcal{S}$, then to obtain the state of $\mathcal{S}$ at time t we take the partial trace over the degrees of freedom of $\mathcal{R}$,

$$\rho(t) := \mathrm{tr}_\mathcal{R}(U_t^\lambda(\rho \otimes \omega_\mathcal{R})). \tag{1.2}$$

Note that the action of U_t^λ can be extended to the whole space of the trace class operators $B^1(\mathcal{H}_\mathcal{S} \otimes \mathcal{H}_\mathcal{R})$. Recall that $B^1(\mathcal{H}_\mathcal{S} \otimes \mathcal{H}_\mathcal{R})$ is a Banach space under the norm $\|\cdot\|_1 = \mathrm{tr}|\cdot|$ and U_t^λ is a one parameter strongly continuous group of isometries on $B^1(\mathcal{H}_\mathcal{S} \otimes \mathcal{H}_\mathcal{R})$. If we introduce the operator

$$P: B^1(\mathcal{H}_\mathcal{S} \otimes \mathcal{H}_\mathcal{R}) \to B^1(\mathcal{H}_\mathcal{S}) \otimes \omega_\mathcal{R} \subset B^1(\mathcal{H}_\mathcal{S} \otimes \mathcal{H}_\mathcal{R}),$$

$$PW := \mathrm{tr}_\mathcal{R}(W) \otimes \omega_\mathcal{R},$$

then P is a projection of norm one and the equation (1.2) can be rewritten

$$\rho(t) \otimes \omega_\mathcal{R} := PU_t^\lambda P(\rho \otimes \omega_\mathcal{R}).$$

Note also that $[U_t^0, P] = 0$. Therefore, we have a setup, where we can apply our results. In the weak coupling limit we obtain completely positive semigroup of contractions which is sometimes called a quantum dynamical Markov semigroup. Hence starting with a fully reversible dynamics for the whole system, we end up with an irreversible evolution of the small subsystem. Now, in the weak coupling approximation, when we study the small system we may exchange complicated object $PU_t^\lambda P$ for a semigroup and use it in order to determine physical quantities. However there is a price to be paid—the results that we get in this approximation are typically the lowest order nonvanishing corrections in the coupling constant to the real quantities.

II. PRELIMINARIES

Notation: Let $\mathcal{X}$ be a Banach space. For a linear operator L on $\mathcal{X}$, $\mathrm{sp}\, L$ denotes its spectrum and $\mathrm{Dom}\, L$ its domain. If Ξ is an isolated bounded subset of $\mathrm{sp}\, L$ then the spectral projection of L onto Ξ, defined by the usual integral formula,[13] is denoted $\mathbf{1}_\Xi(L)$. If e is an isolated point of $\mathrm{sp}\, L$, then we will write $\mathbf{1}_e(L)$ for $\mathbf{1}_{\{e\}}(L)$.

Let $\mathbf{1}^{v v}$ be a distinguished bounded projection on $\mathcal{X}$. It will be convenient to denote $\mathbf{1}^{\overline{v v}} := \mathbf{1} - \mathbf{1}^{v v}$. We also introduce closed subspaces

$$\mathcal{X}^v := \mathbf{1}^{v v}\mathcal{X}, \quad \mathcal{X}^{\overline{v}} := \mathbf{1}^{\overline{v v}}\mathcal{X} = \mathrm{Ker}\, \mathbf{1}^{v v},$$

so that $\mathcal{X}$ is decomposed into a direct sum

$$\mathcal{X} = \mathcal{X}^v \oplus \mathcal{X}^{\overline{v}}. \tag{2.1}$$

Any operator H on $\mathcal{X}$ satisfying

$$\mathrm{Dom}(H) = (\mathrm{Dom}(H) \cap \mathcal{X}^v) \oplus (\mathrm{Dom}(H) \cap \mathcal{X}^{\overline{v}})$$

can be written with respect to the decomposition (2.1) as

$$H=\begin{bmatrix} H^{vv} & H^{v\overline{v}} \\ H^{\overline{v}v} & H^{\overline{v}\overline{v}} \end{bmatrix} = H^{vv}+H^{v\overline{v}}+H^{\overline{v}v}+H^{\overline{v}\overline{v}}. \tag{2.2}$$

Obviously $H^{vv}=\mathbf{1}^{vv}H\mathbf{1}^{vv}$, etc. In particular

$$\mathbf{1}:=\begin{bmatrix} \mathbf{1}^{vv} & 0 \\ 0 & \mathbf{1}^{\overline{v}\overline{v}} \end{bmatrix}.$$

For $e\in i\mathbb{R}$ and for $\alpha\geqslant 0$ we denote

$$\mathbf{Wedge}(e,\alpha):=\{z\in\mathbb{C}:\operatorname{Re} z>0,|\operatorname{Im}(z-e)|\leqslant\alpha\operatorname{Re} z\}.$$

III. MAIN RESULTS

Let L_0 be the generator of a one parameter strongly continuous group of isometries $t\mapsto e^{tL_0}$ on the Banach space $\mathcal{X}$. Recall that L_0 is norm closed, norm densely defined, conservative operator (i.e., both L_0 and $-L_0$ are dissipative) and $\operatorname{sp} L_0\subset i\mathbb{R}$.[3,6]

Let $\mathbf{1}^{vv}$ be a distinguished projection on $\mathcal{X}$ such that $\|\mathbf{1}^{vv}\|=1$. Assume that $\mathbf{1}^{vv}$ commutes with L_0 or equivalently $[\mathbf{1}^{vv},e^{tL_0}]=0$ for all t. Then the operator L_0 written with respect to the decomposition (2.1) has the form

$$L_0=\begin{bmatrix} L_0^{vv} & 0 \\ 0 & L_0^{\overline{v}\overline{v}} \end{bmatrix}. \tag{3.1}$$

We write for shortness $E:=L_0^{vv}$. Note that E generates a one parameter strongly continuous group of isometries on $\mathcal{X}^v$.

Let Q with $\operatorname{Dom} L_0\subset\operatorname{Dom} Q$ be another operator that we will treat as a perturbation of L_0. Fix $\lambda_0>0$. We assume that for $0\leqslant\lambda<\lambda_0$ the operator

$$L_\lambda:=L_0+\lambda Q,$$

defined on $\operatorname{Dom} L_\lambda=\operatorname{Dom} L_0$ is the generator of a one parameter strongly continuous semigroup of contractions on $\mathcal{X}$.

We will assume that the off-diagonal elements of Q, i.e., $Q^{\overline{v}v}$ and $Q^{v\overline{v}}$ are bounded. We also assume that for all $0\leqslant\lambda<\lambda_0$ operator $E+\lambda Q^{vv}$ generates a group of isometries on $\mathcal{X}^v$.

Note that if L_λ with bounded $Q^{\overline{v}v}$ and $Q^{v\overline{v}}$ generates a group of isometries then $E+\lambda Q^{vv}$ generates a group of isometries on $\mathcal{X}^v$.

A. Van Hove limit—stationary approach

In this section we discuss the van Hove limit under the assumptions involving the resolvent of L_λ. The statement of our result is similar to the statement of the results of Davies, which we recall later.

1. Van Hove limit with the first order term

Theorem 3.1: *Assume that for all* $0\leqslant\lambda<\lambda_0$ *:*

(i) *For all* $\xi>0$ *we have* $\xi\notin\operatorname{sp}(L_\lambda^{\overline{v}\overline{v}})$,
(ii) *there exists an operator* $\Gamma_0\in B(\mathcal{X}^v)$ *such that, for any* $\xi>0$,

$$\Gamma_0:=\lim_{\lambda\searrow 0} Q^{v\overline{v}}(\lambda^2\xi\mathbf{1}^{\overline{v}\overline{v}}-L_\lambda^{\overline{v}\overline{v}})^{-1}Q^{\overline{v}v}. \tag{3.2}$$

[*Note that the right-hand side (RHS) of (3.2) may depend on* ξ*. We assume that it does not*].

Let

$$A_{\lambda,0} := E + \lambda Q^{vv} + \lambda^2 \Gamma_0. \tag{3.3}$$

Then the following holds:

(1) Γ_0 *generates a semigroup of contractions on* $\mathcal{X}^v$.
(2) $A_{\lambda,0}$ *generates a semigroup of contractions on* $\mathcal{X}^v$.
(3) *For each* $\xi > 0$,

$$\lim_{\lambda \searrow 0} (\mathbf{1}^{vv}(\xi 1 - \lambda^{-2} L_\lambda)^{-1} \mathbf{1}^{vv} - (\xi \mathbf{1}^{vv} - \lambda^{-2} A_{\lambda,0})^{-1}) = 0. \tag{3.4}$$

(4) *For any* $f \in C_0([0,\infty[)$

$$\lim_{\lambda \searrow 0} \int_0^\infty f(\sigma)(\mathbf{1}^{vv} e^{\sigma \lambda^{-2} L_\lambda} \mathbf{1}^{vv} - e^{\sigma \lambda^{-2} A_{\lambda,0}}) \mathrm{d}\sigma = 0. \tag{3.5}$$

Note that above we use the notation $(z\mathbf{1}^{\overline{vv}} - L_\lambda^{\overline{vv}})^{-1}$ for the inverse of the operator $z\mathbf{1}^{\overline{vv}} - L_\lambda^{\overline{vv}}$ restricted to $\mathcal{X}^{\overline{v}}$. We will often use a similar notation without a comment.

2. Van Hove limit without the first order term

In this section we describe two versions of the van Hove limit without the first order term. In the first we either work at the resolvents or smear out the dynamics in time. In the second, we work at the dynamics pointwise in time. The statement of the second result is essentially the same as that of Davies, however assumptions are different.

We will need the following additional assumptions.

Assumption 3.A: $\mathrm{sp}\, E$ *is a finite set.*

Note that Assumption 3.A implies that we can write

$$\mathbf{1}^{vv} = \sum_{e \in \mathrm{sp}\, E} \mathbf{1}_e(E).$$

Assumption 3.B: $Q^{vv} = 0$.

Theorem 3.2: *Let Assumptions 3.A and 3.B hold. Assume additionally that*

(i) *for* $0 \leqslant \lambda < \lambda_0$, *for each* $e \in \mathrm{sp}\, E$ *and for all* $\xi > 0$ *we have* $e + \xi \notin \mathrm{sp}(L_\lambda^{\overline{vv}})$,
(ii) *there exists an operator* $\Gamma \in B(\mathcal{X}^v)$ *such that, for any* $\xi > 0$,

$$\Gamma := \sum_{e \in \mathrm{sp}\, E} \lim_{\lambda \searrow 0} \mathbf{1}_e(E) Q^{v\overline{v}}((e + \lambda^2 \xi)\mathbf{1}^{\overline{vv}} - L_\lambda^{\overline{vv}})^{-1} Q^{\overline{v}v} \mathbf{1}_e(E). \tag{3.6}$$

[*Note that the RHS of (3.6) may depend on* ξ. *We assume that it does not*].

(iii) *For any* $e, e' \in \mathrm{sp}\, E$, $e \neq e'$ *and* $\xi > 0$,

$$\lim_{\lambda \searrow 0} \lambda \mathbf{1}_e(E) Q^{v\overline{v}}((e + \lambda^2 \xi)\mathbf{1}^{\overline{vv}} - L_\lambda^{\overline{vv}})^{-1} Q^{\overline{v}v} \mathbf{1}_{e'}(E) = 0,$$

$$\lim_{\lambda \searrow 0} \lambda \mathbf{1}_{e'}(E) Q^{v\overline{v}}((e + \lambda^2 \xi)\mathbf{1}^{\overline{vv}} - L_\lambda^{\overline{vv}})^{-1} Q^{\overline{v}v} \mathbf{1}_e(E) = 0.$$

Then the following holds:

(1) Γ *generates semigroup of contractions on* $\mathcal{X}^v$,
(2) $[E, \Gamma] = 0$,
(3) *for each* $\xi > 0$ *we have*

$$\lim_{\lambda \searrow 0} \sum_{e \in \mathrm{sp}\, E} \mathbf{1}_e(E) \mathbf{1}^{vv} (\xi 1 - \lambda^{-2}(L_\lambda - e1))^{-1} \mathbf{1}^{vv} = (\xi \mathbf{1}^{vv} - \Gamma)^{-1}, \tag{3.7}$$

(4) *for any* $f \in C_0([0,\infty[)$,

$$\lim_{\lambda\searrow 0}\int_0^\infty f(\sigma)(e^{-\sigma\lambda^{-2}E}\mathbf{1}^{vv}e^{\sigma\lambda^{-2}L_\lambda}\mathbf{1}^{vv}-e^{\sigma\Gamma})\mathrm{d}\sigma=0. \tag{3.8}$$

Theorem 3.3: *Let assumptions 3.A and 3.B hold. Assume additionally that*

(i) *for* $0\leqslant\lambda<\lambda_0$ *and all* $\xi\in\mathbb{C}$, $\mathrm{Re}\,\xi>0$, *we have* $\xi\notin\mathrm{sp}(L_\lambda^{\overline{vv}})$,

(ii) *for all* $\alpha_0\geqslant 0$ *and for any* $\xi\in\mathrm{Wedge}(0,\alpha_0)$, *there exists an operator* $\Gamma\in B(\mathcal{X}^v)$ *such that,*

$$\Gamma:=\sum_{e\in\mathrm{sp}\,E}\lim_{\lambda\searrow 0}\mathbf{1}_e(E)Q^{v\overline{v}}((e+\lambda^2\xi)\mathbf{1}^{\overline{vv}}-L_\lambda^{\overline{vv}})^{-1}Q^{\overline{v}v}\mathbf{1}_e(E), \tag{3.9}$$

[*Note that the RHS of (3.9) may depend on* ξ. *We assume that it does not*].

(iii) *For each* $e\in\mathrm{sp}\,E$ *we have*

$$\sup_{\mathrm{Re}\,\xi>0;0\leqslant\lambda<\lambda_0}\|Q^{v\overline{v}}((e+\lambda^2\xi)\mathbf{1}^{\overline{vv}}-L_\lambda^{\overline{vv}})^{-1}Q^{\overline{v}v}\|<\infty.$$

Then,

(1) *all statemants of the Theorem 3.2 hold. Besides (3) holds in a stronger form, for* $\alpha_0\geqslant 0$ *the formula (3.7) is valid for each* $\xi\in\mathrm{Wedge}(0,\alpha_0)$.

(2) *Let* $\psi\in\mathcal{X}^v$. *For* $\sigma\geqslant 0$ *we have*

$$\lim_{\lambda\searrow 0}(e^{-\sigma\lambda^{-2}E}\mathbf{1}^{vv}e^{\sigma\lambda^{-2}L_\lambda}\mathbf{1}^{vv}-e^{\sigma\Gamma})\psi=0 \tag{3.10}$$

uniformly for $\sigma\in[\tau_0,\tau_1]$ *for any fixed* $0<\tau_0\leqslant\tau_1<\infty$.

B. Van Hove limit—time-dependent approach

In this section we discuss the van Hove limit under the assumptions involving the dynamics. In Theorem 3.4 we recall the original approach to the van Hove limit due to Davies.[4–6] (Strictly speaking, Davies assumed that the perturbation Q is bounded. In Theorem 3.4 we impose slightly less restrictive assumptions, which can be handled by an essentially the same proof.)

Let L_0, Q, and $\mathbf{1}^{vv}$ be the same as before. Clearly, $L_\lambda^{\overline{vv}}$ generates a semigroup on $\mathcal{X}^{\overline{v}}$. Therefore, we can define the operator

$$K(\lambda,\tau):=\int_{x=0}^{\lambda^{-2}\tau}e^{-xL_\lambda^{vv}}Q^{v\overline{v}}e^{xL_\lambda^{\overline{vv}}}Q^{\overline{v}v}\,\mathrm{d}x. \tag{3.11}$$

The following theorem describes the van Hove limit for the dynamics in both cases—with and without the first order term.

Theorem 3.4: *Assume additionally that*

(i) *for all* $\tau_1>0$ *there is a constant* $C>0$ *such that* $\|K(\lambda,\tau)\|<C$ *for* $|\lambda|\leqslant 1$ *and* $0\leqslant\tau\leqslant\tau_1$.

(ii) *There exists bounded operator* K *on* $\mathcal{X}^v$ *such that if* $0<\tau_0\leqslant\tau_1<\infty$ *then*

$$\lim_{\lambda\searrow 0}(\sup_{\tau_0\leqslant\tau\leqslant\tau_1}\|K(\lambda,\tau)-K\|)=0.$$

Then the following holds:

(1)

$$\lim_{\lambda\searrow 0}\Big(\sup_{0\leqslant t\leqslant\tau_1}\|\mathbf{1}^{vv}e^{t\lambda^{-2}L_\lambda}\mathbf{1}^{vv}-e^{t\lambda^{-2}(E+\lambda Q^{vv}+\lambda^2K)}\|\Big)=0. \tag{3.12}$$

(2) *If additionally Assumptions 3.A and 3.B hold then*

$$\lim_{\lambda \searrow 0} \left(\sup_{0 \leqslant t \leqslant \tau_1} \| e^{-t\lambda^{-2}E} \mathbf{1}^{vv} e^{t\lambda^{-2}L_\lambda} \mathbf{1}^{vv} - e^{tK^\natural} \| \right) = 0, \tag{3.13}$$

where

$$K^\natural := \sum_{e \in \mathrm{sp}\, E} \mathbf{1}_e(E) K \mathbf{1}_e(E) = \lim_{a \to \infty} \frac{1}{2a} \int_{-a}^{a} e^{tE} K e^{-tE}\, \mathrm{d}t.$$

Let us recall how the operators $K(\lambda, \tau)$ are motivated. If we treat the off-diagonal elements of L_λ as a (bounded) perturbation of the diagonal part of L_λ then, by a well-known formula, we have

$$e^{tL_\lambda} = e^{t(L_\lambda^{vv} + L_\lambda^{\overline{vv}})} + \lambda \int_{s=0}^{t} e^{(t-s)(L_\lambda^{vv} + L_\lambda^{\overline{vv}})} (Q^{v\overline{v}} + Q^{\overline{v}v}) e^{sL_\lambda}\, \mathrm{d}s.$$

Using this formula one gets

$$\mathbf{1}^{vv} e^{\lambda^{-2}\tau L_\lambda} \mathbf{1}^{vv} = \mathbf{1}^{vv} e^{\lambda^{-2}\tau L_\lambda^{vv}} + \int_{\sigma=0}^{\tau} \mathbf{1}^{vv} e^{\lambda^{-2}(\tau-\sigma)L_\lambda^{vv}} K(\lambda, \tau - \sigma) \mathbf{1}^{vv} e^{\lambda^{-2}\sigma L_\lambda} \mathbf{1}^{vv}\, \mathrm{d}\sigma.$$

Now we discuss how one can obtain the van Hove limit for the resolvents under time-dependent assumptions. In fact we show when one can use both stationary and time-dependent approaches. We will concentrate on the case without the first order term.

Theorem 3.5: *Let Assumptions 3.A and 3.B hold. Assume additionally that*

(i) *for* $0 \leqslant \lambda < \lambda_0$ *and all* $z \in \mathbb{C}$, $\mathrm{Re}\, z > 0$ *we have* $z \notin \mathrm{sp}(L_\lambda^{\overline{vv}})$,

(ii) $\int_0^\infty \sup_{0 \leqslant \lambda < \lambda_0} \| Q^{v\overline{v}} e^{sL_\lambda^{\overline{vv}}} Q^{\overline{v}v} \| \mathrm{d}s < \infty$,

(iii) *for any* $s > 0$, $\lim_{\lambda \searrow 0} Q^{v\overline{v}} e^{sL_\lambda^{\overline{vv}}} Q^{\overline{v}v} = Q^{v\overline{v}} e^{sL_0^{\overline{vv}}} Q^{\overline{v}v}$.

Then

(1) *The assumptions of both Theorem 3.2 and Theorem 3.4 hold. Moreover, we have*

$$K^\natural = \Gamma.$$

(2) *The following limits exist, coincide and equal to* Γ:

$$\lim_{\epsilon \searrow 0} \sum_{e \in \mathrm{sp}\, E} \mathbf{1}_e(E) Q^{v\overline{v}} ((e + \epsilon)\mathbf{1}^{\overline{vv}} - L_0^{\overline{vv}})^{-1} Q^{\overline{v}v} \mathbf{1}_e(E)$$

$$= \lim_{\epsilon \searrow 0} \sum_{e \in \mathrm{sp}\, E} \int_0^\infty e^{-\epsilon s} \mathbf{1}_e(E) Q e^{sL_0} Q e^{-sL_0} \mathbf{1}_e(E) \mathrm{d}s. \tag{3.14}$$

Note that the assumptions of Theorem 3.5 are stronger than that of Theorem 3.3 and Theorem 3.4 (2).

The operator (3.14) is often called the level shift operator. It is used to describe the second order shift of eigenvalues of L_λ.[7,9–11]

IV. PROOFS

Lemma 4.1: For $0 \leqslant \lambda < \lambda_0$ *the operator*

$$\widetilde{L}_\lambda = \begin{bmatrix} 0 & \lambda Q^{v\overline{v}} \\ \lambda Q^{\overline{v}v} & L_0^{\overline{vv}} + \lambda Q^{\overline{v}v} \end{bmatrix}$$

defined on $\mathrm{Dom}(\widetilde{L}_\lambda) = \mathcal{X}^v \oplus \mathrm{Dom}(L_0^{\overline{vv}})$ *generates a semigroup of contractions on* $\mathcal{X}$.

Proof: Let $0 \leqslant \lambda < \lambda_0$. The operator $\widetilde{L}_\lambda$ is densely defined. By the Lumer-Phillips theorem

(Theorem 3.1.16 in Ref. 3) it is sufficient to show that (I) $\widetilde{L}_\lambda$ is dissipative, (II) for some $\epsilon>0$ we have $\epsilon \notin \mathrm{sp}(\widetilde{L}_\lambda)$.

Step (I): For $0\leqslant\lambda$ the operator,

$$Z := L_\lambda - L_\lambda^{v\overline{v}}$$

with the domain $\mathrm{Dom}(Z)=\mathrm{Dom}(E)\oplus\mathrm{Dom}(L_0^{\overline{v}\overline{v}})$ is densely defined and dissipative. Hence, by Proposition 3.1.15 in Ref. 3, Z is closable and its closure is dissipative. But the closure of Z coincides with $\widetilde{L}_\lambda$.

Step (II): For $0\leqslant\lambda<\lambda_0$ the operator $L_\lambda-\lambda(Q^{v\overline{v}}+Q^{\overline{v}v})$ generates a semigroup such that for $\mathrm{Re}\, z>\|\lambda(Q^{v\overline{v}}+Q^{\overline{v}v})\|$ we have $z\notin \mathrm{sp}(L_\lambda-\lambda(Q^{v\overline{v}}+Q^{\overline{v}v}))$ and

$$\|(z\mathbf{1}-(L_\lambda-\lambda(Q^{v\overline{v}}+Q^{\overline{v}v})))^{-1}\|\leqslant(\mathrm{Re}\, z-\|\lambda(Q^{v\overline{v}}+Q^{\overline{v}v})\|)^{-1}.$$

Hence, for all $\epsilon>\epsilon_0$ for some ϵ_0 large enough,

$$\|(\epsilon\mathbf{1}-(\widetilde{L}_\lambda-\lambda(Q^{v\overline{v}}+Q^{\overline{v}v})))^{-1}(\lambda(Q^{v\overline{v}}+Q^{\overline{v}v}))\|<1.$$

Hence, by the Neumann theorem, $\epsilon\mathbf{1}-\widetilde{L}_\lambda$ is invertible for all $\epsilon\geqslant\epsilon_0$, and so $\epsilon\notin\mathrm{sp}(\widetilde{L}_\lambda)$. □

By the Feshbach projection method,[1,2,7,8] if $z\notin\mathrm{sp}(L_\lambda)\cup\mathrm{sp}(L_\lambda^{\overline{v}\overline{v}})$ then the restricted resolvent is given by

$$\mathbf{1}^{vv}(z\mathbf{1}-L_\lambda)^{-1}\mathbf{1}^{vv}=G_v^{-1}(z),$$

where

$$G_v(z)=z\mathbf{1}^{vv}-E-\lambda Q^{vv}-\lambda^2Q^{v\overline{v}}(z\mathbf{1}^{\overline{v}\overline{v}}-L_\lambda^{\overline{v}\overline{v}})^{-1}Q^{\overline{v}v}.$$

Hence

$$\mathbf{1}^{vv}(\xi-\lambda^{-2}L_\lambda)^{-1}\mathbf{1}^{vv}=\lambda^2G_v^{-1}(\lambda^2\xi).$$

In what follows we will use these facts without a comment. (See Refs. 4 and 15–17.)

Proof of Theorem 3.1:

(1) By Lemma 4.1, the operator $\widetilde{L}_\lambda$ generates a semigroup of contractions, which for $\xi>0$ implies

$$\|(\xi\mathbf{1}^{vv}-\lambda^2Q^{v\overline{v}}(\xi\mathbf{1}^{\overline{v}\overline{v}}-L_\lambda^{\overline{v}\overline{v}})^{-1}Q^{\overline{v}v})^{-1}\|=\|\mathbf{1}^{vv}(\xi\mathbf{1}-\widetilde{L}_\lambda)^{-1}\mathbf{1}^{vv}\|\leqslant\xi^{-1}.$$

Hence, for all $\xi>\xi_0>0$, the operator $(\xi\mathbf{1}^{vv}-Q^{v\overline{v}}(\lambda^2\xi\mathbf{1}^{\overline{v}\overline{v}}-L_\lambda^{\overline{v}\overline{v}})^{-1}Q^{\overline{v}v})^{-1}$ is uniformly bounded. We know that for any $\xi>0$,

$$\lim_{\lambda\searrow0}(\xi\mathbf{1}^{\overline{v}\overline{v}}-Q^{v\overline{v}}(\xi\lambda^2\mathbf{1}^{\overline{v}\overline{v}}-L_\lambda^{\overline{v}\overline{v}})^{-1}Q^{\overline{v}v})=\xi\mathbf{1}^{\overline{v}\overline{v}}-\Gamma_0. \tag{4.1}$$

Therefore, for all $\xi>\xi_0$, the operator $\xi\mathbf{1}^{vv}-\Gamma_0$ is invertible on $\mathcal{X}^v$ and

$$\|(\xi\mathbf{1}^{vv}-\Gamma_0)^{-1}\|\leqslant\xi^{-1}.$$

Hence Γ_0 generates a semigroup of contractions on $\mathcal{X}^v$ (Theorem 2.21 and Corollary 2.22 in Ref. 6).

(2) Let $0\leqslant\lambda<\lambda_0$. Since $E+\lambda Q^{vv}$ generates a group of isometries and Γ_0 is bounded and dissipative then the result follows from Theorem 3.1.32 in Ref. 3.

(3) Let $0<\lambda<\lambda_0$. Recall that for $\xi>0$,

$$\|\lambda^2G_v^{-1}(\lambda^2\xi)\|\leqslant\xi^{-1}, \tag{4.2}$$

$$\|(\xi \mathbf{1}^{v\bar{v}} - \lambda^{-2} A_{\lambda,0})^{-1}\| \leqslant \xi^{-1}, \tag{4.3}$$

$$\lim_{\lambda \searrow 0} Q^{v\bar{v}} (\lambda^2 \xi \mathbf{1}^{\bar{v}\bar{v}} - L_\lambda^{\bar{v}\bar{v}})^{-1} Q^{\bar{v}\bar{v}} = \Gamma_0. \tag{4.4}$$

For any $\xi > 0$ we have

$$\begin{aligned} &\|\mathbf{1}^{vv}(\xi \mathbf{1} - \lambda^{-2} L_\lambda)^{-1} \mathbf{1}^{vv} - (\xi \mathbf{1}^{vv} - \lambda^{-2} A_{\lambda,0})^{-1}\| \\ &\quad = \|\lambda^2 G_v^{-1}(\lambda^2 \xi)(Q^{v\bar{v}}(\lambda^2 \xi \mathbf{1}^{\bar{v}\bar{v}} - L_\lambda^{\bar{v}\bar{v}})^{-1} Q^{\bar{v}\bar{v}} - \Gamma_0)(\xi \mathbf{1}^{vv} - \lambda^{-2} A_{\lambda,0})^{-1}\|. \end{aligned}$$

Hence by (4.2)–(4.4) the RHS of the above expression tends to zero as λ tends to zero.

(4) For $\xi > 0$, by the Laplace transform, we have

$$\mathbf{1}^{vv}(\xi \mathbf{1} - \lambda^{-2} L_\lambda)^{-1} \mathbf{1}^{vv} - (\xi \mathbf{1}^{vv} - \lambda^{-2} A_{\lambda,0})^{-1} = \int_0^\infty e^{-\xi\sigma} (\mathbf{1}^{vv} e^{\lambda^{-2}\sigma L_\lambda} \mathbf{1}^{vv} - e^{\lambda^{-2}\sigma A_{\lambda,0}}) \mathrm{d}\sigma.$$

Hence by (3.4) we get

$$\lim_{\lambda \searrow 0} \int_0^\infty e^{-\xi\sigma} (\mathbf{1}^{vv} e^{\lambda^{-2}\sigma L_\lambda} \mathbf{1}^{vv} - e^{\lambda^{-2}\sigma A_{\lambda,0}}) \mathrm{d}\sigma = 0. \tag{4.5}$$

By the Stone–Weierstrass theorem, the family of functions

$$[0, \infty[\ni \sigma \mapsto e^{-\xi\sigma} \in \mathbb{R}, \quad \xi > 0$$

forms an algebra which is dense in continuous functions of compact support on $[0, \infty[$. This fact together with (4.5) implies (3.5). □

Lemma 4.2: Let E be the generator of a group of isometries. Let e be an isolated point in $\mathrm{sp}(E)$. *Then e is a semisimple eigenvalue which means $E\mathbf{1}_e(E) = e\mathbf{1}_e(E)$ and $\|\mathbf{1}_e(E)\| = 1$.*

Proof: Let e be an isolated point in $\mathrm{sp}(E)$. Then for any $\epsilon > 0$,

$$\|((e + \epsilon)\mathbf{1}^{vv} - E)^{-1}\| \leqslant \epsilon^{-1}. \tag{4.6}$$

So for $z \in \{z \in \mathbb{C} : \mathrm{dist}(e, z) < \delta\} \setminus \{e\}$ for some $\delta > 0$ we have

$$(z\mathbf{1}^{vv} - E)^{-1} = \mathbf{1}_e(E)(z - e)^{-1} + h(z), \tag{4.7}$$

where h is an analytic function on $\{z \in \mathbb{C} : \mathrm{dist}(e, z) < \delta\}$. Hence e is semisimple. But (4.7) also implies that

$$\lim_{\epsilon \searrow 0} \epsilon((e + \epsilon)\mathbf{1}^{vv} - E)^{-1} = \mathbf{1}_e(E)$$

and hence, by (4.6), we get $\|\mathbf{1}_e(E)\| = 1$. □

For an isolated point $e \in \mathrm{sp}\, E$ let us write for shortness

$$\mathbf{1}^{ee} := \mathbf{1}_e(E), \quad \mathbf{1}^{\underline{e}\underline{e}} := \mathbf{1}^{vv} - \mathbf{1}_e(E),$$

$$\mathcal{X}^e := \mathrm{Ran}\, \mathbf{1}_e(E), \quad \mathcal{X}^{\underline{e}} := \mathrm{Ran}\, \mathbf{1}^{\underline{e}\underline{e}}$$

then

$$\mathcal{X}^v = \mathcal{X}^e \oplus \mathcal{X}^{\underline{e}}. \tag{4.8}$$

If $e', e \in \mathrm{sp}\, E$ and $A \in B(\mathcal{X}^v)$ then we denote $A^{e'e} := \mathbf{1}^{e'e'} A \mathbf{1}^{ee}$.

Proof of Theorem 3.2: (2) follows immediately if we note that Lemma 4.2 implies $E = \Sigma_{e \in \mathrm{sp}\, E} e\mathbf{1}_e(E)$ and that we have $\Gamma := \Sigma_{e \in \mathrm{sp}\, E} \mathbf{1}_e(E) \Gamma \mathbf{1}_e(E)$.

(3) Let $e \in \mathrm{sp}\, E$. Set

$$G_\lambda(\xi,e) := \xi \mathbf{1}^{v v} + \lambda^{-2}(e\mathbf{1}^{v v} - E) - Q^{v\bar{v}}((\lambda^2\xi + e)\mathbf{1}^{\bar{v}\bar{v}} - L_\lambda^{\bar{v}\bar{v}})^{-1}Q^{\bar{v}v}.$$

For $\xi > 0$ we have

$$G_\lambda(\xi,e)^{-1} = \mathbf{1}^{v v}(\xi + \lambda^{-2}(e - L_\lambda))^{-1}\mathbf{1}^{v v}.$$

This and the dissipativity of L_λ implies the bound

$$\|G_\lambda(\xi,e)^{-1}\| \leqslant \xi^{-1}. \tag{4.9}$$

Write for shortness G instead of $G_\lambda(\xi,e)$.

Decompose $G = G_{\mathrm{diag}} + G_{\mathrm{off}}$ into its diagonal and off-diagonal part,

$$G_{\mathrm{diag}} := \sum_{e' \in \mathrm{sp}\, E} \mathbf{1}^{e'e'} G \mathbf{1}^{e'e'},$$

$$G_{\mathrm{off}} := \sum_{e' \in \mathrm{sp}\, E} \mathbf{1}^{e'e'} G \mathbf{1}^{\underline{e}'\underline{e}'} = \sum_{e' \in \mathrm{sp}\, E} \mathbf{1}^{\underline{e}'\underline{e}'} G \mathbf{1}^{e'e'}.$$

First we would like to show that for $\xi > 0$ and small enough λ, G_{diag} is invertible. By the Neumann theorem, it is easy to see that $\mathbf{1}^{\underline{e}\underline{e}} G_{\mathrm{diag}}$ is invertible on $\mathrm{Ran}\, \mathbf{1}^{\underline{e}\underline{e}}$ for small enough λ. Moreover, we have

$$\|\mathbf{1}^{\underline{e}\underline{e}} G_{\mathrm{diag}}^{-1}\| \leqslant c\lambda^2. \tag{4.10}$$

It is more complicated to prove that $\mathbf{1}^{ee} G_{\mathrm{diag}}$ is invertible on $\mathrm{Ran}\, \mathbf{1}^{ee}$.

We fix $\xi > 0$. We know that G is invertible and $\|G^{-1}\| \leqslant \xi^{-1}$. Hence we can write

$$G_{\mathrm{diag}} G^{-1} = 1 - G_{\mathrm{off}} G^{-1}.$$

Therefore

$$\mathbf{1}^{ee} G_{\mathrm{diag}} G^{-1} = \mathbf{1}^{ee} - \mathbf{1}^{ee} G_{\mathrm{off}} \mathbf{1}^{\underline{e}\underline{e}} G^{-1},$$

$$\mathbf{1}^{\underline{e}\underline{e}} G_{\mathrm{diag}} G^{-1} = \mathbf{1}^{\underline{e}\underline{e}} - \mathbf{1}^{\underline{e}\underline{e}} G_{\mathrm{off}} G^{-1}. \tag{4.11}$$

The latter identity can be for small enough λ transformed into

$$\mathbf{1}^{\underline{e}\underline{e}} G^{-1} = G_{\mathrm{diag}}^{-1} \mathbf{1}^{\underline{e}\underline{e}} - G_{\mathrm{diag}}^{-1} \mathbf{1}^{\underline{e}\underline{e}} G_{\mathrm{off}} G^{-1}. \tag{4.12}$$

We insert (4.12) into the first identity of (4.11) to obtain

$$\mathbf{1}^{ee} G_{\mathrm{diag}} G^{-1} = \mathbf{1}^{ee} - \mathbf{1}^{ee} G_{\mathrm{off}} \mathbf{1}^{\underline{e}\underline{e}} G_{\mathrm{diag}}^{-1} + \mathbf{1}^{ee} G_{\mathrm{off}} \mathbf{1}^{\underline{e}\underline{e}} G_{\mathrm{diag}}^{-1} G_{\mathrm{off}} G^{-1}. \tag{4.13}$$

We multiply (4.13) from the right by $\mathbf{1}^{ee}$ to get

$$\mathbf{1}^{ee} G_{\mathrm{diag}} \mathbf{1}^{ee} G^{-1} \mathbf{1}^{ee} = \mathbf{1}^{ee} + \mathbf{1}^{ee} G_{\mathrm{off}} \mathbf{1}^{\underline{e}\underline{e}} G_{\mathrm{diag}}^{-1} G_{\mathrm{off}} G^{-1} \mathbf{1}^{ee}. \tag{4.14}$$

Now, using

$$\lim_{\lambda \searrow 0} \|\lambda G_{\mathrm{off}}\| = 0, \tag{4.15}$$

(4.9) and (4.10) we obtain

$$\lim_{\lambda \searrow 0} \mathbf{1}^{ee} G_{\mathrm{off}} \mathbf{1}^{\underline{e}\underline{e}} G_{\mathrm{diag}}^{-1} G_{\mathrm{off}} G^{-1} \mathbf{1}^{ee} = 0.$$

Thus, for small enough λ,

$$\mathbf{1}^{ee}G_{\mathrm{diag}}B_1 = \mathbf{1}^{ee},$$

where

$$B_1 := \mathbf{1}^{ee}G^{-1}\mathbf{1}^{ee}(\mathbf{1}^{ee} + \mathbf{1}^{ee}G_{\mathrm{off}}\mathbf{1}^{\underline{ee}}G_{\mathrm{diag}}^{-1}G_{\mathrm{off}}G^{-1}\mathbf{1}^{ee})^{-1}.$$

Similarly, for small enough λ, we find B_2 such that

$$B_2\mathbf{1}^{ee}G_{\mathrm{diag}} = \mathbf{1}^{ee}.$$

This implies that $\mathbf{1}^{ee}G_{\mathrm{diag}}$ is invertible on $\mathrm{Ran}\,\mathbf{1}^{ee}$.

Next, we can write

$$G^{-1} = G_{\mathrm{diag}}^{-1} - G_{\mathrm{diag}}^{-1}G_{\mathrm{off}}G_{\mathrm{diag}}^{-1} + G_{\mathrm{diag}}^{-1}G_{\mathrm{off}}G_{\mathrm{diag}}^{-1}G_{\mathrm{off}}G^{-1}.$$

Hence

$$\mathbf{1}^{ee}G^{-1} = \mathbf{1}^{ee}G_{\mathrm{diag}}^{-1}(\mathbf{1} - G_{\mathrm{off}}\mathbf{1}^{\underline{ee}}G_{\mathrm{diag}}^{-1} + G_{\mathrm{off}}\mathbf{1}^{\underline{ee}}G_{\mathrm{diag}}^{-1}G_{\mathrm{off}}G^{-1}). \tag{4.16}$$

Therefore, for a fixed ξ, by (4.9), (4.10), and (4.15), we see that as $\lambda \searrow 0$ we have

$$-G_{\mathrm{off}}\mathbf{1}^{\underline{ee}}G_{\mathrm{diag}}^{-1} + G_{\mathrm{off}}\mathbf{1}^{\underline{ee}}G_{\mathrm{diag}}^{-1}G_{\mathrm{off}}G^{-1} \to 0.$$

Therefore, for small enough λ, we can invert the expression in the prentheses of (4.16). Consequently,

$$\begin{aligned}\mathbf{1}^{ee}(G_{\mathrm{diag}}^{-1} - G^{-1}) = \mathbf{1}^{ee}G^{-1}&(1 - G_{\mathrm{off}}\mathbf{1}^{\underline{ee}}G_{\mathrm{diag}}^{-1} + G_{\mathrm{off}}\mathbf{1}^{\underline{ee}}G_{\mathrm{diag}}^{-1}G_{\mathrm{off}}G^{-1})^{-1}\\ &\times (G_{\mathrm{off}}\mathbf{1}^{\underline{ee}}G_{\mathrm{diag}}^{-1} - G_{\mathrm{off}}\mathbf{1}^{\underline{ee}}G_{\mathrm{diag}}^{-1}G_{\mathrm{off}}G^{-1}).\end{aligned} \tag{4.17}$$

Therefore, for a fixed ξ, by (4.9), (4.10), and (4.15), we see that as $\lambda \searrow 0$ we have

$$\mathbf{1}^{ee}(G_{\mathrm{diag}}^{-1} - G^{-1}) \to 0. \tag{4.18}$$

Equations (4.9) and (4.18) imply that $\mathbf{1}^{ee}G_{\mathrm{diag}}^{-1}$ is uniformly bounded as $\lambda \searrow 0$. We know that

$$\mathbf{1}^{ee}G_{\mathrm{diag}} \to \mathbf{1}^{ee}\xi - \mathbf{1}^{ee}\Gamma. \tag{4.19}$$

Therefore, $\xi\mathbf{1}^{ee} - \mathbf{1}^{ee}\Gamma$ is invertible on $\mathrm{Ran}\,\mathbf{1}^{ee}$ and

$$\mathbf{1}^{ee}G_{\mathrm{diag}}^{-1} \to (\mathbf{1}^{ee}\xi - \mathbf{1}^{ee}\Gamma)^{-1}.$$

Using again (4.18) we see that

$$\mathbf{1}^{ee}G^{-1} \to (\mathbf{1}^{ee}\xi - \mathbf{1}^{ee}\Gamma)^{-1}. \tag{4.20}$$

Summing up (4.20) over e we obtain

$$\sum_{e\in \mathrm{sp}\,E} \mathbf{1}^{ee}G_{\lambda}(\xi,e)^{-1} \to (\xi\mathbf{1}^{vv} - \Gamma)^{-1}, \tag{4.21}$$

which ends the proof of (3).

(1) We have

$$\sum_{e\in \mathrm{sp}\,E} \mathbf{1}^{ee}G_{\lambda}(\xi,e)^{-1} = \sum_{e\in \mathrm{sp}\,E}\int_0^{\infty} e^{-t(\xi+\lambda^{-2}e)}\mathbf{1}^{ee}e^{tL_{\lambda}/\lambda^2}\mathbf{1}^{vv}\,\mathrm{d}t = \int_0^{\infty} e^{-t\xi}e^{-tE/\lambda^2}\mathbf{1}^{vv}e^{tL_{\lambda}/\lambda^2}\mathbf{1}^{vv}\,\mathrm{d}t. \tag{4.22}$$

Clearly, $\|e^{-tE/\lambda^2}\mathbf{1}^{vv}e^{tL_{\lambda}/\lambda^2}\mathbf{1}^{vv}\| \leqslant 1$. Therefore,

$$\left\| \sum_{e \in \operatorname{sp} E} \mathbf{1}^{ee} G_\lambda(\xi,e)^{-1} \right\| \leqslant \xi^{-1}.$$

Hence, by (4.21),

$$\|(\xi \mathbf{1}^{vv} - \Gamma)^{-1}\| \leqslant \xi^{-1},$$

which means that Γ is the generator of a semigroup of contractions.

(4) To prove this we repeat the argument used in the proof of Theorem 3.1.

Proof of Theorem 3.3:

(1) Follows by a simple modification of the argument used in Theorem 3.2.

(2) For $e \in \operatorname{sp} E$ and for $\operatorname{Re} \xi > 0$ we denote

$$G_\lambda(\xi,e) := \xi \mathbf{1}^{vv} + \lambda^{-2}(e\mathbf{1}^{vv} - E) - Q^{v\overline{v}}((\lambda^2\xi + e)\mathbf{1}^{\overline{v}\overline{v}} - L_\lambda^{\overline{v}\overline{v}})^{-1} Q^{\overline{v}v}.$$

Obviously

$$G_\lambda(\xi,e)^{-1} = \mathbf{1}^{vv}(\xi + \lambda^{-2}(e - L_\lambda))^{-1}\mathbf{1}^{vv}$$

and

$$\|G_\lambda(\xi,e)^{-1}\| \leqslant \operatorname{Re} \xi^{-1}. \tag{4.23}$$

Let $\psi \in \mathcal{X}^v$. Let $\omega_0 > 0$ and $\sigma \geqslant 0$. By the inverse Laplace transform (Ref. 12 Chap. XI) and by the proof of Theorem 3.2, uniformly for $0 < \tau_0 \leqslant \sigma \leqslant \tau_1$, we get

$$\begin{aligned}
&(e^{-\sigma\lambda^{-2}E}\mathbf{1}^{vv}e^{\sigma\lambda^{-2}L_\lambda}\mathbf{1}^{vv} - e^{\sigma\Gamma})\psi \\
&\quad = \frac{1}{2\pi i} \lim_{R\to\infty} \int_{\omega_0 + i[-R,R]} e^{\sigma\xi} \sum_{e \in \operatorname{sp} E} (\mathbf{1}^{ee}((\xi + \lambda^{-2}e)\mathbf{1} - \lambda^{-2}L_\lambda)^{-1}\mathbf{1}^{vv} - (\xi\mathbf{1}^{ee} - \Gamma^{ee})^{-1})\psi \, \mathrm{d}\xi \\
&\quad = \frac{1}{2\pi i} \sum_{e \in \operatorname{sp} E} \lim_{R\to\infty} \int_{-R}^{R} f_\lambda(y,e) i \, \mathrm{d}y,
\end{aligned}$$

where

$$f_\lambda(y,e) := e^{\sigma(\omega_0 + iy)}(\mathbf{1}^{ee}G_\lambda(\omega_0 + iy,e)^{-1} - ((\omega_0 + iy)\mathbf{1}^{ee} - \Gamma^{ee})^{-1})\psi.$$

For each $e \in \operatorname{sp} E$,

$$\left\| \frac{d}{dy} f_\lambda(y,e) \right\| \leqslant e^{\sigma\omega_0} 2(\sigma\omega_0^{-1} + \omega_0^{-2})\|\psi\|.$$

This shows that the family $f_\lambda(y,e)$ is equicontinuous as $\lambda \to 0$.

For any fixed $R > 0$ if only $\alpha_0 = (R+1)/\omega_0$ then $\xi = \omega_0 + iy \in \operatorname{Wedge}(0,\alpha_0)$ hence, by (1), we get the pointwise convergence $f_\lambda(y,e) \to 0$ as $\lambda \searrow 0$ for $y \in [-R,R]$. Finally pointwise convergence together with equicontinuity implies uniform convergence on compacts, so for any fixed $R > 0$,

$$\lim_{\lambda \searrow 0} \int_{-R}^{R} f_\lambda(y,e)\psi i \, \mathrm{d}y = \int_{-R}^{R} \lim_{\lambda \searrow 0} f_\lambda(y,e)\psi i \, \mathrm{d}y = 0.$$

To end the proof it is sufficient to show that for each $e \in \operatorname{sp} E$,

$$\lim_{R\to\infty} \sup_{0 \leqslant \lambda < \lambda_0} \left\| \int_{|y|>R} f_\lambda(y,e) i \, \mathrm{d}y \right\| = 0.$$

Since Γ^{ee} is independent of λ we need only to show that

$$\lim_{R\to\infty}\sup_{0\leqslant\lambda<\lambda_0}\left\|\int_{|y|>R} e^{\sigma(\omega_0+iy)}\mathbf{1}^{ee}G_\lambda(\omega_0+iy,e)^{-1}\psi\,\mathrm{d}y\right\|=0. \tag{4.24}$$

Decompose $G_\lambda(\xi,e)$ into its diagonal and off-diagonal part,

$$G_{\mathrm{diag}}:=\sum_{e'\in\mathrm{sp}\,E}\mathbf{1}^{e'e'}G_\lambda(\xi,e)\mathbf{1}^{e'e'}=\xi\mathbf{1}^{ee}-T_\lambda(\xi,e)^{ee}+\sum_{e'\in\mathrm{sp}\,E;e'\neq e}((\xi-\lambda^{-2}(e'-e))\mathbf{1}^{e'e'}$$
$$-T_\lambda(\xi,e)^{e'e'}),$$

$$G_{\mathrm{off}}:=\sum_{e'\in\mathrm{sp}\,E}\mathbf{1}^{e'e'}G_\lambda(\xi,e)\mathbf{1}^{e'\underline{e}'}=\sum_{e'\in\mathrm{sp}\,E}\mathbf{1}^{e'\underline{e}'}G_\lambda(\xi,e)\mathbf{1}^{e'e'}=\sum_{e'\in\mathrm{sp}\,E}T_\lambda(\xi,e)^{e'\underline{e}'},$$

where

$$T_\lambda(\xi,e):=Q^{v\overline{v}}((\lambda^2\xi+e)\mathbf{1}^{\overline{v}\overline{v}}-L_0^{\overline{v}\overline{v}}-\lambda Q^{\overline{v}\overline{v}})^{-1}Q^{\overline{v}v}.$$

By the assumption for each $e\in\mathrm{sp}\,E$

$$\sup_{\mathrm{Re}\,\xi>0;0\leqslant\lambda<\lambda_0}\|T_\lambda(\xi,e)\|<C<\infty. \tag{4.25}$$

In the rest of the proof we write for shortness $G=G_\lambda(\xi,e)$ and $T=T_\lambda(\xi,e)$.

Fix $e\in\mathrm{sp}\,E$ and let $\xi:=\omega_0+iy$. Fix $\omega_0>C+1$. Then, by the Neumann theorem, the operator $\mathbf{1}^{ee}G_{\mathrm{diag}}=\xi\mathbf{1}^{ee}-T^{ee}$ is invertible on $\mathcal{X}^e$ and we have

$$\|(\xi\mathbf{1}^{ee}-T^{ee})^{-1}\|\leqslant(|y|-C)^{-1}\quad\text{for }|y|>C. \tag{4.26}$$

Note that for each $e'\in\mathrm{sp}\,E$, $e'\neq e$ the operator $\lambda^{-2}(e'-e)\mathbf{1}^{e'e'}$ generates a group of isometries on $\mathcal{X}^{e'}$. Hence the operator $\mathbf{1}^{e'e'}G_{\mathrm{diag}}=(\xi-\lambda^{-2}(e'-e))\mathbf{1}^{e'e'}-T^{e'e'}$ is invertible on $\mathcal{X}^{e'}$ and we have

$$\|((\xi-\lambda^{-2}(e'-e))\mathbf{1}^{e'e'}-T^{e'e'})^{-1}\|\leqslant(\omega_0-C)^{-1}<1. \tag{4.27}$$

This shows that G_{diag} is invertible on $\mathcal{X}^v$. We have

$$\mathbf{1}^{ee}G^{-1}=\mathbf{1}^{ee}G_{\mathrm{diag}}^{-1}(\mathbf{1}^{ee}-G_{\mathrm{off}}\mathbf{1}^{\underline{e}e}G^{-1})=\xi^{-1}(\mathbf{1}^{ee}+T^{ee}(\xi\mathbf{1}^{ee}-T^{ee})^{-1})(\mathbf{1}^{ee}-G_{\mathrm{off}}\mathbf{1}^{\underline{e}e}G^{-1})$$
$$=\xi^{-1}(\mathbf{1}^{ee}+T^{ee}(\xi\mathbf{1}^{ee}-T^{ee})^{-1})(\mathbf{1}^{ee}-G_{\mathrm{off}}\mathbf{1}^{\underline{e}e}G_{\mathrm{diag}}^{-1}+G_{\mathrm{off}}\mathbf{1}^{\underline{e}e}G_{\mathrm{diag}}^{-1}G_{\mathrm{off}}\mathbf{1}^{ee}G^{-1}).$$

Now, using (4.23) and (4.25)–(4.27), we get for $|y|>C$,

$$\|\xi^{-1}T^{ee}(\xi\mathbf{1}^{ee}-T^{ee})^{-1}(\mathbf{1}^{ee}-G_{\mathrm{off}}\mathbf{1}^{\underline{e}e}G^{-1})\|\leqslant D_1(\omega_0^2+y^2)^{-1/2}(|y|-C)^{-1}$$

$$\|\xi^{-1}G_{\mathrm{off}}\mathbf{1}^{\underline{e}e}G_{\mathrm{diag}}^{-1}G_{\mathrm{off}}\mathbf{1}^{ee}G^{-1}\|\leqslant D_1(\omega_0^2+y^2)^{-1/2}(|y|-C)^{-1}$$

for some $D_1>0$ independent of λ. Hence to prove (4.24) if suffices to show that

$$\lim_{R\to\infty}\sup_{|\lambda|<\lambda_0}\left\|\int_{|y|>R}e^{\sigma(\omega_0+iy)}(\omega_0+iy)^{-1}(\mathbf{1}^{ee}-G_{\mathrm{off}}\mathbf{1}^{\underline{e}e}G_{\mathrm{diag}}^{-1})\psi\,\mathrm{d}y\right\|=0.$$

The first term in the above expression is independent of λ hence we need only to consider the second term. We have

$$\mathbf{1}^{\underline{e}e}G_{\mathrm{diag}}^{-1}=\sum_{e'\in\mathrm{sp}\,E;e'\neq e}(\xi-\lambda^{-2}(e'-e))^{-1}(\mathbf{1}^{e'e'}+T^{e'e'}((\xi-\lambda^{-2}(e'-e))\mathbf{1}^{e'e'}-T^{e'e'})^{-1}).$$

Hence, by (4.25) and (4.27), we get

$$\|e^{\sigma(\omega_0+iy)}(\omega_0+iy)^{-1}G_{\mathrm{off}}\mathbf{1}^{\underline{ee}}G_{\mathrm{diag}}^{-1}\| \leqslant D_2 g(y)g(y-\lambda^{-1}\,\mathrm{Im}(e'-e)) \tag{4.28}$$

for some $D_2>0$ independent of λ, where

$$\mathbb{R} \ni y \mapsto g(y) := (\omega_0^2+y^2)^{-1/2} \in \mathbb{R}.$$

By the Hölder inequality

$$\int_{|y|>R} g(y)g(y-\lambda^{-1}\,\mathrm{Im}(e'-e))\mathrm{d}y \leqslant \|g\|_{L^2(]-\infty,-R]\cup[R,\infty[,\mathrm{dx})}\|g\|_{L^2(\mathbb{R},\mathrm{dx})} \to 0. \tag{4.29}$$

Now, by (4.28) and (4.29), we get

$$\left\| \int_{|y|>R} e^{\sigma(\omega_0+iy)}(\omega_0+iy)^{-1}G_{\mathrm{off}}\mathbf{1}^{\underline{ee}}G_{\mathrm{diag}}^{-1}\psi\,\mathrm{d}y \right\| \to 0$$

independently of λ. This ends the proof of (3.10). □

Proof of Theorem 3.5: Set

$$f(s) := \sup_{|\lambda|<\lambda_0} \|Q^{v\overline{v}}e^{sL_\lambda^{\overline{vv}}}Q^{\overline{v}v}\|.$$

We know that $f(t)$ is integrable.

For any $e \in i\mathbb{R}$ and $\xi \geqslant 0$ we can dominate the integrand in the integral,

$$F_\lambda(e,\xi) := \int_0^\infty Q^{v\overline{v}}e^{sL_\lambda^{\overline{vv}}}Q^{\overline{v}v}e^{-(e+\lambda^2\xi)s}\,\mathrm{d}s = Q^{v\overline{v}}(\mathbf{1}^{\overline{vv}}(e+\lambda^2\xi)-L_\lambda^{\overline{vv}})^{-1}Q^{\overline{v}v} \tag{4.30}$$

by $f(s)$. Hence, using the dominated convergence theorem we see that $F_\lambda(e,\xi)$ is continuous at $\lambda=0$ and $\xi\geqslant 0$. But

$$\sum_{e\in\mathrm{sp}\,E}\mathbf{1}_e(E)F_0(e,0)\mathbf{1}_e(E) = \sum_{e\in\mathrm{sp}\,E}\lim_{\lambda\to 0}\mathbf{1}_e(E)Q^{v\overline{v}}(\mathbf{1}^{\overline{vv}}(e+\lambda^2\xi)-L_\lambda^{\overline{vv}})^{-1}Q^{\overline{v}v}\mathbf{1}_e(E) = \Gamma.$$

Recall (3.11), the definition of $K(\lambda,t)$,

$$K(\lambda,t) := \int_0^{\lambda^{-2}t} e^{-sE}Q^{v\overline{v}}e^{sL_\lambda^{\overline{vv}}}Q^{\overline{v}v}\,\mathrm{d}s.$$

Its integrand can also be dominated by $f(s)$. Hence, using again the dominated convergence theorem, we see that, for $\lambda\to 0$, $K(\lambda,t)$ is convergent to

$$K = \int_0^\infty e^{-sE}Q^{v\overline{v}}e^{sL_0^{\overline{vv}}}Q^{\overline{v}v}\,\mathrm{d}s.$$

Therefore,

$$K^\natural = \sum_{e\in\mathrm{sp}\,E}\mathbf{1}_e(E)\int_0^\infty e^{-es}Q^{v\overline{v}}e^{sL_0^{\overline{vv}}}Q^{\overline{v}v}\,\mathrm{d}s\,\mathbf{1}_e(E) = \sum_{e\in\mathrm{sp}\,E}1_e(E)F_0(e,0)\mathbf{1}_e(E).$$

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Wigner measures dynamics in a Coulomb potential

Sahbi Keraani[a)]
IRMAR, Université de Rennes 1, Campus de Beaulieu, 35 042 Rennes Cedex, France

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In this paper, we are concerned with the propagation of the Wigner measure of a family of solutions to the semiclassical Schrödinger evolution equation with potential having Coulomb-type singularities in *three* space dimensions. We prove that after *collision* the Wigner measure is reflected by the potential singularities under the *regularized flow* as in classical mechanics. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1924705]

I. INTRODUCTION AND RESULTS

We consider the semiclassical Schrödinger evolution equation

$$i\varepsilon\partial_t v^\varepsilon = H^\varepsilon v^\varepsilon, \quad (t,x) \in \mathbb{R}\times\mathbb{R}^d,$$
$$v^\varepsilon(0,x) = v_I^\varepsilon(x) \in L^2(\mathbb{R}^d). \tag{1.1}$$

Here, ε is a small parameter and v_I^ε is a bounded family of $L^2(\mathbb{R}^d)$. The semiclassical Schrödinger operator $H^\varepsilon = -(\varepsilon^2/2)\Delta + U(x)$ is assumed to be self-adjoint on $L^2(\mathbb{R}^d)$. The self-adjointness of H^ε implies the following conservation law:

$$\int_{\mathbb{R}^d} |v^\varepsilon(t,x)|^2 \mathrm{d}x = \int_{\mathbb{R}^d} |v_I^\varepsilon(x)|^2 \mathrm{d}x, \quad \forall\, t \in \mathbb{R}.$$

A main question in the semiclassical theory is to calculate the homogenized density $\eta(t,x)$ (the limit as positive Radon measure when ε goes to 0) of the quadratic quantity

$$\eta^\varepsilon = |v^\varepsilon(t,x)|^2,$$

called *quantum position density*.

A basic tool in this context is some positive measure in the phase space called *Wigner measure*. It was developed independently by Gérard[3] and Lions and Paul.[10] Roughly speaking, and under appropriate assumptions on the family of the initial data v_I^ε, the homogenized density $\eta(t,x)$ is obtained as the moment in ξ-space of the Wigner measure associated to (v_t^ε). [Note that, throughout this paper, v_t^ε denotes the function $x \mapsto v^\varepsilon(t,x)$.]

$$\eta(t,x) = \int_{\mathbb{R}^d_\xi} \nu_t(x, \mathrm{d}\xi).$$

The main advantage of this approach is that this measure can be calculated by solving a transport equation with initial data related to v_I^ε.

In Ref. 3 (see also Refs. 6 and 10) it has been shown that if the potential is smooth then

a)Electronic mail: sahbi.keraani@univ-rennes1.fr

$$\nu_t = \phi_t(\nu_I), \tag{1.2}$$

where ϕ_t is the classical classical Hamiltonian flow $\exp(tH_p)$ of

$$p = \frac{|\xi|^2}{2} + U(x)$$

and ν_I is the Wigner measure of v_I^ε.

In the context of frequency sets (see, e.g., Ref. 12), a classical result of propagation similar to (1.2) is well known. In *three* space dimensions, an interesting extension of this result to a potential with Coulomb-type singularities has been performed by Gérard and Knauf.[2] In fact, these authors have proved that the frequency set of the solution to (1.1) with $d=3$ and $U=-1/|x|$, is reflected by the Coulomb center $x=0$ under the regularized trajectories of the classical mechanics (see Sec. III for precise definitions). Gérard and Knauf's technique is based on the idea of applying to the quantum problem a method of regularization used in the corresponding classical problem in celestial mechanics and known as *Kustaanheimo-Stiefel* transformation (see Sec. III).

The main purpose of this paper is to perform the same extension in the context of Wigner measures. More precisely, by making use of similar arguments to those carried out in Ref. 2 in the context of frequency sets, and some refined lemmas on propagation of Wigner measures, we attempt to describe the dynamics of the Wigner measure associated to the solution to the semiclassical Schrödinger evolution equation

$$\begin{aligned} i\varepsilon\partial_t v^\varepsilon &= -\frac{\varepsilon^2}{2}\Delta v^\varepsilon - \frac{v^\varepsilon}{|x|} + V(x)v^\varepsilon, \quad (t,x) \in \mathbb{R}\times\mathbb{R}^3, \\ v^\varepsilon(0,x) &= v_I^\varepsilon(x), \end{aligned} \tag{1.3}$$

where V is a smooth real potential with sufficient decay at infinity and v_I^ε is a bounded family in $L^2(\mathbb{R}^3)$. [In this paper we do not discuss the optimal assumptions on V. We assume always that V has all the needed properties (for example, we need some control of V at infinity in order to guarantee that Hamiltonian is self-adjoint).]

Before going further into details, we fix some notations.

Notation: (i) $\dot{\mathbb{R}}^d := \mathbb{R}^d\backslash\{0\}$.

(ii) If Ω *is an open subset of* $\mathbb{R}^d$ *then* $\mathbf{T}^*(\Omega) := \Omega\times\mathbb{R}^d$.

We now recall the definition and the basic properties of Wigner measures that we use in the coming analysis. For more details, the reader is referred to Refs. 3, 6, and 10.

For $a \in \mathcal{S}(\mathbb{R}^d\times\mathbb{R}^d)$ we define the ε-dependent family of pseudo-differential operators $A^\varepsilon = a(x,\varepsilon D)$ by

$$a(x,\varepsilon D)u(x) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d_\xi}\int_{\mathbb{R}^d_y} a(x,\varepsilon\xi)e^{i(x-y)\xi}u(y)\mathrm{d}y\,\mathrm{d}\xi,$$

for every $u \in \mathcal{S}'$. Notice that for every family (u^ε) bounded in $L^2(\mathbb{R}^d)$ we have

$$\limsup_{\varepsilon\to 0}\|a(x,\varepsilon D)u^\varepsilon\|_{L^2(\mathbb{R}^d_x)} \leqslant \|a\|_{L^\infty}\limsup_{\varepsilon\to 0}\|u^\varepsilon\|_{L^2(\mathbb{R}^d_x)}.$$

The following basic result is due to Gérard[3] and Lions and Paul.[10]

Theorem 1.1 (Refs. 3 and 10): *Let* (ψ^ε) *be a bounded family in* $L^2(\mathbb{R}^d)$. *Then there are a subsequence, still denoted by* ψ^ε, *and a positive Radon measure* ν *on* $\mathbf{T}^*(\mathbb{R}^d)$, *such that*

$$\langle a(x,\varepsilon D)\psi^\varepsilon,\psi^\varepsilon\rangle \xrightarrow[\varepsilon\to 0]{} \int_{\mathbb{R}^d_x\times\mathbb{R}^d_\xi} a(x,\xi)\nu(\mathrm{d}x\,\mathrm{d}\xi) \tag{1.4}$$

for every $a \in \mathcal{S}(\mathbb{R}^d\times\mathbb{R}^d)$. *Moreover,*

$$\|\nu\|_{\mathcal{M}} \leqslant \limsup_{\varepsilon\to 0}\|\psi^{\varepsilon}\|_{L^2(\mathbb{R}^d_x)},$$

where $\|\cdot\|_{\mathcal{M}}$ *denotes the norm in the space of bounded Radon measures*.

In this context, μ is called *Wigner* measure of (ψ^{ε}). The bounded family (ψ^{ε}) is said to be *pure* if the extraction of a subsequence in (1.4) is not needed.

The proof of the existence is based essentially on an argument of separability of the space $\mathcal{S}(\mathbb{R}^d\times\mathbb{R}^d)$. The positivity can be proved in several ways; in Ref. 3 the proof uses a Gärding inequality and in Ref. 4 a more elementary proof is given, where a Bochner–Schwartz theorem is used. In Ref. 10 the proof relies on some Gaussian regularization trick.

Remark 1.2: Theorem 1 holds for every family (ψ^{ε}) *bounded in* $L^2_{\mathrm{loc}}(\Omega)$, *where* $\Omega\subset\mathbb{R}^d$ *is an open set. In this case* μ *is locally bounded on* Ω_x *and globally bounded on* $\mathbb{R}^d_{\xi}$.

To describe the relationship between Wigner measure and the weak limit of $|\psi^{\varepsilon}|^2$, we need the two following definitions.

Definition 1.3: (1) *A bounded family* (ψ^{ε}) *in* $L^2(\mathbb{R}^d)$ *is said to be* ε*-oscillatory as* ε *goes to 0 if the following property holds for every continuous, compactly supported function* φ *on* $\mathbb{R}^d$:

$$\limsup_{\varepsilon\to 0}\int_{|\xi|\geqslant R/\varepsilon}|\widehat{\varphi\psi^{\varepsilon}}(\xi)|^2\mathrm{d}\xi \xrightarrow[R\to+\infty]{} 0.$$

(2) *A bounded family* (ψ^{ε}) *in* $L^2(\mathbb{R}^d)$ *is said to be compact at infinity as* ε *goes to 0 if*

$$\limsup_{\varepsilon\to 0}\int_{|x|\geqslant R}|\psi^{\varepsilon}(x)|^2\mathrm{d}x \xrightarrow[R\to+\infty]{} 0.$$

Under the above definitions we have the following.

Proposition 1.4 (Refs. 3 and 10): *Let* (ψ^{ε}) *be a bounded family in* $L^2(\mathbb{R}^d)$ *with Wigner measure* μ. *Then*

(1) *The measure* μ *is bounded on* $\mathbb{R}^d\times\mathbb{R}^d$ *and, if* $|\psi^{\varepsilon}|^2 \rightharpoonup m$ *as measure on* $\mathbb{R}^d$, *we have, in the sense of positive measure,*

$$\int_{\mathbb{R}^d}\mu(\cdot,\mathrm{d}\xi)\leqslant m,$$

with equality if and only if (ψ^{ε}) *is* ε*-oscillatory*.

(2) *We have*

$$\mu(\mathbb{R}^d\times\mathbb{R}^d)\leqslant\limsup_{\varepsilon\to 0}\int_{\mathbb{R}^d}|\psi^{\varepsilon}(x)|^2\mathrm{d}x,$$

with equality if and only if (ψ^{ε}) *is* ε*-oscillatory and compact at infinity*.

The Wigner measure is defined independently of the coordinates.

Proposition 1.5 (Ref. 5): *Let* θ *be a* $\mathcal{C}^{\infty}$*-diffeomorphism from* Ω_1 *onto* Ω_2. *Suppose that* (ψ_2^{ε}) *is a pure bounded family in* $L^2_{\mathrm{loc}}(\Omega_2)$. *Then* $\psi_1^{\varepsilon}:=\psi_2^{\varepsilon}\circ\theta$ *is a pure bounded family in* $L^2_{\mathrm{loc}}(\Omega_1)$ *and the Wigner measure* ν_1 *of the family* (ψ_1^{ε}) *is given by*

$$\nu_1=|\det\theta'|^{-1}\Theta^{-1}(\nu_2),$$

where ν_2 *is the Wigner measure of the family* (ψ_2^{ε}) and Θ *is the canonical transformation on* $\mathbf{T}^*(\Omega_1)$ *given by*

$$(x,\xi)\mapsto(\theta(x),{}^T\theta'^{-1}(x)\xi)^3.$$

[Note that ${}^TA$ are used to denote the transposed of a matrix A.]

Consider a particle with mass 1 moving in three-dimensional space according to the laws of classical mechanics, subject to a perturbed Coulomb potential

$$U(x) = -\frac{1}{|x|} + V.$$

The classical motion of the particle is described by the Hamiltonian system

$$\dot{\mathbf{x}} = \boldsymbol{\xi}$$

$$\dot{\boldsymbol{\xi}} = -\frac{\mathbf{x}}{|\mathbf{x}|^3} - \nabla V(\mathbf{x}), \tag{1.5}$$

$$(\mathbf{x}, \xi)_{|_{t=0}} = (x_0, \xi_0) \in \dot{\mathbb{R}}^3 \times \mathbb{R}^3.$$

The standard ODE theory yields a unique maximal solution to (1.5) on some interval $[0, t^*[$. If $t^* < +\infty$, then there is *a collision*: the particle hits the singularity of the potential in finite time t^*. A natural question in such a situation is how one can extend the trajectory after the collision time.

Let us consider the one-dimension motion in the special case of purely Coulomb potential (i.e., $V \equiv 0$) and zero Kepler energy

$$h_K := \frac{1}{|x_0|} - \frac{|\xi_0|^2}{2} = 0.$$

By assuming $\mathbf{x}(t) \geqslant 0$, the equation of motion is reduced to

$$\dot{\mathbf{x}}(t) = \sqrt{\frac{2}{\mathbf{x}(t)}},$$

which yields $\mathbf{x}(t) = Ct^{2/3}$. The particle comes in from the infinity, is reflected at the central mass, and rejected to infinity. The outgoing leg of its path is symmetrical with respect to the incoming leg.

With this example in mind, we define an *extension* of the trajectory after collision as follows: take $(x_0, \xi_0) \in \mathbf{T}^*(\dot{\mathbb{R}}^3)$ and assume that the classical trajectory reaches the origin $x = 0$ at finite time t^*. Then, the extension of this trajectory after t^* is obtained by adding the branch of the trajectory of the same particle ejected from $x = 0$, with infinite velocity in the opposite of the incoming direction.

To make this definition more precise, let us first notice that the direction of collision, when it happens, is well defined. Indeed, we have the following:

Lemma 1.6: Assume that the solution of (1.5) *collides with the origin* $x = 0$ *in a finite time* t^*. *Then, there exists a unique* $v = v(x_0, \xi_0, t^*) \in \mathbb{R}^3$, *such that*

$$\frac{\boldsymbol{\xi}(t)}{|\boldsymbol{\xi}(t)|} \xrightarrow[t \to (t^*)^-]{} v.$$

See Appendix B for the proof of this fact.

With these notations the definition of the extended trajectories can be given by

Definition 1.7: The extended flow is the mapping $\tilde{\phi}: \mathbb{R}_t \times \mathbf{T}^*(\dot{\mathbb{R}}^3) \to \mathbf{T}^*(\dot{\mathbb{R}}^3)$ *defined by*

$$\tilde{\phi}_t(x_0, \xi_0) = \begin{cases} \phi_t(x_0, \xi_0) & \text{if } t < t^* \\ \hat{\phi}_t(x_0, \xi_0) & \text{if } t > t^*, \end{cases}$$

where $\phi_t(x_0, \xi_0)$ *is the usual Hamiltonian trajectory and* $\hat{\phi}_t(x_0, \xi_0)$ *is the trajectory of the same particle ejected from* $x = 0$ *at* $t = t^*$ *with infinite velocity in the direction* $-v(x_0, \xi_0, t^*)$.

The extended trajectory is formed by two legs: the incoming one, which ends up in $x = 0$ with infinite velocity in the direction $v(x_0, \xi_0, t^*)$ and the outgoing one, which starts from $x = 0$ with

infinite velocity in the opposite direction $-v(x_0,\xi_0,t^*)$. For the case of many collisions on the same trajectory we iterate the process of extension described above. For purely Coulomb potential, the extended trajectory is obtained by following backward the incoming collision trajectory. This extension corresponds physically to an elastic bounce. Note that, outside the collision, the extended flow is the same as the usual one.

In the sequel we *denote* by $\mathrm{Coll}_t=\{(x,\xi)\in \mathbf{T}^*(\dot{\mathbb{R}}^3):\Pi_x(\tilde{\phi}_s(x,\xi))\underset{s\to t}{\to}0\}$ the collisions set at time t.

The main result of this paper can be stated as follows.

Theorem 1.8: *Take v_I^ε to be a bounded pure family in $L^2(\mathbb{R}^3)$, ε-oscillatory and compact at infinity, such that ν_I is supported in $\mathbf{T}^*(\dot{\mathbb{R}}^3)$. Let v^ε be the solution of* (1.3) *with initial data v_I^ε. Then one has:*

(i) *the family v_t^ε is pure on $\dot{\mathbb{R}}^3$ and its Wigner measure ν_t satisfies*

$$\nu_{t|_{x\neq 0}}=\tilde{\phi}_t(\nu_{I|_{\mathbb{R}^3\setminus \mathrm{Coll}_t}}).$$

(ii) *If $\nu_I(\mathrm{Coll}_t)=0$, then the family v_t^ε is pure, ε-oscillatory and compact at infinity. In addition,*

$$\nu_t=\tilde{\phi}_t(\nu_I).$$

Some remarks are in order.

Remark 1.9: The proof of the main theorem is based on two essential arguments. The first one is the fundamental fact that the extended trajectory coincides with the regularized trajectory defined by Kustaanheimo–Stiefel transformation in the context of the regularization theory in celestial mechanics (see Lemma 3.4 below). The second main argument is a new result of propagation of Wigner measure through singular regions (see Lemma 2.2 below for precise statement).

Remark 1.10: Main theorem holds for a potential displaying several Coulomb-type singularities

$$\sum_{i=1}^{N}\frac{c_i}{|x-x_i|}+V,$$

where $x_i\in\mathbb{R}^3$, $c_i\in\mathbb{R}$ for $i=1,\ldots,N$ and V is a smooth real bounded potential. The definition 1.7 can be generalized in a natural way to a potential of this type.

Remark 1.11: It is an open problem to describe ν_t over $x=0$. Even the question of uniqueness of ν_t (if (v_t^ε) is pure on $\mathbb{R}^3$ or not) is not solved.

The plan of the rest of the paper is as follows. In Sec. II some lemmas related to the propagation of Wigner measures are formulated. In Sec. III we recall the definitions and some properties of the regularized flows and the KS-transformation and we prove some preliminary results needed to the proof of the main theorem of this work, which is given in Sec. III. In the Appendixes some technical lemmas are proved.

II. PROPAGATION OF WIGNER MEASURES

We consider the initial values problem

$$\begin{aligned}&\varepsilon D_t u^\varepsilon+P^\varepsilon u^\varepsilon=0,\quad (t,x)\in\mathbb{R}^{1+d},\\ &u^\varepsilon(0,x)=u_I^\varepsilon(x),\end{aligned}\tag{2.1}$$

where $P^\varepsilon=p(x,\varepsilon D_x)$ is a semiclassical differential operator and (u_I^ε) is a bounded family in $L^2(\mathbb{R}^d)$. The self-adjointness of P^ε implies the conservation of the L^2 norm of the family of solution (u^ε). Thus, the family (u_t^ε) is bounded in $L^2(\mathbb{R}^d)$ for every $t\in\mathbb{R}$ [recall that, throughout this paper, (u_t^ε) denotes the function $x\mapsto u^\varepsilon(t,x)$] and the family (u^ε) is bounded in $L^2_{\mathrm{loc}}(\mathbb{R}_t\times\mathbb{R}_x^d)$. This allows us to

define two types of Wigner measures associated to the family (u^ε) of solutions to (2.1). The first one, $\mu=\mu(\mathrm{d}x\,\mathrm{d}t\,\mathrm{d}\xi\,\mathrm{d}\tau)$, is obtained by microlocalization in the space–time variable. The second one, $\mu_t=\mu_t(\mathrm{d}x\,\mathrm{d}\xi)$, is obtained by microlocalization in the space variable at fixed time.

Proposition 2.1: Take (u_I^ε) *to be a bounded pure family in* $L^2(R^d)$, *ε-oscillatory and compact at infinity. Let* (u^ε) *be the solution of* (2.1) *with initial data* $u^\varepsilon(0,x)=u_I^\varepsilon(x)$. *Then*:

(i) *For every* $t\in R$ *the family* (u_t^ε) *is pure, ε-oscillatory and compact at infinity. In addition,* μ_t *is given by*

$$\mu_t=\phi_t(\mu_I),$$

where ϕ_t *is the classical classical Hamiltonian flow* $\exp(tH_p)$ *of* p.

(ii) $\mu=dt\otimes\delta_{(\tau+p(x,\xi))}\otimes\phi_t(\mu_I)$.

We consider a family $(u^\varepsilon)\in L^2(\mathbb{R}^d)$ of solutions to

$$P^\varepsilon u^\varepsilon=0, \tag{2.2}$$

where $P^\varepsilon=p(x,\varepsilon D_x)$ is an ε-pseudodifferential operator with smooth real symbol. It is well known (see Refs. 3 and 10) that if the family (u^ε) is bounded in $L^2_{\mathrm{loc}}(\mathbb{R}^d)$ then any Wigner measure associated to this family is transported by the bicharacteristic of p. More precisely,

$$\mathrm{supp}(\mu)\subset\{(x,\xi)\in\mathbf{T}^*(\mathbb{R}^d):p(x,\xi)=0\}\ \text{and}\ H_p\mu=0,$$

where $H_p=\nabla_\xi p.\nabla_x-\nabla_x p.\nabla_\xi$, is the Hamiltonian field associated to p. This result remains true if the (u^ε) is bounded in $L^2_{\mathrm{loc}}(\Omega)$, where Ω is an open set of $\mathbb{R}^d$ provided that all the bicharacteristics of p starting from Ω are contained in Ω. In this paragraph we consider the case where some bicharacteristic of p starting from Ω cross some "black box" F in which the measure μ is not defined. More precisely, we prove the following refined lemma on the propagation of Wigner measure.

Lemma 2.2: Let $(u^\varepsilon)\in L^2(\mathbb{R}^d)$ *be a family of solutions to* $P^\varepsilon u^\varepsilon=0$, *where* $P^\varepsilon=p(x,\varepsilon D_x)$ *is an ε-pseudodifferential operator with smooth real symbol. Assume that*

(H1) (u^ε) *is bounded in* $L^2_{\mathrm{loc}}(\Omega)$, *for some open set* $\Omega\subset\mathbb{R}^d$.

(H2) *There exists an integer* ℓ, *such that* $(\varepsilon^\ell u^\varepsilon)$ *is bounded in* $L^2_{\mathrm{loc}}(\mathbb{R}^d)$.

Let μ *denote the Wigner measure of* $(u^\varepsilon_{|\Omega})$. *Then, for every* $\omega\Subset\mathbf{T}^*(\Omega)$ *and every* $s_0\in\mathbb{R}$, *such that* $\omega_{s_0}=\phi_{s_0}(\omega)\Subset\mathbf{T}^*(\Omega)$, *we have*

$$\mu_{|\omega_{s_0}}=\phi_{s_0}(\mu_{|\omega}),$$

where ϕ_t *is the classical Hamiltonian flow* $\exp(tH_p)$ *of* p.

Proof: Take $\psi\in\mathcal{C}_0^\infty(\mathbf{T}^*(\omega_{s_0}))$ be an arbitrary fixed function. Our aim is to show that

$$\langle\psi(x,\varepsilon D)u^\varepsilon,u^\varepsilon\rangle\xrightarrow[\varepsilon\to0]{}\int_{\mathbf{T}^*(\omega)}\psi(\phi_{s_0}(x,\xi))\mu(\mathrm{d}x\,\mathrm{d}\xi). \tag{2.3}$$

We use a classical argument of propagation of singularities in microlocal analysis. We introduce a new variable $s\in\mathbb{R}$ and we consider u^ε as depending also on this new variable. The family (u^ε) is solution of the following evolution equation with respect to s:

$$\varepsilon D_s u^\varepsilon+P^\varepsilon u^\varepsilon=0.$$

One constructs an operator $\Psi^\varepsilon(s,x,\varepsilon D_x)$, so that

$$[\varepsilon D_s + P^\varepsilon, \Psi^\varepsilon(s,x,\varepsilon D_x)] = \mathcal{O}(\varepsilon^\infty) \text{ in } \mathcal{L}(L^2([-s_0,0]\times\mathbb{R}^d)),$$

$$\Psi^\varepsilon(0,x,\varepsilon D_x) = \psi(x,\varepsilon D_x).$$

To meet these conditions, the operator $\Psi^\varepsilon(s,\cdot,\cdot)$ is chosen as a formal series in the following form:

$$\Psi^\varepsilon = \sum_{j\geqslant 0} \varepsilon^j \psi_j(s,x,\varepsilon D).$$

The construction of such operator is similar to that carried out in Ref. 7 (Chap. XXIII) in the context of propagation of wave front. We will use essentially the following three facts:

(i) For every $s\in\mathbb{R}$, one has

$$\psi_0(s,x,\xi) = \psi(\phi_{-s}(x,\xi)). \tag{2.4}$$

(ii) For every $j\geqslant 0$ and every $s\in\mathbb{R}$,

$$\text{supp}(\psi_j(s,\cdot)) \subset \phi_s(\text{supp}(\psi)).$$

(iii) The partial sum $\Psi_k^\varepsilon = \Sigma_{j=0}^k \varepsilon^j \psi_j$ verifies

$$\|[\varepsilon D_s + P^\varepsilon, \Psi_k^\varepsilon(s,x,\varepsilon D)]\|_{\mathcal{L}(L^2([-s_0,0]\times\mathbb{R}^d))} = \mathcal{O}(\varepsilon^{k+1}).$$

Under the above notations, we have

$$(\varepsilon D_s + P^\varepsilon)\Psi_k^\varepsilon u^\varepsilon = f_k^\varepsilon, \tag{2.5}$$

where $f_k^\varepsilon = [\varepsilon D_s + P^\varepsilon, \Psi_k^\varepsilon]u^\varepsilon$. By construction and (H2), it follows that

$$\|f_k^\varepsilon\|_{L^2([-s_0,0]\times\mathbb{R}^d)} \leqslant \|[\varepsilon D_s + P^\varepsilon, \Psi_k^\varepsilon]\|_{\mathcal{L}(L^2([-s_0,0]\times\mathbb{R}^d))} \|u^\varepsilon\|_{L^2([-s_0,0]\times\mathbb{R}^d)} \lesssim \varepsilon^{k+1-\ell}. \tag{2.6}$$

However, from (2.5), it ensues

$$\frac{\mathrm{d}}{\mathrm{d}s}\langle \Psi_k^\varepsilon(s,x,\varepsilon D_x)u^\varepsilon, u^\varepsilon\rangle = \frac{i}{\varepsilon}\langle f_k^\varepsilon, u^\varepsilon\rangle.$$

Since the family of s-dependent operators $\Psi_k^\varepsilon(s,x,\varepsilon D_x)$ is bounded in $\mathcal{L}(L^2(\mathbb{R}^d))$ uniformly in $(s,\varepsilon)\in[-s_0,0]\times]0,1]$, and by using (2.6) and (H2), we get

$$\left|\frac{\mathrm{d}}{\mathrm{d}s}\langle \Psi_k^\varepsilon(s,x,\varepsilon D_x)u^\varepsilon, u^\varepsilon\rangle\right| = \mathcal{O}(\varepsilon)$$

uniformly in $s\in[-s_0,0]$ for $k>2\ell$. This yields, in particular,

$$|\langle \Psi_k^\varepsilon(-s_0,x,\varepsilon D_x)u^\varepsilon, u^\varepsilon\rangle - \langle \Psi_k^\varepsilon(0,x,\varepsilon D_x)u^\varepsilon, u^\varepsilon\rangle| = \mathcal{O}(\varepsilon),$$

that is

$$\lim_{\varepsilon\to 0}\langle \Psi_k^\varepsilon(-s_0,x,\varepsilon D_x)u^\varepsilon, u^\varepsilon\rangle = \lim_{\varepsilon\to 0}\langle \Psi_k^\varepsilon(0,x,\varepsilon D_x)u^\varepsilon, u^\varepsilon\rangle.$$

Since $\Psi_k^\varepsilon(0,\cdot) = \psi$, this gives

$$\lim_{\varepsilon\to 0}\langle \Psi_k^\varepsilon(-s_0,x,\varepsilon D_x)u^\varepsilon, u^\varepsilon\rangle = \lim_{\varepsilon\to 0}\langle \psi(x,\varepsilon D_x)u^\varepsilon, u^\varepsilon\rangle. \tag{2.7}$$

On the other hand, since, for every $j\in\{1,\ldots,k\}$, $\text{supp}(\psi_j(-s_0,\cdot,\cdot))\subset\mathbf{T}^*(\omega)$ and (u^ε) is bounded in $L^2_{\text{loc}}(\Omega)$, the family $(\psi_j(-s_0,x,\varepsilon D_x)u^\varepsilon)$ is bounded in $L^2(\mathbb{R}^d)$. [Recall that

$\mathrm{supp}(\psi_j(-s_0,\cdot,\cdot,\cdot)) \subset \phi_{-s_0}(\mathrm{supp}(\psi))$ and $\mathrm{supp}(\psi) \subset \phi_{s_0}(\mathbf{T}^*(\omega))$.] Thus, we infer

$$\lim_{\varepsilon\to 0}\langle \Psi_k^\varepsilon(-s_0,x,\varepsilon D_x)u^\varepsilon,u^\varepsilon\rangle = \lim_{\varepsilon\to 0}\langle \psi_0(-s_0,x,\varepsilon D_x)u^\varepsilon,u^\varepsilon\rangle. \tag{2.8}$$

This fact and (2.7) imply

$$\lim_{\varepsilon\to 0}\langle \psi(x,\varepsilon D_x)u^\varepsilon,u^\varepsilon\rangle = \lim_{\varepsilon\to 0}\langle \psi(-s_0,x,\varepsilon D_x)u^\varepsilon,u^\varepsilon\rangle. \tag{2.9}$$

Since $\psi_0(-s_0,x,\xi)=\psi(\phi_{s_0}(x,\xi))$ is supported in $\mathbf{T}^*(\omega)$, then by definition of the Wigner measure it follows that

$$\lim_{\varepsilon\to 0}\langle \psi(-s_0,x,\varepsilon D_x)u^\varepsilon,u^\varepsilon\rangle = \int_{\mathbf{T}^*(\omega)} \psi_0(-s_0,x,\xi))\,\nu(\mathrm{d}x\,\mathrm{d}\xi). \tag{2.10}$$

Putting together (2.4), (2.9), and (2.10), one obtains

$$\lim_{\varepsilon\to 0}\langle \psi^\varepsilon(x,\varepsilon D_x)u^\varepsilon,u^\varepsilon\rangle = \int_{\mathbf{T}^*(\omega)} \psi(\phi_{s_0}(x,\xi))\,\nu(\mathrm{d}x\,\mathrm{d}\xi),$$

which is (2.3). □

III. REGULARIZED FLOWS AND KS-TRANSFORMATION

The classical motion of a particle subject to a Coulomb potential

$$-\frac{1}{|x|}+V(x)$$

is described by the following Hamiltonian system:

$$\begin{aligned}\dot{x}(t)&=\xi(t),\\ \dot{\xi}(t)&=-\frac{x(t)}{|x(t)|^3}-\nabla V(x(t)).\end{aligned} \tag{3.1}$$

This system is singular at the origin since the attraction force of the central mass is infinite at this point. It is a very unpleasant fact, namely from the numerical point of view. It is thus interesting to transform the singular system (3.1) into a regular one. This procedure is called *regularization*. It is an old theory in celestial mechanics starting with the paper of Euler[1] in 1767. The principle of this theory is to eliminate, by an appropriate change of space–time coordinates, the singularities of the vectors fields solutions of (3.1) and to obtain an equation of motion which is regular for the considered collision. [Note that the purpose of the regularization theory is to obtain a regular differential equation of motion and not regular solutions.] The planar perturbed problem was regularized by Levi-Civita[9] and the spatial case by Kustaanheimo.[8] The *Kustaanheimo–Stiefel* transformation (abbreviated to KS-transformation) is the basic idea in the spatial case. In Secs. III A and III B we recall the regularized flows and the KS transformation (see Ref. 13 for more details).

A. Regularized flows

Without details we single out the explicit construction of the regularized flows provided by Kustaanheimo–Stiefel transformation. For more details the reader is referred to Ref. 13 (Chaps. II, X). For $z\in\dot{\mathbb{R}}^4$ one sets

$$L(z)=\begin{pmatrix} z_1 & -z_2 & -z_3 & z_4 \\ z_2 & z_1 & -z_4 & -z_3 \\ z_3 & z_4 & z_1 & z_2 \\ z_4 & -z_3 & z_2 & -z_1 \end{pmatrix}, \quad \Lambda(z)=\begin{pmatrix} z_1 & -z_2 & -z_3 & z_4 \\ z_2 & z_1 & -z_4 & -z_3 \\ z_3 & z_4 & z_1 & z_2 \end{pmatrix}. \tag{3.2}$$

The matrix L, called KS-matrix, satisfies

$$L^T(z)L(z)=|z|^2 I.$$

The KS-transformation is the mapping of $\mathbb{R}^4$ onto the physical space $\mathbb{R}^3$ of Cartesian coordinates x_1,x_2,x_3, given by $x=\Lambda(z)z$. This may be written explicitly

$$x_1=z_1^2-z_2^2-z_3^2+z_4^2, \quad x_2=2(z_1z_2-z_3z_4), \quad x_3=2(z_1z_3+z_2z_4).$$

From this it follows that

$$|x|=|\Lambda(z)z|=|z|^2. \tag{3.3}$$

To construct the regularized trajectory starting from the point $(x_0,\xi_0)\in \mathbf{T}^*(\dot{\mathbb{R}}^3)$, one proceeds as follows. First, one chooses $(z_0,\zeta_0)\in \mathbf{T}^*(\dot{\mathbb{R}}^4)$ satisfying

$$x_0=\Lambda(z_0)z_0, \quad \xi_0=\frac{1}{2|z_0|^2}\Lambda(z_0)\zeta_0. \tag{3.4}$$

One denotes

$$\Lambda^*(z_0,\zeta_0):=\left(\Lambda(z_0)z_0,\frac{1}{2|z_0|^2}\Lambda(z_0)\zeta_0\right). \tag{3.5}$$

The pair $(z_0,\zeta_0)\in \mathbf{T}^*(\dot{\mathbb{R}}^4)$ satisfying (3.4) is not unique, but the regularized flow defined below does not depend on the choice of (z_0,ζ_0) (see Ref. 13 Lemma 2, p. 236). [In order to apply this lemma we have to check that (z_0,ζ_0) belongs to the zero level of the bilinear form: $\ell(z,\zeta)=\langle\overline{z},\zeta\rangle$, where $\overline{z}:=(z_4,-z_3,z_2,-z_1)$. Since $L(z_0)\overline{z_0}=(0,0,0,|z_0|^2)$, then the expression of ζ_0 (3.6) yields $\ell(z_0,\zeta_0)=\langle 2L^T(z_0)(\xi_0,0),\overline{z_0}\rangle=2\langle(\xi_0,0),L(z_0)\overline{z_0}\rangle=0$.] Note that, after having chosen z_0, ζ_0 is uniquely determined by

$$\zeta_0=2L^T(z_0)(\xi_0,0), \tag{3.6}$$

where $(\xi_0,0)$ is the four-vector obtained from ξ_0 by adding the fourth component of value zero and L is as in (3.2). Second, one constructs the integral curves $(\mathbf{t}(s),\mathbf{z}(s),\boldsymbol{\tau}(s),\boldsymbol{\zeta}(s))$ of the Hamiltonian

$$\tilde{p}(t,z,\tau,\zeta)=\tau|z|^2+\tfrac{1}{8}|\zeta|^2-1+W(z) \tag{3.7}$$

starting from $(0,z_0,-p(x_0,\xi_0),\zeta_0)$, where

$$p=\frac{1}{2}|\xi|^2-\frac{1}{|x|}+V(x)$$

is the classical Hamiltonian and $W(z):=|z|^2V(\Lambda(z)z)$. One easily verifies that $\tilde{p}(t_0,z_0,\tau_0,\zeta_0)=0$. The proof of the following lemma is given in Appendix A.

Lemma 3.1: The t-component of every bicharacteristic of $\tilde{p}$ is a bijection from $\mathbb{R}$ onto $\mathbb{R}$.

The regularized flow is defined by

Definition 3.2: The regularized flow is the mapping $\tilde{\phi}:\mathbb{R}_t\times\mathbf{T}^*(\dot{\mathbb{R}}^3)\to\mathbf{T}^*(\dot{\mathbb{R}}^3)$ defined by

$$\tilde{\phi}_t(x_0,\xi_0):=\Lambda^*(\mathbf{z}(s),\boldsymbol{\zeta}(s)) \tag{3.8}$$

where s satisfies $\mathbf{t}(s)=t$. [The existence and uniqueness of s is assured by Lemma 3.1.]

Remark 3.3: Note that Λ^* *is not defined for* $z=0$*; and then* $\tilde{\phi}_t(x_0,\xi_0)$ *exists only if* $\mathbf{z}(s)\neq 0$ [*with* $s=\mathbf{t}^{-1}(t)$]. *Thus, every* (x_0,ξ_0,t) *where* (x_0,ξ_0) *is on a collision orbit and t the collision time are implicitly excluded from the definition* [*for them no such* $\tilde{\phi}_t(x_0,\xi_0)$ *exist*].

For a seek of notations we decompose ϕ_t (and $\tilde{\phi}_t$) as

$$\phi_t(x,\xi)=(\phi_t^1(x,\xi),\phi_t^2(x,\xi)),\quad \phi_t^1=\prod_x(\phi_t),\quad \phi_t^2=\prod_\xi(\phi_t). \tag{3.9}$$

In the proof of the main theorem we use the following

Lemma 3.4: The extended trajectories coincide with the regularized ones.

The proof of this lemma is given in Appendix B.

B. KS-transformation

We begin this section by recalling (see also Ref. 13, p. 32) the explicit construction of the local "inverse" of the KS-transformation. One adds a dummy variable $\theta\in S^1:=[0,2\pi[$. One denotes

$$\Omega=\mathbb{R}^3\setminus\{x\in\mathbb{R}^3: x_2=x_3=0, x_1<0\}. \tag{3.10}$$

Over Ω we consider $\chi: S^1\times\Omega\to\mathbb{R}^4$ defined by

$$z_1=\frac{1}{\sqrt{2}}(x_1+|x|)^{1/2}\cos\theta,$$

$$z_2=\frac{1}{\sqrt{2}}(x_1+|x|)^{-1/2}(x_2\cos\theta+x_3\sin\theta),$$

$$z_3=\frac{1}{\sqrt{2}}(x_1+|x|)^{-1/2}(x_3\cos\theta-x_2\sin\theta),$$

$$z_4=\frac{1}{\sqrt{2}}(x_1+|x|)^{1/2}\sin\theta.$$

Remark that, for a fixed $x\in\dot{\mathbb{R}}^3$, the set $\{\chi(x,\theta),\theta\in S^1\}$ is a curve in $\dot{\mathbb{R}}^4$. Such a curve, which is called the *fiber* in $\mathbb{R}^4$ over x, is mapped by the KS-transform onto the single point x.

Remark 3.5: One denotes

$$\tilde{\Omega}=\mathbb{R}^3\setminus\{x\in\mathbb{R}^3: x_2=x_3=0, x_1>0\}.$$

There exists a "local inverse" $\tilde{\chi}$ *of the KS-transformation defined over* $\tilde{\Omega}$*. In our proof we use these two "local inverses" and a partition of unity to cover* $\dot{\mathbb{R}}^3$*. Since the discussion is the same for* χ *and* $\tilde{\chi}$ *we will work only with* χ*.*

One can check easily that

$$\det(\chi'(\theta,x))=\frac{1}{8|x|}, \tag{3.11}$$

for every $(\theta,x)\in S^1\times\dot{\mathbb{R}}^3$.

One defines the mapping $\Gamma: S^1\times\mathbf{T}^*(\Omega)\mapsto\mathbf{T}^*(\mathbb{R}^4)$ by

$$\Gamma(x,\xi,\theta) = (\chi(x,\theta), 2L^T(\chi(x,\theta))(\xi,0)), \tag{3.12}$$

where L is defined by (3.2) and $(\xi,0)$ is the four-vector obtained from ξ by adding the fourth component of value zero. Under the notations (3.5) and (3.12), we have

$$\Lambda^*(\Gamma(x,\xi,\theta)) = (x,\xi)$$

for every $\theta \in S^1$. Also it is not hard to see that

$$^T(\chi'(x,\theta))^{-1}(\xi,0) = 2L^T(\chi(x,\theta))(\xi,0) \tag{3.13}$$

for every $(\theta,x,\xi) \in S^1 \times \mathbf{T}^*(\dot{\mathbb{R}}^3)$.

The following lemmas will be useful in the proof of the main theorem.

Lemma 3.6: Take $(x,\xi) \in \mathbf{T}^*(\Omega)$ *and* $\theta \in [0,2\pi[$ *to be fixed. Let* $\Phi_s^\theta(x,\xi)$ *denote the classical flow associated to* $\tilde{p}$ *defined by* (3.7) *starting from the point* $(0,-p(x,\xi),\Gamma(x,\xi,\theta))$. [Note that for greater convenience, we will sometimes denote the point in phase space by (t,τ,z,ζ) instead of (t,z,τ,ζ).] *Then there exists* $\kappa > 0$, *such that*

$$\Phi_s^\theta(x,\xi) = (\mathbf{t}(s), -p(x,\xi), \Gamma(\phi_{\mathbf{t}(s)}(x,\xi), \theta + \alpha(x,\xi,\mathbf{t}(s)))), \tag{3.14}$$

for every $s \in]-\kappa,\kappa[$. *Here,* $\mathbf{t}(s)$ *is the inverse of the function* $\mathbf{t}^{-1}$ *given by*

$$\mathbf{t}^{-1}(t) = \int_0^t \frac{1}{|\phi_s^1(x,\xi)|} \mathrm{d}s \tag{3.15}$$

and

$$\alpha(x,\xi,t) := \int_0^t G(\phi_{t'}(x,\xi))\mathrm{d}t',$$

where

$$G(x,\xi) = \frac{x_2\xi_3 - x_3\xi_2}{2(x_1 + |x|)|x|}.$$

Proof: The number κ is chosen sufficiently small, such that (3.14) makes sense. More precisely, we take κ, such that $\phi_{\mathbf{t}(s)}(x,\xi)$ belongs to $\mathbf{T}^*(\Omega)$ for every $s \in]-\kappa,\kappa[$. Since $\phi_{\mathbf{t}(0)}(x,\xi) = \phi_0(x,\xi) = (x,\xi) \in \mathbf{T}^*(\Omega)$ then κ_0 is well defined. By a straightforward computation we can check that (3.14) defines a solution to the Hamiltonian system of $\tilde{p}$ with initial data $\Phi_0^\theta(x,\xi) = (0, -p(x,\xi),\Gamma(x,\xi,\theta))$. Let us remark finally that the application $(x,\xi) \mapsto \kappa(x,\xi)$ is continuous from $\mathbf{T}^*(\Omega)$ onto $]0,+\infty[$. □

Remark 3.7: For large times the expression of $\Phi_s^\theta(x,\xi)$ *is not explicit. Nevertheless, since* $\mathrm{d}\tilde{p}/\mathrm{d}t = 0$, *the* τ*-component is always equal to* $-p(x,\xi)$.

Lemma 3.8: Let Θ *be the canonical transformation*

$$\Theta(t,\tau,x,\theta,\xi,\beta) = (t,\tau,\chi(x,\theta), {}^T(\chi'(x,\theta))^{-1}(\xi,\beta)) \tag{3.16}$$

and $\Phi_s^\theta(x,\xi)$ *the classical flow associated to* $\tilde{p}$ *defined by* (3.7) *starting from the point* $(0, -p(x,\xi),\Gamma(x,\xi,\theta))$. *Then, for every* $\theta \in S^1$ *and every* $s \in \mathbb{R}$, *we have*

$$\prod_{(x,\xi)} [\Theta^{-1}(\Phi_s^\theta(x,\xi))] = \Lambda^*\left(\prod_{(z,\zeta)} (\Phi_s^\theta(x,\xi))\right),$$

where Λ^* *is defined by* (3.5).

See Appendix C for the proof of this lemma.

IV. PROOF OF THE MAIN THEOREM

On $\mathbb{R}_t \times \mathbb{R}^4_z$ we define the transformed function u by

$$u^\varepsilon(t,z) = v^\varepsilon(t, \Lambda(z)z). \tag{4.1}$$

It is easy to check that the mapping $f \mapsto \widetilde{f}$ defined by $\widetilde{f}(z) = f(\Lambda(z)z)$ is isometric from $L^2(\mathbb{R}^3)$ onto $L^2(\mathbb{R}^4, 8|z|^2 \mathrm{d}z)$. An explicit computation yields

Lemma 4.1: (cf. Ref. 2): If v^ε is a solution to (1.3)*, then the function u^ε defined by* (4.1) *satisfies the following equation in $\mathcal{D}'(\mathbb{R}_t \times \mathbb{R}^4_z)$:*

$$i\varepsilon |z|^2 \partial_t u^\varepsilon = -\frac{\varepsilon^2}{8} \Delta_z u^\varepsilon - u^\varepsilon + W(z) u^\varepsilon, \tag{4.2}$$

where $W(z) := |z|^2 V(\Lambda(z)z)$.

The change of variable $x = \Lambda(z)z$ and conservation laws of Eq. (1.3) give

$$\int_{\mathbb{R}^4} |z u^\varepsilon(t,\cdot)|^2 \mathrm{d}z = \frac{1}{8} \int_{\mathbb{R}^3} |v^\varepsilon(t,\cdot)|^2 \mathrm{d}x = \frac{1}{8} \int_{\mathbb{R}^3} |v_I^\varepsilon(x)|^2 \mathrm{d}x.$$

Thus, the family (u^ε) is bounded in $L^2_{\mathrm{loc}}(\mathbb{R}_t \times \dot{\mathbb{R}}^4)$, and we may define a locally bounded Wigner measure on $\mathbf{T}^*(\mathbb{R}_t \times \dot{\mathbb{R}}^4)$ associated to the family $(u^\varepsilon_{|z\neq 0})$. This measure will be denoted by μ. The strategy of the proof is to give a complete description of μ and use the transformation rule of the Wigner measure by the diffeomorphism χ to determine ν_t above $x \neq 0$. Over $x = 0$, we use the principle of conservation of the total mass.

Step 0: In order to use the KS-transform and its local inverse we have to make some extra hypotheses on ν_I. These hypotheses do not break the generality. More precisely, without any loss of generality *we may take v_I^ε to be a bounded pure family in $L^2(\mathbb{R}^d)$, ε-oscillatory and compact at infinity, such that*

$$\|v_I^\varepsilon\|_{H^2(\mathbb{R}^3)} = \mathcal{O}(\varepsilon^{-2}), \tag{4.3}$$

and ν_I is compactly supported in $\mathbf{T}^*(\Omega)$, where Ω is defined by (3.10). Indeed, since $\nu_I(\{0\} \times \mathbb{R}^3_\xi) = 0$ there exists [since $\dot{\mathbb{R}}^3 \times \mathbb{R}^3 = \cup_{v \in S^2} \{sv, s > 0\} \times \mathbb{R}^3_\xi$ is a noncountable disjoint union,] a half line $D^+ = \{sv_0, s \geqslant 0\}$, such that $\nu_I(D^+ \times \mathbb{R}^3_\xi) = 0$. By rotation we may take $D^+ = \{x, x_2 = x_3 = 0, x_1 < 0\} = \mathbb{R}^3 \backslash \Omega$. We introduce the following family of bump functions ψ_k,

$$|\psi_k| \leqslant 1,$$

$$\psi_k(\xi) = 1, \quad |\xi| \leqslant k,$$

$$\psi_k(\xi) = 0, \quad |\xi| \geqslant 2k.$$

Also, we introduce the family ϕ_k,

$$|\phi_k| \leqslant 1,$$

$$\phi_k(x) = 1, \quad \{|x| \leqslant k\} \cap \left\{ -\frac{1}{k} \leqslant x_1, \sqrt{|x_2|^2 + |x_3|^2} \geqslant \frac{1}{k} \right\},$$

$$\phi_k(x) = 0, \quad \{|x| \geqslant 2k\} \cup \left\{ -\frac{1}{2k} \leqslant x_1, \sqrt{|x_2|^2 + |x_3|^2} \leqslant \frac{1}{2k} \right\}.$$

We take

$$v_{I(k)}^{\varepsilon} = \psi_k(\varepsilon D)\phi_k(x)v_I^{\varepsilon}.$$

Under these notations, we have

$$\lim_{\varepsilon\to 0}\|v_{I(k)}^{\varepsilon} - v_I^{\varepsilon}\|_{L^2(\mathbb{R}^3)}^2 = \int (1-\psi_k(\xi)\phi(x))^2 \nu_I(\mathrm{d}x\,\mathrm{d}\xi) \underset{k\to\infty}{\to} 0. \tag{4.4}$$

In the last line we have used the dominated convergence theorem and the fact that $\nu_I(D^+\times\mathbb{R}^3_\xi)=0$.

Let v_k^{ε} be the solution of the Cauchy problem (1.3) with initial data $v_{I(k)}^{\varepsilon}$. From L^2-conservation law and (4.4) it follows that

$$\lim_{\varepsilon\to 0}\|v_k^{\varepsilon}(t,\cdot) - v^{\varepsilon}(t,\cdot)\|_{L^2(\mathbb{R}^3)} = \lim_{\varepsilon\to 0}\|v_{I(k)}^{\varepsilon} - v_I{}^{\varepsilon}\|_{L^2(\mathbb{R}^3)} \underset{k\to\infty}{\to} 0.$$

So, it holds that, for every $t\in\mathbb{R}$,

$$\|\nu_k(t) - \nu_t\|_{\mathcal{M}} \underset{k\to\infty}{\to} 0, \tag{4.5}$$

where $\nu_k(t)$ denotes the Wigner measure associated to $(v_k)^{\varepsilon}(t,\cdot))$ and $\|\cdot\|_{\mathcal{M}}$ the norm in the space of bounded Radon measures. Once the main theorem is proved for the families v_k^{ε}, $k=1,2,\ldots$, it follows for the family v_I^{ε} by (4.5).

Observe finally that since $\psi_k\in\mathcal{C}_0^{\infty}(\mathbb{R}^3)$ then the family (v_k^{ε}) of initial data belongs to $H^2(\mathbb{R}^3)$, for every $k=1,2,\ldots$. Furthermore, it satisfies

$$\|v_{I(k)}^{\varepsilon}\|_{H^2(\mathbb{R}^3)} = \mathcal{O}(\varepsilon^{-2}).$$

The rest of our proof will proceed in three steps.

Step 1: In this short paragraph we give a description of ν_t for small times (before the collision). We choose κ_0 as the minimum over $\mathrm{supp}(\nu_I)$ of the $\kappa(x,\xi)$ defined by Lemma 3.6. Notice that κ_0 is strictly positive because the mapping $(x,\xi)\mapsto\kappa(x,\xi)$ is continuous and the support of ν_I is assumed to be compact. It is evident that

$$\nu_t = \phi_t(\nu_I), \quad t\in\,]-\kappa_0,\kappa_0[,$$

and, thanks to Proposition 2.1,

$$\nu = \mathrm{d}t\otimes\delta_{\tau+p(x,\xi)}\otimes\phi_t(\nu_I), \quad t\in\,]-\kappa_0,\kappa_0[,$$

with ϕ_t denoting the classical Hamiltonian flow of

$$p = \frac{1}{2}|\xi|^2 - \frac{1}{|x|} + V.$$

In order to use the transform χ we consider v^{ε} as a function depending also on the variable θ. The associated Wigner measure becomes

$$\nu_t(\mathrm{d}\theta\,\mathrm{d}\beta\,\mathrm{d}x\,\mathrm{d}\xi) = \mathrm{d}\theta\otimes\delta_{\beta=0}\otimes\nu_t(\mathrm{d}x\,\mathrm{d}\xi), \quad t\in\,]-\kappa_0,\kappa_0[,$$

where $\mathrm{d}\theta$ denotes the Lebesgue measure on $[0,2\pi[$ and $\delta_{\beta=0}$ is the Dirac mass in β the dual variable of θ. In particular,

$$\nu_t(\mathrm{d}\theta\,\mathrm{d}\beta\,\mathrm{d}x\,\mathrm{d}\xi) = \mathrm{d}\theta\otimes\delta_{\beta=0}\otimes\phi_t(\nu_I), \quad t\in\,]-\kappa_0,\kappa_0[,$$

and

$$\nu(\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}\theta\,\mathrm{d}\tau\,\mathrm{d}\xi\,\mathrm{d}\beta) = \mathrm{d}\theta\otimes\delta_{\beta=0}\otimes\mathrm{d}t\otimes\delta_{\tau+p(x,\xi)}\otimes\phi_t(\nu_I), \quad t\in\,]-\kappa_0,\kappa_0[. \tag{4.6}$$

Step 2: This step is devoted to the description of the Wigner measure μ associated to (u^ε). The main result is the following

Proposition 4.2: Under the notation (3.12), *we have*

$$\mu(\mathrm{d}z\,\mathrm{d}t\,\mathrm{d}\zeta\,\mathrm{d}\tau)=\frac{1}{8}\int_0^{2\pi}(\Phi_t^\theta(\nu_I)\otimes \mathrm{d}t)\mathrm{d}\theta, \tag{4.7}$$

where $\Phi_s^\theta(x,\xi)$ *denotes the classical trajectory of the Hamiltonian* $\tilde{p}$ *starting from the point* $(0, -p(x,\xi),\Gamma(x,\xi,\theta))$

Proof: The idea is simple: we use the explicit expression (4.6) and the transformation rule of the Wigner measure by the diffeomorphism χ to determine μ for a small time, and then use Lemma 2.2 to propagate the local explicit information to all the time. We start with the following

Lemma 4.3: The identity (4.7) *holds for* $t\in\,]-\kappa_0,\kappa_0[$.

Proof: We have to prove that

$$\int a(t,\tau,z,\zeta)\mu(\mathrm{d}t\,\mathrm{d}\tau\,\mathrm{d}z\,\mathrm{d}\zeta)=\frac{1}{8}\int_0^{2\pi}\int_{\mathbb{R}_t}\int a(\Phi_t^\theta(x,\xi))\,\nu_I(\mathrm{d}x\,\mathrm{d}\xi)\mathrm{d}t\,\mathrm{d}\theta \tag{4.8}$$

for every $a\in\mathcal{C}_0^\infty(\mathbf{T}^*(]-\kappa_0,\kappa_0[\times\dot{\mathbb{R}}^4))$.

Since $\nu_{|_{]-\kappa_0,\kappa_0[}}$ is supported in $\mathbf{T}^*(]-\kappa_0,\kappa_0[\times S^1\times\Omega)$ we may use transformation rule of the Wigner measure by the diffeomorphism $(t,x,\theta)\mapsto(t,\chi(x,\theta))$. This transformation yields

$$\mu=\Theta(|\det(\chi'(x,\theta))|\nu),\quad t\in\,]-\kappa_0,\kappa_0[\tag{4.9}$$

where Θ is the canonical transformation given by (3.16). From (3.11) it follows that

$$\mu=\Theta\left(\frac{1}{8|x|}\nu\right),\quad t\in\,]-\kappa_0,\kappa_0[. \tag{4.10}$$

Since ν is supported in $\beta=0$ then we have to deal only with the values of Θ on $\beta=0$. Using (3.13), one obtains

$$\Theta(t,\tau,x,\theta,\xi,0)=(t,\tau,\chi(x,\theta),2L^T(\chi(x,\theta))(\xi,0))=(t,\tau,\Gamma(x,\xi,\theta)). \tag{4.11}$$

Putting together (4.6) and (4.9)–(4.11), it follows that

$$\int a(t,\tau,z,\zeta)\mu(\mathrm{d}t\,\mathrm{d}\tau\,\mathrm{d}z\,\mathrm{d}\zeta)=\int\frac{1}{8|\phi_t^1(x,\xi)|}a(t,-p(x,\xi),\Gamma(\phi_t(x,\xi),\theta))\,\nu_I(\mathrm{d}x\,\mathrm{d}\xi)\mathrm{d}t\,\mathrm{d}\theta, \tag{4.12}$$

where $\phi_t^1(x,\xi)=\Pi_x\phi_t(x,\xi)$. Since Γ is periodic in the variable θ, the right-hand side (RHS) of (4.12) does not change if we replace θ by $\theta+\alpha(x,\xi,t)$, where $\alpha(x,\xi,t)$ is defined in Lemma 3.6 (α is well defined because $t\in\,]-\kappa_0,\kappa_0[$). This implies

$$(4.12)=\int\frac{1}{8|\phi_t^1(x,\xi)|}a(t,-p(x,\xi),\Gamma(\phi_t(x,\xi),\theta+\alpha(x,\xi,t)))\,\nu_I(\mathrm{d}x\,\mathrm{d}\xi)\mathrm{d}t\,\mathrm{d}\theta.$$

For every fixed $(x,\xi)\in\mathrm{supp}(\nu_I)$ we make the change of variables $s=\mathbf{t}^{-1}(t)$ [defined by (3.15)] in the last integral. This gives

$$(4.12)=\int\frac{1}{8}a(\mathbf{t}(s),-p(x,\xi),\Gamma(\phi_{\mathbf{t}(s)}(x,\xi),\theta+\alpha(x,\xi),\mathbf{t}(s)))\,\nu_I(\mathrm{d}x\,\mathrm{d}\xi)\mathrm{d}s\,\mathrm{d}\theta.$$

Recall that the number κ_0 is chosen so that the conditions of Lemma 3.6 are satisfied for all $(x,\xi)\in\mathrm{supp}(\nu_I)$. In particular, one has

$$(\mathbf{t}(s), -p(x,\xi), \Gamma(\phi_{\mathbf{t}(s)}(x,\xi), \theta + \alpha(x,\xi,\mathbf{t}(s)))) = \Phi_s^\theta(x,\xi),$$

which yields

$$\int a(t,\tau,z,\zeta)\mu(\mathrm{d}t\,\mathrm{d}\tau\,\mathrm{d}z\,\mathrm{d}\zeta) = \frac{1}{8}\int_0^{2\pi}\int\int a(\Phi_s^\theta(x,\xi))\,\nu_I(\mathrm{d}x\,\mathrm{d}\xi)\mathrm{d}s\,\mathrm{d}\theta$$

as claimed. This concludes the proof of Lemma 4.3 □

Our next task is to use Lemma 2.2 to extend the local result provided by (4.7) to all $\mathbf{T}^*(\mathbb{R}_t \times \dot{\mathbb{R}}^4)$. The family (u^ε) is solution of

$$\tilde{p}(t,x,\varepsilon D_t, \varepsilon D_x)u^\varepsilon = 0,$$

where $\tilde{p}$ is the smooth symbol given by (3.7). Also, (u^ε) is bounded in $L^2_{\mathrm{loc}}(\mathbb{R}_t \times \mathbb{R}^d \backslash F)$ where $F = \mathbb{R}_t \times \{0\}$. Thus, the hypothesis (H1) of Lemma 2.2 is satisfied. In the next lemma we prove that (u^ε) satisfies the hypothesis (H2) with $l=6$.

Lemma 4.4: The family (u^ε) *defined by* (4.1) *satisfies*

$$\|u^\varepsilon\|_{L^\infty(\mathbb{R}_t, L^2(\mathbb{R}^4_z))} = \mathcal{O}(\varepsilon^{-6}). \tag{4.13}$$

Proof: Recall that, as explained in the beginning of this section, the initial family v_I^ε is bounded in $L^2(\mathbb{R}^d)$ and belongs to $H^2(\mathbb{R}^3)$, with

$$\|v_I^\varepsilon\|_{H^2(\mathbb{R}^3)} = \mathcal{O}(\varepsilon^{-2}).$$

By change of variable and conservation laws of the equation (1.3), we have

$$\int_{\mathbb{R}^4} |z u^\varepsilon(t,\cdot)|^2 \mathrm{d}z = \frac{1}{8}\int_{\mathbb{R}^3} |v^\varepsilon(t,\cdot)|^2 \mathrm{d}x = \frac{1}{8}\int_{\mathbb{R}^3} |v_I^\varepsilon(x)|^2 \mathrm{d}x,$$

for every $t \in \mathbb{R}$. Thereby, we estimate

$$\int_{\mathbb{R}^4} |u^\varepsilon(t,\cdot)|^2 \mathrm{d}z \leqslant \int_{|z|\leqslant 1} |u^\varepsilon(t,\cdot)|^2 \mathrm{d}z + \int_{|z|\geqslant 1} |z|^2 |u^\varepsilon(t,\cdot)|^2 \mathrm{d}z \lesssim \|u^\varepsilon(t,\cdot)\|^2_{L^\infty(\mathbb{R}^3)} + \|v_I^\varepsilon\|^2_{L^2(\mathbb{R}^3)}$$

for every $t \in \mathbb{R}$. From the explicit formula (4.1), it follows that

$$\|u^\varepsilon(t,\cdot)\|_{L^\infty(\mathbb{R}^4)} = \|v^\varepsilon(t,\cdot)\|_{L^\infty(\mathbb{R}^3)} \tag{4.14}$$

for every $t \in \mathbb{R}$. However, via Sobolev embedding, we obtain

$$\|v^\varepsilon(t,\cdot)\|_{L^\infty(\mathbb{R}^3)} \lesssim \|v^\varepsilon(t,\cdot)\|_{H^2(\mathbb{R}^3)}$$

for every $t \in \mathbb{R}$. Hence, in order to prove (4.13), it suffices to prove

$$\|v^\varepsilon(t,\cdot)\|_{L^\infty(\mathbb{R}_t, H^2(\mathbb{R}^3))} \lesssim \varepsilon^{-4}\|v_I^\varepsilon\|_{H^2}. \tag{4.15}$$

Observe that v^ε is solution to

$$i\partial_t v^\varepsilon = A_\varepsilon v^\varepsilon, \quad v^\varepsilon_{|t=0} = v_I^\varepsilon, \tag{4.16}$$

where

$$A_\varepsilon = \left(\frac{\varepsilon}{2}\Delta - \frac{1}{\varepsilon|x|} + V(x)\right).$$

Since the domain of A_ε is $H^2(\mathbb{R}^3)$ (see for example Ref. 11), it ensues

$$\|v^\varepsilon(t,\cdot)\|_{L^\infty(\mathbb{R}_t,L^2(\mathbb{R}^3))}+\|A_\varepsilon v^\varepsilon(t,\cdot)\|_{L^\infty(\mathbb{R}_t,L^2(\mathbb{R}^3))}\leqslant\|v_I^\varepsilon\|_{H^2}. \tag{4.17}$$

However, since

$$\Delta=\frac{2}{\varepsilon}A_\varepsilon+\frac{2}{\varepsilon^2}\frac{1}{|x|}-\frac{2}{\varepsilon^2}V(x),$$

we have

$$\|v^\varepsilon(t,\cdot)\|_{L^\infty_t(H^2(\mathbb{R}^3))}\lesssim\|v^\varepsilon(t,\cdot)\|_{L^\infty_t(L^2(\mathbb{R}^3))}+\frac{1}{\varepsilon}\|A_\varepsilon v^\varepsilon(t,\cdot)\|_{L^\infty_t(L^2(\mathbb{R}^3))}+\frac{1}{\varepsilon^2}\left\|\frac{v^\varepsilon(t,\cdot)}{|x|}\right\|_{L^\infty(\mathbb{R}_t,L^2(\mathbb{R}^3))}$$
$$+\frac{1}{\varepsilon^2}\|Vv^\varepsilon(t,\cdot)\|_{L^\infty(\mathbb{R}_t,L^2(\mathbb{R}^3))}. \tag{4.18}$$

Since V is bounded, we get

$$\|Vv^\varepsilon(t,\cdot)\|_{L^\infty(\mathbb{R}_t,L^2(\mathbb{R}^3))}\leqslant\|v^\varepsilon(t,\cdot)\|_{L^\infty(\mathbb{R}_t,L^2(\mathbb{R}^3))}. \tag{4.19}$$

Also, Hardy inequality gives

$$\left\|\frac{v^\varepsilon(t,\cdot)}{|x|}\right\|_{L^\infty(\mathbb{R}_t,L^2(\mathbb{R}^3))}\lesssim\|\nabla v^\varepsilon(t,\cdot)\|_{L^\infty(\mathbb{R}_t,L^2(\mathbb{R}^3))}\lesssim\delta\varepsilon^2\|v^\varepsilon\|_{L^\infty(\mathbb{R}_t,H^2(\mathbb{R}^3))}+\frac{C_\delta}{\varepsilon^2}\|v^\varepsilon\|_{L^\infty(\mathbb{R}_t,L^2(\mathbb{R}^3))}. \tag{4.20}$$

Choosing δ small and combining (4.18) and (4.20), we infer

$$\|v^\varepsilon(t,\cdot)\|_{L^\infty(\mathbb{R}_t,H^2(\mathbb{R}^3))}\lesssim\varepsilon^{-4}(\|v^\varepsilon(t,\cdot)\|_{L^\infty(\mathbb{R},L^2)}+\|A_\varepsilon v^\varepsilon(t,\cdot)\|_{L^\infty(\mathbb{R},L^2)}). \tag{4.21}$$

The statement (4.15) is then the combination of (4.17) and (4.21). □

To close the proof of Proposition 4.2, it remains to be proven that the small interval $]-\kappa_0,\kappa_0[$ contains all the information on μ. In other words, we have to check that the union of the Hamiltonian curves of $\tilde{p}$ starting from $\mathbf{T}^*(]-\kappa_0,\kappa_0[\times\dot{\mathbb{R}}^4)$ contains $\mathrm{supp}(\mu)$. This follows from the fact that $\mathrm{supp}(\mu)$ is contained in the characteristic set of $\tilde{p}$ and that the t-component of every bicharacteristic of $\tilde{p}$ is a bijection from $\mathbb{R}$ onto $\mathbb{R}$ (remember Lemma 3.1). □

Step 3: In this final step we give the description of the measure ν_t over $x\neq 0$. In order to use the "local inverse" of KS-transformation we write any test function $a\in\mathcal{C}_0^\infty(\mathbf{T}^*(S^1\times\mathbb{R}_t\times\dot{\mathbb{R}}^3))$ as $a=a_1+a_2$, such that $a_1\in\mathcal{C}_0^\infty(\mathbf{T}^*(S^1\times\mathbb{R}_t\times\Omega))$ and $a_2\in\mathcal{C}_0^\infty(\mathbf{T}^*(S^1\times\mathbb{R}_t\times\tilde{\Omega}))$. Since the functions a_1 and a_2 are treated in the same manner, we assume that $a_2=0$ and we will treat a_1 only. By using the explicit formula (4.7) and the inverse of the transformation Θ given by (3.16), we get

$$\int a(t,\tau,x,\xi,\theta,\beta)\,\nu(\mathrm{d}\tau\,\mathrm{d}x\,\mathrm{d}\xi\,\mathrm{d}\theta\,\mathrm{d}\beta)=\;=\int\left|\prod_z(\Phi_t^\theta(x,\xi))\right|^2 a(\Theta^{-1}(\Phi_t^\theta(x,\xi)))\,\nu_I(\mathrm{d}x\,\mathrm{d}\xi)\mathrm{d}t\,\mathrm{d}\theta. \tag{4.22}$$

Let $\mathbf{t}(s)$ denote the t-component of $\Phi_t^\theta(x,\xi)$. The Hamiltonian system yields

$$\dot{\mathbf{t}}(s)=\left|\prod_z(\Phi_t^\theta(x,\xi))\right|^2.$$

By making the change of variables $\mathbf{t}(s)=t$ on the RHS of (4.22), one obtains

$$\int a(t,\tau,x,\xi,\theta,\beta)\,\nu(\mathrm{d}\tau\,\mathrm{d}x\,\mathrm{d}\xi\,\mathrm{d}\theta\,\mathrm{d}\beta) = \int a(\Theta^{-1}(\Phi^{\theta}_{\mathbf{t}^{-1}(t)}(x,\xi)))\,\nu_I(\mathrm{d}x\,\mathrm{d}\xi)\mathrm{d}t\,\mathrm{d}\theta. \tag{4.23}$$

We do not need to calculate all the expression $\Theta^{-1}(\Phi^{\theta}_{\mathbf{t}^{-1}(t)}(x,\xi)))$. In fact, since v^{ε} does not depend on θ, the (θ,β)-component of ν is $d\theta\otimes\delta_{\beta=0}$. We take then a test function a which does not depend on (θ,β). Remark 3.7 says that

$$\prod_{t,\tau}\Theta^{-1}(\Phi^{\theta}_{\mathbf{t}^{-1}(t)}(x,\xi)) = (t,-p(x,\xi)).$$

Finally, Lemma 3.8 yields

$$\prod_{x,\xi}\Theta^{-1}(\Phi^{\theta}_{\mathbf{t}^{-1}(t)}(x,\xi)) = \Lambda^{*}\Bigg(\prod_{(z,\zeta)}(\Phi^{\theta}_{\mathbf{t}^{-1}(t)}(x,\xi))\quad.$$

Thus, the identity (4.23) becomes

$$2\pi\int a(t,\tau,x,\xi)\,\nu(\mathrm{d}t\,\mathrm{d}\tau\,\mathrm{d}x\,\mathrm{d}\xi) = \int_0^{2\pi}\int\int a\Big(t,-p(x,\xi),\ \Lambda^{*}\Big(\prod_{(z,\zeta)}(\Phi^{\theta}_{\mathbf{t}^{-1}(t)}(x,\xi))\Big)\Big)\,\nu_I(\mathrm{d}x\,\mathrm{d}\xi)\mathrm{d}t\,\mathrm{d}\theta. \tag{4.24}$$

However, by definition 3.2, we have

$$\Lambda^{*}\Big(\prod_{(z,\zeta)}(\Phi^{\theta}_{\mathbf{t}^{-1}(t)}(x,\xi))\Big) = \tilde{\phi}_t(x,\xi), \tag{4.25}$$

for *every* $\theta\in S^1$. Thus, (4.24) becomes

$$\int a(t,\tau,x,\xi)\,\nu(\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}\tau\,\mathrm{d}\xi) = \int\int a(t,-p(x,\xi),\tilde{\phi}_t(x,\xi))\,\nu_I(\mathrm{d}x\,\mathrm{d}\xi)\mathrm{d}t,$$

for every $a\in\mathcal{C}_0^{\infty}(\mathbf{T}^{*}(\mathbb{R}\times\dot{\mathbb{R}}^3))$. From this, one concludes that, as a function of (t,x)-variable, (v^{ε}) is pure on $\mathbb{R}\times\dot{\mathbb{R}}^3$. Furthermore, the Wigner measure is given by

$$\nu(\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}\tau\,\mathrm{d}\xi) = \mathrm{d}t\otimes\delta_{\tau+p(x,\xi)}\otimes\tilde{\phi}_t(\nu_I)_{|_{x\neq 0}}. \tag{4.26}$$

Let $\tilde{\nu}_t$ be a Wigner measure [we do not know if there exists only one—the uniqueness (and then the fact that (v^{ε}) is pure over $\dot{\mathbb{R}}^3$) will follow from the explicit formula (4.27)] associated to (v^{ε}) over $\dot{\mathbb{R}}^3$. According to (4.26), one obtains easily

$$\tilde{\nu}_t = \tilde{\phi}_t(\nu_I)_{|_{x\neq 0}}.$$

But

$$\tilde{\phi}_t(\nu_I)_{|_{x\neq 0}} = \tilde{\phi}_t(\nu_{I_{|_{\mathbb{R}^3\setminus\mathrm{Coll}_t}}}),$$

which yields

$$\tilde{\nu}_t = \tilde{\phi}_t(\nu_{I_{|_{\mathbb{R}^3\setminus\mathrm{Coll}_t}}}). \tag{4.27}$$

If ν_t is a Wigner measure associated to (v^{ε}) on $\mathbb{R}^3$ then

$$\nu_{t|_{x\neq 0}} = \tilde{\nu}_t = \tilde{\phi}_t(\nu_{I_{|_{\mathbb{R}^3\setminus\mathrm{Coll}_t}}}).$$

Nevertheless we do not know if ν_t is unique [if (v^{ε}) is pure on $\mathbb{R}^3$ or not]. This achieves the proof of the statement (i) of the main theorem.

The statement (ii) of the main theorem is a direct application of the conservation of the total mass. Indeed, if $\nu_I(\mathrm{Coll}_t(\nu_I))=0$ then the statement (i) of the main theorem yields

$$\nu_{t|_{x\neq 0}} = \tilde{\phi}_t(\nu_I). \tag{4.28}$$

Then it remains to prove that $\nu_{t|_{x=0}}=0$. First, one has

$$\|\nu_{t|_{x\neq 0}}\|_{\mathcal{M}} \leqslant \|\nu_t\|_{\mathcal{M}}.$$

second from (4.28), it ensues

$$\|\nu_{t|_{x\neq 0}}\|_{\mathcal{M}} = \|\tilde{\phi}_t(\nu_I)\|_{\mathcal{M}} = \|\nu_I\|_{\mathcal{M}} = \limsup_{\varepsilon\to 0}\|v_I^\varepsilon\|_{L^2(\mathbb{R}^3)}.$$

The latter equality follows from Proposition 1.4 and the assumptions on the family of initial data v_I^ε. Using again Proposition 1.4 and the conservation of the L^2-norm, one gets

$$\|\nu_t\|_{\mathcal{M}} \leqslant \limsup_{\varepsilon\to 0}\|v^\varepsilon(t,\cdot)\|_{L^2(\mathbb{R}^3)} = \limsup_{\varepsilon\to 0}\|v_I^\varepsilon\|_{L^2(\mathbb{R}^3)}.$$

This yields

$$\|\nu_{t|_{x\neq 0}}\|_{\mathcal{M}} = \|\nu_t\|_{\mathcal{M}},$$

which means that $\nu_{t|_{x=0}}\equiv 0$ and so

$$\nu_t = \nu_{t|_{x\neq 0}} = \tilde{\phi}_t(\nu_I).$$

The purity, ε-oscillation, and compactness at infinity of the family v_t^ε follows directly from the explicit expression of ν_t, and the conservation of the total mass (remember Proposition 1.4). This concludes the proof of Theorem 1.8. ■

APPENDIX A: PROOF OF LEMMA 3.1

Let $(t_0,z_0,\tau_0,\zeta_0)\in \mathbf{T}^*(\mathbb{R}\times\dot{\mathbb{R}}^4)$ satisfying $\tilde{p}(t_0,z_0,\tau_0,\zeta_0)=0$ and $(\mathbf{t}(s),\mathbf{z}(s),\boldsymbol{\tau}(s),\boldsymbol{\zeta}(s))$ be the classical trajectory of the Hamiltonian $\tilde{p}$ starting from (t_0,z_0,τ_0,ζ_0):

$$\dot{\mathbf{z}} = \frac{1}{4}\boldsymbol{\zeta}(s),$$

$$\dot{\boldsymbol{\zeta}}(s) = -2\boldsymbol{\tau}(s)\mathbf{z}(s) - \nabla W(\mathbf{z}(s)),$$

$$\dot{\mathbf{t}}(s) = |\mathbf{z}(s)|^2,$$

$$\dot{\boldsymbol{\tau}}(s) = 0,$$

$$(\mathbf{t},\mathbf{z},\boldsymbol{\tau},\boldsymbol{\zeta})_{|_{s=0}} = (t_0,z_0,\tau_0,\zeta_0). \tag{A1}$$

We have to prove that

$$\mathbf{t}(s) \underset{s\to\pm\infty}{\to} \pm\infty \tag{A2}$$

and that $s\mapsto\mathbf{t}(s)$ is an injection. Since $\dot{\mathbf{t}}(s)=|\mathbf{z}(s)|^2$ then the failure of (A2) means that $\mathbf{z}\in\mathbf{L}^2(]-\infty,0])$ or $\mathbf{z}\in\mathbf{L}^2([0,+\infty[)$. Assume, for example, that $\mathbf{z}\in\mathbf{L}^2([0,+\infty[)$, and let w a smooth real valued function, so that

$$w(s) = 0, \quad s \leqslant -1, \quad w(s) = 1, \quad s \geqslant 0.$$

We set

$$\mathbf{y}(s) = w(s)\mathbf{z}(s)$$

First, since $\mathbf{z} \in \mathbf{L}^2([0,+\infty[)$ then $y \in \mathbf{L}^2(\mathbb{R})$. Second, the equation of motion yields

$$\ddot{\mathbf{z}}(s) = -\frac{\tau_0}{2}\mathbf{z}(s) - \frac{1}{4}\nabla W(\mathbf{z}(s)), \tag{A3}$$

which implies that $\ddot{\mathbf{z}} \in \mathbf{L}^2([0,+\infty[)$. Thus, $\ddot{\mathbf{y}} \in \mathbf{L}^2(\mathbb{R})$ and so $\mathbf{y} \in \mathbf{H}^2$. This implies, in particular, that

$$|\dot{\mathbf{y}}(s)| + |\mathbf{y}(s)| \underset{s\to+\infty}{\to} 0,$$

and then

$$|\dot{\mathbf{z}}(s)| + |\mathbf{z}(s)| \underset{s\to+\infty}{\to} 0, \tag{A4}$$

However, (A1) and the conservation of the classical Hamiltonian give

$$\tau_0|\mathbf{z}(s)|^2 + 2|\dot{\mathbf{z}}(s)|^2 + W(\mathbf{z}(s)) = 1,$$

which contradicts (A4) (remember that $W(0)=0$) and proves (A2). On the other hand, since $\dot{\mathbf{t}}(s) = |\mathbf{z}(s)|^2$, if $s \mapsto \mathbf{t}(s)$ is not injective then there exists a nontrivial interval $[s_1, s_2]$, such that $z(s) = 0$, for every $s \in [s_1, s_2]$. This implies, also, that $\boldsymbol{\zeta}(s) = 4\dot{\mathbf{z}}(s) = 0$ and yields a contradiction with the conservation of the classical Hamiltonian as above. Hence, $s \mapsto \mathbf{t}(s)$ is an injection, as claimed. This concludes the proof of Lemma 3.1. □

APPENDIX B: PROOF OF LEMMA 3.4

It is easy to check (see Ref. 13, Chap. X) that outside the set $\{s \in \mathbb{R} : \mathbf{z}(s) = 0\}$ the transformation (3.8) defines a solution to the system

$$\begin{aligned} \dot{\mathbf{x}}(t) &= \boldsymbol{\xi}(t), \\ \dot{\boldsymbol{\xi}}(t) &= -\frac{\mathbf{x}(t)}{|\mathbf{x}(t)|^3} - \nabla V(\mathbf{x}(t)). \end{aligned} \tag{B1}$$

More precisely, if one writes

$$\{s \in \mathbb{R} : \mathbf{z}(s) \neq 0\} = \underbrace{[0, s_1^*[}_{I_*^1} \cup \underbrace{]s_1^*, s_2^*[}_{I_*^2} \cup \underbrace{]s_2^*, s_3^*[}_{I_*^3} \cup \ldots$$

then the transformation (3.8) is well defined on every I_*^i and $\tilde{\phi}_t(x_0, \xi_0)$ is a solution to the system (B1). [Let us note here that collision times cannot accumulate. In fact, the collision orbits are either periodic or go to spacial infinity in both time directions.] Furthermore, in I_*^1 the transformed $\tilde{\phi}_t(x_0, \xi_0)$ coincides with the regular solution of (B1) with initial data (x_0, ξ_0). Also, we have

$$s_1^* = \int_0^{t_1^*} \frac{1}{|\phi_t^1(x_0, \xi_0)|} \mathrm{d}t,$$

where t_1^* is the first collision time of the classical trajectory $\phi_t(x_0, \xi_0)$ starting from (x_0, ξ_0) with the potential center $x=0$. Let $(\tilde{\mathbf{x}}(t), \tilde{\boldsymbol{\xi}}(t)) := \tilde{\phi}_t(x_0, \xi_0)$ denotes the regularized trajectory starting from (x_0, ξ_0). The proof of Lemma 3.4 and Lemma 1.6 [Since $\tilde{\boldsymbol{\xi}}(t) = \boldsymbol{\xi}(t)$ for $t < t_1^*$ then the existence of the limit

$$\lim_{t\to(t_1^*)^-}\frac{\tilde{\boldsymbol{\xi}}(t)}{|\tilde{\boldsymbol{\xi}}(t)|}$$

proves Lemma 1.6] is equivalent to the existence of both limits

$$\lim_{t\to(t_1^*)^-}\frac{\tilde{\boldsymbol{\xi}}(t)}{|\tilde{\boldsymbol{\xi}}(t)|} \quad \text{and } \lim_{t\to(t_1^*)^+}\frac{\tilde{\boldsymbol{\xi}}(t)}{|\tilde{\boldsymbol{\xi}}(t)|},$$

and the equality

$$\lim_{t\to(t_1^*)^+}\frac{\tilde{\boldsymbol{\xi}}(t)}{|\tilde{\boldsymbol{\xi}}(t)|} = -\lim_{t\to(t_1^*)^-}\frac{\tilde{\boldsymbol{\xi}}(t)}{|\tilde{\boldsymbol{\xi}}(t)|}.$$

Since $\mathbf{t}(s)$ is a continuous and increasing function, then

$$\mathbf{t}(s)\to(t_1^*)^{\pm} \Leftrightarrow s\to(s_1^*)^{\pm}.$$

Thus, by definition, we have

$$\lim_{t\to(t_1^*)^{\pm}}\frac{\tilde{\boldsymbol{\xi}}(t)}{|\tilde{\boldsymbol{\xi}}(t)|} = \lim_{s\to(s_1^*)^{\pm}}\frac{\Lambda(\mathbf{z}(s))\boldsymbol{\zeta}(s)}{|\Lambda(\mathbf{z}(s))\boldsymbol{\zeta}(s)|}.$$

Then, to conclude the proof of the lemma, it suffices to prove that the function $s\mapsto\Lambda(\mathbf{z}(s))\boldsymbol{\zeta}(s)$ has a nonzero derivative in $s=s_1^*$. A direct computation yields

$$\frac{\mathrm{d}}{\mathrm{d}s}(\Lambda(\mathbf{z}(s))\boldsymbol{\zeta}(s))_{|s=s_1^*} = \Lambda(\dot{\mathbf{z}}(s_1^*))\boldsymbol{\zeta}(s_1^*) + \Lambda(\mathbf{z}(s_1^*))\dot{\boldsymbol{\zeta}}(s_1^*) = \frac{1}{4}\Lambda(\boldsymbol{\zeta}(s_1^*))\boldsymbol{\zeta}(s_1^*).$$

In the last line we have used $\mathbf{z}(s_1^*)=0$. Thus, we have only to check that $\Lambda(\boldsymbol{\zeta}(s_1^*))\boldsymbol{\zeta}(s_1^*)\neq 0$. On the one hand, in view of (3.3), we have

$$|\Lambda(\boldsymbol{\zeta}(s_1^*))\boldsymbol{\zeta}(s_1^*)| = |\boldsymbol{\zeta}(s_1^*)|^2.$$

On the other hand, the conservation of Hamiltonian implies

$$\tilde{p}(\mathbf{z}(s_1^*),\mathbf{t}(s_1^*),\boldsymbol{\zeta}(s_1^*),\boldsymbol{\tau}(s_1^*)) = \tilde{p}(\mathbf{z}(0),\mathbf{t}(0),\boldsymbol{\zeta}(0),\boldsymbol{\tau}(0)) = 0.$$

Since $\mathbf{z}(s_1^*)=0$ we get $\frac{1}{8}|\boldsymbol{\zeta}(s_1^*)|^2=1$ as desired. Finally, we obtain

$$\lim_{t\to(t_1^*)^{\pm}}\frac{\tilde{\boldsymbol{\xi}}(t)}{|\tilde{\boldsymbol{\xi}}(t)|} = \pm\frac{\Lambda(\boldsymbol{\zeta}(s_1^*))\boldsymbol{\zeta}(s_1^*)}{8}.$$

where $\mathbf{t}(s_1^*)=t_1^*$. Further collisions $(t_2^*,t_3^*,\ldots)$ are treated in the same way. This closes the proof of Lemma 3.4.

APPENDIX C: PROOF OF LEMMA 3.8

One denotes $\Pi_{(z,\zeta)}\Phi_s^{\theta}(x,\xi)=(\mathbf{z}(s),\boldsymbol{\zeta}(s))$. Recall that Θ^{-1} is given by

$$\Theta^{-1}(t,\tau,z,\zeta) = (t,\tau,\chi^{-1}(z),{}^{\mathrm{T}}[(\chi^{-1})'(z)]^{-1}(\zeta)).$$

It is clear that $\Pi_x(\chi^{-1}(\mathbf{z}(s)))=\Lambda(\mathbf{z}(s))\mathbf{z}(s)$. Hence, we have to prove that

$$^{T}[(\chi^{-1})'(\mathbf{z}(s))]^{-1}(\boldsymbol{\zeta}(s)) = \frac{1}{2|\mathbf{z}(s)|^2}(\Lambda(\mathbf{z}(s))\boldsymbol{\zeta}(s),0). \tag{C1}$$

By a straightforward computation we get

$$^{T}[(\chi^{-1})'(z)]^{-1} = \frac{1}{2|z|^2}\begin{pmatrix} z_1 & -z_2 & -z_3 & z_4 \\ z_2 & z_1 & -z_4 & -z_3 \\ z_3 & z_4 & z_1 & z_2 \\ 0 & 0 & 0 & 0 \end{pmatrix} + A(z), \tag{C2}$$

where $A(z)$ is a matrix with lines of the form

$$L_i = a_i(z)(z_4 \ -z_3 \ -z_2 \ z_1). \tag{C3}$$

Here $a_i:\mathbb{R}^4\to\mathbb{R}$, $i=1,2,3,4$ are given functions. Thus, in order to prove (C1), it suffices to show that the bilinear quantity

$$l(z,\zeta) = z_4\zeta_1 - z_3\zeta_2 + z_2\zeta_3 - z_1\zeta_4 \tag{C4}$$

is a first integral of the Hamiltonian $\tilde{p}$, and $l(\Gamma(x,\xi,\theta))=0$ for every $(\theta,x,\xi)\in S^1\times\mathbf{T}^*(\dot{\mathbb{R}}^3)$. This is a well-known fact (see Ref. 13 Lemma 2, p. 236). This achieves the proof of lemma 3.8.

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Equilibrium positions, shape invariance and Askey–Wilson polynomials

Satoru Odake
Department of Physics, Shinshu University, Matsumoto 390-8621, Japan

Ryu Sasaki
Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan

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We show that the equilibrium positions of the Ruijsenaars–Schneider–van Diejen systems with the trigonometric potential are given by the zeros of the Askey–Wilson polynomials with five parameters. The corresponding single particle quantum version, which is a typical example of "discrete" quantum mechanical systems with a q-shift type kinetic term, is shape invariant and the eigenfunctions are the Askey–Wilson polynomials. This is an extension of our previous study, which established the "discrete analogue" of the well-known fact; the equilibrium positions of the Calogero systems are described by the Hermite and Laguerre polynomials, whereas the corresponding single particle quantum versions are shape invariant and the eigenfunctions are the Hermite and Laguerre polynomials. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1927080]

I. INTRODUCTION

The Calogero–Sutherland systems[1] and their integrable deformation called the Ruijsenaars–Schneider–van Diejen systems[2,3] have many attractive features at both classical and quantum mechanical levels. In our recent papers,[4,5] the equilibrium positions of the classical Ruijsenaars–Schneider–van Diejen systems were studied. The equilibrium positions of the Calogero–Sutherland systems are described by the zeros of the classical orthogonal polynomials, the Hermite, Laguerre, Chebyshev, Legendre, Gegenbauer, and Jacobi polynomials.[6–8] Since the Ruijsenaars–Schneider–van Diejen systems are deformation of the Calogero–Sutherland systems, it is expected that the equilibrium positions of the Ruijsenaars–Schneider–van Diejen systems are described by some deformation of these classical orthogonal polynomials. This is indeed the case and we obtained the deformed Hermite, Laguerre, and Jacobi polynomials.[5] These deformed orthogonal polynomials fit in the Askey-scheme of the hypergeometric orthogonal polynomials;[9,10] (i) rational potential cases, one and two parameter deformation of the Hermite polynomials are a special case of the Meixner–Pollaczek polynomial and a special case of the continuous Hahn polynomial, and two and three parameter deformation of the Laguerre polynomials are the continuous dual Hahn polynomial and the Wilson polynomial, (ii) trigonometric potential cases, several one parameter deformation of the Jacobi polynomials are special cases of the Askey–Wilson polynomial. The Askey–Wilson polynomial has five parameters,[11] but the deformed Jacobi polynomials obtained in Ref. 5 have only three parameters. A natural question arises; find (integrable) multiparticle systems whose equilibrium positions are described by the Askey–Wilson polynomials with five parameters.

Shape invariance is an important ingredient of many exactly solvable quantum mechanics.[12–14] In another recent paper of ours,[15] the shape invariance of "discrete" quantum mechanical single particle systems, whose kinetic term causes a shift of the coordinate in the imaginary direction, are discussed. The eigenfunctions of these shape invariant systems are a special case of the Meixner–Pollaczek polynomial, a special case of the continuous Hahn polynomial, the continuous dual Hahn polynomial and the Wilson polynomial. These polynomials have all appeared in the above discussion about the equilibrium positions, in which we have one more

polynomial, the Askey–Wilson polynomial. This gives the second question; are the quantum mechanical single particle systems, whose eigenstates are the Askey–Wilson polynomial, shape invariant or not?

We will answer the above two questions in this paper. The answer to the first question is found by the same method given in Ref. 5, i.e., numerical analysis, functional equation, and three-term recurrence. The second question is answered affirmatively by using the properties of the Askey–Wilson polynomials and similar discussion in Ref. 15 with replacement of a shift operator by a q-shift operator.

This paper is organized as follows. In Sec. II, the classical equilibria of the Ruijsenaars–Schneider–van Diejen system are studied. For a suitable choice of the elementary potential functions, the equilibrium positions are given by the zeros of the Askey–Wilson polynomials with five parameters. In Sec. III we discuss the shape invariance of "discrete" quantum mechanical single particle systems with a q-shift type kinetic term. After discussing general theory, we present an explicit example of such shape invariant systems, in which eigenstates are described by the Askey–Wilson polynomials. The final section is for a summary and comments.

II. MULTIPARTICLE SYSTEMS: EQUILIBRIUM POSITIONS

Let us consider the equilibrium positions of the classical Ruijsenaars–Schneider–van Diejen systems with the trigonometric potential,[2,3] which are integrable deformation of the celebrated Calogero–Sutherland systems of exactly solvable multiparticle quantum mechanics. Its classical Hamiltonian corresponding to the BC root system is the following:[3]

$$H(p,q)=\sum_{j=1}^{n}\left(\cosh p_j\sqrt{V_j(q)V_j^*(q)}-\frac{1}{2}(V_j(q)+V_j^*(q))\right), \tag{1}$$

$$V_j(q)=w(q_j)\prod_{\substack{k=1\\k\neq j}}^{n}v(q_j-q_k)v(q_j+q_k)\quad(j=1,\ldots,n), \tag{2}$$

$$v(x)=\frac{\sin(x-ig_0)}{\sin x}, \tag{3}$$

$$w(x)=\frac{\sin(x-ig_1)}{\sin x}\frac{\sin(x-ig_2)}{\sin x}\frac{\cos(x-ig_3)}{\cos x}\frac{\cos(x-ig_4)}{\cos x}, \tag{4}$$

where $q={}^t(q_1,\ldots,q_n)$ and $p={}^t(p_1,\ldots,p_n)$ are the coordinates and conjugate momenta, and g_j $(j=0,\ldots,4)$ are the real positive coupling constants. The potentials V_j and V_j^* are complex conjugate of each other. Our convention of a complex conjugate function is the following: for an arbitrary function $f(x)=\Sigma_n a_n x^n$ $(a_n\in\mathbb{C})$, we define $f^*(x)=\Sigma_n a_n^* x^n$. Here c^* is the complex conjugation of a number $c\in\mathbb{C}$. Note that $f^*(x)$ is not the complex conjugation of $f(x)$, $(f(x))^*=f^*(x^*)$. This is relevant for considering complex variables in Sec. III. The equilibrium positions $p=0$, $q=\overline{q}$ are determined by the condition[4]

$$V_j(\overline{q})=V_j^*(\overline{q})>0\quad(j=1,2,\ldots,n). \tag{5}$$

This equation *without inequality* is rewritten in the Bethe ansatz type equation

$$\prod_{\substack{k=1\\k\neq j}}^{n}\frac{v(\overline{q_j}-\overline{q_k})v(\overline{q_j}+\overline{q_k})}{v^*(\overline{q_j}-\overline{q_k})v^*(\overline{q_j}+\overline{q_k})}=\frac{w^*(\overline{q_j})}{w(\overline{q_j})}. \tag{6}$$

Note that $\overline{q_j}=0,\pi/2$ is excluded in (5) but allowed in (6).

By the same method given in Ref. 5 (numerical analysis, functional equation, and three-term recurrence), we can show that the equilibrium positions $\{\overline{q_j}\}$ are given by the zeros of the Askey–Wilson polynomial[11] (we follow the notation of Koekoek and Swarttouw[10]) $p_n(x;a,b,c,d|q) \propto \Pi_{j=1}^{n}(x-\cos 2\overline{q_j})$ with the following parameters (while preparing the paper, the authors became aware of a paper by van Diejen,[16] in which the same result was presented):

$$q = e^{-2g_0}, \quad (a,b,c,d) = (e^{-2g_1}, e^{-2g_2}, -e^{-2g_3}, -e^{-2g_4}). \tag{7}$$

The outline of derivation is as follows. The functional equation for $f(x)=\Pi_{j=1}^{n}(x-\cos 2\overline{q_j})$ is the same as Eq. (A.4) ($\epsilon=-1$) in Ref. 5 with [this form of $g(x)$ is obtained by using some empirical knowledge based on numerical analysis]

$$\begin{aligned} h(x) = {} & \left(\frac{q^{-1}-q}{2}x - i\left(1+\frac{q^{-1}+q}{2}\right)\sqrt{1-x^2}\right)\left(\frac{a^{-1}-a}{2}(1+x) + i\left(1+\frac{a^{-1}+a}{2}\right)\sqrt{1-x^2}\right) \\ & \times \left(\frac{b^{-1}-b}{2}(1+x) + i\left(1+\frac{b^{-1}+b}{2}\right)\sqrt{1-x^2}\right)\left(\frac{c-c^{-1}}{2}(1-x) - i\left(1-\frac{c+c^{-1}}{2}\right)\sqrt{1-x^2}\right) \\ & \times \left(\frac{d-d^{-1}}{2}(1-x) - i\left(1-\frac{d+d^{-1}}{2}\right)\sqrt{1-x^2}\right), \end{aligned} \tag{8}$$

$$\begin{aligned} g_n(x) = {} & \frac{(1+a)(1+b)(1-c)(1-d)(1+q)(1-x^2)}{8abcdq^{n+1}}(4q(1+abcdq^{2n-1})x^2 \\ & - 2q^n(abc+abd+acd+bcd+(a+b+c+d)q)x - (1+q) \\ & \times (1+q-q^{n+1}-(ab+ac+ad+bc+bd+cd)q^n - q^{n-1}(1-q^n-q^{n+1})abcd)), \end{aligned} \tag{9}$$

and $\sqrt{\delta}=(1-q)/(1+q)$. The three-term recurrence $f_{n+1}(x)=(x-a_n)f_n(x)-b_nf_{n-1}(x)$ for the monic Askey–Wilson polynomial can be found in the literature, for example, Eq. (3.1.5) in Ref. 10. Then Eq. (A.7) in Ref. 5 holds because the functions $X_n(x), Y_n(x)$ of (A.13), (A.14) in Ref. 5 vanish for these a_n, b_n, and $g_n(x)$. Therefore we obtain Proposition A.3, A.4 in Ref. 5.

Remark 1: The models studied in Ref. 5 are special cases of this model. For example,

$$B, \quad \text{Eq. (2.75) in Ref. 5,} \quad (g_0,g_1,g_2,g_3,g_4) = \left(g_L, \tfrac{1}{2}g_S, \tfrac{1}{2}g_S, 0, 0\right),$$

$$C', \quad \text{Eq. (2.78) in Ref. 5,} \quad (g_0,g_1,g_2,g_3,g_4) = \left(g_S, \tfrac{1}{2}g_L, \tfrac{1}{2}g_L, \tfrac{1}{2}g_L, \tfrac{1}{2}g_L\right),$$

$$B'C, \quad \text{Eq. (2.79) in Ref. 5,} \quad (g_0,g_1,g_2,g_3,g_4) = (g_M, g_S, g_L, g_L, 0),$$

due to the following trigonometic formulas:

$$\frac{\sin(x-ig)}{\sin x} = \cosh g(1 - i\tanh g \cot x), \quad \frac{\cos(x-ig)}{\cos x} = \cosh g(1 + i\tanh g \tan x),$$

$$\cosh 2g(1 - i\tanh 2g \cot 2x) = \frac{\sin(2x-i2g)}{\sin 2x} = \frac{\sin(x-ig)}{\sin x}\frac{\cos(x-ig)}{\cos x}.$$

Remark 2: Ismail *et al.* studied the q-Strum Liouville problems and the Bethe ansatz equation of the *XXZ* model.[17] A special case of their results states that the zeros of Askey–Wilson polynomial $p_n(x;a,b,c,d|q) \propto \Pi_{j=1}^{n}(x-\cos 2\overline{q_j})$ with the parameters

$$q = e^{-2g_0}, \quad (a,b,c,d) = (e^{-2g_1}, e^{-2g_2}, e^{-2g_3}, e^{-2g_4}), \tag{10}$$

satisfies the Bethe ansatz type equation (6) with ($g_j > 0$)

$$v(x)=\frac{\sin(x-ig_0)}{\sin x},\quad w(x)=\frac{\sin(x-ig_1)}{\sin x}\frac{\sin(x-ig_2)}{\sin x}\frac{\sin(x-ig_3)}{\sin x}\frac{\sin(x-ig_4)}{\sin x}. \tag{11}$$

However this does not mean that $\{\overline{q_j}\}$ are equilibrium positions of the system (1) with (11), because $V_j(\overline{q})$ is not positive in this case. Moreover the $\cot^4 x$ term in $w(x)$ (11) appears too singular to give a satisfactory quantum Hamiltonian.

III. SINGLE PARTICLE SYSTEMS: SHAPE INVARIANCE

Next let us consider the shape invariance of the "discrete" quantum mechanical single particle systems with a q-shift type kinetic term. The argument is parallel to that given in Ref. 15, in which discrete quantum systems with a shift-type kinetic term are discussed.

In this section we use variables θ, x, and z, which are related as

$$0\leqslant\theta\leqslant\pi,\quad x=\cos\theta,\quad z=e^{i\theta}. \tag{12}$$

The dynamical variable is 2θ and the inner product is $(f(\theta),g(\theta))=\int_0^\pi d\theta\, f(\theta)^* g(\theta)$. We denote $D=D_z\stackrel{\text{def}}{=}z(d/dz)$. Then q^D is a q-shift operator, $q^D f(z)=f(qz)$. Note that

$$\int_0^\pi d\theta=\int_{-1}^1\frac{dx}{\sqrt{1-x^2}},\quad -i\frac{d}{d\theta}=z\frac{d}{dz}=D,\quad f(z)^*=f^*(z^{-1}). \tag{13}$$

For a real constant q $(0<q<1)$ and a function $V(z)=V(z;\boldsymbol{\lambda},q)$ with a set of real parameters $\boldsymbol{\lambda}$, let us consider the following Hamiltonian $H=H(z;\boldsymbol{\lambda},q)$:

$$H\stackrel{\text{def}}{=}\tfrac{1}{2}\sqrt{V(z)}q^D\sqrt{V^*(z^{-1})}+\tfrac{1}{2}\sqrt{V^*(z^{-1})}q^{-D}\sqrt{V(z)}-\tfrac{1}{2}(V(z)+V^*(z^{-1})). \tag{14}$$

The eigenvalue equation reads

$$H\phi_n=\mathcal{E}_n\phi_n, \tag{15}$$

with eigenfunctions $\phi_n(z)=\phi_n(z;\boldsymbol{\lambda},q)$ and eigenvalues $\mathcal{E}_n=\mathcal{E}_n(\boldsymbol{\lambda},q)$ $(n=0,1,\ldots)$ (we assume non-degeneracy $\mathcal{E}_0<\mathcal{E}_1<\cdots$). The kinetic term causes a q-shift in the variable z. This Hamiltonian is factorized and consequently positive semidefinite,

$$H=A^\dagger A, \tag{16}$$

$$A=A(z;\boldsymbol{\lambda},q)\stackrel{\text{def}}{=}\frac{1}{\sqrt{2}}(q^{D/2}\sqrt{V^*(z^{-1})}-q^{-D/2}\sqrt{V(z)}), \tag{17}$$

$$A^\dagger=A(z;\boldsymbol{\lambda},q)^\dagger\stackrel{\text{def}}{=}\frac{1}{\sqrt{2}}(\sqrt{V(z)}q^{D/2}-\sqrt{V^*(z^{-1})}q^{-D/2}), \tag{18}$$

where † denotes the Hermitian conjugation with respect to the above inner product. The ground state ϕ_0 is the function annihilated by A,

$$A\phi_0=0\quad(\Rightarrow H\phi_0=0,\ \mathcal{E}_0=0). \tag{19}$$

Explicitly this equation reads

$$\sqrt{V^*(q^{-1/2}z^{-1})}\phi_0(q^{1/2}z)=\sqrt{V(q^{-1/2}z)}\phi_0(q^{-1/2}z). \tag{20}$$

The other eigenfunctions can be obtained in the form

$$\phi_n(z)\propto P_n(z)\phi_0(z), \tag{21}$$

where $P_n(z)=P_n^{(\boldsymbol{\lambda},q)}(z)$ is a Laurent polynomial in z (for the explicit example below, it is the Askey–Wilson polynomial in x). This $P_n(z)$ satisfies

$$\widetilde{H}P_n = \mathcal{E}_n P_n. \tag{22}$$

Here $\widetilde{H}=\widetilde{H}(z;\boldsymbol{\lambda},q)$ is a similarity transformed Hamiltonian in terms of the ground state wave function ϕ_0,

$$\widetilde{H} \stackrel{\text{def}}{=} \phi_0^{-1} \circ H \circ \phi_0 = \tfrac{1}{2}V(z)q^D + \tfrac{1}{2}V^*(z^{-1})q^{-D} - \tfrac{1}{2}(V(z) + V^*(z^{-1})). \tag{23}$$

Corresponding to the factorization of H (16), $\widetilde{H}$ is also factorized,

$$\widetilde{H} = BC, \tag{24}$$

$$C = C(z,q) = \tfrac{1}{2}(q^{D/2} - q^{-D/2}), \tag{25}$$

$$B = B(z;\boldsymbol{\lambda},q) = V(z)q^{D/2} - V^*(z^{-1})q^{-D/2}. \tag{26}$$

Let us define a new set of wave functions $\phi_{1,n}(z)=\phi_{1,n}(z;\boldsymbol{\lambda},q)$,

$$\phi_{1,n} \stackrel{\text{def}}{=} A\phi_n \quad (n = 1,2,\dots). \tag{27}$$

As a consequence of the factorization, they form eigenfunctions of a new Hamiltonian $H_1 = H_1(z;\boldsymbol{\lambda},q)$,

$$H_1 = AA^\dagger \tag{28}$$

with the same eigenvalues $\{\mathcal{E}_n\}$,

$$H_1\phi_{1,n} = AA^\dagger A\phi_n = A\mathcal{E}_n\phi_n = \mathcal{E}_n\phi_{1,n} \quad (n = 1,2,\dots). \tag{29}$$

To consider the shape invariance of H, we try to find the operators A_1, $A_1^\dagger$ and a real constant $\mathcal{E}_1$ satisfying

$$H_1 = AA^\dagger = A_1^\dagger A_1 + \mathcal{E}_1, \tag{30}$$

$$A_1 = A_1(z;\boldsymbol{\lambda},q) \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}}(q^{D/2}\sqrt{V_1^*(z^{-1})} - q^{-D/2}\sqrt{V_1(z)}), \tag{31}$$

$$A_1^\dagger = A_1(x;\boldsymbol{\lambda},q)^\dagger \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}}(\sqrt{V_1(z)}q^{D/2} - \sqrt{V_1^*(z^{-1})}q^{-D/2}). \tag{32}$$

In other words, given $V(z)=V(z;\boldsymbol{\lambda},q)$, find a new potential $V_1(z)=V_1(z;\boldsymbol{\lambda},q)$ satisfying

$$V_1(z)V_1^*(q^{-1}z^{-1}) = V(q^{1/2}z)V^*(q^{-1/2}z^{-1}), \tag{33}$$

$$V_1(z) + V_1^*(z^{-1}) = V(q^{-1/2}z) + V^*(q^{-1/2}z^{-1}) + 2\mathcal{E}_1. \tag{34}$$

If V_1 has the same functional form as V with another set of parameters $\boldsymbol{\lambda}'$ (e.g, q-shifted $\boldsymbol{\lambda}$),

$$V_1(z;\boldsymbol{\lambda},q) \propto V(z;\boldsymbol{\lambda}',q), \tag{35}$$

then it is shape invariant. Suppose V_1 has the form

$$V_1(z) = V(q^{1/2}z)g(z), \tag{36}$$

with an as yet unspecified function $g(z)$, the above conditions (33) and (34) get slightly simplified,

$$g(z)g^*(q^{-1}z^{-1}) = 1, \tag{37}$$

$$V(q^{1/2}z)g(z) + V^*(q^{1/2}z^{-1})g^*(z^{-1}) = V(q^{-1/2}z) + V^*(q^{-1/2}z^{-1}) + 2\mathcal{E}_1. \tag{38}$$

If the desired V_1 is found, we can construct $H_2, H_3, \ldots$ by repeating the same step. We illustrate this procedure by taking the Askey–Wilson polynomial as an example.

Let us take V as

$$V(z) = V(z;\boldsymbol{\lambda},q) = \frac{(1-az)(1-bz)(1-cz)(1-dz)}{(1-z^2)(1-qz^2)}, \tag{39}$$

where $\boldsymbol{\lambda}=(a,b,c,d)$. For simplicity we assume $-1<a,b,c,d<1$. Note that $V^*(z)=V(z)$. The ground state (19) is given by[10]

$$\phi_0(z) = \phi_0(z;\boldsymbol{\lambda},q) \propto \sqrt{w(z;\boldsymbol{\lambda},q)} \stackrel{\text{def}}{=} \left| \frac{(z^2;q)_\infty}{(az,bz,cz,dz;q)_\infty} \right| \tag{40}$$

$$= \sqrt{\frac{(z^2,z^{-2};q)_\infty}{(az,az^{-1},bz,bz^{-1},cz,cz^{-1},dz,dz^{-1};q)_\infty}}, \tag{41}$$

where $(a_1,\ldots,a_m;q)_\infty = \prod_{j=1}^m \prod_{n=0}^\infty (1-a_jq^n)$. Excited states have the form (21) $\phi_n(z) \propto P_n(z)\phi_0(z)$, and (22) implies that $P_n(z)$ is proportional to the Askey–Wilson polynomial,[10]

$$P_n(z) = P_n^{(\boldsymbol{\lambda},q)}(z) \propto p_n(x;a,b,c,d;q), \tag{42}$$

$$\mathcal{E}_n = \mathcal{E}_n(\boldsymbol{\lambda},q) = \tfrac{1}{2}q^{-n}(1-q^n)(1-abcdq^{n-1}), \tag{43}$$

which is an orthogonal polynomial,

$$\int_{-1}^{1} \frac{\mathrm{d}x}{\sqrt{1-x^2}} w(z;\boldsymbol{\lambda},q) p_n(x;a,b,c,d|q) p_m(x;a,b,c,d|q) \propto \delta_{nm}, \tag{44}$$

namely $(\phi_n,\phi_m) \propto \delta_{nm}$. By denoting $p_n(x;a,b,c,d|q) = P_n(z;\boldsymbol{\lambda},q)$, the factorization (24) gives the forward and backward shift relations [(3.1.8) and (3.1.10) in Ref. 10],

$$C(z;q)P_n(z;\boldsymbol{\lambda},q) = -\mathcal{E}_n(\boldsymbol{\lambda},q)q^{n/2}(z-z^{-1})P_{n-1}(z;q^{1/2}\boldsymbol{\lambda},q), \tag{45}$$

$$-B(z;\boldsymbol{\lambda},q)q^{n/2}(z-z^{-1})P_{n-1}(z;q^{1/2}\boldsymbol{\lambda},q) = P_n(z;\boldsymbol{\lambda},q). \tag{46}$$

It is easy to check that V_1 in the form (36) with

$$g(z) = q^{-1}\frac{1-q^2z^2}{1-z^2} \tag{47}$$

satisfies (37) and (38), and it becomes

$$V_1(z;\boldsymbol{\lambda},q) = V(q^{1/2}z)g(z) = q^{-1}V(z;q^{1/2}\boldsymbol{\lambda},q), \tag{48}$$

and $\mathcal{E}_1$ is

$$\mathcal{E}_1(\boldsymbol{\lambda},q) = \tfrac{1}{2}q^{-1}(1-q)(1-abcd). \tag{49}$$

Therefore we have shape invariance, (48) and

$$A_1(z;\boldsymbol{\lambda},q) = q^{-1/2}A(z;q^{1/2}\boldsymbol{\lambda},q), \tag{50}$$

$$H_1(z;\boldsymbol{\lambda},q) = q^{-1}H(z;q^{1/2}\boldsymbol{\lambda},q) + \mathcal{E}_1(\boldsymbol{\lambda},q). \tag{51}$$

We write down important formulas once again,

$$A(z;\boldsymbol{\lambda},q)\phi_0(z;\boldsymbol{\lambda},q)=0, \tag{52}$$

$$A(z;\boldsymbol{\lambda},q)A(z;\boldsymbol{\lambda},q)^\dagger = q^{-1}A(z;q^{1/2}\boldsymbol{\lambda},q)^\dagger A(z;q^{1/2}\boldsymbol{\lambda},q)+\mathcal{E}_1(\boldsymbol{\lambda},q). \tag{53}$$

Starting from $V_0=V$, $H_0=H$, $\phi_{0,n}=\phi_n$, let us define V_s, H_s, $\phi_{s,n}$ $(n\geqslant s\geqslant 0)$ step by step,

$$V_{s+1}(z;\boldsymbol{\lambda},q)\stackrel{\text{def}}{=}q^{-1}V_s(z;q^{1/2}\boldsymbol{\lambda},q), \tag{54}$$

$$H_{s+1}(z;\boldsymbol{\lambda},q)\stackrel{\text{def}}{=}A_s(z;\boldsymbol{\lambda},q)A_s(z;\boldsymbol{\lambda},q)^\dagger+\mathcal{E}_s(\boldsymbol{\lambda},q), \tag{55}$$

$$\phi_{s+1,n}(z;\boldsymbol{\lambda},q)\stackrel{\text{def}}{=}A_s(z;\boldsymbol{\lambda},q)\phi_{s,n}(z;\boldsymbol{\lambda},q). \tag{56}$$

Here A_s and $A_s^\dagger$ are defined by

$$A_s(z;\boldsymbol{\lambda},q)\stackrel{\text{def}}{=}\frac{1}{\sqrt{2}}\left(q^{D/2}\sqrt{V_s^*(z^{-1};\boldsymbol{\lambda},q)}-q^{-D/2}\sqrt{V_s(z;\boldsymbol{\lambda},q)}\right), \tag{57}$$

$$A_s(z;\boldsymbol{\lambda},q)^\dagger\stackrel{\text{def}}{=}\frac{1}{\sqrt{2}}\left(\sqrt{V_s(z;\boldsymbol{\lambda},q)}q^{D/2}-\sqrt{V_s^*(z^{-1};\boldsymbol{\lambda},q)}q^{-D/2}\right). \tag{58}$$

As a consequence of the shape invariance (53), we obtain for $n\geqslant s\geqslant 0$,

$$V_s(z;\boldsymbol{\lambda},q)=q^{-s}V(z;q^{s/2}\boldsymbol{\lambda},q), \tag{59}$$

$$A_s(z;\boldsymbol{\lambda},q)=q^{-s/2}A(z;q^{s/2}\boldsymbol{\lambda},q),\quad A_s(z;\boldsymbol{\lambda},q)^\dagger=q^{-s/2}A(z;q^{s/2}\boldsymbol{\lambda},q)^\dagger, \tag{60}$$

$$H_s(z;\boldsymbol{\lambda},q)=A_s(z;\boldsymbol{\lambda},q)^\dagger A_s(z;\boldsymbol{\lambda},q)+\mathcal{E}_s(\boldsymbol{\lambda},q)=q^{-s}H(z;q^{s/2}\boldsymbol{\lambda},q)+\mathcal{E}_s(\boldsymbol{\lambda},q), \tag{61}$$

$$\mathcal{E}_{s+1}(\boldsymbol{\lambda},q)=\mathcal{E}_s(\boldsymbol{\lambda},q)+q^{-s}\mathcal{E}_1(q^{s/2}\boldsymbol{\lambda},q), \tag{62}$$

$$H_s(z;\boldsymbol{\lambda},q)\phi_{s,n}(z;\boldsymbol{\lambda},q)=\mathcal{E}_n(\boldsymbol{\lambda},q)\phi_{s,n}(z;\boldsymbol{\lambda},q), \tag{63}$$

$$A_s(z;\boldsymbol{\lambda},q)\phi_{s,s}(z;\boldsymbol{\lambda},q)=0, \tag{64}$$

$$A_s(z;\boldsymbol{\lambda},q)^\dagger\phi_{s+1,n}(z;\boldsymbol{\lambda},q)=(\mathcal{E}_n(\boldsymbol{\lambda},q)-\mathcal{E}_s(\boldsymbol{\lambda},q))\phi_{s,n}(z;\boldsymbol{\lambda},q). \tag{65}$$

The relation (62) means that $\{\mathcal{E}_n\}$ is calculable from $\mathcal{E}_1$ (49). In other words, the spectrum is determined by the shape invariance.

From (56) and (65) we obtain the formulas,

$$\phi_{s,n}(z;\boldsymbol{\lambda},q)=A_{s-1}(z;\boldsymbol{\lambda},q)\cdots A_1(z;\boldsymbol{\lambda},q)A_0(z;\boldsymbol{\lambda},q)\phi_n(z;\boldsymbol{\lambda},q), \tag{66}$$

$$\phi_n(z;\boldsymbol{\lambda},q)=\frac{A_0(z;\boldsymbol{\lambda},q)^\dagger}{\mathcal{E}_n(\boldsymbol{\lambda},q)-\mathcal{E}_0(\boldsymbol{\lambda},q)}\frac{A_1(z;\boldsymbol{\lambda},q)^\dagger}{\mathcal{E}_n(\boldsymbol{\lambda},q)-\mathcal{E}_1(\boldsymbol{\lambda},q)}\cdots\frac{A_{n-1}(z;\boldsymbol{\lambda},q)^\dagger}{\mathcal{E}_n(\boldsymbol{\lambda},q)-\mathcal{E}_{n-1}(\boldsymbol{\lambda},q)}\phi_{n,n}(z;\boldsymbol{\lambda},q). \tag{67}$$

The former (66) gives the eigenfunction $\phi_{s,n}$ of the sth Hamiltonian H_s along the isospectral line with energy $\mathcal{E}_n$, starting from ϕ_n of the original Hamiltonian H by repeated application of the A operators. The latter (67), on the other hand, expresses the nth eigenfunction ϕ_n of the original Hamiltonian, starting from the explicitly known ground state $\phi_{n,n}$ of the nth Hamiltonian H_n by repeated application of the $A^\dagger$ operators. Since (61) implies $\phi_{n,n}(z;\boldsymbol{\lambda},q)\propto\phi_0(z;q^{n/2}\boldsymbol{\lambda},q)$, ϕ_n is expressed in terms of ϕ_0 and V. The latter formula (67) could also be understood as the generic form of the Rodrigue's formula for the orthogonal polynomials. The situation is depicted in Fig. 1.

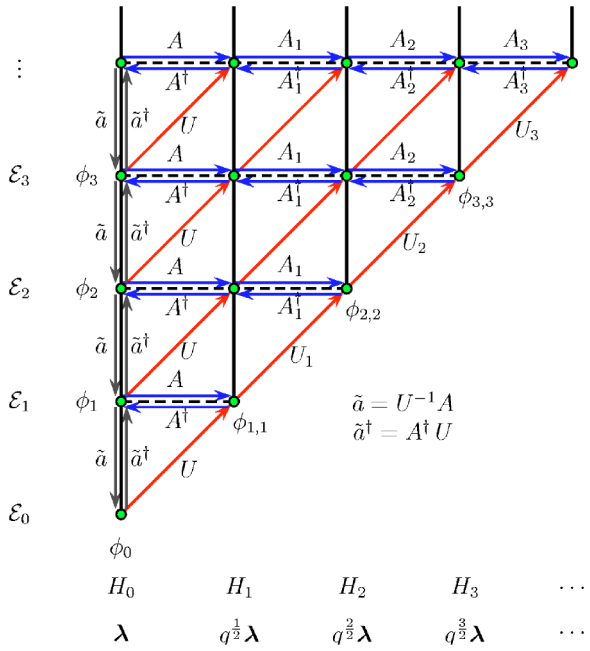

FIG. 1. A schematic diagram of the energy levels and the associated Hamiltonian systems together with the definition of the A and $A^\dagger$ operators and the creation ($\tilde{a}^\dagger$) and annihilation ($\tilde{a}$) operators. The parameter set is indicated below each Hamiltonian.

The operator A acts to the right and $A^\dagger$ to the left along the horizontal (*isospectral*) line. They should not be confused with the *annihilation* and *creation* operators, which act along the vertical line of a given Hamiltonian H_s going from one energy level $\mathcal{E}_n$ to another $\mathcal{E}_{n\pm1}$.

In order to define the annihilation and creation operators, let us introduce normalized basis $\{\hat{\phi}_{s,n}\}_{n\geqslant s}$ for each Hamiltonian H_s. Ordinarily, the phase of each element of an orthonormal basis could be completely arbitrary. In the present case, however, the eigenfunctions are orthogonal polynomials. That is, they are real and the relations among different degree members are governed by the three-term recurrence relations. So the phases of $\{\hat{\phi}_{s,n}\}_{n\geqslant s}$ are fixed. Let us introduce a unitary (in fact an orthogonal) operator U_s mapping the sth orthonormal basis $\{\hat{\phi}_{s,n}\}_{n\geqslant s}$ to the $(s+1)$th $\{\hat{\phi}_{s+1,n}\}_{n\geqslant s+1}$ (see Fig. 1 and, for example, Refs. 14 and 18),

$$U_s\hat{\phi}_{s,n} = \hat{\phi}_{s+1,n+1}, \quad U_s^\dagger\hat{\phi}_{s+1,n+1} = \hat{\phi}_{s,n}. \tag{68}$$

We denote that $U_0 = U$. Roughly speaking U changes the parameters from $\boldsymbol{\lambda}$ to $q^{1/2}\boldsymbol{\lambda}$. Let us introduce an annihilation $\tilde{a}$ and a creation operator $\tilde{a}^\dagger$ for the Hamiltonian H as follows:

$$\tilde{a} = \tilde{a}(z;\boldsymbol{\lambda},q) \stackrel{\text{def}}{=} U^\dagger A(z;\boldsymbol{\lambda},q), \quad \tilde{a}^\dagger = \tilde{a}(z;\boldsymbol{\lambda},q)^\dagger \stackrel{\text{def}}{=} A(z;\boldsymbol{\lambda},q)^\dagger U. \tag{69}$$

It is straightforward to derive

$$H = \tilde{a}^\dagger\tilde{a}, \tag{70}$$

$$[\tilde{a},\tilde{a}^\dagger]\hat{\phi}_n(z;\boldsymbol{\lambda},q) = (\mathcal{E}_{n+1}(\boldsymbol{\lambda},q) - \mathcal{E}_n(\boldsymbol{\lambda},q))\hat{\phi}_n(z;\boldsymbol{\lambda},q). \tag{71}$$

IV. SUMMARY AND COMMENTS

In this paper we have studied the equilibrium positions of the Ruijsenaars–Schneider–van Diejen systems with the trigonometric potential and shown that for a suitable choice of the

elementary potential functions they are given by the zeros of the Askey–Wilson polynomials with five parameters (see Sec. II). The equation for the equilibrium positions (5) (without the positivity condition) can be written in the Bethe ansatz type equation (6). The Bethe ansatz is a powerful method for solvable models, and solving the Bethe ansatz equation or clarifying the properties of its solutions are very important. Ismail *et al.* studied Bethe ansatz equations for spin *s XXZ* models from the *q*-Sturm–Liouville problem point of view.[17] This kind of approach would shed light on the Bethe ansatz(-type) equations.

We have also studied the shape invariance of "discrete" quantum mechanical single particle systems with a *q*-shift type kinetic term. As an example of this shape invariance, we present such a system whose eigenfunctions are the Askey–Wilson polynomials. In this example $V(z)$ is a rational function of z (trigonometric function of θ), but the method works for a wider class of functions. In ordinary quantum mechanics there is the Crum's theorem,[13] which states a construction of the associated isospectral Hamiltonians H_s and their eigenfunctions $\phi_{s,n}$ (Fig. 1) even if the system has no shape invariance. The construction of H_s and $\phi_{s,n}$ given in this paper and Ref. 15 needs shape invariance. A "discrete" analogue of the Crum's theorem, namely similar construction without shape invariance, would be very helpful, if it exists.

We comment on the shape invariance of the Askey–Wilson polynomials with a small number of parameters, $p_n(x;a,b,1,-1)$. In this case $V(z)$ in (14) is

$$V(z;\boldsymbol{\lambda},q)=\frac{(1-az)(1-bz)}{1-qz^2},\quad \boldsymbol{\lambda}=(a,b). \tag{72}$$

By taking a form (36) with the same $g(z)$ (47), the conditions (37) and (38) are satisfied, and we have

$$V_1(z;\boldsymbol{\lambda},q)=q^{-1}V(q^{-1/2}z;q\boldsymbol{\lambda},q),\quad \mathcal{E}_1(\boldsymbol{\lambda},q)=\tfrac{1}{2}(q^{-1}-1)(1+ab). \tag{73}$$

Since $D_z=z(d/dz)$ is invariant under the rescaling of z, $D_z=D_{\alpha z}$, the Hamiltonian is shape invariant,

$$H_1(z,\boldsymbol{\lambda},q)=q^{-1}H(q^{-1/2}z;q\boldsymbol{\lambda},q)+\mathcal{E}_1(\boldsymbol{\lambda},q). \tag{74}$$

The sth Hamiltonian and the spectrum are given by

$$H_s(z;\boldsymbol{\lambda},q)=q^{-s}H(q^{-s/2}z;q^s\boldsymbol{\lambda},q)+\mathcal{E}_s(\boldsymbol{\lambda},q), \tag{75}$$

$$\mathcal{E}_s(\boldsymbol{\lambda},q)=\mathcal{E}_{s-1}(\boldsymbol{\lambda},q)+q^{-(s-1)}\mathcal{E}_1(q^{s-1}\boldsymbol{\lambda},q)=\tfrac{1}{2}q^{-s}(1-q^s)(1+abq^{s-1}). \tag{76}$$

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Erratum: Quantum-mechanical scattering in exterior domains with impenetrable boundaries and short-range potentials [J. Math. Phys. 45, 1426 (2004)]

A. W. Sáenz[a)]
Physics Department, Catholic University of America, Washington DC 20064 and Naval Research Laboratory, Washington DC 22375

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The following corrections should be made on p. 1444 of Appendix A.

(1) After the displayed equation for $\|f\|_{1,A}$ in the second paragraph, insert the definition: $H_0^1(A)$ denotes the completion of the complex space $C_0^\infty(A)$ in the norm $\|\cdot\|_{1,A}$.

(2) The first line of the third paragraph should begin with the definition: Let $A(r)=\{x\in A:\|x\|_A<r\}$.

(3) In the second line of the third paragraph, "$\partial f/\partial x_i|A(R)\in L^2(A(r))$" should read "$\Delta f|A(r)\in L^2(A(r))$."

(4) In the fourth line of the third paragraph, "$\|\cdot\|_{1,A(r)}$" should read "$\|\cdot\|_{\Delta,A(r)}$."

(5) In the sixth line of the third paragraph, "$\partial f/\partial x_i|A(r)\in L^2(A(r))$" should read "$\partial f/\partial x_i|A(r)\in L^2(A(r))(i=1,\ldots,\nu)$."

[a)]Electronic mail: saenz@dave.nrl.navy.mil

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Hybrid states of two and three level atoms

Claude Billionnet[a)]
Centre de Physique Théorique, Ecole Polytechnique, 91128 Palaiseau Cedex, France

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We calculate atom-photon resonances in the Wigner-Weisskopf model, admitting two photons and choosing a particular coupling function. We also present a rough description of the set of resonances in a model for a three-level atom coupled to a scalar-photon field. We give a general picture of matter-field resonances that these results fit into. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1935428]

I. INTRODUCTION

In recent years there has been a renewed interest for atom-radiation states in nonrelativistic quantum electrodynamics. After the rigorous proof[1] of the existence, for small coupling constants, of resonances (singularities of an analytic continuation of the Hamiltonian resolvent), resonances coming from the naked-atom-Hamiltonian eigenvalues, many studies have been concentrated on the study of the Hamiltonian spectrum and more particularly on the existence of the fundamental state in various models,[2–7] for arbitrary coupling constants. This latter question is a nontrivial problem since it has long been known that negative Hamiltonian eigenvalues may appear when the coupling constant increases.[8,9] In preceding works (see Ref. 10, and references therein), for our part, we were interested in a method for calculating resonances for arbitrary values of the coupling constant. It is a way of catching the above-mentioned particular eigenvalues. The result we obtained can be generally stated as follows. The coupling of a discrete-level system S to a zero-mass field does not only shift the level energies into the complex plane. Certainly these energies become resonances. But the coupling also creates other poles of the resolvent (or of its continuations), which have to be placed on the same footing as the preceding ones. For certain values of physical parameters of S, or certain values of the $(S+field)$ coupling constant, these latter poles may be eigenvalues of the coupled-system Hamiltonian. (In this article, the word resonance will refer to such a pole or, by extension, to an eigenvalue, when there is an obvious possible continuous transition from the one to the other.)

The presence of these poles is well-known for an atom or a molecule in an environment in which the only emitted or absorbed photons are monochromatic (lasers or cavities). Indeed, for a two-level atom with energies e_0 and e_1, and photons with energy e_1-e_0, the upper level is split into two levels by the coupling, when at most one photon is considered[9] (vacuum-field Rabi splitting). The coupling increases the number of Hamiltonian eigenvalues because it splits the degeneracy of each of the eigenvalues $e_1, 2e_1-e_0, \cdots, e_1+n(e_1-e_0), \cdots$ of the uncoupled atom-photon system. This phenomenon occurs in different but analogous situations: for instance the coupling of an exciton to the mode of a cavity,[11,12] and it can be detected by spectroscopic means. It is also present in electron-phonon interactions.[13,14] Let us note that the final number of atom-photon states is simply a consequence of the combination of discrete atom states with discrete photon states.

Many papers have studied the coupling of a two-level system to another system which has either discrete levels or a continuum of levels, often focusing on the continuous transition from the

a)Electronic mail: billionnet@cpht.polytechnique.fr

vacuum Rabi splitting to the Fermi's golden rule.[15,16] In the present work, a splitting is exhibited also in the continuum case. The eigenstates of the naked atom we are used to are thus but a small part of all the possible states.

In fact, the appearance of new resonances when the system S is coupled to a field is a general phenomenon whose explanation is given in Sec. II. It is, of course, not due to the smallness of the photon-state width. A numerical method, explained and illustrated in previous publications, enabled us to study and calculate these resonances in various simple models: S was either a harmonic oscillator[17] or a two-level atom. But in this latter case, we almost always limited ourselves to considering physical states with at most one photon.

A reason to carry on with the study is that the new resonances appearing with the coupling might play a role for systems having a large spatial extension: for instance Rydberg atoms or, a case maybe more important, molecular orbitals of big molecules. Indeed, in a very simplified model for an interaction of S with the field, a model in which the spatial extension δ of S may be varied (S is a charged harmonic oscillator whose mass and spring constant may be varied), we noted that some among the poles we speak about come to the negative real axis when δ gets large enough,[18] in comparison with the length scale of the problem, namely the wavelength of the transition from the first excited state to the fundamental one. These poles then correspond to stable states and are therefore important states. Their wave function can be written: it is a mixing of electron and photon states. Analogous phenomena may be expected for more complex extended systems. Besides, the treatment of strong coupling is also interesting for applications in nuclear physics.

From the theoretical point of view, it is thus important to be able to start the study of the resonances in the two following situations: a system with more than two levels and, in the case of two levels, a system with several (non monochromatic) photons. Section III deals with this second question. To the best of our knowledge, it is tackled in the literature only when the fundamental state question is discussed.[4] Here we calculate some mixed (or hybrid) states with several photons, or the resonances which correspond to them. Section IV tackles the same problem for three-level atoms, but since the situation is more complicated, we limit ourselves to a qualitative description of the numerous resonances. Both studies lead to the reasonable conjecture that the number of resonances should be roughly the product of the number of atom states by the number of independent radiation states actually coupled to the atom.

II. NOTATION OF THE RESONANCES

We need a precise notation for the different poles.

It will follow from a very general argument, which also explains why every atomic level should give rise to a double infinity of resonances. Let us consider a material quantum system S whose Hamiltonian, H_S, has eigenstates $|0\rangle$, $|1\rangle$, $|2\rangle$,..., with energies $e_0, e_1, e_2, \ldots$. Let us suppose that this system is coupled to the field of a massless boson, here the photon. We denote the state-space of the ($S+$*field*)-system by $\mathcal{E}$.

Let us consider a very general form for the Hamiltonian of the coupled system:

$$H(\lambda) = H_S \otimes 1 + 1 \otimes H_{\mathrm{rad}} + \lambda V, \tag{2.1}$$

where H_{rad} is the energy operator for the photon field and $\lambda\ V$ represents the coupling of S to the field. Let us introduce the auxiliary Hamiltonian.

$$H(\lambda, \mu) = H_S \otimes 1 + \mu 1 \otimes H_{\mathrm{rad}} + \lambda V, \tag{2.2}$$

where μ is a parameter which may be zero or positive.

If $\mu = 0$ and $\lambda = 0$, the energy levels $e_0, e_1, \ldots$ are infinitely degenerated (in $\mathcal{E}$), as the number of photons accompanying state $|m\rangle$ may be any integer and, moreover, the dimension of the space of possible photon states is infinite. Thus the dimension of the eigenspace $\mathcal{H}_i$ associated with the eigenvalue e_i of $H(0,0)$ is infinite. Let us underline the fact that the degeneracy we speak about here is different from the one we mentioned in the second paragraph of the introduction.

The idea underlying our present study, as well as the preceding ones, is to perturb $H(0,0)$ with respect to λ and μ successively. *A priori*, the perturbation with respect to λ removes the degeneracy, although it may be only partially, in some particular cases. This leads to the following notation.

Notation 1: $\zeta_{i,1}(\lambda), \zeta_{i,2}(\lambda), \ldots$ *denote the* $\mathbb{N}^2(=\mathbb{N})$ *eigenvalues of* $H(\lambda,0)$ *which tend to* e_i *when* λ *tends to* 0.

The choice of the second index, or an equivalent choice, will be described in the different contexts.

The perturbation with respect to μ then leads us to the following notation for the resonances we are interested in.

Notation 2: When we have selected, in a way which remains to be defined, one pole among those of the resolvent of $H(\lambda,\mu)$ *which tend to* $\zeta_{i,j}(\lambda)$ *when* μ *tends to* 0, *we denote it by* $z_{i,j}(\lambda,\mu)$.

There are two reasons for having to make a selection. The first one is that if the $\zeta_{i,j}$'s remain degenerated, and this will be the case in the model of Sec. III (see Proposition 3.2), then the degeneracy may be removed for $\mu \neq 0$; in other words, for $\mu \neq 0$, there may be several resonances (or eigenvalues) going to the same $\zeta_{i,j}$ when μ goes to 0. (See a more precise description at the beginning of Sec. III D 2.) The one we call $z_{i,j}(\lambda,\mu)$ will be a particular one, selected in a way which will be made precise in the context. The second reason is that the matrix elements of $[z - H(\lambda,\mu)]^{-1}$ are multivalued functions of z for $\mu \neq 0$. Therefore, two poles of two different determinations may have the same limit when μ goes to 0. However, we assume that there is only one pole tending to $\zeta_{i,j}$ for a given determination, once the first choice has been made. This will enable us to get the $z_{i,j}(\lambda,\mu)$'s by numerical calculus, starting from their germs $\zeta_{i,j}(\lambda)$'s. The notations of the poles of the different branches of the resolvent matrix elements will be made precise later on, by adding an upper index which refers to the determination (see Sec. III D 2 c).

III. HYBRID STATES FOR A TWO-LEVEL ATOM IN THE WIGNER-WEISSKOPF MODEL

Two resonances (distinct or not, see below) are well-known in the Wigner–Weisskopf model (recalled in Sec. III A), or in the Friedrichs model, which describe a two-level atom coupled to the field of a massless scalar boson.[4,8,9] These resonances can be seen without considering two-photon states. One can be associated, for small coupling constants, to the excited state of the atom; the other one is an eigenvalue corresponding to a stable state which differs from the unperturbed fundamental state. This eigenvalue appears when the coupling constant gets large enough. (Up to recently, it was not clear whether these two resonances were two occurrences of the same resonance or not. In fact this depends on the parameters of the physical system, but in any case it can be shown that there are actually two different resonances,[10] for a given value of the coupling constant.) In this section we want to study other resonances by taking into account several photons. The existence of such states is already alluded to in Ref. 4, where Theorem 2.2 shows that the ground state of the coupled system must take several-photon states into account. In a particular coupling, we will construct two of these states or resonances. It is the subject of Sec. III D 2. In accordance with the general notations introduced in Sec. II, they will be denoted by $z_{0,2}(\lambda,1)$ and $z_{1,2}(\lambda,1)$, tending, respectively, to the energies 0 and 1 of the naked atom. The index 2 will be explained later on.

A. The model and some notations

The atom state space is $\mathbb{C}^2$. The fundamental state is $|0\rangle := (1,0)$, with energy $e_0 = 0$ and the excited state is $|1\rangle := (0,1)$, with energy $e_1 = 1$. In the $\{|0\rangle, |1\rangle\}$ basis, the annihilation operator is $a = \left(\begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix}\right)$. The field state space is $\mathcal{F} := \oplus_{n=0}^{\infty} \mathcal{F}_n$, as usual, with $\mathcal{F}_0 := \mathbf{C}$ and $\mathcal{F}_n := L^2(\mathbb{R})^{\vee n}$. Let g be in $L^2(\mathbb{R})$ with $\|g\|_2 = 1$ and $c(\overline{g})$, $c^*(g)$ be the operators annihilating and creating a (scalar) photon in state g. If $\hat{\omega}$ denotes the multiplication operator by the function $|k|$, acting in $L^2(\mathbb{R})$, the energy operator in $\mathcal{F}, d\Gamma(\hat{\omega})$, is denoted by H_{rad}.

The Hamiltonian of the model is

$$H(\lambda) := a^*a \otimes 1 + 1 \otimes H_{\mathrm{rad}} + \lambda(a^* \otimes c(\overline{g}) + a \otimes c^*(g)). \tag{3.1}$$

In order to have the mixed states appear readily, we introduce

$$H(\lambda,\mu) := a^*a \otimes 1 + \mu 1 \otimes H_{\mathrm{rad}} + \lambda(a^* \otimes c(\overline{g}) + a \otimes c^*(g)). \tag{3.2}$$

Note that $H(\lambda,\mu)$ is unitarily equivalent to the Hamiltonian obtained through replacing g in (3.1) by its unitarily scale transformed $g_\mu(p) := \mu^{-1/2} g(\mu^{-1}p)$. Introducing the parameter μ is thus not so arbitrary as it may seem since μ is in some way related to the width of the coupling function. But note that the position of the peak of g is also moved. This is a departure from a study which would start with monochromatic photons and enlarge the width of their spectrum little by little, without changing the position of the peak.

This Hamiltonian has invariant subspaces. To describe them and, in the same way, prepare the notations for Sec. IV, let us set $\mathcal{H}^{(1)}_{\mathrm{rad}}$, the space spanned by g; $\mathcal{F}^{(1)}_n := (\mathcal{H}^{(1)}_{\mathrm{rad}})^{\vee n}$, the space of n photon states, but each photon being in state g; $\mathcal{E}_0 := |0\rangle \otimes \mathcal{F}_0$, and for $n \geqslant 1$, $\mathcal{E}_n := |0\rangle \otimes \mathcal{F}_n \oplus |1\rangle \otimes \mathcal{F}_{n-1}$, a space we call the "$n$-excitation space"; $\mathcal{E}^{(1)}_n := |0\rangle \otimes \mathcal{F}^{(1)}_n \oplus |1\rangle \otimes \mathcal{F}^{(1)}_{n-1}$, $n \geqslant 1$, $\mathcal{E}^{(1)}_0 = \mathcal{E}_0$; $\mathcal{E}^{(1)} := \oplus_0^\infty \mathcal{E}^{(1)}_n$, $\mathcal{E} := \oplus_0^\infty \mathcal{E}_n$.

We will often use the notation $|n,\varphi\rangle$ for $|n\rangle \otimes \varphi$, if $|n\rangle$ is an atom state and $\varphi \in \mathcal{F}$.

Lemma: $\mathcal{E}_n$ is invariant by $H(\lambda,\mu)$, for all $n \geqslant 0$ and all $\mu \geqslant 0$; $\mathcal{E}^{(1)}_n \subset \mathcal{E}_n$ is invariant by $H(\lambda,0)$, for all $n \geqslant 0$.

As we said when we introduced Notations 1 and 2 in Sec. II, the method for studying the resonances of $H(\lambda,\mu)$ is a numerical method in which μ takes greater and greater values, starting from 0. So we begin with giving some properties of $H(\lambda,0)$.

B. Construction of resonances of $H(\lambda,\mu)$ from eigenvalues of $H(\lambda,0)$: Setting up

Proposition 3.1: $H(\lambda,0)\downarrow_{\mathcal{E}^{(1)}}$, the restriction of $H(\lambda,0)$ to $\mathcal{E}^{(1)}$, has a double infinity of eigenvalues

$$\zeta_{0,n}(\lambda) = 2^{-1}(1 - \sqrt{1 + 4n\lambda^2}), \quad \zeta_{1,n}(\lambda) = 2^{-1}(1 + \sqrt{1 + 4n\lambda^2}). \tag{3.3}$$

For each n, an eigenvector of $H(\lambda,0)\downarrow_{\mathcal{E}^{(1)}}$ associated with $\zeta_{i,n}(\lambda)$ is

$$\phi^{(0)}_{i,n} := (1 + n\lambda^2 \zeta^{-2}_{i,n}(\lambda))^{-1}(|1, g^{\otimes(n-1)}\rangle + \sqrt{n}\lambda\zeta^{-1}_{i,n}(\lambda)|0, g^{\otimes n}\rangle) \in \mathcal{E}^{(1)}_n. \tag{3.4}$$

Proof: $\mathcal{E}^{(1)}_n$, two dimensional, is invariant by $H(\lambda,0)$. (3.3) is thus obtained through diagonalizing a two-by-two matrix. ■

The choice of the first index in the notation of the eigenvalues is in accordance with the principle stated at the end of Sec. II. By the choice of the second index, we indicate that the eigenvector belongs to $\mathcal{E}^{(1)}_n$.

We note that only some part of the double degeneracy mentioned in Sec. II is removed here. Indeed, each $\zeta_{i,n}(\lambda)$ is still degenerated, since adding an arbitrary number of photons whose states are orthogonal to g to some state does not change the energy of this state. This follows from $[H(\lambda,0), 1 \otimes c^*(h)] = 0$, when the scalar product (g,h) vanishes. Let us develop this in order to introduce some notations.

Let $g_1, g_2, \ldots$ be a basis of functions orthogonal to g. For $p \geqslant 1$, let $\mathcal{G}_{0,p}$ be the subspace of $\mathcal{E}$ spanned by

$$\phi^{(n_1,n_2,\ldots)}_{0,n} := \prod_{i=1}^{\infty} (1 \otimes c^*(g_i))^{n_i} \phi^{(0)}_{0,p} \in \mathcal{E}_n \tag{3.5}$$

when n varies from p to infinity; n_i are k non-negative integers, k being arbitrary and

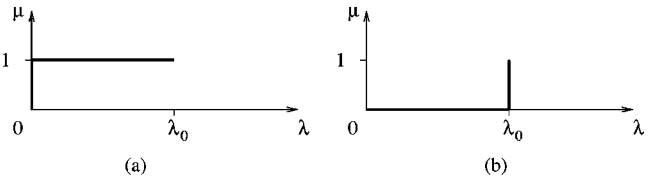

FIG. 1. Two paths enabling to construct two unnecessarily identical resonances.

$$\sum_{i=1}^{k} n_i = n - p.$$

In the same way, let $\mathcal{G}_{1,p}$ be the subspace spanned by

$$\phi_{1,n}^{(n_1,n_2,\ldots)} := \prod_{i=1}^{\infty} (1 \otimes c^*(g_i))^{n_i} \phi_{1,p}^{(0)} \in \mathcal{E}_n. \tag{3.6}$$

Proposition 3.2: For generic λ *values,* $\mathcal{G}_{i,p}$ *is the eigenspace of* $H(\lambda,0)$ *associated with the eigenvalue* $\zeta_{i,p}$*, for* $i=0,1$ *and* $p \geqslant 1$.

See hints for the proof in Appendix B 1, which is devoted to the proof of an analogous property.

Let us thus note that eigenstates of $H(\lambda,0)$ associated with $\zeta_{i,n}$ not only are not n-photon states but are neither necessarily n-excitation states. This complicates the picture of these eigenvalues and of the resonances $z_{i,n}(\lambda,\mu)$ they give rise to.

To be complete, let us still mention that 0 is an eigenvalue of $H(\lambda,0)$, with, if $\Sigma n_i = n$, n arbitrary, the associated eigenvectors

$$\phi_{0,0}^{(n_1,n_2,\ldots)} := \prod_{i=1}^{\infty} (1 \otimes c^*(g_i))^{n_i} |0\rangle \otimes \Omega \in \mathcal{E}_n. \tag{3.7}$$

where Ω denotes the vacuum state in $\mathcal{F}$.

Let us now turn to the μ variation, in order to define and construct resonances $z_{0,1}(\lambda,\mu)$, $z_{0,2}(\lambda,\mu),\ldots$ and $z_{1,1}(\lambda,\mu)$, $z_{1,2}(\lambda,\mu),\ldots$, from their germs $\zeta_{i,j}(\lambda)$ (for the notation, see Notation 2 in Sec. II).

This construction, as we said, is purely numerical for the moment. It goes step-by-step, starting from $\mu=0$. We do not look for any existence theorem nor for a complete description, difficult to get because of the complicated structure of the set of resonances. We just want to obtain numerical values for resonances which have not been considered up to now, and might be important.

This requires a particular choice for g. Before that, let us nevertheless give some general indications.

C. General remarks about the poles of the resolvent of $H(\lambda,\mu)$

In front of so many resonances, it is natural to ask oneself the question: when we consider $H(\lambda,1)$, which resonance is the one we are used to, that is to say is there any which could be "associated" with the excited state $|1\rangle$? Without going into detail here, let us explain shortly why the issue is not simple. In particular, given a value λ_0 of the coupling constant, even a small one, why $z_{1,1}(\lambda_0,\mu)$ is not necessarily the resonance we are used to. The resonance we are used to is obtained through restricting $H(\lambda,\mu)$ to $\mathcal{E}_1$ and following the resonance which sits at 1 for $\mu=1$ and $\lambda=0$. We follow it as λ increases from 0 to λ_0. Since its position at $\lambda=0$ does not depend on μ, it amounts to following the resonance along the path of Fig. 1(a), from its value 1 at the origin of the path.

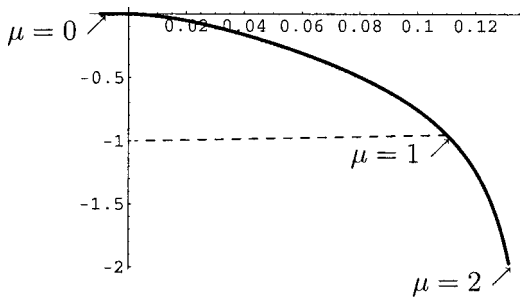

FIG. 2. The resonance $z_{0,1}(0.1,\mu)$, for $\mu \in [0,2]$, first in $\mathbb{R}^-$, then in the second sheet of the complex plane.

It is the usual perturbative approach, in which there is no need to introduce μ. On the contrary, $z_{1,1}(\lambda_0,1)$, also defined with $\mathcal{E}_1$ (see Sec. III D 1 b), is the limit of $z_{1,1}(\lambda_0,\mu)$, when μ increases from 0 (then $z_{1,1}(\lambda_0,0)=\zeta_{1,1}(\lambda_0)$) to 1. Since $\zeta_{1,1}(\lambda_0)$, by definition, tends to 1 when λ_0 tends to 0, $z_{1,1}(\lambda_0,1)$ is the resonance obtained through following the resonance along the path of Fig. 1(b), from the value 1 at the origin of this path. Now, in some examples, functions $z_{0,1}(\lambda,\mu)$ and $z_{1,1}(\lambda,\mu)$ are two branches of a unique analytic 2-variable function, which, even when restricted to $\mathbb{R}^2$, has branch points. These real branch points may lie inside the rectangle $[0,\lambda_0]\times[0,1]$ of the (λ,μ) plane, so that the two previous values of the resonances at the common end $(\lambda_0,1)$ of the two previous paths may be different. The λ and μ variations do not necessarily commute.[10] (Let us note here that it is thus dangerous to move λ and μ simultaneously without caution, as we did it for instance in the second paragraph of Sec. III of Ref. 17.) This phenomenon is at the origin of the remark in parentheses in the first paragraph of the present Sec. III.

This seems to be a drawback of the introduction of parameter μ. But this introduction enables us to see resonances for the physical Hamiltonian ($\mu=1$) which the perturbative approach does not give so easily. Indeed, when λ is the only parameter and when it is varied from λ_0 to 0, the continuous variation of the resonance siting at $z_{i,1}(\lambda_0,\mu)$ for $\lambda=\lambda_0$ may lead to 1, but also to infinity, or to a pole of g (see Fig. 2, where the pole is $-i$). The result depends on μ and g. But these two latter limits are too singular points to start a calculation in their neighborhood.

Since the difficulties of a general study are due to branch points whose positions depend on g, we choose a particular g. We now come back to the study of the announced particular case.

D. Construction of resonances of $H(\lambda,\mu)$ from eigenvalues of $H(\lambda,0)$. Calculations for a particular g

We fix the coupling constant at 0.1 and take the particular function we already used:[10]

$$g(p) = \sqrt{\frac{2}{\pi}}\frac{p}{1+p^2}. \tag{3.8}$$

This is a simple rational function which exhibits the type of singularity that actual coupling functions may have. (See, for instance, matrix elements of the interaction Hamiltonian for hydrogenic atoms in the electromagnetic field.[19])

In Sec. III D 1, we recall the definition of $z_{0,1}(\lambda,\mu)$ and $z_{1,1}(\lambda,\mu)$ and the known formulas through which they are obtained. We give their values for various μ and λ. We use them later on. Then, in Sec. III D 2, we define resonances $z_{0,2}(\lambda,\mu)$ and $z_{1,2}(\lambda,\mu)$ and give some approximate values. An evaluation of the errors is given in Appendix A.

1. Brief review about two resonances obtained with only one photon: $z_{0,1}(0.1,\mu)$ and $z_{1,1}(0.1,\mu)$

They are poles of $\langle 1\otimes\Omega|[z-H\downarrow_{\mathcal{E}_1}]^{-1}|1\otimes\Omega\rangle$ or of its analytic continuation.

TABLE I. Values of $z_{0,1}(0.1,\mu)$, for some values of μ below $\mu_c(0.1)$.

$10^3\,\mu$	0	0.1	1	3	6	6.2	6.36	6.366
$10^4\,z_{0,1}(0.1,\mu)$	−99	−94	−68	−34	−2.5	−1.1	0.04	0.001

Resonance $z_{0,1}(0.1,\mu)$.

For $\Im z>0$, the above mentioned matrix element is[20] $[f(\lambda,\mu,z)]^{-1}$, where

$$f(\lambda,\mu,z) := z-1-2\lambda^2\int_0^\infty \frac{g(p)^2}{z-\mu p}\mathrm{d}p. \tag{3.9}$$

Therefore, $z_{i,1}(0.1,\mu)$ are zeros of $f(\lambda,\mu,.)$, a function defined in the cut plane $\mathbb{C}/\mathbb{R}^+$, or of its analytic continuation through the cut, clockwise.[9,20,21] For $\mu\leqslant\mu_c(\lambda):=2\lambda^2\int_0^\infty g(p)^2/p\mathrm{d}p$, $f(\lambda,\mu,.)$ has only one zero; it is on the negative real axis and is 0 if and only if $\mu=\mu_c(\lambda)$. When μ tends to 0, it tends to $\zeta_{0,1}(0.1)$ and therefore we denote it by $z_{0,1}(0.1,\mu)$. We recall that the corresponding normalized eigenvector, which we denote by $\phi^{(0)}_{0,1}(\lambda,\mu)$, is proportional to

$$\psi^{(0)}_{0,1}(\lambda,\mu) := |1,\Omega\rangle+\lambda\left|0,\frac{g}{z_{0,1}(\lambda,\mu)-\mu|p|}\right\rangle. \tag{3.10}$$

For $\mu>\mu_c(\lambda)$, $z_{0,1}(\lambda,.)$ is defined as a zero of the analytic continuation

$$f_+(\lambda,\mu,z) := z-1-2\lambda^2\int_0^\infty \frac{g(p)^2}{z-\mu p}\mathrm{d}p+4i\pi\frac{\lambda^2}{\mu}g\left(\frac{z}{\mu}\right)^2 \tag{3.11}$$

of $f(\lambda,\mu,.)$, clockwise through the cut. When $\mu\to\mu_c(\lambda)$, it connects to the values for $\mu<\mu_c(\lambda)$. For μ varying from 0 to 2, some values of $z_{0,1}(0.1,\mu)$ are given in Table I and Fig. 2.

The physical value for $\mu=1$ is $0.11-0.95\,i$. For $\mu=0$, $z_{0,1}(0.1,0)=\zeta_{0,1}(0.1)\simeq-0.0099$; the graph goes through 0 for $\mu\simeq 6.36\ 10^{-3}$ and $z_{0,1}(0.1,2)=0.13-1.97\,i$.

In order to connect these results to the usual perturbative treatment, we drew a dashed line in Fig. 2. It describes the continuous move of the resonance which sits at the point $z_{0,1}(0.1,1)$ for $\lambda=0.1$, when λ decreases from this value to 0. One can see that the limit is not 1, the energy of the naked excited state, but $-i$, a pole of g. This makes a difference with what occurs for $z_{1,1}(\lambda,1)$, as we will see it just below. To distinguish the two behaviors, we called a resonance which, as a function of the only λ variable, does not tend to the excited state energy when λ tends to 0 a "nonstandard" resonance.[10] Be careful that a resonance may be standard for some μ's and nonstandard for others.

Resonance $z_{1,1}(0.1,\mu)$

It is another zero of $f_+(\lambda,\mu,.)$, which tends to $\zeta_{1,1}(0.1)$, when $\mu\to 0$. Its displacement when μ varies is given by the full line of Fig. 3.

We have $z_{1,1}(0.1,0)=1.0099$, $z_{1,1}(0.1,1)=0.997-0.010\,i$, $z_{1,1}(0.1,2)=0.995-0.0032\,i$. It can

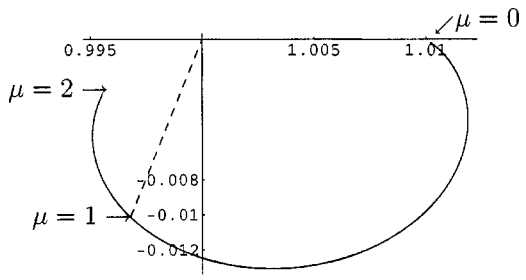

FIG. 3. $z_{1,1}(0.1,\mu)$, in the second sheet, for $\mu\in[0,2]$ (full line).

be shown that the resonance which sits at point $z_{1,1}(\lambda,1)$ for $\lambda=0.1$ moves continuously to 1 along the dashed line of Fig. 3 when λ goes to 0. Therefore, referring to the discussion of Sec. III C, we can say that $z_{1,1}(0.1,1)$ is the resonance usually associated with the excited state of the naked atom.

We now come to the original part of this Sec. III.

2. Two other resonances, obtained with two photons

Among the various resonances tending to $\zeta_{i,2}(\lambda)$ when μ goes to 0, we select poles of matrix elements of $[z-H(\lambda,\mu)\downarrow_{\mathcal{E}_2}]^{-1}$, or of one of their analytic continuation. Note that another choice among those mentioned after Notation 2 would have been to look for poles of matrix elements of $[z-H(\lambda,\mu)\downarrow_{\mathcal{E}_3}]^{-1}$, since we have eigenvectors of $H(\lambda,0)$ in $\mathcal{E}_3$ associated with the same eigenvalue $\zeta_{i,2}(\lambda)$: for instance $(1\otimes c^*(g_1))\phi_{i,2}$. But we make no claim to being complete. We just want to give an example of two resonances which are not considered usually.

Two new difficulties now appear. The first one is that, contrary to the $\mathcal{E}_1$-sector case, resonances in the $\mathcal{E}_2$ sector are given by zeros of a function $D(\lambda,\mu,.)$ which is no longer explicit, since we will see that it is the sum of a series. Up to now, we can only calculate these zeros approximately, through cutting the series after the first non trivial term. The zeros of this truncated function are the approximate values we consider, for the resonances in this sector.

The second difficulty is that this truncated function has several branch points; as a consequence, it has several analytic continuations. There is no reason why it should not be the same for $D(\lambda,\mu,.)$ itself, although it is possible. Therefore, when considering a zero, one must tell which branch is in question; we give a notation for the zeros of the various branches later on.

a. These resonances as zeros of a function $D(\lambda,\mu,.)$.

In $\mathcal{E}_2$, looking for the eigenvalues leads to the following proposition.

Proposition 3.3: (Eigenvalues of $H(\lambda,\mu)\downarrow_{\mathcal{E}_2}$ as zeros of a multivalued function) λ *being fixed and* μ *and* z *being two parameters satisfying* $\mu>0$ *and* $z\in\mathbb{R}^-$, *let* $\mathcal{D}_{\mu,z}$ *be the Fredholm function (see Ref. 22, p. 68) associated with the integral equation*

$$\varphi_{\lambda,\mu}(p)-\lambda^2\int K_{\mu,z}(p,q)\varphi_{\lambda,\mu}(q)\mathrm{d}q=0, \tag{3.12}$$

with

$$K_{\mu,z}(p,q)=\frac{g(p)\overline{g}(q)}{(z-1-\mu|p|-\lambda^2(T_{\mu,z}g)(p))(z-\mu(|p|+|q|))}, \tag{3.13}$$

where

$$(T_{\mu,z}f)(p)=\int\frac{\overline{g}(q')f(q')}{z-\mu(|p|+|q'|)}\mathrm{d}q'. \tag{3.14}$$

Let $z\to D(\lambda,\mu,z)$ *be the multivalued function which, for* $z\in\mathbb{R}^-$, *equals* $\mathcal{D}_{\mu,z}(\lambda^2)$.

In the case where one of the zeros of $D(\lambda,\mu,.)$ *is real negative, this zero is an eigenvalue of* $H(\lambda,\mu)$. *Let us denote it by* $\xi_{0,2}(\lambda,\mu)$. *The associated eigenvector is in* $\mathcal{E}_2$, *proportional to*

$$\psi_{0,2}^{(0)}(\lambda,\mu):=|1,\varphi_{\lambda,\mu}\rangle+\sqrt{2}\lambda\left|0,\frac{g\vee\varphi_{\lambda,\mu}}{\xi_{0,2}(\lambda,\mu)-\mu(|p_1|+|p_2|)}\right\rangle, \tag{3.15}$$

where $\varphi_{\lambda,\mu}$ *is a solution of*

$$\varphi_{\lambda,\mu}(p)-\lambda^2\int K_{\mu,\xi_{0,2}(\lambda,\mu)}(p,q)\varphi_{\lambda,\mu}(q)\mathrm{d}q=0. \tag{3.16}$$

Proof: $|1,\varphi_{\lambda,\mu}\rangle+|0,\chi_{\lambda,\mu}\rangle$ is an eigenvector of $H(\lambda,\mu)\downarrow_{\mathcal{E}_2}$ associated with the eigenvalue z if and only if (3.12) holds and $\chi_{\lambda,\mu}=\sqrt{2}\lambda(z-\mu(|p_1|+|p_2|))^{-1}g\vee\varphi_{\lambda,\mu}$. According to Fredholm's theory,

TABLE II. Four resonances (approximate values for two of them), for $\lambda = 0.1$ and $\mu = 1$.

$z_{0,1}$	$0.13 - 1.97i$
$z^1_{0,2}$	$0.216 - 1.9i$
$z_{1,1}$	$0.997 - 0.010i$
$z^1_{1,2}$	$1.043 - 1.127i$

(3.12) has a nontrivial solution only if $D_{\mu,z}(\lambda^2)=0$. The proposition follows from the fact that (3.14) and (3.13) are defined if z is a negative number. ■

Remark: If μ is set to 0 in (3.12)–(3.14), one finds that (3.12) implies $z=\zeta_{i,2}(\lambda)$. If the continuity with respect to μ could be proved, we would get that the limit of $\xi_{0,2}(\lambda,\mu)$ when μ goes to 0 is $\zeta_{0,2}(\lambda)$. We do not know how to prove this at the moment, since we do not know all the zeros of $D(\lambda,\mu,.)$. Nevertheless, the result of the approximate calculation of Sec. III D 2 d is along this line. That is why we eventually change notation $\xi_{0,2}(\lambda,\mu)$ for $z^1_{0,2}(\lambda,\mu)$, according to Notation 2. (The upper index is explained later on.)

To switch from eigenvalues to resonances, let us take $h \in L^2(\mathbb{R}^2)$, z s.t. $\Im z > 0$ and $\psi := |1,h\rangle$. Let us introduce $H_{\mu,z}(p,q,\lambda^2)$, the resolvent kernel of Eq. (3.12) (see Ref. 22, p. 63). It can be shown that

$$(\psi,[z - H(\lambda,\mu)]^{-1}\psi) = 1 - \lambda^2 \int H_{\mu,z}(p,q,\lambda^2)\overline{h}(p)h(q)\mathrm{d}p\mathrm{d}q. \tag{3.17}$$

We know (Ref. 22, pp. 58 and 63) that the only singular points of $H_{\mu,z}(p,q,.)$ are the solutions of $\mathcal{D}_{\mu,z}(\lambda)=0$. The zeros of analytic continuations of function $D(\lambda,\mu,.)$ of Proposition 3.3 will thus give us poles of the left-hand side of (3.17), that is to say resonances.

The calculation will be an approximate one. The result for $\mu=1$ is given by lines two and four of Table II.

b. Zeros of $D(\lambda,\mu,.)$ approached by zeros of a function $D^{(1)}(\lambda,\mu,.)$

Proposition 3.4: For

$$z < 0, \quad D(\lambda,\mu,z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} C_n(\lambda,\mu,z)$$

with $C_0=1$

$$C_n(\lambda,\mu,z) = \lambda^{2n} \int D_n(\mu,z,p_1,\ldots,p_n)\mathrm{d}p_1\cdots\mathrm{d}p_n \tag{3.18}$$

and, for $1 \leqslant n \leqslant 3$,

$$D_n(\mu,z,p_1,\ldots,p_n) = \mu^{-n} \prod_{i=1}^{i=n} \frac{|g(p_i)|^2}{f(\lambda,\mu,z-\mu|p_i|)\left(\dfrac{z}{\mu} - 2|p_i|\right)} \prod_{i<j} \frac{(|p_i| - |p_j|)^2}{\left(\dfrac{z}{\mu} - (|p_i| + |p_j|)\right)^2}. \tag{3.19}$$

Proof: The D_n's are determinants given by Fredholm's theory. We calculated them for $n \leqslant 3$; the result is given in (3.19). ■

The analytic structure (poles, branch points) of $D(\lambda,\mu,.)$ is difficult to determine. Indeed, $D(\lambda,\mu,.)$ is a series of terms each of which has a different analytic structure. Moreover, this structure is not simple. Therefore we will limit ourselves with replacing the search for zeros of $D(\lambda,\mu,z)$ by the search for the zeros of the sum of the first two terms of the series:

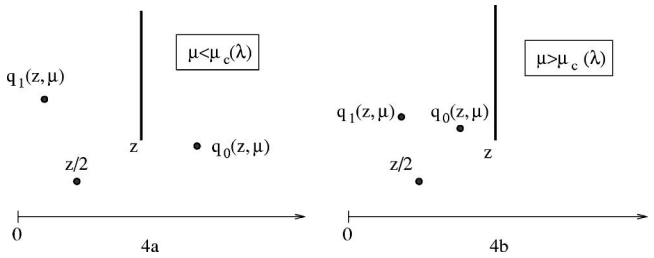

FIG. 4. Branch point and poles of $\psi(\lambda,\mu,z,.)$, defined by (3.21′).

$$D^{(1)}(\lambda,\mu,z) := 1 - C_1(\lambda,\mu,z). \tag{3.20}$$

The first corrections to this approximation are discussed in Appendix A. From Proposition 3.3, we get, if $\mu \neq 0$,

$$D^{(1)}(\lambda,\mu,z) = 1 - \frac{2\lambda^2}{\mu}\int_0^\infty \psi(\lambda,\mu,z,q)\mathrm{d}q, \tag{3.21}$$

where

$$\psi(\lambda,\mu,z,q) := \frac{g(\mu^{-1}q)^2}{(z-2|q|)f(\lambda,\mu,z-|q|)} \tag{3.21′}$$

and $D^{(1)}(\lambda,0,z)=(z(z-1)-\lambda^2)^{-1}(z(z-1)-2\lambda^2)$.

c. Analytic properties of $D^{(1)}$.

Proposition 3.5: For $\mu\neq 0$, $D^{(1)}(\lambda,\mu,.)$ *has at least three branch points:* 0, $z_{0,1}(\lambda,\mu)$ *and* $z_{1,1}(\lambda,\mu)$.

Proof: Let us recall that $f(\lambda,\mu,.)$ is analytic in the complex plane cut along $\mathbb{R}^+$, with a branch point at 0. The analytic continuation from the upper half-plane has a pole at $-i\mu$. An explicit expression of f in the upper half-plane is, for $z\neq i\mu$,

$$f(\lambda,\mu,z) = z - 1 + \lambda^2\frac{2\mu^3+\mu^2\pi z+2\mu z^2-\pi z^3+4\mu z^2(\log\mu-\log(-z))}{\pi(\mu^2+z^2)^2}. \tag{3.22}$$

The continuation clockwise across the cut, which we denote by $f_+(\lambda,\mu,z)$, is obtained through adding $4i\pi(\lambda^2/\mu)g(\mu^{-1}z)^2$ to the above expression. It is convenient to rather introduce the function $\hat{f}(\lambda,\mu,z)$ which coincides with $f(\lambda,\mu,z)$ in the upper half-plane and has a cut along $i\mathbb{R}^-$.

For $\Im z>0$, the poles of $\psi(\lambda,\mu,z,.)$ [see (3.21′)] in the complex plane cut along $z+i\mathbb{R}^+$ are $\pm i\mu$, $z/2$ and $q_i(z,\mu,\lambda):=z-z_{i,1}(\lambda,\mu)$. Depending on whether μ is smaller or greater than $\mu_c(\lambda)$, the z-dependent poles sit at places schematically shown in Fig. 4.

This follows from the position of $z_{i,1}(\lambda,\mu)$, given by the curves in Figs. 2 and 3. If $\mu=\mu_c(\lambda)$, the pole $q_0(z,\mu)$ coincides with z. (In Fig. 4, z has a positive real part, but it could be negative, as well.)

When z enters the lower half-plane along a path γ (for instance the dotted lines in Figs. 7 and 8), the integration path in (3.21) may have to be deformed in order to be kept away from some of the three poles or from the branch point z of $\psi(\lambda,\mu,z,.)$. Two different paths γ and γ' will not necessarily yield the same result. For instance, if γ crosses $z_{i,1}(\lambda,\mu)+\mathbb{R}^+$, $q_i(z,\mu)$ crosses $\mathbb{R}^+$; the integration path has thus to be deformed, whereas it is not the case if γ crosses $z_{i,1}(\lambda,\mu)-\mathbb{R}^+$. As a consequence, $z_{0,1}(\lambda,\mu)$ and $z_{1,1}(\lambda,\mu)$ are branch points.

If z comes to $z_{0,1}(\lambda,\mu)$ [respectively, $z_{1,1}(\lambda,\mu)$], then the pole $q_0(z,\mu)$ (respectively, $q_1(z,\mu)$) comes to 0 and the integral in (3.21) is singular.

To describe the various branches of $D^{(1)}$ readily, we need a notation for the homotopy classes of paths in $X_{\lambda,\mu}:=\mathbb{C}\backslash\{0,z_{0,1}(\lambda,\mu),z_{1,1}(\lambda,\mu)\}$. (Two paths are homotopic if they can be continu-

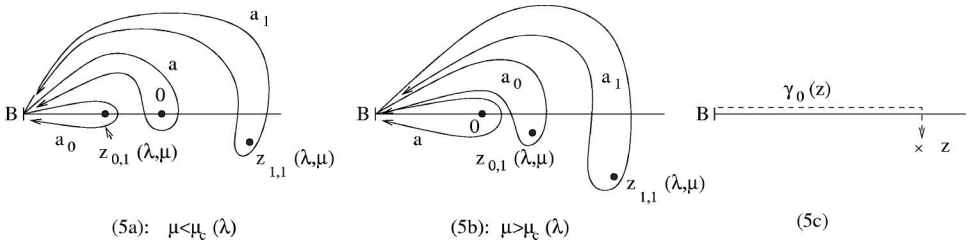

FIG. 5. Fundamental paths in the z plane.

ously deformed into one another, in $X_{\lambda,\mu}$.) Depending on whether μ is smaller or greater than $\mu_c(\lambda)$, the relative position of the three branch points is different. We refer to Fig. 5 for the definition of the fundamental class of paths a, a_0, a_1. The base point B is chosen real and smaller than $\zeta_{0,2}(\lambda)$.

The path $\gamma_0(z)$ is defined as the polyline going through points B, $B+i\epsilon$, $\Re(z)+i\epsilon$ and ending at z, for an arbitrary $\epsilon>0$. Every path γ from B to z can be expressed by means of a, a_0, a_1, and $\gamma_0(z)$. It defines a homotopy class $[\gamma_0(z)^{-1}\gamma] \in \pi_1(X_{\lambda,\mu})$. Conversely, with each class $[l]$ of $\pi_1(X_{\lambda,\mu})$, we can associate the homotopy class of paths $\gamma_0(z)l$ going from B to z. With each pair consisting of $[l]$ in $\pi_1(X_{\lambda,\mu})$ and z, we can associate the analytic continuation in z of $D^{(1)}(\mu,.)$ along the path $\gamma_0(z)l$. We denote the value at the end of the path by $D^{(1)}_{[l]}(\mu,z)$. From now on, we will omit to mention the λ variable (which has been fixed to 0.1.) We denote by $z^{[l]}(\mu)$ a point such that $D^{(1)}_{[l]}(\mu, z^{[l]}(\mu))=0$. When μ varies, we assume that this point varies continuously. It is denoted by $z^{[l]}_{i,2}(\mu)$ if its limit when μ goes to 0 is ζ_i.

These $z^{[l]}_{i,2}(\mu)$ are approximate values for the resonances we are considering. Regarding their physical meaning, we refer to the short comment in Sec. III E.

We now give some values of these functions for various μ values.

d. Values of resonance $z^{[l]}_{0,2}(\mu)$.

(i) $\mu < 6.3662\times 10^{-3}$

(a) $[l]=1$. For μ close to 0, we look for a zero of $D^{(1)}(\mu,.)$ in the neighborhood of $\zeta_{0,2}=-1.96\times 10^{-2}$. $D^{(1)}(\mu,.)$ is well defined by (3.21) in the neighborhood of every negative real number. A calculation on a computer yields negative real zeros of this expression, for μ small (see Table III, first column). When μ increases up to a certain value $\mu^a_{c,2}$, close to $\mu_c := \mu_c(10^{-1})$, the same formula still gives a negative real zero. The first column of Table III gives its values for $0 \leqslant \mu \leqslant 6.3662\times 10^{-3} \simeq \mu_c$.

Through comparing Table III with Table I, one sees that this zero is smaller than $z_{0,1}(\mu)$. In accordance with the notations of the end of Sec. III D 2 c, and with the upper index 1

TABLE III. Values of $z^1_{0,2}(\mu)$, for some values of μ below μ_c.

$10^3\ \mu$	$10^4\, z^1_{0,2}(\mu)$	$\frac{C_2}{2}(\mu, z^1_{0,2}(\mu))$	$\frac{M_3}{6}(\mu, z^1_{0,2}(\mu))$	$\frac{M_4}{24}(\mu, z^1_{0,2}(\mu))$	$\partial_z C_1(\mu, z^1_{0,2}(\mu))$
0	−196	0	0	0	103.9
0.1	−185.5	1.65×10^{-3}	3.95×10^{-6}	1.04×10^{-8}	105.3
1	−135.7	13.14×10^{-3}	10^{-4}	6.26×10^{-7}	116
3	−69.8	0.038	7.93×10^{-4}	10^{-5}	143.8
6	−9.3	0.099	7.7×10^{-3}	3.68×10^{-4}	247.1
6.2	−6.6	0.106	9.3×10^{-3}	5.2×10^{-4}	265.3
6.36	−4.4	0.111	1.09×10^{-2}	7.1×10^{-4}	284.2
6.3662	−4.328	0.112	1.10×10^{-2}	7.17×10^{-4}	285

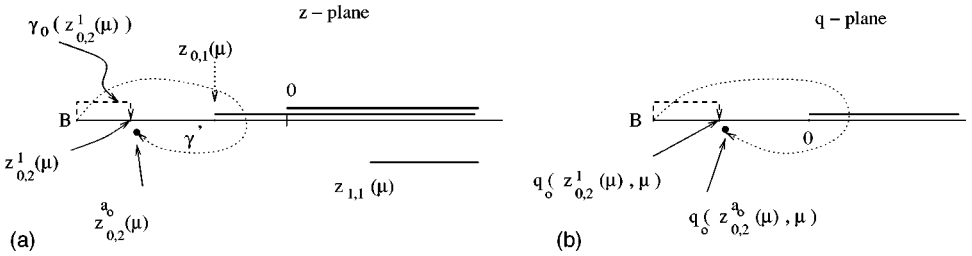

FIG. 6. Paths defining resonances $z^{[l]}_{0,2}(\mu)$ for $\mu<6\times10^{-3}$.

denoting the unity element in $\pi_1(X_\mu)$, this zero may then be denoted by $z^1_{0,2}(\mu)$, since the branch point $z_{0,1}(\mu)$ does not belong to the interval $Bz^1_{0,2}(\mu)$. Figure 6(a) shows the three cuts of $D^{(1)}(\mu,.)$ for $\mu<6.3662\times10^{-3}$ and this zero $z^1_{0,2}(\mu)$.

It has not been possible to determine the place of $\mu^a_{c,2}$ with respect to $\mu_c(10^{-1})$. We will come back to this point in Appendix A when we estimate the errors made in the approximation.

(b) $[l]=a_0$: *a zero associated with another branch*. Figure 6(a) also schematically shows another zero: $z^{[a_0]}_{0,2}(\mu)$. The notation indicates that this value is now the zero of the continuation of $D^{(1)}(\mu,.)$ along the path $\gamma':=\gamma_0(z^{[a_0]}_{0,2}(\mu))a_0$, a path which goes around the branch point $z_{0,1}(\mu)$. Figure 6(b) shows the two paths followed by $q_0(z,\mu)$ when z goes along $\gamma_0(z^{(1)}_{0,2}(\mu))$ or γ'.

This $z^{a_0}_{0,2}(\mu)$, also close to $\zeta_{0,2}$ for $\mu\simeq0$, is a zero of $D^{(1)}_{a_0}(\mu,.)$ which, for $\Re(z)<0$ (and also for $\Re(z)>0,\Im(z)>0$), reads

$$D^{(1)}_{a_0}(\mu,z)=1-\frac{2\lambda^2}{\mu}\int_0^\infty\frac{g(\mu^{-1}q)^2}{(z-2|q|)f(\mu,z-|q|)}dq+4i\pi\frac{\lambda^2}{\mu}\frac{g(q_0(z,\mu)/\mu)^2}{(z-2q_0(z,\mu))\partial_z f(z_{0,1}(\mu,\lambda),\mu,\lambda)} \tag{3.23}$$

with $\lambda=0.1$. This zero is no longer real.

(ii) For $\mu\simeq\mu_c$, things are not clear.

(iii) For $\mu>7\times10^{-3}$, the branch point $z_{0,1}$ of $D^{(1)}$ is in $\{z;\Re(z)>0,\Im(z)<0\}$ (see Fig. 2); it is shown in Fig. 7. Among the various analytic continuations of $D^{(1)}$ across $\mathbb{R}^+$, we consider $D^{(1)}_1$. Expressions are given in the following [formula (3.24) and the two last lines of the section]. The zero of $D^{(1)}_1$, denoted by $z^1_{0,2}(\mu)$, follows the curve of Fig. 7 when μ varies from 7×10^{-3} to 1. For $\mu=1$, the way $D^{(1)}$ is analytically continued to the zero of $D^{(1)}_1$ is shown by the dotted line.

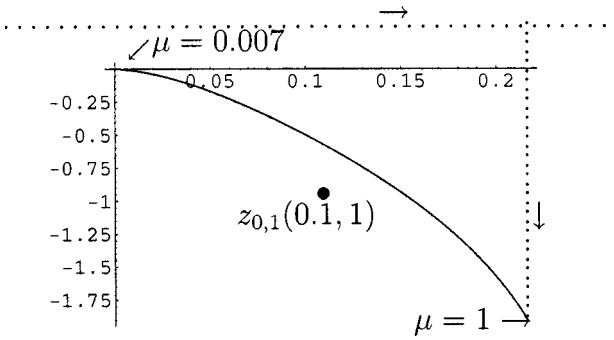

FIG. 7. $z^1_{0,2}(\mu)$ in the complex plane, for $\mu\in[0.007,1]$.

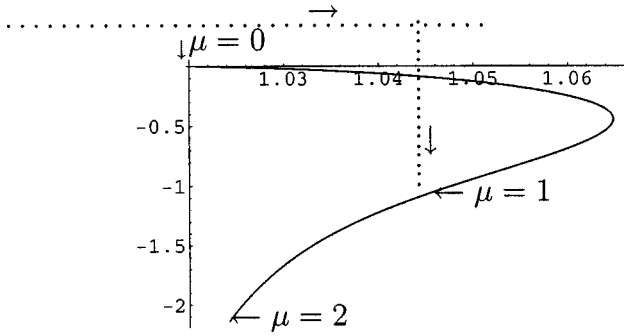

FIG. 8. $z^1_{0,2}(\mu)$, in the complex plane, for $\mu \in [310^{-4}, 2]$.

For $\mu = 7\times10^{-3}$, $z^1_{0,2}(\mu) = 2.8\times10^{-4} - 2.4\times10^{-5}i$, close to 0. Values of $z^1_{0,2}(\mu)$ for μ between 6.37×10^{-3} and 7×10^{-3} are difficult to get. Actually, their determination is not useful since $z^1_{0,2}(\mu)$ is only an approximate value of the exact resonance. We have $z^1_{0,2}(0.1,1) = 0.216 - 1.9i$. For $\Im z < 0$, $\Re(z) > 0$ and $\mu > 7.35\times10^{-3}$, still with $\lambda = 0.1$,

$$D^{(1)}_1(\mu,z) = 1 - \frac{2\lambda^2}{\mu}\left(\int_{[0,\Re(z)]\cup[\Re(z),z]} \frac{g^2(\mu^{-1}q)}{(z-2q)f_+(\mu,z-q)} + \int_{[0,\Re(z)]\cup[\Re(z),z]} \frac{g^2(\mu^{-1}q)}{(z-2q)f(\mu,z-q)}\right.$$
$$\left. + i\pi g^2\left(\frac{z}{2\mu}\right) f_+(\mu,z/2)^{-1} + 2i\pi g^2\left(\frac{z-z_{0,1}(\mu)}{\mu}\right)(2z_{0,1}(\mu)-z)^{-1}\partial_z f_+(\mu,z_{0,1}(\mu))^{-1}\right). \tag{3.24}$$

This formula is derived from (3.21) in the following way: when z enters the quadrant $\{z;\Re(z) > 0, \Im(z) < 0\}$, the cut in Fig. 4(b) drags the integration contour along, which yields the first two terms. The last two terms come from the residues of the poles $z/2$ and $q_0(z,\mu)$ which cross $\mathbb{R}^+$ [$q_1(z,\mu)$ does not cross $\mathbb{R}^+$]. For 10^3 $\mu \in [7, 7.3]$, the expression of $D^{(1)}_1(\mu,z)$ does not contain the residue term at q_0 since $\gamma_0(z^1_{0,2}(\mu))$ does not cross $z_{0,1}(\mu)+\mathbb{R}^+$.

e. Values of resonance $z^1_{1,2}(\mu)$.

It can be shown numerically that the zero of $D^{(1)}_1(\mu,.)$ which tends to $\zeta_{1,2}$ when μ tends to 0, denoted by $z^1_{1,2}(\mu)$, is a zero in $\{z;\Re(z) > 0, \Im(z) < 0\}$ of $\Delta(\mu,.)$, where

$$\Delta(\mu,z) := 1 - \frac{2\lambda^2}{\mu}\left(\int_{[0,\Re(z)]\cup[\Re(z),z]} \frac{g^2(\mu^{-1}q)}{(z-2q)f_+(\mu,z-q)} + \int_{[0,\Re(z)]\cup[\Re(z),z]} \frac{g^2(\mu^{-1}q)}{(z-2q)f(\mu,z-q)}\right.$$
$$+ i\pi g^2\left(\frac{z}{2\mu}\right) f_+(\mu,z/2)^{-1} + 2i\pi g^2\left(\frac{z-z_{0,1}(\mu)}{\mu}\right)(2z_{0,1}(\mu)-z)^{-1}\partial_z f_+(\mu,z_{0,1}(\mu))^{-1}$$
$$\left. + 2i\pi g^2\left(\frac{z-z_{1,1}(\mu)}{\mu}\right)(2z_{1,1}(\mu)-z)^{-1}\partial_z f_+(\mu,z_{1,1}(\mu))^{-1}\right). \tag{3.25}$$

$\Delta(\mu,z)$ is the expression of $D^{(1)}_1(\mu,z)$ in the neighborhood of the considered zero, but not everywhere in the lower half-plane; for example, these two functions differ at a point z such that $\Im(z) < \Im(z_{0,1}(\mu))$. The variation of $z^1_{1,2}(\mu)$ with μ is given by Fig. 8.

This resonance starts from $2^{-1}(1+\sqrt{1+8\lambda^2}) = 1.019\,62$ for $\mu = 0$ and goes through 1.043–1.127 i for $\mu = 1$. We note that this value is much farther from the real axis than the resonance $z_{1,1}(0.1,1)$ of sector $\mathcal{E}_1$. As in Fig. 7, the dotted line in Fig. 8 indicates the path of the analytic continuation of $D^{(1)}$ to the zero (of $D^{(1)}_1$), for $\mu = 1$. The origin is a branch point. The other two branch points, $z_{0,1}(0.1,1)$ and $z_{1,1}(0.1,1)$, whose values are recalled in Table II, cannot be drawn at the scale on the figure.

E. Conclusion of Sec. III

Table II gathers the four results we obtained for $\lambda=0.1$ and $\mu=1$. It gives four resonances among all those of the physical (i.e., $\mu=1$) Hamiltonian, when the function g is given by (3.8).

We see that the usual resonance $z_{1,1}$ is the only one near the real axis. This resonance represents what the excited state of the naked atom has become, due to the coupling of the atom with the field. The state is now unstable and its lifetime is in inverse proportion to $\Im z_{1,1}$. Other resonances are more than a hundred times farther from the real axis. However, for small values of μ, they approach the real axis, as it can be seen from Figs. 2, 7, and 8, or Table III. Therefore, resonances for small μ may play an important role. Now, in the harmonic-oscillator example mentioned in the introduction, what plays the role of parameter μ is δ^{-1}, the inverse of the spatial extension of the states, measured relatively to the wavelength of the transition from the excited state to the fundamental state of the naked atom. Thus, for extended states, μ is small, and we recover our motivation for the study of all the resonances of atom-field Hamiltonians.

One should of course discuss which of these resonances have a physical meaning and make this meaning precise, through finding actual situations in which these resonances or eigenvalues can be seen readily. We mean situations in which the photons are not monochromatic. The physical meaning should appear quite easily in the case of eigenvectors of the Hamiltonian. In $\mathcal{E}_1$ [see (3.10), Table I, and Fig. 2], we have an example of such a state. Regarding the restriction of $H(\lambda,\mu)$ to $\mathcal{E}_2$, we found approximate real values for the resonances. But we have not shown that (real) eigenvalues do exist. The study has to be carried on. Now, as pure resonances are concerned, we think that their study cannot simply be an academic question, since eigenvectors change continuously into resonances when parameters of the physical system are varied.

In any case, the two-level model is perhaps too simple to find a concrete application. The next section is a step toward more realistic models.

IV. HYBRID STATES FOR A THREE-LEVEL ATOM COUPLED TO PHOTONS

To be in a position to describe mixed states in more realistic models, we not only must be able to consider several photons (or bosons, in a more general setting), as in Sec. III, but we must also be able to consider several atomic or molecular levels. The present section is a preliminary study devoted to mixed states when S is a three-level atom coupled to the radiation by a Hamiltonian of type (2.2).

The reason why the study is only a preliminary one is that there comes some additional difficulty, together with those already mentioned in Sec. III: for $\mu \geqslant 0$, none of the spaces with a bounded excitation number is stable by the evolution operator, contrary to the two-level case. This is due to the possibility of the transition from the state consisting of the atom in state $|0\rangle$ and one photon to the state $|2\rangle$, the photon being absorbed ($|2\rangle$ is the second excited state). In this transition the excitation number (defined in Sec. III A) increases. For this reason, the determination of the Hamiltonian eigenvalues is already not simple for $\mu=0$. Since we assume that the structure of the resonance set will roughly be conserved when μ takes nonzero values, we must study the ($\mu=0$)-problem first. This is the subject of this Sec. IV. The displacement of these resonances when μ becomes nonzero will not be examined in the paper. (A typical result is illustrated by Fig. 12.)

A. Notations and Hamiltonian

The atom has three levels with energies $e_0=0$, e_1, and e_2, corresponding to states $|0\rangle$, $|1\rangle$, and $|2\rangle$. f_{01}, f_{12}, and f_{02} being three normalized functions in $L^2(\mathbb{R})$, the Hamiltonian is

$$H(\lambda,\mu) := H_0(\lambda,\mu) + \lambda_{02}V \tag{4.1}$$

with

$$\begin{aligned} H_0(\lambda,\mu) := {} & (e_1|1\rangle\langle 1| + e_2|2\rangle\langle 2|) \otimes 1 + \mu 1 \otimes H_{\mathrm{rad}} + \lambda_{01}(|1\rangle\langle 0| \otimes c(\overline{f_{01}}) + |0\rangle\langle 1| \otimes c^*(f_{01})) \\ & + \lambda_{12}(|2\rangle\langle 1| \otimes c(\overline{f_{12}}) + |1\rangle\langle 2| \otimes c^*(f_{12})) \end{aligned} \tag{4.2}$$

$$V := |2\rangle\langle 0| \otimes c(\overline{f_{02}}) + |0\rangle\langle 2| \otimes c^*(f_{02}), \tag{4.3}$$

where H_{rad} is as in Sec. III A. Transition $|0\rangle \to |2\rangle$ is distinguished from $|0\rangle \to |1\rangle$ and $|1\rangle \to |2\rangle$ for a physical reason and also to prepare a perturbative calculus.

We use the following notations, modeled on those of Sec. III A. Regarding the photons, we denote the Fock space by $\mathcal{F}$, the n-photon space by $\mathcal{F}_n$, the vacuum state by Ω, and we set

$\mathcal{H}^{(2)}_{\mathrm{rad}}$: the space spanned by f_{01}, f_{12}, $\mathcal{F}^{(2)}_n := (\mathcal{H}^{(2)}_{\mathrm{rad}})^{\vee n}$: the n photon-state space, but each photon being restricted to be in $\mathcal{H}^{(2)}_{\mathrm{rad}}$ and $\mathcal{F}^{(2)} := \oplus_n \mathcal{F}^{(2)}_n$.

$\mathcal{H}^{(3)}_{\mathrm{rad}}$: the space spanned by f_{01}, f_{12}, f_{02}, $\mathcal{F}^{(3)}_n := (\mathcal{H}^{(3)}_{\mathrm{rad}})^{\vee n}$ (each photon is restricted to be in $\mathcal{H}^{(3)}_{\mathrm{rad}}$) and $\mathcal{F}^{(3)} := \oplus_n \mathcal{F}^{(3)}_n$.

Regarding the atom-photon system, $\mathcal{E}_n$ and $\mathcal{E}$ have been defined in Sec. III A. We set

$$\mathcal{E}^{(k)}_1 := |0\rangle \otimes \mathcal{F}^{(k)}_1 \oplus |1\rangle \otimes \mathcal{F}^{(k)}_0, \quad k = 2,3$$

$$\mathcal{E}^{(k)}_n := |0\rangle \otimes \mathcal{F}^{(k)}_n \oplus |1\rangle \otimes \mathcal{F}^{(k)}_{n-1} \oplus |2\rangle \otimes \mathcal{F}^{(k)}_{n-2}, \quad k = 2,3, \quad n \geqslant 2$$

$$\mathcal{E}^{(k)} := \bigoplus_{n=0}^{\infty} \mathcal{E}^{(k)}_n$$

$$\lambda := (\lambda_{01}, \lambda_{12}, \lambda_{02}).$$

We also introduce $s_0 := (f_{01}, f_{02})$, $s_1 := (f_{01}, f_{12})$, $s_2 := (f_{02}, f_{12})$.

We will use the letter ϕ to indicate eigenvectors of $H_0(\lambda, 0)$; *a priori*, they depend on λ_{01} and λ_{12}. We will use χ to indicate eigenvectors of $H(\lambda, 0)$; they also depend on λ_{02}.

We aim at getting the eigenvalues of $H(\lambda, 0)$, an operator which we simply write $H(\lambda)$, from now on. When the variable μ is not mentioned, it will be assumed to be 0.

To this end, we take up the idea mentioned in Sec. II consisting in perturbing $H(0)$ through introducing the interaction step by step. The doubly infinite degeneracy of the eigenvalues e_0, e_1, and e_2 of $H(0)$, due to the arbitrariness of the number of photons and the arbitrariness of the state of each photon in the corresponding eigenvectors, is partially removed at each step. The first perturbation will be the addition of the λ_{01} and λ_{12} terms of (4.2) to $H(0)$. It is described in Sec. IV B. The second perturbation will be the supplementary addition of λ_{02} V. It is described in Sec. IV C.

B. Perturbation with respect to λ_{01} and λ_{12}: First splitting of e_0, e_1, and e_2

Here we are interested in $H_0(\lambda) := H_0(\lambda, 0)$; the interaction $\lambda_{02} V$ is switched off. First, in $\mathcal{E}_0$, $|0, \Omega\rangle$, is an eigenvector associated with the eigenvalue 0.

1. Three eigenvectors of $H_0(\lambda)$ in the 1-excitation space $\mathcal{E}^{(2)}_1$ and the three associated eigenvalues

The space $\mathcal{E}^{(2)}_1$, three-dimensional, is invariant by $H_0(\lambda)$. It is the direct sum of the eigensubspaces $|1\rangle \otimes \mathcal{F}^{(2)}_0$ and $|0\rangle \otimes \mathcal{F}^{(2)}_1$ of $H_0(0)$, associated with the eigenvalues e_1 and e_0, respectively, and dim. $\mathcal{F}^{(2)}_0 = 1$ and dim. $\mathcal{F}^{(2)}_1 = 2$. The first perturbation will shift e_1 and split e_0 into two eigenvalues, as it is represented in the first two columns of Fig. 9.

The eigenvalues obtained through the first perturbation and the associated eigenvectors are given by the following proposition.

Proposition 4.1: In $\mathcal{E}^{(2)}_1$, if $f_{01} \neq f_{12}$, $H_0(\lambda)$ has three eigenvalues:

$$(\zeta_{0,1})_1(\lambda_{01}, \lambda_{12}) = 2^{-1}(e_1 - \sqrt{e_1^2 + 4\lambda_{01}^2}), \tag{4.4}$$

$$(\zeta_{0,1})_2(\lambda_{01}, \lambda_{12}) = 0, \tag{4.5}$$

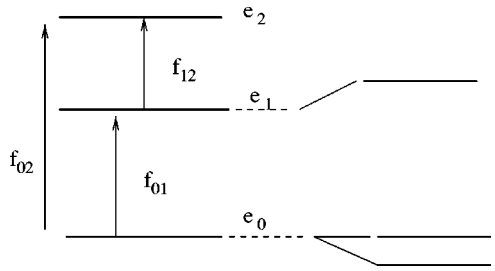

FIG. 9. Levels associated with eigenvectors of $H_0(\lambda)$ in $\mathcal{E}_1^{(2)}$, therefore without any spectator photon.

$$\zeta_{1,1}(\lambda_{01},\lambda_{12}) = 2^{-1}(e_1 + \sqrt{e_1^2 + 4\lambda_{01}^2}). \tag{4.6}$$

The associated normalized eigenvectors are

$$(\phi_{0,1}^{(0)})_1(\lambda_{01},\lambda_{12}) = (1 + (\zeta_{0,1})_1^{-2}\lambda_{01}^2)^{-1/2}(|1,\Omega\rangle + (\zeta_{0,1})_1^{-1}\lambda_{01}|0,f_{01}\rangle), \tag{4.7}$$

$$(\phi_{0,1}^{(0)})_2(\lambda_{01},\lambda_{12}) = (1 - |s_1|^2)^{-1/2}|0,f_{12} - s_1 f_{01}\rangle, \tag{4.8}$$

$$\phi_{1,1}^{(0)}(\lambda_{01},\lambda_{12}) = (1 + (\zeta_{1,1})^{-2}\lambda_{01}^2)^{-1/2}(|1,\Omega\rangle + (\zeta_{1,1})^{-1}\lambda_{01}|0,f_{01}\rangle). \tag{4.9}$$

The calculus is straightforward since the dimension of $\mathcal{E}_1^{(2)}$ is three. ■

To the second order with respect to λ, we get $(\zeta_{0,1})_1 = -(1/e_1)\lambda_{01}^2$ and $\zeta_{1,1} = e_1 + (1/e_1)\lambda_{01}^2$. Note that the perturbed eigenvalues (4.4)–(4.6) do not depend on λ_{12}. They tend to 0, 0, and e_1, respectively, if λ_{01} tends to 0. The notation $\zeta_{i,p}$ is thus in accordance with the rules stated in Sec. II, as far as the first index is concerned; index i refers to the unperturbed level in the following way: $\lim_{\lambda_{01}\to 0}(\zeta_{0,1})_j = 0$, $\lim_{\lambda_{01}\to 0}\zeta_{1,1} = e_1$. To distinguish perturbed eigenvalues which tend to the same e_i if $(\lambda_{01},\lambda_{12}) \to (0,0)$, we chose to put the index p, indicating that the eigenvectors are in $\mathcal{E}_p$ (as in Sec. III B). Since several eigenvalues with the same indices i and p may still have the same limit when $(\lambda_{01},\lambda_{12})$ tends to (0,0), an additional index j is used to number them.

We have $(\phi_{0,1}^{(0)})_1(\lambda_{01},\lambda_{12}) \to -|0,f_{01}\rangle$ and $\phi_{1,1}^{(0)}(\lambda_{01},\lambda_{12}) \to |1,\Omega\rangle$, if λ_{01} tends to 0.

If $f_{01} = f_{12}$, the dimension of $\mathcal{E}_1^{(2)}$ is two and the eigenvector $(\phi_{0,1}^{(0)})_2$ disappears.

As we said before, these eigenvalues are actually infinitely degenerated; indeed, adding photons whose states are orthogonal to $\{f_{01},f_{12}\}$ gives an eigenstate with the same energy, since the energy of the photons is not taken into account in $H_0(\lambda)$. Let us state this fact precisely, with some notations which will be useful later on.

2. Other eigenvectors of $H_0(\lambda)$ in the $(n+1)$-excitation space $\mathcal{E}_{n+1}$, $n>0$, associated with the same eigenvalues

Proposition 4.2: Let $g_1,g_2,\ldots$ be an orthonormal basis of functions orthogonal to f_{01} and f_{12}.
(i) Let $\mathcal{G}_{0,1,1}$ be the subspace of $\mathcal{E}$ spanned by the normalized vectors

$$(\phi_{0,n+1}^{(n_1,n_2,\ldots)})_1 := \prod_{i=1}^{\infty}(n_i!)^{-1/2}(1\otimes c^*(g_i))^{n_i}(\phi_{0,1}^{(0)})_1, \tag{4.10}$$

where the n_i's are k nonnegative integers and k is arbitrary. These vectors are in $\mathcal{E}_{n+1}$ if $n = \sum_{i=1}^{k} n_i$. For generic values of λ_{01} and λ_{12}, $\mathcal{G}_{0,1,1}$ is the eigenspace of $H_0(\lambda)$ associated with eigenvalue $(\zeta_{0,1})_1$

(ii) If $f_{01} \neq f_{12}$, let us set $g_0 := (1-|s_1|^2)^{-1/2}$ $(f_{12} - s_1 f_{01})$ and let $f_{01}^{\perp}$ be the subspace of $\mathcal{H}_{\mathrm{rad}}$ orthogonal to f_{01}, spanned by the g_i's, $i = 0,1,\cdots$. The eigenspace of $H_0(\lambda)$ associated with eigenvalue $(\zeta_{0,1})_2$ is $|0\rangle \otimes \mathcal{F}(f_{01}^{\perp})$, where $\mathcal{F}(f_{01}^{\perp})$ is the Fock space built with $f_{01}^{\perp}$. We set

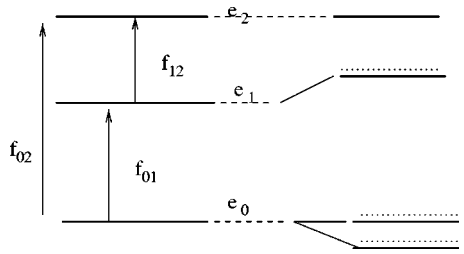

FIG. 10. Levels of Fig. 9, with eigenvectors of $H_0(\lambda)$ in $\mathcal{E}_2$; at most one spectator photon.

$$(\phi_{0,n+1}^{(n_0,n_1,\ldots)})_2 := \prod_{i=0}^{\infty} (n_i!)^{-1/2} (1 \otimes c^*(g_i))^{n_i} (\phi_{0,1}^{(0)})_2. \tag{4.11}$$

(iii) Last, let $\mathcal{G}_{1,1}$ be the subspace of $\mathcal{E}$ spanned by the normalized vectors

$$\phi_{1,n+1}^{(n_1,n_2,\ldots)} := \prod_{i=1}^{\infty} (n_i!)^{-1/2} (1 \otimes c^*(g_i))^{n_i} \phi_{1,1}^{(0)}. \tag{4.12}$$

For generic values of λ_{01} and λ_{12}, $\mathcal{G}_{1,1}$ is the eigenspace of $H_0(\lambda)$ associated with eigenvalue $\zeta_{1,1}$.

That $\Pi_{i=1}^{\infty}(1 \otimes c^*(g_i))^{n_i}$ $(\phi_{0,1}^{(0)})_1$, $\Pi_{i=0}^{\infty}(1 \otimes c^*(g_i))^{n_i}$ $(\phi_{0,1}^{(0)})_2$ and $\Pi_{i=1}^{\infty}(1 \otimes c^*(g_i))^{n_i}$ $\phi_{1,1}^{(0)}$ are eigenvectors follows from the fact that $[1 \otimes c^*(g), H_0(\lambda)] = 0$ if g is orthogonal to $\mathcal{H}_{\text{rad}}^{(2)}$. In Appendix B 1, we explain how the whole eigenspace can be determined, for each of the three eigenvalues.■

Let g [which is no longer function (3.8)] be a linear combination of the g_i's. A photon in such a state will be called a spectator photon. Proposition 4.2 may be stated in the following terms: the three eigenvalues are twice infinitely degenerated; first through the number of spectator photons (the n variable), and second through the infinity of possible states for each spectator photon (the g variable). In the level diagrams, if we symbolize the degeneracy of an eigenvalue (due to the possibility of one spectator photon in the eigenvector) by a dotted line, then in the case where at most one spectator photon is present, the degeneracy of the levels may be represented in Fig. 10 (dotted lines are slightly shifted from the level for reading purpose).

The degeneracy of the eigenvalue is greater if we admit eigenvectors with a greater number of spectator-photons, with all their possible states.

But considering a total number of photons greater than one yields other eigenvalues. For instance, we claim that eigenvectors in $\mathcal{E}_2$ different from $|2,0\rangle$ are not necessarily built with eigenvectors in $\mathcal{E}_1$ and a spectator photon. We are going to see that the set of perturbed eigenvalues coming from one given unperturbed energy e_i changes when the number of photons coupled to the atom changes. This was already the case for the two-level atom of Sec. III (see for instance Proposition 3.1 of Sec. III B, for $\mu = 0$, where the eigenvalue depended on the space in which the eigenvector was looked for).

3. Other eigenvectors of $H_0(\lambda)$ in $\mathcal{E}_{n+1}$ and other eigenvalues

In this section, we assume $f_{01} \neq f_{12}$.

Proposition 4.3: $H_0(\lambda)$ has an infinity of eigenvalues different from $(\zeta_{0,1})_1$, $(\zeta_{0,1})_2$, and $\zeta_{1,1}$.

PROOF: $\mathcal{E}_n$ is invariant by $H_0(\lambda)$. The subspace $\mathcal{E}_n^{(2)}$ of $\mathcal{E}_n$ is also invariant. Let us first consider $\mathcal{E}_2^{(2)}$, six dimensional. If the coupling constants are small, there are six eigenvalues: when λ_{01} and λ_{12} tend to 0, one of them tends to e_2 (it is denoted by $\zeta_{2,2}$), two tend to e_1 [denoted by $(\zeta_{1,2})_1$ and $(\zeta_{1,2})_2$] and three, one of which is zero, tend to 0 [denoted by $(\zeta_{0,2})_1 = 0$, $(\zeta_{0,2})_2$ and $(\zeta_{0,2})_3$]. They are obtained through diagonalizing a six by six matrix (see Appendix B 2). The calculation is straightforward although the result has not a simple expression. In this two-excitation space, that two eigenvalues tend to e_1 is due to the fact that there are two possible photon states, and that three eigenvalues tend to 0 is due to the fact that there are three possible independent states for the two

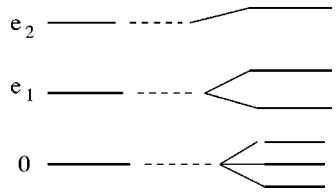

FIG. 11. Levels associated with eigenvectors of $H_0(\lambda)$ in $\mathcal{E}_2^{(2)}$, without any spectator photon.

photons. The eigenvector associated with $(\zeta_{0,2})_1=0$ is $|0,g_0\vee g_0\rangle$; we met it under the form $(\phi_{0,1}^{(1,0,\ldots)})_2$ [see (4.11)].

We already found other eigenvectors in the same space $\mathcal{E}_2$. They were built from eigenvectors in $\mathcal{E}_1^{(2)}$. They are for instance $(\phi_{0,1}^{(1,0,\ldots)})_1$ and $\phi_{1,1}^{(1,0,\ldots)}$, with notations of Proposition 4.2; they are in $\mathcal{E}_2^{(3)}$ if $g_1\in\mathcal{H}_{\mathrm{rad}}^{(3)}$. The corresponding eigenvalues, $(\zeta_{0,1})_1$ and $\zeta_{1,1}$, are different from the six we just saw (see Appendix B 2), except possibly for particular values of λ.

Since the notations are a bit heavy, we again represent the levels in Fig. 11.

The changes in the levels e_0, e_1, and e_2 of Figs. 10 and 11 cannot be superimposed on one another, in general. Both are to be considered in describing the levels of $H_0(\lambda)$.

To complete the study, we have to take an arbitrary number of photons into account. The study of the spectrum of $H_0(\lambda)$ is completed when one has also considered eigenvectors in $\mathcal{E}_3^{(2)}$, $\mathcal{E}_4^{(2)}$, etc.; They give new levels. Eventually, there is a very great number of levels. Let $S(n,p)$ be the number of independent symmetric states that can be formed with n photons, each photon being in p possible states. Let us consider $1,2,\ldots,n$ photons successively. The fundamental state is split into a doublet, a triplet, …, a $S(n,2)$ multiplet. If we look for all possible states, all these levels must be considered. As regards level 1, a shift, then a doublet, a triplet, …, a $S(n-1,2)$ multiplet. Lastly, for level 2, we get no change, then a shift, a doublet, …, a $S(n-2,2)$ multiplet. To be complete, let us recall level $e_0=0$, with eigenvector $|0,\Omega\rangle$. ■

The doubly infinite degeneracy due to spectator-photons still remains. With the six eigenvalues $\zeta_{2,2}$, $(\zeta_{1,2})_1$, and $(\zeta_{1,2})_2$, and last $(\zeta_{0,2})_1$, $(\zeta_{0,2})_2$, and $(\zeta_{0,2})_3$, are associated eigenvectors $\phi_{2,2}^{(0)}$, $(\phi_{1,2}^{(0)})_1$, and $(\phi_{1,2}^{(0)})_2$), and last $(\phi_{0,2}^{(0)})_1$, $(\phi_{0,2}^{(0)})_2$, and $(\phi_{0,2}^{(0)})_3$. As previously, through application of $(1\otimes c^*(g))^n$ with g orthogonal to $\{f_{01},f_{12}\}$, or more generally application of $\Pi(1\otimes c^*(g_i))^{n_i}$, one gets other eigenvectors associated with the same eigenvalues. In the same way that we built Fig. 10 from Fig. 9, we could illustrate this degeneracy graphically through adding dotted lines in Fig. 11.

Let us come back to our initial problem, which is to determine the spectrum of $H(\lambda)$, at least roughly. It may be expected that the perturbation $\lambda_{02}V$ partially removes the degeneracy of each of the six above-mentioned eigenvalues, as well as degeneracies of the same type, for instance those of the three eigenvalues $(\zeta_{0,1})_1$, $(\zeta_{0,1})_2$, and $\zeta_{1,1}$ that we obtained previously. It is this simpler question that we now examine. We are going to show that the coupling $\lambda_{02}\,V$ splits the first three levels of Fig. 10, eigenvalues $(\zeta_{0,1})_1$, $(\zeta_{0,1})_2$, and $\zeta_{1,1}$ of Proposition 4.2, into an infinity of levels and calculate the splittings of $(\zeta_{0,1})_1$ and $\zeta_{1,1}$, at the lowest order in λ_{02}.

C. Perturbation with respect to λ_{02}: Second removal of degeneracy

We are now interested in $H(\lambda)$. The function f_{02} comes into play. Hence we assume that the first vector of the basis $g_1,g_2,\ldots$ of Proposition 4.2 is in $\mathcal{H}_{\mathrm{rad}}^{(3)}$. The g_i's, $i>1$ are thus orthogonal to $\mathcal{H}_{\mathrm{rad}}^{(3)}$. We saw that the $(\phi_{i,p}^{(q,0,\ldots)})_k$, $q=0,1,\ldots$, which are in $\mathcal{E}^{(3)}$, are associated with a unique eigenvalue $(\zeta_{i,p})_k$. In the simple cases $(i,p)=(1,1)$ and $(i,p,k)=(0,1,1)$, we are going to show that the degeneracy is removed. We calculate the approximations of order two in λ_{02} of those eigenvalues of $H(\lambda)$ which tend to $(\zeta_{i,p})_k$ when λ_{02} tends to 0. These eigenvalues depend on q. The approximations are denoted by $(z_{i,p}^{(q)})_k^{(\leqslant 2)}$. The corresponding eigenvectors are denoted by $(\chi_{i,p}^{(q)})_k$ and their second-order approximations by $(\chi_{i,p}^{(q)})_k^{(\leqslant 2)}$. We will have

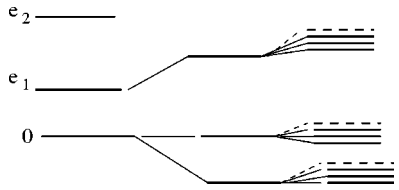

FIG. 12. Qualitative description of the perturbation of Fig. 10 first levels, due to the $\lambda_{02}\,V$ term: ($g_{i_1}=g_1$). (In the last columns, the additional degeneracy is not mentioned.)

$$\lim_{\lambda_{02}\to 0}(\chi_{i,p}^{(q)})_k^{(\leqslant 2)}=(\phi_{i,p}^{(q,0,\ldots)})_k=(1\otimes c^*(g_1))^q(\phi_{i,p}^{(0)})_k. \tag{4.13}$$

(Here, z does not have the same meaning as in Sec. III; μ remains zero.)

Note that, if $\chi\in\mathcal{H}^{(3)}$ is an eigenvector of $H(\lambda)$, then for every g orthogonal to $\mathcal{H}_{\mathrm{rad}}^{(3)}$, $(1\otimes(c^*(g))^n)\chi$ is still an eigenvector, associated with the same eigenvalue. This second degeneracy removal is thus only very partial.

We assume that $p=1$ and we limit ourselves to perturbing $(\zeta_{0,1})_1$, $(\zeta_{0,1})_2$ if $f_{01}\neq f_{12}$, and $\zeta_{1,1}$. If $f_{01}\neq f_{12}$, the diagram in Fig. 10 transforms into the one of Fig. 12. The case of $(\zeta_{0,1})_2$ is particular as we will see later on. Note that the exact eigenvector $(\chi_{i,p}^{(q)})_k$ is no longer in $\mathcal{E}_{q+1}^{(3)}$ but in $\oplus_{r=0}^{\infty}\mathcal{E}_{r+1}^{(3)}$. More precisely, we have

Proposition 4.4: Through the perturbation $\lambda_{02}\,V$*, each of the eigenvalues* $(\zeta_{0,1})_1(\lambda_{01},\lambda_{12})$ *and* $\zeta_{1,1}(\lambda_{01},\lambda_{12})$ *is at least split into an infinity of eigenvalues* $(z_{0,1}^{(n)})_1(\lambda)$ *and* $z_{1,1}^{(n)}(\lambda)$*, given at second order in* λ_{02} *by the following formulas:*

$$(i)\ (z_{0,1}^{(n)})_1^{\leqslant 2}(\lambda)=(\zeta_{0,1})_1(\lambda_{01},\lambda_{12})+\lambda_{02}^2\left(1+n!\frac{\lambda_{01}^2}{(\zeta_{0,1})_1^2}\right)^{-1}A_{0,1,1}^{(n)}(\lambda_{01},\lambda_{12}) \tag{4.14}$$

with, if $f_{01}\neq f_{12}$,

$$A_{0,1,1}^{(n)}(\lambda_{01},\lambda_{12}):=n\frac{\lambda_{01}^4|(f_{02},g_1)|^2}{((\zeta_{0,1})_1)^2(\lambda_{12}^2(\zeta_{0,1})_1+\lambda_{01}^2((\zeta_{0,1})_1-e_2))}, \tag{4.15}$$

where $|(f_{02},g_1)|$ *can be expressed with the* s_i*'s, and, if* $f_{01}=f_{12}$*, and thus* $g_1=(1+|s_0|^2)^{-\frac{1}{2}}(f_{02}-s_0f_{01})$,

$$A_{0,1,1}^{(n)}(\lambda_{01},\lambda_{12}):=\frac{\lambda_{01}^4}{((\zeta_{0,1})_1)^2(\lambda_{12}^2(\zeta_{0,1})_1+\lambda_{01}^2((\zeta_{0,1})_1-e_2))}(n|(f_{02},g_1)|^2+|s_0|^2). \tag{4.16}$$

(ii) $(z_{1,1}^{(n)})^{\leqslant 2}$ *is obtained through replacing* $(\zeta_{0,1})_1$ *by* $\zeta_{1,1}$ *in expressions giving* $(z_{0,1}^{(n)})_1^{\leqslant 2}$.

(iii) $(\zeta_{0,1})_2$*, which is more degenerated than the two previous eigenvalues, is also split. The second-order approximations of the perturbed eigenvalues,* $(z_{0,1}^{(n,m}\,)_2^{\leqslant 2}$*, now depending on two indices, are obtained through the vanishing of an infinite order determinant.*

The broad lines of the proof are given in Appendix B 3, together with the method for calculating the corresponding eigenvectors $(\chi_{0,1}^{(n)})_1^{\leqslant 2}(\lambda)$, $(\chi_{0,1}^{(n,m)})_2^{\leqslant 2}(\lambda)$, and $(\chi_{1,1}^{(n)})^{\leqslant 2}(\lambda)$.

D. Conclusion of Sec. IV

Section IV C described the splitting of the eigenvalues $(\zeta_{0,1})_1$, $(\zeta_{0,1})_2$, and $\zeta_{1,1}$ of Proposition 4.2. It gave a small part of the spectrum of $H(\lambda,0)$, described in the second column of Fig. 12. In view of these results one may reasonably surmise the following points.

This splitting of the levels of the second column of Fig. 9 (or 10) will reproduce for those of the second column of Fig. 11, which are different. In other terms, the degeneracy of the latter levels, due to spectator photons, will also be removed by the coupling $\lambda_{02}V$. More generally, each level multiplet which was mentioned at the end of the proof of Proposition 4.3 is also split when

the interaction is totally switched on. This rough description of the two level splittings we get by successively taking the two parts of the interaction Hamiltonian into account eventually yields quite a complicated spectrum for $H(\lambda,0)$. But the reason of the great number of levels is simple; it is recalled in Sec. V.

When μ increases from 0, we expect that the eigenvalues we found move into eigenvalues or resonances of $H(\lambda,\mu)$. The set of these eigenvalues or resonances thus likely has the same rich structure.

V. GENERAL CONCLUSION

Results of Secs. III and IV fit into the same frame. They lead us to expect that the number of eigenstates or resonances of the atom-photon system is formally, apart from accidental degeneracy or boundary-condition effects, the product of the dimensions of the atom state space and the field state space. The description is complicated because of the multivaluedness of the resolvent matrix elements, as functions of the λ and μ parameters. This picture may be illustrated through the following argument: if the energy of each level of the isolated atom is considered as an eigenvalue of $H_{\text{atom}}\otimes 1_{\text{field}}$, this level is twice infinitely degenerated (number of photons and state of each photon). This degeneracy is removed with the actual Hamiltonian which describes the coupling of the atom to the field. The shift of the naked-atom levels by the coupling of the atom to the photon field is thus not the main feature in the change in the Hamiltonian "spectrum." The main feature is more the emergence of numerous resonances, as in the monochromatic-photon case.

For a two-level atom and Hamiltonian (3.1) (Sec. III), only one photon state comes into play. The subspace of $\mathcal{H}_{\text{rad}}$ to be considered is $\mathcal{H}_{\text{rad}}^{(1)}$ and the two degeneracies which are removed, same energy for states $|0,0\rangle$, $|0,g\rangle,\ldots$, $|0,g^{\vee n}\rangle,\ldots$ on the one hand and $|1,0\rangle$, $|1,g\rangle,\ldots$, $|1,g^{\vee n}\rangle,\ldots$ on the other hand, only concern the number of photons. A great degeneracy remains since adding photons in states orthogonal to the distinguished g state do not change the energies.

For a three-level atom, the number of coupling functions in the Hamiltonian is greater and this forced us to start to pay attention to different photon states. As a consequence, the just mentioned degeneracy now starts being removed.

For a real atom, with its infinity of levels, the splitting will still be greater. Our perturbative treatment illustrates how the different photon states may be taken into account successively. Calculations will of course be impossible if some physically justified simplifications are not made.

The present limits of the study are the following.

Section III described resonances for a realistic Hamiltonian ($\mu\neq 0$), but for a system with only two levels. However, even in that simplified case, we are far from having found all the resonances since we considered only one or two excitation spaces, $\mathcal{E}_1$ or $\mathcal{E}_2$. It would be necessary to take more than two photons into account. But the resonances are then given by more and more complicated equations.

In Sec. IV, to be able to present a qualitative description of resonances in a three-level system, we had to work in the limit $\mu=0$. This first stage seems unavoidable to us if one wants to solve the question completely. Doing this, we were able to take an infinity of photons into account. But the calculations are only carried to the second order in λ_{02} and also the displacement of the resonances when μ becomes non-zero is just qualitatively mentioned.

However, we have seen that these partial results give new information about hybrid states which are present in matter-field interactions such as the interaction to which we borrowed our terminology: the interaction of atoms (or molecules) with the electromagnetic field. We hope that concrete problems will justify approximations making calculations possible.

APPENDIX A. ESTIMATION OF CORRECTIVE TERMS IN THE FREDHOLM EXPANSION OF PROPOSITION 3.4

Proposition: Set $\varphi_2(\mu,z,p,q):=\mu^2 D_2(\mu,z,p,q)$ *and*

$$\varphi_3(\mu,z,p,q):=\frac{|g(p)||g(q)|(1+|p|)^{1/4}(1+|q|)^{1/4}(|p|-|q|)^2}{|f(z-\mu|p|)|^{1/2}|f(z-\mu|q|)|^{1/2}\left|\frac{z}{\mu}-2|p|\right|^{1/2}\left|\frac{z}{\mu}-2|q|\right|^{1/2}\left|\frac{z}{\mu}-|p|-|q|\right|^{2}}$$

$$\varphi_4(\mu,z,p,q) := \frac{|g(p)|^{2/3}|g(q)|^{2/3}(1+|p|)^{1/4}(1+|q|)^{1/4}(|p|-|q|)^2}{|f(z-\mu|p|)|^{1/3}|f(z-\mu|q|)|^{1/3}\left|\frac{z}{\mu}-2|p|\right|^{1/3}\left|\frac{z}{\mu}-2|q|\right|^{1/3}\left|\frac{z}{\mu}-|p|-|q|\right|^2}$$

defined for $z<0$. *we have*

$$C_2(\lambda,\mu,z) = (\lambda^2/\mu)^2\|\varphi_2(\mu,z,.,.)\|_1, \tag{A1}$$

$$|C_3(\lambda,\mu,z)| < M_3(\lambda,\mu,z) := 4(\lambda^2/\mu)^3\|\varphi_3(\mu,z,.,.)\|_3^3. \tag{A2}$$

Assuming that (3.19) also holds for $n=4$, *we also have*

$$|C_4(\lambda,\mu,z)| < M_4(\lambda,\mu,z) := 4^2(\lambda^2/\mu)^4\|\varphi_4(\mu,z,.,.)\|_6^6. \tag{A3}$$

Proof: Use (3.19) and Hölder's inequalities. ■

We omit λ, which is fixed to 0.1. Table III gives values for $C_2(\mu,z_{0,2}^1(\mu))$, $M_3(\mu,z_{0,2}^1(\mu))$, $M_4(\mu,z_{0,2}^1(\mu))$, and $\partial_z C_1(\mu,z_a^{(2)}(\mu))$, from

$$\partial_z C_1(\mu,z) = -\lambda^2\int\frac{|g(p)|^2}{f(\mu,z-\mu|p|)(z-2\mu|p|)}\left(\frac{1}{f(\mu,z-\mu|p|)}-\frac{1}{z-2\mu|p|}\right)dp$$
$$-\lambda^2\int\int\frac{|g(p)|^2|g(q)|^2dpdq}{f^2(\mu,z-\mu|p|)(z-2\mu|p|)(z-\mu(p+q))^2}.$$

By definition $C_1(\mu,z_{0,1}^1(\mu))=1$. We see how the terms of the Fredholm expansion decrease with the order.

For $\mu=\mu_c$, $D(\mu_c,0)$ is close to 0. Let us recall that we have $f(\lambda,\mu_c(\lambda),0)=0$. It would be interesting to see whether $D(\mu_c,0)$ vanishes or not. To try and answer this question, let us estimate the error we made in calculating the zero of $D(\mu,.)$ by the truncated series. Let us consider the following expansion of $D(\mu,.)$ near $z_{0,2}^1(\mu)$:

$$1-C_1(\mu,z_{0,2}^1(\mu))-(z-z_{0,2}^1(\mu))\partial_z C_1(\mu,z_{0,2}^1(\mu))+\frac{1}{2}C_2(\mu,z_{0,2}^1(\mu))+\frac{1}{2}(z-z_{0,2}^1(\mu))\partial_z C_2(\mu,z_{0,2}^1(\mu))$$
$$-\frac{1}{6}(C_3(\mu,z_{0,2}^1(\mu))+(z-z_{0,2}^1(\mu))\partial_z C_3(\mu,z_{0,2}^1(\mu))).$$

Let us assume that terms $(z-z_{0,2}^1(\mu))\partial_z C_2(\mu,z_{0,2}^1(\mu))$ and $(z-z_{0,2}^1(\mu))\partial_z C_3(\mu,z_{0,2}^1(\mu))$ can be neglected. Then the correction to the zero is

$$\frac{1}{\partial_z C_1(\mu,z_{0,2}^1(\mu))}\left(-\frac{1}{2}C_2(\mu,z_{0,2}^1(\mu))+\frac{1}{6}C_3(\mu,z_{0,2}^1(\mu))\right)$$

whose principal term is of the order of 4×10^{-4}. Since it is precisely the order of $z_{0,2}^1(\mu_c)$, it is not possible to answer the question.

APPENDIX B: SKETCHES OF PROOFS OF RESULTS IN THE THIRD-LEVEL CASE

1. Sketch of the proof of Proposition 4.2

Let $\Phi := |2,F_n\rangle+|1,F_{n+1}\rangle+|0,F_{n+2}\rangle$ be an eigenvector of $H_0(\lambda)$ in $\mathcal{E}_{n+2}$ associated with z, one of the two eigenvalues $(\zeta_{0,1})_1$ or $\zeta_{1,1}$. It can be shown that

$$(z-e_2)^{-1}\lambda_{12}^2(f_{12},F_{n+1})\vee f_{12} = z^{-1}\lambda_{01}^2(f_{01},F_{n+1})\vee f_{01}, \tag{B1.1}$$

where

$$(f_{12},F_{n+1})(p_1,p_2,\ldots,p_n)=\int \overline{f}_{12}(p)F_{n+1}(p,p_1,p_2,\ldots,p_n)\mathrm{d}p,$$

$$(f^{\vee n}\vee h)(p_1,p_2,\ldots,p_{n+1})=\frac{1}{n+1}\sum_{i=1}^{n+1}\left(\prod_{j\neq i}^{n+1}f(p_j)\right)h(p_i).$$

From (B1.1), through decomposing F_{n+1} on a basis of the $(n+1)$-photon space built with f_{01},f_{12}, and the g_i's, we get that F_{n+1} is a sum of states $\Pi_{i=1}^{\infty}(c^*(g_i))^{n_i}\Omega$ with $\Sigma_i n_i=n+1$. From relations expressing that Φ is an eigenvector, we derive $F_n=0$ and, if $z\neq 0$, $F_{n+2}=z^{-1}\sqrt{n+2}\lambda_{01}F_{n+1}\vee f_{01}$; this implies that Φ is in $\mathcal{G}_{0,1,1}$ if $z=(\zeta_{0,1})_1$ or in $\mathcal{G}_{1,1}$ if $z=\zeta_{1,1}$. Hence (i) and (iii).

If $z=(\zeta_{0,1})_2=0$, then Φ is an eigenvector if and only if $F_n=0$, $F_{n+1}=0$ and $(f_{01},F_{n+2})=0$. Hence (ii).

2. The six eigenvalues $\zeta_{2,2}$, $(\zeta_{1,2})_1$, $(\zeta_{1,2})_2$, $(\zeta_{0,2})_1$, $(\zeta_{0,2})_2$ and $(\zeta_{0,2})_3$, with eigenvectors in $\mathcal{E}_2^{(2)}$

The space spanned by vectors

$$|2,\Omega\rangle,\quad |1,f_{12}\rangle,\quad |1,f_{01}\rangle,\quad |0,f_{12}\vee f_{01}\rangle,\quad |0,f_{01}\vee f_{01}\rangle$$

is invariant. Through adding $|0,f_{12}\vee f_{12}\rangle$, we get a basis of $\mathcal{E}_2^{(2)}$, in which the matrix of H_0 is

$$\begin{pmatrix} e_2 & \lambda_{12} & s_1\lambda_{12} & 0 & 0 & 0 \\ \lambda_{12} & e_1 & 0 & \frac{\lambda_{01}}{\sqrt{2}} & 0 & \sqrt{2}s_1\lambda_{01} \\ 0 & 0 & e_1 & s_1\frac{\lambda_{01}}{\sqrt{2}} & \sqrt{2}\lambda_{01} & 0 \\ 0 & \sqrt{2}\lambda_{01} & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{2}\lambda_{01} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

One of the eigenvalues is 0 and the eigenvector is the one mentioned in the text. The other eigenvalues are the ζ's for which

$$\zeta(\zeta-e_1)(\zeta(\zeta-e_1)(\zeta-e_2)-3\lambda_{01}^2(\zeta-e_2)-\lambda_{12}^2\zeta)+\zeta\lambda_{01}^2(2\lambda_{01}^2+(2-|s_1|^2)\lambda_{12}^2)-2e_2\lambda_{01}^4$$

vanishes. Neglecting fourth-order terms, we get the following solutions at second order in λ:

$$(\zeta_{0,2}^0)_2=0,\quad (\zeta_{0,2}^0)_3=-\frac{3}{e_1}\lambda_{01}^2,\quad (\zeta_{1,2}^0)_1=e_1,\quad (\zeta_{1,2}^0)_2=e_1+\frac{3}{e_1}\lambda_{01}^2+\frac{1}{e_1-e_2}\lambda_{12}^2,$$

$$\zeta_{2,2}^0=e_2+\frac{1}{e_2-e_1}\lambda_{12}^2.$$

This proves that these eigenvalues are different from those found in $\mathcal{E}_1^{(2)}$.

3. Sketch of the proof of Proposition 4.4.

Let us use Kato's method[23] to determine the three (infinite) sets of perturbed eigenvalues which tend to each of the unperturbed eigenvalues. (See a short account in Ref. 24.)

(i) Let us first consider $(\zeta_{0,1})_1$. The unperturbed eigenspace is $\mathcal{G}_{0,1,1}$ (Proposition 4.2). Let $P_0^{0,1,1}$ be the projector on this space and $Q_0^{0,1,1}=1-P_0^{0,1,1}$. We need operator $\tilde{Q}_0^{0,1,1}$ which is sometimes written as $Q_0^{0,1,1}[(\zeta_{0,1})_1-H_0]^{-1}Q_0^{0,1,1}$; for $x\in\mathcal{E}$, it is defined by $\tilde{Q}_0^{0,1,1}x=Q_0^{0,1,1}z$, where z is

any vector in $\mathcal{E}$ satisfying $[(\zeta_{0,1})_1 - H_0]z = Q_0^{0,1,1}x$. Let $\mathcal{H}_{0,1,1}$ be the direct sum of the eigenspaces associated with eigenvalues of $H(\lambda)$ which tend to $(\zeta_{0,1})_1$ when λ_{02} tends to 0. Let $P^{0,1,1}(\lambda_{02})$ be the projector on $\mathcal{H}_{0,1,1}$. Therefore $\lim_{\lambda_{02}\to 0} P^{0,1,1}(\lambda_{02}) = P_0^{0,1,1}$. We assume that $P_0^{0,1,1}$ and $P^{0,1,1}(\lambda_{02})$ establish one-to-one correspondences $\mathcal{H}_{0,1,1} \to \mathcal{G}_{0,1,1}$ and $\mathcal{G}_{0,1,1} \to \mathcal{H}_{0,1,1}$. Set

$$L_{0,1,1} = P_0^{0,1,1} H P^{0,1,1} P_0^{0,1,1} \text{ and } K_{0,1,1} = P_0^{0,1,1} P^{0,1,1} P_0^{0,1,1}. \tag{B3.1}$$

We recall[24] the expansion of $P^{0,1,1}$: with $S^{(0)} := -P_0^{0,1,1}$ and $S^{(k)} := (\tilde{Q}_0^{0,1,1})^k$,

$$P^{0,1,1} = P_0^{0,1,1} - \sum_n \lambda_{02}^n \sum_{k_i \geqslant 0,\ k_0+\cdots+k_n=n} S^{(k_0)} V S^{(k_1)} \cdots V S^{(k_n)}. \tag{B3.2}$$

A necessary and sufficient condition for $\chi \in \mathcal{H}_{0,1,1}$ to be an eigenvector of $H(\lambda)$ associated with the eigenvalue z is that there exists $\phi \in \mathcal{G}_{0,1,1}$ satisfying $\chi = P^{0,1,1}\phi$ and

$$L_{0,1,1}\phi = z K_{0,1,1}\phi. \tag{B3.3}$$

$L_{0,1,1}$ and $K_{0,1,1}$ are operators in $\mathcal{G}_{0,1,1}$ and the problem of the perturbation of $(\zeta_{0,1})_1$ is turned into finding such z. We still have a degeneracy due to photon-states in $(\mathcal{H}_{\text{rad}}^{(3)})^{\perp}$; indeed, if ϕ is a solution for (B3.3), then $\Pi_{i\geqslant 2}(1 \otimes c^*(g_i))^{n_i}\phi$ is still a solution. Thus we are not going to look for all ϕ's, but only for those in an invariant subspace of $\mathcal{G}_{0,1,1}$. Lemmas B3.1 to B3.6 prepare the calculation of eigenvalues into which $(\zeta_{0,1})_1$ splits. The result for $\zeta_{1,1}$ will be obtained through a simple change in the notations. The splitting of $(\zeta_{0,1})_2$ is just outlined.

Let g_1 be the function of $\mathcal{H}_{\text{rad}}^{(3)}$ orthogonal to $\mathcal{H}_{\text{rad}}^{(2)}$ and let $\mathcal{G}_{0,1,1}^{(1)}$ be the subspace of $\mathcal{G}_{0,1,1}$ spanned by $(1 \otimes c^*(g_1))^n\ (\phi_{0,1}^{(0)})_1$, $n \geqslant 0$. Let us denote the approximations of $K_{0,1,1}$ and $L_{0,1,1}$ to order q in λ_{02} by $K_{0,1,1}^{\leqslant q}$ and $L_{0,1,1}^{\leqslant q}$.

Lemma B3.1: For all q, $\mathcal{G}_{0,1,1}^{(1)}$ is invariant by $K_{0,1,1}^{\leqslant q}$ and $L_{0,1,1}^{\leqslant q}$.

PROOF: Operators $1 \otimes c^*(g_1)$ and V sent $\mathcal{E}^{(3)}$ into $\mathcal{E}^{(3)}$, since functions orthogonal to $\mathcal{H}_{\text{rad}}^{(3)}$ do not play any part. Now, $P_0^{0,1,1}$ sends $\mathcal{E}^{(3)}$ into $\mathcal{G}_{0,1,1}^{(1)} \subset \mathcal{E}^{(3)}$. Thus, if X is any endomorphism of $\mathcal{E}^{(3)}$, $P_0^{0,1,1} X P_0^{0,1,1}$ is an endomorphism of $\mathcal{G}_{0,1,1}^{(1)}$. $Q_0^{0,1,1}$ also leaves $\mathcal{E}^{(3)}$ invariant. The same is true for $\tilde{Q}_0^{0,1,1}$ and therefore for $P^{0,1,1}$. Hence the lemma. ■

Expressions to the second order in λ_{02} of $L_{0,1,1}$ and $K_{0,1,1}$ are

$$K_{0,1,1}^{\leqslant 2} = P_0^{0,1,1} - \lambda_{02}^2 P_0^{0,1,1} V (\tilde{Q}_0^{0,1,1})^2 V P_0^{0,1,1}, \tag{B3.4}$$

$$L_{0,1,1}^{\leqslant 2} = (\zeta_{0,1})_1 K_1^{\leqslant 2} + \lambda_{0,2}^2 P_0^{0,1,1} V \tilde{Q}_0^{0,1,1} V P_0^{0,1,1}. \tag{B3.5}$$

To calculate $K_{0,1,1}^{\leqslant 2}(\phi_{0,n+1}^{(n)})_1$ and $L_{0,1,1}^{\leqslant 2}(\phi_{0,n+1}^{(n)})_1$, we need the following lemma.

Lemma B3.2:

$$V(\phi_{0,n+1}^{(n)})_1 = |2, (\varphi_{0,1}^{(n)})_1\rangle \tag{B3.6}$$

with $(\varphi_{0,1}^{(0)})_1 = N_1 \lambda_{01}/(\zeta_{0,1})_1 \overline{s_0}$ *and, for* $n \geqslant 1$,

$$(\varphi_{0,1}^{(n)})_1 = N_1 \frac{\lambda_{01}}{(\zeta_{0,1})_1} (\overline{s_0} g_1^{\vee n} + n(f_{02}, g_1) f_{01} \vee g_1^{\vee n-1}), \tag{B3.7}$$

where $N_1 = (1 + (\zeta_{0,1})_1^{-2}\lambda_{01}^2)^{-1/2}$.

Lemma B3.3: $K_{0,1,1}^{\leqslant 2}$ and $L_{0,1,1}^{\leqslant 2}$ are diagonal in the basis $(\phi_{0,n+1}^{(n)})_1$ of $\mathcal{G}_{0,1,1}^{(1)}$.

Proof: $V(\phi_{0,n+1}^{(n)})_1 \in \mathcal{E}_{n+2}$, since $(\phi_{0,n+1}^{(0)})_1$ has no component on $|2\rangle \otimes \mathcal{F}$. Through using $\tilde{Q}_0^{0,1,1}\mathcal{E}_{n+2}^{(3)} \subset \mathcal{E}_{n+2}^{(3)}$, we then get

$$(\tilde{Q}_0^{0,1,1} V P_0^{0,1,1} (\phi_{0,n+1}^{(n)})_1, \tilde{Q}_0^{0,1,1} V P_0^{0,1,1} (\phi_{0,m+1}^{(m)})_1) = 0, \quad \text{if } m \neq n$$

and $K_{0,1,1}^{\leqslant 2}$ is diagonal. The same is true for $L_{0,1,1}^{\leqslant 2}$. ■

Lemma B3.4: Let us set $u_{1,n} := \tilde{Q}_0^{0,1,1} V(\phi_{0,n+1}^{(n)})_1$ *and define* $\kappa_{1,n}$, $\theta_{1,n+1}$ *and* $h_{1,n+2}$ *by* $u_{1,n} = |2,\kappa_{1,n}\rangle + |1,\theta_{1,n+1}\rangle + |0,h_{1,n+2}\rangle$. *We denote the expression of* z *to the second order in* λ_{02} *by* $(z_{0,1}^{(n)})_1^{\leqslant 2}$. *We have*

$$(z_{0,1}^{(n)})_1^{\leqslant 2} = (\zeta_{0,1})_1 + \lambda_{02}^2((\varphi_{0,1}^{(n)})_1, \kappa_{1,n}). \tag{B3.8}$$

Proof: From Lemma B3.3, it follows that $(\phi_{0,n+1}^{(n)})_1$ are eigenvectors of $L_{0,1,1}^{\leqslant 2}$ and $K_{0,1,1}^{\leqslant 2}$, associated with eigenvalues which we denote by $(l_0^{(n)})_1^{\leqslant 2}$ and $(k_0^{(n)})_1^{\leqslant 2}$ respectively. Vectors ϕ in $\mathcal{G}_{0,1,1}^{(1)}$ satisfying $(L_{0,1,1}^{\leqslant 2} - zK_{0,1,1}^{\leqslant 2})\phi = 0$ are necessarily these $(\phi_{0,n+1}^{(n)})_1$; the corresponding z-value, for each n, is $((k_{0,1}^{(n)})_1^{\leqslant 2})^{-1}(l_{0,1}^{(n)})_1^{\leqslant 2}$. Through using (B3.4) and (B3.6), we get

$$(k_{0,1}^{(n)})_1^{\leqslant 2} = ((\phi_{0,n+1}^{(n)})_1, K_{0,1,1}^{\leqslant 2}(\phi_{0,n+1}^{(n)})_1) = 1 - \lambda_{02}^2 \|u_{1,n}\|^2,$$

$$(l_{0,1}^{(n)})_1^{\leqslant 2} = (\zeta_{0,1})_1(1 - \lambda_{02}^2\|u_{1,n}\|^2) + \lambda_{02}^2(V(\phi_{0,n+1}^{(n)})_1, u_{1,n}). \tag{B3.9}$$

As a consequence,

$$(l_{0,1}^{(n)})_1^{\leqslant 2} = (\zeta_{0,1})_1(1 - \lambda_{02}^2\|u_{1,n}\|^2) + \lambda_{02}^2((\varphi_{0,1}^{(n)})_1, \kappa_{1,n}). \tag{B3.10}$$

Hence (B3.8) holds since $1 - \|u_{1,n}\|^2$ is to be replaced by 1, to the considered approximation. ■

Lemma B3.5:

(a) Let us set

$$M_1 := \left(\frac{\lambda_{12}^2}{(\zeta_{0,1})_1 - e_2} + \frac{\lambda_{01}^2}{(\zeta_{0,1})_1} \right)^{-1}.$$

For $n \geqslant 0$, *a vector* v *satisfying* $[(\zeta_{0,1})_1 - H_0]v = |2,(\sigma_{0,1}^{(n)})_1\rangle$ *is* $v_{1,n} = |2,\kappa'_{1,n}\rangle + |1,\theta'_{1,n+1}\rangle + |0,h'_{1,n+2}\rangle$ *with*

$$\kappa'_{1,n} = \frac{(\varphi_{0,1}^{(n)})_1}{(\zeta_{0,1})_1 - e_2} + \sqrt{n+1}\lambda_{12}\frac{(f_{12},\theta'_{1,n+1})}{(\zeta_{0,1})_1 - e_2}. \tag{B3.11}$$

$$h'_{1,n+2} = \sqrt{n+2}\lambda_{01}\frac{\theta'_{1,n+1} \vee f_{01}}{(\zeta_{0,1})_1}, \tag{B3.12}$$

$$\theta'_{1,n+1} = N_1\sqrt{n+1}\frac{\lambda_{01}\lambda_{12}}{((\zeta_{0,1})_1 - e_2)(\zeta_{0,1})_1}(s_0(\theta'_{1,n+1})^{(1)} + n(f_{02},g_1)(\theta'_{1,n+1})^{(2)}), \tag{B3.13}$$

where, if $f_{01} \neq f_{12}$,

$$(\theta'_{1,n+1})^{(1)} = \frac{(\zeta_{0,1})_1 - e_2}{\lambda_{12}^2}\frac{1}{1-|s_1|^2}(s_1 f_{01} - f_{12}) \vee g_1^{\vee n}, \tag{B3.14}$$

$$(\theta'_{1,1})^{(2)} = 0, \quad (\theta'_{1,n+1})^{(2)} = \frac{M_1}{2(1-|s_1|^2)}(s_1 f_{01} \vee f_{01} - 2f_{01} \vee f_{12}) + \overline{s_1} f_{12} \vee f_{12}) \vee g_1^{\vee n-1}. \tag{B3.15}$$

If $f_{01} = f_{12}$,

$$(\theta'_{1,n+1})^{(1)} = -M_1 f_{01} \vee g_1^{\vee n}, \tag{B3.16}$$

$$(\theta'_{1,1})^{(2)} = 0, \quad (\theta'_{1,n+1})^{(2)} = -\tfrac{1}{2}M_1 f_{01} \vee f_{01} \vee g_1^{\vee(n-1)}. \tag{B3.17}$$

(b) $u_{1,n}$ *of Lemma* B3.4 *is equal to* $v_{1,n}$

Proof: Relations (B3.11) and (B3.12) are obtained through projecting the equality defining v on $|2\rangle\otimes\mathcal{H}_{\rm rad}$ and $|0\rangle\otimes\mathcal{H}_{\rm rad}$, respectively. The projection on $|1\rangle\otimes\mathcal{H}_{\rm rad}$ implies that $\theta'_{1,n+1}$ satisfies

$$\mathcal{L}_{1,n+1}\theta'_{1,n+1}=\frac{\sqrt{n+1}\lambda_{12}}{(\zeta_{0,1})_1-e_2}(\varphi^{(n)}_{0,1})_1\vee f_{12}, \tag{B3.18}$$

where

$$\mathcal{L}_{1,n+1}\theta'_{1,n+1}:=-\frac{(n+1)\lambda_{12}^2}{(\zeta_{0,1})_1-e_2}f_{12}\vee(f_{12},\theta'_{1,n+1})-\frac{(n+1)\lambda_{0,1}^2}{(\zeta_{0,1})_1}f_{01}\vee(f_{01},\theta'_{1,n+1}). \tag{B3.19}$$

For $n\geqslant 1$, $(\varphi^{(n)}_{0,1})_1$, given by (B3.7) is decomposed into two parts. Hence we introduce two functions $(\theta'_{1,n+1})^{(1)}$ and $(\theta'_{1,n+1})^{(2)}$ satisfying

$$\mathcal{L}_{1,n+1}(\theta'_{1,n+1})^{(1)}=g_1^{\vee n}\vee f_{12}, \tag{B3.20}$$

$$\mathcal{L}_{1,n+1}(\theta'_{1,n+1})^{(2)}=g_1^{\vee(n-1)}\vee f_{01}\vee f_{12}, \tag{B3.21}$$

so that a solution of (B3.18) will be given by (B3.13). To prove (a) if $f_{01}\neq f_{12}$, we check that (B3.14) satisfies (B3.20) and that (B3.15) satisfies (B3.21). We proceed in the same way with (B3.16) and (B3.17), if $f_{01}=f_{12}$, (B3.18) and (B3.19) being still true. Only $(\theta_{1,n+1})^{(1)}$ plays a part if $n=0$.

To prove (b), we note that vectors in $\mathcal{G}_{0,1,1}$ are linear combinations of $|1,g_{i_1}\vee\cdots\vee g_{i_n}\rangle$ and $|0,f_{01}\vee g_{i_1}\vee\cdots\vee g_{i_n}\rangle$. Since (a) implies that $\theta'_{1,n+1}$ is a sum of symmetric products of terms one of which at least is in $\mathcal{H}^{(2)}_{\rm rad}$, we have $(\theta'_{1,n+1},g_{i_1}\vee\cdots\vee g_{i_{n+1}})=0$ and $(h'_{1,n+2},f_{01}\vee g_{i_1}\vee\cdots\vee g_{i_{n+1}})=0$. As a consequence, $|2,\kappa'_{1,n}\rangle$, $|1,\theta'_{1,n+1}\rangle$, and $|0,h'_{1,n+2}\rangle$ are orthogonal to $\mathcal{G}_{0,1,1}$ and $u_{1,n}=Q_0^{0,1,1}v_{1,n}=v_{1,n}$. ■

Lemma B3.6: Take $n\geqslant 0$. *For* $f_{01}\neq f_{12}$,

$$((\varphi^{(n)}_{0,1})_1,\kappa_{1,n})=nN_1^2\frac{\lambda_{01}^4|(f_{02},g_1)|^2}{((\zeta_{0,1})_1)^2(\lambda_{12}^2(\zeta_{0,1})_1+\lambda_{01}^2((\zeta_{0,1})_1-e_2))}. \tag{B3.22}$$

For $f_{01}=f_{12}$,

$$((\varphi^{(n)}_{0,1})_1,\kappa_{1,n})=N_1^2\frac{\lambda_{01}^4}{((\zeta_{0,1})_1)^2(\lambda_{12}^2(\zeta_{0,1})_1+\lambda_{01}^2((\zeta_{0,1})_1-e_2))}(n|(f_{02},g_1)|^2+|s_0|^2). \tag{B3.22$'$}$$

Proof: Use (B3.7) and Lemma (B3.5). ■

Formulas (4.14) and (4.15) then follow from (B3.10) and (B3.22). In the same way, (4.16) follows from (B3.22′).

(ii) All that has been written up to now can be transposed from $(\zeta_{0,1})_1$ to $\zeta_{1,1}$, with the following changes

$$P_0^{0,1,1}\to P_0^{1,1},\quad P^{0,1,1}\to P^{1,1},\quad Q_0^{0,1,1}\to Q_0^{1,1},\quad \tilde{Q}_0^{0,1,1}\to\tilde{Q}_0^{1,1},\quad \mathcal{H}_{0,1,1}\to\mathcal{H}_{1,1},$$

$$(\phi^{(n)}_{0,n+1})_1\to\phi^{(n)}_{1,n+1},\quad \mathcal{G}_{0,1,1}\to\mathcal{G}_{1,1},\quad \mathcal{G}^{(1)}_{0,1,1}\to\mathcal{G}^{(1)}_{1,1},\quad (\varphi^{(n)}_{0,1})_1\to\varphi^{(n)}_{1,1},$$

$$(k^{(n)}_{0,1})_1\to k^{(n)}_{1,1},\quad (l^{(n)}_{0,1})_1\to l^{(n)}_{1,1},\quad (z^{(n)}_{0,1})_1^{\leqslant 2}\to(z^{(n)}_{1,1})^{\leqslant 2}.$$

N_1, M_1, $(\varphi^{(n)}_{0,1})_1$ are thus also changed, as well as $\mathcal{L}_{1,n+1}$ and the solutions $\theta_{1,n+1}$ $h_{1,n+2}$ and $\kappa_{1,n}$.

One then get (ii) of Proposition 4.4.

(iii) Let us come on now to the splitting of $(\zeta_{0,1})_2$, an eigenvalue which is zero and exists only if $f_{01}\neq f_{12}$. The issue is more complicated due to the fact that the unperturbed eigenspace of

interest is no longer just spanned by the $\Pi(1\otimes c^*(g_1))^n(\phi^{(0)}_{0,1})_2$. It is spanned by the $|0,\Pi(c^*(g_i))^{n_i}\Omega\rangle$, with $i=0$ or 1. Let us denote this space by $\mathcal{G}$. Let $P_0^{0,1,2}$ be the projector on $\mathcal{G}$. With $K^{\leqslant 2}_{0,1,2}$ and $L^{\leqslant 2}_{0,1,2}$ defined as in (B3.4) and (B3.5), we can see that $L^{\leqslant 2}_{0,1,2}$ has nonvanishing matrix elements between say $g_0^{\vee p}\vee g_1^{\vee(p+2)}$ and $g_0^{\vee(p+1)}\vee g_1^{\vee(p+1)}$, or between $g_0^{\vee(p+1)}\vee g_1^{\vee(p+1)}$ and $g_0^{\vee(p+2)}\vee g_1^{\vee(p)}$ or also between $g_0^{\vee(p+2)}\vee g_1^{\vee(p)}$ and $g_0^{\vee(p+3)}\vee g_1^{\vee(p-1)}$. This makes the computation of the z's satisfying $\det(L^{\leqslant 2}_{0,1,2}-zK^{\leqslant 2}_{0,1,2})=0$ more intricate and we don't calculate them here.

This completes the proof of Proposition 4.4. ■

Eigenvectors $(\chi^{(n)}_{0,1})^{(2)}_1$, $(\chi^{(n)}_{1,1})^{(2)}$ are obtained from the correspondences $\mathcal{G}_{0,1,1}\to\mathcal{H}_{0,1,1}$, and $\mathcal{G}_{1,1}\to\mathcal{H}_{1,1}$, through the second order expansion of operators $P^{0,1,1}(\lambda_{02})$ and $P^{1,1}(\lambda_{02})$ which perform these correspondences. For example, we get (see Ref. 24, p. 614)

$$(\chi^{(n)}_{0,1})^{(2)}_1=(\phi^{(n)}_{0,n+1})_1+\lambda_{02}^2(-P_0^{0,1,1}V(\tilde{Q}_0^{0,1,1})^2V+\tilde{Q}_0^{0,1,1}V\tilde{Q}_0^{0,1,1}V)(\phi^{(n)}_{0,n+1})_1.$$

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Principal bundle structure of quantum adiabatic dynamics with a Berry phase which does not commute with the dynamical phase

David Viennot[a)]
Observatoire de Besançon (CNRS UMR 6091), 41 bis Avenue de l'Observatoire, BP1615, 25010 Besançon cedex, France

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A geometric model is proposed to describe the Berry phase phenomenon when the geometric phase does not commute with the dynamical phase. The structure used is a principal composite bundle in which the adiabatic transport appears as a horizontal lift. The formulation is applied to a simple quantum dynamical system controlled by two lasers. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Principal bundle theory is a classic tool of modern theoretical physics. The notation (P,M,G,π) will be used throughout this paper to designate a principal bundle on the right-hand side with base space M, total space P, structure group G, and projection π. First we quote an important result of principal bundle theory. Suppose that P is endowed with a connection described by the gauge potential A^σ associated to the local section $\sigma \in \Gamma(M,P)$. Let $\mathcal{C}$ be a curve in M, parametrized by the function $[0,1] \ni t \mapsto \gamma(t) \in M$. Then the horizontal lift of $\mathcal{C}$ at the point $\sigma(\gamma(0))$ is given by

$$P \ni p(t) = \sigma(\gamma(t))\mathbb{P}e^{-\int_0^t A^\sigma(\gamma(t))}, \tag{1}$$

where $\mathbb{P}$ is the path-ordering operator and $\mathbb{P}e^{-\int_0^t A^\sigma(\gamma(t))} \in G$ acts on P by the group canonical right action.

In 1984, Berry[1] proved, in the context of the standard adiabatic approximation, that the wave function of a quantum dynamical system takes the form

$$\psi(t) = e^{-\imath\hbar^{-1}\int_0^t E_a(\vec{R}(t'))\mathrm{d}t' - \int_0^t \langle a,\vec{R}(t')|\partial_{t'}|a,\vec{R}(t')\rangle \mathrm{d}t'}|a,\vec{R}(t)\rangle, \tag{2}$$

where E_a is a nondegenerate instantaneous eigenvalue isolated from the rest of the Hamiltonian spectrum with instantaneous eigenvector $|a,\vec{R}(t)\rangle$ and $\vec{R}$ is a set of classical control parameters used to model the time-dependent environment of the system. The set of all configurations of $\vec{R}$ is supposed to form a $\mathcal{C}^\infty$-manifold $\mathcal{M}$. The important result is the presence of the extra phase term, called the Berry phase $e^{-\int_0^t \langle a,\vec{R}(t')|\partial_{t'}|a,\vec{R}(t')\rangle \mathrm{d}t'}$. Simon[2] later found the mathematical structure which models the Berry phase phenomenon, namely a principal bundle with base space $\mathcal{M}$ and with structure group U(1). If we eliminate the dynamical phase by a gauge transformation which involves redefining the eigenvector at each time, then the expression (2) is the horizontal lift of the curve $\mathcal{C}$ described by $t \mapsto \vec{R}(t)$ with the gauge potential $A = \langle a,\vec{R}|\mathrm{d}_{\mathcal{M}}|a,\vec{R}\rangle$. If $\mathcal{C}$ is closed then the Berry phase $e^{-\oint_{\mathcal{C}} A} \in \mathrm{U}(1)$ is the holonomy of the horizontal lift.

In 1987, Aharonov and Anandan[3] proved that geometric phases such as the Berry phase are not solely attached to the adiabatic approximation but appear in a more general context. Let

[a)]Electronic mail: viennot@obs-besancon.fr

$t \mapsto \psi(t)$ be a wave function such that $\psi(T)=e^{\imath\phi}\psi(0)$ and $H(t)$ be the Hamiltonian of the system. Suppose that the Hilbert space is n-dimensional (the case $n=+\infty$ is not excluded); then the wave function defines a closed curve $\mathcal{C}$ in the complex projective space $\mathbb{C}P^{n-1}$. If one redefines the wave function such that $\tilde{\psi}(T)=\tilde{\psi}(0)$ then

$$\psi(t) = e^{-\imath\hbar^{-1}\int_0^t \langle\tilde{\psi}(t')|H(t')|\tilde{\psi}(t')\rangle \mathrm{d}t' - \int_0^t \langle\tilde{\psi}(t')|\partial_{t'}|\tilde{\psi}(t')\rangle \mathrm{d}t'} \tilde{\psi}(t). \tag{3}$$

The extra phase in addition to the dynamical phase is called the Aharonov-Anandan phase (or nonadiabatic Berry phase). We can eliminate the dynamical phase by a gauge transformation; then the Aharonov-Anandan phase appears as the horizontal lift of $\mathcal{C}$ in the principal bundle with base space $\mathbb{C}P^{n-1}$, the structure group U(1) and with the $(2n-1)$-dimensional sphere S^{2n-1} as total space. The Berry-Simon model and the Aharonov-Anandan model are related by the universal classifying theorem of principal bundles;[4,5] more precisely, the Aharonov-Anandan principal bundle is a universal bundle for the Berry-Simon principal bundle.

The two geometric phases described above are called Abelian because they are related to the Abelian group U(1). In 1984, Wilczek and Zee[6] produced a non-Abelian Berry phase phenomenom in the context of the adiabatic approximation. Let $E_a(\vec{R}(t))$ be an M-fold degenerate instantaneous eigenvalue isolated from the rest of the spectrum and $\{|a,i,\vec{R}(t)\rangle\}_{i=1,\ldots,M}$ be an orthonormal basis for the associated eigensubspace. Suppose that the initial state is $\psi(0)=|a,i,\vec{R}(0)\rangle$; then the wave function is

$$\psi(t) = \sum_{j=1}^{M} e^{-\imath\hbar^{-1}\int_0^t E_a(\vec{R}(t'))\mathrm{d}t'} \left[\mathbb{T} e^{-\int_0^t A(\vec{R}(t'))}\right]_{ji} |a,j,\vec{R}(t)\rangle, \tag{4}$$

where the matricial 1-form A has the elements $A_{ij}=\langle a,i,\vec{R}|\mathrm{d}_{\mathcal{M}}|a,j,\vec{R}\rangle$ and $\mathbb{T}$ is the time-ordering operator. By elimination of the dynamical phase, this expression becomes a horizontal lift of the curve $\mathcal{C}$ described by $t \mapsto \vec{R}(t)$ into a principal bundle with base space $\mathcal{M}$ and structure group U(M). If $\mathcal{C}$ is closed then $\mathbb{P}e^{-\oint_{\mathcal{C}} A(\vec{R})} \in U(M)$ is the holonomy of the horizontal lift.

In 1994, Bohm and Mostafazadeh[7] constructed a non-Abelian Aharonov-Anandan phase as the universal bundle of the preceding one. Let $P(t)$ be an M-fold degenerate projector such that $P(T)=P(0)$. $t \mapsto P(t)$ defines a closed curve $\mathcal{C}$ in the Grassmanian manifold $G_M(\mathbb{C}^n)$. If one chooses a local section of the bundle $[V_M(\mathbb{C}^n), G_M(\mathbb{C}^n), \mathrm{U}(M), \pi_{V_M(\mathbb{C}^n)}]$ [where $V_M(\mathbb{C}^n)$ is the Stiefel manifold] $s(P)=\{\phi_1(P),\ldots,\phi_M(P)\}$, then the evolution of the wave function for which $\psi(0)=\phi_i(0)$ is given by

$$\psi(t) = \sum_{j,k=1}^{M} \left[\mathbb{T} e^{-\imath\hbar^{-1}\int_0^t E(t')\mathrm{d}t'}\right]_{jk} \left[\mathbb{T} e^{-\int_0^t A(t')}\right]_{ki} \phi_j(t), \tag{5}$$

where $A_{ij}=\langle\phi_i|\mathrm{d}_{G_M(\mathbb{C}^n)}|\phi_j\rangle$, $E_{ij}(t)=\langle\phi_i(t)|H(t)|\phi_j(t)\rangle$, and where we suppose that $\forall t$ $\left[\int_0^t E(t')\mathrm{d}t', \int_0^t A(t')\right]=0$. By eliminating the dynamical phase, we obtain a horizontal lift in the universal bundle.

The gauge potentials defined in the four previous cases have the particular form $A=U^{\dagger}\mathrm{d}U$ where U is a $M\times n$ matrix († denotes the transconjugation). A connection with such a gauge potential is called a Stiefel connection. It is in fact the form of the universal connection in the universal bundle, a form which is unique, since Narasimhan and Ramaman[8] proved that all universal connections can be written in this form. Then the above four examples of geometric phase each have an explicit Stiefel structure.

In the previous example, the dynamical phase commutes with the geometric phase, but this is not the case in general. More usually we have $\mathbb{T}e^{-\imath\hbar^{-1}\int_0^t E(t')\mathrm{d}t' - \int_0^t A(t')} \neq \mathbb{T}e^{-\imath\hbar^{-1}\int_0^t E(t')\mathrm{d}t'} \mathbb{T}e^{-\int_0^t A(t')}$ and it is then impossible to eliminate the dynamical phase and to obtain a simple geometric structure which reduces the phenomenom to a horizontal lift in a principal bundle.

Sardanashvily introduced[9,10] a model based on a vector composite bundle, so as to obtain a geometric structure which can describe both the dynamical and the geometric phases when they do not commute. His formulation defines the covariant derivative

$$\nabla_h \psi = (\partial_t + \mathcal{A}_\mu(h(t),t)(\partial_t h^\mu(t)) + \imath\hbar^{-1}\mathcal{H}(h(t),t))\psi, \tag{6}$$

where h is a map from $\mathbb{R}$ to $\mathcal{M}$ (the manifold of classical parameters), and $\mathcal{A}$ and $\mathcal{H}$ are bounded operators. This leads to the result that if a section ψ is an integral section of the connection (i.e., $\nabla_h \psi = 0$) then

$$\psi(t) = \mathbb{T} e^{-\int_0^t (\mathcal{A}_\mu \partial_{t'} h^\mu + \imath\hbar^{-1}\mathcal{H}) \mathrm{d}t'} \psi(0). \tag{7}$$

Sardanashvily finally claims that if one can think of the equation $\nabla_h \psi = 0$ as being the Schrödinger equation of a quantum system depending on the parameter $h(t)$, then $\mathcal{A}$ generates the Berry phase and $\mathcal{H}$ generates the dynamical phase. We now explain why we are not in agreement with this claim. First his whole analysis is made in the framework of a vector bundle. This is basically not incorrect; however the Berry phase is usually described in the framework of a principal bundle and its associated vector bundle, giving a principal structure which is more rich. Also, the definition of the covariant derivative used by Saradanashvily is only indirectly justified by noting that it gives a correct final result. More precisely, Sardanashvily does not explicitly define $\mathcal{A}$ and $\mathcal{H}$, whereas the adiabatic potential and the dynamical phase have well-defined matricial expressions. Finally, Eq. (7) is not the expression of a dynamical phase added to a geometric phase, because the expression of Sardanashvily is of the form $\psi(t) = U_{\mathrm{Sar}}(t)\psi(\mathbf{0})$, whereas the expression of a parallel transport with geometric phase is of the form $\psi(t) = U_{\mathrm{phase}}(t)\tilde{\psi}(\mathbf{t})$ where $\tilde{\psi}(\mathbf{t})$ is a known function or a known basis set dependent on the time (in the case of the Berry phase it is the instantaneous eigenvector basis set). This known function (or basis set) defines the local section used to describe the horizontal lift. Then U_{Sar} is not a non-Abelian phase but is the evolution operator. Consequently we have $\imath\hbar\mathcal{A}_\mu \partial_t h^\mu + H = H$, where H is the Hamiltonian of the system, which is split into two parts $\mathcal{A}$ and $\mathcal{H}$. Since Sardanashvily does not define $\mathcal{A}$, this spliting is totally arbitrary. Moreover, if A is the generator of the Berry phase and E is the generator of the dynamical phase, we have $\imath\hbar A + E \neq H$. Thus the affirmation of Sardanashvily in Ref. 9, namely "$\mathcal{A}$ is responsible for the Berry phase phenomenon" appears to be unjustified.

In this paper we construct a geometric structure to give a correct description of the transport when the Berry phase does not commute with the dynamical phase. We apply Sardanashvily's idea of using a composite bundle, but we take a principal structure in place of the vector structure. We thus construct a connection consistent with the geometric model of the adiabatic transport and with the bundle formulation of nonrelativistic quantum dynamics. Our approach reveals that the noncommutativity of A and E introduces a modified gauge structure. Similar modifications of the gauge have been used by Attal in Ref. 11 in a treatment of the non-Abelian gerbes connection. (We note that in the literature of fiber bundle theory the words "gerbe" and "sheaf" are used by various authors to name the same mathematical entity.) He introduced a gauge theory with generalized Cartan structure equations $F = \mathrm{d}A + \frac{1}{2}[A,A] + B$ and $G = \mathrm{d}B + [A,B]$, and a Bianchi identity $\mathrm{d}G + [A,G] = [F,B]$ where A is a 1-form, B and F are 2-forms, and G is a 3-form. In the same way, Larsson,[12] in his treatment of the Yang-Baxter equation with non-Abelian gerbes, found a gauge theory with the usual Cartan equation and the usual Bianchi identity, but limited by restrictions concerning the possible gauge transformations. It should be stressed that the modified gauge theory induced by the noncommutativity of A and E in our approach is similar to the modified gauge theories of Attal and Larsson which are induced by noncommutativity in the gerbes.

This paper is organized as follows. Section II introduces the generalized adiabatic theorem with a Berry phase which does not commute with the dynamical phase. Section III is devoted to some remarks about the principal composite bundles constituting the fundamental structure of our model. Section IV presents the geometric model used for the description of quantum adiabatic dynamics. Finally, Sec. V presents an application to a simple quantum dynamical system. Different quantum dynamical aspects of this system are presented in our geometric representation.

A note about some of the notation used here: the symbol "≃" between two manifolds denotes that the two manifolds are diffeomorphic, the symbol "↪" denotes an inclusion between two sets and "$\Omega^n M$" denotes the set of the n-differential forms of the manifold M.

II. GENERALIZED ADIABATIC TRANSPORT

Theorem 1: *Let $U(t,0)$ be an evolution operator of a quantum dynamical system governed by the self-adjoint Hamiltonian $H(t)$. Let $\{E_a(t)\}_a$ and $\{|a,t\rangle\}_a$ be the instantaneous eigenvalues and eigenvectors of $H(t)$. We suppose that there exists a set of indices I such that the projector $P_m(t)=\Sigma_{a\in I}|a,t\rangle\langle a,t|$ satisfies the adiabatic condition*

$$\mathrm{U}(t,0)P_m(0) = P_m(t)\mathrm{U}(t,0) \tag{8}$$

(to satisfy this assumption, see for example, Nenciu's adiabatic theorem[13]). If at $t=0$ the wave function is $\psi(0)=|a,0\rangle$ (with $a\in I$) then at time t we have

$$\psi(t) = \sum_{b\in I} U_{ba}(t)|b,t\rangle \tag{9}$$

with the matrix

$$U(t) = \mathbb{T}e^{-\imath\hbar^{-1}\int_0^t E(t')\mathrm{d}t' - \int_0^t A(t')}. \tag{10}$$

Here $A_{ab}(t)=\langle a,t|\partial_t|b,t\rangle \mathrm{d}t$ and we also have $\forall a,b\in I\ E_{ab}(t)=E_a(t)\delta_{a,b}$.

Proof: The condition (8) states that the evolution is inside Ran P_m so that for all t the wave function can be expanded on the basis set $(|a,t\rangle)_{a\in I}$. This justifies the use of Eq. (9), in which U is a unitary matrix (the unitarity of U results from the normalization of the wave function). The use of Eq. (9) in the Schrödinger equation leads to the result

$$\sum_b \imath\hbar\dot{U}_{ba}(t)|b,t\rangle + \sum_b \imath\hbar U_{ba}(t)\partial_t|b,t\rangle = \sum_b U_{ba}(t)E_b(t)|b,t\rangle. \tag{11}$$

By projecting this expression on $\langle c,t|$ we obtain

$$\imath\hbar\dot{U}_{ca} + \sum_b \imath\hbar U_{ba}\langle c,t|\partial_t|b,t\rangle = U_{ca}E_c \tag{12}$$

which leads to the result

$$(\dot{U}U^{-1})_{cd} = \sum_a \dot{U}_{ca}U^{-1}_{ad} \tag{13}$$

$$= -\sum_a \imath\hbar^{-1}E_c U_{ca}U^{-1}_{ad} - \sum_{a,b}\langle c,t|\partial_t|b,t\rangle U_{ba}U^{-1}_{ad} \tag{14}$$

$$= -\imath\hbar^{-1}E_c(UU^{-1})_{cd} - \sum_b \langle c,t|\partial_t|b,t\rangle (UU^{-1})_{bd} \tag{15}$$

$$= -\imath\hbar^{-1}E_c\delta_{cd} - \langle c,t|\partial_t|d,t\rangle. \tag{16}$$

■

This expression manifestly displays a matrix dynamical phase and a matrix geometric phase, in other words a non-Abelian dynamical phase and a non-Abelian geometric phase. In general $[E,A]\neq 0$. If the Hamiltonian is time-dependent with respect to some classical control parameters $\vec{R}$ which describe a $\mathcal{C}^\infty$-differentiable manifold $\mathcal{M}$, then we can rewrite the non-Abelian phase (10). For a dynamics $H(\vec{R}(t))$ described by a path $\mathcal{C}$ in $\mathcal{M}$ we can set

$$U(\mathcal{C}) = \mathbb{T}e^{-\imath\hbar^{-1}\int_0^t E(\vec{R}(t'))\mathrm{d}t' - \oint_{\mathcal{C}} A(\vec{R})} \tag{17}$$

with $A(\vec{R})_{ab} = \langle a, \vec{R} | \mathrm{d}_{\mathcal{M}} | b, \vec{R} \rangle$, where $d_{\mathcal{M}}$ is the exterior differential of $\mathcal{M}$.

III. PRINCIPAL COMPOSITE BUNDLES

A. Definition of a composite bundle

A composite bundle is defined by five kinds of data, three manifolds (P^+, S, and R) and two surjective maps $\pi_+ : P^+ \to S$ and $\pi_S : S \to R$. We denote the composite bundle by $P^+ \to S \to R$. We assert that a composite bundle is a principal composite bundle if $S \to R$ is a locally trivial fiber bundle with as typical fiber a manifold $M : (S, R, M, \pi_S)$, and if $P^+ \to S$ is a principal bundle with as structure group a Lie group $G : (P^+, S, G, \pi_+)$. $\forall y \in R$, we have $\pi_S^{-1}(y) \simeq M$ and we denote by χ_y^S the associated fiber diffeomorphism. We suppose that S has a structure of a cell complex; then $\pi_S^{-1}(y)$ and M are cell complexes. The theorem of universal classification of principal bundles (see Refs. 4 and 5) is used to define the universal bundle (U, B, G, π_U) where B is the classifying space of M, ϱ_U the universal map from M to B, and $\varrho_U \circ \chi_y^S$ the universal map from $\pi_S^{-1}(y)$ to B. We finally define the principal bundle (P, M, G, π_P) such that the following diagram commutes:

$$\begin{array}{ccccccc}
P^+ & \xleftarrow{\ \hookrightarrow\ } & \chi_y^{S*}P & \xleftarrow{\chi_y^{S*}} & P & \xleftarrow{\varrho_U^*} & U \\
\downarrow{\scriptstyle \pi_+} & & \downarrow{\scriptstyle \pi_{P_y}} & & \downarrow{\scriptstyle \pi_P} & & \downarrow{\scriptstyle \pi_U} \\
S & \xleftarrow{\ \hookrightarrow\ } & \pi_S^{-1}(y) & \xrightarrow{\chi_y^S} & M & \xrightarrow{\varrho_U} & B
\end{array}$$

where $P = \varrho_U^* U$ and $\chi_y^{S^*} P = (\varrho_U \circ \chi_y^S)^* U$. We know that U is independent of $\chi_y^{S^*} P$ and thus independent of y. Moreover, since χ_y^S is a diffeomorphism then $\chi_y^{S^*}$ is a principal bundle isomorphism, so that $\chi_y^{S^*} P = \pi_+^{-1}(\pi_S^{-1}(y))$ and $\pi_{P_y} = \pi_{+1\chi_y^{S^*}P}$. Let U^i be an open local chart on M. We consider the local trivialization of (P, M, G, π_P) over U^i, $\phi_P^i : U^i \times G \to \pi_P^{-1}(U^i)$; then the local trivialization of $(\chi_y^{S^*} P, \pi_S^{-1}(y), G, \pi_{P_y})$ is $\phi_P^i[y] = \chi_y^{S^*} \phi_P^i : \chi_y^{S^{-1}}(U^i) \times G \to \pi_+^{-1}(\chi_y^{S^{-1}}(U^i))$. Let V^j be an open local chart of R, ϕ_S^j be the local trivialization of (S, R, M, π_S) over V^j, and ϕ_+^j be the local trivialization of (P^+, S, G, π_+) over $\pi_S^{-1}(V^j)$. It is clear that the local trivializations are related by

$$\phi_+^j : \begin{array}{l} \pi_S^{-1}(V^j) \times G \to \pi_+^{-1}(\pi_S^{-1}(V^j)) \\ (s, g) \mapsto \phi_P^i[\mathrm{Pr}_1\, \phi_S^{j-1}(s)](\mathrm{Pr}_2\, \phi_S^{j-1}(s), g), \end{array}$$

where we have supposed that $\mathrm{Pr}_2\, \phi_S^{j^{-1}}(s) \in U^i$. Pr_1 and Pr_2 are the canonical projections of $R \times M$ over R and M. We call (P, M, G, π_P) the structure bundle of the composite bundle.

Finally one can define a principal bundle related to the principal composite bundle. Consider the map

$$\phi_{++}^{ij} : \begin{array}{l} U^i \times V^j \times G \to P^+ \\ (x, y, g) \mapsto \phi_+^j(\phi_S^j(y, x), g) = \phi_P^i[y](x, g). \end{array}$$

This map is a local trivialization of a principal bundle $(P^+, M \times R, G, \pi_{++})$ with $\pi_{++} = \phi_S^{-1} \circ \pi_+$. It is called the total bundle of the principal composite bundle.

Let $x \in U^i$ be a fixed point of M. Define the map

$$\phi_Q^j[x] : \begin{array}{l} V^j \times G \to P^+ \\ (y, g) \mapsto \phi_{++}^{ij}(x, y, g). \end{array}$$

If we consider this map as a local trivialization, it defines a principal bundle (Q_x, R, G, π_{G_x}) with $\pi_{Q_x} = \mathrm{Pr}_1 \circ \phi_Q^j[x]^{-1}$. We call it the transversal bundle of the principal composite bundle. The situation is schematically summarized in Fig. 1.

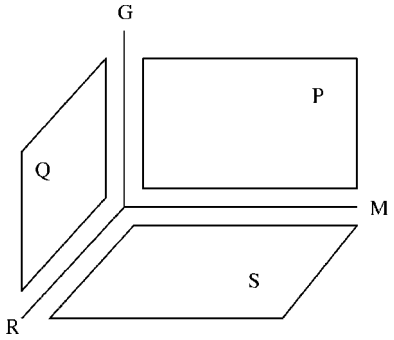

FIG. 1. Scheme of a composite bundle. P^+ is the three-dimensional space delimited by the three planes.

B. Connection on a principal composite bundle

Consider a principal composite bundle $P^+ \to S \to R$. (P^+, S, G, π_+) and $(P^+, M\times R, G, \pi_{++})$ have the structures of principal bundles. We can then define a common connection for these bundles. Let $\omega \in \Omega^1(P^+, \mathfrak{g})$ be the connection 1-form ($\mathfrak{g}$ denotes the Lie algebra of the group G). Let $\sigma^{ij}_{M\times R} \in \Gamma(U^i \times V^i, P^+)$ be a local section of the principal bundle $(P^+, M\times R, G, \pi_{++})$. The gauge potential of this bundle is by definition $A^{ij}_{M\times R} = \omega \circ \sigma^{ij}_{M\times R_*} \in \Omega^1(M\times R, \mathfrak{g})$. Let $\sigma^j_S \in \Gamma(\pi^{-1}(V^j), P^+)$ be a local section of the bundle (P^+, S, G, π_+). In order to simplify the passage from one bundle to another one, the two sections are chosen to be compatible, i.e., $\forall s \in \pi_S^{-1}(V^j)$, $\sigma^j_S(s) = \sigma^{ij}_{M\times R}(\phi^{j^{-1}}_S(s))$ [we suppose that $\mathrm{Pr}_1\, \phi^{j^{-1}}_S(s) \in U^i$], and $\forall (x,y) \in U^i \times V^j$, $\sigma^{ij}_{M\times R}(x,y) = \sigma^j_S(\phi^j_S(x,y))$. Using these relations the gauge potential of the bundle (P^+, S, G, π_+) is $A^j_S = \sigma^{j^*}_{S_*}\omega = \phi^{j^{-1}*}_S\, \sigma^{ij}_{M\times R}{}^*\omega = \phi^{j^{-1}*}_S A^{ij}_{M\times R} \in \Omega^1(S, \mathfrak{g})$.

$\chi^S_y : P \to \pi_+^{-1}(\pi_S^{-1}(y))$ is a diffeomorphism, then [remark about the notation: the first star $\chi^{S^*}_y$ denotes the map induced by χ^S_y in the principal bundles over $\pi_S^{-1}(y)$ and M, the second star $\chi^{S^{**}}_y$ denotes the map induced by $\chi^{S^*}_y$ in the cotangent bundles of P and $\chi^{S^*}_y P$] $\chi^{S^{**}}_y : \Omega^*(\pi_+^{-1}(\pi_S^{-1}(y))) \to \Omega^* P$. Let $i_y : \pi_+^{-1}(\pi_S^{-1}(y)) \hookrightarrow P^+$ be the canonical injection. We define a family of connections of (P, M, G, π_P) by $\omega_y = \chi^{S^{**}}_y\, i^*_y \omega \in \Omega^1(P, \mathfrak{g})$, for $y \in R$. Let $\sigma^i_M \in \Gamma(U^i, P)$ be a local section which is supposed to be compatible with the section of P^+: $\forall x \in M$, $\sigma^i_M(x) = \chi^{S^{*-1}}_y \sigma^{ij}_{M\times R}(x,y)$ (this section depends on y). The gauge potential is $A^i_y(x) = \sigma^i_M{}^*\omega_y = \sigma^{ij}_{M\times R}{}^* \chi^{S^{*-1}}_y\, \chi^{S^{**}}_y\, i^*_y \omega = j^*_y A^{ij}_{M\times R}(x,y) \in \Omega^1(M, \mathfrak{g})$, where $j_y : \begin{smallmatrix} M \to M\times R \\ x \mapsto (x,y) \end{smallmatrix}$.

Finally, let $i_x : \pi_{++}^{-1}(x,R) \hookrightarrow P^+$ be the canonical injection. $\omega_x = i^*_x \omega$ is a connection of the transversal bundle (Q_x, R, G, π_{Q_x}). Let $j_x : \begin{smallmatrix} R \to M\times R \\ y \mapsto (x,y) \end{smallmatrix}$, so that $A_x = j^*_x A_{M\times R} \in \Omega^1(R, \mathfrak{g})$ is the gauge potential of this bundle.

C. Horizontal lift in a principal composite bundle

In the theory of principal bundles, the notion of a horizontal lift of a curve of the base space is fundamental. In a principal composite bundle $P^+ \to S \to R$, there exists a natural generalization of this notion, but the horizontal lift concerns a section of the base bundle (S, R, M, π_S). Let $h \in \Gamma(\ell_R, S)$ be a section, where ℓ_R is a curve in R. h defines a curve $\mathcal{C}$ in $M\times R$ parametrized by $y \in R$ with the function $\phi^{j^{-1}}_S(h(y))$ (to simplify the discussion we suppose that $\ell_R \subset V^j$). Let $i_h : h(\ell_R) \hookrightarrow S$ be the canonical injection. We consider the local section $\sigma^h \in \Gamma(\mathcal{C}, P^+)$ of the bundle $(P^+, M\times R, G, \pi_{++})$ defined by $\sigma^h = \sigma^j_S \circ \phi^j_S$, $\forall y \in R$, $\sigma^h(\phi^{j^{-1}}_S(h(y))) = \sigma^j_S(h(y))$. Then the horizontal lift of h is defined as the usual horizontal lift of $\mathcal{C}$ in the total bundle of the composite bundle,

$$g_h = \mathbb{P} e^{-\int_{\mathcal{C}} A^{\sigma^h}_{M\times R}} = \mathbb{P} e^{-\int_{h(\ell_R)} i_h^* A^j_S} = \mathbb{P} e^{-\int_{\ell_R} h^* A^j_S} \tag{18}$$

IV. GEOMETRIC STRUCTURES OF GENERALIZED ADIABATIC TRANSPORT

Consider again the generalized adiabatic transport characterized by the non-Abelian phase (17) in the framework of our quantum mechanical study. The quantum dynamical system is described by a self-adjoint Hamiltonian $t \mapsto H(\vec{R}(t),t)$ in a separable Hilbert space $\mathcal{H}$ where $\vec{R}$ is a set of classical parameters which evolve adiabatically with respect to the quantum proper time. These parameters form a $\mathcal{C}^\infty$-differential manifold $\mathcal{M}$. $t \mapsto \vec{R}(t)$ represents a particular dynamics described by a curve $\mathcal{C}$ in $\mathcal{M}$. To have a more general description, we assume that the dynamics possesses a part which changes rapidly and which cannot be modeled by a classical parameter. The Hamiltonian then has an explicit dependence on t besides having the adiabatic parameters $\vec{R}(t)$.

To control the physical processes it is necessary to model numerous different dynamics, without fixing any particular path in the classical parameter manifold and without fixing the duration of the evolution. Hence we must consider the generic Hamiltonian

$$H: \begin{array}{c} \mathcal{M} \times \mathbb{R} \to \mathcal{L}(\mathcal{H}) \\ (\vec{R},t) \mapsto H(\vec{R},t) \end{array} \tag{19}$$

To study this dynamical system, we should separate the dynamical and the geometric contributions to the dynamics. To do this we fix $t \in \mathbb{R}$ in a first step and obtain a purely adiabatic (geometric) evolution $\vec{R} \mapsto H(\vec{R},t)$. Next we fix $\vec{R} \in \mathcal{M}$ and obtain a purely quantum dynamical evolution $t \mapsto H(\vec{R},t)$. These two steps are analyzed successively in the next sections A and B.

A. The fiber bundle of the geometry

Let $t_0 \in \mathbb{R}$ be fixed. $\vec{R} \mapsto H(\vec{R},t_0)$ is the Hamiltonian of an adiabatic system. We suppose that $\{E_a(\vec{R},t_0)\}_{a \in I}$ are M point eigenvalues of $H(\vec{R},t_0)$ which form a group which is isolated from the rest of the H spectrum, and we denote by $\{|a,\vec{R},t_0\rangle\}_{a \in I}$ the corresponding eigenvectors [the case of a globally degenerate eigenvalue is not excluded, but in this case $\exists a,b \in I$ such that $\forall \vec{R} E_a(\vec{R},t_0) = E_b(\vec{R},t_0)$ where $(|a,\vec{R},t_0\rangle, |b,\vec{R},t_0\rangle)$ is an orthonormal basis of the eigensubspace]. The case of an isolated degeneracy (an eigenvalue crossing) for which $\exists \vec{R}$ such that $E_a(\vec{R},t_0) = E_b(\vec{R},t_0)$ can also be included. The works of Berry,[1] Simon,[2] Wilczek and Zee[6] assert that the adiabatic evolution is described mathematically by using a principal bundle $(P,\mathcal{M},U(M),\pi_P)$ where the connection is represented by the gauge potential $A \in \Omega^1(\mathcal{M},\mathfrak{u}(M))$,

$$A_{ab}(\vec{R},t_0) = \langle a,\vec{R},t_0|\mathrm{d}_{\mathcal{M}}|b,\vec{R},t_0\rangle. \tag{20}$$

Here $\mathrm{d}_{\mathcal{M}}$ is the exterior differential of $\mathcal{M}$. This expression is associated with the section of the associated vector bundle $\vec{R} \mapsto (|a,\vec{R},t_0\rangle)_{a \in I}$.

By introducing the eigenvector-matrix $T(\vec{R},t_0) \in \mathcal{M}_{\dim \mathcal{H} \times M}(\mathbb{C})$, we can write $A = T^\dagger \mathrm{d}T$, giving a Stiefel connection in agreement with the Narasimhan-Ramaman theorem (see Refs. 14 and 8). It is evident that after a change of section $(\forall a\ |a,\vec{R},t_0\rangle \rightsquigarrow g(\vec{R})|a,\vec{R},t_0\rangle$ with $g(\vec{R}) \in U(M))$ the gauge potential satisfies the usual relation

$$\tilde{A}(\vec{R},t_0) = g(\vec{R})^{-1} A(\vec{R},t_0) g(\vec{R}) + g(\vec{R})^{-1} \mathrm{d}_{\mathcal{M}} g(\vec{R}). \tag{21}$$

Note that a family of connections $\{A(\vec{R},t) \in \Omega^1(\mathcal{M},\mathfrak{u}(M))\}_{t \in \mathbb{R}}$ is generated if t is continuously modified. If $\mathcal{C}$ is a closed curve in $\mathcal{M}$, then its horizontal lift is characterized by a Wilson loop,

$$W(\mathcal{C},t_0) = \mathbb{P} e^{-\oint_{\mathcal{C}} A_\mu(\vec{R},t_0)\mathrm{d}R^\mu}. \tag{22}$$

If the adiabatic bundle is not trivial then $W(\mathcal{C},t_0) \neq 1$ is the holonomy of the horizontal lift which is called the Berry phase.

B. The fiber bundle of the dynamics

Consider now a fixed point $\vec{R}_0 \in \mathcal{M}$. $t \mapsto H(\vec{R}_0, t)$ is the Hamiltonian describing the quantum dynamics in a static environment which is characterized by the fixed parameters $\vec{R}_0$. Let $t_0, t_1 \in \mathbb{R}$; the evolution of the system between t_0 and t_1 which is described by the evolution operator $U(\vec{R}_0, t_0, t_1)P_m(t_0) \in \mathcal{U}(\mathrm{Ran}\, P_m) \simeq U(M)$ which is assumed to satisfy the adiabatic condition (8), while also being the solution of the Schrödinger equation

$$\imath\hbar \frac{\partial}{\partial t} U(\vec{R}_0, t_0, t) = H(\vec{R}_0, t) U(\vec{R}_0, t_0, t) \tag{23}$$

with $U(\vec{R}_0, t_0, t_0) = 1$. It is well known that the solution of this equation is

$$U(\vec{R}_0, t_0, t_1) = \mathbb{T} e^{-\imath\hbar^{-1} \int_{t_0}^{t_1} H(\vec{R}_0, t)\mathrm{d}t}. \tag{24}$$

Expressions (22) and (24) are very similar, and an interpretation of the quantum dynamics as a parallel transport has been developed by Asorey *et al.*[15] in the general framework of infinite-dimensional Hilbert space and by Iliev[16] in the context of a general fiber bundle model of non-relativistic quantum mechanics. In the context of the adiabatic condition (8) the evolution is condensed into an M-dimensional space, leading to a description which involves a principal bundle $(Q_{\vec{R}_0}, \mathbb{R}, U(M), \pi_{Q_{\vec{R}_0}})$ and its associated vector bundle $(E_{\vec{R}_0}, \mathbb{R}, \mathbb{C}^M, \pi_{E_{\vec{R}_0}})$, with a state appearing as a section of the vector bundle $\psi \in \Gamma(\mathbb{R}, E_{\vec{R}_0})$.

Suppose that $\psi \in \Gamma(\mathbb{R}, E_{\vec{R}_0})$ is a solution of the Schrödinger equation. Let $\tilde{\psi}(t) = U(t)\psi(t)$ be a change of section such that

$$\imath\hbar \frac{\partial}{\partial t} \tilde{\psi}(t) = \tilde{H}(\vec{R}_0, t)\tilde{\psi}(t). \tag{25}$$

Inserting $\tilde{\psi}(t) = U(t)\psi$ into Eq. (25) leads to the result

$$\imath\hbar \frac{\partial}{\partial t} \psi(t) = (U(t)^{-1} \tilde{H}(\vec{R}_0, t) U(t) - \imath\hbar U(t)^{-1} \dot{U}(t))\psi \tag{26}$$

so that

$$\imath\hbar^{-1} \tilde{H}(\vec{R}_0, t) = U(t)\imath\hbar^{-1} H(\vec{R}_0, t) U(t)^{-1} + \dot{U}(t) U(t)^{-1} \tag{27}$$

and, finally,

$$\imath\hbar^{-1} \tilde{H}(\vec{R}_0, t)\mathrm{d}t = U(t)\imath\hbar^{-1} H(\vec{R}_0, t)\mathrm{d}t U(t)^{-1} + (\mathrm{d}_t U(t)) U(t)^{-1}, \tag{28}$$

where d_t is the exterior differential of $\mathbb{R}$: $\mathrm{d}_t f(t) = (\partial f / \partial t)\mathrm{d}t$. Equation (28) is the familiar formula of gauge transformation theory, and $\imath\hbar^{-1} H(\vec{R}_0, t)\mathrm{d}t \in \Omega^1(\mathbb{R}, \mathfrak{u}(M))$ is the gauge potential of $(Q_{\vec{R}_0}, \mathbb{R}, U(M), \pi_{Q_{\vec{R}_0}})$. $\psi \in \Gamma(\mathbb{R}, E_{\vec{R}_0})$ is horizontal if the covariant differential $D\psi = \mathrm{d}_t\psi + \imath\hbar^{-1} H(\vec{R}_0, t)\psi\, \mathrm{d}t$ is zero, i.e., if ψ obeys the Schrödinger equation. A horizontal lift of the curve $[t_0, t_1] \subset \mathbb{R}$ is well characterized by the expression (24).

Let $U_{\mathrm{dyn}}(M)$ be the set of maps from $\mathbb{R}$ to $U(M)$ which satisfies the Schrödinger-von Neumann equation [we note that this equation is the analogue for unitary operators of the equation associated to the Hermitian dynamical invariants (see Ref. 17), which are used by Mostafazadeh in Ref. 18 to define the non-Abelian nonadiabatic geometric phases]

$$\imath\hbar \dot{U}(t) = [U(t), H(\vec{R}_0, t)]. \tag{29}$$

In the framework of the adiabatic condition (8), the previous gauge potential is not used, because (24) is not the expression for the dynamical phase factor appearing in Ref. 19. Let $\{E_a(\vec{R}_0, t)\}_{a \in I}$

be the M isolated eigenvalues of $H(\vec{R}_0,t)$ and $\{|a,\vec{R}_0,t\rangle\}_{a\in I}$ be the corresponding eigenvectors. Let $E(\vec{R}_0,t)$ be the matrix such that $E(\vec{R}_0,t)_{ab}=E_a(\vec{R}_0,t)\delta_{ab}$. It is clear that $E(\vec{R}_0,t)_{ab}=\langle a,\vec{R}_0,t|H(\vec{R}_0,t)|b,\vec{R}_0,t\rangle$. A gauge transformation: $\forall a\in I$, $|\alpha,\vec{R}_0,t\rangle=U(t)|a,\vec{R}_0,t\rangle$, leads to

$$\tilde{E}_{\alpha\beta}(\vec{R}_0,t)=\langle\alpha,\vec{R}_0,t|H(\vec{R}_0,t)|\beta,\vec{R}_0,t\rangle \tag{30}$$

$$=\langle a,\vec{R}_0,t|U(t)^{-1}H(\vec{R}_0,t)U(t)|b,\vec{R}_0,t\rangle \tag{31}$$

$$=\langle a,\vec{R}_0,t|U(t)^{-1}U(t)H(\vec{R}_0,t)|b,\vec{R}_0,t\rangle+\langle a,\vec{R}_0,t|U(t)^{-1}[H(\vec{R}_0,t),U(t)]|b,\vec{R}_0,t\rangle \tag{32}$$

$$=\langle a,\vec{R}_0,t|H(\vec{R}_0,t)|b,\vec{R}_0,t\rangle+\langle a,\vec{R}_0,t|U(t)^{-1}[H(\vec{R}_0,t),U(t)]|b,\vec{R}_0,t\rangle \tag{33}$$

$$=\langle\alpha,\vec{R}_0,t|U(t)H(\vec{R}_0,t)U(t)^{-1}|\beta,\vec{R}_0,t\rangle+\langle\alpha,\vec{R}_0,t|[H(\vec{R}_0,t),U(t)]U(t)^{-1}|\beta,\vec{R}_0,t\rangle \tag{34}$$

$$=(U(t)H(\vec{R}_0,t)U(t)^{-1})_{\alpha\beta}+([H(\vec{R}_0,t),U(t)]U(t)^{-1})_{\alpha\beta}. \tag{35}$$

Thus we have

$$\tilde{E}=UEU^{-1}+[H,U]U^{-1}. \tag{36}$$

E does not satisfy the usual gauge transformation formula. But if we take $U\in U_{\mathrm{dyn}}(M)$ we obtain

$$\imath\hbar^{-1}\tilde{E}(\vec{R}_0,t)\mathrm{d}t=U(t)\imath\hbar^{-1}E(\vec{R}_0,t)\mathrm{d}tU(t)^{-1}+(\mathrm{d}_tU(t))U(t)^{-1} \tag{37}$$

we see that $\imath\hbar^{-1}E(\vec{R}_0,t)\mathrm{d}t\in\Omega^1(\mathbb{R},\mathfrak{u}(M))$ is a gauge potential of the principal bundle $(Q_{\vec{R}_0},\mathbb{R},U(M),\pi_{\vec{Q}_{\vec{R}_0}})$ but with a restriction of the gauge transformations to the set $U_{\mathrm{dyn}}(M)$ of the sections of $(Q_{\vec{R}_0},\mathbb{R},U(M),\pi_{\vec{Q}_{\vec{R}_0}})$ which are horizontal for the connection $\imath\hbar^{-1}H(\vec{R}_0,t)\mathrm{d}t$. The horizontal lift of $[t_0,t_1]\subset\mathbb{R}$ is then

$$D(\vec{R}_0,t_0,t_1)=\mathbb{T}e^{-\imath\hbar^{-1}\int_{t_0}^{t_1}E(\vec{R}_0,t)\mathrm{d}t} \tag{38}$$

which is effectively the dynamical term of (17).

The expression for the gauge potential is associated with the section of the associated vector bundle $t\mapsto(|a,\vec{R}_0,t\rangle)_{a\in I}$.

C. The composite bundle of the geodynamics and its connection

The discussion in the two preceding sections A and B suggests that the appropriate entities to give a correct description of the geometric structure of the geodynamical evolution characterized by the expression (17) would be the principal composite bundle $P^+\to S\to\mathbb{R}$ with structure bundle $(P,\mathcal{M},U(M),\pi_P)$, base bundle $(S,\mathbb{R},\mathcal{M},\pi_S)$, transversal bundles $(Q_{\vec{R}},\mathbb{R},U(M),\pi_{Q_{\vec{R}}})$ and total bundle $(P^+,\mathcal{M}\times\mathbb{R},U(M),\pi_{++})$. Note that, following the treatment of Sec. II, the structures of $(P,\mathcal{M},U(M),\pi_P)$, $(Q_{\vec{R}},\mathbb{R},U(M),\pi_{Q_{\vec{R}}})$ and of $(S,\mathbb{R},\mathcal{M},\pi_S)$ completely determine $(P^+,\mathcal{M}\times\mathbb{R},U(M),\pi_{++})$. P and $Q_{\vec{R}}$ have been introduced in the preceding paragraph. By fixing $t_0\in\mathbb{R}$ arbitrarily, the transition functions (to define a principal bundle, there are three equivalent ways, by invoking the local trivializations, by invoking the transition functions or by invoking the fiber diffeomorphisms) $g^{ij}(\vec{R},t_0)\in U(M)$ of P are obtained by setting $g^{ij}_{ab}(\vec{R})=\langle a,\vec{R},t_0,i|b,\vec{R},t_0,j\rangle$ where i and j represent two possible conventions in the matrix representation of the eigenvectors (see the example of Berry phase in Ref. 19). The topology of the bundle S is determined by the

map χ_t^S, for which P_t as defined by the transition functions $T(\vec{R},t,i)^\dagger T(\vec{R},t,j)$ is such that $\chi_t^{S^*} P = \chi_t^{S^*} P_{t_0} = P_t$. Clearly, if we consider $|a,\vec{R},t\rangle$ as a section of $\mathcal{M}$ with values in the associated vector bundle of P_t, then we have

$$\chi_{t*}^S |a,\vec{R},t_0\rangle = |a,\vec{R},t\rangle \Leftrightarrow \chi_{t*}^S = U(\vec{R},t_0,t), \tag{39}$$

$U(\vec{R},t_0,t)$ is defined by Eq. (24), and χ_{t*}^S is the map induced by χ_t^S in the sections.

This naturally leads us to take as the gauge potential of $(P_+,\mathcal{M}\times\mathbb{R},U(M),\pi_{++})$ the quantity

$$A_{\mathcal{M}\times\mathbb{R}}(\vec{R},t) = A(\vec{R},t) + \imath\hbar^{-1}E(\vec{R},t)\mathrm{d}t \in \Omega^1(\mathcal{M}\times\mathbb{R},\mathfrak{u}(M)) \tag{40}$$

with A being defined by Eq. (20). Note that we can use this expression because the two local sections used to express the gauge potentials are compatible. Introducing $j_t: \overset{\mathcal{M}\to\mathcal{M}\times\mathbb{R}}{\vec{R}\mapsto(\vec{R},t)}$ and $j_{\vec{R}}: \overset{\mathbb{R}\to\mathcal{M}\times\mathbb{R}}{t\mapsto(\vec{R},t)}$ we have $A(\vec{R},t_0)=j_{t_0}^* A_{\mathcal{M}\times\mathbb{R}}(\vec{R},t_0)$ and $\imath\hbar^{-1}E(\vec{R}_0,t)\mathrm{d}t = j_{\vec{R}_0}^* A_{\mathcal{M}\times\mathbb{R}}(\vec{R}_0,t)$.

As a gauge potential is locally defined, and as S is locally diffeomorphic to $\mathcal{M}\times\mathbb{R}$, we can write $A_S(\vec{R},t)=A_\mu(\vec{R},t)\mathrm{d}R^\mu + \imath\hbar^{-1}E(\vec{R},t)\mathrm{d}t \in \Omega^1(S,\mathfrak{u}(M))$. Let $h\in\Gamma([0,t_1],S)$ be a section. h defines a curve $\mathcal{C}$ in $\mathcal{M}\times\mathbb{R}$, where $\mathcal{L}=h([0,t_1])$ is a closed path described in $\mathcal{M}$ by $R^\mu(t)=h^\mu(t)$. Consider the pullback of h,

$$\Omega^* S \to \Omega^* \mathbb{R}$$

$$h^*: \mathrm{d}R^\mu \mapsto \frac{\partial h^\mu}{\partial t}\mathrm{d}t.$$

$$\mathrm{d}t \mapsto \mathrm{d}t$$

Then we have

$$(h^* A_S)(t) = A_\mu(h(t),t)\frac{\partial h^\mu}{\partial t}\mathrm{d}t + \imath\hbar^{-1}E(h(t),t)\mathrm{d}t. \tag{41}$$

Using expression (18), the horizontal lift of h is characterized by [with the notation $h(t)=\vec{R}(t)$]

$$g_h = \mathbb{P}e^{-\int_{\mathcal{C}} A_{\mathcal{M}\times\mathbb{R}}(\vec{R},t)} = \mathbb{T}e^{-\int_0^{t_1} A_\mu(\vec{R}(t),t)[\partial R^\mu(t)/\partial t]\mathrm{d}t - \imath\hbar^{-1}\int_0^{t_1} E(\vec{R}(t),t)\mathrm{d}t}. \tag{42}$$

Suppose now that we do not have a fast evolution in addition to the adiabatic evolution, in such a way that $H(\vec{R},t)$ has no explicit time dependence; then we have

$$g_h = \mathbb{T}e^{-\oint_{\mathcal{L}} A_\mu(\vec{R})\mathrm{d}R^\mu - \imath\hbar^{-1}\int_0^{t_1} E(\vec{R}(t))\mathrm{d}t} \tag{43}$$

which is the expression for the non-Abelian phase in (17).

Note that the connection A_S of $(P^+,S,U(M),\pi_+)$ is restricted to the gauge transformations of the form $U(M)\ni g(\vec{R},t)=g(\vec{R})U(t)$, where $g(\vec{R})$ is a map from $\mathcal{M}$ to $U(M)$ without restrictive conditions and where $U(t)\in U_{\mathrm{dyn}}(M)$. We thus have a principal structure but with a restricted choice of gauges.

It should be stressed that in $Q_{\vec{R}}$ we introduce the local fiberd coordinates (t,γ^j) where (γ^j) is a system of coordinates of $U(M)$. In the same way we introduce the fiberd coordinates of P (R^μ,γ^j) and the fiberd coordinates of P^+ (R^μ,t,γ^j). By calling on the theorem of Ehresmann (see Ref. 19), it is possible to construct a connection 1-form with gauge potential $A_{\mathcal{M}\times\mathbb{R}}$. Let $\sigma \in \Gamma(\mathcal{M}\times\mathbb{R},P^+)$ be the section used to express the gauge potential $A_{\mathcal{M}\times\mathbb{R}}$. $\forall(\vec{R},t,\gamma)\in P^+$, let $g(\vec{R},t,\gamma)$ such that $(\vec{R},t,\gamma)=\sigma(\vec{R},t)g(\vec{R},t,\gamma)$. The connection 1-form of P^+ is

$$\omega_+(\vec{R},t,\gamma) = g(\vec{R},t,\gamma)^{-1}A_\mu(\vec{R},t)g(\vec{R},t,\gamma)\mathrm{d}R^\mu + \imath\hbar^{-1}g(\vec{R},t,\gamma)^{-1}E(\vec{R},t)g(\vec{R},t,\gamma)\mathrm{d}t$$
$$+ g(\vec{R},t,\gamma)^{-1}\frac{\partial}{\partial R^\mu}g(\vec{R},t,\gamma)\mathrm{d}R^\mu + g(\vec{R},t,\gamma)^{-1}\frac{\partial}{\partial t}g(\vec{R},t,\gamma)\mathrm{d}t + g(\vec{R},t,\gamma)^{-1}\frac{\partial}{\partial \gamma^j}g(\vec{R},t,\gamma)\mathrm{d}\gamma^j$$

the connection 1-form of P for a fixed t_0 is

$$\omega_P(\vec{R},\gamma) = g(\vec{R},t_0,\gamma)^{-1}A_\mu(\vec{R},t_0)g(\vec{R},t_0,\gamma)\mathrm{d}R^\mu + g(\vec{R},t_0,\gamma)^{-1}\frac{\partial}{\partial R^\mu}g(\vec{R},t_0,\gamma)\mathrm{d}R^\mu$$
$$+ g(\vec{R},t_0,\gamma)^{-1}\frac{\partial}{\partial \gamma^j}g(\vec{R},t_0,\gamma)\mathrm{d}\gamma^j$$

and the connection 1-form of $Q_{\vec{R}_0}$ for a fixed $\vec{R}_0$ is

$$\omega_{Q_{\vec{R}_0}}(t,\gamma) = \imath\hbar^{-1}g(\vec{R}_0,t,\gamma)^{-1}E(\vec{R}_0,t)g(\vec{R}_0,t,\gamma)\mathrm{d}t + g(\vec{R}_0,t,\gamma)^{-1}\frac{\partial}{\partial t}g(\vec{R}_0,t,\gamma)\mathrm{d}t$$
$$+ g(\vec{R}_0,t,\gamma)^{-1}\frac{\partial}{\partial \gamma^j}g(\vec{R}_0,t,\gamma)\mathrm{d}\gamma^j$$

we can see then that $\omega_{P^+} \neq \omega_P + \omega_{Q_{\vec{R}}}$.

D. A pseudo-Stiefel structure

In the preceding section C we considered a fiber bundle with a restriction concerning the allowed gauge transformations. If we give up this restriction we must deal with the nonstandard equation (36) of gauge tranformation theory, $\tilde{E} = UEU^{-1} + [H,U]U^{-1}$. In order to find a structure associated with this formula we first consider the bundle $(Q_{\vec{R}_0}, \mathbb{R}, U(M), \pi_{Q_{\vec{R}_0}})$ endowed with the gauge potential $\imath\hbar^{-1}H(\vec{R}_0,t)\mathrm{d}t$. This gauge potential satisfies the correct gauge transformation formula and it is then possible to define a covariant differential $D_{Q_{\vec{R}_0}}$. Let $\psi \in \Gamma(\mathbb{R}, E_{\vec{R}_0})$ be a section of the associated vector bundle. We have

$$D_{Q_{\vec{R}_0}}\psi = \partial_t\psi\,\mathrm{d}t + \imath\hbar^{-1}H\psi\,\mathrm{d}t. \tag{44}$$

Let $U \in \Gamma(\mathbb{R}, Q_{\vec{R}_0})$ be a section from $\mathbb{R}$ to $Q_{\vec{R}_0}$ considered as the space of the operators of $E_{\vec{R}_0}$; then we have

$$D_{Q_{\vec{R}_0}}U = \partial_t U\,\mathrm{d}t + \imath\hbar^{-1}[H,U]\mathrm{d}t. \tag{45}$$

With $D_{Q_{\vec{R}_0}}$ we define a differential in $\mathcal{M}\times\mathbb{R}$,

$$\tilde{D}\eta(\vec{R},t) = \mathrm{d}_{\mathcal{M}}\eta(\vec{R},t) + D_{Q_{\vec{R}}}\eta(\vec{R},t). \tag{46}$$

We can then define a gauge potential in the style of Stiefel but with the differential $\tilde{D}$ in place of $\mathrm{d}_{\mathcal{M}\times\mathbb{R}}$. We set

$$A_+ = T^\dagger \tilde{D} T, \tag{47}$$

where T is the matrix of the eigenvectors of H. Note that $\tilde{D}^2 \neq 0$ so that the connection is not rigourously a Stiefel one. $|b,\vec{R},t\rangle \in \Gamma(\mathcal{M}\times\mathbb{R}, E_+)$ is a section of the associated vector bundle of P^+, so that

$$\tilde{D}|b,\vec{R},t\rangle = d_{\mathcal{M}}|b,\vec{R},t\rangle + d_t|b,\vec{R},t\rangle + \imath\hbar^{-1}H(\vec{R},t)|b,\vec{R},t\rangle \mathrm{d}t \tag{48}$$

and

$$A_{+ab} = \langle a,\vec{R},t|d_{\mathcal{M}}|b,\vec{R},t\rangle + \langle a,\vec{R},t|\partial_t|b,\vec{R},t\rangle \mathrm{d}t + \imath\hbar^{-1}\langle a,\vec{R},t|H(\vec{R},t)|b,\vec{R},t\rangle \mathrm{d}t \tag{49}$$

so that we have

$$A_+ = A + A_0 + \imath\hbar^{-1}E\mathrm{d}t, \tag{50}$$

where A is the adiabatic gauge potential defined by Eq. (20) and A_0 is the matrix with elements $\langle a,\vec{R},t|\partial_t|b,\vec{R},t\rangle \mathrm{d}t$, namely the expression of a Berry gauge potential for the variable t when $\vec{R}$ is fixed. Considering A_+ as a gauge potential of $(P^+,\mathcal{M}\times\mathbb{R},U(M),\pi_{++})$, the horizontal lift of $h \in \Gamma(\mathbb{R},\mathcal{M})$ is characterized by

$$g_h = \mathbb{T}e^{-\int_0^{t_1} A_\mu(\vec{R}(t),t)[\partial h^\mu(t)/\partial t]-\int_0^{t_1} A_0(\vec{R}(t),t)\mathrm{d}t-\imath\hbar^{-1}\int_0^{t_1} E(\vec{R}(t),t)\mathrm{d}t}. \tag{51}$$

Note that this equation is identical to (10) if one considers the change of variable $t\to(\vec{R}(t),t)$.

Consider a gauge transformation, it is clear that

$$\hat{A}_+ = \hat{A} + \hat{A}_0 + \imath\hbar^{-1}\hat{E}\,\mathrm{d}t \tag{52}$$

$$= UAU^{-1} + (\mathrm{d}_{\mathcal{M}}U)U^{-1} + UA_0U^{-1} + (\mathrm{d}_tU)U^{-1} + U\imath\hbar^{-1}E\,\mathrm{d}t\,U^{-1} + \imath\hbar^{-1}[H,U]U^{-1} \tag{53}$$

$$= UA_+U^{-1} + (\mathrm{d}_{\mathcal{M}}U + \mathrm{d}_tU + \imath\hbar^{-1}[H,U])U^{-1} \tag{54}$$

$$= UA_+U^{-1} + (\tilde{D}U)U^{-1}. \tag{55}$$

A_+ satisfies a gauge transformation formula analogous to the usual one but with the replacement of $\mathrm{d}_{\mathcal{M}\times\mathbb{R}}$ by $\tilde{D}$. The use of the pseudodifferential $\tilde{D}$ modifies the gauge field theory. Let the curvature F_+ be

$$F_+ = \tilde{D}A_+ + A_+\wedge A_+ \tag{56}$$

$$= \mathrm{d}_{\mathcal{M}\times\mathbb{R}}A_+ + A_+\wedge A_+ + \imath\hbar^{-1}[E\,\mathrm{d}t,A_+] \tag{57}$$

$$= \mathrm{d}_{\mathcal{M}\times\mathbb{R}}A_+ + A_+\wedge A_+ + \imath\hbar^{-1}[E\,\mathrm{d}t,A]. \tag{58}$$

Let $B=\imath\hbar^{-1}[E\,\mathrm{d}t,A]\in\Omega^2(\mathcal{M}\times\mathbb{R},\mathfrak{g})$ be the curving. B is the field which characterizes the noncommutativity between the dynamical and the geometric phases. Note that F_+-B is a standard curvature which satisfies the usual Bianchi identity and the usual Cartan structure equation. Using the standard covariant differential associated with A_+ we obtain the generalized Cartan equations

$$F_+ = \mathrm{d}_{\mathcal{M}\times\mathbb{R}}A_+ + A_+\wedge A_+ + B, \tag{59}$$

$$G = \mathrm{d}_{\mathcal{M}\times\mathbb{R}}B + [A_+,B]. \tag{60}$$

$G\in\Omega^3(\mathcal{M}\times\mathbb{R},\mathfrak{g})$ is called the fake curvature.

The fake-curvature satisfies a pseudo-Bianchi identity.

Property 1: Let G be a fake-curvature defined by generalized Cartan structure equations; then

$$\mathrm{d}_{\mathcal{M}\times\mathbb{R}}G + [G,A_+] = [F_+,B]. \tag{61}$$

Proof:

$$\mathrm{d}G = \mathrm{d}A_+ \wedge B - A_+ \wedge \mathrm{d}B - \mathrm{d}B \wedge A_+ - B \wedge \mathrm{d}A_+, \tag{62}$$

$$[F,B] - [G,A_+] = F_+ \wedge B - B \wedge F_+ - G \wedge A_+ - A_+ \wedge G \tag{63}$$

$$= \mathrm{d}A_+ \wedge B + A_+ \wedge A_+ \wedge B + B \wedge B - B \wedge \mathrm{d}A_+ - B \wedge A_+ \wedge A_+ - B \wedge B - \mathrm{d}B \wedge A_+ - A_+ \wedge B \wedge A_+ + B \wedge A_+ \wedge A_+ - A_+ \wedge \mathrm{d}B - A_+ \wedge A_+ \wedge B + A_+ \wedge B \wedge A_+ \tag{64}$$

$$= \mathrm{d}A_+ \wedge B - B \wedge \mathrm{d}A_+ - \mathrm{d}B \wedge A_+ - A_+ \wedge \mathrm{d}B. \tag{65}$$

■

V. ILLUSTRATION: THE EXAMPLE OF A SIMPLE QUANTUM DYNAMICAL SYSTEM

This final section illustrates the formal concepts introduced in the preceding sections by using a concrete physical example taken from atomic physics. We consider a particular three-level atom interacting with two lasers. Before explaining how the model illustrates the formal theory of the preceding sections we give a brief description of three-level systems.

A. Preliminary discussion

We consider a three-level quantum system, described by the Hilbert space $\mathcal{H} = \mathbb{C}^3$. The generic form of a three-level Hamiltonians is

$$H = x^i \lambda_i, \quad i = 0, \ldots, 8, \tag{66}$$

where λ_0 is the identity matrix of $\mathcal{H} = \mathbb{C}^3$ and $\{\lambda_i\}_{i=1,\ldots,8}$ are the Gell-Mann matrices,

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -\imath & 0 \\ \imath & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

$$\lambda_5 = \begin{pmatrix} 0 & 0 & -\imath \\ 0 & 0 & 0 \\ \imath & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\imath \\ 0 & \imath & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

The Gell-Mann matrices can be considered as the generators of the Lie algebra $\mathfrak{su}(3)$. Moreover we introduce the following matrices:

$$\mu_1 = \lambda_3 + \frac{1}{\sqrt{3}}\lambda_8 + \frac{2}{3}\lambda_0, \tag{67}$$

$$\mu_2 = -\lambda_3 + \frac{1}{\sqrt{3}}\lambda_8 + \frac{2}{3}\lambda_0, \tag{68}$$

$$\mu_3 = -\frac{1}{\sqrt{3}}\lambda_8 + \frac{2}{3}\lambda_0. \tag{69}$$

It is clear that $\{\lambda_i, \mu_j\}_{i=1,2,4,5,6,7;j=1,2,3}$ generate the Lie algebra $\mathfrak{u}(3)$. We are interested in particular Hamiltonians of the form

$$H = x^1\lambda_1 + x^2\lambda_2 + x^6\lambda_6 + x^7\lambda_7 + \tilde{x}\mu_2. \tag{70}$$

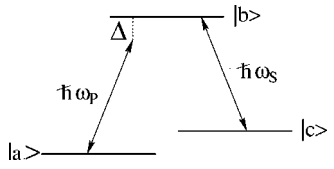

FIG. 2. Scheme of the three-level atom.

Since $\{\lambda_4, \lambda_5, \mu_1, \mu_2\}$ are the generators of the Lie algebra $\mathfrak{u}(2)$ as a subalgebra of $\mathfrak{u}(3)$, then the Hamiltonian (70) is an element of $\mathfrak{u}(3)/\mathfrak{u}(2)$ [this is a vector space quotient; $\mathfrak{u}(2)$ is not an ideal of $\mathfrak{u}(3)$ and so $\mathfrak{u}(3)/\mathfrak{u}(2)$ is a vector space without the Lie algebra structure]. In other words the Hamiltonian (70) characterized by $(x^1, x^2, x^6, x^7, \tilde{x})$ is determined by a point of the manifold $\mathrm{U}(3)/\mathrm{U}(2)$, and we know (see Ref. 4) that

$$\mathrm{U}(3)/\mathrm{U}(2) = \mathrm{SU}(3)/\mathrm{SU}(2) = S^5. \tag{71}$$

Thus, the control parameter space associated with a Hamiltonian of the form (70) can always be chosen as a submanifold of the 5-sphere S^5.

B. A concrete example: a three-level atom interacting with lasers

We consider a three-level atom in the Λ configuration interacting with two lasers, denoted by P (for pump) and S (for Stokes). The three bare states of the atom are labelled by $|a\rangle$, $|b\rangle$, and $|c\rangle$. The control parameters of the system are the amplitudes and the phases of the lasers S and P. We denote by ω_P the frequency of the laser P which is quasiresonant with the transition $|a\rangle \to |b\rangle$, with the detuning Δ. The laser S of frequency ω_S is supposed to be in perfect resonance with the transition $|b\rangle \to |c\rangle$, see Fig. 2.

The dressed Hamiltonian of the system in the rotating wave approximation (RWA) is (see, for example Ref. 20)

$$H = \frac{\hbar}{2}\begin{pmatrix} 0 & We^{\iota\beta} & 0 \\ We^{-\iota\beta} & 2\Delta & Ve^{\iota\alpha} \\ 0 & Ve^{-\iota\alpha} & 0 \end{pmatrix}, \tag{72}$$

where $W = |\langle a|\vec{\mu}\cdot\vec{E}_P|b\rangle|$ and $V = |\langle b|\vec{\mu}\cdot\vec{E}_S|c\rangle|$, $\vec{E}_P$ and $\vec{E}_S$ being the laser amplitudes and $\vec{\mu}$ being the electric dipole moment of the atom. To simplify the notation, we set $\Delta = 1$. The Hamiltonian H is of the form (70) and we can compute the three eigenvalues of H,

$$E_1 = 0, \tag{73}$$

$$E_2 = \frac{\hbar}{2}(1 - \sqrt{1 + V^2 + W^2}), \tag{74}$$

$$E_3 = \frac{\hbar}{2}(1 + \sqrt{1 + V^2 + W^2}). \tag{75}$$

We see that $E_1 = E_2$ if $V = 0$ and $W = 0$, and moreover

$$\inf_{V,W} \mathrm{dist}(\{E_1, E_2(V,W)\}; E_3(V,W)) = \hbar. \tag{76}$$

Let $P_1(W,V,\alpha,\beta)$, $P_2(W,V,\alpha,\beta)$, and $P_3(W,V,\alpha,\beta)$ be the eigenprojectors associated with E_1, E_2, and E_3. It is evident that for all particular dynamics $t \mapsto (W(t), V(t), \alpha(t), \beta(t))$ the Hamiltonian $H(t)$ and the decomposition $\mathrm{Spe}(H(t)) = \sigma_0(t) \cup \sigma_\perp(t)$ satisfy the assumptions of Nenciu's adiabatic theorem (see Ref. 13), where $\sigma_0(t) = \{E_1, E_2(t)\}$ and $\sigma_\perp(t) = \{E_3(t)\}$ and with

$\inf_t \mathrm{dist}(\sigma_0(t),\sigma_\perp(t)) \geqslant \hbar$. In accordance with Nenciu's theorem, we have at the adiabatic limit [this limit is approximately obtained if the variations of $(W(t),V(t))$ are slow with respect to the proper quantum time $\inf_t[\hbar/E_3(t)-E_1]$; for classical parameters such as W or V this hypothesis is consistent]

$$U(t,0)P_m(0) = P_m(t)U(t,0), \tag{77}$$

where $U(t,0)$ is the evolution operator associated with $H(t)$ and $P_m(t)=P_1(t)+P_2(t)$. We can apply the formalism of the previous part with Ran P_m ($\dim \mathrm{Ran}\, P_m=2$), for all particular dynamics.

The eigenvectors of H can be chosen as follows for $V\neq 0$ and $W\neq 0$:

$$|1,(\alpha,\beta,W,V)\rangle = \frac{1}{\sqrt{1+\frac{V^2}{W^2}}}\begin{pmatrix} -e^{\imath(\alpha+\beta)}\frac{V}{W} \\ 0 \\ 1 \end{pmatrix}, \tag{78}$$

$$|2,(\alpha,\beta,W,V)\rangle = \frac{1}{\sqrt{1+\frac{W^2}{V^2}+\frac{(1-\sqrt{1+V^2+W^2})^2}{V^2}}}\begin{pmatrix} e^{\imath(\alpha+\beta)}\frac{W}{V} \\ e^{\imath\alpha}\frac{(1-\sqrt{1+V^2+W^2})}{V} \\ 1 \end{pmatrix}, \tag{79}$$

$$|3,(\alpha,\beta,W,V)\rangle = \frac{1}{\sqrt{1+\frac{W^2}{V^2}+\frac{(1+\sqrt{1+V^2+W^2})^2}{V^2}}}\begin{pmatrix} e^{\imath(\alpha+\beta)}\frac{W}{V} \\ e^{\imath\alpha}\frac{(1+\sqrt{1+V^2+W^2})}{V} \\ 1 \end{pmatrix}. \tag{80}$$

Let $r=\sqrt{1+V^2+W^2}$ and (θ,φ) be such that $W=r\sin\varphi\cos\theta$, $V=r\sin\varphi\sin\theta$ and $r\cos\varphi=1$ ($\theta\in\,]0,\pi/2[$ and $\varphi\in\,]0,\pi/2[$). With these variables we can write

$$|1,(\alpha,\beta,\theta,\varphi)\rangle = \begin{pmatrix} -e^{\imath(\alpha+\beta)}\sin\theta \\ 0 \\ \cos\theta \end{pmatrix}, \tag{81}$$

$$|2,(\alpha,\beta,\theta,\varphi)\rangle = \begin{pmatrix} e^{\imath(\alpha+\beta)}\frac{\sin\varphi\cos\theta}{\sqrt{1-\cos\varphi}} \\ e^{\imath\alpha}\sqrt{1-\cos\varphi} \\ \frac{\sin\varphi\sin\theta}{\sqrt{1-\cos\varphi}} \end{pmatrix}. \tag{82}$$

Let $(\alpha,\beta,\gamma,\theta,\varphi)$ be the angles which generate S^5. The submanifold of S^5 defined by

$$0<\varphi<\frac{\pi}{2},$$

$$0<\theta<\frac{\pi}{2},$$

$$\gamma = 0,$$

is the control manifold; in the following we denote it by S^4_+.

C. The composite bundle modelling the quantum dynamical system

We will now apply the theoretical construction introduced in the preceding sections. First we note that the choice of the eigenvectors (81) and (82) is not unique. They can be

$$|i\rangle^{NE} = \begin{pmatrix} e^{\iota(\alpha+\beta)}* \\ e^{\iota\alpha}* \\ * \end{pmatrix}, \tag{83}$$

where $*$ replace the functions of (θ,φ) in the expressions of $|1\rangle$ (81) or $|2\rangle$ (82). By another choice of phase convention we can choose the following eigenvectors:

$$|i\rangle^{NW} = \begin{pmatrix} e^{\iota\alpha}* \\ e^{\iota(\alpha-\beta)}* \\ e^{-\iota\beta}* \end{pmatrix}, \quad |i\rangle^{SE} = \begin{pmatrix} e^{\iota\beta}* \\ * \\ e^{-\iota\alpha}* \end{pmatrix}, \quad |i\rangle^{SW} = \begin{pmatrix} * \\ e^{-\iota\beta}* \\ e^{-\iota(\alpha+\beta)}* \end{pmatrix}. \tag{84}$$

These different conventions are associated with four open local charts of S^4_+, $U^{NE} = \{(\alpha,\beta,\theta,\varphi) \in S^4_+ \,|\, \alpha \in]-\pi/2-\epsilon, \pi/2+\epsilon[, \beta \in]-\pi/2-\epsilon, \pi/2+\epsilon[$, $U^{NW} = \{(\alpha,\beta,\theta,\varphi) \in S^4_+ \,|\, \alpha \in]-\pi/2-\epsilon, \pi/2+\epsilon[, \beta \in]\pi/2-\epsilon, 3\pi/2+\epsilon[$, $U^{SE} = \{(\alpha,\beta,\theta,\varphi) \in S^4_+ \,|\, \alpha \in]\pi/2-\epsilon, 3\pi/2+\epsilon[, \beta \in]-\pi/2-\epsilon, \pi/2+\epsilon[$, and $U^{SW} = \{(\alpha,\beta,\theta,\varphi) \in S^4_+ \,|\, \alpha \in]\pi/2-\epsilon, 3\pi/2+\epsilon[, \beta \in]\pi/2-\epsilon, 3\pi/2+\epsilon[$, where ϵ is a small parameter. The set $\{U^i\}_{i=NE,NW,SE,SW}$ is an atlas of S^4_+. We want to construct the principal bundle of the geometric phase. Let $T^i = (|1\rangle^i, |2\rangle^i) \in \mathcal{M}_{3\times 2}(\mathbb{C})$ be the matrix of eigenvectors selected by the adiabatic theorem ($i = NE, NW, SE, SW$). We set $\vec{R} = (\alpha,\beta,\theta,\varphi) \in S^4_+$,

$$\forall i,j, \forall \vec{R} \in U^i \cap U^j, \quad g^{ij}(\vec{R}) = T^i(\vec{R})^\dagger T^j(\vec{R}) \in \mathrm{U}(2). \tag{85}$$

The functions g^{ij} are the transition functions of the principal bundle of the geometry $(P, S^4_+, \mathrm{U}(2), \pi_P)$. More precisely we have

$$g^{NE,NW} = g^{SE,SW} = e^{\iota\beta}, \quad g^{NE,SE} = g^{NW,SW} = e^{\iota\alpha}, \quad g^{NE,SW} = e^{\iota(\alpha+\beta)}. \tag{86}$$

Note that $\forall i,j\ g^{ij} \in \mathrm{U}(1) \subset \mathrm{U}(2)$, because the two eigenvectors are never globally degenerate in $U^i \cap U^j$. These functions define completely the total space P of the principal bundle of the geometry. Indeed let $\sim$ be the equivalence relation on $S^4_+ \times \mathrm{U}(2)$ defined by

$$(x,k) \sim (y,h) \text{ if } x = y \text{ and if } \exists\, i,j \text{ such that } x \in U^i \cap U^j \text{ and } k = hg^{ij}.$$

The total space is the quotient manifold $P = S^4_+ \times \mathrm{U}(2)/\sim$. Let $\pi_\sim : S^4_+ \times \mathrm{U}(2) \to P$ be the projection associated to $\sim$, then π_P is defined by the commutative diagram

$$\begin{array}{ccc} S^4_+ \times U(2) & \xrightarrow{\pi_\sim} & P \\ & {\scriptstyle \mathrm{Pr}_1} \searrow \quad \swarrow {\scriptstyle \pi_P} & \\ & S^4_+ & \end{array}$$

The principal bundle of the geometry $(P, S^4_+, \mathrm{U}(2), \pi_P)$ is then completely defined. Moreover it is the structure bundle of the principal composite bundle of the geodynamics. The connection on P is obtained by the gauge potential

$$\forall \vec{R} \in U^i, \quad A^i = T^i(\vec{R})^\dagger \mathrm{d}_{S^4} T^i(\vec{R}) \in \Omega^1(S^4_+, \mathfrak{u}(2)) \tag{87}$$

with $A^j = (g^{ij})^{-1} A^i g^{ij} + (g^{ij})^{-1} \mathrm{d}_{S^4} g^{ij}$ in $U^i \cap U^j$. Let $\{\sigma_i\}_{i=1,2,3}$ be the Pauli matrices [generators of $\mathfrak{su}(2)$] and σ_0 be the identity of $\mathbb{C}^2$, with

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The calculus of the gauge potential shows that

$$A^{NE} = \imath \frac{\sin\varphi}{\sqrt{1-\cos\varphi}} \sigma_2 \, \mathrm{d}\theta - \frac{\imath}{2\sqrt{2}} \frac{\sin(2\theta)\sin\varphi}{\sqrt{1-\cos\varphi}} \sigma_1 (\mathrm{d}\alpha + \mathrm{d}\beta) + \imath \sin\theta \frac{\sigma_3 + \sigma_0}{2} (\mathrm{d}\alpha + \mathrm{d}\beta)$$
$$+ \frac{\imath}{2} \frac{\cos^2\theta \sin^2\varphi}{1-\cos\varphi} \frac{\sigma_0 - \sigma_3}{2} (\mathrm{d}\alpha + \mathrm{d}\beta) + \frac{\imath}{2}(1-\cos\varphi) \frac{\sigma_0 - \sigma_3}{2} \mathrm{d}\alpha. \tag{88}$$

The transversal bundle for $\vec{R} = (\alpha, \beta, \theta, \varphi) \in S^4_+$ fixed is the trivial bundle of the dynamics $(\mathbb{R} \times \mathrm{U}(2), \mathbb{R}, \mathrm{U}(2), \mathrm{Pr}_1)$ endowed with the connection

$$\forall t \in \mathbb{R}, E(\vec{R}, t) = \frac{\imath}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 - \dfrac{1}{\cos\varphi} \end{pmatrix} \mathrm{d}t. \tag{89}$$

Let χ^S_t be the fiber diffeomorphism of the base bundle $(S, \mathbb{R}, S^4_+, \pi_S)$. By definition we have $P_t = \chi_t^{S^*} P$, but the Hamiltonian H does not have an explicit dependence on t. Then it is clear that $\forall t \in \mathbb{R}$, $P_t = P$ and then χ^S_t is the identity map. We conclude that $\pi_S^{-1}(t) = S^4_+$ and then $S = S^4_+ \times \mathbb{R}$. The base bundle is the trivial bundle $(S^4_+ \times \mathbb{R}, \mathbb{R}, S^4_+, \mathrm{Pr}_2)$. The local trivializations of the total bundle are

$$\phi^{ij}_{++}(\vec{R}, t, g) = \phi^i_P[t](\vec{R}, g) = \phi^i_P(\vec{R}, g) \tag{90}$$

because P_t is independent of t. Let $\{U^i \times \mathbb{R}\}_{i=NE,NW,SE,SW}$ be the atlas of $S^4_+ \times \mathbb{R}$, $\forall (\vec{R}, t) \in (U^i \cap U^j) \times \mathbb{R}$ we have the transition functions of the total space P^+ of the total bundle by $g^{ij}_{++}(\vec{R}, t) = g^{ij}(\vec{R})$. Then it is clear that $P^+ = P \times \mathbb{R}$, the total bundle of the geodynamics is then $(P \times \mathbb{R}, S^4_+ \times \mathbb{R}, \mathrm{U}(2), (\pi_P \circ \mathrm{Pr}_1) \times \mathrm{Pr}_2)$. Note that the triviality of the fibration on the time is due to the nonexplicit dependence of H on t. When this is not the case, then the base bundle is not trivial.

D. Different aspects of the quantum dynamical system in our formalism

All the ingredients of the composite bundle formalism have now been explicitly identified for our example. We now want to consider a particular dynamics in order to complete the description of the quantum dynamical system in our composite bundle representation. In order to simplify and to clarify the discussion, we consider a dynamics such that $\forall t \ \alpha = \beta = 0$ (chart U^{NE}) and we use the orginal variables (W, V) in place of (θ, φ); this restricted manifold is denoted by $\mathcal{M}$ in this paragraph. In the sequel $\mu = 1, 2$, $R^1 = W$, $R^2 = V$ and $R^0 = t$. In these conditions, the gauge potential of the total bundle P^+ over $\mathcal{M}$ is

$$A_+ = \imath\hbar^{-1} E(W, V)\mathrm{d}t + A(W, V) = \frac{\imath}{2}(1 - \sqrt{1 + V^2 + W^2})(\sigma_0 - \sigma_3)\mathrm{d}t$$
$$+ \frac{\imath\sigma_2}{\sqrt{2}\sqrt{1 + \dfrac{V^2}{W^2}}\sqrt{\dfrac{1 + V^2 + W^2 - \sqrt{1 + V^2 + W^2}}{V^2}}} \left(\frac{\mathrm{d}W}{W} - \frac{\mathrm{d}V}{V} \right). \tag{91}$$

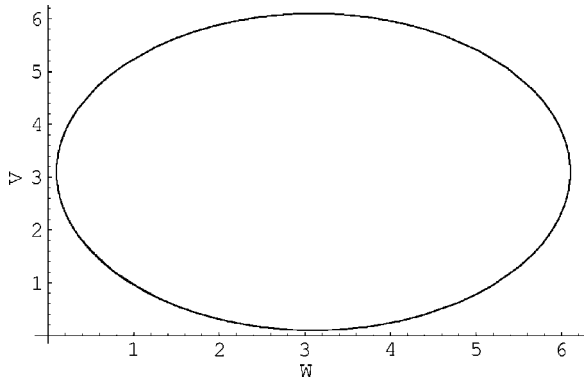

FIG. 3. The path induced by γ in $\mathcal{M}$.

We consider the dynamics described by $\gamma \in \Gamma([t_0=-25, T=90], \mathcal{M}\times\mathbb{R})$ defined by $\gamma(t) = (3\cos(2\pi(t-25)/90)+3.1, 3\sin(2\pi(t-25)/90)+3.1)$ (the units are arbitrary). γ induces a path $\mathcal{C}$ in $\mathcal{M}\times\mathbb{R}$. (See Fig. 3.)

The horizontal lift of $\mathcal{C}$ defines the holonomy operator

$$\forall t \in [t_0, T], \quad J^{\gamma,t_0,t} = \mathbb{P}e^{-\imath\hbar^{-1}\int_{t_0}^{t} E(\gamma(t'))\mathrm{d}t' - \int_0^t A_\mu(\gamma(t'))\mathrm{d}\gamma^\mu(t')/\mathrm{d}t'\mathrm{d}t'} \in \Gamma(\mathcal{M}\times\mathbb{R}, P^+). \tag{92}$$

Let $(E^+, \mathcal{M}\times\mathbb{R}, \mathbb{C}^2, \pi_{E^+})$ be the associated vector bundle of P^+ by the action of U(2) on $\mathbb{C}^2$ defined by the matrix product. The states of the system are described by the $\mathcal{C}^\infty(\mathcal{M}\times\mathbb{R}, \mathbb{C})$-module $\Gamma(\mathcal{M}\times\mathbb{R}, E^+)$, which is the space of the sections of E^+. At $t=0$ we suppose that $\psi(0) = (1/\sqrt{2}) \times (|1, \gamma(0)\rangle + |2, \gamma(0)\rangle)$; then for all $t \geqslant t_0$

$$\psi(t) = \sum_{b=1,2} \frac{1}{\sqrt{2}} ([J^{\gamma,t_0,t}]_{b,1} + [J^{\gamma,t_0,t}]_{b,2}) |b, \gamma(t)\rangle \in \Gamma(C, E^+). \tag{93}$$

The state space $\Gamma(\mathcal{M}\times\mathbb{R}, E^+)$ is endowed with the $\mathcal{C}^\infty(\mathcal{M}\times\mathbb{R}, \mathbb{C})$-valued inner product

$$\forall \chi, \phi \in \Gamma(\mathcal{M}\times\mathbb{R}, E^+), \quad \langle\chi|\phi\rangle_{E^+}(\vec{R}, t) = \langle\chi(\vec{R}, t)|\phi(\vec{R}, t)\rangle_{\mathbb{C}^2} \tag{94}$$

$\forall i = 1, 2$ $|i, \vec{R}\rangle \in \Gamma(\mathcal{M}\times\mathbb{R}, E^+)$ [in the composite bundle representation it is the canonical basis $|1\rangle = \binom{1}{0}$ and $|2\rangle = \binom{0}{1}$]. With the scalar product we obtain the instantaneous occupation probabilities of the eigenlevel E_1 and $E_2(V, W)$,

$$P_i(t) = |\langle i|\psi\rangle_{E^+}(\gamma(t), t)|^2. \tag{95}$$

These probabilities are drawn in Fig. 4.

In Sec. IV, we have introduced some fields F_+, B and G in $\mathcal{M}\times\mathbb{R}$ associated with the structure of the composite bundle. An illustration of these fields are shown in Fig. 5.

Let $(V^+, \mathcal{M}\times\mathbb{R}, u(2), \pi_{V^+})$ be the associated vector bundle of P^+ by the adjoint action Ad of U(2) on u(2) ($\mathrm{Ad}(U)X = U^{-1}XU$, $\forall U \in U(2)$, $\forall X \in \mathfrak{u}(2)$). The algebra $\Gamma(\mathcal{M}\times\mathbb{R}, V^+)$ endowed with the Lie bracket

$$\forall A, B \in \Gamma(\mathcal{M}\times\mathbb{R}, V^+), \quad [A, B]_{V^+}(\vec{R}, t) = [A(\vec{R}, t), B(\vec{R}, t)]_{u(2)} \tag{96}$$

is the observables space. In our example of a three level system, a set of observables has a particular importance. Let $S_i = \frac{1}{2}\lambda_i$ for $i = 1, \ldots, 8$, and let $S_i(t) = U(t, t_0) S_i U(t, t_0)^\dagger$, where $U(t, t_0)$ is the evolution operator associated with the Schrödinger equation. The role of the set of operators $S_i(t)$ for a three level system has been extensively studied by Ho, Chu *et al.*[21–23] Let ρ_0 be the density matrix of the initial condition of the system. We introduce the vector $\vec{\mathcal{S}}(t) \in \mathbb{R}^8$ such that

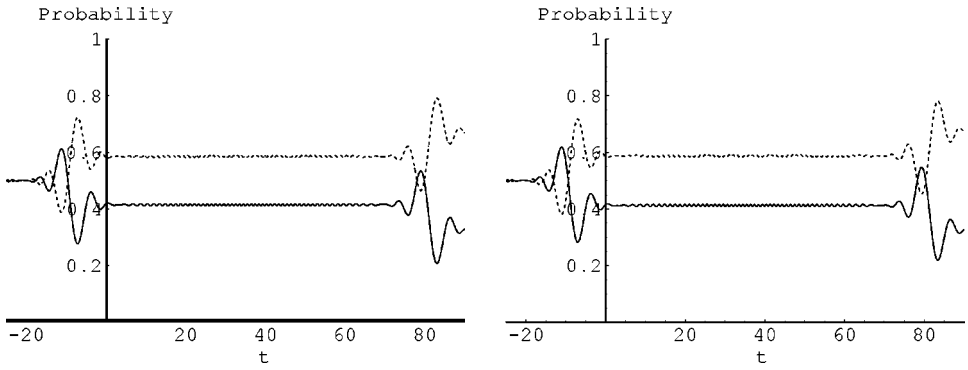

FIG. 4. Left, occupation probabilities of the state $|1\rangle$ (plain line), $|2\rangle$ (dash line), and $|3\rangle$ (strong line) computed by direct integration of the Schrödinger equation in $\mathbb{C}^3$. Right; occupation probabilities of the state $|1\rangle$ (full line), and $|2\rangle$ (dashed line) computed with the formula (93) based on the holonomy operator of the composite bundle. We see that the results obtained by the use of the holonomy operator are in perfect agreement with the direct integration. Moreover the left figure reveals that the level 3 is never occupied, in agreement with its adiabatic elimination in the bundle representation.

$S_i(t)=\mathrm{tr}(\rho_0 S_i(t))$ [the average value of the observable $S_i(t)$]. $\vec{\mathcal{S}}(t)$ is called a coherent vector. From the trajectory of this vector we can obtain information about the dynamical system (for a complete exposition of this subject see Refs. 21–23). Within an approach using our bundle formalism the analogues of the observables $S_i(t)$ are

$$S_i(\vec{R}) = T(\vec{R})^{\dagger} S_i T(\vec{R}) \in \Gamma(\mathcal{M}\times\mathbb{R}, u(2)), \tag{97}$$

and the coherent vector $\vec{\mathcal{S}}(t)$ is obtained by (in our quantum system $\rho_0=|\psi(0)\rangle\langle\psi(0)|$

$$S_i(t) = \langle\psi|S_i\psi\rangle_{E^+}(\gamma(t),t). \tag{98}$$

Figure 6 illustrates the computation of $\mathcal{S}$ in the composite bundle formalism.

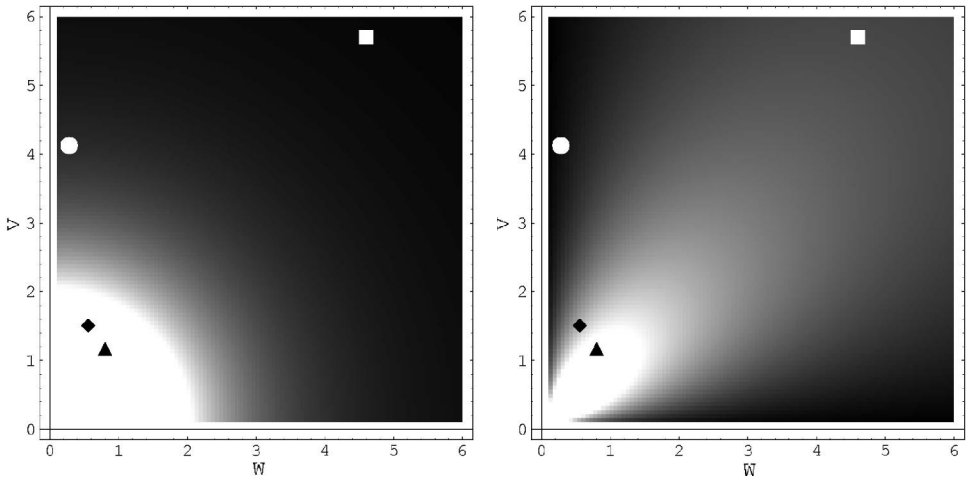

FIG. 5. Left, the (1, 2)-matrix element of $(F_+)_{12}$ with respect to $\mathcal{M}$. Right, the (1, 1)-matrix element of G_{012} with respect to $\mathcal{M}$. The white area is characterized by a strong field intensity whereas the black area corresponds to vanishing fields (arbitrary units). We have moreover indicated some points of the path $\mathcal{C}$, ○, $t=-25$; ◇, $t=-12$; □, $t=40$; and △, $t=80$. By comparison with Fig. 4 we see that the wave function changes significantly only when the control parameters are localized in the strong field area. This shows that these fields are related to the dynamical properties of the quantum system.

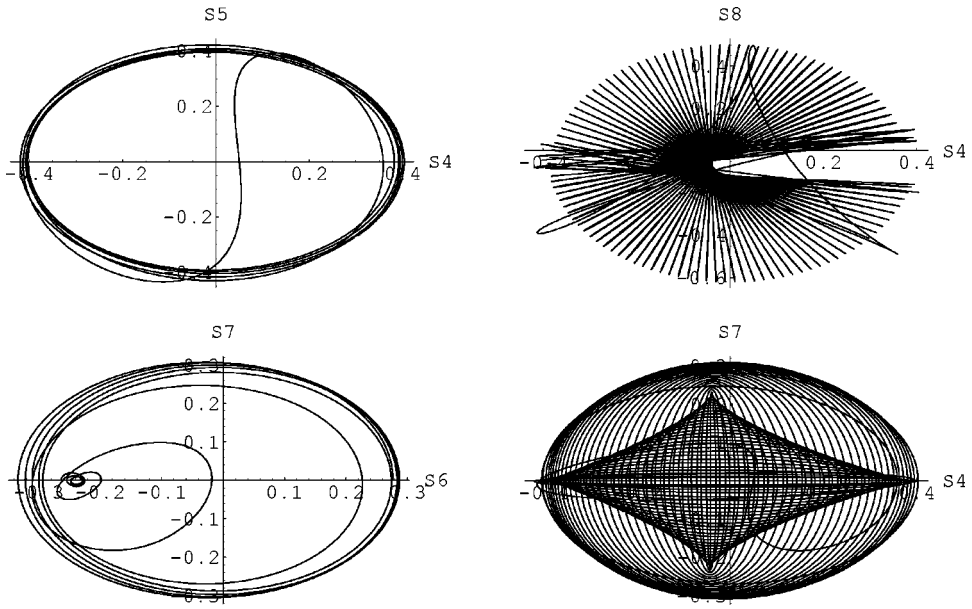

FIG. 6. Trajectories of the coherent vector $\vec{\mathcal{S}}(t)$ projected in different planes, for different time intervals, computed in the composite bundle representation.

The example of the three-level system shows that we can use the composite principal bundle representation to obtain all the physical ingredients of the quantum dynamics. This formalism, coupled with a numerical procedure to compute the holonomy operator, could be used as a powerful method to study a more complex quantum dynamical system.

VI. CONCLUSION

The principal composite bundle appears as a highly appropriate structure to describe the adiabatic transport with a Berry phase which does not commute with the dynamical phase. Nevertheless the use of the standard gauge theory requires us to restrict the gauge transformations to the sections which satisfy the Schrödinger-Von Neumann equation. This feature reveals that it is impossible to describe quantum dynamics with a purely geometric model without a dynamical postulate. If one does not accept any restriction on the gauge transformations, the price to pay is the implementation of an unusual gauge theory which introduces, in addition to the curvature, a field, the curving B, which is precisely the commutator of A with H. It is remarkable that such a situation is very similar to the gauge fields of non-Abelian gerbes, but with the important difference that in the non-Abelian gerbe theory, B does not have values in the Lie algebra g (see Ref. 11). (See Refs. 24–26.)

One can easily generalize this description to the problem of the non-Abelian Aharonov-Anandan phase which does not commute with the dynamical phase; this is done by replacing the principal bundle $(P,\mathcal{M},U(M),\pi_P)$ by the universal principal bundle $(V_M(\mathbb{C}^n),G_M(\mathbb{C}^n),U(M),\pi_U)$. The analysis of Bohm and Mostatazadeh[7] has effectively showed that $(V_M(\mathbb{C}^n),G_M(\mathbb{C}^n),U(M),\pi_U)$ is the universal bundle of $(P,\mathcal{M},U(M),\pi_P)$, and our work demonstrates that the same relationship exists between the adiabatic composite bundle and the universal composite bundle.

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Canonical quantization of SU(3) Skyrme model in a general representation

D. Jurčiukonis[a] and E. Norvaišas[b]
Vilnius University Institute of Theoretical Physics and Astronomy, Goštauto 12, Vilnius 01108, Lithuania

D. O. Riska[c]
Helsinki Institute of Physics and Department of Physical Sciences, University of Helsinki, Helsinki 00014, Finland

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A complete canonical quantization of the SU(3) Skyrme model performed in the collective coordinate formalism in general irreducible representations. In the case of SU(3) the model differs qualitatively in different representations. The Wess-Zumino-Witten term vanishes in all self-adjoint representations in the collective coordinate method for separation of space and time variables. The canonical quantization generates representation dependent quantum mass corrections, which can stabilize the soliton solution. The standard symmetry breaking mass, which in general leads to representation mixing, degenerates to the SU(2) form in all self-adjoint representations. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The Skyrme model is a nonlinear field theory, with localized finite energy soliton solutions, which may be quantized as fermions.[1,2] The semiclassically quantized Skyrme model has proven useful for baryon phenomenology as a realization of the large color limit of QCD.[3] The original model was defined for a unitary field $\mathrm{U}(\mathbf{x},t)$ that belongs to fundamental representation of SU(2). The boundary condition $\mathrm{U}\to\mathbb{1}$ as $|\mathbf{x}|\to\infty$ implies that the unitary field represents a mapping from $S^3\to S^3$, the integer valued winding number of which classifies the solitonic sectors of the model and may be interpreted as the baryon number. The model has subsequently been directly generalized the SU(3) and SU(N),[4] in which case the field $\mathrm{U}(\mathbf{x},t)$ is described by group valued functions with semiclassical quantization.

Both the SU(2) and SU(3) Skyrme versions of the model have been quantized canonically in Refs. 5 and 6 in the collective coordinate formalism. The canonical quantization procedure leads to quantum corrections to the skyrmion mass, which restore the stability of the soliton solutions that is lost in the semiclassical quantization. This method has subsequently been generalized to unitary fields $\mathrm{U}(\mathbf{x},t)$ that belong to general representations of the SU(2),[7–9] along with a demonstration that the quantum corrections, which stabilize the soliton solutions, are representation dependent.

The aim of the present paper is to extend the canonically quantized Skyrme model to general irreducible representations (irrep) of SU(3). The motivation is the absence of any *a priori* reason to restrict collective chiral models to the fundamental representation of the group. The focus here is on the mathematical aspects of the model, and on the derivation of both the Hamiltonian density and the Hamiltonian, in order to elucidate their representation dependence. The possible phenom-

[a]Electronic mail: darius@itpa.lt
[b]Electronic mail: norvaisas@itpa.lt
[c]Electronic mail: riska@pcu.helsinki.fi

enological applications both in hyperon and hypernuclear phenomenology as well as in the Skyrme model description of the quantum Hall effect[10] and Bose-Einstein condensates,[11] are not elaborated.

In contrast to the case of SU(2), the solutions to the SU(3) Skyrme model depend in an essential way on the dimension. Remarkably the Wess–Zumino–Witten (WZW) term vanishes in all self-adjoint irreps of SU(3), as it is proportional to the cubic Casimir operator $C_3^{\mathrm{SU}(3)}$ in the collective coordinate method for separation of the dependence on space and time variables. In the self-adjoint irreps the symmetry breaking mass term in the model reduces to the SU(2) form.

After some preliminary definitions in Sec. II below, the main part of this paper is organized as follows. In Sec. III, the classical treatment of the Skyrme model in a general irrep of SU(3) is reviewed. In Sec. IV, the quantum Skyrme model is constructed *ab initio* in the collective coordinates framework. In Sec. V, the WZW term is taken into account and the left and right transformation generators are derived from the Lagrangian. The Lagrangian and Hamiltonian density operators are given explicitly in terms of generators. In Sec. VI, the symmetry breaking terms are considered in the collective coordinates framework. Section VII contains a summarizing discussion. A number of relevant mathematical details are given in the Appendix.

II. DEFINITIONS FOR THE UNITARY SU(3) SOLITON FIELD

The unitary field $\mathrm{U}(\mathbf{x},t)$ is defined for general irreps (λ,μ) of SU(3) in addition to the fundamental representation (1, 0). The related Young tableaux are denoted $[\lambda_1,\lambda_2,\lambda_3]$, where $\lambda=\lambda_1-\lambda_2$, $\mu=\lambda_2-\lambda_3$. A group element is specified by the eight real parameters $\alpha^i(\mathbf{x},t)$. The unitary field is expressed in the form of Wigner D matrices for SU(3) in (λ,μ) irrep as

$$\mathrm{U}(\mathbf{x},t)=D^{(\lambda,\mu)}(\alpha^i(\mathbf{x},t)). \tag{2.1}$$

The one-form of the unitary field belongs to the Lie algebra of SU(3). The one-forms may be determined by the functions $C_i^{(Z,I,M)}(\alpha)$ and $C_i'^{(Z,I,M)}(\alpha)$, the explicit expressions for which depend on the specific group parametrization,

$$\begin{aligned}\partial_i U U^\dagger &= \left(\frac{\partial}{\partial\alpha^i}U\right)U^\dagger = C_i^{(Z,I,M)}(\alpha)\langle|J^{(1,1)}_{(Z,I,M)}|\rangle,\\ U^\dagger\partial_i U &= U^\dagger\frac{\partial}{\partial\alpha^i}U = C_i'^{(Z,I,M)}(\alpha)\langle|J^{(1,1)}_{(Z,I,M)}|\rangle.\end{aligned} \tag{2.2}$$

The parameters spin I, and its projections M and Z, which is related to hypercharge as $Y=-2Z$, specify the basis states of irrep (1,1).

The parameterization for the SU(3) model, and the expressions of the differential Casimir operator in terms of the Euler angles, has been proposed by Yabu and Ando.[12] The SU(3) generators are defined as components of irreducible tensors (1, 1) and may be expanded in terms of the Gell-Man generators Λ_k,

$$J^{(1,1)}_{(0,0,0)}=-\tfrac{1}{2}\Lambda_8,\quad J^{(1,1)}_{(0,1,0)}=\tfrac{1}{2}\Lambda_3,$$

$$J^{(1,1)}_{(0,1,1)}=-\frac{1}{2\sqrt{2}}(\Lambda_1+i\Lambda_2),\quad J^{(1,1)}_{(0,1,-1)}=\frac{1}{2\sqrt{2}}(\Lambda_1-i\Lambda_2),$$

$$J^{(1,1)}_{\left(-\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)}=\frac{1}{2\sqrt{2}}(\Lambda_4+i\Lambda_5),\quad J^{(1,1)}_{\left(-\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right)}=\frac{1}{2\sqrt{2}}(\Lambda_6+i\Lambda_7),$$

$$J^{(1,1)}_{\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)} = -\frac{1}{2\sqrt{2}}(\Lambda_6 - i\Lambda_7), \quad J^{(1,1)}_{\left(\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right)} = \frac{1}{2\sqrt{2}}(\Lambda_4 - i\Lambda_5). \tag{2.3}$$

In the case of the fundamental representation the Λ_k matrices generators reduce to the standard Gell-Mann matrices λ_i. Although the generators (2.3) are non-Hermitian, $(J^{(1,1)}_{(Z,I,M)})^\dagger = (-1)^{Z+M} J^{(1,1)}_{(-Z,I,-M)}$, the commutation relations nevertheless have the simple form,

$$\left[J^{(1,1)}_{(Z',I',M')}, J^{(1,1)}_{(Z'',I'',M'')}\right] = \sum_{(Z,I,M)} -\sqrt{3}\begin{bmatrix} (1,1) & (1,1) & (1,1)_a \\ (Z',I',M') & (Z'',I'',M'') & (Z,I,M) \end{bmatrix} J^{(1,1)}_{(Z,I,M)}. \tag{2.4}$$

Here the coefficient on the right-hand side (rhs) of Eq. (2.4) is a Clebsch-Gordan coefficient of SU(3), the explicit expressions for which are given in Ref. 13. The index a in the Clebsch-Gordan coefficient denotes that only antisymmetric irrep couplings are included.

For the specification of the basis states in a general irrep (λ,μ) the parameters (z,j,m), where the hypercharge is $y=\frac{2}{3}(\mu-\lambda)-2z$, are employed. The basis state parameters satisfy the inequalities,

$$\begin{gathered} j-m \geqslant 0, \quad j-z \geqslant 0, \\ j+m \geqslant 0, \quad j+z \geqslant 0, \\ \lambda+z-j \geqslant 0, \quad \mu-z-j \geqslant 0, \end{gathered} \tag{2.5}$$

where the left-hand sides are integers. The generators (2.3) act on the basis states as follows:

$$J^{(1,1)}_{(0,0,0)}\left|\begin{matrix}(\lambda,\mu)\\ z,j,m\end{matrix}\right\rangle = -\frac{\sqrt{3}}{2}y\left|\begin{matrix}(\lambda,\mu)\\ z,j,m\end{matrix}\right\rangle, \quad J^{(1,1)}_{(0,1,-1)}\left|\begin{matrix}(\lambda,\mu)\\ z,j,m\end{matrix}\right\rangle = \sqrt{\tfrac{1}{2}(j+m)(j-m+1)}\left|\begin{matrix}(\lambda,\mu)\\ z,j,m-1\end{matrix}\right\rangle,$$

$$J^{(1,1)}_{(0,1,0)}\left|\begin{matrix}(\lambda,\mu)\\ z,j,m\end{matrix}\right\rangle = m\left|\begin{matrix}(\lambda,\mu)\\ z,j,m\end{matrix}\right\rangle, \quad J^{(1,1)}_{(0,1,1)}\left|\begin{matrix}(\lambda,\mu)\\ z,j,m\end{matrix}\right\rangle = -\sqrt{\tfrac{1}{2}(j-m)(j+m+1)}\left|\begin{matrix}(\lambda,\mu)\\ z,j,m+1\end{matrix}\right\rangle,$$

$$\begin{aligned} J^{(1,1)}_{\left(-\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)}\left|\begin{matrix}(\lambda,\mu)\\ z,j,m\end{matrix}\right\rangle = &\sqrt{\frac{(\lambda+z-j)(\mu-z+j+2)(j-z+1)(j+m+1)}{2(2j+1)(2j+2)}}\left|\begin{matrix}(\lambda,\mu)\\ z-\frac{1}{2},j+\frac{1}{2},m+\frac{1}{2}\end{matrix}\right\rangle \\ &-\sqrt{\frac{(\lambda+z+j+1)(\mu-z-j+1)(j+z)(j-m)}{4j(2j+1)}}\left|\begin{matrix}(\lambda,\mu)\\ z-\frac{1}{2},j-\frac{1}{2},m+\frac{1}{2}\end{matrix}\right\rangle, \end{aligned}$$

$$\begin{aligned} J^{(1,1)}_{\left(\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right)}\left|\begin{matrix}(\lambda,\mu)\\ z,j,m\end{matrix}\right\rangle = &-\sqrt{\frac{(\lambda+z+j+2)(\mu-z-j)(z+j+1)(j-m+1)}{2(2j+1)(2j+2)}}\left|\begin{matrix}(\lambda,\mu)\\ z+\frac{1}{2},j+\frac{1}{2},m-\frac{1}{2}\end{matrix}\right\rangle \\ &+\sqrt{\frac{(\lambda+z-j+1)(\mu-z+j+1)(j-z)(j+m)}{4j(2j+1)}}\left|\begin{matrix}(\lambda,\mu)\\ z+\frac{1}{2},j-\frac{1}{2},m-\frac{1}{2}\end{matrix}\right\rangle, \end{aligned}$$

$$\begin{aligned} J^{(1,1)}_{\left(-\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right)}\left|\begin{matrix}(\lambda,\mu)\\ z,j,m\end{matrix}\right\rangle = &\sqrt{\frac{(\lambda+z-j)(\mu-z+j+2)(j-z+1)(j-m+1)}{2(2j+1)(2j+2)}}\left|\begin{matrix}(\lambda,\mu)\\ z-\frac{1}{2},j+\frac{1}{2},m-\frac{1}{2}\end{matrix}\right\rangle \\ &+\sqrt{\frac{(\lambda+z+j+1)(\mu-z-j+1)(j+z)(j+m)}{4j(2j+1)}}\left|\begin{matrix}(\lambda,\mu)\\ z-\frac{1}{2},j-\frac{1}{2},m-\frac{1}{2}\end{matrix}\right\rangle, \end{aligned}$$

$$J^{(1,1)}_{(\frac{1}{2},\frac{1}{2},\frac{1}{2})}\left|\begin{matrix}(\lambda,\mu)\\ z,j,m\end{matrix}\right\rangle = -\sqrt{\frac{(\lambda+z+j+2)(\mu-z-j)(j+z+1)(j+m+1)}{2(2j+1)(2j+2)}}\left|\begin{matrix}(\lambda,\mu)\\ z+\frac{1}{2},j+\frac{1}{2},m+\frac{1}{2}\end{matrix}\right\rangle - \sqrt{\frac{(\lambda+z-j+1)(\mu-z+j+1)(j-z)(j-m)}{4j(2j+1)}}\left|\begin{matrix}(\lambda,\mu)\\ z+\frac{1}{2},j-\frac{1}{2},m+\frac{1}{2}\end{matrix}\right\rangle. \tag{2.6}$$

The basis states are chosen such that the generators $J^{(1,1)}_{(0,1,0)}$ and $J^{(1,1)}_{(0,0,0)}$, as well as the Casimir operator of the SU(2) subgroup $\hat{C}^{\mathrm{SU}(2)}=\Sigma(-1)^M J^{(1,1)}_{(0,1,M)}J^{(1,1)}_{(0,1,-M)}$, are diagonal and thus provide a labelling of the basis states,

$$\hat{C}^{\mathrm{SU}(2)}\left|\begin{matrix}(\lambda,\mu)\\ z,j,m\end{matrix}\right\rangle = j(j+1)\left|\begin{matrix}(\lambda,\mu)\\ z,j,m\end{matrix}\right\rangle. \tag{2.7}$$

III. THE CLASSICAL SU(3) SKYRME MODEL

The action of the Skyrme model in SU (3) is taken to have the form

$$S=\int \mathrm{d}^4x(\mathcal{L}_{\mathrm{Sk}}+\mathcal{L}_{\mathrm{SB}})+S_{\mathrm{WZ}}, \tag{3.1}$$

where the chirally symmetric Lagrangian density is[1]

$$\mathcal{L}_{\mathrm{Sk}}=-\frac{f_\pi^2}{4}\mathrm{Tr}\{\mathbf{R}_\mu\mathbf{R}^\mu\}+\frac{1}{32e^2}\mathrm{Tr}\{[\mathbf{R}_\mu,\mathbf{R}_\nu][\mathbf{R}^\mu,\mathbf{R}^\nu]\}. \tag{3.2}$$

Here the right chiral current is defined as

$$\mathbf{R}_\mu=(\partial_\mu U)U^\dagger=\partial_\mu\alpha^i C_i^{(A)}(\alpha)\langle|J^{(1,1)}_{(A)}|\rangle. \tag{3.3}$$

The greek characters indicate differentiation with respect to space-time variables $\partial_\mu=\partial/\partial x^\mu$ in the metric $\mathrm{diag}(\eta_{\alpha\beta})=(1,-1,-1,-1)$. The only parameters of the model are f_π and e. The symmetry breaking term $\mathcal{L}_{\mathrm{SB}}$ and Wess-Zumino-Witten action S_{WZ} are specified below.

Upon substitution of (3.3) into (3.2) the classical Lagrangian density may be expressed in terms of the group parameters α^i as

$$\mathcal{L}_{\mathrm{Sk}}=\frac{3}{32N}\dim(\lambda,\mu)C_2^{\mathrm{SU}(3)}(\lambda,\mu)\Bigg\{-f_\pi^2(-1)^A\partial_\mu\alpha^i C_i^{(A)}(\alpha)\partial^\mu\alpha^{i'}C_{i'}^{(-A)}(\alpha) + \frac{3}{8e^2}\cdot(-1)^A\partial_\mu\alpha^i C_i^{(A^1)}(\alpha)\partial_\nu\alpha^{i'}C_{i'}^{(A^2)}(\alpha)\partial^\mu\alpha^{i''}C_{i''}^{(A^3)}(\alpha)\partial^\nu\alpha^{i'''}C_{i'''}^{(A^4)}(\alpha)\begin{bmatrix}(1,1) & (1,1) & (1,1)_a\\ (A^1) & (A^2) & (A)\end{bmatrix} \times\begin{bmatrix}(1,1) & (1,1) & (1,1)_a\\ (A^3) & (A^4) & (-A)\end{bmatrix}\Bigg\}. \tag{3.4}$$

In the last SU(3) Clebsch-Gordan coefficients only the antisymmetric irrep coupling is included and there is no summation over irrep multiplicity. The capital italic character indices (A) denote the state label (Z,I,M), $(-A)$ denotes $(-Z,I,-M)$ and $(-1)^A=(-1)^{Z+M}$. The dependence on group irrep appear as an overall factor because

$$\mathrm{Tr}\langle(\lambda,\mu)|J^{(1,1)}_{(A)}J^{(1,1)}_{(B)}|(\lambda,\mu)\rangle=(-1)^A\tfrac{1}{8}\dim(\lambda,\mu)C_2^{\mathrm{SU}(3)}(\lambda,\mu)\,\delta_{(A),(-B)}, \tag{3.5}$$

where $\dim(\lambda,\mu)=\frac{1}{2}(\lambda+1)(\mu+1)(\lambda+\mu+2)$ is a dimension of irrep. Above $C_2^{\mathrm{SU}(3)}(\lambda,\mu)=\frac{1}{3}(\lambda^2+\mu^2+\lambda\mu+3\lambda+3\mu)$ is an eigenvalue of the quadratic Casimir operator of SU(3),

$$\hat{C}_2^{\mathrm{SU}(3)}(\lambda,\mu) = (-1)^{Z+M} J^{(1,1)}_{(Z,I,M)} J^{(1,1)}_{(-Z,I,-M)}. \tag{3.6}$$

The time component of the conserved topological current in the Skyrme model represents the baryon number density which in terms of the variables $\alpha^i(x,t)$ takes the form

$$\begin{aligned} B^0(x) &= \frac{1}{24\pi^2 N}\epsilon^{0ikl}\,\mathrm{Tr}\,(\partial_i U)U^\dagger(\partial_k U)U^\dagger(\partial_l U)U^\dagger \\ &= \frac{(-1)^A}{2^7\sqrt{3}\pi^2 N}\dim(\lambda,\mu)C_2^{\mathrm{SU}(3)}(\lambda,\mu)\varepsilon^{abc}\partial_a\alpha^i C_i^{(A)}(\alpha) \\ &\quad\times \partial_b\alpha^{i'} C_{i'}^{(A')}(\alpha)\partial_c\alpha^{i''} C_{i''}^{(A'')}(\alpha)\begin{bmatrix}(1,1) & (1,1) & (1,1)_a\\ (A') & (A'') & (-A)\end{bmatrix}. \end{aligned} \tag{3.7}$$

For the classical chiral symmetric Skyrme model the dependence on the irrep is contained in the overall factor N. The normalization factor,

$$N = \tfrac{1}{4}\dim(\lambda,\mu)C_2^{\mathrm{SU}(3)}(\lambda,\mu), \tag{3.8}$$

is chosen so that the smallest nontrivial baryon number equals unity, $B=\int \mathrm{d}^3x\, B^0(x)=1$. The dynamics of the system are independent of the overall factor in the Lagrangian. Therefore in the classical case the Skyrme model defined in arbitrary irrep is equivalent to the Skyrme model in the fundamental representation (1, 0), for which $N=1$.

The classical soliton solution of the hedgehog type for (λ,μ) irrep of the SU(3) group may be expressed as direct sum of hedgehog ansätze in SU(2) irreps.[8] The SU(2) representations embedded in the (λ,μ) irrep are defined by the canonical $\mathrm{SU}(3)\supset\mathrm{SU}(2)$ chain. The hedgehog generalization takes the form

$$\exp i(\sigma\cdot\hat{x})F(r) \to U_0(\hat{x},F(r)) = \exp i2(J^{(1,1)}_{(0,1,\cdot)}\cdot\hat{x})F(r) = \sum_{z,j}^{(\lambda,\mu)} \oplus D^j(\varkappa), \tag{3.9}$$

where σ are Pauli matrices and $\hat{x}$ is the unit vector. The Euler angles of the SU(2) subgroup in terms of polar angles φ ,θ and the chiral angle function $F(r)$ are

$$\begin{aligned} \varkappa^1 &= \varphi - \arctan(\cos\theta\tan F(r)) - \pi/2, \\ \varkappa^2 &= -2\arcsin(\sin\theta\sin F(r)), \\ \varkappa^3 &= -\varphi - \arctan(\cos\theta\tan F(r)) + \pi/2. \end{aligned} \tag{3.10}$$

The normalization factor (3.8) ensures that the baryon number density for the hedgehog skyrmion in a general irrep has the usual form,

$$B^0(x) = \frac{1}{24\pi^2 N}\epsilon^{0ikl}\,\mathrm{Tr}(\partial_i U_0)U_0^\dagger(\partial_k U_0)U_0^\dagger(\partial_l U_0)U_0^\dagger = -\frac{1}{2\pi^2}\frac{\sin^2 F(r)}{r^2}F'(r). \tag{3.11}$$

With the hedgehog ansatz (3.9), and after renormalization with the factor (3.8), the Lagrangian density (3.2) reduces to the following simple form:

$$\mathcal{L}_{\mathrm{cl}}[F(r)] = -\mathcal{M}_{\mathrm{cl}}(F(r)) = -\left\{\frac{f_\pi^2}{2}\left(F'^2 + \frac{2}{r^2}\sin^2 F\right) + \frac{1}{8e^2}\frac{\sin^2 F}{r^2}\left(2F'^2 + \frac{\sin^2 F}{r^2}\right)\right\}. \tag{3.12}$$

Variation of the classical hedgehog soliton mass leads to standard differential equation for the chiral angle $F(r)$.

The SU(3) chiral symmetry breaking term of Lagrangian density is defined here as

$$\mathcal{L}_{\mathrm{SB}} = -\mathcal{M}_{\mathrm{SB}} = -\frac{1}{N}\frac{f_\pi^2}{4}[m_0^2\,\mathrm{Tr}\{U+U^\dagger-2\mathbb{1}\} - 2m_8^2\,\mathrm{Tr}\{(U+U^\dagger)J^{(1,1)}_{(0,0,0)}\}]. \tag{3.13}$$

This form is chosen so that it reduces to the mass term of the π, K, η mesons when the unitary field $\mathrm{U}(\mathbf{x},t)=\exp[(i/f_\pi)\varphi_k\Lambda_k]$ is expanded around the classical vacuum $U=\mathbb{1}$,

$$\mathcal{L}_{\mathrm{SB}} = -\tfrac{1}{2}m_\pi^2(\varphi_1^2+\varphi_2^2+\varphi_3^2) - \tfrac{1}{2}m_K^2(\varphi_4^2+\varphi_5^2+\varphi_6^2+\varphi_7^2) - \tfrac{1}{2}m_\eta^2\varphi_8^2 + \cdots . \tag{3.14}$$

For arbitrary irrep the coefficients in the symmetry breaking term can be readily obtained as

$$m_0^2 = \tfrac{1}{3}(m_\pi^2+2m_K^2), \quad m_8^2 = \frac{10}{3\sqrt{3}}\frac{C_2^{\mathrm{SU(3)}}(\lambda,\mu)}{C_3^{\mathrm{SU(3)}}(\lambda,\mu)}(m_\pi^2-m_K^2), \tag{3.15}$$

where

$$C_3^{\mathrm{SU(3)}}(\lambda,\mu) = \tfrac{1}{9}(\lambda-\mu)(2\lambda+\mu+3)(2\mu+\lambda+3), \tag{3.16}$$

is the eigenvalue of the cubic Casimir operator of SU(3).

For the self-adjoint irreps $\lambda=\mu$ the symmetry breaking part of Lagrangian (3.13) is proportional to $m_0^2=\frac{1}{4}m_\pi^2$ only. The Gell-Mann-Okubo mass formula,

$$m_\pi^2 + 3m_\eta^2 - 4m_K^2 = 0, \tag{3.17}$$

is satisfied in all but the self-adjoint irreps.

IV. QUANTIZATION OF THE SKYRMION

The direct quantization of the Skyrme model even in the case of SU(2) leads to rather complicated equations.[7] Here the collective coordinates[3] for the unitary field U in (λ,μ) irrep are employed for the separation of the variables, which depend on the temporal and spatial coordinates:

$$\mathrm{U}(\hat{x},F(r),\mathbf{q}(t)) = A(\mathbf{q}(t))U_0(\hat{x},F(r))A^\dagger(\mathbf{q}(t)). \tag{4.1}$$

Because of form of the ansatz U_0 (3.9), the unitary field U is invariant under right U(1) transformation of the $A(\mathbf{q}(t))=D^{(\lambda,\mu)}(\mathbf{q}(t))$ matrix, defined as

$$A(\mathbf{q}(t)) \to A(\mathbf{q}(t))\exp\beta J^{(1,1)}_{(0,0,0)}. \tag{4.2}$$

Thus the seven-dimensional homogeneous space SU(3)/U(1), which is specified by the seven real, independent parameters $q^k(t)$, must be considered. The mathematical structure of the Skyrme model and its quantization problems on the coset space SU(3)/U(1) have been examined by several authors.[14,16] The canonical quantization procedure for the SU(3) Skyrme model in the fundamental representation has been considered by Fujii *et al.*[6] Here the attention is on the representation dependence of the model. The Lagrangian (3.2) is considered quantum mechanically *ab initio*. The generalized coordinates $q^k(t)$ and velocities $(\mathrm{d}/\mathrm{d}t)q^k(t)=\dot{q}^k(t)$ satisfy the commutation relations

$$[\dot{q}^k,q^l] = -if^{kl}(q), \tag{4.3}$$

where $f^{kl}(q)$ are functions only of q^k, and the form of which will be determined below. The commutation relation between a velocity component $\dot{q}^k$ and arbitrary function $G(q)$ is given by

$$[\dot{q}^k,G(q)] = -i\sum_r f^{kr}(q)\partial_r G(q). \tag{4.4}$$

For the time derivative the usual Weyl ordering is adopted,

$$\partial_0 G(q) = \frac{1}{2}\left\{ \dot{q}^k, \frac{\partial}{\partial q^k} G(q) \right\}. \tag{4.5}$$

The operator ordering is fixed by the form of the Lagrangian (3.2), without further ordering ambiguity. The curly brackets denote an anticommutator.

The ansatz (4.1) is then substituted in the Skyrme Lagrangian (3.2) followed by an integration over the spatial coordinates. The Lagrangian is then obtained in terms of collective coordinates and velocities. For the derivation of the canonical momenta it is sufficient to restrict the consideration to terms of second order in the velocities here (the terms of first order vanish). This leads to

$$\begin{aligned} L_{\mathrm{Sk}} \approx & -\int \mathrm{d}r\, r^2 \Bigg[\sum_M (-1)^M \{\dot{q}^i, C_i'^{(0,1,M)}(q)\}\{\dot{q}^{i'}, C_{i'}'^{(0,1,-M)}(q)\} \\ & \times \frac{\pi}{3}\sin^2 F\left(f_\pi^2 + \frac{1}{e^2}\left(F'^2 + \frac{1}{r^2}\sin^2 F \right)\right) + \sum_{Z,M} (-1)^{Z+M} \left\{ \dot{q}^i, C_i'\left(Z,\tfrac{1}{2},M\right)(q)\right\}\left\{ \dot{q}^{i'}, C_{i'}'\left(-Z,\tfrac{1}{2},-M\right)(q)\right\} \\ & \times \frac{\pi}{4}(1-\cos F)\left(f_\pi^2 + \frac{1}{4e^2}\left(F'^2 + \frac{2}{r^2}\sin^2 F\right)\right)\Bigg] \\ \approx & \frac{1}{2}\dot{q}^\alpha g_{\alpha\beta}(q,F)\dot{q}^\beta + [(\dot{q})^0\text{-order term}] \\ \approx & \frac{1}{8}\{\dot{q}^\alpha, C_\alpha'^{(A)}(q)\} E_{(A)(B)}(F)\{\dot{q}^\beta, C_\beta'^{(B)}(q)\} + [(\dot{q})^0\text{-order term}]. \end{aligned} \tag{4.6}$$

The Lagrangian (4.6) is normalized by the factor (3.8). The metric tensor takes the form

$$g_{\alpha\beta}(q,F) = C_\alpha'^{(A)}(q) E_{(A)(B)}(F) C_\beta'^{(B)}(q), \tag{4.7}$$

where

$$E_{(Z,I,M)(Z',I',M')}(F) = -(-1)^{Z+M} a_I(F)\, \delta_{Z,-Z'}\, \delta_{I,I'}\, \delta_{M,-M'}. \tag{4.8}$$

Here the soliton moments of inertia are given as integrals over the dimensionless variable $\tilde{r} = e f_\pi r$,

$$a_0(F) = 0, \tag{4.9a}$$

$$a_{\frac{1}{2}}(F) = \frac{1}{e^3 f_\pi}\tilde{a}_{\frac{1}{2}}(F) = \frac{1}{e^3 f_\pi} 2\pi \int \mathrm{d}\tilde{r}\, \tilde{r}^2 (1-\cos F)\left[1 + \frac{1}{4}F'^2 + \frac{1}{2\tilde{r}^2}\sin^2 F\right], \tag{4.9b}$$

$$a_1(F) = \frac{1}{e^3 f_\pi}\tilde{a}_1(F) = \frac{1}{e^3 f_\pi}\frac{8\pi}{3}\int \mathrm{d}\tilde{r}\, \tilde{r}^2 \sin^2 F\left[1 + F'^2 + \frac{1}{r^2}\sin^2 F\right]. \tag{4.9c}$$

The canonical momentum, which is conjugate to q^β, is defined as

$$p_\beta^{(0)} = \frac{\partial L_{\mathrm{Sk}}}{\partial \dot{q}^\beta} = \frac{1}{2}\{\dot{q}^\alpha, g_{\alpha\beta}\}. \tag{4.10}$$

The canonical commutation relations

$$[q^\alpha, q^\beta] = [p_\alpha^{(0)}, p_\beta^{(0)}] = 0, \tag{4.11}$$

$$[p_\beta^{(0)}, q^\alpha] = -i\delta_{\alpha\beta},$$

then yield the following explicit form for the functions $f^{\alpha\beta}(q)$:

$$f^{\alpha\beta}(q) = (g_{\alpha\beta})^{-1} = C'^{\alpha}_{\overline{(A)}}(q) E^{\overline{(A)}\overline{(B)}}(F) C'^{\beta}_{\overline{(B)}}(q), \tag{4.12}$$

where

$$E^{\overline{(Z,I,M)}\overline{(Z',I',M')}}(F) = -(-1)^{Z+M} \frac{1}{a_I(F)} \delta_{Z,-Z'} \delta_{I,I'} \delta_{M,-M'}. \tag{4.13}$$

Note that here $E^{(0)(0)}(F)$ is left undefined. The summation over the indices $\overline{(A)}$ denotes summation over the basis states (Z,I,M) of irrep (1, 1), excluding the state (0, 0, 0). It proves convenient to introduce the reciprocal function matrix $C'^{\alpha}_{\overline{(A)}}(q)$, the properties of which are described in the Appendix. The commutation relations of the momenta (4.11) ensure the choice of parameters q^α on the manifold SU(3)/U(1) (see Ref. 5). Here there is no need for explicit parametrization of q^α.

After determination of function $f^{\alpha\beta}(q)$ the following explicit expression $A^\dagger \dot{A}$ obtains

$$\begin{aligned} A^\dagger \dot{A} &= \frac{1}{2} D^{(\lambda,\mu)}(-q)\{\dot{q}^\alpha, \partial_\alpha D^{(\lambda,\mu)}(q)\} \\ &= \frac{1}{2}\{\dot{q}^\alpha, C'^{(A)}_\alpha(q)\}\langle |J^{(1,1)}_{(A)}| \rangle - \frac{1}{2} i E^{\overline{(A)}\overline{(B)}}(F) C'^{\beta}_{\overline{(B)}}(q) C'^{(0)}_\beta(q) (\langle |J^{(1,1)}_{(0)} J^{(1,1)}_{\overline{(A)}}| \rangle + \langle |J^{(1,1)}_{\overline{(A)}} J^{(1,1)}_{(0)}| \rangle) \\ &\quad - \frac{3}{8} i E^{\overline{(A)}\overline{(B)}}(F) C'^{\alpha}_{\overline{(A)}}(q) C'^{(0)}_\alpha(q) C'^{\beta}_{\overline{(B)}}(q) C'^{(0)}_\beta(q) \sum_{z,j}^{(\lambda,\mu)} \oplus\, y^2 \mathbb{1}_{z,j} \\ &\quad + \frac{i}{2a_{\frac{1}{2}}(F)} C_2^{\mathrm{SU}(3)}(\lambda,\mu)\mathbb{1} + i \sum_{z,j}^{(\lambda,\mu)} \oplus \left(\frac{C^{\mathrm{SU}(2)}(j)}{2a_1(F)} - \frac{C^{\mathrm{SU}(2)}(j) + \frac{3}{4}y^2}{2a_{\frac{1}{2}}(F)} \right) \mathbb{1}_{z,j}. \end{aligned} \tag{4.14}$$

Here $\mathbb{1}$ is the unit matrix in the (λ,μ) irrep of SU(3) and $\mathbb{1}_{z,j}$ are unit matrices in the SU(2) irreps. Note that the inverse of the rotation represented by $D^{(\lambda,\mu)}(q)$ is denoted $D^{(\lambda,\mu)}(-q)$.

The field expression (4.1) is substituted in the Lagrangian density (3.2) in order to obtain the explicit expression in terms of collective coordinates and space coordinates. Some expressions with SU(3) group generators, that are useful for this purpose, are presented in the Appendix. After some lengthy manipulation the complete expression of the Skyrme model Lagrangian density is obtained as

$$\begin{aligned} \mathcal{L}_{\mathrm{Sk}} &= \frac{1}{4}\dim(\lambda,\mu) C_2^{\mathrm{SU}(3)}(\lambda,\mu) \Bigg\{ -\frac{(1-\cos F)}{16}\left[f_\pi^2 + \frac{1}{4e^2}\left(F'^2 + \frac{2}{r^2}\sin^2 F \right)\right] \\ &\quad \times \sum_{Z,M} (-1)^{Z+M} \left\{ \dot{q}^\alpha, C'^{\left(Z,\frac{1}{2},M\right)}_\alpha(q) \right\} \left\{ \dot{q}^\beta, C'^{\left(Z,\frac{1}{2},M\right)}_\beta(q) \right\} - \frac{\sin^2 F}{8}\left[f_\pi^2 + \frac{1}{e^2}\left(F'^2 + \frac{1}{r^2}\sin^2 F \right)\right] \\ &\quad \times \sum_{Z,M} [(-1)^M \{\dot{q}^\alpha, C'^{(0,1,M)}_\alpha(q)\}\{\dot{q}^{\alpha'}, C'^{(0,1,M)}_{\alpha'}(q)\} - (\{\dot{q}^\alpha, C'^{(0,1,\cdot)}_\alpha(q)\}\cdot\hat{x})(\{\dot{q}^{\alpha'}, C'^{(0,1,\cdot)}_{\alpha'}(q)\}\cdot\hat{x})] \\ &\quad - \mathcal{M}_{\mathrm{cl}} - \Delta\mathcal{M}_1 - \Delta\mathcal{M}_2 - \Delta\mathcal{M}_3 - \Delta\mathcal{M}'(q) \Bigg\}. \end{aligned} \tag{4.15}$$

Here the following notation has been introduced:

$$\Delta\mathcal{M}_1(F) = -\frac{\sin^2 F}{30a_1^2(F)}\left[f_\pi^2(12\sin^2 F\cdot C_2^{\mathrm{SU}(3)}(\lambda,\mu) - 16\sin^2 F + 15) + \frac{1}{2e^2}\left(2F'^2(12\cos^2 F\cdot \right.\right.$$
$$\left.\left.\times C_2^{\mathrm{SU}(3)}(\lambda,\mu) + 16\sin^2 F - 1) + \frac{\sin^2 F}{r^2}(6C_2^{\mathrm{SU}(3)}(\lambda,\mu) + 7)\right)\right], \tag{4.16a}$$

$$\Delta\mathcal{M}_2(F) = -\frac{(1-\cos F)}{20a_{\frac{1}{2}}^2(F)}\left[f_\pi^2(6(1-\cos F)\cdot C_2^{\mathrm{SU}(3)}(\lambda,\mu) + 3\cos F + 2)\right.$$
$$\left. + \frac{1}{4e^2}\left(F'^2(6(1+\cos F)\cdot C_2^{\mathrm{SU}(3)}(\lambda,\mu) - 3\cos F + 2) + 10\frac{\sin^2 F}{r^2}\right)\right], \tag{4.16b}$$

$$\Delta\mathcal{M}_3(F) = -\frac{\sin^2 F}{30a_1(F)a_{\frac{1}{2}}(F)}\left[f_\pi^2(12(1-\cos F)\cdot C_2^{\mathrm{SU}(3)}(\lambda,\mu) + 16\cos F - 1)\right.$$
$$\left. + \frac{1}{2e^2}\left(F'^2(4\cos F\cdot(3C_2^{\mathrm{SU}(3)}(\lambda,\mu) - 4) + 15) + 15\frac{\sin^2 F}{r^2}\right)\right], \tag{4.16c}$$

$$\Delta\mathcal{M}'(F,q) = -\frac{3(1-\cos F)}{16a_{\frac{1}{2}}^2(F)}\left[f_\pi^2 + \frac{1}{4e^2}\left(F'^2 + \frac{2}{r^2}\sin^2 F\right)\right]$$
$$\times((-1)^{\bar{\bar{A}}}C'^{\alpha}_{(\bar{\bar{A}})}(q)C'^{(0)}_{\alpha}(q)C'^{\beta}_{(-\bar{\bar{A}})}(q)C'^{(0)}_{\beta}(q) + 4). \tag{4.16d}$$

[The "4" in the last bracket on the last row is missing in the corresponding expression in Ref. 6, the consequence of which is the appearance of a spurious term $-3/8a_{1/2}(F)$ in Eq. (69b) of that paper (there are some minor misprints in that equation as well).] The notation $(\bar{\bar{A}})$ indicates that only the states for which $I=\frac{1}{2}$ and $Z=\pm\frac{1}{2}$ are included. The $\Delta\mathcal{M}_k(F)$ terms may be interpreted as quantum mass corrections to the Lagrangian density. The $\Delta\mathcal{M}'(F,q)$ term depends on the quantum variables q^i and is an operator on the configuration space.

The integration (4.17) over the space variables and normalization by factor (3.8) gives the Lagrangian,

$$L_{\mathrm{Sk}} = \int \mathcal{L}_{\mathrm{Sk}}\mathrm{d}^3x = \frac{1}{8}\{\dot{q}^i, C_i'^{(\bar{A})}(q)\}E_{(\bar{A})(\bar{B})}\{\dot{q}^{i'}, C_{i'}'^{(\bar{B})}(q)\} - M_{\mathrm{cl}} - \Delta M_1 - \Delta M_2 - \Delta M_3 - \Delta M'(q)$$
$$= -\frac{1}{8a_{\frac{1}{2}}(F)}(-1)^{\bar{A}}\{\dot{q}^i, C_i'^{(\bar{A})}(q)\}\{\dot{q}^{i'}, C_{i'}'^{(-\bar{A})}(q)\} - \frac{1}{8}\left(\frac{1}{a_1(F)} - \frac{1}{a_{\frac{1}{2}}(F)}\right)(-1)^M$$
$$\times\{\dot{q}^i, C_i'^{(0,1,M)}(q)\}\{\dot{q}^{i'}, C_{i'}'^{(0,1,-M)}(q)\} - M_{\mathrm{cl}} - \Delta M_1 - \Delta M_2 - \Delta M_3 - \Delta M'(q). \tag{4.17}$$

Here $M_{\mathrm{cl}} = (f_\pi/e)\tilde{M}_{\mathrm{cl}} = \int \mathrm{d}^3x\, \mathcal{M}_{\mathrm{cl}}(F)$, $\Delta M_k = e^3 f_\pi \Delta\tilde{M}_k = \int \mathrm{d}^3x\, \Delta\mathcal{M}_k(F)$, and $\Delta M'(q) = \int \mathrm{d}^3x\, \Delta\mathcal{M}'(q)$, where $\tilde{M}_{\mathrm{cl}}$ and $\tilde{M}_k$ are integrals over the dimensionless variable.

V. STRUCTURE OF THE LAGRANGIAN AND THE HAMILTONIAN

The Wess-Zumino-Witten (WZW) action is given as an integral over the five dimensional manifold M^5, the boundary of which is the compactified space-time, $\partial M^5 = M^4 = S^3 \times S^1$. This term is necessary to account for the anomalies in QCD.[14] The standard form for this term is

$$S_{\mathrm{WZ}}(U) = -\frac{iN_c}{240\pi^2 N'}\int_{M^5} \mathrm{d}^5x\, \epsilon^{\mu\nu\lambda\rho\sigma}\,\mathrm{Tr}\, R_\mu R_\nu R_\lambda R_\rho R_\sigma, \tag{5.1}$$

where N_c is the number of colors and N' is a normalization factor. The derivation of the contribution of the Wess-Zumino-Witten term to the effective Lagrangian in the framework of the collective coordinate formalism is given in Ref. 15. By application of Stoke's theorem it takes the following form in a general dimension:

$$\begin{aligned} L_{\mathrm{WZ}}(q,\dot{q}) &= -\frac{iN_c}{24\pi^2 N'}\int_{M^3} \mathrm{d}^3x\, \epsilon^{mjk}\,\mathrm{Tr}[(\partial_m U_0)U_0^\dagger(\partial_j U_0)U_0^\dagger(\partial_k U_0)U_0^\dagger J^{(1,1)}_{(0,0,0)}]\frac{1}{2}\{\dot{q}^\alpha, C'^{(0)}_\alpha(q)\} \\ &= -\frac{iN_c}{2\sqrt{3}\pi^2 N'}\int_{M^3} \mathrm{d}^3x \frac{\sin^2 F(r)}{r^2}F'(r)\sum_{z,j}^{(\lambda,\mu)} yj(j+1)(2j+1)\frac{1}{2}\{\dot{q}^\alpha, C'^{(0)}_\alpha(q)\} \\ &= -\lambda'\frac{i}{2}\{\dot{q}^\alpha, C'^{(0)}_\alpha(q)\}. \end{aligned} \tag{5.2}$$

Here

$$\lambda' = \frac{\sqrt{3}N_c B}{40N'}\dim(\lambda,\mu)C_3^{\mathrm{SU(3)}}(\lambda,\mu). \tag{5.3}$$

The coefficient λ' depends on the representation (λ,μ). For all self-adjoint irreps $\lambda=\mu$ the WZW term vanishes. Following Witten[14] the normalization factor is chosen to be $N'=\dim(\lambda,\mu)\times C_3^{\mathrm{SU(3)}}(\lambda,\mu)/20$ so that $\lambda'=N_cB/2\sqrt{3}$. In the fundamental representation $N'=1$. Here the coefficient λ' only serves to constrain the states of the system. Because the cubic Casimir operator $C_3^{\mathrm{SU(3)}}$ (3.16) vanishes in the self-adjoint representations, it follows that the WZW term (5.2) also vanishes in those representations.

The Lagrangian of the system, with inclusion of the WZW term is

$$L' = L_{\mathrm{Sk}} + L_{\mathrm{WZ}}. \tag{5.4}$$

There are seven collective coordinates. The momenta p_α that are canonically conjugate to q^α are defined as

$$p_\alpha = \frac{\partial L'}{\partial \dot{q}^\alpha} = \frac{1}{2}\{\dot{q}^\beta, g_{\beta\alpha}) - i\lambda' C'^{(0)}_\alpha(q). \tag{5.5}$$

These satisfy the canonical commutation relations (4.11). The WZW term may be considered as an external potential in the system.[16] The seven right transformation generators may be defined as

$$\hat{R}_{\overline{(A)}} = \frac{i}{2}\{p_\alpha + \lambda' i C'^{(0)}_\alpha(q), C'^{\alpha}_{\overline{(A)}}(q)\} = \frac{i}{2}\{\dot{q}^\beta, C'^{(\overline{B})}_\beta(q)\}E_{\overline{(B)}\overline{(A)}}. \tag{5.6}$$

The commutation rules for the generators (5.6) and their action on the $D^{(\lambda,\mu)}$ matrices are given in the Appendix. It is convenient to define an eighth transformation generator formally as[6]

$$\hat{R}_{(0)} = -\lambda'. \tag{5.7}$$

The SU(2) subalgebra of the operators $\hat{R}_{(0,1,M)}$ satisfies the standard SU(2) commutation conditions and may be interpreted as spin generators (Appendix). The eight left transformation generators may be defined as

$$\hat{L}_{(B)} = \tfrac{1}{2}\{\hat{R}_{(A)}, D^{(1,1)}_{(A)(B)}(-q)\}. \tag{5.8}$$

The transformation properties and commutation relations for the left and right transformation generators are given in the Appendix.

The effective Lagrangian, which includes the WZW term takes the form,

$$\begin{aligned} L_{\text{eff}} &= \frac{1}{2a^{\frac{1}{2}}_{\frac{1}{2}}(F)}(-1)^{\bar{A}}\hat{R}_{(A)}\hat{R}_{(-\bar{A})} + \left(\frac{1}{2a_1(F)} - \frac{1}{2a^{\frac{1}{2}}_{\frac{1}{2}}(F)}\right)(\hat{R}_{(0,1,\cdot)}\cdot\hat{R}_{(0,1,\cdot)}) - \lambda'\frac{i}{2}\{\dot{q}^{\alpha}, C'^{(0)}_{\alpha}(q)\} \\ &\quad - M_{\text{cl}} - \Delta M_1 - \Delta M_2 - \Delta M_3 - \Delta M'(q) \\ &= \frac{1}{2a^{\frac{1}{2}}_{\frac{1}{2}}(F)}((-1)^{A}\hat{L}_{(A)}\hat{L}_{(-A)} - \lambda'^2) + \left(\frac{1}{2a_1(F)} - \frac{1}{2a^{\frac{1}{2}}_{\frac{1}{2}}(F)}\right) \\ &\quad \times(\hat{R}_{(0,1,\cdot)}\cdot\hat{R}_{(0,1,\cdot)}) - \lambda'\frac{i}{2}\{\dot{q}^{\alpha}, C'^{(0)}_{\alpha}(q)\} - \Delta M_1 - \Delta M_2 - \Delta M_3 - M_{\text{cl}}. \end{aligned} \tag{5.9}$$

Note that the $\Delta M'(q)$ term which depends on quantum variables due to introducing left translation generators [see (A13)] in the Lagrangian expression (5.9) vanishes.

For the purpose of obtaining Euler-Lagrange equations that are consistent with the canonical equation of motion of the Hamiltonian, the general method of quantization on a curved space developed by Sugano *et al.*[17] is employed, in which the following auxiliary function is introduced:

$$\begin{aligned} Z(q) &= -\frac{1}{16}f^{ab}f^{cd}f^{ek}(\partial_a g_{cd})(\partial_b g_{ek}) - \frac{1}{4}\partial_a(f^{ab}f^{cd}\partial_b g_{cd}) - \frac{1}{4}\partial_a\partial_b f^{ab} \\ &= -\frac{1}{4}\partial_b C'^{\,a}_{(A)}(q)E^{(\bar{A})(\bar{B})}\partial_a C'^{\,b}_{(B)}(q) + \frac{3}{16a^{\frac{1}{2}}_{\frac{1}{2}}(F)}((-1)^{\bar{A}}C'^{(0)}_{a}(q)C'^{\,a}_{(\bar{A})}(q)C'^{\,b}_{(-\bar{A})}(q)C'^{(0)}_{b}(q) + 4). \end{aligned} \tag{5.10}$$

With this the covariant kinetic term may be defined as

$$\begin{aligned} 2K &= \frac{1}{2}\{p_{\alpha} + i\lambda C'^{(0)}_{\alpha}(q), \dot{q}^{\alpha}\} - Z(q) \\ &= \frac{1}{a^{\frac{1}{2}}_{\frac{1}{2}}(F)}((-1)^{A}\hat{L}_{(A)}\hat{L}_{(-A)} - \lambda'^2) + \left(\frac{1}{a_1(F)} - \frac{1}{a^{\frac{1}{2}}_{\frac{1}{2}}(F)}\right)(\hat{R}_{(0,1,\cdot)}\cdot\hat{R}_{(0,1,\cdot)}). \end{aligned} \tag{5.11}$$

According to the prescription[17] the effective Hamiltonian [with the constraint (5.7)] is constructed in the standard form as

$$H = \tfrac{1}{2}\{p_{\alpha}, \dot{q}^{\alpha}\} - L_{\text{eff}} - Z(q) = K + \Delta M_1 + \Delta M_2 + \Delta M_3 + M_{\text{cl}}. \tag{5.12}$$

Upon renormalization the Lagrangian density (4.15) may be reexpressed in terms of left and right transformation generators. The effective Hamiltonian density without the symmetry breaking term in turn takes the form

$$\begin{aligned} \mathcal{H}_{\text{Sk}} &= \frac{(1-\cos F)}{4a^{2}_{\frac{1}{2}}(F)}\left[f_{\pi}^2 + \frac{1}{4e^2}\left(F'^2 + \frac{2}{r^2}\sin^2 F\right)\right][(-1)^{A}\hat{L}_{(A)}\hat{L}_{(-A)} - (\hat{R}_{(0,1,\cdot)}\cdot\hat{R}_{(0,1,\cdot)}) - \lambda'^2] \\ &\quad + \frac{\sin^2 F}{2a_1^2(F)}\left[f_{\pi}^2 + \frac{1}{e^2}\left(F'^2 + \frac{1}{r^2}\sin^2 F\right)\right][(\hat{R}_{(0,1,\cdot)}\cdot\hat{R}_{(0,1,\cdot)}) - (\hat{R}_{(0,1,\cdot)}\cdot\hat{x})(\hat{R}_{(0,1,\cdot)}\cdot\hat{x})] \\ &\quad + \Delta\mathcal{M}_1 + \Delta\mathcal{M}_2 + \Delta\mathcal{M}_3 + \mathcal{M}_{\text{cl}}. \end{aligned} \tag{5.13}$$

The products of spin operators $\hat{R}_{(0,1,M)}$ may be separated into scalar and tensorial terms as

$$(\hat{R}_{(0,1,\cdot)}\cdot\hat{R}_{(0,1,\cdot)})-(\hat{R}_{(0,1,\cdot)}\cdot\hat{x})(\hat{R}_{(0,1,\cdot)}\cdot\hat{x})=\frac{2}{3}(\hat{R}_{(0,1,\cdot)}\cdot\hat{R}_{(0,1,\cdot)})-\frac{4\pi}{3}Y^{*}_{2,M+M'}(\vartheta,\varphi)\times\begin{bmatrix}1 & 1 & 2\\ M & M' & M+M'\end{bmatrix}\hat{R}_{(0,1,M)}\hat{R}_{(0,1,M')},\quad(5.14)$$

where $Y_{l,M}(\vartheta,\varphi)$ is a spherical harmonic and the factor in the square brackets on the right-hand side is an SU(2) Clebsch-Gordan coefficient.

The covariant kinetic term (5.11) is a differential operator constructed from SU(3) left and SU(2) right transformation generators. The eigenstates of the Hamiltonian (5.12) are

$$\left|\begin{matrix}(\Lambda,M)\\ Y,T,M_T;Y',S,M_S\end{matrix}\right\rangle=\sqrt{\dim(\Lambda,M)}D^{*(\Lambda,M)}_{(Y,T,M_T)(Y',S,M_S)}(q)|0\rangle.\quad(5.15)$$

Here the quantity D on the right-hand side is the complex conjugate Wigner matrix elements of (Λ,M) irrep of SU(3) in terms of quantum variables q^k. The topology of the eigenstates can be nontrivial and the quantum states contain an eighth "unphysical" quantum variable q^0.

The matrix elements of the Hamiltonian density (5.13) for states with spin $S>\frac{1}{2}$ are not spherical and those states consequently have quadrupole moments. In the case $S=\frac{1}{2}$ the matrix element of the second rank operator on the right-hand side of (5.14) vanishes.

VI. THE SYMMETRY BREAKING MASS TERM

The chiral symmetry breaking mass term for the SU(3) soliton was defined (3.13). With the ansatz (4.1) in (3.13) the symmetry breaking density operator for the general irrep (λ,μ) obtains

$$\mathcal{L}_{\mathrm{SB}}=-\mathcal{M}_{\mathrm{SB}}=-\frac{1}{N}\frac{f_\pi^2}{4}[m_0^2\,\mathrm{Tr}\{U_0+U_0^\dagger-2\mathbb{1}\}-2m_8^2\,\mathrm{Tr}\{(U_0+U_0^\dagger)J^{(1,1)}_{(0,0,0)}\}D^{(1,1)}_{(0)(0)}(-q)].\quad(6.1)$$

The operator (6.1) contains the matrix elements $D^{(1,1)}$, which depend on the quantum variables q^α. In this form this operator mixes the representations (Λ,M) of the eigenstates of the Hamiltonian.[18] The physical states of the system with symmetry breaking term therefore in principle must be calculated by diagonalization of the Hamiltonian. Since the mass term is a minor part of the Lagrangian it may be considered as a perturbation in the SU(3) representation (Λ,M).

For a given irrep (λ,μ), in which the Lagrangian is defined, the symmetry breaking term depends on the chiral angle $F(r)$ as

$$\begin{aligned}\mathrm{Tr}\{U_0+U_0^\dagger-2\mathbb{1}\}&=2\sum_{z,j}^{(\lambda,\mu)}\left(\sum_{m=-j}^{j}\cos 2mF(r)\right)-2\dim(\lambda,\mu)\\&=2\,\frac{\sin(1+\lambda)F(r)+\sin(1+\mu)F(r)-\sin(\lambda+\mu+2)F(r)}{2\sin F(r)-\sin 2F(r)}-2\dim(\lambda,\mu).\end{aligned}\quad(6.2)$$

Further development of the expression (6.1) leads to

$$\mathrm{Tr}\{(U_0+U_0^\dagger)J^{(1,1)}_{(0,0,0)}\} = 2\sum_{z,j}^{(\lambda,\mu)} 2\sqrt{3}\left[\frac{1}{3}(\lambda-\mu)+z\right]\left(\sum_{m=-j}^{j}\cos 2mF(r)\right)$$

$$= \frac{2\sqrt{3}}{2\sin F(r)-\sin 2F(r)}\times\left\{\frac{1}{2}(1+\mu)(\sin(1+\mu)F(r)-\sin(\lambda+\mu+2)F(r))\right.$$

$$+\frac{1}{3}(\lambda-\mu)(\sin(1+\lambda)F(r)+\sin(1+\mu)F(r)-\sin(\lambda+\mu+2)F(r))$$

$$+\frac{1}{2}(1+\lambda)[(\sin F(r)-\sin(2+\mu)F(r))\cos\lambda F(r)$$

$$\left.-(\cos F(r)-\cos(2+\mu)F(r))\sin\lambda F(r)]\right\}. \tag{6.3}$$

For high irrep (λ,μ) the dependence of the symmetry breaking term on the chiral angle $F(r)$ differs significantly from that in the fundamental representation (1, 0). In that representation the symmetry breaking term takes the standard form

$$\mathcal{M}_{\mathrm{SB}} = f_\pi^2(1-\cos F)\left[m_0^2+\frac{1}{\sqrt{3}}m_8^2 D^{(1,1)}_{(0)(0)}(-q)\right]. \tag{6.4}$$

In the case of (2, 0) representation the expression is

$$\mathcal{M}_{\mathrm{SB}} = \frac{1}{5}f_\pi^2\left[(1-\cos F+2\sin^2 F)m_0^2-(1-\cos F-4\sin^2 F)\frac{m_8^2}{\sqrt{3}}D^{(1,1)}_{(0)(0)}(-q)\right]. \tag{6.5}$$

Note that in both cases the asymptotical behavior at large distance of the symmetry breaking terms are different.

VII. DISCUSSION

Above the SU(3) Skyrme model was quantized canonically in the framework of the collective coordinate formalism for representations of arbitrary dimension. This leads to the complete quantum mechanical structure of the model on the homogeneous space SU(3)/U(1). The results extend those obtained earlier in the fundamental representation for SU(2) and SU(3) (Refs. 5 and 6) and those obtained in general representations of SU(2).[7–9] The explicit representation dependence of the quantum corrections to the Skyrme model Lagrangian was derived. This dependence is nontrivial, especially for the Wess-Zumino-Witten and the symmetry breaking terms. The operators that form the Hamiltonian were shown to have well-defined group-theoretical properties.

The choice of the irrep that is used for the unitary field depends on the phenomenological aspects of the physical system to which the model is applied. Formally the variation of the irrep can be interpreted as modification of the Skyrme model. The representation dependence of the Wess-Zumino-Witten term was shown to be absorbable into a normalization factor, with exception of the self-adjoint irreps in which this term vanishes. The symmetry breaking term has different functional dependence on chiral angle $F(r)$ in different irreps. In case of self-adjoint representations the symmetry breaking term, which is proportional to the m_8^2 coefficient also vanishes.

The effective Hamiltonian (5.12) commutes with the left transformation generators $\hat{L}_{(A)}$ and the right transformation (spin) generators $\hat{R}_{(0,1,M)}$,

$$[\hat{L}_{(A)},H]=[\hat{R}_{(0,1,M)},H]=0, \tag{7.1}$$

which ensures that the states (5.15) are the eigenstates of the effective Hamiltonian.

The symmetry breaking term does, however, not commute with the left generators,

$$[\hat{L}_{\left(Z,\frac{1}{2},M\right)}, M_{\mathrm{SB}}] \neq 0, \tag{7.2}$$

and therefore this term mix the states in different representations (Λ, M).

A result of this investigation is the tensor term (5.15) in the Hamiltonian density operator (5.14). Because of the tensor operator the states with spin $S > \frac{1}{2}$ have quadrupole moments.

Consider finally the energy functional of the quantum skyrmion in the states of (Λ, M) irrep. The problem is simplified if the symmetry breaking term that leads to representation mixing is dropped,

$$E(F) = \frac{C_2^{\mathrm{SU}(3)}(\Lambda, M) - \lambda'^2}{a_{\frac{1}{2}}(F)} + \left(\frac{1}{a_1(F)} - \frac{1}{a_{\frac{1}{2}}(F)}\right) S(S+1) + \Delta M_1 + \Delta M_2 + \Delta M_3 + M_{\mathrm{cl}}. \tag{7.3}$$

The variational condition for the energy is

$$\frac{\delta E(F)}{\delta F} = 0, \tag{7.4}$$

with the usual boundary conditions $F(0) = \pi$, $F(\infty) = 0$. At large distances this equation reduces to the asymptotic form

$$\tilde{r}^2 F'' + 2\tilde{r}F' - (2 + \tilde{m}^2\tilde{r}^2)F = 0, \tag{7.5}$$

where the quantity $\tilde{m}^2$ is defined as

$$\tilde{m}^2 = -e^4 \left(\frac{1}{4\tilde{a}^2_{\frac{1}{2}}(F)} (C_2^{\mathrm{SU}(3)}(\Lambda, M) - S(S+1) - \lambda'^2 + 1) + \frac{2\,S(S+1)+3}{3\tilde{a}_1^2(F)} + \frac{8\Delta\tilde{M}_1 + 4\Delta\tilde{M}_3}{3\tilde{a}_1(F)} \right.$$
$$\left. + \frac{\Delta\tilde{M}_3 + 2\Delta\tilde{M}_2}{2\tilde{a}_{\frac{1}{2}}(F)} + \frac{1}{\tilde{a}_1(F)\tilde{a}_{\frac{1}{2}}(F)} \right). \tag{7.6}$$

The corresponding asymptotic solution takes the form

$$F(\tilde{r}) = k\left(\frac{\tilde{m}^2}{\tilde{r}} + \frac{1}{\tilde{r}^2}\right) \exp(-\tilde{m}\tilde{r}). \tag{7.7}$$

The quantum corrections depends on the irrep (λ, μ) to which the unitary field $\mathrm{U}(\mathbf{x}, t)$ belongs as well as on the state irrep (Λ, M) and spin S. This bears on the stability of quantum skyrmion, the requirement of stability of which the integrals (4.9b) and (4.9c) and ΔM_k converge. This requirement is satisfied only if $\tilde{m}^2 > 0$. That condition is only satisfied in the presence of the negative quantum mass corrections ΔM_k. It is the absence of this term, which leads to the instability of the skyrmion in the semiclassical approach[9] in the SU(2) case. Note that in the quantum treatment the chiral angle $F(\tilde{r})$ has the asymptotic exponential behavior (7.7) even in the chiral limit.

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APPENDIX A

The functions $C'^{(\bar{A})}_{\alpha}(q)$ defined in (2.2) are siebenbeins which constitute nonsingular 7×7 matrices. We can introduce the reciprocal functions $C'^{\alpha}_{(\bar{B})}(q)$ by

$$\sum_{\overline{A}} C'^{(\overline{A})}_{\alpha}(q)\cdot C'^{\beta}_{\underline{(A)}}(q)=\delta_{\alpha\beta}, \tag{A1a}$$

$$\sum_{\alpha} C'^{(\overline{A})}_{\alpha}(q)\cdot C'^{\alpha}_{\underline{(B)}}(q)=\delta_{\overline{(A)}\overline{(B)}}. \tag{A1b}$$

Here $(\overline{A})$ and $(\overline{B})$ denote the basis of the irrep (1, 1), with exception for the state (0, 0, 0). The $C'^{\alpha}_{(0)}(q)$ are not defined.

The properties of the functions $C'^{(K)}_{\alpha}(q)$ follow from $\partial_\alpha\partial_\beta D^{(\lambda,\mu)}=\partial_\beta\partial_\alpha D^{(\lambda,\mu)}$:

$$\partial_\beta C'^{(K)}_{\alpha}(q)-\partial_\alpha C'^{(K)}_{\beta}(q)-\sqrt{3}\begin{bmatrix}(1,1) & (1,1) & (1,1)_a\\ (K') & (K'') & (K)\end{bmatrix}C'^{(K')}_{\beta}(q)C'^{(K'')}_{\alpha}(q)=0, \tag{A2}$$

and are correct for all states (K) including (0, 0, 0). The following properties of the functions $C'^{\alpha}_{\underline{(K)}}(q)$ are useful:

$$\begin{aligned}&C'^{\alpha}_{\underline{(K')}}(q)\partial_\alpha C'^{\beta}_{\underline{(K'')}}(q)-C'^{\alpha}_{\underline{(K'')}}(q)\partial_\alpha C'^{\beta}_{\underline{(K')}}(q)+\sqrt{3}\begin{bmatrix}(1,1) & (1,1) & (1,1)_a\\ \overline{(K')} & \overline{(K'')} & \overline{(K)}\end{bmatrix}C'^{\beta}_{\underline{(K)}}(q)\\ &\quad=\sqrt{3}z''C'^{(0)}_{\alpha}(q)C'^{\alpha}_{\underline{(K')}}(q)C'^{\beta}_{\underline{(K'')}}(q)-\sqrt{3}z'C'^{(0)}_{\alpha}(q)C'^{\alpha}_{\underline{(K'')}}(q)C'^{\beta}_{\underline{(K')}}(q).\end{aligned} \tag{A3}$$

In Sec. V the right transformation generators (5.6) are defined with the following commutation relations:

$$\begin{aligned}[\hat{R}_{\overline{(A')}},\hat{R}_{\overline{(A'')}}]=&-\sqrt{3}\begin{bmatrix}(1,1) & (1,1) & (1,1)_a\\ \overline{(A')} & \overline{(A'')} & \overline{(A)}\end{bmatrix}\hat{R}_{\overline{(A)}}+\sqrt{3}z''\{C'^{\alpha}_{\underline{(A')}}(q)C'^{(0)}_{\alpha}(q),\hat{R}_{\overline{(A'')}}\}\\ &-\sqrt{3}z'\{C'^{\alpha}_{\underline{(A'')}}(q)C'^{(0)}_{\alpha}(q),\hat{R}_{\overline{(A')}}\}.\end{aligned} \tag{A4}$$

The SU(2) subalgebra of the generators $\hat{R}_{(0,1,M)}$ satisfies the standard SU(2) commutation relations. These may be interpreted as spin operators because its acting on unitary field (4.1) can be realized as a spatial rotation of skyrmion only,

$$[\hat{R}_{(0,1,M)},A(q)U_0(x)A(q)^{\dagger}]=A(q)[J^{(1,1)}_{(0,1,M)},U_0(x)]A^{\dagger}(q). \tag{A5}$$

The transformation rule for irrep matrices is

$$[\hat{R}_{\overline{(K)}},D^{(\lambda,\mu)}_{(A)(A')}(q)]=D^{(\lambda,\mu)}_{(A)(A'')}(q)\left\langle\begin{matrix}(\lambda,\mu)\\ A''\end{matrix}\middle|J^{\underline{(1,1)}}_{(K)}\middle|\begin{matrix}(\lambda,\mu)\\ A'\end{matrix}\right\rangle-\frac{\sqrt{3}}{2}y'C'^{\alpha}_{\underline{(K)}}(q)C'^{(0)}_{\alpha}(q)D^{(\lambda,\mu)}_{(A)(A')}(q). \tag{A6}$$

The eight left transformation generators are defined as

$$\hat{L}_{(B)}=\frac{1}{2}\{\hat{R}_{(A)},D^{(1,1)}_{(A)(B)}(-q)\}=\frac{i}{2}\{p_\beta+\lambda iC'^{(0)}_{\beta}(q),K^{\beta}_{(B)}(q)\}+\lambda D^{(1,1)}_{(0)(B)}(-q), \tag{A7}$$

where

$$K^{\beta}_{(B)}(q)=C'^{\beta}_{\underline{(A)}}(q)D^{\underline{(1,1)}}_{(A)(B)}(-q), \tag{A8}$$

the properties of which follows from (A3):

$$K^{\beta''}_{(B'')}(q)\partial_{\beta''}K^{\beta'}_{(B')}(q)-K^{\beta''}_{(B')}(q)\partial_{\beta''}K^{\beta'}_{(B'')}(q)=\sqrt{3}\begin{bmatrix}(1,1) & (1,1) & (1,1)_a\\ (B'') & (B') & (B)\end{bmatrix}K^{\beta'}_{(B)}(q). \tag{A9}$$

By making use of (A4) it may be proven that

$$[\hat{L}_{(B')},\hat{L}_{(B'')}]=\sqrt{3}\begin{bmatrix}(1,1) & (1,1) & (1,1)_a\\ (B') & (B'') & (B)\end{bmatrix}\hat{L}_{(B)}. \tag{A10}$$

The three right transformation generators or spin operators $\hat{R}_{(0,1,M)}$ commute with the left transformation generators,

$$[\hat{R}_{(0,1,M)},\hat{L}_{(B)}]=0. \tag{A11}$$

The left transformation rules for the irrep matrices are

$$\begin{aligned}[\hat{L}_{(B)},D^{(\lambda,\mu)}_{(A')(A)}(q)] &= \langle A'|J^{(1,1)}_{(B)}|A''\rangle D^{(\lambda,\mu)}_{(A'')(A)}(q)\\ &-\frac{\sqrt{3}}{2}y_A\cdot D^{(1,1)}_{(0)(B)}(-q)D^{(\lambda,\mu)}_{(A')(A)}(q)-\frac{\sqrt{3}}{2}y_A\cdot C'^{(0)}_{\alpha}(q)C'^{\alpha}_{(B')}(q)D^{(1,1)}_{(B')(B)}(-q)D^{(\lambda,\mu)}_{(A')(A)}(q).\end{aligned} \tag{A12}$$

It is straightforward to derive the following result:

$$(-1)^B\hat{L}_{(B)}\hat{L}_{(-B)}=(-1)^{\bar{A}}\hat{R}_{(A)}\hat{R}_{(-\bar{A})}+\lambda'^2-\tfrac{3}{4}-\tfrac{3}{16}(-1)^{\bar{A}}C'^{(0)}_{\alpha}(q)C'^{\alpha}_{(\bar{A})}(q)C'^{(0)}_{\beta}(q)C'^{\beta}_{(-\bar{A})}(q). \tag{A13}$$

For the derivation of the Lagrangian density the following expressions are needed:

$$E^{(\bar{A})(\bar{B})}(F)J^{(1,1)}_{(A)}J^{(1,1)}_{(B)}=-\frac{1}{a_{\frac{1}{2}}(F)}\hat{C}^{\mathrm{SU}(3)}_2+\left(\frac{1}{a_{\frac{1}{2}}(F)}-\frac{1}{a_1(F)}\right)\hat{C}^{\mathrm{SU}(2)}+\frac{1}{a_{\frac{1}{2}}(F)}(J^{(1,1)}_{(0,0,0)})^2, \tag{A14}$$

$$\begin{aligned}E^{(\bar{A})(\bar{B})}(F)D^{I}_{(\bar{B'})(\bar{B})}(\hat{x},F(r))J^{(1,1)}_{(A)}J^{(1,1)}_{(B')} &= -\frac{\cos F}{a_{\frac{1}{2}}(F)}\hat{C}^{\mathrm{SU}(3)}_2+\left(\frac{\cos F}{a_{\frac{1}{2}}(F)}-\frac{\cos 2F}{a_1(F)}\right)\hat{C}^{\mathrm{SU}(2)}+\frac{\cos F}{a_{\frac{1}{2}}(F)}(J^{(1,1)}_{(0,0,0)})^2\\ &+i\left(\frac{\sin 2F}{a_1(F)}+\frac{\sin F}{a_{\frac{1}{2}}(F)}\right)(J^{(1,1)}_{(0,1,\cdot)}\cdot\hat{x})-2\frac{\sin^2 F}{a_1(F)}(J^{(1,1)}_{(0,1,\cdot)}\cdot\hat{x})\\ &\times(J^{(1,1)}_{(0,1,\cdot)}\cdot\hat{x}).\end{aligned} \tag{A15}$$

Here $D^{I}_{(\bar{B'})(\bar{B})}(\hat{x},F(r))$ is a Wigner matrix of the SU(2). The summation is over SU(2) representations $I=\frac{1}{2}$, 1 and the corresponding bases,

$$E^{(\bar{A})(\bar{B})}(F)\begin{bmatrix}(1,1) & (1,1) & (1,1)_a\\ (\bar{A}) & (0,1,u) & (\bar{C})\end{bmatrix}J^{(1,1)}_{(B)}J^{(1,1)}_{(\bar{C})}=\frac{1}{\sqrt{3}}\left(\frac{1}{2a_{\frac{1}{2}}(F)}+\frac{1}{a_1(F)}\right)J^{(1,1)}_{(0,1,u)}, \tag{A16}$$

$$\begin{aligned}&E^{(\bar{A})(\bar{B})}(F)\begin{bmatrix}(1,1) & (1,1) & (1,1)_a\\ (\bar{A}) & (0,1,u) & (\bar{C})\end{bmatrix}D^{I}_{(\bar{C'})(\bar{C})}(\hat{x},F(r))J^{(1,1)}_{(B)}J^{(1,1)}_{(C')}\\ &=\frac{1}{\sqrt{3}}\Bigg\{-[J^{(1,1)}_{(0,1,\cdot)}\times\hat{x}]_u\left(\frac{\sin F}{2a_{\frac{1}{2}}(F)}+i\frac{2\sin^2 F}{a_1(F)}(J^{(1,1)}_{(0,1,\cdot)}\cdot\hat{x})\right)\\ &-i\left(\frac{\sin F}{2a_{\frac{1}{2}}(F)}\hat{C}^{\mathrm{SU}(3)}_2-\left(\frac{\sin F}{2a_{\frac{1}{2}}(F)}-\frac{\sin 2F}{a_1(F)}\right)\hat{C}^{\mathrm{SU}(2)}-\frac{\sin F}{2a_{\frac{1}{2}}(F)}(J^{(1,1)}_{(0,0,0)})^2\right)\hat{x}_u\end{aligned}$$

$$+\left(\frac{\cos 2F}{a_1(F)}+\frac{\cos F}{2a_{\frac{1}{2}}(F)}+i\frac{\sin 2F}{a_1(F)}(J^{(1,1)}_{(0,1,\cdot)}\cdot\hat{x})\right)J^{(1,1)}_{(0,1,u)}\Bigg\}. \tag{A17}$$

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Changes in nonlinear potential scattering theory in electron gases brought about by reducing dimensionality

N. H. March
Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium; Oxford University, Oxford, England; and Donostia International Physics Center (DIPC), E-20080 San Sebastian, Spain

I. A. Howard
Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium

I. Nagy
Department of Theoretical Physics, Institute of Physics, Technical University of Budapest, H-1521 Budapest, Hungary; and Donostia International Physics Center (DIPC), E-20080 San Sebastian, Spain

P. M. Echenique
Donostia International Physics Center (DIPC), E-20080 San Sebastian, Spain; and Departamento de Fisica de Materiales, Facultad de Ciencias-Quimicas, Apto. 1072, E-20080 San Sebastian, Spain

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Recent work has shown the essential equivalence of stopping power, force-force correlation function, and phase-shift analysis for nonlinear potential scattering in a three-dimensional electron gas. In the present study, we first demonstrate that the above situation is markedly different when the scattering occurs from a localized potential in a two-dimensional (2D) electron gas. Only to second order in the potential do the three methods referred to above precisely agree. However, all these methods can still be applied in 2D, some fully nonlinear evaluation proving possible. The one-dimensional case is also discussed, albeit more briefly. Scattering from a two-center modeling of the localized potential is also calculated, but now only in the Born approximation, due to the added complication of a noncentral potential. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1947118]

I. INTRODUCTION

Following a vast body of experimental and theoretical studies on three-dimensional metals and alloys,[1,2] attention more recently has focused on two-dimensional systems of itinerant electrons. As an immediate example, on the (111) surfaces of noble metals, e.g., Au, Ag, and Cu, quasiparticles form a two-dimensional electron gas. This has been investigated experimentally by cold scanning tunneling microscopy.[3,4] Turning to physical properties associated with such two-dimensional electron gases (2DEG), the present paper will have as its focus the scattering in such assemblies of the itinerant electrons from localized impurity centers. Then, it is natural enough to proceed with the discussion for spin-compensated impurity systems. However, it is highly relevant to note that both theoretical[5] and experimental[6] studies have appeared recently. In the former, the 2DEG was considered in the presence of a single magnetic impurity (e.g., Co) and the additional scattering phase shift induced by the charge of the Co ion and its specially extended displaced electronic density distribution.[5] Subsequently, scanning tunneling microscopy was employed[6] to measure the phase shift that surface-state electrons suffer when scattering from a single magnetic impurity, which forms a Kondo state.

This is the context then which has motivated the present theoretical study. This follows the earlier discussions,[7,8] of a few aspects of the stopping power of a 2DEG for heavy particles. Two

results utilized there form a valuable starting point for the present study of such a two-dimensional system. First, the transport (tr) cross section is given in the partial wave representation as

$$\sigma_{tr}(k_F) = \frac{4}{k_F} \sum_{m=0}^{\infty} \sin^2[\delta_m(k_F) - \delta_{m+1}(k_F)], \tag{1.1}$$

where k_F denotes the Fermi wave number of the electron gas, related to the Fermi energy E_F by

$$E_F = k_F^2/2. \tag{1.2}$$

In Eq. (1.1), the scattering phase shifts at the Fermi level are denoted by $\delta(k_F)$ for the different partial waves ($m=0,1,\ldots$, etc.). We are interested further in the stopping power $\mathrm{d}E/\mathrm{d}x$ say, at $T=0$, to which the present treatment is restricted, for a heavy ion moving with velocity $\mathbf{v}$. This is related in a direct fashion, as set out in Ref. 7 for slow ions, to the transport cross section σ_{tr} in Eq. (1.1) above

$$\frac{\mathrm{d}E}{\mathrm{d}x} = n_0 v v_F \sigma_{tr}(k_F), \tag{1.3}$$

in which n_0 and v_F are, respectively, the areal density and Fermi velocity of the 2DEG.

The outline of the present investigation is then as follows. In Sec. II below, a force-force correlation function formula, due to Rousseau, Stoddart, and March (RSM),[2,9] in three dimensions, is first adapted to two dimensions. We comment here on the three-dimensional (3D) result. There, the total potential which scatters the electrons is denoted by $V(\mathbf{r})$, and this generates a Dirac density matrix $\gamma(\mathbf{r}_1,\mathbf{r}_2,E)$, which is such that its diagonal element, say $\gamma(\mathbf{r},\mathbf{r},E)$, denotes the integrated local density of electronic states. Correlating the force $-\partial V(\mathbf{r})/\partial \mathbf{r}$ at points $\mathbf{r}_1$ and $\mathbf{r}_2$ via $\partial\gamma(\mathbf{r}_1,\mathbf{r}_2,E)/\partial E$, which is then a generalized density of states, it can readily be shown, when $V(\mathbf{r})$ is assumed to be a central potential $V(r) \equiv V(|\mathbf{r}|)$, to be related to the phase shifts $\delta_l(E)$ for scattering off $V(r)$, via the radial wave functions $R_l(r,E)$ from which the density matrix is constructed. The 3D force-force correlation function formula of RSM is then exactly equivalent to the phase-shift scattering cross section for impurity resistivity of Huang,[10] as shown by one of us.[11] In Sec. II, this 3D situation will be contrasted with that in 2D. Adapting the RSM formula in 3D then leads to the 2D analog set out in Eq. (2.1) below, where account is taken of the Fermi statistics of electrons by considering, as in 3D, that scattering is on the Fermi surface, corresponding to Fermi energy E_F. The 2D phase shift result derived in Eq. (2.15) below for the force-force correlation function is demonstrated here to be distinct from the stopping power in 2D already set out in Eqs. (1.1) and (1.3). This is in contrast to the equivalence of the force-force correlation function and the scattering cross section in 3D which we have discussed above.

Section III is then devoted to studying at some length the Born approximation to this force-force correlation function. In this section, contact is then made with Eqs. (1.1) and (1.3) above. In Sec. IV further illustrations are given by using linear-response formalism for the induced density in 2D. The one-dimensional case of scattering is outlined in Sec. V. Finally, additional and more technical details are summarized in four Appendixes at the end of the paper.

II. FORCE-FORCE CORRELATION FUNCTION IN A TWO-DIMENSIONAL ELECTRON GAS

As indicated above, let us take as starting point a definition of the force-force correlation function in two dimensions as

$$\langle \mathbf{F}\cdot\mathbf{F}\rangle = \int d\mathbf{r}_1 d\mathbf{r}_2 \frac{\partial V(\mathbf{r}_1)}{\partial \mathbf{r}_1}\cdot\frac{\partial V(\mathbf{r}_2)}{\partial \mathbf{r}_2}\left[\frac{\partial \gamma(\mathbf{r}_1,\mathbf{r}_2,E)}{\partial E}\right]^2_{E=E_F}. \tag{2.1}$$

Evidently the two forces $-\partial V(\mathbf{r})/\partial \mathbf{r}$ at two-dimensional position vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ are correlated via the off-diagonal local density of states $N(E,\mathbf{r}_1,\mathbf{r}_2)\equiv \partial\gamma/\partial E$ evaluated at the Fermi level E_F, γ as defined above being the off-diagonal integrated density of states.

As emphasized in three dimensions by Rousseau *et al.*,[9] the merit of the corresponding two-dimensional form in Eq. (2.1) is that it is defined for potentials $V(\mathbf{r})$ of lower than circular symmetry. However, it is a valuable starting point in calculating the force-force correlation function $\langle \mathbf{F}\cdot\mathbf{F}\rangle$ in Eq. (2.1) to treat the case of circular symmetry, i.e., $V(\mathbf{r})=V(|\mathbf{r}|)=V(r)$. This is the objective of the present section. For this limiting case of $V(r)$ with circular symmetry, we shall draw also on the treatments by Adhikari[12] and by Tang and Thouless.[13]

Beginning then with the wave function $\psi(r,\theta)$ in polar coordinates defined by $x=r\cos\theta$ and $y=r\sin\theta$, one can write in the asymptotic region, far from the origin of the scattering potential energy $V(r)$, that $\psi(r,\theta)$ consists of a plane wave, propagating say along the x axis, plus a scattered outgoing wave. Both Refs. 12 and 13 adopt the form

$$\psi(r,\theta)_{r\to\infty} \to \exp(ikx) + \sqrt{i/k} f_k(\theta)\frac{\exp(ikr)}{\sqrt{r}}, \tag{2.2}$$

where $f_k(\theta)$ denotes the scattering amplitude. This result (2.2) follows asymptotically from the Schrödinger equation

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \psi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2} + k^2\psi = U\psi, \tag{2.3}$$

where $k^2=2mE/\hbar^2$ and $U(r)=2mV(r)/\hbar^2$. In this case of circular symmetry $V(r)$, one can separate the variables r and θ by writing

$$\psi(r,\theta) = R(r)\Theta(\theta), \tag{2.4}$$

to find

$$\frac{d^2\Theta}{d\theta^2} + m^2\Theta = 0. \tag{2.5}$$

Hence, we have now wave functions of the form following from Eq. (2.4) plus the physically significant solution of Eq. (2.5) as

$$\psi_m(\mathbf{r}_1) = \exp(im\theta_1)R(k_F r_1). \tag{2.6}$$

Returning to the definition (2.1), we can write the energy derivative of the Dirac matrix γ in terms of $\psi_m(\mathbf{r}_1)$ and the energies E_i generated by the one-body Hamiltonian H given by

$$H = -\frac{1}{2}\nabla^2 + V(r), \tag{2.7}$$

as

$$\frac{\partial\gamma}{\partial E} = \sum_i \psi_i^*(\mathbf{r}_1)\psi_i(\mathbf{r}_2)\delta(E-E_i), \tag{2.8}$$

with the complex conjugate satisfying

$$\frac{\partial \gamma^*}{\partial E} = \sum_j \psi_j(\mathbf{r}_1)\psi_j^*(\mathbf{r}_2)\delta(E-E_j). \tag{2.9}$$

Thus, from Eqs. (2.8) and (2.9) it follows that

$$\left|\frac{\partial \gamma}{\partial E}\right|^2_{E=E_F} = \sum_{i,j} \psi_i^*(k_F\mathbf{r}_1)\psi_j(k_F\mathbf{r}_1)\psi_i(k_F\mathbf{r}_2)\psi_j^*(k_F\mathbf{r}_2). \tag{2.10}$$

Replacing i, j by m, m', it follows from Eq. (2.1) for isotropic scattering potentials that

$$\langle \mathbf{F}\cdot\mathbf{F}\rangle = \int r_1 r_2 \frac{\partial V(r_1)}{\partial r_1}\frac{\partial V(r_2)}{\partial r_2}\cos(\theta_2-\theta_1)\left|\frac{\partial \gamma}{\partial E}\right|^2_{E=E_F} \mathrm{d}r_1\,\mathrm{d}r_2\,\mathrm{d}\theta_1\,\mathrm{d}\theta_2. \tag{2.11}$$

Using the wave functions (2.6), the angular integration in Eq. (2.11) becomes, after some manipulation

$$\begin{aligned}&\frac{1}{2}\sum_{m,m'}\int_0^{2\pi}\int_0^{2\pi}[\exp(i(\theta_2-\theta_1))+\exp(-i(\theta_2-\theta_1))][\exp(i(m-m')\theta_2)\exp(-i(m-m')\theta_1)]\mathrm{d}\theta_1\,\mathrm{d}\theta_2\\ &\quad = 2\pi^2\sum_{m,m'}[\delta(m'=m+1)+\delta(m'=m-1)].\end{aligned} \tag{2.12}$$

Using Eqs. (2.12) and (2.6) in Eq. (2.11), and performing the summation over m' then yields

$$\begin{aligned}\langle \mathbf{F}\cdot\mathbf{F}\rangle = 2\pi^2\sum_m \int_{r_1} r_1\frac{\partial V(r_1)}{\partial r_1}R_m^*(k_Fr_1)[R_{m+1}(k_Fr_1)+R_{m-1}(k_Fr_1)]\mathrm{d}r_1\int_{r_2} r_2\frac{\partial V(r_2)}{\partial r_2}R_m(k_Fr_2)\\ \times[R_{m+1}^*(k_Fr_2)+R_{m-1}^*(k_Fr_2)]\mathrm{d}r_2.\end{aligned} \tag{2.13}$$

Using the result of Tang and Thouless[13] that

$$\int rR_{m+1}^*(kr)\frac{\partial V(r)}{\partial r}R_m(kr)\mathrm{d}r = -\frac{k}{\pi}\exp(\delta_m-\delta_{m+1})\sin(\delta_{m+1}-\delta_m) \tag{2.14}$$

then gives

$$\begin{aligned}\langle \mathbf{F}\cdot\mathbf{F}\rangle &= \frac{(2\pi)^2}{2}\left(\frac{k}{\pi}\right)^2\sum_m[\exp(-i(\delta_m-\delta_{m+1}))\sin(\delta_{m+1}-\delta_m)+\exp(i(\delta_{m-1}-\delta_m))\sin(\delta_m-\delta_{m-1})]\\ &\quad\times[\exp(i(\delta_m-\delta_{m+1}))\sin(\delta_{m+1}-\delta_m)+\exp(-i(\delta_{m-1}-\delta_m))\sin(\delta_m-\delta_{m-1})]\\ &= k^2\sum_m[1-\cos(2(\delta_{m+1}-\delta_{m-1}))].\end{aligned} \tag{2.15}$$

The above analysis is analogous to that of Huang[10] in terms of partial waves of orbital angular momentum quantum number l in 3D; there, only the phase shifts δ_l with $k=k_F$ are required, where k_F is the Fermi wave number (independent of l). This two-dimensional result for the force-force correlation function with $V(\mathbf{r})=V(|\mathbf{r}|)$ appears to be new. It must be stressed that this phase-shift result (2.15) for $\langle \mathbf{F}\cdot\mathbf{F}\rangle$ is distinct from the stopping power in Eqs. (1.1) and (1.3).

Though we do not have an analog of Eq. (2.15) for $\langle \mathbf{F}\cdot\mathbf{F}\rangle$ when the isotropy of $V(\mathbf{r})$ is relaxed, it is of immediate interest to treat this more general case in the Born approximation, and this is the essential content of the following section.

III. FORCE-FORCE CORRELATION FUNCTION IN TWO DIMENSIONS IN THE BORN APPROXIMATION

To calculate $\langle \mathbf{F}\cdot\mathbf{F}\rangle$ in Eq. (2.1) to $\mathcal{O}(V^2)$ for a potential $V(\mathbf{r})$ without circular symmetry, we can make the crucial simplifying approximation that the Dirac density matrix γ in Eq. (2.1) is replaced by its two-dimensional free-electron counterpart $\gamma_0(\mathbf{r}_1,\mathbf{r}_2,E)$. This we obtain following the approach of March and Murray[14,15] in their three-dimensional density matrix perturbation theory, based on the scattering potential $V(r)$ above embedded in an initially uniform free-electron gas. Their main achievement was to start from the canonical, or Bloch density matrix $C(\mathbf{r}_1,\mathbf{r}_2,\beta)$, defined for the one-body Hamiltonian (2.7) having eigenfunctions $\psi_i(\mathbf{r})$ and corresponding eigenvalues ϵ_i as

$$C(\mathbf{r}_1,\mathbf{r}_2,\beta)=\sum_{\text{all}i}\psi_i^*(\mathbf{r}_1)\psi_i(\mathbf{r}_2)\exp(-\beta\epsilon_i):\ \beta=(k_BT)^{-1}. \tag{3.1}$$

The (zero-temperature) Dirac density matrix appearing in Eq. (2.1) is then related to the C matrix in Eq. (3.1) by

$$C(\mathbf{r}_1,\mathbf{r}_2,\beta)=\beta\int_0^\infty \gamma(\mathbf{r}_1,\mathbf{r}_2,E)\exp(-\beta E)\mathrm{d}E. \tag{3.2}$$

A. Free-electron results in two dimensions

It is well known that in D dimensions the free-electron canonical density matrix is given by

$$C_0(\mathbf{r}_1,\mathbf{r}_2,\beta,D)=\frac{1}{(2\pi\beta)^{D/2}}\exp\left(-\frac{|\mathbf{r}_1-\mathbf{r}_2|^2}{2\beta}\right). \tag{3.3}$$

March and Murray were concerned with the three-dimensional case, for which they obtained the Dirac matrix as

$$\gamma_0(\mathbf{r}_1,\mathbf{r}_2,E)_{D=3}=\frac{k_F^3}{2\pi^2}\frac{j_1(k|\mathbf{r}_1-\mathbf{r}_2|)}{k|\mathbf{r}_1-\mathbf{r}_2|}, \tag{3.4}$$

where $j_1(x)$ is the first-order spherical Bessel function $(\sin x - x\cos x)/x^2$, and we have written Eq. (3.4) for single occupied levels.

To obtain the two-dimensional analog, we need the inverse Laplace transform of C_0/β, according to Eq. (3.2), where C_0 is given by Eq. (4.4) with $D=2$. This can be found from Ref. 16 as

$$\gamma_0(\mathbf{r}_1,\mathbf{r}_2,E)=\frac{1}{2\pi}\frac{\sqrt{2E}}{|\mathbf{r}_1-\mathbf{r}_2|}J_1(\sqrt{2E}|\mathbf{r}_1-\mathbf{r}_2|). \tag{3.5}$$

Fortunately, the energy derivative $\partial\gamma/\partial E$ appearing in the force-force formula (2.1) is more compact, and follows after a short calculation using properties of Bessel functions as

$$\frac{\partial\gamma_0(\mathbf{r}_1,\mathbf{r}_2,E)}{\partial E}=\frac{1}{2\pi}J_0(\sqrt{2E}|\mathbf{r}_1-\mathbf{r}_2|). \tag{3.6}$$

An immediate check on the result (3.6) is the density of states $N(E)$ obtained by setting $\mathbf{r}_2=\mathbf{r}_1$ in Eq. (3.6), the result being simply the constant $1/2\pi$ since $J_0(0)=1$. This result (3.6), in conjunction with Eq. (4.7) below, is used in Appendix A to derive the linear response function in two dimensions.

Returning to Eq. (2.1), the force-force correlation function, B denoting the Born approximation, is given, apart from a multiplicative factor, explicitly in terms of the scattering potential $V(\mathbf{r})$ by making use of Eq. (3.6) as

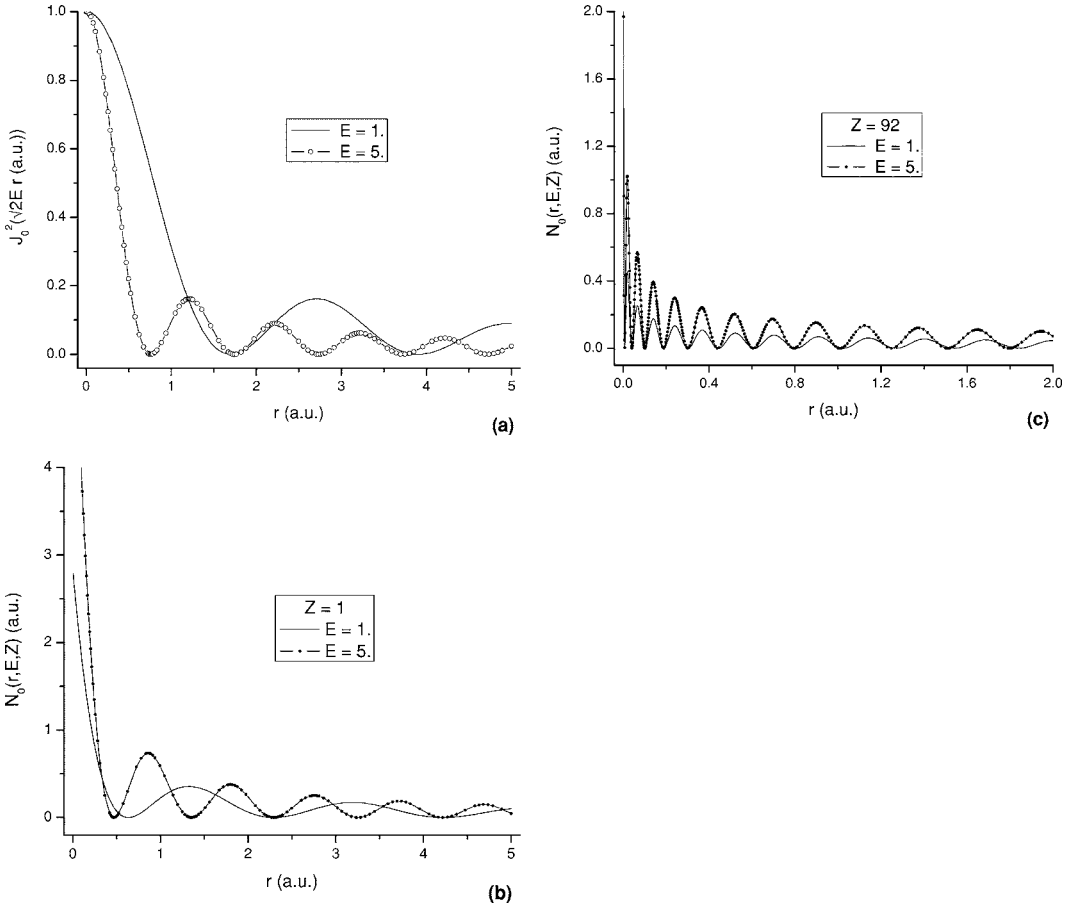

FIG. 1. (a) Plot of $J_0^2(\sqrt{2E}r)$ appearing in force-force correlation function set out in Eq. (3.7), versus r, for two values of E [compare also Eq. (D4)]. Other curves shown are (b) and (c) the s-state ($m=0$) component of the local density of states $N_0(r,E,Z)$ generated by a bare Coulomb potential ($-Z/r$) embedded in a two-dimensional electron gas, for $Z=1$ and 92 and the same two values of energy E as in the plot of J_0^2. Apart from an unimportant normalization factor, J_0^2 is the limit of $N_0(r,E,Z)$ as Z tends to zero.

$$\langle \mathbf{F}\cdot\mathbf{F}\rangle_B \propto \int d\mathbf{r}_1\, d\mathbf{r}_2 \frac{\partial V(\mathbf{r}_1)}{\partial \mathbf{r}_1}\cdot\frac{\partial V(\mathbf{r}_2)}{\partial \mathbf{r}_2} J_0^2(\sqrt{2E}|\mathbf{r}_1-\mathbf{r}_2|). \tag{3.7}$$

Some examples relating to Eq. (3.7) are set out in Appendixes C and D below. By way of illustration, we show in Fig. 1 a plot of $J_0^2(\sqrt{2E}r)$ versus r for two values of E. For comparison, we show the local density of states $N_0(r,E,Z)$ for the bare Coulomb potential energy $-Ze^2/r$ given in Eq. (C3), which reduces to $J_0^2(\sqrt{2E}r)$ when $Z=0$, apart from an unimportant normalization factor.

B. Scattering from a model two-center potential in two dimensions and in Born approximation

Dimers of impurities on nonmagnetic substrates provide a very active research field in scanning tunneling spectroscopy at the atomic scale.[17] This activity motivates the present subsection on the role of reduced dimensionality in associated scattering processes.

Consider the case of two equivalent scattering centers in a 2D electron gas. Let $\mathbf{R}$ be the vector joining the centers, $\mathbf{n}_0$ a unit vector in the direction of incidence, $\mathbf{n}_1$ a unit vector in the direction of scattering, and $\mathbf{k}$ the scattering wave vector of electrons. Due to the Fermi statistics $\mathbf{k}=\mathbf{k}_F$ is, in fact, the practically important value. As a first approximation we regard the two centers as scattering independently but coherently. Therefore, the result obtained will be generally

valid (even for strong scattering by the single center) if $kR \gg 1$. Following closely the standard[18,19] derivation in the 3D case, one obtains for the 2D differential cross section the following expression, in this so-called independent-atom approximation:

$$d\sigma(k,\theta)d\theta = 2|f_k(\theta)|^2(1+\cos[k(\mathbf{n}_0-\mathbf{n}_1)\cdot\mathbf{R}])d\theta, \tag{3.8}$$

where $\cos\theta = \mathbf{n}_0\cdot\mathbf{n}_1$. The function $f_k(\theta)$ is given in Eq. (2.2).

Practically, due to the random orientations of dimers (diclusters), the averaged cross section $d\sigma_{av}(k,\theta)$ is required. Therefore, we average over all orientations of the vector $\mathbf{R}$ in 2D by using Eqs. (3.715.18) of Ref. 20 and obtain

$$d\sigma_{av}(k,\theta)d\theta = 2|f_k(\theta)|^2[1+J_0(qR)]d\theta, \tag{3.9}$$

in which $q=2k\sin(\theta/2)$, the momentum transfer. In the first-order Born approximation the scattering amplitude $f_k^B(\theta)$ is related simply to the Fourier transform of the single-atom screened potential $V(q)$. Thus, in this case we have

$$|f_k^B(\theta)|^2 = \frac{1}{2\pi k}|V(q)|^2. \tag{3.10}$$

For the $kR \gg 1$ condition, Eq. (3.9) is applicable also for stronger scattering using partial-wave expansion.[12,13] In the so-called leading ($m=0$) phase-shift approximation, one gets the usual expression

$$|f_k(\theta)|^2 = \frac{2}{\pi k}\sin^2(\delta_0(k)). \tag{3.11}$$

If the unitary limit, as prescribed by the 2D Friedel sum rule,[8] is a valid approximation, one may use $\delta_0=\pi/2$ in Eqs. (3.11) and (3.9).

Various angular integrals of $d\sigma_{av}(k,\theta)$ need, in the leading phase-shift method, only a simple averaging of the $J_0[2k\sin(\theta/2)R]$ factor. Applying the standard expansion

$$J_0(qR) = \sum_{m=-\infty}^{\infty} J_m^2(kR)\exp(im\theta), \tag{3.12}$$

in Eq. (3.9), the total (t) cross section becomes

$$\sigma_{av}^t(k) = \frac{8}{k}\sin^2(\delta_0(k))(1+[J_0(kR)]^2), \tag{3.13}$$

for this case. This quantity may prove useful in estimating the dephasing time due to elastic scattering of surface-state electrons by dimer impurities.

Other angle-weighted cross sections (transport, diffusion) require more detailed, but feasible, calculations for the important 2D case.

IV. LINEAR RESPONSE FUNCTION GIVING THE DISPLACED FERMION DENSITY AROUND A "PERTURBING POTENTIAL" $V(\mathbf{r})$ IN A TWO-DIMENSIONAL UNIFORM ELECTRON GAS

Though our main purpose has been to evaluate the force-force correlation function defined in Eq. (2.1) to all orders in the scattering potential $V(|\mathbf{r}|)$ in Eq. (2.13), and to illustrate this by presenting numerical results at the Born level, it seemed of interest, in view of the usefulness of the March-Murray result[14,15] for the density $\rho(\mathbf{r})$ in three dimensions, namely

$$\rho_{3d}(\mathbf{r}) - \rho_0 = \text{const.} \times \int d\mathbf{r}' V(\mathbf{r}') \frac{j_1(2k_F|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|^2}, \tag{4.1}$$

where $\rho_0 = k_F^3/6\pi^2$, and the constant is given in Eq. (A2), to obtain the corresponding two-dimensional result. This then is the purpose of the present section. We shall take as starting point the work of Stoddart, March, and Stott,[21] who write Eq. (4.1) more generally as

$$\Delta\rho(\mathbf{r}) = \int d\mathbf{r}' V(\mathbf{r}') F(|\mathbf{r}-\mathbf{r}'|, E), \tag{4.2}$$

where

$$\frac{\partial F}{\partial E} = 2\,\mathrm{Re}\left[G(\mathbf{r},\mathbf{r}',E) \frac{\partial \gamma(\mathbf{r},\mathbf{r}',E)}{\partial E} \right]. \tag{4.3}$$

Thus, to obtain the two-dimensional counterpart of Eq. (4.1), we shall write, for the uniform gas, that

$$\frac{\partial F_0(\mathbf{r},\mathbf{r}',E)}{\partial E} = 2 \frac{\partial \gamma_0(\mathbf{r},\mathbf{r}',E)}{\partial E}\,\mathrm{Re}[G_0(\mathbf{r},\mathbf{r}',E)]. \tag{4.4}$$

Here, G_0 is the free-particle Green function in two dimensions. This is related to the canonical density matrix $C_0(\mathbf{r},\mathbf{r}',\beta)$ discussed above by

$$\mathcal{L} C_0(\mathbf{r},\mathbf{r}',\beta) = G_0(\mathbf{r},\mathbf{r}',-E). \tag{4.5}$$

With C_0 again given by Eq. (3.3) with $D=2$, the Laplace transform $\mathcal{L}$ above can be obtained as

$$\mathcal{L} C_0(\mathbf{r},\mathbf{r}',\beta) = \frac{K_0(\sqrt{2E}|\mathbf{r}-\mathbf{r}'|)}{\pi} \tag{4.6}$$

where $K_0(x)$ is the modified Bessel function.[16] Using Eqs. (4.5) and (4.6), we thus find

$$G_0(\mathbf{r},\mathbf{r}',E) = \frac{K_0(i\sqrt{2E}|\mathbf{r}-\mathbf{r}'|)}{\pi}. \tag{4.7}$$

Since $\partial\gamma_0/\partial E$ is known in terms of J_0 from Eq. (3.6), we have $\partial F_0/\partial E$ by appealing to Eq. (4.4). We note that Zhang[22] has obtained a more compact form in **k**-space, although he then invokes the Meijer function in the **r**-space representation we focus on in the present study. The above theory is extended somewhat in Appendix A.

V. ONE-DIMENSIONAL SCATTERING

Having contrasted nonlinear scattering in 2D and 3D electron gases from a localized potential, we turn, albeit briefly, to consider what further changes are introduced by dimensionality reduction to the case of 1D. We follow March and Murray,[14,15] who dealt completely with 3D plane wave perturbation theory, by starting from the integral equation derived from the well-known Bloch equation[23] for the canonical density matrix $C(x,x_0,\beta)$, where

$$C(x,x_0,\beta) = \sum_{\text{all}\,i} \psi_i(x)\psi_i^*(x_0)\exp(-\beta\epsilon_i). \tag{5.1}$$

In Eq. (5.1), $\psi_i(x)$ and the corresponding eigenvalues ϵ_i satisfy

$$H\psi_i = \epsilon_i \psi_i, \tag{5.2}$$

where the one-dimensional Hamiltonian is simply

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x). \tag{5.3}$$

Evidently, completeness yields from Eq. (5.1) at $\beta=0$

$$C(x,x_0,0) = \delta(x-x_0), \tag{5.4}$$

and this is built in the integral form of the Bloch equation, namely

$$C(x,x_0,\beta) = C_0(x,x_0,\beta) - \int_0^\beta d\beta_1 \int dx_1 C_0(x,x_1,\beta-\beta_1)V(x_1)C(x_1,x_0,\beta_1). \tag{5.5}$$

In Eq. (5.5), C_0 is the free-particle density matrix[23]

$$C_0(x,x_0,\beta) = \frac{1}{\sqrt{2\pi\beta}}\exp\left(-\frac{(x-x_0)^2}{2\beta}\right). \tag{5.6}$$

The β_1 integration can be removed by a Laplace transform on β ($\rightarrow E$) to yield ($C\rightarrow\tilde{C}$)

$$\tilde{C}(x,x_0,E) = \tilde{C}_0(x,x_0,E) - \int \mathrm{d}x_1\, \tilde{C}_0(x,x_1,E)V(x_1)\tilde{C}(x_1,x_0,E). \tag{5.7}$$

The Laplace transform of Eq. (5.6) is readily obtained as[24]

$$\tilde{C}_0(x,x_0,E) \equiv \mathcal{L}C_0(x,x_0,\beta) = \frac{1}{\sqrt{2E}}\exp(-\sqrt{2E}|x-x_0|). \tag{5.8}$$

If in Eq. (5.7) we then work to first order in the "perturbing" potential $V(x)$, we find

$$\tilde{C}(x,x_0,E) = \frac{1}{\sqrt{2E}}\exp(-\sqrt{2E}|x-x_0|) - \frac{1}{2E}\int \mathrm{d}x_1\, V(x_1)\exp(-\sqrt{2E}\{|x-x_1|+|x_1-x_0|\}). \tag{5.9}$$

Inverting the Laplace transform ($E\rightarrow\beta$) in Eq. (5.9) readily yields

$$C(x,x_0,\beta) = \frac{1}{\sqrt{2\pi\beta}}\exp\left(-\frac{(x-x_0)^2}{2\beta}\right) - \frac{1}{2}\int \mathrm{d}x_1\, V(x_1)\mathrm{erfc}\left(\sqrt{\frac{2}{\beta}}\frac{\{|x-x_1|+|x_1-x_0|\}}{2}\right). \tag{5.10}$$

The Dirac density matrix $\gamma(x,x_0,E)$ then follows as the inverse Laplace transform of $C(x,x_0,\beta)/\beta$, and is given by

$$\gamma(x,x_0,E) = \frac{\sin(\sqrt{2E}|x-x_0|)}{\pi|x-x_0|} - \int \mathrm{d}x_1\, V(x_1)\left[\frac{1}{2} - \frac{\mathrm{Si}(\sqrt{2E}\{|x-x_1|+|x_1-x_0|\})}{\pi}\right], \tag{5.11}$$

which is the 1D analog of the first-order 3D result of March and Murray.[14,15]

Of course, one obvious difference between 2D and 3D scattering and the 1D case to be discussed further below is that in the 1D system there are only two discrete directions for scattering: forward and backward along a line. Below, we restrict our discussion to symmetric localized potentials $V(x)$ satisfying

$$V(x) = V(-x). \tag{5.12}$$

The 1D analog of the customary Lippmann-Schwinger equation takes the form

$$\psi_k(x) = \phi_k(x) + \int_{-\infty}^{\infty} G_0(x,x')V(x')\psi_k(x')\mathrm{d}x', \tag{5.13}$$

where $\phi_k(x)$ is the free-particle wave function $\exp(ikx)$. The one-dimensional Green function $G_0(x,x')$ is given by

$$G_0(x,x') = -\frac{i}{2k}\exp(ik|x-x'|), \tag{5.14}$$

which is readily verified to be the Laplace transform ($\mathcal{L}$) of the canonical density matrix (3.3) with respect to β for the case $D=1$, since

$$\mathcal{L}C = G_0(x,x'):E = k^2. \tag{5.15}$$

Using Eq. (5.14) in (5.13), the following asymptotic form of $\psi_k(x)$ results:

$$\psi_k(x) \to \exp(ikx) + \frac{i}{k}f_k(\epsilon)\exp(ikx), \tag{5.16}$$

where $f_k(\epsilon)$ is the analog of the scattering amplitude in higher dimensions. However, as discussed above, there are but two scattering directions in 1D, corresponding to $\epsilon=\pm 1$. This is to be contrasted with the continuum of scattering angles in both 2D and 3D. The differential cross sections in these two directions in the 1D case are given by

$$\sigma_\epsilon = \frac{1}{k^2}|f_k(\epsilon)|^2, \tag{5.17}$$

while the total cross section σ takes the form

$$\sigma = \frac{1}{k^2}[|f_k(+1)|^2 + |f_k(-1)|^2]. \tag{5.18}$$

To press the analogy with higher dimensions, we have now just two partial waves. For potentials satisfying Eq. (5.12), these two partial waves are distinct, with even and odd parity. It is to be noted that the cross section σ, in principle an observable, has units of length L squared in 3D, L in 2D, and is dimensionless according to Eq. (5.18) in 1D.

Analogs of the optical theorem and the unitarity relation again exist, paralleling here the 2D and 3D scattering, but we shall not go into further detail. It is worth adding, in concluding this brief discussion of 1D scattering, that the above can be usefully illustrated for a potential $V(x)$ which is the Dirac delta function (see the discussion in 3D in Ref. 25), but we shall not go into further detail since the 3D example was treated fully for a similar, completely localized, scattering center.

VI. DISCUSSION AND FUTURE DIRECTIONS

Our principal aim has been to demonstrate the effect of dimensionality reduction on the 3D results given earlier[25] for nonlinear scattering by a localized potential. For the 2D case, which is the main focus of the present study, it is striking that the stopping power problem summarized in Eqs. (1.1) and (1.3) turns out, beyond the Born approximation, to be distinct from the force-force correlation function $\langle \mathbf{F}\cdot\mathbf{F}\rangle$ defined in Eq. (2.1) in 2D. These are essentially identical to all orders in the localized scattering potential V in 3D. It is possible in 2D that there are "frictional effects" in surfaces, the theory of which has been discussed by d'Agliano and co-workers,[26] which may mirror $\langle \mathbf{F}\cdot\mathbf{F}\rangle$, but it remains to be proved that this latter correlation function is indeed an observable in 2D, whereas it is established that this is the case, though not distinct from stopping power or transport cross section, in 3D. Here, we believe for the first time, $\langle \mathbf{F}\cdot\mathbf{F}\rangle$ in Eq. (2.1) has been

calculated analytically in terms of phase shifts at the Fermi level, and is given for 2D in Eq. (2.13). This is evidently closely related to, but nevertheless distinct from, Eq. (1.1) in terms of the same input information, for the transport cross section.

Further directions of interest for the future, which were already touched on in the Introduction, are scattering in essentially two dimensions from a single magnetic impurity. Here, the spin-dependent theoretical approach of Stoddart and March[27] may well find application, and the two-dimensional version should prove of considerable interest for the future.

APPENDIX A: r-SPACE LINEAR RESPONSE FUNCTION $F(|\mathbf{r}-\mathbf{r}'|,E)$ IN TWO DIMENSIONS

The object of this appendix is to give the two-dimensional form of the result of March and Murray[14]

$$\Delta\rho(\mathbf{r},E)=\int F_{3d}(|\mathbf{r}-\mathbf{r}'|,E)V(\mathbf{r}')\mathrm{d}\mathbf{r}', \tag{A1}$$

for the displaced charge below energy E created by a perturbing potential $V(\mathbf{r})$ inserted into an initially uniform electron gas. The result of Ref. 14 was explicitly [compare Eq. (4.1)]

$$F_{3d}(R,E)=-\frac{mE}{\pi^3\hbar^2}\frac{j_1(2\sqrt{2E}R)}{R^2}. \tag{A2}$$

Below, we derive an analogous form to Eq. (A2) in two dimensions. As shown by Stoddart, March, and Stott,[21] for the uniform Fermi gas as the unperturbed system, $\partial F(R,E)/\partial E$ is given by Eq. (4.3) of the main text, where the free-electron 2D Green function has been given in Eq. (4.7) in terms of the Bessel function K_0. Likewise, $\partial\gamma/\partial E$ is known in 2D in terms of J_0 from Eq. (3.6), and inserting these results into Eq. (4.3) and forming the energy derivative yields, after using the identity

$$\mathrm{Re}[K_0(ikR)]=-Y_0(kR)/2\pi, \tag{A3}$$

the result

$$F(R,E)=-\frac{1}{2\pi}\int^E J_0(\sqrt{2E}R)Y_0(\sqrt{2E}R)\mathrm{d}E. \tag{A4}$$

Performing the integration, one finds

$$F(R,E)=-\frac{E}{2\pi}[J_0(\sqrt{2E}R)Y_0(\sqrt{2E}R)+J_1(\sqrt{2E}R)Y_1(\sqrt{2E}R)]+f(R). \tag{A5}$$

But, the energy-independent function $f(R)$ must be zero since $\Delta\rho(R,E=0)=0$, and thus, for the displaced charge at the origin $\Delta\rho(0,E)$, one obtains

$$\Delta\rho(0,E)=-ZE\int_0^\infty [J_0(\sqrt{2E}r)Y_0(\sqrt{2E}r)+J_1(\sqrt{2E}r)Y_1(\sqrt{2E}r)]\mathrm{d}r, \tag{A6}$$

for the case of the bare Coulomb potential, by way of illustration. From Ref. 20, we have

$$\int_0^\infty J_\nu(ax)Y_\nu(ax)\mathrm{d}x=-\frac{1}{2a},\quad [\nu>-1/2,a>0], \tag{A7}$$

and hence

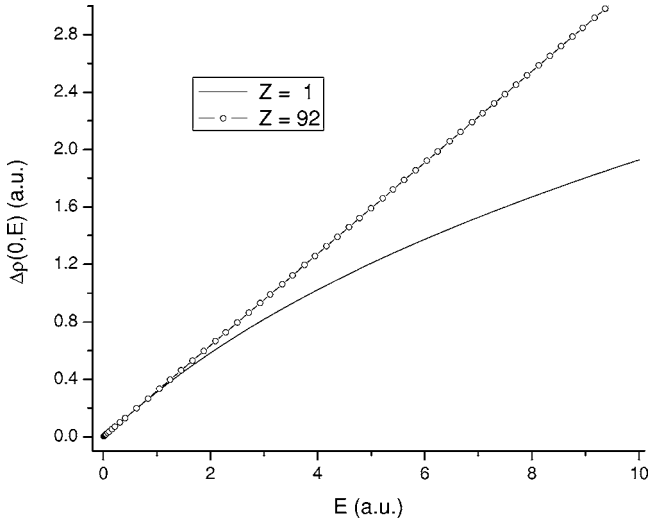

FIG. 2. Displaced charge $\Delta\rho(0,E)$ at nucleus, resulting from a bare Coulomb potential $(-Z/r)$ embedded in a two-dimensional electron gas, for $Z=1$ and 92, versus energy E, as given in Eq. (A9).

$$\Delta\rho(0,E) = \frac{ZE}{\sqrt{2E}} = Z\sqrt{\frac{E}{2}}, \quad E \neq 0. \tag{A8}$$

In fact, for $V=-Z/r$, this result (A8) has the fully nonlinear generalization

$$\Delta\rho(0,E) = \frac{E}{\pi}\tanh\left(\frac{Z\pi}{\sqrt{2E}}\right), \tag{A9}$$

which is equivalent to Eq. (A8) to first order in Z. Equation (A9) is plotted as a function of energy E for $Z=1$ and $Z=92$ in Fig. 2. The following appendix adds some further nonlinear results associated still with the unscreened Coulomb potential.

APPENDIX B: SOME FURTHER PROPERTIES GENERATED BY THE BARE COULOMB POTENTIAL IN TWO DIMENSIONS

The real-space Schrödinger equation in plane polar coordinates (r,θ) reads

$$\left[-\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{B1}$$

where, writing

$$\psi(\mathbf{r}) = R(r)\Theta(\theta), \tag{B2}$$

we have

$$\Theta(\theta) = \frac{1}{\sqrt{2\pi}}\exp(im\theta). \tag{B3}$$

The corresponding radial equation, with $E=-k_0^2$, say, is

$$\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} + \left[\frac{2}{r} - k_0^2 - \frac{m^2}{r^2}\right]R = 0. \tag{B4}$$

The normalized wave functions are then

$$\psi_{nm}(\mathbf{r}) = \sqrt{\frac{k_0^3(n-|m|)!}{\pi(n+|m|)!}}(2k_0r)^{|m|}\exp(-k_0r)L_{n-|m|}^{2|m|}(2k_0r)\exp(im\theta), \tag{B5}$$

where L as usual denotes the associated Laguerre polynomial.

In three dimensions, Heilmann and Lieb[28] (HL) calculated the total density of the entire spectrum of bound states of the hydrogen atom. Below, we note one property for the two-dimensional case that is much simpler than for the three-dimensional case, namely the density $\rho_\infty(r)$ at $r=0$. Using the definition in two dimensions that

$$\rho_\infty(r) = \sum_{n=0}^{\infty}\sum_{m\leqslant n}\psi^*(\mathbf{r})\psi(\mathbf{r}), \tag{B6}$$

one has from Eq. (B5) the result

$$\rho_\infty(r) = \sum_{n=0}^{\infty}\sum_{m\leqslant n}\frac{k_0^3(n-|m|)!}{\pi(n+|m|)!}(2k_0r)^{2|m|}\exp(-2k_0r)[L_{n-|m|}^{2|m|}(2k_0r)]^2. \tag{B7}$$

At $r=0$, the above summation simplifies (because only $m=0$ terms contribute) to

$$\rho_\infty(0) = \sum_{n=0}^{\infty}\frac{k_0^3}{\pi}, \tag{B8}$$

where the bound-state energy levels are given by

$$E = -k_0^2 = -\frac{1}{(n+1/2)^2}. \tag{B9}$$

Using the summation in Ref. 16, namely

$$(1-2^{-n})\zeta(n) = \sum_{k=0}^{\infty}(2k+1)^{-n}, \tag{B10}$$

with $n=3$ yields the closed result

$$\rho_\infty(0) = \frac{7}{\pi}\zeta(3), \tag{B11}$$

where ζ denotes the Riemann zeta function. This result can be further generalized to N closed shells as

$$\rho_N(0) = \frac{7}{\pi}\zeta(3) + \frac{\Psi(2,N+3/2)}{2\pi}, \tag{B12}$$

and Fig. 3 shows a plot of this equation as a function of N. The value $\rho_\infty(0)$ is solely due to the spherically symmetric wave functions corresponding to $m=0$ (s states) and hence $\rho_\infty(0)=\rho_{\infty s}(0)$.

Kato's theorem, discussed by one of us in Ref. 29, has then the generalization to D dimensions for nuclear charge Ze given by

$$\left.\frac{\partial\rho(r)}{\partial r}\right|_{r=0} = \left. -\frac{4Z}{(D-1)}\rho_s(r)\right|_{r=0}, \tag{B13}$$

and means that, for $Z=1$ and $D=2$

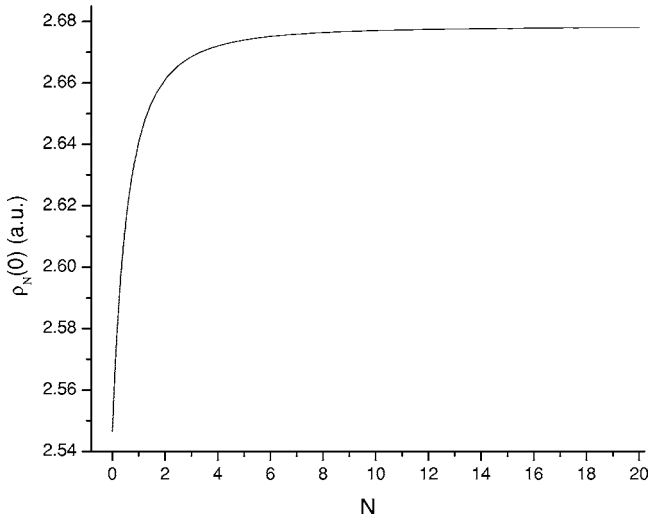

FIG. 3. Plot of electron density $\rho_N(0)$ at the nucleus given by Eq. (B12) for a two-dimensional hydrogen-like atom, versus the number of closed shells N.

$$\left.\frac{\partial\rho(r)}{\partial r}\right|_{r=0} = -\frac{28}{\pi}\zeta(3). \tag{B14}$$

This implies, in particular, that after differentiating $\rho_\infty(r)$ in Eq. (B7) with respect to r, the summation over m can be performed and the result then relates to the s-like ($m=0$) density according to Eq. (B13).

APPENDIX C: DIFFERENTIAL EQUATION SATISFIED BY THE DIAGONAL LOCAL DENSITY OF STATES $N(r,E)$ FOR THE $m=0$ COMPONENT

Denoting the $m=0$ component of the local density of states by $N_0(r,E,Z)$, we have the differential equation, with primes denoting derivatives with respect to r, as

$$\frac{r^2}{2E}N_0''' + \frac{3r}{2E}N_0'' + \left[4r\left(r+\frac{1}{E}\right)+\frac{1}{2E}\right]N_0' + \left[4\left(r+\frac{1}{2E}\right)+\frac{1}{2E}\left(4+\frac{1}{r}\right)\right]N_0 = 0. \tag{C1}$$

Dropping the "potential energy" term $1/r$, one can readily verify that Eq. (C1) is satisfied by the free-electron result

$$N_0(r,E,Z=0) = \text{const.} \times [J_0(\sqrt{2E}r)]^2. \tag{C2}$$

The physical solution (with $V(r)=-Z/r$ now the 2D Coulomb potential) of Eq. (C1) is

$$N_0(r,E,Z) = \text{const.} \times \frac{\mathcal{M}(-iZ/k,0,i2kr)^2}{r}, \tag{C3}$$

where $\mathcal{M}$ denotes the Whittaker function (see also Fig. 1 of the main text).

APPENDIX D: COULOMB LOCAL DENSITY OF STATES AND FREE-ELECTRON LIMIT

In the main text we proved that

$$\frac{\partial\gamma_0}{\partial E} = \frac{1}{2\pi}J_0(\sqrt{2E}|\mathbf{r}-\mathbf{r}'|), \tag{D1}$$

which we now expand in terms of angular functions $\exp(im\phi)$, where $\cos(\phi)=\mathbf{r}\cdot\mathbf{r}'/rr'$, to write

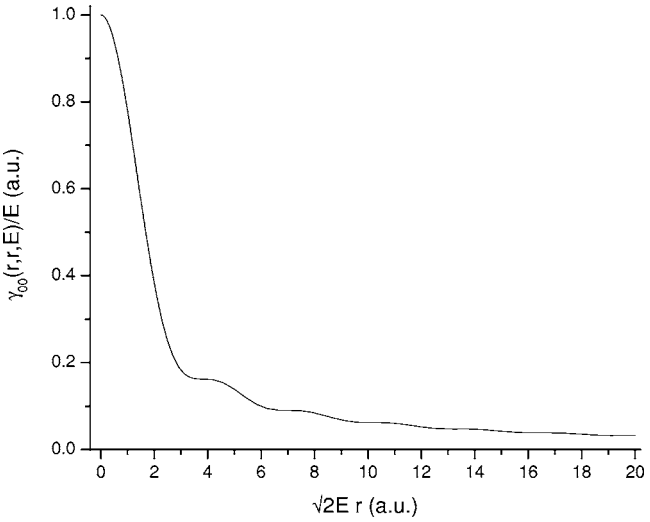

FIG. 4. s-state ($m=0$) electron density $\gamma_{00}(r,r,E)$ for a two-dimensional free electron gas, as given by Eq. (D6). Actual plot is $\gamma_{00}(r,r,E)/E$ versus $\sqrt{2E}r$.

$$\frac{\partial\gamma_0}{\partial E}=\sum_{m=-\infty}^{\infty}\frac{\partial\gamma_{0m}(r,r')}{\partial E}\exp(im\phi). \tag{D2}$$

Then, it follows directly from Eqs. (D1) and (D2) above that

$$\frac{\partial\gamma_{00}(r,r')}{\partial E}=\frac{1}{2\pi}\int_0^{2\pi}J_0(\sqrt{2E}|\mathbf{r}-\mathbf{r}'|)d\phi. \tag{D3}$$

From Ref. 20, Eq. 6.684.1, we have that the integral on the right-hand side of Eq. (D3) is a product of Bessel functions of order zero, and hence we obtain explicitly

$$\frac{\partial\gamma_{00}(r,r')}{\partial E}=J_0(\sqrt{2E}r)J_0(\sqrt{2E}r'). \tag{D4}$$

Performing the energy integration, and using the physical boundary condition that $\partial\gamma_{00}/\partial E\to 0$ as $E\to 0$, we find the $m=0$ component of the Dirac density matrix for the free-electron gas in 2D as

$$\gamma_{00}(r,r',E)=\frac{\sqrt{2E}}{(r'^2-r^2)}[r'J_0(\sqrt{2E}r)J_1(\sqrt{2E}r')-rJ_0(\sqrt{2E}r')J_1(\sqrt{2E}r)]. \tag{D5}$$

Taking the limit of Eq. (D5) as $r'\to r$ yields

$$\gamma_{00}(r,r,E)=E[J_0^2(\sqrt{2E}r)+J_1^2(\sqrt{2E}r)]. \tag{D6}$$

This result (D6) is plotted in Fig. 4 as a function of r for two different values of the energy E.

1. Coulomb analogue

For the continuous spectrum of the hydrogen-like atom with $V(r)=-Z/r$ in two dimensions, the radial wave function corresponding to $m=0$ is

$$R_0(kr) = C_{k0} \exp(-ikr)\,{}_1F_1(iZ/k + 1/2, 1, i2kr), \tag{D7}$$

where ${}_1F_1$ denotes the confluent hypergeometric function, and hence, apart from a multiplying factor which can depend on energy and Z, we can write the analog of Eq. (D4) in the limit $r \to r'$ as

$$\left.\frac{\partial \gamma_{m=0}(r,r',Z)}{\partial E}\right|_{r'=r} = \left|{}_1F_1(iZ/k + 1/2, 1, i2kr)\right|^2 : k = \sqrt{2E}. \tag{D8}$$

Allowing $Z \to 0$ in Eq. (D8), we can make use of the identity (Ref. 20, Eq. 9.215.3)

$${}_1F_1(b + 1/2, 2p + 1, i2z) = \Gamma(p+1)\left(\frac{Z}{2}\right)^{-p} \exp(iz) J_p(z), \tag{D9}$$

for the case $p=0$ to verify that, apart from a factor already referred to, Eq. (D8) correctly leads back to the free-electron result (D4) in the limit $Z \to 0$ and $r'=r$.

The force-force correlation function formula can then be written explicitly as a quadrature involving $(\partial V(r_1)/\partial \mathbf{r}_1)\cdot(\partial V(r_2)/\partial \mathbf{r}_2)$ multiplied by $(\partial \gamma_{m=0}/\partial E)^2 = R_0(kr_1)R_0(kr_2)$, the analog if the higher terms for $m \neq 0$ in Eq. (D2) are assumed small for the Coulomb case. However, the detail proliferates and we shall therefore not give it.

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Spectral and localization properties for the one-dimensional Bernoulli discrete Dirac operator

César R. de Oliveira[a] and Roberto A. Prado[b]
Departamento de Matemática–UFSCar, São Carlos, SP, 13560-970 Brazil

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An one-dimensional (1D) Dirac tight-binding model is considered and it is shown that its nonrelativistic limit is the 1D discrete Schrödinger model. For random Bernoulli potentials taking two values (without correlations), for typical realizations and for all values of the mass, it is shown that its spectrum is pure point, whereas the zero mass case presents dynamical delocalization for specific values of the energy. The massive case presents dynamical localization (excluding some particular values of the energy). Finally, for general potentials the dynamical moments for distinct masses are compared, especially the massless and massive Bernoulli cases. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1948328]

I. INTRODUCTION

Besides the huge amount of mathematical works on spectral problems related to the one-dimensional (1D) Dirac model,[4,26] in physics it has also been used in comparative studies of relativistic and nonrelativistic electron-localization phenomena,[2] in relativistic investigations of electrical conduction in disordered systems,[21] in the construction of supertransparent models with supersymmetric structures[25] and in relativistic tunnelling problems.[20]

In this paper a discrete version of the 1D Dirac model is discussed, which can be interpreted as a relativistic version of the well-known tight-binding Schrödinger Hamiltonian (with $\hbar=1$),

$$(H\psi)_n = -\frac{1}{2m}(\Delta\psi)_n + V_n\psi_n = \frac{1}{2m}(-\psi_{n+1} - \psi_{n-1} + 2\psi_n) + V_n\psi_n. \tag{1}$$

The model was first reported in Ref. 11 and this work is its very expanded and mathematical detailed version. Consider a particle of mass $m \geqslant 0$ in the one-dimensional lattice $\mathbb{Z}$ under the real site potential $\tilde{V}=(V_n)$. The proposed 1D Dirac tight-binding operator is

$$\mathbb{D}(m,c) = \mathbb{D}_0(m,c) + \tilde{V}\,\mathrm{Id}_2 = c\mathcal{B} + mc^2\sigma_3 + \tilde{V}\,\mathrm{Id}_2, \tag{2}$$

with $c>0$ representing the speed of light,

$$\mathcal{B} = \begin{pmatrix} 0 & d^* \\ d & 0 \end{pmatrix},$$

σ_3 the usual Pauli matrix, Id_2 the 2×2 identity matrix and d the finite difference operator (a discrete counterpart of the first derivative) defined by

$$(d\psi)_n = \psi_{n+1} - \psi_n.$$

$(d^*\psi)_n = \psi_{n-1} - \psi_n$ is the adjoint of d so that $\mathbb{D}_0(m,c) = c\mathcal{B} + mc^2\sigma_3$ is a bounded self-adjoint operator acting on $\ell^2(\mathbb{Z};\mathbb{C}^2)$ and its square is

[a]Electronic mail: oliveira@dm.ufscar.br
[b]Electronic mail: rap@dm.ufscar.br

$$\mathbb{D}_0(m,c)^2 = \begin{pmatrix} c^2 dd^* + m^2c^4 & 0 \\ 0 & c^2 dd^* + m^2c^4 \end{pmatrix}.$$

This equality is reminiscent of the relation between momentum $\vec{p}$ and energy E in relativistic quantum mechanics,[4] given by $E^2 = c^2\vec{p}^2 + m^2c^4$. Denoting by $\sigma(A)$ the spectrum of a self-adjoint operator A, it is well known that $\sigma(-\Delta) = [0,4]$, and since $d^*d = dd^* = -\Delta$,

$$\sigma(\mathbb{D}_0(m,c)) = [-c\sqrt{4 + m^2c^2}, -mc^2] \cup [mc^2, c\sqrt{4 + m^2c^2}].$$

In case the potential $\tilde{V}$ is a bounded sequence, $\mathbb{D}(m,c)$ is also a bounded self-adjoint operator acting on $\ell^2(\mathbb{Z};\mathbb{C}^2)$.

It will be shown that the nonrelativistic limit of the resolvent of the discrete Dirac operator (2) is the resolvent of discrete Schrödinger operator (1) (when projected on a proper subspace; see Sec. II). This is an important support for such Dirac model.

The study of quantum transport depends, of course, on the admitted definitions. In the physics literature terms like "extended states" and "zero Lyapunov exponents" have been used to crudely designate quantum transport. For instance, in Ref. 27 it was claimed that "extended states" were found in one-dimensional Schrödinger systems with off-diagonal randomness, but in Ref. 24 it was argued that although the localization length diverges the "transmission coefficient" vanishes as the system size goes to infinity. Up to recently, in the mathematical literature pure point spectrum (sometimes with exponentially decaying eigenfunctions) was considered synonymous of absence of transport. Currently the transport has been probed via the time behavior of the moments of the position operator, and in this work this idea will be followed. See ahead for precise definitions and related comments.

One of the goals of this paper is to study the phenomenon called dynamical localization (in the sense of time-boundedness of all moments of the position operator) for the Bernoulli-Dirac model, that is, the model (2) with the site potentials V_n, $n \in \mathbb{Z}$, being independent identically distributed Bernoulli random variables taking the values $\pm V$, $V > 0$. In this case it will be shown that almost surely the spectrum of $\mathbb{D}(m,c)$ is pure point for all values of the mass, the massive case has dynamical localization (excluding some particular values of the energy for which a more careful analysis is needed) and the zero mass case presents dynamical delocalization (that is, absence of localization) for specific values of the energy.

The problem of dynamical localization has been intensively studied during the last years, especially in the case of random discrete and continuous Schrödinger operators (in particular for the Bernoulli-Anderson model, that is, the Schrödinger model with Bernoulli potentials); see Refs. 10, 14, and 16 and references therein. What one usually proves is the so-called exponential localization,[1,6,28] i.e., pure point spectrum and exponentially decaying eigenfunctions. On the other hand, it is also known that exponential localization does not imply dynamical localization;[12] it is usually needed a precise control of the decay of the eigenfunctions, called SULE,[12,16] that can be obtained through the method of multiscale analysis, a technique set out by Fröhlich and Spencer.[14,15]

One motivation for studying dynamical localization for the Bernoulli-Dirac operator comes from the random dimer model,[10,13] i.e., the Bernoulli-Anderson model with the site energies V_n assigned for pairs of lattices, $V_{2n} = V_{2n+1} = \pm V$ for all n. This model almost surely presents pure point spectrum for all values of $V \neq 0$.[10] It was also numerically found in Ref. 13 and rigorously shown in Refs. 10 and 18 the existence of *critical energies* (in the sense of Ref. 18; see ahead) at which the Lyapunov exponent vanishes; dynamical localization was obtained in Ref. 10 only after projecting onto closed energy intervals not containing such critical energies. Despite the similarity between the transfer matrices of the two models, it is not immediate the adaptation of the localization (delocalization) results to the Bernoulli-Dirac model and each step needs to be verified; here, many points will not be detailed when they follow exactly the same lines of their Schrödinger counterpart.

With respect to nontrivial quantum transport, probed via dynamical delocalization (unbounded moments of the position operator), it was found in random polymer models[18] and in random

palindrome models[7] (both including the important random dimer model), due to existence of critical energies.[18] Recently, for 1D discrete Schrödinger operators, Damanik, Sütő, and Tcheremchantsev[9] have developed a general method which allows one to derive quantum dynamical lower bounds from upper bounds on the growth of norms of transfer matrices, and they applied this method to some substitution, Sturmian and prime models, among others. Damanik, Lenz, and Stolz[8] presented an extension of this method to 1D continuous Schrödinger operators, with application to the continuous Bernoulli-Anderson model. Another method to obtain quantum transport from upper bounds on transfer matrix was lately developed by Germinet, Kiselev, and Tcheremchantsev,[17] with application to Schrödinger operators with random decaying potentials, providing examples of Schrödinger operator with point spectrum and nontrivial quantum transport.

In the zero mass case, the one-dimensional Bernoulli-Dirac model presented here has pure point spectrum and nontrivial quantum transport for potentials with no correlations nor decaying properties (see Sec. III). This phenomenon does not take place in the corresponding Schrödinger tight-binding model,[16] and this also motivates the interest to better understanding the Dirac case. Presumably, this tight-binding model is the simplest one presenting such phenomenon.

Now the localization results for the Bernoulli-Dirac model will be briefly summarized. By using as the main tool a particular form of Furstenberg theorem (Lemma 2 ahead), it is shown (see Theorems 2, 3, and 4) that the Lyapunov exponent $\gamma_m(E)$ is strictly positive for the energies $E \in \sigma(\mathbb{D}(m,c))$, except for $E=\pm V$, $V\in(0,c]$, $V\neq c/\sqrt{2}$, in the case $m=0$; and if $m\geqslant 0$ for $(E_V=0, V=c\sqrt{2+m^2c^2})$ and the four energy-potential pairs $(E_V=\pm c\sqrt{2+m^2c^2}\pm c/\sqrt{2}, V=c/\sqrt{2})$.

For all energies E for which $\gamma_m(E)>0$, an initial estimate for localization (Lemma 4) and the Wegner's estimate (Lemma 3) will be checked; by adapting the method multiscale analysis[14,16,28] to this model, it will be shown (see Theorems 2 and 3) that for typical realizations the spectrum of $\mathbb{D}(m,c)$ is pure point and the corresponding eigenfunctions are semiuniformly exponentially localized (SULE).[12,16] This and the results of Ref. 16 [properly adapted to $\mathbb{D}(m,c)$] imply dynamical localization.

In the massless ($m=0$) case, the values $E=\pm V$ with $V\in(0,c]$, $V\neq c/\sqrt{2}$, are critical energies for the operator $\mathbb{D}(0,c)$ and this implies (almost surely) upper boundedness for the transfer matrices in the vicinity of these energies (see Lemmas 5 and 6). By adapting the ideas of Ref. 18 (see also Ref. 9) to $\mathbb{D}(0,c)$ it will follow (see Theorem 5) that for an initial spinor Ψ well localized in space, there is $0<C_q<\infty$ such that

$$\int_0^\infty \frac{1}{T} e^{-2t/T} M_\Psi^{(q)}(0,t)\mathrm{d}t \geqslant C_q T^{q-1/2},$$

for almost all realization of the potential (or exponent $q-1$ instead of $q-1/2$ for every realization), where (X is the usual position operator)

$$M_\Psi^{(q)}(m,t) := \langle e^{-i\mathbb{D}(m,c)t}\Psi, |X|^q e^{-i\mathbb{D}(m,c)t}\Psi\rangle,$$

i.e., there is nontrivial quantum transport despite the absence of a continuous component in the spectrum of $\mathbb{D}(0,c)$.

In the case of the set of pairs $(E_V=\pm c\sqrt{2+m^2c^2}\pm c/\sqrt{2}, V=c/\sqrt{2})$ and $(E_V=0, V=c\sqrt{2+m^2c^2})$ it is shown (see Theorem 4) that the Lyapunov exponent γ_m vanishes, but it was not possible to give an answer about dynamical localization for them. Nevertheless, for these cases there is a general dynamical upper bound (in fact valid for all potentials $\widetilde{V}$) established in Theorem 6.

For distinct masses $m,m'\geqslant 0$, but m close to m', it is expected that the moments $M_\Psi^{(q)}(m,t)$ follow closely the moments $M_\Psi^{(q)}(m',t)$ (both with the same potential), at least for a small period of time. The final result to be reported is an inequality confirming such expectative; by making use of DuHamel's formula, it will be shown (see Theorem 7) that, for the initial state Ψ with only one nonzero component, there exists $K_q>0$ so that, for all $t>0$,

$$|M_\Psi^{(q)}(m,t) - M_\Psi^{(q)}(m',t)| \leqslant K_q|m-m'|c^2t^{q+2}.$$

In particular, for the Bernoulli-Dirac model this relation with $m'=0$ gives quantitatively an estimate of how, for small times, the dynamics of the localized regime follows the delocalized one (see also Corollary 1 in Sec. VI).

This paper is organized as follows: In Sec. II the nonrelativistic limit for the discrete Dirac model (2) is discussed. In Sec. III the results about spectral properties of such model, dynamical localization (delocalization) and a dynamical upper bound for moments are presented, whose proofs appear in Sec. V. In Sec. IV some tools used in those proofs are collected. Finally, in the Sec. VI the dynamical moments with different masses are compared; in particular the dynamics of the massless and massive Dirac-Bernoulli cases.

II. NONRELATIVISTIC LIMIT

In this section consider $\mathbb{D}(m,c)$ with $m>0$ fixed and c as a parameter. For simplicity, $\mathbb{D}(c)$ will denote $\mathbb{D}(m,c)$, which is supposed to be self-adjoint with (real) potential $\tilde{V}$.

The nonrelativistic limit means c going to infinity, and since the rest energy mc^2 is a purely relativistic quantity, (as usual) it must be subtracted before taking this limit. The norm convergence of the resolvent operators $(\mathbb{D}(c)-mc^2-z)^{-1}$, for $z\in\mathbb{C}\backslash\mathbb{R}$ will be considered. Λ below is the projector onto the subspace of "positive energies," and so ΛH_∞ corresponds to the Schrödinger operator (1). It is interesting to compare the approach presented here with the one in Ref. 11.

Theorem 1: *If* $z\in\mathbb{C}\backslash\mathbb{R}$, *then*

$$\lim_{c\to\infty}(\mathbb{D}(c)-mc^2-z)^{-1} = \Lambda(H_\infty - z)^{-1},$$

where $\Lambda=\frac{1}{2}(Id_2+\sigma_3)$ *and* $H_\infty=(\mathcal{B}^2/2m)+\tilde{V}\Lambda$, *and the limit is in the norm of bounded operators.*

Lemma 1: If $z\in\mathbb{C}\backslash\mathbb{R}$, *then*

$$(\mathbb{D}(c)-mc^2-z)^{-1} = \left(\Lambda+\frac{c\mathcal{B}+z}{2mc^2}\right)S(c)\left(\mathrm{Id}+\tilde{V}\frac{c\mathcal{B}+z}{2mc^2}S(c)\right)^{-1}, \tag{3}$$

where Id is the identity operator and

$$S(c) = \left(H_\infty - z - \frac{z^2}{2mc^2}\right)^{-1} = \left(\mathrm{Id}-\frac{z^2}{2mc^2}(H_\infty-z)^{-1}\right)^{-1}(H_\infty-z)^{-1}. \tag{4}$$

Proof: Note that

$$(\mathbb{D}_0(c)+mc^2+z)(\mathbb{D}_0(c)-mc^2-z) = c^2\mathcal{B}^2 - 2mc^2z - z^2.$$

Hence

$$(\mathbb{D}_0(c)-mc^2-z)^{-1} = \frac{\mathbb{D}_0(c)+mc^2+z}{2mc^2}\left(\frac{\mathcal{B}^2}{2m}-z-\frac{z^2}{2mc^2}\right)^{-1} = \left(\Lambda+\frac{c\mathcal{B}+z}{2mc^2}\right)S_0 \tag{5}$$

with $S_0=[(\mathcal{B}^2/2m)-z-(z^2/2mc^2)]^{-1}$. On the other hand, by using the operator relation

$$(A+B)^{-1} = (\mathrm{Id}-A^{-1}B)^{-1}A^{-1}$$

with $A=(\mathcal{B}^2/2m)-z-(z^2/2m)$ and $B=\tilde{V}\Lambda$, one obtains

$$S(c) = S_0(\mathrm{Id}+\tilde{V}\Lambda S_0)^{-1}. \tag{6}$$

Therefore, by (5) and (6) it is found that

$$(\mathbb{D}(c)-mc^2-z)^{-1}=(\mathbb{D}_0(c)-mc^2-z)^{-1}(\mathrm{Id}+\tilde{V}(\mathbb{D}_0(c)-mc^2-z)^{-1})^{-1}$$
$$=\left(\Lambda+\frac{c\mathcal{B}+z}{2mc^2}\right)S_0\left(\mathrm{Id}+\tilde{V}\Lambda S_0+\tilde{V}\frac{c\mathcal{B}+z}{2mc^2}S_0\right)^{-1}$$
$$=\left(\Lambda+\frac{c\mathcal{B}+z}{2mc^2}\right)S(c)\left(\mathrm{Id}+\tilde{V}\frac{c\mathcal{B}+z}{2mc^2}S(c)\right)^{-1}.$$

□

Proof (Theorem 1): Since $(H_\infty-z)^{-1}$ is bounded for $z\in\mathbb{C}\backslash\mathbb{R}$ and

$$\left\|\frac{z^2}{2mc^2}(H_\infty-z)^{-1}\right\|<1$$

for c sufficiently large, one can expand

$$S(c)=\sum_{n=0}^{\infty}\left(\frac{z^2}{2mc^2}(H_\infty-z)^{-1}\right)^n(H_\infty-z)^{-1}, \tag{7}$$

where the sum is convergent in the operator norm.

For any fixed $z\in\mathbb{C}\backslash\mathbb{R}$ and c sufficiently large,

$$\left\|T(c):=\tilde{V}\frac{c\mathcal{B}+z}{2mc^2}S(c)\right\|<1$$

and so

$$(\mathrm{Id}+T(c))^{-1}=\sum_{n=0}^{\infty}(-T(c))^n. \tag{8}$$

Replacing (7) and (8) into (3) one obtains the expansion

$$(\mathbb{D}(c)-mc^2-z)^{-1}=\sum_{n=0}^{\infty}\frac{R_n(z)}{c^n}$$

with

$$R_0(z)=\Lambda(H_\infty-z)^{-1},$$

$$R_1(z)=\Lambda(H_\infty-z)^{-1}\frac{\mathcal{B}}{2m}+\frac{\mathcal{B}}{2m}(H_\infty-z)^{-1}\Lambda,$$

and so on, and the sum is convergent in the operator norm. The result then follows. □

III. LOCALIZATION RESULTS

Consider the family of Dirac operators,

$$\mathbb{D}_\omega(m,c)=\begin{pmatrix}mc^2 & cd^*\\ cd & -mc^2\end{pmatrix}+V_\omega\,\mathrm{Id}_2,\quad \omega\in\Omega=\{-V,V\}^{\mathbb{Z}}, \tag{9}$$

on $\ell^2(\mathbb{Z};\mathbb{C}^2)$, where $V_\omega(n)$, $n\in\mathbb{Z}$, are i.i.d. Bernoulli random variables taking the values $\pm V$, $V>0$, with common (nontrivial) probability measure μ and product measure $\boldsymbol{P}=\Pi_{n\in\mathbb{Z}}\mu(V_\omega(n))$. Let $P^\omega_{I,m}$ be the spectral projector of $\mathbb{D}_\omega(m,c)$ onto the interval $I\subset\mathbb{R}$.

Denote by $\delta_n^{\pm}$ the elements of the canonical position basis of $\ell^2(\mathbb{Z};\mathbb{C}^2)$, for which all entries are $\binom{0}{0}$ except at the nth entry, which is given by $\binom{1}{0}$ and $\binom{0}{1}$ for the superscript indices $+$ and $-$, respectively. If $\Psi=\binom{\psi^+}{\psi^-}$ is a solution of the eigenvalue equation

$$(\mathbb{D}_\omega(m,c)-E)\Psi=0,$$

then it is simple to check that

$$\begin{pmatrix}\psi^+(n+1)\\ \psi^-(n)\end{pmatrix}=T_m^{V_\omega(n)}(E)\begin{pmatrix}\psi^+(n)\\ \psi^-(n-1)\end{pmatrix},$$

with

$$T_m^V(E)=\begin{pmatrix}1+\dfrac{m^2c^4-(E-V)^2}{c^2} & \dfrac{mc^2+E-V}{c}\\ \dfrac{mc^2-E+V}{c} & 1\end{pmatrix}.$$

The transfer matrix from site k to site n is introduced by

$$T_m^{\omega}(E;n,k)=T_m^{V_\omega(n-1)}(E)T_m^{V_\omega(n-2)}(E)\cdots T_m^{V_\omega(k)}(E),\quad n>k$$

and $T_m^{\omega}(E;n,n)=\mathrm{Id}_2$. For $q>0$, let $|X|^q$ be the moment of order q of the position operator on $\ell^2(\mathbb{Z};\mathbb{C}^2)$, i.e.,

$$|X|^q\Psi=\sum_n |n|^q(\langle\delta_n^+,\Psi\rangle\delta_n^+ + \langle\delta_n^-,\Psi\rangle\delta_n^-).$$

Definition 1: The operator $\mathbb{D}_\omega(m,c)$ is dynamically localized on a spectral interval I if for all $q>0$ and for all exponentially decaying initial state $\Psi\in\ell^2(\mathbb{Z};\mathbb{C}^2)$,

$$\sup_t M_{\Psi,I,\omega}^{(q)}(m,t):=\sup_t\langle P_{I,m}^{\omega}e^{-i\mathbb{D}_\omega(m,c)t}\Psi,|X|^qP_{I,m}^{\omega}e^{-i\mathbb{D}_\omega(m,c)t}\Psi\rangle<\infty,$$

***P** almost surely (**P**-a.s.). Otherwise $\mathbb{D}_\omega(m,c)$ is dynamically delocalized on I. If $I=\sigma(\mathbb{D}_\omega(m,c))$, then $M_{\Psi,I,\omega}^{(q)}(m,t)$ will be denoted by $M_{\Psi,\omega}^{(q)}(m,t)$.*

It is important to notice that although the Dirac operator acts on spinors, its eigenvalue equation, in the transfer matrix form, looks exactly like the equation for a one-dimensional Schrödinger operator acting on scalar valued functions, with the transfer matrix being in $\mathrm{SL}(2,\mathbb{R})$. Hence the methods used in studies of the usual one-dimensional Anderson model, as Furstenberg's theorem, can be applied for this Dirac model; see Secs. IV and V.

The localization results are gathered in the following set of theorems.

Theorem 2: *Let $(\mathbb{D}_\omega(m,c))_{\omega\in\Omega}$ be as in (9) and $V\in(0,c],V\neq c/\sqrt{2}$. Then, **P** almost surely, the Lyapunov exponent,*

$$\gamma_m(E)=\lim_{n\to\infty}\frac{1}{|n|}\ln\|T_m^{\omega}(E;n,1)\|$$

exists, is independent of ω, and

(i) (i.1) $\gamma_m(E\neq\pm V)>0$ for $m\geqslant 0$,
(i.2) $\gamma_m(E=\pm V)>0$ for $m>0$,
(i.3) $\gamma_0(E=\pm V)=0$.

(ii) *Let $m\geqslant 0$; then **P**-a.s. $\sigma(\mathbb{D}_\omega(m,c))$ is pure point.*

(iii) (iii.1) *Let $m>0$. Then **P**-a.s. the operator $\mathbb{D}_\omega(m,c)$ is dynamically localized on its spectrum.*

(iii.2) *For any closed interval* $I \subset \sigma(\mathbb{D}_\omega(0,c))$, *with* $\pm V \notin I$, *the operator* $\mathbb{D}_\omega(0,c)$ *is dynamically localized on* I.

Theorem 3: *Let* $(\mathbb{D}_\omega(m,c))_{\omega\in\Omega}$ *be as in (9),* $m \geqslant 0$ *and* $V > c, V \neq c\sqrt{2+m^2c^2}$. *Then,* ***P****a.s. the spectrum of* $\mathbb{D}_\omega(m,c)$ *is pure point and this operator is dynamically localized on its spectrum.*

Theorem 4: *Let* $(\mathbb{D}_\omega(m,c))_{\omega\in\Omega}$ *be as in (9),* $m \geqslant 0$ *and* $V = c/\sqrt{2}$ (*respectively*, $V = c\sqrt{2+m^2c^2}$). *Then the same conclusions of Theorem 2 (respectively, Theorem 3) hold except at the four possibilities of energies* $E_V = \pm c\sqrt{2+m^2c^2} \pm c/\sqrt{2}$ (*respectively*, $E_V = 0$). [*The point is that* $E_V = \pm c\sqrt{2+m^2c^2} \pm c/\sqrt{2}$ (*respectively*, $E_V = 0$) *are energies so that* $\gamma_m(E_V) = 0$.]

For the next result it is convenient to use the average dynamical moments

$$A^{(q)}_{\Psi,\omega}(m,T) := \int_0^\infty \frac{1}{T} e^{-2t/T} M^{(q)}_{\Psi,\omega}(m,t)\mathrm{d}t, \tag{10}$$

defined for $m \geqslant 0$ and $T > 0$. The main reason for working with this kind of Laplace transform average is relation (14) ahead.

Theorem 5 (massless case): *Let* $(\mathbb{D}_\omega(0,c))_{\omega\in\Omega}$ *be as in (9) and* $V \in (0,c]$, $V \neq c/\sqrt{2}$. *Then, for* $q > 0$ *and* Ψ *with only one nonzero component, there exists* $0 < C_q(\omega) < \infty$ *such that, for* $T > 0$,

(i) $A^{(q)}_{\Psi,\omega}(0,T) \geqslant C_q(\omega) T^{q-1/2}$ ***P****-a.s.*,
(ii) $A^{(q)}_{\Psi,\omega}(0,T) \geqslant C_q(\omega) T^{q-1}$ *for every* ω,

i.e., $\mathbb{D}_\omega(0,c)$ *is not dynamically localized on its spectrum.*

The following theorem establishes very general upper bounds for the dynamical moments of the position operator; notice that it holds for any potential sequence $\widetilde{V}$ and is not restricted to the Bernoulli case.

Theorem 6: *Let* $\mathbb{D}(m,c)$ *be as in (2),* $m \geqslant 0$ *and* Ψ *with only one nonzero component (so in the domain of* $|X|^q$ *for all* $q > 0$). *Then for any* $q \in \mathbb{N}$ *there exists* $0 < K_q(\widetilde{V},m,c) < \infty$ *such that*

$$M^{(q)}_\Psi(m,t) \leqslant K_q(\widetilde{V},m,c) t^q, \quad t \geqslant 1.$$

Remark: It is possible to adjust the constant K_q so that the above upper bound holds for $t \geqslant \varepsilon$ for any given $\varepsilon > 0$, instead of just $t \geqslant 1$. Since $M^{(q)}_\Psi(m,t) \geqslant M^{(q')}_\Psi(m,t)$ for $q \geqslant q'$, it is evident that $M^{(q)}_\Psi(m,t) \leqslant K_{\lceil q \rceil}(\widetilde{V},m,c) t^{\lceil q \rceil}$ for real q.

IV. TOOLS

In this section some tools and notations that will be used in the proofs of the results presented in Sec. III are collected. For studying the positivity of the Lyapunov exponent γ_m, $m \geqslant 0$, the following particular form of Furstenberg theorem[5] will be used.

Lemma 2: Let $\mathcal{G}_m(E)$ *be the smallest closed subgroup of* $SL(2,\mathbb{R})$ *generated by the matrices* $T^V_m(E)$ *and* $T^{-V}_m(E)$. *Then* $\gamma_m(E) > 0$ *if*

(i) $\mathcal{G}_m(E)$ *is not compact, and*
(ii) *there is no probability measure on* $P(\mathbb{R}^2)$ *(the set of all the directions of* $\mathbb{R}^2$*) that is invariant under the action of* $\mathcal{G}_m(E)$, *which is equivalent to the statement, the orbit* $\mathcal{G}_m(E)\cdot\tilde{x} := \{T\cdot\tilde{x}, T \in \mathcal{G}_m(E)\}$ *of each direction* $\tilde{x} \in P(\mathbb{R}^2)$ *contains at least three elements.*

If $L > 0$, $n \in \mathbb{Z}$, consider the finite subset of $\mathbb{Z}$,

$$\Lambda_L(n) = \left\{ k \in \mathbb{Z} : |k-n| \leqslant \frac{L}{2} \right\}$$

with boundary

$$\partial\Lambda_L(n)=\{(k,k'):k\in\Lambda_L(n),k'\notin\Lambda_L(n),|k-k'|=1\}.$$

Denote by $\mathbb{D}_\omega^{\Lambda_L(n)}(m,c)$ the operator $\mathbb{D}_\omega(m,c)$ restricted to $\ell^2(\Lambda_L(n);\mathbb{C}^2)$ with zero boundary conditions outside $\Lambda_L(n)$.

The matrix elements of an operator $\mathcal{O}$ on $\ell^2(\mathbb{Z};\mathbb{C}^2)$ are given by

$$\mathcal{O}_{nk}=\begin{pmatrix}\langle\delta_n^+,\mathcal{O}\delta_k^+\rangle & \langle\delta_n^+,\mathcal{O}\delta_k^-\rangle\\ \langle\delta_n^-,\mathcal{O}\delta_k^+\rangle & \langle\delta_n^-,\mathcal{O}\delta_k^-\rangle\end{pmatrix}$$

with "norm"

$$\|\mathcal{O}_{nk}\|^2=|\langle\delta_n^+,\mathcal{O}\delta_k^+\rangle|^2+|\langle\delta_n^+,\mathcal{O}\delta_k^-\rangle|^2+|\langle\delta_n^-,\mathcal{O}\delta_k^+\rangle|^2+|\langle\delta_n^-,\mathcal{O}\delta_k^-\rangle|^2.$$

Now two important results required for the multiscale analysis are described. The first one is the Wegner's estimate, adapted from Ref. 6 to the discrete Dirac operator (details will be omitted, since they are long and very similar to the Schrödinger case).

Lemma 3: Let $\mathbb{D}_\omega(m,c)$ *be as in (9) and I a compact energy interval. For any* $\theta\in(0,1)$ *and* $\tau>0$ *there exist* $L_0=L_0(I,\theta,\tau,m)>0$ *and* $a=a(I,\theta,\tau,m)>0$ *such that*

$$\boldsymbol{P}\{\omega:\mathrm{dist}(E,\sigma(\mathbb{D}_\omega^{\Lambda_L(0)}(m,c)))\leqslant e^{-\tau L^\theta}\}\leqslant e^{-aL^\theta}$$

for all $E\in I$ *and* $L\geqslant L_0$.

The second result is the initial estimate for localization, adapted from Ref. 28 (details omitted).

Lemma 4: Let $\mathbb{D}_\omega(m,c)$ *be as in (9),* $\epsilon>0$ *and* $\theta\in(0,1)$. *For each* $E_0\in\mathbb{R}$, $E_0\notin\sigma(\mathbb{D}_\omega^{\Lambda_L(0)}(m,c))$ *with* $\gamma_m(E_0)>\epsilon$, *there exist* $L_0=L_0(E_0,\epsilon,\theta,m)>0$ *and* $r=r(E_0,\epsilon,\theta,m)>0$ *such that*

$$\boldsymbol{P}\{\omega:\|(\mathbb{D}_\omega^{\Lambda_L(0)}(m,c)-E_0)_{0k}^{-1}\|\leqslant e^{-(\gamma_m(E_0)-\epsilon)L/2}\ \forall\ k\in\partial\Lambda_L(0)\}\geqslant 1-e^{-rL^\theta}$$

for all $L\geqslant L_0$.

In order to obtain dynamical localization from the multiscale analysis, the following properties of $\mathbb{D}_\omega(m,c)$ are useful.

(P1) With respect to the spectral measure of $\mathbb{D}_\omega(m,c)$, almost every energy is a generalized eigenvalue, i.e., with polynomially bounded eigenvector (see Ref. 3 and 22).

(P2) If $E\notin\sigma(\mathbb{D}_\omega^{\Lambda_L(n)}(m,c))$ and $\Psi\in\ell^2(\mathbb{Z};\mathbb{C}^2)$ so that $\mathbb{D}_\omega(m,c)\Psi=E\Psi$, then

$$\Psi(n)=-(\mathbb{D}_\omega^{\Lambda_L(n)}(m,c)-E)_{nl_1}^{-1}\begin{pmatrix}0 & c\\ 0 & 0\end{pmatrix}\Psi(l_1-1)-(\mathbb{D}_\omega^{\Lambda_L(n)}(m,c)-E)_{nl_2}^{-1}\begin{pmatrix}0 & 0\\ c & 0\end{pmatrix}\Psi(l_2+1),$$

with $\{(l_1,l_1-1),(l_2,l_2+1)\}=\partial\Lambda_L(n)$.

Property (P2) follows after defining the *boundary operator* $\mathcal{F}_{\Lambda_L(n)}$ by its matrix elements

$$(\mathcal{F}_{\Lambda_L(n)})_{jk}=\begin{cases}-\begin{pmatrix}0 & c\\ 0 & 0\end{pmatrix} & \text{if } j-1=k,\quad j\in\Lambda_L(n),\quad k\notin\Lambda_L(n),\\ -\begin{pmatrix}0 & 0\\ c & 0\end{pmatrix} & \text{if } j+1=k,\quad j\in\Lambda_L(n),\quad k\notin\Lambda_L(n),\\ \begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix} & \text{otherwise},\end{cases}$$

noting that $l^2(\mathbb{Z};\mathbb{C}^2)=l^2(\Lambda_L(n);\mathbb{C}^2)\oplus l^2(\mathbb{Z}\setminus\Lambda_L(n);\mathbb{C}^2)$ and

$$\mathbb{D}_\omega(m,c)=\mathbb{D}_\omega^{\Lambda_L(n)}(m,c)+\mathbb{D}_\omega^{\mathbb{Z}\setminus\Lambda_L(n)}(m,c)-\mathcal{F}_{\Lambda_L(n)}.$$

In the zero mass case ($m=0$) the operators $\mathbb{D}_\omega(0,c)$, $\omega\in\Omega$, presents critical energies $E_V=\pm V$ for $V\in(0,c]$, $V\neq c/\sqrt{2}$, as defined in Ref. 18, since either $T_0^V(V)=\mathrm{Id}_2$ and $T_0^{-V}(V)$ is elliptic [that is, $|\mathrm{trace}\ T_0^{-V}(V)|<2$] or $T_0^{-V}(-V)=\mathrm{Id}_2$ and $T_0^V(-V)$ is elliptic. Thus there exists a real invertible matrix Q such that

$$QT_0^{\pm V}(E_V)Q^{-1}=\begin{pmatrix}\cos(\eta_\pm) & -\sin(\eta_\pm)\\ \sin(\eta_\pm) & \cos(\eta_\pm)\end{pmatrix}.$$

Since the eigenvalues of this matrix are $e^{i\eta_\pm}$ and $e^{-i\eta_\pm}$, for both of the above cases one has $\eta_+-\eta_-\neq k\pi$, $k\in\mathbb{Z}$ (a condition required in Ref. 18). By using the modified Prüfer variables, phase shifts, oscillatory sums, large deviation estimates as in Ref. 18, one obtains the following result.

Lemma 5 (massless case): Let $\lambda>0$ be arbitrary. Then there are $b>0$ and $C<\infty$ such that for every $N\in\mathbb{N}$, there exists a set $\Omega_N(\lambda)\subset\Omega$ with $\mathbf{P}(\Omega_N(\lambda))\leqslant Ce^{-bN^\lambda}$ and

$$\|T_0^\omega(E;n,k)\|\leqslant C$$

for all $\omega\in\Omega\backslash\Omega_N(\lambda)$, $0\leqslant k\leqslant n\leqslant N$, and $E\in[E_V-N^{-\lambda-1/2},E_V+N^{-\lambda-1/2}]$.

On the other hand, since $\|QT_0^{\pm V}(E_V)Q^{-1}\|=1$, expanding $T_0^{\pm V}(E_V+\epsilon)$ into powers of ϵ one obtains

$$\|QT_0^{\pm V}(E_V+\epsilon)Q^{-1}\|\leqslant 1+a|\epsilon|$$

for $|\epsilon|\leqslant\delta$, $0<a<\infty$, and one deduces the following.

Lemma 6 (massless case): For $\delta>0$ there exists $C<\infty$ such that for all $n,k\in\mathbb{Z}$ and $E\in[E_V-\delta,E_V+\delta]$,

$$\|T_0^\omega(E;n,k)\|\leqslant Ce^{C\delta|n-k|}.$$

An inductive argument shows that, for $\zeta\in\mathbb{C}$ and $m\geqslant 0$,

$$T_m^\omega(E+\zeta;n,k)=T_m^\omega(E;n,k)-\zeta\sum_{l=k}^{n-1}T_m^\omega(E+\zeta;n,l+1)S_\zeta^\omega(E;l)T_m^\omega(E;l,k),\tag{11}$$

where

$$S_\zeta^\omega(E;l)=\frac{\zeta}{c^2}\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}+\frac{1}{c}\begin{pmatrix}\frac{2}{c}(E-V_\omega(l)) & -1\\ 1 & 0\end{pmatrix}.$$

Now, for $z\in\mathbb{C}\backslash\mathbb{R}$ and $m\geqslant 0$, introduce the two-components Green's function

$$\begin{pmatrix}G_{m,\omega}^+(z;n)\\ G_{m,\omega}^-(z;n)\end{pmatrix}=\begin{pmatrix}\langle\delta_n^+,(\mathbb{D}_\omega(m,c)-z)^{-1}\delta_0^+\rangle\\ \langle\delta_n^-,(\mathbb{D}_\omega(m,c)-z)^{-1}\delta_0^+\rangle\end{pmatrix},$$

so that

$$(\mathbb{D}_\omega(m,c)-z)\begin{pmatrix}G_{m,\omega}^+(z;n)\\ G_{m,\omega}^-(z;n)\end{pmatrix}=\delta_0^+(n).$$

By using transfer matrices, one obtains for $n\leqslant 0$,

$$\begin{pmatrix}G_{m,\omega}^+(z;n)\\ G_{m,\omega}^-(z;n-1)\end{pmatrix}=T_m^\omega(z;n,0)\begin{pmatrix}G_{m,\omega}^+(z;0)\\ G_{m,\omega}^-(z;-1)\end{pmatrix}\tag{12}$$

and for $n\geqslant 1$,

$$\begin{pmatrix} G^{+}_{m,\omega}(z;n) \\ G^{-}_{m,\omega}(z;n-1) \end{pmatrix} = T^{\omega}_{m}(z;n,1)\begin{pmatrix} G^{+}_{m,\omega}(z;1) \\ G^{-}_{m,\omega}(z;0) \end{pmatrix}. \tag{13}$$

For $z=E+i/T(T>0)$ and $m\geqslant 0$, it is also valid the following identity (adapted from Lemma 3.2 in Ref. 19):

$$A^{(q)}_{\delta^{+}_{0},\omega}(m,T) = \frac{1}{2\pi T}\sum_{n\in\mathbb{Z}}|n|^{q}\int_{\mathbb{R}}(|G^{+}_{m,\omega}(z;n)|^{2}+|G^{-}_{m,\omega}(z;n)|^{2})\mathrm{d}E. \tag{14}$$

V. LOCALIZATION PROOFS

In this section the proofs of Theorems 2–6 are presented.

Proof (Theorems 2 and 3): The strategy of the proof is based on Ref. 10, where the random dimer Schrödinger operator was studied. Since for the discrete Dirac operator there are the particular role played by the mass and some different possibilities for the transfer matrices, a rather detailed proof will be presented. The idea is to show that given $\epsilon>0$, $I\subset\sigma(\mathbb{D}_{\omega}(m,c))$ a compact energy interval not containing the excluded V values, then for each $0<\gamma<\gamma_{m}(I):=\inf\{\gamma_{m}(E):E\in I\}$ there exist a constant $C(\omega,\epsilon,\gamma)$ and, for each eigenfunction $\varphi_{j,\omega}=\binom{\varphi^{+}_{j,\omega}}{\varphi^{-}_{j,\omega}}$ with energy $E_{j,\omega}\in I$, a "center" $z_{j,\omega}\in\mathbb{Z}$, such that

$$\|\varphi_{j,\omega}(n)\|\leqslant C(\omega,\epsilon,\gamma)e^{\gamma|z_{j,\omega}|^{\epsilon}}e^{-\gamma|n-z_{j,\omega}|},\quad \forall\, n\in\mathbb{Z}. \tag{15}$$

If Ψ decays exponentially with rate $\theta_{0}>0$ and if $q>0$, it is known that (15) (that is, SULE condition) implies the existence of a constant $C_{\Psi}(m,I,\omega)$ so that

$$\sup_{t} M^{(q)}_{\Psi,I,\omega}(m,t)\leqslant C_{\Psi}(m,I,\omega),\quad \boldsymbol{P}\text{-}a.s.,$$

i.e., $\mathbb{D}_{\omega}(m,c)$ is dynamically localized on I (see Sec. II in Ref. 16).

To prove (ii) and (15), it is sufficient to show strict positivity of the Lyapunov exponent, because in this case Lemmas 3 and 4 hold. By using the multiscale analysis[28] together with (P1) and (P2), one can then follow the proof of Theorem 3.1 in Ref. 16 [properly adapted to $\mathbb{D}_{\omega}(m,c)$] to obtain (ii) and (15) (details will be omitted).

Now the proof of (i). It follows from Furstenberg and Kesten theorem[5] that, $\boldsymbol{P}$-*a.s.* the Lyapunov exponent γ_{m} exists and is independent of ω.

Consider first the energies $E\neq\pm V$ and it will be proven that $\gamma_{m}(E\neq\pm V)>0$ for all $m\geqslant 0$ and for all $E\in\sigma(\mathbb{D}_{\omega}(m,c))$. Let $\mathcal{G}_{m}(E)$ be as in the Lemma 2. Set $\alpha=E-V$, $\beta=E+V$ and rename $T^{V}_{m}(E)=T^{(\alpha)}_{m}$, $T^{-V}_{m}(E)=T^{(\beta)}_{m}$. In the present case $\alpha\neq 0$ and $\beta\neq 0$.

Since the problem is symmetric in α and β, the proof is reduced to the study of three cases,

(a) $T^{(\alpha)}_{m}$ and $T^{(\beta)}_{m}$ are elliptic ($|\mathrm{trace}\ T^{(\alpha)}_{m}|<2, |\mathrm{trace}\ T^{(\beta)}_{m}|<2$),
(b) $T^{(\alpha)}_{m}$ is parabolic ($|\mathrm{trace}\ T^{(\alpha)}_{m}|=2$),
(c) $T^{(\alpha)}_{m}$ is hyperbolic ($|\mathrm{trace}\ T^{(\alpha)}_{m}|>2$).

Note that in cases (b) and (c) the group $\mathcal{G}_{m}(E)$ is not compact.

Case (a): Since $T^{(\alpha)}_{m}$ and $T^{(\beta)}_{m}$ are both elliptic, then $|\alpha|,|\beta|\in(mc^{2},c\sqrt{4+m^{2}c^{2}})$. In this case such matrices do not commute. Since the operator

$$T^{(\alpha)}_{m}T^{(\beta)}_{m}(T^{(\alpha)}_{m})^{-1}(T^{(\beta)}_{m})^{-1}$$

built from two noncommuting elliptic elements is hyperbolic, it follows that $\mathcal{G}_{m}(E)$ is not compact. Moreover, note that

$$\operatorname{trace}(T_m^{(\alpha)})^2 = \frac{\alpha^4}{c^4} - \left(2m^2 + \frac{4}{c^2}\right)\alpha^2 + m^2c^2(4 + m^2c^2) + 2$$

(analogous for $T_m^{(\beta)}$). Hence, if $\alpha^2 \neq 2c^2 + m^2c^4$ or $\beta^2 \neq 2c^2 + m^2c^4$, then $T_m^{(\alpha)}$ and $(T_m^{(\alpha)})^2$ or $T_m^{(\beta)}$ and $(T_m^{(\beta)})^2$ are elliptic. Since elliptic elements have no fixed points in $P(\mathbb{R}^2)$, it follows that for any $\tilde{x} \in P(\mathbb{R}^2)$, $\mathcal{G}_m(E)\cdot\tilde{x}$ contains at least the three elements $\tilde{x}$, $T_m^{(\alpha)}\cdot\tilde{x}$, $(T_m^{(\alpha)})^2\cdot\tilde{x}$ or $\tilde{x}$, $T_m^{(\beta)}\cdot\tilde{x}$, $(T_m^{(\beta)})^2\cdot\tilde{x}$. Therefore, by Lemma 2, $\gamma_m(E) > 0$. If, on the other hand, $\alpha^2 = 2c^2 + m^2c^4$ and $\beta^2 = 2c^2 + m^2c^4$, then $E = 0$ and $V = c\sqrt{2 + m^2c^2}$, which is one of the excluded pairs described in Theorem 4.

Case (b): Suppose $T_m^{(\alpha)}$ is parabolic, that is, $|\alpha| = mc^2$ or $|\alpha| = c\sqrt{4 + m^2c^2}$. First the possibility $\alpha = mc^2$ will be discussed (the case $\alpha = -mc^2$ is similar). In this case

$$T_m^{(\alpha)} = \begin{pmatrix} 1 & 2mc \\ 0 & 1 \end{pmatrix}, \quad \text{and so } (T_m^{(\alpha)})^n = \begin{pmatrix} 1 & 2nmc \\ 0 & 1 \end{pmatrix}.$$

Denote by $\{e_1, e_2\}$ the canonical basis of $\mathbb{R}^2$. By taking a vector $x = x_1e_1 + x_2e_2$, and setting $\tilde{x}$ for its direction, one concludes that $\lim_{n\to\infty}(T_m^{(\alpha)})^n\cdot\tilde{x} = \tilde{e}_1$. If ν is a probability measure that is invariant under the action of $\mathcal{G}_m(E)$, and if $f \in C_0^\infty(P(\mathbb{R}^2))$, by Lebesgue's dominated convergence theorem one has

$$f(\tilde{e}_1) = \lim_{n\to\infty} \int f((T_m^{(\alpha)})^n \cdot \tilde{x}) \mathrm{d}\nu(\tilde{x}).$$

This means that $\nu = \delta_{\tilde{e}_1}$. But the matrix $T_m^{(\beta)}$ does not leave invariant the direction $\tilde{e}_1$ since

$$T_m^{(\beta)}e_1 = \left(1 + \frac{m^2c^4 - \beta^2}{c^2}\right)e_1 + \frac{-\beta + mc^2}{c}e_2 \quad \text{and } \beta \neq mc^2.$$

Thus it is proven that there is no invariant measure under the action of $\mathcal{G}_m(E)$. Therefore, by Lemma 2 one gets $\gamma_m(E) > 0$.

Consider now the possibility $\alpha = c\sqrt{4 + m^2c^2}$ (the case $\alpha = -c\sqrt{4 + m^2c^2}$ is similar). In this case an eigenvector of

$$T_m^{(\alpha)} = \begin{pmatrix} -3 & mc + \sqrt{4 + m^2c^2} \\ mc - \sqrt{4 + m^2c^2} & 1 \end{pmatrix}$$

is given by $v_1 = (mc + \sqrt{4 + m^2c^2}/2, 1)$. Picking $v_2 = (-mc + \sqrt{4 + m^2c^2}/2, -1)$ a vector orthogonal to v_1, the matrix $T_m^{(\alpha)}$ in the basis $\{v_1, v_2\}$ is

$$\begin{pmatrix} -1 & -4 - m^2c^2 + mc\sqrt{4 + m^2c^2} \\ 0 & -1 \end{pmatrix}.$$

Repeating the previous calculation for this case, one obtains $\nu = \delta_{\tilde{v}_1}$. But $T_m^{(\beta)}$ does not leave invariant the direction $\tilde{v}_1$ except for $\beta = 0$ or $\beta = c\sqrt{4 + m^2c^2} = \alpha$, which are excluded since the first condition yields $E = -V$ and the second one $V = 0$. Thus it is proven that there is no invariant measure and, by Lemma 2, $\gamma_m(E) > 0$.

Case (c): Suppose now that $T_m^{(\alpha)}$ is hyperbolic (so $|\alpha| < mc^2$ or $|\alpha| > c\sqrt{4 + m^2c^2}$). It is sufficient to study the orbit of the eigendirections of $T_m^{(\alpha)}$, namely

$$e_m^\epsilon = \begin{pmatrix} \alpha^2 - m^2c^4 + \epsilon\sqrt{(\alpha^2 - m^2c^4)(\alpha^2 - m^2c^4 - 4c^2)} \\ 2c(\alpha - mc^2) \end{pmatrix}, \quad \epsilon = \pm 1.$$

If $T_m^{(\beta)}$ is hyperbolic then the orbit of e_m^ϵ is infinite. Hence $\gamma_m(E) > 0$ by Lemma 2. If $T_m^{(\beta)}$ is parabolic, it is again case (b). Finally, suppose that $T_m^{(\beta)}$ is elliptic. If $T_m^{(\beta)}\tilde{e}_m^{\ \epsilon} \neq \tilde{e}_m^{\ -\epsilon}$, then $T_m^{(\beta)}\tilde{e}_m^{\epsilon}$ cannot belong to the eigendirections of $T_m^{(\alpha)}$ and its orbit is infinite. Hence $\gamma_m(E) > 0$ by Lemma 2. If $T_m^{(\beta)}\tilde{e}_m^{\ \epsilon} = \tilde{e}_m^{\ -\epsilon}$, then simple calculations lead to the equations

$$\left(1+m^2c^2-\frac{\beta^2}{c^2}\right)(\alpha^2-m^2c^4+\epsilon u)=4(m^2c^4-\beta\alpha)+(\alpha^2-m^2c^4-\epsilon u)$$

with $\epsilon=\pm 1$ and $u=\sqrt{(\alpha^2-m^2c^4)(\alpha^2-m^2c^4-4c^2)}\neq 0$. It implies $\beta^2=2c^2+m^2c^4$ and $\alpha=\beta\pm c\sqrt{2}$, which means $V=c/\sqrt{2}$ and $E=\pm c\sqrt{2+m^2c^2}-c/\sqrt{2}$. The symmetric case where one assumes that $T_m^{(\beta)}$ is hyperbolic leads naturally to $\alpha^2=2c^2+m^2c^4$ and $\beta=\alpha\pm c\sqrt{2}$, which means $V=c/\sqrt{2}$ and $E=\pm c\sqrt{2+m^2c^2}+c/\sqrt{2}$. Those are excluded pairs that will be discussed in the proof of Theorem 4.

Consider now the energy $E=V$ (the case $E=-V$ is analogous). Note that $\alpha=0$ and $\beta=2V$. First the case $m>0$ will be discussed. The two possible transfer matrices are

$$T_m^{(\alpha)}=\begin{pmatrix}1+m^2c^2 & mc\\ mc & 1\end{pmatrix} \quad \text{and} \quad T_m^{(\beta)}=\begin{pmatrix}1+\dfrac{m^2c^4-4V^2}{c^2} & \dfrac{mc^2+2V}{c}\\ \dfrac{mc^2-2V}{c} & 1\end{pmatrix}.$$

Observe that $T_m^{(\alpha)}$ and $T_m^{(\beta)}$ do not commute, and that $T_m^{(\alpha)}$ is hyperbolic. It is enough to study this case for $\beta=c\sqrt{4+m^2c^2}$ ($T_m^{(\beta)}$ is parabolic). The eigendirections of $T_m^{(\alpha)}$ are

$$e_m^{\delta}=\begin{pmatrix}\dfrac{mc+\delta\sqrt{4+m^2c^2}}{2}\\ 1\end{pmatrix}, \quad \delta=\pm 1.$$

The matrices $T_m^{(\alpha)}$ and $T_m^{(\beta)}$ in the basis $\{e_m^1,e_m^{-1}\}$ are given, respectively, by

$$\begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_{-1}\end{pmatrix} \quad \text{and} \quad \begin{pmatrix}-1 & 4+m^2c^2-mc\sqrt{4+m^2c^2}\\ 0 & -1\end{pmatrix},$$

with

$$\lambda_1\lambda_{-1}=\left(1+\frac{m^2c^2}{2}+\frac{mc\sqrt{4+m^2c^2}}{2}\right)\left(1+\frac{m^2c^2}{2}-\frac{mc\sqrt{4+m^2c^2}}{2}\right)=1.$$

Suppose that $T_m^{(\alpha)}$ occurs with probability $0<p<1$ and $T_m^{(\beta)}$ occurs with probability $1-p$. Denote by n_α (respectively, n_β) the number of times that $T_m^{(\alpha)}$ (respectively, $T_m^{(\beta)}$) occurs in the product $T_m^{\omega}(E;n,1)$. Supposing, without loss of generality, that $T_m^{V_\omega(1)}(E)=T_m^{(\alpha)}$, one has

$$T_m^{\omega}(E;n,1)=\begin{pmatrix}\lambda_1^{n_\alpha} & C_nP(\lambda_1,\lambda_{-1})\\ 0 & \lambda_{-1}^{n_\alpha}\end{pmatrix},$$

***P**-a.s.*, where C_n is a constant and $P(\lambda_1,\lambda_{-1})$ is a polynomial in λ_1 and λ_{-1}. Thus,

$$\|T_m^{\omega}(E;n,1)\|\geqslant\left\|\begin{pmatrix}\lambda_1^{n_\alpha}\\ 0\end{pmatrix}\right\|=\lambda_1^{n_\alpha}, \quad \lambda_1>1,$$

and therefore ***P**-a.s.*

$$\gamma_m(E=V)=\lim_{n\to\infty}\frac{1}{|n|}\ln\|T_m^{\omega}(E;n,1)\|\geqslant(\ln\lambda_1)\lim_{n\to\infty}\frac{n_\alpha}{|n|}=(\ln\lambda_1)p>0.$$

Now the case $m=0$ will be treated. In this case

$$T_0^{(\alpha)}=\mathrm{Id}_2 \quad \text{and} \quad T_0^{(\beta)}=\begin{pmatrix}1-4V^2/c^2 & 2V/c\\ -2V/c & 1\end{pmatrix}.$$

One then finds

$$\lim_{n\to\infty} \|(T_0^{(\beta)})^n\|^{1/n} = 1$$

if $V \in (0,c]$ and

$$\lim_{n\to\infty} \|(T_0^{(\beta)})^n\|^{1/n} > 1$$

if $V > c$. Hence, if $V \in (0,c]$, $V \neq c/\sqrt{2}$,

$$\gamma_0(E=V) = \lim_{n\to\infty} \frac{n_\beta}{|n|} \ln\|(T_0^{(\beta)})^{n_\beta}\|^{1/n_\beta} = (1-p)\ln 1 = 0,$$

and $\gamma_0(E=V) > 0$ if $V > c$. □

Proof (Theorem 4): By analyzing the proof of Theorems 2 and 3 observe that for $V=c/\sqrt{2}$ (respectively, $V=c\sqrt{2+m^2c^2}$) one has $\gamma_m(E_V \neq \pm c\sqrt{2+m^2c^2} \pm c/\sqrt{2}) > 0$ [respectively, $\gamma_m(E_V \neq 0) > 0$] and then the same conclusions of Theorem 2 (respectively, Theorem 3) hold. It remains to show that γ_m vanishes at the pairs $(V=c\sqrt{2+m^2c^2}, E_V=0)$ and $(V=c/\sqrt{2}, E_V = \pm c\sqrt{2+m^2c^2} \pm c/\sqrt{2})$. Note that in all cases $E_V \in \sigma(\mathbb{D}_\omega(m,c))$ $\boldsymbol{P}$-*a.s.*.

First it will be treated the case $(V=c/\sqrt{2}, E_V=-c\sqrt{2+m^2c^2}-c/\sqrt{2})$ (the others three excluded cases with $V=c/\sqrt{2}$ are similar). In this case one has $\beta=-c\sqrt{2+m^2c^2}$ and $\alpha=\beta-c\sqrt{2}$. The eigenvectors of $T_m^{(\alpha)}$ are given by

$$\begin{pmatrix} \dfrac{2c-\sqrt{2}\beta+\epsilon\sqrt{4c^2+2m^2c^4-2\sqrt{2}c\beta}}{\beta-c\sqrt{2}-mc^2} \\ 1 \end{pmatrix}, \quad \epsilon = \pm 1,$$

and by looking at the matrices in the basis given by these two vectors, the study is reduced to products of matrices of the following two types:

$$\begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & \kappa_- \\ \kappa_+ & 0 \end{pmatrix}$$

with $\lambda_+\lambda_- = 1$ and $\kappa_+\kappa_- = -1$, where

$$\lambda_\pm = -1 + \frac{\sqrt{2}\beta}{c} \pm \frac{\sqrt{4c^2+2m^2c^4-2\sqrt{2}c\beta}}{c}$$

and

$$\kappa_\pm = \left(-\frac{\beta}{c}+mc\right)\left(\frac{2c-\sqrt{2}\beta \pm \sqrt{4c^2+2m^2c^4-2\sqrt{2}c\beta}}{\beta-c\sqrt{2}-mc^2}\right)+1.$$

Moreover,

$$(T_m^{(\beta)})^2 = \begin{pmatrix} -1 & mc+\beta/c \\ mc-\beta/c & 1 \end{pmatrix}^2 = -\mathrm{Id}_2.$$

Therefore the proof that $\gamma_m(E_V=-c\sqrt{2+m^2c^2}-c/\sqrt{2}, V=c/\sqrt{2})=0$ is analogous to the Schrödinger case (see the proof of Theorem 2.4 in Ref. 10).

Now consider the excluded case $(V=c\sqrt{2+m^2c^2}, E_V=0)$. In this case $\alpha^2=\beta^2=2c^2+m^2c^4$. Since $\alpha \neq \beta$ (otherwise $V=0$), then $\alpha=-\beta=\pm c\sqrt{2+m^2c^2}$. Noting that $(T_m^{(\alpha)})^2=(T_m^{(\beta)})^2=-\mathrm{Id}_2$ and $T_m^{(\alpha)}T_m^{(\beta)}$ is hyperbolic, the proof that $\gamma_m(E_V=0, V=c\sqrt{2+m^2c^2})=0$ is again similar to the corresponding Schrödinger case (see the proof of Theorem 2.4 in Ref. 10). □

Proof (Theorem 5): (i) It is sufficient to prove the theorem for $\Psi=\delta_0^+$. Given $\lambda>0$, there exists $b'>0$ and by Lemma 5 there are $b>0$ and $C<\infty$ such that, by applying Lemma 5 for N

$=[b'T]$, together with the relation (11) for $m=0$ and $\zeta=i/T$, one concludes that there exists a set $\Omega_N(\lambda)\subset\Omega$ with $\boldsymbol{P}(\Omega_N(\lambda))\leqslant Ce^{-bN^{\lambda}}$ and

$$\|T_0^{\omega}(E+i/T;n,1)\|\leqslant C \tag{16}$$

for all $\omega\in\Omega\backslash\Omega_N(\lambda)$, $1\leqslant n\leqslant N$, and $E\in I_V=[E_V-N^{-\lambda-1/2},E_V+N^{-\lambda-1/2}]$.

Supposing that

$$|G^+_{0,\omega}(E+i/T;1)|^2+|G^-_{0,\omega}(E+i/T;0)|^2\geqslant B_1(\omega)>0,$$

it follows from (13) and

$$\|T_0^{\omega}(E+i/T;n,1)^{-1}\|=\|T_0^{\omega}(E+i/T;n,1)\|$$

that

$$\max\{|G^+_{0,\omega}(E+i/T;n)|^2,|G^-_{0,\omega}(E+i/T;n-1)|^2\}\geqslant\frac{B_1(\omega)}{2\|T_0^{\omega}(E+i/T;n,1)\|^2}. \tag{17}$$

Thus, replacing (16) and (17) into (14), $\boldsymbol{P}$-*a.s.* one has

$$A^{(q)}_{\delta_0^+,\omega}(0,T)\geqslant\frac{1}{2\pi T}\sum_{0\leqslant n\leqslant[b'T]}n^q\int_{I_V}\frac{B_1(\omega)}{2C^2}\mathrm{d}E\geqslant B_q(\omega)T^qN^{-\lambda-1/2}\geqslant C_q(\omega)T^{q-1/2-\lambda}$$

for some constant $C_q(\omega)>0$.

If, on the other hand,

$$|G^+_{0,\omega}(E+i/T;0)|^2+|G^-_{0,\omega}(E+i/T;-1)|^2\geqslant B_2(\omega)>0,$$

then one gets this estimate in the same way, but based on (12) instead of (13). Since $\lambda>0$ is arbitrary, this finishes the proof.

(ii) It follows from the above arguments by using Lemma 6. □

Proof (Theorem 6): The arguments will be a variation of Ref. 23. Define the operator

$$p:=i[\mathbb{D}(m,c),X]=ci\begin{pmatrix}0 & -d^*-1\\ d+1 & 0\end{pmatrix}$$

with $[\cdot,\cdot]$ denoting the commutator. Note that p is self-adjoint and bounded. Set

$$X(t)=e^{i\mathbb{D}(m,c)t}Xe^{-i\mathbb{D}(m,c)t}\quad\text{and}\quad p(t)=e^{i\mathbb{D}(m,c)t}pe^{-i\mathbb{D}(m,c)t},$$

so that

$$\frac{d}{\mathrm{d}t}X(t)=i[\mathbb{D}(m,c),X(t)]=e^{i\mathbb{D}(m,c)t}i[\mathbb{D}(m,c),X]e^{-i\mathbb{D}(m,c)t}=p(t).$$

Hence

$$X(t)=X+\int_0^t p(s)\mathrm{d}s.$$

Using this relation, the boundedness $\|p(t)\|=\|p\|<\infty$ for all t, Cauchy-Schwarz inequality, and keeping only the dominant terms for large t, it follows that for $t\geqslant 1$ and $q\in\mathbb{N}$, there exists $C_q(\tilde{V},m,c)>0$ so that

$$M_{\Psi}^{(q)}(m,t) = \langle \Psi, |X(t)|^q \Psi \rangle \leqslant C_q(\tilde{V},m,c) \int_0^t \cdots \int_0^t \langle \Psi, p(s_1)\cdots p(s_q)\Psi \rangle \mathrm{d}s_1 \cdots \mathrm{d}s_q \leqslant C_q(\tilde{V},m,c)$$
$$\times \|p\|^q t^q = K_q(\tilde{V},m,c) t^q.$$

□

VI. DYNAMICAL COMPARISON

The aim of this section is to compare the dynamical moments $M_{\Psi}^{(q)}(m,t)$, as in Definition 1, for different masses and general potentials, in particular for the massless and massive Bernoulli cases.

Theorem 7: *Let $\mathbb{D}(m,c)$ and $\mathbb{D}(m',c)$ be Dirac operators on $l^2(\mathbb{Z},\mathbb{C}^2)$ defined as in (2) with the same potential $\tilde{V}$, and let Ψ be with only one nonzero component. Given $T>0$, there exists a constant $B_q>0$ so that*

$$\sup_{0\leqslant t\leqslant T} |M_{\Psi}^{(q)}(m,t) - M_{\Psi}^{(q)}(m',t)| \leqslant B_q |m-m'| c^2 T^{q+2}. \tag{18}$$

Proof: Observe that for $m=m'$ the result is immediate. Suppose $m \neq m'$. For the proof it will be assumed that $m>0$, $m'=0$ and $\Psi = \delta_0^+$ (the case $m>0$, $m'>0$ and Ψ as in the hypotheses is similar).

For fixed $\alpha>0$ consider the Banach space

$$B_\alpha := \{\Phi \in l^2(\mathbb{Z},\mathbb{C}^2) : \|\Phi\|_\alpha = \sup_{k\in\mathbb{Z}} e^{\alpha|k|}(|\langle \delta_k^+, \Phi\rangle| + |\langle \delta_k^-, \Phi\rangle|) < \infty\}.$$

Since $\mathbb{D}(m,c)$ is a bounded operator on B_α, it follows that

$$|\langle \delta_n^+, e^{-i\mathbb{D}(m,c)t}\delta_0^+\rangle| + |\langle \delta_n^-, e^{-i\mathbb{D}(m,c)t}\delta_0^+\rangle| \leqslant \|e^{-i\mathbb{D}(m,c)t}\delta_0^+\|_\alpha e^{-n\alpha} \leqslant e^{-n\alpha + t\|\mathbb{D}(m,c)\|_\alpha}. \tag{19}$$

For $k\in\mathbb{N}$ denote by X^k the restriction of the position operator X to the set $\{n\in\mathbb{Z}: |n|\leqslant k\}$ and by $M_{\delta_0^+}^{(q),k}(m,t)$ the corresponding dynamical moments. Then, for all times $t \leqslant \alpha k/2\|\mathbb{D}(m,c)\|_\alpha$, using (19) one has

$$|M_{\delta_0^+}^{(q)}(m,t) - M_{\delta_0^+}^{(q),k}(m,t)| = \sum_{|n|>k} |n|^q (|\langle \delta_n^+, e^{-i\mathbb{D}(m,c)t}\delta_0^+\rangle|^2 + |\langle \delta_n^-, e^{-i\mathbb{D}(m,c)t}\delta_0^+\rangle|^2)$$
$$\leqslant C_1(q) k^q e^{-k\alpha + 2t\|\mathbb{D}(m,c)\|_\alpha} \leqslant C_1(q) k^q. \tag{20}$$

Furthermore, it follows by DuHamel's formula that

$$M_{\delta_0^+}^{(q),k}(m,t) - M_{\delta_0^+}^{(q),k}(0,t) = -i\int_0^t \langle \delta_0^+, e^{i\mathbb{D}(m,c)t}|X^k|^q e^{-i\mathbb{D}(m,c)(t-s)}(\mathbb{D}(m,c)-\mathbb{D}(0,c))e^{-i\mathbb{D}(0,c)s}\delta_0^+\rangle \mathrm{d}s$$
$$+ i\int_0^t \langle \delta_0^+, e^{i\mathbb{D}(m,c)(t-s)}(\mathbb{D}(m,c)-\mathbb{D}(0,c))e^{i\mathbb{D}(0,c)s}|X^k|^q e^{-i\mathbb{D}(0,c)t}\delta_0^+\rangle \mathrm{d}s.$$

Hence, for $t\leqslant \alpha k/2\|\mathbb{D}(m,c)\|_\alpha$, using (19), the fact of the operator $e^{i\mathbb{D}(m,c)t}$ on $\ell^2(\mathbb{Z};\mathbb{C}^2)$ be unitary and Cauchy-Schwarz, it is found that

$$|M_{\delta_0^+}^{(q),k}(m,t) - M_{\delta_0^+}^{(q),k}(0,t)| \leqslant C_2(q) mc^2 k^{q+1} t e^{-k\alpha + t\|\mathbb{D}(m,c)\|_\alpha} \leqslant C_2(q) mc^2 \frac{\alpha}{2\|\mathbb{D}(m,c)\|_\alpha} k^{q+2}. \tag{21}$$

Thus, by (20) and (21),

$$|M^{(q)}_{\delta_0^+}(m,t) - M^{(q)}_{\delta_0^+}(0,t)| \leqslant B_q mc^2 \frac{\alpha}{2\|\mathbb{D}(m,c)\|_\alpha} k^{q+2},$$

for all times $t \leqslant \alpha k/2\|\mathbb{D}(m,c)\|_\alpha$.

Now, for each $T>0$ choose k to be the smallest integer such that

$$k \geqslant \frac{2\|\mathbb{D}(m,c)\|_\alpha}{\alpha} T.$$

Therefore, for all $t \leqslant T$,

$$|M^{(q)}_{\delta_0^+}(m,t) - M^{(q)}_{\delta_0^+}(0,t)| \leqslant B_q mc^2 T^{q+2}.$$

□

With respect to the Bernoulli-Dirac model (9), the relation (18) with $m>0$ and $m'=0$ gives an estimate of how, for small times and/or sufficiently small mass, the dynamics of the localized regime follows the delocalized one. In terms of the average dynamical moments $A^{(q)}_{\Psi,\omega}(m,T)$ defined in (10) one has the following.

Corollary 1: Let $(\mathbb{D}_\omega(m,c))_{\omega\in\Omega}$ *be as in (9),* $m \geqslant 0$ *and* $V \in (0,c]$, $V \neq c/\sqrt{2}$, *and let* Ψ *be with only one nonzero component. Then, for each* $q>0$, ***P****-a.s. there is* $\widetilde{C}_{q,\omega}>0$ *so that*

$$\left| 1 - \frac{A^{(q)}_{\Psi,\omega}(m,t)}{A^{(q)}_{\Psi,\omega}(0,t)} \right| \leqslant \widetilde{C}_{q,\omega} mc^2 t^{5/2}, \quad t>0.$$

Notice that the power exponent on the right-hand side of this expression does not depend on q.

Proof: By Theorem 7 with $m>0$ and $m'=0$, it follows that for all $t>0$,

$$|A^{(q)}_{\Psi,\omega}(m,t) - A^{(q)}_{\Psi,\omega}(0,t)| \leqslant \Gamma(q+3) C_{q,\omega} mc^2 t^{q+2},$$

with Γ the usual gamma function. By Theorem 5(i) there is $0<B_q(\omega)<\infty$ such that

$$A^{(q)}_{\Psi,\omega}(0,t) \geqslant B_q(\omega) t^{q-1/2}, \quad \textbf{\textit{P}}\text{-}a.s.,$$

and the result follows with $\widetilde{C}_{q,\omega}=\Gamma(q+3)C_{q,\omega}/B_q(\omega)$. □

Remark: By using Theorem 6 one gets (for $q \in \mathbb{N}$),

$$|M^{(q)}_{\Psi}(m,t) - M^{(q)}_{\Psi}(m',t)| \leqslant \widetilde{K}_q(\omega,m,m',c) t^q,$$

but with no expression for the constant $\widetilde{K}_q(\omega,m,m',c)$. The price paid for the explicit dependence on the masses and light speed c in Theorem 7 is the larger exponent $q+2$ instead of just q. In the same way, the exponent $5/2$ in Corollary 1 could be replaced by $3/2$, but with no precise dependence of the resulting multiplicative constant on m and c.

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k-component *q*-deformed charge coherent states and their nonclassical properties

X.-M. Liu[a)]
Department of Physics, Beijing Normal University, Beijing 100875, China[b)] *and Physique Nucléaire Théorique et Physique Mathématique, Université Libre de Bruxelles, Campus de la Plaine CP229, Boulevard du Triomphe, B-1050 Brussels, Belgium*

C. Quesne[c)]
Physique Nucléaire Théorique et Physique Mathématique, Université Libre de Bruxelles, Campus de la Plaine CP229, Boulevard du Triomphe, B-1050 Brussels, Belgium

F. Song
Department of Physics, Beijing Normal University, Beijing 100875, China

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k-component *q*-deformed charge coherent states are constructed, their (over)completeness proved and their generation explored. The *q*-deformed charge coherent states and the even (odd) *q*-deformed charge coherent states are the two special cases of them as *k* becomes 1 and 2, respectively. A *D*-algebra realization of the $SU_q(1,1)$ generators is given in terms of them. Their nonclassical properties are studied and it is shown that for $k \geqslant 3$, they exhibit two-mode *q*-antibunching, but neither $SU_q(1,1)$ squeezing, nor one- or two-mode *q*-squeezing. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1951607]

I. INTRODUCTION

The coherent states introduced by Schrödinger[1] and Glauber[2] are the eigenstates of the boson annihilation operator, and have widespread applications in the fields of physics.[3–7] However, in all the cases the quanta involved are uncharged. In 1976, Bhaumik *et al.*[4,8,9] constructed the boson coherent states which, carrying definite charge, are the eigenstates of both the pair boson annihilation operator and the charge operator. These kind of states are the so-called charge coherent states. Based on this work, the charge coherent states for SU(2),[10] SU(3),[11] and arbitrary compact Lie groups[12] were also put forward.

The concept of charge coherent states has proved to be very useful in many areas, such as elementary particle physics,[9,13–17] quantum field theory,[12,18,19] nuclear physics,[20] thermodynamics,[21–23] quantum mechanics,[24] and quantum optics.[25–27] Moreover, some schemes for generating charge coherent states in quantum optics were proposed.[25,26,28,29]

As is well known, the even and odd coherent states,[30] which are the two orthonormalized eigenstates of the square of the boson annihilation operator, play an important role in quantum optics.[31–33] An extension of the even and odd coherent states is to define the *k*-component coherent states,[34,35] which are the k ($k \geqslant 1$) orthonormalized eigenstates of the kth power of the boson annihilation operator. The coherent states and the even (odd) ones are the two special cases of the *k*-component coherent states as *k* becomes 1 and 2, respectively. Inspired by the above idea, in Ref. 36 one of the authors (X.-M.L.) has generalized the charge coherent states to the even and odd charge coherent states, defined as the two orthonormalized eigenstates of both the square of the pair boson annihilation operator and the charge operator; in Ref. 37 he has further extended the

[a)]Author to whom correspondence should be addressed. Electronic mail: liuxm@bnu.edu.cn
[b)]Address for correspondence.
[c)]Electronic mail: cquesne@ulb.ac.be

even and odd charge coherent states to the k-component charge coherent states, defined as the k orthonormalized eigenstates of both the kth power of the pair boson annihilation operator and the charge operator. The charge coherent states and the even (odd) ones are the two special cases of the k-component charge coherent states as k becomes 1 and 2, respectively.

On the other hand, quantum groups,[38,39] introduced as a mathematical description of deformed Lie algebras, have given the possibility of generalizing the notion of coherent states to the case of q-deformations.[40–44] A q-deformed harmonic oscillator[40,45] was defined in terms of q-boson annihilation and creation operators, the latter satisfying the quantum Heisenberg-Weyl algebra,[40,45,46] which plays an important role in quantum groups. The q-deformed coherent states introduced by Biedenharn[40] are the eigenstates of the q-boson annihilation operator. Such states have been well studied,[41,42,47,48] and widely applied to quantum optics and mathematical physics.[44,49–53] Furthermore, the q-deformed charge coherent states[54,55] were constructed as the eigenstates of both the pair q-boson annihilation operator and the charge operator.

A natural extension of the q-deformed coherent states is provided by the even and odd q-deformed coherent states,[56] which are the two orthonormalized eigenstates of the square of the q-boson annihilation operator. In a previous paper,[57] motivated by the above idea, the authors (X.-M.L. and C.Q.) have generalized the q-deformed charge coherent states to the even and odd q-deformed charge coherent states, defined as the two orthonormalized eigenstates of both the square of the pair q-boson annihilation operator and the charge operator. A further extension of the even and odd q-deformed coherent states is given by the k-component q-deformed coherent states,[58,59] which are the k orthonormalized eigenstates of the kth power of the q-boson annihilation operator. The q-deformed coherent states and the even (odd) ones are the two special cases of the k-component q-deformed coherent states as k becomes 1 and 2, respectively. In a parallel way, it is very desirable to generalize the even and odd q-deformed charge coherent states to the k-component q-deformed charge coherent states, defined as the k orthonormalized eigenstates of both the kth power of the pair q-boson annihilation operator and the charge operator. The q-deformed charge coherent states and the even (odd) ones are the two special cases of the k-component q-deformed charge coherent states as k becomes 1 and 2, respectively.

This paper is arranged as follows. In Sec. II, the k-component q-deformed charge coherent states are constructed. Their completeness is proved in Sec. III. Section IV is devoted to generating them. In Sec. V, they are used to provide a D-algebra realization of the $\mathrm{SU}_q(1,1)$ generators. Their nonclassical properties, such as $\mathrm{SU}_q(1,1)$ squeezing, single- or two-mode q-squeezing, and two-mode q-antibunching, are studied in Sec. VI. Section VII contains a summary of the results.

II. k-COMPONENT q-DEFORMED CHARGE COHERENT STATES

Two mutually commuting q-deformed harmonic oscillators are defined in terms of two pairs of independent q-boson annihilation and creation operators a_i, a_i^+ $(i=1,2)$, together with corresponding number operators N_i, satisfying the quantum Heisenberg-Weyl algebra

$$a_i a_i^+ - q a_i^+ a_i = q^{-N_i}, \tag{1}$$

$$[N_i, a_i^+] = a_i^+, \quad [N_i, a_i] = -a_i, \tag{2}$$

where q is a positive real deformation parameter. The operators a_i, a_i^+, and N_i act in the Fock space with basis $|n\rangle_i$, $(n=0, 1, 2, \ldots)$, such that

$$a_i|0\rangle_i = 0, \quad |n\rangle_i = \frac{(a_i^+)^n}{\sqrt{[n]!}}|0\rangle_i, \tag{3}$$

where

$$[n]! \equiv [n]_q! = [n]_q[n-1]_q \cdots [1]_q, \quad [0]! = 1, \tag{4}$$

$$[n]_q = \frac{q^n - q^{-n}}{q - q^{-1}} \equiv [n]. \tag{5}$$

Their action on the basis states is given by

$$a_i|n\rangle_i = \sqrt{[n]}|n-1\rangle_i, \quad a_i^+|n\rangle_i = \sqrt{[n+1]}|n+1\rangle_i, \quad N_i|n\rangle_i = n|n\rangle_i. \tag{6}$$

Note that $[n]$ is invariant under $q \leftrightarrow 1/q$. In the following, $[n]$ will refer to the q-deformed n defined by (5) corresponding to the base q. If the base is different, then it will be indicated explicitly.

The q-boson operators a_i and a_i^+ can be constructed from the conventional boson annihilation and creation operators b_i, b_i^+ in the following way:[60]

$$a_i = \sqrt{\frac{[N_i+1]}{N_i+1}}\, b_i, \quad a_i^+ = b_i^+ \sqrt{\frac{[N_i+1]}{N_i+1}}, \tag{7}$$

where $N_i = b_i^+ b_i$. It is worth noticing that $[N_i] = a_i^+ a_i$.

The operators $a_1(a_1^+)$ and $a_2(a_2^+)$ are assigned the "charge" quanta 1 and -1, respectively. Thus the charge operator is given by

$$Q = N_1 - N_2. \tag{8}$$

In view of the fact that

$$[Q, (a_1 a_2)^k] = 0, \tag{9}$$

where k is a positive integer ($k=1, 2, 3, \ldots$), we may seek the k-component q-deformed charge coherent states, which are the k orthonormalized eigenstates of both the kth power $(a_1 a_2)^k$ of the pair q-boson annihilation operator $a_1 a_2$ and the charge operator Q.

Let $|m,n\rangle = |m\rangle_1 |n\rangle_2$ denote the basis states of two-mode Fock space, where $|m\rangle_1$ and $|n\rangle_2$ are the eigenstates of N_1 and N_2 corresponding to the eigenvalues m and n, respectively. They satisfy the completeness relation

$$\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} |m,n\rangle\langle m,n| = I. \tag{10}$$

We now consider the following states:

$$\begin{aligned} |\xi, \underline{q}, k\rangle_j &= N_{k\underline{q}}^j \sum_{p=\max(0,-\underline{q}/k)}^{\infty} \frac{\xi^{kp+j+\min(0,\underline{q})}}{\{[kp+j]\,![kp+j+\underline{q}]\,!\}^{1/2}} |kp+j+\underline{q}, kp+j\rangle \\ &= \begin{cases} N_{k\underline{q}}^j \sum_{n=0}^{\infty} \dfrac{\xi^{kn+j}}{\{[kn+j]\,![kn+j+\underline{q}]\,!\}^{1/2}} |kn+j+\underline{q}, kn+j\rangle, & \underline{q} \geqslant 0, \\ N_{k\underline{q}}^j \sum_{n=0}^{\infty} \dfrac{\xi^{kn+j}}{\{[kn+j]\,![kn+j-\underline{q}]\,!\}^{1/2}} |kn+j, kn+j-\underline{q}\rangle, & \underline{q} \leqslant 0, \end{cases} \end{aligned} \tag{11}$$

where $j = 0, 1, \ldots, k-1$, ξ is a complex number, $\underline{q}$ is a fixed integer, and $N_{k\underline{q}}^j$ are normalization factors given by

$$N_{k\underline{q}}^j \equiv N_{k\underline{q}}^j(|\xi|^2) = \left\{ \sum_{n=0}^{\infty} \frac{(|\xi|^2)^{kn+j}}{[kn+j]\,![kn+j+|\underline{q}|]!} \right\}^{-1/2}. \tag{12}$$

As can be verified by explicit calculations, these states satisfy the relations

$$(a_1a_2)^k|\xi,\underline{q},k\rangle_j=\xi^k|\xi,\underline{q},k\rangle_j,\quad Q|\xi,\underline{q},k\rangle_j=\underline{q}|\xi,\underline{q},k\rangle_j,\quad {}_j\langle\xi,\underline{q},k|\xi,\underline{q},k\rangle_{j'}=\delta_{jj'}. \tag{13}$$

It indicates that $|\xi,\underline{q},k\rangle_j$ $(j=0,1,\ldots,k-1)$ in (11) are exactly the k orthonormalized eigenstates of both the operator $(a_1a_2)^k$ and Q corresponding to the eigenvalues ξ^k and $\underline{q}$, respectively. Obviously, $\underline{q}$ is the charge number which the states $|\xi,\underline{q},k\rangle_j$ carry.

Therefore, the k states of (11) are just what we want, that is to say, they are the k-component q-deformed charge coherent states. In the limit $q\to 1$, they reduce to the usual k-component charge coherent states constructed by the author (X.-M.L.).[37]

According to (11), for $k=1$, we obtain

$$\begin{aligned}|\xi,\underline{q},1\rangle_0&=N_{\underline{q}}\sum_{p=\max(0,-\underline{q})}^{\infty}\frac{\xi^{p+\min(0,\underline{q})}}{\{[p]!\,[p+\underline{q}]!\,\}^{1/2}}|p+\underline{q},p\rangle\\&=\begin{cases}N_{\underline{q}}\sum_{n=0}^{\infty}\dfrac{\xi^n}{\{[n]!\,[n+\underline{q}]!\,\}^{1/2}}|n+\underline{q},n\rangle, & \underline{q}\geqslant 0,\\ N_{\underline{q}}\sum_{n=0}^{\infty}\dfrac{\xi^n}{\{[n]!\,[n-\underline{q}]!\,\}^{1/2}}|n,n-\underline{q}\rangle, & \underline{q}\leqslant 0,\end{cases}\\&\equiv|\xi,\underline{q}\rangle\end{aligned} \tag{14}$$

where

$$N_{\underline{q}}\equiv N^0_{1\underline{q}}(|\xi|^2)=\left\{\sum_{n=0}^{\infty}\frac{(|\xi|^2)^n}{[n]!\,[n+|\underline{q}|]!}\right\}^{-1/2}. \tag{15}$$

It is evident that $|\xi,\underline{q},1\rangle_0(\equiv|\xi,\underline{q}\rangle)$ are exactly the so-called q-deformed charge coherent states given in Ref. 54.

According to (11), for $k=2$, we obtain

$$\begin{aligned}|\xi,\underline{q},2\rangle_j&=N^j_{2\underline{q}}\sum_{p=\max(0,-\underline{q}/2)}^{\infty}\frac{\xi^{2p+j+\min(0,\underline{q})}}{\{[2p+j]!\,[2p+j+\underline{q}]!\,\}^{1/2}}|2p+j+\underline{q},2p+j\rangle\\&=\begin{cases}N^j_{2\underline{q}}\sum_{n=0}^{\infty}\dfrac{\xi^{2n+j}}{\{[2n+j]!\,[2n+j+\underline{q}]!\,\}^{1/2}}|2n+j+\underline{q},2n+j\rangle, & \underline{q}\geqslant 0,\\ N^j_{2\underline{q}}\sum_{n=0}^{\infty}\dfrac{\xi^{2n+j}}{\{[2n+j]!\,[2n+j-\underline{q}]!\,\}^{1/2}}|2n+j,2n+j-\underline{q}\rangle, & \underline{q}\leqslant 0,\end{cases}\end{aligned} \tag{16}$$

where $j=0$, 1. It is evident that $|\xi,\underline{q},2\rangle_0$ $(|\xi,\underline{q},2\rangle_1)$ are exactly the so-called even (odd) q-deformed charge coherent states obtained by the authors (X.-M.L. and C.Q.).[57]

From (11), it follows that

$${}_j\langle\xi,\underline{q},k|\xi',\underline{q}',k\rangle_{j'}=N^j_{k\underline{q}}(|\xi|^2)N^j_{k\underline{q}}(|\xi'|^2)[N^j_{k\underline{q}}(\xi^*\xi')]^{-2}\delta_{\underline{q}\underline{q}'}\delta_{jj'}. \tag{17}$$

This further shows that, for the same value of k, the states $|\xi,\underline{q},k\rangle_j$ are orthogonal to one another with respect to both the subscript j and the charge number $\underline{q}$. However, they are nonorthogonal with respect to the parameter ξ.

For the mean values of the operators N_1 and N_2, there exists the relation

$${}_j\langle\xi,\underline{q},k|N_1|\xi,\underline{q},k\rangle_j=\underline{q}+{}_j\langle\xi,\underline{q},k|N_2|\xi,\underline{q},k\rangle_j. \tag{18}$$

In terms of the k-component q-deformed charge coherent states, the q-deformed charge coherent states can be expanded as

$$|\xi,\underline{q}\rangle = N_{\underline{q}}\left[\sum_{j=0}^{k-1}(N_{k\underline{q}}^{j})^{-1}|\xi,\underline{q},k\rangle_j\right], \tag{19}$$

where the normalization factors are such that

$$N_{\underline{q}}^{-2} = \sum_{j=0}^{k-1}(N_{k\underline{q}}^{j})^{-2}. \tag{20}$$

III. COMPLETENESS OF *k*-COMPONENT *q*-DEFORMED CHARGE COHERENT STATES

Let us begin with some q-deformed formulas which are useful in the proof of completeness of the k-component q-deformed charge coherent states. The q-deformed Bessel function of (integer) order ν may be defined by[61]

$$J_\nu(q,x) = \sum_{k=0}^{\infty}\frac{(-1)^k}{[k]\,![\nu+k]!}\left(\frac{x}{\sqrt{q}[2]_{\sqrt{q}}}\right)^{\nu+2k}, \tag{21}$$

where $[n]_{\sqrt{q}}$ is defined as in Eq. (5) except for replacing q by $\sqrt{q}$. An integral representation of the q-deformed modified Bessel function of order ν is given by[62]

$$K_\nu(q,x) = \frac{1}{[2]_{\sqrt{q}}}\left(\frac{x}{[2]_{\sqrt{q}}}\right)^{\nu}\int_0^{\infty} d_q t\,\frac{1}{t^{\nu+1}}e_q(-t)e_q\left(-\frac{x^2}{([2]_{\sqrt{q}})^2 t}\right), \tag{22}$$

where $d_q t$ is a standard q-integration,[47,63,64] and $e_q(x)$ is a q-exponential function[47]

$$e_q(x) = \begin{cases}\displaystyle\sum_{n=0}^{\infty}\frac{x^n}{[n]!} & \text{for } x > -\zeta,\\ 0 & \text{otherwise},\end{cases} \tag{23}$$

with $-\zeta$ being the largest zero of $e_q(x)$. Then, it follows that[62]

$$\int_0^{\infty} d_{\sqrt{q}}u\, u^{2p+\nu+1}K_\nu(q,[2]_{\sqrt{q}}u) = \frac{[\nu+p]\,![p]!}{([2]_{\sqrt{q}})^2}. \tag{24}$$

We now prove that the k-component q-deformed charge coherent states form an (over)complete set, that is to say

$$\sum_{\underline{q}=-\infty}^{\infty}\int\frac{d_q^2\xi}{\pi}\phi_{\underline{q}}(\xi)N_{\underline{q}}^2\left[\sum_{j=0}^{k-1}(N_{k\underline{q}}^{j})^{-2}|\xi,\underline{q},k\rangle_{j\,j}\langle\xi,\underline{q},k|\right] \equiv \sum_{\underline{q}=-\infty}^{\infty} I_{\underline{q}} = I, \tag{25}$$

where

$$d_q^2\xi = |\xi|d_{\sqrt{q}}|\xi|\mathrm{d}\theta, \quad \xi = |\xi|e^{i\theta}, \tag{26}$$

and

$$\phi_{\underline{q}}(\xi) = \frac{([2]_{\sqrt{q}})^2}{2}(-\mathrm{i})^{\underline{q}}J_{\underline{q}}(q,\mathrm{i}\sqrt{q}[2]_{\sqrt{q}}|\xi|)K_{\underline{q}}(q,[2]_{\sqrt{q}}|\xi|). \tag{27}$$

Note that the integral over θ is a standard integration while that over $|\xi|$ is a q-integration.

In fact, for $\underline{q}\geqslant 0$, we have

$$
\begin{aligned}
I_{\underline{q}} &= \int \frac{d_{\underline{q}}^2\xi}{\pi}\phi_{\underline{q}}(\xi)N_{\underline{q}}^2\sum_{j=0}^{k-1}\sum_{n,m}\frac{\xi^{kn+j}\xi^{*km+j}|kn+j+\underline{q},kn+j\rangle\langle km+j+\underline{q},km+j|}{\{[kn+j]![kn+j+\underline{q}]![km+j]![km+j+\underline{q}]!\}^{1/2}} \\
&= \int_0^\infty \frac{d_{\sqrt{\bar{q}}}|\xi|}{\pi}\frac{([2]_{\sqrt{\bar{q}}})^2}{2}|\xi|^{\underline{q}+1}K_{\underline{q}}(q,[2]_{\sqrt{\bar{q}}}|\xi|)\sum_{j=0}^{k-1}\sum_{n,m}|\xi|^{k(n+m)+2j}\int_{-\pi}^{\pi}\mathrm{d}\theta\, e^{\mathrm{i}k(n-m)\theta} \\
&\quad\times\frac{|kn+j+\underline{q},kn+j\rangle\langle km+j+\underline{q},km+j|}{\{[kn+j]![kn+j+\underline{q}]![km+j]![km+j+\underline{q}]!\}^{1/2}} \\
&= \int_0^\infty d_{\sqrt{\bar{q}}}|\xi|([2]_{\sqrt{\bar{q}}})^2|\xi|^{\underline{q}+1}K_{\underline{q}}(q,[2]_{\sqrt{\bar{q}}}|\xi|)\times\sum_{j=0}^{k-1}\sum_{n=0}^{\infty}\frac{(|\xi|^2)^{kn+j}|kn+j+\underline{q},kn+j\rangle\langle kn+j+\underline{q},kn+j|}{[kn+j]![kn+j+\underline{q}]!} \\
&= \sum_{n=0}^{\infty}\frac{([2]_{\sqrt{\bar{q}}})^2}{[n]![n+\underline{q}]!}|n+\underline{q},n\rangle\langle n+\underline{q},n|\int_0^\infty d_{\sqrt{\bar{q}}}|\xi||\xi|^{2n+\underline{q}+1}K_{\underline{q}}(q,[2]_{\sqrt{\bar{q}}}|\xi|) \\
&= \sum_{n=0}^{\infty}|n+\underline{q},n\rangle\langle n+\underline{q},n|. \qquad (28)
\end{aligned}
$$

Similarly, for $\underline{q}\leqslant 0$, we get

$$
I_{\underline{q}} = \sum_{n=0}^{\infty}|n,n-\underline{q}\rangle\langle n,n-\underline{q}|. \qquad (29)
$$

Consequently, we derive

$$
\begin{aligned}
\sum_{\underline{q}=-\infty}^{\infty} I_{\underline{q}} &= \sum_{n=0}^{\infty}\left(\sum_{\underline{q}=-\infty}^{-1}|n,n-\underline{q}\rangle\langle n,n-\underline{q}| + \sum_{\underline{q}=0}^{\infty}|n+\underline{q},n\rangle\langle n+\underline{q},n|\right) \\
&= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}|m,n\rangle\langle m,n| = I. \qquad (30)
\end{aligned}
$$

Hence, the k-component q-deformed charge coherent states are qualified to make up an (over) complete representation. It should be mentioned that $I_{\underline{q}}$ represents the resolution of unity in the subspace where $Q=\underline{q}$.

In the two special cases of $k=1$ and $k=2$, the above demonstration gives the proof of completeness of the q-deformed charge coherent states[65] and the even (odd) q-deformed charge coherent states,[57] respectively.

IV. GENERATION OF *k*-COMPONENT *q*-DEFORMED CHARGE COHERENT STATES

The k-component q-deformed coherent states, defined as the k orthonormalized eigenstates of the kth power of the q-boson annihilation operator, can be expanded in the single-mode Fock space as[58,59]

$$
|\xi,k\rangle_j = N_k^j\sum_{n=0}^{\infty}\frac{\xi^{kn+j}}{\sqrt{[kn+j]!}}|kn+j\rangle, \qquad (31)
$$

where $j=0,1,\ldots,k-1$ and

$$
N_k^j \equiv N_k^j(|\xi|^2) = \left\{\sum_{n=0}^{\infty}\frac{(|\xi|^2)^{kn+j}}{[kn+j]!}\right\}^{-1/2}. \qquad (32)
$$

As a special case, for $k=1$, $|\xi,1\rangle_0$ are exactly the q-deformed coherent states, i.e.,

$$|\xi,1\rangle_0 = e_q^{-1/2}(|\xi|^2)\sum_{n=0}^{\infty}\frac{\xi^n}{\sqrt{[n]!}}|n\rangle \equiv |\xi\rangle. \tag{33}$$

The *k*-component *q*-deformed charge coherent states can also be obtained from the states (31) and (33) according to the following expression:

$$|\xi,\underline{q},k\rangle_j = \begin{cases} N_{k\underline{q}}^j e_q^{1/2}(|\xi_1|^2)[N_k^j(|\xi_2|^2)]^{-1}\xi_1^{-\underline{q}}\displaystyle\int_{-\pi}^{\pi}\frac{d\alpha}{2\pi}e^{+i\underline{q}\alpha}|e^{-i\alpha}\xi_1\rangle\otimes|e^{i\alpha}\xi_2,k\rangle_j, & \underline{q}\geqslant 0, \\ N_{k\underline{q}}^j e_q^{1/2}(|\xi_1|^2)[N_k^j(|\xi_2|^2)]^{-1}\xi_1^{+\underline{q}}\displaystyle\int_{-\pi}^{\pi}\frac{d\alpha}{2\pi}e^{-i\underline{q}\alpha}|e^{i\alpha}\xi_2,k\rangle_j\otimes|e^{-i\alpha}\xi_1\rangle, & \underline{q}\leqslant 0, \end{cases} \tag{34}$$

where $\xi=\xi_1\xi_2$. Such a representation is very useful since the properties of *q*-deformed coherent states and *k*-component *q*-deformed coherent states can now be employed in a study of the properties of *k*-component *q*-deformed charge coherent states. The expression for the latter given in (34) has a very simple group-theoretical interpretation, in (34) one suitably averages over the U(1)-group (caused by the charge operator Q) action on the product of *q*-deformed coherent states and *k*-component *q*-deformed coherent states, which then projects out the $Q=\underline{q}$ charge subspace contribution.

It is easy to see that in the limit $q\to 1$, the above discussion gives back the corresponding results for the usual *k*-component charge coherent states obtained in Ref. 37, and that in the two special cases of $k=1$ and $k=2$, it gives the corresponding results for the *q*-deformed charge coherent states[54] and the even (odd) *q*-deformed charge coherent states,[57] respectively.

V. *D*-ALGEBRA REALIZATION OF $SU_q(1,1)$ GENERATORS

As is well known, the coherent state *D*-algebra[6,66] is a mapping of quantum observables onto a differential form that acts on the parameter space of coherent states, and has a beautiful application in the reformulation of the entire laser theory in terms of *C*-number differential equations.[67] We shall construct the *D*-algebra realization of the *q*-deformed $SU_q(1,1)$ generators corresponding to the unnormalized *k*-component *q*-deformed charge coherent states, defined by

$$\|\underline{q}\rangle_j \equiv \|\xi,\underline{q},k\rangle_j = (N_{k\underline{q}}^j)^{-1}|\xi,\underline{q},k\rangle_j. \tag{35}$$

Let $\|\underline{q}\rangle$ denote a column vector composed of $\|\underline{q}\rangle_j$ $(j=0,1,\ldots,k-1)$, i.e.,

$$\|\underline{q}\rangle \equiv \begin{bmatrix} \|\underline{q}\rangle_0 \\ \|\underline{q}\rangle_1 \\ \vdots \\ \|\underline{q}\rangle_{k-1} \end{bmatrix}. \tag{36}$$

The action of the operators a_i, a_i^+ and N_i on this column vector can be written in the matrix form,

$$
\begin{array}{ll}
\text{Positive } Q & \text{Negative } Q \\
a_1\|\underline{q}\rangle = \|\underline{q}-1\rangle & a_1\|\underline{q}\rangle = \xi M\|\underline{q}-1\rangle \\
a_2\|\underline{q}\rangle = \xi M\|\underline{q}+1\rangle & a_2\|\underline{q}\rangle = \|\underline{q}+1\rangle \\
a_1^+\|\underline{q}\rangle = \xi^{-\underline{q}}\dfrac{d}{d_q\xi}\xi^{\underline{q}+1}\|\underline{q}+1\rangle & a_1^+\|\underline{q}\rangle = \dfrac{d}{d_q\xi}N\|\underline{q}+1\rangle \\
a_2^+\|\underline{q}\rangle = \dfrac{d}{d_q\xi}N\|\underline{q}-1\rangle & a_2^+\|\underline{q}\rangle = \xi^{\underline{q}}\dfrac{d}{d_q\xi}\xi^{-\underline{q}+1}\|\underline{q}-1\rangle \\
N_1\|\underline{q}\rangle = \left(\xi\dfrac{d}{\mathrm{d}\xi}+\underline{q}\right)\|\underline{q}\rangle & N_1\|\underline{q}\rangle = \xi\dfrac{d}{\mathrm{d}\xi}\|\underline{q}\rangle \\
N_2\|\underline{q}\rangle = \xi\dfrac{d}{\mathrm{d}\xi}\|\underline{q}\rangle & N_2\|\underline{q}\rangle = \left(\xi\dfrac{d}{\mathrm{d}\xi}-\underline{\mathrm{q}}\right)\|\underline{q}\rangle,
\end{array}
\tag{37}
$$

where $d/\mathrm{d}\xi$ is a standard differential operator, whereas $d/d_q\xi$ is a q-differential one,[42,47,64] defined by

$$
\frac{d}{d_q\xi}f(\xi) = \frac{f(q\xi)-f(q^{-1}\xi)}{q\xi-q^{-1}\xi}, \tag{38}
$$

and

$$
M = \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}, \quad N = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{bmatrix}. \tag{39}
$$

Obviously, N is both the inverse and the transpose of M. It is worth noticing that $M^k=N^k=I$, and $M^\alpha N^\beta=N^\beta M^\alpha$ for integers α,β.

The q-deformed $\mathrm{SU}_q(1,1)$ algebra consists of three generators K_0, K_+, and K_-, satisfying the commutation relations

$$
[K_+,K_-] = -[2K_0], \quad [K_0,K_\pm] = \pm K_\pm, \tag{40}
$$

and is realized in terms of the two-mode q-boson operators as

$$
K_- = a_1a_2, \quad K_+ = a_1^+a_2^+, \quad K_0 = \tfrac{1}{2}(N_1+N_2+1). \tag{41}
$$

Actually, the k-component q-deformed charge coherent states are also the k orthonormalized eigenstates of the kth power of K_-.

The D-algebra of the $\mathrm{SU}_q(1,1)$ generators A may be defined for the action on the ket coherent states (36) or for that on the corresponding bras as

$$
A\|\underline{q}\rangle = D^k(A)\|\underline{q}\rangle, \tag{42}
$$

$$
\langle\underline{q}\|A = D^b(A)\langle\underline{q}\|, \tag{43}
$$

respectively. Using (37) and (41), we get for the former

$$
D^k(K_-) = \xi M, \tag{44}
$$

$$
D^k(K_+) = \xi^{-|\underline{q}|}\frac{d}{d_q\xi}\xi^{|\underline{q}|+1}\frac{d}{d_q\xi}N, \tag{45}
$$

$$D^k(K_0) = \frac{1}{2}\left(2\xi\frac{d}{d\xi} + |\underline{q}| + 1\right)I, \tag{46}$$

while the latter can be obtained from the adjoint relation

$$D^b(A) = [D^k(A^+)]^*. \tag{47}$$

Thus, the D-algebra of the $SU_q(1,1)$ generators corresponding to the unnormalized k-component q-deformed charge coherent states has been realized in a q-differential-operator matrix form.

From (36), (39), (42), and (44), we clearly see that by the successive actions of the operator a_1a_2, each component of the k-component q-deformed charge coherent states, apart from normalization, can be transformed into another in this way, $|\xi,\underline{q},k\rangle_0 \to |\xi,\underline{q},k\rangle_{k-1} \to |\xi,\underline{q},k\rangle_{k-2} \to \cdots \to |\xi,\underline{q},k\rangle_1 \to |\xi,\underline{q},k\rangle_0$. Actually, a_1a_2 plays the role of a rotating operator among these k-component states.

It is easy to check that in the limit $q \to 1$, the above discussion gives back the corresponding results for the usual k-component charge coherent states obtained in Ref. 37, and that in the two special cases of $k=1$ and $k=2$, it gives the corresponding results for the q-deformed charge coherent states[65] and the even (odd) q-deformed charge coherent states,[57] respectively.

VI. NONCLASSICAL PROPERTIES OF *k*-COMPONENT *q*-DEFORMED CHARGE COHERENT STATES

In Ref. 57, the authors (X.-M.L. and C.Q.) have examined the even and odd q-deformed charge coherent states for some nonclassical properties, such as $SU_q(1,1)$ squeezing, single- or two-mode q-squeezing, and two-mode q-antibunching. In this section, we will study the nonclassical properties of the k-component q-deformed charge coherent states with $k \geqslant 3$.

A. $SU_q(1,1)$ squeezing

In analogy with the definition of SU(1,1) squeezing,[68] we have introduced $SU_q(1,1)$ squeezing[57] in terms of the Hermitian q-deformed quadrature operators

$$X_1 = \frac{K_+ + K_-}{2}, \quad X_2 = \frac{i(K_+ - K_-)}{2}, \tag{48}$$

which satisfy the commutation relation

$$[X_1, X_2] = \frac{i}{2}[2K_0] \tag{49}$$

and the uncertainty relation

$$\langle(\Delta X_1)^2\rangle\langle(\Delta X_2)^2\rangle \geqslant \tfrac{1}{16}|\langle[2K_0]\rangle|^2. \tag{50}$$

A state is said to be $SU_q(1,1)$ squeezed if

$$\langle(\Delta X_i)^2\rangle < \tfrac{1}{4}|\langle[2K_0]\rangle| \quad (i = 1 \text{ or } 2). \tag{51}$$

Let us now calculate the fluctuations (variances) of X_1 and X_2 with respect to the k-component q-deformed charge coherent states. Using (41)–(44) and (47), we get

$${}_0\langle\xi,\underline{q},k|K_+K_-|\xi,\underline{q},k\rangle_0 = |\xi|^2(N^0_{k\underline{q}})^2/(N^{k-1}_{k\underline{q}})^2, \tag{52}$$

$${}_m\langle\xi,\underline{q},k|K_+K_-|\xi,\underline{q},k\rangle_m = |\xi|^2(N^m_{k\underline{q}})^2/(N^{m-1}_{k\underline{q}})^2, \quad m = 1,2,\ldots,k-1. \tag{53}$$

In the meantime, for the states $|\xi,\underline{q},k\rangle_j$ $(k \geqslant 3)$, it always follows that

$$ {}_j\langle \xi,\underline{q},k|K_-|\xi,\underline{q},k\rangle_j = {}_j\langle \xi,\underline{q},k|K_-^2|\xi,\underline{q},k\rangle_j = 0, \quad j=0,1,\ldots,k-1. \tag{54} $$

Therefore, for $|\xi,\underline{q},k\rangle_0$ and $|\xi,\underline{q},k\rangle_m$ $(m=1,2,\ldots,k-1)$, the fluctuations are given by

$$ \begin{aligned} {}_0\langle \xi,\underline{q},k|(\Delta X_1)^2|\xi,\underline{q},k\rangle_0 &= {}_0\langle \xi,\underline{q},k|(\Delta X_2)^2|\xi,\underline{q},k\rangle_0 \\ &= \tfrac{1}{4}{}_0\langle \xi,\underline{q},k|[2K_0]|\xi,\underline{q},k\rangle_0 + \tfrac{1}{2}|\xi|^2(N_{k\underline{q}}^0)^2/(N_{k\underline{q}}^{k-1})^2, \end{aligned} \tag{55} $$

$$ \begin{aligned} {}_m\langle \xi,\underline{q},k|(\Delta X_1)^2|\xi,\underline{q},k\rangle_m &= {}_m\langle \xi,\underline{q},k|(\Delta X_2)^2|\xi,\underline{q},k\rangle_m \\ &= \tfrac{1}{4}{}_m\langle \xi,\underline{q},k|[2K_0]|\xi,\underline{q},k\rangle_m + \tfrac{1}{2}|\xi|^2(N_{k\underline{q}}^m)^2/(N_{k\underline{q}}^{m-1})^2. \end{aligned} \tag{56} $$

Consequently, for $k\geqslant 3$, we find

$$ \begin{aligned} {}_j\langle \xi,\underline{q},k|(\Delta X_1)^2|\xi,\underline{q},k\rangle_j &= {}_j\langle \xi,\underline{q},k|(\Delta X_2)^2|\xi,\underline{q},k\rangle_j \\ &\geqslant \tfrac{1}{4}{}_j\langle \xi,\underline{q},k|[2K_0]|\xi,\underline{q},k\rangle_j, \quad j=0,1,\ldots,k-1. \end{aligned} \tag{57} $$

The inequalities in (57) say that there is no $\mathrm{SU}_q(1,1)$ squeezing in the k-component q-deformed charge coherent states with $k\geqslant 3$. However, there is such squeezing in the even and odd q-deformed charge coherent states.[57]

It is easy to verify that the q-deformed charge coherent states satisfy the equality in (50) and that $\langle(\Delta X_1)^2\rangle=\langle(\Delta X_2)^2\rangle$. This point has been observed in Ref. 57. Therefore, the q-deformed charge coherent states are not $\mathrm{SU}_q(1,1)$ squeezed.

B. Single-mode *q*-squeezing

In analogy with the definition of single-mode squeezing,[27] we have introduced single-mode q-squeezing[57] in terms of the Hermitian q-deformed quadrature operators for the individual modes

$$ Y_1 = \frac{a_1^+ + a_1}{2}, \quad Y_2 = \frac{i(a_1^+ - a_1)}{2}, $$

$$ Z_1 = \frac{a_2^+ + a_2}{2}, \quad Z_2 = \frac{i(a_2^+ - a_2)}{2}, \tag{58} $$

which satisfy the commutation relations

$$ [Y_1,Y_2] = \frac{i}{2}[a_1,a_1^+], \quad [Z_1,Z_2] = \frac{i}{2}[a_2,a_2^+], \tag{59} $$

and the uncertainty relations

$$ \langle(\Delta Y_1)^2\rangle\langle(\Delta Y_2)^2\rangle \geqslant \tfrac{1}{16}|\langle[a_1,a_1^+]\rangle|^2, \quad \langle(\Delta Z_1)^2\rangle\langle(\Delta Z_2)^2\rangle \geqslant \tfrac{1}{16}|\langle[a_2,a_2^+]\rangle|^2. \tag{60} $$

A state is said to be single-mode q-squeezed if

$$ \langle(\Delta Y_i)^2\rangle < \tfrac{1}{4}|\langle[a_1,a_1^+]\rangle|, \quad \langle(\Delta Z_i)^2\rangle < \tfrac{1}{4}|\langle[a_2,a_2^+]\rangle| \quad (i=1 \text{ or } 2). \tag{61} $$

For the states $|\xi,\underline{q},k\rangle_j$ $(k\geqslant 1)$, it always follows that

$$ {}_j\langle a_1\rangle_j = {}_j\langle a_2\rangle_j = {}_j\langle a_1^2\rangle_j = {}_j\langle a_2^2\rangle_j = {}_j\langle a_1^+a_2\rangle_j = 0, \quad j=0,1,\ldots,k-1. \tag{62} $$

Thus, the fluctuations are given by

$$
\begin{aligned}
{}_j\langle \xi,\underline{q},k|(\Delta Y_1)^2|\xi,\underline{q},k\rangle_j &= {}_j\langle \xi,\underline{q},k|(\Delta Y_2)^2|\xi,\underline{q},k\rangle_j \\
&= \tfrac{1}{4}\{{}_j\langle \xi,\underline{q},k|[a_1,a_1^+]|\xi,\underline{q},k\rangle_j + 2{}_j\langle \xi,\underline{q},k|a_1^+a_1|\xi,\underline{q},k\rangle_j\} \\
&> \tfrac{1}{4}{}_j\langle \xi,\underline{q},k|[a_1,a_1^+]|\xi,\underline{q},k\rangle_j, \qquad (63)
\end{aligned}
$$

$$
\begin{aligned}
{}_j\langle \xi,\underline{q},k|(\Delta Z_1)^2|\xi,\underline{q},k\rangle_j &= {}_j\langle \xi,\underline{q},k|(\Delta Z_2)^2|\xi,\underline{q},k\rangle_j \\
&= \tfrac{1}{4}\{{}_j\langle \xi,\underline{q},k|[a_2,a_2^+]|\xi,\underline{q},k\rangle_j + 2{}_j\langle \xi,\underline{q},k|a_2^+a_2|\xi,\underline{q},k\rangle_j\} \\
&> \tfrac{1}{4}{}_j\langle \xi,\underline{q},k|[a_2,a_2^+]|\xi,\underline{q},k\rangle_j. \qquad (64)
\end{aligned}
$$

This shows that there is no single-mode q-squeezing in the k-component q-deformed charge coherent states with $k \geqslant 1$. As two special cases, there is no such q-squeezing in the q-deformed charge coherent states[65] and the even (odd) q-deformed charge coherent states[57] as k becomes 1 and 2, respectively.

C. Two-mode q-squeezing

In analogy with the definition of two-mode squeezing,[69] we have introduced two-mode q-squeezing[57] in terms of the Hermitian q-deformed quadrature operators for the two modes

$$
W_1 = \frac{Y_1 + Z_1}{\sqrt{2}} = \frac{1}{\sqrt{8}}(a_1^+ + a_2^+ + a_1 + a_2), \quad W_2 = \frac{Y_2 + Z_2}{\sqrt{2}} = \frac{i}{\sqrt{8}}(a_1^+ + a_2^+ - a_1 - a_2), \qquad (65)
$$

which satisfy the commutation relation

$$
[W_1, W_2] = \tfrac{1}{4}i\{[a_1,a_1^+] + [a_2,a_2^+]\} \qquad (66)
$$

and the uncertainty relation

$$
\langle(\Delta W_1)^2\rangle\langle(\Delta W_2)^2\rangle \geqslant \tfrac{1}{64}|\langle[a_1,a_1^+]\rangle + \langle[a_2,a_2^+]\rangle|^2. \qquad (67)
$$

A state is said to be two-mode q-squeezed if

$$
\langle(\Delta W_i)^2\rangle < \tfrac{1}{8}|\langle[a_1,a_1^+]\rangle + \langle[a_2,a_2^+]\rangle| \quad (i = 1 \text{ or } 2). \qquad (68)
$$

For the states $|\xi,\underline{q},k\rangle_j$ $(k \geqslant 2)$, the fluctuations are given by

$$
\begin{aligned}
{}_j\langle \xi,\underline{q},k|(\Delta W_1)^2|\xi,\underline{q},k\rangle_j &= {}_j\langle \xi,\underline{q},k|(\Delta W_2)^2|\xi,\underline{q},k\rangle_j \\
&= \tfrac{1}{2}\{{}_j\langle \xi,\underline{q},k|(\Delta Y_1)^2|\xi,\underline{q},k\rangle_j + {}_j\langle \xi,\underline{q},k|(\Delta Z_1)^2|\xi,\underline{q},k\rangle_j\} = \tfrac{1}{2}\{{}_j\langle \xi,\underline{q},k| \\
&\quad \times(\Delta Y_2)^2|\xi,\underline{q},k\rangle_j + {}_j\langle \xi,\underline{q},k|(\Delta Z_2)^2|\xi,\underline{q},k\rangle_j\} \\
&= \tfrac{1}{8}\{{}_j\langle \xi,\underline{q},k|[a_1,a_1^+]|\xi,\underline{q},k\rangle_j + {}_j\langle \xi,\underline{q},k|[a_2,a_2^+]|\xi,\underline{q},k\rangle_j \\
&\quad + 2{}_j\langle \xi,\underline{q},k|a_1^+a_1|\xi,\underline{q},k\rangle_j + 2{}_j\langle \xi,\underline{q},k|a_2^+a_2|\xi,\underline{q},k\rangle_j\} \\
&> \tfrac{1}{8}\{{}_j\langle \xi,\underline{q},k|[a_1,a_1^+]|\xi,\underline{q},k\rangle_j + {}_j\langle \xi,\underline{q},k|[a_2,a_2^+]|\xi,\underline{q},k\rangle_j\}. \qquad (69)
\end{aligned}
$$

This shows that there is no two-mode q-squeezing in the k-component q-deformed charge coherent states with $k \geqslant 2$. As a special case, there is no such q-squeezing in the even and odd q-deformed charge coherent states[57] as k becomes 2. However, there is such q-squeezing in the q-deformed charge coherent states.[65]

D. Two-mode q-antibunching

In analogy with the definition of two-mode antibunching,[36] we have introduced a two-mode q-correlation function as[57]

$$g^{(2)}(0) \equiv \frac{\langle (a_1^+ a_2^+)^2 (a_1 a_2)^2 \rangle}{\langle a_1^+ a_2^+ a_1 a_2 \rangle^2} = \frac{\langle :([N_1][N_2])^2: \rangle}{\langle [N_1][N_2] \rangle^2} = \frac{\langle K_+^2 K_-^2 \rangle}{\langle K_+ K_- \rangle^2}, \tag{70}$$

where a_i and a_i^+ represent the annihilation and creation operators of q-deformed photons of a deformed light field and $::$ denotes normal ordering. We call $g^{(2)}(0)$ the two-mode q-correlation degree. Physically, $g^{(2)}(0)$ is a measure of q-deformed two-photon correlations in the q-deformed two-mode field and is related to the q-deformed two-photon number distributions. A state is said to be two-mode q-antibunched if

$$g^{(2)}(0) < 1. \tag{71}$$

Let us now study the two-mode q-antibunching effect for the k-component q-deformed charge coherent states with $k \geqslant 3$. First, for $k \geqslant 3$, one can easily obtain the following relations:

$${}_0\langle \xi, \underline{q}, k | K_+^2 K_-^2 | \xi, \underline{q}, k \rangle_0 = |\xi|^4 (N_{k\underline{q}}^0)^2 / (N_{k\underline{q}}^{k-2})^2, \tag{72}$$

$${}_1\langle \xi, \underline{q}, k | K_+^2 K_-^2 | \xi, \underline{q}, k \rangle_1 = |\xi|^4 (N_{k\underline{q}}^1)^2 / (N_{k\underline{q}}^{k-1})^2, \tag{73}$$

$${}_l\langle \xi, \underline{q}, k | K_+^2 K_-^2 | \xi, \underline{q}, k \rangle_l = |\xi|^4 (N_{k\underline{q}}^l)^2 / (N_{k\ \underline{q}}^{l-2})^2, \quad l = 2,3,\ldots,k-1. \tag{74}$$

According to (52), (53), and (72)–(74), the two-mode q-correlation degrees of the k-component q-deformed charge coherent states can be obtained as follows:

$$g_0^{(2)}(0) = \frac{{}_0\langle \xi, \underline{q}, k | K_+^2 K_-^2 | \xi, \underline{q}, k \rangle_0}{({}_0\langle \xi, \underline{q}, k | K_+ K_- | \xi, \underline{q}, k \rangle_0)^2} = \frac{(N_{k\underline{q}}^{k-1})^4}{(N_{k\underline{q}}^0)^2 (N_{k\underline{q}}^{k-2})^2}, \tag{75}$$

$$g_1^{(2)}(0) = \frac{{}_1\langle \xi, \underline{q}, k | K_+^2 K_-^2 | \xi, \underline{q}, k \rangle_1}{({}_1\langle \xi, \underline{q}, k | K_+ K_- | \xi, \underline{q}, k \rangle_1)^2} = \frac{(N_{k\underline{q}}^0)^4}{(N_{k\underline{q}}^1)^2 (N_{k\underline{q}}^{k-1})^2}, \tag{76}$$

$$g_l^{(2)}(0) = \frac{{}_l\langle \xi, \underline{q}, k | K_+^2 K_-^2 | \xi, \underline{q}, k \rangle_l}{({}_l\langle \xi, \underline{q}, k | K_+ K_- | \xi, \underline{q}, k \rangle_l)^2} = \frac{(N_{k\underline{q}}^{l-1})^4}{(N_{k\underline{q}}^{l-2})^2 (N_{k\underline{q}}^l)^2}, \quad l = 2,3,\ldots,k-1. \tag{77}$$

Evidently, the following relation exists:

$$\prod_{j=0}^{k-1} g_j^{(2)}(0) = 1. \tag{78}$$

We shall prove that for $k \geqslant 3$, the k-component q-deformed charge coherent states show two-mode q-antibunching.

From (12) and (75), it follows that

$$g_0^{(2)}(0) = \frac{f(x)}{x^k \varphi(x)},$$

where

$$f(x) = \sum_{m=0}^{\infty} \left\{ \sum_{n=0}^{m} \frac{1}{[kn]\,![kn + |\underline{q}|]\,![km - kn + k - 2]\,![km - kn + k - 2 + |\underline{q}|]!} \right\} x^{km},$$

$$\varphi(x)=\sum_{m=0}^{\infty}\left\{\sum_{n=0}^{m}\frac{1}{[kn+k-1]![kn+k-1+|\underline{q}|]![km-kn+k-1]![km-kn+k-1+|\underline{q}|]!}\right\}x^{km}$$

and $x=|\xi|^2$. For $k\geqslant 3$, we have

$$\sum_{n=0}^{m}\frac{1}{[kn]![kn+|\underline{q}|]![km-kn+k-2]![km-kn+k-2+|\underline{q}|]!}$$
$$>\sum_{n=0}^{m}\frac{1}{[kn+k-1]![kn+k-1+|\underline{q}|]![km-kn+k-1]![km-kn+k-1+|\underline{q}|]!},$$

and thus $f(x)>\varphi(x)$ when $x>0$. Hence, $g_0^{(2)}(0)>1$ when $0<x\leqslant 1$. However, when $x>1$, the following inequality,

$$\frac{f(x)}{x^k\varphi(x)}<1,\quad \text{i.e.}, x^k>\frac{f(x)}{\varphi(x)},$$

may have real roots. Consequently, in the region of $x>1$, for arbitrary fixed values of $\underline{q}$ and q, there surely exists some range of x values such that

$$g_0^{(2)}(0)=\frac{f(x)}{x^k\varphi(x)}<1.$$

To make the above statement clear, we plot $g_0^{(2)}(0)$ against x for various k, $\underline{q}$, and q in Fig. 1.

From (12) and (76), it follows that

$$g_1^{(2)}(0)=\frac{x^k f_1(x)}{\varphi_1(x)},$$

where

$$f_1(x)=\sum_{m=0}^{\infty}\left\{\sum_{n=0}^{m}\frac{1}{[kn+1]![kn+1+|\underline{q}|]![km-kn+k-1]![km-kn+k-1+|\underline{q}|]!}\right\}x^{km},$$

$$\varphi_1(x)=\sum_{m=0}^{\infty}\left\{\sum_{n=0}^{m}\frac{1}{[kn]![kn+|\underline{q}|]![km-kn]![km-kn+|\underline{q}|]!}\right\}x^{km}.$$

Apparently,

$$\sum_{n=0}^{m}\frac{1}{[kn+1]![kn+1+|\underline{q}|]![km-kn+k-1]![km-kn+k-1+|\underline{q}|]!}$$
$$<\sum_{n=0}^{m}\frac{1}{[kn]![kn+|\underline{q}|]![km-kn]![km-kn+|\underline{q}|]!},$$

so that $f_1(x)<\varphi_1(x)$. Therefore, $g_1^{(2)}(0)<x^k$, namely, $g_1^{(2)}(0)<1$ as $x\leqslant 1$.

From (12) and (77), it follows that

$$g_l^{(2)}(0)=\frac{f_2(x)}{\varphi_2(x)},$$

where

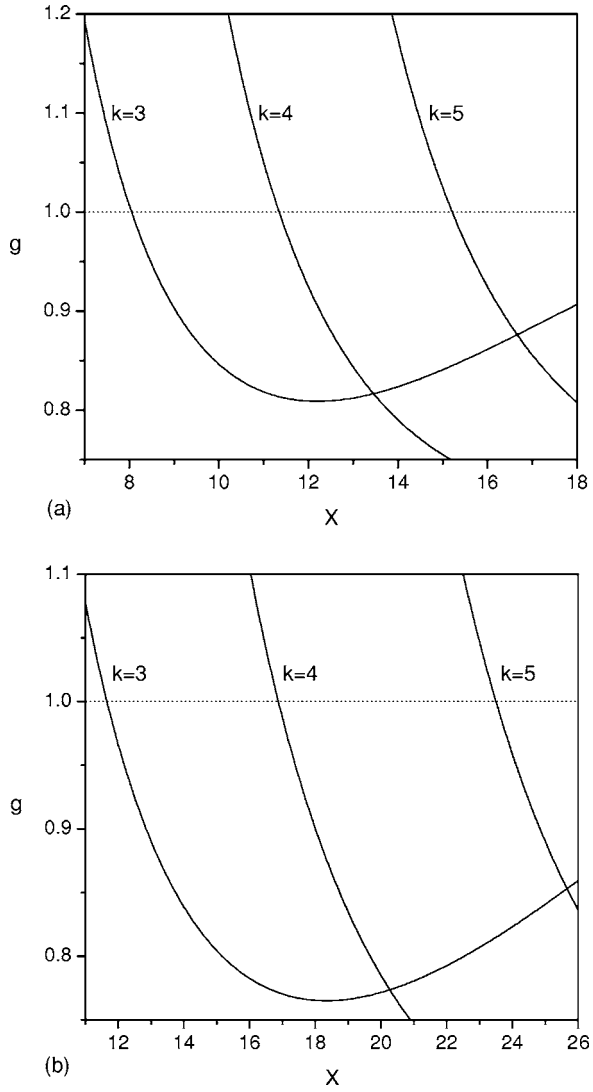

FIG. 1. $g\,[\equiv g_0^{(2)}(0)]$ against x for $k=3$, 4, 5, with (a) $\underline{q}=\pm 2$, $q=0.9$ and (b) $\underline{q}=\pm 3$, $q=0.8$.

$$f_2(x)=\sum_{m=0}^{\infty}\left\{\sum_{n=0}^{m}\frac{1}{[kn+l-2]\,![kn+l-2+|\underline{q}|]\,![km-kn+l]\,![km-kn+l+|\underline{q}|]!}\right\}x^{km},$$

$$\varphi_2(x)=\sum_{m=0}^{\infty}\left\{\sum_{n=0}^{m}\frac{1}{[kn+l-1]\,![kn+l-1+|\underline{q}|]\,![km-kn+l-1]\,![km-kn+l-1+|\underline{q}|]!}\right\}x^{km}.$$

Obviously,

$$f_2(x)<\frac{1}{[l-2]\,![l-2+|\underline{q}|]\,![l]\,![l+|\underline{q}|]!}\sum_{m=0}^{\infty}(m+1)x^{km},$$

$$\varphi_2(x) > \sum_{m=0}^{\infty} \frac{(m+1)x^{km}}{\{[km+l-1]![km+l-1+|\underline{q}|]!\}^2} > \frac{1}{\{[l-1]![l-1+|\underline{q}|]!\}^2}.$$

Thus, we obtain

$$g_l^{(2)}(0) < \frac{\{[l-1]![l-1+|\underline{q}|]!\}^2}{[l-2]![l-2+|\underline{q}|]![l]![l+|\underline{q}|]!} \sum_{m=0}^{\infty} (m+1)x^{km}.$$

For $x<1$, it reads

$$\sum_{m=0}^{\infty} (m+1)x^{km} = \frac{1}{(1-x^k)^2}.$$

Therefore, as $x<1$, we get

$$g_l^{(2)}(0) < \frac{[l-1][l-1+|\underline{q}|]}{[l][l+|\underline{q}|]} \frac{1}{(1-x^k)^2}.$$

As a result, if $x^k \leqslant 1-\{[l-1][l-1+|\underline{q}|]/[l][l+|\underline{q}|]\}^{1/2}$, then

$$g_l^{(2)}(0) < 1, \quad l=2,3,\ldots,k-1.$$

From the above discussion, we see that for $k \geqslant 3$, the two-mode q-correlation degrees $g_j^{(2)}(0)$ $(j=0,1,\ldots,k-1)$ can be less than 1 over some particular range of x values. This indicates that two-mode q-antibunching exists for the k-component q-deformed charge coherent states with $k \geqslant 3$. The same situation occurs for the even and odd q-deformed charge coherent states.[57] However, for the q-deformed charge coherent states we have $g^{(2)}(0)=1$ so that no two-mode q-antibunching exists.

It can be shown that in the limit $q \to 1$, the nonclassical properties of the usual k-component charge coherent states, studied in Ref. 37, are retrieved as expected.

VII. SUMMARY

Let us sum up the results obtained in the present paper.

(1) The k-component q-deformed charge coherent states, defined as the k $(k \geqslant 1)$ orthonormalized eigenstates of both the kth power of the pair q-boson annihilation operator and the charge operator, have been constructed and their (over)completeness proved. Such q-deformed states become the usual k-component charge coherent states in the limit $q \to 1$. They become the q-deformed charge coherent states and the even (odd) q-deformed charge coherent states in the two special cases of $k=1$ and $k=2$, respectively.

(2) The k-component q-deformed charge coherent states have been shown to be generated by a suitable average over the U (1)-group (caused by the charge operator) action on the product of q-deformed coherent states and k-component q-deformed coherent states.

(3) The D-algebra of the $SU_q(1,1)$ generators corresponding to the k-component q-deformed charge coherent states has been realized in a q-differential-operator matrix form.

(4) For $k \geqslant 3$, the k-component q-deformed charge coherent states have been shown to exhibit two-mode q-antibunching, but neither $SU_q(1,1)$ squeezing, nor single- or two-mode q-squeezing.

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Stargenfunctions, generally parametrized systems and a causal formulation of phase space quantum mechanics

Nuno Costa Dias[a] and João Nuno Prata[b]
Departamento de Matemática, Universidade Lusófona de Humanidades e Tecnologias, Av. Campo Grande, 376, 1749-024 Lisboa, Portugal

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We address the deformation quantization of generally parametrized systems displaying a natural time variable. The purpose of this exercise is twofold: first, to illustrate through a pedagogical example the potential of quantum phase space methods in the context of constrained systems and particularly of generally covariant systems. Second, to show that a causal representation for quantum phase space quasidistributions can be easily achieved through general parametrization. This result is succinctly discussed. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1948327]

I. INTRODUCTION

Generally covariant systems are a particular kind of dynamical systems in which time is included among the canonical variables.[1] The state of the system evolves along orbits parametrized by an unphysical scalar parameter. The formalism is invariant under reparametrizations of this parameter (for this reason these systems are also called general parametrized systems) leading to a gauge symmetry, which in the Hamiltonian formulation is implemented by a first class (Hamiltonian) constraint. One of the most striking properties of generally covariant theories is that the Hamiltonian is identically zero on the constraint hypersurface. Consequently there is no standard Hamiltonian time evolution (which coincides exactly with the gauge transformation). Instead, dynamics is to be found among the relations between the canonical variables that are determined by the Hamiltonian constraint.[2–4] In other words, dynamics is the unfolding of the gauge transformation. The most famous example of a generally covariant theory is, of course, general relativity.[5–7]

Upon quantization these systems display a number of technical and conceptual problems which, motivated by the quest to quantize general relativity, have been intensively studied in the literature. Since the publication of Dirac's seminal work on the quantization of constrained systems,[8] several quantization programs have been developed with the aim of refining Dirac's approach and making it suitable to address the generally covariant case.[1,6,9–11] In spite of this, several important problems concerning the quantization of these systems (the problem of time, the observables' problem and the measurement problem, just to mention a few) are still lacking a definitive answer.[3,4,10]

One quantization program that has only been scarcely explored in this context is the deformation approach.[12–22] And this regardless of the fact that the deformation quantization method displays some remarkable features that make it especially suitable to address the generally covariant case.[23–25] On the one hand, the deformation approach leads to a formulation of quantum mechanics in terms of classical-like objects. The theory lives in phase space and mimics the structure of classical statistical mechanics. The state of the system is described by a phase space

[a]Electronic mail: ncdias@mail.telepac.pt
[b]Electronic mail: joao.prata@ulusofona.pt

quasidistribution and observables are also functionals on the phase space. From the deformation point of view quantization amounts to the substitution of the standard product of functions by a noncommutative star product.[21,22] The theory has been proved useful when addressing a wide range of fields of research ranging from topics in nonrelativistic quantum mechanics[16,26–29] to some current developments in M-theory.[30–32] In the context of generally covariant systems it has been advocated that the relation between classical statistical and standard operator quantum mechanics should be emphasized when approaching the quantization of these systems.[33] The point of view is that the problems besetting their quantization, being to a large extent conceptual ones, may receive key physical insights from the more intuitive classical statistical analysis. From this perspective the deformation methods seem to be especially suited.

On the technical side the deformation approach acquired the status of a powerful mathematical theory not displaying any of the subtleties of the path integral or canonical quantization prescriptions. Most remarkable is the fact that the theory is able to generate the quantum version of a classical system living on a generic (possibly curved) Poisson or sympletic manifold.[34–37] Of special relevance for generally covariant systems is that the deformation approach displays some powerful tools to address the quantum eigenvalue problem, the most meaningful of which being a covariant formalism unifying all distinct phase space representations of the eigenvalue problem,[21,38,39] a formal solution of a generic stargenvalue equation[19,40] and a set of efficient methods to determine the semiclassical expansion of the stargenfunctions.[41,42]

In this paper we aim at providing a pedagogical incursion into some of these methods by studying the deformation quantization of a special simple kind of generally covariant systems, those obtained by parametrizing an originally noncovariant version of the system. The parametrization procedure leads to a formulation of the dynamics living on an enlarged phase space where the physical time is incorporated as a canonical variable.[1] The existence of such a natural time variable considerably simplifies the (technical and conceptual) analysis of the dynamical structure of the system. For this reason these models have been used[1,3,4] to test a set of quantization techniques and interpretative prescriptions aiming at addressing the far more difficult problem of quantizing "already parametrized systems" of which the most significant example is general relativity.

The Hamiltonians of these models (as in the general case) are identically zero on the constraint hypersurface. At the quantum level the imposition of this constraint determines the physical states of the system. In the deformation context the imposition of first class constraints yields a stargenvalue equation[19,43] and so the physical states are the zero stargenfunctions of the Hamiltonian symbol. We are then able to apply the powerful tools of the deformation approach to study the quantum eigenvalue problem. A complete characterization of the physical states will be provided in three different phase space representations. In particular, we obtain a representation where the dynamics of the quasidistribution (with respect to the physical time variable) is dictated by the classical Liouville equation. This is an interesting side result that shows that through general parametrization a causal formulation for the distributional sector of quantum mechanics is made possible. More generally we find that the remarkable parallelism between classical statistical mechanics and phase space quantum mechanics carries on intact to the generally covariant setting, a property that establishes a promising starting point for the future research on the deformation quantization of generally covariant systems.

II. COVARIANT WIGNER QUANTUM MECHANICS

The aim of this section is to review the main structures of the covariant formulation of the deformation quantization procedure. Our analysis will be restricted to the case of flat phase space as we will be dealing only with systems of this sort. The reader should refer to Refs. 36 and 38 for a more detailed presentation of these results and to Refs. 35 and 37 for the generalization of the formalism to the nonflat case. An important part of this section [Eqs. (9)–(15)] focuses on the covariant generalization of the $*$-genvalue equation, once again, just for the flat case. This is a topic that will play an important role latter on.

Before proceeding and to avoid future misunderstandings let us make the following remark:

Throughout the paper the word *covariant* will be used in two different contexts, to designate the invariance under time reparametrizations of the original classical system and to designate the invariance under general coordinate transformations of the Moyal plane. The aim of this paper is to present the deformation quantization of a generally covariant (parametrized) classical system. We use the covariant version of the deformation quantization procedure (a subject where this paper makes no original contribution) because this leads to a larger set of possible quantum phase space representations, among which we will find the causal representation presented in Sec. IV.

Let us then settle down the preliminaries. We consider a N-dimensional dynamical system, its classical formulation living on the flat phase space T^*M. A set of global canonical coordinates $(\{q_i,p_i,i=1,\ldots,N\})$ can then be defined on T^*M in terms of which the sympletic structure reads $w=\mathrm{d}q_i\wedge\mathrm{d}p_i$. Upon quantization the set $\{\hat{q}_i\}$ constitutes a complete set of commuting observables. Let us introduce the vector notation $\hat{\vec{q}}=(\hat{q}_1,\ldots,\hat{q}_N)$ and designate by $|\vec{q}\rangle$ the general eigenstate of $\hat{\vec{q}}$ associated to the array of eigenvalues $\vec{q}$ and spanning the Hilbert space $\mathcal{H}$ of the system. Let also $\mathcal{A}(\mathcal{H})$ be the algebra of quantum observables over $\mathcal{H}$ and $\mathcal{A}(T^*M)$ the algebra of classical functions over the classical phase space T^*M. Let $(\vec{Q},\vec{P})$ be a second set of phase space coordinates, related to $(\vec{q},\vec{p})$ by a generic phase space diffeomorphism (not necessarily canonical), $\vec{q}=\vec{q}(\vec{Q},\vec{P})$ and $\vec{p}=\vec{p}(\vec{Q},\vec{P})$. The covariant Weyl transform,[38]

$$
\begin{aligned}
&W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}:\mathcal{A}(\mathcal{H})\to\mathcal{A}(T^*M),\\
&\hat{A}\to W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}(\hat{A})=\hbar^N\int \mathrm{d}^N\vec{x}\int \mathrm{d}^N\vec{y}\,e^{-i\vec{p}(\vec{Q},\vec{P})\cdot\vec{y}}\delta(\vec{x}-\vec{q}(\vec{Q},\vec{P}))\left\langle \vec{x}+\frac{\hbar}{2}\vec{y}|\hat{A}|\vec{x}-\frac{\hbar}{2}\vec{y}\right\rangle,
\end{aligned}
\tag{1}
$$

where $|\vec{x}\pm(\hbar/2)\vec{y}\rangle$ are eigenstates of $\hat{\vec{q}}$, yields the entire structure of covariant phase space quantum mechanics. The map $W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}$ can be applied both to an observable $\hat{A}$ as well as to the density matrix $|\psi(t)\rangle\langle\psi(t)|$. In the first case it yields the $^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}$-Weyl symbol $A'(\vec{Q},\vec{P})=W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}(\hat{A})$ of the original quantum operator and, in the second case, the celebrated Wigner function $f'_W(\vec{Q},\vec{P},t)=[1/(2\pi\hbar)^N]W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}(|\psi(t)\rangle\langle\psi(t)|)$. Notice that if $(\vec{Q},\vec{P})=(\vec{q},\vec{p})$ then the covariant map $W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}$ reduces to the standard Weyl transform in the variables $(\vec{q},\vec{p})$. In this case we will use the notation $W_{(\vec{q},\vec{p})}$ to designate $W^{(\vec{q},\vec{p})}_{(\vec{q},\vec{p})}$. Notice also that $A'(\vec{Q},\vec{P})=A(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))$ where $A(\vec{q},\vec{p})=W_{(\vec{q},\vec{p})}(\hat{A})$ and the same relation is valid for the Wigner function. The covariant Weyl map implements the transformation $(\vec{q},\vec{p})\to(\vec{Q},\vec{P})$ as a coordinate transformation in quantum phase space and defines a covariant star-product $*'_{(\vec{Q},\vec{P})}$ and Moyal bracket $[,]_{M'_{(\vec{Q},\vec{P})}}$ (Refs. 21 and 38) $(\hat{A},\hat{B}\in\mathcal{A}(H))$,

$$
\begin{aligned}
&W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}(\hat{A}\hat{B})=W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}(\hat{A})*'_{(\vec{Q},\vec{P})}W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}(\hat{B}),\\
&W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}\left(\frac{1}{i\hbar}[\hat{A},\hat{B}]\right)=[W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}(\hat{A}),W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}(\hat{B})]_{M'_{(\vec{Q},\vec{P})}},
\end{aligned}
\tag{2}
$$

which display the functional form

$$
A'(\vec{Q},\vec{P})*'_{(\vec{Q},\vec{P})}B'(\vec{Q},\vec{P})=A'(\vec{Q},\vec{P})e^{(i\hbar/2)\overleftarrow{\nabla}'_i J'^{ij}_{(\vec{Q},\vec{P})}\overrightarrow{\nabla}'_j}B'(\vec{Q},\vec{P}),
$$

$$[A'(\vec{Q},\vec{P}),B'(\vec{Q},\vec{P})]_{M'_{(\vec{Q},\vec{P})}}=\frac{2}{\hbar}A'(\vec{Q},\vec{P})\sin\left(\frac{\hbar}{2}\overleftarrow{\nabla}'_i J'^{ij}_{(\vec{Q},\vec{P})}\overrightarrow{\nabla}'_j\right)B'(\vec{Q},\vec{P}), \tag{3}$$

where the covariant derivative is given by (let $O'^i=P_i$, $O^i=p_i$, $i=1,\ldots,N$; $O'^i=Q_{i-N}$, $O^i=q_{i-N}$, $i=N+1,\ldots,2N$)

$$\nabla'_i A'=\partial'_i A', \quad \nabla'_i\nabla'_j A'=\partial'_i\partial'_j A'-\Gamma'^k_{ij}\partial'_k A', \quad \partial'_i=\partial/\partial O'^i, \quad i,j,k=1,\ldots,2N, \tag{4}$$

and

$$J'^{ij}_{(\vec{Q},\vec{P})}(\vec{Q},\vec{P})=\frac{\partial O'^i}{\partial O^k}\frac{\partial O'^j}{\partial O^l}J^{kl}_{(\vec{q},\vec{p})}, \quad \Gamma'^i_{jk}(\vec{Q},\vec{P})=\frac{\partial O'^i}{\partial O^b}\frac{\partial^2 O^b}{\partial O'^j\,\partial O'^k}, \tag{5}$$

are the symplectic structure and Poisson connection associated with the coordinates $(\vec{Q},\vec{P})$, respectively. Finally, notice that in Eq. (5) we explicitly took into account the phase space flat structure.

When formulated in terms of these structures Wigner mechanics becomes fully invariant under the action of general phase space diffeomorphisms,

$$A'(\vec{Q},\vec{P})*'_{(\vec{Q},\vec{P})}B'(\vec{Q},\vec{P})=A(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))*_{(\vec{q},\vec{p})}B(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})) \quad \forall_{A,B\in\mathcal{A}(T^*M)}, \tag{6}$$

the covariant generalization of the Moyal and stargenvalue equations reading

$$\frac{\partial f'_W}{\partial t}=[H',f'_W]_{M'_{(\vec{Q},\vec{P})}},$$

$$A'(\vec{Q},\vec{P})*'_{(\vec{Q},\vec{P})}\rho'_{a;b}(\vec{Q},\vec{P})=a\rho'_{a;b}(\vec{Q},\vec{P}), \tag{7}$$

$$\rho'_{a;b}(\vec{Q},\vec{P})*'_{(\vec{Q},\vec{P})}A'(\vec{Q},\vec{P})=b\rho'_{a;b}(\vec{Q},\vec{P}),$$

where $\rho'_{a;b}(\vec{Q},\vec{P})$ is the a-left and b-right $*'_{(\vec{Q},\vec{P})}$-genfunction of $A'(\vec{Q},\vec{P})$. These equations transform covariantly under arbitrary phase space diffeomorphisms yielding, in any coordinates, identical mathematical solutions and thus identical physical predictions,

$$P(A'(\vec{Q},\vec{P};t)=a)=\int \mathrm{d}^N\vec{Q}\int \mathrm{d}^N\vec{P}(\det J'^{ij}_{(\vec{Q},\vec{P})})^{-1/2}\rho'_{a;a}(\vec{Q},\vec{P})f'_W(\vec{Q},\vec{P};t). \tag{8}$$

Let us consider the stargenvalue equation (7) in more detail. Let $\{\hat{A}_1,\ldots,\hat{A}_N\}$ and $\{\hat{B}_1,\ldots,\hat{B}_N\}$ be two sets of commuting observables satisfying $[\hat{A}_i,\hat{B}_j]=i\hbar\,\delta_{ij}$. Let $A'_i(\vec{Q},\vec{P})=W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}(\hat{A}_i)$ and $B'_i(\vec{Q},\vec{P})=W^{(\vec{q},\vec{p})}_{(\vec{Q},\vec{P})}(\hat{B}_i)$. Then the simultaneous solution of

$$\begin{aligned}A'_i(\vec{Q},\vec{P})*'_{(\vec{Q},\vec{P})}\rho'_{a_1,\ldots,a_N;b_1,\ldots,b_N}(\vec{Q},\vec{P})&=a_i\rho_{a_1,\cdots,a_N;b_1,\ldots,b_N}(\vec{Q},\vec{P}),\\ \rho'_{a_1,\ldots,a_N;b_1,\ldots,b_N}(\vec{Q},\vec{P})*'_{(\vec{Q},\vec{P})}A'_i(\vec{Q},\vec{P})&=b_i\rho_{a_1,\ldots,a_N;b_1,\ldots,b_N}(\vec{Q},\vec{P}), \quad i=1,\ldots,N\end{aligned} \tag{9}$$

is given by[19]

$$\rho'_{a_1,\ldots,a_N;b_1,\ldots,b_N}(\vec{Q},\vec{P})\equiv\Delta_{*'_{(\vec{Q},\vec{P})}}(A'_1,\ldots,A'_N;a_1,\ldots,a_N;b_1,\ldots,b_N)=\prod_{i=1}^{N}*'_{(\vec{Q},\vec{P})}\rho'_{a_i;b_i}(\vec{Q},\vec{P}), \tag{10}$$

$$\rho'_{a_i;b_i}(\vec{Q},\vec{P}) \equiv \Delta_{*'_{(\vec{Q},\vec{P})}}(A'_i;a_i;b_i) = \frac{1}{2\pi} e^{(i/\hbar)(b_i-a_i)B'_i(\vec{Q},\vec{P})} *'_{(\vec{Q},\vec{P})} \int \mathrm{d}k\, e^{ik(A'_i(\vec{Q},\vec{P})-b_i)}_{*'_{(\vec{Q},\vec{P})}}, \tag{11}$$

where $\Pi^N_{i=i*'_{(\vec{Q},\vec{P})}}$ is the N-fold star-product and the star-exponential $e^{ikA'_i(\vec{Q},\vec{P})}_{*'_{(\vec{Q},\vec{P})}} \equiv E_{*'_{(\vec{Q},\vec{P})}}(k,\vec{Q},\vec{P})$ is defined as the solution of the differential problem, $(\partial/\partial k)E_{*'_{(\vec{Q},\vec{P})}}(k,\vec{Q},\vec{P}) = iA'_i(\vec{Q},\vec{P}) *'_{(\vec{Q},\vec{P})} E_{*'_{(\vec{Q},\vec{P})}}(k,\vec{Q},\vec{P})$ and $E_{*'_{(\vec{Q},\vec{P})}}(0,\vec{Q},\vec{P}) = 1$, which is unique for the Weyl symbol $A'_i(\vec{Q},\vec{P})$ of a generic self-adjoint operator $\hat{A}_i$ (a result that is just the Weyl-Wigner translation of an equivalent result in operator quantum mechanics[44]). Furthermore $E_{*'_{(\vec{Q},\vec{P})}}(k,\vec{Q},\vec{P}) = \Sigma^{+\infty}_{n=1}[(ik)^n/n!]\Pi^n_{j=1*'_{(\vec{Q},\vec{P})}} A'_i(\vec{Q},\vec{P})$ whenever k is in the radius of convergence of the series, which justifies the notation used in Eq. (11). We also introduced the $*$-delta notation $\Delta_{*'_{(\vec{Q},\vec{P})}}(A'_1,\ldots,A'_N;a_1,\ldots,a_N;b_1,\ldots,b_N)$ that will be extensively used later on. Notice that the stargenfunctions $\rho'_{a_1,\ldots,a_N;b_1,\ldots,b_N}(\vec{Q},\vec{P})$ are the $\frac{(\vec{q},\vec{p})}{(\vec{Q},\vec{P})}$-Weyl transform of the projectors $|a_1,\ldots,a_N\rangle\langle b_1,\ldots,b_N|$ where $|a_1,\ldots,a_N\rangle$ and $|b_1,\ldots,b_N\rangle$ are simultaneous eigenvectors of $\hat{A}_i, i=1,\ldots,N$. Moreover the stargenfunctions $\rho'_{a_i;b_i}(\vec{Q},\vec{P})$ are the $\frac{(\vec{q},\vec{p})}{(\vec{Q},\vec{P})}$-Weyl transform of the projector

$$|a_i\rangle\langle b_i| = \int \mathrm{d}\vec{z}\,|a_i,\vec{z}\rangle\langle b_i,\vec{z}| = \frac{1}{2\pi}\int \mathrm{d}k\, e^{(i/\hbar)(b_i-a_i)\hat{B}_i} e^{ik(\hat{A}_i-b_i)}, \tag{12}$$

where $\vec{z}=(a_1,\ldots,a_{i-1},a_{i+1},\ldots,a_N)$ is the $N-1$ array of degeneracy indices. The Weyl transform of the first identity in Eq. (12) yields the inverse relation of Eq. (10),

$$\rho'_{a_i;b_i}(\vec{Q},\vec{P}) = \int \mathrm{d}a_1 \cdots \mathrm{d}a_{i-1}\,\mathrm{d}a_{i+1} \cdots \mathrm{d}a_N\, \rho'_{a_1,\ldots,a_i,\ldots,a_N;a_1,\ldots,b_i,\ldots,a_N}(\vec{Q},\vec{P}). \tag{13}$$

Finally, the diagonal elements $\rho'_{a_i;a_i}(\vec{Q},\vec{P})$ are given by

$$\rho'_{a_i;a_i}(\vec{Q},\vec{P}) = \frac{1}{2\pi}\int \mathrm{d}k\, e^{ik(A'_i(\vec{Q},\vec{P})-a_i)}_{*'_{(\vec{Q},\vec{P})}} = \Delta_{*'_{(\vec{Q},\vec{P})}}(A'_i;a_i;a_i) \equiv \Delta_{*'_{(\vec{Q},\vec{P})}}(A'_i-a_i), \tag{14}$$

this being the object that enters the probability functional (8). The stargenfunctions (10) and (11) transform as scalars under arbitrary phase space coordinate transformations. For instance $\rho'_{a_i;a_i}(\vec{Q},\vec{P})$ satisfies

$$\rho'_{a_i;a_i}(\vec{Q},\vec{P}) = \Delta_{*'_{(\vec{Q},\vec{P})}}(A'_i(\vec{Q},\vec{P})-a_i) = \Delta_{*_{(\vec{q},\vec{p})}}(A_i(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))-a_i) = \rho_{a_i;a_i}(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})), \tag{15}$$

where $\rho_{a_i;a_i}(\vec{q},\vec{p})$ is the diagonal solution of the stargenvalue equation in the $(\vec{q},\vec{p})$-representation.

Last, we should point out that the former results (in the presented form) are valid whenever we are able to provide the complete sets of commuting observables $\{\hat{A}_i\}$ and $\{\hat{B}_i\}$. In fact this restriction can be considerably weakened. It is crucial to the overall approach that the complete set $\{\hat{A}_i\}$ exists, but the requirement on the existence of the set $\{\hat{B}_i\}$ can be discarded, while preserving the validity of Eqs. (8), (10), (13), and (14) exactly and that of Eqs. (11) and (12) under slight modifications. This is the case, for instance, when $\hat{A}_i$ displays a discrete spectrum. The reader should refer to Ref. 19 for a detailed presentation of these results.

III. DEFORMATION QUANTIZATION OF A PARAMETRIZED NONRELATIVISTIC SYSTEM

Let us consider an arbitrary N-dimensional dynamical system with configuration variables $\vec{q}=(q_1,\ldots,q_N)$, described by the Lagrangian $L_0(\vec{q},\mathrm{d}\vec{q}/\mathrm{d}t)$. Starting from the standard action $S=\int \mathrm{d}t\, L_0(\vec{q},\mathrm{d}\vec{q}/\mathrm{d}t)$ we impose the time reparametrization invariance by introducing an unphysical time τ and promoting t to a configuration variable. The action is now rewritten as[1]

$$S=\int \mathrm{d}\tau\, \dot{t} L_0\left(\vec{q},\frac{\dot{\vec{q}}}{\dot{t}}\right), \tag{16}$$

where the overdot represents the derivative with respect to τ. The Legendre transform yields the Hamiltonian formulation living in a $(2N+2)$-dimensional phase space spanned by the canonical variables $t,P_t,\vec{q},\vec{p}$ where $P_t=\partial L/\partial \dot{t}$, $p_i=\partial L/\partial \dot{q}_i$, $i=1,\ldots,N$ and $L(t,\dot{t},\vec{q},\dot{\vec{q}})=\dot{t}L_0(\vec{q},\dot{\vec{q}}/\dot{t})$. This, as expected, is a "zero-Hamiltonian" system,

$$H=\lambda\phi, \quad \phi=P_t+H_0(\vec{q},\vec{p}), \tag{17}$$

where ϕ is a first class constraint, λ is a Lagrange multiplier, and H_0 is the Hamiltonian associated to the original Lagrangian L_0.

Dirac's quantization procedure imposes the constraint as a restriction on the space of physical states, $\hat{\phi}|\psi\rangle=0$. In the density matrix formulation this equation reads

$$\hat{\phi}|\psi\rangle\langle\psi|=|\psi\rangle\langle\psi|\hat{\phi}=0. \tag{18}$$

To find the complete specification of its solutions, and according to the general method of Sec. II, the first step is to introduce the complete set of observables $\{\hat{\phi},\hat{\vec{A}}=(\hat{A}_1,\ldots,\hat{A}_N)\}$ and the set of operators $\hat{\vec{B}}=(\hat{B}_1,\ldots,\hat{B}_N)$, generators of translations in the spectrum of $\hat{\vec{A}}$, satisfying $[\hat{A}_j,\hat{B}_k]=i\hbar\delta_{jk}$ and $[\hat{\phi},\hat{B}_k]=0, j,k=1,\ldots,N$. We easily find that

$$\hat{A}_j=\hat{F}_j(\hat{\vec{q}},\hat{\vec{p}},-\hat{t}), \quad \hat{B}_k=\hat{G}_k(\hat{\vec{q}},\hat{\vec{p}},-\hat{t}), \tag{19}$$

where $\hat{F}_j(\hat{\vec{q}},\hat{\vec{p}},t)$ and $\hat{G}_k(\hat{\vec{q}},\hat{\vec{p}},t)$ are the solutions of the original Heisenberg equations,

$$\frac{\partial \hat{F}_j}{\partial t}=[\hat{F}_j,\hat{H}_0], \quad \frac{\partial \hat{G}_k}{\partial t}=[\hat{G}_k,\hat{H}_0], \quad j,k=1,\ldots,N \tag{20}$$

together with the initial conditions $\hat{F}_j(\hat{\vec{q}},\hat{\vec{p}},0)=\hat{q}_j$ and $\hat{G}_k(\hat{\vec{q}},\hat{\vec{p}},0)=\hat{p}_k$, satisfy the aforementioned requirements. $\hat{\vec{A}}$ and $\hat{\vec{B}}$ are the quantum histories of the system.

The phase space representation of Eq. (18) is determined by the Weyl transform. We may write

$$\phi *_{(t,\phi,\vec{A},\vec{B})} f_W(t,\phi,\vec{A},\vec{B})=f_W(t,\phi,\vec{A},\vec{B})*_{(t,\phi,\vec{A},\vec{B})}\phi=0 \tag{21}$$

by using the map $W_{(t,\phi,\vec{A},\vec{B})}$ or equivalently

$$\phi(t,P_t,\vec{q},\vec{p})*_{(t,P_t,\vec{q},\vec{p})} f_W(t,P_t,\vec{q},\vec{p})=f_W(t,P_t,\vec{q},\vec{p})*_{(t,P_t,\vec{q},\vec{p})}\phi(t,P_t,\vec{q},\vec{p})=0 \tag{22}$$

by using the map $W_{(t,P_t,\vec{q},\vec{p})}$. We start by considering the simplest representation, which is provided by Eq. (21). In this case the Wigner function is a left and right zero $(t,\phi,\vec{A},\vec{B})$-stargenfunction of the constraint symbol ϕ. To determine f_W explicitly we will follow the procedure described in Sec. II. From Eqs. (10), (11), and (14), the fundamental zero stargenfunctions of the Hamiltonian constraint (which will be designated by $\rho_{\vec{a},\vec{b}}$) are given by

$$\rho_{\vec{a},\vec{b}}(t,\phi,\vec{A},\vec{B}) = \Delta_{*_{(t,\phi,\vec{A},\vec{B})}}(\phi,\vec{A};h=0,\vec{a};h=0,\vec{b})$$

$$= \Delta_{*_{(t,\phi,\vec{A},\vec{B})}}(\phi) *_{(t,\phi,\vec{A},\vec{B})} \Delta_{*_{(t,\phi,\vec{A},\vec{B})}}(\vec{A};\vec{a};\vec{b}) = \Delta_{*_{(t,\phi,\vec{A},\vec{B})}}(\phi) \prod_{j=1}^{N} {}_{*_{(t,\phi,\vec{A},\vec{B})}}$$

$$\{e^{(i/\hbar)(b_j-a_j)B_j}_{*_{(t,\phi,A,B)}} *_{(t,\phi,\vec{A},\vec{B})} \Delta_{*_{(t,\phi,\vec{A},\vec{B})}}(A_j - b_j)\}$$

$$= \delta(\phi) *_{(t,\phi,\vec{A},\vec{B})} \prod_{j=1}^{N} \{e^{(i/\hbar)(b_j-a_j)B_j} *_{(t,\phi,\vec{A},\vec{B})} \delta(A_j - b_j)\}$$

$$= \delta(\phi) \prod_{j=1}^{N} \left\{ \frac{1}{2\pi} \sum_{n=0}^{+\infty} \frac{1}{n!} \left(\frac{-i\hbar}{2} \right)^n e^{(i/\hbar)(b_j-a_j)B_j} \left[\frac{i}{\hbar}(b_j - a_j) \frac{\partial}{\partial A_j} \right]^n \int \mathrm{d}k \, e^{ik(A_j-b_j)} \right\}$$

$$= \frac{\delta(\phi)}{(2\pi)^N} \prod_{j=1}^{N} \left\{ e^{(i/\hbar)(b_j-a_j)B_j} \int \mathrm{d}k \sum_{n=0}^{+\infty} \frac{1}{n!} \left[\frac{i}{2} k(b_j - a_j) \right]^n e^{ik(A_j-b_j)} \right\}$$

$$= \delta(\phi) \prod_{j=1}^{N} \left\{ e^{(i/\hbar)(b_j-a_j)B_j} \frac{1}{2\pi} \int \mathrm{d}k \, e^{ik[A_j-b_j+(b_j/2)-(a_j/2)]} \right\}$$

$$= \delta(\phi) \prod_{j=1}^{N} \left\{ e^{(i/\hbar)(b_j-a_j)B_j} \delta\left(A_j - \frac{a_j}{2} - \frac{b_j}{2} \right) \right\} = \delta(\phi) e^{(i/\hbar)(\vec{b}-\vec{a})\cdot\vec{B}} \delta\left(\vec{A} - \frac{\vec{a}+\vec{b}}{2} \right), \quad (23)$$

where $\Pi_{j=1*_{(t,\phi,\vec{A},\vec{B})}}^{N}$ stands for the N-fold star-product and $\Pi_{j=1}^{N}$ for the standard N-fold product of functions. The stargenfunctions $\rho_{\vec{a},\vec{b}}(t,\phi,\vec{A},\vec{B})$ are simultaneously solutions of Eq. (21) and

$$A_j *_{(t,\phi,\vec{A},\vec{B})} \rho_{\vec{a},\vec{b}}(t,\phi,\vec{A},\vec{B}) = a_j \rho_{\vec{a},\vec{b}}(t,\phi,\vec{A},\vec{B}),$$

$$\rho_{\vec{a},\vec{b}}(t,\phi,\vec{A},\vec{B}) *_{(t,\phi,\vec{A},\vec{B})} A_j = b_j \rho_{\vec{a},\vec{b}}(t,\phi,\vec{A},\vec{B}), \quad j = 1,\ldots,N. \quad (24)$$

Notice that the diagonal elements $\vec{a}=\vec{b}$ fully identify a history of the system, $\rho_{\vec{a},\vec{a}}(t,\phi,\vec{A},\vec{B}) = \delta(\phi)\Pi_{j=1}^{N}\delta(A_j - a_j)$. It is also straightforward to realize that the fundamental stargenfunctions (23) are the $(t,\phi,\vec{A},\vec{B})$-Weyl transform of the projectors,

$$|h=0,\vec{a}\rangle\langle h=0,\vec{b}| = \hat{\Delta}(\hat{\phi}) \prod_{j=1}^{N} \{e^{(i/\hbar)(b_j-a_j)\hat{B}_j} \hat{\Delta}(\hat{A}_j - b_j)\}, \quad (25)$$

where the general ket satisfies

$$\hat{\phi}|h,\vec{x}\rangle = h|h,\vec{x}\rangle \quad \text{and } \hat{A}_j|h,\vec{x}\rangle = x_j|h,\vec{x}\rangle \quad (26)$$

and

$$\hat{\Delta}(\hat{\phi}) = \int \mathrm{d}\vec{x}|h=0,\vec{x}\rangle\langle h=0,\vec{x}| = \frac{1}{2\pi} \int \mathrm{d}k \, e^{ik\hat{\phi}}, \quad (27)$$

is the operator analogue of (14). The most general solution of Eq. (21) is a linear combination of the fundamental solutions (23):

$$f_W(t,\phi,\vec{A},\vec{B}) = \frac{1}{(2\pi\hbar)^N} \int \mathrm{d}\vec{a} \int \mathrm{d}\vec{b} \, C(\vec{a}) C^*(\vec{b}) \rho_{\vec{a},\vec{b}}(t,\phi,\vec{A},\vec{B}), \quad (28)$$

where $C(\vec{a})$ obeys the normalization condition that is induced by the normalization of the Wigner function. Let us then calculate its norm,

$$\iiint \mathrm{d}t\,\mathrm{d}\phi\,\mathrm{d}\vec{A}\,\mathrm{d}\vec{B}\,f_W(t,\phi,\vec{A},\vec{B}) = \frac{1}{(2\pi\hbar)^N}\iiint \mathrm{d}t\,\mathrm{d}\vec{A}\,\mathrm{d}\vec{B}\int \mathrm{d}\vec{a}\int \mathrm{d}\vec{b}\,C(\vec{a})C^*(\vec{b})\prod_{j=1}^{N} e^{(i/\hbar)(b_j-a_j)B_j}\delta$$

$$\left(A_j - \frac{a_j+b_j}{2}\right) = \int \mathrm{d}t\int \mathrm{d}\vec{a}\int \mathrm{d}\vec{b}\,C(\vec{a})C^*(\vec{b})\delta(\vec{b}-\vec{a})$$

$$= \int \mathrm{d}t\int \mathrm{d}\vec{a}\,C(\vec{a})C^*(\vec{a}). \tag{29}$$

The divergence of the previous integral indicates that we are integrating over the gauge orbits thus spoiling the normalization of the Wigner function. In this case this is quite simple to correct. In fact we just have to introduce the phase space measure $\mathrm{d}\mu = \mathrm{d}\phi\,\mathrm{d}\vec{A}\,\mathrm{d}\vec{B}$ and use it from now on whenever we must integrate the Wigner function. The procedure corresponds to cutting the gauge orbits through a single time hypersurface. With this measure the Wigner function satisfies

$$\int \mathrm{d}\mu\, f_W = 1, \quad \forall\, t \tag{30}$$

provided the parameters $C(\vec{a})$ satisfy $\int \mathrm{d}\vec{a}|C(\vec{a})|^2 = 1$. The proper normalization of the Wigner function determines a phase space measure and a restriction on the factors $C(\vec{a})$. These parameters display a natural physical interpretation. To see this explicitly let us calculate the probabilities for the output of a measurement of $\vec{A}$. The general $\vec{x} = (x_1, \ldots, x_N)$ left and right stargenfunction of $\vec{A}$ (and simultaneously y left and right stargenfunction of the constraint) is

$$\rho_{y,\vec{x};y,\vec{x}} = \Delta_{*_{(t,\phi,\vec{A},\vec{B})}}(\phi,\vec{A};y,\vec{x};y,\vec{x}) = \Delta_{*_{(t,\phi,\vec{A},\vec{B})}}(\phi - y)\prod_{j=1}^{N} {}_{*_{(t,\phi,\vec{A},\vec{B})}}\Delta_{*_{(t,\phi,\vec{A},\vec{B})}}(A_j - x_j)$$

$$= \delta(\phi - y)\prod_{j=1}^{N}\delta(A_j - x_j) = \delta(\phi - y)\,\delta(\vec{A} - \vec{x}). \tag{31}$$

Therefore, the probability density for $\vec{A} = \vec{x}$ and $\phi = y$ is given by

$$\mathcal{P}(\phi = y, \vec{A} = \vec{x}) = \int \mathrm{d}\mu\, f_W(t,\phi,\vec{A},\vec{B})\,\delta(\phi - y)\,\delta(\vec{A} - \vec{x}) = \int \mathrm{d}\vec{B}\, f_W(t,y,\vec{x},\vec{B})$$

$$= \frac{1}{(2\pi\hbar)^N}\int \mathrm{d}\vec{B}\iint \mathrm{d}\vec{a}\,\mathrm{d}\vec{b}\,C(\vec{a})C^*(\vec{b})\,\delta(y)\prod_{j=1}^{N}\left\{e^{(i/\hbar)(b_j-a_j)B_j}\delta\left(x_j - \frac{a_j+b_j}{2}\right)\right\}$$

$$= \iint \mathrm{d}\vec{a}\,\mathrm{d}\vec{b}\,C(\vec{a})C^*(\vec{b})\,\delta(\vec{b}-\vec{a})\,\delta\left(\vec{x} - \frac{\vec{a}+\vec{b}}{2}\right)\delta(y) = |C(\vec{x})|^2\delta(y) \tag{32}$$

from where it follows:

$$P(\phi = y, \vec{A} = \vec{x}) = \lim_{\epsilon\to 0^+}\int_{y-\epsilon}^{y+\epsilon}\mathrm{d}y'\,\mathcal{P}(\phi = y', \vec{A} = \vec{x}) = |C(\vec{x})|^2\delta_{y,0}. \tag{33}$$

It is clear from the previous equation that the term $|C(\vec{x})|^2$ represents the probability for the system to be found in the history $\vec{A} = \vec{x}$. Under the measurement of $\vec{A}$ with output $\vec{x}$ the Wigner function will indeed collapse to the state,

$$\rho_{0,\vec{x};0,\vec{x}} = \delta(\phi)\,\delta(\vec{A}-\vec{x}). \tag{34}$$

Let us also point out that in the $(t,\phi,\vec{A},\vec{B})$ representation the Wigner function is static both with respect to the external time τ and to the physical time t. In fact from Eqs. (23) and (28) we see that $(\partial/\partial t)f_W=0$.

The former results can now be easily translated to the $(t,P_t,\vec{q},\vec{p})$ representation where the intention is to solve Eq. (22). The two representations are related by the unitary transformation:

$$t(t,P_t,\vec{q},\vec{p}) = U^{-1}*_{(t,P_t,\vec{q},\vec{p})}t*_{(t,P_t,\vec{q},\vec{p})}U = t,$$

$$\begin{aligned}
\phi(t,P_t,\vec{q},\vec{p}) &= W_{(t,P_t,\vec{q},\vec{p})}(\hat{\phi}) = U^{-1}*_{(t,P_t,\vec{q},\vec{p})}P_t*_{(t,P_t,\vec{q},\vec{p})}U = P_t + H_0(\vec{q},\vec{p}),\\
A_j(t,\vec{q},\vec{p}) &= W_{(t,P_t,\vec{q},\vec{p})}(\hat{A}_j) = U^{-1}*_{(t,P_t,\vec{q},\vec{p})}q_j*_{(t,P_t,\vec{q},\vec{p})}U, \quad j=1,\ldots,N,\\
B_j(t,\vec{q},\vec{p}) &= W_{(t,P_t,\vec{q},\vec{p})}(\hat{B}_j) = U^{-1}*_{(t,P_t,\vec{q},\vec{p})}p_j*_{(t,P_t,\vec{q},\vec{p})}U, \quad j=1,\ldots,N,
\end{aligned} \tag{35}$$

where $U=e^{(i/\hbar)H_0(\vec{q},\vec{p})t}_{*_{(t,P_t,\vec{q},\vec{p})}}$. The fundamental stargenfunctions are

$$\begin{aligned}
\rho_{\vec{a},\vec{b}}(t,P_t,\vec{q},\vec{p}) &= \Delta_{*_{(t,P_t,\vec{q},\vec{p})}}(\phi,\vec{A};h=0,\vec{a};h=0,\vec{b}) = \Delta_{*_{(t,P_t,\vec{q},\vec{p})}}(P_t+H_0(\vec{q},\vec{p}))\prod_{j=1}^{N}{}_{*_{(t,P_t,\vec{q},\vec{p})}}\\
&\{e^{(i/\hbar)(b_j-a_j)B_j(t,\vec{q},\vec{p})}_{*_{(t,P_t,\vec{q},\vec{p})}}*_{(t,P_t,\vec{q},\vec{p})}\Delta_{*_{(t,P_t,\vec{q},\vec{p})}}(A_j(t,\vec{q},\vec{p})-b_j)\},
\end{aligned} \tag{36}$$

which in general do not simplify any further as in Eq. (23). These stargenfunctions are the $(t,P_t,\vec{q},\vec{p})$-Weyl transform of the projector (25). The most general solution of (22) is then

$$f_W(t,P_t,\vec{q},\vec{p}) = \frac{1}{(2\pi\hbar)^N}\int \mathrm{d}\vec{a}\,\mathrm{d}\vec{b}\,C(\vec{a})C^*(\vec{b})\rho_{\vec{a},\vec{b}}(t,P_t,\vec{q},\vec{p}) \tag{37}$$

and can be obtained directly from the Wigner function (28) by applying the unitary transformation (35). Hence, $f_W(t,P_t,\vec{q},\vec{p})$ is properly normalized for the phase space measure $\mathrm{d}\mu=\mathrm{d}P_t\,\mathrm{d}\vec{q}\,\mathrm{d}\vec{p}$ provided the coefficients $C(\vec{a})$ satisfy the normalization $\int \mathrm{d}\vec{a}\,C(\vec{a})C^*(\vec{a})=1$. Notice that in general the Wigner function does not have support exclusively on the classical constraint hypersurface. This is due to the nonlocal character of the $*$-delta functions in Eq. (36). Notice also that f_W does not evolve with respect to the external time τ but it displays the standard time evolution with respect to the canonical time t,

$$\begin{aligned}
\frac{\partial f_W(t,P_t,\vec{q},\vec{p})}{\partial\tau} &= [H(t,P_t,\vec{q},\vec{p}),f_W(t,P_t,\vec{q},\vec{p})]_{M_{(t,P_t,\vec{q},\vec{p})}} = 0 \Leftrightarrow \frac{\partial f_W(t,P_t,\vec{q},\vec{p})}{\partial t}\\
&= [H_0(\vec{q},\vec{p}),f_W(t,P_t,\vec{q},\vec{p})]_{M_{(\vec{q},\vec{p})}}.
\end{aligned} \tag{38}$$

We conclude that the $(t,P_t,\vec{q},\vec{p})$ representation yields the extended phase space Schrödinger picture for the quantum generally covariant system. Likewise the $(t,\phi,\vec{A},\vec{B})$ representation provides the phase space Heisenberg picture.

IV. CAUSAL REPRESENTATION

We now study another possible phase space representation of the system. The first step is to specify a set of classical phase space coordinates $(t,P_t,\vec{Q},\vec{P})$. Let us define the phase space diffeomorphism by

$$t = t, \quad P_t = \phi - H_0(\vec{A},\vec{B}), \quad \vec{Q} = \vec{Q}(t,\vec{A},\vec{B}), \quad \vec{P} = \vec{P}(t,\vec{A},\vec{B}), \tag{39}$$

where $H_0(\vec{A},\vec{B}) = W_{(\vec{A},\vec{B})}(\hat{H}_0) = W_{(\vec{q},\vec{p})}(\hat{H}_0)|_{\vec{q}=\vec{A}\wedge\vec{p}=\vec{B}}$ and $\vec{Q}(t,\vec{A},\vec{B}), \vec{P}(t,\vec{A},\vec{B})$ satisfy

$$\frac{\partial \vec{Q}(t,\vec{A},\vec{B})}{\partial t} = \{\vec{Q}(t,\vec{A},\vec{B}), H_0(\vec{A},\vec{B})\}_{(\vec{A},\vec{B})}, \quad \frac{\partial \vec{P}(t,\vec{A},\vec{B})}{\partial t} = \{\vec{P}(t,\vec{A},\vec{B}), H_0(\vec{A},\vec{B})\}_{(\vec{A},\vec{B})} \tag{40}$$

together with the initial conditions $\vec{Q}(0,\vec{A},\vec{B}) = \vec{A}$ and $\vec{P}(0,\vec{A},\vec{B}) = \vec{B}$. That is $\vec{Q}(t,\vec{A},\vec{B})$ and $\vec{P}(t,\vec{A},\vec{B})$ constitute the *classical* time evolution of the deparametrized system. The transformation (39) is canonical and can be easily inverted. It yields

$$t = t, \quad \phi = \phi'(t,P_t,\vec{Q},\vec{P}) = P_t + H_0(\vec{Q},\vec{P}), \quad \vec{A} = \vec{A}'(t,\vec{Q},\vec{P}), \quad \vec{B} = \vec{B}'(t,\vec{Q},\vec{P}), \tag{41}$$

where this time $H_0(\vec{Q},\vec{P}) = W_{(\vec{q},\vec{p})}(\hat{H}_0)|_{\vec{q}=\vec{Q}\wedge\vec{p}=\vec{P}}$ and $\vec{A}'(t,\vec{Q},\vec{P}), \vec{B}'(t,\vec{Q},\vec{P})$ satisfy

$$\frac{\partial \vec{A}'(t,\vec{Q},\vec{P})}{\partial t} = \{H_0(\vec{Q},\vec{P}), \vec{A}'(t,\vec{Q},\vec{P})\}_{(\vec{Q},\vec{P})}, \quad \frac{\partial \vec{B}'(t,\vec{Q},\vec{P})}{\partial t} = \{H_0(\vec{Q},\vec{P}), B'(t,\vec{Q},\vec{P})\}_{(\vec{Q},\vec{P})} \tag{42}$$

together with the initial conditions $\vec{A}'(0,\vec{Q},\vec{P}) = \vec{Q}$ and $\vec{B}'(0,\vec{Q},\vec{P}) = \vec{P}$. This means that the *functions* $\vec{A}'(t,\vec{Q},\vec{P})$ and $\vec{B}'(t,\vec{Q},\vec{P})$ are the classical histories of the system. We should point out that in general the two functions $\vec{A}'(t,\vec{Q},\vec{P})$ and $\vec{A}(t,\vec{q},\vec{p})$ given by Eqs. (41) and (35), respectively, as well as $\vec{B}'(t,\vec{Q},\vec{P})$ and $\vec{B}(t,\vec{q},\vec{p})$, display different functional forms (they are, respectively, the classical and the quantum Weyl-Wigner histories of the system). To make this point explicit, we introduced the prime notation which is in agreement with the fact that $\vec{A}'(t,\vec{Q},\vec{P}) = W^{(t,\phi,\vec{A},\vec{B})}_{(t,P_t,\vec{Q},\vec{P})}(\hat{\vec{A}})$, $\vec{B}'(t,\vec{Q},\vec{P}) = W^{(t,\phi,\vec{A},\vec{B})}_{(t,P_t,\vec{Q},\vec{P})}(\hat{\vec{B}})$, and $\phi'(t,P_t,\vec{Q},\vec{P}) = W^{(t,\phi,\vec{A},\vec{B})}_{(t,P_t,\vec{Q},\vec{P})}(\hat{\phi})$. Finally, let us concisely designate the transformation (41) by $\vec{T}: \mathbb{R}^{(2N+2)} \to \mathbb{R}^{(2N+2)}$; $(t,P_t,\vec{Q},\vec{P}) \to (t,\phi,\vec{A},\vec{B}) = \vec{T}(t,P_t,\vec{Q},\vec{P})$.

The transformation $\vec{T}$ is canonical but in general it does not preserve either the star-product or the Moyal bracket. Using the generalized Weyl transform $W^{(t,\phi,\vec{A},\vec{B})}_{(t,P_t\vec{Q},\vec{P})}$ we find a phase space representation of the eigenvalue equation (18),

$$\phi'(t,P_t,\vec{Q},\vec{P}) *'_{(t,P_t,\vec{Q},\vec{P})} f'_W(t,P_t,\vec{Q},\vec{P}) = f'_W(t,P_t,\vec{Q},\vec{P}) *'_{(t,P_t,\vec{Q},\vec{P})} \phi'(t,P_t,\vec{Q},\vec{P}) = 0, \tag{43}$$

where the $*'_{(t,P_t,\vec{Q},\vec{P})}$ is the covariant star-product given by (3) with

$$J'^{ij}_{(t,P_t,\vec{Q},\vec{P})} = J^{ij}_{(t,\phi,\vec{A},\vec{B})} \quad \text{and } \Gamma'^{i}_{jk} = \frac{\partial O'^{i}}{\partial O^{b}} \frac{\partial^2 O^{b}}{\partial O'^{j}\, \partial O'^{k}}, \tag{44}$$

where $O^b \in \{t,\phi,\vec{A},\vec{B}\}$ and $O'^i \in \{t,P_t,\vec{Q},\vec{P}\}$. The solutions of Eq. (43) can be read from Eqs. (23) and (28),

$$f'_W(t,P_t,\vec{Q},\vec{P}) = \frac{1}{(2\pi\hbar)^N} W^{(t,\phi,\vec{A},\vec{B})}_{(t,P_t,\vec{Q},\vec{P})}(|\psi\rangle\langle\psi|) = \frac{1}{(2\pi\hbar)^N} \int \mathrm{d}\vec{a} \int \mathrm{d}\vec{b}\; C(\vec{a}) C^*(\vec{b}) \rho'_{\vec{a},\vec{b}}(t,P_t,\vec{Q},\vec{P}), \tag{45}$$

where

$$\rho'_{\vec{a},\vec{b}}(t,P_t,\vec{Q},\vec{P}) = \Delta_{*'_{(t,P_t,\vec{Q},\vec{P})}}(\phi'(t,P_t,\vec{Q},\vec{P}),\vec{A}'(t,\vec{Q},\vec{P});h=0,\vec{a};h=0,\vec{b})$$

$$= \Delta_{*'_{(t,P_t,\vec{Q},\vec{P})}}(\phi'(t,P_t,\vec{Q},\vec{P}))\prod_{j=1}^{N} {}_{*'_{(t,P_t,\vec{Q},\vec{P})}}\Delta_{*'_{(t,P_t,\vec{Q},\vec{P})}}(A'_j(t,\vec{Q},\vec{P}),a_j,b_j) = \Delta_{*_{(t,\phi,\vec{A},\vec{B})}}$$

$$(\phi'(t,P_t,\vec{Q},\vec{P}))\prod_{j=1}^{N} {}_{*_{(t,\phi,\vec{A},\vec{B})}}\{e^{(i/\hbar)(b_j-a_j)B'_j(t,\vec{Q},\vec{P})}_{*_{(t,\phi,\vec{A},\vec{B})}} *_{(t,\phi,\vec{A},\vec{B})}\Delta_{*_{(t,\phi,\vec{A},\vec{B})}}(A'_j(t,\vec{Q},\vec{P})-b_j)\}$$

$$= \delta(\phi'(t,P_t,\vec{Q},\vec{P}))\prod_{j=1}^{N}\left\{e^{(i/\hbar)(b_j-a_j)B'_j(t,\vec{Q},\vec{P})}\delta\left(A'_j(t,\vec{Q},\vec{P})-\frac{a_j+b_j}{2}\right)\right\}$$

$$= \delta(\phi'(t,P_t,\vec{Q},\vec{P}))e^{i/\hbar(\vec{b}-\vec{a})\cdot\vec{B}'(t,\vec{Q}\vec{P})}\delta\left(\vec{A}'(t,\vec{Q},\vec{P})-\frac{\vec{a}+\vec{b}}{2}\right). \tag{46}$$

The Wigner function satisfies

$$f'_W(t,P_t,\vec{Q},\vec{P}) = f_W(t,\phi'(t,P_t,\vec{Q},\vec{P}),\vec{A}'(t,\vec{Q},\vec{P}),\vec{B}'(t,\vec{Q},\vec{P})), \tag{47}$$

where f_W is given by Eq. (28). Furthermore and since the coordinate transformation is canonical we have

$$\mathrm{d}\mu = \mathrm{d}\phi\,\mathrm{d}\vec{A}\,\mathrm{d}\vec{B} = \delta(t)\mathrm{d}t\,\mathrm{d}\phi\,\mathrm{d}\vec{A}\,\mathrm{d}\vec{B} = \delta(t)\mathrm{d}t\,\mathrm{d}P_t\,\mathrm{d}\vec{Q}\,\mathrm{d}\vec{P} = \mathrm{d}P_t\,\mathrm{d}\vec{Q}\,\mathrm{d}\vec{P}, \tag{48}$$

and the Wigner function obeys the proper normalization, $\int \mathrm{d}\mu\, f'_W = 1$. Also notice that both the diagonal and the nondiagonal stargenfunctions (and thus also the Wigner function) have support only on the classical constraint hypersurface, a property that it is not shared by the previous representation (36) and (37).

Finally, let us briefly elaborate on the dynamical structure of the system in this representation. It is clear from Eq. (43) that the Wigner function is static,

$$\frac{\partial}{\partial\tau}f'_W(t,P_t,\vec{Q},\vec{P};\tau) = [H'(t,P_t,\vec{Q},\vec{P}),f'_W(t,P_t,\vec{Q},\vec{P};\tau)]_{M'_{(t,P_t,\vec{Q},\vec{P})}}$$

$$= \lambda[\phi'(t,P_t,\vec{Q},\vec{P}),f'_W(t,P_t,\vec{Q},\vec{P};\tau)]_{M'_{(t,P_t,\vec{Q},\vec{P})}} = 0, \tag{49}$$

confirming the typical picture of frozen dynamics. However, the Wigner function does evolve with respect to the physical time t. From Eqs. (42) and (47) we have

$$\frac{\partial}{\partial t}f'_W(t,P_t,\vec{Q},\vec{P}) = \frac{\partial f_W}{\partial\phi}(\vec{T}(t,P_t,\vec{Q},\vec{P}))\frac{\partial\phi'}{\partial t} + \sum_{j=1}^{N}\frac{\partial f_W}{\partial A_j}(\vec{T}(t,P_t,\vec{Q},\vec{P}))\frac{\partial A'_j}{\partial t} + \sum_{j=1}^{N}\frac{\partial f_W}{\partial B_j}(\vec{T}(t,P_t,\vec{Q},\vec{P}))\frac{\partial B'_j}{\partial t}$$

$$= \sum_{j=1}^{N}\frac{\partial f_W}{\partial A_j}(\vec{T}(t,P_t,\vec{Q},\vec{P}))\{H_0,A'_j\}_{(t,P_t,\vec{Q},\vec{P})} + \sum_{j=1}^{N}\frac{\partial f_W}{\partial B_j}(\vec{T}(t,P_t,\vec{Q},\vec{P}))\{H_0,B'_j\}_{(t,P_t,\vec{Q},\vec{P})}$$

$$= \{H_0,f'_W\}_{(t,P_t,\vec{Q},\vec{P})}, \tag{50}$$

reproducing the classical Liouville equation $\{H',f'_W\}_{(t,P_t,\vec{Q},\vec{P})}=0$.

We see that the $\frac{(t,\phi,\vec{A},\vec{B})}{(t,P_t,\vec{Q},\vec{P})}$-representation of the system leads to an interesting mathematical picture; the Hamiltonian vector field lives on the extended phase space and is given by

$$\xi_H = \lambda \left\{ \frac{\partial}{\partial t} + \sum_{j=1}^{N} \frac{\partial H_0}{\partial P_j}\frac{\partial}{\partial Q_j} - \sum_{j=1}^{N} \frac{\partial H_0}{\partial Q_j}\frac{\partial}{\partial P_j} \right\}. \tag{51}$$

The flows of this vector field define lines in phase space. These lines cross each time hypersurface once and only once; they are the histories of the system. These histories are one-dimensional hypersurfaces that can be identified by the values of the $1+2N$ constants of motion, $\phi, \vec{A}, \vec{B}$. Along these lines the Wigner distribution function is constant. However, the correlations between the canonical variables, namely between $\vec{Q}$ and t, do change and time evolution is imprinted on these correlations. The interesting point is that this picture is not of the classical description but of the quantum mechanical instead.

A natural question is what happened to the quantum content of the theory? What happened to the interfering trajectories and to the nonlocal behavior? The answer is that the quantum features have been completely removed from the distributional sector and are now exclusively placed in the observables' sector of the theory. This can be checked explicitly by applying the proper generalized Weyl transform to one of the fundamental operators of the system. We have for instance,

$$W^{(t,\phi,\vec{A},\vec{B})}_{(t,P_t,\vec{Q},\vec{P})}(\hat{q}_1) = q_1(t,\phi,\vec{A},\vec{B})|_{(t,\phi,\vec{A},\vec{B})=\vec{T}(t,P_t,\vec{Q},\vec{P})} = q_1(t,\phi'(t,P_t,\vec{Q},\vec{P}),A'(t,\vec{Q},\vec{P}),B'(t,\vec{Q},\vec{P})), \tag{52}$$

leading to the time evolution

$$\begin{aligned} \frac{\mathrm{d}q_1}{\mathrm{d}t} &= \frac{\partial q_1}{\partial t} + \frac{\partial q_1}{\partial \phi}\frac{\partial \phi'}{\partial t} + \sum_{j=1}^{N} \frac{\partial q_1}{\partial A_j}\frac{\partial A'_j}{\partial t} + \sum_{j=1}^{N} \frac{\partial q_1}{\partial B_j}\frac{\partial B'_j}{\partial t} = [q_1, H_0]_{M_{(\vec{A},\vec{B})}} - \sum_{j=1}^{N} \frac{\partial q_1}{\partial A_j}\{A'_j, H_0\}_{(\vec{Q},\vec{P})} \\ &\quad - \sum_{j=1}^{N} \frac{\partial q_1}{\partial B_j}\{B'_j, H_0\}_{(\vec{Q},\vec{P})} = [q_1, H_0]_{M_{(\vec{A},\vec{B})}} - \{q_1, H_0\}_{(\vec{A},\vec{B})}, \end{aligned} \tag{53}$$

where the identity $\partial q_1/\partial t = [q_1, H_0]_{M_{(\vec{A},\vec{B})}}$ follows from Eq. (20) [or alternatively from Eq. (35)], we used the fact that ϕ' is time independent and that the transformation $(\vec{Q},\vec{P}) \to (\vec{A},\vec{B})$ is canonical. Equation (53) does in fact constitute a quantum correction to the classical statistical description where we have

$$\frac{\partial \rho}{\partial t} = \{H_0, \rho\} \quad \text{and} \quad \frac{\mathrm{d}q_1}{\mathrm{d}t} = 0. \tag{54}$$

Notice that in the classical description $\vec{Q} = \vec{q}, \vec{P}, = \vec{p}$ and $\vec{q}(t,\phi'(t,P_t,\vec{q},\vec{p}),\vec{A}'(t,\vec{q},\vec{p}),\vec{B}'(t,\vec{q},\vec{p})) = \vec{q}$.

We finally conclude by pointing out that a causal representation can also be obtained for deparametrized systems by using an explicit "time dependent phase space representation" where the star-product and Moyal bracket are themselves (scalar) time dependent.[39] In this approach we apply a time dependent generalization of the Weyl map to the density matrix formulation of the deparametrized system and obtain a phase space causal representation of the Wigner function, which is formally identical to the one described by Eqs. (45), (46), and (52), although t is a canonical variable in the former equations and an external scalar parameter in the approach of Ref. 39. Accordingly, the two resulting quasidistributions live on different phase spaces. In spite of this the two formulations are consistent with each other leading to the single conclusion that a phase space formulation of quantum mechanics where the distributional sector displays a fully classical causal structure is made possible through a suitable choice of representation. This may either be a (scalar) time dependent representation in the deparametrized phase space or a history representation in the generally covariant setting.

V. EXAMPLE

To illustrate our previous results let us consider the simple system composed by two coupled particles and described by the Hamiltonian

$$H_0 = \frac{p_1^2}{2M} + \frac{p_2^2}{2m} + kq_1p_2^2, \tag{55}$$

where (q_1,p_1) are the canonical variables of the particle of mass M, (q_2,p_2) those of the particle of mass m and k is a coupling constant.

The generally covariant version of this system is obtained by promoting t to a canonical variable and imposing the time reparametrization invariance. The extended Hamiltonian formulation of the system lives on a six-dimensional phase space spanned by the canonical variables $t,P_t,\vec{q}=(q_1,q_2),\vec{p}=(p_1,p_2)$ which satisfy the commutation relations $\{t,P_t\}=1,\{q_i,p_j\}=\delta_{ij},i,j=1,2$, all others being zero. Upon quantization the system is described by the "zero Hamiltonian,"

$$\hat{H} = \lambda\hat{\phi}, \quad \hat{\phi} = \hat{P}_t + \hat{H}_0 = \hat{P}_t + \frac{\hat{p}_1^2}{2M} + \frac{\hat{p}_2^2}{2m} + k\hat{q}_1\hat{p}_2^2, \tag{56}$$

where $\hat{\phi}$ is the first class Hamiltonian constraint and λ is a Lagrange multiplier. In standard the Dirac formulation the physical states of this system are the wave functions ψ solutions of the constraint equation

$$\hat{\phi}|\psi\rangle = 0. \tag{57}$$

We now address the deformation quantization of the system. As in the main text, three distinct quantum phase space representations will be presented.

(1) *The map $W_{(t,P_t,\vec{q},\vec{p})}$ and the generally covariant Schrödinger picture*. The Weyl map $W_{(t,P_t,\vec{q},\vec{p})}$ yields the $(t,P_t,\vec{q},\vec{p})$-constraint symbol

$$\phi = W_{(t,P_t,\vec{q},\vec{p})}(\hat{\phi}) = P_t + \frac{p_1^2}{2M} + \frac{p_2^2}{2m} + kq_1p_2^2 \tag{58}$$

and the quantum phase space version of the Hamiltonian constraint (57) is given by

$$\phi(t,P_t,\vec{q},\vec{p}) *_{(t,P_t,\vec{q},\vec{p})} f_W(t,P_t,\vec{q},\vec{p}) = f_W(t,P_t,\vec{q},\vec{p}) *_{(t,P_t,\vec{q},\vec{p})} \phi(t,P_t,\vec{q},\vec{p}) = 0. \tag{59}$$

The solutions of this right and left stargenvalue equation are given by Eqs. (36) and (37) and they do not easily simplify any further. It is worth noticing that due to the nonlocal character of the $*$-product the phase space quasidistribution f_W will have support on phase-space regions which are not classically allowed. One can easily calculate the evolution of f_W with respect to the physical time t. From Eq. (59) we have

$$\begin{aligned}\frac{\partial f_W}{\partial\tau} = \lambda[\phi,f_W]_{M_{(t,P_t,\vec{q},\vec{p})}} = 0 \Leftrightarrow \frac{\partial f_W}{\partial t} = [H_0,f_W]_{M_{(\vec{q},\vec{p})}} \Leftrightarrow \frac{\partial f_W}{\partial t} \\ = \{H_0,f_W\}_{(\vec{q},\vec{p})} + \frac{\hbar^2}{24}\left[2\left\{2kp_2,\frac{\partial^2 f_W}{\partial q_2\,\partial p_1}\right\}_{(\vec{q},\vec{p})} - \left\{2kq_1,\frac{\partial^2 f_W}{\partial q_2^2}\right\}_{(\vec{q},\vec{p})}\right]\end{aligned} \tag{60}$$

which is obviously not of the form of the Liouville equation. Consequently, the Wigner function does not display a classical causal structure.

(2) *The map $W_{(t,\phi,\vec{A},\vec{B})}$ and the generally covariant Heisenberg picture*. Following the approach of Sec. III our first step is to determine the quantum histories associated to $\hat{H}$. We easily find that [check Eqs. (19) and (20)]

$$\hat{A}_1 = \hat{q}_1 - \frac{\hat{p}_1}{M}\hat{t} - \frac{k}{2M}\hat{p}_2^2\hat{t}^2,$$

$$\hat{B}_1 = \hat{p}_1 + k\hat{p}_2^2\hat{t},$$

$$\hat{A}_2 = \hat{q}_2 - \left\{\frac{\hat{p}_2}{m} + 2k\hat{q}_1\hat{p}_2\right\}\hat{t} + \frac{k}{M}\hat{p}_1\hat{p}_2\hat{t}^2 + \frac{k^2}{3M}\hat{p}_2^3\hat{t}^3,$$

$$\hat{B}_2 = \hat{p}_2 \tag{61}$$

satisfy the requisites following Eq. (18), i.e., $\hat{A}_j, \hat{B}_j, j=1, 2$ commute with the constraint $\hat{\phi}$ and with $\hat{t}$ and furthermore they satisfy the Heisenberg algebra $[\hat{A}_1, \hat{B}_1]=[\hat{A}_2, \hat{B}_2]=i\hbar$, all other commutators being zero. Since $[\hat{t}, \hat{\phi}]=i\hbar$ the set $\{\hat{t}, \hat{\phi}, \hat{\vec{A}}=(\hat{A}_1, \hat{A}_2), \hat{\vec{B}}=(\hat{B}_1, \hat{B}_2)\}$ is a complete set of fundamental operators for this system.

Using the Weyl map $W_{(t,\phi,\vec{A},\vec{B})}$ we find the Heisenberg phase space representation of the constraint equation (57),

$$\phi *_{(t,\phi,\vec{A},\vec{B})} f_W(t,\phi,\vec{A},\vec{B}) = f_W(t,\phi,\vec{A},\vec{B}) *_{(t,\phi,\vec{A},\vec{B})} \phi = 0. \tag{62}$$

The fundamental solutions of this equation $\rho_{\vec{a},\vec{b}}$ [where $\vec{a}=(a_1, a_2)$ and $\vec{b}=(b_1, b_2)$], and also satisfying

$$A_j *_{(t,\phi,\vec{A},\vec{B})} \rho_{\vec{a},\vec{b}} = a_j \rho_{\vec{a},\vec{b}}, \quad \rho_{\vec{a},\vec{b}} *_{(t,\phi,\vec{A},\vec{B})} A_j = b_j \rho_{\vec{a},\vec{b}}, \quad j = 1,2 \tag{63}$$

are given by

$$\rho_{\vec{a},\vec{b}}(t,\phi,\vec{A},\vec{B}) = \delta(\phi) e^{(i/\hbar)\{(b_1-a_1)B_1+(b_2-a_2)B_2\}} \delta\left(A_1 - \frac{a_1+b_1}{2}\right)\delta\left(A_2 - \frac{a_2+b_2}{2}\right). \tag{64}$$

And the Wigner function, solution of (62), is just a Hermitian combination of the fundamental solutions. We have

$$f_W(t,\phi,\vec{A},\vec{B}) = \frac{1}{2\pi\hbar}\int \mathrm{d}\vec{a} \int \mathrm{d}\vec{b}\, C(\vec{a}) C^*(\vec{b}) \rho_{\vec{a},\vec{b}}(t,\phi,\vec{A},\vec{B}), \tag{65}$$

where $C(\vec{a})$ obeys to the normalization condition that is induced by the normalization of the Wigner function, $\int \mathrm{d}\vec{a}|C(\vec{a})|^2=1$. The Wigner function satisfies Eq. (62) which implies that $\partial f_W/\partial\tau=0$. We also have from Eq. (64) that $\partial f_W/\partial t=0$. That is, the Wigner function is static both with respect to the unphysical scalar parameter as well as to the physical time. This is an expected result since, in this representation, the Wigner quasidistribution is an exclusive function of observables of the system (the histories), i.e., of quantities that commute with the Hamiltonian constraint.

On the other hand, in this representation, the stargenfunctions of the fundamental variables $\hat{t}$, $\hat{\vec{q}}$, and $\hat{\vec{p}}$ do evolve with respect to the physical time. For instance (let $|x\rangle$ be the general eigenket of $\hat{q}_1$ with associated eigenvalue x),

$$g_x(t,\phi,\vec{A},\vec{B}) = W_{(t,\phi,\vec{A},\vec{B})}(|x\rangle\langle x|) = \Delta_{*_{(t,\phi,\vec{A},\vec{B})}}(q_1(t,\vec{A},\vec{B}) - x) = \frac{1}{2\pi}\int \mathrm{d}k\, e^{ik(q_1(t,\vec{A},\vec{B})-x)}_{*_{(t,\phi,\vec{A},\vec{B})}}$$

$$= \frac{1}{2\pi}\int \mathrm{d}k\, e^{ik(q_1(t,\vec{A},\vec{B})-x)} = \delta(q_1(t,\vec{A},\vec{B}) - x), \tag{66}$$

where $q_1(t,\vec{A},\vec{B})$ can be easily derived from Eq. (61), $q_1(t,\vec{A},\vec{B}) = W_{(t,\phi,\vec{A},\vec{B})}(\hat{q}_1(\hat{t},\hat{\vec{A}},\hat{\vec{B}})) = A_1 + (B_1/M)t - (k/2M)B_2^2t^2$. Hence, $g_x(t,\phi,\vec{A},\vec{B})$ satisfies

$$\frac{\partial}{\partial t}g_x(t,\phi,\vec{A},\vec{B}) = [g_x(t,\phi,\vec{A},\vec{B}), H_0(\vec{A},\vec{B})]_{M_{(\vec{A},\vec{B})}} = \{g_x(t,\phi,\vec{A},\vec{B}), H_0(\vec{A},\vec{B})\}_{(\vec{A},\vec{B})}, \tag{67}$$

where $H_0(\vec{A},\vec{B}) = W_{(\vec{A},\vec{B})}(\hat{H}_0) = (B_1^2/2M) + (B_2^2/2m) + kA_1B_2^2$. We conclude that the Weyl transform $W_{(t,\phi,\vec{A},\vec{B})}$ casts the phase space dynamics in the Heisenberg picture. Accordingly, the time dependence is exclusively displayed by the observable (stargenfunction) sector of the theory.

(3) *The map* $W^{(t,\phi,\vec{A},\vec{B})}_{(t,P_t,\vec{q},\vec{p})}$ *and the generally covariant causal picture*. Following the prescription of Sec. IV let us introduce a set of phase space coordinates $[t, P_t, \vec{Q}=(Q_1,Q_2), \vec{P}=(P_1,P_2)]$ defined by Eqs. (39) and (40). We get $t=t$, $P_t = \phi - H_0(\vec{A},\vec{B})$, and

$$\begin{cases} Q_1 = A_1 + \dfrac{B_1}{M}t - \dfrac{k}{2M}B_2^2t^2 \\ P_1 = B_1 - kB_2^2t \\ Q_2 = A_2 + \left\{\dfrac{B_2}{m} + 2kA_1B_2\right\}t \\ \quad + \dfrac{k}{M}B_1B_2t^2 - \dfrac{k^2}{3M}B_2^3t^3 \\ P_2 = B_2 \end{cases} \Leftrightarrow \begin{cases} A_1 = Q_1 - \dfrac{P_1}{M}t - \dfrac{k}{2M}P_2^2t^2, \\ B_1 = P_1 + kP_2^2t, \\ A_2 = Q_2 - \left\{\dfrac{P_2}{m} + 2kQ_1P_2\right\}t \\ \quad + \dfrac{k}{M}P_1P_2t^2 + \dfrac{k^2}{3M}P_2^3t^3, \\ B_2 = P_2. \end{cases} \tag{68}$$

We notice that $\vec{Q}(t,\vec{A},\vec{B})$ and $\vec{P}(t,\vec{A},\vec{B})$ coincide with $W_{(t,\phi,\vec{A},\vec{B})}(\hat{\vec{q}}), W_{(t,\phi,\vec{A},\vec{B})}(\hat{\vec{p}})$, respectively [this is an easy result that follows from Eq. (61)], i.e., the classical and the quantum histories of this system are exactly the same. Indeed, Eq. (68) solves both the Moyal and the Hamiltonian equations of motion. In the notation of Sec. IV we have $\vec{A}' = \vec{A}$ and $\vec{B}' = \vec{B}$ (one should notice that this result is not valid in general). Hence, for this system, we are not required to introduce a second set of "classical coordinates" and can simplify the notation by making $Q_j = q_j$ and $P_j = p_j$, $j=1, 2$.

We now consider the action of the generalized Weyl map $W^{(t,\phi,A,B)}_{(t,P_t,\vec{q},\vec{p})}$. The associated covariant star-product $*'_{(t,P_t,\vec{q},\vec{p})}$ and Moyal bracket $[,]_{M_{(t,P_t,\vec{q},\vec{p})}}$ are characterized by (let $O'^1 = P_t$, $O'^2 = p_1$, $O'^3 = p_2$, $O'^4 = t$, $O'^5 = q_1$, $O'^6 = q_2$, $O^1 = \phi$, $O^2 = B_1$, $O^3 = B_2$, $O^4 = t$, $O^5 = A_1$, $O^6 = A_2$ and $i,j = 1,\ldots,6$) [check Eq. (5)]

$$J'^{ij}_{(\vec{q},\vec{p})} = J^{ij}_{(\vec{q},\vec{p})},$$

$$\Gamma'^1_{22} = -\Gamma'^5_{24} = -\Gamma'^5_{42} = \frac{1}{M}, \quad \Gamma'^1_{24} = \Gamma'^1_{42} = -\Gamma'^5_{44} = \frac{k}{M}p_2^2, \quad \Gamma'^1_{33} = 2kA_1(t,\vec{q},\vec{p}),$$

$$\Gamma'^1_{34} = \Gamma'^1_{43} = -\Gamma'^6_{44} = -\frac{2k}{M}p_1p_2, \quad \Gamma'^1_{35} = \Gamma'^1_{53} = \Gamma'^2_{34} = \Gamma'^2_{43} = -\Gamma'^6_{45} = -\Gamma'^6_{54} = 2kp_2, \tag{69}$$

$$\Gamma'^{1}_{44}=\frac{k^2}{M}p_2^4,\quad \Gamma'^{2}_{33}=-\Gamma'^{6}_{35}=-\Gamma'^{6}_{53}=2kt,\quad \Gamma'^{5}_{33}=\Gamma'^{6}_{23}=\Gamma'^{6}_{32}=\frac{k}{M}t^2,$$

$$\Gamma'^{5}_{34}=\Gamma'^{5}_{43}=\frac{k}{M}p_2t,\quad \Gamma'^{6}_{33}=\frac{2k^2}{M}p_2t^3,\quad \Gamma'^{6}_{34}=\Gamma'^{6}_{43}=-\frac{1}{m}-2kA_1(t,\vec{q},\vec{p})$$

all other Christoffel symbols being zero.

In this representation the constraint equation reads

$$(P_t+H_0(\vec{q},\vec{p}))*'_{(t,P_t,\vec{q},\vec{p})}f'_W(t,P_t,\vec{q},\vec{p})=f'_W(t,P_t,\vec{q},\vec{p})*'_{(t,P_t,\vec{q},\vec{p})}(P_t+H_0(\vec{q},\vec{p}))=0, \tag{70}$$

where $H_0(\vec{q},\vec{p})=W^{(t,\phi,\vec{A},\vec{B})}_{(t,P_t,\vec{q},\vec{p})}(\hat{H}_0)$ is given by Eq. (54). The fundamental solutions of Eq. (70) are given by

$$\begin{aligned}\rho'_{\vec{a},\vec{b}}(t,P_t,\vec{q},\vec{p})&=\Delta_{*'_{(t,P_t,\vec{q},\vec{p})}}(\phi(t,P_t,\vec{q},\vec{p}),\vec{A}(t,\vec{q},\vec{p});h=0,\vec{a};h=0,\vec{b})\\&=\delta(\phi(t,P_t,\vec{q},\vec{p}))e^{(i/\hbar)(\vec{b}-\vec{a})\cdot\vec{B}(t,\vec{q},\vec{p})}\delta\left(\vec{A}(t,\vec{q},\vec{p})-\frac{\vec{a}+\vec{b}}{2}\right).\\&=\delta(P_t+H_0(\vec{q},\vec{p}))e^{(i/\hbar)\{(b_1-a_1)(p_1+kp_2^2t)+(b_2-a_2)p_2\}}\delta\left(q_1-\frac{p_1}{M}t-\frac{k}{2M}p_2^2t^2-\frac{a_1+b_1}{2}\right)\\&\quad\times\delta\left(q_2-\left\{\frac{p_2}{m}+2kq_1p_2\right\}t+\frac{k}{M}p_1p_2t^2+\frac{k^2}{3M}p_2^3t^3-\frac{a_2+b_2}{2}\right)\end{aligned} \tag{71}$$

and the Wigner function is once again a Hermitian combination of the fundamental solutions $\rho'_{\vec{a},\vec{b}}$,

$$f'_W(t,P_t,\vec{q},\vec{p})=\frac{1}{(2\pi\hbar)^N}W^{(t,\phi,\vec{A},\vec{B})}_{(t,P_t,\vec{q},\vec{p})}(|\psi\rangle\langle\psi|)=\frac{1}{(2\pi\hbar)^N}\int \mathrm{d}\vec{a}\int \mathrm{d}\vec{b}\; C(\vec{a})C^*(\vec{b})\rho'_{\vec{a},\vec{b}}(t,P_t,\vec{q},\vec{p}). \tag{72}$$

It is related with the $(t,\phi,\vec{A},\vec{B})$ representation by

$$f'_W(t,P_t,\vec{q},\vec{p})=f_W(0,\phi(t,P_t,\vec{q},\vec{p}),\vec{A}(t,\vec{q},\vec{p}),\vec{B}(t,\vec{q},\vec{p})), \tag{73}$$

where f_W is given by Eqs. (64) and (65). We conclude that (1) The support of f'_W is confined to the classically allowed regions [check Eq. (71)] and (2) its evolution with respect to the physical time satisfies the Liouville equation

$$\frac{\partial f'_W}{\partial t}=\sum_{j=1}^{2}\frac{\partial f_W}{\partial A_j}\frac{\partial A_j}{\partial t}+\sum_{j=1}^{2}\frac{\partial f_W}{\partial B_j}\frac{\partial B_j}{\partial t}=\sum_{j=1}^{2}\frac{\partial f_W}{\partial A_j}\{H_0,A_j\}_{(\vec{q},\vec{p})}+\sum_{j=1}^{2}\frac{\partial f_W}{\partial B_j}\{H_0,B_j\}_{(\vec{q},\vec{p})}=\{H_0,f'_W\}_{(\vec{q},\vec{p})}. \tag{74}$$

Hence, in this representation the quantum behavior is displayed by the stargenfunction sector alone. However, for this system, we also have (let $z=q_1,p_1\vee p_2$ and $|z_0\rangle$ be a generic eigenket of $\hat{z}$ with associated eigenvalue z_0)

$$\begin{aligned}W^{(t,\phi,\vec{A},\vec{B})}_{(t,P_t,\vec{q},\vec{p})}(|z_0\rangle\langle z_0|)&=\Delta_{*'(t,P_t,\vec{q},\vec{p})}(z-z_0)=\Delta_{*(t,\phi,\vec{A},\vec{B})}(z(t,\vec{A},\vec{B})-z_0)|_{\vec{A}=\vec{A}(t,\vec{q},\vec{p})\wedge\vec{B}=\vec{B}(t,\vec{q},\vec{p})}\\&=\delta(z(t,\vec{A},\vec{B})-z_0)|_{\vec{A}=\vec{A}(t,\vec{q},\vec{p})\wedge\vec{B}=\vec{B}(t,\vec{q},\vec{p})}=\delta(z-z_0),\end{aligned} \tag{75}$$

where in the third step we used the fact that $e^{ik(z(t,\vec{A},\vec{B})-z_0)}_{*_{(t,\phi,A,B)}}=e^{ik(z(t,\vec{A},\vec{B})-z_0)}$ for $z=q_1,p_1\vee p_2$ [a simple result that follows from Eq. (61)]. Hence, the former three fundamental stargenfunctions display a

classical structure and satisfy $(\partial/\partial t)\Delta_{*'(t,P_t,q,p)}(z-z_0)=0$. We conclude that for this system, in this representation, the nontrivial (quantum) behavior is displayed by the stargenfunction $z=q_2$ alone.

VI. CONCLUSIONS

We addressed the deformation quantization of the nonrelativistic particle in the generally parametrized form and provided the complete specification of its physical quantum states in three different phase space representations. We proved that in one of these representations the distributional sector of the system displays a classical causal structure. This result confirms a similar conclusion that has been recently obtained for a generic nonrelativistic deparametrized system and reinforces the point of view that the De Broglie-Bohm formulation is not the unique possible causal formulation of quantum mechanics. In the De Broglie-Bohm theory[45–47] the source of quantum behavior is the quantum potential determining a causal (although not fully classical) dynamics for the quasidistribution. Furthermore, the theory also displays a nontrivial quantum correction to the momentum stargenfunction. On the other hand, in the "causal covariant formulation" presented here the quantum effects have been completely removed from the distributional sector (which now displays a fully classical causal structure) and the price to pay was the appearance of some further (quantum) corrections on the observable's sector of the theory.

We finish by recalling the point of view according to which the relation between the classical statistical and the quantum mechanical formulations of generally covariant systems should be further explored as it may provide key physical insights into some of the conceptual problems displayed by the quantum version of these systems. From this perspective the deformation methods seem to be especially suited. We proved that (at least for the simplest case of the parametrized nonrelativistic particle) the formal similarities between classical statistical and phase space quantum mechanics carry on intact to the generally covariant context. This close analogy is obviously superior to the one displayed by the standard operator formulation, and supports the point of view that the deformation methods should be further explored as an alternative, conceptually simpler approach to the quantization of generally covariant systems.

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Quantum phase space for the one-dimensional hydrogen atom on the hyperbola

George S. Pogosyan
Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, 141980, Moscow Region, Russia and Departamento de Matemáticas, CUCEI, Universidad de Guadalajara, Av. Corregidora 500, Guadalajara, Jalisco, México

Luis Edgar Vicent[a)]
Facultad de Ciencias, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Cuernavaca, Morelos 62251, México

Kurt Bernardo Wolf[b)]
Centro de Ciencias Físicas, Universidad Nacional Autónoma de México, Apartado Postal 48-3, Cuernavaca, Morelos 62251, México

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We obtain the solution of the one-dimensional hydrogen atom on the hyperbola by transforming its Schrödinger equation into the modified Pöschl-Teller equation. We write explicitly the wave functions both in configuration and momentum space, and check the contraction limit of the system to the flat space model. Finally, we find the closed form of the Wigner function for the states of this system. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1945767]

I. INTRODUCTION

One-dimensional hydrogen atom is customarily called the quantum system described by the Hamiltonian

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{1}{|x|} \tag{1}$$

(using units so that $e=m=\hbar=1$), and the point $x=0$ is *excluded* from the range of the operator. This is the so-called regularization, at the limit $\alpha \to 0$, of the Coulomb-type potentials

$$V(x,\alpha) = -\frac{1}{|x|+\alpha}, \quad \alpha > 0. \tag{2}$$

At first sight it may seem that a system with the Hamiltonian (1) is physically unremarkable and technically easy to solve. But this is not true. The one-dimensional hydrogen atom models a real hydrogen atom present in an extremely strong magnetic field, for instance in astrophysics, where the field of a pulsar is $B \approx 10^{12}$. In such situations, the atomic sizes perpendicular to the field are much smaller than the longitudial sizes.[1,2] In contrast to the real three-dimensional hydrogen atom, the one-dimensional system (1) demands more delicacy in the mathematical methods needed to understand the spectrum and complete eigenfunction set of the corresponding Schrödinger equation.[3]

The one-dimensional hydrogen atom was first investigated in 1959 by Loudon.[4] He proved that the spectrum of the one-dimensional hydrogen atom contains a ground state $E_0=-\infty$ and an infinite number of doubly degenerate excited states, even and odd solutions, defined over the

[a)]Electronic mail: vicent@fis.unam.mx
[b)]Electronic mail: bwolf@fis.unam.mx

whole x axis. This degeneracy is very strange since it contradicts one of the basic principles of (one-dimensional) quantum mechanics.[1] In Ref. 5, Andrews explained the double degeneracy observing that the strong singularity at $x=0$ absolutely isolates the two regions of the system, $x<0$ and $x>0$. The "Andrews mechanism" states that the probability for the particle in the left side to penetrate the right side or *vice versa* is zero. (See Refs. 6 and 7 where this *space-spliting effect* is studied further.) For all finite values of the energy Loudon found two independent solutions; the degeneracy of the eigenvalues has been explained in terms of hidden symmetry group $O(2)$,[6,8,9] and even in terms supersymmetry.[10–12] These papers contain three noncontradicting models to explain the same phenomenon. Indeed, during the last three decades this model has been the subject of intensive discussion and study, but there is still controversy in the interpretation of some of its features (see the literature contained in Ref. 13).

Analogs of the hydrogen atom on the spaces with constant positive or negative curvature were introduced by Schrödinger[14] and Infeld[15] in three and more dimensions. In this article we analyze the one-dimensional hydrogen atom analog on the upper branch of a hyperbola of pseudoradius R, defined by

$$\mathcal{H}^1 := \{s_1, s_2 \in \Re | s_2^2 - s_1^2 = R^2 > 0, s_2 \geqslant R\}, \tag{3}$$

where $\boldsymbol{s}=(s_2, s_1)$ are Cartesian coordinates in the ambient pseudo-Euclidean space. We have seen in a recent work[16] that spaces of constant curvature $1/R$ provide parametrized families of models which properly contract to the previously known ones as $R \to \infty$. The one-dimensional hydrogen atom on the sphere was recently analyzed for the circle $\mathcal{S}^1$ in the work of Mardoyan *et al.*[17] The hyperbolic case is studied here; it is connected by a transformation of coordinates to the Pöschl-Teller potential;[18] it participates thus in the representation theory of the three-dimensional Lorentz group (Ref. 19, Sec. 6.5); and has served as a model for scattering phenomena in systems with mixed (discrete and continuous) spectra.[20] Finally, it is an exactly solvable problem, so its eigenfunctions are expected (and confirmed) to be expressible in terms of special functions, particularly Gauss hypergeometrics ${}_2F_1$.

Physical interest leads us to extend the analysis of this one-dimensional system to phase space by means of the Wigner distribution function.[21] The phase space model that contains a hyperbolic position subspace was introduced in Ref. 16 for $N \geqslant 1$ dimensions. (See also Ref. 22 where phase space and the Wigner distribution are defined for N-sphere position spaces.) It is constructed from a complete set of solutions of the Schrödinger equations in configuration and momentum spaces. And it turns out that also the Wigner function can be expressed in terms of hypergeometric and other elementary special functions.

The Coulomb potential of the one-dimensional hydrogen atom on the hyperbola $\mathcal{H}^1$ in (3) is

$$V(\boldsymbol{s}) = -\frac{\kappa}{R}\frac{s_2}{|s_1|} \leqslant \frac{\kappa}{R}, \tag{4}$$

where κ is the coupling constant. This system belongs to the well-known class with superintegrable potentials on constant curvature spaces,[23,24] which is here restricted to one spatial dimension.

The organization of this paper is as follow: In sec. II we detail the method used to find the wave functions of this system in configuration space, and the corresponding wave functions in momentum space are obtained in Sec. III; in Sec. IV we verify the flat-space contraction limit. Section V is devoted to the calculation of the Wigner functions of the eigenstates of this system.

II. SOLUTIONS ON THE HYPERBOLA

Following Ref. 25, we shall use the map from the space $s=\{(s_1, s_2) \in \Re^2\}$ to the space $u=\{(u_1, u_2) \in \Re^2\}$ given by

$$s_1 = (\text{sign } u_1)\sqrt{u_2^2 - u_1^2}\frac{u_1^2}{2u_2}, \quad s_2 = \sqrt{u_2^2 - u_1^2}\left(u_2 - \frac{u_1^2}{2u_2}\right), \tag{5}$$

which satisfies

$$s_2^2 - s_1^2 = (u_2^2 - u_1^2)^2. \tag{6}$$

The relation between the distance elements in s- and u-spaces through the map (5) is

$$\mathrm{d}\boldsymbol{s} \,.\, \mathrm{d}\boldsymbol{s} = (u_2^2 - u_1^2)\left[\frac{(\boldsymbol{u}\cdot\mathrm{d}\boldsymbol{u})^2}{u_2^2} - \frac{u_1^2}{u_2^2}\mathrm{d}\boldsymbol{u}\cdot\boldsymbol{u}\right] + 3(\boldsymbol{u}\cdot\mathrm{d}\boldsymbol{u})^2. \tag{7}$$

From (6) we see that when the point $\boldsymbol{s}=(s_1,s_2)$ lies on the upper branch of the hyperbola of pseudoradius R, then $\boldsymbol{u}=(u_1,u_2)$ belongs to the upper branch of another hyperbola in u-space: $u_2^2-u_1^2=D^2$, with the pseudoradius $D=\sqrt{R}$. Thus in particular (5) corresponds to a transformation between the one-dimensional s- and u-hyperbolic spaces $\mathcal{H}^1$. From (7), for the points on the hyperbolas, the line elements are then related through

$$\frac{\mathrm{d}\boldsymbol{s}\cdot\mathrm{d}\boldsymbol{s}}{R} = -\frac{u_1^2}{u_2^2}\mathrm{d}\boldsymbol{u}\cdot\mathrm{d}\boldsymbol{u}. \tag{8}$$

This mapping is conformal, i.e., it conserves angles between lines.

Choosing the ordinary hyperbolic coordinates on s-space, their transformation (5) to u-space is

$$s_1 = R\sinh\tau, \quad s_2 = R\cosh\tau, \tag{9}$$

$$u_1 = \pm D\sqrt{e^{2\tau}-1}, \quad u_2 = De^{\tau}, \quad 0 \leqslant \tau < \infty. \tag{10}$$

This transformation is one-to-one between the points of the two $\mathcal{H}^1$ spaces, and a trivial case of the series of Hurwitz-type quadratic transformations between oscillator systems in two, four, and eight dimensions, and Coulomb systems in two, three, and five dimensions, respectively.[25,26] The line elements in the s- and u-hyperbolas are then

$$\mathrm{d}s = R\,\mathrm{d}\tau, \quad \mathrm{d}u = \frac{De^{\tau}}{\sqrt{e^{2\tau}-1}}\mathrm{d}\tau, \tag{11}$$

and so they are related by

$$\frac{\mathrm{d}s}{R} = \mathrm{d}\tau = \frac{u_1}{u_2}\frac{\mathrm{d}u}{D}. \tag{12}$$

Taking into account that $R=D^2$, the relation between the inner products defining the Hilbert space on the s- and u-hyperbolas is

$$(\Psi_1,\Psi_2)_{\mathcal{H}^1} \coloneqq \int_{\mathcal{H}^1}\mathrm{d}s\Psi_1^*(s)\Psi_2^*(s) = D\int_{\mathcal{H}^1}\frac{u_1}{u_2}\mathrm{d}u\Psi_1^*(s(u))\Psi_2^*(s(u)) =: (\Phi_1,\Phi_2)_{\mathcal{H}^1}, \tag{13}$$

for the renormalized functions

$$\Phi(u) \coloneqq \sqrt{D|u_2/u_1|}\Psi(s(u)). \tag{14}$$

In order to compare the dynamics in the two hyperbolic spaces, we write the one-dimensional Laplace-Beltrami operators on the s-hyperbola in the coordinates (9),

$$\Delta_{\mathrm{LB}}^{(s)} = \frac{1}{R^2}\left(s_1\frac{\partial}{\partial s_2} + s_2\frac{\partial}{\partial s_1}\right)^2 = \frac{1}{R^2}\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}, \tag{15}$$

while on the u-hyperbola this operator is

$$\Delta_{\mathrm{LB}}^{(u)} = \frac{1}{D^2}\left(u_1\frac{\partial}{\partial u_2} + u_2\frac{\partial}{\partial u_1}\right)^2 = \frac{2}{D^2}\sqrt{\sinh\,\tau}e^{-\pi/2}\frac{\mathrm{d}}{\mathrm{d}\tau}\sqrt{\sinh\,\tau}e^{-\pi/2}\frac{\mathrm{d}}{\mathrm{d}\tau}. \tag{16}$$

With the identification (14) we find that the operators $\Delta_{\mathrm{LB}}^{(s)}$ and $\Delta_{\mathrm{LB}}^{(u)}$ are related by

$$\Delta_{\mathrm{LB}}^{(s)} = \left(\left|\frac{u_1}{u_2}\right|\right)^{1/2}\left\{\frac{u_2^2}{u_1^2}\frac{1}{D^2}\left[\Delta_{\mathrm{LB}}^{(u)} - \frac{3/4}{u_1^2} + \frac{1/4}{u_2^2}\right]\right\}\left(\left|\frac{u_1}{u_2}\right|\right)^{-1/2}. \tag{17}$$

The Schrödinger equation describing the nonrelativistic motion on the one-dimensional hyperbolic space $\mathcal{H}^1$ under the potential (4), written in terms of the Laplace-Beltrami operator $\Delta_{\mathrm{LB}}^{(s)}$, has the form

$$-\frac{1}{2}\Delta_{\mathrm{LB}}^{(s)}\Psi(\boldsymbol{s}) - \frac{\kappa}{R}\left(\frac{s_2}{|s_1|} - 1\right)\Psi(\boldsymbol{s}) = E\Psi(\boldsymbol{s}), \tag{18}$$

where E is the total energy of the system, and we have added the constant κ/R to the Coulomb potential in order to have bound states with negative energy. The transformation (5) and the substitutions (14) and (17) convert the Schrödinger equation (18) of the one-dimensional hydrogen atom into that of the singular oscillator whose parameters depend on the pseudoradius $R=D^2$ and the energy E,

$$-\frac{1}{2}\Delta_{\mathrm{LB}}^{(u)}\Phi(\boldsymbol{u}) + \left(\frac{\kappa_1^2 - \frac{1}{4}}{u_2^2} - \frac{\kappa_2^2 - \frac{1}{4}}{u_1^2}\right)\Phi(\boldsymbol{u}) = \lambda^2\Phi(\boldsymbol{u}), \tag{19}$$

$$\lambda^2 = -R(RE + \kappa), \quad k_1^2 = -2R(RE - \kappa), \quad k_2^2 = 1. \tag{20}$$

As in the case of the flat space where the corresponding transformation establishes the connection between the one-dimensional Coulomb system and an oscillator system with a centrifugal barrier,[6] in the case of the hyperbola (5) with the coordinates (9) and (10), the change of variables

$$e^{\tau} = \cosh\,\alpha, \tag{21}$$

transforms Eq. (19) into the *modified Pöschl-Teller* equation,

$$-\frac{1}{2}\frac{d^2\Phi}{d\alpha^2} + \left(-\frac{\kappa_1^2 - \frac{1}{4}}{\cosh^2\,\alpha} + \frac{\kappa_2^2 - \frac{1}{4}}{\sinh^2\,\alpha}\right)\Phi = \lambda^2\Phi, \tag{22}$$

where $u_1>0$ and $u_1<0$ correspond to $\alpha>0$ and $\alpha<0$ respectively. In Fig. 1 we show the one-dimensional hydrogen atom potential with five bound states shown as energy levels [see $E_n^{R,\kappa}$ in Eq. (30) ahead], and the Pöschl-Teller potentials that correspond to them through the parameters in Eq. (20). We remark this *duality* where for each energy level of the hydrogen atom one has a different Pöschl-Teller potential, whose coupling constant k_1 is thus quantized. These Schrödinger equations exhibit singularities in the potentials $\sim u_1^{-2} = 1/R\,\sinh^2\,\tau$ which disconnect the $u_1<0$ and $u_1>0$ halves of the plane (u_1, u_2).[5–7] In the two half-planes there are two potential wells which are mirror images of each other and separated by an impenetrable barrier, as shown in the figure. Correspondingly, the singularity of the potential (4) at $s_1=0$ splits the physical s-space in such a way that the particle on the upper branch of the hyperbola can be located either on the left-hand side $s_1<0$, or on the right-hand side $s_1>0$. Correspondingly, the motion in u-space takes place in only one of the two wells, so we must consider separately the Schrödinger equation (19) in each of these two regions, that we indicate by right (R) and left (L), as

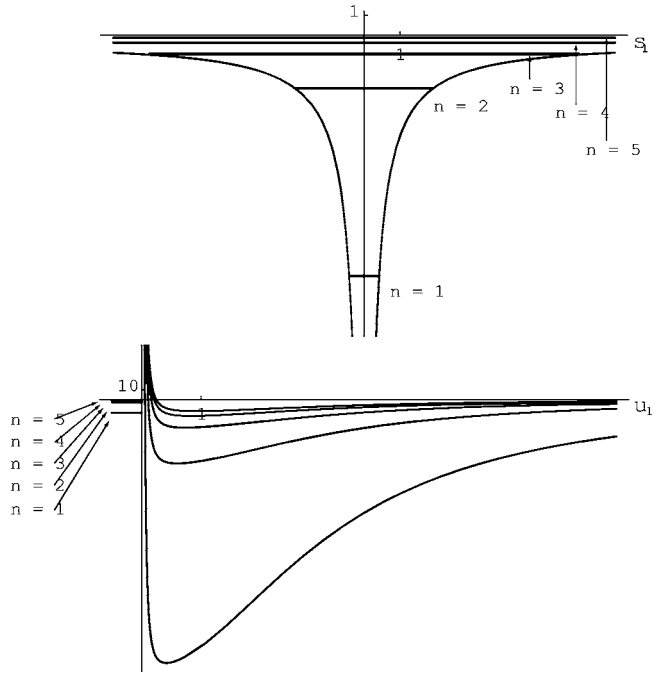

FIG. 1. Top: Panel The one-dimensional hydrogen atom potential (4) for $R=10$ and $\kappa=5$, showing all the energy levels, $n=1$, 2, 3, 4, and 5. The *physical* coordinate s_1 is related to the ensuing variable τ through $s_1=R\sinh\tau$. Bottom panel: The Pöschl-Teller potentials corresponding to the energy levels of the top figure (for $n=1$, 2, 3, 4, 5, $R=10$ and $\kappa=5$). The deeper potentials correspond to lower n's. The energy levels of the corresponding eigenstates are shown by horizontal lines to the left of the vertical axis. The coordinate u_1 is related to the variable τ by $u_1(\tau)=\sqrt{R(e^{2\tau}-1)}$.

$$\Phi^{\mathrm{R}}(u_1,u_2)=\Theta(u_1)f(u_1,u_2),\quad \Phi^{\mathrm{L}}(u_1,u_2)=\Theta(-u_1)g(u_1,u_2), \tag{23}$$

where $g(u_1,u_2)=f(-u_1,u_2)$ and $\Theta(x)=0,\frac{1}{2}$ and 1, for $x<0,x=0$ and $x>0$, respectively, is the Heaviside Θ-function.

The solutions of the Pöschl-Teller equation (22) are a well-known set of functions, one of whose outstanding properties is to serve as coupling (Clebsch-Gordan or Wigner) coefficients for the three-dimensional Lorentz group in the parabolic subgroup reduction,[19] between its discrete and continuous representation series. The coefficients k_1,k_2 in (22) are the Bargmann indices of the Lorentz group, which are determined by the two representations being coupled, and the energy eigenvalues determine the coupled representation, which can belong to the discrete or to the continuous series. In the present case $k_1>k_2+1$, the full spectrum of the one-dimensional hydrogen atom corresponds to the coupling of a discrete lower-bound and a discrete upper-bound representations: $D^+_{k_1}\otimes D^-_{k_2}=\Sigma_{k=0}^{K}D^+_k\oplus\int_0^\infty \mathrm{d}\kappa C_q$. The Clebsch-Gordan series yields here a finite number $K=\lfloor\frac{1}{2}(k_1-k_2-1)\rfloor$ of discrete representations ($\lfloor x\rfloor$ denotes the integer part of x), and a generalized integral over the continuous series representations $q=k(1-k),k=-\frac{1}{2}+ir$ and $r\in\Re$.

For $\alpha>0$, the wave functions that solve (22) are[19,23,24]

$$\Phi_n(\alpha)=A_n(\sinh\alpha)^{1/2+k_2}(\cosh\alpha)^{2n-k_1+1/2}\times {}_2F_1(-n,-n+k_1;1+k_2;\tanh^2\alpha), \tag{24}$$

$$A_n=\sqrt{\frac{2k_1(k_1-2n-k_2-1)\Gamma(k_1-n)\Gamma(n+1+k_2)}{D^2(2n+1+k_2)n\,!\,[\Gamma(1+k_2)]^2\Gamma(k_1-n-k_2)}}. \tag{25}$$

For these bound states, the eigenvalues λ are quantized as

$$\lambda = k_2 - k_1 + 2n + 1 > 0, \quad n = 0,1,\ldots,\left\lfloor \tfrac{1}{2}(k_1 - k_2 - 1)\right\rfloor, \tag{26}$$

and so bound state solutions exist only for $k_1 - k_2 > 1$. The normalization constant A_n in (25) is computed from the requirement of square integrability of the wave functions for $\alpha > 0$ under the inner product (13). We are reminded by (23) that there are right and left solutions for $\alpha \in \Re$, namely

$$\Phi^R(\alpha) = \Theta(\alpha)\Phi_n(|\alpha|), \quad \Phi^L(\alpha) = \Theta(-\alpha)\Phi_n(|\alpha|). \tag{27}$$

So, after replacement of $d\tau = \tanh\alpha\, d\alpha$ and $u_1/u_2 = \tanh\alpha$, the normalization condition can be expressed as

$$R\int_0^\infty d\tau |\Psi_n^R(\tau)|^2 = D\int_0^\infty d\alpha |\Psi_n^R(\alpha)|^2 \tanh^2\alpha = 1. \tag{28}$$

Finally, we note that the wave functions (24) can be written in terms of Jacobi polynomials of degree n, indices (k_2, k_1), and argument $\cosh 2\alpha$, including other factors of powers $\frac{1}{2} - k_1$ and $\frac{1}{2} + k_2$ of $\cosh\alpha$ and $\sinh\alpha$, respectively.[19]

Now we are ready to construct the eigenfunctions and energy eigenvalues of the one-dimensional hydrogen atom. Comparing (20) and (26), and replacing $n \mapsto n-1$, we find that for

$$k_1 = n + \rho_n, \quad \rho_n := \kappa R/n = \rho/n, \tag{29}$$

with $\rho := \kappa R$, the energy spectrum is

$$E_n^{R,\kappa} = -\frac{n^2}{2R^2} - \frac{\kappa^2}{2n^2} + \frac{\kappa}{R}, \quad n = 1,2,\ldots,\lfloor\sqrt{\rho}\rfloor. \tag{30}$$

Returning to the variable $\tau = \ln\cosh\alpha$ of (21), we express the bound state wave functions $\Psi^{\mathrm{R}}_{n\rho_n}(\tau)$ which describe the particle in the right ($\tau > 0$) and left ($\tau < 0$) regions, in the form

$$\Psi^{\mathrm{R,L}}_{n\rho_n}(\tau) = \Theta(\pm\tau)\sqrt{\frac{\rho_n(\rho_n^2 - n^2)}{R}}\, 2\sinh|\tau| e^{(n-1-\rho_n)|\tau|}\, {}_2F_1\left(-n+1, 1+\rho_n; 2; 1-e^{-2|\tau|}\right), \tag{31}$$

$$= \Theta(\pm\tau)\frac{2^n}{n}\sqrt{\frac{\rho_n(\rho_n^2 - n^2)}{R}}(\sinh|\tau|)^n e^{-\rho_n|\tau|} P_{n-1}^{(-n-\rho_n, -n+\rho_n)}\left(-\coth|\tau|\right), \tag{32}$$

where $P_{n-1}^{(\alpha,\beta)}(x)$ is a Jacobi polynomial and we have added ρ_n as an explicit parameter in the functions. Thus we find that all excited bound states ($n \geqslant 1$) of the one-dimensional hydrogen atom are doubly degenerate—as in the model on flat space. To find the ground state of this $\mathcal{H}^1$-system one must solve the Schrödinger equation for an "inoculating" potential,[4] but this boundary case lies outside our present scope. In Fig. 2 we show on configuration space the five bound wave functions of the system in the previous figure.

III. SOLUTIONS IN MOMENTUM SPACE

From the wave functions on the τ-space for the R- and L-regions, we introduce the two wave functions on momentum space $p \in \Re$, $\tilde{\Psi}^{\mathrm{R}}_{n,\rho_n}(p)$ and $\tilde{\Psi}^{L}_{n,\rho_n}(p)$ [see (23)] by means of the Fourier integral transform

$$\tilde{\Psi}^{\mathrm{R,L}}_{n,\rho_n}(p) = \sqrt{\frac{R}{2\pi}}\int_{-\infty}^{+\infty} d\tau\, e^{-ipR\tau}\Psi^{\mathrm{R,L}}_{n,\rho_n}(\tau). \tag{33}$$

For the positive-τ region, replacing the explicit form (31) of the wave function $\tilde{\Psi}^{\mathrm{R}}_{n,\rho n}(\tau)$ into Eq. (33), we obtain

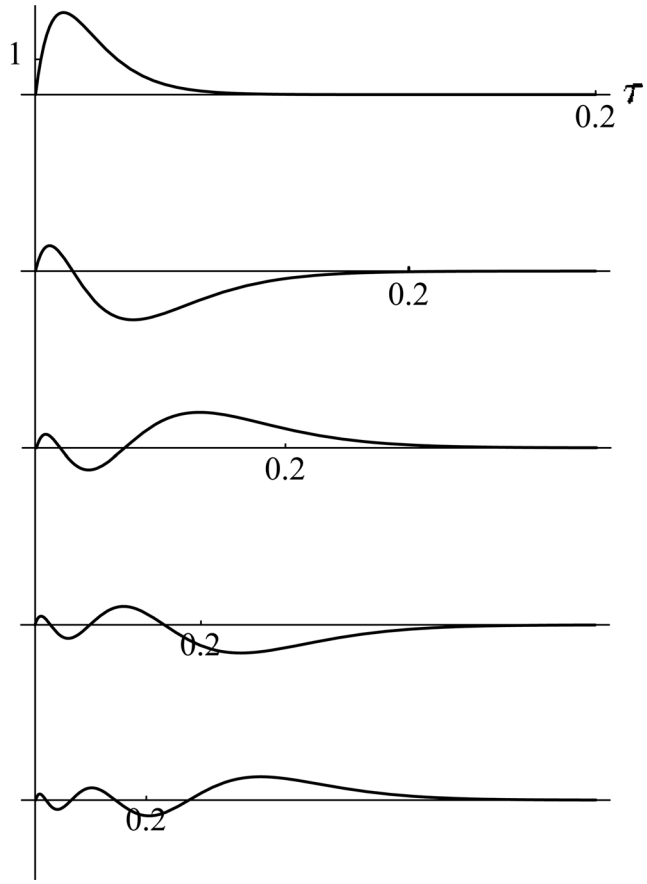

FIG. 2. Wave functions of the one-dimensional hydrogen atom on the right half of hyperbolic configuration space, for the levels $n=1$, 2, 3, 4, and 5 (from top to bottom). The horizontal axis is the variable $\tau>0$ (related to the physical coordinate through $s_1=R\sinh\tau$); for visibility, it has been rescaled by a factor of 3/2 between successive levels. The plots were generated from Eq. (31).

$$\tilde{\Psi}^{\mathrm{R}}_{n,\rho n}(p)=\sqrt{\frac{2\rho n(\rho_n^2-n^2)}{\pi}}\int_0^\infty \mathrm{d}\tau\sinh\tau e^{(n-1-\rho n-ipR)\tau}\times {}_2F_1(-n+1,1+\rho n;2;1-e^{-2\tau}), \tag{34}$$

$$=\sqrt{\frac{\rho_n(\rho_n^2-n^2)}{8\pi}}\frac{\Gamma\left(\frac{1}{2}[\rho_n-n+ipR]\right)}{\Gamma\left(\frac{1}{2}[\rho_n-n+ipR]+2\right)}$$
$$\times {}_2F_1\left(-n+1,1+\rho_n;\tfrac{1}{2}(\rho_n-n+ipR)+2;1\right), \tag{35}$$

where we have used the formula [Ref. 27, Eq. (10) on p. 110]

$$\int_0^\infty \mathrm{d}t\, e^{-\alpha t}(\sinh t)^\gamma=\frac{\Gamma\left(\frac{1}{2}[\alpha-\gamma]\right)\Gamma(\gamma+1)}{2^{\gamma+1}\Gamma\left(\frac{1}{2}[\alpha+\gamma]+1\right)}. \tag{36}$$

Finally, with the help of the Gauss identity for the ${}_2F_1(a,b;c;1)$ and using

$$\frac{\Gamma(z)}{\Gamma(z-n)}=(-1)^n\frac{\Gamma(1+n-z)}{\Gamma(1-z)}, \tag{37}$$

the result (35) can be written in the form

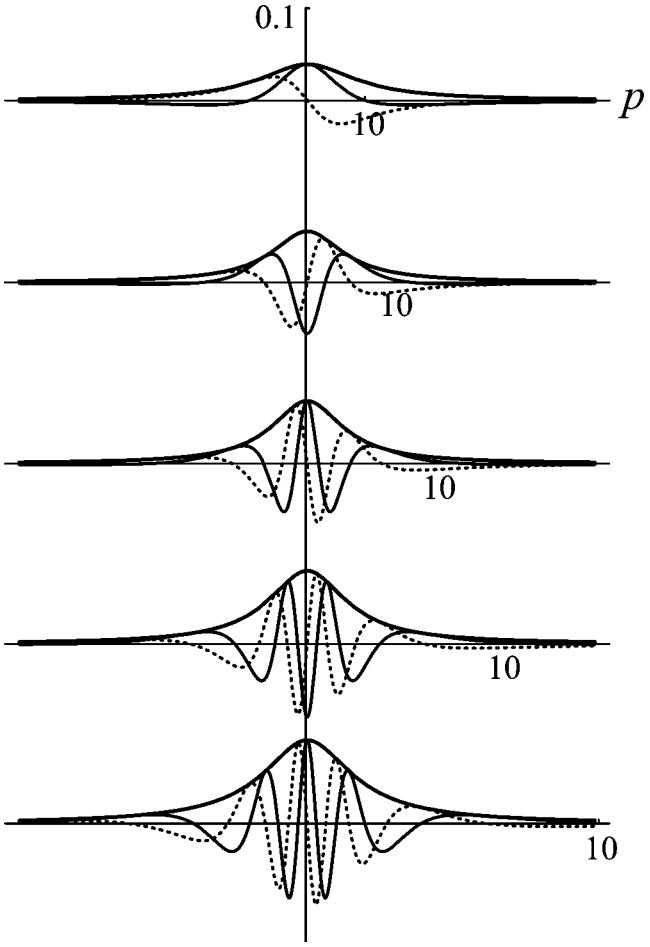

FIG. 3. Wave functions in momentum space of the one-dimensional hydrogen atom on the hyperbola, for $n=1$, 2, 3, 4, and 5 (from top to bottom, corresponding to those on configuration space in the previous figure). Real and imaginary parts of the function are indicated by thin continuous and dashed lines; the modulus by thick continuous lines. For visibility, the axes have been rescaled by 2/3 between successive levels—the proportion inverse to that of the previous figure. The plots were generated from Eq. (38).

$$\tilde{\Psi}^{\mathrm{R,L}}_{n,\rho_n}(p)=[\tilde{\Psi}^{\mathrm{L,R}}_{n,\rho_n}(p)]^*=\frac{(-1)^{n+1}}{4}\sqrt{\frac{\rho_n(\rho_n^2-n^2)}{2\pi}}\frac{\Gamma\left(\frac{1}{2}[\rho_n-n\pm ipR]\right)}{\Gamma\left(\frac{1}{2}[\rho_n-n\mp ipR]+1\right)}\frac{\Gamma\left(\frac{1}{2}[\rho_n+n\mp ipR]\right)}{\Gamma\left(\frac{1}{2}[\rho_n+n\pm ipR]+1\right)}. \tag{38}$$

For the particular case $n=1$, the preceding expression simplifies to

$$\tilde{\Psi}^{\mathrm{R,L}}_{1,\rho}(p)=\sqrt{\frac{\rho(\rho^2-1)}{2\pi}}\frac{1}{(\rho-1\pm ipR)(\rho+1\pm ipR)}. \tag{39}$$

In Fig. 3 we show the wave functions of the hyperbolic hydrogen atom in momentum space, for the levels $n=1$, 2, 3, 4, and 5, of the previous figure.

IV. CONTRACTION TO FLAT SPACE

The contraction of the hyperbola $\mathcal{H}^1$ to flat space $\mathfrak{R}$ is obtained considering the limit $R\to\infty$. In this case, the energy spectrum (30) for finite n becomes the energy spectrum of the one-dimensional standard hydrogen atom:[4]

$$E_n^{\kappa} = \lim_{R\to\infty} E_n^{R,\kappa} = -\frac{\kappa^2}{2n^2}, \quad n = 1,2,\ldots . \tag{40}$$

The bound-state wave functions of the one-dimensional hydrogen atom on the hyperbola given by (31) in the limit $R\to\infty$ converge to the well-known Coulomb wave functions different from zero on of the region $x>0$ or $x<0$. Their contraction is

$$\lim_{R\to\infty} \Psi_{n,\rho_n}^{\mathrm{R,L}}\left(\frac{x}{R}\right) = \Theta(\pm x)\frac{2\kappa^{3/2}}{n^{3/2}}|x|e^{-\kappa|x|/n}{}_1F_1\left(-n+1;2;\frac{2\kappa|x|}{n}\right) \tag{41}$$

$$= \Theta(\pm x)\frac{2\kappa^{3/2}}{n^{5/2}}|x|e^{-\kappa|x|/n}L_{n-1}^1\left(\frac{2\kappa|x|}{n}\right), \tag{42}$$

where $L_n^{\alpha}(x)$ is a generalized Laguerre polynomials.[27]

The bound-state wave functions in momentum representation, in (38) will contract to functions on the circle (which is the Hopf sphere for the one-dimensional case). In order to compute the contraction limit $R\to\infty$ for these functions we use the Stirling asymptotic formula for the gamma functions to prove that

$$\begin{aligned}\lim_{R\to\infty} \sqrt{R}\tilde{\psi}_{n,\rho_n}^{\mathrm{R,L}}(p) &= \frac{(-1)^{n+1}}{\sqrt{2\pi}}\frac{p_n^{3/2}}{p_n^2+p^2}\left(\frac{p_n \mp ip}{p_n \pm ip}\right)^n \\ &= \frac{(-1)^{n+1}}{\sqrt{2\pi}}\frac{p_n^{3/2}}{p_n^2+p^2}\exp\left(\mp 2in\arctan\frac{p}{p_n}\right) = \frac{(-1)^{n+1}}{\sqrt{2\pi p_n}}(1+\cos\theta_n)e^{\mp in\theta_n},\end{aligned} \tag{43}$$

where $n=1, 2,\ldots$, and

$$p_n := \sqrt{-2E_n^{\kappa}} = \frac{\kappa}{n}, \quad \tan\frac{1}{2}\theta_n = \frac{p}{p_n} = \frac{n}{\kappa}p. \tag{44}$$

The limit in Eq. (43) coincides with the momentum wave functions found in Ref. 8.

V. WIGNER DISTRIBUTION FUNCTION

We now construct the Wigner distribution function for the states of the one-dimensional hydrogen atom in hyperbolic space. According to the definition of the Wigner function on momentum space,[16] we have

$$W(\Psi_{n,p_n}^{\mathrm{R,L}}|\tau,p) = \frac{R}{2\pi}\int_{-\infty}^{\infty} dp'\,\tilde{\Psi}_{n,p_n}^{\mathrm{L,R}}\left(p-\tfrac{1}{2}p'\right)^* e^{iRp'\tau}\tilde{\Psi}_{n,p_n}^{\mathrm{R,L}}\left(p+\tfrac{1}{2}p'\right) \tag{45}$$

$$= W(\Psi_{n,p_n}^{\mathrm{L,R}}|-\tau,p), \tag{46}$$

where the last equality follows from (38).

Let us first consider the particular case $n=1$. Using the explicit form of the wave function $\tilde{\Psi}_{1,\rho}^{\mathrm{R}}$ given in (39), we can write

$$W(\Psi_{1,\rho}^{\mathrm{R}}|\tau,p) = \frac{\rho(\rho^2-1)}{16i\pi^2}\int_{-i\infty}^{i\infty} dz\,\frac{e^{-4y\tau}}{\left|\left(\frac{1}{2}[\rho-1+ipR]-y\right)\left(\frac{1}{2}[\rho+1+ipR]-y\right)\right|^2}. \tag{47}$$

The integrand on (47) has four poles in the upper complex half-plane, at the points $y_{1,2}=\frac{1}{2}(\rho-1\pm ipR)$ and $y_{3,4}=\frac{1}{2}(\rho+1\pm ipR)$. After complex integration, using the residue theorem, we obtain

$$W(\Psi^{\mathrm{R}}_{1,\rho}|\tau,p)=\frac{\rho(\rho^2-1)}{2\pi(pR)}e^{-2\rho\tau}\mathrm{Im}\frac{\sinh 2\tau(1+ipR)}{1+ipR}. \tag{48}$$

The Wigner function for the left-side solutions $\Psi^{\mathrm{L}}_{1,\rho}$ is obtained, according to (46), reversing the sign of τ in the exponential factor in (48), to $e^{+2\rho\tau}$. Using the last expression, it is easy to check the marginal properties for this particular case, that is

$$\int_{-\infty}^{\infty}\mathrm{d}p\ W(\Psi^{\mathrm{R}}_{1,\rho}|\tau,p)=|\Psi^{\mathrm{R}}_{1,\rho}(\tau)|^2,\quad \int_0^{\infty}\mathrm{d}\tau\ W(\Psi^{\mathrm{R}}_{1,\rho}|\tau,p)=|\tilde{\Psi}^{\mathrm{R}}_{1,\rho}(p)|^2. \tag{49}$$

We can now tackle the computation of the Wigner function for the general-n bound wave functions $\Psi^{\mathrm{R,L}}_{n,\rho_n}(\tau)$, whose momentum representation $\tilde{\Psi}^{\mathrm{R,L}}_{n,\rho_n}(p)$ is given by (38). Replacing the explicit forms in (45) with $y:=-i\frac{1}{2}p'R$, we obtain

$$\begin{aligned}W(\Psi^{\mathrm{R}}_{n,\rho_n}|\tau,p)&=\frac{\rho_n(\rho_n^2-n^2)}{16i\pi^2}\int_{-i\infty}^{i\infty}\mathrm{d}y\left|\frac{\Gamma\left(\frac{1}{2}[\rho_n-1+ipR]-y\right)\Gamma\left(\frac{1}{2}[\rho_n-1+ipR]+n+y\right)}{\Gamma\left(\frac{1}{2}[\rho_n+1+ipR]+y\right)\Gamma\left(\frac{1}{2}[\rho_n+1+ipR]+n-y\right)}\right|^2 e^{-4y\tau}\\&=(-1)^{n+1}\frac{\rho_n(\rho_n^2-n^2)\Gamma(\rho_n)}{4\pi n!\,\Gamma(\rho_n-n+1)}e^{-2(\rho_n-n)\tau}\times\mathrm{Re}\left[\frac{\Gamma(-n+ipR)\Gamma(\rho_n+ipR)e^{-2i\pi pR}}{\Gamma(1+ipR)\Gamma(\rho_n-n+1+ipR)}\right.\\&\left.\times\,{}_4F_3\left(\begin{matrix}-n,-n+ipR,\rho_n,\rho_n+ipR\\1+ipR,\rho_n-n+1,\rho_n-n+1+ipR\end{matrix}\middle|e^{-4\tau}\right)\right].\end{aligned} \tag{50}$$

The Wigner functions for the left-side wave functions $\Psi^{\mathrm{L}}_{n,\rho_n}$ are obtained from (46) through changing the sign of τ in the three exponentials of the general result (50). In Fig. 4 we show the Wigner functions of the states in the previous two figures, for $n=1$, 2, 3, 4, and 5. We note in the figure that the number of zeros of the configuration-space function on $\tau>0$ axis can be seen from the Wigner plot in Fig. 4 by counting the changes of sign of the phase space function along the $\tau>0$ axis. The absolute square of the momentum wave functions are symmetric and bell-shaped, with their width increasing with n.

VI. CONCLUSIONS

We obtained the bound-state wave functions of the one-dimensional hydrogen atom on the hyperbola $\mathcal{H}^1$ by solving the Schrödinger equation in configuration space. As in the flat case, we have shown that their double degeneracy is explained by the Andrews mechanism of space-splitting. We have found that the two independent position wave functions in the regions $u_1>0$ and $u_1<0$ are expressible in terms of Gauss hypergeometric functions ${}_2F_1$ (or Jacobi polynomials) as expected. This is in contrast with the flat one-dimensional case where the wave functions are written in terms of the associated Laguerre polynomials $L^1_{n-1}(\gamma|x|)\,\gamma>0$, i.e., ${}_1F_1(-n+1;\gamma|x|)$ confluent hypergeometric functions [see Eq. (31) and Ref. 4]. The wave functions in momentum representation were obtained through the usual Fourier transform method, and it was surprising that these could be written in the closed form also, in terms of ordinary Gamma functions. And we verified that in the $R\to\infty$ contraction limit, the hyperbolic system becomes the well-known one on flat space.

The simple form of the momentum wave functions allowed us to construct the Wigner distribution function of this model in closed analytic form, and to check its correctness through the marginal projections. We note that the above-noted expressions for the Wigner functions in the hydrogen atom model are considerably simpler than those for the one-dimensional *oscillator* on $\mathcal{H}^1$, found in Ref. 16, which have the form of two sums over Gauss hypergeometrics. As expected, Fig. 4 shows that with increasing energy the states show larger spread of probability at greater distances. The pointed-triangle shapes of the main peak of the Wigner function and its regions of negativity follow the pattern of Wigner functions for bound states of other potentials having a mixed spectra.[28]

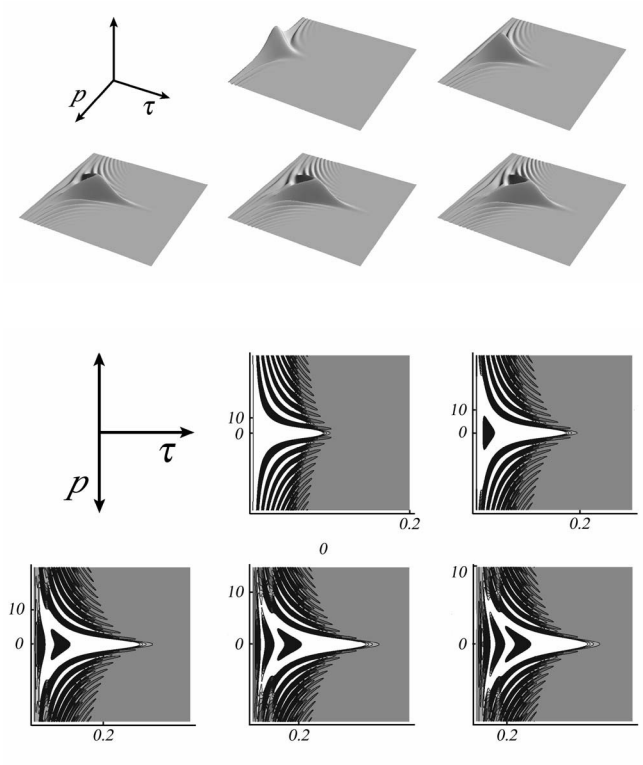

FIG. 4. Top panel: Wigner functions of the one-dimensional hydrogen atom states on phase space (τ,p), $\tau>0$, for the levels $n=1$, 2, 3, 4, and 5 of the previous two figures (left to right and top to bottom). Bottom panel: Contour plots on phase space of the previous Wigner functions, with emphasis on distinguishing their positive (white) and negative (black) regions. As in the previous two figures, the axes are rescaled by reciprocal factors to frame the oscillatory behavior of the functions.

We leave for future consideration important issues such as the hidden symmetry group and the supersymmetrization of the one-dimensional hydrogen atom on the hyperbola and on the circle.

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Non-Abelian conversion and quantization of nonscalar second-class constraints

I. Batalin and M. Grigoriev
Tamm Theory Department, Lebedev Physics Institute, Leninsky prospect 53, 119991 Moscow, Russia

S. Lyakhovich
Tomsk State University, prospect Lenina 36, 634050 Tomsk, Russia

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We propose a general method for the deformation quantization of any second-class constrained system on a symplectic manifold. The constraints determining an arbitrary constraint surface are in general defined only locally and can be components of a section of a nontrivial vector bundle over the phase-space manifold. The covariance of the construction with respect to the change of the constraint basis is provided by introducing a connection in the "constraint bundle," which becomes a key ingredient of the conversion procedure for the nonscalar constraints. Unlike in the case of scalar second-class constraints, no Abelian conversion is possible in general. Within the BRST framework, a systematic procedure is worked out for converting nonscalar second-class constraints into non-Abelian first-class ones. The BRST-extended system is quantized, yielding an explicitly covariant quantization of the original system. An important feature of second-class systems with nonscalar constraints is that the appropriately generalized Dirac bracket satisfies the Jacobi identity only on the constraint surface. At the quantum level, this results in a weakly associative star-product on the phase space. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1935430]

I. INTRODUCTION

The quantization problem is usually understood as that of constructing a quantum theory for a given classical system, at the same time preserving important properties of the system such as locality and global symmetries. This additional requirement is crucial. Indeed, formally one can always find a representation such that all the constraints are solved, gauge symmetries are just shift symmetries, and the Poisson bracket has the canonical form. But in doing so one usually destroys locality and global symmetries. It is the problem of the quantization of relativistic local field theories that initiated the development of sophisticated quantization methods applicable to systems with non-Abelian and open gauge algebras.[1–4]

From this point of view, the problem of quantizing curved phase space appears as a problem of constructing quantization in a way that is explicitly covariant with respect to the arbitrary change of phase-space coordinates. Given such a method (at the level of deformation quantization at least) one can always find quantization in each coordinate patch and then glue everything together. Similar to the curved phase-space quantization problem is the one of quantizing an arbitrary constraint surface. Any surface can be represented by independent equations (constraints) but in general only locally. In fact, one can always assume that the surface is the zero locus of a section of a vector bundle over the phase space. The quantization problem for arbitrary constrained systems can then be reformulated as the problem of constructing quantization that is explicitly covariant with respect to the basis of constraints. In this paper, we restrict ourselves to the case of second-class constraints and address the problem of constructing a quantization scheme that is explicitly covariant with respect to the change of phase-space coordinates and the constraint basis.

A general framework that allows us to quantize second-class constraints at the same footing as first-class ones is the well-known *conversion*—the procedure that converts the original second-class constraints into first-class ones by introducing extra variables known as conversion variables. At least locally in the phase space, any second-class constraints can be converted into Abelian ones, and therefore the Abelian conversion is sufficient for most applications. The situation changes drastically if one wants the quantization to be explicitly covariant with respect to the change of the constraint basis. Indeed, by changing the constraint basis one can always make the converted constraints non-Abelian. The additional price one has to pay for covariance is the appearance of a connection in the vector bundle associated with the constraints. This is reminiscent of the quantization of systems with curved phase space, where phase-space covariance requires introducing a symplectic connection on the phase space. In fact, this is more than a coincidence.

The coordinate and constraint basis covariance appear to be intimately related within the quantization methods developed in Refs. 5 and 6 (see also Refs. 7 and 8). Indeed, the key ingredient of these methods is the embedding of the system into the cotangent bundle over its phase space. In the natural coordinate system x^i, p_i, the embedding constraints $p_i=0$ are nonscalar.[7] In this example, the reparametrization covariance in the original phase space translates into the covariance with respect to the basis of constraints p_i. In Ref. 8, this approach was extended to general second-class constrained systems with constraints being scalar functions.

In this paper, we extend the method in Ref. 8 to the case where the second-class constraint surface is an arbitrary symplectic submanifold of the phase space, not necessarily defined by zero locus of the set of any independent scalar functions. Considering the quantization problem for the constrained systems whose classical dynamics evolves on the constraint surface, one has to take care of the geometry of the tubular neighborhood of the constrained submanifold. The geometry of the entire phase space is irrelevant for this problem. In its turn, any tubular neighborhood of the submanifold can be identified with the normal bundle over the submanifold. For coisotropic submanifolds (first-class constrained systems), the corresponding approach to quantization was considered in Ref. 9. It then follows that an arbitrary constrained submanifold can be considered a zero locus of a section of the appropriate vector bundle over the phase space. Moreover, in practical physical problems, the second-class constraints can appear from the outset as components of a section of some bundle over the original phase space rather than scalar functions. This leads naturally to the concept of constrained systems with nonscalar constraints.

By considering the original nonscalar constraints θ_α at the same footing with the constraints p_i determining the embedding into $T^*\mathcal{M}$, we achieve a globally defined description for general second-class systems. Using the appropriate non-Abelian conversion procedure and subsequent BRST quantization, we then arrive at the formulation of the quantum theory (at the level of deformation quantization) that is explicitly covariant under the reparametrizations of the original phase space and under the changing of the constraint basis. We note that the nonscalar first-class constraints were also considered in Ref. 10 in a different framework.

The conventional approach to second-class systems is based on the Dirac bracket—a Poisson bracket on the entire phase space, which is determined by constraints and for which the constraint surface is a symplectic leaf. This allows considering the Poisson algebra of observables as a Dirac bracket algebra of phase-space functions modulo those vanishing on the constrained submanifold. From this point of view, the quantization problem can be understood as that of quantizing a degenerate Poisson bracket. However, outside the constraint surface, the Dirac bracket is not invariant under the change of the constraint basis and therefore is not well defined in the case of nonscalar constraints. The Dirac bracket bivector can be invariantly continued from the constraint surface under certain natural conditions, although the price is that the Jacobi identity is in general satisfied only in the weak sense, i.e., on the constrained submanifold. In the non-Abelian conversion framework such a covariant generalization of the Dirac bracket is naturally determined by the Poisson bracket of observables of the converted system. We note that weak brackets were previously studied in various contexts in Refs. 11–14.

At the quantum level, the lack of Jacobi identity for the covariant Dirac bracket results in a

phase-space star product that is not associative in general. Within the non-Abelian conversion approach developed in the paper, this star product naturally originates from the quantum multiplication of BRST-invariant extensions of phase-space functions. In the BRST cohomology, we obtain an associative star product that is identified with the quantum deformation of the classical algebra of observables (functions on the constraint surface). In particular, the associativity of the phase-space star-product is violated only by the terms vanishing on the constraint surface.

The quantization method developed in this paper can be viewed as an extension of the Fedosov quantization scheme[15,6] to systems whose constrained submanifolds are defined by nonscalar constraints and whose phase spaces, as a result, carry a weak Poisson structure. We note that gauge systems with a weak Poisson structure can be alternatively quantized[14] using the Kontsevich formality theorem.

II. GEOMETRY OF CONSTRAINED SYSTEMS WITH LOCALLY DEFINED CONSTRAINTS

We consider a constrained system on a general symplectic manifold $(\omega, \mathcal{M})$. The constrained system is defined on $\mathcal{M}$ by specifying a submanifold $\Sigma \subset \mathcal{M}$ such that the restriction $\omega|_\Sigma$ of the symplectic form to the constraint surface has a constant rank. If Σ is coisotropic, the constrained system is called first class. A constrained system is called second class if the restriction $\omega|_\Sigma$ of the symplectic form is invertible on Σ.

Let us assume for a moment that Σ is determined by constraints $\theta_\alpha = 0$ that are globally defined functions on $\mathcal{M}$; then $\{\theta_\alpha, \theta_\beta\}|_\Sigma = 0$ ($\{\theta_\alpha, \theta_\beta\}|_\Sigma$ is invertible) iff the system is first (respectively, second) class. The converse is also true, but *only locally*: if a constrained system is first (respectively, second) class, then locally there exist independent functions θ_α determining the constraint surface Σ by $\theta_\alpha = 0$ and any such functions satisfy $\{\theta_\alpha, \theta_\beta\}|_\Sigma = 0$ (respectively, $\{\theta_\alpha, \theta_\beta\}|_\Sigma$ is invertible).

The dynamics of a constrained system on $\mathcal{M}$ is assumed evolving on the constraint surface $\Sigma \subset \mathcal{M}$. At the quantum level, a tubular neighborhood of Σ gets involved in describing dynamics. In its turn, it is a standard geometrical fact that any such neighborhood is diffeomorphic to a vector bundle over Σ. Indeed, in each neighborhood $U^{(i)}$ of a point of Σ one can pick a coordinate system $x^a_{(i)}$, $\theta^{(i)}_\alpha$ such that $\Sigma \cap U^{(i)}$ is singled out by $\theta^{(i)}_\alpha = 0$ and on the intersection of two such neighborhoods $U^{(i)}$ and $U^{(j)}$

$$x^a_{(i)} = X^a_{(ij)}(x_{(j)}), \quad \theta^{(i)}_\alpha = (\phi^{(ij)})^\beta_\alpha \theta^{(j)}_\beta \tag{2.1}$$

with some functions $X^a_{(ij)}(x)$ and $\phi^{(ij)}(x)$. Functions $(\phi^{ij})^\alpha_\beta$ can be identified with transition functions of a vector bundle $V^*(\Sigma)$ over Σ (we use the notation for a dual bundle to make notations convenient in what follows). Under the identification of an open neighborhood of Σ with the vector bundle $V^*(\Sigma)$, coordinates θ_α are identified with constraint functions on $\mathcal{M}$. In particular, Σ goes to the zero section of $V^*(\Sigma)$. Note that the constraints θ_α, being understood as functions on $\mathcal{M}$, are defined only locally. If there exist globally defined constraints then $V^*(\Sigma)$ is trivial.

It can be useful to pull back the vector bundle $V^*(\Sigma)$ to the vector bundle $V^*(\mathcal{M})$ over $\mathcal{M}$. Functions θ_α are then naturally identified with the components of a globally defined section θ of $V^*(\mathcal{M})$. At the same time Σ is nothing else than a submanifold of points where θ vanishes. These arguments motivate the following concept of a constrained system.

Definition 2.1: A constrained system with nonscalar constraints is a triple $(\mathcal{M}, V^*(\mathcal{M}), \theta)$ *where the* $\mathcal{M}$*-symplectic manifold with a symplectic form* ω*,* $V^*(\mathcal{M})$*-vector bundle over* $\mathcal{M}$*, and* θ *is a fixed section of* $V^*(\mathcal{M})$*. It is assumed that vanishing points of* θ *are regular and form a submanifold* $\Sigma \subset \mathcal{M}$ *(constraint surface) such that* $\omega|_\Sigma$ *has a constant rank.*

The definitions of first- and second-class constrained systems still stand because they are formulated entirely in the intrinsic terms of the constraint surface Σ, making use only of the rank of $\omega|_\Sigma$ irrespectively of the way of defining Σ.

Several comments are in order:

(i) Another possibility to consider an arbitrary constraint surface keeping at the same time constraints as globally defined functions is to use overcomplete sets of constraints (i.e., reducible constraints with different terminology). However, depending on a particular system this can be a complicated task. Moreover, even if the constraints are reducible it can also be useful to allow them to be nonscalar.

(ii) As we have seen, any submanifold $\Sigma \subset \mathcal{M}$ can be represented as a surface of regular vanishing points of a section of a vector bundle over $\mathcal{M}$. Note, however, that by taking arbitrary constraints $\theta^{(i)}_{\alpha}$ in each neighborhood $U^{(i)}$, one does not necessarily arrive at a vector bundle. Indeed, in the intersection $U^{(i)} \cap U^{(j)}$ one still has

$$\theta^{(i)}_{\alpha} = (\phi^{(ij)})^{\beta}_{\alpha}\theta^{(j)}_{\beta}. \tag{2.2}$$

But functions $(\phi^{(ij)})^{\beta}_{\alpha}$ are defined only up to terms of the form $(\chi^{(ij)})^{\beta\gamma}_{\alpha}\theta_{\gamma}$ with $(\chi^{(ij)})^{\beta\gamma}_{\alpha} = -(\chi^{(ij)})^{\gamma\beta}_{\alpha}$. As a consequence, functions $(\phi^{(ij)})^{\beta}_{\alpha}$ satisfy the cocycle condition also up to terms proportional to θ,

$$(\phi^{(ik)})^{\gamma}_{\alpha}(\phi^{(kj)})^{\beta}_{\gamma} = (\phi^{(ij)})^{\beta}_{\alpha} + \cdots . \tag{2.3}$$

This means that only appropriately chosen constraints can be identified with components of a section of a vector bundle over $\mathcal{M}$. What differential geometry tells us is that such a choice always exists.

III. CONNECTIONS AND SYMPLECTIC STRUCTURES ON VECTOR BUNDLES

In what follows we need some geometrical facts on the connections and symplectic structures on the appropriately extended cotangent bundle over a symplectic manifold. Now let $\mathcal{M}$ be a symplectic manifold and $\mathcal{W}(\mathcal{M}) \to \mathcal{M}$ be a symplectic vector bundle over $\mathcal{M}$. Also let e_A be a local frame [locally defined basic sections of $\mathcal{W}(\mathcal{M})$] and $\mathcal{D}$ be the symplectic form on the fibers of $\mathcal{W}(\mathcal{M})$. The components of $\mathcal{D}$ with respect to e_A are determined by $\mathcal{D}_{AB} = \mathcal{D}(e_A, e_B)$.

It is well known (see, e.g., Ref. 6) that any symplectic vector bundle admits a symplectic connection. Let Γ and $\boldsymbol{\nabla}$ denote a symplectic connection and the corresponding covariant differential in $\mathcal{W}(\mathcal{M})$. The compatibility condition reads as

$$\boldsymbol{\nabla}\mathcal{D} = 0, \quad \partial_i \mathcal{D}_{AB} - \Gamma^{C}_{iA}\mathcal{D}_{CB} - \Gamma^{C}_{iB}\mathcal{D}_{AC} = 0, \tag{3.1}$$

where the coefficients Γ^{C}_{iA} of Γ are determined as

$$\boldsymbol{\nabla} e_A = dx^i \, \Gamma^{C}_{iA} e_C. \tag{3.2}$$

It is useful to introduce the following connection 1-form:

$$\Gamma_{AB} = dx^i \, \Gamma_{AiB}, \quad \Gamma_{AiB} = \mathcal{D}_{AC}\Gamma^{C}_{iB}. \tag{3.3}$$

Then compatibility condition (3.1) is rewritten as

$$d\mathcal{D}_{AB} = \Gamma_{AB} - \Gamma_{BA}, \quad \partial_i \mathcal{D}_{AB} - \Gamma_{AiB} + \Gamma_{BiA} = 0. \tag{3.4}$$

As a consequence of the condition, one arrives at the following property of the connection 1-form Γ_{AB}:

$$d\Gamma_{AB} = d\Gamma_{BA}. \tag{3.5}$$

Consider the following direct sum of vector bundles:

$$\mathcal{E}_0 = \mathcal{W}(\mathcal{M}) \oplus T^*\mathcal{M}, \tag{3.6}$$

where $T^*\mathcal{M}$ denotes a cotangent bundle over $\mathcal{M}$. Let x^i, p_j and Y^A be standard local coordinates on $\mathcal{E}_0$ (x^i are local coordinates on $\mathcal{M}$, p_j are standard coordinates on the fibers of $T^*\mathcal{M}$, and Y^A are

coordinates on the fibers of $\mathcal{W}(\mathcal{M})$ corresponding to the local frame e_A). Assume in addition that $\mathcal{M}$ is equipped with a closed 2-form ω (not necessarily nondegenerate).

Considered as a manifold that $\mathcal{E}_0$ can be equipped with the following symplectic structure:

$$\omega^{\mathcal{E}_0} = \pi^* \omega + 2\, dp_i \wedge dx^i + \mathcal{D}_{AB} dY^A \wedge dY^B + d\Gamma_{AB}\, Y^A Y^B - 2\Gamma_{AB} \wedge dY^A\, Y^B, \tag{3.7}$$

where $\pi^*\omega$ is the 2-form ω on $\mathcal{M}$ pulled back by the bundle projection $\pi: \mathcal{E}_0 \to \mathcal{M}$. One can directly check that 2-form (3.7) is well defined. Indeed, it can be brought to the standard explicitly covariant form, similar to that of the supersymplectic manifolds[16]

$$\omega^{\mathcal{E}_0} = \pi^* \omega + 2\, dp_i \wedge dx^i + \mathcal{D}_{AB}\, \boldsymbol{\nabla} Y^A \wedge \boldsymbol{\nabla} Y^B + \mathcal{R}_{AB} Y^A Y^B. \tag{3.8}$$

Here, $\boldsymbol{\nabla} Y^A = dY^A + \Gamma^A_C Y^C$, and $\mathcal{R}_{AB} = \mathcal{R}_{ij;AB} dx^i \wedge dx^j$ denotes the curvature of Γ:

$$\begin{aligned} \mathcal{R}_{ij;AB} &= \mathcal{D}_{AC} \mathcal{R}^C_{ijB} = \mathcal{D}_{AC} (\partial_i \Gamma^C_{jB} - \partial_j \Gamma^C_{iB} + \Gamma^C_{iD} \Gamma^D_{jB} - \Gamma^C_{jD} \Gamma^D_{iB}) \\ &= \partial_i \Gamma_{AjB} - \partial_j \Gamma_{AiB} + \Gamma_{CiA} \mathcal{D}^{CD} \Gamma_{DjB} - \Gamma_{CjA} \mathcal{D}^{CD} \Gamma_{DiB}. \end{aligned} \tag{3.9}$$

The last equality follows from the nondegeneracy of $\mathcal{D}_{AB}$ and compatibility condition (3.4). Also, it is straightforward to show that the 2-form (3.7) is exact, besides the first term:

$$\omega^{\mathcal{E}} = \pi^* \omega + d[2p_i\, dx^i + Y^A \mathcal{D}_{AB}\, \boldsymbol{\nabla} Y^B]. \tag{3.10}$$

Analyzing the structure on the rhs of (3.10), one can see that an arbitrary (not necessarily symplectic) connection $\overset{0}{\Gamma}$ can be taken to construct the close 2-form on $\mathcal{E}$ in (3.10). It turns out that the resulting 2-form still has the structure (3.7), with Γ given by

$$\Gamma_{AB} = \frac{1}{2}(d\mathcal{D}_{AB} + \overset{0}{\Gamma}_{AB} + \overset{0}{\Gamma}_{BA}). \tag{3.11}$$

It is easy to see that connection Γ is by construction compatible with the sympletric structure $\mathcal{D}$ for any connection $\overset{0}{\Gamma}$. In addition, if $\overset{0}{\Gamma}$ was taken symplectic it would bring $\Gamma = \overset{0}{\Gamma}$.

The Poisson bracket on $\mathcal{E}_0$ corresponding to the symplectic form (3.7) is determined by the following basic relations:

$$\begin{gathered} \{p_i, x^j\}_{\mathcal{E}_0} = -\delta^j_i, \quad \{p_i, p_j\}_{\mathcal{E}_0} = \omega_{ij}(x) + \frac{1}{2}\mathcal{R}_{ij;AB}(x) Y^A Y^B, \\ \{Y^A, Y^B\}_{\mathcal{E}_0} = \mathcal{D}^{AB}(x), \quad \{p_i, Y^A\}_{\mathcal{E}_0} = \Gamma^A_{iB}(x) Y^B, \end{gathered} \tag{3.12}$$

with all the others vanishing: $\{x^i, Y^A\}_{\mathcal{E}_0} = \{x^i, x^j\}_{\mathcal{E}_0} = 0$.

IV. EMBEDDING AND CONVERSION AT THE CLASSICAL LEVEL

A. Embedding

Consider a second-class constrained system $(\mathcal{M}, V^*(\mathcal{M}), \theta)$ with locally defined constraints θ_α [i.e., θ_α are components of a section θ of $V^*(\mathcal{M})$ with respect to a local frame e^α]. Let $T^*_\omega \mathcal{M}$ be a cotangent bundle equipped with the modified symplectic structure $2\, dp_i \wedge dx^i + \pi_0^* \omega$, where ω is a symplectic form on $\mathcal{M}$ and $\pi_0: T^*_\omega \mathcal{M} \to \mathcal{M}$ is the canonical projection.

The embedding of $\mathcal{M}$ into $T^*_\omega \mathcal{M}$ as a zero section is a symplectic map, i.e., a restriction of symplectic form $2\, dp_i \wedge dx^i + \pi_0^* \omega$ to the submanifold $\mathcal{M}$ is ω. Moreover, constrained system $(\mathcal{M}, V^*(\mathcal{M}), \theta)$ is equivalent to the constrained system $(T^*_\omega \mathcal{M}, W^*(\mathcal{M}), \Theta)$, where $W^*(\mathcal{M})$ is a direct sum $W^*(\mathcal{M}) = T^*\mathcal{M} \oplus V^*(\mathcal{M})$ considered as a vector bundle over $T^*_\omega(\mathcal{M})$ and components of Θ with respect to the local frame dx^i, e^α are $-p_i, \theta_\alpha$ (in other words, locally, the constraints are

given by $-p_i=0$ and $\theta_\alpha=0$). Indeed, by solving constraints $-p_i=0$ one arrives at the starting point constrained system. At this stage the construction here repeats the one from Ref. 8, with the only difference being that constraints θ_α are now defined only locally.

B. Non-Abelian conversion

Given second-class constraints Θ_A, one can always find an appropriate extension of the phase space by introducing conversion variables Y^A whose Poisson bracket relations have the form $\{Y^A, Y^B\}=\mathcal{D}^{AB}$, with $\mathcal{D}^{AB}$ invertible. Then one can find converted constraints T_A in the extended phase space, satisfying

$$\{T_A, T_B\} = U_{AB}^C T_C, \quad T_A|_{Y=0} = \Theta_A. \tag{4.1}$$

The resulting first-class system with constraints T_A is equivalent to the original second-class one and is called converted system. For second-class constraints that are scalar functions on the phase space one can always assume the conversion to be Abelian, i.e. with vanishing functions U_{AB}^C (see Ref. 17 for a detailed discussion of the conversion and the existence theorem for the Abelian conversion).

For the nonscalar constraints one naturally wants to build converted constraints in the invariant way, i.e., independently of a particular choice of the constraint basis. As we will see momentarily this forces one to consider, in general, a non-Abelian conversion.

To see this, one first needs to introduce conversion variables in a geometrically covariant way. It is useful to take as conversion variables the coordinates on the fibers of the bundle $W(\mathcal{M})$ dual to the bundle $W^*(\mathcal{M})=T^*\mathcal{M}\oplus V^*(\mathcal{M})$ associated to constraints $\theta_\alpha, -p_i$. The phase space is then

$$\mathcal{E}_0 = T^*_\omega \mathcal{M} \oplus W(\mathcal{M}), \quad W(\mathcal{M}) = V(\mathcal{M}) \oplus T\mathcal{M}. \tag{4.2}$$

We introduce unified notation e_A and Y^A for the local frame and coordinates on the fibers of $W(\mathcal{M})$, respectively. In the adapted basis Y^A is split into Y^i and Y^α.

Given a connection $\overline{\Gamma}$ in $V(\mathcal{M})$, one can equip $W(\mathcal{M})$ with the following fiberwise symplectic structure:

$$\mathcal{D}_{ij} = \omega_{ij}, \quad \mathcal{D}_{i\alpha} = -\mathcal{D}_{\alpha i} = \overline{\nabla}_i \theta_\alpha = \partial_i \theta_\alpha - \overline{\Gamma}^\beta_{i\alpha}\theta_\beta, \quad \mathcal{D}_{\alpha\beta} = 0. \tag{4.3}$$

In what follows we also need the explicit form of its inverse $\mathcal{D}^{AC}$, $\mathcal{D}^{AC}\mathcal{D}_{CB}=\delta^A_B$

$$\begin{gathered} \mathcal{D}^{\alpha\beta} = \Delta^{\alpha\beta}, \quad \mathcal{D}^{i\beta} = -\omega^{il}\mathcal{D}_{l\gamma}\Delta^{\gamma\beta}, \\ \mathcal{D}^{ij} = \omega^{ij} - \omega^{ik}\mathcal{D}_{k\alpha}\Delta^{\alpha\beta}\mathcal{D}_{l\beta}\omega^{lj}, \end{gathered} \tag{4.4}$$

where we introduced $\Delta^{\alpha\beta}$ as follows:

$$\Delta^{\alpha\gamma}\Delta_{\gamma\beta} = \delta^\alpha_\beta, \quad \Delta_{\alpha\beta} = \mathcal{D}_{i\alpha}\omega^{ij}\mathcal{D}_{j\beta}. \tag{4.5}$$

Δ is invertible on Σ by assumption (recall that its invertibility is a part of the defining property of second-class constraints). It is then invertible in some neighborhood of Σ and we assume that it is invertible on the entire $\mathcal{M}$.

Note that $\mathcal{D}^{ij}$ determines a bivector field on $\mathcal{M}$ that coincides on Σ with the conventional Dirac bracket. The latter bracket is not well defined beyond Σ if the constraints are not scalars. The bracket determined by $\mathcal{D}^{ij}$ in (4.4) can therefore be understood as a covariant generalization of the Dirac bracket to the case of nonscalar constraints. It is straightforward to check that the covariant Dirac bracket satisfies Jacobi identity modulo terms vanishing on Σ.

Furthermore, one can equip $W(\mathcal{M})$ with the symplectic connection compatible with the fiberwise symplectic form. This is achieved as follows. First, one picks a linear symplectic connection $\overline{\Gamma}_{\mathcal{M}}$ on the symplectic manifold $\mathcal{M}$ and equips $W(\mathcal{M})$ with the direct sum connection $\overset{0}{\Gamma}$ determined by

$$\overset{0}{\nabla} e_i = (\overline{\Gamma}_{\mathcal{M}})_i^j e_j, \quad \overset{0}{\nabla} e_\alpha = (\overline{\Gamma})_\alpha^\beta e_\beta, \tag{4.6}$$

where $\overset{0}{\nabla}$ denotes the covariant differential determined by $\overset{0}{\Gamma}$. Given "bare" connection $\overset{0}{\nabla}$ in $W(\mathcal{M})$ one then arrives at the symplectic connection Γ using (3.11). In its turn the symplectic connection in $W(\mathcal{M})$ determines a symplectic structure $\omega^{\mathcal{E}_0}$ on $\mathcal{E}_0$ in accordance to the general formula (3.7). The associated Poisson bracket reads as

$$\begin{gathered}\{p_i, x^j\} = -\delta_i^j, \quad \{p_i, p_j\} = \omega_{ij}(x) + \frac{1}{2} R_{ij;AB}(x) Y^A Y^B, \\ \{Y^A, Y^B\} = \mathcal{D}^{AB}(x), \quad \{p_i, Y^A\} = \Gamma_{iB}^A(x) Y^B.\end{gathered} \tag{4.7}$$

Here and in what follows we drop the superscript of the Poisson bracket on the extended phase space whenever it cannot lead to confusions. Note that the embedding of $T^*_\omega \mathcal{M}$ into $\mathcal{E}_0$ is symplectic. This implies that coordinates Y^A can be treated as second-class constraints (they can also be understood as gauge conditions for the converted system). Considered together with constraints Θ_A they determine a constrained system on $\mathcal{E}_0$ that is equivalent to the original constrained system on $\mathcal{M}$.

Since we are interested in the non-Abelian conversion, it is preferable to work in terms of the BFV-BRST formalism from the very beginning. To this end we introduce ghost variables $\mathcal{C}^A$ and $\mathcal{P}^A$ with the transformation law determined by that of components of a section of $W(\mathcal{M})$ and $W^*(\mathcal{M})$, respectively. One can consistently assume canonical Poisson bracket relations,

$$\{\mathcal{P}_A, \mathcal{C}^B\} = -\delta_A^B, \tag{4.8}$$

and brackets between $\mathcal{C}^A$ and $\mathcal{P}^A$ and all other variables vanishing. Note that in order for Poisson brackets between ghosts and other variables to remain vanishing when passing from one neighborhood to another momenta p_i should transform inhomogeneously. This means that the extended phase space is $\mathcal{E} = T^*_\omega(\Pi W(\mathcal{M})) \oplus W(\mathcal{M})$ with $W(\mathcal{M})$ in the second summand considered as a vector bundle over $\Pi W(\mathcal{M})$. Here and below Π indicates that the Grassmann parity of the fibers of a vector bundle is reversed. Note also that the extended phase space $\mathcal{E}$ is not anymore a vector bundle over $\mathcal{M}$ because p_i transform in an inhomogeneous way.

In the BRST language the conversion problem can be formulated as follows. Given "bare" generating function $\overline{\Omega}$ whose expansion with respect to the ghosts variables starts with given second-class constraints Θ_A,

$$\overline{\Omega} = \mathcal{C}^A \Theta_A + \cdots, \quad gh(\overline{\Omega}) = 1. \tag{4.9}$$

The conversion implies finding BRST charge satisfying

$$\{\Omega, \Omega\} = 0, \quad gh(\Omega) = 1, \quad \Omega|_{Y=0} = \overline{\Omega}. \tag{4.10}$$

Note that Ω and $\overline{\Omega}$ are assumed to be globally defined functions on the entire extended phase space and its submanifold determined by $Y^A = 0$, respectively.

Now we describe conversion of the second-class constraints $\Theta_A = \{-p_i, \theta_\alpha\}$. Taking into account their transformation properties a natural anzatz for a generating function $\overline{\Omega}$ is as follows:

$$\overline{\Omega} = -\mathcal{C}^i p_i + \mathcal{C}^\alpha \theta_\alpha + \mathcal{C}^i (\overline{\Gamma})^\alpha_{i\beta} \mathcal{C}^\beta \mathcal{P}_\alpha . \tag{4.11}$$

Indeed, the nonlinear in ghosts term coming from the transformation law for p_i is compensated by the term coming from inhomogeneous contribution in the transformation law for the connection coefficients. This is exactly the point. In order for the generating function $\overline{\Omega}$ as well as BRST charge Ω to be globally defined functions, one needs to introduce the terms nonlinear in ghosts. In terms of constraints, this implies that the conversion is non-Abelian.

C. Existence and construction of the classical BRST charge

In the standard BFV-BRST formalism the BRST charge and BRST-invariant observables are constructed by expanding in homogeneity degree in ghost momenta. The existence of a nilpotent BRST charge is ensured by Homological Perturbation Theory[18] with the relevant operator being Koszul–Tate differential associated with the constraints. At the same time, within the Abelian conversion procedure the effective first-class constraints, BRST charge, and BRST-invariant observables are constructed by expanding in homogeneity degree in conversion variables, and all these quantities are to be found order by order in these variables.

In the case of non-Abelian conversion it is then natural to take as an expansion degree the total homogeneity in ghost momenta $\mathcal{P}_A$ and conversion variables Y^A:

$$\deg Y^A = \deg \mathcal{P}_A = 1, \quad \deg x^i = \deg p_i = \deg \mathcal{C}^A = 0 . \tag{4.12}$$

Accordingly, Ω decomposes as

$$\Omega = \sum_{s=0} \Omega_s, \quad \Omega_0 = \mathcal{C}^\alpha \theta_\alpha - \mathcal{C}^i p_i, \quad \Omega_1 = \mathcal{C}^i (\overline{\Gamma})^\alpha_{i\beta} \mathcal{C}^\beta \mathcal{P}_\alpha + \cdots , \tag{4.13}$$

where we have explicitly kept the term from the first-order contribution that is needed for covariance. The required BRST charge satisfying (4.10) is to be constructed order by order in the degree. To this end one first needs to satisfy the master equation to zeroth order in the degree, which implies finding Ω_1. A "minimal" form of Ω_1 that satisfies a master equation to the zeroth order can be taken as

$$\Omega_1 = \mathcal{C}^i (\overline{\Gamma})^\alpha_{i\beta} \mathcal{C}^\beta \mathcal{P}_\alpha - \mathcal{C}^A \mathcal{D}_{AB} Y^B . \tag{4.14}$$

In constructing BRST charge it is also useful to restrict ourselves to the following class of phase-space functions: let $\mathfrak{U}^0$ be the space of formal power series in Y^A, ghosts $\mathcal{C}^A$, and ghost momenta $\mathcal{P}_\alpha$ with coefficients being smooth functions in x^i. In other words we forbid dependence on p_i and $\mathcal{P}_i$. The space $\mathfrak{U}^0$ is closed under the multiplication and the Poisson bracket (both operations can be naturally defined for formal power series). Algebra $\mathfrak{U}^0$ decomposes with respect to the degree (4.12) as $\mathfrak{U}^0 = \oplus_{s \geqslant 0} \mathfrak{U}^0_s$ so that an element of $\mathfrak{U}^0_s$ has the form

$$a = \sum_{p \geqslant 0, q \geqslant 0}^{p+q=s} (a_{pq})^{\alpha_1 \cdots \alpha_q}_{A_1 \cdots A_p} Y^{A_1} \cdots Y^{A_p} \mathcal{P}_{\alpha_1} \cdots \mathcal{P}_{\alpha_q}, \quad a_{pq} = a_{pq}(x, \mathcal{C}) . \tag{4.15}$$

Since the BRST charge and BRST-invariant observables are to be constructed by expanding in the degree (4.12) the lowest degree term $-\delta$ in the expansion of $\{\Omega, \cdot\}$ plays a role of the nilpotent operator determining homological perturbation theory. Considered acting on elements from $\mathfrak{U}^0$, operator δ is completely determined by $\overline{\Omega}$ and is given by degree -1 operator

$$\delta = \mathcal{C}^A \frac{\partial}{\partial Y^A} + \theta_\alpha \frac{\partial}{\partial \mathcal{P}_\alpha}. \tag{4.16}$$

It is therefore a sum of the standard Koszul–Tate operator $\delta_K = \theta_\alpha(\partial/\partial \mathcal{P}_\alpha)$ associated with original constraints θ_α and the operator $\mathcal{C}^A(\partial/\partial Y^A)$ that determines a homological perturbation theory in the Abelian conversion framework and in the Fedosov quantization.

To proceed with the conversion we need to introduce a version of the contracting homotopy operator determined by

$$\delta^* f_{pq} = \frac{1}{p+q} Y^A \frac{\partial}{\partial \mathcal{C}^A} f_{pq}, \quad p+q \neq 0, \quad \delta^* f_{00} = 0, \quad \delta^{*2} \equiv 0, \tag{4.17}$$

for an element $f_{pq} \in \mathfrak{U}^0$ that is homogeneous in $\mathcal{C}^A$ and Y^A of orders p and q, respectively. Operators δ and δ^* satisfy

$$\delta^* \delta a + \delta \delta^* a = a - a|_{\mathcal{C}=Y=0}. \tag{4.18}$$

Proposition 4.1: There exists a classical BRST charge Ω, $\mathrm{gh}(\Omega)=1$ *satisfying master equation* $\{\Omega,\Omega\}=0$, *boundary conditions (4.13) and (4.14), and such that* $\Omega_s \in \mathfrak{U}^0_s$ *for* $s \geqslant 2$. *In addition, given* Ω_0 *and* Ω_1 *such a BRST charge is unique provided* $\delta^* \Omega_s = 0$ *for all* $s \geqslant 2$.

Proof: The Poisson bracket on $\mathcal{E}$ can also be expanded with respect to the degree as

$$\{\cdot,\cdot\} = \{\cdot,\cdot\}_{-2} + \{\cdot,\cdot\}_{-1} + \{\cdot,\cdot\}_0 + \{\cdot,\cdot\}_2 \tag{4.19}$$

(terms with other degrees vanish), where each term is a bilinear first-order differential operator of definite degree. In particular,

$$\{f,g\}_{-2} = f \frac{\overleftarrow{\partial}}{\partial Y^A} \mathcal{D}^{AB} \frac{\partial}{\partial Y^B} g. \tag{4.20}$$

The master equation at order n in degrees implies

$$\{\Omega_0, \Omega_{n+2}\}_{-2} + \{\Omega_0, \Omega_{n+1}\}_{-1} + \{\Omega_1, \Omega_{n+1}\}_{-2} + B_n = 0, \tag{4.21}$$

where B_n depends on Ω_s with $s \leqslant n$ only and is given explicitly by

$$B_n = \sum_{0 \geqslant p,q \geqslant n}^{p+q+s=n} \{\Omega_p, \Omega_q\}_s. \tag{4.22}$$

In fact, the first term in (4.21) vanishes because Ω_0 does not depend on Y and the equation takes the form

$$\delta \Omega_{n+1} = B_n. \tag{4.23}$$

This equation can always be solved by $\Omega_{n+1} = \delta^* B_n$ using (4.18), $B_n|_{\mathcal{C}=Y=0}=0$, and the consistency condition $\delta B_n = 0$. The later is fulfilled provided the master equation holds to lowest orders, i.e., that Ω_s for $s \leqslant n$ are such that

$$\{\overset{(n)}{\Omega}, \overset{(n)}{\Omega}\} \in \bigoplus_{s \geqslant n} \mathfrak{U}^0_s, \quad \overset{(n)}{\Omega} = \sum_{s=0}^{n} \Omega_s. \tag{4.24}$$

Indeed, consider the following identity:

$$\{\overset{(n)}{\Omega},\{\overset{(n)}{\Omega},\overset{(n)}{\Omega}\}\}=0. \tag{4.25}$$

Next, observe that $\{\overset{(n)}{\Omega},\overset{(n)}{\Omega}\}=B_n+\cdots$ with dots denoting terms from $\mathfrak{U}^0_{\geqslant n+1}$ and, finally, check that to order $n-1$ in the degree this identity gives $\delta B_n=0$.

This solution for Ω_{n+1} obviously belongs to $\mathfrak{U}^0$ and satisfies $\delta^*\Omega_{n+1}=0$. Conversely, Eq. (4.23) has a unique solution Ω_{n+1} satisfying $\Omega_{n+1}\in\mathfrak{U}^0_{n+1}$, $\delta^*\Omega_{n+1}=0$, and $\mathrm{gh}(\Omega_{n+1})=1$. □

D. Classical observables and weak Dirac bracket

We show that observables of the original system on $\mathcal{M}$ are isomorphic to observables of the BFV-BRST system on $\mathcal{E}$. The latter are understood as cohomology of the adjoint action,

$$Q=\{\Omega,\cdot\} \tag{4.26}$$

of the BRST charge.

Proposition 4.2: Let $f_0=f_0(x,\mathcal{C})$ be any Y and $\mathcal{P}$-independent function. Then there exists $f\in\mathfrak{U}^0$ such that

$$\{\Omega,f\}=0,\quad f|_{Y=\mathcal{P}=0}=f_0,\quad \mathrm{gh}(f)=\mathrm{gh}(f_0). \tag{4.27}$$

If, in addition, $\delta^*(f-f_0)=0$ and $\mathrm{gh}(f)\geqslant 0$, then f is a unique BRST-invariant extension of f_0. Moreover, if $f,\tilde{f}\in\mathfrak{U}^0$ both satisfy (4.27) with the same function f_0, then $f-\tilde{f}=Qh$ for some function $h\in\mathfrak{U}^0$.

Proof: The proof is standard and follows by expanding $Qf=0$ with respect to degree (4.12) and using the fact that δ cohomology is trivial in nonzero degree. The later statement obviously holds provided cohomology of the standard Koszul–Tate operator $\delta_K=\theta_\alpha(\partial/\partial\mathcal{P}_\alpha)$ vanishes in nonzero degree in $\mathcal{P}_\alpha$. Locally, operator δ_K is known to have vanishing cohomology in nonzero degree, provided constraints θ_α satisfy standard regularity assumptions. This also holds globally, as can be shown by using a suitable partition of unity. □

Let f_0 and g_0 be two inequivalent observables of the original system, i.e. $f_0|_\Sigma-g_0|_\Sigma\neq 0$. It then follows from the explicit form of Ω that their BRST-invariant extensions f and g determined by Proposition **4.2** are not equivalent, i.e., $f-g\neq\{\Omega,h\}$ for any h. This means that observables of the original system are observables of the BFV-BRST system. In fact, one can show that these systems are equivalent in the sense that the Poisson algebra of inequivalent observables of the original system (i.e., the algebra of functions on Σ equipped with the Poisson bracket) is isomorphic to the Poisson algebra of ghost number zero BRST cohomology of the BFV-BRST system. Now we restrict ourselves to a little bit weaker equivalence statement. Namely, we show that this holds for BRST cohomology evaluated in $\mathfrak{U}^0$ (Q obviously maps $\mathfrak{U}^0$ to itself).

Proposition 4.3: Let f be an arbitrary function from $\mathfrak{U}^0$ satisfying $Qf=0$. Then $f=Qh$ for some h iff $f|_\Sigma=f|_{\theta_\alpha=\mathcal{C}^A=Y^A=\mathcal{P}_\alpha=0}=0$.

Proof: Let $f_0=f|_{Y=\mathcal{P}=0}$. Condition $f|_\Sigma=f_0|_\Sigma=0$ implies that there exist $f_0^\alpha(x)$ and $f_{0A}(x,\mathcal{C})$, such that

$$f_0=\theta_\alpha f_0^\alpha+\mathcal{C}^A f_{0A}, \tag{4.28}$$

and their transformation properties can be assumed to be those of sections of $V(\mathcal{M})$ and $W^*(\mathcal{M})$, respectively. One can then check that

$$(Qh)|_{Y=\mathcal{P}=0}=f_0,\quad h=-\mathcal{P}_\alpha f_0^\alpha-Y^A f_{0A}, \tag{4.29}$$

because $f_0=-\delta h$ and $(Qh)|_{\mathfrak{U}^0_0}=-\delta h$ for $h\in\mathfrak{U}^0_1$. Proposition **4.2** then implies that there exists $h'\in\mathfrak{U}^0$ such that $f=Q(h+h')$. □

To summarize, we have the following.

Theorem 4.1: *The BRST cohomology of $Q=\{\Omega,\cdot\}$ evaluated in $\mathfrak{U}^0$ are given by*

$$H^n(Q,\mathfrak{U}^0) = C^\infty(\Sigma), \quad n = 0,$$
$$H^n(Q,\mathfrak{U}^0) = 0, \quad n \neq 0. \tag{4.30}$$

The fact that all the physical observables can be taken elements of $\mathfrak{U}^0$ suggests that we consider $\mathfrak{U}^0$ as a fundamental object replacing the algebra of functions on the entire extended phase space. This can be consistently done in spite of the fact that the BRST charge Ω and the ghost charge $\mathcal{G}=\mathcal{C}^A\mathcal{P}_A$ do not belong to $\mathfrak{U}^0$. Indeed, from a more general point of view, a classical BFV-BRST system is determined by (i) Poisson algebra with a not necessarily nondegenerate Poisson structure, which is also graded with the ghost degree, (ii) Odd nilpotent BRST differential Q of ghost number 1 that differentiates both the product of functions and the Poisson bracket, and (iii) differential V (determining evolution) of zero ghost number that differentiates both the product and the Poisson bracket and satisfies $[Q,V]=0$. The standard Hamiltonian BFV-BRST system fits this definition with $Q=\{\Omega,\cdot\}$ and $V=\{H,\cdot\}$, with H denoting a Hamiltonian. Such a generalization of the Hamiltonian BFV-BRST theory was recently studied in Ref. 14. Note also that in the Lagrangian context this corresponds to theories described by the BRST differential not necessarily generated by a master action and an antibracket. Theories of this type were recently considered in Ref. 19.

From this slightly more general point of view, the Poisson algebra $\mathfrak{U}^0$ is a BFV-BRST system because Q and the ghost number operator preserve $\mathfrak{U}^0$. The notion of a generalized BFV-BRST system can be extended to the quantum case by replacing the Poisson algebra with the star-product algebra. It can also be generalized further in the sense that the bracket can be allowed to satisfy the Jacobi identity only up to Q-exact terms as well as V can preserve the bracket only weakly.[14]

Let us give some further comments concerning the Poisson bracket of BRST observables. In the case where Ω is Abelian (see Ref. 8 for a detailed discussion of this case) Proposition **4.2** establishes an isomorphism between the algebra of functions of x^i and functions of x^i, Y^A satisfying $\{\Omega,\cdot\}=0$ and $\delta^*\cdot=0$. The later algebra (understood as a subalgebra in $\mathfrak{U}^0$) is closed under the Poisson bracket in $\mathfrak{U}^0$. The Poisson bracket in this algebra determines a Poisson bracket on $\mathcal{M}$ that can be easily seen to coincide with the Dirac bracket associated to second-class constraints θ_α.

In the present case Ω explicitly depends on $\mathcal{P}_\alpha$ and one is forced to consider δ^* and $\{\Omega,\cdot\}$-closed functions from $\mathfrak{U}^0$ that are now allowed to depend also on $\mathcal{C}^A$ and $\mathcal{P}_\alpha$. However, this algebra is not anymore closed under the Poisson bracket and therefore a direct counterpart of the Dirac bracket fails to satisfy the Jacobi identity outside Σ in this case. Indeed, finding unique lifts $f,g\in\mathfrak{U}^0$ of two phase-space functions f_0 and g_0, evaluating their Poisson bracket, and putting $Y=\mathcal{P}=0$ one finds a bracket on $\mathcal{M}$ that coincides with the standard Dirac bracket when $\theta_\alpha=0$. Explicitly, the bracket reads as

$$\{f_0,g_0\}_D = \partial_i f_0 \mathcal{D}^{ij}\,\partial_j g_0 = \partial_i f_0\,\omega^{ij}\,\partial_j g_0 - \partial_i f_0\,\omega^{il}\overline{\nabla}_l\theta_\alpha\Delta^{\alpha\beta}\overline{\nabla}_k\theta_\beta\omega^{kj}\,\partial_j g_0, \tag{4.31}$$

where

$$\overline{\nabla}_i\theta_\alpha = \partial_i\theta_\alpha - \overline{\Gamma}^\beta_{i\alpha}\theta_\beta, \quad \Delta^{\alpha\gamma}\Delta_{\gamma\beta}=\delta^\alpha_\beta, \quad \Delta_{\alpha\beta}=\overline{\nabla}_i\theta_\alpha\omega^{ij}\overline{\nabla}_j\theta_\beta. \tag{4.32}$$

This bracket can be considered as a direct generalization of the standard Dirac bracket. Unlike the later this generalized bracket does not depend on the choice of constraint basis and therefore is well defined outside Σ in the case of nonscalar constraints. The Jacobi identity for the bracket (4.31) is violated by the terms proportional to the curvature $\overline{R}^\alpha_{ij\beta}$ of the connection $\overline{\nabla}$ and to the constraints θ_α. So it is inevitably a weak bracket if the bundle $V(\mathcal{M})$ does not admit a flat connection.

E. Dirac connection

As we have seen, the construction imposes no constraints on the connection Γ^A_{iB} entering the Poisson bracket on $\mathcal{E}$ but the compatibility with the symplectic from $\mathcal{D}_{AB}$. A symplectic connection

always exists and can be obtained, starting from an arbitrary connection in $W(\mathcal{M})$, e.g., using (3.11). Let us, nevertheless, give an explicit form of the particular symplectic connection, which, as we are going to see, also has some additional properties.

To this end let us consider an explicit form of the compatibility condition $\nabla\mathcal{D}=0$,

$$\partial_i\omega_{jk}-\Gamma_{jik}+\Gamma_{kij}=0,$$

$$\partial_i\overline{\nabla}_j\theta_\alpha-\Gamma_{ji\alpha}+\Gamma_{\alpha ij}=0, \tag{4.33}$$

$$\Gamma_{\alpha i\beta}-\Gamma_{\beta i\alpha}=0.$$

A minimal solution having correct transformaion properties reads as

$$\Gamma_{\alpha i\beta}=0,\quad \Gamma_{ji\alpha}=\mathcal{D}_{j\beta}(\overline{\Gamma})^\beta_{i\alpha},$$
$$\Gamma_{ijk}=(\overline{\Gamma}_{\mathcal{M}})_{ijk},\quad \Gamma_{\alpha ij}=-\overline{\nabla}_i\overline{\nabla}_j\theta_\alpha, \tag{4.34}$$

where $\overline{\nabla}_i\overline{\nabla}_j\theta_\alpha=\overline{\nabla}_i\mathcal{D}_{j\alpha}=\partial_i\mathcal{D}_{j\alpha}-\Gamma^\beta_{i\alpha}\mathcal{D}_{j\beta}$.

It is easy to see that if $V(\mathcal{M})$ is trivial and one takes $\overline{\Gamma}=0$ then (4.34) coincides with the Dirac connection introduced in Ref. 8. In fact, connection (4.34) possesses similar properties with respect to the weak Dirac bracket. To see this let us write down this connection in terms of the coefficients with upper indices,

$$\Gamma^j_{ik}=\omega^{jl}((\overline{\Gamma}_{\mathcal{M}})_{lik}+\mathcal{D}_{l\gamma}\Delta^{\gamma\alpha}\hat{\nabla}_i\hat{\nabla}_k\theta_\alpha),\quad \Gamma^j_{i\alpha}=0,$$
$$\Gamma^\alpha_{ij}=-\Delta^{\alpha\beta}\hat{\nabla}_i\hat{\nabla}_j\theta_\beta,\quad \Gamma^\beta_{i\alpha}=\overline{\Gamma}^\beta_{i\alpha}, \tag{4.35}$$

where $\hat{\nabla}_i\theta_\alpha=\overline{\nabla}_i\theta_\alpha$ and $\hat{\nabla}_i\hat{\nabla}_j\theta_\alpha=\partial_i\mathcal{D}_{j\alpha}-\overline{\Gamma}^\beta_{i\alpha}\mathcal{D}_{j\beta}-(\overline{\Gamma}_{\mathcal{M}})^k_{ji}\mathcal{D}_{k\alpha}$. Connection Γ in $W(\mathcal{M})$ determines a connection $\Gamma_{\mathcal{D}}$ in $T\mathcal{M}$ whose coefficients are Γ^j_{ik}. It follows from $\nabla\mathcal{D}^{AB}=0$ and $\Gamma^j_{i\alpha}=0$ that

$$(\nabla_{\mathcal{D}})_i\mathcal{D}^{jk}=\partial_i\mathcal{D}^{jk}+\Gamma^j_{il}\mathcal{D}^{lk}+\Gamma^k_{il}\mathcal{D}^{jl}=0, \tag{4.36}$$

which means that the Dirac bivector is covariantly constant with respect to the connection $\Gamma_{\mathcal{D}}$. One then concludes that $\Gamma_{\mathcal{D}}$ can be considered a generalization of the Dirac connection introduced in Ref. 8.

Note that $\Gamma_{\mathcal{D}}$ is, in general, not symmetric and its torsion is proportional to the curvature of $\overline{\Gamma}$. On the constraint surface this connection coincides with the Dirac connection in Ref. 8. Similar arguments then show that $\Gamma_{\mathcal{M}}$ can be restricted to Σ and its restriction is a symplectic connection on Σ considered as a symplectic manifold.

There is an ambiguity in Γ that is described by an arbitrary 1-form with values in the symmetric tensor square of the bundle $W^*(\mathcal{M})$ (in components, a general symplectic connection has the form $\Gamma_{AiB}=\Gamma^{\text{fixed}}_{AiB}+\gamma_{AiB}$, with $\gamma_{AiB}-\gamma_{BiA}=0$). One can try to find additional conditions restricting the ambiguity in the connection. In particular, it seems natural to formulate an invariant criterion allowing to single out a symplectic connection in $W(\mathcal{M})$ that after restricting to $T\mathcal{M}\subset W(\mathcal{M})$ would respect the Dirac bracket (4.31) on $\mathcal{M}$.

Such a condition can be seen from analyzing the conversion procedure. To demostrate this, we note that the term in Ω_2 of the form $\mathcal{C}^i\gamma_{AiB}Y^AY^B$ can be absorbed into the redefinition of p_i, which, in turn, leads to the adjustment of the symplectic connection $\Gamma_{AiB}\to\Gamma_{AiB}+\gamma_{AiB}$. It is then natural to choose the connection such that the respective contribution to Ω_2 vanishes, i.e., the connection that is not modified by the conversion. For Ω satisfying conditions of the second part of Proposition **4.1**, this implies that

$$(\delta^*\{-\mathcal{C}^i p_i + \mathcal{C}^i \overline{\Gamma}^{\beta}_{i\alpha}\mathcal{C}^{\alpha}\mathcal{P}_{\beta}, C^A\mathcal{D}_{AB}Y^B\})|_{\mathcal{C}^{\alpha}=0} = 0. \tag{4.37}$$

This gives the following conditions on Γ:

$$\begin{gathered}\partial_i\omega_{jk} - \Gamma_{jik} + \partial_k\omega_{ji} - \Gamma_{jki} + \Gamma_{ijk} + \Gamma_{kji} = 0,\\ \partial_i\mathcal{D}_{j\alpha} - \mathcal{D}_{i\beta}\overline{\Gamma}^{\beta}_{j\alpha} - \Gamma_{ji\alpha} + \Gamma_{ij\alpha} + \Gamma_{\alpha ji} = 0,\\ \Gamma_{\alpha i\beta} + \Gamma_{\beta i\alpha} = 0.\end{gathered} \tag{4.38}$$

If one takes $\Gamma_{ijk}=(\overline{\Gamma}_{\mathcal{M}})_{ijk}$, where $(\overline{\Gamma}_{\mathcal{M}})_{ijk}$ are coefficients of a fixed symmetric symplectic connection on $\mathcal{M}$, then Eqs. (4.33) and (4.38) have a unique solution given by

$$\begin{gathered}\Gamma_{\alpha i\beta} = 0, \quad \Gamma_{ji\alpha} = \mathcal{D}_{j\beta}(\overline{\Gamma})^{\beta}_{i\alpha} + \frac{1}{3}\overline{R}^{\beta}_{ji\alpha}\theta_{\beta},\\ \Gamma_{ijk} = (\overline{\Gamma}_{\mathcal{M}})_{ijk}, \quad \Gamma_{\alpha ij} = -\overline{\boldsymbol{\nabla}}_i\overline{\boldsymbol{\nabla}}_j\theta_{\alpha} - \frac{1}{3}\overline{R}^{\beta}_{ij\alpha}\theta_{\beta},\end{gathered} \tag{4.39}$$

where $\overline{R}^{\beta}_{ij\alpha}\theta_{\beta}=-[\overline{\boldsymbol{\nabla}}_i,\overline{\boldsymbol{\nabla}}_j]\theta_{\alpha}$. Note that the consistency of (4.33) and (4.38) together with $d\omega=0$ requires $\Gamma_{ijk}-\Gamma_{ikj}=0$.

This connection differs from the one in (4.34) by the terms proportional to $\overline{R}^{\beta}_{ij\alpha}\theta_{\beta}$. It also determines a connection $\Gamma'_{\mathcal{D}}$ on $\mathcal{M}$, which coincides with $\Gamma_{\mathcal{D}}$ on Σ. In particular, $\Gamma'_{\mathcal{D}}$ is compatible with the Dirac bracket only weakly in general.

V. CONVERSION AT THE QUANTUM LEVEL

A. Quantization of the extended phase space

At the quantum level we concentrate on the algebra $\hat{\mathfrak{U}}^0=\mathfrak{U}^0\otimes[[\hbar]]$ and its extension $\hat{\mathfrak{U}}$ obtained by allowing the dependence on p_i and $\mathcal{P}_i$ through the following combinations (see Ref. 8 for details):

$$\mathbf{P} = \mathcal{C}^i(-p_i + \overline{\Gamma}^{\alpha}_{i\beta}\mathcal{C}^{\beta}\mathcal{P}_{\alpha}), \quad \mathbf{G} = \mathcal{C}^i\mathcal{P}_i. \tag{5.1}$$

A general element of $\hat{\mathfrak{U}}$ has the form

$$a = \mathbf{P}^r\mathbf{G}^s a_0, \quad r = 0,1, \quad s = 0,1,\ldots,\dim(\mathcal{M}), \quad a_0 \in \hat{\mathfrak{U}}^0. \tag{5.2}$$

The algebra $\hat{\mathfrak{U}}$ is closed under ordinary multiplication and the Poisson bracket. Moreover, it can be directly quantized. To this end one first quantizes $\hat{\mathfrak{U}}^0$ by introducing the Weyl star product according to

$$\begin{aligned}(a\star b)(x,Y,\mathcal{C},\mathcal{P},\hbar) = \Bigg\{&(a(x,Y_1,\mathcal{C}_1,\mathcal{P}_2,\hbar))\exp\Bigg(-\frac{i\hbar}{2}\Bigg(\mathcal{D}^{AB}\frac{\tilde{\partial}}{\partial Y_1^A}\frac{\partial}{\partial Y_2^B} - \frac{\tilde{\partial}}{\partial\mathcal{C}_1^{\alpha}}\frac{\partial}{\partial\mathcal{P}_{\alpha}^2}\\ &- \frac{\tilde{\partial}}{\partial\mathcal{P}_{\alpha}^1}\frac{\partial}{\partial\mathcal{C}_2^{\alpha}}\Bigg)\Bigg)b(x,Y_2,\mathcal{C}_2,\mathcal{P}_2,\hbar)\Bigg\}\Bigg|_{Y_1=Y_2=Y,\mathcal{C}_1=\mathcal{C}_2=\mathcal{C},\mathcal{P}_1=\mathcal{P}_2=\mathcal{P}},\end{aligned} \tag{5.3}$$

where $\mathcal{P}$ stands for $\mathcal{P}_{\alpha}$ only. This star product can then be extended from $\hat{\mathfrak{U}}^0$ to $\hat{\mathfrak{U}}$. Here we give only those formulas that we really need in what follows (we refer to Refs. 8 and 7 for further details of such an extension):

$$\frac{i}{\hbar}[\mathbf{P},a]=\mathcal{C}^i\left(\frac{\partial}{\partial x^i}-\overline{\Gamma}^{\beta}_{i\alpha}\mathcal{C}^{\alpha}\frac{\partial}{\partial\mathcal{C}^{\beta}}+\overline{\Gamma}^{\alpha}_{i\beta}\mathcal{P}_{\beta}\frac{\partial}{\partial\mathcal{P}^{\beta}}-\Gamma^{B}_{iA}Y^{B}\frac{\partial}{\partial Y^{A}}\right)a,\quad a\in\hat{\mathfrak{U}}^0,$$

$$\frac{i}{\hbar}[\mathbf{P},\mathbf{P}]=-i\hbar\mathcal{C}^i\mathcal{C}^j\left(\omega_{ij}+\overline{R}^{\beta}_{ij\alpha}\mathcal{C}^{\alpha}\mathcal{P}_{\beta}+\frac{1}{2}\mathcal{R}_{ijAB}Y^AY^B\right),\tag{5.4}$$

$$\frac{i}{\hbar}[\mathbf{G},a]=-\mathcal{C}^i\frac{\partial}{\partial\mathcal{C}^i}+\mathcal{P}_i\frac{\partial}{\partial\mathcal{P}_i},\quad a\in\hat{\mathfrak{U}}^0.$$

Note that these relations are sufficient to consistently consider $\hat{\mathfrak{U}}^0$ as a star-product algebra underlying the BFV-BRST system at the quantum level in the sense described in **4.4** after the Theorem **4.1**.

On $\hat{\mathfrak{U}}$ we introduce the following degree:

$$\deg Y^A=\deg\mathcal{P}_A=\deg p_i=1,\quad \deg\mathcal{C}^A=\deg x^i=0,\quad \deg\hbar=2.\tag{5.5}$$

One then decomposes $\hat{\mathfrak{U}}^0$ and $\hat{\mathfrak{U}}$ with respect to the degree as

$$\hat{\mathfrak{U}}^0=\bigoplus_{s=0}\hat{\mathfrak{U}}^0_s,\tag{5.6}$$

and similarly for $\hat{\mathfrak{U}}$. The star product is also decomposed into homogeneous components with respect to degree

$$\star=\star_0+\star_1+\star_2+\cdots.\tag{5.7}$$

In particular, $\star_0$ contains an ordinary product, a Weyl product in the sector of Y variables, and the component of the product that takes $\mathbf{P}$ with itself into $-\imath\hbar\mathcal{C}^i\mathcal{C}^j\omega_{ij}$.

Let us note that the choice of the degree is not unique. The one we are using is convenient for general proofs but perhaps is not the most suitable for computations because it is not preserved by the star product in $\hat{\mathfrak{U}}^0$. From this point of view one can consider another degree for which $\deg\mathcal{C}^A=1$ and gradings of other variables left unchanged.

B. Quantum BRST charge

Now we are going to show the existence of the quantum BRST charge satisfying

$$[\hat{\Omega},\hat{\Omega}]=0,\quad \mathrm{gh}(\hat{\Omega})=1,\tag{5.8}$$

together with the condition $\hat{\Omega}|_{\hbar=0}=\Omega$. Here and below $[\cdot,\cdot]$ stands for the graded commutator with respect to the star multiplication in $\hat{\mathfrak{U}}$, which is also decomposed into homogeneous component with respect to the degree. A degree s component of the commutator is denoted by $[\cdot,\cdot]_s$.

It follows from the standard deformation theory and the vanishing of Q cohomology in nonzero ghost number that quantum BRST charge exists. However, instead of deforming the classical BRST charge we construct the quantum one from scratch. To this end we show that the quantum master equation (5.8) has a solution satisfying the following boundary conditions:

$$\hat{\Omega}_0=\mathcal{C}^{\alpha}\theta_{\alpha},\quad \hat{\Omega}_1=\mathbf{P}-\mathcal{C}^A\mathcal{D}_{AB}Y^B=-\mathcal{C}^ip_i+\mathcal{C}^i\overline{\Gamma}^{\alpha}_{i\beta}\mathcal{C}^{\beta}\mathcal{P}_{\alpha}-\mathcal{C}^A\mathcal{D}_{AB}Y^B.\tag{5.9}$$

Proposition 5.1: Equation (5.8) has a solution satisfying boundary condition (5.9) and $\hat{\Omega}_s\subset\hat{\mathfrak{U}}^0_s$ for $s\geqslant 2$. *Under the additional condition* $\delta^*\hat{\Omega}_s=0$, $s\geqslant 2$ *the solution is unique.*

Proof: Proof is completely standard once degree is prescribed. The only thing to check is that with boundary conditions (5.9), the master equation holds at orders 0, 1, and 2, which is straightforward. The rest follows by induction, using that

$$[\hat{\Omega}_0, a]_0 = 0, \quad \frac{1}{i\hbar}([\hat{\Omega}_0, a]_1 + [\hat{\Omega}_1, a]_0) = \delta a, \tag{5.10}$$

for any $a \in \hat{\mathfrak{U}}^0$. Here, $[\cdot, \cdot]_s$ denotes the degree s component of the star commutator. □

C. Quantum BRST observables and weakly associative star product

Given a nilpotent quantum BRST charge one can consider the cohomology group of its adjoint action $\hat{Q} = (i/\hbar)[\hat{\Omega}, \cdot]$. It follows from the standard deformation theory and Theorem **4.1** that any classical BRST cohomology class determines a quantum one. In fact it also follows that

$$H^n(\hat{Q}, \hat{\mathfrak{U}}^0) \cong H^n(Q, \mathfrak{U}^0) \otimes [[\hbar]]. \tag{5.11}$$

It is nevertheless useful to explicitly construct representatives of the quantum BRST cohomology classes. Similarly to the classical case this is achieved by finding a lift of functions of x^i, $\mathcal{C}^A$ to BRST-invariant elements of $\hat{\mathfrak{U}}^0$. We have the following.

Proposition 5.2: For any $f_0 = f_0(x, \mathcal{C}, \hbar)$ there exists $f \in \hat{\mathfrak{U}}^0$, such that

$$[\Omega, f] = 0, \quad \mathrm{gh}(f) = \mathrm{gh}(f_0), \quad f|_{Y=\mathcal{P}=0} = f_0. \tag{5.12}$$

If in addition f is such that $\delta^*(f - f_0) = 0$ and $\mathrm{gh}(f) \geqslant 0$, then f is a unique quantum BRST-invariant extension of f_0. Moreover, if f and $\tilde{f}$ both satisfy (5.12) *with the same f_0, then $f - \tilde{f} = [\hat{\Omega}, h]$ for some $h \in \hat{\mathfrak{U}}^0$.*

Proof: The proof is standard once the degree is prescribed. That equation holds to lowest order and follows from $\delta f_0 = 0$. □

If $f, g \in \hat{\mathfrak{U}}^0$ are unique BRST-invariant extensions of functions $f_0(x)$ and $g_0(x)$ determined by Proposition **5.2**, then one can define a bilinear operation,

$$f_0 \star_D g_0 = (f \star g)|_{Y=\mathcal{P}=0}. \tag{5.13}$$

This operation is not an associative product in general. However, it determines the associative star product on Σ. Indeed, BRST cohomology can be identified with functions on Σ while quantum multiplication in $\hat{\mathfrak{U}}^0$ determines a quantum multiplication in the cohomology. By choosing different lifts from functions on $\mathcal{M}$ to $\hat{\mathfrak{U}}^0$ one can describe different extensions of the associative star products on Σ to, in general, a nonassociative product on $\mathcal{M}$.

As a final remark, we comment on the emergence of weak Poisson brackets and weak star products in the context of constrained systems. In dynamics, and especially in what concerns the deformations and quantization of classical dynamical systems, the Poisson geometry is stereotypically considered the most fundamental structure of the theory. But whenever a constrained or a gauge system is considered, the dynamics, as such, does not require a Poisson algebra to exist for all functions on the entire phase-space manifold. Only the space of physical quantities has to carry a Poisson structure, and hence the geometry of the entire manifold turns out to have a weaker structure than the Poisson one. As we have seen, this is the case with nonscalar second-class constraints. The BRST theory was originally worked out as a tool for quantizing systems with gauge symmetries defined by weakly integrable distributions. Now, as is seen, the idea of BRST cohomology allows one to quantize systems whose Poisson algebra is also weak.

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Local superfield Lagrangian BRST quantization

D. M. Gitman[a)]
Instituto de Física, Universidade de São Paulo, Caixa Postal 66318-CEP, 05315-970 São Paulo, S.P., Brazil

P. Yu. Moshin[b)]
Instituto de Física, Universidade de São Paulo, Caixa Postal 66318-CEP, 05315-970 São Paulo, S.P., Brazil and Tomsk State Pedagogical University, 634041 Tomsk, Russia

A. A. Reshetnyak[c)]
Tomsk State Pedagogical University, 634041 Tomsk, Russia

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A θ-local formulation of superfield Lagrangian quantization in non-Abelian hypergauges is proposed on the basis of an extension of general reducible gauge theories to special superfield models with a Grassmann parameter θ. We solve the problem of describing the quantum action and the gauge algebra of an L-stage-reducible superfield model in terms of a BRST charge for a formal dynamical system with first-class constraints of $(L+1)$-stage reducibility. Starting from θ-local functions of the quantum and gauge-fixing actions, with an essential use of Darboux coordinates on the antisymplectic manifold, we construct a superfield generating functionals of Green's functions, including the effective action. We present two superfield forms of BRST transformations, considered as θ-shifts along vector fields defined by Hamiltonian-like systems constructed in terms of the quantum and gauge-fixing actions and an arbitrary θ-local boson function, as well as in terms of corresponding fermion functionals, through Poisson brackets with opposite Grassmann parities. The gauge independence of the S-matrix is proved. The Ward identities are derived. Connection is established with the BV method, the multilevel Batalin-Tyutin formalism, as well as with the superfield quantization scheme of Lavrov, Moshin, and Reshetnyak, extended to the case of general coordinates. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1938707]

I. INTRODUCTION

The construction of superfield counterparts of the Lagrangian[1] and Hamiltonian[2,3] quantization schemes for gauge theories on the basis of BRST symmetry[4] has been covered in a number of papers.[5–7] These works are based on nontrivial (represented by the operator $D=\partial_\theta+\theta\partial_t$, $[D,D]_+=2\partial_t$) and trivial relations between the even t and odd θ components of supertime.[8] In Refs. 5–7, the geometric interpretation[9] of BRST transformations is realized by special translations in superspace, which originally provided a basis for the superspace description[10] of quantum theories of Yang–Mills type.

It should be noted that superfield quantization is closely related to generalized Poisson sigma-models,[11] described from a superfield geometric viewpoint in Ref. 12, and then developed algorithmically by Batalin and Marnelius in Ref. 13. The geometry of $D=2$ supersymmetric sigma-models[14] with an arbitrary, $N\geqslant 1$, number of Grassmann coordinates has been adapted to the classical and quantum description of $D=1$ sigma-models by Hull, and, independently, to the

[a)]Electronic mail: gitman@dfn.if.usp.br
[b)]Electronic mail: moshin@dfn.if.usp.br
[c)]Electronic mail: reshet@tspu.edu.ru

construction of the partition function for $N=2$, by Gozzi *et al.*[15] Quantization with a single fermion supercharge, $Q(t,\theta)$, containing the BRST charge and the unitarizing Hamiltonian,[5] was recently extended to $N=2$ (non-space–time) supersymmetries,[16] and then, in Ref. 17, to the case of an arbitrary number of supercharges, $Q^k(t,\theta^1,\ldots,\theta^N)$, $k=1,\ldots,N$, depending on Grassmann variables θ^k. The superfield modification[18] of the procedure[5] reveals a close interplay between the quantum action of the Batalin–Vilkovisky (BV) method[1] and the BRST charge of the Batalin–Fradkin–Vilkovisky (BFV) method.[2] Finally, note that the superfield approach is used in the description of second-class constrained systems as gauge models[19] as well as in the second quantization of gauge theories.[20]

The Lagrangian superfield partition function of Ref. 5 is derived from the Hamiltonian partition function through functional integration over so-called Pfaffian ghosts and momenta. On the other hand, the quantization rules (Refs. 6 and 7) present a superfield modification of the BV formalism by including non-Abelian hypergauges.[21] The corresponding hypergauge functions enter a gauge-fixing action which obeys (following the ideas of Ref. 22) the same generating equation that holds for the quantum action,[6,7] except that the first-order operator V in this equation is replaced by the first-order operator U (these operators are crucial ingredients of Refs. 6 and 7 from the viewpoint of a superspace interpretation of BRST transformations).

The formalism (Refs. 6 and 7) provides a comparatively detailed analysis of superfield quantization (BRST invariance, S-matrix gauge-independence). This analysis is based on solutions to the generating equations; however, a detailed correspondence between these solutions and a gauge model is not established. To achieve a better understanding of the quantum properties based on solutions of the superfield generating equations, it is natural to equip the formalism (Refs. 6 and 7) with an *explicit superfield description* of gauge algebra structure functions that determine a given model. So far, this problem has remained unsolved. For instance, the definition of a classical action of superfields, $\mathcal{A}^i(\theta)=A^i+\lambda^i\theta$, on a superspace with coordinates (x^μ,θ), $\mu=0,\ldots,D-1$, as an integral of a nontrivial odd density, $\mathcal{L}(\mathcal{A}(x,\theta),\partial_\mu\mathcal{A}(x,\theta),\ldots;x,\theta)\equiv\mathcal{L}(x,\theta)$, is a problem for every given model. Here, by trivial densities $\mathcal{L}(x,\theta)$ we understand those of the form

$$\int \mathrm{d}^D x\,\mathrm{d}\theta\mathcal{L}(x,\theta)=\int \mathrm{d}\theta\theta S_0(\mathcal{A}(\theta))=S_0(A),$$

where $S_0(A)$ is a usual classical action.

A peculiar feature of the vacuum functional Z and generating functional of Green's functions $Z[\Phi^*]$ in the formalism (Refs. 6 and 7) is the dependence of the gauge fermion $\Psi[\Phi]$ and quantum action $S[\Phi,\Phi^*]$ on the components λ^A of superfields $\Phi^A(\theta)$ in the multiplet $(\Phi^A,\Phi^*_A)(\theta)=(\phi^A+\lambda^A\theta,\phi^*_A-\theta J_A)$, where $(\phi^A,\phi^*_A,\lambda^A,J_A)$ are the complete set of variables of the BV method. Another peculiarity of Refs. 6 and 7 is that, due to the manifest structure of $\Phi^*_A(\theta)$ and $Z[\Phi^*]$, an effective action Γ with the standard Ward identity $(\Gamma,\Gamma)=0$ in terms of a superantibracket[6] can be introduced by a Legendre transformation of $\ln Z[\Phi^*]$ with respect to $P_1(\theta)\Phi^*_A(\theta)$,

$$\Gamma[P_0(\Phi,\Phi^*)]=\frac{\hbar}{i}\ln Z[\Phi^*]+\partial_\theta\{[P_1(\theta)\Phi^*_A(\theta)]\Phi^A(\theta)\},\quad \Phi^A(\theta)=-\frac{\hbar}{i}\frac{\delta\ln Z[\Phi^*]}{\delta(P_1(\theta)\Phi^*_A(\theta))}. \tag{1}$$

[The objects $P_1(\theta)$ and $\delta/\delta(P_1(\theta)\Phi^*_A(\theta))$ are, respectively, an element of the system of projectors $\{P_a(\theta)=\delta_{a0}(1-\theta\partial_\theta)+\delta_{a1}\theta\partial_\theta, a=0,1\}$, acting on the supermanifold with coordinates $(\Phi^A,\Phi^*_A)(\theta)$, and a superfield variational derivative with respect to $P_1(\theta)\Phi^*_A(\theta)$.] Although noncontradictory, such an introduction of Γ violates the superfield content of the variables. By violating the superfield content, we understand the fact that the derivative of $Z[\Phi^*]$, which defines the effective action through a Legendre transformation, is taken with respect to only one superfield component, namely, the θ-component of $\Phi^*_A(\theta)$, so that the resulting effective action depends only on ϕ^A and ϕ^*_A, which can be formally expressed as $P_0(\theta)(\Phi^A,\Phi^*_A)(\theta)=(\phi^A,\phi^*_A)$.

In this paper, we propose a local formalism of superfield Lagrangian quantization in which the quantities of an initial classical theory are realized in the framework of a *θ-local superfield model* (LSM). The idea of LSM is to represent the objects of a gauge theory (classical action, generators

of gauge transformations, etc.) in terms of θ-local functions, trivially related to the space–time coordinates, in the sense that (as compared to the formalism—Ref. 5) the derivatives with respect to the even t and odd θ component of supertime are taken independently. Using an analogy with classical mechanics (or classical field theory), we reproduce the dynamics and gauge invariance (in particular, BRST transformations) of the initial theory (the one with $\theta=0$) in terms of θ-local equations, called *Lagrangian* and *Hamiltonian systems* (LS, HS) with a dynamical odd time θ, which implies that this coordinate enters a LS or HS not as a parameter but as part of a differential operator ∂_θ that describes the θ-evolution of a system.

On the basis of the suggested formalism, we circumvent the peculiarities of the functionals Z and $Z[\Phi^*]$ in Refs. 6 and 7 as well as solve the following problems:

1. We develop a *dual description* of an arbitrary reducible LSM of Ref. 18 in the case of irreducible gauge theories (with bosonic classical fields and parameters of gauge transformations), in terms of a BRST charge related to a (formal) dynamical system with first-class constraints of a higher stage of reducibility. By dual description, we understand such a treatment of a gauge model that interrelates the Lagrangian and Hamiltonian formulations (the latter understood in the sense of formal dynamical systems).

2. An HS constructed from θ-local quantities, i.e., a quantum action, a gauge-fixing action, and an arbitrary bosonic function, encodes (through a θ-local antibracket) both BRST and so-called anticanonical-like transformations, in terms of a universal set of equations underlying the gauge-independence of the S-matrix. This set of equations is generated, in terms of an even superfield Poisson bracket, by a linear combination of fermionic functionals corresponding to the mentioned θ-local quantities, e.g., the quantum and gauge-fixing actions as well as the bosonic function.

3. For the first time in the framework of superfield approach, we introduce a *superfield effective action* (also in the case of non-Abelian hypergauges).

4. We extend the superfield quantization of Refs. 6 and 7 to the case of general coordinates on the manifold of super(anti)fields and establish a relation with the proposed local quantization.

The paper is organized as follows. In Sec. II, a Lagrangian formulation of a LSM is proposed as an extension of a usual model of classical fields A^i, $i=1,\ldots,n=n_+ + n_-$, to a θ-local theory, defined on the odd tangent bundle $T_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}} \equiv \Pi T\mathcal{M}_{\mathrm{CL}} = \{\mathcal{A}^I, \partial_\theta \mathcal{A}^I\}$, $I=1,\ldots,N=N_+ + N_-$, $(n_+,n_-) \leqslant (N_+,N_-)$. [$\Pi$ denotes the exchange operation of the coordinates of a tangent fiber bundle $T\mathcal{M}_{\mathrm{CL}}$ over a configuration $\mathcal{A}^I$ into the coordinates of the opposite Grassmann parity,[23] and N_+,N_-, are the numbers of bosonic and fermionic fields, among which there may exist superfields corresponding to the ghosts of the minimal sector in the BV quantization scheme (in terms of the condensed notation[24] used in this paper).] The superfields $(\mathcal{A}^I, \partial_\theta \mathcal{A}^I)$ are defined in a superspace $\mathcal{M} = \tilde{\mathcal{M}} \times \tilde{P}$ parametrized by (z^M, θ), where the space–time coordinates $z^M \subset i \subset I$ include Lorentz vectors and spinors of the superspace $\tilde{\mathcal{M}}$. We investigate the superfield equations of motion, introduce the notions of reducible *general* and *special* superfield gauge theories, and apply Noether's first theorem to θ-translations. Section III is devoted to the Hamiltonian formulation of a LSM on the odd cotangent bundle $T^*_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}} \equiv \Pi T^*\mathcal{M}_{\mathrm{CL}} = \{\mathcal{A}^I, \mathcal{A}^*_I\}$. Here, we establish a connection to the Lagrangian formalism and investigate the existence of a Noether integral, related to θ-translations, which leads to the validity of a θ-local master equation. The quantization rules are given in Sec. IV. In particular, we construct the dual description of a LSM and define a generating functional of Green's functions, $\mathrm{Z}(\theta)$, and an effective action, $\Gamma(\theta)$, using an invariant description of super(anti)fields on a general antisymplectic manifold. An essential feature in introducing $\mathrm{Z}(\theta)$ and $\Gamma(\theta)$ is a choice of Darboux coordinates $(\varphi,\varphi^*)(\theta)$ compatible with the properties of the quantum action. In Sec. V, on the basis of a component form of the local superfield quantization, we establish its connection with the first-level formalism,[21] with the BV method, and with an extension of the superfield scheme (Refs. 6 and 7). In Sec. VI, we discuss the results of the present work.

In addition to DeWitt's condensed notation,[24] we partially use the conventions of Refs. 6 and 7. We distinguish between two types of superfield derivatives: the right (left) variational derivative $\delta_{(l)}F/\delta\Phi^A(\theta)$ of a functional F, and the right (left) derivative $\partial_{(l)}\mathcal{F}(\theta)/\partial\Phi^A(\theta)$ of a function $\mathcal{F}(\theta)$

for a fixed θ. Derivatives with respect to super(anti)fields and their components are understood as right (left), for instance, $\delta/\delta\Phi^*_A(\theta)$ or $\delta/\delta\lambda^A$, while the corresponding left (right) derivatives are labeled by the subscript $l(r)$. For right-hand derivatives with respect to $\mathcal{A}^I(\theta)$, with a fixed θ, we use the notation $\mathcal{F}_{,I}(\theta)\equiv\partial\mathcal{F}(\theta)/\partial\mathcal{A}^I(\theta)$. The $\delta(\theta)$-function and integration over θ are given, respectively, by $\delta(\theta)=\theta$ and left-hand differentiation over θ. We refer to a function $\mathcal{F}(\theta)$, regarded as an element of the superalgebra $C^\infty(T_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}})$, as a $C^\infty(T_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}})$-function. The rank of an even θ-local supermatrix $K(\theta)$ with Z_2-grading ε is characterized by a pair of numbers $\overline{m}=(m_+,m_-)$, where m_+ (m_-) is the rank of the Bose–Bose (Fermi–Fermi) block of the θ-independent part of the supermatrix $K(\theta)$: $\mathrm{rank}\|K(\theta)\|=\mathrm{rank}\|K(0)\|$. With respect to the same Grassmann parity ε, we understand the dimension of a smooth supersurface, also characterized by a pair of numbers, in the sense of the definition (Ref. 25) of a supermanifold, so that the above pair coincides with the corresponding numbers of the Bose and Fermi components of $z^i(0)$, being the θ-independent parts of local coordinates $z^i(\theta)$ parametrizing this supersurface. On these pairs, we consider the operations of component addition, $\overline{m}+\overline{n}=(m_++n_+,m_-+n_-)$, and comparison,

$$\overline{m}=\overline{n}\Leftrightarrow m_\pm=n_\pm,\quad \overline{m}>\overline{n}\Leftrightarrow(m_+>n_+,m_-\geqslant n_-)\ \text{or}\ (m_+\geqslant n_-,m_+>n_-).$$

II. ODD-TIME LAGRANGIAN FORMULATION

The basic objects of the Lagrangian formulation of a LSM are a *Lagrangian action* S_{L}: $T_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}}\times\{\theta\}\to\Lambda_1(\theta;\mathbb{R})$, being a $C^\infty(T_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}})$-function taking values in a real Grassmann algebra $\Lambda_1(\theta;\mathbb{R})$, and (independently) a functional $Z[\mathcal{A}]$, whose θ-density is defined with accuracy up to an arbitrary function $f((\mathcal{A},\partial_\theta\mathcal{A})(\theta),\theta)\in\ker\{\partial_\theta\}$, $\vec{\varepsilon}(f)=\vec{0}$,

$$Z[\mathcal{A}]=\partial_\theta S_{\mathrm{L}}(\theta),\quad \vec{\varepsilon}(Z)=\vec{\varepsilon}(\theta)=(1,0,1),\quad \vec{\varepsilon}(S_{\mathrm{L}})=\vec{0}. \tag{2}$$

The values $\vec{\varepsilon}=(\varepsilon_P,\varepsilon_{\overline{J}},\varepsilon)$, $\varepsilon=\varepsilon_P+\varepsilon_{\overline{J}}$, of Z_2-grading, with the auxiliary components $\varepsilon_{\overline{J}}$, ε_P related to the respective coordinates (z^M,θ) of a superspace $\mathcal{M}$, are defined on superfields $\mathcal{A}^I(\theta)$ by the relation $\vec{\varepsilon}(\mathcal{A}^I)=((\varepsilon_P)_I,(\varepsilon_{\overline{J}})_I,\varepsilon_I)$. Note that $\mathcal{M}$ may be realized as the quotient of a symmetry supergroup $J=\overline{J}\times P$, $P=\exp(i\mu p_\theta)$, for the functional $Z[\mathcal{A}]$, where μ and p_θ are, respectively, a nilpotent parameter and a generator of θ-shifts, whereas $\overline{J}$ is chosen as the space–time SUSY group. The quantities $\varepsilon_{\overline{J}}$, ε_P are the respective Grassmann parities of the coordinates of representation spaces of the supergroups $\overline{J}$, P. The introduced objects allow one to achieve a correct incorporation of the spin-statistic relation into operator quantization.

Among the objects $S_{\mathrm{L}}(\theta)$ and $Z[\mathcal{A}]$, invariant under the action of a J-superfield representation T restricted to $\overline{J}$, $T|_{\overline{J}}$, it is only $S_{\mathrm{L}}(\theta)$ that transforms nontrivially (in view of the J-scalar nature of $Z[\mathcal{A}]$) with respect to the total representation T under $\mathcal{A}^I(\theta)\to\mathcal{A}'^I(\theta)=(T|_{\overline{J}}\mathcal{A})^I(\theta-\mu)$,

$$\delta S_{\mathrm{L}}(\theta)=S_{\mathrm{L}}(\mathcal{A}'(\theta),\partial_\theta\mathcal{A}'(\theta),\theta)-S_{\mathrm{L}}(\theta)=-\mu\left[\frac{\partial}{\partial\theta}+P_0(\theta)(\partial_\theta U)(\theta)\right]S_{\mathrm{L}}(\theta). \tag{3}$$

Here, we have introduced the nilpotent operator $(\partial_\theta U)(\theta)=\partial_\theta\mathcal{A}^I(\theta)\partial_l/\partial\mathcal{A}^I(\theta)=[\partial_\theta,U(\theta)]_-$, $U(\theta)=P_1\mathcal{A}^I(\theta)\partial_l/\partial\mathcal{A}^I(\theta)$.

Assuming the existence of a critical superfield configuration for $Z[\mathcal{A}]$, one presents the dynamics of an LSM in terms of superfield Euler–Lagrange equations:

$$\frac{\delta_l Z[\mathcal{A}]}{\delta\mathcal{A}^I(\theta)}=\left[\frac{\partial_l}{\partial\mathcal{A}^I(\theta)}-(-1)^{\varepsilon_I}\partial_\theta\frac{\partial_l}{\partial(\partial_\theta\mathcal{A}^I(\theta))}\right]S_{\mathrm{L}}(\theta)\equiv\mathcal{L}^l_I(\theta)S_{\mathrm{L}}(\theta)=0, \tag{4}$$

equivalent, in view of $\partial^2_\theta\mathcal{A}^I(\theta)\equiv0$, to a LS characterized by $2N$ formally second-order differential equations in θ,

$$\partial_\theta^2 \mathcal{A}^J(\theta) \frac{\partial_l^2 S_{\mathrm{L}}(\theta)}{\partial(\partial_\theta \mathcal{A}^I(\theta))\partial(\partial_\theta \mathcal{A}^J(\theta))} \equiv \partial_\theta^2 \mathcal{A}^J(\theta)(S_{\mathrm{L}}'')_{IJ}(\theta) = 0,$$

$$\Theta_I(\theta) \equiv \frac{\partial_l S_{\mathrm{L}}(\theta)}{\partial \mathcal{A}^I(\theta)} - (-1)^{\varepsilon_I}\left[\frac{\partial}{\partial\theta}\frac{\partial_l S_{\mathrm{L}}(\theta)}{\partial(\partial_\theta \mathcal{A}^I(\theta))} + (\partial_\theta U)(\theta)\frac{\partial_l S_{\mathrm{L}}(\theta)}{\partial(\partial_\theta \mathcal{A}^I(\theta))}\right] = 0. \tag{5}$$

The *Lagrangian constraints* $\Theta_I(\theta) = \Theta_I(\mathcal{A}(\theta), \partial_\theta \mathcal{A}(\theta), \theta)$ restrict the setting of the Cauchy problem for the LS and may be functionally dependent, as first-order equations in θ.

Provided that there exists (at least locally) a supersurface $\Sigma \subset \mathcal{M}_{\mathrm{CL}}$ such that

$$\Theta_I(\theta)|_\Sigma = 0, \quad \dim \Sigma = \overline{M}, \quad \operatorname{rank}\|\mathcal{L}_J^l(\theta)[\mathcal{L}_I^l(\theta)S_{\mathrm{L}}(\theta)(-1)^{\varepsilon_I}]\|_\Sigma = \overline{N} - \overline{M}, \tag{6}$$

there exist $M = M_+ + M_-$ independent identities:

$$\int \mathrm{d}\theta \frac{\delta Z[\mathcal{A}]}{\delta \mathcal{A}^I(\theta)} \hat{\mathcal{R}}^I_{\mathcal{A}_0}(\theta;\theta_0) = 0, \quad \hat{\mathcal{R}}^I_{\mathcal{A}_0}(\theta;\theta_0) = \sum_{k\geqslant 0} ((\partial_\theta)^k \delta(\theta - \theta_0)) \hat{\mathcal{R}}^I_{k\mathcal{A}_0}(\mathcal{A}(\theta), \partial_\theta \mathcal{A}(\theta), \theta). \tag{7}$$

The generators $\hat{\mathcal{R}}^I_{\mathrm{A}_0}(\theta;\theta_0)$ of *general gauge transformations*,

$$\delta_g \mathcal{A}^I(\theta) = \int \mathrm{d}\theta_0 \hat{\mathcal{R}}^I_{\mathcal{A}_0}(\theta;\theta_0)\xi^{\mathcal{A}_0}(\theta_0), \quad \vec{\varepsilon}(\xi^{\mathcal{A}_0}) = \vec{\varepsilon}_{\mathcal{A}_0}, \quad \mathcal{A}_0 = 1, \ldots, \quad M_0 = M_{0+} + M_{0-},$$

that leave $Z[\mathcal{A}]$ invariant, are functionally dependent under the assumption of locality and $\overline{J}$-covariance, provided that

$$\operatorname{rank}\left\|\sum_{k\geqslant 0} \hat{\mathcal{R}}^I_{k\mathcal{A}_0}(\theta)(\partial_\theta)^k\right\|_\Sigma = \overline{M} < \overline{M}_0.$$

The dependence of $\hat{\mathcal{R}}^I_{\mathcal{A}_0}(\theta;\theta_0)$ implies the existence (on solutions of the LS) of proper zero-eigenvalue eigenvectors, $\hat{\mathcal{Z}}^{\mathcal{A}_0}_{\mathcal{A}_1}(\mathcal{A}(\theta_0), \partial_{\theta_0}\mathcal{A}(\theta_0), \theta_0; \theta_1)$, with a structure analogous to $\hat{\mathcal{R}}^I_{\mathcal{A}_0}(\theta;\theta_0)$ in (7), which exhaust the zero-modes of the generators, and are dependent in case

$$\operatorname{rank}\left\|\sum_k \hat{\mathcal{Z}}^{\mathcal{A}_0}_{k\mathcal{A}_1}(\theta_0)(\partial_{\theta_0})^k\right\|_\Sigma = \overline{M}_0 - \overline{M} < \overline{M}_1.$$

As a result, the relations of dependence for eigenvectors that define a general L_g-stage reducible LSM are given by

$$\int \mathrm{d}\theta' \hat{\mathcal{Z}}^{\mathcal{A}_{s-2}}_{\mathcal{A}_{s-1}}(\theta_{s-2};\theta')\hat{\mathcal{Z}}^{\mathcal{A}_{s-1}}_{\mathcal{A}_s}(\theta';\theta_s) = \int \mathrm{d}\theta' \Theta_J(\theta')\mathcal{L}^{\mathcal{A}_{s-2}J}_{\mathcal{A}_s}((\mathcal{A}, \partial_\theta \mathcal{A})(\theta_{s-2}), \theta_{s-2}, \theta';\theta_s),$$

$$\overline{M}_{s-1} > \sum_{k=0}^{s-1}(-1)^k \overline{M}_{s-k-2} = \operatorname{rank}\left\|\sum_{k\geqslant 0} \hat{\mathcal{Z}}^{\mathcal{A}_{s-2}}_{\mathcal{A}_{s-1}}(\theta_{s-2})(\partial_{\theta_{s-2}})^k\right\|_\Sigma,$$

$$\overline{M}_{L_g} = \sum_{k=0}^{L_g}(-1)^k \overline{M}_{L_g - k - 1} = \operatorname{rank}\left\|\sum_{k\geqslant 0} \hat{\mathcal{Z}}^{\mathcal{A}_{L_g-1}}_{\mathcal{A}_{L_g}}(\theta_{L_g-1})(\partial_{\theta_{L_g-1}})^k\right\|_\Sigma,$$

$$\vec{\varepsilon}(\hat{\mathcal{Z}}^{\mathcal{A}_s}_{\mathcal{A}_{s+1}}) = \vec{\varepsilon}_{\mathcal{A}_s} + \vec{\varepsilon}_{\mathcal{A}_{s+1}} + (1,0,1), \quad \hat{\mathcal{Z}}^{\mathcal{A}_{-1}}_{\mathcal{A}_0}(\theta_{-1};\theta_0) \equiv \hat{\mathcal{R}}^I_{\mathcal{A}_0}(\theta_{-1};\theta_0),$$

$$\mathcal{L}^{\mathcal{A}_{-1}J}_{\mathcal{A}_1}(\theta_{-1},\theta';\theta_1) \equiv \mathcal{K}^{IJ}_{\mathcal{A}_1}(\theta_{-1},\theta';\theta_1) = -(-1)^{(\varepsilon_I+1)(\varepsilon_J+1)}\mathcal{K}^{JI}_{\mathcal{A}_1}(\theta',\theta_{-1};\theta_1), \tag{8}$$

for $s=1,\ldots,L_g$, $\mathcal{A}_s=1,\ldots,M_s=M_{s+}+M_{s-}$, $\overline{M}\equiv\overline{M}_{-1}$. For $L_g=0$, the LSM is an irreducible *general gauge theory*.

In case a LSM admits the form $S_{\mathrm{L}}(\theta)=T(\partial_\theta\mathcal{A}(\theta))-S(\mathcal{A}(\theta),\theta)$, the functions $\Theta_I(\theta)$ are given in the extended configuration space $\mathcal{M}_{\mathrm{CL}}\times\{\theta\}$ by

$$\Theta_I(\theta)=-S_{,I}(\mathcal{A}(\theta),\theta)(-1)^{\varepsilon_I}=0, \tag{9}$$

being the extremals of the functional $S_0(A)=S(\mathcal{A}(0),0)$, corresponding to $\theta=0$. Condition (6) and identities (7) take the usual form (in case $\theta=0$)

$$\mathrm{rank}\|S_{,IJ}(\mathcal{A}(\theta),\theta)\|_\Sigma=\overline{N}-\overline{M},\quad S_{,I}(\mathcal{A}(\theta),\theta)\mathcal{R}^{I}_{0\mathcal{A}_0}(\mathcal{A}(\theta),\theta)=0, \tag{10}$$

with linearly-dependent (for $\overline{M}_0>\overline{M}$) generators of *special gauge transformations*,

$$\delta\mathcal{A}^I(\theta)=\mathcal{R}^{I}_{0\mathcal{A}_0}(\mathcal{A}(\theta),\theta)\xi_0^{\mathcal{A}_0}(\theta),$$

that leave invariant only $S(\theta)$, in contrast to $T(\theta)$. The dependence of generators $\mathcal{R}_{0\mathcal{A}_0}{}^{I}(\theta)$, as well as of their zero-eigenvalue eigenvectors $\mathcal{Z}^{\mathcal{A}_0}_{\mathcal{A}_1}(\mathcal{A}(\theta),\theta)$, and so on, can also be expressed by special relations of reducibility for $s=1,\ldots,L_g$, namely,

$$\mathcal{Z}^{\mathcal{A}_{s-2}}_{\mathcal{A}_{s-1}}(\mathcal{A}(\theta),\theta)\mathcal{Z}^{\mathcal{A}_{s-1}}_{\mathcal{A}_s}(\mathcal{A}(\theta),\theta)=S_{,J}(\theta)\mathcal{L}^{\mathcal{A}_{s-2}J}_{\mathcal{A}_s}(\mathcal{A}(\theta),\theta),\quad \vec{\varepsilon}(\mathcal{Z}^{\mathcal{A}_{s-1}}_{\mathcal{A}_s})=\vec{\varepsilon}_{\mathcal{A}_{s-1}}+\vec{\varepsilon}_{\mathcal{A}_s},$$

$$\mathcal{Z}^{\mathcal{A}_{-1}}_{\mathcal{A}_0}(\theta)\equiv\mathcal{R}^{I}_{0\mathcal{A}_0}(\theta),\quad \mathcal{L}^{\mathcal{A}_{-1}J}_{\mathcal{A}_1}(\theta)\equiv\mathcal{K}^{IJ}_{\mathcal{A}_1}(\theta)=-(-1)^{\varepsilon_I\varepsilon_J}\mathcal{K}^{JI}_{\mathcal{A}_1}(\theta). \tag{11}$$

For $\overline{M}_{L_g}=\Sigma_{k=0}^{L_g}(-1)^k\overline{M}_{L_g-k-1}=\mathrm{rank}\|\mathcal{Z}^{\mathcal{A}_{L_{g-1}}}_{\mathcal{A}_{L_g}}\|_\Sigma$, relations (9)–(11) determine a *special gauge theory* of L_g-stage reducibility. The gauge algebra of such a theory is θ-locally embedded into the gauge algebra of a general gauge theory with the functional $Z[\mathcal{A}]=\partial_\theta(T(\theta)-S(\theta))$, which implies the relation between the eigenvectors

$$\hat{\mathcal{Z}}^{\mathcal{A}_{s-1}}_{\mathcal{A}_s}(\mathcal{A}(\theta_{s-1}),\theta_{s-1};\theta_s)=-\delta(\theta_{s-1}-\theta_s)\mathcal{Z}^{\mathcal{A}_{s-1}}_{\mathcal{A}_s}(\mathcal{A}(\theta_{s-1}),\theta_{s-1}) \tag{12}$$

and the fact that the structure functions of the gauge algebra of a special gauge theory may depend on $\partial_\theta\mathcal{A}^I(\theta)$ only parametrically. Note that an extended (as compared to $\{P_a(\theta)\}$, $a=0,1$) system of projectors onto $C^\infty(T_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}})\times\{\theta\}$, $\{P_0(\theta),\theta\partial/\partial\theta,U(\theta)\}$, selects from (11) two kinds of gauge algebras: one with structure equations and functions $S(\mathcal{A}(\theta))$, $\mathcal{Z}^{\mathcal{A}_{s-1}}_{\mathcal{A}_s}(\mathcal{A}(\theta))$ not depending on θ in an explicit form; another with the standard relations for the gauge algebra of a reducible model with quantities $S_0(A)$, $\mathcal{Z}^{\alpha_{s-1}}_{\alpha_s}(A)$, in case $\theta=0$, $(\varepsilon_P)_I=(\varepsilon_P)_{\mathcal{A}_s}=0$, $s=1,\ldots,L_g$, and under the assumption of completeness of the reduced generators $\mathcal{R}^{i}_{\alpha_0}(\mathcal{A}(\theta))$ and eigenvectors $\mathcal{Z}^{\alpha_{s-1}}_{\alpha_s}(\mathcal{A}(\theta))$; see Sec. IV A.

An extension of a usual field theory to a θ-local LSM permits one to apply Noether's first theorem[26] to the invariance of the density $d\theta S_{\mathrm{L}}(\theta)$ with respect to global θ-translations as symmetry transformations of the superfields $\mathcal{A}^I(\theta)$ and coordinates (z^M,θ), $(\mathcal{A}^I,z^M,\theta)\to(\mathcal{A}^I,z^M,\theta+\mu)$. By direct verification, one establishes that the function

$$S_E((\mathcal{A},\partial_\theta\mathcal{A})(\theta),\theta)\equiv\frac{\partial S_{\mathrm{L}}(\theta)}{\partial(\partial^r_\theta\mathcal{A}^I(\theta))}\partial^r_\theta\mathcal{A}^I(\theta)-S_{\mathrm{L}}(\theta) \tag{13}$$

is a LS integral of motion, i.e., a conserved quantity under the θ-evolution, in case there holds the equation

$$\frac{\partial}{\partial\theta}S_{\mathrm{L}}(\theta)+2(\partial_\theta U)(\theta)S_{\mathrm{L}}(\theta)\Big|_{\mathcal{L}^I_I S_{\mathrm{L}}=0}=0. \tag{14}$$

In contrast to its analogue in a t-local field theory, the energy $E(t)$, the function $S_E(\theta)$ is a LS integral also in the case of an explicit dependence on θ. This fact takes place in case $S_{\mathrm{L}}(\theta)$ admits the structure

$$S_{\mathrm{L}}((\mathcal{A},\partial_\theta\mathcal{A})(\theta),\theta)=S^0_{\mathrm{L}}(\mathcal{A},\partial_\theta\mathcal{A})(\theta)-2\theta(\partial_\theta U)(\theta)S^0_{\mathrm{L}}(\theta),\vec{\varepsilon}(S^0_{\mathrm{L}})=\vec{0}. \tag{15}$$

III. ODD-TIME HAMILTONIAN FORMULATION

Independently, a LSM can be formulated in terms of a *Hamiltonian action*, being a $C^\infty(T^*_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}})$-function, S_{H}: $T^*_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}}\times\{\theta\}\to\Lambda_1(\theta;\mathbb{R})$, depending on superantifields $\mathcal{A}^*_I(\theta)=(A^*_I-\theta J_I)$, included in the local coordinates of $T^*_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}}$: $\Gamma^P_{\mathrm{CL}}(\theta)=(\mathcal{A}^I,\mathcal{A}^*_I)(\theta)$, $\vec{\varepsilon}(\mathcal{A}^*_I)=\vec{\varepsilon}(\mathcal{A}^I)+(1,0,1)$. The equivalence of the Lagrangian and Hamiltonian formulations is implied by the nondegeneracy of the supermatrix $\|(S''_{\mathrm{L}})_{IJ}(\theta)\|$ given by (5), in the framework of a Legendre transformation of $S_{\mathrm{L}}(\theta)$ with respect to $\partial^r_\theta\mathcal{A}^I(\theta)$,

$$S_{\mathrm{H}}(\Gamma_{\mathrm{CL}}(\theta),\theta)=\mathcal{A}^*_I(\theta)\partial^r_\theta\mathcal{A}^I(\theta)-S_{\mathrm{L}}(\theta),\ \mathcal{A}^*_I(\theta)=\frac{\partial S_{\mathrm{L}}(\theta)}{\partial(\partial^r_\theta\mathcal{A}^I(\theta))}, \tag{16}$$

where $S_{\mathrm{H}}(\Gamma_{\mathrm{CL}}(\theta),\theta)$ coincides with $S_E(\theta)$ in terms of the $T^*_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}}$-coordinates.

The dynamics of a LSM is given by a *generalized Hamiltonian system* of $3N$ first-order equations in θ, equivalent to the LS equations in (5), and expressed through a θ-local antibracket $(\cdot,\cdot)_\theta$, namely,

$$\begin{gathered}\partial^r_\theta\Gamma^P_{\mathrm{CL}}(\theta)=(\Gamma^P_{\mathrm{CL}}(\theta),S_{\mathrm{H}}(\theta))_\theta,\quad \Theta^{\mathrm{H}}_I(\Gamma_{\mathrm{CL}}(\theta),\theta)=\Theta_I(\mathcal{A}(\theta),\partial_\theta\mathcal{A}(\Gamma_{\mathrm{CL}}(\theta),\theta),\theta)=0,\\ (\mathcal{F}_1(\theta),\mathcal{F}_2(\theta))_\theta\equiv\frac{\partial\mathcal{F}_1(\theta)}{\partial\mathcal{A}^I(\theta)}\frac{\partial\mathcal{F}_2(\theta)}{\partial\mathcal{A}^*_I(\theta)}-\frac{\partial_r\mathcal{F}_1(\theta)}{\partial\mathcal{A}^*_I(\theta)}\frac{\partial_l\mathcal{F}_2(\theta)}{\partial\mathcal{A}^I(\theta)},\ \mathcal{F}_t(\theta)\in C^\infty(\Pi T^*\mathcal{M}_{\mathrm{CL}}),\quad t=1,2\end{gathered} \tag{17}$$

with *Hamiltonian constraints* $\Theta^{\mathrm{H}}_I(\Gamma_{\mathrm{CL}}(\theta),\theta)$. The latter coincide with half of the equations of the HS proper, due to transformations (16) and their consequences:

$$\Theta^{\mathrm{H}}_I(\Gamma_{\mathrm{CL}}(\theta),\theta)=-\partial^r_\theta\mathcal{A}^*_I(\theta)-S_{\mathrm{H},I}(\theta)(-1)^{\varepsilon_I}. \tag{18}$$

Formula (18) establishes the equivalence of an HS with a generalized HS, and hence with a LS in the corresponding [formal, in view of the degeneracy conditions (6)] setting ($\theta=0$, $k=\mathrm{CL}$) of the Cauchy problem for integral curves $\hat{\mathcal{A}}^I(\theta)$, $\hat{\Gamma}^P_k(\theta)$,

$$(\hat{\mathcal{A}}^I,\partial^r_\theta\hat{\mathcal{A}}^I)(0)=(\overline{\mathcal{A}^I},\overline{\partial^r_\theta\mathcal{A}^I}),\quad \hat{\Gamma}^P_k(0)=(\overline{\mathcal{A}^I},\overline{\mathcal{A}^*_I}):\overline{\mathcal{A}^*_I}=P_0\left[\frac{\partial S_{\mathrm{L}}(\theta)}{\partial(\partial^r_\theta\mathcal{A}^I(\theta))}\right](\overline{\mathcal{A}^I},\overline{\partial^r_\theta\mathcal{A}^I}), \tag{19}$$

where we have ignored the continuous part of I. The equivalence between an HS and a generalized HS is valid due to the coincidence (mutual inclusion) of the corresponding sets of solutions. Indeed, the solutions of a generalized HS are included into those of an HS by construction, while the reverse is valid due to (18).

The HS is defined through a variational problem for a functional identical to $Z[\mathcal{A}]$,

$$Z_{\mathrm{H}}[\Gamma_k]=\int\mathrm{d}\theta\left[\frac{1}{2}\Gamma^P_k(\theta)\omega^k_{PQ}(\theta)\partial^r_\theta\Gamma^Q_k(\theta)-S_{\mathrm{H}}(\Gamma_k(\theta),\theta)\right],$$

$$\omega_k^{PQ}(\theta) \equiv (\Gamma_k^P(\theta), \Gamma_k^Q(\theta))_\theta, \quad \omega_k^{PD}(\theta)\omega_{DQ}^k(\theta) = \delta^P{}_Q. \tag{20}$$

Definitions (9)–(11) remain the same for special gauge theories, while definitions (7) and (8), in the case of general gauge theories of L_g-stage reducibility, are transformed by the rule

$$\hat{\mathcal{Z}}_{\mathrm{H}\mathcal{A}_s}^{\mathcal{A}_{s-1}}(\Gamma_k(\theta_{s-1}), \theta_{s-1}; \theta_s) = \hat{\mathcal{Z}}_{\mathcal{A}_s}^{\mathcal{A}_{s-1}}(\mathcal{A}(\theta_{s-1}), \partial_{\theta_{s-1}}\mathcal{A}(\Gamma_k(\theta_{s-1}), \theta_{s-1}), \theta_{s-1}; \theta_s), \quad s = 0, \ldots, L_g. \tag{21}$$

Equation (14), transformations (16) and their consequence $(\partial/\partial\theta)(S_\mathrm{L} + S_\mathrm{H})(\theta) = 0$ imply the invariance of $S_\mathrm{H}(\theta)$ under θ-shifts along arbitrary solutions $\hat{\Gamma}_k^P(\theta)$, or, equivalently, along an $(\varepsilon_P, \varepsilon)$-odd vector field $\mathbf{Q}(\theta) = \mathrm{ad}S_\mathrm{H}(\theta) \equiv (S_\mathrm{H}(\theta), \cdot)_\theta$. Hence,

$$\delta_\mu S_\mathrm{H}(\theta)|_{\hat{\Gamma}_k(\theta)} = \mu\left[\frac{\partial}{\partial\theta}S_\mathrm{H}(\theta) - (S_\mathrm{H}(\theta), S_\mathrm{H}(\theta))_\theta\right] = 0, \quad \delta_\mu S_\mathrm{H}(\theta) = \mu\partial_\theta S_\mathrm{H}(\theta) \tag{22}$$

holds true, provided that $S_\mathrm{H}(\theta)$ can be presented, according to (14), in the form

$$S_\mathrm{H}\big(\Gamma_k(\theta), \theta\big) = S_\mathrm{H}^0(\Gamma_k(\theta)) + \theta\big(S_\mathrm{H}^0(\Gamma_k(\theta)), S_\mathrm{H}^0(\Gamma_k(\theta))\big)_\theta, \tag{23}$$

where $(\partial_\theta U)(\theta)S_\mathrm{L}(\theta) = 1/2(S_\mathrm{H}(\theta), S_\mathrm{H}(\theta))_\theta$, and $S_\mathrm{H}^0(\Gamma_k(\theta))$ is the Legendre transform of $S_\mathrm{L}^0(\theta)$, defined by (15).

If $S_\mathrm{H}(\theta)$ or $S_\mathrm{L}(\theta)$ does not depend on θ explicitly, then Eq. (22) or (14) implies the fulfillment of the equation $(S_\mathrm{H}(\theta), S_\mathrm{H}(\theta))_\theta = 0$, or $(\partial_\theta U)(\theta)S_\mathrm{L}(\theta)|_{\hat{\mathcal{A}}(\theta)} = 0$, which has no counterpart in a *t*-local field theory, and imposes the known condition[1] that $S_\mathrm{H}(\theta)$ or $S_\mathrm{L}(\theta)$ be proper, although for a LSM at the classical level. In this case, a θ-superfield integrability (introduced by analogy with the treatment of Ref. 16) of the HS in (17) is guaranteed by the standard properties of the antibracket, including the Jacobi identity:

$$(\partial_\theta^r)^2\Gamma_k^P(\theta) = \tfrac{1}{2}(\Gamma_k^P(\theta), (S_\mathrm{H}(\Gamma_k(\theta)), S_\mathrm{H}(\Gamma_k(\theta)))_\theta)_\theta = 0. \tag{24}$$

This fact ensures the validity on $C^\infty(T^*_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}} \times \{\theta\})$ of the θ-translation formula

$$\delta_\mu \mathcal{F}(\theta)|_{\hat{\Gamma}_k(\theta)} = \mu\left[\frac{\partial}{\partial\theta} - \mathrm{ad}\, S_\mathrm{H}(\theta)\right]\mathcal{F}(\theta) \equiv \mu\check{s}^l(\theta)\mathcal{F}(\theta), \tag{25}$$

as well as the nilpotency of a BRST-like generator of θ-shifts along $\mathbf{Q}(\theta)$, $\check{s}^l(\theta)$.

Depending on the realization of additional properties of a gauge theory (see Sec. IV), we shall henceforth assume the validity of

$$\Delta^k(\theta)S_\mathrm{H}(\theta) = 0, \quad \Delta^k(\theta) \equiv \tfrac{1}{2}(-1)^{\varepsilon(\Gamma^Q)}\omega_{QP}^k(\theta)(\Gamma_k^P(\theta), (\Gamma_k^Q(\theta), \cdot)_\theta)_\theta. \tag{26}$$

Equation (26) is equivalent to a vanishing divergence of the vector field $\mathbf{Q}(\theta)$, namely,

$$\mathrm{div}(\partial_\theta^r\Gamma_k(\theta)|_{\hat{\Gamma}_k(\theta)}) = \frac{\partial_r}{\partial\Gamma_k^P(\theta)}(\partial_\theta^r\Gamma_k^P(\theta)|_{\hat{\Gamma}_k(\theta)}) = 2\Delta^k(\theta)S_\mathrm{H}(\theta) = 0. \tag{27}$$

This condition is trivial for the symplectic counterpart of formula (27). The validity of the *Hamiltonian master equation* $(S_\mathrm{H}(\theta), S_\mathrm{H}(\theta))_\theta = 0$ in case $(\partial/\partial\theta)S_\mathrm{H}(\theta) = 0$ justifies the interpretation of the equivalent equation in (14), for $(\partial/\partial\theta)S_\mathrm{L}(\theta) = 0$, $(\partial_\theta U)(\theta)S_\mathrm{L}(\theta)|_{\mathcal{L}_I^l S_\mathrm{L} = 0} = 0$, as a *Lagrangian master equation.*

IV. LOCAL SUPERFIELD QUANTIZATION

In order to set up the rules of local superfield quantization for a gauge model, we should first extract such a model from a general LSM. Then we should consider a procedure of constructing a quantum action for the restricted LSM, and, finally, investigate the possibility (inherent in the

θ-local approach) of a *dual description* of the LSM in terms of the quantities of the BFV formalism.

A. Superfield quantum action in initial coordinates

In this section, we transform the reducibility relations of a *restricted* special LSM into a sequence of new gauge transformations for the ghost superfields of the minimal sector. Together with the gauge transformations of the classical superfields $\mathcal{A}^i(\theta)$, extracted from $\mathcal{A}^I(\theta)$, the new gauge transformations are translated into a Hamiltonian system related to the initial restricted HS. A requirement of superfield integrability for the resulting HS produces a deformation of the θ-local Hamiltonian in powers of the ghosts and superantifields of the minimal sector, and leads to a quantum action, and, independently, to a gauge-fixing action (Sec. IV C), subject to different θ-local master equations.

Given the standard distribution of ghost number[1] for $\Gamma^P_{\mathrm{CL}}(\theta)$, $\mathrm{gh}(\mathcal{A}^*_I)=-1-\mathrm{gh}(\mathcal{A}^I)=-1$, the choice $\mathrm{gh}(\theta,\partial_\theta)=(-1,1)$ implying the absence of ghosts among $\mathcal{A}^I$, and, in particular, the relations $(\varepsilon_P)_I=0$, the quantization rules consist, first, in restricting a LSM (in both Lagrangian and Hamiltonian formulations) by

$$\left(\mathrm{gh},\frac{\partial}{\partial\theta}\right)S_{\mathrm{H(L)}}(\theta)=(0,0). \tag{28}$$

Given the existence of a potential term in $S_{\mathrm{H(L)}}(\theta)$, $S(\mathcal{A}(\theta),0)=\mathcal{S}(\mathcal{A}(\theta))$, and the absence in $S_{\mathrm{H(L)}}(\theta)$ of a dimensional constants with a nonzero ghost number, solutions of Eq. (28) select from a LSM a usual gauge model with a classical action $S_0(A)$ in which the fields A^i are extended to $\mathcal{A}^i(\theta)$. Then the generalized HS in (17) is transformed into a θ-integrable system defined in $\Pi T^*\mathcal{M}_{\mathrm{cl}}=\{\Gamma^p_{\mathrm{cl}}(\theta)\}=\{(\mathcal{A}^i,\mathcal{A}^*_i)(\theta)\}$, with $\Theta^{\mathrm{H}}_i(\mathcal{A}(\theta))=\Theta_i(\mathcal{A}(\theta))$,

$$\partial^r_\theta\Gamma^p_{\mathrm{cl}}(\theta)=(\Gamma^p_{\mathrm{cl}}(\theta),S_0(\mathcal{A}(\theta)))_\theta,\quad \Theta^{\mathrm{H}}_i(\mathcal{A}(\theta))=-(-1)^{\varepsilon_i}S_{0,i}(\mathcal{A}(\theta)). \tag{29}$$

The restricted special gauge transformations $\delta\mathcal{A}^i(\theta)=\mathcal{R}^i_{0\alpha_0}(\mathcal{A}(\theta))\xi^{\alpha_0}_0(\theta)$, $\vec{\varepsilon}(\xi^{\alpha_0}_0(\theta))=\vec{\varepsilon}_{\alpha_0}$, with the condition $(\varepsilon_P)_{\alpha_0}=0$, are embedded by the substitution $\xi^{\alpha_0}_0(\theta)=d\tilde{\xi}^{\alpha_0}_0(\theta)=\mathcal{C}^{\alpha_0}(\theta)d\theta$, $\alpha_0=1,\ldots,m_0=m_{0-}+m_{0+}$, into a Hamiltonian system with $2n$ equations for unknown $\Gamma^p_{\mathrm{cl}}(\theta)$, with the Hamiltonian $S^0_1(\Gamma_{\mathrm{cl}},C_0)(\theta)=(\mathcal{A}^*_i\mathcal{R}_{0\alpha0}^{\ i}(\mathcal{A})\mathcal{C}^{\alpha_0})(\theta)$. A union of this system with the HS in (29), extended to $2(n+m_0)$ equations, has the form

$$\partial^r_\theta\Gamma^{p_{[0]}}_{[0]}(\theta)=(\Gamma^{p_{[0]}}_{[0]}(\theta),S^0_{[1]}(\theta))_\theta,\quad S^0_{[1]}(\theta)=(S_0+S^0_1)(\theta),\quad \Gamma^{p_{[0]}}_{[0]}\equiv(\Gamma^p_{\mathrm{cl}},\Gamma^{p_0}_0),\Gamma^{p_0}_0\equiv(\mathcal{C}^{\alpha_0},\mathcal{C}^*_{\alpha_0}). \tag{30}$$

By virtue of (11), the function $S^0_1(\theta)$ is invariant, modulo $S_{0,i}(\theta)$, under special gauge transformations of ghost superfields $\mathcal{C}^{\alpha_0}(\theta)$, with arbitrary functions $\xi^{\alpha_1}_1(\theta)$, $(\varepsilon_P)_{\alpha_1}=0$, on the superspace $\mathcal{M}$:

$$\delta\mathcal{C}^{\alpha_0}(\theta)=\mathcal{Z}^{\alpha_0}_{\alpha_1}(\mathcal{A}(\theta))\xi^{\alpha_1}_1(\theta),\ (\vec{\varepsilon},\mathrm{gh})\xi^{\alpha_1}_1(\theta)=(\vec{\varepsilon}_{\alpha_1}+(1,0,1),1). \tag{31}$$

Making the substitution $\xi^{\alpha_1}_1(\theta)=d\tilde{\xi}^{\alpha_1}_1(\theta)=\mathcal{C}^{\alpha_1}(\theta)d\theta$, $\alpha_1=1,\ldots,m_1$, and an enlargement of m_0 first-order equations in θ, with respect to the unknowns $\mathcal{C}^{\alpha_0}(\theta)$ in transformations (31), to an HS of $2m_0$ equations with the Hamiltonian $S^1_1(\mathcal{A},\mathcal{C}^*_0,\mathcal{C}_1)(\theta)=(\mathcal{C}^*_{\alpha_0}\mathcal{Z}^{\alpha_0}_{\alpha_1}(\mathcal{A})\mathcal{C}^{\alpha_1})(\theta)$, we obtain a system of the form (30), written for $\partial^r_\theta\Gamma^{p_0}_0(\theta)$. The enlargement of the union of the latter HS with Eq. (30) is formally identical to the system (30) under the replacement

$$(\Gamma^{p_{[0]}}_{[0]},S^0_{[1]})\to(\Gamma^{p_{[1]}}_{[1]},S^1_{[1]}):\{\Gamma^{p_{[1]}}_{[1]}=(\Gamma^{p_{[0]}}_{[0]},\Gamma^{p_1}_1),\Gamma^{p_1}_1=(\mathcal{C}^{\alpha_1},\mathcal{C}^*_{\alpha_1}),S^1_{[1]}=S^0_{[1]}+S^1_1\}.$$

The iteration sequence related to a reformulation of the special gauge transformations of ghosts $\mathcal{C}^{\alpha_0}\ldots$, $\mathcal{C}^{\alpha_{s-2}}$, obtained from (possibly) enhanced relations (11), leads, for an L-stage-reducible restricted LSM at the sth step with $0<s\leqslant L$ and $\Gamma^p_{cl}\equiv\Gamma^{p_{-1}}_{-1}$, to invariance transformations for $S_1^{s-1}(\theta)$, modulo $S_{0,i}(\theta)$, namely,

$$\delta\mathcal{C}^{\alpha_{s-1}}(\theta)=\mathcal{Z}^{\alpha_{s-1}}_{\alpha_s}(\mathcal{A}(\theta))\xi_s^{\alpha_s}(\theta),\quad (\vec{\varepsilon},\mathrm{gh})\xi_s^{\alpha_s}(\theta)=(\vec{\varepsilon}_{\alpha_s}+s(1,0,1),s),\quad (\varepsilon_P)_{\alpha_s}=0,$$

$$S_1^{s-1}(\theta)=(\mathcal{C}^*_{\alpha_{s-2}}\mathcal{Z}^{\alpha_{s-2}}_{\alpha_{s-1}}(\mathcal{A})C^{\alpha_{s-1}})(\theta),\quad \left(\mathrm{gh},\frac{\partial}{\partial\theta}\right)S_1^{s-1}(\theta)=(0,0). \tag{32}$$

[From $\mathrm{gh}(\mathcal{A}^I)=0$ in Eq. (28), with $(\varepsilon_P)_{\mathcal{A}_s}=(\varepsilon_P)_I=0$, $s=0,\ldots,L_g$, it follows that the values of $\overline{m}$, $\overline{m_s}$ may be both larger and smaller than the corresponding values $\overline{M}$, $\overline{M_s}$, in contrast to the values of $\overline{n}$, $\overline{N}$. Indeed, for a restricted LSM, the presence of additional gauge symmetries is possible; therefore, we suppose that (possibly) enhanced sets of restricted functions $\mathcal{R}^i_{0\,\alpha_0}(\theta)$, $\mathcal{Z}^{\alpha_{s-1}}_{\alpha_s}(\theta)$ exhaust, correspondingly, on the surface $S_{0,i}(\theta)=0$, the zero-modes of both the Hessian $S_{0,ij}(\theta)$ and $\mathcal{Z}^{\alpha_{s-2}}_{\alpha_{s-1}}(\theta)$. As a consequence, this implies that the final stage of reducibility for a restricted model L is different from L_g.] The substitution $\xi_s^{\alpha_s}(\theta)=d\tilde{\xi}_s^{\alpha_s}(\theta)=\mathcal{C}^{\alpha_s}(\theta)d\theta$, $\alpha_s=1,\ldots,m_s=m_{s-}+m_{s+}$, transforms special gauge transformations (32) into m_{s-1} equations for unknown $\mathcal{C}^{\alpha_{s-1}}(\theta)$, extended by the introduction of superantifields $\mathcal{C}^*_{\alpha_{s-1}}(\theta)$ to an HS:

$$\partial^r_\theta\Gamma^{p_{s-1}}_{s-1}(\theta)=(\Gamma^{p_{s-1}}_{s-1}(\theta),S_1^s(\theta))_\theta,\quad S_1^s(\theta)=(\mathcal{C}^*_{\alpha_{s-1}}\mathcal{Z}^{\alpha_{s-1}}_{\alpha_s}(\mathcal{A})\mathcal{C}^{\alpha_s})(\theta),\quad \Gamma^{p_{s-1}}_{s-1}=(\mathcal{C}^{\alpha_{s-1}},\mathcal{C}^*_{\alpha_{s-1}}). \tag{33}$$

Having combined the system (33) with an HS of the same form, although with $\partial^r_\theta\Gamma^{p_{[s-1]}}_{[s-1]}(\theta)$ and the Hamiltonian $S^{s-1}_{[1]}(\theta)=(S_0+\Sigma_{r=0}^{s-1}S_1^r)(\theta)$, and having expressed the result for $2(n+\Sigma_{r=0}^s m_r)$ equations with $S^s_{[1]}(\theta)=(S^{s-1}_{[1]}+S_1^s)(\theta)$, we obtain, by induction, the following HS:

$$\partial^r_\theta\Gamma^{p_{[L]}}_{[L]}(\theta)=(\Gamma^{p_{[L]}}_{[L]}(\theta),S^L_{[1]}(\theta))_\theta,\quad S^L_{[1]}(\theta)=S_0(\mathcal{A}(\theta))+\sum_{s=0}^{L}(\mathcal{C}^*_{\alpha_{s-1}}\mathcal{Z}^{\alpha_{s-1}}_{\alpha_s}(\mathcal{A})\mathcal{C}^{\alpha_s})(\theta). \tag{34}$$

The function $S^L_{[1]}(\theta)$, subject to the condition of a proper θ-local solution of the classical master equation,[1] with the antibracket extended in $\Pi T^*\mathcal{M}_k=\{\Gamma^{p_{[L]}}_{[L]}(\theta)\equiv\Gamma^{p_k}_k(\theta)=(\Phi^{A_k},\Phi^*_{A_k})(\theta),A_k=1,\ldots,n+\Sigma_{r=0}^L m_r,k=\min\}$, is a solution of the master equation with accuracy up to $O(C^{\alpha_s})$, modulo $S_{0,i}(\theta)$. The integrability of the HS in (34) is guaranteed by a double deformation of $S^L_{[1]}(\theta)$: first in powers of $\Phi^*_{A_k}(\theta)$ and then in powers of $\mathcal{C}^{\alpha_s}(\theta)$, in the framework of the existence theorem[27] for the classical master equation in the minimal sector:

$$(S_{\mathrm{H};k}(\Gamma_k(\theta)),S_{\mathrm{H};k}(\Gamma_k(\theta)))_\theta=0,\quad \left(\vec{\varepsilon},\mathrm{gh},\frac{\partial}{\partial\theta}\right)S_{\mathrm{H};k}(\Gamma_k(\theta))=(\vec{0},0,0),\quad k=\min. \tag{35}$$

The proposed superfield algorithm for constructing the function $S_{\mathrm{H};\min}(\theta)$ may be considered as a superfield version of the Koszul–Tate complex resolution.[28]

Let us consider an extension of $S_{\mathrm{H};\min}(\theta)$ to $S_{\mathrm{H};k}(\theta)=S_{\mathrm{H};\min}(\theta)+\Sigma_{s=0}^L\Sigma_{s'=0}^s(\mathcal{C}^*_{s'\,\alpha_s}\mathcal{B}^{\alpha_s}_{s'})(\theta)$, being a proper solution[1] in $\Pi T^*\mathcal{M}_k=\{\Gamma^{p_k}_k(\theta)\}$,

$$\Gamma^{p_k}_k(\theta)=(\Gamma^{p_{\min}}_{\min},\mathcal{C}^{\alpha_s}_{s'},\mathcal{B}^{\alpha_s}_{s'},\mathcal{C}^*_{s'\,\alpha_s},\mathcal{B}^*_{s'\,\alpha_s})(\theta),\quad s'=0,\ldots,s,\quad s=0,\ldots,L,$$

$$(\vec{\varepsilon},\mathrm{gh})\mathcal{C}^{\alpha_s}_{s'}(\theta)=(\vec{\varepsilon}_{\alpha_s}+(s+1)(1,0,1),2s'-s-1)=(\vec{\varepsilon},\mathrm{gh})\mathcal{B}^{\alpha_s}_{s'}(\theta)+((1,0,1),-1)$$

[henceforth we assume $k=\mathrm{ext}$ and take into account that $(\vec{\varepsilon},\mathrm{gh})\Phi^*_{A_k}(\theta)=-((1,0,1),1)-(\vec{\varepsilon},\mathrm{gh})\Phi^{A_k}(\theta)$], with the pyramids of ghosts and Nakanishi–Lautrup superfields, and with a

deformation in the Planck constant $\hbar$. Then $S_{\mathrm{H};k}(\theta)$ determines the quantum action $S^{\Psi}_{\mathrm{H}}(\Gamma(\theta),\hbar)$, e.g., in case of an Abelian hypergauge defined as an anticanonical phase transformation:

$$\Gamma^{p_k}_k(\theta)\to\Gamma'^{p_k}_k(\theta)=\left(\Phi^{A_k}(\theta),\Phi^*_{A_k}(\theta)-\frac{\partial\Psi(\Phi(\theta))}{\partial\Phi^{A_k}(\theta)}\right):S^{\Psi}_{\mathrm{H}}(\Gamma(\theta),\hbar)=e^{\mathrm{ad}\Psi}S_{\mathrm{H};k}(\Gamma_k(\theta),\hbar). \tag{36}$$

The functions $(S^{\Psi}_{\mathrm{H}},S_{\mathrm{H};k})(\theta,\hbar)$ obey Eqs. (26) and (35) in case the $\hbar$-deformation of $S_{\mathrm{H;min}}(\theta)$ is a solution of these equations. It is known that this choice of equations ensures the integrability of a nonequivalent HS constructed from S^{Ψ}_{H}, $S_{\mathrm{H};k}$, as well as the anticanonical [preserving the volume element $dV_k(\theta)=\Pi_{p_k}d\Gamma^{p_k}_k(\theta)$] nature of this change of variables, corresponding to a θ-shift by a constant parameter μ along the corresponding HS solutions. In its turn, the quantum master equation

$$\Delta^k(\theta)\exp\left[\frac{i}{\hbar}E(\theta,\hbar)\right]=0,\quad E\in\{S^{\Psi}_{\mathrm{H}},S_{\mathrm{H};k}\} \tag{37}$$

determines a nonintegrable HS, with the respective anticanonical change of variables preserving $d\hat{V}_k(\theta)=\exp[(i/\hbar)E(\theta,\hbar)]dV_k(\theta)$. It is the latter nonintegrable HS with the Hamiltonian $S^{\Psi}_{\mathrm{H}}(\theta,\hbar)$ that is crucial, for $\theta=0$, in the BV formalism. This HS defines in $\Pi T^*\mathcal{M}_k$ a θ-local, but not nilpotent, generator of BRST transformations, $\tilde{s}^{l(\Psi)}(\theta)$, which is associated with its θ-nonintegrable consequence:

$$\partial^r_\theta(\Phi^{A_k},\Phi^*_{A_k})(\theta)=((\Phi^{A_k}(\theta),S^{\Psi}_{\mathrm{H}}(\theta,\hbar))_\theta,0),\quad \tilde{s}^{l(\Psi)}(\theta)=\frac{\partial}{\partial\theta}+\frac{\partial_r S^{\Psi}_{\mathrm{H}}(\theta,\hbar)}{\partial\Phi^*_{A_k}(\theta)}\frac{\partial_l}{\partial\Phi^{A_k}(\theta)}. \tag{38}$$

B. Duality between the BV and BFV superfield quantities

An embedding of a restricted LSM gauge algebra, described by $S_{\mathrm{H;min}}(\theta)$ and Eq. (35), into the gauge algebra of a general gauge theory in the Lagrangian formalism, see Eqs. (7)–(12), can be effectively realized by means of dual functional counterparts, with the opposite $(\varepsilon_P,\varepsilon)$-parity, of the action and antibracket, by analogy with the approach of Refs. 12 and 18. To this end, let us consider the functional

$$Z_k[\Gamma_k]=-\partial_\theta S_{\mathrm{H};k}(\theta),\quad(\vec{\varepsilon},\mathrm{gh})Z_k=((1,0,1),1)$$

on the supermanifold $\Pi T(\Pi T^*\mathcal{M}_k)=\{(\Gamma^{p_k}_k,\partial_\theta\Gamma^{p_k}_k)(\theta),k=\min\}$ with natural $(\varepsilon_P,\varepsilon)$-even, symplectic, and $(\varepsilon_P,\varepsilon)$-odd Poisson structures. These structures define an $(\varepsilon_P,\varepsilon)$-even functional $\{\cdot,\}$ with canonical pairs $\{(\Phi^{A_k}_k,\partial_\theta\Phi^*_{A_k}),(\partial_\theta\Phi^{A_k}_k,\Phi^*_{A_k})\}(\theta)$, and $(\varepsilon_P,\varepsilon)$-odd θ-local, $(\cdot,\cdot)^{(\Gamma_k,\partial_\theta\Gamma_k)}_\theta$, Poisson brackets. The latter act on the superalgebra $C^\infty(\Pi T(\Pi T^*\mathcal{M}_k)\times\theta)$ and provide a lifting of the antibracket $(\cdot,\cdot)_\theta$ defined on $\Pi T^*\mathcal{M}_k$. For arbitrary functionals $F_t[\Gamma_k]=\partial_\theta\mathcal{F}_t((\Gamma_k,\partial_\theta\Gamma_k)(\theta),\theta)$, $t=1,2$, one has the following correspondence between the Poisson brackets of opposite Grassmann grading:

$$\{F_1,F_2\}=\int\mathrm{d}\theta\left[\frac{\delta F_1}{\delta\Phi^{A_k}(\theta)}\frac{\delta F_2}{\delta\Phi^*_{A_k}(\theta)}-\frac{\delta_r F_1}{\delta\Phi^*_{A_k}(\theta)}\frac{\delta_l F_2}{\delta\Phi^{A_k}(\theta)}\right]=\int\mathrm{d}\theta(\mathcal{F}_1(\theta),\mathcal{F}_2(\theta))^{(\Gamma_k,\partial_\theta\Gamma_k)}_\theta,$$
$$(\mathcal{F}_1(\theta),\mathcal{F}_2(\theta))^{(\Gamma_k,\partial_\theta\Gamma_k)}_\theta\equiv[(\mathcal{L}_{A_k}\mathcal{F}_1)\mathcal{L}^{*A_k}\mathcal{F}_2-(\mathcal{L}^{*A_k}_r\mathcal{F}_1)\mathcal{L}^l_{A_k}\mathcal{F}_2](\theta), \tag{39}$$

where the Euler–Lagrange superfield derivative, e.g., with respect to $\Phi^*_{A_k}(\theta)$, for a fixed θ, has the form $\mathcal{L}^{*A_k}(\theta)=\partial/\partial\Phi^*_{A_k}(\theta)-(-1)^{\varepsilon_{A_k}+1}\partial_\theta\cdot\partial/\partial(\partial_\theta\Phi^*_{A_k}(\theta))$.

By construction, the functional Z_k is nilpotent:

$$\{Z_k, Z_k\} = \int \mathrm{d}\theta (S_{\mathrm{H};k}(\theta), S_{\mathrm{H};k}(\theta))_\theta = 0, \quad k = \min, \tag{40}$$

and, due to the absence of the additional time coordinate, is formally related to the BRST charge of a dynamical system with first-class constraints.[2] Indeed, after identifying $(\Gamma_k, \partial_\theta \Gamma_k)(0)$ with the phase-space coordinates of the minimal sector, canonical with respect to the $(\varepsilon_P, \varepsilon)$-even brackets in the framework of the BFV method[2] for first-class constrained systems of $(L+1)$-stage reducibility,

$$\begin{gathered}(q^i, p_i) = (\mathcal{A}^i, \partial_\theta \mathcal{A}_i^*)(0), \quad (C^{A_s}, \mathcal{P}_{A_s}) = \left((\partial_\theta^r \mathcal{C}^{\alpha_{s-1}}, \mathcal{C}^{\alpha_s}), (\mathcal{C}^*_{\alpha_{s-1}}, \partial_\theta \mathcal{C}^*_{\alpha_s})\right)(0), \\ A_s = (\alpha_{s-1}, \alpha_s), \quad s = 0, \ldots, L, \quad (C^{A_{L+1}}, \mathcal{P}_{A_{L+1}}) = (\partial_\theta^r \mathcal{C}^{\alpha_L}, \mathcal{C}^*_{\alpha_L})(0),\end{gathered} \tag{41}$$

the functional Z_k takes the form

$$Z_k[\Gamma_k] = T_{A_0}(q,p) C^{A_0} + \sum_{s=1}^{L+1} \mathcal{P}_{A_{s-1}} Z^{A_{s-1}}_{A_s}(q) C^{A_s} + O(C^2). \tag{42}$$

With allowance for the gauge algebra structure functions of the original L-stage-reducible restricted LSM described by the enhanced Eq. (11), the constraints $T_{A_0}(q,p)$ and the set of $(L+1)$-stage-reducible eigenvectors $Z^{A_{s-1}}_{A_s}(q)$ are defined by (the symbol T below stands for transposition)

$$\begin{gathered}T_{A_0}(q,p) = (S_{0,i}(q), -p_i \mathcal{R}_{0\ \alpha_0}^{\ i}(q)), \quad Z^{A_{s-1}}_{A_s}(q) = \mathrm{diag}(\mathcal{Z}^{\alpha_{s-2}}_{\alpha_{s-1}}, \mathcal{Z}^{\alpha_{s-1}}_{\alpha_s})(q), \\ s = 1, \ldots, L, \quad (Z^{A_L}_{A_{L+1}})^T(q) = (\mathcal{Z}^{\alpha_{L-1}}_{\alpha_L}, 0)^T(q),\end{gathered} \tag{43}$$

$$\begin{gathered}Z^{A_{s-2}}_{A_{s-1}} Z^{A_{s-1}}_{A_s} = T_{B_0} L^{A_{s-2} B_0}_{A_s}(q,p), \quad s = 1, \ldots, \quad L+1, \quad Z^{A_{-1}}_{A_0} \equiv T_{A_0}, \quad L^{A_{s-2}\beta_0}_{A_s} = 0, \\ L^{A_{s-2} j}_{A_s} = \mathrm{diag}(\mathcal{L}^{\alpha_{s-3} j}_{\alpha_{s-1}}, \mathcal{L}^{\alpha_{s-2} j}_{\alpha_s}), \quad \mathcal{L}^{\alpha_{-2} j}_{\alpha_0} = \mathcal{L}^{\alpha_{L-1} j}_{\alpha_{L+1}} = 0, \quad \mathcal{L}^{\alpha_{-1} j}_{\alpha_1}(q,p) = (-1)^{\varepsilon_j + 1} p_i \mathcal{K}^{ji}_{\alpha_1}(q).\end{gathered} \tag{44}$$

Relations (39)–(44) generalize, to the case of arbitrary reducible theories, the results of Ref. 18 concerning a dual description (for $\varepsilon_i = \varepsilon_{\alpha_0} = L = 0$) of the quantum action and classical master equation in terms of a nilpotent BRST charge.

By the rule (41), the variables $(\mathcal{C}^*_{s'\alpha_s}, \mathcal{B}^*_{s'\alpha_s}, \mathcal{B}^{\alpha_s}_{s'})(\theta)$ are identical to the respective ghost momenta $\mathcal{P}_{s'A_s}$, Lagrangian multipliers $\lambda_{s'A_s}$, and their conjugate momenta $\pi^{A_s}_{s'}$ in Ref. 2. Then a comparison of the superfields $\mathcal{C}^{\alpha_s}_{s'}(\theta)$, $s' = 0, \ldots, s$, selected from the nonminimal configuration space of an L-stage-reducible LSM, with the coordinates $C^{A_s}_{s'}$ selected from the nonminimal phase space of the corresponding $(L+1)$-stage-reducible dynamical system[2] demonstrates the only possible embedding of $\Pi T(\Pi T^* \mathcal{M}_{\mathrm{ext}})$ into the phase space of the BFV method. Indeed, for the coordinates $C^{A_{L+1}}_0$, $\mathrm{gh}(C^{A_{L+1}}_0) = -L-2$, there exists no preimage among $(\mathcal{C}^{\alpha_s}_{s'}, \partial_\theta \mathcal{C}^{\alpha_s}_{s'})(0)$, because the ghost number spectrum for the latter variables is bounded from below:

$$\min \mathrm{gh}(\mathcal{C}^{\alpha_s}_{s'}, \partial_\theta \mathcal{C}^{\alpha_s}_{s'}) = \mathrm{gh}(\mathcal{C}^{\alpha_L}_0) = -L-1.$$

As a consequence, the nilpotent functional $Z_k[\Gamma_k] = -\partial_\theta S_{\mathrm{H};k}(\theta)$, $k = \mathrm{ext}$, is embedded into the total BRST charge constructed by the prescription of Ref. 2.

It should be noted that the systems constructed with respect to the Hamiltonians $S^\Psi_{\mathrm{H}}(\Gamma(\theta), \hbar)$ and $S_{\mathrm{H};k}(\theta)$, $k = \min$, ext, are equivalently described by dual fermion functionals $Z_k[\Gamma_k]$ and $Z^\Psi[\Gamma] = -\partial_\theta S^\Psi_{\mathrm{H}}(\Gamma(\theta), \hbar)$, in terms of even Poisson brackets, for instance,

$$\partial^r_\theta \Gamma^p(\theta) = (\Gamma^p(\theta), S^\Psi_{\mathrm{H}}(\Gamma(\theta),\hbar))_\theta = -\{\Gamma^p(\theta), Z^\Psi[\Gamma]\}. \tag{45}$$

Thereby, BRST transformations in the Lagrangian formalism with Abelian hypergauges can be encoded by a formal BRST charge, $Z^\Psi[\Gamma]$, related to $Z_k[\Gamma_k]$, $k=\mathrm{ext}$, by a phase canonical transformation with the $(\varepsilon_P,\varepsilon)$-even phase $F^\Psi[\Phi]=\partial_\theta\Psi(\Phi(\theta))$,

$$Z^\Psi[\Gamma] = e^{\overline{\mathrm{ad}}F^\Psi} Z_k[\Gamma_k], \quad \overline{\mathrm{ad}}F^\Psi \equiv \{F^\Psi, \cdot\}. \tag{46}$$

On the assumption that an additional gauge invariance does not appear in deriving the restricted LSM from the initial general gauge theory, i.e., $\overline{m_s} \leqslant \overline{M_s}$, and, therefore, $L \leqslant L_g$, the problem of including the restricted LSM gauge algebra into the initial gauge algebra, defined by (2), (7), and (8), is solved with the help of a nilpotent functional on $\Pi T(\Pi T^*\mathcal{M}_k)=\{(\Gamma^{P_k}_k, \partial_\theta\Gamma^{P_k}_k)(\theta), \Gamma^{P_k}_k(\theta) = (\Gamma^{P_{\mathrm{CL}}}_{\mathrm{CL}}, \mathcal{C}^{\mathcal{A}_s}, \mathcal{C}^*_{\mathcal{A}_s})(\theta), s=0,1,\ldots,L_g, k=\mathrm{MIN}\}$, namely,

$$\hat{Z}_k[\Gamma_k] = Z[\mathcal{A}] + \sum_{s=0}^{L_g}\left[\int \mathrm{d}\theta_{s-1}\mathrm{d}\theta_s \mathcal{C}^*_{\mathcal{A}_{s-1}}(\theta_{s-1})\hat{\mathcal{Z}}^{\mathcal{A}_{s-1}}_{\mathcal{A}_s}(\theta_{s-1};\theta_s)\mathcal{C}^{\mathcal{A}_s}(\theta_s)(-1)^{\varepsilon_{\mathcal{A}_{s-1}}+s} + O(C^{\mathcal{A}_s})\right]$$

$$= \int \mathrm{d}\theta S_{\mathrm{L};k}((\Gamma_k, \partial_\theta\Gamma_k)(\theta),\theta). \tag{47}$$

Given the superfields $\mathcal{C}^{\mathcal{A}_s}$ introduced as simple ghosts $\mathcal{C}^{\alpha_s}$, although used for a description of a general gauge algebra, a representation of solutions to the generating equation $\{\hat{Z}_k,\hat{Z}_k\}=0$ as expansions in powers of $\mathcal{C}^{\mathcal{A}_s}$ can be controlled by an additional *generalized ghost number*, gh_g, $\mathrm{gh}_g(\hat{Z}_k)=0$, coinciding with the standard ghost number only in the sector of $(\Phi^{A_{\mathrm{MIN}}}, \Phi^*_{A_{\mathrm{MIN}}})(0)$, for $\mathrm{gh}(\mathcal{A}^I, C^{\mathcal{A}_s})=(0,1+s)$, and having the spectrum

$$\mathrm{gh}_g(\mathcal{A}^I, C^{\mathcal{A}_s}) = (0,1+s), \quad \mathrm{gh}_g(\Phi^*_{A_{\mathrm{MIN}}}) = -1 - \mathrm{gh}_g(\Phi^{A_{\mathrm{MIN}}}), \quad \mathrm{gh}_g(\theta,\partial_\theta) = (0,0).$$

Conditions (28), applied to $S_{\mathrm{L};k}(\theta)$ in case $(\varepsilon_P)_{\mathcal{A}_s}=(\varepsilon_P)_I=0$, $s=0,\ldots,L_g$, extract from $\hat{Z}_k$ the functional Z_k in (42), so that the $(\varepsilon_P,\varepsilon)$-even θ-density $S_{\mathrm{L};k}(\theta)$ lifts the function $S_{\mathrm{H};k}(\theta) \in C^\infty(\Pi T^*\mathcal{M}_{\mathrm{min}})$ to the superalgebra $C^\infty(\Pi T(\Pi T^*\mathcal{M}_{\mathrm{MIN}})\times\theta)$. In general, $S_{\mathrm{L};k}(\theta)$ does not obey the generalized master equation (35) with the antibracket (39) acting on $C^\infty(\Pi T(\Pi T^*\mathcal{M}_{\mathrm{MIN}}) \times\theta)$,

$$(S_{\mathrm{L};k}(\theta), S_{\mathrm{L};k}(\theta))^{(\Gamma_k,\partial_\theta\Gamma_k)}_\theta = \tilde{f}((\Gamma_k,\partial_\theta\Gamma_k)(\theta),\theta), \quad \tilde{f}(\theta) \in \ker\{\partial_\theta\}, \quad k=\mathrm{MIN}. \tag{48}$$

C. Local quantization

Leaving aside the realization of a reducible LSM on $\Pi T^*\mathcal{M}_{\mathrm{ext}}$, we now suppose that the model is described by a quantum action, $W(\theta,\hbar)=W(\theta)$, defined on an arbitrary antisymplectic manifold $\mathcal{N}$ without connection, $\dim\mathcal{N}=\dim\Pi T^*\mathcal{M}_{\mathrm{ext}}=\overline{n}+(n_-,n_+) +\Sigma^L_{r=0}(2r+3)(\overline{m_r} +(m_{r-},m_{r+}))$, with local coordinates $\Gamma^p(\theta)$ and a density function $\rho(\Gamma(\theta))$. A local antibracket, an invariant volume element, $\mathrm{d}\mu(\Gamma(\theta))$, and a nilpotent second-order operator, $\Delta^{\mathcal{N}}(\theta)$, are defined in terms of an $(\varepsilon_P,\varepsilon)$-odd Poisson bivector, $\omega^{pq}(\Gamma(\theta))=(\Gamma^p(\theta),\Gamma^q(\theta))^{\mathcal{N}}_\theta$, namely,

$$\mathrm{d}\mu(\Gamma(\theta)) = \rho(\Gamma(\theta))\mathrm{d}\Gamma(\theta),\ \Delta^{\mathcal{N}}(\theta) = \tfrac{1}{2}(-1)^{\varepsilon(\Gamma^q)}\rho^{-1}\omega_{qp}(\theta)\big(\Gamma^p(\theta),\rho(\Gamma^q(\theta),\ \cdot)^{\mathcal{N}}_\theta\big)^{\mathcal{N}}_\theta. \tag{49}$$

The definition of a generating functional of Green's functions $Z((\partial_\theta\varphi^*,\varphi^*,\partial_\theta\varphi,\mathcal{I})(\theta))\equiv Z(\theta)$ as a path integral, for a fixed θ, is possible, within perturbation theory, by introducing on $\mathcal{N}$ the Darboux coordinates, $\Gamma^p(\theta)=(\varphi^a,\varphi^*_a)(\theta)$, in a vicinity of solutions of the equations $\partial W(\theta)/\partial\Gamma^p(\theta)=0$, so that $\rho=1$ and $\omega^{pq}(\theta)=\mathrm{antidiag}(-\delta^a_b,\delta^a_b)$. The function

$$Z(\theta) = \int d\mu(\tilde{\Gamma}(\theta)) d\Lambda(\theta) \exp\{(i/\hbar)[W(\tilde{\Gamma}(\theta),\hbar) + X((\tilde{\varphi},\tilde{\varphi}^* - \varphi^*,\Lambda,\Lambda^*)(\theta),\hbar)|_{\Lambda^*=0} - ((\partial_\theta \varphi_a^*)\tilde{\varphi}^a + \tilde{\varphi}_a^* \partial_\theta^r \varphi^a - \mathcal{I}_a \Lambda^a)(\theta)]\} \tag{50}$$

depends on an extended set of sources,

$$(\partial_\theta \varphi_a^*, \partial_\theta^r \varphi^a, \mathcal{I}_a)(\theta) = (-J_a, \lambda^a, I_{0a} + I_{1a}\theta),$$

$$(\vec{\varepsilon}, \mathrm{gh}) \partial_\theta \varphi_a^* = (\vec{\varepsilon}, \mathrm{gh}) \mathcal{I}_a + ((1,0,1),1) = (\vec{\varepsilon}, -\mathrm{gh}) \varphi^a,$$

to the superfields $(\varphi^a, \varphi_a^*, \Lambda^a)(\theta)$, where $\Lambda^a(\theta) = (\lambda_0^a + \lambda_1^a \theta)$ are Lagrangian multipliers to independent non-Abelian hypergauges, see Ref. 21,

$$G_a(\Gamma(\theta)), a = 1, \ldots, \quad k = n + \sum_{r=0}^{L} (2r+3) m_r, \quad k = k_+ + k_-,$$

$$\mathrm{rank} \| \partial G_a(\theta) / \partial \Gamma^p(\theta) \|_{\partial W / \partial \Gamma = G = 0} = \overline{l}, \quad l = l_+ + l_- = k.$$

The functions $G_a(\Gamma(\theta))$, $(\vec{\varepsilon}, \mathrm{gh}) G_a = (\vec{\varepsilon}, \mathrm{gh}) \mathcal{I}_a$, determine a boundary condition for the gauge-fixing action, $X(\theta) = X((\Gamma, \Lambda, \Lambda^*)(\theta), \hbar)$,

$$\partial_r X(\theta) / \partial \Lambda^a(\theta)|_{\Lambda^* = \hbar = 0} = G_a(\theta),$$

defined on the direct sum $\mathcal{N}_{\mathrm{tot}} = \mathcal{N} \oplus \Pi T^* \mathcal{K}$ of the manifolds $\mathcal{N}$ and $\Pi T^* \mathcal{K} = \{(\Lambda^a, \Lambda_a^*)(\theta)\}$. Hypergauges in involution, $(G_a(\theta), G_b(\theta))_\theta^{\mathcal{N}} = G_c(\theta) U_{ab}^c(\Gamma(\theta))$, obey different types of unimodularity relations,[21] depending on a set of equations for which $X(\theta)$ may be a solution, independent from $W(\theta)$, in terms of the antibracket $(\cdot,\cdot)_\theta = (\cdot,\cdot)_\theta^{\mathcal{N}} + (\cdot,\cdot)_\theta^{\mathcal{K}}$ and the operator $\Delta(\theta) = (\Delta^{\mathcal{N}} + \Delta^{\mathcal{K}})(\theta)$, trivially lifted from $\mathcal{N}$ to $\mathcal{N}_{\mathrm{tot}}$,

$$1)\ (E(\theta), E(\theta))_\theta = 0, \quad \Delta(\theta) E(\theta) = 0;\ 2)\ \Delta(\theta) \exp\left[\frac{i}{\hbar} E(\theta)\right] = 0, \quad E \in \{W, X\}. \tag{51}$$

The functions $G_a(\theta)$, assumed to be solvable with respect to $\varphi_a^*(\theta)$, determine a Lagrangian surface, $\mathcal{Q} = \{(\varphi^*, \Lambda)(\theta)\} \subset \mathcal{N}_{\mathrm{tot}}$, on which the restriction $X(\theta)|_{\mathcal{Q}}$ is nondegenerate. Given this, integration over $(\tilde{\varphi}^*, \Lambda)(\theta)$ in Eq. (50) determines a function, for $\partial_\theta \varphi^a = \mathcal{I}_a = 0$, whose restriction to the Lagrangian surface $\{\varphi(\theta)\} \subset \mathcal{N}$ is also nondegenerate.

In view of the properties of $(W, X)(\theta)$, one can introduce an effective action $\Gamma(\theta) \equiv \Gamma(\varphi, \varphi^*, \partial_\theta^r \varphi, \mathcal{I})(\theta)$ defined, in the usual manner, by means of a Legendre transformation of $\ln Z(\theta)$ with respect to $\partial_\theta \varphi_a^*(\theta)$,

$$\Gamma(\theta) = \frac{\hbar}{i} \ln Z(\theta) + ((\partial_\theta \varphi_a^*) \varphi^a)(\theta), \quad \varphi^a(\theta) = -\frac{\hbar}{i} \frac{\partial_l \ln Z(\theta)}{\partial(\partial_\theta \varphi_a^*(\theta))}. \tag{52}$$

The analysis of the properties of $(Z, \Gamma)(\theta)$ is based on the following θ-nonintegrable Hamiltonian-like system, which contains an arbitrary $(\varepsilon_P, \varepsilon)$-even $C^\infty(\mathcal{N}_{\mathrm{tot}})$-function, $R(\theta) = R((\tilde{\Gamma}, \Lambda, \Lambda^*) \times (\theta), \hbar)$, with a vanishing ghost number:

$$\partial_\theta^r \tilde{\Gamma}^p(\theta) = -i\hbar\, T^{-1}(\theta) (\tilde{\Gamma}^p(\theta), T(\theta) R(\theta))_\theta|_{\Lambda^* = 0},$$

$$\partial_\theta^r \Lambda^a(\theta) = -2i\hbar\, T^{-1}(\theta) (\Lambda^a(\theta), T(\theta) R(\theta))_\theta|_{\Lambda^* = 0},$$

$$\partial^r_\theta(\varphi^*_a,\Lambda^*_a)(\theta)=0, \tag{53}$$

where the function $T((\tilde{\Gamma},\Lambda,\Lambda^*)(\theta),\hbar)\equiv T(\theta)$ has the form $T(\theta)=\exp[(i/\hbar)(W-X)(\theta)]$. Let us enumerate the properties of $(\mathrm{Z},\Gamma)(\theta)$.

1. The integrand in (50) is invariant, for $\partial_\theta\varphi^*=\partial_\theta\varphi=\mathcal{I}=0$, with respect to the *superfield BRST transformations*

$$\tilde{\Gamma}_{\mathrm{tot}}(\theta)=(\tilde{\Gamma},\Lambda,\Lambda^*)(\theta)\to(\tilde{\Gamma}_{\mathrm{tot}}+\delta_\mu\tilde{\Gamma}_{\mathrm{tot}})(\theta),\ \delta_\mu\tilde{\Gamma}_{\mathrm{tot}}(\theta)=\ (\partial^r_\theta\tilde{\Gamma}_{\mathrm{tot}})|_{\check{\Gamma}_{\mathrm{tot}}}\mu, \tag{54}$$

having the form of a θ-shift by a constant parameter μ along an arbitrary solution $\check{\Gamma}_{\mathrm{tot}}(\theta)$ of the system (53), or, equivalently, along a vector field determined by the right-hand side of (53), for $R(\theta)=1$. Here, the arguments of $(W,X)(\theta)$ are the same as in definition (50). The above statement can be verified with the help of the identities

$$\partial_r X(\theta)/\partial F(\theta)|_{\Lambda^*=0}=\partial_r(\,X(\theta)|_{\Lambda^*=0})/\partial F(\theta),\quad F\in\{\Gamma^p,\Lambda^a\}.$$

Notice that the system (53), for $R(\theta)=\mathrm{const}$, admits the integral $(W+X)(\theta)$ in case W and X obey the first system in (51).

2. The vacuum function $\mathrm{Z}_X(\theta)\equiv\mathrm{Z}(0,\varphi^*,0,0)(\theta)$ is gauge-independent, namely, it does not change when $X(\theta)$ is replaced by an $(X+\Delta X)(\theta)$ subject to the same system in (51) that holds for $X(\theta)$ and conforming to nondegeneracy on the surface $\mathcal{Q}$. Indeed, this hypothesis implies that the variation $\Delta X(\theta)$ obeys a system of linearized equations with a nilpotent operator $Q_j(X)$, $j=1,2$,

$$Q_j(X)\Delta X(\theta)=0,\ \delta_{j1}\Delta(\theta)\Delta X(\theta)=0;\ Q_j(X)=\mathrm{ad}X(\theta)-\delta_{j2}(i\hbar\Delta(\theta)), \tag{55}$$

where j is identical to the number that labels that system in Eq. (51) for which $X(\theta)$ is a solution. Using the fact that solutions $X(\theta)$ of every system in (51) are proper, one can prove, by analogy with the theorems of Ref. 29, that the cohomologies of the operator $Q_j(X)$ on the functions $f(\Gamma_{\mathrm{tot}}(\theta))\in C^\infty(\mathcal{N}_{\mathrm{tot}})$ vanishing for $\Gamma_{\mathrm{tot}}(\theta)=0$ are trivial. Hence, the general solution of Eq. (55) has the form

$$\Delta X(\theta)=Q_j(X)\Delta Y(\theta),\ \left(\vec{\varepsilon},\mathrm{gh},\frac{\partial}{\partial\theta}\right)\Delta Y(\theta)=((1,0,1),-1,0),\ \ \Delta Y(\theta)|_{\Gamma_{\mathrm{tot}}=0}=0, \tag{56}$$

with a certain $\Delta Y(\theta)$. Now, making in $\mathrm{Z}_{X+\Delta X}(\theta)$ a change of variables induced by a θ-shift by a constant μ, related to the system (53), and choosing

$$2R(\theta)\mu=\Delta Y(\theta),$$

we find that $\mathrm{Z}_{X+\Delta X}(\theta)=\mathrm{Z}_X(\theta)$, and conclude that the S-matrix is gauge-independent in view of the equivalence theorem.[30] [Properties 1, 2 of $\mathrm{Z}_X(\theta)|_{\varphi^*=0}$ are valid for arbitrary $\rho(\theta)$, $\Gamma^p(\theta)$ on the manifold $\mathcal{N}$.]

The above proof shows, due to (54), that the system (53) encodes the BRST transformations for $R(\theta)=\mathrm{const}$, as well as continuous anticanonical-like transformations in an infinitesimal form, with the scalar fermionic generating function $R(\theta)\mu$, where $R(\theta)$ is arbitrary and μ is constant.

Equivalently, following the ideas of Sec. IV B, the above characteristics of the generating functional of Green's functions can be derived from a Hamiltonian-like system presented in terms of an even superfield Poisson bracket in general coordinates,

$$\partial^r_\theta\tilde{\Gamma}^p(\theta)=-\{\tilde{\Gamma}^p(\theta),Z^W[\tilde{\Gamma}]-(Z^X+i\hbar Z^R)[\tilde{\Gamma}_{\mathrm{tot}}]\}|_{\Lambda^*=0},$$

$$\partial^r_\theta\Lambda^a(\theta)=-2\{\Lambda^a(\theta),Z^W[\tilde{\Gamma}]-(Z^X+i\hbar Z^R)[\tilde{\Gamma}_{\mathrm{tot}}]\}|_{\Lambda^*=0},$$

$$\partial_\theta^r(\varphi_a^*,\Lambda_a^*)(\theta)=0 \tag{57}$$

with a linear combination of fermionic functionals related to the above actions and a bosonic function by the rule

$$Z^E[\Gamma_{\mathrm{tot}}]=-\partial_\theta E(\Gamma_{\mathrm{tot}}(\theta),\hbar),\quad E\in\{W,X,R\}. \tag{58}$$

If the actions $(W,X)(\theta)$ obey the first system in (51), then the functionals Z^W, Z^X, formally playing the role of the usual and *gauge-fixing* BRST charges, are nilpotent with respect to the even Poisson bracket $\{\cdot,\cdot\}=\{\cdot,\cdot\}^{\Pi TM}+\{\cdot,\cdot\}^{\Pi TK}$. Here, for instance, the first bracket in the sum is defined on arbitrary functionals on $\Pi TM\times\{\theta\}$, via a θ-local extension of the odd bracket $(\cdot,\cdot)_\theta^{\Pi TM}$ in (39), as follows:

$$\begin{aligned}&\{F_1,F_2\}^{\Pi TM}\equiv\int \mathrm{d}\theta\frac{\delta_r F_1}{\delta\Gamma^p(\theta)}\omega^{pq}(\Gamma(\theta))\frac{\delta_l F_2}{\delta\Gamma^q(\theta)}=\partial_\theta(\mathcal{F}_1(\theta),\mathcal{F}_2(\theta))_\theta^{\Pi TM},\\&(\mathcal{F}_1(\theta),\mathcal{F}_2(\theta))_\theta^{\Pi TM}\equiv((\mathcal{L}_p^r\mathcal{F}_1)\omega^{pq}(\Gamma(\theta))\mathcal{L}_q^l\mathcal{F}_2)(\theta),\quad F_t[\Gamma]=\partial_\theta\mathcal{F}_t((\Gamma,\partial_\theta\Gamma)(\theta),\theta),\end{aligned} \tag{59}$$

where $\mathcal{L}_q^l(\theta)$ is the left-hand Euler–Lagrange superfield derivative with respect to $\Gamma^q(\theta)$. [The antibracket $(\cdot,\cdot)_\theta^{\Pi TM}$, identical, for $\mathcal{N}=\Pi TM_k$, with $(\cdot,\cdot)_\theta^{(\Gamma_k,\partial_a\Gamma_k)}$, $k=$ext, in (39) lifts the operator $\Delta^{\mathcal{N}}$ in (49) to the nilpotent operator $\Delta^{\Pi TM}$ acting in $C^\infty(\Pi TM\times\{\theta\})$, defined exactly as $\Delta^{\mathcal{N}}(\theta)$, although in terms of the antibracket (59).]

Therefore, as in the case of the HS in (45), we arrive at an interpretation of BRST transformations, for a gauge theory with non-Abelian hypergauges in Lagrangian formalism, in terms of the formal "BRST charges" Z^W, Z^X, as well as in terms of the functional Z^R and the even Poisson bracket. [The construction of the latter bracket is different from that of Ref. 5, where an odd superfield Poisson bracket was derived from a (t,θ)-local even bracket; however, it is similar to the construction of Ref. 18; see Eq. (27).] The system (57) encodes the BRST transformations, for $Z^R=0$, as well as the BRST and continuous canonical-like transformations with the bosonic generating functional $Z^R\mu$, for an arbitrary Z^R and a constant μ.

3. The functions $(\mathrm{Z},\Gamma)(\theta)$ obey the Ward identities

$$\begin{aligned}&\left[\left\{\partial_\theta\varphi_a^*(\theta)-\left(\frac{\partial W}{\partial\tilde{\varphi}^a(\theta)}\right)\left(i\hbar\frac{\partial_l}{\partial(\partial_\theta\varphi^*)},i\hbar\frac{\partial_r}{\partial(\partial_\theta^r\varphi)}\right)\right\}\frac{\partial_l}{\partial\varphi_a^*(\theta)}+\frac{i}{\hbar}\mathcal{I}_a(\theta)\frac{\partial_l}{\partial\Lambda_a^*(\theta)}\right.\\&\left.X\left(i\hbar\frac{\partial_l}{\partial(\partial_\theta\varphi^*)},i\hbar\frac{\partial_r}{\partial(\partial_\theta^r\varphi)}-\varphi^*,\frac{\hbar}{i}\frac{\partial_l}{\partial\mathcal{I}},\Lambda^*\right)\Big|_{\Lambda_a^*=0}\right]\mathrm{Z}(\theta)=0,\end{aligned} \tag{60}$$

$$\begin{aligned}&\mathcal{I}_a(\theta)\frac{\partial_l}{\partial\Lambda_a^*(\theta)}\;X\left(\varphi^b+i\hbar(\Gamma''^{-1})^{bc}\frac{\partial_l}{\partial\varphi^c},i\hbar\frac{\partial_r}{\partial(\partial_\theta^r\varphi)}-\frac{\partial_r\Gamma}{\partial(\partial_\theta^r\varphi)}-\varphi^*,\frac{\partial_l\Gamma}{\partial\mathcal{I}}+\frac{\hbar}{i}\frac{\partial_l}{\partial\mathcal{I}},\Lambda^*\right)\Big|_{\Lambda_a^*=0}-\left[\left(\frac{\partial W}{\partial\tilde{\varphi}^a(\theta)}\right)\right.\\&\left.\times\left(\varphi^b+i\hbar(\Gamma''^{-1})^{bc}\frac{\partial_l}{\partial\varphi^c},i\hbar\frac{\partial_r}{\partial(\partial_\theta^r\varphi)}-\frac{\partial_r\Gamma}{\partial(\partial_\theta^r\varphi)}\right)\right]\frac{\partial_l\Gamma(\theta)}{\partial\varphi_a^*(\theta)}+\frac{1}{2}(\Gamma(\theta),\Gamma(\theta))_\theta^{(\Gamma)}=0,\end{aligned} \tag{61}$$

with the notation

$$\Gamma''_{ab}(\theta)\equiv\frac{\partial_l}{\partial\varphi^a(\theta)}\frac{\partial_r}{\partial\varphi^b(\theta)}\Gamma(\theta),\quad \Gamma''_{ac}(\theta)(\Gamma''^{-1})^{cb}(\theta)=\delta_a{}^b.$$

In the symmetric form of these identities, we have extended the standard set of sources $\partial_\theta\varphi_a^*(\theta)$ used in the definition of the generating functional of Green's functions in Abelian hypergauges.

The technique used in deriving the above identities is analogous to the corresponding procedure of Refs. 31 and 32 applied, in the framework of the BV[1] and Batalin–Lavrov–Tyutin[29]

methods, to the problem of gauge dependence in theories with composite fields. Thus, identities (60) and (61) follow from the corresponding system in (51) for $(W,X)(\theta)$. For instance, making the functional averaging of the second system in (51) for $X(\theta)$,

$$\int \mathrm{d}\Lambda(\theta)\mathrm{d}\mu(\tilde{\Gamma}(\theta))\exp\left[\frac{i}{\hbar}(W-(\partial_\theta\varphi_a^*)\tilde{\varphi}^a-\tilde{\varphi}_a^*\partial_\theta^r\varphi^a+\mathcal{I}_a\Lambda^a)(\theta)\right]$$
$$\times\left\{\Delta(\theta)\exp\left[\frac{i}{\hbar}X((\tilde{\varphi},\tilde{\varphi}^*-\varphi^*,\Lambda,\Lambda^*)(\theta),\hbar)\right]\right\}_{\Lambda^*=0}=0, \tag{62}$$

and integrating by parts in (62), with allowance for $(\partial/\partial\tilde{\varphi}^*+\partial/\partial\varphi^*)X(\theta)=0$, we obtain identity (60). Identities (60) and (61) take the standard form in case $\partial_\theta\varphi^a=\mathcal{I}_a(\theta)=\theta=0$, which becomes more involved due to the quantities $(\partial_\theta W(\theta)/\partial\tilde{\varphi}^a(\theta))$, in the case of non-Abelian hypergauges.

In the special case of Abelian hypergauges, $G_A((\Phi,\Phi^*)(\theta))=\Phi_A^*(\theta)-\partial\Psi(\Phi(\theta))/\partial\Phi^A(\theta)=0$, corresponding to the change of variables (36), for $(\varphi,\varphi^*,W)=(\Phi,\Phi^*,S_{\mathrm{H;ext}})$, $\partial_\theta\Phi^A=\mathcal{I}_A=0$ (locally, $\mathcal{N}=\Pi T^*\mathcal{M}_{\mathrm{ext}}$), the object $\mathrm{Z}(\partial_\theta\Phi^*,\Phi^*)(\theta)$ takes the form

$$\mathrm{Z}(\partial_\theta\Phi^*,\Phi^*)(\theta)=\int \mathrm{d}\Phi(\theta)\exp\left\{\frac{i}{\hbar}[S_{\mathrm{H}}^{\Psi}(\Gamma(\theta),\hbar)-((\partial_\theta\Phi_A^*)\Phi^A)(\theta)]\right\}. \tag{63}$$

A θ-local BRST transformation for $\mathrm{Z}(\partial_\theta\Phi^*,\Phi^*)(\theta)$ is given, for an HS defined on $\Pi T^*\mathcal{M}_{\mathrm{ext}}$, with the Hamiltonian $S_{\mathrm{H}}^{\Psi}(\theta,\hbar)$ and a solution $\check{\Gamma}(\theta)$, by the change of variables

$$\Gamma^p(\theta)\to\Gamma^{(1)p}(\theta)=\exp[\mu s^{l(\Psi)}(\theta)]\Gamma^p(\theta),\quad s^{l(\Psi)}(\theta)\equiv\frac{\partial}{\partial\theta}-\mathrm{ad}S_{\mathrm{H}}^{\Psi}(\theta,\hbar). \tag{64}$$

Transformation (64) with a constant μ is anticanonical, with

$$\mathrm{Ber}\left\|\frac{\partial\Gamma^{(1)}(\theta)}{\partial\Gamma(\theta)}\right\|=\mathrm{Ber}\left\|\frac{\partial\Phi^{(1)}(\theta)}{\partial\Phi(\theta)}\right\|=1,$$

provided that $S_{\mathrm{H}}^{\Psi}(\theta,\hbar)$ is subject to the first system in (51).

The obvious permutation rule of the functional integral, $\varepsilon(\mathrm{d}\Phi(\theta))=0$,

$$\partial_\theta\int \mathrm{d}\Phi(\theta)\mathcal{F}((\Phi,\Phi^*)(\theta),\theta)=\int \mathrm{d}\Phi(\theta)\left[\frac{\partial}{\partial\theta}+(\partial_\theta V)(\theta)\right]\mathcal{F}(\theta),\ (\partial_\theta V)(\theta)=\partial_\theta\Phi_A^*(\theta)\frac{\partial}{\partial\Phi_A^*(\theta)},$$

yields, for $i\hbar\partial_\theta^r\ln\mathrm{Z}(\theta)=(\partial_\theta\Phi_A^*\partial_\theta^r\Phi^A)(\theta)-\partial_\theta^r\Gamma(\theta)$, the following relations:

$$\partial_\theta\mathrm{Z}(\theta)|_{\check{\Gamma}(\theta)}=(\partial_\theta V)(\theta)\mathrm{Z}(\theta)=0,\qquad \partial_\theta^r\Gamma(\theta)|_{\check{\Gamma}(\theta)}=(\Gamma(\Gamma(\theta)),\Gamma(\Gamma(\theta)))_\theta=0. \tag{65}$$

When deriving Eq. (65), we have taken into account the fact that the functional averaging of the HS with respect to $\mathrm{Z}(\theta)$ and $\Gamma(\theta)$ has the form

$$\langle\partial_\theta^r\Gamma^p\rangle|_{\mathrm{Z}}=\left(\frac{\hbar}{i}\mathrm{Z}^{-1}\frac{\partial\mathrm{Z}(\theta)}{\partial\Phi_A^*(\theta)},-\partial_\theta\Phi_A^*(\theta)\right),\quad \langle\partial_\theta^r\Gamma^p\rangle=(\langle\Gamma^p(\theta)\rangle,\Gamma(\langle\Gamma(\theta)\rangle))_\theta=\partial_\theta^r\langle\Gamma^p\rangle, \tag{66}$$

without the sign of average in (65) for $\check{\Gamma}^p(\theta)$ and $\Gamma^p(\theta)$. Expressions (65) relate the explicit form of the Ward identities in a theory with Abelian hypergauges to the invariance of the generating functional of Green's functions with respect to the superfield BRST transformations.

V. CONNECTION BETWEEN LAGRANGIAN QUANTIZATIONS

The problem of establishing a correspondence between a LSM and a usual gauge theory can be solved on the basis of a component form of the local quantization in the following two ways: one is applicable to an arbitrary LSM, another applies to theories of Yang–Mills type. This makes

it possible to establish a relation of the local superfield scheme with the known formulations of Lagrangian quantization,[1,21] as well as with an extension (proposed in the following) of the superfield method[6,7] to the case of general coordinates.

A. Component formulation and its relation to Batalin–Vilkovisky, Batalin–Tyutin, and superfield methods

The objects of θ-local quantization in the Lagrangian and Hamiltonian formulations are related to the conventional description of a gauge theory by means of a component representation of the variables $\Gamma^{P_{\mathrm{MIN}}}_{\mathrm{MIN}}$, $\Gamma^{p_k}_k$, Λ^a, $\mathcal{I}_a$, $\Gamma^{p_k}_k(\theta)=\Gamma^{p_k}_{0k}+\Gamma^{p_k}_{1k}\theta$, $k=\mathrm{tot}$, under the restriction $\theta=0$, for instance, $(\mathcal{M},\mathcal{N}_k,\Lambda^a,\mathcal{I}_a)\to(\widetilde{\mathcal{M}},\ \mathcal{N}_k|_{\theta=0}=\{\Gamma^{p_k}_{0k}\},\lambda^a_0,I_{0a})$. Extracting a standard field model from a classical description of a general gauge theory can be effected, in addition to $\theta=0$, by various kinds of eliminating the functions $\partial_\theta\mathcal{A}^I(\theta)$, $\mathcal{A}^*_I(\theta)$, as well as the superfields $\mathcal{A}^I(\theta)$ that contain objects with an incorrect spin-statistics relation, $\varepsilon_P(\mathcal{A}^I)\neq 0$. A possible way of such elimination is provided by the conditions $\mathrm{gh}(\mathcal{A}^I)=-1-\mathrm{gh}(\mathcal{A}^*_I)=0$, $(\varepsilon_P)_I=0$, and $(\mathrm{gh},\partial/\partial\theta)S_{\mathrm{L(H)}}(\theta)=(0,0)$, mentioned in Sec. IV A. Another possibility is related to superfield BRST transformations for theories of Yang–Mills type,[10,33,34] in which a Lagrangian classical action $S_{\mathrm{LYM}}(\theta)=S_{\mathrm{L}}(\mathcal{A},\mathcal{D}_\theta\mathcal{A},\widetilde{\mathcal{A}},\mathcal{D}_\theta\widetilde{\mathcal{A}})(\theta)$ is defined in terms of generalized Yang–Mills superfields, $\mathcal{A}^{Bu}(z)$, $\mathcal{A}^{Bu}=(\mathcal{A}^{\mu u},\mathcal{C}^u)$, $u=1,\ldots,r$, and matter superfields, $\widetilde{\mathcal{A}}(z)=(\Psi^\varrho,\overline{\Psi}^\sigma,\varphi^f,\varphi^{+g})(z)$, where Ψ^ϱ, $\overline{\Psi}^\sigma$, ϱ, $\sigma=1,\ldots,k_1$, are spinor superfields, and φ^g, φ^{+h}, g, $h=1,\ldots,k_2$, are spinless ones. The superfields $\mathcal{A}^{Bu}(z)$ and $\widetilde{\mathcal{A}}(z)$ are defined on the superspace $\mathcal{M}=\mathbb{R}^{1,3}\times\widetilde{P}=\{z^B=(x^\mu,\theta)\}$ and take values, respectively, in the adjoint and vector representation spaces of an r-parametric Lie group. The action $S_{\mathrm{LYM}}(\theta)$ can be written as

$$S_{\mathrm{LYM}}(\theta)=\int \mathrm{d}^4x\left[\frac{1}{4}\mathcal{G}_{BC}{}^u\mathcal{G}^{CBu}(-1)^{\varepsilon_B}-i\overline{\Psi}^\sigma\gamma^B\nabla_{B\varrho}{}^\sigma\Psi^\varrho-\overline{\nabla}_{Bg}{}^h\varphi^{+g}\nabla^{Bh}{}_f\varphi^f+M(\widetilde{\mathcal{A}})\right](z), \tag{67}$$

with an $\widetilde{\mathcal{A}}(z)$-local gauge-invariant polynomial $M(\widetilde{\mathcal{A}})$, containing no derivatives over z^B. In expression (67), we have introduced the superfield strength $\mathcal{G}_{BC}{}^u=i[\mathcal{D}_B,\mathcal{D}_C]^u=\partial_B\mathcal{A}^u_C-(-1)^{\varepsilon_B\varepsilon_C}\partial_C\mathcal{A}^u_B+f^{uvw}\mathcal{A}^v_B\mathcal{A}^w_C$, $\partial_B=(\partial_\mu,\partial_\theta)$ and the following covariant derivatives, expressed through the matrix elements of the Hermitian generators $\Gamma^u=\mathrm{diag}(T^u,\overline{T^u},\tau^\mu,\overline{\tau^\mu})$ of the corresponding Lie algebra:

$$(\mathcal{D}^{uv}_B,\nabla_{B\varrho}{}^\sigma,\nabla_{Bf}{}^e,\overline{\nabla}_{Bh}{}^g)=\partial_B(\delta^{uv},\delta^\sigma_\varrho,\delta^e_f,\delta^g_h)+(f^{uwv},-i(T^w)^\sigma_\varrho,-i(\tau^w)^e_f,-i(\overline{\tau^w})^g_h)\mathcal{A}^w_B, \tag{68}$$

where the coupling constant is absorbed into the completely antisymmetric structure coefficients f^{uvw}. We have also used a generalization of Dirac's matrices, $\gamma^B=(\gamma^\mu,\gamma^\theta)$, $\gamma^\theta=(\gamma^\theta)^+=\xi\mathbb{I}_4$, with a Grassmann scalar ξ, $(\vec{\varepsilon},\mathrm{gh})\xi=((1,0,1),-1)$. The $\vec{\varepsilon}$-grading and ghost number are nonvanishing for the superfields $(\Psi,\overline{\Psi},\mathcal{C}^u)$, namely, $\vec{\varepsilon}(\Psi,\overline{\Psi})=(0,1,1)$, $\vec{\varepsilon}(\mathcal{C}^u)=(1,0,1)$, $\mathrm{gh}(\mathcal{C}^u)=1$. The functional $Z[\mathcal{A},\widetilde{\mathcal{A}}]=\partial_\theta S_{\mathrm{LYM}}(\theta)$ is invariant under the infinitesimal general gauge transformations

$$\delta_g\mathcal{A}^I(\theta)=\delta_g(\mathcal{A}^{Bu};\widetilde{\mathcal{A}})(z)=-\int \mathrm{d}^5z_0(\mathcal{D}^{Buv}(z)(-1)^{\varepsilon_B};i\Gamma^v\widetilde{\mathcal{A}}(z)(-1)^{\varepsilon(\widetilde{\mathcal{A}})})\delta(z-z_0)\xi^v(z_0), \tag{69}$$

with arbitrary bosonic $(\vec{\varepsilon}_{\mathcal{A}_0}=\vec{0})$ functions $\xi^v(z_0)$ on $\mathcal{M}$, and with functionally independent generators $\hat{\mathcal{R}}^I_{\mathcal{A}_0}(\theta,\theta_0)\equiv\hat{\mathcal{R}}^I_{A_0}(\mathcal{A}(\theta),\theta,\theta_0)$. The condensed indices I, $\mathcal{A}_0$ of the theory in question, $(I;\mathcal{A}_0)=((B,u,\delta,\epsilon,f,h,x);(v,x_0))$, conform to the relations, $\overline{N}>\overline{n}$, $\overline{M}=\overline{m}$, $(\overline{m},\overline{M})=(\overline{m}_0,\overline{M}_0)$, provided that

$$\overline{N}=(4r+2k_2,r+8k_1),\quad \overline{M}=(r,0),\quad \overline{n}=\overline{N}-(0,r),$$

which holds for a reduced theory with the action [for $\theta=0$, the functional $S_{\mathrm{YM}}(0)=S_{0\mathrm{YM}}$ coincides with the corresponding classical action of Ref. 36] $S_{\mathrm{YM}}(\theta)=-S_{\mathrm{LYM}}(\mathcal{A},0,\widetilde{\mathcal{A}},0)(\theta)$ on $\mathcal{M}_{\mathrm{cl}}$

$=\{A^{\mu u},\tilde{\mathcal{A}}\}(z)$, in view of special *horizontality conditions* for the strength $\mathcal{G}_{BC}{}^{u}$ and certain subsidiary conditions for the matter superfields $\tilde{\mathcal{A}}(z)$ in Refs. 10 and 33,

$$\mathcal{G}_{BC}{}^{u}(z)=\mathcal{G}_{\mu\nu}{}^{u}(z),\quad (\nabla_{\theta\eta}^{\delta}\Psi^{\eta},\overline{\nabla}_{\theta\varrho}^{\sigma}\overline{\Psi}^{\varrho},\nabla_{\theta e}^{f}\varphi^{e},\overline{\nabla}_{\theta g}^{h}\overline{\varphi}^{g})(z)=(0,0,0,0). \tag{70}$$

To extract a standard component model defined on $\mathcal{M}_{\mathrm{cl}}|_{\theta=0}$ from a Hamiltonian LSM, it is sufficient to eliminate, for $\theta=0$, the antifields $\mathcal{A}_I^*(\theta)$ of a theory of Yang–Mills type, by analogy with the prescription (70), i.e., by taking into account the relation between $\mathcal{A}_I^*(\theta)$ and $\partial_\theta\mathcal{A}^I(\theta)$: see Sec. III and the final remarks (item 1) of the Conclusion.

For the restricted LSM used in the Feynman rules of Sec. IV, the reduction to the model of the multilevel formalism of Ref. 21 is realized by the conditions

$$\theta=0,\quad \partial_\theta\varphi_a^*=\partial_\theta\varphi^a=\varphi_a^*=\mathcal{I}_a=0. \tag{71}$$

In this case, the identification $(\rho,\omega^{pq})(\Gamma_0)=(M,E^{pq})(\Gamma_0)$ implies the coincidence of $(\cdot,\cdot)_\theta|_{\theta=0}$ and $\Delta(0)$ with their counterparts of Ref. 21. Then the first-level functional integral $Z^{(1)}$ and its symmetry transformations[21]

$$Z^{(1)}=\int \mathrm{d}\lambda_0\mathrm{d}\Gamma_0 M(\Gamma_0)\exp\left\{\frac{i}{\hbar}(W(\Gamma_0)+G_a(\Gamma_0)\lambda_0^a)\right\},$$

$$\delta\Gamma_0^p=(\Gamma_0^p,-W+G_a\lambda_0^a)\mu,$$

$$\delta\lambda_0^a=(-U_{cb}^a\lambda_0^b\lambda_0^c(-1)^{\varepsilon_c}+2i\hbar V_b^a\lambda_0^b+2(i\hbar)^2\tilde{G}^a)\mu,$$

coincide (λ_0^a being replaced by the notation π^a of Ref. 21), respectively, with $\mathrm{Z}_X(0)|_{\varphi_0^*=0}$ and the BRST transformations $\delta_\mu\Gamma_{0\,\mathrm{tot}}$ (having the opposite signs) generated by the system (53) for $R(\theta)=1$. This coincidence is guaranteed by the choice of $X(\theta)$ in the form

$$X(\theta)=\left\{G_a(\Gamma)\Lambda^a-\Lambda_a^*\left[\tfrac{1}{2}U_{cb}^a(\Gamma)\Lambda^b\Lambda^c(-1)^{\varepsilon_c}-i\hbar V_b^a(\Gamma)\Lambda^b-(i\hbar)^2\tilde{G}^a(\Gamma)\right]\right\}(\theta)+o(\Lambda^*), \tag{72}$$

where $(V_b^a,\tilde{G}^a)(\theta)$, together with $(U_{cb}^a,G_a)(\theta)$, define the unimodularity relations.[21] The relation of the θ-local quantization to the generating functional of Green's function $Z[J,\phi^*]$ of the BV method[1] is obvious from the identification $\mathrm{Z}(\partial_\theta\Phi^*,\Phi^*)(0)=Z[J,\phi^*]$ in (63), where the action $S_H^\Psi(\Gamma_0,\hbar)$ of (36) obeys Eq. (37).

Another aspect of the restriction $\theta=0$ is that an arbitrary function $\mathcal{F}(\theta)=\mathcal{F}((\Gamma,\partial_\theta\Gamma)(\theta),\theta)\in C^\infty(\Pi T\mathcal{N}\times\{\theta\})$ is represented by a functional $F[\Gamma]$ of the superfield methods[6,7] (in case $\Gamma^p=(\Phi^A,\Phi_A^*)$, see Sec. I)

$$F[\Gamma]=\int \mathrm{d}\theta\theta\mathcal{F}(\theta)=\mathcal{F}(\Gamma(0),\partial_\theta\Gamma,0)\equiv\mathcal{F}(\Gamma_0,\Gamma_1). \tag{73}$$

In the first place, formula (73) implies the independence of $F[\Gamma]$ from $\partial_\theta^r\Gamma^p(\theta)=\Gamma_1^p$, in case $F(\theta)=F(\Gamma(\theta),\theta)$. Second, formula (73) is fundamental in establishing a relation between the θ-local antibracket $(\cdot,\cdot)_\theta^{\mathcal{N}}$ and operator $\Delta^{\mathcal{N}}(\theta)$, acting on $C^\infty(N\times\{\theta\})$, with a generalization to arbitrary $(\Gamma,\omega^{pq},\rho)(\theta)$ of the flat functional operations $(\cdot,\cdot)$, Δ of Refs. 6 and 7, identical to their counterparts of the BV method in case $\Gamma^p=(\Phi^A,\Phi_A^*)$, $\omega^{pq}(\Gamma(\theta))=\mathrm{antidiag}(-\delta_B^A,\delta_B^A)$, $\rho(\theta)=1$, and in case of a different odd Poisson bivector, $\tilde{\omega}^{pq}(\Gamma(\theta),\theta')=(1+\theta'\partial_\theta)\omega^{pq}(\theta)$. The correspondence follows from

$$(\mathcal{F}(\theta),\mathcal{G}(\theta))_\theta^{\mathcal{N}}|_{\theta=0}=\frac{\delta_r\mathcal{F}(\Gamma_0)}{\delta\Gamma_0^p}\omega^{pq}(\Gamma_0)\frac{\delta_l\mathcal{G}(\Gamma_0)}{\delta\Gamma_0^q}=(F[\Gamma],G[\Gamma])^{\mathcal{N}},$$

$$(F[\Gamma],G[\Gamma])^{\mathcal{N}}=\partial_\theta\left[\frac{\delta_r F[\Gamma]}{\delta\Gamma^p(\theta)}\partial_{\theta'}\left(\tilde{\omega}^{pq}(\Gamma(\theta),\theta')\frac{\delta_l G[\Gamma]}{\delta\Gamma^q(\theta')}\right)\right](-1)^{\varepsilon(\Gamma^p)+1}, \tag{74}$$

$$\begin{gathered}\Delta^{\mathcal{N}}(\theta)\mathcal{F}(\theta)|_{\theta=0}=\Delta^{\mathcal{N}}(0)\mathcal{F}(\Gamma_0)=\Delta^{\mathcal{N}}F[\Gamma],\\ \Delta^{\mathcal{N}}=\tfrac{1}{2}(-1)^{\varepsilon(\Gamma^q)}\partial_\theta\partial_{\theta'}[\rho^{-1}[\Gamma]\tilde{\omega}_{qp}(\theta',\theta)(\Gamma^p(\theta),\rho[\Gamma](\Gamma^q(\theta'),\cdot)^{\mathcal{N}})^{\mathcal{N}}],\end{gathered} \tag{75}$$

where $(\rho[\Gamma],\tilde{\omega}_{pq}(\theta',\theta))=(\rho(\Gamma_0),\theta'\theta\omega_{pq}(\theta))$ and

$$\int \mathrm{d}\theta''\tilde{\omega}^{pd}(\theta',\theta'')\tilde{\omega}_{dq}(\theta'',\theta)=\theta\delta^p{}_q.$$

When establishing the correspondence with the operations $(\cdot,\cdot)$ and Δ of Refs. 6 and 7 in (74) and (75), we have used a relation between the superfield and component derivatives:

$$\delta_l/\delta\Gamma^p(\theta)=(-1)^{\varepsilon(\Gamma^p)}(\theta\delta_l/\delta\Gamma^p_0-\delta_l/\delta\Gamma^p_1),\quad \Gamma^p_1=(\lambda^A,-(-1)^{\varepsilon_A}J_A).$$

In general coordinates, the action of the sum and difference $\partial_\theta(V\pm U)^{\mathcal{N}}(0)$ for $\mathcal{N}=\Pi T^*\mathcal{M}_{\mathrm{ext}}|_{\theta=0}$ reduced to

$$\partial_\theta(V\pm U)(0)=\partial_\theta\Phi^*_A(\theta)\partial/\partial\Phi^*_A(0)\pm\partial_\theta\Phi^A(\theta)\partial_l/\partial\Phi^A(0),$$

is identical to the action of the generalized sum and difference of their counterparts V, U in Ref. 6:

$$\begin{gathered}\partial_\theta(V-(-1)^tU)^{\mathcal{N}}(\theta)\mathcal{F}(\theta)|_{\theta=0}=(\mathcal{S}^t(\theta),\mathcal{F}(\theta))^{\mathcal{N}}_\theta|_{\theta=0}=(V-(-1)^tU)^{\mathcal{N}}F[\Gamma]=(S^t[\Gamma],F[\Gamma])^{\mathcal{N}},\\ t=1,2,\\ \mathcal{S}^t(\theta)=(\partial_\theta\Gamma^p)\omega^t_{pq}(\Gamma(\theta))\Gamma^q(\theta),\quad S^t[\Gamma]=\partial_\theta\{\Gamma^p(\theta)\partial_{\theta'}\partial_\theta[\tilde{\omega}^t_{pq}(\theta,\theta')\Gamma^q(\theta')]\}=\mathcal{S}^t(0),\end{gathered} \tag{76}$$

where the functions $\omega^t_{pq}(\theta),\tilde{\omega}^t_{pq}(\theta,\theta')$, identical with $\omega_{pq}(\theta)$ and $\tilde{\omega}_{pq}(\theta,\theta')$ for $t=1$, are defined by

$$\tilde{\omega}^t_{pq}(\theta,\theta')=\theta\theta'\omega^t_{pq}(\theta')=-(-1)^{t+\varepsilon(\Gamma^p)\varepsilon(\Gamma^q)}\tilde{\omega}^t_{qp}(\theta',\theta),\quad \omega^t_{pq}(\theta)=(-1)^{\varepsilon(\Gamma^p)\varepsilon(\Gamma^q)+t}\omega^t_{qp}(\theta).$$

The $\vec{\varepsilon}$-bosonic quantities $\mathcal{S}^t(\theta)$ and $S^t[\Gamma]$ with a vanishing ghost number play the role of the symmetric Sp(2)-tensor S_{ab} $(a,b=1,2)$ and anti-Hamiltonian S_0 of Ref. 35, which define (in terms of extended antibrackets) the first-order operators of the modified triplectic algebra. In this case, the additional functions $\omega^2_{pq}(\theta),\tilde{\omega}^2_{pq}(\theta,\theta')$ may be considered as quantities that define another nonantisymplectic (non-Riemannian) nondegenerate structure on $\mathcal{N}$. The θ-local functional operators $\{\Delta^{\mathcal{N}},V^{\mathcal{N}},U^{\mathcal{N}}\}(\theta)$ anticommute for a fixed θ,

$$[E^{\mathcal{N}}_i(\theta),E^{\mathcal{N}}_j(\theta)]_+=0,\ i,j=1,2,3,\quad (E_1,E_2,E_3)=(\Delta,V,U), \tag{77}$$

provided that $\mathcal{S}^t(\theta)$ or $S^t[\Gamma]$ is subject to

$$\Delta^{\mathcal{N}}(\theta)\mathcal{S}^t(\theta)=0,\quad (\mathcal{S}^u(\theta),\mathcal{S}^v(\theta))^{\mathcal{N}}_\theta=0,\quad t,u,v=1,2. \tag{78}$$

Relations (78), which hold, due to Eqs. (74)–(77), also for functional objects (those without a θ-dependence), follow from the well-known properties of the antibracket (*bilinearity, graded antisymmetry, Leibniz rule, Jacobi identity*), and from the rule of antibracket differentiation by the operator $\Delta^{\mathcal{N}}(\theta)$. The system (78) determines the geometry of $\mathcal{N}$ by restricting the choice of both quantities $\omega^t_{pq}(\theta),\tilde{\omega}^t_{pq}(\theta,\theta')$. Notice that a solution of Eq. (78) always exists, for instance, $\omega^t_{pq}(\theta)=\mathrm{antidiag}(\delta^A_B,(-1)^t\delta^A_B)$.

B. Superfield functional quantization in general coordinates

Let us consider a generalization of the vacuum functional of the superfield method,[6,7] namely,

$$Z^{\mathcal{N}}_{X'} = \int \mathrm{d}\mu[\Gamma] q^{\mathcal{N}}[\Gamma] \exp\left\{ \frac{i}{\hbar}(W' + X' + \varkappa_2 S^2)[\Gamma] \right\}, \tag{79}$$

where $\varkappa_2$ is an arbitrary real number; W', X' are the quantum and gauge-fixing actions, defined on $\mathcal{N}$ and subject to the equations

$$\tfrac{1}{2}(W', W')^{\mathcal{N}} + \mathcal{V}W' = i\hbar\Delta^{\mathcal{N}}W', \quad \tfrac{1}{2}(X', X')^{\mathcal{N}} + \mathcal{U}X' = i\hbar\Delta^{\mathcal{N}}X', \tag{80}$$

while the integration measure and the weight functional $q^{\mathcal{N}}[\Gamma]$ have the form

$$\mathrm{d}\mu[\Gamma] = \rho[\Gamma]\tilde{\mathrm{d}}\Gamma, \quad \tilde{\mathrm{d}}\Gamma = \mathrm{d}\Gamma_0 \mathrm{d}\Gamma_1, \quad q^{\mathcal{N}}[\Gamma] = \delta(G^{\mathcal{V}}_{a_1}(\Gamma(\theta))), \quad a_1 = 1, \ldots, \quad \dim_+ \mathcal{N}. \tag{81}$$

In (80), we have introduced a two-parameter set $\mathcal{U}(\varkappa_1, \varkappa_2)$, $\mathcal{V}(\varkappa_1, \varkappa_2)$ of anticommuting operators,

$$\mathcal{U} = \tfrac{1}{2}(-1)^t \varkappa_t (S^t[\Gamma], \cdot)^{\mathcal{N}}, \quad \mathcal{V} = \tfrac{1}{2}\varkappa_t (S^t[\Gamma], \cdot)^{\mathcal{N}}, \tag{82}$$

satisfying, together with $\Delta^{\mathcal{N}}$, the algebra (77), for arbitrary real numbers $\varkappa_t$, whose choice admissible for the existence of the functional integral fixes the form of $Z^{\mathcal{N}}_{X'}$. This choice also fixes Eq. (80), the admissible boundary conditions for W', X', and the form of the *additional hypergauge conditions*, $G^{\mathcal{V}}_{a_1}(\Gamma(\theta)) = 0$, which are required to retain the explicit superfield form of the vacuum functional. The independent functions $G^{\mathcal{V}}_{a_1}(\Gamma(\theta))$ are equivalent to the set of functions $\mathcal{V}\Gamma^p(\theta)$: $G^{\mathcal{V}}_{a_1}(\theta_1) = \partial_\theta[Y_{a_1 p}(\Gamma(\theta_1), \theta)\mathcal{V}\Gamma^p(\theta)]$ with certain $Y_{a_1 p}(\theta_1, \theta)$ such that

$$\mathrm{rank}\left\| P_0(\theta)\frac{\delta_l E_t(\theta_1)}{\delta\Gamma^q(\theta)} \right\|_{\delta W'/\delta\Gamma = \delta X'/\delta\Gamma = G^{\mathcal{V}} = 0} = (L^{\mathcal{V}}_t, \dim_+\mathcal{N} - L^{\mathcal{V}}_t), \quad (E_1, E_2) = (G^{\mathcal{V}}_{a_1}, \mathcal{V}\Gamma^p), \tag{83}$$

for some integers $L^{\mathcal{V}}_1$, $L^{\mathcal{V}}_2$: $0 \leqslant L^{\mathcal{V}}_1$, $L^{\mathcal{V}}_2 \leqslant \dim_+ \mathcal{N}$.

The basic properties of the functional $Z^{\mathcal{N}}_{X'}$ are analogous to properties 1, 2 of $Z(\theta)$ in (50), which are encoded by a Hamiltonian-like system with an arbitrary functional $R[\Gamma]$, $(\vec{\varepsilon}, \mathrm{gh})R = (\vec{0}, 0)$,

$$\partial^r_\theta \Gamma^p(\theta) = \frac{\hbar}{i} T^{-1}[\Gamma](\Gamma^p(\theta), T[\Gamma]R)^{\mathcal{N}}, \quad T[\Gamma] = \exp\left[\frac{i}{\hbar}(W' - X' + \varkappa_1 S^1) \right]. \tag{84}$$

For instance, the *superfield BRST transformations* $\delta_\mu \Gamma^p(\theta) = \partial^r_\theta \Gamma^p(\theta)\mu$ for $Z^{\mathcal{N}}_{X'}$ are derived from (84), with $R = 1$, and from the additional equations

$$(G^{\mathcal{V}}_{a_1}(\Gamma(\theta)), W' - X' + \varkappa_1 S^1)^{\mathcal{N}} = 0 \Leftrightarrow \delta_\mu G^{\mathcal{V}}_{a_1}(\Gamma(\theta)) = 0, \tag{85}$$

which ensure the BRST invariance of $q^{\mathcal{N}}$. In order to be valid for any gauge theory with an admissible action, Eq. (85) imposes strong restrictions on all the quantities $Y_{a_1 p}(\theta_1, \theta)$, $\tilde{\omega}^t_{pq}(\theta, \theta')$, and consequently on the geometry of $\mathcal{N}$. For example, the constant functions $Y_{a_1 p}(\theta_1, \theta)$, $\tilde{\omega}^t_{pq}(\theta, \theta')$ belong to solutions of Eq. (85). We, however, do not restrict the consideration to this special case, assuming that Eq. (85) is fulfilled for any W', X'. Some remarks are in order concerning the status of the functional $q^{\mathcal{N}}[\Gamma]$. Here, we do not consider the possibility of presenting the functions $G^{\mathcal{V}}_{a_1}(\theta)$ by an integral over new additional superfields $\Lambda^{a_1}(\theta)$, following in part the prescription of Ref. 21 that introduces so-called "unimodularity involution relations" for $G^{\mathcal{V}}_{a_1}(\theta)$ and modifies the BRST transformations for the extended set of variables $(\Gamma^p, \Lambda^{a_1})(\theta)$.

Choosing

$$(\varkappa_t,\Gamma^p,\rho,\tilde{\omega}^t_{pq}(\theta,\theta'),Y_{a_1p}(\theta_1,\theta))=(1,(\Phi^A,\Phi^*_A),1,\theta\theta'\,\mathrm{antidiag}(\delta^A_B,(-1)^t\delta^A_B),\delta(\theta_1-\theta)\delta_{Ap}), \tag{86}$$

we obtain

$$(\mathcal{V},\mathcal{U},S^2,q^{\mathcal{N}})=(V,U,\partial_\theta(\Phi^*_A\Phi^A)(\theta),\delta(J_A)), \tag{87}$$

where $(V,U)=(-1)^{\varepsilon_A}\partial_\theta(-\Phi^*_A(\theta)\partial_\theta\delta/\delta\Phi^*_A(\theta),\Phi^A(\theta)\partial_\theta\delta_l/\delta\Phi^A(\theta))$, according to Ref. 6, and hence $Z^{\mathcal{N}}_{X'}$, as well as Eq. (80), and BRST transformations, implied by (84) for $R=1$, coincide, respectively, with the vacuum functional Z,

$$Z=\int \mathrm{d}\Phi\mathrm{d}\Phi^*\delta(\partial_\theta\Phi^*(\theta))\exp\left\{\frac{i}{\hbar}(W[\Phi,\Phi^*]+X[\Phi,\Phi^*]+\partial_\theta(\Phi^*_A\Phi^A))\right\},$$

with the equations $1/2(W,W)+VW=i\hbar\Delta W$, $1/2(X,X)-UX=i\hbar\Delta X$, for $W=W'$, $X=X'$, and with the BRST symmetry transformations[7] for Z (having the opposite signs in the r.h.s.)

$$\delta\Phi^A(\theta)=\mu U\Phi^A(\theta)+(\Phi^A(\theta),X-W)\mu,\quad \delta\Phi^*_A(\theta)=\mu V\Phi^*_A(\theta)+(\Phi^*_A(\theta),X-W)\mu.$$

In particular, choosing X in terms of the gauge fermion $\Psi[\Phi]=\Psi(\phi,\lambda)$, $X[\Phi,\Phi^*]=U\Psi[\Phi]$, first realized in Ref. 6, we obtain the generating functional of Green's functions $Z[\Phi^*]$ used in Sec. I in order to determine the superfield effective action in Abelian hypergauges.

A complete correspondence between $Z^{\mathcal{N}}_{X'}$ and the functional $Z_X(0)|_{\varphi^*_0=0}$ in (50) can be established as follows: First, the functional $\varkappa_2S^2$ is represented as $(1/2)(1+(-1)^t)\varkappa_tS^t$, so that the redefined actions

$$W''=W'+\tfrac{1}{2}\varkappa_tS^t,\ X''=X'+\tfrac{1}{2}(-1)^t\varkappa_tS^t \tag{88}$$

obey Eq. (80) without the operators $\mathcal{V}$ and $\mathcal{U}$. Second, the actions $W(\theta)$ in (50) and $W''[\Gamma]$, as well as the quantities $X(\theta)|_{\Lambda^*=0}$ in (50) and $X''[\Gamma]$, are related by formula (73). Third, the solvability of the hypergauges $G_a[\Gamma]$ with respect to the fields $\varphi^*_a(\theta)$, on condition that $\Lambda^a(\theta)=\partial^r_\theta\varphi^a(\theta)$, implies, together with the previous restriction, a linear dependence of $X''[\Gamma]$ on $\Lambda^a(\theta)$ and its independence from $\partial_\theta\varphi^*_a(\theta)$. Next, one should take into account the structure of the generating equation for $X''[\Gamma]$, as well as the second system in (51) with (72) for $X(\theta)$, and the fact that the corresponding systems (84) and (53), encoding the BRST transformations, coincide with each other. The latter requires the commutativity of $G_a[\Gamma]$ and the triviality of the unimodularity relations, i.e., $\Delta^{\mathcal{N}}G_a=V^a_b=\tilde{G}^a=0$. Finally, the measure $\mathrm{d}\mu[\Gamma]q^{\mathcal{N}}$ in (79) is made identical to $\mathrm{d}\mu(\Gamma(\theta))\mathrm{d}\Lambda(\theta)|_{\theta=0}$ in (50) by the choice $q^{\mathcal{N}}=\delta(\partial_\theta\varphi^*(\theta))$. This choice can be realized by $(\varkappa_t,\tilde{\omega}^t_{pq}(\theta,\theta'),a_1,Y_{a_1p}(\theta_1,\theta))=(1,\theta\theta'\,\mathrm{antidiag}(\delta^a_b,(-1)^t\delta^a_b),a,\delta(\theta_1-\theta)\delta_{a_1p})$.

VI. CONCLUSION

Let us summarize the main results of the present work:

We have proposed a θ-local description of an arbitrary reducible superfield theory as a natural extension of a usual gauge theory, defined on a configuration space $\mathcal{M}_{\mathrm{cl}}|_{\theta=0}$ of classical fields A^i, to a superfield model defined on extended cotangent, $T^*_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}}\times\{\theta\}$, and tangent, $T_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}}\times\{\theta\}$, odd bundles, in respective Hamiltonian and Lagrangian formulations. It is shown that the conservation under a θ-evolution (defined by a Hamiltonian or Lagrangian system providing a superfield extension of the usual extremals) of a Hamiltonian action $S_H((\mathcal{A},\mathcal{A}^*)(\theta),\theta)$, or, equivalently, of an odd counterpart of energy, $S_E((\mathcal{A},\partial_\theta\mathcal{A})(\theta),\theta)$, is equivalent, in view of Noether's first theorem, to the validity of a Hamiltonian or Lagrangian master equation, respectively.

Using non-Abelian hypergauges, we have constructed a θ-local superfield formulation of Lagrangian quantization for a reducible gauge model, extracted from a general superfield model by the conditions of a manifest θ-independence of the classical action and the vanishing of ghost number and auxiliary Grassmann parity (related to θ) for the action and $\mathcal{A}^I(\theta)$. In particular, we

have proposed a new superfield algorithm for constructing a first approximation to the quantum action in powers of ghosts of the minimal sector, on the basis of interpreting the reducibility relations as special gauge transformations of ghosts for an HS with the Hamiltonian chosen as the quantum action. To investigate the properties of BRST invariance and gauge-independence in a superfield form, for the introduced generating functionals of Green's functions (including the effective action), we have used *two equivalent* Hamiltonian-like systems. The first system is defined by a θ-local antibracket, in terms of a quantum action, a gauge-fixing action, and an arbitrary θ-local boson function, while the second (dual) system is defined by an even Poisson bracket, in terms of fermion functionals corresponding to the above functions. The two systems allow one to describe the BRST transformations and the continuous (anti)canonical-like transformations in a manner analogous to the relation between these transformations in the superfield Hamiltonian formalism.[5] We emphasize that, as a basis for the local quantization, we have intensely used the first-level formalism of Ref. 21, whose main ingredient is the vacuum functional (however, without recourse to the gauge-fixing action in a manifest form).

We have considered the problem of a *dual description* for an L-stage reducible gauge theory in terms of a BRST charge for a formal dynamical system with first-class constraints of $(L+1)$-stage reducibility. It is shown that this problem is a particular case of embedding a reducible special gauge theory into a general gauge theory of the same stage of reducibility.

We have proposed an extension of functional superfield quantization[6,7] to the case of general antisymplectic manifold without connection. It is shown that the condition of anticommutativity for all operators as well as the requirement of a correct transformation of the path integral measure impose strong restrictions on the geometry of the manifold as well as on *additional hypergauge conditions* that determine the measure.

We have established the coincidence of the first-level functional integral $Z^{(1)}$ in Ref. 21 with the local vacuum function of the proposed quantization scheme, in case $\theta=0$ and $\varphi^*(\theta)=0$, $Z_X(0)|_{\varphi_0^*=0}$. A correspondence is found between $Z_X(0)|_{\varphi_0^*=0}$ and the vacuum functional $Z_{X'}^{\mathcal{N}}$ of the proposed extension of the superfield quantization.[6,7] It is shown that the above functionals coincide only in Abelian hypergauges, with a trivial choice of the additional hypergauge conditions.

From the obtained results there follow the generating functional of Green's functions and the effective action of the first-level formalism.[21] It is observed that in case the quantum action $W'[\Gamma]$ depends on the superfields $\partial_\theta\Gamma^p(\theta)$, or the gauge-fixing action $X'[\Gamma]$ depends on the same superfields more than linearly, the functional $Z_{X'}^{\mathcal{N}}$ differs from $Z_X(0)|_{\varphi_0^*=0}$ exactly as the functional Z in Ref. 7 differs from $Z^{(1)}$ in Ref. 21.

In connection with the discussed points, the following open problems seem to be of interest:

1. One could obtain a Hamiltonian formulation of a LSM from a Lagrangian formulation in the case of a degenerate Hessian supermatrix $(S_L'')_{IJ}(\theta)$ in (5), and consider its relation to the standard component description of a model. In this case, Dirac's algorithm in terms of a θ-local antibracket, under the conservation of primary constraints in the course of θ-evolution along a vector field defined by an HS with a primary Hamiltonian in terms of antifields, would determine all antisymplectic constraints for the classical superfields $\Gamma^P_{\mathrm{CL}}(\theta)$. Among these constraints, there may exist a subsystem of second-class ones, in the case of the degeneracy of the supermatrix $\|\mathcal{L}^l_J(\theta_1)[\mathcal{L}^l_I(\theta_1)S_{\mathrm{L}}(\theta_1)(-1)^{\varepsilon_I}]\|_\Sigma$ in (6). It is interesting to apply the BFV method to construct, in terms of a θ-local Dirac's antibracket (the prescription for the first-level functional integral in terms of Dirac's antibracket was considered in Ref. 21), $(\cdot,\cdot)_{\theta D}$, a triplet of θ-local quantities $\widetilde{S}_{\mathrm{H}}(\theta)$, $\widetilde{\Omega}(\theta),\widetilde{\Psi}(\theta)$: $(\varepsilon_P,\varepsilon)$-even functions $\widetilde{S}_{\mathrm{H}}(\theta)$, $\widetilde{\Omega}(\theta)$, commuting with respect to $(\cdot,\cdot)_{\theta D}$ [by analogy with the Hamilton function and the BFV-BRST charge in a t-local field theory] and an $(\varepsilon_P,\varepsilon)$-odd function $\widetilde{\Psi}(\theta)$, which encodes the dynamics of a LSM and its first-class constraint algebra, as well as fixes the "gauge" arbitrariness in a space larger than $T^*_{\mathrm{odd}}\mathcal{M}_{\mathrm{CL}}\times\{\theta\}$. In this connection, it seems interesting to consider the question of how the construction of $\widetilde{S}_{\mathrm{H}}(\theta)$, $\widetilde{\Omega}(\theta)$ and of the "unitarizing Hamiltonian" $\widetilde{\mathcal{S}}_{\mathrm{H}}(\theta)=\widetilde{S}_{\mathrm{H}}(\theta)+(\widetilde{\Omega}(\theta),\widetilde{\Psi}(\theta))_{\theta D}$ is related to the quantum action of the BV method.

2. From the solution of the dual problem of Sec. IV B, found within the classical description,

there arise two natural questions: "How does the operator formulation of a formal dynamical system with a nilpotent BRST charge and a quantum counterpart of the even Poisson bracket correspond to the Lagrangian quantization of a gauge model?" and "What is related, in a Lagrangian formulation, to the formal supercommutator and the Hilbert space of states?" The mentioned problems appear to be related to the correspondence found in Ref. 37 between Poisson brackets and their operator counterparts of the opposite parity.

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On a classification of irreducible almost commutative geometries. III

Jan-Hendrik Jureit[a] and Chtistoph Stephan[b]
Centre de Physique Théoretique, CNRS-Luminy, Case 907, 13288 Marseille Cedex 9, France; Université de Provence; and Universität Kiel

Thomas Schücker[c]
Centre de Physique Théoretique, CNRS-Luminy, Case 907, 13288 Marseille Cedex 9, France; Université de Provence

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We extend a classification of irreducible, almost commutative geometries whose spectral action is dynamically nondegenerate to internal algebras that have four simple summands. © *2005 American Institute of Physics.*
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I. INTRODUCTION

A Yang-Mills-Higgs model is specified by choosing a real compact Lie group describing the gauge bosons and three unitary representations describing the left- and right-handed fermions and the Higgs scalars. Connes[1] remarks that the set of all Yang-Mills-Higgs models comes in two classes, Fig.1. The first is tiny and contains all those models that derive from gravity by generalizing Riemannian to almost commutative geometry. The intersections of this tiny class with the classes of left-right symmetric, grand unified, or supersymmetric Yang-Mills-Higgs models are all empty. However, the tiny class does contain the standard model of electromagnetic, weak, and strong forces with an arbitrary number of colors.

The first class is tiny, but still infinite and difficult to assess. We have started putting some order into this class. The criteria we apply are heteroclitic.[2]

Two criteria are simply motivated by simplicity: we take the internal algebra to be simple, or with two, three,… simple summands, we take the internal triple to be irreducible.

Two criteria are motivated from perturbative quantum field theory of the nongravitational part in flat time space: vanishing Yang-Mills anomalies and dynamical nondegeneracy. The latter imposes that the number of possible fermion mass equalities be restricted to the minimum, and that they be stable under renormalization flow. The origin of these mass equalities is the following. In almost commutative geometry, the fermionic mass matrix is the "Riemannian metric" of internal space, and as such becomes a dynamical variable. Its "Einstein equation" is the requirement that the fermionic mass matrix minimize the Higgs potential. Indeed, in almost commutative geometry, the Higgs potential is the "Einstein-Hilbert action" of internal space.

Two criteria are motivated from particle phenomenology: We want the fermion representation to be complex under the little group in each of its irreducible components, because we want to distinguish particles from antiparticles by means of unbroken charges. We want possible massless fermions to remain neutral under the little group, i.e., not to couple to massless gauge bosons.

Two criteria are motivated from the hope that, one day, we will have a unified quantum theory of all forces: vanishing mixed gravitational Yang-Mills anomalies and again dynamical nondegeneracy.

[a]Electronic mail: jureit@cpt.univ-mrs.fr>
[b]Electronic mail: Stephan@cpt.univ-mrs.fr
[c]Electronic mail: schucker@cpt.univ-mrs.fr

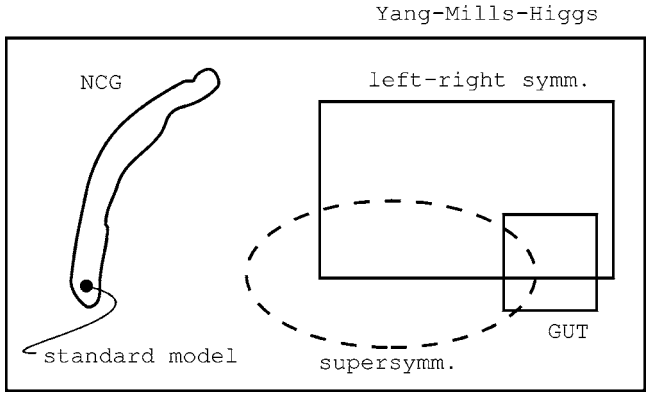

FIG. 1. Pseudoforces from noncommutative geometry.

Our analysis is based on a classification of all finite spectral triples by means of Krajewski diagrams[3] and centrally extended spin lifts of the automorphism group of their algebras.[4] The central extension serves two purposes: (i) It makes the spin lift of complex algebras $M_n(\mathbb{C})$ well defined. (ii) It allows the corresponding $U(n)$ anomalies to cancel.

Of course, we started with the case of a simple internal algebra. Here, there is only one contracted, irreducible Krajewski diagram and all induced Yang-Mills-Higgs models are dynamically degenerate.

The second case concerns algebras with two simple summands. It admits three contracted, irreducible Krajewski diagrams, one of them being a direct sum of two diagrams from the first case. The corresponding triples induce two Yang-Mills-Higgs models which are dynamically nondegenerate and anomaly free: SU(2) with a doublet of left-handed fermions and a singlet of right-handed fermions. The Higgs scalar is a doublet. Therefore, the little group is trivial, $SU(2)\rightarrow\{1_2\}$, and the fermion representation is real under the little group. The second model is the SO(2) submodel of the first.

The case of three summands has 41 contracted, irreducible diagrams plus direct sums. Its combinatorics is on the limit of what we can handle without a computer. There are only four induced models satisfying all criteria: The first is the standard model with C colors, $C\geqslant 2$, $SU(2)\times U(1)\times SU(C)$, with one generations of leptons and quarks and one colorless SU(2) doublet of scalars. The three others are submodels, $SO(2)\times U(1)\times SU(C)$, $SU(2)\times U(1)\times SO(C)$, and $SU(2)\times U(1)\times USp(C/2)$ and must have $C\geqslant 2$; the last submodel of course requires C even, $C\geqslant 4$.

In the following we push our classification to four summands. For simplicity we will only consider diagrams made of letter-changing arrows, i.e., we exclude arrows of type $a\bar{a}$ because, in the first three cases, these arrows always produced degeneracy. When the algebra is simple, of course all arrows are of this type and all models were degenerate. All direct sum diagrams in cases 2 and 3 necessarily contain such arrows. For two summands, there is only one contracted, irreducible diagram, which is not a direct sum and which is made of letter changing arrows; for three summands there are 30 such diagrams.

For four summands, a well-educated computer[5] tells us that there are 22 contracted, irreducible diagrams made of letter-changing arrows and which are not direct sums. They are shown in Fig. 2. We have two pleasant surprises: (i) the number of these diagrams is small; (ii) there are only two ladder diagrams, diagrams 18 and 19, i.e., diagrams with vertically aligned arrows, and all other diagrams have no subdiagrams of ladder form. We will see that these other diagrams are easily dealt with.

II. STATEMENT OF THE RESULT

Consider a finite, real, S^0-real, irreducible spectral triple whose algebra has four simple summands and the extended lift as described in Ref. 4. Consider the list of all Yang-Mills-Higgs models induced by these triples and lifts. Discard all models that have either

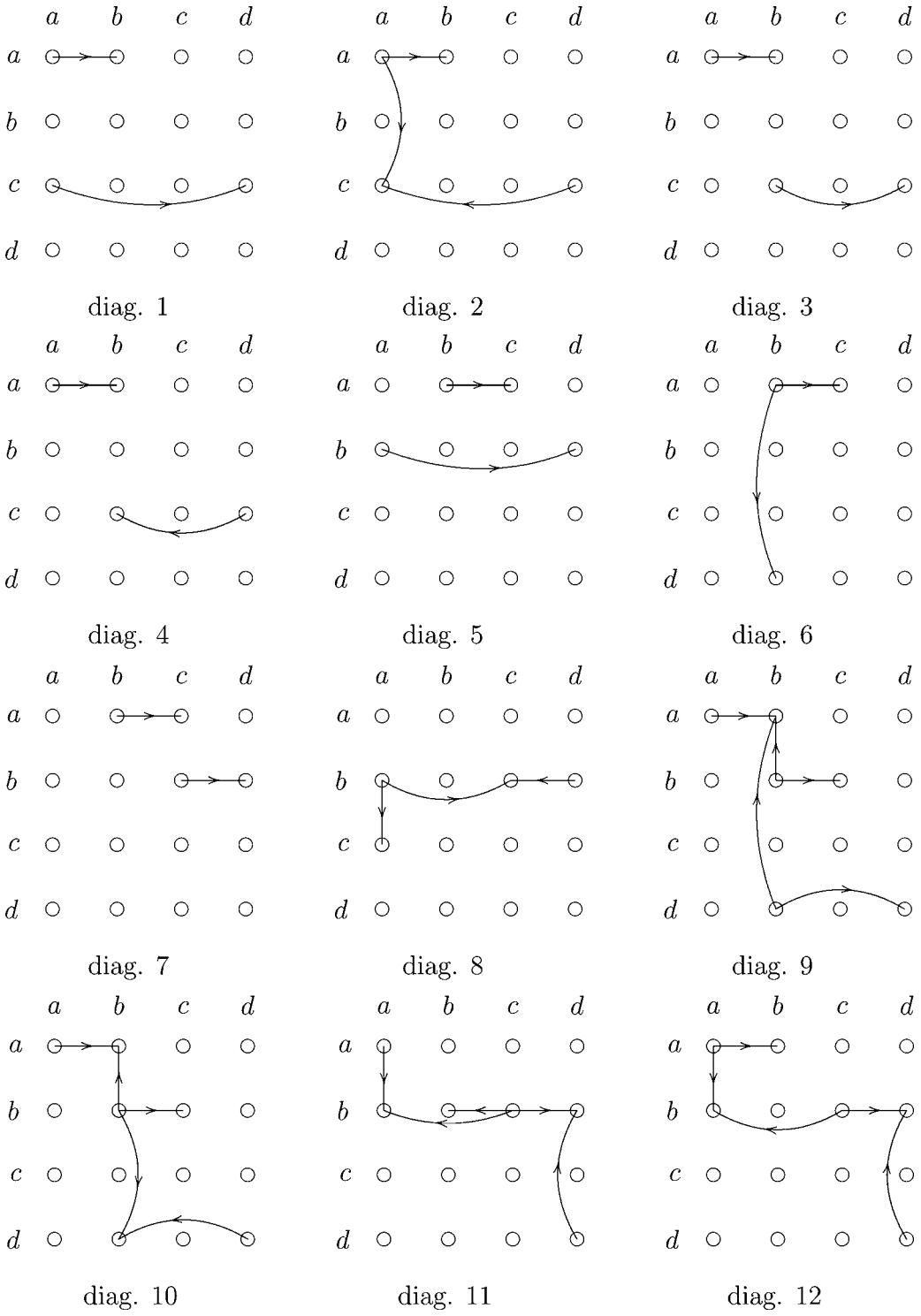

FIG. 2. Four simple summands produce 22 contracted, irreducible diagrams made of letter changing arrows and which are not direct sums.

(i) a dynamically degenerate fermionic mass spectrum;
(ii) Yang-Mills or gravitational anomalies;
(iii) a fermion multiplet whose representation under the little group is real or pseudoreal,

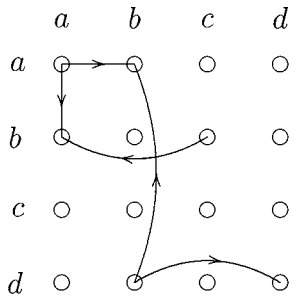

diag. 13

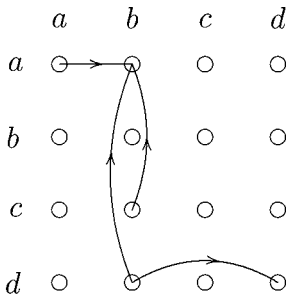

diag. 14

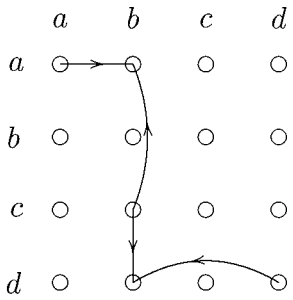

diag. 15

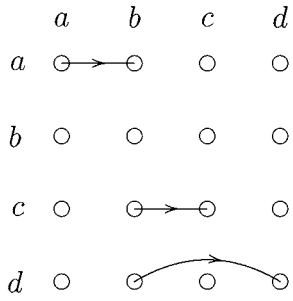

diag. 16

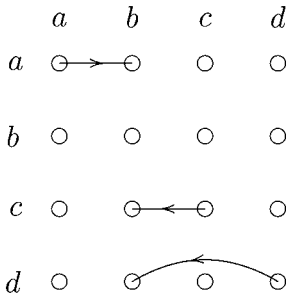

diag. 17

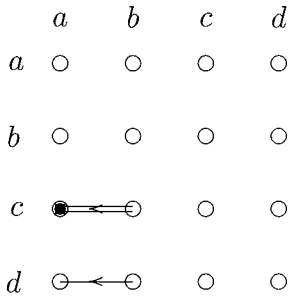

diag. 18

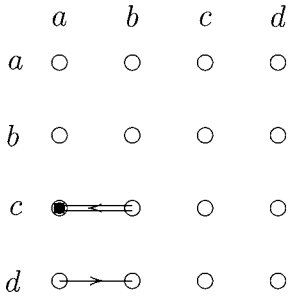

diag. 19

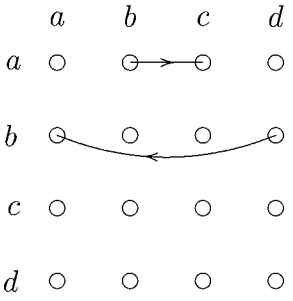

diag. 20

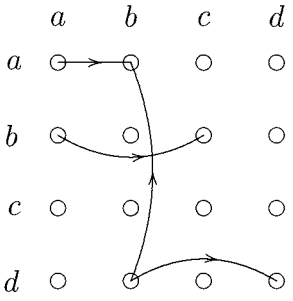

diag. 21

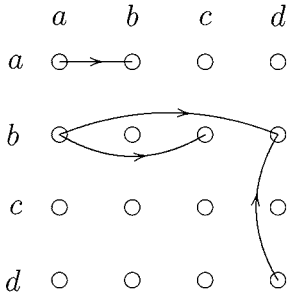

diag. 22

FIG. 2. (*Continued*).

(iv) or a massless fermion transforming nontrivially under the little group.

The remaining models are the following: C is the number of colors, the gauge group is on the left-hand side of the arrow, the little group on the right-hand side

$C=3, 5\ldots$

$$\frac{\mathrm{SU}(2)\times\mathrm{U}(1)\times\mathrm{SU}(C)}{\mathbb{Z}_2\times\mathbb{Z}_C}\to\frac{\mathrm{U}(1)\times\mathrm{SU}(C)}{\mathbb{Z}_C}.$$

The left-handed fermions transform according to a multiplet $\underline{2}\otimes\underline{C}$ with hypercharge $q/(2C)$ and a multiplet $\underline{C}$ with hypercharge $-q/2$. The right-handed fermions sit in two multiplets $\underline{C}$ with hypercharges $q(1+C)/(2C)$ and $q(1-C)/(2C)$ and one singlet with hypercharge $-q$, $q\in\mathbb{Q}$. The elements in $\mathbb{Z}_2\times\mathbb{Z}_C$ are embedded in the center of $\mathrm{SU}(2)\times\mathrm{U}(1)\times\mathrm{SU}(C)$ as

$$\left(\exp\frac{2\pi ik}{2}1_2,\exp[2\pi i(Ck-2\ell)/q],\exp\frac{2\pi i\ell}{C}1_p\right),\quad k=0,1,\quad \ell=0,1,\ldots,C-1.$$

The Higgs scalar transforms as an SU(2) doublet, SU(C) singlet and has hypercharge $-q/2$.

With the number of colors $C=3$, this is the standard model with one generation of quarks and leptons.

We also have in our list two submodels of the above model defined by the subgroups

$$\frac{\mathrm{SO}(2)\times\mathrm{U}(1)\times\mathrm{SU}(C)}{\mathbb{Z}_2\times\mathbb{Z}_C}\to\frac{\mathrm{U}(1)\times\mathrm{SU}(C)}{\mathbb{Z}_C},$$

$$\frac{\mathrm{SU}(2)\times\mathrm{U}(1)\times\mathrm{SO}(C)}{\mathbb{Z}_2}\to\mathrm{U}(1)\times\mathrm{SO}(C).$$

They have the same particle content as the standard model; in the first case only the $W^{\pm}$ bosons are missing, in the second case roughly half the gluons are lost.

$C=2, 4\ldots$

$$\frac{\mathrm{SU}(2)\times\mathrm{U}(1)\times\mathrm{SU}(C)}{\mathbb{Z}_C}\to\frac{\mathrm{U}(1)\times\mathrm{SU}(C)}{\mathbb{Z}_C},$$

with the same particle content as for odd C. But, now we have three possible submodels

$$\frac{\mathrm{SO}(2)\times\mathrm{U}(1)\times\mathrm{SU}(C)}{\mathbb{Z}_C}\to\frac{U(1)\times\mathrm{SU}(C)}{\mathbb{Z}_C},$$

$$\mathrm{SU}(2)\times\mathrm{U}(1)\times\mathrm{SO}(C)\to\mathrm{U}(1)\times\mathrm{SO}(C),$$

$$\frac{\mathrm{SU}(2)\times\mathrm{U}(1)\times\mathrm{USp}(C/2)}{\mathbb{Z}_2}\to\frac{U(1)\times\mathrm{USp}(C/2)}{\mathbb{Z}_2}.$$

electro-strong

$$\mathrm{U}(1)\times\mathrm{SU}(C)\to\mathrm{U}(1)\times\mathrm{SU}(C).$$

The fermionic content is $\underline{C}\oplus\underline{1}$, one quark and one charged lepton. The two fermion masses are arbitrary but different and nonvanishing. The number of colors is greater than or equal to 2, the two charges are arbitrary but vectorlike; of course the lepton charge must not vanish. There is no scalar and no symmetry breaking.

III. DIAGRAM BY DIAGRAM

We will use the following letters to denote algebra elements and unitaries: Let $\mathcal{A}=M_A(\mathbb{C})\oplus M_B(\mathbb{C})\oplus M_C(\mathbb{C})\oplus M_D(\mathbb{C})\ni(a,b,c,d)$. The extended lift is defined by

$$L(u,v,w,z) \coloneqq \rho(\hat{u},\hat{v},\hat{w},\hat{z})J\rho(\hat{u},\hat{v},\hat{w},\hat{z})J^{-1}, \tag{1}$$

with

$$\hat{u} \coloneqq u(\det u)^{q_{11}}(\det v)^{q_{12}}(\det w)^{q_{13}}(\det z)^{q_{14}} \in U(A), \tag{2}$$

$$\hat{v} \coloneqq v(\det u)^{q_{21}}(\det v)^{q_{22}}(\det w)^{q_{23}}(\det z)^{q_{24}} \in U(B), \tag{3}$$

$$\hat{w} \coloneqq w(\det u)^{q_{31}}(\det v)^{q_{32}}(\det w)^{q_{33}}(\det z)^{q_{34}} \in U(C), \tag{4}$$

$$\hat{z} \coloneqq z(\det u)^{q_{41}}(\det v)^{q_{42}}(\det w)^{q_{43}}(\det z)^{q_{44}} \in U(D), \tag{5}$$

and unitaries $(u,v,w,z) \in U(M_A(\mathbb{C}) \oplus M_B(\mathbb{C}) \oplus M_C(\mathbb{C}) \oplus M_D(\mathbb{C}))$. It is understood that, for instance, if $A=1$ we set $u=1$ and $q_{j1}=0$, $j=1$, 2,3,4. If $M_A(\mathbb{C})$ is replaced by $M_A(\mathbb{R})$ or $M_{A/2}(\mathbb{H})$, we set $q_{j1}=0$ and $q_{1j}=0$.

Diagram 1 yields

$$\rho_L = \begin{pmatrix} b \otimes 1_A & 0 \\ 0 & d \otimes 1_C \end{pmatrix}, \quad \rho_R = \begin{pmatrix} a \otimes 1_A & 0 \\ 0 & {}^{\alpha}a \otimes 1_C \end{pmatrix},$$

$$\rho_L^c = \begin{pmatrix} 1_B \otimes {}^{\alpha'}a & 0 \\ 0 & 1_D \otimes c \end{pmatrix}, \quad \rho_R^c = \begin{pmatrix} 1_A \otimes {}^{\alpha'}a & 0 \\ 0 & 1_A \otimes c \end{pmatrix}, \tag{6}$$

and

$$\mathcal{M} = \begin{pmatrix} M_1 \otimes 1_A & 0 \\ 0 & M_2 \otimes 1_C \end{pmatrix}, \quad M_1 \in M_{B\times A}(\mathbb{C}), \quad M_2 \in M_{D\times A}(\mathbb{C}). \tag{7}$$

The parameters α and α' take values ± 1 and distinguish between fundamental representation and its complex conjugate: ${}^{1}a \coloneqq a$, ${}^{-1}a \coloneqq \bar{a}$. The color algebras consist of a's and c's. The a's are broken and therefore we must have $A=1$. We want at most one massless Weyl fermion, which leaves us with three possibilities. The first is $B=2$, $D=1$. The fluctuations read

$$\varphi_1 = \sum_j r_j \hat{v}_j M_1 \hat{u}_j^{-1}, \quad \varphi_2 = \sum_j r_j \hat{z}_j M_2 {}^{\alpha}\hat{u}_j^{-1}. \tag{8}$$

We can decouple the two scalars φ_1 and φ_2 by means of the fluctuation: $r_1=\frac{1}{2}$, $\hat{u}_1=1$, $\hat{v}_1=1_2$, $\hat{w}_1=1_C$, $\hat{z}_1=1$, $r_2=\frac{1}{2}$, $\hat{u}_2=1$, $\hat{v}_2=-1_2$, $\hat{w}_2=1_C$, $\hat{z}_2=1$. Since the arrows M_1 and M_2 are disconnected, the Higgs potential is a sum of a potential in φ_1 and of a potential in φ_2. The minimum is $\mathring{\varphi}_1 = \mu(4\lambda)^{-1/2}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\mathring{\varphi}_2 = \mu(4\lambda)^{-1/2}$, and the model is dynamically degenerate.

The same accidents happen for the second possibility, $B=1$, $D=2$. We are left with the third possibility, $B=D=1$. Anomaly cancellations imply that the fermion couplings are vectorial: $q_{13}=q_{23}$, $q_{43}=\alpha q_{13}$, and there is no spontaneous symmetry breaking, $\mathrm{SU}(C)\times\mathrm{U}(1) \to \mathrm{SU}(C)\times\mathrm{U}(1)$. The model describes electro-strong forces with one charged lepton, one quark, and no scalar. The masses of both fermions are arbitrary but nonvanishing, the electric charges are arbitrary, nonvanishing for the lepton, and the number of colors C is arbitrary, $C \geqslant 2$.

Diagrams 3, 4, and **7** are treated in the same way and produce only the electro-strong model.

Diagram 2 yields

$$\rho_L = \begin{pmatrix} b \otimes 1_A & 0 \\ 0 & {}^{\alpha}a \otimes 1_C \end{pmatrix}, \quad \rho_R = \begin{pmatrix} a \otimes 1_A & 0 \\ 0 & d \otimes 1_C \end{pmatrix}, \tag{9}$$

$$\rho_L^c = \begin{pmatrix} 1_B \otimes^{\alpha'} a & 0 \\ 0 & 1_A \otimes c \end{pmatrix}, \quad \rho_R^c = \begin{pmatrix} 1_A \otimes^{\alpha'} a & 0 \\ 0 & 1_D \otimes c \end{pmatrix},$$

and

$$\mathcal{M} = \begin{pmatrix} M_1 \otimes 1_A & 0 \\ 1_A \otimes M_3 & M_2 \otimes 1_C \end{pmatrix}, \quad M_1 \in M_{B\times A}(\mathbb{C}), \quad M_2 \in M_{A\times D}(\mathbb{C}), \quad M_3 \in M_{C\times A}(\mathbb{C}). \tag{10}$$

If $M_3=0$ diagram 2 is treated as diagram 1. We consider the case $M_3 \neq 0$. Then, the first-order axiom implies $\alpha=1$. The color algebras consist of a's and c's. Both are broken and we take $A=C=1$. Then, $\mathcal{M}$ is of rank two or less. If we want at most one massless Weyl fermion, we must take $B=2$ and $D=1$ or $B=1$ and $D=2$. Anomaly cancellations then imply that the doublet of fermions does not couple to the determinant of the 2×2 unitary, "the hypercharge of the doublet is zero." On the other hand, the little group turns out either trivial or U(1). In the latter case the neutrino sitting in the doublet is charged under this U(1).

Diagram 5 has no unbroken color and fails as the first possibility of diagram 1, $B=2$, $D=1$.

Diagram 6 has color a and b; both are broken, implying $A=B=1$. Then, we must have $C=D=1$ to avoid two or more neutrinos.

Diagram 8 yields

$$\rho_L = \begin{pmatrix} a \otimes 1_C & 0 \\ 0 & c \otimes 1_B \end{pmatrix}, \quad \rho_R = \begin{pmatrix} a \otimes 1_A & 0 \\ 0 & d \otimes 1_C \end{pmatrix}, \tag{11}$$

$$\rho_L^c = \begin{pmatrix} 1_A \otimes^{\gamma} c & 0 \\ 0 & 1_C \otimes b \end{pmatrix}, \quad \rho_R^c = \begin{pmatrix} 1_A \otimes b & 0 \\ 0 & 1_D \otimes b \end{pmatrix},$$

and

$$\mathcal{M} = \begin{pmatrix} 1_A \otimes M_1 & 0 \\ M_3 \otimes 1_B & M_2 \otimes 1_B \end{pmatrix}, \quad M_1 \in M_{C\times B}(\mathbb{C}), \quad M_2 \in M_{C\times D}(\mathbb{C}), \quad M_3 \in M_{C\times A}(\mathbb{C}). \tag{12}$$

We suppose that M_3 does not vanish; otherwise, diagram 8 is treated as diagram 1. Broken color implies $A=B=1$. Neutrino counting leaves two possibilities, $C=1$ and $D=2$ or $C=D=2$. The first possibility is disposed of as in diagram 2. For the second possibility, anomaly cancellations imply that the determinants of the 2×2 unitaries w and z do not couple to the right-handed fermions.

Diagrams 14, 15, 16, and **17** share the fate of diagram 6.

Diagram 9 yields

$$\rho_L = \begin{pmatrix} b \otimes 1_A & 0 & 0 \\ 0 & c \otimes 1_B & 0 \\ 0 & 0 & d \otimes 1_D \end{pmatrix}, \quad \rho_R = \begin{pmatrix} a \otimes 1_A & 0 & 0 \\ 0 & {}^{\beta_1} b \otimes 1_B & 0 \\ 0 & 0 & {}^{\beta_2} b \otimes 1_D \end{pmatrix}, \tag{13}$$

$$\rho_L^c = \begin{pmatrix} 1_B \otimes^{\alpha'} a & 0 & 0 \\ 0 & 1_C \otimes^{\beta'} b & 0 \\ 0 & 0 & 1_D \otimes^{\delta'} d \end{pmatrix}, \quad \rho_R^c = \begin{pmatrix} 1_A \otimes^{\alpha'} a & 0 & 0 \\ 0 & 1_B \otimes^{\beta'} b & 0 \\ 0 & 0 & 1_B \otimes^{\delta'} d \end{pmatrix},$$

and

$$\mathcal{M}=\begin{pmatrix} M_1\otimes 1_A & 1_B\otimes M_4 & 1_B\otimes M_5 \\ 0 & M_2\otimes 1_B & 0 \\ 0 & 0 & M_3\otimes 1_D \end{pmatrix},$$

with $M_1\in M_{B\times A}(\mathbb{C})$, $M_2\in M_{C\times D}(\mathbb{C})$, $M_3\in M_{D\times B}(\mathbb{C})$, $M_4\in M_{A\times B}(\mathbb{C})$, $M_5\in M_{A\times D}(\mathbb{C})$. If M_4 is nonzero β_1 must be 1, and if M_5 is nonzero β_2 must be 1. From broken color and neutrino counting, we have $A=B=D=1$ and $C=2$. Vanishing anomalies imply that the first and the third fermion have vectorlike hypercharges, while the hypercharges of the second fermion are zero. It is therefore neutral under the little group U(1).

Diagrams 10, 11, 12, and **13** fail in the same way.

Diagram 18 produces the following triple:

$$\rho_L=\begin{pmatrix} a\otimes 1_C & 0 \\ 0 & {}^{\alpha}a\otimes 1_D \end{pmatrix},\quad \rho_R=\begin{pmatrix} b\otimes 1_C & 0 & 0 \\ 0 & {}^{\beta_1}\bar{b}\otimes 1_C & 0 \\ 0 & 0 & {}^{\beta_2}\bar{b}\otimes 1_D \end{pmatrix},$$

$$\rho_L^c=\begin{pmatrix} 1_A\otimes c & 0 \\ 0 & 1_A\otimes d \end{pmatrix},\quad \rho_R^c=\begin{pmatrix} 1_B\otimes c & 0 & 0 \\ 0 & 1_B\otimes c & 0 \\ 0 & 0 & 1_B\otimes d \end{pmatrix},$$

and

$$\mathcal{M}=\begin{pmatrix} M_1\otimes 1_C & M_2\otimes 1_C & 0 \\ 0 & 0 & M_3\otimes 1_D \end{pmatrix},\quad M_1,M_2,M_3\in M_{A\times B}(\mathbb{C}). \tag{14}$$

Counting neutrinos leaves two possibilities, $A=2$ and $B=1$, or $A=1$ and $B=1$. If the neutrino is to be neutral under the little group, we must have $D=1$ for the first possibility and $C=1$ for the second.

The first possibility has two U(1)'s if $C\geqslant 2$ and all four algebras consist of matrices with complex entries. They are parametrized by $\det u$ and by $\det w$. For $(\alpha,\beta_1,\beta_2)=+++,-++,++-$, and $-+-$, anomaly cancellations imply that the fermionic hypercharges of both U(1)'s are proportional

$$q_{11}=-\frac{1}{2},\quad q_{21}=Cp,\quad q_{31}=p,\quad q_{41}=-Cp, \tag{15}$$

$$q_{13}=0,\quad q_{23}=Cq,\quad q_{33}=q-\frac{1}{C},\quad q_{43}=-Cq, \tag{16}$$

with $p,\ q\in\mathbb{Q}$. Consequently, one linear combination of the two generators decouples from the fermions and is absent from the spectral action. This is similar to what happens to the scalar in the electro-strong model of diagram 1. The hypercharges of the remaining generator are those of the standard model with C colors. In the remaining four cases $(\alpha,\beta_1,\beta_2)=+-+,--+,+--$, and $---$, all ten fermionic hypercharges vanish and the three leptons are neutral under the little group. Finally, the cases where some of the four summands consist of matrices with real or quaternionic entries are treated as in the situation with three summands, and they produce the same submodels of the standard model.

The first possibility with $C=1$ has only one U(1). For the four sign assignments: $(\alpha,\beta_1,\beta_2)=+++,-++,++-$, and $-+-$, we find anomaly free lifts with nontrivial little group. For example,

for the first assignment, we get $q_{11}=-1/2$, $q_{21}=p$, $q_{31}=-p$, and $q_{41}=-p$, with $p\in\mathbb{Q}$. All four assignments produce the electro-weak model $(\mathrm{SU}(2)\times\mathrm{U}(1))/\mathbb{Z}_2\to\mathrm{U}(1)$ of protons, neutrons, neutrinos, and electrons.

The second possibility, $A=B=C=1$, contains at least one chiral lepton with vanishing hypercharge and therefore neutral under the little group.

Diagram 19 gives the same results as diagram 18.

In **diagrams 20, 21**, and **22**, the elements a and b must be matrices with complex entries to allow for conjugate representations. Without both the fundamental representation and its complex conjugate, these diagrams would violate the condition that every nonvanishing entry of the multiplicity matrix of a (blown-up) Krajewski diagram must have the same sign as its transposed element if the latter is not zero. Diagram 20 is treated and fails as diagram 2; diagrams 21 and 22 are treated and fail as diagram 13.

At this point we have exhausted all diagrams of Fig. 2.

IV. CONCLUSION AND OUTLOOK

For three summands there was essentially one irreducible spectral triple satisfying all items on our shopping list: the standard model with one generation of quarks and leptons and an arbitrary number of colors (greater than or equal to 2). We say "essentially" because a few submodels of the standard model can be obtained. Going to four summands adds precisely one model, the electro-strong model for one massive quark with an arbitrary number of colors and one massive, charged lepton. Note that this is the first appearance of a spectral triple without any Higgs scalar and without symmetry breaking.

We still have to prove that spectral triples in four summands involving letter-preserving arrows like $a\ \bar{a}$ do not produce any model compatible with our shopping list.

We are curious to know what happens in five (and more) summands. Here, ladder diagrams do not exist and we may speculate that our present list of models exhausts our shopping list also in any number of summands.

Anyhow, two questions remain: Who ordered three colors? Who ordered three generations?

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Seiberg-Witten equations in R^4: Lie symmetries, particular solutions, integrability

Dmitriy V. Aleynikov[a)]
B.I. Stepanov Institute of Physics, National Academy of Sciences of Belarus, 68 F. Skaryna Avenue, 220072 Minsk, Belarus

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It is shown that the 11-parameter automorphism group of Lie algebra of four-dimensional Euclidean group is a maximal Lie symmetries group of the Seiberg-Witten equations in R^4. Particular explicit solutions which are invariant under SO(3) subgroups of the maximal Lie symmetries group are constructed. It is established that Seiberg-Witten equations do not possess the Painlevé property. Nevertheless, SO(3) invariant solutions obtained are turned to admit a characteristic singularity structure. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The Seiberg-Witten, or Abelian monopole, equations introduced in Ref. 1, following up with Ref. 2, play a significant role in the quantum gauge field theory and can be used as a powerful tool in the analysis of four manifolds.[3] These equations have arisen in the context of the *S*-duality between $N=2$ SUSY pure gauge Yang-Mills theory and $N=2$ supersymmetric Abelian theory, the latter including not only gauge fields but matter ones.[2,4] The Witten twist leads the SUSY pure gauge Yang-Mills theory to the Witten-Donaldson topological theory.[5] The weakly coupled region of field space in this theory is described by (anti)self-dual Yang-Mills instanton equations. The Seiberg-Witten equations describe the dynamics of "twisted" $N=2$ supersymmetric Abelian gauge fields with weakly coupling constant.[1,6] The more precise relationship between Donaldson theory, counting instantons, and dual Seiberg-Witten theory, counting monopoles, is explored in Ref. 7. So, the Seiberg-Witten equations, to some extent, are "dual" to Yang-Mills instanton equations. The problems of duality and topological aspects of low dimensional reduction of these theories have been studied in Refs. 8,9.

In light of these results, we note some properties of self-dual Yang-Mills equations. It was shown in Ref. 10 that the SU(2) self-dual Yang-Mills equations pass the Painlevé test for integrability.[11] Moreover, experience has shown that many well-known integrable equations are the reductions of the Yang-Mills equations.[12–15] These facts led to the famous Ward hypothesis.[13,14] The Seiberg-Witten equations have been linked to integrable systems by means of prepotentials (Refs. 16 and 17 and references therein). Some equations of the Painlevé type were obtained from the non-Abelian generalization of monopole equations.[18,19] However, the integrability of the Seiberg-Witten equations was not investigated.

Besides, the Abelian monopole equations are referred to in the context of zero-eigenvalue solutions to the Euclidean Dirac equation in external gauge field. The general ansatz of zero modes of the Abelian Dirac operator in three dimensional Euclidean space was proposed in Ref. 20. By exploiting this result, some particular solutions to the Seiberg-Witten equations in R^3 were found.[21,22] Furthermore, the Freund's equations were proposed which differ from Seiberg-Witten ones in the sign of the quadratic term.[22] It was shown in Ref. 23 that conformal group of three-

[a)]Electronic mail: aleynik@dragon.bas-net.by

dimensional Euclidean space is a maximal group of Lie symmetries of the Seiberg-Witten equations in R^3. Particular explicit solutions which are invariant under some subgroups of conformal group were constructed.

This paper deals with the Seiberg-Witten equations in four dimensional Euclidean space. The maximal group of Lie symmetries and particular solutions of this equations will be constructed. Besides, it will be shown that Seiberg-Witten equations do not possess the Painlevé property. Strictly speaking, we should define equations on compact manifolds. However, an arbitrary manifold M is defined by introducing a set of Euclidean-type neighborhoods covering M. In other words, a manifold is constructed by pasting together many pieces of Euclidean space. In turn, this paper is devoted to a study of the local properties of the Seiberg-Witten equations. Our point of view does not concern with the global topological aspects of Seiberg-Witten theory. Connections between Painlevé analysis and global aspects have been studied in Ref. 24.

II. SEIBERG-WITTEN AND FREUND'S EQUATIONS IN R^4

The Seiberg-Witten equations as well as Freund's ones are a set of coupled PDEs in four dimensions for the Abelian vector potential A_ν and the two-component spinor field $\tilde{\psi}$. Following Ref. 22, we write the Seiberg-Witten (Freund's) equations as

$$\gamma^\mu(i\partial_\mu - eA_\mu)\psi = 0,$$

$$\epsilon(ie/2)\overline{\psi}(\sigma^{\mu\nu})^+\psi = (F^{\mu\nu})^+, \tag{1}$$

$$\partial^\mu A^\nu - \partial^\nu A^\mu = F^{\mu\nu}.$$

Here the bispinor ψ is

$$\psi = \begin{pmatrix} \tilde{\psi} \\ 0 \end{pmatrix};$$

$\epsilon = \pm 1$; μ, $\nu = 0,1,2,3$; γ^ν are the Dirac matrices satisfying $\{\gamma^\mu, \gamma^\nu\} = -2g^{\mu\nu}I_4$; $\sigma^{\mu\nu} = 1/2[\gamma^\mu, \gamma^\nu]$. $\overline{\psi}$ means the Hermitian conjugate bispinor. We use the usual summation convention throughout, repeated indices are summed if one index is "up" and one is "down." For $\epsilon = 1$, these equations will be the Seiberg-Witten ones. In the case $\epsilon = -1$, we will think of the equations (1) as the Freund's equations. With the Euclidean metric $g^{\mu\nu}$ of signature $(-,-,-,-)$ the Dirac matrices can be represented in the form

$$\gamma^0 = \begin{pmatrix} 0 & \sigma^0 \\ \sigma^0 & 0 \end{pmatrix}, \quad \gamma^k = \begin{pmatrix} 0 & -i\sigma^k \\ i\sigma^k & 0 \end{pmatrix},$$

where $\sigma^0 = I_2$ and σ^k are the Pauli matrices; $k = 1,2,3$. Then

$$(\sigma_{\mu\nu})^+ = 1/2(\sigma_{\mu\nu} + (1/2)\varepsilon_{\mu\nu\rho\lambda}\sigma^{\rho\lambda}) = \frac{1}{2}(\delta_{\mu\rho}\delta_{\nu\lambda} - \delta_{\nu\rho}\delta_{\mu\lambda} + \varepsilon_{\mu\nu\rho\lambda})\begin{pmatrix} \sigma^\rho\sigma^\lambda & 0 \\ 0 & 0 \end{pmatrix}$$

and the self-dual tensor $(F^{\mu\nu})^+$ is given by

$$(F^{\mu\nu})^+ = 1/2(F^{\mu\nu} + (1/2)\varepsilon^{\mu\nu\rho\sigma}F_{\rho\sigma}),$$

where $\varepsilon^{\mu\nu\rho\sigma}$ is a totally antisymmetric tensor with $\varepsilon_{0123} = 1$ and δ is a Kronecker symbol. As has been shown in Ref. 25, the gauge vector field A^μ can be related to the spinor field ψ by

$$A^{\nu}=\frac{ie}{2\bar{\psi}\psi}[\partial_{\mu}(\bar{\psi}\gamma^{\mu}\gamma^{\nu}\psi)+2\bar{\psi}\partial^{\nu}\psi]. \tag{2}$$

This relation follows from the equations

$$\gamma^{\mu}(i\partial_{\mu}-eA_{\mu})\psi=0,$$

$$\bar{\psi}\gamma^{\mu}(i\overleftarrow{\partial}_{\mu}+eA_{\mu})=0,$$

which are equivalent to

$$i\bar{\psi}\gamma^{\nu}\gamma^{\mu}\partial_{\mu}\psi=e\bar{\psi}\gamma^{\nu}\gamma^{\mu}\psi A_{\mu},$$

$$i\partial_{\mu}(\bar{\psi})\gamma^{\mu}\gamma^{\nu}\psi=-e\bar{\psi}\gamma^{\mu}\gamma^{\nu}\psi A_{\mu}.$$

Using the property $\{\gamma^{\mu},\gamma^{\nu}\}=-2g^{\mu\nu}I_4$ leads us to the equation (2). The curvature $F^{\mu\nu}$ is

$$F^{\mu\nu}=\frac{ie}{2(\bar{\psi}\psi)}[\partial^{\mu}\partial_{\rho}(\bar{\psi}\gamma^{\rho}\gamma^{\nu}\psi)-\partial^{\nu}\partial_{\rho}(\bar{\psi}\gamma^{\rho}\gamma^{\mu}\psi)+2(\partial^{\mu}\bar{\psi})(\partial^{\nu}\psi)-2(\partial^{\nu}\bar{\psi})(\partial^{\mu}\psi)]$$
$$+\frac{ie}{2(\bar{\psi}\psi)^2}[\partial^{\nu}(\bar{\psi}\psi)(2\bar{\psi}\partial^{\mu}\psi+\partial_{\rho}(\bar{\psi}\gamma^{\rho}\gamma^{\mu}\psi))-\partial^{\mu}(\bar{\psi}\psi)(2\bar{\psi}\partial^{\nu}\psi+\partial_{\rho}(\bar{\psi}\gamma^{\rho}\gamma^{\nu}\psi))]. \tag{3}$$

The second equation of (1) defines the projection of Kustaanheimo-Stiefel bundle $R^4/\{0\}\rightarrow R^3/\{0\}$, ψ being a total space and $F^{+}_{\mu\nu}$ being a base manifold.[20,26] (The Kustaanheimo-Stiefel bundle is isomorphic to Hopf one.) Within this framework the solutions to the Seiberg-Witten equations can be represented as the local sections

$$\tilde{\psi}=\begin{cases}\tilde{\psi}_N, & f\neq -f^3,\\ \tilde{\psi}_S, & f\neq f^3,\end{cases} \tag{4}$$

where

$$\tilde{\psi}_N=\frac{1}{\sqrt{2(f+f^3)}}\begin{pmatrix}f+f^3\\ f^1+\mathrm{i}f^2\end{pmatrix},\quad \tilde{\psi}_S=\frac{1}{\sqrt{2(f-f^3)}}\begin{pmatrix}f^1-\mathrm{i}f^2\\ f-f^3\end{pmatrix},$$

and the local connections

$$A^{\nu}=\begin{cases}A^{\nu}_N, & f\neq -f^3,\\ A^{\nu}_S, & f\neq f^3.\end{cases} \tag{5}$$

Here $F^{01}+F^{23}=f^1$, $F^{02}+F^{31}=f^2$, $F^{03}+F^{12}=f^3$, and $f=\sqrt{-f^kf_k}=\sqrt{(f^1)^2+(f^2)^2+(f^3)^2}$.

It can be verified using the equations (2), (4), and (5) that

$$\psi_N=e^{i\alpha}\psi_S,\quad A^{\nu}_N=A^{\nu}_S-\partial^{\nu}\alpha,\quad \text{where}\quad \alpha=\arctan(f^2/f^1).$$

Using the equations (3) and (4) one can rewrite the second equation of (1) in the form

$$\tfrac{1}{2}(\varepsilon^{\lambda j\rho k}(\partial_{\lambda}f_j)(\partial_{\rho}f_k)+(\partial_kf^j)(\partial_jf^k)-(\partial_jf^j)(\partial_kf^k))f^i+\varepsilon^{ik\sigma j}((\partial_{\sigma}f^m)(\partial_mf_j)-(\partial_mf^m)(\partial_{\sigma}f_j)$$
$$-\varepsilon_{\sigma\lambda n\rho}(\partial^{\lambda}f^n)(\partial^{\rho}f_j))f_k+(f^kf_k)\partial_{\rho}\partial^{\rho}f^i-f_j(\partial^{\rho}f^j)(\partial_{\rho}f^i)+2\epsilon(-f^kf_k)^{3/2}f^i=0. \tag{6}$$

We note that greek indices can take the four values (0, 1, 2, 3). Italic indices take the three values (1, 2, 3). As speaking above the ε-tensor has its usual meaning.

So, we obtain the second order nonlinear differential equations in four independent and three dependent variables. The gauge ambiguity is removed.

III. LIE SYMMETRIES AND PARTICULAR SOLUTIONS

One of the most useful methods for determining particular explicit solutions to partial differential equations is to reduce them to ordinary differential equations which are invariant under some subgroups of maximal Lie symmetry group. For this purpose we need to construct the infinitesimal Lie algebra generators. Using the method described in Ref. 27 gives (see the Appendix)

$$M_{\nu\mu} = x_\nu \partial_\mu - x_\mu \partial_\nu + (\delta_{\nu i}\delta_{\mu j} - \delta_{\nu j}\delta_{\mu i} + \varepsilon_{\nu\mu ij}) f^i \frac{\partial}{\partial f_j}, \tag{7}$$

$$P_\nu = \partial_\nu, \tag{8}$$

$$D = x^\mu \partial_\mu - 2 f^i \frac{\partial}{\partial f^i}. \tag{9}$$

The commutation relations of generators (7)–(9) are

$$[M_{\nu\mu}, M_{\rho\sigma}] = g_{\nu\sigma} M_{\mu\rho} + g_{\mu\rho} M_{\nu\sigma} - g_{\nu\rho} M_{\mu\sigma} - g_{\mu\sigma} M_{\nu\rho},$$

$$[M_{\nu\mu}, P_\sigma] = g_{\mu\sigma} P_\nu - g_{\nu\sigma} P_\mu,$$

$$[M_{\nu\mu}, D] = 0,$$

$$[P_\mu, D] = P_\mu,$$

$$[P_\nu, P_\mu] = 0.$$

We note that $g_{\nu\mu} = -\delta_{\nu\mu}$. So, the generators (7)–(9) reproduce the infinitesimal transformations of $T^4 \ltimes (SO(4) \otimes D)$ automorphism group of Lie algebra of four-dimensional Euclidean group. The group obtained has the structure of a semidirect product, namely, the semidirect product of the translation group T^4 and $SO(4) \otimes D$ group, the latter being the direct product of the rotation group SO(4) and the dilatation group D. Generators $M_{\nu\mu}$, P_ν, and D determine infinitesimal rotations, shifts and dilatation, respectively. Note in particular that (7)–(9) generate fiber-preserving transformations, meaning that the transformations in x^μ do not depend on the coordinates f^i.

The symmetry group $T^4 \ltimes (SO(4) \otimes D)$ of four dimensional Seiberg-Witten equations does not include the inversions in spite of the fact that the initial fields ψ and A_ν are massless. The theorem proven in Ref. 28 states that an arbitrary Poincaré (Euclidean) invariant equation for massless fields are conformally invariant "by default." In general, the latter fact holds for linear equations such as massless Dirac and Maxwell ones.[29] Since the Seiberg-Witten equations contain the nonlinear quadratic term, the Euclidean invariance does not give rise to the conformal one. It is interesting to note that the inversions are nonlinear transformations. So, the invariance under nonlinear transformations is removed. We must note that Yang-Mills equations are conformal invariant.[30,31] Moreover, the conformal invariance is not removed by coupling of Yang-Mills fields with massless scalar fields[32] or massless Dirac fields.[33]

Consider the solutions of (6) which are invariant under SO(3) subgroups of $T^4 \ltimes (SO(4) \otimes D)$ or, more precisely, SO(4). It should be noted that subgroups are determined up to inner automorphisms of maximal symmetry group. So, a class of adjoint subgroups can be associated

with a subgroup $\mathrm{SO}(3):\widetilde{\mathrm{SO}}(3)=g\mathrm{SO}(3)g^{-1}$, where g is an arbitrary element of $\mathrm{T}^4\ltimes(\mathrm{SO}(4)\otimes\mathrm{D})$ group. There are three nonequivalent SO(3) subgroups of SO(4) group. One of them can be generated by vector fields

$$M_{ij}=x_i\partial_j-x_j\partial_i+f_i\frac{\partial}{\partial f^j}-f_j\frac{\partial}{\partial f^i}.$$

The solutions to the Witten-Seiberg equations which are invariant under the SO(3) subgroup generated by vector fields M_{ij} and the solutions which are invariant under some adjoint subgroup to this SO(3) group were constructed in Ref. 23. The SO(3) invariant solutions are turned out to be a monopolelike ones.

The second SO(3) subgroup is generated by vector fields $M^-_{\nu\mu}=M_{\nu\mu}-\frac{1}{2}\varepsilon_{\nu\mu\lambda\tau}M^{\lambda\tau}$,

$$M^-_{\nu\mu}=x_\nu\partial_\mu-x_\mu\partial_\nu-\tfrac{1}{2}\varepsilon_{\nu\mu\lambda\tau}(x^\lambda\partial^\tau-x^\tau\partial^\lambda).$$

It is evidently that f^i, $i=1,2,3$ and $r=\sqrt{-x^\mu x_\mu}$ are group invariants. By Lie's reduction method the equations (6) are reduced to the ordinary differential equations in the three dependent variables f^i and the independent variable r,

$$(-f^jf_j)\left(\frac{\mathrm{d}^2f^i}{\mathrm{d}r^2}+\frac{3}{r}\frac{\mathrm{d}f^i}{\mathrm{d}r}\right)+\frac{1}{2}\frac{\mathrm{d}(f^jf_j)}{\mathrm{d}r}\frac{\mathrm{d}f^i}{\mathrm{d}r}+2\epsilon(-f^jf_j)^{3/2}f^i=0.$$

These equations with $\epsilon=1$ admit the solution

$$f^i=\pm\frac{2\hat{u}^i}{r^2}=\mp\frac{2\hat{u}^i}{x^\nu x_\nu}, \tag{10}$$

where $\hat{u}^i$ is an arbitrary constant unit vector, $\hat{u}^i\hat{u}_i=-1$.

The finite transformations $\exp(\varphi M^-_{\nu\mu})$ of this subgroup are

$$x^\sigma\mapsto x^\sigma\cos\phi+(x^\nu g^{\mu\sigma}-x^\mu g^{\nu\sigma}+\varepsilon^{\nu\mu\sigma\lambda}x_\lambda)\sin\phi,$$

$$f^i\mapsto f^i.$$

It is evidently that

$$\widetilde{f}^i(x^\sigma)\equiv G(\exp(\varphi M^-_{\nu\mu}))f^i(x^\sigma)\equiv\exp(\varphi M^-_{\nu\mu})f^i(\exp(-\varphi M^-_{\nu\mu})x^\sigma)=f^i(\exp(-\varphi M^-_{\nu\mu})x^\sigma)=f^i(x^\sigma)$$

for the solutions (10).

The third SO(3) subgroup is generated by vector fields $M^+_{\nu\mu}=M_{\nu\mu}+\frac{1}{2}\varepsilon_{\nu\mu\lambda\tau}M^{\lambda\tau}$,

$$M^+_{\nu\mu}=x_\nu\partial_\mu-x_\mu\partial_\nu+\tfrac{1}{2}\varepsilon_{\nu\mu\lambda\tau}(x^\lambda\partial^\tau-x^\tau\partial^\lambda)+2(\delta_{\nu i}\delta_{\mu j}-\delta_{\nu j}\delta_{\mu i}+\varepsilon_{\nu\mu ij})f^i\frac{\partial}{\partial f_j}.$$

As in the previous case the variable $r=\sqrt{-x^\mu x_\mu}$ is a group invariant. The next three invariants have the form $F_i=\Omega_{ij}f^j$, where Ω_{ij} is the orthogonal matrix

$$\Omega_{ij}=\frac{1}{x^\mu x_\mu}(-\delta_{ij}x^\nu x_\nu+2\delta_{ij}x^kx_k+2x_ix_j-\varepsilon_{ijk\mu}x^kx^\mu).$$

We recall that greek indices can take the four values (0, 1, 2, 3). Italic indices take the three values (1, 2, 3). It can be verified by direct calculation that $M^+_{\nu\mu}F^i=0$. The equations (6) are reduced to the ordinary differential equations

$$(-F^jF_j)\left(\frac{\mathrm{d}^2F^i}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}F^i}{\mathrm{d}r}-\frac{12}{r^2}F^i\right)+\frac{1}{2}\frac{\mathrm{d}(F^jF_j)}{\mathrm{d}r}\left(\frac{\mathrm{d}F^i}{\mathrm{d}r}+\frac{2F^i}{r}\right)+2\epsilon(-F^jF_j)^{3/2}F^i=0.$$

The solutions to the latter equations with $\epsilon=1$ are

$$F^i=\pm\frac{4\hat{v}^i}{r^2}=\mp\frac{4\hat{v}^i}{x^\nu x_\nu},$$

where $\hat{v}^i$ is an arbitrary constant unit vector, $\hat{v}^i\hat{v}_i=-1$. Then

$$f^i=\pm\frac{4\hat{w}^i}{r^2}=\mp\frac{4\hat{w}^i}{x^\nu x_\nu}, \tag{11}$$

where

$$\hat{w}_i=\Omega_{ij}^{-1}\hat{v}^j=\frac{1}{x^\mu x_\mu}(-\delta_{ij}x^\nu x_\nu+2\delta_{ij}x^kx_k+2x_ix_j+\varepsilon_{ijk\mu}x^kx^\mu)\hat{v}^j.$$

To avoid difficulties we write out the finite transformations $\exp(\varphi M^+_{\nu\mu})$ in component form. Thus, $\exp(\varphi M^+_{21})=\exp(\varphi M^+_{30})$ is given by

$$x^0\mapsto x^0\cos\varphi-x^3\sin\varphi,\quad x^3\mapsto x^3\cos\varphi+x^0\sin\varphi,$$

$$x^1\mapsto x^1\cos\varphi-x^2\sin\varphi,\quad x^2\mapsto x^2\cos\varphi+x^1\sin\varphi,$$

$$f^1\mapsto f^1\cos 2\varphi-f^2\sin 2\varphi,\quad f^2\mapsto f^2\cos 2\varphi+f^1\sin 2\varphi,$$

$$f^3\mapsto f^3.$$

For $\exp(\varphi M^+_{13})=\exp(\varphi M^+_{20})$ we have

$$x^0\mapsto x^0\cos\varphi-x^2\sin\varphi,\quad x^2\mapsto x^2\cos\varphi+x^0\sin\varphi,$$

$$x^1\mapsto x^1\cos\varphi+x^3\sin\varphi,\quad x^3\mapsto x^3\cos\varphi-x^1\sin\varphi,$$

$$f^1\mapsto f^1\cos 2\varphi+f^3\sin 2\varphi,\quad f^3\mapsto f^3\cos 2\varphi-f^1\sin 2\varphi,$$

$$f^2\mapsto f^2.$$

The transformation $\exp(\varphi M^+_{32})=\exp(\varphi M^+_{10})$ is defined by

$$x^0\mapsto x^0\cos\varphi-x^1\sin\varphi,\quad x^1\mapsto x^1\cos\varphi+x^0\sin\varphi,$$

$$x^2\mapsto x^2\cos\varphi-x^3\sin\varphi,\quad x^3\mapsto x^3\cos\varphi+x^2\sin\varphi,$$

$$f^2\mapsto f^2\cos 2\varphi-f^3\sin 2\varphi,\quad f^3\mapsto f^3\cos 2\varphi+f^2\sin 2\varphi,$$

$$f^1\mapsto f^1.$$

It can be verified that

$$\tilde{f}^i(x^\sigma) \equiv G(\exp(\varphi M^+_{\nu\mu}))f^i(x^\sigma) \equiv \exp(\varphi M^+_{\nu\mu})f^i(\exp(-\varphi M^+_{\nu\mu})x^\sigma) = f^i(x^\sigma)$$

for the functions (11). This implies that the solutions (11) are invariant under finite transformations $\exp(\varphi M^+_{\nu\mu})$.

The point that we wish to emphasize is that a class of solutions containing 11 parameters can be obtained from some initial particular solution by transformations of the $T^4 \ltimes (SO(4) \otimes D)$ group. In turn, both the equations (6) and group transformations are gauge independent. For this reason, none of the parameters are removable by gauge transformation. These parameters are interpreted as degrees of freedom of field configurations. In contrast, the gauge transformations of instanton solutions of self-dual Yang-Mills equations remove the degrees of freedom generated by inversion subgroup of the conformal symmetry group.[34,35]

An interesting property of Seiberg-Witten equations can be pointed out. The four dimensional Seiberg-Witten equations are reduced to the three dimensional ones through some differential constraints, namely $\partial_i f^i = 0$ and $\partial_0 f^j = 0$.[22,23] We have already mentioned that the reduced three dimensional Seiberg-Witten equations are invariant under 10-parameter conformal group of three dimensional Euclidean space as well as under shifts along x^0. So, the $T^4 \ltimes (SO(4) \otimes D)$ group goes over into the $SO(4,1) \otimes T^0$ one.

Indeed, let us copy out the generators of SO(4,1) group obtained in Ref. 23,

$$M_{ij} = x_i\partial_j - x_j\partial_i + f_i\frac{\partial}{\partial f^j} - f_j\frac{\partial}{\partial f^i},$$

$$P_i = \partial_i,$$

$$\tilde{D} = x^j\partial_j - 2f^i\frac{\partial}{\partial f^i},$$

$$K_i = -2x_i x^j\partial_j + x^j x_j\partial_i + 4x_i f^j\frac{\partial}{\partial f^j} - 2f_i x^j\frac{\partial}{\partial f^j} + 2x^j f_j\frac{\partial}{\partial f^i}.$$

It is evident that the violation of symmetry caused by dimensional reduction does not change the number of group parameters. The generators K_i of three dimensional inversions occur instead of the generators M_{0i}. We must note that although the $SO(4,1) \otimes T^0$ group is the symmetry group of the reduced equations, but there is no straightforward reduction procedure which transforms the generators of the $T^4 \ltimes (SO(4) \otimes D)$ group to the generators K_i.

IV. PAINLEVÉ ANALYSIS

The Painlevé property for partial differential equations[11] is believed to be a sufficient condition for integrability.[36] A partial differential equation has the Painlevé property when the solutions of the equation are single valued about the movable singularity manifolds. These manifolds are determined by conditions of the form $Z(x_1,\ldots,x_n)=0$, where Z is an analytic function of n complex variables. So, if Seiberg-Witten (Freund's) equations (6) had the Painlevé property, the solutions to the equations (6) would be represented by the power expansion

$$f^i = \frac{1}{Z^p}\sum_{q=0}^{\infty} a^i_q Z^q, \tag{12}$$

where p is an integer. The expansion (12) contains an arbitrary analytic function $Z=Z(x^\mu)$ determining a singularity manifold $M=\{x^\mu : Z(x^\mu)=0\}$ and five arbitrary analytic functions $a^i_q = a^i_q(x^\mu)$ for some values of q. These values are resonances.

To determine the leading power p, one can take

$$f^i = \frac{a^i}{Z^p},$$

$$\partial_\nu f^i = \frac{\partial_\nu a^i}{Z^p} - \frac{p a^i \partial_\nu Z}{Z^{p+1}},$$

$$\partial^\nu \partial_\nu f^i = \frac{\partial^\nu \partial_\nu a^i}{Z^p} - \frac{2p(\partial_\nu a^i)(\partial^\nu Z) + p a^i \partial^\nu \partial_\nu Z}{Z^{p+1}} + \frac{p(p+1) a^i (\partial_\nu Z)(\partial^\nu Z)}{Z^{p+2}}.$$

By setting the leading term of (6) equal to zero we get

$$\frac{p(a^k a_k)(\partial_\nu Z)(\partial^\nu Z) a^i}{Z^{3p+2}} = -\epsilon \frac{2(-a^k a_k)^{3/2} a^i}{Z^{4p}}.$$

As a consequence, we have

$$p = 2, \quad (-a^k a_k)^{1/2} = \epsilon (\partial^\nu Z)(\partial_\nu Z). \tag{13}$$

The vector function $\hat{a}^i = a^i/(-a_i a^i)^{1/2}$, $\hat{a}_i \hat{a}^i = -1$ is arbitrary.

We note that the Witten-Seiberg equations are equivalent to the Freund's ones up to change of variables $x^\mu \to \mathrm{i} x^\mu$. Without loss of a generality we choose $\epsilon = -1$.

Resonances can be found by setting

$$f^i = \frac{a^i + \omega^i Z^n}{Z^2},$$

$$\partial_\nu f^i = \cdots + \frac{(n-2)\omega^i Z^n - 2a^i}{Z^3} \partial_\nu Z,$$

$$\partial^\nu \partial_\nu f^i = \cdots + \frac{6a^i + (n-2)(n-3)\omega^i Z^n}{Z^4} (\partial^\nu Z)(\partial_\nu Z).$$

Collecting terms which involve ω^i leads us to the linear equations

$$-((a^k a_k)(n-1)(n-2)\omega^i + 2(n+2)a^i (a^k \omega_k))(\partial^\nu Z)(\partial_\nu Z) = (-a^k a_k)^{1/2} (6a^i (a^k \omega_k) + 2(a^k a_k)\omega^i),$$

or

$$2(n-1)a^i (a^k \omega_k) + n(n-3)\omega^i (a^k a_k) \equiv \Lambda^i_k \omega^k = 0.$$

It then follows from $\det \Lambda^i_k = 0$ that

$$\det \Lambda^i_k = (-a^k a_k)^3 (n+1) n^2 (n-2)(n-3)^2 = 0.$$

So, resonances occur at $n = 0,2,3$. This indicates that the solutions f^i do not have an algebraic movable singularity. However, a logarithmic movable singularitity can occur.

For further purpose it is sufficient to consider the four leading terms of (12),

$$f^i = \frac{a^i}{Z^2} + \frac{b^i}{Z} + c^i + d^i Z. \tag{14}$$

Substitution of (14) into (6) gives

$$6a^i(a^kb_k)(\partial_\rho Z)(\partial^\rho Z)-2(a^ka_k)(a^i\partial_\rho\partial^\rho Z+(\partial^\rho a^i)(\partial_\rho Z))+2(a^ka_k)((\partial^i Z)(\partial_j a^j)-(\partial_j Z)(\partial^i a^j)+\varepsilon^{i\nu\rho j}(\partial_\nu Z)$$
$$\times(\partial_\rho a_j))+a^i(\partial_\rho Z)\partial^\rho(a^ka_k)+a^j(\partial_j Z)\partial^i(a^ka_k)-a^j(\partial^i Z)\partial_j(a^ka_k)-\varepsilon^{ij\rho\sigma}a_j(\partial_\rho Z)\partial_\sigma(a^ka_k)$$
$$+6a^i(-a^ka_k)^{1/2}a^jb_j-2b^i(-a^ka_k)^{3/2}=0. \tag{15}$$

The vector function b^i is uniquely determined,

$$b^i=\frac{1}{(-a^ka_k)^{1/2}}\Bigg(a^i\partial^\rho\partial_\rho Z+(\partial^\rho a^i)\partial_\rho Z-\varepsilon^{i\nu\rho j}(\partial_\nu Z)(\partial_\rho a_j)-(\partial^i Z)(\partial_j a^j)+(\partial_j Z)(\partial^i a^j)$$
$$+\frac{1}{2(a^ka_k)}(2a^i(\partial^\nu Z)\partial_\nu(a^ka_k)+\varepsilon^{ij\rho\sigma}a_j(\partial_\rho Z)\partial_\sigma(a^ka_k)+a^j(\partial^i Z)\partial_j(a^ka_k)-a^j(\partial_j Z)\partial^i(a^ka_k))\Bigg). \tag{16}$$

The compatibility condition at $n=2$ is

$$-2(-a^ka_k)^{1/2}((a^ja_j)c^i-a^i(a^jc_j))=\Delta^i, \tag{17}$$

where

$$\Delta^i=(a^ka_k)(\partial^\rho\partial_\rho a^i-b^i\partial^\rho\partial_\rho Z)-(a^kb_k)(5b^i(\partial^\rho Z)(\partial_\rho Z)+4a^i\partial^\rho\partial_\rho Z)+a^i(\partial^\rho Z)(\partial_\rho Z)(b^kb_k)-3\hat{a}^i(a^kb_k)^2$$
$$-5(a^kb_k)(\partial^\rho Z)(\partial_\rho a^i)-\partial^\rho(a^ka_k)(\partial_\rho a^i)/2+b^i(\partial^\rho Z)\partial_\rho(a^ka_k)/2+2a^i(\partial^\rho Z)\partial_\rho(a^kb_k)+(\partial_j(a^ka_k)(\partial^i a^j)$$
$$-\partial^i(a^ka_k)(\partial_j a^j)-\varepsilon^{i\nu\rho j}\partial_\nu(a^ka_k)(\partial_\rho a_j))/2-3(a^kb_k)((\partial_j Z)(\partial^i a^j)-(\partial^i Z)(\partial_k a^k)-\varepsilon^{i\nu\rho j}(\partial_\nu Z)(\partial_\rho a_j))$$
$$+2(a^j(\partial_j Z)\partial^i(a^kb_k)-a^j(\partial^i Z)\partial_j(a^kb_k)-\varepsilon^{ij\nu\rho}a_j(\partial_\nu Z)\partial_\rho(a^kb_k))-(b^j(\partial_j Z)\partial^i(a^ka_k)-b^j(\partial^i Z)\partial_j(a^ka_k)$$
$$-\varepsilon^{ij\nu\rho}b_j(\partial_\nu Z)\partial_\rho(a^ka_k))/2-2(a^ka_k)((\partial_j Z)(\partial^i b^j)-(\partial^i Z)(\partial_k b^k)-\varepsilon^{i\nu\rho j}(\partial_\nu Z)(\partial_\rho b_j))$$
$$+\varepsilon_{jl\rho m}a^jb^l((\partial^i Z)(\partial^\rho a^m)-(\partial^\rho Z)(\partial^i a^m)+\varepsilon^{i\tau\sigma\rho}(\partial_\tau Z)(\partial_\sigma a^m))+\varepsilon_{kl\rho m}a^k((\partial^i a^l)(\partial^\rho a^m)-(\partial^\rho a^l)(\partial^i a^m)$$
$$+\varepsilon^{i\tau\sigma\rho}(\partial_\tau a^l)(\partial_\sigma a^m))/2.$$

The condition (17) is not compatible because $a_i\Delta^i\neq 0$ for arbitrary functions $\hat{a}^i$ and Z. For the compatible condition (17) to occur, a logarithmic term must be included into the expansion (12). So, a logarithmic movable singularity holds. For this reason, the Seiberg-Witten (Freund's) equations do not possess the Painlevé property.

It is interesting to note that the expansion (14) can be rewritten as

$$f^i=\partial^\mu(\partial_\mu(\ln Z)\hat{a}^i)-\varepsilon^{ij\mu\nu}(\partial_\mu(\ln Z)(\partial_\nu\hat{a}_j)+\varepsilon_{\mu\nu\rho\sigma}\partial^\rho(\ln Z)(\partial^\sigma\hat{a}_j))+c^i+d^iZ.$$

The latter fact follows from (13) and (16). Consider the expansion (12) with $a^i_q\equiv 0$ for $q\geqslant 2$ (so-called truncated expansion). We can think of

$$f^i=\partial^\mu(\partial_\mu(\ln Z)\hat{a}^i)-\varepsilon^{ij\mu\nu}(\partial_\mu(\ln Z)(\partial_\nu\hat{a}_j)+\varepsilon_{\mu\nu\rho\sigma}\partial^\rho(\ln Z)(\partial^\sigma\hat{a}_j)) \tag{18}$$

as a change of variables f^i in the equations (6). According to Ref. 37, the truncation (18) gives an available ansatz for particular solutions to the equations (6). Substitution of the truncation (18) into the equations (6) leads to a set of differential constraints for $\hat{a}^i$ and Z. The resulting overdetermined system requires separate analysis.

We note in conclusion that the solutions (10) correspond to (18) with $\hat{a}^i=\hat{u}^i$ and $Z=(-x^\mu x_\mu)^{\mp 1/2}$. In turn, for the solutions (11) we have $Z=(-x^\mu x_\mu)^{\mp 1}$ and $\hat{a}^i=\hat{w}^i$.

The monopolelike solutions obtained in Ref. 21 correspond to (18) with $Z=(-x^ix_i)^{\pm 1/4}$ and $\hat{a}^i=x^i/(-x^jx_j)^{1/2}$.

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APPENDIX

The infinitesimal Lie group transformations have the form[27]

$$L = \xi^{\nu}\partial_{\nu} + \varphi^{i}\frac{\partial}{\partial f^{i}}, \tag{A1}$$

where ξ and φ depend on x^{μ}, f^{j}.

The second prolongation $\mathrm{pr}^{2} L$ of vector field (A1) is

$$\mathrm{pr}^{2} L = L + \Phi^{i\nu}\frac{\partial}{\partial h^{i\nu}} + \Phi^{i\nu\mu}\frac{\partial}{\partial h^{i\nu\mu}},$$

where

$$\Phi^{i\nu} = D^{\nu}(\varphi^{i} - \xi_{\mu}h^{i\mu}) + \xi_{\rho}h^{i\rho\nu}$$

and

$$\Phi^{i\nu\mu} = D^{\nu\mu}(\varphi^{i} - \xi_{\sigma}h^{i\sigma}) + \xi_{\rho}h^{i\rho\nu\mu}.$$

Here $h^{i\nu}=\partial^{\nu}f^{i}$, $h^{i\nu\mu}=\partial^{\nu}\partial^{\mu}f^{i}$, D^{ν} is the total derivative operator

$$D^{\mu}P(x^{\mu},f^{i}) = \partial^{\mu}P + (\partial^{\mu}f^{i})\frac{\partial P}{\partial f^{i}}$$

for arbitrary function $P(x^{\mu},f^{i})$.

It is convenient to denote the equations (6) by $W(f^{i},h^{i\mu},h^{i\mu\nu})=0$. These equations are invariant under infinitesimal transformations (A1) if

$$\mathrm{pr}^{2} L[W(f^{i},h^{i\mu},h^{i\mu\nu})] = 0 \tag{A2}$$

for all solutions of (6). The infinitesimal condition (A2) leads to the differential constraints

$$\frac{\partial\xi^{\mu}}{\partial f^{i}} = \frac{\partial\varphi^{i}}{\partial x^{\mu}} = \frac{\partial^{2}\xi^{\rho}}{\partial x^{\nu}\,\partial x^{\mu}} = \frac{\partial\varphi^{i}}{\partial f^{k}\,\partial f^{m}} = 0, \quad \frac{\partial\varphi^{k}}{\partial f_{m}} + \frac{\partial\varphi^{m}}{\partial f_{k}} = -2\delta^{km}\frac{\varphi^{j}f_{j}}{f^{i}f_{i}},$$

$$\partial_{\mu}\xi_{\nu} + \partial_{\nu}\xi_{\mu} = -\delta_{\mu\nu}\frac{\partial\varphi^{i}}{\partial f_{i}}, \quad \frac{\partial\varphi^{i}}{\partial f_{j}} = \frac{1}{2}\varepsilon^{ijk\mu}\partial_{\mu}\xi_{k} - \partial^{i}\xi^{j} - \frac{1}{4}\delta^{ij}\partial_{\nu}\xi^{\nu}.$$

The functions which satisfy these constraints are

$$\xi^{\nu} = s^{\nu\mu}x_{\mu} + sx^{\nu} + s^{\nu}, \tag{A3}$$

$$\varphi^{i} = s^{ij}f_{j} - \varepsilon^{ij\rho\sigma}s_{\rho\sigma}f_{j}, \tag{A4}$$

where $s^{\mu\nu}=-s^{\nu\mu}$, s^{ν} and s are arbitrary constants. Substituting (A3) and (A4) into (A1) gives

$$L = s^{\mu\nu}M_{\mu\nu} + s^{\nu}P_{\nu} + sD.$$

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A generalization of Connes-Kreimer Hopf algebra

Jungyoon Byun
Mathematics, University of Pennsylvania, Philadelphia, Pennsylvania 19104

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"Bonsai" Hopf algebras, introduced here, are generalizations of Connes-Kreimer Hopf algebras, which are motivated by Feynman diagrams and renormalization. We show that we can find operad structure on the set of bonsais. We introduce a differential on these bonsai Hopf algebras, which is inspired by the tree differential. The cohomologies of these are computed here, and the relationship of this differential with the appending operation $*$ of Connes-Kreimer Hopf algebras is investigated. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1951591]

I. MOTIVATION

Kreimer (1998) discovered a Hopf algebra structure on Feynman diagrams and the forest formula of perturbative quantum field theory. Connes and Kreimer (1999) suggested the representation of Feynman graphs using rooted tree diagrams and represented the Hopf algebra structure with the notion of cuts of tree diagrams. That expression is as follows: let us consider a Feynman diagram in ϕ^3 theory as in Fig. 1.

Figure 1 is a 1-loop graph. Now let us look at another loop having subloops in Fig. 2.

In Kreimer's expression of a Feynman diagram using decorated rooted trees (Connes and Kreimer, 1999), if the loop of Fig. 1 is labeled 1 (in Kreimer's context, this label indicates a specific shape of loop. So, later in this paper, if every loop in the Feynman diagram has the same shape, we do not need this label), the loop of Fig. 2 is expressed as in Fig. 3. In Fig. 2, the loops labeled 2 are immediate subloops of loop 1, and the loop 3 is an immediate subloop of the lower loop 2 and not of loop 1.

In the Connes and Kreimer context, we call a connected rooted tree, which corresponds to a connected Feynman graph, a *tree* and we call a diagram of trees having more than one connected component a *forest*.

The Connes-Kreimer Hopf algebra $\mathcal{H}_K$ is a Hopf algebra with forests of rooted trees as basis elements (see Sec. III for details).

In Fig. 2, the author observed that the biggest loop cannot include more than three immediate subloops of the shape of Fig. 1. Hence, in the tree diagram, the vertex labeled 1 cannot have more than three subsidiary vertices labeled 1, and so the rooted tree of Fig. 3 cannot have a ramification number (or arity, branch number) greater than 3 at the root.

So, in the ϕ^3 theory in which the only allowed loop is that of Fig. 1, the corresponding tree diagrams are forbidden to have ramification number greater than 3. The theory of such ramification number bounded trees is our main interest in this paper. We will call them *bonsais*.

For a more precise description of Feynman diagrams, let us consider the positions of subloops in a loop. For the loops having subloops like Fig. 2, in the context of Connes and Kreimer (unpublished), sometimes we need to indicate which subloop is shrinking and what position is available for a subloop. For that, we label each corner of the loop in Fig. 4 and change that loop into a tree as shown in Fig. 4, by expressing a subloop as a subsidiary vertex in the tree diagram and attaching the labels representing the subloop positions to the edges.

The tree diagram of Fig. 4 asssigns the numbers of the occupied corners in the big loop to edges of the tree. Note that there is no edge numbered 2. This means there is no subloop on the corner 2. We easily see that, in this expression, the left tree of Fig. 5 is allowed but the right tree of Fig. 5 is not.

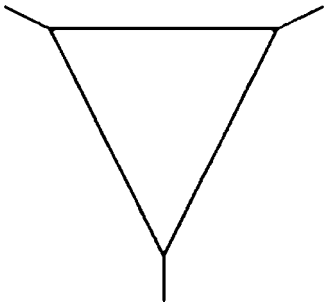

FIG. 1.

II. MAIN RESULTS

Definition 2.1: *We define a Hopf algebra which has the same operations as in the Connes-Kreimer Hopf algebra, and whose basis elements are forests of* trees having ramification numbers at each vertex smaller than or equal to m and under each vertex v, each subsidiary edge of v has labels from $1,2,\ldots,m$ without duplication. *We call this Hopf algebra the* m-bonsai Hopf algebra $\mathcal{H}_{b,m}$. In $\mathcal{H}_{b,m}$, *each tree is called a* m-bonsai.

As in Connes and Kreimer (1999), we can show the following.

Theorem 2.1: $\mathcal{H}_{b,m}$ *is a Hopf algebra*.

As in Connes and Kreimer (1999), when we define an *appending operation*,

$$T * T' = \Sigma \text{ (a bonsai obtained by connecting the root of } T \text{ to a vertex } v \text{ of } T' \text{ with one edge, where the added edge has every possible label)}.$$

(An example of the $*$ operation is in Fig. 11.)

Theorem 2.2: *The operation* $*$ *is pre-Lie, and we have* $\mathcal{H}_{b,m}=\mathcal{U}(\mathcal{L})^{\vee}$, *where* $V^{\vee}$ *is the dual of* V.

In the m-bonsai Hopf algebra, the set of m-bonsais has a structure of an operad, thus there is a natural analog of the tree differential [as in Markl, Shnider, and Stasheff (2002)]. We call it the *vertex-appending differential* ∂ (Definition 9.1).

Then, mainly using the Künneth theorem, we can calculate the cohomology groups of ∂ as follows.

Theorem 2.3: *In m-bonsai*,

$$H^i(\mathcal{H}_{b,m},\partial) = \begin{cases} k\frac{(mn)!}{((m-1)n+1)!n!} & \text{if } i=(2m-1)n+1,\ n\geqslant 0, \\ 0 & \text{otherwise}. \end{cases}$$

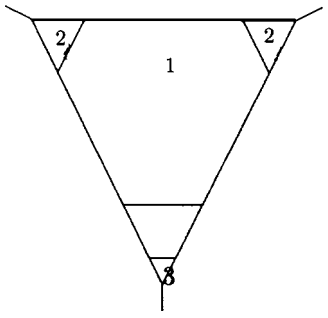

FIG. 2.

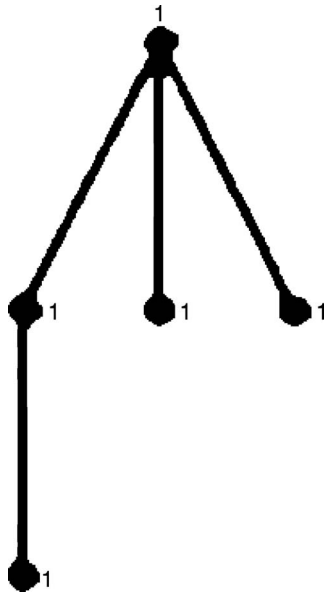

FIG. 3.

Here, $(mn)!/[(m-1)n+1]!n!$ is the number of rooted trees consisting of n of m-corollas, which is called the m-Catalan number. When $m=2$, this number is just the Catalan number. Representatives of H^i are Σ (a bonsai obtained by appending edges to all tips of a rooted tree every vertex of which except tips has ramification number m, one edge to each tip, with every possible label).

When we define $T_1 *_1 T_2$, which is the deviation from ∂ being a derivation of $*$ as

$$T_1 *_1 T_2 = (\partial T_1) * T_2 + T_1 * (\partial T_2) - \partial(T_1 * T_2),$$

we have the following.

Theorem 2.4: *With coefficients mod 2,*

$$T_1 *_1 T_2 = \Sigma \text{ (}a \text{ bonsai obtained by connecting a tip } v \text{ of } T_2 \text{ and the root of } T_1 \text{ with one--edge, and attaching an edge to } v\text{, added edge have every admissible label)} + \Sigma \text{ (}a \text{ bonsai obtained by connecting a nontip of } T_2 \text{ and the root of } T_1 \text{ with two--edge ladder, having every possible label)}$$

and

$$\partial(T_1 *_1 T_2) = (\partial T_1) *_1 T_2 + T_1 *_1 (\partial T_2).$$

We provide an example in Fig. 6.

Now, let us consider another Hopf algebra, having the same operations but the trees having ramification numbers at each vertex smaller than or equal to m but no edge labels, and call it

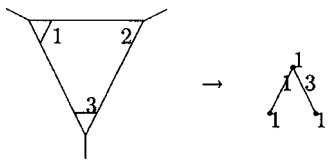

FIG. 4.

FIG. 5.

clear-edged m-bonsai Hopf algebra $\mathcal{H}_{c,m}$. (In other words, a clear-edged m-bonsai is an m-bonsai without edge labels.)

Clear-edged m-bonsai Hopf algebras still represent Feynman graphs, actually more physically relevant, and also appear in the tree diagrams of "open-closed homotopy algebra (OCHA)" [Kajiura and Stasheff (unpublished)].

Then we can define the *vertex-appending differential* similarly to the case of m-bonsai. For example, in planar clear-edged 3-bonsai, we can get an example like Fig. 7.

The cohomology groups of the vertex-appending differential in clear-edged bonsai are not as easy to calculate as in m-bonsai and we have just partial results as follows:

We first define a specific form of bonsai S called "seedling" (Definition 11.3), and then we define the complexes $(\mathbf{C}^{S,*},\partial)$. Then we can show that the cohomology of the whole bonsai complex $H^i=\oplus H^i(S)$, where the sum is over all seedlings.

By the definition of seedling, when $S_1,S_2,\ldots,S_n$ are seedlings, the new bonsai S obtained by appending the roots of each S_i's to a single new root is a seedling again. There is an example in Fig. 8.

On the way to find the relationship of $H(S)$ and $H(S_1),\ldots,H(S_n)$, we have a definition of a bonsai called *grafting seedlings* $(n;T_1,\ldots,T_{n+1};S_1,\ldots,S_n)$ (Definition 11.6), a complex $\{\mathbf{K}^i(gs(n;T_1,\ldots,T_{n+1};S_1,\ldots,S_n))\}$ (Definition 11.8) and the following.

Theorem 2.5: *When* $H^i(gs(n;T_1,\ldots,T_{n+1};S_1,\ldots,S_n))$ *is the ith cohomology group of the complex* $\mathbf{K}^i(gs(n;T_1,\ldots,T_{n+1};S_1,\ldots,S_n))$, *the ith cohomology group* H^i *of clear-edged m-bonsai is*

$$H^i=\bigoplus_{S\ \text{is a grafting seedling}} H^i(S),$$

and

$$H^i(gs(n;T_1,\ldots,T_{n+1};S_1,\ldots,S_n))=\bigoplus_{j_1+\ldots+j_n=i-m}[H^{i_1}(S_1)\otimes\cdots\otimes H^{i_n}(S_n)]^{\oplus N},$$

where N is combinatorially all determined and

$$P=\deg T_1+\cdots+\deg T_n.$$

Finally, as in the case of m-bonsai, we have again the following.

Theorem 2.6: *For any clear-edged m-bonsai* T_1 *and* T_2, $\partial(T_1*_1T_2)=(\partial T_1)*_1T_2+T_1*_1\partial T_2$ *with coefficients mod 2.*

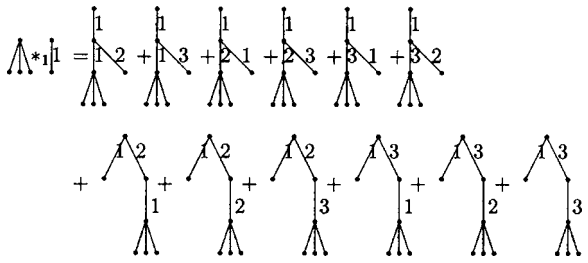

FIG. 6.

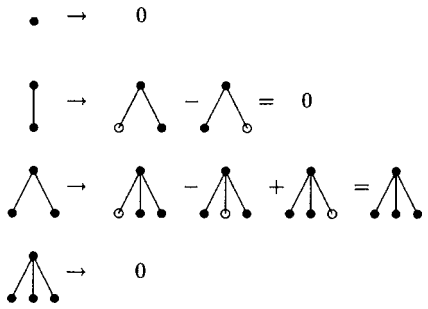

FIG. 7.

III. BONSAI HOPF ALGEBRA

As seen in the last section, loops in Feynman diagrams of a specific theory have a maximum number of immediate subloops. In the example of the preceeding section, the maximum number is 3 and each edge of the tree diagram corresponding to a Feynman diagram has label 1, 2 or 3.

From this motivation, we define the following.

Definition 3.1: A simple cut *of rooted tree is a cut of edges such that at any vertex of T, the path between it and the root has at most one cut, $P_c(T)$ is the part of T cut off by c and $R_c(T)$ is the part of T remaining after cut c.*

Definition 3.2: Let $\mathcal{H}_{b,m}$ be the vector space having as its basis the forests consisting of trees whose vertices have ramification numbers $\leqslant m$ and whose edges are labeled by numbers in $1,2,\ldots,m$.

We equip this $\mathcal{H}_{b,m}$ with operations, as in Connes and Kreimer (1999),

$$(\textit{multiplication})\ m(T_1T_2\cdots T_m,S_1S_2\cdots S_n)=T_1\cdots T_mS_1\cdots S_n \quad (T_i,S_j \textit{ are trees, } m \textit{ is commutative}), \tag{1}$$

$$(\textit{diagonal})\ \Delta(T)=T\otimes 1+\sum_c P_c(T)\otimes R_c(T)\ (T \textit{ is a tree}),$$

$$\Delta(T_1\cdots T_n)=\Delta(T_1)\cdots\Delta(T_n), \tag{2}$$

$$(\textit{antipode})\ S(T)=-\sum_c S(P_c(T))R_c(T)\ (T \textit{ is a tree}),$$

$$S(1)=1,\ S(v)=-v\ (\textit{where } v \textit{ is the one-vertex bonsai}),$$

$$S(T_1\cdots T_n)=S(T_n)\cdots S(T_1), \tag{3}$$

where c runs over simple cuts of T including $c=\emptyset$, and a counit function

$$\epsilon:\mathcal{H}_{b,m}\to\mathcal{H}_{b,m} \quad \textit{such that } \epsilon(1)=1 \quad \textit{and} \quad \epsilon(f)=0 \quad \textit{if a forest } f\neq 1. \tag{4}$$

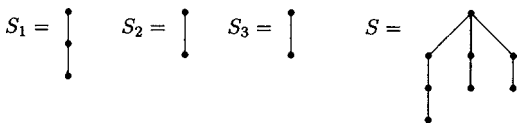

FIG. 8.

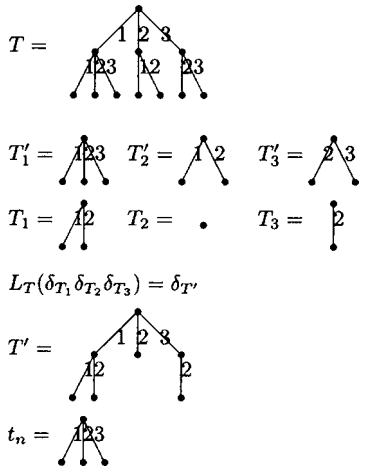

FIG. 9.

We call the rooted tree T an m-bonsai *and* $\mathcal{H}_{b,m}$ *the m*-bonsai Hopf algebra.

It will be proved in the next section that this vector space $\mathcal{H}_{b,m}$ is actually a Hopf algebra.

Definition 3.3: Sometimes we will ignore the positions of subloops in Feynman graphs and use trees without labels on edges. Then the trees in the forests corresponding to the Feynman graphs have no label on their edges. In this case, we denote the vector space having a basis consisting of forests of planar trees as $\mathcal{H}_{c,m}$*, where m is the maximum of ramification number of each vertex in the trees of the forests in* $\mathcal{H}_{c,m}$*. We equip* $\mathcal{H}_{c,m}$ *with operations* (1)–(4) *in Definition 3.2. Then we call that Hopf algebra* planar clear-edged *m*-bonsai Hopf algebra.

IV. BASIC RESULTS RELATED TO HOPF ALGEBRAS

In order to develop a basic theorem related to Lie algebras, let us adapt Connes and Kreimer (1999) to our bonsai language and get some basic results.

In order to prove that our Hopf algebras are actually Hopf algebras and derive some algebraic results, let us give another expression of bonsai Hopf algebras and their elements.

First we give the following.

Definition 4.1: For a bonsai T, deg(*T*) *is the number of vertices of T*.

For each p, we let Σ_p be the set of bonsai T such that $\deg(T) \leqslant p$ with the restriction of ramification numbers by m, and let $\mathcal{H}_p$ be the polynomial commutative algebra generated by the symbols,

$$\delta_T, \quad T \in \Sigma_p. \tag{5}$$

We define a coproduct on $\mathcal{H}_p$ by

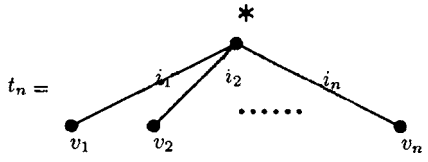

FIG. 10.

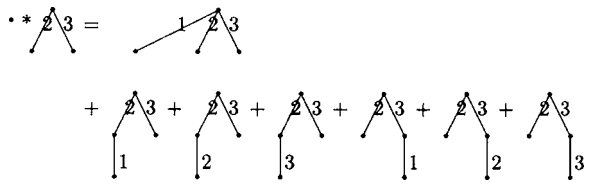

FIG. 11.

$$\Delta\delta_T = \delta_T \otimes 1 + \sum_c \left(\prod_{P_c(T)} \delta_{T_i} \right) \otimes \delta_{R_c(T)}, \tag{6}$$

where the last sum is over all simple cuts including $c=\emptyset$, while the product $\Pi_{P_c(T)}$ is over the cut branches. Sometimes $\Pi_{P_c(T)}\delta_{T_i}$ is written $\delta_{P_c(T)}$. The antipodal map S is given as

$$S(1) = 1, \tag{7}$$

$$S(\delta_T) = -\delta_T - \sum_{\text{simple cuts } c\neq\emptyset \text{ of } T} S(\delta_{P_c(T)})\delta_{R_c(T)}. \tag{8}$$

We let $\mathcal{H}_{b,m}=\cup\mathcal{H}_p$ and extend the maps on $\mathcal{H}_p$ to $\mathcal{H}_{b,m}$. Coassociativity of Δ and $m((S\otimes \mathrm{id})\Delta)=\epsilon$ can be shown just by introducing the notion of double cuts of T. But in order to emphasize the algebraic aspect of the definition, let us give another proof of the following theorem.

Theorem 4.1: Δ *is coassociative*.

Proof: It is enough to check

$$(\mathrm{id}\otimes\Delta)\Delta\delta_T = (\Delta\otimes\mathrm{id})\Delta\delta_T \quad \forall\, T\in\Sigma_p, \tag{9}$$

where T is a tree in $\mathcal{H}_{b,m}$. Define $L_T:\mathcal{H}_{b,m}\to\mathcal{H}_{b,m}$ as follows: Let $T'_1,\ldots,T'_n$ be the subsidiary branches of the root of T in T. Let T_{n_i} be a subtree of T'_{n_i} whose root is the root of T'_{n_i}. Define T' to be the tree obtained by appending T_{n_i}'s to a new root $*$ and the edge connecting $*$ and the root of T_{n_i} is labeled the same as the edge connecting the root of T and the root of T'_{n_i}. Then $L_T(\delta_{T_{n_1}}\cdots\delta_{T_{n_p}})=\delta_{T'}$. If some T_j is not a subsidiary branch of the root in T, $L_T(\delta_{T_1}\cdots\delta_{T_n})$ is 0. (An example of this notation is in Fig. 9.)

First let us show that

$$\Delta\circ L_T(a) = L_T(a)\otimes 1 + (\mathrm{id}\otimes L_T)\circ\Delta(a), \tag{10}$$

where $a=\delta_{T_1}\delta_{T_2}\cdots\delta_{T_n}$ and $T_1,\ldots,T_n$ are all subsidiary branches of the root of T in T so that $L_T(a)=\delta_T$. From (6), we get

$$\Delta(L_T(a)) - L_T(a)\otimes 1 = \sum_c \left(\prod_{P_c} \delta_{T'_i} \right) \otimes \delta_{R_c}, \tag{11}$$

where all simple cuts of T (including $c=\emptyset$) are allowed. Moreover,

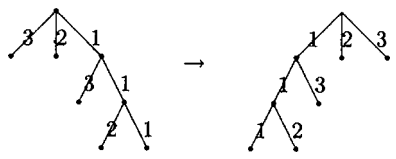

FIG. 12.

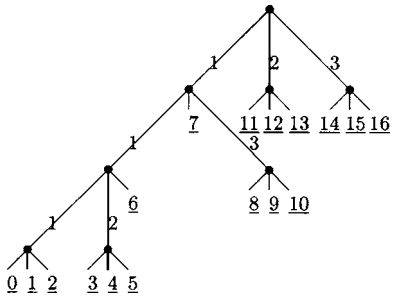

FIG. 13.

$$\Delta(a) = \prod_{i=1}^{n} \left(\delta_{T_i} \otimes 1 + \sum_{c_i} \left(\prod_{P_{c_i}} \delta_{T_{i_j}''} \right) \otimes \delta_{R_{c_i}} \right), \tag{12}$$

where again all simple cuts c_i of T_i are allowed.

Let t_n be the corolla with root $*$ and n other vertices v_i labeled by $i_1, \ldots, i_n$, where i_j is the label of the edge in T connecting the root of T and the vertex of T_j', all directly connected to the root $*$, as in Fig. 10.

We view t_n in an obvious way as a subgraph of the tree T, where $*$ is the root of T and the vertex v_i is the root of T_i, i.e., we can get T by attaching the root of T_i to the vertex v_i of t_n. Given a simple cut c of T we get by restriction to the corolla subgraph $t_n \subset T$ a cut of t_n. It is characterized by the subset $I = \{i \,|\, (*, v_i) \in c\} \subset \{1, \ldots, m\}$. The simple cut c is uniquely determined by the restriction c_i of c to each subtree T_i'. Thus the simple cuts c_i of T are in one to one correspondence with the various terms of the expression (12), namely the $\Pi_{k \in I}(\delta_{T_k} \otimes 1) \Pi_{i \in \{1,\ldots,m\}-I} \Pi_{P_{c_i}} \delta_{T_{i_j}''} \otimes \delta_{R_{c_i}}$. So, applying $\mathrm{id} \otimes L$ to (12) and comparing with (11), we get (10).

Now let us show (10) by induction. We have,

$$\Delta \delta_\bullet = \delta_\bullet \otimes 1 + 1 \otimes \delta_\bullet, \tag{13}$$

where $\bullet$ is the one-vertex bonsai, so that $\mathcal{H}_1$ is coassociative. Let us assume that $\mathcal{H}_n$ is coassociative and prove it for $\mathcal{H}_{n+1}$. It is enough to check (9) for the generators δ_T, with $\deg(T) \leqslant n+1$. We have $\delta_T = L_T(\delta_{T_1} \delta_{T_2} \cdots \delta_{T_m}) = L_T(a)$ where the degrees of all T_j are $\leqslant n$, i.e., $a \in \mathcal{H}_n$. Using (10) we can replace $\Delta \delta_T$ by

$$L_T(a) \otimes 1 + (\mathrm{id} \otimes L_T) \Delta(a), \tag{14}$$

where Δ is the coassociative coproduct in $\mathcal{H}_n$.

The first term of (9) is then

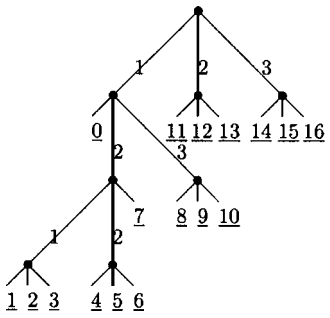

FIG. 14.

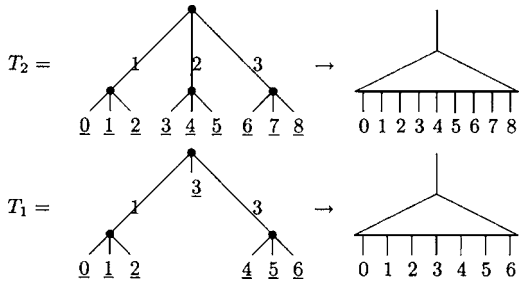

FIG. 15.

$$(\mathrm{id} \otimes \Delta)(L_T(a) \otimes 1 + (\mathrm{id} \otimes L_T)\Delta(a)) = L_T(a) \otimes 1 \otimes 1 + \Sigma a_{(1)} \otimes \Delta \circ L_T a_{(2)}, \tag{15}$$

where $\Delta(a) = \Sigma a_{(1)} \otimes a_{(2)}$, which by (10) gives

$$L_T(a) \otimes 1 \otimes 1 + \Sigma a_{(1)} \otimes L_T a_{(2)} \otimes 1 + \Sigma a'_{(1)} \otimes a'_{(2)} \otimes L_T a'_{(3)}, \tag{16}$$

where

$$(\Delta \otimes \mathrm{id})\Delta(a) = (\mathrm{id} \otimes \Delta)\Delta(a) = \Sigma a'_{(1)} \otimes a'_{(2)} \otimes a'_{(3)} \tag{17}$$

by induction hypothesis on n, since $a \in \mathcal{H}_n$.

The second term of (9) is $\Delta \circ L(a) \otimes 1 + \Sigma \Delta a_{(1)} \otimes L a_{(2)}$, which by (10) gives,

$$L(a) \otimes 1 \otimes 1 + \Sigma a_{(1)} \otimes L a_{(2)} \otimes 1 + \Sigma a'_{(1)} \otimes a'_{(2)} \otimes L a'_{(3)}. \tag{18}$$

Thus we conclude that Δ is coassociative.

Theorem 4.2: $m((S \otimes \mathrm{id})\Delta) = \epsilon$.

Proof: We have $m((S \otimes \mathrm{id})\Delta)(1) = m(S \otimes \mathrm{id})(1 \otimes 1) = S(1)1 = 1 = \epsilon(1)$. And when $\delta_T \neq 1$,

$$\begin{aligned} m((S \otimes \mathrm{id})\Delta)(\delta_T) &= m\left((S \otimes \mathrm{id})\left(\delta_T \otimes 1 + \sum_{\text{simple cuts } c} \delta_{P_c(T)} \otimes \delta_{R_c(T)}\right)\right) = S(\delta_T) \\ &\quad + m\left(\sum_{\text{simple cuts } c} S(\delta_{P_c(T)}) \otimes \delta_{R_c(T)}\right) = S(\delta_T) + \sum_{\text{simple cuts } c} S(\delta_{P_c(T)})\delta_{R_c(T)} = 0, \end{aligned} \tag{19}$$

where the last equality is by the definition of the antipodal map S.

V. LIE ALGEBRA $\mathcal{L}^1$

Let $\mathcal{L}^1 \subset \mathcal{H}^\vee_{b,m}$ be the linear space having basis $\{Z_T | T \in \mathcal{H}_{b,m}$ is a tree$\}$, where δ_T is defined as

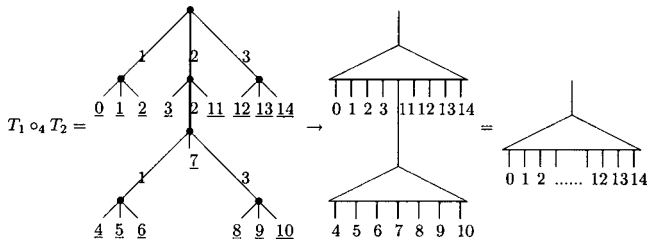

FIG. 16.

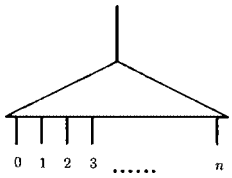

FIG. 17.

$$\langle Z_T, \delta_T \rangle = 1 \tag{20}$$

and

$$\langle Z_T, P(\delta_{T_i}) \rangle = (\partial / \partial \delta_T P)(0) \tag{21}$$

for each rooted tree T.

We introduce an operation on $\mathcal{L}^1$ by

$$Z_{T_1} * Z_{T_2} = \sum_T n(T_1, T_2; T) Z_T, \tag{22}$$

where the integer $n(T_1, T_2; T)$ is determined as the number of simple cuts c with cardinality $|c| = 1$ of bonsai T such that the cut branch is T_1 while the remaining trunk is T_2.

With a notational abuse such as $T = Z_T$, we have an example of $*$ in Fig. 11.

In this section, we will show that $\mathcal{L}^1$ is a Lie algebra and the Hopf algebra $\mathcal{H}_{b,m}$ is the dual of the enveloping algebra of $\mathcal{L}^1$.

Theorem 5.1: $\deg(T)$ defines a grading of the Lie algebra $\mathcal{L}^1$.

Proof: If we write $Z_{T_1} * Z_{T_2} = \Sigma\, Z_T$, then the number of vertices in T is the sum of numbers of vertices in T_1 and T_2.

Definition 5.1: We define the bracket $[Z_{T_1}, Z_{T_2}] = Z_{T_1} * Z_{T_2} - Z_{T_2} * Z_{T_1}$.

Theorem 5.2: *(a) The bracket of the previous definition makes* $\mathcal{L}^1$ *a Lie algebra. (b) The Hopf algebra* $\mathcal{H}_{b,m}$ *is the dual of the enveloping algebra of the Lie algebra* $\mathcal{L}^1$.

First we define the associator

$$A(T_1, T_2, T_3) := Z_{T_1} * (Z_{T_2} * Z_{T_3}) - (Z_{T_1} * Z_{T_2}) * Z_{T_3}. \tag{23}$$

and see the following.

Lemma 1: $A(T_1, T_2, T_3) = \Sigma n(T_1, T_2, T_3; T) Z_T$, where the integer $n(T_1, T_2, T_3; T)$ is the number of simple cuts c of T such that the number of elements $|c|$ of c is 2 and the two branches cut out from T_3 by c are T_1, T_2 while the remaining trunk $R_c(T) = T_3$.

Proof: When we evaluate (23) against Z_T we get the coefficient

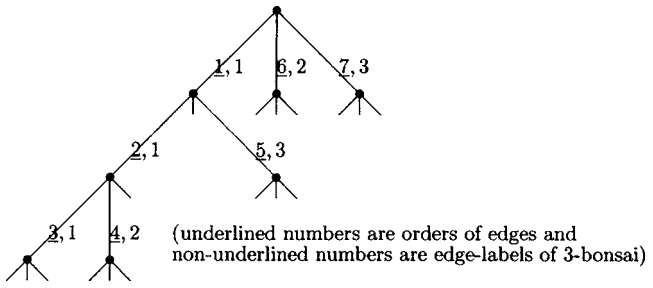

FIG. 18.

$$\sum_{T'} n(T_1,T';T)n(T_2,T_3;T') - \sum_{T''} n(T_1,T_2;T'')n(T'',T_3;T). \tag{24}$$

The first term corresponds to pairs of cuts, c, c' of T with $|c|=|c'|=1$ and where c' is a cut of $R_c(T)$. These pairs of cuts fall into two classes either $c\cup c'$ is an admissible cut or it is not. The second sum corresponds to pairs of cuts c_1, c_1' of T such that $|c_1|=|c_1'|=1$, $R_{c_1}(T)=T_3$ and c_1' is a cut of $P_{c_1}(T)$. In such a case $c_1\cup c_1'$ is never an admissible cut so the difference (24) amounts to subtracting from the first sum the pairs c, c' such that $c\cup c'$ is not an admissible cut. This gives

$$A(T_1,T_2,T_3) = \sum_T n(T_1,T_2,T_3;T)Z_T, \tag{25}$$

where $n(T_1,T_2,T_3;T)$ is the number of admissible cuts c of T of cardinality 2 such that the two cut branches are T_1 and T_2, and T_3 is the remaining trunk.

Now for the theorem, we have the following.

Proof: (a) By the lemma, it is clear that

$$A(T_1,T_2,T_3) = A(T_2,T_1,T_3). \tag{26}$$

Now compute $[[Z_{T_1},Z_{T_2}],Z_{T_3}]+[[Z_{T_2},Z_{T_3}],Z_{T_1}]+[[Z_{T_3},Z_{T_1}],Z_{T_2}]$. We can write it as a sum of 12 terms,

$$\begin{aligned}(T_1*T_2)*T_3 - (T_2*T_1)*T_3 - T_3*(T_1*T_2) + T_3*(T_2*T_1) + (T_2*T_3)*T_1 - (T_3*T_2)*T_1\\ - T_1*(T_2*T_3) + T_1*(T_3*T_2) + (T_3*T_1)*T_2 - (T_1*T_3)*T_2 - T_2*(T_3*T_1)\\ + T_2*(T_1*T_3) = -A(T_1,T_2,T_3) + A(T_2,T_1,T_3) - A(T_3,T_1,T_2) + A(T_3,T_2,T_1) - A(T_2,T_3,T_1)\\ + A(T_1,T_3,T_2) = 0.\end{aligned} \tag{27}$$

(b) Let P and Q be polynomials of δ_T's. By the definition of Z_T, Z_T vanishes when paired with any monomial $\delta_{T_1}^{n_1}\cdots\delta_{T_k}^{n_k}$ except when this monomial is δ_T. Since $P\to P(0)$ is the counit ϵ of $\mathcal{H}_{b,m}$ and since Z_T satisfies

$$\langle Z_T,PQ\rangle = (\partial/\partial\delta_T PQ)(0) = (\partial/\partial\delta_T P)(0)Q(0) + P(0)(\partial/\partial\delta_T Q)(0) = \langle Z_T,P\rangle\epsilon(Q) + \epsilon(P)\langle Z_T,Q\rangle, \tag{28}$$

it follows that the coproduct of Z_T is

$$\Delta Z_T = Z_T\otimes 1 + 1\otimes Z_T. \tag{29}$$

The product of two elements of $\mathcal{H}_{b,m}^\vee$ is defined by

$$\langle Z_1Z_2,P\rangle = \langle Z_1\otimes Z_2,\Delta P\rangle. \tag{30}$$

Since the commutator of two derivations is still a derivation, the subspace of $\mathcal{H}_{b,m}^\vee$ satisfying (36) is stable under bracket. What remains is to show that

$$Z_{T_1}Z_{T_2} - Z_{T_2}Z_{T_1} = [Z_{T_1},Z_{T_2}], \tag{31}$$

where $[Z_{T_1},Z_{T_2}]=Z_{T_1}*Z_{T_2}-Z_{T_2}*Z_{T_1}$ by definition.

Let $\mathcal{H}_0=\mathrm{Ker}\,\epsilon$ be the augmentation ideal of $\mathcal{H}_{b,m}$. By definition of Δ,

$$\Delta\delta_T = \delta_T\otimes 1 + 1\otimes\delta_T + R_T, \tag{32}$$

where $R_T\in\mathcal{H}_0\otimes\mathcal{H}_0$. In fact, we have

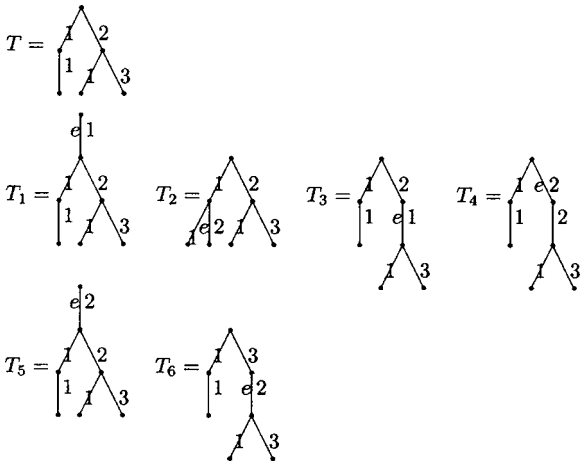

FIG. 19.

$$R_T = \sum_c \delta_{T'_c} \otimes \delta_{T_c} \tag{33}$$

modulo $(\mathcal{H}_0)^2 \otimes \mathcal{H}_0$, where c varies among single cuts of the bonsai tree T, where T_c is the trunk of T that contains the root, and T'_c is the tree which remains. When we compute

$$\langle Z_{T_1} Z_{T_2}, \delta_T \rangle = \langle Z_{T_1} \otimes Z_{T_2}, \Delta \delta_T \rangle, \tag{34}$$

the only part which contributes comes from R_T and it counts the number of ways of obtaining T from T_1 and T_2, which gives (31).

If a map f satisfies

$$\langle f, PQ \rangle = \langle f, P \rangle \epsilon(Q) + \epsilon(P) \langle f, Q \rangle, \tag{35}$$

f is determined by $f(\delta_T) = \langle f, \delta_T \rangle$'s and each of them is a scalar. Since $f(\delta_T) = \Sigma_{T'} f(\delta_{T'}) Z_{T'}(\delta_T)$, f has the form $\Sigma f(\delta_T) Z_T$. Hence $\{Z_T\}$ is a basis of the subspace of $\mathcal{H}^\vee_{b,m}$ consisting of the vectors f satisfying (35).

Since every Z_T satisfies (35) by (28) and $f \in \mathcal{H}^\vee_{b,m}$ satisfies (35) if and only if f satisfies

$$\Delta f = f \otimes 1 + 1 \otimes f, \tag{36}$$

we have $\mathcal{L}^1 = Prim(\mathcal{H}^\vee_{b,m})$ and they are isomorphic as Lie algebras. Since $\mathcal{H}^\vee_{b,m}$ is connected and cocommutative, by the Milnor-Moore theorem, $\mathcal{H}^\vee_{b,m} = \mathcal{U}(Prim(\mathcal{H}^\vee_{b,m})) = \mathcal{U}(\mathcal{L}^1)$ and so $\mathcal{H}_{b,m} = \mathcal{U}(\mathcal{L}^1)^\vee$.

$$d^0(\ \cdot \otimes 1) = e' \left\lfloor 1 \otimes e_{1,1} \right. \ + \ e' \left\lfloor 2 \otimes e_{1,2} \right.$$

$$d^1(\ e' \left\lfloor 1 \otimes e_{1,1}) = \begin{matrix} e'' \\ e' \end{matrix} \left\lfloor \begin{matrix} 1 \\ 1 \end{matrix} \right. \otimes e_{1,1} \wedge e_{2,1} \ + \ \begin{matrix} e' \\ e'' \end{matrix} \left\lfloor \begin{matrix} 1 \\ 1 \end{matrix} \right. \otimes e_{2,1} \wedge e_{1,1}$$

$$+ \ \begin{matrix} e'' \\ e' \end{matrix} \left\lfloor \begin{matrix} 2 \\ 1 \end{matrix} \right. \otimes e_{1,2} \wedge e_{2,1} \ + \ \begin{matrix} e' \\ e'' \end{matrix} \left\lfloor \begin{matrix} 1 \\ 2 \end{matrix} \right. \otimes e_{2,2} \wedge e_{1,1}$$

FIG. 20.

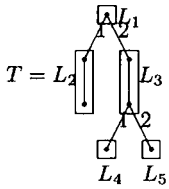

L_1 only grows upward by ii) of Definition 7.1.

FIG. 21.

VI. OPERAD OF *m*-BONSAI

Now let us consider operad theory with respect to the m-bonsai Hopf algebra structure. As seen in the preceding section, for trees $T, T' \in \mathcal{H}_{b,m}$ we can define $T * T'$ and this is a (left) pre-Lie operation. The map $T \mapsto Z_T$ is a pre-Lie isomorphism from the space spanned by trees to $\mathcal{L}^1$. In $\mathcal{H}_{b,m}$, we denote this $\mathcal{L}^1$ as $\mathcal{L}_{b,m}$. We will sometimes allow a notational abuse such as $T = Z_T$ from now on.

Let us start from a rudimentary idea. Every bonsai in $\mathcal{H}_{b,m}$ has a unique form in which for each vertex, its subsidiary edges are arranged so that the lower edge label is on the left of the higher edge label as in Fig. 12.

We can number the possible positions in the bonsai of Fig. 12 to append other bonsais as in Fig. 13, the example in $\mathcal{L}_{b,3}$ (the orders of possible appending positions are underlined). When the labeling of Fig. 13 is changed into that of Fig. 14, then the numbering of possible appending positions is also changed.

Then, by taking the standard form of bonsai and ordering the possible positions of appending, we can get the transform of a bonsai into the broomstick diagram used in Markl, Shnider, and Stasheff (2002) like Fig. 15, again in $\mathcal{L}_{b,3}$.

So, we can define $T_1 \circ_i T_2$ as appending T_1 to T_2 at the ith appending position of T_2, and for T_2 and T_1 in Fig. 15, $T_1 \circ_4 T_2$ is given as in Fig. 16.

Then obviously, this $\circ_i$ satisfies the definition of *pre-Lie system* of Gerstenhaber (1963) [it is called *nonsymmetric pseudo-operad* in Markl, Shnider, and Stasheff (2002), but it has a difference in the convention of grading]. When we use the pseudo-operad later, we will give an extra definition, which we give here.

Definition 6.1: When $\{V_i\}$ *is a graded module over a field* k *and* $\circ_i = \circ_i(m,n) : V_m \otimes V_n \to V_{m+n}$ *is an operation satisfying; when* f^m, g^n, *and* h^p *are in* V_m, V_n, *and* V_p, *respectively*,

$$h^p \circ_j (g^n \circ_i f^m) = \begin{cases} g^n \circ_{i+p} (h^p \circ_j f^m) & \text{if } 0 \leqslant j \leqslant i-1, \\ (h^p \circ_{j-i} g^n) \circ_i f^m & \text{if } i \leqslant j \leqslant n+i, \end{cases} \tag{37}$$

then $\{\{V_i\}, \circ_i\}$ *is called a* (left) pre-Lie system.

[In Gerstenhaber (1963) the right pre-Lie system is defined, but we define and use the left pre-Lie system. This is mainly intended for the theory related to Hopf algebra we will argue later.] By the broomstick diagrams shown in Figs. 15 and 16, we have the following.

Definition 6.2: When $W_{m,n}$ *is the vector subspace of* $\mathcal{L}_{b,m}$ *generated by the trees having the number* n *of possible appending positions, and* $T_1 \circ_i T_2$ *is appending* T_1 *to* T_2 *at the appending position* i *of* T_2, *then* $\{\{W_{m,n}\}, \circ_i\}$ *is a left pre-Lie system. It is called* m-bonsai pre-Lie system. *For*

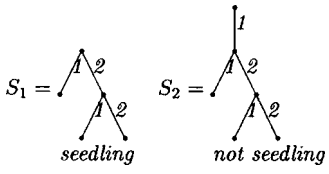

FIG. 22.

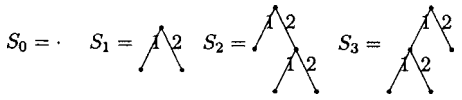

FIG. 23.

trees T which are basis elements of $W_{m,n}$, *n is called the appending degree of T, and denoted* $\deg_{ap}(T)$.

(Graphically, a basis element of $W_{m,n}$ has the broomstick representation like Fig. 17.)

VII. BRANCH-FIXED DIFFERENTIAL

In the next several sections, following the oracle of Markl, Shnider, and Stasheff (2002), we will define some complexes related to bonsais. To get the analogy of the *cobar complex* and the *tree differential* in Sec. 3.1 of Markl, Shnider, and Stasheff (2002), first let us give an order of edges of a bonsai as in Fig. 18, i.e., starting from the root, sweeping around the bonsai counterclockwise and numbering the edges. We call this order the *traversing order*. In the traversing order, e_{k,l_k} is a vector representing the kth edge of a tree T, such that $1 \leqslant l_k \leqslant m$ is the edge label of the kth edge.

Second, let us define a vector space $\mathbf{C}^n$ having basis $T \otimes e_{1,l_1} \wedge \cdots \wedge e_{k,l_k}$, where T is a m-bonsai (not forest) having n edges and the pairs k, l_k run over the labels of edges of T. (If T is a vertex, i.e., a connected bonsai without any edge, then $e_{1,l_1} \wedge \cdots \wedge e_{k,l_k}$ is the constant unit 1.) For later use, we denote this $e_{1,l_1} \wedge \cdots \wedge e_{k,l_k}$ as $\det(T)$ and call it the *determinant term* of T, and call $T \otimes \det(T)$ a *determinanted bonsai*. So the basis element corresponding to the bonsai T of Fig. 18 is $T \otimes e_{1,1} \wedge e_{2,1} \wedge e_{3,1} \wedge e_{4,2} \wedge e_{5,3} \wedge e_{6,2} \wedge e_{7,3} = T \otimes \det(T)$. Let us denote $\mathbf{C} = \oplus \mathbf{C}^m$. Once we define d, we call this complex $(\mathbf{C}, d)$ the *bonsai cobar complex* after the *cobar complex* of Markl, Shnider, and Stasheff (2002).

Third, let us define a map $d^i : \mathbf{C}^i \to \mathbf{C}^{i+1}$ and show that $d^{i+1} \circ d^i = 0$ as follows.

Definition 7.1: Let T be an m-bonsai. Let T′ be a bonsai such that we can obtain T by contracting an edge e′ from T′ and the following conditions are satisfied.

(i) *T′ does not have more branching vertices (i.e., vertices which have the ramification numbers >1) than T,*
(ii) *e′ is not attatched to a branching vertex of T so that e′ becomes a subsidiary edge of that branching vertex.*

We call this T′ a branch-fixed extension *of T.*

For example, for the 3-bonsai T in Fig. 19, T_1, T_3, T_5, and T_6 are all branch-fixed extension of T, but T_2 [violating (i)] and T_4 [violating (ii)] are not.

Then we define $d^i : C^i \to C^{i+1}$ as follows: when $T \in \mathbf{C}^i$,

$$d^i(T) = \sum T' \otimes e'_{j,l_j} \wedge e'_{1,l_1} \wedge \cdots \wedge \widehat{e'_{j,l_j}} \wedge \cdots \wedge e'_{i+1,l_{i+1}}, \tag{38}$$

where the sum runs over T', which is a branch-fixed extension of T having an edge e added to T and that e is denoted e'_{j,l_j} in the edge-ordering of T'.

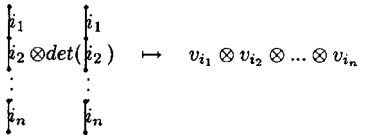

FIG. 24.

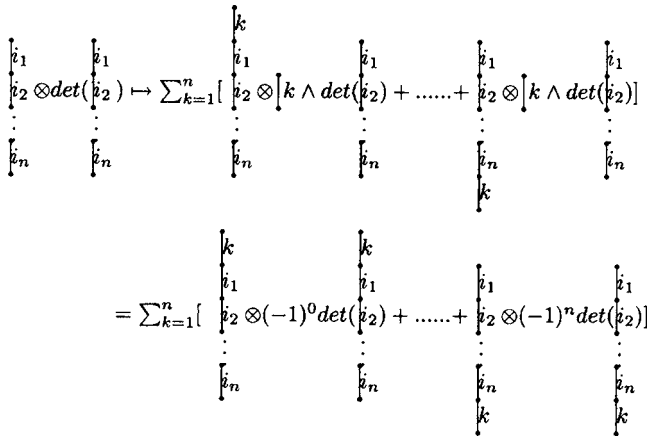

FIG. 25.

Theorem 7.1: $d^{i+1}\circ d^i=0$.

Proof: Suppose T'' is a branch-fixed extension of a bonsai T' with added edge e'', which is a branch-fixed extension of T with added edge e'. Then, when e'' is e''_{j,l_j} and e' is e''_{k,l_k} in the edge ordering of T'' and $d^{i+1}\circ d^i(T)$ is written as $\Sigma S\otimes f_{1,p_1}\wedge\cdots\wedge f_{i+2,p_{i+2}}$, where S runs over the bonsais obtained by attaching two edges as given in (i) and (ii) in Definition 7.1 and f_{i,p_i}'s are the edges of $S, T''\otimes e''_{1,l_1}\wedge\cdots\wedge e''_{i+2,l_{i+2}}$ can be obtained only in two ways.

(i) Adding e' first to T, then the component of $T''\otimes e''_{1,l_1}\wedge\cdots\wedge e''_{i+2,l_{1+2}}$ is $T''\otimes e''_{j,l_j}\wedge e''_{k,l_k}\wedge e''_{1,l_1}\wedge\cdots\wedge\widehat{e''_{j,l_j}}\wedge\cdots\wedge\widehat{e''_{k,l_k}}\wedge\cdots\wedge e''_{i+2,l_{i+2}}$.

(ii) Adding e'' first to T, then the component of $T''\otimes e''_{1,l_1}\wedge\cdots\wedge e''_{i+2,l_{1+2}}$ is $T''\otimes e''_{k,l_k}\wedge e''_{j,l_j}\wedge e''_{1,l_1}\wedge\cdots\wedge\widehat{e''_{j,l_j}}\wedge\cdots\wedge\widehat{e''_{k,l_k}}\wedge\cdots\wedge e''_{i+2,l_{i+2}}$.

Since the orders of e''_{k,l_k} and e''_{j,l_j} are different in the wedge products, the sum of two terms in (i) and (ii) is 0, and this is true for all components of $d^{i+1}\circ d^i(T)$. Hence $d^{i+1}\circ d^i=0$.

We call this boundary map d^i the *branch-fixed differential*. A simple example is given in Fig. 20. We will study the cohomology of this $\{d^i\}$, but before that, following Markl, Shnider, and Stasheff (2002), let us see an important property of this bonsai complex in the next section.

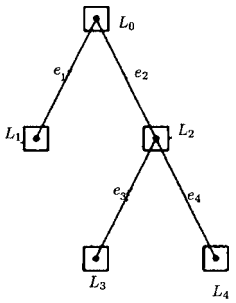

FIG. 26.

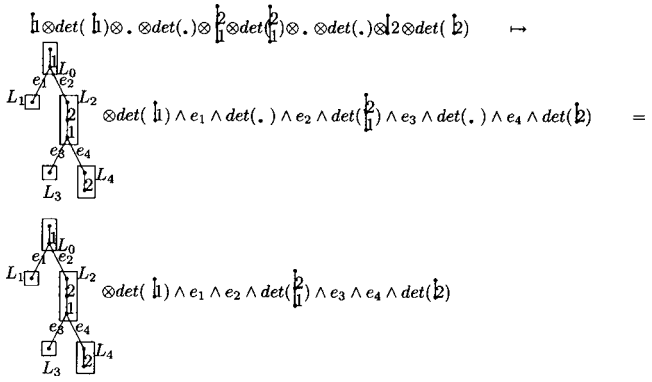

FIG. 27.

VIII. COHOMOLOGY OF BRANCH-FIXED DIFFERENTIAL

In this section, we study the cohomology theory of the cochain complex $\{C^i, d^i\}$, where C^i is the bonsai cobar complex and d^i is the branch-fixed differential. We will define a kind of bonsai called *seedling* and a complex $\{\mathbf{C}^{S,j}, d^{i+j}\}_{j\geq 0}$ called *thread* and show that the cohomology groups of $\{C^i, d^i\}$ are the direct sum of cohomology groups of threads $\{\mathbf{C}^{S,j}, d^{i+j}\}_{j\geq 0}$.

First, let us give some definitions.

Definition 8.1: A bonsai every vertex, of which has the ramification number 0 or 1, is called a ladder. *In other words, a ladder is a bonsai which has no branching vertex.*

Definition 8.2: If a bonsai T has an edge, a vertex v which is an end of only one edge and is not the root, is called a tip. *If a bonsai T is a one-vertex bonsai, the root v is a tip.*

By the definition of d^i, all terms in $d^i(T)$ are of the form $\pm T' \otimes e \wedge \det(T)$, where T' runs over bonsais obtained by adding an edge e to T so that (i) and (ii) of Definition 7.1 hold. So T' has the form of extending a subladder of T which does not contain the subsidiary edges of branching vertices, as in the example of Fig. 21, boxed subladders of which are denoted $L_1, L_2, \ldots, L_5$.

So, the action of d^i on $T \otimes \det(T)$ is by extending a ladder of T, getting an edge e and changing $\det(T)$ into $e \wedge \det(T)$. Acting by d^i's on $T \otimes \det(T)$, the possible bonsais appearing in the $d^i(T)$ are obtained by extending a subladder of T as in the example of Fig. 21.

Keeping this intuitive fact in mind, we have some definitions.

Definition 8.3: A seedling *is an m-bonsai all of whose vertices other than tips are branching vertices. For example, in 2-bonsai, S_1 of Fig. 22 is a seedling, but S_2 is not, because the root vertex is not a branching vertex. In other words, a seedling is a bonsai which cannot be obtained from another bonsai by adding an edge so that (i) and (ii) of Definition 7.1 are satisfied.*

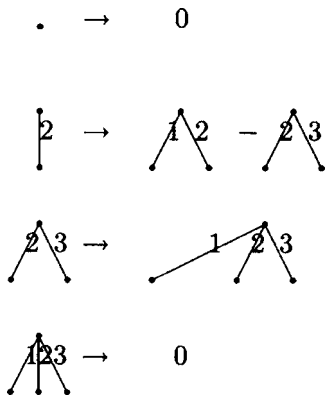

FIG. 28.

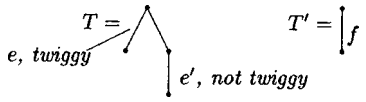

FIG. 29.

Definition 8.4: Let $\mathbf{C}^{S,0}$ *be the submodule of* $\mathcal{C}^i$, *where S is a seedling and i is the number of edges of S, generated by* $S \otimes \det(S)$. *Let* $\mathbf{C}^{S,j}(j \geqslant 0)$ *be the submodule of* $\mathcal{C}^{i+j}$ *generated by* $T \otimes \det(T)$, *where T is an m-bonsai obtained by adding j edges to S so that (i) and (ii) of Definition 7.1 are satisfied.*

Then, every $\mathcal{C}^i$ is the direct sum of some $\mathbf{C}^{S,j}$'s and $d(\mathbf{C}^{S,j}) \subset \mathbf{C}^{S,j+1}$. For example, in 2-bonsai, when S_0, S_1, S_2, and S_3 are as given in Fig. 23, we have

$$\mathcal{C}^0 = \mathbf{C}^{S_0,0},$$

$$\mathcal{C}^1 = \mathbf{C}^{S_0,1},$$

$$\mathcal{C}^2 = \mathbf{C}^{S_0,2} \oplus \mathbf{C}^{S_1,0},$$

$$\mathcal{C}^3 = \mathbf{C}^{S_0,3} \oplus \mathbf{C}^{S_1,1},$$

$$\mathcal{C}^4 = \mathbf{C}^{S_0,4} \oplus \mathbf{C}^{S_1,2} \oplus \mathbf{C}^{S_0,3} \oplus \mathbf{C}^{S_1,1},$$

$$\mathcal{C}^5 = \mathbf{C}^{S_0,5} \oplus \mathbf{C}^{S_1,3} \oplus \mathbf{C}^{S_0,3} \oplus \mathbf{C}^{S_1,1},$$

$$\cdots . \tag{39}$$

Definition 8.5: For a given seedling S, when i is the number of edges of S, $\{\mathbf{C}^{S,j}, d^{i+j}\}_{j \geqslant 0}$ *is called a* thread *of S.*

So the cohomology groups of $\{\mathcal{C}^i, d^i\}$ are the direct sum of cohomology groups of threads $\{\mathbf{C}^{S,j}, d^{i+j}\}_{j \geqslant 0}$.

Let us look into each of these threads. For $\mathbf{C}^{S_0,0}$, where S_0 is a vertex, $\mathbf{C}^{S_0,i}$ is the module with the basis $\{T \otimes \det(T)\}$, where T is a ladder with i edges and the boundary maps extend the ladders by adding an edge e and replacing $\det(T)$ with $e \wedge \det(T)$. Let us consider a chain complex which is isomorphic to the thread $\mathbf{C}^{S_0,0}$ of the ladder S_0. For any m-bonsai, consider a vector space V which has a basis $\{v_1, \ldots, v_m\}$, and let $V_n = V^{\otimes n} (n \geqslant 1)$. Then we define a map $\delta^n : V^n \to V^{n+1}$ as

$$v_{i_1} \otimes v_{i_2} \otimes \cdots \otimes v_{i_n} \mapsto \sum_{k=1}^{m} v_k \otimes v_{i_1} \otimes v_{i_2} \otimes \cdots \otimes v_{i_n} + \sum_{k=1}^{m} (-1)^1 v_{i_1} \otimes v_k \otimes v_{i_2} \otimes \cdots \otimes v_{i_n} + \cdots$$
$$+ \sum_{k=1}^{m} (-1)^n v_{i_1} \otimes \cdots \otimes v_{i_{n-1}} \otimes v_{i_n} \otimes v_k, \tag{40}$$

and it is easily seen that this δ^n is a boundary map, so we have made $\{V^n, \delta^n\}$ a cochain complex.

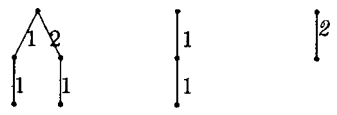

FIG. 30.

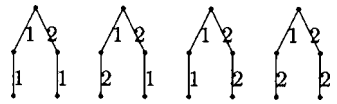

FIG. 31.

By the cochain map f as in Fig. 24, the cochain complexes $\{\mathbf{C}^{S_0,n}, d^n\}$ and $\{V^n, \delta^n\}$ are isomorphic, since d^n acts as in Fig. 25, that is, we have $f \circ \delta^n = d^n \circ f$.

In $\{V^n, \delta^n\}_{n \geqslant 1}$, by the definition of δ^n, inductively we have

$$\delta((v_1 \otimes \cdots \otimes v_i) \otimes v) = \delta(v_1 \otimes \cdots \otimes v_i) \otimes v + (-1)^{i+1}(v_1 \otimes \cdots \otimes v_i) \otimes v \otimes \sum_{k=1}^{m} v_k, \tag{41}$$

where $v_1 \otimes \cdots \otimes v_i \in V^i$ and $v \in V$. Suppose $\delta(\Sigma_{k=1}^m v_k' \otimes v_k) = 0$ where $v_k' \in V^i$, then we have

$$\sum_{k=1}^{m} \delta(v_k') \otimes v_k + (-1)^{i+1}\left(\sum_{k=1}^{m} v_k' \otimes v_k\right) \otimes \sum_{l=1}^{m} v_l = \sum_{l=1}^{m} \left\{ \delta(v_l') - (-1)^k \left(\sum_{k=1}^{m} v_k' \otimes v_k\right)\right\} \otimes v_l = 0. \tag{42}$$

Therefore, we have $(\Sigma_{k=1}^m v_k' \otimes v_k) = (-1)^k \delta(v_l')$ and it is a coboundary. So, $\{V^n, \delta^n\}$ is acyclic, and so is $\{\mathbf{C}^{S_0,n}, d^n\}$.

Here, we can directly calculate $H^0(\mathbf{C}^{S_0,*}) = 0$, since the boundary map image of a one-vertex bonsai is the sum of one-edge bonsais over all labels $1, 2, \ldots, n$. So $\{\mathbf{C}^{S_0,n}, d^n\}$ is acyclic with $H^0 = 0$.

Now for an arbitrary seedling S, when S has n edges, there are $n+1$ vertices and each vertex other than the root has one and only one edge whose branch end is that vertex. When we order the edges of a bonsai T with the shape S as in Fig. 13 and denote them as e_l's $(l = 1, 2, \ldots, n)$, we can denote the branch-end vertex of e_l as v_l and denote the root v_0. Then the bonsais which appear in the basis of $\mathbf{C}^{S,j}$ are obtained by extending the vertices of T into upward-growing ladders, and each ladder grown from v_l is denoted as L_l, as in the example of Fig. 26.

To get the cohomology of $\mathbf{C}^{S,j}$, let us consider the complexes $\mathbf{C}_k^{S_0,p}$, where $k = 0, \ldots, n$ and each of $\mathbf{C}_k^{S_0,p}$ is a copy of $\mathbf{C}^{S_0,p}$, i.e., each of $\mathbf{C}_k^{S_0,p}$ has the basis $\{L_k^p \otimes \det(L_k^p)\}$, where L_k^p is a ladder with p edges. Then we have an isomorphism F between

$$\mathbf{D}^l = \bigoplus_{p_0 + \cdots + p_n = l} \mathbf{C}_0^{S_0,p_0} \otimes \cdots \otimes \mathbf{C}_n^{S_0,p_n} \tag{43}$$

and $\mathbf{C}^{S,l}$ given by

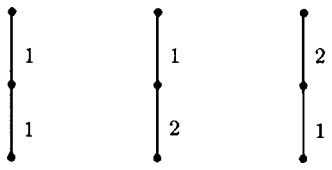

FIG. 32.

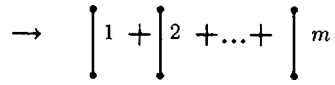

FIG. 33.

$$L_0^{p_0} \otimes \det(L_0^{p_0}) \otimes \cdots \otimes L_n^{p_n} \otimes \det(L_n^{p_n}) \mapsto \Sigma \text{ (the bonsai obtained by setting } L_i^{p_0} \text{ into the place of vertex } v_i) \otimes \det(L_0^{p_0}) \wedge e_1 \wedge \det(L_1^{p_1}) \wedge \cdots \wedge e_n \wedge \det(L_n^{p_n}) \tag{44}$$

as in the example of Fig. 27, for the seedling of Fig. 26.

From now on, we write $L_i^{p_i}$ just as L_i for convenience of writing.

In $T \otimes \det(T) \in \mathbf{C}^{S,l}$, $\det(T)$ is

$$\det(L_0) \wedge e_{1,k_1} \wedge \det(L_1) \wedge \cdots \wedge e_{n,k_n} \wedge \det(L_n), \tag{45}$$

where k_l is the label of the edge e_l, and $d^n(T \otimes \det(T))$ is

$$\Sigma \text{ (a bonsai } T' \text{ obtained by adding an edge } f \text{ to one of the } L_i) \otimes f \wedge \det(T)$$

and this is

$$\begin{aligned} &\Sigma \text{ (a bonsai } T' \text{ obtained by adding an edge } f \text{ to one of } L_i) \\ &\quad \otimes f \wedge \det(L_0) \wedge e_{1,k_1} \wedge \det(L_1) \wedge \cdots \wedge e_{n,k_n} \wedge \det(L_n) \\ &= \Sigma \text{ (a bonsai } T' \text{ obtained by adding an edge } f \text{ to one of } L_i) \\ &\quad \otimes (-1)^{\beta} \det(L_0) \wedge e_{1,k_1} \wedge \det(L_1) \wedge \cdots \wedge e_{i,k_i} \wedge f \wedge \det(L_i) \wedge \cdots \wedge e_{n,k_n} \wedge \det(L_n), \end{aligned}$$

where $\beta = (\deg(L_0)+1)+(\deg(L_1)+1)+\cdots+(\deg(L_{i-1})+1)$.

Here, $\det(T')$ is obtained by replacing $\det(L_i)$ with $f \wedge \det(L_i)$ in (45), and we get the sign $(-1)^{\beta}$ since when f is added to L_i, in the ordering of edges of T', the edges of $L_j (j=0,1,\ldots,i-1)$ and edges $e_1, e_2, \ldots, e_i$ are prior to the edges of L_i. So we can conclude that $d(T \otimes \det(T))$ is the sum of $(-1)^{\deg(L_0)+1+\cdots+\deg(L_{i-1})+1} T' \otimes \det(T')$, where T' is the bonsai obtained by adding an edge in the subladder L_i.

Thus, when we construct a coboundary map ∂^l for $\{\mathbf{D}^l\}$, acting on $\mathbf{C}_1^{S_0,p_1} \otimes \cdots \otimes \mathbf{C}_n^{S_0,p_n}$ by

$$\begin{aligned} \partial^l(L_0 \otimes \det(L_0) \otimes \cdots \otimes L_n \otimes \det(L_n)) &= d(L_0 \otimes \det(L_0)) \otimes L_1 \otimes \det(L_1) \otimes \cdots \otimes L_n \otimes \det(L_n) \\ &+ (-1)^{\deg(L_0)+1} L_0 \otimes \det(L_0) \otimes d(L_1 \otimes \det(L_1)) \otimes \cdots \otimes L_n \otimes \det(L_n) + \cdots \\ &+ (-1)^{(\deg(L_0)+1)+\cdots+(\deg(L_{n-1})+1)} L_0 \otimes \det(L_0) \otimes L_1 \otimes \det(L_1) \otimes \cdots \otimes d(L_n \otimes \det(L_n)), \end{aligned}$$

the isomorphism F becomes a cochain isomorphism between $\{\mathbf{D}^l\}$ and $\{\mathbf{C}^{S,l}\}$, and since each $\{\mathbf{C}_k^{S_0,p_k}\}$ is acyclic and $H^0=0$, by the Künneth theorem, $\{\mathbf{D}^l\}$ is acyclic and $H^0=0$, and so is $\{\mathbf{C}^{S,l}\}$.

Then, by a Künneth argument, every thread of $\{\mathbf{C}^{S,j}, d^{i+j}\}$ (i is the number of edges of S) is acyclic with $H^0=0$, and so we have the following.

Theorem 8.1: *$\{\mathcal{C}^n, d^n\}$ is acyclic.*

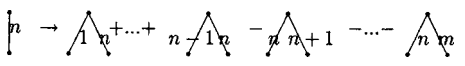

FIG. 34.

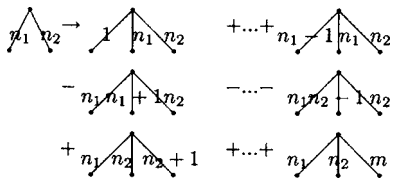

FIG. 35.

IX. VERTEX-APPENDING DIFFERENTIAL

In this section, we consider a differential, different from the ladder-extension. Again, all bonsais of this section are m-bonsais.

Definition 9.1: We define the vertex-appending differential ∂ *as follows; consider a determinanted bonsai* $T\otimes\det(T)$. *Then* $\partial(T\otimes\det(T))$ *is the sum of* $T'\otimes e\wedge\det(T)$, *where* T' *is a bonsai obtained by*

(i) *appending a vertex to* T,
(ii) *except to tips of* T,

and so, getting an edge e.

If there is no available appending position an a bonsai, the map ∂ *assigns 0 to that bonsai.*

For example, in 3-bonsai, we have an example like Fig. 28 (in bonsais, determinant terms are omitted). (Note that one vertex in the first example is also a tip and the fourth bonsai is a cocycle).

First, we have the following.

Theorem 9.1: $\partial^{i+1}\circ\partial^{i}=0$. *That is,* ∂ *is actually a differential.*

Proof: This proof is almost the same as that of Theorem 7.1. Suppose T'' is obtained by appending a vertex to T' with added edge e'' so that (i) and (ii) of Definition 9.1 are satisfied, where T' is obtained by appending a vertex to T with added edge e' so that (i) and (ii) of Definition 9.1 are satisfied. Here, if T' has no available position to append a vertex, then $\partial(T')=0$, so $T''=0$. Otherwise, when e'' is e''_{j,l_j} and e' is e''_{k,l_k} in the edge ordering of T'', in $\partial^{i+1}\circ\partial^{i}(T)$ hits the component $T''\otimes e''_{1,l_1}\wedge\cdots\wedge e''_{i+2,l_{i+2}}$ just by adding the edge e' and e'' to T, and it can be done only in two ways.

(i) Adding e' first to T, then the component of $T''\otimes e''_{1,l_1}\wedge\cdots\wedge e''_{i+2,l_{1+2}}$ is $T''\otimes e''_{j,l_j}\wedge e''_{k,l_k}\wedge e''_{1,l_1}\wedge\cdots\wedge\widehat{e''_{j,l_j}}\wedge\cdots\wedge\widehat{e''_{k,l_k}}\wedge\cdots\wedge e''_{i+2,l_{i+2}}$.
(ii) Adding e'' first to T, then the component of $T''\otimes e''_{1,l_1}\wedge\cdots\wedge e''_{i+2,l_{1+2}}$ is $T''\otimes e''_{k,l_k}\wedge e''_{j,l_j}\wedge e''_{1,l_1}\wedge\cdots\wedge\widehat{e''_{j,l_j}}\wedge\cdots\wedge\widehat{e''_{k,l_k}}\wedge\cdots\wedge e''_{i+2,l_{i+2}}$.

Since the order of e''_{k,l_k} and e''_{j,l_j} are different in the wedge products, the sum of the two terms in (i) and (ii) is 0. This is true for all components of $\partial^{i+1}\circ\partial^{i}(T)$, and so $\partial^{i+1}\circ\partial^{i}=0$. □

9.1. Definition of seedling: By the definition of ∂^{i}, all terms in $\partial^{i}(T)$ are of the form $\pm T'$

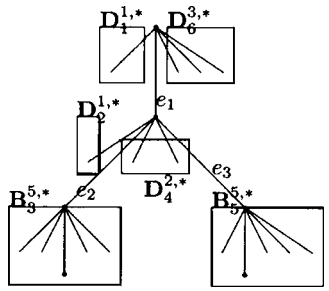

FIG. 36.

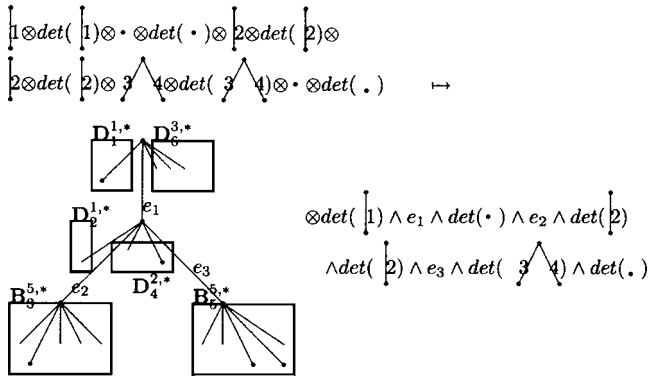

FIG. 37.

$\otimes e \wedge \det(T)$, where T' runs over bonsais obtained by adding an edge e to T so that (i) and (ii) of Definition 9.1 hold. So T' has the form of appending a vertex to a vertex of T which is not a tip. Having this intuitive fact in mind, let us present some definitions and reorganize the cochain complex of bonsais.

Definition 9.2: For a bonsai T, an edge e of T is called twiggy *if it is at the end of a branch and the opposite end of the tip is a branching vertex. In Fig. 29, e is twiggy in T and e′ is not, and f is not a twiggy edge of T′.*

Definition 9.3: A bonsai which has no twiggy edge is called a vertex-appending seedling. *In this section, we will call this just a* seedling. *The left bonsai in Fig. 35 is not a seedling, and the ones in Fig. 30 are all seedlings in 2-bonsai. Note that the one-vertex bonsai is a seedling. Intuitively, a seedling is a bonsai which cannot be obtained by adding edges like (i) and (ii) of Definition 9.1.*

Definition 9.4: For two seedlings S and S′, we define an equivalence relation $S \sim S'$ if S is obtained by changing labels of branch-end edges of S′. For example, all four seedlings in Fig. 31 are equivalent, and so are the first and second seedlings of Fig. 32, but the first and third seedlings of Fig. 32 are not equivalent.

Let us try the same trick as in the proof of acyclicity of the branch-fixed differential. When S is a seedling, let $\mathbf{C}^{[S],0}$ be the subspace of the determinanted m-bonsai space having $\{T \otimes \det(T)\}$ as the basis, where T is in the equivalence class $[S]$ of S by $\sim$. And let $\mathbf{C}^{[S],i+1}$ be the space with the basis $\{T' \otimes \det(T')\}$, where T' is obtained by adding an edge to T, where $\{T \otimes \det(T)\}$ is the basis of $\mathbf{C}^{S,i}$, as (i) and (ii) of Definition 9.1. Every bonsai is obtained by adding some edges to a seedling as given in Definition 9.1 and if S and S' are not equivalent seedlings, then the bonsais obtained by adding edges to S and S' as given in Definition 9.1 are not equivalent; the space of determinant bonsais is the direct sum of $\mathbf{C}^{[S],i}$. Then, since $\partial(\mathbf{C}^{[S],i}) \subset \mathbf{C}^{[S],i+1}$, the cohomology groups of determinant bonsais by the differential ∂ is the direct sum of cohomology groups of the threads $\{\mathbf{C}^{[S],i}\}$.

9.2. The cohomology groups of the vertex-appending differential: First let us consider a coboundary complex $\{\mathbf{D}^{m,i}\}$ consisting of corollas, such that each corolla is an m-bonsai, and the boundary map is the vertex-appending differential, but in this complex, appending to the one-vertex bonsai is allowed, so we must be careful not to be confused with the definition of the above

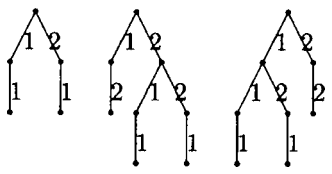

FIG. 38.

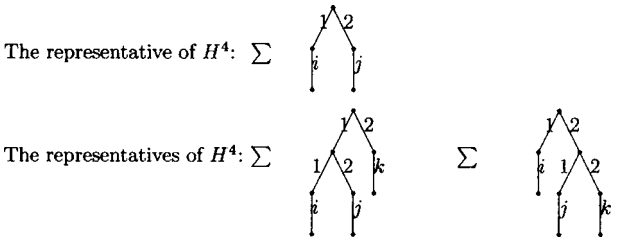

FIG. 39.

vertex-appending differential. By the definition of $\partial^i: \mathbf{D}^{m,i} \to \mathbf{D}^{m,i+1}$, all terms in $\partial^i(T)$ are of the form $\pm T' \otimes e \wedge \det(T)$, where T' runs over bonsais obtained by adding one vertex as defined in Definition 9.1. Since appending to a tip is forbidden, every ∂^i is appending a vertex to the root of a corolla. Now let us show some boundary map sequences of the thread starting from one vertex. For one vertex, ∂^0 acts as in Fig. 33.

For the one-edge corolla, ∂^1 acts as in Fig. 34, where $1 \leqslant n \leqslant m$, and for the two-edge corolla, ∂^2 acts as in Fig. 35, where $1 \leqslant n_1 < n_2 \leqslant m$, and so on.

This sequence of coboundary maps is the same as that of the reduced cohomology of the $(m-1)$-simplex with vertices $v_1, v_2, \ldots, v_m$, once we identify the corolla with labels $i_1, i_2, \ldots, i_k$ with the simplex generated by vertices $v_{i_1}, v_{i_2}, \ldots, v_{i_k}$. So the cohomology groups of this thread of boundary maps is acyclic, and the lowest degree group is trivial. Let us denote the module having the basis consisting of one vertex having m available positions of vertex appending as $\mathbf{D}^{m,0}$, and the module having the basis consisting of corollae with n edges as shown above $\mathbf{D}^{m,n}$. Also, let $\{\mathbf{B}^{m,n}\}$ be a cochain complex defined by $\mathbf{B}^{m,n} = \mathbf{D}^{m,n+1}$ for later convenience. Then $\{\mathbf{B}^{m,n}\}$ is acyclic and $H^0 = k$, where k is the base field, since the cohomology of $\{\mathbf{B}^{m,n}\}$ is isomorphic to the cohomology (not the reduced cohomology) of the $(m-1)$-simplex.

9.3. The case of general seedlings: Now let us show an example.

Lemma 2: *Any complex* $\{\mathbf{C}^{[S],i}\}$ *is isomorphic to it, which is represented as a direct sum of tensor products of* $\{\mathbf{D}^{m,i}\}$*'s and* $\{\mathbf{B}^{m,i}\}$*'s (as in the proof of acyclicity of the branch-fixed differential).*

In 5-bonsai, the seedling S in Fig. 36 can get twiggy edges at the positions of the twigs shown in the picture which are grouped as surrounded by squares.

Note that, in Fig. 36 adding an edge to each square is the same as attaching an edge to the corolla at the vertex at which the square is appended, each corolla corresponds to the module that is written on each square (in Fig. 36, $\mathbf{D}_i^{m,*}$ is isomorphic to $\mathbf{D}^{m,*}$ and $\mathbf{B}_i^{m,*}$ is isomorphic to $\mathbf{B}^{m,*}$).

Keeping this in mind, we can define modules $\{\mathbf{D}^l\}$ and an isomorphism F of them with $\{\mathbf{C}^{[S],i}\}$ like the following:

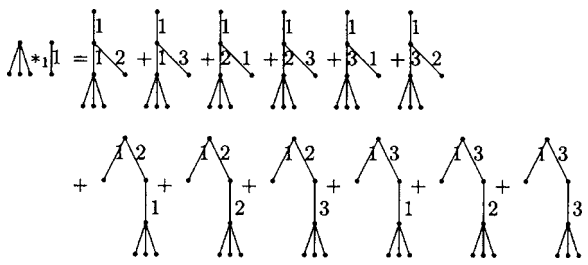

FIG. 40.

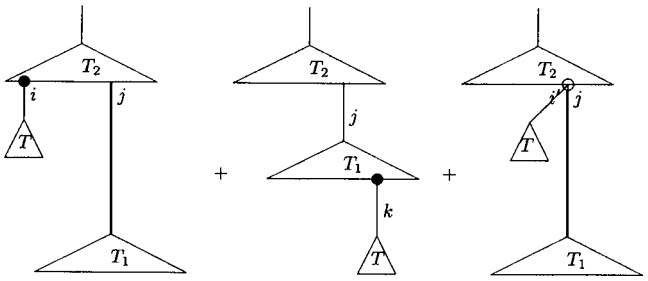

FIG. 41.

$$\mathbf{D}^l = \bigoplus_{p_1+\cdots+p_6=l} \mathbf{D}_1^{1,p_1} \otimes \mathbf{D}_2^{1,p_2} \otimes \mathbf{B}_3^{5,p_3} \otimes \mathbf{D}_4^{2,p_4} \otimes \mathbf{B}_5^{5,p_5} \otimes \mathbf{D}_6^{3,p_6} \tag{46}$$

and when $\mathbf{M}_1=\mathbf{D}_1^{1,p_1}$, $\mathbf{M}_2=\mathbf{D}_2^{1,p_2}$, $\mathbf{M}_3=\mathbf{B}_3^{5,p_3}$, $\mathbf{M}_4=\mathbf{D}_4^{2,p_4}$, $\mathbf{M}_5=\mathbf{B}_5^{5,p_5}$ and $\mathbf{M}_6=\mathbf{D}_6^{3,p_6}$, the map $F:\mathbf{D}^l \to \mathbf{C}^{[S],l}$ is defined as, when $c_i \in \mathbf{M}_i$ is a corolla,

$$\begin{aligned} &c_1 \otimes \det(c_1) \otimes \cdots \otimes c_6 \otimes \det(c_6) \mapsto \\ &\quad \Sigma \text{ (the bonsai obtained by attaching } c_i \text{ to the square corresponding to } \mathbf{M}_i) \\ &\quad \otimes \det(c_1) \wedge e_1 \wedge \det(c_2) \wedge e_2 \wedge \det(c_3) \wedge \det(c_4) \wedge e_3 \wedge \det(c_5) \wedge \det(c_6) \end{aligned} \tag{47}$$

as in the example of Fig. 37.

Then in $T \otimes \det(T) \in \mathbf{C}^{S,l}$, $\det(T)$ is

$$\det(c_1) \wedge e_{1,k_1} \wedge \det(c_2) \wedge e_{2,k_2} \wedge \det(c_3) \wedge \det(c_4) \wedge e_{3,k_3} \wedge \det(c_5) \wedge \det(c_6), \tag{48}$$

where k_l is the label of the edge e_l, and $\partial^n(T \otimes \det(T))$ is

$$\begin{aligned} &\Sigma \text{ (a bonsai } T' \text{ obtained by adding an edge } f \text{ to one of } c_i) \otimes f \wedge \det(T) \\ &\quad = \Sigma \text{ (a bonsai } T' \text{ obtained by adding an edge } f \text{ to one of } c_i) \\ &\qquad \otimes f \wedge \det(c_1) \wedge e_{1,k_1} \wedge \det(c_2) \wedge e_{2,k_2} \wedge \det(c_3) \wedge \det(c_4) \wedge e_{3,k_3} \wedge \det(c_5) \wedge \det(c_6) \\ &\quad = \Sigma \text{ (a bonsai } T' \text{ obtained by adding an edge } f \text{ to } c_1) \\ &\qquad \otimes f \wedge \det(c_1) \wedge e_{1,k_1} \wedge \det(c_2) \wedge e_{2,k_2} \wedge \det(c_3) \wedge \det(c_4) \wedge e_{3,k_3} \wedge \det(c_5) \wedge \det(c_6) \\ &\qquad + \Sigma \text{ (a bonsai } T' \text{ obtained by adding an edge } f \text{ to } c_2) \otimes (-1)^{\deg(c_1)+1} \det(c_1) \wedge e_{1,k_1} \\ &\qquad \wedge f \wedge \det(c_2) \wedge e_{2,k_2} \wedge \det(c_3) \wedge \det(c_4) \wedge e_{3,k_3} \wedge \det(c_5) \wedge \det(c_6) \\ &\qquad + \Sigma \text{ (a bonsai } T' \text{ obtained by adding an edge } f \text{ to } c_3) \otimes (-1)^{(\deg(c_1)+1)+(\deg(c_2)+1)} \end{aligned}$$

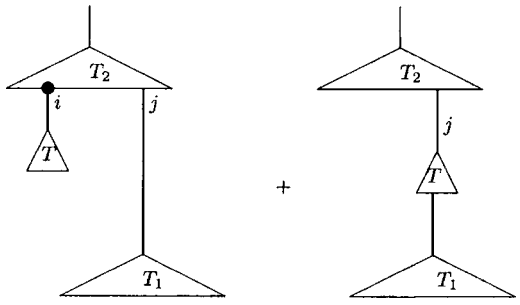

FIG. 42.

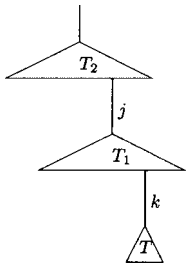

FIG. 43.

$$\det(c_1) \wedge e_{1,k_1} \wedge \det(c_2) \wedge e_{2,k_2} \wedge f \wedge \det(c_3) \wedge \det(c_4) \wedge e_{3,k_3} \wedge \det(c_5) \wedge \det(c_6)$$

$$+ \Sigma \text{ (a bonsai } T' \text{ obtained by adding an edge } f \text{ to } c_4)$$

$$\otimes (-1)^{(\deg(c_1)+1)+(\deg(c_2)+1)+(\deg(c_3)+0)}$$

$$\times \det(c_1) \wedge e_{1,k_1} \wedge \det(c_2) \wedge e_{2,k_2} \wedge \det(c_3) \wedge f \wedge \det(c_4) \wedge e_{3,k_3} \wedge \det(c_5) \wedge \det(c_6)$$

$$+ \Sigma \text{ (a bonsai } T' \text{ obtained by adding an edge } f \text{ to } c_5)$$

$$\otimes (-1)^{(\deg(c_1)+1)+(\deg(c_2)+1)+(\deg(c_3)+0)+(\deg(c_4)+1)}$$

$$\det(c_1) \wedge e_{1,k_1} \wedge \det(c_2) \wedge e_{2,k_2} \wedge \det(c_3) \wedge \det(c_4) \wedge e_{3,k_3} \wedge f \wedge \det(c_5)$$

$$\wedge \det(c_6) + \Sigma \text{ (a bonsai } T' \text{ obtained by adding an edge } f \text{ to } c_6)$$

$$\otimes (-1)^{(\deg(c_1)+1)+(\deg(c_2)+1)+(\deg(c_3)+0)+(\deg(c_4)+1)+(\deg(c_5)+0)} \det(c_1) \wedge e_{1,k_1}$$

$$\wedge \det(c_2) \wedge e_{2,k_2} \wedge \det(c_3) \wedge \det(c_4) \wedge e_{3,k_3} \wedge \det(c_5) \wedge f \wedge \det(c_6). \tag{49}$$

So, when $m_1=\deg(c_1)+1$, $m_2=\deg(c_2)+1$, $m_3=\deg(c_3)+0$, $m_4=\deg(c_4)+1$, and $m_5=\deg(c_5)+0$, we can write $\partial(T\otimes\det(T))$ as

$$+ \Sigma \text{ (a bonsai } T' \text{ obtained by adding an edge } f \text{ to } c_i)$$

$$\otimes (-1)^{m_1+\cdots+m_{i-1}} \det(c_1) \wedge e_{1,k_1} \wedge \cdots \wedge (f \wedge \det(c_i)) \wedge \cdots \wedge \det(c_6).$$

Hence, when we define the coboundary map on $\{\mathbf{D}^l\}$ as

$$c_1 \otimes \cdots \otimes c_6 \mapsto \Sigma(-1)^{\beta_i} c_1 \otimes \cdots \otimes \partial(c_i) \otimes \cdots \otimes c_6, \tag{50}$$

where $\beta_i=m_1+\cdots+m_{i-1}$ and $\beta_1=0$, the map F defined in (47) becomes a cochain isomorphism of $\{\mathbf{D}^l\}$ and $\{\mathbf{C}^{[S],l}\}$. Then by the Künneth theorem, the cohomology of the cochain complex $\{\mathbf{D}^l\}$ is

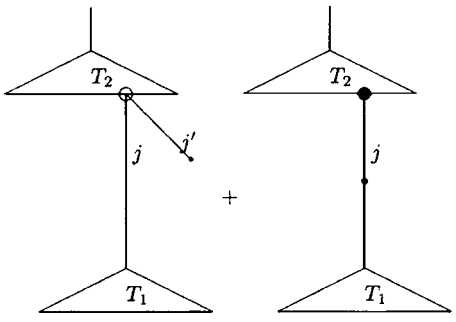

FIG. 44.

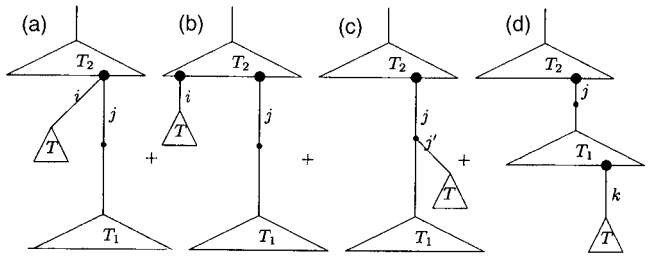

FIG. 45.

expressed as the sum of $H^{q_1}(\mathbf{M}_1)\otimes\cdots\otimes H^{q_6}(\mathbf{M}_6)$ for some q_i's, and since $H^i(\mathbf{M}_1)=H^i(\mathbf{D}^{1,*})=0$ for any i, the cohomology of $\mathbf{C}^{[S],l}$ for S of Fig. 36 is acyclic.

Definition 9.5: As shown for the example of Fig. 36, for any seedling S, we have a cochain complex as in (46) *and an isomorphism F of it with* $\mathbf{C}^{[S],l}$ *as in* (47). *We call this cochain complex as in* (46) *the* tensor product representation *of* $\mathbf{C}^{[S],l}$.

Then, whether $\{\mathbf{C}^{[S],l}\}$ is acyclic or not depends on whether its tensor product representation contains $\mathbf{D}^{m,*}$. As shown in Fig. 36, $\mathbf{B}^{m,*}$ appears only at the branch-end edges of a seedling, and $\mathbf{D}^{m,*}$ appears only at the available positions of vertex-appending other than at branch-end edges. So, the only case where $\{\mathbf{C}^{[S],l}\}$ is not acyclic is that the bonsai obtained by deleting all branch-end edges of S is a cocycle, i.e., that bonsai has no available position of vertex appending and so there is no room for $\mathbf{D}^{m,*}$ on S, like the bonsais of Fig. 38, in 2-bonsai. The only nontrivial cohomology group of $\{\mathbf{C}^{[S],l}\}$ is $H^0=k$ by Künneth theorem, where k is the base field, since all $H^0(\mathbf{B}^{m,i})=k$.

In m-bonsai, every cocycle C is a planar tree, all of whose vertices which are not branch-ends have ramification number m, so if C contains n corollas with m edges, it has $mn+1$ vertices, n of those vertices have m successors and $(mn+1)-n$ of those vertices have 0 successors, i.e., are the endpoints of edges, in the language of Stanley (1999). Then, by Theorem 5.3.10 of Stanley (1999), the number of such C is

$$\frac{1}{mn+1}\binom{mn+1}{(mn+1)-n,\ldots,n} \tag{51}$$

which is $(mn)!/((m-1)n+1)!n!$. A seedling S is obtained by adding one edge to every branch-end vertex of C and C has $(mn+1)-n$ branch-end vertices. So S has $mn+((mn+1)-n)=(2m-1)n+1$ vertices. Thus we have the following.

Theorem 9.2: *The cohomology groups* H^i *of m-bonsai Hopf algebra by the vertex-appending differential is*

$$H^i=\begin{cases} k\frac{(mn)!}{((m-1)n+1)!n!} & \text{if } i=(2m-1)n+1, n\geqslant 0,\\ 0 & \text{otherwise.}\end{cases}$$

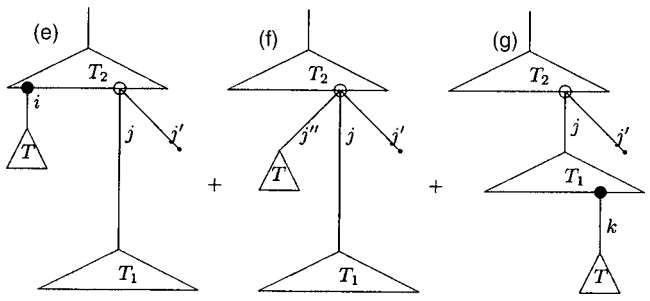

FIG. 46.

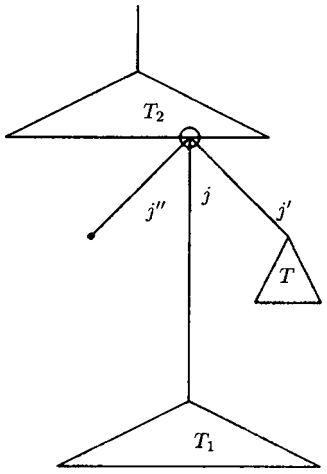

FIG. 47.

In 2-bonsai, the representatives of H^i are as in Fig. 39.

X. APPENDING OPERATION $*$ AND ITS DEVIATION

Over a general base field k for a bonsai Hopf algebra, it is not so easy to find a good algebraic relationship between $\partial(T_1 * T_2)$ and $(\partial T_1) * T_2 \pm T_1 * (\partial T_2)$ where ∂ is the vertex-appending differential, mainly because of the signs of determinant bonsais. But if k has characteristic 2, we do not need to consider signs. Moreover, the vertex-appending differential becomes just appending of a vertex, taking no consideration of determinant terms, but it is still a boundary map by the same argument as in the preceding section. Then the relation of $\partial(T_1 * T_2)$ and $(\partial T_1) * T_2 + T_1 * (\partial T_2)$ becomes much simpler. In this section, we consider only the case where the characteristic of k is 2.

Let us define the binary operation $*_1$ by

$$\partial(T_1 * T_2) = (\partial T_1) * T_2 + T_1 * (\partial T_2) + T_1 *_1 T_2 \tag{52}$$

and call this operation $*_1$ the *first deviation* of the operation $*$. We let $*_2$ be defined by

$$\partial(T_1 *_1 T_2) = (\partial T_1) *_1 T_2 + T_1 *_1 (\partial T_2) + T_1 *_2 T_2 \tag{53}$$

and call this operation the *second deviation* of the operation $*$. We define third, fourth, etc., deviations iteratively. Note that $*_2$ is the first deviation of $*_1$.

First, for the appending operation $*$, we have the following.

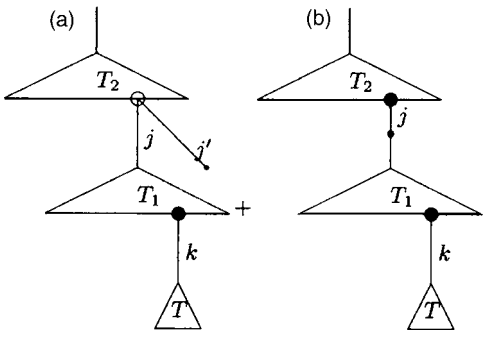

FIG. 48.

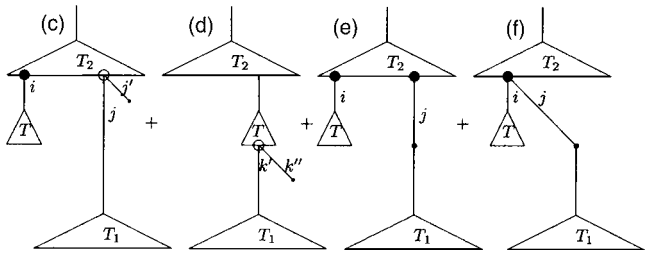

FIG. 49.

Theorem 10.1: *In bonsai Hopf algebra, with its base field of characteristic 2,* $T_1 *_1 T_2$ *is the sum of all* T' 's, *where* T' *is any bonsai obtained by connecting a tip* v *of* T_2 *and the root of* T_1 *with one edge and attatch another edge to that vertex of* T_2, *or by connecting a nontip of* T_2 *and the root of* T_1 *with a length-2 ladder. In both cases, the edges added to* T_1 *and* T_2 *are allowed to have all possible labels, as in the example in 3-bonsai of Fig. 40.*

Proof: Let us use a graphical illustration. Bonsais which are summands of $\partial(T_1 * T_2)$ are as in Fig. 41, where T_1 and T_2 and the appended vertex are drawn as broomsticks, and i, j, and k are indices of twigs and $T_1 * T_2$ is the sum of these two kinds of bonsai over i, j, and k. In this proof, the black circles in the pictures represent the twigs at nontips of bonsais, and the white circles represent the twigs at tips of bonsais. Here, i is on the vertices of T_2 which are not tips, and k is on the vertices of T_1 which are not tips and i' is on the vertices of T_2 which are tips, but not tips in $\partial(T_1 * T_2)$ since the connecting edge is attached.

The bonsais which are summands of $T_1 * \partial T_2$ are as in Fig. 42. On the right-hand bonsai of Fig. 42, the label of the edge connecting T and T_1 can be anything out of $1, 2, \ldots, m$.

The bonsais which are summands of $\partial T_1 * T_2$ are as in Fig. 43. Then the discrepancy between $\partial(T_1 * T_2)$ and $\partial T_1 * T_2 + T_1 * \partial T_2$ is the sum of the third bonsai of Fig. 41 and the second bonsai of Fig. 42, which gives the wanted formula.

Theorem 10.2: Mod 2, *for any m-bonsais* T_1 *and* T_2, *we have* $T_1 *_2 T_2 = 0$. *In other words,* $\partial(T_1 *_1 T_2) = \partial T_1 *_1 T_2 + T_1 *_1 \partial T_2$.

Proof: Bonsais which are summands of $T_1 *_1 T_2$ are those in Fig. 44, which represent the bonsais obtained by connecting T_1 and T_2 with one edge and attaching another edge and obtained by connecting T_1 and T_2 with a length-2 ladder. As in the proof of the previous theorem, a black circle represents a nontip of a bonsai and a white circle represents a tip of a bonsai.

The bonsais in $\partial(T_1 *_1 T_2)$ obtained by ∂ acting on the left-hand bonsai in Fig. 44 are those in Fig. 45, and the bonsais obtained by ∂ acting on the right-hand bonsai in Fig. 44 are those in Fig. 46. In both pictures, the broomstick lettered T is a one-vertex bonsai which is appended by the vertex-appending differential ∂.

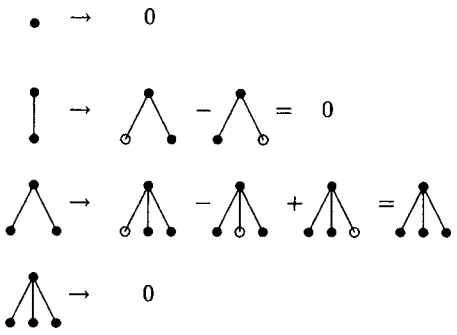

FIG. 50.

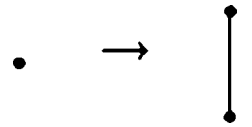

FIG. 51.

The bonsais in $\partial(T_1 *_1 T_2)$ corresponding to the left-hand bonsai in Fig. 44 are like Fig. 45, and the ones corresponding to the right-hand one are like Fig. 46. For later use, we denote those bonsais A, B,…,G as assigned in the figures. In both pictures, the broomstick lettered T is a one-vertex bonsai which is appended by the vertex-appending differential ∂.

For the bonsai F, actually we have a term like Fig. 47 also in $\partial(T_1 *_1 T_2)$, and since we are working mod 2, the bonsais looking like F are all canceled. So we have F=0.

Now, the bonsais in $\partial(T_1) *_1 T_2$ are as in Fig. 48. Let us denote them as a and b.

The bonsais in $T_1 *_1 \partial(T_2)$ are like those in Fig. 49, where we denote the bonsais as c, d, e, and f.

In Figs. 45–49, we have a=G, b=D, c=E, d=C, e=B, and f=A. We already showed that F=0, so we have $\partial(T_1 *_1 T_2) = \partial(T_1) *_1 T_2 + T_1 *_1 \partial(T_2)$. □

XI. PLANAR CLEAR-EDGED *m*-BONSAI AND ITS DERIVATIVE

In planar clear-edged m-bonsai, we can define a differential and calculate some cohomologies as for m-bonsai.

Definition 11.1: For the planar clear-edged m-bonsai, we define the vertex-appending differential ∂ *as follows. Consider a determinant planar clear-edged m-bonsai* $T \otimes \det(T)$. *Then* $\partial(T \otimes \det(T))$ *is the sum of* $T' \otimes \wedge \det(T)$, *where* T' *is a planar clear-edged m-bonsai obtained by*

(i) *appending a vertex to* T,
(ii) *except to tips of* T,

and so, getting an edge e.

If there is no available appending position on a bonsai, the map assigns 0 to that bonsai.

For example, in planar clear-edged 3-bonsai, we can get an example like Fig. 50 (in bonsais of Fig. 50, determinant terms are omitted). (Note that one vertex in the first example is also a tip and the third bonsai is a cocycle. In the picture, appended vertices are drawn as open vertices, not indicating colors.)

And by the totally same argument as for edge-numbered bonsai, we get the following.

Theorem 11.1: $\partial^{i+1} \circ \partial^i = 0$. *That is,* ∂ *is a differential.*

Now let us consider the cohomology groups of this differential. First let us consider a cochain complex $\{\mathbf{D}^i\}$ consisting of corollas, with the boundary map $\bar{\partial}$ being the vertex-appending differential, but in this complex, appending to the one-vertex bonsai is allowed. Here, let us denote as $\mathbf{D}^0$ the module having the basis consisting of one vertex, and as $\mathbf{D}^n$ the one-dimensional module having the basis consisting of the corolla with n edges as shown above. By the definition of ∂^i, all terms in $\partial^i(T)$ are of the from $\pm T' \otimes e \wedge \det(T)$, where T' runs over bonsais obtained by adding one vertex as defined in Definition 11.1. Since appending to an edge-end is forbidden, every ∂^i is appending a vertex to the root of a corolla. Now let us show some boundary map sequences of the thread starting from one vertex. For one vertex, ∂^0 acts as in Fig. 51.

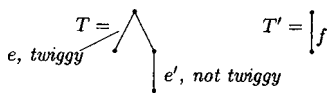

FIG. 52.

FIG. 53.

For the one-edge corolla, ∂^1 acts as in the second map of Fig. 50, for the two-edge corolla, ∂^2 acts as in the third map of Fig. 50, and so on.

This sequence of coboundary maps is

$$k \xrightarrow{id} k \xrightarrow{0} k \xrightarrow{id} k \xrightarrow{0} \cdots \tag{54}$$

where k is the base field.

So the cohomology groups of this thread of boundary maps is acyclic, and the lowest degree group is trivial.

Also, let $\{\mathbf{B}^n\}$ be a cochain complex defined by $\mathbf{B}^n=\mathbf{D}^{n+1}$ for later convenience. Then $\{\mathbf{B}^n\}$ is acyclic and $H^0=k$, where k is the base field.

Now let us consider the general case. By the definition of ∂^i, all terms in $\partial^i(T)$ are of the form $\pm T' \otimes e \wedge \det(T)$, where T' runs over bonsais obtained by adding an edge e to T so that (i) and (ii) of Definition 11.1 hold. So T' has the form of appending a vertex to a vertex of T other than a tip. Having this intuitive fact in mind, let us present some definitions and reorganize the cochain complex of bonsais.

Definition 11.2: For a bonsai T, an edge e of T is called twiggy *if it is at the end of a branch and the opposite end of the tip is a branching vertex. In Fig. 52, e is twiggy in T and e′ is not, and f is not a twiggy edge of T′.*

Definition 11.3: A bonsai which has no twiggy edge is called a vertex-appending seedling. *In this section, we will just call this* seedling. *The bonsais in Fig. 53 are all seedlings. Note that the one-vertex bonsai is a seedling. Intuitively, a seedling is a bonsai which cannot be obtained by adding edges like (i) and (ii) of Definition 9.1.*

11.1. *Cohomology groups of ∂ when m=∞:* Let us try the same trick as in the proof of acyclicity of the branch-fixed differential.

Definition 11.4: When S is a seedling, let $\mathbf{C}^{S,0}$ *be the subspace of the determinant planar clear-edged ∞-bonsai space having* $\{S \otimes \det(S)\}$ *as the basis. And let* $\mathbf{C}^{S,i+1}$ *be the space with the basis* $\{T' \otimes \det(T')\}$, *where T′ is obtained by adding an edge to T, where* $\{T \otimes \det(T)\}$ *is the basis of* $\mathbf{C}^{S,i}$, *as (i) and (ii) of Definition 11.1. Then since every bonsai is obtained by adding some edges to a seedling as given in Definition 11.1 and if S and S′ are different seedlings, then the bonsais obtained by adding edges to S and S′ as given in Definition 11.1 are different, the space of determinant bonsais is the direct sum of the* $\mathbf{C}^{S,i}$. *We call this complex* $\{\mathbf{C}^{S,i}\}$ *a* thread *starting from S.*

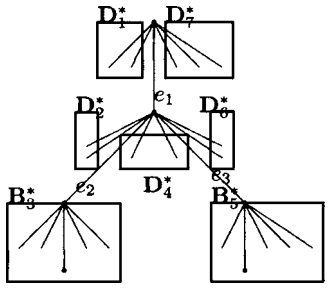

FIG. 54.

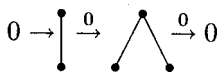

FIG. 55.

Then, since $\partial(\mathbf{C}^{S,i}) \subset \mathbf{C}^{S,i+1}$, the cohomology groups of determinant bonsais by the differential ∂ are the direct sum of cohomology groups of the threads $\{\mathbf{C}^{S,i}\}$.

Now let us show through an example that, for any thread $\{\mathbf{C}^{S,i}\}$, we can get a cochain complex which is isomorphic to it, obtained from the direct sums of tensor products of $\{\mathbf{D}^i\}$'s and $\{\mathbf{B}^i\}$'s as in the proof of acyclicity of branch-fixed differential. In 5-bonsai, the seedling S in Fig. 54 can have twiggy edges at the positions of the twigs shown in the picture, and those twigs are grouped as surrounded by squares.

Note that, in Fig. 54, adding edges to the corolla in each square is the same as attaching edges to the vertex at which the square is appended, each corolla corresponds to the module that is written on each square (in Fig. 54, $\mathbf{D}_i^{m,*}$ is isomorphic to $\mathbf{D}^{m,*}$ and $\mathbf{B}_i^{m,*}$ is isomorphic to $\mathbf{B}^{m,*}$).

Then, as in Sec. XI, we can get the cochain isomorphism of $\{\mathbf{C}^{S,i}\}$ and $\mathbf{D}_1^* \otimes \mathbf{D}_2^* \otimes \mathbf{B}_3^* \otimes \mathbf{D}_4^* \otimes \mathbf{B}_5^* \otimes \mathbf{D}_6^* \otimes \mathbf{D}_7^*$, and use Künneth's theorem. Since the cohomology of $\{\mathbf{D}^*\}$ is acyclic with trivial base degree cohomology, it is clear that any $\{\mathbf{C}^{S,*}\}$ whose tensor product representation has $\{\mathbf{D}^*\}$ is acyclic with trivial base degree cohomology. The only seedlings having no $\{\mathbf{D}^*\}$ are the first two bonsais of Fig. 50, i.e., the one-vertex bonsai v and the one-edge bonsai e. Since v is a cocycle, we have $H^0 = k$ and since $\mathbf{C}^{e,*} = \mathbf{B}^*$, we have $H^1 = H^0(\mathbf{B}^*) = k$. This illustrates a general argument. Thus we have the following.

Theorem 11.2: *The cohomology groups H^i of the planar clear-edged m-bonsai Hopf algebra by vertex-appending differential are*

$$H^i = \begin{cases} k & \text{if } i = 0 \text{ or } 1, \\ 0 & \text{otherwise}. \end{cases}$$

11.2. *Cohomology groups of ∂ when $m < \infty$: terminology*. In this section, let us consider the cohomology groups in case $m < \infty$. It is not as easy as in the preceding section to get a simple tensor product representation of a thread $\{\mathbf{C}^{S,i}\}$ when each vertex has the upper bound m of ramification number. So we need to change our strategy for the case of $m < \infty$. Since every $\{\mathbf{C}^{S,i}\}$ is finite dimensional, we can calculate the cohomology groups by considering a finite number of bonsais. So from now on, we develop an "inductive strategy" for calculating the cohomology groups of the thread $\{\mathbf{C}^{S,i}\}$ for any given S.

Let us illustrate the basic idea of the " inductive strategy" using an example. In 2-bonsai, let S_i be the ladder of length i. Then the cohomology $H^j(S_1)$ of $\{\mathbf{C}^{S_1,j}\}$ is, by a sequence as in Fig. 55, $H^1(S_1) = H^2(S_2) = k$, the base field.

Let us find an inductive step to get $H^i(S_{j+1})$'s from $H^i(S_j)$'s, so that we can get the cohomology group of every $\{\mathbf{C}^{S_i,j}\}$.

As in Fig. 56, when T is a linear combination of m-bonsais, the other two expressions of Fig. 56 represent linear combinations of bonsais obtained by attaching a bonsai to the roots of bonsais which are the components of T.

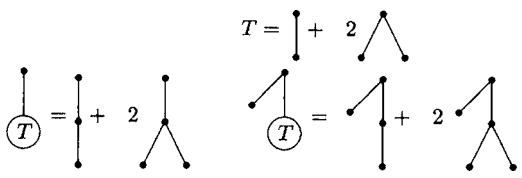

FIG. 56.

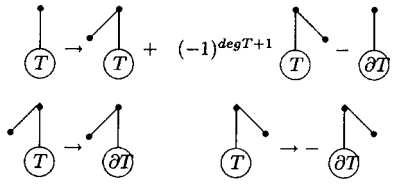

FIG. 57.

Then, when T is a linear combination of bonsais in $\{\mathbf{C}^{S_i,j}\}$ in 2-bonsai, the map ∂ on $\{\mathbf{C}^{S_{i+1},j}\}$ is expressed in Fig. 57.

From Fig. 57, we can find that the kernel of ∂ on $\{\mathbf{C}^{S_{i+1},j}\}$ is generated by the linear combinations of bonsais shown in Fig. 58 in which $T \in \ker \partial$ and $\partial T' = \partial T'' = T$, and that the image of ∂ on $\{\mathcal{C}^{S^{i+1},j}\}$ is generated by the linear combinations of bonsais shown in Fig. 59.

So we can write

$$\frac{\ker \partial}{\operatorname{im} \partial} = \frac{\langle A,B,C\rangle}{\langle a,b,c\rangle}. \tag{55}$$

In A, we have $\partial T=0$, $\partial T' = T$ and $\partial T'' = T$, so we have $A-a=(-1)^{\deg T''+1}C$. Hence we have C is generated by A and a. Also, in c, when $T' = \partial T$, we have $a-b=(-1)^{\deg T}c$. So c is generated by a and b. So we have

$$\frac{\ker \partial}{\operatorname{im} \partial} = \frac{\langle A,B\rangle}{\langle a,b\rangle}. \tag{56}$$

In Fig. 58, $\partial T'' = T$. So A in Fig. 58 can be redrawn as Fig. 60.

Since $\partial T' = \partial T'' = T$, we have $\partial(T' - T'') = 0$ and so A can be rewritten as $B+a$. Hence we have

$$\frac{\ker \partial}{\operatorname{im} \partial} = \frac{\langle B+a,B\rangle}{\langle a,b\rangle} = \frac{\langle a,B\rangle}{\langle a,b\rangle} = \frac{\langle a\rangle \oplus \langle B\rangle}{\langle a\rangle \oplus \langle b\rangle} = \frac{\langle B\rangle}{\langle b\rangle}. \tag{57}$$

Obviously, $\langle B\rangle/\langle b\rangle$ is isomorphic to the cohomology group of $\mathbf{C}^{S_i,j}$. Since B and b have two more edges than bonsais in $\mathbf{C}^{S_i,j}$, we can see the following.

Theorem 11.3: *When $H^j(S_i)$ is the jth cohomology group of the thread $\mathbf{C}^{S_i,j}$, $H^{j+2}(S_{i+1}) = H^j(S_i)$.*

As in the previous theorem, we can generalize the process of getting the cohomology of the thread starting from S' which is obtained by attaching the root of a seedling S to a tip of a corolla, when the cohomology of the thread starting from S is already known. Let us define some terminology. We first define a kind of "seedling."

Definition 11.5: We define a grafting seedling *as a bonsai defined as one of the following:*

(1) *a seedling*,
(2) *a bonsai obtained by attaching even-arity corollas to vertices of a seedling S which are more than two edges from any tip, and by replacing branch-end edges of S to even-arity corollas.*

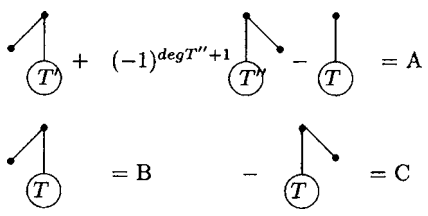

FIG. 58.

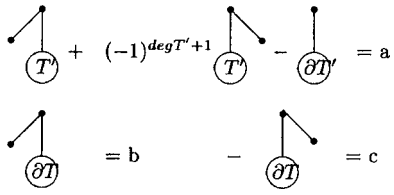

FIG. 59.

In Fig. 61, the first three bonsais are grafting seedlings and the last is not.

Definition 11.6: A grafting seedling $gs(n;T_1,T_2,\dots,T_{n+1};S_1,S_2,\dots,S_n)$, *which we call a* grafting seedling *is constructed like the following: In the corollas C with arity n, the corollas* $T_1,T_2,\dots,T_{n+1}$ *of* even *arities are attached so that the root of* T_1 *is attached to the root of C on the left of the leftmost edge of C, the root of* T_2 *is attached to the root of C between the first leftmost edge and the second leftmost edge of C,…, and so on, and the grafting seedlings* $S_1,S_2,\dots,S_n$ *are attached so that the root of* S_1 *is attached to the tip of the first leftmost edge of C, the root of* S_2 *is attached to the tip of the second leftmost edge of C, …, and so on, as in Fig. 62 in 6-bonsai.*

Note that the grafting seedling defined here is different from the seedling we used until now.

Definition 11.7: We define the relation $T_1 \to T_2$ *of clear-edged m-bonsais* T_1 *and* T_2 *as follows:*

(i) T_2 *is a nonzero component of* ∂T_1 *and* T_2 *is obtained by attaching one edge to the* root *of* T_1 *or*

(ii) T_2 *is obtained by attaching an edge to a nonroot vertex of* T_1.

In 3-bonsai, we have examples as in Fig. 63.

Definition 11.8: We define the relation $T_1 \Rightarrow T_1'$ *if there is a sequence of m-bonsais such that* $T_1 \to T_2 \to \cdots \to T_n = T_1'$ *or* $T_1 = T_1'$.

Let $\mathbf{K}(gs(n;T_1,\dots,T_{n+1};S_1,\dots,S_n))$ *be the vector space generated by the bonsais* T' *such that* $gs(n;T_1,\dots,T_{n+1};S_1,\dots,S_n) \Rightarrow T'$. *Also, when S is a grafting seedling and* $\mathbf{C}$ *is the cochain complex of m-bonsai, we define* $\mathbf{K}^i(S) := \mathbf{C}^i \cap \mathbf{K}(S)$.

Theorem 11.4: *When S is a grafting seedling and* $H^i(S)$ *is the ith cohomology group of the thread* $\{\mathbf{K}^i(S)\}$, *the ith cohomology group* H^i *of m-bonsai is*

$$H^i = \bigoplus_{S \text{ is a grafting seedling}} H^i(S).$$

Proof: We have

$$\mathbf{C} = \bigoplus_{S \text{ is a grafting seedling}} \mathbf{K}(S)$$

since (i) there is no T such that $T \Rightarrow T'$, $T \neq T'$, and T' is a grafting seedling and (ii) if two grafting seedlings S and S' are not equal, then $\mathbf{K}(S) \cap \mathbf{K}(S') = \emptyset$. Also we have $\partial \mathbf{K}^i(S) \subset \partial \mathbf{K}^{i+1}(S)$. So we get the wanted result. □

11.3. The cohomology groups for each $\{\mathbf{K}^i(gs(n;T_1,\dots,T_{n+1};S_1,\dots,S_n))\}$*:* Now we must cal-

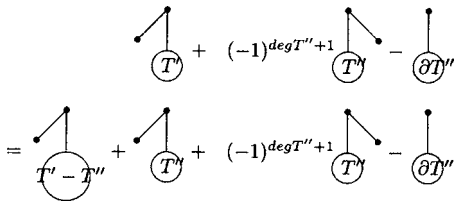

FIG. 60.

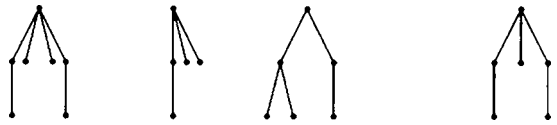

FIG. 61.

culate the cohomology groups for $\{\mathbf{K}^i(gs(n;T_1,\ldots,T_{n+1};S_1,\ldots,S_n))\}$. First let us define some notation.

Definition 11.9: For any integer $n\geqslant 0$, the cochain complex $\{\mathbf{D}^j_{2n}\}$ is defined as follows: when $j=2n$ or $2n+1$, $\mathbf{D}^j_{2n}$ is a one-dimensional vector space with the basis $\{C_j\}$, where C_j is the corolla of arity j (when $j=0$, C_j is the one-vertex bonsai), and otherwise, $\mathbf{D}^j_{2n}=0$. And when $j=2n$, the boundary map $\partial:\mathbf{D}^j_{2n}\to\mathbf{D}^{j+1}_{2n}$ is given by $C_j\mapsto C_{j+1}$ and otherwise, $\partial=0$.

To calculate the cohomology groups of $\{\mathbf{K}^i(gs(n;T_1,\ldots,T_{n+1};S_1,\ldots,S_n))\}$, we use a similar type of tensor product representation as in Sec. XI.

Definition 11.10: Let $B(n;U_1,\ldots,U_{n+1};V_1,\ldots,V_n)$ be the bonsai obtained by replacing T_i by U_i and S_i by V_i in $gs(n;T_1,\ldots,T_{n+1};S_1,\ldots,S_n)$, where U_i is the corolla C_k of arity $k=deg\ T_i$ or deg T_i+1 (i.e., U_i is a basis element of $\{\mathbf{D}_{deg\ T_i}\}$) and V_i is a bonsai in the thread $\{\mathbf{C}^{S_i,i}\}$ starting from S_i (see section 11.2).

Let us define the cochain complexes $\{\mathbf{D}_i\}$ and $\{\mathbf{E}_i\}$ as $\{\mathbf{D}_{\deg\ T_i}\}$ and $\{\mathbf{C}(S_i)\}$. Then we can define an isomophism P from $\mathbf{K}^i(S)$ to $\mathbf{L}^i=\mathbf{D}_1^{i_1}\otimes\mathbf{E}_1^{j_1}\otimes\cdots\otimes\mathbf{D}_n^{i_n}\otimes\mathbf{E}_n^{j_n}\otimes\mathbf{D}_{n+1}^{i_{n+1}}$ where $i_1+\cdots+i_{n+1}+j_1+\cdots+j_n+n=i$ and $i_1+\cdots+i_{n+1}+n\leqslant m$, by sending $B(n;U_1,\ldots,U_{n+1};V_1,\ldots,V_n)$ to $U_1\otimes V_1\otimes\cdots\otimes U_n\otimes V_n\otimes U_{n+1}$. The differential d in $\mathbf{L}$ is defined as, when $\deg U_1+\cdots+\deg U_{n+1}<m-n$,

$$\begin{aligned}d(U_1\otimes V_1\otimes U_2\otimes V_2\otimes\cdots\otimes U_n\otimes V_n\otimes U_{n+1}) &= \partial U_1\otimes V_1\otimes U_2\otimes V_2\otimes\cdots\otimes U_n\otimes V_n\\ &\otimes U_{n+1}+U_1\otimes(-1)^{p_1}\partial V_1\otimes U_2\otimes V_2\otimes\cdots\otimes U_n\otimes V_n\otimes U_{n+1})+U_1\otimes V_1\otimes(-1)^{q_1}\partial U_2\\ &\otimes V_2\otimes\cdots\otimes U_n\otimes V_n\otimes U_{n+1})+U_1\otimes V_1\otimes U_2\otimes(-1)^{p_2}\partial V_2\otimes\cdots\otimes U_n\otimes V_n\otimes U_{n+1})\\ &+\cdots+U_1\otimes V_1\otimes U_2\otimes V_2\otimes\cdots\otimes U_n\otimes V_n\otimes(-1)^{q_n}\partial U_{n+1},\end{aligned}$$

where $p_i=\deg U_1+\deg V_1+\cdots+\deg U_{i-1}+\deg V_{i-1}+\deg U_i+i$ and $q_i=\deg U_1+\deg V_1+\cdots+\deg U_i+\deg V_i+i$, and if $\deg U_1+\cdots+\deg U_{n+1}=m-n$,

$$\begin{aligned}d(U_1\otimes V_1\otimes U_2\otimes V_2\otimes\cdots\otimes U_n\otimes V_n\otimes U_{n+1}) &= \partial U_1\otimes V_1\otimes U_2\otimes V_2\otimes\cdots\otimes U_n\otimes V_n\\ &\otimes U_{n+1}+U_1\otimes V_1\otimes(-1)^{q_1}\partial U_2\otimes V_2\otimes\cdots\otimes U_n\otimes V_n\otimes U_{n+1})+\cdots+U_1\otimes V_1\otimes U_2\otimes V_2\\ &\otimes\cdots\otimes U_n\otimes V_n\otimes(-1)^{q_n}\partial U_{n+1}).\end{aligned}$$

Then by the definition of ∂ in $\mathbf{C}$, the isomorphism P is a cochain complex isomorphism from $(\mathbf{K}^i(S),\partial)$ to $(\mathbf{L}^i,d)$.

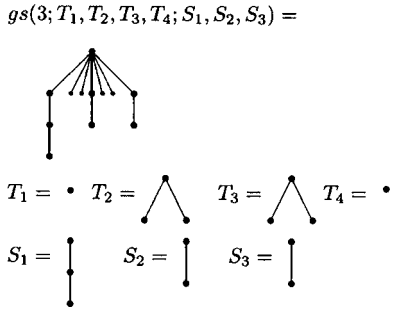

FIG. 62.

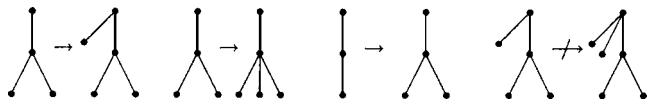

FIG. 63.

Now let us define a double complex $\{\mathbf{M}^i \otimes \mathbf{N}^j\}^{i,j}$ where $\mathbf{M}^i = \Sigma \mathbf{D}_1^{i_1} \otimes \cdots \otimes \mathbf{D}_{n+1}^{i_{n+1}}$ where $i_1, \ldots, i_{n+1}$ satisfy $i_1 + \cdots + i_{n+1} + n = i$ and $i \leqslant m$, and $\mathbf{N}^j = \Sigma_{j_1+\cdots+j_n=j} \mathbf{E}_1^{j_1} \otimes \cdots \otimes \mathbf{E}_n^{j_n}$ where $j_1, \ldots, j_n$ satisfy $j_1 + \cdots + j_n = j$, and differentials $\bar{\partial}_1$ and $\bar{\partial}_2$ are

$$\begin{aligned}\bar{\partial}_1(U_1 \otimes U_2 \otimes \cdots \otimes U_{n+1} \otimes V_1 \otimes \cdots \otimes V_n) &= \partial U_1 \otimes U_2 \otimes \cdots \otimes U_{n+1} \otimes V_1 \otimes \cdots \otimes V_n + U_1 \\ &\otimes (-1)^{q_1} \partial U_2 \otimes \cdots \otimes U_{n+1} \otimes V_1 \otimes \cdots \otimes V_n + \cdots + U_1 \otimes U_2 \otimes \ldots \otimes (-1)^{q_n} \partial U_{n+1} \otimes V_1 \\ &\otimes \ldots \otimes V_n\end{aligned}$$

where $U_1 \otimes \cdots \otimes U_{n+1} \in \mathbf{M}^j (j < m)$ (if $j \geqslant m$, since $\mathbf{M}^j = 0$, $\bar{\partial}_1 = 0$), and

$$\begin{aligned}\bar{\partial}_2(U_1 \otimes \cdots \otimes U_{n+1} \otimes V_1 \otimes V_2 \otimes \cdots \otimes V_n) &= U_1 \otimes \cdots \otimes U_{n+1} \otimes (-1)^{p_1} \partial V_1 \otimes V_2 \otimes \cdots \otimes V_n \\ &+ U_1 \otimes \cdots \otimes U_{n+1} \otimes V_1 \otimes (-1)^{p_2} \partial V_2 \otimes \cdots \otimes V_n) + \cdots + U_1 \otimes \cdots \otimes U_{n+1} \otimes V_1 \otimes V_2 \\ &\otimes \cdots \otimes (-1)^{p_n} \partial V_n.\end{aligned}$$

Then each of $\bar{\partial}_1$ and $\bar{\partial}_2$ is a differential of Künneth products of $\{\mathbf{D}_{2n}^i\}$'s and $\{\mathbf{C}^{S,j}\}$'s, respectively. Let $\bar{\partial} = \bar{\partial}_1 + \bar{\partial}_2$. When the bijection $Q: \{\mathbf{L}^i\} \to \{\mathbf{M}^i \otimes \mathbf{N}^j\}$ is given by $U_1 \otimes V_1 \otimes \cdots \otimes U_n \otimes V_n \otimes U_{n+1} \mapsto U_1 \otimes \cdots \otimes U_{n+1} \otimes V_1 \otimes \cdots \otimes V_n$, immediately by the definitions of d and $\bar{\partial}$, we have

$$\bar{\partial} \circ Q = Q \circ d. \tag{58}$$

Hence $\bar{\partial}$ satisfies $\bar{\partial} \circ \bar{\partial} = 0$. So we have $0 = \bar{\partial} \circ \bar{\partial} = \bar{\partial}_1 \circ \bar{\partial}_1 + \bar{\partial}_1 \circ \bar{\partial}_2 + \bar{\partial}_2 \circ \bar{\partial}_1 + \bar{\partial}_2 \circ \bar{\partial}_2 = \bar{\partial}_1 \circ \bar{\partial}_2 + \bar{\partial}_2 \circ \bar{\partial}_1$, therefore $\{\mathbf{M}^i \otimes \mathbf{N}^j\}$ is a double complex. Also, by (58), Q induces the cochain complex isomorphism $(\{\mathbf{L}^i\}, d) \to (\{\mathbf{M}^i \otimes \mathbf{N}^j\}, \bar{\partial})$. So by the isomorphism $Q \circ P, (\{\mathbf{K}(gs(n; T_1, \ldots T_{n+1}; S_1, \ldots, S_n))\}, \partial)$ and $(\{\mathbf{M} \otimes \mathbf{N}\}, \bar{\partial})$ are isomorphic. In order to calculate the cohomology of $(\{\mathbf{K}^i(gs(n; T_1, \ldots, T_{n+1}; S_1, \ldots, S_n))\})$, we can use the cohomology groups $(\{\mathbf{M} \otimes \mathbf{N}\}, \bar{\partial})$. Let us use the spectral sequence starting with $\bar{\partial}_1$.

Since $\bar{\partial}_1$ acts only on $\{\mathbf{M}^i\}$, we can write $E_1^{i,j} = H_{\bar{\partial}_1}(\{\mathbf{M}^i \otimes \mathbf{N}^j\}) = H_{\bar{\partial}_1}^i(\{\mathbf{M}\}) \otimes \mathbf{N}^j$, and similarly, since $\bar{\partial}_2$ acts only on $\{\mathbf{N}^j\}$, we can write $E_2^{i,j} = H_{\bar{\partial}_2}(E_1) = H_{\bar{\partial}_1}^i(\{\mathbf{M}\}) \otimes H_{\bar{\partial}_2}^j(\{\mathbf{N}\})$. Since $\bar{\partial}_2$ is a Künneth product of $\mathbf{E}_i$'s, $H_{\bar{\partial}_2}(\{\mathbf{N}\})$ is the Künneth product $H(\mathbf{E}_1) \otimes \cdots \otimes H(\mathbf{E}_n) = H(S_1) \otimes \cdots \otimes H(S_n)$. But as we can see in the definition of $\bar{\partial}_1$, it is not exactly the canonical differential of Künneth product, so the calculation of $H(\{\mathbf{M}\})$ takes some more consideration.

When $i < m$, $\mathbf{M}^i = \oplus_{i_1+\cdots+i_{n+1}=i-n} \mathbf{D}_1^{i_1} \otimes \cdots \otimes \mathbf{D}_{n+1}^{i_{n+1}}$ and $\bar{\partial}_1$ is a Künneth differential. So when $i < m, H_{\bar{\partial}_1}^i(\{\mathbf{M}\})$ is a Künneth product of $H(\{\mathbf{D}_j\})$'s, and so it is 0, since each $\{\mathbf{D}_j\}$ is acyclic.

When $i > m, \mathbf{M}^j = 0$. So when $i \geqslant m, \bar{\partial}_1 = 0$ on $\mathbf{M}^i$ and $H_{\bar{\partial}_1}^i(\{\mathbf{M}\}) = 0 (i > m)$.

Let us calculate $H_{\bar{\partial}_1}^m(\{\mathbf{M}\}) = \ker \bar{\partial}_1|_{\mathbf{M}^m} / im \bar{\partial}_1|_{\mathbf{M}^{m-1}}$.

First, if $(i_1 + 1) + \cdots + (i_{n+1} + 1) + n < m, \mathbf{M}^m = 0$. So, $H_{\bar{\partial}_1}^m(\{\mathbf{M}\}) = 0$.

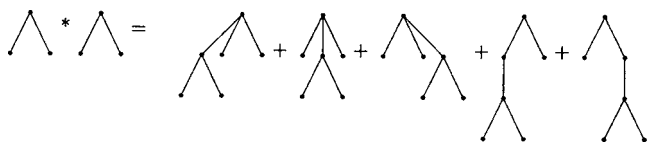

FIG. 64.

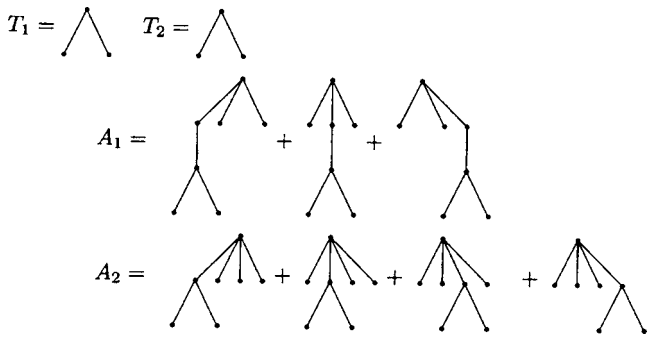

FIG. 65.

Suppose that $(i_1+1)+\cdots+(i_{n+1}+1)+n \geqslant m$. Since the clear-edged m-bonsai is a vector space over the field k, we just need to calculate the dimension of H^m. We have

$$\dim(H^m_{\bar{\partial}_1}(\{\mathbf{M}\})) = \dim\left(\ker \bar{\partial}_1\big|_{\mathbf{M}^m}\right) - \dim\left(\operatorname{im} \bar{\partial}_1\big|_{\mathbf{M}^{m-1}}\right), \tag{59}$$

$$\dim\left(\ker \bar{\partial}_1\big|_{\mathbf{M}^m}\right) = \dim(\mathbf{M}^m), \tag{60}$$

and

$$\dim\left(\operatorname{im} \bar{\partial}_1\big|_{\mathbf{M}^{m-1}}\right) = \dim(\mathbf{M}^{m-1}) - \dim\left(\ker \bar{\partial}_1\big|_{\mathbf{M}^{m-1}}\right). \tag{61}$$

Since

$$H^j_{\bar{\partial}_1}(\{\mathbf{M}\}) = 0 \text{ when } j < m, \tag{62}$$

we have

$$\dim\left(\ker \bar{\partial}_1\big|_{\mathbf{M}^{m-1}}\right) = \dim\left(\operatorname{im} \bar{\partial}_1\big|_{\mathbf{M}^{m-2}}\right) = \dim(\mathbf{M}^{m-2}) - \dim\left(\ker \bar{\partial}_1\big|_{\mathbf{M}^{m-2}}\right), \tag{63}$$

and so, by (59)–(63),

$$\begin{aligned}\dim(H^m_{\bar{\partial}_1}(\{\mathbf{M}\})) &= \dim(\mathbf{M}^m) - \left(\dim(\mathbf{M}^{m-1}) - \dim\left(\ker \bar{\partial}_1\big|_{\mathbf{M}^{m-1}}\right)\right) = \dim(\mathbf{M}^m) - \dim(\mathbf{M}^{m-1}) \\ &\quad + \dim(\mathbf{M}^{m-2}) - \dim\left(\ker \bar{\partial}_1\big|_{\mathbf{M}^{m-2}}\right).\end{aligned} \tag{64}$$

Continuing like this, we have

$$\dim(H^m_{\bar{\partial}_1}(\{\mathbf{M}\})) = \dim(\mathbf{M}^m) - \dim(\mathbf{M}^{m-1}) + \dim(\mathbf{M}^{m-2}) - \dim(\mathbf{M}^{m-3}) + \cdots \tag{65}$$

and since $\mathbf{M}^i = 0$ if $i < n+P$ where

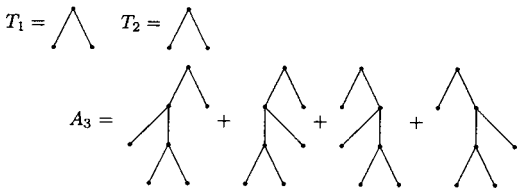

FIG. 66.

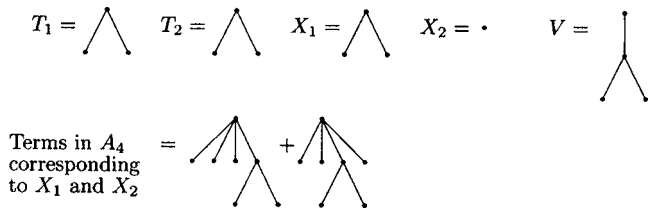

FIG. 67.

$$P = \deg T_1 + \cdots + \deg T_{n+1}, \tag{66}$$

we have

$$\dim(H^m_{\bar{\partial}_1}(\{\mathbf{M}\})) = \dim(\mathbf{M}^m) - \dim(\mathbf{M}^{m-1}) + \ldots + (-1)^{m-(n+P)} \dim(\mathbf{M}^{n+P}). \tag{67}$$

Let N be the number and let us calculate it. By the definition of $\mathbf{M}^i$, its dimension is that of

$$\bigoplus_{i_1+\cdots+i_{n+1}+n=i} \mathbf{D}_1^{i_1} \otimes \cdots \otimes \mathbf{D}_n^{i_n}. \tag{68}$$

Every $\mathbf{D}_k^{i_k}$ is one-dimensional when $p_k = i_k - \deg T_k$ is 0 or 1, and 0 otherwise. So the above direct sum is

$$\bigoplus_{p_1+\ldots+p_{n+1}+P+n=i} \mathbf{D}_1^{p_1+\deg T_1} \otimes \cdots \otimes \mathbf{D}_n^{p_n+\deg T_n}. \tag{69}$$

Hence, $\dim(\mathbf{M}^i)$ is the number of $(p_1, \ldots, p_{n+1})$'s satisfying $p_1+\cdots+p_{n+1}+P+n=i$ and each p_k is 0 or 1. Hence

$$\dim(\mathbf{M}^i) = \binom{n+1}{i-P-n} \tag{70}$$

and

$$N = \binom{n+1}{m-P-n} - \binom{n+1}{(m-1)-P-n} + \cdots + (-1)^{m-P-n}\binom{n+1}{0}.$$

Now we have

$$E_2^{i,j} = \begin{cases} \oplus_{j_1+\cdots+j_n=j} k^N \otimes H^{j_1}(S_1) \otimes \cdots \otimes H^{j_n}(S_n) & \text{if } i = m \\ 0 & \text{otherwise.} \end{cases}$$

Since $E_2^{i,j}=0$ except when $j=m$, every "knight's move map" on $E^{i,j}$'s is trivial. So the spectral sequence collapses and we have $H^n_{\bar{\partial}} = \oplus_{i+j=n} E^{i,j} = \oplus_{j_1+\cdots+j_n=n-m} k^N \otimes H^{j_1}(S_1) \otimes \cdots \otimes H^{j_n}(S_n)$, and since

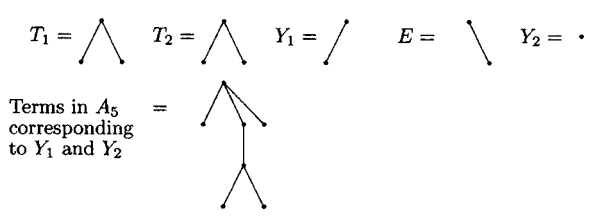

FIG. 68.

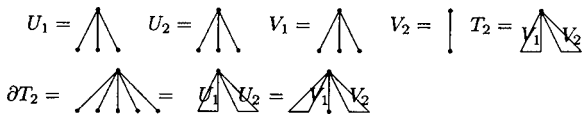

FIG. 69.

$$k^N \otimes H^{j_1}(S_1) \otimes \ldots \otimes H^{j_n}(S_n) = (H^{j_1}(S_1) \otimes \ldots \otimes H^{j_n}(S_n))^{\oplus N}, \tag{71}$$

we finally have the following.

Theorem 11.5: *When* $H^i(gs(n;T_1,\ldots,T_{n+1};S_1,\ldots,S_n))$ *is the ith cohomology group of the thread* $\mathbf{K}^i(gs(n;T_1,\ldots,T_{n+1};S_1,\ldots,S_n))$, *the ith cohomology group* H^i *of clear-edged m-bonsai is*

$$H^i = \bigoplus_{S \text{ is a grafting seedling}} H^i(S).$$

And, if $P=\deg T_1+\cdots+\deg T_n<m-2n+1$, *then* $H^i(gr(n;T_1,\ldots,T_{n+1};S_1,\ldots,S_n))=0$. *Otherwise*,

$$H^i(gr(n;T_1,\ldots,T_{n+1};S_1,\ldots,S_n)) = \bigoplus_{j_1+\ldots+j_n=n-m} [H^{j_1}(S_1) \otimes \cdots \otimes H^{j_n}(S_n)]^{\oplus N},$$

where

$$N = \binom{n+1}{m-P-n} - \binom{n+1}{(m-1)-P-n} + \cdots + (-1)^{m-(n+P)}\binom{n+1}{0}.$$

XII. DIFFERENTIAL AND APPENDING OF CLEAR-EDGED BONSAI

Let us consider the relationship between the appending operation $*$ on the clear-edged m-bonsai Hopf algebra $\mathcal{H}_{c,m}$ and the vertex appending differential ∂. We work mod 2 again. First, the operation $T_1 * T_2$ is the sum of all m-bonsais obtained by connecting the root of T_1 and a vertex of T_2 with an edge, as illustrated for 3-bonsai in Fig. 64.

In this section, we will show that $T_1 *_2 T_2 = 0$ for every T_1 and T_2 as in Sec. X.

Temporarily in this section, we use a differential $\bar{\partial}$ of corollas which is the same as ∂ except $\bar{\partial}(v)=e$, where v is the one-vertex bonsai and e is the one-edge bonsai.

12.1 Brief table of contents: In this section, first we will describe $T_1 *_1 T_2$ for each of the following cases when T_2 is a corolla, by dividing the cases as follows;

(i) when $\partial T_2 \neq 0$ and $\deg(T_2) \leqslant m-2$,
(ii) when $\partial T_2 \neq 0$ and $\deg(T_2) = m-1$,
(iii) when $\partial T_2 = 0$ and $\deg(T_2) \leqslant m-2$,
(iv) when $\partial T_2 = 0$ and $\deg(T_2) = m-1$,

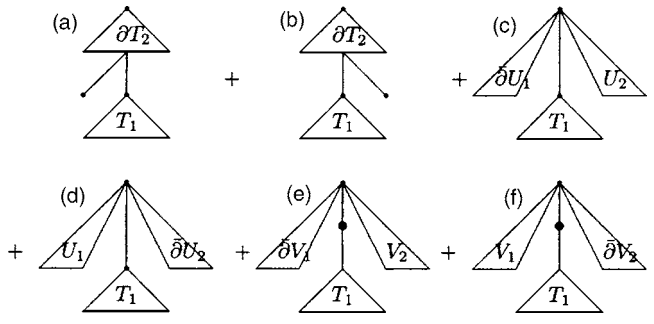

FIG. 70.

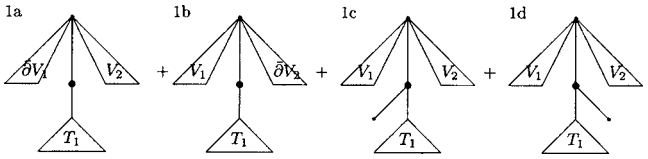

FIG. 71.

(v) when $\deg(T_2)=m$.

Second, we will show that $T_1 *_2 T_2$ for each of the following cases when T_2 is a corolla:

(i) when $\partial T_2 \neq 0$ and $\deg(T_2) \leqslant m-3$,
(ii) when $\partial T_2 \neq 0$ and $\deg(T_2)=m-2$,
(iii) when $\partial T_2 \neq 0$ and $\deg(T_2)=m-1$,
(iv) when $\partial T_2=0$ and $\deg(T_2) \leqslant m-2$,
(v) when $\partial T_2=0$ and $\deg(T_2)=m-1$,
(vi) when $\deg(T_2)=m$.

Finally, we show that $T_1 *_2 T_2$ for a general T_2.

12.2. $T_1 *_1 T_2$ when T_2 is a corolla: For clear-edged bonsai, since it is not an operad, we cannot use broomstick diagrams for graphical proof. Let us look into $T_1 *_1 T_2$ by dividing the cases of ∂T_2 and $\deg(T_2)$.

12.2.1. When $\partial T_2 \neq 0$ and $deg(T_2) \leqslant m-2$: If T_1 is not the one-vertex bonsai, then $(\partial T_1) * T_2$ is the sum of terms in $\partial(T_1 * T_2)$ obtained by attaching edges to T_1. So $T_1 *_1 T_2 = (\partial T_1) * T_2 + T_1 * (\partial T_2) - \partial(T_1 * T_2)$ ("−" in this equation is in fact "+", since we are working mod 2),

$$T_1 * (\partial T_2)$$

$+\Sigma$ [a term in $\partial(T_1 * T_2)$ which is obtained by attaching an edge to a vertex of $T_1 * T_2$ not in T_1 so that (i) and (ii) of Definition 11.1 is satisfied].

Then the first summand is the sum of (i) bonsais A_1 obtained by connecting a nonroot vertex of ∂T_2 and the root of T_1 with an edge, which is depicted as in the first equation of Fig. 65 in 3-bonsai and (ii) bonsais A_2 obtained by connecting the root of ∂T_2 and the root of T_1 with an edge, which is depicted as in the second equation in Fig. 65 in 3-bonsai.

The second summand is the sum of A_3, A_4, and A_5, where A_3, A_4, and A_5 are as follows.

A_3 is the sum of bonsais obtained by connecting a vertex v of T_2 and the root of T_1 with one edge and attaching an edge to v, as in Fig. 66 in 3-bonsai.

A_4: Bonsais B obtained as follows: suppose that T_2 is constructed by attaching the roots of corollas X_1 and X_2 so that X_1 is on the left and X_2 is on the right. Then B is obtained by attaching the roots of $\bar{\partial} X_1$, V, and X_2 from the left or X_1, V, and $\bar{\partial} X_2$ from the left, where V is obtained by attaching the root of T_1 to the lower vertex of the one-edge clear-edged bonsai, illustrated in Fig. 67. In Fig. 67, the first term of A_4 is constructed by $\bar{\partial} X_1$, V, and X_2, and the second term is constructed by X_1, V, and $\bar{\partial} X_2$.

A_5: Bonsais B obtained as follows: Suppose T_2 is constructed by attaching the roots of bonsais Y_1, E, and Y_2 from the left, where Y_1 and Y_2 are corollas and E is the one-edge bonsai. Then B is

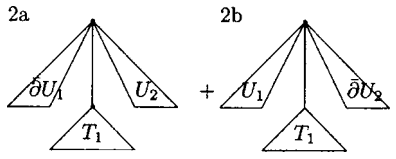

FIG. 72.

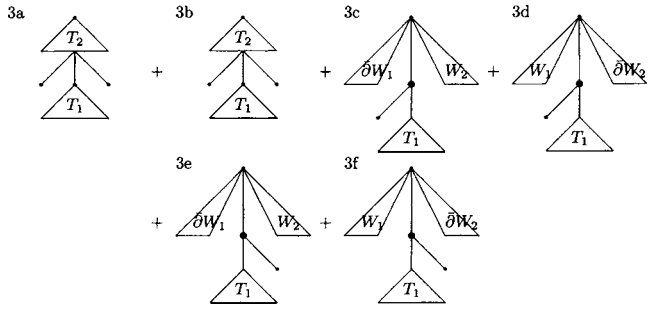

FIG. 73.

constructed by attaching the roots of $\bar{\partial}Y_1$, V, and Y_2 from the left or Y_1, V, and $\bar{\partial}Y_2$ from the left, where V is obtained by connecting the root of T_1 to the lower vertex of E with one edge. This is illustrated in Fig. 68.

If T_1 is the one-vertex bonsai, A_2 becomes 0, since it is equal to $\partial\partial T_2$. And $A_3=0$, since it is twice a multiple of the bonsais obtained by attaching the root of the two-edge corolla to a tip of T_2 (note that we are working mod 2). Also, $A_4=\partial\partial T_2=0$. So $T_1*_1T_2=A_1+A_5$.

12.2.2. When $\partial T_2\neq 0$ and $deg(T_2)=m-1$: When T_1 is not the one-vertex bonsai. This is almost the same as the previous case, but we cannot add more than one edge to the root of T_2. So $T_1*_1T_2$ is the sum of the terms A_1, A_3, and A_5.

When T_1 is the one-vertex bonsai, $A_3=0$, since it is twice a multiple of the bonsais obtained by attaching the root of the two-edge corolla to a tip of T_2 (note that we are working mod 2). So $T_1*_1T_2=A_1+A_5$.

12.2.3. When $\partial T_2=0$ and $deg(T_2)\leqslant m-2$: When T_1 is not the one-vertex bonsai. As in the first case, $T_1*_1T_2=(\partial T_1)*T_2+T_1*(\partial T_2)-\partial(T_1*T_2)$ is

$$T_1*(\partial T_2)$$

$+\Sigma$ [a term in $\partial(T_1*T_2)$ that is obtained by attaching an edge to a vertex of T_1*T_2 not in T_1 so that (i) and (ii) of Definition 11.1 is satisfied]

Here $\partial T_2=0$. So we just have the latter summand in $T_1*_1T_2$. As in the first case again, we have $T_1*_1T_2=A_3+A_4+A_5$.

When T_1 is the one-vertex bonsai: $A_3=0$, since it is a twice multiple of the bonsais obtained by attaching the root of the two-edge corolla to a tip of T_2 (note that we are working mod 2). Also, $A_4=\partial\partial T_2=0$. Hence, $T_1*_1T_2=A_5$.

12.2.4. When $\partial T_2=0$ and $deg(T_2)=m-1$: When T_1 is not the one-vertex bonsai. This is almost the same as the previous case, but we cannot add more than one edge to the root of T_2. So $T_1*_1T_2$ is the sum of the terms A_3 and A_5.

When T_1 is the one-vertex bonsai, $A_3=0$, since it is a twice multiple of the bonsais obtained by attaching the root of the two-edge corolla to a tip of T_2 (note that we are working mod 2). Hence, $T_1*_1T_2=A_5$.

12.2.5. When $deg(T_2)=m$: When T_1 is not the one-vertex bonsai. This is almost the same as the previous case, but we cannot add any more edges to the root of T_2. So $T_1*_1T_2$ is A_3.

When T_1 is the one-vertex bonsai, $A_3=0$, since it is twice a multiple of the bonsais obtained by attaching the root of the two-edge corolla to a tip of T_2 (note that we are working in mod 2). Hence, $T_1*_1T_2=0$.

12.3. $T_1*_2T_2$ when T_2 is a corolla: For each case in the preceding section, let us show that $T_1*_2T_2=0$.

12.3.1. When $\partial T_2\neq 0$ and $deg(T_2)\leqslant m-3$: In this case, we have $deg(\partial T_2\leqslant m-2)$ and $\partial(\partial T_2)=0$. And as in the first case of the preceding section, $T_1*_2T_2$ is

$$T_1*_1(\partial T_2)$$

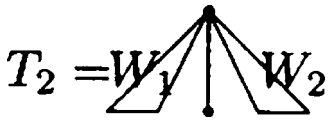

FIG. 74.

$+\Sigma$ [a term in $\partial(T_1 *_1 T_2)$ obtained by attaching an edge to a vertex of $T_1 * T_2$ not in T_1, so that (i) and (ii) of Definition 11.1 are satisfied].

When T_1 is not the one-vertex bonsai, by the third case of the preceding section, $T_1 *_1 (\partial T_2)$ is $A_3+A_4+A_5$, and by the first case of the preceding section, the sum of the terms in $\partial(T_1 *_1 T_2)$ obtained by attaching an edge to a vertex not in T_1 is $\hat{\partial}(T_1 *_1 T_2)=\hat{\partial}A_1+\hat{\partial}A_2+\hat{\partial}A_3+\hat{\partial}A_4+\hat{\partial}A_5$, where $\hat{\partial}X$, when X is a sum of terms in $T_1 *_1 T_2$, is the sum of the bonsais in ∂X obtained by attaching an edge to a vertex which is not originally in T_1.

In order to show that $T_1 *_2 T_2 = T_1 *_1 \partial T_2 + \hat{\partial}(T_1 *_1 T_2)=0$ pictorially, let us introduce a picture convention. In Fig. 69, where T_2 is a corolla with 4 edges, each triangle represents a corolla (including the one-vertex bonsai).

With this pictorial convention, we can draw $T_1 *_1 \partial T_2 = A_3+A_4+A_5$ as in Fig. 70, like A+B+C+D+E+F.

In $\hat{\partial}(T_1 *_1 T_2)$, $\hat{\partial}A_1$ can be drawn as in Fig. 71.

$\hat{\partial}A_2$ is as in Fig. 72.

$\hat{\partial}A_3$ is as in Fig. 73, where W_1 and W_2 are as in Fig. 74.

$\hat{\partial}A_4$ can be drawn as in Fig. 75.

And $\hat{\partial}A_5$ can be drawn as in Fig. 76.

Then we can get the pairs which are canceled as follows; A and 1c, B and 1d, C and 2a, D and 2b, E and 1a, F and 1b, 3a and 3b, 3c and 5e, 3d and 5f, 3e and 5g, 3f and 5h, 4b and 4c, 5b and 5c. 4a, 4d, 5a, and 5d are 0, because they have $\overline{\partial}^2$ in it. (Since 4b and 4c cancel each other, $\hat{\partial}A_4 = 0$.)

And every bonsai in Figs. 70–76 is in one of those pairs. So $T_1 *_2 T_2 = 0$.

When T_1 is the one-vertex bonsai: Since $T_1 *_1 T_2 = A_3+A_5$, it is the sum of A, B, E, and F. And since $T_1 *_1 T_2 = A_1+A_5$, we have $\hat{\partial}(T_1 *_1 T_2)=\hat{\partial}A_1+\hat{\partial}A_5$, and it is the sum of the bonsais in Fig. 71 and Fig. 76. So as above, we have $T_1 *_1 T_2 = 0$.

12.3.2. When $\partial T_2 \neq 0$ and $deg(T_2)=m-2$: When T_1 is not the one-vertex bonsai. We have $\partial(\partial T_2)=0$ and $\deg(\partial T_2)=m-1$. So we have $T_1 *_1 \partial T_2 = A_3+A_5$ and $\hat{\partial}(T_1 *_1 T_2)=\hat{\partial}(A_1+A_2+A_3+A_4+A_5)$. So the $T_1 *_2 T_2$ is the sum of the bonsais A, B, E, and F of Fig. 70 and the bonsais in Figs. 71–73 and Figs. 75 and 76 (2a and 2b are 0, since the valences at the roots are $m+1$). So as in the above case, $T_1 *_2 T_2 = 0$.

When T_1 is not the one-vertex bonsai, $T_1 *_1 \partial T_2 = A_5$ and $\hat{\partial}(T_1 *_1 T_2)=\hat{\partial}(A_1+A_5)$. So $T_1 *_2 T_2$ is the sum of the bonsais E and F of Fig. 70 and the bonsais in Figs. 71 and 76.

12.3.3. When $\partial T_2 \neq 0$ and $deg(T_2)=m-1$: In this case and others, we will just write down what $T_1 *_1 \partial T_2$ and $\hat{\partial}(T_1 *_1 T_2)$ are. In each case, as above, the bonsais in $T_1 *_2 T_2$ all cancel out.

In this case, $\partial(\partial T_2)=0$ and $\deg(\partial T_2)=m$.

When T_1 is not the one-vertex bonsai: $T_1 *_1 \partial T_2 = A_3+A_5$ and $\hat{\partial}(T_1 *_1 T_2)=\hat{\partial}(A_1+A_3+A_5)$.

When T_1 is the one-vertex bonsai, $T_1 *_1 \partial T_2 = A_5$ and $\hat{\partial}(T_1 *_1 T_2)=\hat{\partial}(A_1+A_5)$.

12.3.4. When $\partial T_2 = 0$ and $deg(T_2) \leqslant m-2$: In this case, $\partial T_2 = 0$ and $\deg(T_2) \leqslant m-2$.

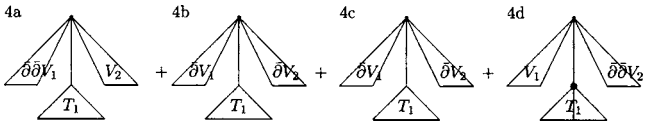

FIG. 75.

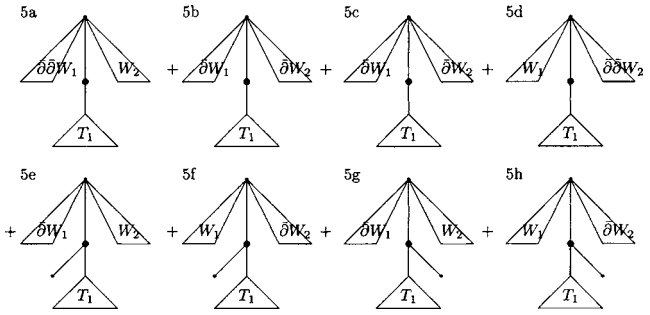

FIG. 76.

When T_1 is not the one-vertex bonsai, $T_1 *_1 \partial T_2 = 0$ and $\hat{\partial}(T_1 *_1 T_2) = \hat{\partial}(A_3 + A_4 + A_5)$.

When T_1 is the one-vertex bonsai, $T_1 *_1 \partial T_2 = 0$ and $\hat{\partial}(T_1 *_1 T_2) = \hat{\partial}(A_5)$.

12.3.5. When $\partial T_2 = 0$ and $deg(T_2) = m-1$: In this case, $\partial T_2 = 0$ and $\deg(T_2) = m-1$.

When T_1 is not the one-vertex bonsai, $T_1 *_1 \partial T_2 = A_3 + A_5$ and $\hat{\partial}(T_1 *_1 T_2) = \hat{\partial}(A_3 + A_5)$.

When T_1 is the one-vertex bonsai, $T_1 *_1 \partial T_2 = 0$ and $\hat{\partial}(T_1 *_1 T_2) = \hat{\partial}(A_5)$.

12.3.6. When $deg(T_2) = m$: In this case, $\partial T_2 = 0$ and $\deg(T_2) = m$.

When T_1 is not the one-vertex bonsai, $T_1 *_1 \partial T_2 = 0$ and $\hat{\partial}(T_1 *_1 T_2) = \hat{\partial}(A_3 + A_5)$.

When T_1 is the one-vertex bonsai, $T_1 *_1 \partial T_2 = 0$ and $\hat{\partial}(T_1 *_1 T_2) = 0$.

12.4. $T_1 *_2 T_2$ for general T_2: Now let us consider the case where T_2 is a general m-bonsai, not only a corolla. First, let us give an expression of a general m-bonsai as a concatenation of corollas. When we have a general clear-edged m-bonsai T as in Fig. 77, we first enumerate the nontip vertices of T in traversing order (cf. Sec. VII), as in Fig. 78, and for each nontip vertex numbered i, denote the corollas attached to that vertex as $T_{i1}, T_{i2}, \ldots, T_{im_i}$ from the left, and denote the given bonsai as $T(T_{11}, \ldots, T_{1m_1}; \ldots; T_{k1}, \ldots, T_{km_k})$, where k is the number of nontip vertices of T.

In Fig. 78, the given bonsai T is

$$T(T_{11}, T_{12}, T_{13}, T_{14}; T_{21}; T_{31}; T_{41}, T_{42}, T_{43}; T_{51}; T_{61}). \tag{72}$$

Now let $T = T(T_{11}, \ldots, T_{1m_1}; \ldots; T_{k1}, \ldots, T_{km_k})$ and just for convenience of algebra, let us denote T as $T(T_1, T_2, \ldots, T_m)$, where $T_1 = T_{11}, T_2 = T_{12}, \ldots, T_k = T_{km_k}$. Then we have $\partial T = \Sigma_i T(T_1, \ldots, \bar{\partial} T_i, \ldots, T_m)$ and $S * T = \Sigma_i T(T_1, \ldots, S * T_i, \ldots, T_m)$. So we have, by the definitions of $\hat{\partial}$, $\bar{\partial}$, and $*$,

$$\begin{aligned} S *_1 T &= S * \partial T + \hat{\partial}(S * T) = \sum_i T(T_1, \ldots, S * \bar{\partial} T_i, \ldots, T_m) + \sum_{i \neq j} T(T_1, \ldots, \bar{\partial} T_i, \ldots, S * T_j, \ldots, T_m) \\ &\quad + \sum_i T(T_1, \ldots, \hat{\partial}(S * T_i), \ldots, T - m) + \sum_{i \neq j} T(T_1, \ldots, \bar{\partial} T_i, \ldots, S * T_j, \ldots, T_m) \\ &= \sum_i T(T_1, \ldots, S * \bar{\partial} T_i, \ldots, T_m) + \sum_i T(T_1, \ldots, \hat{\partial}(S * T_i), \ldots, T - m) = \sum_i T(T_1, \ldots, S *_1 T_i, \ldots, T_m). \end{aligned} \tag{73}$$

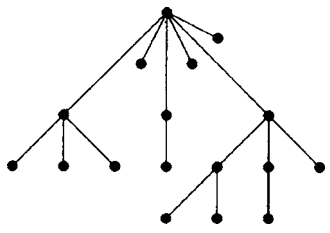

FIG. 77.

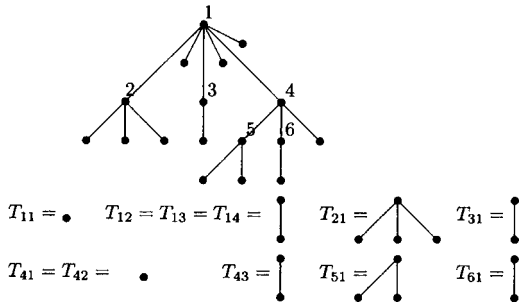

FIG. 78.

Similarly, we have

$$S*_2T = S*_1 \partial T + \hat{\partial}(S*_1T) = \sum_i T(T_1,\ldots,S*_1\bar{\partial}T_i,\ldots,T_m) + \sum_{i\neq j} T(T_1,\ldots,\bar{\partial}T_i,\ldots,S*_1T_j,\ldots,T_m)$$

$$+ \sum_i T(T_1,\ldots,\hat{\partial}(S*_1T_i),\ldots,T-m) + \sum_{i\neq j} T(T_1,\ldots,\bar{\partial}T_i,\ldots,S*_1T_j,\ldots,T_m) \tag{74}$$

$$= \sum_i T(T_1,\ldots,S*_1\bar{\partial}T_i,\ldots,T_m) + \sum_i T(T_1,\ldots,\hat{\partial}(S*_1T_i),\ldots,T-m) = \sum_i T(T_1,\ldots,S*_2T_i,\ldots,T_m) = 0. \tag{75}$$

So we have

Theorem 12.1:: *Mod2, for any clear-edged m-bonsai* T_1 *and* T_2, *we have* $T_1*_2T_2=0$.

XIII. FURTHER DIRECTION

In the next paper of the author, we will investigate a generalization of the *m*-bonsai Hopf algebra, its differentials and cohomology groups. Also we will investigate some possibility of generalization of the appending operation $*$.

Also see Bergbauer and Kreimer (unpublished), Harrivel (unpublished), and Pachter and Sturmfels (unpublished).

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Bosonic color-flavor transformation for the special unitary group

Yi Wei
Department of Physics, Yale University, New Haven, Connecticut 06520-8120

Tilo Wettig
Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

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We extend Zirnbauer's color-flavor transformation in the bosonic sector to the color group $\mathrm{SU}(N_c)$. Because the flavor group $\mathrm{U}(N_b,N_b)$ is noncompact, the algebraic method by which the original color-flavor transformation was derived leads to a useful result only for $2N_b \leqslant N_c$. Using the character expansion method, we obtain a different form of the transformation in the extended range $N_b \leqslant N_c$. This result can also be used for the color group $\mathrm{U}(N_c)$. The integrals to which the transformation can be applied are of relevance for the recently proposed boson-induced lattice gauge theory. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1951627]

I. INTRODUCTION

In 1996, Zirnbauer[1] invented a generalized Hubbard-Stratonovitch transformation which trades an integration over a "color" gauge group for an integration over a certain supersymmetric coset space, or "flavor" space. Although the transformation was originally derived to study disordered systems in condensed matter physics, the terminology comes from lattice gauge theory because the integral over the gauge group to which the color-flavor transformation is applied is precisely of the form of a one-link integral in lattice gauge theory at infinite coupling.

The fields that appear in the transformation carry two types of indices that will be referred to as color and flavor indices. The number of colors is denoted by N_c, and the numbers of bosonic and fermionic flavors are denoted by N_b and N_f, respectively. Zirnbauer derived versions of the color-flavor transformation for the three color groups $\mathrm{U}(N_c)$, $\mathrm{O}(N_c)$, and $\mathrm{Sp}(2N_c)$.[1] In his original work, the flavor space contained an equal number of bosonic and fermionic degrees of freedom, but it is possible to relax this constraint.[2] Convergence requirements then place an upper bound on the difference between the number of bosons and fermions. For the case of $\mathrm{U}(N_c)$, this bound is given by $2(N_b-N_f) \leqslant N_c$.

The color-flavor transformation has been used in a number of physical applications, e.g., in the derivation of a field theory for the random flux model by Altland and Simons[3] and in the construction of chiral Lagrangians for lattice gauge theories by Nagao and Nishigaki.[4] In the latter paper, the calculations were done for the above-mentioned color groups. However, in quantum chromodynamics (QCD) the color group is SU(3). To be able to apply the color-flavor transformation to this very important physical case, a variant of the transformation for the special unitary group needed to be derived. Following earlier work by Budczies and Shnir,[5,6] this was done in Refs. 7 and 8 in the fermionic sector, i.e., for $N_b=0$. The result was then applied to lattice QCD in Refs. 8 and 9.

As mentioned above, the color-flavor transformation can only be applied to the one-link integral of lattice gauge theory if the gauge coupling is infinite. Fortunately, it is possible to go beyond the infinite-coupling limit. A gauge action (Yang-Mills action in the continuum or Wilson action on the lattice) can be induced by coupling auxiliary fields to the gauge field (still at infinite coupling) and integrating out these extra fields. This idea, which is known as "induced QCD," has been considered in various forms in the literature.[10–15] For example, the job can be done by a

number N_h of heavy auxiliary fermions with common mass m_h in the combined limit $N_h \to \infty$, $m_h \to \infty$ such that the ratio N_h/m_h^4 is constant, and this constant can then be related to the strength of the induced gauge coupling.

So far, the color-flavor transformation for SU(N_c) has only been derived in the fermionic sector, for three reasons, (a) physical quarks are fermions, (b) a gauge action can be induced by auxiliary fermions alone, and (c) the calculation is somewhat easier for fermions than for bosons. There seemed to be no special need for a bosonic variant of the transformation until Budczies and Zirnbauer suggested a new method to induce the gauge action using auxiliary bosons.[16] Their approach has the advantage of requiring only a small number (essentially equal to N_c) of auxiliary fields. However, to be able to use their method in lattice QCD, one requires an SU(N_c) variant of the color-flavor transformation that accommodates both fermions (the physical quarks) and bosons (to induce the gauge action).

As a first step towards this goal, we found it useful to consider the purely bosonic case with $N_f=0$ for which we will present results in this paper. Our results can be applied to study a boson-induced gauge theory without physical quarks. Focusing on the bosonic sector allows us to separate the complications due to the fact that the fields are bosonic from those due to the supersymmetric framework. This is the main motivation for the present paper. The supersymmetric case will be addressed in a separate paper.

The convergence requirement mentioned above is irrelevant for the purely fermionic case in which $N_b=0$ since the inequality is always satisfied. However, it becomes relevant for the purely bosonic case. We obtain a "standard" form of the color-flavor transformation if the condition $2N_b \leqslant N_c$ is satisfied. In the extended range $N_b \leqslant N_c$ we derive a different form of the transformation. Interestingly, for $N_b < N_c$ our results for SU(N_c) are identical to those for gauge group U(N_c), and we therefore obtain new results for U(N_c) in the range $N_b < N_c < 2N_b$. [The physical reason behind this is the observation that one cannot make baryons out of bosonic quarks if $N_b < N_c$. Such "bosonic baryons" must contain at least as many flavors as colors, see, e.g., Eq. (22) below.] For $N_b > N_c$ we have not been able to simplify our formal result to be useful in applications.

This paper is organized as follows. We first state our results in Sec. II. In Sec. III, we use the algebraic method of Refs. 1 and 7 to derive our general result for the bosonic color-flavor transformation. In Sec. IV, we use a different approach, the character expansion method, to derive an alternative form of the bosonic color-flavor transformation. We close with a brief discussion of possible applications and open problems. The appendix contains derivations of several intermediate results as well as a number of examples for the results from both approaches.

II. STATEMENT OF RESULTS

Let ψ_a^i, $\bar{\psi}_a^i$, φ_a^i, and $\bar{\varphi}_a^i$ be complex bosonic variables that carry a color index (superscript i running from 1 to N_c) and a flavor index (subscript a running from 1 to N_b). The bar denotes complex conjugation. Summation over repeated indices is implied here and throughout the paper unless indicated otherwise. Using the algebraic method of Refs. 1 and 7, we obtain

$$\int_{\mathrm{SU}(N_c)} \mathrm{d}U \exp(\bar{\psi}_a^i U^{ij} \psi_a^j + \bar{\varphi}_a^i U^{\dagger ij} \varphi_a^j) = \int_{|ZZ^\dagger| \leqslant 1} \frac{\mathrm{d}Z\, \mathrm{d}Z^\dagger}{\det^{2N_b - N_c}(1 - ZZ^\dagger)} \times \exp(\bar{\psi}_a^i Z_{ab} \varphi_b^i + \bar{\varphi}_a^i Z_{ab}^\dagger \psi_b^i) \sum_{Q=0}^{\infty} \chi_Q, \tag{1}$$

where

$$\chi_0 = \mathcal{C}_0, \quad \chi_{Q>0} = \mathcal{C}_Q(\det{}^Q \mathcal{M} + \det{}^Q \mathcal{N}), \tag{2}$$

the $N_c \times N_c$ matrices $\mathcal{M}$ and $\mathcal{N}$ are defined by $\mathcal{M}^{ij} = \bar{\psi}_a^i (1 - ZZ^\dagger)_{ab} \psi_b^j$ and $\mathcal{N}^{ij} = \bar{\varphi}_a^i (1 - Z^\dagger Z)_{ab} \varphi_b^j$, and the coefficients $\mathcal{C}_Q$ are computed in Appendix B.

The integration on the left-hand side (LHS) of Eq. (1) is over $\mathrm{SU}(N_c)$ matrices U distributed according to the Haar measure $\mathrm{d}U$, normalized such that the group volume is unity. The integration on the right-hand side (RHS) of that equation is over complex $N_b \times N_b$ matrices Z, with the restriction that all eigenvalues of $ZZ^\dagger$ are less than or equal to 1. These matrices parametrize the noncompact coset space $\mathrm{U}(N_b,N_b)/[\mathrm{U}(N_b)\times\mathrm{U}(N_b)]$ (the reason to choose this particular parametrization is given at the end of Sec. III E). The corresponding invariant integration measure is given by[17]

$$\mathrm{d}\mu(Z,Z^\dagger) = \frac{\mathrm{d}Z\,\mathrm{d}Z^\dagger}{\det(1-ZZ^\dagger)^{2N_b}} \quad \text{with } \mathrm{d}Z\,\mathrm{d}Z^\dagger = \prod_{a,b=1}^{N_b} \mathrm{d}\,\mathrm{Re}\,Z_{ab}\mathrm{d}\,\mathrm{Im}\,Z_{ab}. \tag{3}$$

Note that the $N_c \times N_c$ matrices $\mathcal{M}$ and $\mathcal{N}$ can be thought of as products of three matrices of dimension $N_c \times N_b$, $N_b \times N_b$, and $N_b \times N_c$, respectively. The resulting matrix is of full rank only if $N_b \geqslant N_c$. For $N_b < N_c$, we therefore have $\det \mathcal{M} = \det \mathcal{N} = 0$,[18] and the transformation simplifies to

$$\int_{\mathrm{SU}(N_c)} \mathrm{d}U \exp(\bar{\psi}^i_a U^{ij} \psi^j_a + \bar{\varphi}^i_a U^{\dagger ij} \varphi^j_a) = \mathcal{C}_0 \int_{|ZZ^\dagger|\leqslant 1} \frac{\mathrm{d}Z\,\mathrm{d}Z^\dagger}{\det^{2N_b-N_c}(1-ZZ^\dagger)} \exp(\bar{\psi}^i_a Z_{ab} \varphi^i_b + \bar{\varphi}^i_a Z^\dagger_{ab} \psi^i_b) \tag{4}$$

with a constant $\mathcal{C}_0$ given in Eq. (B5). This agrees with the result for the color group $\mathrm{U}(N_c)$ in Ref. 2.

Equation (1) looks similar to the result for the fermionic sector presented in Ref. 7. There are two major differences, however. First, due to the nilpotency of Grassmann variables the sum over Q in Eq. (1) only went up to N_f in the fermionic case, whereas it extends to infinity now. Second, the invariant measure of the coset space $\mathrm{U}(N_b,N_b)/[\mathrm{U}(N_b)\times\mathrm{U}(N_b)]$ in Eq. (3) diverges at the boundary, giving rise to convergence issues which we discuss now.

For $2N_b \leqslant N_c$, the divergence of the measure is canceled by the factor of $\det^{N_c}(1-ZZ^\dagger)$ in the integrand of Eq. (1). In this case the result (4) applies and is free from divergences. For $N_b < N_c < 2N_b$, the integral over Z in Eq. (4) diverges. For $N_b = N_c$, the integral over Z in Eq. (1) diverges for $Q < N_b$, whereas for $N_b > N_c$, it diverges for all Q. Of course, the final result for the RHS of Eqs. (1) and (4) must be finite, so whatever divergence arises from the integration over Z will be canceled by a similar divergence in the integral for the corresponding (inverse) constant $\mathcal{C}_Q^{-1}$, see Eq. (56). A finite ratio could in principle be obtained by a suitable regularization and limiting procedure, but it is not clear to us whether this would lead to a simple final result (an explicit example for such a limiting procedure is given in Appendix D 3).

Instead, we have used the character expansion method[19–21] to derive a different form of the color-flavor transformation and obtain for $N_b < N_c$

$$\int_{\mathrm{SU}(N_c)} \mathrm{d}U \exp(\bar{\psi}^i_a U^{ij} \psi^j_a + \bar{\varphi}^i_a U^{\dagger ij} \varphi^j_a) = \prod_{n=0}^{N_c-N_b-1} \frac{(N_b+n)!}{n!} \int_{\mathrm{U}(N_b)} \mathrm{d}V \det{}^{N_b-N_c}(VB) \times \exp(\bar{\psi}^i_a V_{ab} \varphi^i_b + \bar{\varphi}^i_a V^\dagger_{ab} \psi^i_b), \tag{5}$$

where the $N_b \times N_b$ matrix B is defined by $B_{ab} = \varphi^i_a \bar{\psi}^i_b$. Note that the integration on the RHS is over the unitary group with the normalized Haar measure $\mathrm{d}V$. Equation (5) is also valid if the integration on the LHS is over the color group $\mathrm{U}(N_c)$ and, to the best of our knowledge, represents a new result for this case.

The corresponding result for $N_b = N_c$ reads

$$\int_{\mathrm{SU}(N_c)} \mathrm{d}U \exp(\bar{\psi}_a^i U^{ij} \psi_a^j + \bar{\varphi}_a^i U^{\dagger ij} \varphi_a^j) = \sum_{Q=0}^{\infty} \tilde{\chi}_Q \int_{\mathrm{U}(N_b)} \mathrm{d}V \det{}^{-Q}(VB) \exp(\bar{\psi}_a^i V_{ab} \varphi_b^i + \bar{\varphi}_a^i V_{ab}^\dagger \psi_b^i) \tag{6}$$

with

$$\tilde{\chi}_0 = 1, \quad \tilde{\chi}_{Q>0} = \det{}^Q M + \det{}^Q N, \tag{7}$$

the matrix B as defined above, and $N_c \times N_c$ matrices M and N defined by $M^{ij} = \psi_a^i \bar{\psi}_a^j$ and $N^{ij} = \varphi_a^i \bar{\varphi}_a^j$. Note that we are not allowed to change the order of summation and integration in Eq. (6), see Sec. IV C. If the integration on the LHS of Eq. (6) is over $\mathrm{U}(N_c)$, only the $Q=0$ term contributes on the RHS, see Eq. (77). The integral over $\mathrm{U}(N_b)$ in Eqs. (5) and (6) can be done analytically,[22–24] resulting in a determinant involving modified Bessel functions, but we do not display this result here because Eqs. (5) and (6) are to be viewed as transformations.

As mentioned in the introduction, for $N_b > N_c$ we have not been able to obtain a simple form of the color-flavor transformation in which the divergences have been eliminated.

III. BOSONIC COLOR-FLAVOR TRANSFORMATION: ALGEBRAIC METHOD

The basic idea of the algebraic approach to the color-flavor transformation is to construct two projection operators onto the subspace of Fock space (to be defined below) which is invariant under the action of the color group $\mathrm{SU}(N_c)$. One such projector is implemented by integrating over the color group. The other one is obtained by integrating over a certain coset of the flavor group $\mathrm{U}(N_b, N_b)$. Identification of the two projection operations then leads to Eq. (1). In this section, we shall use this algebraic approach to derive the bosonic color-flavor transformation. We closely follow Refs. 1, 7, and 8 whenever possible.

A. Fock space, Lie algebras, and Lie groups

We introduce two sets of bosonic creation and annihilation operators $\{\bar{c}_a^i, c_a^i\}$ and $\{\bar{d}_a^i, d_a^i\}$, where $i = 1, \ldots, N_c$ and $a = 1, \ldots, N_b$. As mentioned above, we shall refer to the upper index as "color" and to the lower index as "flavor." The Fock vacuum $|0\rangle$ is defined by the requirement that $c_a^i|0\rangle = d_a^i|0\rangle = 0$ for all combinations of i and a, and the Fock space is generated by acting on $|0\rangle$ with the $\bar{c}_a^i$ and $\bar{d}_a^i$. In the following, the two sets of particles created by the $\bar{c}_a^i$ and $\bar{d}_a^i$ will be referred to as particles and antiparticles, respectively.

For simplicity of notation, we also introduce the unified operators $\{\bar{c}_A^i, c_A^i\}$ defined by

$$c_A^i = \begin{cases} c_A^i & \text{for } 1 \leqslant A \leqslant N_b, \\ \bar{d}_{A-N_b}^i & \text{for } N_b < A \leqslant 2N_b, \end{cases}$$

$$\bar{c}_A^i = \begin{cases} \bar{c}_A^i & \text{for } 1 \leqslant A \leqslant N_b, \\ -d_{A-N_b}^i & \text{for } N_b < A \leqslant 2N_b. \end{cases} \tag{8}$$

They satisfy the usual commutation relations for bosonic operators,

$$[c_A^i, \bar{c}_B^j] = \delta^{ij} \delta_{AB}. \tag{9}$$

Next we define operators $E_{AB}^{ij} = \bar{c}_A^i c_B^j$. Simple algebra reveals that they satisfy the commutation relations

$$[E_{AB}^{ij}, E_{CD}^{k\ell}] = \delta_{BC} \delta^{kj} E_{AD}^{i\ell} - \delta_{AD} \delta^{i\ell} E_{CB}^{kj}, \tag{10}$$

and hence they are generators of the Lie algebra $\mathrm{gl}(2N_c N_b)$.

The Lie algebra $\mathrm{gl}(2N_cN_b)$ has two commuting subalgebras that are important for our proof, namely $\mathrm{gl}(2N_b)$, which is generated by the color-singlet operators

$$\left\{ \mathcal{G}_{AB} \equiv \sum_{i=1}^{N_c} E_{AB}^{ii} \right\}, \tag{11}$$

and $\mathrm{sl}(N_c)$, which is generated by the flavor-singlet operators

$$\left\{ \mathcal{E}^{ij} \equiv \sum_{A=1}^{2N_b} E_{AA}^{ij}; i \neq j \right\},$$

$$\left\{ \mathcal{H}^i \equiv \sum_{A=1}^{2N_b} E_{AA}^{ii} - \frac{1}{N_c} \sum_{j=1}^{N_c} \sum_{A=1}^{2N_b} E_{AA}^{jj}; i = 1, \ldots, N_c \right\}. \tag{12}$$

Note that only $N_c - 1$ of the generators $\mathcal{H}^i$ are linearly independent.

The action of the group $\mathrm{GL}(2N_cN_b)$ and its subgroups on the Fock space is defined by exponential mapping, i.e., for all $g \in \mathrm{GL}(2N_cN_b)$ we define a map $g \mapsto T_g$ from group elements to operators by[1,8]

$$T_g = \exp[\bar{c}_A^i (\ln g)_{AB}^{ij} c_B^j]. \tag{13}$$

Following Zirnbauer,[1] one can show that the map $g \mapsto T_g$ is well-defined and a homomorphism of $\mathrm{GL}(2N_cN_b)$,

$$T_g T_h = T_{gh}. \tag{14}$$

Therefore it furnishes a (reducible) representation of $\mathrm{GL}(2N_cN_b)$.

In the following, we will consider the action of the subgroups $\mathrm{SU}(N_c)$ (the color group) and $\mathrm{U}(N_b,N_b)$ (the flavor group) of $\mathrm{GL}(2N_cN_b)$ on the Fock space. The corresponding subalgebras $\mathrm{sl}(N_c)$ and $\mathrm{gl}(2N_b)$ have been given above. What are the reasons to single out these two subgroups? For the color group the reason is simple. The integration on the LHS of Eq. (1) is over $\mathrm{SU}(N_c)$. For the flavor group, the choice of the noncompact subgroup $\mathrm{U}(N_b,N_b)$ is not immediately obvious at this point but will become clear as we proceed. We shall see below that the color-neutral sector of Fock space is noncompact in the bosonic case, as opposed to the fermionic case in which it was compact. Attempts to work with the compact subgroup $\mathrm{U}(2N_b)$ do not lead to useful results. Also, when Eq. (1) is used in applications, one wants the resulting integrals over the bosonic variables to converge, and this requirement necessitates a noncompact integration domain on the RHS of that equation.[1,25–27]

Under the action of the subgroups $\mathrm{SU}(N_c)$ and $\mathrm{U}(N_b,N_b)$, the operators c_A^i and $\bar{c}_A^i$ transform as follows:

$$g \in \mathrm{SU}(N_c): \quad T_g c_A^i T_g^{-1} = (g^{-1})^{ij} c_A^j, \quad T_g \bar{c}_A^i T_g^{-1} = \bar{c}_A^j g^{ji}, \tag{15}$$

$$g \in \mathrm{U}(N_b,N_b): \quad T_g c_A^i T_g^{-1} = g_{AB}^{-1} c_B^i, \quad T_g \bar{c}_A^i T_g^{-1} = \bar{c}_B^i g_{BA}, \tag{16}$$

which can be shown using the Baker-Campbell-Hausdorff formula.

B. Bose coherent states and projection onto the color-neutral sector

We call a vector $|\mathcal{N}\rangle$ in the Fock space color neutral if it is invariant under $\mathrm{SU}(N_c)$ transformations, i.e., $T_U|\mathcal{N}\rangle = |\mathcal{N}\rangle$ for all $U \in \mathrm{SU}(N_c)$. The subspace of Fock space spanned by these invariant vectors is called the color-neutral subspace or sector.

The following argument closely parallels Ref. 8. With the complex bosonic variables ψ_a^i, $\bar{\psi}_a^i$, φ_a^i, and $\bar{\varphi}_a^i$ introduced in Sec. II Bose coherent states are defined as

$$|\Psi\rangle = \exp(\bar{c}^i_a \psi^i_a + \bar{d}^i_a \bar{\varphi}^i_a)|0\rangle, \quad \langle\Psi| = \langle 0|\exp(\bar{\psi}^i_a c^i_a + \varphi^i_a d^i_a). \tag{17}$$

They span the entire Fock space (or its dual). Using Eq. (15) we find

$$\langle\Psi|T_U|\Psi\rangle = \exp(\bar{\psi}^i_a U^{ij} \psi^j_a + \bar{\varphi}^i_a U^{\dagger ij} \varphi^j_a). \tag{18}$$

The LHS of Eq. (1) can therefore be written as

$$\mathcal{Z} = \int_{\mathrm{SU}(N_c)} \mathrm{d}U \exp(\bar{\psi}^i_a U^{ij} \psi^j_a + \bar{\varphi}^i_a U^{\dagger ij} \varphi^j_a) = \langle\Psi|P|\Psi\rangle, \tag{19}$$

where we have introduced the operator P defined by

$$P = \int_{\mathrm{SU}(N_c)} \mathrm{d}U \, T_U. \tag{20}$$

This operator annihilates all states that are not color neutral, while leaving color-neutral states invariant [recall that the volume of $\mathrm{SU}(N_c)$ is unity]. Therefore, it is a projector onto the color-neutral sector. As advertised above, it is one possible representation of such a projector, and we will now derive an alternative form.

C. Action of the flavor group in the color-neutral sector

By definition, color-neutral vectors $|\mathcal{N}\rangle$ are annihilated by all generators of $\mathrm{sl}(N_c)$, i.e., $\mathcal{E}^{ij}|\mathcal{N}\rangle = 0$ and $\mathcal{H}^i|\mathcal{N}\rangle = 0$. Using Eq. (12) and the commutation relations (9), this requirement leads to

$$\left(\sum_{a=1}^{N_b} \bar{c}^i_a c^j_a - \sum_{a=1}^{N_b} \bar{d}^j_a d^i_a \right) |\mathcal{N}\rangle = \delta^{ij} Q |\mathcal{N}\rangle, \tag{21}$$

where Q is an integer. Clearly, the color-neutral sector contains the vacuum. For $i=j$, the operator on the LHS of Eq. (21) counts the difference in the number of particles and antiparticles for each color, the difference being equal to Q.

The color-neutral sector can be generated by acting on the vacuum state with three types of operators,

$$\text{type-1a}, \quad \bar{c}^i_a \bar{d}^i_b,$$

$$\text{type-2a}, \quad \epsilon_{i_1 \cdots i_{N_c}} \bar{c}^{i_1}_{a_1} \bar{c}^{i_2}_{a_2} \cdots \bar{c}^{i_{N_c}}_{a_{N_c}},$$

$$\text{type-2b}, \quad \epsilon_{i_1 \cdots i_{N_c}} \bar{d}^{i_1}_{b_1} \bar{d}^{i_2}_{b_2} \cdots \bar{d}^{i_{N_c}}_{b_{N_c}}, \tag{22}$$

where ϵ denotes the totally antisymmetric Levi-Civita symbol which ensures that the resulting state is invariant under $\mathrm{SU}(N_c)$ transformations. In addition, the following types of operators make transformations in the color-neutral sector:

$$\text{type-1b}, \quad c^i_a d^i_b,$$

$$\text{type-1c}, \quad \bar{c}^i_a c^i_b,$$

$$\text{type-1d}, \quad d_a^i \bar{d}_b^i. \tag{23}$$

When acting on a color-neutral state, type-1 operators do not change the Q value of that state, whereas type-2a (type-2b) operators increase (decrease) the Q value by one. Note, however, that for $N_b < N_c$ the type-2 operators do not exist, which makes it impossible to generate a vector in a nonzero Q sector. The range of Q is therefore given by

$$Q = \begin{cases} -\infty, \ldots, \infty & \text{for } N_b \geqslant N_c, \\ 0 & \text{for } N_b < N_c. \end{cases} \tag{24}$$

[In the case of $N_b < N_c$, we are back to the bosonic color-flavor transformation for the group $\mathrm{U}(N_c)$.[2] The Lie algebra of $\mathrm{U}(N_c)$ has an extra U(1) generator, and by requiring invariance under $\mathrm{U}(N_c)$, this U(1) generator eliminates all nonzero Q sectors.]

The action of the flavor group on the Fock space is defined by Eq. (13) with $g \in \mathrm{U}(N_b, N_b)$. We now choose the color-neutral sector to be the carrier space of this representation. The type-1 operators are the generators of the flavor group and do not change the Q value of a given state. Therefore, under the action of the flavor group, the color-neutral sector decomposes into invariant subspaces labeled by Q, which we shall call "Q sectors." As mentioned above, a Q sector contains Q more particles than antiparticles for each color.

We now prove that the flavor group acts irreducibly in a given Q sector.[1] For this we need to show that from any given state in the Q sector we can reach any other state by the action of the flavor group. Equivalently, we can single out a particular state $|\psi_Q\rangle$, defined by

$$|\psi_{Q>0}\rangle = (\epsilon_{i_1 \cdots i_{N_c}} \bar{c}_1^{i_1} \bar{c}_2^{i_2} \cdots \bar{c}_{N_c}^{i_{N_c}})^Q |0\rangle,$$

$$|\psi_{Q=0}\rangle = |0\rangle,$$

$$|\psi_{Q<0}\rangle = (\epsilon_{i_1 \cdots i_{N_c}} \bar{d}_1^{i_1} \bar{d}_2^{i_2} \cdots \bar{d}_{N_c}^{i_{N_c}})^Q |0\rangle, \tag{25}$$

and show that (i) starting from this state, we can reach any other state, and (ii) from that state we can return to $|\psi_Q\rangle$, using type-1 operators only.

An arbitrary vector in a given Q sector, which we should be able to reach from $|\psi_Q\rangle$, is obtained by acting on the vacuum with the appropriate number of type-1a operators and Q more type-2a than type-2b operators. There are already Q ($-Q$) unpaired type-2a (type-2b) operators associated with $|\psi_Q\rangle$, so what remains are pairs consisting of a type-2a and a type-2b operator. Such a pair can be expanded in terms of type-1a operators as

$$\epsilon_{i_1 \cdots i_{N_c}} \bar{c}_{a_1}^{i_1} \bar{c}_{a_2}^{i_2} \cdots \bar{c}_{a_{N_c}}^{i_{N_c}} \epsilon_{j_1 \cdots j_{N_c}} \bar{d}_{b_1}^{j_1} \bar{d}_{b_2}^{j_2} \cdots \bar{d}_{b_{N_c}}^{j_{N_c}} = \sum_{\sigma \in S_{N_c}} \mathrm{sgn}(\sigma) \bar{c}_{a_1}^{i_1} \bar{d}_{\sigma(b_1)}^{i_1} \cdots \bar{c}_{a_{N_c}}^{i_{N_c}} \bar{d}_{\sigma(b_{N_c})}^{i_{N_c}} \tag{26}$$

and is therefore in the algebra of the flavor group. The type-1c and type-1d operators obey the commutation relations

$$[\bar{c}_a^i c_{b_1}^i, \epsilon_{i_1 \cdots i_{N_c}} \bar{c}_{b_1}^{i_1} \bar{c}_{b_2}^{i_2} \cdots \bar{c}_{b_{N_c}}^{i_{N_c}}] = \epsilon_{i_1 \cdots i_{N_c}} \bar{c}_a^{i_1} \bar{c}_{b_2}^{i_2} \cdots \bar{c}_{b_{N_c}}^{i_{N_c}},$$

$$[d_{b_1}^i \bar{d}_a^i, \epsilon_{i_1 \cdots i_{N_c}} \bar{d}_{b_1}^{i_1} \bar{d}_{b_2}^{i_2} \cdots \bar{d}_{b_{N_c}}^{i_{N_c}}] = \epsilon_{i_1 \cdots i_{N_c}} \bar{d}_a^{i_1} \bar{d}_{b_2}^{i_2} \cdots \bar{d}_{b_{N_c}}^{i_{N_c}}. \tag{27}$$

Thus, they enable us to change the flavor indices of the type-2 operators. We can thus reach any state in a given Q-sector by acting with the corresponding number and subtypes of type-1 operators on $|\psi_Q\rangle$. Furthermore, type-1a operators can be undone by type-1b operators, while type-1c and type-1d operators can undo themselves. We can therefore go from an arbitrary state in the Q

sector back to $|\psi_Q\rangle$. In other words, $|\psi_Q\rangle$ is a cyclic vector in the Q sector under the action of the flavor group, which implies irreducibility.

D. Generalized coherent states and projection onto the color-neutral sector

Generalized coherent states are described in detail in Ref. 28. They are useful for our purposes because they allow a resolution of the identity operator. For a Lie group G and an irreducible representation T_g, a set of generalized coherent states is obtained by acting on a state $|\psi_T\rangle$ in the carrier space of T_g with all elements of T_g. This results in the set $\{T_g|\psi_T\rangle\}$ which, in general, is overcomplete. If H is the maximal subgroup of G such that $T_h|\psi_T\rangle \propto |\psi_T\rangle$ for all $h \in H$, the subgroup H is called the isotropy subgroup of $|\psi_T\rangle$, and the set of generalized coherent states can be parametrized without overcounting by the elements of the coset space G/H. (If the subgroup H is not maximal, some overcounting remains.)

We now set $G=\mathrm{U}(N_b,N_b)$ and consider the representation T_g of Eq. (13) (with $g \in G$) which acts irreducibly in a given Q sector. For the starting vector we choose the vector $|\psi_Q\rangle$ defined in Eq. (25), resulting in the (overcomplete) set of generalized coherent states $\{T_g|\psi_Q\rangle\}$. The identity operator in this Q sector is then given by[28]

$$\mathbb{1}_Q = C_Q \int_G \mathrm{d}g\, T_g|\psi_Q\rangle\langle\psi_Q|T_g^{-1}, \tag{28}$$

where $\mathrm{d}g$ is the invariant measure of $\mathrm{U}(N_b,N_b)$ and C_Q is a normalization factor defined by

$$C_Q^{-1} = \frac{1}{N_Q}\int_G \mathrm{d}g\langle\psi_Q|T_g|\psi_Q\rangle\langle\psi_Q|T_g^{-1}|\psi_Q\rangle. \tag{29}$$

Here, N_Q is the norm of $|\psi_Q\rangle$,

$$N_Q = \langle\psi_Q|\psi_Q\rangle = \prod_{n=0}^{N_c-1}\frac{(|Q|+n)!}{n!}. \tag{30}$$

A detailed calculation of N_Q is given in Appendix A.

Note that the integrals in Eqs. (28) and (29) are divergent for $2N_b > N_c$ as discussed in Sec. II. A regularization procedure is necessary to show that their ratio is finite, see, e.g., Appendix D 3. We return to this issue at the end of Sec. III F.

The operator in Eq. (28) annihilates all states that are not color neutral, as well as color-neutral states corresponding to a different value of Q. Thus, it is a projector onto the Q sector. We can therefore write the projector onto the color-neutral sector as

$$P = \bigoplus_Q \mathbb{1}_Q, \tag{31}$$

where the sum runs over the values of Q given in Eq. (24). Identifying this projection operator with the one in Eq. (20) yields

$$\mathcal{Z} = \sum_Q \mathcal{Z}_Q$$

with

$$\mathcal{Z}_Q = \langle\Psi|\mathbb{1}_Q|\Psi\rangle = \langle 0|\exp(\bar{\psi}^i_a c^i_a + \varphi^i_a d^i_a)\mathbb{1}_Q \exp(\bar{c}^i_a \psi^i_a + \bar{d}^i_a \bar{\varphi}^i_a)|0\rangle. \tag{32}$$

E. Parametrization of the coherent states

The maximal compact subgroup of the flavor group $G=\mathrm{U}(N_b,N_b)$ is $H=H_+\times H_-=\mathrm{U}(N_b)\times\mathrm{U}(N_b)$ with elements $h=\mathrm{diag}(h_+,h_-)$, where $h_\pm \in \mathrm{U}(N_b)$. The corresponding Fock operators are

$$T_h = \exp[\bar{c}^i_a (\ln h_+)_{ab} c^i_b - d^i_a (\ln h_-)_{ab} \bar{d}^i_b]. \tag{33}$$

For $Q=0$, these operators stabilize the vacuum,

$$T_h|0\rangle = \exp(-N_c \operatorname{tr} \ln h_-)|0\rangle = (\det{}^{-N_c} h_-)|0\rangle, \tag{34}$$

and therefore the set of coherent states for $Q=0$ can be parametrized without overcounting by the elements of the noncompact coset space $S=G/H=\mathrm{U}(N_b,N_b)/[\mathrm{U}(N_b)\times U(N_b)]$. (We will use the same coset space also for $Q\neq 0$, see Sec. III G.)

To arrive at this parametrization, we first use the canonical projection $\pi: G \mapsto G/H$ which assigns to each $g \in G$ the corresponding equivalence class gH. We then choose a representative group element $s(\pi(g))$ from each equivalence class and write an arbitrary group element g as the product $g=s(\pi(g))h(g)$. The coset element $s(\pi(g))$ can be parametrized using projective coordinates Z, see Eqs. (5.8n) and (5.28) in Chap. 9 of Ref. 29,

$$s(\pi(g)) \equiv s(Z,Z^\dagger) = \begin{pmatrix} (1-ZZ^\dagger)^{-1/2} & Z(1-Z^\dagger Z)^{-1/2} \\ Z^\dagger(1-ZZ^\dagger)^{-1/2} & (1-Z^\dagger Z)^{-1/2} \end{pmatrix} = \begin{pmatrix} 1 & Z \\ 0 & 1 \end{pmatrix} \begin{pmatrix} (1-ZZ^\dagger)^{1/2} & 0 \\ 0 & (1-Z^\dagger Z)^{-1/2} \end{pmatrix} \times \begin{pmatrix} 1 & 0 \\ Z^\dagger & 1 \end{pmatrix}. \tag{35}$$

Here, Z is an $N_b \times N_b$ complex matrix with the constraint $|ZZ^\dagger| \leqslant 1$. We have $s=s^\dagger$ and $s^{-1}=s(-Z,-Z^\dagger)$. Also, $s(Z,Z^\dagger)$ satisfies the pseudounitarity condition $s\,\mathrm{diag}(\mathbb{1}_{N_b},-\mathbb{1}_{N_b})s^\dagger=\mathrm{diag}(\mathbb{1}_{N_b},-\mathbb{1}_{N_b})$. Using the decomposition (35), the Fock space operator corresponding to $s(Z,Z^\dagger)$ becomes

$$T_{s(Z,Z^\dagger)} = \exp(\bar{c}^i_a Z_{ab} \bar{d}^i_b) \exp\left[\tfrac{1}{2}\bar{c}^i_a \ln(1-ZZ^\dagger)_{ab} c^i_b + \tfrac{1}{2} d^i_a \ln(1-Z^\dagger Z)_{ab} \bar{d}^i_b\right] \exp(-d^i_a Z^\dagger_{ab} c^i_b). \tag{36}$$

The coset space G/H has a G-invariant measure[17] that has already been given in Eq. (3). We can therefore use Eq. (14) to rewrite the integral (28) over G as an integral over H and $S=G/H$,

$$\mathbb{1}_Q = C_Q \int_G \mathrm{d}g\, T_g |\psi_Q\rangle\langle\psi_Q| T_g^{-1} = C_Q \int_{G/H} \mathrm{d}\mu(Z,Z^\dagger) \int_H \mathrm{d}h\, T_s T_h |\psi_Q\rangle\langle\psi_Q| T_h^{-1} T_s^{-1}. \tag{37}$$

The Haar measure $\mathrm{d}h$ of H is normalized to unity.

We pause briefly to explain the reason behind the choice of the coset-space parametrization (35).[1] In the language of lattice gauge theory, the left-hand side of Eq. (1) is a one-link integral with fields $\bar{\psi}$, φ at one end of the link and fields $\bar{\varphi}$, ψ at the other end (the notation is a bit misleading but in line with Refs. 1 and 7). Note that the gauge fields U and $U^\dagger$ couple bosonic fields that live on opposite ends of the link. On the right-hand side of Eq. (1), the matrices Z and $Z^\dagger$ couple bosonic fields that live on the same end of the link. This is a highly desirable feature since, when Eq. (1) is applied to a lattice with many links, the ensuing integral over the bosonic fields has a simpler structure. Other parametrizations of the coset space do not lead to this feature.

F. Calculation of $\mathcal{Z}_0$

For $Q=0$, Eq. (34) tells us that the integration over H in Eq. (37) is trivial, and we are left with

$$\mathcal{Z}_0 = C_0 \int_{G/H} \mathrm{d}\mu(Z,Z^\dagger) \langle 0|\exp(\bar{\psi}^i_a c^i_a + \varphi^i_a d^i_a) T_s|0\rangle\langle 0|T_s^{-1} \exp(\bar{c}^i_a \psi^i_a + \bar{d}^i_a \bar{\varphi}^i_a)|0\rangle. \tag{38}$$

Defining the notation $|Z\rangle = \exp(\bar{c}^i_a Z_{ab} \bar{d}^i_b)|0\rangle$ and $\langle Z| = \langle 0|\exp(d^i_a Z^\dagger_{ab} c^i_b)$, we find

$$T_s|0\rangle = \det{}^{N_c/2}(1-ZZ^\dagger)|Z\rangle \tag{39}$$

and

$$\langle 0|\exp(\bar{\psi}^i_a c^i_a + \varphi^i_a d^i_a)T_s|0\rangle\langle 0|T_s^{-1}\exp(\bar{c}^i_a\psi^i_a + \bar{d}^i_a\bar{\varphi}^i_a)|0\rangle = \det{}^{N_c}(1-ZZ^\dagger)\langle 0|\exp(\bar{\psi}^i_a c^i_a + \varphi^i_a d^i_a)|Z\rangle$$
$$\times\langle Z|\exp(\bar{c}^i_a\psi^i_a + \bar{d}^i_a\bar{\varphi}^i_a)|0\rangle = \det{}^{N_c}(1-ZZ^\dagger)\exp(\bar{\psi}^i_a Z_{ab}\varphi^i_b + \bar{\varphi}^i_a Z^\dagger_{ab}\psi^i_b). \tag{40}$$

Thus

$$\mathcal{Z}_0 = C_0\int_{|ZZ^\dagger|\leqslant 1} D(Z,Z^\dagger)\exp(\bar{\psi}^i_a Z_{ab}\varphi^i_b + \bar{\varphi}^i_a Z^\dagger_{ab}\psi^i_b) \tag{41}$$

with

$$D(Z,Z^\dagger) = \frac{\mathrm{d}Z\,\mathrm{d}Z^\dagger}{\det{}^{2N_b-N_c}(1-ZZ^\dagger)}. \tag{42}$$

Not surprisingly, this is the same result as in Ref. 2 for the color group $\mathrm{U}(N_c)$. From Eq. (29) we have

$$C_0^{-1} = \frac{1}{N_0}\int_G \mathrm{d}g\langle 0|T_g|0\rangle\langle 0|T_g^{-1}|0\rangle = \int_{|Z^\dagger Z|\leqslant 1} D(Z,Z^\dagger). \tag{43}$$

An explicit calculation of C_0 is given in Appendix B.

Note that for $2N_b > N_c$, $D(Z,Z^\dagger)$ becomes divergent at the boundary of the integration domain. This divergence is due to the noncompactness of the symmetric space $\mathrm{U}(N_b,N_b)/[\mathrm{U}(N_b)\times\mathrm{U}(N_b)]$ and is a feature of the bosonic color-flavor transformation. In Ref. 1, this divergence is canceled by the measure of the fermionic degrees of freedom, and the noncompact supersymmetric coset space has a flat measure if there is an equal number of bosons and fermions. In the fermionic case,[7] the integral on the RHS is over the compact symmetric space $\mathrm{U}(2N_f)/[\mathrm{U}(N_f)\times\mathrm{U}(N_f)]$, and there is no divergence problem.

Note also that for $2N_b > N_c$, there are divergences in both numerator and denominator of the above formula. Apart from $D(Z,Z^\dagger)$, the integrands are analytic on the entire coset space, therefore the divergences in numerator and denominator are of the same degree and the ratio must be finite. We will show this for a simple example in Appendix D 3. However, in the general case it is not obvious how to cancel the divergences, and even if it were possible, the resulting expressions might not be simple enough to be useful in applications. That is why in Sec. IV we will use another method to extend the range of N_b in which all terms in the transformation are finite.

G. Calculation of $\mathcal{Z}_Q$ for $Q \neq 0$

Let us start with the case of $Q > 0$; the case of $Q < 0$ follows analogously. Similar to Ref. 7, the idea is to relate the state $|\psi_Q\rangle$ to $|0\rangle$ by the action of the creation operators. Starting from the integrand of Eq. (32), we perform the following manipulations:

$$\begin{aligned}
&\langle 0|\exp(\bar{\psi}^i_a c^i_a + \varphi^i_a d^i_a)T_g|\psi_Q\rangle\langle\psi_Q|T_g^{-1}\exp(\bar{c}^i_a\psi^i_a + \bar{d}^i_a\bar{\varphi}^i_a)|0\rangle = \langle 0|\exp(\bar{\psi}^i_a c^i_a + \varphi^i_a d^i_a)\\
&\quad\times(\epsilon_{i_1\cdots i_{N_c}}T_g\bar{c}^{i_1}_1 T_g^{-1}T_g\bar{c}^{i_2}_2 T_g^{-1}\cdots T_g\bar{c}^{i_{N_c}}_{N_c}T_g^{-1})^Q T_g|0\rangle\\
&\quad\times\langle 0|T_g^{-1}(\epsilon_{i_1\cdots i_{N_c}}T_g c^{i_1}_1 T_g^{-1}T_g c^{i_2}_2 T_g^{-1}\cdots T_g c^{i_{N_c}}_{N_c}T_g^{-1})^Q\exp(\bar{c}^i_a\psi^i_a + \bar{d}^i_a\bar{\varphi}^i_a)|0\rangle\\
&= \det{}^{N_c}(1-ZZ^\dagger)\exp(\bar{\psi}^i_a Z_{ab}\varphi^i_b + \bar{\varphi}^i_a Z^\dagger_{ab}\psi^i_b)\\
&\quad\times[(\epsilon_{i_1\cdots i_{N_c}}\hat{\bar{\psi}}^{i_1}_{a^1_1}\cdots\hat{\bar{\psi}}^{i_{N_c}}_{a^1_{N_c}})\cdots(\epsilon_{j_1\cdots j_{N_c}}\hat{\bar{\psi}}^{j_1}_{a^Q_1}\cdots\hat{\bar{\psi}}^{j_{N_c}}_{a^Q_{N_c}})]\Gamma^{(a^1_1\cdots a^1_{N_c})\cdots(a^Q_1\cdots a^Q_{N_c})}_{(1\cdots N_c)\cdots(1\cdots N_c)}\\
&\quad\times[(\epsilon_{i'_1\cdots i'_{N_c}}\hat{\psi}^{i'_1}_{b^1_1}\cdots\hat{\psi}^{i'_{N_c}}_{b^1_{N_c}})\cdots(\epsilon_{j'_1\cdots j'_{N_c}}\hat{\psi}^{j'_1}_{b^Q_1}\cdots\hat{\psi}^{j'_{N_c}}_{b^Q_{N_c}})]\bar{\Gamma}^{(b^1_1\cdots b^1_{N_c})\cdots(b^Q_1\cdots b^Q_{N_c})}_{(1\cdots N_c)\cdots(1\cdots N_c)}.
\end{aligned} \tag{44}$$

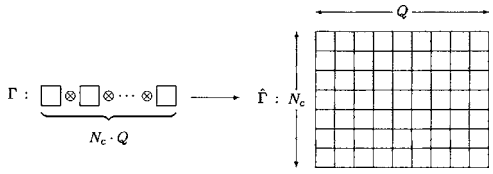

FIG. 1. The (reducible) product of fundamental representations of $\mathrm{U}(N_b)$ contains an irreducible representation of $\mathrm{U}(N_b)$ with symmetric color indices and antisymmetric flavor indices. Here $Q>0$.

In the first step, we have used Eq. (25) and inserted $T_g^{-1}T_g$ between each pair of creation and annihilation operators. In the second step, which involves a tedious but straightforward calculation, we have used the transformation properties of the Fock space operators given in Eq. (16), the Baker-Campbell-Hausdorff formula, and the coset decomposition of the group elements, $g=s(Z,Z^\dagger)h(g)$. We have also defined

$$\hat{\bar{\psi}}^i_a=\bar{\psi}^i_b(1-ZZ^\dagger)^{1/2}_{ba},\quad \hat{\psi}^i_a=(1-ZZ^\dagger)^{1/2}_{ab}\psi^i_b \tag{45}$$

and

$$\Gamma^{(a_1^1\cdots a_{N_c}^1)\cdots(a_1^Q\cdots a_{N_c}^Q)}_{(b_1^1\cdots b_{N_c}^1)\cdots(b_1^Q\cdots b_{N_c}^Q)}=(h_{+a_1^1b_1^1}\cdots h_{+a_{N_c}^1b_{N_c}^1})\cdots(h_{+a_1^Qb_1^Q}\cdots h_{+a_{N_c}^Qb_{N_c}^Q}). \tag{46}$$

The hypermatrix Γ represents the direct product of $N_c\cdot Q$ fundamental representations of $H_+=\mathrm{U}(N_b)$, see Fig. 1. Note that H_- does not appear here. Inserting Eq. (44) into Eq. (32), we obtain

$$\begin{aligned}\mathcal{Z}_Q=C_Q\int_{G/H}\mathrm{d}\mu(Z,Z^\dagger)\int_H\mathrm{d}h\langle 0|\exp(\bar{\psi}^i_ac^i_a+\varphi^i_ad^i_a)T_{s(Z,Z^\dagger)}T_h|\psi_Q\rangle\langle\psi_Q|T_h^{-1}T^{-1}_{s(Z,Z^\dagger)}\\ \times\exp(\bar{c}^i_a\psi^i_a+\bar{d}^i_a\bar{\varphi}^i_a)|0\rangle=\int_{|ZZ^\dagger|\leqslant 1}D(Z,Z^\dagger)\exp(\bar{\psi}^i_aZ_{ab}\varphi^i_b+\bar{\varphi}^i_aZ^\dagger_{ab}\psi^i_b)\chi_Q,\end{aligned} \tag{47}$$

where we have defined

$$\begin{aligned}\chi_Q=C_Q\{(\epsilon_{i_1\cdots i_{N_c}}\hat{\bar{\psi}}^i_{a_1^1}\cdots\hat{\bar{\psi}}^{i_{N_c}}_{a_{N_c}^1})\cdots(\epsilon_{j_1\cdots j_{N_c}}\hat{\bar{\psi}}^{j_1}_{a_1^Q}\cdots\hat{\bar{\psi}}^{j_{N_c}}_{a_{N_c}^Q})\}\\ \times\{(\epsilon_{i'_1\cdots i'_{N_c}}\hat{\psi}^{i'_1}_{b_1^1}\cdots\hat{\psi}^{i'_{N_c}}_{b_{N_c}^1})\cdots(\epsilon_{j'_1\cdots j'_{N_c}}\hat{\psi}^{j'_1}_{b_1^Q}\cdots\hat{\psi}^{j'_{N_c}}_{b_{N_c}^Q})\}\\ \times\int_{\mathrm{U}(N_b)}\mathrm{d}h_+[\Gamma^{(a_1^1\cdots a_{N_c}^1)\cdots(a_1^Q\cdots a_{N_c}^Q)}_{(1\cdots N_c)\cdots(1\cdots N_c)}\bar{\Gamma}^{(b_1^1\cdots b_{N_c}^1)\cdots(b_1^Q\cdots b_{N_c}^Q)}_{(1\cdots N_c)\cdots(1\cdots N_c)}].\end{aligned} \tag{48}$$

It follows from the definition of Γ that the term in square brackets is totally symmetric under the exchange of a^i_a with $a^{i'}_a$ and of b^i_a with $b^{i'}_a$. Because of the contraction with the totally antisymmetric tensor ϵ, the terms in curly brackets are totally antisymmetric under the exchange of a^i_a with $a^i_{a'}$ and of b^i_a with $b^i_{a'}$. Therefore, after the contractions of the a^i_a's and b^i_a's, only terms with the correct symmetry properties survive, i.e., symmetric in color and antisymmetric in flavor. In other words, when the (reducible) direct-product representation Γ is decomposed into irreducible representations, only the irreducible representation $\hat{\Gamma}$ shown in Fig. 1 contributes to χ_Q.

This observation enables us to perform the integration over H_+ in the same way as in Ref. 7. We use the group theoretic result that for irreducible unitary representations Γ^r and $\Gamma^{r'}$ of a compact Lie group G,

$$\int_G \mathrm{d}g\, \bar{\Gamma}^r_{ab}\Gamma^{r'}_{a'b'} = \frac{1}{d_r}\delta_{aa'}\delta_{bb'}\delta^{rr'}\int_G \mathrm{d}g, \tag{49}$$

where d_r is the dimension of Γ^r. The group volume of $\mathrm{U}(N_b)$ is normalized to unity as mentioned above.

Comparing Eq. (48) with Eq. (41) of Ref. 7, we realize that we can use (a slightly modified version of) the result in Eq. (46) of that reference and thus obtain

$$\chi_Q = \frac{(N_c!)^Q}{d^{N_b}_{N_c,Q}(Q!)^{N_c}} C_Q \det{}^Q \mathcal{M}, \tag{50}$$

where we have defined the $N_c \times N_c$ matrix $\mathcal{M}$ by $\mathcal{M}^{ij} = \bar{\psi}^i_a(1-ZZ^\dagger)_{ab}\psi^j_b$. The symbol $d^{N_b}_{N_c,Q}$ denotes the dimension of the irreducible representation of $\mathrm{U}(N_b)$ specified by a Young diagram with N_c rows and Q columns, i.e., of the representation $\hat{\Gamma}$ in Fig. 1. (For $N_b \leqslant N_c$, this dimension is equal to 1.) We will see in a moment that the prefactor of $C_Q \det{}^Q \mathcal{M}$ in Eq. (50) is in fact irrelevant.

We now use Eq. (29) to calculate the normalization factor C_Q. Using similar methods as in the calculation of χ_Q, we obtain

$$\begin{aligned}
\langle\psi_Q|T_g|\psi_Q\rangle &= \det{}^{N_c/2}(1-ZZ^\dagger)\langle\psi_Q|\{(\epsilon_{i_1\cdots i_{N_c}}\bar{c}^{\,i_1}_{c^1_1}\cdots\bar{c}^{\,i_{N_c}}_{c^1_{N_c}})\cdots(\epsilon_{j_1\cdots j_{N_c}}\bar{c}^{\,j_1}_{c^Q_1}\cdots\bar{c}^{\,j_{N_c}}_{c^Q_{N_c}})\}|0\rangle \\
&\quad\times[(1-ZZ^\dagger)^{1/2}_{c^1_1 a^1_1}\cdots(1-ZZ^\dagger)^{1/2}_{c^1_{N_c}a^1_{N_c}}]\cdots[(1-ZZ^\dagger)^{1/2}_{c^Q_1 a^Q_1}\cdots(1-ZZ^\dagger)^{1/2}_{c^Q_{N_c}a^Q_{N_c}}] \\
&\quad\times[h_{+_{a^1_1 1}}\cdots h_{+_{a^1_{N_c}N_c}}]\cdots[h_{+_{a^Q_1 1}}\cdots h_{+_{a^Q_{N_c}N_c}}] = N_Q \det{}^{N_c/2}(1-ZZ^\dagger)\Gamma^{(a^1_1\cdots a^1_{N_c})\cdots(a^Q_1\cdots a^Q_{N_c})}_{(1\cdots N_c)\cdots(1\cdots N_c)} \\
&\quad\times\sum_{\sigma_1\cdots\sigma_Q}[\mathrm{sgn}(\sigma_1)(1-ZZ^\dagger)^{1/2}_{\sigma_1(1)a^1_1}\cdots(1-ZZ^\dagger)^{1/2}_{\sigma_1(N_c)a^1_{N_c}}] \\
&\quad\times\cdots[\mathrm{sgn}(\sigma_Q)(1-ZZ^\dagger)^{1/2}_{\sigma_Q(1)a^Q_1}\cdots(1-ZZ^\dagger)^{1/2}_{\sigma_Q(N_c)a^Q_{N_c}}],
\end{aligned} \tag{51}$$

where we have used $N_Q = \langle\psi_Q|\psi_Q\rangle$. The symbol σ and the symbol ρ in the equation below denote elements of the permutation group S_{N_c}. Analogously, we find

$$\begin{aligned}
\langle\psi_Q|T_g^{-1}|\psi_Q\rangle &= N_Q \det{}^{N_c/2}(1-ZZ^\dagger)\bar{\Gamma}^{(b^1_1\cdots b^1_{N_c})\cdots(b^Q_1\cdots b^Q_{N_c})}_{(1\cdots N_c)\cdots(1\cdots N_c)}\sum_{\rho_1\cdots\rho_Q}[\mathrm{sgn}(\rho_1)(1-ZZ^\dagger)^{1/2}_{b^1_1\rho_1(1)} \\
&\quad\times\cdots(1-ZZ^\dagger)^{1/2}_{b^1_{N_c}\rho_1(N_c)}]\cdots[\mathrm{sgn}(\rho_Q)(1-ZZ^\dagger)^{1/2}_{b^Q_1\rho_Q(1)}\cdots(1-ZZ^\dagger)^{1/2}_{b^Q_{N_c}\rho_Q(N_c)}].
\end{aligned} \tag{52}$$

Combining these two results, we have from Eq. (29),

$$\begin{aligned}
C_Q^{-1} &= \frac{1}{N_Q}\int_{\mathrm{U}(N_b,N_b)}\mathrm{d}g\langle\psi_Q|T_g|\psi_Q\rangle\langle\psi_Q|T_g^{-1}|\psi_Q\rangle = N_Q\int_{|ZZ^\dagger|\leqslant 1}\mathrm{d}\mu(Z,Z^\dagger)\det{}^{N_c}(1-ZZ^\dagger) \\
&\quad\times\sum_{\sigma_1\cdots\sigma_Q}[\mathrm{sgn}(\sigma_1)(1-ZZ^\dagger)^{1/2}_{\sigma_1(1)a^1_1}\cdots(1-ZZ^\dagger)^{1/2}_{\sigma_1(N_c)a^1_{N_c}}]\cdots[\mathrm{sgn}(\sigma_Q)(1-ZZ^\dagger)^{1/2}_{\sigma_Q(1)a^Q_1} \\
&\quad\times\cdots(1-ZZ^\dagger)^{1/2}_{\sigma_Q(N_c)a^Q_{N_c}}]\sum_{\rho_1\cdots\rho_Q}[\mathrm{sgn}(\rho_1)(1-ZZ^\dagger)^{1/2}_{b^1_1\rho_1(1)}\cdots(1-ZZ^\dagger)^{1/2}_{b^1_{N_c}\rho_1(N_c)}] \\
&\quad\times\cdots[\mathrm{sgn}(\rho_Q)(1-ZZ^\dagger)^{1/2}_{b^Q_1\rho_Q(1)}\cdots(1-ZZ^\dagger)^{1/2}_{b^Q_{N_c}\rho_Q(N_c)}] \\
&\quad\times\int_{\mathrm{U}(N_b)}\mathrm{d}h_+\Gamma^{(a^1_1\cdots a^1_{N_c})\cdots(a^Q_1\cdots a^Q_{N_c})}_{(1\cdots N_c)\cdots(1\cdots N_c)}\bar{\Gamma}^{(b^1_1\cdots b^1_{N_c})\cdots(b^Q_1\cdots b^Q_{N_c})}_{(1\cdots N_c)\cdots(1\cdots N_c)}.
\end{aligned} \tag{53}$$

The integration over $\mathrm{U}(N_b)$ is of the same type as in the calculation of χ_Q, and using the same method we obtain

$$C_Q^{-1} = \frac{N_Q (N_c!)^Q}{d_{N_c,Q}^{N_b} (Q!)^{N_c}} \int_{|ZZ^\dagger| \leqslant 1} D(Z,Z^\dagger) \det{}^Q (1 - ZZ^\dagger)_{[N_c]}, \tag{54}$$

where $(1-ZZ^\dagger)_{[N_c]}$ denotes the upper left $N_c \times N_c$ block of the $N_b \times N_b$ matrix $(1-ZZ^\dagger)$. Recall that nonzero Q sectors only exist for $N_b \geqslant N_c$, so this notation always makes sense.

We now combine Eqs. (47), (50), and (54) to obtain for $Q>0$,

$$\mathcal{Z}_Q = \mathcal{C}_Q \int_{|ZZ^\dagger| \leqslant 1} D(Z,Z^\dagger) \exp(\bar{\psi}_a^i Z_{ab} \varphi_b^i + \bar{\varphi}_a^i Z_{ab}^\dagger \psi_b^i) \det{}^Q \mathcal{M}, \tag{55}$$

where we have defined

$$\mathcal{C}_Q^{-1} = N_Q \int_{|ZZ^\dagger| \leqslant 1} D(Z,Z^\dagger) \det{}^Q (1 - ZZ^\dagger)_{[N_c]}. \tag{56}$$

The explicit calculation of this integral is performed in Appendix B. As anticipated, the nontrivial prefactors in Eqs. (50) and (54) have dropped out.

For $Q<0$, the calculation proceeds in exact analogy, and we obtain

$$\mathcal{Z}_Q = \mathcal{C}_{|Q|} \int_{|ZZ^\dagger| \leqslant 1} D(Z,Z^\dagger) \exp(\bar{\psi}_a^i Z_{ab} \varphi_b^i + \bar{\varphi}_a^i Z_{ab}^\dagger \psi_b^i) \det{}^{|Q|} \mathcal{N}, \tag{57}$$

where the $N_c \times N_c$ matrix $\mathcal{N}$ is defined by $\mathcal{N}^{ij} = \bar{\varphi}_a^i (1 - Z^\dagger Z)_{ab} \varphi_b^j$. This completes the derivation of Eq. (1).

A number of concrete examples illustrating the transformation are given in Appendix D 1. In particular, in Appendix D 3 we consider an example where the integration measure diverges, and show how this problem can be solved in a simple case.

H. Generalization to unequal flavor numbers

So far we only considered the case in which particles and antiparticles have equal flavor numbers, i.e., $N_{b+}=N_{b-}=N_b$, where N_{b+} (N_{b-}) denotes the number of flavors of the particles (antiparticles). In practice this constraint may not be present. It is not difficult to see how our method can be extended to the general case in which $N_{b+} \neq N_{b-}$. The flavor group is then $\mathrm{U}(N_{b+},N_{b-})$, and the integral on the RHS of Eq. (1) is over the noncompact symmetric space $\mathrm{U}(N_{b+},N_{b-})/[\mathrm{U}(N_{b+}) \times \mathrm{U}(N_{b-})]$. All results derived in earlier parts of this section are still valid with some minor changes, (1) the complex matrix Z has dimension $N_{b+} \times N_{b-}$, (2) replace $2N_b$ by $N_{b+}+N_{b-}$ in the integration measure, and (3) choose the range of Q accordingly. For example, if $N_{b-} < N_c$ and $N_{b+} \geqslant N_c$, there are no Q_- sectors, and we sum over $Q \geqslant 0$ and set $\mathcal{N}=0$ in our results. We give a concrete example with $N_{b+} \neq N_{b-}$ in Appendix D 2.

IV. BOSONIC COLOR-FLAVOR TRANSFORMATION: CHARACTER EXPANSION METHOD

In this section, we use the character expansion method[19] to derive an alternative form of the bosonic color-flavor transformation which is free from divergences in the range $N_b \leqslant N_c$. We will also make use of the results of Refs. 20 and 21.

A. Setup of the calculation

In the last section, we have traded the integral over the compact color group for an integral over a noncompact manifold parametrized by an $N_b \times N_b$ complex matrix Z. Employing a singular value decomposition, this matrix can be written as

$$Z = U\Lambda V, \tag{58}$$

where $U \in \mathrm{U}(N_b)$, $V \in \mathrm{U}(N_b)/\mathrm{U}^{N_b}(1)$, and Λ is a diagonal matrix with real entries, the so-called radial coordinates, satisfying $0 \leqslant \Lambda_a \leqslant 1$. The divergence problem we met in the last section is caused by the integration over the submanifold spanned by the radial coordinates. Specifically, the divergence of highest degree occurs at the boundary, $\Lambda_a = 1$ for all a, and the entire information that is needed to complete the color-flavor transformation resides in the boundary. A natural question to ask at this point is whether the integration over the radial coordinates can be avoided. To answer this question, we integrate over the two compact unitary groups first. At the same time, we relax the constraints on the radial coordinates by replacing Λ with an arbitrary complex matrix.

Our strategy is as follows. We first perform the integration over the color group on the LHS of the transformation explicitly using the character expansion method. Next we compute an integral over a compact subgroup of the flavor group with a manifestly color-invariant integrand. We then complete the transformation by observing that the two integrals are equal.

We define two rectangular $N_c \times N_b$ matrices Ψ and Φ by

$$\Psi = (\psi_a^i), \quad \Phi = (\varphi_a^i). \tag{59}$$

The integrand on the LHS of Eq. (1) can then be rewritten as

$$\exp(\bar{\psi}_a^i U^{ij} \psi_a^j + \bar{\varphi}_a^i U^{\dagger ij} \varphi_a^j) = \exp(\mathrm{tr}\, UM + \mathrm{tr}\, U^\dagger N), \tag{60}$$

where we have defined two $N_c \times N_c$ matrices M and N by

$$M = (M^{ij}) = (\psi_a^i \bar{\psi}_a^j) = \Psi\Psi^\dagger, \quad N = (N^{ij}) = (\varphi_a^i \bar{\varphi}_a^j) = \Phi\Phi^\dagger. \tag{61}$$

In the following, we consider irreducible representations of $\mathrm{GL}(m)$ (for various values of m) labeled by

$$r = (r_1, r_2, \ldots, r_m) \quad \text{with integers} \quad r_1 \geqslant r_2 \geqslant \cdots \geqslant r_m \geqslant 0, \tag{62}$$

where r_j is the number of boxes in row j of the corresponding Young diagram. Using Eq. (3.5) of Ref. 20, we have

$$\exp(\mathrm{tr}\, UM) = \sum_r \alpha_r^{(0)} \chi_r(UM), \quad \exp(\mathrm{tr}\, U^\dagger N) = \sum_{r'} \alpha_{r'}^{(0)} \chi_{r'}(U^\dagger N), \tag{63}$$

where the sums are over all irreducible representations of $\mathrm{GL}(N_c)$ of the form (62). For a given representation r, we have[20]

$$\alpha_r^{(\nu)} = \det\left[\frac{1}{(r_j - \nu + i - j)!}\right] = \left[\prod_{i=1}^{N_c} \frac{(N_c - i)!}{(k_i - \nu)!}\right] d_r \quad \text{with } k_i = N_c + r_i - i, \tag{64}$$

where i and j run from 1 to N_c, ν is an additional integer which we shall need later on, d_r is the dimension of the representation r, given by Weyl's formula

$$d_r = \left[\prod_{n=1}^{N_c - 1} n!\right]^{-1} \Delta(k_1, \ldots, k_{N_c}), \tag{65}$$

and $\Delta(k_1, \ldots, k_{N_c}) = \prod_{i<j}(k_i - k_j)$ is the Vandermonde determinant. We then obtain

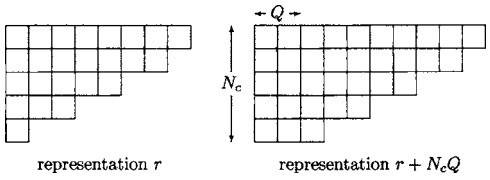

FIG. 2. Irreducible representations r and $r+N_cQ$.

$$\int_{\mathrm{SU}(N_c)} \mathrm{d}U \exp(\mathrm{tr}\, UM + \mathrm{tr}\, U^\dagger N) = \sum_{rr'} \alpha_r^{(0)} \alpha_{r'}^{(0)} \int_{\mathrm{SU}(N_c)} \mathrm{d}U\, \chi_r(UM)\chi_{r'}(U^\dagger N)$$
$$= \sum_{rr'} \alpha_r^{(0)} \alpha_{r'}^{(0)} \int_{\mathrm{SU}(N_c)} \mathrm{d}U\, U_r^{ij} M_r^{ji} \bar{U}_{r'}^{kl} N_{r'}^{kl}, \tag{66}$$

where we use the notation U_r for the matrix corresponding to the representation r specified by a given Young diagram, an example of which is shown on the left-hand part of Fig. 2. On the right-hand part of Fig. 2, we show a Young diagram that has Q more columns, each containing N_c boxes, than the Young diagram for r. (Here we assume $Q \geqslant 0$.) We denote the corresponding representation by $r+N_cQ$. Note that for $\mathrm{SU}(N_c)$, these two representations are identical. We have the orthogonality relation

$$\int_{\mathrm{SU}(N_c)} \mathrm{d}U\, U_r^{ij} \bar{U}_{r'}^{kl} = \frac{1}{d_r} \delta^{ik} \delta^{jl} \delta_{r',r+N_cQ}. \tag{67}$$

From Eq. (64) it is clear that

$$\alpha_{r+N_cQ}^{(0)} = \alpha_r^{(-Q)}. \tag{68}$$

Furthermore, for all $g \in \mathrm{GL}(N_c)$ we have[30]

$$g_{r+N_cQ}^{ij} = g_r^{ij} \det{}^Q g. \tag{69}$$

Rewriting the sum over r and r' in Eq. (66) as a sum over r and Q, we obtain

$$\int_{\mathrm{SU}(N_c)} \mathrm{d}U \exp(\bar{\psi}_a^i U^{ij} \psi_a^j + \bar{\varphi}_a^i U^{\dagger ij} \varphi_a^j) = \sum_r \frac{\alpha_r^{(0)} \alpha_r^{(0)}}{d_r} \chi_r(MN) + \sum_{Q=1}^{\infty} (\det{}^Q M$$
$$+ \det{}^Q N) \sum_r \frac{\alpha_r^{(0)} \alpha_r^{(-Q)}}{d_r} \chi_r(MN). \tag{70}$$

The sums over r can be done analytically, resulting in an expression involving determinants of modified Bessel functions,[21] but we shall not need this explicit result and therefore do not quote it here.

Note that in the case of color group $\mathrm{U}(N_c)$ only the $Q=0$ term is nonzero in Eq. (67), and therefore only the first term contributes on the RHS of Eq. (70). This observation will allow us to read off results for $\mathrm{U}(N_c)$ from those for $\mathrm{SU}(N_c)$ in Secs. IV B and IV C.

We now turn to the RHS of Eq. (1) and first define two $N_b \times N_b$ matrices

$$B = (B_{ab}) = (\varphi_a^i \bar{\psi}_b^i) = [\Psi^\dagger \Phi]^T, \quad C = (C_{ab}) = (\psi_a^i \bar{\varphi}_b^i) = [\Phi^\dagger \Psi]^T. \tag{71}$$

We then consider the integral

$$\int_{U(N_b)} dU \int_{U(N_b)} dV \det{}^{-Q}(UAVB)\exp[\bar{\psi}^i_a (UAV)_{ab}\varphi^i_b + \bar{\varphi}^i_a (V^\dagger D U^\dagger)_{ab}\psi^i_b]$$

$$= \int_{U(N_b)} dU \int_{U(N_b)} dV \det{}^{-Q}(UAVB)\exp[\mathrm{tr}(UAVB) + \mathrm{tr}(CV^\dagger D U^\dagger)], \tag{72}$$

where A and D are two arbitrary $N_b \times N_b$ matrices. Using Ref. 21, we have for $AD=I$, i.e., A is the inverse of D,

$$(72) = \sum_s \frac{\alpha_s^{(0)}\alpha_s^{(-Q)}}{d_s^2}\chi_s(AD)\chi_s(BC) = \sum_s \frac{\alpha_s^{(0)}\alpha_s^{(-Q)}}{d_s}\chi_s(BC), \tag{73}$$

where the sum is over all irreducible representations s of $\mathrm{GL}(N_b)$ of the form (62), and we have used $d_s=\chi_s(I)$.

In Appendix C we prove the following identity for $\delta=N_c-N_b\geqslant 0$,

$$\sum_r \frac{\alpha_r^{(0)}\alpha_r^{(-Q)}}{d_r}\chi_r(MN) = \prod_{n=0}^{\delta-1}\frac{(N_b+n)!}{(Q+n)!}\sum_s \frac{\alpha_s^{(0)}\alpha_s^{(-Q-\delta)}}{d_s}\chi_s(BC), \tag{74}$$

where the sums on the LHS and the RHS are over all irreducible representations of $\mathrm{GL}(N_c)$ and $\mathrm{GL}(N_b)$, respectively, that are of the form (62). Using this identity, we can now relate Eqs. (70) and (73). We consider separately the cases $N_b<N_c$, $N_b=N_c$, and $N_b>N_c$.

B. $N_b<N_c$

For $N_b<N_c$, the matrices M and N are not of full rank, i.e., we have $\det M=\det N=0$. The terms multiplied by $\det M$ and $\det N$ in Eq. (70) are finite.[21] Thus, only the $Q=0$ term in Eq. (70) survives, and we obtain

$$(70) = \sum_r \frac{\alpha_r^{(0)}\alpha_r^{(0)}}{d_r}\chi_r(MN) = \prod_{n=0}^{\delta-1}\frac{(N_b+n)!}{n!}\sum_s \frac{\alpha_s^{(0)}\alpha_s^{(-\delta)}}{d_s}\chi_s(BC), \tag{75}$$

where we have used Eq. (74). This is already in the form of Eq. (73) with $Q=\delta=N_c-N_b$. We can further simplify the integral in Eq. (72) by choosing $A=D=I$ and using the invariance of the Haar measure to eliminate U from the integrand. This yields

$$\int_{\mathrm{SU}(N_c)} dU \exp(\bar{\psi}^i_a U^{ij}\psi^j_a + \bar{\varphi}^i_a U^{\dagger ij}\varphi^j_a) = \prod_{n=0}^{N_c-N_b-1}\frac{(N_b+n)!}{n!}\int_{U(N_b)} dV \det{}^{N_b-N_c}(VB)$$
$$\times\exp(\bar{\psi}^i_a V_{ab}\varphi^i_b + \bar{\varphi}^i_a V^\dagger_{ab}\psi^i_b) \tag{5}$$

as stated in Sec. II. If in the above expression one wants to take the limit of $\det B\to 0$, the integral over V needs to be done first. This procedure yields a finite result, see the example in Appendix E 3.

The result (5) is also valid if the integration on the LHS is over the color group $\mathrm{U}(N_c)$. This follows immediately from the remarks made after Eq. (70) and from the fact that the terms with $Q>0$ do not contribute on the RHS of Eq. (70).

C. $N_b=N_c$

For $N_b=N_c$ the matrices M and N are of full rank, and all terms in Eq. (70) contribute. Equation (74) now becomes trivial,

$$\sum_r \frac{\alpha_r^{(0)}\alpha_r^{(-Q)}}{d_r}\chi_r(MN) = \sum_s \frac{\alpha_s^{(0)}\alpha_s^{(-Q)}}{d_s}\chi_s(BC). \tag{76}$$

We again simplify the integral in Eq. (72) by choosing $A=D=I$ and using the invariance of the Haar measure to arrive at

$$\int_{\mathrm{SU}(N_c)} \mathrm{d}U \exp(\bar{\psi}_a^i U^{ij}\psi_a^j + \bar{\varphi}_a^i U^{\dagger ij}\varphi_a^j) = \sum_{Q=0}^{\infty} \tilde{\chi}_Q \int_{U(N_b)} \mathrm{d}V \det{}^{-Q}(VB)\exp(\bar{\psi}_a^i V_{ab}\varphi_b^i + \bar{\varphi}_a^i V_{ab}^\dagger \psi_b^i) \tag{6}$$

with $\tilde{\chi}_0=1$ and $\tilde{\chi}_{Q>0}=\det{}^Q M+\det{}^Q N$ as stated in Sec. II. If the $\det B\to 0$ limit is desired, the integral over V needs to be done first as mentioned at the end of the preceding section. If $\det{}^{-Q}(VB)$ is combined with the terms in $\tilde{\chi}_{Q>0}$, we obtain $\beta^Q+1/\bar{\beta}^Q$ with $\beta=\det\Psi/\det(\Phi V)$. This shows that we are not allowed to change the order of summation and integration in Eq. (6), since the resulting geometric series would diverge for one of the two terms.

If the integration on the LHS of Eq. (6) is over the color group $\mathrm{U}(N_c)$, only the $Q=0$ term contributes on the RHS as explained after Eq. (70), and we obtain for $N_b=N_c$,

$$\int_{U(N_c)} \mathrm{d}U \exp(\bar{\psi}_a^i U^{ij}\psi_a^j + \bar{\varphi}_a^i U^{\dagger ij}\varphi_a^j) = \int_{U(N_b)} \mathrm{d}V \exp(\bar{\psi}_a^i V_{ab}\varphi_b^i + \bar{\varphi}_a^i V_{ab}^\dagger \psi_b^i), \tag{77}$$

see also Sec. 6 of Ref. 16.

D. $N_b>N_c$

In this case the $N_c\times N_c$ matrices M and N are of full rank, whereas the $N_b\times N_b$ matrices B and C are of rank N_c with N_b-N_c eigenvalues equal to zero so that $\det B=\det C=0$. We now have $\delta=N_c-N_b<0$. Using similar arguments as in Appendix C but in the reverse direction, we obtain instead of Eq. (74),

$$\begin{aligned}\sum_r \frac{\alpha_r^{(0)}\alpha_r^{(-Q)}}{d_r}\chi_r(MN) &= C_{|\delta|}\sum_s \frac{\alpha_s^{(0)}\alpha_s^{(|\delta|-Q)}}{d_s}\chi_s(BC)\\ &= C_{|\delta|}\int_{U(N_b)} \mathrm{d}U \int_{U(N_b)} \mathrm{d}V \det{}^{|\delta|-Q}(UAVB)\exp[\mathrm{tr}(UAVB)+\mathrm{tr}(CV^\dagger DU^\dagger)]\\ &= C_{|\delta|}\int_{U(N_b)} \mathrm{d}V \det{}^{|\delta|-Q}(VB)\exp[\mathrm{tr}(VB)+\mathrm{tr}(CV^\dagger)]\end{aligned} \tag{78}$$

with

$$C_{|\delta|} = \prod_{n=1}^{|\delta|}\frac{(Q-n)!}{(N_b-n)!}, \tag{79}$$

where in the last step in Eq. (78) we have again set $A=D=I$ and used the invariance of the Haar measure to eliminate U from the integrand. Note that this expression is only valid for $Q\geqslant|\delta|=N_b-N_c$. Although $\det B=0$ appears with a nonpositive power, the RHS of Eq. (78) must be finite because the LHS is. This fact can be established explicitly by a suitable limiting procedure.

For $0\leqslant Q<|\delta|$, the integral over $\mathrm{U}(N_b)$ in Eq. (78) is zero because $\det B=0$ appears with a positive power. For this range of Q, we cannot replace the corresponding terms in Eq. (70) by integrals over $\mathrm{U}(N_b)$ and therefore cannot complete the transformation. Thus, it seems that the character expansion method does not yield a useful result for $N_b>N_c$.

V. CONCLUSIONS AND OUTLOOK

We have generalized Zirnbauer's color-flavor transformation in the bosonic sector to the special unitary group $\mathrm{SU}(N_c)$. Because the flavor group $\mathrm{U}(N_b,N_b)$ is noncompact, divergences arise if the number of bosonic flavors is too large. This has already been noted in Refs. 2 and 16 where the gauge group was $\mathrm{U}(N_c)$ and results were given for $2N_b \leqslant N_c$. We have found a "standard" result for the color-flavor transformation in the same range, and an alternative form of the transformation in the extended range $N_b \leqslant N_c$. [A special case of this result for $N_b=N_c$ and color group $\mathrm{U}(N_c)$ has already been given in Ref. 16.] For $N_b<N_c$, the results for $\mathrm{SU}(N_c)$ are identical to those for $\mathrm{U}(N_c)$ because only the sector with $Q=0$ contributes.

The results of the present paper can be applied to study a boson-induced $\mathrm{SU}(N_c)$ lattice gauge theory analogous to the $\mathrm{U}(N_c)$ gauge theory discussed in Ref. 16. We hope that other applications will arise, e.g., in the field of disordered and/or chaotic systems.

One obvious open problem is to obtain a manifestly convergent result for $N_b>N_c$. While the divergences that appear in numerator and denominator of our formal result (1) can always be canceled in special cases, see Appendix D 3, the general case is difficult to deal with. The character expansion method, which led to a convergent result in the extended range $N_b \leqslant N_c$, fails for $N_b>N_c$ since it cannot generate the terms with $0 \leqslant Q<N_b-N_c$ on the RHS of Eq. (70) in terms of integrals over (a subgroup of) the flavor group. However, as stated earlier and in Ref. 16, all necessary information resides in the boundary of the coset space $\mathrm{U}(N_b,N_b)/[\mathrm{U}(N_b)\times\mathrm{U}(N_b)]$, so it is conceivable that an explicit result in terms of an integration over this boundary might yet be obtained.

The other open problem is the extension of the present results to the supersymmetric case in which both fermionic and bosonic flavors are present. In this case the divergence of the integration measure due to the bosonic degrees of freedom can be canceled by the contribution of the fermions to the measure, as long as sufficiently many fermions are included. The physically interesting case is $N_c=3$ (the gauge group of QCD), $N_f \geqslant 2$ (the number of physical quark flavors), and $N_b=N_c$ (the lower bound for N_b so that the bosons induce the correct gauge action[16]). In this case, the convergence requirement $2(N_b-N_f) \leqslant N_c$ is satisfied. However, the supersymmetric case raises other issues which will be addressed in a separate paper.

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APPENDIX A: NORMALIZATION OF GENERALIZED SLATER STATES

In this section, we calculate the norm, $N_Q=\langle\psi_Q|\psi_Q\rangle$, of the state $|\psi_Q\rangle$ defined in Eq. (25). We first assume $Q \geqslant 0$ and discuss the case of $Q<0$ at the end of this section. The vacuum is normalized by definition so that $N_0=1$. For $Q=1$, $|\psi_Q\rangle$ is the Slater state with the well-known norm $N_1=N_c!$.

Let us mention in passing that N_Q corresponds to the complete contraction of all permutations of totally antisymmetric tensors of the form

$$N_Q=\sum_{\{\sigma_s\}} \epsilon^{i_1^1 i_2^1 \cdots i_{N_c}^1} \cdots \epsilon^{i_1^Q i_2^Q \cdots i_{N_c}^Q} \epsilon_{i_1^{\sigma_1(1)} i_2^{\sigma_2(1)} \cdots i_{N_c}^{\sigma_{N_c}(1)}} \cdots \epsilon_{i_1^{\sigma_1(Q)} i_2^{\sigma_2(Q)} \cdots i_{N_c}^{\sigma_{N_c}(Q)}}, \tag{A1}$$

where the sum is over N_c copies of the permutation group S_Q, i.e., $\sigma_s \in S_Q$, $s=1,\ldots,N_c$. To the best of our knowledge, N_Q was not known previously for $Q>1$.

To prove Eq. (30), we study a different version of the color-flavor transformation in which the flavor group is $\mathrm{U}(N_b)$ with $N_b=N_c$. Note that the flavor group is compact now. We follow the same

method as in Sec. III but keep only the particles created by the $\bar{c}^i_a$ and discard the antiparticles created by the $\bar{d}^i_a$. The flavor group $\mathrm{U}(N_b)$ is then generated by $\{\widetilde{\mathcal{G}}_{ab}=\bar{c}^i_a c^i_b\}$. The state $|\psi_Q\rangle$ is still defined as in Eq. (25). The projector onto the Q-sector is now

$$\mathbb{1}_Q = \widetilde{C}_Q \int_{U(N_b)} \mathrm{d}g\, \widetilde{T}_g |\psi_Q\rangle\langle\psi_Q| \widetilde{T}_g^{-1} \tag{A2}$$

with the normalized Haar measure $\mathrm{d}g$ of $\mathrm{U}(N_b)$ and $\widetilde{T}_g=\exp(\bar{c}^i_a(\ln g)_{ab}c^i_b)$. For $N_b=N_c$, we have by explicit calculation

$$\widetilde{T}_g|\psi_Q\rangle = (\det{}^Q g)|\psi_Q\rangle. \tag{A3}$$

Using this equation, the normalization constant $\widetilde{C}_Q$, see also Eq. (29), simplifies to

$$\widetilde{C}_Q = N_Q\left[\int_{U(N_b)} \mathrm{d}g \langle\psi_Q|\widetilde{T}_g|\psi_Q\rangle\langle\psi_Q|\widetilde{T}_g^{-1}|\psi_Q\rangle\right]^{-1} = N_Q[N_Q^2]^{-1} = \frac{1}{N_Q}. \tag{A4}$$

Next we consider the following integral and perform manipulations similar to those in Sec. III:

$$\begin{aligned}
\int_{\mathrm{SU}(N_c)} \mathrm{d}U \exp(\bar{\psi}^i_a U^{ij}\psi^j_a) &= \int_{\mathrm{SU}(N_c)} \mathrm{d}U \langle 0|\exp(\bar{\psi}^i_a c^i_a)\exp(\bar{c}^i_a U^{ij}\psi^j_a)|0\rangle \\
&= \sum_{Q=0}^{\infty} \langle 0|\exp(\bar{\psi}^i_a c^i_a)\mathbb{1}_Q \exp(\bar{c}^i_a\psi^i_a)|0\rangle \\
&= \sum_{Q=0}^{\infty} \widetilde{C}_Q \int_{U(N_b)} \mathrm{d}g \langle 0|\exp(\bar{\psi}^i_a c^i_a)\widetilde{T}_g|\psi_Q\rangle\langle\psi_Q|\widetilde{T}_g^{-1}\exp(\bar{c}^i_a\psi^i_a)|0\rangle \\
&= \sum_{Q=0}^{\infty} \frac{1}{N_Q}\langle 0|\exp(\bar{\psi}^i_a c^i_a)|\psi_Q\rangle\langle\psi_Q|\exp(\bar{c}^i_a\psi^i_a)|0\rangle = \sum_{Q=0}^{\infty}\frac{1}{N_Q}\det{}^Q M,
\end{aligned} \tag{A5}$$

where M is an $N_c\times N_c$ matrix, $M^{ij}=\psi^i_a\bar{\psi}^j_a$, and we have again used Eq. (A3). However, we can also use the character expansion method[19,20] to do this integral. Using the same notation as in Sec. IV, we obtain

$$\begin{aligned}
\int_{\mathrm{SU}(N_c)} \mathrm{d}U \exp(\bar{\psi}^i_a U^{ij}\psi^j_a) &= \int_{\mathrm{SU}(N_c)} \mathrm{d}U \exp(\mathrm{tr}\, UM) = \int_{\mathrm{SU}(N_c)} \mathrm{d}U \sum_r \alpha^{(0)}_r \chi_r(UM) \\
&= \sum_r \alpha^{(0)}_r M^{ji}_r \int_{\mathrm{SU}(N_c)} \mathrm{d}U\, U^{ij}_r = \sum_{Q=0}^{\infty} \alpha^{(0)}_{r=N_cQ} \det{}^Q M.
\end{aligned} \tag{A6}$$

In the last step, we have used the facts that

$$\int_{\mathrm{SU}(N_c)} \mathrm{d}U\, U^{ij}_r = \begin{cases} 1, & r = N_cQ, \\ 0, & \text{else}, \end{cases} \tag{A7}$$

where $r=N_cQ$ denotes the (one-dimensional) irreducible representation of $\mathrm{GL}(N_c)$ specified by a Young diagram with N_c rows and Q columns, and that for all $M\in\mathrm{GL}(N_c)$ we have $M^{ij}_{r=N_cQ}=\det{}^Q M$, see Eq. (69). (Note that in the one-dimensional representation $r=N_cQ$ the indices i and j only take the value 1.) From Eq. (64) we obtain with $d_{r=N_cQ}=1$,

$$\alpha^{(0)}_{r=N_cQ} = \prod_{n=0}^{N_c-1} \frac{n!}{(Q+n)!}. \tag{A8}$$

Comparing Eqs. (A5) and (A6) we arrive at Eq. (30), valid for $Q \geqslant 0$. The calculation for $Q<0$ proceeds in complete analogy by working with the antiparticles instead of the particles, and the result for this case can be obtained by the replacement $Q \to -Q$ in the expression for N_Q.

APPENDIX B: CALCULATION OF THE $\mathcal{C}_Q$

In this section, we do the integral in Eq. (56). This is an example of so-called Hua-type integrals that were studied by Hua a long time ago[17] and recently extended by Neretin.[31] Here, we follow the method introduced in Ref. 17. We first consider the case of $N_b \geqslant N_c$ and $Q \geqslant 0$, and then give a result for $N_b < N_c$ and $Q=0$.

Using Eq. (42), Eq. (56) becomes

$$\mathcal{C}_Q^{-1} = N_Q \int_{|ZZ^\dagger|\leqslant 1} \frac{\mathrm{d}Z\, \mathrm{d}Z^\dagger}{\det^{2N_b-N_c}(1-ZZ^\dagger)} \det{}^Q(1-ZZ^\dagger)_{[N_c]}. \tag{B1}$$

We now write the matrix Z as $Z=(Z_{N_b,N_b-1}, q)$, where Z_{N_b,N_b-1} is an $N_b \times (N_b-1)$ matrix and q is a single column. We then have

$$1-ZZ^\dagger = 1 - Z_{N_b,N_b-1} Z^\dagger_{N_b,N_b-1} - qq^\dagger. \tag{B2}$$

Since $|1-Z_{N_b,N_b-1}Z^\dagger_{N_b,N_b-1}| \geqslant 0$, i.e., the matrix has real and non-negative eigenvalues, we write $1-Z_{N_b,N_b-1}Z^\dagger_{N_b,N_b-1}=\Gamma\Gamma^\dagger$ and define $q=\Gamma w$. Then

$$\mathrm{d}q\, \mathrm{d}q^\dagger = |\det \Gamma|^2\, \mathrm{d}w\, \mathrm{d}w^\dagger = \det(1 - Z_{N_b,N_b-1}Z^\dagger_{N_b,N_b-1})\mathrm{d}w\, \mathrm{d}w^\dagger. \tag{B3}$$

On the other hand,

$$\det(1-ZZ^\dagger) = \det[\Gamma(1-ww^\dagger)\Gamma^\dagger] = (1-w^\dagger w)\det(1 - Z_{N_b,N_b-1}Z^\dagger_{N_b,N_b-1}),$$

where we have used $\det(1-ww^\dagger)=(1-w^\dagger w)$. Applying the same procedure to Z_{N_b,N_b-1} and so on, we obtain

$$\begin{aligned}
[\mathcal{C}_Q N_Q]^{-1} &= \int_{|ZZ^\dagger|\leqslant 1} \frac{\mathrm{d}Z\, \mathrm{d}Z^\dagger}{\det^{2N_b-N_c}(1-ZZ^\dagger)} \det{}^Q(1-ZZ^\dagger)_{[N_c]} = \prod_{i=1}^{N_c} \int_{w_i^\dagger w_i \leqslant 1} \mathrm{d}w_i\, \mathrm{d}w_i^\dagger (1 \\
&\quad - w_i^\dagger w_i)^{N_c-N_b+Q-i} \prod_{j=N_c+1}^{N_b} \int_{w_j^\dagger w_j \leqslant 1} \mathrm{d}w_j\, \mathrm{d}w_j^\dagger (1-w_j^\dagger w_j)^{N_c-N_b-j} \\
&= \prod_{i=1}^{N_c} \pi^{N_b} \frac{(N_c-N_b+Q-i)!}{(N_c+Q-i)!} \prod_{j=N_c+1}^{N_b} \pi^{N_b} \frac{(N_c-N_b-j)!}{(N_c-j)!}.
\end{aligned} \tag{B4}$$

From this equation, which was derived for $N_b \geqslant N_c$, we see that for $N_b > N_c$, the above integral diverges for all $Q \geqslant 0$, whereas for $N_b=N_c$, it diverges for $Q<N_b$.

For $N_b<N_c$, only the $Q=0$ sector exists, and we obtain from a very similar and even simpler calculation

$$\mathcal{C}_0^{-1} = C_0^{-1} = \pi^{N_b^2} \prod_{n=1}^{N_b} \frac{(N_c-N_b-n)!}{(N_c-n)!}, \tag{B5}$$

which is finite for $2N_b \leqslant N_c$ but diverges for $N_b < N_c < 2N_b$.

APPENDIX C: PROOF OF IDENTITY (74)

We have $\mathrm{tr}(MN)=\mathrm{tr}(\Psi\Psi^\dagger\Phi\Phi^\dagger)=\mathrm{tr}(\Phi^\dagger\Psi\Psi^\dagger\Phi)=\mathrm{tr}(\Phi^\dagger\Psi\Psi^\dagger\Phi)^T=\mathrm{tr}(BC)$, which proves the identity immediately for $N_b=N_c$. In the following, we assume $\delta=N_c-N_b>0$ and prove the identity by an iterative procedure.

The semipositive definite $N_b\times N_b$ matrix $BC=(\Phi^\dagger\Psi\Psi^\dagger\Phi)^T$ has N_b eigenvalues that we denote by λ_a^2 with $a=1,\ldots,N_b$. From linear algebra[18] we know that the $N_c\times N_c$ matrix $MN=\Psi\Psi^\dagger\Phi\Phi^\dagger$ has N_b eigenvalues equal to those of BC and $\delta=N_c-N_b$ eigenvalues equal to zero. We denote the eigenvalues of MN by μ_i^2, with $\mu_i=\lambda_i$ for $1\leqslant i\leqslant N_b$. For the purpose of this proof, we start with nonzero values μ_i for $N_b<i\leqslant N_c$ and let them go to zero one by one, starting with μ_{N_c}. Weyl's character formula is[17]

$$\chi_{(r_1,r_2,\ldots,r_{N_c})}(MN)=\frac{\det(\mu_i^{2(N_c+r_j-j)})}{\Delta(\mu^2)}=\frac{\det(\mu_i^{2k_j})}{\Delta(\mu^2)}, \tag{C1}$$

where the k_j have been defined in Eq. (64) and Δ again denotes the Vandermonde determinant. We have

$$\lim_{\mu_{N_c}\to 0}\Delta_{N_c}(\mu^2)=\lim_{\mu_{N_c}\to 0}\prod_{i<j}^{N_c}(\mu_i^2-\mu_j^2)=\Delta_{N_c-1}(\mu^2)\prod_{i=1}^{N_c-1}\mu_i^2, \tag{C2}$$

where the index on Δ denotes the number of eigenvalues involved. Similarly, we introduce the notation $\det_m(\mu_i^{2k_j})$ to denote the determinant of the $m\times m$ upper-left submatrix of the matrix $(\mu_i^{2k_j})$, i.e., i and j run from 1 to m instead of from 1 to N_c. Note that for $\mu_{N_c}\to 0$, $\det_{N_c}(\mu_i^{2k_j})$ is nonvanishing only if $k_{N_c}=0$ or, equivalently, $r_{N_c}=0$, in which case we have

$$\lim_{\mu_{N_c}\to 0}\det_{N_c}(\mu_i^{2k_j})=\det_{N_c-1}(\mu_i^{2k_j'})\prod_{i=1}^{N_c-1}\mu_i^2, \tag{C3}$$

where

$$k_j'=r_j+(N_c-1)-j\quad\text{with } j=1,\ldots,N_c-1. \tag{C4}$$

We conclude that for $\mu_{N_c}=0$, $\chi_r(MN)$ is nonzero only for representations of $\mathrm{GL}(N_c)$ with Young diagram $r=(r_1\geqslant\cdots\geqslant r_{N_c}=0)$. We thus obtain

$$\begin{aligned}\lim_{\mu_{N_c}\to 0}\sum_r\frac{\alpha_r^{(0)}\alpha_r^{(-Q)}}{d_r}\chi_r(MN)&=\sum_{r_1\geqslant\cdots\geqslant r_{N_c}=0}\frac{\alpha_r^{(0)}\alpha_r^{(-Q)}}{d_r}\frac{\det_{N_c-1}(\mu_i^{2k_j'})}{\Delta_{N_c-1}(\mu^2)}\\&=\prod_{n=1}^{N_c-1}n!\sum_{k_1>\cdots>k_{N_c}=0}\det_{N_c}\left(\frac{1}{k_j!(k_j-N_c+Q+i)!}\right)\frac{\det_{N_c-1}(\mu_i^{2k_j'})}{\Delta_{N_c-1}(\mu^2)},\end{aligned} \tag{C5}$$

where we have used Eqs. (64) and (65). From Eq. (64) with $k_{N_c}=0$ we have

$$\det_{N_c}\left(\frac{1}{k_j!(k_j-N_c+Q+i)!}\right)=\frac{d^{\mathrm{GL}(N_c)}_{(r_1,\ldots,r_{N_c-1},0)}}{\prod_{j=1}^{N_c-1}k_j!}\prod_{i=1}^{N_c}\frac{(N_c-i)!}{(k_i+Q)!}. \tag{C6}$$

From Eq. (65) we find that

$$d^{\mathrm{GL}(N_c)}_{(r_1,\ldots,r_{N_c-1},0)} = \frac{\prod_{j=1}^{N_c-1} k_j}{(N_c-1)!} d^{\mathrm{GL}(N_c-1)}_{(r_1+1,\ldots,r_{N_c-1}+1)}. \tag{C7}$$

Hence, for $\mu_{N_c}=0$, and thus $k_{N_c}=0$, we obtain from (C6), (C7), and (64),

$$\det_{N_c}\left(\frac{1}{k_j!(k_j-N_c+Q+i)!}\right) = \frac{1}{Q!}\det_{N_c-1}\left(\frac{1}{k_j'!(k_j'-(N_c-1)+(Q+1)+i)!}\right). \tag{C8}$$

Putting everything together, we arrive at

$$\lim_{\mu_{N_c}\to 0}\sum_r \frac{\alpha_r^{(0)}\alpha_r^{(-Q)}}{d_r}\chi_r(MN) = \frac{(N_c-1)!}{Q!}\sum_{r'}\frac{\alpha_{r'}^{(0)}\alpha_{r'}^{(-Q-1)}}{d_{r'}}\chi_{r'}(MN), \tag{C9}$$

where the sum on the RHS is over all irreducible representations $r'=(r_1\geqslant\cdots\geqslant r_{N_c-1}\geqslant 0)$ of $\mathrm{GL}(N_c-1)$. Repeating this procedure $\delta=N_c-N_b$ times, we obtain our identity

$$\sum_r \frac{\alpha_r^{(0)}\alpha_r^{(-Q)}}{d_r}\chi_r(MN) = \prod_{n=0}^{\delta-1}\frac{(N_b+n)!}{(Q+n)!}\sum_s \frac{\alpha_s^{(0)}\alpha_s^{(-Q-\delta)}}{d_s}\chi_s(BC), \tag{74}$$

where the sum on the RHS is over all irreducible representations s of $\mathrm{GL}(N_b)$ of the form (62), and where we have again used $\mathrm{tr}(MN)=\mathrm{tr}(BC)$.

APPENDIX D: EXAMPLES FOR THE ALGEBRAIC RESULT

1. $N_c=2$, $N_b=1$

We parametrize elements of SU(2) as

$$U=\begin{pmatrix} e^{i\lambda}\cos\theta & -e^{i\eta}\sin\theta \\ e^{-i\eta}\sin\theta & e^{-i\lambda}\cos\theta \end{pmatrix} \quad \text{with } 0\leqslant\theta\leqslant\frac{\pi}{2},\quad 0\leqslant\lambda,\eta<2\pi. \tag{D1}$$

The corresponding normalized Haar measure is $\mathrm{d}U=(1/2\pi^2)\sin\theta\cos\theta\,\mathrm{d}\theta\,\mathrm{d}\lambda\,\mathrm{d}\eta$. Performing the integral on the LHS of Eq. (4), we obtain

$$\int_{\mathrm{SU}(2)}\mathrm{d}U\exp(\bar\psi^i U^{ij}\psi^j+\bar\varphi^i U^{\dagger ij}\varphi^j) = \sum_{n=0}^{\infty}\frac{1}{n!(n+1)!}(\bar\psi^1\psi^1\bar\varphi^1\varphi^1+\bar\psi^2\psi^2\bar\varphi^2\varphi^2+\bar\psi^1\psi^2\bar\varphi^2\varphi^1 + \bar\psi^2\psi^1\bar\varphi^1\varphi^2)^n. \tag{D2}$$

For the RHS of Eq. (4), we have with $\mathcal{C}_0=1/\pi$,

$$\frac{1}{\pi}\int_{|z|\leqslant 1}\mathrm{d}z\,\mathrm{d}\bar z\exp[(\bar\psi^1\varphi^1+\bar\psi^2\varphi^2)z+(\bar\varphi^1\psi^1+\bar\varphi^2\psi^2)\bar z] = \frac{1}{\pi}\int_0^1 r\,\mathrm{d}r\int_0^{2\pi}\mathrm{d}\theta\exp[(\bar\psi^1\varphi^1+\bar\psi^2\varphi^2)re^{i\theta} + (\bar\varphi^1\psi^1+\bar\varphi^2\psi^2)re^{-i\theta}] = \sum_{n=0}^{\infty}\frac{1}{n!(n+1)!}(\bar\psi^1\psi^1\bar\varphi^1\varphi^1+\bar\psi^2\psi^2\bar\varphi^2\varphi^2+\bar\psi^1\psi^2\bar\varphi^2\varphi^1+\bar\psi^2\psi^1\bar\varphi^1\varphi^2)^n \tag{D3}$$

in agreement with Eq. (D2).

2. $N_c=N_{b+}=2$, $N_{b-}=0$

In this example we check the argument we made in Sec. III H for $N_{b+}\neq N_{b-}$. To have $N_{b-}=0$ we simply set $\bar\varphi_a^i=\varphi_a^i=0$. Using the same parametrization for SU(2) as in Appendix D 1, we calculate the integral on the LHS of Eq. (1),

$$\int_{\mathrm{SU}(2)} \mathrm{d}U \exp(\bar{\psi}_a^i U^{ij} \psi_a^j) = \sum_{n=0}^{\infty} \frac{1}{n!(n+1)!} (\bar{\psi}_1^1 \psi_1^1 \bar{\psi}_2^2 \psi_2^2 + \bar{\psi}_1^2 \psi_1^2 \bar{\psi}_2^1 \psi_2^1 - \bar{\psi}_1^1 \psi_1^2 \bar{\psi}_2^2 \psi_2^1 - \psi_1^1 \bar{\psi}_1^2 \bar{\psi}_2^1 \psi_2^2)^n. \tag{D4}$$

In this case we must sum over Q from zero to infinity on the RHS. The integral over the coset space U(2)/U(2) amounts to evaluating the integrand at the single point $Z=0$. From Eqs. (56) and (30), we have $\mathcal{C}_Q = 1/N_Q = 1/[Q!(Q+1)!]$ and thus obtain

$$\mathrm{RHS} = \sum_{Q=0}^{\infty} \frac{1}{Q!(Q+1)!} \det{}^Q \mathcal{M} = \sum_{Q=0}^{\infty} \frac{1}{Q!(Q+1)!} (\bar{\psi}_1^1 \psi_1^1 \bar{\psi}_2^2 \psi_2^2 + \bar{\psi}_1^2 \psi_1^2 \bar{\psi}_2^1 \psi_2^1 - \bar{\psi}_1^1 \psi_1^2 \bar{\psi}_2^2 \psi_2^1 - \psi_1^1 \bar{\psi}_1^2 \bar{\psi}_2^1 \psi_2^2)^Q \tag{D5}$$

in agreement with Eq. (D4), where we have used $\mathcal{M}^{ij} = \bar{\psi}_a^i \psi_a^j$.

3. $N_c = N_b = 1$

In this example, we run into the divergence problem discussed in Secs. II and III. The LHS of Eq. (1) is simple because the integral over SU(1) reduces to evaluating the integrand at unity,

$$\int_{\mathrm{SU}(1)} \mathrm{d}U \exp(\bar{\psi}^i U^{ij} \psi^j + \bar{\varphi}^i U^{\dagger ij} \varphi^j) = \exp(\bar{\psi}\psi + \bar{\varphi}\varphi). \tag{D6}$$

The RHS of Eq. (1) is a sum over Q. For $Q=0$ we have

$$\mathcal{C}_0^{-1} = \int_{|z|\leqslant 1} \frac{\mathrm{d}z\, \mathrm{d}\bar{z}}{1 - z\bar{z}} = 2\pi \int_0^1 \frac{r\, \mathrm{d}r}{1 - r^2} \tag{D7}$$

and

$$\int_{|z|\leqslant 1} \frac{\mathrm{d}z\, \mathrm{d}\bar{z}}{1 - z\bar{z}} \exp(\bar{\psi} z \varphi + \bar{\varphi} \bar{z} \psi) = 2\pi \sum_{n=0}^{\infty} \frac{(\bar{\psi}\psi\bar{\varphi}\varphi)^n}{(n!)^2} \int_0^1 \frac{r^{2n+1}\, \mathrm{d}r}{1 - r^2}. \tag{D8}$$

We now change the upper limit in the integral to $1-\epsilon$ and let $\epsilon \to 0$ to obtain

$$\mathcal{C}_0 \int_{|z|\leqslant 1} \frac{\mathrm{d}z\, \mathrm{d}\bar{z}}{1 - z\bar{z}} \exp(\bar{\psi} z \varphi + \bar{\varphi} \bar{z} \psi) = \sum_{n=0}^{\infty} \frac{(\bar{\psi}\psi\bar{\varphi}\varphi)^n}{(n!)^2}. \tag{D9}$$

For $Q \geqslant 1$, there are no divergences, and we have

$$\int_{|z|\leqslant 1} \frac{\mathrm{d}z\, \mathrm{d}\bar{z}}{(1 - z\bar{z})^{2N_b - N_c - Q}} \exp(\bar{\psi} z \varphi + \bar{\varphi} \bar{z} \psi) = \pi \sum_{n=0}^{\infty} \frac{(Q-1)!}{n!(n+Q)!} (\bar{\psi}\psi\bar{\varphi}\varphi)^n. \tag{D10}$$

Collecting all terms and using $\mathcal{C}_Q = 1/[\pi(Q-1)!]$, we find for the RHS of Eq. (1),

$$\int_{|ZZ^\dagger|\leqslant 1} D(Z, Z^\dagger) \exp(\bar{\psi}_a^i Z_{ab} \varphi_b^i + \bar{\varphi}_a^i Z_{ab}^\dagger \psi_b^i) \sum_{Q=0}^{\infty} \chi_Q = \sum_{n=0}^{\infty} \sum_{Q=0}^{\infty} \frac{1}{n!(n+Q)!} [(\bar{\psi}\psi)^Q + (\bar{\varphi}\varphi)^Q - \delta_{Q0}] \times (\bar{\psi}\psi\bar{\varphi}\varphi)^n = \exp(\bar{\psi}\psi + \bar{\varphi}\varphi), \tag{D11}$$

where the last step requires some rearrangements of the terms in the sums. We see that the transformation works although for $Q=0$ the normalization factor and the integral on the RHS of the transformation are divergent. After those infinities have been canceled, the finite ratio gives the

correct result. However, as mentioned at the end of Sec. III F, it is not trivial to obtain a simple result for the general case.

APPENDIX E: EXAMPLES FOR THE CHARACTER EXPANSION RESULT

1. $N_c=N_b=1$

Although this example was already considered in Appendix D 3, we revisit it here to check our result obtained using the character expansion method. Again, the LHS equals $\exp(\bar{\psi}\psi+\bar{\varphi}\varphi)$. From Eq. (6) we have

$$\sum_{Q=0}^{\infty}\tilde{\chi}_Q\int_0^{2\pi}\frac{\mathrm{d}\theta}{2\pi}(Be^{i\theta})^{-Q}\exp(\bar{\psi}e^{i\theta}\varphi+\bar{\varphi}e^{-i\theta}\psi)=\sum_{Q=0}^{\infty}[(\bar{\psi}\psi)^Q+(\bar{\varphi}\varphi)^Q-\delta_{Q0}]\sum_{n=0}^{\infty}\frac{1}{n!(n+Q)!}(\bar{\psi}\psi\bar{\varphi}\varphi)^n$$
$$=\exp(\bar{\psi}\psi+\bar{\varphi}\varphi) \tag{E1}$$

as in Eq. (D11), where we have used $M=\psi\bar{\psi}$, $N=\varphi\bar{\varphi}$, and $B=\varphi\bar{\psi}$. We see that the transformation (6) works and that, unlike in Appendix D 3, we do not have any divergence problem.

2. $N_c=N_b=2$

In this case we also have $2N_b>N_c$, and therefore divergences would arise in Eq. (1). We now check our result (6) in which no divergence appears. Using the parametrization of SU(2) in Appendix D 1, we perform the integral on the LHS,

$$\int_{\mathrm{SU}(2)}\mathrm{d}U\exp(\bar{\psi}^i_aU^{ij}\psi^j_a+\bar{\varphi}^i_aU^{\dagger ij}\varphi^j_a)=\sum_{n=0}^{\infty}\frac{1}{n!(n+1)!}(\det M+\det N+\mathrm{tr}\,MN)^n \tag{E2}$$

with M and N given by Eq. (61) and B and C given by Eq. (71). To do the integral on the RHS, we parametrize U(2) by multiplying the matrix in Eq. (D1), which we now call V, by a phase $e^{i\phi}$, with $0\leqslant\phi<2\pi$. The corresponding normalized Haar measure is $\mathrm{d}V=(1/4\pi^3)\sin\theta\cos\theta\,\mathrm{d}\theta\,\mathrm{d}\lambda\,\mathrm{d}\eta\,\mathrm{d}\phi$. We then obtain

$$\sum_{Q=0}^{\infty}\tilde{\chi}_Q\int_{\mathrm{U}(2)}\mathrm{d}V\det{}^{-Q}(VB)\exp(\bar{\psi}^i_aV_{ab}\varphi^i_b+\bar{\varphi}^i_aV^{\dagger}_{ab}\psi^i_b)=\sum_{n=0}^{\infty}\frac{1}{n!(n+1)!}(\det M+\det N+\mathrm{tr}\,BC)^n \tag{E3}$$

with $\tilde{\chi}_Q$ defined in Eq. (7). The two results agree. In the derivation of Eqs. (E2) and (E3) we have used $\det(BC)=\det(MN)$ and $\mathrm{tr}(BC)=\mathrm{tr}(MN)$.

3. $N_c=2$, $N_b=1$

Let us check our result (5). The LHS is given by Eq. (D2). On the RHS we have

$$\prod_{n=0}^{N_c-N_b-1}\frac{(N_b+n)!}{n!}\int_{\mathrm{U}(N_b)}\mathrm{d}V\det{}^{N_b-N_c}(VB)\exp(\bar{\psi}^i_aV_{ab}\varphi^i_b+\bar{\varphi}^i_aV^{\dagger}_{ab}\psi^i_b)=\int_0^{2\pi}\frac{\mathrm{d}\theta}{2\pi}(Be^{i\theta})^{-1}\exp(Be^{i\theta}$$
$$+Ce^{-i\theta})=\sum_{n=0}^{\infty}\frac{1}{n!(n+1)!}(\bar{\psi}^1\psi^1\bar{\varphi}^1\varphi^1+\bar{\psi}^2\psi^2\bar{\varphi}^2\varphi^2+\bar{\psi}^1\psi^2\bar{\varphi}^2\varphi^1+\bar{\psi}^2\psi^1\bar{\varphi}^1\varphi^2)^n, \tag{E4}$$

where we have used $B=\varphi^1\bar{\psi}^1+\varphi^2\bar{\psi}^2$ and $C=\psi^1\bar{\varphi}^1+\psi^2\bar{\varphi}^2$. Thus, the RHS agrees with the result in Eq. (D2).

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Integration of massive states as contractions of nonlinear σ models

L. Andrianopoli[a)]
Centro E. Fermi, Compendio Viminale, I-00184 Rome, Italy

S. Ferrara[b)]
Department of Physics, Theory Division CERN, CH 1211 Geneva 23, Switzerland and INFN, Laboratori Nazionali di Frascati, Italy

M. A. Lledó[c)] and O. Maciá[d)]
Departament de Física Teòrica, Universitat de València and IFIC C/Dr. Moliner, 50, E-46100 Burjassot (València), Spain

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We consider the contraction of some nonlinear σ models which appear in effective supergravity theories. In particular we consider the contractions of maximally symmetric spaces corresponding to $N=1$ and $N=2$ theories, as they appear in certain low energy effective supergravity actions with mass deformations. The contraction procedure is shown to describe the *integrating out* of massive modes in the presence of interactions, as it happens in many supergravity models after spontaneous supersymmetry breaking. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Supergravity theories with mass deformations have recently received some attention because of their relation to flux compactifications (for a review see, e.g., Ref. 1) or Scherk–Schwarz generalized dimensional reduction.[2]

For $N \geqslant 2$ local supersymmetry, the supergravity theories admit mass deformations that always correspond to gauged supergravities.[3,4] The mass parameters may be chosen in such a way that a low energy effective Lagrangian for the massless sector can be singled out by deleting the massive modes.

This procedure is usually discussed in the framework of consistent truncations of field theories,[5] but here we want to show that the same phenomenon may arise as well as a *contraction*. The basic argument is that the limiting situation of a mass scale asymptotically large is equivalent to the contraction of some group structure.

Suppose the group structure is a nonlinear σ model related to a maximally symmetric space G/H where G is noncompact and H its maximally compact subgroup.[6,7] One can make an Inönü-Wigner contraction[8] of the group G with respect to a subgroup G'. Let $H'=H\cap G'$. We can induce a contraction G/H to a manifold which will have G'/H' embedded in it. The contracted manifold has the same dimension as the original one (as it happens for contractions of algebras and groups), but with a metric that will be essentially different. An example of this are the contractions of the hyperboloid SU(1, 1)/U(1). If the contraction is made with respect to the subgroup U(1) one

[a)]Electronic mail: Laura.Andrianopoli@cern.ch
[b)]Electronic mail: Sergio.Ferrara@cern.ch
[c)]Electronic mail: Maria.Lledo@ific.uv.es
[d)]Electronic mail: Oscar.Macia@ific.uv.es

obtains the flat metric, whereas if the contraction is made with respect to SO(1, 1) one obtains an hyperbolic sheet, with one translational isometry. We will see in detail how to compute the metrics in these and other cases.

There are other types of contractions that do not fit in the scheme described previously, but that may have physical interest. If G/H is a symmetric space of the noncompact type, it inherits a group structure through the Iwasawa decomposition of G

$$G = G_S \times H.$$

Then $G/H \approx G_S$ is the solvable Lie group associated to G.[6,7,9] Note that G_S depends on the real (noncompact) form of G. We can then consider contractions in which G/H goes to $G'/H' \ltimes \mathbb{R}^n$ (where $\ltimes$ stands for the semidirect product of groups) with $\dim(G/H)=\dim(G'/H')+n$, independently of the fact that G' is a subgroup of G or not. The physical interpretation of these contractions is as a (super)-Higgs mechanism,[10] where the massive modes are described by $\mathbb{R}^n$ degrees of freedom while the fields which remain massless are in G'/H'.[11] Indeed, because of the semidirect product structure, it is always consistent to set to zero (which, in this case, would correspond to integrate out) the elements of $\mathbb{R}^n$, since $\mathbb{R}^n$ is an invariant subalgebra of $G'/H' \ltimes \mathbb{R}^n$.[12] We will consider several examples and discuss their physical applications.

The paper is organized as follows.

In Sec. II we describe the solvable algebras related to symmetric spaces

$$\frac{\mathrm{SO}(1,1+n)}{\mathrm{SO}(1+n)}, \quad \frac{\mathrm{SU}(1,1+n)}{\mathrm{U}(1)\times\mathrm{SU}(1+n)}, \quad \frac{\mathrm{SO}(2,2+n)}{\mathrm{SO}(2)\times\mathrm{SO}(2+n)}, \quad \frac{\mathrm{U}(2,2+n)}{\mathrm{U}(2)\times\mathrm{U}(2+n)}, \tag{1}$$

and how these algebras are embedded one into the other. We also compute the metric of these spaces in the solvable parametrization. We show a couple of examples where these spaces are related to one another by gauging some isometries in the corresponding supergravity models followed by an integration of the massive modes.

In Sec. III we study some contractions of the solvable algebras introduced and we show how they are related among themselves. We compute the contracted metric by first giving a *deformation* of it in terms of a parameter ϵ. The limits $\epsilon \to 1$ and $\epsilon \to 0$ correspond to the original and the contracted spaces, respectively. For an arbitrary $\epsilon \neq 0$, the groups are isomorphic but we will see that it is not possible, in general, to reabsorb the parameter into a redefinition of the coordinates of the coset space. This means that the spaces at $\epsilon \neq 0$ are not isometric. We will show this phenomenon in detail. We will see how it is possible to interpret the gauging and integrating procedure of the examples treated in Sec. II as a contraction followed by a quotienting by a submanifold.

In Sec. IV we describe the super Higgs phenomenon associated to an effective $N=2$ supergravity theory with scalar manifold

$$\frac{\mathrm{SU}(1,1+n)}{(\mathrm{U}(1)\times\mathrm{SU}(1+n))}\times\frac{\mathrm{U}(2,2+n)}{(\mathrm{U}(2)\times\mathrm{U}(2+n))},$$

relating it to the contraction procedure described in previous sections.

In the Appendix we explain in more detail the parametrization chosen to study these sigma models.

II. SYMMETRIC SPACES, SOLVABLE PARAMETRIZATIONS AND EMBEDDINGS

We first illustrate the calculation of the solvable Lie algebra associated to a symmetric space of the noncompact type with the simplest example in (1). Essentially one has to diagonalize simultaneously the elements of the maximal abelian subalgebra in the space $\mathfrak{p}$ of the Cartan decomposition

$$\mathfrak{g} = \mathfrak{h} + \mathfrak{p}, \quad \mathfrak{g} = \mathrm{Lie}(G), \quad \mathfrak{h} = \mathrm{Lie}(H).$$

A. Solvable parametrization of SO(1,1+*n*)/SO(1+*n*)

We consider the Lie algebra of $\mathrm{SO}(1,1+n)$, $\mathfrak{so}(1,1+n)$. In the fundamental representation, an element of it is given by

$$X=\begin{pmatrix} & & b_1 \\ & A & \vdots \\ & & b_{n+1} \\ b_1 \cdots b_{n+1} & & 0 \end{pmatrix}, \quad A=-A^T,$$

where A is an antisymmetric $(n+1)\times(n+1)$ matrix. The Cartan decomposition of $\mathfrak{g}=\mathfrak{so}(1,1+n)$ is

$$\mathfrak{g}=\mathfrak{k}+\mathfrak{p}, \quad \mathfrak{k}=\mathfrak{so}(1+n)=\left\{\begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix}\right\}, \quad \mathfrak{p}=\left\{\begin{pmatrix} 0 & b \\ b^T & 0 \end{pmatrix}\right\}.$$

It is easy to see that the coset has rank one. We choose the element

$$H=\begin{pmatrix} & & 0 & 0 \\ & 0 & \vdots & \vdots \\ & & 0 & 0 \\ 0\cdots 0 & & 0 & 1 \\ 0\cdots 0 & & 1 & 0 \end{pmatrix}$$

as the generator of the maximal abelian subalgebra in $\mathfrak{p}$. We must diagonalize h to obtain the reduced root pattern. This is easier by noting the following decomposition

$$\mathfrak{so}(1,n+1)\rightarrow\mathfrak{so}(1,1)+\mathfrak{so}(n)+\mathbf{n}^+ +\mathbf{n}^-,$$

where

$$\mathfrak{so}(1,1)=\mathrm{span}\{H\}, \quad \mathbf{n}^{\pm}=\left\{\begin{pmatrix} & & & b_1 & \mp b_1 \\ & & 0 & \vdots & \vdots \\ & & & b_n & \mp b_n \\ -b_1 & \cdots & -b_n & 0 & 0 \\ \mp b_1 & \cdots & \mp b_n & 0 & 0 \end{pmatrix}\right\},$$

and a vector in $\mathbf{n}^{\pm}$ has charge ± 1 with respect to H. In this decomposition the algebra shows a $\mathfrak{so}(1,1)$ grading ($\mathfrak{so}(n)$ has degree 0), and $\mathbf{n}^{\pm}$ are nilpotent (in particular, abelian) subalgebras. The solvable Lie algebra associated to the coset $\mathrm{SO}(1,1+n)/\mathrm{SO}(1+n)$ is then

$$\mathfrak{solv}\left(\frac{\mathrm{SO}(1,1+n)}{\mathrm{SO}(1+n)}\right)=\mathrm{span}\{H\}\ltimes\mathbf{n}^+, \tag{2}$$

with commutation rules

$$[H,X_i]=X_i, \quad i=1,\ldots,n \quad \text{(the rest zero)}.$$

Finally, the Iwasawa decomposition of the Lie algebra is

$$\mathfrak{so}(1,1+n)=\mathfrak{so}(1+n)+\mathfrak{solv}\left(\frac{\mathrm{SO}(1,1+n)}{\mathrm{SO}(1+n)}\right).$$

We choose a coset representative of the following form:

$$L = e^{u_i X_i} e^{\varphi H}, \quad L^{-1} = e^{-\varphi H} e^{-u_i X_i}.$$

We will see that this kind of splitting of the generators is specially useful. The pull back of the Maurer-Cartan form on the group to the coset space, $L^{-1}\mathrm{d}L$, decomposes as

$$L^{-1}\mathrm{d}L = (L^{-1}\mathrm{d}L)_{\mathfrak{k}} + (L^{-1}\mathrm{d}L)_{\mathfrak{p}}.$$

The first term is the connection on the K bundle $G \to G/K$, with $K=\mathrm{SO}(1+n)$ (spin bundle and spin connection) and the second term is the vielbein of G/K.

The metric is then computed as

$$\mathrm{d}s^2 = \langle (L^{-1}\mathrm{d}L)_{\mathfrak{p}}, (L^{-1}\mathrm{d}L)_{\mathfrak{p}} \rangle$$

where $\langle , \rangle$ is the Cartan-Killing form on $\mathfrak{g}$. Using the relation

$$e^{\alpha X} Y e^{-\alpha X} = Y e^{\alpha \beta}, \quad \text{provided } [X,Y] = \beta Y,$$

it is easy to see that the metric becomes

$$\mathrm{d}s^2 = \mathrm{d}\varphi^2 + e^{-2\varphi} \sum_i \mathrm{d}u_i^{\,2}. \tag{3}$$

This metric has the translational isometries $u_i \to u_i + c_i$ which are a maximal abelian ideal of the solvable Lie algebra (see the Appendix). In this case the ideal is $\mathcal{I}=\mathrm{span}\{X_i\}$.

It is now easy to go to the largest space in (1). It has only rank two and the rest of the solvable algebras can be seen as subalgebras of this. In fact we have a chain of embeddings of the solvable Lie algebras which implies a chain of embeddings of the corresponding symmetric spaces.

B. Solvable parametrization of U(2,2+*n*)/U(2)×U(2+*n*)

An element of the Lie algebra $\mathfrak{su}(2,2+n)$ can be written as

$$X = \begin{pmatrix} A_{2\times 2} & B_{2\times(2+n)} \\ B^{\dagger}_{(2+n)\times 2} & D_{(2+n)\times(2+n)} \end{pmatrix}, \quad A^{\dagger} = -A, \quad D^{\dagger} = -D,$$

and the Cartan decomposition of $\mathfrak{su}(2,2+n)=\mathfrak{h}+\mathfrak{p}$ is

$$\mathfrak{h} = \left\{ \begin{pmatrix} A_{2\times 2} & 0 \\ 0 & D_{(2+n)\times(2+n)} \end{pmatrix} \right\}, \quad \mathfrak{p} = \left\{ \begin{pmatrix} 0 & B_{2\times(2+n)} \\ B^{\dagger}_{(2+n)\times 2} & 0 \end{pmatrix} \right\}.$$

A maximal abelian subalgebra of $\mathfrak{p}$ has dimension 2, and so the coset has rank two. We can choose for example, as maximal abelian subalgebra, the one generated by the matrices

$$H_+ = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \cdots & \vdots & & & & \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad H_- = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & i & 0 & 0 & \cdots & 0 \\ 0 & -i & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \cdots & \vdots & & & & \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}$$

The solvable algebra can be shown to be generated by

$$\mathfrak{s}_4 = \mathfrak{solv}\left(\frac{\mathrm{U}(2,2+n)}{\mathrm{U}(2)\times \mathrm{U}(2+n)} \right) = \mathrm{span}\{H_+, H_-\} + \mathrm{span}\{Z^{ia}, Y^{ia}, T^{2,0}, T^{0,2}, S_{\alpha}^{(1,1)}, S_{\alpha}^{(1,-1)}\}, \tag{4}$$

where $i=1,2$, $a=1,\ldots n$, $\alpha=1,2$, with commutation rules

$$[Z^{ia},Z^{jb}]=\epsilon^{ij}\delta^{ab}T^{(2,0)},$$

$$[Y^{ia},Y^{jb}]=\epsilon^{ij}\delta^{ab}T^{(0,2)},$$

$$[Z^{ia},Y^{jb}]=\delta^{ab}(\delta^{ij}S_2^{(1,1)}+\epsilon^{ij}S_1^{(1,1)}),$$

$$[Y^{ia},S_1^{(1,-1)}]=Z^{ia},$$

$$[Y^{ia},S_2^{(1,-1)}]=\epsilon^{ij}Z^{ja},$$

$$[T^{(0,2)},S_\alpha^{(1,-1)}]=2S_\alpha^{(1,1)},$$

$$[S_\alpha^{(1,1)},S_\beta^{(1,-1)}]=\delta_{\alpha\beta}T^{(2,0)},$$

$$[H_+,Z^{ia}]=Z^{ia},$$

$$[H_-,Y^{ia}]=Y^{ia}. \tag{5}$$

The rest of the commutators with the Cartan generators H_+ and H_- are indicated by the upper indices (h_+,h_-). All the other commutators are zero.

Based on this solvable algebra, we choose the following parametrization for the coset representative of $\mathrm{U}(2,2+n)/(\mathrm{U}(2)\times\mathrm{U}(2+n))$ (In the appendix we show that the generators $T^{(2,0)}$, $T^{(0,2)}$, $S_\alpha^{(1,1)}$, and Z^{1a} correspond to true global *translational isometries*.):

$$L(t,\tilde{t},\tilde{s}_\alpha,s_\alpha,z_{ia},y_{ia},\psi,\phi)=A(t,\tilde{t},\tilde{s}_\alpha,z_{1a})B(s_\alpha,z_{2a},y_{ia})C(\psi,\phi), \tag{6}$$

where

$$A=\exp(tT^{(2,0)}+\tilde{t}\,T^{(0,2)}+\tilde{s}_\alpha S_\alpha^{(1,1)}+z_{1a}Z^{1a}),$$

$$B=\exp(s_1S_1^{(1,-1)})\exp(s_2S_2^{(1,-1)})\exp(z_{2a}Z^{2a})\exp(y_{2a}Y^{2a})\exp(y_{1a}Y^{1a}),$$

$$C=\exp(\psi H_+ +\phi H_-).$$

The Maurer Cartan form is

$$\begin{aligned}L^{-1}\mathrm{d}L=&\,e^{-2\psi}(s_\alpha\mathrm{d}\tilde{s}_\alpha+(s_1^2+s_2^2)\mathrm{d}\tilde{t}+\mathrm{d}t+z_{2a}\mathrm{d}z_{1a})T^{(2,0)}+e^{-2\phi}(\mathrm{d}\tilde{t}-y_{1a}\mathrm{d}y_{2a})T^{(0,2)}\\&+e^{-(\phi+\psi)}\big(y_{1a}y_{2a}\mathrm{d}s_1+\tfrac{1}{2}(y_1^2+y_2^2)\mathrm{d}s_2+\mathrm{d}\tilde{s}_1+2s_1\mathrm{d}\tilde{t}-\epsilon_{ij}y_{ia}\mathrm{d}z_{ja}\big)S_1^{(1,1)}\\&+e^{-(\phi+\psi)}\big(y_{1a}y_{2a}\mathrm{d}s_2-\tfrac{1}{2}(y_1^2+y_2^2)\mathrm{d}s_1+\mathrm{d}\tilde{s}_2+2s_2\mathrm{d}\tilde{t}+\delta_{ij}y_{ia}\mathrm{d}z_{ja}\big)S_2^{(1,1)}\\&+e^{-\psi}(-y_{1a}\mathrm{d}s_1+y_{2a}\mathrm{d}s_2+\mathrm{d}z_{1a})Z^{1a}+e^{-\psi}(-y_{2a}\mathrm{d}s_1-y_{1a}\mathrm{d}s_2+\mathrm{d}z_{2a})Z^{2a}+e^{\phi-\psi}\mathrm{d}s_\alpha S_\alpha^{(1,-1)}\\&+e^{-\phi}\mathrm{d}y_{ia}Y^{ia}+\mathrm{d}\psi H_+ +\mathrm{d}\phi H_-.\end{aligned} \tag{7}$$

The metric of the coset is computed now as $\langle(L^{-1}\mathrm{d}L)_\mathfrak{p},(L^{-1}\mathrm{d}L)_\mathfrak{p}\rangle$. On the tangent space to the identity, this gives the following inner product:

$$\langle X,X\rangle=\begin{cases}1 & \text{for } X=H_\pm,T^{(2,0)},T^{(0,2)}\\ \dfrac{1}{2} & \text{for } X=S_1^{(1,1)},S_2^{(1,1)},S_1^{(1,-1)},S_2^{(1,-1)},Y^{1a},Y^{2a},Z^{1a},Z^{2a},\end{cases}$$

and the rest zero.

For $n=0$ we obtain the reduced expression

$$\begin{aligned}
ds^2 &= d\phi^2 + d\psi^2 + e^{-4\psi} dt dt + 2e^{-4\psi} s_1 dt d\tilde{s}_1 + 2e^{-4\psi} s_2 dt d\tilde{s}_2 + 2e^{-4\psi}(s_2^2 + s_1^2) dt d\tilde{t} \\
&+ \frac{1}{2}(e^{-2(\psi+\phi)} + 2e^{-4\psi} s_1^2) d\tilde{s}_1 d\tilde{s}_1 + 2e^{-4\psi} s_2 s_1 d\tilde{s}_1 d\tilde{s}_2 + 2e^{-4\psi} s_1 (e^{2(\psi-\phi)} + s_2^2 + s_1^2) d\tilde{s}_1 d\tilde{t} \\
&+ \frac{1}{2}(e^{-2(\psi+\phi)} + 2e^{-4\psi} s_2^2) d\tilde{s}_2 d\tilde{s}_2 + 2e^{-4\psi} s_2 (e^{2(\psi-\phi)} + s_2^2 + s_1^2) d\tilde{s}_2 d\tilde{t} + \frac{1}{2} e^{2(\phi-\psi)} ds_2 ds_2 \\
&+ \frac{1}{2} e^{2(\phi-\psi)} ds_1 ds_1 + e^{-4(\psi+\phi)}(e^{2\psi} + e^{2\phi}(s_1^2 + s_2^2))^2 d\tilde{t} d\tilde{t}. \qquad (8)
\end{aligned}$$

For arbitrary n we obtain (for this and the rest of the calculations of different metrics we have used the program MATHEMATICA, Version 5.1, Wolfram Research, Inc., Champaign, IL, 2004.) (sum over repeated indices is understood, and we have used the short-hand notation $y_1^2 = y_{1a} y_{1a}$):

$$\begin{aligned}
ds^2 &= d\phi^2 + d\psi^2 + e^{-4\psi} dt dt + 2e^{-4\psi} s_1 dt d\tilde{s}_1 + 2e^{-4\psi} s_2 dt d\tilde{s}_2 + 2e^{-4\psi} z_{2a} dt dz_{1a} + 2e^{-4\psi}(s_2^2 \\
&+ s_1^2) dt d\tilde{t} \\
&+ \frac{1}{2}(e^{-2(\psi+\phi)} + 2e^{-4\psi} s_1^2) d\tilde{s}_1 d\tilde{s}_1 + 2e^{-4\psi} s_2 s_1 d\tilde{s}_1 d\tilde{s}_2 + \frac{1}{2} e^{-2(\psi+\phi)}(y_1^2 + y_2^2) d\tilde{s}_1 ds_2 \\
&+ e^{-2(\psi+\phi)} y_{1a} y_{2a} d\tilde{s}_1 ds_1 - e^{-2(\psi+\phi)} y_{1a} d\tilde{s}_1 dz_{2a} + (2e^{-4\psi} s_1 z_{2a} + e^{-2(\psi+\phi)} y_{2a}) d\tilde{s}_1 dz_{1a} \\
&+ 2e^{-4\psi} s_1 (e^{2(\psi-\phi)} + s_2^2 + s_1^2) d\tilde{s}_1 d\tilde{t} + \frac{1}{2}(e^{-2(\psi+\phi)} + 2e^{-4\psi} s_2^2) d\tilde{s}_2 d\tilde{s}_2 + e^{-2(\psi+\phi)} y_{1a} y_{2a} d\tilde{s}_2 ds_2 \\
&- \frac{1}{2} e^{-2(\psi+\phi)}(y_1^2 + y_2^2) d\tilde{s}_2 ds_1 + e^{-2(\psi+\phi)} y_{2a} d\tilde{s}_2 dz_{2a} + (2e^{-4\psi} s_2 z_{2a} + e^{-2(\psi+\phi)} y_{1a}) d\tilde{s}_2 dz_{1a} \\
&+ 2e^{-4\psi} s_2 (e^{2(\psi-\phi)} + s_2^2 + s_1^2) d\tilde{s}_2 d\tilde{t} + \frac{1}{8} e^{-2(\psi+\phi)}(4e^{4\phi} + 4e^{2\phi}(y_1^2 + y_2^2) + 4(y_{1a} y_{2a})^2 + (y_1^2 + y_2^2) \\
&\times (y_1^2 + y_2^2)) ds_\alpha ds_\alpha - \frac{1}{2} e^{-2(\psi+\phi)}(2e^{2\phi} y_{1b} + (-2(y_{1a} y_{2a}) y_{2b} + (y_1^2 + y_2^2) y_{1b})) ds_2 dz_{2b} \\
&+ \frac{1}{2} e^{-2(\psi+\phi)}(2e^{2\phi} y_{2b} + (2(y_{1a} y_{2a}) y_{1b} + (y_1^2 + y_2^2) y_{2b})) ds_2 dz_{1b} \\
&+ e^{-2(\psi+\phi)}(y_2^2 s_1 + 2y_{2a} s_2 y_{1a} + s_1 y_1^2) ds_2 d\tilde{t} - \frac{1}{2} e^{-2(\psi+\phi)}(2e^{2\phi} y_{2b} + (2(y_{1a} y_{2a}) y_{1b} \\
&+ (y_1^2 + y_2^2) y_{2b})) ds_1 dz_{2b} - \frac{1}{2} e^{-2(\psi+\phi)}(2e^{2\phi} y_{1b} + (-2(y_{1a} y_{2a}) y_{2b} + (y_1^2 + y_2^2) y_{1b})) ds_1 dz_{1b} \\
&- e^{-2(\psi+\phi)}(y_1^2 s_2 - 2y_{1a} s_1 y_{2a} + s_2 y_2^2) ds_1 d\tilde{t} - \frac{1}{2} e^{-2(\phi+\psi)} \epsilon_{ij} \epsilon_{mn} (y_{ia} y_{jb}) dz_{ma} dz_{nb} \\
&+ \frac{1}{2} e^{-2(\psi+\phi)}(e^{2\phi} \delta_{ab} + (y_{1a} y_{1b} + y_{2a} y_{2b})) dz_{2a} dz_{2b} - e^{-2(\psi+\phi)}(2y_1 s_1 - 2s_2 y_2) dz_2 d\tilde{t} \\
&+ \frac{1}{2} e^{-4\psi}(e^{2\psi} \delta_{ab} + 2z_{2a} z_{2b} + e^{2(\psi-\phi)}(y_{1a} y_{1b} + y_{2a} y_{2b})) dz_{1a} dz_{1b} + (2e^{-4\psi}(s_2^2 + s_1^2) z_{2a} \\
&+ 2e^{-2(\psi+\phi)}(y_{1a} s_2 + s_1 y_{2a})) dz_{1a} d\tilde{t} + e^{-4(\psi+\phi)}(e^{2\psi} + e^{2\phi}(s_1^2 + s_2^2))^2 d\tilde{t} d\tilde{t} - 2e^{-4\phi} y_{1a} d\tilde{t} dy_{2a} \\
&+ \frac{1}{2} e^{-4\phi}(e^{2\phi} \delta_{ab} + 2y_{1a} y_{1b}) dy_{2a} dy_{2b} + \frac{1}{2} e^{-2\phi} dy_{1a} dy_{1a}. \qquad (9)
\end{aligned}$$

C. Chain of embeddings

We have the following chain of solvable Lie algebras

$$\mathfrak{s}_4 = \mathfrak{solv}\left(\frac{\mathrm{U}(2,2+n)}{\mathrm{U}(2)\times\mathrm{U}(2+n)}\right) \quad (\text{see}(3)),$$

$$\mathfrak{s}_3 = \mathfrak{solv}\left(\frac{\mathrm{SO}(2,2+n)}{\mathrm{SO}(2)\times\mathrm{SO}(2+n)}\right) = \mathrm{span}\{H_+,H_-\} + \mathrm{span}\{Z^{1a},Y^{1a},S_2^{(1,1)},S_2^{(1,-1)}\},$$

$$\mathfrak{s}_2 = \mathfrak{solv}\left(\frac{\mathrm{SU}(1,1+n)}{\mathrm{U}(1+n)}\right) = \mathrm{span}\{H_+ + H_-\} + \mathrm{span}\{Z^{1a},Y^{1a},S_2^{(1,1)}\},$$

$$\mathfrak{s}_1 = \mathfrak{solv}\left(\frac{\mathrm{SO}(1,1+n)}{\mathrm{SO}(1+n)}\right) = \mathrm{span}\{H_+ + H_-\} + \mathrm{span}\{Y^{1a}\}, \tag{10}$$

with $\mathfrak{s}_i \subset_{\mathrm{sub}} \mathfrak{s}_{i+1}$. Following the same procedure than in the previous examples, one can show that these solvable Lie algebras correspond to the following chain of symmetric spaces:

$$\frac{\mathrm{SO}(1,1+n)}{\mathrm{SO}(1+n)} \subset \frac{\mathrm{SU}(1,1+n)}{\mathrm{U}(1+n)} \subset \frac{\mathrm{SO}(2,2+n)}{\mathrm{SO}(2)\times\mathrm{SO}(2+n)} \subset \frac{\mathrm{U}(2,2+n)}{\mathrm{U}(2)\times\mathrm{U}(2+n)}. \tag{11}$$

Notice that in this chain we have

$$\frac{G_i}{H_i} \subset \frac{G_{i+1}}{H_{i+1}}$$

with

$$G_1 \subset G_2, \quad H_1 \subset H_2,$$

$$G_3 \subset G_4, \quad H_3 \subset H_4,$$

$$G_1 \subset G_3, \quad H_1 \subset H_3,$$

$$G_2 \subset G_4, \quad H_2 \subset H_4,$$

but G_2 is not in G_3 nor H_2 in H_3 for generic n.

The solvable parametrization (6) allows us to compute the metric of the spaces in (11) by imposing different restrictions on (9).

For the coset $\mathrm{SO}(2,2+n)/(\mathrm{SO}(2)\times\mathrm{SO}(2+n))$, we have

$$z_{2a} = y_{2a} = t = \tilde{t} = \tilde{s}_1 = s_2 = 0,$$

so the metric is

$$\begin{aligned} \mathrm{d}s^2 = {} & \mathrm{d}\phi^2 + \mathrm{d}\psi^2 + \tfrac{1}{2}e^{-2(\psi+\phi)}\mathrm{d}\tilde{s}_2\mathrm{d}\tilde{s}_2 - \tfrac{1}{2}e^{-2(\psi+\phi)}y_1^2\mathrm{d}\tilde{s}_2\mathrm{d}s_1 + e^{-2(\psi+\phi)}y_{1a}\mathrm{d}\tilde{s}_2\mathrm{d}z_{1a} + \tfrac{1}{8}e^{-2(\psi+\phi)}(4e^{4\phi}+(y_1^2)^2 \\ & + 4e^{2\phi}y_1^2)\mathrm{d}s_1\mathrm{d}s_1 - \tfrac{1}{2}e^{-2(\psi+\phi)}y_{1a}(2e^{2\phi}+y_1^2)\mathrm{d}s_1\mathrm{d}z_{1a} + \tfrac{1}{2}e^{-4\psi}(e^{2\psi}\delta_{ab} + e^{2(\psi-\phi)}y_{1a}y_{1b})\mathrm{d}z_{1a}\mathrm{d}z_{1b} \\ & + \tfrac{1}{2}e^{-2\phi}\mathrm{d}y_{1a}\mathrm{d}y_{1a}. \end{aligned} \tag{12}$$

Imposing the constraints $s_1 = \phi - \psi = 0$, we obtain the metric on $\mathrm{SU}(1,1+n)/\mathrm{U}(1+n)$,

$$ds^2 = 2d\phi^2 + \tfrac{1}{2}e^{-4\phi}d\tilde{s}_2 d\tilde{s}_2 + e^{-4\phi}y_{1a}d\tilde{s}_2 dz_{1a} + \tfrac{1}{2}e^{-4\phi}(e^{2\phi}\delta_{ab} + y_{1a}y_{1b})dz_{1a}dz_{1b} + \tfrac{1}{2}e^{-2\phi}dy_{1a}dy_{1a}, \tag{13}$$

and imposing $z_{1a}=\tilde{s}_2=0$, we obtain the metric for $SO(1,1+n)/SO(1+n)$:

$$ds^2 = 2d\phi^2 + \tfrac{1}{2}e^{-2\phi}dy_{1a}dy_{1a} \tag{14}$$

which, up to a rescaling of the coordinates, corresponds to (3).

We can further impose $y_{1n}=0$ to obtain the same form than (14) but with $a=1,\ldots,n-1$. It is the metric of $SO(1,n)/SO(n)$.

D. Truncations and integration of massive modes

Let us consider a sigma model described by the metric (14). As we have seen, this model has n translational isometries corresponding to the coordinates y_{1a}. We may consider gauging one of these isometries, say y_{1n}. We introduce a gauge field $A=A_\mu dx^\mu$ and substitute dy_{1n} by the covariant differential

$$Dy_{1n} = dy_{1n} + gA.$$

We redefine the connection by a gauge transformation

$$\hat{A} = A + \frac{1}{g}dy_{1n},$$

which will not change the kinetic term for A. Substituting this definition in the metric we obtain

$$ds^2 = 2d\phi^2 + \frac{1}{2}e^{-2\phi}\sum_{a=1}^{n-1} dy_{1a}dy_{1a} + \frac{1}{2}e^{-2\phi}g^2\hat{A}^2.$$

We see that the effect of the gauging is absorbing the field y_{1n} to give mass to the gauge vector. Moreover, in this model $\hat{A}$ is decoupled from the rest of fields (except for the warping factor $e^{-2\phi}$), so setting $\hat{A}=0$ is consistent with the equations of motion. After the truncation the sigma model becomes $SO(1,n)/SO(n)$. This is explained by the mathematical identity

$$\mathfrak{solv}\left(\frac{SO(1,1+n)}{SO(1+n)}\right) = \mathfrak{solv}\left(\frac{SO(1,1+n-k)}{SO(1+n-k)}\right) \ltimes \mathbb{R}^k$$

which is a consequence of (2).

We want to consider now the model SU(1, 2)/U(2), with metric (13) for $n=1$. Note that $\tilde{s}_2$ and z_1 are translational isometries. As before, we can gauge them by introducing abelian connections A^1, A^2 with covariant differentials

$$d\tilde{s}_2 \to D\tilde{s}_2 = d\tilde{s}_2 + k_1 A^1,$$

$$dz_1 \to Dz_1 = dz_1 + k_2 A^2.$$

We define the gauge-transformed connections

$$\hat{A}^1 = A^1 + \frac{1}{k_1}d\tilde{s}_2,$$

$$\hat{A}^2 = A^2 + \frac{1}{k_2}dz_1.$$

By substituting this definition, we can see that in the metric there will appear the terms

$$ds^2 = \cdots + \tfrac{1}{2}e^{-4\phi}(k_1)^2(\hat{A}^1)^2 + \cdots + \tfrac{1}{2}e^{-2\phi}(k_2)^2(\hat{A}^2)^2 + \cdots \ .$$

So, as before, the effect of the gauging has been to give mass to the vectors by absorbing the modes associated to the translational isometries.

Nevertheless, in this case other interactions are present. By assuming that the mass of the vectors is big enough we can take their kinetic terms to zero, and then we obtain algebraic equations for $\hat{A}^1$, $\hat{A}^2$. A straightforward calculation shows that, after the elimination of these fields the metric that remains is SO(1, 2)/SO(2), that is Eq. (14) with $n=1$.

The difference between the two models here described is that in the first case the integration of the massive modes is exact (that is, it is a consistent truncation of the theory), while in the second case a limiting process is involved (masses $\to\infty$).

In the next section we will see that these integrations can be modeled by a *contraction* of the metric of the initial manifold, followed by a *quotienting* of the manifold by a submanifold.

III. CONTRACTIONS OF GROUPS AND COSET SPACES

A. Contraction of a Lie algebra with respect to a subalgebra

We describe the Inönü-Wigner contraction of an algebra with respect to a subalgebra. Let $\mathfrak{g}$ be an arbitrary, finite dimensional Lie algebra with commutator $[,]$ and let $\mathfrak{g}=\mathfrak{g}_1+\mathfrak{g}_2$, with $\mathfrak{g}_1$ a subalgebra. We define the following family of linear maps

$$\phi_\epsilon : \mathfrak{g} \to \mathfrak{g},$$

$$x = x_1 \oplus x_2 \to x = x_1 \oplus \epsilon x_2,$$

labeled by a real parameter ϵ, In matrix form, the map and its inverse ($\epsilon \neq 0$) are block diagonal

$$\phi_\epsilon = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \epsilon\mathbb{1} \end{pmatrix}, \quad \phi_\epsilon^{-1} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \frac{1}{\epsilon}\mathbb{1} \end{pmatrix}.$$

We can define a new commutator

$$[X,Y]_\epsilon = \phi_\epsilon^{-1}([\phi_\epsilon(X), \phi_\epsilon(Y)]), \quad X,Y \in \mathfrak{g}.$$

$[,]_\epsilon$ is a *deformed bracket*, but of a simple form, since for $\epsilon \neq 0$ is, by construction, isomorphic to the bracket with $\epsilon=1$. We define the *contraction* of $\mathfrak{g}$ with respect to the subalgebra $\mathfrak{g}_1$ as a Lie algebra with the same supporting vector space $\mathfrak{g}_c \approx \mathfrak{g}$ and with commutator

$$[X,Y]_c = \lim_{\epsilon\to 0} \phi_\epsilon^{-1}([\phi_\epsilon(X), \phi_\epsilon(Y)]), \quad X,Y \in \mathfrak{g}. \tag{15}$$

This bracket is well defined but, since ϕ_0 is not invertible, $[,]_c$ will not be, in general, isomorphic to the original bracket.

B. Representations of the contracted algebra

We consider now a representation of $\mathfrak{g}$ on a finite dimensional vector space W

$$R(X): W \to W, \quad X \in \mathfrak{g}$$

and assume that $W=W_1 \oplus W_2$ with W_1 an invariant subspace under the action of the subalgebra $\mathfrak{g}_1$. As before, we define a one parameter family of linear maps

$$\psi_\epsilon : W \to W,$$

$$w = w_1 \oplus w_2 \rightarrow w = w_1 \oplus \epsilon w_2,$$

so

$$\psi_\epsilon = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \epsilon\mathbb{1} \end{pmatrix}, \quad \psi_\epsilon^{-1} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \frac{1}{\epsilon}\mathbb{1} \end{pmatrix}.$$

Let us denote

$$R_\epsilon(X) = \psi_\epsilon^{-1} \circ R(\phi_\epsilon(X)) \circ \psi_\epsilon, \quad X \in \mathfrak{g}.$$

R_ϵ is a representation of the deformed algebra. It is easy to check that the map R_c

$$R_c(X) = \lim_{\epsilon \to 0} R_\epsilon(X)$$

is a representation of $\mathfrak{g}_c$ on W.

Notice that $\psi_\epsilon = \phi_\epsilon$ for the adjoint representation.

C. Generalized contractions

The map ϕ_ϵ can in fact be more general than the one considered before, the only constraint being that the bracket in (15) is well defined. The conditions for this to happen were studied in Ref. 13 and are called *generalized Inönü-Wigner contractions*. They are also a particular example of *algebra expansions*.[14]

We will use particular examples of generalized contractions where the brackets can be seen explicitly to have a well defined limit. We will not describe the general theory of these contractions, for which we refer to the original paper, Ref. 13.

D. Deformations and contractions of the metric: Some examples

As we have seen, we can always contract an algebra $\mathfrak{g}$ with respect to a subalgebra $\mathfrak{g}'$. The contracted algebra, $\mathfrak{g}_c$ will have always the structure of a semidirect product

$$\mathfrak{g}_c = \mathfrak{g}' \ltimes \mathbb{R}^n.$$

In chain (10) we have described subalgebras of $\mathfrak{s}_4$, so we can contract each algebra $\mathfrak{s}_i$ with respect to $\mathfrak{s}_j$ with $j < i$

Since the solvable Lie algebras are related to the corresponding symmetric spaces, we are going to define a procedure to contract the symmetric spaces. We will start with a representation R_ϵ of the deformed Lie algebra, and compute the coset representative as in (6) with this new representation. From this, one can compute a deformed vielbein and a deformed metric. This procedure will introduce the parameter ϵ in the metric, so we will have a uniparametric family of metrics. Then, we can take the limit $\epsilon \rightarrow 0$.

We are interested in the simple examples presented in Sec. II D. The first one is trivial, since the contraction of $\mathfrak{s}_1$ for arbitrary n by the subalgebra $\mathfrak{s}_1$ for $n-1$ has no effect, giving again $\mathfrak{s}_1$ for n.

Let us see how this works with the next example. We start with the algebra $\mathfrak{so}\mathfrak{l}\mathfrak{v}(\mathrm{SU}(1,2)/\mathrm{U}(2))$ (which is $\mathfrak{s}_2$ for $n=1$) and we will work out the contraction with respect to $\mathfrak{so}\mathfrak{l}\mathfrak{v}(\mathrm{SO}(1,2)/\mathrm{SO}(2))$ which is ($\mathfrak{s}_1$ for $n=1$).

$$\mathfrak{s}_2(n=1) = \mathrm{span}\{H_1 = H_+ + H_-\} + \mathrm{span}\{Z^1, Y^1, S_1^{(1,1)}\}, \tag{16}$$

$$\mathfrak{s}_1(n=1) = \mathrm{span}\{H_1\} + \mathrm{span}\{Y^1\}. \tag{17}$$

It is convenient to write explicitly the commutation rules

$$[H_1,Z^1]=Z^1,\quad [H_1,Y^1]=Y^1,\quad [H_1,S_1^{(1,1)}]=2S_1^{(1,1)},\quad [Z^1,Y^1]=S_1^{(1,1)}.$$

The deformed algebra is

$$[H_1,Z^1]_\epsilon=Z^1,\quad [H,Y^1]_\epsilon=Y^1,\quad [H_1,S_1^{(1,1)}]_\epsilon=2S_1^{(1,1)},\quad [Z^1,Y^1]_\epsilon=\epsilon S_1^{(1,1)}\to 0.$$

The contracted algebra has the property that the only elements in $\mathfrak{g}'$ that act on the abelian factor $\mathbb{R}^n$ are the elements of the commuting subalgebra of $\mathfrak{p}$. In our case this subalgebra is $H_1=H_+ +H_-$. This property will translate in a particularly simple form of the metric.

We consider the three-dimensional representation (induced from the fundamental of $\mathfrak{su}(1,2)$). We decompose the representation space as

$$\mathbb{C}^3=V_1\oplus V_2,\quad V_1=\left\{\begin{pmatrix} v_1\\ 0\\ v_3\end{pmatrix}\right\},\quad V_2=\left\{\begin{pmatrix} 0\\ v_2\\ 0\end{pmatrix}\right\},$$

being V_1 an invariant subspace under the subalgebra (17) and consider the linear map $\psi_\epsilon(e_1\oplus e_2)=e_1\oplus\epsilon e_2$. Then we have a three dimensional representation of the deformed algebra,

$$R_\epsilon(H_1)=\begin{pmatrix} 0 & 0 & 1\\ 0 & 0 & 0\\ 1 & 0 & 0\end{pmatrix},$$

$$R_\epsilon(Z^1)=\begin{pmatrix} 0 & i & 0\\ i\epsilon^2 & 0 & -i\epsilon^2\\ 0 & i & 0\end{pmatrix}\to\begin{pmatrix} 0 & i & 0\\ 0 & 0 & 0\\ 0 & i & 0\end{pmatrix},$$

$$R_\epsilon(Y^1)=\begin{pmatrix} 0 & 1 & 0\\ -\epsilon^2 & 0 & \epsilon^2\\ 0 & 1 & 0\end{pmatrix}\to\begin{pmatrix} 0 & 1 & 0\\ 0 & 0 & 0\\ 0 & 1 & 0\end{pmatrix},$$

$$R_\epsilon(S_1^{(1,1)})=-\epsilon\begin{pmatrix} i & 0 & 0\\ 0 & i & 0\\ 0 & 0 & -2i\end{pmatrix}\to 0.$$

We compute now the vielbein and the metric in the way that we indicated in Sec. II. Notice that the Euclidean metric that we put on the solvable Lie algebra with the deformed bracket is *the same* as the one for $\epsilon=1$. In this way the normal metric Lie algebras (in the terminology of Ref. 9) are not isomorphic, nor are isometric the corresponding Riemannian spaces. We obtain then a true deformation of the metric.

The result is

$$ds^2=2d\phi^2+\tfrac{1}{2}e^{-4\phi}d\tilde{s}_2d\tilde{s}_2+\epsilon^2e^{-4\phi}y_1d\tilde{s}_2dz_1+\tfrac{1}{2}e^{-4\phi}(e^{2\phi}+\epsilon^4y_1^2)dz_1dz_1+\tfrac{1}{2}e^{-2\phi}dy_1dy_1,\quad (18)$$

which can be compared with (13) for $\epsilon=1$.

For $\epsilon\to 0$ we get

$$ds^2=\left(2d\phi^2+\tfrac{1}{2}e^{-2\phi}dy_1dy_1\right)+\tfrac{1}{2}e^{-2\phi}dz_1dz_1+\tfrac{1}{2}e^{-4\phi}d\tilde{s}_2d\tilde{s}_2.\quad (19)$$

The first two factors correspond to (14). The remaining modes appear decoupled except for warping factors of type $e^{a\phi}/2$. Then, imposing the constraints $z_1=0=\tilde{s}_2$ is always a consistent truncation of the contracted sigma model (19). We see with this simple example that integrating

out massive modes can be geometrically modeled by a contraction of the sigma model, followed by a quotienting by the decoupled modes.

It is instructive to compute Ricci tensor of the deformed metric (18). We obtain (in the ordered basis $\phi, y_1, z_1, \tilde{s}_2$)

$$R^a_b(\epsilon) = \begin{pmatrix} -6 & 0 & 0 & 0 \\ 0 & -2(2+\epsilon^4) & 0 & 0 \\ 0 & 0 & -2(2+\epsilon^4) & 0 \\ 0 & 0 & 8y_1\epsilon^2(\epsilon^4-1) & 2(-4+\epsilon^4) \end{pmatrix}. \tag{20}$$

We see that for arbitrary ϵ it is not an Einstein space. In the relevant limits

$$R^a_b(1) = \begin{pmatrix} -6 & 0 & 0 & 0 \\ 0 & -6 & 0 & 0 \\ 0 & 0 & -6 & 0 \\ 0 & 0 & 0 & -6 \end{pmatrix}, \quad R^a_b(0) = \begin{pmatrix} -6 & 0 & 0 & 0 \\ 0 & -4 & 0 & 0 \\ 0 & 0 & -4 & 0 \\ 0 & 0 & 0 & -8 \end{pmatrix}.$$

For $\epsilon=1$ we have an Einstein space, but not for arbitrary ϵ. It becomes clear from this simple example that the deformation cannot be reabsorbed by a change of coordinates.

We consider now the Inönu-Wigner contraction of $\mathfrak{s}_4$ with respect to $\mathfrak{s}_3$. For simplicity, we take $n=1$, so we have $\mathfrak{s}_4=\mathfrak{s}_3+\mathfrak{g}$ where

$$\mathfrak{s}_3 = \mathrm{span}\{H_+, H_-, S_2^{(1,1)}, S_1^{(1,-1)}, Y^1, Z^1\},$$

$$\mathfrak{g} = \mathrm{span}\{T^{(2,0)}, T^{(0,2)}, S_1^{(1,1)}, S_2^{(1,-1)}, Y^2, Z^2\}.$$

Differently from the first example, we use the adjoint representation to introduce the parameter ϵ. The result for the metric is

$$\begin{aligned}
\mathrm{d}s^2 = {} & \mathrm{d}\phi^2 + \mathrm{d}\psi^2 + e^{-4\psi}\mathrm{d}t\mathrm{d}t + 2e^{-4\psi}s_1\mathrm{d}t\mathrm{d}\tilde{s}_1 + 2e^{-4\psi}s_2\mathrm{d}t\mathrm{d}\tilde{s}_2 + 2e^{-4\psi}z_2\mathrm{d}t\mathrm{d}z_1 + 2e^{-4\psi}(s_2^2\epsilon^2 \\
& + s_1^2)\mathrm{d}t\mathrm{d}\tilde{t} \\
& + \tfrac{1}{2}(e^{-2(\psi+\phi)} + 2e^{-4\psi}s_1^2)\mathrm{d}\tilde{s}_1\mathrm{d}\tilde{s}_1 + 2e^{-4\psi}s_2s_1\mathrm{d}\tilde{s}_1\mathrm{d}\tilde{s}_2 + \tfrac{1}{2}e^{-2(\psi+\phi)}(y_1^2 + y_2^2\epsilon^2)\mathrm{d}\tilde{s}_1\mathrm{d}s_2 \\
& + e^{-2(\psi+\phi)}y_1y_2\mathrm{d}\tilde{s}_1\mathrm{d}s_1 - e^{-2(\psi+\phi)}y_1\mathrm{d}\tilde{s}_1\mathrm{d}z_2 + (2e^{-4\psi}s_1z_2 + e^{-2(\psi+\phi)}y_2)\mathrm{d}\tilde{s}_1\mathrm{d}z_1 \\
& + 2e^{-4\psi}s_1(e^{2(\psi-\phi)} + s_2^2\epsilon^2 + s_1^2)\mathrm{d}\tilde{s}_1\mathrm{d}\tilde{t} + \tfrac{1}{2}(e^{-2(\psi+\phi)} + 2e^{-4\psi}s_2^2)\mathrm{d}\tilde{s}_2\mathrm{d}\tilde{s}_2 + e^{-2(\psi+\phi)}y_1y_2\epsilon^2\mathrm{d}\tilde{s}_2\mathrm{d}s_2 \\
& - \tfrac{1}{2}e^{-2(\psi+\phi)}(y_1^2 + y_2^2\epsilon^2)\mathrm{d}\tilde{s}_2\mathrm{d}s_1 + e^{-2(\psi+\phi)}y_2\epsilon^2\mathrm{d}\tilde{s}_2\mathrm{d}z_2 + (2e^{-4\psi}s_2z_2 + e^{-2(\psi+\phi)}y_1)\mathrm{d}\tilde{s}_2\mathrm{d}z_1 \\
& + 2e^{-4\psi}s_2(e^{2(\psi-\phi)}\epsilon^2 + s_2^2\epsilon^2 + s_1^2)\mathrm{d}\tilde{s}_2\mathrm{d}\tilde{t} + \tfrac{1}{8}e^{-2(\psi+\phi)}(4e^{4\phi} + y_1^4 + (2\epsilon^2 + 4\epsilon^4)y_1^2y_2^2 + y_2^4\epsilon^4 \\
& + 4e^{2\phi}(y_1^2 + y_2^2\epsilon^4))\mathrm{d}s_2\mathrm{d}s_2 - \tfrac{1}{2}e^{-2(\psi+\phi)}y_1(2e^{2\phi} + y_1^2 - (2\epsilon^4 - \epsilon^2)y_2^2)\mathrm{d}s_2\mathrm{d}z_2 + \tfrac{1}{2}e^{-2(\psi+\phi)}y_2 \\
& \times(2e^{2\phi}\epsilon^2 + (2\epsilon^2 + 1)y_1^2 + y_2^2\epsilon^2)\mathrm{d}s_2\mathrm{d}z_1 + e^{-2(\psi+\phi)}(y_2^2s_1\epsilon^2 + 2y_2s_2y_1\epsilon^4 + s_1y_1^2)\mathrm{d}s_2\mathrm{d}\tilde{t} \\
& + \tfrac{1}{8}e^{-2(\psi+\phi)} \\
& \times(4e^{4\phi} + y_1^4 + (2\epsilon^2 + 4)y_1^2y_2^2 + y_2^4\epsilon^4 + 4e^{2\phi}(y_1^2 + y_2^2))\mathrm{d}s_1\mathrm{d}s_1 - \tfrac{1}{2}e^{-2(\psi+\phi)} \\
& \times y_2(2e^{2\phi} + (2+\epsilon^2)y_1^2 + y_2^2\epsilon^4)\mathrm{d}s_1\mathrm{d}z_2 - \tfrac{1}{2}e^{-2(\psi+\phi)}y_1(2e^{2\phi} + y_1^2 - (2-\epsilon^2)y_2^2)\mathrm{d}s_1\mathrm{d}z_1 \\
& - e^{-2(\psi+\phi)}(y_1^2s_2\epsilon^2 - 2y_1s_1y_2 + s_2y_2^2\epsilon^4)\mathrm{d}s_1\mathrm{d}\tilde{t} + \tfrac{1}{2}e^{-2(\psi+\phi)}(e^{2\phi} + y_1^2 + y_2^2\epsilon^4)\mathrm{d}z_2\mathrm{d}z_2 \\
& - e^{-2(\psi+\phi)}(2y_1s_1 - 2s_2y_2\epsilon^4)\mathrm{d}z_2\mathrm{d}\tilde{t} + \tfrac{1}{2}e^{-4\psi}(e^{2\psi} + 2z_2^2 + e^{2(\psi-\phi)}(y_1^2 + y_2^2))\mathrm{d}z_1\mathrm{d}z_1 \\
& + (2e^{-4\psi}(s_2^2\epsilon^2 + s_1^2)z_2 + 2e^{-2(\psi+\phi)}(y_1s_2\epsilon^2 + s_1y_2))\mathrm{d}z_1\mathrm{d}\tilde{t}(e^{-4\phi} + 2e^{-2(\phi+\psi)}(s_1^2 + s_2^2\epsilon^4)
\end{aligned}$$

$$+ e^{-4\psi}(s_1^4 + 2s_1^2 s_2^2\epsilon^2 + s_2^4\epsilon^4))\mathrm{d}\tilde{t}\mathrm{d}\tilde{t} - 2e^{-4\phi}y_1\mathrm{d}\tilde{t}\mathrm{d}y_2 + \tfrac{1}{2}e^{-4\phi}(e^{2\phi} + 2y_1^2)\mathrm{d}y_2\mathrm{d}y_2 + \tfrac{1}{2}e^{-2\phi}\mathrm{d}y_1\mathrm{d}y_1$$
$$+ e^{-2(\phi+\psi)}y_1y_2\ (\epsilon^2 - 1)\mathrm{d}z_1\mathrm{d}z_2) + \tfrac{1}{2}e^{-2\psi}y_1y_2(1 - \epsilon^2)(2 + e^{-2\phi}(y_1^2 + y_2^2\epsilon^2))\mathrm{d}s_1\mathrm{d}s_2, \tag{21}$$

which can be compared with (9) for $\epsilon=1$. For $\epsilon=0$ it becomes

$$\begin{aligned}
\mathrm{d}s^2 = &\big(\mathrm{d}\phi^2 + \mathrm{d}\psi^2 + \tfrac{1}{2}e^{-4\psi}(e^{-2(\phi-\psi)} + 2s_2^2)\mathrm{d}\tilde{s}_2^2 - \tfrac{1}{2}e^{-2(\phi+\psi)}y_1^2\mathrm{d}\tilde{s}_2\mathrm{d}s_1 + (e^{-2(\phi+\psi)}y_1 \\
&+ 2e^{-4\psi}s_2z_2)\mathrm{d}\tilde{s}_2\mathrm{d}z_1 \\
&+ \tfrac{1}{8}e^{-2(\phi+\psi)}(4e^{4\phi} + y_1^4 + 4y_1^2y_2^2 + 4e^{2\phi}(y_1^2 + y_2^2))\mathrm{d}s_1^2 - \tfrac{1}{2}e^{-2(\phi+\psi)}y_1(2e^{2\phi} + y_1^2 - 2y_2^2)\mathrm{d}s_1\mathrm{d}z_1 \\
&+ \tfrac{1}{2}e^{-4\psi}(e^{2\psi} + e^{-2(\phi-\psi)}(y_1^2 + y_2^2) + 2z_2^2)\mathrm{d}z_1^2 + \tfrac{1}{2}e^{-2\phi}\mathrm{d}y_1^2\big) + e^{-4\psi}\mathrm{d}t^2 + e^{-4(\phi+\psi)}(e^{2\psi} \\
&+ e^{2\phi}s_1^2)^2\mathrm{d}\tilde{t}^2 + \tfrac{1}{2}e^{-4\psi}(e^{-2(\phi-\psi)} + 2s_1^2)\mathrm{d}\tilde{s}_1^2 + \tfrac{1}{8}e^{-2(\phi+\psi)}(2e^{2\phi} + y_1^2)^2\mathrm{d}s_2^2 + \tfrac{1}{2}e^{-4\phi}(e^{2\phi} + 2y_1^2)\mathrm{d}y_2^2 \\
&+ \tfrac{1}{2}e^{-2(\phi+\psi)}(e^{2\phi} + y_1^2)\mathrm{d}z_2^2 + 2e^{-4\psi}s_1^2\mathrm{d}t\mathrm{d}\tilde{t} + 2e^{-4\psi}s_1\mathrm{d}t\mathrm{d}\tilde{s}_1 + 2e^{-4\psi}s_2\mathrm{d}t\mathrm{d}\tilde{s}_2 + 2e^{-4\psi}z_2\mathrm{d}t\mathrm{d}z_1 \\
&+ 2e^{-2(\phi+2\psi)}s_1(e^{2\psi} + e^{2\phi}s_1^2)\mathrm{d}\tilde{t}\mathrm{d}\tilde{s}_1 + 2e^{-4\psi}s_1^2s_2\mathrm{d}\tilde{t}\mathrm{d}\tilde{s}_2 + 2e^{-2(\phi+\psi)}s_1y_1y_2\mathrm{d}\tilde{t}\mathrm{d}s_1 \\
&+ e^{-2(\phi+\psi)}s_1y_1^2\mathrm{d}\tilde{t}\mathrm{d}s_2 - 2e^{-4\phi}y_1\mathrm{d}\tilde{t}\mathrm{d}y_2 + 2e^{-2(\phi+2\psi)}s_1(e^{2\psi}y_2 + e^{2\phi}s_1z_2) \\
&\times\mathrm{d}\tilde{t}\mathrm{d}z_1 - 2e^{-2(\phi+\psi)}s_1y_1\mathrm{d}\tilde{t}\mathrm{d}z_2 + 2e^{-4\psi}s_1s_2\mathrm{d}\tilde{s}_1\mathrm{d}\tilde{s}_2 + e^{-2(\phi+\psi)}y_1y_2\mathrm{d}\tilde{s}_1\mathrm{d}s_1 + \tfrac{1}{2}e^{-2(\phi+\psi)}y_1^2\mathrm{d}\tilde{s}_1\mathrm{d}s_2 \\
&+ e^{-4\psi}(e^{-2(\phi-\psi)}y_2 + 2s_1z_2)\mathrm{d}\tilde{s}_1\mathrm{d}z_1 - e^{-2(\phi+\psi)}y_1\mathrm{d}\tilde{s}_1\mathrm{d}z_2 + \tfrac{1}{2}e^{-2(\phi+\psi)}y_1(2e^{2\phi} + y_1^2)y_2\mathrm{d}s_1\mathrm{d}s_2 \\
&- e^{-2(\phi+\psi)}y_2(e^{2\phi} + y_1^2)\mathrm{d}s_1\mathrm{d}z_2 - \tfrac{1}{2}e^{-2(\phi+\psi)}y_1(2e^{2\phi} + y_1^2)\mathrm{d}s_2\mathrm{d}z_2 + \tfrac{1}{2}e^{-2(\phi+\psi)}y_1^2y_2\mathrm{d}s_2\mathrm{d}z_1 \\
&- e^{-2(\phi+\psi)}y_1y_2\mathrm{d}z_1\mathrm{d}z_2
\end{aligned} \tag{22}$$

We can compare the first five lines of (22) with (12). They are different, but the extra terms are zero when imposing the constraints

$$z_2 = y_2 = t = \tilde{t} = \tilde{s}_1 = s_2 = 0.$$

This means that there is an isometric embedding of $\mathrm{SO}(2,3)/(\mathrm{SO}(2)\times\mathrm{SO}(3))$ in the manifold with the metric (22). We can improve this result by making use of a generalized contraction, that gives a simpler contracted metric. We will do that in the next section.

E. Generalized contractions: Some examples

1. Generalized contraction of $\mathbf{U(2,3)/(U(2)\times U(3))}$

We consider the following decomposition of s_4,

$$\mathfrak{s}_4 = \mathfrak{g}_0 + \mathfrak{g}_1 + \mathfrak{g}_2 + \mathfrak{g}_3,$$

where

$$\mathfrak{g}_0 = \mathrm{span}\{H_+, H_-, S_2^{(1,1)}, S_1^{(1,-1)}, Y^1, Z^1, T^{(2,0)}\},$$

$$\mathfrak{g}_1 = \mathrm{span}\{S_1^{(1,1)}\}, \quad \mathfrak{g}_2 = \mathrm{span}\{T^{(0,2)}, Z^2\}, \quad \mathfrak{g}_3 = \mathrm{span}\{S_2^{(1,-1)}, Y^2\}$$

and the linear map

$$\begin{array}{ccc} \mathfrak{s}_4 & \xrightarrow{\phi_\epsilon} & \mathfrak{s}_4 \\ e_0 + e_1 + e_2 + e_3 & \longrightarrow & e_0 + \epsilon e_1 + \epsilon^2 e_2 + \epsilon^3 e_3 \end{array} \quad \text{with } e_i \in \mathfrak{g}_i.$$

Equation (15) gives a deformed bracket that has a well defined limit when $\epsilon\to 0$. We write here the contracted bracket. The only surviving commutators from (5) when $\epsilon\to 0$ are

$$[Z^1, Y^1] = S_2^{(1,1)},$$

$$[Y^1, S_1^{(1,-1)}] = Z^1,$$

$$[H_+, Z^i] = Z^i,$$

$$[H_-, Y^i] = Y^i,$$

so the contracted algebra has as a subalgebra

$$\mathfrak{solo}\left(\frac{\mathrm{SO}(2,3)}{\mathrm{SO}(2)\times\mathrm{SO}(3)}\right) = \mathrm{span}\{H_+, H_-\} + \mathrm{span}\{Z^1, Y^1, S_2^{(1,1)}, S_1^{(1,-1)}\}$$

in semidirect product with $\mathbb{R}^6 = \mathrm{span}\{Z^2, Y^2, T^{(0,2)}, T^{2,0}, S_1^{(1,1)}, S_2^{(1,-1)}\}$, where the only generators that act on $\mathbb{R}^6$ are H_+ and H_-.

We use the adjoint representation of the deformed algebra to compute the deformed metric. The result is

$$\begin{aligned}
\mathrm{d}s^2 &= \mathrm{d}\phi^2 + \mathrm{d}\psi^2 + e^{-4\psi}\mathrm{d}t\mathrm{d}t + 2e^{-4\psi}s_1\epsilon\mathrm{d}t\mathrm{d}\tilde{s}_1 + 2e^{-4\psi}s_2\epsilon^3\mathrm{d}t\mathrm{d}\tilde{s}_2 + 2e^{-4\psi}z_2\epsilon^2\mathrm{d}t\mathrm{d}z_1 \\
&+ 2e^{-4\psi}(s_2^2\epsilon^2 + s_1^2\epsilon^8)\mathrm{d}t\mathrm{d}\tilde{t} + \tfrac{1}{2}(e^{-2(\psi+\phi)} + 2e^{-4\psi}s_1^2\epsilon^2)\mathrm{d}\tilde{s}_1\mathrm{d}\tilde{s}_1 + 2e^{-4\psi}s_2s_1\epsilon^4\mathrm{d}\tilde{s}_1\mathrm{d}\tilde{s}_2 \\
&+ \tfrac{1}{2}e^{-2(\psi+\phi)}(y_1^2\epsilon^2 + y_2^2\epsilon^8)\mathrm{d}\tilde{s}_1\mathrm{d}s_2 + e^{-2(\psi+\phi)}y_1y_2\epsilon^2\mathrm{d}\tilde{s}_1\mathrm{d}s_1 - e^{-2(\psi+\phi)}y_1\epsilon\mathrm{d}\tilde{s}_1\mathrm{d}z_2 \\
&+ (2e^{-4\psi}s_1z_2\epsilon^3 + e^{-2(\psi+\phi)}y_2\epsilon^2)\mathrm{d}\tilde{s}_1\mathrm{d}z_1 + 2e^{-4\psi}s_1(e^{2(\psi-\phi)}\epsilon + s_2^2\epsilon^9 + s_1^2\epsilon^3)\mathrm{d}\tilde{s}_1\mathrm{d}\tilde{t} \\
&+ \tfrac{1}{2}(e^{-2(\psi+\phi)} + 2e^{-4\psi}s_2^2\epsilon^6)\mathrm{d}\tilde{s}_2\mathrm{d}\tilde{s}_2 + e^{-2(\psi+\phi)}y_1y_2\epsilon^6\mathrm{d}\tilde{s}_2\mathrm{d}s_2 - \tfrac{1}{2}e^{-2(\psi+\phi)}(y_1^2 + y_2^2\epsilon^6)\mathrm{d}\tilde{s}_2\mathrm{d}s_1 \\
&+ e^{-2(\psi+\phi)}y_2\epsilon^5\mathrm{d}\tilde{s}_2\mathrm{d}z_2 + (2e^{-4\psi}s_2z_2\epsilon^5 + e^{-2(\psi+\phi)}y_1)\mathrm{d}\tilde{s}_2\mathrm{d}z_1 \\
&+ 2e^{-4\psi}s_2(e^{2(\psi-\phi)}\epsilon^5 + s_2^2\epsilon^{11} + s_1^2\epsilon^5)\mathrm{d}\tilde{s}_2\mathrm{d}\tilde{t} + \tfrac{1}{8}e^{-2(\psi+\phi)}(4e^{4\phi} + y_1^4\epsilon^4 + (4\epsilon^{12} + 2\epsilon^{10})y_1^2y_2^2 \\
&+ y_2^4\epsilon^{16} \\
&+ 4e^{2\phi}(y_1^2\epsilon^2 + y_2^2\epsilon^{12}))\mathrm{d}s_2\mathrm{d}s_2 - \tfrac{1}{2}e^{-2(\psi+\phi)}y_1(2e^{2\phi}\epsilon + y_1^2\epsilon^3 - (2\epsilon^{11} - \epsilon^9)y_2^2)\mathrm{d}s_2\mathrm{d}z_2 \\
&+ \tfrac{1}{2}e^{-2(\psi+\phi)}y_2(2e^{2\phi}\epsilon^6 + (\epsilon^2 + 2\epsilon^6)y_1^2 + y_2^2\epsilon^{10})\mathrm{d}s_2\mathrm{d}z_1 + e^{-2(\psi+\phi)}(y_2^2s_1\epsilon^9 + 2y_2s_2y_1\epsilon^{11} + s_1y_1^2\epsilon^3) \\
&\times\mathrm{d}s_2\mathrm{d}\tilde{t} + \tfrac{1}{8}e^{-2(\psi+\phi)}(4e^{4\phi} + y_1^4 + (4\epsilon^4 + 2\epsilon^6)y_1^2y_2^2 + y_2^4\epsilon^{12} + 4e^{2\phi}(y_1^2 + y_2^2\epsilon^2))\mathrm{d}s_1\mathrm{d}s_1 \\
&\times - \tfrac{1}{2}e^{-2(\psi+\phi)}y_2(2e^{2\phi}\epsilon + (2\epsilon^3 + \epsilon^5)y_1^2 + y_2^2\epsilon^{11})\mathrm{d}s_1\mathrm{d}z_2 - \tfrac{1}{2}e^{-2(\psi+\phi)}y_1(2e^{2\phi} + y_1^2 - (2\epsilon^4 - \epsilon^6)y_2^2) \\
&\times\mathrm{d}s_1\mathrm{d}z_1 - e^{-2(\psi+\phi)}(y_1^2s_2\epsilon^5 - 2y_1s_1y_2\epsilon^3 + s_2y_2^2\epsilon^{11})\mathrm{d}s_1\mathrm{d}\tilde{t} + \tfrac{1}{2}e^{-2(\psi+\phi)}(e^{2\phi} + y_1^2\epsilon^2 + y_2^2\epsilon^{10}) \\
&\times\mathrm{d}z_2\mathrm{d}z_2 - e^{-2(\psi+\phi)}(2y_1s_1\epsilon^2 - 2s_2y_2\epsilon^{10})\mathrm{d}z_2\mathrm{d}\tilde{t} + \tfrac{1}{2}e^{-4\psi}(e^{2\psi} + 2z_2^2\epsilon^4 + e^{2(\psi-\phi)}(y_1^2 + y_2^2\epsilon^2)) \\
&\times\mathrm{d}z_1\mathrm{d}z_1 + (2e^{-4\psi}(s_2^2\epsilon^{10} + s_1^2\epsilon^4)z_2 + 2e^{-2(\psi+\phi)}(y_1s_2\epsilon^3 + s_1y_2\epsilon^5))\mathrm{d}z_1\mathrm{d}\tilde{t} \\
&+ (e^{4\psi} + e^{4\phi}(s_1^4\epsilon^4 + 2s_1^2s_2^2\epsilon^{10} + s_2^4\epsilon^{16}) + 2e^{2(\phi+\psi)}(s_1^2\epsilon^2 + s_2^2\epsilon^{10}))\mathrm{d}\tilde{t}\mathrm{d}\tilde{t} - 2e^{-4\phi}y_1\epsilon\mathrm{d}\tilde{t}\mathrm{d}y_2 \\
&+ \tfrac{1}{2}e^{-4\phi}(e^{2\phi} + 2y_1^2\epsilon^2)\mathrm{d}y_2\mathrm{d}y_2 + \tfrac{1}{2}e^{-2\phi}\mathrm{d}y_1\mathrm{d}y_1 + e^{-2(\phi+\psi)}y_1y_2(\epsilon^5 - \epsilon^3)\mathrm{d}z_1\mathrm{d}z_2 \\
&+ \tfrac{1}{2}e^{-2\psi}y_1y_2(2(\epsilon^2 - \epsilon^6) + (\epsilon^4 - \epsilon^6)(y_1^2 + y_2^2\epsilon^6))\mathrm{d}s_1\mathrm{d}s_2. \qquad (23)
\end{aligned}$$

And for $\epsilon = 0$ it becomes

$$\begin{aligned}
\mathrm{d}s^2 &= \mathrm{d}\phi^2 + \mathrm{d}\psi^2 + \tfrac{1}{2}e^{-2(\psi+\phi)}\mathrm{d}\tilde{s}_2^2 - \tfrac{1}{2}e^{-2(\psi+\phi)}y_1^2\mathrm{d}\tilde{s}_2\mathrm{d}s_1 + e^{-2(\psi+\phi)}y_1\mathrm{d}\tilde{s}_2\mathrm{d}z_1 \\
&+ \tfrac{1}{8}e^{-2(\psi+\phi)}(4e^{4\phi} + y_1^4 + 4e^{2\phi}y_1^2)\mathrm{d}s_1^2 - \tfrac{1}{2}e^{-2(\psi+\phi)}y_1(2e^{2\phi} + y_1^2)\mathrm{d}s_1\mathrm{d}z_1 \\
&+ \tfrac{1}{2}e^{-4\psi}(e^{2\psi} + e^{2(\psi-\phi)}y_1^2)\mathrm{d}z_1^2 + \tfrac{1}{2}e^{-2\phi}\mathrm{d}y_1^2 + e^{-4\psi}\mathrm{d}t^2 + e^{-4\phi}\mathrm{d}\tilde{t}^2 + \tfrac{1}{2}e^{-2(\phi+\psi)}\mathrm{d}\tilde{s}_1^2 + \tfrac{1}{2}e^{2(\phi-\psi)}\mathrm{d}s_2^2 \\
&+ \tfrac{1}{2}e^{-2\phi}\mathrm{d}y_2^2 + \tfrac{1}{2}e^{-2\psi}\mathrm{d}z_2^2.
\end{aligned}$$

The first three lines reproduce (12) for $n=1$, and the rest of the terms are flat up to factors $e^{(a\phi+b\psi)}$. The physical meaning of this limit remains unclear at this moment, but it relates two different sigma models in what can be a generalized procedure of integrating out some modes.

2. Generalized contraction of $\mathbf{U(2,1+n)/(U(2)\times U(1+n))}$

We show here another example of generalized contraction that has an application in a physically interesting theory.

Let us denote $H_1=H_+ + H_-$. Then the commutation rules of $\mathfrak{s}_2$ are

$$[H_1, Z^{1a}] = Z^{1a}, \quad [H_1, Y^{1a}] = Y^{1a}, \quad [H_1, S_2^{(1,1)}] = 2S_2^{(1,1)}, \quad [Z^{1a}, Y^{1b}] = S_2^{(1,1)}.$$

Consider the subalgebras of $\mathfrak{s}_4$

$$\mathfrak{s}_2' = \mathrm{span}\{H_+, Z^{ia}, T^{(2,0)}\}, \quad s_2'' = \mathrm{span}\{H_-, Y^{ia}, T^{(0,2)}\},$$

with commutation rules

$$[H_+, Z^{ia}] = Z^{ia}, \quad [H_+, T^{(2,0)}] = 2T^{(2,0)}, \quad [Z^{ia}, Z^{jb}] = \delta^{ab}\epsilon^{ij}T^{(2,0)} \quad \text{for } \mathfrak{s}_2',$$

$$[H_-, Y^{ia}] = Y^{ia}, \quad [H_-, T^{(0,2)}] = 2T^{(0,2)}, \quad [Y^{ia}, Y^{jb}] = \delta^{ab}\epsilon^{ij}T^{(0,2)} \quad \text{for } s_2''.$$

We have that $\mathfrak{s}_2 \simeq \mathfrak{s}_2' \simeq \mathfrak{s}_2''$ but $[\mathfrak{s}_2', \mathfrak{s}_2''] \neq 0$, so $\mathfrak{s}_2' \oplus \mathfrak{s}_2''$ is not a subalgebra of $\mathfrak{s}_4$. Nevertheless, one can find a generalized contraction of $\mathfrak{s}_4$ which has $\mathfrak{s}_2' \oplus \mathfrak{s}_2''$ as a subalgebra. We consider the decomposition,

$$\mathfrak{s}_4 = \mathfrak{g}_0 + \mathfrak{g}_1 + \mathfrak{g}_2,$$

where

$$\mathfrak{g}_0 = \mathrm{span}\{H_+, H_-\}, \quad \mathfrak{g}_1 = \mathrm{span}\{Y^{ia}, Z^{ia}, S_\alpha^{(1,1)}\}, \quad \mathfrak{g}_2 = \{T^{(0,2)}, T^{(2,0)}, S_\alpha^{(1,-1)}\},$$

and the linear map

$$\begin{array}{ccc} \mathfrak{s}_4 & \xrightarrow{\phi_\epsilon} & \mathfrak{s}_4 \\ e_0 + e_1 + e_2 & \longrightarrow & e_0 + \epsilon e_1 + \epsilon^2 e_2 \end{array} \qquad e_i \in \mathfrak{g}_i. \tag{24}$$

The contracted Lie algebra, with commutator given by (15) is well defined. It is worthy to see the commutators of the contracted algebra:

$$[Z^{ia}, Z^{jb}]_\epsilon = \epsilon^{ij}\delta^{ab}T^{(2,0)},$$

$$[Y^{ia}, Y^{jb}]_\epsilon = \epsilon^{ij}\delta^{ab}T^{(0,2)},$$

$$[Z^{ia}, Y^{jb}]_\epsilon = \epsilon\delta^{ab}(\delta^{ij}S_2^{(1,1)} + \epsilon^{ij}S_1^{(1,1)}),$$

$$[Y^{ia}, S_1^{(1,-1)}]_\epsilon = \epsilon^2 Z^{ia},$$

$$[Y^{ia}, S_2^{(1,-1)}]_\epsilon = \epsilon^2\epsilon^{ij}Z^{ja},$$

$$[T^{(0,2)}, S_\alpha^{(1,-1)}]_\epsilon = \epsilon^3 2S_\alpha^{(1,1)},$$

$$[S_\alpha^{(1,1)}, S_\beta^{(1,-1)}]_\epsilon = \epsilon\delta_{\alpha\beta}T^{(2,0)},$$

$$[H_+, Z^{ia}]_\epsilon = Z^{ia},$$

$$[H_-, Y^{ia}]_\epsilon = Y^{ia}. \tag{25}$$

showing explicitly $\mathfrak{s}_2' \oplus \mathfrak{s}_2''$ as a subalgebra when $\epsilon \to 0$. We use the adjoint representation to compute the metric, as in the previous examples. The result is

$$\begin{aligned}
ds^2 = {} & d\phi^2 + d\psi^2 + e^{-4\psi} dt dt + 2e^{-4\psi} \epsilon s_1 dt d\tilde{s}_1 + 2e^{-4\psi} \epsilon s_2 dt d\tilde{s}_2 + 2e^{-4\psi} z_{2a} dt dz_{1a} \\
& + 2e^{-4\psi} \epsilon^4 (s_2^2 + s_1^2) dt d\tilde{t} + \tfrac{1}{2}(e^{-2(\psi+\phi)} + 2e^{-4\psi} \epsilon^2 s_1^2) d\tilde{s}_1 d\tilde{s}_1 + 2e^{-4\psi} \epsilon^2 s_2 s_1 d\tilde{s}_1 d\tilde{s}_2 + \tfrac{1}{2} e^{-2(\psi+\phi)} \\
& \times \epsilon^3 (y_1^2 + y_2^2) d\tilde{s}_1 ds_2 + e^{-2(\psi+\phi)} \epsilon^3 y_{1a} y_{2a} d\tilde{s}_1 ds_1 - e^{-2(\psi+\phi)} \epsilon y_{1a} d\tilde{s}_1 dz_{2a} \\
& + \epsilon (2e^{-4\psi} s_1 z_{2a} + e^{-2(\psi+\phi)} y_{2a}) d\tilde{s}_1 dz_{1a} + 2e^{-4\psi} \epsilon^3 s_1 (e^{2(\psi-\phi)} + \epsilon^2 (s_2^2 + s_1^2)) d\tilde{s}_1 d\tilde{t} \\
& + \tfrac{1}{2}(e^{-2(\psi+\phi)} + 2e^{-4\psi} \epsilon^2 s_2^2) d\tilde{s}_2 d\tilde{s}_2 + e^{-2(\psi+\phi)} \epsilon^3 y_{1a} y_{2a} d\tilde{s}_2 ds_2 - \tfrac{1}{2} e^{-2(\psi+\phi)} \epsilon^3 (y_1^2 + y_2^2) d\tilde{s}_2 ds_1 \\
& + e^{-2(\psi+\phi)} \epsilon y_{2a} d\tilde{s}_2 dz_{2a} + \epsilon (2e^{-4\psi} s_2 z_{2a} + e^{-2(\psi+\phi)} y_{1a}) d\tilde{s}_2 dz_{1a} + 2e^{-4\psi} \epsilon^3 s_2 (e^{2(\psi-\phi)} + \epsilon^2 (s_2^2 + s_1^2)) \\
& \times d\tilde{s}_2 d\tilde{t} + \tfrac{1}{8} e^{-2(\psi+\phi)} (4e^{4\phi} + 4e^{2\phi} \epsilon^4 (y_1^2 + y_2^2) + 4\epsilon^6 (y_{1a} y_{2a})^2 + \epsilon^6 (y_1^2 + y_2^2)(y_{1b}^2 + y_{2b}^2)) ds_\alpha ds_\alpha \\
& - \tfrac{1}{2} e^{-2(\psi+\phi)} \epsilon^2 (2e^{2\phi} y_{1b} + \epsilon^2 (-2(y_{1a} y_{2a}) y_{2b} + (y_1^2 + y_2^2) y_{1b})) ds_2 dz_{2b} + \tfrac{1}{2} e^{-2(\psi+\phi)} \epsilon^2 \\
& \times (2e^{2\phi} y_{2b} + \epsilon^2 (2(y_{1a} y_{2a}) y_{1b} + (y_1^2 + y_2^2) y_{2b})) ds_2 dz_{1b} + e^{-2(\psi+\phi)} \epsilon^6 (y_2^2 s_1 + 2 y_{2a} s_2 y_{1a} \\
& + s_1 y_1^2) ds_2 d\tilde{t} \\
& - \tfrac{1}{2} e^{-2(\psi+\phi)} \epsilon^2 (2e^{2\phi} y_{2b} + \epsilon^2 (2(y_{1a} y_{2a}) y_{1b} + (y_1^2 + y_2^2) y_{2b})) ds_1 dz_{2b} - \tfrac{1}{2} e^{-2(\psi+\phi)} \\
& \times \epsilon^2 (2e^{2\phi} y_{1b} + \epsilon^2 (-2(y_{1a} y_{2a}) y_{2b} + (y_{1a}^2 + y_{2a}^2) y_{1b})) ds_1 dz_{1b} \\
& - e^{-2(\psi+\phi)} \epsilon^6 (y_{1a}^2 s_2 - 2 y_{1a} s_1 y_{2a} + s_2 y_{2a}^2) ds_1 d\tilde{t} - \tfrac{1}{2} e^{-2(\phi+\psi)} \epsilon_{ij} \epsilon_{mn} \epsilon^2 (y_{ia} y_{jb}) dz_{ma} dz_{nb} + \tfrac{1}{2} e^{-2(\psi+\phi)} \\
& \times (e^{2\phi} \delta_{ab} + \epsilon^2 (y_{1a} y_{1b} + y_{2a} y_{2b})) dz_{2a} dz_{2b} - e^{-2(\psi+\phi)} \epsilon^4 (2y_1 s_1 - 2s_2 y_2) dz_2 d\tilde{t} \\
& + \tfrac{1}{2} e^{-4\psi} (e^{2\psi} \delta_{ab} + 2 z_{2a} z_{2b} + e^{2(\psi-\phi)} \epsilon^2 (y_{1a} y_{1b} + y_{2a} y_{2b})) dz_{1a} dz_{1b} + \epsilon^4 (2e^{-4\psi} (s_2^2 + s_1^2) z_{2a} \\
& + 2e^{-2(\psi+\phi)} (y_{1a} s_2 + s_1 y_{2a})) dz_{1a} d\tilde{t} + e^{-4(\psi+\phi)} (e^{4\psi} + e^{2(\phi+\psi)} \epsilon^6 (s_1^2 + s_2^2) + e^{4\phi} \epsilon^8 (s_1^2 + s_2^2)^2) d\tilde{t} d\tilde{t} \\
& - 2e^{-4\phi} y_{1a} d\tilde{t} dy_{2a} + \tfrac{1}{2} e^{-4\phi} (e^{2\phi} \delta_{ab} + 2 y_{1a} y_{1b}) dy_{2a} dy_{2b} + \tfrac{1}{2} e^{-2\phi} dy_{1a} dy_{1a}.
\end{aligned} \tag{26}$$

In the contraction limit $\epsilon \to 0$ the metric reduces to

$$\begin{aligned}
ds^2 = {} & \left(d\phi^2 + e^{-4\phi} d\tilde{t} d\tilde{t} - 2e^{-4\phi} y_{1a} d\tilde{t} dy_{2a} + \tfrac{1}{2} e^{-4\phi} (e^{2\phi} \delta_{ab} + 2 y_{1a} y_{1b}) dy_{2a} dy_{2b} + \tfrac{1}{2} e^{-2\phi} dy_{1a} dy_{1a} \right) \\
& + \left(d\psi^2 + e^{-4\psi} dt dt + 2e^{-4\psi} z_{2a} dt dz_{1a} + \tfrac{1}{2} e^{-4\psi} (e^{2\psi} \delta_{ab} + 2 z_{2a} z_{2b}) dz_{1a} dz_{1b} + \tfrac{1}{2} e^{-2\psi} dz_{2a} dz_{2a} \right) \\
& + \tfrac{1}{2} e^{-2(\psi+\phi)} d\tilde{s}_\alpha d\tilde{s}_\alpha + \tfrac{1}{2} e^{-2(\psi+\phi)} ds_\alpha ds_\alpha.
\end{aligned}$$

By comparison with (13) we can see, after a suitable renaming of the coordinates and a rescaling by a global constant factor, that this is the metric on

$$\left(\frac{\mathrm{SU}(1,1+N)}{\mathrm{U}(1+N)} \times \frac{\mathrm{SU}(1,1+N)}{\mathrm{U}(1+N)} \right) \ltimes \mathbb{R}^4.$$

IV. SUPER HIGGS MECHANISM IN SUPERGRAVITY: GEOMETRIC INTERPRETATION

We consider an $N=2$ supergravity model coupled to $n+2$ hypermultiplets and $n+1$ vector multiplets. This model can be obtained as an $N=2$ phase of the compactification of type IIB supergravity on the $N=4$ orientifold $T^6/\mathbb{Z}_2$.[15,16] Indeed, when certain fluxes are turned on, has an $N=3$ phase obtained after the integration of the massive gravitino multiplet. The theory describing

the $N=3$ massless modes can be further Higgsed to an $N=2$ phase by turning on other suitable fluxes and further integration.[17] The scalar manifold for the $N=2$ theory is[11]

$$\mathcal{M}_Q \times \mathcal{M}_{SK} = \frac{\mathrm{U}(2,2+n)}{\mathrm{U}(2)\times \mathrm{U}(2+n)} \times \frac{\mathrm{SU}(1,1+n)}{\mathrm{U}(1+n)}.$$

Here n refers to the brane degrees of freedom. The special geometry and symplectic basis that describe this model have been discussed in Ref. 18.

The $N=2$ model can also be Higgsed to $N=1,0$ phases by still turning on fluxes. This corresponds in the supergravity language to gauge two translational isometries of the quaternionic manifold. In the parametrization that we have used before (26) it is manifest that the coordinates $\tilde{s}_\alpha$ correspond to two translational isometries, generated by $S_\alpha^{(1,1)}$, and we used the two bulk vector fields to gauge them.

When the gauge interactions are switched on, the σ-model Lagrangian gets modified by the minimal coupling prescription, with

$$\mathrm{d}\tilde{s}_\alpha \to D\tilde{s}_\alpha = \mathrm{d}\tilde{s}_\alpha + k_{\alpha,\Lambda} A^\Lambda, \quad \Lambda = 0,1,\ldots,n+1$$

and we may choose the constants $k_{1,0}\neq 0$, $k_{2,1}\neq 0$ and the rest zero. Then the Higgs mechanism takes place, as we described in Sec. II D, with the $\tilde{s}_\alpha$ contributing to the longitudinal components of the massive vectors

$$\hat{A}^0_\mu = A^0_\mu + \frac{1}{k_{1,0}}\partial_\mu \tilde{s}_1, \quad \hat{A}^1_\mu = A^1_\mu + \frac{1}{k_{2,1}}\partial_\mu \tilde{s}_2.$$

From Eq. (7) we can see that the kinetic term of these modes is

$$\begin{aligned}\mathrm{ds}^2 = \cdots + e^{-4\psi}(s_\alpha D\tilde{s}_\alpha + (s_1^2+s_2^2)\mathrm{d}\tilde{t} + \mathrm{d}t + z_{2a}\mathrm{d}z_{1a})^2 + \tfrac{1}{2}e^{-2(\psi+\phi)}\big(D\tilde{s}_1 + y_{1a}y_{2a}\mathrm{d}s_1 + \tfrac{1}{2}(y_1^2+y_2^2)\mathrm{d}s_2 \\ + 2s_1\mathrm{d}\tilde{t} - \epsilon_{ij}y_{ia}\mathrm{d}z_{ja}\big)^2 + \tfrac{1}{2}e^{-2(\psi+\phi)}\big(D\tilde{s}_2 + y_{1a}y_{2a}\mathrm{d}s_2 - \tfrac{1}{2}(y_1^2+y_2^2)\mathrm{d}s_1 + 2s_2\mathrm{d}\tilde{t} + \delta_{ij}y_{ia}\mathrm{d}z_{ja}\big)^2 + \cdots .\end{aligned}$$

After the substitution

$$D\tilde{s}_\alpha \to k_{\alpha,\Lambda}\hat{A}^\Lambda = B^\Lambda$$

the kinetic term for the vectors remains unchanged, whereas mass terms appear for the vectors $\hat{A}^\Lambda$, with masses $k_{0,1}$ and $k_{1,2}$. The modes $\tilde{s}_\alpha$ disappear from the Lagrangian.

In the large mass limit, the massive fields $B^\Lambda_\mu = m\hat{A}^\Lambda_\mu$ appear in the Lagrangian through expressions of the type

$$(B_\mu + f_\mu)^2,$$

where f_μ is some interaction of the massless modes.[11] The B's are Lagrange multipliers and their equations of motions make these terms to vanish.

The $N=2$ gauged theory has a scalar potential stabilizing two additional scalars which in our parametrization correspond to the coordinates s_α.[19] These fields acquire also a mass through the potential. In the large mass limit, these fields become Lagrange multipliers and the potential is such that their field equations set them to zero.

After performing these integrations, the metric becomes the one of the symmetric space

$$\frac{\mathrm{SU}(1,1+n)}{\mathrm{U}(1+n)} \times \frac{\mathrm{SU}(1,1+n)}{\mathrm{U}(1+n)}.$$

Now we see that this example fits with the contraction performed in Sec. III E. We can see that the terms set to zero in the metric by taking the limit $\epsilon \to 0$ are precisely the terms eliminated by the integration procedure. The modes that have become massive are the modes in $\mathbb{R}^4$ in the decomposition

$$\mathfrak{so}[\mathfrak{v}]\left(\frac{\mathrm{U}(2,2+n)}{\mathrm{U}(2)\times\mathrm{U}(2+n)}\right)\to\mathfrak{so}[\mathfrak{v}]\left(\frac{\mathrm{SU}(1,1+n)}{\mathrm{U}(1+n)}\times\frac{\mathrm{SU}(1,1+n)}{\mathrm{U}(1+n)}\right)\ltimes\mathbb{R}^4.$$

Since $\mathbb{R}^4$ is an invariant subgroup of the contracted group, the quotient

$$\mathfrak{so}[\mathfrak{v}]\left(\frac{\mathrm{SU}(1,1+n)}{\mathrm{U}(1+n)}\times\frac{\mathrm{SU}(1,1+n)}{\mathrm{U}(1+n)}\right)\ltimes\mathbb{R}^4/\mathbb{R}^4\approx\mathfrak{so}[\mathfrak{v}]\left(\frac{\mathrm{SU}(1,1+n)}{\mathrm{U}(1+n)}\times\frac{\mathrm{SU}(1,1+n)}{\mathrm{U}(1+n)}\right),$$

is a (solvable) group, associated to the symmetric space. So in the geometrical picture the integration of the massive modes is again modeled by a contraction and a quotient by an invariant subgroup.

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APPENDIX: ABOUT SOLVABLE LIE ALGEBRAS AND TRANSLATIONAL ISOMETRIES

A Lie algebra $\mathfrak{s}$ is solvable if the chain of ideals

$$\mathfrak{s}^{(0)}=\mathfrak{s},\quad \mathfrak{s}^{(1)}=[\mathfrak{s},\mathfrak{s}],\ldots,\mathfrak{s}^{(p)}=[\mathfrak{s}^{(p-1)},\mathfrak{s}^{(p-1)}],\ldots$$

has $\mathfrak{s}^{(p+1)}=0$ for some integer p. It is possible to prove[7] that a Lie algebra $\mathfrak{s}$ is solvable if and only if there is a chain of ideals $\mathfrak{i}_{i+1}\subset\mathfrak{i}_i$ with $\mathfrak{i}_i/\mathfrak{i}_{i+1}$ an abelian algebra, $\mathfrak{i}_0=\mathfrak{s}$ and $\mathfrak{i}_{p+1}=0$ for some p. It is clear that $\mathfrak{i}_p=0$ is an abelian ideal.

Example A.1

As an example, let us consider $\mathfrak{s}=\mathfrak{s}_4$ so

$$\mathfrak{i}_0=\mathfrak{s}_4,$$

$$\mathfrak{i}_1=[\mathfrak{i}_0,\mathfrak{i}_0]=\mathrm{span}\{Z^{ia},Y^{ia},T^{2,0},T^{0,2},S_\alpha^{(1,1)},S_\alpha^{(1,-1)}\},$$

$$\mathfrak{i}_2=[\mathfrak{i}_1,\mathfrak{i}_1]=\mathrm{span}\{Z^{ia},T^{2,0},T^{0,2},S_\alpha^{(1,1)}\},$$

$$\mathfrak{i}_3=[\mathfrak{i}_2,\mathfrak{i}_2]=\mathrm{span}\{T^{2,0}\}.$$

Notice that it is possible to substitute $\mathfrak{i}_3$ in the chain by the maximal abelian ideal

$$\mathfrak{i}_3'=\mathrm{span}\{T^{2,0},T^{0,2},S_\alpha^{(1,1)},Z^{1a}\},$$

or by this other one (with the same dimension)

$$\mathfrak{i}''_3 = \mathrm{span}\{T^{2,0}, T^{0,2}, S_\alpha^{(1,1)}, Z^{2a}\},$$

so the chain is not unique. ■

One can also show that $\mathfrak{s}^{(1)}$ is a nilpotent Lie algebra. The unique simply connected group associated to a nilpotent Lie algebra is exponential (the exp map is a diffeomorphism of the Lie algebra into the Lie group).[7]

Let $\mathfrak{g}$ be a Lie algebra and $\mathfrak{t}$ an abelian subalgebra. Let $\{X_i\}$ be a basis of $\mathfrak{t}$ and $\{Y_\alpha\}$ a basis of a complementary space to $\mathfrak{t}$. In a neighborhood of the identity, we have the exponential map

$$L(u^i, v^\alpha) = e^{u^i X_i} e^{v^\alpha Y_\alpha}. \tag{A1}$$

The Maurer-Cartan form is

$$L^{-1}\mathrm{d}L = e^{-v^\alpha Y_\alpha} X_i e^{v^\alpha Y_\alpha} \mathrm{d}u^i + e^{-v^\alpha Y_\alpha} \mathrm{d}(e^{v^\alpha Y_\alpha}).$$

From this expression, one can see that the local expression of the Maurer-Cartan form does not depend on the coordinates u^i. Whenever the group G with Lie algebra $\mathfrak{g}$ is diffeomorphic to $\mathbb{R}^n \times M$, with $\mathbb{R}^n$ parametrized by u^i (in other words, the coordinates u^i are global), we will say that the generators X_i are *translational isometries*.

We consider now the solvable algebras associated to the non compact symmetric spaces by the Iwasawa decomposition and explore the translational isometries in the corresponding symmetric spaces. The solvable Lie algebras are always a semidirect product

$$\mathfrak{s} = \mathfrak{a} \ltimes \mathfrak{n},$$

where $\mathfrak{a}$ is abelian (it contains the non compact Cartan elements) and $\mathfrak{s}^{(1)} = \mathfrak{n}$ is the nilpotent part. The non compact symmetric spaces are simply connected, so they are, in each case, the unique simply connected group associated to the corresponding solvable algebra. We denote it by

$$S = A \ltimes N, \quad \text{with } \mathrm{Lie}(A) = \mathfrak{a} \text{ and } \mathrm{Lie}(N) = \mathfrak{n},$$

and A and N being simply connected as well[6] (and hence, exponential). As a manifold,

$$S = A \times N = \exp(\mathfrak{a}) \times \exp(\mathfrak{n}). \tag{A2}$$

Let us now consider the factor N in (A2). We want to prove that the generators in the abelian ideal are translational isometries. Let $\mathfrak{n} = \mathfrak{n}_1 + \mathfrak{n}_2$, with $\mathfrak{n}_1$ an abelian ideal and $\mathfrak{n}_2$ any complementary subspace. We have that the map

$$\mathfrak{n} \to N,$$

$$(X_1, X_2) \to \exp(X_1 + X_2)$$

is a diffeomorphism. We want to show that, equally, the map

$$\mathfrak{n} \to N,$$

$$(X_1, X_2) \to \exp X_1 \exp X_2$$

is a diffeomorphism. It is enough to prove that any element $\exp(Y_1 + Y_2)$ can be written as $\exp X_1 \exp X_2$ for some $X_i \in \mathfrak{n}_i$. We notice that

$$\exp X_1 \exp X_2 = \exp\left(X_1 + X_2 + \tfrac{1}{2}[X_1, X_2] + \cdots\right) = \exp(X_2 + X_1'), \quad \text{with } X_1' \in \mathfrak{n}_1.$$

We take $Y_2 = X_2$, and the equation $Y_1 = X_1'$ can be solved for some $X_1 \in \mathfrak{n}_1$.

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Near threshold expansion of Feynman diagrams

E. Mendels[a)]
Schenkkade 221, The Hague, 2595 AT Den Haag, The Netherlands

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The near threshold expansion of Feynman diagrams is derived from their configuration space representation, by performing all x integrations. The general scalar Feynman diagram is considered, with an arbitrary number of external momenta, an arbitrary number of internal lines and an arbitrary number of loops, in n dimensions and all masses may be different. The expansions are considered both below and above threshold. Rules, giving real and imaginary part, are derived. Unitarity of a sunset diagram with I internal lines is checked in a direct way by showing that its imaginary part is equal to the phase space integral of I particles. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1947119]

I. INTRODUCTION

In the usual approach of quantum field theory,[1–4] the successive terms in perturbation theory are represented by diagrams that are given by Feynman rules in momentum space. The most simple Feynman diagram is the zero loop diagram of Fig. 1. Several particles may come in and out, only the sum $\mathbf{p}$ of their momenta is of interest. The momentum space expression of Fig. 1 is

$$\frac{1}{\mathbf{p}^2 - m^2 + i\varepsilon}. \tag{1.1}$$

The one loop diagram (Fig. 2) is given by the momentum space expression

$$\int \mathrm{d}\mathbf{k} \frac{i}{(\mathbf{k}^2 - m_1^2 + i\varepsilon)\{(\mathbf{p}-\mathbf{k})^2 - m_2^2 + i\varepsilon\}}, \tag{1.2}$$

which is logarithmic divergent in four dimensions. The $i\varepsilon$'s may be transformed away by a Wick rotation, dimensional regularization may be introduced and the internal momentum may be integrated away. Integration over one Feynman parameter is left. In this way, (1.2) becomes[5]

$$(1.2) = \pi^{\nu}\Gamma(\nu-2)\int_0^1 \mathrm{d}y\{-y(1-y)\mathbf{p}^2 + ym_1^2 + (1-y)m_2^2\}^{\nu-2}. \tag{1.3}$$

The minus sign in the integrand comes from the inverse Wick rotation at the end of the calculations, which transforms p into ip.

The ν is a continuous variable and (1.3) must be considered in the limit

$$\varepsilon = \nu - \tfrac{1}{2}n \to 0, \tag{1.4}$$

where n is the number of dimensions. The logarithmic divergence of (1.2) in four dimensions is visible through the Γ-function in front,

[a)]Electronic mail: emendels@zonnet.nl

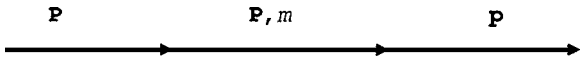

FIG. 1. Zero loop diagram.

$$(1.3) = \frac{\pi^2}{\varepsilon} + \pi^2 \int_0^1 \mathrm{d}y \, \ln\{-y(1-y)p^2 + ym_1^2 + (1-y)m_2^2\}. \tag{1.5}$$

Finally, the integration over y may be done,

$$(1.5) = \frac{\pi^2}{\varepsilon} + \pi^2\left(\frac{p^2 + m_1^2 - m_2^2}{2p^2}\right)\ln m_1^2 + \pi^2\left(\frac{p^2 + m_2^2 - m_1^2}{p^2}\right)\ln m_2^2 - 2\pi^2 + 2\pi^2\frac{a}{p^2}\mathrm{arctg}\left(\frac{p^2 + m_1^2 - m_2^2}{a}\right) + 2\pi^2\frac{a}{p^2}\mathrm{arctg}\left(\frac{p^2 + m_2^2 - m_1^2}{a}\right), \tag{1.6}$$

with

$$a = \sqrt{-(p + m_1 + m_2)(p - m_1 + m_2)(p + m_1 - m_2)(p - m_1 - m_2)}. \tag{1.7}$$

If the absolute value of the argument of the arctangents in (1.6) is smaller than 1, their series expansion is given by

$$\mathrm{arctg}\left(\frac{p^2 + m_1^2 - m_2^2}{a}\right) = \left(\frac{p^2 + m_1^2 - m_2^2}{a}\right) - \frac{1}{3}\left(\frac{p^2 + m_1^2 - m_2^2}{a}\right)^3 + \cdots . \tag{1.8a}$$

If it is larger than 1, the series expansion is given by

$$\mathrm{arctg}\left(\frac{p^2 + m_1^2 - m_2^2}{a}\right) = \frac{\pi}{4} - \left(\frac{a}{p^2 + m_1^2 - m_2^2}\right) + \frac{1}{3}\left(\frac{a}{p^2 + m_1^2 - m_2^2}\right)^3 - \cdots . \tag{1.8b}$$

The two-loop diagram (Fig. 3) is represented in momentum space by

$$\int \mathrm{d}\mathbf{k}_1 \, \mathrm{d}\mathbf{k}_2 \frac{i^2}{(\mathbf{k}_1^2 - m_1^2 + i\varepsilon)(\mathbf{k}_2^2 - m_2^2 + i\varepsilon)\{(\mathbf{p} - \mathbf{k}_1 - \mathbf{k}_2)^2 - m_3^2 + i\varepsilon\}}. \tag{1.9}$$

In four dimensions, it is quadratic divergent and contains subintegrals that are logarithmic divergent. The expression becomes after regularization and integration over the internal momenta,

$$(1.9) = \pi^{2\nu}\Gamma(3 - 2\nu) \int \mathrm{d}y_1 \, \mathrm{d}y_2 \{y_1y_2 + y_1y_3 + y_2y_3\}^{-\nu} \times\left(-\frac{y_1y_2y_3p^2}{y_1y_2 + y_1y_3 + y_2y_3} + y_1m_1^2 + y_2m_2^2 + y_3m_3^2\right)^{2\nu-3} \tag{1.10}$$

with

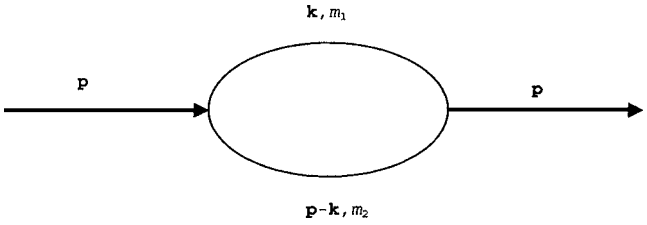

FIG. 2. One loop diagram.

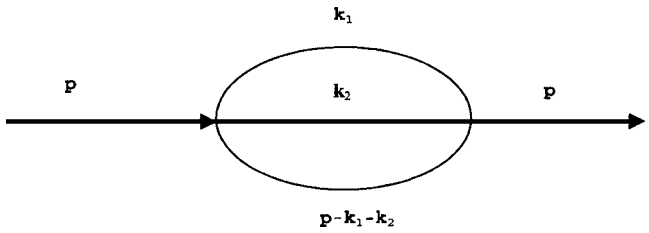

FIG. 3. Two loop diagram.

$$y_3 = 1 - y_1 - y_2. \tag{1.11}$$

One of the infinities is visible through the Γ-function in front. Other infinities become visible only after cumbersome partial integrations over the Feynman parameters y_1 and y_2 and introduction of master integrals to which they are reduced.[6,7]

The cut in the complex $(\Sigma m - p)$ plane, causing an imaginary part above threshold, is not clearly visible in (1.2), nor in (1.5). It becomes manifest in (1.6), after having done the y integration. In the two loop case, it is not visible at all, neither in (1.9), nor in (1.10).

Unitarity implies that the imaginary part of diagrams with two vertices and I internal lines should be equal to the phase space integral of I particles. This relation is valid in the zero loop case of Fig. 1,

$$\frac{1}{\mathbf{p}^2 - m^2 + i\varepsilon} = PP\frac{1}{\mathbf{p}^2 - m^2} - i\pi\delta(\mathbf{p}^2 - m^2). \tag{1.12}$$

On the right-hand side (rhs), both a real and an imaginary part is seen. The latter is given by

$$2\Im\left(\frac{1}{\mathbf{p}^2 - m^2 + i\varepsilon}\right) = -2\pi\int \mathrm{d}\mathbf{k}\ \delta(\mathbf{p} - \mathbf{k})\,\theta(k_0)\,\delta(\mathbf{k}^2 - m^2). \tag{1.13}$$

Indeed, the rhs is the one-particle phase space integral, up to a factor 2π.

In the one loop case of Fig. 2, unitarity is not clear from (1.2) or (1.3). It is seen from (1.8a), which is real if $p < m_1 + m_2$, but if $p > m_1 + m_2$, an imaginary part appears, coming from the $\pi/4$ term in (1.8b),

$$\Im(1.6) = -\frac{\pi^3\theta(p - m_1 - m_2)\sqrt{(p + m_1 + m_2)(p - m_1 + m_2)(p + m_1 - m_2)(p - m_1 - m_2)}}{p^2}. \tag{1.14}$$

On the other hand, the two-particle phase space integral in four dimensions is given by[8]

$$\int \mathrm{d}\mathbf{k}_1\,\mathrm{d}\mathbf{k}_2\ \delta(\mathbf{p} - \mathbf{k}_1 - \mathbf{k}_2)\,\delta(\mathbf{k}_1^2 - m_1)\,\delta(\mathbf{k}_2^2 - m_2^2)\,\theta(k_1^0)\,\theta(k_2^0)$$
$$= \frac{\pi\theta(p - m_1 - m_2)\sqrt{(p + m_1 + m_2)(p - m_1 + m_2)(p + m_1 - m_2)(p - m_1 - m_2)}}{2p^2}. \tag{1.15}$$

Indeed,

$$2(1.14) = -(2\pi)^2(1.15) \tag{1.16}$$

which means unitarity of the one loop diagram in four dimensions.

In the two loop case, the imaginary part of (1.10) is not easily found and if there are near threshold expansions from which it possibly may be derived,[9] it is not clear that it is equal to the three particle phase space integral. On the other hand, if the three particle phase space integral is computed,[10] it is not clear that it equals the imaginary part of (1.10).

To our opinion, it is an unsatisfactory situation that zero loop Feynman rules are given in momentum space, that must be replaced by one loop rules in terms of Feynman parameters that must be replaced once again by rules that work in the case of more loops. Moreover, it is an unsatisfactory situation that real and imaginary parts are not clearly visible in the usual expressions of Feynman diagrams. Finally, it is an unsatisfactory situation that unitarity is not obviously seen in the usual expressions of Feynman diagrams.

It would be more satisfactory if final rules could be derived, that do not have to be redefined twice. For this reason, it has been proposed[11] to describe Feynman diagrams in terms of configuration space parameters, which are structure conserving and, therefore, do not mix different kinds of infinities.

In the configuration space formalism, internal and external lines of a diagram correspond to Bessel functions with a pure imaginary argument. In the case of sunset diagrams, only one integration variable x is needed. On the other hand, these same Bessel functions appear in the configuration space expression of phase space integrals.[12,13] The *integrands* of sunset diagrams and phase space integrals are equal, only the *ranges* of the x integration are different. By this fact, unitarity is built into the formalism in a natural way.

The **x** space formalism has been extended from sunset diagrams to general Feynman diagrams, which implies integration over several configuration space parameters $\mathbf{x}^j$ and over the angles between them.[14]

The purpose of the present paper is to complete the work and to perform all integrations. Rules are derived that immediately give the final result, including cuts, disentangled poles, real and imaginary parts.

The formulas are complicated in the case of a general diagram, summation variables with three and sometimes four indices must be used. To our opinion, this situation is preferable above a formalism, where infinities, cuts and unitarity are hidden in the integration variables and which too is complicated.

The formalism is general, i.e., it is applicable on diagrams with any number of internal lines, any number of vertices, any number of loops in any dimension and all internal and external masses may be different. Scalar fields are considered, but introduction of spin does not give complications since spin leads to matrices and derivatives that do not affect the essential structure of the formulas.

II. SERIES EXPANSION OF SUNSET DIAGRAMS

In order to understand the way of working of the formalism, we consider first dimensionally regularized diagrams with two vertices and I internal lines (so-called sunset, sunrise or water melon diagrams). They are represented in x space by the expression

$$F_2^I \prod \frac{(m^j)^{2b^j}}{\Gamma(\alpha^j)} \int_0^\infty \mathrm{d}x\, x^{2\nu-1} i_b(px) k_{bj}(m^j x), \tag{2.1}$$

with notation

$$\prod = \prod_{1 \leqslant j \leqslant I} \tag{2.2}$$

and front factor

$$F_2^I = \frac{(2\pi^{\frac{1}{2}n})^{I+1}}{(2\pi)^n}. \tag{2.3}$$

Equation (2.1) is obtained from the corresponding momentum space expression after a Wick transformation and n dimensional Fourier transformations of the propagators according to

$$\int \mathrm{d}\mathbf{k}^j \frac{e^{-i\mathbf{k}^j\cdot\mathbf{x}}}{(\mathbf{k}^{j^2} + m^{j^2})^{\alpha^j}} = \frac{2\pi^{\frac{1}{2}n} m^{2b^j}}{\Gamma(\alpha^j)} k_{b^j}(m^j x), \tag{2.4}$$

with

$$b^j = \tfrac{1}{2}n - \alpha^j. \tag{2.5}$$

Thereupon, one inverse n dimensional Fourier transformation has been performed. After integration of an exponential over its angles and an inverse Wick transformation according to

$$\int \mathrm{d}\hat{\mathbf{x}}\, e^{i\mathbf{p}\cdot\mathbf{x}} = 2\pi^{\frac{1}{2}n} \mathrm{j}_b(px) \overset{p\to ip}{\longrightarrow} 2\pi^{\frac{1}{2}n} i_b(px), \tag{2.6}$$

with

$$b = \tfrac{1}{2}n - 1, \tag{2.7}$$

the result (2.1) is obtained.[11] The various factors 2 and π in (2.3) are remnants of all these actions.

The functions $i_b(px)$ and $k_{b^j}(m^j x)$ are, up to a factor, modified Bessel functions of the first and third kind,[15] respectively. Details are summarized in Appendix A. In the case of integer b and b^j, the near zero expansions are given by

$$i_b(z) = j_b(iz) = \sum_{k=0}^{\infty} \frac{1}{k\,!\,(b+k)!} \left(\frac{z}{2}\right)^{2k}, \tag{2.8a}$$

$$k_{b^j}(z) = \sum_{0\leqslant k^j\leqslant\infty} K^j \left(\frac{z}{2}\right)^{2k^j} + \sum_{0\leqslant k^j\leqslant\infty} L^j \left(\frac{z}{2}\right)^{2k^j} \ln\left(\frac{z}{2}\right) + \sum_{0\leqslant k^j\leqslant b^j-1} M^j \left(\frac{z}{2}\right)^{-2b^j+2k^j}. \tag{2.8b}$$

K^j, L^j, and M^j are building stones of the functions $k_{b^j}(z)$; they depend on the summation variable k^j and, according to Appendix A, they are given by

$$K^j \equiv K_{b^j}(k^j) = \frac{(-)^{b^j+1}}{k^j\,!\,(b^j+k^j)!} \left\{ \left(\gamma - \frac{1}{1} - \frac{1}{2} - \cdots - \frac{1}{k^j}\right) + \left(\gamma - \frac{1}{1} - \frac{1}{2} - \cdots - \frac{1}{k^j+b^j}\right) \right\},$$
$$(\gamma = 0.577\,215\,664\,9), \tag{2.9a}$$

$$L^j \equiv L_{b^j}(k^j) = \frac{(-)^{b^j+1}}{k^j\,!\,(b^j+k^j)!}, \tag{2.9b}$$

$$M^j \equiv M_{b^j}(k^j) = \frac{(-)^{k^j}(b^j-k^j-1)!}{2k^j!}. \tag{2.9c}$$

As indicated in (2.8b), the summation over k^j is from 0 to ∞ if it concerns K^j or L^j and from 0 to b^j-1 if it concerns M^j.

To compute the integral (2.1), it must be split according to

$$\int_0^\infty \mathrm{d}x = \int_0^X \mathrm{d}x + \int_X^\infty \mathrm{d}x, \tag{2.10}$$

where X is arbitrary. In the $\int_X^\infty \mathrm{d}x$ integral, the asymptotic expansions (A6a) for $k_{bj}(m^j x)$ and (A6f) for $i_b(px)$ are inserted,

$$\begin{aligned}\prod \int_X^\infty \mathrm{d}x\, x^{2\nu-1} i_b(px) k_{bj}(m^j x) = &\sum_{\substack{0\leqslant k^j<H^j \\ 0\leqslant k<H}} \prod \frac{\pi^{(I-1)/2} 2^{2b+2\Sigma b^c}(b,k)(b^j,k^j) e^{-i\pi\left(b+\frac{1}{2}\right)}}{(2p)^{b+k+\frac{1}{2}}(2m^j)^{b^j+k^j+\frac{1}{2}}} \\ &\times \int_X^\infty \mathrm{d}x\, e^{-\left(\Sigma m^c+p\right)x} x^{2\nu-\left(b+k+\frac{1}{2}\right)-\Sigma\left(b^c+k^c+\frac{1}{2}\right)-1} \\ &+ \sum_{\substack{0\leqslant k^j<H^j \\ 0\leqslant k<H}} \prod \frac{\pi^{(I-1)/2} 2^{2b+2\Sigma b^c}(b,k)(b^j,k^j)}{(2p)^{b+k+\frac{1}{2}}(2m^j)^{b^j+k^j+\frac{1}{2}}} \\ &\times \int_X^\infty \mathrm{d}x\, e^{-\left(\Sigma m^c-p\right)x} x^{2\nu-\left(b+k+\frac{1}{2}\right)-\Sigma\left(b^c+k^c+\frac{1}{2}\right)-1} + \text{rest term},\end{aligned} \tag{2.11}$$

with notation

$$\sum = \sum_{1\leqslant c\leqslant I}, \tag{2.12a}$$

$$(b,k) = \frac{\Gamma\left(b+k+\frac{1}{2}\right)}{k!\,\Gamma\left(b-k+\frac{1}{2}\right)}. \tag{2.12b}$$

Though asymptotic expansions of Bessel functions are used,[16–18] it should be remembered that they do not converge in even dimensional spaces[15] (the asymptotic series do converge and even are finite in odd dimensional spaces). Nonetheless, these expansions make sense if their meaning is realized,[19] for a given H and H^j in (2.11), X may be chosen sufficiently large to make the rest term arbitrary small and to make the $X\to\infty$ integrals arbitrary accurate. For this reason, near ∞ integrals over the asymptotic series must be combined with near 0 integrals over expansions that are convergent in the neighborhood of 0.

The integrals of (2.11) make sense only if the exponentials in the integrand are decreasing, i.e., if

$$\sum m^c - p > 0. \tag{2.13}$$

By introducing the parameter

$$\Lambda = \left(\sum m^c - p\right)X \tag{2.14}$$

and choosing Λ large with respect to the asymptotic coefficients (b,H) and (b^j,H^j) of (2.12b), both integrals of (2.11) are small and (2.1) can be computed by doing the integration from 0 to Λ only,

$$F_2^I \prod (m^j)^{2b^j} \int_0^\infty \mathrm{d}x\, x^{2\nu-1} i_b(px) k_{bj}(m^j x) \cong F_2^I \prod \frac{(\mu^j)^{2b^j}}{\left(\sum m^c - p\right)^{2\left(\nu-\Sigma b^c\right)}} \int_0^\Lambda \mathrm{d}\xi\, \xi^{2\nu-1} i_b(\rho\xi) k_{bj}(\mu^j \xi), \tag{2.15}$$

with

$$\rho = \frac{p}{\sum m^c - p}, \tag{2.16a}$$

$$\mu^j = \frac{m^j}{\sum m^c - p}. \tag{2.16b}$$

III. BELOW THRESHOLD

The Bessel function expansions (2.8) must be inserted into the rhs of (2.15) and integration is performed with use of Appendix D.

In the case of the one loop diagram of Fig. 2, the result is

$$\begin{aligned}
&\frac{F_2^2(\mu^1)^{2b^1}(\mu^2)^{2b^2}}{(m^1+m^2-p)^{2(\nu-b^1-b^2)}} \int_0^\Lambda \mathrm{d}\xi\, \xi^{2\nu-1} i_b(\rho\xi) k_{b^1}(\mu^1\xi) k_{b^2}(\mu^2\xi) \\
&\quad = \sum_{k,k^1,k^2} \frac{2^{2\nu} F_2^2 \rho^{2k} (\mu^1)^{2(b^1+k^1)} (\mu^2)^{2(b^2+k^2)}}{(m^1+m^2-p)^{2(\nu-b^1-b^2)} k!\,(b+k)!} \\
&\qquad \times \left\{ F^{11} \ln\left(\frac{\mu^1\Lambda}{2}\right) \ln\left(\frac{\mu^2\Lambda}{2}\right) + F^{10} \ln\left(\frac{\mu^1\Lambda}{2}\right) + F^{01} \ln\left(\frac{\mu^2\Lambda}{2}\right) + F^{00} \right\}.
\end{aligned} \tag{3.1}$$

The coefficients F^{11}, F^{10}, F^{01}, and F^{00} depend on the summation variables k^j and are expressed in terms of the functions K^j, L^j, and M^j of (2.9),

$$F^{11} = \frac{L^1 L^2 (\Lambda/2)^N}{N}, \tag{3.2a}$$

$$F^{10} = -\frac{L^1 L^2 (\Lambda/2)^N}{(N)^2} + \frac{L^1 K^2 (\Lambda/2)^N}{N} + \frac{L^1 M^2 (\Lambda/2)^{(N-2b^2)}}{(N-2b^2)}, \tag{3.2b}$$

$$F^{01} = -\frac{L^1 L^2 (\Lambda/2)^N}{(N)^2} + \frac{K^1 L^2 (\Lambda/2)^N}{N} + \frac{M^1 L^2 (\Lambda/2)^{(N-2b^1)}}{(N-2b^1)}, \tag{3.2c}$$

$$\begin{aligned}
F^{00} = {} & \frac{L^1 L^2 (\Lambda/2)^N}{(N)^3} - \frac{K^1 L^2 (\Lambda/2)^N}{(N)^2} - \frac{M^1 L^2 (\Lambda/2)^{N-2b^1}}{(N-2b^1)^2} - \frac{L^1 K^2 (\Lambda/2)^N}{(N)^2} - \frac{L^1 M^2 (\Lambda/2)^{(N-2b^2)}}{(N-2b^2)} \\
& - \frac{K^1 L^2 (\Lambda/2)^N}{(N)^2} - \frac{M^1 L^2 (\Lambda/2)^{(N-2b^1)}}{(N-2b^1)^2} + \frac{K^1 K^2 (\Lambda/2)^N}{N} + \frac{K^1 M^2 (\Lambda/2)^{(N-2b^2)}}{(N-2b^2)} + \frac{M^1 K^2 (\Lambda/2)^{N-2b_1}}{(N-2b^1)} \\
& + \frac{M^1 M^2 (\Lambda/2)^{N-2b^1-2b^2}}{(N-2b^1-2b^2)},
\end{aligned} \tag{3.2d}$$

with

$$N = 2(\nu + k + k^1 + k^2). \tag{3.3}$$

In the case of four dimensions ($\nu=2$) and propagator exponent 1 ($\nu - b^j = 1$), an infinity appears in (3.2d) through the denominator factor $(N - 2b^1 - 2b^2)$. It corresponds to the infinity in (1.5).

The formula's (3.1), (3.2), and (3.3) may be generalized to sunset diagrams with I internal lines,

$$\prod \frac{F_2^I (\mu^j)^{2b^j}}{\left(\sum m^c - p\right)^{2(\nu - \Sigma b^c)}} \int_0^\Lambda \mathrm{d}\xi\, \xi^{2\nu-1} i_b(\rho\xi) k_{bj}(\mu^j \xi)$$

$$= \sum_{k,k^j} \prod \frac{2^{2\nu} F_2^I \rho^{2k} (\mu^j)^{2(b^j + k^j)}}{\left(\sum m^c - p\right)^{2(\nu - \Sigma b^c)} k!\,(b+k)!} \sum_{0 \leqslant f^j \leqslant 1} F^{f^1 \cdots f^j} \left\{ \ln\left(\frac{\mu^j \Lambda}{2}\right) \right\}^{f^j}, \tag{3.4}$$

with

$$F^{f^1 \cdots f^j} = \sum_{f^j \leqslant g^j \leqslant h^j \leqslant 1} \prod \frac{(-)^G G!\,(K^j)^{(1-h^j)(1-g^j)} (L^j)^{g^j} (M^j)^{(1-g^j)h^j}}{\left\{N - 2\sum (1-g^c) h^c b^c\right\}^{1+G}} \left(\frac{\Lambda}{2}\right)^{N - 2\Sigma(1-g^c)h^c b^c}, \tag{3.5}$$

where

$$G = \sum (g^c - f^c), \tag{3.6a}$$

$$N = 2\left(\nu + k + \sum_{1 \leqslant c \leqslant I} k^c\right). \tag{3.6b}$$

To (3.4) must be added the $\Lambda \to \infty$ integrals (2.11) which may help convergence and may be computed by means of the formulas of Appendix C. The latter integrals are arbitrary small for sufficiently large Λ.

IV. ABOVE THRESHOLD

The threshold at $p = \Sigma m^c$ appears through the logarithmic factors in (3.1) and (3.4). It is a direct consequence of the requirement (2.13) that the asymptotic integrands (2.11) should decrease exponentially.

Analytical continuation to above threshold, i.e., to

$$p > \sum m, \tag{4.1}$$

is obtained after replacement of $(\Sigma m - p)$ by $(p - \Sigma m)$ in (3.1) and (3.4). Terms that are even in $(\Sigma m - p)$ remain unchanged by this replacement, odd terms transform into their opposite and a term $i\pi$ is added to a logarithmic factor,

$$\left(\sum m - p\right)^{2k} \to \left(p - \sum m\right)^{2k}, \tag{4.2a}$$

$$\left(\sum m - p\right)^{2k+1} \to -\left(p - \sum m\right)^{2k+1}, \tag{4.2b}$$

$$\ln\left(\sum m - p\right) \to \ln\left(p - \sum m\right) + i\pi. \tag{4.2c}$$

Imaginary terms appear by these transformations through the factor

$$\sum_{0\leqslant f^i\leqslant 1} F^{f^1,f^2}\left\{\ln\left(\frac{\mu^1\Lambda}{2}\right)\right\}^{f^1}\left\{\ln\left(\frac{\mu^2\Lambda}{2}\right)\right\}^{f^2}.$$

In the one loop case,

$$\begin{aligned}
&F^{11}\ln\left(\frac{\mu^1\Lambda}{2}\right)\ln\left(\frac{\mu^2\Lambda}{2}\right)+F^{10}\ln\left(\frac{\mu^1\Lambda}{2}\right)+F^{01}\ln\left(\frac{\mu^2\Lambda}{2}\right)+F^{00}\\
&\quad=F^{1,1}\ln\left(\frac{\mu^1\Lambda}{2}\right)\ln\left(\frac{\mu^2\Lambda}{2}\right)-\pi^2F^{1,1}+F^{1,0}\ln\left(\frac{\mu^1\Lambda}{2}\right)+F^{0,1}\ln\left(\frac{\mu^2\Lambda}{2}\right)\\
&\quad+i\pi\left\{F^{1,1}\ln\left(\frac{\mu^1\Lambda}{2}\right)+F^{1,1}\ln\left(\frac{\mu^2\Lambda}{2}\right)+F^{1,0}+F^{0,1}\right\}.
\end{aligned}\tag{4.3}$$

V. THE GENERAL FEYNMAN DIAGRAM

A general Feynman diagram, with V vertices and I internal lines, is written in terms of configuration space parameters as[14]

$$\frac{(2\pi^{\frac{1}{2}n})^I}{(2\pi)^{n(V-1)}}\prod\frac{(m_i^j)^{2b_i^j}(m_{i',i}^j)^{2b_{i',i}^j}}{\Gamma(\alpha_i^j)\Gamma(\alpha_{i',i}^j)}\int \mathrm{d}\mathbf{x}_i\, e^{i\mathbf{p}_i\cdot\mathbf{x}_i}k_{b_i^j}(m_i^jx_i)k_{b_{i',i}^j}(m_{i',i}^j|\mathbf{x}_i-\mathbf{x}_{i'}|)\tag{5.1}$$

with notation

$$\prod=\prod_{\substack{1\leqslant i\leqslant V-1\\ 1\leqslant i'<i\\ j}}.\tag{5.2}$$

Internal lines and their corresponding masses wear three indices, the two subscripts i', i indicate the vertices that they are connecting, the superscript j counts the lines between these vertices.

The number of integration vectors $\mathbf{x}_i$ is $V-1$, one less than the number of vertices. The external momenta are given by $V-1$ vectors $\mathbf{p}_i$, the momentum $\mathbf{p}_V$ is given by momentum conservation,

$$\sum_{1\leqslant i\leqslant V}\mathbf{p}_i=0.\tag{5.3}$$

The elaboration of (5.1) goes along the same lines as in the case of Sec. II. It will turn out that the final result is a generalization of the result (3.4) for sunset diagrams.

The integrand of (5.1) contains both functions like $k_{b_i}(m_ix_i)$, with a simple argument, and functions like $k_{b_{i',i}}(m_{i',i}|\mathbf{x}_i-\mathbf{x}_{i'}|)$, with a composed argument. Because of the latter functions, the integration range of (5.1) must be divided into $V!$ subregions. $(V-1)!$ of them are of the kind

$$0<x_1<x_2<\cdots<x_{V-1}<X+\text{permutations},\tag{5.4a}$$

with arbitrary X, and $V!-(V-1)!$ subregions are of the kind

$$0<x_1<x_2<\cdots<X<\cdots<x_{V-1}<\infty.\tag{5.4b}$$

In the subregions of (5.4b), the functions $k_{b_{i',i}}$ with a composed argument are split according to (A8) and the integral (5.1) contains a sum of products of three factors,

$$(5.1) = F_V^I \sum \prod \frac{(m_i^j)^{2b_i^j}(m_{i',i}^j)^{2b_{i',i}^j}}{\Gamma(\alpha_i^j)\Gamma(\alpha_{i',i}^j)} A(r_{i',i}^j) R_1(r_{i',i}^j) R_2(r_{i',i}^j), \tag{5.5}$$

with front factor

$$F_V^I = \frac{(2\pi^{\frac{1}{2}n})^{I+V-1}}{(2\pi)^{n(V-1)}}. \tag{5.6}$$

$A(r_{i',i}^j)$ is an angular factor given in (B8b), $R_1(r_{i',i}^j)$ and $R_2(r_{i',i}^j)$ are radial factors given by (C1a) and (C1b).

The radial integrals are meaningful only if the integrands are decreasing exponentials. From the formulas of Appendix C, it is seen that the latter condition is satisfied below all thresholds, i.e., if

$$\sum m - \sum p \equiv \min_V \left\{ \sum_{a \in V, b \notin V} \left(\sum_c m_{a,b}^c - p_b \right) \right\} > 0, \tag{5.7}$$

where V is a set of vertices and $\min_V$ is the minimum over all possible sets. Under the condition (5.7), integrals in the subregions (5.4b) can be made arbitrary small if

$$\Lambda \equiv \left(\sum m - \sum p \right) X \tag{5.8}$$

is chosen sufficiently large.

The nondisappearing integrals in the subregions (5.4a) are computed by splitting the composed functions $\mathrm{k}_{b_{i',i}}(m_{i',i}|\mathbf{x}_i - \mathbf{x}_{i'}|)$ according to (A11), which leads to a simpler formula than (A8). Integral (5.1) is written in these subregions as the sum over products of an angular and a radial factor according to

$$(5.1) \cong F_V^I \sum \prod \frac{r_{i',i}!}{\Gamma(\alpha_i^j)\Gamma(\alpha_{i',i}^j) r_{i',i}^j!} A(q_i; r_{i',i}) R(q^i; r_{i',i}), \tag{5.9}$$

with

$$r_{i',i} = \sum_c r_{i',i}^c, \tag{5.10a}$$

$$(2\pi^{\frac{1}{2}n})^{V-1} A(q_i, r_{i',i}) = \prod \int \mathrm{d}\hat{\mathbf{x}}_i \frac{(2\hat{\mathbf{p}}_i \cdot \hat{\mathbf{x}}_i)^{q_i}}{q_i!} \frac{(2\hat{\mathbf{x}}_{i'} \cdot \hat{\mathbf{x}}_i)^{r_{i',i}}}{r_{i',i}!} \tag{5.10b}$$

and

$$\begin{aligned} R(q_i; r_{i',i}^j) \equiv & \sum_{l_{i',i}^j=0}^{\infty} \prod \frac{2^{2\nu(V-1)}(-)^{l_{i',i}^j}}{l_{i',i}^j!} p_i^{q_i} (m_i^j)^{2b_i^j} (m_{i',i}^j)^{2(b_{i',i}^j + l_{i',i}^j + r_{i',i}^j)} \\ & \times \int_{0<x_1<\cdots<x_{V-1}<X} d\frac{x_i}{2} \left(\frac{x_i}{2} \right)^{2\nu-1+q_i+2\Sigma l_{i,a}^c + \Sigma r_{a,i} + \Sigma r_{i,a}} k_{b_i^j}(m_i^j x_i) k_{b_{i',i}^j + l_{i',i}^j + r_{i',i}^j}(m_{i',i}^j x_i) \\ & + \text{permutations}. \end{aligned} \tag{5.10c}$$

Summation Σ in the exponent is defined in (B5).

Integral (5.10b) is computed in (B4b) and (5.10c) is computed by insertion of (A3c). The final result is a generalization of the result (3.4) for sunset diagrams,

$$(5.1) \cong \frac{2^{2\nu(V-1)}F_V^I}{\left(\sum m-\sum p\right)^{2\{\nu(V-1)-\Sigma b_a^c-\Sigma b_{a,b}^c\}}}\sum_{k,l,q,r}\prod\frac{r_{i',i}!}{\Gamma(\alpha_i^j)\Gamma(\alpha_{i',i}^j)r_{i',i}^j}A(q_i;r_{i',i})\rho_i^{q_i}\frac{(-)^{l_{i',i}^j}}{l_{i',i}^j}(\mu_i^j)^{2(b_i^j+k_i^j)}$$

$$\times(\mu_{i',i}^j)^{2(b_{i',i}^j+l_{i',i}^j+r_{i',i}^j+k_{i',i}^j)}\sum_{f=0}^{1}F^{f_i^j,f_{i',i}^j}\left\{\ln\left(\frac{\mu_i^j\Lambda}{2}\right)\right\}^{f_i^j}\left\{\ln\left(\frac{\mu_{i',i}^j\Lambda}{2}\right)\right\}^{f_{i',i}^j}, \tag{5.11}$$

with

$$\rho_i=\frac{p_i}{\left(\sum m-\sum p\right)},\quad \mu_i^j=\frac{m_i^j}{\left(\sum m-\sum p\right)},\quad \mu_{i',i}^j=\frac{m_{i',i}^j}{\left(\sum m-\sum p\right)}, \tag{5.12a}$$

and

$$F^{f_i^j,f_{i',i}^j}=\sum_{f\leqslant g_{;V-2}\cdots\leqslant g_{;1}\leqslant g\leqslant h\leqslant 1}\prod\frac{(-)^{G_i}G_i!}{\left(\sum\limits_{1\leqslant a\leqslant i}N_a\right)^{1+G_i}}(K_i^j)^{(1-g_i^j)(1-h_i^j)}(L_i^j)^{g_i^j}(M_i^j)^{(1-g_i^j)h_i^j}(K_{i',i}^j)^{(1-g_{i',i}^j)(1-h_{i',i}^j)}$$

$$\times(L_{i',i}^j)^{g_{i',i}^j}(M_{i',i}^j)^{(1-g_{i',i}^j)h_{i',i}^j}\left(\frac{\Lambda}{2}\right)^{\sum\limits_{1\leqslant a\leqslant V-1}N_a}+\text{permutations}. \tag{5.12b}$$

$F^{f_i^j,f_{i',i}^j}$ depends on the summation variables k,l,q,r through the factors K_i^j, L_i^j, M_i^j, through the factors

$$K_{i',i}^j\equiv K_{b_{i',i}^j+l_{i',i}^j+r_{i',i}^j}(k_{i',i}^j),\quad L_{i',i}^j\equiv L_{b_{i',i}^j+l_{i',i}^j+r_{i',i}^j}(k_{i',i}^j),\quad M_{i',i}^j\equiv M_{b_{i',i}^j+l_{i',i}^j+r_{i',i}^j}(k_{i',i}^j), \tag{5.13}$$

all defined according to (2.9), and through the factors $\Sigma_{1\leqslant a\leqslant i}N_a$ with

$$N_i=2\nu+q_i+2\sum k_i^c+2\sum k_{a,i}^c+2\sum l_{i,a}^c+\sum r_{a,i}^c+\sum r_{i,a}^c$$
$$-2\sum h_i^c(1-g_i^c)b_i^c-\sum h_{a,i}^c(1-g_{a,i}^c)(b_{a,i}^c+l_{a,i}^c+r_{a,i}^c), \tag{5.14}$$

where summation Σ is according to the convention of (B5). G_i is computed in Appendix D,

$$G_i=\sum_{\substack{1\leqslant a\leqslant i\\ c}}(g_{a;i-1}^c-g_{a;i}^c)+\sum_{\substack{1\leqslant a'<a\leqslant i\\ c}}(g_{a',a;i-1}^c-g_{a',a;i}^c), \tag{5.15}$$

where g_i^j, $g_{i',i}^j$, $g_{i;i''}^j$, $g_{i',i;i''}^j$, f_i^j, and $f_{i',i}^j(i'<i\leqslant i''<V-1)$ are summation variables running from 0 to 1 and

$$g_{i;i-1}^j\equiv g_i^j, \tag{5.16a}$$

$$g_{i',i;i-1}^j\equiv g_{i',i}^j, \tag{5.16b}$$

$$g_{i;V-1}^j\equiv f_i^j, \tag{5.16c}$$

$$g_{i',i;V-1}^j\equiv f_{i',i}^j. \tag{5.16d}$$

$\Sigma_{f\leqslant g_{;V-2}\cdots\leqslant g_{;1}\leqslant g\leqslant h\leqslant 1}$ in (5.12b) means summation under the conditions

$$f_i^j\leqslant g_{i;V-2}^j\leqslant\cdots\leqslant g_{i;i}^j\leqslant g_i^j\leqslant h_i^j\leqslant 1, \tag{5.17a}$$

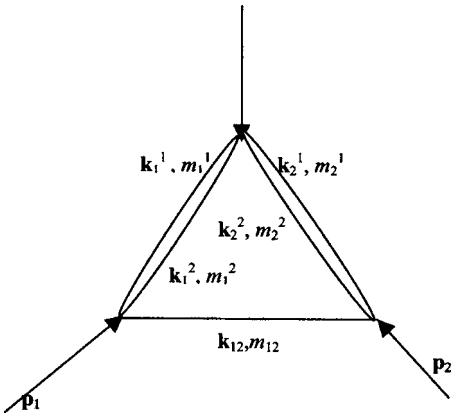

FIG. 4. A diagram with three vertices and five internal lines.

$$f^j_{i',i} \leqslant g^j_{i',i;V-2} \leqslant \cdots \leqslant g^j_{i',i;i} \leqslant g^j_{i',i} \leqslant h^j_{i',i} \leqslant 1, \tag{5.17b}$$

Σ_k means summation over all k^j_i and $k^j_{i',i}$ from 0 to ∞, if they are appearing through factors K and L, the summation is from 0 to b^j_i-1 and $b^j_i+l^j_i+r^j_i-1$, respectively, if they are appearing through a factor M.

Equation (5.11) is a generalization of formula (3.4) for sunset diagrams. It is a sum of terms that have factors K, L, and M, defined in (2.8) and (2.9), in the numerator. Instead of a power of one denominator factor N in (3.4), (5.10c) leads to $V-1$ denominator factors $\Sigma^i_{a=1}N_a(i=1,2,\ldots,V-1)$, which all, in turn, may have higher powers, caused by integration over logarithms. The various terms of (5.12b) may be described by the following features:

(i) The first term consists of I factors L in the numerator. The exponent of x_i in (5.10c) becomes, after integration, a factor $\Sigma^i_{a=1}N_a$, in the denominator. The factor in front is 0! .
(ii) Integration of terms with factors L gives, because of the logarithm of (2.8b), both a term with a logarithm and a term without logarithm.
(iii) In the latter case, the power of the corresponding factors $\Sigma^i_{a=1}N_a$ increases by 1, as well as the argument of the faculty in front, and the sign of the term changes.
(iv) Further terms are obtained after replacement of factors L by K, M or combinations in terms with an increased power of $\Sigma^i_{a=1}N_a$. Each replacement lowers the power of $\Sigma^i_{a=1}N_a$ by 1 as well as the argument of the faculty in front, and changes the sign of the term.
(v) A factor M in the numerator implies addition of a term $-2b$ or $-2(b+l+r)$ to the corresponding N_a in the denominator. If two or more of these terms are added, poles in the complex ν plane may appear.

The integrals in the regions (5.4b), which may be computed by means of the formulas of Appendix C, must be added to (5.11) to help convergence. The latter integrals are arbitrary small for sufficiently large Λ.

Analytical continuation from the region (5.7) to other regions of the complex $(\Sigma m-\Sigma p)$ plane is obtained according to the rules of (4.2).

As an example, we demonstrate a diagram with three vertices and five internal lines according to Fig. 4.

The expression is

$$\frac{(2\pi^{1/2n})^5}{(2\pi)^{2n}} \frac{(m_1^1)^{2b_1^1}(m_1^2)^{2b_1^2}(m_2^1)^{2b_2^1}(m_2^2)^{2b_2^2}(m_{1,2})^{2b_{1,2}}}{\Gamma(\alpha_1^1)\Gamma(\alpha_1^2)\Gamma(\alpha_2^1)\Gamma(\alpha_2^2)\Gamma(\alpha_{1,2})}$$

$$\times \int d\mathbf{x}_1\, d\mathbf{x}_2\, e^{i\mathbf{p}_1\cdot\mathbf{x}_1} e^{i\mathbf{p}_2\cdot\mathbf{x}_2} k_{b_1^1}(m_1^1 x_1) k_{b_1^2}(m_1^2 x_1) k_{b_2^1}(m_2^1 x_2) k_{b_2^2}(m_2^2 x_2) k_{b_{1,2}}(m_{1,2}|\mathbf{x}_1-\mathbf{x}_2|) \tag{5.18}$$

and the region of the radial integrations is divided into subregions $0<x_1<x_2<X$, $0<x_1<X$

$<x_2$, $0<X<x_1<x_2$, and permutations of x_1 and x_2. $(\Sigma m-\Sigma p)$ is given by

$$\left(\sum m-\sum p\right)\equiv \min\begin{cases}(m_1^1+m_1^2+m_{1,2}-p_1),\\ (m_2^1+m_2^2+m_{12}-p_2),(m_1^1+m_1^2+m_2^1+m_2^2-p_1-p_2).\end{cases} \tag{5.19}$$

The contribution of the subregions $0<x_1<X<x_2$, $0<X<x_1<x_2$, and permutations can be made arbitrary small by choosing

$$\Lambda=\left(\sum m-\sum p\right)X \tag{5.20}$$

sufficiently large. In this case, only the two regions $0<x_1<x_2<X$ and $0<x_2<x_1<X$ contribute. In the latter subregions, (5.18) is factorized into an angular and a radial part,

$$(5.18)\cong \frac{(2\pi^{1/2n})^7}{(2\pi)^{2n}\Gamma(\alpha_1^1)\Gamma(\alpha_1^2)\Gamma(\alpha_2^1)\Gamma(\alpha_2^2)\Gamma(\alpha_{12})}A(q_1,q_2,r_{12})R(q_1,q_2,r_{12}) \tag{5.21}$$

with

$$A(q_1,q_2,r_{12})=\frac{1}{(2\pi^{\frac{1}{2}n})^2}\int \mathrm{d}\hat{\mathbf{x}}_1\,\mathrm{d}\hat{\mathbf{x}}_2\frac{(2\hat{\mathbf{p}}_1\cdot\hat{\mathbf{x}}_1)^{q_1}}{q_1!}\frac{(2\hat{\mathbf{p}}_2\cdot\hat{\mathbf{x}}_2)^{q_2}}{q_2!}\frac{(2\hat{\mathbf{x}}_1\cdot\hat{\mathbf{x}}_2)^{r_{1,2}}}{r_{1,2}!}$$

$$=\sum_{q_{1,2},p_{1,2}}{}'\frac{(2\hat{\mathbf{p}}_1\cdot\hat{\mathbf{p}}_2)^{p_{1,2}}}{\frac{1}{2}(n+q_1+r_{1,2})!\,\frac{1}{2}(n+q_2+q_{1,2})!\,\frac{1}{2}(q_1-q_{1,2})!\,\frac{1}{2}(q_2-p_{1,2})!\,\frac{1}{2}(r_{1,2}-q_{1,2})!\,\frac{1}{2}(q_{1,2}-p_{1,2})!\,p_{1,2}!} \tag{5.22a}$$

(Σ' means summation over $q_{1,2}$ and $p_{1,2}$ under the condition that the arguments of the faculties in the denominator are integers) and

$$\begin{aligned}R(q_1,q_2,r_{12})=&\sum_{l_{1,2}}\frac{2^{4\nu}p_1^{q_1}p_2^{q_2}(m_1^1)^{2b_1^1}(m_1^2)^{2b_1^2}(m_2^1)^{2b_2^1}(m_2^2)^{2b_2^2}(-)^{l_{1,2}}(m_{1,2})^{2(b_{1,2}+l_{1,2}+r_{1,2})}}{l_{1,2}!}\\ &\times\int_{0<x_1<x_2<X}d\frac{x_1}{2}d\frac{x_2}{2}\left(\frac{x_1}{2}\right)^{2\nu+q_1+2l_{1,2}+r_{1,2}-1}\left(\frac{x_2}{2}\right)^{2\nu+q_2+r_{1,2}-1}\\ &\times k_{b_1^1}(m_1^1x_1)k_{b_1^2}(m_1^2x_1)k_{b_2^1}(m_2^1x_2)k_{b_1^2}(m_2^2x_2)k_{b_{1,2}+l_{1,2}+r_{1,2}}(m_{1,2}x_2)+\text{permutation}.\end{aligned} \tag{5.22b}$$

The rhs of (5.22b) is computed with use of Appendix D. The final result is

$$(5.18) \cong \sum \frac{2^{4\nu} F_3^5 A(q_1,q_2,r_{1,2}) \rho_1^{q_1} \rho_2^{q_2} (\mu_1^1)^{2(b_1^1+k_1^1)} (\mu_1^2)^{2(b_1^2+k_1^2)} (\mu_2^1)^{2(b_2^1+k_2^1)} (\mu_2^2)^{2(b_2^2+k_2^2)} (-)^{l_{1,2}} (\mu_{1,2})^{2(b_{1,2}+l_{1,2}+r_{1,2}+k_{1,2})}}{\left(\sum m - \sum p\right)^{4\nu-2(b_1^1+b_1^2+b_2^1+b_2^2+b_{1,2})} l_{1,2}!}$$

$$\times \left\{ \begin{array}{l} \left\{ \frac{L_1^1 L_1^2 L_2^1 L_2^2 L_{1,2}}{N_1(N_1+N_2)} \right\} \ln\left(\frac{\mu_1^1\Lambda}{2}\right) \ln\left(\frac{\mu_1^2\Lambda}{2}\right) \ln\left(\frac{\mu_2^1\Lambda}{2}\right) \ln\left(\frac{\mu_2^2\Lambda}{2}\right) \ln\left(\frac{\mu_{1,2}\Lambda}{2}\right) \left(\frac{\Lambda}{2}\right)^{N_1+N_2} \\ + \left\{ \begin{array}{l} -\frac{L_1^1 L_1^2 L_2^1 L_2^2 L_{1,2}}{N_1^2(N_1+N_2)} - \frac{L_1^1 L_1^2 L_2^1 L_2^2 L_{1,2}}{N_1(N_1+N_2)^2} \\ + \frac{K_1^1 L_1^2 L_2^1 L_2^2 L_{1,2}}{N_1(N_1+N_2)} + \frac{M_1^1 L_1^2 L_2^1 L_2^2 L_{1,2}}{(N_1-2b_1^1)(N_1+N_2)} + \cdots \end{array} \right\} \ln\left(\frac{\mu_1^2\Lambda}{2}\right) \ln\left(\frac{\mu_2^1\Lambda}{2}\right) \ln\left(\frac{\mu_2^2\Lambda}{2}\right) \ln\left(\frac{\mu_{1,2}\Lambda}{2}\right) \left(\frac{\Lambda}{2}\right)^{N_1+N_2} \\ + \left\{ -\frac{L_1^1 L_1^2 L_2^1 L_2^2 L_{1,2}}{N_1(N_1+N_2)^2} + \frac{L_1^1 L_1^2 K_2^1 L_2^2 L_{1,2}}{N_1(N_1+N_2)} + \cdots \right\} \ln\left(\frac{\mu_1^1\Lambda}{2}\right) \ln\left(\frac{\mu_1^2\Lambda}{2}\right) \ln\left(\frac{\mu_2^2\Lambda}{2}\right) \ln\left(\frac{\mu_{1,2}\Lambda}{2}\right) \left(\frac{\Lambda}{2}\right)^{N_1+N_2} \\ + \left\{ \frac{L_1^1 L_1^2 M_2^1 L_2^2 L_{1,2}}{N_1(N_1+N_2-2b_2^1)} + \cdots \right\} \ln\left(\frac{\mu_1^1\Lambda}{2}\right) \ln\left(\frac{\mu_1^2\Lambda}{2}\right) \ln\left(\frac{\mu_2^2\Lambda}{2}\right) \ln\left(\frac{\mu_{1,2}\Lambda}{2}\right) \left(\frac{\Lambda}{2}\right)^{N_1+N_2-2b_2^1} \\ + \left\{ \frac{2!\, L_1^1 L_1^2 L_2^1 L_2^2 L_{1,2}}{N_1(N_1+N_2)^3} - \frac{L_1^1 L_1^2 L_2^1 K_2^2 L_{1,2}}{N_1(N_1+N_2)^2} + \cdots \right\} \ln\left(\frac{\mu_1^1\Lambda}{2}\right) \ln\left(\frac{\mu_1^2\Lambda}{2}\right) \ln\left(\frac{\mu_2^1\Lambda}{2}\right) \left(\frac{\Lambda}{2}\right)^{N_1+N_2} \\ + \left\{ -\frac{L_1^1 L_1^2 L_2^1 K_2^2 M_{1,2}}{N_1\{N_1+N_2-2(b_{1,2}+l_{1,2}+r_{1,2})\}^2} + \cdots \right\} \ln\left(\frac{\mu_1^1\Lambda}{2}\right) \ln\left(\frac{\mu_1^2\Lambda}{2}\right) \ln\left(\frac{\mu_2^1\Lambda}{2}\right) \left(\frac{\Lambda}{2}\right)^{N_1+N_2-2(b_{1,2}+l_{1,2}+r_{1,2})} \\ + \left\{ -\frac{L_1^1 L_1^2 L_2^1 M_2^2 M_{1,2}}{N_1\{N_1+N_2-2(b_2^2+b_{1,2}+l_{1,2}+r_{1,2})\}^2} + \cdots \right\} \ln\left(\frac{\mu_1^1\Lambda}{2}\right) \ln\left(\frac{\mu_1^2\Lambda}{2}\right) \ln\left(\frac{\mu_2^1\Lambda}{2}\right) \left(\frac{\Lambda}{2}\right)^{N_1+N_2-2(b_2^2+b_{1,2}+l_{1,2}+r_{1,2})} \end{array} \right\}$$

$$+ \text{many similar terms} + \text{permutations}, \tag{5.23}$$

with

$$N_1 = 2\nu + q_1 + 2k_1^1 + 2k_1^2 + 2l_{1,2} + r_{1,2}, \tag{5.24a}$$

$$N_2 = 2\nu + q_2 + 2k_2^1 + 2k_2^2 + 2k_{1,2} + r_{1,2}. \tag{5.24b}$$

VI. UNITARITY

The S matrix must satisfy the unitarity relation

$$S^\dagger S = I. \tag{6.1}$$

In terms of the T-matrix, which is defined by

$$S = I - i\delta\left(\sum p\right) T, \tag{6.2}$$

(6.1) is written as

$$2\Im(T) \equiv i(T^\dagger - T) = -\delta\left(\sum p\right) T^\dagger T. \tag{6.3}$$

In the case of sunset diagrams, their imaginary part must be equal to the integral over positive energy states with momenta that are on the mass shell, which is the phase space integral.

The n dimensional Laplace transform of $\theta(k^0)\delta(\mathbf{k}^2 - m^2)$ is found by using the integral representation (A14),[13]

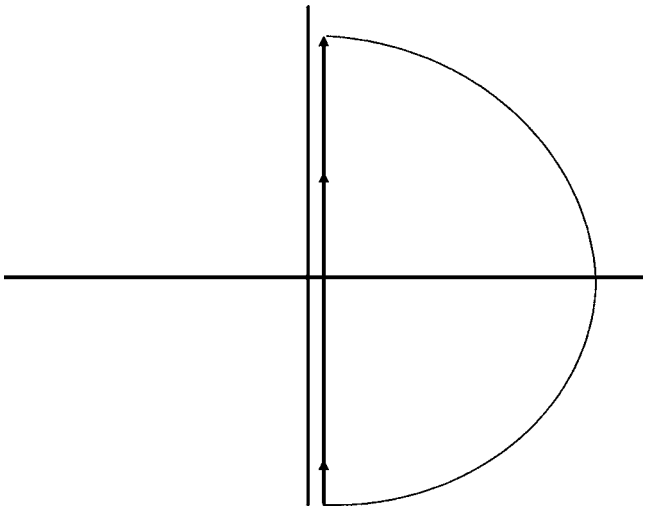

FIG. 5. Integration path to the right.

$$\int_0^\infty \mathrm{d}\mathbf{k}\, e^{-\mathbf{x}\cdot\mathbf{k}}\theta(k^0)\,\delta(\mathbf{k}^2-m^2) = \frac{\pi^{(n-1)/2}}{\Gamma\left(\frac{n-1}{2}\right)}\int_m^\infty \mathrm{d}k^0\, e^{-xk^0}(k^{0^2}-m^2)^{(n-3)/2}$$

$$= \frac{\pi^{(n-1)/2}(m^2)^{(n/2)-1}}{\Gamma\left(\frac{n-1}{2}\right)}\int_1^\infty \mathrm{d}t\, e^{-mxt}(t^2-1)^{(n-3)/2}$$

$$= \pi^{(n/2)-1}(m^2)^{(n/2)-1}k_{(n/2)-1}(mx). \tag{6.4}$$

Applying (6.4) on a product of factors $\theta(k^0)\delta(\mathbf{k}^2-m^2)$ and taking afterwards the inverse n dimensional Laplace transformation, which is an inverse K transform according to (A15), it follows that[12,13]

$$(2\pi)^I \prod \int \mathrm{d}\mathbf{k}^j\ \delta\Big(\mathbf{p}-\sum \mathbf{k}^c\Big)\theta(k_0^j)\,\delta(\mathbf{k}^{j^2}-m^{j^2}) = \frac{F_2^I}{i}\prod (m^j)^{2b^j}\int_{c-i\infty}^{c+i\infty}\mathrm{d}x\, x^{n-1}i_b(px)k_{bj}(m^jx), \tag{6.5}$$

with

$$b = b^j = \tfrac{1}{2}n - 1, \tag{6.6a}$$

$$c > 0, \tag{6.6b}$$

and F_2^I is given in (2.3). The left-hand side (lhs) of (6.5) is, up to a factor $(2\pi)^I$, the I particle phase space integral.

We remark that (6.5) is obtained by Laplace transformations followed by an n dimensional inverse Laplace transformation in the same way as (2.1) is obtained from the momentum space representation by Fourier transformations followed by an n dimensional inverse Fourier transformation. The integrands of (6.5) and (2.1) are equal, the integrals differ by the path of integration.

In the case $p<\Sigma m$, it is seen that (6.5) is 0, by closing the contour to the right of the complex $(\Sigma m-p)$ plane and by remarking that the integrand vanishes towards ∞ (Fig. 5).

In the case $p>\Sigma m$, the integral does not vanish near infinity towards the left-hand side of the complex plane, since the decreasing asymptotic behavior of the integrand is restricted by the

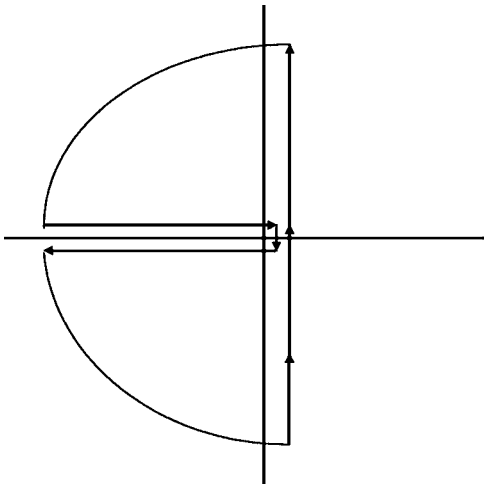

FIG. 6. Integration path to the left.

values of the argument of the integration variable, as indicated in (A6). The integrand vanishes near ∞ only if crossing the negative axis is avoided. Hence, the path of integration must be closed according to Fig. 6. The contribution from the near zero part and that of the near infinity circle are both 0. The contribution along the negative real axis from $-\infty \rightarrow -0$ is equal to the complex conjugate of the $-0 \rightarrow -\infty$ integration.

Hence, we conclude that

$$(6.5) = -F_2^I \prod (m^j)^{2b^j} \int_0^\infty \mathrm{d}x\, x^{n-1} 2\Im\left\{\prod i_{(n/2)-1}(px) k_{(n/2)-1}(m^j x)\right\}. \tag{6.7}$$

After interchanging integral and $\Im$ operation, the unitarity relation

$$2\Im(2.1) = -(2\pi)^I \prod \int \mathrm{d}\mathbf{k}^j\, \delta\left(\mathbf{p} - \sum \mathbf{k}^j\right) \theta(k_0^j)\, \delta(\mathbf{k}^{j^2} - m^{j^2}) \tag{6.8}$$

of a sunset diagram is obtained. It is in agreement with (1.13) and (1.16).

VII. CONVERGENCE

Expansions with many summation variables occurred in the preceding sections and convergence of these series must be discussed.

In the used formulas, faculties of summation variables appear in the denominator, which helps convergence. Also factors like $(-)^k$ and $(-)^l$ may promote convergence.

A point of concern is a Γ function of summation variables in the numerator, like in the factor

$$\frac{(-)^{l^j_{i',i}} M^j_{i',i}}{l^j_{i',i}!} = \frac{(-)^{k^j_{i',i}+l^j_{i',i}} \Gamma(b^j_{i',i} + l^j_{i',i} + r^j_{i',i} - k^j_{i',i})}{2k^j_{i',i}!\, l^j_{i',i}!}. \tag{7.1}$$

Its origin is (A11) where the function $k_b(m|x_i - x_{i'}|)$ with a composed argument is split. Since this Bessel function is analytical, it is not dangerous in itself. Only integration in a region where the argument is zero may cause divergences. These correspond to the ultraviolet divergences in momentum space.

In the case of functions $k_b(mx)$ with simple argument, divergences were appearing through factors of the kind

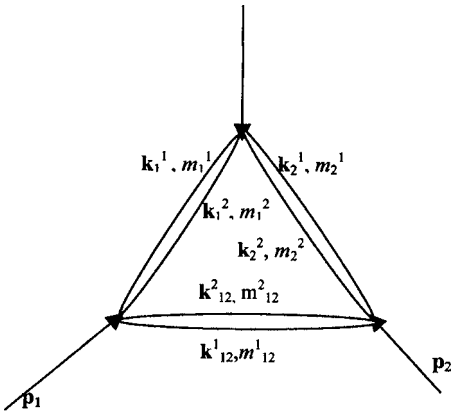

FIG. 7. A diagram with three vertices and six internal lines.

$$\frac{1}{N} = \frac{1}{2\nu - 2\sum b + 2\sum k + \cdots}. \tag{7.2}$$

In the case of functions with a composed argument, the divergences come from integration in the region where $|\mathbf{x}_i - \mathbf{x}_{i'}| = 0$. These manifest by divergence of the summation over the variable $l_{i',i}$. For this reason, the method of Sec. V is applicable only on diagrams like Fig. 4, where composed k-functions correspond to single connected vertices, which add only one term $-2b$ to the denominator of (7.2).

There is a freedom of choice of the configuration space parameters. Transformations like

$$\mathbf{x}_i \rightarrow \mathbf{x}_i + \mathbf{x}_{i'} \tag{7.3}$$

are possible. By such transformations, it may be tried to manage that all multiple connected vertices correspond to simple k functions. This has been done in the case of Fig. 4. However, there are cases where such transformations cannot be found, like the diagram of Fig. 7.

A division of the integral range, finer than in (5.4a), is needed, $(V+1)!$ subregions of the kind

$$x_1 < x_2 < |\mathbf{x}_1 - \mathbf{x}_2| < X \text{ and permutations} \tag{7.4}$$

must be considered and more complicated angle integrations must be performed. This procedure has been discussed in Ref. 14. Fortunately, diagrams like Fig. 7 are not used in today's physics.

A second source of divergences are integrations in the neighborhood of ∞. They correspond to infrared divergences in momentum space. By caring that the asymptotic behavior of the integrand is exponential decreasing, this kind of infinity is avoided.

In the preceding sections, the above-mentioned restrictions have been treated by separating out the corresponding divergences. Hence, the general expression (5.1) is convergent up to the divergences that have been separated out, and so is its expansion (5.11).

The working of the splitting procedure of (2.10) may be elucidated in the case of $\int_0^\infty \mathrm{d}x\, x^{2\nu-1} k_\beta(x)$ with $\nu=2$ and $\beta=1$. The integral is known exactly,[15]

$$\int_0^\infty \mathrm{d}x\, x^{2\nu-1} k_\beta(x) = 2^{2\nu-2}\Gamma(\nu)\Gamma(\nu-\beta). \tag{7.5}$$

On the other hand, we may work out

$$\int_0^\infty \mathrm{d}x\, x^3 k_1(x) = \int_0^\Lambda \mathrm{d}x\, x^3 k_1(x) + \int_\Lambda^\infty \mathrm{d}x\, x^3 k_1(x). \tag{7.6}$$

Insertion of the expansion (A3) into the first term of the rhs and application of (D1) yields

$$\int_0^\Lambda \mathrm{d}x\, x^{2\nu-1} k_1(x) = \sum_{k=0}^{\infty} \frac{2^{2\nu}\left\{\left(\gamma - \frac{1}{1} - \frac{1}{2} - \frac{1}{3} \cdots - \frac{1}{k}\right) + \left(\gamma - \frac{1}{1} - \frac{1}{2} - \frac{1}{3} \cdots - \frac{1}{k} - \frac{1}{k+1}\right)\right\}\left(\frac{\Lambda}{2}\right)^{2\nu+2k}}{k\,!\,(k+1)\,!\,(2\nu+2k)}$$
$$+ \sum_{k=0}^{\infty} \frac{2^{2\nu}\left(\frac{\Lambda}{2}\right)^{2\nu+2k} \ln\left(\frac{\Lambda}{2}\right)}{k\,!\,(k+1)\,!\,(2\nu+2k)} - \sum_{k=0}^{\infty} \frac{2^{2\nu}\left(\frac{\Lambda}{2}\right)^{2\nu+2k} \ln\left(\frac{\Lambda}{2}\right)}{k\,!\,(k+1)\,!\,(2\nu+2k)^2} + \frac{1}{2(2\nu-2)}\left(\frac{\Lambda}{2}\right)^{2\nu-2}. \tag{7.7}$$

Insertion of the asymptotic expansion (A6a) into the second term of the rhs of (7.6) yields

$$\int_\Lambda^\infty \mathrm{d}x\, x^{2\nu-1} k_1(x) \cong \left\{\sqrt{\pi} \sum_{k=0}^{H-1} 2^{\frac{1}{2}-k}(1,k)\right\} \int_\Lambda^\infty \mathrm{d}x\, x^{2\nu-k-\frac{5}{2}} e^{-x}, \tag{7.8}$$

on which (C7) may be applied.

We take the number of terms of the asymptotic series 15 $(H=15)$, $\gamma=0.577\,215\,664\,9$, and find

Λ	$\int_0^\Lambda \mathrm{d}x\, x^3 k_1(x)$	$\int_\Lambda^\infty \mathrm{d}x\, x^3 k_1(x)$	$\int_0^\Lambda \mathrm{d}x\, x^3 k_1(x) + \int_\Lambda^\infty \mathrm{d}x\, x^3 k_1(x)$
2	1.969921963	1.204499139	3.174421102
5	3.734552813	0.26544653	3.999999343
10	3.995697337	0.004301964	3.99999301
15	3.999745608	0.0000503234	3.999795931
20	3.951797003	−0.0000460393	3.951750964
23	2.799347994	−0.008824087	2.781523907

It is seen that for $10<\Lambda<15$ the first integral alone approaches the exact answer 4 of (7.5). For smaller Λ's, the asymptotic integral may help convergence. Apparently, the calculations are not sufficiently accurate for $\Lambda<3$ and $\Lambda>20$.

ACKNOWLEDGMENT

The author thanks Professor J. Smit for a useful discussion.

APPENDIX A: BESSEL FUNCTIONS

Most of the formulas of this appendix are found in the textbook by Watson[15] for the functions $J_\beta(z)$, $I_\beta(z)$, $K_\beta(z)$, $H_\beta^{(1)}(z)$, and $H_\beta^{(2)}(z)$. In this paper, use has been made of functions $j_\beta(z)$, $i_\beta(z)$, $k_\beta(z)$, $h_\beta^+(z)$, and $h_\beta^-(z)$ that differ from them by a factor $(z/2)^\beta$ according to

$$j_\beta(z) = \left(\frac{z}{2}\right)^{-\beta} J_\beta(z) = \sum_{k=0}^{\infty} \frac{(-)^k}{k\,!\,\Gamma(1+\beta+k)}\left(\frac{z}{2}\right)^{2k}, \tag{A1a}$$

$$i_\beta(z) = \left(\frac{z}{2}\right)^{-\beta} I_\beta(z) = \sum_{k=0}^{\infty} \frac{1}{k\,!\,\Gamma(1+\beta+k)}\left(\frac{z}{2}\right)^{2k}, \tag{A1b}$$

$$k_\beta(z)=\left(\frac{z}{2}\right)^{-\beta}K_\beta(z)=\frac{\pi}{2\sin\pi\beta}\sum_{k=0}^{\infty}\left\{\frac{1}{k!\,\Gamma(1-\beta+k)}\left(\frac{z}{2}\right)^{-2\beta+2k}-\frac{1}{k!\,\Gamma(1+\beta+k)}\left(\frac{z}{2}\right)^{2k}\right\}, \tag{A1c}$$

$$h_\beta^{+}(z)=\left(\frac{z}{2}\right)^{-\beta}H_\beta^{(1)}(z)=\frac{-i}{\sin\pi\beta}\sum_{k=0}^{\infty}(-)^k\left\{\frac{1}{k!\,\Gamma(1-\beta+k)}\left(\frac{z}{2}\right)^{-2\beta+2k}-\frac{e^{-i\pi\beta}}{k!\,\Gamma(1+\beta+k)}\left(\frac{z}{2}\right)^{2k}\right\}, \tag{A1d}$$

$$h_\beta^{-}(z)=\left(\frac{z}{2}\right)^{-\beta}H_\beta^{(2)}(z)=\frac{i}{\sin\pi\beta}\sum_{k=0}^{\infty}(-)^k\left\{\frac{1}{k!\,\Gamma(1-\beta+k)}\left(\frac{z}{2}\right)^{-2\beta+2k}-\frac{e^{i\pi\beta}}{k!\,\Gamma(1+\beta+k)}\left(\frac{z}{2}\right)^{2k}\right\}. \tag{A1e}$$

If it is supposed that

$$\beta=b+\varepsilon, \tag{A2}$$

where b is integer, (A1) becomes in the limit $\varepsilon\to 0$,

$$j_b(z)=\sum_{k=0}^{\infty}\frac{(-)^k}{k!\,(b+k)!}\left(\frac{z}{2}\right)^{2k}, \tag{A3a}$$

$$i_b(z)=j_b(iz)=\sum_{k=0}^{\infty}\frac{1}{k!\,(b+k)!}\left(\frac{z}{2}\right)^{2k}, \tag{A3b}$$

$$k_b(z)=K_b(k)\left(\frac{z}{2}\right)^{2k}+L_b\left(\frac{z}{2}\right)^{2k}\ln\left(\frac{z}{2}\right)+M_b(k)\left(\frac{z}{2}\right)^{-2b+2k}, \tag{A3c}$$

$$h_b^{+}(z)=j_b(z)+iy_b(z), \tag{A3d}$$

$$h_b^{-}(z)=j_b(z)-iy_b(z), \tag{A3e}$$

with the notation

$$y_b(z)=\frac{-(-)^k 2}{\pi}\left\{(-)^bK_b(k)\left(\frac{z}{2}\right)^{2k}+(-)^bL_b\left(\frac{z}{2}\right)^{2k}\ln\left(\frac{z}{2}\right)+M_b(k)\left(\frac{z}{2}\right)^{-2b+2k}\right\}, \tag{A4a}$$

$$K_b(k)=\frac{(-)^{b+1}}{k!\,(b+k)!}\left\{\left(\gamma-\frac{1}{1}-\frac{1}{2}-\cdots-\frac{1}{k}\right)+\left(\gamma-\frac{1}{1}-\frac{1}{2}-\cdots-\frac{1}{k+b}\right)\right\},$$
$$(\gamma=0.577\,215\,664\,9), \tag{A4b}$$

$$L_b(k)=\frac{(-)^{b+1}}{k!\,(b+k)!}, \tag{A4c}$$

$$M_b(k)=\frac{(-)^k(b-k-1)!}{2\,.\,k!}. \tag{A4d}$$

From here, we see that

$$h_b^+(iz) = \frac{2i(-)^{b+1}}{\pi} k_b(z), \tag{A5a}$$

$$h_b^-(iz) = 2i_b(z) - \frac{2i(-)^{b+1}}{\pi} k_b(z). \tag{A5b}$$

The asymptotic behavior of the functions $k_\beta(z)$, $h_\beta^+(z)$, $h_\beta^-(z)$, $h_\beta^+(iz)$, and $h_\beta^-(iz)$ is given by

$$k_\beta(z) = e^{-z}\left\{\sum_{k=0}^{H-1} \frac{\sqrt{\pi}2^{2\beta}(\beta,k)}{(2z)^{\beta+k+\frac{1}{2}}} + O(z^{-H})\right\} \quad \left(-\frac{3}{2}\pi < \arg z < \frac{3}{2}\pi\right), \tag{A6a}$$

$$h_\beta^+(z) = \frac{2^{2\beta+1}e^{-\frac{1}{2}i\pi\left(\beta+\frac{1}{2}\right)}e^{iz}}{\sqrt{\pi}}\left\{\sum_{k=0}^{H-1} \frac{i^k(\beta,k)}{(2z)^{\beta+k+\frac{1}{2}}} + O(z^{-H})\right\} \quad (-\pi < \arg z < 2\pi), \tag{A6b}$$

$$h_\beta^-(z) = \frac{2^{2\beta+1}e^{\frac{1}{2}i\pi\left(\beta+\frac{1}{2}\right)}e^{-iz}}{\sqrt{\pi}}\left\{\sum_{k=0}^{H-1} \frac{(-i)^k(\beta,k)}{(2z)^{\beta+k+\frac{1}{2}}} + O(z^{-H})\right\} \quad (-2\pi < \arg z < \pi), \tag{A6c}$$

$$h_\beta^+(iz) = \frac{2^{2\beta+1}e^{-i\pi\left(\beta+\frac{1}{2}\right)}e^{-z}}{\sqrt{\pi}}\left\{\sum_{k=0}^{H-1} \frac{(\beta,k)}{(2z)^{\beta+k+\frac{1}{2}}} + O(z^{-H})\right\} \quad \left(-\frac{3}{2}\pi < \arg z < \frac{3}{2}\pi\right), \tag{A6d}$$

$$h_\beta^-(iz) = \frac{2^{2\beta+1}e^{z}}{\sqrt{\pi}}\left\{\sum_{k=0}^{H-1} \frac{(-)^k(\beta,k)}{(2z)^{\beta+k+\frac{1}{2}}} + O(z^{-H})\right\} \quad \left(-\frac{5}{2}\pi < \arg z < \frac{1}{2}\pi\right), \tag{A6e}$$

$$i_\beta(z) = \frac{2^{2\beta}}{\sqrt{\pi}}\left\{\sum_{k=0}^{H-1} \frac{(-)^k(\beta,k)e^{z}}{(2z)^{\beta+k+\frac{1}{2}}} + \sum_{k=0}^{H-1} \frac{(\beta,k)e^{-i\pi\left(\beta+\frac{1}{2}\right)}e^{-z}}{(2z)^{\beta+k+\frac{1}{2}}} + O(z^{-H})\right\} \quad \left(-\frac{3}{2}\pi < \arg z < \frac{1}{2}\pi\right), \tag{A6f}$$

where $(\beta,0)=1$ and

$$(\beta,k) = \frac{\Gamma\left(\beta+k+\frac{1}{2}\right)}{k!\,\Gamma\left(\beta-k+\frac{1}{2}\right)} = \frac{\left\{\beta^2-\left(\frac{1}{2}\right)^2\right\}\left\{\beta^2-\left(\frac{3}{2}\right)^2\right\}\cdots\left\{\beta^2-\left(\frac{2k-1}{2}\right)^2\right\}}{k!}, \tag{A7}$$

if $k>0$.

The function $k_b(m|\mathbf{x}-\mathbf{y}|)$ may be split according to

$$k_\beta(m|\mathbf{x}-\mathbf{y}|) = \Gamma(\beta)\sum_{l=0}^{\infty}(\beta+l)C_l^\beta(\hat{\mathbf{x}}\cdot\hat{\mathbf{y}})\left(\frac{m^2xy}{4}\right)^l i_{\beta+l}(mx)k_{\beta+l}(my) \tag{A8}$$

if

$$x < y, \tag{A9}$$

where $\hat{\mathbf{x}}\cdot\hat{\mathbf{y}}$ is the cosine of the angle between $\mathbf{x}$ and $\mathbf{y}$ and $C_k^\beta(\hat{\mathbf{x}}\cdot\hat{\mathbf{y}})$ are Gegenbauer polynomials, defined by

$$C_l^\beta(\hat{\mathbf{x}}\cdot\hat{\mathbf{y}}) \equiv \sum_r{}' \frac{(-)^{(l-r)/2}\Gamma\left(\beta+\frac{l+r}{2}\right)(2\hat{\mathbf{x}}\cdot\hat{\mathbf{y}})^r}{\Gamma(\beta)\frac{l-r}{2}!\,r!}. \tag{A10}$$

Σ' means summation under the condition that $(l-r)/2$ is integer. A direct splitting into Bessel functions and cosines is[11]

$$k_\beta(m|\mathbf{x}-\mathbf{y}|) = \sum_{l,r=0}^{\infty} \frac{(-)^l}{l!}\left(\frac{mx}{2}\right)^{r+2l}\left(\frac{my}{2}\right)^r \frac{(2\hat{\mathbf{x}}\cdot\hat{\mathbf{y}})^r}{r!} k_{\beta+l+r}(my) \tag{A11}$$

if

$$x < y. \tag{A12}$$

An integral representation is

$$k_\beta(z) = \frac{1}{2}\int_0^\infty \mathrm{d}\rho\, \rho^{-\beta} e^{-\rho} e^{-z^2/4\rho}, \tag{A13}$$

which establishes the connection between configuration space and Feynman parameters.[14]

Another integral representation is

$$k_\beta(z) = \frac{\sqrt{\pi}}{\Gamma\left(\beta+\frac{1}{2}\right)}\int_1^\infty \mathrm{d}t\, e^{-zt}(t^2-1)^{\beta-\frac{1}{2}}. \tag{A14}$$

If the k_β transform of a function $R(p)$ is defined by

$$S(x) = 2\pi^{\frac{1}{2}n-1}\int_0^\infty \mathrm{d}p\, p^{n-1} k_{\frac{1}{2}n-1}(px) R(p), \tag{A15a}$$

then $R(p)$ is found by the inverse transformation[20]

$$R(p) = \frac{1}{i\pi^{\frac{1}{2}n}2^{n-2}}\int_{c-i\infty}^{c+i\infty} \mathrm{d}x\, x^{n-1} i_{\frac{1}{2}n-1}(px) S(x). \tag{A15b}$$

APPENDIX B: ANGULAR INTEGRATIONS

Integration over n dimensional Euclidean space of a product of cosines is done by using the formula[21,22]

$$\int \mathrm{d}\hat{\mathbf{x}}(\hat{\mathbf{x}}\cdot\mathbf{q}_1)^{q_1}(\hat{\mathbf{x}}\cdot\mathbf{q}_2)^{q_2}\cdots(\hat{\mathbf{x}}\cdot\mathbf{q}_{V-1})^{q_{V-1}} = \sum_{q_i}\frac{q_1!\,q_2!\cdots q_{V-1}!}{(q_1+q_2+\cdots q_{V-1})!}\int \mathrm{d}\hat{\mathbf{x}}\,\hat{\mathbf{x}}\cdot(\mathbf{q}_1+\mathbf{q}_2+\cdots + \mathbf{q}_{V-1})^{q_1+q_2+\cdots q_{V-1}}. \tag{B1}$$

Integration of the rhs yields

$$\prod_{1<i\leqslant V-1}\int \mathrm{d}\hat{\mathbf{x}}_1 \frac{(2\hat{\mathbf{p}}_\mathbf{1}\cdot\hat{\mathbf{x}}_1)^{q_1}}{q_1!}\frac{(2\hat{\mathbf{x}}_1\cdot\hat{\mathbf{x}}_i)^{r_{1,i}}}{r_{1,i}!} = \sum{}' \frac{2\pi^{\frac{1}{2}n}}{\Gamma\left(\frac{n+q_1+r_{1,2}+\cdots+r_{1,V-1}}{2}\right)\frac{q_1-\sum_{1<a\leqslant V-1} q_{1,a}}{2}!}$$
$$\prod_{1<i\leqslant V-1}\frac{(2\hat{\mathbf{p}}_\mathbf{1}\cdot\hat{\mathbf{x}}_i)^{q_{1,i}}}{\frac{r_{1,i}-q_{1,i}-\sum_{1<a<i} q^1_{a,i}-\sum_{i<a\leqslant V-1} q^1_{i,a}}{2}!\, q_{1,i}!}$$
$$\prod_{1\leqslant i'<i\leqslant V-1}\frac{(2\hat{\mathbf{x}}_{i'}\cdot\hat{\mathbf{x}}_i)^{q^1_{i',i}}}{q^1_{i',i}!}, \tag{B2}$$

where Σ' means summation over the variables $q_{1,i}$ and $q^1_{i,i''}$ $(1<i<i''\leqslant V-1)$ from 0 to ∞ in such a way that the arguments of the faculties in the denominator are integers.

Multiple application of (B2) yields

$$\prod\int \mathrm{d}\hat{\mathbf{x}}_i \frac{(2\hat{\mathbf{p}}_i\cdot\hat{\mathbf{x}}_i)^{q_i}}{q_i!}\frac{(2\hat{\mathbf{x}}_{i'}\cdot\hat{\mathbf{x}}_i)^{r^j_{i',i}}}{r^j_{i',i}!} = \frac{(2\pi^{\frac{1}{2}n})^{V-1}r_{i',i}!}{\prod_j r^j_{i',i}!}A(q_i,r_{i',i}), \tag{B3}$$

with notation of Π according to (5.2) and

$$r_{i',i} = \sum_c r^c_{i',i}. \tag{B4a}$$

The angular factor in (B3) is given by

$$A(q_i,r_{i',i}) = \sum{}' \prod$$
$$\frac{\left(r_{i',i}+\sum q^c{}_{i',i}\right)!\left(q_{i',i}+\sum q_{i'}{}^c{}_i\right)!\,(2\hat{\mathbf{p}}_{i'}\cdot\hat{\mathbf{p}}_i)^{p_{i',i}+\Sigma q_{i',i}{}^c}}{\Gamma\left(\frac{n+q_i+\sum r_{i,a}+\sum q^c{}_{i,b}+\sum q_{a,i}+\sum q_a{}^c{}_i}{2}\right)\overline{q_i}!\,\overline{r_{i',i}}!\,\overline{q_{i',i}}!\,r_{i',i}!\,q_{i',i}!\,p_{i',i}!\,q^{i'}{}_{i,i''}!\,q_{i'}{}^i{}_{i''}!\,q_{i',i}{}^{i''}!} \tag{B4b}$$

where we used summation variables $q^{i'}{}_{i,i''}$, $q_{i'}{}^i{}_{i''}$, and $q_{i',i}{}^{i''}$ $(1\leqslant i'<i<i''\leqslant V-1)$ with three indices and summation notation

$$\sum r_{i,a} = \sum_{a=i+1}^{V-1} r_{i,a},\quad \sum q_{a,i} = \sum_{a=1}^{i-1} q_{a,i},\quad \sum q^c{}_{i,b} = \sum_{c=1}^{i-1}\sum_{b=i+1}^{V-1} q^c{}_{i,b},$$

$$\sum q_a{}^c{}_i = \sum_{a=1}^{c-1}\sum_{c=2}^{i-1} q_a{}^c{}_i,\quad \sum q_{i',i}{}^c = \sum_{c=i+1}^{V-1} q_{i',i}{}^c,\quad \text{etc.} \tag{B5}$$

Furthermore,

$$\overline{q_i} = \frac{q_i-\sum q_{i,a}-\sum p_{a,i}}{2}, \tag{B6a}$$

$$\overline{r}_{i',i} = \frac{r_{i',i} + \sum q^{a}{}_{i',i} - q_{i',i} - \sum q^{i'}{}_{a,i} - \sum q^{i'}{}_{i,a}}{2}, \tag{B6b}$$

$$\overline{q}_{i',i} = \frac{q_{i',i} + \sum q_{i'}{}^{a}{}_{i} - p_{i',i} - \sum q_{a,i'}{}^{i} - \sum q_{i',a}{}^{i}}{2}. \tag{B6c}$$

Σ' means summation over the variables $p_{i',i}$, $q_{i',i}$, $q^{i'}{}_{i,i''}$, $q_{i'}{}^{i}{}_{i''}$, and $q_{i',i}{}^{i''}$ from 0 to ∞ in such a way that $\overline{q}_i$, $\overline{q}_{i',i}$, and $\overline{r}_{i',i}$ are integers. Summation over $\overline{q}_i$ yields Bessel functions,

$$\prod \int \mathrm{d}\hat{\mathbf{x}}_i \, e^{i\mathbf{p}_i\cdot\mathbf{x}_i} \frac{(2\hat{\mathbf{x}}_{i'}\cdot\hat{\mathbf{x}}_i)^{r^j_{i',i}}}{r^j_{i',i}!} = \frac{(2\pi^{\frac{1}{2}n})^{V-1} r_{i',i}!}{\prod_j r^j_{i',i}!} \sum{}' A(r_{i',i}) \left(\frac{ip_ix_i}{2}\right)^{s_i - \Sigma\overline{r}_{i,a} - \Sigma\overline{q}_{a,i} - \Sigma q^{i}{}_{a,b} - \Sigma q_{a,b}{}^{i}} j_{(n/2)-1+s_i}(p_ix_i) \tag{B7}$$

with

$$\begin{aligned} s_i &= \frac{\sum q_{i,a} + \sum p_{a,i} + \sum r_{i,a} + \sum q^{c}{}_{i,a} + \sum q_{a,i} + \sum q_{a}{}^{c}{}_{i}}{2} \\ &= \overline{r}_{i,a} + 2\overline{q}_{i,a} + \overline{q}_{a,i} + p_{i,a} + p_{a,i} + q^{i}{}_{a,b} - q_{i}{}^{a}{}_{b} + q_{a,i}{}^{c} + q_{i,a}{}^{c} + q_{a,b}{}^{i} \end{aligned} \tag{B8a}$$

and

$$A(r^j_{i',i}) = \prod \frac{\left(r_{i',i} + \sum q^{c}{}_{i',i}\right)! \left(q_{i',i} + \sum q_{i'}{}^{c}{}_{i}\right)! (2\hat{\mathbf{p}}_{i'}\cdot\hat{\mathbf{p}}_i)^{p_{i',i} + \Sigma q_{i',i}{}^{c}}}{\overline{r}_{i',i}!\, \overline{q}_{i',i}!\, r_{i',i}!\, q_{i',i}!\, p_{i',i}!\, q^{i'}{}_{i,i''}!\, q_{i'}{}^{i}{}_{i''}!\, q_{i',i}{}^{i''}!}. \tag{B8b}$$

APPENDIX C: RADIAL $\Lambda \to \infty$ INTEGRATIONS

The radial factors $R_1(r^j_{i',i})$ and $R_2(r^j_{i',i})$, appearing in (5.5) as result of integrations in the subregions (5.4b), may be expressed, using (A8) and (B7), in terms of Bessel functions. They become

$$R_1(r^j_{i',i}) = \sum{}' \prod \frac{2^{2\nu}(-)^{\frac{l^j_{i',a} - r^j_{i',a} + l^j_{i,i''} - r^j_{i,i''}}{2}} (m^j_{i',i})^{2l^j_{i',i}} \left(b^j_{i',i} + l^j_{i',i}\right)\left(b^j_{i,i''} + l^j_{i,i''}\right) \Gamma\left(b^j_{i',i} + \frac{l^j_{i',i} + r^j_{i',i}}{2}\right) \Gamma\left(b^j_{i,i''} + \frac{l^j_{i,i''} + r^j_{i,i''}}{2}\right)}{\left(\frac{l^j_{i',i} - r^j_{i',i}}{2}\right)! \left(\frac{l^j_{i,i''} - r^j_{i,i''}}{2}\right)!}$$

$$\times \int_{0<x_1<\ldots<x_f<X} d\frac{x_i}{2} \left(\frac{ip_ix_i}{2}\right)^{s_i - \sum\overline{r}_{i,a} - \sum\overline{q}_{a,i} - \sum q^{i}{}_{a,b} - \sum q_{a,b}{}^{i}} \left(\frac{x_i}{2}\right)^{2\nu - 1 + \sum l^{c}_{i,a} + \sum l^{c}_{a,i}}$$

$$\times i_{\frac{n}{2}-1+s_i}(p_ix_i) k_{b^j_i}(m^j_i x_i) k_{b^j_{i',i} + l^j_{i',i}}(m^j_{i',i}x_i) i_{b^j_{i,i''} + l^j_{i,i''}}(m^j_{i,i''}x_i) + \texttt{permutations}, \tag{C1a}$$

which may be computed after insertion of the near zero expansions (A3b) and (A3c), and

$$R_2(r^j_{i',i}) = \sum{}' \prod \frac{2^{2\nu}(-)^{\frac{l^j_{i',i}-r^j_{i',i}+l^j_{i,i''}-r^j_{i,i''}}{2}}(m^j_{i',i})^{2l^j_{i',i}}\left(b^j_{i',i}+l^j_{i',i}\right)\left(b^j_{i,i''}+l^j_{i,i''}\right)\Gamma\left(b^j_{i',i}+\frac{l^j_{i',i}+r^j_{i',i}}{2}\right)\Gamma\left(b^j_{i,i''}+\frac{l^j_{i,i''}+r^j_{i,i''}}{2}\right)}{\left(\frac{l^j_{i',i}-r^j_{i',i}}{2}\right)!\left(\frac{l^j_{i,i''}-r^j_{i,i''}}{2}\right)!}$$

$$\times \int_{X<x_{f+1}<\ldots<x_{F-1}<\infty} d\frac{x_i}{2}\left(\frac{ip_ix_i}{2}\right)^{s_i-\sum\bar{r}_{i,a}-\sum\bar{q}_{a,i}-\sum q^j{}_{a,b}-\sum q_{a,b}{}^i}\left(\frac{x_i}{2}\right)^{2\nu-1+\sum l^i_{i,a}+\sum l^i_{a,i}}$$

$$\times i_{\frac{n}{2}-1+s_i}(p_ix_i)k_{b^j_i}(m^j_ix_i)k_{b^j_{i',i}+l^j_{i',i}}(m^j_{i',i}x_i)i_{b^j_{i,i''}+l^j_{i,i''}}(m^j_{i,i''}x_i)+\texttt{permutations}. \tag{C1b}$$

Insertion of the asymptotic expansions (A6) into (C1b) yields incomplete Γ functions. The power of x_i is restricted since terms s_i and $l^j_{i',i}$ in the exponent are cancelled by terms s_i and $l^j_{i',i}$ in the order of the Bessel functions.

The rhs of (C1b) is computed by use of the following formulas:

$$\int_X^\infty \mathrm{d}x_1\, e^{-M_1x}x_1^{\rho_1-1} = M^{-\rho_1}\sum_{0\leqslant k_1\leqslant H_1-1}\frac{\Gamma(\rho_1)}{\Gamma(\rho_1-k_1)}e^{-M_1X}(M_1X)^{-k_1-1} + M^{-H_1-1}\frac{\Gamma(\rho_1)}{\Gamma(\rho_1-H_1)}\int_X^\infty \mathrm{d}x_1\, e^{-M_1x}x_1^{\rho_1-H_1-1}. \tag{C2}$$

If ρ_1 is positive integer, the series on the rhs is finite. If ρ_1 is positive noninteger, H_1 is chosen $\geqslant\rho_1$ so that the exponent of x_1 in the integrand is negative.

In both cases and also in the case $\rho_1\leqslant 0$ the rhs is restricted according to

$$\int_X^\infty \mathrm{d}x_1\, e^{-M_1x}x_1^{\rho_1-1} \leqslant M_1^{-\rho_1}\sum_{0\leqslant k_1\leqslant H_1}\frac{\Gamma(\rho_1)}{\Gamma(\rho_1-k_1)}\Lambda^{\rho_1-k_1-1}e^{-\Lambda}, \tag{C3}$$

where

$$\Lambda = M_1X. \tag{C4}$$

Multiple application of this formula yields

$$\prod_{1\leqslant i\leqslant g}\int_{X<x_1\cdots<x_g<\infty}\mathrm{d}x_i\, e^{-M_ix}x_i^{\rho_i-1}$$

$$\leqslant\left(\sum_{1\leqslant a\leqslant g}M_a\right)^{-\Sigma_{1\leqslant a\leqslant g}\rho_a}\sum_{0\leqslant k_i\leqslant H_i}\frac{\Gamma\left(\sum_{i\leqslant a\leqslant g}\rho_a-\sum_{i<a\leqslant g}k_a-g+i\right)}{\Gamma\left(\sum_{i\leqslant a\leqslant g}(\rho_a-k_a)-g+i\right)} \times\left(\frac{\sum_{1\leqslant a\leqslant g}M_a}{\sum_{i\leqslant a\leqslant g}M_a}\right)^{-1-k_i}\Lambda^{\Sigma_{1\leqslant a\leqslant g}\rho_a-k_a-g}e^{-\Lambda}. \tag{C5}$$

It is seen that (C3) and (C5) can be made arbitrary small by choosing Λ sufficiently large.

By application of

$$\int_X^\infty dx_1\, e^{-M_1 x_1} x_1^{\rho_1 - 1} = M_1^{\rho_1}\Gamma(\rho_1) - \int_0^X dx_1\, e^{-M_1 x_1} x_1^{\rho_1 - 1}, \tag{C6}$$

the incomplete Γ functions with integer or half-integer arguments may be computed by the following expansions:

$$\int_X^\infty dx_1\, e^{-M_1 x} x_1^{\rho_1 - 1} = \mathsf{P}_{\rho_1} + \mathsf{Q}_{\rho_1} \sum_{\substack{l=0 \\ l \neq -\rho_1}}^{\infty} \frac{(-)^l \Lambda^{\rho_1 + l}}{l\,!\,(\rho_1 + l)}, \tag{C7}$$

where

$$\mathsf{P}_{\rho_1} = (\rho_1 - 1)\,! \quad \text{and } \mathsf{Q}_{\rho_1} = -1 \quad \text{if } \rho_1 \text{ positive integer}, \tag{C8a}$$

$$\mathsf{P}_{\rho_1} = 0 \quad \text{and } \mathsf{Q}_{\rho_1} = 1 \quad \text{if } \rho_1 \text{ nonpositive integer}, \tag{C8b}$$

$$\mathsf{P}_{\rho_1} = \frac{\sqrt{\pi}(2\rho_1 - 1)!}{\left(\rho_1 - \frac{1}{2}\right)!\, 2^{2\rho_1 - 1}} \quad \text{and } \mathsf{Q}_{\rho_1} = -1 \quad \text{if } \rho_1 \text{ positive half-integer}, \tag{C8c}$$

$$\mathsf{P}_{\rho_1} = \frac{\sqrt{\pi}(-)^{\frac{1}{2} - r}\left(\frac{1}{2} - \rho_1\right)!\, 2^{1 - 2\rho_1}}{(1 - 2\rho_1)!} \quad \text{and } \mathsf{Q}_{\rho_1} = -1 \quad \text{if } \rho_1 \text{ negative half-integer}. \tag{C8d}$$

Multiple application of (C7) and (C8) yields

$$\begin{aligned} \prod_{1 \leqslant i \leqslant g} \int_{X < x_1 < \cdots < x_g}^\infty dx_i\, e^{-M_i x} x_i^{\rho_i - 1} &= \mathsf{P}_{\rho_1} \cdots \mathsf{P}_{\rho_g} M_1^{-\rho_1} \cdots M_g^{-\rho_g} \\ &+ \mathsf{P}_{\rho_1} \cdots \mathsf{P}_{\rho_{g-1} + \rho_g + l_g} \mathsf{Q}_{\rho_g} M_1^{-\rho_1} \cdots M_{g-1}^{-\rho_{g-1} - \rho_g} \frac{\left(-\frac{M_g}{M_{g-1}}\right)^{l_g}}{l_g\,!\,(\rho_g + l_g)} \\ &+ 2^g - 1 \quad \text{terms where factors } \mathsf{P}_{\rho_i} \text{ have been replaced by factors } \mathsf{Q}_{\rho_i}. \end{aligned} \tag{C9}$$

Equation (C9) may be inserted into (C1b).

APPENDIX D: RADIAL $0 \to \Lambda$ INTEGRATIONS

Multiple application of

$$\prod_j \int_0^\Lambda d\xi_1\, \xi_1^{N_1 - 1} \{\ln(\mu_1^j \xi_1)\}^{g_1^j} = \sum_{0 \leqslant g_{1;1}^j \leqslant g_1^j} \prod_j \frac{g_1^j\,!\,(-)^{\sum_c (g_1^c - g_{1;1}^c)} \sum_c (g_1^c - g_{1;1}^c)!}{g_{1;1}^j\,!\,(g_1^j - g_{1;1}^j)\,!\, N_1^{1 + \sum_c (g_1^c - g_{1;1}^c)}} \{\ln(\mu_1^j \Lambda)\}^{g_{1;1}^j} \Lambda^{N_1} \tag{D1}$$

gives

$$\prod \int_{0 < \xi_1 < \xi_2 < \cdots < \xi_{V-1} < \Lambda} d\xi_i\, \xi_i^{N_i - 1} (\ln \mu_i^j \xi_i)^{g_i^j}$$

$$= \sum_{0\leqslant f_i^j\leqslant g_{i;V-2}^j\cdots\leqslant g_{i,i}^j\leqslant g_i^j} \prod_{1\leqslant i\leqslant i''\leqslant V-1} \frac{(-)^{G_i} G_i\,!\, g_i^j!}{(g_{i;i''-1}^j - g_{i;i''}^j)\,!\left(\sum_{1\leqslant a\leqslant i} N_a\right)^{1+G_i}} (\ln \mu_i^j \Lambda)^{f_i^j} \Lambda^{\sum_{1\leqslant a\leqslant V-1} N_a}, \tag{D2}$$

with

$$G_i = \sum_{\substack{1\leqslant a\leqslant i \\ c}} (g_{a;i-1}^c - g_{a;i}^c), \tag{D3}$$

where $g_{i;i''}^j$ are summation variables if $i\leqslant i''\leqslant V-1$ and

$$g_{i;i-1}^j \equiv g_i^j, \tag{D4a}$$

$$g_{i;V-1}^j \equiv f_i^j. \tag{D4b}$$

In the case

$$0 \leqslant g_i^j \leqslant 1, \tag{D5}$$

all summation variables are 0 or 1 and (D2) takes the form

$$\prod \int_{0<\xi_1<\xi_2<\cdots<\xi_{V-1}<\Lambda} \mathrm{d}\xi_i\, \xi_i^{N_i-1} (\ln \mu_i^j \xi_i)^{g_i^j}$$

$$= \sum_{0\leqslant f_i^j\leqslant g_{i;V-2}^j\cdots\leqslant g_{i;i}^j\leqslant g_i^j} \prod_{\substack{1\leqslant i\leqslant V-1 \\ j}} \frac{(-)^{G_i} G_i!}{\left(\sum_{1\leqslant a\leqslant i} N_a\right)^{1+G_i}} (\ln \mu_i^j \Lambda)^{f_i^j} \Lambda^{(\Sigma_{1\leqslant a\leqslant V-1} N_a)}. \tag{D6}$$

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Laplacian in the hyperbolic space H_n and linearization stability of the Einstein equation for Robertson-Walker models

Lluís Bruna and Joan Girbau
Universitat Autónoma de Barcelona, Edificí C, Bellasterra (Barcelona), 08193, Spain

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We prove that some operators related to the rough Laplacian in the hyperbolic space give isomorphisms between Sobolev spaces of 1-forms. By using these results we prove that the Einstein equation of the hyperbolic Robertson-Walker cosmological model is linearization stable. We also study the linearization stability for Robertson-Walker models, $V=S\times I$, with S compact, complete, having either constant negative or zero curvature. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Let $\tilde{g}$ be a Lorentz metric. Denote by $\mathrm{Ric}(\tilde{g})$ the Ricci tensor of $\tilde{g}$, by $R(\tilde{g})$ the scalar curvature of $\tilde{g}$, and by $G(\tilde{g})=\mathrm{Ric}(\tilde{g})-(1/2)R(\tilde{g})\tilde{g}$ the Einstein tensor. The Einstein equation with this notation takes the following form:

$$G(\tilde{g})=\chi\tilde{T}, \tag{1}$$

where $\tilde{T}$ is the stress-energy tensor and χ is a constant. We set tildes over Lorentz metrics and over stress-energy tensors in order to indicate that we deal with a four-dimensional manifold. The letters without tildes will be used for three-dimensional manifolds. One often begins with an initial stress-energy tensor, $\tilde{T}_0$, and an initial Lorentz metric, $\tilde{g}_0$, satisfying $\tilde{G}(\tilde{g}_0)=\chi\tilde{T}_0$ and is interested in finding metrics $\tilde{g}$ close to $\tilde{g}_0$ which are solutions of (1) for a given $\tilde{T}$ close to $\tilde{T}_0$. In order to solve this problem, it can sometimes be useful to linearize the equation (1) at the initial metric $\tilde{g}_0$. When the solutions of the linearized equation do really approximate exact solutions of the true equation, we will say that the Einstein equation is linearization stable at the initial metric $\tilde{g}_0$. An exact version of this concept will be given in what follows.

This paper deals with the problem of linearization stability of the Einstein equation in the case where the initial pair $(\tilde{g}_0,\tilde{T}_0)$ consists of the metric and the stress-energy tensor of a Robertson-Walker cosmological model. The Lorentz manifold corresponding to this model is the product $V=S\times I$, where I is an interval in $\mathbb{R}$, $(S,\hat{g}_0)$ is a Riemannian manifold of constant curvature, and $\tilde{g}_0$ is a Lorentz metric of the form $\tilde{g}_0=-\mathrm{d}t^2+\zeta^2(t)\hat{g}_0$ (t is the coordinate of I). The tensor $\tilde{T}_0$ takes the form $\tilde{T}_0=(\rho+p)\mathrm{d}t\otimes\mathrm{d}t+p\tilde{g}_0$. Generally, it is assumed that S is complete and simply connected. Then S should necessarily be either the Euclidean space $\mathbb{R}^3$, the hyperbolic space $\mathbb{H}_3$, or the sphere S^3.

In our papers, Refs. 7 and 8, we have shown that the Euclidean Robertson-Walker model is linearization stable for the Einstein equation and that the spherical model of positive curvature is not. The remaining case to be studied is that of a hyperbolic Robertson-Walker model. In this paper, we will show (Theorem 1) that such a model is linearization stable. For this purpose, we will use a result (Theorem 2) on the Laplace operator in a hyperbolic space proved in the Appendix. Theorem 1 combined with the results in our earlier papers, Refs. 7 and 8, may suggest that the fact whether or not a Robertson-Walker model is linearization stable can be related to the fact

whether or not the Riemannian manifold S is compact. In fact, when the curvature is negative or zero then S is not compact and the model is linearly stable, while when the curvature is positive then S is compact and the model is not linearly stable. This is the case when S is simply connected, but if we drop this condition, Theorem 3 makes it clear that the fact that the Einstein equation of the model is linearization stable has nothing to do with S being compact.

It is quite well known that any complete n-dimensional Riemannian manifold S of constant curvature is always a quotient X/Γ, where X is either the Euclidean space $\mathbb{R}^n$, or the hyperbolic space $\mathbb{H}_n$, or the sphrere S^n, and Γ is a discrete subgroup of the group of isometries of X acting in a free and properly discontinuous manner. In our case, S has dimension 3. In Theorem 3, we will study Robertson-Walker cosmological models, $V=S\times I$, where S is compact, complete, having either constant negative curvature ($S=\mathbb{H}_3/\Gamma$) or curvature zero ($S=\mathbb{R}^3/\Gamma$). We will show that there is stability when the curvature is negative, and there is not when the curvature is zero. This will make it clear that stability has nothing to do with compactness since the manifolds are compact in either of these cases. In fact, when S is compact the existence of Killing vectors is the first reason of instability.

II. WHAT TYPES OF DEFORMATIONS OF THE INITIAL MODEL WE WILL CONSIDER

Let $(V,\tilde{g}_0,\tilde{T}_0)$ be an initial Robertson-Walker model. The aim of the paper is to consider small deformations $\tilde{T}=\tilde{T}_0+\delta\tilde{T}$ of the initial tensor $\tilde{T}_0$ and metrics $\tilde{g}$ close to $\tilde{g}_0$ such that $G(\tilde{g})=\chi\tilde{T}$, and establish what conditions should be satisfied by the initial model for the equation $G(\tilde{g})=\tilde{T}_0+\delta\tilde{T}$ to be linearly stable at the point $\tilde{g}_0$. For this purpose, we must first specify to what class of tensors the deformations $\tilde{T}=\tilde{T}_0+\delta\tilde{T}$ of $\tilde{T}_0$ should belong.

First we introduce some notation and recall a few topics on this subject. From now on V will always stand for the manifold $V=S\times I$, where both the initial metric $\tilde{g}_0$ and the initial tensor $\tilde{T}_0$ are defined. t will denote the coordinate of I. For a fix $t_0\in I$ consider the hypersurface M of V given by $M=S\times\{t_0\}$. Let now $\tilde{g}$ be a Lorentz metric on V close to $\tilde{g}_0$. Denote by g the Riemannian metric on M obtained by restricting $\tilde{g}$ to M and write k for twice the second fundamental quadratic form of M with respect to the metric $\tilde{g}$. Indicate by n the vector field of V with support on M, orthogonal to M at each point, satisfying $\tilde{g}(n,n)=-1$ and $\tilde{g}(n,\partial_t)<0$. Define the function F and the 1-form X on M as follows:

$$F=-\frac{1}{\chi}G(\tilde{g})(n,n)$$
$$X=\frac{1}{\chi}\,i(n)G(\tilde{g})\big|_M, \tag{2}$$

where $i(n)G(\tilde{g})|_M$ means the inner contraction of $G(\tilde{g})$ by n, acting over tangent vectors to M. If $\tilde{T}$ is a stress-energy tensor related to $\tilde{g}$ through the Einstein equation (1), then $F=-\tilde{T}(n,n)$, $X=i(n)\tilde{T}|_M$. Finally, let $\mathcal{H}(g,k)$ and $\mathcal{V}(g,k)$ be the function and the 1-form on M defined as follows:

$$\mathcal{H}(g,k)=\tfrac{1}{8}(k\cdot k-\mathrm{tr}_g^2\,k-4R),$$
$$\mathcal{V}(g,k)_i=\tfrac{1}{2}\nabla^r(k_{ir}-(\mathrm{tr}_g k)g_{ir}).$$

Then it is well known that the following formulas hold:

$$\mathcal{H}(g,k)=\chi F,$$
$$\mathcal{V}(g,k)=\chi X. \tag{3}$$

The type of stress-energy tensors is normally fixed in advance depending on the type of matter considered. For example, the class of stress-energy tensors for perfect fluids is of the form $\tilde{T}=(\rho+p)u^*\otimes u^*+p\tilde{g}$, where p and ρ are functions and u^* is the 1-form associated with a vector field u by means of the metric $\tilde{g}$, satisfying $\tilde{g}(u,u)=-1$. Here, p is a known function of ρ, $p=p(\rho)$ (state equation). We do not fix any concrete value for the variables u, ρ, and $\tilde{g}$ (we do fix the form of the tensor). In general, we can assume that $\tilde{T}$ is a known function of the metric $\tilde{g}$ and of m scalar or vector fields $\Omega_1,\ldots,\Omega_m$, called *matter fields*. In the case of perfect fluids, these variables $\Omega_1,\ldots,\Omega_m$ would be ρ and the vector field u [the latter with the constraint $\tilde{g}(u,u)=-1$]. Since by (1) $\tilde{T}$ is proportional to G, the stress-energy tensor must satisfy $\mathrm{div}_{\tilde{g}}\,\tilde{T}=0$.

Let us focus briefly on the Cauchy problem for the Einstein equation. Consider the manifold $V=S\times I$ without any metric. Let us give a function $\tilde{T}=\tilde{T}(\tilde{g},\Omega_1,\ldots,\Omega_m)$, where $\Omega_1,\ldots,\Omega_m$ are scalar or vector fields on V called *matter fields*, whose concrete values are unknown for us (they are variables). Moreover, let us give a vector field n of V with support in M, transversal to M. Let us give on M a pair (g,k) of symmetric tensor fields of order 2 such that g is positive definite. Let us also give on M values $\omega_1,\ldots,\omega_m$ of the variables $\Omega_1,\ldots,\Omega_m$. Suppose that F and X are the function and the 1-form on M given by $F=-\tilde{T}(n,n)$, $X=i(n)\tilde{T}|_M$. Assume that the data $g,k,\omega_1,\ldots,\omega_m$ on M are such that the two pairs (g,k) and (F,X) satisfy the constraints (3). We ask (Cauchy problem) whether we can find with these data a neighborhood U of M on V, unique values $\Omega_1,\ldots,\Omega_m$ of the matter fields on U and a unique Lorentz metric $\tilde{g}$ on U in such a way that the following conditions be satisfied:

(i) $\tilde{g}$ and $\tilde{T}$ satisfy $G(\tilde{g})=\chi\tilde{T}$ and $\mathrm{div}_{\tilde{g}}\,\tilde{T}=0$,
(ii) n is normal to M with respect to the metric $\tilde{g}$ and $\tilde{g}(n,n)=-1$,
(iii) $\tilde{g}$ restricted to M is g,
(iv) k is twice the second quadratic form of M with respect to the metric $\tilde{g}$,
(v) we have $\Omega_i=\omega_i$ for $i=1,\ldots,m$ over M.

If this happens, that is, if the initial data over M enable us to uniquely retrieve the metric $\tilde{g}$ and the matter fields $\Omega_1,\ldots,\Omega_m$ in a neighborhood of M in V and the solution $(\tilde{g},\Omega_i)$ depends continuously on the initial data (g,k,ω_i), we will say that the Cauchy problem *is well-posed*.

The Cauchy problem for the Einstein equation is a very wide and difficult field of research. It is clear that the above Cauchy problem will not be well posed if no additional assumptions are made. For example, in the case of perfect fluids where $\tilde{T}$ has the form $\tilde{T}=(\rho+p)u^*\otimes u^*+p\tilde{g}$ the Cauchy problem would be well posed if the following additional assumptions were made (see, e.g., Refs. 5,20 or 14):

(1) there exists a positive constant C satisfying $\rho\geqslant C>0$,
(2) p is a known function of ρ (state equation) which can never be negative on the interval $[C,+\infty)$,
(3) $p(\rho)$ belongs to the class C^1 and the derivative $p'(\rho)$ satisfies $0<p'(\rho)<1$.

Since we are going to work with Cauchy data throughout this paper, we will need the Cauchy problem to be well posed. Therefore the tensors $\tilde{T}=\tilde{T}_0+\delta\tilde{T}$ close to $\tilde{T}_0$ we will consider in what follows will be the tensors for perfect fluids satisfying the above-mentioned conditions (1)–(3). These tensors are parametrized by ρ and u, with the condition $\tilde{g}(u,u)=-1$. The initial tensor $\tilde{T}_0$ (which will correspond to the parameters ρ_0, u_0, and $\tilde{g}_0$) should be that of a Robertson-Walker model.

Since (for the Cauchy problem) the transversal field n over M should be defined in advance, we will always take $n=\partial_t$ on M for any set of Cauchy data (g,k,ρ,u). This means that for the Lorentz metrics $\tilde{g}$ we are going to consider (solutions of the Cauchy problem) the vector n will always coincide with ∂_t over M. This is by no means restrictive since if $\tilde{g}$ is an arbitrary metric and n is its unitary normal field over M, we can always find a diffeomorphism $\varphi:U\to U$, where U is

a neighborhood of M in V, such that φ is the identity over M and transforms n into ∂_t at each point of M. Then $\varphi^*\tilde{g}$ is a metric isometric to $\tilde{g}$ and satisfying the required condition (its n is ∂_t).

If u is a velocity field of a stress-energy tensor $\tilde{T}$ of the type we consider then u restricted to M will be of the form $u=q\partial_t+v$, where q is a scalar $\geqslant 0$ and v is a vector field tangent to M. The condition $\tilde{g}(u,u)=-1$ over M is written as $q=\sqrt{1+g(v,v)}$. Therefore (g,ρ,v) determine the tensor $\tilde{T}$ over M. The pair (F,X) is given as a function of (g,ρ,v) by the following formulas:

$$F = -\tilde{T}(\partial_t,\partial_t) = -(\rho + p(\rho))(1 + g(v,v)) + p(\rho),$$

$$X_i = X(\partial/\partial x^i) = \tilde{T}(\partial_t,\partial/\partial x^i) = -(\rho + p(\rho))\sqrt{1 + g(v,v)}v_i. \tag{4}$$

We will take the Cauchy data belonging to appropriate Sobolev spaces we now describe. Denote by $\mathcal{F}_s(M)$, $\Omega_s(M)$, and $\mathcal{S}_s(M)$, respectively, the Sobolev spaces of functions, of 1-forms and of covariant symmetric tensors of order 2 whose degree of regularity is s. For example, $\mathcal{F}_s(M)$ will be the space of all functions belonging $L^2(M)$ whose weak derivatives up to order s belong to $L^2(M)$. Given an initial function f_0 on M belonging to C^∞, we will denote by $\mathcal{F}_s(f_0)$ the set of functions of the form $f=f_0+h$ with $h\in\mathcal{F}_s(M)$. The set $\mathcal{F}_s(f_0)$ is topologized by imposing the condition that the map $f\to h=f-f_0$ from $\mathcal{F}_s(f_0)$ to $\mathcal{F}_s(M)$ should be a homeomorphism. In a similar way, given a 1-form ω_0 on M belonging to C^∞, the set $\Omega_s(\omega_0)$ is defined as the set of 1-forms ω satisfying $\omega-\omega_0\in\Omega_s(M)$. Given a covariant symmetric 2-tensor α_0 belonging to C^∞, we define $\mathcal{S}_s(\alpha_0)$ in an analogous way. The Cauchy data (g,k,ρ,v) will be taken in the Sobolev space $\mathcal{S}_s(g_0)\times\mathcal{S}_s(k_0)\times\mathcal{F}_{s-2}(\rho_0)\times\Omega_{s-1}(v_0)$, where s is a positive integer to be chosen below and (g_0,k_0,ρ_0,v_0) are the Cauchy data corresponding to the Robertson-Walker's initial metric $\tilde{g}_0$ and the initial tensor $\tilde{T}_0$. To be precise, $g_0=\zeta^2(t_0)\hat{g}_0$, $k_0=2\{\dot{\zeta}(t_0)/\zeta(t_0)\}g_0$, ρ_0 is the initial density, and $v_0=0$.

Let F and X be functions of g, ρ, and v defined by (4). Let

$$\begin{gathered} H:\mathcal{S}_s(g_0)\times\mathcal{F}_{s-2}(\rho_0)\times\Omega_{s-1}(v_0) \longrightarrow \mathcal{S}_s(g_0)\times\mathcal{F}_{s-2}(F_0)\times\Omega_{s-1}(X_0), \\ (g,\rho,v) \longrightarrow (g,F,X). \end{gathered} \tag{5}$$

It follows from formula (4) that the linear tangent map to H at the point (g_0,ρ_0,v_0) is

$$(DH)_{(g_0,\rho_0,v_0)}:\mathcal{S}_s(M)\times\mathcal{F}_{s-2}(M)\times\Omega_{s-1}(M) \longrightarrow \mathcal{S}_s(M)\times\mathcal{F}_{s-2}(M)\times\Omega_{s-1}(M),$$

$$(h,f,v) \longrightarrow (h,-f,-(\rho_0+p_0)v).$$

Since ρ_0+p_0 is positive, the above map is an isomorphism. By the inverse function theorem in Banach spaces, the map H can be inverted in a neighborhood of the initial data. Consider the map Ψ obtained by composition of the following maps:

$$(g,k) \longrightarrow (g,(1/\chi)\mathcal{H}(g,k),(1/\chi)\gamma(g,k)) \xrightarrow{H^{-1}} (g,\rho,v) \xrightarrow{\pi} (\rho,v) \tag{6}$$

(where π is the canonical projection). The map Ψ maps $\mathcal{S}_s(g_0)\times\mathcal{S}_s(k_0)$ to $\mathcal{F}_{s-2}(\rho_0)\times\Omega_{s-1}(v_0)$ and is defined in a neighborhood of (g_0,k_0) only. It assigns to any pair (g,k) [close to (g_0,k_0)] the unique pair (ρ,v) satisfying the constrains conditions

$$\begin{aligned} \mathcal{H}(g,k) &= \chi F(g,\rho,v), \\ \gamma(g,k) &= \chi X(g,\rho,v). \end{aligned} \tag{7}$$

We have mentioned in the introduction that we are interested in those metrics $\tilde{g}$ close to $\tilde{g}_0$ which are solutions of (1) for a given $\tilde{T}$ close to $\tilde{T}_0$. However, this cannot be formulated in such

a way. We cannot take an arbitrary $\tilde{T}$ close to $\tilde{T}_0$ and look for the metrics $\tilde{g}$ satisfying $G(\tilde{g})=\chi\tilde{T}$ since, on one hand, the expression for $\tilde{T}$ contains the metric and, on the other hand, $\tilde{T}$ should anyway satisfy the extra condition $\mathrm{div}_{\tilde{g}}\tilde{T}=0$. A correct way of expressing the initial idea (for perfect fluids) is to give a pair (ρ,v) on M (corresponding to the distribution of the matter at $t=t_0$) and acquire about the pairs (g,k) satisfying $\Psi(g,k)=(\rho,v)$. Then the data (g,k,ρ,v) over M completely define $\tilde{g}$ and $\tilde{T}$ satisfying $G(\tilde{g})=\chi\tilde{T}$. The Einstein equation is then replaced by (7).

Remark 1: In our setting, we have demanded that all deformations $\tilde{T}_0+\delta T$ of the initial tensor correspond to perfect fluids. We do this for the sake of clarity in our exposition; however, this is not crucial. What is crucial indeed is that we work with a class of tensors containing the perfect fluids and for which the Cauchy problem would be well posed. For example, Lichnerowicz introduced,[15] a class of fluids he called *holonomous media* whose stress-energy tensor has the form $\tilde{T}=ru^*\otimes u^*+\theta$, where u^* is the 1-form associated to a unitary field u $[\tilde{g}(u,u)=-1]$, r is a positive scalar called *pseudodensity* and where θ is a covariant symmetric 2-tensor whose divergence is the gradient of a function K. Perfect fluids are a particular case of holonomous media with $r=\rho+p$ and $\theta=p\tilde{g}$. If we consider holonomous media whose pseudodensity r and whose function K are both functions of some variable τ (parametrizing both functions), then one can prove that if the function $r(\tau)$ is positive over the whole domain, if $r(\tau)$ and $K(\tau)$ belong to C^1, if the derivative K' is positive and $r'/K'>2$, then the Cauchy problem is well posed for the Cauchy data (g,k,τ,v). In these holonomous media one can work with Cauchy data. Therefore one could consider deformations $\tilde{T}_0+\delta T$ of the initial tensor corresponding to holonomous media, for example.

III. THE NOTION OF LINEAR STABILITY OF THE EINSTEIN EQUATION WITH MATTER

Linear stability of the Einstein equation in the vacuum has been considered in detail in the literature (Refs. 10–13, 1, and 17–19). An interesting bibliography on the subject can be found in Ref. 16. In this case, one begins with an initial Lorentz metric $\tilde{g}_0$ satisfying $G(\tilde{g}_0)=0$ and is interested in metrics $\tilde{g}$ close to $\tilde{g}_0$ which are also solutions of the equation $G(\tilde{g})=0$. Formulated in terms of Cauchy data in appropriate Sobolev spaces, this leads to the following situation: One has a differentiable map $f:X\to Y$ between two Banach spaces, a particular solution $x=x_0$ of the equation $f(x)=0$ is known, and the problem is to find solutions x close to x_0. The classical definition of linearization stability in this case looks as follows: The equation $f(x)=0$ is linearization stable at the point x_0 if for any solution h of the linearized equation $D_{x_0}f(h)=0$ there exists a curve $\lambda\to x(\lambda)$ of solutions of $f(x)=0$ which is tangent to h at x_0. However, the situation in the case of the Einstein equation with matter is not the same. Here, for some $y_0\in Y$, we know $x_0\in X$ such that $f(x_0)=y_0$ and for y close to y_0 we are interested in finding solutions x (close to x_0) of the equation $f(x)=y$. If we take $q=y-y_0$, we would like that for any solution h of the linearized equation $D_{x_0}f(h)=q$, x_0+h would be always close to an exact solution of the equation $f(x)=y$. If this is the case, we will say that the equation $f(x)=y$ is linearization stable at the point x_0. We will make this definition more precise in what follows. Let us observe by now that the difference with the case of vacuum is that we are interested in obtaining not only solutions of $f(x)=y_0$ through linearization for a fixed y_0 (which will be $y_0=0$ in the case of vacuum), but also the solutions of $f(x)=y$ for any y close to y_0. Although we have already given in Ref. 7 a correct definition of linearization stability for this case we shall give here a more simple and clear version.

Definition 1: Let $f:U\to Y$ be a continuously differentiable map of an open set U in a Banach space X to a Banach space Y. Let $x_0\in U$ and $y_0=f(x_0)$. For any $q\in Y$ consider

$$H_q=\{x\in U \text{ solution of } f(x)=y_0+q\},$$

$$L_q=\{x\in U: x=x_0+h,\quad h \text{ solution of } D_{x_0}f(h)=q\}.$$

Let $\mathcal{K}$ be a closed vector subspace of Y. We will say that the equation $f(x)=y_0+q$ is linearization stable at x_0 in the direction of the subspace $\mathcal{K}$ if there exist a neighborhood V of the origin in $\mathcal{K}$,

a neighborhood W of the origin in $L=\ker D_{x_0}f$, a neighborhood U' of x_0, $U'\subset U$, and continuously differentiable maps φ and ψ,

$$\begin{array}{cccc} \mathcal{K}\times L & U & \mathcal{K}\times L & U \\ \cup & \cup & \cup & \cup \end{array}$$

$$\varphi: V\times W \longrightarrow U' \quad \varphi: V\times W \longrightarrow U'$$

such that for any $q\in V$ the maps

$$\varphi_q: W \longrightarrow H_q\cap U', \quad \psi_q: W \longrightarrow L_q\cap U',$$

$$z \longrightarrow \varphi(q,z), \quad z \longrightarrow \psi(q,z)$$

are differentiable bijections having differentiable inverses (that is, they are respective parametrizations of $H_q\cap U'$ and $L_q\cap U'$) satisfying $\varphi_0(0)=x_0$ and $\psi_0(0)=x_0$. Moreover, for any $q\in V$ and any $z\in W$ the error $E_q(z)=\varphi_q(z)-\psi_q(z)$ committed in considering $\psi_q(z)$ instead of $\varphi_q(z)$ satisfies

$$\lim_{(z,q)\to(0,0)} \frac{E_q(z)}{\sqrt{\|z\|^2+\|q\|^2}}=0. \tag{8}$$

Intuitively, this definition consists in demanding that for any $q\in\mathcal{K}$ close to zero the set H_q of solutions of the equation $f(x)=y_0+q$ and the set L_q of solutions of the linearized equation be parametrizable by the same vector space of parameters L in such a way that the error $E_q(z)$ committed in considering the solution of the linearized equation corresponding to the parameter z instead of the true solution corresponding to the same parameter satisfies condition (8). Observe that if the subspace $\mathcal{K}$ of Y is $\mathcal{K}=\{0\}$, Definition 1 coincides with the classical definition for the vacuum.

Definition 2: With the same notations as those in Definition 1, if $f(x)=y$ is linearization stable at the initial point x_0 in the direction of $\mathcal{K}=Y$, we will simply say that it is linearization stable at this point.

In Ref. 7, the following sufficient condition for linearization stability was proved. *If $L=\ker D_{x_0}$ has a topologic supplement and if the map $D_{x_0}f: X\to Y$ is surjective, then f is linearization stable at the point x_0.*

We will have to apply these tools to the particular case where the space X is $X=\mathcal{S}_s(g_0)\times\mathcal{S}_s(k_0)$, the space Y is $Y=\mathcal{F}_{s-2}(\rho_0)\times\Omega_{s-1}(v_0)$, and f is the map Ψ defined in (6). We will take as the degree of regularity s of Sobolev spaces any integer $s>4$. Then all the elements of the Sobolev spaces appearing in our study will be differentiable elements of the class C^1.

IV. STABILITY IN THE CASE OF A HYPERBOLIC RW MODEL

Theorem 1: *Suppose that the initial pair $(\tilde{g}_0,\tilde{T}_0)$ consists of the metric and the stress-energy tensor of a Robertson-Walker (RW) cosmological model, $V=S\times I$, where S is the hyperbolic space $\mathbb{H}_3$. In this case, the Einstein equation is linearization stable.*

Proof: We need only show that the map $D_{(g_0,k_0)}\Psi$ is surjective and has a splitting kernel. Let Φ be the map

$$\Phi: \mathcal{S}_s(g_0)\times\mathcal{S}_s(k_0) \longrightarrow \mathcal{F}_{s-2}(\rho_0)\times\omega_{s-1}(v_0),$$

$$(g,k) \longrightarrow (\mathcal{H}(g,k),\gamma(g,k)).$$

Let J be the map of the space $\mathcal{F}_{s-2}(M)\times\Omega_{s-1}(M)$ into the same space defined by $J=(\mathrm{id},1/(\rho_0+p_0)\mathrm{id})$. By definition (6) of Ψ, we deduce that $D_{(g_0,k_0)}\Psi=-(1/\chi)J\circ D_{(g_0,k_0)}\Phi$. Therefore we need only see that

$$D_{(g_0,k_0)}\Phi:\mathcal{S}_s(M)\times\mathcal{S}_s(M)\to\mathcal{F}_{s-2}(M)\times\Omega_{s-1}(M)$$

is surjective and has a splitting kernel. For simplicity of our notation, we denote the initial pair (g_0,k_0) by (g,k). The map $D_{(g,k)}\Phi$ is calculated in Ref. 7. It is clear that $D_{(g,k)}\Phi=D_{(g,k)}\mathcal{H}\times D_{(g,k)}\gamma$. If we set $g'=g+h$, $k'=k+K$ and take the linear part in (h,K) of the expressions $\mathcal{H}(g',k')$ and $\gamma(g',k')$, we obtain the formulas for $D_{(g,k)}\mathcal{H}$ and $D_{(g,k)}\gamma$ as functions of the variables (h,K) appearing at the end of p. 5128 in Ref. 7. Since the k corresponding to the initial model is $k=2Cg$, where $C=\dot{\zeta}(t_0)/\zeta(t_0)$, and the Ricci tensor of g is $2cg/\zeta(t_0)^2$, where c is the constant curvature of the model (-1 for the hyperbolic space, but we make no assumptions over c by the moment), these expressions are

$$D_{(g,k)}\mathcal{H}(h,K)=\frac{1}{8}\left[\left(16C^2+\frac{8c}{\zeta(t_0)^2}\right)\mathrm{tr}(h)-8C\,\mathrm{tr}(K)-4\nabla^i\nabla^j h_{ij}+4\nabla^i\nabla_i\,\mathrm{tr}(h)\right],$$

$$D_{(g,k)}\gamma(h,K)_i=\tfrac{1}{2}[\nabla^j K_{ij}-\partial_i\,\mathrm{tr}(K)+2C\partial_i\,\mathrm{tr}(h)-2C\nabla^j h_{ji}]. \tag{9}$$

We are now interested in those pairs (h,K) having the form $h=g\tau$, $K=-2L_Yg+2(\mathrm{div}\,Y)g+2C\tau g$, where τ and Y are a function and a vector field on M. By substituting in (9) these expressions for h and K, we will have the following expressions for $D_{(g,k)}\mathcal{H}$ and for $D_{(g,k)}\gamma$ as functions of the variables τ, Y:

$$D_{(g,k)}\mathcal{H}(Y,\tau)=\left(\frac{3c}{\zeta^2(0)}\tau-2C\,\mathrm{div}\,Y-\Delta\tau\right),$$

$$D_{(g,k)}\gamma(Y,\tau)=(\delta L_Yg), \tag{10}$$

where as usual $\Delta\tau$ denotes $-\nabla^i\nabla_i\tau$ (the Laplace operator of τ) and δL_Yg denotes the 1-form whose components are $(\delta L_Yg)_i=-\nabla^j(L_Yg)_{ij}$ (the operator δ is the Hodge operator, applied here to a symmetric 2-tensor). In order to prove surjectivity of $D_{(g,k)}\Phi$, we use the following result whose proof can be found in the Appendix.

Theorem 2: *For any real number $q\geqslant 0$, the following two maps,*

$$\mathcal{F}_s(\mathbb{H}_3)\to\mathcal{F}_{s-2}(\mathbb{H}_3),\quad \mathcal{X}_s(\mathbb{H}_3)\to\Omega_{s-2}(\mathbb{H}_3),$$

$$\tau\to\Delta\tau+q\tau,\quad Y\to\delta L_Yg,$$

are isomorphisms [$\mathcal{X}_s(\mathbb{H}_3)$ *denotes here the Sobolev space of degree of regularity s of vector fields over the hyperbolic space* $\mathbb{H}_3$].

We will use this theorem for proving surjectivity of $D_{(g,k)}\Phi$. Given $(f,\omega)\in\mathcal{F}_{s-2}(M)\times\Omega_{s-2}(M)$, there exists, by Theorem 2, $Y\in\mathcal{X}_s(M)$ such that $\delta L_Yg=\omega$. By the same theorem, there exists $\tau\in\mathcal{F}_s(M)$ such that

$$\Delta\tau+\frac{3}{\zeta(t_0)^2}\tau=-2C\,\mathrm{div}\,Y-f.$$

By (10), we will then have (taking into account that now $c=-1$)

$$(D_{(g,k)}\Phi)(\tau,Y)=((D_{(g,k)}\mathcal{H})(\tau,Y),(D_{(g,k)}\gamma)(\tau,Y))=(f,\omega).$$

We need only see that the kernel of $D_{(g,k)}\Phi$ has a topological supplement. For any pair (h,K), consider the only pair (h',K') satisfying $h'=2g\tau$, $K'=-2L_Yg+2\,\mathrm{div}(Y)g+2C\tau g$ such that $(D_{(g,k)}\Phi)(h,K)=(D_{(g,k)}\Phi)(h',K')$ [it is unique since $D_{(g,k)}\Phi$ is an isomorphism over the pairs (h',K')]. Then

$$(h,K) = (h - h', K - K') + (h', K')$$

gives the required splitting. □

V. NOT SIMPLY CONNECTED RW MODELS

In this section, we will assume that the initial pair $(\tilde{g}_0, \tilde{T}_0)$ consists of the metric and the stress-energy tensor of a Robertson-Walker model, $V = S \times I$, where $(S, \hat{g})$ is a complete Riemannian manifold of constant sectional curvature. We will restrict here to the case where S is compact of curvature $\leqslant 0$ (since the compact case of curvature >0 is the sphere already studied). If the curvature is zero, S will be a plate torus, $S = \mathbb{R}^3/\Gamma$, where Γ is a group of translations. If the curvature is negative, we have $S = \mathbb{H}_3/\Gamma$, where Γ is a certain discrete subgroup of isometries of $\mathbb{H}_3$. For these models, we have the following.

Theorem 3: *If the initial pair $(\tilde{g}_0, \tilde{T}_0)$ corresponds to a RW model, $V = S \times I$, where S is a plate torus, then there exists no closed vector subspace $\mathcal{K}$ of $\mathcal{F}_{s-2}(\rho_0) \times \Omega_{s-1}(0)$ such that the map*

$$\Psi : \mathcal{S}_s(g_0) \times \mathcal{S}_s(k_0) \to \mathcal{F}_{s-2}(\rho_0) \times \Omega_{s-1}(0)$$

defined in (6) is linearization stable at the initial pair (g_0, k_0) in the direction of $\mathcal{K}$ (observe that in RW models we have $v_0 = 0$). However, if the initial pair corresponds to a RW model, $V = S \times I$, where S is a compact, complete, orientable Riemannian manifold of negative constant curvature, then Ψ is linearization stable at the initial pair.

Proof: By Definition 1, if $f : U \to Y$ is linearization stable at a point $x_0 \in U$ in the direction of a certain closed vector subspace of Y, the set $\{x \in U$: solving $f(x) = y_0 + q\}$ is a differentiable manifold whose parametrization is given by Definition 1. In particular, taking $q = 0$, the set $\{x \in U$: solving $f(x) = y_0\}$ is a differentiable manifold. We will apply this to the map Ψ when y_0 is the initial pair $(\rho_0, 0)$. In order to prove instability, it will be sufficient to prove that the set $\{(g,k)$ fulfilling $\Psi(g,k) = (\rho_0, 0)\}$ is not a differentiable manifold. Since, by (5) and (4), we have $H(g_0, \rho_0, 0) = (g_0, -\rho_0, 0)$, it follows from the definition of Ψ given in (6) that the above set is the set of pairs (g,k) such that $F(g,k) = -\rho_0$, $X(g,k) = 0$. Therefore the instability will be proved if we check that the set $\{(g,k)$ such that $\Phi(g,k) = (-\chi\rho_0, 0)\}$ is not a differentiable manifold.

Let us change variables according to $(g,k) \to (g,p)$, where $p = k - (\mathrm{tr}_g k)g$ and let us express Φ using variables (g,p),

$$\Phi : (g,p) \to (\mathcal{H}(g,p), \gamma(g,p)).$$

Let $D_{(g_0,p_0)}\Phi$ be the linear map tangent to Φ at the initial pair (g_0, p_0). As we have already done in the preceding section, we denote for brevity the initial pair (g_0, p_0) by (g,p) and by (g', p') the pairs close to (g,p). Set $g' = g + h$, $p' = p + P$. This is the same notation as that on pp. 5134 and 5135 of Ref. 8. The linear map $D_{(g,p)}\Phi$ induces a map

$$D_{(g,p)}\Phi : \mathcal{S}_\infty(M) \times \mathcal{S}_\infty(M) \to \mathcal{F}_\infty(M) \times \Omega_\infty(M). \tag{11}$$

If M is compact (which is the case we consider now), following Ref. 8 we introduce a scalar product $\langle\ ,\ \rangle$ on $\mathcal{S}_\infty(M) \times \mathcal{S}_\infty(M)$ defined by

$$\langle (h,P), (h',P') \rangle = \int_M (h,P)_x \cdot (h',P')_x \, \mathrm{d}v,$$

where $\mathrm{d}v$ is the volume element in M and $(h,P)_x . (h',P')_x$ is the inner product defined for each $x \in M$ by the formula

$$(h,P)_x \cdot (h',P')_x = g^{ir}(x) g^{js}(x) [h_{ir}(x) h'_{js}(x) + P_{ir}(x) + P'_{js}(x)].$$

In a similar way, $\mathcal{F}_\infty(M) \times \Omega_\infty(M)$ is endowed with the scalar product

$$\langle (f,Y),(f',Y')\rangle = 4\int_M f(x)f'(x)\mathrm{d}v + 4\int_M g^*(Y,Y')_x\,\mathrm{d}v,$$

where g^* is the scalar product induced by g over 1-forms. The map (11) has an adjoint with respect to these scalar products

$$(D_{(g,p)}\Phi)^*:\mathcal{F}_\infty(M)\times\Omega_\infty(M)\longrightarrow \mathcal{S}_\infty(M)\times\mathcal{S}_\infty(M),$$

$$(f,Y)\longrightarrow (A(f,Y),B(f,Y))$$

which induces a map between the corresponding Sobolev spaces. The expressions for $D_{(g,p)}\Phi$, $D^2_{(g,p)}\Phi$, and $(D_{(g,p)}\Phi)^*$ are given by formulas (3), (4), and (6) in Ref. 8, p. 5133. In order to apply these formulas, one should recall that in a RW model one has $k=2Cg$ with $C=\dot{\zeta}(t_0)/\zeta(t_0)$, $p=k-\mathrm{tr}_g(k)g=-4Cg$, $\mathcal{R}(g)=2cg/\zeta(t_0)^2$, where $c=0,1,-1$ is the constant curvature of the model. One should also take into account that $\gamma(g,p)=\chi X(\rho_0,0)=0$. Then formula (6) in Ref. 8 giving $(A,B)=(D_{(g,p)}\Phi)^*(f,Y)$ yields

$$A(f,Y)=\left(8C^2+\frac{4c}{\zeta^2(0)}\right)fg-4CL_Yg-2\,\mathrm{Hess}(f)-2(\Delta f)g,$$

$$B(f,Y)=2Cfg-L_Yg. \tag{12}$$

It is proved in Ref. 8, p. 5133, that if $\mathcal{C}=\{(g',k')$ satisfying $\Phi(g',k')=-(\chi\rho_0,0)\}$ is a differentiable manifold, then

$$\langle (D^2_{(g,p)}\Phi)(h,P),(f,Y)\rangle = 0, \tag{13}$$

for all $(f,Y)\in\mathcal{F}_\infty(M)\times\Omega_\infty(M)$ belonging to $\mathrm{Ker}(D_{(g,p)}\Phi)^*$ and all (h,P) belonging to $\mathrm{Ker}\,D_{(g,p)}\Phi$. Therefore in order to see that $\mathcal{C}$ is not a differentiable manifold, it will suffice to find $(h,P)\in\mathrm{Ker}\,D_{(g,p)}\Phi$ and $(f,Y)\in\mathrm{Ker}(D_{(g,p)}\Phi)^*$ which fail to satisfy (13). For this purpose, we take a pair (f,Y) having $f=0$ and Y to be a Killing vector field. Then (12) implies that $(0,Y)\in\mathrm{Ker}(D_{(g,p)}\Phi)^*$. By the same argument as that in Ref. 8, p. 5135, one can readily obtain

$$\langle (D^2_{(g,p)}\Phi)(h,P),(0,Y)\rangle = -\int_M(\nabla_Y h\cdot P)\mathrm{d}v - 2\int_M Y^i\nabla_r(h^{rs}P_{is})\mathrm{d}v. \tag{14}$$

Take an atlas on the torus $\mathbb{T}_3=\mathbb{R}^3/\Gamma$ where the coordinates of any local chart are induced by the canonical coordinates of $\mathbb{R}^3$ (coordinate changes will be given by translations). In these coordinates, $\hat{g}_{ij}=\delta_{ij}$ and $\partial_i=\partial/\partial x^i$ are Killing fields. Denote by x, y, z the three coordinates x^1, x^2, x^3 and take $Y=\partial_x$, $h=\partial_x\otimes\partial_y+\partial_y\otimes\partial_x$, $P=x(\partial_x\otimes\partial_y+\partial_y\otimes\partial_x)-z(\partial_y\otimes\partial_z+\partial_z\otimes\partial_y)$. Then h and P have zero trace and divergence. This makes (h,P) belong to $\mathrm{Ker}\,D_{(g,p)}\Phi$, as one can see by applying formula (13) in Ref. 8, p. 5136, to this concrete pair (h,P) and taking into account that $\nabla_i\nabla_j h^{ij}=0$. In fact,

$$\nabla_i\nabla_j h^{ij}=\partial_i(\nabla_j h^{ij})-\Gamma^m_{ij}\nabla_m h^{ij}+\Gamma^i_{im}\nabla_j h^{mj}+\Gamma^j_{im}\nabla_j h^{mi}.$$

The second and fourth terms are opposed. Thus $\nabla_i\nabla_j h^{ij}=0$ because $\mathrm{div}(h)=0$.

On the other hand, one has $\nabla_Y h=0$. Therefore the first integral in (14) equals zero. Calculating the second term in (14) we have

$$Y^i\nabla_r(h^{rs}P_{is})=Y^i\nabla_1(h^{12}P_{i2})+Y^i\nabla_2(h^{21}P_{i1})=Y^1\nabla_1(h^{12}P_{12})=\nabla_1P_{12}=\partial_x(x)=1.$$

Then

$$\int_{\mathbb{T}_3} Y^i \nabla_r (h^{rs} P_{is}) \mathrm{d}v = \mathrm{vol}(\mathbb{T}_3) \neq 0.$$

This proves the first part of the theorem.

Let us now consider the case of a RW model, $V = S \times I$, where S is a compact complete orientable Riemannian manifold of constant negative curvature. By the Berger-Ebin theorem,[3] if one of the two operators $D_{(g,p)}\Phi$ or $(D_{(g,p)}\Phi)^*$ has injective symbol, then the following splitting holds:

$$\Omega_{s-1} \times \mathcal{F}_{s-2} = \mathrm{Image}(D_{(g,p)}\Phi) \oplus \ker(D_{(g,p)}\Phi)^*.$$

Then the fact that $D_{(g,p)}\Phi$ is surjective is equivalent to the fact that $(D_{(g,p)}\Phi)^*$ is injective. For each $x \in M$ and $\xi \in T_x(M)^*$, we calculate the symbol of $(D_{(g,p)}\Phi)^*$,

$$\sigma_L(x,\xi): T_x(M) \times \mathbb{R} \longrightarrow (S_2 \times S_2),$$

$$(X, f) \longrightarrow (\alpha, \beta).$$

In order to find expressions for α and β we apply formulas (12) recalling that $(L_X g)_{ij} = \nabla_i X_j + \nabla_j X_i$, $(\mathrm{Hess}\, f)_{ij} = \nabla_i \nabla_j f$ i $\Delta f = -\nabla^i \nabla_i f$. Then we have

$$\alpha_{rs} = -2\xi_r \xi_s f - 2\xi \cdot \xi f g_{rs},$$

$$\beta_{rs} = -\xi_r X_s - \xi_s X_r.$$

This implies that $\mathrm{tr}(\alpha) = g^{rs}\alpha_{rs} = -8(\xi.\xi)f$. If we assume that $\alpha = 0$, then $\mathrm{tr}(\alpha) = 0$. Since $\xi.\xi \neq 0$, this implies $f = 0$. Since $\xi \neq 0$, we can take a basis $\{\omega^1, \omega^2, \omega^3\}$ in $T_x(M)^*$ such that $\omega^1 = \xi$. The components of ξ in this basis are $\xi = (1,0,0)$. If we assume that $\beta = 0$, then $\xi_r X_s = -\xi_s X_r$. By applying this to $r = 1$ and $s = 2,3$ we obtain $X_2 = X_3 = 0$. Finally, $0 = \beta_{11} = -2\xi_1 X_1 = -2X_1$. Therefore the symbol $\sigma_L(x,\xi)$ is injective. Let us now prove that $(D_{(g,p)}\Phi)^*$ is also injective. If we take $B = 0$ in (12), we obtain $L_X g = 2Cfg$. Substitute this into the expression of $A(f,X)$ to obtain

$$A(f,X) = -\frac{4}{\zeta(t_0)^2} fg - 2\,\mathrm{Hess}(f) - 2(\Delta f) g.$$

If $A = 0$, then $\mathrm{tr}(A) = 0$ and the above expression implies that $\Delta f + (3/\zeta(t_0)^2) f = 0$. Then perform scalar multiplication of this equality by f to obtain

$$\langle \mathrm{d}f, \mathrm{d}f \rangle + \frac{3}{\zeta(t_0)^2} \langle f, f \rangle = 0.$$

This implies that $f = 0$. Coming back to (12) we obtain $L_X g = 0$. This means that the kernel of $(D_{(g,p)}\Phi)^*$ is formed by those pairs which are written as $(0,X)$, where X is a Killing field. On the other hand, any compact Riemannian manifold whose Ricci tensor is negative definite does not have Killing vectors.[4] This means that our operator $(D_{(g,p)}\Phi)^*$ is injective. □

APPENDIX: OPERATORS RELATED TO THE LAPLACIAN OF THE HYPERBOLIC SPACE

In this Appendix, we prove two theorems (Theorem 4 and Theorem 5) which enable us to obtain the two isomorphisms in Theorem 2. The proofs rely heavily on the results and the techniques in Ref. 9 (see also Ref. 6).

1. Notations

The manifold M we will work with will be the n-dimensional hyperbolic space $\mathbb{H}_n$. We will always denote by g the Riemannian metric on M of constant curvature -1. We will denote the components of the covariant differential $\nabla\alpha$ of a p-tensor α by $\nabla_i\alpha_{i_1\cdots i_p}$. The notation $\nabla^{(k)}$ is used for the kth iterate of ∇.

If α and β are two covariant tensors of order p indicate by (α,β) the function defined coordinatewise by $\alpha^{i_1\cdots i_p}\beta_{i_1\cdots i_p}$. This definition does not depend on the coordinates chosen. Write $\langle\alpha,\beta\rangle=\int_M(\alpha,\beta)\mathrm{d}v$, where $\mathrm{d}v$ is the volume element. Naturally, $\langle\alpha,\beta\rangle$ is only defined when the above integral is finite. Denote $|\alpha|=\sqrt{(\alpha,\alpha)}$ and $\|\alpha\|=\sqrt{\langle\alpha,\alpha\rangle}$.

The metric adjoint ∇^* of ∇ is defined by $\langle\nabla\alpha,\beta\rangle=\langle\alpha,\nabla^*\beta\rangle$ for any p-tensor α and any $(p+1)$-tensor β belonging to the class C^∞ and having compact support. The operator $\Delta_R=\nabla^*\nabla$ is called the rough Laplacian and is defined over all covariant p-tensors. It follows from the definition that Δ_R is self-adjoint and positive. The coordinatewise expressions of ∇^* and Δ_R are the following:

$$(\nabla^*\alpha)_{i_1\cdots i_{p-1}}=-\nabla^j\alpha_{ji_1\cdots i_{p-1}},\quad (\Delta_R\alpha)_{i_1\cdots i_p}=-\nabla^j\nabla_j\alpha_{i_1\cdots i_p}.$$

Observe that the expression of ∇^* coincides with that of the Hodge operator δ (the metric adjoint of the exterior differential d). The latter, however, is defined only over p-forms (antisymmetrics), while ∇^* is defined over all covariant p-tensors. Observe also that the operator denoted by δ in Theorem 2 is in fact the operator ∇^* since it operates over a 2-tensor (not antisymmetric).

We will say that a p-covariant tensor α over M is of L^2 type if its coefficients in any local chart are measurable functions with respect to the measure $\mathrm{d}v$ and, moreover, the function $|\alpha|$ belongs to $L^2(\mathrm{d}v)$, that is, $\|\alpha\|<+\infty$. Denote by $L^2_p(M)$ the space of p-forms belonging to L^2.

Given $\omega\in L^2_p(M)$, we will say that ω has a generalized or weak kth order covariant derivative $\nabla^{(k)}\omega$ in L^2 if for any covariant tensor β of order $p+k$ belonging to the class C^∞ and having compact support we have

$$|\langle\omega,(\nabla^*)^{(k)}\beta\rangle|\leqslant C\|\beta\|$$

for some positive constant C. Then the map $\beta\to\langle\omega,(\nabla^*)^{(k)}\beta\rangle$ is continuous and therefore there exists a unique element $f\in L^2_{p+k}(M)$ such that $\langle\omega,(\nabla^*)^{(k)}\beta\rangle=\langle f,\beta\rangle$. This f is taken to be $\nabla^{(k)}\omega$.

Let $L^2_{p,s}(M)$ be the space of L^2 p-forms ω such that $\nabla^{(k)}\omega$ belongs to L^2 for $k\leqslant s$. We will assume that this space is endowed with the norm

$$\|\omega\|_s=\left(\sum_{k=0}^{s}\|\nabla^{(k)}\omega\|^2\right)^{1/2}.$$

Denote by $\mathcal{D}_p(M)$ the space of C^∞ p-forms on M having compact support. It is clear that $\mathcal{D}_p(M)\subset L^2_{p,s}(M)$. Denote by $H^s_p(M)$ the closure of $\mathcal{D}_p(M)$ in $L^2_{p,s}(M)$. Aubin proved,[2] under certain assumptions, including the case we are interested in (curvature -1 and complete manifold) that one has $H^s_p(M)=L^2_{p,s}(M)$, that is, the density of $\mathcal{D}_p(M)$ in $L^2_{p,s}(M)$. An explicit proof of this fact can be found for our case in Ref. 9.

2. Proof of the first isomorphism in Theorem 2

Given $q\in\mathbb{R}$, $q\geqslant 0$ and $p\in\mathbb{Z}$, $0\leqslant p\leqslant n$, consider the operator $T=\Delta_R+qI$ (where I is the identity operator) acting on p-forms in $M=\mathbb{H}_n$. For any integer $s\geqslant 0$, T yields a continuous operator $T:H^{s+2}_p(M)\to H^s_p(M)$. If $\alpha\in H^{s+2}_p$, $T\alpha$ should be interpreted in the sense of weak derivatives. That is, $T\alpha$ is the unique element in L^2 such that

$$\langle T\alpha,\beta\rangle=\langle\alpha,T^*\beta\rangle=\langle\alpha,T\beta\rangle$$

for any $\beta\in\mathcal{D}_p$ (T is self-adjoint and $T^*=T$). The fact that $\alpha\in H^{s+2}_p$ implies that $T\alpha\in H^s_p$. We shall prove the following.

Theorem 4: *The linear map*

$$T{:}H_p^{s+2} \to H_p^s, \tag{A1}$$

where $T=\Delta_R+qI$, *is a topological isomorphism.*

If we take into account that the rough Laplacian Δ_R coincides with the De Rham Laplacian $\Delta=\delta d$ on functions, the first isomorphism in Theorem 2 appears to be a particular case of Theorem 4 with $p=0$ and $n=3$. The proof of Theorem 4 we will carry out in the sequel (for any p, not only for $p=0$) will give us a hint on the proof of the second isomorphism in Theorem 2.

Proof: As we have already said, (A1) is continuous. The fact that (A1) is injective follows from the fact that $T\alpha$ belongs to $H_p^0=L_p^2$ for $\alpha \in H_p^{s+2} \subset H_p^2$ and we have

$$\langle T\alpha, \alpha\rangle = \langle \Delta_R\alpha, \alpha\rangle + q\langle \alpha, \alpha\rangle. \tag{A2}$$

Since $\langle \Delta_R\alpha, \alpha\rangle > 0$ if $\alpha \neq 0$ and since $q \geqslant 0$, $T\alpha=0$ implies $\alpha=0$. Therefore we should check that (A1) is surjective and has a continuous inverse. The latter is written as $\|\alpha\|_{s+2} \leqslant \text{const}\|T\alpha\|_s \,\forall\, \alpha \in H_p^{s+2}$. We will prove both statements by induction on s. Let us begin with $s=0$.

Consider the scalar product B in H_p^1 defined by the formula

$$B[\alpha,\beta] = \langle \nabla\alpha, \nabla\beta\rangle + q\langle \alpha, \beta\rangle.$$

Denote by $\|\ \|_B$ the norm induced by this scalar product. If $q>0$, this norm coincides with the Sobolev norm $\|\ \|_1$, if $q=0$, this, however, is not the case. Let us see that $T{:}H_p^2 \to H_p^0$ is surjective. Given $f \in H_p^0$, we would like to find $\omega \in H_p^2$ such that $T\omega=f$. Consider the liner map $L{:}H_p^1 \to \mathbb{R}$ defined by $L(\beta)=\langle f, \beta\rangle$. It is well known that we have $\|\beta\| \leqslant \text{const}\|\nabla\beta\|$ in the hyperbolic space (see Ref. 9, p. 155). Therefore

$$|L(\beta)| = |\langle f, \beta\rangle| \leqslant \|f\|\,\|\beta\| \leqslant \text{const}\,\|f\|\,\|\nabla\beta\| \leqslant \text{const}\,\|f\|\,\|\beta\|_B.$$

This means that L is continuous with respect to the topology in H_p^1 induced by $\|\ \|_B$. Therefore there exists a unique $\omega \in H_p^1$ such that $L(\beta)=B[\omega,\beta] \,\forall\, \beta$. That is,

$$\langle \nabla\omega, \nabla\beta\rangle + q\langle \omega, \beta\rangle = \langle f, \beta\rangle.$$

If $\beta \in \mathcal{D}_p$, this is equivalent to

$$\langle \omega, (\Delta_R + qI)\beta\rangle = \langle f, \beta\rangle$$

which is the same as saying that $T\omega=f$ (T operates over L^2 elements in the sense of weak derivatives). It remains to see that $\omega \in H_p^2$. Since ω and $\Delta_R\omega$ belong to $L_p^2=H_p^0$, Lemma 3.3 in Ref. 9 implies that $\omega \in H_p^2$. We should still check that $\|\alpha\|_2 \leqslant \text{const}\,\|T\alpha\| \,\forall\, \alpha \in H_p^2$. Proposition 2.3 in Ref. 9 gives $\|\alpha\|_2 \leqslant \text{const}\,\|\Delta_R\alpha\|$. Then

$$\|\alpha\|_2 \leqslant \text{const}\,\|\Delta_R\alpha\| = \text{const}\,\|T\alpha - q\alpha\| \leqslant \text{const}\,\|T\alpha\| + \text{const}\,\|\alpha\|. \tag{A3}$$

Now (A2) implies that $\|\alpha\|^2 \leqslant \text{const}\langle T\alpha, \alpha\rangle \leqslant \text{const}\|T\alpha\|\,\|\alpha\|$. Therefore $\|\alpha\| \leqslant \text{const}\,\|T\alpha\|$. Substitute this into (A2) to obtain $\|\alpha\|_2 \leqslant \text{const}\,\|T\alpha\|$ as is required.

Take any $s>0$ and let us prove that (A1) is surjective. Given $f \in H_p^s \subset H_p^{s-1}$, the induction assumption implies that there exists a unique $\omega \in H_p^{s+1} \subset H_p^s$ satisfying $T\omega=f$. We would like to see that $\omega \in H_p^{s+2}$. Since $f=T\omega=\Delta_R\omega+q\omega$, we have $\Delta_R\omega \in H_p^s$, because ω and f belong to H_p^s, and Lemma 3.3 in Ref. 9 gives $\omega \in H_p^{s+2}$. It remains to prove the inequality $\|\alpha\|_{s+2} \leqslant \text{const}\,\|T\alpha\|_s \,\forall\, \alpha \in H_p^{s+2}$. By Proposition 2.3 in Ref. 9, we have $\|\alpha\|_{s+2} \leqslant \text{const}\,\|\Delta_R\alpha\|_s$. Therefore it will suffice to check that $\|\Delta_R\alpha\|_s \leqslant \text{const}\,\|T\alpha\|_s$. We will also prove this fact by induction on s. We have

$$\begin{aligned}\|\Delta_R\alpha\|_s = \|T\alpha - q\alpha\|_s \leqslant \|T\alpha\|_s + q\|\alpha\|_s \leqslant \|T\alpha\|_s + q\|\alpha\|_{s+1} \leqslant \|T\alpha\|_s + \text{const}\,\|\Delta_R\alpha\|_{s-1}\\ \leqslant (\text{by induction hyp.}) \leqslant \|T\alpha\|_s + \text{const}\,\|T\alpha\|_{s-1} \leqslant \text{const}\,\|T\alpha\|_s.\end{aligned}$$

□

3. A sketch of the proof of the second isomorphism in Theorem 2

Denote by F the operator defined on vector fields X by $F(X)=\nabla^* L_X g$, where $L_X g$ denotes the Lie derivative of g with respect to the vector field X. If we identify vector fields with 1-forms through the metric, F is an operator transforming 1-forms into 1-forms. In a local chart, $L_X g$ is expressed as follows:

$$(L_X g)_{ij} = \nabla_i X_j + \nabla_j X_i.$$

Then

$$F(X)_j = (\nabla^* L_X g)_j = -\nabla^i \nabla_i X_j - \nabla^i \nabla_j X_i = (\Delta_R X)_j - (\nabla^i \nabla_j - \nabla_j \nabla^i) X_i - \nabla_j \nabla^i X_i.$$

Since the curvature of the hyperbolic space is constant and equals -1, the Ricci identity reads $(\nabla^i \nabla_j - \nabla_j \nabla^i) X_i = -(n-1) X_j$. On the other hand, the term $-\nabla_j \nabla^i X_i$ is $(\mathrm{d}\delta X)_j$. Therefore

$$F = \Delta_R + (n-1)I + \mathrm{d}\delta.$$

This formula shows that F is a self-adjoint and positive operator. For any integer $s \geqslant 0$, F yields a continuous operator $F: H_1^{s+2}(M) \to H_1^s(M)$.

Theorem 5: *For any $s \in \mathbb{Z}$, $s \geqslant 0$, the map*

$$F: H_1^{s+2}(M) \to H_1^s(M). \tag{A4}$$

is a topological isomorphism.

The second isomorphism in Theorem 2 is a particular case of this theorem when the dimension n of the hyperbolic space is 3. If the expression of F did not contain the term $\mathrm{d}\delta$, Theorem 5 would be a particular case of Theorem 4 (with $p=1$). The term $\mathrm{d}\delta$ appearing in the expression of F is an order 2 operator and therefore makes the situation a bit more complex. We will prove Theorem 5 following the same method as that used in the proof of Theorem 4. In order to adapt that method to the present situation, we need a result similar to Lemma 3.3 in Ref. 9 for the operator $G = \Delta_R + \mathrm{d}\delta$. To be exact, we need the following proposition.

Proposition 1: If $\alpha \in H_1^s(M)$ and $G(\alpha) = \Delta_R \alpha + \mathrm{d}\delta\alpha \in H_1^s(M)$, then $\alpha \in H_1^{s+2}(M)$ and there exist positive constants such that for all α under the above assumptions the following inequalities hold:

(a) $\|\Delta_R \alpha\|_s \leqslant \mathrm{const}\, \|G(\alpha)\|_s$,
(b) $\|\alpha\|_{s+2} \leqslant \mathrm{const}\, \|G(\alpha)\|_s$.

With this proposition, the proof of Theorem 5 simply follows the lines of that of Theorem 4. Indeed we have the following.

Proof of Theorem 5: Since

$$\langle F(\alpha), \alpha \rangle = \langle \nabla \alpha, \nabla \alpha \rangle + \langle \delta\alpha, \delta\alpha \rangle + (n-1)\langle \alpha, \alpha \rangle, \tag{A5}$$

for all $\alpha \in H_1^{s+2}$, it is clear that $F(\alpha)=0$ implies $\alpha=0$. In order to see that (A4) is surjective and has a continuous inverse, the induction on s is used. Let us check the case of $s=0$. Consider the scalar product B in H_1^1 defined by

$$B[\alpha, \beta] = \langle \nabla \alpha, \nabla \beta \rangle + \langle \delta\alpha, \delta\beta \rangle + (n-1)\langle \alpha, \beta \rangle.$$

Given $f \in H_1^0$, in order to find $\omega \in H_1^2$ satisfying $F(\omega) = f$, we consider the map $L: H_1^1 \to \mathbb{R}$ defined by $L(\beta) = \langle f, \beta \rangle$. Here, we have $|L(\beta)| \leqslant \mathrm{const}\, \|f\|\, \|\beta\|_B$ as has already happened in Theorem 4 proving that L is continuous with respect to the norm $\|\ \|_B$. Therefore there exists a unique $\omega \in H_1^1$ such that $L(\beta) = B[\omega, \beta]$. Then

$$\langle \nabla \omega, \nabla \beta \rangle + \langle \delta\omega, \delta\beta \rangle + (n-1)\langle \alpha, \beta \rangle = \langle f, \beta \rangle.$$

If $\beta \in \mathcal{D}_1$, this is written as $\langle \omega, F(\beta) \rangle = \langle f, \beta \rangle$ meaning that $F(\omega) = f$ (since F is self-adjoint and operates on L^2 elements in the sense of weak derivatives). Since ω and $G(\omega)$ belong to $L_1^2 = H_1^0$,

Proposition 1 implies that $\omega \in H_1^2$ as is required. The inequality $\|\alpha\|_2 \leqslant \text{const}\,\|F(\alpha)\|$ for all $\alpha \in H_1^2$ is then proved in the following way:

$$\|\alpha\|_2 \leqslant (\text{by (b) in Proposition 1}) \leqslant \text{const}\,\|G(\alpha)\| = \text{const}\,\|F(\alpha) - (n-1)\alpha\| \leqslant \text{const}\,(\|F(\alpha)\| + \|\alpha\|). \tag{A6}$$

By (A5), we have $\|\alpha\|^2 \leqslant \text{const}\,\langle F(\alpha), \alpha\rangle \leqslant \text{const}\,\|F(\alpha)\|\,\|\alpha\|$. Then one has $\|\alpha\| \leqslant \text{const}\,\|F(\alpha)\|$. Substitute this into (A6) to obtain the required inequality. The proof by induction corresponding to any $s>0$ is also carried out following the lines of the proof of Theorem 4. ■

Observe that we have used only inequality (b) among inequalities (a) and (b) in Proposition 1. In fact, (a) is only required to prove (b).

The only thing we need to complete the proof of Theorem 5 is to prove Proposition 1.

4. Preliminary material for the proof of Proposition 1

Before proceeding to the proof of Proposition 1 we will need the following lemma.

Lemma 1: For any integer $s \geqslant 0$ there exists a constant such that

$$\|\Delta_R \omega\|_s \leqslant \text{const}\,\|G(\omega)\|_s$$

for any $\omega \in H_1^{s+2}(M)$.

In order to prove this lemma, we will need the following two lemmas.

Lemma 2: Let (M,g) be an n-dimensional Riemannian manifold of constant curvature K. If α is a covariant p-tensor and σ is a permutation of the indices $\{1,\ldots,s\}$, let $\sigma(\nabla^{(s)}\alpha)$ be the covariant $(p+s)$-tensor defined as follows:

$$\sigma(\nabla^{(s)}\alpha)(X_1,\ldots,X_s,Y_1,\ldots,Y_p) = (\nabla^{(s)}\alpha)(X_{\sigma(1)},\ldots,X_{\sigma(s)},Y_1,\ldots,Y_p).$$

Then, given an integer $s \geqslant 2$ and a permutation σ of the indices $\{1,\ldots,s\}$, there exists a constant such that the formula

$$\|\sigma(\nabla^{(s)}\alpha) - \nabla^{(s)}\alpha\| \leqslant \text{const}\,\|\alpha\|_{s-2},$$

holds for any covariant p-tensor α having compact support and belonging to the class C^∞.

Proof: Let τ be the transposition of the two successive indices k and $k+1$,

$$\tau:\{1,\ldots,k,k+1,\ldots,s\} \to \{1,\ldots,k+1,k,\ldots,s\}$$

(any permutation can be expressed as a product of transpositions). In a local chart, the components of $\tau(\nabla^{(s)}\alpha)$ will be

$$\tau(\nabla^{(s)}\alpha)_{i_1\cdots i_s j_1\cdots j_p} = \nabla_{i_1}\cdots\nabla_{i_{k+1}}\nabla_{i_k}\cdots\nabla_{i_s}\alpha_{j_1\cdots j_p}.$$

Since the curvature K is constant, the Ricci identity implies that for any r-tensor β

$$(\nabla_i\nabla_j - \nabla_j\nabla_i)\beta_{i_1\cdots i_r} = K(g_{ii_1}\beta_{ji_2\cdots i_r} - g_{ji_1}\beta_{ii_2\cdots i_r}) + \cdots + K(g_{ii_r}\beta_{i_1\cdots i_{r-1}j} - g_{ji_r}\beta_{i_1\cdots i_{r-1}i}).$$

Set

$$\beta_{i_{k+2}\cdots i_s j_1\cdots j_p} = \nabla_{i_{k+2}}\cdots\nabla_{i_s}\alpha_{j_1\cdots j_p}.$$

Taking into account that the covariant differential of the metric tensor g equals zero one obtains that $(\tau(\nabla^{(s)}\alpha) - \nabla^{(s)}\alpha)_{i_1\cdots i_s j_1\cdots j_p}$ will be the sum of $2((s-k-1)+p)$ terms having the form

$$\pm K g_{\sigma(i_1)\sigma(i_2)}\nabla_{\sigma(i_3)}\cdots\nabla_{\sigma(i_s)}\alpha_{j_1\cdots j_p},$$

where σ is a certain permutation of the indices $\{1,\ldots,s\}$. Since all of these terms contain $s-2$ derivatives, the norm $\|\sigma(\nabla^{(s)}\alpha) - \nabla^{(s)}\alpha\|$ will be controlled by $\|\alpha\|_{s-2}$. □

Lemma 3: Let (M,g) be a Riemannian manifold of constant curvature K. Given an integer

$s \geqslant 0$, there exists a constant such that the formula

$$\|(\nabla^{(s)}\Delta_R - \Delta_R\nabla^{(s)})\alpha\| \leqslant \text{const}\,\|\alpha\|_s$$

holds for any covariant p-tensor α having compact support and belonging to the class C^∞.

This lemma is readily obtained from the previous lemma.

Proof of Lemma 1: Since $\mathcal{D}_1(M)$ is dense in $H_1^{s+2}(M)$ and the operators Δ_R and G are continuous in the Sobolev norm, it is enough to prove the inequality for $\omega \in \mathcal{D}_1(M)$. We proceed by induction on s. In order to obtain the required result for $s=0$, we must prove that $\|\Delta_R\omega\| \leqslant \text{const}\,\|(\Delta_R + \mathrm{d}\delta)\omega\|$. We have

$$\langle(\Delta_R + \mathrm{d}\delta)\omega, (\Delta_R + \mathrm{d}\delta)\omega\rangle \geqslant \langle\Delta_R\omega, \Delta_R\omega\rangle + 2\langle\mathrm{d}\delta\omega, \Delta_R\omega\rangle. \tag{A7}$$

In hyperbolic spaces of constant curvature $=-1$ the rough Laplacian is related to the De Rham Laplacian $\Delta = \mathrm{d}\delta + \delta\mathrm{d}$ by $\Delta_R = \Delta + (n-1)I$. Then

$$\langle\mathrm{d}\delta\,\omega, \Delta_R\omega\rangle = \langle\mathrm{d}\delta\,\omega, \mathrm{d}\delta\,\omega + \delta\,\mathrm{d}\omega + (n-1)\omega\rangle = \langle\mathrm{d}\delta\,\omega, \mathrm{d}\delta\,\omega\rangle + \langle\mathrm{d}\delta\,\omega, \delta\,\mathrm{d}\omega\rangle + (n-1)\langle\mathrm{d}\delta\,\omega, \omega\rangle.$$

Among the three terms on the right-hand side, the first term and the third term are $\geqslant 0$ while the second equals zero since

$$\langle\mathrm{d}\delta\,\omega, \delta\,\mathrm{d}\omega\rangle = \langle\mathrm{d}\,\mathrm{d}\delta\omega, \mathrm{d}\omega\rangle = 0.$$

So $<\mathrm{d}\delta\omega, \Delta_R\omega>$ is $\geqslant 0$. Then (A7) implies

$$\|(\Delta_R + \mathrm{d}\delta)\omega\|^2 = \langle(\Delta_R + \mathrm{d}\delta)\omega, (\Delta_R + \mathrm{d}\delta)\omega\rangle \geqslant \langle\Delta_R\omega, \Delta_R\omega\rangle = \|\Delta_R\omega\|^2,$$

which is the required result.

Assume that the result is proved for $s-1$ and let us prove it for s. We have

$$\langle\nabla^{(s)}(\Delta_R + \mathrm{d}\delta)\omega, \nabla^{(s)}(\Delta_R + \mathrm{d}\delta)\omega\rangle \geqslant \langle\nabla^{(s)}\Delta_R\omega, \nabla^{(s)}\Delta_R\omega\rangle + 2\langle\nabla^{(s)}\,\mathrm{d}\delta\omega, \nabla^{(s)}\Delta_R\omega\rangle. \tag{A8}$$

In order to complete the proof, we need the following lemma describing the last term in the above inequality.

Lemma 4: $<\nabla^{(s)}\mathrm{d}\delta\,\omega, \nabla^{(s)}\Delta_R\omega>$ can be expressed as the sum of two terms $T_1 + T_2$, where $T_1 \geqslant 0$ and T_2 satisfy the inequality

$$|T_2| \leqslant \text{const}\,\|\omega\|_{s+1}^2.$$

Assume that Lemma 4 is proved and let us see how the proof of Lemma 1 is completed. Inequality (A8) implies

$$\langle\nabla^{(s)}(\Delta_R + \mathrm{d}\delta)\omega, \nabla^{(s)}(\Delta_R + \mathrm{d}\delta)\omega\rangle \geqslant \langle\nabla^{(s)}\Delta_R\omega, \nabla^{(s)}\Delta_R\omega\rangle + 2T_2.$$

Then we obtain

$$\begin{aligned}\langle\nabla^{(s)}\Delta_R\omega, \nabla^{(s)}\Delta_R\omega\rangle &\leqslant \langle\nabla^{(s)}(\Delta_R + \mathrm{d}\delta)\omega, \nabla^{(s)}(\Delta_R + \mathrm{d}\delta)\omega\rangle + 2|T_2| \\ &\leqslant \|\nabla^{(s)}(\Delta_R + \mathrm{d}\delta)\omega\|^2 + \text{const}\,\|\omega\|_{s+1}^2.\end{aligned}$$

By Proposition 2.3 in Ref. 9, we have $\|\omega\|_{s+1} \leqslant \text{const}\,\|\Delta_R\omega\|_{s-1}$ and, by the induction assumption, $\|\Delta_R\omega\|_{s-1} \leqslant \|(\Delta_R + \mathrm{d}\delta)\omega\|_{s-1}$. Hence

$$\|\nabla^{(s)}\Delta_R\omega\|^2 \leqslant \|\nabla^{(s)}(\Delta_R + \mathrm{d}\delta)\omega\|^2 + \text{const}\,\|(\Delta_R + \mathrm{d}\delta)\omega\|_{s-1}^2 \leqslant \text{const}\,\|(\Delta_R + \mathrm{d}\delta)\omega\|_s^2$$

which proves Lemma 1. □

It remains to prove Lemma 4.

Proof of Lemma 4: The local scalar product of $\nabla^{(s)}\,\mathrm{d}\delta\,\omega$ by $\nabla^{(s)}\Delta_R\omega$ is

$$(\nabla^{(s)}\,\mathrm{d}\delta\,\omega,\nabla^{(s)}\Delta_R\omega)=(\nabla_{i_1}\cdots\nabla_{i_s}\nabla_i\nabla^k\omega_k)(\nabla^{i_1}\cdots\nabla^{i_s}\nabla^r\nabla_r\omega^i). \tag{A9}$$

Permute the derivatives $\nabla_{i_1}\cdots\nabla_{i_s}\nabla_i$ in the first factor in order to place ∇_i first. We obtain

$$\nabla_{i_1}\cdots\nabla_{i_s}\nabla_i\nabla^k\omega_k=\nabla_i\nabla_{i_1}\cdots\nabla_{i_s}\nabla^k\omega_k+A(\omega)_{ii_1\cdots i_s},$$

where $A(\omega)$ is a globally defined $(s+1)$-tensor. By substituting into (A9), we have

$$(\nabla^{(s)}\,\mathrm{d}\delta\,\omega,\nabla^{(s)}\Delta_R\omega)=(\nabla_i\nabla_{i_1}\cdots\nabla_{i_s}\nabla^k\omega_k)(\nabla^{i_1}\cdots\nabla^{i_s}\nabla^r\nabla_r\omega^i)+(A(\omega),\nabla^{(s)}\Delta_R\omega).$$

Adding a divergence we pass the derivation ∇_i from the first factor to the second factor,

$$(\nabla^{(s)}\,\mathrm{d}\delta\,\omega,\nabla^{(s)}\Delta_R\omega)=-(\nabla_{i_1}\cdots\nabla_{i_s}\nabla^k\omega_k)(\nabla_i\nabla^{i_1}\cdots\nabla^{i_s}\nabla^r\nabla_r\omega^i)+\mathrm{div}+(A(\omega),\nabla^{(s)}\Delta_R\omega). \tag{A10}$$

As before

$$\nabla_i\nabla_{i_1}\cdots\nabla_{i_s}\nabla^r\nabla_r\omega^i=\nabla_{i_1}\cdots\nabla_{i_s}\nabla_i\nabla^r\nabla_r\omega^i+B(\omega)_{i_1\cdots i_s},$$

where $B(\omega)$ is a globally defined s-tensor. Substitute this result into (A10) to obtain

$$\begin{aligned}(\nabla^{(s)}\,\mathrm{d}\delta\,\omega,\nabla^{(s)}\Delta_R\omega)=&-(\nabla_{i_1}\cdots\nabla_{i_s}\nabla^k\omega_k)(\nabla^{i_1}\cdots\nabla^{i_s}\nabla_i\nabla^r\nabla_r\omega^i)+(\nabla^{(s)}\delta\omega,B(\omega))\\&+\mathrm{div}+(A(\omega),\nabla^{(s)}\Delta_R\omega).\end{aligned} \tag{A11}$$

Finally, passing the Laplacian $\Delta_R=-\nabla^r\nabla_r$ in front of all,

$$\nabla^{i_1}\cdots\nabla^{i_s}\nabla_i\nabla^r\nabla_r\omega^i=\nabla^r\nabla_r\nabla^{i_1}\cdots\nabla^{i_s}\nabla_i\omega^i+C(\omega)_{i_1\cdots i_s},$$

where $C(\omega)$ is a globally defined s-tensor. By (25), we obtain

$$\begin{aligned}(\nabla^{(s)}\,\mathrm{d}\delta\,\omega,\nabla^{(s)}\Delta_R\omega)=&-(\nabla_{i_1}\cdots\nabla_{i_s}\nabla^k\omega_k)(\nabla^r\nabla_r\nabla^{i_1}\cdots\nabla^{i_s}\nabla_i\omega^i)+(\nabla^{(s)}\delta\omega,C(\omega))+(\nabla^{(s)}\delta\omega,B(\omega))\\&+\mathrm{div}+(A(\omega),\nabla^{(s)}\Delta_R\omega).\end{aligned}$$

Integrating over the whole manifold,

$$\langle\nabla^{(s)}\,\mathrm{d}\delta\,\omega,\nabla^{(s)}\Delta_R\omega\rangle=\langle\nabla^{(s)}\delta\omega,\Delta_R\nabla^{(s)}\delta\omega\rangle+\langle\nabla^{(s)}\delta\omega,C(\omega)+B(\omega)\rangle+\langle A(\omega),\nabla^{(s)}\Delta_R\omega\rangle.$$

Define now

$$T_1=\langle\nabla^{(s)}\delta\omega,\Delta_R\nabla^{(s)}\delta\omega\rangle,\quad T_2=\langle\nabla^{(s)}\delta\omega,C(\omega)+B(\omega)\rangle+\langle A(\omega),\nabla^{(s)}\Delta_R\omega\rangle.$$

It is clear that $T_1\geqslant 0$. It remains to see that T_2 satisfies the inequality in the lemma. It is not difficult to check, using Lemmas 2 and 3, that every term appearing in the definition of T_2 satisfies this inequality. □

5. Proof of Proposition 1

We first give a naive and simple proof of Proposition 1.

A naive proof: Lemma 1 assures that for any integer $s\geqslant 0$ there exists a constant such that

$$\|\Delta_R\omega\|_s\leqslant\mathrm{const}\,\|G(\omega)\|_s \tag{A12}$$

for any $\omega\in\mathcal{D}_1$. Since the space $\mathcal{D}_1$ is dense in H_1^s, one should expect that inequality (A12) also holds for $\alpha\in H_1^s$. Therefore, since $G(\alpha)\in H_1^s$ means that $\|G(\alpha)\|_s$ is finite, (A12) implies that $\|\Delta_R\alpha\|_s$ is finite and then $\Delta_R\alpha\in H_1^s$. Now Lemma 3.3 in Ref. 9 states that $\alpha\in H_1^{s+2}$ and $\|\alpha\|_{s+2}\leqslant\mathrm{const}\,\|\Delta_R\alpha\|_s$. Then inequality (A12) enables us to write $\|\alpha\|_{s+2}\leqslant\mathrm{const}\,\|G(\alpha)\|_s$. □

Nevertheless, the fact that (A12) holds for $\omega\in\mathcal{D}_1$ does not imply in a simple way that it will also hold for $\alpha\in H_1^s$. In fact, Lemma 1 assures only that (A12) holds for $\alpha\in H_1^{s+2}$. The more

difficult task is to show that $\nabla^{s+1}\alpha$ and $\nabla^{s+2}\alpha$ belong to L^2. For this purpose a delicate regularization argument in hyperbolic space is needed. In order to obtain a rigorous proof of Proposition 1, we first deal with a particular case of it.

A particular case of Proposition 1. Proposition 1 holds for 1-forms α belonging to the class C^∞.

Proof of the particular case: We start with a sequence $\{\chi_m\}$ of C^∞-functions on M with compact support, $\chi_m \in \mathcal{D}(M)$, (an *exhausting sequence*) such that $\chi_m \nearrow 1$ and $|\nabla^{(k)}\chi_m(x)| \leqslant c_k$ for all m and all $x \in M$. In Ref. 9 is verified that such a sequence really exists when $M=\mathbb{H}_n$. Also it is proved that given a C^∞ form $\alpha \in H_1^s(M)$ then $\chi_m\alpha \to \alpha$ in $H_1^s(M)$.

As usual we use induction on s. Let us begin with the case $s=0$. Let $\alpha_m=\chi_m\alpha$. We have $\alpha_m \in \mathcal{D}_1(M)$. Since $G=\Delta_R+\mathrm{d}\delta=\nabla^*\nabla+\mathrm{d}\delta$,

$$\langle G(\alpha_m), \alpha_m\rangle = \langle \nabla\alpha_m, \nabla\alpha_m\rangle + \langle \delta\alpha_m, \delta\alpha_m\rangle.$$

This implies

$$\langle \nabla\alpha_m, \nabla\alpha_m\rangle \leqslant \langle G(\alpha_m), \alpha_m\rangle.$$

Develop each member of the previous inequality. Since $\nabla\alpha_m=\nabla(\chi_m\alpha)=(\nabla\chi_m)\otimes\alpha+\chi_m\nabla\alpha$, the pointwise inner product $(\nabla\alpha_m, \nabla\alpha_m)$ is

$$\begin{aligned}(\nabla\alpha_m, \nabla\alpha_m) &= (\nabla\chi_m\otimes\alpha, \nabla\chi_m\otimes\alpha) + (\chi_m\nabla\alpha, \chi_m\nabla\alpha) + 2(\nabla\chi_m\otimes\alpha, \chi_m\nabla\alpha)\\ &= |\mathrm{d}\chi_m|^2|\alpha|^2 + \chi_m^2|\nabla\alpha|^2 + 2(\mathrm{d}\chi_m\otimes\alpha, \chi_m\nabla\alpha),\end{aligned}$$

On the other hand, we have

$$\begin{aligned}G(\chi_m\alpha) = \chi_m G(\alpha) + (\Delta_R\chi_m)\alpha - C_{23}(\nabla^{(2)}\chi_m\otimes\alpha) - 2C_{12}(\mathrm{d}\chi_m\otimes\nabla\alpha)\\ - C_{13}(\mathrm{d}\chi_m\otimes\nabla\alpha) + (\delta\alpha)\mathrm{d}\chi_m,\end{aligned} \tag{A13}$$

where, for example, C_{12} means the operator obtained at each point $x \in M$ by contraction through the metric between the first and second factor of $\otimes^3 T_x(M)^*$. The above formula can be proved by making a trivial coordinatewise calculation. Then

$$\begin{aligned}(G(\alpha_m), \alpha_m) = (G(\chi_m\alpha), \chi_m\alpha) = \chi_m^2(G(\alpha), \alpha) + \chi_m\Delta_R\chi_m(\alpha, \alpha) - \chi_m(\nabla^{(2)}\chi_m, \alpha\otimes\alpha)\\ - 2\chi_m(\nabla\alpha, \mathrm{d}\chi_m\otimes\alpha) - \chi_m(\nabla\alpha, \alpha\otimes\mathrm{d}\chi_m) - \chi_m\delta\alpha(\mathrm{d}\chi_m, \alpha).\end{aligned}$$

The inequality $\langle\nabla\alpha_m, \nabla\alpha_m\rangle \leqslant \langle G(\alpha_m), \alpha_m\rangle$ writes

$$\begin{aligned}\int \{|\mathrm{d}\chi_m|^2|\alpha|^2 + |\chi_m|^2|\nabla\alpha|^2 + 4\chi_m(\mathrm{d}\chi_m\otimes\alpha, \nabla\alpha)\}\mathrm{d}v\\ \leqslant \int \{|\chi_m|^2(G(\alpha), \alpha) + \chi_m\Delta_R\chi_m|\alpha|^2 - \chi_m(\nabla^{(2)}\chi_m, \alpha\otimes\alpha)\\ - \chi_m(\nabla\alpha, \alpha\otimes\mathrm{d}\chi_m) - \chi_m\delta\alpha(\mathrm{d}\chi_m, \alpha)\}\mathrm{d}v.\end{aligned}$$

We know that χ_m, $|\mathrm{d}\chi_m|$, $|\nabla^{(2)}\chi_m|$, and $|\Delta_R\chi_m|$ are bounded (for all $x \in M$) by a constant independent of m, hence

$$|(\mathrm{d}\chi_m\otimes\alpha, \nabla\alpha)| \leqslant \text{const}\,|\alpha||\nabla\alpha|, \quad |(\nabla^{(2)}\chi_m, \alpha\otimes\alpha)| \leqslant \text{const}\,|\alpha|^2,$$

$$|\delta\alpha||(\mathrm{d}\chi_m, \alpha)| \leqslant \text{const}\,|\alpha||\nabla\alpha|.$$

Let I_m be the integral $\int_M |\chi_m|^2|\nabla\alpha|^2\,\mathrm{d}v$, (finite because $\chi_m \in \mathcal{D}$). Since $\alpha, G(\alpha) \in H_p^0(M)$ the global products $\langle G\alpha, \alpha\rangle$ and $\langle\alpha, \alpha\rangle$ are finite, and hence one deduces from the previous inequality that

$$I_m \leqslant \text{const}\left(\langle G(\alpha),\alpha\rangle + \langle \alpha,\alpha\rangle + \int |\chi_m||\alpha||\nabla\,\alpha|\mathrm{d}v\right). \tag{A14}$$

The Schwarz inequality asserts that

$$\int |\chi_m||\alpha|\,|\nabla\,\alpha|\mathrm{d}v \leqslant \left\{\int |\chi_m|^2|\nabla\,\alpha|^2\mathrm{d}v\right\}^{1/2}\left\{\int |\alpha|^2\mathrm{d}v\right\}^{1/2} = I_m^{1/2}\|\alpha\|.$$

If x, y, and ε are real numbers, we have

$$(y-2\varepsilon x)^2 = y^2 + 4\varepsilon^2x^2 - 4\varepsilon xy \geqslant 0,$$

whence

$$xy \leqslant \varepsilon x^2 + \frac{y^2}{4\varepsilon}.$$

For a fixed ε, this inequality holds for all x, y. This means that

$$I_m^{1/2}\|\alpha\| \leqslant \varepsilon I_m + \frac{\|\alpha\|^2}{4\varepsilon}.$$

For a fixed ε, this holds for all I_m and $\|\alpha\|$. Then we obtain

$$\int_M \chi_m|\alpha||\nabla\,\alpha|\mathrm{d}v \leqslant \varepsilon I_m + \frac{\|\alpha\|^2}{4\varepsilon}.$$

Take ε such that $0<\varepsilon<1$. Then expression (A14) yields (by collecting in the first member all the terms containing I_m)

$$I_m = \int |\chi_m|^2|\nabla\,\alpha|^2\,\mathrm{d}v \leqslant \text{const}\,(\langle G(\alpha),\alpha\rangle + \|\alpha\|^2).$$

But $\langle G(\alpha),\alpha\rangle \leqslant \|G(\alpha)\|\,\|\alpha\| \leqslant (1/2)(\|G(\alpha)\|^2+\|\alpha\|^2)$. Therefore

$$I_m = \int |\chi_m|^2|\nabla\,\alpha|^2\,\mathrm{d}v \leqslant \text{const}\,(\|\alpha\|^2 + \|G(\alpha)\|^2).$$

By the dominated convergence theorem [which can be applied since both $\|\alpha\|$ and $\|G(\alpha)\|$ are finite because α and $G(\alpha)$ belong to $H_1^0(M)=L_1^2(M)$], we have that $\int|\nabla\alpha|^2\,\mathrm{d}v$ is finite. That is, $\nabla\alpha \in L_1^2(M)$. Then $\alpha\in H_1^1(M)$. Therefore we know that the sequence $\{\alpha_m\}$ converges to α in the norm of $H_1^1(M)$. In particular, $\{\nabla\alpha_m\}$ converges to $\nabla\alpha$ in $L_1^2(M)$. Since, on the other hand, $G(\alpha)\in L_1^2(M)$, $\{G(\alpha_m)\}$ converges to $G(\alpha)$ in $L_1^2(M)$. We can then pass to the limit in inequality $\langle\nabla\alpha_m,\nabla\alpha_m\rangle \leqslant \langle G(\alpha_m),\alpha_m\rangle$ to obtain

$$\langle\nabla\alpha,\nabla\,\alpha\rangle \leqslant \langle G(\alpha),\alpha\rangle.$$

This implies that

$$\|\nabla\,\alpha\|^2 \leqslant \|G(\alpha)\|\,\|\alpha\| \leqslant (1/2)(\|G(\alpha)\|^2+\|\alpha\|^2).$$

From expression (A13) one obtains

$$\|G(\alpha_m)\|^2 \leqslant \text{const}\,(\|G(\alpha)\|^2+\|\alpha\|^2).$$

This inequality will enable us to establish that $\Delta_R\alpha\in L_1^2(M)$. The inequality in Lemma 1 gives

$$\|\Delta_R\alpha_m\|^2 \leqslant \text{const}\,\|G\alpha_m\|^2 \leqslant \text{const}\,(\|G\alpha\|^2 + \|\alpha\|^2).$$

As one can easily check

$$\Delta_R\alpha_m = \Delta_R(\chi_m\alpha) = (\Delta_R\chi_m)\alpha + \chi_m\Delta_R\alpha - 2C_{12}(d\chi_m \otimes \nabla\,\alpha), \tag{A15}$$

and therefore

$$\|\chi_m\Delta_R\alpha\| \leqslant \|\Delta_R\alpha_m\| + \|\alpha\Delta_R\chi_m\| + 2\|d\chi_m \otimes \nabla\,\alpha\|.$$

Since $\{\chi_m\}$ is an exhausting sequence and $(\|G(\alpha)\|^2+\|\alpha\|^2)$ controls the norm $\|\nabla\alpha\|$ as well as $\|\Delta_R\alpha_m\|$, we have

$$\int \chi_m^2|\Delta_R\alpha|^2\,\mathrm{d}v \leqslant \text{const}\,(\|G(\alpha)\|^2 + \|\alpha\|^2).$$

Then, by the dominated convergence theorem, the integral $\int|\Delta_R\alpha|^2\,\mathrm{d}v$ is finite. That is, $\Delta_R\alpha \in L_1^2(M)$. Therefore we can apply Lemma 3.3 in Ref. 9 giving $\alpha\in H_1^2(M)$ and $\|\alpha\|_2 \leqslant \text{const}\,\|\Delta_R\alpha\|$. Once we know that $\Delta_R\alpha\in L_1^2(M)$, we can take limits in the inequality $\|\Delta_R\alpha_m\| \leqslant \text{const}\,\|G(\alpha_m)\|$ and obtain $\|\Delta_R\alpha\|\leqslant\text{const}\,\|G(\alpha)\|$. Combining this results with earlier ones, we have

$$\|\alpha\|_2 \leqslant \text{const}\,\|\Delta_R\alpha\| \leqslant \text{const}\,\|G(\alpha)\|,$$

completing the proof of the lemma for $s=0$.

Let us suppose that the particular case of Proposition 1 holds for $s-1$. Since α and $G(\alpha)$ belong to $H_1^s(M)\subset H_1^{s-1}(M)$ then by the induction assumption, $\alpha\in H_1^{s+1}(M)$, $\|\alpha\|_{s+1} \leqslant \text{const}\,\|G(\alpha)\|_{s-1}$, and $\|\Delta_R\alpha\|_{s-1}\leqslant\text{const}\,\|G(\alpha)\|_{s-1}$. Next we try to control $\|\Delta_R\alpha_m\|_s$ by the finite quantities $\|G(\alpha)\|_s$ and $\|\alpha\|_{s+1}$. Write (A13) ordering the terms by the order of derivatives of α they contain,

$$G(\chi_m\alpha)_i = \chi_m G(\alpha)_i - 2(\nabla_k\chi_m)(\nabla^k\alpha_i) - (\nabla_k\chi_m)(\nabla_i\alpha^k) - (\nabla^k\alpha_k)(\nabla_i\chi_m) + (\Delta_R\chi_m)\alpha_i - (\nabla_i\nabla_k\chi_m)\alpha^k.$$

Then

$$\nabla^{(s)}G(\alpha_m) = \nabla^{(s)}G(\chi_m\alpha) = \chi_m\nabla^{(s)}G(\alpha) + T,$$

where T denotes the sum of terms containing less than s derivatives of $G(\alpha)$ and of terms containing less than $s+2$ derivatives of α. The local inner product of $\nabla^{(s)}G(\alpha_m)$ by itself will be

$$(\nabla^{(s)}G(\alpha_m),\nabla^{(s)}G(\alpha_m)) = \chi_m^2(\nabla^{(s)}G(\alpha),\nabla^{(s)}G(\alpha)) + (T,T) + 2\chi_m(\nabla^{(s)}G(\alpha),T).$$

Integrate this expression over M to obtain

$$\begin{aligned}\|\nabla^{(s)}G(\alpha_m)\|^2 &= \int_M |\chi_m|^2|\nabla^{(s)}G(\alpha)|^2\,\mathrm{d}v + \|T\|^2 + 2\int_M |\chi_m|(\nabla^{(s)}G(\alpha),T)\mathrm{d}v \\ &\leqslant \text{const}\,\|\nabla^{(s)}G(\alpha)\|^2 + \|T\|^2 + \text{const}\,|\langle\nabla^{(s)}G(\alpha),T\rangle|.\end{aligned}$$

Since

$$|\langle\nabla^{(s)}G(\alpha),T\rangle| \leqslant \|\nabla^{(s)}G(\alpha)\|\,\|T\| \leqslant \tfrac{1}{2}(\|\nabla^{(s)}G(\alpha)\|^2 + \|T\|^2)$$

and $\|T\|^2\leqslant\text{const}\,(\|\alpha\|_{s+1}^2+\|G(\alpha)\|_{s-1}^2)$ we get

$$\|G(\alpha_m)\|_s^2 = \|\nabla^{(s)}G(\alpha_m)\|^2 + \|G(\alpha_m)\|_{s-1}^2 \leqslant \text{const}\,(\|G(\alpha)\|_s^2 + \|\alpha\|_{s+1}^2).$$

Lemma 1 gives $\|\Delta_R\alpha_m\|_s\leqslant\text{const}\,\|G(\alpha_m)\|_s$. Then

$$\|\Delta_R \alpha_m\|_s^2 \leqslant \text{const}\,(\|G(\alpha)\|_s^2 + \|\alpha\|_{s+1}^2). \tag{A16}$$

Using formula (A13) and applying to $\nabla^{(s)}\Delta_R\alpha_m$ the same argument as that applied to I_m, we conclude that

$$\int |\chi_m|^2 |\nabla^{(s)}\Delta_R\alpha|^2 \, dv \leqslant \text{const}\,(\|\Delta_R\alpha\|_{s-1}^2 + \|G(\alpha)\|_s^2 + \|\alpha\|_{s+1}^2).$$

By the induction assumption, $\|\Delta_R\alpha\|_{s-1}^2 \leqslant \text{const}\,\|G(\alpha)\|_{s-1}^2 \leqslant \text{const}\,\|G(\alpha)\|_s^2$ and $\|\alpha\|_{s+1}^2 \leqslant \text{const}\,\|G(\alpha)\|_{s-1}^2 \leqslant \text{const}\,\|G(\alpha)\|_s^2$. Then

$$\int \chi_m^2 |\nabla^{(s)}\Delta_R\alpha|^2 \, dv \leqslant \text{const}\,\|G(\alpha)\|_s.$$

This proves that $\int |\nabla^{(s)}\Delta_R\alpha|^2 \, dv$ is finite and

$$\int |\nabla^{(s)}\Delta_R\alpha|^2 \, dv \leqslant \text{const}\,\|G(\alpha)\|_s.$$

Hence

$$\|\Delta_R\alpha\|_s^2 = \int |\nabla^{(s)}\Delta_R\alpha|^2 \, dv + \|\Delta_R\alpha\|_{s-1}^2 \leqslant \text{const}\,\|G(\alpha)\|_s^2.$$

Lemma 3.3 in Ref. 9 then gives $\alpha \in H_1^{s+2}(M)$ and

$$\|\alpha\|_{s+2} \leqslant \text{const}\,\|\Delta_R\alpha\|_s \leqslant \text{const}\,\|G(\alpha)\|_s$$

completing the proof. □

Final part of the proof of Proposition 1: We have to approximate forms α in $H_1^s(\mathbb{H}_n)$ with $G(\alpha) \in H_1^s(\mathbb{H}_n)$ by C^∞ forms with the same properties. This is achieved via the hyperbolic regularization (see Ref. 9). There one defines for any $\varepsilon > 0$ the hyperbolic convolution $C_\varepsilon\alpha$ of a form α by

$$(C_\varepsilon\alpha)(x) = \int_{\mathbb{H}^n} \alpha(y) \wedge \star\,\delta_\varepsilon(x,y).$$

Here $\star$ stands for Hodge operator. Each $C_\varepsilon\alpha$ is a C^∞ 1-form on $\mathbb{H}^n$ invariant for all isometries, that is, $C_\varepsilon(\varphi\alpha) = \varphi(C_\varepsilon\alpha)\,\forall\,\varphi \in \text{Iso}(\mathbb{H}_n)$. It is proved that $C_\varepsilon\alpha \in H_1^s(\mathbb{H}_n)$, that

$$\|C_\varepsilon\alpha\|_s \leqslant \text{const}\,\|\alpha\|_s \tag{A17}$$

and that $C_\varepsilon\alpha$ tends to α in $H_1^s(\mathbb{H}_n)$ as $\varepsilon \to 0$.

The operator $G = \Delta_R + d\delta$ in $\mathbb{H}^n$ commutes with all isometries, that is, if φ is an isometry then $G(\varphi^*(\alpha)) = \varphi^*(G(\alpha))$, because all the operators involved are defined in terms of the metric. Then one can show that C_ε commutes with G. Since $\alpha \in H_1^s(\mathbb{H}_n)$, the inequality (A17) gives $C_\varepsilon\alpha \in H_1^s(\mathbb{H}_n)$ for all ε. Since, on the other hand, $G(\alpha) \in H_1^s(\mathbb{H}_n)$, we have in a similar manner that $C_\varepsilon(G(\alpha)) \in H_1^s(\mathbb{H}_n)$. The particular case of Proposition 1 applied to $C_\varepsilon\alpha$ and to $G(C_\varepsilon\alpha) = C_\varepsilon(G(\alpha))$ gives $C_\varepsilon\alpha \in H_1^{s+2}(\mathbb{H}_n)$. Let us prove that (by varying ε) $\{C_\varepsilon\alpha\}$ is a Cauchy sequence in the space $H_1^{s+2}(\mathbb{H}_n)$. For this purpose, we apply the particular case of Proposition 1 to the difference $C_\varepsilon\alpha - C_{\varepsilon'\alpha}$. We have

$$\|C_\varepsilon\alpha - C_{\varepsilon'}\alpha\|_{s+2} \leqslant \text{const}\,\|G(C_\varepsilon\alpha - C_{\varepsilon'}\alpha)\|_s \leqslant \text{const}\,\|C_\varepsilon G(\alpha) - C_{\varepsilon'}G(\alpha)\|_s. \tag{A18}$$

Since $G(\alpha)$ and $C_\varepsilon G(\alpha)$ belong to $H_1^s(\mathbb{H}_n)$ and $C_\varepsilon G(\alpha)$ converges in this space to $G(\alpha)$ as $\varepsilon \to 0$, we have that $\{C_\varepsilon G(\alpha)\}$ is a Cauchy sequence in $H_1^s(\mathbb{H}_n)$ and then (A18) implies that $\{C_\varepsilon\alpha\}$ is also a Cauchy sequence in $H_1^{s+2}(\mathbb{H}_n)$. Since this space is complete, this Cauchy sequence has a

limit $\beta \in H_1^{s+2}(\mathbb{H}_n) \subset H_1^s(\mathbb{H}_n)$. Let us see that this limit coincides with α. Since the convergence in the norm $\| \|_{s+2}$ is stronger than that in the norm $\| \|_s$, β will also be the limit of $\{C_\varepsilon \alpha\}$ in the norm $\| \|_s$. This limit, however, was α. Therefore $\alpha = \beta$ and $\alpha \in H_1^{s+2}(\mathbb{H}_n)$. Finally, by taking limits in the inequalities

$$\|C_\varepsilon \alpha\|_{s+2} \leqslant \text{const} \, \|G(C_\varepsilon \alpha)\|_s = \text{const} \, \|C_\varepsilon G(\alpha)\|_s,$$

$$\|\Delta_R C_\varepsilon \alpha\|_s \leqslant \text{const} \, \|G(C_\varepsilon \alpha)\|_s = \text{const} \, \|C_\varepsilon G(\alpha)\|_s,$$

we obtain

$$\|\alpha\|_{s+2} \leqslant \text{const} \, \|G(\alpha)\|_s,$$

$$\|\Delta_R \alpha\|_s \leqslant \text{const} \, \|G(\alpha)\|_s.$$

□

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Birkhoff's theorem in Lovelock gravity

Robin Zegers[a)]
LPT, Université de Paris-Sud, Bât. 210, 91405 Orsay Cedex, France and APC[b)],
11 Place Marcelin Berthelot, F-75231 Paris Cedex 05, France

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We show that the solutions of the Lovelock equations with spherical, planar, or hyperbolic symmetry are locally isometric to the corresponding static Lovelock black hole. As a consequence, these solutions are locally static: they admit an additional Killing vector that can either be space-like or time-like, depending on the position. This result also holds in the presence of an abelian gauge field, in which case the solutions are locally isometric to a charged static black hole. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1960798]

In four-dimensional general relativity, it is well known that the spherically symmetric solutions of Einstein's field equations in the vacuum are locally isometric to the Schwarzschild solution—this is Birkhoff's theorem, see e.g., Ref. 1. As a consequence, these solutions are locally static outside the horizon and a spherically symmetric source does not radiate gravitational waves. In this letter, we extend Birkhoff's theorem to Lovelock gravity.

Lovelock theory is the most general classical theory of gravity leading to second order field equations and conserved energy momentum, in D dimensions. The corresponding field equations without matter sources read[2]

$$\sum_{k=0}^{[(D-1)/2]} \alpha_k \mathcal{E}_{(k)a} = 0, \tag{1}$$

where the brackets stand for the integer part, the α_k are real constants and the $\mathcal{E}_{(k)a}$ (with $a=1,\ldots,D$) are given by

$$\mathcal{E}_{(k)a} = \left(\bigwedge_{l=1}^{k} \Omega^{a_{2l-1}a_{2l}} \right) \wedge \theta^{*}_{aa_1\cdots a_{2k}}, \tag{2}$$

which is of order k in the curvature 2 form $\Omega^a{}_b = \frac{1}{2} R^a{}_{bcd} \theta^c \wedge \theta^d$. Finally, $\theta^{*}_{a_1\cdots a_k}$ is the Hodge dual of $\theta^{a_1} \wedge \cdots \wedge \theta^{a_k}$, the basis of the space of k forms $\Omega^{(k)}(TM)$, and we thus have

$$\theta^{*}_{a_1\cdots a_k} = \frac{1}{(D-k)!} \epsilon_{a_1\cdots a_k a_{k+1}\cdots a_D} \theta^{a_{k+1}} \wedge \cdots \wedge \theta^{a_D}. \tag{3}$$

When $D=4$, Eq. (1) reduces to Einstein equations ($k=1$) with a cosmological constant α_0, whilst for $D=5$, the Gauss–Bonnet term ($k=2$) must be added. For arbitrary D, the static spherically symmetric solutions of (1) were found in Ref. 3 and their extension to planar and hyperbolic symmetry is given in Ref. 4. All these solutions belong to a one parameter family and read

[a)]Electronic mail: robin.zegers@th.u-psud.fr
[b)]UMR 7164 (CNRS, Université Paris 7, CEA, Observatoire de Paris).

$$g = -h(r)dt^2 + \frac{dr^2}{h(r)} + r^2\bar{g}_{(D-2,K)}, \tag{4}$$

where h is given as a root of a polynomial that depends on the Lovelock coupling constants α_k and on the mass parameter μ, and $\bar{g}_{(D-2,K)}$ is the $(D-2)$-dimensional metric with spherical $(K=1)$, planar $(K=0)$ or hyperbolic $(K=-1)$ symmetry and hence with isometry groups $SO(D-1)$, E_{D-2} or $SO(1,D-2)$ respectively. Notice that, in addition to these isometries, the solutions (4) also admit ∂_t as a Killing vector and this can either be space-like when $h<0$ or time-like when $h>0$, so that g is locally static. This family contains static black holes, with one or more horizons.[5] These horizons can be spherical as in the Schwarzschild case, but also planar or hyperbolic, yielding a much richer topology as for topological black holes.[6] Though solutions of the form (4) do not only describe static black holes, we shall refer to them as static Lovelock black hole solutions. Now, we shall prove the following.

Theorem: *The $\mathcal{C}^2$ solutions of the Lovelock field equations without matter (1), with spherical, planar or hyperbolic symmetry are locally isometric to the corresponding static Lovelock black hole solutions (4).*

Before proceeding with the proof, note that this theorem implies that the solutions of (1), with spherical, planar or hyperbolic symmetry are also locally static; by which we mean that they have an additional Killing vector that is locally time-like. In the specific case of Einstein–Gauss–Bonnet gravity, this theorem was already proven in Refs. 7–9.

Proof: We begin with a D-dimensional space-time with spherical, planar or hyperbolic symmetry. We thus consider a Lorentzian manifold (M,g) admitting, respectively, $SO(D-1)$, E_{D-2}, or $SO(1,D-2)$ as an isometry group with $(D-2)$-dimensional space-like orbits Σ. For all point $P \in M$, if Σ_P is the orbit of P, the tangent space T_PM can be decomposed into $T_PM = T_P\Sigma_P \oplus (T_P\Sigma_P)^\perp$. Then, let $\Sigma_P^\perp$ be the set of all the geodesics passing through P that are tangent to $(T_P\Sigma_P)^\perp$. Locally, $\Sigma_P^\perp$ is a two-dimensional submanifold of M that is perpendicular to the orbit Σ_P. Thus, on taking (∂_t, ∂_z) as a coordinate basis of $T\Sigma^\perp$ and making use of the conformal flatness of the two-dimensional submanifold $\Sigma^\perp$, one can write

$$g = A^2(t,z)(-dt^2 + dz^2) + R^2(t,z)\bar{g}_{(D-2,K)}, \tag{5}$$

where $\bar{g}_{(D-2,K)}$ is the metric over the orbits of the corresponding isometry group. Since these orbits are invariant under their isometry group, they are homogeneous and have constant induced curvature

$$\bar{\Omega}^i{}_j = K\bar{\theta}^i \wedge \bar{\theta}_j, \tag{6}$$

where $i,j=1,\ldots,D-2$, $\bar{\theta}^i$ is the orthonormal frame adapted to $\bar{g}_{(D-2,K)}$,

$$\bar{g}_{(D-2,K)} = \delta_{ij}\bar{\theta}^i \otimes \bar{\theta}^j, \tag{7}$$

and $\bar{\theta}^i \wedge \bar{\theta}^j$ is the resulting basis of the space of 2 forms on the orbits, $\Omega^{(2)}(T\Sigma)$. It will be useful to introduce the conformal coordinates

$$u = \frac{z+t}{2} \quad \text{and} \quad v = \frac{z-t}{2}, \tag{8}$$

together with the following parametrization of the metric:

$$g = e^{2\nu(u,v)}(du \otimes dv + dv \otimes du) + B^2(u,v)\bar{g}_{(D-2,K)}. \tag{9}$$

We define the associated orthonormal frame

$$\theta^\mu = e^{\nu(u,v)}du, \tag{10}$$

$$\theta^v = e^{\nu(u,v)}dv, \tag{11}$$

$$\theta^i = B(u,v)\bar{\theta}^i, \tag{12}$$

so that

$$g = 2\theta^{(u} \otimes \theta^{v)} + \delta_{ij}\theta^i \otimes \theta^j. \tag{13}$$

In this basis, indices are raised and lowered using

$$\eta_{ab} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \delta_{ij} \end{pmatrix}. \tag{14}$$

Given a torsion-free metric connection ∇, one can define a connection 1 form $\omega^a{}_b$, such that $\omega_{ab}=-\omega_{ba}$ and $d\theta^a=-\omega^a{}_b\wedge\theta^b$. From the latter, it is straightforward to derive the components of the connection 1 form. The curvature 2 form then follows from

$$\Omega^a{}_b = d\omega^a{}_b + \omega^a{}_c \wedge \omega^c{}_b, \tag{15}$$

yielding

$$\Omega^u{}_u = -\Omega^v{}_v = \frac{2\nu_{uv}}{e^{2\nu}}\theta^v \wedge \theta^u, \tag{16}$$

$$\Omega^i{}_u = \frac{1}{Be^{2\nu}}[(B_{uu} - 2B_u\nu_u)\theta^u \wedge \theta^i + B_{uv}\theta^v \wedge \theta^i], \tag{17}$$

$$\Omega^i{}_v = \frac{1}{Be^{2\nu}}[B_{uv}\theta^u \wedge \theta^i + (B_{vv} - 2B_v\nu_v)\theta^v \wedge \theta^i], \tag{18}$$

$$\Omega^i{}_j = \bar{\Omega}^i{}_j - \frac{2B_uB_v}{B^2e^{2\nu}}\theta^i \wedge \theta^j = \frac{K - 2B_uB_ve^{-2\nu}}{B^2}\theta^i \wedge \theta^j, \tag{19}$$

where $f_{u(v)}=\partial_{u(v)}f$. Now, the projection of the u (respectively, v) components of (1) onto θ^*_v (respectively, θ^*_u) yields the integrability conditions

$$P'\left[\frac{K - 2B_uB_ve^{-2\nu}}{B^2}\right](B_{uu} - 2B_u\nu_u) = 0 \tag{20}$$

$$P'\left[\frac{K - 2B_uB_ve^{-2\nu}}{B^2}\right](B_{vv} - 2B_v\nu_v) = 0, \tag{21}$$

where

$$P[X] \equiv \sum_{k=0}^{[(D-1)/2]} \frac{\alpha_k}{(D-2k-1)!}X^k \tag{22}$$

and a prime stands for a derivative with respect to the unique argument of a function. Notice how (20) and (21) factorize as a product of a polynomial, times the integrability conditions one gets from pure Einstein gravity.[10] Up to the possible vanishing of P', Einstein and Lovelock gravities thus obey the same integrability conditions and the theorem will hold. The projection of the u (respectively v) component of (1) onto θ^*_u (respectively θ^*_v) then yields a further equation

$$P\left[\frac{K-2B_uB_ve^{-2\nu}}{B^2}\right]-\frac{2}{(D-1)}P'\left[\frac{K-2B_uB_ve^{-2\nu}}{B^2}\right]\left(\frac{1}{Be^{2\nu}}\left(B_{uv}-2\frac{B_uB_v}{B}\right)+\frac{K}{B^2}\right)=0. \quad (23)$$

Finally, the i component of (1) only projects onto θ_i^* giving

$$(D-1)(D-2)P\left[\frac{K-2B_uB_ve^{-2\nu}}{B^2}\right]-\frac{2}{Be^{2\nu}}P'\left[\frac{K-2B_uB_ve^{-2\nu}}{B^2}\right]\left(\frac{(2D-5)}{B}(Ke^{2\nu}-2B_uB_v)\right.$$
$$\left.+(2D-6)B_{uv}+2B\nu_{uv}\right)+\frac{4}{B^2e^{4\nu}}P''\left[\frac{K-2B_uB_ve^{-2\nu}}{B^2}\right]\left(\left(B_{uv}-2\frac{B_uB_v}{B}+\frac{Ke^{2\nu}}{B}\right)^2\right.$$
$$\left.-(B_{uu}-2B_u\nu_u)(B_{vv}-2B_v\nu_v)\right)=0. \quad (24)$$

Equations (20), (21), (23), and (24) form the full set of Lovelock equations. From the integrability conditions (20) and (21), we distinguish two classes of solutions

- class I for which $P'[(K-2B_uB_ve^{-2\nu})/B^2]=0$ and
- class II for which $P'[(K-2B_uB_ve^{-2\nu})/B^2]\neq 0$.

For class I,

$$K-2B_uB_ve^{-2\nu}=\lambda B^2, \quad (25)$$

where λ is one of the real roots of P' and is thus a function of the α_k. On using Eq. (23), it follows that $P[\lambda]=0$, whilst Eq. (24) is trivially satisfied since (25) implies that

$$\left(B_{uv}-2\frac{B_uB_v}{B}+\frac{Ke^{2\nu}}{B}\right)^2=(B_{uu}-2B_u\nu_u)(B_{vv}-2B_v\nu_v). \quad (26)$$

The solutions thus read

$$g=\frac{2B_uB_v}{K-\lambda B^2}(du\otimes dv+dv\otimes du)+B^2\bar{g}_{(D-2,K)}, \quad (27)$$

where B is an arbitrary function of its two arguments u and v. For all harmonic B, a couple of new coordinates (t,r) can be defined on $\Sigma^\perp$, so that $r=B$ and $dt=(B_u\,du-B_v\,dv)/(K-\lambda B^2)$. In these coordinates, the solutions actually reduce to

$$g=-(K-\lambda r^2)dt^2+\frac{dr^2}{K-\lambda r^2}+r^2\bar{g}_{(D-2,K)}, \quad (28)$$

which is just a spherical, planar or hyperbolic slicing of dS_D or adS_D.[11] The fine-tuning condition $P[\lambda]=0$ must hold, so that a space-time of constant curvature λ is an acceptable solution of the Lovelock equations (1). Birkhoff's theorem thus holds for class I solutions.

For class II, the integrability conditions (20) and (21) yield

$$B(u,v)=H(F(u)+G(v)) \quad \text{and} \quad e^{2\nu(u,v)}=H'F'G', \quad (29)$$

where H, F, and G are three functions that depend only on one argument and a prime denotes the derivative of a function with respect to its single argument. To all functions F and G, one can associate a new set of coordinates $\tilde{u}=F(u)$ and $\tilde{v}=G(v)$ on $\Sigma^\perp$. Further, trading the $(\tilde{u},\tilde{v})$ conformal coordinates for time-like $\tilde{t}=\tilde{u}+\tilde{v}$ and space-like $\tilde{z}=\tilde{u}-\tilde{v}$, the metric can be rewritten as

$$g=2H'(\tilde{z})(-d\tilde{t}^2+d\tilde{z}^2)+H^2(\tilde{z})\bar{g}_{(D-2,K)}, \quad (30)$$

which has a time-like Killing vector $\partial_{\tilde{t}}$ in all neighborhood where $H'(\tilde{z})>0$ and is thus locally static. In particular, setting $r=H(\tilde{z})$, we can put it into the following form:

$$g = -h(r)dt^2 + \frac{dr^2}{h(r)} + r^2 \bar{g}_{(D-2,K)}, \tag{31}$$

where $h(r)=2H'(\tilde{z})$ solves Eq. (23),

$$P\left[\frac{K-h}{r^2}\right] - \frac{1}{D-1}P'\left[\frac{K-h}{r^2}\right]\left(\frac{h'}{r} + \frac{2(K-h)}{r^2}\right) = 0. \tag{32}$$

The latter can be integrated, yielding

$$P\left[\frac{K-h}{r^2}\right] = \frac{\mu}{r^{D-1}}, \tag{33}$$

where μ is a real constant. Let $\Lambda(\alpha_0, \ldots, \alpha_{[(D-1)/2]})$ denote a real root of $P[X]$, as a function of the Lovelock couplings, so that we can write

$$h(r) = K - r^2\Lambda\left(\alpha_0 - \frac{\mu}{r^{D-1}}, \alpha_1, \ldots, \alpha_{[(D-1)/2]}\right). \tag{34}$$

The metric (31), with h given by (34), is the static Lovelock black hole found in Refs. 3 and 4. Birkhoff's theorem thus holds for class II solutions. ■

As we shall now see, this result still holds in the presence of an abelian gauge field that is invariant under the chosen isometry group. Such a gauge field has a 1 form potential $A(u,v) = L(u,v)du + M(u,v)dv$ and therefore

$$F = dA = \frac{M_u - L_v}{e^{2\nu}}\theta^u \wedge \theta^v. \tag{35}$$

This of course implies that $dF=0$. From $d*F=0$, on the other hand, it follows that

$$F = \frac{Q}{B^{(D-2)}}\theta^u \wedge \theta^v, \tag{36}$$

where Q is a real constant. The integrability conditions (20) and (21) are unchanged, but there is no class I solution if $Q \neq 0$. We are thus left with class II, which is still free of any fine-tuning, and for which Eq. (32) becomes

$$P\left[\frac{K-h}{r^2}\right] = \frac{\mu}{r^{D-1}} - \frac{Q^2}{r^{2D-4}} \tag{37}$$

as it is now sourced by the stress-energy of the gauge field. In the end, the metric is still of the form (31), but now, h is given by

$$h(r) = K - r^2\Lambda\left(\alpha_0 - \frac{\mu}{r^{D-1}} + \frac{Q^2}{r^{2D-4}}, \alpha_1, \ldots, \alpha_{[(D-1)/2]}\right). \tag{38}$$

This is the Lovelock analog of the Reissner–Nordstrøm black hole of general relativity.[3,5] Class II solutions are the only solutions of the Lovelock equations, coupled to a non-vanishing abelian gauge field, with spherical, planar, or hyperbolic symmetry and they are locally static.

Though the set of Killing vectors of space times with spherical, planar, or hyperbolic symmetry, *a priori* reduces to the generators of their respective isometry groups $SO(D-1)$, E_{D-2}, or $SO(1,D-2)$, we have shown that the solutions of the Lovelock equations with these symmetries admit an additional Killing vector that enlarges their isometry group, so that they reduce to locally static space times. The static Lovelock black holes therefore span the whole set of solutions of the Lovelock equations without matter or in the presence of an abelian gauge field, with spherical, planar or hyperbolic symmetry.

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The Kepler problem with anisotropic perturbations

Florin Diacu[a)]
Pacific Institute for the Mathematical Sciences, Department of Mathematics and Statistics, University of Victoria, P.O. Box 3045 STN CSC, Victoria, BC, Canada V8W 3P4

Ernesto Pérez-Chavela[b)]
Departamento de Matemáticas, Universidad Autónoma Metropolitana-Iztapalapa, Apdo. 55534, México, D.F., México

Manuele Santoprete[c)]
Department of Mathematics, University of California, Irvine, Irvine, California 92697

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We study a two-body problem given by the sum of the Newtonian potential and an anisotropic perturbation that is a homogeneous function of degree $-\beta$, $\beta \geqslant 2$. For $\beta > 2$, the sets of initial conditions leading to collisions/ejections and the one leading to escapes/captures have positive measure. For $\beta > 2$ and $\beta \neq 3$, the flow on the zero-energy manifold is chaotic. For $\beta = 2$, a case we prove integrable, the infinity manifold of the zero-energy level has heteroclinic connections with the collision manifold. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1952580]

I. INTRODUCTION

In the past three centuries, celestial mechanics has stimulated the development of many branches of mathematics.[11,13] This trend continues, and even its most basic question, known as the *two-body problem* or the *Kepler problem*, still attracts the vivid interest of mathematicians and physicists, both in its classical form[1] and in more recent versions.

Among the latter are the problems raised by *quasihomogeneous* potentials, given by the sum of homogeneous functions, and problems set in *anisotropic* spaces, for which the interaction law is different in each direction of the space. For quasihomogeneous problems the terminology and the first qualitative results were introduced in the mid-1990s;[9,12,21] this potential unifies several dynamical laws, including those of Newton, Coulomb, Manev, Schwarzschild, Lennard-Jones, Birkhoff and others. The anisotropic case is more related to physics, and was initiated by Gutzwiller in the 1970s[17,18] for the quantization of classical ergodic systems. Among Gutzwiller's goals was also that of finding connections between classical and quantum mechanics. A combination of the quasihomogeneous and anisotropic aspects shows up in the anisotropic Manev problem, whose dynamics contains classical, quantum and relativistic features.[6,10,14,15]

In the present paper we consider a version of the Kepler problem, which combines two of the above characteristics, isotropy and anisotropy. The potential [see formula (3)] is the sum of the classical Keplerian potential and an anisotropic perturbation, the latter being a homogeneous function of degree $-\beta$, $\beta \geqslant 2$ that depends on a parameter $\mu > 1$ measuring the strength of the anisotropy. This is the first analysis of a *quasihomogeneous* potential that mixes isotropic and anisotropic components. For previously studied problems, all terms have been either isotropic or anisotropic. As we will see, this case has some surprising dynamical properties, often very different from the ones that characterize potentials whose terms are not mixed.

[a)]Electronic mail: diacu@math.uvic.ca
[b)]Electronic mail: epc@xanum.uam.mx
[c)]Electronic mail: msantopr@math.uci.edu

Such mixed potentials can be used to understand the dynamics of satellites around oblate planets or the motion of stars around black holes. Here, however, we are not interested in applications. Our endeavours are restricted to mathematical results.

In Sec. II we introduce the basic notations, the equations of motion, and set into evidence the symmetries of the problem. In Sec. III we begin the study of the case $\beta>2$, define the collision manifold, which is an essential qualitative tool, and perform a geometric study of the flow in the neighborhood of collisions. We classify all collision-ejection orbits and prove that the set of initial conditions leading to them has positive measure. We achieve this while studying the flow on and near the collision manifold in terms of McGehee-type coordinates.

In Sec. IV we investigate the existence of heteroclinic orbits on the collision manifold for potentials with $\mu>1$ and $\beta=2+[2/(1+2k)]$ or $\beta=2+[1/(1+k)]$. The main result of this section is that for an open and dense set of μ values, saddle-saddle connections do not exist on the collision manifold. Section V deals with capture and escape orbits in the zero-energy case. We show that the infinity manifold has two circles of normally hyperbolic equilibria, one attractive and one repelling. This proves the existence of infinitely many capture and escape orbits.

In Sec. VI we consider the case $\beta=2$, which we show to be integrable. Apparently this is quite surprising since the anisotropic Manev problem, which resembles this case except for the anisotropy of the Newtonian term, is nonintegrable.[3,15] But as we will show, the surprise element vanishes once we look at the problem in the larger context of the Hamilton-Jacobi theory. In Sec. VII we study the flow on and near the collision manifold and see that its qualitative behavior is similar to that of the anisotropic Manev problem.

In Sec. VIII we prove the existence of heteroclinic orbits connecting the collision and infinity manifolds in the zero-energy case for $\beta=2$.

In Sec. IX we consider a perturbative approach of the problem. The perturbation function of the Hamiltonian is a homogeneous function of degree $-\beta$ with $\beta>3/2$. We end the paper with Sec. X, in which we apply the Melnikov method to show that for every $\beta\neq 2,3$, the flow on the zero-energy manifold is chaotic.

II. EQUATIONS OF MOTION AND SYMMETRIES

Consider the Hamiltonian

$$H_\beta(\mathbf{q},\mathbf{p}) = \tfrac{1}{2}\mathbf{p}^2 + U_\beta(\mathbf{q}), \tag{1}$$

where $\mathbf{q}=(x,y)$ and $\mathbf{p}=(p_x,p_y)$. The equations of motion are

$$\dot{\mathbf{q}} = \mathbf{p},$$

$$\dot{\mathbf{p}} = -\nabla U_\beta(\mathbf{q}), \tag{2}$$

where U_β is a potential of the form

$$U_\beta(x,y) = -\frac{1}{\sqrt{x^2+y^2}} - \frac{b}{(\mu x^2+y^2)^{\beta/2}}, \tag{3}$$

with the constants $\beta\geqslant 2$, $\mu\geqslant 1$, and $b>0$. The symmetries of (2) are given by the following analytic diffeomorphisms in the extended phase space:

$$\text{Id:}\quad (x,y,p_x,p_y,t)\to(x,y,p_x,p_y,t),$$

$$S_0\text{:}\quad (x,y,p_x,p_y,t)\to(x,y,-p_x,-p_y,-t),$$

$$S_1\text{:}\quad (x,y,p_x,p_y,t)\to(x,-y,-p_x,p_y,-t),$$

$$
\begin{aligned}
S_2&: \quad (x,y,p_x,p_y,t) \to (-x,y,p_x,-p_y,-t),\\
S_3&: \quad (x,y,p_x,p_y,t) \to (-x,-y,-p_x,-p_y,t),\\
S_4&: \quad (x,y,p_x,p_y,t) \to (-x,y,-p_x,p_y,t),\\
S_5&: \quad (x,y,p_x,p_y,t) \to (x,-y,p_x,-p_y,t),\\
S_6&: \quad (x,y,p_x,p_y,t) \to (-x,-y,p_x,p_y,-t),
\end{aligned}
\tag{4}
$$

where Id is the identity. These diffeomorphisms form a group that is isomorphic to $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2$.[14,22] Invariance under these symmetries implies that if $\gamma(t)$ is a solution of (2), then also $S_i(\gamma(t))$ is a solution for $i\in\{0,1,2,3,4,5,6\}$.

III. THE COLLISION MANIFOLD FOR $\beta>2$

We will further express the equations of motion in McGehee-type coordinates,[8,20] which are suitable for understanding the motion near collision. The transformations are given step by step as follows. Take

$$
\begin{aligned}
r &= \sqrt{x^2+y^2},\\
\theta &= \arctan\frac{y}{x},\\
\tilde{v} &= r\dot{r} = (xp_x + yp_y),\\
\tilde{u} &= r^2\dot{\theta} = (xp_y - yp_x),
\end{aligned}
\tag{5}
$$

rescale $\tilde{v}$ and $\tilde{u}$ by

$$
v = r^{(\beta-2)/2}\tilde{v}, \quad u = r^{(\beta-2)/2}\tilde{u},
$$

and then rescale the time variable using the transformation

$$
\frac{\mathrm{d}t}{\mathrm{d}\tau} = r^{\beta/2+1}.
$$

The equations of motion take the form

$$
\begin{aligned}
r' &= rv,\\
v' &= \frac{\beta-2}{2}v^2 + r^{\beta-1} + 2hr^{\beta} - \frac{b(\beta-2)}{\Delta^{\beta/2}},\\
\theta' &= u,\\
u' &= \frac{\beta-2}{2}uv + \frac{b\beta(\mu-1)\sin 2\theta}{2\Delta^{(\beta+2)/2}},
\end{aligned}
\tag{6}
$$

where $\Delta=\mu\cos^2\theta+\sin^2\theta$ and the prime denotes differentiation with respect to the independent time variable τ. For simplicity, we keep the same notation for the dependent variables.

In these coordinates, the energy integral $H_\beta=h$ [see Eq. (1)], takes the form

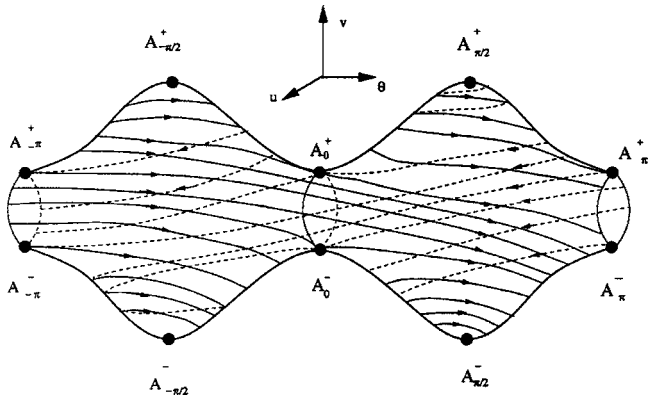

FIG. 1. The collision manifold C for $\beta>2$.

$$u^2+v^2-2r^{\beta-1}-\frac{2b}{\Delta^{\beta/2}}=2hr^{\beta}. \tag{7}$$

We define the collision manifold (see Fig. 1) as

$$C=\left\{ (r,v,\theta,u)\middle|\ r=0,\ u^2+v^2=\frac{2b}{\Delta^{\beta/2}}\right\}. \tag{8}$$

Notice that C is homeomorphic to a torus. The flow on this manifold is given by the system

$$v'=\frac{\beta-2}{2}(-u^2),$$

$$\theta'=u,$$

$$u'=\frac{\beta-2}{2}uv+\frac{b\beta(\mu-1)\sin 2\theta}{2\Delta^{(\beta+2)/2}}. \tag{9}$$

We can now prove the following results.

Proposition 3.1: All the equilibrium points of system (6) lie on the collision manifold C and are given by

$$r=0,\quad v=\pm\sqrt{\frac{2b}{\Delta^{\beta/2}}},\quad \theta=0,\ \pi/2,\ 3\pi/2,\quad u=0.$$

Proof: It is obvious that the above points are equilibria for the flow defined by (6). To check that there are no equilibria outside the collision manifold, from the first equation in (6) with $r\neq 0$ we see that $v=0$ and from the third equation in (6) that $u=0$. So, if there are equilibrium points with $r\neq 0$, they must be on the zero velocity curve (ZVC); substituting these values in (7), we obtain that the ZVC exists just for $h<0$, it is given by

$$r^{\beta-1}+\frac{b}{\Delta^{\beta/2}}=-hr^{\beta}. \tag{10}$$

Solving the equation $v'=0$ in (6), we are led to

$$r^{\beta-1} - \frac{b(\beta-2)}{\Delta^{\beta/2}} = -2hr^{\beta}. \tag{11}$$

But (10) and (11) have no common solutions for $h<0$, therefore there are no equilibria outside the collision manifold. □

Proposition 3.2: The flow on the collision manifold C is gradientlike (i.e., increasing) with respect to the $(-v)$*-coordinate*.

Proof: Since $\beta>2$, we see from the first equation in (9) that $v'<0$ except at equilibria, therefore the flow on C increases with respect to $-v$, so is gradientlike relative to it. □

To match the sign of v and the value of θ, we denote the equilibria on C by $A_0^{\pm}$, $A_{\pi/2}^{\pm}$, $A_{\pi}^{\pm}$, and $A_{3\pi/2}^{\pm}$, respectively. Observe that $\Delta(0)=\Delta(\pi)=\mu$ and $\Delta(\pi/2)=\Delta(3\pi/2)=1$. With this notation, we can describe the following properties of the flow.

Theorem 3.1: *On the collision manifold C, the equilibria* $A_0^{\pm}$ *and* $A_{\pi}^{\pm}$ *are saddles,* $A_{\pi/2}^{+}$ *and* $A_{3\pi/2}^{+}$ *are sources and* $A_{\pi/2}^{-}$ *and* $A_{3\pi/2}^{-}$ *are sinks. Outside C, the equilibria* A_0^{+}, A_{π}^{+}, $A_{\pi/2}^{+}$, *and* $A_{3\pi/2}^{+}$ *have a local one-dimensional unstable analytic manifold, whereas* A_0^{-}, A_{π}^{-}, $A_{\pi/2}^{-}$, *and* $A_{3\pi/2}^{-}$ *have a local one-dimensional stable analytic manifold. All these equilibrium points are hyperbolic*.

Proof: Consider the function

$$F(r,v,\theta,u) = u^2 + v^2 - 2r^{\beta-1} - \frac{2b}{\Delta^{\beta/2}} - 2hr^{\beta} = 0.$$

According to Eq. (7), the surface of constant energy M_h defined by the equation

$$F(r,\theta,v,u) = 0$$

is a three-dimensional manifold. At every point B of M_h, the tangent space is given by

$$T_B F = \{\,(r,v,\theta,u) \,|\, \nabla F(B)\cdot(r,v,\theta,u) = 0\}.$$

At any equilibrium point A, the tangent space is defined by

$$T_A F = \{\,(r,\theta,v,u) | v = 0\}.$$

A straightforward computation shows that at the equilibria $A_0^{\pm}$ and $A_{\pi}^{\pm}$ the linearized system corresponding to (6) has the matrix

$$\begin{bmatrix} \pm\sqrt{\dfrac{2b}{\mu^{\beta/2}}} & 0 & 0 & 0 \\ 0 & (\beta-2)\pm\left(\sqrt{\dfrac{2b}{\mu^{\beta/2}}}\right) & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & \dfrac{b\beta(\mu-1)}{\mu^{\beta+2/2}} & \pm\dfrac{(\beta-2)}{2}\left(\sqrt{\dfrac{2b}{\mu^{\beta/2}}}\right) \end{bmatrix},$$

therefore the linear part of the vector field (6) restricted to $T_{A_{0,\pi}}^{+,-}$ is given by

$$L = \begin{pmatrix} \pm\sqrt{\dfrac{2b}{\mu^{\beta/2}}}r \\ 0 \\ u \\ \dfrac{b\beta(\mu-1)}{\mu^{\beta+2/2}}\theta + \pm\dfrac{(\beta-2)}{2}\left(\sqrt{\dfrac{2b}{\mu^{\beta/2}}}\right)u \end{pmatrix}.$$

As a basis for the tangent space $T_{A_{0,\pi}}^{+,-}$, we take the vectors

$$\xi_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \xi_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad \xi_3 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \tag{12}$$

The representation of the linear part L relative to this basis is given by the matrix

$$J^* = \begin{pmatrix} \pm\sqrt{\dfrac{2b}{\mu^{\beta/2}}} & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \dfrac{b\beta(\mu-1)}{\mu^{\beta+2/2}} & \pm\dfrac{(\beta-2)}{2}\left(\sqrt{\dfrac{2b}{\mu^{\beta/2}}}\right) \end{pmatrix}.$$

The characteristic polynomial shows that all eigenvalues are real and that the equilibrium is a saddle in each case.

At the equilibria $A^{\pm}_{\pi/2}$ and $A^{\pm}_{3\pi/2}$, the same linearized system has the matrix

$$\begin{bmatrix} \pm\sqrt{2b} & 0 & 0 & 0 \\ 0 & (\beta-2)\pm(\sqrt{2b}) & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -b\beta(\mu-1) & \pm\dfrac{(\beta-2)}{2}(\sqrt{2b}) \end{bmatrix}.$$

Using the vectors given in (12) as a basis for the tangent space $T^{+,-}_{A_{\pi/2,3\pi/2}}$, the linear part is given by the matrix

$$J^* = \begin{pmatrix} \pm\sqrt{2b} & 0 & 0 \\ 0 & 0 & 1 \\ 0 & b\beta(\mu-1) & \pm\dfrac{(\beta-2)}{2}(\sqrt{2b}) \end{pmatrix}.$$

The eigenvalues at $A^{+}_{\pi/2}$ and at $A^{+}_{3\pi/2}$ are

$$\sqrt{2b}, \quad \frac{(\beta-2)}{2}(\sqrt{2b}) + \sqrt{\frac{b}{2}[(\beta-2)^2 - 8\beta(\mu-1)]},$$

and

$$\frac{(\beta-2)}{2}(\sqrt{2b}) - \sqrt{\frac{b}{2}[(\beta-2)^2 - 8\beta(\mu-1)]}.$$

This means that all of them are positive or have positive real part. At $A^{-}_{\pi/2}$ and $A^{-}_{3\pi/2}$ the eigenvalues are all negative or have negative real part. □

Corollary 3.1: The set of initial conditions leading to collisions or ejections has positive measure.

Proof: The equilibrium points $A^{-}_{\pi/2}$ ($A^{+}_{\pi/2}$) and $A^{-}_{3\pi/2}$ ($A^{+}_{3\pi/2}$) are sinks (sources) for the global flow, therefore their basin of attraction (repulsion) is a three-dimensional set of collision (ejection) orbits. □

Remark 3.1. If $0<\mu<(\beta+2)^2/8\beta$, all the eigenvalues are real and positive. If $\mu>(\beta+2)^2/8\beta$, there are two complex eigenvalues with positive real part, so some orbits have the spiraling property, i.e., engage into an infinite spin. For example, to have spiraling orbits in the

case $\beta=3$, it is necessary that $\mu>\frac{25}{24}$. Therefore when μ is sufficiently close to 1, no spiraling orbits exist.

Remark 3.2: The inequalities in Remark 3.1 do not depend on the parameter b.

Remark 3.3: For μ close enough to 1, though the set of collision orbits has positive measure, there are no spiralling orbits.

IV. SADDLE-SADDLE CONNECTIONS ON C

Using ideas similar to those found in Ref. 7, we will further study the existence of saddle-saddle connections on C for $\mu>1$ and β of the form

$$\beta=2+\frac{2}{1+2k} \quad \text{and} \quad \beta=2+\frac{1}{1+k},$$

k integer, $k\neq-1$. The reason for choosing these values of β will be clarified below. In the proof we restrict ourselves to the cases $\beta=3,4$. This is because the method requires the computation of an integral for each value of k, and each integral must be computed separately. But the principle is the same for every such k.

To show that there are no heteroclinic connections is sufficient to prove that the stable and unstable manifolds of corresponding fixed points miss each other. We will show that this holds true for most values of $\mu>1$.

It is now convenient to introduce different coordinates on C. Since C is homeomorphic to a torus, we can describe the flow using angle variables. With the transformations

$$u=\frac{\sqrt{2b}}{\Delta^{\beta/4}}\sin\psi,$$

$$v=\frac{\sqrt{2b}}{\Delta^{\beta/4}}\cos\psi, \tag{13}$$

we can rewrite the flow on the equations of motion (9) on C as

$$\begin{aligned}\theta'&=\frac{\sqrt{2b}}{\Delta^{\beta/4}}\sin\psi,\\ \psi'&=\frac{\beta-2}{2}\frac{\sqrt{2b}}{\Delta^{\beta/4}}\sin\psi+\frac{d}{d\tau}\left(\frac{\sqrt{2b}}{\Delta^{\beta/4}}\right)\frac{\Delta^{\beta/4}}{\sqrt{2b}}\cot\psi,\end{aligned} \tag{14}$$

where

$$\frac{d}{d\tau}\left(\frac{\sqrt{2b}}{\Delta^{\beta/4}}\right)=\frac{\beta(\mu-1)\sqrt{2b}}{4\Delta^{(\beta+4)/4}}\sin 2\theta. \tag{15}$$

The equilibrium points in the variables (θ,ψ) are $A^-_{\pm\pi/2}=(\pm\pi/2,0)$, $A^+_{\pm\pi/2}=(\pm\pi/2,\pi)$, $A^-_0=(0,0)$, $A^+_0=(0,\pi)$, $A^-_\pi=(\pi,0)$, and $A^+_\pi=(\pi,\pi)$.

Notice that if $\mu=1$ (the isotropic case), the collision manifold is a torus for which the upper and lower circles C^+ and C^- consist of fixed points. The equations (14) take the form

$$\theta'=\sqrt{2b}\sin\psi,$$

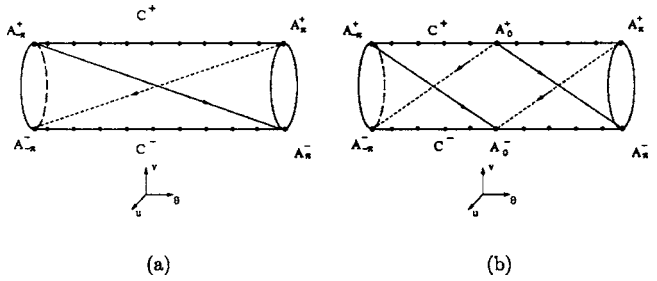

FIG. 2. The collision manifold and the heteroclinic connections for (a) $\mu=1$, $\beta=3$ and for (b) $\mu=1$, $\beta=4$.

$$\psi' = \frac{\beta-2}{2}\sqrt{2b}\sin\psi. \tag{16}$$

It is easy to see that in this case there are heteroclinic orbits that connect the critical points A_0^+ to A_π^- and A_π^+ to A_0^- when

$$\beta = 2 + \frac{2}{1+2k},$$

k integer, $k\neq -1$, and connect the critical points $A_{-\pi}^+$ to A_π^- and A_π^+ to $A_{-\pi}^-$ when

$$\beta = 2 + \frac{1}{1+k},$$

k integer, $k\neq -1$.

Figure 2(a) depicts the collision manifold for $\mu=1$ and $\beta=3$ and the heteroclinic connections on it, while Fig. 2(b) does the same for $\mu=1$ and $\beta=4$.

In the following we will show that if $\mu-1=\epsilon>0$ and small, such saddle-saddle connections are broken and the same result holds for an open dense set of $\mu-1=\epsilon>0$.

Theorem 4.2: *For $\beta=3$ and for an open and dense set of real numbers $\mu>1$, the unstable manifolds at $A_{-\pi}^-$ and A_π^- miss the stable manifolds at A_π^+ and $A_{-\pi}^+$. For $\beta=4$ and for an open and dense set of real numbers $\mu>1$, the unstable manifolds at A_0^+ and $A_{-\pi}^+$ miss the stable manifolds at A_π^- and A_0^-.*

Proof: Dividing the first of equations (14) by the second one we have

$$\frac{\mathrm{d}\psi}{\mathrm{d}\theta} = \frac{d}{\mathrm{d}\tau}\left(\frac{\sqrt{2b}}{\Delta^{\beta/4}}\right)\frac{\Delta^{\beta/2}}{2b}\frac{\cos\psi}{\sin^2\psi} + \left(\frac{\beta-2}{2}\right) = F_\beta(\theta,\psi,\epsilon), \tag{17}$$

where $\epsilon=\mu-1$ and $\Delta=1+\epsilon\cos^2\theta$.

First consider $\beta=3$, and the unstable manifolds $W_3^u(-\pi,0)=W_3^u(\pi,0)$. When $\epsilon=0$, $W_3^s(\pi,\pi)$ matches $W_3^u(-\pi,0)$. Consider the branch of $W_3^u(-\pi,0)$ which contains $(0,\pi/2)$. This curve lies along the line

$$-2\psi+\theta=-\pi. \tag{18}$$

When ϵ varies, this branch of the unstable manifold $W_3^u(-\pi,0)$ varies smoothly on C. Let $\zeta^3(\theta,\epsilon)$ denote the ψ-coordinate of this curve, satisfying $\zeta^3(-\pi,\epsilon)=0$.

Now let $\beta=4$ and $W_4^u(-\pi,0)=W_4^u(\pi,0)$. When $\epsilon=0$, $W_4^s(-\pi,0)$ matches $W_4^u(0,\pi)$. Consider the branch of $W_4^u(-\pi,0)$ that contains $(-\pi/2,\pi/2)$. This curve lies along the line

$$-2\psi+2\theta=-2\pi. \tag{19}$$

As ϵ varies, this branch of $W_4^u(-\pi,0)$ varies smoothly on C. Let $\zeta^4(\theta,\epsilon)$ denote the ψ-coordinate of this curve, satisfying $\zeta^4(-\pi,\epsilon)=0$. Now we need the following result, which we will prove at the end of this demonstration.

Lemma 4.1: With the above notations, $(\partial/\partial\epsilon)\zeta^3(0,0)=3/4\pi>0$ *and* $(\partial/\partial\epsilon)\zeta^4(-\pi/2,0)=\pi/2>0$.

From this lemma it follows that $\zeta^3(0,\epsilon)>0$ and $\zeta^4(0,\epsilon)>0$ for $\epsilon>0$ small. Thus, it is easy to show that $v_{1+\epsilon}(0,\zeta^l(0,\epsilon))>0$, where $l=3,4$. Equations (17) are reversed by the transformation

$$(\theta,\psi)\to(-\theta,\pi-\psi). \tag{20}$$

If $\beta=3$, the unstable manifold through $(-\pi,0)$ is mapped onto the stable manifold through (π,π). Hence the stable manifold intersects the line $\theta=0$ at some point $(0,\psi_0)$ such that $v_{1+\epsilon}(0,\psi_0)<0$. Consequently the stable manifold misses the unstable one for $\epsilon>0$ small.

Moreover the stable and unstable manifolds intersect only for a discrete set of ϵ, since they vary analytically with ϵ.

Furthermore equations (17) are reversed by the transformation

$$(\theta,\psi)\to(-\theta-\pi,\pi-\psi). \tag{21}$$

If $\beta=4$, the unstable manifold through $(-\pi,0)$ is mapped onto the stable manifold through $(0,\pi)$. Hence the stable manifold intersects the line $\theta=0$ at some point $(0,\psi_0)$ such that $v_{1+\epsilon}(0,\psi_0)<0$ and the stable manifold misses the unstable one for $\epsilon>0$ small.

Moreover the stable and unstable manifolds intersect only for a discrete set of ϵ, since they vary analytically with ϵ.

Similar arguments can be applied to the remaining stable and unstable manifolds. This concludes the proof of Proposition 4.1. □

Proof of Lemma 4.1: Observe that ζ^β satisfies the equation

$$\zeta^\beta(\theta,\epsilon)=\int_{-\pi}^{\theta}F_\beta(\eta,\zeta^\beta(\eta),\epsilon)\mathrm{d}\eta, \tag{22}$$

where F_β is given by (17). For ϵ small we can write

$$\zeta^\beta=\zeta_0^\beta(\theta)+\epsilon\zeta_1^\beta(\theta)+O(\epsilon^2). \tag{23}$$

We also have

$$\begin{aligned}\zeta_0^3(\theta)&=(1/2)\theta+\pi/2,\\ \zeta_0^4(\theta)&=\theta+\pi.\end{aligned} \tag{24}$$

To compute $\zeta_1(\theta)$, we can use the Taylor expansion of (22) with respect to ϵ and find

$$\zeta_1^\beta(\theta)=\int_{-\pi}^{\theta}\left(\frac{\partial}{\partial\epsilon}F_\beta(\eta,\zeta_0^\theta(\eta),0)+\frac{\partial}{\partial\psi}F_\beta(\eta,\zeta_0^\beta(\eta),0)\zeta_1^\beta(\eta)\right)\mathrm{d}\eta. \tag{25}$$

Standard computations show that

$$\frac{\partial}{\partial\epsilon}F_\beta(\eta,\zeta_0^\beta(\eta),\epsilon)=\frac{\beta}{2}\frac{\cos(\eta)\sin(\eta)\cos(\zeta_0^\beta(\eta))}{\sin(\zeta_0^\beta(\eta))}+O(\epsilon) \tag{26}$$

and that

$$\frac{\partial}{\partial \psi} F_\beta(\eta, \zeta_0^\beta(\eta), \epsilon) = O(\epsilon). \tag{27}$$

We can now compute $\zeta_1^\beta(\theta)$ as follows:

$$\zeta_1^\beta(\theta) = \int_{-\pi}^{\theta} \left(\frac{\partial}{\partial \epsilon} F_\beta + \frac{\partial}{\partial \psi} F_\beta \zeta_1 \right) \mathrm{d}\eta = \frac{\beta}{2} \int_{-\pi}^{\theta} \frac{\cos(\eta)\sin(\eta)\cos(\zeta_0^\beta(\eta))}{\sin(\zeta_0^\beta(\eta))} \mathrm{d}\eta. \tag{28}$$

When $\beta=3$,

$$\zeta_1^3(\theta) = \frac{3}{2} \int_{-\pi}^{\theta} \frac{\cos(\eta)\sin(\eta)\cos(\eta/2+\pi/2)}{\sin(\eta/2+\pi/2)} \mathrm{d}\eta = -\frac{9}{2} \cos\left(\frac{1}{2}\theta\right) \sin\left(\frac{1}{2}\theta\right) + \frac{3}{4}\theta + 3\left(\cos\left(\frac{1}{2}\theta\right)\right)^3 \sin\left(\frac{1}{2}\theta\right) + \frac{3}{4}\pi \tag{29}$$

and, in particular, for $\theta=0$, we have

$$\zeta_1^3(0) = \frac{3}{4}\pi = \frac{\partial}{\partial \epsilon} \zeta^3(0,0). \tag{30}$$

When $\beta=4$,

$$\zeta_1^4(\theta) = \frac{3}{2} \int_{-\pi}^{\theta} \frac{\cos(\eta)\sin(\eta)\cos(\eta+\pi)}{\sin(\eta+\pi)} \mathrm{d}\eta = \cos(\theta)\sin(\theta) + \theta + \pi \tag{31}$$

and, in particular, for $\theta=-\pi/2$, we have

$$\zeta_1^4\left(-\frac{\pi}{2}\right) = \frac{\pi}{2} = \frac{\partial}{\partial \epsilon} \zeta^4\left(-\frac{\pi}{2}, 0\right). \tag{32}$$

This concludes the proof of Lemma 4.1. □

V. ESCAPE AND CAPTURE SOLUTIONS FOR $h=0$

We will further study escape (capture) solutions, i.e., the ones for which $r \to \infty$ when $t \to \infty$ ($t \to -\infty$). From the energy relation (7), we can see that for $h<0$, the radial coordinate r is bounded by the zero velocity curve ($u=0, v=0$), so escapes exist only for $h \geqslant 0$. We restrict our analysis to the case $h=0$, in which the energy relation (7) takes the form

$$u^2 + v^2 = 2r^{\beta-1} + \frac{2b}{\Delta^{\beta/2}}. \tag{33}$$

With the transformations

$$\rho = r^{-1}, \quad \bar{v} = \rho^{(\beta-1)/2} v, \quad \bar{u} = {}^{(\beta-1)/2} u,$$

the energy relation becomes

$$\bar{u}^2 + \bar{v}^2 = 2 + \frac{2b}{\Delta^{\beta/2}} \rho^{\beta-1}. \tag{34}$$

We define the *infinity manifold* I_0 as

$$I_0 = \{ (\rho, \bar{v}, \theta, \bar{u}) \mid \rho = 0,\ \bar{u}^2 + \bar{v}^2 = 2 \}. \tag{35}$$

Since the variable $\theta \in S^1$, the infinity manifold I_0 is a torus.

Remark 5.4: The infinity manifold I_0 is independent of the parameter β.

After rescaling the time τ with the transformation $\mathrm{d}\tau=\rho^{(\beta-1)/2}\,\mathrm{d}s$, the equations (6) take the form

$$\frac{\mathrm{d}\rho}{\mathrm{d}s}=-\rho\bar{v},$$

$$\frac{\mathrm{d}\bar{v}}{\mathrm{d}s}=-\frac{1}{2}\bar{v}^2=\frac{b(\beta-2)}{\Delta^{\beta/2}}\rho^{\beta-1}+1,$$

$$\frac{\mathrm{d}\theta}{\mathrm{d}s}=\bar{u},$$

$$\frac{\mathrm{d}\bar{u}}{\mathrm{d}s}=-\frac{1}{2}\bar{u}\bar{v}+\frac{b\beta(\mu-1)\sin 2\theta}{2\Delta^{\beta+2/2}}\rho^{\beta-1}. \tag{36}$$

Equations (34) and (36) are well defined on the boundary $\rho=0$. Consequently, the phase space of the coordinates $(\rho,\bar{v},\theta,\bar{u})$ can be analytically extended to contain the manifold I_0. Since $\mathrm{d}\rho/\mathrm{d}s=0$ for $\rho=0$, this manifold is invariant under the flow.

Proposition 5.3: All the equilibrium solutions of the flow given by (36) lie on the infinity manifold I_0 and they form two circles of equilibria given by

$$\rho=0,\quad \bar{v}=\pm\sqrt{2},\quad \theta\in S^1,\quad \bar{u}=0.$$

Proof: It is obvious that any point of the above circles is an equilibrium orbit. If $\bar{v}=0$ in (36), by the third equation we have that $\bar{u}=0$, but this is a contradiction with the energy relation given by (34). This proves the result. □

On the infinity manifold I_0, the equations of motion take the form

$$\frac{\mathrm{d}\bar{v}}{\mathrm{d}s}=-\tfrac{1}{2}\bar{v}^2+1=\bar{u}^2/2,$$

$$\frac{\mathrm{d}\theta}{\mathrm{d}s}=\bar{u},$$

$$\frac{\mathrm{d}\bar{u}}{\mathrm{d}s}=-\tfrac{1}{2}\bar{u}\bar{v}. \tag{37}$$

We can now prove the following properties.

Proposition 5.4: The flow on I_0 is gradientlike with respect to the $\bar{v}$-coordinate.

Proof: From the first equation in (37), we obtain that $\bar{v}'>0$ except at equilibria, which proves the gradientlike property. □

In agreement with the sign of $\bar{v}$, and by similarity with the collision manifold for $\mu=1$ studied in Sec. IV, we also denote the equilibria on I_0 as $C^{\pm}$, respectively.

Theorem 5.3: *On the infinity manifold I_0, the two circles of equilibria C^+ and C^- are normally hyperbolic. C^+ corresponds to a sink, whereas C^- corresponds to a source. The escape orbits are the ones having C^+ as an ω-limit, whereas capture orbits are the ones having C^- as an α-limit.*

Proof: The proof is similar to the one of Theorem 3.1, so we will only sketch the main steps. From Eq. (34), we define

$$G(\rho,\bar{v},\theta,\bar{u}) = \bar{u}^2 + \bar{v}^2 - 2 - \frac{2b}{\Delta^{\beta/2}}\rho^{\beta-1} = 0.$$

Then I_∞ is the three-dimensional manifold given by $G^{-1}(0)$. To study the tangent spaces to this manifold at the equilibria, we use as a basis the same vectors (12). Then the linear representation of the vector field (36) at any equilibrium C^+ and C^- is given by the matrix

$$\begin{pmatrix} -v_0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & \dfrac{-v_0}{2} \end{pmatrix}.$$

Notice that for C^+, $v_0=\sqrt{2}$ and for C^-, $v_0=-\sqrt{2}$. In the former case two eigenvalues are negative and one is zero, whereas in the latter case two eigenvalues are positive and one is zero. This completes the proof of the normal hyperbolicty and shows the existence of infinitely many escape orbits and capture orbits. □

The next result, which is a direct consequence of Theorem 5.3, characterizes the flow on the infinity manifold.

Corollary 5.2: For $h=0$, the infinity manifold I_0 is foliated by heteroclinic orbits between C^- to C^+.

The flow on I_0 given by Eqs. (37) is easy to draw. Because on I_0, $\bar{u}^2+\bar{v}^2=2$, we can introduce the angular variable ψ with the transformation

$$\bar{u} = \sqrt{2}\cos\psi, \quad \bar{v} = \sqrt{2}\sin\psi.$$

On I_0, the equations of motion take the form

$$\dot{\psi} = -2\sqrt{2}\cos\psi, \quad \dot{\theta} = \sqrt{2}\cos\psi.$$

From here we obtain that

$$\frac{d\psi}{d\theta} = -2.$$

On I_0 we can also study the projection of the flow on the $v-\theta$ plane, which is given by

$$\frac{dv}{d\theta} = \frac{\sqrt{2-v^2}}{2},$$

whose solution is $v(\theta)=\sqrt{2}\sin[(\theta+k)/2]$, where k is a constant determined by the initial condition.

VI. INTEGRABILITY FOR $\beta=2$

We will further study the problem for $\beta=2$ and deal with a Hamiltonian (1) of the form

$$H_2 = \frac{1}{2}\mathbf{p}^2 - \frac{1}{\sqrt{x^2+y^2}} - \frac{b}{\mu x^2+y^2}. \tag{38}$$

With the notation $\epsilon=\mu-1$, the Hamiltonian expressed in polar coordinates becomes

$$H_2 = \frac{p_r^2}{2} + \frac{p_\theta^2}{2r^2} - \frac{1}{r} - \frac{b}{r^2(1+\epsilon\cos^2(\theta))}. \tag{39}$$

The corresponding system is integrable since it admits another first integral independent of the Hamiltonian, namely

$$G = \frac{p_\theta^2}{2} - \frac{b}{1 + \epsilon \cos^2(\theta)}. \tag{40}$$

Indeed,

$$\{H_2, G\} = \frac{\partial H_2}{\partial \theta}\frac{\partial G}{\partial p_\theta} - \frac{\partial H_2}{\partial p_\theta}\frac{\partial G}{\partial \theta}, \tag{41}$$

and since

$$\frac{\partial H_2}{\partial \theta} = -\frac{\epsilon b \sin(2\theta)}{r^2(1 + \epsilon \cos^2(\theta))^2}, \quad \frac{\partial H_2}{\partial p_\theta} = \frac{p_\theta}{r^2} \tag{42}$$

and

$$\frac{\partial G}{\partial \theta} = -\frac{\epsilon b \sin(2\theta)}{(1 + \epsilon \cos^2(\theta))^2}, \quad \frac{\partial G}{\partial p_\theta} = p_\theta \tag{43}$$

the Poisson's bracket is $\{H_2, G\}=0$, also G and H_2 are linearly independent.

The existence of the integral G is not surprising. Indeed it is well known[19] that given the Hamiltonian

$$\bar{H} = \frac{p_r^2}{2} + \frac{p_\theta^2}{2r^2} + U(r, \theta), \tag{44}$$

the corresponding Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + \bar{H}\left(r, \theta; \frac{\partial S}{\partial r}, \frac{\partial S}{\partial \theta}\right) = 0 \tag{45}$$

[where $S=S(r, \theta, t)$ is the action expressed as function of the coordinates and time, $\partial S/\partial r=p_r$ and $\partial S/\partial \theta=p_\theta$] can be solved by separation of variables if the potential energy is of the form

$$U = a(r) + \frac{b(\theta)}{r^2}. \tag{46}$$

Since the Hamiltonian is time independent we take $S(r, \theta, t)=S_0(r, \theta)-Et$ (where E is a constant), and the Hamilton-Jacobi equation for S_0 becomes

$$\frac{1}{2}\left(\frac{\partial S}{\partial r}\right)^2 + a(r) + \frac{1}{2r^2}\left[\left(\frac{\partial S}{\partial \theta}\right)^2 + 2b(\theta)\right] = E. \tag{47}$$

Looking for a solution of the form

$$S_0 = S_1(r) + S_2(\theta), \tag{48}$$

we find for S_1 and S_2 the equations

$$\left(\frac{dS_2}{d\theta}\right)^2 + 2b(\theta) = 2G,$$

$$\frac{1}{2}\left(\frac{dS_1}{dr}\right)^2 + a(r) + \frac{2G}{2r^2} = E, \tag{49}$$

which define two independent integrals. Solving these equations leads to a solution of the Hamilton-Jacobi equations and thus to a general solution of the equations of motion. The above technique applies to the Hamiltonian H_2 and to the additional integral G.

This approach also shows that the Hamiltonian system given by H_2 is integrable by quadratures. The same conclusion can be reached by directly applying the Liouville-Arnold theorem.[2]

VII. THE COLLISION MANIFOLD FOR $\beta=2$

For $\beta=2$ the equation of motion (6) in McGehee coordinates can be written as

$$r' = rv,$$

$$v' = 2r^2h + r,$$

$$\theta' = u,$$

$$u' = \epsilon b \sin(2\theta)\Delta^{-2}, \tag{50}$$

where the prime denotes differentiation with respect to τ and $\Delta=1+\epsilon\cos^2(\theta)$. In McGehee coordinates, the energy relation takes the form

$$u^2 + v^2 - 2r - 2b\Delta^{-1} = 2r^2h, \tag{51}$$

where h is the energy constant. The first integral G can be written as

$$g = \tfrac{1}{2}(u^2 - 2b\Delta^{-1}), \tag{52}$$

where g is also constant along orbits.

The vector field (50) is analytic on the boundary $r=0$, since r no longer occurs in the denominators of the vector field. The collision manifold reduces to

$$C = \{(r,\theta,v,u): r = 0,\ u^2 + v^2 = 2b\Delta^{-1}\}. \tag{53}$$

This shows that C is homeomorphic to a torus. The restriction of equations (50) to C yields the system

$$v' = 0,$$

$$\theta' = u,$$

$$u' = \epsilon b\Delta^{-2}\sin 2\theta. \tag{54}$$

All nonequilibrium orbits on C are periodic. Comparing the collision manifold and vector field above with the corresponding ones in Ref. 6, we see that the collision manifold and the flow for $\beta=2$ are identical to the ones of the anisotropic Manev problem.

VIII. HETEROCLINIC ORBITS FOR $\beta=2$ AND $h=0$

The main goal of this section is to study the infinity manifold for $h=0$ and the heteroclinic orbits that connect the collision and infinity manifold. First notice that for $h<0$ the motion is bounded and therefore there is no infinity manifold. More precisely, we have the following result.

Proposition 8.5: If $h<0$ the motion is bounded by the zero velocity curve

$$r_0 = \frac{-1+\sqrt{1-4hb\Delta^{-1}}}{2h}, \quad v=0,\ \theta,\ u=0. \tag{55}$$

Proof: Obviously $u=0$ and $v=0$ if and only if $u^2+v^2=0$. Also $v=0$ implies $r'=0$. Using the energy relation we can draw the conclusion that $u^2+v^2=0$ if and only if $2r^2h+2r+2b\Delta^{-1}=0$. This quadratic equation has the solutions

$$r = \frac{-1 \pm \sqrt{1 - 4hb\Delta^{-1}}}{2h}. \tag{56}$$

Since $r \geqslant 0$ and $h < 0$ the only valid solution r_0 is the one with the minus sign. This shows that (55) is the zero velocity curve. The fact that the motion is bounded by this curve follows from the fact that if $r > r_0$ then $u^2 + v^2 < 0$. □

To describe the behavior of the solution at infinity we need to study the equations (36) with $\beta = 2$ and $h = 0$, that is

$$\dot{\rho} = -\rho\bar{v},$$

$$\dot{\bar{v}} = -\tfrac{1}{2}\bar{v}^2 + 1,$$

$$\dot{\theta} = \bar{u},$$

$$\dot{\bar{u}} = -\tfrac{1}{2}\bar{v}\bar{u} + \epsilon b\rho \sin 2\theta\Delta^{-2}, \tag{57}$$

where the dot denotes differentiation with respect to the time variable s. The energy relation is

$$\bar{u}^2 + \bar{v}^2 - 2 - 2b\rho\Delta^{-1} = 0 \tag{58}$$

and the other first integral can be written as

$$\bar{u}^2 - 2b\rho\Delta^{-1} = 2\rho g. \tag{59}$$

The infinity manifold is a two-manifold embedded in $\mathbb{R}^3 \times S^1$ given by the equations

$$I_0 = \{ (\rho, \bar{v}, \theta, \bar{u}) | \rho = 0,\ \bar{u}^2 + \bar{v}^2 = 2 \}, \tag{60}$$

i.e., the points in phase space that satisfy the condition $\rho = 0$ and the energy relation. This shows that I_0 is a torus $S^1 \times S^1$.

The first two equations of the system (57) are independent from the others, and we would like to determine ρ and $\bar{v}$. If we set $\bar{v} = \pm\sqrt{2}$, then $\rho = \exp(\mp\sqrt{2}(s - s_0))$ is a solution of the two equations mentioned above. If $\bar{v} = \pm\sqrt{2}$ the energy integral (58) gives the condition

$$\bar{u} = \pm\sqrt{2b\rho\Delta^{-1}}. \tag{61}$$

Moreover the previous condition and Eq. (59) impose $g = 0$. Differentiating (61) with respect to s we obtain

$$\dot{\bar{u}} = \pm\sqrt{2b}\left(\frac{\Delta^{-1/2}}{2\rho^{1/2}}\dot{\rho} + \frac{\epsilon}{2}\bar{u}\sqrt{\rho\Delta}\frac{\sin 2\theta}{\Delta^2}\dot{\theta}\right) \tag{62}$$

and using the first equation in (57) and Eq. (61) it follows that

$$\dot{\bar{u}} = -\tfrac{1}{2}\bar{v}\bar{u} + \epsilon b\rho \sin 2\theta\Delta^{-2}. \tag{63}$$

This shows that system (57) admits solutions with $\bar{v} = \pm\sqrt{2}$.

The other solutions of the first two equations of the system (57) can be found by dividing the second equation by the first. This leads to the equation

$$\frac{\dot{\bar{v}}}{\dot{\rho}} = \frac{1}{2}\frac{\bar{v}}{\rho} - \frac{1}{\rho\bar{v}}, \tag{64}$$

which can be solved by separating the variables. This leads to

$$\int_{\rho_0}^{\rho} \frac{\mathrm{d}\xi}{\xi} = \int_{\bar{v}_0}^{z} \frac{z\,\mathrm{d}z}{\frac{1}{2}z^2 - 1} \tag{65}$$

and consequently yields

$$\rho = \left(\frac{\rho_0}{\bar{v}_0^2 - 2}\right)(\bar{v}^2 - 2), \tag{66}$$

where ρ_0 and v_0 are initial conditions and $\rho \geqslant 0$, since $\rho < 0$ has no physical meaning. Now we can prove the following result relative to the heteroclinic solutions connecting the infinity and the collision manifolds.

Theorem 8.4: *The solutions whose ω-limit set belongs to the infinity manifold have the α-limit set contained in the collision manifold. In particular, the following properties take place:*

(1) *If* $\bar{v} = \sqrt{2}$ $(\bar{v} = -\sqrt{2})$, *the above solutions belong to the unstable (stable) manifold of one of the periodic orbits on the equator of the collision manifold.*

(2) *If* $0 < \sqrt{1/k} < \sqrt{2b}$ *and* $\sqrt{1/k} \neq \sqrt{2b/\mu}$ *with* $k = \rho_0/(\bar{v}_0^2 - 2)$, *the above solutions belong to the unstable (stable) manifold of the periodic orbits on the collision manifold with* $v = \sqrt{1/k}$ $(v = -\sqrt{1/k})$.

(3) *If* $\sqrt{1/k} = \sqrt{2b/\mu}$ $(-\sqrt{1/k} = \sqrt{2b/\mu})$, *then the above solutions belong to the unstable (stable) manifold of one of the fixed points* A_0^+, A_π^+ (A_0^-, A_π^-).

(4) *If* $\sqrt{1/k} = \sqrt{2b}$ $(-\sqrt{1/k} = \sqrt{2b})$, *then the above solutions belong to the unstable (stable) manifold of one of the fixed points* $A_{-\pi/2}^+$, $A_{\pi/2}^+$ $(A_{-\pi/2}^-, A_{\pi/2}^+)$.

Proof: To prove (1) observe that $v = \bar{v}/\rho^{1/2} = \pm\sqrt{2}/\rho^{1/2}$. Thus $\lim_{s\to\infty} v = \lim_{s\to\infty} \pm\sqrt{2}/\rho^{1/2} = \lim_{\tau\to\infty} \pm\sqrt{2}/\rho^{1/2} = \lim_{\tau\to\infty} v = 0$, since $\lim_{s\to\infty} \tau = \infty$. To prove (2), (3), and (4) we consider the limit $\lim_{\tau\to\infty} v$, which with the help of Eq. (66) becomes

$$\lim_{\tau\to\infty} v = \lim_{\tau\to\infty} \frac{\bar{v}}{\rho^{1/2}} = \pm \lim_{\tau\to\infty} \sqrt{\frac{\rho + 2k}{k}}\rho^{-1/2} = \pm\sqrt{\frac{1}{k}}.$$

Moreover from the energy relation $\bar{u}^2 + \bar{v}^2 - 2 - 2b\rho/\Delta = 0$ and the fact that $\bar{v}^2 = (\rho + 2k)/k$ it is easy to see that

$$\bar{u}^2 = -\rho\left(\frac{1}{k} - \frac{2b}{\Delta}\right),$$

and since $\rho > 0$ and $\bar{u}^2 \geqslant 0$, we have

$$\frac{1}{k} \leqslant \frac{2b}{\Delta} \leqslant 2b.$$

Consequently we have shown that

$$0 < \sqrt{\frac{1}{k}} \leqslant \sqrt{2b}. \tag{67}$$

In particular it is clear that when $\sqrt{1/k} = \sqrt{2b/\mu}$ $(-\sqrt{1/k} = \sqrt{2b/\mu})$ the solutions lie on the unstable (stable) manifold of one of the fixed points A_0^+, A_π^+ (A_0^-, A_π^-). Similarly when $\sqrt{1/k} = \sqrt{2b}$ $(-\sqrt{1/k} = \sqrt{2b})$, the solutions lie on the unstable (stable) manifold of one of the fixed points $A_{-\pi/2}^+$, $A_{\pi/2}^+$ $(A_{-\pi/2}^-, A_{\pi/2}^-)$. In the remaining cases the solutions lie on the unstable (stable) manifold of the periodic orbits on the collision manifold with $v = \sqrt{1/k}$ $(v = -\sqrt{1/k})$. □

IX. A PERTURBATIVE APPROACH

In this and the next section we study the appearance of chaos on the zero-energy manifold for the system of Hamiltonian H_β given by Eq. (1). In order to do that we study the problem for small values of ϵ and b and we use an extension of the Melnikov method that is briefly illustrated in the following section. Consider the Hamiltonian

$$\mathcal{H}_\beta = \frac{1}{2}\mathbf{p}^2 - \frac{1}{r} - \frac{b}{r^\beta} + \epsilon b \frac{\beta \cos^2 \theta}{2r^\beta} \equiv \mathcal{H}^0 + b\mathcal{W}^1_\beta(r,\theta) + \epsilon b \mathcal{W}^2_\beta(r,\theta), \tag{68}$$

where $\beta > 3/2$, $b \ll 1$, $\epsilon \ll 1$. This is the original Hamiltonian H_β [defined in (1)] truncated to the second order in ϵ and b. Consider, as in Ref. 5, the parabolic solutions of the unperturbed ($\epsilon = 0, b = 0$) problem (68), defined by the Hamiltonian $\mathcal{H}^0$ of the classical Kepler problem that are on the zero-energy manifold and play the role of homoclinic solutions corresponding to the critical point at infinity, i.e., $r = \infty$, $\dot{r} = 0$. These solutions satisfy the equations

$$\dot{r} = \pm \frac{\sqrt{2r - k^2}}{r}, \quad \dot{\theta} = \frac{k}{r^2}, \tag{69}$$

where $k \neq 0$ is the (constant) angular momentum and the sign $-$ (respectively, $+$) holds for $t < 0$ (respectively, $t > 0$). From (69) we get

$$\pm t = \frac{k^2 + r}{3}\sqrt{2r - k^2} + \text{const},$$

$$\theta = \pm 2 \arctan \frac{\sqrt{2r - k^2}}{\sqrt{k^2}} + \text{const}. \tag{70}$$

We denote by

$$R = R(t) \quad \text{and } \Theta = \Theta(t) \tag{71}$$

the expressions giving the dependence of r and of θ on the time t. These are obtained by "inverting" the equations (70) with the conditions $R(0) = r_{\min} = k^2/2$ and $\Theta(0) = 0$. Let us emphasize that, as in Ref. 5, it is not necessary to have the explicit form of these functions. But it is important to remark that $R(t)$ is even and $\Theta(t)$ is odd, both in the time variable. The choice $\Theta(0) = 0$ correspond to selecting the solution describing the parabola with axis coinciding with the x axis and going to infinity when $x \to -\infty$.

The parabolic orbits can also be described in parametric form.[19] If $p = k^2 \neq 0$, we can write

$$r = \frac{p}{2}(1 + \eta^2), \quad t = \frac{p^{3/2}}{2}\eta\left(1 + \frac{\eta^2}{3}\right), \quad \eta = \tan\frac{\theta}{2}. \tag{72}$$

We also have

$$\cos 2\theta = 2\frac{(1 - \eta^2)^2}{(1 + \eta^2)^2} - 1. \tag{73}$$

We will further use these remarks to apply the Melnikov method.

X. THE MELNIKOV METHOD

Consider the problem defined in (68). The homoclinic manifold, i.e., the set of solution of the unperturbed equation which are doubly asymptotic to $r = \infty$, $\dot{r} = 0$, is given for each value $k \neq 0$ of the angular momentum by the two-dimensional manifold described by the family of solutions $r = R(t - t_0)$, $\vartheta = \Theta(t - t_0) + \theta_0$, where $R(t)$ and $\Theta(t)$ have been defined in (71), with arbitrary t_0, θ_0.

It is clear from Eq. (68) that the first order in b of the perturbation (i.e., the term $b\mathcal{W}_\beta^1$) does not contribute to the Melnikov integrals. This is because the perturbed Hamiltonian truncated at the first order, i.e., $\mathcal{H}_0+b\mathcal{W}_\beta^1$, is integrable and, at this order, the positively and negatively asymptotic sets coincide. Furthermore, for the same reason, the terms in b^n for $n\geqslant 2$ do not contribute to the Melnikov integral. Consequently the first nonvanishing terms of the Melnikov integrals are of order ϵb.

The perturbation resulting from a small anisotropy vanishes as $r\to\infty$ since $\mathcal{W}_\beta^2(r,\theta)\sim 1/r^\beta$ with $\beta>3/2$. This guarantees, among other things, the integrability of the Melnikov integrals and the applicability of the aforementioned method.[5] This allows us to write the first nonvanishing effect on the Melnikov integral in the same form as in Ref. 5, with the difference that here we can drop the dependence on time,

$$M_1(\theta_0)=\int_{-\infty}^{+\infty}\left[\dot{R}(t)\frac{\partial\mathcal{W}_\beta^2(R(t),\Theta(t)+\theta_0)}{\partial r}+\dot{\Theta}(t)\frac{\partial\mathcal{W}_\beta^2(R(t),\Theta(t)+\theta_0)}{\partial\theta}\right]\mathrm{d}t=0, \tag{74}$$

$$M_2(\theta_0)=\int_{-\infty}^{+\infty}\frac{\partial\mathcal{W}_\beta^2(R(t),\Theta(t)+\theta_0)}{\partial\theta}\mathrm{d}t=0. \tag{75}$$

Since the perturbation $\mathcal{W}_\beta^2$ vanishes as $t\to\pm\infty$, the first Melnikov condition can be written as

$$M_1(\theta_0)=\int_{-\infty}^{+\infty}\frac{\partial\mathcal{W}_\beta^2(R(t),\Theta(t)+\theta_0)}{\partial t}\mathrm{d}t\equiv 0. \tag{76}$$

The above integral is identically zero because the perturbation $\mathcal{W}_\beta^2$ is not time dependent. This simplifies our discussion since we must only find the solutions of (75). Such solutions correspond, at the order ϵb, to intersections of the positively and negatively asymptotic sets of the critical point at infinity. If one such solution exists then there are infinitely many. Moreover, if the solutions correspond to simple zeroes of $M_2(\theta_0)$, the intersection is transversal and, for ϵ and b sufficiently small, higher order terms are not going to destroy the intersection.

It is significant to remark, and easy to verify, that these conditions can be written also in terms of the first integrals of the unperturbed problem as

$$M_1(\theta_0)=\int_{-\infty}^{+\infty}\{H_0,\mathcal{W}_\beta^2\}(\cdots)\mathrm{d}t=0 \tag{77}$$

and

$$M_2(\theta_0)=\int_{-\infty}^{+\infty}\{K,\mathcal{W}_\beta^2\}(\cdots)\mathrm{d}t=0, \tag{78}$$

where $(\cdots)$ represents the homoclinic orbit.

This resembles some properties obtained for the Gyldén problem[5,16] and is related to the symmetries of the problem. In the Gyldén problem there is a perturbation that does not depend on the angle θ, but depends on time. This means that the perturbation destroys the time homogeneity, so the Hamiltonian is not an integral of motion anymore, but does not destroy the rotational invariance, so the angular momentum is still conserved. Therefore the only one condition is given by (74). However, the anisotropy destroys the rotational symmetry but not the homogeneity of time, so we are left with the condition (75).

Here the Melnikov condition for M_2 becomes

$$M_2(\theta_0) = \frac{\beta}{2}\int_{-\infty}^{+\infty} \frac{\sin[2(\Theta(t)+\theta_0)]}{R(t)^\beta} \mathrm{d}t = 0. \tag{79}$$

Using some trigonometry the integral can be written as

$$M_2(\theta_0) = I_1 \cos 2\theta_0 + I_2 \sin 2\theta_0, \tag{80}$$

where I_1 and I_2 are defined by

$$I_1 = \frac{\beta}{2}\int_{-\infty}^{+\infty} \frac{\sin 2\Theta(t)}{R(t)^\beta} \mathrm{d}t,$$

$$I_2 = \frac{\beta}{2}\int_{-\infty}^{+\infty} \frac{\cos 2\Theta(t)}{R(t)^\beta} \mathrm{d}t. \tag{81}$$

Recall that $R(t)$ is an even function of time and $\Theta(t)$ is an odd function. This implies that the integrand of I_1 is an odd function. Therefore $I_1 \equiv 0$, and M_2 can be rewritten as

$$M_2(\theta_0) = I_2 \sin 2\theta_0. \tag{82}$$

Thus $M_2(\theta_0)$ has infinitely many simple zeroes, provided that $I_2 \neq 0$. To complete the proof we must verify that $I_2 \neq 0$. We compute I_2 using the parametric form of the parabolic orbits defined in Eqs. (72). Since $\mathrm{d}t = (p^{3/2}/2)(1+\eta^2)\mathrm{d}\eta$, we can write

$$I_2 = 2^{\beta-1} p^{3/2-\beta} \frac{\beta}{2}\int_{-\infty}^{+\infty} \frac{1}{(1+\eta^2)^{\beta-1}} \left(\frac{2(1-\eta^2)^2}{(1+\eta)^2} - 1 \right) \mathrm{d}\eta. \tag{83}$$

Computing the integral, we find that

$$I_2 = \frac{2^{\beta-1} p^{3/2-\beta}}{2\Gamma(\beta-1)} \sqrt{\pi} \left[\Gamma\left(\beta - \frac{3}{2}\right) \left(\frac{3}{2(\beta-1)\beta} - 1 \right) + 2\frac{\Gamma\left(\beta+\frac{1}{2}\right) - \Gamma\left(\beta-\frac{1}{2}\right)}{(\beta-1)\beta} \right], \tag{84}$$

where $\Gamma(z)$ is Euler's gamma function. Thus $I_2(\beta)$ is an analytic function in β for $\beta > 3/2$, since $\Gamma(z)$ is analytic for $z > 0$. Recall that the gamma function can be expressed as

$$\Gamma(z) = \lim_{n\to\infty} \frac{n!\, n^z}{z(z+1)\cdots(z+n)} \tag{85}$$

if $z \neq 0, -1, -2, -3, \ldots$. Using this form of the gamma function, and letting $A = 2^{\beta-2} p^{3/2-\beta}$, we find that

$$\begin{aligned} I_2 &= A \lim_{n\to\infty} n^{3/2} \sqrt{\pi} \frac{\beta(\beta+1)(\beta+2)\cdots(\beta-1+n)}{\left(\beta-\frac{3}{2}\right)\left(\beta-\frac{1}{2}\right)\cdots\left(\beta-\frac{1}{2}+n\right)} (\beta^2 - 5\beta + 6) \\ &= \frac{A\sqrt{\pi}\,\Gamma\left(\beta+\frac{1}{2}\right)}{(\beta-1)\left(\beta-\frac{3}{2}\right)\left(\beta-\frac{1}{2}\right)\Gamma(\beta-1)} (\beta^2 - 5\beta + 6), \end{aligned} \tag{86}$$

which is zero if and only if $\beta^2 - 5\beta + 6 = 0$, since the gamma function $\Gamma(z)$ is always positive for $z > 0$ and therefore the first factor never vanishes. Consequently I_2 vanishes if and only if $\beta^2 - 5\beta + 6 = 0$, namely for $\beta = 2$ or $\beta = 3$, see Fig. 3.

This proves that for every $\beta > 3/2$, $\beta \neq 2, 3$, and ϵ small, the system given by the Hamiltonian $\mathcal{H}_\beta$ of Eq. (68) exhibits chaotic dynamics on the zero energy manifold induced by an infinite sequence of intersections on the Poincaré section of the positively and negatively asymptotic sets of the critical point at infinity. Moreover, if ϵ and b are sufficiently small, one can consider the

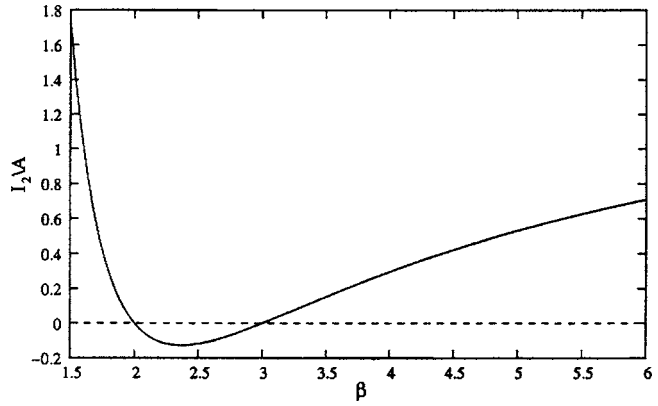

FIG. 3. I_2/A as a function of β.

Hamiltonian H_β of Eq. (1) and the simple zeroes of the Melnikov function cannot be destroyed by the higher-order terms of the perturbation. Therefore chaos persists for the Hamiltonian system of Hamiltonian (1). This proves the following.

Theorem 10.5: For every $\beta > 3/2$, $\beta \neq 2, 3$, *and* ϵ *small, the system given by the Hamiltonian* H_β *defined by Eq. (1) exhibits chaotic dynamics on the zero energy manifold.*

This type of chaotic behavior is induced by a chain of infinitely many intersections of the positively and negatively asymptotic sets to the critical point at infinity. The Smale-Birkhoff theorem does not directly apply to this situation, which is degenerate. But it is well known that the existence of Smale horseshoes and positive topological entropy can arise in the case of nonhyperbolic equilibria.[4]

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Boundedness, invariant algebraic surfaces and global dynamics for a spectral model of large-scale atmospheric circulation

Dan Dobrovolschi[a)]
National Institute of Meteorology and Hydrology, Sos. Bucuresti-Ploiesti 97, 013686 Bucuresti, Rumania

Jaume Llibre[b)]
Departament de Matemàtiques, Universitat Autónoma de Barcelona, 08193 Bellaterra, Barcelona, Spain

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We consider a three-dimensional quadratic system S in $\mathbb{R}^3$ with six parameters which appears in geophysical fluid dynamics (atmospheric blocking). In this paper we start its systematic study from the point of view of dynamical systems. First, we reduce the number of its parameters from six to three. Thus, we must study a three-dimensional quadratic system with three parameters, which recalls us the famous Lorenz-63 system. Traditionally, system S has been studied by considering two subcases, called the conservative and the dissipative case, as the parameter responsible for dissipation is zero or not. In the conservative case, we reduce system S to systems without parameters. Among these there are two interesting systems: one is homeomorphic to the simple pendulum, and the other is a perturbation of it. In the latter system the saddle point corresponding to topographic instability is connected to two homoclinic orbits to it. In the dissipative case we prove that all trajectories of system S enter in an ellipsoid for any values of the parameters. We characterize their invariant algebraic surfaces of degree 2, and for those systems having such invariant algebraic surfaces we describe their global phase portraits. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1955448]

I. INTRODUCTION

In this paper we consider the following quadratic system in $\mathbb{R}^3$

$$\dot{x} = az - b(x - c),$$

$$\dot{y} = -(dx - e)z - by,$$

$$\dot{z} = (dx - e)y - fx - bz, \tag{1}$$

where a, b, c, d, e, and f are arbitrary real parameters and the overdot denotes differentiation with respect to time t. We start the systematic study of its flow from the point of view of dynamical systems. System (1) with positive parameters is a subsystem of Charney DeVore (CdV) model, well known in geophysical fluid dynamics, and describes topographically driven disturbances of an atmospheric zonal flow. The CdV model is a quadratic system in $\mathbb{R}^6$ introduced by Charney and DeVore in 1979 as a truncation of the equations describing barotropic atmospheric flow over topography. They found that more than one stable equilibrium state may occur for a given external

[a)]Electronic mail: danidbrv@yahoo.com
[b)]Electronic mail: jllibre@mat.uab.es

force, and that these equilibrium states are analogues of the observed large-scale preferent states of the atmospheric circulation. For more details, see Ref. 2. This work has been considered by many researchers in geophysical fluid dynamics (see Refs. 24, 15–17, 32, 6, 7, 13, 14, and 4). The CdV model in $\mathbb{R}^6$ or its extensions up to $\mathbb{R}^{25}$ have been studied by numerical methods.

Another quadratic system which models the general atmospheric circulation is the famous Lorenz-84 model:[22]

$$\dot{x} = -y^2 - z^2 - ax + aF, \quad \dot{y} = xy - bxz - y + G, \quad \dot{z} = bxy + xz - z, \tag{2}$$

where F and G are forcing terms due to the average north-south temperature contrast and the earth-sea temperature contrast, respectively. For more details on physical interpretation of the variables x, y, z and of suitable choices of parameters a and b, see e.g., Ref. 22. Both systems (1) and (2) are spectrally truncated versions of Navier-Stokes equations. However, system (1) is a barotropic quasigeostrophic model, whereas system (2) is a geostrophic baroclinic model, i.e., a more general one. Values of parameters F and G for which system (2) is chaotic are known. For instance, if $a=1/4$, $b=4$, $F=8$ and $G=1$, i.e., winter conditions for the forcing terms, then the behavior of system (2) is chaotic.[29] Thus, the study of bifurcations and strange attractors for system (2) is more advanced than for system (1). For example, a comprehensive bifurcation analysis of system (2) is presented in Ref. 26. It is shown that the system admits a codimension-two saddle-node Hopf bifurcation. Nontrivial limit sets in the form of a chaotic attractor or repeller are found in some parameter ranges. Their presence implies an increased unpredictability of the system of parameter values corresponding to the winter season. In Ref. 1 system (2) is studied by using a three-dimensional Poincaré mapping, depending on the forcing parameters F and G of the system and on the relative amplitude of the oscillating part of the forcing. In order to simulate seasonal effects, F and G are subject to periodic forcing where the period is one year. It is showed that system (2) displays periodicity, quasiperiodicity, and strange attractors. The transitions of the attractors are explained in terms of codimension one bifurcations (saddle-node and Hopf). In Ref. 29 van Veen investigated the atmosphere-ocean interaction at midlatitudes in a low-order climate model (van Veen model, hereafter). This model combines the Lorenz-84 model for the atmosphere on a fast time scale and a box model for the ocean on a slow time scale; the ocean is forced strongly by the atmosphere and the feedback to the atmosphere is weak, but capable of producing decadal variability in atmospheric observables. The physical focus of Ref. 29 is on the interplay of the short time scale variability of the atmospheric component and the long time scale of the oceanic component. The mathematical focus is on periodic and chaotic solutions of the Lorenz-84 model and on intermittency in van Veen model. The most recent paper on six-component CdV model is Ref. 4. Its authors provide support for the hypothesis that regime transitions are related to heteroclinic connections. By parameter tuning, the Hopf bifurcation corresponding to barotropic instability can be made to coincide with one of the saddle-node bifurcations that are due to the topography in the model. Heteroclinic connections and homoclinic orbits connected to equilibria are related to such a bifurcation. In this paper we have not performed a bifurcation analysis of system (1) as our approach logically precedes such a study.

In this paper we begin the systematic analytic study of the subsystem (1) in $\mathbb{R}^3$ of the CdV model. Our first step is to reduce system (1) to a system whose dynamics is either easy to analyze, or has at most three parameters instead of six. This is done in Sec. II. In Sec. III we describe the phase portraits of the systems to which system (1) is reduced excepting system (18), whose dynamics is difficult to describe exhaustively. However, in Sec. IV we prove that all solutions of system (18) enter in an ellipsoid for any values of its three parameters. In Sec. V we characterize the invariant algebraic surfaces of degree 2 for system (18). In Sec. VI, we describe the phase portraits of system (18) having these invariant algebraic surfaces. To this end, we use that the existence of invariant algebraic surfaces implies the existence of semipermeable surfaces; i.e., the trajectories cross these surfaces always in the same direction. Finally in Sec. VII we compare our results with the previous ones.

II. REDUCED FORMS OF SYSTEM (1)

In this section we transform system (1) by rescalings and changes of variables to one of the following 12 systems: (3)–(7), (9)–(12), and (16)–(18). The advantage is that the transformed system, either has an easy dynamics to analyze, or has at most three parameters instead of the initial six parameters. We prove this in Lemmas 1–4.

When specifying the change of variables, we always denote new variables in uppercase X,Y,Z and old variables in lowercase x,y,z. For brevity, and when no confusion is possible, we rewrite the new system using lowercase letters as well.

Lemma 1: We consider system (1). If $b=0$ *and* $d=0$, *then system (1) is equivalent to the linear system* $\dot{\mathbf{x}}=L\mathbf{x}$ *where*

(a) *if* $e^2+af<0$, *then*

$$L=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{3}$$

(b) *if* $e^2+af>0$, *then*

$$L=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{4}$$

(c) *if* $e^2+af=0$ *and* $e\neq 0$, *then*

$$L=\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \tag{5}$$

(d) *if* $e=0$, $af=0$ *and* $a^2+f^2\neq 0$, *then*

$$L=\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{6}$$

(e) *if* $e=a=f=0$, *then*

$$L=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}=O_3. \tag{7}$$

Proof: If $b=d=0$ then system (1) becomes $\dot{\mathbf{x}}=A\mathbf{x}$ with

$$A=\begin{pmatrix} 0 & 0 & a \\ 0 & 0 & e \\ -f & -e & 0 \end{pmatrix}.$$

Its real Jordan normal form J_A depends on the sign of e^2+af. If $e^2+af<0$, then

$$J_A=\begin{pmatrix} 0 & 0 & 0 \\ 0 & \sqrt{r} & 0 \\ 0 & 0 & -\sqrt{r} \end{pmatrix},$$

where $r=-(e^2+af)>0$. After a time rescaling, we obtain (3). If $e^2+af>0$, then

$$J_A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\sqrt{r} \\ 0 & \sqrt{r} & 0 \end{pmatrix},$$

where now $r=e^2+af$. Using again a time rescaling, we get (4). If $e^2+af=0$ then we have three cases: (i) $e\neq 0$, (ii) $e=0$ and $a^2+f^2\neq 0$, and (iii) $e=a=f=0$.

Case (i): Since $e\neq 0$ and $e^2+af=0$, the parameters a and f are also nonzero. In particular, $f=-e^2/a$, and the matrix A becomes

$$B = \begin{pmatrix} 0 & 0 & a \\ 0 & 0 & e \\ e^2/a & -e & 0 \end{pmatrix}.$$

The matrix B has the zero as an eigenvalue of algebraic multiplicity three, and geometric multiplicity one. By standard procedure,

$$B = P^{-1}AP = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \tag{8}$$

where P is the matrix whose columns are generalized eigenvectors of A. Now we put the last matrix of (8) in the form (5) doing the change of variables $X=z, Y=y, Z=x$.

Case (ii): If $e=f=0$ and $a\neq 0$, then by a rescaling we get (6). If $e=a=0$ and $f\neq 0$, then after the change of variables $X=-z, Y=y, Z=x$, we obtain (6).

Case (iii): If $e=a=f=0$, then obviously $L=A=O_3$, and we have (7). ■

Lemma 2: We consider system (1). Assume $b=0$ and $d\neq 0$. Then system (1) reduces to system S where

(a) *if $ef=0$ and $a\neq 0$, then S is*

$$\dot{x}=z, \quad \dot{y}=-xz, \quad \dot{z}=xy; \tag{9}$$

(b) *if $ef=0$ and $a=0$, then S is*

$$\dot{x}=0, \quad \dot{y}=-xz, \quad \dot{z}=xy; \tag{10}$$

(c) *if $ef\neq 0$ and $a\neq 0$, then S is*

$$\dot{x}=z, \quad \dot{y}=-xz, \quad \dot{z}=xy-1; \tag{11}$$

(d) *if $ef\neq 0$ and $a=0$, then S is*

$$\dot{x}=0, \quad \dot{y}=-xz, \quad \dot{z}=xy-1. \tag{12}$$

Proof: Since $b=0$ and $d\neq 0$, after rescaling the time parameter $T=dt$, system (1) becomes

$$\dot{x}=a_1z, \quad \dot{y}=-(x-e_1)z, \quad \dot{z}=(x-e_1)y-f_1x, \tag{13}$$

where $a_1=a/d$, $e_1=e/d$, $f_1=f/d$. The change of variables $X=x-e_1$, $Y=y-f_1$ transforms system (13) into

$$\dot{x}=a_1z, \quad \dot{y}=-xz, \quad \dot{z}=xy-e_1f_1. \tag{14}$$

Assume $ef=0$. Then $e_1f_1=0$. If $a=0$ then $a_1=0$, and system (14) is system (10). If $a\neq 0$ then $a_1\neq 0$, and system (14) becomes system (9) after the rescaling $Y=a_1y$, $Z=a_1z$. If $ef\neq 0$ and $a=0$, then also $e_1f_1\neq 0$ and $a_1=0$. By the rescaling $Y=hy$, $Z=hz$, where $h=1/(e_1f_1)$, we get system (12) from system (14). If $ef\neq 0$ and $a\neq 0$ then also $e_1f_1\neq 0$ and $a_1\neq 0$. System (14) becomes system (11) after the rescaling $X=\alpha x$, $Y=\beta y$, $Z=\gamma z$, $T=\delta t$ where $\alpha=1/\delta$, $\beta=\gamma=\delta/(e_1f_1)$, and δ is

a fixed nonzero real number such that $\delta^3=a_1e_1f_1$. ■

For the remaining of this section we assume $b\neq 0$, and we denote

$$a_1=a/b,\quad d_1=d/b,\quad e_1=e/b,\quad f_1=f/b. \tag{15}$$

Lemma 3: We consider system (1). *If* $b\neq 0$ *and* $d=0$, *then system* (1) *is becomes*

$$\dot{x}=-x+a_1z+c,\quad \dot{y}=-y+e_1z,\quad \dot{z}=-z-f_1x-e_1y, \tag{16}$$

where a_1, e_1, f_1 *are given in* (15).

Proof: Since $b\neq 0$ and $d=0$, system (1) becomes system (16) after rescaling the time ($T=bt$). ■

Lemma 4: We consider system (1). *Assume* $bd\neq 0$. *We recall the notation introduced in* (15) *for* a_1, d_1, e_1 *and* f_1. *We denote* $c_1=cd_1-e_1$, $f_2=f_1/d_1$, $r=-a_1f_1$, $c_2=re_1$.

(a) *If* $a=0$, *then system* (1) *reduces to*

$$\dot{x}=-x,\quad \dot{y}=-y-(x+c_1)z,\quad \dot{z}=-z+(x+c_1)y-f_2x-cf_1, \tag{17}$$

(b) *If* $a\neq 0$, *then system* (1) *becomes*

$$\dot{x}=-x+y+c_1,\quad \dot{y}=-y+rx-xz+c_2,\quad \dot{z}=-z+xy. \tag{18}$$

Proof: After rescaling the time ($T=bt$) system (1) becomes

$$\dot{x}=a_1z-x+c,\quad \dot{y}=-(d_1x-e_1)z-y,\quad \dot{z}=(d_1x-e_1)y-f_1x-z. \tag{19}$$

(a) If $a=0$ then $a_1=0$. After the changes of variables $X=d_1x-e_1$ and $X=x-c_1$, system (19) becomes system (17). (b) If $a\neq 0$ then $a_1\neq 0$. System (19) is transformed into system (18) after the following four changes of variables: $X=d_1x-e_1$; $Y=a_1d_1y$, $Z=a_1d_1z$; $Y=z$, $Z=y$; and $Z=-z$. ■

III. PHASE PORTRAITS OF SYSTEM (1)

In this section we describe all the phase portraits of the systems to which system (1) is reduced with the exception of system (18); i.e., systems (3)–(7), (9)–(12), (16), and (17). First of all, we introduce a definition and some notations. Consider the differential system $\dot{\mathbf{x}}=f(\mathbf{x})$ with $\mathbf{x}=(x,y,z)$ in $\mathbb{R}^3$, $f:\mathbb{R}^3\to\mathbb{R}^3$, and suppose that it has two first integrals, H_1 and H_2. If the set $\{\mathbf{x}\in\mathbb{R}^3$: rank $M<2\}$, where

$$M=\begin{pmatrix} \dfrac{\partial H_1}{\partial x} & \dfrac{\partial H_1}{\partial y} & \dfrac{\partial H_1}{\partial z} \\ \dfrac{\partial H_2}{\partial x} & \dfrac{\partial H_2}{\partial y} & \dfrac{\partial H_2}{\partial z} \end{pmatrix},$$

has zero Lebesgue measure in $\mathbb{R}^3$, then we say that H_1 and H_2 are *linearly independent*.

We denote by I_{h_i} the h_i-level sets of the first integrals H_i (i=1,2); i.e.

$$I_{h_i}:=\{(x,y,z)\in\mathbb{R}^3: H_i(x,y,z)=h_i\}\quad (i=1,2)$$

where h_i (i=1,2) are arbitrary real numbers. We also denote $I_{h_1,h_2}=I_{h_1}\cap I_{h_2}$.

System (3): The set of singular points is the x axis. In the yz plane, the orbits are the axes and hyperbolas, because system (3) restricted to this plane is a linear saddle. All the planes $x=$constant are copies of the flow in the plane $x=0$.

System (4): As before, the set of singular points is the x axis. In the yz plane, the phase portrait is given by concentric circles, because system (4) restricted to this plane is a linear center. All the planes $x=$constant are copies of the flow in the plane $x=0$.

System (5): The set of singular points is the x axis. Clearly, the function z is a first integral. So, the planes $z=C$, with $C\in\mathbb{R}$, are invariant by the flow. System $\dot{x}=y$, $\dot{y}=C$ with $C\neq 0$ is equivalent

to $\dot{x}=y$, $\dot{y}=1$. This system has the first integral $y^2/2-x=$constant. Consequently, each plane $z=C$, with $C\neq 0$, is filled with these parabolas. The plane $z=0$ is filled with straight lines parallel to the x axis.

System (6): The set of singular points is the xy plane. Clearly, y is a first integral. Thus, all the planes $y=$constant are copies of the flow in the plane $y=0$. In this plane the flow is given by the system $\dot{x}=z$, $\dot{z}=0$. Therefore, the plane $y=0$ is filled with straight lines parallel to the x-axis, which is formed by singular points.

System (7): The whole space $\mathbb{R}^3$ is filled with singular points.

System (9): It is easy to see that $H_1(x,y,z)=y^2+z^2$ and $H_2(x,y,z)=x^2+2y$ are linearly independent first integrals.

The set I_{h_1} is empty if $h_1<0$, I_{h_1} is the x axis filled with singular points if $h_1=0$, and I_{h_1} is a cylinder of radius $\sqrt{h_1}$ around the x axis if $h_1>0$.

The set of finite singular points of system (9) is the union of the x and y axes.

The set I_{h_1,h_2} is empty if $h_1=0$ and $h_2<0$, it is a singular point (the origin (0, 0, 0)) if $h_1=h_2=0$, and it is formed by two singular points $((-\sqrt{h_2},0,0)$ and $(\sqrt{h_2},0,0))$ if $h_1=0$ and $h_2>0$.

We note that the sets I_{h_2} and $\mathcal{P}_{h_2}\times\mathbb{R}$, where $\mathcal{P}_{h_2}=\{(x,y,0)\in\mathbb{R}^3: x^2+2y=h_2\}$, are homeomorphic.

Proposition 5: For $h_1>0$ the flow on the cylinder I_{h_1} is as follows: I_{h_1,h_2} is empty if $h_2<-2\sqrt{h_1}$; it is the center $\{(0,-\sqrt{h_1},0)\}$ if $h_2=-2\sqrt{h_1}$; it is a periodic orbit if $-2\sqrt{h_1}<h_2<2\sqrt{h_1}$; it is formed by the saddle $\{(0,\sqrt{h_1},0)\}$ and two homoclinic orbits to this saddle if $h_2=2\sqrt{h_1}$; and finally, it is formed by two periodic orbits if $h_2>2\sqrt{h_1}$.

Proof: In the xy plane, the parabola $\mathcal{P}_{h_2}$ intersects the y-axis at the point $(0,h_2/2)$. For $h_1>0$ the cylinder I_{h_1} intersects the xy plane into the pair of parallel lines $y^2=h_1$. For $h_2=-2\sqrt{h_1}$, the intersection $I_{h_1}\cap\mathcal{P}_{h_2}\times\mathbb{R}$ is the point $(0,-\sqrt{h_1},0)$. For $-2\sqrt{h_1}<h_2<2\sqrt{h_1}$, the intersection of the cylinder I_{h_1} with the topological plane $\mathcal{P}_{h_2}\times\mathbb{R}$ is a topological circle. For $h_2=2\sqrt{h_1}$, $I_{h_1}\cap\mathcal{P}_{h_2}\times\mathbb{R}$ is a union of two topological circles, both of them containing the singular point $\{(0,\sqrt{h_1},0)\}$. For $h_2>2\sqrt{h_1}I_{h_1}\cap\mathcal{P}_{h_2}\times\mathbb{R}$ is a union of two disjoint topological circles. ■

We note that, when we fix $h_1>0$, the phase portraits of system (9) and of the simple pendulum are exactly the same. Since both systems have the same separatrix configuration, by a theorem of Neumann,[23] it follows that both phase portraits are topologically equivalent.

Note that system (9) also appears in Refs. 18 and 25 in the context of a dynamo problem under the form

$$\dot{x}=y,\quad \dot{y}=x-xz,\quad \dot{z}=xy.$$

However, this is system (9), after two changes of variables ($Z=z-1$, and $Y=-z$, $Z=y$).

System (10): We can check that $H_1(x,y,z)=y^2+z^2$ and $H_2(x,y,z)=x$ are linearly independent first integrals. The set I_{h_1} is empty if $h_1<0$, I_{h_1} is the x axis filled with singular points if $h_1=0$, and I_{h_1} is a cylinder of radius $\sqrt{h_1}$ around the x axis if $h_1>0$. The set I_{h_2} is the plane $\{x=h_2\}$.

The set of finite singular points of system (10) is the union of the yz plane with the x axis. The set I_{0,h_2} is the singular point $(h_2,0,0)$ for all h_2.

Proposition 6: For $h_1>0$ the flow on the cylinder I_{h_1} is as follows: I_{h_1,h_2} is a periodic orbit if $h_2\neq 0$ and it is a circle filled with singular points if $h_2=0$.

Proof: For any h_2, I_{h_1,h_2} is the circle $y^2+z^2=h_1, x=h_2$. When $h_2=0$ the circle is contained in the plane $x=0$, which is entirely formed by singular points. ■

System (11): Two linearly independent first integrals of system (11) are $H_1(x,y,z)=(x+1)^2+(y+1)^2+z^2$ and $H_2(x,y,z)=x^2+2y$. The description of the topology of I_{h_1} is the following: I_{h_1} is empty if $h_1<0$, I_{h_1} is the singular point $(-1,-1,0)$ if $h_1=0$, and I_{h_1} is the sphere of center $(-1,-1,0)$ and radius $\sqrt{h_1}$ if $h_1>0$.

The set of finite singular points of system (11) is the hyperbola $\mathcal{H}:=\{(x,y,z)\in\mathbb{R}^3: xy=1, z$

$=0\}$. We denote by $\mathcal{C}_{h_1}:=\{(x,y,z)\in\mathbb{R}^3:(x+1)^2+(y+1)^2=h_1,z=0\}$ the circle of center $(-1,-1,0)$ and radius $\sqrt{h_1}$ contained in the plane $z=0$, and by $\mathcal{P}_{h_2}:=\{(x,y,z)\in\mathbb{R}^3:x^2+2y=h_2,z=0\}$ a parabola in the plane $z=0$.

We note that $I_{h_1}\cap\{z=0\}=\mathcal{C}_{h_1}$ and $I_{h_2}\cap\{z=0\}=\mathcal{P}_{h_2}$. Moreover, since $I_{h_2}=\{(x,y,z)\in\mathbb{R}^3:(x,y)\in\mathcal{P}_{h_2}\}$, we can denote I_{h_2} by $\mathcal{P}_{h_2}\times\mathbb{R}$.

We provide the phase portrait of system (11) in $\mathbb{R}^3$, describing it on every sphere of center $(-1,-1,0)$. We distinguish three cases according to the values of $h_1>0$.

For $0<h_1<8$, the circle $\mathcal{C}_{h_1}$ intersects the hyperbola $\mathcal{H}$ in two points, which are singular points of system (11). They are situated in the quadrant $\{x<0,y<0\}$, and we denote them by $P_1=(x_1,y_1,0)$, and $P_4=(x_4,y_4,0)$ where $x_4<x_1<0$. We also denote $h_{21}:=H_2(x_1,y_1,0)$, and $h_{24}:=H_2(x_4,y_4,0)$. We claim that $h_{21}<h_{24}$. Indeed, a direct computation yields $h_{24}-h_{21}=(x_4-x_1)(x_1+x_4-2/x_1x_4)$. Since both factors are strictly negative, we get that $h_{24}-h_{21}>0$.

Proposition 7: For $0<h_1<8$ *the phase portrait on the sphere* I_{h_1} *consists of two singular points,* $I_{h_1,h_{21}}=\{P_1\}$, *and* $I_{h_1,h_{24}}=\{P_4\}$, *which are centers, and of periodic orbits* $I_{h_1h_2}$ *for* $h_{21}<h_2<h_{24}$.

Proof: For $h_2=h_{21}$ the set $I_{h_1}\cap\mathcal{P}_{h_2}\times\mathbb{R}$ is the point P_1 (in other words, the parabola $\mathcal{P}_{h_2}$ is tangent to the circle $\mathcal{C}_{h_1}$ at P_1). For $h_{21}<h_2<h_{24}$ the intersection of the sphere I_{h_1} with the topological plane $\mathcal{P}_{h_2}\times\mathbb{R}$ is a topological circle. For $h_2=h_{24}$, the set $I_{h_1}\cap\mathcal{P}_{h_2}\times\mathbb{R}$ is the point P_2 (in other words, $\mathcal{P}_{h_2}$ is tangent to $\mathcal{C}_{h_1}$ at P_4). ■

For $h_1=8$, the circle $\mathcal{C}_8$ intersects the hyperbola $\mathcal{H}$ in three points, which are singular points of system (11). Two of them are situated in the quadrant $\{x<0,y<0\}$, denoted by $P_1=(x_1,y_1,0)$, and $P_4=(x_4,y_4,0)$ with $x_4<x_1<0$, and one is situated in the quadrant $\{x>0,y>0\}$, denoted by $P_2=(x_2,y_2,0)$ where $x_2>0$. We also denote $h_{2i}:=H_2(x_i,y_i,0)$, for $i=1,2,4$.

We claim that $h_{21}<h_{22}<h_{24}$. We prove these inequalities by using the equation $h_{2i}-h_{2j}=(x_i-x_j)(x_i+x_j-2/x_ix_j)$, for $i\neq j$ equal to 1,2,4, and by computing the abscissas x_1, and x_2.

Both abscissas are solutions of the same equation, $(x+1/x+1)^2=9$, but $x_1<0$ while $x_2>0$. Thus, x_1 is the greatest negative solution of the equation $x+1/x+1=-3$, while x_2 is the unique positive solution of the equation $x+1/x+1=3$. Direct computation yields $x_1=-2+\sqrt{3}$, and $x_2=1$.

Therefore, the first inequality is true, because

$$h_{22}-h_{21}=\frac{(x_1-1)^2}{-x_1}(x_1+2)$$

is strictly positive, as all its factors.

The second inequality also holds, because

$$h_{24}-h_{22}=(x_4-1)^2\frac{x_4+2}{x_4}$$

and the ratio is strictly positive (by direct computation it is equal to $2\sqrt{3}-3$, because $x_4=-2-\sqrt{3}$).

Proposition 8: For $h_1=8$ *the phase portrait over the sphere* I_{h_1} *consists of three singular equilibrium points* P_1,P_2,P_4 *and of periodic orbits. The singular points* $P_1(x_1,y_{1,0})=I_{h_1,h_{21}}$ *and* $P_4(x_4,y_{4,0})=I_{h_1,h_{24}}$ *are centers and the singular point* $P_2(x_2,y_{2,0})=I_{h_1,h_{22}}$ *with* $x_4<x_1<0<x_2<1$ *has a homoclinic orbit to it. The local phase portrait of* P_2 *is formed by the union of two hyperbolic sectors. The periodic orbits are obtained for* $h_{21}<h_2<h_{22}$ *and* $h_{22}<h_2<h_{24}$.

Proof: It follows from the statements below: (i) for $h_2=h_{21}$ or h_{24}, the set $I_8\cap\mathcal{P}_{h_2}\times\mathbb{R}$ is formed by the point P_1 or P_4, respectively, (in other words, for $h_2=h_{21}$ or h_{24} the parabola $\mathcal{P}_{h_2}$ is tangent to the circle $\mathcal{C}_8$ at P_1, respectively at P_4); (ii) for $h_{21}<h_2<h_{22}$, and $h_{22}<h_2<h_{24}$, the intersection of the sphere I_8 with the topological plane $\mathcal{P}_{h_2}\times\mathbb{R}$ is a topological circle; (iii) for $h_2=h_{22}$, $I_8\cap\mathcal{P}_{h_2}\times\mathbb{R}$ is a topological circle containing the singular point P_2.

With respect to the statement on the local phase portrait of P_2, in addition to (ii) and (iii), we note that for $h_2=h_{22}$, $\mathcal{P}_{h_2}$ and $\mathcal{C}_8$ share the same tangent at the common point P_2, namely $x+y$

$-2=0$. We also note that $\mathcal{P}_{h_{22}}$ intersects the y-axis at the point of coordinates $(0,3/2)$ and the x-axis at the point of coordinates $(\sqrt{3},0)$, while $\mathcal{C}_8$ intersects the y-axis at the point of coordinates $(0,\sqrt{7}-1)$ and the x-axis at the point of coordinates $(\sqrt{8}-1,0)$. Note that $\sqrt{7}-1>3/2$ and $\sqrt{7}-1<\sqrt{3}$. We now prove that $\mathcal{P}_{h_{22}}$ is below the circle $\mathcal{C}_8$ in the first quadrant for $0<x<1$, and above it for $x>1$. This fact reduces to show that $\sqrt{8-(1+x)^2}-(5-x^2)/2\geqslant 0$ for $0<x<1$, and that the opposite inequality holds for $1<x<\sqrt{7}-1$. Therefore, it suffices to prove $(x-1)^3(x+3)\leqslant 0$ for $0<x<1$, and the opposite inequality for $1<x<\sqrt{7}-1$, which is evident. ■

For $h_1>8$, the circle $\mathcal{C}_{h_1}$ intersects the hyperbola $\mathcal{H}$ in four points, which are singular points of system (11). Two of them are situated in the quadrant $\{x<0,y<0\}$, denoted by $P_1=(x_1,y_1,0)$, and $P_4=(x_4,y_4,0)$ where $x_4<x_1<0$, and the other two are in the quadrant $\{x>0,y>0\}$, denoted by $P_2=(x_2,y_2,0)$, and $P_3=(x_3,y_3,0)$ where $0<x_2<x_3$. We also denote $h_{2i}:=H_2(x_i,y_i,0)$, for $i=1,2,3,4$. We claim that $h_{21}<h_{22}<h_{23}<h_{24}$.

We prove these inequalities by using the equation $h_{2i}-h_{2j}=(x_i-x_j)(x_i+x_j-2/x_ix_j)$, for $i\neq j$ equal to 1,2,3,4 and by computing the abscissas $x_i, i=1,2,3,4$.

The abscissas are obtained by elementary computations: $2x_4=-1-r-\sqrt{(r+3)(r-1)}$, $2x_1=-1-r+\sqrt{(r+3)(r-1)}$, $2x_2=-1+r-\sqrt{(r-3)(r+1)}$, $2x_3=-1+r+\sqrt{(r-3)(r+1)}$, where $r:=\sqrt{1+h_1}>3$ because $h_1>8$.

The inequality $h_{21}<h_{22}$ holds because $x_2-x_1>0$ and $x_1+x_2-2/x_1x_2>0$. Indeed, $x_2>0>x_1$ implies the first inequality, and the fact that $-2/x_1x_2>0$. Thus, it is sufficient to prove that $x_1+x_2>0$. By using the above expressions of x_1 and x_2 as a function of r, we have $x_1+x_2>0$ if and only if $12(1+h_1)+13>0$, which holds because $h_1>8$.

The inequality $h_{22}<h_{23}$ holds because x_2 and x_3 are the roots of the quadratic equation $x^2+(1-r)x+1=0$, and by Viète equations we have $x_2+x_3=r-1$ and $x_2x_3=1$, hence $h_{23}-h_{22}=(x_3-x_2)(x_2+x_3-2/x_2x_3)=(x_3-x_2)(r-3)>0$, because $x_3>x_2$ and $r>3$.

The inequality $h_{23}<h_{24}$ holds because both factors of $h_{24}-h_{23}$, (i.e. x_4-x_3 and x_3+x_4-2/x_3x_4), are strictly negative. The first one is strictly negative because $x_3>0>x_4$. In order to prove that the second one is also strictly negative we use the following three statements:

(a) $r>3$ implies that $x_3>1$;
(b) $r>3$ implies that $-x_4>x_3+1$;
(c) If a and b are real numbers such that $b>a+1$ and $a>1$, then $a-b+2/ab<0$.

Since $r>3$ implies $\sqrt{(r-3)(r+1)}>0>-r+3$, i.e. $2x_3>2$, and (a) follows.

From $r>3>0$ we get that $r^2+2r-3>r^2-2r-3>0$, which implies that $\sqrt{r^2+2r-3}>\sqrt{r^2-2r-3}$, hence $-2x_4>2x_3+2$. So (b) is proved.

On one hand, $b>a+1$ and $a>1$ implies $ab>a(a+1)>2$. On the other hand, $b>a+1$ implies $2>2/(b-a)$. Thus, $ab>2/(b-a)$. The last inequality is equivalent to the desired one, because $b-a>1>0$. Hence, (c) follows.

Now $x_3+x_4-2/x_3x_4<0$ follows from (c) for $a=x_3$ and $b=-x_4$. The proof of $h_{23}<h_{24}$ is complete.

Proposition 9: For $h_1>8$ the phase portrait over the sphere I_{h_1} is as follows: $I_{h_1,h_{21}}=\{P_1\}$ is a center; for $h_{21}<h_2<h_{22}$, I_{h_1,h_2} is a periodic orbit; $I_{h_1,h_{22}}$ is formed by the saddle P_2 and two homoclinic orbits to this saddle; for $h_{22}<h_2<h_{23}$, I_{h_1,h_2} is formed by two periodic orbits; $I_{h_1h_{23}}$ is formed by the center P_3 and a periodic orbit; for $h_{23}<h_2<h_{24}$, I_{h_1,h_2} is a periodic orbit; and finally, $I_{h_1,h_{24}}=\{P_4\}$ is a center.

Proof: For $h_2=h_{21}$ (respectively, h_{24}) the set $I_{h_1}\cap\mathcal{P}_{h_2}\times\mathbb{R}$ is the point P_1 (respectively, P_4). In other words, for $h_2=h_{21}$ (respectively h_{24}) the parabola $\mathcal{P}_{h_2}$ is tangent to the circle $\mathcal{C}_{h_1}$ at P_1 (respectively, at P_4). For $h_{21}<h_2<h_{22}$ the intersection of the sphere I_{h_1} with the topological plane $\mathcal{P}_{h_2}\times\mathbb{R}$ is a topological circle. For $h_2=h_{22}$, the set $I_{h_1}\cap\mathcal{P}_{h_2}\times\mathbb{R}$ is a union of two topological circles, both of them containing the singular point P_2. For $h_{22}<h_2<h_{23}$ the set $I_{h_1}\cap\mathcal{P}_{h_2}\times\mathbb{R}$ is union of two disjoint topological circles. For $h_2=h_{23}$ the set $I_{h_1}\cap\mathcal{P}_{h_2}\times\mathbb{R}$ is the union of the point P_3 with a topological circle which does not contain P_3. For $h_{23}<h_2<h_{24}$ the set $I_{h_1}\cap\mathcal{P}_{h_2}\times\mathbb{R}$ is a topological circle. ■

System (12): Clearly, x is a first integral. The flow of system (12) has the same pattern in every plane $x=x_0$ with $x_0\neq 0$. It suffices to analyze the two-dimensional system: $\dot{y}=-x_0z$, $\dot{z}=x_0y-1$. There are two cases: $x_0=0$ and $x_0\neq 0$. If $x_0=0$ then the system becomes $\dot{y}=0$, $\dot{z}=-1$. Its flow on the yz plane consists of the straight lines $y=y_0$, on which the orientation of the flow is opposite to the z axis. If $x_0\neq 0$ then, since the linear part at its singular point is given by the matrix

$$\begin{pmatrix} 0 & -x_0 \\ x_0 & 0 \end{pmatrix},$$

we have a global center.

System (16): Denote $\Delta=a_1f_1+e_1^2$ and $f_4=f_1/(1+e_1^2)$. The following statements hold:

(a) If $\Delta<-1$, then its singular point has a two-dimensional stable manifold and a one-dimensional unstable one.
(b) If $\Delta>-1$, then its singular point is a global attractor.
(c) If $\Delta=-1$ and $c\neq 0$, then there are no singular points.
(d) If $\Delta=-1$ and $c=0$, then the set of singular points is the straight line (a_1z,e_1z,z) with arbitrary z. Every one of these singular points is contained in an invariant plane $f_1x+e_1y+z=h$, for a convenient constant h. In each of these planes the corresponding singular point is a global attractor.

Now we prove the above statements. The singular points of system (16) are given by the equations

$$(1+\Delta)/(1+e_1^2)x=c, \quad y=-e_1f_4x, \quad z=-f_1f_4x. \tag{20}$$

If $\Delta\neq -1$, then clearly system (16) has a unique singular point S. Now we prove statements (a) and (b). To this purpose, we consider the linear part A of the vector field of system (16) at the singular point S

$$A=\begin{pmatrix} -1 & 0 & a_1 \\ 0 & -1 & e_1 \\ -f_1 & -e_1 & -1 \end{pmatrix},$$

and we study its eigenvalues. The characteristic equation is $(1+\lambda)((1+\lambda)^2+\Delta)=0$. It is therefore sufficient to prove that if $\Delta\neq -1$, then the roots of the equation in λ $(1+\lambda)^2=-\Delta$ have the real parts strictly negative. If $\Delta<-1$, then the eigenvalues of matrix A are -1, $-1-\sqrt{-\Delta}$ and $-1+\sqrt{-\Delta}$. Thus, all of them are real, two of them being strictly negative and one strictly positive. Statement (a) is proved by the Hartman–Grobman Theorem. If $-1<\Delta\leqslant 0$, then the eigenvalues of the matrix A are given by the same formulas as before but now they are all strictly negative. If $\Delta>0$ then the eigenvalues of A are -1, and $-1\pm i\sqrt{\Delta}$. All of them have strictly negative real part. Statement (b) is proved. If $\Delta=-1$ and $c\neq 0$, then equations (20) have no solution. Statement (c) follows. If $\Delta=-1$ and $c=0$, then equations (20) have the solution $(x,-e_1f_4x,-f_4x)$ with arbitrary x. At each singular point, the associated eigenvalues are $0,-1,-2$. The linear center eigenspace (i.e., corresponding to the zero eigenvalue) is the straight line (a_1z,e_1z,z) with z arbitrary in $\mathbb{R}$. The linear stable eigenspace corresponding to eigenvalues -1 and -2 is $f_1x+e_1y-z=0$. Clearly, in our case, $H=f_1x+e_1y-z$ is a first integral of system (16). The planes $f_1x+e_1y+z=h$, where h is an arbitrary constant, are parallel and on each of these planes the corresponding singular point is a global attractor.

System (17): This system has only one finite singular point, namely $(0,-c_1f_3,f_3)$ where $f_3=-cf_1/(1+c_1^2)$. Now we prove that $(0,-c_1f_3,f_3)$ is a global attractor of system (17) in $\mathbb{R}^3$. Since $\dot{x}=-x$, it follows that if $(x(t),y(t),z(t))$ is an orbit passing through the point (x_0,y_0,z_0) at $t=0$, then $x(t)=e^{-t}x_0$. Thus, all trajectories of system (17) tends towards the plane $x=0$ when $t\to\infty$; and if $x_0=0$, then $x(t)=0$ for all t. On the other hand, in the plane $x=0$ the singular point $(0,-c_1f_3,f_3)$ is a global attractor, because on the plane $x=0$ the system is $\dot{y}=-y-c_1z$, $\dot{z}=-z+c_1y-cf_1$, and the

eigenvalues of the singular point $(c_1 f_3, -f_3)$ are $-1 \pm i|c_1|$. Consequently, the singular point $(0, -c_1 f_3, f_3)$ is a global attractor of $\mathbb{R}^3$.

IV. BOUNDEDNESS OF SOLUTIONS FOR SYSTEM (18)

The goal of this section is to prove that all trajectories of system (18) enter in an ellipsoid, i.e., all ω-limit sets of the orbits of (18) are contained in that ellipsoid.

We first introduce some notation. If $\mathcal{E}$ is the ellipsoid $\mathcal{E}: x^2/a^2+y^2/b^2+z^2/c^2=1$ then its *exterior* is the set $\text{Ext}\,\mathcal{E}: x^2/a^2+y^2/b^2+z^2/c^2>1$, its *interior* is the set $\text{Int}\,\mathcal{E}: x^2/a^2+y^2/b^2+z^2/c^2<1$. We also denote $\mathcal{E}^- = \text{Int}\,\mathcal{E} \cup \mathcal{E}$. Consider now the differential equation

$$\dot{\mathbf{x}} = d\mathbf{x}/dt = f(\mathbf{x}), \quad \mathrm{x} \text{ in } \mathbb{R}^n. \tag{21}$$

The *orbital derivative* of a differentiable function $V: \mathbb{R}^n \mapsto \mathbb{R}$ along the vector field f parameterized by t is the scalar product $L_t V(\mathbf{x}) = \text{grad}\, V(\mathbf{x}) \cdot f(\mathbf{x})$. The *orbit* of (21) starting from the point $\mathbf{x}$ is denoted by $\varphi_t(\mathbf{x})$ where φ_t is the *flow* of (21). A point $\mathbf{y}$ is an *ω-limit point* of the orbit $\varphi_t(\mathbf{x})$ through the point $\mathbf{x}$ if there exists a sequence of numbers $t_1 < t_2 < t_3 < \cdots$ such that $\lim_{n\to\infty} t_n = \infty$ and $\lim_{n\to\infty} \varphi_{t_n}(\mathbf{x}) = \mathbf{y}$. The *$\omega$-limit set* of the orbit $\varphi_t(\mathbf{x})$, denoted $\omega(\varphi_t(\mathbf{x}))$, is the set of its all ω-limit points.

Theorem 10: *We consider the differential equation $\dot{\mathbf{x}} = f(\mathbf{x})$, where $f: \mathbb{R}^3 \mapsto \mathbb{R}^3$ is a C^1 function, a differentiable function $V: \mathbb{R}^3 \mapsto \mathbb{R}$, and an ellipsoid $\mathcal{E}$ in $\mathbb{R}^3$ such that $L_t V(\mathbf{x}) < 0$ for $\mathbf{x}$ in $\text{Ext}\,\mathcal{E}$. Then $\omega(\varphi_t(\mathbf{x})) \subseteq \mathcal{E}^-$ for any $\mathbf{x}$ in $\mathbb{R}^3$.*

Remark: This result is similar and more general than the well-known Lyapunov's Stability Theorem, the role of the singular point being played by the ellipsoid. Our proof follows the Chicone's one[3] for the mentioned theorem.

Proof of Theorem 10: Let $\mathbf{x} \in \mathbb{R}^3$ and $\xi \in \omega(\varphi_t(\mathbf{x}))$. We want to prove that $\xi \in \mathcal{E}^-$. Assume the contrary. Then $\xi \in \text{Ext}\,\mathcal{E}$. Since $\xi \in \omega(\varphi_t(\mathbf{x}))$, there is a monotone increasing sequence of numbers $\{t_n\} \to \infty$ such that $\varphi_{t_n}(\mathbf{x}) \to \xi \in \text{Ext}\,\mathcal{E}$. Therefore, there is some natural number N such that $\varphi_{t_n}(\mathbf{x}) \in \text{Ext}\,\mathcal{E}$ for any $n \geqslant N$. By the continuity of function V, $V(\varphi_{t_n}(\mathbf{x})) \to V(\xi)$. By hypothesis, the function $t \mapsto V(\varphi_t(\mathbf{x}))$ is strictly decreasing for $\varphi_t(\mathbf{x}) \in \text{Ext}\,\mathcal{E}$. Thus, $V(\varphi_{t_n}(\mathbf{x})) \geqslant V(\xi)$ for any $n \geqslant N$. On the other hand, $\lim V(\varphi_{t_N+t_n}(\mathbf{x})) = \lim V(\varphi_{t_N}(\varphi_{t_n}(\mathbf{x}))) = V(\varphi_{t_N}(\xi)) < V(\xi)$. Consequently, there is some natural number $q \geqslant N$ such that $V(\varphi_{t_N+t_q}(\mathbf{x})) < V(\xi)$. There is also a natural number $m > N$ such that $t_m > t_N + t_q$. For this number we get $V(\varphi_{t_m}(\mathbf{x})) < V(\varphi_{t_N+t_q}((x))) < V(\xi) \leqslant V(\varphi_{t_m}((x)))$, i.e., a contradiction. The assumption that $\xi \notin \mathcal{E}^-$ is false. The proof is completed.■

Lemma 11: Consider system (18). Then for any $\alpha > 0$ and $\beta > 0$ there is a differentiable function $V_{\alpha,\beta}: \mathbb{R}^3 \mapsto \mathbb{R}$ and an ellipsoid $\mathcal{E}_{\alpha,\beta}$ in $\mathbb{R}^3$ such that

$$L_t V_{\alpha,\beta}(x,y,z) < 0 \quad \textit{for } (x,y,z) \textit{ in } \textit{Ext}\,\mathcal{E}_{\alpha,\beta}. \tag{22}$$

Proof: Let $\alpha > 0$ and $\beta > 0$ be fixed, and take

$$V_{\alpha,\beta}(x,y,z) = \alpha x^2 + \beta y^2 + \beta(z - (r + \alpha/\beta))^2 - R_V, \tag{23}$$

where

$$R_V = (\alpha + \beta r)^2/\beta. \tag{24}$$

Clearly, the function $V_{\alpha,\beta}(x,y,z)$ is differentiable. It follows that

$$\frac{1}{2} L_t V_{\alpha,\beta}(x,y,z) = -\alpha(x - c_1/2)^2 - \beta(y - c_2/2)^2 - \beta\left(z - \frac{\alpha + \beta r}{2\beta}\right)^2 + R_L, \tag{25}$$

where

$$R_L = \alpha c_1^2/4 + \beta c_2^2/4 + R_V/4. \tag{26}$$

Now it is easy to see that $L_t V_{\alpha,\beta}(x,y,z) < 0$ for any $(x,y,z) \in \text{Ext}\,\mathcal{E}_{\alpha,\beta}$ where $\mathcal{E}_{\alpha,\beta}$ is the ellipsoid

$$\mathcal{E}_{\alpha,\beta}: \alpha(x-c_1/2)^2+\beta(y-c_2/2)^2+\beta\left(z-\frac{\alpha+\beta r}{2\beta}\right)^2=R_L. \tag{27}$$

In short, we found the function $V_{\alpha,\beta}(x,y,z)$ and the ellipsoid $\mathcal{E}_{\alpha,\beta}$ satisfying (22). ■

The main result of this section follows directly from Lemma 11 and Theorem 10.

Theorem 12. *Let φ_t be the flow of system* (18). *Then, there exists an ellipsoid $\mathcal{E}$ in $\mathbb{R}^3$ such that $\omega(\varphi_t(\mathbf{x}))\subseteq\mathcal{E}^-$ for any $\mathbf{x}$ in $\mathbb{R}^3$.*

Remark: In fact, for any $\alpha>0$ and $\beta>0$ fixed there exists such an ellipsoid.

V. QUADRATIC INVARIANT ALGEBRAIC SURFACES FOR SYSTEM (18)

This section has two parts. In the first part we prove the proposition below. In the second part of this section we discuss the nature of the surface f obtained in Proposition 13(d). We also prove some general results in Lemma 17 about limit sets of quadratic systems with constant cofactor and apply them to our case.

Proposition 13: Let χ be the vector field associated to system (18); *i.e.*,

$$\mathcal{X}=(-x+y+c_1)\frac{\partial}{\partial x}+(-y+rx-xz+c_2)\frac{\partial}{\partial y}+(-z+xy)\frac{\partial}{\partial z}.$$

If

$$f=\sum_{d=0}^{2}\sum_{\substack{i+j+k=d,\\ 0\leqslant i,j,k\leqslant 2}} a_{ijk}x^iy^jz^k \tag{28}$$

in $\mathbb{R}[x,y,z]$ is such that

$$\mathcal{X}f=Kf, \tag{29}$$

for some polynomial K in $\mathbb{R}[x,y,z]$, then

(a) $K=k_0\in\mathbb{R}$;
(b) *if* $k_0\neq -2$, *then* $f=0$;
(c) *if* $k_0=-2$ *and* $c_2\neq -rc_1$, *then* $f=0$;
(d) *if* $k_0=-2$ *and* $c_2=-rc_1$, *then* $f=a(-r(x-c_1)^2+y^2+z^2)$, *where a is an arbitrary real constant.*

Let $f\in\mathbb{R}[x,y,z]\backslash\mathbb{R}$. The algebraic surface $f(x,y,z)=0$ is called an *invariant algebraic surface* of system (18) if equation (29) holds for some real polynomial $K(x,y,z)$, which is called the *cofactor* of the surface $f=0$. For simplicity, we will refer to the surface $f=0$ only by f.

We separate the main parts of the proof of Proposition 13 into two steps.

Step 1: We prove that each cofactor for system (18) is constant. First, we recall the definition of the weight of a polynomial as introduced in Ref. 28. Next, we prove the properties we need in Lemma 14. Finally, in Lemma 15 we prove that each cofactor for system (18) is constant.

The *weight of a monomial* $Cx^ay^bz^c$ is $a+2b+2c$, and the *weight of a nonzero polynomial* is the largest of the weights of its constituent monomials. For any polynomial f of degree d, and any integer $n\geqslant 0$ we denote by W_nf, and by G_df, the sum of those monomials of f which have weight exactly n, and degree exactly d, respectively. We say that a polynomial is *weight homogeneous of weight w* if it is the sum of monomials of weight w. By $w(f)$, and by $\deg(f)$, we denote the weight, and the degree of polynomial f, respectively.

Lemma 14: The following statements hold

(a) $w(\chi f)\leqslant w(f)+1$ *for any polynomial f*
(b) $w(fg)=w(f)+w(g)$ *for any two polynomials f and g.*
If f is a polynomial of degree d_0 and $w_0=w(G_{d_0}f)$ then
(c) $W_{w_0+1}G_{d_0+1}\chi f=W_{w_0+1}G_{d_0+1}\chi(W_{w_0}G_{d_0}f)$;

(d) $W_{w_0}G_{d_0}f=x^n\phi(y,z)$ *where* $n=2d_0-w_0$ *and* ϕ *is a homogeneous polynomial of degree* $m=w_0-d_0$.

Proof: Statements (*a*) and (*b*) follow from the fact that they hold for mononomials, and from the definition of the weight of a polynomial.

(*c*) Denote by $S_{w<w_0}f$, and by $S_{d<d_0}f$, the sum of the monomials in f which have weight strictly less than w_0, and degree strictly less than d_0, respectively. Then, $G_{d_0}f=W_{w_0}G_{d_0}f+S_{w<w_0}f$, since $w_0=w(G_{d_0}f)$, and $f=G_{d_0}f+S_{d<d_0}f$. Consequently, $\chi f=\chi(W_{w_0}G_{d_0}f+S_{w<w_0}f+S_{d<d_0}f)$. Any term of $\chi(S_{w<w_0}f)$ is of weight at most w_0, and any term of $\chi(S_{d<d_0}f)$ is of degree at most d_0, because the vector field χ increases weight and degree by at most one (as proved in (a)). Therefore, the third statement is proved.

(d) Clearly, $W_{w_0}G_{d_0}f$ is a finite sum of terms of the form $C_ix^{a_i}y^{b_i}z^{c_i}$ with $a_i+b_i+c_i=d_0$ and $a_i+2b_i+2c_i=w_0$ for any i. Therefore, we have $a_i=2d_0-w_0=n$ and $b_i+c_i=w_0-d_0=m$ for any i. The proof is completed. ■

Lemma 15: If f and K are polynomials such that (29) *holds, then K is constant.*

Proof: The idea is to use the fact that if $\mathcal{X}f=Kf$, then

$$w(\mathcal{X}f)=w(Kf) \tag{30}$$

and

$$W_{w_0+1}G_{d_0+1}\mathcal{X}f=W_{w_0+1}G_{d_0+1}(Kf), \tag{31}$$

where we denote $\deg(f)=d_0$ and $w(G_{d_0}f)=w_0$. Clearly, from (30) and Lemma 14 (*a*) and (*b*) we get $w(K)\leqslant 1$, i.e., $K=k_{100}x+k_0$. It suffices now to show that (31) implies $k_{100}=0$. To this purpose, we look more carefully at the terms of Eq. (31). By Lemma 14 (*c*) and (*d*), the left term is $W_{w_0+1}G_{d_0+1}\mathcal{X}f=W_{w_0+1}G_{d_0+1}\mathcal{X}(W_{w_0}G_{d_0})f=W_{w_0+1}G_{d_0+1}\mathcal{X}(x^n\phi)=x^{n+1}(y(\partial\phi/\partial z)-z(\partial\phi/\partial y))$. The right term of (31) is $W_{w_0+1}G_{d_0+1}(Kf)=W_{w_0+1}G_{d_0+1}(k_{100}xf)=W_{w_0+1}(k_{100}xG_{d_0}f)=k_{100}xW_{w_0}(G_{d_0}f)=k_{100}x^{n+1}\phi$. Therefore, Eq. (31) reduces to

$$y\frac{\partial\phi}{\partial z}-z\frac{\partial\phi}{\partial y}=k_{100}\phi, \tag{32}$$

where $\phi(y,z)$ is a homogeneous polynomial of degree m. The change of variables $\eta=y+iz$, $\zeta=y-iz$ transforms (32) into

$$i\left(\eta\frac{\partial\psi}{\partial\eta}-\zeta\frac{\partial\psi}{\partial\zeta}\right)=k_{100}\psi, \tag{33}$$

with $\phi(\eta,\zeta)$ a homogeneous polynomial of degree m. Then, the solutions of Eq. (33) are of the from $\phi=C\eta^{m-\mu}\zeta^{\mu}$ for some integer μ with $0\leqslant\mu\leqslant m$ and $k_{100}=i(m-2\mu)$. Since k_{100} must be real, $m=2\mu$. So, $k_{100}=0$. ■

Remark: The method of proof is taken from Ref. 28, where the same result was proved for Lorenz system. Note that the result holds not merely for quadratic but for arbitrary polynomials f.

Remark: We remark that from Eq. (33) we can get additional information interesting in itself about the degree of its solutions. More precisely, m is even. Hence the polynomial ϕ in Lemma 14(*d*) is of even degree.

Step 2: If f is a quadratic polynomial (28), K is constant and both satisfy (29), now we shall prove that statements (*b*)–(*d*) of Proposition 13 hold.

Let f be a quadratic polynomial (28), $K=k_0$ constant and both satisfying (29). Clearly, (29) is a polynomial equation in $\mathbb{R}[x,y,z]$. The coefficients a_{ijk} of the polynomial f will be determined by comparing the coefficients of equal degree of the polynomials $\mathcal{X}f$ and Kf. In order to write the corresponding equations, it is more convenient to write each polynomial of Eq. (29) as a sum of its homogeneous parts. Given a polynomial $A\in\mathbb{R}[x,y,z]$ of degree m, we denote by H_lA its homogeneous part of degree l, for any $0\leqslant l\leqslant m$. Before computing the homogeneous parts of

polynomials $\mathcal{X}f$ and Kf we need to compute the partial derivatives of f. Here and after, we denote by f_x, f_y and f_z the derivatives of f with respect to x, y and z, respectively,

$$f_x = 2a_{200}x + a_{110}y + a_{101}z + a_{100},$$

$$f_y = a_{110}x + 2a_{020}y + a_{011}z + a_{010},$$

$$f_z = a_{101}x + a_{011}y + 2a_{002}z + a_{001}.$$

Therefore, $\mathcal{X}f=\Sigma_{l=0}^{3}H_l\mathcal{X}f$ where

$$H_3\mathcal{X}f = -xz(a_{110}x + 2a_{020}y + a_{011}z) + xy(a_{101}x + a_{011}y + 2a_{002}z),$$

$$H_2\mathcal{X}f = (-x+y)(2a_{200}x + a_{110}y + a_{101}z) + (rx-y)(a_{110}x + 2a_{020}y + a_{011}z) - z(a_{101}x + a_{011}y + 2a_{002}z),$$

$$H_1\mathcal{X}f = a_{100}(-x+y) + c_1(2a_{200}x + a_{110}y + a_{101}z) + a_{010}(rx-y) + c_2(a_{110}x + 2a_{020}y + a_{011}z) - a_{001}z,$$

$$H_0\mathcal{X}f = c_1a_{100} + c_2a_{010},$$

and $Kf=\Sigma_{l=0}^{3}H_lKf$ where

$$H_3Kf = 0,$$

$$H_2Kf = k_0H_2f,$$

$$H_1Kf = k_0H_1f,$$

$$H_0Kf = a_0k_0.$$

Writing that $H_l\mathcal{X}f=H_lKf$ for each $l=0,\ldots,3$, we get, respectively, for $l=3$

$$a_{110} = a_{101} = a_{011} = 0, \tag{34}$$

$$a_{002} = a_{020}; \tag{35}$$

for $l=2$

$$(k_0+2)a_{200} = 0, \tag{36}$$

$$(k_0+2)a_{020} = 0, \tag{37}$$

$$2a_{200} + 2ra_{020} = -a_{001}, \tag{38}$$

$$a_{010} = 0; \tag{39}$$

for $l=1$

$$2c_1a_{200} = (k_0+1)a_{100}, \tag{40}$$

$$2c_2a_{020} = -a_{100}, \tag{41}$$

$$(k_0+1)a_{001}=0; \tag{42}$$

for $l=0$

$$c_1a_{100}=k_0a_0. \tag{43}$$

Proof of Proposition 13: Statement (*a*) follows from Lemma 15. Statement (*b*) is obtained directly from Eqs. (34)–(43). Statements (*c*) and (*d*) can be proved simultaneously. Indeed, $k_0=-2$ by hypothesis. From Eqs. (34)–(43) we get

$$a_{001}=0, \tag{44}$$

$$a_{200}=-ra_{020}, \tag{45}$$

$$2c_1a_{200}=-a_{100}, \tag{46}$$

$$2c_2a_{020}=-a_{100}, \tag{47}$$

$$c_1a_{100}=-2a_0. \tag{48}$$

Now we combine (45) and (46) and get

$$-2rc_1a_{020}=-a_{100}. \tag{49}$$

By using (49) and (48) we deduce $a_0=-rc_1^2a_{020}$. From (49) and (47) we obtain $(rc_1+c_2)a_{020}=0$. Now statements (*c*) and (*d*) easily follow. This concludes the proof of Proposition 13. ■

From Proposition 13 follows immediately.

Corollary 16: Consider system (18).

(a) *If* $c_2=-rc_1$, *then* $f=-r(x-c_1)^2+y^2+z^2$ *is the only quadratic invariant algebraic surface for system* (18). *Moreover, its cofactor is* $K=-2$.
(b) *If* $c_2\neq -rc_1$ *then there are no quadratic invariant algebraic surfaces for system* (18).

Remark: The nature of the invariant algebraic surface is as follows. If $r<0$ then $\mathcal{S}$ reduces to the point $(c_1,0,0)$. If $r=0$ then $\mathcal{S}$ becomes the x-axis. If $r>0$ then $\mathcal{S}$ is a cone.

Remark: We consider a general quadratic system on $\mathbb{R}^3$

$$\dot{\mathbf{x}}=F(\mathbf{x}), \tag{50}$$

and $U\subset\mathbb{R}^3$ an open set. We say that an analytic function $I(x,y,z,t):U\times\mathbb{R}\mapsto\mathbb{R}$ is an *invariant* of system (50) if $I(x,y,z,t)=$constant for all values of t for which the solution $(x(t),y(t),z(t))$ is defined and contained in U.

Lemma 17: We consider the quadratic system (50) *on* $\mathbb{R}^3$ *and assume that the system has an invariant algebraic surface* f *of constant cofactor* K. *If* γ *is an orbit, we denote by* $\omega(\gamma)$ *its* ω*-limit set. We also denote by* $\mathcal{F}$ *the surface* $f=0$ *in* $\mathbb{R}^3$. *Then*

(a) $I=fe^{-Kt}$ *is an invariant of system* (50),
(b) *If* $K<0$ *then* $\omega(\gamma)\subset\mathcal{F}$ *for any orbit* γ, and
(c) *If* $K>0$ *then* $\alpha(\gamma)\subset\mathcal{F}$ *for any orbit* γ.

Proof: (a) We denote the vector field associated to (50) by $\mathcal{X}=X(\partial/\partial x)+Y(\partial/\partial y)+Z(\partial/\partial z)$. For $I=I(\mathbf{x}(t),t)$ we denote $\mathrm{d}I/\mathrm{d}t=X(\partial I/\partial x)+Y(\partial I/\partial y)+Z(\partial I/\partial z)+\partial I/\partial t$. Clearly, $\mathrm{d}I/\mathrm{d}t=e^{-Kt}(\mathrm{d}f/\mathrm{d}t-Kf)=0$.

(b) Let γ be an orbit of system (50). By (a) we have $fe^{-Kt}=$constant. In particular, $\lim_{t\to+\infty}fe^{-Kt}$ is finite. But $\lim_{t\to+\infty}e^{-Kt}=+\infty$. Therefore, we must have $\lim_{t\to+\infty}f(\mathbf{x}(t))=0$. Let P

$\in \omega(\gamma)$. Then there exists a sequence $\{t_n\} \to +\infty$ such that $\{\mathbf{x}(t_n)\} \to P$. It follows that $\{f(\mathbf{x}(t_n))\} \to f(P)$, because the function f is continuous. Consequently, $f(P)=0$. Thus, $P \in \mathcal{F}$.

(c) The proof is similar to that of (b). ■

In our case, if $c_2=-rc_1$ then $I=fe^{2t}$ is an invariant of system (18) and the ω-limit set of any orbit is the surface $-r(x-c_1)^2+y^2+z^2=0$.

VI. SYSTEM (18) WITH $c_1=c_2=0$

We note that if $c_1=c_2=0$, then system (18) is the particular case $s=b=1$ of the famous Lorenz system (63):

$$\dot{x}=-x+y, \quad \dot{y}=-y+rx-xz, \quad \dot{z}=-z+xy. \tag{51}$$

Although the Lorenz system has been intensively studied, most of the papers are concerned with the parameter values $s=10$, $b=8/3$, and r fixed to 28 or varying from 0 to ∞. We will study the Lorenz system for $s=b=1$ and $r \in \mathbb{R}$ arbitrary. More precisely, in this section we determine the phase portrait of system (51) in Theorems 18, 19, and 20.

Since $c_2=-rc_1=0$, from Corollary 16 system (51) possesses the algebraic invariant surface $f=-rx^2+y^2+z^2$ with cofactor -2. Let $\mathcal{X}$ be the vector field associated to system (51), and let φ_t be its flow. Then

$$\mathcal{X}f=-2rx\dot{x}+2y\dot{y}+2z\dot{z}=(-2rx,2y,2z)\cdot(\dot{x},\dot{y},\dot{z}) \tag{52}$$

is precisely the scalar product $\pi(x,y,z)$ between the normal vector to the surface $S_k:-rx^2+y^2+z^2=k$ (k is an arbitrary constant) at a given point $\mathbf{x}=(x,y,z)$ and the tangent to the trajectory $\varphi_t(\mathbf{x})$. Therefore, for a given surface S_k, this scalar product is constant and equal to $-2k$, having the same sign for every point of S_k. In other words, each surface S_k is crossed by the flow φ_t in the same direction. This direction depends on the sign of the constant k. Such surfaces are called *semipermeable*, and for instance in the Lorenz system has been used in Refs. 10 and 11.

Theorem 18: If $r<1$ then the origin is a global attractor of system (51).

Proof: If $r<0$ then take $k>0$. The surface $S_k:-rx^2+y^2+z^2=k$ is an ellipsoid such that the scalar product (52) is strictly negative at any point of S_k. Therefore, for any $k>0$, all trajectories of system (51) enter into the ellipsoid S_k. When $k \to 0$ the ellipsoid S_k shrinks to the origin, therefore it is a global attractor. If $0 \leqslant r<1$ then, following Ref. 25, we consider the function $W(x,y,z)=x^2+y^2+z^2$. Clearly, $L_tW=-2(x^2-(r+1)xy+y^2+z^2)=-2((x-(r+1)y/2)^2+(r+3)(1-r)y^2/4+z^2)<0$ for $-3<r<1$. Also $W(0,0,0)=0$. Therefore W is a global Lyapunov function for the singular point (0,0,0), consequently it is a global attractor. ■

Theorem 19: If $r=1$ then the origin is a global attractor of system (51).

Proof: If $r=1$ then system (51) becomes:

$$\dot{x}=y-x, \quad \dot{y}=-y+x-xz, \quad \dot{z}=-z+xy. \tag{53}$$

The origin is its only finite singular point. Consider the family of surfaces $S_k:-x^2+y^2+z^2=k$. When $k=0$, S_0 is a cone surrounding the x axis. When $k>0$, S_k is a hyperboloid of one sheet also surrounding the x axis, and S_0 is in the interior of S_k for all $k>0$. When $k<0$, S_k is a hyperboloid of two sheets whose line joining the foci is the x axis, and S_k is inside the cone S_0. We prove the theorem in two steps.

Step 1: Now we prove that any trajectory starting at a point which is not on the cone S_0 tends to this cone as time $t \to \infty$. We take $k>0$ arbitrary and fixed, and consider a point P on S_k. Then the scalar product

$$(-2x,2y,2z)\cdot(-x+y,-y+x-xz,-z+xy)=-2k$$

is strictly negative. The normal to S_k is directed outward S_k, so the tangent to the trajectory which passes through the point P must be directed inward the hyperboloid S_k with $k>0$. Similarly, when $k<0$, the tangent to the trajectory is directed outward the hyperboloid of two sheets S_k. So, Step

1 is proved. Another way to show it is using the invariant $H(x,y,z,t)=(x^2-y^2-z^2)\exp 2t$ of system (53), see the definition for Eq. (50). From Lemma 17(b) we conclude Step 1.

Step 2: Here, we prove that any trajectory starting on the cone S_0 tends to the origin of $\mathbb{R}^3$. Now we study the flow on the cone $x^2=y^2+z^2$. Clearly, this cone is invariant. On it, the system becomes

$$\dot{y}=-y+(1-z)\sqrt{y^2+z^2}, \quad \dot{z}=-z+y\sqrt{y^2+z^2}.$$

Passing to polar coordinates $y=r\cos\theta$, $z=r\sin\theta$, we get $\dot{r}=r(\cos\theta-1)$, $\dot{\theta}=r-\sin\theta$, if we are on the half-cone $x>0$; and $\dot{r}=r(-\cos\theta-1)$, $\dot{\theta}=-(r-\sin\theta)$, if we are on the half-cone $x<0$. Note that always $\dot{r}<0$ (it is 0 when $\theta=0$, but then $\dot{\theta}$ is not zero), so over the cone r always decreases with the time. In other words, the flow over the cone tends to the origin when time $t\to\infty$. In short, for this system we have proved that the origin is a global attractor. ■

Theorem 20: *If $r>1$ then we consider the cone $S_0: rx^2=y^2+z^2$, and denote S_0^+ (S_0^-) the positive (negative) half-cone S_0 with $x>0$ ($x<0$). On S_0^+ the system has two singular points, the origin O and $C_+=(\sqrt{r-1},\sqrt{r-1},r-1)$. The global flow of system* (51) *on the half-cone S_0^+ is as follows. Let γ^s and γ^u be the two separatrices of O, the stable and the unstable, respectively. Then, if we denote by $\alpha(\gamma)$ and $\omega(\gamma)$ the α- and ω-limit sets of the orbit γ, we have*

$$\alpha(O)=\omega(O)=O, \quad \alpha(C_+)=\omega(C_+)=C_+,$$

$$\alpha(\gamma^s)=\infty, \quad \omega(\gamma^s)=O, \quad \alpha(\gamma^u)=O, \quad \omega(\gamma^u)=C_+,$$

$$\alpha(\gamma)=\infty, \quad \omega(\gamma)=C_+,$$

for any orbit γ on the half-cone S_0^+ different from O, C_+, γ^s, and γ^u. The flow on the negative half-cone S_0^- is obtained by using the symmetry $(x,y,z)\to(-x,-y,z)$.

Proof: The origin is locally unstable because one of its eigenvalues is positive whereas the other two are negative. Indeed, its eigenvalues are the roots of the equation $(a+1)((a+1)^2-r)=0$, i.e. $-1<0, -1-\sqrt{r}<0$, and $-1+\sqrt{r})>0$. However, $C_\pm$ are locally stable for any $r>1$. Clearly, their eigenvalues are the roots of the equation $(a+2)(a^2+a+r-1=0)$, and their real part is always negative.

As in the case $r=1$, there is a family of semipermeable surfaces, $S_k: -rx^2+y^2+z^2=k$. For every $k>0$ ($k<0$) the tangent to the trajectory through a point on the surface S_k is directed inwardly (outwardly). Consequently, trajectories which start at a point which is not on the cone S_0 tend to it.

The cone $S_0: rx^2=y^2+z^2$ is invariant. Now we study the flow on this cone. Passing to polar coordinates, $y=\rho\cos\theta$, $z=\rho\sin\theta$, for $x>0$ we obtain the system

$$\dot{\rho}=\rho(\sqrt{r}\cos\theta-1), \quad \dot{\theta}=\frac{1}{\sqrt{r}}(\rho-r\sin\theta), \tag{54}$$

with $\rho\geqslant 0$ and $\theta\in\mathbb{S}^1$. We denote by S_0^+ the positive half-cone S_0 with $x>0$.

Step 1: We study the finite singular points of system (54). They are given by the equations (i) $\rho=0$, $\sin\theta=0$; and (ii) $\cos\theta=1/\sqrt{r}$, $\rho=r\sin\theta$. Equation (i) gives the following pairs (ρ,θ): (0, 0) and $(0,\pi)$; both of them correspond to the origin. Equation (ii) gives only the point $(\sqrt{r(r-1)},\theta)$ with $\cos\theta=1/\sqrt{r}$, $\sin\theta=\sqrt{(r-1)/r}>0$. The value of θ corresponding to $\sin\theta<0$ is not acceptable since it would give $\rho=r\sin\theta<0$.

The eigenvalues of the third point are given by the equation $a^2+a+r-1=0$, i.e. they are $(-1\pm\sqrt{5-4r})/2$ for $1<r\leqslant 5/4$ and $(-1\pm i\sqrt{-(5-4r)})/2$ for $r>5/4$. Therefore this point is a local attractor: a stable node if $1<r\leqslant 5/4$, and a stable focus if $r>5/4$.

Step 2: Now we determine the local phase portrait at the origin of system (54). When passing to polar coordinates (ρ,θ), the origin blows up to the circle $\rho=0$ ($\theta\in[0,2\pi[$). On this circle there

are two singular points: (0, 0) and $(0,\pi)$. The topological type of each of them can be determined using the Hartman-Grobman Theorem.

For the point (0, 0) the linearized flow has the associated matrix

$$\begin{pmatrix} \sqrt{r}-1 & 0 \\ \dfrac{1}{\sqrt{r}} & -\sqrt{r} \end{pmatrix},$$

with eigenvalues $-\sqrt{r}$ and $\sqrt{r}-1$ and corresponding eigenvectors $u_1=(0,1)$ and $u_2=(2r-\sqrt{r},1)$. Thus, the point (0, 0) is a saddle with stable manifold tangent to the direction u_1, and unstable manifold tangent to the direction u_2.

Similarly, the point $(0,\pi)$ is a saddle with stable manifold tangent to the direction $v_1=(-2r-\sqrt{r},1)$, and unstable manifold tangent to the direction $v_2=(0,1)$.

Finally, we can contract the circle $\rho=0$ to the origin to obtain the local phase portrait. The origin has two separatrices (one stable and one unstable) and two hyperbolic sectors.

Step 3: Now we study system (54) at infinity. Doing the change of variables $u=1/\rho$, system (54) becomes

$$\mathrm{d}u/\mathrm{d}t=-u(\sqrt{r}\cos\theta-1),\quad \mathrm{d}\theta/\mathrm{d}t=(1/u-r\sin\theta)/\sqrt{r}. \tag{55}$$

where $u>0$, $\theta\in\mathbb{S}^1$. After the time reparameterization $\mathrm{d}t=u\mathrm{d}s$, system (55) becomes

$$\mathrm{d}u/\mathrm{d}s=-u^2(\sqrt{r}\cos\theta-1),\quad \mathrm{d}\theta/\mathrm{d}s=(1-ru\sin\theta)/\sqrt{r}. \tag{56}$$

where $u\in\mathbb{R}$, $\theta\in\mathbb{S}^1$. The study of system (54) at infinity is now reduced to the study of system (56) at $u=0$. (We need system (56) instead of system (55) because the circle $u=0$ is invariant for system (56), whereas system (55) is not defined at $u=0$).

Note that the circle $u=0$ is an invariant curve of system (56). Moreover, it is a closed curve and it does not contain any singular points. Therefore, $u=0$ is a periodic orbit of system (56). We shall prove that $u=0$ is an unstable periodic orbit for system (56). System (56) can be written as

$$\mathrm{d}u/\mathrm{d}\theta=-u^2\sqrt{r}(\sqrt{r}\cos\theta-1)/(1-ru\sin\theta), \tag{57}$$

where $u\in\mathbb{R}$, $\theta\in\mathbb{S}^1$. Instead of studying the stability of the periodic orbit $u=0$ for system (57), which is hard to integrate, we note that if $u(t)$ is a solution of system (57) such that $\sup|u(t)|$ is sufficiently small, then $|u(t)r\sin\theta|<1$ for all t. Consequently, by using that $1/(1-x)=1+x+O(x^2)$ for $|x|<1$, we have that if $u(t)$ is a solution of system (57) such that $\sup|u(t)|$ is sufficiently small, then $u(t)$ satisfies

$$\mathrm{d}u/\mathrm{d}\theta=-\sqrt{r}u^2(\sqrt{r}\cos\theta-1)+O(u^3). \tag{58}$$

Solving Eq. (58) after omitting the terms of $O(u^3)$, we get the solution $u(\theta)=1/(r\sin\theta-\sqrt{r}\theta+1/u(0))$. Here $u(0)>0$ has to be small enough in order to insure that $u(t)\geqslant 0$ for all $\theta\in[0,2\pi]$. Since $u(2\pi)=1/-2\pi\sqrt{r}+1/u(0)>u(0)$, $u=0$ is an unstable periodic orbit for system (58), and consequently also unstable for systems (57) and (56). In short, the infinity of system (54) is unstable.

Step 4: Now we prove that system (54) has no periodic orbits. This follows from Bendixson's criterion (see Ref. 31), because the vector field of system (54) has constant divergence, equal to -1 in the whole plane $(\rho,\theta)\in\mathbb{R}_+\times\mathbb{S}^1$.

Step 5: Now if we summarize the results obtained for the global flow on the half-cone S_0^+, we get the conclusions of the statement of the theorem. ■

VII. DISCUSSION OF RESULTS

(1) System (1) belongs to a special class of quadratic systems which we describe now. It is known[9,6] that by spectral expansion and truncation, the governing equations of most fluid dynamical problems can be reduced to a quadratic system of N ordinary differential equations

$$\dot{x}_i = \sum_{j,k=1}^{N} a_{ijk} x_j x_k - \sum_{j=1}^{N} b_{ij} x_j + c_i \quad (i = 1, \ldots, N). \tag{59}$$

Hereafter, N is the truncation number. The indices i,j,k are ranging between 1 and N. The *quadratic coefficients* a_{ijk}, the *linear coefficients* b_{ij}, and the *forcing coefficients* c_i are real numbers. The overdot denotes differentiation with respect to time t. We denote $X=(x_1,x_2,\ldots,x_N)$. As usual, when $N=3$ we write x,y,z instead of x_1,x_2,x_3, respectively. Following the terminology of Ref. 9, we call the quadratic coefficients a_{ijk} *conservative* if

$$\sum_{i,j,k=1}^{N} a_{ijk} x_i x_j x_k = 0 \tag{60}$$

and not all of them are zero. System (59) is called a *forced system* if not all of its forcing coefficients c_i are zero. System (59) is called *dissipative* if its linear coefficients are such that

$$\sum_{i,j=1}^{N} b_{ij} x_i x_j > 0 \tag{61}$$

for any $X \neq 0$. Finally, system (59) is a *forced dissipative* system if it is forced and dissipative at the same time. It is known[9] that all trajectories of such a system eventually enter a ball and never leave it again.

An example of a forced dissipative system is the following one:

$$\dot{x} = s(y-x), \quad \dot{y} = -y - sx - xz, \quad \dot{z} = -bz + xy - b(r+s), \tag{62}$$

which is obtained from the famous Lorenz system[21]

$$\dot{x} = s(y-x), \quad \dot{y} = -y + rx - xz, \quad \dot{z} = -bz + xy. \tag{63}$$

by the change of variables $X=x, Y=y, Z=z-r-s$ (here, the parameters s,b,r are strictly positive).

According to the above definition, system (1) is also forced dissipative after imposing some restrictions on the parameters. For instance, condition (61) holds for system (1) if $b>0$ and $b^2+e^2+af>0$. If $r<1$ then system (18) is forced dissipative and therefore all its trajectories eventually enter an ellipsoid. However, in Theorem 12 we prove that system (18) has this property for any r.

Regarding the relation between system (1) and Lorenz system, we note that both of them are spectrally truncated versions of some partial differential equations. More precisely, system (63) originates in the coupled Navier-Stokes and heat equations, modeling the Rayleigh-Bénard convection problem, i.e., Eq. (5.31a,b) of Ref. 9, whereas system (1) arises from the nonlinear barotropic quasigeostrophic potential vorticity equation, i.e., Eq. (6.14) of Ref. 9. However, unlike system (63), system (1) includes the effects of topography and of Earth's rotation.

(2) If $b=0$ and parameters a,d,e,f are all strictly positive, then we reduced system (1) to system (11). This case is also considered in Refs. 2, 6, 7, and 9. However our approach leads to a complete description of the phase portrait. We also considered the cases when a,d,e,f are nonpositive. We proved that if $b=ef=0$ and $d\neq 0$, then system (1) is reduced to (9); i.e., to the simple pendulum.

(3) If $b\neq 0$ then we reduce system (1) to systems (16)–(18). If the other parameters are nonnegative, then systems (16) and (17) have only one singular point. It is a global attractor, in accordance with known results.[2,6,7,9] Also, system (18) has at most three singular points. It remains

to characterize first, if system (18) has only one singular point when it is a global attractor; and second if system (18) has three singular points, when two of them are stable and one is unstable. It was stated in Ref. 6 that this second question holds for system (1) when all its parameters are strictly positive. We have obtained this result in Theorem 20 in the case $c_1=c_2=0$ for any $r>1$.

(4) We proved that system (18) possesses the quadratic invariant algebraic surface $f=-r(x-c_1)^2+y^2+z^2=0$ if and only if $c_2=-rc_1$. A similar result holds for Lorenz system.[20]

(5) Knowing the invariant algebraic surface helps to determine the phase portrait of the system. As an application, we describe the phase portrait of system (18) when $c_1=c_2=0$ in Sec. VI.

(6) 1—In Ref. 6 DeSwart found that the singular points of system (1) for $b=c=0$ are of the form $(\bar{x},f\bar{x}/(\mathrm{d}\bar{x}-e),0)$ where $\bar{x}$ is an arbitrary real number. Moreover, if

$$e/d<\bar{x}<(aef)^{1/3}/d+e/d, \tag{64}$$

then the equilibrium point $(\bar{x},f\bar{x}/(\mathrm{d}\bar{x}-e),0)$ is unstable, because one of the eigenvalues of the Jacobian matrix of the system at this equilibrium point becomes positive. The number aef in (64) is nonzero only if a parameter related to amplitude topography is nonzero. Thus, the occurence of unstable equilibrium points of this type is physically interpreted as topographic instability.

In our approach we obtain that the singular points of system (11), which is the physically interesting reduced form of the above-mentioned system in the conservative case $b=c=0$, are of the form $(\bar{x},1/\bar{x},0)$ where $\bar{x}$ is an arbitrary real (nonzero) number. The eigenvalues of the Jacobian matrix of the system at $(\bar{x},1/\bar{x},0)$ are given by the equation $\Lambda(\Lambda^2-a)=0$ where $a=(1-\bar{x}^3)/\bar{x}$. Thus, if $0<\bar{x}<1$ then one of these eigenvalues is positive, and the equilibrium point $(\bar{x},1/\bar{x},0)$ is unstable. Condition $0<\bar{x}<1$ corresponds to Eq. (64) found in Ref. 6.

From Propositions 7, 8, and 9 we see that system (11) has singular points $(\bar{x},1/\bar{x},0)$ with $0<\bar{x}<1$ only when $h_1>8$; in this case, the equilibrium point P_2, which is a saddle point with two homoclinic orbits to it, is unstable and corresponds to topographic instability. This is a nice and new connection between topographic instability and homoclinic orbits. Such homoclinic orbits could be remnants of heteroclinic orbits of the six-component CdV model, in accordance with Ref. 4.

2—In Ref. 2 Charney and DeVore suggested that flow regimes should be identified with equilibrium solutions of the equations describing the evolution of large-scale atmospheric flow. In Ref. 4 it is suggested that regime transitions in deterministic atmosphere models are related to the existence of heteroclinic connections between these regimes. A characteristic property of the atmosphere is its *vacillation* behavior, i.e., the irregular fluctuation of atmospheric circulation between different preferent flow regimes which are also called weather regimes.[7]

Recall the dynamics of system (11) on the sphere I_{h_1}: for $0<h_1<8$ there are only two equilibria (flow regimes) which are centers, i.e., stable but not asymptotically stable, and all other orbits are periodic. As h_1 increases, new equilibria appear. When $h_1=8$, a third equilibrium occurs, and it is unstable, with a homoclinic orbit to it and with two hyperbolic sectors in a neighborhood of it. The point which are now on the homoclinic orbit where previously situated on a periodic orbit. When $h_1>8$, a fourth equilibrium point appears; it is a center, whereas the third equilibrium point is still unstable (a saddle with two homoclinic orbits to it).

Since system (11) has only periodic and homoclinic orbits, there are no transitions between equilibria. Thus, system (11) cannot model vacillation behavior. However, not any equilibrium point of an atmospheric model can be identified with a weather regime.[5] For instance, some conditions such as the presence of forcing and dissipation, are necessary.[8] Future work is necessary to clarify the role of homoclinic and heteroclinic orbits in transitions between weather regimes (when an equilibrium of a given model of atmospheric circulation (59) represents a weather regime? when a heteroclinic orbit between such equilibria represents a transition between weather regimes?).

3—We note that when $b=c=0$, system (1) can be interpreted as a Volterra gyrostat with two pairs of gyrostatic terms corresponding to rotation and topography effects (see Ref. 12).

(7) The problem of finding the values of parameters of a given quadratic system for which the system is chaotic, if such values do exist, is still open. Such values, but not all of them are known for Lorenz-63 model,[21] and for Lorenz-84 model,[29] but not for system (1).

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Integrability of the Bianchi IX system

Jaume Llibre[a)]
Departament de Matemàtiques, Universitat Autónoma de Barcelona, 08193 Bellaterra, Barcelona, Spain

Clàudia Valls[b)]
Departamento de Matemática, Instituto Superior Técnico, Av. Rovisco Pais 1049-001, Lisboa, Portugal

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In this paper we apply the Darboux theory of integrability to the classical Bianchi IX system. Thus, we provide a complete description of the Darboux polynomials, exponential factors, rational first integrals, and Darboux first integrals, for the classical Bianchi IX system. © *2005 American Institute of Physics.*
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I. INTRODUCTION TO THE PROBLEM

The Bianchi IX model can be written as the Hamiltonian system (see Ref. 8):

$$\dot{q}_1 = 12q_1(p_1q_1 - p_2q_2 - p_3q_3),$$

$$\dot{q}_2 = 12q_2(-p_1q_1 + p_2q_2 - p_3q_3),$$

$$\dot{q}_3 = 12q_3(-p_1q_1 - p_2q_2 + p_3q_3),$$

$$\dot{p}_1 = -12p_1(p_1q_1 - p_2q_2 - p_3q_3) - \tfrac{1}{3}(q_1 - q_2 - q_3),$$

$$\dot{p}_2 = -12p_2(-p_1q_1 + p_2q_2 - p_3q_3) - \tfrac{1}{3}(-q_1 + q_2 - q_3),$$

$$\dot{p}_3 = -12p_3(-p_1q_1 - p_2q_2 + p_3q_3) - \tfrac{1}{3}(-q_1 - q_2 + q_3), \tag{1}$$

in $\mathbb{R}^6$ with the Hamiltonian

$$G = 6(p_1^2q_1^2 + p_2^2q_2^2 + p_3^2q_3^2 - 2p_1q_1p_2q_2 - 2p_1q_1p_3q_3 - 2p_2q_2p_3q_3) + \frac{1}{6}(q_1^2 + q_2^2 + q_3^2 - 2q_1q_2 - 2q_1q_3 - 2q_2q_3).$$

This system has been throughly investigated from the point of view of integrability by using different methods for studying the existence of first integrals. One of these methods is the Painlevé test (see, for instance, Refs. 10, 5, and 6) where the authors prove that the solutions of the equation of motion do not have movable critical points and conjecture that system (1) is integrable. Later on, in Ref. 7 the same authors of Ref. 6 find new arguments, this time against the integrability. Another method is the numerical computation of the Lyapunov exponents (see Ref. 1), where the authors also conjecture the integrability of system (1). In Ref. 8 the authors, by means of sym-

[a)]Electronic mail: jllibre@mat.uab.es
[b)]Electronic mail: cvalls@math.ist.utl.pt

plectic geometrical techniques, prove that system (1) is locally integrable. In Ref. 12 it is shown that system (1) is not completely integrable in the Birkhoff sense. We also want to mention the work of Ref. 13, where the author proves that the Hamiltonian system (1) is not completely integrable with rational first integrals (see Theorem 2 in the following) using techniques from the differential Galois theory.

We say that the functions $F_1,\dots,F_n$ are in *involution* if $\{F_i,F_j\}=0$ for all $i\neq j$, where $\{\cdot,\cdot\}$ denotes the Poisson bracket. Moreover, they are *independent* if the one forms $dF_1,\dots,dF_n$ are linearly independent over a full Lebesgue measure subset of the common definition domain of F_j for $j=1,\dots,n$. By definition, a Hamiltonian system with n degrees of freedom having n independent first integrals in involution is *(completely) integrable*.

A *rational first integral* of system (1) is a rational function f which is constant over the trajectories of system (1), where it is defined.

The aim of this paper is to study the integrability of system (1) by using the Darboux theory of integrability (see Refs. 9 and 11). The main results of this paper are the following Theorems 1 and 3.

Theorem 1: *All rational first integrals of system* (1) *are rational functions in the variable G*.

As a corollary of Theorem 1 we obtain the following result given in Ref. 13.

Theorem 2: *The Hamiltonian system* (1) *is not completely integrable with rational first integrals*.

Note that Theorem 1 is stronger than Theorem 2.

Writing system (1) as

$$\dot{x}_j = X_j(x_1,\dots,x_6), \quad j=1,\dots,6, \tag{2}$$

we have the following three definitions.

A *Darboux polynomial* of system (1) is a polynomial $f\in\mathbb{C}[x_1,\dots,x_6]\backslash\mathbb{C}$ such that

$$\frac{\mathrm{d}f}{\mathrm{d}t}=\sum_{j=1}^{6}X_j\frac{\partial f}{\partial x_j}=Kf,$$

for some polynomial $K\in\mathbb{C}[x_1,\dots,x_6]$ called the *cofactor*. Taking into account the degrees of the polynomials which appear in the previous equation, it follows easily that the degree of the cofactor is at most 2. Note that $f=0$ is an invariant algebraic hypersurface for the flow of system (2).

Note that a *polynomial first integral* of system (1) is a Darboux polynomial with cofactor zero.

An *exponential factor* F of the polynomial differential system (1) is a function $F=\exp(f/g)\notin\mathbb{C}$ with $f,g\in\mathbb{C}[x_1,\dots,x_6]$ satisfying that

$$\frac{\mathrm{d}F}{\mathrm{d}t}=\sum_{j=1}^{6}X_j\frac{\partial F}{\partial x_j}=LF,$$

for some polynomial $L\in\mathbb{C}[x_1,\dots,x_6]$ of degree at most 2. See Proposition 7 for more details about the exponential factors.

A first integral G of system (1) is called *Darboux* if G is of the form

$$G=f_1^{\lambda_1}\dots f_p^{\lambda_p}F_1^{\mu_1}\dots F_q^{\mu_q},$$

where $f_1,\dots,f_p$ are Darboux polynomials, $F_1,\dots,F_q$ are exponential factors and $\lambda_j,\mu_k\in\mathbb{C}$, for $j=1,\dots,p$, $k=1,\dots,q$.

We note that for real polynomial differential systems, as system (1), when we look for their Darboux first integrals we use in general complex Darboux polynomials and complex exponential factors. This is due to the fact that these objects appear in pairs (one and its conjugate), and this forces that the Darboux first integral becomes real. For more details see Ref. 3.

The second main result of this paper is the following.

Theorem 3: *All Darboux first integrals of system (1) are of the form*

$$P_1^{\lambda_1} \cdots P_r^{\lambda_r} \exp(Q/R),$$

where P_i, Q, *and* R *are polynomials in* $\mathbb{C}[G]$ *and* $\lambda_i \in \mathbb{C}$ *for* $i=1,\ldots,r$.

This paper is organized as follows. In Sec. II we state some preliminary and basic results on the Darboux theory of integrability that will be used through the paper. In Sec. III we reduce the study of the Bianchi IX system to a homogeneous differential system. In Sec. IV we see that it is sufficient to study the homogeneous Darboux polynomials. In Secs. V and VI we analyze the homogeneous polynomial first integrals and the homogeneous Darboux polynomials with nonzero cofactor, respectively. Finally, in Sec. VII, we prove the main results of this paper.

II. PRELIMINARIES

We consider a differential system with polynomial right–hand sides

$$\dot{x}_j = X_j(x_1, \ldots, x_n), \quad j = 1, \ldots, n. \tag{3}$$

of degree m, i.e., $m=\max\{\deg X_j : j=1,\ldots,n\}$, defined in an open subset of $\mathbb{R}^n$. The proof of the next results can be found in Refs. 2–4, with the exception of Proposition 6 which can be proved easily.

Proposition 4: Let f *be a polynomial and* $f=\Pi_{j=1}^{s} f_j^{\alpha_j}$ *its decomposition into irreducible factors in* $\mathbb{C}[x_1,\ldots,x_n]$. *Then,* f *is a Darboux polynomial if and only if all the* f_j *are Darboux polynomials. Moreover, if* K *and* K_j *are the cofactors of* f *and* f_j, *then* $K=\Sigma_{j=1}^{s}\alpha_j K_j$.

Theorem 5: *Suppose that the differential polynomial system (3) defined in* $\mathbb{R}^n$ *of degree* m *admits* p *invariant algebraic hypersurfaces* $f_i=0$ *with cofactors* K_i *for* $i=1,\ldots,p$ *and* q *exponential factors* $F_j=\exp(g_j/h_j)$ *with cofactors* L_j *for* $j=1,\ldots,q$. *Then, there exist* λ_j, $\mu_j \in \mathbb{C}$ *not all zero such that* $\Sigma_{i=1}^{p}\lambda_i K_i + \Sigma_{j=1}^{q}\mu_j L_j = 0$ *if and only if the following real (multivalued) function of Darboux type*

$$f_1^{\lambda_1} \ldots f_p^{\lambda_p} F_1^{\mu_1} \ldots F_q^{\mu_q},$$

substituting $f_i^{\lambda_i}$ *by* $|f_i|^{\lambda_i}$ *if* $\lambda_i \in \mathbb{R}$, *is a first integral of system (3).*

Proposition 6: The existence of a rational first integral for a polynomial differential system (3) implies either the existence of a polynomial first integral, or the existence of two Darboux polynomials having the same nonzero cofactor.

Proposition 7: If $F=\exp(h/g)$ *is an exponential factor for the polynomial differential system (3) and* g *is not a constant polynomial, then* $g=0$ *is an invariant algebraic hypersurface of system (3) with multiplicity higher than 1.*

III. REDUCTION TO A HOMOGENEOUS DIFFERENTIAL SYSTEM

We do two changes of variables, the change $(q_1,q_2,q_3,p_1,p_2,p_3) \to (y_1,y_2,y_3,z_1,z_2,z_3)$ given by

$$y_i = q_i, \quad z_i = p_i q_i, \quad i = 1,2,3; \tag{4}$$

and the change $(y_1,y_2,y_3,z_1,z_2,z_3,t) \to (6y_1,6y_2,6y_3,z_1,z_2,z_3,t/12)$. In these last variables system (1) becomes

$$\begin{aligned}
\dot{y}_1 &= y_1(z_1 - z_2 - z_3),\\
\dot{y}_2 &= y_2(-z_1 + z_2 - z_3),\\
\dot{y}_3 &= y_3(-z_1 - z_2 + z_3),\\
\dot{z}_1 &= -y_1(y_1 - y_2 - y_3),
\end{aligned} \tag{5}$$

$$\dot{z}_2 = -y_2(-y_1 + y_2 - y_3),$$

$$\dot{z}_3 = -y_3(-y_1 - y_2 + y_3).$$

System (5) has the first integral:

$$H = \tfrac{1}{2}(z_1^2 + z_2^2 + z_3^2 - 2z_1z_2 - 2z_1z_3 - 2z_2z_3) + \tfrac{1}{2}(y_1^2 + y_2^2 + y_3^2 - 2y_1y_2 - 2y_1y_3 - 2y_2y_3).$$

Of course, H is the first integral G in the new variables.

Lemma 8: The following statements hold.

(a) *If* $f(y_1,y_2,y_3,z_1,z_2,z_3)$ *is a rational first integral of system (5), then* $f(q_1,q_2,q_3,p_1q_1,p_2q_2,p_3q_3)$ *is a rational first integral of system (1).*
(b) *If* $f(q_1,q_2,q_3,p_1,p_2,p_3)$ *is a rational first integral of system (1), then* $f(y_1,y_2,y_3,z_1/y_1,z_2/y_2,z_3/y_3)$ *is a rational first integral of system (5).*

Proof: (a) is immediate. Now we prove (b). If $f(q_1,q_2,q_3,p_1,p_2,p_3)$ is a rational first integral of system (1), this means that $f(q_1,q_2,q_3,p_1,p_2,p_3) = f_1(q_1,q_2,q_3,p_1,p_2,p_3)/f_2(q_1,q_2,q_3,p_1,p_2,p_3)$, with f_1 and f_2 polynomials. From (4), we define

$$\bar{f}(y_1,y_2,y_3,z_1,z_2,z_3) = f_1\left(y_1,y_2,y_3,\frac{z_1}{y_1},\frac{z_2}{y_2},\frac{z_3}{y_3}\right)/f_2\left(y_1,y_2,y_3,\frac{z_1}{y_1},\frac{z_2}{y_2},\frac{z_3}{y_3}\right).$$

Therefore, multiplying f_1 and f_2 by $y_1^{N_1}y_2^{N_2}y_3^{N_3}$ where, for $i=1,2,3$, $N_i=\max\{N_i^1,N_i^2\}$ with N_i^1 the maximum degree of f_1 in the variable p_i, and N_i^2 the maximum degree of f_2 in the variable p_i, we have that $\bar{f}(y_1,y_2,y_3,z_1,z_2,z_3)$ is also a rational first integral of system (5). ■

By Lemma 8, if we prove that the unique rational first integrals of system (5) are functions of H, Theorem 1 will be proved. Therefore, to prove Theorem 1, it is enough to prove the following result.

Theorem 9: *For system (5) the unique rational first integrals are rational functions in the variable* H.

For proving Theorem 9, we need previously to study the Darboux polynomials of system (5) with zero cofactor (i.e., the polynomial first integrals) and with nonzero cofactor. We will do that in the next three sections. In the first one we will see that it is sufficient to study the homogeneous Darboux polynomials. Finally, in Sec. VII we prove Theorem 9.

IV. REDUCTION TO HOMOGENEOUS DARBOUX POLYNOMIALS

The equation defining a Darboux polynomial f for system (5) is

$$\dot{y}_1\frac{\partial f}{\partial y_1} + \dot{y}_2\frac{\partial f}{\partial y_2} + \dot{y}_3\frac{\partial f}{\partial y_3} + \dot{z}_1\frac{\partial f}{\partial z_1} + \dot{z}_2\frac{\partial f}{\partial z_2} + \dot{z}_3\frac{\partial f}{\partial z_3} = Kf,$$

where the cofactor $K=a_0+a_1y_1+a_2y_2+a_3y_3+a_4z_1+a_5z_2+a_6z_3$.

Lemma 10: Any Darboux polynomial f *of system* (5) *has a cofactor of the form*

$$K = a_1y_1 + a_2y_2 + a_3y_3 + a_4z_1 + a_5z_2 + a_6z_3. \tag{6}$$

Proof: See Ref. 14 where the authors prove Lemma 10 in a more general context of arbitrary homogeneous polynomial systems. ■

Proposition 11: We write f *in sum of its homogeneous parts as* $f=f_1+\cdots+f_n$. *Then,* f *is a Darboux polynomial of system* (5) *with cofactor* K *if and only if for all* $j=1,\ldots,n$, f_j *is a Darboux polynomial of system* (5) *with cofactor* K.

Proof: See Ref. 14 where the authors prove Proposition 11 in a more general context of arbitrary homogeneous polynomial systems. ■

Proposition 12: System (5) *has exactly three irreducible Darboux polynomials of degree* 1,

namely y_1, y_2, *and* y_3.

Proof: It follows easily from the definition of Darboux polynomial. ■

Let $\tau:\mathbb{C}[y_1,y_2,y_3,z_1,z_2,z_3]\to\mathbb{C}[y_1,y_2,y_3,z_1,z_2,z_3]$ be the automorphism

$$\tau(y_i)=-y_i,\quad \tau(z_i)=z_i,\quad i=1,2,3;$$

and let $\sigma:\mathbb{C}[y_1,y_2,y_3,z_1,z_2,z_3]\to\mathbb{C}[y_1,y_2,y_3,z_1,z_2,z_3]$ be the automorphism

$$\sigma(y_1)=y_2,\quad \sigma(y_2)=y_3,\quad \sigma(y_3)=y_1,\quad \sigma(z_1)=z_2,\quad \sigma(z_2)=z_3,\quad \sigma(z_3)=z_1.$$

Proposition 13: If g is an irreducible (homogeneous) Darboux polynomial of degree >1 *for system* (5) *with cofactor K given by* (6), *then* $f=(g\cdot\sigma g\cdot\sigma^2 g)\cdot\tau(g\cdot\sigma g\cdot\sigma^2 g)$ *is a (homogeneous) Darboux polynomial invariant by* τ *and* σ *with a cofactor of the form* $2(a_4+a_5+a_6)(z_1+z_2+z_3)$. *If the cofactor of g is zero, then the cofactor of f is also zero. Moreover,* y_i *is not a factor f for i* $=1,2,3$.

Proof: Since system (5) is invariant under τ, σ, and σ^2, τg is a Darboux polynomial of system (5) with cofactor $\tau(K)$. Moreover, by Proposition 4, $g\cdot\sigma g\cdot\sigma^2 g$ is also a Darboux polynomial of (5) with cofactor $K+\sigma(K)+\sigma^2(K)$. Therefore, again by Proposition 4, the cofactor of f is $2(a_4+a_5+a_6)(z_1+z_2+z_3)$.

Finally, y_i is not a factor f for $i=1,2,3$, otherwise some y_i would be a factor of g, and g is irreducible of degree >1. ■

In Proposition 13 the parenthesis in the word homogeneous means that the statement of the proposition holds if g is homogeneous, as if it is not.

V. HOMOGENEOUS POLYNOMIAL FIRST INTEGRALS

In this section we study the homogeneous polynomial first integrals of system (5), or equivalently its homogeneous Darboux polynomials with zero cofactor.

Proposition 14: If f is a homogeneous polynomial first integral of degree n even for system (5) restricted to $y_1=0$, $z_1=0$, *then* $f=\sum_{k=0}^{n/2}a_k H_1^k H_2^{n/2-k}$ *with*

$$H_1=\tfrac{1}{2}(z_2-z_3)^2+\tfrac{1}{2}(y_2-y_3)^2,\quad H_2=y_2y_3. \tag{7}$$

Proof: Let f be a homogeneous polynomial first integral of degree n even of system (5) restricted to $y_1=0$, $z_1=0$. Then f satisfies

$$(z_2-z_3)\left(y_2\frac{\partial f}{\partial y_2}-y_3\frac{\partial f}{\partial y_3}\right)-(z_2-z_3)\left(y_2\frac{\partial f}{\partial z_2}-y_3\frac{\partial f}{\partial z_3}\right)=0. \tag{8}$$

By direct computation, it is straightforward to prove that H_1, H_2, and linear combinations of them are the unique polynomial first integrals of system (5) restricted to $y_1=0$, $z_1=0$ of degree $n=2$. So, the proposition is proved if $n=2$. Assume, by induction, that it is proved until degree $n-2$ and we shall prove it for degree n. We denote by $\bar{f}_2=f(0,y_3,z_2,z_3)$. Then, restricting (8) to $y_2=0$, we get that $\bar{f}_2$ is a first integral of the system

$$\dot{z}_2=0,\quad \dot{y}_3=y_3(z_3-z_2),\quad \dot{z}_3=-y_3^2. \tag{9}$$

Now, we do the linear change of variables $x_1=z_2$, $x_2=z_2-z_3+iy_3$ and $x_3=z_2-z_3-iy_3$. In these new variables system (9) becomes

$$\dot{x}_1=0,\quad \dot{x}_2=-\tfrac{1}{2}(x_2-x_3)x_2,\quad \dot{x}_3=\tfrac{1}{2}(x_2-x_3)x_3. \tag{10}$$

Since the change of variables is linear, if we have a polynomial first integral of system (10) we have a polynomial first integral of system (9) and vice versa.

Let $g=g(x_1,x_2,x_3)$ be a polynomial first integral of system (10). Then, after dividing by $(x_2-x_3)/2$, g satisfies

$$-x_2\frac{\partial g}{\partial x_2}+x_3\frac{\partial g}{\partial x_3}=0. \tag{11}$$

The general solution of this linear partial differential equation is an arbitrary function of x_2x_3. Since we are only interested in the homogeneous polynomial solutions of degree n of (11) in the variables x_1, x_2, x_3, g must be a polynomial in x_2x_3 with coefficients polynomials in the variable x_1. Thus, we have

$$\bar{f}_2=\sum_{l+2k=n} a_{l,k}z_2^l((z_2-z_3)^2+y_3^2)^k.$$

Now, taking the notation $\bar{f}_3=f(y_2,0,z_2,z_3)$, restricting (8) to $y_3=0$ and proceeding as for $\bar{f}_2$, we get that $\bar{f}_3$ has the form

$$\bar{f}_3=\sum_{l+2k=n} b_{l,k}z_3^l((z_2-z_3)^2+y_2^2)^k.$$

We note that for $y_2=y_3=0$, $\bar{f}_2$ restricted to $y_3=0$ and $\bar{f}_3$ restricted to $y_2=0$ must coincide. Thus, we get the relation

$$\sum_{l+2k=n} a_{l,k}z_2^l(z_2-z_3)^{2k}=\sum_{l+2k=n} b_{l,k}z_3^l(z_2-z_3)^{2k}. \tag{12}$$

We claim that

$$a_{l,k}=b_{l,k}=0, \quad \text{for all } l>0 \text{ and } a_{0,n/2}=b_{0,n/2}. \tag{13}$$

First, we prove the claim for $l=n$ ($n\geqslant 2$). To do it, we restrict (12) to $z_2=z_3$. Then, we get $a_{n,0}z_2^n=b_{n,0}z_3^n$, which obviously implies $a_{n,0}=b_{n,0}=0$. Suppose that the claim is true for $l=n,\ldots,n-2m$ with $0\leqslant m<(n-2)/2$. Then, we want to prove it for $l=n-2(m+1)$. Clearly, by induction hypothesis, (12) is equal to

$$\sum_{l+2k=n,l\leqslant n-2m} a_{l,k}z_2^l(z_2-z_3)^{2k}=\sum_{l+2k=n,l\leqslant n-2m} b_{l,k}z_3^l(z_2-z_3)^{2k}. \tag{14}$$

In the equality (12), we substitute the equality (14), so it remains as the terms with $k>m$. Therefore, we can remove the common factor $(z_2-z_3)^{2m+2}$, and (12) becomes

$$\sum_{l+2k=n,k>m} a_{l,k}z_2^l(z_2-z_3)^{2(k-m-1)}=\sum_{l+2k=n,k>m} b_{l,k}z_3^l(z_2-z_3)^{2(k-m-1)}.$$

So, $a_{l,k}=b_{l,k}=0$ for $l=n-2(m+1)$. Thus, by induction hypothesis, (12) reduces to $a_{0,n/2}(z_2-z_3)^n=b_{0,n/2}(z_2-z_3)^n$, which obviously implies $a_{0,n/2}=b_{0,n/2}$ and finishes the proof of the claim. Therefore, from (13) we get $\bar{f}_2=a_{0,n/2}((z_2-z_3)^2+y_3^2)^{n/2}$ and $\bar{f}_3=b_{0,n/2}((z_2-z_3)^2+y_2^2)^{n/2}$.

Now, by the Newton's binomial formula, we get

$$((z_2-z_3)^2+y_2^2+y_3^2)^{n/2}=((z_2-z_3)^2+y_3^2)^{n/2}+y_2^2g_1,$$

$$((z_2-z_3)^2+y_2^2+y_3^2)^{n/2}=((z_2-z_3)^2+y_2^2)^{n/2}+y_3^2g_2,$$

where g_1 and g_2 are of homogeneous polynomial of degree $n-2$. Then, using this and the fact that $\bar{f}_2$ is the restriction of f to $y_2=0$, we can write

$$f=\bar{f}_2+y_2g_3=a_{0,n/2}((z_2-z_3)^2+y_2^2+y_3^2)^{n/2}+y_2g_4+y_2y_3g_5,$$

where g_4,g_5 are polynomials, and g_4 does not depend on y_3. In an analogous way, since $\bar{f}_3$ is the restriction of f to $y_3=0$, we can write

$$f = a_{0,n/2}((z_2 - z_3)^2 + y_2^2 + y_3^2)^{n/2} + y_3 g_6 + y_2 y_3 g_7,$$

where g_6 and g_7 are polynomials, and g_6 does not depend on y_2. Then, equating these two expressions for f we obtain $y_2 g_4 - y_3 g_6 = y_2 y_3 (g_5 - g_7)$, which obviously yields $g_4 = g_6 = 0$ and $g_7 = g_5$. Thus, since $(z_2 - z_3)^2 + y_2^2 + y_3^2 = 2(H_1 + H_2)$, also by the Newton's binomial formula, we obtain

$$f = a_{0,n/2}((z_2 - z_3)^2 + y_2^2 + y_3^2)^{n/2} + y_2 y_3 g_5 = 2^{n/2} a_{0,n/2} H_1^{n/2} + y_2 y_3 g_8,$$

for some homogeneous polynomial g_8. Then, since f, $y_2 y_3$ and H_1 are first integrals of system (5) restricted to $y_1 = 0$, $z_1 = 0$, we have that g_8 is also a first integral of system (5) restricted to $y_1 = 0$, $z_1 = 0$ of degree $n-2$. Hence, by induction assumption, g_8 can be written as in the statement of the proposition, with n replaced by $n-2$. Therefore, the proposition follows for f. ■

Proposition 15: If f is a homogeneous polynomial first integral of degree n even for system (5) *restricted to* $y_1 = 0$, *then* $f = \Sigma_{l+2k=n} a_{l,k} z_1^l H_3^k$ *with*

$$H_3 = \frac{1}{2}(z_1^2 + z_2^2 + z_3^2 - 2z_1 z_2 - 2z_1 z_3 - 2z_2 z_3) + \frac{1}{2}(y_2 - y_3)^2.$$

Proof: Let f be a homogeneous polynomial first integral of degree n even of system (5) restricted to $y_1 = 0$, then f satisfies

$$y_2(-z_1 + z_2 - z_3)\frac{\partial f}{\partial y_2} + y_3(-z_1 + z_3 - z_2)\frac{\partial f}{\partial y_3} - (y_2 - y_3)\left(y_2 \frac{\partial f}{\partial z_2} - y_3 \frac{\partial f}{\partial z_3}\right) = 0.$$

By direct computation, it is straightforward to prove that the unique first integrals of degree 2 of system (5) restricted to $y_1 = 0$, are z_1^2, H_3 and linear combinations of them. So, the proposition is proved if $n = 2$ and we can assume that $n \geqslant 4$. Moreover, we assume, by induction, that it is proved until degree $n-2$ and we shall prove it for degree n.

We first consider the restriction of system (5) to $y_1 = 0$, $z_1 = 0$. Any homogeneous polynomial first integral f of system (5) of degree n even restricted to $y_1 = 0$, $z_1 = 0$ satisfies (8) with f replaced by $\bar{f}$, where $\bar{f} = \bar{f}(y_2, y_3, z_2, z_3) = f(y_2, y_3, 0, z_2, z_3)$.

By Proposition 14, we have that $\bar{f} = \Sigma_{2k+2m=n} a_{k,m} H_1^k H_2^m$, where H_1 was introduced in (7), and $a_{k,m} \in \mathbb{C}$. Since $\bar{f}$ is the restriction of f to $z_1 = 0$, is also a homogeneous polynomial of degree n, and $H_3 = H_1 + \frac{1}{2} z_1 (z_1 - 2z_2 - 2z_3)$, we get that

$$f = \sum_{2k+2m=n} a_{k,m} H_3^k H_2^m + z_1 g_3, \tag{15}$$

with $g_3 = g_1 + g_2$ a homogeneous polynomial of degree $n-1$.

Now, since f, z_1, and H_3 are first integrals of system (5) restricted to $y_1 = 0$, we obtain, after simplifying by z_1, that

$$\frac{\mathrm{d}g_3}{\mathrm{d}t} = 2 \sum_{2k+2m=n} a_{k,m} m H_3^k H_2^m, \tag{16}$$

where this expression is evaluated along a solution of system (5) restricted to $y_1 = 0$. We write $g_3 = \bar{g}_3 + z_1 g_4$, where $\bar{g}_3$ is a homogeneous polynomial of degree $n-1$ and g_4 is a homogeneous polynomial of degree $n-2$. Further, $\bar{g}_3$ satisfies (16) restricted to $z_1 = 0$, that is

$$\frac{d\bar{g}_3}{dt} = 2 \sum_{2k+2m=n} a_{k,m} m H_1^k H_2^m, \tag{17}$$

where this expression is evaluated along a solution of system (5) restricted to $y_1 = 0$, $z_1 = 0$. Now, we claim that

$$\bar{g}_3 = y_2 y_3 h_1 \quad \text{for some polynomial } h_1 = h_1(z_2, z_3, y_2, y_3). \tag{18}$$

To prove (18), we restrict (17) to $y_2=0$ and denote by $\tilde{g}_3$ the restriction of $\bar{g}_3$ to $y_2=0$. Then, if we introduce the variables $x_1=z_2$, $x_2=z_2-z_3+iy_3$, $x_3=z_2-z_3-iy_3$, and denote $\tilde{g}_3(z_2,z_3,y_3)=G(x_1,x_2,x_3)$, we get, after dividing by $(x_2-x_3)/2$, that G satisfies (11) with g replaced by G. Thus, the same arguments used in the proof of Proposition 14 imply that $\tilde{g}_3=\Sigma_{l+2k=n-1}c_{l,k}z_2^l((z_2-z_3)^2+y_3^2)^k$. Further, if we denote by $\hat{g}_3$ the restriction of $\bar{g}_3$ to $y_3=0$, then proceeding as for $\tilde{g}_3$ we get that $\hat{g}_3=\Sigma_{l+2k=n-1}d_{l,k}z_3^l((z_2-z_3)^2+y_2^2)^k$. We note that for $y_2=y_3=0$, $\tilde{g}_3$ restricted to $y_3=0$ and $\hat{g}_3$ restricted to $y_2=0$ must coincide. Thus we get the relation

$$\sum_{l+2k=n-1} c_{l,k} z_2^l (z_2 - z_3)^{2k} = \sum_{l+2k=n-1} d_{l,k} z_3^l (z_2 - z_3)^{2k}. \tag{19}$$

We claim that

$$c_{l,k} = d_{l,k} = 0 \quad \text{for all } l \geqslant 1. \tag{20}$$

Proceeding exactly in the same way as in the proof of claim (13) we can prove by induction that $c_{l,k}=d_{l,k}=0$ for $l\geqslant 3$. Then, (19) reduces to $c_{1,(n-2)/2}z_2(z_2-z_3)^{n-2}=d_{1,(n-2)/2}z_3(z_2-z_3)^{n-2}$ which clearly implies $c_{1,(n-2)/2}=d_{1,(n-2)/2}=0$ and finishes the proof of the claim. Therefore from (20), we get that $\tilde{g}_3=\hat{g}_3=0$. Now, using that $\tilde{g}_3$ is the restriction of $\bar{g}_3$ to $y_2=0$ and $\hat{g}_3$ is the restriction of $\bar{g}_3$ to $y_3=0$, we can write $\bar{g}_3$ in the two following forms $\bar{g}_3=y_2G_0$ and $\bar{g}_3=y_3G_1$, where G_0, G_1 are polynomials. Then, equating the two expressions for $\bar{g}_3$ we readly obtain $\bar{g}_3=y_2y_3h_1$ for some polynomial h_1. Thus, the claim (18) is proved.

Now, from (18) and (16), and after dividing by $H_2=y_2y_3$ we get

$$\frac{\mathrm{d}h_1}{\mathrm{d}t} = 2 \sum_{2k+2m=n, m\geqslant 1} a_{k,m} m H_1^k H_2^{m-1}. \tag{21}$$

We claim that

$$a_{k,m} = 0,\ h_1 = (y_2 y_3)^m h_{m+1} \quad \text{for } m = 1, \ldots, n/2 \tag{22}$$

where h_{m+1} are polynomials.

First, we prove the claim (22) for $m=1$. To do it, we restrict (21) to $y_2=0$. Then, taking the notation $\tilde{h}_1$ for the restriction of h_1 to $y_2=0$, using the variables x_1,x_2,x_3 introduced previously, and denoting $F(x_1,x_2,x_3)=\tilde{h}_1(z_2,z_3,y_3)$ we get

$$\frac{x_2 - x_3}{2}\left(-x_2\frac{\partial F}{\partial x_2} + x_3\frac{\partial F}{\partial x_3}\right) = a_{(n-2)/2,1}\left(\frac{1}{2}x_2x_3\right)^{(n-2)/2} \tag{23}$$

Evaluating (23) on $x_2=x_3$, we get $a_{(n-2)/2,1}=0$. Since (21) is of the same type as (17) replacing $\bar{g}_3$ by h_1, the same arguments used for $\bar{g}_3$ imply that $h_1=y_2y_3h_2$ for some polynomial h_2. This proves the claim for $m=1$.

Now, assume the claim is true for $1\leqslant m\leqslant j$ with $0<j<n/2$. Then, we want to prove it for $m=j+1$. Clearly, by induction hypotheses $h_1=(y_2y_3)^jh_{j+1}$ and since y_2y_3 is a first integral of system (5) restricted to $y_1=0$, $z_1=0$, after simplifying by $(y_2y_3)^j$, (21) is equal to

$$\frac{dh_{j+1}}{dt} = 2 \sum_{2k+2m=n, m\geqslant j+1} a_{k,m} m H_1^k H_2^{m-j-1} = 2 \sum_{2k+2m=n, k\leqslant n/2-(j+1)} a_{k,m} m H_1^k H_2^{m-j-1}.$$

Now, repeating for h_{j+1} the arguments we did for h_1 in the case $m=1$, we get that $a_{n/2-j-1,j+1}=0$ and $h_{j+1}=y_2y_3h_{j+2}$ for some polynomial h_{j+2}. Hence, the claim is proved.

In short, using the claim (22) we have, $\bar{g}_3=(y_2y_3)^{n/2+1}h_{n/2+1}$, which due to the fact that the degree of $\bar{g}_3$ is $n-1$ we get that $h_{n/2+1}=0$ and thus $\bar{g}_3=0$. Further, applying the claim (22) to (15), we obtain $f=a_{n/2,0}H_3^{n/2}+z_1^2g_4$. Then, since f, H_3, and z_1 are first integrals of system (5) restricted to

$y_1=0$, we have that g_4 is also a first integral of system (5) restricted to $y_1=0$ of degree $n-2$. Hence, by induction assumption g_4 can be written as in the statement of the proposition with n replaced by $n-2$. Therefore, the proposition follows for f. ■

VI. HOMOGENEOUS DARBOUX POLYNOMIALS WITH NONZERO COFACTOR

The objective of this section is to study the homogeneous Darboux polynomials of system (5) with nonzero cofactor.

Proposition 16. System (5) has no homogeneous Darboux polynomials invariant by τ and σ with cofactor $K=a(z_1+z_2+z_3)$, $a\in\mathbb{C}\backslash\{0\}$ that are coprime with y_1, y_2, and y_3.

Proof: Let f be a homogeneous Darboux polynomial invariant by τ and σ with cofactor $K=a(z_1+z_2+z_3)$, $a\in\mathbb{C}\backslash\{0\}$ that is coprime with y_1, y_2, and y_3. By Proposition 12, the degree n of f satisfies that $n>1$, and by assumptions, y_i is not a factor f for $i=1,2,3$. Now, the proof of the proposition will be completed if we reach a contradiction. We write $f_0=f_0(y_2,y_3,z_1,z_2,z_3)=f(0,y_2,y_3,z_1,z_2,z_3)$. Since y_1 is not a factor f, then $f_0\neq 0$. We separate the proof in two different cases.

Case 1: f_0 is not divisible by y_2. In this case, we can write $f_{0,0}=f_0(0,y_3,z_1,z_2,z_3)$. Then, the polynomial $f_{0,0}$ is a Darboux polynomial of system (5) restricted to $y_1=y_2=0$ and thus, it satisfies the equation

$$y_3(-z_1-z_2+z_3)\frac{\partial f_{0,0}}{\partial y_3}-y_3^2\frac{\partial f_{0,0}}{\partial z_3}=a(z_1+z_2+z_3)f_{0,0}. \tag{24}$$

Hence, from (24) and since $a\neq 0$, $f_{0,0}$ is divisible by y_3. We write $f_{0,0}=y_3^m g$ where $1\leqslant m\leqslant n$, $\deg(g)=n-m$, $g\neq 0$ and g is not divisible by y_3. We have that $m<n$; otherwise, $f_{0,0}=by_3^n$ with $b\in\mathbb{C}\backslash\{0\}$, and from (24) we get a contradiction. From (24) and Proposition 4, we obtain that g is a Darboux polynomial of system (5) restricted to $y_1=y_2=0$ satisfying

$$y_3(-z_1-z_2+z_3)\frac{\partial g}{\partial y_3}-y_3^2\frac{\partial g}{\partial z_3}=[a(z_1+z_2+z_3)+m(z_1+z_2-z_3)]g.$$

Hence, if $m<n$ then g is divisible by y_3, a contradiction. Thus, Case 1 is not possible.

Case 2: f_0 is divisible by y_2. In this case, we write $f_0=y_2^m g$ where $1\leqslant m\leqslant n$, $\deg(g)=n-m$, $g\neq 0$ and g is not divisible by y_2. We have that $m<n$; otherwise, $f_0=by_2^m$ with $b\in\mathbb{C}\backslash\{0\}$ and $y_2(-z_1+z_2-z_3)\partial f_0/\partial y_2=a(z_1+z_2+z_3)f_0$, a contradiction. Since f_0 and y_2 are Darboux polynomials of system (5) restricted to $y_1=0$, from Proposition 4, g is also a Darboux polynomial of system (5) restricted to $y_1=0$ satisfying

$$\begin{aligned}&y_2(-z_1+z_2-z_3)\frac{\partial g}{\partial y_2}+y_3(-z_1-z_2+z_3)\frac{\partial g}{\partial y_3}-y_2(y_2-y_3)\frac{\partial g}{\partial z_2}-y_3(-y_2+y_3)\frac{\partial g}{\partial z_3}\\&\quad=[a(z_1+z_2+z_3)-m(-z_1+z_2-z_3)]g.\end{aligned}$$

We write $g_0=g(0,y_3,z_1,z_2,z_3)$. Since g is not divisible by y_2 we have that $g_0\neq 0$. Moreover, g_0 is a Darboux polynomial of system (5) restricted to $y_1=y_2=0$, and g_0 satisfies

$$y_3(-z_1-z_2+z_3)\frac{\partial g_0}{\partial y_3}-y_3^2\frac{\partial g_0}{\partial z_3}=[a(z_1+z_2+z_3)-m(-z_1+z_2-z_3)]g_0. \tag{25}$$

Hence, g_0 is divisible by y_3 and we can write $g_0=y_3^l h$, where $1\leqslant l\leqslant n-m$, $h\neq 0$ and h is not divisible by y_3. We have that $l<n-m$; otherwise, $g_0=by_3^{n-m}$ with $b\in\mathbb{C}\backslash\{0\}$, and we get a contradiction using (25). Again from (25) and Proposition 4, we have that

$$y_3(-z_1-z_2+z_3)\frac{\partial h}{\partial y_3}-y_3^2\frac{\partial h}{\partial z_3}=[(a+m+l)z_1+(a-m+l)z_2+(a+m-l)z_3]h. \tag{26}$$

Note that since $m\neq 0$ and $l\neq 0$, then $(a+m+l)z_1+(a-m+l)z_2+(a+m-l)z_3\neq 0$. Hence, from (26), we get that h must be divisible by y_3, a contradiction. Thus, Case 2 is not possible. ■

VII. PROOF OF THE MAIN RESULTS

The next two results will play a main role in the proofs of Theorems 1 and 3, our main results.

Theorem 17. *All homogeneous Darboux polynomials of degree n with zero cofactor (i.e., homogeneous polynomial first integrals of degree n) for system (5) are of the form* $aH^{n/2}$ *with n even and* $a\in\mathbb{C}\backslash\{0\}$.

Proof: Let g be a homogeneous polynomial first integral of system (5) of degree n. By Proposition 13, $f=(g\cdot\sigma g\cdot\sigma^2 g)\cdot\tau(g\cdot\sigma g\cdot\sigma^2 g)$ is a homogeneous polynomial first integral invariant by τ and σ of degree equal to $6n$. We claim that there exists a polynomial h such that

$$f=a_{3n}H^{3n}+y_1y_2y_3h. \tag{27}$$

From Proposition 15 (with n replaced by $6n$) and since f is invariant by σ, we have that there exist a homogeneous polynomial g_3 such that

$$f=\sum_{l+k=3n}a_{l,k}z_1^{2l}H_3^k+y_1g_3=\sum_{l+k=3n}a_{l,k}z_2^{2l}H_4^k+y_2\cdot\sigma g_3=\sum_{l+k=3n}a_{l,k}z_3^{2l}H_5^k+y_3\cdot\sigma^2 g_3, \tag{28}$$

where $H_4=\sigma H_3$ and $H_5=\sigma^2 H_3$.

Restricting (28) to $y_1=y_2=y_3=0$, we get the

$$\sum_{l+k=3n}a_{l,k}z_1^{2l}\bar{H}^k=\sum_{l+k=3n}a_{l,k}z_2^{2l}\bar{H}^k=\sum_{l+k=3n}a_{l,k}z_3^{2l}\bar{H}^k,$$

where $\bar{H}=\frac{1}{2}(z_1^2+z_2^2+z_3^2-2z_1z_2-2z_1z_3-2z_2z_3)$. These equalities between polynomials in the variables $\bar{H}$, z_1, z_2 and z_3 imply that $a_{l,k}=0$ for $l>0$. Therefore, from the first equation of (28) we have

$$f=a_{0,3n}H_3^{3n}+y_1g_3. \tag{29}$$

Since $H=H_3+\frac{1}{2}y_1(y_1-2y_2-2y_3)=H_3+y_1h$, we obtain that $H_3^{3n}=H^{3n}+y_1T_1$, where T_1 is a homogeneous polynomial of degree $n-1$. Therefore, taking into account that H is invariant by σ, (29) can be written in the three equivalent forms,

$$f=a_{0,3n}H^{3n}+y_1f^3=a_{0,3n}H^{3n}+y_2\cdot\sigma f^3=a_{0,3n}H^{3n}+y_3\cdot\sigma^2 f^3, \tag{30}$$

where f^3 is a homogeneous polynomial of degree $6n-1$. Now, equating the three identities of (30), it follows that the claim (27) is proved.

From (27) and since f and H are invariant by σ and τ, it follows that $h=\sigma h=-\tau h$. Moreover, since f and H are first integrals of system (5), we have

$$0=\frac{d}{dt}(y_1y_2y_3h)=y_1y_2y_3\left(-(z_1+z_2+z_3)h+\frac{dh}{dt}\right),$$

on the solutions of system (5). Therefore, h is either 0, or a Darboux polynomial of system (5) with cofactor $K=z_1+z_2+z_3$. Therefore, the polynomial $h^2=-h\cdot\tau h$ is a Darboux polynomial of system (5) with cofactor $2K$ (see Proposition 4) invariant by σ and by τ.

From Proposition 16, if $h\neq 0$, then $h^2=Py_1^{n_1}y_2^{n_2}y_3^{n_3}$ with P a Darboux polynomial of system (5) with zero cofactor and n_1,n_2,n_3 nonnegative integers satisfying $n_1+n_2+n_3\geqslant 1$, because $2K$ is nonzero. Since h^2 is a Darboux polynomial of cofactor $2K$, using Proposition 4 we get

$$\frac{dh^2}{dt} = [z_1(n_1 - n_2 - n_3) + z_2(-n_1 + n_2 - n_3) + z_3(-n_1 - n_2 + n_3)]h^2 = 2(z_1 + z_2 + z_3)h^2.$$

Therefore, $n_1 = n_2 = n_3 = -2$, a contradiction with the fact that $n_1 + n_2 + n_3 \geqslant 1$. Thus, $h^2 = 0$, that is, $h = 0$ and consequently from (27), $f = a_{3n}H^{3n}$. Hence, since H is irreducible, by the definition of f, it follows that $3n$ must be even, i.e., n must be even and g is of the form $aH^{n/2}$. So, the theorem is proved. ■

Theorem 18. *For system (5) the unique irreducible homogeneous Darboux polynomials with nonzero cofactor are* y_1, y_2, and y_3.

Proof: By Proposition 12, if g is an irreducible homogeneous Darboux polynomial of degree 1, it must be y_1, y_2, or y_3. Now, assume that g is an irreducible homogeneous Darboux polynomial of degree $n > 1$ for system (5) with nonzero cofactor K of the form (6). Then, from Proposition 13, we can assume that $f = (g \cdot \sigma g \cdot \sigma^2 g) \cdot \tau(g \cdot \sigma g \cdot \sigma^2 g)$ is a homogeneous Darboux polynomial invariant by τ and σ, with degree $6n$ and nonzero cofactor of the form $2(a_4 + a_5 + a_6)(z_1 + z_2 + z_3)$ and such that y_i is not a factor f for $i = 1, 2, 3$. From Proposition 16, we get that $a_4 + a_5 + a_6 = 0$, otherwise we have a contradiction. Hence, f is a homogeneous polynomial first integral of system (5). By Theorem 17, f is of the form aH^{3n} with n even and $a \in \mathbb{C}\backslash\{0\}$. Therefore, from the definition of f and since H and g are irreducible and invariant for σ and τ, it follows that $g = bH^{n/2}$, in contradiction with the fact that the cofactor of g is not zero. ■

Now we prove Theorem 9, that as it was shown in Sec. III is equivalent to prove Theorem 5.

Proof of Theorem 9: By Theorems 17 and 18, it follows that every Darboux polynomial of system (5) is of the form $y_1^m y_2^n y_3^l P_H$ with cofactor

$$K = (m - n - l)z_1 + (n - m - l)z_2 + (l - m - n)z_3, \tag{31}$$

where m, n, and l are nonnegative integers, and P_H is some polynomial of the variable H.

From Proposition 6 and Theorem 17, the existence of a rational first integral which is not a function of H, implies the existence of two coprime Darboux polynomials with the same nonzero cofactor. So, the first integral must be of the form $R/S = y_1^{m_1} y_2^{n_1} y_3^{l_1} P_H / (y_1^{m_2} y_2^{n_2} y_3^{l_2} Q_H)$ with at most one m_i, n_i, and l_i nonzero, and the cofactors of R and S must be equal.

Suppose that m_1, n_1, and l_2 are the possible nonzero exponents. Then, according to Eq. (31), the equality of the cofactors of R and S imply that

$$(m_1 - n_1 + l_2)z_1 + (n_1 - m_1 + l_2)z_2 - (l_2 + m_1 + n_1)z_3 = 0.$$

Hence, $m_1 = n_1 = l_2 = 0$. All the other combinations with the possible non-zero exponents, also end showing that the six exponents are zero. In short, the only rational first integrals are rational functions in the variable H. ■

The equation defining the exponential factor $F = \exp(h/g)$ with cofactor L is

$$\dot{y}_1 \frac{d}{dy_1}\frac{h}{g} + \dot{y}_2 \frac{d}{dy_2}\frac{h}{g} + \dot{y}_3 \frac{d}{dy_3}\frac{h}{g} + \dot{z}_1 \frac{d}{dz_1}\frac{h}{g} + \dot{z}_2 \frac{d}{dz_2}\frac{h}{g} + \dot{z}_3 \frac{d}{dz_3}\frac{h}{g} = L, \tag{32}$$

where we have simplified the common factor F, and

$$L = b_0 + b_1 y_1 + b_2 y_2 + b_3 y_3 + b_4 z_1 + b_5 z_2 + b_6 z_3. \tag{33}$$

According to Proposition 7 and Theorems 17 and 18, if system (5) has exponential factors, they must be of the form $\exp(h/(y_1^{n_1} y_2^{n_2} y_3^{n_3}))$, $\exp(h/(y_1^{n_1} y_2^{n_2} y_3^{n_3} P_H))$, where h and P_H are polynomials in $\mathbb{C}[y_1, y_2, y_3, z_1, z_2, z_3]$ and $\mathbb{C}[H]$, respectively; and n_1, n_2, and n_3 are nonnegative integers.

We shall need the following auxiliary result.

Proposition 19: The unique irreducible homogeneous Darboux polynomials with non-zero cofactor of system (5) restricted to $y_1 = z_1 = 0$ *are* y_2 *and* y_3.

Proof: It follows by direct computations that if g is an irreducible homogeneous Darboux polynomial of degree 1 for system (5) restricted to $y_1 = z_1 = 0$, it must be y_2 or y_3. Now, assume that g is an irreducible homogeneous Darboux polynomial of degree $n > 1$ for system (5) restricted to

$y_1=z_1=0$ with nonzero cofactor K of the form (6) restricted to $y_1=z_1=0$. Then, we can assume that $f=(g\cdot\sigma g)\cdot\tau(g\cdot\sigma g)$ is a homogeneous Darboux polynomial invariant by τ and σ, with degree $4n$, nonzero cofactor of the form $2(a_5+a_6)(z_2+z_3)$ and such that y_2 and y_3 are not factors f. Repeating the arguments used in the proof of Proposition 16 with $y_1=z_1=0$, we get that $a_5+a_6=0$, otherwise we have a contradiction. Hence, f is a homogeneous polynomial first integral of system (5) restricted to $y_1=z_1=0$. By Proposition 14 (with n replaced by $4n$), f is of the form $f=\sum_{k=0}^{2n}a_kH_1^kH_2^{n/2-k}$, with n even and $a_k\in\mathbb{C}\backslash\{0\}$. Therefore, from the definition of f it follows that $g=g(H_1,H_2)$, in contradiction with the fact that the cofactor of g is not zero. ■

Proposition 20: The unique exponential factors of system (5) are of the form $\exp(P)$ *and* $\exp(P/Q)$, *where P and Q are polynomials in $\mathbb{C}[H]$. Moreover, such exponential factors have cofactor zero.*

Proof: We start showing that if system (5) has an exponential factor of the form $\exp(h/Q^\lambda)$, with $\lambda\in\{0,1\}$, then h is a polynomial in H. Since Q is a Darboux polynomial with cofactor zero (by Proposition 7), applying (32) with $h/g=h/Q$ we get

$$\dot{y}_1\frac{\mathrm{d}h}{\mathrm{d}y_1}+\dot{y}_2\frac{\mathrm{d}h}{\mathrm{d}y_2}+\dot{y}_3\frac{\mathrm{d}h}{\mathrm{d}y_3}+\dot{z}_1\frac{\mathrm{d}h}{\mathrm{d}z_1}+\dot{z}_2\frac{\mathrm{d}h}{\mathrm{d}z_2}+\dot{z}_3\frac{\mathrm{d}h}{\mathrm{d}z_3}=LQ^\lambda, \tag{34}$$

with L given by (33). Taking $y_1=y_2=y_3=0$ in (34), since $H_{|y_1=y_2=y_3=0}\neq 0$, it holds that $b_0=b_4=b_5=b_6=0$. Restricting (34) to $y_1=y_2=0$ and $z_3=z_1+z_2$, we get

$$-y_3^2\frac{\partial h}{\partial z_3}_{|y_1=y_2=0,z_3=z_1+z_2}=y_3b_3Q(\bar{H})^\lambda, \tag{35}$$

where $\bar{H}=-2z_1z_2+\frac{1}{2}y_3^2$. From (35) we obtain that either $b_3=0$ or $Q(\bar{H})$ must be divisible by y_3. This last case is impossible and then $b_3=0$. In a similar way, restricting (34) to $y_1=y_3=0$, $z_2=z_1+z_3$ we get $b_2=0$, and restricting (34) to $y_2=y_3=0$ and $z_1=z_2+z_3$ we get $b_1=0$. Thus we have $L=0$. Therefore, from (34), h is a polynomial first integral. From Proposition 11, we can assume h is a homogeneous polynomial first integral and then, from Theorem 17, h is a polynomial function of H.

Suppose that $\exp(h/(y_1^{n_1}y_2^{n_2}y_3^{n_3}P^\lambda))$ is an exponential factor of system (5), where n_1,n_2,n_3 are nonnegative integers with at least one of them positive, $\lambda\in\{0,1\}$ and h is coprime with y_1, y_2, y_3 and P. Of course, P is a polynomial in the variable H. Then, h satisfies

$$\dot{y}_1\frac{\partial h}{dy_1}+\dot{y}_2\frac{\partial h}{dy_2}+\dot{y}_3\frac{\partial h}{dy_3}-\left(\frac{\dot{y}_1}{y_1}n_1+\frac{\dot{y}_2}{y_2}n_2+\frac{\dot{y}_3}{y_3}n_3\right)h+\dot{z}_1\frac{\partial h}{dz_1}+\dot{z}_2\frac{\partial h}{dz_2}+\dot{z}_3\frac{\partial h}{dz_3}=Ly_1^{n_1}y_2^{n_2}y_3^{n_3}P^\lambda, \tag{36}$$

where we have simplified the common factor $\exp(h/(y_1^{n_1}y_2^{n_2}y_3^{n_3}P^\lambda))$ and multiplied by $y_1^{n_1}y_2^{n_2}y_3^{n_3}P^\lambda$.

Without loss of generality, we can assume that $n_1>0$. Taking $y_1=0$ in (36) and denoting by $\bar{h}$ the restriction of h to $y_1=0$, we conclude that $\bar{h}$ satisfies

$$\dot{y}_2\frac{\partial\bar{h}}{dy_2}+\dot{y}_3\frac{\partial\bar{h}}{dy_3}+\dot{z}_2\frac{\partial\bar{h}}{dz_2}+\dot{z}_3\frac{\partial\bar{h}}{dz_3}=(z_1(n_1-n_2-n_3)+z_2(-n_1+n_2-n_3)+z_3(-n_1-n_2+n_3))\bar{h}. \tag{37}$$

Since by hypothesis h is coprime with y_1, we have that $\bar{h}\neq 0$. We consider two different cases:

Case 1: $\bar{h}$ is not divisible by z_1. In this case, we write $\bar{h}_0=\bar{h}(y_2,y_3,0,z_2,z_3)$. Then, $\bar{h}_0\neq 0$ and $\bar{h}_0$ satisfies (37) restricted to $z_1=0$, that is

$$\dot{y}_2\frac{\partial \bar{h}_0}{dy_2}+\dot{y}_3\frac{\partial \bar{h}_0}{dy_3}+\dot{z}_2\frac{\partial \bar{h}_0}{dz_2}+\dot{z}_3\frac{\partial \bar{h}_0}{dz_3}=(z_2(-n_1+n_2-n_3)+z_3(-n_1-n_2+n_3))\bar{h}_0. \tag{38}$$

Since $n_1>0$, $z_2(-n_1+n_2-n_3)+z_3(-n_1-n_2+n_3)\neq 0$. Thus, since $\bar{h}_0\neq 0$, Eq. (38) implies that $\bar{h}_0$ is a Darboux polynomial of system (5) restricted to $y_1=z_1=0$. From Proposition 19, we obtain that $\bar{h}_0=Ry_2^{m_2}y_3^{m_3}$, with R a Darboux polynomial with zero cofactor of system (5) restricted to $y_1=z_1=0$, and m_2 and m_3 are nonnegative integers such that $m_2+m_3>0$. Substituting $\bar{h}_0=Py_2^{m_2}y_3^{m_3}$ in (38), we get that $(m_2-m_3)(z_2-z_3)=z_2(-n_1+n_2-n_3)+z_3(-n_1-n_2+n_3)$ which implies $n_1=0$, in contradiction with the fact that $n_1>0$.

Case 2: $\bar{h}$ is divisible by z_1. In this case, we write $\bar{h}=z_1^n g$ where $\deg(g)=\deg(\bar{h})-n$ and $0\leqslant n\leqslant \deg(\bar{h})$. Further, $g\neq 0$ and g is not divisible by z_1. Then, since z_1 is a first integral of system (5) restricted to $y_1=0$, then g satisfies (37). Thus, if we set $g_0=g(y_2,y_3,0,z_2,z_3)$, then $g_0\neq 0$ and g_0 satisfies (38). Hence, applying to g_0 the arguments we used for $\bar{h}$ in Case 1, we get a contradiction. This completes the proof of the proposition. ■

Proof of Theorem 3: From Theorems 5, 17, and 18 and Proposition 20, if system (5) has a Darboux first integral G, then

$$G=y_1^{\lambda_1}y_2^{\lambda_2}y_3^{\lambda_3}P_1^{\mu_1}\cdots P_r^{\mu_r}\exp(Q/R)\quad \text{with } \lambda_1,\lambda_2,\lambda_3,\mu_i\in\mathbb{C},$$

where P, Q, and R are polynomials in the variable H, and $i=1,\ldots,r$. Since G and H are first integrals and the cofactors of P_i and $\exp(P/R)$ are zero, using Theorem 5, it must hold $(\lambda_1-\lambda_2-\lambda_3)z_1+(\lambda_2-\lambda_1-\lambda_3)z_2+(\lambda_3-(\lambda_1-\lambda_2)z_3=0$. This implies $\lambda_1=\lambda_2=\lambda_3=0$, and completes the proof of the theorem. ■

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Multiple states and hysteresis for type I superconductors

Y. Du[a)]
School of Mathematics, Statistics and Computer Science, University of New England, Armidale, NSW2351, Australia, and Department of Mathematics, Qufu Normal University, Qufu, People's Republic of China

X. B. Pan[b)]
Department of Mathematics, East China Normal University, Shanghai 200062, People's Republic of China

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For type I superconductors with penetration parameter λ below a certain critical value, the existence of multiple local minimizers of the energy functional is shown. The behavior of these minimizers is examined when the Ginzburg–Landau parameter is small, and a hysteresis phenomenon is demonstrated. In contrast to the case investigated by X. B. Pan [J. Math. Phys. **44**, 2639 (2003)] where λ is above the critical value, the results presented in this paper show that type I superconductors with λ below the critical value have higher critical magnetic field H_c, and exhibit more complicated superconducting behavior. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1938747]

I. INTRODUCTION

The following functional:

$$\mathcal{G}[\psi,\mathcal{A}] := \int_\Omega \left\{ |\nabla \psi - i\mathcal{A}\psi|^2 + \frac{\kappa^2}{2\lambda^2}(1-|\psi|^2)^2 \right\} dx + \lambda^2 \int_{\mathbb{R}^3} |\mathrm{curl}\, \mathcal{A} - \mathcal{H}|^2 dx$$

is a rescaled version of the Gibbs free energy in the Ginzberg–Landau theory (see for instance Refs. 1 and 2), which can be derived from the original Ginzburg–Landau energy functional by performing a series of changes of variables. It can also be obtained from the functional given in Ref. 3 [Eq. (1.3)] by letting $\kappa=\lambda\sqrt{\mu}$. According to the Ginzburg–Landau theory[4] (also see Refs. 5–11), the critical points $(\psi,\mathcal{A})$ of this functional (in a space to be specified in Sec. III), namely the solutions of the Euler equations associated with this functional, describe the superconducting behavior of a superconductor occupying a bounded domain $\Omega\subset\mathbb{R}^3$ with penetration parameter λ and Ginzburg–Landau parameter κ, subjected to an applied magnetic field $\mathcal{H}$. Here ψ is a complex-valued function known as the order parameter, and $\mathcal{A}$ is a real-valued vector field called the magnetic potential. Superconductors with $\kappa<1/\sqrt{2}$ are called type I superconductors and those with $\kappa>1/\sqrt{2}$ are termed type II. It is well known that for type I superconductors there is a critical magnetic field H_c, below which the material will be in the so-called superconducting Meissner state, but above which it will be in the normal state where no superconductivity is observed. In the Ginzburg–Landau theory, a critical point $(\psi,\mathcal{A})$ with $\psi(x)\equiv 0$ indicates that the sample is in the normal state, and *a critical point* $(\psi,\mathcal{A})$ *where* $|\psi(x)|$ *is close to a positive constant everywhere on the whole domain corresponds with the Meissner state*.

We consider in this paper a type I superconductor with small κ, and subjected to an applied magnetic field of the form $\mathcal{H}=\sigma\mathbf{h}$, where $\mathbf{h}$ is a fixed unit vector in $\mathbb{R}^3$, and σ is a real parameter representing the strength of the applied field. One tends to believe that minimizers with a small

[a)]Electronic mail: ydu@turing.une.edu.au
[b)]Electronic mail: xbpan@math.ecnu.edu.cn

value of κ have simpler behavior, and may expect a simple transition from the Meissner state to the normal state as the applied field varies. The results in Ref. 3 show that the phase transition is simple if λ is greater than a critical value $\lambda(\mathbf{h})$. In this paper we shall show that the phase transition is not simple if $\lambda<\lambda(\mathbf{h})$; we will provide estimates for the critical value H_c, examine the change of state of the superconductor as the applied field crosses H_c, and discuss a hysteresis phenomenon.

We assume throughout this paper that Ω is a simply connected and bounded domain in $\mathbb{R}^3$ and has smooth boundary $\partial\Omega$. For the given applied field $\mathcal{H}=\sigma\mathbf{h}$, letting $\mathcal{A}=\sigma\mathbf{A}$, we have

$$\mathcal{G}[\psi,\mathcal{A}]=\mathcal{G}_\sigma[\psi,\mathbf{A}],$$

where

$$\mathcal{G}_\sigma[\psi,\mathbf{A}]:=\int_\Omega\left\{|\nabla_{\sigma\mathbf{A}}\psi|^2+\frac{\kappa^2}{2\lambda^2}(1-|\psi|^2)^2\right\}\mathrm{d}x+\lambda^2\sigma^2\int_{\mathbb{R}^3}|\mathrm{curl}\,\mathbf{A}-\mathbf{h}|^2\mathrm{d}x. \tag{1.1}$$

Here and in the following, we will let ν denote the outward unit normal of $\partial\Omega$, and we shall use the usual notations

$$\nabla_{\mathcal{A}}\psi=\nabla\psi-i\psi\mathcal{A},$$

$$\nabla_{\mathcal{A}}^2\psi=(\nabla-i\mathcal{A})^2\psi=\Delta\psi-i(2\mathcal{A}\cdot\nabla\psi+\psi\,\mathrm{div}\,\mathcal{A})-|\mathcal{A}|^2\psi.$$

Let $\mathbf{F_h}$ be a smooth vector field associated with the above-mentioned given unit vector $\mathbf{h}$ such that

$$\mathrm{curl}\,\mathbf{F_h}=\mathbf{h},\quad \mathrm{div}\,\mathbf{F_h}=0\quad \text{in } \mathbb{R}^3. \tag{1.2}$$

It is easily seen that such $\mathbf{F_h}$ is uniquely determined up to a harmonic gradient (namely, the gradient field of a real-valued harmonic function). For convenience of later discussions, we fix such an $\mathbf{F_h}$ so that

$$\int_\Omega\mathbf{F_h}\mathrm{d}x=\mathbf{0}.$$

It is known that for large σ, the only minimizers of $\mathcal{G}_\sigma$ are

$$(\psi,\mathbf{A})=(0,\mathbf{F_h}+\nabla\phi),$$

where ϕ is an arbitrary real-valued smooth function (see Refs. 3, 12, and 13). We will henceforth call $(0,\mathbf{F_h})$ the trivial solution or trivial critical point of $\mathcal{G}_\sigma$; it corresponds to the normal state of the superconductor. Let us define the critical field H_c by

$$H_c=H_c(\mathbf{h};\kappa,\lambda)=\inf\{\sigma>0:(0,\mathbf{F_h})\text{ is a global minimizer of }\mathcal{G}_\sigma\}. \tag{1.3}$$

[In Ref. 3 a definition of the critical field $H_c(\mathbf{h},\kappa,\mu)$ regarding the functional considered there was given. In the present paper we fix λ and examine the value of H_c for $\kappa=\lambda\varepsilon$, $\varepsilon\to0$. Therefore it is more convenient to treat H_c as a function of $\mathbf{h}$, λ, and κ. The critical field $H_c(\mathbf{h},\kappa,\mu)$ defined in Ref. 3 and the critical field $H_c(\mathbf{h};\kappa,\lambda)$ defined in the present paper are related by the equality $H_c(\mathbf{h};\kappa,\lambda)=H_c(\mathbf{h},\kappa,(\kappa/\lambda)^2)$.]

Clearly for any $0<\sigma<H_c$, $\mathcal{G}_\sigma$ has a nontrivial global minimizer, indicating that the sample is in the superconducting state.

The value of $H_c(\mathbf{h};\kappa,\lambda)$ was estimated in Ref. 3 (Theorem 1). Two positive numbers $a(\mathbf{h})$ and $\lambda(\mathbf{h})$, both depending only on $\mathbf{h}$ and Ω, were introduced there in order to describe the estimates [see also Eqs. (2.3) and (2.8) in Sec. II for the definition]. In particular, it has been shown that, for small $\kappa>0$,

$$H_c(\mathbf{h};\kappa,\lambda) = a(\mathbf{h})\frac{\kappa}{\lambda} + o(\kappa) \quad \text{for fixed } \lambda \geqslant \lambda(\mathbf{h}). \tag{1.4}$$

In fact, for the case $\lambda > \lambda(\mathbf{h})$, the following better estimate has been established in Ref. 3 (Theorem 4.1):

$$H_c(\mathbf{h};\kappa,\lambda) = a(\mathbf{h})\frac{\kappa}{\lambda} + O(\kappa^3) \quad \text{as } \kappa \to 0.$$

Moreover, the asymptotic behavior of the global minimizers of $\mathcal{G}_\sigma$ with $\sigma = a\kappa/\lambda$ with $0 < a < a(\mathbf{h})$ and $\kappa \to 0$ has also been established in Ref. 3 (see Theorem 2 there for details), which, together with Theorem 5.3 in this paper, have the following physical explanation. (We should mention that the actual mathematical results in Theorem 5.3 are more complicated, but their physical meaning is well described by the statement given in Conclusion A.)

Conclusion A: For type I superconductors with small Ginzburg–Landau parameter κ *and penetration parameter* $\lambda \geqslant \lambda(\mathbf{h})$, *and subjected to the applied magnetic field* $\mathcal{H} = \sigma\mathbf{h}$, *there exists a critical field* H_c *such that*,

(i) *as the applied field increases, the Meissner state is a global minimizer of the Ginzburg–Landau energy for* $0 < \sigma < H_c$, *and disappears for* $\sigma > H_c$;
(ii) *as the applied field decreases, the normal state is a global minimizer for* $\sigma > H_c$, *and becomes unstable when* $0 < \sigma < H_c$.

The case where $0 < \lambda < \lambda(\mathbf{h})$ and κ being small is not covered by the above results in Ref. 3, and it will be examined in this paper. To state our results we need two positive constants $C(\lambda)$ and $a^*(\lambda)$ with the property

$$a(\mathbf{h}) < a^*(\lambda) < C(\lambda), \tag{1.5}$$

which depend only on λ, $\mathbf{h}$, and Ω; see Lemmas 2.2 and 2.3 for the definitions. We shall see that, in contrast to (1.4), the value of $H_c(\mathbf{h};\kappa,\lambda)$ is significantly larger when $0 < \lambda < \lambda(\mathbf{h})$.

Theorem 1: *Let* $\mathbf{h}$ *be a unit vector and* $0 < \lambda < \lambda(\mathbf{h})$. *For small* $\kappa > 0$ *we have*

$$H_c(\mathbf{h};\kappa,\lambda) = a^*(\lambda)\frac{\kappa}{\lambda} + o(\kappa). \tag{1.6}$$

Here for fixed $\mathbf{h}$ *and* λ, $\lim_{\kappa\to 0} o(\kappa)/\kappa = 0$.

We shall also show that the sample exhibits rather different and interesting superconducting behavior when $0 < \lambda < \lambda(\mathbf{h})$, see Theorems 5.2 and 6.1. The physical explanation of these results can be stated as follows.

Conclusion B: For type I superconductors with small Ginzburg–Landau parameter κ *and penetration parameter* $\lambda < \lambda(\mathbf{h})$, *and subjected to the applied magnetic field* $\mathcal{H} = \sigma\mathbf{h}$, *there exist three critical fields* H_{sc}, H_c, *and* H_{sh} *satisfying*

$$H_{sc} < H_c < H_{sh} \tag{1.7}$$

such that

(i) *as the applied field increases, the Meissner state is a global minimizer of the Ginzburg–Landau energy for* $0 < \sigma < H_c$, *remains stable (a local minimizer) for* $H_c \leqslant \sigma < H_{sh}$, *and disappears for* $\sigma > H_{sh}$;
(ii) *as the applied field decreases, the normal state is a global minimizer for* $\sigma > H_c$, *remains stable (a local minimizer) for* $H_{sc} < \sigma \leqslant H_c$, *and becomes unstable when* $0 < \sigma < H_{sc}$.

Moreover,

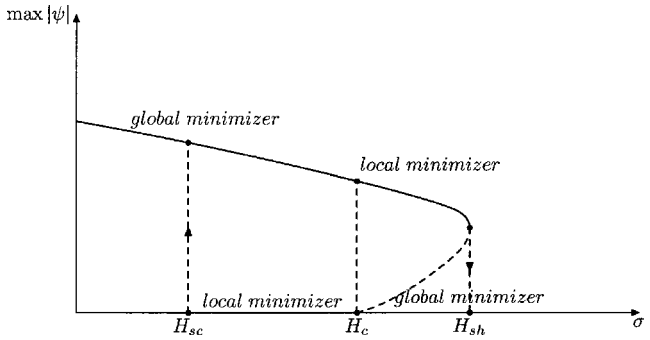

FIG. 1. Bifurcation and hysteresis for $0<\lambda<\lambda(\mathbf{h})$.

$$H_{sc} \sim a(\mathbf{h})\frac{\kappa}{\lambda}, \quad H_c \sim a^*(\lambda)\frac{\kappa}{\lambda}, \quad H_{sh} \sim C(\lambda)\frac{\kappa}{\lambda} \quad \text{for small } \kappa. \tag{1.8}$$

Remark 1.2. We believe that Conclusion B suggests a hysteresis phenomenon for type I superconductors with small penetration length $\lambda<\lambda(\mathbf{h})$: As the applied field increases from below H_c, the superconductor remains in the Meissner state until the field reaches H_{sh}, then it jumps to the normal state once the applied field increases past H_{sh}. On the other hand, as the applied field is lowered from above H_c, the superconductor is in normal state until the field reaches H_{sc}, then it jumps to the Meissner state once the magnetic field decreases past H_{sc}. These are sometimes called *superheating* and *subcooling*, respectively. We illustrate this in Fig. 1 (see Remark 5.4 for further details).

We should point out that the hysteresis phenomena described in Remark 1.2 are only natural physical explanations of our mathematical results. The actual mathematical results in Theorems 5.2 and 6.1 are more complicated. We would like to mention that an interesting hysteresis phenomenon for type II superconductors under an applied field near H_{C_1} has been analyzed by Lin and Du;[14] see also Ref. 15 for discussions related to the super-heating phenomenon for a similar situation to Ref. 14.

Remark 1.3: Comparing our results in the present paper for the case $0<\lambda<\lambda(\mathbf{h})$ with the results obtained in Ref. 3 for $\lambda\geqslant\lambda(\mathbf{h})$, we see that $\lambda(\mathbf{h})$ is a critical value for the penetration parameter λ. The superconducting behavior makes an important change between the cases $\lambda>\lambda(\mathbf{h})$ and $\lambda<\lambda(\mathbf{h})$, with more complicated behavior occurring when $0<\lambda<\lambda(\mathbf{h})$.

Remark 1.4: It is customary to perform the rescaling of the Ginzburg–Landau energy functional in a way that the parameter λ is reduced to 1. In that setting, the change in the value of λ in the present paper is translated into the change of the domain size of the sample, and our results can be roughly described as follows: Conclusion A applies when the sample is below a certain critical size, and Conclusion B applies if the sample is above that critical size. For a more accurate statement see the Appendix (Conclusion C). We would like to mention that A. Geim *et al.*[16] discovered numerous phase transitions of superconductors whose character changes rapidly with size and temperature. In particular, a sample can be either type I or type II depending on its size. Superconductivity for samples with small size has been studied by Aftalion and Dancer[17] and Aftalion and Du.[18] We should mention that Ginzburg–Landau equations in one-dimensional domains have been studied by many authors, and many interesting phenomena have been discovered; see for instance Bolley and Helffer,[19] Hastings and Troy,[20] and Aftalion and Troy.[21] We should also mention that the vortices of the minimizers of Ginzburg–Landau functional for large κ have been extensively studied; see for instance Bethuel *et al.*,[22] Lin,[23] and Sandier and Serfaty.[24]

Now we sketch the general scheme of the proof of our main results. The main part of the proof is to classify all critical points of the functional $\mathcal{G}_\sigma$ with $\sigma=a\varepsilon$ and $\kappa=\lambda\varepsilon$, and study their minimality, where $a>0$ is fixed, and $\varepsilon>0$ is small. We prove that when ε is small, all nontrivial critical points $(\psi_\varepsilon,\mathbf{A}_\varepsilon)$ have expansions

$$\psi_\varepsilon \sim e^{ic_\varepsilon}\rho^{1/2}(1+ia\varepsilon w^\rho), \quad \mathbf{A}_\varepsilon \sim \mathbf{A}^\rho + O(\varepsilon),$$
$$\mathcal{G}_{a\varepsilon}[\psi_\varepsilon, \mathbf{A}_\varepsilon] = \varepsilon^2 F(a,\rho) + O(\varepsilon^3), \tag{1.9}$$

where $(w^\rho, \mathbf{A}^\rho)$ satisfies Eq. (2.11), and ρ is a root of the equation

$$f(a,\rho) = 1, \tag{1.10}$$

where $f(a,\rho)$ and $F(a,\rho)$ are functions defined by the integrals involving w^ρ and $\nabla\mathbf{A}^\rho$, see (2.13). Note that $(w^\rho, \mathbf{A}^\rho)$ depends also on λ, and hence $f(a,\rho)$ depends on λ through w^ρ and $\mathbf{A}^\rho$. The detailed information about the roots of (1.10) has been given in Ref. 3, which is useful to classify all the critical points of $\mathcal{G}_{a\varepsilon}$. If $\lambda \geqslant \lambda(\mathbf{h})$, then (1.10) has exactly one root $\rho(a)$ for all $0 < a < C(\lambda)$. If $0 < \lambda < \lambda(\mathbf{h})$, then (1.10) has exactly one root when $0 < a < a(\mathbf{h})$ and has exactly two roots $\rho_*(a)$ and $\rho(a)$ when $a(\mathbf{h}) < a < C(\lambda)$. Moreover, we shall show that $\rho(a)$ is a minimizer of the function $F(a,\cdot)$ and $\rho_*(a)$ is a maximizer of $F(a,\cdot)$. Using this fact and the expansions in (1.9) we are able to prove the local minimality of the critical points with $\rho = \rho(a)$. These local minimizers describe the Meissner state of type I superconductors, and their existence is proved by minimizing a new functional

$$g_{a,\varepsilon}[\rho, w, \mathbf{A}] = \frac{1}{\varepsilon^2}\mathcal{G}_{a\varepsilon}[\rho^{1/2}(1+ia\varepsilon w), \mathbf{A}].$$

The existence of unstable critical points corresponding to $\rho_*(a)$ can be proved by using the well-known Mountain Pass Lemma,[25] but the details will be omitted. To examine the minimality of the normal state $(0, \mathbf{F_h})$, we need uniform estimates of the lowest eigenvalue of the operator $-\nabla^2_{\varepsilon_n \mathbf{A}_n}$, where $\mathbf{A}_n \to \mathbf{F_h}$ in $W^{1,2}(\Omega, \mathbb{R}^3)$.

The rest of the paper is organized as follows. In Sec. II, we collect some notations and results from Ref. 3, which clarify the results previously mentioned, and more importantly, play an essential role in our discussions to follow. In Sec. III, we collect some elliptic estimates for weak solutions of the Ginzburg–Landau equations. These estimates are already known for global minimizers. In Sec. IV we obtain a family of nontrivial local minimizers and also determine the local minimality and uniqueness in a chosen gauge of the normal state $(0, \mathbf{F_h})$. In Sec. V, we obtain a classification of all possible critical points of the energy functional, and this helps us to determine, in Sec. VI, the region of the parameters where the local minimizers are global minimizers, which in turn leads to a description for the critical value H_c and an explanation of the hysteresis phenomenon around H_c. Theorem 1.1 will be obtained in Sec. VI as a corollary of Theorem 6.1. In the Appendix we give a brief discussion about the effect of the size of a sample on its superconducting behavior.

II. PRELIMINARIES

In this section we introduce the various constants that have been used in stating our results in the introduction, namely, $\omega(\mathbf{h})$, $a(\mathbf{h})$, $\lambda(\mathbf{h})$, $a^*(\lambda)$, and $C(\lambda)$. We shall also introduce the constants $\rho(a)$ and $\rho_*(a)$ that depend on a parameter a. The numbers $\rho(a)$ and $\rho_*(a)$ will play an important role in our study.

Recall that $\mathbf{h}$ is a unit vector in $\mathbb{R}^3$ and $\mathbf{F_h}$ is a fixed vector field satisfying (1.2) and $\int_\Omega \mathbf{F_h} dx = \mathbf{0}$. Let

$$\omega(\mathbf{h}) = \inf_{\phi \in W^{1,2}(\Omega)} \fint_\Omega |\nabla \phi - \mathbf{F_h}|^2 dx, \tag{2.1}$$

where $\fint_\Omega = |\Omega|^{-1}\int_\Omega$ and $|\Omega|$ denotes the volume of Ω. It is well known that $\omega(\mathbf{h})$ is achieved by a real-valued function $w_\mathbf{h}$ which satisfies

$$\Delta w_{\mathbf{h}} = 0 \quad \text{in } \Omega, \quad \frac{\partial w_{\mathbf{h}}}{\partial \nu} = \mathbf{F}_{\mathbf{h}} \cdot \nu \quad \text{on } \partial\Omega. \tag{2.2}$$

Such $w_{\mathbf{h}}$ is unique if we further require $\int_\Omega w_{\mathbf{h}} dx = 0$. We define

$$a(\mathbf{h}) = \omega(\mathbf{h})^{-1/2}. \tag{2.3}$$

Lemma 2.1: (Ref. 3, Lemma 2.1) Let $\mu(\varepsilon \mathbf{F}_{\mathbf{h}})$ denote the lowest eigenvalue of the problem

$$-\nabla^2_{\varepsilon \mathbf{F}_{\mathbf{h}}} \phi = \mu\phi \quad \text{in } \Omega, \quad (\nabla_{\varepsilon \mathbf{F}_{\mathbf{h}}} \phi) \cdot \nu = 0 \quad \text{on } \partial\Omega.$$

Then

$$\mu(\varepsilon \mathbf{F}_{\mathbf{h}}) = \omega(\mathbf{h})\varepsilon^2 + O(\varepsilon^3) \quad \text{as } \varepsilon \to 0. \tag{2.4}$$

A simple application of Lemma 2.1 yields the following result (see Ref. 3, Theorem 3.2):

$$\liminf_{\varepsilon \to 0^+} \frac{H_c(\mathbf{h}, \lambda\varepsilon, \lambda)}{\varepsilon} \geqslant a(\mathbf{h}) \quad \text{uniformly for } \lambda \in (0, \infty). \tag{2.5}$$

Let

$$D^{1,2}(\mathbb{R}^3) = \{\phi \in L^1_{\text{loc}}(\mathbb{R}^3) : |\nabla \phi| \in L^2(\mathbb{R}^3)\},$$

and for $\phi \in D^{1,2}(\mathbb{R}^3)$ define $\|\phi\|_{1,2} = \|\nabla \phi\|_{L^2(\mathbb{R}^3)}$. It is well known that, after identifying functions that differ by a constant, $D^{1,2}(\mathbb{R}^3)$ is a Hilbert space under the norm $\|\cdot\|_{1,2}$. We denote by $\mathbf{D}^{1,2}(\mathbb{R}^3)$ the corresponding space of vector fields in $\mathbb{R}^3$. Let us recall the following well-known formula

$$\|\mathbf{B}\|^2_{1,2} = \int_{\mathbb{R}^3} |\nabla \mathbf{B}|^2 dx = \int_{\mathbb{R}^3} \{|\text{curl } \mathbf{B}|^2 + |\text{div } \mathbf{B}|^2\} dx, \quad \mathbf{B} \in \mathbf{D}^{1,2}(\mathbb{R}^3). \tag{2.6}$$

The definition of $\lambda(\mathbf{h})$ involves the following problem:

$$\text{curl}^2 \mathbf{U} = (\nabla w_{\mathbf{h}} - \mathbf{F}_{\mathbf{h}})\chi_\Omega, \quad \text{div } \mathbf{U} = 0 \quad \text{in } \mathbb{R}^3, \quad \mathbf{U} \in \mathbf{D}^{1,2}(\mathbb{R}^3). \tag{2.7}$$

It has been proved in Ref. 3 (Lemma 3.4) that (2.7) has a solution and it belongs to $C^{1+\alpha}_{\text{loc}}(\mathbb{R}^3, \mathbb{R}^3)$ for any $\alpha \in (0,1)$. Moreover, it is unique up to an additive constant vector. Let $\mathbf{U}_{\mathbf{h}}$ be the solution of (2.7) such that $\int_\Omega \mathbf{U}_{\mathbf{h}} dx = \mathbf{0}$. For convenience we introduce the notation

$$\mathbf{D}^{1,2}(\mathbb{R}^3, \text{div}, \Omega) = \left\{ \mathbf{A} \in \mathbf{D}^{1,2}(\mathbb{R}^3) : \text{div } \mathbf{A} = 0 \text{ in } \mathbb{R}^3, \quad \int_\Omega \mathbf{A} dx = \mathbf{0} \right\}.$$

Therefore $\mathbf{F}_{\mathbf{h}}, \mathbf{U}_{\mathbf{h}} \in \mathbf{D}^{1,2}(\mathbb{R}^3, \text{div}, \Omega)$. We define

$$\lambda(\mathbf{h}) = \frac{\sqrt{2}a(\mathbf{h})}{\sqrt{|\Omega|}} \|\text{curl } \mathbf{U}_{\mathbf{h}}\|_{L^2(\mathbb{R}^3)}. \tag{2.8}$$

To define $a^*(\lambda)$ and $C(\lambda)$, we need to introduce the following functional for given constants $\lambda > 0$ and $\rho \geqslant 0$:

$$J_\rho[w, \mathbf{A}] = \lambda^2 \int_{\mathbb{R}^3} |\text{curl } \mathbf{A} - \mathbf{h}|^2 dx + \rho \int_\Omega |\nabla w - \mathbf{A}|^2 dx, \quad (w, \mathbf{A}) \in Y, \tag{2.9}$$

where

$$Y = \left\{ (w,\mathbf{A}) : w \in W^{1,2}(\Omega,\mathbb{C}), \int_\Omega w \mathrm{d}x = 0;\ \mathbf{A} - \mathbf{F_h} \in \mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div},\Omega) \right\}. \tag{2.10}$$

Let

$$\widetilde{Y} := \{(w,\widetilde{\mathbf{A}}) : \widetilde{\mathbf{A}} = \mathbf{A} - \mathbf{F_h}, (w,\mathbf{A}) \in Y\}.$$

We observe that $\widetilde{Y}$ is a Hilbert space with norm

$$\|(w,\widetilde{\mathbf{A}})\|_{\widetilde{Y}} := (\|w\|^2_{W^{1,2}(\Omega,\mathbb{C})} + \|\widetilde{\mathbf{A}}\|^2_{1,2})^{1/2}.$$

In what follows, we write

$$(w_n,\mathbf{A}_n) \to (w^*,\mathbf{A}^*) \quad \text{in } Y$$

if and only if $(w_n - w^*, \mathbf{A}_n - \mathbf{A}^*)$ converges to $(0,\mathbf{0})$ in the Hilbert space $\widetilde{Y}$.

It was shown in Ref. 3 (Sec. III) that, for any $\rho > 0$, the following problem has a unique solution $(w^\rho,\mathbf{A}^\rho) \in Y$:

$$\begin{gathered} \Delta w = 0 \quad \text{in } \Omega; \\ \lambda^2 \operatorname{curl}^2 \mathbf{A} = \rho(\nabla w - \mathbf{A})\chi_\Omega \quad \text{in } \mathbb{R}^3; \\ \frac{\partial w}{\partial \nu} = \mathbf{A}\cdot\nu \quad \text{on } \partial\Omega, \\ \mathbf{A} - \mathbf{F_h} \in \mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div}), \end{gathered} \tag{2.11}$$

and it is the unique global minimizer of $J_\rho[w,\mathbf{A}]$ over the set Y defined previously [note that any solution of (2.11) in Y necessarily has w real valued; therefore the result in Ref. 3, which is stated for real-valued w only, applies to our more general setting here.] When $\rho=0$, clearly the global minimum of J_0 is achieved by $(w,\mathbf{F_h})$ with $w \in W^{1,2}(\Omega,\mathbb{C})$ arbitrary. However, $(w_\mathbf{h},\mathbf{F_h})$ is the unique solution of (2.11) in Y when $\rho=0$. We define, for $\rho=0$, $(w^0,\mathbf{A}^0)=(w_\mathbf{h},\mathbf{F_h})$. It is easily seen that

$$(w^\rho,\mathbf{A}^\rho) \to (w^0,\mathbf{A}^0) \quad \text{as } \rho \to 0.$$

For given $a>0$, the solutions $\rho \in [0,1]$ of

$$a^2 \int_\Omega |\nabla w^\rho - \mathbf{A}^\rho|^2 \mathrm{d}x + \rho = 1 \tag{2.12}$$

will be useful in proving our main results of this paper. Write

$$f(a,\rho) = a^2 \int_\Omega |\nabla w^\rho - \mathbf{A}^\rho|^2 \mathrm{d}x + \rho. \tag{2.13}$$

It is proved in Ref. 3 (Sec. III) that f is C^2 for $a>0$ and $\rho>0$, and

$$\frac{\partial f}{\partial \rho}(a,0^+) = 1 - \left(\frac{a}{a(\mathbf{h})}\right)^2 \left(\frac{\lambda(\mathbf{h})}{\lambda}\right)^2, \quad \frac{\partial^2 f}{\partial \rho^2}(a,\rho) > 0. \tag{2.14}$$

Clearly for $a>0$,

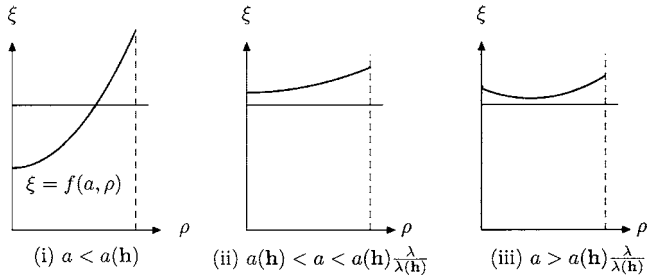

FIG. 2. Graph of $f(a,\rho)$ with $\lambda>\lambda(\mathbf{h})$.

$$f(a,0)=\left(\frac{a}{a(\mathbf{h})}\right)^2, \quad f(a,1)>1. \tag{2.15}$$

Using (2.14) and (2.15), the following result was proved in Ref. 3, Lemma 3.5.

Lemma 2.2: Suppose $0<\lambda<\lambda(\mathbf{h})$. *Then the following conclusions hold.*

(i) *There exists a constant* $C(\lambda)>a(\mathbf{h})$ *such that (2.12) has no solution if* $a>C(\lambda)$; *it has a unique solution* $\rho_0\in(0,1)$ *if* $a=C(\lambda)$.

(ii) *If* $0<a<C(\lambda)$, *(2.12) has a maximal solution* $\rho(a)\in(0,1)$, *and*

$$\lim_{a\to 0^+}\rho(a)=1, \qquad \lim_{a\to C(\lambda)^-}\rho(a)=\rho_0.$$

(iii) *If* $a(\mathbf{h})\leqslant a<C(\lambda)$, *(2.12) has exactly one more solution* $\rho_*(a)$,

$$0<\rho_*(a)<\rho(a) \quad \text{for all } a\in(a(\mathbf{h}),C(\lambda)),$$

$$\rho_*(a(\mathbf{h}))=0, \qquad \lim_{a\to C(\lambda)^-}\rho_*(a)=\rho_0.$$

(iv) *If* $0<a<a(\mathbf{h})$, $\rho(a)$ *is the only solution of (2.12).*

The results of Lemma 3.5 in Ref. 3 also discuss the case $\lambda>\lambda(\mathbf{h})$. Since this part is not used in this paper, we will not recall its full details, but only illustrate it in Fig. 2 above, which provides an interesting comparison to the conclusions in Lemma 2.2 (illustrated by Fig. 3).

Let

$$I(a)=\int_0^{\rho(a)}[f(a,\rho)-1]\mathrm{d}\rho. \tag{2.16}$$

Lemma 2.3: Suppose $0<\lambda<\lambda(\mathbf{h})$. *Then* $I(a)$ *is continuous and strictly increasing for* $a\in(0,C(\lambda))$, *and there exists a unique* $a^*=a^*(\lambda)\in(a(\mathbf{h}),C(\lambda))$ *such that* $I(a^*)=0$.

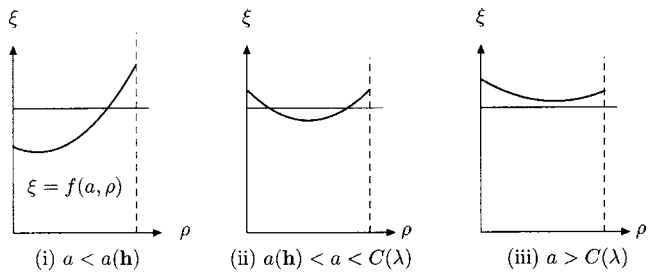

FIG. 3. Graph of $f(a,\rho)$ with $0<\lambda<\lambda(\mathbf{h})$.

Proof: Note that $\rho_*(a)$ and $\rho(a)$ also depend on λ but we regard $\lambda \in (0, \lambda(\mathbf{h}))$ as fixed in the following analysis. Since

$$\frac{\partial f}{\partial a}(a,\rho) > 0, \quad \frac{\partial f}{\partial \rho}(a,\rho_*(a)) < 0, \quad \frac{\partial f}{\partial \rho}(a,\rho(a)) > 0,$$

we apply the implicit function theorem to the solutions $\rho=\rho_*(a)$ and $\rho=\rho(a)$ of the equation

$$f(a,\rho) = 1 \tag{2.17}$$

to find that $\rho_*(a)$ and $\rho(a)$ are C^2 functions for $a \in (a(\mathbf{h}), C(\lambda))$ and $(0, C(\lambda))$, respectively, and

$$\rho_*{}'(a) > 0 \quad \text{for } a(\mathbf{h}) \leqslant a < C(\lambda), \quad \rho'(a) < 0 \quad \text{for } 0 < a < C(\lambda).$$

Note that $I(a)$ is a continuously differentiable function of $a \in (0, C(\lambda))$, and

$$I'(a) = \int_0^{\rho(a)} \frac{\partial f}{\partial a}(a,\rho)\mathrm{d}\rho > 0.$$

When $0<\lambda<\lambda(\mathbf{h})$, it follows from (2.13) (see also Ref. 3, proof of Lemma 3.5) that

$$f(a(\mathbf{h}),0) = f(a(\mathbf{h}),\rho(a(\mathbf{h})) = 1, \quad \text{and } f(a(\mathbf{h}),\rho) < 1 \quad \text{for all} \quad 0 < \rho < \rho(a(\mathbf{h})).$$

Hence $I(a(\mathbf{h}))<0$. On the other hand, we have (see Ref. 3, proof of Lemma 3.5)

$$f(C(\lambda),\rho) > 1 \quad \text{for all } 0 \leqslant \rho < \rho_0,$$

where ρ_0 is the positive number given in Lemma 2.2. So $I(C(\lambda))>0$. Since $I(a)$ is continuous and strictly increasing, there exists a unique $a^*=a^*(\lambda) \in (a(\mathbf{h}), C(\lambda))$ such that $I(a^*)=0$. □

Let us define

$$F(a,\rho) = \frac{|\Omega|}{2}(1-\rho)^2 + a^2 J_\rho[w^\rho, \mathbf{A}^\rho], \tag{2.18}$$

where $(w^\rho, \mathbf{A}^\rho)$ is the unique solution of (2.11) in Y. By Remark 3.8 of Ref. 3,

$$\frac{\partial F}{\partial \rho}(a,\rho) = |\Omega|(f(a,\rho) - 1),$$

where $f(a,\rho)$ is the function given in (2.13). Therefore, for fixed $a \in (a(\mathbf{h}), C(\lambda))$, $F(a,\rho)$ is strictly increasing for $\rho \in (0, \rho_*(a))$, strictly decreasing for $\rho \in (\rho_*(a), \rho(a))$, and strictly increasing for $\rho > \rho(a)$. Hence $\rho_*(a)$ is a local maximizer of $F(a,\cdot)$ and $\rho(a)$ is a local minimizer of $F(a,\cdot)$. By a similar consideration, for fixed $a \in (0, a(\mathbf{h})]$, $\rho(a)$ is a local minimizer of $F(a,\cdot)$. This fact is a key element in our study.

From the previous equality (2.16) and the fact $F(a,0)=|\Omega|/2$, we have

$$F(a,\rho(a)) - F(a,0) = |\Omega| I(a). \tag{2.19}$$

It follows that $F(a,\rho(a))-F(a,0)$ is a strictly increasing function of a in $[0, C(\lambda)]$ and has a unique zero at $a=a^*(\lambda)$.

III. ELLIPTIC ESTIMATES OF CRITICAL POINTS

We first introduce the spaces in which minimizers of $\mathcal{G}_\sigma$ are sought. Let $W^{1,2}(\Omega, \mathbb{C})$ be the Sobolev space of all complex-valued functions defined on Ω, and let

$$\mathcal{W}(\Omega) = \{(\psi, \mathbf{A}) : \psi \in W^{1,2}(\Omega, \mathbb{C}), \mathbf{A} - \mathbf{F}_\mathbf{h} \in \mathbf{D}^{1,2}(\mathbb{R}^3)\}.$$

Our minimization problem for $\mathcal{G}_\sigma[\psi, \mathbf{A}]$ is

$$\inf_{(\psi,\mathbf{A})\in\mathcal{W}(\Omega)} \mathcal{G}_\sigma[\psi,\mathbf{A}]. \tag{3.1}$$

It is standard to show that (3.1) is always achieved by a minimizer $(\psi,\mathbf{A})$ which satisfies (in the weak sense)

$$\begin{gathered} -\nabla_{\sigma\mathbf{A}}^2\psi=\frac{\kappa^2}{\lambda^2}(1-|\psi|^2)\psi \quad \text{in } \Omega,\\ \operatorname{curl}^2\mathbf{A}=\frac{1}{\lambda^2\sigma}\operatorname{Im}(\bar{\psi}\nabla_{\sigma\mathbf{A}}\psi)\chi_\Omega \quad \text{in } \mathbb{R}^3,\\ (\nabla_{\sigma\mathbf{A}}\psi)\cdot\nu=0 \quad \text{on } \partial\Omega,\\ (\psi,\mathbf{A})\in\mathcal{W}(\Omega), \end{gathered} \tag{3.2}$$

where ν denotes the unit outward normal of $\partial\Omega$ and χ_Ω is the characteristic function of Ω. To be more precise, by a weak solution to (3.2) we mean a pair $(w,\mathbf{A})\in\mathcal{W}(\Omega)$ satisfying

$$\int_\Omega \nabla_{\sigma\mathbf{A}}\psi\cdot\overline{\nabla_{\sigma\mathbf{A}}\phi}\,dx=\frac{\kappa^2}{\lambda^2}\int_\Omega(1-|\psi|^2)\psi\bar{\phi}\,dx, \quad \text{for all } \phi\in W^{1,2}(\Omega,\mathbb{C}),$$

$$\int_{\mathbb{R}^3}\operatorname{curl}(\mathbf{A}-\mathbf{F_h})\cdot\operatorname{curl}\mathbf{B}\,dx=\frac{1}{\lambda^2\sigma}\int_\Omega\operatorname{Im}(\bar{\psi}\nabla_{\sigma\mathbf{A}}\psi)\cdot\mathbf{B}\,dx, \quad \text{for all } \mathbf{B}\in\mathbf{C}_0^\infty(\mathbb{R}^3,\mathbb{R}^3).$$

It is well known that $\mathcal{G}_\sigma$ is invariant under the gauge transformation

$$(\psi,\mathbf{A})\to(\tilde{\psi},\tilde{\mathbf{A}}),$$

where $\tilde{\psi}=\psi e^{i\sigma\eta}$, $\tilde{\mathbf{A}}=\mathbf{A}-\sigma\nabla\eta$, and where η is an arbitrary smooth and real-valued function. By replacing $\mathbf{A}$ by $\mathbf{A}+\nabla\eta$, where $\eta=\eta_0-x\cdot(\int_\Omega\mathbf{A}dx)$, and η_0 is the unique solution of

$$-\Delta\eta_0=\operatorname{div}\mathbf{A}\in L^2(\mathbb{R}^3), \quad \eta_0\in W^{1,2}(\mathbb{R}^3),$$

we may require that

$$\operatorname{div}\mathbf{A}=0 \quad \text{and} \quad \int_\Omega\mathbf{A}dx=\mathbf{0}$$

in (3.1). Let

$$\mathcal{W}_0(\Omega,\operatorname{div})=\left\{(\psi,\mathbf{A})\in\mathcal{W}(\Omega):\operatorname{div}\mathbf{A}=0 \text{ in } \mathbb{R}^3,\int_\Omega\mathbf{A}dx=0\right\}.$$

Then (3.1) is equivalent to

$$\inf_{(\psi,\mathbf{A})\in\mathcal{W}_0(\Omega,\operatorname{div})}\mathcal{G}_\sigma[\psi,\mathbf{A}]. \tag{3.3}$$

Lemma 3.1: If $(\psi,\mathbf{A})\in\mathcal{W}_0(\Omega,\operatorname{div})$ *is a weak solution to* (3.2), *then there exists a constant vector* $\mathbf{v}\in\mathbb{R}^3$ *such that* $\mathbf{A}-\mathbf{F_h}-\mathbf{v}\in W^{1,2}(\mathbb{R}^3,\mathbb{R}^3)$.

Proof: Let $\mathbf{f}$ denote the right-hand side of the second equation in (3.2). Then $\mathbf{f}\in L^{3/2}(\mathbb{R}^3)$ and, due to the facts

$$\operatorname{div} \mathbf{A} = \operatorname{div} \mathbf{F_h} = 0, \quad \operatorname{curl}^2 \mathbf{F_h} = \mathbf{0},$$

the second equation in (3.2) can be written as

$$-\Delta(\mathbf{A} - \mathbf{F_h}) = \mathbf{f} \text{ in } \mathbb{R}^3.$$

It is well-known that the problem

$$-\Delta \mathbf{V} = \mathbf{f} \text{ in } \mathbb{R}^3, \quad \mathbf{V} \in W^{2,3/2}(\mathbb{R}^3, \mathbb{R}^3)$$

has a unique solution $\mathbf{V_f}$. Let $\mathbf{v} = (\mathbf{A} - \mathbf{F_h}) - \mathbf{V_f}$. Then $\mathbf{v}$ is a harmonic vector-valued function on $\mathbb{R}^3$ with $|\nabla \mathbf{v}| \in L^2(\mathbb{R}^3)$. It follows that $\mathbf{v}$ is a constant vector. By the Sobolev imbedding theorem we find $\mathbf{A} - \mathbf{F_h} - \mathbf{v} = \mathbf{V_f} \in W^{1,2}(\mathbb{R}^3, \mathbb{R}^3)$. □

Now we give some estimates for the critical points of $\mathcal{G}_\sigma$, which will be used in later sections for $\kappa = \lambda\varepsilon$, where λ is fixed and $\varepsilon > 0$ is small. Similar estimates have already been established for global minimizers, see Ref. 3 (Lemma 3.3) and Ref. 26 (Proposition 4.2 in two-dimensional case).

Lemma 3.2: Let $(\psi, \mathbf{A})$ *be a critical point of* $\mathcal{G}_\sigma$ *in* $\mathcal{W}_0(\Omega, \operatorname{div})$. *Then there exist positive constants* C_0 *and* $C(\lambda, \kappa/\lambda)$, *with* C_0 *depending only on* Ω *and* $\mathbf{h}$, *and* $C(\lambda, \kappa/\lambda)$ *depending only on* Ω, $\mathbf{h}$, λ *and upper bound of* κ/λ, *such that*

(i) $\|\nabla_{\sigma\mathbf{A}}\psi\|_{L^2(\Omega)} \leq \kappa/\lambda \|\psi\|_{L^2(\Omega)}$;

(ii) $\|\nabla_{\sigma\mathbf{A}}\psi\|_{L^\infty(\Omega)} \leq C(\lambda, \kappa/\lambda)(1 + \sqrt{\sigma})\|\psi\|_{L^\infty(\Omega)}$;

(iii) $\|\nabla(\mathbf{A} - \mathbf{F_h})\|_{L^2(\mathbb{R}^3)} \leq C_0 \kappa/\lambda^3 \sigma$;

(iv) $\|\mathbf{A} - \mathbf{F_h}\|_{L^2(\Omega)} \leq C_0 \kappa/\lambda^3 \sigma$.

(v) *For any* $0 < \alpha < 1$, $\psi \in C^{2+\alpha}(\bar{\Omega})$, $\mathbf{A} \in C^{1+\alpha}(\bar{\Omega})$, *and for any* $R > 0$ *such that* $\bar{\Omega} \subset B_R$, *there exists a positive constant* $C_{\alpha,R}$ *depending only on* Ω, $\mathbf{h}$, α *and* R, *such that, for* $q = 3/(1 - \alpha)$,

$$\|\nabla(\mathbf{A} - \mathbf{F_h})\|_{C^\alpha(B_R)} \leq C_{\alpha,R}\left\{\frac{\kappa}{\lambda^3\sigma} + \frac{1}{\lambda^2\sigma}\|\bar{\psi}\nabla_{\sigma\mathbf{A}}\psi\|_{L^q(\Omega)}\right\}. \tag{3.4}$$

Proof: It is well known (see Ref. 9) that $|\psi(x)| \leq 1$ in Ω. Multiplying the first equation in (3.2) by $\bar{\psi}$ and integrating over Ω yields

$$\int_\Omega |\nabla_{\sigma A}\psi|^2 dx = \frac{\kappa^2}{\lambda^2}\int_\Omega (1 - |\psi|^2)|\psi|^2 dx \leq \frac{\kappa^2}{\lambda^2}\int_\Omega |\psi|^2 dx,$$

which gives (i).

To prove (iii), we use Lemma 3.1 to find a constant vector $\mathbf{v}$ such that

$$\mathbf{V} := \mathbf{A} - \mathbf{F_h} - \mathbf{v} \in W^{1,2}(\mathbb{R}^3, \mathbb{R}^3).$$

In particular, $\mathbf{A} - \mathbf{F_h} \in W^{1,2}(\Omega, \mathbb{R}^3)$. Let

$$\mathbf{f} = \frac{1}{\lambda^2\sigma}\operatorname{Im}(\bar{\psi}\nabla_{\sigma\mathbf{A}}\psi)\chi_\Omega.$$

The weak formulation of the second equation in (3.2) gives

$$\int_{\mathbb{R}^3} \operatorname{curl}(\mathbf{A} - \mathbf{F_h}) \cdot \operatorname{curl} \mathbf{B} dx = \int_\Omega \mathbf{f} \cdot \mathbf{B} dx,$$

for all $\mathbf{B} \in C_0^\infty(\mathbb{R}^3, \mathbb{R}^3)$. Since $\mathbf{V} \in W^{1,2}(\mathbb{R}^3, \mathbb{R}^3)$, we can choose $\mathbf{B}_j \in C_0^\infty(\mathbb{R}^3, \mathbb{R}^3)$ such that

$$\|\mathbf{B}_j - \mathbf{V}\|_{W^{1,2}(\mathbb{R}^3,\mathbb{R}^3)} \to 0 \quad \text{as } j \to \infty.$$

It follows that

$$\int_{\mathbb{R}^3} |\text{curl}(\mathbf{A} - \mathbf{F_h})|^2 \mathrm{d}x = \int_\Omega \mathbf{f} \cdot \mathbf{V} \mathrm{d}x.$$

Therefore, for an arbitrary positive constant δ_0 we have

$$\int_{\mathbb{R}^3} |\text{curl}(\mathbf{A} - \mathbf{F_h})|^2 \mathrm{d}x \leqslant \frac{1}{\delta_0} \int_\Omega |\mathbf{f}|^2 \mathrm{d}x + \delta_0 \int_\Omega |\mathbf{V}|^2 \mathrm{d}x.$$

Since $\mathbf{V} \in W^{1,2}(\mathbb{R}^3, \mathbb{R}^3)$, using Hölder's inequality and the Sobolev inequality we deduce

$$\int_\Omega |\mathbf{V}|^2 \mathrm{d}x \leqslant |\Omega|^{2/3} \|\mathbf{V}\|^2_{L^6(\Omega)} \leqslant |\Omega|^{2/3} \|\mathbf{V}\|^2_{L^6(\mathbb{R}^3)} \leqslant C_1 \| \nabla \mathbf{V}\|^2_{L^2(\mathbb{R}^3)} = C_1 \int_{\mathbb{R}^3} |\text{curl}(\mathbf{A} - \mathbf{F_h})|^2 \mathrm{d}x.$$

Hence

$$\int_{\mathbb{R}^3} |\text{curl}(\mathbf{A} - \mathbf{F_h})|^2 \mathrm{d}x \leqslant \frac{1}{\delta_0} \int_\Omega |\mathbf{f}|^2 \mathrm{d}x + C_1 \delta_0 \int_{\mathbb{R}^3} |\text{curl}(\mathbf{A} - \mathbf{F_h})|^2 \mathrm{d}x.$$

Choose $\delta_0 = 1/(2C_1)$, we find

$$\int_{\mathbb{R}^3} | \nabla (\mathbf{A} - \mathbf{F_h})|^2 \mathrm{d}x = \int_{\mathbb{R}^3} |\text{curl}(\mathbf{A} - \mathbf{F_h})|^2 \mathrm{d}x \leqslant 4C_1 \int_\Omega |\mathbf{f}|^2 \mathrm{d}x.$$

In view of (i), we find (iii) is true.

Since $\int_\Omega (\mathbf{A} - \mathbf{F_h}) \mathrm{d}x = \mathbf{0}$, we can apply Poincarè inequality to obtain (iv) from (iii) (replacing C_0 by a larger constant if necessary).

(v) was essentially proved in Ref. 3 (Lemma 3.3). In fact, it was proved in Ref. 3 that, for $\Omega \subset B_r \subset B_R$,

$$\| \nabla (\mathbf{A} - \mathbf{F_h})\|_{C^\alpha(B_r)} \leqslant C(r, R, \alpha) \{ \|\text{curl}(\mathbf{A} - \mathbf{F_h})\|_{L^2(\mathbb{R}^3)} + \|\mathbf{f}\|_{L^q(B_R)} \}.$$

Using this, (i) and (iii) we get (v) immediately.

To prove (ii), we first use (iv) and apply the L^∞ estimate of elliptic equations to prove the conclusion for bounded σ, then apply the blow-up argument used in Ref. 26 (Proposition 4.2) to prove the conclusion for large σ. □

IV. LOCAL MINIMIZERS

Throughout this section we assume $\kappa = \lambda\varepsilon$ and $\sigma = a\varepsilon$, where $\lambda > 0$ and $a > 0$ are fixed, and ε is small. If $0 < a < a(\mathbf{h})$, then by the theory in Ref. 3 [see (2.5) previously displayed], besides the trivial critical point $(0, \mathbf{F_h})$, $\mathcal{G}_{a\varepsilon}$ has a nontrivial global minimizer in $\mathcal{W}_0(\Omega, \text{div})$ for all small $\varepsilon > 0$. In this section, we shall show that if $0 < \lambda < \lambda(\mathbf{h})$, then for each $a \in [a(\mathbf{h}), C(\lambda))$, the functional $\mathcal{G}_{a\varepsilon}$ also has a nontrivial local minimizer when $\varepsilon > 0$ is small. If $a \in (a^*(\lambda), C(\lambda))$, then $\mathcal{G}_{a\varepsilon}$ has a third (unstable) critical point (see Remark 4.4 and Lemma 5.1). We will further give a description of the way of the change of the local minimality and uniqueness, up to an additive constant vector in the vector potential, of the trivial solution $(0, \mathbf{F_h})$, when a changes. The results presented in this Section will be crucial in Sec. VI.

Let us recall from Sec. II that if we fix $\lambda \in (0, \lambda(\mathbf{h}))$, then (2.12) has exactly one positive solution $\rho(a)$ if $0 < a < a(\mathbf{h})$, and has exactly two nonnegative solutions $\rho_*(a) < \rho(a)$ if $a(\mathbf{h}) \leqslant a < C(\lambda)$. For convenience of presentation, we extend the definition of $\rho_*(a)$ and $\rho(a)$ by letting

$$\rho_*(a) = 0 \quad \text{if } 0 < a \leqslant a(\mathbf{h}), \quad \rho(0) = 1;$$
$$\rho_*(C(\lambda)) = \rho(C(\lambda)) = \rho_0, \tag{4.1}$$

where $\rho_0 \in (0,1)$ is the number given in Lemma 2.2. Then $\rho_*(a)$ is continuous on $[0, C(\lambda)]$ and is C^2 and strictly increasing in $(a(\mathbf{h}), C(\lambda))$, and $\rho(a)$ is continuous on $[0, C(\lambda)]$ and is C^2 and strictly decreasing in $(0, C(\lambda))$.

In the following we assume

$$0 < \lambda < \lambda(\mathbf{h}), \quad \kappa = \lambda\varepsilon, \quad \sigma = a\varepsilon, \tag{4.2}$$

where λ is fixed, $\varepsilon > 0$ is small and $a > 0$. We look for a local minimizer of $\mathcal{G}_{a\varepsilon}$ with ψ of the form

$$\psi = \rho^{1/2}(1 + ia\varepsilon w), \tag{4.3}$$

where $0 < \rho \leqslant 1$, $w \in W^{1,2}(\Omega, \mathbb{C})$. Let us define

$$g_{a,\varepsilon}[\rho, w, \mathbf{A}] = \frac{1}{\varepsilon^2}\mathcal{G}_{a\varepsilon}[\rho^{1/2}(1 + ia\varepsilon w), \mathbf{A}], \tag{4.4}$$

and let

$$Y_R = \{(w, \mathbf{A}) \in Y : \|(w, \mathbf{A} - \mathbf{F_h})\|_{\tilde{Y}} < R\},$$

$$\partial Y_R = \{(w, \mathbf{A}) \in Y : \|(w, \mathbf{A} - \mathbf{F_h})\|_{\tilde{Y}} = R\}.$$

Lemma 4.1: We have

$$g_{a,\varepsilon}[\rho, w, \mathbf{A}] = \frac{|\Omega|}{2}(1 - \rho)^2 + a^2 J_\rho[w, \mathbf{A}] + O(\varepsilon), \tag{4.5}$$

where the error term $O(\varepsilon)$ has the following property: For any given $R > 0$, there exists a constant $M(R) > 0$ such that

$$|O(\varepsilon)| \leqslant M(R)\varepsilon \quad \textit{for all } a \in [0, R], \quad \rho \in [0,1], \quad (w, \mathbf{A}) \in Y_R. \tag{4.6}$$

Proof: The conclusion is proved by a direct calculation. In fact for ψ given in (4.3), $\kappa = \lambda\varepsilon$ and $\sigma = a\varepsilon$ we have

$$|\nabla_{a\varepsilon\mathbf{A}}\psi|^2 = a^2\rho\varepsilon^2\{|\nabla w - \mathbf{A}|^2 - 2a\varepsilon\mathfrak{I}(\bar{w}\mathbf{A}(\nabla w - \mathbf{A})) + a^2\varepsilon^2|w\mathbf{A}|^2\},$$

$$\frac{1}{2}(1 - |\psi|^2)^2 = \frac{(1-\rho)^2}{2} + a\rho(1-\rho)\varepsilon[2\mathfrak{I}(w) - a\varepsilon|w|^2] + \frac{a^2\rho^2\varepsilon^2}{2}[2\mathfrak{I}(w) - a\varepsilon|w|^2]^2.$$

So we have

$$\begin{aligned}\frac{1}{\varepsilon^2}\mathcal{G}_{a\varepsilon}[\psi, \mathbf{A}] &= \frac{|\Omega|}{2}(1-\rho)^2 + a^2 J_\rho[w, \mathbf{A}] - 2a\rho\varepsilon\int_\Omega \{a^2\mathfrak{I}(\bar{w}\mathbf{A}(\nabla w - \mathbf{A})) - (1-\rho)\mathfrak{I}(w)\}\mathrm{d}x \\ &\quad + a^2\rho\varepsilon^2\int_\Omega \left\{a^2|w\mathbf{A}|^2 - (1-\rho)|w|^2 + \frac{\rho}{2}[2\mathfrak{I}(w) - a\varepsilon|w|^2]^2\right\}\mathrm{d}x \\ &= \frac{|\Omega|}{2}(1-\rho)^2 + a^2 J_\rho[w, \mathbf{A}] + \varepsilon q_a[\rho, w, \mathbf{A}],\end{aligned}$$

where

$$q_a[\rho,w,\mathbf{A}] = -2a\rho\int_\Omega \{a^2\mathfrak{I}(\bar{w}\mathbf{A}(\nabla w-\mathbf{A}))-(1-\rho)\mathfrak{I}(w)\}\mathrm{d}x$$
$$+a^2\rho\varepsilon\int_\Omega\left\{a^2|w\mathbf{A}|^2-(1-\rho)|w|^2+\frac{\rho}{2}[2\mathfrak{I}(w)-a\varepsilon|w|^2]^2\right\}\mathrm{d}x.$$

Using the Sobolev imbedding theorems and Hölder's inequality we can easily show that

$$M(R)=\sup_{a\in[0,R],\rho\in[0,1],(w,\mathbf{A})\in Y_R}|q_a[\rho,w,\mathbf{A}]|<\infty. \tag{4.7}$$

Hence the conclusion is true. □

Let us introduce the notation

$$I_{a,\varepsilon_0}=(\rho(a)-\varepsilon_0,\rho(a)+\varepsilon_0). \tag{4.8}$$

Lemma 4.2: Assume (4.2) *holds and let* $g_{a,\varepsilon}[\rho,w,\mathbf{A}]$ *be defined by* (4.4). *Given a small constant* $\delta>0$ *and a large constant* $R_0>0$, *there exist positive constants* $R>R_0$, ε_0, *and* ε^*, *all depending on* δ *and* R_0, *such that for each* $\varepsilon\in(0,\varepsilon^*)$ *and each* $a\in[\delta,C(\lambda)-\delta]$, *the infimum*

$$\inf_{I_{a,\varepsilon_0}\times Y_R} g_{a,\varepsilon}[\rho,w,\mathbf{A}]$$

is achieved by some $(\rho_\varepsilon^a,w_\varepsilon^a,\mathbf{A}_\varepsilon^a)\in I_{a,\varepsilon_0}\times Y_R$. *Moreover we have*

$$\lim_{\varepsilon\to0^+}\rho_\varepsilon^a=\rho(a)\quad\text{and}\quad\lim_{\varepsilon\to0^+}\|(w_\varepsilon^a-w^{\rho(a)},\mathbf{A}_\varepsilon^a-\mathbf{A}^{\rho(a)})\|_{\tilde{Y}}=0, \tag{4.9}$$

and they hold uniformly for $a\in[\delta,C(\lambda)-\delta]$.

Proof: It follows from Lemma 2.2 that given a small number $\delta>0$, we can find $\varepsilon_0>0$ depending on δ such that

$$\rho(a)-\varepsilon_0>\rho_*(a)\quad\text{and}\quad\rho(a)+\varepsilon_0<1\quad\text{for all } a\in[\delta,C(\lambda)-\delta].$$

By the properties of $F(a,\rho)$, we can find $\delta_0>0$ such that

$$F(a,\rho(a))+\delta_0\leqslant\min\{F(a,\rho(a)-\varepsilon_0),F(a,\rho(a)+\varepsilon_0)\},\quad\text{for all } a\in[\delta,C(\lambda)-\delta]. \tag{4.10}$$

We now divide our proof into several steps.

Step 1: There exist $\varepsilon_1>0$ *and* $R>R_0$ *such that if* $a\in[\delta,C(\lambda)-\delta]$ *and* $\varepsilon\in(0,\varepsilon_1)$ *are fixed, then for each* $\rho\in[\rho(a)-\varepsilon_0,\rho(a)+\varepsilon_0]$, *the functional* $g_{a,\varepsilon}[\rho,\cdot,\cdot]$ *has a minimizer* $(w_\varepsilon^\rho,\mathbf{A}_\varepsilon^\rho)$ *in* Y_R, *namely*

$$g_{a,\varepsilon}[\rho,w_\varepsilon^\rho,\mathbf{A}_\varepsilon^\rho]=\min_{(w,\mathbf{A})\in Y_R}g_{a,\varepsilon}[\rho,w,\mathbf{A}].$$

We easily see from the definition (2.9) for $J_\rho[w,\mathbf{A}]$ that for a fixed $\rho\in\bar{I}_{a,\varepsilon_0}=[\rho(a)-\varepsilon_0,\rho(a)+\varepsilon_0]$,

$$J_\rho[w,\mathbf{A}]\geqslant J_{\rho(a)-\varepsilon_0}[w,\mathbf{A}]\to\infty\quad\text{as }\|(w,\mathbf{A}-\mathbf{F_h})\|_{\tilde{Y}}\to\infty.$$

On the other hand, for the given $\delta>0$, we have

$$\sup_{a\in[\delta,C(\lambda)-\delta],\rho\in\bar{I}_{a,\varepsilon_0}}F(a,\rho)<\infty.$$

Therefore, we can find $R>R_0$ large enough so that whenever $(w,\mathbf{A})\in Y$ satisfies $\|(w,\mathbf{A}-\mathbf{F_h})\|_{\tilde{Y}}\geqslant R$, we have

$$a^2 J_\rho[w,\mathbf{A}] > \sup_{\rho\in I_{a,\varepsilon_0}} F(a,\rho)+1 \quad \text{for all a} \in [\delta, C(\lambda)-\delta].$$

We may assume that

$$R > 1 + \max_{\rho\in[0,1]} \|(w^\rho, \mathbf{A}^\rho - \mathbf{F_h})\|_{\tilde{Y}}.$$

For this R, we choose $\varepsilon_1 > 0$ small enough so that $O(\varepsilon)$ in (4.5) satisfies

$$|O(\varepsilon)| \leqslant 1/2 \quad \text{for all a} \in [0,R], \quad \rho \in [0,1], \quad \varepsilon \in (0,\varepsilon_1), \quad (w,\mathbf{A}) \in Y_R.$$

Then for any fixed $a \in [\delta, C(\lambda)-\delta]$, $\varepsilon \in (0,\varepsilon_1)$, and $\rho \in [\rho(a)-\varepsilon_0, \rho(a)+\varepsilon_0]$, we have

$$g_{a,\varepsilon}[\rho,w,\mathbf{A}] > \sup_{\rho\in I_{a,\varepsilon_0}} F(a,\rho)+1 > g_{a,\varepsilon}[\rho,w^\rho,\mathbf{A}^\rho] \quad \text{for all } (w,\mathbf{A}) \in \partial Y_R, \tag{4.11}$$

and

$$g_{a,\varepsilon}[\rho,w,\mathbf{A}] > F(a,\rho) - \frac{1}{2} \quad \text{for all } (w,\mathbf{A}) \in Y_R. \tag{4.12}$$

From (4.12) we know that for a, ρ, and ε as chosen previously,

$$\inf_{(w,\mathbf{A})\in Y_R} g_{a,\varepsilon}[\rho,w,\mathbf{A}] \geqslant F(a,\rho) - \frac{1}{2}$$

and hence it is finite. Let $(w_n,\mathbf{A}_n)$ be a minimizing sequence of $g_{a,\varepsilon}[\rho,\cdot,\cdot]$ on Y_R, namely:

$$g_{a,\varepsilon}[\rho,w_n,\mathbf{A}_n] \to \inf_{(w,\mathbf{A})\in Y_R} g_{a,\varepsilon}[\rho,w,\mathbf{A}],$$

and let

$$\psi_n = \rho^{1/2}(1 + ia\varepsilon w_n).$$

Since $\|\mathbf{A}_n - \mathbf{F_h}\|_{\mathbf{D}^{1,2}(\mathbb{R}^3)} \leqslant R$, we may assume that

$$\operatorname{curl} \mathbf{A}_n - \mathbf{h} \to \mathbf{B}_0.$$

weakly in $L^2(\mathbb{R}^3)$ as $n\to\infty$. On the other hand, using the condition $\int_\Omega \mathbf{A}_n dx = \mathbf{0}$ and the Sobolev imbedding theorems on bounded sets, and a standard diagonal argument, and passing to a subsequence if necessary, we may assume that $\mathbf{A}_n$ converges strongly in $L^4(B_r)$ and weakly in $W^{1,2}(B_r,\mathbb{R}^3)$ to some $\mathbf{A}_0$ for all balls $B_r \subset \mathbb{R}^3$. It follows that $\mathbf{B}_0 = \operatorname{curl} \mathbf{A}_0 - \mathbf{h}$ and $\int_\Omega \mathbf{A}_0 dx = \mathbf{0}$. Thus

$$\operatorname{curl} \mathbf{A}_n - \mathbf{h} \to \operatorname{curl} \mathbf{A}_0 - \mathbf{h}$$

weakly in $L^2(\mathbb{R}^3)$ as $n\to\infty$.

Since $\{\psi_n\}$ is bounded in $W^{1,2}(\Omega,\mathbb{C})$, we can apply the Sobolev imbedding theorems to conclude that after passing to a subsequence, $\phi_n \to \phi_0$ weakly in $W^{1,2}(\Omega,\mathbb{C})$ and strongly in $L^4(\Omega)$ as $n\to\infty$, and $\psi_0 = \rho^{1/2}(1+ia\varepsilon w_0)$. It now follows easily that

$$\mathcal{G}_{a\varepsilon}[\psi_0,\mathbf{A}_0] \leqslant \lim_{n\to\infty} \mathcal{G}_{a\varepsilon}[\psi_n,\mathbf{A}_n],$$

and hence

$$g_{a,\varepsilon}[\rho,w_0,\mathbf{A}_0] \leqslant g_{a,\varepsilon}[\rho,w_n,\mathbf{A}_n] = \inf_{(w,\mathbf{A})\in Y_{R_0}} g_{a,\varepsilon}[\rho,w,\mathbf{A}].$$

Clearly we have $(w_0,\mathbf{A}_0) \in \bar{Y}_{R_0}$. From (4.11), $(w_0,\mathbf{A}_0) \in Y_{R_0}$. Therefore we have

$$g_{a,\varepsilon}[\rho, w_0, \mathbf{A}_0] = \inf_{(w,\mathbf{A}) \in Y_{R_0}} g_{a,\varepsilon}[\rho, w, \mathbf{A}].$$

Letting $(w_\varepsilon^\rho, \mathbf{A}_\varepsilon^\rho) = (w_0, \mathbf{A}_0)$, the conclusion in step 1 is proved.

Step 2: We have

$$\lim_{\varepsilon \to 0^+} \|(w_\varepsilon^\rho, \mathbf{A}_\varepsilon^\rho) - (w^\rho, \mathbf{A}^\rho)\|_{\tilde{Y}} = 0,$$

and it holds uniformly for $a \in [\delta, C(\lambda) - \delta]$ *and* $\rho \in \bar{I}_{a,\varepsilon_0}$.

We first prove the convergence for fixed a and ρ. Let ε_n be a sequence converging to 0, and we may assume that each ε_n is small enough so that there is a minimizer $(w_{\varepsilon_n}^\rho, \mathbf{A}_{\varepsilon_n}^\rho)$ as given in step 1. To simplify the notations we let $(w_n, \mathbf{A}_n)$ denote this minimizer. Clearly it suffices to show that there exists a subsequence, still denoted by $(w_n, \mathbf{A}_n)$, such that $\|(w_n, \mathbf{A}_n) - (w^\rho, \mathbf{A}^\rho)\|_{\tilde{Y}} \to 0$ as $n \to \infty$.

By (4.5), we see that $(w_n, \mathbf{A}_n)$ is also a minimizing sequence of $J_\rho[w, \mathbf{A}]$ over Y_R. Then a similar argument as used in step 1 shows that after passing to a subsequence,

$$\operatorname{curl} \mathbf{A}_n - \mathbf{h} \to \operatorname{curl} \mathbf{A}_0 - \mathbf{h} \quad \text{weakly in } L^2(\mathbb{R}^3),$$

$$\mathbf{A}_n \to \mathbf{A}_0 \quad \text{strongly in } L^4(\Omega),$$

$$w_n \to w_0 \quad \text{weakly in } W^{1,2}(\Omega, \mathbb{C}) \text{ and strongly in } L^4(\Omega).$$

It is then standard to obtain

$$J_\rho[w_0, \mathbf{A}_0] \leqslant \lim_{n \to \infty} J_\rho[w_n, \mathbf{A}_n] = \inf_{Y_R} J_\rho[w, \mathbf{A}].$$

Since $(w_0, \mathbf{A}_0) \in \bar{Y}_R$, we necessarily have

$$J_\rho[w_0, \mathbf{A}_0] = \inf_{Y_R} J_\rho[w, \mathbf{A}] = \lim_{n \to \infty} J_\rho[w_n, \mathbf{A}_n]. \tag{4.13}$$

As we know from Sec. II that $(w^\rho, \mathbf{A}^\rho)$ is the unique global minimizer of J_ρ, and by our choice of R, $(w^\rho, \mathbf{A}^\rho) \in Y_R$, so we must have $(w_0, \mathbf{A}_0) = (w^\rho, \mathbf{A}^\rho)$. From (4.13), we find

$$\lim_{n \to \infty} J_\rho[w_n, \mathbf{A}_n] = J_\rho[w^\rho, \mathbf{A}^\rho].$$

It follows that

$$\lim_{n \to \infty} \int_{\mathbb{R}^3} |\operatorname{curl} \mathbf{A}_n - \mathbf{h}|^2 \mathrm{d}x = \int_{\mathbb{R}^3} |\operatorname{curl} \mathbf{A}^\rho - \mathbf{h}|^2 \mathrm{d}x, \tag{4.14}$$

and

$$\lim_{n \to \infty} \int_\Omega |\nabla w_n - \mathbf{A}_n|^2 \mathrm{d}x = \int_\Omega |\nabla w^\rho - \mathbf{A}^\rho|^2 \mathrm{d}x. \tag{4.15}$$

The limit in (4.14) implies that $\operatorname{curl} \mathbf{A}_n - \operatorname{curl} \mathbf{A}_0$ converges to $\mathbf{0}$ strongly in $L^2(\mathbb{R}^3)$. Since $\operatorname{div}(\mathbf{A}_n - \mathbf{A}^\rho) = 0$, we find $\|\mathbf{A}_n - \mathbf{A}^\rho\|_{\mathbf{D}^{1,2}(\mathbb{R}^3)}$ converges to 0. From (4.15) and the fact that ∇w_n converges to ∇w^ρ weakly in $L^2(\Omega)$ and $\mathbf{A}_n - \mathbf{A}^\rho$ converges to $\mathbf{0}$ strongly in $L^2(\Omega)$, we easily deduce

$$\lim_{n\to\infty}\int_\Omega |\nabla w_n|^2 dx = \int_\Omega |\nabla w^\rho|^2 dx.$$

Recalling $\int_\Omega w_n dx = 0$, we deduce $w_n \to w^\rho$ strongly in $W^{1,2}(\Omega)$. This proves the claimed convergence for fixed a and ρ.

To show that the convergence is uniform in a and ρ, we observe that if in the previous argument we replace (a,ρ) by (a_n,ρ_n) with $a_n \to a$ and $\rho_n \to \rho$, then using (4.5) and (4.6) we find that

$$g_{a_n,\varepsilon_n}[\rho_n, w_n, \mathbf{A}_n] = \frac{|\Omega|}{2}(1-\rho_n)^2 + a_n^2 J_{\rho_n}[w_n, \mathbf{A}_n] + o(1) = \frac{|\Omega|}{2}(1-\rho)^2 + a^2 J_\rho[w_n, \mathbf{A}_n] + o(1).$$

Hence $(w_n, \mathbf{A}_n)$ is a minimizing sequence of $J_\rho[w, \mathbf{A}]$ in Y_R, and the proof follows the same line as the previous one. This finishes the proof for step 2.

Step 3: There exists $\varepsilon^* > 0$ such that for each $\varepsilon \in (0, \varepsilon^*)$ and each $a \in [\delta, C(\lambda) - \delta]$,

$$g_{a,\varepsilon}[\rho, w, \mathbf{A}] > g_{a,\varepsilon}[\rho(a), w^{\rho(a)}, \mathbf{A}^{\rho(a)}] \quad \text{for all } (\rho, w, \mathbf{A}) \in \partial(I_{a,\varepsilon_0} \times Y_R). \tag{4.16}$$

By (4.5) and (4.6) we can find $\varepsilon_2 \in (0, \varepsilon_1]$ so that for $a \in [\delta, C(\lambda) - \delta]$, $\varepsilon \in (0, \varepsilon_2)$, and $\rho \in I_{a,\varepsilon_0}$, one has

$$F(a,\rho) - \frac{\delta_0}{3} < g_{a,\varepsilon}[\rho, w^\rho, \mathbf{A}^\rho] < F(a,\rho) + \frac{\delta_0}{3}, \tag{4.17}$$

where δ_0 is given in (4.10). By (4.11), we see that (4.16) holds if $(\rho, w, \mathbf{A}) \in I_{a,\varepsilon_0} \times (\partial Y_R)$ whenever $\varepsilon \in (0, \varepsilon_1)$. Consider now the remaining case $(\rho, w, \mathbf{A}) \in (\partial I_{a,\varepsilon_0}) \times Y_R$. Let ρ^* stand for either $\rho(a) - \varepsilon_0$ or $\rho(a) + \varepsilon_0$. Then for $(w, \mathbf{A}) \in Y_R$,

$$g_{a,\varepsilon}[\rho^*, w, \mathbf{A}] \geqslant g_{a,\varepsilon}[\rho^*, w_\varepsilon^{\rho^*}, \mathbf{A}_\varepsilon^{\rho^*}].$$

By the conclusion in step 2 and (4.5) and (4.6), we have

$$\lim_{\varepsilon \to 0^+} g_{a,\varepsilon}[\rho^*, w_\varepsilon^{\rho^*}, \mathbf{A}_\varepsilon^{\rho^*}] = F(a, \rho^*).$$

Therefore we can find $\varepsilon_3 \in (0, \varepsilon_2]$ such that

$$g_{a,\varepsilon}[\rho^*, w_\varepsilon^{\rho^*}, \mathbf{A}_\varepsilon^{\rho^*}] > F(a,\rho^*) - \frac{\delta_0}{3} \quad \text{for all } \varepsilon \in (0, \varepsilon_3).$$

Therefore,

$$g_{a,\varepsilon}[\rho^*, w, \mathbf{A}] > F(a,\rho^*) - \frac{\delta_0}{3} \quad \text{for all } \varepsilon \in (0, \varepsilon_3), \quad (w, \mathbf{A}) \in Y_R.$$

In view of (4.10) and (4.17), we obtain from the above inequality that for $\varepsilon \in (0, \varepsilon_3)$,

$$g_{a,\varepsilon}[\rho^*, w, \mathbf{A}] > F(a, \rho(a)) + \frac{2\delta_0}{3} > g_{a,\varepsilon}[\rho(a), w^{\rho(a)}, \mathbf{A}^{\rho(a)}] + \frac{\delta_0}{3}.$$

Therefore we can choose $\varepsilon^* = \varepsilon_3$ and the proof for step 3 is complete.

We would like to remark that the conclusion of step 3 also follows from the independent argument in the proof for (4.9) in step 4 below. However, the argument gives a better idea on how ε^* is chosen, and indeed we feel it makes the idea of the entire proof of this lemma more transparent.

Step 4: Completion of the proof.

By (4.12), we know that the infimum

$$\inf_{(\rho,w,\mathbf{A})\in I_{a,\varepsilon_0}\times Y_R} g_{a,\varepsilon}[\rho,w,\mathbf{A}]$$

is finite. Let $(\rho_n,w_n,\mathbf{A}_n)$ be a minimizing sequence. We may assume that $\rho_n\to\rho_\varepsilon$ as $n\to\infty$. Then

$$g_{a,\varepsilon}[\rho_n,w_n,\mathbf{A}_n]=g_{a,\varepsilon}[\rho_\varepsilon,w_n,\mathbf{A}_n]+o(1).$$

Therefore $(w_n,\mathbf{A}_n)$ must be a minimizing sequence of $g_{a,\varepsilon}[\rho_\varepsilon,\cdot,\cdot]$ over Y_R. From the argument in step 1 we know that after passing to a subsequence,

$$\|(w_n,\mathbf{A}_n)-(w_\varepsilon,\mathbf{A}_\varepsilon)\|_{\tilde{Y}}\to 0 \quad \text{as } n\to\infty,$$

where $(w_\varepsilon,\mathbf{A}_\varepsilon)\in Y_R$ and is a minimizer of $g_{a,\varepsilon}[\rho_\varepsilon,\cdot,\cdot]$ in Y_R. It follows that

$$\lim_{n\to\infty} g_{a,\varepsilon}[\rho_n,w_n,\mathbf{A}_n]=g_{a,\varepsilon}[\rho_\varepsilon,w_\varepsilon,\mathbf{A}_\varepsilon].$$

Therefore, $(\rho_\varepsilon,w_\varepsilon,\mathbf{A}_\varepsilon)$ is a minimizer of $g_{a,\varepsilon}$ on $\bar{I}_{a,\varepsilon_0}\times\bar{Y}_R$. It follows from step 3 that this minimizer does not locate on the boundary of $I_{a,\varepsilon_0}\times Y_R$, and hence is a local minimizer of $g_{a,\varepsilon}$ on $I_{a,\varepsilon_0}\times Y_R$.

It remains to prove (4.9). We first prove (4.9) for a fixed a. Let ε_n be a sequence converging to 0 and let $(\rho_n,w_n,\mathbf{A}_n)$ denote $(\rho_{\varepsilon_n},w_{\varepsilon_n},\mathbf{A}_{\varepsilon_n})$. We may assume that $\rho_n\to\rho$ as $n\to\infty$. Using (4.5) and (4.6), we obtain

$$g_{a,\varepsilon_n}[\rho_n,w_n,\mathbf{A}_n]=\frac{|\Omega|}{2}(1-\rho)^2+a^2J_\rho[w_n,\mathbf{A}_n]+o(1). \tag{4.18}$$

Therefore, $(w_n,\mathbf{A}_n)$ is a minimizing sequence of $J_\rho[w,\mathbf{A}]$ over Y_R. Now the argument in the proof of step 2 shows that

$$\|(w_n,\mathbf{A}_n)-(w^\rho,\mathbf{A}^\rho)\|_{\tilde{Y}}\to 0 \quad \text{as } n\to\infty.$$

It follows from (4.18) that

$$\lim_{n\to\infty} g_{a,\varepsilon_n}[\rho_n,w_n,\mathbf{A}_n]=F(a,\rho).$$

Note that $\rho\in\bar{I}_{a,\varepsilon_0}$. If $\rho\neq\rho(a)$, we have $F(a,\rho)>F(a,\rho(a))$; and by (4.5) and (4.6),

$$\lim_{n\to\infty} g_{a,\varepsilon_n}[\rho(a),w^{\rho(a)},\mathbf{A}^{\rho(a)}]=F(a,\rho(a))<F(a,\rho).$$

Hence for all large n,

$$g_{a,\varepsilon_n}[\rho_n,w_n,\mathbf{A}_n]>g_{a,\varepsilon_n}[\rho(a),w^{\rho(a)},\mathbf{A}^{\rho(a)}].$$

But this inequality contradicts the assumption that $(\rho_n,w_n,\mathbf{A}_n)$ is a minimizer of g_{a,ε_n} over $I_{a,\varepsilon_0}\times Y_R$. Therefore we must have $\rho=\rho(a)$. It follows that the entire original sequence $(\rho_n,w_n,\mathbf{A}_n)$ converges to $(\rho(a),w^{\rho(a)},\mathbf{A}^{\rho(a)})$ in the obvious sense.

Finally we can apply the argument used in step 2 to show that (4.9) holds uniformly in a. The details are omitted. □

Let us define

$$Z_{a,\varepsilon}=\{(\psi,\mathbf{A}):\psi=z(1+ia\varepsilon w),\quad z\in\mathbb{C},\quad |z|^2\in I_{a,\varepsilon_0},\quad (w,\mathbf{A})\in Y_R\}.$$

Now we can state the main result in this section.

Proposition 4.3: Under assumption (4.2), *for any small* $\delta>0$ *and large* $R_0>0$, *there exist* $R>R_0$, $\varepsilon_0>0$, *and* $\varepsilon^*>0$ *such that, for each* $a\in[\delta,C(\lambda)-\delta]$ *and* $\varepsilon\in(0,\varepsilon^*)$, *the functional* $\mathcal{G}_{a\varepsilon}$ *has a nontrivial local minimizer* $(\psi_\varepsilon^a,\mathbf{A}_\varepsilon^a)$, *and*

$$\mathcal{G}_{a\varepsilon}[\psi_\varepsilon^a, \mathbf{A}_\varepsilon^a] = \inf_{(\psi,\mathbf{A})\in Z_{a,\varepsilon}} \mathcal{G}_{a\varepsilon}[\psi, \mathbf{A}].$$

Moreover, we have

(i) $\psi_\varepsilon^a = \sqrt{\rho_\varepsilon^a}(1 + ia\varepsilon w_\varepsilon^a)$, *where* $(\rho_\varepsilon^a, w_\varepsilon^a, \mathbf{A}_\varepsilon^a) \in I_{a,\varepsilon_0} \times Y_R$;
(ii) $\lim_{\varepsilon\to 0} \rho_\varepsilon^a = \rho(a)$, $\lim_{\varepsilon\to 0} \|(w_\varepsilon^a, \mathbf{A}_\varepsilon^a) - (w^{\rho(a)}, \mathbf{A}^{\rho(a)})\|_{\tilde{Y}} = 0$ *uniformly in* $a \in [\delta, C(\lambda) - \delta]$.

Proof: Note that the set

$$\{(\psi, \tilde{\mathbf{A}}) : \tilde{\mathbf{A}} = \mathbf{A} - \mathbf{F_h}, \quad (\psi, \mathbf{A}) \in Z_{a,\varepsilon}\}$$

is an open set in the space $W^{1,2}(\Omega, \mathbb{C}) \times \mathbf{D}^{1,2}(\mathbb{R}^3, \mathrm{div}, \Omega)$ with $(\psi_\varepsilon^a, \mathbf{A}_\varepsilon^a - \mathbf{F_h})$ lying in its interior, or speaking loosely, $Z_{a,\varepsilon}$ is an open set in $\mathcal{W}_0(\Omega, \mathrm{div})$ containing $(\psi_\varepsilon^a, \mathbf{A}_\varepsilon^a)$. Also note that

$$\mathcal{G}_\sigma[\psi, \mathbf{A}] = \mathcal{G}_\sigma[z\psi, \mathbf{A}] \quad \text{for all } z \in \mathbb{C} \text{ with } |z| = 1.$$

Thus $(\psi, \mathbf{A}) \in Z_{a,\varepsilon}$ is a local minimizer of $\mathcal{G}_{a\varepsilon}$ with $\psi = \sqrt{\rho}(1 + ia\varepsilon w)$ if and only if $(\rho, w, \mathbf{A})$ is a local minimizer of $g_{a,\varepsilon}$. Therefore Proposition 4.3 follows directly from Lemma 4.2. □

Remark 4.4: From Lemma 4.2 and Proposition 4.3 we find that, under assumption (4.2) we have:

(i) *for any fixed* $a \in (0, C(\lambda))$, *there exists a constant* $\varepsilon_a > 0$ *such that* $\mathcal{G}_{a\varepsilon}$ *has a nontrivial local minimizer* $(\psi_\varepsilon^a, \mathbf{A}_\varepsilon^a)$ *for all* $0 < \varepsilon < \varepsilon_a$.
(ii) *if* $a \in (a^*(\lambda), C(\lambda))$ *is fixed, then for all small* $\varepsilon > 0$, *the energy functional* $\mathcal{G}_{a\varepsilon}(\psi, \mathbf{A})$ *has two local minima:* $(0, \mathbf{F_h})$ *and* $(\psi_\varepsilon, \mathbf{A}_\varepsilon)$. *It is possible to use the well-known mountain pass theorem to show that, in this case,* $\mathcal{G}_{a\varepsilon}$ *has a third critical point* $(\psi_\varepsilon^*, \mathbf{A}_\varepsilon^*)$; *and if we write*

$$\psi_\varepsilon^* = \alpha_\varepsilon^*(1 + ia\varepsilon w_\varepsilon^*),$$

where

$$\alpha_* = \fint_\Omega \psi_\varepsilon^* dx,$$

then as $\varepsilon \to 0$,

$$|\alpha_\varepsilon^*|^2 \to \rho_*(a), \quad \|(w_\varepsilon^*, \mathbf{A}_\varepsilon^*) - (w^{\rho_*(a)}, \mathbf{A}^{\rho_*(a)})\|_{\tilde{Y}} \to 0.$$

We will discuss this point further in the next section (see Lemma 5.1).

We next examine the change of local minimality and uniqueness, up to an additive constant vector in the vector potential, of $(0, \mathbf{F_h})$ as a varies. To this end, we need an estimate of the lowest eigenvalue $\mu(\varepsilon\mathbf{A})$ for small ε which holds uniformly in $\mathbf{A}$, where $\mu(\mathbf{A})$ denotes the lowest eigenvalue of the problem

$$-\nabla_{\mathbf{A}}^2 \phi = \mu\phi \quad \text{in } \Omega, \quad (\nabla_{\mathbf{A}}\phi) \cdot \nu = 0 \quad \text{on } \partial\Omega. \tag{4.19}$$

The following estimate is an extension of Lemma 2.1.

Lemma 4.5. Suppose that $\{\mathbf{A}_n\}$ *is a sequence of vector fields in* $W^{1,2}(\Omega, \mathbb{R}^3)$ *such that*

$$\mathrm{div}\, \mathbf{A}_n = 0, \quad \int_\Omega \mathbf{A}_n dx = \mathbf{0}, \quad \lim_{n\to\infty} \|\mathbf{A}_n - \mathbf{F_h}\|_{W^{1,2}(\Omega,\mathbb{R}^3)} = 0.$$

Then for any positive sequence $\varepsilon_n \to 0$, *we have*

$$\lim_{n\to\infty} \frac{\mu(\varepsilon_n \mathbf{A}_n)}{\varepsilon_n^2} = \omega(\mathbf{h}), \tag{4.20}$$

where $\mu(\varepsilon_n \mathbf{A}_n)$ *is the lowest eigenvalue of* (4.19) *for* $\mathbf{A}=\varepsilon_n \mathbf{A}_n$.

Proof: In the proof C denotes a generic constant which varies from line to line but is independent of n. Let $\mu_n=\mu(\varepsilon_n \mathbf{A}_n)$ and let ϕ_n be a corresponding eigenfunction satisfying $\|\phi_n\|_{W^{1,2}(\Omega,\mathbb{C})}=1$. Let

$$\psi_n = 1 + i\varepsilon_n w_{\mathbf{h}},$$

where $w_{\mathbf{h}}$ is the function given in Sec. II that achieves $\omega(\mathbf{h})$. Using the variational characterization of $\mu(\varepsilon_n \mathbf{A}_n)$, we obtain

$$\frac{\mu_n}{\varepsilon_n^2} \leqslant \frac{\int_\Omega |\nabla_{\varepsilon_n \mathbf{A}_n} \psi_n|^2 \mathrm{d}x}{\varepsilon_n^2 \int_\Omega |\psi_n|^2 \mathrm{d}x} = \frac{\int_\Omega (|\nabla w_{\mathbf{h}} - \mathbf{A}_n|^2 + \varepsilon_n^2 |w_{\mathbf{h}} \mathbf{A}_n|^2)\mathrm{d}x}{\int_\Omega (1+\varepsilon_n^2 |w_{\mathbf{h}}|^2)\mathrm{d}x} \to \omega(\mathbf{h})$$

as $n \to \infty$. Therefore, after passing to a subsequence, we have $\mu_n=\lambda_n \varepsilon_n^2$ with $\lambda_n \to \lambda_0 \in [0, \omega(\mathbf{h})]$.

Since $\operatorname{div} \mathbf{A}_n=0$, the equation for ϕ_n can be written in the form

$$\begin{aligned} -\Delta \phi_n &= \mu_n \phi_n - 2i\varepsilon_n \mathbf{A}_n \cdot \nabla \phi_n - \varepsilon_n^2 |\mathbf{A}_n|^2 \phi_n \quad \text{in } \Omega, \\ \frac{\partial \phi_n}{\partial \nu} &= i\varepsilon_n \phi_n \mathbf{A}_n \cdot \nu \quad \text{on } \partial\Omega. \end{aligned} \tag{4.21}$$

Applying the Agmon–Douglis–Nirenberg L^p theory for elliptic equations (see Ref. 27, Theorem 15.2) to (4.21) we have, for $1<p<\infty$,

$$\|\phi_n\|_{W^{2,p}(\Omega,\mathbb{C})} \leqslant C_1 (\|f_n\|_{L^p(\Omega)} + \|\eta_n\|_{W^{1/2,p}(\partial\Omega)} + \|\phi_n\|_{L^p(\Omega)}), \tag{4.22}$$

where C_1 depends only on Ω,

$$f_n = \mu_n \phi_n - 2i\varepsilon_n \mathbf{A}_n \cdot \nabla \phi_n - \varepsilon_n^2 |\mathbf{A}_n|^2 \phi_n,$$

$$\eta_n = i\varepsilon_n \phi_n \mathbf{A}_n \cdot \nu,$$

and $\|\cdot\|_{W^{1/2,p}(\partial\Omega)}$ is the trace norm defined by

$$\|\eta\|_{W^{1/2,p}(\partial\Omega)} = \inf_{\phi \in W^{1,2}(\Omega), \gamma(\phi)=\eta} \|\phi\|_{W^{1,p}(\Omega)},$$

where γ is the trace operator. Since $\|\mathbf{A}_n\|_{W^{1,2}(\Omega,\mathbb{R}^3)}$ is bounded and $\int_\Omega \mathbf{A}_n \mathrm{d}x=\mathbf{0}$, we deduce from the standard Sobolev imbedding theorems that $\{\mathbf{A}_n\}$ is bounded in $L^6(\Omega)$. Similarly, since $\{\phi_n\}$ is bounded in $W^{1,2}(\Omega,\mathbb{C})$, it is bounded in $L^6(\Omega)$. Using Hölder's inequality we find

$$\|f_n\|_{L^{3/2}(\Omega)} \leqslant C, \quad \|\eta_n\|_{W^{1/2,3/2}(\partial\Omega)} \leqslant C. \tag{4.23}$$

To obtain the second inequality in (4.23) note that

$$\|\eta_n\|_{W^{1/2,3/2}(\partial\Omega)} \leqslant C\varepsilon_n \|\phi_n \mathbf{A}_n\|_{W^{1,3/2}(\Omega,\mathbb{R}^3)},$$

and

$$\begin{aligned} \|\nabla(\phi_n \mathbf{A}_n)\|_{L^{3/2}(\Omega)} &\leqslant \|\phi_n \nabla \mathbf{A}_n\|_{L^{3/2}(\Omega)} + \|\mathbf{A}_n \nabla \phi_n\|_{L^{3/2}(\Omega)} \\ &\leqslant \|\phi_n\|_{L^6(\Omega)} \|\nabla \mathbf{A}_n\|_{L^2(\Omega)} + \|\mathbf{A}_n\|_{L^6(\Omega)} \|\nabla \phi_n\|_{L^2(\Omega)}. \end{aligned}$$

Recall that $\|\phi_n\|_{W^{1,2}(\Omega,\mathbb{C})}=1$. From (4.22) and (4.23) we have

$$\|\phi_n\|_{W^{2,3/2}(\Omega,\mathbb{C})} \leqslant C.$$

This implies, by the Sobolev imbedding theorems again, that $\{\phi_n\}$ is precompact in $W^{1,2}(\Omega,\mathbb{C})$. Hence, after passing to a subsequence, we may assume that

$$\phi_n \to \phi_0 \quad \text{in } W^{1,2}(\Omega,\mathbb{C}) \text{ as } n \to \infty,$$

and $\|\phi_0\|_{W^{1,2}(\Omega,\mathbb{C})}=1$. Using this and (4.21), we find that ϕ_0 satisfies the following equation:

$$-\Delta\phi_0 = 0 \quad \text{in } \Omega, \quad \frac{\partial\phi_0}{\partial\nu} = 0 \quad \text{on } \partial\Omega.$$

It follows that ϕ_0 is a constant c_0, and $|c_0|$ is uniquely determined by $\|\phi_0\|_{W^{1,2}(\Omega,\mathbb{C})}=1$. Without loss of generality we may assume that c_0 is a positive number.

Now we define

$$\alpha_n = \int_\Omega \phi_n \mathrm{d}x, \quad \tilde{\phi}_n = \frac{\phi_n - \alpha_n}{\varepsilon_n}.$$

From (4.21) we obtain the equation for $\tilde{\phi}_n$:

$$\begin{aligned} -\Delta\tilde{\phi}_n &= \varepsilon_n\lambda_n\phi_n - 2i\mathbf{A}_n\cdot\nabla\phi_n - \varepsilon_n|\mathbf{A}_n|^2\phi_n \quad \text{in } \Omega, \\ \frac{\partial\tilde{\phi}_n}{\partial\nu} &= i\phi_n\mathbf{A}_n\cdot\nu \quad \text{on } \partial\Omega. \end{aligned} \tag{4.24}$$

Let

$$\tilde{f}_n = \varepsilon_n\lambda_n\phi_n - 2i\mathbf{A}_n\cdot\nabla\phi_n - \varepsilon_n|\mathbf{A}_n|^2\phi_n,$$

$$\tilde{\eta}_n = i\phi_n\mathbf{A}_n\cdot\nu.$$

Since $\int_\Omega\tilde{\phi}_n\mathrm{d}x=0$, the L^p theory for elliptic equations[27,28] applied to (4.24) implies

$$\|\tilde{\phi}_n\|_{W^{2,3/2}(\Omega,\mathbb{C})} \leqslant C_2(\|\tilde{f}_n\|_{L^2(\Omega)} + \|\tilde{\eta}_n\|_{W^{1/2,3/2}(\partial\Omega)}), \tag{4.25}$$

where C_2 depends only on Ω. Similar to (4.23) we have

$$\|\tilde{f}_n\|_{L^{3/2}(\Omega)} \leqslant C, \quad \|\tilde{\eta}_n\|_{W^{1/2,3/2}(\partial\Omega)} \leqslant C.$$

Thus we have

$$\|\tilde{\phi}_n\|_{W^{2,3/2}(\Omega,\mathbb{C})} \leqslant C.$$

In particular, $\{\tilde{\phi}_n\}$ is precompact in $W^{1,2}(\Omega,\mathbb{C})$. After passing to a subsequence again, we may assume $\tilde{\phi}_n \to \tilde{\phi}_0$ in $W^{1,2}(\Omega,\mathbb{C})$ as $n\to\infty$, and then find from (4.24),

$$-\Delta\tilde{\phi}_0 = 0 \quad \text{in } \Omega, \quad \frac{\partial\tilde{\phi}_0}{\partial\nu} = ic_0\mathbf{F}_\mathbf{h}\cdot\nu \quad \text{on } \partial\Omega.$$

Comparing this with (2.2) we see that $\tilde{\phi}_0/(ic_0)$ satisfies the same equation as $w_\mathbf{h}$. Moreover, since $\int_\Omega\tilde{\phi}_n\mathrm{d}x=0$, we have $\int_\Omega\tilde{\phi}_0\mathrm{d}x=0$. It follows from the uniqueness of $w_\mathbf{h}$ that $\tilde{\phi}_0=ic_0w_\mathbf{h}$, i.e.,

$$\tilde{\phi}_n \to ic_0w_\mathbf{h} \quad \text{in } W^{1,2}(\Omega,\mathbb{C}) \text{ as } n\to\infty.$$

Let us now write

$$\tilde{\phi}_n = i\beta_n w_{\mathbf{h}} + \varepsilon\hat{\phi}_n, \quad \beta_n = -\frac{i\int_\Omega w_{\mathbf{h}}\tilde{\phi}_n \mathrm{d}x}{\int_\Omega |w_{\mathbf{h}}|^2 \mathrm{d}x}.$$

We easily see that $\beta_n \to c_0$ as $n \to \infty$. Moreover, from (4.24) we find that $\hat{\phi}_n$ satisfies

$$\begin{aligned} -\Delta\hat{\phi}_n &= \lambda_n\phi_n - 2i\mathbf{A}_n\cdot\nabla\tilde{\phi}_n - |\mathbf{A}_n|^2\phi_n \quad \text{in } \Omega, \\ \frac{\partial\hat{\phi}_n}{\partial\nu} &= i\tilde{\phi}_n\mathbf{A}_n\cdot\nu + i\varepsilon_n^{-1}[\alpha_n\mathbf{A}_n - \beta_n\mathbf{F}_{\mathbf{h}}]\cdot\nu \quad \text{on } \partial\Omega. \end{aligned} \tag{4.26}$$

Integrating the first equation of (4.26) over Ω, we obtain

$$\lambda_n\int_\Omega \phi_n \mathrm{d}x = \int_\Omega (|\mathbf{A}_n|^2\phi_n + 2i\mathbf{A}_n\cdot\nabla\tilde{\phi}_n - \Delta\hat{\phi}_n)\mathrm{d}x.$$

Since

$$\int_{\partial\Omega}\mathbf{A}_n\cdot\nu \mathrm{d}S = \int_\Omega \operatorname{div}\mathbf{A}_n \mathrm{d}x = 0$$

and

$$\int_{\partial\Omega}\mathbf{F}_{\mathbf{h}}\cdot\nu \mathrm{d}s = \int_\Omega \operatorname{div}\mathbf{F}_{\mathbf{h}}\mathrm{d}x = 0,$$

from the second equality in (4.26) we have

$$\int_\Omega \Delta\hat{\phi}_n \mathrm{d}x = \int_{\partial\Omega}\frac{\partial\hat{\phi}_n}{\partial\nu}\mathrm{d}S = \int_{\partial\Omega} i\tilde{\phi}_n\mathbf{A}_n\cdot\nu \mathrm{d}S + i\varepsilon_n^{-1}\int_{\partial\Omega}[\alpha_n\mathbf{A}_n\cdot\nu - \beta_n\mathbf{F}_{\mathbf{h}}\cdot\nu]\mathrm{d}S = \int_{\partial\Omega} i\tilde{\phi}_n\mathbf{A}_n\cdot\nu \mathrm{d}S.$$

Since $\mathbf{A}_n \to \mathbf{F}_{\mathbf{h}}$ in $W^{1,2}(\Omega,\mathbb{R}^3)$ and $\tilde{\phi}_n \to ic_0 w_{\mathbf{h}}$ as $n\to\infty$, we deduce

$$\int_\Omega \mathbf{A}_n\cdot\nabla\tilde{\phi}_n \mathrm{d}x \to ic_0\int_\Omega \mathbf{F}_{\mathbf{h}}\cdot\nabla w_{\mathbf{h}}\mathrm{d}x = ic_0\int_{\partial\Omega} w_{\mathbf{h}}\mathbf{F}_{\mathbf{h}}\cdot\nu \mathrm{d}S = ic_0\int_{\partial\Omega} w_{\mathbf{h}}\frac{\partial w_{\mathbf{h}}}{\partial\nu}\mathrm{d}S = ic_0\int_\Omega |w_{\mathbf{h}}|^2\mathrm{d}x,$$

$$\int_{\partial\Omega} i\tilde{\phi}_n\mathbf{A}_n\cdot\nu \mathrm{d}S \to -\int_{\partial\Omega} c_0 w_{\mathbf{h}}\mathbf{F}_{\mathbf{h}}\cdot\nu \mathrm{d}S = -c_0\int_\Omega |w_{\mathbf{h}}|^2\mathrm{d}x,$$

$$\int_\Omega |\mathbf{A}_n|^2\phi_n \mathrm{d}x \to \int_\Omega |\mathbf{F}_{\mathbf{h}}|^2 c_0 \mathrm{d}x.$$

We thus obtain

$$\lambda_0 c_0|\Omega| = \lim_{n\to\infty}\lambda_n\int_\Omega \phi_n \mathrm{d}x = c_0\int_\Omega (|\mathbf{F}_{\mathbf{h}}|^2 - |\nabla w_{\mathbf{h}}|^2)\mathrm{d}x = c_0\int_\Omega |\nabla w_{\mathbf{h}} - \mathbf{F}_{\mathbf{h}}|^2\mathrm{d}x = c_0\omega(\mathbf{h})|\Omega|.$$

Therefore,

$$\lambda_0 = \omega(\mathbf{h}).$$

This completes the proof. □

Now we fix a small $\varepsilon > 0$, and examine the minimality of $(0, \mathbf{F_h})$ when a changes. Note that, for any constant vector $\mathbf{c}$, $(0, \mathbf{F_h} + \mathbf{c})$ is a critical point of $\mathcal{G}_{a\varepsilon}$. In the following we consider the uniqueness of local minimizers in the space $\mathcal{W}_0(\Omega, \mathrm{div})$, in which the vector component is normalized so that the integral average over Ω is zero. Let

$$W_r := \{(\psi, \mathbf{A}) \in \mathcal{W}_0(\Omega, \mathrm{div}) : \|\psi\|_{W^{1,2}(R^3,\mathbb{C})} < r, \quad \|\mathbf{A} - \mathbf{F_h}\|_{\mathbf{D}^{1,2}(\mathbb{R}^3)} < r\}. \tag{4.27}$$

Proposition 4.6: Under assumption (4.2), for any small $\delta > 0$, there exist $\varepsilon_* > 0$, $r > 0$, and $L > 0$ such that, for every $\varepsilon \in (0, \varepsilon_*)$ being fixed,

(i) *if $a \in (0, a(\mathbf{h}) - \delta]$, then $(0, \mathbf{F_h})$ is not a local minimizer of $\mathcal{G}_{a\varepsilon}$ in $\mathcal{W}_0(\Omega, \mathrm{div})$;*
(ii) *if $a(\mathbf{h}) + \delta \leqslant a \leqslant L$, then $(0, \mathbf{F_h})$ is a local minimizer of $\mathcal{G}_{a\varepsilon}$ in $\mathcal{W}_0(\Omega, \mathrm{div})$, and it is the only critical point in W_r;*
(iii) *if $a \geqslant L$, then $(0, \mathbf{F_h})$ is the only critical point of $\mathcal{G}_{a\varepsilon}$ in $\mathcal{W}_0(\Omega, \mathrm{div})$, and hence it is the global minimizer.*

Proof: Conclusion (i) has been proved in Ref. 3. In fact, for $0 < a < a(\mathbf{h}) - \delta$, let $\phi_{a\varepsilon}$ be an eigenfunction associated with the lowest eigenvalue $\mu(a\varepsilon \mathbf{F_h})$. For small $\varepsilon > 0$, we can use (2.4) to show that for all small $t > 0$,

$$\mathcal{G}_{a\varepsilon}[t\phi_{a\varepsilon}, \mathbf{F_h}] < \frac{\varepsilon^2}{2}|\Omega| = \mathcal{G}_{a\varepsilon}[0, \mathbf{F_h}].$$

Conclusion (iii) is a consequence of Theorem 4.1 in Ref. 12. In fact it follows from Ref. 12 that there exists $L > 0$ such that, if $a \geqslant L$, then the only critical points are the normal solutions $(0, \mathbf{F_h} + \mathbf{c})$, where $\mathbf{c}$ is a constant vector. Since $(0, \mathbf{F_h} + \mathbf{c}) \in \mathcal{W}_0(\Omega, \mathrm{div})$ we must have $\mathbf{c} = \mathbf{0}$. (Note that the scaling we use in the present paper is different to that used in Ref. 12.)

To prove conclusion (ii) we use Lemma 4.5 to find $\varepsilon_1 > 0$ and $r_1 > 0$ small so that the lowest eigenvalue $\mu(a\varepsilon \mathbf{A})$ of (4.19) for $a\varepsilon \mathbf{A}$ satisfies

$$\mu(a\varepsilon \mathbf{A}) > \left(\frac{a(\mathbf{h})}{a(\mathbf{h}) + \delta/2}\right)^2 \omega(\mathbf{h}) a^2 \varepsilon^2 = \left(\frac{a\varepsilon}{a(\mathbf{h}) + \delta/2}\right)^2 \tag{4.28}$$

whenever $a\varepsilon \in (0, \varepsilon_1)$ and $\|\mathbf{A} - \mathbf{F_h}\|_{W^{1,2}(\Omega,\mathbb{R}^3)} < r_1$. Since $\int_\Omega \mathbf{A} \mathrm{d}x = \int_\Omega \mathbf{F_h} \mathrm{d}x = \mathbf{0}$, there exists a constant C such that

$$\|\mathbf{A} - \mathbf{F_h}\|_{W^{1,2}(\Omega,\mathbb{R}^3)} \leqslant C\|\mathbf{A} - \mathbf{F_h}\|_{\mathbf{D}^{1,2}(\mathbb{R}^3)}.$$

Therefore, if we choose $r = r_1/C$ and $\varepsilon_* = \varepsilon_1/L$, then for $\varepsilon \in (0, \varepsilon_*)$ and $a \in [a(\mathbf{h}) + \delta, L]$, we have, for any $(\psi, \mathbf{A}) \in W_r$ with $\psi \not\equiv 0$,

$$\mathcal{G}_{a\varepsilon}[\psi, \mathbf{A}] - \mathcal{G}_{a\varepsilon}[0, \mathbf{F_h}] \geqslant \mu(a\varepsilon \mathbf{A}) \int_\Omega |\psi|^2 \mathrm{d}x - \varepsilon^2 \int_\Omega |\psi|^2 \mathrm{d}x \geqslant \varepsilon^2 \left[\left(\frac{a(\mathbf{h}) + \delta}{a(\mathbf{h}) + \delta/2}\right)^2 - 1\right] \int_\Omega |\psi|^2 \mathrm{d}x > 0$$

It follows that $(0, \mathbf{F_h})$ is a local minimizer in W_r.

With ε, r, and a chosen as above, we now suppose that (ψ_0, A_0) is an arbitrary critical point of $\mathcal{G}_{a\varepsilon}$ in W_r. We show that $\psi_0 \equiv 0$. Otherwise, from Lemma 3.2 (i) we have $\mu(a\varepsilon \mathbf{A}_0) \leqslant \varepsilon^2$. However, from (4.28) and the choice of a we have

$$\mu(a\varepsilon \mathbf{A}_0) > \left(\frac{a(\mathbf{h}) + \delta}{a(\mathbf{h}) + \delta/2}\right)^2 \varepsilon^2 > \varepsilon^2.$$

Therefore we necessarily have $\psi_0 = 0$. From (3.2) we find

$$\operatorname{curl}^2 \mathbf{A}_0 = \mathbf{0} \text{ in } \mathbb{R}^3, \quad \mathbf{A}_0 - \mathbf{F_h} \in \mathbf{D}^{1,2}(\mathbb{R}^3, \operatorname{div}, \Omega).$$

Thus $\mathbf{B} \equiv \mathbf{A}_0 - \mathbf{F_h}$ satisfies

$$\Delta \mathbf{B} = \mathbf{0} \text{ in } \mathbb{R}^3, \quad \int_{\mathbb{R}^3} |\nabla \mathbf{B}|^2 dx = 0.$$

Hence $\mathbf{B}$ is a constant vector. Since $\int_\Omega \mathbf{B} dx = \int_\Omega (\mathbf{A}_0 - \mathbf{F_h}) dx = \mathbf{0}$, we have $\mathbf{B} = \mathbf{0}$, namely $\mathbf{A}_0 = \mathbf{F_h}$. This completes the proof. □

V. CLASSIFICATION OF NONTRIVIAL SOLUTIONS

We show in this section that, under assumption (4.2), for all small $\varepsilon > 0$, the nontrivial critical points of $\mathcal{G}_{a\varepsilon}$ can be easily classified according to the value of a. To this end, we let $(\psi_n, \mathbf{A}_n) \in \mathcal{W}_0(\Omega, \operatorname{div})$ be an arbitrary nontrivial critical point of $\mathcal{G}_{a_n \varepsilon_n}$, namely, it is a weak solution of the following system

$$\begin{aligned} &-\nabla^2_{a_n \varepsilon_n \mathbf{A}} \psi = \varepsilon^2 (1 - |\psi|^2)\psi \quad \text{in } \Omega, \\ &\operatorname{curl}^2 \mathbf{A} = \frac{1}{\lambda^2 a_n \varepsilon_n} \operatorname{Im}(\bar{\psi} \nabla_{a_n \varepsilon_n \mathbf{A}} \psi) \chi_\Omega \quad \text{in } \mathbb{R}^3, \\ &(\nabla_{a_n \varepsilon_n \mathbf{A}} \psi) \cdot \nu = 0 \quad \text{on } \partial\Omega, \\ &(\psi, \mathbf{A}) \in \mathcal{W}_0(\Omega, \operatorname{div}), \end{aligned} \tag{5.1}$$

and $\psi \equiv 0$. Due to the gauge invariance, for any complex number z_n with $|z_n| = 1$, $(z_n \psi_n, \mathbf{A}_n)$ is also a critical point. We assume that ψ_n is uniquely chosen from this gauge invariant class so that

$$\alpha_n = \int_\Omega \psi_n dx \geqslant 0. \tag{5.2}$$

Lemma 1.5: Assume $\varepsilon_n \to 0$, $a_n \to a$, *where* $0 < a < \infty$. *Let* $(\psi_n, \mathbf{A}_n) \in \mathcal{W}_0(\Omega, \operatorname{div})$ *be a nontrivial critical point of* $\mathcal{G}_{a_n \varepsilon_n}$ *where* ψ_n *satisfies* (5.2). *Then we necessarily have* $a \leqslant C(\lambda)$. *Moreover,* $\alpha_n > 0$ *for all large* n; *and if we write*

$$\psi_n = \alpha_n (1 + i a_n \varepsilon_n w_n),$$

then the following conclusions hold.

(i) *If* $0 < a < a(\mathbf{h})$, *then, as* $n \to \infty$,

$$\alpha_n \to \rho(a)^{1/2}, \quad \|(w_n, \mathbf{A}_n) - (w^{\rho(a)}, \mathbf{A}^{\rho(a)})\|_{\tilde{Y}} \to 0.$$

(ii) *If* $a(\mathbf{h}) \leqslant a < C(\lambda)$, *then, as* $n \to \infty$, *subject to a subsequence, either*

$$\alpha_n \to \rho(a)^{1/2}, \quad \|(w_n, \mathbf{A}_n) - (w^{\rho(a)}, \mathbf{A}^{\rho(a)})\|_{\tilde{Y}} \to 0,$$

or

$$\alpha_n \to \rho_*(a)^{1/2}, \quad \|(w_n, \mathbf{A}_n) - (w^{\rho_*(a)}, \mathbf{A}^{\rho_*(a)})\|_{\tilde{Y}} \to 0.$$

(iii) *If* $a = C(\lambda)$, *then, as* $n \to \infty$,

$$\alpha_n \to \rho_0^{1/2}, \quad \|(w_n, \mathbf{A}_n) - (w^{\rho_0}, \mathbf{A}^{\rho_0})\|_{\tilde{Y}} \to 0.$$

Proof: In the proof C, C_1, C_2, etc., denote generic positive constants which may be dependent

of Ω, $\mathbf{h}$, and λ but are independent of n. Let $(\psi_n, \mathbf{A}_n) \in \mathcal{W}_0(\Omega, \mathrm{div})$ be a critical point of $\mathcal{G}_{a_n\varepsilon_n}$. From Lemma 3.1, there exists a constant vector $\mathbf{v}_n \in \mathbb{R}^3$ such that

$$\mathbf{B}_n := \mathbf{A}_n - \mathbf{F}_\mathbf{h} - \mathbf{v}_n \in W^{1,2}(\mathbb{R}^3, \mathbb{R}^3).$$

In particular, $\mathbf{A}_n - \mathbf{F}_\mathbf{h} \in W^{1,2}(\Omega, \mathbb{R}^3)$.

Step 1. $\{(\psi_n, \mathbf{A}_n - \mathbf{F}_\mathbf{h})\}$ *is bounded in* $W^{1,2}(\Omega, \mathbb{C}) \times \mathbf{D}^{1,2}(\mathbb{R}^3, \mathrm{div}, \Omega)$.

It is well known (see Ref. 9) that $|\psi_n(x)| \leqslant 1$ in Ω. From Lemma 3.2 (with $\kappa = \lambda\varepsilon$ and $\sigma = a\varepsilon$) we see that

$$\int_\Omega |\nabla_{a_n\varepsilon_n \mathbf{A}_n} \psi_n|^2 \mathrm{d}x \leqslant \varepsilon_n^2 |\Omega|, \quad \| \nabla (\mathbf{A}_n - \mathbf{F}_\mathbf{h}) \|_{L^2(\mathbb{R}^3)} \leqslant C_1. \tag{5.3}$$

In particular

$$\|\mathbf{A}_n\|_{W^{1,2}(\Omega, \mathbb{R}^3)} \leqslant C_2. \tag{5.4}$$

From the first and third equations in (5.1) we see that ψ_n is a weak solution of the following equation

$$-\Delta\psi = 2ia_n\varepsilon_n \mathbf{A}_n \cdot \nabla \psi_n + g_n \text{ in } \Omega, \quad \frac{\partial \psi}{\partial \nu} = h_n \text{ on } \partial\Omega, \tag{5.5}$$

where

$$g_n = a_n^2 \varepsilon_n^2 |\mathbf{A}_n|^2 \psi_n + \varepsilon_n^2 (1 - |\psi_n|^2) \psi_n,$$

$$h_n = ia_n\varepsilon_n (\mathbf{A}_n \cdot \nu) \psi_n.$$

Multiplying (5.5) by $\bar{\psi}_n$, integrating over Ω and using the Sobolev imbedding theorems we find

$$\int_\Omega |\nabla \psi_n|^2 \mathrm{d}x = \int_\Omega \{2ia_n\varepsilon_n \mathbf{A}_n \cdot \nabla \psi_n + g_n\} \bar{\psi}_n \mathrm{d}x + \int_{\partial\Omega} h_n \bar{\psi}_n \mathrm{d}S.$$

From (5.4) and using the fact $\|\psi_n\|_{L^\infty(\Omega)} \leqslant 1$, we have

$$\|g_n\|_{L^2(\Omega)} \leqslant C_3\varepsilon_n^2, \quad \|h_n\|_{L^2(\partial\Omega)} \leqslant C_4\varepsilon_n,$$

$$\left| \int_\Omega 2ia_n\varepsilon_n \mathbf{A}_n \cdot \nabla \psi_n \bar{\psi}_n \mathrm{d}x \right| \leqslant C_5\varepsilon_n \int_\Omega |\mathbf{A}_n| |\nabla \psi_n| \mathrm{d}x \leqslant C_5\varepsilon_n \|\mathbf{A}_n\|_{L^2(\Omega)} \|\nabla \psi_n\|_{L^2(\Omega)}$$
$$\leqslant C_6\varepsilon_n \|\nabla \psi_n\|_{L^2(\Omega)}.$$

From these inequalities we have

$$\|\psi_n\|^2_{W^{1,2}(\Omega,\mathbb{C})} = \int_\Omega |\nabla \psi_n|^2 \mathrm{d}x + \int_\Omega |\psi_n|^2 \mathrm{d}x \leqslant C_7\varepsilon_n \|\psi_n\|_{W^{1,2}(\Omega,\mathbb{C})} + |\Omega|.$$

Hence there exists a constant $C_8 > 0$ such that, for all n,

$$\|\psi_n\|_{W^{1,2}(\Omega,\mathbb{C})} \leqslant C_8.$$

The proof for step 1 is complete.

Step 2: The asymptotic limit of $(\psi_n, \mathbf{A}_n)$.

We now use the equations for ψ_n and $\mathbf{A}_n$ to find their limits as $n \to \infty$. Let

$$\delta_n = \|\psi_n\|_{W^{1,2}(\Omega,\mathbb{C})}, \quad \hat{\psi}_n = \frac{\psi_n}{\delta_n}.$$

From Step 1, we may assume

$$\delta_n \to \delta_0 \geqslant 0, \quad \alpha_n \to \alpha \geqslant 0.$$

We obtain from (5.5) the equation for $\hat{\psi}_n$:

$$\begin{aligned} -\Delta\hat{\psi}_n &= 2ia_n\varepsilon_n\mathbf{A}_n\cdot\nabla\hat{\psi}_n + a_n^2\varepsilon_n^2|\mathbf{A}_n|^2\hat{\psi}_n + \varepsilon_n^2(1-\delta_n^2|\hat{\psi}_n|^2)\hat{\psi}_n \quad \text{in } \Omega, \\ \frac{\partial\hat{\psi}_n}{\partial\nu} &= ia_n\varepsilon_n\hat{\psi}_n\mathbf{A}_n\cdot\nu \quad \text{on } \partial\Omega. \end{aligned} \tag{5.6}$$

From the conclusion obtained in step 1 and the fact $\int_\Omega \mathbf{A}_n \mathrm{d}x = \mathbf{0}$ we see that $\{\mathbf{A}_n\}$ is bounded in $W^{1,2}(\Omega,\mathbb{R}^3)$. Also note that $\|\hat{\psi}_n\|_{W^{1,2}(\Omega,\mathbb{C})}=1$. Thus the right-hand side of the first equation in (5.6) is bounded in $L^{3/2}(\Omega)$, and the right side of the second equation in (5.6) is bounded in $W^{1/2,3/2}(\partial\Omega)$. Therefore the L^p estimate used for (4.21) [see (4.22)] can be applied to (5.6) to conclude that $\{\hat{\psi}_n\}$ is bounded in $W^{2,3/2}(\Omega,\mathbb{C})$. After passing to a subsequence, $\hat{\psi}_n$ converges to some $\hat{\psi}_0$ in $W^{1,2}(\Omega,\mathbb{C})$ and

$$-\Delta\hat{\psi}_0 = 0 \quad \text{in } \Omega, \quad \frac{\partial\hat{\psi}_0}{\partial\nu} = 0 \quad \text{on } \partial\Omega.$$

Therefore $\hat{\psi}_0 \equiv c_0$, a nonzero constant satisfying $\|c_0\|_{W^{1,2}(\Omega,\mathbb{C})}=1$. From (5.2) we deduce

$$c_0 = \lim_{n\to\infty}\frac{\alpha_n}{\delta_n} \geqslant 0.$$

Therefore $c_0 = 1/\sqrt{|\Omega|}$. It follows that for all large n, $\alpha_n > 0$. We assume from now on that $\alpha_n > 0$ for all $n \geqslant 1$. Thus we have

$$\hat{\psi}_n \to c_0 \text{ in } W^{1,3/2}(\Omega,\mathbb{C}) \text{ as } n\to\infty, \quad \lim_{n\to\infty}\frac{\alpha_n}{\delta_n} = c_0 = \frac{1}{\sqrt{|\Omega|}}. \tag{5.7}$$

Define

$$\tilde{\psi}_n = \frac{1}{\alpha_n\varepsilon_n}(\psi_n - \alpha_n). \tag{5.8}$$

We find from (5.6) that

$$\begin{aligned} -\Delta\tilde{\psi}_n &= \frac{\delta_n}{\alpha_n}[2ia_n\mathbf{A}_n\cdot\nabla\hat{\psi}_n + a_n^2\varepsilon_n|\mathbf{A}_n|^2\hat{\psi}_n + \varepsilon_n(1-\delta_n^2|\hat{\psi}_n|^2)\hat{\psi}_n] \quad \text{in } \Omega, \\ \frac{\partial\tilde{\psi}_n}{\partial\nu} &= \frac{\delta_n}{\alpha_n}[ia_n\hat{\psi}_n\mathbf{A}_n\cdot\nu] \quad \text{on } \partial\Omega. \end{aligned} \tag{5.9}$$

From $\lim_{n\to\infty}\delta_n/\alpha_n = 1/c_0 > 0$, $\|\hat{\psi}_n\|_{W^{1,2}(\Omega,\mathbb{C})}=1$, and using (5.4), we see that the right-hand side of the first equation in (5.9) is uniformly bounded in $L^{3/2}(\Omega)$, and the right-hand side of the second equation in (5.9) is uniformly bounded in $W^{1/2,3/2}(\partial\Omega)$. Note that $\int_\Omega \tilde{\psi}_n \mathrm{d}x = 0$. So the L^p estimate used for (4.24) [see (4.25)] can now be applied to (5.9) to conclude that $\{\tilde{\psi}_n\}$ is uniformly bounded in $W^{2,3/2}(\Omega,\mathbb{C})$. Therefore, after passing to a subsequence again, we have,

$$\tilde{\psi}_n \to \tilde{\psi}_0 \quad \text{in } W^{1,2}(\Omega,\mathbb{C}) \text{ as } n \to \infty.$$

Now we look at the equation for $\mathbf{A}_n$:

$$-\Delta \mathbf{A}_n = \operatorname{curl}^2 \mathbf{A}_n = \frac{\delta_n^2}{\lambda^2 a_n} \operatorname{Im}\left[\bar{\hat{\psi}}_n\left(\frac{\alpha_n}{\delta_n}\nabla \tilde{\psi}_n - i a_n \mathbf{A}_n \hat{\psi}_n\right)\right]\chi_\Omega. \tag{5.10}$$

From the conclusion obtained in step 1 and the fact $\int_\Omega \mathbf{A}_n dx = \mathbf{0}$, we know that $\{\mathbf{A}_n\}$ is bounded in $W^{1,2}_{\mathrm{loc}}(\mathbb{R}^3,\mathbb{R}^3)$. Using the Hölder inequality we see that the right-hand side of (5.10) is bounded in $L^{3/2}_{\mathrm{loc}}(\mathbb{R}^3)$. Then the standard interior L^p estimates of elliptic equations imply that $\{\mathbf{A}_n\}$ is bounded in $W^{2,3/2}_{\mathrm{loc}}(\mathbb{R}^3,\mathbb{R}^3)$. Using the Sobolev imbedding theorem and a standard diagonal argument we find that, after passing to a subsequence, we have

$$\mathbf{A}_n \to \mathbf{A}_0 \text{ in } W^{1,2}_{\mathrm{loc}}(\mathbb{R}^3,\mathbb{R}^3) \text{ as } n \to \infty.$$

On the other hand, from Lemma 3.1 we know that $\mathbf{B}_n = \mathbf{A}_n - \mathbf{F_h} - \mathbf{v}_n$ is a bounded sequence in $W^{1,2}(\mathbb{R}^3,\mathbb{R}^3)$. Therefore, after passing to a subsequence, it converges to some $\mathbf{B}_0$ weakly in $W^{1,2}(\mathbb{R}^3,\mathbb{R}^3)$. In particular, $\operatorname{curl} \mathbf{B}_n = \operatorname{curl}(\mathbf{A}_n - \mathbf{F_h})$ converges weakly in $L^2(\mathbb{R}^3)$ to $\operatorname{curl} \mathbf{B}_0$. Therefore, we necessarily have

$$\operatorname{curl}(\mathbf{A}_0 - \mathbf{F_h}) = \operatorname{curl} \mathbf{B}_0 \in L^2(\mathbb{R}^3).$$

Recall that we have assumed that $\alpha_n \to \alpha \geqslant 0$. Then we use (5.7), (5.9), and (5.10) to obtain

$$\begin{gathered} -\Delta \tilde{\psi}_0 = 0 \quad \text{in } \Omega, \\ \operatorname{curl}^2 \mathbf{A}_0 = \frac{\alpha^2}{\lambda^2 a} \operatorname{Im}[\nabla \tilde{\psi}_0 - i a \mathbf{A}_0)]\chi_\Omega \quad \text{in } \mathbb{R}^3, \\ \frac{\partial \tilde{\psi}_0}{\partial \nu} = i a \mathbf{A}_0 \cdot \nu \quad \text{on } \partial\Omega, \\ \mathbf{A}_0 - \mathbf{F_h} \in \mathbf{D}^{1,2}(\mathbb{R}^3,\operatorname{div},\Omega). \end{gathered} \tag{5.11}$$

Let

$$\phi_0 := \frac{\tilde{\psi}_0}{ia}.$$

From (5.11) we see that ϕ_0 satisfies

$$-\Delta \phi_0 = 0 \quad \text{in } \Omega, \quad \frac{\partial \phi_0}{\partial \nu} = \mathbf{A}_0 \cdot \nu \quad \text{on } \partial\Omega. \tag{5.12}$$

Since $\int_\Omega \phi_0 dx = 0$, from (5.12) we see immediately that ϕ_0 is real valued. From (5.11) we see that $\mathbf{A}_0$ satisfies

$$\lambda^2 \operatorname{curl}^2 \mathbf{A}_0 = \alpha^2(\nabla \phi_0 - \mathbf{A}_0)\chi_\Omega \text{ in } \mathbb{R}^3, \quad \mathbf{A}_0 - \mathbf{F_h} \in \mathbf{D}^{1,2}(\mathbb{R}^3,\operatorname{div},\Omega). \tag{5.13}$$

Comparing (5.12) and (5.13) with (2.11), we realize that

$$(\phi_0,\mathbf{A}_0) = (w^{\alpha^2},\mathbf{A}^{\alpha^2}).$$

Summarizing, we have proved that, subject to a subsequence,

$$\psi_n = \alpha_n(1+\varepsilon_n\tilde{\psi}_n), \quad \alpha_n \to \alpha \geqslant 0, \quad \|(\tilde{\psi}_n, \mathbf{A}_n) - (iaw^{\alpha^2}, \mathbf{A}^{\alpha^2})\|_{\tilde{Y}} \to 0. \tag{5.14}$$

Step 3: The value of α and completion of the proof.

Let $\tilde{\psi}_n$ be defined in (5.8), and for $\rho > 0$ let

$$\psi_n^\rho = \rho(1+\varepsilon_n\tilde{\psi}_n).$$

We know that $(\psi_n^\rho, \mathbf{A}_n)$ is a critical point of $\mathcal{G}_{a_n\varepsilon_n}$ when $\rho = \alpha_n$. It follows that

$$\frac{\partial}{\partial\rho}\mathcal{G}_{a_n\varepsilon_n}[\psi_n^\rho, \mathbf{A}_n]|_{\rho=\alpha_n} = 0 \quad \text{for all } n \geqslant 1.$$

A direct calculation gives

$$\frac{\partial}{\partial\rho}\mathcal{G}_{a_n\varepsilon_n}[\psi_n^\rho, \mathbf{A}_n] = 2\varepsilon_n^2\rho\left\{\int_\Omega |\nabla\tilde{\psi}_n - ia_n\mathbf{A}_n(1+\varepsilon_n\tilde{\psi}_n)|^2 dx - \int_\Omega (1-\rho^2|1+\varepsilon_n\tilde{\psi}_n|^2)|1+\varepsilon_n\tilde{\psi}_n|^2 dx\right\}.$$

It follows by taking $\rho = \alpha_n$ that

$$\int_\Omega |\nabla\tilde{\psi}_n - ia_n\mathbf{A}_n(1+\varepsilon_n\tilde{\psi}_n)|^2 dx = \int_\Omega (1-\alpha_n^2|1+\varepsilon_n\tilde{\psi}_n|^2)|1+\varepsilon_n\tilde{\psi}_n|^2 dx.$$

Letting $n \to \infty$ and using (5.14), we obtain

$$a^2\int_\Omega |\nabla w^{\alpha^2} - \mathbf{A}^{\alpha^2}|^2 dx = (1-\alpha^2)|\Omega|.$$

Therefore $\rho = \alpha^2 \geqslant 0$ is a solution to (2.12). By Lemma 2.2, we must have

$$a \leqslant C(\lambda), \tag{5.15}$$

and

$$\alpha = \begin{cases} \rho(a)^{1/2} & \text{if } a \in (0, a(\mathbf{h})) \\ \rho(a)^{1/2} \text{ or } \rho_*(a)^{1/2} & \text{if } a \in [a(\mathbf{h}), C(\lambda)) \\ \rho_0^{1/2} & \text{if } a = C(\lambda). \end{cases} \tag{5.16}$$

In view of (5.14), we find all the conclusions in our theorem follow from the previous formulas for α. □

Let us define

$$N_r^\rho = \{(\psi, \mathbf{A}) : \psi = z(1+ia\varepsilon w), \quad z \in \mathbb{C}, \quad ||z|^2 - \rho| + \|(w - w^\rho, \mathbf{A} - \mathbf{A}^\rho)\|_{\tilde{Y}} < r\}. \tag{5.17}$$

From Lemma 5.1 and Proposition 4.6 (iii), we immediately obtain the following result.

Theorem 5.2: *Under assumption (4.2), for any given small $\delta > 0$ and $r > 0$, there exists $\varepsilon_* > 0$ so that for every $\varepsilon \in (0, \varepsilon_*)$ being fixed, the following conclusions hold.*

(i) *If $\delta \leqslant a \leqslant a(\mathbf{h}) - \delta$ and if $(\psi, \mathbf{A}) \in \mathcal{W}_0(\Omega, \text{div})$ is a nontrivial critical point of $\mathcal{G}_{a\varepsilon}$, then $(\psi, \mathbf{A}) \in N_r^{\rho(a)}$.*

(ii) *If $a(\mathbf{h}) - \delta \leqslant a \leqslant C(\lambda) - \delta$ and if $(\psi, \mathbf{A}) \in \mathcal{W}_0(\Omega, \text{div})$ is a nontrivial critical point of $\mathcal{G}_{a\varepsilon}$, then either $(\psi, \mathbf{A}) \in N_r^{\rho(a)}$ or $(\psi, \mathbf{A}) \in N_r^{\rho_*(a)}$.*

(iii) *If $C(\lambda) - \delta \leqslant a \leqslant C(\lambda) + \delta$ and if there exists any nontrivial critical point $(\psi, \mathbf{A}) \in \mathcal{W}_0(\Omega, \text{div})$ of $\mathcal{G}_{a\varepsilon}$, then either $(\psi, \mathbf{A}) \in N_r^{\rho(a)}$ or $(\psi, \mathbf{A}) \in N_r^{\rho_*(a)}$. Here if $C(\lambda) \leqslant a \leqslant C(\lambda) + \delta$, we define $\rho(a) = \rho^*(a) = \rho_0$, where ρ_0 is the positive number given in Lemma 2.2.*

(iv) *If $a \geqslant C(\lambda) + \delta$, then $(0, \mathbf{F_h})$ is the only critical point of $\mathcal{G}_{a\varepsilon}$ in $\mathcal{W}_0(\Omega, \text{div})$.*

Recall that the existence of multiple critical points of $\mathcal{G}_{a\varepsilon}$ for $0<\lambda<\lambda(\mathbf{h})$ is essentially due to the existence of multiple positive solutions of Eq. (2.17). When $\lambda\geqslant\lambda(\mathbf{h})$, it has been shown in Ref. 3 (Lemma 3.5) that (2.17) has a unique positive solution $\rho(a)$ if $0<a<a(\mathbf{h})$, a unique non-negative solution $\rho=0$ if $a=a(\mathbf{h})$, and has no non-negative solutions if $a>a(\mathbf{h})$. Also note that it follows from Ref. 12 (Theorem 4.1) that $(0,\mathbf{F_h})$ is the only critical point of $\mathcal{G}_{a\varepsilon}$ in $\mathcal{W}_0(\Omega,\mathrm{div})$ if a is large. Using these facts and applying the arguments used in Lemma 5.1, we have the following.

Theorem 5.3: *Assume that*

$$\lambda\geqslant\lambda(\mathbf{h})\ \textit{is fixed},\quad \kappa=\lambda\varepsilon,\quad \sigma=a\varepsilon,\quad \textit{where } \varepsilon>0\ \textit{is small}. \tag{5.18}$$

For any given small $\delta>0$ and $r>0$, there exists $\varepsilon_*>0$ so that for every $\varepsilon\in(0,\varepsilon_*)$ being fixed, the following conclusions hold.

(i) *If $\delta\leqslant a\leqslant a(\mathbf{h})-\delta$, then the global minimizer of $\mathcal{G}_{a\varepsilon}$ over $\mathcal{W}_0(\Omega,\mathrm{div})$ is nontrivial, and lies in $N_r^{\rho(a)}$.*

(ii) *If $a(\mathbf{h})-\delta\leqslant a\leqslant a(\mathbf{h})+\delta$ and if there exists any nontrivial critical point $(\psi,\mathbf{A})\in\mathcal{W}_0(\Omega,\mathrm{div})$ of $\mathcal{G}_{a\varepsilon}$, then $(\psi,\mathbf{A})\in N_r^{\rho(a)}$. Here if $a(\mathbf{h})\leqslant a\leqslant a(\mathbf{h})+\delta$, we define $\rho(a)=0$.*

(iii) *If $a\geqslant a(\mathbf{h})+\delta$, then $(0,\mathbf{F_h})$ is the only critical point of $\mathcal{G}_{a\varepsilon}$ in $\mathcal{W}_0(\Omega,\mathrm{div})$.*

Remark 5.4: The results in this section and Remark 4.6 suggest that, under assumption (4.2), for fixed small $\varepsilon>0$, the set of nontrivial critical points of $\mathcal{G}_{a\varepsilon}(\psi,\mathbf{A})$ in the space of $(a,\psi,\mathbf{A})$ can be described by a bifurcation diagram (see Fig. 1):

(i) *A branch of nontrivial critical points bifurcates from the trivial solution branch*

$$\{(a,0,\mathbf{F_h}):0<a<+\infty\}$$

at $a=\varepsilon^{-2}\mu(a\varepsilon\mathbf{F_h})$, the value of which is approximately equal to $a(\mathbf{h})$ for small ε.

(ii) *Along this branch of nontrivial solutions the value of a initially increases until it reaches some critical value $C_\varepsilon(\lambda)$, which is approximately equal to $C(\lambda)$ for small ε, then the branch bends back, i.e., the value of a decreases when the branch is further continued, until a reaches 0.*

This bifurcation diagram is very much similar in nature to the curve

$$\{(a,\rho):(a,\rho)\ \textit{satisfies}\ (2.12)\},$$

i.e., the solution curve of $f(a,\rho)=1$, in the (a,ρ) plane.

VI. GLOBAL MINIMIZERS AND HYSTERESIS

In this section, under assumption (4.2), we fix a small $\varepsilon>0$ and determine the global minimizers of $\mathcal{G}_{a\varepsilon}$ according to the value of a. We will also explain how our results suggest a hysteresis phenomenon. We use the notations from previous sections. In particular, $a^*(\lambda)$ denotes the unique zero point of the function $I(a)$, see Lemma 2.3; $Z_{a,\varepsilon}$ denotes the set defined in Sec. IV, and N_r^ρ denotes the set defined in (5.17).

Theorem 6.1: *Under assumption (4.2), for any given small constants $\delta>0$ and $r>0$, there exists $\varepsilon_*>0$ such that for every $\varepsilon\in(0,\varepsilon_*)$ being fixed, we have:*

(i) *if $\delta\leqslant a\leqslant a^*(\lambda)-\delta$, then the local minimizer $(\psi_\varepsilon^a,\mathbf{A}_\varepsilon^a)$ obtained in Proposition 4.3 is a global minimizer of $\mathcal{G}_{a\varepsilon}$ over $\mathcal{W}_0(\Omega,\mathrm{div})$, and any other global minimizer, if it exists, must belong to $N_r^{\rho(a)}$;*

(ii) *if $a\geqslant a^*(\lambda)+\delta$, then $(0,\mathbf{F_h})$ is the only global minimizer of $\mathcal{G}_{a\varepsilon}$ in $\mathcal{W}_0(\Omega,\mathrm{div})$.*

Proof. From (4.5) and (4.6) we have

$$g_{a,\varepsilon}[\rho, w^{\rho}, \mathbf{A}^{\rho}] = F(a,\rho) + O(\varepsilon), \tag{6.1}$$

where $F(a,\rho)$ was defined in (2.18). From Lemma 2.3 and (2.19) we have

$$F(a,\rho(a)) - F(a,0) = I(a)|\Omega| \begin{cases} \leqslant I(a^*(\lambda) - \delta)|\Omega| < 0 & \text{if } 0 < a \leqslant a^*(\lambda) - \delta \\ \geqslant I(a^*(\lambda) + \delta)|\Omega| > 0 & \text{if } a^*(\lambda) + \delta \leqslant a \leqslant C(\lambda). \end{cases}$$

Let us define, for small $\delta > 0$,

$$\sigma_1(\delta) = -I(a^*(\lambda) - \delta)|\Omega|,$$

$$\sigma_2 \delta = I(a^*(\lambda) + \delta)|\Omega|, \tag{6.2}$$

$$\sigma_0(\delta) = \frac{1}{2}\min\{\sigma_1, \sigma_2\}.$$

Then $\sigma_j(\delta) > 0$ for small $\delta > 0$, and we have

$$F(a,\rho(a)) - F(a,0) \begin{cases} \leqslant -\sigma_1 & \text{if } 0 < a \leqslant a^*(\lambda) - \delta \\ \geqslant \sigma_2 & \text{if } a^*(\lambda) + \delta \leqslant a \leqslant C(\lambda). \end{cases} \tag{6.3}$$

Moreover, we have

$$F(a,\rho_*(a)) \geqslant \max\{F(a,0), F(a,\rho(a))\} \quad \text{if } 0 < a \leqslant C(\lambda), \tag{6.4}$$

see the discussion after the proof of Lemma 4.1. Due to (6.1), we can choose $\varepsilon_1 > 0$, $\delta_1 \in (0,\delta]$ and $r_1 \in (0,r]$ small enough so that for every $\varepsilon \in (0,\varepsilon_1)$ and $a \in [\delta, C(\lambda) + \delta_1]$, the conclusions in Theorem 5.2 holds with (δ, r) replaced by (δ_1, r_1), and

$$N_{r_1}^{\rho(a)} \subset Z_{a,\varepsilon}, \tag{6.5}$$

$$|\varepsilon^{-2}\mathcal{G}_{a\varepsilon}[\psi, \mathbf{A}] - F(a,\rho(a))| < \sigma_0 \quad \text{for all } (\psi, \mathbf{A}) \in N_{r_1}^{\rho(a)}, \tag{6.6}$$

$$|\varepsilon^{-2}\mathcal{G}_{a\varepsilon}[\psi, \mathbf{A}] - F(a,\rho_*(a))| < \sigma_0 \quad \text{for all } (\psi, \mathbf{A}) \in N_{r_1}^{\rho_*(a)}. \tag{6.7}$$

Here, as in Theorem 5.2, we understand that $\rho(a) = \rho_*(a) = \rho_0$ for $a \geqslant C(\lambda)$.

Suppose $\delta \leqslant a \leqslant a^*(\lambda) - \delta$. We shall show that the critical point $(\psi_\varepsilon^a, \mathbf{A}_\varepsilon^a)$ obtained in Proposition 4.3 is a global minimizer of $\mathcal{G}_{a\varepsilon}$ over $\mathcal{W}_0(\Omega, \mathrm{div})$. To prove, let $(\psi^*, \mathbf{A}^*)$ be any global minimizer of $\mathcal{G}_{a\varepsilon}$. By Theorem 5.2, we find either $(\psi^*, \mathbf{A}^*) = (0, \mathbf{F_h})$ or $(\psi^*, \mathbf{A}^*) \in N_{r_1}^{\rho(a)}$ or $(\psi^*, \mathbf{A}^*) \in N_{r_1}^{\rho_*(a)}$. To determine which case must occur, we estimate the energy in each case. Clearly

$$\varepsilon^{-2}\mathcal{G}_{a\varepsilon}[0, \mathbf{F_h}] = F(a,0).$$

By (6.2)–(6.7), we obtain

$$\varepsilon^{-2}\mathcal{G}_{a\varepsilon}[\psi^*, \mathbf{A}^*] \begin{cases} > F(a,0) + \sigma_0 & \text{if } (\psi^*, \mathbf{A}^*) \in N_{r_1}^{\rho_*(a)} \\ < F(a,0) - \sigma_0 & \text{if } (\psi^*, \mathbf{A}^*) \in N_{r_1}^{\rho(a)}. \end{cases}$$

Therefore we must have $(\psi^*, \mathbf{A}^*) \in N_{r_1}^{\rho(a)}$. Recall from Proposition 4.3 that $(\psi_\varepsilon^a, \mathbf{A}_\varepsilon^a)$ is a global minimizer of $\mathcal{G}_{a\varepsilon}$ over the set $Z_{a,\varepsilon}$. In view of (6.5), we have the inequality $\mathcal{G}_{a\varepsilon}[\psi_\varepsilon^a, \mathbf{A}_\varepsilon^a] \leqslant \mathcal{G}_{a\varepsilon}[\psi^*, \mathbf{A}^*]$. Since $(\psi^*, \mathbf{A}^*)$. is a global minimizer, the equality must hold, and hence $(\psi_\varepsilon^a, \mathbf{A}_\varepsilon^a)$ is a global minimizer.

Next, assume $a \geqslant a^*(\lambda)+\delta$. We shall show that $(0,\mathbf{F_h})$ is the only global minimizer of $\mathcal{G}_{a\varepsilon}$ over $\mathcal{W}_0(\Omega,\mathrm{div})$. Let $(\psi^*,\mathbf{A}^*)$ be a global minimizer. By Theorem 5.2, we find that $(\psi^*,\mathbf{A}^*)=(0,\mathbf{F_h})$ if $\varepsilon \in (0,\varepsilon_1)$ and $a \geqslant C(\lambda)+\delta_1$. In the remaining case $a \in [a^*(\lambda)+\delta, C(\lambda)+\delta_1]$, if $(\psi^*,\mathbf{A}^*) \neq (0,\mathbf{F_h})$, then Theorem 5.2 tells us that either $(\psi^*,\mathbf{A}^*) \in N_{r_1}^{\rho(a)}$ or $(\psi^*,\mathbf{A}^*) \in N_{r_1}^{\rho_*(a)}$. In either case, we can use (6.2)–(6.7) to deduce

$$\varepsilon^{-2}\mathcal{G}_{a\varepsilon}[\psi^*,\mathbf{A}^*] \geqslant F(a,0)+\sigma_0 = \varepsilon^{-2}\mathcal{G}_{a\varepsilon}[0,\mathbf{F_h}]+\sigma_0.$$

This contradiction shows that we must have $(\psi^*,\mathbf{A}^*)=(0,\mathbf{F_h})$. Therefore, if we take $\varepsilon_*=\varepsilon_1$, then both (i) and (ii) hold. □

Proof of Theorem 1.1: It follows from Theorem 6.1 immediately. □

Hysteresis: We are now in a position to explain how our results suggest a hysteresis phenomenon under assumption (4.2), see Fig. 1.

We first consider the change of superconducting behavior of the sample when the applied magnetic field is increased from below H_c.

(i) When $\sigma=a\varepsilon$ with $a<a^*(\lambda)$, $(\psi_\varepsilon^a,\mathbf{A}_\varepsilon^a)$ is a (nontrivial) global minimizer, which indicates that the sample is in a superconducting state.

(ii) As a increases across $a^*(\lambda)$, $(0,\mathbf{F_h})$ becomes a global minimizer but is uniformly away from $(\psi_\varepsilon^a,\mathbf{A}_\varepsilon^a)$ by a positive distance; moreover $(\psi_\varepsilon^a,\mathbf{A}_\varepsilon^a)$ remains to be a local minimizer until a is increased further to $C(\lambda)$, and after which this local minimizer disappears.

Therefore it seems reasonable to believe that the superconducting state of the sample does not jump to the normal state $(0,\mathbf{F_h})$ when a first crosses $a^*(\lambda)$, rather it remains to be represented by the local minimizer until a approaches $C(\lambda)$, then the state of the sample jumps to the normal state. This suggests that there is super-heating at $\sigma=H_{sh}\sim C(\lambda)\varepsilon$.

Next we consider the situation that the superconductor changes from the normal state to a superconducting state when the magnetic field is decreased from above H_c.

(i) Suppose we initially have $\sigma=a\varepsilon$ with $a>a^*(\lambda)$. Then $(0,\mathbf{F_h})$ is the global minimizer, which indicates that the sample is in the normal state.

(ii) As a decreases across $a^*(\lambda)$, $(0,\mathbf{F_h})$ loses its status as a global minimizer but it remains to be a local minimizer until a approaches $a(\mathbf{h})$; and the global minimizer $(\psi_\varepsilon^a,\mathbf{A}_\varepsilon^a)$ is uniformly away from $(0,\mathbf{F_h})$ by a positive distance.

Therefore it is reasonable to believe that the sample remains in the normal state when a decreases across $a^*(\lambda)$ until a approaches $a(\mathbf{h})$, then the state of the sample jumps to a superconducting state represented by the global minimizer $(\psi_\varepsilon^a,\mathbf{A}_\varepsilon^a)$. This suggests that sub-cooling occurs at $\sigma=H_{sc}\sim a(\mathbf{h})\varepsilon$.

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APPENDIX

Let us write the functional (1.1) by $\mathcal{G}_\sigma[\psi,\mathbf{A},\lambda,\Omega]$ to indicate the dependence on the domain Ω and the parameter λ. Let us introduce

$$\Omega_\lambda=\lambda^{-1}\Omega, \quad \psi_\lambda(y)=\psi(\lambda y), \quad \mathbf{A}_\lambda(y)=\lambda^{-1}\mathbf{A}(\lambda y), \quad \tau=\lambda^2\sigma. \tag{A1}$$

A simple computation shows

$$\mathcal{G}_\sigma[\psi,\mathbf{A},\lambda,\Omega]=\lambda\mathcal{G}_\tau[\psi_\lambda,\mathbf{A}_\lambda,1,\Omega_\lambda], \tag{A2}$$

where

$$\mathcal{G}_\tau[\phi,\mathbf{B},1,\Omega_\lambda]=\int_{\Omega_\lambda}\left\{|\nabla_{\tau\mathbf{B}}\phi|^2+\frac{\kappa^2}{2}(1-|\phi|^2)^2\right\}\mathrm{d}y+\tau^2\int_{\mathbb{R}^3}|\mathrm{curl}\,\mathbf{B}-\mathbf{h}|^2\mathrm{d}y.$$

Given a unit vector $\mathbf{h}$, let $H_c(\mathbf{h};\kappa,\lambda,\Omega)$ denote the critical field for Ω defined in (1.3). From (A2) we see that $\mathcal{G}_\sigma$ has a nontrivial minimizer if and only if $\mathcal{G}_{\lambda^2\sigma}$ has a nontrivial minimizer. Hence

$$H_c(\mathbf{h};\kappa,1,\Omega_\lambda)=\lambda^2H_c(\mathbf{h};\kappa,\lambda,\Omega). \tag{A3}$$

Let $\mathbf{F_h}$ be the vector field defined in (1.2), and let $w_\mathbf{h}$ and $\mathbf{U_h}$ be defined in (2.2) and (2.7) with respect to Ω. Set

$$\mathbf{F}_{\mathbf{h},\lambda}(y)=\frac{1}{\lambda}\mathbf{F_h}(\lambda y),\quad w_{\mathbf{h},\lambda}(y)=\frac{1}{\lambda^2}w_\mathbf{h}(\lambda y),\quad \mathbf{U}_{\mathbf{h},\lambda}(y)=\frac{1}{\lambda^2}\mathbf{U_h}(\lambda y).$$

Then $\mathbf{F}_{\mathbf{h},\lambda}$, $w_{\mathbf{h},\lambda}$, and $\mathbf{U}_{\mathbf{h},\lambda}$ satisfy (1.2), (2.2), and (2.7) for Ω_λ, respectively. Let $\omega(\mathbf{h},\Omega)$, $a(\mathbf{h},\Omega)$, and $\lambda(\mathbf{h},\Omega)$ be the numbers defined for Ω in (2.1), (2.3), and (2.8), respectively. We have

$$\omega(\mathbf{h},\Omega_\lambda)=\frac{1}{\lambda^2}\omega(\mathbf{h},\Omega),\quad a(\mathbf{h},\Omega_\lambda)=\lambda a(\mathbf{h},\Omega). \tag{A4}$$

Thus

$$\lambda(\mathbf{h},\Omega_\lambda)=\lambda(\mathbf{h},\Omega). \tag{A5}$$

Let $(w^\rho,\mathbf{A}^\rho)$ be the unique solution of (2.11) for Ω and define

$$w^\rho_\lambda(y)=\frac{1}{\lambda^2}w^\rho(\lambda y),\quad \mathbf{A}^\rho_\lambda(y)=\frac{1}{\lambda}\mathbf{A}^\rho(\lambda y).$$

Then $(w^\rho_\lambda,\mathbf{A}^\rho_\lambda)$ satisfies

$$\begin{cases}\Delta w^\rho_\lambda=0 & \text{in } \Omega_\lambda,\\ \mathrm{curl}^2\,\mathbf{A}^\rho_\lambda=\rho(\nabla w^\rho_\lambda-\mathbf{A}^\rho_\lambda)\chi_{\Omega_\lambda} & \text{in } \mathbb{R}^3,\\ \dfrac{\partial w^\rho_\lambda}{\partial\nu}=\mathbf{A}^\rho_\lambda\cdot\nu & \text{on } \partial\Omega_\lambda,\\ \mathbf{A}^\rho_\lambda-\mathbf{F}_{\mathbf{h},\lambda}\in\mathbf{D}^{1,2}(\mathbb{R}^3,\mathrm{div}).\end{cases} \tag{A6}$$

Let $f(a,\rho,\Omega)$ denote the function defined in (2.13) for Ω and $\rho(a,\Omega)$ denote the maximal solution of (2.12) for Ω. Using (A5) we find

$$f(a\lambda,\rho,\Omega_\lambda)=f(a,\rho,\Omega),\quad \rho(a\lambda,\Omega_\lambda)=\rho(a,\Omega).$$

Hence

$$I(a\lambda,\Omega_\lambda)=I(a,\Omega),$$

where $I(a,\Omega)$ denotes the function defined in (2.16) for Ω. Therefore, if $a^*(\lambda,\Omega)$ denotes the zero of $I(a,\Omega)$ given in Lemma 2.3, we have

$$a^*(\lambda,\Omega_\lambda)=\lambda a^*(\lambda,\Omega). \tag{A7}$$

Finally, let $C(\lambda,\Omega)$ be the number given in Lemma 2.2 for Ω such that $f(a,\cdot,\Omega)$ has no zero for $a>C(\lambda,\Omega)$. We have

$$C(\lambda,\Omega_\lambda)=\lambda C(\lambda,\Omega). \tag{A8}$$

Moreover,

$$a(\mathbf{h},\Omega_\lambda)<a^*(\lambda,\Omega_\lambda)<C(\lambda,\Omega_\lambda). \tag{A9}$$

From (1.4), (1.6), and the previous discussions we have

Theorem A1: *For small* κ,

$$H_c(\mathbf{h};\kappa,1,\Omega_\lambda)\sim\begin{cases}a(\mathbf{h},\Omega_\lambda)\kappa & \text{if } \lambda\geqslant\lambda(\mathbf{h},\Omega_\lambda)\\ a^*(\lambda,\Omega_\lambda)\kappa & \text{if } 0<\lambda<\lambda(\mathbf{h},\Omega_\lambda).\end{cases} \tag{A10}$$

Now we can state Conclusions A and B as follows.

Conclusion C: Let Ω *be a bounded, smooth and simply-connected domain in* $\mathbb{R}^3$. *For type I superconductors with small Ginzburg–Landau parameter* κ, *occupying* $\Omega_\lambda=\lambda^{-1}\Omega$, *and subjected to the applied magnetic field* $\mathcal{H}=\sigma\mathbf{h}$, *we have the following conclusions.*

(a) *If* $\lambda\geqslant\lambda(\mathbf{h},\Omega_\lambda)$, *there exists a critical field* H_c *such that,*

- (i) *the Meissner state is a global minimizer of the Ginzburg–Landau energy for* $0<\sigma<H_c$, *and disappears for* $\sigma>H_c$;
- (ii) *the normal state is a global minimizer for* $\sigma>H_c$, *and becomes unstable when* $0<\sigma<H_c$.

Moreover, for small κ,

$$H_c\sim a(\mathbf{h},\Omega_\lambda)\kappa.$$

(b) *If* $0<\lambda<\lambda(\mathbf{h},\Omega_\lambda)$, *there exist three critical fields* $H_{sc}<H_c<H_{sh}$, *such that*,

- (i) *the Meissner state is a global minimizer of the Ginzburg–Landau energy for* $0<\sigma<H_c$, *remains stable (a local minimizer) for* $H_c\leqslant\sigma<H_{sh}$, *and disappears for* $\sigma>H_{sh}$;
- (ii) *the normal state is a global minimizer for* $\sigma>H_c$, *remains stable (a local minimizer) for* $H_{sc}<\sigma\leqslant H_c$, *and becomes unstable when* $0<\sigma<H_{sc}$.

Moreover, for small κ,

$$H_{sc}\sim a(\mathbf{h},\Omega_\lambda)\kappa,\quad H_c\sim a^*(\lambda,\Omega_\lambda)\kappa,\quad H_{sh}\sim C(\lambda,\Omega_\lambda)\kappa.$$

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Dynamical clusters of infinite particle dynamics

V. A. Malyshev[a)]
Vadim Malyshev, Domaine de Voluceau, INRI, B.P. 105, Le Chesnay Cedex, 78153, France

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For any system $\{i\}$ of particles with the trajectories $x_i(t)$ in R^d on a finite time interval $[0,\tau]$ we define the interaction graph G. Vertices of G are the particles, there is an edge between two particles i and j iff for some $t\in[0,\tau]$ the distance between particles i and j is not greater than some constant. We undertake a detailed study of this graph for infinite particle dynamics and prove exponential estimates for its finite connected components. This also solves continuous percolation problem for complicated geometrical objects—the tubes around particle trajectories. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1955513]

I. INTRODUCTION

We undertake a detailed study of the interaction graph for infinite particle dynamics and prove exponential estimates for its finite clusters. Cluster properties of classical infinite-particle dynamics is a folklor notion now, cluster dynamics was discussed in Ref. 1. In more general sense, weak dependence of far away particle trajectories plays substantial role in many papers, see e.g., Refs. 2–5. For classical (deterministic or stochastic) dynamics, the cluster property reveals a clear geometric picture, where the system of infinite particles is subdivided into random finite subsets (clusters) which do not interact with each other on a fixed time interval. Thus the dynamics is reduced to finite particle dynamics. The new feature of this article is that we describe clusters in detail combinatorially and give combinatorial estimates of their probabilities. This solves continuous percolation problem for complicated geometrical objects—the tubes around particle trajectories.

Note that cluster property can have also different (but related) meaning: decay of correlations, existence of quasiparticles, especially for the quantum case, see Ref. 6, we do not pursue this issue here.

We assume that at time 0, for any cube Λ, Poisson point field with density ρ is given. Thus the number $N(\Lambda)$ of particles in Λ has Poisson distribution with $\langle N(\Lambda)\rangle/|\Lambda|=\rho$. The initial velocities $v_i(0)$ of the particles are assumed to be independently and identically distributed. Random initial configuration of coordinates $x_i(0)$ and velocities $v_i(0)$ is denoted by $\omega=\omega_\Lambda$.

We assume that for any cube Λ and any fixed number of particles $N(\Lambda)$ some finite particle dynamics in Λ is given. Here we mean by this that for (almost) any initial coordinates $x_i(0)$ and velocities $v_i(0)$ the trajectories $x_i(t)=x_i^{(\Lambda)}(t)$ are uniquely defined on the time interval $[0,\tau]$, they are assumed to be piecewise smooth (then the velocities $v_i(t)=\mathrm{d}x_i(t)/\mathrm{d}t$ are defined a.e.).

We further fix on some $r>0$. We call the tube (or r tube) $T_i(\tau)$ of the particle i the r-neighborhood of its trajectory $x_i(t,\omega)$, $0\leqslant t\leqslant\tau$. We say that two particles i, j interact at time t if

$$\mathrm{dist}(x_i(t),x_j(t))\leqslant 2r$$

that is if the closed r neighborhoods of $x_i(t)$ and $x_j(t)$ (the time t slices of the corresponding tubes) intersect. Then

a)Electronic mail: vadim.malyshev@inria.fr

$$s_{ij} = \min\{t:\mathrm{dist}(x_i(t),x_j(t)) \leqslant 2r\}$$

is called the first interaction time of particles i and j.

To define dynamical clusters we consider (for any τ) the following finite random graphs $G^\Lambda = G^\Lambda(\tau) = G^\Lambda(\tau,\omega)$. Vertices of G^Λ are the particles. We can assume that they are labelled by the initial coordinates of the particles. Two vertices are connected by an edge if on the time interval $[0,\tau]$ these two particles interact at least at one time moment. The sets of vertices of connected components of $G^\Lambda = G^\Lambda(\tau)$ are called dynamical clusters in Λ (or simply clusters) if τ and Λ are fixed. Equivalently, the connected components are the same as the topological connected components of the union of all tubes $T = \cup T_i(\tau)$ in $\Lambda \times [0,\tau]$.

Within this general setting, sufficient for our purpose, we have to do three additional assumptions:

(1) For simplicity of presentation we assume translation invariance of the dynamics and periodic boundary conditions and that the particle i moves freely on the time interval $(t,t+s)$

$$x_i(t+s] = x_i(t) + v_i(t+0)s$$

if for any $t' \in (t,t+s)$ this particle does not interact with other particles.

(2) We assume that for any two particles i,j their first interaction times $s_{ij} = s_{ij}(\omega)$ are all different a.s. This holds trivially in many known dynamical models.

(3) Our main assumption is that the velocities are uniformly bounded, that is for some constant $v^0 > 0$ and any i and $t \in [0,\tau]$

$$|v_i(t)| \leqslant v^0.$$

This is a very simplifying assumption. However, even under such condition the combinatorics of clusters is not easy. I hope that the obtained estimates allow to weaken essentially this condition.

Remark 1.1: Note that our dynamics is very general—we do not even assume that the particle trajectories are related for different Λ. We could even take, with some precautions. any metric space instead of R^d with trajectories satisfying Lipschitz condition

$$\mathrm{dist}(x(t),x(t')) \leqslant v^0|t-t'|.$$

At the same time we could consider the infinite particle system directly in R^d with the same existence assumptions (1)–(3).

Physical intuition and percolation theory: If the velocities are uniformly bounded then on the time interval $[0,\tau]$ the tube of a particle belongs to the ball of radius $v^0\tau + r$ with the center in its initial coordinate. The results from continuous percolation theory, see Refs. 7–9, tell us that the infinite system of balls of radius $v^0\tau + r$ around Poisson points in R^d a.s. has no infinite clusters for ρ small. More exactly, simple space scaling shows that if ρ does not exceed $\alpha_0(v^0\tau + r)^{-d}$ for some fixed factor $\alpha_0 > 0$ sufficiently small, then all clusters are finite a.s. Moreover, exponential cluster estimates hold. However this result is too rough for our purpose.

Physics tells us that the correct answer is given by the Boltzman–Grad (BG) scaling. Note that the volume λ swept up by the particle, that is the volume of its tube, is of the order $v^0\tau r^{d-1}$, where $v^0\tau$ is the length of the trajectory and r^{d-1} is of the order of the circular section of the tube. Heuristically, for the densities smaller than $\alpha_0\lambda^{-1}$, the limiting dynamical clusters should be finite a.s. The reason is that $N(\Lambda)$ particles sweep up the volume $v^0\tau r^{d-1}N(\Lambda)$ which should be small compared to Λ.

We give the proof here. As far as I know, this does not follow from the existing results in continuous percolation theory. One of the reasons is that the particle tubes are not independent volumes around the Poisson points.

For obvious reasons we assume that $v^0\tau \gg r$, that is $v^0\tau > C_1 r$ for some C_1 sufficiently large. Otherwise, the percolation properties of the initial configuration of balls of radius r would prevail.

Moreover, exactly under this condition the BG volume $v_0\tau r^{d-1}+r^d$ is much smaller than the volume $(v_0\tau+r)^d$, and our result is stronger than the one obtained from continuous percolation theory.

Result: Denote $P_k^\Lambda(\tau|x)$ the conditional probability that, under the condition that there is a particle at the point x, the cluster, containing this particle, has exactly k particles. Then the following exponential estimate holds.

Theorem 1.2: *There are constants* C, $\alpha_0>0$ *such that for any* τ, v^0, r *and*

$$\rho=\frac{N(\Lambda)}{\Lambda}=\alpha(\tau v^0 r^{d-1})^{-1} \tag{1.1}$$

with $0<\alpha<\alpha_0$ *and any* k *we have, uniformly in* Λ *and in* x,

$$P_k^\Lambda(\tau|x)\leqslant(C\alpha)^{k-1}. \tag{1.2}$$

Corollary: If for any $t\in[0,\tau]$ the thermodynamic limit of the dynamics (that is $\lim_{\Lambda\to\infty}x^{(\Lambda)}\times(t)$ exists, then all clusters in R^d are finite and the exponential estimates (1.2) hold for $P_k(\tau)=\lim_{\Lambda\to\infty}P_k^\Lambda(\tau|x)$.

Under our general dynamics one cannot prove the existence of thermodynamic limit (it may not even exist). However, there are many results, obtained in a different way, concerning the existence of the thermodynamic limit.[2,4,10,11] In the last section we give an example of the (random) dynamics which satisfies our conditions.

To prove the theorem one has to decribe somehow the set of possible clusters. There are combinatorial and geometric aspects in the description of the set of clusters. The idea of the proof is to separate these two aspects. Combinatorial part consists of describing possible "collision schemes," that is the order in which particles interact at the first time. The central difficulty lies in the estimation of the number of such schemes.

II. TREES DESCRIBING THE DYNAMICS OF CLUSTERS

Dynamical clusters grow in time. Here we describe this growth in combinatorial terms.

A. Labeled trees

Assume that $N(\Lambda)$ particles together with their initial coordinates and velocities (that is a point ω in our probability space) are given in the volume Λ. Then by assumption 1 the trajectories of particles are uniquely defined. For given ω, any $t\in[0,\tau]$ and any set A of $N=N(A)\leqslant N(\Lambda)$ particles consider the subgraph $G_A(t)=G_A(t,\omega)$ of $G(t)=G(\tau)$. Then there is a finite number of moments t when the structure of this subgraph changes (the number of edges increases). We will be interested only in the moments when some connected components join together.

Denote $A_{-j}, j=1,2,\ldots,N_1\leqslant N$, the connected components of $G_A(0)$. Assume first, for convenience, that $N_1=N$, that is all these connected components are the one-point subsets of A.

Denote

$$0<t_1<\cdots<t_l<\cdots<t_{N-1}\leqslant\tau$$

all moments when the number of connected components decreases (by assumption 2 it decreases by 1). Denote A_k, $k>0$, the connected component which appeared at time t_k. It is a union of two nonintersecting connected components $A_{i(k)}$ and $A_{j(k)}$ for some $i(k)$, $j(k)<k$. One can say that t_k is the first collision time of the clusters $A_{i(k)}$ and $A_{j(k)}$. For example, $t_1=t_1(\omega)$ is the first moment when a pair of particles from A begin to interact. Thus the cluster A_1 consists of two vertices.

Now define the tree $T(A)=T(A,\omega)$ with $2N-1$ vertices. N vertices of this tree are labeled by the initial coordinates $x_1(0),\ldots,x_N(0)$, that is by clusters of $G_A(0)$. Denote this set of vertices V_0. Let us agree that to all vertices of V_0 time moment 0 is assigned. Other $N-1$ vertices are labeled by time moments t_i (or by the clusters A_i). Denote this set of vertices $V_1=\{1,\ldots,N-1\}$. If A_k is the union of connected components $A_{i(k)}$ and $A_{j(k)}$ then we draw a directed edge from $i(k)$ to k and

directed edge from $j(k)$ to k. Now V_0 can be defined as the set of vertices having no ingoing edges. The level of the vertex w is defined to be the maximal length of the (directed) paths from V_0 to w. Thus the vertices of level 0 are exactly the vertices of V_0.

Define the complete order R on V_1: $w<w'$ iff $t(w)<t(w')$. Note that this complete order is compatible with the natural partial order on the tree defined as: $w<w'$ iff $A_w \subset A_{w'}$.

At time t_k the connected component A_k appears because some particle from $A_{i(k)}$ and some particle from $A_{j(k)}$ interact at time t_k. Denote the pair of vertices from V_0, corresponding to these two particles, as $f(i(k)), f(j(k)) \in V_0$, where $f: V_1 \to V_0$ is the function, which to any $w \in V_1$ assigns an element of A_w.

Thus, each cluster with N points defines a tree T, some complete order relation R, defined by the time moments t_k, on the set V_1, and a function $f(w)$, which assigns to each vertex w a vertex $f(w)$ of level 0, lying under w.

Formally we did not assume that the particles from A do not interact with particles outside A on time interval $[0,\tau]$. However further we will consider the trees only for this case.

B. Unlabeled structured trees

There is a continuum of the labeled trees, introduced previously. Note that all trees $T(A,\omega)$ have the following property: each vertex (except those of level 0) has exactly two adjacent vertices of lower level. Denote the corresponding class of unlabeled trees $\mathcal{T}(N)$, N is thus the number of zero level vertices. Note that the number of trees in $\mathcal{T}(N)$ does not exceed C^N for some absolute constant $C>0$ and that for any (directed) unlabeled tree $T \in \mathcal{T}(N)$ the sets $V_0=V_0(T)$, $V_1=V_1(T)$ are uniquely defined.

The triple

$$\mathbf{B} = (T,R,f)$$

will be our underlying combinatorial structure. Here $T \in \mathcal{T}(N)$, R is a complete order on $V_1(T)$ and function f on $V_1(T)$, where $f(w)$ is a directed path p from V_0 to w.

Now consider the set $\mathcal{B}(N)$ of equivalence classes of such triples under isomorphisms ψ of trees respecting the complete order R and such that $\psi f = f\psi$. Note that the number of elements in $\mathcal{B}(N)$ is finite for any N. The elements of $\mathcal{B}(N)$ can be called collision schemes (of cluster formation).

The following diagram shows unique collision schemes for $N=2,3$ and all 3 collision schemes for $N=4$:

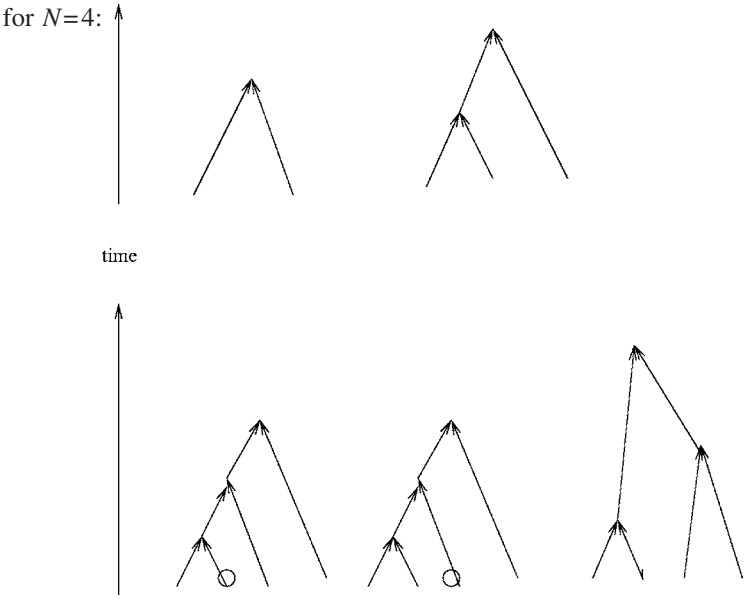

On the first two isomorphic trees for $N=4$ the small circles show the particle of the left-most cluster which interacts at time t_3 with the right-most particle.

C. Main combinatorial estimate

Note first, that in the following sections one of the vertices of V_0 will be specified. This vertex will correspond to the particle situated in some fixed point x. One could agree that the isomorphisms, introduced previously, respect the specified vertices. Choice of the specified vertex gives factor N in combinatorial estimates. It is neglectable in the foregoing estimates, and we do not consider it in this section.

For any T we shall get an upper bound for $|\mathcal{B}(T,N)|$, the number of triples from $\mathcal{B}(N)$ with given T.

Let $K(T)\leqslant(N-1)!$ be the number of ordering R. For any vertex w let D_w be the number of elements in the subcluster A_w In total this gives the factor

$$D(T)=\prod_{w=1}^{N-1} D_w.$$

The main combinatorial estimate is the following result, which is interesting in its own.

Lemma 2.1: For any tree T

$$|\mathcal{B}(T,N)|\leqslant Q(T,N)=K(T)D(T)<C^N N! \tag{2.1}$$

for some absolute constant $C>0$.

Proof: The first inequality is evident. To prove the second we need the following notation. Let S_k, S_l be two completely ordered sets with k and l elements correspondingly. Denote $R(k,l)$ the number of complete orderings of the set $S_k\cup S_l$ which do not change the order inside S_k and inside S_l. Take, for example, $k\leqslant l$, then

$$R(k,l)=2\sum_{i=1}^{k} C_{k-1}^{i-1}C_{l-1}^{i-1}.$$

In fact, we can split each of S_k and S_l on $i=1,\ldots,k$ consecutive nonempty groups and arrange these groups in a sequence in alternative order. For example, S_k can be split on i consecutive parts by putting $i-1$ walls on $k-1$ empty places between consecutive elements of S_k, that gives the factor C_{k-1}^{i-1}.

For any tree T, $|T|=N$, we have the recurrent relation

$$Q(T,N)=NQ(k,T_1)Q(N-k,T_2)R(k,N-k) \tag{2.2}$$

if under the root vertex of T there are trees T_1 and T_2 with $|T_1|=k$, $|T_2|=N-k$ correspondingly. For $q=\log_2 Q$ we have

$$q(T,N)=\log N+q(k,T_1)+q(N-k,T_2)+\log R(k,N-k). \tag{2.3}$$

One can easily get uniform estimates separately for $K(T)\leqslant N!$ and $D(T)\leqslant N!$, but it is too rough, because there are cases where $K(T)=N!$, $D(T)=C^N$ and vice versa. This is seen from the following two examples. In the first one for the sequence of subclusters

$$\{1,2\},\{1,2,3\},\ldots,\{1,2,\ldots,N-1\}$$

we have $K(T)=1$, $D(T)=(N-1)!$.

From the second example one sees, moreover, that the estimate (2.1) cannot be improved. Put $N=2^n$ and consider the tree T with 2^{n-k} vertices on levels $k=0,\ldots,n$. Denote $Q(n)=K(T)D(T)$. We have the recurrent relation

$$Q(n) = 2^{2n}Q^2(n-1)R(2^{n-1},2^{n-1}).$$

It follows

$$Q(n) \leqslant 2^{2n}Q^2(n-1)a\frac{2^N}{\sqrt{N}}$$

for some constant $a>0$. For $q(n)=\log_2 Q(n)$ this gives for $n \geqslant 2$

$$q(n) \leqslant 2q(n-1) + 2^n + bn, q(1) = 1$$

for some constant $b>0$. The solution of this inequality is

$$q(n) \leqslant \sum_{k=1}^{n} 2^k(2^{n-k} + b(n-k)) = n2^n + b2^n\sum_{k=1}^{n}(n-k)2^{-n+k} = (n+c)2^n$$

for some $c>0$. This gives

$$Q(N) \leqslant 2^{N\log N + cN}.$$

Now we come to the general case. Put $Q(N)=P(N)N!$, then from (2.2) we get

$$P(N) \leqslant NP(k)P(N-k)r(k,N-k),$$

where

$$r(k,N-k) = \frac{2\sum_{i=1}^{k} C_{k-1}^{i-1}C_{N-k-1}^{i-1}}{C_N^k}$$

for some $k \leqslant [N/2]$. For $p(N)=\log P(N)$ we have

$$p(N) = p(k) + p(N-k) + a(v),$$

$$a(v) = a(k,N-k) = \log(Nr(k,N-k)).$$

This equation can be solved explicitely as

$$p(N) = \sum_{v} a(v).$$

To make estimation of this sum we need some notation and results. In the inductive procedure for a given tree T we will distinguish vertices of type A or B, where correspondingly $k \in [\alpha[N/2],[N/2]]$ and $k \in [0,\alpha[N/2]]$ where $\alpha=1-\varepsilon$ for some small $\varepsilon>0$. Denote their numbers N_A and N_B correspondingly. We have $N_A+N_B=N-1$.

Introduce the depth $m(v)$ of the vertex v of the tree—the distance from the root vertex. It is clear that $\log N \leqslant m(v) \leqslant N$. The A-depth $m_A(v)$ of the A-vertex v is the number of A vertices on the path from it to the root. We have

$$m_A(v) < \log_b N, \quad b = \tfrac{1}{2}(1+\epsilon). \tag{2.4}$$

The number

$$\sharp(v{:}m_A(v) = m) < c^m, \quad c = 2(1+\epsilon). \tag{2.5}$$

Denote $N(v)$ the number of level 0 vertices under v. We have

$$c_-^{m(v)} < N(v) < Nc_+^{m(v)}, \tag{2.6}$$

where

$$c_- = \tfrac{1}{2}(1-\epsilon), \quad c_+ = \tfrac{1}{2}(1+\epsilon).$$

We will need some inequalities.

(1) For any k,N

$$\frac{2\sum_{i=1}^{k} C_{k-1}^{i-1} C_{N-k-1}^{i-1}}{C_N^k} \leqslant 1. \tag{2.7}$$

This can be proved by simple combinatorial argument. Take four intervals $1,2,[3,k+1],[k+2;N]$. Then we choose k elements from these two intervals. The number $2C_{k-1}^{i-1}C_{N-k-1}^{i-1}$ gives only restricted choice: we choose one of the first two elements (factor of 2), $i-1$ elements from the last interval (factor C_{N-k-1}^{i-1}) and $k-i$ elements from the third interval (factor C_{k-1}^{i-1}).

(2) (Large deviation estimate) We will use the asymptotics

$$\log C_N^{\alpha N} \sim H(\alpha)N, H(\alpha) = -\alpha \log \alpha - (1-\alpha)\log(1-\alpha).$$

Then for $\gamma \leqslant \beta \leqslant \frac{1}{2}$ the maximum of

$$\log C_{\beta N}^{\gamma N} + \log C_{(1-\beta)N}^{\gamma N}$$

is attained for γ satisfying

$$\frac{1}{\beta}\log\frac{\beta-\gamma}{\gamma} + \frac{1}{1-\beta}\log\frac{1-\beta-\gamma}{\gamma} = 0.$$

In fact,

$$\log C_{\beta N}^{\gamma N} + \log C_{(1-\beta)N}^{\gamma N} \sim N\left(H\left(\frac{\gamma}{\beta}\right)\beta + H\left(\frac{\gamma}{1-\beta}\right)(1-\beta)\right),$$

$$\frac{d}{d\gamma}\left(H\left(\frac{\gamma}{\beta}\right)\beta + H\left(\frac{\gamma}{1-\beta}\right)(1-\beta)\right) = \frac{1}{\beta}\log\frac{\beta-\gamma}{\gamma} + \frac{1}{1-\beta}\log\frac{1-\beta-\gamma}{\gamma}.$$

Then by large deviation principle for any $k \sim \beta N$, $\beta < \frac{1}{2}$

$$\log r(k, N-k) < (1-\delta)^N. \tag{2.8}$$

We estimate $a_v < N$ for B vertices and $a_v < N(v)c_+^{m(v)}$ for A vertices. Using the bounds (2.4)–(2.7) we get the proof. □

III. GEOMETRY AND PROBABILITY OF CLUSTERS

In the previous section we assigned to any ω and any cluster A the triple $\mathbf{B}=\mathbf{B}(\omega,A)$. Here we follow inverse way: for any triple $\mathbf{B} \in \mathcal{B}(\mathbf{N})$ we describe the set of ω and the set of clusters A, containing given point x, such that $\mathbf{B}=\mathbf{B}(\omega,A)$.

Note that in finite volume Λ any cluster is finite, thus for any x

$$\sum_{k=1}^{\infty} P_k^{\Lambda}(\tau|x) = 1.$$

To prove the theorem we will describe the set of initial configurations containing k particles $X = (x_1(0), v_1(0), \ldots, x_k(0), v_k(0))$ which would give a cluster with exactly k particles, if other particles in Λ were not taken into account. We estimate by 1 the conditional probability (given X) that

there are no other particles, which could interact with the particles of the cluster on the time interval $[0,\tau]$. We get these estimates uniformly in Λ and x.

For any $\mathbf{B}=(T,R,f)$ and any sequence $0<t_1<\cdots<t_{N-1}\leqslant\tau$ define the set $I(\mathbf{B},t_1,\ldots,t_{N-1})$ of initial configurations ω of particles such that there exists a set $A,|A|=N$, among them (containing some particle at x) such that A defines a cluster, $N(A)=N$ and $\mathbf{B}(A,\omega)=\mathbf{B}$. The order of t_k, of course, should be compatible with the order R. Denote

$$I(\mathbf{B}) = \cup_{t_1,\ldots,t_{N-1}} I(\mathbf{B},t_1,\ldots,t_{N-1}).$$

We use the estimate

$$P_N^{\Lambda}(\tau|x) \leqslant \sum_{\mathbf{B}} P(I(\mathbf{B})|x).$$

In the previous section we have proved the factorial estimate of the number of terms in the sum $\Sigma_{\mathbf{B}}$. Thus from Lemma 1 and the following Lemma 2 the theorem follows.

Lemma 3.1: The following bound holds uniformly in $\mathbf{B}$

$$P(I(\mathbf{B})|x) \leqslant \frac{(C\alpha)^{N-1}}{N!}$$

for some absolute constant $C>0$.

The proof of this lemma is an easy (but unwieldy) matter and will be given in the next section. It is based on simple geometric considerations with piecewise smooth trajectories and simple facts about Poisson point fields.

IV. PROOF OF LEMMA 2

It is very instructive to understand first the proof for $N=2,3$. Anyway, this is the first step of the inductive procedure below.

A. Two particle cluster

For $N=2$ we have the only tree and the only $\mathbf{B}$. We have to describe geometrically all two particle clusters

Let two particles 1 and 2 have initial velocities v_1 and v_2 correspondingly. Assume that the initial coordinate of particle 1 is $x_1(0)=x$. For any r denote $S_r(x)$ the $(d-1)$-dimensional sphere of radius r and centre $x\in R^d$, let $B_r(x)$ be the corresponding d-dimensional ball. Put $S_r=S_r(0)$ and $B_r=B_r(0)$.

At the first collision time t_1 the particles 1 and 2 should be at the points $x_1(t_1)=x_1(0)+t_1v_1$ and $x_2(t_1)=x_1(0)+t_1v_1+y_1$ correspondingly, where y_1 is any point on the sphere S_{2r}, such that for any $0\leqslant t<t_1$ the spheres $S_r(x_1(0)+tv_1)$ and $S_r(x_2(0)+tv_2)$ do not intersect. This event $G_1(t_1,y_1)$ can also be defined as the event that initially at the point $x_2(0)=x+y_1+t_1(v_1-v_2)$ there is a particle. In other words the relative initial coordinate $x_2(0)-x_1(0)$ of the particle 2 is

$$z_{12}(0) = x_2(0) - x_1(0) = y_1 + t_1(v_1 - v_2).$$

Thus $x_2(0)$, for given $v_1,v_2,t_1,x_1(0)$, should be in a subset of the sphere

$$u_1(t_1) = S_{2r}(x + t_1(v_1 - v_2)) = S_{2r} + x + t_1(v_1 - v_2)$$

in R^d.

Consider the majorizing event

$$G_1(t_1) = \cup_{y_1\in S_{2r}} G_1(t_1,y_1)$$

that there is at least one particle in $u_1(t_1)$. The union

$$G = \cup_{t_1 \in [0,\tau]} G(t_1)$$

is the event that initially there is at least one particle in the union

$$U = \cup_{t_1 \in [0,\tau]} u_1(t_1)$$

which is a closed subset of Λ, parametrized (not one-to-one) by $[0,\tau] \times S_{2r}$. The volume of U does not exceed $C\tau v^0 r^{d-1}$, uniformly in v_1, v_2 (here the boundedness of velocities is used), where C_d is some absolute constant. That is obtained by integration in t_1. Thus the probability that initially there is a particle in this volume does not exceed

$$1 - \exp(-C_d \alpha).$$

This gives the bound $C_d \alpha$ if α is small.

Note that we estimated the conditional probability for given v_1 and v_2, we should now integrate over the velocity distributions

$$\int \int \mathrm{d}\mu(v_1)\mu(v_2),$$

where μ is the initial velocity distribution.

Given the initial coordinates of the two particles, we estimate from above the conditional probability that there are no more particles in their vicinity so that they could interact with them on the time interval $(0,\tau]$, by 1.

B. Three particle cluster

For general N, and in particular for $N=3$, we should only describe the set of relative coordinates of all particles. Then we choose one particle and put its coordinate equal x (this will give a nonessential factor N), thus shifting correspondingly all configuration.

For $N=3$ we also have the unique $\mathbf{B}=(T,R,f)$. Denote velocities of the particles (say 1 and 2) colliding at time t_1 correspondingly v_1, v_2. We can assume that at time t_2 the particle 3, having velocity v_3 collides with particle 1.

Introduce the events $G_1(y_1,t_1), G_1(t_1)$ exactly as in the case of two particles. Let $x_1(s) = x_1(s;y_1)$ be the trajectory of particle 1 for $s \in [t_1,t_2]$, it depends on y_1 (or on $x_2(0)$). Introduce the conditional (given t_1, y_1) event $G_2(t_2,y_2;t_1,y_1)$ that at the moment of collision of the particle 3 with particle 1

$$x_3(t_2) = x_1(t_2) + y_2, y_2 \in S_{2r}.$$

In other words

$$x_3(0) = x_1(t_2) + y_2 - v_3 t_2.$$

Consider the events

$$G_2(t_2;y_1,t_1) = \cup_{y_2 \in S_{2r}} G_2(t_2,y_2;t_1,y_1),$$

$$G_2([s,s'];t_1,y_1) = \cup_{t_2 \in [s,s']} G_2(t_2;t_1,y_1).$$

Using the independence property of Poisson point field, we can estimate, uniformly in y_1, the probability of the event $G_2([t_2,t_2+\mathrm{d}t_2];t_1,y_1)$ as

$$\rho C v^0 r^{d-1} \mathrm{d}t_2.$$

Thus the probability of the event

$$\cup_{s_1\in[t_1,t_1+dt_1]}\cup_{s_2\in[t_2,t_2+dt_2]}(G_1(y_1,s_1)\cap G_2(s_2;t_1,y_1))$$

can be estimated as

$$\rho C v^0 r^{d-1} dt_1 \rho C v^0 r^{d-1} dt_2.$$

Put also

$$G=\cup_{t_1\in[0,\tau]}(G_1(y_1,t_1)\cap G_2(t_1,y_1))=\cup_{t_1\in[0,\tau]}\cup_{t_2\in[t_1,\tau]}(G_1(y_1,t_1)\cap G_2(t_2;t_1,y_1)).$$

Then the probability of the latter event G is estimated by

$$\int_0^\tau C\rho v^0 r^{d-1} dt_1 \int_{t_1}^\tau C\rho v^0 r^{d-1} dt_2 = (C\rho v^0 r^{d-1})^2 \frac{\tau^2}{2!}.$$

C. General case

Assume now for any N that **B** and the velocities $v_1,\dots,v_N$ of the particles are fixed. We should describe the possible initial coordinates $x_1(0),\dots,x_N(0)$ which give rise to a cluster with N particles. The emergence of the cluster occurs as a sequence of $N-1$ conditional events

$$G_1(t_1,y_1),\dots,G_k(t_k,y_k;t_{k-1},y_{k-1};\dots;t_1,y_1),\dots,G_{N-1}(t_{N-1},y_{N-1};t_{N-2},y_{N-2};\dots;t_1,y_1)$$

at the moments $t_1,\dots,t_{N-1}$. We define these events inductively.

Our inductive assumption is that after step k the vectors $y_1,\dots,y_k\in S_{2r}$ and the events $G_1,\dots,G_k$ are defined. Moreover, there are $m(k)=N-k$ maximal (that is not contained in other clusters) clusters $A_{k,1},\dots,A_{k,m(k)}$ at time t_k, as on each step the number of clusters decreases by 1. For each $i=1,\dots,m(k)$, denote a vertex of the tree, corresponding to the cluster $A_{k,i}$, by i. Assume that at time moment t_{k+1} the clusters $A_{k,i(k+1)}$ and $A_{k,j(k+1)}$ (the choice of these clusters is unique as dictated by **B**) collide and the colliding particles be $f(i(k+1))$ and $f(j(k+1))$. Moreover, after k steps the initial relative coordinates inside all maximal clusters are fixed, they enter the definition of the events $G_1,\dots,G_k$.

Thus at time t_{k+1} the particle $f(i(k+1))$ will be at the point $x_{f(i(k+1))}(t_{k+1})$, the trajectory $x_{f(i(k+1))}(s)$ on the time interval $[t_k,t_{k+1}]$ depends in a rather complicated way on the relative coordinates inside the cluster $A_{i(k+1)}$ and in a simple way (translation invariance) on the initial coordinate $x_{f(i(k+1))}(0)$. Then the particle $f(j(k+1))$ will be at the point $x_{f(i(k+1))}(t_{k+1})+y_{k+1}$. Thus the initial coordinate of the particle $f(j(k+1))$ is

$$x_{f(i(k+1))}(t_{k+1})+y_{k+1}-x^{(0)}_{f(j(k+1))}(t_{k+1}),$$

where the upper index 0 means that the initial coordinate of the particle $f(j(k+1))$ is 0, and the relative coordinates inside this cluster were fixed in the inductive process. Here we use the translation invariance of the dynamics. It follows that we know now the initial relative coordinate of the particles $f(i(k+1))$ and $f(j(k+1))$, thus all relative initial coordinates inside the new cluster $A_{k+1}=A_{k,i(k+1)}\cup A_{k,j(k+1)}$.

We have, as in case $N=3$, the inductive estimates

$$\rho C v^0 r^{d-1} dt_k$$

for the probabilites of the events

$$G_k([t_k,t_k+dt_k])=\cup_{y_k\in S_{2r}}\cup_{s_k\in[t_k,t_k+dt_k]}G_k(s_k,y_k;t_{k-1},y_{k-1};\dots;t_1,y_1)$$

uniformly in $t_{k-1},y_{k-1},\dots,t_1,y_1$. Then for the product of events

$$\cap_{k=1}^{N-1} G_k([t_k, t_k + \mathrm{d}t_k])$$

we get the estimate

$$\prod_{k=1}^{N-1} \rho C v^0 r^{d-1} \mathrm{d}t_k.$$

Then, using the known formula

$$\int_0^\tau \cdots \int_{t_{N-3}}^\tau \int_{t_{N-2}}^\tau \mathrm{d}t_{N-1} \cdots \mathrm{d}t_1 = \int_0^\tau \cdots \int_0^{t_3} \int_0^{t_2} \mathrm{d}t_1 \cdots \mathrm{d}t_{N-1} = \frac{\tau^{N-2}}{(N-2)!}$$

we get the estimate of Lemma 2.

We assumed throughout the proof that the graph $G_A(0)$ has no clusters other than one-point clusters. If however there are some clusters at time zero, then the proof proceeds along the same lines. Moreover, it is easy to see, using our assumption $r \ll v^0 \tau$, that the cluster probability will be even smaller.

V. EXAMPLE OF DYNAMICS

Here we give an example of dynamics "with chemical reactions," satisfying the above general conditions. This dynamics however will be a random dynamics. In this dynamics randomness occurs because of random initial conditions and random interaction rules of dynamics.

Define first the finite volume dynamics. There are $N(\Lambda) < \infty$ particles in the cube Λ, each particle is characterized at time $t \in R_+$ by its coordinate $x(t) \in \Lambda \subset R^d$, velocity $v(t) \in R^d$ and type $q(t) \in \{1, \ldots, Q\}$. Initial coordinates $x_i(0)$ are distributed uniformly in Λ. The vectors $(q_i(0), v_i(0))$ are independently distributed with densities $p_q(v)$

$$\sum_q \int p_q(v) \mathrm{d}v = 1.$$

We will define a continuous time Markov process $(x_i(t), v_i(t), q_i(t) : i = 1, 2, \ldots, N)$ together with initial data $(x_i(0), v_i(0), q_i(0) : i = 1, 2, \ldots, N)$. It is a mixture of piecewise linear movement for the coordinates and random jumps for the velocities and types. We will not write down the generator of this process, but rather describe it more intuitively. The coordinates are defined as

$$x_i(t, \omega) = x_i(0, \omega) + \int_0^t v_i(t, \omega) \mathrm{d}t.$$

At the same time, any pair of particles i and j (independently of other pairs) at any time interval $(t, t+dt)$ can change their types and velocities with rates

$$\lambda(q_i(t) \,.\, v_i(t), q_j(t) \,.\, v_j(t), x_i(t) - x_j(t)) \chi_{2r}(x_i(t) - x_j(t)),$$

where $\chi_{2r}(x) = 1$ if $|x| \leqslant 2r$, and 0 otherwise. Functions λ are assumed to be bounded. As a result of this jump coordinates do not change, but types and velocities change

$$(q_i, v_i, q_j, v_j) = (q_i, v_i, q_j, v_j)(t) \to (q_i', v_i', q_j', v_j') = (q_i', v_i', q_j', v_j')(t + 0)$$

via conditional probability densities $P(q_i', v_i', q_j', v_j' \,|\, q_i, v_i, q_j, v_j)$ so that for any q_i, v_i, q_j, v_j we have

$$\sum_{q_i', q_j'} \int P(q_i', v_i', q_j', v_j' | q_i, v_i, q_j, v_j) dv_i' dv_j' = 1.$$

Our main assumption that velocities are uniformly bounded that is

$$P(q_i',v_i',q_j',v_j'|q_i,v_i,q_j,v_j)=0$$

if v_i' or v_j' exceed some constant $v^0>0$.

Thus, the velocities and types are piecewise constant on $[0,\infty]$, jumps occur at discrete time moments

$$0<t_1(\omega)<\cdots<t_k(\omega)<\cdots\ .$$

The process is well defined—$x_i(t,\omega)$ exist for any initial data and are piecewise linear a.s. This means that between the jumps the particles move freely with constant velocities $v_i(t)=\mathrm{d}x_i(t)/\mathrm{d}t$ defined a.e.

All previous results for the deterministic dynamics hold for this random dynamics with piecewise random trajectories as well. In this example, from this one can easily prove, in particular, the existence of the thermodynamic limit for small times. This limit coincides with the directly and similarly defined infinite particle dynamics.

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Coupled dielectric waveguides: variational estimations

O. P. Melnichuk and I. Yu. Popov
Department of Higher Mathematics, St.-Petersburg State University of Information Technologies, Mechanics and Optics, Sablinskaya 14, St.-Petersburg, 197101, Russia

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Two dielectric waveguides coupled through small windows are considered. In the case of single coupling window we prove the existence of an eigenvalue below the threshold. It's estimation is obtained. If there is the periodic set of coupling windows a band below the threshold exists. Using variational estimations of the band edges we prove that there exists a gap between the band and the threshold. This result shows that the system has a property of photonic band gap material (photonic crystal). It can be used for construction of optical fiber systems. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1933046]

I. INTRODUCTION

Photonic band gap materials (also called photonic crystals) have attracted a lot of attention lately. The reason of this is a wealth of expected (and partly achieved) applications. Probably the main feature of these materials is the existence of a gap (stopband) in the frequency spectrum of propagating electromagnetic waves.[1] In spite of the fact that there is a great number of experimental and numerical investigations of photonic crystals, theoretical studies are far from being completed (see, e.g., Refs. 2 and 3). That is why it is interesting to analyze the corresponding systems from the point of theoretical investigations. In this paper we will discuss the system of three dielectric layers. The central layer has large permittivity. Electromagnetic waves, which passed along the layers, are considered. Analysis reduces to investigation of two possible polarizations when the electric field or correspondingly, magnetic field is orthogonal to the boundary. In each case the problem reduces to the scalar equation for the electric field (correspondingly, magnetic field). If electric field E is orthogonal to the system plane, one obtains a two-dimensional Helmholtz equation in the orthogonal cross section of the system, $-\Delta E=\lambda\varepsilon(y)E$, where $\lambda=(\omega/c)^2$, ω, wave frequency; c, speed of light; $\varepsilon(y)$, permittivity. Let us take layers of dielectric material with permittivity of $\varepsilon=\varepsilon_1$, separated by a narrow (with width 2δ) central layer with large $\varepsilon=\varepsilon_2\gg\varepsilon_1$. And there is a number of small slots (with width $2a$) in the central layer. In the case of a single narrow window (with width $2a$) in the central strip it was shown in Refs. 2 and 4 that under the assumption that $\varepsilon\delta\to 0$ or $\varepsilon\delta\to$const ($\varepsilon=\varepsilon_2-\varepsilon_1$) (i.e., for high contrast), the spectrum of the Helmholtz operator splits into two parts. One part is related with the transport properties of a narrow dielectric waveguide. The second one is close to the spectrum of the Helmholtz operator for the domain with the narrow strip replaced by a line with the Dirichlet boundary condition. Variational estimation of the bound state close to the threshold for the Dirichlet case was obtained in Refs. 5 and 6. In the case of the periodic system of narrow windows (with width $2a$) in the central strip of zero width, the asymptotics of the band edges was obtained in Ref. 7. Variational estimates of the band were obtained in Ref. 8.

The present paper has the following structure. At first, we describe the idea of the proof of the existence of eigenvalue below the threshold. We use the variational approach and the proof reduces to the obtaining of the corresponding estimations. The second section is devoted to the method of the trial function construction and to the description of the way of the main ratio estimation. The next section contains the proof of the eigenvalue existence for the case of single coupling window (the geometry of the system is shown in Fig. 1). Then we consider the case of the periodic set of coupling windows (see Fig. 2). Here we prove that there exists a band below the

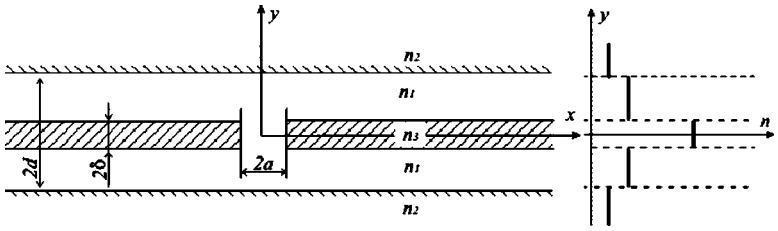

FIG. 1. Three-layer dielectric waveguide with a single coupling window.

threshold and obtain variational estimation of the gap. Note that this band belongs to the part of the spectrum which is close to the spectrum of the corresponding Dirichlet problem (see above). Thus, the described system has the spectral property which is analogous to that of a photonic crystal. The appendix contains some calculations, which are omitted in the main text.

II. THE METHOD OF THE PROOF

It is assumed that in the corresponding three-dimensional problem we deal with polarized monochromatic light (the case of TE modes is considered, i.e., $E_x=0$) passes along x axis. The layers are unbounded in the directions of x and z. Under these assumptions, mode solutions for a one-layer planar waveguide (with the refraction index n) are obtained from the Helmholtz equation for E_z [harmonic dependence on time t ($e^{i\omega t}$) is taken into account],

$$\frac{\partial^2 E_z}{\partial y^2} + \frac{\partial^2 E_z}{\partial x^2} + n^2 k_0^2 E_z = 0, \tag{1}$$

where $k_0=\omega\sqrt{\varepsilon_0\mu_0}$ and $n^2=\varepsilon/\varepsilon_0$. For the harmonic dependence of E_z on x and time t, $e^{i(\omega t-\lambda x)}$, one gets

$$\frac{\partial^2 E_z}{\partial y^2} + (n^2 k_0^2 - \lambda^2) E_z = 0, \tag{2}$$

where λ^2 is an eigenvalue of the corresponding boundary problem. Mode solutions for a multilayer waveguide are obtained by matching together the solutions for each layer. We take

$$E_z = \Psi(x,y).$$

Then for each layer we can write

$$\frac{\partial^2 \Psi_i}{\partial y^2} + (n_i^2 k_0^2 - \lambda^2)\Psi = 0,$$

where $i=1,2,3$—the number of the layer. Eigenfunction Ψ can be constructed using Ψ_1, Ψ_2, and Ψ_3. It satisfies the equation

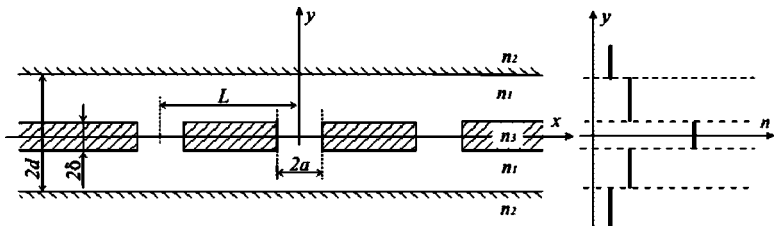

FIG. 2. Three-layer dielectric waveguide with the periodic set of coupling windows.

$$\frac{\partial^2\Psi}{\partial y^2} + (n^2k_0^2 - \lambda^2)\Psi = 0, \tag{3}$$

where

$$n = \begin{cases} n_1, & y \in [-d,-\delta] \cup [\delta,d], \\ n_2, & y \in [-\infty,-d] \cup [d,\infty], \\ n_3, & y \in [-\delta,\delta]. \end{cases} \tag{4}$$

Our system is symmetric. Hence, it is sufficient to analyze the system only for $y \geqslant 0$. The boundary conditions at $y=\delta$ and $y=d$ are

$$\begin{aligned} \Psi_2|_{(y=d)} &= \Psi_1|_{(y=d)}, \quad \left.\frac{\partial\Psi_2}{\partial y}\right|_{(y=d)} = \left.\frac{\partial\Psi_1}{\partial y}\right|_{(y=d)}, \\ \Psi_3|_{(y=\delta)} &= \Psi_1|_{(y=\delta)}, \quad \left.\frac{\partial\Psi_3}{\partial y}\right|_{(y=\delta)} = \left.\frac{\partial\Psi_1}{\partial y}\right|_{(y=\delta)}, \end{aligned} \tag{5}$$

where $\Psi_1 = \Psi|_{(\delta \leqslant y \leqslant d)}$, $\Psi_2 = \Psi|_{(d \leqslant y \leqslant \infty)}$, $\Psi_3 = \Psi|_{(0 \leqslant y \leqslant \delta)}$. We will construct an approximation of the eigenfunction $\hat{\Psi}$ for the case when there exists coupling windows as a perturbation of Ψ. That is in the corresponding two-dimensional problem the function $\hat{\Psi}$ satisfies the equation $H\hat{\Psi} - n^2k_0^2\hat{\Psi} = 0$, where $H = -\Delta$ is the Laplacian with the matching conditions at the interfaces. In accordance with the variational principles if there exists a trial function $\hat{\Psi}$ (satisfying the matching conditions at the interfaces) such that the following ratio is negative:

$$\frac{(H\hat{\Psi},\hat{\Psi}) - \|\hat{\Psi}\sqrt{n^2k_0^2 - \lambda^2}\|^2}{\|\hat{\Psi}\|^2} \leqslant 0, \tag{6}$$

then there exists an eigenvalue Λ^2 less than the threshold, $\Lambda^2 < \lambda^2$. Note that we work in the orthogonal subspace to the subspace corresponding to the first branch of the continuous spectrum (with zero lower bound), i.e., $\hat{\Psi}$ satisfies the orthogonality condition. Thus, the idea is to find a trial function $\hat{\Psi}$ which makes the ratio

$$\frac{M(\hat{\Psi})}{\|\hat{\Psi}\|^2} \tag{7}$$

negative, where

$$M(\hat{\Psi}) = (H\hat{\Psi},\hat{\Psi}) - \|\hat{\Psi}\sqrt{n^2k_0^2 - \lambda^2}\|^2. \tag{8}$$

We take the trial function $\hat{\Psi}$ as

$$\hat{\Psi} = F + G, \tag{9}$$

where

$$F = \alpha v(y) f(x), \tag{10}$$

$$v(y) = \begin{cases} N_3 \sin(\mu y), & y \in [0,\delta], \\ N_1 \cos(\nu y) + M_1 \sin(\nu y), & y \in [\delta,d], \\ N_2 e^{-\gamma(y-d)}, & y \in [d,\infty], \end{cases} \tag{11}$$

$$\gamma = \sqrt{\lambda^2 - n_2^2 k_0^2}, \quad \nu = \sqrt{\lambda^2 - n_1^2 k_0^2}, \quad \mu = \sqrt{n_3^2 k_0{}^2 - \lambda^2}, \tag{12}$$

$$G = \eta r(y) g(x), \tag{13}$$

$$r(y) = \begin{cases} e^{-\pi y/2a} + t_1, & y \in [0, d/2], \\ \dfrac{2t_2}{d}(d - y), & y \in [d/2, d], \\ 0, & y \in [d, \infty], \end{cases} \tag{14}$$

where α, η are free parameters of the trial function, 2δ is the width of the central layer, $2d$ is the width of the three-layered waveguide,

$$t_1 = \frac{2}{\pi d}\left[e^{-\pi d/4a}\left(4a + \frac{\pi d}{2}\right) - 4a \right],$$

$$t_2 = \frac{2}{\pi d}[e^{-\pi d/4a}(4a + \pi d) - 4a].$$

The functions $v(y)$ and $r(y)$ are y symmetrical. t_1 and t_2 are chosen in such a way that the corresponding functions satisfy the orthogonality condition

$$\int_{-d}^{d} v(y)dy = 0, \quad \int_{-d}^{d} r(y)dy = 0.$$

The functions $f(x)$ and $g(x)$ will be defined later. Now it is important that in general the values of $f(x)$ and $g(x)$ are complex. In the case of a single narrow window these functions will meet the requirements

$$f(\infty) = f(-\infty) = 0,$$

$$g(\infty) = g(-\infty) = 0. \tag{15}$$

In the case of the periodic system of narrow windows (with period L), these functions will meet Bloch's condition

$$f(x + L) = e^{i\theta L} f(x),$$

$$g(x + L) = e^{i\theta L} g(x). \tag{16}$$

Lemma 1: The trial function $\hat{\Psi}$ defined in (9)–(16) satisfies the following condition:

$$(H\hat{\Psi}, \hat{\Psi}) = \|\hat{\Psi}_x\|^2 + \|\hat{\Psi}_y\|^2. \tag{17}$$

Proof: Here we mark $\hat{\Psi}$ as Ψ for simplification. We can write

$$(H\Psi, \Psi) = \int\int \frac{\partial^2 \Psi}{\partial^2 x} \overline{\Psi}\, \mathrm{d}x\, \mathrm{d}y + \int\int \frac{\partial^2 \Psi}{\partial^2 y} \overline{\Psi}\, \mathrm{d}x\, \mathrm{d}y. \tag{18}$$

Using integration by parts we can write the first term in (18) as

$$\int\int \frac{\partial^2\Psi}{\partial^2 x}\overline{\Psi}\,dx\,dy = \int\int \frac{\partial^2(F+G)}{\partial^2 x}(\overline{F}+\overline{G})dx\,dy$$
$$= \int_{-\infty}^{\infty} \frac{\partial(F+G)}{\partial x}(\overline{F}+\overline{G})\Big|_{X_{\min}}^{X_{\max}} dy + \int_{-\infty}^{\infty}\int_{X_{\min}}^{X_{\max}} \frac{\partial(F+G)}{\partial x}\frac{\partial(\overline{F}+\overline{G})}{\partial x}dx\,dy$$
$$= \int_{-\infty}^{\infty} \frac{\partial(F+G)}{\partial x}(\overline{F}+\overline{G})\Big|_{X_{\min}}^{X_{\max}} dy + \|\Psi_x\|^2, \tag{19}$$

and the second term in (18) as

$$\int\int \frac{\partial^2\Psi}{\partial^2 y}\overline{\Psi}\,dx\,dy = \int\int \frac{\partial^2(F+G)}{\partial^2 y}(\overline{F}+\overline{G})dx\,dy$$
$$= \int_{X_{\min}}^{X_{\max}} \frac{\partial(F+G)}{\partial y}(\overline{F}+\overline{G})\Big|_{-\infty}^{\infty} dx + \int_{X_{\min}}^{X_{\max}}\int_{-\infty}^{\infty} \frac{\partial(F+G)}{\partial y}\frac{\partial(\overline{F}+\overline{G})}{\partial y}dx\,dy$$
$$= \int_{X_{\min}}^{X_{\max}} \frac{\partial(F+G)}{\partial y}(\overline{F}+\overline{G})\Big|_{-\infty}^{\infty} dx + \|\Psi_y\|^2. \tag{20}$$

It follows from the definitions (10)–(14) that

$$v(\infty) = v(-\infty) = 0, \quad r(\infty) = r(-\infty) = 0.$$

Then the first term on the right-hand side of (20) is equal to zero

$$\frac{\partial(F+G)}{\partial y}(\overline{F}+\overline{G})\Big|_{y=-\infty}^{y=\infty} = 0.$$

At last, we need to calculate the first term on the right-hand side of (19). In the case of a single narrow window we have

$$X_{\min} = -\infty, \quad X_{\max} = \infty,$$

then from conditions (15)

$$\frac{\partial(F+G)}{\partial x}(\overline{F}+\overline{G})\Big|_{X_{\min}}^{X_{\max}} = \frac{\partial(F+G)}{\partial x}(\overline{F}+\overline{G})\Big|_{x=-\infty}^{x=\infty} = 0.$$

In the case of the periodic system of narrow windows we have

$$X_{\min} = -L/2, \quad X_{\max} = L/2,$$

then from the conditions (16)

$$\frac{\partial(F+G)}{\partial x}(\overline{F}+\overline{G})\Big|_{X_{\min}}^{X_{\max}} = \frac{\partial(F+G)}{\partial x}(\overline{F}+\overline{G})\Big|_{x=-L/2}^{x=L/2} = 0.$$

Q.E.D.

It's easy to see, that $\hat{\Psi}$ is symmetrical in y direction, so we will take interval $0 \leqslant y \leqslant \infty$.

Lemma 2: The form $M(\Psi)$ for the trial function $\hat{\Psi}$ defined in (9)–(14) can be represented as follows:

$$M(\hat{\Psi}) = \|F_x\|^2 + \|G_x\|^2 + \|G_y\|^2 + \int_0^d \int_{X_{\min}}^{X_{\max}} (\overline{F}_x \overline{G}_x + F_x G_x)\mathrm{d}x\,\mathrm{d}y - \|G\sqrt{n^2k_0^2 - \lambda^2}\|^2$$
$$- \int_{X_{\min}}^{X_{\max}} [\overline{F}_y(x,0)\overline{G}(x,0) + F_y(x,0)G(x,0)]\mathrm{d}x. \tag{21}$$

Proof: We get from (8), by Lemma 1, after some calculations

$$M(\hat{\Psi}) = \|\hat{\Psi}_x\|^2 + \|\hat{\Psi}_y\|^2 - \|\hat{\Psi}\sqrt{n^2k_0^2 - \lambda^2}\|^2 = \|F_x\|^2 + \|G_x\|^2 + \|G_y\|^2 + \int_0^d \int_{X_{\min}}^{X_{\max}} (\overline{F}_y \overline{G}_y + F_y G_y)\mathrm{d}x\,\mathrm{d}y$$
$$+ \int_0^d \int_{X_{\min}}^{X_{\max}} (\overline{F}_x \overline{G}_x + F_x G_x)\mathrm{d}x\,\mathrm{d}y - \left[\|G\sqrt{n^2k_0^2 - \lambda^2}\|^2 + \int_0^d \int_{X_{\min}}^{X_{\max}} (\overline{FG} + FG)(n^2k_0^2 \right.$$
$$\left. - \lambda^2)\mathrm{d}x\,\mathrm{d}y \right]. \tag{22}$$

Using integration by parts, we reduce the first integral in the previous formula to the following expression:

$$\int_0^d \int_{X_{\min}}^{X_{\max}} (\overline{F}_y \overline{G}_y + F_y G_y)\mathrm{d}x\,\mathrm{d}y = \int_0^d \int_{X_{\min}}^{X_{\max}} \overline{F}_y \overline{G}_y\,\mathrm{d}x\,\mathrm{d}y + \int_0^d \int_{X_{\min}}^{X_{\max}} F_y G_y\,\mathrm{d}x\,\mathrm{d}y$$
$$= - \int_{X_{\min}}^{X_{\max}} [\overline{F}_y(x,0)\overline{G}(x,0) + F_y(x,0)G(x,0)]\mathrm{d}x$$
$$- \int_{X_{\min}}^{X_{\max}} \int_0^d (\overline{F}_{yy}\overline{G} + F_{yy}G)\mathrm{d}y\,\mathrm{d}x, \tag{23}$$

where

$$\int_{X_{\min}}^{X_{\max}} [\overline{F}_y(x,d)\overline{G}(x,d) + F_y(x,d)G(x,d)] = 0,$$

because $G(x,d) = \overline{G}(x,d) = 0$. The absolute value of the last term in (23) is equal to the absolute value of the last term in (22)

$$\int_0^d \int_{X_{\min}}^{X_{\max}} [\overline{F}_{yy}\overline{G} + F_{yy}G]\mathrm{d}y\,\mathrm{d}x = -\alpha\eta \int_0^d r(y)v(y)(n^2k_0^2 - \lambda^2)\mathrm{d}y \int_{X_{\min}}^{X_{\max}} [\overline{f}(x)\overline{g}(x) + f(x)g(x)]\mathrm{d}x, \tag{24}$$

$$\int_0^d \int_{X_{\min}}^{X_{\max}} [\overline{FG} + FG](n^2k_0^2 - \lambda^2)\mathrm{d}x\,\mathrm{d}y = \alpha\eta \int_0^d r(y)v(y)(n^2k_0^2 - \lambda^2)\mathrm{d}y \int_{X_{\min}}^{X_{\max}} [\overline{f}(x)\overline{g}(x) + f(x)g(x)]\mathrm{d}x. \tag{25}$$

To obtain (21) it is necessary to substitute (23)–(25) into (22). Q.E.D.

This lemma will help us to estimate the ratio (7) for two different cases of the system geometry (a single narrow window and the periodic system of narrow windows).

III. THE CASE OF SINGLE NARROW WINDOW

We will analyze here a two-dimensional three-layered dielectric waveguide with one narrow window (width $2a$) in the central layer (Fig. 1). In this case for the full definition of $\hat{\Psi}$ in (9) we choose

$$f(x) = \min\{1, e^{-q(|x|-a)}\}, \tag{26}$$

$$g(x) = \begin{cases} \cos(\pi x/2a), & x \in [-a,a], \\ 0, & x \in [-\infty,-a] \cup [a,\infty]. \end{cases} \tag{27}$$

Theorem 1: The ratio (7) is negative for the trial function $\hat{\Psi}$ described in (9)–(14), (26), and (27), and

$$\frac{M(\hat{\Psi})}{\|\hat{\Psi}\|^2} \leqslant -\frac{a^4 2^9 N_3^4}{\pi^6 \mu^4 (1+\epsilon)^2 N_{vv}^2}, \tag{28}$$

where N_3, N_{vv} are positive constants, $\epsilon \sim e^{-\pi d/2a}$.

Proof: For the proof we need to estimate all terms in (21), Lemma 2. At first, we estimate $\|G_y\|^2$, $\|G_x\|^2$, $\|G\|^2$, and $\|G\sqrt{n^2k_0^2-\lambda^2}\|^2$,

$$\|G_x\|^2 = \int_{-a}^{a}\int_{0}^{\infty} G_x^2 \,\mathrm{d}y\,\mathrm{d}x < \tfrac{1}{2}\pi\eta^2(1+\epsilon),$$

$$\|G\|^2 = \eta^2 \int_0^\infty r(y)^2 \,\mathrm{d}y \int_{-a}^{a} g(x)^2 \,\mathrm{d}x, \tag{29}$$

$$\|G\sqrt{n^2k_0^2-\lambda^2}\|^2 = \eta^2 \int_0^\infty r(y)^2 (n(y)^2k_0^2-\lambda^2)\mathrm{d}y \int_{-a}^{a} g(x)^2 \,\mathrm{d}x < \eta^2\nu^2\frac{a^2}{\pi}\left(1+\frac{32a}{3d\pi}\right),$$

where $\epsilon > 0$ and $\epsilon \sim e^{-\pi d/2a}$. Then we estimate $\|F_x\|^2$,

$$\|F_x\|^2 = \int_{-\infty}^{\infty}\int_{0}^{\infty} \overline{F}_x F_x \,\mathrm{d}y\,\mathrm{d}x = \alpha^2 \int_0^\infty v(y)^2 \,\mathrm{d}y \int_{-\infty}^{\infty} \overline{f}_x(x) f_x(x)\mathrm{d}x = \alpha^2 N_{vv} q,$$

where N_{vv} is some non-negative constant. The calculations of the integrals in (21) (Lemma 2) gives us

$$\begin{aligned}\int_{-a}^{a} G(x,0)[\overline{F}_y(x,0) + F_y(x,0)]\mathrm{d}x &= \alpha\eta \int_{-a}^{a} r(0)v(0)g(x)(\overline{f}(x) + f(x))\mathrm{d}x \\ &= \alpha\eta N_3 \int_{-a}^{a} g(x)(\overline{f}(x) + f(x))\mathrm{d}x = \alpha\eta N_3 \frac{8a}{\pi},\end{aligned} \tag{30}$$

$$\int_0^d \int_{-a}^{a} G_x(\overline{F}_x + F_x)\mathrm{d}x\,\mathrm{d}y = \alpha\eta \int_0^\infty r(y)v(y)\mathrm{d}y \int_{-a}^{a} g_x(x)(\overline{f}_x(x) + f_x(x))\mathrm{d}x = 0, \tag{31}$$

due to the equality $f_x(x) = 0$ on the interval $[-a,a]$. Now we can write the estimation of $M(\hat{\Psi})$. After the substitution of (29)–(31) into (21) we get

$$M(\hat{\Psi}) \leqslant \frac{\pi\eta^2}{2}(1+\epsilon) + \alpha^2 N_{vv} q - \alpha\eta \frac{N_3}{\mu}\frac{8a}{\pi}. \tag{32}$$

α, η, and q are free parameters and one can choose their values by an appropriate way. To get the upper boundary of the ratio (7) we minimize (32) by η (η^* is corresponding minimizing value),

$$\eta^* = \frac{\alpha a 2^3 N_3}{\mu\pi^2(1+\epsilon)},$$

$$M(\hat{\Psi}) \leqslant -\frac{\alpha^2 a^2 2^5 N_3^2}{\pi^3\mu^2(1+\epsilon)} + \alpha^2 N_{vv} q. \tag{33}$$

The estimation of $\|\hat{\Psi}\|^2$ is

$$\|\hat{\Psi}\|^2 \leqslant 2\|F\|^2_{a<x<\infty} + 2\|F\|^2_{-a<x<a} + 2\|G\|^2_{-a<x<a} = 2(\|F\|^2_{a<x<\infty} + \|F\|^2_{-a<x<a}) + 2a\eta^2\|r\|^2, \tag{34}$$

where

$$\|F\|^2_{-a<x<a} = \alpha^2 N_{vv}\int_{-a}^{a} \overline{f(x)} f(x)\mathrm{d}x = \alpha^2 N_{vv} 2a,$$

$$\|F\|^2_{a<x<\infty} = \alpha^2 N_{vv}\int_{a}^{\infty} \overline{f(x)} f(x)\mathrm{d}x = \alpha^2 N_{vv}\frac{1}{2q}.$$

The estimation of the ratio (7) follows from (32) and (34)

$$\frac{M(\Psi)}{\|\Psi\|^2} \leqslant -\frac{a^2 2^6 N_3^2}{\pi^3\mu^2(1+\epsilon)N_{vv}} q + 2q^2. \tag{35}$$

Now we need to choose the parameter q. Therefore we minimize the last ratio estimation by q (q^* is the corresponding minimizing value),

$$q^* = \frac{a^2 2^4 N_3^2}{\pi^3\mu^2(1+\epsilon)N_{vv}},$$

$$\frac{M(\Psi)}{\|\Psi\|^2} \leqslant -\frac{a^4 2^9 N_3^4}{\pi^6\mu^4(1+\epsilon)^2 N_{vv}^2}. \tag{36}$$

Q.E.D.

Thus, we have proved that there exists a bound state below the threshold and simultaneously obtained it's estimation.

IV. THE CASE OF THE PERIODIC SET OF NARROW WINDOWS

In this section we estimate the ratio (7) for three-layer dielectric waveguide with the periodic set of narrow windows (of widths $2a$) in the central layer (Fig. 2). The trial function $\hat{\Psi}$ in this case satisfies the Bloch's condition,

$$\hat{\Psi}(x+nL,y) = e^{i\theta nL}\hat{\Psi}(x,y), \tag{37}$$

where θ is the quasimomentum, L is a period, $-\pi/L \leqslant \theta \leqslant \pi/L$. It is sufficient to describe the trial function $\hat{\Psi}$ on the segment $[-L/2, L/2]$ (one period). According to (9)–(14) and (16), functions $f(x)$ and $g(x)$ satisfies the Bloch's condition. Let

$$f(x) = \sum_{n=-\infty}^{\infty} f_i(x,n)e^{-i\theta nL}, \tag{38}$$

where

$$f_i(x,n) = \begin{cases} e^{q(x+a)-qLn}, & x \in [nL - L/2, nL - a], \\ 1, & x \in [nL - a, nL + a], \\ e^{-q(x-a)+qLn}, & x \in [nL + a, nL + L/2]. \end{cases}$$

The function $f(x)$ on the segment $[-L/2, L/2]$ is described in the following manner:

$$f(x)_{[-L/2,-a]} = e^{q(x+a)} + e^{q(x+a)}A + e^{-q(x-a)}B,$$

$$f(x)_{[-L/2,-a]} = 1 + e^{q(x+a)}A + e^{-q(x-a)}B, \tag{39}$$

$$f(x)_{[-L/2,-a]} = e^{-q(x-a)} + e^{q(x+a)}A + e^{-q(x-a)}B,$$

where

$$A = \sum_{n=1}^{\infty} e^{-qnL-i\theta n} = \frac{e^{-qL-i\theta L}}{1 - e^{-qL-i\theta L}}, \tag{40}$$

$$B = \sum_{n=-1}^{-\infty} e^{qnL-i\theta n} = \frac{e^{-qL+i\theta L}}{1 - e^{-qL+i\theta L}}, \tag{41}$$

and

$$\overline{A} = B, \quad \overline{B} = A, \quad A^2 = B^2 = AB. \tag{42}$$

Let

$$g(x) = \sum_{-\infty}^{\infty} \chi_{[nL-a,nL+a]}e^{-i\theta nL} \cos\left(\frac{\pi(x - nL)}{2a}\right), \tag{43}$$

where $\chi_{[nL-a,nL+a]}$ is the characteristic function of the interval $[nL-a, nL+a]$.

Lemma 3: The functions $f(x)$ and $g(x)$, defined in (38) and (43), satisfy the Bloch's condition.

Proof: For the functions $f(x)$ and $g(x)$ we have

$$f(x+L) = \sum_{n=-\infty}^{\infty} f_i(x + (n+1)L)e^{-i\theta nL} = e^{i\theta L}f(x),$$

$$g(x+L) = \sum_{n=-\infty}^{\infty} \chi_{[nL-a,nL+a]}e^{-i\theta nL} \cos\left(\frac{\pi(x - (n-1)L)}{2a}\right) = e^{-i\theta L}g(x).$$

Q.E.D.

Theorem 2: For the trial function $\hat{\Psi}$, defined in (9)–(14), (38), and (43), the ratio (7) is negative, and

$$\frac{M(\hat{\Psi})}{\|\hat{\Psi}\|^2} \leqslant -ac, \tag{44}$$

where c is some non-negative constant.

Proof: For the proof we need to estimate all terms in (21), Lemma 2. Estimations of $\|G_y\|^2$, $\|G_x\|^2$, $\|G\|^2$, and $\|G\sqrt{n^2k_0^2-\lambda^2}\|^2$ will not change in the case of the periodic system of narrow windows, so we can get them from (29), Theorem 1. We need to calculate other terms in (21). At first, we estimate $\|F_x\|^2$,

$$\|F_x\|^2 = \int_{-L/2}^{L/2}\int_0^\infty \overline{F}_x F_x \,\mathrm{d}y\,\mathrm{d}x = \alpha^2 \int_0^\infty v(y)^2\,\mathrm{d}y \int_{-L/2}^{L/2} \overline{f}_x(x) f_x(x)\mathrm{d}x = \alpha^2 N_{vv} q e^{2qa}\Phi_1(A,B), \tag{45}$$

where

$$\Phi_1(A,B) = 2AB[\sinh(qL) - \sinh(2qa) - qL + 2qa] - (A+B)[qL - 2qa + e^{-qL} - e^{-2qa}] - [e^{-qL} - e^{-2qa}] \geqslant 0,$$

and the constant N_{vv} is non-negative. Then we write the estimations of integral terms in (21),

$$\begin{aligned}\int_{-a}^{a} G(x,0)[\overline{F}_y(x,0) + F_y(x,0)]\mathrm{d}x &= \alpha\eta\int_a^a r(0)v(0)g(x)(\overline{f}(x) + f(x))\mathrm{d}x \\ &= \alpha\eta N_3 \int_{-a}^{a} g(x)(\overline{f}(x) + f(x))\mathrm{d}x = \alpha\eta N_3 \\ &\quad \left[\frac{8a}{\pi} + \frac{8e^{qa}(A+B)a\pi\cosh(qa)}{4q^2a^2+\pi^2}\right],\end{aligned} \tag{46}$$

$$\begin{aligned}\int_0^d\int_{-a}^{a} G_x(\overline{F}_x + F_x)\mathrm{d}x\,\mathrm{d}y &= \alpha\eta\int_0^\infty r(y)v(y)\mathrm{d}y\int_{-a}^{a} g_x(x)(\overline{f}_x(x) + f_x(x))dx \\ &= \alpha\eta a N_{vr}\int_{-a}^{a} g_x(x)(\overline{f}_x(x) + f_x(x))\mathrm{d}x \\ &= \alpha\eta a N_{vr}\left[-\frac{8q^2e^{qa}(A+B)\pi a\cosh(qa)}{4q^2a^2+\pi^2}\right],\end{aligned} \tag{47}$$

where constants N_3, N_{vr} are non-negative. Now we can write the estimation of $M(\hat{\Psi})$. After substitution of (29) and (45)–(47) into (21) we get

$$M(\Psi) \leqslant \frac{\pi\eta^2}{4}(1+2\epsilon) + \alpha^2 N_{vv} q e^{2qa}\Phi_1(A,B) - \alpha\eta\left[N_3\frac{8a}{\pi} + \Phi_2(A,B)(N_3 + aN_{vr}q^2)\right], \tag{48}$$

where

$$\Phi_2(A,B) = \frac{8e^{qa}(A+B)a\pi\cosh(qa)}{4q^2a^2+\pi^2}.$$

Now we need to choose the parameter η. Therefore, we minimize the right-hand part of $M(\hat{\Psi})$ by η (η^* is the minimizing value),

$$\eta^* = 2\frac{\alpha(8N_3a + \Phi_2(A,B)\pi[N_3 + aN_{vr}q^2])}{\pi^2(1+2\epsilon)},$$

$$M(\hat{\Psi}) \leqslant \alpha^2\left(-\frac{(8N_3a + \Phi_2(A,B)\pi[N_3 + aN_{vr}q^2])^2}{\pi^3(1+2\epsilon)} + N_{vv}qe^{2qa}\Phi_1(A,B)\right). \tag{49}$$

The estimation of $\|\hat{\Psi}\|^2$ has the form

$$\|\hat{\Psi}\|^2 \leqslant 2\|F\|^2_{a<x<(L/2)} + 2\|F\|^2_{-a<x<a} + 2\|G\|^2_{-a<x<a} = 2(\|F\|^2_{a<x<(L/2)} + \|F\|^2_{-a<x<a}) + 2a\eta^2\|r\|^2, \tag{50}$$

where

$$\|F\|^2_{-a<x<a} = \alpha^2 N_{vv}\int_{-a}^{a}\overline{f(x)}f(x)\mathrm{d}x = \alpha^2 N_{vv}\Phi_3(A,B),$$

$$\Phi_3(A,B) = 2a + 4e^{qa}(A+B)\frac{\sinh(qa)}{q} + 2e^{2qa}AB\left(2a + \frac{\sinh(2qa)}{q}\right), \tag{51}$$

and

$$\|F\|^2_{a<x<L/2} = \alpha^2 N_{vv}\int_{a}^{L/2}\overline{f(x)}f(x)\mathrm{d}x = \alpha^2 N_{vv}\tfrac{1}{2}e^{2qa}\Phi_4(A,B),$$

$$\Phi_4(A,B) = \frac{(-e^{-qL} + e^{-2qa})}{q} + (A+B)\left[L - 2a + \frac{(-e^{-qL} + e^{-2qa})}{q}\right] + 2AB\left[L - 2a + \frac{(\sinh(qL) - \sinh(2qa))}{q}\right]. \tag{52}$$

The theorem must be proved for all values of the quasimomentum θ. It is easy to see that the parameter θ is in the functions $\Phi_i(A,B)$ only. So we need to calculate the expressions $(A+B)$ and (AB),

$$(A+B) = -\frac{\cosh(Lq) - \sinh(Lq) - \cos(L\theta)}{\cosh(Lq) - \cos(L\theta)}, \tag{53}$$

$$(AB) = \frac{\cosh(Lq) - \sinh(Lq)}{2\cosh(Lq) - 2\cos(L\theta)}. \tag{54}$$

Note, that when $q\to 0$, $\theta\to 0$ the denominator tends to zero. Hence, this case should be treated especially. Let q be sufficiently small (e.g., $q\sim a^2$), but not equal to zero. Then we can expand the right-hand sides of formulas (53) and (54) in series (by q)

$$(A+B) = -\left[1 - \frac{Lq + \frac{1}{6}L^3q^3 + \frac{1}{120}L^5q^5 + O(q^7)}{1 + \frac{1}{2}L^2q^2 + \frac{1}{24}L^4q^4 + O(q^6) - \cos(L\theta)}\right],$$

$$(AB) = \frac{1}{2}\frac{1 - Lq + \frac{1}{2}L^2q^2 - \frac{1}{6}L^3q^3 + \frac{1}{24}L^4q^4 - \frac{1}{120}L^5q^5 + O(q^6)}{1 + \frac{1}{2}L^2q^2 + \frac{1}{24}L^4q^4 + O(q^6) - \cos(L\theta)},$$

where $-\pi\leqslant L\theta\leqslant\pi$. Here we split the proof into two parts, when $L\theta\neq 2\pi n$ and when $L\theta\to 2\pi n$. In the first case $\cos(L\theta)\neq 1$, then

$$(A+B) = -\left(1 - \frac{Lq + O(q^3)}{1 - \cos(L\theta) + \frac{1}{2}L^2q^2 + O(q^4)}\right) \sim -C_1(\theta),$$

$$(AB) = \frac{1}{2}\frac{1 - Lq + O(q^2)}{1 - \cos(L\theta) + \frac{1}{2}L^2q^2 + O(q^4)} \sim C_2(\theta),$$

where $0 < C_1(\theta) < 1$, $0 < C_2(\theta)$. Then

$$\Phi_1 = 2(AB)[\sinh(qL) - \sinh(2qa) - qL + 2qa] - (A+B)[qL - 2qa + e^{-qL} - e^{-2qa}] - [e^{-qL} - e^{-2qa}]$$
$$\sim q(L-2a) + O(q^2), \tag{55}$$

$$\Phi_2 = \frac{8e^{qa}(A+B)a\pi\cosh(qa)}{4q^2a^2 + \pi^2} \sim -8\frac{aC_1(\theta)}{\pi}(1+a), \tag{56}$$

$$\Phi_3 = 2a + 4e^{qa}(A+B)\frac{\sinh(qa)}{q} + 2e^{2qa}AB\left(2a + \frac{\sinh(2qa)}{q}\right)$$
$$\sim a(2 - 4C_1(\theta) + 8C_2(\theta)) + 4a^2q(-C_1(\theta) + 4C_2(\theta)) + O(q^2a^3) > 0, \tag{57}$$

$$\Phi_4 = \frac{(-e^{-qL} + e^{-2qa})}{q} + (A+B)\left[L - 2a + \frac{(-e^{-qL} + e^{-2qa})}{q}\right]$$
$$+ 2AB\left[L - 2a + \frac{(\sinh(qL) - \sinh(2qa))}{q}\right]$$
$$\sim (2L - 4a)[-C_1(\theta) + 2C_2(\theta)] + q[-C_1(\theta)(-1/2L^2 + 2a^2) + L - 2a] + O(q^2) > 0. \tag{58}$$

At last, we have from (49), (55), and (56),

$$M(\hat{\Psi}) \leqslant \alpha^2\left(-\frac{a^2 2^6[N_3 - C_1(\theta)(1+a)(N_3 + aN_v r q^2)]^2}{\pi^3(1+2\epsilon)} + N_{vv}q^2e^{2qa}(L-2a)\right). \tag{59}$$

And the denominator $\|\hat{\Psi}\|^2$ is

$$\|\hat{\Psi}\|^2 \leqslant \alpha^2 2N_{vv}[\Phi_3 + 1/2e^{2qa}\Phi_4] = \alpha^2 2N_{vv}C_\psi(\theta) > 0, \tag{60}$$

where

$$C_\psi(\theta) = a[2 - 4C_1(\theta) + 8C_2(\theta)] + 1/2e^{2qa}(2L - 4a)[-C_1(\theta) + 2C_2(\theta)] + O(q) > 0.$$

From (59) and (60) we get the ratio

$$\frac{M(\hat{\Psi})}{\|\Psi\|^2} \leqslant -\frac{a^2 2^6[N_3 - C_1(\theta)(1+a)(N_3 + aN_{vr}q^2)]^2}{\pi^3(1+2\epsilon)N_{vv}2C_\psi(\theta)} + \frac{q^2e^{2qa}(L-2a)}{2C_\psi(\theta)}. \tag{61}$$

Thus for

$$q^2 < \frac{a^2 2^6[N_3 - C_1(\theta)(1+a)(N_3 + aN_{vr}q^2)]^2}{\pi^3(1+2\epsilon)N_{vv}e^{2qa}(L-2a)} \tag{62}$$

and $L\theta \neq 0$ the theorem is proved. In the case $L\theta \to 0$ we expand $\cos(L\theta)$ in series in expressions $(A+B)$ and (AB),

$$(A+B) \sim -\left[1 - \frac{Lq + O(q^3)}{1/2(L^2q^2 + L^2\theta^2) + O(q^6 + \theta^6)}\right], \tag{63}$$

$$(AB) \sim \frac{1}{2}\frac{1}{1/2(L^2q^2 + L^2\theta^2) + O(q^6 + \theta^6)}, \tag{64}$$

If θ is sufficiently small like q or q^2 (or even if $\theta=0$) we can write

$$(A+B) \sim \frac{1}{Lq}C_1, \tag{65}$$

$$(AB) \sim \frac{1}{L^2q^2}C_2, \tag{66}$$

where C_1, C_2 are non-negative. In this case it is difficult to see the dependencies of θ. Here we calculate an estimation of the ratio (7) as a constant for all $L\theta < q$. Let us see the $\Phi_i(A,B)$ calculations

$$\Phi_1 \leqslant 2(L-2a)q + O(q^2),$$

$$\Phi_2 = \frac{8aC_1}{\pi Lq} + O(1),$$

$$\Phi_3 = \frac{8aC_2}{L^2q^2} + \frac{4a}{Lq}\left(\frac{4aC_2}{L} + C_1\right) + O(1),$$

$$\Phi_4 = 4C_2\frac{L-2a}{L^2q^2} + 2C_1\frac{L-2a}{Lq} + O(1),$$

and then the ratio estimation is

$$\frac{M(\hat{\Psi})}{\|\hat{\Psi}\|^2} \leqslant -\frac{2^4aC_1^2(1+\epsilon_1)}{\pi^2(1+2\epsilon)2N_{vv}(8C_2 + O(q))} + \frac{q^4e^{2qa}(L-2a)}{a(8C_2 + O(q))}, \tag{67}$$

where $\epsilon_1 \sim aq^2$. Then for

$$q^4 < \frac{2^3a^2C_1^2(1+\epsilon_1)}{\pi^2(1+2\epsilon)N_{vv}e^{2qa}(L-2a)}$$

the theorem is proved. The dependence of the ratio

$$\frac{M(\hat{\Psi})}{\|\hat{\Psi}\|^2}$$

for the trial function $\hat{\Psi}$ of the quasimomentum θ and the parameter q is shown in Figs. 3 and 4. One can see that there is a specific behavior near the points $2\pi n$. That is why we consider the ratio in neighborhoods of these points separately. The figures show that the ratio is strongly negative for all values of θ. Theorem 2 gives us a more precise result—an estimation for the gap. Summarizing the results for different θ, we obtain the following estimation of the ratio for the trial function:

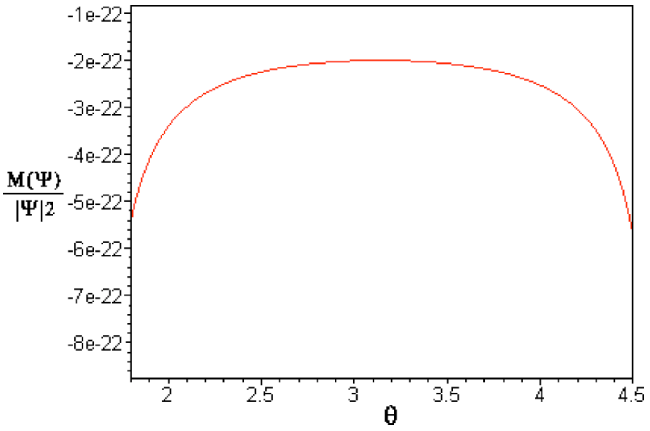

FIG. 3. The dependence of the ratio $M(\hat{\Psi})/\|\hat{\Psi}\|^2$ on the quasimomentum θ for $q=10^{-8}$.

$$\frac{M(\Psi)}{\|\Psi\|^2} \leqslant -ac, \quad c = \frac{2C_1^2(1+\epsilon_1)}{\pi^2(1+2\epsilon)N_{vv}(8C_2+O(q))}. \tag{68}$$

The assumptions which we made are sufficient and not necessary. We assume that the separating layer is strongly narrow, but there is no assumption concerning the very high dielectric contrasts as in the work of Kuchment and co-workers.[2,4]

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APPENDIX

Here we place the formulas, that are not in the main text, but which are useful for the reader's understanding of the proofs.

Calculations of $M(\hat{\Psi})$ in Lemma 2 are as follows:

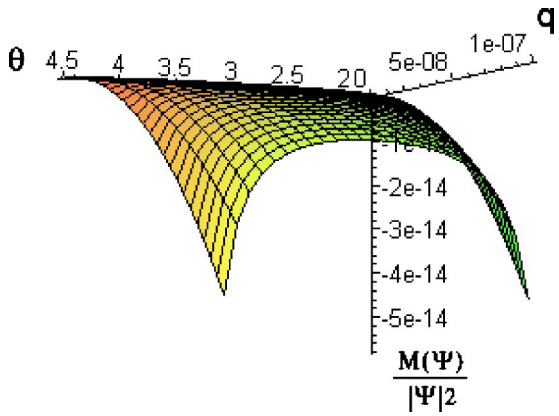

FIG. 4. The dependence of the ratio $M(\hat{\Psi})/\|\hat{\Psi}\|^2$ on the quasimomentum θ and parameter q.

$$M(\hat{\Psi}) = \|\hat{\Psi}_x\|^2 + \|\hat{\Psi}_y\|^2 - \|\hat{\Psi}\sqrt{n^2k_0^2 - \lambda^2}\|^2 = \|F_x\|^2 + \|G_x\|^2 + \int_0^d \int_{-\infty}^{\infty} \overline{F_x}\overline{G_x} + F_xG_x \,\mathrm{d}x\,\mathrm{d}y + \|F_y\|^2$$
$$+ \|G_y\|^2 + \int_0^d \int_{-\infty}^{\infty} \overline{F_y}\overline{G_y} + F_yG_y \,\mathrm{d}x\,\mathrm{d}y - \|F\sqrt{n^2k_0^2 - \lambda^2}\|^2 - \|G\sqrt{n^2k_0^2 - \lambda^2}\|^2$$
$$- \int_0^d \int_{-\infty}^{\infty} (\overline{FG} + FG)\sqrt{n^2k_0^2 - \lambda^2}\mathrm{d}x\,\mathrm{d}y = \|F_x\|^2 + \|G_x\|^2 + \|G_y\|^2 + \int_0^d \int_{-\infty}^{\infty} \overline{F_y}\overline{G_y} + F_yG_y \,\mathrm{d}x\,\mathrm{d}y$$
$$+ \int_0^d \int_{-\infty}^{\infty} \overline{F_x}\overline{G_x} + F_xG_x \,\mathrm{d}x\,\mathrm{d}y - \left[\|G\sqrt{n^2k_0^2 - \lambda^2}\|^2 + \int_0^d \int_{-\infty}^{\infty} (\overline{FG} + FG)(n^2k_0^2 - \lambda^2)\mathrm{d}x\,\mathrm{d}y \right], \tag{A1}$$

where

$$\int_0^d \int_{-\infty}^{\infty} \overline{F_y}\overline{G_y} + F_yG_y \,\mathrm{d}x\,\mathrm{d}y = \int_0^d \int_{-\infty}^{\infty} \overline{F_y}\overline{G_y} \,\mathrm{d}x\,\mathrm{d}y + \int_0^d \int_{-\infty}^{\infty} F_yG_y \,\mathrm{d}x\,\mathrm{d}y$$
$$= \int_{-\infty}^{\infty} \left[F_yG|_0^d - \int_0^d \overline{F_{yy}}\overline{G}\,\mathrm{d}y \right]\mathrm{d}x + \int \left[F_yG|_0^d - \int F_{yy}G\,\mathrm{d}y \right]\mathrm{d}x$$
$$= \int_{-\infty}^{\infty} (\overline{F_y}\overline{G} + F_yG)|_0^d \,\mathrm{d}x - \int_{-\infty}^{\infty} \int_0^d (\overline{F_{yy}}\overline{G} + F_{yy}G)\mathrm{d}y\,\mathrm{d}x$$
$$= -\int_{-\infty}^{\infty} [\overline{F_y}(x,0)\overline{G}(x,0) + F_y(x,0)G(x,0)]\mathrm{d}x$$
$$- \int_{-\infty}^{\infty} \int_0^d (\overline{F_{yy}}\overline{G} + F_{yy}G)\mathrm{d}y\,\mathrm{d}x. \tag{A2}$$

Calculations of $\|G\sqrt{n^2k_0^2-\lambda^2}\|^2$ are as follows:

$$\|G\sqrt{n^2k_0^2 - \lambda^2}\|^2 = \eta^2 \int_0^{\infty} r(y)^2(n(y)^2k_0^2 - \lambda^2)\mathrm{d}y \int_{-a}^{a} g(x)^2 \,\mathrm{d}x < \eta^2\nu^2\frac{a^2}{\pi}\left(1 + \frac{32a}{3d\pi}\right), \tag{A3}$$

where

$$\int_0^{\infty} r(y)^2(n(y)^2k_0^2 - \lambda^2)\mathrm{d}y = \nu^2 \int_0^{\infty} r(y)^2 \,\mathrm{d}y < \nu^2\frac{a}{\pi}\left(1 + \frac{32a}{3d\pi}\right), \tag{A4}$$

and

$$\int_{-a}^{a} g(x)^2 \,\mathrm{d}x = \int_{-a}^{a} \cos\left(\frac{\pi x}{2a}\right)^2 \mathrm{d}x = a. \tag{A5}$$

The integral of $v(y)^2$ is used to calculate the norms $\|F\|^2$ and $\|F_y\|^2$, which are used in Theorem 1 and Theorem 2. In the proofs we mark the value of this integral as N_{vv}. Calculations of the integral are

$$N_{vv} = \int_0^\infty v(y)^2\,\mathrm{d}y = N_3^2\int_0^\delta \sin(\mu y)^2\,\mathrm{d}y + (N_1+M_1)^2\int_\delta^d \cos(\nu y - arg)^2\,\mathrm{d}y + N_2^2\int_d^\infty e^{-2\gamma(y-d)}\,\mathrm{d}y$$
$$= N_3^2\frac{1}{2}\left(\frac{1}{2\mu}\sin(2\mu\delta) + 2\delta\right) + N_2^2\frac{1}{2\gamma} + (N_1+M_1)^2\frac{1}{2}\left(\frac{1}{2\mu}(\sin(2(\mu d - arg)) - \sin(2(\mu\delta - arg))) + (d-\delta)\right), \tag{A6}$$

where $N_{vv} \geqslant 0$. In the case of a single coupling window for the norm $\|f(x)\|^2$ we have

$$\int_{-\infty}^{\infty} \overline{f_x}(x) f_x(x)\mathrm{d}x = \int_{-a}^{a} \overline{f_x}(x) f_x(x)\mathrm{d}x + 2\int_{-\infty}^{-a} \overline{f_x(x)} f_x(x)\mathrm{d}x = q. \tag{A7}$$

And in the case of the periodic set of coupling windows we have

$$\int_{-L/2}^{L/2} \overline{f_x}(x) f_x(x)\mathrm{d}x = \int_{-a}^{a} \overline{f_x}(x) f_x(x)\mathrm{d}x + 2\int_{-L/2}^{-a} \overline{f_x}(x) f_x(x)\mathrm{d}x$$
$$= \int_{-a}^{a} q^2 e^{2qa}(2AB\cosh(2qx) - A^2 - B^2) + 2\int_{-L/2}^{-a} q^2 e^{2qa}(2AB\cosh(2qx) - A^2 - B^2$$
$$- A - B + (A+B+1)e^{2qx})$$
$$= -2qe^{2qa}[-AB\sinh(2qa) + qa(A^2+B^2)] + qe^{2qa}[-2AB(\sinh(2qa) - \sinh(qL))$$
$$+ (2qa - qL)(B^2 + A^2 + A + B)] + qe^{2qa}[(e^{-2qa} - e^{-qL})(A+B+1)]$$
$$= qe^{2qa}[2AB(\sinh(qL) - \sinh(2qa) - qL + 2qa) - (qL - 2qa + e^{-qL} - e^{-2qa})$$
$$\times(A+B)] - qe^{2qa}[e^{-qL} - e^{-2qa}] = qe^{2qa}\Phi_1(A,B), \tag{A8}$$

where $\Phi_1(A,B) \geqslant 0$. The integral of $v(y)r(y)$ is used in both theorems and known as constant N_{vr},

$$\int_0^d v(y)r(y)\mathrm{d}y = \int_0^\delta N_3\sin(\mu y)e^{-\pi y/2a}\,\mathrm{d}y + \int_\delta^{d/2}(N_1\cos(\nu y) + M_1\sin(\nu y))e^{-\pi y/2a}\,\mathrm{d}y$$
$$+ \int_{d/2}^{d}(N_1\cos(\nu y) + M_1\sin(\nu y))2\left(1 - \frac{y}{d}\right)e^{-\pi d/4a}\,\mathrm{d}y$$
$$= \int_0^\delta N_3\sin(\mu y)e^{-\pi y/2a}\,\mathrm{d}y + (N_1+M_1)\int_\delta^{d/2}\cos(\nu y - arg)e^{-\pi y/2a}\,\mathrm{d}y + (N_1+M_1)$$
$$\int_{d/2}^{d}\cos(\nu y - arg)2\left(1 - \frac{y}{d}\right)e^{-\pi d/4a}\,\mathrm{d}y, \tag{A9}$$

where

$$N_3\int_0^\delta \sin(\mu y)e^{-\pi y/2a}\,\mathrm{d}y = N_3\frac{2a}{\pi^2 + 4\mu^2a^2}(2a\mu - e^{-\pi\delta/2a}[\pi\sin(\mu\delta) + 2\mu a\cos(\mu\delta)]), \tag{A10}$$

$$(N_1 + M_1)\int_{\delta}^{d/2} \cos(\nu y - arg)e^{-\pi y/2a}\,dy$$

$$= (N_1 + M_1)\frac{2a}{\pi^2 + 4\nu^2 a^2}(e^{-\pi d/4a}(-\pi\cos(1/2\,\nu d - arg) + 2a\nu\sin(1/2\,\nu d - arg)) - e^{-\pi\delta/2a}(-\pi\cos(\nu\delta - arg) + 2a\nu\sin(\nu\delta - arg)))$$

$$= (N_1 + M_1)\frac{2a}{\pi^2 + 4\nu^2 a^2}\left(e^{-\pi\delta/2a}(\pi\cos(\nu\delta - arg) - 2a\nu\sin(\nu\delta - arg)) + \epsilon_1\right), \tag{A11}$$

$$(N_1 + M_1)\int_{d/2}^{d} \cos(\nu y - arg)2\left(1 - \frac{y}{d}\right)e^{-\pi d/4a}\,dy = (N_1 + M_1)\frac{e^{-\pi d/4a}}{\nu^2 d}(-2\cos(\nu d - arg) - \sin(1/2\,\nu d - arg)\nu d + 2\cos(1/2\,\nu d - arg)) = (N_1 + M_1)\epsilon_1, \tag{A12}$$

where $\epsilon_1 \sim e^{-\pi d/4a}$. So,

$$\int_0^d v(y)r(y)dy = aN_{vr}. \tag{A13}$$

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Weak Hopf algebras corresponding to Cartan matrices

Shilin Yang[a)]
College of Applied Sciences, Beijing University of Technology, Beijing 100022, People's Republic of China

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We replace the group of grouplike elements of the quantized enveloping algebra $U_q(\mathfrak{g})$ of a finite dimensional semisimple Lie algebra $\mathfrak{g}$ by some regular monoid and get the weak Hopf algebra $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$. It is a subclass of weak Hopf algebras but not Hopf algebras. Then we devote to constructing a basis of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ and determine the group of weak Hopf algebra automorphisms of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ when q is not a root of unity. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1933063]

I. INTRODUCTION

Recently, many mathematicians are interested in generalizations of Hopf algebras, of which importance has been recognized in both mathematics and physics. One way is to introduce the notion of a weak coproduct, such that $\Delta(1) \neq 1 \otimes 1$, which was motivated by the study of symmetries in low dimensional quantum field theory. This resulted in the definition of weak Hopf algebras, introduced by Böhm, Nill, and Szlachányi (see, for example, Ref. 3). Since they are not bialgebras, but almost bialgebras, there were also axioms required to define a weak antipode, differing slightly from the usual notion of a Hopf algebra. The face algebras[7] and generalized Kac algebras[19] are examples of this class of weak Hopf algebras.

It is possible to define a weak antipode on a given bialgebra. This was introduced by Li in Ref. 11. By definition, a bialgebra $\mathcal{H}=(H,\mu,\eta,\Delta,\varepsilon)$ over a field k together with the identity map id in $\hom_k(H,H)$ is called a *weak Hopf algebra* if there exists $T \in \hom_k(H,H)$ such that $\mathrm{id}*T*\mathrm{id}=\mathrm{id}$ and $T*\mathrm{id}*T=T$ where $*$ is the convolution product. The map T is called a weak antipode. It is noted that the notion of Hopf algebras, and left or right Hopf algebras are included in this class of weak Hopf algebras (see Refs. 17, 16, and 6). Another typical example is the weak quantum algebras $\mathfrak{w}\mathfrak{sl}_q(2)$ and $v\mathfrak{sl}_q(2)$ constructed in Ref. 12. It is the generalization by replacing the set of grouplike elements of $U_q(\mathfrak{sl}_2)$ by the set of some regular monoid, where $U_q(\mathfrak{sl}_2)$ is the quantized enveloping algebra corresponding to three-dimensional semisimple Lie algebra. The basis and some properties of $\mathfrak{w}\mathfrak{sl}_q(2)$ [respectively, $v\mathfrak{sl}_q(2)$] were studied in Ref. 12. Recently, Aizawa and Isaac[1] gave a description of weak Hopf algebra $\mathfrak{w}\mathfrak{sl}_q^d(n)$ in general, which is corresponding to the known Hopf algebra $U_q(\mathfrak{sl}_n)$.

Our aim is to give more nontrivial examples for weak Hopf algebras in the sense of Li. Following the idea,[1,12] we would like to extend this construction to the more general one $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ corresponding to arbitrary finite dimensional semisimple Lie algebra $\mathfrak{g}$.

Thanks to the definition of quantum group $U_q(\mathfrak{g})$ defined by Refs. 13 and 9, we can also replace the group $G(U_q(\mathfrak{g}))$ of grouplike elements by some regular monoid and get the weak Hopf algebra $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$, which is resulted from quantum group $U_q(\mathfrak{g})$.[12,9,13] This successful construction provides us with a subclass of weak Hopf algebras but not Hopf algebras. As does the classic quantum group $U_q(\mathfrak{g})$, we will determine the basis and the group of weak Hopf algebra automorphisms of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$.

To determine the basis of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$, we first show that $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ can be written as a direct sum of its two ideals and one of them is just isomorphic to the classic quantum group $U_q(\mathfrak{g})$. Then we apply

a)Electronic mail: slyang@bjut.edu.cn

the PBW theorem for $U_q(\mathfrak{g})$ to describe a basis of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$. If q is not a root of unity, the group of Hopf algebra automorphisms of $U_q(\mathfrak{g})$ was determined in Ref. 4. The case when q is a root of unity, was considered in recent work.[15] In the present paper, we will determine the group of weak Hopf algebra automorphisms of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ under the condition that q is not a root of unity. The method is to apply the result of Ref. 4, Corollary 4.3, and some technical lemmas.

The paper is organized as follows.

In Sec. II, we give some notations and the definition of weak Hopf algebra $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$. The ideal to construct the algebra $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ and some basic properties are described. In Sec. III, we give the comultiplication of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ in order that it is a weak Hopf algebra but not a Hopf alegbra. The proof is somewhat basic and direct. In Sec. IV, we describe the basis of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ by the technique of Lusztig's constructing PBW basis of $U_q(\mathfrak{g})$. In the final section, we study and determine the group of Hopf automorphisms of $U_q(\mathfrak{g})$.

II. WEAK QUANTUM ALGEBRAS $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$

In this paper, we always assume that k is a field of characteristic 0. Let $\mathfrak{g}$ be a finite dimensional semisimple Lie algebra. For the simplicity, we can assume that $\mathfrak{g}$ is also simple. Then there is a finite positive symmetrizable Cartan matrix $\mathcal{C}=(a_{ij})_{n\times n}$ corresponding to it (see Ref. 8).

Now we let R be the root system of $\mathfrak{g}$ and we fix a basis $I=\{\alpha_1,\ldots,\alpha_n\}$ of R. Let W be the Weyl group of R. It is well known that there is a unique W-invariant scalar product $(,)$ on the vector space generated by R over the reals such that $(\alpha,\alpha)=2$ for all short roots α in R. Set for each $\alpha_i\in I$, $1\leqslant i\leqslant n$

$$d_i=\frac{(\alpha_i,\alpha_i)}{2}.$$

It is noted that $(\alpha_i,\alpha_j)=d_ia_{ij}=d_ja_{ji}$.

Let $q\in k$ and $q_i=q^{d_i}$, $1\leqslant i\leqslant n$. It is assumed that $q_i\neq\pm1, 0$ for all i. For an indeterminate x and an integer m, let

$$[m]_x=\frac{x^m-x^{-m}}{x-x^{-1}},\quad [m]!_x=[m]_x\cdots[1]_x,\quad [0]_x!=1,$$

and

$$\begin{bmatrix} m \\ s \end{bmatrix}_x=\frac{[m]!_x}{[s]!_x[m-s]!_x}.$$

One can review the definition of the quantized enveloping algebra $U_q=U_q(\mathfrak{g})$ by referring to Refs. 10, 9, and 13. For the completeness, we describe it here as follows. The algebra $U_q(\mathfrak{g})$ generated by $4n$ generators $e_i,f_i,k_i,k_i^{-1}(1\leqslant i\leqslant n)$ with the relations

$$k_ik_j=k_jk_i,\quad k_ik_i^{-1}=k_i^{-1}k_i=1, \tag{2.1}$$

$$k_ie_jk_i^{-1}=q_i^{a_{ij}}e_j,\quad k_if_jk_i^{-1}=q_i^{-a_{ij}}f_j, \tag{2.2}$$

$$e_if_j-f_je_i=\delta_{ij}\frac{k_i-k_i^{-1}}{q_i-q_i^{-1}}, \tag{2.3}$$

$$\sum_{s=0}^{1-a_{ij}}(-1)^s\begin{bmatrix} 1-a_{ij} \\ s \end{bmatrix}_{q_i}e_i^{1-a_{ij}-s}e_je_i^s=0,\quad \text{if } i\neq j, \tag{2.4}$$

$$\sum_{s=0}^{1-a_{ij}} (-1)^s \begin{bmatrix} 1-a_{ij} \\ s \end{bmatrix}_{q_i} f_i^{1-a_{ij}-s} f_j f_i^s = 0, \quad \text{if } i \neq j. \tag{2.5}$$

To generalize the invertibility condition (2.1), one way is to weaken the invertibility to regularity, in which instead of $\{k_i, k_i^{-1}\}$ by a pair $\{K_i, \overline{K_i}\}$ for all $1 \leqslant i \leqslant n$ subjecting to some relations. For example, we can introduce a projector J such that

$$J = K_i \overline{K_i} = \overline{K_i} K_i,$$

$$JK_i = K_i, \quad \overline{K_i} J = \overline{K_i},$$

$$J\overline{K_i} = \overline{K_i}, \quad K_i J = K_i$$

for $1 \leqslant i \leqslant n$. To generalize other relations of the definition, we need some terminologies for simplicity. For example, if E_i satisfies

$$K_j E_i = q_i^{a_{ij}} E_i K_j, \quad E_i \overline{K_j} = q_i^{a_{ij}} \overline{K_j} E_i, \quad \forall\, j, \tag{2.6}$$

we say E_i is type 1. Moreover, if E_i satisfies

$$K_j E_i \overline{K_j} = q_i^{a_{ij}} E_i, \quad \forall\, j, \tag{2.7}$$

we say E_i is type 2. The same convention holds for F_i by replacing E_i with F_i and a_{ij} with $-a_{ij}$ in the above relations.

We borrow some notations from Ref. 1, $2n$ simple generators E_i and F_i are listed by starting with the E_i followed by the F_i, where a 1 is to indicate the use of a type 1 generator and a 0 is to indicate the use of a type 2 generator. Then we write down a list of 0's and 1's in the order corresponding to the generators determined by their type. This gives a sequence d containing 0 and 1 in a binary representation of length $2n$. It is noted that d contains all the information on the relations with the generators E_i and F_j, all $K_j/\overline{K_j}$, and J. We write d in terms of its binary expansion,

$$\mathsf{d} = (\kappa_1, \ldots, \kappa_n | \overline{\kappa_1}, \ldots, \overline{\kappa_n})$$

where the bar separates the values representing the E_i and F_i, and where the κ_i and $\overline{\kappa_i}$ have values of either 0 or 1. Accordingly, we can say E_i and F_i, $\alpha_i \in I$ are type d in an obvious sense.

Now we can write down this generalization explicitly as follows.

Definition 2.1: The algebra $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$ *is generated by the* $4n+1$ *variables* $E_i, F_i, K_i, \overline{K_i} (1 \leqslant i \leqslant n)$ *and* J *with the following relations: for all* $1 \leqslant i,j \leqslant n$,

$$J = K_i \overline{K_i}, \tag{2.8}$$

$$K_i \overline{K_j} = \overline{K_j} K_i, \quad K_i K_j = K_j K_i, \quad \overline{K_i}\,\overline{K_j} = \overline{K_j}\,\overline{K_i}, \tag{2.9}$$

$$JK_i = K_i, \quad J\overline{K_i} = \overline{K_i}, \tag{2.10}$$

$$E_i, \quad F_i \text{ are type } \mathsf{d}, \tag{2.11}$$

$$E_i F_j - F_j E_i = \delta_{ij} \frac{K_i - \overline{K_i}}{q_i - q_i^{-1}}, \tag{2.12}$$

$$\sum_{s=0}^{1-a_{ij}} (-1)^s \begin{bmatrix} 1-a_{ij} \\ s \end{bmatrix}_{q_i} E_i^{1-a_{ij}-s} E_j E_i^s = 0, \quad \text{if } i \neq j, \tag{2.13}$$

$$\sum_{s=0}^{1-a_{ij}} (-1)^s \begin{bmatrix} 1-a_{ij} \\ s \end{bmatrix}_{q_i} F_i^{1-a_{ij}-s} F_j F_i^s = 0, \quad \text{if } i \neq j. \tag{2.14}$$

The algebra $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$ *is said to be a* d*-type* weak quantum algebra *associated to Lie algebra* $\mathfrak{g}$.

It is easy to see that there are 2^{2n} possible weak quantum algebras $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$ corresponding to the sequence d in total.

It is easy to see that (2.9) and (2.10) generalize the relation (2.1), and the relations (2.11) and (2.12) generalize the corresponding relations (2.2) and (2.3). The notations P_i $(1 \leqslant i \leqslant n)$ are defined by

$$P_i^k = \begin{cases} K_i^k, & k > 0, \\ J, & k = 0, \\ \overline{K}_i^{-k}, & k < 0. \end{cases}$$

It is easy to see that P_i^k satisfy the regularity conditions

$$P_i^k P_i^{-k} P_i^k = P_t^k \tag{2.15}$$

for all $k \in \mathbb{Z}$.

There are some properties for $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$ which are used later.

Lemma 2.2: The idempotent J *is in the center of* $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$.

Proof: Indeed, for K_j and $\overline{K}_j$, it follows from (2.9) and (2.10). For instance,

$$K_j J = K_j K_j \overline{K}_j = K_j \overline{K}_j K_j = J K_j.$$

For E_j, if it is type 1, then we have

$$J E_j = K_i \overline{K}_i E_j = q_i^{-a_{ij}} K_i E_j \overline{K}_i = E_j J$$

by (2.6) if E_i is type 2,

$$J E_i = K_i \overline{K}_i E_i = q_i^{-2} K_i \overline{K}_i K_i E_i \overline{K}_i = q_i^{-2} K_i E_i \overline{K}_i = q_i^{-2} K_i E_i \overline{K}_i K_i \overline{K}_i = E_i J$$

by (2.7). Hence, $JE_i = E_i J$ for all $i = 1, 2, \ldots, n$. The same argument for F_i by (2.11). □

If E_i is type 2, hence $K_j E_i \overline{K}_j = q_i^{a_{ij}} E_i$ for all $1 \leqslant j \leqslant n$, then

$$K_j E_i = K_j J E_i = K_j E_i J = K_j E_i \overline{K}_j K_j = q_i^{a_{ij}} E_i K_j$$

and $E_i \overline{K}_j = q_i^{a_{ij}} \overline{K}_j E_i$. Similarly, if F_i is type 2, we have

$$K_j F_i = q_i^{-a_{ij}} F_i K_j, \quad F_i \overline{K}_j = q_i^{-a_{ij}} \overline{K}_j F_i.$$

Now, it is straightforward to check by induction that E_i (respectively, F_i), $1 \leqslant i \leqslant n$, is type 1 or type 2, the following relations hold in $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$:

$$E_i^m K_j^n = q_i^{-mna_{ij}} K_i^n E_i^m, \quad F_i^m K_j^n = q_i^{mna_{ij}} K_j^n F_i^m,$$

$$E_i^m \overline{K}_j^n = q_i^{mna_{ij}} \overline{K}_j^n E_i^m, \quad F_i^m \overline{K}_j^n = q_i^{-mna_{ij}} \overline{K}_j^n F_i^m. \tag{2.16}$$

In particular, we have

$$E_i^m K_i^n = q_i^{-2mn} K_i^n E_i^m, \quad F_i^m K_i^n = q_i^{2mn} K_i^n F_i^m,$$
$$E_i^m \overline{K_i^n} = q_i^{2mn} \overline{K_i^n} E_i^m, \quad F_i^m \overline{K_i^n} = q_i^{-2mn} \overline{K_i^n} F_i^m. \tag{2.17}$$

III. THE WEAK HOPF ALGEBRA STRUCTURE OF $\mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g})$

To make the d-type weak quantum algebra $\mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g})$ be a weak Hopf algebra, we define three maps,

$$\Delta: \mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g}) \to \mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g}) \otimes \mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g}),$$

$$\varepsilon: \mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g}) \to k,$$

$$T: \mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g}) \to \mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g}),$$

as follows:

$$\Delta(K_i) = K_i \otimes K_i, \tag{3.1}$$

$$\Delta(\overline{K_i}) = \overline{K_i} \otimes \overline{K_i}, \tag{3.2}$$

$$\Delta(J) = J \otimes J, \tag{3.3}$$

$$\Delta(E_i) = \begin{cases} 1 \otimes E_i + E_i \otimes K_i, & E_i \text{ is type 1}, \\ J \otimes E_i + E_i \otimes K_i, & E_i \text{ is type 2}, \end{cases} \tag{3.4}$$

$$\Delta(F_i) = \begin{cases} F_i \otimes 1 + \overline{K_i} \otimes F_i, & F_i \text{ is type 1}, \\ F_i \otimes J + \overline{K_i} \otimes F_i, & F_i \text{ is type 2}, \end{cases} \tag{3.5}$$

$$\varepsilon(E_i) = \varepsilon(F_i) = 0, \quad \varepsilon(K_i) = \varepsilon(\overline{K_i}) = 1, \quad \varepsilon(J) = 1,$$

while the map T has the form

$$T(1) = 1, \tag{3.6}$$

$$T(E_i) = -E_i \overline{K_i}, \tag{3.7}$$

$$T_i(F_i) = -K_i F_i, \tag{3.8}$$

$$T(K_i) = \overline{K_i}, \tag{3.9}$$

$$T(\overline{K_i}) = K_i, T(J) = J. \tag{3.10}$$

Then we extend them to the whole $\mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g})$.

In Ref. 1, Sec IV, the authors investigated the algebra $\mathfrak{ws}\mathfrak{l}_q^{\mathrm{d}}(n)$ and claimed that $\mathfrak{ws}\mathfrak{l}_q^{\mathrm{d}}(n)$ is a weak Hopf algebra, of which no proof was given. In general, we yield the following.

Theorem 3.1: (Ref. 1, Sec. IV) $\mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g})$ *is a noncommutative and noncocommutative weak Hopf algebra with the weak antipode T, but not a Hopf algebra.*

In Ref. 1, the authors gave a classification in some sense of weak Hopf algebras corresponding to $U_q(\mathfrak{sl}_n)$. Similarly, we can follow the idea[1] to describe the isomorphism classes of weak Hopf algebras $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$. As a consequence, we have a lot of nontrivial examples of weak Hopf algebras for various sequences d.

The theorem follows from Lemma 3.2 and Lemma 3.3 below.

Lemma 3.2: $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$ *is a bialgebra with comultiplication* Δ *and counit* ε.

Proof: It can be shown by direct calculation that the following relations hold:

$$\Delta(K_i)\Delta(\overline{K_j}) = \Delta(\overline{K_j})\Delta(K_i),$$

$$\Delta(J) = \Delta(K_i)\Delta(\overline{K_i}),$$

$$\Delta(J)\Delta(K_i) = \Delta(K_i),$$

$$\Delta(J)\Delta(\overline{K_i}) = \Delta(\overline{K_i}),$$

$$\varepsilon(K_i)\varepsilon(\overline{K_j}) = \varepsilon(\overline{K_i})\varepsilon(K_j),$$

$$\varepsilon(J)\varepsilon(K_i) = \varepsilon(K_i),$$

$$\varepsilon(J)\varepsilon(\overline{K_i}) = \varepsilon(\overline{K_i}),$$

$$\varepsilon(\overline{K_i})\varepsilon(E_i) = q^{-2}\varepsilon(E_i)\varepsilon(\overline{K_i}),$$

$$\varepsilon(\overline{K_i})\varepsilon(F_i) = q^{2}\varepsilon(F_i)\varepsilon(\overline{K_i}),$$

$$\varepsilon(E_i)\varepsilon(F_j) - \varepsilon(F_j)\varepsilon(E_i) = \delta_{ij}\frac{\varepsilon(K_i) - \varepsilon(\overline{K_i})}{q_i - q_i^{-1}}.$$

If E_i is type 1, then

$$\Delta(K_j)\Delta(E_i) = (K_j \otimes K_j)(1 \otimes E_i + E_i \otimes K_i) = K_j \otimes K_jE_i + K_jE_i \otimes K_jK_i = q_i^{a_{ij}}K_j \otimes E_iK_j + q_i^{a_{ij}}E_iK_j \otimes K_iK_j = q_i^{a_{ij}}\Delta(E_i)\Delta(K_j);$$

if E_i is type 2, then

$$\Delta(K_j)\Delta(E_i)\Delta(\overline{K_j}) = (K_j \otimes K_j)(J \otimes E_i + E_i \otimes K_i)(\overline{K_j} \otimes \overline{K_j}) = K_j\overline{K_j} \otimes K_jE_i\overline{K_j} + K_jE_i\overline{K_j} \otimes K_jK_i\overline{K_j} = q_i^{a_{ij}}J \otimes E_i + q_i^{a_{ij}}E_i \otimes K_i = q_i^{a_{ij}}\Delta(E_i).$$

Therefore, Δ keeps the relation (2.11) for E_i's. The similar argument can show that Δ also keeps the relation (2.11) for F_i's.

Now we examine the identity

$$\Delta(E_i)\Delta(F_j) - \Delta(F_j)\Delta(E_i) = \delta_{ij}\frac{\Delta(K_i) - \Delta(\overline{K_i})}{q_i - q_i^{-1}}.$$

The following cases should be considered:

(1) E_i is type 1 and F_i is type 1,

(2) E_i is type 1 and F_i is type 2,
(3) E_i is type 2 and F_i is type 1,
(4) E_i is type 2 and F_i is type 2.

For the case (2), it is noted that

$$E_i\overline{K_j} = q_i^{a_{ij}}\overline{K_j}E_i = q^{d_i a_{ij}}\overline{K_j}E_i = q^{(\alpha_i,\alpha_j)}\overline{K_j}E_i$$

and

$$K_iF_j = K_iF_jJ = K_iF_j\overline{K_j}K_i = q_j^{-a_{ji}}F_jK_i = q^{-d_ja_{ji}}F_jK_i = q^{-(\alpha_i,\alpha_j)}F_jK_i.$$

The later identity holds since $K_iJ=K_i$ and J is central in $\mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g})$. Then, it is easy to see that

$$\begin{aligned}\Delta(E_i)\Delta(F_j) - \Delta(F_j)\Delta(E_i) &= \overline{K_j}\otimes(E_iF_j - F_jE_i) + (E_iF_j - F_jE_i)\otimes K_i \\ &= \delta_{ij}\overline{K_j}\otimes\frac{K_i - \overline{K_i}}{q_i - q_i^{-1}} + \delta_{ij}\frac{K_i - \overline{K_i}}{q_i - q_i^{-1}}\otimes K_i \\ &= \delta_{ij}\frac{K_i\otimes K_i - \overline{K_i}\otimes\overline{K_i}}{q_i - q_i^{-1}} = \delta_{ij}\frac{\Delta(K_i) - \Delta(\overline{K_i})}{q_i - q_i^{-1}}.\end{aligned}$$

We have shown that Δ keeps the relation (2.12) for the case (2). For the other cases the proof is similar. To see the map Δ keeps the quantum Serre relations (2.13) and (2.14), we should consider several cases according to the type of $\{E_i,E_j\}$ or $\{F_i,F_j\}$ $(i\neq j)$. In fact, for each case, the argument is more or less the same as the case of $U_q(\mathfrak{g})$ (see Ref. 9, pp. 67 and 68).

Therefore, Δ and ε can be extended to algebra morphisms from $\mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g})$ to $\mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g})\otimes\mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g})$ and from $\mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g})$ to k, respectively.

By the above relations it can be shown that

$$(\Delta\otimes\mathrm{id})\Delta(X) = (\mathrm{id}\otimes\Delta)\Delta(X),$$

$$(\varepsilon\otimes\mathrm{id})\Delta(X) = (\mathrm{id}\otimes\varepsilon)\Delta(X) = X$$

for any $X=E_i,F_i,K_i$ or $\overline{K_i}$. Let μ and η be the product and the unit of $\mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g})$, respectively, then $(\mathfrak{w}_q^{\mathrm{d}}(\mathfrak{g}),\mu,\eta,\Delta,\varepsilon)$ becomes a bialgebra. □

It is easy to see that

$$T(\overline{K_i})T(K_j) = T(K_j)T(\overline{K_i}),$$

$$T(J)T(K_i) = T(K_i),$$

$$T(J)T(\overline{K_i}) = T(\overline{K_i}),$$

$$T(F_j)T(E_i) - T(E_i)T(F_j) = \delta_{ij}\frac{T(K_i) - T(\overline{K_i})}{q_i - q_i^{-1}},$$

and E_i is either type 1 or type 2, the map T keeps the antirelation of (2.11). The argument for F_i is similar. Moreover, T also keeps the antirelation for quantum Serre relations. For example, for $1\leqslant i,j\leqslant n$ with $i\neq j$, let $r=1-a_{ij}$, we have

$$\sum_{s=0}^{r}(-1)^s\begin{bmatrix} r \\ s \end{bmatrix}_{q_i} T(E_i)^s T(E_j)T(E_i)^{r-s} = \sum_{s=0}^{r}(-1)^s\begin{bmatrix} r \\ s \end{bmatrix}_{q_i} (-1)^{r+1}(E_i\overline{K_i})^s(E_j\overline{K_j})(E_i\overline{K_i})^{r-s}$$

$$= -q_j^2 q_i^{r^2+r+ra_{ij}}\overline{K_i^r}\,\overline{K_j}\sum_{s=0}^{r}(-1)^{r-s}\begin{bmatrix} r \\ s \end{bmatrix}_{q_i} E_i^s E_j E_i^{r-s} = 0.$$

Here we use the formulas (2.16) and (2.17). The argument for F_i is similar. Therefore, T can be extended to an antialgebra morphism from $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ to $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$, respectively.

Recall that the convolution product in the bialgebra $(\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g}),\mu,\eta,\Delta,\varepsilon)$ is defined in the similar way to the standard one (see, e.g., Ref. 10) as

$$(f * g)(X) = \mu(f\otimes g)\Delta(X) \tag{3.11}$$

for all $f,g\in \mathrm{Hom}(\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g}),\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g}))$ and $X\in\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$. It is noted that if E_i is type 2, then

$$JE_i = K_i\overline{K_i}E_i = q_i^{-2}K_i\overline{K_i}K_iE_i\overline{K_i} = q_i^{-2}K_iE_i\overline{K_i} = E_i.$$

The same argument shows that $F_iJ=F_iJ=F_i$ if F_i is type 2. Let id denote identity map in $\hom_k(\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g}),\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g}))$.

Lemma 3.3: Let X be E_i,F_i,K_i, or $\overline{K_i}$, then

$$(\mathrm{id} * T * \mathrm{id})(X) = \mathrm{id}(X),$$

$$(T * \mathrm{id} * T)(X) = T(X).$$

Proof: It is easy for $X=K_i,\overline{K_i}$. We consider $X=E_i$, as an example. We set

$$\Delta_2 = (\mathrm{id}\otimes\Delta)\circ\Delta.$$

If E_i is type 1, then

$$\Delta_2(E_i) = 1\otimes 1\otimes E_i + 1\otimes E_i\otimes K_i + E_i\otimes K_i\otimes K_i.$$

It follows that

$$(\mathrm{id} * T * \mathrm{id})(E_i) = T(1)E_i + T(E_i)K_i + E_iT(K_i)K_i = E_i - E_i\overline{K_i}K_i + E_i\overline{K_i}K_i = \mathrm{id}(E_i),$$

and

$$(T * \mathrm{id} * T)(E_i) = T(1)T(E_i) + T(1)E_iT(K_i) + T(E_i)K_iT(K_i)$$
$$= -E_i\overline{K_i} + E_i\overline{K_i} - E_i\overline{K_i}K_i\overline{K_i} = -E_i\overline{K_i} = T(E_i).$$

If E_i is type 2, then

$$\Delta_2(E_i) = J\otimes J\otimes E_i + J\otimes E_i\otimes K_i + E_i\otimes K_i\otimes K_i.$$

It is also deduced that

$$(\mathrm{id} * T * \mathrm{id})(E_i) = J\ T(J)E_i + JT(E_i)K_i + E_iT(K_i)K_i = JE_i - E_i\overline{K_i}K_i + E_i\overline{K_i}K_i = JE_i = \mathrm{id}(E_i)$$

since $JE_i=E_i$, and

$$(T * \mathrm{id} * T)(E_i) = T(J)JT(E_i) + T(J)E_iT(K_i) + T(E_i)K_iT(K_i)$$
$$= -E_i\overline{K_i} + E_i\overline{K_i} - E_i\overline{K_i}K_i\overline{K_i} = -E_i\overline{K_i} = T(E_i).$$

As for F_i, the argument is similar. The proof of the lemma is finished. □

In order to conclude that the antipode axioms hold on arbitrary elements, the following two facts are to be used:

(a) the coproducts of the generators are bilinear expressions of generators;
(b) one of $(\mathrm{id}*T)(X)$ and $T*\mathrm{id}(X)$ is a central element of $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$ for X being the generators $K_i, \overline{K_i}, E_i, F_i$.

The fact (a) is obvious. To see (b), we note the fact that $(\mathrm{id}*T)(X)=\varepsilon(X)J$ for $X=K_i, \overline{K_i}, E_i$ $(1\leqslant i\leqslant n)$ and F_i of type 2. Hence $(\mathrm{id}*T)(X)$ is in the center of $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$. However, if $X=F_i$ is type 1, the $(\mathrm{id}*T)(X)=(1-J)F_i$ may not be a central element, but $(T*\mathrm{id})(F_i)=\varepsilon(F_i)J$ is in the center. Similarly, $(T*\mathrm{id})(X)$ for $X=K_i, \overline{K_i}, F_i$ $(1\leqslant i\leqslant n)$ and E_i is of type 2, in the center of $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$. However, if $X=E_i$ is type 1, the $(T*\mathrm{id})(X)=(1-J)E_i$ may not be a central element, but $(\mathrm{id}*T)\times(E_i)$ is in the center of $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$. This means that (b) holds.

It is noted that $E_i(1-J)F_j=F_j(1-J)E_i$ for all $i,j\in\{1,2,\ldots,n\}$ by the relation (2.12). Therefore, if E_i (respectively, F_i) is type 1, $(T*\mathrm{id})(E_i)$ [respectively, $(\mathrm{id}*T)(F_i)$] commutates with all F_j (respectively, all E_j), and $K_j, \overline{K_j}$ $(1\leqslant j\leqslant n)$.

We should show the claim that if

$$(\mathrm{id}*T*\mathrm{id})(x)=x, \quad (T*\mathrm{id}*T)(x)=T(x),$$

$$(\mathrm{id}*T*\mathrm{id})(y)=y, \quad (T*\mathrm{id}*T)(y)=T(y),$$

for all x and y being generators $E_i, F_i, K_i, \overline{K_i}$, then

$$(\mathrm{id}*T*\mathrm{id})(xy)=xy, \quad (T*\mathrm{id}*T)(xy)=T(xy).$$

However, it is considerably direct by the above facts. Now, that the antipode axioms hold on arbitrary elements is obvious by induction.

If we assume that with the operations $\mu,\eta,\Delta,\varepsilon$ the algebra $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$ would possess an antipode S so as to become a Hopf algebra, then S should satisfy $(S*\mathrm{id})(J)=\eta\varepsilon(J)$, and it would follow that $S(J)J=1$ and J is invertible. It is impossible since $J(1-J)=0$. This implies that $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$ is not a Hopf algebra with the above operators. The proof of Theorem 3.1 is finished. □

It should be noted that if $\mathfrak{g}=\mathfrak{sl}_n$, the algebra $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$ is just the mixtures $\mathfrak{wsl}_q^d(n)$ in Ref. 1. In particular, if $\mathfrak{g}=\mathfrak{sl}_2$, $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$ where $\mathsf{d}=(1|1)$ [respectively, $\mathsf{d}=(0|0)$] coincides with $\mathfrak{wsl}_q(2)$ [respectively, $v\mathfrak{sl}_q(2)$] given in Ref. 12.

IV. THE BASIS OF $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$

One can find the relationship between $U_q(\mathfrak{g})$ and the quantum algebra $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$ as follows.

Proposition 4.1: $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})/\langle J-1\rangle\cong U_q(\mathfrak{g})$.

Proof: It is obvious by cancelling K_i. □

In fact, we can give a more explicit relationship between $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$ and $U_q(\mathfrak{g})$. For this purpose, we let $w_q=\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})J$ and $\overline{w_q}=\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})(1-J)$. We have the following decomposition.

Proposition 4.2: As algebras $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})=w_q\oplus\overline{w_q}$. *Moreover,* $w_q\cong U_q(\mathfrak{g})$ *as Hopf algebras*.

Proof: Noting that J is a central idempotent, we see that w_q and $\overline{w_q}$ are ideals of $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$. It follows that

$$\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})=w_q\oplus\overline{w_q}$$

as algebras. Moreover, it is easy to see that w_q is generated by $E_iJ, F_iJ, K_i, \overline{K_i}$, and J subject to the relations (2.8)–(2.10) and

$$K_i(E_jJ)=q_i^{a_{ij}}(E_jJ)K_i, \quad \overline{K_i}(E_jJ)=q_i^{-a_{ij}}(E_jJ)\overline{K_i}, \tag{4.1}$$

$$K_i(F_jJ) = q_i^{-a_{ij}}(F_jJ)K_i, \quad \overline{K_i}(F_jJ) = q_i^{a_{ij}}(F_jJ)\overline{K_i}, \tag{4.2}$$

$$(E_iJ)(F_jJ) - (F_jJ)(E_iJ) = \delta_{ij}\frac{K_i - \overline{K_i}}{q_i - q_i^{-1}}, \tag{4.3}$$

$$\sum_{s=0}^{1-a_{ij}} (-1)^s \begin{bmatrix} 1-a_{ij} \\ s \end{bmatrix}_{q_i} (E_iJ)^{1-a_{ij}-s}(E_jJ)(E_iJ)^s = 0, \quad \text{if } i \neq j, \tag{4.4}$$

$$\sum_{s=0}^{1-a_{ij}} (-1)^s \begin{bmatrix} 1-a_{ij} \\ s \end{bmatrix}_{q_i} (F_iJ)^{1-a_{ij}-s}(F_jJ)(F_iJ)^s = 0, \quad \text{if } i \neq j. \tag{4.5}$$

Here J can be viewed as the identity of w_q. At this point of view w_q becomes a Hopf algebra, in which the comultiplication Δ is

$$\Delta(E_iJ) = J \otimes E_iJ + E_iJ \otimes K_i,$$

$$\Delta(F_iJ) = F_iJ \otimes J + \overline{K_i} \otimes F_iJ,$$

$$\Delta(K_i) = K_i \otimes K_i, \quad \Delta(\overline{K_i}) = \overline{K_i} \otimes \overline{K_i}.$$

The counit ε is

$$\varepsilon(E_iJ) = \varepsilon(F_iJ) = 0, \quad \varepsilon(K_i) = \varepsilon(\overline{K_i}) = 1.$$

The antipode S is

$$S(E_iJ) = -(E_iJ)\overline{K_i}, \quad S(F_iJ) = -K_i(F_iJ), \quad S(K_i) = \overline{K_i}, \quad S(\overline{K_i}) = K_i.$$

Let ρ be the algebra morphism from $U_q(\mathfrak{g})$ to w_q defined by

$$\rho(e_i) = E_iJ, \quad \rho(f_i) = F_iJ, \quad \rho(k_i) = K_i, \quad \rho(k_i^{-1}) = \overline{K_i}.$$

It is straightforward to see that ρ is a Hopf algebra isomorphism. □

For the ideal $\overline{w_q}$ of $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$, some conventions should be noted. Let

$$\mathsf{d} = (\kappa_1, \ldots, \kappa_n | \overline{\kappa_1}, \ldots, \overline{\kappa_n})$$

be a binary sequence. If κ_i (respectively, $\overline{\kappa_i}$), $1 \leqslant i \leqslant n$ is zero, and hence that E_i (respectively, F_i) is type 2, then $E_i(1-J)=0$ [respectively, $F_i(1-J)=0$]; if κ_i (respectively, $\overline{\kappa_i}$), $1 \leqslant i \leqslant n$ is nonzero, and hence that E_i (respectively, F_i) is type 1, then $E_i(1-J) \neq 0$ [respectively, $F_i(1-J) \neq 0$]. Let

$$\mathfrak{d} = \{i | \kappa_i \neq 0\} \text{ and } \overline{\mathfrak{d}} = \{i | \overline{\kappa_i} \neq 0\}$$

and

$$X_i = E_i(1-J), \quad Y_j = F_j(1-J),$$

where $i \in \mathfrak{d}$, $j \in \overline{\mathfrak{d}}$. It is easy to see that $\{X_i, Y_j | i \in \mathfrak{d}, j \in \overline{\mathfrak{d}}\} \cup \{1-J\}$ generate the ideal $\overline{w_q}$ with enjoying the first relation

$$X_iY_j = Y_jX_i \text{ for all } i \in \mathfrak{d}, j \in \overline{\mathfrak{d}} \tag{4.6}$$

from the relation (2.12).

To see what other relations X_i and Y_i enjoy, we consider the following two extreme cases:

(1) The case

$$\overline{\mathsf{d}} := (\underbrace{1,\cdots,1}_{n\text{copies}}|\underbrace{1,\cdots,1}_{n\text{copies}}).$$

In this case, $\mathfrak{d}=\{1,\ldots,n\}$ and $\overline{\mathfrak{d}}=\{1,\ldots,n\}$. From the quantum Serre relations (2.13) and (2.14), we get that

$$\sum_{s=0}^{1-a_{ij}}(-1)^s\begin{bmatrix}1-a_{ij}\\ s\end{bmatrix}_{q_i}(X_i)^{1-a_{ij}-s}X_j(X_i)^s=0,\ \text{if } i\neq j, \tag{4.7}$$

$$\sum_{s=0}^{1-a_{ij}}(-1)^s\begin{bmatrix}1-a_{ij}\\ s\end{bmatrix}_{q_i}(Y_i)^{1-a_{ij}-s}Y_j(Y_i)^s=0,\ \text{if } i\neq j, \tag{4.8}$$

and other relations corresponding to (2.8)–(2.11) would be vanished automatically. This means that the ideal $\overline{w_q}$ can be understood as an algebra generated by X_i, Y_i, $1\leqslant i\leqslant n$, with an identity $1-J$ subject to the relations (4.6)–(4.8).

(2) The case

$$\underline{\mathsf{d}} := (\underbrace{0,\cdots,0}_{n\text{copies}}|\underbrace{0,\cdots,0}_{n\text{copies}}).$$

In this case, $\mathfrak{d}$ and $\overline{\mathfrak{d}}$ are empty and $\overline{w_q}=k(1-J)$.

In general, three cases should be considered,

(1) $\mathfrak{d}\neq\emptyset$ and $\overline{\mathfrak{d}}=\emptyset$,
(2) $\mathfrak{d}=\emptyset$ and $\overline{\mathfrak{d}}\neq\emptyset$,
(3) $\mathfrak{d}\neq\emptyset$ and $\overline{\mathfrak{d}}\neq\emptyset$.

In the first case, as an algebra $\overline{w_q}$ is generated by X_i, $i\in\mathfrak{d}$ with an identity $1-J$ subject to the relations (4.7) with $i,j\in\mathfrak{d}$. In the second case, as an algebra $\overline{w_q}$ is generated by Y_i, $i\in\overline{\mathfrak{d}}$ with an identity $1-J$ subject to the relations (4.8) with $i,j\in\overline{\mathfrak{d}}$. In the third case, $\overline{w_q}$ can be viewed as an algebra generated by X_i, Y_j, $i\in\mathfrak{d}$, $j\in\overline{\mathfrak{d}}$ with an identity $1-J$ subject to the relations (4.6)–(4.8).

To consider the PBW basis of $\mathfrak{w}_q^{\mathsf{d}}(\mathfrak{g})$, we need some knowledge of braid groups. We define a simple reflection s_i by

$$s_i(\alpha_j)=\alpha_j-a_{ij}\alpha_i$$

for all i and j. Let W be the Weyl group of R; it is the subgroup of $\mathrm{GL}(\mathbb{Z}^n)$ generated by the refelctions $s_i(1\leqslant i\leqslant n)$. Let $\ell(w)$ be the usual length function on W with respect to the generators $\{s_1,\ldots,s_n\}$. Let R^+ be the set of positive roots of R with respect to the set of simple roots Π and $\ell_0=|R^+|$. For each pair $1\leqslant i,\ j\leqslant n$ with $i\neq j$, we let $r=-a_{ij}$.

As is known in Ref. 9, for each $1\leqslant i\leqslant n$, there is a unique automorphism $T_i: U_q(\mathfrak{g})\to U_q(\mathfrak{g})$ such that

$$T_i(e_i)=-f_ik_i, T_i(f_i)=-k_i^{-1}e_i,$$

$$T_i(k_\mu)=k_{s_i(\mu)},$$

$$T_i(e_j)=\sum_{k=0}^{r}(-1)^iq_i^{-k}e_i^{(r-i)}e_je_i^{(i)},$$

$$T_i(f_j) = \sum_{k=0}^{r} (-1)^i q_i^k f_i^{(i)} f_j f_i^{(r-i)}.$$

They are called Lusztig's symmetries. It is well known that $\{T_i | 1 \leqslant i \leqslant n\}$ satisfies the braid relations, that is

$$T_i T_j T_i = T_j T_i T_j, \quad \text{if } s_i s_j \text{ of order } 2,$$

$$T_i T_j T_i T_j = T_j T_i T_j T_i, \quad \text{if } s_i s_j \text{ of order } 4,$$

$$T_i T_j T_i T_j T_i T_j = T_j T_i T_j T_i T_j T_i, \quad \text{if } s_i s_j \text{ of order } 6.$$

Therefore, the above facts allow us to define for each $w \in W$ an automorphism T_w of $U_q(\mathfrak{g})$ as follows. For $w=1$ set $T_1=1$ (the identity). For $w \neq 1$ choose a reduced expression $w=s_{i_1}\cdots s_{i_m}$ and set

$$T_w = T_{i_1} \cdots T_{i_m}.$$

It is independent of the reduced expression. Let U_q^+ (respectively, U_q^- and U_q^0) be the subalgebra of $U_q(\mathfrak{g})$ generated by e_i (respectively, f_i and k_i, k_i^{-1}), $1 \leqslant i \leqslant n$. Let w_0 be the longest element in W and let $w_0 = s_{i_1}\cdots s_{i_t}$ be a reduced expression. Let $\mathbb{N}$ be the set of non-negative numbers. According to this order we denote $a=(a_t,\ldots,a_1) \in \mathbb{N}^{\ell_0}$ and

$$e^a = T_{i_1} \cdots T_{i_{t-1}}(e_{i_t}^{a_t}) \cdots T_{i_1} T_{i_2}(e_{i_3}^{a_3}) T_{i_1}(e_{i_2}^{a_2}) e_{i_1}^{a_1}. \tag{4.9}$$

The following theorem is well known.

Theorem 4.3: (cf. Ref. 9, Theorem 8.24) *The elements* e^a (respectively, f^a) *for* $a \in \mathbb{N}^{\ell_0}$, *are linearly independent and a basis of* U_q^+ (respectively, U_q^-).

We note that the multiplication map

$$U_q^- \otimes U_q^0 \otimes U_q^+ \to U_q(\mathfrak{g}), \quad u_1 \otimes u_2 \otimes u_3 \to u_1 u_2 u_3 \tag{4.10}$$

is an isomorphism of vector spaces.

For $s=(s_1,s_2,\ldots,s_n) \in \mathbb{Z}^n$, we define

$$P^s = P_1^{s_1} P_2^{s_2} \cdots P_n^{s_n}.$$

First, let us examine two examples.

Example 4.4: The set

$$\{F^b P^s E^a J | a,b \in \mathbb{N}^{\ell_0}, s \in \mathbb{Z}^n\} \cup \{F^b E^a (1-J) | a,b \in \mathbb{N}^{\ell_0}\}$$

forms a basis of $\overline{\mathfrak{w}_q^{\mathfrak{d}}}(\mathfrak{g})$.

Proof: Let w_q^0 be the subalgebra generated by $\{K_i, \overline{K_i} | 1 \leqslant i \leqslant n\}$. It is easy to see that P^s ($s \in \mathbb{Z}$) forms a basis of w_q^0.

Let w_q^+ (respectively, w_q^-) denote the subalgebra generated by $E_i J$ (respectively, $F_i J$), $1 \leqslant i \leqslant n$.

We replace e_{i_k} where $k=1,\ldots,t$ on the right-hand side of (4.9) by $E_{i_k} J$ [respectively, $E_{i_k}(1-J)$], and the corresponding left-hand side by $(EJ)^a$ [resppectively, $(E(1-J))^a$]. By Theorem 4.3 the set $\{(EJ)^a | a \in \mathbb{N}^{\ell_0}\}$ [respectively, $\{(FJ)^b | b \in \mathbb{N}^{\ell_0}\}$] forms a basis of w_q^+ (respectively, w_q^-). It is easy to see that

$$(FJ)^b P^s (EJ)^a = F^b P^s E^a J.$$

It follows from (4.10) that

$$\{F^aP^sE^bJ|a,b\in\mathbb{N}^{\ell_0},s\in\mathbb{Z}^n\}$$

forms a basis of w_q.

Similarly, $\{F^aE^b(1-J)|a,b\in\mathbb{N}^{\ell_0}\}$ forms a basis of $\overline{w_q}$. The proof is completed by Proposition 4.2. □

In a similar way we can get the following.

Example 4.5: The set

$$\{F^bP^sE^aJ|a,b\in\mathbb{N}^{\ell_0},s\in\mathbb{Z}^n\}\cup\{1-J\}$$

forms a basis of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$.

In general, let both i and j be in $\mathfrak{d}$ or in $\overline{\mathfrak{d}}$, we say that $i\sim j$ if there exist some sequence $i=\gamma_1,\ldots,\gamma_p=j$ in $\mathfrak{d}$, where γ_p is in $\mathfrak{d}$ or $\overline{\mathfrak{d}}$, p is some positive integer, such that $(\alpha_{\gamma_i},\alpha_{\gamma_{i+1}})\neq 0$ for all $i=1,\ldots,p-1$. This is an equivalent relation. Let $\mathfrak{s}$ and $\overline{\mathfrak{s}}$ be the set of equivalent classes on $\mathfrak{d}$ and $\overline{\mathfrak{d}}$, respectively. If $\mathfrak{e}$ is an element in $\mathfrak{s}$ or $\overline{\mathfrak{s}}$, it is obvious that $C_{\mathfrak{e}}=(a_{ij})_{i,j\in\mathfrak{e}}$ is also a symmetrizable Cartan matrix. If $\mathfrak{e}_1\neq\mathfrak{e}_2$ in $\mathfrak{s}$ or $\overline{\mathfrak{s}}$ and $i\in\mathfrak{e}_1$ and $j\in\mathfrak{e}_2$, then $E_iE_j=E_jE_i$ and $F_iF_j=F_jF_i$, and hence $X_iX_j=X_jX_i$ and $Y_iY_j=Y_jY_i$, respectively. Let $W_{\mathfrak{e}}$ be the Weyl group corresponding to the equivalent class $\mathfrak{e}$ on $\mathfrak{d}$ or $\overline{\mathfrak{d}}$. Let $w_0^{\mathfrak{e}}=s_{i_1}\cdots s_{i_{t_{\mathfrak{e}}}}$ be the longest element in $W_{\mathfrak{e}}$. Let $\ell_{\mathfrak{e}}=|w_0^{\mathfrak{e}}|=t_{\mathfrak{e}}$. We denote $a_{\mathfrak{e}}=(a_{t_{\mathfrak{e}}},\ldots,a_1)$ according to this order and

$$X_{\mathfrak{e}}^{a_{\mathfrak{e}}}=T_{i_1}\cdots T_{i_{t_{\mathfrak{e}}-1}}(E_{i_{t_{\mathfrak{e}}}}^{a_{t_{\mathfrak{e}}}})\cdots T_{i_1}T_{i_2}(E_{i_3}^{a_3})T_{i_1}(E_{i_2}^{a_2})E_{i_1}^{a_1}(1-J),\tag{4.11}$$

$$Y_{\mathfrak{e}}^{a_{\mathfrak{e}}}=T_{i_1}\cdots T_{i_{t_{\mathfrak{e}}-1}}(F_{i_{t_{\mathfrak{e}}}}^{a_{t_{\mathfrak{e}}}})\cdots T_{i_1}T_{i_2}(F_{i_3}^{a_3})T_{i_1}(F_{i_2}^{a_2})F_{i_1}^{a_1}(1-J).\tag{4.12}$$

It is noted that

$$X_iY_j=Y_jX_i$$

for all $i\in\mathfrak{d}$, $j\in\overline{\mathfrak{d}}$, and

$$\mathfrak{d}=\cup_{\mathfrak{e}\in\mathfrak{s}}\mathfrak{e},\quad \overline{\mathfrak{d}}=\cup_{\mathfrak{e}\in\overline{\mathfrak{s}}}\overline{\mathfrak{e}},$$

one sees that

$$\left\{\prod_{\mathfrak{e}\in\mathfrak{s}}X_{\mathfrak{e}}^{a_{\mathfrak{e}}}\prod_{\overline{\mathfrak{e}}\in\overline{\mathfrak{s}}}Y_{\overline{\mathfrak{e}}}^{b_{\overline{\mathfrak{e}}}}\middle|a_{\mathfrak{e}}\in\mathbb{N}^{\ell_{\mathfrak{e}}},b_{\overline{\mathfrak{e}}}\in\mathbb{N}^{\ell_{\overline{\mathfrak{e}}}}\right\}$$

forms a basis of $\overline{w_q}$. By Proposition 4.2 and the discussion above, we have the following.

Theorem 4.6: *The notations are kept as above. Then the set*

$$\{F^bP^sE^aJ|a,b\in\mathbb{N}^{\ell_0},s\in\mathbb{Z}^n\}\cup\left\{\prod_{\mathfrak{e}\in\mathfrak{s}}X_{\mathfrak{e}}^{a_{\mathfrak{e}}}\prod_{\overline{\mathfrak{e}}\in\overline{\mathfrak{s}}}Y_{\overline{\mathfrak{e}}}^{b_{\overline{\mathfrak{e}}}}\middle|a_{\mathfrak{e}}\in\mathbb{N}^{\ell_{\mathfrak{e}}},b_{\overline{\mathfrak{e}}}\in\mathbb{N}^{\ell_{\overline{\mathfrak{e}}}}\right\}$$

forms a basis of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$.

It is mentioned that the set

$$\{E^aP^sF^aJ|a,b\in\mathbb{N}^{\ell_0},s\in\mathbb{Z}^n\}\cup\left\{\prod_{\mathfrak{e}\in\mathfrak{s}}X_{\mathfrak{e}}^{a_{\mathfrak{e}}}\prod_{\overline{\mathfrak{e}}\in\overline{\mathfrak{s}}}Y_{\overline{\mathfrak{e}}}^{b_{\overline{\mathfrak{e}}}}\middle|a_{\mathfrak{e}}\in\mathbb{N}^{\ell_{\mathfrak{e}}},b_{\overline{\mathfrak{e}}}\in\mathbb{N}^{\ell_{\overline{\mathfrak{e}}}}\right\}$$

also forms a basis of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$.

Let us recall some basic facts used below. Let C be a coalgebra. If the set $\{C_n\}_{n\geqslant 0}$ of subspaces of C satisfies

(1) $C_n\subseteq C_{n+1}$ and $C=\cup_{n\geqslant 0}C_n$

(2) $\Delta(C_n) \subseteq \Sigma_{i=0}^{n} C_i \otimes C_{n-i}$,

then the set $\{C_n\}_{n\geqslant 0}$ is said to be a coalgebra filtration of C.

The following lemma is well known.

Lemma 4.7: (Ref. 14, Lemma 5.5.1) *Let H be a bialgebra which contains subspaces $A_0 \subset A_1$ such that*

(1) *A_0 is a (unital) subalgebra of H and A_1 is a left, and a right A_0-module*;
(2) *A_1 generates H as an algebra, and $1 \in A_0$*;
(3) *$\Delta A_0 \subseteq A_0 \otimes A_0$ and $\Delta(A_1) \subseteq A_1 \otimes A_0 + A_0 \otimes A_1$.*

Then, if we set $A_n = (A_1)^n$ for all $n \geqslant 1$, $\{A_n\}$ is a coalgebra filtration of H and $A_0 \supseteq H_0$, where H_0 is the coradical of H.

The element $x \in \mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ is said to be a grouplike element if $\Delta(x) = x \otimes x$. The set $G = G(\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g}))$ of all grouplike elements of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ can be determined.

A semigroup S is called regular, if for every $x \in S$, there exists a $y \in S$ such that $xyx = x$ and $yxy = y$ and a monoid is a semigroup with identity.

Proposition 4.8: The set of all grouplike elements is $G = \{P^s | s \in \mathbb{Z}^n\} \cup \{1\}$, which forms a regular monoid under the multiplication of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$.

Proof: Let G be the setup as above. Let $A_0 = kG$ and

$$A_1 = A_0\left(\sum_i kE_i + kF_i + A_0\right)A_0.$$

It is easy to see that $A_0 \subset A_1$ satisfies the hypotheses of Lemma 4.7 and $A_0 \subseteq H_0$. Hence $H_0 = A_0$. □

It is mentioned that $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ is a pointed bialgebra with the coradical kG by Proposition 4.8.

V. THE AUTOMORPHISM GROUP OF $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$

If $(A, m, \mu, \Delta, \varepsilon, T)$ is a (weak) Hopf algebra, then a (weak) Hopf algebra automorphism $\varphi: A \to A$ is an invertible algebra homomorphism satisfying

$$(\varphi \otimes \varphi) \circ \Delta = \Delta \circ \varphi,$$

$$\varepsilon = \varepsilon \circ \varphi,$$

$$\varphi \circ T = T \circ \varphi.$$

The group of Hopf algebra automorphisms of $U_q(\mathfrak{g})$ was determined by several authors. See, for example, Refs. 4 and 15. Inspired by these considerations, we would like to determine the group of weak Hopf algebra automorphisms of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ where q is not a root of unity.

Let $N = (k^*)^n$, and for $a = (a_1, \ldots, a_n) \in N$, we define a map $\phi_a: U_q(\mathfrak{g}) \to U_q(\mathfrak{g})$ by

$$\phi_a(k_i) = k_i, \quad \phi_a(e_i) = a_i e_i, \quad \phi_a(f_i) = a_i^{-1} f_i.$$

It is straightfoward to check that ϕ_a is a Hopf algebra automorphism of $U_q(\mathfrak{g})$. It is called N the group of diagonal automorphisms of $U_q(\mathfrak{g})$.

Recall that the Dynkin diagram of $\mathfrak{g}$ is the weight graph Γ with vertices $\mathfrak{n} = \{1, 2, \ldots, n\}$ such that vertices i and j are connected by $a_{ij}a_{ji}$ edges, and vertex i carries weight d_i. Let σ be a automorphsim of Dynkin diagram Γ, that is σ is a bijection of $\mathfrak{n}$ and

$$d_i a_{ij} = d_{\sigma(i)} a_{\sigma(i)\sigma(j)}$$

for all $1 \leqslant i, j \leqslant n$. If this is the case, there is an automorphism of Hopf algebra $U_q(\mathfrak{g})$, also denoted by σ, given by

$$\sigma(k_i) = k_{\sigma(i)}, \quad \sigma(e_i) = e_{\sigma(i)}, \quad \sigma(f_i) = f_{\sigma(i)}.$$

We denote by H the group of automorphisms of the Dynkin diagram. Also, H acts on N by the rules $\sigma\cdot a=(a_{\sigma(1)},\ldots,a_{\sigma(n)})$ and we have $\phi_a\sigma=\sigma\phi_{\sigma\cdot a}$. We will base on the following theorem to investigate the group of automorphisms of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$.

Theorem 5.1: (Ref. 4, Corollary 4.3; Ref. 18, Theorem 2.1) *The group of Hopf algebra automorphism of $U_q(\mathfrak{g})$ is the semidirect product $N\rtimes H$ of the group of diagonal automorphism N by the group of diagram automorphisms H.*

Moreover, we also need some basic lemmas.

Lemma 5.2: *If $x,y\in\overline{w_q}$, $a_x,b_y\neq 0$ and*

$$\Delta(x)=1\otimes x+x\otimes K_i+a_x(1-J)\otimes E_iJ,$$

$$\Delta(y)=\overline{K_i}\otimes y+y\otimes 1+b_yF_iJ\otimes(1-J),$$

then $x=a_xE_i(1-J)$ and $y=b_yF_i(1-J)$.

Proof: The notations $\mathfrak{d}$ and $\overline{\mathfrak{d}}$ are as in Sec. IV. Let $W_{\mathfrak{d}}$ be the Weyl group corresponding to $\mathfrak{d}$ and $w_{\mathfrak{d}}=s_{i_1}\cdots s_{i_{t_{\mathfrak{d}}}}$ be the longest element in $W_{\mathfrak{d}}$ and $\ell_{\mathfrak{d}}=t_{\mathfrak{d}}$. Similarly, we have the Weyl group $W_{\overline{\mathfrak{d}}}$, $w_{\overline{\mathfrak{d}}}=s_{j_1}\cdots s_{j_{t_{\overline{\mathfrak{d}}}-1}}$, $\ell_{\overline{\mathfrak{d}}}$ for the support set $\overline{\mathfrak{d}}$ in an obvious sense.

Let $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})^+$ be the sub-bialgebra of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ generated by E_i, $1\leqslant i\leqslant n$ and the set G of group-likes of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$. Let $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})^-$ be the sub-bialgebra of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ generated by F_i, $1\leqslant i\leqslant n$ and G. We define a $\mathbb{N}[I]$-algebra gradation on $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})^+$ [respectively, $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})^-$] such that E_j^s (respectively, F_j^s) are homogeneous of degree $s\alpha_j\in\mathbb{N}[I]$ for $s\in\mathbb{N}$, $1\leqslant j\leqslant n$. We also set $\deg K_j=\deg\overline{K_j}=\deg J=0$ for all j. According to this gradation, $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})^+$ [respectively, $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})^-$] is also a graded coalgebra. It is obvious that $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})^+(1-J)\subset\overline{w_q}$ has a basis $\{E^a(1-J)|a\in\mathbb{N}^{\ell_{\mathfrak{d}}}\}$. Similarly, $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})^-(1-J)\subset\overline{w_q}$ has a basis $\{F^b(1-J)|b\in\mathbb{N}^{\ell_{\overline{\mathfrak{d}}}}\}$.

It is easy to see the elements $E^a(1-J)$, $F^b(1-J)$ have a gradation $|a|$ and $|b|$, where

$$|a|=a_1\alpha_1+a_2s_{i_1}(\alpha_{i_2})+\cdots+a_{t_{\mathfrak{d}}}s_{i_1}s_{i_2}\cdots s_{i_{t_{\mathfrak{d}}-1}}(\alpha_{i_{t_{\mathfrak{d}}}}),$$

$$|b|=b_1\alpha_1+b_2s_{j_1}(\alpha_{j_2})+\cdots+b_{t_{\mathfrak{d}}}s_{j_1}s_{j_2}\cdots s_{j_{t_{\overline{\mathfrak{d}}}-1}}(\alpha_{i_{j_{\mathfrak{d}}}}).$$

Let

$$x=\sum_{a\in\mathbb{N}^{\ell_{\mathfrak{d}}},b\in\mathbb{N}^{\ell_{\overline{\mathfrak{d}}}}}x(a,b)E^aF^b(1-J)\in\overline{w_q},$$

where $\{E^aF^b(1-J)\}$ are linear independent. We have

$$\Delta(x)=\sum_{\substack{a\in\mathbb{N}^{\ell_{\mathfrak{d}}},b\in\mathbb{N}^{\ell_{\overline{\mathfrak{d}}}}\\ |s|+|t|=|a|\\ |x|+|y|=|b|}}x(a,b)a(s,t)b(x,y)E^sF^x\overline{K_{|y|}}\otimes E^tK_{|s|}F^y-\sum_{\substack{a\in\mathbb{N}^{\ell_{\mathfrak{d}}},b\in\mathbb{N}^{\ell_{\overline{\mathfrak{d}}}}\\ |s|+|t|=|a|\\ |x|+|y|=|b|}}x(a,b)a(s,t)b(x,y)E^sF^x\overline{K_{|y|}}J$$
$$\otimes E^tK_{|s|}F^yJ.$$

Hence,

$$\Delta(x) = \sum_{\substack{a\in\mathbb{N}^{\ell_\mathfrak{d}}, b\in\mathbb{N}^{\ell_\mathfrak{d}^-} \\ |x|+|y|=|b| \\ |a'|=|a|,|y|\neq 0}} x(a,b)a(0,a')b(x,y)F^x\overline{K}_{|y|}\otimes E^{a'}F^y(1-J)$$
$$+ \sum_{\substack{a\in\mathbb{N}^{\ell_\mathfrak{d}}, b\in\mathbb{N}^{\ell_\mathfrak{d}^-} \\ |s|+|t|=|a| \\ |b'|=|b|,|s|\neq 0}} x(a,b)a(s,t)b(b',0)E^sF^{b'}(1-J)\otimes E^tK_{|s|}$$
$$+ \sum_{\substack{a\in\mathbb{N}^{\ell_\mathfrak{d}}, b\in\mathbb{N}^{\ell_\mathfrak{d}^-} \\ |a'|=|a| \\ |b'|=|b|}} x(a,b)a(0,b')b(b',0)F^{b'}\otimes E^{a'} - \sum_{\substack{a\in\mathbb{N}^{\ell_\mathfrak{d}}, b\in\mathbb{N}^{\ell_\mathfrak{d}^-} \\ |a'|=|a| \\ |b'|=|b|}} x(a,b)a(0,b')b(b',0)F^{b'}J$$
$$\otimes E^{a'}J.$$

On the other hand, by the assumption we have

$$\Delta(x) = 1\otimes \sum_{a\in\mathbb{N}^{\ell_\mathfrak{d}}, b\in\mathbb{N}^{\ell_\mathfrak{d}^-}} x(a,b)E^aF^b(1-J) + \sum_{a\in\mathbb{N}^{\ell_\mathfrak{d}}, b\in\mathbb{N}^{\ell_\mathfrak{d}^-}} x(a,b)E^aF^b(1-J)\otimes K_i + a_x(1-J)\otimes E_iJ.$$

Comparing the above identities, we conclude that all $b=0$. Now we can rewrite x as

$$x = \sum_{a\in\mathbb{N}^{\ell_\mathfrak{d}}} x(a)E^a(1-J) \in \overline{w}_q$$

and

$$\sum_{\substack{a\in\mathbb{N}^{\ell_\mathfrak{d}} \\ |s|+|t|=|a| \\ |s|\neq 0}} x(a)a(s,t)E^s(1-J)\otimes E^tK_{|s|} + \sum_{\substack{a\in\mathbb{N}^{\ell_\mathfrak{d}} \\ |a'|=|a|}} x(a)1\otimes E^{a'} - \sum_{\substack{a\in\mathbb{N}^{\ell_\mathfrak{d}} \\ |a'|=|a|}} x(a)J\otimes E^{a'}J$$
$$= \sum_{\substack{a\in\mathbb{N}^{\ell_\mathfrak{d}} \\ |s|+|t|=|a| \\ |s|\neq 0}} x(a)a(s,t)E^s(1-J)\otimes E^tK_{|s|} + 1\otimes \sum_{\substack{a\in\mathbb{N}^{\ell_\mathfrak{d}} \\ |a'|=|a|}} x(a)E^{a'}(1-J) + \sum_{a\in\mathbb{N}^{\ell_\mathfrak{d}}} x(a)(1-J)\otimes E^{a'}J$$
$$= 1\otimes \sum_{a\in\mathbb{N}^{\ell_\mathfrak{d}}} x(a)E^a(1-J) + \sum_{a\in\mathbb{N}^{\ell_\mathfrak{d}}} x(a)E^a(1-J)\otimes K_i + a_x(1-J)\otimes E_iJ.$$

Also, comparing the above identity, we conclude that $|a|=|a'|=i$, and hence $x=x(a)E_i(1-J)$. It follows that $x(a)=a_x$. The argument for F_i is similar. □

Lemma 5.3: Let φ be a Hopf algebra automorphism of w_q (the identity is J). Then there exists a unique way to extend φ to $\mathfrak{w}_q^\mathfrak{d}(\mathfrak{g})$ such that φ is an automorphism of weak Hopf algebra $\mathfrak{w}_q^\mathfrak{d}(\mathfrak{g})$.

Proof: Let φ be the automorphism of Hopf algebra w_q. By Lemma 5.1, the map φ is

$$K_i\to K_{\sigma(i)},\quad \overline{K_i}\to\overline{K}_{\sigma(i)},\quad E_iJ\to a_{\sigma(i)}E_{\sigma(i)}J,\quad F_iJ\to a_{\sigma(i)}^{-1}F_{\sigma(i)}J$$

for some automorphism σ of Dynkin diagram. Assume that φ can be extended to $\mathfrak{w}_q^\mathfrak{d}(\mathfrak{g})$ such that φ is an automorphism of $\mathfrak{w}_q^\mathfrak{d}(\mathfrak{g})$ as weak Hopf algebras. We must find suitable images of $\varphi(E_i(1-J))$ and $\varphi(F_i(1-J))$. For example, if E_i is type 2, we do nothing since $E_i(1-J)=0$. Assume that E_i is type 1 and $\varphi(E_i(1-J))=x$, then $x\neq 0$, $x\in\overline{w}_q$, and

$$\varphi(E_i) = \varphi(E_iJ + E_i(1-J)) = a_{\sigma(i)}E_{\sigma(i)}J + x.$$

Since φ is a coalgebra homomorphism, we have

$$a_{\sigma(i)}E_{\sigma(i)}J \otimes K_{\sigma(i)} + a_{\sigma(i)}J \otimes E_{\sigma(i)}J + \Delta(x) = (a_{\sigma(i)}E_{\sigma(i)}J + x) \otimes K_{\sigma(i)} + 1 \otimes (a_{\sigma(i)}E_{\sigma(i)}J + x).$$

It follows that

$$\Delta(x) = x \otimes K_{\sigma(i)} + 1 \otimes x + a_{\sigma(i)}(1-J) \otimes E_{\sigma(i)}J.$$

By Lemma 5.2, $x = a_{\sigma(i)}E_{\sigma(i)}(1-J)$. Similarly, we can get that $\varphi(F_i(1-J)) = a_{\sigma(i)}^{-1}F_{\sigma(i)}(1-J)$ if F_i is type 1, and nothing is done if F_i is of type 2. Of course, $\varphi(1)=1$. The lemma is proved. □

For $a=(a_1,\ldots,a_n) \in N$, we define a map $\phi_a : \mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g}) \to \mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ by

$$\phi_a(K_i) = K_i, \quad \phi_a(\overline{K_i}) = \overline{K_i}, \quad \phi_a(E_i) = a_iE_i, \quad \phi_a(F_i) = a_i^{-1}F_i.$$

It is straightfoward to check that ϕ_a is a weak Hopf algebra automorphism of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$. If $\sigma \in H$, then there is an automorphism of weak algebra $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$, also denoted by σ, given by

$$\sigma(K_i) = K_{\sigma(i)}, \quad \sigma(\overline{K_i}) = \overline{K}_{\sigma(i)}, \quad \sigma(E_i) = E_{\sigma(i)}, \quad \sigma(F_i) = F_{\sigma(i)}.$$

Recall that there is an action of H on N by the rules $\sigma \cdot a = (a_{\sigma(1)},\ldots,a_{\sigma(n)})$ and $\phi_a\sigma = \sigma\phi_{\sigma\cdot a}$.

Let $\mathrm{Aut}(\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g}))$ be the group of automorphisms of weak Hopf algebra $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$. The group $\mathrm{Aut}(\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g}))$ can be determined by the following theorem.

Theorem 5.4: $\mathrm{Aut}(\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})) = N \rtimes H$.

Proof: Theorem A in Ref. 4 is the key to determine the group of automorphisms of Hopf algebra. But we do not know whether it is true or not for bialgebras (see Ref. 5); we cannot directly apply Theorem A to get the result.

Let $\varphi \in \mathrm{Aut}(\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g}))$, since φ sends group-likes to group-likes, we have $\varphi(J) = P^s$ for some $s \in \mathbb{Z}^n$ by Proposition 4.8. If $s \neq 0$, since $J^2 = J$ we have $P^{2s} = P^s$, hence $P^s = J$ it follows that $P^sJ = J$. It is a contradiction for Theorem 4.6. Therefore, $s=0$ and $\varphi(J) = J$.

According to Proposition 4.2, $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g}) = w_q \oplus \overline{w_q}$ and $w_q \cong U_q(\mathfrak{g})$ as Hopf algebras, where the notations w_q and $\overline{w_q}$ as before.

Let $\mathrm{inj}_q : w_q \to \mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$ be the inclusion defined by

$$J \to J, \quad E_iJ \to E_iJ, \quad F_iJ \to F_iJ, \quad K_i \to K_i, \quad \overline{K_i} \to \overline{K_i},$$

and then extend it by linearity. It is easy to see that inj_q is a weak Hopf algebra injection by Proposition 4.2. Let $\varphi \in \mathrm{Aut}(\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g}))$, we see that $w_q = \mathrm{im}(\varphi \circ \mathrm{inj}_q)$ since $\varphi(J) = J$. This implies that $\varphi \circ \mathrm{inj}_q$ is an automorphism of Hopf algebra w_q and $\varphi \circ \mathrm{inj}_q \in N \rtimes H$ by Theorem 5.1. That is, the map $\varphi|_{w_q}$ is

$$K_i \to K_{\sigma(i)}, \quad \overline{K_i} \to \overline{K}_{\sigma(i)}, \quad E_iJ \to a_{\sigma(i)}E_{\sigma(i)}J, \quad F_iJ \to a_{\sigma(i)}^{-1}F_{\sigma(i)}J.$$

This implies that φ is

$$K_i \to K_{\sigma(i)}, \quad \overline{K_i} \to \overline{K}_{\sigma(i)}, \quad E_i \to a_{\sigma(i)}E_{\sigma(i)}, \quad F_i \to a_{\sigma(i)}^{-1}F_{\sigma(i)}$$

by Lemma 5.2. Hence $\varphi \in N \rtimes H$ and $\mathrm{Aut}(\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})) \subseteq N \rtimes H$. On the other hand, it is obvious that $N \rtimes H \subseteq \mathrm{Aut}(\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g}))$. The proof is completed. □

The more interesting problem is to determine the algebraic group of $\mathfrak{w}_q^{\mathfrak{d}}(\mathfrak{g})$. It is mentioned that Ref. 2 contributed to determine $\mathrm{Aut}_{\mathrm{Alg}}(U_q^+(\mathfrak{g}))$. A basic idea to approach the group $\mathrm{Aut}_{\mathrm{Alg}}(U_q^+(\mathfrak{g}))$ is to study its actions on natural sets.

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On the uniqueness of solutions to gauge covariant Poisson equations with compact Lie algebras

Christofer Cronström[a)]
Department of Physical Sciences, Theoretical Physics Division FIN-00014, University of Helsinki, Finland

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It is shown, under rather general smoothness conditions on the gauge potential, which takes values in an arbitrary semisimple compact Lie algebra **g**, that if a (**g**-valued) solution to the gauge-covariant Laplace equation exists, which vanishes at spatial infinity, in the cases of 1,2,3,…, space dimensions, then the solution is identically zero. This result is also valid if the Lie algebra is merely compact. Consequently, a solution to the gauge-covariant Poisson equation is uniquely determined by its asymptotic radial limit at spatial infinity. In the cases of one or two space dimensions a related result is proved, namely that if a solution to the gauge-covariant Laplace equation exists, which is unbounded at spatial infinity, but with a certain dimension-dependent condition on the asymptotic growth of its norm, then the solution in question is a covariant constant. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1935427]

I. INTRODUCTION

Let **g** denote a semisimple compact Lie algebra and let Φ and $\mathcal{F}$ denote two **g**-valued functions on an n-dimensional Euclidean space R^n. Points in R^n are denoted by $x := (x^1, x^2, \ldots, x^n)$. The covariant Poisson equation is then the following:

$$\sum_{k=1}^{n} \boldsymbol{\nabla}_k(A)\boldsymbol{\nabla}^k(A)\Phi(x) = \mathcal{F}(x), \tag{1}$$

where $\boldsymbol{\nabla}_k(A)$ denotes the following gauge-covariant gradient,

$$\boldsymbol{\nabla}_k(A) := \partial_k + i[A_k,] \equiv \frac{\partial}{\partial x^k} + i[A_k(x),]. \tag{2}$$

In definition (2), the symbol $A := (A_1(x), A_2(x), \ldots, A_n(x))$ is a **g**-valued gauge potential,[1] and the symbol $[\ ,\ ]$ stands for the commutator of **g**-valued quantities. The covariant gradient with an upper index k, $\boldsymbol{\nabla}^k(A)$, is defined as follows:

$$\boldsymbol{\nabla}^k(A) := -\boldsymbol{\nabla}_k(A). \tag{3}$$

Other quantities with upper space indices are defined similarly; viz., if V_k is any quantity with a lower (subscript) space index, then its counterpart with an upper (superscript) space index V^k is given as follows:

$$V^k := -V_k, \quad k = 1,2,\ldots,n. \tag{4}$$

The covariant Poisson equation (1) is a second-order elliptic system of partial differential equations, which, together with appropriate boundary conditions, is supposed to determine the

a)Electronic mail: Christofer.Cronstrom@Helsinki.fi.

quantity $\Phi(x)$, when the inhomogeneous term $\mathcal{F}(x)$ and gauge potential $A(x)$, respectively, are given. These quantities are supposed to satisfy appropriate regularity conditions. We will return to the question of regularity conditions subsequently.

The Lie algebra $\mathbf{g}$ is specified by the (real-valued) structure constants $f_{ab}{}^{c}$ in the commutation relations of the Lie algebra generators T_a, $a=1,2,\ldots,\dim \mathbf{g}$,

$$[T_a,T_b]=if_{ab}{}^{c}T_c, \quad a,b=1,2,\ldots,\dim \mathbf{g}. \tag{5}$$

Here and in what follows, a summation of repeated Lie algebra indices, i.e., letters from the beginning of the Latin alphabet, over the range $1,2,\ldots,\dim \mathbf{g}$ is implied, unless otherwise stated.

From now on we will identify the Lie algebra generators with some specific Hermitian matrix representatives. For the purposes of this paper it does not matter which representation is chosen; in physical applications the choice of representations is related to the question of what types of other fields are coupled to the gauge fields, a question that is not our concern here.

Any $\mathbf{g}$-valued quantity is in the linear span of the generators T_a, thus

$$\Phi(x)=\Phi^a(x)T_a, \quad \mathcal{F}(x)=\mathcal{F}^a(x)T_a, \quad A_k(x)=A_k^a(x)T_a, \tag{6}$$

where all the components Φ^a, $\mathcal{F}^a$, and A_k^a are *real*.

The covariant Poisson equation (1) can naturally be written as a system of partial differential equations for the real-valued components Φ^a. Using the commutator algebra (5) one readily obtains the following system of equations:

$$\partial_k\partial^k\Phi^a-2f_{bc}{}^{a}A^{kb}\partial_k\Phi^c-f_{bc}{}^{a}(\partial_kA^{kb})\Phi^c+f_{bd}{}^{a}f_{ec}{}^{d}A_k^bA^{ke}\Phi^c=\mathcal{F}^a. \tag{7}$$

In the previous equation, summation over repeated space indices, one lower and one upper, is also implied.

For our purposes the compact matrix notation in Eq. (1) is preferable, and this will be used in what follows.

The gauge-covariant Poisson equation (1) on R^3 is one of the field equations (for fixed time) in either pure Yang–Mills theory, or Yang–Mills theory coupled to matter fields,[1] in four-dimensional Minkowski space. The gauge field $G_{\mu\nu}$ in Yang–Mills theory is as follows:

$$G_{\mu\nu}=\partial_\nu A_\mu-\partial_\mu A_\nu-i[A_\mu,A_\nu], \tag{8}$$

where Greek indices are Minkowski-space indices in the range (0, 1, 2, 3). The field equations are

$$\boldsymbol{\nabla}_\nu(A)G^{\mu\nu}(A)=j^\mu_{(m)}, \quad \mu=0,1,2,3, \tag{9}$$

where $j^\mu_{(m)}$ is a matter current constructed out of matter fields, e.g., fermionic and scalar fields.

The $\mu=0$ case of the equations (9) is Gauss' law,

$$\boldsymbol{\nabla}_k(A)G^{0k}=j^0_{(m)}, \tag{10}$$

which written in terms of the gauge potential components, is as follows:

$$\boldsymbol{\nabla}_k(A)\boldsymbol{\nabla}^k(A)A^0=j^0_{(m)}+\boldsymbol{\nabla}_k(A)\dot{A}^k, \tag{11}$$

where

$$\dot{A}_k(x)\equiv\partial_0A_k(x). \tag{12}$$

One physical application of the covariant Poisson equation (1) on R^3 is thus the implementation of Gauss' law by solving the equation (11) for the quantity A^0, with $j^0_{(m)}$ and $\dot{A}^k$ considered as known quantities. For this purpose one needs both existence and uniqueness theorems for equations of the form (1).

We will state and prove our main uniqueness theorems in detail for the equation (1) in Secs. III and IV. However, before that we collect in the next section a number of facts related to gauge transformations and inner products for semisimple compact Lie algebras that we need in the proofs.

II. ON GAUGE TRANSFORMATIONS AND LIE ALGEBRA INNER PRODUCTS

Let G denote the Lie group corresponding to the compact or semisimple compact Lie algebra defined by the equations (5) and let ω denote a mapping from R^n to G. In the vicinity of the unit element in G any such G-valued element ω can be obtained by exponentiating the Lie algebra, i.e.,

$$\omega(x) = e^{i\alpha^a T_a}, \tag{13}$$

where the parameters $\alpha^a(x), a=1,2,\ldots,\dim \mathbf{g}$ are sufficiently smooth real-valued functions that vary over a finite range.

A gauge transformation of a gauge potential $A \overset{\omega}{\rightarrow} A^\omega$ is then defined as follows for any sufficiently smooth G-valued function $\omega(x)$:

$$A_k(x) \overset{\omega}{\rightarrow} A_k^\omega(x) = \omega^{-1}(x)A_k(x)\omega(x) + i(\partial_k \omega^{-1}(x))\omega(x). \tag{14}$$

Let $U(x)$ be any differentiable $\mathbf{g}$-valued function and $\omega(x)$ likewise any differentiable G-valued function. Using Eq. (14), one readily shows that

$$\omega^{-1}(x)(\boldsymbol{\nabla}_k(A)U(x))\omega(x) = \boldsymbol{\nabla}_k(A^\omega)(\omega^{-1}(x)U(x)\omega(x)). \tag{15}$$

Applying the transformation (15) to the gauge-covariant Poisson equation (1), one obtains

$$\sum_{k=1}^{n} \boldsymbol{\nabla}_k(A^\omega)\boldsymbol{\nabla}^k(A^\omega)(\omega^{-1}(x)\Phi(x)\omega(x)) = \omega^{-1}(x)\mathcal{F}(x)\omega(x), \tag{16}$$

a result that will be used later.

If our Lie algebra is semisimple and compact, we use the following quantities h_{ab} as our Lie algebra metric. The quantities h_{ab} are defined in terms of the structure constants $f_{ab}{}^c$ as follows:

$$h_{ab} = -f_{ab'}{}^{c'} f_{bc'}{}^{b'}. \tag{17}$$

This is the so-called Killing form multiplied with -1 for convenience. It is known[2] that the form (17) is nondegenerate, and, furthermore, positive definite, if and only if the Lie algebra is semisimple and compact. The form (17) thus has an inverse, which we denote by h^{ab},

$$h^{ab}h_{bc} = \delta_c^a. \tag{18}$$

The form h_{ab} (h^{ab}) is used to lower (raise) Lie algebra indices.

For any two $\mathbf{g}$-valued quantities $U=U^aT_a$ and $V=V^aT_a$ we thus define their inner product (U,V) as follows:

$$(U,V) = h_{ab}U^aV^b. \tag{19}$$

The inner product (19) is invariant under the adjoint action of the group, i.e.,

$$(U,V) = (\omega^{-1}U\omega, \omega^{-1}V\omega), \quad \forall\ \omega \in G. \tag{20}$$

The norm $\|\ \|_g$ of any Lie algebra-valued quantity U is defined in terms of the inner product,

$$\|U\|_g := \sqrt{(U,U)}. \tag{21}$$

We also need the fact that for any three **g**-valued quantities U, V, and W the quantity $(U,[V,W])$ is cyclically symmetric,

$$(U,[V,W]) = (V,[W,U]) = (W,[U,V]) \tag{22}$$

The equations (22) follow directly from the fact that the quantities f_{abc} are antisymmetric under the interchange of any indices.

An immediate consequence of Eqs. (22) is the following useful identity:

$$\partial_k(U,V) = (\boldsymbol{\nabla}_k(A)U,V) + (U,\boldsymbol{\nabla}_k(A)V). \tag{23}$$

This identity is valid for any two differentiable **g**-valued quantities U and V and a smooth gauge potential A.

We finally note that one may drop the condition of semisimplicity above and require only the condition of compactness of the Lie algebra. One is still then guaranteed the existence of an inner product $(\ ,\ )$ in the Lie algebra that is positive definite and satisfies the condition (22) of cyclic symmetry.[3] In the considerations below one only needs these properties of the Lie algebra inner product. The results derived below are therefore also valid for the case of only compact Lie algebras, and not only for the case of *both* semisimple and compact Lie algebras.

III. UNIQUENESS THEOREMS IN THE CASES $n=1$ AND $n=2$

A. The one-dimensional case

In the case of one space dimension, the gauge-covariant Poisson equation (1) is fairly trivial. We nevertheless give a brief analysis also of this case for completeness. In one space dimension Eq. (1) becomes the following:

$$\boldsymbol{\nabla}_1(A)\boldsymbol{\nabla}^1(A)\Phi(x) = \mathcal{F}(x), \tag{24}$$

where we now use the notation x instead of x^1 for simplicity.

We then choose a G-valued quantity ω such that

$$A_1^{\omega}(x) \equiv \omega^{-1}(x)A_1(x)\omega(x) + i\left(\frac{d}{dx}\omega^{-1}(x)\right)\omega(x) = 0. \tag{25}$$

The condition (25) is equivalent to the differential equation

$$\frac{d}{dx}\omega(x) = -iA_1(x)\omega(x). \tag{26}$$

For any smooth gauge potential $A_1(x)$, the (matrix) differential equation (26) has a G-valued solution, determined apart from a constant initial value at some appropriate point in R^1. Then, applying a transform of the type given in Eq. (16) to Eq. (24), with the quantity ω determined by Eq. (26), one obtains

$$\frac{d^2}{dx^2}(\omega^{-1}\Phi\omega) = (\omega^{-1}\mathcal{F}\omega). \tag{27}$$

The question of uniqueness of the solution(s) to Eq. (27) is related to the number of solutions of the homogeneous equation corresponding to Eq. (27) under appropriate boundary conditions. The homogeneous equation in question,

$$\frac{d^2}{dx^2}(\omega^{-1}\Phi_h\omega) = 0, \tag{28}$$

has the general solution

$$\Phi_h(x) = \omega(x)\alpha\omega^{-1}(x)x + \omega(x)\beta\omega^{-1}(x), \tag{29}$$

where α and β are arbitrary constant **g**-valued quantities.

If it is required to find solutions $\Phi(x)$ to Eq. (24), which is equivalent to Eq. (27), which grow less rapidly than linearly with x for large x, then the following boundary condition at infinity must hold,

$$\lim_{|x|\to\infty} \frac{1}{x}\|\Phi(x)\|_g = 0. \tag{30}$$

Hence the difference of any two such solutions, which satisfies the homogeneous equation (28), and which is of the form Φ_h given in Eq. (29) above, must satisfy the condition

$$\lim_{|x|\to\infty} \frac{1}{x}\|\Phi_h(x)\|_g = \lim_{|x|\to\infty} \frac{1}{x}\sqrt{(\alpha,\alpha)x^2 + 2(\alpha,\beta)x + (\beta,\beta)} = 0. \tag{31}$$

Thus one must set $\alpha=0$ in Eq. (29). Hence, if a solution to Eq. (24) exists, which satisfies the condition (30), then the solution is unique apart from an additive *covariant constant*, i.e., a solution to the homogeneous equation of the form

$$\Phi_h(x) = \omega(x)\beta\omega^{-1}(x). \tag{32}$$

The solution (32) satisfies the condition of covariant constancy,

$$\boldsymbol{\nabla}_1(A)\Phi_h(x) = 0, \tag{33}$$

as a consequence of the condition (26) which determines the quantity ω.

Likewise, if one requires solutions which vanish at infinity, i.e., which satisfy the conditions

$$\lim_{|x|\to\infty} \|\Phi(x)\|_g = 0, \tag{34}$$

then one must have $\alpha=\beta=0$ in Eq. (29). Thus, if a solution to Eq. (24) exists, which satisfies the condition (34), then the solution is unique.

We can summarize the discussion above as follows.

Theorem 3.1: Assume that the gauge-covariant Poisson equation in one space dimension, Eq. (24), has a solution in the classic sense, i.e., a solution that is twice continuously differentiable in any finite interval in R^1, for a given smooth gauge potential $A_1(x)$ and for a given inhomogeneous term $\mathcal{F}(x)$, satisfying appropriate smoothness and asymptotic conditions in R^1. If such a solution grows less rapidly than linearly with increasing x, i.e., satisfies the condition (30), then the solution is unique apart from an additive covariant constant. Furthermore, if such a solution vanishes asymptotically in the sense of condition (34), then the solution is unique.

B. The two-dimensional case

We will now consider the gauge-covariant Poisson equation (1) in two-dimensional space R^2. We assume that this equation has solutions that are twice continuously differentiable in any finite domain in R^2, for a given smooth gauge potential $\mathbf{(}A_1(x^1,x^2),A_2(x^1,x^2)\mathbf{)}$ and a given inhomogeneous term $\mathcal{F}(x^1,x^2)$, which is supposed to satisfy appropriate smoothness and asymptotic conditions. Let there be two such solutions Φ_A and Φ_B, say. Then their difference,

$$\Phi_C := \Phi_A - \Phi_B, \tag{35}$$

satisfies the gauge-covariant Laplace equation, i.e., the homogeneous equation,

$$\boldsymbol{\nabla}_k(A)\boldsymbol{\nabla}^k(A)\Phi_C(x) = 0, \tag{36}$$

where summation over the space-index k in the range (1, 2) is implied here and in what follows. We then consider the quantity

$$-\nabla^2(\Phi_C,\Phi_C) \equiv \partial_k \partial^k(\Phi_C,\Phi_C). \tag{37}$$

Using the previously established formula (23) and Eq. (36), one obtains

$$-\nabla^2(\Phi_C,\Phi_C) = 2(\boldsymbol{\nabla}_k(A)\Phi_C, \boldsymbol{\nabla}^k(A)\Phi_C). \tag{38}$$

We then express the ∇^2 operator in terms of polar coordinates (r,θ) in the plane R^2,

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}. \tag{39}$$

Integrating equation (38) over the variable θ in the range $(0,2\pi)$ one obtains

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right)\int_0^{2\pi} d\theta(\Phi_C,\Phi_C) = -2\int_0^{2\pi} d\theta(\boldsymbol{\nabla}_k(A)\Phi_C, \boldsymbol{\nabla}^k(A)\Phi_C). \tag{40}$$

We now consider Eq. (40) as an ordinary differential equation for the quantity $\int d\theta(\Phi_C,\Phi_C)$ as if the right-hand side of the equation were a known quantity. The general solution to this equation is then the following:

$$\int_0^{2\pi} d\theta(\Phi_C,\Phi_C) = \alpha \log r + \beta - 2(\log r)\int_0^r dr'\, r' \int_0^{2\pi} d\theta(\boldsymbol{\nabla}_k(A)\Phi_C, \boldsymbol{\nabla}^k(A)\Phi_C) + 2\int_0^r dr'\, r'(\log r') \int_0^{2\pi} d\theta(\boldsymbol{\nabla}_k(A)\Phi_C, \boldsymbol{\nabla}^k(A)\Phi_C), \tag{41}$$

where α and β are real constants.

In view of the assumed smoothness of the gauge potential A and assumed regularity of the solution Φ_C to the original equation (36), in particular in the vicinity of the origin $r=0$ in R^2, one readily concludes that the terms involving integrals in the expression (41) cannot generate logarithmic singularities at $r=0$, which could cancel the term $\alpha \log r$ in that expression. The logarithmic singularity in (41) must be expelled, and this can then only be achieved by setting $\alpha=0$. Hence, the general solution to the equation (40) when the regularity conditions at $r=0$ are taken into account, is

$$\int_0^{2\pi} d\theta(\Phi_C,\Phi_C) = \beta - 2(\log r)\int_0^r dr'\, r'\left(1 - \frac{\log r'}{\log r}\right)\int_0^{2\pi} d\theta(\boldsymbol{\nabla}_k(A)\Phi_C, \boldsymbol{\nabla}^k(A)\Phi_C), \tag{42}$$

where we now can identify the constant β as follows:

$$\beta = \left[\int_0^{2\pi} d\theta(\Phi_C,\Phi_C)\right]_{r=0} = 2\pi \|\Phi_C(0)\|_g^2. \tag{43}$$

We then consider the asymptotic properties of the solutions Φ_C. Let us impose the condition

$$\lim_{r\to\infty} \frac{1}{\log r}\int_0^{2\pi} d\theta(\Phi_C,\Phi_C) = 0. \tag{44}$$

Then Eq. (42) implies that

$$\lim_{r\to\infty} \int_0^r dr'\, r'\left(1 - \frac{\log r'}{\log r}\right)\int_0^{2\pi} d\theta(\boldsymbol{\nabla}_k(A)\Phi_C, \boldsymbol{\nabla}^k(A)\Phi_C) = 0. \tag{45}$$

The vanishing of the integral (45) in the limit $r\to\infty$ implies that the integrand must vanish, since the integrand is nonpositive (for $r>1$) in view of convention (3) and the positive definiteness of the Lie algebra inner product. But then, necessarily,

$$\nabla^k(A)\Phi_C = 0, \quad k = 1,2, \tag{46}$$

i.e., Φ_C is a covariant constant.

We can thus infer from the result above that if the gauge-covariant Poisson equation in R^2 has a twice continuously differentiable solution Φ, such that (Φ,Φ) is dominated by $\log r$ for large values of r, or more precisely, if the solution satisfies an asymptotic condition of the form (44), then the solution is unique apart from an additive covariant constant. Let us note, however, that the existence of a nonzero covariant constant in two (or more) dimensions places certain restrictions on the gauge potential A, which are related to the internal holonomy group.[4]

If one requires a more stringent asymptotic condition on the solutions to the gauge covariant Laplace equation than condition (44), namely the condition

$$\lim_{r\to\infty} \int_0^{2\pi} d\theta(\Phi_C,\Phi_C) \equiv \lim_{r\to\infty} \int_0^{2\pi} d\theta \|\Phi_C\|_g^2 = 0, \tag{47}$$

then Eqs. (42) and (43) imply as before that Eq. (46) is in force, but also that

$$\left[\int_0^{2\pi} d\theta(\Phi_C,\Phi_C)\right]_{r=0} = 0. \tag{48}$$

Taken together, Eqs. (46) and (48) imply that

$$\Phi_C(x^1,x^2) \equiv 0. \tag{49}$$

We have now demonstrated that the only solution to the gauge-covariant Laplace equation in two dimensions that vanishes at spatial infinity in the sense given by Eq. (47), is the identically vanishing solution. This gives rise to a uniqueness theorem for such solutions Φ to the inhomogeneous gauge-covariant Poisson equation, which have a given asymptotic behavior Φ^{as} at spatial infinity, or, more precisely, which satisfy a boundary condition of the form

$$\lim_{r\to\infty} \int_0^{2\pi} d\theta \|\Phi - \Phi^{\mathrm{as}}\|_g = 0. \tag{50}$$

Namely, suppose that there exist two solutions, Φ_A and Φ_B, say, to the gauge-covariant Poisson equation in two dimensions, which satisfy a boundary condition of the form (50) with some appropriate given asymptotic function Φ^{as}. Then their difference Φ_C satisfies the gauge-covariant Laplace equation (36) and the following boundary condition:

$$\begin{aligned} 0 &\leqslant \lim_{r\to\infty} \int_0^{2\pi} d\theta \|\Phi_C\|_g^2 = \lim_{r\to\infty} \int_0^{2\pi} d\theta \|\Phi_A - \Phi_B\|_g^2 = \lim_{r\to\infty} \int_0^{2\pi} d\theta \|(\Phi_A - \Phi^{\mathrm{as}}) - (\Phi_B - \Phi^{\mathrm{as}})\|_g^2 \\ &\leqslant \lim_{r\to\infty} \int_0^{2\pi} d\theta (\|\Phi_A - \Phi^{\mathrm{as}}\|_g + \|\Phi_B - \Phi^{\mathrm{as}}\|_g)^2 = 0. \end{aligned} \tag{51}$$

But then, in accordance with the reasoning above, Eq. (49) must be in force, i.e., $\Phi_A \equiv \Phi_B$. Thus, if a solution to the gauge-covariant Poisson equation in R^2 exists that has a given asymptotic limit in the sense given in Eq. (50), then the solution is unique.

We summarize the results obtained above on the gauge-covariant Poisson equation on R^2 as *Theorem 3.2*.

Theorem 3.2: Assume that the gauge-covariant Poisson equation in two space dimensions has a solution in the classic sense, i.e., a solution that is twice continuously differentiable in any finite domain in R^2, for a given smooth gauge potential $\mathbf{(}A_1(x^1,x^2),A_2(x^1,x^2)\mathbf{)}$ and for a given inhomogeneous term $\mathcal{F}(x^1,x^2)$, satisfying appropriate smoothness and asymptotic conditions in R^2.

If the squared norm $\|\Phi\|_g^2$ of such a solution grows less rapidly than logarithmically with increasing distance from the origin in R^2, i.e., satisfies the condition (44), then the solution is unique apart from an additive covariant constant.

Furthermore, if such a solution has a given asymptotic radial limit Φ^{as} in the sense of condition (50), then the solution is unique.

IV. UNIQUENESS THEOREM IN THE CASES $n \geqslant 3$

The analysis of the uniqueness of solutions to the gauge-covariant Poisson equation (1) in the cases $n \geqslant 3$ proceeds much in the same way as in the two-dimensional case considered in the previous section. Thus, we assume that the equation (1) has at least two solutions: $\Phi_A(x)$ and $\Phi_B(x)$, say, which are twice continuously differentiable in any finite domain in R^n, for any given sufficiently smooth gauge potential $\mathbf{(}A_1(x), A_2(x), \ldots, A_n(x)\mathbf{)}$ and given inhomogeneous term $\mathcal{F}(x)$, which satisfies appropriate smoothness and asymptotic conditions in R^n. We consider the difference $\Phi_C(x)$ of these solutions,

$$\Phi_C(x) = \Phi_A(x) - \Phi_B(x). \tag{52}$$

The function $\Phi_C(x)$ satisfies the gauge-covariant Laplace equation,

$$\sum_{k=1}^{n} \boldsymbol{\nabla}_k(A)\boldsymbol{\nabla}^k(A)\Phi_C = 0, \tag{53}$$

as well as such regularity and asymptotic conditions that follow from those conditions of a similar nature that are supposed to be valid for the solutions $\Phi_A(x)$ and $\Phi_B(x)$. In the equation (53) we have for clarity reinstated the explicit summation over the space index k and continue to use this notation below.

Again, using the previously established formula (23) and the equation (53), one obtains

$$\nabla^2(\Phi_C, \Phi_C) = -2\sum_{k=1}^{n} (\boldsymbol{\nabla}_k(A)\Phi_C, \boldsymbol{\nabla}^k(A)\Phi_C). \tag{54}$$

We then use spherical coordinates[5] on R^n,

$$x^1 = r \sin\theta_{n-1} \ldots \sin\theta_2 \sin\theta_1$$

$$x^2 = r \sin\theta_{n-1} \ldots \sin\theta_2 \cos\theta_1$$

$$\vdots$$

$$x^{n-1} = r \sin\theta_{n-1} \cos\theta_{n-2}$$

$$x^n = r \cos\theta_{n-1}, \tag{55}$$

where

$$r \geqslant 0, \quad 0 \leqslant \theta_1 < 2\pi, \quad 0 \leqslant \theta_k \leqslant \pi, \quad k \neq 1. \tag{56}$$

The Laplace operator ∇^2 expressed in terms of the spherical coordinates above is as follows:

$$\nabla^2 = \frac{1}{r^{n-1}}\frac{\partial}{\partial r}r^{n-1}\frac{\partial}{\partial r} + \frac{1}{r^2 \sin^{n-2}\theta_{n-1}}\frac{\partial}{\partial \theta_{n-1}}\sin^{n-2}\theta_{n-1}\frac{\partial}{\partial \theta_{n-1}} + \frac{1}{r^2 \sin^2\theta_{n-1}\sin^{n-3}\theta_{n-2}}\frac{\partial}{\partial \theta_{n-2}}\sin^{n-3}\theta_{n-2}\frac{\partial}{\partial \theta_{n-2}} + \cdots + \frac{1}{r^2 \sin^2\theta_{n-1}\cdots\sin^2\theta_2}\frac{\partial^2}{\partial \theta_1^2}. \tag{57}$$

We still need the invariant (normalized) measure $d\Omega_n$ on the sphere S^{n-1} in terms of the spherical coordinates above,

$$d\Omega_n = \frac{\Gamma\left(\frac{n}{2}\right)}{2\pi^{n/2}}\sin^{n-2}\theta_{n-1}\ldots\sin\theta_2\, d\theta_1\ldots d\theta_{n-1}. \tag{58}$$

Using the formulas (57) and (58), one obtains the following result from Eq. (54):

$$\frac{1}{r^{n-1}}\frac{\partial}{\partial r}\left(r^{n-1}\frac{\partial}{\partial r}\int d\Omega_n(\Phi_C,\Phi_C)\right) = -2\sum_{k=1}^{n}\int d\Omega_n(\boldsymbol{\nabla}_k(A)\Phi_C,\boldsymbol{\nabla}^k(A)\Phi_C), \tag{59}$$

where the integration over the angular variables $\theta_k, k=1,2,\ldots,n-1$ is over the complete range specified in (56). The equation (59) is now considered an ordinary differential equation for the quantity $\int d\Omega_n(\Phi_C,\Phi_C)$, under the assumption that the right-hand side of Eq. (59) is a known quantity. The general solution to Eq. (59) is then the following:

$$\int d\Omega_n(\Phi_C,\Phi_C) = \alpha r^{2-n} + \beta + \frac{2r^{2-n}}{n-2}\int_0^r dr'\, r'^{n-1}\int d\Omega_n\sum_{k=1}^{n}(\boldsymbol{\nabla}_k(A)\Phi_C,\boldsymbol{\nabla}^k(A)\Phi_C) - \frac{2}{n-2}\int_0^r dr'\, r'\int d\Omega_n\sum_{k=1}^{n}(\boldsymbol{\nabla}_k(A)\Phi_C,\boldsymbol{\nabla}^k(A)\Phi_C), \tag{60}$$

where α and β are so far undetermined real constants.

We now recall that the solutions Φ_C are supposed to be twice differentiable in any finite domain in R^n, in particular, in the vicinity of the origin $r=0$ in R^n. Moreover, the gauge potential A is supposed to be smooth, in particular near $r=0$ in R^n. From these conditions follow the estimates below, valid near $r=0$,

$$\left|\int_0^r dr'\, r'^{n-1}\int d\Omega_n\sum_{k=1}^{n}(\boldsymbol{\nabla}_k(A)\Phi_C,\boldsymbol{\nabla}^k(A)\Phi_C)\right| = O(r^n) \tag{61}$$

and

$$\left|\int_0^r dr'\, r'\int d\Omega_n\sum_{k=1}^{n}(\boldsymbol{\nabla}_k(A)\Phi_C,\boldsymbol{\nabla}^k(A)\Phi_C)\right| = O(r^2). \tag{62}$$

From the esimates (61) and (62) and the equation (60), it then follows that

$$\int d\Omega_n(\Phi_C,\Phi_C) = \alpha r^{2-n} + \beta + O(r^2), \tag{63}$$

in the vicinity of $r=0$. But the solution Φ_C is supposed to be regular, in particular near $r=0$. The singularity at $r=0$ that appears to be present in the general solution (60) must be made to disappear, and this can only happen if

$$\alpha = 0 \tag{64}$$

in Eq. (60), in accordance with the estimate (63). Then it also follows that

$$\beta = \left[\int d\Omega_n(\Phi_C, \Phi_C) \right]_{r=0} = \|\Phi_C(0)\|_g^2. \tag{65}$$

Using the conditions (64) and (65), one then finally obtains the following result:

$$\int d\Omega_n(\Phi_C, \Phi_C) = \|\Phi_C(0)\|_g^2 - \frac{2}{n-2} \int_0^r dr'\, r' \left(1 - \left(\frac{r'}{r} \right)^{n-2} \right) \int d\Omega_n \sum_{k=1}^{n} (\boldsymbol{\nabla}_k(A)\Phi_C, \boldsymbol{\nabla}^k(A)\Phi_C). \tag{66}$$

Let us emphasize that the equation (66) is a relation that is valid for any twice differentiable solution Φ_C to the gauge-covariant Laplace equation (53) with a smooth gauge potential A.

Assume now the following boundary condition at spatial infinity for the solution Φ_C to the gauge-covariant Laplace equation (53),

$$\lim_{r \to \infty} \int d\Omega_n(\Phi_C, \Phi_C) = 0. \tag{67}$$

In view of the convention (3) and the positive definiteness of the inner product (,), the condition (67) and the relation (66) together imply that

$$\boldsymbol{\nabla}^k(A)\Phi_C = 0, \quad k = 1, 2, \ldots, n, \tag{68}$$

and that

$$\|\Phi_C(0)\|_g^2 = 0. \tag{69}$$

But the conditions (68) and (69) then finally imply that

$$\Phi_C \equiv 0. \tag{70}$$

We have thus shown that the only twice differentiable solution Φ_C to the gauge-covariant Laplace equation (53) with a smooth gauge potential A, which vanishes at spatial infinity in the sense of the condition (67), is the identically vanishing solution (70).

The result above gives rise to a uniqueness theorem for the solutions to the gauge-covariant Poisson equation (1) in a space R^n of $n \geqslant 3$ dimensions, just as in the two-dimensional case. Namely, consider the following boundary conditions:

$$\lim_{r \to \infty} \int d\Omega_n \|\Phi - \Phi^{\mathrm{as}}\|_g = 0. \tag{71}$$

As has essentially already been demonstrated in the two-dimensional case, then the difference Φ_C, Eq. (52), of any two solutions Φ_A and Φ_B satisfying the asymptotic condition (71), vanishes at spatial infinity in the sense of Eq. (67). The difference in question also satisfies the gauge-covariant Laplace equation (53), and vanishes therefore identically, as has just been demonstrated above. Hence the solution to the gauge-covariant Poisson equation (1) is unique if one imposes the boundary conditions (71).

We summarize the result above as the following theorem of uniqueness:

Theorem 4: Assume that the gauge-covariant Poisson equation (1) in $n \geqslant 3$ space dimensions has a solution in the classic sense, i.e., a solution that is twice continuously differentiable in any finite domain in R^n, for a given smooth gauge potential $\mathbf{(}A_1(x), A_2(x), \ldots, A_n(x)\mathbf{)}$ and for a given inhomogeneous term $\mathcal{F}(x)$, satisfying appropriate smoothness and asymptotic conditions in R^n. If, furthermore, such a solution has a given asymptotic limit Φ^{as} in the sense of condition (71), then

the solution is *unique*.

V. SUMMARY AND DISCUSSION

In this paper a uniqueness theorem has been proved for the gauge-covariant Poisson equation in n-dimensional space R^n. The theorem has been obtained by considering the homogeneous counterpart of the Poisson equation in question, i.e., the gauge-covariant Laplace equation. It has been shown that the only solution to the gauge-covariant Laplace equation, which is twice continuously differentiable in any finite domain in R^n, and that vanishes at infinity, is the zero solution. This then proves the uniqueness of that solution of the corresponding Poisson equation, which satisfies appropriate conditions of regularity and has a given asymptotic radial limit.

In one or two dimensions the asymptotic conditions can be relaxed; it has been shown that in these cases the solutions, which may be unbounded at infinity, are unique apart from an additive covariant constant, even if one does not specify the asymptotic behavior of the solutions, but merely imposes certain specific limitations on the asymptotic growth of the solutions.

We have not touched upon the question of the existence of solutions in this paper. Such questions have been analyzed in depth in the three-dimensional case in a recent paper by Salmela,[6] who uses modern functional analytic methods in his study. The principal existence theorem proved by Salmela in R^3 is briefly as follows. There exists a weak solution to Eq. (1), which vanishes at infinity, provided that the Lie algebra norms of the potential components A_k are locally square integrable, and provided that the inhomogeneous term $\mathcal{F}(x)$ in that equation satisfies the following condition:

$$\int_{R^3} d^3x(1+|\mathbf{x}|^2)^{(1+\sigma)/2}\|\mathcal{F}\|_g^2 < \infty, \tag{72}$$

where σ is a number that can be chosen in the range $0<\sigma\leqslant 1$. It has further been shown by Salmela that solutions with nontrivial asymptotic behavior also exist under less stringent conditions than condition (72). Namely, if one can construct a function Φ_{as} such that

$$\int_{R^3} d^3x(1+|\mathbf{x}|^2)^{(1+\sigma)/2}\|\mathcal{F}-\boldsymbol{\nabla}_k(A)\boldsymbol{\nabla}^k(A)\Phi_{\text{as}}\|_g^2 < \infty, \tag{73}$$

then Eq. (1) has a weak solution,

$$\Phi(x) = Y(x) + \Phi_{\text{as}}(x), \tag{74}$$

where the quantity Y, which vanishes in the limit $|\mathbf{x}|\to\infty$, satisfies the equation

$$\boldsymbol{\nabla}_k(A)\boldsymbol{\nabla}^k(A)Y(x) = \mathcal{F}(x) - \boldsymbol{\nabla}_k(A)\boldsymbol{\nabla}^k(A)\Phi_{\text{as}}(x). \tag{75}$$

For more details we refer to the aforementioned paper by Salmela,[6] which also contains extensive references to physical applications of the gauge-covariant Poisson equations in R^3.

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A Wannier function made from distributed Gaussians

Hasan Karabulut
Rize Faculty of Arts and Sciences, Physics Department, Karadeniz Technical University, 53100 Rize/Turkey

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A new Wannier function made from distributed Gaussians is reported. Convolution integrals of the Wannier functions are studied and analytical expressions for the convolution integral are given. A new expression for a set of coefficients introduced in an earlier publication [J. Math. Phys. **38**, 4815 (1997)] is derived. Using this new expression, the peculiar behavior of another set of coefficients introduced in the same publication in a particular limit is explained. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1946529]

I. INTRODUCTION

Distributed Gaussians are a set of identical Gaussians positioned with equal intervals. They are widely used as a basis set in variational calculations in molecular vibrations. The widespread use of this basis started in chemical physics computations by an important paper of Hamilton and Light.[1]

The Wannier functions are used in solid-state physics as orthogonal and localized basis sets.[2] One can make Wannier functions from any basis set formed by shifting a localized function at equal intervals. In particular, Wannier[3] reported a set of Wannier functions made from distributed Gaussians. Itakutti *et al.*[4] also reported Wannier functions made from distributed Gaussians, but they constructed them numerically and did not provide analytical expressions for the Gaussian coefficients.

In a paper[5] (hereafter called Paper 1) on distributed Gaussians, we introduced a set of orthogonal functions that are linear combinations of distributed Gaussians and called them distributed Gaussian polynomials. We also introduced a set of Wannier functions made from distributed Gaussians and suggested a general procedure to construct Wannier functions made from distributed Gaussians. At that time it escaped our attention that normalized distributed Gaussian polynomials become a Wannier function set in a particular limit. This is one of the results reported in this paper.

Other than introducing a Wannier function, we also introduced some sets of coefficients in Paper 1.[5] In this paper I study convolution integrals of Wannier functions and as a product of this, I introduce an expression for a set of coefficients called σ_n in Paper 1. Using this result, I explain peculiar behavior of another set of coefficients called $e_n(y)$ in Paper 1 as $y \to 1/4$.

In the next section I list some results from Paper 1 that are needed in the following sections. I felt it necessary to list them to make the new results in the following sections understandable. There are a couple of results that were stated in Paper 1 for a specific case, but here the more general statements are made. One important point that was unnoticed in Paper 1 is also stated in this section. The rest of the section are the results of Paper 1.

In this paper the Gaussians are written as $g_n(x)=\mathrm{e}^{-c^2(x-n)^2}=\mathrm{q}^{(x-n)^2}$, where $q=\mathrm{e}^{-c^2}$ and c^{-1} is related to the width of the Gaussians. In the text we will use mostly expressions with q. But there are some formulas that do not look pretty when c is replaced with $\sqrt{\ln(1/q)}$ in them. So some formulas contain both c and q and when you see them just remember that $q=\mathrm{e}^{-c^2}$.

In the Introduction above "we" refers to myself, Dr. Karabulut, and Professor Sibert, who are the authors of Paper 1. In the rest of the paper, as in a lecturing mode, "we" refers to me, Dr. Karabulut, and the audience.

II. SOME RESULTS GIVEN IN PAPER 1

Consider a chain of Gaussians

$$g_n(x) = g(x-n) = \mathrm{e}^{-c^2(x-n)^2} = \mathrm{q}^{(x-n)^2} \quad (n = 0,1,2,\ldots,\infty), \tag{1}$$

where $q = e^{-c^2}$. A set of orthogonal functions constructed from them was given in Paper 1[5] as

$$\Phi_n(x) = \sum_{k=0}^{n} \frac{(q;q)_n}{(q;q)_k (q;q)_{n-k}} (-1)^k \mathrm{q}^{-k/2} g_k(x); \quad (n = 0,1,2,\ldots,\infty), \tag{2}$$

where

$$(q;q)_k = (1-q)(1-q^2)(1-q^3)\cdots(1-q^k), \tag{3}$$

for $k>0$ and $(q;q)_0 \equiv 1$. We call these functions distributed Gaussian polynomials. They satisfy the recurrence relation[5]

$$\mathrm{q}^{-2x}\Phi_n(x) = d_{n-1}^n \Phi_{n-1}(x) + d_n^n \Phi_n(x) + d_{n+1}^n \Phi_{n+1}(x), \tag{4}$$

where d_{n-1}^n, d_n^n, and d_{n+1}^n are

$$d_{n+1}^n = -q^{-2(n+1/4)}, \tag{5}$$

$$d_n^n = (1+q-q^{n+1})q^{-2(n+1/4)}, \tag{6}$$

$$d_{n-1}^n = -(q-q^{n+1})q^{-2(n+1/4)}. \tag{7}$$

We can make Wannier functions from the distributed Gaussians. Wannier[3] reported one such Wannier function set and another one was reported in Paper 1. Appendix A of Karabulut[6] gives a short account of Bloch and Wannier functions and their properties. A set of Wannier functions made from distributed Gaussians can be written as

$$W_n(x) = \sum_{m=-\infty}^{\infty} c_m g(x-n-m), \tag{8}$$

where the c_m are

$$c_m = \int_0^1 \frac{\mathrm{e}^{\mathrm{i}\Theta(t)}}{\sqrt{Z(t)}} \mathrm{e}^{\mathrm{i}2\pi m t} \mathrm{d}t. \tag{9}$$

Here, $\Theta(t)$ is an arbitrary periodic $(\Theta(t+1)=\Theta(t))$ phase factor and $Z(t)$ is the norm of the unnormalized Bloch function

$$Z(t) = \int_0^1 \left| \sum_{n=-\infty}^{\infty} \mathrm{e}^{i2\pi n t} g(x-n) \right|^2 \mathrm{d}x. \tag{10}$$

Using the Poisson summation formula [cf. Eq. (A1) in Ref. 6] we get the expressions

$$Z(t) = \sqrt{\frac{\pi}{2c^2}} \sum_{n=-\infty}^{\infty} \mathrm{e}^{i2\pi n t} \mathrm{q}^{n^2/2}, \tag{11}$$

$$= \frac{\pi}{c^2} \sum_{n=-\infty}^{\infty} \mathrm{e}^{-2(\pi/c)^2(t-n)^2}. \tag{12}$$

The equality of the middle expression to the last is known as the Jacobi identity, which is simply the Fourier series of the periodic function in the last equation. Note also that $Z(t)$ is periodic with a period unity. An infinite number of different Wannier functions can be constructed from Gaussians. Different choices of the phase factor $\mathrm{e}^{\mathrm{i}\Theta(t)}$ yield different Wannier functions.

From Eq. (9), the c_n are the Fourier coefficients of the periodic function $\mathrm{e}^{\mathrm{i}\Theta(t)}/\sqrt{Z(t)}$. Therefore, if we know the Gaussian coefficients c_n of the Wannier functions, we can obtain the phase factor $\mathrm{e}^{\mathrm{i}\Theta(t)}$ as follows:

$$\mathrm{e}^{\mathrm{i}\Theta(t)} = \sqrt{Z(t)} \sum_{m=-\infty}^{\infty} c_m \mathrm{e}^{-\mathrm{i}2\pi mt}. \tag{13}$$

This function must have a unit modulus

$$\left|e^{\mathrm{i}\Theta(t)}\right|^2 = Z(t) \sum_{n=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}2\pi nt} \xi_n = 1, \tag{14}$$

where the ξ_n are defined as

$$\xi_n = \sum_{m=-\infty}^{\infty} c_m c_{m+n}. \tag{15}$$

The coefficients ξ_n are symmetrical: $\xi_n = \xi_{-n}$. From Eq. (14) it is seen that the ξ_n are the Fourier coefficients of the periodic function $1/Z(t)$. Here, we obtain an interesting result. *Since the $Z(t)$ does not depend on the phase factor $\mathrm{e}^{\mathrm{i}\Theta(t)}$ chosen, the coefficients ξ_n should be independent of the phase factor too, in spite of the fact that the c_n coefficients in the defining relation, Eq. (15), depend on the phase factor. Hence, the ξ_n are the same for all Wannier functions made from Gaussians*. This important point was not stated in Paper 1.

The expression for $Z(t)$ given in Eqs. (11) and (12) and the fact that ξ_n are the Fourier coefficients of $1/Z(t)$ give us an integral representation for the ξ_n

$$\xi_n = \int_0^1 \frac{\mathrm{e}^{-\mathrm{i}2\pi nt}}{Z(t)} \mathrm{d}t = \sqrt{\frac{2c^2}{\pi}} \int_{-1/2}^{1/2} \frac{\cos(2\pi nt)}{\sum_{m=-\infty}^{\infty} \mathrm{q}^{m^2/2} \mathrm{e}^{\mathrm{i}2\pi mt}} \mathrm{d}t. \tag{16}$$

In Paper 1 the Wannier functions $W_n(x) = L_0^+(x-n)/\sqrt{w_\infty}$ were introduced. The $L_0^+(x)$ is given as

$$L_0^+(x) = \sum_{m=-\infty}^{\infty} b_n g(x-n), \tag{17}$$

where b_n are defined as

$$b_n = q^{-1/16} N(q) (-1)^n \mathrm{q}^{(|n|+n/2)} \alpha_n(q), \tag{18}$$

and the factor α_n are

$$\alpha_n(q) = \sum_{j=0}^{\infty} (-1)^j \mathrm{q}^{j(j+2|n|+1)}. \tag{19}$$

The factor $q^{-1/16}N(q)$ is the normalization factor to ensure $L_0^+(1/4) = 1$, which requires

$$q^{-1/16}N(q)\left(\sum_{n=-\infty}^{\infty}(-1)^n q^{(|n|+n/2)}\alpha_n(q)q^{(1/4-n)^2}\right)=1. \tag{20}$$

From this, the factor $N(q)$ is found as

$$N(q)=\left(\sum_{n=-\infty}^{\infty}(-1)^n q^{|n|}\alpha_n(q)q^{n^2}\right)^{-1}. \tag{21}$$

We prefer to define the normalization factor this way because the $N(q)$ will reappear in the formulas in the following sections. The $|n|$ is the absolute value of n. The $L_0^+(x-n)$ were called the "infinite chain Lagrange functions" in Paper 1. They satisfy the Lagrange function property $L_0^+(n+1/4)=\delta_{n0}$. In Paper 1 the w_∞ was defined as "the weights for the infinite chain quadrature," and it was given as

$$w_\infty=\frac{1}{\sum_{n=-\infty}^{\infty}(-1)^n e^{-2(\pi/c)^2 n^2}}. \tag{22}$$

Since $c_n=b_n/\sqrt{w_\infty}$ are the Gaussian coefficients in the Wannier function, the ξ_n coefficients can be expressed as $(\Sigma_{m=-\infty}^{\infty}b_m b_{m+n}\cdot)/w_\infty$. The coefficients $\Sigma_{m=-\infty}^{\infty}b_m b_{m+n}$ were called σ_n in Paper 1 and hence $\sigma_n=w_\infty\xi_n$.

Given a Wannier function $W_0(x)=\Sigma_{n=-\infty}^{\infty}a_n g(x-n)$, from Eq. (13), the $1/\sqrt{Z(t)}$ can be expressed as

$$\frac{1}{\sqrt{Z(t)}}=e^{-i\Phi(t)}\sum_{m=-\infty}^{\infty}a_m e^{-i2\pi mt}, \tag{23}$$

where $\Phi(t)$ is the phase associated with this Wannier function. Setting this for $1/\sqrt{Z(t)}$ and taking the general phase $\Theta(t)=\Phi(t)+\Gamma(t)$ in Eq. (9), we get

$$c_n=\sum_{m=-\infty}^{\infty}a_{n-m}\left(\int_0^1 e^{i\Gamma(t)}e^{i2\pi mt}dt\right). \tag{24}$$

The c_n are Gaussian coefficients of another Wannier function. Choosing $\Gamma(t)$ arbitrarily, we can generate many other Wannier functions. The integral in this expression is calculable for many phase factors $\Gamma(t)$; therefore, if we know one Wannier function Gaussian coefficients we can produce many other Wannier functions using it. Examples were given in Paper 1.

The results in Eqs. (13) and (24) were actually given in Paper 1 for the specific case of $W_n(x)=L_0^+(x-n)/\sqrt{w_\infty}$. But, the statements that they hold for arbitrary Wannier functions were not made in Paper 1.

III. A NEW WANNIER FUNCTION SET MADE FROM DISTRIBUTED GAUSSIANS

In this section we introduce a new Wannier function set made from distributed Gaussians. For this we need to normalize the distributed Gaussian polynomials, which was an important omission in Paper 1.

A. Normalization of the distributed Gaussian polynomials

Consider the integral

$$\int_{-\infty}^{\infty}\Phi_n(x)q^{-2x}\Phi_{n-1}(x)dx=d_n^{n-1}\|\Phi_n\|^2=d_{n-1}^{n}\|\Phi_{n-1}\|^2, \tag{25}$$

where $\|\Phi_n\|^2=\int_{-\infty}^{\infty}\Phi_n^2(x)dx$ and Eq. (4) and the orthogonality are invoked. Writing this as

$$\|\Phi_n\| = \|\Phi_{n-1}\| \sqrt{\frac{d_{n-1}^n}{d_n^{n-1}}}, \tag{26}$$

using the relations in Eqs. (5)–(7), and iterating this relation, we get

$$\|\Phi_n\| = \left(\frac{\pi}{2c^2}\right)^{1/4} q^{-n/2} \sqrt{(q,q)_n}. \tag{27}$$

This relation is useful for obtaining the normalized functions $\Phi_n(x)/\|\Phi_n\|$.

B. The new Wannier functions

The orthonormal functions $\Phi_n(x)/\|\Phi_n\|$ are written as

$$\Phi_n(x)/\|\Phi_n\| = \left(\frac{2c^2}{\pi}\right)^{1/4} \sum_{k=0}^{n} \frac{\sqrt{(q;q)_n}}{(q;q)_k (q;q)_{n-k}} (-1)^k \mathrm{q}^{(n-k)/2} g_k(x). \tag{28}$$

Because of the orthogonality relation the $\Phi_n(x)$ is orthogonal to $\Phi_0(x), \ldots, \Phi_{n-1}(x)$. This means that $\Phi_n(x)$ is orthogonal to all Gaussians $g(x-m)$ for $0 \leqslant m \leqslant n-1$. By shifting the normalized $\Phi_n(x)$ to the left by n (i.e., $\Phi_n(x+n)/\|\Phi_n\|$), we get a function orthogonal to Gaussians $g(x-m)$ with $-n \leqslant m \leqslant -1$. When we take the limit $n \to \infty$, the resulting function becomes orthogonal to all Gaussians centered on the negative integers and it is normalized by construction. In the above equation (28) the sign of the Gaussian centered at $x=n$ is $(-1)^n$. To make it positive, we multiply by $(-1)^n$ before taking the limit. The limit is

$$\Omega^-(x) = \lim_{n\to\infty} (-1)^n \Phi_n(x+n)/\|\Phi_n\|, \tag{29}$$

$$= \frac{(2c^2/\pi)^{1/4}}{\sqrt{(q;q)_\infty}} \sum_{m=0}^{\infty} \frac{(-1)^m}{(q;q)_m} \mathrm{q}^{m/2} g(x+m). \tag{30}$$

This function is orthogonal to all of the Gaussians $g(x-n)$ for $n<0$ and it is normalized.

Now, let us consider the integral

$$\int_{-\infty}^{\infty} \Omega^-(x-n)\Omega^-(x-m)\mathrm{d}x. \tag{31}$$

Since $\Omega^-(x)$ is normalized this integral is unity for $n=m$. For $n \neq m$ let us assume $n>m$ without loss of generality. Then, $\Omega^-(x-n)$ is orthogonal to all the Gaussians $g(x-k)$ for $k<n$. The $\Omega^-(x-m)$ contains Gaussians up to $g(x-m)$ and since $m<n$ the $\Omega^-(x-n)$ is orthogonal to all of them. Therefore, the integral vanishes for $n \neq m$. This argument proves that the $\Omega^-(x-n)$ functions are Wannier functions satisfying

$$\int_{-\infty}^{\infty} \Omega^-(x-n)\Omega^-(x-m)\mathrm{d}x = \delta_{nm}. \tag{32}$$

We have a minus sign on the $\Omega^-(x-n)$ for a purpose. The functions $\Omega^-(x)$ are a linear combination of the Gaussians centered on the negative integers and zero. The mirror symmetry of it, $\Omega^+(x)=\Omega^-(-x)$, is a linear combination of Gaussians centered on the positive integers and zero. The $\Omega^+(x-n)$ also satisfy the orthonormality conditions and they are equally valid Wannier functions. We use $\pm$ superscripts to distinguish them.

$\Omega^\pm(x)$ are related to the q-special functions that mathematicians study. The functions

$$E_q^{(\alpha)}(z) = \sum_{n=0}^{\infty} \frac{q^{\alpha n^2/2}}{(q,q)_n} z^n, \tag{33}$$

are introduced in Floreanini *et al.*[7] and some of their properties are studied in Atakishiyev.[8] They are some form of one parameter q-exponential functions and the $E_q^{(\alpha)}((1-q)z)$ reduces to e^z in the limit $q \to 1$. The Wannier functions constructed above can be expressed in terms of $E_q^{(\alpha)}(z)$ for $\alpha=2$ and $z=-q^{(1/2+2x)}$ as

$$\Omega^-(x) = \frac{(2c^2/\pi)^{1/4}}{\sqrt{(q;q)_\infty}} q^{x^2} E_q^{(2)}(-q^{(1/2+2x)}). \tag{34}$$

We showed that the $\Omega^{\pm}(x)$ are Wannier functions. Now, we can write the corresponding phase factor. The Gaussian coefficients in the $\Omega^+(x)$ are

$$c_n = \begin{cases} (2c^2/\pi)^{1/4}(-1)^n \mathrm{q}^{n/2}/(q;q)_n \sqrt{(q;q)_\infty} & n \geqslant 0 \\ 0 & n < 0 \end{cases}. \tag{35}$$

Then, from Eq. (13) the phase factor can be expressed as

$$\mathrm{e}^{\mathrm{i}\Theta(t)} = \left(\frac{2c^2}{\pi}\right)^{1/4} \sqrt{\frac{Z(t)}{(q;q)_\infty}} \sum_{m=0}^{\infty} (-1)^m \frac{\mathrm{q}^{m/2}}{(q;q)_m} \mathrm{e}^{-\mathrm{i}2\pi m t}. \tag{36}$$

From Eqs. (15) and (35), the ξ_n coefficients are expressed as

$$\xi_n = \sqrt{\frac{2c^2}{\pi}} \frac{(-1)^n}{(q;q)_\infty} \mathrm{q}^{|n|/2} \sum_{m=0}^{\infty} \frac{\mathrm{q}^m}{(q;q)_m (q;q)_{m+|n|}}. \tag{37}$$

The phase factor for the $\Omega^-(x)$ is the complex conjugate of the phase of $\Omega^+(x)$.

IV. THE CONVOLUTION INTEGRAL AND A NEW EXPRESSION FOR THE ξ_n COEFFICIENTS

Consider the convolution integral of the Wannier functions

$$I_q(z) = \int_{-\infty}^{\infty} W_0(x) W_0(x+z) \mathrm{d}x, \tag{38}$$

$$= \sqrt{\frac{\pi}{2c^2}} \sum_{n=-\infty}^{\infty} \xi_n \mathrm{q}^{(z-n)^2/2}. \tag{39}$$

Since the ξ_n is independent of the phase factor $\mathrm{e}^{\mathrm{i}\Theta(t)}$, the $I_q(z)$ is the same for all of the Wannier functions made from Gaussians. The Fourier transforms of $I_q(z)$ and $W_0(x)$ are

$$I_q^F(k) = \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}kz2\pi} I_q(z) \mathrm{d}z \tag{40}$$

$$W_0^F(k) = \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}kx2\pi} W_0(x) \mathrm{d}x. \tag{41}$$

From the convolution theorem of Fourier transforms, we have

$$I_q^F(k) = |W_0^F(k)|^2. \tag{42}$$

For a given localized function $u(x)$, the function set $u(x/d-n)$ for $(n=-\infty,\ldots,\infty)$ is called a distributed basis set made from $u(x)$. Here, d is the distance between the basis functions. In a recent paper Karabulut[6] has introduced a quantity $r(k,d)$ called the representation power, which is an effective measure of the ability of a distribution basis set to span a given function. The $r(k,d)$ turns out to be equal to $|W_0^F(kd)|^2$, where the $W_0^F(k)$ is the Fourier transform of the Wannier function made from the $u(x-n)$, $(n=-\infty,\ldots,\infty)$ set. Since the $r(k,d)$ is a property of the basis function $u(x)$ itself, it is absolutely necessary that $|W_0^F(k)|^2$ be independent of the phase factor $e^{i\Theta(t)}$. The $I_q^F(kd)$ is actually the representation power $r(k,d)$ and it is a very important quantity in the formalism presented in Karabulut.[6]

After these remarks about the significance of the convolution integral, we will derive three different representations for the $I_q(z)$. This function must have zeros at all the nonzero integers due to the orthogonality of Wannier functions, and it is a linear combination of Gaussians with a different width. It must be unity at $z=0$ due to the normalization of the Wannier functions. Since such Gaussians are a polynomial of $q^{-z}=e^{c^2z}$, we can immediately write an infinite product representation

$$I_q(z)=q^{z^2/2}\prod_{n=1}^{\infty}\left(\frac{q^{-z}-q^{-n}}{1-q^{-n}}\right)\left(\frac{q^{z}-q^{-n}}{1-q^{-n}}\right). \tag{43}$$

This product is a linear combination of Gaussians and it vanishes at all nonzero integers. It takes unity value for $z=0$. It is also symmetrical just like $I_q(z)$ is due to the symmetry of the ξ_n coefficients. So, it is the right function.

Another function that has the right zeros can be expressed as

$$I_q(z)=\kappa\frac{\sum_{n=-\infty}^{\infty}(-1)^n q^{(z-n-1/2)^2/2}}{q^{-z/2}-q^{z/2}}. \tag{44}$$

The coefficient κ is chosen to satisfy $I_q(0)=1$. This function also satisfies all of the properties of the $I_q(z)$ and, although it may not be obvious at first glance, it is also a linear combination of Gaussians centered at integers. To find the coefficients, we equate

$$\sum_{n=-\infty}^{\infty}h_n q^{(z-n)^2/2}=\frac{\sum_{n=-\infty}^{\infty}(-1)^n q^{(z-n-1/2)^2/2}}{q^{-z/2}-q^{z/2}}, \tag{45}$$

to obtain the following difference equation for the h_n:

$$h_{n-1}q^{-(n-1/2)}-h_n=(-1)^{n+1}q^{1/8}q^{-n/2}. \tag{46}$$

Solving this and putting it back into Eq. (44) we can write the $I_q(z)$ as

$$I_q(z)=N(\sqrt{q})\sum_{n=-\infty}^{\infty}(-1)^n\alpha_n(\sqrt{q})q^{|n|/2}q^{(z-n)^2/2}, \tag{47}$$

where the $N(q)$ is the function introduced in Eq. (21). The factor $N(\sqrt{q})$ ensures the normalization condition $I_q(0)=1$. Comparing this to Eq. (39), we find

$$\xi_n=\sqrt{\frac{2c^2}{\pi}}N(\sqrt{q})(-1)^n\alpha_n(\sqrt{q})q^{|n|/2}. \tag{48}$$

This is the explicit expression for the ξ_n coefficients we are looking for. The $\alpha_n(q)$ coefficients rapidly approach unity as $|n|$ gets larger. Hence, ξ_n decays as $q^{|n|/2}$ for large $|n|$ values. This result is not transparent from the other definition of ξ_n in Eq. (15).

It is interesting that the infinite chain Lagrange functions given in Eqs. (17), (18), (19), and (21) can be written as

$$L_0^+(x) = \mathrm{q}^{(x-1/4)/2} I_{q^2}(x - 1/4). \tag{49}$$

This is due to the fact that they both are square integrable functions having equally spaced zeros. For a function made from a linear combination of distributed Gaussians, once we fix the positions of zeros as $x_n = n + \delta$, where $-1/2 < \delta < 1/2$ and $n \neq 0$, and require that the function is square integrable, it is fixed up to a normalization factor. In the above formula the $\delta = 1/4$ for $L_0^+(x)$ and zero for $I_{q^2}(x)$. All such normalizable functions with equally spaced zeros can be expressed as $(\mathrm{const})\mathrm{q}^{2\delta(x-\delta)} I_{q^2}(x-\delta)$.

There are some identities we can derive from the ξ_n expression given in Eq. (48). Comparing Eq. (48) with Eq. (16), we get an interesting identity

$$\int_{-1/2}^{1/2} \frac{\cos(2\pi n t)}{\sum_{m=-\infty}^{\infty} q^{m^2/2} \mathrm{e}^{\mathrm{i}2\pi m t}} \mathrm{d}t = N(\sqrt{q})(-1)^n \alpha_n(\sqrt{q}) q^{|n|/2}. \tag{50}$$

Comparing Eqs. (48) and (37), we obtain

$$\sum_{m=0}^{\infty} \frac{q^m}{(q;q)_m (q;q)_{m+|n|}} = N(\sqrt{q})(q;q)_\infty \alpha_n(\sqrt{q}). \tag{51}$$

Finally, taking $n \to \infty$ limit of the above equation we obtain

$$\sum_{m=0}^{\infty} \frac{q^m}{(q;q)_m} = N(\sqrt{q})((q;q)_\infty)^2. \tag{52}$$

There is also another representation for the $I_q(z)$ function which shows how the $I_q(z)$ behaves. The nominator of Eq. (45) is periodic with period two, and it can be expressed as a Fourier series. The Fourier coefficients can be evaluated with the help of the Poisson summation formula. Then, we get another representation for the $I_q(z)$ as

$$I_q(z) = G(z)/G(0), \tag{53}$$

where the $G(z)$ is

$$G(z) = \sum_{n=0}^{\infty} (-1)^n \frac{\sin(2n+1)\pi z}{\sinh(c^2 z/2)} \mathrm{e}^{-(2n+1)^2 \pi^2 / 2c^2}, \tag{54}$$

and the $G(0)$ is

$$G(0) = \frac{2\pi}{c^2} \sum_{n=0}^{\infty} (-1)^n (2n+1) \mathrm{e}^{-(2n+1)^2 \pi^2 / 2c^2}. \tag{55}$$

For low values of c ($c < 1$ for example), only the $n = 0$ term is significant. For $c = 1$ the ratio of the $n = 1$ term to the $n = 0$ term is of order $\mathrm{e}^{-4\pi^2}$ and the second and higher terms are totally negligible. Therefore, the $I_q(z)$ is

$$I_q(z) \approx \frac{c^2}{2\pi} \frac{\sin \pi z}{\sinh(c^2 z/2)}, \tag{56}$$

to a high accuracy. The $I_q(z)$ decays as $\mathrm{e}^{-c^2|z|/2}$ asymptotically and in the limit $c \to 0$ ($q \to 1$) it approaches $\sin(\pi z)/\pi z$.

V. THE BEHAVIOR OF THE $e_n(y)$ COEFFICIENTS

Consider the sum

$$R(x,y) = \sum_{n=-\infty}^{\infty} \frac{L_0^+(x-n)}{\sqrt{w_\infty}} \frac{L_0^+(y-n)}{\sqrt{w_\infty}}, \tag{57}$$

$$= \frac{1}{w_\infty} \sum_{m=-\infty}^{\infty} e_m(y) \mathrm{q}^{(x-m)^2}, \tag{58}$$

where $e_n(y)$ is given as

$$e_n(y) = w_\infty \sum_{m=-\infty}^{\infty} \xi_m \mathrm{q}^{(y+m-n)^2}. \tag{59}$$

Let us recall at this point that $L_0^+(x)/\sqrt{w_\infty}$ is a Wannier function. Because of the Lagrange function property $L_0^+(n+1/4)=\delta_{n0}$ of the infinite chain Lagrange functions $L_0^+(x-n)$, if we set $y=1/4$ in the $R(x,y)$ only the $n=0$ term is nonzero and we get $L_0^+(x)/w_\infty$ result for the sum. Since the Gaussian coefficients of $L_0^+(x)$ are the b_n coefficients given in Eqs. (18), (19), and (21), the $e_n(y)$ coefficients approach the b_n coefficients as $y \to 1/4$. The b_n coefficients decay three times faster exponentially for positive indices than negative indices, and the $L_0^+(x)$ is an asymmetric function. The slower exponent (for $n<0$) is $-c^2|n|/2$ and the faster exponent (for $n>0$) is $-3c^2n/2$, as can be seen from Eq. (18). The $\ln|e_n(y)|$ coefficients versus n for $y=0.24$, $y=0.2499$, and $y=0.249\,999$ was plotted in Paper 1 (Fig. 1), and from the graph it was clear that for $n>0$ the $|e_n(y)|$ decays with the faster exponent for some time and after a visibly sharp turning point it starts decaying with the slower exponent. The turning point goes to infinity as $y \to 1/4$, and exactly at $y=1/4$ it decays with the faster exponent for all $n>0$. We (the authors) were not able to explain this behavior in Paper 1 because our new expression for the ξ_n coefficients was not available. Now that it is available, let us explain.

Consider the $e_n(y)$ coefficients

$$e_n(y) = w_\infty N(\sqrt{q}) \sum_{m=-\infty}^{\infty} (-1)^n \alpha_m(\sqrt{q}) \mathrm{q}^{|m|/2} \mathrm{q}^{(y+m-n)^2}, \tag{60}$$

for $n \gg 1$ and $y \approx 1/4$. Here, the constant $w_\infty N(\sqrt{q})$ is unimportant to the discussion. For large n, only m values near n contribute significantly. For large m values only the first two terms of the $\alpha_m(\sqrt{q})$ expansion

$$\alpha_m(\sqrt{q}) = 1 - \mathrm{q}^{|m|+1} + \text{higher order}, \tag{61}$$

are important. Then, the $e_n(y)$ can be written as

$$e_n(y) = w_\infty N(\sqrt{q}) \sum_{m=-\infty}^{\infty} (-1)^n \mathrm{q}^{|m|/2} \mathrm{q}^{(y+m-n)^2} \tag{62}$$

$$- w_\infty N(\sqrt{q}) q \sum_{m=-\infty}^{\infty} (-1)^n \mathrm{q}^{3|m|/2} \mathrm{q}^{(y+m-n)^2} + \text{H.O.}, \tag{63}$$

where H.O. stands for higher order terms. Now, since we assume that $n \gg 1$, the terms with negative values of m are order of $\mathrm{q}^{n^2/2}$ smaller than the terms making the main contribution around $m \approx n$. Therefore, replacing $\mathrm{q}^{|m|/2}$ and $\mathrm{q}^{3|m|/2}$ with $\mathrm{q}^{m/2}$ and $\mathrm{q}^{3m/2}$ we make an error of order $\mathrm{q}^{n^2/2}$, which is insignificant for large n but makes the sums manageable. We also expand the Gaussians

as $q^{(y+m-n)^2}=q^{y^2}q^{2y(m-n)}q^{(m-n)^2}$ and change the summation index from m to $m\rightarrow m+n$. Then, $e_n(y)$ becomes

$$e_n(y)\approx\left(w_\infty N(\sqrt{q})q^{y^2}\sum_{m=-\infty}^{\infty}(-1)^m q^{(1+4y)m/2}q^{m^2}\right)(-1)^n q^{n/2}$$
$$-\left(w_\infty N(\sqrt{q})q^{y^2+1}\sum_{m=-\infty}^{\infty}(-1)^m q^{(3/2+4y)m/2}q^{m^2}\right)(-1)^n q^{3n/2}+\text{H.O.} \tag{64}$$

The sum in the first parenthesis vanishes as $y\rightarrow 1/4$. To see this, consider the Jacobi triple product formula[9]

$$\sum_{n=-\infty}^{\infty}x^n q^{n^2}=\prod_{n=0}^{\infty}(1-q^{2n+2})(1+xq^{2n+1})(1+x^{-1}q^{2n+1}), \tag{65}$$

where $|q|<1$. If we take $x=-q^{(1+4y)/2}$, then the sum in the first parenthesis of Eq. (64) can be written as an infinite product. The term $(1+x^{-1}p^{2n+1})$ for $n=0$ becomes $(1-q^{(1-4y)/2})$, and this vanishes as $y\rightarrow 1/4$. Therefore, all other terms in the product can be seen as a constant factor when $y\approx 1/4$. The sum in the second parenthesis in Eq. (64) does not vanish for $y=1/4$; therefore, the entire sum can be taken as another constant for $y\approx 1/4$. The $e_n(y)$ can be written as

$$e_n(y)\approx[K_1(1-q^{(1-4y)/2})q^{n/2}+K_2 q^{3n/2}](-1)^n+\text{H.O.} \tag{66}$$

$$\approx[K_1(c^2/2)(1-4y)q^{n/2}+K_2 q^{3n/2}](-1)^n+\text{H.O.} \tag{67}$$

Here, K_1 and K_2 are two constants. In the second expression above, we took the Taylor series expansion of $q^{(1-4y)/2}$ and ignored the terms beyond the first two.

When y is very close to $1/4$, the second term dominates for the lower values of n but, as n gets larger, the first term begins to dominate. The higher order terms decay faster than $q^{3n/2}$ exponentially and they quickly die out, leaving the race between the two terms given above. Therefore, the $\ln(|e_n(y)|)$ versus n graph is a straight line for lower values of n with a slope $-3c^2/2$. After a visibly sharp turning point the graph becomes another straight line with a slope $-c^2/2$. This graph was given in Paper 1 (Fig. 1) without an explanation to why it behaves that way. Here, we have a clear explanation.

The turning point occurs for the n value where the two terms are approximately equal. This happens at $n\approx-\ln(|K_1c^2(1-4y)/2K_2|)/c^2$, which says that the turning point increases linearly with $-\ln(|1-4y|)/c^2$. Therefore, as $y\rightarrow 1/4$, the turning point goes to infinity, and exactly at $y=1/4$ the $e_n(y)$ decays with the faster exponent for all positive indices. The logarithmic dependence of the turning point to $|1-4y|$ explains why the turning point moves so slowly as $y\rightarrow 1/4$, which was clear from Fig. 1 given in Paper 1.

VI. SUMMARY

In this paper we obtained a new expression for the integrals of the squared distributed Gaussian polynomials and showed how to normalize them, a result that was missing in Paper 1. Using the normalized distributed Gaussian polynomials, we took a particular limit of them and constructed a new Wannier function set made from distributed Gaussians. There are only three Wannier functions made from distributed Gaussians in the literature to our knowledge; the one constructed by Wannier,[3] the one reported in Paper 1[5] as the normalized infinite chain Lagrange functions $(L_0^{\pm}(x-n)/\sqrt{w_\infty})$, and the one presented in this paper $(\Omega^{\pm}(x))$.

In addition to reporting a new Wannier function, we studied convolution integral of the Wannier functions and found three different representations for it. We have also presented a new expression for the ξ_n coefficients. The new expression is simpler in appearance than the first

prescription $\Sigma_{m=-\infty}^{\infty} c_{n+m} c_m$, and it also gives the asymptotic behavior of the ξ_n coefficients which is not easy to see from the $\Sigma_{m=-\infty}^{\infty} c_{n+m} c_m$ summation. The new expression also made it possible to explain the peculiar behavior of the $e_n(y)$ coefficients as $y \to 1/4$.

We also found some identities given in Eqs. (50), (51), and (52) as a result of discovery of a new Wannier function. They seem to result from the fact that the distributed Gaussians can be written as polynomials, and there is a quadrature to integrate Gaussians on an infinite chain. We leave it to mathematicians to assess the significance of these strange identities.

Using the Gaussian coefficients of the three reported Wannier functions and using the result stated in Eq. (24), one can construct many Wannier function sets depending on arbitrary number of parameters. Of course the target in this game is to construct the Wannier functions with the desired properties. I have been searching for the Wannier functions made from distributed Gaussians that satisfy

$$\int_{-\infty}^{\infty} W_n(x) \mathrm{e}^{2c^2 \eta x} W_m(x) \mathrm{d}x = \mathrm{e}^{2c^2 \eta (n+\epsilon(\eta))} \delta_{nm}, \tag{68}$$

in addition to the usual orthogonality condition

$$\int_{-\infty}^{\infty} W_n(x) W_m(x) \mathrm{d}x = \delta_{nm}. \tag{69}$$

The normalized infinite chain Lagrange functions $W_n(x) = L_0^+(x-n)/\sqrt{w_\infty}$ reported in Paper 1 is an example of this for $\eta = 1$ and $\epsilon(\eta) = 1/4$. I have not been able to find them for a general η value. In addition to the beauty of the mathematics involved, they are related to the discrete variable representation methods used in chemical physics calculations and hence they might have some practical value.

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Four-dimensional indefinite Kähler Osserman manifolds

Eduardo García-Río[a)]
Faculty of Mathematics, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain

Zoran Rakić[b)]
Faculty of Mathematics, University of Belgrade, Studentski trg 16, pp. 550, 11001 Belgrade, Serbia & Montenegro

M. E. Vázquez-Abal[c)]
Faculty of Mathematics, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain

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It is shown that a four-dimensional Kähler metric is pointwise Osserman if and only if it is either of constant holomorphic sectional curvature or a Ricci flat complex surface. Examples of Kähler Osserman metrics with nilpotent Jacobi operators of all possible degrees are given. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1938727]

I. INTRODUCTION

Pseudo-Riemannian metrics of signature other than Lorentzian and more specially, Ricci-flat indefinite Kähler metrics have received considerable attention in mathematical physics, mainly since the work of Ooguri and Vafa.[19] Indefinite Kähler Einstein metrics on complex surfaces have been classified by Petean[21] and more recently scalar flat indefinite Kähler surfaces have been considered by Kamada.[14] A classification of four-dimensional Lie groups admitting Ricci flat indefinite Kähler metrics have been obtained by Ovando.[20]

To a large extent, the geometry of a pseudo-Riemannian manifold (M,g) is the study of the curvature $R \in \otimes^4 T^*M$ which is defined by the Levi-Civita connection ∇. A pseudo-Riemannian manifold (M,g) is said to be *Osserman* if the eigenvalues of the Jacobi operators are constant on the unit pseudo-sphere bundles $S^{\pm}(M)$. Any two-point homogeneous space is Osserman and the converse is true in the Riemannian ($\dim M \neq 16$) and Lorentzian settings.[7,17,18,2,9] However there exist many nonsymmetric Osserman pseudo-Riemannian metrics in other signatures (cf. Refs. 10 and 12) and even symmetric Osserman spaces which are not of rank-one.[11,22] Moreover, besides the results in Refs. 3 and 11 a description of all four-dimensional Osserman metrics is not yet complete in dimension four.[5,15]

An algebraic curvature tensor in a four-dimensional vector space is Osserman if and only if it is Einstein self-dual for some orientation. Since self-duality and anti-self-duality are well understood in the Kähler setting, we obtain in Sec. II a complete description of the Osserman algebraic curvature tensors which may be Kähler for some complex structure. Based on those results, we show in Sec. III that a pointwise Osserman four-dimensional Kähler metric is either of constant holomorphic sectional curvature or Ricci flat. This should be contrasted with the general situation, where Osserman metrics exist whose Jacobi operators are nondiagonalizable with eigenvalues $\alpha = 4\beta \neq 0$.[8] Finally, part of Sec. III is dedicated to the construction of Osserman Kähler metrics, showing that all possible degrees of nilpotency of the Jacobi operators are realized at the differentiable level.

[a)]Electronic mail: xtedugr@usc.es
[b)]Electronic mail: zrakic@matf.bg.ac.yu
[c)]Electronic mail: meva@zmat.usc.es

II. KÄHLER OSSERMAN ALGEBRAIC CURVATURE TENSORS

Here we will work in the pure algebraic level. Let V be a four-dimensional real vector space. Let $\mathcal{R}(V)\subset\otimes^4 V^*$ be the space of all *algebraic curvature tensors*, i.e., those tensors R having the symmetries of the curvature tensor R:

$$\begin{aligned} &R(x,y,z,w)=R(z,w,x,y)=-R(y,x,z,w),\\ &R(x,y,z,w)+R(y,z,x,w)+R(z,x,y,w)=0. \end{aligned} \tag{1}$$

If V is equipped with an indefinite inner product $\langle,\rangle$, then the Ricci and scalar curvatures of R are defined by

$$\mathrm{Ric}(x,y)=\mathrm{tr}(z\mapsto R(x,z)y),\quad \mathrm{Sc}=\mathrm{tr}\,\mathrm{Ric},$$

where the traces are considered with respect to $\langle,\rangle$. Moreover, the Weyl conformal curvature W is given by

$$\begin{aligned} W(x,y,z,w)=R(x,y,z,w)&+\frac{\mathrm{Sc}}{12}\{g(x,z)g(y,w)-g(y,z)g(x,w)\}\\ &-\frac{1}{2}\{\mathrm{Ric}_0(x,z)g(y,w)-\mathrm{Ric}_0(y,x)g(x,w)+g(x,z)\mathrm{Ric}_0(y,w)-g(y,x)\mathrm{Ric}_0(x,w)\}, \end{aligned}$$

where Ric_0 denotes the traceless Ricci tensor,

$$\mathrm{Ric}_0(x,y)=\mathrm{Ric}(x,y)-\frac{\mathrm{Sc}}{4}g(x,y).$$

Considering the algebraic curvature tensor R as an endomorphism of $\Lambda^2(V)$, we have the following well-known $O(2,2)$-decomposition

$$R\equiv\frac{\mathrm{Sc}}{12}\mathrm{Id}_{\Lambda^2(V)}+\frac{1}{2}\mathrm{Ric}_0+W{:}\Lambda^2(V)\to\Lambda^2(V). \tag{2}$$

Further if V is equipped with an orthogonal *complex structure* J, i.e., a linear endomorphism satisfying $J^2=-\mathrm{id}$ and $\langle Jx,Jy\rangle=\langle x,y\rangle$, a preferred orientation is given to $(V,J,\langle,\rangle)$ and the Hodge star operator $*:\Lambda^2(V)\to\Lambda^2(V)$ is defined by $\alpha\wedge *\beta=\langle\alpha,\beta\rangle$ vol for arbitrary two-forms α and β, where vol is the volume form of V and $\langle,\rangle$ denote the inner product on $\Lambda^2(V)$ induced from that in V. Since the inner product is of signature $(--++)$, $\Lambda^2(V)$ splits as $\Lambda^2(V)=\Lambda^2_+\oplus\Lambda^2_-$, where $\Lambda^2_\pm$ denotes the ±1-eigenspaces of the Hodge star operator, that is $\Lambda^2_\pm=\{\alpha\in\Lambda^2(V)/*\alpha=\pm\alpha\}$. Then we have a further splitting for the Weyl curvature tensor and (2) becomes

$$R\equiv\frac{\mathrm{Sc}}{12}\mathrm{Id}_{\Lambda^2(V)}+\frac{1}{2}\mathrm{Ric}_0+W_+ +W_-, \tag{3}$$

where $W_\pm=\frac{1}{2}(W\pm *W)$.

An algebraic curvature tensor on an oriented vector space is said to be *self-dual* (respectively, *anti-self-dual*) if $*W=W$, that is $W_-=0$ (respectively, $*W=-W$, that is $W_+=0$).[15] Self-dual algebraic curvature tensors are of interest when considering Osserman-type properties in view of the following

Theorem 1 (Refs. 1 and 13): *Let R be an algebraic curvature tensor on a four-dimensional vector space $(V,\langle,\rangle)$. The following are equivalent*

(i) *R is Osserman.*
(ii) *There is a choice of orientation on V such that R is Einstein self-dual.*

As a matter of notation, an algebraic curvature tensor on a Hermitian vector space $(V,J,\langle,\rangle)$ is

said to be a *Kähler algebraic curvature tensor* if and only if it satisfies

$$R(x,y,Jz,Jw) = R(Jx,Jy,z,w) = R(x,y,z,w). \tag{4}$$

Let $\{e_1,e_2,e_3,e_4\}$ be an orthonormal basis of $(V,J,\langle,\rangle)$ such that $Je_1=e_2$, $Je_3=e_4$ and, as a convention, we will assume e_1 and e_2 to be timelike while e_3 and e_4 are spacelike vectors. Now, local basis of the spaces of self-dual and anti-self-dual two-forms can be constructed as

$$\Lambda^2_{\pm} = \langle\{E_1^{\mp},E_2^{\mp},E_3^{\mp}\}\rangle,$$

where

$$E_1^{\mp} = \frac{e^1\wedge e^2 \mp e^3\wedge e^4}{\sqrt{2}},\ E_2^{\mp} = \frac{e^1\wedge e^3 \mp e^2\wedge e^4}{\sqrt{2}},\ E_3^{\mp} = \frac{e^1\wedge e^4 \pm e^2\wedge e^3}{\sqrt{2}}.$$

Observe that the induced metric on $\Lambda^2_{\pm}$ is of signature $(+--)$, in opposition to the positive definite case. Indeed $\langle E_1^{\mp},E_1^{\mp}\rangle=1$, $\langle E_2^{\mp},E_2^{\mp}\rangle=-1$, $\langle E_3^{\mp},E_3^{\mp}\rangle=-1$.

Denote by Ω the Kähler two-form associated to the indefinite Hermitian structure $(V,J,\langle,\rangle)$, defined by $\Omega(x,y)=\langle Jx,y\rangle$. Observe that with respect to the orthonormal basis above the Kähler form is given by $\Omega=-e^1\wedge e^2+e^3\wedge e^4$, which shows that Ω is a spacelike anti-self-dual two-form. It is worth remarking here that Ω and J induce opposite orientations on V in the $(--++)$-setting, while the orientations agree and Ω is a self-dual form in the positive definite case. Now, a characterization of Osserman Kähler algebraic curvature tensors can be obtained from Theorem 1 as follows.

Theorem 2: *Let R be an algebraic curvature tensor on a four-dimensional neutral vector space $(V,\langle,\rangle)$. Then R is Kähler Osserman with respect to some orthogonal complex structure J on V if and only if one of the following hold*

(i) R is an Einstein anti-self-dual algebraic curvature tensor, i.e.,

$$R = \frac{\mathrm{Sc}}{12}\mathrm{Id}_{\Lambda^2(V)} + W_-, \quad \textit{where } W_- = \frac{\mathrm{Sc}}{12}\begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

(ii) R is a Ricci flat self-dual algebraic curvature tensor, i.e.,

$$R = \begin{pmatrix} W_+ & 0 \\ 0 & 0 \end{pmatrix}.$$

Moreover, an algebraic curvature tensor as in (i) determines a unique Kähler two-form, defined by the eigenspace corresponding to the distinguished eigenvalue of W_-, but algebraic curvature tensors given by (ii) are Kähler with respect to any positively oriented complex structure.

Proof: Recall from Theorem 1 that R is Osserman if and only if it is Einstein and self-dual or anti-self-dual. In the special framework of four-dimensional Kähler geometry the self-duality and anti-self-duality conditions are quite well understood. First of all recall that since the metric is indefinite of signature $(--++)$, the anti-self-dual part of a Kähler algebraic curvature tensor satisfies

$$W_- = \frac{\mathrm{Sc}}{12}\begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

which shows that a Kähler algebraic curvature tensor is self-dual if and only if the scalar curvature vanishes. Hence, a self-dual Kähler algebraic curvature tensor is Osserman if and only if it is Ricci flat.

Recall that the space $\Lambda^2(V)$ on a neutral Hermitian vector space $(V,J,\langle,\rangle)$ decomposes into the J-invariant and J-anti-invariant subspaces $\Lambda^2(V)=\Lambda^{\text{inv}}\oplus\Lambda^{\text{anti}}$, where

$$\Lambda^{\text{inv}}=\{\alpha\in\Lambda^2(V)/\alpha(Jx,Jy)=\alpha(x,y)\},$$

$$\Lambda^{\text{anti}}=\{\alpha\in\Lambda^2(V)/\alpha(Jx,Jy)=-\alpha(x,y)\}.$$

Then $\Lambda^2(V)=\Lambda^2_+\oplus\Lambda^2_-$ also decomposes as

$$\Lambda^2_+=\Lambda^{\text{inv}}_0,\ \Lambda^2_-=\mathbb{R}\Omega\oplus\Lambda^{\text{anti}},$$

where Λ^{inv}_0 denotes the J-invariant two-forms orthogonal to Ω. Considering the induced map $J:\Lambda^2(V)\to\Lambda^2(V)$ defined by $J(x\wedge y)=Jx\wedge Jy$, an algebraic curvature tensor $R:\Lambda^2(V)\to\Lambda^2(V)$ is Kähler, i.e., it satisfies (4), if and only if $R\circ J=R$.

Hence, if a Kähler algebraic curvature tensor is self-dual, then it follows from (3) that the whole algebraic curvature tensor becomes

$$R=\begin{pmatrix}W_+ & 0\\ 0 & 0\end{pmatrix} \tag{5}$$

and any such algebraic curvature tensor is invariant by $J:\Lambda^2(V)\to\Lambda^2(V)$, and thus Kähler for any positively oriented orthogonal complex structure.

For a non-Ricci-flat Kähler algebraic curvature tensor, the Osserman condition is equivalent to anti-self-duality, i.e., $W_+=0$. Now, note that the self-dual part of the Weyl curvature tensor in neutral signature $(--++)$ represents the Bochner tensor,[5] and thus R is a Bochner-flat Einstein algebraic curvature tensor, from where it immediately follows that R is of constant holomorphic sectional curvature. Moreover, any algebraic curvature tensor given as in (i) is Kähler with respect to an orthogonal complex structure if and only if J is defined by the distinguished eigenvalue of W_-. □

Remark 3: A Ricci-flat Kähler Osserman algebraic curvature tensor is determined by the Jordan normal form of W_+. Moreover, since the induced inner product on $\Lambda^2_\pm$ is of Lorentzian signature, four different possibilities may occur for the self-dual curvature operator $\langle\hat{W}_+\alpha,\beta\rangle=W_+(\alpha,\beta)$ as follows (cf. Ref. 3)

(Ia) The self-dual curvature operator $\hat{W}_+$ is diagonalizable, i.e.,

$$\hat{W}_+=\begin{pmatrix}b+c & 0 & 0\\ 0 & -b & 0\\ 0 & 0 & -c\end{pmatrix}.$$

(Ib) The self-dual curvature operator $\hat{W}_+$ has a complex eigenvalue, i.e.,

$$\hat{W}_+=\begin{pmatrix}a & b & 0\\ -b & a & 0\\ 0 & 0 & -2a\end{pmatrix}.$$

(II) The self-dual curvature operator $\hat{W}_+$ has a double root of its minimal polynomial, i.e,

$$\hat{W}_+=\begin{pmatrix}a\pm 1 & \pm 1 & 0\\ \mp 1 & a\mp 1 & 0\\ 0 & 0 & -2a\end{pmatrix}.$$

(III) The self-dual curvature operator $\hat{W}_+$ has a triple root of its minimal polynomial, i.e,

$$\hat{W}_+ = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}}{2} \\ 0 & -\frac{\sqrt{2}}{2} & 0 \end{pmatrix}.$$

III. KÄHLER OSSERMAN METRICS

Although the structure of the Kähler Osserman algebraic curvature tensors is completely determined in Theorem 2, the situation is more complex as concerns the differentiable level. An algebraic curvature tensor is said to be *Jordan–Osserman* if the normal Jordan form of the Jacobi operators is constant on $S^{\pm}(V)$. It follows from the results in Ref. 3 that any Osserman algebraic curvature tensor is Jordan–Osserman in dimension four, but such equivalence is no longer true in higher dimensions (see, for example Ref. 4). Passing from the algebraic to the differentiable level the corresponding notions arise. A pseudo-Riemannian manifold is said to be *Osserman* (respectively, *Jordan–Osserman*) if the eigenvalues of the Jacobi operators (respectively, their normal Jordan forms) are constant on the pseudo-unit sphere bundles $S^{\pm}(M)$. The *pointwise* Osserman and Jordan–Osserman conditions correspond to the possibility of the eigenvalues and the Jordan normal form to vary from point to point on the manifold. Hence we have the following

Theorem 4: *A four-dimensional Kähler metric is pointwise Osserman if and only if it is an indefinite complex space form or a Ricci flat Kähler surface. Moreover, the Jacobi operators of a Jordan–Osserman four-dimensional Kähler metric which is not of constant holomorphic sectional curvature are nilpotent of degree two or three.*

Proof: It follows from Ref. 3, Sec. 5 that a four-dimensional Kähler Osserman manifold whose Jacobi operators are diagonalizable must be locally an indefinite complex space form. Moreover, no Jordan–Osserman four-manifold whose Jacobi operators have complex roots may exist (cf. Ref. 3, Theorem 6.4). Therefore only cases II and III in Remark 3 remain for consideration. Since the manifold is Ricci flat the Jacobi operators are three-step nilpotent for type III Jordan–Osserman metrics. Moreover, if the Jacobi operators are of type II it follows from Ref. 3 Corollary 7.3 that the Jacobi operators have a unique eigenvalue or two distinct eigenvalues α and $\beta=4\alpha$. Hence, the Ricci flatness implies that the Jacobi operators are two-step nilpotent.

Remark 5: It has been shown in Ref. 3 that a type II Jordan–Osserman four-manifold admits a parallel two-dimensional null plane field, and hence the metric corresponds to those discussed by Walker.[23] Further note the existence of Walker metrics which are Osserman but not Ricci flat. Indeed, any para-Kähler metric is necessarily Walker and therefore the class of Walker metrics contains that of paracomplex space forms.

Remark 6: Compact complex surfaces admitting a Ricci flat Kähler metric have been classified by Petean,[21] who showed that any such surface must be a complex torus, a hyperelliptic surface or a primary Kodaira surface. Moreover, he constructed explicit examples of Ricci flat Kähler metrics on any of such surfaces. It should be remarked that all examples in Ref. 21 are either flat or otherwise they have two-step nilpotent Jacobi operators.

Remark 7: Recently, left invariant Kähler structures on simply connected Lie groups have been classified in Ref. 20. It has been shown by Ovando that any such Ricci flat indefinite Kähler structure corresponds to one of the following:

- $\mathfrak{aff}(\mathbb{C})$

  The Lie algebra structure is given by $[e_1,e_3]=e_3$, $[e_1,e_4]=e_4$, $[e_2,e_3]=e_4$ and $[e_2,e_4]=-e_3$, the left-invariant metric is given by $a_{14}(e^1\otimes e^3-e^2\otimes e^4)-a_{13}(e^1\otimes e^4+e^2\otimes e^3)-s(e^1\otimes e^1+e^2\otimes e^2)$ and the complex structure satisfies $Je_2=e_1$, $Je_3=e_4$.

- $\mathfrak{r}_{4,-1,-1}$

  The Lie algebra structure is given by $[e_1,e_4]=-e_1$, $[e_2,e_4]=e_2$ and $[e_3,e_4]=e_3$, the left-invariant metric is given by $a_{13}(e^1\otimes e^2-e^3\otimes e^4)-a_{12}(e^1\otimes e^3+e^2\otimes e^4)-s(e^1\otimes e^1+e^4\otimes e^4)$ and the complex structure satisfies $Je_2=e_3$, $Je_4=e_1$.
- $\mathfrak{d}_{4,2}$

  The Lie algebra structure is given by $[e_1,e_2]=e_3$, $[e_1,e_4]=-2e_1$, $[e_2,e_4]=e_2$ and $[e_3,e_4]=-e_3$, the left-invariant metric is given by $a_{14}(e^1\otimes e^2+e^3\otimes e^4)+s(e^2\otimes e^2+e^4\otimes e^4)$ and the complex structure satisfies $Je_1=e_3$, $Je_2=e_4$.

Now, it follows after some calculations that in all the three cases above the Jacobi operators are two-step nilpotent or they vanish (if and only if $s=0$).

Kähler metrics with three-step nilpotent Jacobi operators

Four-dimensional indefinite Kähler Osserman manifolds with two-step nilpotent Jacobi operators are already known in the literature,[4] but there are only a few examples of Osserman four-manifolds with three-step nilpotent Jacobi operators (cf. Refs. 6 and 10). Moreover, the fact that locally symmetric four-dimensional Osserman manifolds may not have three-step nilpotent Jacobi operators[11] could suggest the nonexistence of Kähler Osserman metrics whose Jacobi operators are nilpotent of degree three.

A Walker manifold is a triple $(M,g,\mathcal{D})$ of an n-dimensional manifold, an indefinite metric g, and an r-dimensional parallel null distribution $\mathcal{D}$. Of special interest are manifolds admitting a field of null planes of maximum dimensionality ($r=n/2$). Since the dimension of a null plane is $r\leqslant\frac{1}{2}n$, the lowest possible case of a Walker metric is that of $(--++)$-manifolds admitting a field of parallel null two-planes. A canonical form for such metrics has been obtained by Walker in Ref. 23, showing the existence of suitable coordinates (x_1,x_2,x_3,x_4), where the metric expresses as

$$g_{(x,y,z,t)}=\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & a(x_1,x_2,x_3,x_4) & c(x_1,x_2,x_3,x_4) \\ 0 & 1 & c(x_1,x_2,x_3,x_4) & b(x_1,x_2,x_3,x_4) \end{pmatrix}, \tag{6}$$

for some functions $a(x_1,x_2,x_3,x_4)$, $b(x_1,x_2,x_3,x_4)$, and $c(x_1,x_2,x_3,x_4)$. Further note that the plane field $\mathcal{D}$ is strictly parallel (i.e., there exists two orthogonal null parallel vector fields) if and only if the defining functions satisfy $a(x_3,x_4)$, $b(x_3,x_4)$, $c(x_3,x_4)$ and in such case coordinates can be specialized to obtain $a\equiv c\equiv 0$, $b(x_3,x_4)$ (cf. Ref. 23).

It follows after some straightforward calculations that the Levi-Civita connection of a Walker metric is given by

$$\nabla_{\partial_1}\partial_3=\tfrac{1}{2}a_1\partial_1+\tfrac{1}{2}c_1\partial_2,$$

$$\nabla_{\partial_1}\partial_4=\tfrac{1}{2}c_1\partial_1+\tfrac{1}{2}b_1\partial_2,$$

$$\nabla_{\partial_2}\partial_3=\tfrac{1}{2}a_2\partial_1+\tfrac{1}{2}c_2\partial_2,$$

$$\nabla_{\partial_2}\partial_4=\tfrac{1}{2}c_2\partial_1+\tfrac{1}{2}b_2\partial_2,$$

$$\nabla_{\partial_3}\partial_3=\tfrac{1}{2}\{a_3+ca_2+aa_1\}\partial_1+\tfrac{1}{2}\{2c_3-a_4+ba_2+ca_1\}\partial_2-\tfrac{1}{2}a_1\partial_3-\tfrac{1}{2}a_2\partial_4,$$

$$\nabla_{\partial_3}\partial_4 = \tfrac{1}{2}\{a_4 + cc_2 + ac_1\}\partial_1 + \tfrac{1}{2}\{b_3 + bc_2 + cc_1\}\partial_2 - \tfrac{1}{2}c_1\partial_3 - \tfrac{1}{2}c_2\partial_4,$$

$$\nabla_{\partial_4}\partial_4 = \tfrac{1}{2}\{2c_4 - b_3 + cb_2 + ab_1\}\partial_1 + \tfrac{1}{2}\{b_4 + bb_2 + cb_1\}\partial_2 - \tfrac{1}{2}b_1\partial_3 - \tfrac{1}{2}b_2\partial_4, \tag{7}$$

where a_k means partial derivative

$$\frac{\partial}{\partial x_k}a(x_1,x_2,x_3,x_4)$$

and ∂_k denotes the coordinate vector field $\partial/\partial k$, $k=1,\ldots,4$.

A g-orthogonal almost complex structure J on a Walker four-manifold is said to be proper if it defines a standard generator of a positive $\pi/2$ rotation on $\mathcal{D}$,[16] i.e., $J\partial_1=\partial_2$ and $J\partial_2=-\partial_1$. The whole almost complex structure can be recovered from this property to obtain in the canonical coordinates

$$J\partial_1 = \partial_2, \quad J\partial_2 = -\partial_1,$$

$$J\partial_3 = -c\partial_1 + \tfrac{1}{2}(a-b)\partial_2 + \partial_4, \tag{8}$$

$$J\partial_4 = \tfrac{1}{2}(a-b)\partial_1 + c\partial_2 - \partial_3.$$

Further note that the indefinite almost Hermitian structure (g,J) is Kähler if and only if[16]

$$a_1 = -b_1 = c_2 \quad a_2 = -b_2 = -c_1. \tag{9}$$

Next, let R denote the curvature tensor, taken with the sign convention $R(X,Y)=\nabla_{[X,Y]} - [\nabla_X,\nabla_Y]$. A straightforward calculation from (7) using (9) shows that the curvature tensor of a Kähler Walker metric is given by the following (see also Ref. 16, Appendix 1):

$$R_{1331} = R_{1342} = R_{1414} = R_{1432} = R_{2323} = R_{2442} = \tfrac{1}{2}c_{12},$$

$$R_{1341} = R_{1323} = R_{1442} = R_{2324} = \tfrac{1}{2}c_{11},$$

$$R_{1334} = R_{2434} = \tfrac{1}{2}(c_{24} - c_{13}),$$

$$R_{1434} = R_{2343} = \tfrac{1}{2}(c_{23} + c_{14}),$$

$$R_{3434} = \tfrac{1}{4}\{4c_{34} - 2a_{44} - 2b_{33} - (a_3 + 3b_3 - 2c_4)c_2 - (b_4 + 3a_4 - 2c_3)c_1 - (a+b)c_2^2 - (a+b)c_1^2\}. \tag{10}$$

Theorem 8: *A Kähler Walker metric* (6)–(8) *is Osserman if and only if the coefficient functions satisfy*

$$a(x_1,x_2,x_3,x_4) = x_1P(x_3,x_4) + x_2Q(x_3,x_4) + \xi(x_3,x_4),$$

$$b(x_1,x_2,x_3,x_4) = -x_1P(x_3,x_4) - x_2Q(x_3,x_4) + \eta(x_3,x_4), \tag{11}$$

$$c(x_1,x_2,x_3,x_4) = -x_1Q(x_3,x_4) + x_2P(x_3,x_4) + \gamma(x_3,x_4)$$

for any functions $P(x_3,x_4)$, $Q(x_3,x_4)$ *satisfying*

$$P_3 - Q_4 = 0 \tag{12}$$

and arbitrary functions $\xi(x_3,x_4)$, $\eta(x_3,x_4)$, and $\gamma(x_3,x_4)$. Moreover the Jacobi operators have zero eigenvalues and they satisfy one of the following

(i) The Jacobi operators vanish at those points where $P_4+Q_3=0$ and

$$(P^2+Q^2)(\xi+\eta)+P(\xi_3+3\eta_3-2\gamma_4)-Q(\eta_4+3\xi_4-2\gamma_3)+2(\xi_{44}-2\gamma_{34}+\eta_{33})=0,$$

(ii) the Jacobi operators are two-step nilpotent if and only if $P_4+Q_3=0$ and

$$(P^2+Q^2)(\xi+\eta)+P(\xi_3+3\eta_3-2\gamma_4)-Q(\eta_4+3\xi_4-2\gamma_3)+2(\xi_{44}-2\gamma_{34}+\eta_{33})\neq 0,$$

(iii) The Jacobi operators are three-step nilpotent otherwise.

Proof: As a matter of notation, let Ric and Sc denote the Ricci tensor and the scalar curvature of (M,g), defined by $\mathrm{Ric}(X,Y)=\mathrm{trace}\{Z\to R(X,Z)Y\}$ and $\mathrm{Sc}=\mathrm{trace\ Ric}$. Now it follows from (10) that the Ricci tensor and the scalar curvature of a Kähler Walker metric satisfies

$$\mathrm{Ric}_{13}=\mathrm{Ric}_{24}=c_{12},$$

$$\mathrm{Ric}_{14}=-\mathrm{Ric}_{23}=c_{11},$$

$$\mathrm{Ric}_{33}=c_{23}+c_{14}+\tfrac{1}{2}\{(a-b)c_{12}-2cc_{11}\}, \tag{13}$$

$$\mathrm{Ric}_{44}=c_{23}+c_{14}-\tfrac{1}{2}\{(a-b)c_{12}-2cc_{11}\},$$

$$\mathrm{Ric}_{34}=\tfrac{1}{2}\{2cc_{12}+(a-b)c_{11}\},$$

$$\mathrm{Sc}=4c_{12}. \tag{14}$$

Now, since any Osserman manifold is necessarily Einstein, a straightforward calculation from (13) shows that the Einstein tensor

$$G=\mathrm{Ric}-\frac{\mathrm{Sc}}{4}g$$

vanishes (equivalently the metric is Einstein) if and only if the following hold

$$\begin{gathered} G_{14}=-G_{23}=c_{11}\equiv 0,\\ G_{33}=c_{14}+c_{23}-\tfrac{1}{2}\{(a+b)c_{12}+2cc_{11}\}\equiv 0,\\ G_{34}=\tfrac{1}{2}(a-b)c_{11}\equiv 0,\\ G_{44}=c_{14}+c_{23}-\tfrac{1}{2}\{(a+b)c_{12}-2cc_{11}\}\equiv 0. \end{gathered} \tag{15}$$

Next note from (9) that $a_{11}+a_{22}=0$ for any Kähler Walker metric, and thus it follows from (15) and (9) that $a_{11}=a_{22}=a_{12}\equiv 0$, $c_{11}=c_{22}=c_{12}\equiv 0$, and $b_{11}=b_{22}=b_{12}\equiv 0$. Now, those conditions together with the Kähler ones at (9) show that the metric (6) must be necessarily given by (11). Now, a straightforward calculation shows that (15) reduces to

$$G_{33}=G_{44}=-Q_4+P_3\equiv 0, \tag{16}$$

which shows (12).

Now, in order to analyze the Osserman property, it is convenient to consider the normalized Jacobi operators $J_R(X)=g(X,X)^{-1}R_X$, where for any non-null vector $X=\Sigma X_i\partial_i$, the Jacobi operators $R_X=R(X,\cdot,)X$ of a metric (11) satisfying (12) are given by

$$R_X=\begin{pmatrix} A & B \\ 0 & {}^tA \end{pmatrix}, \tag{17}$$

where A and B are 2×2-matrices and moreover

$$A=\tfrac{1}{2}(P_4+Q_3)\begin{pmatrix} X_3X_4 & X_4^2 \\ -X_3^2 & -X_3X_4 \end{pmatrix}. \tag{18}$$

This shows that the characteristic polynomial of the Jacobi operators satisfy $\det(R_X-\lambda\mathrm{id})=\lambda^4$ and thus metrics (11) and (12) are Osserman with zero eigenvalues for the Jacobi operators.

Moreover, in order to analyze the minimal polynomial of the Jacobi operators, observe that $J_R(X)^{(3)}=0$ and that

$$J_R(X)^{(2)}=-\frac{1}{4}g(X,X)^{-1}(P_4+Q_3)^2\begin{pmatrix} 0 & 0 & X_4^2 & -X_3X_4 \\ 0 & 0 & -X_3X_4 & X_3^2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Moreover, assuming $P_4+Q_3=0$, the Jacobi operators reduce to

$$R_X=-\frac{1}{4}\Xi\begin{pmatrix} 0 & 0 & X_4^2 & -X_3X_4 \\ 0 & 0 & -X_3X_4 & X_3^2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

where

$$\Xi=(P^2+Q^2)(\xi+\eta)+P(\xi_3+3\eta_3-2\gamma_4)-Q(\eta_4+3\xi_4-2\gamma_3)+2(\xi_{44}-2\gamma_{34}+\eta_{33})$$

from where the result follows. □

Remark 9: As a consequence of Theorem 8 we have plenty of examples of Kähler Osserman metrics whose Jacobi operators are three-step nilpotent. Indeed, any metric

$$a(x_1,x_2,x_3,x_4)=x_1P(x_3,x_4)+x_2Q(x_3,x_4),$$

$$b(x_1,x_2,x_3,x_4)=-x_1P(x_3,x_4)-x_2Q(x_3,x_4),$$

$$c(x_1,x_2,x_3,x_4)=-x_1Q(x_3,x_4)+x_2P(x_3,x_4)$$

is Kähler Osserman if and only if the functions P and Q satisfy $P_3-Q_4=0$. Moreover, the corresponding Jacobi operators vanish (equivalently the metric is flat) if and only if $P_4+Q_3=0$. Otherwise the Jacobi operators are three-step nilpotent.

Remark 10: The Ricci operator $\langle\hat{\mathrm{Ric}}(X),Y\rangle=\mathrm{Ric}(X,Y)$ of a metric (6) satisfying the Kähler conditions (9) is given by

$$\hat{\mathrm{Ric}} = \begin{pmatrix} c_{12} & -c_{11} & c_{14}+c_{23}-\frac{1}{2}(a+b)c_{12} & -\frac{1}{2}(a+b)c_{11} \\ c_{11} & c_{12} & \frac{1}{2}(a+b)c_{11} & c_{14}+c_{23}-\frac{1}{2}(a+b)c_{12} \\ 0 & 0 & c_{12} & c_{11} \\ 0 & 0 & -c_{11} & c_{12} \end{pmatrix}$$

and hence the Ricci curvatures satisfy

$$\lambda = c_{12} \pm \sqrt{-c_{11}^2}. \tag{19}$$

Moreover, since the scalar curvature satisfies $\mathrm{Sc}=4c_{12}$, proceeding as in Theorem 8 it follows that a Kähler metric (6)–(9) is self-dual if and only if it is given by

$$a(x_1,x_2,x_3,x_4) = -2x_1x_2T(x_3,x_4) + x_1P(x_3,x_4) + x_2Q(x_3,x_4) + \xi(x_3,x_4),$$

$$b(x_1,x_2,x_3,x_4) = 2x_1x_2T(x_3,x_4) - x_1P(x_3,x_4) - x_2Q(x_3,x_4) + \eta(x_3,x_4),$$

$$c(x_1,x_2,x_3,x_4) = (x_1^2-x_2^2)T(x_3,x_4) - x_1Q(x_3,x_4) + x_2P(x_3,x_4) + \gamma(x_3,x_4).$$

Hence any self-dual metric as above has Ricci curvatures $\pm 2T(x_3,x_4)\sqrt{-1}$. Further note that even in case the Ricci curvatures are vanishing (i.e., $T\equiv 0$), the Ricci operator becomes

$$\hat{\mathrm{Ric}} = \begin{pmatrix} 0 & 0 & P_3-Q_4 & 0 \\ 0 & 0 & 0 & P_3-Q_4 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

which is nondiagonalizable unless (12) holds.

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On Explicit point multimonopoles in SU(2) gauge theory

Alexander D. Popov[a)]
Institut für Theoretische Physik, Universität Hannover, Appelstraße 2, 30167 Hannover, Germany

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It is well known that the Dirac monopole solution with the U(1) gauge group embedded into the group SU(2) is equivalent to the SU(2) Wu–Yang point monopole solution having no Dirac string singularity. We consider a multicenter configuration of m Dirac monopoles and n antimonopoles and its embedding into SU(2) gauge theory. Using geometric methods, we construct an explicit solution of the SU(2) Yang–Mills equations which generalizes the Wu–Yang solution to the case of m monopoles and n antimonopoles located at arbitrary points in $\mathbb{R}^3$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1939987]

I. INTRODUCTION

Abelian magnetic monopoles play a key role in the dual superconductor mechanism of confinement[1] which has been confirmed by many numerical simulations of the lattice gluodynamics (see, e.g., Refs. 2 and 3 and references therein). Due to a dominant role of Abelian monopoles in the confinement phenomena, it is important to better understand how they arise in nonabelian pure gauge theories.

A spherically symmetric monopole solution of the SU(2) pure gauge field equations was obtained by Wu and Yang in 1969.[4] This solution is singular at the origin and smooth on $\mathbb{R}^3 - \{0\}$. Initially it was thought that it is genuinely nonabelian, yet later it was shown[5] that this solution is nothing but the Abelian Dirac monopole[6] in disguise. Note that the gauge potential of the finite-energy spherically symmetric 't Hooft–Polyakov monopole[7] approaches just the Wu–Yang gauge potential for large $r^2 = x^a x^a$.

In this article, we generalize the Wu-Yang solution to a configuration describing m monopoles and n antimonopoles with arbitrary locations in $\mathbb{R}^3$. This explicit solution to the Yang—Mills equations can also be used as a guide to the asymptotic $r \to \infty$ behavior of unknown finite-energy solutions in the Yang–Mills–Higgs theory, whose form for small r is determined by multiplying the solution by arbitrary functions and minimizing the energy functional, as was proposed in Ref. 8.

II. GENERIC U(1) CONFIGURATIONS

We consider the configuration of m Dirac monopoles and n antimonopoles located at points $\vec{a}_i = \{a_i^1, a_i^2, a_i^3\}$ with $i = 1, \ldots, m$ and $i = m+1, \ldots, m+n$, respectively. There are delta-function sources for the magnetic field at these points.

Let us introduce the following two regions in $\mathbb{R}^3$:

$$R^3_{N,m+n} := \mathbb{R}^3 - \{ \bigcup_{i=1}^{m+n} (x^1 = a_i^1, \quad x^2 = a_i^2, \quad x^3 \leqslant a_i^3) \},$$

[a)]On leave from Bogoliubov Laboratory of Theoretical Physics, JINR, Dubna, Russia; Electronic mail: popov@itp.uni-hannover.de

$$R^3_{S,m+n} := \mathbb{R}^3 - \{\bigcup_{i=1}^{m+n}(x^1 = a^1_i, \quad x^2 = a^2_i, \quad x^3 \geqslant a^3_i)\}. \tag{1}$$

For simplicity we restrict ourselves to the *generic* case

$$a^{1,2}_i \neq a^{1,2}_j \quad \text{for} \quad i \neq j, \tag{2}$$

when

$$R^3_{N,m+n} \cup R^3_{S,m+n} = \mathbb{R}^3 - \{\vec{a}_1, \ldots, \vec{a}_{m+n}\}, \tag{3}$$

and the two open sets are enough for describing the previous (m,n) configuration. Namely, the generic configuration of m Dirac monopoles and n antimonopoles is described by the gauge potentials

$$A^{N,m+n} = \sum_{j=1}^{m} A^{N,j} + \sum_{j=m+1}^{m+n} \overline{A}^{N,j}, \quad A^{S,m+n} = \sum_{j=1}^{m} A^{S,j} + \sum_{j=m+1}^{m+n} \overline{A}^{S,j}, \tag{4}$$

where $A^{N,m+n}$ and $A^{S,m+n}$ are well defined on $R^3_{N,m+n}$ and $R^3_{S,m+n}$, respectively. Here

$$A^{N,j} = A^{N,j}_a \mathrm{d}x^a \quad \text{with} \quad A^{N,j}_1 = \frac{\mathrm{i}x^2_j}{2r_j(r_j + x^3_j)}, \quad A^{N,j}_2 = -\frac{\mathrm{i}x^1_j}{2r_j(r_j + x^3_j)}, \quad A^{N,j}_3 = 0, \tag{5}$$

$$A^{S,j} = A^{S,j}_a \mathrm{d}x^a \quad \text{with} \quad A^{S,j}_1 = -\frac{\mathrm{i}x^2_j}{2r_j(r_j - x^3_j)}, \quad A^{S,j}_2 = \frac{\mathrm{i}x^1_j}{2r_j(r_j - x^3_j)}, \quad A^{S,j}_3 = 0, \tag{6}$$

where

$$x^c_j = x^c - a^c_j, \quad r^2_j = \delta_{ab} x^a_j x^b_j, \quad a,b,c = 1,2,3, \tag{7}$$

and $\overline{A}^{N,j} = -A^{N,j}$, $\overline{A}^{S,j} = -A^{S,j}$. On the intersection $R^3_{N,m+n} \cap R^3_{S,m+n}$ we have

$$A^{N,m+n} = A^{S,m+n} + \mathrm{d}\ln\left(\prod_{i=1}^{m}\left(\frac{\overline{y_i}}{y_i}\right)^{1/2}\prod_{j=m+1}^{m+n}\left(\frac{y_j}{\overline{y_j}}\right)^{1/2}\right), \tag{8}$$

where $y_j = x^1_j + \mathrm{i}x^2_j$ and overbar denotes a complex conjugation.

Remark: Note that in the case when $a^{1,2}_i = a^{1,2}_j$ for some $i \neq j$, one has to introduce more than two open sets covering the space $\mathbb{R}^3 - \{\vec{a}_1, \ldots, \vec{a}_{m+n}\}$ and define gauge potentials on each of these sets as well as transition functions on their intersections. However, for the case $\vec{a}_1 = \cdots = \vec{a}_{m+n} = \vec{a}$ the two sets (1) are again enough to cover $\mathbb{R}^3 - \{\vec{a}\}$ and the gauge potential (4)–(6) will describe $m-n$ monopoles (if $m > n$) or $n-m$ antimonopoles (if $m < n$) sitting on top of each other.

One can simplify expressions (4)–(8) by introducing functions of coordinates

$$w_j := \frac{y_j}{r_j - x^3_j} = \mathrm{e}^{\mathrm{i}\varphi_j}\cot\frac{\vartheta_j}{2}, \quad v_j := \frac{1}{w_j} = \frac{\overline{y_j}}{r_j + x^3_j} = \mathrm{e}^{-\mathrm{i}\varphi_j}\tan\frac{\vartheta_j}{2}, \tag{9}$$

where

$$x^1_j = r_j \sin\vartheta_j \cos\varphi_j, \quad x^2_j = r_j \sin\vartheta_j \sin\varphi_j, \quad x^3_j = r_j \cos\vartheta_j. \tag{10}$$

Note that $w_i \to \infty$ for $x^{1,2} \to a^{1,2}_i$, $x^3 \geqslant a^3_i$, and $v_i \to \infty$ for $x^{1,2} \to a^{1,2}_i$, $x^3 \leqslant a^3_i$. In terms of w_j and v_j the gauge potentials (4)–(6) have the form

$$A^{N,m+n} = \sum_{i=1}^{m} \frac{1}{2(1 + v_i\overline{v_i})}(\overline{v_i}\,\mathrm{d}v_i - v_i\,\mathrm{d}\overline{v_i}) + \sum_{i=m+1}^{m+n} \frac{1}{2(1 + v_i\overline{v_i})}(v_i\,\mathrm{d}\overline{v_i} - \overline{v_i}\,\mathrm{d}v_i), \tag{11}$$

$$A^{S,m+n}=\sum_{i=1}^{m}\frac{1}{2(1+w_i\overline{w_i})}(\overline{w_i}\,\mathrm{d}w_i-w_i\,\mathrm{d}\overline{w_i})+\sum_{i=m+1}^{m+n}\frac{1}{2(1+w_i\overline{w_i})}(w_i\,\mathrm{d}\overline{w_i}-\overline{w_i}\,\mathrm{d}w_i). \tag{12}$$

On the intersection $R^3_{N,m+n}\cap R^3_{S,m+n}$ of two domains (1) these configurations are related by the transformation

$$A^{N,m+n}=A^{S,m+n}+\mathrm{d}\ln\left(\prod_{i=1}^{m}\left(\frac{\overline{w_i}}{w_i}\right)^{1/2}\prod_{j=m+1}^{m+n}\left(\frac{w_j}{\overline{w_j}}\right)^{1/2}\right), \tag{13}$$

since $\overline{y_i}/y_i=\overline{w_i}/w_i$. Note that the transition function in (13) can also be written in terms of v_i by using the relation $v_i/\overline{v_i}=\overline{w_i}/w_i$.

For the Abelian curvature $F^{D,m+n}$ we have

$$\begin{aligned}F^{D,m+n}=\mathrm{d}A^{N,m+n}&=-\sum_{i=1}^{m}\frac{\mathrm{d}v_i\wedge\mathrm{d}\overline{v_i}}{(1+v_i\overline{v_i})^2}+\sum_{i=m+1}^{m+n}\frac{\mathrm{d}v_i\wedge\mathrm{d}\overline{v_i}}{(1+v_i\overline{v_i})^2}\\&=-\sum_{i=1}^{m}\frac{\mathrm{d}w_i\wedge\mathrm{d}\overline{w_i}}{(1+w_i\overline{w_i})^2}+\sum_{i=m+1}^{m+n}\frac{\mathrm{d}w_i\wedge\mathrm{d}\overline{w_i}}{(1+w_i\overline{w_i})^2}=\mathrm{d}A^{S,m+n}.\end{aligned} \tag{14}$$

It is not difficult to see that $F^{D,m+n}$ is singular only at points $\{\vec{a}_1,\ldots,\vec{a}_{m+n}\}$, where monopoles and antimonopoles are located.

III. POINT SU(2) CONFIGURATIONS

The generalization of the Wu–Yang SU(2) monopole[4] to a configuration describing m monopoles and n antimonopoles can be obtained as follows. Let us multiply Eq. (13) by the Pauli matrix σ_3 and rewrite it as

$$A^{N,m+n}\sigma_3=f^{(m,n)}_{NS}A^{S,m+n}\sigma_3(f^{(m,n)}_{NS})^{-1}+f^{(m,n)}_{NS}\mathrm{d}(f^{(m,n)}_{NS})^{-1}, \tag{15}$$

where

$$f^{(m,n)}_{NS}=\begin{pmatrix}\displaystyle\prod_{i=1}^{m}\left(\frac{w_i}{\overline{w_i}}\right)^{1/2}\prod_{j=m+1}^{m+n}\left(\frac{\overline{w_j}}{w_j}\right)^{1/2} & 0\\ 0 & \displaystyle\prod_{i=1}^{m}\left(\frac{\overline{w_i}}{w_i}\right)^{1/2}\prod_{j=m+1}^{m+n}\left(\frac{w_j}{\overline{w_j}}\right)^{1/2}\end{pmatrix}. \tag{16}$$

It can be checked by direct calculation that the transition matrix (16) can be split as

$$f^{(m,n)}_{NS}=(g^{(m,n)}_{N})^{-1}g^{(m,n)}_{S}, \tag{17}$$

where the 2×2 unitary matrices

$$g^{(m,n)}_{N}=\frac{1}{(1+\prod_{i=1}^{m+n}v_i\overline{v_i})^{1/2}}\begin{pmatrix}\displaystyle\prod_{j=1}^{m}v_j\prod_{k=m+1}^{m+n}\overline{v_k} & 1\\ -1 & \displaystyle\prod_{j=1}^{m}\overline{v_j}\prod_{k=m+1}^{m+n}v_k\end{pmatrix} \tag{18}$$

and

$$g_S^{(m,n)} = \frac{1}{(1+\prod_{i=1}^{m+n} w_i\overline{w_i})^{1/2}} \begin{pmatrix} 1 & \prod_{j=1}^{m} \overline{w_j} \prod_{k=m+1}^{m+n} w_k \\ -\prod_{j=1}^{m} w_j \prod_{k=m+1}^{m+n} \overline{w_k} & 1 \end{pmatrix} \tag{19}$$

are well defined on $R^3_{N,m+n}$ and $R^3_{S,m+n}$, respectively. Using formulas (9) and (10), one can rewrite these matrices in the coordinates x_i^a with explicit dependence on moduli $\vec{a}_i$ for $i=1,\ldots,m+n$.

Substituting (17) into (15), we obtain

$$A^{N,m+n} g_N^{(m,n)} \sigma_3 (g_N^{(m,n)})^\dagger + g_N^{(m,n)} \mathrm{d}(g_N^{(m,n)})^\dagger = A^{S,m+n} g_S^{(m,n)} \sigma_3 (g_S^{(m,n)})^\dagger + g_S^{(m,n)} \mathrm{d}(g_S^{(m,n)})^\dagger =: A^{(m,n)}_{su(2)}, \tag{20}$$

where by construction $A^{(m,n)}_{\mathrm{su}(2)}$ is well defined on $R^3_{N,m+n} \cup R^3_{S,m+n} = \mathbb{R}^3 - \{\vec{a}_1,\ldots,\vec{a}_{m+n}\}$. Geometrically, the existence of splitting (17) means that Dirac's nontrivial U(1) bundle over $\mathbb{R}^3 - \{\vec{a}_1,\ldots,\vec{a}_{m+n}\}$ trivializes when being embedded into an SU(2) bundle. The matrices (18) and (19) define this trivialization since $f_{NS}^{(m,n)} \mapsto \widetilde{f}_{NS}^{(m,n)} = g_N^{(m,n)} f_{NS}^{(m,n)} (g_S^{(m,n)})^{-1} = \mathbf{1}_2$.

Remark: Recall that we consider generic configurations with conditions (2). In the case of $a_i^{1,2}$ coinciding for some $i \neq j$, one has $R^3_{N,m+n} \cup R^3_{S,m+n} \neq \mathbb{R}^3 - \{\vec{a}_1,\ldots,\vec{a}_{m+n}\}$ and the gauge potential (20) can have singularities outside $R^3_{N,m+n} \cup R^3_{S,m+n}$. For example, in the case $m=2$, $n=0$, $a_1^{1,2} = a_2^{1,2} = 0$, and $a_1^3 = -a_2^3 = a$, the gauge potential describing two separated monopoles will be singular on the interval $-a \leqslant x^3 \leqslant a$. To have nonsingular $A^{(2,0)}_{\mathrm{su}(2)}$ one should consider $a_1^{1,2} \neq a_2^{1,2}$ or to use three open sets covering $\mathbb{R}^3 - \{\vec{a}_1, \vec{a}_2\}$ instead of two ones.

The field strength for the configuration (20) is given by

$$F^{(m,n)}_{\mathrm{su}(2)} = \mathrm{d}A^{(m,n)}_{\mathrm{su}(2)} + A^{(m,n)}_{\mathrm{su}(2)} \wedge A^{(m,n)}_{\mathrm{su}(2)} = \mathrm{i} F^{D,m+n} Q_{(m,n)}, \tag{21}$$

where the su(2)-valued matrix

$$Q_{(m,n)} := -\mathrm{i} g_N^{(m,n)} \sigma_3 (g_N^{(m,n)})^\dagger = -\mathrm{i} g_S^{(m,n)} \sigma_3 (g_S^{(m,n)})^\dagger \tag{22}$$

is well defined on $R^3_{N,m+n} \cup R^3_{S,m+n}$. It is easy to see that $Q^2_{(m,n)} = -1$ and $Q_{(m,n)}$ may be considered as the generator of the group U(1) embedded into SU(2). Then the Abelian nature of the configuration (20) and (21) becomes obvious. Further, for

$$A^{(m,n)}_{\mathrm{su}(2)} = A^{(m,n)}_a \mathrm{d}x^a, \quad F^{(m,n)}_{\mathrm{su}(2)} = \tfrac{1}{2} F^{(m,n)}_{ab} \mathrm{d}x^a \wedge \mathrm{d}x^b \tag{23}$$

one can easily show that

$$\partial_a F^{(m,n)}_{ab} + [A^{(m,n)}_a, F^{(m,n)}_{ab}] = \mathrm{i}(\partial_a F^{D,m+n}_{ab}) Q_{(m,n)} \tag{24}$$

and therefore on the space $\mathbb{R}^3 - \{\vec{a}_1,\ldots,\vec{a}_{m+n}\}$ we have

$$\partial_a F^{(m,n)}_{ab} + [A^{(m,n)}_a, F^{(m,n)}_{ab}] = 0, \tag{25}$$

which follows from the field equations describing m Dirac monopoles and n antimonopoles. Note that the solution (20)–(23) of the SU(2) gauge theory can be embedded in any larger gauge theory following, e.g., Ref. 9.

IV. POINT MONOPOLES VIA RIEMANN–HILBERT PROBLEMS

Here we want to rederive the described configurations by solving a matrix Riemann-Hilbert problem. For simplicity, we restrict ourselves to the case of m monopoles.

Let us consider the Bogomolny equations[10]

$$F_{ab} = \epsilon_{abc} D_c \chi, \tag{26}$$

where $D_c = \partial_c + [A_c, \cdot]$ and the fields $A_a, F_{ab} = \partial_a A_b - \partial_b A_a + [A_a, A_b]$ and χ take values in the Lie algebra $u(q)$. Obviously, in the Abelian case $D_c\chi = \partial_c \chi$. Note that for the gauge fields $F^{D,m}$ given by (14) we have

$$F^{D,m}_{ab} = \epsilon_{abc} \partial_c \phi^{(m)} \quad \text{with} \quad \phi^{(m)} = \sum_{k=1}^{m} \frac{\mathrm{i}}{2r_k}. \tag{27}$$

Analogously, for the field $F^{(m)}_{ab}$ from (23) we have

$$F^{(m)}_{ab} = \epsilon_{abc} D_c \Phi^{(m)} \quad \text{with} \quad \Phi^{(m)} = \mathrm{i}\phi^{(m)} Q_{(m)}, \tag{28}$$

where $\phi^{(m)}$ is given in (27) and $Q_{(m)}$ in (22). Thus, both U(1) and SU(2) multimonopoles as well as (m,n) configurations (11)–(14) and (20)–(22) can be considered as solutions of the Bogomolny equations (26). In fact, the second order pure Yang–Mills equations for $F^{D,m}_{ab}$ and $F^{(m)}_{ab}$ can be obtained by differentiating (27) and (28), respectively. Moreover, in pure SU(2) Yang–Mills theory in (3+1)-dimensional Minkowski space, one can choose the component A_0 of the gauge potential $A = A_0 \mathrm{d}t + A_a \, \mathrm{d}x^a$ to be nonzero and proportional to $\Phi^{(m)}$ (the Abelian case is similar). Then the configuration $\{A^{(m)}_0, A^{(m)}_a\}$ will be a static multidyon solution of the Yang–Mills equations.

Recall that the Bogomolny equations (26) can be obtained as the compatibility conditions of the linear system

$$\left[D_{\bar{y}} - \frac{\lambda}{2}(D_3 + \mathrm{i}\chi) \right] \psi = 0, \quad \left[\frac{1}{2}(D_3 - \mathrm{i}\chi) + \lambda D_y \right] \psi = 0, \tag{29}$$

where $D_{\bar{y}} = \frac{1}{2}(D_1 + \mathrm{i}D_2)$, $D_y = \frac{1}{2}(D_1 - \mathrm{i}D_2)$, and the auxiliary $q \times q$ matrix $\psi(x^a, \lambda)$ depends holomorphically on a new variable $\lambda \in U \subset \mathbb{C}P^1$. Such matrices ψ can be found via solving a parametric Riemann–Hilbert problem which is formulated in the monopole case as follows.[11] Suppose we are given a $q \times q$ matrix f_{+-} depending holomorphically on

$$\eta = y - 2\lambda x^3 - \lambda^2 \bar{y} \tag{30}$$

and λ for $\lambda \in U_+ \cap U_-$, where $U_+ = \mathbb{C}P^1 - \{\infty\}$ and $U_- = \mathbb{C}P^1 - \{0\}$. Then for each fixed $(x^a) \in \mathbb{R}^3$ and $\lambda \in S^1 \subset U_+ \cap U_-$ one should factorize this matrix-valued function,

$$f_{+-}(x,\lambda) = \psi_+^{-1}(x,\lambda)\psi_-(x,\lambda), \tag{31}$$

in such a way that ψ_+ and ψ_- extend holomorphically in λ onto subsets of U_+ and U_-, respectively. In order to insure that $A^\dagger_a = -A_a$ and $\chi^\dagger = -\chi$ in (29) with $\psi = \psi_\pm$ one should also impose the (reality) conditions

$$f^\dagger_{+-}(x, -\bar{\lambda}^{-1}) = f_{+-}(x,\lambda), \quad \psi^\dagger_+(x, -\bar{\lambda}^{-1}) = \psi^{-1}_-(x,\lambda). \tag{32}$$

After finding such $\psi_\pm$ for an educated guess of f_{+-}, one can get A_a and χ from the linear system (29) with the matrix function ψ_+ or ψ_- instead of ψ. Namely, from (29) we get

$$A_{\bar{y}} := \frac{1}{2}(A_1 + \mathrm{i}A_2) = \psi_+ \partial_{\bar{y}} \psi_+^{-1}|_{\lambda=0}, \quad A_3 - \mathrm{i}\chi = \psi_+ \partial_3 \psi_+^{-1}|_{\lambda=0}, \tag{33}$$

$$A_y := \frac{1}{2}(A_1 - \mathrm{i}A_2) = \psi_- \partial_y \psi_-^{-1}|_{\lambda=\infty}, \quad A_3 + \mathrm{i}\chi = \psi_- \partial_3 \psi_-^{-1}|_{\lambda=\infty}. \tag{34}$$

For more details see Refs. 11 and 12 and references therein.

The construction of U(1) multimonopole solutions via solving the Riemann–Hilbert problem for the function

$$f_{+-}^{D,m}=\frac{\lambda^m}{\prod_{k=1}^m \eta_k}=:\rho_m \quad \text{with} \quad \eta_k=\eta-h(a_k^1,a_k^2,a_k^3,\lambda)=(1-\lambda^2)x_k^1+\mathrm{i}(1+\lambda^2)x_k^2-2\lambda x_k^3 \tag{35}$$

was discussed in Ref. 12 and here we describe only the SU(2) case. The ansatz for $f_{+-}^{(m)}$ which satifies (32) only for odd m was written down in Appendix C of Ref. 12. Here we introduce the ansatz

$$f_{+-}^{(m)}=\begin{pmatrix}\rho_m & \lambda^{-m}\\ (-1)^m\lambda^m & \rho_m^{-1}+(-1)^m\rho_m^{-1}\end{pmatrix} \tag{36}$$

satisfying the reality condition (32) for any m. It is not difficult to see that

$$f_{+-}^{(m)}=\begin{pmatrix}1 & 0\\ (-1)^m\lambda^m\rho_m^{-1} & 1\end{pmatrix}\begin{pmatrix}f_{+-}^{D,m} & 0\\ 0 & (f_{+-}^{D,m})^{-1}\end{pmatrix}\begin{pmatrix}1 & \lambda^{-m}\rho_m^{-1}\\ 0 & 1\end{pmatrix}\sim\begin{pmatrix}f_{+-}^{D,m} & 0\\ 0 & (f_{+-}^{D,m})^{-1}\end{pmatrix}, \tag{37}$$

where the diagonal matrix in (37) describes the Dirac line bundle L [the U(1) gauge group] embedded into the rank 2 complex vector bundle [the SU(2) gauge group] as $L\oplus L^{-1}$. This gives another proof of the equivalence of U(1) and SU(2) point monopole configurations (see Ref. 12 for more details). Furthermore, the matrix (36) can be split as follows:

$$f_{+-}^{(m)}=(\psi_+^{(m)})^{-1}\psi_-^{(m)}, \tag{38}$$

where

$$\psi_+^{(m)}=\hat{\psi}_+^{(m)}\begin{pmatrix}1 & 0\\ (-1)^{m+1}\lambda^m\rho_m^{-1} & 1\end{pmatrix}, \quad \psi_-^{(m)}=\hat{\psi}_-^{(m)}\begin{pmatrix}1 & -\lambda^{-m}\rho_m^{-1}\\ 0 & 1\end{pmatrix}, \tag{39}$$

$$\hat{\psi}_+^{(m)}=g_S^{(m)}\begin{pmatrix}\psi_+^{S,m} & 0\\ 0 & (\psi_+^{S,m})^{-1}\end{pmatrix}, \quad \hat{\psi}_-^{(m)}=g_N^{(m)}\begin{pmatrix}\psi_-^{N,m} & 0\\ 0 & (\psi_-^{N,m})^{-1}\end{pmatrix}, \tag{40}$$

$$\psi_+^{S,m}=\prod_{i=1}^m\psi_+^S(x_i^a,\lambda), \quad \psi_+^S(x_i^a,\lambda)=\xi_+(x_i^a)-\lambda\xi_+^{-1}(x_i^a)\overline{y_i}, \quad \xi_+(x_i^a)=(r_i-x_i^3)^{1/2}, \tag{41}$$

$$\psi_-^{N,m}=\prod_{i=1}^m\psi_-^N(x_i^a,\lambda), \quad (\psi_-^N(x_i^a,\lambda))^{-1}=\xi_-(x_i^a)\overline{y_i}+\lambda^{-1}\xi_-^{-1}(x_i^a), \quad \xi_-(x_i^a)=(r_i+x_i^3)^{-1/2}. \tag{42}$$

The explicit form of $g_N^{(m)}$ and $g_S^{(m)}$ is given in (18) and (19). Note that both $\psi_\pm^{(m)}$ and $\hat{\psi}_\pm^{(m)}$ satisfy the reality conditions (32).

Formulas (38)–(42) solve the parametric Riemann–Hilbert problem for our $f_{+-}^{(m)}$ restricted to a contour on $\mathbb{C}P^1$ which avoids all zeros of the function $\Pi_{k=1}^m\eta_k$. Substituting (39)–(42) into formulas (33) and (34), we get

$$A_{\bar{y}}^{(m)}=\hat{g}_S^{(m)}\partial_{\bar{y}}(\hat{g}_S^{(m)})^{-1}, \quad A_y^{(m)}=\hat{g}_N^{(m)}\partial_y(\hat{g}_N^{(m)})^{-1}, \quad A_3^{(m)}=g_S^{(m)}\partial_3(g_S^{(m)})^\dagger=g_N^{(m)}\partial_3(g_N^{(m)})^\dagger, \tag{43}$$

$$\chi^{(m)}=\frac{\mathrm{i}}{2}(\hat{g}_S^{(m)}\partial_3(\hat{g}_S^{(m)})^{-1}-\hat{g}_N^{(m)}\partial_3(\hat{g}_N^{(m)})^{-1}), \tag{44}$$

where

$$\hat{g}_S^{(m)} = g_S^{(m)} \begin{pmatrix} \xi_+ & 0 \\ 0 & \xi_+^{-1} \end{pmatrix} \text{ with } \quad g_S^{(m)} = \frac{1}{(\prod_{i=1}^m (r_i - x_i^3)^2 + \prod_{i=1}^m y_i \overline{y_i})^{1/2}} \begin{pmatrix} \prod_{j=1}^m (r_j - x_j^3) & \prod_{j=1}^m \overline{y_j} \\ -\prod_{j=1}^m y_j & \prod_{j=1}^m (r_j - x_j^3) \end{pmatrix}, \tag{45}$$

$$\hat{g}_N^{(m)} = g_N^{(m)} \begin{pmatrix} \xi_-^{-1} & 0 \\ 0 & \xi_- \end{pmatrix} \text{ with } \quad g_N^{(m)} = \frac{1}{(\prod_{i=1}^m (r_i + x_i^3)^2 + \prod_{i=1}^m y_i \overline{y_i})^{1/2}} \begin{pmatrix} \prod_{j=1}^m \overline{y_j} & \prod_{j=1}^m (r_j + x_j^3) \\ -\prod_{j=1}^m (r_j + x_j^3) & \prod_{j=1}^m y_j \end{pmatrix} \tag{46}$$

and

$$\xi_+ = \prod_{k=1}^m \xi_+(x_k^a) = \prod_{k=1}^m (r_k - x_k^3)^{1/2}, \quad \xi_- = \prod_{k=1}^m \xi_-(x_k^a) = \prod_{k=1}^m (r_k + x_k^3)^{-1/2}. \tag{47}$$

It is not difficult to see that the configuration (43) coincides with (20) and $\chi^{(m)}$ from (44) with $\Phi^{(m)}$ from (28). Thus, we have derived SU(2) multimonopole point-like solutions via a parametric Riemann–Hilbert problem.

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Nonlocal symmetries and the Kaup–Kupershmidt equation

Enrique G. Reyes[a)]
Departamento de Matemáticas y Ciencias de la Computación, Universidad de Santiago de Chile, Casilla 307 Correo 2, Santiago, Chile

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Computational and geometric aspects of nonlocal (infinitesimal) symmetries of nonlinear partial differential equations are considered. In particular, the relation of nonlocal symmetries with classical, generalized and internal symmetries is briefly discussed. A nonlocal symmetry for the Kaup–Kupershmidt equation is introduced and studied in some detail. Some explicit particular solutions are found with its help, and a Darboux-like transformation is also obtained. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1939988]

I. INTRODUCTION

Let $\Xi(x,t,u,\ldots)=0$ be a scalar partial differential equation. An infinitesimal (generalized) symmetry of $\Xi=0$ is a smooth function G depending on x, t, u and a finite number of derivatives of u such that for any solution $u(x,t)$ to $\Xi=0$, the deformed function $u(x,t)+\tau G(x,t)$ is also a solution to first order in τ. At least at a formal level[5,10,34] an infinitesimal generalized symmetry G allows one to generate new solutions from old ones, and indeed, if G depends at most on x, t, u and u_x, one can find a one-parameter group of transformations on the space of first order jets of the trivial bundle $(x,t,u)\mapsto(x,t)$ which "sends solutions to solutions."[26,32,34]

The adjective "infinitesimal" will be omitted hereafter. It is of great interest to extend the symmetry concept, since symmetries are of fundamental importance in the theory of differential equations.[34] A natural generalization is provided by *nonlocal symmetries*, first studied rigorously by Vinogradov and Krasil'shchik[45]: In analogy with the generalized symmetry case, by a nonlocal symmetry of $\Xi(x,t,u,\ldots)=0$ one means, intuitively (a formal definition will be given in Sec. III) a function G which depends on x, t, u, a finite number of x derivatives of u *and for example integrals of u*, such that for any solution $u(x,t)$ of $\Xi=0$, the function $u(x,t)+\tau G(u(x,t))$ is also a solution to first order in τ.

That these symmetries are important has been gradually acknowledged in the literature on geometric aspects of differential equations. For example, they were used in the important paper[45] to generate the hierarchy of Korteweg-de-Vries equations and to derive the Hopf–Cole transformation from symmetry considerations; in the late 1980s they were employed by Bluman *et al.*[9] and Bluman and Kumei[8] to find linearizing transformations for nonlinear partial differential equations, and by Akhatov *et al.*[3] to obtain group classification results and special solutions for equations of thermal conductivity and gas dynamics; in 1992, Fushchych and Tychnin[12] used them to classify linearizable equations. Nonlocal symmetries also appear naturally in integrable systems,[2,11] symmetry reduction of ordinary differential equations,[1] and in the theory of recursion operators.[3,15,16,20,26]

A satisfactory geometric formulation of nonlocal symmetries taking into account the requirement that a symmetry—be it local or not—should (at least formally) transform solutions into solutions, has been developed by Krasil'shchik and Vinogradov, see Refs. 45 and 24–26, and references therein. Their theory is based on an extension, also due to them, of the formal geometry of partial differential equations,[5,26,34] the theory of "coverings" and "diffieties." Explicit compu-

[a)]Electronic mail: ereyes@lauca.usach.cl; ereyes@fermat.usach.cl

tations of nonlocal symmetries (in the Krasil'shchik-Vinogradov sense) appear in Refs. 45 and 26, and have been also carried out by Galas[13] (for KdV, Harry Dym, and AKNS), Leo *et al.*[27,28] (for KdV and Harry Dym), and Reyes[41,42] (for Camassa-Holm, Hunter-Saxton, and KdV). Galas' work has been further considered in Ref. 43. In the papers (Refs. 13, 27, 28, and 41–43) it is also shown how to use these new symmetries to obtain Darboux transformations and/or special solutions for the equations at hand.

It is interesting and natural to study the existence of nonlocal symmetries for equations other than the ones considered in (Refs. 13, 27, 28, 41, and 42) since, in contradistinction with generalized symmetries,[5,26,34] finding them is not an algorithmic task. For instance, the nonlocal symmetries appearing in the articles just cited depend not simply on integrals of the dependent variables, but on solutions to nontrivial first order systems of differential equations.

The goals of this article are to review some aspects of nonlocal symmetries in a form as concrete as possible, to make some preliminary remarks on their relation with other types of symmetries, and to present a new nontrivial example of the theory. A short review of classical, generalized and internal symmetries is in Sec. II (three main classes of *local* symmetries, see Refs. 5 and 14) and nonlocal symmetries are discussed in Sec. III. Although the author's debt to the work of I. Krasil'shchik and A. Vinogradov[24–26] is evident, the presentation of nonlocal symmetries appearing in this work is slightly different to the one in these references, as it does not rely explicitly on the formal differential geometry of infinite dimensional manifolds and their coverings. The article then focuses on the Kaup-Kupershmidt equation

$$q_t = q_{xxxxx} + 5qq_{xxx} + \frac{25}{2}q_x q_{xx} + 5q^2 q_x. \tag{1}$$

Eq. (1) has been chosen because to the author's knowledge no fifth order equation has been considered before from the point of view of nonlocal symmetries, and also because this particular equation has proven to be difficult to analyze by standard means: Kaup[21] introduced Eq. (1) in 1980 and found a solitary wave solution for it using inverse scattering techniques, but its N-soliton solutions have been found only in the last four years,[19,30,37,38,31,46] and other classes of exact solutions for (1) do not appear to have been much considered at all, except perhaps for Refs. 17 and 47.

The Kaup–Kupershmidt equation and its nonlocal symmetry are studied in Sec. IV. As is the case in Refs. 13, 27, 28, 41, and 42, this nonlocal symmetry depends on solutions to first order systems of differential equations determined by (1). Finally, in Sec. V a Darboux-like transformation for Eq. (1) is deduced from the computations carried out in Sec. IV, and some particular solutions are explicitly constructed, using again the results of Sec. IV.

Below and henceforth, independent variables will be denoted by $x^1,\dots,x^n$ and dependent variables by $u^1,\dots,u^m$. The space of dependent and independent variables will be denoted by E. Partial derivatives

$$\frac{\partial^k u^\alpha}{\partial x^{j_1}\cdots\partial x^{j_k}} \tag{2}$$

with respect to (not necessarily different) independent variables $x^{j_1},\dots,x^{j_k}$ will be denoted by $u^\alpha_{x^{j_1}\cdots x^{j_k}}$ or simply by $u^\alpha_{j_1,\dots,j_k}$, and of course u^α_0 will be identified with u^α. Multi-indices will be also used, following the conventions of Ref. 34: A multi-index J will be **either** an *unordered* k-tuple of integers $J=(j_1,\dots,j_k)$, $1\leqslant j_1,\dots,j_k\leqslant n$, with *length* $\#J=k$ indicating how many derivatives are being taken, **or** $J=0$. In the second case, the length of J is $\#J=0$. In this notation, the derivative (2) will be represented simply by u^α_J.

II. ON LOCAL SYMMETRIES OF DIFFERENTIAL EQUATIONS

A. Classical symmetries

Let $\Xi_a(x^i,u^\alpha,\dots,u^\alpha_J)=0$ be an nth order system of partial differential equations, and let V be a vector field on the space E,

$$V=\sum_{i=1}^{n}\xi^i(x^j,u^\beta)\frac{\partial}{\partial x^i}+\sum_{\alpha=1}^{m}\varphi^\alpha(x^j,u^\beta)\frac{\partial}{\partial u^\alpha}.$$

The nth *prolongation* of V is given by the formula

$$pr^{(n)}V=\sum_{i=1}^{n}\xi^i\frac{\partial}{\partial x^i}+\sum_{\alpha=1}^{m}\sum_{0\leqslant\#J\leqslant n}\varphi^\alpha_J\frac{\partial}{\partial u^\alpha_J}, \tag{3}$$

where the functions φ^α_J are obtained inductively by means of

$$\varphi^\alpha_{Ji}=D_i\varphi^\alpha_J-\sum_{k=1}^{n}D_i(\xi^k)u^\alpha_{Jk},\quad \varphi^\alpha_0=\varphi^\alpha, \tag{4}$$

and the *total derivatives* D_i are the formal derivations

$$D_i=\frac{\partial}{\partial x^i}+u^\alpha_i\frac{\partial}{\partial u^\alpha}+u_{i_1i}\frac{\partial}{\partial u^\alpha_{i_1}}+u_{i_1i_2i}\frac{\partial}{\partial u^\alpha_{i_1i_2}}+\cdots. \tag{5}$$

The vector V is a *classical symmetry* of $\Xi_a=0$ if the equations $pr^{(n)}V(\Xi_a)=0$ hold whenever $u^\alpha(x^i)$ is a solution to $\Xi_a=0$.[5,10,26,34] It can be rigorously proven[34] that if V is a classical symmetry, and the system $\Xi_a=0$ satisfies some mild technical conditions, for each value of τ the transformation $x^i\mapsto x^i(\tau)$, $u^\alpha\mapsto u^\alpha(\tau)$ determined by the flow equations:

$$\frac{dx^i}{d\tau}=\xi^i(x^j,u^\beta),\quad \frac{du^\alpha}{d\tau}=\varphi^\alpha(x^j,u^\beta), \tag{6}$$

sends solutions of $\Xi_a=0$ to solutions of the same system.

B. Generalized symmetries

A *differential function* is a smooth function depending on the variables x^i, u^α, and a finite number of partial derivatives of u^α.[34] *Generalized vector fields* on the space E are first order operators of the form

$$V=\sum_{i=1}^{n}\xi^i\frac{\partial}{\partial x^i}+\sum_{\alpha=1}^{m}\varphi^\alpha\frac{\partial}{\partial u^\alpha},$$

in which the functions ξ^i and φ^α are arbitrary differential functions.[5,34] In analogy with II.A., V is a *generalized symmetry* of the system $\Xi_a=0$ if and only if $prV(\Xi_a)=0$ whenever $u^\alpha(x^i)$ is a solution of $\Xi_a=0$, in which prV is now the *infinite prolongation* of the generalized vector field V,

$$prV=\sum_{i=1}^{n}\xi^i\frac{\partial}{\partial x^i}+\sum_{\alpha=1}^{m}\sum_{\#J\geqslant 0}\varphi^\alpha_J\frac{\partial}{\partial u^\alpha_J}, \tag{7}$$

and the functions φ^α_J are given as before by Eq. (4). It can be proven that it is enough[5,26,34] to consider generalized symmetries of the form

$$V = \sum_{\alpha=1}^{m} G^{\alpha} \frac{\partial}{\partial u^{\alpha}}. \tag{8}$$

In this case the condition $prV(\Xi_a)=0$ says that the "infinitesimal deformation" $u^{\alpha}(x^i) + \tau G^{\alpha}(u^{\alpha}(x^i))$ solves $\Xi_a=0$ to first order in τ whenever $u^{\alpha}(x^i)$ is a solution of $\Xi_a=0$, and one recovers the preliminary definition of generalized symmetries given in the Introduction. If $u_0^{\alpha}(x^i)$ is a solution to $\Xi_a=0$ and V is a generalized symmetry as in (8), then for any τ the solution $u^{\alpha}(x^i,\tau)$ to the Cauchy problem

$$\frac{\partial u^{\alpha}}{\partial \tau} = G^{\alpha}, \quad u^{\alpha}(x^i,0) = u_0^{\alpha}(x^i) \tag{9}$$

is also a solution to $\Xi_a=0$.[34] In spite of the formal character of this result,[5,10,34] generalized symmetries are of great interest: they are an essential ingredient of Noether's theorem[34] and, they are one of the most important indicators of integrability available for partial differential equations.[32,34]

C. Internal symmetries

In order to introduce internal symmetries one has to dwell a little deeper on the geometry of differential equations.[5,26,34]

Assume that E has a trivial bundle structure, $E=X\times U\to X$, in which X is the space of variables x^i and U is the space of variables u^{α}. Let J^NE be the Nth order jet bundle of E equipped with local coordinates

$$(x^1,\ldots,x^n,u^1,\ldots,u^m,u^1_{j_1},\ldots u^m_{j_1},\ldots,u^1_{j_1j_2\ldots j_k},\ldots,u^m_{j_1j_2\ldots j_k}),$$

in which $J=(j_1,j_2,\ldots,j_k)$ runs over all multi-indices of length at most N, and let $J^{\infty}E$ be the *infinity jet bundle* of E equipped with coordinates

$$(x^1,\ldots,x^n,u^1,\ldots,u^m,u^1_1,\ldots u^m_n,\ldots,u^1_{j_1j_2\ldots j_k},\ldots,u^m_{j_1j_2\ldots j_k},\ldots) \tag{10}$$

in which $J=(j_1,j_2,\ldots,j_k)$ runs now over *all* multi-indices of length $\#J\geqslant 0$.

An Nth order system $\Xi_a=0$ defines a locus in J^NE, and one assumes that this locus can be restricted to a submanifold S^N of J^NE which fibers over X. The kth *prolongation* of $\Xi_a=0$, $k\geqslant 1$, is the system of differential equations

$$D_K\Xi_a = 0, \quad 0 \leqslant \#K \leqslant k \tag{11}$$

in which $D_K=D_{k_1}D_{k_2}\cdots D_{k_p}$ if $K=(k_1,\ldots,k_p)$. For each $k\geqslant 1$ one restricts the locus in $J^{N+k}E$ determined by (11) to a submanifold S^{N+k} of $J^{N+k}E$, and one further assumes that S^{N+k} fibers over S^{N+k-1}. The "tower" $S^N\leftarrow S^{N+1}\leftarrow\cdots$ determines a sub-bundle S^{∞} of $J^{\infty}E$ locally described by the set of points (10) that satisfy $\Xi_a=0$ and all its differential consequences (11). This subbundle is called the *equation manifold* of the system $\Xi_a=0$.

A few facts on the geometry of $J^{\infty}E$ need to be recalled: Smooth functions on $J^{\infty}E$ are the differential functions defined before, and vector fields on $J^{\infty}E$ are formal series

$$X = A_i \frac{\partial}{\partial x^i} + \sum_{\#J\geqslant 0} B_J^{\alpha} \frac{\partial}{\partial u_J^{\alpha}}, \tag{12}$$

in which A_i, B_J^{α} are differential functions. Differential k-forms are finite linear combinations of terms $Adx^{i_1}\wedge\cdots\wedge dx^{i_p}\wedge du_{J_1}^{\alpha_1}\wedge\cdots\wedge du_{J_q}^{\alpha_q}$ in which $p+q=k$ and A is smooth. A differential form ω is a *contact form* if $j^{\infty}(s)^*\omega=0$ for all local sections $s:(x^i)\mapsto(x^i,u^{\alpha}(x^i))$ of E, in which $j^{\infty}(s)$ is the *infinite prolongation* of s given by $j^{\infty}(s)(x^i)=(x^i,u^{\alpha}(x^i),\ldots,u_J^{\alpha}(x^i),\ldots)$. The space of contact forms on $J^{\infty}E$ will be denoted by $C(J^{\infty}E)$.

All the foregoing constructions remain valid, via pull-back, on the equation manifold S^∞ of a system of partial differential equations $\Xi_a=0$.

An (infinitesimal) *contact transformation* is a vector field X on $J^\infty E$ such that $X(C(J^\infty E))\subseteq C(J^\infty E)$ (that is, the Lie derivative of any contact form with respect to X is again a contact form). A contact transformation X is an *external* symmetry of a system of differential equations $\Xi_a=0$ if $X(\Xi_a)=0$ on solutions to $\Xi_a=0$. An *internal* symmetry of $\Xi_a=0$ is a vector field X *on* S^∞ such that $X(C(S^\infty))\subseteq C(S^\infty)$ (Refs. 5, 14, and 26, and references therein), in which $C(S^\infty)$ denotes the space of contact forms on S^∞.

If $\Xi_a=0$ is of order N, one defines *mutatis mutandis* contact transformations on $J^N E$ and internal symmetries on S^N. The following basic result holds.[5]

Theorem 1. *Let $\Xi_a=0$ be a system of equations of order N and let W be a vector field on S^N. If W is an internal symmetry and $V=\pi(W)$ is the projection of W to the bundle E, then V is a generalized symmetry of the system $\Xi_a=0$.* Moreover, $W=(prV)|_{S^N}$.

An "S^∞" version of this result is in Ref. 26 and references therein. The precise relations among classical, generalized and internal symmetries, however, are quite subtle.[5,14] For instance,[5] if a system $\Xi_a=0$ satisfies a technical condition, then every internal symmetry on S^N is obtained by restriction to S^N of a *first order* generalized symmetry of $\Xi_a=0$.

One would argue that nonlocal symmetries should be properly considered as generalizing the class of *internal* symmetries. Some comments to support this point of view are at the end of Sec. III.

III. NONLOCAL SYMMETRIES

The discussion of nonlocal symmetries given in this section is an operational version of the deep geometric theory of Krasil'shchik and Vinogradov.[45,24–26] There are at least two reasons why one would consider their viewpoint as the most satisfactory theory of nonlocalities for differential equations: First, their approach is completely general; there are no a priori restrictions on the *form* nonlocal objects may take, as it happens for instance in Refs. 10 and 20. Second, Krasil'shchik and Vinogradov take naturally into account the fact that there are examples of nonlocal symmetries[13,22,27,28,41,42] which make sense *only if defined on solutions* of a given differential equation.

The following notation will be used: For some extra variables δ_b (to be identified below with new dependent variables) and smooth functions Y_{ib} depending on x^i, u^α, δ_b, and x^i derivatives of u^α, one sets

$$\tilde{D}_i = D_i + \sum_{b=1}^{N} Y_{ib}\frac{\partial}{\partial \delta_b}, \tag{13}$$

and for a given system $\Xi_a=0$ of partial differential equations one defines

$$\widetilde{\Xi}_* = \left(\sum_L \frac{\partial \Xi_a}{\partial u_L^\alpha}\tilde{D}_L\right) = \begin{pmatrix} \dfrac{\partial \Xi_1}{\partial u^1} + \cdots + \dfrac{\partial \Xi_1}{\partial u_I^1}\tilde{D}_I & \dfrac{\partial \Xi_1}{\partial u^2} + \cdots + \dfrac{\partial \Xi_1}{\partial u_J^2}\tilde{D}_J & \cdots \\ \dfrac{\partial \Xi_2}{\partial u^1} + \cdots + \dfrac{\partial \Xi_2}{\partial u_K^1}\tilde{D}_K & \cdots & \cdots \\ \vdots & & \end{pmatrix}. \tag{14}$$

Definition 1: Let $\Xi_a(x^i,u^\alpha,\ldots,u^\alpha_{J_a})=0$ $(i=1,\ldots,n;\ \alpha=1,\ldots,m)$ *be a system of partial differential equations and let* $\{\gamma_b : b=1,2,\ldots,N\}$ *be a new collection of dependent variables. An ordered* $(m+N)$*-tuple of functions* (G^α,H_b)*, depending on the variables* x^i, u^α, γ_b *and finite numbers of* x^i *derivatives of* u^α*, is a nonlocal symmetry of* $\Xi_a=0$ *if there exist functions* X_{ib} *depending on* x^i, u^α, γ_b and x^i*-derivatives of* u^α*, such that the equations*

$$\tilde{D}_i(X_{jb}) = \tilde{D}_j(X_{ib}), \quad i,j=1,2,\ldots,n, \quad b=1,2,\ldots,N, \tag{15}$$

$$\widetilde{\Xi}_*(G) = 0, \tag{16}$$

$$\widetilde{D}_i(H_b) = \widetilde{D}_\tau(X_{ib}), \tag{17}$$

hold whenever $u^\alpha(x^i)$ *is a solution to* $\Xi_a = 0$.

The operators $\widetilde{D}_i$ *are defined as in* (13) *with* Y_{ib} *replaced by the functions* X_{ib} *and* δ_b *replaced by the functions* γ_b*; the matrix* $\widetilde{\Xi}_*$ *in Eq.* (16) *is the matrix* (14) *determined by the system of equations* $\Xi_a = 0$ *and the operators* $\widetilde{D}_i$*; the vector G is* $(G^1, G^2, \ldots, G^m)^t$*; and finally, the operator* $\widetilde{D}_\tau$ *appearing in* (17) *is given by*

$$\widetilde{D}_\tau = \sum_{\alpha=1}^{m} \sum_{\#K \geqslant 0} \widetilde{D}_K(G^\alpha) \frac{\partial}{\partial u_K^\alpha} + \sum_{c=1}^{N} H_c \frac{\partial}{\partial \gamma_c}. \tag{18}$$

The new dependent variables γ_b are the "nonlocal variables," the operators $\widetilde{D}_i$ *satisfying Eq.* (15) are the new total derivatives of the theory, and the corresponding matrix $\widetilde{\Xi}_*$ is the nonlocal version of the *formal linearization* of the system $\Xi_a = 0$. The space $\widetilde{N}$ described locally as the set of coordinates $(x^i, u^\alpha, \ldots, u_J^\alpha, \ldots, \gamma_b)$ and equipped with total derivative operators $\widetilde{D}_i$ satisfying Eq. (15), is said to be a *covering* of the equation manifold S^∞ of the system $\Xi_a = 0$.

Note that Eq. (16) depends only on the functions G^α and the symmetry of equations at hand. Following Krasil'shchik and Vinogradov[24,26,45] one says that the functions G^α are the *shadow* of the nonlocal symmetry (G^α, H_b). It is important to stress that, basically due to the amazing freedom one has to define nonlocal objects (see, e.g.. Refs. 18, 22, and 44), there is no general algorithmic method to find shadows, in contradistinction with the local theory as explained in Refs. 10, 26, and 34.

Example 1: The Kaup–Kupershmidt equation,

$$q_t = q_{xxxxx} + 5qq_{xxx} + (25/2)q_x q_{xx} + 5q^2 q_x, \tag{19}$$

is the integrability condition of the linear problem $\Psi_x = X\Psi$ and $\Psi_t = T\Psi$, in which X and T are given by[33]

$$X = \begin{bmatrix} 0 & 1/(4\lambda^2) \\ -\lambda^2 q & 0 \end{bmatrix} \tag{20}$$

and

$$T = \begin{bmatrix} -(q_{xxx}/4 + qq_x) & (q_{xx}/2 + q^2)/(4\lambda^2) \\ -\lambda^2(q_{xxxx} + 9qq_{xx}/2 + 4q_x^2 + q^3) & q_{xxx}/4 + qq_x \end{bmatrix}. \tag{21}$$

Set $\Psi = (\alpha, \delta)^t$. Then, one checks (using Anderson's VESSIOT package, for instance, see Ref. 4) that

$$G = \alpha^3 \delta \tag{22}$$

is a shadow of a nonlocal symmetry for (19).

An important issue is to motivate Definition 1: First, one should certainly modify the total derivative operators D_i defined in (5), since one wishes to introduce new dependent variables (the "nonlocal variables" of the theory) and total derivatives should take them into account. The operators $\widetilde{D}_i$ appearing in Definition 1 are these new total derivatives, and since one expects $\widetilde{D}_j\widetilde{D}_i = \widetilde{D}_i\widetilde{D}_j$, the equations $\widetilde{D}_i(X_{jb}) = \widetilde{D}_j(X_{ib})$ should hold *on solutions to* $\Xi_a = 0$.

Now, the total derivatives $\widetilde{D}_i$ satisfy $\widetilde{D}_i(\gamma_b) = X_{ib}$, and these equations are compatible because (15) holds. Since *on solutions to the system of equations* $\Xi_a = 0$ the total derivatives $\widetilde{D}_i$ should become ordinary partial derivatives, one concludes that the equations

$$\frac{\partial \gamma_b}{\partial x^i} = X_{ib} \tag{23}$$

should hold for each index b whenever $u^\alpha(x^i)$ is a solution to $\Xi_a=0$. These compatible equations specify the relation between the variables u^α and γ_b whenever $u^\alpha(x^i)$ is a solution to $\Xi_a=0$.

Next, if (G^α, H_b) is a nonlocal symmetry, the deformed variables $u^\alpha+\tau G^\alpha$ should satisfy $\Xi_a=0$ to first order in τ, as in the generalized symmetry case. This means that the equation

$$\frac{\partial \Xi_a}{\partial u^\alpha} u^\alpha_\tau + \frac{\partial \Xi_a}{\partial u^\alpha_{i_1}} u^\alpha_{i_1\tau} + \cdots + \frac{\partial \Xi_a}{\partial u^\alpha_J} u^\alpha_{J_\tau} = 0 \tag{24}$$

should hold whenever $u^\alpha(x^i)$ is a solution to $\Xi_a=0$ and $u^\alpha_\tau = G^\alpha$. Computing $u^\alpha_{i\tau} = u^\alpha_{\tau i}$ on solutions $u^\alpha(x^i)$, one finds

$$u^\alpha_{i\tau} = \frac{\partial G^\alpha}{\partial x^i} = \frac{\partial G^\alpha}{\partial x^i} + \frac{\partial G^\alpha}{\partial u^\beta} u^\beta_i + \cdots + \frac{\partial G^\alpha}{\partial u^\beta_K} u^\beta_{Ki} + \frac{\partial G^\alpha}{\partial \gamma_b} \gamma_{b,i} \tag{25}$$

$$= D_i G^\alpha + \sum_{b=1}^{N} X_{ib} \frac{\partial G^\alpha}{\partial \gamma_b} = \tilde{D}_i G^\alpha. \tag{26}$$

Hence, Eq. (24) becomes

$$\frac{\partial \Xi_a}{\partial u^\alpha} G^\alpha + \frac{\partial \Xi_a}{\partial u^\alpha_{i_1}} \tilde{D}_{i_1} G^\alpha + \cdots + \frac{\partial \Xi_a}{\partial u^\alpha_J} \tilde{D}_J G^\alpha = 0$$

for each index a, and so Eq. (16) should hold.

Finally, not only the dependent variables u^α are deformed, but also the nonlocal variables γ_b—related to u^α by Eq. (23)—change as u^α change (see e.g., Refs. 13, 27, 28, 41, and 42). This change is measured by the deformation $\gamma_b \mapsto \gamma_b + \tau H_b$. One expects that for each index b the function $\gamma_b + \tau H_b$ satisfies (23) to first order in τ whenever $u^\alpha(x^i)$ is a solution to $\Xi_a=0$. Equivalently,

$$\frac{\partial H_b}{\partial x^i} = \frac{\partial X_{ib}}{\partial \tau} \tag{27}$$

whenever $u^\alpha(x^i)$ is a solution to $\Xi_a=0$ and $\gamma_{b,\tau}=H_b$. Expanding one finds,

$$\frac{\partial H_b}{\partial x^i} = \frac{\partial H_b}{\partial x^i} + \frac{\partial H_b}{\partial u^\alpha} u^\alpha_i + \frac{\partial H_b}{\partial u^\alpha_{i_1}} u^\alpha_{i_1 i} + \cdots + \frac{\partial H_b}{\partial u^\alpha_J} u^\alpha_{Ji} + \cdots + \frac{\partial H_b}{\partial \gamma_c} \gamma_{c,i} = D_i H_b + \frac{\partial H_b}{\partial \gamma_c} X_{ic} = \tilde{D}_i H_b$$

and

$$\begin{aligned} \frac{\partial X_{ib}}{\partial \tau} &= \frac{\partial X_{ib}}{\partial u^\alpha} u^\alpha_\tau + \frac{\partial X_{ib}}{\partial u^\alpha_{i_1}} u^\alpha_{i_1\tau} + \cdots + \frac{\partial X_{ib}}{\partial u^\alpha_J} u^\alpha_{J_\tau} + \cdots + \frac{\partial X_{ib}}{\partial \gamma_c} \gamma_{c\tau} \\ &= \frac{\partial X_{ib}}{\partial u^\alpha} G^\alpha + \frac{\partial X_{ib}}{\partial u^\alpha_{i_1}} \tilde{D}_{i_1} G^\alpha + \cdots + \frac{\partial X_{ib}}{\partial u^\alpha_J} \tilde{D}_J G^\alpha + \frac{\partial X_{ib}}{\partial \gamma_c} H_c = \tilde{D}_\tau X_{ib} \end{aligned}$$

that is, (27) is precisely Eq. (17).

The foregoing discussion tells one how to construct nonlocal symmetries *starting from a shadow* G^α: In the process of finding G^α one also finds a collection of new dependent variables ξ_d, and a corresponding collection of compatible equations

$$\frac{\partial \xi_d}{\partial x^i} = Z_{id}(x^i, u^\alpha, u^\alpha_{x^j}, \ldots, u^\alpha_{x^{j_1}\ldots x^{j_i}}, \xi_d), \tag{28}$$

stating how these new variables are related to the original variables u^α. One has to see how ξ_d change as u^α change under the deformation $u^\alpha \mapsto u^\alpha + \tau G^\alpha$. Formally differentiate (28) with respect to τ, and simplify using $u^\alpha_\tau = G^\alpha$. One obtains a compatible system of first order equations for $\xi_{d,\tau}$ of the form

$$\frac{\partial \xi_{d,\tau}}{\partial x^i} = \widetilde{Z}_{id}(x^i, u^\alpha, u^\alpha_{x^k}, \ldots, u^\alpha_{x^{k_1}\ldots x^{k_i}}, \xi_d, \xi_{d,\tau}), \tag{29}$$

which has to be solved for $\xi_{d,\tau}$ assuming (28). If (29) has a solution in terms of x^i, u^α,..., u^α_J, and ξ_d, one is done. If not, add new dependent variables, η_e say, related to u^α and ξ_d by further compatible differential equations

$$\frac{\partial \eta_e}{\partial x^i} = Y_{ie}(x^i, u^\alpha, u^\alpha_{x^j}, \ldots, u^\alpha_{x^{j_1}\ldots x^{j_i}}, \xi_d, \eta_e), \tag{30}$$

and write $\xi_{d,\tau} = F_d(x^i, u^\alpha, \ldots, u^\alpha_{x^{k_1}\ldots x^{k_d}}, \xi_d, \eta_e)$. Now find $\eta_{e,\tau}$, and so on. Eventually one will obtain a set of new dependent variables collectively called γ_b, a corresponding set of functions X_{ib} and compatible equations

$$\frac{\partial \gamma_b}{\partial x^i} = X_{ib}(x^i, u^\alpha, u^\alpha_{x^j}, \ldots, u^\alpha_{x^{j_1}\ldots x^{j_i}}, \gamma_c), \tag{31}$$

and a corresponding set of infinitesimal variations of the form

$$\frac{\partial \gamma_b}{\partial \tau} = H_b(x^i, u^\alpha, \ldots, u^\alpha_{x^{k_1}\ldots x^{k_b}}, \gamma_c). \tag{32}$$

Define total derivatives $\widetilde{D}_i$ by (13) with functions Y_{ib} replaced by X_{ib}. Then, (G^α, H_b) is a bona fide nonlocal symmetry. It is a theorem due to Khorkova, see Refs. 25 and 26 and references therein, that one can always construct a nonlocal symmetry starting from a shadow. Examples appear in Refs. 10, 13, 25, 27, 28, 41, and 42.

Example 2: It was proven in Ref. 45 that

$$G = (2S_x - uS)\mathrm{e}^{-(1/2)\int u \mathrm{d}x}, \tag{33}$$

in which S satisfies $S_t = S_{xx}$, is a shadow of a nonlocal symmetry of Burgers equation $u_t = u_{xx} + uu_x$. Consider an extra dependent variable γ_1 defined by the compatible equations $\gamma_{1,x} = u = X_{11}$ and $\gamma_{1,t} = u_x + \frac{1}{2}u^2 = X_{21}$, and set $G^1 = (2S_x - uS)\exp(-(1/2)\gamma_1)$. Compute $\gamma_{1,\tau x} = \gamma_{1,x\tau} = u_\tau = (2S_x - uS)\mathrm{e}^{-(1/2)\gamma_1} = (2S\mathrm{e}^{-(1/2)\gamma_1})_x$. Thus, $\gamma_{1,\tau} = 2S\exp\left(-\frac{1}{2}\gamma_1\right)$, and one can define $H_1 = 2S\exp\left(-\frac{1}{2}\gamma_1\right)$. The deformations $u \mapsto u + \tau G^1$ and $\gamma_1 \mapsto \gamma_1 + \tau H_1$ satisfy the equations

$$u_t = u_{xx} + uu_x, \quad \gamma_{1,x} = u, \quad \gamma_{1,t} = u_x + \tfrac{1}{2}u^2$$

to first order in τ, and (G^1, H_1) is therefore a nonlocal symmetry for Burgers equation. This example is further examined in Refs. 10, 25, and 39.

Now consider flows of nonlocal symmetries. First of all, one has the following.

Proposition 1: Let $\Xi_a(x^i, u^\alpha, \ldots) = 0$ *be a system of partial differential equations. Assume that* $\{\gamma_b\}$ *is a finite set of nonlocal variables and that* $\widetilde{D}_i = D_i + \Sigma X_{ib}\partial/\partial\gamma_b$ *satisfy Eq.* (15). If G^α *and* H_b *are functions depending on the variables* x^i, u^α, γ_b *and finite numbers of* x^i *derivatives of* u^α *such that* (G^α, H_b) *is a nonlocal symmetry of* $\Xi_a = 0$, *the vector field*

$$G^\alpha \frac{\partial}{\partial u^\alpha} + H_b \frac{\partial}{\partial \gamma_b} \tag{34}$$

is a generalized symmetry of the augmented system

$$\Xi_a = 0, \quad \frac{\partial \gamma_b}{\partial x^i} = X_{ib}. \tag{35}$$

Conversely, if (34) is a generalized symmetry of the system (35), (G^α, H_b) *is a nonlocal symmetry of* $\Xi_a = 0$.

Proof: The vector field (34) is a generalized symmetry of the system (35) if and only if the linearized equations

$$\Xi_{a,\tau} = 0, \quad \frac{\partial}{\partial \tau}\left(\frac{\partial \gamma_b}{\partial x^i}\right) = X_{ib,\tau} \tag{36}$$

with $u^\alpha_\tau = G^\alpha$ and $\gamma_{b,\tau} = H_b$ are satisfied whenever $u^\alpha(x^i)$ and $\gamma_b(x^i)$ are solutions to (35). But, as it can be seen from Eq. (25), the equation $\Xi_{a,\tau} = 0$ is precisely $\tilde{\Xi}_*(G^\alpha)^T = 0$, and this equation holds because (G^α, H_b) is a nonlocal symmetry. Also, the second equation appearing in (36) is equivalent to $H_{b,x^i} = X_{ib,\tau}$ on solutions to (35), and the discussion following Eq. (27) shows that this condition holds if (G^α, H_b) is a nonlocal symmetry. The converse is also clear. □

Example 3: The nonlinear thermal conductivity equation

$$u_t = \left(\frac{u_x}{1+u^2}\right)_x \tag{37}$$

is discussed by Akhatov *et al.*[3] It follows from the analysis of Ref. 3 that the differential function $G = 1 + u^2 + v u_x$, in which v is a potential defined by the equations

$$v_x = u, \quad v_t = \frac{v_{xx}}{1+v_x^2}, \tag{38}$$

is the shadow of a nonlocal symmetry for (37). Proceeding as in Example 2 one easily obtains the genuine nonlocal symmetry $(1 + u^2 + v u_x, x + v v_x)$, and therefore one can conclude that the system of equations (37) and (38), possess the first order generalized symmetry

$$(1 + u^2 + v u_x)\frac{\partial}{\partial u} + (x + v v_x)\frac{\partial}{\partial v}.$$

One says that a nonlocal symmetry is *of type* Γ if it depends on a finite number of nonlocal variables $\Gamma = \{\gamma_b\}$. The following corollary is immediate from Proposition 1 and the well known fact that generalized symmetries of a given system of equations form a Lie algebra:[26,34,36]

Corollary 1: Let $\Xi_a(x^i, u^\alpha, \ldots) = 0$ *be a system of partial differential equations. Assume that* $\Gamma = \{\gamma_b\}$ *is a finite set of nonlocal variables and that* $\tilde{D}_i = D_i + \Sigma X_{ib} \partial / \partial \gamma_b$ *satisfy Eq. (15). Then, the set of all nonlocal symmetries of type* Γ *of* $\Xi_a = 0$ *forms a Lie algebra.*

Remark 1: It seems it was generally believed that a much stronger form of Corollary 1 should hold, namely, that the collection of evolutionary vector fields (8) with coefficients depending on *arbitrary* nonlocal variables should form a Lie algebra. Sanders and Wang, (see Ref. 36, and references therein) showed that this is in fact not true, as these vector fields *do not* satisfy the Jacobi identity. Olver *et al.*[36] and Olver[35] have recently developed a formal calculus of nonlocal evolutionary vector fields of a very general kind which does not suffer of this handicap. Some comments on the problem of equipping the collection of "all" nonlocal symmetries of a given equation with a Lie algebra structure appear in Ref. 25.

Corollary 2: If $u_0^\alpha(x^i)$ *and* $\gamma_b^0(x^i)$ *are solutions to the augmented system (35), the Cauchy problem*

$$\frac{\partial u^\alpha}{\partial \tau} = G^\alpha, \quad \frac{\partial \gamma_b}{\partial \tau} = H_b,$$

$$u^\alpha(x^i,0)=u_0^\alpha(x^i),\quad \gamma_b(x^i,0)=\gamma_b^0(x^i),$$

determines one-parameter family of solutions to the augmented system (35). Therefore nonlocal symmetries send solutions to the original system $\Xi_a=0$ *to solutions of the same system.*

A subtler issue concerns the relation between nonlocal and internal symmetries. Consider the shadows of nonlocal symmetries for the Burger and Kaup–Kupershmidt equations introduced in Examples 2 and 1, respectively, and let the equation manifolds of these equations, S^∞_{Burger} and S^∞_{KK} respectively, be submanifolds of the infinite jet bundles $J^\infty E_{\text{Burger}}$ and $J^\infty E_{\text{KK}}$. The vector fields determined by (33) and (22),

$$\left[(2S_x-uS)\exp\left(-\frac{1}{2}\int u dx\right)\right]\frac{\partial}{\partial u} \tag{39}$$

(for Burger's) and

$$\alpha^3\delta\frac{\partial}{\partial u} \tag{40}$$

(for Kaup–Kupershmidt) are quite different:

(a) In the case of (39) it should be possible, intuitively, to add an extra dependent variable u_{-1} satisfying $D_x u_{-1}=u$ to the infinite jet bundle $J^\infty E_{\text{Burger}}$, in which $D_x=\partial/\partial x+u_x\partial/\partial u+u_{xx}\partial/\partial u_x+\cdots$, see Eq. (5). In the Krasil'shchik–Vinogradov scheme[26] this would correspond to building a manifold N equipped with coordinates $(x^i,u,\ldots,u_{-1})$ which "covers" $J^\infty E_{\text{Burger}}$. (As stated in Remark 1, the construction of N as a manifold with a well-defined tangent bundle is not trivial: it is necessary to set up a special formal machinery in order to construct Lie algebras of vector fields with nonlocal coefficients.[36,35]). The vector field (39) would then be a vector field on N *which would restrict* to (a covering of) the equation manifold S^∞_{Burger}, thereby determining a shadow of a nonlocal symmetry of Burger's equation.

(b) On the other hand, it is hard to see how one could make the procedure above work in the Kaup–Kupershmidt case: it does not seem appropriate to consider the variables α and δ appearing in (40) as functions on some universal manifold covering $J^\infty E_{\text{KK}}$. A more natural point of view is to think of the vector field (40) as defined only on a covering of the equation manifold S^∞_{KK}, *independently* of whether or not one can extend it to a vector field on a covering of the infinite jet bundle $J^\infty E_{\text{KK}}$.

Thus, it would seem reasonable to call the nonlocal symmetry induced by (40) an *internal* nonlocal symmetry, and to claim that nonlocal symmetries provide an interesting and natural generalization of the class of (local) *internal* symmetries. One wonders if an analysis like the one performed in Ref. 5 for these symmetries can be made in this nonlocal setting.

IV. THE KAUP-KUPERSHMIDT EQUATION

The theory reviewed in the previous sections will be now applied to the interesting Kaup–Kupershmidt equation[21,30,31,37,38,46]

$$q_t=q_{xxxxx}+5qq_{xxx}+\frac{25}{2}q_xq_{xx}+5q^2q_x. \tag{41}$$

As a first remark, recall from Example 1 that Eq. (41) is the integrability condition of the linear problem[33]

$$\begin{pmatrix}\psi_{1,x}\\ \psi_{2,x}\end{pmatrix}=\begin{bmatrix}0 & 1/(4\eta^2)\\ -\eta^2 q & 0\end{bmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}, \tag{42}$$

$$\begin{pmatrix}\psi_{1,t}\\ \psi_{2,t}\end{pmatrix}=\begin{bmatrix}-(\frac{1}{4}q_{xxx}+qq_x) & (\frac{1}{2}q_{xx}+q^2)/(4\eta^2)\\ -\eta^2(q_{xxxx}+\frac{9}{2}qq_{xx}+4q_x^2+q^3) & \frac{1}{4}q_{xxx}+qq_x\end{bmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}. \tag{43}$$

As is well known, equations which are the integrability condition of linear problems *with parameter*, $\Psi_x=X\Psi$, $\Psi_t=T\Psi$, in which X, T belong to a given (matrix) Lie algebra $\tilde{g}$, are of great interest because, in principle, they can be investigated by means of scattering/inverse scattering techniques.[6,7,21] A key point in this theory, however, is that the parameter must be *intrinsic*[29] and it is generally agreed that this means (at least) that one cannot eliminate it by means of a simple gauge transformation

$$X\mapsto AXA^{-1}+\left[\frac{\partial}{\partial x}A\right]A^{-1},\quad T\mapsto ATA^{-1}+\left[\frac{\partial}{\partial t}A\right]A^{-1}, \tag{44}$$

in which A is an invertible matrix belonging to the Lie group with Lie algebra $\tilde{g}$. In the case at hand, the parameter η appearing in (42) and (43) *can* be removed by applying a gauge transformation (44) with $A\in SL(2,\mathbf{R})$ given simply by

$$A=\begin{bmatrix}\eta & 0\\ 0 & 1/\eta\end{bmatrix}.$$

[And indeed, the linear problem with intrinsic parameter used to analyze Eq. (41) via scattering/inverse scattering is an $sl(3,\mathbf{R})$-valued problem, see Refs. 6, 7, and 21].

However, one would claim that linear problems without parameter may also be of interest. For example, a linear problem with a removable parameter[29] for the Burgers equation yields, nonetheless, the linearizing Hopf–Cole transformation[39,40] and, as it will be seen momentarily, the linear problem (42) and (43) allows one to find a *nontrivial* nonlocal symmetry for the Kaup–Kupershmidt equation which in turn yields nontrivial particular solutions to (41).

The nonlocal symmetry of Kaup–Kupershmidt to be considered here depends on solutions to first order systems of equations determined by Eq. (41) via its $sl(2,\mathbf{R})$-valued associated linear problem (42), (43). These systems can be understood geometrically,[39,40] but they can also be built from scratch:

First, set $\alpha=\psi_2/\psi_1$. The linear problem (42) and (43) yields the Pfaffian system[33]

$$\alpha_x=-\eta^2q-\frac{\alpha^2}{4\eta^2}, \tag{45}$$

$$\alpha_t=-\eta^2q_{xxxx}-\frac{9}{2}\eta^2qq_{xx}-4\eta^2q_x{}^2-\eta^2q^3+\left(\frac{1}{2}q_{xxx}+2qq_x\right)\alpha-\left(\frac{q_{xx}}{8\eta^2}+\frac{q^2}{4\eta^2}\right)\alpha^2, \tag{46}$$

and one checks that (45) and (46) is completely integrable for $\alpha(x,t)$ whenever $q(x,t)$ is a solution to Eq. (41). The function $\alpha(x,t)$ is said to be a *quadratic pseudopotential* for the Kaup–Kupershmidt equation.

Second, write Eq. (46) in the form $U_t=V_x$ for some functions U and V using Eq. (45), and define a potential δ satisfying $\delta_x=U$, $\delta_t=V$ on solutions of Eq. (41). After a straightforward computation, one obtains that δ is determined by the following equations:

$$\delta_x=-\frac{\alpha}{2\eta^2}, \tag{47}$$

$$\delta_t=\frac{1}{2}q_{xxx}+2qq_x-\alpha\left(\frac{q_{xx}}{4\eta^2}+\frac{q^2}{2\eta^2}\right). \tag{48}$$

The proposition below then holds. Its proof is a (rather long) computation which is best performed by using a symbolic computation package such as the MAPLE package VESSIOT:[4]

Proposition 2: With the foregoing notations, the vector field

$$V_G = \alpha \exp(-2\delta)\frac{\partial}{\partial q} \tag{49}$$

is the shadow of a nonlocal symmetry for the Kaup-Kupershmidt equation (41).

One now extends this shadow to a nonlocal symmetry for (41). Set

$$q_\tau = \alpha \exp(-2\delta), \tag{50}$$

and find the variations of α and δ with respect to the parameter τ. Taking τ derivatives in Eq. (45) one obtains

$$\alpha_{x\tau} = -\eta^2 q_\tau - \frac{1}{2\eta^2}\alpha\alpha_\tau = -\eta^2\alpha\exp(-2\delta) - \frac{1}{2\eta^2}\alpha\alpha_\tau.$$

Multiplying by the integrating factor $\exp(\int \alpha/2\eta^2 \mathrm{d}x)$ and using (47), one finds

$$\alpha_\tau = -\frac{2}{3}\eta^4\exp(-2\delta) + C\exp(\delta), \tag{51}$$

in which C is independent of x. Now take derivative with respect to τ in (47):

$$\delta_{x\tau} = -\frac{1}{2\eta^2}\alpha_\tau = \frac{\eta^2}{3}\exp(-2\delta) - \frac{C}{2\eta^2}\exp(\delta).$$

Since the right-hand side of this equation is not a total x derivative, simply define a further potential β by means of

$$\beta_x = \frac{\eta^2}{3}\exp(-2\delta) - \frac{C}{2\eta^2}\exp(\delta) \tag{52}$$

and set

$$\delta_\tau = \beta. \tag{53}$$

In order to determine β one needs to compute $\beta_t = \delta_{\tau t} = \delta_{t\tau}$ taking into account Eqs. (50), (51), and (53). Before doing this, it is instructive to try to find β_τ by differentiating Eq. (52) with respect to τ:

$$\begin{aligned}\beta_{x\tau} &= -2\delta_\tau\frac{\eta^2}{3}\exp(-2\delta) - \frac{C}{2\eta^2}\delta_\tau\exp(\delta)\\ &= -2\beta\left[\frac{\eta^2}{3}\exp(-2\delta) + \frac{C}{4\eta^2}\exp(\delta)\right] = -2\beta\left[\beta_x + \frac{3C}{4\eta^2}\exp(\delta)\right],\end{aligned} \tag{54}$$

in which (52) has been used. The right-hand side of Eq. (54) is not a total x derivative *unless* $C=0$, and if $C=0$, Eq. (54) implies that

$$\beta_\tau = -\beta^2. \tag{55}$$

It follows that $C=0$ is necessary and sufficient for obtaining a nonlocal symmetry with shadow (49) depending only on the nonlocal variables α, δ, and β, in analogy with the examples worked out in Refs. 13, 22, 27, 28, 41, and 42, and this condition will be used henceforth. It seems plausible to conjecture that if $C\neq 0$ one would obtain instead an infinite dimensional extension of the shadow (49). An example of such an extension (for Burger's) is in Ref. 26.

The foregoing discussion implies that the following result holds.

Theorem 2: *Consider the pseudopotential α determined by Eqs.* (45) and (46), *and the*

potential δ *given by* (47) and (48). *Define* β *by means of*

$$\beta_x = \frac{\eta^2}{3}\exp(-2\delta), \tag{56}$$

$$\beta_t = \exp(-2\delta)\left\{\left(-\frac{1}{3}q_{xx} - \frac{5}{12}q^2\right)\eta^2 + \frac{1}{2}\alpha q_x - \frac{3}{8}\frac{\alpha^2 q}{\eta^2} - \frac{3}{64}\frac{\alpha^4}{\eta^6}\right\}. \tag{57}$$

These equations are compatible whenever $q(x,t)$, $\alpha(x,t)$, *and* $\delta(x,t)$ *solve Eqs.* (41) and (45)–(48). *Moreover, the vector field*

$$W = \alpha\exp(-2\delta)\frac{\partial}{\partial q} - \frac{2}{3}\eta^4\exp(-2\delta)\frac{\partial}{\partial \alpha} + \beta\frac{\partial}{\partial \delta} - \beta^2\frac{\partial}{\partial \beta} \tag{58}$$

is a (generalized) symmetry for the compatible system of equations (41), (45)–(48), (56), and (57), *and therefore it determines a bona fide nonlocal symmetry for the Kaup-Kupershmidt equation* (41).

One can check this result independently of the previous discussion, using the MAPLE package VESSIOT.[4] Note that this nonlocal symmetry is of the type called *internal* in the discussion appearing at the end of Sec. III. The interesting problem of studying the Lie algebra structure of all internal nonlocal symmetries of type $\Gamma=\{\alpha,\delta,\beta\}$ for Kaup–Kupershmidt remains open.

The flow of the vector field (58) can be explicitly found: as explained in Sec. II one only needs to solve the system of equations:

$$\frac{\partial q}{\partial \tau} = \alpha\exp(-2\delta); \quad \frac{\partial \alpha}{\partial \tau} = -\frac{2}{3}\eta^4\exp(-2\delta); \tag{59}$$

$$\frac{\partial \delta}{\partial \tau} = \beta; \quad \frac{\partial \beta}{\partial \tau} = -\beta^2; \tag{60}$$

with initial conditions

$$q(x,t,0) = q_0; \quad \alpha(x,t,0) = \alpha_0; \quad \delta(x,t,0) = \delta_0; \quad \beta(x,t,0) = \beta_0, \tag{61}$$

in which q_0, α_0, δ_0, and β_0 are arbitrary particular solutions to the compatible system (41), (45)–(48), (56), and (57). One finds the formulas

$$q(\tau) = \frac{\alpha_0\tau\exp(-2\delta_0)}{\beta_0\tau+1} - \frac{\eta^4\exp(-4\delta_0)}{3(\beta_0\tau+1)^2}\tau^2 + q_0; \tag{62}$$

$$\alpha(\tau) = \frac{-2\eta^4\tau\exp(-2\delta_0)}{3(\beta_0\tau+1)} + \alpha_0; \tag{63}$$

$$\delta(\tau) = \ln|\beta_0\tau+1| + \delta_0; \tag{64}$$

$$\beta(\tau) = \frac{1}{\tau+1/\beta_0}. \tag{65}$$

The theory of Secs. II and III implies the following result:

Corollary 3: Assume that the functions q_0, α_0, δ_0, and β_0 *are arbitrary particular solutions to the compatible system of equations* (41), (45)–(48), (56), and (57). *Then, the function* $q(x,t,\tau)$ *given by Eq.* (62) *solves the Kaup–Kupershmidt equation for any value of the parameter* τ.

V. A DARBOUX TRANSFORM AND PARTICULAR SOLUTIONS TO KAUP–KUPERSHMIDT

A. A Darboux-like transform

Following an observation made by Schiff,[43] the analysis of Sec. IV allows one to find a Darboux-like transformation for Kaup–Kupershmidt. Starting from (62), one simply eliminates α_0 and δ_0 using Eqs. (45), (47), and (56):

$$\begin{aligned} q(\tau) &= q_0 + \frac{\alpha_0 \tau \exp(-2\delta_0)}{\beta_0 \tau + 1} - \frac{\eta^4 \exp(-4\delta_0)}{3(\beta_0 \tau + 1)^2} \tau^2 \\ &= q_0 + \frac{\tau}{\beta_0 \tau + 1}(-2\eta^2)\delta_{0,x} \exp(-2\delta_0) - \frac{1}{3}\tau^2 \frac{(\eta^2 \exp(-2\delta_0))^2}{(\beta_0 \tau + 1)^2} \\ &= q_0 + \frac{\tau \eta^2}{\beta_0 \tau + 1}(\exp(-2\delta_0))_x - \frac{1}{3}\tau^2 \frac{(\eta^2 \exp(-2\delta_0))^2}{(\beta_0 \tau + 1)^2} \\ &= q_0 + \frac{3\tau \beta_{0,xx}}{\beta_0 \tau + 1} - \frac{3\tau^2 \beta_{0,x}^2}{(\beta_0 \tau + 1)^2}, \end{aligned}$$

and therefore $q(\tau)$ and q_0 are related by

$$q(\tau) = q_0 + 3\frac{\partial^2}{\partial x^2} \ln(\beta_0 \tau + 1), \tag{66}$$

in which β_0 is any solution to the compatible system of equations (56) and (57). This is analogous to the Darboux transform for Kaup–Kupershmidt recently discussed in Refs. 31 and 46. Making a slight change of notation, eliminating subscripts and writing $\overline{q} = q(\tau)$ and $B = \beta\tau + 1$, these comments can be stated as follows.

Proposition 3: The Kaup–Kupershmidt equation (41) *is invariant under the transformation* $q \mapsto \overline{q}$, *in which*

$$\overline{q} = q + 3(\ln B)_{xx}. \tag{67}$$

In this equation the functions q and B are related by

$$q = -\frac{B_{xxx}}{B_x} + \frac{3}{4}\left(\frac{B_{xx}}{B_x}\right)^2, \tag{68}$$

and $B(x,t)$ *is a solution to*

$$B_t = -5\frac{B_{xxxx}B_{xx}}{B_x} + \frac{65}{4}\frac{B_{xxx}B_{xx}^2}{B_x^2} - \frac{135}{16}\frac{B_{xx}^4}{B_x^3} + B_{xxxxx} - \frac{15}{4}\frac{B_{xxx}^2}{B_x}. \tag{69}$$

Equations (68) and (69) are found easily from (45), (56), and (57).

B. Examples of particular solutions

For $q_0 = 0$, one obtains the following formulas from Eqs. (45)–(48), (56), and (57):

$$\alpha_0(x,t) = \frac{1}{\dfrac{x}{4\eta^2} + c_\alpha} \tag{70}$$

$$\delta_0(x,t) = -2 \ln\left|\frac{x}{4\eta^2} + c_\alpha\right| + c_\delta \tag{71}$$

$$\beta_0(x,t) = \frac{4}{15}\eta^4 \exp(-2c_\delta)\left(\frac{x}{4\eta^2} + c_\alpha\right)^5 - \frac{3}{64}\frac{1}{\eta^6}\exp(-2c_\delta)t + c_\beta, \tag{72}$$

in which c_α, c_δ, and c_β are constant. Replacing these equations into (62) [or, equivalently, replacing (72) into the transform (66)], one finds the following family of rational solutions to the Kaup–Kupershmidt equation:

$$q(x,t,\tau) = \frac{\left(\frac{x}{4\eta^2} + c_\alpha\right)^3 \exp(-2c_\delta)\tau}{\tau\left[\exp(-2c_\delta)\left(\frac{4\eta^4}{15}\left(\frac{x}{4\eta^2} + c_\alpha\right)^5 - \frac{3}{64}\frac{t}{\eta^6}\right) + c_\beta\right] + 1} - \frac{1}{3}\frac{\left(\frac{x}{4\eta^2} + c_\alpha\right)^8 \exp(-4c_\delta)\tau^2\eta^4}{\left(\tau\left[\exp(-2c_\delta)\left(\frac{4\eta^4}{15}\left(\frac{x}{4\eta^2} + c_\alpha\right)^5 - \frac{3}{64}\frac{t}{\eta^6}\right) + c_\beta\right] + 1\right)^2}. \tag{73}$$

Since the Kaup–Kupershmidt equation is invariant under x and t translations, one can set $c_\alpha = c_\beta = 0$ and, by scaling the parameter τ, one can choose $c_\delta = 0$. The family of solutions (73) is thus equivalent to

$$q(x,t,\tau) = -15\frac{\tau x^3(720\tau t - 15360\eta^6 + x^5\tau)}{(-x^5\tau + 180\tau t - 3840\eta^6)^2}, \tag{74}$$

a rational solution depending on the parameters τ and η. It would be of interest to study it in more detail, perhaps along the lines of Kovalyov's[23] analysis of a class of singular solutions for KdV. Setting $\mu = 3840\eta^6/\tau$, one can write (74) as

$$q(x,t,\mu) = -15\frac{x^3(720t - 4\mu + x^5)}{(-x^5 + 180t - \mu)^2}. \tag{75}$$

The limit $\mu \to \infty$ reproduces the seed solution $q_0 = 0$. On the other hand, note that $\eta = 0$ is a pole of the linear problem (42) and (43), but—reflecting the fact that the parameter η can be "gauged away"—the value $\eta = 0$ (or equivalently, $\mu = 0$) yields a well defined rational solution to Eq. (41).

A second family of solutions which can be obtained from $q_0 = 0$ is the following: Instead of (70)–(72), take $\alpha_0 = 0$, $\delta_0 = 0$, and $\beta_0 = (\eta^2/3)x + c_\beta$. Then, Eq. (62) yields the stationary solution

$$q(x,t,\tau) = \frac{-\eta^4\tau^2}{3\left(\tau\left(\frac{\eta^2}{3}x + c_\beta\right) + 1\right)^2}.$$

Setting $\tau\eta^2 = 3\mu$ and using again the invariance of Kaup–Kupershmidt under x translations, one can write this solution as

$$q(x,\mu) = \frac{-3\mu^2}{(\mu x + 1)^2}. \tag{76}$$

This stationary solution was used in Ref. 46 to obtain examples of "extended" N-soliton solutions to Kaup–Kupershmidt, that is, solutions which approach asymptotically to solitons or to static bell shaped waves as $t \to \infty$.

Assume now that $q_0 = 1/4$ and take $\eta = 1$ for simplicity. The functions α_0, δ_0, and β_0 become

$$\alpha_0 = -\tan\left(\frac{x}{4} + \frac{t}{64}\right), \tag{77}$$

$$\delta_0 = -2\ln\left|\cos\left(\frac{x}{4} + \frac{t}{64}\right)\right|, \tag{78}$$

$$\beta_0 = \frac{1}{24}\sin\left(x + \frac{t}{16}\right) + \frac{1}{3}\sin\left(\frac{x}{2} + \frac{t}{32}\right) + \frac{x}{8} - \frac{5t}{128}. \tag{79}$$

Replacing these functions into (62), one obtains a one-parameter family of trigonometric solutions to Kaup–Kupershmidt,

$$q(x,t,\tau) = \frac{-\cos^4\left(\frac{x}{4} + \frac{t}{64}\right)\tan\left(\frac{x}{4} + \frac{t}{64}\right)\tau}{\tau\left[\frac{1}{24}\sin\left(x + \frac{t}{16}\right) + \frac{1}{3}\sin\left(\frac{x}{2} + \frac{t}{32}\right) + \frac{x}{8} - \frac{5t}{128}\right] + 1} - \frac{1}{3}\frac{\tau^2\cos^8\left(\frac{x}{4} + \frac{t}{64}\right)}{\left(\tau\left[\frac{1}{24}\sin\left(x + \frac{t}{16}\right) + \frac{1}{3}\sin\left(\frac{x}{2} + \frac{t}{32}\right) + \frac{x}{8} - \frac{5t}{128}\right] + 1\right)^2} + \frac{1}{4}. \tag{80}$$

This solution is almost, but not quite, a function of the sum $s = x/4 + t/64$: the potential β_0 (and hence the solution $q(x,t,\tau)$) fails to depend only on s. As is the case with (74), this solution is singular along a curve in the (x,t) plane.

Now consider the solutions appearing from the choices $q_0 = -1/4$ and $\eta = 1$. In this case the functions α_0, δ_0, and β_0 read

$$\alpha_0 = \tanh\left(\frac{x}{4} + \frac{t}{64}\right), \tag{81}$$

$$\delta_0 = -2\ln\left|\cosh\left(\frac{x}{4} + \frac{t}{64}\right)\right|, \tag{82}$$

$$\beta_0 = \frac{1}{24}\sinh\left(x + \frac{t}{16}\right) + \frac{1}{3}\sinh\left(\frac{x}{2} + \frac{t}{32}\right) + \frac{x}{8} - \frac{5t}{128}, \tag{83}$$

and the corresponding one–parameter family of solutions to Kaup–Kupershmidt is

$$q(x,t,\tau)=\frac{\cosh^4\left(\frac{x}{4}+\frac{t}{64}\right)\tanh\left(\frac{x}{4}+\frac{t}{64}\right)\tau}{\tau\left[\frac{1}{24}\sinh\left(x+\frac{t}{16}\right)+\frac{1}{3}\sinh\left(\frac{x}{2}+\frac{t}{32}\right)+\frac{x}{8}-\frac{5t}{128}\right]+1}$$
$$-\frac{1}{3}\frac{\tau^2\cosh^8\left(\frac{x}{4}+\frac{t}{64}\right)}{\left(\tau\left[\frac{1}{24}\sinh\left(x+\frac{t}{16}\right)+\frac{1}{3}\sinh\left(\frac{x}{2}+\frac{t}{32}\right)+\frac{x}{8}-\frac{5t}{128}\right]+1\right)^2}-\frac{1}{4}. \tag{84}$$

Finally, take the stationary solution (76) as seed solution q_0. The functions α_0, δ_0 and β_0 read:

$$\alpha_0=6\frac{\eta^2\mu((\mu x+1)^2+1)}{((\mu x+1)^2-3)(\mu x+1)}, \tag{85}$$

$$\delta_0=-2\ln((\mu x+1)^2-3)+\ln(\mu x+1), \tag{86}$$

$$\beta_0=\frac{1}{3}\eta^2\left(\frac{1}{7}\mu^6x^7+\mu^5x^6+\frac{3}{5}\mu^4x^5-7\mu^3x^4-\mu^2x^3+33x^2\mu-65x-81\frac{1}{(\mu x+1)\mu}\right)-576\mu^4\eta^2t. \tag{87}$$

Setting $\xi=\tau\eta^2$ and using (62) [or the transform (66)], one can write the corresponding family of solutions $q(x,t,\xi,\mu)$ as

$$q(x,t,\xi,\mu)=\frac{6\xi\mu[(\mu x+1)^2-3]^3[(\mu x+1)^2+1]}{(\mu x+1)^3(1/3\xi[P(x,\mu)-81Q(x,\mu)]-576\mu^4\xi t+1)}$$
$$-\frac{1/3\xi^2[(\mu x+1)^2-3]^8}{(1/3\xi[P(x,\mu)-81Q(x,\mu)]-576\mu^4\xi t+1)^2(\mu x+1)^4}-3\frac{\mu^2}{(\mu x+1)^2}, \tag{88}$$

in which

$$P(x,\mu)=\frac{1}{7}\mu^6x^7+\mu^5x^6+\frac{3}{5}\mu^4x^5-7\mu^3x^4-\mu^2x^3+33x^2\mu-65x, \tag{89}$$

$$Q(x,\mu)=\frac{1}{\mu(\mu x+1)}. \tag{90}$$

This solution approaches asymptotically the stationary solution $q(x)=-24/x^2$ as $\mu\to\infty$, whereas the seed solution q_0 is recovered in the limit $t\to\infty$.

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Some results on the eigenfunctions of the quantum trigonometric Calogero–Sutherland model related to the Lie algebra E_6

J. Fernández Núñez and W. García Fuertes
Departamento de Física, Facultad de Ciencias, Universidad de Oviedo, E-33007 Oviedo, Spain

A. M. Perelomov[a)]
Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, E-50009 Zaragoza, Spain

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The quantum trigonometric Calogero–Sutherland models related to Lie algebras admit a parametrization in which the dynamical variables are the characters of the fundamental representations of the algebra. We develop here this approach for the case of the exceptional Lie algebra E_6. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1933088]

I. INTRODUCTION

The so-called Calogero–Sutherland or Calogero–Moser models were introduced by Calogero,[1] who studied, from the quantum standpoint, the dynamics on the infinite line of a set of pairwise interacting particles through rational plus quadratic potentials, and found that the problem was exactly solvable. Soon afterwards, Sutherland[2] arrived to similar results for the quantum problem on the circle, this time with trigonometric interaction, and Moser[3] showed that the classical version of both models enjoyed integrability in the Liouville sense. The identification of the general scope of these discoveries came with the works of Olshanetsky and Perelomov,[4–6] who realized that it was possible to associate models of this kind to all the root systems of the simple Lie algebras, and that all these models were integrable, both in the classical and in the quantum framework;[7,8] see also Ref. 9 for a complete treatment of these topics. Nowadays, there is a widespread interest in this type of integrable system, and many mathematical and physical applications for them have been found, see for instance Ref. 10.

The Calogero-Sutherland Hamiltonian associated to the root system of a simple Lie algebra L can be written as a second-order differential operator whose variables are the characters of the fundamental representations of the algebra. As it was shown in the papers,[11–13] and later in Refs. 14–19 this approach gives the possibility of developing some systematic procedures to solve the Schrödinger equation and determine important properties of the eigenfunctions, such as recurrence relations or generating functions for some subsets of them. For the moment, the approach has been used only for classical algebras of A_n and D_n type, and recently[19] for the exceptional algebra E_6 for a special value of the coupling constant for which the eigenfunctions are proportional to the characters of the ireducible representations of the algebra. The aim of this paper is to show how to generalize the treatment of Ref. 19 to arbitrary values of the coupling constant and to extend some of the particular results found there to the general case.

[a)]On leave of absence from the Institute for Theoretical and Experimental Physics, 117259, Moscow, Russia. Electronic address: Perelomo@dftuz.unizar.es

II. THE CALOGERO–SUTHERLAND MODEL FOR E_6 IN z-VARIABLES

The Hamiltonian operator for the trigonometric Calogero–Sutherland model related to the root system of a simple Lie algebra has the generic form

$$H = \frac{1}{2}(p,p) + \sum_{\alpha \in \mathcal{R}^+} \kappa_\alpha(\kappa_\alpha - 1)\sin^{-2}(\alpha,q),$$

where $\mathcal{R}^+$ is the set of positive roots, q and p are vectors of dimension r=rank of the algebra, (,) is the usual Euclidean scalar product in $\mathbf{R}^r$, and the coupling constants κ_α are such that $\kappa_\alpha = \kappa_\beta$ if $\|\alpha\| = \|\beta\|$. In particular, because E_6 is simply laced (for all details about the structure of E_6 needed to follow the main text, see Appendix A), the Calogero–Sutherland model associated to E_6 depends only on one coupling constant κ. To write H in a more explicit way, it is convenient to use the orthonormal basis $\{e_i, i=1,\ldots,6\}$ which is related to the generating system of the Appendix A through $\varepsilon_i = e_i - \frac{1}{6}\Sigma_{j=1}^6 e_j$. The expression of q and p in this basis is simply $q = \Sigma_{i=1}^6 q_i e_i$, $p = \Sigma_{i=1}^6 p_i e_i$, while the simple roots are given by

$$\alpha_1 = e_1 - e_2,$$

$$\alpha_2 = \frac{1}{2}\left(-1 + \frac{\sqrt{3}}{3}\right)\sum_{j=1}^{3} e_j + \frac{1}{2}\left(1 + \frac{\sqrt{3}}{3}\right)\sum_{j=4}^{6} e_j,$$

$$\alpha_k = e_{k-1} - e_k, \quad k = 3,4,5,6.$$

The q coordinates are assumed to take values in the interval $[0,\pi]$, and therefore the Hamiltonian can be interpreted as describing the dynamics of a system of six particles moving on the circle, but notice that there is not translational invariance. We recapitulate some important facts about this model which follow from the general structure of the quantum Calogero–Sutherland models related to Lie algebras.[8,9] The ground state energy and (non-normalized) wave function are

$$E_0(\kappa) = 2(\rho,\rho)\kappa^2 = 156\kappa^2,$$

$$\Psi_0^\kappa(q) = \prod_{\alpha \in \mathcal{R}^+} \sin^\kappa(\alpha,q),$$

with ρ being the Weyl vector, while the excited states depend on a six-tuple of quantum numbers $\mathbf{m} = (m_1, m_2, m_3, m_4, m_5, m_6)$, and satisfy the Schrödinger equation

$$H\Psi_{\mathbf{m}}^\kappa = E_{\mathbf{m}}(\kappa)\Psi_{\mathbf{m}}^\kappa,$$

$$E_{\mathbf{m}}(\kappa) = 2(\lambda + \kappa\rho, \lambda + \kappa\rho), \tag{1}$$

where λ is the highest weight of the irreducible representation of E_6 labelled by $\mathbf{m}$, i.e., $\lambda = \Sigma_{i=1}^6 m_i \lambda_i$. By substitution in (1) of

$$\Psi_{\mathbf{m}}^\kappa(q) = \Psi_0^\kappa(q)\Phi_{\mathbf{m}}^\kappa(q), \tag{2}$$

we are led to the eigenvalue problem

$$\Delta^\kappa \Phi_{\mathbf{m}}^\kappa = \varepsilon_{\mathbf{m}}(\kappa)\Phi_{\mathbf{m}}^\kappa \tag{3}$$

with

$$\Delta^{\kappa} = -\frac{1}{2}\Delta - \kappa \sum_{\alpha \in \mathcal{R}^+} \mathrm{ctg}(\alpha, q)(\alpha, \nabla_q), \tag{4}$$

and

$$\varepsilon_{\mathbf{m}}(\kappa) = E_{\mathbf{m}}(\kappa) - E_0(\kappa) = 2(\lambda, \lambda + 2\kappa\rho). \tag{5}$$

Taking into account that $A^{-1}_{jk} = (\lambda_j, \lambda_k)$, it is possible to give a more explicit expression for $\varepsilon_{\mathbf{m}}(\kappa)$,

$$\varepsilon_{\mathbf{m}}(\kappa) = 2 \sum_{j,k=1}^{6} A^{-1}_{jk} m_j m_k + 4\kappa \sum_{j,k=1}^{6} A^{-1}_{jk} m_j. \tag{6}$$

Now the main problem is to solve (3). As it has been shown for other algebras,[11–13,17] the best way to do this is to use a set of independent variables which are invariant under the Weyl symmetry of the Hamiltonian, namely the characters $z_k, k = 1, \ldots, 6$, of the six fundamental representations of the Lie algebra E_6. We can infer from (4) the structure of Δ^{κ} when written in the z variables,

$$\Delta^{\kappa} = \sum_{j,k=1}^{6} a_{jk}(z) \partial_{z_j} \partial_{z_k} + \sum_{j=1}^{6} [b_j^{(0)}(z) + \kappa b_j^{(1)}(z)] \partial_{z_j}. \tag{7}$$

As a matter of fact, the eigenfunctions of $\Delta^{(0)}$ and $\Delta^{(1)}$ are (proportional to) the monomial symmetric functions $M_\lambda = \Sigma_{s \in W} \exp[2i(s\lambda, q)]$ (W is the Weyl group) and the characters $\boldsymbol{\chi}_\lambda$ of the irreducible representations of the algebra E_6, respectively.[8] Thus, knowing the characters $z_i = \boldsymbol{\chi}_{\lambda_i}$ of the fundamental representations and the products $z_i z_j$ through the Clebsch–Gordan series for the algebra, we are able to find the Hamiltonian $\Delta^{(1)}$, that is, we obtain the coefficients $a_{jk}(z)$ entering in the expression of all the Hamiltonians Δ^{κ} and also the coefficients $b_j^{(0)}(z) + b_j^{(1)}(z)$. In the previous paper[19] we computed the needed Clebsch–Gordan series and showed these coefficients.

On the other hand, knowing enough monomial symmetric functions in terms of the fundamental characters, $M_\lambda(z)$, we can complete the form of Δ^{κ}, for we know that

$$\Delta^{(0)} M_\lambda = \varepsilon_{\mathbf{m}}(0) M_\lambda = 2(\lambda, \lambda) M_\lambda, \tag{8}$$

a system of linear equations which can be solved for the coefficients $b_j^{(0)}(z)$, $j = 1, \ldots, 6$. To this end, remind that the characters can be expanded as sums of monomial functions,[20]

$$\boldsymbol{\chi}_\lambda = M_\lambda + a_1 M_{\mu_1} + a_2 M_{\mu_2} + \cdots,$$

where the set of μ_k entering in the expansion is easy to determine: they are the dominant weights such that $\mu_i = \lambda - \Sigma_{j=1}^{6} n_j \alpha_j$ with $n_j \geqslant 0$ and $(\mu_i, \alpha_k) \geqslant 0$ for the six simple roots α_k. The coefficients a_k, on the other hand, represent the multiplicities of the weights μ_i in the representation with highest weight λ. Here it will suffice to deal with the following expansions:

$$\boldsymbol{\chi}^{(27)}_{100000} = z_1 = M^{(27)}_{100000},$$

$$\boldsymbol{\chi}^{(78)}_{010000} = z_2 = M^{(72)}_{010000} + aM^{(1)}_{000000},$$

$$\boldsymbol{\chi}^{(351)}_{001000} = z_3 = M^{(216)}_{001000} + bM^{(27)}_{000001},$$

$$\boldsymbol{\chi}^{(2925)}_{000100} = z_4 = M^{(720)}_{000100} + cM^{(270)}_{100001} + dM^{(72)}_{010000} + eM^{(1)}_{000000},$$

$$\boldsymbol{\chi}^{(351)}_{000010} = z_5 = M^{(216)}_{000010} + bM^{(27)}_{100000},$$

$$\chi^{(27)}_{000001} = z_6 = M^{(27)}_{000001},$$

$$\chi^{(650)}_{100001} = z_1 z_6 - z_2 - 1 = M^{(270)}_{100001} + fM^{(72)}_{010000} + gM^{(1)}_{000000}, \tag{9}$$

where the form of χ_{100001} comes from the list in Ref. 19 and the numbers appearing in parentheses as superscripts are either the dimensions of the representations or the dimensions of the linear spaces generated by the orbits of the Weyl group corresponding to the monomial functions. The former can be computed from the Weyl dimension formula, while the latter follow easily from the fact that the Weyl group of the subalgebra of E_6 obtained by removing from the Dynkin diagram the dots corresponding to the weight defining the monomial function acts trivially on such a weight, for instance, removing the dot associated to λ_1 we obtain the Dynkin diagram of D_5, and hence

$$\dim M_{100000} = \frac{|W_{E_6}|}{|W_{D_5}|} = \frac{2^7 \cdot 3^4 \cdot 5}{\frac{1}{2}10!!} = 27,$$

and so on.

While the dimensions shown in (9) suffice for fixing $a=6$, $b=5$, for the computation of remaining multiplicities we need to use the Freudenthal formula[21]

$$n_\mu = \frac{\sum_{\alpha>0} \sum_{k=1}^{\infty} 2n_{\mu+k\alpha}(\mu + k\alpha, \alpha)}{(\lambda + \mu + 2\rho, \lambda - \mu)}. \tag{10}$$

Here n_μ stands for the multiplicity of the weight μ in the representation of highest weight λ, the first sum extends over positive roots, and ρ is the Weyl vector. The application of the Freudenthal formula is quite easy for the representations at stake. Let us see, for instance, how to compute c in (9). In this case $\lambda=\lambda_4$ and $c=n_\mu=n_{\lambda_1+\lambda_6}$. The scalar product of the vector $\beta=\lambda-\mu=\alpha_2+\alpha_3+2\alpha_4+\alpha_5$ with μ is $(\beta,\mu)=0$ and, due to the fact that the length of $\mu+\alpha$, with α a positive root, is $|\mu+\alpha|=(|\mu|^2+2+2(\mu,\alpha))^{\frac{1}{2}}$, the only roots entering in (10) are the positive roots α such that $(\mu,\alpha)=0$, because otherwise $|\mu+\alpha|>|\mu+\beta|=|\lambda|$ and $\mu+\alpha$ would lie outside of the weight diagram for the representation R_λ. Looking at the table of positive roots in Appendix A, we check that there are 12 of them with $(\mu,\alpha)=0$. For all of these, $\mu+\alpha$ lies on the orbit of λ, and thus $n_{\mu+\alpha}=1$. This gives

$$c = n_{\lambda_1+\lambda_6} = 12\frac{2(\mu,\alpha) + 2(\alpha,\alpha)}{(\lambda_4 + \lambda_1 + \lambda_6 + 2\sum_{i=1}^{6} \lambda_i, \alpha_1 + \alpha_3 + 2\alpha_4 + \alpha_5)} = 12\frac{2\cdot 0 + 2\cdot 2}{2 + 2\cdot 5} = 4.$$

To compute d we proceed much in the same way. Now $\mu=\lambda_2$ and $\beta=\lambda-\mu=\alpha_1+\alpha_2+2\alpha_3+3\alpha_4+2\alpha_5+\alpha_6$. It follows that $(\mu,\beta)=1$, and thus only positive roots with $(\mu,\alpha)=0$ or $(\mu,\alpha)=1$ enter in the Freudenthal formula. There are 20 positive roots with $(\mu,\alpha)=1$, and for them $n_{\mu+\alpha}=1$ because they are in the orbit of λ. The number of positive roots with $(\mu,\alpha)=0$ is 15, and for them $\mu+\alpha$ lies in the orbit of $\lambda_1+\lambda_6$, so that their multiplicities are $n_{\mu+\alpha}=4$. This gives $d=n_{\lambda_2}=15$. Once we know c and d, we compute e by balancing dimensions in (9), and obtain $e=45$. A similar use of the Freudenthal formula gives $f=5$, and therefore $g=20$.[22]

With all the coefficients in (9) being fixed, we can now solve for the monomial functions corresponding to the fundamental weights. We find

$$M_{100000} = z_1,$$

$$M_{010000} = z_2 - 6,$$

$$M_{001000} = z_3 - 5z_6,$$

$$M_{000100} = z_4 - 4z_1z_6 + 9z_2 + 9,$$

$$M_{000010} = z_5 - 5z_1,$$

$$M_{000001} = z_6.$$

The remaining step is to substitute these monomials in (8) and to solve the linear system for the coefficients $b_j^{(0)}(z)$; the outcome is

$$b_1^{(0)}(z) = \tfrac{8}{3}z_1, \quad b_2^{(0)}(z) = 4(z_2 - 6), \quad b_3^{(0)}(z) = \tfrac{20}{3}z_3 - 20z_6,$$

$$b_4^{(0)}(z) = 12z_4 - 16z_1z_6 - 24z_2 + 36, \quad b_5^{(0)}(z) = \tfrac{20}{3}z_5 - 20z_1, \quad b_6^{(0)}(z) = \tfrac{8}{3}z_6.$$

With this and the form of $\Delta^{(1)}$ given in Ref. 19, we can now write the full set of coefficients in (7),

$$a_{11}(z) = \tfrac{8}{3}z_1^2 - 4z_3 - 20z_6,$$

$$a_{12}(z) = 2z_1z_2 - 26z_1 - 10z_5,$$

$$a_{13}(z) = \tfrac{10}{3}z_1z_3 + 18 - 12z_2 - 6z_4 - 18z_1z_6,$$

$$a_{14}(z) = 4z_1z_4 + 18z_1 - 10z_1z_2 - 18z_5 - 8z_2z_5 - 8z_3z_6 + 8z_6^2,$$

$$a_{15}(z) = \tfrac{8}{3}z_1z_5 - 10z_3 - 26z_6 - 10z_2z_6,$$

$$a_{16}(z) = \tfrac{4}{3}z_1z_6 - 36 - 12z_2,$$

$$a_{22}(z) = 4z_2^2 - 36 - 12z_2 - 4z_4 - 16z_1z_6,$$

$$a_{23}(z) = 4z_2z_3 - 24z_1^2 + 14z_3 - 8z_1z_5 - 2z_6 - 10z_2z_6,$$

$$a_{24}(z) = 6z_2z_4 - 18z_2 - 12z_2^2 - 10z_1z_3 + 24z_4 - 6z_3z_5 + 26z_1z_6 - 8z_1z_2z_6 - 10z_5z_6,$$

$$a_{25}(z) = 4z_2z_5 - 2z_1 - 10z_1z_2 + 14z_5 - 8z_3z_6 - 24z_6^2,$$

$$a_{26}(z) = 2z_2z_6 - 10z_3 - 26z_6,$$

$$a_{33}(z) = \tfrac{20}{3}z_3^2 + 28z_1 - 24z_1z_2 - 4z_1z_4 + 32z_5 - 8z_2z_5 - 16z_1^2z_6 + 8z_3z_6 - 12z_6^2,$$

$$a_{34}(z) = 8z_3z_4 + 10z_1^2 - 10z_1^2z_2 + 18z_3 - 2z_2z_3 - 6z_1z_2z_5 - 10z_5^2 - 18z_6 + 8z_2z_6 - 10z_2^2z_6 - 8z_1z_3z_6 + 20z_4z_6 + 8z_1z_6^2,$$

$$a_{35}(z) = \tfrac{16}{3}z_3z_5 - 36 + 24z_2 - 12z_2^2 - 10z_1z_3 + 24z_4 - 16z_1z_6 - 8z_1z_2z_6 - 10z_5z_6,$$

$$a_{36}(z) = \tfrac{8}{3}z_3z_6 - 26z_1 - 10z_1z_2 - 10z_5,$$

$$a_{44}(z) = 12z_4^2 - 8z_1^3 - 12z_2^3 + 36z_1z_3 - 12z_1z_2z_3 - 36z_4 + 36z_2z_4 + 16z_1^2z_5 - 36z_3z_5 - 4z_2z_3z_5 - 8z_1z_5^2 - 36z_1z_6 + 28z_1z_2z_6 - 8z_1z_2^2z_6 - 8z_3^2z_6 + 16z_1z_4z_6 + 36z_5z_6 - 12z_2z_5z_6 + 16z_3z_6^2 - 8z_6^3,$$

$$a_{45}(z) = 8z_4z_5 - 18z_1 + 8z_1z_2 - 10z_1z_2^2 - 10z_3^2 + 20z_1z_4 + 18z_5 - 2z_2z_5 + 8z_1^2z_6 - 6z_2z_3z_6 - 8z_1z_5z_6 + 10z_6^2 - 10z_2z_6^2,$$

$$a_{46}(z) = 4z_4z_6 + 8z_1^2 - 18z_3 - 8z_2z_3 - 8z_1z_5 + 18z_6 - 10z_2z_6,$$

$$a_{55}(z) = \tfrac{20}{3}z_5^2 - 12z_1^2 + 32z_3 - 8z_2z_3 + 8z_1z_5 + 28z_6 - 24z_2z_6 - 4z_4z_6 - 16z_1z_6^2,$$

$$a_{56}(z) = \tfrac{10}{3}z_5z_6 + 18 - 12z_2 - 6z_4 - 18z_1z_6,$$

$$a_{66}(z) = \tfrac{8}{3}z_6^2 - 20z_1 - 4z_5,$$

$$b_1(z) = b_1^{(0)}(z) + \kappa b_1^{(1)}(z) = \left(32\kappa + \tfrac{8}{3}\right)z_1,$$

$$b_2(z) = b_2^{(0)}(z) + \kappa b_2^{(1)}(z) = (44\kappa + 4)z_2 + 24(\kappa - 1),$$

$$b_3(z) = b_3^{(0)}(z) + \kappa b_3^{(1)}(z) = \left(60\kappa + \tfrac{20}{3}\right)z_3 + 20(\kappa - 1)z_6,$$

$$b_4(z) = b_4^{(0)}(z) + \kappa b_4^{(1)}(z) = (84\kappa + 12)z_4 + (\kappa - 1)(16z_1z_6 + 24z_2 - 36),$$

$$b_5(z) = b_5^{(0)}(z) + \kappa b_5^{(1)}(z) = \left(60\kappa + \tfrac{20}{3}\right)z_5 + 20(\kappa - 1)z_1,$$

$$b_6(z) = b_6^{(0)}(z) + \kappa b_6^{(1)}(z) = \left(32\kappa + \tfrac{8}{3}\right)z_6.$$

III. COMPUTATION OF POLYNOMIALS AND DEFORMED CLEBSCH–GORDAN SERIES

The eigenfunctions $\Phi_{\mathbf{m}}^{\kappa}(q)$ are polynomials when expressed in z variables, $\Phi_{\mathbf{m}}^{\kappa}(q) = P_{\mathbf{m}}^{\kappa}(z)$. The Schrödinger equation can then be solved by applying a systematic procedure, which is suitable to be implemented in a computer program able to carry out symbolic calculations. We propose two alternative methods to find the Schrödinger eigenfunctions.

(1) Given a weight $n_1\lambda_1 + n_2\lambda_2 + n_3\lambda_3 + n_4\lambda_4 + n_5\lambda_5 + n_6\lambda_6$, let us denote $z^{\mathbf{n}} = z_1^{n_1}z_2^{n_2}z_3^{n_3}z_4^{n_4}z_5^{n_5}z_6^{n_6}$. Thus, Δ^{κ} acting on $z^{\mathbf{n}}$ gives

$$\Delta^{\kappa} z^{\mathbf{n}} = \sum_{\beta \in \Lambda} k_{\beta,\mathbf{n}}(\kappa) z^{\mathbf{n}-\beta}, \tag{11}$$

where Λ includes only integral linear combinations of the simple roots with non-negative coefficients and, of course, in the exponent of (11) we express β in the basis of fundamental weights. In particular, $k_{0,\mathbf{n}}(\kappa) = \varepsilon_{\mathbf{n}}(\kappa)$. The polynomials $P_{\mathbf{m}}(z)$ can be written as

$$P^{\kappa}_{\mathbf{m}}(z) = \sum_{\mu \in Q^+(\mathbf{m})} c_{\mu}(\kappa) z^{\mathbf{m}-\mu}, \quad c_0 = 1,$$

where again the μ in $Q^+(\mathbf{m})$ are integral linear combinations of the simple roots with non-negative coefficients such that they do not give rise to negative powers of the z's. By substituting in the Schrödinger equation we find the iterative formula

$$c_{\mu}(\kappa) = \frac{1}{\varepsilon_{\mathbf{m}}(\kappa) - \varepsilon_{\mathbf{m}-(\mu)}(\kappa)} \sum_{\beta \in \Lambda, \beta \neq 0} k_{\beta,\mathbf{m}-(\mu-\beta)}(\kappa) c_{\mu-\beta}(\kappa).$$

To use this formula in practice, one should take into account the heights of the μ's, because each coefficient c_{μ} can depend only on some of the c_{ν} such that $\mathrm{ht}(\nu) < \mathrm{ht}(\mu)$.

(2) The product $z_1^{m_1} z_2^{m_2} z_3^{m_3} z_4^{m_4} z_5^{m_5} z_6^{m_6}$ can be expanded on the basis of the orthogonal polynomials $P^{\kappa}_{\mathbf{m}}(z)$ as

$$z_1^{m_1} z_2^{m_2} z_3^{m_3} z_4^{m_4} z_5^{m_5} z_6^{m_6} = P^{\kappa}_{\mathbf{m}}(z) + \sum_{\beta \in S_{\mathbf{m}}} n_{\beta}(\kappa) P^{\kappa}_{\mathbf{m}-\beta}(z),$$

where $S_{\mathbf{m}}$ is the set of all integral dominant weights β such that $\mathbf{m}-\beta$ is a linear integral combination of the simple roots with non-negative coefficents, i.e., $\mathbf{m}-\beta$ belongs to the cone of positive roots. Furthermore, the operator $\Delta^{\kappa} - \varepsilon_{\mathbf{n}}(\kappa)$ annihilates the character $P^{\kappa}_{\mathbf{n}}$. Taking this into account, we can obtain the eigenfunctions using the formula

$$P^{\kappa}_{\mathbf{m}} = \left\{ \prod_{\beta \in S_{\mathbf{m}}} (\Delta^{\kappa} - \varepsilon_{\mathbf{m}-\beta}(\kappa)) \right\} z^{\mathbf{m}}.$$

Through any of these methods, it is possible to compute the characters rather quickly. As an illustration, we offer a list of polynomials and monomial functions in Appendix B. For a similar list of characters, see Ref. 19.

Once we have a method for the computation of the polynomials, we can extend it to produce an algorithm for calculating deformed Clebsch–Gordan series for the product of them. Suppose that we want to obtain the series for $P^{\kappa}_{\mathbf{m}} \times P^{\kappa}_{\mathbf{n}}$. We list the possible dominant weights entering in the series arranged by heights

$$P^{\kappa}_{\mathbf{m}} \times P^{\kappa}_{\mathbf{n}} = P^{\kappa}_{\mathbf{m}+\mathbf{n}} + n_{\mu_1}(\kappa) P^{\kappa}_{\mu_1} + n_{\mu_2}(\kappa) P^{\kappa}_{\mu_2} + \cdots .$$

The coefficient $n_{\mu_1}(\kappa)$ is simply the difference between the coefficients of z^{μ_1} in $P^{\kappa}_{\mathbf{m}} \times P^{\kappa}_{\mathbf{n}}$ and in $P^{\kappa}_{\mathbf{m}+\mathbf{n}}$. Then, $n_{\mu_2}(\kappa)$ is the difference between the coefficient of z^{μ_2} in $P^{\kappa}_{\mathbf{m}} \times P^{\kappa}_{\mathbf{n}}$ and the sum of the corresponding coefficients in $P^{\kappa}_{\mathbf{m}+\mathbf{n}}$ and $P^{\kappa}_{\mu_1}$, and so on. As an example, we present a list with all the quadratic deformed Clebsch–Gordan series in Appendix C.

IV. SOME RECURRENCE RELATIONS

The approach we are describing is also useful to find the form of the recurrence relations for products $z_j P^{\kappa}_{\mathbf{m}}(z)$. Considered in full generality, these recurrence relations are extremely complicated, but for some special cases they can be written in explicit form. Let us consider, for instance, the recurrence relation for $z_1 P^{\kappa}_{n\lambda_1}$ with arbitrary n. If we express the weights of the representation R_{λ_1} (which are all the combinations $\varepsilon_i \pm \varepsilon$, $-\varepsilon_i - \varepsilon_j$) in the basis of fundamental weights, we see that there are only three whose coefficients for λ_i, $i \neq 1$, are all non-negative, namely $\lambda_1, -\lambda_1 + \lambda_3$ and $-\lambda_1 + \lambda_6$. Hence, the form of the series should be

$$z_1 P^{\kappa}_{n00000} = P^{\kappa}_{(n+1)00000} + a_n(\kappa) P^{\kappa}_{(n-1)01000} + b_n(\kappa) P^{\kappa}_{(n-1)00001}, \tag{12}$$

where we must fix $a_n(\kappa)$ and $b_n(\kappa)$. Now, solving the Schrödinger equation by means of the first of the two methods described in Sec. III, one finds

$$P^{\kappa}_{n00000} = z_1^n + \frac{(1-n)n}{n+\kappa-1} z_1^{n-2} z_3 + \frac{(1-n)n\kappa(n+5\kappa-2)}{(n+\kappa-1)(n+\kappa-2)(n+4\kappa-1)} z_1^{n-2} z_6 + \cdots ,$$

$$P^{\kappa}_{(n-1)01000} = z_1^{n-1} z_3 + \frac{10\kappa^3 - 5(1+3n)\kappa^2 - 2(-1-9n+5n^2)\kappa - n(2-3n+n^2)}{(n+\kappa-2)(n+\kappa-1)(n+7\kappa)} z_1^{n-1} z_6 + \cdots ,$$

$$P^{\kappa}_{(n-1)00001} = z_1^{n-1} z_6 + \cdots .$$

Substituting in (12), we can solve for $a_n(\kappa)$ and $b_n(\kappa)$ with the results

$$a_n(\kappa) = \frac{n(n+2\kappa-1)}{(n+\kappa)(n+\kappa-1)},$$

$$b_n(\kappa) = \frac{n(n+3\kappa)(n+5\kappa-1)(n+8\kappa-1)}{(n+\kappa-1)(n+4\kappa-1)(n+4\kappa)(n+7\kappa)}.$$

We list below the series of the form $z_1 P^{\kappa}_{n\lambda_k}$ obtained through the same procedure,

$$z_1 P^{\kappa}_{0n0000} = P^{\kappa}_{1n0000} + c_n(\kappa) P^{\kappa}_{0(n-1)0010} + d_n(\kappa) P^{\kappa}_{1(n-1)0000},$$

$$z_1 P^{\kappa}_{00n000} = P^{\kappa}_{10n000} + e_n(\kappa) P^{\kappa}_{00(n-1)100} + f_n(\kappa) P^{\kappa}_{10(n-1)001} + g_n(\kappa) P^{\kappa}_{01(n-1)000},$$

$$z_1 P^{\kappa}_{000n00} = P^{\kappa}_{100n00} + h_n(\kappa) P^{\kappa}_{010(n-1)10} + i_n(\kappa) P^{\kappa}_{001(n-1)01} + j_n(\kappa) P^{\kappa}_{110(n-1)00} + k_n(\kappa) P^{\kappa}_{000(n-1)10},$$

$$z_1 P^{\kappa}_{0000n0} = P^{\kappa}_{1000n0} + l_n(\kappa) P^{\kappa}_{0100(n-1)1} + p_n(\kappa) P^{\kappa}_{0010(n-1)0} + q_n(\kappa) P^{\kappa}_{0000(n-1)1},$$

$$z_1 P^{\kappa}_{00000n} = P^{\kappa}_{10000n} + r_n(\kappa) P^{\kappa}_{01000(n-1)} + s_n(\kappa) P^{\kappa}_{00000(n-1)},$$

where

$$c_n(\kappa) = \frac{n(-1+n+5\kappa)}{(-1+n+\kappa)(n+4\kappa)},$$

$$d_n(\kappa) = \frac{2n(n+2\kappa)(-1+n+6\kappa)(-1+n+8\kappa)(-1+2n+12\kappa)}{(-1+n+\kappa)(-1+n+3\kappa)(n+7\kappa)(-1+2n+11\kappa)(2n+11\kappa)},$$

$$e_n(\kappa) = \frac{n(-1+n+3\kappa)}{(-1+n+\kappa)(n+2\kappa)},$$

$$f_n(\kappa) = \frac{2n(n+2\kappa)(-1+n+4\kappa)(-1+n+6\kappa)(-1+2n+8\kappa)}{(-1+n+\kappa)(-1+n+3\kappa)(n+5\kappa)(-1+2n+7\kappa)(2n+7\kappa)},$$

$$g_n(\kappa) = \frac{n(n+\kappa)(n+3\kappa)(-1+n+5\kappa)(-1+n+6\kappa)(-1+2n+11\kappa)}{(-1+n+\kappa)(-1+n+2\kappa)(n+4\kappa)(n+5\kappa)^2(-1+2n+7\kappa)},$$

$$h_n(\kappa) = \frac{n(-1+n+4\kappa)}{(-1+n+\kappa)(n+3\kappa)},$$

$$i_n(\kappa) = \frac{n(n+\kappa)(-1+n+3\kappa)(-1+n+4\kappa)(-1+2n+7\kappa)}{(-1+n+\kappa)(-1+n+2\kappa)(n+3\kappa)^2(-1+2n+5\kappa)},$$

$$j_n(\kappa) = \frac{6n(n+\kappa)(n+2\kappa)(-1+n+4\kappa)(-1+n+5\kappa)(-1+2n+8\kappa)(-1+3n+11\kappa)}{(-1+n+\kappa)(-1+n+2\kappa)(n+4\kappa)(-1+2n+5\kappa)(2n+7\kappa)(-1+3n+10\kappa)(3n+10\kappa)},$$

$$k_n(\kappa) = \frac{3n(n+\kappa)(n+2\kappa)(-1+n+4\kappa)(-1+n+5\kappa)(2n+5\kappa)(-1+2n+8\kappa)}{(-1+n+\kappa)(-1+n+2\kappa)(n+4\kappa)^2(-1+2n+5\kappa)(-1+2n+6\kappa)(2n+7\kappa)} \times \frac{(-1+2n+9\kappa)(-1+3n+12\kappa)}{(-1+3n+10\kappa)(3n+11)\kappa},$$

$$l_n(\kappa) = \frac{n(-1+n+5\kappa)}{(-1+n+\kappa)(n+4\kappa)},$$

$$p_n(\kappa) = \frac{n(n+\kappa)(-1+n+4\kappa)(-1+n+5\kappa)(-1+2n+9\kappa)}{(-1+n+\kappa)(-1+n+2\kappa)(n+4\kappa)^2(-1+2n+7\kappa)},$$

$$q_n(\kappa) = \frac{2n(n+2\kappa)(n+3\kappa)(-1+n+6\kappa)(-1+n+8\kappa)(-1+2n+12\kappa)}{(-1+n+\kappa)(-1+n+3\kappa)(n+5\kappa)(n+7\kappa)(-1+2n+7\kappa)(2n+11\kappa)}$$

$$r_n(\kappa) = \frac{n(-1+n+6\kappa)}{(-1+n+\kappa)(n+5\kappa)},$$

$$s_n(\kappa) = \frac{n(n+3\kappa)(-1+n+9\kappa)(-1+n+12\kappa)}{(-1+n+\kappa)(-1+n+4\kappa)(n+8\kappa)(n+11\kappa)}.$$

Note that the series $z_6 P^{\kappa}_{n\lambda_j}$ immediately follow by duality.

V. CONCLUSIONS

In this paper, we have shown how to solve the Schrödinger equation for the trigonometric Calogero–Sutherland model related to the Lie algebra E_6 and we have explored some properties of the energy eigenfunctions. The main point is that the use of a Weyl-invariant set of variables, the characters of the fundamental representations, leads to a formulation of the Schrödinger equation by means of a second order differential operator which is simple enough to make feasible a recursive method for the treatment of the spectral problem. The eigenfunctions provide a complete system of orthogonal polynomials in six variables, and these polynomials obey recurrence relations which are deformations of the Clebsch–Gordan series of the algebra. The structure of some of these recurrence relations has been fixed.

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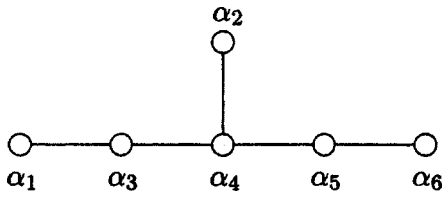

FIG. 1. The Dynkin diagram for the Lie algebra E_6.

APPENDIX A: SUMMARY OF RESULTS ON THE LIE ALGEBRA E_6

In this section, we review some standard facts about the root and weight systems of the Lie algebra E_6, with the aim of fixing the notation and help the reader to follow the rest of the paper. More extensive and sound treatments of these topics can be found in many excellent textbooks, see for instance Refs. 21 and 23.

The complex Lie algebra E_6, the lowest-dimensional one in the E-family of exceptional Lie algebras in the Cartan–Killing classification, has dimension 78 and rank 6, as the name suggests. From the geometrical point of view, it admits (with some subtleties, see Ref. 24) an interpretation which extends the standard-one for the classical algebras, in the same way that these correspond to the isometries of projective spaces over the first three normed division algebras—$\mathrm{SO}(n+1) \simeq \mathrm{Isom}(\mathbf{R}P^n)$, $\mathrm{SU}(n+1) \simeq \mathrm{Isom}(\mathbf{C}P^n)$, $\mathrm{Sp}(n+1) \simeq \mathrm{Isom}(\mathbf{H}P^n)$—$F_4$, E_6, E_7, and E_8 are the Lie algebras of the projective planes over extensions of the octonions, giving rise to the so-called "magic square:" $F_4 \simeq \mathrm{Isom}(\mathbf{O}P^2)$, $E_6 \simeq \mathrm{Isom}[(\mathbf{C}\otimes\mathbf{O})P^2]$, $E_7 \simeq \mathrm{Isom}[(\mathbf{H}\otimes\mathbf{O})P^2]$, $E_8 \simeq \mathrm{Isom}[(\mathbf{O}\otimes\mathbf{O})P^2]$. In physics, the most remarkable role played by E_6 is in the heterotic 10-dimensional $E_8 \times E_8$ superstring theory when the extra six dimensions are compactified to a manifold of SU(3) holonomy. In such a case, one of the E_8 breaks to an E_6 which gives the grand unification group of four-dimensional physics.[25] The Dynkin diagram of E_6, see Fig. 1, encodes the Euclidean relations among the simple roots, which are

$$(\alpha_i, \alpha_i) = 2, \quad i = 1,2,3,4,5,6,$$

$$(\alpha_4, \alpha_i) = -1, \quad i = 2,3,5,$$

$$(\alpha_1, \alpha_3) = (\alpha_5, \alpha_6) = -1,$$

$$(\alpha_i, \alpha_j) = 0, \quad \text{in all other cases.}$$

Therefore, the Cartan matrix reads

$$A = \begin{pmatrix} 2 & 0 & -1 & 0 & 0 & 0 \\ 0 & 2 & 0 & -1 & 0 & 0 \\ -1 & 0 & 2 & -1 & 0 & 0 \\ 0 & -1 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 \end{pmatrix}.$$

We will use a realization of the simple roots in terms of a generating system $\{\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \varepsilon_5, \varepsilon_6, \varepsilon\}$ of $\mathbf{R}^7$ (endowed with the standard Euclidean metric) satisfying $\varepsilon_1+\varepsilon_2+\varepsilon_3+\varepsilon_4+\varepsilon_5+\varepsilon_6=0$, $(\varepsilon_i, \varepsilon_j)=-\frac{1}{6}+\delta_{ij}$, $(\varepsilon, \varepsilon)=\frac{1}{2}$, and $(\varepsilon, \varepsilon_j)=0$.[21] With reference to this system, we have

$$\alpha_1 = \varepsilon_1 - \varepsilon_2, \quad \alpha_2 = \varepsilon_4 + \varepsilon_5 + \varepsilon_6 + \varepsilon,$$

TABLE I. Heights of positive roots.

Height	Positive roots
1	$\alpha_1,\ \alpha_2,\ \alpha_3,\ \alpha_4,\ \alpha_5,\ \alpha_6$
2	$\alpha_1+\alpha_3,\ \alpha_3+\alpha_4,\ \alpha_4+\alpha_5,\ \alpha_5+\alpha_6,\ \alpha_2+\alpha_4$
3	$\alpha_1+\alpha_3+\alpha_4,\ \alpha_3+\alpha_4+\alpha_5,\ \alpha_4+\alpha_5+\alpha_6,\ \alpha_2+\alpha_3+\alpha_4,$ $\alpha_2+\alpha_4+\alpha_5$
4	$\alpha_1+\alpha_3+\alpha_4+\alpha_5,\ \alpha_3+\alpha_4+\alpha_5+\alpha_6,\ \alpha_1+\alpha_2+\alpha_3+\alpha_4,$ $\alpha_2+\alpha_3+\alpha_4+\alpha_5,\ \alpha_2+\alpha_4+\alpha_5+\alpha_6$
5	$\alpha_1+\alpha_3+\alpha_4+\alpha_5+\alpha_6,\ \alpha_1+\alpha_2+\alpha_3+\alpha_4+\alpha_5,$ $\alpha_2+\alpha_3+2\alpha_4+\alpha_5,\alpha_2+\alpha_3+\alpha_4+\alpha_5+\alpha_6$
6	$\alpha_1+\alpha_2+\alpha_3+2\alpha_4+\alpha_5,\ \alpha_1+\alpha_2+\alpha_3+\alpha_4+\alpha_5+\alpha_6,$ $\alpha_2+\alpha_3+2\alpha_4+\alpha_5+\alpha_6$
7	$\alpha_1+\alpha_2+2\alpha_3+2\alpha_4+\alpha_5,\ \alpha_2+\alpha_3+2\alpha_4+2\alpha_5+\alpha_6,$ $\alpha_1+\alpha_2+\alpha_3+2\alpha_4+\alpha_5+\alpha_6$
8	$\alpha_1+\alpha_2+2\alpha_3+2\alpha_4+\alpha_5+\alpha_6,\ \alpha_1+\alpha_2+\alpha_3+2\alpha_4+2\alpha_5+\alpha_6$
9	$\alpha_1+\alpha_2+2\alpha_3+2\alpha_4+2\alpha_5+\alpha_6$
10	$\alpha_1+\alpha_2+2\alpha_3+3\alpha_4+2\alpha_5+\alpha_6$
11	$\alpha_1+2\alpha_2+2\alpha_3+3\alpha_4+2\alpha_5+\alpha_6$

$$\alpha_3=\varepsilon_2-\varepsilon_3,\quad \alpha_4=\varepsilon_3-\varepsilon_4,$$

$$\alpha_5=\varepsilon_4-\varepsilon_5,\quad \alpha_6=\varepsilon_5-\varepsilon_6. \tag{A1}$$

The positive roots, which are given by all linear combinations of the forms

$$\varepsilon_i-\varepsilon_j,\quad \varepsilon_i+\varepsilon_j+\varepsilon_k+\varepsilon,\quad 2\varepsilon,\quad i\neq j\neq k, \tag{A2}$$

can be classified by heights as indicated in Table I. The fundamental weights λ_k follow from the equation $\alpha_i=\Sigma_{j=1}^{4}A_{ji}\lambda_j$. They are

$$\lambda_1=\varepsilon_1+\varepsilon,$$

$$\lambda_2=2\varepsilon,$$

$$\lambda_3=\varepsilon_1+\varepsilon_2+2\varepsilon,$$

$$\lambda_4=\varepsilon_1+\varepsilon_2+\varepsilon_3+3\varepsilon,$$

$$\lambda_5=\varepsilon_1+\varepsilon_2+\varepsilon_3+\varepsilon_4+2\varepsilon,$$

$$\lambda_6=\varepsilon_1+\varepsilon_2+\varepsilon_3+\varepsilon_4+\varepsilon_5+\varepsilon.$$

The geometry of the weight system is summarized by the relations

$$(\lambda_i,\lambda_j)=A_{ij}^{-1},$$

with (A_{ij}^{-1}) being the inverse Cartan matrix. The Weyl vector is

$$\rho = \frac{1}{2} \sum_{\alpha \in \mathcal{R}^+} \alpha = \sum_{i=1}^{6} \lambda_i = 8\alpha_1 + 11\alpha_2 + 15\alpha_3 + 21\alpha_4 + 15\alpha_5 + 8\alpha_6,$$

with $\mathcal{R}^+$ being the set of positive roots of the algebra. The Weyl formula for dimensions applied to the irreducible representation associated to the integral dominant weight $\lambda = m_1\lambda_1 + m_2\lambda_2 + m_3\lambda_3 + m_4\lambda_4 + m_5\lambda_5 + m_6\lambda_6$ gives

$$\dim R_\lambda = \prod_{\alpha \in \mathcal{R}^+} \frac{(\alpha, \lambda + \rho)}{(\alpha, \rho)} = \frac{P}{2^5 \cdot 3^5 \cdot 4^5 \cdot 5^4 \cdot 6^3 \cdot 7^3 \cdot 8^2 \cdot 9 \cdot 10 \cdot 11},$$

where P is a product extended to the set of positive roots in which the root $\alpha = \Sigma_{i=1}^6 c_i \alpha_i$ contributes with a factor $\mathrm{ht}(\alpha) + \Sigma_{i=1}^6 c_i m_i$ where $\mathrm{ht}(\alpha)$ is the height of α. In particular, for the fundamental representations, one finds

$$\dim R_{\lambda_1} = 27, \quad \dim R_{\lambda_2} = 78,$$

$$\dim R_{\lambda_3} = 351, \quad \dim R_{\lambda_4} = 2925,$$

$$\dim R_{\lambda_5} = 351, \quad \dim R_{\lambda_6} = 27.$$

Note that, these dimensions reflect the fact, coming from the $\mathbf{Z}_2$ symmetry (duality) of the Dynkin diagram, that the representations R_{λ_1} and R_{λ_6} are complex conjugates. The same is true for R_{λ_3} and R_{λ_5}, while R_{λ_2} (the adjoint representation) and R_{λ_4} are real.

APPENDIX B: SOME POLYNOMIALS AND MONOMIAL FUNCTIONS

We list here the polynomials up to degree two, and the monomial functions up to degree three. Some of them are omitted for they can be obtained by duality.

Polynomials:

$$P^\kappa_{200000} = z_1^2 - \frac{2z_3}{1+\kappa} - \frac{10\kappa z_6}{(1+\kappa)(1+4\kappa)},$$

$$P^\kappa_{110000} = z_1 z_2 - \frac{5z_5}{1+4\kappa} + \frac{(6 - 95\kappa + 24\kappa^2) z_1}{(1+4\kappa)(2+11\kappa)},$$

$$P^\kappa_{020000} = z_2^2 - \frac{2z_4}{1+\kappa} - \frac{8\kappa z_1 z_6}{(1+\kappa)(1+3\kappa)} + \frac{6(-1+\kappa)(1-\kappa+6\kappa^2) z_2}{(1+\kappa)(1+3\kappa)(3+11\kappa)} + \frac{18(-1+\kappa)(2+13\kappa-7\kappa^2+6\kappa^3)}{(1+\kappa)(1+3\kappa)(2+11\kappa)(3+11\kappa)},$$

$$P^\kappa_{101000} = z_1 z_3 - \frac{3z_4}{1+2\kappa} + \frac{(-2-35\kappa+10\kappa^2) z_1 z_6}{(1+2\kappa)(2+7\kappa)} - \frac{6(-1+\kappa)(2+15\kappa) z_2}{(1+2\kappa)(1+4\kappa)(2+7\kappa)} + \frac{9(-2+17\kappa)}{(1+2\kappa)(1+4\kappa)(2+7\kappa)},$$

$$P^{\kappa}_{011000} = z_2 z_3 - \frac{4z_1 z_5}{1+3\kappa} + \frac{5(-1+\kappa)(-2+3\kappa)z_2 z_6}{(1+3\kappa)(2+7\kappa)} - \frac{4(-1+7\kappa)z_1^2}{(1+3\kappa)(1+5\kappa)} + \frac{6(-4+51\kappa+311\kappa^2+41\kappa^3+105\kappa^4)z_3}{(1+3\kappa)(1+5\kappa)(2+7\kappa)(3+11\kappa)} + \frac{6(-16+17\kappa+673\kappa^2-245\kappa^3+75\kappa^4)z_6}{(1+3\kappa)(1+5\kappa)(2+7\kappa)(3+11\kappa)},$$

$$P^{\kappa}_{002000} = z_3^2 - \frac{2z_1 z_4}{1+\kappa} - \frac{2(-1+\kappa)z_2 z_5}{(1+\kappa)(1+2\kappa)} - \frac{8\kappa z_1^2 z_6}{(1+\kappa)(1+3\kappa)} + \frac{2(-3+7\kappa+49\kappa^2+37\kappa^3+30\kappa^4)z_3 z_6}{(1+\kappa)(1+2\kappa)(1+3\kappa)(3+7\kappa)} - \frac{2(-1+\kappa)\kappa(17+69\kappa)z_1 z_2}{(1+\kappa)(1+2\kappa)(1+3\kappa)(3+7\kappa)} + \frac{(-1+\kappa)(42+291\kappa+478\kappa^2+59\kappa^3+150\kappa^4)z_6^2}{(1+\kappa)(1+2\kappa)(1+3\kappa)(2+7\kappa)(3+7\kappa)} + \frac{12(6+27\kappa+41\kappa^2+103\kappa^3+3\kappa^4)z_5}{(1+\kappa)(1+2\kappa)(1+3\kappa)(2+7\kappa)(3+7\kappa)} - \frac{6(-2-7\kappa+58\kappa^2-433\kappa^3+24\kappa^4)z_1}{(1+\kappa)(1+2\kappa)(1+3\kappa)(2+7\kappa)(3+7\kappa)},$$

$$P^{\kappa}_{100100} = z_1 z_4 - \frac{4z_2 z_5}{1+3\kappa} + \frac{4(-1+\kappa)z_1^2 z_6}{1+5\kappa} - \frac{2(-1+\kappa)(5+21\kappa)z_3 z_6}{(1+3\kappa)^2(1+5\kappa)} + \frac{(1-\kappa)(27+292\kappa+723\kappa^2-270\kappa^3)z_1 z_2}{(1+3\kappa)^2(1+5\kappa)(3+10\kappa)} + \frac{2(7+56\kappa-15\kappa^2)z_6^2}{(1+3\kappa)^2(1+5\kappa)} - \frac{6(34+321\kappa+712\kappa^2+55\kappa^3+750\kappa^4)z_5}{(1+3\kappa)^2(1+5\kappa)(2+7\kappa)(3+10\kappa)} + \frac{3(-1+\kappa)(42+703\kappa+1634\kappa^2-2937\kappa^3-270\kappa^4)z_1}{(1+3\kappa)^2(1+5\kappa)(2+7\kappa)(3+10\kappa)},$$

$$P^{\kappa}_{010100} = z_2 z_4 - \frac{3z_3 z_5}{1+2\kappa} + \frac{4(-1+\kappa)(-1+2\kappa)z_1 z_2 z_6}{(1+2\kappa)(2+5\kappa)} + \frac{6(-1+\kappa)(-1+2\kappa)(-2+5\kappa)z_2^2}{(1+2\kappa)(2+5\kappa)(3+10\kappa)} - \frac{5(\kappa-1)(2+11\kappa)z_1 z_3}{(1+2\kappa)(1+3\kappa)(2+5\kappa)} - \frac{5(\kappa-1)(2+11\kappa)z_5 z_6}{(1+2\kappa)(1+3\kappa)(2+5\kappa)} + \frac{6(\kappa-1)(56+548\kappa+1465\kappa^2+1000\kappa^3+300\kappa^4)z_4}{(1+2\kappa)(1+3\kappa)(2+5\kappa)(3+10\kappa)(4+11\kappa)} + \frac{(-456-2930\kappa+2063\kappa^2+23981\kappa^3-7718\kappa^4+1440\kappa^5)z_1 z_6}{(1+2\kappa)(1+3\kappa)(2+5\kappa)(3+10\kappa)(4+11\kappa)} + \frac{3(272+244\kappa-11336\kappa^2-28933\kappa^3+8109\kappa^4-18036\kappa^5+540\kappa^6)z_2}{(1+2\kappa)(1+3\kappa)(2+5\kappa)(2+7\kappa)(3+10\kappa)(4+11\kappa)} + \frac{18(1-\kappa)(112+1200\kappa+2570\kappa^2-1215\kappa^3+1788\kappa^4+180\kappa^5)}{(1+2\kappa)(1+3\kappa)(2+5\kappa)(2+7\kappa)(3+10\kappa)(4+11\kappa)},$$

$$P^{\kappa}_{001100} = z_3 z_4 - \frac{3z_1 z_2 z_5}{1+2\kappa} - \frac{5(-1+\kappa)z_2^2 z_6}{(1+2\kappa)(1+3\kappa)} + \frac{4(-1+\kappa)(-1+2\kappa)z_1 z_3 z_6}{(1+2\kappa)(2+5\kappa)} - \frac{5(-1+\kappa)z_5^2}{(1+2\kappa)(1+3\kappa)} + \frac{(-42+25\kappa+444\kappa^2+263\kappa^3+150\kappa^4)z_4 z_6}{(1+2\kappa)(1+3\kappa)(2+5\kappa)(3+7\kappa)} - \frac{5(-1+\kappa)(2+11\kappa)z_1^2 z_2}{(1+2\kappa)(1+3\kappa)(2+5\kappa)} + \frac{4(-15-32\kappa+276\kappa^2+626\kappa^3-105\kappa^4+90\kappa^5)z_1 z_6^2}{(1+2\kappa)(1+3\kappa)^2(2+5\kappa)(3+7\kappa)}$$

$$+\frac{2(-1+\kappa)(84+574\kappa+904\kappa^2+69\kappa^3+315\kappa^4)z_2z_3}{(1+2\kappa)(1+3\kappa)(2+5\kappa)^2(3+7\kappa)}$$

$$+\frac{4(1-\kappa)(30+109\kappa-87\kappa^2+158\kappa^3+1680\kappa^4)z_1z_5}{(1+2\kappa)(1+3\kappa)^2(2+5\kappa)^2(3+7\kappa)}$$

$$+\frac{(\kappa-1)(-36-1080\kappa-8095\kappa^2-12988\kappa^3+5847\kappa^4)z_1^2}{(1+2\kappa)(1+3\kappa)^2(2+5\kappa)^2(3+7\kappa)}$$

$$+\frac{2(-1+\kappa)(12+734\kappa+5474\kappa^2+9705\kappa^3-1620\kappa^4+675\kappa^5)z_2z_6}{(1+2\kappa)(1+3\kappa)^2(2+5\kappa)^2(3+7\kappa)}$$

$$+\frac{3(1-\kappa)(1+6\kappa)(44+492\kappa-41\kappa^2+252\kappa^3+45\kappa^4)z_3}{(1+2\kappa)(1+3\kappa)^2(2+5\kappa)^2(3+7\kappa)}$$

$$-\frac{3(-120-3020\kappa-14654\kappa^2+9383\kappa^3+99779\kappa^4-34713\kappa^5+12555\kappa^6+1350\kappa^7)z_6}{(1+2\kappa)(1+3\kappa)^2(2+5\kappa)^2(2+7\kappa)(3+7\kappa)},$$

$$P^{\kappa}_{000200}=z_4^2-\frac{2z_2z_3z_5}{1+\kappa}-\frac{2(-1+\kappa)z_3^2z_6}{(1+\kappa)(1+2\kappa)}-\frac{2(-1+\kappa)z_1z_5^2}{(1+\kappa)(1+2\kappa)}-\frac{2(-1+\kappa)z_1z_2^2z_6}{(1+\kappa)(1+2\kappa)}$$

$$-\frac{2(-1+\kappa)(-1+2\kappa)z_2^3}{(1+\kappa)(1+2\kappa)(1+3\kappa)}+\frac{4(-3+5\kappa+6\kappa^2+4\kappa^3)z_1z_4z_6}{(1+\kappa)(1+2\kappa)(3+5\kappa)}$$

$$-\frac{2(-1+\kappa)(-3+2\kappa+28\kappa^2)z_2z_5z_6}{(1+\kappa)(1+2\kappa)^2(3+5\kappa)}-\frac{2(-1+\kappa)(-3+2\kappa+28\kappa^2)z_1z_2z_3}{(1+\kappa)(1+2\kappa)^2(3+5\kappa)}$$

$$+\frac{6(-1+\kappa)(-15+2\kappa+335\kappa^2+754\kappa^3+436\kappa^4+120\kappa^5)z_2z_4}{5(1+\kappa)(1+2\kappa)^3(1+3\kappa)(3+5\kappa)}$$

$$+\frac{16(-1+\kappa)(3+10\kappa+3\kappa^2+2\kappa^3)z_1^2z_6^2}{(1+\kappa)(1+2\kappa)(2+5\kappa)(3+5\kappa)}-\frac{4(-18-65\kappa-82\kappa^2-109\kappa^3+22\kappa^4)z_3z_6^2}{(1+\kappa)(1+2\kappa)^2(2+5\kappa)(3+5\kappa)}$$

$$-\frac{4(-18-65\kappa-82\kappa^2-109\kappa^3+22\kappa^4)z_1^2z_5}{(1+\kappa)(1+2\kappa)^2(2+5\kappa)(3+5\kappa)}$$

$$-\frac{4(150+1507\kappa+6668\kappa^2+17329\kappa^3+27482\kappa^4+23584\kappa^5+9800\kappa^6+4200\kappa^7)z_3z_5}{5(1+\kappa)(1+2\kappa)^4(1+3\kappa)(2+5\kappa)(3+5\kappa)}$$

$$-\frac{2(-1+\kappa)(6+39\kappa-118\kappa^2-453\kappa^3+70\kappa^4)z_6^3}{(1+\kappa)(1+2\kappa)^2(1+3\kappa)(2+5\kappa)(3+5\kappa)}$$

$$+\frac{2(-1+\kappa)(-30-21\kappa+3383\kappa^2+22456\kappa^3+52408\kappa^4+39680\kappa^5-3216\kappa^6+2880\kappa^7)z_1z_2z_6}{5(1+\kappa)(1+2\kappa)^4(1+3\kappa)(2+5\kappa)(3+5\kappa)}$$

$$-\frac{4(-1+\kappa)(-6-37\kappa+225\kappa^2+1328\kappa^3+1224\kappa^4-616\kappa^5+600\kappa^6)z_5z_6}{(1+\kappa)(1+2\kappa)^4(1+3\kappa)(2+5\kappa)(3+5\kappa)}$$

$$-\frac{2(-1+\kappa)(6+39\kappa-118\kappa^2-453\kappa^3+70\kappa^4)z_1^3}{(1+\kappa)(1+2\kappa)^2(1+3\kappa)(2+5\kappa)(3+5\kappa)}$$

$$+\frac{9(-1+\kappa)(-60-784\kappa-4813\kappa^2-15896\kappa^3-24883\kappa^4-9500\kappa^5+9296\kappa^6+80\kappa^7+1200\kappa^8)z_2^2}{5(1+\kappa)(1+2\kappa)^4(1+3\kappa)(2+5\kappa)^2(3+5\kappa)}$$

$$-\frac{4(-1+\kappa)(-6-37\kappa+225\kappa^2+1328\kappa^3+1224\kappa^4-616\kappa^5+600\kappa^6)z_1z_3}{(1+\kappa)(1+2\kappa)^4(1+3\kappa)(2+5\kappa)(3+5\kappa)}-\frac{Az_1z_6}{a}-\frac{Bz_2}{a}-\frac{Cz_4}{a}+\frac{D}{a},$$

$$P^{\kappa}_{001010} = z_3 z_5 - \frac{4z_1 z_2 z_6}{1+3\kappa} - \frac{9(-1+\kappa)z_2^2}{(1+3\kappa)(1+4\kappa)} + \frac{5(-1+\kappa)(-2+3\kappa)z_1 z_3}{(1+3\kappa)(2+7\kappa)} + \frac{5(-1+\kappa)(-2+3\kappa)z_5 z_6}{(1+3\kappa)(2+7\kappa)}$$
$$+ \frac{24(-1+\kappa+21\kappa^2+9\kappa^3)z_4}{(1+3\kappa)^2(1+4\kappa)(2+7\kappa)} + \frac{(-44+140\kappa+3413\kappa^2+7150\kappa^3-5079\kappa^4+900\kappa^5)z_1 z_6}{(1+3\kappa)^2(1+4\kappa)(2+7\kappa)^2}$$
$$- \frac{36\kappa(16+26\kappa-231\kappa^2+9\kappa^3)z_2}{(1+3\kappa)^2(1+4\kappa)(2+7\kappa)^2} - \frac{108\kappa(6+103\kappa+311\kappa^2-123\kappa^3+63\kappa^4)}{(1+3\kappa)^2(1+4\kappa)(1+5\kappa)(2+7\kappa)^2},$$

$$P^{\kappa}_{100001} = z_1 z_6 - \frac{6z_2}{1+5\kappa} - \frac{9(-1+7\kappa)}{(1+5\kappa)(1+8\kappa)},$$

where the coefficients A, B, C, D, and a are

$$A = 8\kappa(-12-6872\kappa-74937\kappa^2-237510\kappa^3-15495\kappa^4+979026\kappa^5+989844\kappa^6-199504\kappa^7$$
$$+142260\kappa^8+10800\kappa^9),$$

$$B = 18(1-\kappa)(180+2196\kappa+12403\kappa^2+34729\kappa^3+9833\kappa^4-153277\kappa^5-225096\kappa^6-37608\kappa^7$$
$$-36240\kappa^8-3600\kappa^9),$$

$$C = 6(420+6424\kappa+50807\kappa^2+228922\kappa^3+594476\kappa^4+938974\kappa^5+1027217\kappa^6+835680\kappa^7$$
$$+400680\kappa^8+132000\kappa^9+18000\kappa^{10}),$$

$$D = 27(120+1772\kappa+7970\kappa^2+5421\kappa^3+21440\kappa^4+503710\kappa^5+1712910\kappa^6+1652129\kappa^7$$
$$+44920\kappa^8+259768\kappa^9+19840\kappa^{10}+3600\kappa^{11}),$$

$$a = 5(1+\kappa)(1+2\kappa)^4(1+3\kappa)(2+5\kappa)^2(3+5\kappa)(3+7\kappa).$$

Monomial functions:

$$M_{200000} = z_1^2 - 2z_3,$$

$$M_{110000} = z_1 z_2 - 5z_5 + 3z_1,$$

$$M_{020000} = z_2^2 - 2z_4 - 2z_2 - 6,$$

$$M_{101000} = z_1 z_3 - 3z_4 - z_1 z_6 + 6z_2 - 9,$$

$$M_{011000} = z_2 z_3 - 4z_1 z_5 + 5z_2 z_6 + 4z_1^2 - 4z_3 - 16z_6,$$

$$M_{002000} = z_3^2 - 2z_1 z_4 + 2z_2 z_5 - 2z_3 z_6 - 7z_6^2 + 12z_5 + 2z_1,$$

$$M_{100100} = z_1 z_4 - 4z_2 z_5 - 4z_1^2 z_6 + 10z_3 z_6 + 9z_1 z_2 + 14z_6^2 - 34z_5 - 21z_1,$$

$$M_{010100} = z_2 z_4 - 3z_3 z_5 + 2z_1 z_2 z_6 - 2z_2^2 + 5z_1 z_3 + 5z_5 z_6 - 14z_4 - 19z_1 z_6 + 17z_2 + 42,$$

$$M_{001100} = z_3 z_4 - 3z_1 z_2 z_5 + 5z_2^2 z_6 + 2z_1 z_3 z_6 + 5z_5^2 - 7z_4 z_6 + 5z_1^2 z_2 - 10z_1 z_6^2 - 14z_2 z_3 + 10z_1 z_5 - 3z_1^2$$
$$-2z_2 z_6 + 11z_3 + 15z_6,$$

$$M_{000200} = z_4^2 - 2z_2z_3z_5 + 2z_3^2z_6 + 2z_1z_5^2 + 2z_1z_2^2z_6 - 2z_2^3 - 4z_1z_4z_6 - 2z_2z_5z_6 - 2z_1z_2z_3 + 6z_2z_4 - 8z_1^2z_6^2 + 12z_3z_6^2 + 12z_1^2z_5 - 20z_3z_5 + 2z_6^3 + 2z_1z_2z_6 - 4z_5z_6 + 2z_1^3 + 9z_2^2 - 4z_1z_3 - 14z_4 - 18z_2 + 9,$$

$$M_{001010} = z_3z_5 - 4z_1z_2z_6 + 9z_2^2 + 5z_1z_3 + 5z_5z_6 - 12z_4 - 11z_1z_6,$$

$$M_{100001} = z_1z_6 - 6z_2 + 9,$$

$$M_{300000} = z_1^3 - 3z_1z_3 + 3z_4,$$

$$M_{210000} = z_1^2z_2 - 2z_2z_3 - z_1z_5 - z_1^2 + 5z_2z_6 - 5z_3 - 9z_6,$$

$$M_{120000} = z_1z_2^2 - 2z_1z_4 - z_2z_5 + 4z_3z_6 - 4z_6^2 - 8z_1z_2 + 9z_5 + 7z_1,$$

$$M_{030000} = z_2^3 - 3z_2z_4 + 3z_3z_5 - 3z_1z_2z_6 + 3z_4 + 3z_1z_6 - 9,$$

$$M_{201000} = z_1^2z_3 - 2z_3^2 - z_1z_4 - z_1^2z_6 + 4z_2z_5 - 2z_3z_6 - 4z_6^2 + z_1z_2 - z_5 + 8z_1,$$

$$M_{111000} = z_1z_2z_3 - 3z_2z_4 - 4z_1^2z_5 + 6z_3z_5 + 7z_1z_2z_6 - 10z_5z_6 - 12z_2^2 + 4z_1^3 - 19z_1z_3 + 33z_4 + 7z_1z_6 + 15z_2 - 9,$$

$$M_{021000} = z_2^2z_3 - 2z_3z_4 - z_1z_2z_5 + 5z_5^2 + 4z_1z_3z_6 - 8z_4z_6 - 6z_1^2z_2 - 12z_1z_6^2 + 3z_2z_3 + 11z_1z_5 + 14z_1^2 + 18z_2z_6 - 18z_3 - 14z_6,$$

$$M_{102000} = z_1z_3^2 - 2z_1^2z_4 - z_3z_4 + 5z_1z_2z_5 - 5z_5^2 - 5z_2^2z_6 - 5z_1z_3z_6 + 10z_4z_6 + 5z_2z_3 + 4z_1z_6^2 - 3z_1z_5 + 6z_2z_6 - 10z_3 - z_6,$$

$$M_{012000} = z_2z_3^2 - 2z_1z_2z_4 - z_1z_3z_5 + 2z_2^2z_5 + 3z_4z_5 + 4z_1^2z_2z_6 - 9z_2z_3z_6 - 6z_1^2z_3 - 3z_1z_5z_6 - 4z_1z_2^2 + 11z_3^2 + 8z_1z_4 + 2z_1^2z_6 - 2z_2z_6^2 + 6z_2z_5 + 11z_3z_6 - 12z_1z_2 - 6z_6^2 + 19z_5 + 18z_1,$$

$$M_{003000} = z_3^3 - 3z_1z_3z_4 + 3z_4^2 + 3z_1^2z_2z_5 - 3z_2z_3z_5 - 3z_1z_2^2z_6 - 3z_1^2z_3z_6 + 3z_3^2z_6 - 3z_1z_5^2 + 6z_1z_4z_6 + 3z_1^2z_6^2 + 3z_2z_5z_6 + 3z_2^3 + 3z_1z_2z_3 - 9z_2z_4 - 3z_1^2z_5 - 8z_6^3 - 3z_1z_2z_6 + 21z_5z_6 - 21z_4,$$

$$M_{200100} = z_1^2z_4 - 2z_3z_4 - z_1z_2z_5 - 4z_1^3z_6 + 5z_5^2 + 5z_2^2z_6 + 12z_1z_3z_6 - 19z_4z_6 + 4z_1^2z_2 - 11z_2z_3 - 8z_1z_6^2 + 8z_1^2 + 4z_2z_6 - 6z_3 - 7z_6,$$

$$M_{110100} = z_1z_2z_4 - 3z_1z_3z_5 - 4z_2^2z_5 + 6z_4z_5 + 2z_1^2z_2z_6 + 7z_2z_3z_6 + 5z_1^2z_3 - 7z_1z_2^2 - 3z_1z_5z_6 - 15z_3^2 + 2z_1z_4 - 3z_1^2z_6 - z_2z_6^2 + 15z_2z_5 - 6z_3z_6 + 24z_1z_2 + 9z_6^2 - 16z_5 - 28z_1,$$

$$M_{020100} = z_2^2z_4 - 2z_4^2 - z_2z_3z_5 + 4z_3^2z_6 + 4z_1z_5^2 - 6z_1z_4z_6 - 3z_2z_5z_6 - 3z_1z_2z_3 - 8z_1^2z_6^2 + 4z_3z_6^2 + 6z_2z_4 + 4z_1^2z_5 - 8z_3z_5 + 8z_6^3 + 27z_1z_2z_6 + 8z_1^3 - 22z_5z_6 - 19z_2^2 - 22z_1z_3 + 20z_4 - 14z_1z_6 - 4z_2 + 42,$$

$$M_{101100} = z_1z_3z_4 - 3z_4^2 - 3z_1^2z_2z_5 + 4z_2z_3z_5 + 2z_1^2z_3z_6 + 7z_1z_2^2z_6 - 4z_3^2z_6 + 7z_1z_5^2 - 9z_1z_4z_6 - 10z_1^2z_6^2 - 20z_2z_5z_6 - 12z_2^3 + 5z_1^3z_2 - 20z_1z_2z_3 + 12z_3z_6^2 + 45z_2z_4 + 2z_1^2z_5 + 40z_6^3 + 12z_3z_5 + 24z_1z_2z_6 + 3z_1^3 - 92z_5z_6 - 21z_1z_3 - 18z_2^2 + 96z_4 - 7z_1z_6 + 33z_2 - 9,$$

$$M_{011100} = z_2z_3z_4 - 3z_3^2z_5 - 3z_1z_2^2z_5 + 5z_2^3z_6 + 4z_1z_4z_5 + 8z_1z_2z_3z_6 + 7z_2z_5^2 - 22z_2z_4z_6 - 5z_1z_3^2 - 4z_1^2z_5z_6 - 5z_1^2z_2^2 + z_3z_5z_6 - 10z_1z_2z_6^2 + 8z_5z_6^2 + 8z_1^2z_4 - 3z_2^2z_3 + 8z_3z_4 + 19z_1z_2z_5 - 2z_2^2z_6 + 4z_1^3z_6 - 23z_5^2 + z_1z_3z_6 - 4z_1^2z_2 + 8z_4z_6 + 2z_1z_6^2 + 10z_2z_3 - 18z_1z_5 + 17z_1^2 + 3z_2z_6 - 14z_3 - 6z_6,$$

$$M_{002100} = z_3^2z_4 - 2z_1z_4^2 - z_1z_2z_3z_5 + 5z_2z_4z_5 + 4z_1^2z_5^2 + 4z_1^2z_2^2z_6 - 7z_3z_5^2 - 6z_1^2z_4z_6 - 7z_2^2z_3z_6 - 3z_1^2z_2z_3 + 10z_3z_4z_6 - 4z_1z_2^3 - 9z_1z_2z_5z_6 + 6z_2z_3^2 - 8z_1^3z_6^2 + 5z_5^2z_6 + 5z_2^2z_6^2 + 9z_1z_2z_4 + 24z_1z_3z_6^2 + 13z_2^2z_5 + 4z_1^3z_5 - 8z_1z_3z_5 - 8z_4z_6^2 - 4z_1z_6^3 - 18z_4z_5 + 7z_1^2z_2z_6 - 23z_2z_3z_6 + 4z_1z_5z_6 + 8z_1^4 - 29z_1^2z_3 - 20z_2z_6^2 + 4z_1z_2^2 + 16z_3^2 + z_1z_4 + z_1^2z_6 + 10z_2z_5 + 24z_3z_6 - z_1z_2 + 19z_6^2 - 16z_5 - 27z_1,$$

$$M_{100200} = z_1z_4^2 - 2z_1z_2z_3z_5 - z_2z_4z_5 + 2z_1^2z_5^2 + 2z_1z_3^2z_6 + 2z_1^2z_2^2z_6 + 3z_3z_5^2 - 4z_1^2z_4z_6 + 3z_2^2z_3z_6 - 2z_1^2z_2z_3 - 5z_3z_4z_6 - 7z_1z_2^3 - 7z_1z_2z_5z_6 - 3z_2z_3^2 - 8z_1^3z_6^2 + 21z_1z_2z_4 + 14z_1z_3z_6^2 + 7z_2^2z_5 + 12z_1^3z_5 - 25z_1z_3z_5 - z_4z_6^2 + 8z_1z_6^3 + 3z_4z_5 + 13z_1^2z_2z_6 - 19z_2z_3z_6 - 17z_1z_5z_6 + 2z_1^4 - 16z_1^2z_3 - 8z_2z_6^2 + 10z_1z_2^2 + 27z_3^2 - 11z_1z_4 - z_1^2z_6 + 7z_2z_5 + 11z_3z_6 - 31z_1z_2 - 8z_6^2 + 37z_5 + 22z_1,$$

$$M_{010200} = z_2z_4^2 - 2z_2^2z_3z_5 - z_3z_4z_5 + 5z_2z_3^2z_6 + 5z_1z_2z_5^2 - 5z_3^3 - 5z_5^3 + 2z_1z_2^3z_6 - 9z_1z_2z_4z_6 - 5z_2^2z_5z_6 - 5z_1z_3z_5z_6 + 15z_4z_5z_6 - 5z_1z_2^2z_3 - 2z_2^4 + 15z_1z_3z_4 - 6z_1^2z_2z_6^2 + 7z_2z_3z_6^2 + 14z_2^2z_4 - 16z_4^2 + 11z_1z_5z_6^2 + 7z_1^2z_2z_5 - 10z_2z_3z_5 + 11z_1^2z_3z_6 + 4z_1z_2^2z_6 - 12z_1z_5^2 - 12z_3^2z_6 - 17z_1z_4z_6 - 5z_1^2z_6^2 - 10z_1^3z_2 - 10z_2z_6^3 + 29z_2z_5z_6 + 29z_1z_2z_3 + 3z_3z_6^2 + 10z_6^3 - 21z_2z_4 + 3z_1^2z_5 - 34z_3z_5 + 7z_1z_2z_6 - 14z_5z_6 + 10z_1^3 - 14z_1z_3 - 6z_2^2 - 6z_4 - 34z_1z_6 + 38z_2 + 42,$$

$$M_{001200} = z_3z_4^2 - 2z_2z_3^2z_5 + 2z_3^3z_6 - z_1z_2z_4z_5 + 5z_1z_3z_5^2 + 4z_2^2z_5^2 - 7z_4z_5^2 + 5z_1z_2^2z_3z_6 - 7z_2^2z_4z_6 - 9z_1z_3z_4z_6 + 14z_4^2z_6 - 5z_1^2z_2z_5z_6 - 6z_1^2z_3z_6^2 - 5z_1^2z_2^3 - 6z_2z_3z_5z_6 - 5z_1z_2z_3^2 + 15z_1^2z_2z_4 + 6z_3^2z_6^2 + 7z_1^2z_3z_5 + 2z_2^3z_3 + z_2z_3z_4 - 4z_3^2z_5 + 24z_1z_4z_6^2 + 8z_1z_2^2z_5 - 12z_2z_5z_6^2 - 33z_1z_4z_5 + 2z_1^2z_6^3 + 11z_1^3z_2z_6 + 8z_3z_6^3 + 8z_6^4 - 28z_1z_2z_3z_6 + 16z_2z_5^2 + 7z_1^2z_2^2 + 2z_2z_4z_6 - z_1^2z_5z_6 - 6z_3z_5z_6 + 11z_2^2z_3 - 10z_1^3z_3 + 38z_1z_3^2 - 29z_1^2z_4 - 22z_3z_4 - z_1^3z_6 - z_1z_2z_5 - 20z_5z_6^2 - 9z_1z_3z_6 - 20z_1^2z_2 - 5z_2^2z_6 + 22z_5^2 - 3z_4z_6 + 14z_2z_3 - 24z_1z_6^2 + 29z_1z_5 + 10z_2z_6 + 27z_3 + 17z_6,$$

$$M_{000300} = z_4^3 - 3z_2z_3z_4z_5 + 3z_3^2z_5^2 + 3z_1z_2^2z_5^2 + 3z_2^2z_3^2z_6 - 3z_3^2z_4z_6 - 3z_1z_2^2z_4z_6 - 3z_1z_4z_5^2 - 3z_2z_3^3 - 3z_2^3z_5z_6 + 6z_1z_4^2z_6 - 9z_1z_2z_3z_5z_6 - 3z_2z_5^3 + 12z_2z_4z_5z_6 - 3z_1z_2^3z_3 + 3z_3z_5^2z_6 + 9z_1^2z_4z_6^2 + 12z_1z_2z_3z_4 + 3z_2^2z_3z_6^2 + 6z_2^3z_4 - 18z_2z_4^2 + 3z_1^2z_2^2z_5 - 12z_3z_4z_6^2 + 3z_1z_2^2z_5 - 12z_1^2z_4z_5 + 3z_2^2z_6^3 - 4z_1^3z_6^3 + 9z_3z_4z_5 + 3z_1^2z_3^2 + 3z_5^2z_6^2 - 12z_1z_2z_4z_6 + 12z_1z_3z_6^3 - 24z_4z_6^3 - 3z_5^3 + 12z_1^3z_5z_6 - 33z_1z_3z_5z_6 - 3z_3^3 + 3z_1^3z_2^2 - 24z_1^3z_4 + 54z_4z_5z_6 + 54z_1z_3z_4 - 45z_4^2 - 9z_2z_3z_5 - 9z_1z_2^2z_6 - 6z_1z_5z_6^2 - 6z_2z_6^3$$

$$- 6z_1^2z_3z_6 - 6z_1^3z_2 + 27z_1z_4z_6 + 9z_2z_5z_6 + 12z_2^3 + 3z_1^2z_6^2 + 9z_1z_2z_3 + 9z_1^2z_5 - 36z_2z_4 + 9z_3z_6^2 + 9z_3z_5 - 18z_1z_2z_6 + 3z_6^3 + 3z_1^3 + 9z_4 + 9z_1z_6 - 9,$$

$$M_{101010} = z_1z_3z_5 - 3z_4z_5 - 4z_1^2z_2z_6 + 5z_1^2z_3 + 6z_2z_3z_6 + 9z_1z_2^2 + 7z_1z_5z_6 - 10z_3^2 - 13z_1z_4 - 13z_1^2z_6 - 10z_2z_6^2 - 7z_2z_5 + 16z_3z_6 + 50z_6^2 + 11z_1z_2 - 57z_5 - 59z_1,$$

$$M_{011010} = z_2z_3z_5 - 4z_3^2z_6 - 4z_1z_5^2 - 4z_1z_2^2z_6 + 9z_2^3 + 12z_1z_4z_6 + 11z_2z_5z_6 + 11z_1z_2z_3 - 45z_2z_4 + 16z_1^2z_6^2 - 28z_3z_6^2 - 28z_1^2z_5 + 45z_3z_5 - 16z_6^3 - 17z_1z_2z_6 + 45z_5z_6 - 16z_1^3 + 45z_1z_3 - 27z_4 - 3z_1z_6 + 18z_2 - 27,$$

$$M_{002010} = z_3^2z_5 - 2z_1z_4z_5 + 2z_2z_5^2 - z_1z_2z_3z_6 + 3z_2z_4z_6 + 4z_1^2z_5z_6 + 5z_1^2z_2^2 - 9z_3z_5z_6 - 3z_1z_2z_6^2 - 8z_1^2z_4 - 9z_2^2z_3 - 2z_5z_6^2 + 16z_3z_4 - 6z_1z_2z_5 + 7z_5^2 - 12z_1^3z_6 + 8z_2^2z_6 + 37z_1z_3z_6 - 9z_4z_6 + 2z_1^2z_2 + z_1z_6^2 - 27z_2z_3 + 6z_1z_5 + 13z_1^2 - 11z_2z_6 - 14z_3 + 13z_6,$$

$$M_{001110} = z_3z_4z_5 - 3z_1z_2z_5^2 - 3z_2z_3^2z_6 + 5z_3^3 + 4z_1z_2z_4z_6 + 8z_1z_3z_5z_6 + 5z_5^3 + 7z_2^2z_5z_6 + 7z_1z_2^2z_3 - 22z_4z_5z_6 - 4z_1^2z_2z_6^2 - 18z_2^2z_4 + z_2z_3z_6^2 - 22z_1z_3z_4 + 36z_4^2 + z_1^2z_2z_5 - 10z_1z_5z_6^2 + 8z_2z_6^3 - 8z_2z_3z_5 - 10z_1^2z_3z_6 + 8z_3^2z_6 + 8z_1z_5^2 + 9z_2^3 + 52z_1z_4z_6 + 16z_1^2z_6^2 - 40z_2z_5z_6 + 8z_1^3z_2 - 40z_1z_2z_3 - z_3z_6^2 - z_1^2z_5 + 9z_2z_4 + 24z_3z_5 - 23z_1z_2z + 18z_2^2 + 27z_1z_3 + 27z_5z_6 - 63z_4 - 9z_1z_6 - 36z_2 - 27,$$

$$M_{200001} = z_1^2z_6 - 2z_3z_6 - z_1z_2 + 5z_5 - 4z_1,$$

$$M_{110001} = z_1z_2z_6 - 6z_2^2 - 5z_1z_3 - 5z_5z_6 + 21z_4 + 24z_1z_6 - 30z_2 - 9,$$

$$M_{101001} = z_1z_3z_6 - 3z_4z_6 - z_1z_6^2 - 5z_1^2z_2 + 8z_2z_3 + 9z_1z_5 + z_1^2 - 9z_2z_6 + 3z_3 + 2z_6,$$

$$M_{100101} = z_1z_4z_6 - 4z_2z_5z_6 - 4z_1z_2z_3 - 4z_1^2z_6^2 + 9z_2z_4 + 10z_3z_6^2 + 10z_1^2z_5 - 9z_3z_5 - z_1z_2z_6 + 14z_6^3 - 39z_5z_6 + 14z_1^3 - 39z_1z_3 + 27z_4 + 24z_1z_6 - 81.$$

APPENDIX C: DEFORMED QUADRATIC CLEBSCH–GORDAN SERIES

$$P^\kappa_{100000} \times P^\kappa_{100000} = P^\kappa_{200000} + \frac{2}{1+\kappa}P^\kappa_{001000} + \frac{10(1+3\kappa)}{(1+4\kappa)(1+7\kappa)}P^\kappa_{000001},$$

$$P^\kappa_{100000} \times P^\kappa_{010000} = P^\kappa_{110000} + \frac{5}{1+4\kappa}P^\kappa_{000010} + \frac{32(1+2\kappa)(1+12\kappa)}{(1+7\kappa)(1+11\kappa)(2+11\kappa)}P^\kappa_{100000},$$

$$P^{\kappa}_{010000}\times P^{\kappa}_{010000}=P^{\kappa}_{020000}+\frac{2}{1+\kappa}P^{\kappa}_{000100}+\frac{8(1+2\kappa)}{(1+3\kappa)(1+5\kappa)}P^{\kappa}_{100001}+\frac{12(5+84\kappa+255\kappa^2+160\kappa^3)}{(1+5\kappa)^2(1+11\kappa)(3+11\kappa)}P^{\kappa}_{010000}+\frac{144(1+2\kappa)(1+3\kappa)(1+5\kappa)(1+12\kappa)}{(1+7\kappa)(1+8\kappa)(1+11\kappa)^2(2+11\kappa)}P^{\kappa}_{000000},$$

$$P^{\kappa}_{100000}\times P^{\kappa}_{001000}=P^{\kappa}_{101000}+\frac{3}{1+2\kappa}P^{\kappa}_{000100}+\frac{16(1+2\kappa)(1+8\kappa)}{(1+5\kappa)(1+7\kappa)(2+7\kappa)}P^{\kappa}_{100001}+\frac{15(1+\kappa)(1+3\kappa)(1+11\kappa)}{(1+4\kappa)(1+5\kappa)^2(1+7\kappa)}P^{\kappa}_{010000},$$

$$P^{\kappa}_{010000}\times P^{\kappa}_{001000}=P^{\kappa}_{011000}+\frac{4}{1+3\kappa}P^{\kappa}_{100010}+\frac{20(1+\kappa)(1+8\kappa)}{(1+4\kappa)(1+7\kappa)(2+7\kappa)}P^{\kappa}_{010001}+\frac{16(1+2\kappa)}{(1+5\kappa)(1+7\kappa)}P^{\kappa}_{200000}+\frac{20(1+2\kappa)(1+9\kappa)(3+46\kappa+71\kappa^2-8\kappa^3)}{(1+\kappa)(1+4\kappa)^2(1+7\kappa)(1+11\kappa)(3+11\kappa)}P^{\kappa}_{001000}+\frac{80(1+\kappa)(1+2\kappa)(1+3\kappa)(1+12\kappa)}{(1+4\kappa)(1+5\kappa)(1+7\kappa)^2(2+11\kappa)}P^{\kappa}_{000001},$$

$$P^{\kappa}_{001000}\times P^{\kappa}_{001000}=P^{\kappa}_{002000}+\frac{2}{1+\kappa}P^{\kappa}_{100100}+\frac{6(1+\kappa)}{(1+2\kappa)(1+3\kappa)}P^{\kappa}_{010010}+\frac{8(1+2\kappa)}{(1+3\kappa)(1+5\kappa)}P^{\kappa}_{200001}+\frac{4(9+113\kappa+305\kappa^2+231\kappa^3-18\kappa^4)}{(1+\kappa)(1+3\kappa)^2(1+7\kappa)(3+7\kappa)}P^{\kappa}_{001001}+\frac{120(1+\kappa)(1+2\kappa)(2+33\kappa+56\kappa^2)}{(1+4\kappa)(2+5\kappa)(1+7\kappa)(2+7\kappa)(3+10\kappa)}P^{\kappa}_{110000}+\frac{80(1+\kappa)(1+2\kappa)(1+3\kappa)(1+8\kappa)}{(1+4\kappa)(1+5\kappa)(1+7\kappa)^2(2+7\kappa)}P^{\kappa}_{000002}+\frac{80(1+8\kappa)(3+56\kappa+176\kappa^2+108\kappa^3-63\kappa^4)}{(1+4\kappa)^2(1+7\kappa)^2(2+7\kappa)(3+11\kappa)}P^{\kappa}_{000010}+\frac{160(1+\kappa)^2(1+2\kappa)(1+3\kappa)(1+9\kappa)(1+12\kappa)}{(1+4\kappa)^2(1+5\kappa)(1+7\kappa)^3(2+11\kappa)}P^{\kappa}_{100000},$$

$$P^{\kappa}_{100000}\times P^{\kappa}_{000100}=P^{\kappa}_{100100}+\frac{4}{1+3\kappa}P^{\kappa}_{010010}+\frac{6(1+\kappa)(1+7\kappa)}{(1+3\kappa)^2(1+5\kappa)}P^{\kappa}_{001001}+\frac{30(1+\kappa)(1+2\kappa)(1+8\kappa)(2+11\kappa)}{(1+4\kappa)(1+5\kappa)^2(2+7\kappa)(3+10\kappa)}P^{\kappa}_{110000}+\frac{30(1+\kappa)(1+2\kappa)(2+5\kappa)(1+8\kappa)(1+9\kappa)}{(1+4\kappa)^2(1+5\kappa)^2(2+7\kappa)(3+11\kappa)}P^{\kappa}_{000010},$$

$$P^{\kappa}_{010000}\times P^{\kappa}_{000100}=P^{\kappa}_{010100}+\frac{3}{1+2\kappa}P^{\kappa}_{001010}+\frac{12(1+\kappa)(1+6\kappa)}{(1+3\kappa)(1+5\kappa)(2+5\kappa)}P^{\kappa}_{110001}$$
$$+\frac{30(1+\kappa)(1+2\kappa)(2+11\kappa)}{(1+4\kappa)(1+5\kappa)^2(3+10\kappa)}P^{\kappa}_{020000}$$
$$+\frac{20(1+\kappa)(1+2\kappa)(1+8\kappa)}{(1+3\kappa)(1+4\kappa)(1+5\kappa)(2+7\kappa)}P^{\kappa}_{101000}$$
$$+\frac{20(1+\kappa)(1+2\kappa)(1+8\kappa)}{(1+3\kappa)(1+4\kappa)(1+5\kappa)(2+7\kappa)}P^{\kappa}_{000011}$$
$$+\frac{72(1+7\kappa)(1+22\kappa+115\kappa^2+87\kappa^3-45\kappa^4)}{(1+3\kappa)^2(1+5\kappa)^2(1+11\kappa)(4+11\kappa)}P^{\kappa}_{000100}$$
$$+\frac{144(1+\kappa)^2(1+2\kappa)(2+5\kappa)(1+8\kappa)^2}{(1+3\kappa)(1+5\kappa)^3(2+7\kappa)^2(3+11\kappa)}P^{\kappa}_{100001}$$
$$+\frac{60(1+\kappa)(1+2\kappa)^2(1+3\kappa)(2+5\kappa)(1+8\kappa)(1+9\kappa)(1+11\kappa)}{(1+4\kappa)^2(1+5\kappa)^4(1+7\kappa)(2+7\kappa)(3+11\kappa)}P^{\kappa}_{010000},$$

$$P^{\kappa}_{001000}\times P^{\kappa}_{000100}=P^{\kappa}_{001100}+\frac{3}{1+2\kappa}P^{\kappa}_{110010}+\frac{10(1+\kappa)}{(1+3\kappa)(1+4\kappa)}P^{\kappa}_{020001}+\frac{12(1+\kappa)(1+6\kappa)}{(1+3\kappa)(1+5\kappa)(2+5\kappa)}P^{\kappa}_{101001}$$
$$+\frac{10(1+\kappa)}{(1+3\kappa)(1+4\kappa)}P^{\kappa}_{000020}+\frac{72(1+6\kappa)(1+11\kappa+13\kappa^2-5\kappa^3)}{(1+2\kappa)(1+5\kappa)(2+5\kappa)(1+7\kappa)(3+7\kappa)}P^{\kappa}_{000101}$$
$$+\frac{20(1+\kappa)(1+2\kappa)(1+8\kappa)}{(1+3\kappa)(1+4\kappa)(1+5\kappa)(2+7\kappa)}P^{\kappa}_{210000}+\frac{48(1+\kappa)^2(1+2\kappa)(1+8\kappa)}{(1+3\kappa)^2(1+5\kappa)^2(2+7\kappa)}P^{\kappa}_{100002}$$
$$+\frac{6(36+1134\kappa+12624\kappa^2+65771\kappa^3+172189\kappa^4+224179\kappa^5+127295\kappa^6+17700\kappa^7)}{(1+2\kappa)(1+3\kappa)(1+5\kappa)^2(2+5\kappa)^2(1+7\kappa)(3+8\kappa)}$$

$$P^{\kappa}_{011000}+\frac{24(1+\kappa)(42+1024\kappa+7069\kappa^2+17092\kappa^3+13653\kappa^4+720\kappa^5)}{(1+3\kappa)^2(1+5\kappa)^2(3+7\kappa)(3+8\kappa)(4+11\kappa)}P^{\kappa}_{100010}$$

$$+\frac{480(1+\kappa)^2(1+2\kappa)^2(1+6\kappa)(1+8\kappa)}{(1+4\kappa)(1+5\kappa)^3(1+7\kappa)(2+7\kappa)(3+11\kappa)}P^{\kappa}_{200000}$$

$$+\frac{60(1+\kappa)(1+2\kappa)(1+8\kappa)(32+842\kappa+6313\kappa^2+16912\kappa^3+16251\kappa^4+3330\kappa^5)}{(1+3\kappa)(1+4\kappa)(1+5\kappa)^2(2+5\kappa)(1+7\kappa)(2+7\kappa)(3+10\kappa)(4+11\kappa)}P^{\kappa}_{010001}$$

$$+\frac{60(1+\kappa)(1+2\kappa)(2+5\kappa)(1+8\kappa)(1+9\kappa)(3+40\kappa+39\kappa^2-18\kappa^3)}{(1+3\kappa)^2(1+4\kappa)^2(1+5\kappa)^2(1+7\kappa)(2+7\kappa)(3+11\kappa)}P^{\kappa}_{001000}$$

$$+\frac{480(1+\kappa)^2(1+2\kappa)^2(1+3\kappa)(2+5\kappa)(1+8\kappa)(1+9\kappa)(1+12\kappa)}{(1+4\kappa)^2(1+5\kappa)^3(1+7\kappa)^2(2+7\kappa)(2+11\kappa)(3+11\kappa)}P^{\kappa}_{000001},$$

$$P^{\kappa}_{000100}\times P^{\kappa}_{000100}=P^{\kappa}_{000200}+\frac{2}{1+\kappa}P^{\kappa}_{011010}+\frac{6(1+\kappa)}{(1+2\kappa)(1+3\kappa)}P^{\kappa}_{002001}+\frac{6(1+\kappa)}{(1+2\kappa)(1+3\kappa)}P^{\kappa}_{100020}$$
$$+\frac{6(1+\kappa)}{(1+2\kappa)(1+3\kappa)}P^{\kappa}_{120001}+\frac{20(1+\kappa)(1+2\kappa)}{(1+3\kappa)(1+4\kappa)(1+5\kappa)}P^{\kappa}_{030000}$$
$$+\frac{24(1+7\kappa-2\kappa^2)}{(1+2\kappa)(1+5\kappa)(3+5\kappa)}P^{\kappa}_{100101}+\frac{36(1+\kappa)^2(1+13\kappa+16\kappa^2)}{(1+2\kappa)^2(1+3\kappa)(1+5\kappa)(3+7\kappa)}P^{\kappa}_{010011}$$
$$+\frac{36(1+\kappa)^2(1+13\kappa+16\kappa^2)}{(1+2\kappa)^2(1+3\kappa)(1+5\kappa)(3+7\kappa)}P^{\kappa}_{111000}$$
$$+\frac{36(1+\kappa)(40+1064\kappa+7172\kappa^2+16301\kappa^3+13138\kappa^4+940\kappa^5-1800\kappa^6)}{5(2+\kappa)(1+2\kappa)^3(1+5\kappa)^2(2+5\kappa)(4+9\kappa)}P^{001002}_{k}$$
$$+\frac{48(1+\kappa)^2(1+2\kappa)(1+6\kappa)}{(1+3\kappa)^2(1+5\kappa)^2(2+5\kappa)}P^{200002}_{k}+\frac{144(1+\kappa)(1+6\kappa)(1+11\kappa+13\kappa^2-5\kappa^3)}{(1+3\kappa)^2(1+5\kappa)^2(2+5\kappa)(3+7\kappa)}P^{\kappa}_{001002}$$
$$+\frac{144(1+\kappa)(1+6\kappa)(1+11\kappa+13\kappa^2-5\kappa^3)}{(1+3\kappa)^2(1+5\kappa)^2(2+5\kappa)(3+7\kappa)}P^{\kappa}_{200010}$$
$$+\frac{2(195+5540\kappa+49198\kappa^2+163456\kappa^3+239715\kappa^4+157964\kappa^5+57452\kappa^6+26320\kappa^7)}{(1+2\kappa)^4(1+5\kappa)^2(3+7\kappa)(5+11\kappa)}P^{\kappa}_{001010}$$
$$+EP^{\kappa}_{000003}+FP^{\kappa}_{110001}+GP^{\kappa}_{000011}+EP^{\kappa}_{300000}$$
$$+\frac{180(1+\kappa)^2(1+2\kappa)(90+2499\kappa+31155\kappa^2+193684\kappa^3+611355\kappa^4+972155\kappa^5+708750\kappa^6+171000\kappa^7)}{(1+3\kappa)(1+4\kappa)(1+5\kappa)^4(2+5\kappa)^2(3+8\kappa)(3+10\kappa)(5+11\kappa)}P^{\kappa}_{020000}$$
$$+GP^{\kappa}_{101000}+HP^{\kappa}_{000100}+IP^{\kappa}_{100001}$$
$$+\frac{2160(1+\kappa)^2(1+2\kappa)^2(2+5\kappa)(1+8\kappa)(1+9\kappa)(1+22\kappa+115\kappa^2+87\kappa^3-45\kappa^4)}{(1+3\kappa)(1+4\kappa)^2(1+5\kappa)^6(2+7\kappa)(3+11\kappa)(4+11\kappa)}P^{\kappa}_{010000}$$
$$+\frac{4320(1+\kappa)^2(1+2\kappa)^3(1+3\kappa)^2(2+5\kappa)(1+9\kappa)(1+12\kappa)}{(1+4\kappa)^2(1+5\kappa)^3(1+7\kappa)^2(2+7\kappa)(1+11\kappa)(2+11\kappa)(3+11\kappa)}P^{\kappa}_{000000},$$

$$P^{\kappa}_{100000}\times P^{\kappa}_{000010}=P^{\kappa}_{100010}+\frac{5}{1+4\kappa}P^{\kappa}_{010001}+\frac{10(1+\kappa)(1+9\kappa)}{(1+4\kappa)^2(1+7\kappa)}P^{\kappa}_{001000}$$
$$+\frac{32(1+2\kappa)(1+3\kappa)(1+12\kappa)}{(1+5\kappa)(1+7\kappa)^2(2+11\kappa)}P^{\kappa}_{000001},$$

$$P^{\kappa}_{001000}\times P^{\kappa}_{000010}=P^{\kappa}_{001010}+\frac{4}{1+3\kappa}P^{\kappa}_{110001}+\frac{15(1+\kappa)}{(1+4\kappa)(1+5\kappa)}P^{\kappa}_{020000}$$
$$+\frac{20(1+\kappa)(1+8\kappa)}{(1+4\kappa)(1+7\kappa)(2+7\kappa)}P^{\kappa}_{101000}+\frac{20(1+\kappa)(1+8\kappa)}{(1+4\kappa)(1+7\kappa)(2+7\kappa)}P^{\kappa}_{000011}$$
$$+\frac{6(3+40\kappa+39\kappa^2-18\kappa^3)}{(1+2\kappa)(1+3\kappa)^2(1+7\kappa)}P^{\kappa}_{000100}$$
$$+\frac{8(1+2\kappa)(48+1342\kappa+11893\kappa^2+41323\kappa^3+59235\kappa^4+31311\kappa^5)}{(1+3\kappa)(1+5\kappa)(1+7\kappa)^2(2+7\kappa)^2(3+11\kappa)}P^{\kappa}_{100001}$$
$$+\frac{60(1+2\kappa)(1+3\kappa)(1+9\kappa)(3+46\kappa+71\kappa^2-8\kappa^3)}{(1+4\kappa)^2(1+5\kappa)^2(1+7\kappa)^2(3+11\kappa)}P^{\kappa}_{010000}$$

$$+\frac{432(1+\kappa)(1+2\kappa)(1+3\kappa)^2(1+12\kappa)}{(1+5\kappa)(1+7\kappa)^2(1+8\kappa)(1+11\kappa)(2+11\kappa)}P^{\kappa}_{000000},$$

$$P^{\kappa}_{100000}\times P^{\kappa}_{000001}=P^{\kappa}_{100001}+\frac{6}{1+5\kappa}P^{\kappa}_{010000}+\frac{27(1+3\kappa)}{(1+8\kappa)(1+11\kappa)}P^{\kappa}_{000000},$$

where the coefficients E, F, G, H, and I are such that

$$E(1+3\kappa)(1+4\kappa)(1+5\kappa)^2(1+7\kappa)(2+7\kappa)=160(1+\kappa)^2(1+2\kappa)^2(1+8\kappa),$$

$$F(1+2\kappa)(1+3\kappa)(2+3\kappa)(1+5\kappa)^3(2+5\kappa)^2(3+5\kappa)(3+7\kappa)^2(5+11\kappa)=144(1+\kappa)^2(270+10965\kappa+166113\kappa^2+1237287\kappa^3+5078136\kappa^4+12177475\kappa^5+17282049\kappa^6+13976605\kappa^7+5700600\kappa^8+818500\kappa^9),$$

$$G=\frac{720(1+\kappa)^2(1+2\kappa)(1+8\kappa)(8+208\kappa+1312\kappa^2+1877\kappa^3+360\kappa^4-300\kappa^5)}{(2+\kappa)(1+3\kappa)(1+4\kappa)(1+5\kappa)^3(2+5\kappa)(2+7\kappa)(3+8\kappa)(4+11\kappa)},$$

$$H\frac{(1+3\kappa)^2(1+5\kappa)^4(2+5\kappa)^2(1+7\kappa)(3+7\kappa)(3+8\kappa)(4+11\kappa)}{24(1+\kappa)}=444+21566\kappa+436658\kappa^2+4716853\kappa^3+29111132\kappa^4+102644506\kappa^5+195972356\kappa^6+176806835\kappa^7+45083850\kappa^8-6894000\kappa^9+10935000\kappa^{10},$$

$$I(1+3\kappa)^2(1+5\kappa)^5(2+7\kappa)^2(3+8\kappa)(3+11\kappa)(4+11\kappa)=864(1+\kappa)^2(1+2\kappa)(1+8\kappa)(16+626\kappa+8775\kappa^2+55745\kappa^3+172984\kappa^4+268299\kappa^5+193845\kappa^6+48150\kappa^7).$$

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Extensions of representations of the *CAR* algebra to the Cuntz algebra $\mathcal{O}_2$—the Fock and the infinite wedge

Katsunori Kawamura[a)]
Research Institute for Mathematical Sciences, Kyoto University, Kyoto 606-8502, Japan

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Fermions are expressed by polynomials of canonical generators of the Cuntz algebra $\mathcal{O}_2$ and they generate the U(1)-fixed point subalgebra $\mathcal{A}\equiv\mathcal{O}_2^{\mathrm{U}(1)}$ of $\mathcal{O}_2$ by the canonical gauge action. We extend the Fock and the infinite wedge representations of $\mathcal{A}$ to permutative representations of $\mathcal{O}_2$. By these extensions, the boson-fermion correspondence is rewritten by canonical generators of $\mathcal{O}_2$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1939989]

I. INTRODUCTION

Let $\mathcal{A}_0$ be the Clifford algebra generated by fermions $a_n, a_n^*, n\in\mathbf{N}\equiv\{1,2,3,\ldots\}$ which satisfy the canonical anticommutation relations (=*CAR*):

$$a_n a_m^* + a_m^* a_n = \delta_{n,m} I, \quad a_n^* a_m^* + a_m^* a_n^* = a_n a_m + a_m a_n = 0 \tag{1.1}$$

for $n,m\in\mathbf{N}$. $\mathcal{A}_0$ always has unique C*-norm $\|\cdot\|$ and the completion $\mathcal{A}\equiv\overline{\mathcal{A}_0}$ with respect to $\|\cdot\|$ is called the *CAR algebra* in theory of operator algebras.[6] In Refs. 1–4, we construct several polynomial embeddings of $\mathcal{A}$ into the Cuntz algebras $\mathcal{O}_N$. For example, if s_1, s_2 are canonical generators of $\mathcal{O}_2$, that is, they satisfy

$$s_i^* s_j = \delta_{ij} I \quad (i,j=1,2), \quad s_1 s_1^* + s_2 s_2^* = I, \tag{1.2}$$

then

$$a_1 \equiv s_1 s_2^*, \quad a_n \equiv \sum_{J\in\{1,2\}^{n-1}} (-1)^{n_2(J)} s_J s_1 s_2^* s_J^* \quad (n\geqslant 2) \tag{1.3}$$

satisfy (1.1) where $n_2(J)\equiv\Sigma_{l=1}^k (j_l-1)$ and $s_J=s_{j_1}\cdots s_{j_k}$, $s_J^*=s_{j_k}^*\cdots s_{j_1}^*$ for $J=(j_1,\ldots,j_k)$, and $C^*\langle\{a_n\in\mathcal{O}_2 : n\in\mathbf{N}\}\rangle$ coincides with a fixed-point subalgebra $\mathcal{O}_2^{\mathrm{U}(1)}$ of $\mathcal{O}_2$ by the canonical gauge action. Put a linear map ζ on $\mathcal{O}_2$ by

$$\zeta(x)\equiv s_1 x s_1^* - s_2 x s_2^* \quad (x\in\mathcal{O}_2). \tag{1.4}$$

Then $a_n=\zeta(a_{n-1})$ for each $n\geqslant 2$. In this sense, $\{a_n\}_{n\in\mathbf{N}}$ in (1.3) is called the recursive fermion system (=RFS) in $\mathcal{O}_2$.

In this article, we extend the Fock and the infinite wedge representations[12,13] of $\mathcal{A}$ to permutative representations of $\mathcal{O}_2$ under identification of $\mathcal{A}$ as $\mathcal{O}_2^{\mathrm{U}(1)}\subset\mathcal{O}_2$ by (1.3). At first, we give our main theorem for abstract formulations of representations of $\mathcal{A}$.

Theorem 1.1 *(i) Let $(\mathcal{H}_F,\pi_F)$ be the Fock representation of $\mathcal{A}$, that is, $(\mathcal{H}_F,\pi_F)$ is a cyclic representation with a cyclic vector $\Omega\in\mathcal{H}_F$ such that*

$$\pi_F(a_n)\Omega = 0 \quad (\forall n\in\mathbf{N}).$$

Then $(\mathcal{H}_F,\pi_F)$ is extended to an irreducible representation $(\mathcal{H}_F,\tilde{\pi}_F)$ of $\mathcal{O}_2$ defined by

a)Electronic-mail: kawamura@kurims.kyoto-u.ac.jp

$$\tilde{\pi}_F(s_1) \equiv L, \quad \tilde{\pi}_F(s_2) \equiv \pi(a_1^*) \cdot L$$

where L is the one-sided shift operator on $\mathcal{H}_F$ defined by

$$L\Omega \equiv \Omega, \quad L\pi_F(a_{n_1}^* \cdots a_{n_k}^*)\Omega \equiv \pi_F(a_{n_1+1}^* \cdots a_{n_k+1}^*)\Omega$$

for each $n_1, \ldots, n_k \in \mathbf{N}$ and $k \in \mathbf{N}$. (ii) Let $(\Lambda^{\infty/2}V, \pi_{\infty,+})$ be the infinite wedge representation of $\mathcal{A}$, that is, $(\Lambda^{\infty/2}V, \pi_{\infty,+})$ is a cyclic representation with a cyclic vector $|\mathrm{vac}\rangle_+ \in \Lambda^{\infty/2}V$ such that

$$\psi_{-k}|\mathrm{vac}\rangle_+ = \psi_k^*|\mathrm{vac}\rangle_+ = 0 \quad \left(\forall k \in \mathbf{Z} + \tfrac{1}{2}, k > 0\right)$$

where

$$\psi_k \equiv \pi_{\infty,+}(a_{2k+1}), \quad \psi_{-k} \equiv \pi_{\infty,+}(a_{2k}) \quad \left(k \in \mathbf{Z} + \tfrac{1}{2}, k > 0\right) \tag{1.5}$$

and $\mathbf{Z} + \frac{1}{2} \equiv \{n + 1/2 : n \in \mathbf{Z}\}$. Then $(\Lambda^{\infty/2}V, \pi_{\infty,+})$ is extended to an irreducible representation $(\Lambda^{\infty/2}V \oplus \Lambda^{\infty/2}V^*, \Pi)$ of $\mathcal{O}_2$ which satisfies

$$\Pi(s_1 s_2)|\mathrm{vac}\rangle_+ = |\mathrm{vac}\rangle_+.$$

Both representations, $(\mathcal{H}, \tilde{\pi}_F)$ and $(\Lambda^{\infty/2}V \oplus \Lambda^{\infty/2}V^*, \Pi)$, of $\mathcal{O}_2$ in Theorem 1.1 are permutative representations[5,8,9] and they are not equivalent to each other. Well-known Fock and infinite wedge representations are just realizations of those in Theorem 1.1. The extension for a concrete infinite wedge is given Sec. IV.

On the other hand, the boson-fermion correspondence on the infinite wedge representation is given by

$$\alpha_n = \sum_{k \in \mathbf{Z} + \frac{1}{2}} \psi_{k-n}\psi_k^* \quad (n \in \mathbf{Z} \setminus \{0\}). \tag{1.6}$$

$\{a_n\}_{n \in \mathbf{Z}}$ satisfies $\alpha_{-n} = \alpha_n^*$, $\alpha_n\alpha_m - \alpha_m\alpha_n = n \cdot \delta_{n,-m} I$. By identifying s_i and $\Pi(s_i)$ in Theorem 1.1 (ii) and combining (1.3) and (1.5), we have

$$\begin{aligned} \psi_k &= \sum_{J \in \{1,2\}^{2k}} (-1)^{n_2(J)} s_J s_1 s_2^* s_J^* \\ \psi_{-k} &= \sum_{J \in \{1,2\}^{2k-1}} (-1)^{n_2(J)} s_J s_1 s_2^* s_J^* \end{aligned} \quad \left(k \in \mathbf{Z} + \frac{1}{2}, k > 0\right).$$

From these and (1.6), we have a direct expression of bosons by canonical generators of $\mathcal{O}_2$ as follows:

$$\alpha_n = \sum_{l \in \mathbf{N}} \rho^{2l-2}(X_n) + B_n \quad (n \geqslant 1) \tag{1.7}$$

where

$$X_n \equiv \rho(s_1 s_2^* \zeta^{2n}(s_2 s_1^*)) + \zeta^{2n}(s_1 s_2^*) s_2 s_1^* \quad (n \geqslant 1), \tag{1.8}$$

$$B_1 \equiv -s_1 s_2 s_1^* s_2^*, \quad B_n \equiv \rho(B_{n-1}^*) - s_1 \zeta^{2n-2}(s_2 s_1^*) s_2^* \quad (n \geqslant 2), \tag{1.9}$$

ζ is in (1.4) and ρ is the canonical endomorphism of $\mathcal{O}_2$, that is, $\rho(x) \equiv s_1 x s_1^* + s_2 x s_2^*$ for $x \in \mathcal{O}_2$. Further $\alpha_n^*|\mathrm{vac}\rangle_+ = B_n^*|\mathrm{vac}\rangle_+$ for each $n \geqslant 1$.

In Sec. II, we review representations of $\mathcal{A}$ and $\mathcal{O}_2$ and the RFS. In Sec. III, we introduce a branching function system on the space of Maya diagrams and review the infinite wedge space and its dual space. In Sec. IV, we show extensions of the Fock and the infinite wedge representations to $\mathcal{O}_2$. A relation between a branching law of a permutative representation of $\mathcal{O}_2$ and the extension of the infinite wedge is concretely illustrated.

II. RECURSIVE FERMION SYSTEM AND PERMUTATIVE REPRESENTATIONS OF $\mathcal{O}_2$

Both $\mathcal{O}_2$ and the *CAR* algebra

$$CAR \equiv C^*\langle\{a_n : n \in \mathbf{N}\}\rangle$$

($=\mathcal{A}$ in Sec. I) are simple, infinite dimensional, noncommutative C*-algebras.[6,7] Remark that $a_n^* \in CAR$ for each $n \in \mathbf{N}$ by definition of C*-algebra. Unital $*$-homomorphisms (specially, unital $*$-representations) from these algebras to other algebras are always faithful. Algebras which are generated by generators s_1, s_2 in (1.2) and a_n, $n \in \mathbf{N}$ in (1.1) are unique up to $*$-isomorphisms, respectively. Therefore their representations are determined by only operators on a Hilbert space, which satisfy relations of their generators without ambiguity. In this article, a representation and an embedding always mean a unital $*$-representation and a unital $*$-embedding, respectively.

A. Representations of *CAR* and the RFS

We review representations of *CAR* in theory of operator algebras in Ref. 6.

Definition 2.1: Let $(\mathcal{H}, \pi)$ *be a representation of CAR.* (i) $(\mathcal{H}, \pi)$ *is the (abstract)Fock representation of CAR if there is a cyclic unit vector* $\Omega \in \mathcal{H}$ *such that* $\pi(a_n)\Omega = 0$ *for each* $n \in \mathbf{N}$. Ω *is called the vacuum of* $(\mathcal{H}, \pi)$. *We denote* $(\mathcal{H}, \pi)$ *by* $\mathcal{H}_{\mathrm{Fock}}$ *simply.* (ii) $(\mathcal{H}, \pi)$ *is* $P[12]$ *if there is a cyclic unit vector* $\Omega \in \mathcal{H}$ *such that* $\pi(a_{2n-1})\Omega = \pi(a_{2n}^*)\Omega = 0$ $(\forall n \in \mathbf{N})$. (iii) $(\mathcal{H}, \pi)$ *is* $P[21]$ *if there is a cyclic unit vector* $\Omega \in \mathcal{H}$ *such that* $\pi(a_{2n-1}^*)\Omega = \pi(a_{2n})\Omega = 0$ $(\forall n \in \mathbf{N})$.

For consistency with after statements, any Ω in the above is normalized. $\mathcal{H}_{\mathrm{Fock}}$, $P[12]$, $P[21]$ appear in Ref. 5 as components of irreducible decomposition of permutative representation of $\mathcal{O}_2$, which are called "atom." This fact is explained in *Proposition 2.6*.

Proposition 2.2: All of $\mathcal{H}_{\mathrm{Fock}}$, $P[12]$, $P[21]$ *are unique up to unitary equivalences and irreducible. Any two of* $\mathcal{H}_{\mathrm{Fock}}$, $P[12]$, $P[21]$ *are not unitarily equivalent*.

Proof: See (5.18) in Refs. 4 and 5. In the Appendix, their inequivalences are shown. ■

By Proposition 2.2, symbols $\mathcal{H}_{\mathrm{Fock}}$, $P[12]$ and $P[21]$ make sense as equivalence classes of representations. Since fermions are often treated as operators on a concrete Hilbert space, any representation which is different with the Fock representation in only permutation of creations and annihilations and their phase factors, are called the Fock representation, too in such situation. In this article, we do not call such representation by the Fock representation.

We review a concrete example: Put $H \equiv l_2(\mathbf{N})$ and the completely antisymmetric Fock space $F_-(H) \equiv \mathbf{C}\Omega \oplus \bigoplus_{k=1}^{\infty} H^{\wedge k}$, $H^{\wedge k} \equiv P_-^{(k)} H^{\otimes k}$ where $P_-^{(k)}$ is the antisymmetrizer on $H^{\otimes k}$ defined by $P_-^{(k)}(v_1 \otimes \cdots \otimes v_k) \equiv (\sqrt{k!})^{-1/2} \sum_{\sigma \in \mathfrak{S}_k} \mathrm{sgn}(\sigma) \cdot v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(k)}$ for $k \geqslant 1$. We denote $v_1 \wedge \cdots \wedge v_k = P_-^{(k)}(v_1 \otimes \cdots \otimes v_k)$. We see $v_{\sigma(1)} \wedge \cdots \wedge v_{\sigma(k)} = \mathrm{sign}(\sigma)(v_1 \otimes \cdots \otimes v_k)$ for each $\sigma \in \mathfrak{S}_k$. For $f \in H$, define $A^*(f)\Omega \equiv f$, $A^*(f)v \equiv f \wedge v$ for $f \in H$, $v \in H^{\wedge n}$, $n \geqslant 1$. $A(f)$ is defined by the adjoint operator of $A^*(f)$ on $F_-(H)$. We see that $A(f)\Omega = 0$ for each $f \in H$. Then $A(f)A^*(g) + A^*(g)A(f) = \langle f|g\rangle I$ for each f, $g \in H$. For the canonical basis $\{e_n\}_{n \in \mathbf{N}}$ of $H = l_2(\mathbf{N})$, put $\pi_F(a_n) \equiv A(e_n)$ for $n \in \mathbf{N}$. Then $(F_-(H), \pi_F)$ is a representation of *CAR*. $(F_-(H), \pi_F)$ is the (concrete)Fock representation.

Let s_1, s_2 be canonical generators of $\mathcal{O}_2$. Define an embedding

$$\varphi_S : CAR \hookrightarrow \mathcal{O}_2; \quad \varphi_S(a_n) \equiv \zeta^{n-1}(s_1 s_2^*) \quad (n \geqslant 1) \tag{2.1}$$

where ζ is in (1.4). For example, $\varphi_S(a_1) = s_1 s_2^*$, $\varphi_S(a_2) = s_1 s_1 s_2^* s_1^* - s_2 s_1 s_2^* s_2^*$. We call φ_S by the standard embedding of *CAR* into $\mathcal{O}_2$. $C^*\langle\{\varphi_S(a_n)\}_{n \in \mathbf{N}}\rangle = \mathcal{O}_2^{\mathrm{U}(1)} = \{x \in \mathcal{O}_2 : \forall z \in \mathrm{U}(1), \gamma_z(x) = x\} \cong UHF_2$ where γ is the canonical U(1)-action of $\mathcal{O}_2$, $\gamma_z(s_i) \equiv z s_i$ for $z \in \mathrm{U}(1) \equiv \{z \in \mathbf{C} : |z| = 1\}$ and $i = 1, 2$. By identifying a_n and $\varphi_S(a_n)$, a_n's coincide with those in (1.3) and we have the following intertwining relations.

Lemma 2.3: For $n \geqslant 1$,

$$s_1 a_n = a_{n+1} s_1, \quad s_1 a_n^* = a_{n+1}^* s_1, \quad s_2 a_n = -a_{n+1} s_2, \quad s_2 a_n^* = -a_{n+1}^* s_2,$$

$$s_1^* a_{n+1} = a_n s_1^*, \quad s_1^* a_{n+1}^* = a_n^* s_1^*, \quad s_2^* a_{n+1} = -a_n s_2^*, \quad s_2^* a_{n+1}^* = -a_n^* s_2^*.$$

B. Permutative representations of $\mathcal{O}_2$ and their branching laws

Permutative representations of the Cuntz algebras are well-studied.[5,8,9]. We introduce two permutative representations of $\mathcal{O}_2$ according to Ref. 10.

Definition 2.4: A representation $(\mathcal{H}, \pi)$ of $\mathcal{O}_2$ is $P(1)$ (respectively, $P(12)$) if there is a cyclic unit vector $\Omega \in \mathcal{H}$ such that $\pi(s_1)\Omega = \Omega$ (respectively $\pi(s_1 s_2)\Omega = \Omega$). We call Ω by the GP vector of $(\mathcal{H}, \pi)$.

Both $P(1)$ and $P(12)$ exist uniquely up to unitary equivalences, and they are irreducible and not unitarily equivalent each other.

Assume that $(\mathcal{H}, \pi)$ is $P(12)$ of $\mathcal{O}_2$ with the GP vector Ω and α is an automorphism of $\mathcal{O}_2$ defined by $\alpha(s_1) \equiv s_2$, $\alpha(s_2) \equiv s_1$. Define an operator U on $\mathcal{H}$ by

$$U\Omega \equiv \pi(s_2)\Omega, \quad U\pi(s_J)\Omega \equiv \pi(\alpha(s_J)s_2)\Omega \quad (J \in \{1,2\}^k, k \geqslant 1). \tag{2.2}$$

Then U is a unitary which satisfies $U^2 = I$ and $\mathrm{Ad}\, U \circ \pi = \pi \circ \alpha$. In consequence, $(\mathcal{H}, \pi, U)$ is a covariant representation of a C^*-dynamical system $(\mathcal{O}_2, \alpha, \mathbf{Z}_2)$.

Example 2.5: (i) Define a representation $(l_2(\mathbf{N}), \pi_S)$ of $\mathcal{O}_2$ by

$$\pi_S(s_1)e_n \equiv e_{2n-1}, \quad \pi_S(s_2)e_n \equiv e_{2n} \quad (n \in \mathbf{N}).$$

Then $(l_2(\mathbf{N}), \pi_S)$ is $P(1)$. We call $(l_2(\mathbf{N}), \pi_S)$ by the *standard representation* of $\mathcal{O}_2$. (ii) Define a representation $(l_2(\mathbf{N}), \pi_{12})$ of $\mathcal{O}_2$ by

$$\pi_{12}(s_1)e_{2n-1} \equiv e_{4n-1}, \quad \pi_{12}(s_1)e_{2n} \equiv e_{4n-3}, \quad \pi_{12}(s_2)e_n \equiv e_{2n} \quad (n \in \mathbf{N}).$$

The action of s_1, s_2 on the canonical basis of $l_2(\mathbf{N})$ is illustrated as follows:

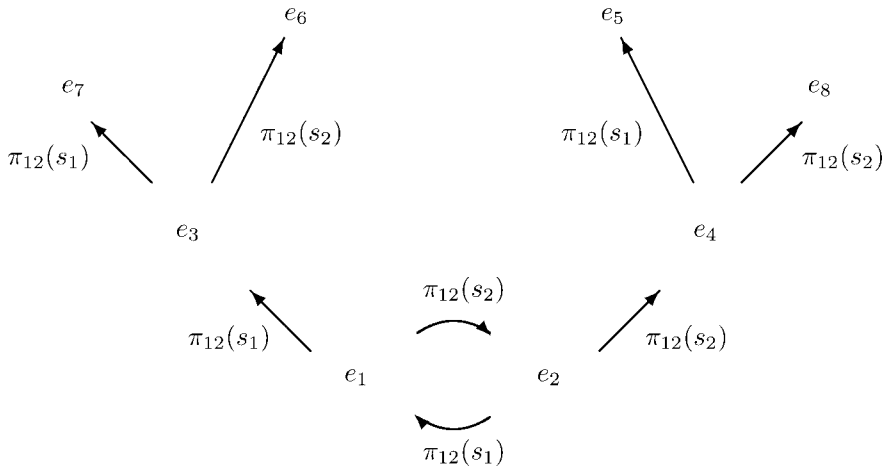

This system looks like the Fock representation with two vacuums e_1 and e_2. This diagram appears in Secs. III and IV again. $(l_2(\mathbf{N}), \pi_{12})$ is $P(12)$. Remark that $\pi_{12}(s_1 s_2)e_1 = e_1$ is expressed as a cycle in the previous diagram. For this type of example, see Ref. 11.

By φ_S in (2.1), we identify *CAR* and a subalgebra $\varphi_S(CAR) = \mathcal{O}_2^{\mathrm{U}(1)} \subset \mathcal{O}_2$. For a representation $(\mathcal{H}, \pi)$ of $\mathcal{O}_2$, we have the restriction $(\mathcal{H}, \pi|_{CAR})$ of $(\mathcal{H}, \pi)$ on *CAR*.

Proposition 2.6: ([2]) The following branching laws hold:

$$P(1)|_{CAR} = \mathcal{H}_{\mathrm{Fock}}, \quad P(12)|_{CAR} = P[12] \oplus P[21].$$

Specially, all of these are irreducible decompositions.

We consider the branching of $P(12)$ on *CAR* more.

Lemma 2.7: Let $(\mathcal{H}, \pi)$ be $P(12)$ of $\mathcal{O}_2$ with the GP vector $\Omega_1 \equiv \Omega$ and put $\Omega_2 \equiv \pi(s_2)\Omega_1$.

Then we have the following:

$$\pi(a_{2k-1})\Omega_1 = 0, \quad \pi(a_{2k})\Omega_1 = (-1)^{k-1}\pi(s_{(12)^{k-1}s_1s_1})\Omega_1,$$

$$\pi(a^*_{2k-1})\Omega_1 = (-1)^{k-1}\pi(s_{(12)^{k-1}s_2s_2})\Omega_1, \quad \pi(a^*_{2k})\Omega_1 = 0,$$

$$\pi(a_{2k-1})\Omega_2 = (-1)^{k-1}\pi(s_{(21)^{k-1}s_1})\Omega_1, \quad \pi(a_{2k})\Omega_2 = 0,$$

$$\pi(a^*_{2k-1})\Omega_2 = 0, \quad \pi(a^*_{2k})\Omega_2 = (-1)^{k}\pi(s_2s_{(12)^{k-1}s_2s_2})\Omega_1$$

for each $k \in \mathbf{N}$.

Proof: By $\pi(\zeta(x)s_2)\Omega_1 = -\pi(s_2x)\Omega_1$ for any $x \in \mathcal{O}_2$, statements hold. ■

Let $V_{12} \equiv \pi(CAR)\Omega_1$, $V_{21} \equiv \pi(CAR)\Omega_2$. Then $\mathcal{H} = V_{12} \oplus V_{21}$ and we see that

	V_{12}	V_{21}
vacuum	Ω_1	Ω_2
creation	a^*_{2k-1}, a_{2k}	a_{2k-1}, a^*_{2k}
annihilation	a_{2k-1}, a^*_{2k}	a^*_{2k-1}, a_{2k}

where $k \in \mathbf{N}$. Specially,

$$\begin{aligned} &\pi(a_1)\Omega_2 = \pi(s_1)\Omega_1, \quad \pi(a_2)\Omega_1 = \pi(s_1s_1)\Omega_1, \\ &\pi(a^*_1)\Omega_1 = \pi(s_2)\Omega_2, \quad \pi(a^*_2)\Omega_2 = -\pi(s_2s_2)\Omega_2. \end{aligned} \tag{2.3}$$

If α is the $\mathbf{Z}_2$ action on $\mathcal{O}_2$ and a_n is the *RFS* in $\mathcal{O}_2$, then $\alpha(a_n) = (-1)^{n-1}a^*_n$. Hence U in (2.2) satisfies

$$U\Omega_1 = \Omega_2, \quad U\Omega_2 = \Omega_1, \quad U\pi(a_K a^*_L)\Omega_1 = (-1)^{|K|_1+|L|_1}\pi(a^*_K a_L)\Omega_2$$

where $a_K \equiv a_{k_1}\cdots a_{k_n}$, $|K|_1 \equiv \Sigma_{i=1}^n(k_i - 1)$ for $K = \{k_1, \ldots, k_n\} \subset \mathbf{N}$. Hence $UV_{12} = V_{21}$.

Example 2.8: (i) In Example 2.5 (i), $\pi_S \circ \varphi_S$ is $\mathcal{H}_{\mathrm{Fock}}$ with the vacuum e_1. See [Ref. 3] for more detail. (ii) In Example 2.5 (ii), we consider $\pi_{12} \circ \varphi_S$. Then $(l_2(2\mathbf{N}-1), \pi_{12} \circ \varphi_S)$ is $P[12]$ and $(l_2(2\mathbf{N}), \pi_{12} \circ \varphi_S)$ is $P[21]$. If we identify a_n and $(\pi_{12} \circ \varphi_S)(a_n)$, then

$$a_{2n-1}e_1 = a^*_{2n}e_1 = a_{2n}e_2 = a^*_{2n-1}e_2 = 0,$$

$$a_{2n}e_1 = (-1)^{n-1}e_{4^{n-1}\cdot 6+1}, \quad a^*_{2n-1}e_1 = (-1)^{n-1}e_{4^{n-1}\cdot 3+1},$$

$$a_{2n-1}e_2 = (-1)^{n-1}e_{4^{n-1}\cdot 3+2}, \quad a^*_{2n}e_2 = (-1)^{n}e_{4^{n-1}\cdot 6+2}$$

for each $n \in \mathbf{N}$. These statements are shown by using $(\pi_{12}(s_1s_2))^m e_n = e_{4^{m(n-1)+1}}$ for each $m, n \in \mathbf{N}$. Specially, when $n_2 > n_1$,

$$a_{2n_1}a_{2n_2}e_1 = (-1)^{n_2-1}e_{3\cdot(2^{2n_2-1}+2^{2n_1-1})+1}.$$

III. A BRANCHING FUNCTION SYSTEM ON THE INFINITE WEDGE

We review a representation of the fermion algebra which is called the *infinite wedge space*[12,13] according to notation in Ref. 13. In order to extend this representation to $\mathcal{O}_2$, we introduce the dual infinite wedge space at once and a branching function system on them.

A. Maya diagram

Denote $\mathbf{Z}+\frac{1}{2}\equiv\{n+\frac{1}{2}:n\in\mathbf{Z}\}$. Put

$$\mathbf{Z}_{+/2}\equiv\{n+1/2:n\in\mathbf{Z},n\geqslant 0\},\quad \mathbf{Z}_{-/2}\equiv\{n-1/2:n\in\mathbf{Z},n\leqslant 0\}.$$

For a subset $S\subset\mathbf{Z}+\frac{1}{2}$, define $\Delta_{\pm}(S)\subset\mathbf{Z}+\frac{1}{2}$ by

$$\Delta_{\pm}(S)\equiv(S\setminus\mathbf{Z}_{\mp/2})\cup(\mathbf{Z}_{\mp/2}\setminus S). \tag{3.1}$$

Remark the sign of both sides.

Definition 3.1: An element in $\mathcal{M}_{\pm}\equiv\{S\subset\mathbf{Z}+\frac{1}{2}:\#\Delta_{\pm}(S)<\infty\}$ *is called a Maya diagram. Specially,* $\mathbf{Z}_{\mp/2}\in\mathcal{M}_{\pm}$ *is called the vacuum in* $\mathcal{M}_{\pm}$.

We see that $\mathcal{M}_{+}\cap\mathcal{M}_{-}=\emptyset$ and $\mathcal{M}_{\pm}=\{-S:S\in\mathcal{M}_{\mp}\}$ where $-S\equiv\{-k:k\in S\}$. There are $\max S$ for any $S\in\mathcal{M}_{+}$ and $\min S$ for any $S\in\mathcal{M}_{-}$, and $\#S=\infty$ for any $S\in\mathcal{M}_{\pm}$. Therefore we can always parameterize as follows: $S=\{t_i:i\in\mathbf{N}\}$ such that $t_i>t_{i+1}$ for $i\geqslant 1$ when $S\in\mathcal{M}_{+}$, and $S=\{t_i:i\in\mathbf{N}\}$ such that $t_i<t_{i+1}$ for $i\geqslant 1$ when $S\in\mathcal{M}_{-}$.

We illustrate $S\in\mathcal{M}_{\pm}$ by a two-sided infinite sequence consisting of symbols ○ and ● along the lattice $\mathbf{Z}+\frac{1}{2}$ as follows: For $S\in\mathcal{M}_{\pm}$, put ○ at $k\in\mathbf{Z}+\frac{1}{2}$ when $k\in S$, and put ● at $k\in\mathbf{Z}+\frac{1}{2}$ when $k\notin S$. For example, if $\{-5/2,-1/2,3/2,7/2\}\subset S$ and $\{-7/2,-3/2,1/2,5/2\}\cap S=\emptyset$, then

⋯	−7/2	−5/2	−3/2	−1/2	1/2	3/2	5/2	7/2	⋯
⋯	•	∘	•	∘	•	∘	•	∘	⋯

By this illustration, $\mathcal{M}_{\pm}$ are the following sets:

$$\mathcal{M}_{+}=\{\cdots\circ\circ*****\bullet\bullet\cdots\},\quad \mathcal{M}_{-}=\{\cdots\bullet\bullet*****\circ\circ\cdots\}$$

where ****** is taken any finite sequence consisting of ○ and ●. Specially,

vacuum	$\mathbf{Z}_{-/2}\in\mathcal{M}_{+}$	$\cdots\circ\circ\circ\circ\bullet\bullet\bullet\bullet\cdots$
dual vacuum	$\mathbf{Z}_{+/2}\in\mathcal{M}_{-}$	$\cdots\bullet\bullet\bullet\bullet\circ\circ\circ\circ\cdots$

B. A branching function system on the space of Maya diagrams

Put the space of all Maya diagrams

$$\mathcal{M}\equiv\mathcal{M}_{+}\cup\mathcal{M}_{-}.$$

We give a branching function system on $\mathcal{M}$. Put $S_{\pm}\equiv S\cap\mathbf{Z}_{\pm/2}$, $S_{+1}\equiv\{k+1:k\in S\}$ and $S_{\pm,+1}\equiv(S_{\pm})_{+1}$. For $S\in\mathcal{M}$, define

$$g_1(S)\equiv-(S_{+,+1}\cup S_{-}\cup\{1/2\}),\quad g_2(S)\equiv-(S_{+,+1}\cup S_{-}). \tag{3.2}$$

Then $g=\{g_1,g_2\}$ is a branching function system on $\mathcal{M}$, that is, g_1 and g_2 are injective maps on $\mathcal{M}$, $g_1(\mathcal{M})\cap g_2(\mathcal{M})=\emptyset$ and $g_1(\mathcal{M})\cup g_2(\mathcal{M})=\mathcal{M}$. Further,

$$g_1(\mathcal{M})=\{S\in\mathcal{M}:-1/2\in S\},\quad g_2(\mathcal{M})=\{S\in\mathcal{M}:-1/2\notin S\},$$

$$g_1^{-1}(S)=-\{(S_{-}\setminus\{-1/2\})_{+1}\cup S_{+}\},\quad g_2^{-1}(S)=-(S_{-,+1}\cup S_{+}).$$

If $\theta(S)\equiv\mathbf{Z}+\frac{1}{2}\setminus S$, then $\theta^2=id$, $\theta(\mathcal{M}_{\pm})=\mathcal{M}_{\mp}$, $\theta(\mathbf{Z}_{\pm/2})=\mathbf{Z}_{\mp/2}$, and $g_2=\theta\circ g_1\circ\theta$.

Lemma 3.2: Denote $S_{\pm n}\equiv\{k\pm n:k\in S\}$, $S_{\pm,+n}\equiv(S_{\pm})_{+n}$. *Then the followings hold:* (i) $(g_1\circ g_2)^n(S)=S_{-,-n}\cup S_{+,+n}\cup\{-1/2,\ldots,-(n-1)-1/2\}$ *for* $n\in\mathbf{N}$. (ii) $(g_1\circ g_2)^{-n}(S)=(S_{-,+n})_{-}\cup S_{+,-n}$ *for* $n\in\mathbf{N}$. (iii) *Put* $h_n(S)\equiv(g_{12}^{n-1}\circ g_1\circ g_2^{-1}\circ(g_{12}^{n-1})^{-1})(S)$ *and* $k_n(S)\equiv(g_{12}^{n-1}\circ g_1\circ g_1\circ(g_{12}^{-1})^n)(S)$ *for* $n\in\mathbf{N}$. *Then*

$$h_n(S) = S \cup \{-(n-1) - 1/2\}, \quad k_n(S) = S \cup \{n - 1 + 1/2\} \quad (n \in \mathbf{N}).$$

We illustrate g by Maya diagrams:

S	$g_1(S)$	$g_2(S)$
$\mathbf{Z}_{-/2}$	$\mathbf{Z}_{+/2} \cup \{-1/2\}$	$\mathbf{Z}_{+/2}$
$\mathbf{Z}_{+/2}$	$\mathbf{Z}_{-/2}$	$\mathbf{Z}_{-/2} \setminus \{-1/2\}$
$\mathbf{Z}_{+/2} \cup \{-1/2\}$	$\mathbf{Z}_{-/2} \cup \{1/2\}$	$(\mathbf{Z}_{-/2} \setminus \{-1/2\}) \cup \{1/2\}$
$\mathbf{Z}_{-/2} \setminus \{-1/2\}$	$(\mathbf{Z}_{+/2} \setminus \{1/2\}) \cup \{-1/2\}$	$\mathbf{Z}_{+/2} \setminus \{1/2\}$
$\vdots$	$\vdots$	$\vdots$

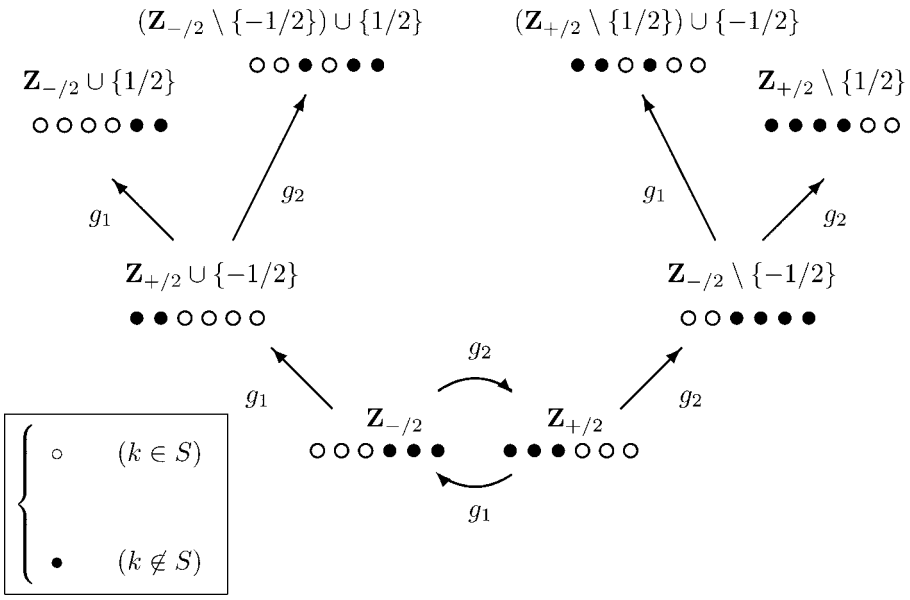

C. The infinite wedge representation of *CAR* and its dual

We introduce the infinite wedge space by a Hilbert space of Maya diagrams. For a set Λ, $l_2(\Lambda)$ is a complex Hilbert space with a complete orthonormal basis $\{e_\lambda\}_{\lambda \in \Lambda}$ and $\dim l_2(\Lambda) = \#\Lambda$.

Definition 3.3: For $\mathcal{M}_\pm$,

$$\Lambda^{\infty/2}V^{\#} \equiv l_2(\mathcal{M}), \quad \Lambda^{\infty/2}V \equiv l_2(\mathcal{M}_+), \quad \Lambda^{\infty/2}V^* \equiv l_2(\mathcal{M}_-)$$

are called the bi-infinite wedge space, the infinite wedge space and the dual infinite wedge space, respectively.

We see that $\Lambda^{\infty/2}V^{\#} = \Lambda^{\infty/2}V \oplus \Lambda^{\infty/2}V^*$. By definition, $\Lambda^{\infty/2}V^{\#}$, $\Lambda^{\infty/2}V$ and $\Lambda^{\infty/2}V^*$ have canonical basis $\{e_S : S \in \mathcal{M}\}$, $\{e_S : S \in \mathcal{M}_+\}$, and $\{e_S : S \in \mathcal{M}_-\}$, respectively. Usually, the symbol $\Lambda^{\infty/2}V$ means a subspace of $l_2(\mathcal{M}_+)$ consisting of finite linear combinations of $\{e_S : S \in \mathcal{M}_+\}$.[12,13] We denote

$$|\mathrm{vac}\rangle_\pm \equiv e_{\mathbf{Z}_{\mp/2}}.$$

Since there are $\max S$ for any $S \in \mathcal{M}_+$ and $\min S$ for any $S \in \mathcal{M}_-$, and $\#S = \infty$ for any $S \in \mathcal{M}_\pm$, we can denote

$$t_1 \wedge t_2 \wedge \cdots = e_S \quad \text{when } S = \{t_i : \forall\, i \in \mathbf{N}, t_i > t_{i+1}\} \in \mathcal{M}_+,$$

$$t_1 \wedge t_2 \wedge \cdots = e_S \quad \text{when } S = \{t_i : \forall\, i \in \mathbf{N}, t_i < t_{i+1}\} \in \mathcal{M}_-.$$

Then we see that

$$|\mathrm{vac}\rangle_+ = \left(-\tfrac{1}{2}\right) \wedge \left(-\tfrac{3}{2}\right) \wedge \left(-\tfrac{5}{2}\right) \wedge \cdots, \quad |\mathrm{vac}\rangle_- = \tfrac{1}{2} \wedge \tfrac{3}{2} \wedge \tfrac{5}{2} \wedge \cdots.$$

For a permutation $\sigma \in \mathfrak{S}_k$ $k \geqslant 2$, define

$$t_{\sigma(1)} \wedge \cdots \wedge t_{\sigma(k)} \wedge t_{k+1} \wedge \cdots \equiv \mathrm{sgn}(\sigma) \cdot t_1 \wedge \cdots \wedge t_k \wedge t_{k+1} \wedge \cdots.$$

By these definitions, "$\wedge$" seems the exterior product of infinite vectors.

Define a family $\{\psi_k\}_{k \in \mathbf{Z}+\frac{1}{2}}$ of operators on $\Lambda^{\infty/2}V^{\#}$ by

$$\psi_k e_S \equiv \begin{cases} (-1)^{d_S(k)} \cdot e_{S \cup \{k\}} & (k \notin S), \\ 0 & (\text{otherwise}) \end{cases} \quad (S \in \mathcal{M})$$

where $d_S(k) \equiv \min\{\#\{x \in S : x > k\}, \#\{x \in S : x < k\}\}$. We simply denote

$$\psi_k e_S = (-1)^{d_S(k)} \cdot \chi_{S^c}(k) \cdot e_{S \cup \{k\}}$$

where χ_{S^c} is the characteristic function on $S^c \equiv \left(\mathbf{Z}+\frac{1}{2}\right) \setminus S$. We can easily check that the definition of ψ_k coincides with the following ordinary definition:

$$\psi_k v = k \wedge v \quad \left(v \in \Lambda^{\infty/2}V^{\#}, k \in \mathbf{Z}+\tfrac{1}{2}\right).$$

Lemma 3.4: (i) The adjoint ψ_k^* of ψ_k is given by

$$\psi_k^* e_S = (-1)^{d_{S \setminus \{k\}}(k)} \cdot \chi_S(k) \cdot e_{S \setminus \{k\}} \quad \left(k \in \mathbf{Z}+\tfrac{1}{2}, S \in \mathcal{M}\right).$$

(ii) $\psi_k \psi_k^* e_S = \chi_S(k) \cdot e_S$ for $k \in \mathbf{Z}+\frac{1}{2}$ and $S \in \mathcal{M}$. (iii) $\psi_k \psi_l^* + \psi_l^* \psi_k = \delta_{kl} I$ for $k, l \in \mathbf{Z}+\frac{1}{2}$ and other anticommutators vanish. We see that

$$\psi_{-k}|\mathrm{vac}\rangle_+ = \psi_k^*|\mathrm{vac}\rangle_+ = 0,$$

$$\psi_k|\mathrm{vac}\rangle_+ = k \wedge |\mathrm{vac}\rangle_+, \quad \psi_{-k}^*|\mathrm{vac}\rangle_+ = (-1)^{k-1/2} \cdot e_{\mathbf{Z}_{-/2} \setminus \{-k\}}$$

for $k \in \mathbf{Z}+\frac{1}{2}$, $k > 0$. In the same way, we see that

	$\Lambda^{\infty/2}V$	$\Lambda^{\infty/2}V^*$
vacuum	$\lvert\mathrm{vac}\rangle_+$	$\lvert\mathrm{vac}\rangle_-$
creation	ψ_{-k}^*, ψ_k	ψ_{-k}, ψ_k^*
annihilation	ψ_{-k}, ψ_k^*	ψ_{-k}^*, ψ_k

where $k \in \mathbf{Z}+\frac{1}{2}$, $k > 0$.

Definition 3.5: A representation $(\Lambda^{\infty/2}V^{\#}, \pi_\infty)$ of CAR defined by

$$\pi_\infty(a_{2n-1}) \equiv \psi_{-n+1/2}, \quad \pi_\infty(a_{2n}) \equiv \psi_{n-1/2} \quad (n \in \mathbf{N}) \tag{3.3}$$

is called the bi-infinite wedge representation of CAR.

On the other hand,

$$\psi_k = \pi_\infty(a_{2k+1}), \quad \psi_{-k} = \pi_\infty(a_{2k}) \quad \left(k \in \mathbf{Z}+\tfrac{1}{2}, k > 0\right). \tag{3.4}$$

Proposition 3.6: (i) The following irreducible decomposition of representations of CAR holds:

$$\Lambda^{\infty/2}V^{\#} = \Lambda^{\infty/2}V \oplus \Lambda^{\infty/2}V^*.$$

(ii) If we denote

$$\pi_{\infty,+} \equiv \pi_\infty|_{\Lambda^{\infty/2}V}, \quad \pi_{\infty,-} \equiv \pi_\infty|_{\Lambda^{\infty/2}V^*},$$

then $(\Lambda^{\infty/2}V, \pi_{\infty,+})$ is $P[12]$ and $(\Lambda^{\infty/2}V^*, \pi_{\infty,-})$ is $P[21]$.

$(\Lambda^{\infty/2}V, \pi_{\infty,+})$ and $(\Lambda^{\infty/2}V^*, \pi_{\infty,-})$ are called the *infinite wedge representation* and the *dual-infinite wedge representation* of *CAR*, respectively.

IV. STANDARD EXTENSIONS OF REPRESENTATIONS OF *CAR*

In order to show extension theorems, we prepare a notion, "standard extension" of a representation of *CAR* to $\mathcal{O}_2$ as follows.

Definition 4.1: Let φ_S be the standard embedding of CAR into $\mathcal{O}_2$ in (2.1). For a representation $(\mathcal{H}, \pi)$ of CAR, $(\tilde{\mathcal{H}}, \tilde{\pi})$ is the standard extension of $(\mathcal{H}, \pi)$ to $\mathcal{O}_2$ if $\mathcal{H}$ is a closed subspace of $\tilde{\mathcal{H}}$ such that

$$(\tilde{\pi} \circ \varphi_S)|_{\mathcal{H}} = \pi. \tag{4.1}$$

A. Standard extension of the Fock representation

Theorem 4.2: *Let $(\mathcal{H}, \pi)$ be the Fock representation of CAR with the vacuum Ω in Definition 2.1. Put two operators $\tilde{\pi}(s_1)$, $\tilde{\pi}(s_2)$ on $\mathcal{H}$ by*

$$\tilde{\pi}(s_1)\Omega \equiv \Omega, \quad \tilde{\pi}(s_1)\pi(a^*_{n_1}\cdots a^*_{n_k})\Omega \equiv \pi(a^*_{n_1+1}\cdots a^*_{n_k+1})\Omega,$$

$$\tilde{\pi}(s_2)\Omega \equiv \pi(a^*_1)\Omega, \quad \tilde{\pi}(s_2)\pi(a^*_{n_1}\cdots a^*_{n_k})\Omega \equiv \pi(a^*_1 a^*_{n_1+1}\cdots a^*_{n_k+1})\Omega$$

for $n_1 < n_2 < \cdots < n_k$, $n_j \in \mathbf{N}$, $j = 1, \ldots, k$, $k \geqslant 1$. Then the followings hold:

(i) *$(\mathcal{H}, \tilde{\pi})$ is a representation of $\mathcal{O}_2$.*
(ii) *$\tilde{\pi} \circ \varphi_S = \pi$.*
(iii) *$(\mathcal{H}, \tilde{\pi})$ is $P(1)$ with the GP vector Ω.*

This proof is given by direct computation and Lemma 2.3. For more detail, see Sec. III C in Ref. 3. Clearly, $(\tilde{\mathcal{H}} \equiv \mathcal{H}, \tilde{\pi})$ in Theorem 4.2 is the standard extension of the Fock representation. Theorem 1 (i) about an operator L follows from Theorem 4.2 as another expression of this extension.

B. Standard extension of the infinite wedge

For $g = \{g_1, g_2\}$ in (3.2), define a representation $(\Lambda^{\infty/2}V^{\#}, \Pi)$ of $\mathcal{O}_2$ by

$$\Pi(s_1)e_S \equiv (-1)^{d_+(S)}e_{g_1(S)}, \quad \Pi(s_2)e_S \equiv (-1)^{d_+(S)}e_{g_2(S)} \quad (S \in \mathcal{M}_+),$$

$$\Pi(s_1)e_S \equiv (-1)^{d'_-(S)}e_{g_1(S)}, \quad \Pi(s_2)e_S \equiv (-1)^{d_-(S)}e_{g_2(S)} \quad (S \in \mathcal{M}_-)$$

where $d_+(S) \equiv \#(S \cap \mathbf{Z}_{+/2}) + \#(\mathbf{Z}_{-/2} \backslash S)$ and $d'_-(S) \equiv \#(\mathbf{Z}_{+/2} \backslash S)$, $d_-(S) \equiv \#(\mathbf{Z}_{+/2} \backslash S) + \#(S \cap \mathbf{Z}_{-/2})$.

Lemma 4.3: When $K = \{k_1, \ldots, k_n\}$ and $L = \{l_1, \ldots, l_m\} \subset \mathbf{Z}_{+/2}$ satisfy $k_1 > \cdots > k_n$ and $l_1 < \cdots < l_m$,

$$\Pi(s_1)|\mathrm{vac}\rangle_+ = \psi_{-1/2}|\mathrm{vac}\rangle_- = e_{\mathbf{Z}_{+/2} \cup \{-1/2\}}, \quad \Pi(s_2)|\mathrm{vac}\rangle_+ = |\mathrm{vac}\rangle_-,$$

$$\Pi(s_1)|\mathrm{vac}\rangle_- = |\mathrm{vac}\rangle_+, \quad \Pi(s_2)|\mathrm{vac}\rangle_- = \psi^*_{-1/2}|\mathrm{vac}\rangle_+ = e_{\mathbf{Z}_{-/2} \backslash \{-1/2\}}.$$

$$\Pi(s_1)e_{\mathbf{Z}_{-/2} \cup K \backslash (-L)} = (-1)^{n+m}e_{\mathbf{Z}_{+/2} \cup (-K^*_{+1}) \backslash L},$$

$$\Pi(s_2)e_{\mathbf{Z}_{-/2} \cup K \backslash (-L)} = (-1)^{n+m}e_{\mathbf{Z}_{+/2} \cup (-K_{+1}) \backslash L},$$

$$\Pi(s_1)e_{\mathbf{Z}_{+/2}\cup(-K)\setminus L} = (-1)^m e_{\mathbf{Z}_{-/2}\cup K\setminus(-L_{+1})},$$

$$\Pi(s_2)e_{\mathbf{Z}_{+/2}\cup(-K)\setminus L} = (-1)^{m+n} e_{\mathbf{Z}_{-/2}\cup K\setminus(-L^*_{+1})}$$

where $K_{+1} \equiv \{k+1 : k \in K\}$ *and* $K^*_{+1} \equiv K_{+1} \cup \{1/2\}$.

Proposition 4.4: (i) $(\Lambda^{\infty/2}V^{\#}, \Pi)$ *is* $P(12)$. *(ii) If* π_∞, $\pi_{\infty,\pm}$ *are in Proposition 3.6, then* $\Pi \circ \varphi_S = \pi_\infty$. *Specially,*

$$(\Lambda^{\infty/2}V, \pi_{\infty,+}) = (\Lambda^{\infty/2}V, (\Pi \circ \varphi_S)|_{\Lambda^{\infty/2}V}) \sim P[12],$$

$$(\Lambda^{\infty/2}V^*, \pi_{\infty,-}) = (\Lambda^{\infty/2}V^*, (\Pi \circ \varphi_S)|_{\Lambda^{\infty/2}V^*}) \sim P[21].$$

Proof: (i) By Lemma 4.3, $\Pi(s_1 s_2)|\mathrm{vac}\rangle_+ = |\mathrm{vac}\rangle_+$. By definition of g_1, g_2, $(\Lambda^{\infty/2}V^{\#}, \Pi)$ is $P(12)$. (ii) Identify $\varphi_S(a_n)$ and a_n for each $n \in \mathbf{N}$. By Lemma 3.2 and Lemma 4.3, we can check the following:

$$\Pi(a_{2n-1})|\mathrm{vac}\rangle_+ = \Pi(a_{2n})|\mathrm{vac}\rangle_- = \Pi(a^*_{2n})|\mathrm{vac}\rangle_+ = \Pi(a_{2n-1})^*|\mathrm{vac}\rangle_- = 0,$$

$$\Pi(a_{2n})|\mathrm{vac}\rangle_+ = \psi_{n-1/2}|\mathrm{vac}\rangle_+, \quad \Pi(a_{2n-1})|\mathrm{vac}\rangle_- = \psi_{-n+1/2}|\mathrm{vac}\rangle_-,$$

$$\Pi(a^*_{2n-1})|\mathrm{vac}\rangle_+ = \psi^*_{-n+1/2}|\mathrm{vac}\rangle_+, \quad \Pi(a^*_{2n})|\mathrm{vac}\rangle_- = \psi^*_{n-1/2}|\mathrm{vac}\rangle_-$$

for each $n \in \mathbf{N}$. By Lemma 4.3, $\Pi(a_n) = \pi_\infty(a_n)$ for each $n \in \mathbf{N}$. ■

The branching law $\Pi|_{CAR} = \pi_{\infty,+} \oplus \pi_{\infty,-}$ is illustrated by Maya diagrams as follows:

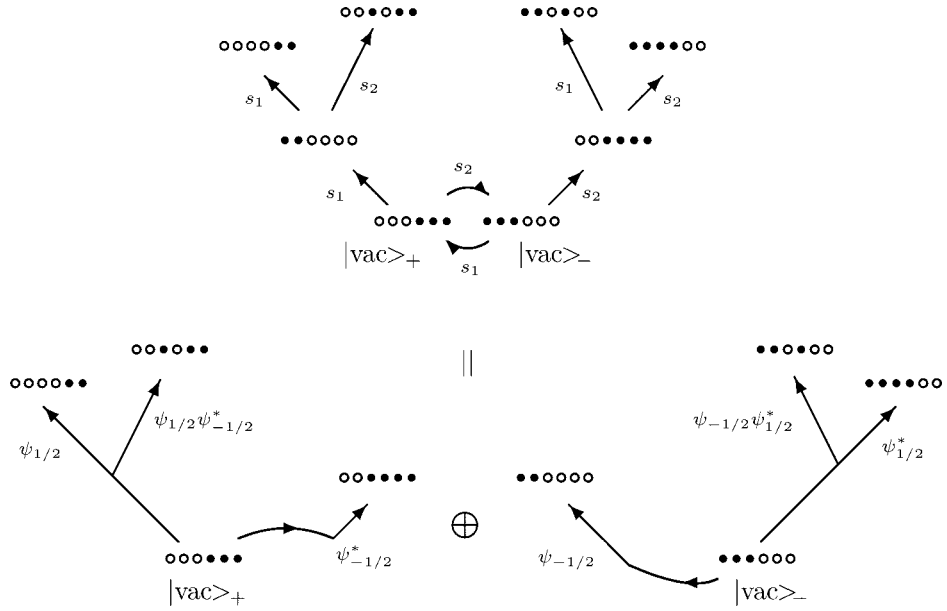

We try to interpret this branching law from a physical standpoint. *Before* the symmetry breaking of $\mathcal{O}_2$ to *CAR*, the vacuum and the dual vacuum are coupled as a cycle: $|\mathrm{vac}\rangle_+ \overset{s_2}{\to} |\mathrm{vac}\rangle_- \overset{s_1}{\to} |\mathrm{vac}\rangle_+$. *After* the symmetry breaking, they are decomposed into two independent vacua of fermions. A $\mathbf{Z}_2$ symmetry between $\Lambda^{\infty/2}V$ and $\Lambda^{\infty/2}V^*$ are just a unitary U in (2.2) on $\Lambda^{\infty/2}V^{\#}$ which satisfies $Us_1U^* = s_2$.

C. Boson-fermion correspondence described by $\mathcal{O}_2$

By using the standard extension of the infinite wedge, we consider correspondence among boson, fermion, and generators of the Cuntz algebra $\mathcal{O}_2$. Under identification of $\Pi(s_i)$ and s_i for $i=1,2$ in Proposition 4.4, we have the following:

$$\psi_k = \zeta^{2k}(s_1 s_2^*), \quad \psi_{-k} = \zeta^{2k-1}(s_1 s_2^*) \quad \left(k \in \mathbf{Z} + \tfrac{1}{2}, k > 0\right)$$

where ζ is in (1.4). From this, we have the following recurrence formulas:

Proposition 4.5:

$$\psi_{1/2} = \zeta(s_1 s_2^*), \quad \psi_{-1/2} = s_1 s_2^*,$$

$$\psi_{k+1} = \zeta^2(\psi_k), \quad \psi_{-k-1} = \zeta^2(\psi_{-k}) \quad \left(k \in \mathbf{Z} + \tfrac{1}{2}, k > 0\right).$$

Intertwining relations are given as follows:

$$s_i \psi_k = (-1)^{i-1} \psi_{-(k+1)} s_i, \quad s_i \psi_{-k} = (-1)^{i-1} \psi_k s_i,$$

$$s_i \psi_k^* = (-1)^{i-1} \psi_{-(k+1)}^* s_i, \quad s_i \psi_{-k}^* = (-1)^{i-1} \psi_k^* s_i$$

for $i=1,2$ and $k \in \mathbf{Z} + \frac{1}{2}$, $k>0$.

Proof of (1.7): If $n \geqslant 0$, then we can decompose

$$\alpha_n = A_n + B_n + C_n$$

where $A_n \equiv \Sigma_{k \in \mathbf{Z}+1/2, k>n} \psi_{k-n} \psi_k^*$, $B_n \equiv \Sigma_{k \in \mathbf{Z}+1/2, n>k>0} \psi_{k-n} \psi_k^*$ and $C_n \equiv \Sigma_{k \in \mathbf{Z}+1/2, k<0} \psi_{k-n} \psi_k^*$. By Proposition 4.5,

$$A_n + C_n = \sum_{l \in \mathbf{N}} \rho^{2n-2}(X_n), \quad X_n \equiv \psi_{1/2} \psi_{n+1/2}^* + \psi_{-n-1/2} \psi_{-1/2}^*$$

where we use $\zeta(x)\zeta(y) = \rho(xy)$ for each $x, y \in \mathcal{O}_2$. This implies (1.8). Further, we have $B_1 = -s_1 s_2 s_1^* s_2^*$,

$$B_{2k} = -\sum_{1 \leqslant l \leqslant k} \rho^{2(l-1)} \{\rho(s_2 \zeta^{4(k-l)}(s_1 s_2^*) s_1^*) + s_1 \zeta^{4(k-l)+2}(s_2 s_1^*) s_2^*\},$$

$$B_{2k+1} = -\rho^{2k}(s_1 s_2 s_1^* s_2^*) - \sum_{1 \leqslant l \leqslant k} \rho^{2(l-1)} \{\rho(s_2 \zeta^{4(k-l)+2}(s_1 s_2^*) s_1^*) + s_1 \zeta^{4(k-l)+4}(s_2 s_1^*) s_2^*\}$$

for each $k \in \mathbf{N}$. Hence the recurrence formula (1.9) of B_n is obtained. ■

Remark that α_n is an unbounded operator on a Hilbert space $\Lambda^{\infty/2} V$ and the previous equations make sense on a dense domain in $\Lambda^{\infty/2} V$.

In the same way, the *energy* defined by

$$H \equiv \sum_{k \in \mathbf{Z}+1/2} k{:}\psi_k \psi_k^*{:} = \sum_{k \in \mathbf{Z}+1/2 : k>0} k(\psi_k \psi_k^* + \psi_{-k}^* \psi_{-k})$$

is rewritten as follows:

$$H = \sum_{l \in \mathbf{N}} (l - 1/2) \rho^{2l-2}(s_1 s_1 s_1^* s_1^* + s_2 s_1 s_1^* s_2^* + s_2 s_2^*).$$

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APPENDIX: INEQUIVALENCES AMONG $\mathcal{H}_{\mathrm{Fock}}$, $P[12]$, $P[21]$

Assume that $\mathcal{H}_{\mathrm{Fock}}$ and $P[12]$ are equivalent. Then there is a cyclic representation $(\mathcal{H},\pi)$ of *CAR* with two cyclic vectors Ω and Ω' such that $\pi(a_n)\Omega=0$ and $\pi(a_{2n-1})\Omega'=\pi(a_{2n}^*)\Omega'=0$ for each $n\in\mathbf{N}$. We identify $\pi(a_n)$ and a_n for each $n\in\mathbf{N}$. We see that $\mathcal{H}$ has a complete orthonormal basis $\{a_F^*\Omega:F\in\mathcal{F}(\mathbf{N})\}$ where $\mathcal{F}(\mathbf{N})$ is the set of all finite subsets of $\mathbf{N}$ and $a_\emptyset^*\equiv I$, $a_F^*\equiv a_{n_1}^*\cdots a_{n_k}^*$ when $F=\{n_1,\ldots,n_k\}$ and $n_1<\cdots<n_k$. Hence we can denote $\Omega'=\Sigma_F c_F a_F^*\Omega$ for suitable $c_F\in\mathbf{C}$. Then there are $n_0\in\mathbf{N}$ and $F_0\in\mathcal{F}(\mathbf{N})$ such that $2n_0\notin F_0$ and $c_{F_0}\neq 0$. This implies

$$a_{2n_0}a_{F_0}^*\Omega=0. \tag{A1}$$

We see that

$$\langle a_n a_F^*\Omega|a_n a_{F'}^*\Omega\rangle=\delta_{F,F'}\cdot\chi_F(n)\cdot\chi_{F'}(n) \tag{A2}$$

for each $(n,F)\in\mathbf{N}\times\mathcal{F}(\mathbf{N})$. By assumption of Ω' and anticommutation relations of a_n's,

$$\|a_{2n}\Omega'\|=\|\Omega'\|\ (\forall n\in\mathbf{N}). \tag{A3}$$

By (A1)–(A3),

$$\|\Omega'\|^2=\|a_{2n_0}\Omega'\|^2=\left\|\sum_F c_F a_{2n_0}a_F^*\Omega\right\|^2\leqslant\sum_{F\neq F_0}|c_F|^2<\|\Omega'\|^2.$$

This is contradiction. Hence $\mathcal{H}_{\mathrm{Fock}}$ and $P[12]$ are not equivalent. In the same way, inequivalences among $\mathcal{H}_{\mathrm{Fock}}$, $P[21]$, and $P[12]$ are shown. ■

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The "Blow up" problem for a quasilinear Schrödinger equation

Boling Guo
Institute of Applied Physics and Computational Mathematics, P.O. Box 8009, Beijing 100088, People's Republic of China

Jianqing Chen[a)]
Institute of Applied Physics and Computational Mathematics, P.O. Box 8009, Beijing 100088, People's Republic of China and School of Mathematics and Computer Science, Fujian Normal University, Fuzhou, 350007, People's Republic of China

Fengqiu Su
Department of Mathematics, Central University of Nationalities, Beijing, 100081, People's Republic of China

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Consider the blow up results for $W^{2,2}(\mathbb{R}^N)$ solutions of a quasilinear Schrödinger equation $iu_t+\Delta u+\beta|u|^{p-2}u+\theta(\Delta|u|^2)u=0$, $u_{|_{t=0}}=u_0(x), x\in\mathbb{R}^N$. When $|x|u_0 \in L^2(\mathbb{R}^N)$, we show that the $W^{2,2}(\mathbb{R}^N)$ solutions must blow up for any $\beta\geqslant 0$, $\theta \in \mathbb{R}$ and some restriction on p. We also show that the radial symmetric solutions in $W^{2,2}(\mathbb{R}^N)$ must blow up at finite time without assuming $|x|u_0\in L^2(\mathbb{R}^N)$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1941089]

I. INTRODUCTION

Porkolab and Goddman[13] have proposed the following nonlinear Schrödinger equation:

$$iu_t + u_{xx} + q(|u|^2)u - (|u|^2)_{xx} = 0, \tag{1.1}$$

and Refs. 15,14 have derived (1.1) for various physical situation. Equations similar to (1.1) in the case of higher spatial dimensions has been derived in the study of theory of superfluids, dissipative quantum mechanics, see Refs. 3,5,6 and the references therein. Considering the model problem

$$\begin{aligned} &iu_t + \Delta u + \beta|u|^{p-2}u + \theta(\Delta|u|^2)u = 0, \quad x \in \mathbb{R}^N, \\ &u_{|_{t=0}} = u_0(x), \quad x \in \mathbb{R}^N, \end{aligned} \tag{QSE}$$

$u:=u(x,t):\mathbb{R}^N\times\mathbb{R}_+\to\mathbb{C}$ is a complex-valued function, $i^2=-1$. β, θ are real constants and $p>2$. $\Delta=\Sigma_{j=1}^N(\partial^2/\partial x_j^2)$ is the standard Laplacian operator.

Mathematical difficulties in the study of problem (QSE) are due to the presence of the quasilinear term $(\Delta|u|^2)u$. There are some results about the existence of stationary solutions of problem (QSE). In a series of works, Liu-Wang-Wang[9,10] have shown the existence of standing waves solutions, i.e., a solution of form $e^{iwt}v(x)$ of (QSE). Local well posedness or global well posedness for small initial data of (QSE) is known, see, e.g., Refs. 6 and 12. However, the general global existence result for the Cauchy problem (QSE) is still open.

In this paper, we study the "blowing up" phenomena for the Cauchy problem (QSE). More precisely, we have the following.

Theorem 1.1: *Suppose that* $u(t)\in W^{2,2}(\mathbb{R}^N)(N\geqslant 1)$ *is a solution of (QSE) and*

[a)]Author to whom correspondence should be addressed: Institute of Applied Physics and Computational Mathematics, P.O. Box 8009(28 Branch), Beijing 100088, People's Republic of China.

(1) $u_0 \in W^{2,2}(\mathbb{R}^N)$, $\beta \geqslant 0$ *and* $4+(4/N) \leqslant p < 2\cdot 2^* := 2\times 2^*$, *here and after*, $2^* = 2N/(N-2)$ *if* $N \geqslant 3$ *and* $2^* = +\infty$ *otherwise*;
(2) $\nabla |u_0|^2 \in L^2(\mathbb{R}^N)$;
(3) $E(0) = \int (|\nabla u_0|^2 - (2\beta/p)|u_0|^p + (\theta/2)|\nabla |u_0|^2|^2) \leqslant 0$;
(4) $\mathrm{Im} \int \bar{u}_0 x \nabla u_0 < 0$ *and* $|x|u_0 \in L^2(\mathbb{R}^N)$;

here and after, $\bar{u}$ *is the complex conjugate of* u. *Then there exists a* $T_0 > 0$ *such that*

$$\lim_{t \to T_0^-} \| \nabla u \|^2_{L^2(\mathbb{R}^N)} = +\infty.$$

So that $\|u\|_{W^{2,2}(\mathbb{R}^N)}$ *blows up in finite time.*

Remark 1.2: (a) When $\theta = 0$, *a similar result has been obtained by Glassey.*[2] *(b) If choosing* $u_0(x) = \lambda e^{-i|x|^2} \varphi(x)$ *with* $\lambda > 0$ *and real-valued function* $\varphi(x) \in \mathcal{S}$, *the Schwartz space of rapidly decreasing functions in* $\mathbb{R}^N$, *then a direct computation gives* $\mathrm{Im} \int \bar{u}_0(x) x \nabla u_0(x) = -2\lambda^2 \int |x|^2 |\varphi|^2$, *so that* (4) *always holds in this case. Since* $p > 4$, (3) *also holds for some* λ *large.*

Note that the existence of T_0 obtained in Theorem 1.1 depends (see the proof of Theorem 1.1) on the existence of $L^2(\mathbb{R}^N)$ norm of $|x|u_0$. If $\int |x|^2 |u_0|^2 = \infty$ (this is possible, say, $u_0 \notin L^2(\mathbb{R}^N, |x|^2\, dx)$), then we cannot get the existence of such T_0. Furthermore, some numerical computations suggest that the weight restriction of $L^2(\mathbb{R}^N, |x|^2\, dx)$ is not necessarily needed for the blow up of solutions, see e.g., Ref. 7, Sec. 5 for the case of $\theta = 0$. Our next purpose is to improve this result. That is, we will remove the restriction of $u_0 \in L^2(\mathbb{R}^N, |x|^2\, dx)$ and prove that the radially symmetric solutions in $W^{2,2}(\mathbb{R}^N)$ [possibly not in $L^2(\mathbb{R}^N, |x|^2\, dx)$] blow up at finite time.

Theorem 1.3: *Suppose that* $u(t) \in W_r^{2,2}(\mathbb{R}^N) = \{u \in W^{2,2}(\mathbb{R}^N); u(x) = u(|x|)\} (N \geqslant 2)$ *is a radially symmetric solution of (QSE) and*

(i) $u_0(x) \in W_r^{2,2}(\mathbb{R}^N)$, $\beta \geqslant 0$ *and* $4+(4/N) \leqslant p \leqslant 6$ *if* $6 < 2\cdot 2^*$ *and* $4+(4/N) \leqslant p < 2\cdot 2^*$ *if* $6 > 2\cdot 2^*$;
(ii) $\nabla |u_0|^2 \in L^2(\mathbb{R}^N)$;
(iii) $E(0) = \int (|\nabla u_0|^2 - (2\beta/p)|u_0|^p + (\theta/2)|\nabla |u_0|^2|^2) < 0$;

then there is T *such that*

$$\lim_{t \to T^-} \| \nabla u \|^2_{L^2(\mathbb{R}^N)} = +\infty.$$

Remark 1.4: When $\theta = 0$, *Ogawa et al.*[11] *have proved the blow up of the radial solution of (QSE) for* $2+(4/N) \leqslant p < \min\{2^*, 6\}$ *and* $N \geqslant 2$.

Remark 1.5: When $\theta = 0$, $p = 2+(4/N)$ *is the critical exponent for the blowing up of Cauchy problem (QSE). When* $\theta \neq 0$, *we need to increase the value of* p. *However, it seems that the presence of quasilinear term can relax the restriction of* p *in some sense since we allow* $p = 6$ *in Theorem 1.3.*

This paper is organized as follows. The forthcoming section is due to the proof of Theorem 1.1. In Sec. III, we give some lemmas which are useful in the proof of Theorem 1.3. The final section contains the proof of Theorem 1.3.

We end this introduction by some notations. Throughout this paper, all integrals are taken over $\mathbb{R}^N$ unless stated otherwise, $W^{k,q}(\mathbb{R}^N)$ and $L^q(\mathbb{R}^N)$ are standard Sobolev spaces with standard norms. $L^2(\mathbb{R}^N, |x|^2\, dx)$ is a weighted Sobolev space. By C we denote a generic positive constant whose value can vary from line to line. Re (Im) denotes the real (imaginary) part for the complex value.

II. PROOF OF THEOREM 1.1

In this section, we will prove Theorem 1.1. The proof suggests that we not only give the existence of blowing up time, but also give an upper bound estimate for the blowing up time. The methods are adapted from those in Glassey,[2] see also Ref. 1, but we need to overcome the additional difficulty created by the quasilinear term.

Proof of Theorem 1.1: Multiplying (QSE) by $\bar{u}$, integrating by parts and taking the imaginary part, we can get that

$$\int |u|^2 = \int |u_0|^2. \tag{2.1}$$

Multiplying (QSE) by $\bar{u}_t$ and taking the real part, we have that

$$\mathrm{Re}\int (\Delta u\bar{u}_t + \beta|u|^{p-2}u\bar{u}_t + \theta(\Delta|u|^2)u\bar{u}_t) = \frac{d}{\mathrm{d}t}\int \left(-\frac{1}{2}|\nabla u|^2 + \frac{\beta}{p}|u|^p - \frac{\theta}{4}|\nabla |u|^2|^2\right) = 0.$$

It follows that

$$E(t) = \int \left(|\nabla u|^2 - \frac{2\beta}{p}|u|^p + \frac{\theta}{2}|\nabla |u|^2|^2\right) = E(0). \tag{2.2}$$

Denote $D(t) = \int r^2|u|^2\,\mathrm{d}x$. We have that

$$\begin{aligned}\frac{\mathrm{d}D(t)}{\mathrm{d}t} &= 2\,\mathrm{Re}\int r^2\bar{u}u_t = -2\,\mathrm{Im}\int r^2\bar{u}\Delta u = 2\,\mathrm{Im}\int (r^2\nabla u\nabla\bar{u} + 2x\bar{u}\nabla u)\\ &= 4\,\mathrm{Im}\int \bar{u}x\nabla u := -4D_1(t),\end{aligned} \tag{2.3}$$

in here $D_1(t) = -\mathrm{Im}\int \bar{u}x\nabla u$.

$$\begin{aligned}\frac{\mathrm{d}D_1(t)}{\mathrm{d}t} &= -\,\mathrm{Im}\int (\bar{u}_t x\nabla u + \bar{u}x\nabla u_t) = \mathrm{Im}\int (2x\nabla\bar{u} + N\bar{u})u_t\\ &= \mathrm{Re}\int (2x\nabla\bar{u} + N\bar{u})(\Delta u + \beta|u|^{p-2}u + \theta(\Delta|u|^2)u).\end{aligned} \tag{2.4}$$

Note that

$$\begin{aligned}\mathrm{Re}\int (2x\nabla\bar{u} + N\bar{u})\Delta u &= -\,\mathrm{Re}\int [\nabla u\nabla(2x\nabla\bar{u}) + N\nabla u\nabla\bar{u}]\\ &= -N\int |\nabla u|^2 - 2\int |\nabla u|^2 - \int x\nabla|\nabla u|^2 = -2\int |\nabla u|^2,\end{aligned} \tag{2.5}$$

$$\begin{aligned}\mathrm{Re}\int (2x\nabla\bar{u} + N\bar{u})|u|^{p-2}u &= N\int |u|^p + \int |u|^{p-2}x\nabla|u|^2 = N\int |u|^p + \frac{2}{p}\int x\nabla|u|^p\\ &= N\int |u|^p + \frac{2}{p}\int xd|u|^p = \frac{N(p-2)}{p}\int |u|^p,\end{aligned} \tag{2.6}$$

$$\begin{aligned}\mathrm{Re}\int (2x\nabla\bar{u} + N\bar{u})(\Delta|u|^2)u &= \mathrm{Re}\int N(\Delta|u|^2)|u|^2 + \int (x\nabla|u|^2)(\Delta|u|^2)\\ &= -N\int |\nabla|u|^2|^2 - \int \nabla|u|^2\nabla(x\nabla|u|^2) = -(N+1)\int |\nabla|u|^2|^2\\ &\quad -\frac{1}{2}\int x\nabla|\nabla|u|^2|^2\end{aligned}$$

$$= -(N+1)\int |\nabla |u|^2|^2 + \frac{N}{2}\int |\nabla |u|^2|^2 = -\frac{N+2}{2}\int |\nabla |u|^2|^2. \tag{2.7}$$

Thus

$$\frac{dD_1(t)}{dt} = -2\int |\nabla u|^2 + \frac{N\beta(p-2)}{p}\int |u|^p - \frac{\theta(N+2)}{2}\int |\nabla |u|^2|^2. \tag{2.8}$$

Combining this with the expression of $E(t)=E(0)\leqslant 0$ and $p\geqslant 4+(4/N)$, we know that

$$\frac{dD_1(t)}{dt} = -\left((N+2)E(t) - N\int |\nabla u|^2 + \frac{(4N+4-Np)\beta}{p}\int |u|^p\right) \geqslant N\int |\nabla u|^2 > 0. \tag{2.9}$$

Therefore

$$D_1(t) \geqslant D_1(0) = -\operatorname{Im}\int \bar{u}_0 x\nabla u_0 > 0. \tag{2.10}$$

It now follows from (2.3) that $dD(t)/dt < 0$ and

$$D(t) \leqslant D(0) = \int r^2|u_0|^2. \tag{2.11}$$

Because of

$$|D_1(t)| = D_1(t) = -\operatorname{Im}\int \bar{u}x\nabla u \leqslant \left(\int r^2|u|^2\right)^{1/2}\left(\int |\nabla u|^2\right)^{1/2} \leqslant D(0)^{1/2}\|\nabla u\|_{L^2(\mathbb{R}^N)}, \tag{2.12}$$

there holds

$$D_1(t)^2 \leqslant D(0)\|\nabla u\|_{L^2}^2 \leqslant \frac{D(0)}{N}\frac{dD_1(t)}{dt}.$$

So $dD_1(t)/dt \geqslant ND_1(t)^2/D(0)$ and $D_1(0) = -\operatorname{Im}\int \bar{u}_0 x\nabla u_0 > 0$. It follows that

$$D_1(t) \geqslant 1\Big/\left(\frac{1}{D_1(0)} - \frac{Nt}{D(0)}\right).$$

Let $T^* = D(0)/ND_1(0)$, then there is $T_0 \leqslant T^*$ such that

$$\lim_{t\to T_0^-}\|\nabla u\|_{L^2}^2 \geqslant \lim_{t\to T_0^-}\frac{D_1(t)}{D(0)^{1/2}} = +\infty. \tag{2.13}$$

So that $\|u\|_{W^{2,2}(\mathbb{R}^N)}$ blows up in finite time. The proof is complete. □

III. SOME LEMMAS

In this section, we state some lemmas which are useful in what follows. The first is about decay property for radially symmetric functions in $W^{1,2}(\mathbb{R}^N)$ which is due to Lin *et al.*[8]

Lemma 3.1: Let u be radially symmetric in $W^{1,2}(\mathbb{R}^N)$ *and* $N\geqslant 2$. *Then for any* $R>0$, *u satisfies*

$$\|u\|_{L^\infty(R<r)} \leqslant CR^{-(N-1)/2}\|u\|_{L^2(R<r)}^{1/2}\|\nabla u\|_{L^2(R<r)}^{1/2}, \tag{3.1}$$

where $r=|x|$ and C is a constant independent of u and R.

Next, we prove a general identity which is a generalization for those obtained in Lin *et al.*[8] in the case of $\theta=0$, see also Refs. 4 and 11.

Lemma 3.2: Suppose that $\Psi=(\Psi_1,\Psi_2,\ldots,\Psi_N)$ is a vector valued function in $(W^{3,\infty}(\mathbb{R}^N))^N$ and $2<p<22^*$. Then the $W^{2,2}(\mathbb{R}^N)$ solution $u(t)$ of (QSE) satisfies

$$\begin{aligned}\operatorname{Im}\int \Psi u_0\nabla\bar{u}_0-\operatorname{Im}\int \Psi u(t)\nabla\bar{u}(t)=\int_0^t\Bigg\{2\operatorname{Re}\int\sum_{k,j}u_k\Psi_{kj}\bar{u}_j+\frac{\beta(2-p)}{p}\int|u|^p(\nabla\cdot\Psi)\\ -\frac{1+\theta}{2}\int|u|^2\Delta(\nabla\cdot\Psi)+\theta\int\sum_{k,j}(|u|^2)_k\Psi_{kj}(|u|^2)_j\\ +\frac{\theta}{2}\int|\nabla|u|^2|^2(\nabla\cdot\Psi)\Bigg\}\mathrm{d}\tau,\end{aligned}\tag{3.2}$$

in here $u_k=(\partial/\partial x_k)u$, $(|u|^2)_k=(\partial/\partial x_k)|u|^2$, and $\Psi_{kj}=\partial/\partial_{x_k}\Psi_j$, all summations are taken from 1 to N.

Proof: Keep the following in mind,

$$iu_t=-\Delta u-\beta|u|^{p-2}u-\theta(\Delta|u|^2)u,\tag{3.3}$$

$$-i\bar{u}_t=-\Delta\bar{u}-\beta|u|^{p-2}\bar{u}-\theta(\Delta|u|^2)\bar{u}.\tag{3.4}$$

Now multiplying (3.3) by $\Psi\bar{u}$ and integrating by parts, we have first that

$$i\int u_t(\Psi\bar{u})=i\frac{d}{\mathrm{d}t}\int\Psi u\nabla\bar{u}-i\int\Psi u\nabla\bar{u}_t.$$

It follows that

$$i\frac{d}{\mathrm{d}t}\int\Psi u\nabla\bar{u}+i\int(\nabla\cdot\Psi)u\bar{u}_t=i\int u_t(\Psi\bar{u})+i\int\Psi u\nabla\bar{u}_t+i\int(\nabla\cdot\Psi)u\bar{u}_t.\tag{3.5}$$

Combining this with (3.3) and (3.4), we get that

$$\begin{aligned}i\frac{d}{\mathrm{d}t}\int\Psi u\nabla\bar{u}+i\int(\nabla\cdot\Psi)u\bar{u}_t=i\int u_t(\Psi\nabla\bar{u})-i\int\bar{u}_t\Psi\nabla u=\int(-\Delta u-\beta|u|^{p-2}u-\theta(\Delta|u|^2)u)\\ \times(\Psi\nabla\bar{u})+\int(-\Delta\bar{u}-\beta|u|^{p-2}\bar{u}-\theta(\Delta|u|^2)\bar{u})(\Psi\nabla u).\end{aligned}\tag{3.6}$$

Direct computations can arrive at

$$\begin{aligned}-\int\Delta u(\Psi\nabla\bar{u})=\int\nabla u\nabla(\Psi\nabla\bar{u})=\int\sum_k u_k\sum_j(\Psi_{kj}\bar{u}_j+\Psi_j\bar{u}_{jk})\\ =\int\sum_{k,j}u_k\Psi_{kj}\bar{u}_j+\int\sum_j\Psi_j\sum_k u_k\bar{u}_{kj},\end{aligned}$$

$$-\int\Delta\bar{u}(\Psi\cdot\nabla u)=\int\sum_{k,j}\bar{u}_k\Psi_{kj}u_j+\int\sum_j\Psi_j\sum_k\bar{u}_k u_{kj},$$

and hence

$$\int [-\Delta u(\Psi\nabla\bar{u})-\Delta\bar{u}(\Psi\cdot\nabla u)]=2\,\mathrm{Re}\int\sum_{k,j}u_k\Psi_{kj}\bar{u}_j+\int\Psi\cdot\nabla|\nabla u|^2$$
$$=2\,\mathrm{Re}\int\sum_{k,j}u_k\Psi_{kj}\bar{u}_j-\int(\nabla\cdot\Psi)|\nabla u|^2. \tag{3.7}$$

Similarly

$$\int(-\beta|u|^{p-2}u(\Psi\nabla\bar{u})-\Delta\bar{u}-\beta|u|^{p-2}\bar{u}(\Psi\nabla u))=\frac{2\beta}{p}\int(\nabla\cdot\Psi)|u|^p, \tag{3.8}$$

$$\int(-\theta(\Delta|u|^2)u(\Psi\nabla\bar{u})-\theta(\Delta|u|^2)\bar{u}(\Psi\nabla u))=-\theta\int(\Delta|u|^2)\Psi\nabla|u|^2=\theta\int\nabla|u|^2\nabla(\Psi\nabla|u|^2)$$
$$=\theta\int\sum_{k,j}(|u|^2)_k\Psi_{kj}(|u|^2)_j-\frac{\theta}{2}\int(\nabla\cdot\Psi)|\nabla|u|^2|^2. \tag{3.9}$$

Therefore

$$i\frac{d}{dt}\int\Psi u\nabla\bar{u}+i\int(\nabla\cdot\Psi)u\bar{u}_t=2\,\mathrm{Re}\int\sum_{k,j}u_k\Psi_{kj}\bar{u}_j-\int(\nabla\cdot\Psi)|\nabla u|^2+\frac{2\beta}{p}\int(\nabla\cdot\Psi)|u|^p$$
$$+\theta\int\sum_{k,j}(|u|^2)_k\Psi_{kj}(|u|^2)_j-\frac{\theta}{2}\int(\nabla\cdot\Psi)|\nabla|u|^2|^2. \tag{3.10}$$

Using (3.4), we know that

$$i\int(\nabla\cdot\Psi)u\bar{u}_t=\int(\nabla\cdot\Psi)(u\Delta\bar{u}+\beta|u|^p+\theta(\Delta|u|^2)|u|^2). \tag{3.11}$$

Similar calculations show that

$$\int(\nabla\cdot\Psi)u\Delta\bar{u}=-\int(\nabla\cdot\Psi)|\nabla u|^2-\int\nabla\bar{u}u\nabla(\nabla\cdot\Psi), \tag{3.12}$$

$$\theta\int(\nabla\cdot\Psi)(\Delta|u|^2)|u|^2=-\theta\int(\nabla\cdot\Psi)|\nabla|u|^2|^2+\frac{\theta}{2}\int\Delta(\nabla\cdot\Psi)|u|^4. \tag{3.13}$$

It follows that

$$i\frac{d}{dt}\int\Psi u\nabla\bar{u}=2\,\mathrm{Re}\int\sum_{k,j}u_k\Psi_{kj}\bar{u}_j+\frac{\beta(2-p)}{p}\int(\nabla\cdot\Psi)|u|^p+\int\nabla\bar{u}u\nabla(\nabla\cdot\Psi)$$
$$+\theta\int\sum_{k,j}(|u|^2)_k\Psi_{kj}(|u|^2)_j+\frac{\theta}{2}\int(\nabla\cdot\Psi)|\nabla|u|^2|^2-\frac{\theta}{2}\int\Delta(\nabla\cdot\Psi)|u|^2. \tag{3.14}$$

Taking real part in (3.14), we get that

$$\int \Psi u_0 \nabla \bar{u}_0 - \int \Psi u \nabla \bar{u} = \int_0^t \Bigg\{ 2\,\mathrm{Re} \int \sum_{k,j} u_k \Psi_{kj} \bar{u}_j + \frac{\beta(2-p)}{p} \int (\nabla \cdot \Psi)|u|^p + \theta \int \sum_{k,j} (|u|^2)_k \Psi_{kj} (|u|^2)_j + \frac{\theta}{2} \int (\nabla \cdot \Psi) |\nabla |u|^2|^2 - \frac{1+\theta}{2} \int \Delta(\nabla \cdot \Psi)|u|^2 \Bigg\} \mathrm{d}\tau. \tag{3.15}$$

This completes the proof. □

IV. PROOF OF THEOREM 1.3

In this section, we will prove Theorem 1.3. The idea is to take a suitable weight function Ψ and use Lemma 3.2, which has been used by Ogawa *et al.*[11] in the case of $\theta=0$. But when $\theta \neq 0$, the method used in Ref. 11 does not work. Hence, here we choose an appropriate weight function Ψ and some estimates. To proceed, we need some preparations.

Let $\phi:[0,\infty)\to\mathbb{R}_+$ be a function with bounded third order derivatives and be such that

$$\phi(s) = \begin{cases} s, & 0 \leqslant s < \frac{1}{2}, \\ s - \left(s - \frac{1}{2}\right)^3, & \frac{1}{2} \leqslant s < \frac{1}{2} + \frac{\sqrt{3}}{3}, \\ \text{smooth}, \phi' < 0, & \frac{1}{2} + \frac{\sqrt{3}}{3} \leqslant s < 2, \\ 0, & 2 \leqslant s, \end{cases}$$

and $\phi'(s) \leqslant 1$. Let m be a large positive constant to be determined later, we set

$$\phi_m(r) = m\phi\left(\frac{r}{m}\right).$$

Clearly

$$\left| \frac{\partial^\alpha}{\partial r^\alpha} \phi_m(r) \right| \leqslant \frac{C_\alpha}{m^{\alpha-1}}, \quad \text{for } \alpha = 0,1,2,3. \tag{4.1}$$

Denote $r=|x|$ and choose Ψ as follows:

$$\Psi(x) = \frac{x}{r}\phi_m(r) \quad \text{and } \Psi_j(x) = \frac{x_j}{r}\phi_m(r).$$

Direct computations show that

$$\Psi_{kj} = \begin{cases} \delta_{kj}, & 0 \leqslant r < \frac{1}{2}m, \\ \left(\frac{\delta_{kj}}{r} - \frac{x_k x_j}{r^3}\right)\phi_m(r) + \frac{x_k x_j}{r^3}\phi_m'(r), & \frac{1}{2}m \leqslant r < \left(\frac{1}{2} + \frac{\sqrt{3}}{3}\right)m, \\ \left(\frac{\delta_{kj}}{r} - \frac{x_k x_j}{r^3}\right)\phi_m(r) + \frac{x_k x_j}{r^3}\phi_m'(r),\ \phi' < 0, & \left(\frac{1}{2} + \frac{\sqrt{3}}{3}\right)m \leqslant r < 2m, \\ 0, & 2m \leqslant r, \end{cases} \tag{4.2}$$

where $k, j = 1, 2, \ldots, N$ and

$$\Delta(\nabla\cdot\Psi)=\sigma(r)$$
$$=\begin{cases}0, & 0\leqslant r<\frac{1}{2}m,\\ \phi_m^{(3)}+(N-1)\left\{\frac{2}{r}\phi_m''+\frac{N-3}{r^2}\phi_m'-\frac{N-3}{r^3}\phi_m\right\}, & \frac{1}{2}m<r<\left(\frac{1}{2}+\frac{\sqrt{3}}{3}\right)m,\\ \phi_m^{(3)}+(N-1)\left\{\frac{2}{r}\phi_m''+\frac{N-3}{r^2}\phi_m'-\frac{N-3}{r^3}\phi_m\right\},\ \phi'<0, & \left(\frac{1}{2}+\frac{\sqrt{3}}{3}\right)m\leqslant r<2m,\\ 0, & 2m\leqslant r.\end{cases}\tag{4.3}$$

Proof of Theorem 1.3: Arguing by a contradiction, we assume $u(t)\in W_r^{2,2}(\mathbb{R}^N)$ and $\|\nabla u\|_{L^2(\mathbb{R}^N)}$ exists globally. Using the fact that

$$\frac{\theta}{2}\int_{r<(m/2)}|\nabla|u|^2|^2=E(t)-\int|\nabla u|^2+\frac{2\beta}{p}\int|u|^p-\frac{\theta}{2}\int_{r>(m/2)}|\nabla|u|^2|^2,$$

we substitute the relations (4.2) and (4.3) into (3.2) to get that

$$\begin{aligned}\mathrm{Im}\int\Psi u_0\nabla\bar{u}_0-\mathrm{Im}\int\Psi u(t)\nabla\bar{u}(t)=\int_0^t\Bigg\{&2\int_{r<(m/2)}|\nabla u|^2+2\int_{r>(m/2)}\phi_m'(r)|\nabla u|^2+(N+2)E(t)\\&-(N+2)\int|\nabla u|^2-\frac{1+\theta}{2}\int_{r>(m/2)}\sigma(r)|u|^2\\&+\frac{2\beta(N+2)}{p}\int|u|^p+\frac{N\beta(2-p)}{p}\int_{r<(m/2)}|u|^p\\&+\frac{\beta(2-p)}{p}\int_{r>(m/2)}\left(\frac{N-1}{r}\phi_m(r)+\phi_m'(r)\right)|u|^p\\&+\theta\int_{r>(m/2)}\left(\frac{3}{2}\phi_m'(r)+\frac{N-1}{2r}\phi_m(r)-\frac{N+2}{2}\right)|\nabla|u|^2|^2\Bigg\}\mathrm{d}\tau.\end{aligned}\tag{4.4}$$

Now from the construction of ϕ, we know that

$$\frac{3}{2}\phi_m'(r)+\frac{N-1}{2r}\phi_m(r)-\frac{N+2}{2}\leqslant 0\quad\text{for } r\geqslant\frac{m}{2}.$$

Equations (4.1) and (4.3) imply that for some positive constant C,

$$|\sigma(r)|\leqslant Cm^{-2}.$$

Combining these with $p\geqslant 4+(4/N)$, we obtain that

$$\begin{aligned}\mathrm{Im}\int\Psi u_0\nabla\bar{u}_0-\mathrm{Im}\int\Psi u(t)\nabla\bar{u}(t)\leqslant\int_0^t\Bigg\{&(N+2)E(t)-N\int|\nabla u|^2+Cm^{-2}\|u\|_{L^2}^2\\&+C\int_{r>(m/2)}|u|^p\Bigg\}\mathrm{d}\tau.\end{aligned}\tag{4.5}$$

Noticing from Lemma 3.1 that

$$\int_{r>(m/2)} |u|^p \leqslant \|u\|^{p-2}_{L^\infty[r>(m/2)]} \int_{r>(m/2)} |u|^2 \leqslant Cm^{[-(N-1)(p-2)/2]} \|u\|^{(p+2)/2}_{L^2[r>(m/2)]} \| \nabla u\|^{(p-2)/2}_{L^2}. \quad (4.6)$$

If $p=6$, then

$$\int_{r>(m/2)} |u|^p \leqslant Cm^{-2(N-1)} \|u\|^4_{L^2[r>(m/2)]} \| \nabla u\|^2_{L^2} \leqslant Cm^{-2(N-1)} \|u\|^4_{L^2} \| \nabla u\|^2_{L^2}. \quad (4.7)$$

Combining with (2.1), we know that the right-hand side of (4.7) can be dominated by $-N\int |\nabla u|^2$ for m large. It follows that there is a positive constant η_1 such that

$$\mathrm{Im} \int \Psi u_0 \nabla \bar{u}_0 - \mathrm{Im} \int \Psi u(t) \nabla \bar{u}(t) \leqslant - \eta_1 t.$$

If $p<6$, then we can apply Young inequality directly to (4.6) that

$$\int_{r>(m/2)} |u|^p \leqslant \varepsilon \| \nabla u\|^2_{L^2} + C_\varepsilon m^{-\gamma} \|u\|^{[(p+2)(6-p)/8]}_{L^2},$$

with $\gamma=(N-1)(p-2)(6-p)/8$. Choosing ε small and using (2.1), we can get that for m large there is a positive constant η_2 such that

$$\mathrm{Im} \int \Psi u_0 \nabla \bar{u}_0 - \mathrm{Im} \int \Psi u(t) \nabla \bar{u}(t) \leqslant - \eta_2 t.$$

Thus in any cases, we have for some positive constant η such that

$$\mathrm{Im} \int \Psi u_0 \nabla \bar{u}_0 - \mathrm{Im} \int \Psi u(t) \nabla \bar{u}(t) \leqslant - \eta t. \quad (4.8)$$

Set $\Phi(r)=\int_0^r \phi_m(s)\mathrm{d}s$. Since $\Phi \in L^\infty(\mathbb{R}^N)$ and

$$\nabla \Phi(r) = \frac{x}{r} \phi_m(r) = \Psi(x),$$

we can use (3.4) to get that

$$\begin{aligned} i \int \Phi u \bar{u}_t &= \int (\Phi u \triangle \bar{u} + \Phi \beta |u|^p + \Phi \theta(\triangle |u|^2)|u|^2) \\ &= - \int \Psi u \nabla \bar{u} - \int \Phi(| \nabla u|^2 - \beta |u|^p - \theta(\triangle |u|^2)|u|^2). \end{aligned} \quad (4.9)$$

Taking the imaginary part in (4.9), we know that

$$\mathrm{Re} \int \Phi u \bar{u}_t = - \mathrm{Im} \int \Psi u \nabla \bar{u}.$$

Since

$$\frac{d}{\mathrm{d}t} \int \Phi |u|^2 = 2 \,\mathrm{Re} \int \Phi u \bar{u}_t \quad \text{for } t \in [0,\infty),$$

we can get that

$$\int \Phi|u|^2 \leqslant -\eta t^2 - 2t\,\mathrm{Im}\int \Psi u_0 \nabla \bar{u}_0 + \int \Phi|u_0|^2. \tag{4.10}$$

Therefore the left-hand side of (4.10) becomes negative at finite time, which implies a contradiction since $\Phi(r)>0$ except when $r=0$. Hence $\|\nabla u\|_{L^2(\mathbb{R}^N)}$ must blow up at finite time. The proof is complete.

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The 1856 lemma of Cayley revisited. I. Infinitesimal generators

Jin Yue[a)]
Department of Mathematics and Statistics, Dalhousie University, Halifax, Nova Scotia, B3H 3J5, Canada

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The result of classical invariant theory commonly referred to as Cayley's lemma is reviewed. Its analog in the invariant theory of Killing tensors defined in pseudo-Riemannian spaces of constant curvature is formulated and proven. Illustrative examples are provided. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Recent years have seen the appearance of new areas of mathematics bridging the gap between classical invariant theory (CIT) and differential geometry. They have brought about novel techniques proving their worth in various areas of mathematical physics, in particular, the theory of *integrable and superintegrable Hamiltonian systems* (see Horwood *et al.*,[12] and the relevant reference therein). At the same time the classical invariant theory of homogeneous polynomials itself resurrected once again through new aspects of the Lie group theory (notably, the generalizations of the moving frames method due to Fels and Olver[8,9] and Kogan,[14] see also the relevant references therein), the rise of the modern computer algebra and new applications in other areas of mathematics (see Hilbert[11] and Olver[24] for a complete review and related references). Thus, McLenaghan *et al.* in their pioneering paper[16] successfully planted the underlying ideas of CIT into the fertile field of the (geometric) study of Killing tensors defined in pseudo-Riemannian manifolds of constant curvature, which ultimately bore the fruit of a new theory (see also Refs. 12, 17, 28, 29, 4, and 18–21). The resulting *invariant theory of Killing tensors* (ITKT) shares many of the same essential features with the original CIT. In light of the fact that "Mathematics is the study of analogies between analogies,"[25] we wish to continue developing ITKT by establishing more analogies with CIT. One of the most famous problems solved by Cayley around the time CIT was conceived was the problem of the determination of the infinitesimal action of $SL(2,\mathbb{R})$ in the vector spaces of the binary forms $\mathcal{Q}^n(\mathbb{R}^2)$ of an *arbitrary degree n*. Interestingly, this was done before the emergence of the formal theory of Lie groups in order to develop a tractable procedure for computing the *invariants* and *covariants* of such vector spaces under the action of $SL(2,\mathbb{R})$. The people working in ITKT routinely encounter similar problems that boil down to finding effective and efficient ways for computing the invariants and covariants of the isometry group action in the vector spaces of Killing tensors defined in pseudo-Riemannian spaces of constant curvature. Of particular importance is the case when the vector spaces in question are the vector spaces of Killing tensors defined in two-dimensional pseudo-Riemannian manifolds. Let $\mathbb{R}^2_1$ be the Minkowski plane. In this paper we formulate and solve the problem of finding the infinitesimal action of the isometry group $I(\mathbb{R}^2_1)$ *in the vector space* $\mathcal{K}^n_0(\mathbb{R}^2_1)$ *of Killing tensors of* arbitrary valence n.

This problem represents a natural analog of the classical problem solved by Arthur Cayley in 1856 (i.e., the so-called *Cayley's Lemma*), while establishing the foundations of CIT.

[a)]Electronic mail: jyue@dal.ca

The paper is organized as follows. In Sec. II we briefly review Cayley's lemma in CIT. In Sec. III we review basic facts about ITKT. An analog of Cayley's lemma in ITKT is formulated and proven in Sec. IV. Finally, in Sec. V we make concluding remarks.

II. CAYLEY'S LEMMA

As is well known, the *main object* of study in CIT is a vector space of homogeneous polynomials under the action of the general linear group (or its subgroups), while the *main problem* is that of the determination of the functions of the parameters of the vector space in question that remain fixed under the action of the group. These functions, called *invariants*, are very useful in solving various classification problems. In this study the vector spaces of particular importance are the spaces of *binary forms*, or homogeneous polynomials of degree n in two variables, originally referred to by Arthur Cayley[3] as *quantics*.

Let $\mathcal{Q}^n(\mathbb{R}^2)$ denote the vector space of binary forms of degree n over the reals. Then the dimension d of the space is $n+1$, and an element $\boldsymbol{Q}(x,y)$ of $\mathcal{Q}^n(\mathbb{R}^2)$ is given by

$$\boldsymbol{Q}(x,y)=\sum_{i=0}^{n}\binom{n}{i}a_i x^{n-i}y^i, \quad (x,y)\in\mathbb{R}^2. \tag{1}$$

The special linear group $SL(2,\mathbb{R})$ acts on the space $\mathcal{Q}^n(\mathbb{R}^2)$ by linear substitutions, which yield the corresponding transformation rules

$$\tilde{a}_i=\tilde{a}_i(a_0,\ldots,a_n,\alpha,\beta,\gamma,\delta), \quad i=0,\ldots,n, \tag{2}$$

where $\alpha,\beta,\gamma,\delta\in\mathbb{R},(\alpha\delta-\beta\gamma=1)$ are local coordinates that parametrize the group. Note dim $SL(2,\mathbb{R})=3$. The formulas (2) can be derived explicitly.[24] The problem reduces to finding all of the $SL(2,\mathbb{R})$-invariants of $\mathcal{Q}^n(\mathbb{R})^2$, or those functions defined over Σ, the parameter space spanned by $(a_0,\ldots,a_n)$, that remain unchanged under the transformations (2):

$$\mathcal{I}=F(\tilde{a}_0,\ldots,\tilde{a}_n)=F(a_0,\ldots,a_n). \tag{3}$$

Note that in the case of $SL(2,\mathbb{R})$ action the invariants appear to be of weight zero due to the condition $\alpha\delta-\beta\gamma=1$.

One way to determine the fundamental invariants is to use the infinitesimal generators of the Lie algebra of the group, by which we mean their counterparts in the parameter space Σ satisfying the same commutator relations as the generators defined in the original space. Thus, a function $F(a_0,\ldots,a_n)$ is an *invariant* if and only if it is annihilated by the generators of the Lie algebra defined in the parameter space Σ. This is a short description of Sophus Lie's *method of the infinitesimal generators*.

Another powerful method, about which we shall not dwell in this article, is Élie Cartan's *method of moving frames*, which has been recently brought back to light.[8,9,23,24,1,2,14,4,28–30]

Arthur Cayley's main contributions to the development of CIT appeared during the period 1854–1878 in his famous "ten memoirs on quantics." Having introduced the notion of an abstract group, he was the first to recognize that the action of a Lie group on a vector space can be investigated by studying its "infinitesimal action," that is the corresponding Lie algebra. In spite of the fact that Cayley thought of this as of something pertinent only to the general linear group and its subgroups, his results in this area may be considered as a precursor to Sophus Lie's theory of abstract Lie groups that was developed later in the 19th century. More specifically, in his "second memoirs on quantics"[3] Arthur Cayley considers (in modern mathematical language) the problem of the determination of the action of the Lie group $SL(2,\mathbb{R})$ on the vector space $\mathcal{Q}^n(\mathbb{R}^2)$ in conjunction with the problem of computing the invariants. The main result is the subject of the following lemma (Cayley,[3] see also Olver[24]).

Lemma 2.1 (Cayley, 1856): *The action of* $SL(2,\mathbb{R})$ *on the vector space* $\mathcal{Q}^n(\mathbb{R}^2)$ *of binary homogeneous polynomials of degree n defined by (1) has the following infinitesimal generators in the corresponding parameter space* Σ:

$$\boldsymbol{V}^{-} = na_1\partial_{a_0} + (n-1)a_2\partial_{a_1} + \cdots + 2a_{n-1}\partial_{a_{n-2}} + a_n\partial_{a_{n-1}},$$

$$\boldsymbol{V}^{0} = -na_0\partial_{a_0} + (2-n)a_1\partial_{a_1} + \cdots + (n-2)a_{n-1}\partial_{a_{n-1}} + na_n\partial_{a_n},$$

$$\boldsymbol{V}^{+} = a_0\partial_{a_1} + 2a_1\partial_{a_2} + \cdots + (n-1)a_{n-2}\partial_{a_{n-1}} + na_{n-1}\partial_{a_n}, \tag{4}$$

where $\partial_{a_i} = \partial/\partial_{a_i}, i = 0, \ldots, n$.

Observe that the vector fields (4) enjoy the following commutator relations:

$$[\boldsymbol{V}^{-}, \boldsymbol{V}^{0}] = -2\boldsymbol{V}^{-}, \quad [\boldsymbol{V}^{+}, \boldsymbol{V}^{0}] = 2\boldsymbol{V}^{+}, \quad [\boldsymbol{V}^{-}, \boldsymbol{V}^{+}] = \boldsymbol{V}^{0}, \tag{5}$$

which confirm that the generators (4) represent the action of $SL(2,\mathbb{R})$ in the parameter space Σ. In view of the above, solving the problem of the determination of the $SL(2,\mathbb{R})$-invariants of $\mathcal{Q}^n(\mathbb{R}^2)$ now amounts to solving the corresponding system of PDEs determined by the generators (4):

$$\boldsymbol{V}^{-}(F) = 0, \quad \boldsymbol{V}^{0}(F) = 0, \quad \boldsymbol{V}^{+}(F) = 0 \tag{6}$$

for a (analytic) function F defined in Σ. The following fundamental theorem on invariants of a regular Lie group aciton (see Olver[24] tells us that the number of fundamental $SL(2,\mathbb{R})$-invariants is $n+1-s$, where $s \leqslant 3$ is the dimension of the orbits (wherever the dimension of the orbits is constant).

Theorem 2.1: *Let G be a Lie group acting regularly on an m-dimensional manifold M with s-dimensional orbits. Then, in a neighborhood N of each point* $x_0 \in M$, *there exist* $m-s$ *functionally independent G-invariants* $\Delta_1, \ldots, \Delta_{m-s}$. *Any other G-invariant* $\mathcal{I}$ *defined near* x_0 *can be locally uniquely expressed as an analytic function of the fundamental invariants through* $\mathcal{I} = F(\Delta_1, \ldots, \Delta_{m-s})$.

Therefore for each particular n the general solution to the system (6) will take the form

$$\mathcal{I} = F(\Delta_1, \ldots, \Delta_{n+1-s}),$$

where $\Delta_i, i = 1, \ldots, n+1-s$ are the fundamental $SL(2,\mathbb{R})$-invariants. To determine s and the subspaces of Σ where the isometry group acts with orbits of the same dimension, one employs the result of the following proposition.[24]

Proposition 2.1: *Let a Lie group G act on X,* *is the corresponding Lie algebra and let* $x \in X$. *The vector space* $S|_x = \mathrm{Span}\{\mathbf{V}_i(x) \,|\, \mathbf{V}_i \in \ \}$ *spanned by all vector fields determined by the infinitesimal generators at x coincides with the tangent space to the orbit* $\mathcal{O}_x$ *of G that passes through x, so* $S|_x = T\mathcal{O}_x|_x$. *In particular, the dimension of* $\mathcal{O}_x$ *equals the dimension of* $S|_x$. *Moreover, the isotropy subgroup* $G_x \subset G$ *has dimension* $\dim G - \dim \mathcal{O}_x = r - s$.

To illustrate the procedure, let us recall a well-known example.[24]

Example 2.1: Consider $\mathcal{Q}^2(\mathbb{R}^2)$-the vector space of quadratic homogeneous polynomials defined over reals. The elements of $\mathcal{Q}^2(\mathbb{R}^2)$ assume

$$Q(x,y) = a_0x^2 + 2a_1xy + a_2y^2 \quad (x,y) \in \mathbb{R}^2. \tag{7}$$

The (local) action of $SL(2,\mathbb{R})$ on the parameter space $\Sigma \simeq \mathbb{R}^3$ generated by a_0, a_1, and a_2 is represented by the vector fields

$$\boldsymbol{V}^{-} = 2a_1\partial_{a_0} + a_2\partial_{a_1},$$

$$\boldsymbol{V}^{0} = 2a_0\partial_{a_0} - 2a_2\partial_{a_2},$$

TABLE I. The settings for the corresponding problems in CIT and ITKT.

Theory	Vector space	Group	Dimension of the space	Dimension of the orbits
CIT	$\mathcal{Q}^n(\mathbb{R}^2)$	$SL(2,\mathbb{R})$	$n+1$	$\leqslant 3$
ITKT	$\mathcal{K}^n(\mathbb{R}^2_1)$	$I(\mathbb{R}^2_1)$	$\frac{1}{2}(n+1)(n+2)$	$\leqslant 3$

$$\boldsymbol{V}^+ = a_0\partial_{a_1} + 2a_1\partial_{a_2}, \tag{8}$$

obtained via the standard technique of exponentiation, which can also be derived from the above lemma. Observe that only two of the vector fields (8) are linearly independent, therefore there is (almost everywhere) $3-2=1$ fundamental invariant. Indeed, solving the system of PDEs (6) yields the solution: $\mathcal{I}=F(\Delta_1)$, where $\Delta_1=a_0a_2-a_1^2$. The group acts with orbits of two types: $a_0=a_1=a_2=0$, an orbit of dimension 0 and the level sets of Δ_1 (i.e., $\Delta_1=0$ and $\Delta_1\neq 0$), both of which are orbits of dimension 2.

Now let us briefly turn our attention to ITKT (for more details see the next section). There the underlying space is a pseudo-Riemannian manifold $(M,\boldsymbol{g})$ of constant curvature. The vector spaces in question are the vector spaces of (generalized) Killing tensors. Our notations are consistent with those introduced in Ref. 16. Thus, $\mathcal{K}_0^n(M)$ denotes the vector space of generalized contravariant Killing tensors of valence n and order zero (or, the standard Killing tensors) defined on $(M,\boldsymbol{g})$. The group acting on $\mathcal{K}_0^n(M)$ is the isometry group $I(M)$ of $(M,\boldsymbol{g})$. Since Cayley's problem concerns binary forms it will be natural to investigate in this respect the Killing tensors of arbitrary valence n defined in pseudo-Riemannian manifolds of dimension two, for example, the Minkowski plane $\mathbb{R}^2_1$. Accordingly, the vector space that we shall study is $\mathcal{K}_0^n(\mathbb{R}^2_1), n\geqslant 1$. A comparison of the two problems is given in Table I. Having made these observations, we are now in the position to formulate an ITKT version of the problem considered by Cayley.[3]

Problem 2.1: Consider the action of $I(\mathbb{R}^2_1)$ *on* $\mathcal{K}_0^n(\mathbb{R}^2_1)$. *Determine a representation of the corresponding Lie algebra* $i(\mathbb{R}^2_1)$ *on the parameter space* Σ of $\mathcal{K}_0^n(\mathbb{R}^2_1)$, $n\geqslant 2$.

In Sec. III we establish the requisite language to be used for solving Problem 2.1 in Sec. IV.

III. INVARIANT THEORY OF KILLING TENSORS

Developed recently as an analog of CIT, the invariant theory of Killing tensors (ITKT) has been first and foremost effectively employed in the study of those integrable and superintegrable Hamiltonian systems[12,16,17,19–21,28] for which the Killing tensors of valence two having normal eigenvectors play a pivotal role. Other applications include classifications of Hamiltonian systems admitting first integrals that are polynomials in the momenta determined by Killing tensors of higher valences.[13,18,29] In what follows, we briefly discuss the main features of the theory.

Let $(M,\boldsymbol{g})$ be an m-dimensional pseudo-Riemannian manifold of constant curvture.

Definition 3.1: A symmetric contravariant tensor $\boldsymbol{K}$ *of valence n defined on* $(M,\boldsymbol{g})$ *is said to be a generalized Killing tensor (GKT) of order p if and only if*

$$[[\ldots[\boldsymbol{K},\boldsymbol{g}],\boldsymbol{g}],\ldots\boldsymbol{g}] = 0 \quad (p+1 \text{ brackets}), \tag{9}$$

where $[,]$ *denotes the Schouten bracket.*

It is easy to see, taking into the account the $\mathbb{R}$-bilinear properties of the Schouten bracket, that GKTs of the same valence and order constitute a *vector space*. We observe next that such a vector space specified by the system of overdetermined PDEs (9) includes the subspace of the standard Killing tensors of valence n defined on $(M,\boldsymbol{g})$ by the system of overdetermined PDEs

$$[\boldsymbol{K},\boldsymbol{g}] = 0. \tag{10}$$

Hence, we conclude that the GKTs of order zero are the standard Killing tensors (KTs). Recall that the concept of a generalized Killing tensor defined on the Minkowski space $\mathbb{R}^m_1$ was introduced by

Nikitin and Prilipko[22] [see also Appendix A of the monograph (Ref. 10)] as generalized symmetries of the Klein-Gordon-Fock equation. In addition, the authors determined the formulas for the dimensions of the vector spaces of GKTs. Alternatively, these tensors have been independently reintroduced in a more general setting by Eastwood[6,7] within the framework of the study of overdetermined systems of PDEs by the methods of representation theory. Thus, it has been demonstrated that the vector space of the solutions of the overdetermined system of PDEs (9) is preserved by the action induced by $SL(m+1,\mathbb{R})$. In this view the author defines such a vector space as an irreducible representation of $\mathfrak{sl}(m+1,\mathbb{R})$ (see also Ref. 15), and then derives the formula for the dimension of the vector space $\mathcal{K}_p^n(M)$ of the generalized Killing tensors of valence n and order p defined on $(M,\boldsymbol{g})$. Thus, the dimension d of the vector space $\mathcal{K}_p^n(M), p\geqslant 0$ is determined by the *Nikitin-Prilipko-Eastwood (NPE) formula* given by

$$d=\dim \mathcal{K}_p^n(M)=\frac{p+1}{m}\binom{n+m-1}{m-1}\binom{p+n+m}{m-1}, \tag{11}$$

where $m=\dim(M,\boldsymbol{g})$. We immediately recognize that for $p=0$ the formula (11) reduces to the *Delong-Takeuchi-Thompson (DTT) formula*.[5,31,32] In this view the elements of $\mathcal{K}_p^n(M)$ are specified by d arbitrary parameters $a_0,\ldots,a_{d-1}$, where d is given by (11).

Example 3.1: Consider the vector space $\mathcal{K}_0^2(\mathbb{R}_1^2)$ of Killing tensors of valence two and order zero defined in Minkowski plane. Solving the Killing tensor equation (10) in the pseudo-Cartesian coordinates (t,x) yields the general formula[17,21]

$$\boldsymbol{K}=\begin{pmatrix} a_0+2a_3x+a_5x^2 & a_1+a_3t+a_4x+a_5tx \\ a_1+a_3t+a_4x+a_5tx & a_2+2a_4t+a_5t^2 \end{pmatrix}. \tag{12}$$

The arbitrary constants of integration $a_0,\ldots,a_5$ represent the dimension of the space $\mathcal{K}_0^2(\mathbb{R}_1^2)$. Formula (12) is an ITKT analog of the general formula (7) in CIT. The three generators of the Lie group $I(\mathbb{R}_1^2)$ acting on $\mathbb{R}_1^2$ are given by (Killing vector fields)

$$\boldsymbol{T}=\partial_t,\quad \boldsymbol{X}=\partial_x,\quad \boldsymbol{H}=x\partial_t+t\partial_x \tag{13}$$

corresponding to translations and hyperbolic rotations, having the commutator relations

$$[\boldsymbol{T},\boldsymbol{X}]=0,\quad [\boldsymbol{T},\boldsymbol{H}]=\boldsymbol{X},\quad [\boldsymbol{X},\boldsymbol{H}]=\boldsymbol{T}. \tag{14}$$

We note that in the case of vector spaces of Killing tensors defined in $\mathbb{R}_1^2$, the generators (13) are not connected via any nontrivial relations. This is also true for any other two-dimensional pseudo-Riemannian manifold of constant curvature. In this view, for a fixed $n\geqslant 1$ the dimension of the corresponding vector space $\mathcal{K}_0^n(\mathbb{R}_1^2)$ can be computed, for example, by employing the well-known formula for the dimension of the space $\mathrm{Sym}^r(M)$ of symmetric $(r,0)$-tensors defined over an m-dimensional manifold:

$$\dim \mathrm{Sym}^r(M)\binom{m+r-1}{r}. \tag{15}$$

Now $m=\dim i(\mathbb{R}_1^2)=3$ and $r=n$. Therefore we have from (15)

$$\dim \mathcal{K}_0^n(\mathbb{R}_1^2)=\tfrac{1}{2}(n+1)(n+2). \tag{16}$$

For spaces of higher dimensions the formula (16) is no longer valid due to the existence of additional nontrivial relations among the generators of the Lie algebra of Killing vectors (i.e., the "syzygy modules problem"[5]). Note the formula (16) agrees with (11). Indeed, (16) is a particular case of (11) corresponding to $p=0,m=2$. Note that for a given vector space $\mathcal{K}_0^n(M), n\geqslant 1$ defined on $(M,\boldsymbol{g})$ the corresponding isometry group $I(M)$ acts as an automorphism: $I(M):\mathcal{K}_0^n(M)\rightarrow\mathcal{K}_0^n(M)$.

This key observation led to the emergence of ITKT.[16] More specifically, the isometry group $I(M)$ acting on M induces the corresponding transformation laws on the parameters $a_0,\ldots,a_{d-1}$ of the vector space $\mathcal{K}_0^n(M)$:

$$\tilde{a}_i = \tilde{a}_i(a_0,\ldots,a_{d-1},g_1,\ldots,g_r), \quad i=0,\ldots,d-1, \tag{17}$$

where $g_1,\ldots,g_r$ are local coordinates on $I(M)$ that parametrize the group, $r=\dim I(M)=\frac{1}{2}m(m+1)$ and d is given by (11). The formulas (17), which we obtain from the standard tensor transformation laws for the elements of the vector space $\mathcal{K}_0^n(M)$ represent the isometry group $I(M)$ action in the vector space.

Clearly, the transformation formulas (17) are analogu of the corresponding transformation formulas in CIT [see, for example, (2)]. It must be mentioned, however, that in the case of ITKT they are computationally more difficult to obtain.

Definition 3.2: A smooth function $\mathcal{I}:\Sigma\to\mathbb{R}$ *defined over the parameter space* Σ *of* $\mathcal{K}_0^n(M)$ *is said to be an* $I(M)$*-invariant of* $\mathcal{K}_0^n(M)$ *if it satisfies the condition*

$$\mathcal{I}=F(a_0,\ldots,a_{d-1})=F(\tilde{a}_0,\ldots,\tilde{a}_{d-1}),$$

under the transformation laws (17).

We remark that in a similar way the ITKT-analogues of the CIT-concepts of a *covariant* and *joint invariant* have been introduced in Ref. 28. In complete analogy with CIT, we can in principle determine the space of $I(M)$-invariants by employing the (Sophus Lie's) method of infinitesimal generators. To do so, one has to determine the (infinitesimal) action of $I(M)$ in the corresponding parameter space Σ.

We note that the procedure originally devised in McLenaghan *et al.*[16] can be effectively employed to derive the generators of the Lie algebra in Σ that is isomorphic to the Lie algebra $i(M)$ of $I(M)$. We briefly review the *MST-procedure* here.

Let $\{\boldsymbol{X}_1,\ldots,\boldsymbol{X}_r\}$ be the generators of the Lie algebra $i(M)$ (Killing vector fields) of the Lie group $I(M)$. Consider Diff Σ, that is the group of all diffeomorphisms on Σ, defining the corresponding space Diff $\mathcal{K}_0^n(M)$, whose elements are determined by the elements of Diff Σ in an obvious way.

Let $\boldsymbol{K}^0\in$ Diff $\mathcal{K}_0^n(M)$. Note $\boldsymbol{K}^0$ is determined by d parameters

$$a_i^0=a_i^0(a_0,\ldots,a_{d-1}), \quad i=0,\ldots,d-1$$

which are functions of $a_0,\ldots,a_{d-1}$. Define now a map π: Diff $\mathcal{K}_0^n(M)\to\mathcal{X}(\Sigma)$ given by

$$\boldsymbol{K}^0\to\sum_{i=0}^{d-1}a_i^0(a_0,\ldots,a_{d-1})\partial_{a_i}. \tag{18}$$

To specify the action of $I(M)$ in Σ, we have to find the counterparts of the generators $\boldsymbol{X}_1,\ldots,\boldsymbol{X}_r$ in $\mathcal{X}(\Sigma)$. Consider the composition $\pi\circ\mathcal{L}$, where $\mathcal{L}$ is the Lie derivative operator. Let $\boldsymbol{K}$ be the general Killing tensor of $\mathcal{K}_0^n(M)$ [see, for example, (12)]. Next define

$$\boldsymbol{V}_i=\pi\circ\mathcal{L}_{\boldsymbol{X}_i}\boldsymbol{K}, \quad i=1,\ldots r. \tag{19}$$

The composition map

$$\pi\circ\mathcal{L}:i(M)\to\mathcal{X}(\Sigma)$$

maps the generators $\boldsymbol{X}_1,\ldots,\boldsymbol{X}_r$ to $\mathcal{X}(\Sigma)$. Finally, we check that the vector fields $\boldsymbol{V}_i, i=1,\ldots,r$ satisfy the same commutator relations as the original $\boldsymbol{X}_i, i=1,\ldots,r$. This can be checked on a case by case basis. We remark that this step is actually redundant, since it has been proven[15] in general that Killing tensors can be expressed as irreducible representations of $GL(n,\mathbb{R})$ so that the vector fields (19) satisfy the same commutator relations as the original generators of $i(M)$. Thus, the Lie algebra generated by (19) is isomorphic to the Lie algebra $i(M)$ of the isometry group $I(M)$ and we

can use (19) to solve the problem of the determination of the $I(M)$-invariants of $\mathcal{K}_0^n(M)$ by solving the corresponding system of PDEs:

$$\boldsymbol{V}_i(F) = 0, \quad i = 1, \ldots, r. \tag{20}$$

The MST-procedure stated above is based on *Lie derivative deformations* of tensors (see, for example, Ref. 27, which is an analog of the standard technique of exponentiation used in CIT to determine corresponding infinitesimal gernerators. We also note that the generators (19) can be alternatively determined from the parameter transformation laws (17), representing the group action in Σ, when the latter are available. It is, however, increasingly difficult, and often impossible to determine (19) using (17) for vector spaces of Killing tensors of higher valence or defined in pseudo-Riemannian manifolds of higher dimensions.

To illustrate the effectiveness of the MST procedure, let us consider the following example.[17,21,28]

Example 3.2: Consider again $\mathcal{K}_0^2(\mathbb{R}_1^2)$, using (12), (13), (18), and (19) we arrive at the corresponding generators:

$$\boldsymbol{V}_1 = a_3\partial_{a_1} + 2a_4\partial_{a_2} + a_5\partial_{a_4},$$

$$\boldsymbol{V}_2 = a_4\partial_{a_1} + 2a_3\partial_{a_0} + a_5\partial_{a_3}, \tag{21}$$

$$\boldsymbol{V}_3 = -2a_1\partial_{a_0} - a_4\partial_{a_3} - (a_0 + a_2)\partial_{a_1} - 2a_1\partial_{a_2} - a_3\partial_{a_4}.$$

It is easy to check that the Lie algebra generated by (21) is isomorphic to the Lie algebra $i(\mathbb{R}_1^2) = \mathcal{K}_0^1(\mathbb{R}_1^2)$ generated by (13). We conclude therefore that the vector fields (21) represent the infinitesimal action of $I(\mathbb{R}_1^2)$ in Σ. Our next observation is that the orbits of the $I(\mathbb{R}_1^2)$-action have dimension three wherever the vector fields (21) are linearly independent. Therefore in that subspace of Σ we expect to derive $6-3=3$ fundamental $I(\mathbb{R}_1^2)$-invariants.

Using the method of characteristics to solve the system (20) defined by the vector fields (21), we arrive at the following result:

Theorem 3.1: *Any algebraic $I(\mathbb{R}_1^2)$-invariant $\mathcal{I}$ of the subspace of the parameter space Σ of $\mathcal{K}_0^2(\mathbb{R}_1^2)$ defined by the condition that the vector fields (21) are linearly independent can be (locally) uniquely expressed as an analytic function*

$$\mathcal{I} = F(\Delta_1, \Delta_2, \Delta_3), \tag{22}$$

where the fundamental invariants $\Delta_i, i = 1, 2, 3$ are given by

$$\Delta_1 = a_5,$$

$$\Delta_2 = (a_0 - a_2)a_5 - a_3^2 + a_4^2,$$

$$\Delta_3 = (a_3^2 + a_4^2 - a_5(a_0 + a_2))^2 - 4(a_5a_1 - a_3a_4)^2. \tag{23}$$

The fundamental $I(\mathbb{R}_1^2)$-invariant Δ_3 presented above was first derived in Ref. 17 and 21 and used to generate *discrete-$I(\mathbb{R}_1^2)$*-invariants, which were in turn employed to classify orthogonal coordinate webs in the Minkowski plane $\mathbb{R}_1^2$. The same problem was solved in Ref. 28 by employing the $I(\mathbb{R}_1^2)$-invariants and covariants of $\mathcal{K}_0^2(\mathbb{R}_1^2)$.

IV. AN ITKT ANALOG OF CAYLEY'S LEMMA

In this section we solve Problem 2.1 presented in Sec. II. The vector space $\mathcal{K}_0^n(\mathbb{R}_1^2)$ appears to be a natural counterpart of the vector space $\mathcal{Q}^n(\mathbb{R}^2)$ in CIT. To proceed, we need to first derive a

general formula for the elements of $\mathcal{K}_0^n(\mathbb{R}_1^2)$ [i.e., an analog of (1)]. Note each $\boldsymbol{K}\in\mathcal{K}_0^n(\mathbb{R}_1^2)$ is determined by the $(n+1)(n+2)/2$ parameters that appear in the $n+1$ components of the form

$$K^{i_1\cdots i_p j_1\cdots j_{n-p}}, \tag{24}$$

where $i_1=\cdots=i_p=1, j_1=\cdots=j_{n-p}=2, p=0,\ldots,n$.

To derive the formulas for the components (24), we solve the Killing tensor equation (10) in pseudo-Cartesian coordinates (t,x), which reduces to the following system of PDEs:

$$\partial_t K^{i_1\cdots i_n}=0, \quad \partial_x K^{j_1\cdots j_n}=0,$$

$$(n-p+1)\partial_x K^{i_1\cdots i_p j_1\cdots j_{n-p}} = p\partial_t K^{i_1\cdots i_{p-1} j_1\cdots j_{n-p+1}}, \tag{25}$$

where $p=0,\ldots,n$. As a consequence of (25), we readily obtain the necessary differential conditions:

$$\begin{aligned} \partial_x^{p+1} K^{i_1\cdots i_p j_1\cdots j_{n-p}}&=0,\\ \partial_t^{n-p+1} K^{i_1\cdots i_p j_1\cdots j_{n-p}}&=0. \end{aligned} \tag{26}$$

Solving the PDEs (25) and (26) we arrive at the following general formulas for the components (the parameters in the formulas are constants of integration):

$$K^{i_1\cdots i_p j_1\cdots j_{n-p}} = \begin{cases} \displaystyle\sum_{i=0}^{n-p}\left[\binom{n-p}{i} t^i \sum_{j=0}^{p}\binom{p}{j} a_{pij}x^j\right] & \text{if } n\geqslant p\geqslant\left[\dfrac{n+1}{2}\right] \\ \displaystyle\sum_{i=0}^{p}\left[\binom{p}{i} x^i \sum_{j=0}^{n-p}\binom{n-p}{j} b_{pij}t^j\right] & \text{if } 0\leqslant p\leqslant\left[\dfrac{n+1}{2}\right] \end{cases}, \tag{27}$$

where the parameters a_{pij}, b_{pij} are to be determined (at this stage they are inserted for mere convenience). We immediately recognize that the formula (27) is the ITKT analog of the general formula (1) exhibited in Sec. II. The parameters a_{pij}, b_{pij} can be determined by following the general procedure of solving the system of PDEs (25). We consider separately two cases: n is even and n is odd.

The parameters of each of the $n+1$ components can be organized into groups in such a way that the parameters of one group are completely determined by the parameters of the other (see the illustrative examples to follow). After relabeling the parameters, we obtain the following two schemes (corresponding to $n=2k$ and $n=2k+1$, respectively), which specify the arrangements of the parameters of the first groups of the components. Once they are specified, the parameters of the other groups can be determined accordingly.

Case 1: $n=2k$

$$\begin{array}{lcccccc} \text{Step } 1: & a_0^1 & a_1^1 & \cdots & a_{n-2}^1 & a_{n-1}^1 & a_n^1, \\ & b_0^1 & b_1^1 & \cdots & b_{n-2}^1 & b_{n-1}^1 & a_n^1; \\ \text{Step } 2: & a_0^2 & a_1^2 & \cdots & a_{n-3}^2 & a_{n-2}^2 & b_{n-1}^1, \\ & b_0^2 & b_1^2 & \cdots & b_{n-3}^2 & a_{n-2}^2 & a_{n-1}^1; \\ & & & \vdots & & & \\ \text{Step } \dfrac{n}{2}: & a_0^{n/2} & a_1^{n/2} & a_2^{n/2} & b_1^{(n-2)/2} & \cdots & b_{(n+2)/2}^1, \\ & b_0^{n/2} & b_1^{n/2} & a_2^{n/2} & a_1^{(n-2)/2} & \cdots & a_{(n+2)/2}^1; \\ \text{Step } (n+2)/2: & a_0^{(n+2)/2} & b_1^{n/2} & b_2^{(n-2)/2} & b_3^{(n-4)/2} & \cdots & b_{n/2}^1. \end{array} \tag{28}$$

Case 2: $n=2k+1$

$$
\begin{array}{lcccccc}
\text{Step } 1: & a_0^1 & a_1^1 & \cdots & a_{n-2}^1 & a_{n-1}^1 & a_n^1, \\
 & b_0^1 & b_1^1 & \cdots & b_{n-2}^1 & b_{n-1}^1 & a_n^1; \\
\text{Step } 2: & a_0^2 & a_1^2 & \cdots & a_{n-3}^2 & a_{n-2}^2 & b_{n-1}^1, \\
 & b_0^2 & b_1^2 & \cdots & b_{n-3}^2 & a_{n-2}^2 & a_{n-1}^1. \\
 & & & \vdots & & & \\
\text{Step } (n-1)/2: & a_0^{(n-1)/2} & a_1^{(n-1)/2} & a_2^{(n-1)/2} & a_3^{(n-1)/2} & \cdots & b_{(n+3)/2}^1, \\
 & b_0^{(n-1)/2} & b_1^{(n-1)/2} & b_2^{(n-1)/2} & a_3^{(n-1)/2} & \cdots & a_{(n+3)/2}^1; \\
\text{Step } (n+1)/2: & a_0^{(n+1)/2} & a_1^{(n+1)/2} & b_2^{(n-1)/2} & b_3^{(n-3)/2} & \cdots & b_{(n+1)/2}^1, \\
 & b_0^{(n+1)/2} & a_1^{(n+1)/2} & a_2^{(n-1)/2} & a_3^{(n-3)/2} & \cdots & a_{(n+1)/2}^1.
\end{array}
\tag{29}
$$

The parameters that appear in the general solution to (27) are now organized in two schemes according the cases of n being even (28) and odd (29) respectively.

More specifically, given $2(n+1)-1$ parameters

$$
a_0^1,\ldots,a_{n-1}^1,a_n^1, \quad b_0^1,\ldots,b_{n-1}^1,a_n^1
$$

we write down the first and the last components of $\boldsymbol{K}\in\mathcal{K}^n(\mathbb{R}_1^2)$:

$$
K^{11\cdots11}=\left[a_0^1+\binom{n}{1}a_1^1x+\binom{n}{2}a_2^1x^2+\cdots+\binom{n}{n-1}a_{n-1}^1x^{n-1}+a_n^1x^n\right],
$$

$$
K^{22\cdots22}=\left[b_0^1+\binom{n}{1}b_1^1t+\binom{n}{2}b_2^1t^2+\cdots+\binom{n}{n-1}b_{n-1}^1t^{n-1}+a_n^1t^n\right].
$$

Next, for $2(n-1)-1$ new parameters

$$
a_0^2,\ldots,a_{n-3}^2,a_{n-2}^2;b_0^2,\ldots,b_{n-3}^2,a_{n-2}^2
$$

we then have the second and penultimate components of $\boldsymbol{K}$ [see (27)], each of which is the sum of two polynomials, the first having been determined by the newly specified parameters and the other by the parameters determined previously,

$$
\begin{aligned}
K^{11\cdots12}=&\left[a_0^2+\binom{n-1}{1}a_1^2x+\cdots+\binom{n-1}{n-2}a_{n-2}^2x^{n-2}+b_{n-1}^1x^{n-1}\right]\\
&+t\left[a_1^1+\binom{n-1}{1}a_2^1x+\cdots+\binom{n-1}{n-2}a_{n-1}^1x^{n-2}+a_n^1x^{n-1}\right],
\end{aligned}
$$

$$
\begin{aligned}
K^{22\cdots21}=&\left[b_0^2+\binom{n-1}{1}b_1^2t+\cdots+\binom{n-1}{n-2}a_{n-2}^2t^{n-2}+a_{n-1}^1t^{n-1}\right]\\
&+x\left[b_1^1+\binom{n-1}{1}b_2^1t+\cdots+\binom{n-1}{n-2}b_{n-1}^1t^{n-2}+a_n^1t^{n-1}\right].
\end{aligned}
$$

To clarify the process more, let us consider the next step (if any). Thus, given $2(n-3)-1$ new parameters

$$
a_0^3,\ldots,a_{n-5}^3,a_{n-4}^3;b_0^3,\ldots,b_{n-5}^3,a_{n-4}^3
$$

we write down the next two components:

$$K^{11\cdots122}=\left[a_0^3+\binom{n-2}{1}a_1^3x+\cdots+\binom{n-2}{n-4}a_{n-4}^3x^{n-4}+\binom{n-2}{n-3}b_{n-3}^2x^{n-3}+b_{n-2}^1x^{n-2}\right]$$
$$+2t\left[a_1^2+\binom{n-2}{1}a_2^2x+\cdots+\binom{n-2}{n-4}a_{n-3}^2x^{n-4}+\binom{n-2}{n-3}a_{n-2}^2x^{n-3}+b_{n-1}^1x^{n-2}\right]$$
$$+t^2\left[a_2^1+\binom{n-2}{1}a_3^1x+\cdots+\binom{n-2}{n-4}a_{n-2}^1x^{n-4}+\binom{n-2}{n-3}a_{n-1}^1x^{n-3}+a_n^1x^{n-2}\right],$$

$$K^{22\cdots211}=\left[b_0^3+\binom{n-2}{1}b_1^3t+\cdots+\binom{n-2}{n-4}a_{n-4}^3t^{n-4}+\binom{n-2}{n-3}a_{n-3}^2t^{n-3}+a_{n-2}^1t^{n-2}\right]$$
$$+2x\left[b_1^2+\binom{n-2}{1}b_2^2t+\cdots+\binom{n-2}{n-4}b_{n-3}^2t^{n-4}+\binom{n-2}{n-3}a_{n-2}^2t^{n-3}+a_{n-1}^1t^{n-2}\right]$$
$$+x^2\left[b_2^1+\binom{n-2}{1}b_3^1t+\cdots+\binom{n-2}{n-4}b_{n-2}^1t^{n-4}+\binom{n-2}{n-3}b_{n-1}^1t^{n-3}+a_n^1t^{n-2}\right].$$

We continue this process in both directions (i.e., going "downwards" and "upwards") until it is terminated in the middle of (27). In this view, counting the steps in both cases, it is easy to see that the dimension of the space $d=\dim \mathcal{K}_0^n(\mathbb{R}_1^2)=\frac{1}{2}(n+1)(n+2), n\geqslant 1$ gets decomposed as follows.

$$d=\begin{cases}[2(n+1)-1]+[2(n-1)-1]+\cdots+[2\times 1-1] & \text{if } n \text{ is even}\\ [2(n+1)-1]+[2(n-1)-1]+\cdots+[2\times 2-1] & \text{if } n \text{ is odd}\end{cases}. \tag{30}$$

The auxiliary problem of finding the general form for the elements $\boldsymbol{K}\in\mathcal{K}_0^n(\mathbb{R}_1^2)$ is therefore completely solved.

We immediately notice that the general solution (12) can be relabeled following the scheme (28) as follows:

$$\mathbf{K}=\begin{pmatrix}a_0^1+2a_1^1x+a_2^1x^2 & (a_0^2+b_1^1x)+t(a_1^1+a_2^1x)\\ (a_0^2+b_1^1x)+t(a_1^1+a_2^1x) & b_0^1+2b_1^1t+a_2^1t^2\end{pmatrix}. \tag{31}$$

To illustrate our results, consider more examples.

Example 4.1: $\mathcal{K}_0^4(\mathbb{R}_1^2)$. Note $d=\dim \mathcal{K}_0^4(\mathbb{R}_1^2)=15$. Following the formula (27) and the coefficient scheme (29),

$$K^{1111}=a_0^1+4a_1^1x+6a_2^1x^2+4a_3^1x^3+a_4^1x^4,$$

$$K^{1112}=(a_0^2+3a_1^2x+3a_2^2x^2+b_3^1x^3)+t(a_1^1+3a_2^1x+3a_3^1x^2+a_4^1x^3),$$

$$K^{1122}=(a_0^3+2b_1^2x+b_2^1x^2)+2t(a_1^2+2a_2^2x+b_3^1x^2)+t^2(a_2^1+2a_3^1x+a_4^1x^2), \tag{32}$$

$$K^{1222}=(b_0^2+3b_1^2t+3a_2^2t^2+a_3^1t^3)+x(b_1^1+3b_2^1t+3b_3^1t^2+a_4^1t^3),$$

$$K^{2222}=b_0^1+4b_1^1t+6b_2^1t^2+4b_3^1t^3+a_4^1t^4.$$

Example 4.2: $\mathcal{K}^5(\mathbb{R}_1^2)$. $d=\dim \mathcal{K}_0^5(\mathbb{R}_1^2)=21$.

$$K^{11111}=a_0^1+5a_1^1x+10a_2^1x^2+10a_3^1x^3+5a_4^1x^4+a_5^1x^5,$$

$$K^{11112}=(a_0^2+4a_1^2x+6a_2^2x^2+4a_3^2x^3+b_4^1x^4)+t(a_1^1+4a_2^1x+6a_3^1x^2+4a_4^1x^3+a_5^1x^4),$$

$$K^{11122} = (a_0^3 + 3a_1^3 x + 3b_2^2 x^2 + b_3^1 x^3) + 2t(a_1^2 + 3a_2^2 x + 3a_3^2 x^2 + b_4^1 x^3) + t^2(a_2^1 + 3a_3^1 x + 3a_4^1 x^2 + a_5^1 x^3),$$

$$K^{11222} = (b_0^3 + 3a_1^3 t + 3a_2^2 t^2 + a_3^1 t^3) + 2x(b_1^2 + 3b_2^2 t + 3a_3^2 t^2 + a_4^1 x^3) + x^2(b_2^1 + 3b_3^1 t + 3b_4^1 t^2 + a_5^1 t^3),$$

$$K^{12222} = (b_0^2 + 4b_1^2 t + 6b_2^2 t^2 + 4a_3^2 t^3 + a_4^1 t^4) + x(b_1^1 + 4b_2^1 t + 6b_3^1 t^2 + 4b_4^1 t^3 + a_5^1 t^4),$$
$$K^{22222} = b_0^1 + 5b_1^1 t + 10b_2^1 t^2 + 10b_3^1 t^3 + 5b_4^1 t^4 + a_5^1 t^5. \tag{33}$$

In principle, following the parameter scheme given above, i.e., using formulas (27)–(29), one can now write down explicitly the general form of the elements of $\mathcal{K}_0^n(\mathbb{R}_1^2)$ for an arbitrary n easily.

To solve Problem 2.1, we employ the MST-procedure[16] outlined in the previous section.

Using the formulas (19) and (27)–(29), we obtain the general formulas for the vector fields representing the infinitesimal action of the isometry group $I(\mathbb{R}_1^2)$ on the parameter space. As above, we have two cases corresponding to (28) and (29), respectively.

Case 1: $n=2k$

$$\begin{aligned}
\boldsymbol{V}_1 = \;& a_1^1\partial_{a_0^2} + a_2^1\partial_{a_1^2} + \cdots + a_{n-1}^1\partial_{a_{n-2}^2} \\
& + 2a_1^2\partial_{a_0^3} + 2a_2^2\partial_{a_1^3} + \cdots + 2a_{n-3}^2\partial_{a_{n-4}^3} \\
& \vdots \\
& + \frac{n}{2}a_1^{\frac{n}{2}}\partial_{a_0^{(n+2)/2}} \\
& + \frac{n+2}{2}b_1^{n/2}\partial_{b_0^{n/2}} + \frac{n}{2}a_2^{n/2}\partial_{b_1^{n/2}} \\
& \vdots \\
& + (n-1)b_1^2\partial_{b_0^2} + (n-2)b_2^2\partial_{b_1^2} + \cdots 2b_{n-2}^2\partial_{bn-3}^2 \\
& + nb_1^1\partial_{b_0^1} + (n-1)b_2^1\partial_{b_1^1} + \cdots + a_n^1\partial_{b_{n-1}^1};
\end{aligned} \tag{34}$$

$$\begin{aligned}
\boldsymbol{V}_2 = \;& b_1^1\partial_{b_0^2} + b_2^1\partial_{b_1^2} + \cdots + b_{n-1}^1\partial_{a_{n-2}^2} \\
& + 2b_1^2\partial_{b_0^3} + 2b_2^2\partial_{b_1^3} + \cdots + 2b_{n-3}^2\partial_{a_{n-4}^3} \\
& \vdots \\
& + \frac{n}{2}b_1^{\frac{n}{2}}\partial_{a_0^{(n+2)/2}} \\
& + \frac{n+2}{2}a_1^{n/2}\partial_{a_0^{n/2}} + \frac{n}{2}a_2^{n/2}\partial_{a_1^{n/2}} \\
& \vdots \\
& + (n-1)a_1^2\partial_{a_0^2} + (n-2)A_2^2\partial_{a_1^2} + \cdots + 2a_{n-2}^2\partial_{an-3}^2 \\
& + na_1^1\partial_{a_0^1} + (n-1)a_2^1\partial_{a_1^1} + \cdots + a_n^1\partial_{a_{n-1}^1};
\end{aligned} \tag{35}$$

$\boldsymbol{V}_3=$

$$
\begin{aligned}
&-na_0^2\partial_{a_0^1}-(n-1)a_1^2\partial_{a_1^1}-\cdots-2a_{n-2}^2\partial_{a_{n-2}^1}-b_{n-1}^1\partial_{a_{n-1}^1}\\
&-[(n-1)a_0^3+a_0^1]\partial_{a_0^2}-\cdots-[2b_{n-3}^2+a_{n-3}^1]\partial_{a_{n-3}^2}\\
&\vdots\\
&-\frac{n}{2}[a_0^{\frac{n}{2}}+b_0^{\frac{n}{2}}]\partial_{a_o^{(n+2)/2}}-\cdots-[a_{n-2}^1+b_{n-2}^1]\partial_{a_{n-2}^2}\\
&\vdots\\
&-[(n-1)b_0^3+b_0^1]\partial_{b_0^2}-\cdots-[2a_{n-3}^2+b_{n-3}^1]\partial_{b_{n-3}^2}\\
&-nb_0^2\partial_{b_0^1}-(n-1)b_1^2\partial_{b_1^1}-\cdots-2a_{n-2}^2\partial_{b_{n-2}^1}-a_{n-1}^1\partial_{b_{n-1}^1}.
\end{aligned}
\tag{36}
$$

Case 2: $n=2k+1$

$\boldsymbol{V}_1=$

$$
\begin{aligned}
&a_1^1\partial_{a_0^2}+a_2^1\partial_{a_1^2}+\cdots+a_{n-1}^1\partial_{a_{n-2}^2}\\
&+2a_1^2\partial_{a_0^3}+2a_2^2\partial_{a_1^3}+\cdots+2a_{n-3}^2\partial_{a_{n-4}^3}\\
&\vdots\\
&+\frac{n+1}{2}a_1^{(n+1)/2}\partial_{b_0^{(n+1)/2}}\\
&+\frac{n+3}{2}b_1^{(n-1)/2}\partial_{b_0^{(n-1)/2}}+\frac{n+1}{2}b_1^{(n-1)/2}\partial_{b_1^{(n-1)/2}}+\frac{n-1}{2}a_3^{(n-1)/2}\partial_{b_2^{(n-1)/2}}\\
&\vdots\\
&+(n-1)b_1^2\partial_{b_0^2}+(n-2)b_2^2\partial_{b_1^2}+\cdots 2a_{n-2}^2\partial_{b_{n-3}^2}\\
&+nb_1^1\partial_{b_0^1}+(n-1)b_2^1\partial_{b_1^1}+\cdots+2b_{n-1}^1\partial_{b_{n-2}^1}+a_n^1\partial_{b_{n-1}^1};
\end{aligned}
\tag{37}
$$

$\boldsymbol{V}_2=$

$$
\begin{aligned}
&b_1^1\partial_{b_0^2}+b_2^1\partial_{b_1^2}+\cdots+b_{n-1}^1\partial_{a_{n-2}^2}\\
&+2b_1^2\partial_{b_0^3}+2b^2\partial_{b_1^3}+\cdots+2b_{n-3}^2\partial_{a_{n-4}^3}\\
&\vdots\\
&+\frac{n+1}{2}a_1^{(n+1)/2}\partial_{a_0^{(n+1)/2}}\\
&+\frac{n+3}{2}a_1^{(n-1)/2}\partial_{a_0^{(n-1)/2}}+\frac{n+1}{2}a_2^{(n+1)/2}\partial_{b_1^{(n-1)/2}}+\frac{n-1}{2}a_3^{(n-1)/2}\partial_{a_2^{(n-1)/2}}\\
&\vdots\\
&+(n-1)a_1^2\partial_{a_0^2}+(n-2)a_2^2\partial_{a_1^2}+\cdots+2a_{n-2}^2\partial_{a_{n-3}^2}\\
&+na_1^1\partial_{a_0^1}+(n-1)a_2^1\partial_{a_1^1}+\cdots+2a_{n-1}^1\partial_{a_{n-2}^1}+a_n^1\partial_{a_{n-1}^1};
\end{aligned}
\tag{38}
$$

$$
\begin{aligned}
\boldsymbol{V}_3 = & \\
& -na_0^2\partial_{a_0^1} - (n-1)a_1^2\partial_{a_1^1} - \cdots 2a_{n-2}^2\partial_{a_{n-2}^1} - b_{n-1}^1\partial_{a_{n-1}^1} \\
& -[(n-1)a_0^3 + a_0^1]\partial_{a_0^2} - \cdots - [2b_{n-3}^2 + a_{n-3}^1]\partial_{a_{n-3}^2} \\
& \vdots \\
& -\left[\frac{n+1}{2}b_0^{\frac{n+1}{2}} + \frac{n-1}{2}a_0^{\frac{n-1}{2}}\right]\partial_{a_0^{(n+1)/2}} \\
& -\frac{n-1}{2}\left[a_1^{\frac{n-1}{2}} + b_1^{\frac{n-1}{2}}\right]\partial_{a_1^{\frac{n+1}{2}}} - \cdots - [a_{n-2}^1 + b_{n-2}^1]\partial_{a_{n-2}^2} \\
& -\left[\frac{n+1}{2}a_0^{\frac{n+1}{2}} + \frac{n-1}{2}b_0^{\frac{n-1}{2}}\right]\partial_{b_0^{\frac{(n+1)}{2}}} \\
& \vdots \\
& -[(n-1)b_0^3 + b_0^1]\partial_{b_0^2} - \cdots - [2a_{n-3}^2 + b_{n-3}^1]\partial_{b_{n-3}^2} \\
& -nb_0^2\partial_{b_0^1} - (n-1)b_1^2\partial_{b_1^1} - \cdots - 2a_{n-2}^2\partial_{b_{n-2}^1} - a_{n-1}^1\partial_{b_{n-1}^1}.
\end{aligned}
\tag{39}
$$

We remark that in both cases the vector fields $\boldsymbol{V}_1, \boldsymbol{V}_2$, and $\boldsymbol{V}_3$ correspond to the generators $\boldsymbol{T}, \boldsymbol{X}$, and $\boldsymbol{H}$ given by (13), respectively. Moreover, it is easy to verify directly that the vector fields $-\boldsymbol{V}_1, -\boldsymbol{V}_2$, and $-\boldsymbol{V}_3$ satisfy the same commutator relations (14) as $\boldsymbol{T}, \boldsymbol{X}$, and $\boldsymbol{H}$. We conclude therefore that $\boldsymbol{V}_i, i=1, 2, 3$ represent the infinitesimal action of the isometry group $I(\mathbb{R}_1^2)$ on the parameter space Σ defined by $\mathcal{K}_0^n(\mathbb{R}_1^2)$ for each $n \geqslant 1$ and we have proven an ITKT analog of Lemma 2.1 of Cayley:[3]

Theorem 4.1: *The action of the isometry group $I(\mathbb{R}_1^2)$ on the vector space $\mathcal{K}_0^n(\mathbb{R}_1^2)$ has the infinitesimal generators (34)–(36) when n is even and (37)–(39) when n is odd.*

Example 4.3: $\mathcal{K}_0^4(\mathbb{R}_1^2)$. Using Theorem 4.1,

$$
\boldsymbol{V}_1 = a_1^1\partial_{a_0^2} + a_2^1\partial_{a_1^2} + a_3^1\partial_{a_2^2} + 2a_1^2\partial_{a_0^3} + 3b_1^2\partial_{b_0^2} + 2a_2^2\partial_{b_1^2} + 4b_1^1\partial_{b_0^1} + 3b_2^1\partial_{b_1^1} + 2b_3^1\partial_{b_2^1} + a_4^1\partial_{b_3^1},
\tag{40}
$$

$$
\boldsymbol{V}_2 = b_1^1\partial_{b_0^2} + b_2^1\partial_{b_1^2} + b_3^1\partial_{a_2^2} + 2b_1^2\partial_{a_0^3} + 3a_1^2\partial_{a_0^2} + 2a_2^2\partial_{a_1^2} + 4a_1^1\partial_{b_0^1} + 3a_2^1\partial_{b_1^1} + 2a_3^1\partial_{b_2^1} + a_4^1\partial_{a_3^1},
\tag{41}
$$

$$
\begin{aligned}
\boldsymbol{V}_3 = & -4a_0^2\partial_{a_0^1} - 3a_1^2\partial_{a_1^1} - 2a_2^2\partial_{a_2^1} - b_3^1\partial_{a_3^1} - (3a_0^3 + a_0^1)\partial_{a_0^2} - (2b_1^2 + a_1^1)\partial_{a_1^2} - 2(a_0^2 + b_0^2)\partial_{a_0^3} - (a_2^1 + b_2^1)\partial_{a_2^2} \\
& -(3a_0^3 + b_0^1)\partial_{b_0^2} - (2a_1^2 + b_1^1)\partial_{b_1^2} - 4b_0^2\partial_{b_0^1} - 3b_1^2\partial_{b_1^1} - 2a_2^2\partial_{b_2^1} - a_3^1\partial_{b_3^1}.
\end{aligned}
\tag{42}
$$

Example 4.4: $\mathcal{K}_0^5(\mathbb{R}_1^2)$. Using again Theorem 4.1,

$$
\begin{aligned}
\boldsymbol{V}_1 = & a_1^1\partial_{a_0^2} + a_2^1\partial_{a_1^2} + a_3^1\partial_{a_2^2} + a_4^1\partial_{a_3^2} + 2a_1^2\partial_{a_0^3} + 2a_2^2\partial_{a_1^3} + 3a_1^3\partial_{b_0^3} + 4b_1^2\partial_{b_0^2} + 3b_2^2\partial_{b_1^2} + 2a_3^2\partial_{b_2^2} + 5b_1^1\partial_{b_0^1} \\
& + 4b_2^1\partial_{b_1^1} + 3b_3^1\partial_{b_2^1} + 2b_4^1\partial_{b_3^1} + a_5^1\partial_{b_4^1},
\end{aligned}
\tag{43}
$$

$$
\begin{aligned}
\boldsymbol{V}_2 = & b_1^1\partial_{b_0^2} + b_2^1\partial_{b_1^2} + b_3^1\partial_{b_2^2} + b_4^1\partial_{a_3^2} + 2b_1^2\partial_{b_0^3} + 2a_2^2\partial_{a_1^3} + 3a_1^3\partial_{a_0^3} + 4a_1^2\partial_{a_0^2} + 3a_2^2\partial_{a_1^2} + 2a_3^2\partial_{a_2^2} + 5a_1^1\partial_{a_0^1} \\
& + 4a_2^1\partial_{a_1^1} + 3a_3^1\partial_{a_2^1} + 2a_4^1\partial_{a_3^1} + a_5^1\partial_{a_4^1},
\end{aligned}
\tag{44}
$$

$$\begin{aligned}\boldsymbol{V}_3 = &-5a_0^2\partial_{a_0^1} - 4a_1^2\partial_{a_1^1} - 3a_2^2\partial_{a_2^1} - 2a_3^2\partial_{a_3^1} - b_4^1\partial_{a_4^1} - (4a_0^3 + a_0^1)\partial_{a_0^2} - (3a_1^3 + a_1^1)\partial_{a_1^2} - (2b_2^2 + a_2^1)\partial_{a_2^2} \\ &- (3b_0^3 + 2a_0^2)\partial_{a_0^3} - 2(b_1^2 + a_1^2)\partial_{a_1^3} - (a_3^1 + b_3^1)\partial_{a_3^2} - (3a_0^3 + 2b_0^2)\partial_{b_0^3} - (4b_0^3 + b_0^1)\partial_{b_0^2} - (3a_1^3 + b_1^1)\partial_{b_1^2} \\ &- (2a_2^2 + b_2^1)\partial_{b_2^2} - 5b_0^2\partial_{b_0^1} - 4b_1^2\partial_{b_1^1} - 3b_2^2\partial_{b_2^1} - 2a_3^2\partial_{b_3^1} - a_4^1\partial_{b_4^1}. \end{aligned} \tag{45}$$

Using the result of Theorem 4.1 one can compute the $I(\mathbb{R}_1^2)$-invariants:

Theorem 4.2: *Any function* $I:\Sigma\to\mathbb{R}$ *is an* $I(\mathbb{R}_1^2)$*-invariant of* $\mathcal{K}_0^n(\mathbb{R}_1^2)$ *if and only if it satisfies the infinitesimal invariance criteria*

$$\boldsymbol{V}_i(I) = 0, \quad i = 1,2,3, \tag{46}$$

where Σ *is the parameter space and* $\boldsymbol{V}_i, i=1, 2, 3$ *are given in Theorem 4.1.*

Corollary 4.1: *The parameter* a_n^1 *[refer to the formulas* (28) and (29) *when n is even and odd, respectively] is a fundamental* $I(\mathbb{R}_1^2)$*-invariant of* $\mathcal{K}_0^n(\mathbb{R}_1^2)$.

In view of Theorem 4.2 the problem of the determination of the space of $I(\mathbb{R}_1^2)$-invariants reduces to solving the system of linear PDEs resulting from the vector fields in Theorem 4.1. For larger values of n the problem becomes very challenging computationally. The method of characteristics may fail, in which case one can employ the method of undetermined coefficients in conjuncture with the result of the fundameatal theorem on invariants of a regular Lie group action (Theorem 2.1), as well as computer algebra. This technique was used with a remarkable success in Horwood *et al.*[12] to solve the problem of the determination of the space of $I(\mathbb{R}^3)$-invariants of $\mathcal{K}_0^2(\mathbb{R}^3)$, where $\mathbb{R}^3$ denotes the Euclidean space.

Theorem 4.1 also entails the corresponding criteria for $I(\mathbb{R}_1^2)$-covariants (see Ref. 28 for more details) of $\mathcal{K}_0^n(\mathbb{R}_1^2)$.

Theorem 4.3: *Let* $\mathcal{K}_0^n(\mathbb{R}_1^2)$ *be the vector space of Killing tensors of valence n defined in the Minkowski plane* $\mathbb{R}_1^2$. *A function* $C:\Sigma\times\mathbb{R}_1^2\to\mathbb{R}$ *is an* $I(\mathbb{R}_1^2)$*-covariant of* $\mathcal{K}^n(\mathbb{R}_1^2)$ *if and only if it satisfies the infinitesimal invariance conditions*

$$\begin{aligned}(\boldsymbol{V}_1 + \boldsymbol{T})(C) &= 0, \\ (\boldsymbol{V}_2 + \boldsymbol{X})(C) &= 0, \\ (\boldsymbol{V}_3 + \boldsymbol{H})(C) &= 0,\end{aligned} \tag{47}$$

where Σ *is the parameter space*, $\boldsymbol{T}$,$\boldsymbol{X}$, *and* $\boldsymbol{H}$ *are given in* (13) *and* $\boldsymbol{V}_i$, $i=1, 2, 3$ *are specified in Theorem 4.1.*

V. CONCLUSIONS

In this article we have formulated and proven an ITKT analog of Cayley's Lemma in CIT. A similar result for the vector space $\mathcal{K}_0^n(\mathbb{R}^2), n\geqslant 1$ (where $\mathbb{R}^2$ denotes the Euclidean plane) can be obtained *mutatis mutandis*. A more challenging problem is to extend the result to two-dimensional spaces of nonzero curvature, namely when the underlying manifold is $\mathbb{S}^2$ (two-sphere) or $\mathbb{H}^2$ (hyperbolic plane). The work in this direction is under way.[1,2,26]

In a forthcoming article[30] we will present a natural continuation of the project initiated here, namely the determination of all fundamental invariants of vector spaces of Killing tensors of arbitrary valence defined in the Minkowski plane, employing the inductive version of the moving frames method.[14]

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Green's function for a Schrödinger operator and some related summation formulas

Attila B. von Keviczky
Department of Mathematics and Statistics, Concordia University, Montréal, Québec, Canada H3G 1M8

Nasser Saad
Department of Mathematics and Statistics, University of Prince Edward Island, Charlottetown, PEI, Canada C1A 4P3

Richard L. Hall
Department of Mathematics and Statistics, Concordia University, Montréal, Québec, Canada H3G 1MB

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Summation formulas are obtained for products of associated Lagurre polynomials by means of the Green's function K for the Hamiltonian $H_0=-d^2/\mathrm{d}x^2+x^2+Ax^{-2}$ $(A>0)$. K is constructed by an application of a Mercer-type theorem that arises in connection with integral equations. The approach introduced in this paper may be useful for the construction of wider classes of generating function. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1952581]

I. INTRODUCTION AND MAIN RESULTS

Since the early development of quantum mechanics, highly singular potentials have attracted much attention. Two main reasons for this are (1) regular perturbation theory can fail badly for such potentials, and (2) in physics one often encounters phenomenological potentials that are strongly singular at the origin such as certain types of nucleon-nucleon interaction, and singular models of fields in arbitrary dimensions. A specific family of singular quantum Hamiltonians known as generalized harmonic oscillators given by

$$H(\lambda)=H_0+\frac{\lambda}{x^\alpha}=-\frac{d^2}{\mathrm{d}x^2}+x^2+\frac{A}{x^2}+\frac{\lambda}{x^\alpha}\quad(A\geqslant 0,\alpha>0,\lambda\geqslant 0)\tag{1.1}$$

and acting in the Hilbert space $L_2(0,\infty)$ have been subject to intensive investigation recently. For a background and brief history of these problems we refer the reader to the summary in Ref. 1. We have shown[1,2] that the set of eigenfunctions of $H_0=H(0)$, namely

$$\psi_n(x)\equiv(-1)^n\sqrt{\frac{2(\gamma)_n}{n!\Gamma(\gamma)}}x^{\gamma-1/2}e^{-x^2/2}\,{}_1F_1(-n;\gamma;x^2)\ \text{with}\ \gamma\equiv 1+\frac{1}{2}\sqrt{1+4A}\quad(n=0,1,2,\ldots),\tag{1.2}$$

constitutes an orthonormal basis for the Hilbert space $L_2(0,\infty)$. Here ${}_1F_1$ stands for the confluent hypergeometric function defined in terms of the associated Laguerre polynomials $L_n^{\gamma-1}(z)$ by

$${}_1F_1(-n;\gamma;z)=\frac{n!}{(\gamma)_n}L_n^{\gamma-1}(z).\tag{1.3}$$

This basis has proven to be useful in providing a complete variational study[1–5] of the spectrum of $H(\lambda)$ for arbitrary fixed $A\geqslant 0$, and λ, $\alpha>0$. The advantage over earlier studies in the Hermite basis $A=0$ was that for $A>0$ the H_0 basis itself derives from a singular problem with the term

A/x^2. In the present paper. we explore another aspect of this basis. We shall prove that the eigenfunctions $\psi_n(x)$ satisfy the following identity:

$$\sum_{n=0}^{\infty} \frac{\psi_n(x)\psi_n(y)}{4n+2\gamma} = \begin{cases} w(x)v(y) & \text{for } 0 \leqslant y \leqslant x, \\ v(x)w(y) & \text{for } 0 \leqslant x \leqslant y. \end{cases} \tag{1.4}$$

where

$$w(x)v(y) = 2^{-1}\sqrt{xy}K_\nu\left(\frac{x^2}{2}\right)I_\nu\left(\frac{y^2}{2}\right), \quad \text{where } \nu = \tfrac{1}{2}(\gamma-1).$$

In particular, we have, for $x=y$, that

$$\sum_{n=0}^{\infty} \frac{|\psi_n(x)|^2}{4n+2\gamma} = 2^{-1}xK_\nu\left(\frac{x^2}{2}\right)I_\nu\left(\frac{x^2}{2}\right). \tag{1.5}$$

Here $I_\nu(x)$ and $K_\nu(x)$ are modified Bessel functions of the first and second kind, respectively. There are direct applications for these identities. An obvious application is that it can been seen as complimentary identity for Watson's famous result[6] (see also, Ref. 7, p. 140, formula 14),

$$\sum_{n=0}^{\infty} \frac{(\gamma)_n}{n!(1+n)} {}_1F_1(-n;\gamma;x)\,{}_1F_1(-n;\gamma;y) = {}_1F_1(1;\gamma;y)\left(\Gamma(\gamma-1)x^{1-\gamma}e^x - \frac{1}{\gamma-1}\,{}_1F_1(1;\gamma;x)\right), \tag{1.6}$$

valid for $x \geqslant y \geqslant 0$. Second, it can be used in theory of coherent states to provide, for example, normalization factors of class of coherent states labeled by confluent hypergeometric functions. Third, there are standard techniques known for generating closed form sums for products of hypergeometric functions and related polynomials, such as Laguerre polynomials. Srivastava *et al.*[8–10] have discussed many different techniques that can be used for such purposes. It is noteworthy that the use of a kernel of a differential equation and a Mercer-type theorem is not an idea that has been well explored in this context. It is our goal in the present paper to show the usefulness of this approach to the construction of generating functions.

In order to prove our main results, we organize the paper as follows. In Sec. II, we introduce two linearly independent solutions of the second-order homogeneous differential equation $H_0u = [-(d^2/dx^2)+(x^2+Ax^{-2})]u=0$. In Sec. III, we construct the Green's function of H_0 and study some of its properties. The majorization of the Kernel operator $K(x,y)$ is investigated in Sec. IV. In Sec. V, we introduce and prove a Mercer-type theorem that allows us to conclude the absolute and uniform convergence of the kernel $K(x,y)$ on the Hilbert space $L_2(0,\infty)$, and consequently prove our main results, Theorem 1 and Theorem 2, from which formulas (1.4) and (1.5) follow immediately.

II. SECOND-ORDER DIFFERENTIAL EQUATION AND ITS SOLUTIONS

If we set $u(z)=z^\alpha\psi(z)$ with $z=\frac{1}{2}x^2$, we can easily show $H_0u=0$ reduces to

$$\frac{d^2\psi}{dz^2} + \frac{\left(2\alpha+\frac{1}{2}\right)}{z}\frac{d\psi}{dz} - \left[1 + \frac{4\alpha\left(\alpha-\frac{1}{2}\right)-A}{4z^2}\right]\psi(z) = 0. \tag{2.1}$$

If we adjust α so that $\psi(z)$ satifies the modified Bessel function

$$\frac{d^2\psi}{dz^2} + z^{-1}\frac{d\psi}{dz} - [\nu^2z^{-2}+1]\psi(z) = 0,$$

we obtain, for $\alpha=\frac{1}{4}$ and $\nu=\frac{1}{4}\sqrt{1+4A}$, and from the basis $\{\sqrt{x}I_\nu(x^2/2), \sqrt{x}K_\nu(x^2/2)\}$, the two linearly independent solutions

$$v(x) = B\sqrt{x}I_\nu\left(\frac{x^2}{2}\right), \quad w(x) = C\sqrt{x}K_\nu\left(\frac{x^2}{2}\right), \tag{2.2}$$

where B and C are constants to be determined. We note that, the Wronskian of $I_\nu(z)$ and $K_\nu(z)$ satisfies [Ref. 6, p. 80, formula (90)]

$$I_\nu(z)K'_\nu(z) - I'_\nu(z)K_\nu(z) = -z^{-1},$$

which equation we divide by $I_\nu^2(z)$ and thereby obtain the derivative of the quotient $(K_\nu/I_\nu)(z)$, namely

$$\left(\frac{K_\nu}{I_\nu}\right)'(z) = z^{-1}I_\nu^{-2}(z).$$

We integrate this expression from z to ∞ [using the properties $K_\nu(\infty)=0$ and $I_\nu(\infty)=\infty$] and thus we arrive at

$$\left(\frac{K_\nu}{I_\nu}\right)(z) = \int_z^\infty \frac{1}{\xi I_\nu^2(\xi)}\mathrm{d}\xi. \tag{2.3}$$

On the other hand, we make the replacements $z=x^2/2$, $K_\nu(x^2/2)=C^{-1}x^{-1/2}w(x)$, and $I_\nu(x^2/2)=B^{-1}x^{-1/2}v(x)$ in the immediately preceding formula, and find

$$\frac{K_\nu(x^2/2)}{I_\nu(x^2/2)} = \frac{B}{C}\times\frac{\omega(x)}{v(x)} = \int_{x^2/2}^\infty \frac{1}{\xi I_\nu^2(\xi)}\mathrm{d}\xi,$$

where in the last integral we make the substitution $I_\nu(\xi)=B^{-1}(2\xi)^{-1/4}v(\sqrt{2\xi})$ thereby giving us

$$\frac{B}{C}\times\frac{w(x)}{v(x)} = \int_{\xi=x^2/2}^\infty \xi^{-1}\left[\frac{v(\sqrt{2\xi})}{B(\sqrt{2\xi})}\right]^{-2}\mathrm{d}\xi = 2B^2\int_{\xi=x^2/2}^\infty \frac{1}{2\xi v^2(\sqrt{2\xi})(2\xi)^{-1/2}}\mathrm{d}\xi = 2B^2\int_{r=x}^\infty \frac{1}{v^2(r)}\mathrm{d}r.$$

The last integral expression was obtained via the substitution $r=\sqrt{2\xi}$. Equating the first expression with the last in the above equations leads to

$$\frac{w(x)}{v(x)} = 2BC\int_{r=x}^\infty \frac{1}{v^2(r)}\mathrm{d}r \quad \text{or equivalently } w(x) = 2BCv(x)\int_{r=x}^\infty \frac{1}{v^2(r)}\mathrm{d}r. \tag{2.4}$$

However, reduction of the order of the original differential equation implies that

$$v(x)\int_{r=x}^\infty \frac{1}{v^2(r)}\mathrm{d}r$$

is the other solution of $H_0u=0$, independent of $v(x)$, which result lets us conclude that $2BC=1$ or $BC=1/2$.

III. MAPPING PROPERTIES OF THE GREEN'S FUNCTION IN $L_2(0,\infty)$

For the operator

$$H_0 = -\frac{d^2}{\mathrm{d}x^2} + (x^2 + Ax^{-2}), \tag{3.1}$$

the linear space $D(H_0)$, consisting of all functions $u\in C^2(0,\infty)\cap C[0,\infty)$ with $u(0)=0$, becomes a normed linear space by setting $\|u\|_\infty \equiv \sup|u([0,\infty))|$. For the Green's function of the linear transformation $H_0: D(H_0)\mapsto C[0,\infty)$, we now formulate a well-known result from the theory of ordi-

nary differential equations, which may be easily arrived at from the properties of Green's function as stated in Refs. 11–13.

Lemma 1: *The differential operator H_0 maps $D(H_0)$ bijectively onto $C[0,\infty)$ by means of $H_0^{-1}: f \mapsto u$, where*

$$(H_0^{-1})f(x) = u(x) \equiv w(x)\int_{\xi=0}^{x} v(\xi)f(\xi)\mathrm{d}\xi + v(x)\int_{\xi=x}^{\infty} w(\xi)f(\xi)\mathrm{d}\xi, \tag{3.2}$$

with $\|H_0^{-1}f\|_\infty \leqslant 4A^{-1/2}\|f\|_\infty$.

Proof: The boundedness of H_0^{-1} is simply a consequence of the inequality

$$v(x)\int_{\xi=x}^{\infty} [v(\xi)]^{-2}\,\mathrm{d}\xi \leqslant \frac{\sqrt{2}}{a}[v(x)]^{-1}, \tag{3.3}$$

where $a \equiv \sqrt[4]{A}$, the value of x where the potential $q_A(x) = x^2 + Ax^{-2}$ assumes its minimum. Indeed, since the function $q_A(x)$ assumes its minimum value $q_A(\sqrt[4]{A}) = 2\sqrt{A} = 2a^2$ at the point $x = a \equiv \sqrt[4]{A}$, we note that

$$v(x) = v(x') + (x-x')v'(x') + \int_{\xi=x'}^{x} (x-\xi)q_A(\xi)v(\xi)\mathrm{d}\xi \quad \text{for } 0 \leqslant x' \leqslant x,$$

and from this directly deduce

$$v(x) \geqslant v(x') + 2a^2\int_{\xi=x'}^{x} (x-\xi)v(\xi)\mathrm{d}\xi \quad \text{for } 0 \leqslant x' \leqslant x.$$

By substituting $v(\xi) \geqslant v(x') + 2a^2\int_{\eta=x'}^{\xi}(\xi-\eta)v(\eta)\mathrm{d}\eta$ into the previous integral inequality, we further arrive at

$$v(x) \geqslant \left\{1 + \frac{1}{2!}2a^2(x-x')^2\right\}v(x') + \frac{1}{3!}(2a^2)^2\int_{\xi=x'}^{x}(x-\xi)^3 v(\xi)\mathrm{d}\xi \quad \text{for } 0 \leqslant x' \leqslant x.$$

Iterating this procedure leads to $v(x) \geqslant v(x')\cosh\sqrt{2a}(x-x')$ for $x \geqslant x' \geqslant 0$. In particular

$$v(x) \geqslant 2^{-1}\exp(\sqrt{2}a(x-x'))v(x') \quad \text{for } x \geqslant x' \text{ and } v(x) \geqslant 2^{-1}\exp(\sqrt{2}a(x-a))v(a) \quad \text{for } x \geqslant a,$$

which can also be written in the form $v(x') \leqslant 2\exp(-\sqrt{2}a(x-x'))v(x)$ for $x \geqslant x' \geqslant 0$ and this in turn leads to

$$\int_{\xi=a}^{x} v(\xi)\mathrm{d}\xi \leqslant \frac{\sqrt{2}}{a}v(x).$$

This result is also evident from the integration of the inequality $v(\xi) \leqslant 2\exp(-\sqrt{2}a(x-\xi))v(x)$ with respect to ξ on the interval (a,x). As a result of $v(\xi) \geqslant 2^{-1}\exp(\sqrt{2}a(\xi-x))v(x)$ for all $\xi \geqslant x$, or by means of $[v(\xi)]^{-2} \leqslant 4\exp(2\sqrt{2}a(x-\xi))[v(x)]^{-2}$, leads to the inequality

$$\int_{\xi=x}^{\infty}[v(\xi)]^{-2}\,\mathrm{d}\xi \leqslant 4\int_{\xi=x}^{\infty}\exp(2\sqrt{2}a(x-\xi))\mathrm{d}\xi \times [v(x)]^{-2} \leqslant \frac{\sqrt{2}}{a}[v(x)]^{-2},$$

which proves (3.3). The injective nature of $H_0^{-1}: C[0,\infty) \to D(H_0)$ is demonstrated as follows. Let $u(x)$ be a solution of $H_0u = 0$ with $u(0) = 0$, whence $u(x) = B\omega(x) + Cv(x)$. On account of the asymptotic behavior of $w(x)$ and $v(x)$ as $x \to 0^+$, namely $w(x)$ and $v(x) \to \infty$ and 0, respectively, as $x \to 0^+$, combined with $\|u\|_\infty < \infty$ leads to $B = 0$, that is to say $u(x) = Cv(x)$; however, the asymptotic behavior of $v(x)$, namely

$$v(x) = \frac{1}{\sqrt{\pi x}} e^{x^2/2}[1 + O(x^2)]$$

as $x \to \infty$, implies that $C=0$. Thus $H_0: D(H_0) \to C[0,\infty)$ is bijective. This completes the proof.■

We have therefore that the Green's function $K(x,y)$ of the differential operator $H_0: D(H_0) \to C[0,\infty)$, which permits us to write the action of H_0^{-1} in terms of integration on $[0,\infty)$, has the integral representation

$$H_0^{-1} f(x) = \int_0^\infty K(x,y) f(y) \mathrm{d}y, \tag{3.4}$$

where

$$K(x,y) = \begin{cases} w(x)v(y) & \text{for } 0 \leqslant y \leqslant x, \\ v(x)w(y) & \text{for } 0 \leqslant x \leqslant y. \end{cases} \tag{3.5}$$

It thus becomes evident that the kernel $K(x,y)$ is a continuous non-negative function on $[0,\infty) \times [0,\infty)$ because, for $\nu = \frac{1}{2}(\gamma - 1) = \frac{1}{4}\sqrt{1+4A}$, $\sqrt{x} I_\nu(x^2/2)$ and $\sqrt{x} K_\nu(x^2/2)$ are continuous on $[0, \infty)$ and $(0, \infty)$, respectively, and, furthermore, both are positive on $(0, \infty)$. Thus $K(x,y)$ is continuous on $[0,\infty) \times [0,\infty) \backslash \{(0,0)\}$.

For the continuity at (0,0) we again turn to the asymptotic behavior of $w(x)$ and $v(x)$ as $x \to 0^+$. In the lower sector $\{(x,y): 0 \leqslant \mathrm{arctg}(y/x) \leqslant \pi/4\}$ of the first quadrant of the (x,y) plane, we have that

$$\begin{aligned} K(x,y) = w(x)v(y) &= \frac{1}{4\pi\nu} x^{1/2-2\nu}[1 + O(x^\epsilon)] y^{1/2+2\nu}[1 + O(y^4)] \\ &= \frac{1}{4\pi\nu} (xy)^{1/2} (y/x)^{2\nu} [1 + O(y^4)][1 + O(x^\epsilon)] \to 0 \quad \text{as} (x,y) \to (0,0), \end{aligned}$$

because in this sector $|y/x| \leqslant 1$. Consequently, $K(x,y)$ is continuous in the lower sector $\{(x,y): 0 \leqslant \mathrm{arctg}(y/x) \leqslant \pi/4\}$, whereas the symmetry of $K(x,y)$, i.e. $K(x,y) = K(y,x)$, guarantees the continuity in upper sector $\{(x,y): \pi/4 \leqslant \mathrm{arctg}(y/x) \leqslant \pi/2\}$ of the first quadrant of the (x,y) plane.

We know further that $H_0 u \equiv -d^2u/\mathrm{d}x^2 + [x^2 + Ax^{-2}]u = 0$ $(A > 0)$ is a symmetric lower semibounded operator in the Hilbert space $L_2(0,\infty)$ with domain of definition consisting of all $L_2(0,\infty)$ functions u vanishing at 0, having absolutely continuous derivative $u' \in L_2(0,\infty)$, on $[0, \infty)$ such that $[x^2 + Ax^{-2}]u(x)$ is also an $L_2(0,\infty)$ function in x. Since the linear manifold $C_0^\infty(0,\infty)$, of all complex valued infinitely differentiable function on $(0, \infty)$ with compact support, lies dense in this domain of definition of H_0 as well as in $L_2(0,\infty)$, we readily conclude that the domain of definition of H_0 is also a dense subset of $L_2(0,\infty)$. Thus H_0 possesses a Friedrichs' extension, which extension we again denote by H_0, and this extension (Ref. 14, Secs. 7.2–7.3 and Ref. 15, p. 335) is a self-adjoint operator in $L_2(0,\infty)$. For $H_0\psi_n = E_n\psi_n$ and because the orthonormalized set of eigenfunctions (1.2) with corresponding eigenvalues $E_n = 4n + 2\gamma = 4n + 2 + \sqrt{1+4A}$ of H_0 forms[1] a complete orthonormal set of functions of the Hilbert space $L_2(0,\infty)$, we shall have that the spectrum of this Friedrichs' extension H_0 is a purely point-spectrum, consisting only of the simple eigenvalues $E_n = 4n + 2\gamma = 4n + 2 + \sqrt{1+4A}$. Thus the spectral family $\{P_\mu: \mu \in \Re\}$ of H_0, which is an "increasing" projection-operator valued Saltus function on the set $\Re$ of real numbers (Ref. 17, p. 92 and Ref. 15, Chap. I, Sec. 7), is

$$P_\mu \equiv \begin{cases} 0 & \text{for } -\infty < \mu < 2\gamma, \\ \psi_0 \otimes \psi_0 & \text{for } 4(0) + 2\gamma \leqslant \mu < 4(1) + 2\gamma, \\ \psi_0 \otimes \psi_0 + \psi_1 \otimes \psi_1 & \text{for } 4(1) + 2\gamma \leqslant \mu < 4(2) + 2\gamma, \\ \psi_0 \otimes \psi_0 + \psi_1 \otimes \psi_1 + \psi_2 \otimes \psi_2 & \text{for } 4(2) + 2\gamma \leqslant \mu < 4(3) + 2\gamma, \\ \cdots, & \\ \sum_{k=0}^{n-1} \psi_k \otimes \psi_k & \text{for } 4(n-1) + 2\gamma \leqslant \mu < 4(n) + 2\gamma, \\ \cdots. & \end{cases} \tag{3.6}$$

For any two $L_2(0,\infty)$ functions ψ and ϕ, the expression $\psi \otimes \phi$ denotes the operator of rank 1 defined by

$$(\phi \otimes \psi) f(x) \equiv \langle f | \psi \rangle \phi(x) = \left[\int_{\xi=0}^{\infty} f(\xi) \overline{\psi(\xi)} \mathrm{d}\xi \right] \times \phi(x) = \int_{\xi=0}^{\infty} (\phi \otimes \psi)(x,\xi) f(\xi) \mathrm{d}\xi, \tag{3.7}$$

with L_2 kernel $(\phi \otimes \psi)(x,y) \equiv \phi(x)\overline{\psi(y)}$ on $L_2(0,\infty)$, which in our case turns out to be an integral operator. It is further clear that the spectral family $\{P_\mu : \mu \in \Re\}$ is increasing in μ, i.e., $P_\lambda \leqslant P_\mu$ for $\lambda \leqslant \mu$, as well as continuous from the right, i.e., $P_\mu = P_{\mu+0}$, in the sense of strong convergence (denoted by $\rightarrow$) in the Hilbert space $L_2(0,\infty)$. Moreover, $P_\mu \rightarrow 0$ or I (the identity operator) according as $\mu \rightarrow -\infty$ or ∞. In consequence, the spectral decomposition (Ref. 15, Sec. 120, p. 320) of our self-adjoint operator H_0 allows H_0 to be represented (as well as functions of H_0) as a Stieltjes integral of μ (functions of μ) with respect to the spectral family $\{P_\mu\}$ on the set $\Re = (-\infty,\infty)$ of real numbers. This turns out to be

$$H_0 = \int_{-\infty}^{\infty} \mu d_\mu P_\mu \tag{3.8}$$

with

$$D(H_0) = \left\{ f \in L_2(0,\infty) : \int_{-\infty}^{\infty} \mu^2 d_\mu \| P_\mu f \|^2 = \sum_{n=0}^{\infty} (4n + 2\gamma)^2 |\langle f | \psi_n \rangle|^2 < \infty \right\}$$

and

$$H_0^{-1} = \int_{-\infty}^{\infty} \mu^{-1} d_\mu P_\mu = \sum_{n=0}^{\infty} (4n + 2\gamma)^{-1} [P_{4n+2\gamma} - P_{4n+2\gamma-0}] = \sum_{n=0}^{\infty} (4n + 2\gamma)^{-1} (\psi_n \otimes \psi_n), \tag{3.9}$$

where $P_{4n+2\gamma} - P_{4n+2\gamma-0} = \psi_n \otimes \psi_n$ is the projection onto the eigenspace (LH) (ψ_n) spanned by the single eigenfunction ψ_n for each of the integers $n \geqslant 0$. The abbreviation (LH) stands for "the linear hull of whatever is between the two brackets to its immediate right," and "linear hull" means the set of all linear combinations. Consequently, the Green's function $K(x,y)$ of the differential operator H_0, namely the kernel of our self-adjoint operator H_0 restricted to the previous domain $D(H_0)$, takes on the form

$$K(x,y) = \sum_{n=0}^{\infty} (4n + 2\gamma)^{-1} (\psi_n \otimes \psi_n)(x,y) = \sum_{n=0}^{\infty} \frac{\psi_n(x)\psi_n(y)}{4n + 2\gamma} \quad \text{a.e. on} [0,\infty) \times [0,\infty) \tag{3.10}$$

with respect to Lebesgue measure on $[0,\infty)^2 = [0,\infty) \times [0,\infty)$, which shall turn out to be a positive L_2 kernel on $[0,\infty)$ with "finite double norm" (Ref. 19, p. 13). Herein we must emphasize the almost everywhere (a.e.) nature of the immediately preceding equality. The finite double norm of kernel $K(x,y)$ is defined as

$$|||K||| \equiv \sqrt{\int_0^\infty \int_0^\infty |K(x,y)|^2 \, dy \, dx} = \sqrt{\sum_{n=0}^{\infty} (4n+2\gamma)^{-2}} < \infty, \tag{3.11}$$

and consequently many of the ideas, but not all, that led to of Mercer's theorem (Ref. 19, p. 127) are applicable. However, because $\Sigma_{n=0}^{\infty}(4n+2\gamma)^{-1}=\infty$, it cannot be expected that all of the results of Mercer's theorem carry over; specifically, K as an operator "on" the Hilbert space $L_2(0,\infty)$ fails to be an operator of trace class.

IV. MAJORIZATION PROPERTY OF THE KERNEL OF OPERATOR K ON $L_2(0,\infty)$

Let us now call the extension of H_0 to all of $L_2(0,\infty)$ the operator K, which is an operator "on" $L_2(0,\infty)$ [instead of "in" $L_2(0,\infty)$]. We may do this, on account (Ref. 19, Theorem 4.5.1, p. 63) of the fact that kernel $K(x,y)$ is an L_2 kernel and therefore the norm relation

$$\|K\| \leqslant |||K||| \equiv \sqrt{\int_0^\infty \int_0^\infty |K(x,y)|^2 \, dy \, dx} = \sqrt{\sum_{n=0}^{\infty} (4n+2\gamma)^{-2}} < \infty, \tag{4.1}$$

guarantees that operator K has domain of definition $D(K)=L_2(0,\infty)$. Herein, $\|K\|$ and $|||K|||$ denote the operator norm of K and double norm of its kernel $K(x,y)$, respectively. The action of K on $L_2(0,\infty)$ is

$$(Kf)(x) = \int_0^\infty K(x,y)f(y)dy = \sum_{n=0}^{\infty} \frac{\langle f|\psi_n\rangle}{4n+2\gamma}\psi_n(x) \quad \text{a.e. in } x \text{ on } [0,\infty), \tag{4.2}$$

and moreover, this operator K on $L_2(0,\infty)$ is also the Friedrichs' extension of H_0. We first consider the kernel $K(x,y)$ as the Green's function of H_0, and note that the completeness of the orthonormal basis $\{\psi_n : n \geqslant 0\}$, where the normalized eigenfunction ψ_n corresponds to the simple eigenvalue $\lambda_n=4n+2\gamma$, entails that

$$\langle Kf|g\rangle = \sum_{n=0}^{\infty} \frac{\langle f|\psi_n\rangle\langle\psi_n|g\rangle}{4n+2\gamma} \quad \text{for all } f \text{ and } g \in L_2(0,\infty). \tag{4.3}$$

In particular, we replace f and g herein by the sequence of $L_2(0,\infty)$ functions $\delta_n(x)$, tending weakly towards the Dirac-δ function $\delta(x)$, defined by

$$\delta_n(x) \equiv n[1-n|x|] \quad \text{for } |x| \leqslant 1/n \text{ and } 0 \text{ otherwise on the set } \Re,$$

where $\Re$ is the set of real numbers. It becomes immediately clear, that out of $\langle Kf|f\rangle$ always exceeding each of the finite sums $\Sigma_{k=0}^{N}[4n+2\gamma]^{-1}|\langle f|\psi_k\rangle|^2$, the inequality

$$\langle K\delta_n(\cdot-x)|\delta_n(\cdot-x)\rangle \geqslant \sum_{k=0}^{N} \frac{\langle\delta_n(\cdot-x)|\psi_n\rangle\langle\psi_n|\delta_n(\cdot-x)\rangle}{4n+2\gamma} \quad \text{for all } N \geqslant 0$$

implies, by way of letting $n\to\infty$ and holding $x\geqslant 0$ fixed, that

$$K(x,x) \geqslant \sum_{k=0}^{N} [4n+2\gamma]^{-1}|\psi_k(x)|^2 \quad \text{for all } N \geqslant 0.$$

Therefore, it follows that

$$\sum_{n=0}^{\infty} \frac{|\psi_n(x)|^2}{4n+2\gamma} \leqslant K(x,x) \quad \text{for all } x \in [0,\infty),$$

where the function $K(x,x)$ has the precise form given by $\left(\nu=\frac{1}{4}\sqrt{1+4A}\right)$

$$K(x,x) = w(x)v(x) = 2^{-1}xI_\nu\left(\frac{x^2}{2}\right)K_\nu\left(\frac{x^2}{2}\right) \tag{4.4}$$

as well as asymptotic behavior as $x \to 0^+$ and ∞, respectively, given by

$$K(x,x) = \begin{cases} \dfrac{1}{\sqrt{1+4A}}x[1+O(x^\epsilon)] & \text{for } x \to 0^+, \\ 2^{-1}x^{-1}[1+O(x^{-2})] & \text{for } x \to \infty. \end{cases} \tag{4.5}$$

V. MERCER THEOREM TYPE PROPERTIES OF THE KERNEL $K(x,y)$

From the asymptotic behavior (4.5) of the majorizing function $K(x,x)$ of $\Sigma_{n=0}^{\infty}[4n+2\gamma]^{-1}|\psi_n(x)|^2$ as well as the continuity of $K(x,x)$ on $[0,\infty)$, we readily see that if we let $M_\infty \equiv \sup\{K(x,x): x \in [0,\infty)\}$, the above asymptotic behavior guarantees that $M_\infty < \infty$, then

$$\sum_{n=0}^{\infty} \frac{|\psi_n(x)|^2}{4n+2\gamma} \leqslant M_\infty \quad \text{for all } x \in [0,\infty). \tag{5.1}$$

It therefore follows that $\Sigma_{n=0}^{\infty}[4n+2\gamma]^{-1}|\psi_n(x)|^2$ converges for all $x \in [0,\infty)$. Moreover, the Cauchy-Schwarz inequality allows us to write for all non-negative integers N that

$$\sum_{n=N}^{\infty} \frac{|\psi_n(x)\psi_n(y)|}{4n+2\gamma} \leqslant \left\{\sum_{n=N}^{\infty} \frac{|\psi_n(x)|^2}{4n+2\gamma}\right\}^{1/2} \times \left\{\sum_{n=N}^{\infty} \frac{|\psi_n(y)|^2}{4n+2\gamma}\right\}^{1/2} \quad \text{for all } x,y \in [0,\infty). \tag{5.2}$$

It further follows that the series $\Sigma_{n=0}^{\infty}[4n+2\gamma]^{-1}\psi_n(x)\psi_n(y)$ converges absolutely, because out of the immediately preceding inequality shall follow

$$\sum_{n=N}^{\infty} \frac{|\psi_n(x)\psi_n(y)|}{4n+2\gamma} \leqslant \left\{\sum_{n=N}^{\infty} \frac{|\psi_n(x)|^2}{4n+2\gamma}\right\}^{1/2} \times \sqrt{M_\infty} \quad \text{for all } x \in [0,\infty),$$

$$\sum_{n=N}^{\infty} \frac{|\psi_n(x)\psi_n(y)|}{4n+2\gamma} \leqslant \left\{\sum_{n=N}^{\infty} \frac{|\psi_n(y)|^2}{4n+2\gamma}\right\}^{1/2} \times \sqrt{M_\infty} \quad \text{for all } y \in [0,\infty). \tag{5.3}$$

Let $\epsilon > 0$. It then follows that, for every $y \in [0,\infty)$, there exists an integer $N = N(y)$ such that

$$\sum_{n=N}^{\infty} \frac{|\psi_n(x)\psi_n(y)|}{4n+2\gamma} \leqslant \epsilon\sqrt{M_\infty} \tag{5.4}$$

for all $x \in [0,\infty)$, provided $N = N(y)$ is chosen sufficiently large; and there exists correspondingly for every $x \in [0,\infty)$ an integer $N = N(x)$ such that

$$\sum_{n=N}^{\infty} \frac{|\psi_n(x)\psi_n(y)|}{4n+2\gamma} \leqslant \epsilon\sqrt{M_\infty} \tag{5.5}$$

for all $x \in [0,\infty)$, provided $N = N(x)$ is chosen sufficiently large. These two statements (5.4) and (5.5) are valid because the series $\Sigma_{n=0}^{\infty}[4n+2\gamma]^{-1}|\psi_n(x)|^2$ is majorized by the constant M_∞ on $[0,\infty)$. Hence we are led to the following Mercer-type theorem.

Theorem 1: *The kernel $K(x,y)$ of the operator K on the Hilbert space $L_2(0,\infty)$ with spectral decomposition $K = \Sigma_{n=0}^{\infty}[4n+2\gamma]^{-1}(\psi_n \otimes \psi_n)$ possesses the following property: the convergence of the series*

$$\sum_{n=0}^{\infty} \frac{\psi_n(x)\psi_n(y)}{4n+2\gamma} = K(x,y) \tag{5.6}$$

is absolute and uniform on every compact subset of $[0,\infty)\times[0,\infty)$.

Proof: The series $\Sigma_{n=0}^{\infty}[4n+2\gamma]^{-1}|\psi_n(x)\psi_n(y)|$ is uniformly convergent in x on $[0,\infty)$ for every $y\geqslant 0$, as well as uniformly convergent in y on $[0,\infty)$ for every $x\geqslant 0$, as evident from (5.4) and (5.5). Therefore $\Sigma_{n=0}^{\infty}[4n+2\gamma]^{-1}\psi_n(x)\psi_n(y)$ represents a continuous function in variable x on $[0,\infty)$ for every $y\geqslant 0$, as, well as a continuous function in variable y on $[0,\infty)$ for every $x\geqslant 0$. For every $L_2(0,\infty)$ function f the Fourier expansion of Kf has the form

$$(Kf)(x) = \int_0^{\infty} K(x,y)f(y)\mathrm{d}y = \sum_{n=0}^{\infty} \frac{\langle f|\psi_n\rangle}{4n+2\gamma}\psi_n(x) \quad \text{a.e. in } x \text{ on } [0,\infty)$$

and possesses the following property:

$$\begin{aligned}\sum_{n=N}^{\infty}\left|\frac{\langle f|\psi_n\rangle}{4n+2\gamma}\psi_n(x)\right| &\leqslant \left\{\sum_{n=N}^{\infty}|\langle f|\psi_n\rangle|^2\right\}^{1/2}\left\{\sum_{n=N}^{\infty}\frac{|\psi_n(x)|^2}{(4n+2\gamma)^2}\right\}^{1/2}\\ &\leqslant \left\{\sum_{n=N}^{\infty}|\langle f|\psi_n\rangle|^2\right\}^{1/2}\left\{\sum_{n=N}^{\infty}\frac{|\psi_n(x)|^2}{(4n+2\gamma)}\right\}^{1/2} \leqslant \left\{\sum_{n=N}^{\infty}|\langle f|\psi_n\rangle|^2\right\}^{1/2}\times\sqrt{M_{\infty}},\end{aligned}$$

and therefore the sum $\Sigma_{n=0}^{\infty}[4n+2\gamma]^{-1}\langle f|\psi_n\rangle\psi_n(x)$ is an absolutely and uniformly convergent series of continuous functions on $[0,\infty)$ whose limit is continuous on $[0,\infty)$, and hence

$$(Kf)(x) = \int_0^{\infty} K(x,y)f(y)\mathrm{d}y = \sum_{n=0}^{\infty} \frac{\langle f|\psi_n\rangle}{4n+2\gamma}\psi_n(x) \quad \text{for all } x[0,\infty).$$

Since in the series $\Sigma_{n=0}^{\infty}[4n+2\gamma]^{-1}(\psi_n\otimes\psi_n)$ the set of kernels $\{(\psi_n\otimes\psi_n): n\geqslant 0\}$ constitutes an orthonormal set of $L_2(0,\infty)$ kernels, the Riesz-Fischer theorem, combined with $K(x,y)=\Sigma_{n=0}^{\infty}[4n+2\gamma]^{-1}(\psi_n\otimes\psi_n)(x,y)$ a.e. on $[0,\infty)\times[0,\infty)$ and the fact that $\Sigma_{n=0}^{\infty}[4n+2\gamma]^{-2}<\infty$, leads to

$$\left|\left\|K-\sum_{n=0}^{\infty}\frac{\psi_n\otimes\psi_n}{4n+2\gamma}\right\|\right| = \left\{\int_0^{\infty}\int_0^{\infty}\left|K(x,y)-\sum_{n=0}^{\infty}\frac{\psi_n(x)\psi_n(y)}{4n+2\gamma}\right|\mathrm{d}y\,\mathrm{d}x\right\}^{1/2} = 0$$

and furthermore to

$$\int_0^{\infty}\left[K(x,y)-\sum_{n=0}^{\infty}\frac{\psi_n(x)\psi_n(y)}{4n+2\gamma}\right]f(y)\mathrm{d}y = 0 \quad \text{for all } f\in L_2(0,\infty).$$

Now let C denote any compact interval $[a,b]$ contained in $[0,\infty)$, and consider the immediately preceding equality for all functions continuous on C and vanishing on $[0,\infty)\backslash C$. Note that these functions belong to $L_2[0,\infty)$. This in turn implies that

$$\int_C\left[K(x,y)-\sum_{n=0}^{\infty}\frac{\psi_n(x)\psi_n(y)}{4n+2\gamma}\right]f(y)\mathrm{d}y = 0$$

for all $x\in C$ and f continuous on C with $f([0,\infty)\backslash C)=0$. By choosing f for any arbitrary, however momentarily, fixed $x\in C$ as follows:

$$f(y) = K(x,y) - \sum_{n=0}^{\infty} \frac{\psi_n(x)\psi_n(y)}{4n+2\gamma} \quad \text{and} \quad f([0,\infty)\setminus C) \equiv 0,$$

where for this fixed $x \in C$ the series represents a continuous function in variable y on set C vanishing on $[0,\infty)\setminus C$, and substituting it into the immediately above equality, we obtain that

$$\int_C \left| K(x,y) - \sum_{n=0}^{\infty} \frac{\psi_n(x)\psi_n(y)}{4n+2\gamma} \right|^2 \mathrm{d}y = 0 \quad \text{for all } x \in C.$$

Because the integrand above is a continuous function of y on the compact subset C, which is an arbitrary finite closed interval contained in $[0, \infty)$, we obtain

$$K(x,y) - \sum_{n=0}^{\infty} \frac{\psi_n(x)\psi_n(y)}{4n+2\gamma} = 0 \quad \text{for all } x,y \in [0,\infty),$$

which, for $x=y \in [0,\infty)$, specifically yields

$$K(x,x) = \sum_{n=0}^{\infty} \frac{|\psi_n(x)|^2}{4n+2\gamma} \quad \text{for all } x \in [0,\infty).$$

We now invoke Dini's theorem, which states "Every monotone sequence of real valued continuous functions on a compact metric space with continuous limit, converges uniformly to its limit." Hence by Dini's theorem (Ref. 17, p.66) the convergence of $K(x,x)=\Sigma_{n=0}^{\infty}[4n+2\gamma]^{-1}|\psi_n(x)|^2$ is therefore uniform on every compact subset of $[0, \infty)$, and therefore the series $\Sigma_{n=0}^{\infty}[4n+2\gamma]^{-1}\psi_n(x)\psi_n(y)$ converges absolutely and uniformly on every compact subset of $[0,\infty)\times[0,\infty)$ with limit $K(x,y)$, i.e., $K(x,y)=\Sigma_{n=0}^{\infty}[4n+2\gamma]^{-1}\psi_n(x)\psi_n(y)$ for all $(x,y)\in[0,\infty)\times[0,\infty)$. This completes the proof. □

Again we note that this is only a Mercer-type theorem, because it makes no conclusion about the operator K or its $L_2(0,\infty)$ kernel $K(x,y)$ being of trace class; whereas Mercer's theorem makes an affirmative statement (Ref. 15, pp. 245–246), see also Refs. 16–19, concerning the trace class nature of operator K. As consequence of this Mercer-type theorem for our Green's function $K(x,y)$, we return to the property of the spectral decomposition of the operator K discussed before, because any complex valued function $W(\mu)$ of the real variable μ on $(-\infty,\infty)$ determines (Ref. 15, Secs. 127 and 128) an operator $W(K)$ in $L_2(0,\infty)$ defined by

$$W(K) = \int_{-\infty}^{\infty} W(\mu) d_\mu P_\mu = \sum_{n=0}^{\infty} W(4n+2\gamma)[P_{4n+2\gamma} - P_{4n+2\gamma-0}] = \sum_{n=0}^{\infty} W(4n+2\gamma)(\psi_n \otimes \psi_n),$$

whose domain of definition $D(W(K))$ consists of all $L_2(0,\infty)$ functions satisfying

$$\int_{-\infty}^{\infty} |W(\mu)|^2 d_\mu < P_\mu f|f\rangle = \int_{-\infty}^{\infty} |W(\mu)|^2 d_\mu \|P_\mu f\|^2 = \sum_{n=0}^{\infty} |W(4n+2\gamma)|^2 |\langle f|\psi_n\rangle|^2 < \infty.$$

It is clearly evident that the operators $W(K)$ are always densely defined, regardless of the function W considered on $\Re=(-\infty,\infty)$, because every domain of definition $D(W(K))$ always contains (LH) $(\psi_n(n\geqslant 0))$. Thus we have that the inverse $[\lambda I-K]^{-1}$ of the operator $\lambda \mathrm{I}-K$, in the normed algebra of bounded linear operators on $L_2(0,\infty)$, comes about from the complex valued function $W(\mu)=[\lambda-\mu]^{-1}$ of the real variable μ and takes the form

$$[\lambda I - K]^{-1} = \int_{-\infty}^{\infty} [\lambda - \mu]^{-1} d_\mu P_\mu = \sum_{n=0}^{\infty} [\lambda - (4n + 2\gamma)]^{-1} [P_{4n+2\gamma} - P_{4n+2\gamma-0}]$$

$$= \sum_{n=0}^{\infty} [\lambda - 4n - 2\gamma]^{-1} (\psi_n \otimes \psi_n),$$

provided $\lambda \notin \sigma(K) = \{4n+2\gamma : n$ a non-negative integer$\}$, namely the spectrum of operator K in the algebra of bounded linear operators on $L_2(0,\infty)$, with continuous kernel

$$[\lambda - \cdot\,]^{-1}(x,y) = \sum_{n=0}^{\infty} \frac{\psi_n(x)\psi_n(y)}{\lambda - 4n - 2\gamma} \quad \text{for all } (x,y) \in [0,\infty) \times [0,\infty),$$

where the convergence is absolute on $[0,\infty)\times[0,\infty)$ and uniform on every compact subset of $[0,\infty)\times[0,\infty)$. We may consequently summarize our results in the following two theorems.

Theorem 2: *The $C[0,\infty)$-function $K(x,x)$ arising out of the Green's function of the differential operator $H_0 = -(d^2/dx^2) + x^2 + Ax^{-2}$ $(A > 0)$ satisfies*

$$\sum_{n=0}^{\infty} \frac{|\psi_n(x)|^2}{4n + 2\gamma} = K(x,x) = w(x)v(x) = 2^{-1} x\, I_{\frac{1}{2}(\gamma-1)}\left(\frac{x^2}{2}\right) K_{\frac{1}{2}(\gamma-1)}\left(\frac{x^2}{2}\right),$$

where $\gamma = 1 + \frac{1}{2}\sqrt{1+4A}$, with uniform convergence on every compact subset of $[0,\infty)$. $K(x,x)$ has the asymptotic behavior

$$K(x,x) = \begin{cases} \dfrac{1}{\sqrt{1+4A}} x[1 + O(x^{\epsilon})] & \text{for } x \to 0^+, \\ 2^{-1} x^{-1}[1 + O(x^{-2})] & \text{for } x \to \infty. \end{cases}$$

Theorem 3: *The continuous kernel $K(x,y)$ on $[0,\infty)\times[0,\infty)$, arising from the Green's function of the differential operator $H_0 = -(d^2/dx^2) + x^2 + Ax^{-2}$ $(A > 0)$ satisfies*

$$K(x,y) = \sum_{n=0}^{\infty} \frac{\psi_n(x)\psi_n(y)}{4n + 2\gamma} = \begin{cases} w(x)v(y) & \text{for } 0 \leqslant y \leqslant x, \\ w(x)w(y) & \text{for } 0 \leqslant x \leqslant y. \end{cases}$$

on $[0,\infty)\times[0,\infty)$ with convergence being absolute and uniform on every compact subset of $[0,\infty)\times[0,\infty)$, where

$$w(x)v(y) = 2^{-1}\sqrt{xy} K_{\frac{1}{2}(\gamma-1)}\left(\frac{x^2}{2}\right) I_{\frac{1}{2}(\gamma-1)}\left(\frac{y^2}{2}\right).$$

.

We further conclude that, for the orthonormal basis $\{\psi_n(x) : n \geqslant 0\}$, (1.2), of the Hilbert space $L_2(0,\infty)$, the two summation formulas (1.4) and (1.5) follows immediately.

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Comparing symmetries and conservation laws of nonlinear telegraph equations

G. W. Bluman[a] and Temuerchaolu[b]
Department of Mathematics, University of British Columbia, Vancouver, BC, Canada V6T 1Z2

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A comparison is made between the symmetries and conservation laws admitted by nonlinear telegraph (NLT) systems. Such systems are not variational. Unlike the situation for variational systems where all conservation laws arise from symmetries, there are many NLT systems that admit more conservation laws than symmetries. The results are summarized in a table which includes the numbers of symmetries and conservation laws for each NLT system. It is also indicated when symmetries map conservation laws to other conservation laws. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1915292]

I. INTRODUCTION

In this paper, we consider the problem of comparing the multipliers of conservation laws and the point symmetries of a given nonlinear system of partial differential equations (PDEs) that is not variational, i.e., whose associated Fréchet derivative is not self-adjoint. As a protypical example, we consider nonlinear telegraph (NLT) systems of the form

$$H_1[u,v] = v_t - F(u)u_x - G(u) = 0,$$

$$H_2[u,v] = u_t - v_x = 0. \tag{1}$$

One physical example related to system (1) is represented by the equations of telegraphy of a two-conductor transmission line with v as the current in the conductors, u as the voltage between the conductors, $G(u)$ as the leakage current per unit length, $F(u)$ as the differential capacitance, t as a spatial variable and x as time.[1] Another physical example related to system (1) is the equation of motion of a hyperelastic homogeneous rod whose cross-sectional area varies exponentially along the rod. Here u is the displacement gradient related to the difference between a spatial Eulerian coordinate and a Lagrangian coordinate x, v is the velocity of a particle displaced by this difference, $G(u)$ is essentially the stress-tensor, $F(u)=\lambda G'(u)$ for some constant λ, and t is time (see Refs. 2 and 3).

A point symmetry

$$x^* = x + \hat{\xi}(x,t,u,v)\varepsilon + O(\varepsilon^2),$$

$$t^* = t + \hat{\tau}(x,t,u,v)\varepsilon + O(\varepsilon^2),$$

$$u^* = u + \hat{\eta}(x,t,u,v)\varepsilon + O(\varepsilon^2),$$

[a]Electronic mail: bluman@math.ubc.ca
[b]Permanent address: Inner Mongolia University of Technology, Hohhot, People's Republic of China. Electronic mail: tmchaolu@impu.edu.cn

$$v^* = v + \hat{\zeta}(x,t,u,v)\varepsilon + O(\varepsilon^2), \tag{2}$$

with corresponding infinitesimal generator (in evolutionary form)

$$X = \eta\partial_u + \zeta\partial_v$$

is admitted by system (1)[4–6] if and only if

$$\left.\begin{aligned} X^{(1)}H_1[u,v]\Big|_{\substack{H_1[u,v]=0,\\ H_2[u,v]=0}} &= 0,\\ X^{(1)}H_2[u,v]\Big|_{\substack{H_1[u,v]=0,\\ H_2[u,v]=0}} &= 0, \end{aligned}\right. \tag{3}$$

where $X^{(1)}$ is the first extension of X and

$$\eta = \hat{\eta}(x,t,u,v) - \hat{\xi}(x,t,u,v)u_x - \hat{\tau}(x,t,u,v)u_t,$$

$$\zeta = \hat{\zeta}(x,t,u,v) - \hat{\xi}(x,t,u,v)v_x - \hat{\tau}(x,t,u,v)v_t.$$

The Fréchet derivative associated with system (1) is the linear operator

$$L[u] = \begin{bmatrix} D_t & -D_x \\ -F'(u)u_x - F(u)D_x - G'(u) & D_t \end{bmatrix}, \tag{4}$$

and it yields the linearized system of (1) given by

$$L[u]\begin{bmatrix}\Phi\\ \Psi\end{bmatrix}\Big|_{\substack{H_1[u,v]=0,\\ H_2[u,v]=0}} = 0 \tag{5}$$

in terms of total derivative operators D_x and D_t. It is easy to show that a point symmetry of system (3) is any solution $(\Phi,\Psi)=(\eta,\zeta)$ of the linearized system (5).

On the other hand, a set of multipliers

$$\xi = \xi(x,t,U,V), \quad \phi = \phi(x,t,U,V), \tag{6}$$

yields a conservation law of system (1) if and only if

$$\left.\begin{aligned} E_U[\xi(x,t,U,V)H_1[U,V] + \phi(x,t,U,V)H_2[U,V]] &\equiv 0,\\ E_V[\xi(x,t,U,V)H_1[U,V] + \phi(x,t,U,V)H_2[U,V]] &\equiv 0, \end{aligned}\right. \tag{7}$$

for *all* differentiable functions $U(x,t)$ and $V(x,t)$, where

$$E_U = \frac{\partial}{\partial U} - D_x\frac{\partial}{\partial U_x} - D_t\frac{\partial}{\partial U_t}, \quad E_V = \frac{\partial}{\partial V} - D_x\frac{\partial}{\partial V_x} - D_t\frac{\partial}{\partial V_t}$$

are Euler operators. One can show that a necessary condition for $\{\xi(x,t,U,V),\phi(x,t,U,V)\}$ to be a set of multipliers for a conservation law of system (1) is that

$$L^*[u]\begin{bmatrix}\xi(x,t,u,v)\\ \phi(x,t,u,v)\end{bmatrix}\Big|_{\substack{H_1[u,v]=0,\\ H_2[u,v]=0}} = 0, \tag{8}$$

where in terms of the Fréchet derivative operator $L[u]$, the adjoint operator $L^*[u]$ is the unique operator having the property that

$$[\alpha,\beta]L[u]\begin{bmatrix}\Phi\\ \Psi\end{bmatrix}-[\Phi,\Psi]L^*[u]\begin{bmatrix}\alpha\\ \beta\end{bmatrix}$$

is a divergence expression for any differentiable functions α, β, Φ, and Ψ.[4,7–9] It is easy to show that for the Fréchet derivative operator $L[u]$ defined by (4), one has

$$L^*[u]=\begin{bmatrix}-D_t & F(u)D_x-G'(u)\\ D_x & -D_t\end{bmatrix}.$$

In the study of physical systems, the importance of conservation laws is well known, including connections with integrability, linearization and modern numerical methods. Conservation laws are intrinsic properties of field equations since they must hold for any posed data. Familiarly, conservation laws are derived from variational principles through Noether's theorem.[4,5] A given system of PDEs (linear or nonlinear) can be directly obtained from a variational principle if and only if its Fréchet derivative is *self-adjoint*,[4,10] i.e., $L^*[u]=L[u]$. Noether's theorem yields a conservation law for any point symmetry (2) that leaves invariant the action functional of the variational principle. This is equivalent to the Euler operator annihilating the scalar product of the multipliers and the given system of PDEs' functions in which solutions (u,v) are replaced by arbitrary differentiable functions (U,V), i.e., system (7). Consequently, any set of multipliers for a conservation law of a system of PDEs having a variational principle must also be admitted symmetries of the given system. Hence, when a system of PDEs has an associated self-adjoint Fréchet derivative, its multipliers for conservation laws are a subset of its admitted symmetries.

It is well known that for a linear system of PDEs, any solution of its adjoint system yields a set of multipliers for a conservation law since for any linear operator L, a divergence expression is yielded by $vLu-uL^*v$. Moreover, from this it follows that if a given nonlinear system of PDEs can be mapped into a linear system by a point or contact transformation, then its infinite number of admitted symmetries exhibit this linear system and its infinite number of multipliers for conservation laws exhibit the adjoint of this linear system.[5,11,12]

It is easy to show that for any $F(u)$ and $G(u)$, the NLT system (1) is *not* self-adjoint. The extra conditions beyond the necessary condition (8) for $\xi(x,t,U,V)$, $\phi(x,t,U,V)$ to be multipliers for a conservation law of system (1) are given in Refs. 7–9. At first sight, one might think that a given system (1) admits more point symmetries (2) which involve four unknowns $\{\hat{\xi},\hat{\tau},\hat{\eta},\hat{\zeta}\}$ than sets of multipliers of the form (6) which involve only two unknowns $\{\xi,\phi\}$. However, we will show that for many NLT systems (1), there are more admitted sets of multipliers of the form (6) than admitted point symmetries (2).

The point symmetry and conservation law classifications of the NLT system (1) have been separately investigated in Refs. 13 and 14, respectively. In Ref. 15, it is shown how to obtain new conservation laws from the action of an admitted symmetry on a known conservation law.

In Sec. II, we give the determining equations for point symmetries and multipliers admitted by NLT systems (1). We present the Symmetry and Conservation Law Classification Table for NLT systems (1) and show that when (1) is not linearizable, there are many cases where it can admit, nontrivially, one symmetry and four, three, two or zero conservation laws as well as cases where it can admit, nontrivially, zero symmetries and four or two conservation laws. We also comment on situations when a symmetry maps a conservation law into another conservation law(s). Further comments are presented in Sec. III.

II. COMPARISON OF SYMMETRIES AND CONSERVATION LAWS FOR NLT SYSTEMS

By inspection, any NLT system (1) obviously admits, as point symmetries, translations $t\to t+\varepsilon_1$, $v\to v+\varepsilon_2$, and $x\to x+\varepsilon_3$, corresponding to admitted infinitesimal generators $X_1=u_t\partial_u+v_t\partial_v$, $X_2=\partial_v$, and $X_3=u_x\partial_u+v_x\partial_v$, respectively, as well as a set of multipliers $(\xi,\phi)=(0,1)$ since the second PDE of any NLT system (1) is written as a conservation law. Any additional admitted point symmetries or sets of multipliers for conservation laws are considered to be nontrivial.

A point symmetry (2) admitted by an NLT system (1) is represented by any solution $\{\hat{\xi}(x,t,u,v),\hat{\tau}(x,t,u,v),\hat{\eta}(x,t,u,v),\hat{\zeta}(x,t,u,v)\}$ of the linear determining system of PDEs[4–6]

$$\hat{\xi}_v - \hat{\tau}_u = 0,$$

$$\hat{\eta}_u - \hat{\psi}_v + \xi_x - \tau_t = 0,$$

$$G(u)\hat{\eta}_v + \hat{\eta}_t - \hat{\psi}_x + G(u)\hat{\tau}_x = 0,$$

$$\hat{\xi}_u - F(u)\hat{\tau}_v = 0,$$

$$\hat{\psi}_u - G(u)\hat{\tau}_u - F(u)\hat{\eta}_v = 0,$$

$$G(u)\hat{\xi}_v + \hat{\xi}_t - F(u)\hat{\tau}_x = 0,$$

$$[\hat{\psi}_v - \hat{\tau}_t - 2G(u)\hat{\tau}_v - \hat{\eta}_u + \hat{\xi}_x]F(u) - F'(u)\hat{\eta} = 0,$$

$$[\hat{\psi}_v - \hat{\tau}_t - G(u)\hat{\tau}_v]G(u) - F(u)\hat{\eta}_x - G'(u)\hat{\eta} + \hat{\psi}_t = 0. \tag{9}$$

The complete solution of the determining system (9) is presented in Ref. 13.

A set of multipliers for a conservation law of an NLT system (1) is represented by any solution $\{\xi(x,t,U,V),\phi(x,t,U,V)\}$ of the linear determining system of PDEs[7,9]

$$\phi_V - \xi_U = 0,$$

$$\phi_U - F(U)\xi_V = 0,$$

$$\phi_x - \xi_t - G(U)\xi_V = 0,$$

$$F(U)\xi_x - \phi_t - G(U)\xi_U - G'(U)\xi = 0. \tag{10}$$

The complete solution of the determining system (10) and the corresponding conservation laws are presented in Ref. 14.

Equivalence transformations[10,11] simplify the symmetry and conservation law classifications of NLT systems (1). In particular, in Refs. 13 and 14, it is shown how to obtain the corresponding conservation law for any $(\overline{F}(u),\overline{G}(u))$ pair related to the conservation law for a given $(F(u),G(u))$ pair through any similarity transformation

$$\overline{F}(u) = \gamma F(\alpha u + \beta), \quad \overline{G}(u) = \delta G(\alpha u + \beta) + \rho. \tag{11}$$

In the following Symmetry and Conservation Law Classification Table (Table I), we list and compare the additional admitted nontrivial symmetries and nontrivial conservation laws for all possible pairs $(F(u),G(u))$, modulo any similarity transformation (11). For each such pair, we indicate the number of additional admitted point symmetries, the number of additional admitted conservation laws, list all such admitted point symmetries in evolutionary form, show where to find such admitted conservation laws in Ref. 14, and state pertinent comments. Most important, in the comments column we indicate where an admitted symmetry can map a conservation law to

TABLE I. Symmetry and conservation law classification table.

$G(u)$	$F(u)$		Number of additional point symmetries; listing of symmetries	Number of additional conservation laws; see Ref. 14 for conservation laws		Comments; symmetry mappings of conservation laws (Ref. 15)
0	Arbitrary	∞	$X=[-A(u,v)u_x+B(u,v)u_t]\partial_u$ $+[-A(u,v)v_x+B(u,v)v_t]\partial_v$ with $A_u=-F(u)B_v, A_v=-B_u$	∞	Multipliers $\xi=a(U,V)$, $\phi=b(U,V)$ with $a_U=b_V$, $F(U)a_V=b_U$	Linearizable by a hodograph transformation; (a,b) system is adjoint of (A,B) system
u	1	∞	$X_\infty=B(x,t)\partial_u-A(x,t)\partial_v$ with $A_x+B_t=0$, $A_t+B_x+B=0$	∞	Multipliers $\xi=b(x,t)$, $\phi=a(x,t)$ with $a_x=b_t$, $a_t=b_x-b$	Linear system; (a,b) system is adjoint of (A,B) system
	u	1	$X=(2u-2xu_x-tu_t)\partial_u$ $+(3v-2xv_x-tv_t)\partial_v$	4	Table 4: Case 1 with $\beta_2=1$, $\beta_1=\beta_3=0$	$t\to t+\varepsilon$ maps (ξ_3,ϕ_3) to additional three (ξ_i,ϕ_i), $i=1,2,4$
	$u^\alpha[\alpha\neq 0,1]$	1	$X=(2u-2\alpha xu_x-\alpha tu_t)\partial_u$ $+[(2+\alpha)v-2\alpha xv_x-\alpha tv_t]\partial_v$	2	Table 1	$t\to t+\varepsilon$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
	$e^{\alpha u}[\alpha\neq 0]$	1	$X=(2-2\alpha xu_x-\alpha tu_t)\partial_u$ $+(\alpha v+2t-2\alpha xv_t)\partial_v$	2	〃	〃
	$u^2+\alpha_1u+\alpha_2$ $[\alpha_1^2\neq 4\alpha_2]$	0		4	Table 4: Case 1 with $\beta_1=1$, $\beta_2=\alpha_1, \beta_3=\alpha_2$	In Ref. 14: in Table 1, $t\to t+\varepsilon$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2); in Table 3, $(t,V)\to(-t,-V)$ maps a *different* (ξ_1,ϕ_1) to a *different* (ξ_2,ϕ_2) than for Table 1
	All other $F(u)$	0		2	Table 1	$t\to t+\varepsilon$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
u^{-1}	u^{-2}	∞	$X=[u^{-1}A(\hat{u},v)u_x$ $-B(\hat{u},v)u_t+A(\hat{u},v)]\partial_u$ $+[u^{-1}A(\hat{u},v)v_x$ $-B(\hat{u},v)v_t]\partial_u$ with $A_v+B_{\hat{u}}=0$, $A_{\hat{u}}+B_v-A=0$ $[\hat{u}=x+\ln u]$	∞	Multipliers $\xi=e^{-x}b(\hat{U},V)$, $\phi=a(\hat{U},V)$ with $a_V-e^{-\hat{U}}b_{\hat{U}}=0$, $a_{\hat{U}}-e^{-\hat{U}}b_V=0$ $[\hat{U}=x+\ln U]$	Linearizable; (a,b) system is adjoint of (A,B) system
	u^{-1}	1	$X=(2xu_x+3tu_t-2u)\partial_u$ $+(2xu_x+3tu_t-v)\partial_v$	4	Table 5: Case 1 with $\beta_2=1$, $\beta_1=\beta_3=0$	$V\to V+\varepsilon$ maps (ξ_3,ϕ_3) to additional three (ξ_i,ϕ_i), $i=1,2,4$

TABLE I. (*Continued.*)

$G(u)$	$F(u)$		Number of additional point symmetries; listing of symmetries	Number of additional conservation laws; see Ref. 14 for conservation laws		Comments; symmetry mappings of conservation laws (Ref. 15)
u^{-1}	$(u+1)/u^2$	1	$X=[2(x+\ln u-1/u)u_x$ $+(3t+2v)u_t-2(u+1)]\partial_u$ $+[2(x+\ln u-1/u)v_x$ $+(3t+2v)v_t-v]\partial_v$	4	Table 5: Case 1 with $\beta_3=0$, $\beta_1=\beta_2=1$	X maps (ξ_3,ϕ_3) to (ξ_2,ϕ_2); $V\to V+\varepsilon$ maps (ξ_3,ϕ_3) to additional three (ξ_i,ϕ_i), $i=1,2,4$
	$(u\pm1)^\beta/u^2$ $[\beta\neq0,1]$	1	$X=[2(\beta x\pm\int F(u)du)u_x$ $+((\beta+2)t\pm2v)u_t$ $-2(u\pm1)]\partial_u$ $+[2(\beta x\pm\int F(u)du)v_x$ $+((\beta+2)t\pm2v)v_t$ $-\beta v]\partial_v$	2	Table 1	$V\to V+\varepsilon$ maps (ξ_2,ϕ_2) to (ξ_1,ϕ_1)
	u^α $[\alpha\neq-1,-2]$	1	$X=[2(2+\alpha)xu_x$ $+(4+\alpha)tu_t-2u]\partial_u$ $+[2(2+\alpha)xu_x$ $+(4+\alpha)tu_t-(2+\alpha)v]\partial_u$	2	〃	〃
	$u^{-2}e^{\alpha u}$ $[\alpha\neq0]$	1	$X=[(2\alpha x+2\int F(u)du)u_x$ $+(\alpha t+2v)u_t-2]\partial_u$ $[(2\alpha x+2\int F(u)du)v_x$ $+(\alpha t+2v)v_t-\alpha v]\partial_v$	2	〃	〃
	$u^{-2}+\alpha_1u^{-1}+\alpha_2$ $[\alpha_1^2\neq4\alpha_2$, $\alpha_2\neq0]$	0		4	Table 5: Case 1 with $\beta_1=1$, $\beta_2=\alpha_1$, $\beta_3=\alpha_2$	In Ref. 14: in Table 1, $V\to V+\varepsilon$ maps (ξ_2,ϕ_2) to (ϕ_1,ϕ_1); in Table 3, $(t,V)\to(-t,-V)$ maps a *different* (ξ_1,ϕ_1) to a *different* (ξ_2,ϕ_2) than for Table 1
	All other $F(u)$	0		2	Table 1	$v\to v+\varepsilon$ maps (ξ_2,ϕ_2) to (ξ_1,ϕ_1)
u^δ $[\delta\neq0,\pm1]$	$u^{\delta-1}$	1	$X=[(\delta-1)tu_t+2u]\partial_u$ $+[(\delta-1)tv_t$ $+(1+\delta)v]\partial_v$	3	Table 3: Case 2 with $\nu=\delta$, $\mu=0$	$t\to t+\varepsilon$ maps (ξ_1,ϕ_1) to (ξ_3,ϕ_3); $V\to V+\varepsilon$ maps (ξ_3,ϕ_2) to (ξ_3,ϕ_3)
	$u^\beta[\beta\neq\delta-1]$	1	$X=[2(\delta-\beta-1)xu_x$ $+(2\delta-\beta-2)tu_t+2u]\partial_u$ $+[2(\delta-\beta-1)xu_x$ $+(2\delta-\beta-2)tv_t$ $+(2+\beta)]\partial_u$	0		
	$u^{\delta-1}+\beta$ $[\beta\neq0]$	0		2	Table 3: Case 2 with $\nu=\delta$, $\mu=\delta^2\beta$	$(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)k

TABLE I. (*Continued.*)

$G(u)$	$F(u)$		Number of additional point symmetries; listing of symmetries		Number of additional conservation laws; see Ref. 14 for conservation laws	Comments; symmetry mappings of conservation laws (Ref. 15)
u^{δ} $[\delta\neq 0,\pm 1]$	$u^{\delta-1}$ $+\kappa(u^{\delta}+\rho)^2$ $[\kappa\neq 0]$	0		2	Table 3: Case 1 with $\gamma=\delta$, $\alpha=\delta^2\kappa$, $\beta=\rho$	〃
$\ln u$	u^{-1}	1	$X=(tu_t-2u)\partial_u$ $+(tv_t-v-2t)\partial_v$	3	Table 3: Case 2 with $\nu=1$, $\mu=0$	X maps (ξ_2,ϕ_2) to (ξ_1,ϕ_1); $t\to t+\varepsilon$ maps (ξ_1,ϕ_1) to (ξ_3,ϕ_3)
	u^{α} $[\alpha\neq -1]$	1	$X=[2(\alpha+1)xu_x+(\alpha+2)tu_t$ $-2u]\partial_u$ $+[2(\alpha+1)xv_x+(\alpha+2)tv_t$ $-(2t+(2+\alpha)v)]\partial_v$	0		
	$u^{-1}+\alpha$ $[\alpha\neq 0]$	0		2	Table 3: Case 2 with $\nu=1$, $\mu=\alpha$	$(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
	u^{-1} $+\kappa(\ln u+\rho)^2$ $[\kappa\neq 0]$	0		2	Table 3: Case 1 with $\gamma=1$, $\alpha=\kappa$, $\beta=\rho$	〃
$\ln^{-1} u$	$1/(u\ln^2 u)$	1	$X=[-2\ln^{-1} uu_x$ $+(t+2v)u_t-2u]\partial_u$ $+[-2\ln^{-1} uv_x$ $+(t+2v)v_t-v]\partial_v$	3	Table 3: Case 2 with $\nu=-1$, $\mu=0$	X maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2); $t\to t+\varepsilon$ maps (ξ_1,ϕ_1) to (ξ_3,ϕ_3)
	$u^{\beta}/\ln^2 u$ $[\beta\neq -1]$	1	$X=2[((\beta+1)x+\int F(u)du)u_x$ $+((\beta+2)t+2v)u_t-2u]\partial_u$ $+2[((\beta+1)x+\int F(u)du)v_x$ $+((\beta+2)t+2v)v_t$ $-(\beta+2)v]\partial_v$	0		
	$1/(u\ln^2 u)+\alpha$ $[\alpha\neq 0]$	0		2	Table 3: Case 2 with $\nu=-1$, $\mu=\alpha$	$(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
	$1/(u\ln^2 u)$ $+\kappa(\ln^{-1} u+\rho)^2$ $[\kappa\neq 0]$	0		2	Table 3: Case 1 with $\gamma=-1$, $\alpha=\kappa$, $\beta=\rho$	〃
e^u	e^u	1	$X=(2+tu_t)\partial_u$ $+(v+tv_t)\partial_v$		Table 6: Case 4 with $\beta_1=\beta_3=0$, $\beta_2=1$	$V\to V+\varepsilon$ maps (ξ_4,ϕ_4) to (ξ_1,ϕ_1); $t\to t+\varepsilon$ maps (ξ_4,ϕ_4) to (ξ_2,ϕ_2); X maps (ξ_4,ϕ_4) to (ξ_3,ϕ_3)

TABLE I. (*Continued.*)

$G(u)$	$F(u)$		Number of additional point symmetries; listing of symmetries	Number of additional conservation laws; see Ref. 14 for conservation laws		Comments; symmetry mappings of conservation laws (Ref. 15)
e^u	$e^{\alpha u}$ $[\alpha\neq 0,1]$	1	$X=[2(\alpha-1)xu_x$ $+(\alpha-2)tu_t-2]\partial_u$ $+[2(\alpha-1)xv_x$ $+(\alpha-2)tv_t-\alpha v]\partial_v$	0		
	$e^u+\alpha$ $[\alpha\neq 0]$	0		4	Table 6: Case 4 with $\beta_1=0$, $\beta_2=1$, $\beta_3=\alpha$	$t\to t+\varepsilon$ maps (ξ_3,ϕ_3) to (ξ_1,ϕ_1); $(t,V)\to(-t,-V)$ maps (ξ_3,ϕ_3) to (ξ_4,ϕ_4) and maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
	$e^{2u}+\alpha_1e^u+\alpha_2$ $[\alpha_1^2\neq 4\alpha_2]$	0		4	Table 6: Case 1 with $\beta_1=1$, $\beta_2=\alpha_1$, $\beta_3=\alpha_2>0$	$(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
					$\xi_1=e^A\sin B$, $\phi_1=e^A(r\cos B$ $-e^U\sin B)$ with $A=a(x+e^U)$ $+\frac{1}{2}(a\alpha_1$ $-1)U$ $+\alpha t-\rho V$, $B=\kappa t+\gamma V-b(x$ $+e_U$ $+\frac{1}{2}\alpha_1U)$; $a,b,r,\alpha,\gamma,\rho,\kappa$ are given in Table 6: Case 2 with $\beta_1=1$, $\beta_2=\alpha_1$, $\beta_3=\alpha_2<0$	$(t,V)\to$ $(t+c_1,\ V+c_2)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2); $(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_3,ϕ_3); $(t,V)\to$ $(-t+c_1,-V+c_2)$ maps (ξ_1,ϕ_1) to (ξ_4,ϕ_4) $[c_1=\alpha_1\pi/2\sqrt{\lvert\alpha_2\rvert}$, $c_2=\sqrt{\lvert\alpha_2\rvert}\pi]$
					Table 6: Case 5 with $\beta_1=1$, $\beta_2=\alpha_1$, $\beta_3=\alpha_2=0$	$t\to t+\varepsilon$ maps (ξ_3,ϕ_3) to (ξ_1,ϕ_1); $(t,V)\to(-t,-V)$ maps (ξ_3,ϕ_3) to (ξ_4,ϕ_4) and maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
	$(e^u+\alpha)^2$ $[\alpha\neq 0]$	0		2	Table 6: Case 3 with $\beta_1=1$, $\beta_2=2\alpha$, $\beta_3=\alpha^2$	$(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)

other conservation laws through the methods presented in Ref. 15. In particular, we show that in many cases the obvious admitted point symmetries $t\to t+\varepsilon_1$ and $v\to v+\varepsilon_2$ are very useful to obtain new conservation laws from a known conservation law.

TABLE I. (*Continued.*)

$G(u)$	$F(u)$		Number of additional point symmetries; listing of symmetries	Number of additional conservation laws; see Ref. 14 for conservation laws		Comments; symmetry mappings of conservation laws (Ref. 15)
$\frac{u^{\delta}\pm 1}{u^{\delta}\mp 1}$ $[\delta\neq 0,\pm 1]$	$\frac{u^{\delta-1}}{(u^{\delta}\mp 1)^2}$	1	$X=\left[\mp\frac{1}{2}\frac{u^{\delta}\pm 1}{u^{\delta}\mp 1}u_x+(t+\delta v)u_t-2u\right]\partial_u+\left[\mp\frac{1}{2}\frac{u^{\delta}\pm 1}{u^{\delta}\mp 1}v_x+(t+\delta v)v_t-(\delta t+v)\right]\partial_v$	3	Table 3: Case 2 with $\nu=\mp 2\delta$, $\mu=0$	X maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2); $t\to t+\varepsilon$, maps (ξ_1,ϕ_1) to (ξ_3,ϕ_3); $V\to V+\varepsilon$, maps (ξ_2,ϕ_2) to (ξ_3,ϕ_3)
	$\frac{u^{\delta+\beta-1}}{(u^{\delta}\mp 1)^2}$ $[\beta\neq 0]$	1	$X=[(2\beta x+\delta\int F(u)du)u_x+((\beta+1)t+\delta v)u_t-2u]\partial_u+[(2\beta x+\delta\int F(u)du)v_x+((\beta+1)t+\delta v)v_t-(\delta t+(\beta+1)v\ ]\partial_v$	0		
	$\frac{u^{\delta-1}}{(u^{\delta}\mp 1)^2}+\alpha$ $[\alpha\neq 0]$	0		2	Table 3: Case 2 with $\nu=\mp 2\delta$, $\mu=(2\delta)^2\alpha$	$(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
	$\frac{u^{\delta-1}}{(u^{\delta}\mp 1)^2}+\kappa\left(\frac{u^{\delta}\pm 1}{u^{\delta}\mp 1}+\rho\right)^2$ $[\kappa\neq 0]$	0		2	Table 3: Case 1 with $\gamma=\mp 2\delta$, $\alpha=(2\delta)^2\kappa$, $\beta=\rho$	〃
$\tan(\delta\ln u)$ $[\delta\neq 0]$	$u^{-1}\sec^2(\delta\ln u)$	1	$X=[-2\tan(\delta\ln u)u_x+(t-2\delta v)u_t-2u]\partial_u+[-2\tan(\delta\ln u)v_x+(t-2\delta v)v_t-(2\delta t+v)]\partial_v$	3	Table 3: Case 2 with $\nu=\delta$, $\mu=0$	X maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2); $t\to t+\varepsilon$, maps (ξ_1,ϕ_1) to (ξ_3,ϕ_3); $V\to V+\varepsilon$, maps (ξ_2,ϕ_2) to (ξ_3,ϕ_3)
	$u^{\beta}\sec^2(\delta\ln u)$ $[\beta\neq -1]$	1	$X=[2((\beta+1)x-\delta\int F(u)du)u_x+((\beta+2)t-2\delta u)u_t-2u]\partial_u+[2((\beta+1)x-\delta\int F(u)du)v_x+((\beta+2)t-2\delta v)v_t+(2\delta t+(\beta+2)v)]\partial_v$	0		
	$\left(\sec^2(\delta\ln u)/u\right)+\alpha$ $[\alpha\neq 0]$	0		2	Table 3: Case 2 with $\nu=\delta$, $\mu=\delta^2\alpha$	$(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
	$\left(\sec^2(\delta\ln u)/u\right)+\kappa[\rho+\tan(\delta\ln u)]^2$ $[\kappa\neq 0]$	0		2	Table 3: Case 1 with $\gamma=\delta$, $\alpha=\delta^2\kappa$, $\beta=\rho$	〃

III. FURTHER DISCUSSION

(1) As can be seen in the Symmetry and Conservation Law Classification Table (Table I), for each $(F(u),G(u))$ pair where the NLT system (1) admits nontrivial conservation laws, there exists

TABLE I. (*Continued.*)

$G(u)$	$F(u)$		Number of additional point symmetries; listing of symmetries	Number of additional conservation laws; see Ref. 14 for conservation laws	Comments; symmetry mappings of conservation laws (Ref. 15)
$\tanh u$	$\operatorname{sech}^2 u$	1	$X=(\tanh u u_x+v u_t-1)\partial_u$ $+(\tanh u v_x+v v_t-t)\partial_v$	4 Table 7: Case 3 with $\beta_1=1$, $\beta_2=\beta_3=0$	$t\to t+\varepsilon$ maps (ξ_4,ϕ_4) to (ξ_i,ϕ_i), $i=1,3$; $V\to V+\varepsilon$, maps (ξ_4,ϕ_4) to (ξ_i,ϕ_i), $i=2,3$; X maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
	$e^{\beta u}\operatorname{sech}^2 u$ $[\beta\neq 0]$	1	$X=[2(\beta x+\int F(u)du)u_x$ $+(\beta t+2v)u_t-2]\partial_u$ $+[2(\beta x+\int F(u)du)v_x$ $+(\beta t+2v)v_t-(2t$ $+\beta v)]\partial_v$	0	
	$\tanh u+\delta$	0		4 Table 7: Case 1 with $\beta_1=0$, $\beta_2=1$, $\beta_3=\delta$, $\lvert\delta\rvert>1$	$(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
				ξ_1 $=e^A\cosh U\cos B$, $\phi_1=\left[(1\right.$ $\left.-\delta)^{1/2}/1\right.$ $\left.+e^{2U}\right]e^A\cosh U$ $\times[\sin B$ $-re^{2U}\cos B]$ with $A=a(x+\frac{1}{2}U)$ $-(\kappa t+\gamma V)$, $B=-b(x+\frac{1}{2}U)$ $-(\alpha t+\rho V)$, $a,b,r,\alpha,\gamma,\rho,\kappa$ are given in Table 7: Case 2 with $\beta_1=0$, $\beta_2=1$, $\beta_3=\delta$, $\lvert\delta\rvert<1$	$(t,V)\to$ $(t+c_1,V+c_2)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2); $(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_3,ϕ_3); $(t,V)\to$ $(-t+c_1,-V+c_2)$ maps (ξ_1,ϕ_1) to (ξ_4,ϕ_4) $[c_1=-\pi/4\sqrt{1-\delta}$, $c_2=(2\delta$ $-1)\pi/4\sqrt{1-\delta}]$
				Table 7: Case 3 with $\beta_1=0$, $\beta_2=1$, $\beta_3=\delta$, $\lvert\delta\rvert=1$	$t\to t+\varepsilon$ maps (ξ_3,ϕ_3) to (ξ_1,ϕ_1); $(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2) and maps (ξ_3,ϕ_3) to (ξ_4,ϕ_4)
	$\tanh^2 u+\delta$ $[\delta\neq -1,0]$	0		4 Table 7: Case 1 with $\beta_1=-1$, $\beta_2=0$, $\beta_3=1+\delta$	$(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)

TABLE I. (*Continued.*)

$G(u)$	$F(u)$	Number of additional point symmetries; listing of symmetries	Number of additional conservation laws; see Ref. 14 for conservation laws	Comments; symmetry mappings of conservation laws (Ref. 15)
$\tanh u$	$\tanh^2 u + \alpha_1 \tanh u + \alpha_2$ $[\alpha_1^2 \neq 4\alpha_2, \alpha_1 \neq 0]$	0	4 Table 7: Case 1 with $\beta_1=-1$, $\beta_2=\alpha_1$, $\beta_3=1+\alpha_2$, $\lvert 1+\alpha_2\rvert > \lvert\alpha_1\rvert$	$(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
			Table 7: Case 2 with $\beta_1=-1$, $\beta_2=\alpha_1<0$, $\beta_3=1+\alpha_2$, $\lvert 1+\alpha_2\rvert < -\alpha_1$	$(t,V)\to(t+c_1,V+c_2)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2); $(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_3,ϕ_3); $(t,V)\to(-t+c_1,-V+c_2)$ maps (ξ_1,ϕ_1) to (ξ_4,ϕ_4) $\left[c_1=\frac{(2+\alpha_1)\pi}{4\sqrt{-(1+\alpha_1+\alpha_2)}},\ c_2=-\frac{(\alpha_1+2\alpha_2)\pi}{4\sqrt{-(1+\alpha_1+\alpha_2)}}\right]$
			$\xi_1 = e^A \cosh^{1+a} u \cos B$, $\phi_1 = \left[\frac{\sqrt{\alpha_1-(1+\alpha_2)}}{1+e^{2U}}\right] e^A \times \cosh^{1+a} U[\sin B - re^{2U}\cos B]$ with $A=a(x-\frac{1}{2}U)-(\kappa t+\gamma V)$, $B=-b(x+\ln\cosh U+\frac{1}{2}\alpha_1 U)-(\alpha t+\rho V)$; $a,b,r,\alpha,\gamma,\rho,\kappa$ are given in Table 7: Case 2 with $\beta_1=-1$, $\beta_2=\alpha_1>0$, $\beta_3=1+\alpha_2$, $\lvert 1+\alpha_2\rvert < \alpha_1$	$(t,V)\to(t+c_1,V+c_2)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2); $(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_3,ϕ_3); $(t,V)\to(-t,+c_1,-V+c_2)$ maps (ξ_1,ϕ_1) to (ξ_4,ϕ_4) $\left[c_1=\frac{(2-\alpha_1)\pi}{4\sqrt{\alpha_1-(1+\alpha_2)}},\ c_2=\frac{(2\alpha_2-\alpha_1)\pi}{4\sqrt{\alpha_1-(1+\alpha_2)}}\right]$

an admitted group of point transformations (discrete and/or continuous) that maps a conservation law to one or more (up to three) new conservation laws for the same $(F(u),G(u))$ pair through use of the work presented in Ref. 15.

TABLE I. (*Continued.*)

$G(u)$	$F(u)$		Number of additional point symmetries; listing of symmetries	Number of additional conservation laws; see Ref. 14 for conservation laws		Comments; symmetry mappings of conservation laws (Ref. 15)
$\tanh u$	$\tanh^2 u + \alpha_1 \tanh u + \alpha_2$ $[\alpha_1^2 \neq 4\alpha_2, \alpha_1 \neq 0]$	0		4	Table 7: Case 3 with $\beta_1=-1$, $\beta_2=\alpha_1$, $\beta_3=1+\alpha_2$, $\lvert\beta_3\rvert=\lvert\alpha_1\rvert$	$t\to t+\varepsilon$ maps (ξ_3,ϕ_3) to (ξ_1,ϕ_1); $(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2) and maps (ξ_3,ϕ_3) to (ξ_4,ϕ_4)
	$(\tanh u+\delta)^2$ $[\delta \neq \pm 1]$	0		2	Table 7: Case 5 with $\beta_1=-1$, $\beta_2=2\delta$, $\beta_3=1+\delta^2$	$(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
	1	0		2	Table 7: Case 5 with $\beta_3=1$ $\beta_1=\beta_2=0$	〃
$\coth u$	$e^{\beta u}\cosh^2 u$	1	See comments	0 or 4	See comments	Symmetries and conservation laws obtained from the the cases where $G(u)=\tanh u$ through equivalence transformation $(x,t,u,v)\to\left(x,t,u+\frac{\pi}{2}i,v\right)$
	$\gamma_1\coth^2 u + \gamma_2\coth u+\gamma_3$	0		2 or 4	See comments	
$\tan u$	$\sec^2 u$	1	$X=(1+\tan u u_x+v u_t)\partial_u + (t+\tan u v_x+v v_t)\partial_v$	4	Table 8: Case 2 with $\beta_1=1$, $\beta_2=\beta_3=0$	$V\to V+\varepsilon$ maps (ξ_1,ϕ_1) to (ξ_i,ϕ_i), $i=2,3$; $t\to t+\varepsilon$ maps (ξ_1,ϕ_1) to ξ_i,ϕ_i, $i=1,3$; X maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)
	$e^{\beta u}\sec^2 u$ $[\beta\neq 0]$	1	$X=[2(\beta x-\int F(u)du)u_x + (\beta t-2v)u_t-2]\partial_u + [2(\beta x-\int F(u)du)v_x + (\beta t-2v)v_t - (2t+\beta v)]\partial_v$	0		
	$\tan u+\delta$	0		4	Table 8: Case 1 with $\beta_1=0$, $\beta_2=1$, $\beta_3=\delta$	$(t,V)\to(-t,-V)$ maps (ξ_1,ϕ_1) to (ξ_2,ϕ_2)

(2) It can happen that a nonvariational system of PDEs can become variational through a differential substitution. For example, the Korteweg–de Vries equation

$$u_t + uu_x + u_{xxx} = 0$$

is not variational but becomes variational after the differential substitution $u=\Gamma_x$. One can show that the differential substitution $(u,v)=(\Gamma_x,\Delta_x)$, leads to an NLT system (1) that is variational if

TABLE I. (*Continued.*)

$G(u)$	$F(u)$		Number of additional point symmetries; listing of symmetries	Number of additional conservation laws; see Ref. 14 for conservation laws	Comments; symmetry mappings of conservation laws (Ref. 15)
$\tan u$	$\tan^2 u+\delta$ $[\delta\neq 0,1]$	0		4 Table 8: Case 2 with $\beta_1=1$, $\beta_2=0$, $\beta_3=\delta-1$	〃
	$\tan^2 u$ $+\alpha_1\tan u+\alpha_2$ $[\alpha_1^2\neq 4\alpha_2, \alpha_1\neq 0]$	0		4 Table 8: Case 1 with $\beta_1=1$, $\beta_2=\alpha_1$, $\beta_3=\alpha_2-1$	〃
	$(\tan u+\delta)^2$	0		2 Table 8: Case 3 with $\beta_1=1$, $\beta_2=2\delta$, $\beta_3=\delta^2-1$	〃
	1	0		2 Table 8: Case 3 with $\beta_3=1$, $\beta_1=\beta_2=0$	〃

and only if $G(u)=\text{const}$ [in this variational case, the NLT system (1) is linearizable by a hodograph transformation].

(3) In general, suppose a system of PDEs with two dependent variables (u,v) and two independent variables (x,t) is not variational but becomes variational through the differential substitution $(u,v)=(\Gamma_x,\Delta_x)$, then an admitted point symmetry

$$\eta=\hat{\eta}(x,t,\Gamma,\Delta)-\hat{\xi}(x,t,\Gamma,\Delta)\Gamma_x-\hat{\tau}(x,t,\Gamma,\Delta)\Gamma_t,$$

$$\zeta=\hat{\eta}(x,t,\Gamma,\Delta)-\hat{\xi}(x,t,\Gamma,\Delta)\Delta_x-\hat{\tau}(x,t,\Gamma,\Delta)\Delta_t,$$

of the variational system would yield multipliers of the form $\{\xi(x,t,U,V),\phi(x,t,U,V)\}$ of the given system, if and only if $\hat{\tau}(x,t,\Gamma,\Delta)=0$ and $\hat{\eta}$, $\hat{\zeta}$ and $\hat{\xi}$ do not depend explicitly on Γ and Δ (otherwise, such a set of multipliers yields a set of nonlocal multipliers and nonlocal symmetries of the given system). Conversely, suppose the given system admits a conservation law resulting from a set of multipliers of the form $\{\xi(x,t,U,V),\phi(x,t,U,V)\}$, then such a set of multipliers yields a point symmetry admitted by the variational system if and only if $\xi_V=\xi_{UU}=\phi_U=\phi_{VV}=0$ [otherwise, such a set of multipliers would yield a local (but not point) symmetry admitted by the variational system].

(4) In general, for a nonvariational system of PDEs, there is a direct connection between conservation laws and symmetries if the system is linear or directly linearizable by a point or contact transformation. For the other exhibited cases, in view of the previous two remarks it would be interesting to investigate if there exist nonlocal symmetries directly connected to the conservation laws.

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Existence of solitary waves for a simplified two fluid system of equations in plasma

Boling Guo
Institute of Applied Physics and Computational Mathematics, Beijing 100088, China

Daiwen Huang
China Academy of Engineering Physics, Beijing 100088, China

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In this paper, we consider a simplified two fluid system of equations in plasma under some conditions. The existence, uniqueness, and the behavior of solitary waves at infinity for the system are proved by ordinary differential equations methods. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1941088]

I. INTRODUCTION

Since the end of 1960s, nonlinear propagation of solitary waves in plasma have been studied extensively. For example, in laser target shooting, people have observed many phenomena such as the density hollow near the critical surface, the vortex solitary wave propagating due to collapse, the solitons emerging when laser beam self-focusing in nonlinear medium, Langmuir soliton emerging from high frequency longitudinal electric field, and optic solitons emerging from high frequency transverse electric fields. With the development of experimental technology, more and more interesting soliton phenomena are observed in the interaction between plasma and laser. At the same time, some results obtained in theoretical study and electronic computer numerical simulations are confirmed by experiments. Here, we refer the readers to Refs. 2, 6, 8, 10, and 11 and references therein.

The system of two-fluid dynamics are composed of equations for electrons and for ions. Here we assume that $\vec{B}=0$, $T_i=0$, $T_e=\text{const}$, then dynamics equations for ions are

$$\frac{\partial n_i}{\partial t}+\nabla\cdot n_i\vec{v_i}=0, \tag{1.1}$$

$$n_iM\left(\frac{\partial\vec{v_i}}{\partial t}+\vec{v_i}\cdot\nabla\vec{v_i}\right)=n_ie\vec{E}, \tag{1.2}$$

dynamics equations for electrons are

$$\frac{\partial n_e}{\partial t}+\nabla\cdot n_e\vec{v_e}=0, \tag{1.3}$$

$$n_em\left(\frac{\partial\vec{v_e}}{\partial t}+\vec{v_e}\cdot\nabla\vec{v_e}\right)=-T_e\nabla n_e-n_e e\vec{E}, \tag{1.4}$$

and Maxwell equations are

$$\nabla\times\vec{E}=0, \tag{1.5}$$

$$\frac{\partial \vec{E}}{\partial t} = -4\pi e(n_i \vec{v_i} - n_e \vec{v_e}), \tag{1.6}$$

where n_i is the number density of ion, n_e the number density of electron, $\vec{v}_i$ the velocity of ion, $\vec{v}_e$ the velocity of electron, M the mass of ion, m the mass of electron, T_i the temperature of ion, T_e the temperature of electron, e is electronic charge, $\vec{E}$ the intensity of the electric field, $\vec{B}$ the intensity of the magnetic field,

$$\nabla = \vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z}.$$

.

Under some technical treatment, (1.1)–(1.7) reduces to the following simplified two-fluid system:

$$\frac{\partial n_i}{\partial t} + \nabla \cdot n_i \vec{v_i} = 0, \tag{1.7}$$

$$n_i M\left(\frac{\partial \vec{v_i}}{\partial t} + \vec{v_i} \cdot \nabla \vec{v_i}\right) = n_i e \vec{E_l}, \tag{1.8}$$

$$\nabla \cdot \vec{E}_l = 4\pi e(n_i - n_l), \tag{1.9}$$

$$\vec{E}_l = -\frac{T_e \nabla n_l}{n_l} - \frac{e^2}{2m\omega_p{}^2} \nabla \overline{\vec{E}_h{}^2}, \tag{1.10}$$

$$\frac{\partial^2 \vec{E_h}}{\partial t^2} - c^{*2}\nabla^2 \vec{E_h} + c^{*2} \nabla \nabla \cdot \vec{E_h} - v_e{}^2 \nabla \nabla \cdot \vec{E_h} = -\frac{4\pi n_l e^2}{m} \vec{E_h}, \tag{1.11}$$

where the suffix l and h are the lower and higher frequency parts respectively, $v_e{}^2 = T_e/m$, $\omega_p = 4\pi n_l e^2/m$, $n_e = n_l + n_h$, c^* the velocity of light, $\overline{\vec{E}_h{}^2} = (1/2T)\int_{t-T}^{t+T} \vec{E}_h{}^2 \mathrm{d}t$. For more details, the readers can refer to Ref. 14. The system of equations (1.7)–(1.11) are self-contained. And it has at least three kinds of waves, the ion acoustic wave, the plasma wave, and the light wave. Each wave contains a nonlinear term producing space coacervation, for the ion acoustic wave it is the transport term $\vec{v}_i \cdot \nabla \vec{v}_i$, while for the plasma wave and the light wave it is the one in Eq. (1.11). Three kinds of waves all contain a dispersion term. For the ion acoustic wave it is the charge separate term $\nabla \cdot \vec{E}_l$, for the plasma wave it is $v_e{}^2 \nabla^2 \vec{E}_h$, and for the light wave it is $c^{*2}\nabla^2 \vec{E}_h$. When the interactions between the nonlinear terms and the dispersion terms reach to a certain equilibrium, the acoustic solitons, the plasma solitons, and the light solitons are produced.

For the simplified system of two-fluid dynamics (1.7)–(1.11), if we take units of the physical quantities as $[t] = (M/4\pi n_0 e^2)^{1/2} = \omega_{p_i}{}^{-1}$, $[x] = (T_e/4\pi n_0 e^2)^{1/2} = \lambda_D$, $[v] = [x]/[t] = (T_e/M)^{1/2}$, $[n_l] = n_0$, $[\phi] = (T_e/e)(E_i - \nabla \phi)$, $[|\epsilon|^2] = 4\pi n_0 T_e$, we can obtain the dimensionless form of the system

$$\frac{\partial n_i}{\partial t} + \nabla \cdot n_i \vec{v_i} = 0, \tag{1.12}$$

$$\frac{\partial \vec{v_i}}{\partial t} + \vec{v_i} \cdot \nabla \vec{v_i} = -\nabla \phi, \tag{1.13}$$

$$\nabla^2\phi = n_l - n_i = \exp(\phi - |\epsilon|^2) - n_i, \tag{1.14}$$

$$n_l = \exp(\phi - |\epsilon|^2), \tag{1.15}$$

$$\frac{2i}{\omega_p}\frac{\partial\epsilon}{\partial t} - \frac{1}{\omega_p^2}\frac{\partial^2\epsilon}{\partial t^2} = -\nu\nabla^2\epsilon + (\exp(\phi - |\epsilon|^2) - 1)\epsilon, \tag{1.16}$$

$$E_l = -\nabla\phi, \tag{1.17}$$

where ϵ is the higher frequency electric field, $\omega_p=(M/m)^{1/2}$, $\nu=1$ if $\overline{E_h}$ is the intensity of the longitudinal field, while $\nu=c^{*2}/v_e^2$ if $\overline{E_h}$ is the intensity of the transverse field.

In the following, we only discuss the one-dimensional case, therefore $\vec{v}_i=v$. Suppose

$$\epsilon(x,t) = \psi(x-ct)\exp(-ipt+iqx), \tag{1.18}$$

and n_i, v, and ϕ are the functions of $\xi=x-ct$. Substituting (1.18) into (1.16) and setting its real part and imaginary part to zero, respectively, we get from (1.12)–(1.14) and (1.16) the plane solitary wave equations

$$\left(\nu - \frac{c^2}{\omega_p^2}\right)\frac{d^2\psi}{d\xi^2} = (\exp(\phi-\psi^2) - 1 + a^2)\psi, \tag{1.19}$$

$$\frac{d^2\phi}{d\xi^2} = \exp(\phi-\psi^2) - \frac{1}{\sqrt{1-\dfrac{2\phi}{c^2}}}, \tag{1.20}$$

$$n_i = \frac{1}{\sqrt{1-\dfrac{2\phi}{c^2}}}, \tag{1.21}$$

$$n_l = \exp(\phi-\psi^2), \tag{1.22}$$

where c is the propagation velocity of the solitary wave, $a^2=\nu q^2-(p/\omega_p)^2-(2p/\omega_p)>0$, $\nu q=(c/\omega_p)[1+(p/\omega_p)]$.

There are many papers which concern the existence of approximate solutions for the equations (1.19)–(1.22), cf. Refs. 5, 6, 10, and 11. For the longitudinal wave $\nu=1$, by expanding n_i, n_l untill ϕ and ψ^2 terms, one has $n_l=1+\phi-\psi^2$, $n_i=1+(\phi/c^2)$. Supposing $n_i=n_l$, one can replace the equation (1.19) (c^2/ω_p^2 is ignored) by the following equation:

$$\frac{d^2\psi}{d\xi^2} = \left(\frac{1}{c^2-1}\psi^2 + a^2\right)\psi. \tag{1.23}$$

Hence the solution of (1.19) and (1.20) are

$$\psi = a\sqrt{2(1-c^2)}\,\operatorname{sech} a\xi \tag{1.24}$$

$$\phi = -2a^2c^2\operatorname{sech}^2 a\xi, \tag{1.25}$$

where $0<c<1$. The single-peaked symmetry solution (1.24) and (1.25) are soliton solutions of Zakharov equations, which is consistent with the numerical calculation for development of the initial wave packet of Zakharov equations and the interactions of solitons made by Makhankov, etc.

By taking higher order terms appropriately from expansions of n_i and n_l, one obtains the Makhanhov-Nishikawa solitary wave solution (ϕ,ψ) where ϕ is symmetric and ψ is antisymmetric. Near the region $c^2\simeq 1$, $0<c<1$, by taking ϕ and ψ of the same order of magnitude and expanding n_i and n_l to quadric terms of ϕ and ψ, one can have the equations

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2}=(\phi+a^2)\psi, \tag{1.26}$$

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}\xi^2}=-\frac{1-c^2}{c^2}\phi--\frac{3-c^4}{2c^4}\phi^2-\psi^2, \tag{1.27}$$

the solution of which is given by

$$\psi=A\ \mathrm{sech}\ a\xi\tanh a\xi, \tag{1.28}$$

$$\phi=B\ \mathrm{sech}^2\ a\xi, \tag{1.29}$$

where $A^2=6a^2[4a^2-1+(1/c^2)]$, $B=-6a^2$, and a, c satisfy $a^2=c^2(1-c^2)/(9-c^4)$.

In the simplified two-fluid system of equations (1.12)–(1.17), by taking the higher frequency oscillatory part as zero, one can obtain soliton in ion acoustic waves, cf. Ref. 6, p. 19. Considering the one-dimensional case, and supposing $T_i=0$, $\vec{v}_i=v_i$, one gets the dimensionless form

$$\frac{\partial n_i}{\partial t}+\frac{\partial n_i v_i}{\partial x}=0, \tag{1.30}$$

$$\frac{\partial v_i}{\partial t}+v_i\frac{\partial v_i}{\partial x}=-\frac{\partial\phi}{\partial x}, \tag{1.31}$$

$$\frac{\partial^2\phi}{\partial x^2}=\exp(\phi)-n_i. \tag{1.32}$$

By letting $\xi=x-ct$ and supposing that $n_i\to 1$, $v_i\to 0$, $\phi\to 0$ as $|x|\to\infty$, one may obtain

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}\xi^2}=\exp(\phi)-\frac{1}{\sqrt{1-\dfrac{2\phi}{c^2}}}, \tag{1.33}$$

$$n_i=\frac{1}{\sqrt{1-\dfrac{2\phi}{c^2}}}, \tag{1.34}$$

$$n_i(c-v_i)=c, \tag{1.35}$$

Assuming that $c>1$, $\delta_c=c-1\ll 1$, one gets the equation

$$\frac{1}{2}\left(\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right)^2=\frac{1}{3}\phi^2(3\delta_c-\phi).$$

The solution of the above equation is

$$\phi = 3(c-1)\operatorname{sech}^2\left(\sqrt{\frac{c-1}{2}}(x-ct)\right), \tag{1.36}$$

where the peak value of the solitary wave is $3(c-1)$. If letting $\xi=\delta_0^{1/2}(x-t)$, $\tau=\delta_0^{3/2}t$, the ion acoustic wave equations (1.30)–(1.32) reduce to the so-called KdV equation.

In the present paper, we are interested in finding the existence of solitary waves for the simplified two-fluid system of equations under some conditions by rigorous mathematical theories. In the equations (1.19) and (1.20), by letting $\varphi=\sqrt{2}\psi$, we can obtain

$$-\omega_0\frac{d^2\varphi}{d\xi^2} = \left[-\exp\left(\phi-\frac{\varphi^2}{2}\right)+1-a^2\right]\varphi, \tag{1.37}$$

$$\frac{d^2\phi}{d\xi^2} = \exp\left(\phi-\frac{\varphi^2}{2}\right) - \frac{1}{\sqrt{1-\dfrac{2\phi}{c^2}}}, \tag{1.38}$$

where $\omega_0=\nu-(c^2/\omega_p^2)>0$. Supposing that $n_i\to 1$, $v_i\to 0$, φ, $\phi\to 0$ as $|x|\to\infty$, in order to solve the equations (1.37) and (1.38) we may consider

$$-\omega_0\frac{d^2\varphi}{d\xi^2} = \left[-\exp\left(\phi-\frac{\varphi^2}{2}\right)+1-a^2\right]\varphi, \quad \text{in } \mathbb{R},$$

$$\frac{d^2\phi}{d\xi^2} = \exp\left(\phi-\frac{\varphi^2}{2}\right) - \frac{1}{\sqrt{1-\dfrac{2\phi}{c^2}}}, \quad \text{in } \mathbb{R}, \quad (P_1)$$

$$\varphi, \quad \phi \in W^{1,2}(\mathbb{R}),$$

where

$$W^{1,2}(\mathbb{R}) := \{u; u \in L^2(\mathbb{R}), \nabla u \in L^2(\mathbb{R})\}$$

with the norm

$$\|u\| := |u|_2 + |\nabla u|_2,$$

where $|.|_2$ denotes the norm in $L^2(\mathbb{R})=\{u; \int_{\mathbb{R}}|u(\xi)|^2\,d\xi<+\infty\}$. We note that if (φ_0,ϕ_0) is a solution for (P_1) when $a\geqslant 1$, then $\varphi_0=0$ (the details will be given in Sec. II). So we can discuss the existence of solutions for the following problem:

$$\frac{d^2\phi}{d\xi^2} = \exp(\phi) - \frac{1}{\sqrt{1-\dfrac{2\phi}{c^2}}},$$
$$\phi\to 0 \quad \text{as } |\xi|\to 0, \quad \exists\, \xi_0 \text{ such that } \phi(\xi_0)>0, \quad 1-\frac{2\phi(\xi_0)}{c^2}>o, \tag{P_2}$$

By ordinary differential equations methods, cf. Refs. 4 and 3, we obtain existence of a nontrivial solution ϕ for (P_2) and the solution is unique up to translations of the origin. Moreover we can prove the exponential decay of the solution at infinity by a standard argument of ordinary differential equations in Ref. 12. Therefore we can obtain a nontrivial solitary wave $(0,\phi)$ for the system of equations (1.12)–(1.17).

In Sec. II, we shall give the main results, Theorems 2.1 and 2.2, and the proof of Theorems 2.1 and 2.2.

II. THE MAIN RESULTS

Now we can state our main results.

Theorem 2.1: If (φ,ϕ) is a solution of (P_1) for $a\geqslant 1$, then $\varphi=0$.

Proof: From the first equation of the system (P_1),

$$-\omega_0\frac{d^2\varphi}{d\xi^2}=\left[-\exp\left(\phi-\frac{\varphi^2}{2}\right)+1-a^2\right]\varphi,\quad \text{in } \mathbb{R},$$

we note that $d^2\varphi/d\xi^2$ and φ have the same sign since $\omega>0$ and $-\exp[\phi-(\varphi^2/2)]+1-a^2<0$ when $a\geqslant 1$. On the other hand, since $\varphi\in W^{1,2}(\mathbb{R})$, by Sobolev embedding theorem (Ref. 1, Theorem 5.4) φ tends to zero as $\xi\to 0$, and φ is continuous, bounded. Thus φ takes either positive maximum or negative minimum, which is impossible because $d^2\varphi/d\xi^2$ and φ have the same sign. Therefore the only possibility left is that $\varphi=0$.

Theorem 2.2: The problem (P_2) has a nontrivial solution ϕ if and only if $1<c<c_0$, where $c_0:=\inf\{c;c>1,-\exp(c^2/2)+c^2+1>0\}$. Furthermore, if $1<c<c_0$, then the solution ϕ is unique up to translations of the origin, and it satisfies (after a suitable translation of the origin) the following:

(i) $\phi(\xi)=\phi(-\xi)$, $\xi\in\mathbb{R}$ (ϕ is radial),
(ii) $\phi(\xi)>0$, $\xi\in\mathbb{R}$,
(iii) $\phi(0)=\xi_1$, $\xi_1:=\inf\{\xi;\xi>0,-\exp(\xi)-c^2\sqrt{1-(2\xi/c^2)}+c^2+1>0\}$,
(iv) $\phi'(\xi)<0$, $\xi>0$, where the prime indicates the derivative,
(v) ϕ, ϕ', ϕ'' have exponential decay at infinity, i.e., there exists C, $\delta>0$ such that

$$0\leqslant\phi(\xi),\ |\phi'(\xi)|,|\phi''(\xi)|\leqslant C\exp(-\delta|\xi|),\quad \xi\in\mathbb{R}.$$

Proof: Under the assumptions of Theorem 2.2, one solution of (P_2) can be obtained as the solution of the initial value problem

$$\frac{d^2\phi}{d\xi^2}=\exp(\phi)-\frac{1}{\sqrt{1-\dfrac{2\phi}{c^2}}}=h(\phi),\qquad (P_3)$$
$$\phi(0)=\xi_1,\quad \phi'(0)=0.$$

The other solutions are obtained by translations, $\phi(\xi)=\phi(\xi+\xi^*),\xi^*\in\mathbb{R}$ being a constant.

By the definition of c_0 and $1<c<c_0$, there exists $\xi_1>0$ such that

$$\xi_1:=\inf\{\xi;\xi>0,-\exp(\xi)-c^2\sqrt{1-(2\xi/c^2)}+c^2+1>0\},\quad h(\xi_1)>0. \tag{2.1}$$

On the other hand, if (2.1) holds, then $H(\xi_1)=-\exp(\xi_1)-c^2\sqrt{1-(2\xi_1/c^2)}+c^2+1=0$, thus $1<c<c_0$.

Let ϕ denote the solution of (P_3). This solution exists and is unique on a certain maximal interval $(-\overline{\xi},\overline{\xi})$. Multiplying the equation in (P_3) by ϕ' and integrating from 0 to ξ yields

$$-\frac{1}{2}\left(\frac{d\phi}{d\xi}\right)^2=-\exp(\phi)-c^2\sqrt{1-\frac{2\phi}{c^2}}+c^2+1,\quad |\xi|<\overline{\xi}. \tag{2.2}$$

A bounded solution of Eq. (2.2) exists if and only if $H(\xi)$ has a root in the interval $(0,c^2/2)$. It is easy to see that $H(0)=H'(0)=0$. In addition, when $c>1$, there is ϕ_0 such that $\phi_0<c^2/2$, $H'(\phi)<0$ for $0<\phi<\phi_0$ and $H'(\phi)>0$ for $\phi_0<\phi<c^2/2$. We can see that $H(\xi)$ have a root in the interval $(0,c^2/2)$ if and only if $H(c^2/2)>0$. And the function $H(c^2/2)=-\exp(c^2/2)+c^2+1$ has exactly one positive root $c_0>1$. In conclusion, we obtain that (P_2) admits the solitary wave solution if and only if $1<c<c_0$.

By ordinary differential equations methods, we can prove $\overline{\xi}=+\infty$, (i), (ii), (iii), (iv), and (v). For more details of the proof of the above statements, one can refer to Refs. 3 and 12.

Remark 2.3: By variational methods, in order to find the solutions for the problem (P_1), we can find the critical points of the following functional:

$$I(\varphi,\phi)=\frac{1}{2}\int\left(\omega_0\left(\frac{\mathrm{d}\varphi}{\mathrm{d}\xi}\right)^2+a^2\varphi^2\right)-\frac{1}{2}\int\left(\left(\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right)^2+b\phi^2\right)-\int F(\varphi,\phi), \tag{2.3}$$

where $b>0$, $F(\varphi,\phi)=e^{\phi-(\varphi^2/2)}-1+c^2\sqrt{1-(2\phi/c^2)}-c^2+\frac{1}{2}\varphi^2-(b\phi^2/2)$, φ, $\phi\in W^{1,2}(\mathbb{R})$, $\int\cdot$ denoting $\int_{\mathbb{R}}\cdot\,\mathrm{d}\xi$. There are three difficulties in considering the existence of critical points of the functional (2.3). The first is the functional (2.3) is not always continuous and differential at all $(\varphi,\phi)\in W^{1,2}(\mathbb{R})\times W^{1,2}(\mathbb{R})$. The second is the functional (2.3) is strongly indefinite in the sense that it is neither bounded from above nor from below even under some compact perturbations. The last is the loss of compactness, that is, the imbedding $W^{1,2}(\mathbb{R})\hookrightarrow L^q(\mathbb{R})(2\leqslant q<2^*=\infty)$ is not compact because $\mathbb{R}$ is an unbounded domain. In Theorem 2.1 and Theorem 2.2, we have proved the existence, the behavior at infinity and uniqueness of solitary waves for (P_1) when $a\geqslant 1$, $1<c<c_0$. For example, if $p=-\omega_p$, then $a=1$. However, we cannot deal with the problem (P_1) when $0<a<1$, $0<c<1$, because the Euler functional (2.3) associated with (P_1) is strongly indefinite. Since the embedding $W^{1,2}_{\mathrm{O}(N)}(\mathbb{R})\hookrightarrow L^q(\mathbb{R})(2\leqslant q<2^*=\infty)$ is not compact $[W^{1,2}_{\mathrm{O}(N)}(\mathbb{R})$ is the set of all spherically symmetric functions in $W^{1,2}(\mathbb{R})]$, we cannot use the method in Ref. 7, where its authors used principle of symmetric criticality and limit index theory to obtain critical points for a strongly indefinite functional. As $F(\varphi,\phi)$ in (2.3) is not always positive or bounded from below, we also cannot use the general linking theorem in Refs. 9 and 13 to obtain the existence of critical points for the functional (2.3). Meanwhile, (0, 0) is a trivial solution for the problem (P_1), the Leray-Schauder fixed point theorem cannot be used to solve the existence of solutions for (P_1). In the future work, we shall consider the problem (P_1) when $0<a<1$, $0<c<1$ by other methods.

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Publisher's Note: "Continuous spin representations from group contraction" [J. Math. Phys. 46, 053515 (2005)]

Abu M. Khan[a] and Pierre Ramond[b]
Institute for Fundamental Theory, Department of Physics, University of Florida, Gainesville, Florida 32611

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This article was originally published with typographical errors in Eq. (51). AIP apologizes for these errors. All online versions of the article have been corrected. The correct version of Eq. (51) follows:

$$W_{\mu\nu}W^{\mu\nu} \text{ and } W=\epsilon_{\rho\mu\nu\sigma\lambda}P^{\rho}M^{\mu\nu}M^{\sigma\lambda}. \tag{51}$$

[a]Electronic mail: amas@phys.ufl.edu
[b]Electronic mail: ramond@phys.ufl.edu

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Publisher's Note: "The Parr formula for the superheating field in a semi-infinite film"[J. Math. Phys. 46, 053513 (2005)]

Pierre Del Castillo[a)]
Laboratoire Amiénois de Mathématiques Fondamentales et Appliquées, CNRS UMR 6140, Université de Picardie Jules Verne, 33 r. Saint-Leu, 80039 Amiens Cedex 1, France

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This article was originally published with typographical errors in a formula within the abstract and in Eq. (93). AIP apologizes for these errors. The online versions of the article have been corrected. The corrected formula within the abstract is as follows:

$$\kappa(h^{\mathrm{sh}}(\kappa))^2 \leqslant 2^{-3/2} + \tfrac{15}{22}\kappa + \mathcal{O}(\kappa^{1+\rho}),\ \rho > 0.$$

The correct version of Eq. (93) follows:

$$S^2 = \tfrac{1}{8}(-8\kappa^2 h^4 \exp(-\sqrt{2}x) - 1 + 24\kappa^2 h^4 + \mathcal{O}(\kappa^{\rho}))\exp(-\sqrt{2}x),\quad \forall\, x \in [0, \kappa^{-\rho}]. \tag{93}$$

[a)]Electronic mail: pierre.delcastillo@u-picardie.fr

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Finite-time stochastic reduction models

Dorje C. Brody
Blackett Laboratory, Imperial College, London SW7 2BZ, United Kingdom

Lane P. Hughston
Department of Mathematics, King's College London, The Strand, London WC2R 2LS, United Kingdom

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A new energy-based stochastic extension of the Schrödinger equation for which the wave function collapses after the passage of a finite amount of time is proposed. An exact closed-form solution to the dynamical equation, valid for all finite-dimensional quantum systems, is presented and used to verify explicitly that reduction of the state vector to an energy eigenstate occurs. A time-change technique is introduced to construct a "clock" variable that relates the asymptotic and the finite-time collapse models by means of a nonlinear transformation. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1990108]

The idea that Brownian motion might play a role in models for the collapse of the wave function was first envisaged by Wiener and Siegel.[1] Although that specific proposal did not in the end fully account for the correct probability law, a number of authors have subsequently proposed and developed dynamical collapse models driven by Brownian motion that have the key property of being compatible with the probabilistic hypotheses of standard quantum mechanics. Progress in this area over the last two decades can be broadly classified into two categories: (a) models based on the idea of "spontaneous localization" of the wave function,[2] and (b) models based on the notion of collapse of the state vector to an energy eigenstate.[3] See, e.g., the articles cited in Ref. 4 for accounts of these approaches.

The energy-based collapse models, with which we are concerned here, have the physical property that the expectation of the future energy of the system is given by the initial energy. It has been argued on phenomenological grounds[5] that the characteristic time scale for collapse to an energy eigenstate in such models is of the order

$$\tau_R \approx \left(\frac{2.8\ \text{MeV}}{\Delta H}\right)^2 \text{s}, \tag{1}$$

where ΔH is the initial energy uncertainty, and it has been demonstrated that the choice (1) is consistent with empirical observations for a number of different examples of quantum systems.[6] The time scale τ_R is indicative of the time it takes for the wave function to reach the immediate vicinity of an energy eigenstate. That is to say, after the passage of several multiples of τ_R, the state of the system is, with a high degree of probability, nearly indistinguishable from one of the energy eigenstates. It should be emphasised, however, that strict collapse, in these models, is achieved only asymptotically in time, and it has hitherto been unknown how to formulate a consistent dynamical collapse model that exhibits a complete reduction of the state vector in a finite period of time.

The purpose of this article is to introduce a new class of energy-based models for which the collapse is completed after the passage of a specified time interval T. Further, we obtain an exact closed-form expression for the state vector process that solves the dynamical equation. We show that, remarkably, the finite-time collapse model and the standard infinite-time collapse models are related by a time transformation of the form

$$\tau(t) = \frac{tT}{T-t}, \tag{2}$$

where t is the clock time of the finite-time collapse model, and τ is the clock time in the asymptotic collapse model. Thus the finite-time collapse model can be viewed as a "fast-forwarded" version of the asymptotic collapse model.

We begin by stating the main results of the paper. *Let the dynamics of the state-vector process* $\{|\psi_t\rangle\}$ *be given by the following stochastic Schrödinger equation:*

$$\mathrm{d}|\psi_t\rangle = -\mathrm{i}\hat{H}|\psi_t\rangle \mathrm{d}t - \tfrac{1}{8}\sigma_t^2(\hat{H}-H_t)^2|\psi_t\rangle \mathrm{d}t + \tfrac{1}{2}\sigma_t(\hat{H}-H_t)|\psi_t\rangle \mathrm{d}W_t. \tag{3}$$

Here

$$H_t = \frac{\langle\psi_t|\hat{H}|\psi_t\rangle}{\langle\psi_t|\psi_t\rangle} \tag{4}$$

is the expectation value of the Hamiltonian $\hat{H}$ *in the state* $|\psi_t\rangle$, $\{W_t\}$ *is the Wiener process, and* $\sigma_t = \sigma T/(T-t)$*, where* σ *is a parameter. Then starting from an arbitrary initial state* $|\psi_0\rangle$ *the wave function collapses to an energy eigenstate at time* T*. Energy is conserved in expectation, and the probability of collapse to a state of energy* E_i $(i=1,2,3,\ldots,n)$ *is in accordance with the Born law*

$$\pi_i = \frac{\langle\psi_0|\hat{\Pi}_i|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}, \tag{5}$$

where $\hat{\Pi}_i$ *is the projection operator onto the Hilbert subspace of states with energy* E_i*.*

Our model (3) contains two parameters, namely, the reduction time T and the energy volatility parameter σ, which has the units $(\text{energy})^{-1}(\text{time})^{-1/2}$. An application of the Ito product rule

$$\mathrm{d}(X_tY_t) = X_t(\mathrm{d}Y_t) + (\mathrm{d}X_t)Y_t + (\mathrm{d}X_t)(\mathrm{d}Y_t) \tag{6}$$

shows that the normalization of $|\psi_t\rangle$ is preserved under (3), so $\mathrm{d}\langle\psi_t|\psi_t\rangle = 0$, and that $\{H_t\}$ satisfies

$$\mathrm{d}H_t = \sigma_t V_t \mathrm{d}W_t, \tag{7}$$

where

$$V_t = \frac{\langle\psi_t|(\hat{H}-H_t)^2|\psi_t\rangle}{\langle\psi_t|\psi_t\rangle} \tag{8}$$

is the energy variance. It follows from (7) that the energy process $\{H_t\}$ has no drift and thus satisfies the conservation law

$$\mathbb{E}[H_u|\{W_s\}_{0\leqslant s\leqslant t}] = H_t \tag{9}$$

for $0\leqslant t\leqslant u$, where $\mathbb{E}[-|\{W_s\}_{0\leqslant s\leqslant t}]$ denotes conditional expectation given the trajectory of the Wiener process from time 0 up to time t.

To verify the collapse property we shall examine the dynamics of the energy variance process $\{V_t\}$. In particular, by use of the Ito rule (6) together with Jensen's inequality we deduce that

$$\bar{V}_t \leqslant V_0 - \int_0^t \sigma_s^2 \bar{V}_s^2 \mathrm{d}s, \tag{10}$$

where $\bar{V}_t = \mathbb{E}[V_t]$ is the unconditional expectation of the energy variance, which is nonnegative. Since $\bar{V}_t \leqslant \bar{V}_s$ for $s\leqslant t$, the inequality (10) remains valid if we replace $\bar{V}_s$ with $\bar{V}_T$ in the integrand. It follows for any $t\leqslant T$ that

$$\bar{V}_t \leqslant V_0 - \sigma^2 \frac{tT}{T-t} \bar{V}_T^2. \tag{11}$$

Now suppose it were the case that $\bar{V}_T > 0$. Then there would exist a time

$$t_0 = \frac{V_0 T}{V_0 + \sigma^2 T \bar{V}_T^2} < T \tag{12}$$

such that the right-hand side of (11) vanishes and hence such that $\bar{V}_{t_0} = 0$. This contradicts our supposition, and hence we conclude that $\bar{V}_T = 0$, and thus $V_T = 0$ with probability one.

To verify the Born law we must show that the conditional transition probability

$$\pi_{it} = \frac{\langle \psi_t | \hat{\Pi}_i | \psi_t \rangle}{\langle \psi_t | \psi_t \rangle} \tag{13}$$

is conserved in expectation, i.e., that $\pi_i = \mathbb{E}[\pi_{it}]$ for $t \leqslant T$. This follows from an application of Ito's rule, which implies that $\mathrm{d}\pi_{it} = \sigma_t (E_i - H_t)\pi_{it} \mathrm{d}W_t$ and thus that $\{\pi_{it}\}$ has no drift. Because $\mathbb{E}[\pi_{iT}]$ is the probability of collapse to a state with energy E_i, the conservation law shows that this is given by the Born probability π_i.

We now proceed to investigate the dynamical equation (3) further, with a view to obtaining a closed-form solution. First we observe that (3) can be cast into an integral form that incorporates the initial condition. In particular, it follows from (3) that

$$|\psi_t\rangle = \hat{U}_t \hat{M}_t^{1/2} |\psi_0\rangle, \tag{14}$$

where $\hat{U}_t = \mathrm{e}^{-\mathrm{i}\hat{H}t}$ is the standard unitary evolutionary operator associated with $\hat{H}$, and

$$\hat{M}_t = \frac{\exp(\hat{H}\int_0^t \sigma_s (\mathrm{d}W_s + \sigma_s H_s \mathrm{d}s) - \frac{1}{2}\hat{H}^2 \int_0^t \sigma_s^2 \mathrm{d}s)}{\exp(\int_0^t \sigma_s H_s (\mathrm{d}W_s + \sigma_s H_s \mathrm{d}s) - \frac{1}{2}\int_0^t \sigma_s^2 H_s^2 \mathrm{d}s)} \tag{15}$$

is a positive operator-valued process. Next we introduce a process $\{W_t^*\}$ defined by

$$W_t^* = W_t + \int_0^t \sigma_s H_s \mathrm{d}s. \tag{16}$$

With respect to the Wiener measure $\mathbb{P}$, under which $\{W_t\}$ is a standard Brownian motion, $\{W_t^*\}$ is a Brownian motion with drift. Therefore, by the well-known theorem of Girsanov there exists a measure $\mathbb{Q}$ with the property that $\{W_t^*\}$ is a $\mathbb{Q}$-Brownian motion for $t \in [0, T)$. Since the dynamical law (3) preserves the normalization of $|\psi_t\rangle$, it follows from (14) that $\langle \psi_0 | \hat{M}_t | \psi_0 \rangle = \langle \psi_0 | \psi_0 \rangle$ for $t \in [0, T)$, and hence that

$$\hat{M}_t = \frac{1}{\Phi_t} \exp\left(\hat{H} \int_0^t \sigma_s \mathrm{d}W_s^* - \frac{1}{2}\hat{H}^2 \int_0^t \sigma_s^2 \mathrm{d}s \right), \tag{17}$$

where

$$\Phi_t = \exp\left(\int_0^t \sigma_s H_s \mathrm{d}W_s^* - \frac{1}{2}\int_0^t \sigma_s^2 H_s^2 \mathrm{d}s \right) = \frac{\langle \psi_0 | \exp(\hat{H}\int_0^t \sigma_s \mathrm{d}W_t^* - \frac{1}{2}\hat{H}^2 \int_0^t \sigma_s^2 \mathrm{d}t) | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle}. \tag{18}$$

We recall that at time t the probability of reduction to a state with energy E_i is given by (13). By use of (14), the commutation relation $[\hat{M}_t, \hat{\Pi}_i] = 0$, and the normalization condition $\langle \psi_0 | \hat{M}_t | \psi_0 \rangle = \langle \psi_0 | \psi_0 \rangle$, it follows then that

$$\pi_{it} = \frac{\langle \psi_0 | \hat{\Pi}_i \hat{M}_t | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle}. \tag{19}$$

Substituting (17) into this relation we thus obtain

$$\pi_{it} = \frac{\langle \psi_0 | \hat{\Pi}_i \exp(\hat{H} \int_0^t \sigma_s \mathrm{d}W_s^* - \frac{1}{2}\hat{H}^2 \int_0^t \sigma_s^2 \mathrm{d}s) | \psi_0 \rangle}{\langle \psi_0 | \exp(\hat{H} \int_0^t \sigma_s \mathrm{d}W_s^* - \frac{1}{2}\hat{H}^2 \int_0^t \sigma_s^2 \mathrm{d}s) | \psi_0 \rangle} = \frac{\pi_i \exp(E_i \int_0^t \sigma_s \mathrm{d}W_s^* - \frac{1}{2}E_i^2 \int_0^t \sigma_s^2 \mathrm{d}s)}{\Sigma_i \pi_i \exp(E_i \int_0^t \sigma_s \mathrm{d}W_s^* - \frac{1}{2}E_i^2 \int_0^t \sigma_s^2 \mathrm{d}s)}. \tag{20}$$

Recalling that $\sigma_s = \sigma T/(T-s)$, we find it convenient now to introduce a process $\{\xi_t\}$ defined by

$$\xi_t = (T-t) \int_0^t \frac{1}{T-s} \mathrm{d}W_s^*. \tag{21}$$

We observe that the right-hand side of (21) is an integral representation for a *Brownian bridge*[7] in the $\mathbb{Q}$ measure. Substituting (21) into (20) we infer that the reduction probability π_{it} can be expressed in terms of the variable ξ_t as follows:

$$\pi_{it} = \frac{\pi_i \exp\left(\frac{\sigma \xi_t E_i T - \frac{1}{2}\sigma^2 E_i^2 t T}{T-t} \right)}{\Sigma_i \pi_i \exp\left(\frac{\sigma \xi_t E_i T - \frac{1}{2}\sigma^2 E_i^2 t T}{T-t} \right)}. \tag{22}$$

Further, on account of the relation $H_t = \Sigma_i E_i \pi_{it}$ for the energy process, we deduce that:

$$H_t = \frac{\Sigma_i \pi_i E_i \exp\left(\frac{\sigma \xi_t E_i T - \frac{1}{2}\sigma^2 E_i^2 t T}{T-t} \right)}{\Sigma_i \pi_i \exp\left(\frac{\sigma \xi_t E_i T - \frac{1}{2}\sigma^2 E_i^2 t T}{T-t} \right)}. \tag{23}$$

In view of the exact solution to the asymptotic collapse model obtained in Ref. 8, the fact that H_t and π_{it} can be expressed as functions of ξ_t and t suggests there might be a simple representation for ξ_t in terms of elementary random data that can be specified without reference to the state-vector process. If so, we can substitute such a representation for ξ_t into (23) to obtain a closed-form solution to the stochastic equation, in place of the integral representation (14) which implicitly depends on $\{|\psi_t\rangle\}$.

We thus proceed as follows: we define a process $\{\beta_t\}$ by the relation

$$\beta_t = \xi_t - \sigma t H_T, \tag{24}$$

where H_T is the terminal value of the energy. We claim that the random variables β_t and H_T are independent. To establish their independence it suffices to verify that

$$\mathbb{E}[\mathrm{e}^{x\beta_t + yH_T}] = \mathbb{E}[\mathrm{e}^{x\beta_t}]\mathbb{E}[\mathrm{e}^{yH_T}] \tag{25}$$

for arbitrary x, y. Using the tower property of conditional expectation we have

$$\mathbb{E}[\mathrm{e}^{x\beta_t + yH_T}] = \mathbb{E}[\mathrm{e}^{x\xi_t}\mathbb{E}[\mathrm{e}^{(y-\sigma t x)H_T} | \xi_t]]. \tag{26}$$

Let us consider the inner expectation $\mathbb{E}[\mathrm{e}^{(y-\sigma t x)H_T} | \xi_t]$. Using expression (22) for the conditional probability distribution of the terminal energy H_T we obtain

$$\mathbb{E}[\mathrm{e}^{(y-\sigma t x)H_T} | \xi_t] = \Phi_t^{-1} \sum_i \pi_i \mathrm{e}^{(y-\sigma t x)E_i} \exp\left(\frac{\sigma \xi_t E_i T - \frac{1}{2}\sigma^2 E_i^2 t T}{T-t} \right).$$

Now $\{\Phi_t\}$ is the density process for changing the measure from $\mathbb{Q}$ to $\mathbb{P}$. That is to say, the expectation $\mathbb{E}$ under $\mathbb{P}$, in which $\{W_t\}$ is a standard Brownian motion, is related to the expectation $\mathbb{E}^{\mathbb{Q}}$ under $\mathbb{Q}$, in which $\{W_t^*\}$ is a standard Brownian motion, according to

$$\mathbb{E}[X_u|\{W_s\}_{0\leqslant s\leqslant t}] = \frac{1}{\Phi_t}\mathbb{E}^{\mathbb{Q}}[\Phi_u X_u|\{W_s\}_{0\leqslant s\leqslant t}], \tag{27}$$

for any random variable X_u that can be expressed as a functional of the trajectory $\{W_s\}_{0\leqslant s\leqslant u}$. Thus making use of the fact that $\{\xi_t\}$ is a Brownian bridge under $\mathbb{Q}$, we deduce, after some rearrangement of terms, that

$$\mathbb{E}[\mathrm{e}^{x\beta_t+yH_T}] = \sum_i \pi_i\, \mathrm{e}^{yE_i}\, \mathrm{e}^{[t(T-t)/2T]x^2}. \tag{28}$$

Here we have used the facts that if g is a zero-mean Gaussian random variable with variance γ^2, then $\mathbb{E}[\mathrm{e}^{xg}]=\mathrm{e}^{(1/2)\gamma^2x^2}$, and that the variance of the Brownian bridge $\{\xi_t\}$ is $t(T-t)/T$. This proves the independence of $\{\beta_t\}$ and H_T.

The result (28) also establishes that under $\mathbb{P}$ the process $\{\beta_t\}$ is Gaussian, and has mean zero and variance $t(T-t)/T$ for $t\in[0,T)$. A similar line of argument shows for $s\leqslant t$ that the covariance of β_s and β_t is

$$\mathrm{Cov}[\beta_s,\beta_t] = s(T-t)/T. \tag{29}$$

Therefore we conclude that $\{\beta_t\}$ is a $\mathbb{P}$-Brownian bridge. As a consequence, there exists a Brownian motion $\{B_t\}$ such that $\{\beta_t\}$ admits an integral representation:

$$\beta_t = (T-t)\int_0^t \frac{1}{T-s}\mathrm{d}B_s. \tag{30}$$

Thus we have verified that the process $\{\xi_t\}$ can be expressed in the form

$$\xi_t = \sigma t H_T + \beta_t, \tag{31}$$

where H_T is the terminal energy, and $\{\beta_t\}$ is an independent Brownian bridge.

Conversely, *given a discrete random variable H_T taking the values $\{E_i\}$ with probability $\{\pi_i\}$, and given an independent Brownian bridge process $\{\beta_t\}$ on the interval $[0,T]$, we can use the ansatz* (31) *as a basis for constructing a closed-form solution to the dynamical equation* (3).

The argument can be sketched as follows. First, given $\{\xi_t\}$ as defined above in terms of H_T and $\{\beta_t\}$, let $\pi_{it}=\mathbb{P}(H_T=E_i|\,\xi_t)$ be the conditional probability that H_T takes the value E_i when the value of ξ_t is specified. It follows by use of the Bayes formula that

$$\mathbb{P}(H_T=E_i|\xi_t) = \frac{\pi_i\rho(\xi_t|H_T=E_i)}{\Sigma_i\pi_i\rho(\xi_t|H_T=E_i)}, \tag{32}$$

where

$$\rho(\xi_t|H_T=E_i) = \sqrt{\frac{T}{2\pi t(T-t)}}\exp\left(-\frac{(\xi_t-\sigma tE_i)^2T}{2t(T-t)}\right). \tag{33}$$

Expression (33) can be deduced from the fact that conditional on $H_T=E_i$ the variable ξ_t in (31) is normally distributed with mean σtE_i and variance $t(T-t)/T$. Thus, we recover the expression (22) for $\{\pi_{it}\}$. Then by an application of Ito calculus we obtain

$$\mathrm{d}\pi_{it} = \sigma_t(E_i-H_t)\pi_{it}\mathrm{d}W_t, \tag{34}$$

where now the process $\{W_t\}$ is *defined* in terms of $\{\xi_t\}$ by the relation

$$W_t = \int_0^t \frac{1}{T-s}(\xi_s - \sigma T H_s)\mathrm{d}s + \xi_t, \tag{35}$$

and $\{H_t\}$ is defined by $H_t = \Sigma_i \pi_{it} E_i$. The process $\{W_t\}$ thus determined turns out to be a standard Brownian motion. This can be demonstrated by showing that $\{W_t\}$ satisfies $\mathbb{E}[W_t|\{W_u\}_{0\leqslant u\leqslant s}] = W_s$ for $s \leqslant t$ and $(\mathrm{d}W_t)^2 = \mathrm{d}t$. Finally, if we write

$$|\phi_i\rangle = \frac{\hat{\Pi}_i|\psi_0\rangle}{\langle\psi_0|\hat{\Pi}_i|\psi_0\rangle^{1/2}} \tag{36}$$

for the standard Lüders states, then the state vector $\{|\psi_t\rangle\}$ that solves (3) can be written in the form

$$|\psi_t\rangle = \mathrm{e}^{-\mathrm{i}\hat{H}t}\sum_i \sqrt{\pi_{it}}|\phi_i\rangle, \tag{37}$$

or, more explicitly,

$$|\psi_t\rangle = \sum_i \frac{\sqrt{\pi_i}\exp\left(-\mathrm{i}E_i t + \frac{1}{2}E_i\sigma_t\xi_t - \frac{1}{4}E_i^2\int_0^t\sigma_s^2\mathrm{d}s\right)}{\sqrt{\Sigma_i \pi_i \exp\left(\frac{1}{2}E_i\sigma_t\xi_t - \frac{1}{4}E_i^2\int_0^t\sigma_s^2\mathrm{d}s\right)}}|\phi_i\rangle, \tag{38}$$

where $\sigma_s = \sigma T/(T-s)$, and $\xi_t = \sigma t H_T + \beta_t$. A straightforward calculation shows that $|\psi_t\rangle \to |\phi_k\rangle$ as $t \to T$, if we set $H_T = E_k$ in (38). By taking the stochastic differential of (38), and using (35), we are led back to the starting point (3), which directly verifies that (38) is the solution to the dynamical equation (3).

We thus conclude that the substitution of (31) in (23) yields a closed-form expression for the energy process in terms of the exogenously specifiable independent data $\{H_T\}$ and $\{\beta_t\}$. As a consequence, we are able to directly simulate the solution to the stochastic equation, as well as the associated energy evolution $\{H_t\}$, for an arbitrary finite-dimensional quantum system.

Next, we remark on the interpretation of the finite-time collapse model (3). First we observe (cf. Ref. 7) that if $\{B_t\}$ is a standard Brownian motion on the interval $[0,T]$, then the process $\{\widetilde{B}_\tau\}$ defined by

$$\widetilde{B}_\tau = \int_0^{\tau T/(\tau+T)} \frac{T}{T-s}\mathrm{d}B_s \tag{39}$$

is a standard Brownian motion on the time interval $[0,\infty)$. In particular, let us introduce a new time variable by the relation $\tau(t) = tT/(T-t)$, and define

$$\eta_\tau = \frac{T}{T-t}\xi_t = \left(1 + \frac{\tau}{T}\right)\xi_{\tau T/(\tau+T)}. \tag{40}$$

Then Eq. (31) can be put into the form

$$\eta_\tau = \frac{\sigma t T H_T}{T-t} + \frac{T\beta_t}{T-t} = \sigma\tau H_T + \int_0^t \frac{T}{T-s}\mathrm{d}B_s, \tag{41}$$

on account of the integral representation (30). Making use of relations (39) and

$$t = \frac{\tau T}{\tau + T}, \tag{42}$$

we thus deduce that

$$\eta_\tau = \sigma\tau H_T + \widetilde{B}_\tau. \tag{43}$$

However, this is the ansatz (cf. Ref. 8) that determines *asymptotic* collapse to an energy eigenstate. That is to say, the expectation $H_\tau = \mathbb{E}[H_T | \eta_\tau]$ determines the energy process $\{H_\tau\}$ associated with the standard energy-based infinite-time collapse models. Therefore, if we take the infinite-time collapse model and replace the time variable t with a clock $\tau(t)$, then as $t \to T$, the clock $\tau(t)$ "ticks" faster and faster. Eventually, in a system for which time is measured by "internal" time t, the collapse takes place in a finite time interval T, whereas in a system for which time is measured by the clock variable $\tau(t)$, the collapse takes place asymptotically as $\tau \to \infty$.

In summary, we have introduced a consistent energy-based collapse model that achieves state reduction in finite time, thus meeting the "challenge" posed in Ref. 9. We have verified the collapse property directly by solving the dynamical equation (3) explicitly for the state-vector process $\{|\psi_t\rangle\}$ in terms of independently specifiable random data. We have also obtained closed form expressions for the energy process $\{H_t\}$ and the reduction probability process $\{\pi_{it}\}$. An argument based on a time-change shows that the finite-time collapse model is related to the infinite-time collapse model by a nonlinear transformation of the time variable.

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No-cloning of nonorthogonal states does not require inner product preserving

Dafa Li[a)]
Department of Mathematical Sciences, Tsinghua University, Beijing 100084, China

Xiangrong Li
Department of Mathematics, University of California, Irvine, California 92697-3875

Hongtao Huang
Electrical Engineering and Computer Science Department, University of Michigan, Ann Arbor, Michigan 48109

Xinxin Li
Department of Computer Science, Wayne State University, Detroit, Michigan 48202

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The no-cloning theorem says there is no quantum copy machine which can copy any one-qubit state. Inner product preserving was always used to prove the no-cloning of nonorthogonal states. In this paper we show that the no-cloning of nonorthogonal states does not require inner product preserving and discuss the minimal properties which a linear operator possesses to copy two different states at the same device. In this paper, we obtain the following necessary and sufficient condition. For any two different states $|\psi\rangle=a|0\rangle+b|1\rangle$ and $|\varphi\rangle=c|0\rangle+d|1\rangle$, assume that a linear operator L can copy them, that is, $L(|\psi,0\rangle)=|\psi,\psi\rangle$ and $L(|\varphi,0\rangle)=|\varphi,\varphi\rangle$. Then the two states are orthogonal if and only if $L(|0,0\rangle)$ and $L(|1,0\rangle)$ are unit length states. Thus we only need linearity and that $L(|0,0\rangle)$ and $L(|1,0\rangle)$ are unit length states to prove the no-cloning of nonorthogonal states. It implies that inner product preserving is not necessary for the no-cloning of nonorthogonal states. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1996327]

I. INTRODUCTION

The no-cloning theorem from the work of Wootters and Zurek said there is no quantum copy machine which can copy any quantum state.[1–3] The authors in Refs. 1 and 4 demonstrated if a quantum copy machine can copy two basis states, then it cannot copy their suppositions. Another version of the no-cloning theorem was stated in Ref. 5. The authors in Refs. 6–8 used inner product preserving to show that nonorthogonal states cannot be cloned by a unitary operator. The no-cloning theorem was extended to mixed states by Barnum *et al.*[3] Some authors presented approximate copies of qubits.[4,8] Mor suggested a type of the no-cloning principle and discussed various cases in which orthogonal states cannot be cloned in principle.[9]

Let $|0\rangle$ and $|1\rangle$ be the basis states of a one-qubit system and $|0,0\rangle$, $|0,1\rangle$, $|1,0\rangle$ and $|1,1\rangle$ be the basis states of a two-qubit system.

Let $|\psi\rangle=a|0\rangle+b|1\rangle$, where a and b are complex and

$$\|a\|^2+\|b\|^2=1. \tag{1}$$

Let $|\varphi\rangle=c|0\rangle+d|1\rangle$, where c and d are complex and

[a)]Electronic mail: dli@math.tsinghua.edu.cn

$$\|c\|^2 + \|d\|^2 = 1. \tag{2}$$

Assume that a linear operator L can copy states $|\psi\rangle$ and $|\varphi\rangle$, that is, $L(|\psi,0\rangle)=|\psi,\psi\rangle$ and $L(|\varphi,0\rangle)=|\varphi,\varphi\rangle$. By tensor product $|\psi,\psi\rangle=(a|0\rangle+b|1\rangle)\otimes(a|0\rangle+b|1\rangle)=a^2|0,0\rangle+ab|0,1\rangle+ab|1,0\rangle+b^2|1,1\rangle$. By the linearity of L, $L(|\psi,0\rangle)=aL(|0,0\rangle)+bL(|1,0\rangle)$. So we get

$$aL(|0,0\rangle) + bL(|1,0\rangle) = a^2|0,0\rangle + ab|0,1\rangle + ab|1,0\rangle + b^2|1,1\rangle. \tag{3}$$

From that $L(|\varphi,0\rangle)=|\varphi,\varphi\rangle$, similarly we get

$$cL(|0,0\rangle) + dL(|1,0\rangle) = c^2|0,0\rangle + cd|0,1\rangle + cd|1,0\rangle + d^2|1,1\rangle. \tag{4}$$

Since $|\psi\rangle$ and $|\varphi\rangle$ are different, the determinant of the coefficient matrix

$$ad - bc \neq 0. \tag{5}$$

Thus from Eqs. (3) and (4) we get by Gramer's rule the following $L(|0,0\rangle)$ and $L(|1,0\rangle)$: $L(|0,0\rangle)=(1/(ad-bc))((a^2d-bc^2)|0,0\rangle+bd(a-c)|0,1\rangle+bd(a-c)|1,0\rangle+bd(b-d)|1,1\rangle)$, $L(|1,0\rangle)=(1/(ad-bc))(ac(c-a)|0,0\rangle+ac(d-b)|0,1\rangle+ac(d-b)|1,0\rangle+(ad^2-b^2c)|1,1\rangle)$.

In this paper $\|x\|$ denotes the norm of $|x\rangle$ or a complex number x. Let $|\alpha\rangle=L(|0,0\rangle)$ and $|\beta\rangle=L(|1,0\rangle)$, $P=\|a^2d-bc^2\|^2+2\|bd(a-c)\|^2+\|bd(b-d)\|^2$ and $Q=\|ac(c-a))\|^2+2\|ac(d-b)\|^2+\|ad^2-b^2c\|^2$. Then

$$\|\alpha\|^2 = P/\|(ad - bc)\|^2 \tag{6}$$

and

$$\|\beta\|^2 = Q/\|(ad - bc)\|^2. \tag{7}$$

II. LEMMA 1

Assume that a linear operator L can copy different states $|\psi\rangle$ and $|\varphi\rangle$. If $|\psi\rangle$ and $|\varphi\rangle$ are orthonormal, then $L(|0,0\rangle)$ and $L(|1,0\rangle)$ are orthonormal.

Proof: First let us prove that $L(|0,0\rangle)$ and $L(|1,0\rangle)$ are unit length states. Since $|\psi\rangle$ and $|\varphi\rangle$ are orthonormal, $\langle\psi|\varphi\rangle=0$, i.e.,

$$a\overline{c} + b\overline{d} = 0 \tag{8}$$

where $\overline{c}$ and $\overline{d}$ are complex conjugates of c and d, respectively. From Eq. (8) we obtain that $\|a\|^2\|c\|^2=\|b\|^2\|d\|^2$. By using Eqs. (1) and (2) $\|a\|^2\|c\|^2=(1-\|a\|^2)(1-\|c\|^2)$. It follows that $\|a\|^2+\|c\|^2=1$. We can as well get $\|b\|^2+\|d\|^2=1$.

We assume that a, b, c, and d are all real. It is not hard to extend the results in this paper to complex a, b, c, and d. Thus we obtain that

$$a^2 + c^2 = 1, \tag{9}$$

$P=(a^2d-bc^2)^2+2(bd(a-c))^2+(bd(b-d))^2$ and $Q=(ac(c-a))^2+2(ac(d-b))^2+(ad^2-b^2c)^2$. In P and Q, simultaneously replacing b^2 by $(1-a^2)$ [see Eq. (1)] and d^2 by $(1-c^2)$ [see Eq. (2)], respectively, P and Q are reduced into the following forms:

$$P = 2 + 2bda^2 + 2bdc^2 - a^2 - c^2 - 4a^2c^2db + 4ac^3 + 4a^3c - 4a^3c^3 - 4ac - 2bd, \tag{10}$$

$$Q = -4a^3c^3 - 4a^2c^2db + a^2 - 2ac + 2ac^3 + 2a^3c + c^2. \tag{11}$$

Let us compute P and Q when $|\psi\rangle$ and $|\varphi\rangle$ are orthogonal. Replacing bd by $-ac$ [see Eq. (8)] and using Eq. (9) in Eqs. (10) and (11), respectively, we obtain that $P=(a^2+c^2)^2=1$ and $Q=(1+2ac)(a^2+c^2)-2ac=1$.

Next let us compute the determinant of the coefficient matrix in Eq. (5) when $|\psi\rangle$ and $|\varphi\rangle$ are orthogonal. Simultaneously replacing b^2 by $(1-a^2)$ [see Eq. (1)] and d^2 by $(1-c^2)$ [see Eq. (2)] and bd by $-ac$ [see Eq. (8)] and using Eq. (9), we derive that $\|ad-bc\|^2=(a^2+c^2)=1$.

From Eqs. (6) and (7) and the above it is easy to get $\|\alpha\|=1$ and $\|\beta\|=1$. That is, $L(|0,0\rangle)$ and $L(|1,0\rangle)$ are unit length states.

Second, we show that $L(|0,0\rangle)$ and $L(|1,0\rangle)$ are orthogonal. After omitting the factor the inner product of $L(|0,0\rangle)$ and $L(|1,0\rangle)$ is $(a^2d-bc^2)ac(c-a)+2bd(a-c)ac(d-b)+bd(b-d)(ad^2-b^2c)$ (replacing b^2 by $(1-a^2)$ [see Eq. (1)] and d^2 by $(1-c^2)$ [see Eq. (2)])

$$=-(a-c)(a^3cd-bd^2ac+b^2dac-ac^3b-b^2d+bd^2)$$

(using $a^2+b^2=1$ and $c^2+d^2=1$)

$$=-(a-c)(d-b)(ac+bd).$$

Equation (8) implies that $L(|0,0\rangle)$ and $L(|1,0\rangle)$ are orthogonal.

Examples: The following combinations of a, b, c, and d satisfy $ac+bd=0$, that is, $|\psi\rangle$ and $|\varphi\rangle$ are orthogonal. It is easy to verify that $\|\alpha\|^2=1=\|\beta\|^2$.

1. $a=\sqrt{2}/2$, $b=\sqrt{2}/2$, $c=\sqrt{2}/2$, $d=-\sqrt{2}/2$.
2. $a=\sqrt{3}/2$, $b=1/2$, $c=1/2$, $d=-\sqrt{3}/2$.
3. $a=3/5$, $b=4/5$, $c=4/5$, $d=-3/5$.

Remark: However, that $L(|0,0\rangle)$ and $L(|1,0\rangle)$ are orthogonal cannot guarantee that $|\psi\rangle$ and $|\varphi\rangle$ are orthogonal. For example, $|\psi\rangle=a|0\rangle+b|1\rangle$ and $|\varphi\rangle=a|0\rangle-b|1\rangle$, where $a^2+b^2=1$ and $a\neq\pm b$. Though $L(|0,0\rangle)$ and $L(|1,0\rangle)$ are orthogonal, $\langle\psi|\varphi\rangle\neq 0$, namely, $|\psi\rangle$ and $|\varphi\rangle$ are not orthogonal.

Corollary: For any two orthogonal states, there is a unitary operator which can copy them.

Proof: Let $|\psi\rangle=a|0\rangle+b|1\rangle$ and $|\varphi\rangle=c|0\rangle+d|1\rangle$ be orthogonal states. Let the truth table be the following matrix L.

	$\|0,0\rangle$	$\|0,1\rangle$	$\|1,0\rangle$	$\|1,1\rangle$
$\|0,0\rangle$	$\frac{a^2d-bc^2}{ad-bc}$	$\frac{bd(a-c)}{ad-bc}$	$\frac{bd(a-c)}{ad-bc}$	$\frac{bd(b-d)}{ad-bc}$
$\|0,1\rangle$	0	$-\sqrt{2}/2$	$\sqrt{2}/2$	0
$\|1,0\rangle$	$\frac{ac(c-a)}{ad-bc}$	$\frac{ac(d-b)}{ad-bc}$	$\frac{ac(d-b)}{ad-bc}$	$\frac{ad^2-b^2c}{ad-bc}$
$\|1,1\rangle$	0	$-\sqrt{2}/2$	$\sqrt{2}/2$	0

It is easy to verify that L is unitary by Lemma 1 and not hard to show that $L(|\psi,0\rangle)=|\psi,\psi\rangle$ and $L(|\varphi,0\rangle)=|\varphi,\varphi\rangle$.

III. LEMMA 2

Assume that a linear operator L can copy two different states $|\psi\rangle$ and $|\varphi\rangle$. If $L(|0,0\rangle)$ and $L(|1,0\rangle)$ are unit length states, then $|\psi\rangle$ and $|\varphi\rangle$ are orthogonal.

Proof: Since $\|\alpha\|=1$, from Eq. (6) we obtain that $P=\|ad-bc\|^2$, and since $\|\beta\|=1$, from Eq. (7) we get that $Q=\|ad-bc\|^2$. Thus $P-Q=0$. Using Eqs. (10) and (11), equation $P-Q=0$ is reduced into the following one:

$$2+2bda^2+2bdc^2-2a^2-2c^2+2ac^3+2a^3c-2ac-2bd=2(a^2+c^2-1)(ac+bd-1)=0.$$

There are two cases. *Case 1*: $a^2+c^2=1$ and *case 2*: $ac+bd=1$. We shall show that in case 1 $|\psi\rangle$ and $|\varphi\rangle$ are orthogonal and case 2 does not occur.

Case 1 in which $a^2+c^2=1$: By simultaneously replacing b^2 by $(1-a^2)$ [see Eq. (1)] and d^2 by

$(1-c^2)$ [see Eq. (2)], it is reduced that $(ac)^2-(bd)^2=(ac)^2-(1-a^2)(1-c^2)=-1+c^2+a^2=0$. Hence $(ac)^2-(bd)^2=(ac-bd)(ac+bd)=0$. There are two subcases.

1.1 *Subcase 1.1*: $ac+bd=0$, that is, $|\psi\rangle$ and $|\varphi\rangle$ are orthogonal.
1.2 *Subcase 1.2*: $ac-bd=0$, that is,

$$ac=bd. \tag{12}$$

We shall show that in subcase 1.2 $|\psi\rangle$ and $|\varphi\rangle$ are also orthogonal. Let us first compute the determinant of the coefficient matrix (5). Simultaneously replacing b^2 by $(1-a^2)$ [see Eq. (1)], d^2 by $(1-c^2)$ [see Eq. (2)] and bd by ac [see Eq. (12)], we derive that $(ad-bc)^2=a^2d^2-2acbd+b^2c^2=a^2(1-c^2)-2ac(ac)+(1-a^2)c^2=a^2-4a^2c^2+c^2$. Using $a^2+c^2=1$, it follows that $(ad-bc)^2=1-4a^2c^2=(1-2ac)(1+2ac)$. By requirement for the determinant of the coefficient matrix in Eq. (5), $(ad-bc)^2=(1-2ac)(1+2ac)\neq 0$.

Next let us compute P in Eq. (10) and Q in Eq. (11) by replacing bd by ac [see Eq. (12)] and using $a^2+c^2=1$. We get that $P=1-8a^3c^3=(1-2ac)(4a^2c^2+2ac+1)$ and $\|\alpha\|^2=(4a^2c^2+2ac+1)/(1+2ac)$; $Q=1-8a^3c^3=(1-2ac)(4a^2c^2+2ac+1)$ and $\|\beta\|^2=(4a^2c^2+2ac+1)/(1+2ac)$. Let $\|\alpha\|^2=\|\beta\|^2=1$. Then $ac=0$. From $ac=bd$, we obtain $ac+bd=0$. In other words, $|\psi\rangle$ and $|\varphi\rangle$ are also orthogonal for subcase 1.2.

Consequently when $a^2+c^2=1$, we derive that $ac+bd=0$, namely, $|\psi\rangle$ and $|\varphi\rangle$ are orthogonal.

Case 2 in which $ac+bd=1$: We shall show that case 2 does not occur. If $ac+bd=1$, then $(ac+bd)^2-1=a^2c^2+2acbd+b^2d^2-1=0$. Simultaneously replacing b^2 by $(1-a^2)$ [see Eq. (1)], d^2 by $(1-c^2)$ [see Eq. (2)] and bd by $(1-ac)$, we infer that $a^2c^2+2ac(1-ac)+(1-a^2)(1-c^2)-1=-(a-c)^2=0$. It follows that $a=c$.

Next let us compute the determinant of the coefficient matrix (5) in the case $ac+bd=1$. Simultaneously replacing b^2 by $(1-a^2)$ [see Eq. (1)], d^2 by $(1-c^2)$ [see Eq. (2)], and bd by $(1-ac)$, we derive that $(ad-bc)^2=a^2d^2-2adbc+b^2c^2=a^2(1-c^2)-2ac(1-ac)+(1-a^2)c^2=(a-c)^2$. By the requirement for the determinant of the coefficient matrix in Eq. (5) $ad-bc\neq 0$, it follows that $a\neq c$.

Therefore this case contradicts our hypothesis for the determinant of the coefficient matrix $ad-bc\neq 0$ in Eq. (5). In other words, case 2 does not happen.

IV. THE NO-CLONING OF NONORTHOGONAL STATES DOES NOT REQUIRE INNER PRODUCT PRESERVING

The authors always used inner product preserving to prove the no-cloning of nonorthogonal states.[6–8] From Lemma 2, it is easy to see that we only need linearity and that $L(|0,0\rangle)$ and $L(|1,0\rangle)$ are unit length states to prove the no-cloning of nonorthogonal states. It shows that inner product preserving is not necessary for the no-cloning of nonorthogonal states.

The following examples show when $|\psi\rangle$ and $|\varphi\rangle$ are not orthogonal, $L(|0,0\rangle)$ and $L(|1,0\rangle)$ are not unit length states. When $a=3/5$, $b=4/5$, $c=3/5$. and $d=-4/5$, $\|\alpha\|^2=18/25$ and $\|\beta\|^2=337/225$; when $a=\sqrt{3}/2$, $b=1/2$, $c=\sqrt{3}/2$, and $d=-1/2$, $\|\alpha\|^2=5/6$, $\|\beta\|^2=3/2$.

V. CLONING LEADS TO INFINITY OF PROBABILITY AMPLITUDE

Let $|\gamma\rangle=c|0\rangle+d|1\rangle$, where $\|c\|^2+\|d\|^2=1$ and $c\neq 0$. Assume that a linear operator L can copy states $|1\rangle$ and $|\gamma\rangle$, that is, $L(|1,0\rangle)=|1,1\rangle$ and $L(|\gamma,0\rangle)=|\gamma,\gamma\rangle$. By the linearity of L and tensor product, it is easy to derive that $L(|0,0\rangle)=c|0,0\rangle+d|0,1\rangle+d|1,0\rangle+|((d^2-d)/c)|1,1\rangle$. Let $d<0$. Then d tends to -1 as c approaches 0 since $\|c\|^2+\|d\|^2=1$. Therefore the norm of probability amplitude $((d^2-d)/c)$ of state $|1,1\rangle$ tends to plus infinity as c approaches 0. For example, when $c=3/5$ and $d=-4/5$, $\|(d^2-d)/c\|=12/5$. It contradicts that the norm of probability amplitude should be 1 or less than 1.

Let $|\phi\rangle=L(|0,0\rangle)$. Then the norm of $|\phi\rangle$ is $\|\phi\|^2=\|c\|^2+\|d\|^2+\|d\|^2+\|(d^2-d)/c\|^2$ and clearly $\|\phi\|>1$. Notice that the norm of $|0,0\rangle$ is 1. It says again that cloning contradicts the norm preserving. For example, when $c=3/5$ and $d=-4/5$, $\|\phi\|=\sqrt{77/45}>1$.

VI. CONCLUSION

As is well known, the no-cloning theorem has far-reaching consequences for quantum information and quantum computing. Nielsen thought "what if we allow cloning devices that are not unitary?" is a good question which has been the subject of much investigation. See page 532 in Ref. 10.

In this paper we demonstrate that it only needs linearity and that $L(|0,0\rangle)$ and $L(|1,0\rangle)$ are unit length states to prove the no-cloning of nonorthogonal states. Clearly we do not require norm preservation for any state. It means that we do not make any use of unitarity. In theory, it is possible to derive a deeper result than the no-cloning principle by using the unitarity. Intuitively it seems that it is easier to implement the operator required in this paper than a unitary operator.

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Quantum channels and representation theory

William Gordon Ritter
Department of Physics, Harvard University, Cambridge, Massachusetts 02138

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In the study of d-dimensional quantum channels ($d \geqslant 2$), an assumption which includes many interesting examples, and which has a natural physical interpretation, is that the corresponding Kraus operators form a representation of a Lie algebra. Physically, this is a symmetry algebra for the interaction Hamiltonian. This paper begins a systematic study of channels defined by representations; the famous Werner-Holevo channel is one element of this infinite class. We show that the channel derived from the defining representation of $\mathfrak{su}(n)$ is a depolarizing channel for all n, but for most other representations this is not the case. Since the standard Bloch sphere only exists for the qubit representation of $\mathfrak{su}(2)$, we develop a consistent generalization of Bloch's technique. By representing the density matrix as a polynomial in Lie algebra generators, we determine a class of positive semidefinite matrices which represent quantum states for various channels defined by finite-dimensional representations of semisimple Lie algebras. We also give a general method for finding positive semidefinite matrices using Lie algebraic trace identities. This includes an analysis of channels based on the exceptional Lie algebra $\mathfrak{g}_2$ and the Clifford algebra. © *2005 American Institute of Physics.*
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I. INTRODUCTION

A quantum channel is a model for a particular snapshot of the time evolution of a density matrix, and especially for the evolution of pure into mixed states. Let $\mathcal{H}$ be a Hilbert space of dimension n, and let $\mathfrak{gl}(\mathcal{H})$ denote the vector space of all linear transformations $\mathcal{H} \to \mathcal{H}$. A map $\mathcal{E}: \mathfrak{gl}(\mathcal{H}) \to \mathfrak{gl}(\mathcal{H})$ is said to be *completely positive* (*CP*) if it is linear and $\mathcal{E} \otimes \mathbf{1}$ is positive on $\mathcal{H} \otimes \mathcal{H}'$ for all $\mathcal{H}'$. The map is said to be *trace-preserving* if $\operatorname{Tr} \mathcal{E}(A) = \operatorname{Tr} A$ for all $A \in \mathfrak{gl}(\mathcal{H})$.

Definition 1: A CPT map *(or* stochastic map *or* channel*) is a completely positive, trace-preserving linear transformation* $\mathcal{E}: \mathfrak{gl}(\mathcal{H}) \to \mathfrak{gl}(\mathcal{H})$.

Of central importance to the current work is a famous theorem of Kraus[1] which gives a simple representation of any quantum channel.

Theorem 1 (Kraus decomposition): *For any quantum channel* $\mathcal{E}$, *there exists a finite set of operators*

$$M_0, M_1, M_2, \ldots, M_k, \quad \text{where } k \leqslant (\dim \mathcal{H})^2,$$

such that

$$\mathcal{E}(\boldsymbol{\rho}) = \sum_{\mu} M_\mu \boldsymbol{\rho} M_\mu^\dagger \quad \text{with} \sum_{\mu} M_\mu^\dagger M_\mu = \mathbf{1}. \tag{1}$$

In this situation, (1) *is called the* Kraus representation, *the* operator sum representation *or the* Stinespring form, *while* $\Sigma_\mu M_\mu^\dagger M_\mu = \mathbf{1}$ *is sometimes called the* normalization condition *and is just the statement that the map is trace preserving.*

A proof of this theorem may be found in the original article of Kraus,[1] or in the book by Nielsen and Chuang.[2] We simply note that the converse, namely that any operator of the form (1)

satisfies the conditions of Definition 1, is clearly true. A stochastic map may also be obtained as the partial trace of a unitary conjugation on a larger space; see Ruskai,[3] Sec. III D for a discussion. The representation (1) is sometimes called the *Stinespring form* since its existence follows from the Stinespring dilation theorem.[4]

This is a general framework, and in order to obtain explicit results, further assumptions are necessary. A mathematically elegant assumption with important physical consequences is that the possible errors introduced in the decoherence process are not arbitrary, but that they correspond to the action of the infinitesimal generators of a Lie group G of continuous symmetries. For example, the *qubit depolarizing channel* is a model of a decohering qubit with an $\mathfrak{su}_2$ symmetry. With probability p an error occurs, which is implemented by one of the generators of the Lie algebra $\mathfrak{su}_2$ in its two-dimensional irreducible representation. These generators admit direct physical interpretations as bit-flip errors, phase-flip errors, or combinations of those. The qubit depolarizing channel admits a beautiful generalization to a channel with k possible errors based on a d-dimensional representation $\mathcal{H}$ of a k-dimensional Lie algebra $\mathfrak{g}$.

The situation just described, in which the error generators live in a matrix representation of a semisimple Lie algebra, arises naturally in the model of Markovian dynamics considered by Lidar, Chuang, and Whaley.[5] This was shown to have important consequences for the possibility of decoherence-free dynamics; see Lidar and Whaley,[6] and references therein for an up-to-date review. The present work may be considered as a further exploration of the consequences of that model.

Suppose the M_μ span the space of Hermitian operators, so that $\mu=0,\ldots,n^2-1$. Define $\lambda_0=\mathbf{1}$ and let λ_a for $a\geqslant 1$ denote the n-dimensional Gell-Mann matrices, which are standard generators for the Lie algebra $\mathfrak{su}_n$. Then $\{\lambda_\mu\}$ is a basis for the space of Hermitian matrices. Taking M_0 proportional to the identity, there exist constants U_{ab} such that $M_a=\Sigma_b U_{ab}\lambda_b$. If U is a unitary matrix, then we may take each M_μ proportional to λ_μ without changing the quantum channel defined by these Kraus operators.

In the latter case, one may readily calculate $\Sigma_\mu M_\mu \rho M_\mu^\dagger$, since ρ itself may be expanded in the λ_μ basis, and the Gell-Mann matrices in any dimension satisfy elegant product identities. This leads to a simple, elegant and explicit formula for the action of the $\mathfrak{su}_n$ channel; if $\rho=(1/d)\mathbf{1}+\Sigma_\mu v_\mu \lambda_\mu$ then the channel multiplies v by a scalar given in Sec. III. This is a wonderful calculational tool, and also has physical significance. A quantum channel models the interaction of a decohering system with its environment, and the identification of the M_μ as generators of a Lie algebra is related to symmetry of the interaction Hamiltonian.[5]

The generalizations of the $\mathfrak{su}_n$ calculations to other Lie algebras and to higher-dimensional representations are illuminating, and have not appeared in the literature before. These cases necessarily have the property that not all of the Hermitian matrices in that dimension are linear combinations of representation matrices, so direct generalization of the calculational method for $\mathfrak{su}_n$ will not work, and a new idea is required. This is the subject of Sec. IV. We give a detailed analysis of the spin-1 representation; however, many of the formulas we use there generalize readily to higher spin. In an interesting twist, the spin-one case turns out to be a generalization of the Werner-Holevo channel. Section V analyzes two channels, based, respectively, on the exceptional algebra $\mathfrak{g}_2$ and the Clifford algebra.

In Sec. VI we generalize some aspects of the Bloch sphere to density matrices constructed from Lie algebra representations. It is shown that for each representation, there is a class of positive semidefinite, Hermitian trace-one density operators parametrized by a closed, bounded (hence compact) submanifold of Euclidean space, which we term the Bloch manifold. Explicit bounds are given on the size of these manifolds. A general method is given for finding the Bloch manifold exactly, using trace identities.

II. QUANTUM CHANNELS FROM LIE ALGEBRA REPRESENTATIONS

This section contains our notations and conventions for the generalized depolarizing channels which will be studied in detail in later sections. The possibility of defining a quantum channel

based on a representation of a compact Lie algebra was mentioned briefly, but never elaborated upon, in a paper of Gregoratti and Werner.[7] In any case, it is not necessary that the Lie algebra be compact.

A. Pure Lie algebra channels

It is a standard convention[8,9] to normalize the canonical generators for the defining representation of $\mathfrak{su}_n$ so that

$$\mathrm{Tr}(\lambda_a \lambda_b) = 2\delta_{ab}. \tag{2}$$

This has the desirable feature that the canonical generators for $n=2$ are the Pauli matrices, and those for $n=3$ are the familiar Gell-Mann matrices, while inserting factors of 2 in certain formulas. With convention (2), these generators will be orthogonal but not orthonormal with respect to the Killing form. We return to this point below.

On a general semisimple Lie algebra, the Killing form K is defined as

$$K(X,Y) = \mathrm{Tr}(\mathrm{ad}(X) \circ \mathrm{ad}(Y): \mathfrak{g} \to \mathfrak{g}),$$

where the trace is taken in the adjoint representation. At the moment we focus on semisimple algebras $\mathfrak{g}$, for which the Killing form is nondegenerate. Let α be an irreducible representation of $\mathfrak{g}$, let X_i be any basis of $\mathfrak{g}$, and let X_i' denote the dual basis with respect to the Killing form. The Casimir operator

$$C_2(\alpha) = \sum_i \alpha(X_i)\alpha(X_i')$$

does not depend on the choice of basis, and by Schur's lemma is proportional to the identity, so we write $C_2(\alpha) = c_2(\alpha)\mathbf{1}$. If X_i is orthonormal with respect to K, then $C_2(\alpha) = \Sigma_i \alpha(X_i)^2$. For reducible representations, $C_2(\alpha)$ may not be proportional to the identity.

Definition 2 (Lie algebra channel: Let $\mathfrak{g}$ *denote a Lie algebra of dimension* k, *with basis* $\{X_i : i = 1, \ldots, k\}$. *Let* α *be an irreducible* $\mathfrak{g}$*-representation on the Hilbert space* $\mathcal{H}$. *The* generalized depolarizing channel *or* Lie algebra channel *is defined to be the channel in which an error occurs conditionally with probability* p, *causing an initial state* $|\psi\rangle \in \mathcal{H}$ *to evolve into an ensemble of the* k *states* $\alpha(X_i)|\psi\rangle$, *all with equal likelihood.*

The Kraus operators for the channel of Definition 2 are given by

$$M_0 = \sqrt{1-p}\mathbf{1}, \quad M_i = \sqrt{\Lambda p}\alpha(X_i), \tag{3}$$

where Λ is a normalization constant which will be fixed momentarily. The operators M_μ are Hermitian if the representation is unitary and if $p \in [0,1]$, and are constrained to satisfy $\Sigma_\mu M_\mu M_\mu = \mathbf{1}$, which fixes the value of the constant Λ appearing in (3). By definition,

$$\sum_\mu M_\mu^2 = (1-p)\mathbf{1} + \Lambda p \sum_i \alpha(X_i)^2.$$

If $\Sigma_i \alpha(X_i)^2 = Z \cdot \mathbf{1}$, where Z is a constant (which in most cases we can take to be real), then

$$\Lambda = \frac{1}{Z}.$$

If X_i is orthonormal with respect to the Killing form, then $Z = c_2(\alpha)$. More generally, if the basis satisfies

$$K(X_i, X_j) = \mathfrak{n}\,\delta_{ij}, \quad \mathfrak{n} > 0,$$

then it can be rescaled to an orthonormal basis by a single constant. In this situation,

$$Z = \mathfrak{n}\, c_2(\alpha), \quad \Lambda = \frac{1}{Z}. \tag{4}$$

Defining the Killing norm by $\|x\|_K^2 = K(x,x)$, we note that if

$$\|X_i\|_K \neq \|X_j\|_K,$$

for some pair of indices i, j, then the normalization condition cannot be satisfied.

What if the representation is reducible? Suppose $\mathcal{H} = V \oplus W$ as a direct sum of irreducible $\mathfrak{g}$-modules, and X_i is orthonormal with respect to K. Then there exist independent constants Z_V and Z_W such that the operator

$$C_2(\alpha) = \sum_i \alpha(X_i)^2 = \begin{pmatrix} Z_V & 0 \\ 0 & Z_W \end{pmatrix}$$

as a block decomposition on $V \oplus W$. If $Z_V \neq Z_W$, then it is not possible for the Kraus operators (3) to give a trace-preserving map. On the other hand, if $Z_V = Z_W$ then they do define a CPT map even though the representation is reducible.

What if $p > 1$? Then $M_0 = i\sqrt{p-1}\mathbf{1}$, and we have

$$\sum_\mu M_\mu M_\mu^\dagger = (2p-1)\mathbf{1}.$$

Thus the map cannot be trace-preserving unless $p = 1$, which is a contradiction. A similar argument shows that $p < 0$ does not give a trace-preserving map. Thus, if we wish to study the framework of Definition 2, then we must limit ourselves to $p \in [0,1]$.

We summarize the results of the last few paragraphs in a theorem.

Theorem 2 (normalization): *Consider the Kraus operators*,

$$M_0 = (1-p)^{1/2}\mathbf{1} \quad \textit{and } M_i = (\Lambda p)^{1/2}\alpha(X_i),$$

for $i = 1, \ldots, k$. *If*

(i) $p \in [0,1]$,
(ii) *The representation* α *of* $\mathfrak{g}$ *is a direct sum of irreducible representations all with the same quadratic Casimir, and*
(iii) $\exists\ \mathfrak{n} > 0$ *such that* $K(X_i, X_j) = \mathfrak{n}\,\delta_{ij}$ *for all* i, j,

then $\Sigma_\mu M_\mu M_\mu = \mathbf{1}$ *with* Λ *given by* Eq. (4). *Conversely, if any of (i)–(iii) is not satisfied, then (except in trivial cases) there does not exist* Λ *s.t.* $\Sigma_\mu M_\mu M_\mu = \mathbf{1}$, *and the M's do not give rise to a quantum channel.*

The coefficients of the M_μ in (3) admit a natural "probability of error" interpretation, but in Sec. II B we investigate the possibility of modifying them to complex coefficients in order to obtain a channel. We find that no new channels arise unless one is willing to promote the coefficients to operators.

Using (1), the Lie algebra channel has the explicit Kraus decomposition

$$\boldsymbol{\rho} \to \mathcal{E}(\boldsymbol{\rho}) = (1-p)\boldsymbol{\rho} + \frac{p}{Z}\sum_{i=1}^{k} \alpha(X_i)\boldsymbol{\rho}\,\alpha(X_i). \tag{5}$$

As is proven in standard textbooks[9] (see Theorem 8.9), the trace of any generator of any representation of a compact simple Lie algebra is zero, so in particular, the $\alpha(X_i)$ are traceless. Moreover, it is clear that this transformation satisfies the defining properties for a quantum channel, given here as Definition 1.

Two operator-sum representations

$$\sum_{\mu} M_{\mu}\boldsymbol{\rho}M_{\mu}^{\dagger} \quad \text{and} \sum_{\nu} N_{\nu}\boldsymbol{\rho}N_{\nu}^{\dagger}$$

describe the same channel if and only if there exists a unitary matrix $U_{\nu\mu}$ such that $N_{\nu}=U_{\nu\mu}M_{\mu}$. Therefore, it is immaterial which basis of the Lie algebra that we use, as long as the two bases are related by a $U(N)$ similarity transformation. As noted in Theorem 2, in order to build a channel satisfying the normalization condition, we are forced to use a basis satisfying "orthonormality," $K(X_i,X_j)=\mathfrak{n}\,\delta_{ij}$. But any two "orthonormal" bases in this sense are related by a unitary transformation, so the CPT map constructed above is independent of the basis chosen for $\mathfrak{g}$.

Given a Lie algebra $\mathfrak{g}$ and a representation α on a vector space of dimension d, the CPT map (5) is a model for decoherence through a d-level noisy quantum channel, with errors that are not completely arbitrary; rather, they transform the state in a way determined by the representation of $\mathfrak{g}$.

The channels (5) have an extremely interesting structure. For a certain subclass of possible Lie algebra representations, the channel (5) has an action which, like the qubit case, is most simply described by a Bloch parametrization with polarization vector $v\in\mathbb{R}^k$, where $k=\dim\mathfrak{g}$. In these cases, we show that (5) decreases the length of v, and so deserves the title generalized depolarizing channel. In other cases of interest, a single Bloch vector is not sufficient, but the action of the channel can be described by similar rescalings of symmetric 2-tensors or higher-rank objects.

A natural step, which we begin in the next section, is to calculate the expression (5) explicitly in certain representations of classical Lie algebras.

Remark 1: When we use the terminology "the $\mathfrak{g}$-channel," where $\mathfrak{g}$ is a semisimple Lie algebra, the fundamental representation of $\mathfrak{g}$ is implied. Examples of fundamental representations include the n-dimensional defining representation of $\mathfrak{su}_n$, and the seven-dimensional irrep of G_2.

It is easy to see that the Lie algebra channel (5) always has the property of being *doubly stochastic*, i.e., $\mathcal{E}(\mathbf{1})=\mathbf{1}$. See, for example, Ref. 7 for further discussion.

B. A note on coefficients and extensions

As discussed prior to Theorem 2, for $p\notin[0,1]$ the transformation defined by (5) is CP but not T, and it is possible to recover a CPT map (channel) only if we consider different coefficients for the Kraus operators (3). To this end, let us first consider

$$M_0=m_0\mathbf{1} \quad \text{and } M_i=\frac{\tilde{m}}{\sqrt{Z}}\alpha(X_i), \tag{6}$$

where m_0, $\tilde{m}\in\mathbb{C}$ are some complex constants. Then to obtain a trace-preserving map, we require

$$\sum_{\mu} M_{\mu}^{\dagger}M_{\mu}=|m_0|^2+|\tilde{m}|^2=1\,.$$

This condition is equivalent to the statement that the point $(m_0,\tilde{m})\in\mathbb{C}^2\cong\mathbb{R}^4$ lies in the unit 3-sphere $S^3\subset\mathbb{R}^4$.

We can now view the coefficients of the Kraus operators (3) as the projection $S^3\to S^1$. Introduce a parameter $q\in[-1,1]$ such that $p=q^2$, and write (3) as $M_0=\pm\sqrt{1-q^2}\mathbf{1}$, and $M_i=(q/\sqrt{Z})\alpha(X_i)$. Then ignoring $\sqrt{Z}$, the coefficients of M_i and M_0 give a point on the unit circle. Further, m_0 and $\tilde{m}$ only enter through the square of their magnitude, so the two additional parameters associated to projecting from the 3-sphere are fictitious, and (5) is in fact the most general channel of this kind.

A nontrivial generalization is obtained by promoting m_0 and $\tilde{m}$ to *operators*. However this "generalization" is a special case of a well-known operation which extends an existing channel $\mathcal{E}_B$ using any set of operators which satisfy the normalization condition (1). Given two sets of Kraus operators $A_1,\ldots,A_r$ and $B_1,\ldots,B_s$ acting on the same vector space and satisfying

$$\sum_{i=1}^{r} A_i^\dagger A_i = \sum_{j=1}^{s} B_j^\dagger B_j = \mathbf{1},$$

we note that the set of operators

$$\{A_1, \ldots, A_{r-1}, B_1 A_r, \ldots, B_s A_r\} \tag{7}$$

also satisfies the normalization condition, because

$$\sum_{j=1}^{s} (B_j A_r)^\dagger B_j A_r = A_r^\dagger A_r.$$

This construction is *natural* with respect to the channel $\mathcal{E}_B$ defined by B_i, in the sense that if $\{B_i'\}$ is another set of Kraus operators defining the same channel, then the channel defined by (7) is also the same. Naturality does not hold for the A operators, but this will not concern us here. We call this procedure *the extension of $\mathcal{E}_B$ by the A operators, on the element A_r.*

For example, one may notice that the operators $Z^{-1/2}\alpha(X_i)$ of the preceding section satisfy the normalization condition since the sum of their squares is a Casimir element, and the normalization constant Z cancels the numerical factor. Consider this the B-channel, and extend it on every element by the same set of Kraus operators. This yields a "double $\mathfrak{g}$-channel" with Kraus operators

$$\left\{ \frac{1}{Z} X_i X_j : i,j = 1, \ldots, k \right\}. \tag{8}$$

These operators generate the image of $\mathfrak{g} \otimes \mathfrak{g}$ under the universal homomorphism expressed in the commutative diagram (18).

This underscores the fact that, aside from the basic examples of quantum channels provided by Sec. II A, many further examples may be obtained by extension, as in (7). As in the basic Lie algebra channels, computations with extended channels are facilitated by the existence of nontrivial identities which exist among the representation matrices. Channel (8) is interesting because for many representations, the matrices $\alpha(X_i)$ do not span the entire space of traceless $d \times d$ matrices, but the set of products $\alpha(X_i)\alpha(X_j)$ spans a subspace of larger dimension. Therefore the extension leading to (8) is a way of generating a channel whose Kraus operators come closer to spanning the space of all matrices in the appropriate dimension. If a density matrix were written as $\rho = \Sigma_{ij} w_{ij} X_i X_j$, and if the representation satisfies an identity for reduction of products of six generators, then one can calculate the action of (8) on ρ explicitly.

We are now in a position to interpret the channel defined by (6) with complex coefficients m_0, $\tilde{m}$ as the extension (7) of the identity channel with the unusual Kraus representation $B_1 = m_0 \mathbf{1}$, $B_2 = \tilde{m}\mathbf{1}$ by the nontrivial Lie algebra channel $A_i = Z^{-1/2}\alpha(X_i)$ on the element B_2. We may use naturality in B to rotate to the case $\tilde{m} = q \in [-1, 1]$ and $m_0 = \pm\sqrt{1-q^2}$ whence we recover (5), so there is no advantage to complexifying the coefficients. Given any channel whose set of Kraus operators do not contain $\mathbf{1}$, we can always extend it so that they do contain the identity by this method.

For the rest of this paper, we will assume that the Kraus operators take the form (3) in order to retain the beautiful probabilistic interpretation given by Definition 2. As we continue, we will keep in mind that extensions are possible, and develop methods which easily generalize.

III. THE $_n$ CHANNEL

A. Bloch methods for $_n$

The $\mathfrak{su}_n$ channel, our first example, is the channel built from the n-dimensional defining representation (also called standard representation) of $\mathfrak{su}_n$. It is simpler than most other channels

studied in this paper, because it admits a complete solution. Its action on any arbitrary input density matrix can be calculated in closed form using the Bloch parametrization, and in all cases it is a depolarizing channel.

One reason for the beauty and simplicity of the $\mathfrak{su}_n$ channel is that any n-dimensional density matrix admits a Bloch vector parametrization in terms of $\mathfrak{su}_n$ generators. This is because $k \equiv \dim(\mathfrak{su}_n) = n^2 - 1$ is only one less than n^2, the dimension over $\mathbb{R}$ of the space of $n \times n$ Hermitian matrices.

Any $n \times n$ Hermitian matrix ρ may be represented as

$$\rho = \frac{1}{n}(\mathrm{tr}(\rho)\mathbf{1} + T), \quad T \in \mathfrak{su}_n,$$

and having chosen a basis X_a for $\mathfrak{su}_n$, it follows that

$$T = \sum_{a=1}^{k} v_a X_a \equiv v \cdot X,$$

for some coefficient vector v. In analogy with the well-known parametrization of the 2×2 density matrices as the interior of a sphere, we will refer to v as the *Bloch vector*.

For $n \geqslant 3$ it may be hard to visualize the geometry of the space of density matrices in terms of the geometry of v. This question was first considered in the $n=3$ case by MacFarlane *et al.*[8] Section VI undertakes a systematic study of the geometry of the space of v which lead to a valid density matrix in various representations. We call this space the *Bloch manifold* and give details of the geometry for a number of important examples, including all representations of $\mathfrak{su}_2$, and the n-dimensional irrep of $\mathfrak{su}_n$.

B. The standard representation

In this section, we take α to be the standard representation of $\mathfrak{su}_n$ on a vector space $\mathcal{H}$ of dimension n. For simplicity, we let X_i denote both the generator of $\mathfrak{su}_n$ and its image under this representation. One could now compute the quadratic Casimir in the standard way using roots and weights, but it will turn out that the value of this Casimir as well as all other properties we will need to obtain a complete solution to the $\mathfrak{su}_n$ channel follow from the single relation

$$X_i X_j = \beta \delta_{ij} \mathbf{1} + \sum_k Q_{ijk} X_k \tag{9}$$

for some constant β and tensor Q_{ijk}. Of course, this relation is just the decomposition of a Hermitian matrix into a trace part with trace $n\beta\delta_{ij}$, and a linear combination of the X_k, which generate the space of traceless matrices.

Elements of the standard basis of $\mathfrak{su}_n$ are called Gell-Mann matrices, and they satisfy

$$\mathrm{Tr}(X_i X_j) = 2\delta_{ij},$$

so $\beta = 2/n$. Many properties of the Q tensor already follow from the single assumption that X_i generate a Lie algebra. It is immediate that $Q_{[ij]k} = i f_{ijk}$ where $[ij]$ denotes antisymmetrization, and f_{ijk} is $1/2$ times the structural tensor of the Lie algebra. It follows that

$$Q_{ijk} = d_{ijk} + i f_{ijk}$$

for some d_{ijk} symmetric in the first two indices. Also, (9) implies

$$\{X_i, X_j\} = \frac{4}{n}\delta_{ij}\mathbf{1} + 2\sum_l d_{ijl} X_l.$$

Multiplying by X_k and taking the trace yields

$$d_{ijk} = \tfrac{1}{4}\mathrm{Tr}(\{X_i, X_j\}X_k),$$

therefore the d-tensor is *completely* symmetric, and interchange of any two indices has the effect of complex conjugating Q. Since $\Sigma_i X_i X_i$ is a multiple of the identity,

$$\sum_i d_{iik} = \frac{1}{2}\mathrm{Tr}\left(\left(\sum_i X_i X_i\right)X_k\right) = 0. \tag{10}$$

It follows from the associativity of matrix multiplication that

$$f_{ijm}f_{klm} = \frac{2}{n}(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}) + d_{ikm}d_{jlm} - d_{jkm}d_{ilm}$$

with a sum over m implied. Contracting j and k and using (10) yields

$$d_{ijm}d_{ljm} = f_{ijm}f_{jlm} + \left(2n - \frac{4}{n}\right)\delta_{il}.$$

By a general property of compact semisimple Lie algebras, the structure constants satisfy

$$f_{ijk}f_{ljk} = n\delta_{il}. \tag{11}$$

Therefore, $d_{ijm}d_{ljm} = [n - (4/n)]\delta_{il}$. Using this and (11), we obtain

$$Q_{ijm}Q_{ljm} = d_{ijm}d_{ljm} - f_{ijm}f_{ljm} = -\frac{4}{n}\delta_{il}. \tag{12}$$

C. Solution of the $_n$ channel

For this basis of $\mathfrak{su}_n$, $Z = 2k/n$, where $k = n^2 - 1$. The action of the channel

$$\boldsymbol{\rho} \to \mathcal{E}(\boldsymbol{\rho}) = (1-p)\boldsymbol{\rho} + \frac{pn}{2k}\sum_{i=1}^{k} X_i \boldsymbol{\rho} X_i$$

on the density matrix

$$\boldsymbol{\rho} = \frac{1}{n}(\mathrm{tr}(\boldsymbol{\rho})\mathbf{1} + v \cdot X)$$

is given by

$$\mathcal{E}(\boldsymbol{\rho}) = \frac{\mathrm{tr}(\boldsymbol{\rho})}{n}\mathbf{1} + \frac{1-p}{n}v \cdot X + \frac{p}{2k}\sum_{i,j} v_j X_i X_j X_i. \tag{13}$$

Using (9) to expand the triple product, we have

$$\sum_{j,i} v_j X_i X_j X_i = \beta v \cdot X + \beta \sum_{i,j} v_a Q_{iji}\mathbf{1} + \sum_{i,j,k,a} v_j Q_{ijk} Q_{kia} X_a.$$

Since $\mathcal{E}(\boldsymbol{\rho})$ has unit trace, it must be the case that $\Sigma_i Q_{iji} = 0$. The same conclusion also follows from (10), but it is amusing to see that $\Sigma_i Q_{iji}$ must vanish because this is a CPT map. Therefore,

$$\mathcal{E}(\boldsymbol{\rho}) = \frac{\mathrm{tr}(\boldsymbol{\rho})}{n}\mathbf{1} + \frac{1-p+p/k}{n}v \cdot X + \frac{p}{2k}\sum_{i,j,k,a} v_j Q_{ijk} Q_{kia} X_a. \tag{14}$$

Using (12), we have finally

$$\mathcal{E}(\boldsymbol{\rho}_v) = \frac{1}{n}(\mathrm{tr}(\boldsymbol{\rho})\mathbf{1} + f(p,n)v \cdot X),$$

where

$$f(p,n) = 1 - p - \frac{p}{k} = \frac{(1-p)n^2 - 1}{n^2 - 1}. \tag{15}$$

In the qubit case, $f(p,2) = 1 - 4p/3$, which is consistent with standard results.

D. Properties of the solution

The $\mathfrak{su}_n$ channel maps an initial density matrix to a linear combination of itself and the identity, i.e., it has the form

$$\Delta_\lambda(\boldsymbol{\rho}) = \lambda\boldsymbol{\rho} + \left(\frac{1-\lambda}{n}\right)\mathbf{1}. \tag{16}$$

This is the standard definition of the n-dimensional depolarizing channel. The information-carrying capacity of this channel was studied in great detail by King,[10] where notably the Amosov-Holevo-Werner[11] conjecture was established for channels which are products of a depolarizing channel with an arbitrary channel. Channels based on representations of semisimple algebras generically do not take the form (16), except possibly on special subsets of the space of density matrices; see Theorem 3.

The depolarizing channel on an n-dimensional Hilbert space satisfies complete positivity if and only if

$$\frac{1}{1-n^2} \leqslant \lambda \leqslant 1.$$

The $\mathfrak{su}_n$ channel has the form (16) for $\lambda = f(p,n)$. Note that the relation

$$\frac{-1}{n^2-1} \leqslant f(p,n) \leqslant 1$$

holds for all $n \geqslant 2$. In fact, $f(p,n)$ saturates both of these inequalities at the endpoints of the allowed range, $0 \leqslant p \leqslant 1$.

Knowing that the $\mathfrak{su}_n$ channel is depolarizing allows an easy calculation of the minimal von Neumann output entropy,

$$S_{\min} = \frac{-np}{1+n}\ln\left(\frac{np}{n^2-1}\right) - \left(1 - \frac{np}{1+n}\right)\ln\left(1 - \frac{np}{1+n}\right),$$

with large n behavior $\lim_{n\to\infty} S_{\min}/\ln(n) = p$.

At the special value $p = 1 - n^{-2}$, the $\mathfrak{su}_n$ channel is a constant map from $\mathbb{R}^{n^2-1}$ into the space of density matrices,

$$\mathcal{E}(\boldsymbol{\rho}_v) = \frac{1}{n}\mathbf{1} \quad \text{for all } v, \quad \text{at } p = p_c \equiv 1 - n^{-2}. \tag{17}$$

Physically, if the probability of error happens to be $p = p_c$, then $\mathfrak{su}_n$-decoherence evolves an arbitrary initial density matrix into a completely uniform ensemble consisting of pure states with equal probabilities. This is the "worst" value of p, in the sense that all information about the initial density matrix has been lost. This result is *stable* in the sense that if p is only approximately equal to the critical value, the initial density matrix decoheres into an approximately uniform ensemble. We will see in Sec. IV that for other Lie algebra channels, there are critical values of p which generalize (17).

IV. OTHER REPRESENTATIONS

A. General remarks

In the n-dimensional standard representation of $\mathfrak{su}_n$, the representation matrices $\alpha(X_i)$ span the space of all traceless Hermitian matrices, and thus an arbitrary initial density matrix can be expressed in terms of the $\alpha(X_i)$ and the identity. As we consider higher-dimensional representations, the representation matrices become increasingly sparse in the space of all traceless matrices, and thus only some fraction of the set of all possible density matrices can be expressed in the form $d_\alpha^{-1}\mathbf{1}+\Sigma_i v_i \alpha(X_i)$. Also for higher-dimensional irreducible representations, (9) does not hold. Therefore, ideas are needed to further extend our analysis to irreps which have higher dimension than the fundamental representation. This is the subject of Sec. IV. Let $d=d_\alpha$ denote the dimension of the representation α, and $\mathfrak{gl}_d$ as usual denotes the associative algebra of all $d\times d$ matrices.

A representation ϕ of $\mathfrak{g}$ lifts to a unique associative algebra homomorphism $\tilde{\phi}$ of the universal enveloping algebra $\mathcal{U}(\mathfrak{g})$, by the universal property most elegantly expressed in the commutative diagram

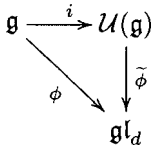

(18)

The action of $\tilde{\phi}$ is simply to convert the tensor product to matrix multiplication, i.e., $\tilde{\phi}(x\otimes y)=\phi(x)\cdot\phi(y)$, etc. The interesting property about this commutative diagram, and one which gives a computational method for Lie algebra channels, is that if ϕ is an irreducible faithful representation and if $\mathfrak{g}$ is a semisimple Lie algebra, then $\tilde{\phi}$ is surjective.

This surjectivity has the consequence that for *any representation* of said Lie algebra, *every* density matrix can be represented as a linear combination of products of the representation matrices. In other words, the calculational method outlined in this section will always work. Before continuing our discussion of this, let us consider a simple but nontrivial example, the spin-1 channel, in complete detail.

B. The spin-1 channel

Consider the spin-1 representation of $\mathfrak{su}_2$. We use standard angular momentum notation, in which

$$J_1=\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix},\quad J_2=\frac{1}{\sqrt{2}}\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix},\quad J_3=\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}.$$

Before generalizing to arbitrary density matrices, we restrict attention to the simpler example of density matrices $\boldsymbol{\rho}$ which are of the form

$$\boldsymbol{\rho}_v=\tfrac{1}{3}(\mathbf{1}+v\cdot J),\quad v\in\mathbb{R}^3. \tag{19}$$

Then

$$\mathcal{E}(\boldsymbol{\rho}_v)=\frac{1}{3}\mathbf{1}+\frac{1-p}{3}v\cdot J+\frac{p}{6}\sum_{a,b}v_b J_a J_b J_a. \tag{20}$$

The relation analogous to (9) does not hold, i.e., J_aJ_b is not a linear combination of $\mathbf{1}$ and $\{J_i: i=1,\ldots,3\}$. In this special case, the triple product appearing in (20) simplifies considerably,

$$J_a J_b J_a = \delta_{ab} J_a \quad \text{(no sum)}, \tag{21}$$

which implies that

$$\mathcal{E}(\boldsymbol{\rho}_v) = \frac{1}{3}\left(\mathbf{1} + \left(1 - \frac{p}{2}\right) v \cdot J\right). \tag{22}$$

This takes the form (19) with $v \to [1-(p/2)]v$. Thus, for 3×3 density matrices admitting a Bloch parametrization, the spin-1 channel scales the Bloch vector by a number between $1/2$ and 1.

Interestingly, we can go further and find a Bloch-type picture of the spin-1 channel on a general density matrix. The six elements of the form

$$J_{(a}J_{b)} \equiv \tfrac{1}{2}(J_a J_b + J_b J_a),$$

together with J_1, J_2, and J_3, span the space of 3×3 matrices. Therefore an arbitrary 3×3 density matrix $\boldsymbol{\rho}$ can be written as

$$\boldsymbol{\rho}_{v,w} = v \cdot J + \sum_{a,b} w_{ab} J_{(a}J_{b)} \tag{23}$$

for some vector v and symmetric tensor w.

We use standard physics normalizations which entail that for the spin-s representation in $d = 2s+1$ dimensional space,

$$\sum_a J_a^2 = \lambda\, \mathbf{1} \quad \Rightarrow \quad \operatorname{tr}(J_a J_b) = \frac{d\lambda}{3}\delta_{ab},$$

where $\lambda = s(s+1)$. Then we have

$$\operatorname{tr}(\boldsymbol{\rho}_{v,w}) = \frac{d\lambda}{3}\operatorname{tr}(w).$$

It follows that in order to have a density matrix, we require $\operatorname{tr}(w) = 3(d\lambda)^{-1}$. For $s=1$, $\operatorname{tr}(w) = 1/2$.

Theorem 3 (action of the spin-1 channel): *The action of the spin-1 channel on the vector and symmetric tensor are $v \to v'$ and $w \to w'$, where*

$$\begin{aligned} v_a &\to v_a{}' = \left(1 - \frac{p}{2}\right) v_a, \\ w_{ab} &\to w_{ab}{}' = \left(1 - \frac{3p}{2}\right) w_{ab} + \frac{p}{4}\delta_{ab}. \end{aligned} \tag{24}$$

Proof: The asymmetric quadruple product identity

$$\sum_i J_i J_j J_k J_i = \delta_{jk}\mathbf{J}^2 - J_k J_j \tag{25}$$

implies the symmetrized identity

$$\sum_i J_i J_{(a} J_{b)} J_i = \delta_{ab}\mathbf{J}^2 - J_{(a}J_{b)}. \tag{26}$$

We refer to identities of the form (25) and (26) as "$4 \to 2$ identities," because they relate degree 4 polynomials in the generators to degree 2 polynomials. Using $4 \to 2$ identities and (21), a straightforward calculation shows that $\mathcal{E}(\boldsymbol{\rho}_{v,w})$ is equal to

$$\left(1-\frac{p}{2}\right)v\cdot J+\left(1-\frac{3p}{2}\right)\sum_{a,b}w_{ab}J_{(a}J_{b)}+p\,\mathrm{tr}(w)\mathbf{1},$$

which implies the stated result, since for spin-1, we have $\mathrm{tr}(w)=1/2$ and $\mathbf{1}=\Sigma_{a,b}\frac{1}{2}\delta_{ab}J_{(a}J_{b)}$. □

Theorem 3 shows that $p=2/3$ is a sort of critical value; the channel at $p=2/3$ maps an arbitrary initial $\boldsymbol{\rho}$ into a density matrix with a Bloch representation; $\mathcal{E}(\boldsymbol{\rho})=d^{-1}(\mathbf{1}+v\cdot J)$. These are a three-dimensional set within the eight-dimensional space of all 3×3 density operators. This is reminiscent of the critical value $p=1-n^{-2}$ for the $\mathfrak{su}_n$ channel, but now there is no value of p for which the channel outputs pure noise.

It is possible to iterate formula (24), with interesting results. Clearly, after n applications of the channel, $v\rightarrow[1-(p/2)]^n v$. Consider a W-state, i.e., a state of the form

$$\boldsymbol{\rho}_w=\sum_{a,b}w_{ab}J_{(a}J_{b)},$$

and let $\mathcal{E}^n$ denote n applications of the spin-1 channel.

Theorem 4 (iteration formula): *The action of $\mathcal{E}^n$ on w is the following:*

$$w\underset{\mathcal{E}^n}{\longrightarrow}F^{(n)}(p)(\mathbf{1}-6w)+w,$$

where $F^{(n)}(p)$ is a degree n polynomial in p, determined as follows. $F^{(1)}(p)=1-3p/2$, and the $F^{(n)}$ for $n>1$ are determined by the recursion relation

$$F^{(n+1)}(p)=\left(1-\frac{3p}{2}\right)F^{(n)}(p)+\frac{p}{4}.$$

Interestingly, this recursion relation has the same coefficients as the transformation (24) of w itself.

C. Higher spin representations

Note that the triple product (21) and quadruple product (25) identities are simply certain elements of the ideal $\mathcal{I}=\ker(\tilde{\phi})$, where $\tilde{\phi}$ is the representation of the universal enveloping algebra, as in (18). The larger this ideal, the more product identities there will be in the representation of interest. For higher spin, we have the following $3\rightarrow 1$ identity in the spin-s representation of $\mathfrak{su}_2$:

$$\sum_{i=1}^{3}J_iJ_aJ_i=(\lambda-1)J_a,\quad \text{where } \lambda=s(s+1). \tag{27}$$

There is also a generalization of the $4\rightarrow 2$ identity valid for general spin-s,

$$\sum_{i=1}^{3}J_iJ_aJ_bJ_i=(\lambda-2)J_aJ_b+\lambda\delta_{ab}\mathbf{1}-J_bJ_a.$$

The latter has the more convenient symmetrized form,

$$\sum_{i=1}^{3}J_iJ_{(a}J_{b)}J_i=(\lambda-3)J_{(a}J_{b)}+\lambda\delta_{ab}\mathbf{1}. \tag{28}$$

Theorem 5 (higher spin channel): *Let J_1, J_2, J_3 be canonical generators for the spin-s representation of $\mathfrak{su}_2$ in dimension $d=2s+1$, and let $\mathcal{E}_s$ denote the spin-s channel. Defining $\boldsymbol{\rho}_{v,w}=v\cdot J+\Sigma_{a,b}w_{ab}J_{(a}J_{b)}$, we have*

$$\mathrm{tr}(\boldsymbol{\rho}_{v,w})=1\Leftrightarrow\ \mathrm{tr}(w)=\frac{3}{d\lambda},$$

where $\lambda = s(s+1)$. *The action of the spin-s channel is*

$$\mathcal{E}_s(\rho_{v,w}) = \left(1 - \frac{p}{\lambda}\right) v \cdot J + \left(1 - \frac{3p}{\lambda}\right) w_{ab} J_{(a} J_{b)} + p \operatorname{tr}(w) \mathbf{1}.$$

Proof: A straightforward application of (27) and (28). □

Thus, the action of the spin channel is more complicated than the scaling of a single vector. It is the scaling of a series of symmetric tensors, by different scale factors. This shows that the spin-s channels are never depolarizing channels.

At the critical value $p = \lambda/3$, the channel maps an arbitrary $\rho_{v,w}$ into a matrix with a Bloch representation,

$$\mathcal{E}_s(\boldsymbol{\rho}_{v,w})\big|_{p=\lambda/3} = \frac{1}{d}\mathbf{1} + \frac{2}{3} v \cdot J.$$

It follows that if $p = \lambda/3$, then the channel maps an initial density matrix of the form (23) with $v = 0$ into pure noise.

For spin-1, an arbitrary density matrix may be represented as (23), and for higher spin, these are a proper submanifold of the convex cone of all density matrices. For spin-3/2, an arbitrary density matrix may be written in the form

$$\sum_{a,b} w_{ab} J_{(a} J_{b)} + \sum_{a,b,c} u_{abc} J_{(a} J_b J_{c)},$$

where w and u are completely symmetric tensors. The U-term is traceless, and so we require the W-term to have trace one. As discussed prior to Theorem 3, this means that $\operatorname{tr}(w) = 3/(d\lambda) = 1/5$.

D. Finding *v* and *w* from *ρ* in higher spin and pure states

In this brief section we show how to invert the relation (23) for the density operator, and find the coefficient vector v and symmetric tensor w. We do the analysis at arbitrary spin, although for spin higher than 1, not all density matrices have the form (23). The methods will generalize assuming the relevant trace identities can be found.

As in Theorem 5, let J_1, J_2, J_3 be canonical generators for the spin-s representation of $\mathfrak{su}_2$. Note that

$$\operatorname{Tr}(J_a J_b) = \frac{1}{3} d\lambda \, \delta_{ab} \quad \text{and} \quad \operatorname{Tr}(J_a J_b J_c) = i \frac{d\lambda}{6} \epsilon_{abc},$$

where $\lambda = s(s+1)$ and $d = 2s+1$, and ϵ_{abc} is the Levi-Civita alternating symbol. It follows immediately from (23) that

$$v_a = \frac{3}{d\lambda} \operatorname{Tr}(\rho J_a).$$

To find w, note the trace identity

$$\operatorname{Tr}(J_{(a} J_{b)} J_{(j} J_{k)}) = f_1(s) \tfrac{1}{2}(\delta_{ak}\delta_{bj} + \delta_{bk}\delta_{aj}) + f_2(s)\delta_{ab}\delta_{jk},$$

where f_i are functions of s, given by

$$f_1 = \operatorname{tr}(J_{(1} J_{2)})^2 = \frac{\lambda d(d^2-4)}{30},$$

$$f_2 = \operatorname{tr}(J_1^2 J_2^2) = \frac{\lambda d(1+2\lambda)}{30}.$$

By calculating $\operatorname{tr}(\rho J_{(j} J_{k)})$, we find

$$w_{jk} = \frac{1}{f_1}\left(\mathrm{tr}(\rho J_{(j}J_{k)}) - f_2\,\mathrm{tr}(w)\,\delta_{jk}\right) = \frac{30}{\lambda d(d^2-4)}\mathrm{tr}(\rho J_{(j}J_{k)}) - \frac{2\lambda+1}{d^2-4}\mathrm{tr}(w)\,\delta_{jk}.$$

For spin-1, $f_1=1/2$, $f_2=1$, and $d\lambda=6$ so

$$v_a = \tfrac{1}{2}\mathrm{tr}(\rho J_a) \quad \text{and } w_{jk} = \mathrm{tr}(\rho J_{(j}J_{k)}) - \tfrac{1}{2}\delta_{jk}.$$

This gives another way to find pure states, if $\rho=|\psi\rangle\langle\psi|$ then

$$v_a = \tfrac{1}{2}\langle J_a\rangle_\psi \quad \text{and } w_{jk} = \langle J_{(j}J_{k)}\rangle_\psi - \tfrac{1}{2}\delta_{jk}. \tag{29}$$

In conclusion, if the pure state $\rho=|\psi\rangle\langle\psi|$ has a representation of the form (23), then we can find its Bloch vector and w-matrix easily.

E. Relation to the Werner-Holevo channel and a new conjecture

Datta[12] has shown that the spin-1 channel at $p=1$ is equivalent to the Werner-Holevo channel[13]

$$\mathcal{E}_{\mathrm{WH}}(\rho) = \frac{1}{d-1}(\mathrm{tr}(\rho)\mathbf{1} - \rho^T). \tag{30}$$

Recall that in our notation, $M_0=\sqrt{1-p}\mathbf{1}$, so taking $p=1$ eliminates the identity from the set of Kraus operators. For $p<1$ and for the spin-s representation with $s>1$, we may view the spin channel as a generalization of the WH channel.

Amosov *et al.*[11] conjectured that ν_q is multiplicative for tensor product channels,

$$\nu_q(\mathcal{E}^{\otimes m}) \equiv \sup_{\Gamma\in\mathcal{D}(\mathcal{H}^{\otimes m})} \|\mathcal{E}^{\otimes m}(\Gamma)\|_q = \nu_q(\mathcal{E})^m, \tag{31}$$

where $\nu_q(\mathcal{E})=\sup_{\gamma\in\mathcal{D}(\mathcal{H})}\|\mathcal{E}(\gamma)\|_q$ is the maximal ℓ_q-norm. Equation (31) is often called the ℓ_q *multiplicativity relation* or the *AHW conjecture*. Giovannetti *et al.*[14] have conjectured that (31) holds for the Werner-Holevo channel when $d\geqslant 2^{q-1}$.

The Werner-Holevo channel became famous as a counterexample to the AHW conjecture.[11] We infer by Datta's equivalence that the spin-1 channel at $p=1$ gives precisely the same counterexample to the AHW conjecture, stated below. Therefore, multiplicativity does not hold generically in Lie algebra channels. Once it was established that the AHW conjecture does not hold for all $q\geqslant 1$, it was natural to conjecture[15] that it holds for $1\leqslant q\leqslant 2$, and this was recently proved for the WH channel by Alicki and Fannes.[16] If this is true, one would expect additional counterexamples with values of q approaching 2. However, none have yet been reported, except for the WH channel which gives a sequence of counterexamples with q increasing from 4.79 as the dimension d increases. Ruskai, in a private communication to the author, suggested the possibility that Lie algebra channels might provide additional counterexamples with special properties.

Conjecture 1: Lie algebra channels generate counterexamples to the AHW conjecture for a sequence of values of q approaching the boundary of the region in q-space where multiplicativity begins to hold for all channels, assuming there is such a region.

A preliminary investigation in this direction seems promising, and we hope to address this more fully in a future paper.

V. EXCEPTIONAL LIE ALGEBRAS AND CLIFFORD ALGEBRAS

A. Channels based on the exceptional algebra G_2

Let e_j $(j=0,\ldots,7)$ denote the standard basis for the octonions $\mathbb{O}$, where e_0 is the unit. Our notation is compatible with that of Baez,[17] and the proofs of our statements about the octonion algebra can be found there. The Lie group G_2 is the automorphism group of $\mathbb{O}$, so the Lie algebra $\mathfrak{g}_2$ is the derivation algebra of the octonions,

$$\mathfrak{g}_2 = \mathfrak{der}(\mathbb{O}).$$

Derivations act trivially on the identity, and the imaginary octonions $\mathrm{Im}(\mathbb{O})$ form the fundamental seven-dimensional irreducible representation of $\mathfrak{g}_2$.

It is known that if $\mathcal{A}$ is an alternative, nonassociative algebra (such as the octonions), any pair of elements $x,y \in \mathcal{A}$ define a derivation $D(x,y):\mathcal{A}\to\mathcal{A}$ by

$$D(x,y)a = [[x,y],a] - 3[x,y,a], \tag{32}$$

where $[a,b,x]$ denotes the associator $(ab)x - a(bx)$. When $\mathcal{A}$ is a normed division algebra, every derivation is a linear combination of derivations of this form. For the octonion algebra, the elements

$$D(e_1,e_i), \quad D(e_2,e_j), \quad \text{and } D(e_4,e_k)$$

for all $i>1$, $j>2$, and $k>4$, are linearly independent and there are 14 such elements, so they are a basis for $\mathfrak{g}_2$. Define the notation

$$d_{i,j} = \tfrac{1}{2}D(e_i,e_j).$$

This is one possible basis for the Lie algebra $\mathfrak{g}_2$, but we will use another more suited for our purposes. The fact[18] that the six-dimensional sphere S^6 may be viewed as a $G_2/\mathrm{SU}(3)$ coset space, implies a corresponding decomposition of the algebra:

$$\mathfrak{g}_2 = \mathfrak{m} + \mathfrak{h}, \quad \mathfrak{h} \cong \mathfrak{su}_3,$$

where $\mathfrak{m}$ is a six-dimensional subspace. We find a basis adapted to this decomposition. The basis vectors for $\mathfrak{m}$ are simply expressed as $m_i = d_{1,i+1}$, while

$$h_1 = d_{12} + 2d_{47}, \quad h_2 = d_{13} - 2d_{46}, \quad h_3 = d_{14} - 2d_{27},$$

$$h_4 = d_{15} + 2d_{26}, \quad h_5 = d_{16} - 2d_{25}, \quad h_6 = d_{17} + 2d_{24},$$

$$h_7 = \sqrt{3}d_{23}, \quad h_8 = d_{23} + 2d_{45}$$

are a basis for $\mathfrak{su}_3$. Let

$$\beta = \frac{i}{\sqrt{24}}\left(\{m_1,\ldots,m_6\} \cup \frac{1}{\sqrt{3}}\{h_1,\ldots,h_8\}\right)$$

denote a corresponding basis for $\mathfrak{g}_2$. Interestingly, β is an orthonormal basis of $\mathfrak{g}_2$ with respect to the trace form on the seven-dimensional representation space,

$$\mathrm{Tr}_{\mathrm{Im}(\mathbb{O})}(\beta_i\beta_j) = \tfrac{1}{2}\delta_{ij}, \quad \text{therefore } \sum_{i=1}^{14} \beta_i^2 = I_7.$$

The $\mathfrak{g}_2$ channel acts as

$$\mathcal{E}(\boldsymbol{\rho}) = (1-p)\boldsymbol{\rho} + p\sum_{i=1}^{14} \beta_i \boldsymbol{\rho}\, \beta_i.$$

Assume $\boldsymbol{\rho}$ has a Bloch representation with $\mathbf{v} \in \mathbb{R}$,[14]

$$\boldsymbol{\rho} = \tfrac{1}{7}(I_7 + \mathbf{v}\cdot\boldsymbol{\beta}), \tag{33}$$

then as an intermediate step,

$$\mathcal{E}(\boldsymbol{\rho}) = \frac{1-p}{7}(I + \mathbf{v}\cdot\boldsymbol{\beta}) + \frac{p}{7}\sum_{i=1}^{14}(\beta_i^2 + v_a\beta_i\beta_a\beta_i).$$

The sum of β_i^2 gives the identity, with a factor of $p/7$ to cancel the $-p/7$, and (miraculously) the term which is cubic in β's vanishes identically. This is due to the following remarkable $3\to 0$ identity

$$\sum_i \beta_i\beta_a\beta_i = 0 \quad \text{for all } a,$$

as may be checked explicitly. Therefore, the $\mathfrak{g}_2$ channel (restricted to its Bloch manifold) is the simplest of all. It is a true depolarizing channel, shrinking its Bloch vector by a factor of $1-p$,

$$\mathcal{E}(\boldsymbol{\rho}) = \tfrac{1}{7}(I + (1-p)\mathbf{v}\cdot\boldsymbol{\beta}).$$

We emphasize, however, that the $\mathfrak{g}_2$ channel is almost certainly *not* a depolarizing channel outside the Bloch manifold, though we have not proven this.

B. Channels based on the Clifford algebra

Let $\langle,\rangle$ be a nondegenerate bilinear form on V, a d-dimensional vector space. A representation of the Clifford algebra associated to $(V,\langle,\rangle)$ is a map $\gamma: V\to\mathfrak{gl}(V)$ satisfying

$$\{\gamma(x),\gamma(y)\} = \langle x,y\rangle\mathbf{1},$$

where the left-hand side is an anticommutator. The representation is *Hermitian* if the image of γ is contained in $H(V)$, the (Hilbert) space of Hermitian operators on V.

Theorem 6 (Clifford algebra channel): *Given a Hermitian representation of the Clifford algebra, and a finite collection of nonzero vectors* $x_1, x_2, \ldots, x_n \in \mathbb{R}^d$, *then*

$$\mathcal{E}_{C\ell}(\boldsymbol{\rho}) \equiv \left(\sum_{i=1}^{n}\langle x_i,x_i\rangle\right)^{-1}\sum_{i=1}^{n}\gamma(x_i)\boldsymbol{\rho}\,\gamma(x_i) \tag{34}$$

is a CPT map.

Proof: The operator is completely positive because it is already in the form of an operator sum representation. We check that it is trace preserving. By cyclicity of the trace,

$$\mathrm{Tr}(\mathcal{E}_{C\ell}(\boldsymbol{\rho})) = \left(\sum_{i=1}^{n}\langle x_i,x_i\rangle\right)^{-1}\sum_{i=1}^{n}\mathrm{Tr}(\boldsymbol{\rho}\,\gamma(x_i)^2).$$

However, $\gamma(x_i)^2 = \frac{1}{2}\{\gamma(x_i),\gamma(x_i)\} = \langle x_i,x_i\rangle\mathbf{1}$ using the Clifford algebra. The sum of such terms decouples from $\mathrm{Tr}(\boldsymbol{\rho})$ and exactly cancels the prefactor.

Although the proof of Theorem 6 is trivial, the result may not be easily obtained by inspecting any of the standard matrix representations. Taking the Weyl representation of the γ matrices in $d=4$, writing out the CPT map $\gamma(x)\boldsymbol{\rho}\gamma(x)+\gamma(y)\boldsymbol{\rho}\gamma(y)$ for general x, y, $\boldsymbol{\rho}$ as an explicit matrix takes a full page.

As we have seen in other examples, the computational methods used in this paper are most effective when an arbitrary density matrix can be written in terms of the generators of the symmetry algebra. For the Weyl representation of the Clifford algebra, there is a convenient basis consisting of antisymmetric combinations of γ matrices, which we summarize in the following:

$\mathbf{1}$	one of these
γ^μ	four of these
$\gamma^{\mu\nu} = \frac{1}{2}[\gamma^\mu,\gamma^\nu] = \gamma^{[\mu}\gamma^{\nu]}$	six of these
$\gamma^{\mu\nu\rho} = \gamma^{[\mu}\gamma^\nu\gamma^{\rho]} = i\epsilon^{\mu\nu\rho\sigma}\gamma_\sigma\gamma^5$	four of these

$$\gamma^{\mu\nu\rho\sigma} = \gamma^{[\mu}\gamma^{\nu}\gamma^{\rho}\gamma^{\sigma]} = -i\epsilon^{\mu\nu\rho\sigma}\gamma^5 \qquad \text{one of these}$$

These 16 matrices form a basis for the space $\mathfrak{gl}(\mathbb{R}^4)$. One can therefore write any 4×4 density matrix as a linear combination of these matrices with coefficients that are tensors of rank 4, and use γ matrix identities to calculate the action of the CPT map (34).

VI. THE BLOCH MANIFOLD

A. General results

The Bloch manifold is a geometrical space which is naturally associated to a certain representation of a semisimple Lie algebra $\mathfrak{g}$, by asking the question, which linear combinations of the generators of $\mathfrak{g}$ in that representation are positive-definite, trace-one Hermitian matrices, i.e., physical states? For any preferred class of matrices (such as those with non-negative eigenvalues) one can define a manifold from a representation in a similarly basis-dependent way, but for the application to quantum physics, we restrict interest to density matrices.

Since the action of the $\mathfrak{su}_n$ channel is most simply expressed as a rescaling of the Bloch vector and any n-level density matrix admits a Bloch representation, all that remains for a complete mathematical description of the $\mathfrak{su}_n$ channel is to know the set of vectors $v \in \mathbb{R}^{n^2-1}$ which correspond to positive-definite matrices.

The simplest example of why this is an important question for other representations is formula (22), which gives the action of the spin-1 channel on density matrices admitting a Bloch representation as

$$\mathcal{E}(\boldsymbol{\rho}_v) = \frac{1}{3}\left(\mathbf{1} + \left(1 - \frac{p}{2}\right) v \cdot J\right).$$

Thus, the spin-1 channel also rescales the Bloch vector and it is of interest to know which Bloch vectors give rise to physical states.

In any representation which has a $3 \to 1$ identity, i.e., an expression for $\Sigma_i \alpha(X_i)\alpha(X_j)\alpha(X_i)$ in terms of the generators $\alpha(X_k)$, it follows that any density matrix admitting a Bloch representation transforms very simply under the action of the Lie algebra channel.

Definition 3 (Bloch manifold): Choose a set of generators $\{X_i\}$ *of a semisimple Lie algebra* $\mathfrak{g}$, *and an irreducible representation* $\alpha: \mathfrak{g} \to \mathfrak{gl}(\mathcal{H})$ *on a* d_α*-dimensional Hilbert space* $\mathcal{H}$. *The* Bloch manifold $\mathcal{V}$ *(in the* X_i *basis) is defined to be the set of vectors* $v \in \mathbb{R}^k$ ($k = \dim \mathfrak{g}$), *such that*

$$\boldsymbol{\rho}(v) = \frac{1}{d_\alpha}\left(\mathbf{1} + \sum_i v_i \alpha(X_i)\right), \tag{35}$$

is a positive semidefinite, Hermitian matrix. A density matrix which can be written in the form (35) *is said to possess a* Bloch representation, *and the point* $v \in \mathcal{V}$ *is said to be a* valid Bloch vector.

Theorem 7 (closure property): *The Bloch manifold is a closed set in* $\mathbb{R}^k$.

Proof: The matrix $\boldsymbol{\rho}(v)$ is positive iff the lowest eigenvalue $\lambda_{\min}$ of $\mathbf{1} + \Sigma_i v_i \alpha(X_i)$ lies in the set $[0, +\infty)$. The lowest eigenvalue of a matrix is a continuous function of the matrix, so $\lambda_{\min}$ is a continuous function of v. The inverse image of the closed set $[0, +\infty)$ must be closed.

Theorem 8 (general Bloch manifold bound): *Let* α *be a d-dimensional representation of* $\mathfrak{g}$, *let* $k = \dim(\mathfrak{g})$, *and let* X_a *be an orthogonal basis of* $\mathfrak{g}$ *with respect to the Killing form. Then for some constant N*,

$$\mathrm{Tr}(\alpha(X_a)\alpha(X_b)) = Nd\ \delta_{ab}.$$

Moreover, if v is a valid Bloch vector, then

$$v^2 \leqslant \frac{d-1}{N}. \tag{36}$$

In the notation of Sec. II, $N=Z/\dim(\mathfrak{g})$.

Proof: The density matrix $\boldsymbol{\rho}=d^{-1}(\mathbf{1}+v_a\alpha(X_a))$ must satisfy $\mathrm{tr}(\boldsymbol{\rho}^2)\leqslant 1$. But

$$\mathrm{tr}(\boldsymbol{\rho}^2)=d^{-1}(1+Nv^2) \tag{37}$$

which implies the desired result. □

If $\{X_j'\}$ is a second basis of $\mathfrak{g}$, related to the original basis by a matrix A, then the Bloch manifold in the X' basis consists of A^T applied to the Bloch manifold in the X basis. If $\det(A)=1$, this yields an isometric copy of the original manifold, but otherwise the manifold has been stretched in some way. We will see examples of Lie algebra representations which are analogous to the qubit representation, in the sense that the Bloch manifold is a closed ball in some preferred basis.

B. The Bloch manifold for all $\mathfrak{su}_2$ representations

As an example, we give the Bloch manifold relevant to the spin-j representation of $\mathfrak{su}_2$. Let I_{2j+1} be the $(2j+1)$-dimensional identity matrix, and the J_i are the standard generators in the spin-j representation. Let $E_{\min}$ denote the lowest eigenvalue of a matrix. Then

$$E_{\min}\left(I_{2j+1}+\sum_{i=1}^{3}v_iJ_i\right)=1-j\|v\|.$$

The next result follows immediately.

Theorem 9: *The valid Bloch vectors for the spin-j representation of* $\mathfrak{su}_2$ *(with the standard basis) are elements of a closed ball in* $\mathbb{R}^3$ *with radius* $1/j$.

Thus, the picture of the Bloch manifold as a closed ball is not necessarily particular to the qubit system, however, it is certainly not *always* a closed ball. As we shall see below, the Bloch manifold for the defining representation of $\mathfrak{su}_n$ with $n>2$ is a proper subset of the analogous closed ball. To complete the $\mathfrak{su}_2$ case, we remark that the radius receives a multiplicative constant if we rescale the generators; however, the radius always scales as one inverse power of the dimension of the representation.

C. A Bloch submanifold from the Cartan subalgebra

We discuss a method which works for any Lie algebra representation and which always gives a nonempty set of positive semidefinite Hermitian trace-one operators which take the form $\rho=d^{-1}(\mathbf{1}+\Sigma_i v_i\alpha(X_i))$. In Bloch space this set is the interior of a convex polyhedron.

Let $H_1,\ldots,H_r$ denote a basis for the Cartan subalgebra of $\mathfrak{g}$, with $r=\mathrm{rank}(\mathfrak{g})$. As they commute, we may simultaneously diagonalize all $\alpha(H_i)$, and let $h_i^{\,j}$ denote the jth diagonal element of $\alpha(H_i)$. Each vector h^j with components $(h_1^{\,j},h_2^{\,j},\ldots,h_r^{\,j})$ is a weight vector for the given representation.

Assume that the basis $\{X_i\}$ has the Cartan generators $H_1,\ldots,H_r$ as its first r elements. Consider $v\in\mathbb{R}^k$ which are zero except for the first r components. Let $\mathcal{P}$ be the set of $v\in\mathbb{R}^r$ such that $\mathbf{1}+\Sigma_{i=1}^r v_i\alpha(H_i)$ is positive semidefinite. The positivity condition is $1+\Sigma_{i=1}^r v_i h_i^{\,j}\geqslant 0(\forall\ j=1,\ldots,d)$. The solutions of each linear inequality $v\cdot h^j\geqslant -1$ define a half-space $\mathbb{H}_j\subset\mathbb{R}^r$, and the valid Bloch vectors lie in their intersection. A bounded intersection of a finite set of half-spaces is called a *polytope*. If one of the weights h^j is the zero vector, it satisfies $v\cdot h^j\geqslant -1$ for all v.

Definition 4: Define the Bloch-Cartan polytope *as*

$$\mathcal{P}=\{v|v\cdot h^j\geqslant -1\ \ \forall\ \ j\}=\bigcap_{j=1}^{d_\alpha}\mathbb{H}_j. \tag{38}$$

For representations of non-Abelian Lie algebras, $\mathcal{P}\subsetneq\mathcal{V}$. *A priori*, an intersection of half-spaces is either a finite or semi-infinite polyhedron; however (36) implies $v^2\leqslant(d-1)/N$, so $\mathcal{P}$ is always bounded. This provides a geometric proof that a semisimple rank r algebra will not have any irreps

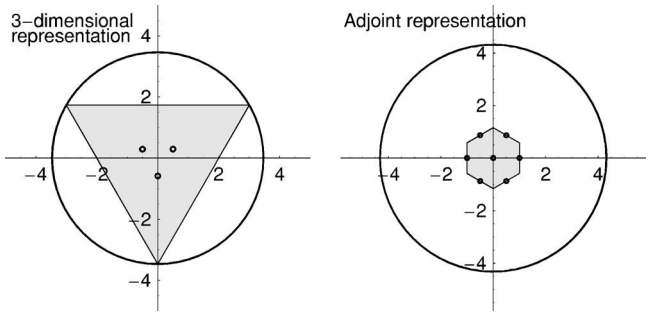

FIG. 1. The shaded region is the intersection of the linear inequalities $v \cdot h^j \geqslant -1$, where h^j are the weight vectors for the indicated representation of $\mathfrak{su}_3$, shown as small circles. Points in the shaded region represent positive semidefinite density matrices. The outer circle shows Bloch vectors which saturate the bound (36).

of dimension smaller than $r+1$, since we need $r+1$ half-spaces to define a finite polyhedron in $\mathbb{R}^r$.

Figure 1 shows two examples for $\mathfrak{su}_3$. This algebra has $r=\mathrm{rank}(\mathfrak{su}_3)=2$ Cartan generators so the Bloch-Cartan polytope can be drawn in $\mathbb{R}^2$. With the conventions of Georgi,[9] the weight vectors h^1, h^2, h^3 for the three-dimensional representation of $\mathfrak{su}_3$ are $\left(\pm\frac{1}{2}, \sqrt{3}/6\right)$ and $(0, -\sqrt{3}/3)$, and the convention $\mathrm{Tr}(T_a T_b)=\frac{1}{2}\delta_{ab}$ for the Gell-Mann matrices implies $N=1/6$. The bound (36) then gives $|v| \leqslant \sqrt{12}$. Note that $v^2=12$ is precisely the circumscribing circle of the polygon. Therefore, in this case our simple method using the Cartan subalgebra produces points up to and including the boundary of the Bloch manifold. These may or may not include pure states. For the adjoint representation $N=3/8$ and the bound (36) gives a boundary circle larger than the polygon by a factor of $\sqrt{14}$.

D. The Bloch manifold for the standard representation of $\mathfrak{su}_n$

We now discuss the structure of the Bloch manifold for the defining representation of $\mathfrak{su}_n$. First, Theorem 8 with $N=2/n$ gives a simple bound,

$$v^2 \leqslant \frac{n(n-1)}{2}. \tag{39}$$

By Descartes' rule of signs, an algebraic equation of degree D with real roots

$$\sum_{j=0}^{D} (-1)^j a_j x^{n-j} = \prod_{i=1}^{D} (x - x_i) = 0, \quad x_i \in \mathbb{R}$$

has all roots non-negative if and only if $a_i \geqslant 0$ for all $i=0,\ldots,D$. Such an equation arises as the characteristic polynomial for a Hermitian matrix. Therefore the Bloch manifold for the n-dimensional irrep of $\mathfrak{su}_n$ is given by the set of $v \in \mathbb{R}^{n^2-1}$ such that the characteristic polynomial $\mathrm{ch}_{\boldsymbol{\rho}(v)}(x)$ has only non-negative coefficients. Some related results for $\mathfrak{su}_n$ were recently reported by Kimura.[19]

The coefficients a_i can be calculated for any specific example using $a_0=1$ and Newton's formula,

$$a_j = \frac{1}{j}\sum_{q=1}^{j} (-1)^{q-1} c_q a_{j-q}, \tag{40}$$

where $c_q=\Sigma_i x_i^q=\mathrm{tr}(\boldsymbol{\rho}(v)^q)$. The largest value of j that we need to consider is $j=d$, the dimension of the Hilbert space.

Naturally, calculating $c_q=\mathrm{tr}(\boldsymbol{\rho}^q)$ reduces to calculating the traces of products of at most q generators of $\mathfrak{su}_n$. Since

$$a_1 = c_1 = 1 \quad \text{and } a_2 = \tfrac{1}{2}(1 - c_2),$$

the condition $a_2 \geqslant 0$ is equivalent to $\operatorname{tr} \boldsymbol{\rho}^2 \leqslant 1$, which leads to (39).

Using (40), the condition $a_3 \geqslant 0$ reduces to $c_3 \geqslant 1/2(3c_2 - 1)$, but c_2 is given by (37), and a similar calculation shows that

$$c_3 \equiv \operatorname{tr} \boldsymbol{\rho}^3 = \frac{1}{n^3}(n + 6v^2 + 2v_a v_b v_c d_{abc}).$$

The calculations up to this point have been valid for $\mathfrak{su}_n$ for all n. To completely solve the problem for $n > 3$, we need to know $c_4, c_5, \ldots, c_n$. However, we can completely calculate the Bloch manifold for the $\mathfrak{su}_3$ channel in closed form. For $n = 3$, we note that

$$\det(v \cdot \lambda) = \tfrac{2}{3} d_{ijk} v_i v_j v_k$$

so the condition $c_3 \geqslant 1/2(3c_2 - 1)$ (for $n = 3$) can be expressed as $\det(v\lambda) > -1$ and $v^2 \leqslant 1 + \det(v\lambda)$. Therefore, the Bloch manifold for the **3** of $\mathfrak{su}_3$ admits the following expression, beautiful in its simplicity:

$$\mathcal{V}_{\mathfrak{su}_3} = \{v \in \mathbb{R}^8 : v^2 \leqslant \min(3, 1 + \det(v\lambda))\}. \tag{41}$$

E. Bloch manifold for the seven of G_2.

In our calculation of the $\mathfrak{g}_2$ channel, we explicitly constructed a basis β of $\mathfrak{g}_2$ using its definition as $\mathfrak{Der}(\mathbb{O})$. This basis was normalized so that

$$\sum_a \beta_a^2 = \mathbf{1}, \quad \operatorname{tr}(\beta_a \beta_b) = \frac{1}{2}\delta_{ab}.$$

Theorem 8 gives

$$|v| \leqslant 2\sqrt{21}.$$

This proves that the $\mathfrak{g}_2$ Bloch manifold is contained in a closed ball of radius about 9.2. However, the true radius is much smaller, as we will now show. By $\mathfrak{g}_2$ symmetry, the β's satisfy the identity

$$\operatorname{tr}(v\beta)^q = 0, \quad (\forall\ v \in \mathbb{R}^{14}), \quad q \text{ odd},$$

where $v\beta = \Sigma_i v_i \beta_i$. Further, for certain even values of q, $\operatorname{tr}(v\beta)^q$ may have a simple expression. For example,

$$\operatorname{tr}(v\beta)^2 = \frac{v^2}{2}, \quad \operatorname{tr}(v\beta)^4 = (\operatorname{tr}(v\beta)^2)^2 = \frac{v^4}{4}. \tag{42}$$

The $\mathfrak{g}_2$ trace identity $\operatorname{tr}(v\beta)^4 = (\operatorname{tr}(v\beta)^2)^2$ is not easy to prove. It is true because for $\mathfrak{g}_2$ and some other algebras, every fourth-order Casimir invariant is expressible in terms of the second-order invariant, as shown by Okubo.[20] Recently a simpler proof, together with other interesting trace identities, was given by Macfarlane and Pfeiffer,[21] see their Eq. (4.36).

Enforcing $c_3 \geqslant 1/2(3c_2 - 1)$ gives a refinement,

$$|v| \leqslant 2\sqrt{7} \approx 5.3.$$

Requiring $a_4 \geqslant 0$ gives $v^2 \leqslant 8(10 - \sqrt{65})$, so $|v| \leqslant 3.93$. The coefficients are such that $a_5 \geqslant 0$ for all v, and $\operatorname{tr}(v\beta)^n$ for $n \geqslant 6$ has no simple expression analogous to (42), so we have taken the simple analysis of the $\mathfrak{g}_2$ Bloch manifold as far as it will go.

F. Pure states in the Bloch manifold

Let the representation matrices be denoted by $X_a, a=1,\ldots,k$. If v is in the Bloch manifold, so that

$$\boldsymbol{\rho}_v = d^{-1}\left(\mathbf{1} + \sum_a v_a X_a\right)$$

is a density matrix, it is particularly easy to determine whether $\boldsymbol{\rho}$ is pure. If the products $X_a X_b$ are linearly independent from X_a (i.e., there is no $2\to 1$ identity) then $\boldsymbol{\rho}^2 \neq \boldsymbol{\rho}$ and the state is never pure.

On the other hand, if the representation has a $2\to 1$ identity of the type satisfied by the fundamental representation of $\mathfrak{su}_n$,

$$X_a X_b = \beta \delta_{ab}\mathbf{1} + \sum_c Q_{abc} X_c, \tag{43}$$

then there can be pure states, and we have a complete characterization of them.

Theorem 10 (pure Bloch states): *If the* $2\to 1$ *identity* (43) *holds, then a Bloch state* $\boldsymbol{\rho}_v$ *is pure if and only if*

$$1 + \beta v^2 = d \quad \textit{and} \sum_{a,b} v_a v_b Q_{abc} = \left(1 - \frac{2}{d}\right) v_c,$$

for all $c=1,\ldots,k$.

Proof: This follows from $\boldsymbol{\rho}_v{}^2 = (1/d^2)(1+\beta v^2)\mathbf{1} + (1/d^2)\Sigma_{abc}(2v_c + v_a v_b Q_{abc})X_c$. □

It is interesting to see how Theorem 10 specializes to $d=2$. In that case, $Q_{abc}=0$ and also $1 - 2/d = 0$, so the second equation is always satisfied. The first equation amounts to $v^2 = 1/\beta$, and $\beta = 1$, so this just says that v is on the boundary of the Bloch sphere, which is the well-known characterization of pure states.

Unfortunately, $2\to 1$ identities almost never hold, excepting of course the fundamental representation of $\mathfrak{su}_n$, because products $X_a X_b$ tend to be linearly independent from the representation matrices X_a if the dimension of the vector space is large enough to allow this.

G. Summary of Bloch manifold technology

The Bloch manifold is defined to contain the positive-semidefinite density matrices and is given (in a certain basis) by the solution of a system of polynomial inequalities in the components of the Bloch vector v. These inequalities come from enforcing positivity of the density matrix, $\boldsymbol{\rho}_v \geqslant 0$. It is easy to see that the Bloch manifold is bounded within a ball, by enforcing the inequality $\mathrm{tr}(\boldsymbol{\rho}^2) \leqslant 1$. The Bloch manifold for the **3** of $\mathfrak{su}_3$ can be calculated exactly, and also in principle for $\mathfrak{g}_2$. In the latter case, it is bounded within a ball of radius < 3.93. In any representation of any Lie algebra, if a $2\to 1$ identity (43) holds, then pure states lie on the surface of a sphere of squared radius $(d-1)/\beta$.

What we have defined and studied here should rightly be called the *linear Bloch manifold*, because already for the spin-1 channel, one needs to represent the density matrix as $v\cdot J + \Sigma_{a,b} w_{ab} J_{(a} J_{b)}$. So the full geometry of the space of 3×3 density matrices is described by placing nontrivial conditions on both v and w, and similar remarks apply in higher dimensions.

The positivity constraint $\boldsymbol{\rho} \geqslant 0$ can always be solved by the method of Sec. VI D, but its complete solution requires knowledge of $\mathrm{tr}(\boldsymbol{\rho}^q)$ for all $q \leqslant d$ for a d-dimensional quantum system. Also, $\boldsymbol{\rho}$ itself may not be representable as a linear combination of generators, but will require products of m generators where m grows with the dimension. Thus to apply the method of Sec. VI D, one needs a trace identity for a product of md generators. The study of such identities is an active branch of research.[21]

VII. CONCLUSIONS

The main results are as follows:

(1) Definition 2 and Theorem 2 which define the Lie algebra channel and provide conditions for this channel to be trace-preserving (and hence physically realizable),
(2) identification of the $\mathfrak{su}(n)$ channel (in its standard representation) as a depolarizing channel,
(3) computation of the action of the $\mathfrak{su}(2)$ channel in its Three-dimensional representation (the spin-1 case) on a general Hermitian 3×3 matrix, and on some special pure states,
(4) definition and analysis of channels based on the exceptional Lie algebra $\mathfrak{g}_2$ and the Clifford algebra,
(5) a description of the positive semidefinite matrices which represent quantum states for various Lie algebra channels, and a general method for proving positivity from Lie algebraic trace identities.

In conclusion, the mathematical problems posed by quantum information theory and, more generally, by finite-dimensional quantum systems often involve computations which are most easily handled using techniques from representation theory of Lie algebras. In many cases, the feasibility of these calculations rests on the availability of trace identities,[20,21] of which many are known but surely many more remain to be discovered.

It is remarkable and unexpected by this author how much the theory of quantum channels and the classical theory of Lie algebras seem to dovetail. In some cases, classical results about Lie algebras receive independent proofs based on physical intuition. This is surely a math/physics bridge.

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On approximately symmetric informationally complete positive operator-valued measures and related systems of quantum states

Andreas Klappenecker[a)]
Department of Computer Science, Texas A&M University, College Station, Texas 77843-3112

Martin Rötteler[b)]
NEC Laboratories America, Inc., Princeton, New Jersey 08540

Igor E. Shparlinski[c)]
Department of Computing, Macquarie University, Sydney, NSW 2109, Australia

Arne Winterhof[d)]
Johann Radon Institute for Computational and Applied Mathematics, Austrian Academy of Sciences Altenbergerstr. 69, 4040 Linz, Austria

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We address the problem of constructing positive operator-valued measures (POVMs) in finite dimension n consisting of n^2 operators of rank one which have an inner product close to uniform. This is motivated by the related question of constructing symmetric informationally complete POVMs (SIC-POVMs) for which the inner products are perfectly uniform. However, SIC-POVMs are notoriously hard to construct and, despite some success of constructing them numerically, there is no analytic construction known. We present two constructions of approximate versions of SIC-POVMs, where a small deviation from uniformity of the inner products is allowed. The first construction is based on selecting vectors from a maximal collection of mutually unbiased bases and works whenever the dimension of the system is a prime power. The second construction is based on perturbing the matrix elements of a subset of mutually unbiased bases. Moreover, we construct vector systems in $\mathbb{C}^n$ which are almost orthogonal and which might turn out to be useful for quantum computation. Our constructions are based on results of analytic number theory. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1998831]

I. INTRODUCTION

A. Background

A basic question in quantum mechanics is how to obtain information about the state of a given physical system by using suitable measurements. Even in the case when many identically prepared copies of the system are available, it is a nontrivial task to devise a measurement procedure that uniquely identifies the given quantum state from the statistical data produced by the measurements. Note that this holds true even in the case where the complete statistics, that is, the probabilities for the different measurement outcomes, is known.

[a)]Electronic mail: klappi@cs.tamu.edu
[b)]Electronic mail: mroetteler@nec-labs.com
[c)]Electronic mail: igor@ics.mq.edu.au
[d)]Electronic mail: arne.winterhof@oeaw.ac.at

We next describe the possible measurements of the quantum system in more detail and first remark that all systems considered in this paper are of finite dimension n. If the state of the quantum system is given by an $n \times n$ density matrix, then the complete measurement statistics of one fixed *von Neumann measurement* is not sufficient to reconstruct the state. Indeed, this follows from the fact that the statistics of a fixed von Neumann measurement determines at most $n-1$ real parameters (specified by the probabilities of the measurement outcomes), whereas a general density matrix is determined by n^2-1 free real parameters.

In fact, it is possible to perform a more general measurement procedure on a quantum system, namely a *positive operator-valued measure*, or POVM for short (see Refs. 33 and 34). A POVM is described by a collection of positive operators $E_i \geqslant 0$, called POVM elements, that partition the identity, that is, $\Sigma_i E_i = I_n$. If the state of the quantum system is given by the density matrix ρ, then the probability p_i to observe outcome i in the POVM is given by the Born rule

$$p_i = \mathrm{tr}(\rho E_i), \tag{1}$$

where $\mathrm{tr}(A)$ denotes the trace of a complex matrix A. The task is to devise a POVM with operators E_i such that the state ρ is uniquely specified by the probabilities p_i in (1). The POVM is then called *informationally complete*, or simply an IC-POVM, and they appear to have been first studied in Ref. 38. A particularly interesting question is whether a POVM exists on $\mathbb{C}^n$ that consists of n^2 POVM elements E_i of rank one. Counting the number of parameters determined by the measurement, we see that n^2 is indeed the minimal possible number of such POVM elements. In this case E_i is a subnormalized projector, that is, $E_i = \Pi_i / n$ for projectors $\Pi_i = |\psi_i\rangle\langle\psi_i|$ corresponding to some vectors $|\psi_i\rangle$ in $\mathbb{C}^n$. In Ref. 12 it has been shown that IC-POVMs exist in all dimensions and in Ref. 15 a method has been given how to construct IC-POVMs by taking a fixed fiducial start vector $|\psi\rangle$ and taking the orbit of this vector under a (projective) group operation.

As an example of this type, consider the normalized states $|\psi_1\rangle, \ldots, |\psi_4\rangle$ defined as follows:

$$|\psi_1\rangle = \frac{1}{3}\begin{pmatrix} 1 \\ 2+2i \end{pmatrix}, \quad |\psi_2\rangle = \frac{1}{3}\begin{pmatrix} 2+2i \\ 1 \end{pmatrix},$$

$$|\psi_3\rangle = \frac{1}{3}\begin{pmatrix} 1 \\ -2-2i \end{pmatrix}, \quad |\psi_4\rangle = \frac{1}{3}\begin{pmatrix} 2+2i \\ -1 \end{pmatrix}.$$

Then the rank one operators defined by $E_i = 1/2|\psi_i\rangle\langle\psi_i|$ are given by

$$E_1 = \frac{1}{18}\begin{pmatrix} 1 & 2-2i \\ 2+2i & 8 \end{pmatrix}, \quad E_2 = \frac{1}{18}\begin{pmatrix} 8 & 2+2i \\ 2-2i & 1 \end{pmatrix},$$

$$E_3 = \frac{1}{18}\begin{pmatrix} 1 & -2+2i \\ -2-2i & 8 \end{pmatrix}, \quad E_4 = \frac{1}{18}\begin{pmatrix} 8 & -2-2i \\ -2+2i & 1 \end{pmatrix},$$

and it can be verified easily that $E_1+E_2+E_3+E_4 = I_4$ is the identity matrix and that the matrices E_1, E_2, E_3, E_4 are linearly independent. For the possible inner products between two POVM elements E_i and E_j where $i \neq j$ we obtain that $\mathrm{tr}(E_i E_j) \in \{4/81, 49/324\}$.

Our goal is to find IC-POVMs on $\mathbb{C}^n$ such that $n^2\mathrm{tr}(E_i E_j)$ is "small" for distinct POVM elements $E_i = |\psi_i\rangle\langle\psi_i|/n$ and $E_j = |\psi_j\rangle\langle\psi_j|/n$. In Sec. I C we make precise what we mean by the inner products being small and briefly summarize previous work on the problem.

B. Notation

We use the Landau notation to compare the asymptotics of two functions $f, g: \mathbb{N} \to \mathbb{C}$. We recall that $f(n) = o(g(n))$ means $\lim_{n\to\infty} f(n)/g(n) = 0$. Furthermore, $f(n) = O(g(n))$ means that there exists a constant $c > 0$, such that $|f(n)| \leqslant c g(n)$ for all $n \geqslant 1$. Throughout the paper, the implied

constants in the symbols "o" and "O" may occasionally, where obvious, depend on an integer parameter d and a small real parameter $\varepsilon>0$, and are absolute otherwise.

For an integer $n\geqslant 1$ we denote by $\mathbb{C}^n$ the n-dimensional vector space over the complex numbers $\mathbb{C}$. For two vectors $|\psi\rangle=(a_1,\ldots,a_n)\in\mathbb{C}^n$ and $|\varphi\rangle=(b_1,\ldots,b_n)\in\mathbb{C}^n$, we use

$$\langle\psi|\varphi\rangle=\sum_{i=1}^{n}\bar{a}_i b_i$$

to denote their inner product. We also define $\delta_{i,j}=1$ if $i=j$ and 0 otherwise. We denote the identity matrix of size $n\times n$ by I_n, the all-ones matrix of size n by $J_n=[1]_{i,j=1}^{n}$. We use $\mathrm{diag}(a_1,\ldots,a_n)$ to denote the $n\times n$ diagonal matrix which has $a_1,\ldots,a_n$ on the main diagonal. For matrices A and B, we use $A\oplus B$ to denote their block-diagonal direct sum.

For a real z and an integer m we use the notation $\mathbf{e}_m(z)=\exp(2\pi\iota z/m)$, where $\iota=\sqrt{-1}$.

We use $\mathbb{F}_q$ to denote the finite field of q elements, and we also assume that for a prime p, the field $\mathbb{F}_p$ is represented by the set $\{0,\ldots,p-1\}$.

As we have mentioned, we use $\mathrm{tr}(A)$ to denote the trace of a complex matrix A. On the other hand, for an element $a\in\mathbb{F}_q$ we use $\mathrm{Tr}_{\mathbb{F}_q/\mathbb{F}_p}(a)$ to denote its trace in the prime subfield $\mathbb{F}_p$ of $\mathbb{F}_q$ (see Ref. 31). That is, if $q=p^m$ for a prime p and a positive integer m, then

$$\mathrm{Tr}_{\mathbb{F}_q/\mathbb{F}_p}(a)=\sum_{j=0}^{m-1}a^{p^j}.$$

C. Previously known results

A particularly appealing case of IC-POVMs arises when, furthermore, all of the inner products of the vectors $|\psi_i\rangle$ are small. An extremal case in this sense arises when we are given a system of n^2 normalized vectors $\{|\psi_i\rangle: i=1,\ldots,n^2\}$ in $\mathbb{C}^n$ for which

$$|\langle\psi_i|\psi_j\rangle|^2=\frac{1}{n+1},\quad 1\leqslant i<j\leqslant n^2. \tag{2}$$

Indeed, for any system of k vectors $|\psi_1\rangle,\ldots,|\psi_k\rangle$ in $\mathbb{C}^n$ for which the absolute values of pairwise inner products are constant $|\langle\psi_i|\psi_j\rangle|^2=\alpha$, where $\alpha\in\mathbb{R}$ (for $1\leqslant i<j\leqslant k$), the so-called special bound holds[23] which says that $k\leqslant n(1-\alpha)/(1-n\alpha)$. Specializing $\alpha=1/(n+1)$ we obtain that n^2 is the largest possible number of vectors satisfying (2).

A system of vectors as in (2), respectively the corresponding POVMs, are called *symmetric informationally complete POVMs*, or SIC-POVMs for short. They have several very desirable properties; see Ref. 12 for a discussion in the context of the quantum de Finetti theorem and more generally in their Bayesian approach to quantum mechanics and its interpretation.[11] Furthermore, see Refs. 18 and 19 for their role in establishing the quantumness of a Hilbert space and the related question about optimal intercept-resend eavesdropping attacks on quantum cryptographic schemes. Explicit analytical constructions of sets satisfying (2) have been given for dimensions $n=2,3,4,5$ in Ref. 50, Sec. 3.4, and Ref. 41, for dimension $n=6$ in Ref. 20, for dimensions $n=7,19$ in Ref. 1, and for dimension $n=8$, see Ref. 24. While it has been conjectured that SIC-POVMs exist in all dimensions (Ref. 50, Sec. 3.4, or Ref. 41) and numerical evidence exists for dimensions up to 45 (see Ref. 41), it is a difficult task to explicitly construct systems of vectors which satisfy (2). There are no known infinite families of SIC-POVMs and, in fact, it is not even clear if there are SIC-POVMs for infinitely many n.

D. Our results

In the first part (Sec. II) of this paper we relax condition (2) on the inner products slightly and allow that

$$|\langle\psi_i|\psi_j\rangle|^2 \leqslant \frac{1+o(1)}{n}, \quad 1 \leqslant i < j \leqslant n^2. \tag{3}$$

The purpose of the first part of this paper is to show that infinite families of systems of n^2 normalized vectors which satisfy (3) and give rise to IC-POVMs exist. We call the rank one projectors obtained from such systems of vectors *approximately symmetric informationally complete POVMs*, or ASIC-POVMs for short. Here we show that when $n=p^r$ is a power of a prime p, ASIC-POVMs can be constructed.

In the second part (Sec. III) of the paper we explore properties of other approximately symmetric vector systems where we do not require the properties of completeness and informational completeness but require the property of approximate symmetry. We also relax (3) further by allowing that the inner products be bounded from above by $|\langle\psi_i|\psi_j\rangle| \leqslant (2+o(1))/\sqrt{n}$ and by dropping the requirement that the vectors give rise to a POVM. This additional freedom then allows us to construct bases in all dimensions n. Besides their general mathematical interest in constructing such vector systems they might be useful in quantum cryptographic scenarios which generalize the BB84 setting,[7] such as the protocols described in Refs. 8, 39, and 40. See also Ref. 14 for an analysis of general schemes for quantum key distribution where the sender uses arbitrary quantum states and the receiver's measurement is replaced by a POVM.

Besides approximations to SIC-POVMs we also consider approximations to *mutually unbiased bases* (MUBs). Since we also need MUBs for our construction of ASIC-POVMs we briefly recall their definition. A maximal set of MUBs is given by a set of n^2+n vectors in $\mathbb{C}^n$ which are the elements of $n+1$ orthonormal bases $\mathcal{B}_k=\{|\psi_{k,1}\rangle, \ldots, |\psi_{k,n}\rangle\}$ of $\mathbb{C}^n$ where $k=0, \ldots, n$. Hence,

$$\langle\psi_{k,i}|\psi_{k,j}\rangle = \delta_{i,j}, \tag{4}$$

and the defining property is the mutual unbiasedness, given by

$$|\langle\psi_{k,i}|\psi_{\ell,j}\rangle| = \frac{1}{\sqrt{n}} \tag{5}$$

for $0 \leqslant k, \ell \leqslant n$, $k \neq \ell$, and $1 \leqslant i, j \leqslant n$. Starting from Refs. 26, 42, and 49, an extensive growing body of research explores MUBs and their constructions (see Refs. 2, 4, 6, 13, 17, 21, 27, 36, 37, and 48 and references therein). However, so far maximally sets of $n+1$ MUBs in dimension n are only known to exist in any dimension $n=p^r$ which is a power of a prime $p \geqslant 3$ (see Ref. 27 for an overview and some of such constructions). The main construction is based on Gaussian sums and in the case of prime $n=p$ can be described as

$$|\psi_{k,j}\rangle = \frac{1}{\sqrt{p}}(\mathbf{e}_p(ku^2+ju))_{u=1}^p, \quad 1 \leqslant k,j \leqslant p,$$

and also $\mathcal{B}_0$ being a standard orthonormal basis, that is, $|\psi_{0,j}\rangle=(\delta_{j,u})_{u=1}^p$.

One can use additive characters over an arbitrary finite field to extend this construction to an arbitrary prime power $n=p^r$. However, the condition that $n=p^r$ is a prime power is still somewhat too restrictive and unnatural for quantum computation. So a natural question arises whether MUBs exist for every positive integer n. In the second part we consider vector systems where we relax the conditions (3) and (5). We use exponential sums to construct vector systems for any dimension n which

- satisfy (4) but instead of (5) all other inner products are $O(n^{-1/4})$;
- are normalized but instead of (2) all other inner products are at most $(2+o(1))n^{-1/2}$.

We call vector systems of n^2+n vectors in $\mathbb{C}^n$ which satisfy (4), and instead of (5) the condition

$$|\langle\psi_i|\psi_j\rangle|^2 \leqslant \frac{1+o(1)}{n}, \quad 1 \leqslant i < j \leqslant n^2+n,$$

approximately mutually unbiased bases, or AMUBs for short.

We also construct some vector systems using multiplicative and mixed character sums, which

- satisfy (4) and, assuming some natural and widely believed conjecture on the distribution of primes in arithmetic progressions, all other inner products are $O(n^{-1/2}\log n)$;
- in the special case of $n=p-1$, where p is a prime, form AMUBs.

Interestingly, our arguments use both the classical bound of Weyl[47] (see also Refs. 25 and 43) as well as the more recent, but no less celebrated, bounds of Weil[45] (see also Refs. 30, 31, and 46). Besides exponential sum techniques we also use some recent results about the gaps between prime numbers from Ref. 3. We conclude with some conjectures and open questions concerning our constructions in Sec. IV.

II. CONSTRUCTING ASIC-POVMS

A. Preliminaries

We begin by giving a definition of the vectors and associated rank one operators we are interested in.

Definition 1 (ASIC-POVMs): Suppose that n is a positive integer. Let $\mathcal{A}=\{|\psi_i\rangle : i=1,\ldots,n^2\}$ *be a set of vectors in* $\mathbb{C}^n$. *Let* $\mathcal{E}=\{E_i=|\psi_i\rangle\langle\psi_i|/n : i=1,\ldots,n^2\}$ *be the corresponding set of subnormalized projection operators. If* $\mathcal{E}$ *satisfies the conditions*

(i) $\Sigma_{i=1}^{n^2} E_i = I_n$ (completeness/POVM condition),
(ii) *the matrices* E_i *are linearly independent as elements of* $\mathbb{C}^{n\times n}$ (informational completeness), *and*
(iii) $|\langle\psi_i|\psi_j\rangle|^2 = n^2\,\mathrm{tr}(E_iE_j) \leqslant (1+o(1))n^{-1}$ *for* $1\leqslant i<j\leqslant n^2$ (approximate symmetry),

then we call $\mathcal{E}$ *an* approximately symmetric informationally complete POVM, *or ASIC-POVM for short*.

We remark that, in fact, sometimes we also refer to the corresponding set $\mathcal{A}$ as an ASIC-POVM.

In the subsequent sections, we present two different constructions that give rise to infinite families of ASIC-POVMs. The first construction is based on the observation that a set of $n+1$ mutually unbiased bases in $\mathbb{C}^n$ gives rise to an IC-POVM, cf. Refs. 26 and 49. However, this IC-POVM consists of n^2+n rank-one operators; thus, it is an overcomplete generating set of the vector space of all $n\times n$ matrices. In our first construction in Sec. II C we show how to select n^2 projectors that allow us to derive an ASIC-POVM. The second construction in Sec. II D starts from all vectors contained in n of the $n+1$ MUBs. We show that by slightly perturbing the components of these vectors it is possible to obtain an ASIC-POVM.

B. POVMs and frames

Suppose that $\mathcal{A}=\{|\psi_i\rangle \in \mathbb{C}^n 1\leqslant i\leqslant n^2\}$ is a system of n^2 vectors of unit norm, such that $\mathcal{A}$ spans $\mathbb{C}^n$ and the associated subnormalized projectors $E_i=|\psi_i\rangle\langle\psi_i|/n$ satisfy $n^2\,\mathrm{tr}(E_iE_j)=(1+o(1))n^{-1}$ whenever $i\neq j$.

We would like to have that the subnormalized projectors E_i form a POVM, but, unfortunately, the completeness relation $\Sigma_{i=1}^{n^2}E_i=I_n$ is in general not satisfied. However, there is a way to fix this using a technique described in Ref. 12: Define a positive semidefinite Hermitian operator G by

$$G = \sum_{i=1}^{n^2} E_i.$$

Since $\mathcal{A}$ spans $\mathbb{C}^n$, the inequality $\langle\varphi|G|\varphi\rangle = \Sigma_i |\langle\psi_i|\varphi\rangle|^2 > 0$ holds for any nonzero vector $|\varphi\rangle$ in $\mathbb{C}^n$, so G is even positive definite. It follows that G^{-1} exists and is positive definite, and we can form the uniquely determined positive definite square root $G^{-1/2}$. The n^2 rank-one operators

$$\mathcal{E} = \{F_i = G^{-1/2} E_i G^{-1/2} : 1 \leqslant i \leqslant n^2\}$$

form a POVM, since $\Sigma_i F_i = G^{-1/2} G G^{-1/2} = I_n$.

Clearly, if the operators E_i are linearly independent, then so are the operators F_i. Therefore, the procedure preserves information completeness.

In general, if we switch from the rank-one operators E_i to the rank-one operators F_i, then $\mathrm{tr}(F_i F_j) \leqslant (1+o(1))/n^3$ might not hold for some $i \neq j$. However, if G^{-1} is close to the identity matrix, then approximate symmetry is preserved as well.

We now mention some connections between POVMs and the theory of frames.[5,9,16]

Definition 2 (Frames): A set $\mathcal{F} = \{|\psi_i\rangle : 1 \leqslant i \leqslant N\}$ of vectors in $\mathbb{C}^n$ is called a frame *if there exist real numbers a and b, with $0 < a \leqslant b$, such that*

$$a\langle\varphi|\varphi\rangle \leqslant \sum_{i=1}^{N} |\langle\varphi|\psi_i\rangle|^2 \leqslant b\langle\varphi|\varphi\rangle$$

holds for all $|\varphi\rangle \in \mathbb{C}^n$.

If $a=b$, then the frame is called a tight frame, *and if $a=b=1$, then the frame is called a* Parseval frame.

We can associate with the frame $\mathcal{F}$ its *frame operator* $G = \Sigma_{k=1}^{N} |\psi_k\rangle\langle\psi_k|$. If we are given a frame $\mathcal{F}$ with frame operator G, then

$$\mathcal{G} = \{G^{-1/2}|v\rangle : |v\rangle \in \mathcal{F}\}$$

is a Parseval frame (see Ref. 10, Theorem 4.2). The projectors associated with $\mathcal{G}$ form a POVM, since $\Sigma_{v\in\mathcal{F}} G^{-1/2}|v\rangle\langle v|G^{-1/2} = G^{-1/2} G G^{-1/2} = I$ holds.

If we have a Parseval frame $\mathcal{G}$ in $\mathbb{C}^n$ with n^2 elements such that the associated projection operators are linearly independent and the frame elements satisfy the approximate symmetry (3), then by definition the projectors corresponding to the frame $\mathcal{G}$ form an ASIC-POVM.

C. Construction I: Pruning MUBs

The first construction of ASIC-POVMs is based on the idea to select a suitable collection of n^2 vectors from a set of n^2+n vectors that form a maximal set of $n+1$ mutually unbiased bases of $\mathbb{C}^n$. Our goal is to choose n^2 vectors such that the corresponding projection operators are linearly independent. We recall a known fact that belongs to the folklore of mutually unbiased bases; it is implicitly contained in Refs. 26 and 49, and more explicitly in Ref. 22, and our proof is based on the latter.

Lemma 3: Suppose that $\mathcal{B}_a = \{v_{a,b} : 0 \leqslant b < n\}$, with $0 \leqslant a \leqslant n$, are $n+1$ mutually unbiased bases of $\mathbb{C}^n$, and let

$$\mathcal{P} = \{|v_{a,b}\rangle\langle v_{a,b}| : 0 \leqslant a \leqslant n, 0 \leqslant b < n\}$$

denote the associated set of n^2+n projectors. The n^2 projection operators in $\mathcal{P}^* = \{|v_{a,b}\rangle \times \langle v_{a,b}| : (a,b) = (0,0)$ or $b \neq 0\} \subset \mathcal{P}$ are linearly independent.

Proof: First, suppose that a linear relation

$$\sum_{a=0}^{n}\sum_{b=0}^{n-1}\gamma_{a,b}|v_{a,b}\rangle\langle v_{a,b}| = 0 \tag{6}$$

holds for some $\gamma_{a,b}\in\mathbb{C}$. We are going to show that this has some rather strong consequences for the coefficients $\gamma_{a,b}$. If we apply the projection operators from $\mathcal{P}$ and take the trace, then we obtain a linear system of equations $A\mathbf{g}=0$, where

$$A = [\mathrm{tr}(|v_{a,b}\rangle\langle v_{a,b}||v_{c,d}\rangle\langle v_{c,d}|)]_{(a,b),(c,d)}$$

and $\mathbf{g}=(\gamma_{a,b})$ is a column vector. The matrix A is block circulant,

$$A = \begin{pmatrix} I_n & \frac{1}{n}J_n & \cdots & \frac{1}{n}J_n & \frac{1}{n}J_n \\ \frac{1}{n}J_n & I_n & \cdots & \frac{1}{n}J_n & \frac{1}{n}J_n \\ \ddots & \ddots & & \ddots & \ddots \\ \frac{1}{n}J_n & \frac{1}{n}J_n & \cdots & \frac{1}{n}J_n & I_n \end{pmatrix},$$

with $n\times n$ identity matrices in the diagonal blocks, and multiples of the $n\times n$ all-one matrix in the off-diagonal blocks.

If we subtract two equations in $A\mathbf{g}=0$ that belong to the same block row, then we find that $\gamma_{a,b}=\gamma_{a,d}$ holds for all $0\leqslant b,d<n$ and all indices a. Therefore, the coefficients $\gamma_{a,b}$ do not depend on the value of b.

Finally, suppose that the left-hand side of (6) consists of a linear combination of projectors belonging to the set $\mathcal{P}^*$, meaning that the coefficients $\gamma_{a,b}=0$ when $a\neq 0$ and $b=0$. It follows that $\gamma_{a,b}=0$ holds whenever $a\neq 0$, since $\gamma_{a,b}=\gamma_{a,0}$ by our previous observation. Therefore, the left-hand side of (6) reduces to

$$\sum_{b=0}^{n-1}\gamma_{0,b}|v_{0,b}\rangle\langle v_{0,b}| = \sum_{b=0}^{n-1}\gamma_{0,0}|v_{0,b}\rangle\langle v_{0,b}| = 0.$$

Thus, we must have $\gamma_{0,0}=0$. Therefore, we can conclude that the projectors in P^* are linearly independent, as claimed. □

We also recall the basic construction of MUBs in prime power dimension; see, for instance, Refs. 27 and 49.

Lemma 4: Let q be a power of a prime $p\geqslant 3$. Define

$$|\psi_{a,b}\rangle = q^{-1/2}(\mathbf{e}_p(\mathrm{Tr}_{\mathbb{F}_q/\mathbb{F}_p}(ax^2+bx)))_{x\in\mathbb{F}_q}\in\mathbb{C}^q.$$

Then the standard basis $\mathcal{B}_0$ together with the bases $\mathcal{B}_a=\{|\psi_{a,b}\rangle : b\in\mathbb{F}_q\}$, $a\in\mathbb{F}_q$, form a set of $q+1$ mutually unbiased bases of $\mathbb{C}^q$.

Our first construction of ASIC-POVMs is given in the next theorem.

Theorem 5: *Let q be a power of a prime $p\geqslant 3$. Let*

$$|\psi_{a,b}\rangle = q^{-1/2}(\mathbf{e}_p(\mathrm{Tr}_{\mathbb{F}_q/\mathbb{F}_p}(ax^2+bx)))_{x\in\mathbb{F}_q}\in\mathbb{C}^q$$

for all $(a,b)\in\mathbb{F}_q\times\mathbb{F}_q^{\times}$ and $|\psi_{a,0}\rangle=(\delta_{a,x})_{x\in\mathbb{F}_q}$ for all $a\in\mathbb{F}_q$. We define $E_{a,b}=|\psi_{a,b}\rangle\langle\psi_{a,b}|/q$ and

$$G = \sum_{a\in\mathbb{F}_q}\sum_{b\in\mathbb{F}_q}E_{a,b}.$$

Then the set $\{F_{a,b}: a,b\in\mathbb{F}_q\}$, with $F_{a,b}=G^{-1/2}E_{a,b}G^{-1/2}$, is an ASIC-POVM.

Proof: The linear independence of the operators $E_{a,b}$ follows from Lemma 3. It remains to

show that the matrix G^{-1} is close to the identity and that $F_{a,b}=G^{-1/2}|\psi_{a,b}\rangle\langle\psi_{a,b}|G^{-1/2}$ indeed forms an ASIC-POVM. First, we explicitly compute the frame operator G. We have

$$G=\frac{1}{q}\sum_{(a,b)\in\mathbb{F}_q\times\mathbb{F}_q^\times}|\psi_{a,b}\rangle\langle\psi_{a,b}|+\frac{1}{q}I_q=\frac{1}{q^2}\Bigg(\sum_{x,y,a,b\in\mathbb{F}_q}\mathbf{e}_p(\mathrm{Tr}_{\mathbb{F}_q/\mathbb{F}_p}(a(x^2-y^2)+b(x-y)))|x\rangle\langle y|$$

$$-\sum_{x,y,a\in\mathbb{F}_q}\mathbf{e}_p(\mathrm{Tr}_{\mathbb{F}_q/\mathbb{F}_p}(a(x^2-y^2)))|x\rangle\langle y|\Bigg)+\frac{1}{q}I_q.$$

We notice that $\langle x|G|x\rangle=1$ for $x\in\mathbb{F}_q$, $\langle x|G|-x\rangle=-1/q$ for $x\in\mathbb{F}_q^\times$, and $\langle x|G|y\rangle=0$ for $x,y\in\mathbb{F}_q$ with $x\neq\pm y$. Therefore, we can express the operator G in the form

$$G=I_q-\frac{1}{q}Q+\frac{1}{q}|0\rangle\langle 0|,\quad\text{where } Q=\sum_{x\in\mathbb{F}_q}|x\rangle\langle -x|.$$

Using the structure of G, it follows that the inverse is given by

$$G^{-1}=\left(1+\frac{1}{q^2-1}\right)I_q+\frac{q}{q^2-1}Q-\frac{1}{q-1}|0\rangle\langle 0|.$$

Observe that the set of vectors $\{|\psi_{a,b}\rangle:(a,b)\in\mathbb{F}_q\times\mathbb{F}_q^\times\}$ is invariant under Q, since $Q|\psi_{a,b}\rangle=|\psi_{a,-b}\rangle$. Recall that by Lemma 4 the bounds

$$|\langle\psi_{a,b}|\psi_{c,d}\rangle|\leqslant q^{-1/2}$$

hold, whenever $(a,b)\neq(c,d)$. Defining $|\tilde{\psi}_{a,b}\rangle=G^{-1/2}|\psi_{a,b}\rangle$ we get

$$F_{a,b}=G^{-1/2}E_{a,b}G^{-1/2}=|\tilde{\psi}_{a,b}\rangle\langle\tilde{\psi}_{a,b}|/q$$

and obtain that

$$q^2\mathrm{tr}(F_{a,b}F_{c,d})=|\langle\tilde{\psi}_{a,b}|\tilde{\psi}_{c,d}\rangle|^2=|\langle\psi_{a,b}|G^{-1}|\psi_{c,d}\rangle|^2\leqslant\left|\left(1+\frac{1}{q^2-1}\right)\langle\psi_{a,b}|\psi_{c,d}\rangle\right|^2+\left|\left(\frac{q}{q^2-1}\right)\right.$$

$$\left.\times\langle\psi_{a,b}|\psi_{c,-d}\rangle\right|^2+\left(\frac{1}{q(q-1)}\right)^2\leqslant\frac{1}{q}\left(1+\frac{1}{q^2-1}\right)^2+\frac{1}{q}\left(\frac{q}{q^2-1}\right)^2+\left(\frac{1}{q(q-1)}\right)^2$$

$$=\frac{1+o(1)}{q}.$$

This shows that the rank-one operators $F_{a,b}$ form an ASIC-POVM. □

D. Construction II: Perturbing MUBs

We now describe a second, different, method to obtain a set of n^2 vectors such that the corresponding projectors span the space of all $n\times n$ matrices. This construction of ASIC-POVMs works for all dimensions n such that n is an odd prime number.

We note that all arithmetic operations in any expression involving elements of $\mathbb{F}_p$ and real numbers are performed over the real numbers (where each element of $\mathbb{F}_p$ is represented by an integer in the range $[0,p-1]$). For example, for a real $r\in\mathbb{R}$ and $a,x\in\mathbb{F}_p$, the power r^{ax} means r^u, where the integer $u=ax$ can be of size $(p-1)^2$.

Theorem 6: *Let p be an odd prime number, and let $0<r<1$ be a real number. For $a,b\in\mathbb{F}_p$ define*

$$|\varphi_{a,b}\rangle=\sqrt{\frac{1-r^{2a}}{1-r^{2pa}}}(r^{ax}\mathbf{e}_p(ax^2+bx))_{x\in\mathbb{F}_p}\in\mathbb{C}^p,$$

and let $E_{a,b}=|\varphi_{a,b}\rangle\langle\varphi_{a,b}|/p$. *Then the* $E_{a,b}$ *are linearly independent. Furthermore, let*

$$G=\sum_{a,b\in\mathbb{F}_p}E_{a,b}.$$

Then for $r=1-p^{-3}$ *the set* $\{F_{a,b}:a,b\in\mathbb{F}_p\}$, *with* $F_{a,b}=G^{-1/2}E_{a,b}G^{-1/2}$, *is an ASIC-POVM*.

Proof: First, we show that the matrices $E_{a,b}$ are linearly independent. Note that instead of considering the normalized vectors $|\varphi_{a,b}\rangle$ it is possible to consider the vectors $|\tilde{\varphi}_{a,b}\rangle=(r^{ax}\mathbf{e}_p(ax^2+bx))_{x\in\mathbb{F}_p}$ and to show that the corresponding projectors $\tilde{E}_{a,b}=|\tilde{\varphi}_{a,b}\rangle\langle\tilde{\varphi}_{a,b}|$ are linearly independent.

We use the technique introduced in Ref. 15 to check whether the matrices $\tilde{E}_{a,b}$ are linearly independent. To each $n\times n$ matrix $\tilde{E}_{a,b}$ we associate a state $|\tilde{E}_{a,b}\rangle$ which is simply the rowwise concatenation of the entries of $\tilde{E}_{a,b}$ as a vector of length n^2. Then the matrices $\tilde{E}_{a,b}$ are linearly independent if and only if the matrix $S=(1/p)\Sigma_{a,b\in\mathbb{F}_p}|\tilde{E}_{a,b}\rangle\langle\tilde{E}_{a,b}|$ has full rank. We obtain

$$pS=\sum_{a,b\in\mathbb{F}_p}|\tilde{E}_{a,b}\rangle\langle\tilde{E}_{a,b}|=\sum_{\substack{a\in\mathbb{F}_p\\x,y,u,v\in\mathbb{F}_p}}r^{a(x+y+u+v)}\mathbf{e}_p(a(x^2-y^2-u^2+v^2))\times\sum_{b\in\mathbb{F}_p}\mathbf{e}_p(b(x-y-u+v))|x,y\rangle$$

$$\times\langle u,v|=p\sum_{\substack{a\in\mathbb{F}_p\\x,y,u,v\in\mathbb{F}_p}}r^{a(x+y+u+v)}\mathbf{e}_p(a(x^2-y^2-u^2+v^2))\,\delta_{x-y,u-v}|x,y\rangle\langle u,v|.$$

The rows of S are labeled by pairs (x,y), with $x,y\in\mathbb{F}_p$, and the columns by pairs (u,v), with $u,v\in\mathbb{F}_p$. We first note that S can be written as a block-diagonal matrix of p submatrices, each of size $p\times p$, if the rows and columns of S are suitably rearranged. For $0\leqslant i\leqslant(p-1)$, we define the sets $\mathcal{L}_i=\{(x,x+i):x\in\mathbb{F}_p\}$ (we treat i as an element of $\mathbb{F}_p$ so $x+i$ is computed in $\mathbb{F}_p$, too). We now order the rows and columns according to the list $\mathcal{L}=\cup_{i=0}^{p-1}\mathcal{L}_i$. With respect to this basis we obtain that

$$S=A_0\oplus A_1\oplus\cdots\oplus A_{p-1},$$

with $p\times p$ matrices

$$A_i=\left[\sum_{a\in\mathbb{F}_p}r^{a(x+y+u+v)}\mathbf{e}_p(a(x^2-y^2-u^2+v^2))\right]_{x,u\in\mathbb{F}_p},$$

where $y=x+i$ and $v=u+i$. Hence, we obtain that

$$A_i=\left[\sum_{a\in\mathbb{F}_p}r^{2a(x+u+i)}\mathbf{e}_p(2ai(u-x))\right]_{x,u\in\mathbb{F}_p}$$

and have to show that this matrix is invertible for $0\leqslant i\leqslant(p-1)$. In order to do so, we first observe that $x\mapsto x-i/2$ defines a permutation of the rows of any $p\times p$ matrix and that similarly $u\mapsto u-i/2$ defines a permutation of the columns (hereafter $i/2$ is computed in $\mathbb{F}_p$). Applying both the row and the column permutation to A_i we obtain the matrix

$$B_i=\left[\sum_{a\in\mathbb{F}_p}r^{2a(x+y)}\mathbf{e}_p(2ai(u-x))\right]_{x,u\in\mathbb{F}_p}.$$

Note further that $x\mapsto x/2$ and $y\mapsto y/2$ induce permutations of the rows and columns of any $p\times p$ matrix. Applying this to B_i we obtain the matrix

$$C_i=\left[\sum_{a\in\mathbb{F}_p}r^{a(u+x)}\mathbf{e}_p(ai(u-x))\right]_{x,u\in\mathbb{F}_p}=\left[\sum_{a\in\mathbb{F}_p}(r^x\mathbf{e}_p(-ix))^a(r^u\mathbf{e}_p(iu))^a\right]_{x,u\in\mathbb{F}_p}$$

$$=[(r\mathbf{e}_p(-i))^{xk}]_{x,k=0}^{p-1}\times[(r\mathbf{e}_p(i))^{\ell u}]_{\ell,u=0}^{p-1}.$$

Since $|r\mathbf{e}_p(i)|=|r\mathbf{e}_p(-i)|=r$ and $0<r<1$, by the property of Vandermonde matrices[32] we conclude that C_i is invertible for all $i=0,\ldots,p-1$, which implies that the matrices B_i, A_i, and finally S are invertible. Arguing as in the proof of Theorem 5 we have established the informational completeness of the projectors corresponding to the normalized vectors $|\varphi_{a,b}\rangle$.

Next, for $r=1-p^{-3}$ we derive the bound

$$|\langle\varphi_{a,b}|\varphi_{c,d}\rangle| \leqslant \frac{1+o(1)}{\sqrt{p}}, \quad (a,b)\neq(c,d). \tag{7}$$

We have

$$|\langle\varphi_{a,b}|\varphi_{c,d}\rangle| = \sqrt{\frac{1-r^{2a}}{1-r^{2pa}}}\sqrt{\frac{1-r^{2c}}{1-r^{2pc}}}\left|\sum_{x\in\mathbb{F}_p} r^{(a+c)x}\mathbf{e}_p(\alpha x^2+\beta x)\right|, \tag{8}$$

where $\alpha=a-c$ and $\beta=c-d$.

We frequently use that $r^t=1+O(t/p^3)$ for any $t=O(p^3)$. In particular,

$$\begin{aligned}\sqrt{\frac{1-r^{2a}}{1-r^{2pa}}}\sqrt{\frac{1-r^{2c}}{1-r^{2pc}}} &= \left(\sum_{x\in\mathbb{F}_p} r^{2ax}\right)^{-1/2}\left(\sum_{x\in\mathbb{F}_p} r^{2cx}\right)^{-1/2} \leqslant \left(\sum_{x\in\mathbb{F}_p} r^{2px}\right)^{-1}\\ &= (p(1+O(1/p)))^{-1} = (1+o(1))p^{-1}.\end{aligned}$$

Furthermore,

$$\begin{aligned}\left|\sum_{x\in\mathbb{F}_p} r^{(a+c)x}\mathbf{e}_p(\alpha x^2+\beta x)\right| &\leqslant \left|\sum_{x\in\mathbb{F}_p}(1+O(1/p))\mathbf{e}_p(\alpha x^2+\beta x)\right| \leqslant \left|\sum_{x\in\mathbb{F}_p}\mathbf{e}_p(\alpha x^2+\beta x)\right| + O(1)\\ &\leqslant \sqrt{p}+O(1).\end{aligned}$$

Substituting the above bounds in (8), we derive (7).

Next, we note that $E_{a,b}=|\varphi_{a,b}\rangle\langle\varphi_{a,b}|/p$ and $G=\Sigma_{a,b\in\mathbb{F}_p}E_{a,b}$. We now compute the frame operator G and show that G^{-1} is close to the identity. Similarly to the proof of Theorem 5, this implies that $F_{a,b}=G^{-1/2}E_{a,b}G^{-1/2}$ indeed forms an ASIC-POVM. We have

$$\begin{aligned}G &= \left(\sum_{\substack{a,b\in\mathbb{F}_p\\ x,y,\in\mathbb{F}_p}} \frac{1-r^{2a}}{p(1-r^{2pa})} r^{a(x+y)}\mathbf{e}_p(a(x^2-y^2)+b(x-y))|x\rangle\langle y|\right)\\ &= \left(\sum_{\substack{a\in\mathbb{F}_p\\ x,y,\in\mathbb{F}_p}} \frac{1-r^{2a}}{1-r^{2pa}} r^{a(x+y)}\mathbf{e}_p(a(x^2-y^2))\,\delta_{x,y}|x\rangle\langle y|\right) = \operatorname{diag}\left(\sum_{a\in\mathbb{F}_p}\frac{1-r^{2a}}{1-r^{2pa}}r^{2ax} : x\in\mathbb{F}_p\right).\end{aligned}$$

Recalling that $r=1-p^{-3}$, from the Taylor expansion we obtain that

$$\frac{1-r^{2a}}{1-r^{2pa}} = \frac{1+o(1)}{p}.$$

Hence

$$\sum_{a\in\mathbb{F}_p}\frac{1-r^{2a}}{1-r^{2pa}}r^{2ax} = \frac{1+o(1)}{p}\sum_{a\in\mathbb{F}_p} r^{2ax} = \frac{1+o(1)}{p}(p+O(1)) = 1+o(1).$$

Finally, we deduce that

$$p^2\operatorname{tr}(F_{a,b}F_{c,d}) = |\langle\widetilde{\varphi}_{a,b}|\widetilde{\varphi}_{c,d}\rangle|^2 = |\langle\varphi_{a,b}|G^{-1}|\varphi_{c,d}\rangle|^2 = (1+o(1))|\langle\varphi_{a,b}|\varphi_{c,d}\rangle|^2 = \frac{1+o(1)}{p},$$

which implies that the rank-one operators $F_{a,b}$ form an ASIC-POVM. □

III. RELAXED MUBs AND SIC-POVMs

A. Motivation

The constructions in the previous sections required the existence of $n+1$ mutually unbiased bases in $\mathbb{C}^n$. Currently, it is not known whether such extremal sets of mutually unbiased bases exist when n is divisible by two distinct primes. We show that approximately mutually unbiased bases exists in all dimensions. Furthermore, we show that if we slightly relax the ASIC-POVM condition, then we can obtain in any dimension systems of vectors that approximate SIC-POVMs. For these constructions, we need some results about the distribution of primes and bounds on exponential sums, which we summarize below.

These constructions work in any dimension n but attain its maximal strength for n of a certain arithmetic structure. In particular, if $n=p-1$ for a prime p, then we show the existence of AMUBs in $\mathbb{C}^n$. It is not known whether maximal sets of MUBs in these dimensions exist.

Besides the general mathematical interest in the vector systems derived in this section, we expect that our approach and the new technique introduced in the following will lend themselves to some further applications in quantum information processing.

B. Analytic number theory background

First of all we recall a remarkable result of Ref. 3 on gaps between consecutive primes.

Lemma 7: For any sufficiently large x, any interval of the form $[x-x^{0.525},x]$ contains a prime number.

We now need some bounds of exponential sums with polynomials.

Let p be a prime number and let $\mathbb{F}_p$ be a field of p elements. We always assume that $\mathbb{F}_p$ is represented by the elements $\{0,\ldots,p-1\}$.

The following statement is a variant of the celebrated *Weil bound* (see Example 12 of Appendix 5 of Ref. 46 as well as Theorem 3 of Chap. 6 in Ref. 30 and Theorem 5.41 and comments to Chap. 5 of Ref. 31).

Lemma 8: Let χ be a nontrivial multiplicative character of $\mathbb{F}_p$ of order s. Suppose that $G(X)\in\mathbb{F}_p[X]$ is not, up to a nonzero multiplicative constant, an sth power in $\mathbb{F}_p[X]$. Then for any polynomial $F(X)\in\mathbb{F}_p[X]$ of degree d we have

$$\left|\sum_{u=1}^{p}\mathbf{e}_p(F(u))\chi(G(u))\right|\leqslant(d+\nu-1)p^{1/2},$$

where ν is the number of distinct roots of G in the algebraic closure of $\mathbb{F}_p$.

We now use Lemma 8 to estimate some mixed exponential sums with two exponential functions.

Lemma 9: Let $F(X)\in\mathbb{F}_p[X]$ be of degree $d\geqslant 2$. Then, for any integer k,

$$\left|\sum_{u=1}^{p}\mathbf{e}_p(F(u))\mathbf{e}_n(ku)\right|=\begin{cases}O(p^{2/3}), & \text{if } d=2,\\ O(p^{3/4}), & \text{if } d\geqslant 3.\end{cases}$$

Proof: Because each term in our sum is of absolute value $|\mathbf{e}_p(F(u))\mathbf{e}_n(ku)|=1$, for every integer $v\geqslant 0$ we have

$$\sum_{u=1}^{p}\mathbf{e}_p(F(u))\mathbf{e}_n(ku)=\sum_{u=1}^{p}\mathbf{e}_p(F(u+v))\mathbf{e}_n(k(u+v))+O(v).$$

Thus for every positive integer m we have

$$m\sum_{u=1}^{p}\mathbf{e}_p(F(u))\mathbf{e}_n(ku)=\sum_{v=0}^{m-1}\sum_{u=1}^{p}\mathbf{e}_p(F(u+v))\mathbf{e}_n(k(u+v))+O(m^2).$$

Therefore

$$\left|\sum_{u=1}^{p}\mathbf{e}_p(F(u))\mathbf{e}_n(ku)\right|\leqslant\frac{1}{m}W+O(m), \tag{9}$$

where

$$W=\left|\sum_{u=1}^{p}\sum_{v=0}^{m-1}\mathbf{e}_p(F(u+v))\mathbf{e}_n(k(u+v))\right|=\left|\sum_{u=1}^{p}\mathbf{e}_n(ku)\sum_{v=0}^{m-1}\mathbf{e}_p(F(u+v))\mathbf{e}_n(kv)\right|$$
$$\leqslant\sum_{u=1}^{p}\left|\sum_{v=0}^{m-1}\mathbf{e}_p(F(u+v))\mathbf{e}_n(kv)\right|.$$

By the Cauchy inequality we obtain

$$W^2\leqslant p\sum_{u=1}^{p}\left|\sum_{v=0}^{m-1}\mathbf{e}_p(F(u+v))\mathbf{e}_n(kv)\right|^2=p\sum_{v,w=0}^{m-1}\mathbf{e}_n(k(v-w))\sum_{u=1}^{p}\mathbf{e}_p(F(u+v)-F(u+w)).$$

We now examine the polynomial $F_{v,w}(U)=F(U+v)-F(U+w)$. By the Taylor formula we have

$$F_{v,w}(U)=F(U+v)-F(U+w)=\sum_{\nu=0}^{d-1}\frac{F^{(\nu)}(v)-F^{(\nu)}(w)}{\nu!}U^{\nu}.$$

Clearly $F^{(d-1)}(v)=F^{(d-1)}(w)$ is possible only for $v=w$. For such m pairs of v and w we estimate the sum over u trivially as p. Otherwise we estimate these sums as $(d-2)p^{1/2}$ by Lemma 8, getting

$$W^2=\begin{cases}O(mp^2), & \text{if } d=2,\\ O(mp^2+m^2p^{3/2}), & \text{if } d\geqslant 3.\end{cases}$$

Thus by (9)

$$\left|\sum_{u=1}^{p}\mathbf{e}_p(F(u))\mathbf{e}_n(ku)\right|=\begin{cases}O(m^{-1/2}p+m), & \text{if } d=2,\\ O(m^{-1/2}p+p^{3/4}+m), & \text{if } d\geqslant 3.\end{cases}$$

Taking $m=\lceil p^{2/3}\rceil$ we conclude the proof.

We also need a special case of the classical *Weyl bound* which we present in the following form (see Lemma 3.6 of Ref. 25 or Lemma 2.4 of Ref. 43 for a similar statement in full generality).

Lemma 10: Let $F(X)\in\mathbb{F}_p[X]$ be of degree $d\geqslant 2$. Then for any fixed $\varepsilon>0$ and any integer $h\leqslant p$,

$$\left|\sum_{u=1}^{h}\mathbf{e}_p(F(u))\right|=O\left(h^{1+\varepsilon}\left(\frac{1}{h}+\frac{1}{p}+\frac{p}{h^d}\right)^{1/2^{d-1}}\right).$$

C. Arbitrary dimensions

We now describe a construction of a vector system, which satisfies (4) exactly and also gives a certain approximation to (5). In fact we are able to get n^d+1 (rather than $n+1$) orthogonal bases with this property, where $d\geqslant 1$ is any integer.

Let $\mathcal{F}_d$ be the set of polynomials of the form

$$f(X) = \sum_{\nu=2}^{d+1} a_\nu X^\nu$$

with integer coefficients in the range $0 \leqslant a_\nu \leqslant n-1$, $\nu = 2, \ldots, d+1$. Thus $\#\mathcal{F}_d = n^d$. Let p be the smallest prime with $p \geqslant n$. For each $f \in \mathcal{F}_d$ we consider the basis

$$\mathcal{B}_f = \{|\psi_{f,1}\rangle, \ldots, |\psi_{f,n}\rangle\}, \quad \text{where } |\psi_{f,i}\rangle = \frac{1}{\sqrt{n}}(\mathbf{e}_p(f(u))\mathbf{e}_n(iu))_{u=1}^n. \tag{10}$$

Theorem 11: *For any integer $d \geqslant 1$, the standard basis and the n^d bases $\mathcal{B}_f$, $f \in \mathcal{F}_d$, given by* (10) *are orthonormal and satisfy also*

$$\langle \psi_{g,j} | \psi_{f,i} \rangle = \begin{cases} O(n^{-1/3}), & \text{if } d = 1, \\ O(n^{-1/4}), & \text{if } d \geqslant 2, \end{cases}$$

where $f, g \in \mathcal{F}_d \cup \{0\}$, $f \neq g$, $1 \leqslant i, j \leqslant n$.

Proof: The orthonormality of each basis follows from the identity

$$\langle \psi_{f,j} | \psi_{f,i} \rangle = \frac{1}{n} \sum_{u=1}^{n} \mathbf{e}_n((i-j)u) = \delta_{i,j}.$$

Clearly, if $f \in \mathcal{F}_d$ and $g = 0$ (or $f = 0$ and $g \in \mathcal{F}_d$) then $|\langle \psi_{g,j} | \psi_{f,i} \rangle| = n^{-1/2}$. Thus it remains to estimate

$$\langle \psi_{g,j} | \psi_{f,i} \rangle = \frac{1}{n} \sum_{u=1}^{n} \mathbf{e}_p(f(u) - g(u))\mathbf{e}_n((i-j)u)$$

for $f, g \in \mathcal{F}_d$, $f \neq g$ and $1 \leqslant i, j \leqslant n$.

Because

$$|\mathbf{e}_n(f(u) - g(u) + (i-j)u)| = 1$$

and by Lemma 7 we have

$$\begin{aligned} \frac{1}{n} \sum_{u=1}^{n} \mathbf{e}_p(f(u) - g(u))\mathbf{e}_n((i-j)u) &= \frac{1}{n} \sum_{u=1}^{p} \mathbf{e}_p(f(u) - g(u))\mathbf{e}_n((i-j)u) + O\left(\frac{|p-n|}{n}\right) \\ &= \frac{1}{n} \sum_{u=1}^{p} \mathbf{e}_p(f(u) - g(u))\mathbf{e}_n((i-j)u) + O(n^{-0.475}). \end{aligned}$$

Hence,

$$\langle \psi_{g,j} | \psi_{f,i} \rangle = \frac{1}{n} \sum_{u=1}^{p} \mathbf{e}_p(f(u) - g(u))\mathbf{e}_n((i-j)u) + O(n^{-0.475}).$$

Because $f(X) - g(X)$ is a polynomial of degree at least 2, Lemma 9 yields

$$\sum_{u=1}^{p} \mathbf{e}_p(f(u) - g(u))\mathbf{e}_n((i-j)u) = \begin{cases} O(p^{2/3}) = O(n^{2/3}), & d = 1, \\ O(p^{3/4}) = O(n^{3/4}), & d \geqslant 2, \end{cases}$$

which concludes the proof. □

As before, let p be the smallest prime with $p \geqslant n$. We consider n^2 vectors

$$\mathcal{B} = \{|\psi_f\rangle : f \in \mathcal{F}_2\}, \quad \text{where } |\psi_f\rangle = \frac{1}{\sqrt{n}}(\mathbf{e}_p(f(u)))_{u=1}^n. \tag{11}$$

Theorem 12: *Let p be the smallest prime with $p \geqslant n$. Then, the vector system $\mathcal{B}$ of n^2 vectors given by* (11) *is normalized and also satisfies*

$$|\langle \psi_g | \psi_f \rangle| \leqslant (2 + O(n^{-1/10}))n^{-1/2},$$

where $f, g \in \mathcal{F}_2$, $f \neq g$.

Proof: Obviously, we have

$$|\langle \psi_f | \psi_f \rangle| = 1, \quad f \in \mathcal{F}_2.$$

Put $h = p - n$. Then for $f, g \in \mathcal{F}_2$, $f \neq g$, we have

$$|\langle \psi_g | \psi_f \rangle| = \frac{1}{n} \left| \sum_{u=1}^{n} \mathbf{e}_p(f(u) - g(u)) \right| \leqslant \frac{1}{n} \left| \sum_{u=1}^{p} \mathbf{e}_p(f(u) - g(u)) \right| + \frac{1}{n} \left| \sum_{u=1}^{h} \mathbf{e}_p(f(n+u) - g(n+u)) \right|.$$

By Lemmas 8 and 10 we have

$$\begin{aligned} |\langle \psi_g | \psi_f \rangle| &\leqslant 2p^{1/2}n^{-1} + O\left(h^{1+\varepsilon} n^{-1} \left(\frac{1}{h} + \frac{1}{p} + \frac{p}{h^3} \right)^{1/4} \right) \\ &= 2p^{1/2}n^{-1} + O(n^{-1}(h^{3/4+\varepsilon} + h^{1+\varepsilon}p^{-1/4} + h^{1/4+\varepsilon}p^{1/4})). \end{aligned}$$

By Lemma 7 we see that $h = O(p^{0.525})$, therefore

$$h^{3/4+\varepsilon} + h^{1+\varepsilon}p^{-1/4} + h^{1/4+\varepsilon}p^{1/4} = O(p^{2/5}) = O(n^{2/5})$$

for sufficiently small ε and sufficiently large p. Noting that

$$p^{1/2} = (n + O(n^{0.525}))^{1/2} = n^{1/2}(1 + O(n^{-0.475}))^{1/2} = n^{1/2} + O(n^{0.2625})$$

we finish the proof. □

D. Special dimensions

Here we give some improvements of the constructions of Sec. III C for the values of n for which the smallest prime p with $p \equiv 1 \pmod{n}$ is sufficiently small.

Let p be the smallest prime such that $p \equiv 1 \pmod{n}$. Let $\mathcal{X}_n$ be the set of n characters of order n modulo p and $\mathcal{U}_n$ be the subgroup of residues of order n in $\mathbb{F}_p^\times$. In particular $\#\mathcal{U}_n = n$. It is known that $\mathcal{X}_n$ is a cyclic group, so for some character $\chi \in \mathcal{X}_n$ all other characters of $\mathcal{X}_n$ are given be the powers χ^i, $i = 1, \ldots, n$.

For $f \in \mathbb{F}_p[X]$ of degree at most d and the above character $\chi \in \mathcal{X}_n$ we define

$$\mathcal{B}_f = \{|\psi_{f,1}\rangle, \ldots, |\psi_{f,n}\rangle\} \quad \text{where } |\psi_{f,i}\rangle = \frac{1}{\sqrt{n}} (\mathbf{e}_p(f(u))\chi(u)^i)_{u \in \mathcal{U}_n}. \tag{12}$$

Let $\mathcal{G}_d$ be the set of polynomials of the form

$$f(X) = \sum_{\nu=1}^{d} a_\nu X^\nu,$$

with integer coefficients in the range $0 \leqslant a_\nu \leqslant n-1$, $\nu = 2, \ldots, d+1$.

Theorem 13: *For any integer $d \geqslant 1$, the standard basis and the n^d bases $\mathcal{B}_f$, $f \in \mathcal{G}_d$, given by* (12) *are orthonormal and satisfy also*

$$|\langle \psi_{g,j} | \psi_{f,i} \rangle| \leqslant dp^{1/2}n^{-1},$$

where $f, g \in \mathcal{F}_d \cup \{0\}$, $f \neq g$, $1 \leqslant i, j \leqslant n$.

Proof: We have

$$\langle \psi_{f,j} | \psi_{f,i} \rangle = \frac{1}{n} \sum_{u \in \mathcal{U}_n} \chi(u)^{i-j} = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases} \qquad 1 \leqslant i,j \leqslant n.$$

We also have

$$\langle \psi_{g,j} | \psi_{f,i} \rangle = \frac{1}{n} \sum_{u \in \mathcal{U}_n} \mathbf{e}_p(f(u) - g(u)) \chi(u)^{i-j} = \frac{1}{p-1} \sum_{x=0}^{p-1} \mathbf{e}_p(f(x^{(p-1)/n}) - g(x^{(p-1)/n})) \chi(x^{(p-1)/n})^{i-j}.$$

Now, using Lemma 8, we conclude the proof. □

Corollary 14: Let p be a prime and let n=p−1. Then an AMUB exists in dimension n.

Proof: We apply Theorem 13 for $p=n+1$ and for $d=1$. Hence, we have n^2+1 orthonormal bases such that inner products between their components are all bounded by $(n+1)^{1/2}n^{-1}=n^{-1/2}+O(n^{-1})$. □

IV. REMARKS AND OPEN QUESTIONS

The questions about finding SIC-POVMs and MUBs can be reformulated as a spherical design question in the vector space $\mathbb{C}^n$ (see Zauner's thesis[50] and also Refs. 28 and 41). Thus it is possible that the techniques of Ref. 29, as well as of more recent works (see a very inspiring survey[35]), may apply to the problem of constructing systems of n^2 equiangular lines in $\mathbb{C}^n$, that is, SIC-POVMs. In fact, it is quite possible that with some adjustments they may also apply to MUBs.

It is widely believed, see Ref. 44, but remains unproved, that the smallest prime $p \equiv 1 \pmod{n}$ satisfies the bound

$$p = O(n \log^2 n).$$

In this case, the bound of Theorem 13 becomes $O(n^{-1/2} \log n)$. Thus, it is quite possible that the construction of Sec. III D is always superior to those of Sec. III C.

Finally, we remark that many of the results of this paper remain unchanged if one uses prime powers $q=p^r$ (and thus general finite fields $\mathbb{F}_q$) instead of just primes p. In particular, Corollary 14 holds true in this more general setting. Hence, in summary, we have shown that ASIC-POVMs and AMUBs exist for any prime power dimension q. Moreover, we have shown that approximate versions of mutually unbiased bases and SIC-POVMs exist in any dimension if we are slightly more liberal about our constraints on the angles.

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Geometry of the Schrödinger equation and stochastic mass transportation

Stephan Völlinger
Mathematical Stochastics, Eckerstraβe 1, Freiburg, Germany

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The Schrödinger equation is deduced from a geometric principle. Lagrange, Hamilton-Jacobi, and Hamilton formalisms are defined almost analogously to the deterministic case, which can be identified as geometric optic. The form of these formalisms is identical to the deterministic formalisms. Furthermore, it will be shown how the deterministic case is "superficial" to the stochastic one if Planck's constant is very small. An elementary proof of Heisenberg's uncertainty relation finishes the paper. © *2005 American Institute of Physics.*
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I. INTRODUCTION AND STATEMENT OF THE MAIN RESULT

The Austrian physician Erwin Schrödinger, who discovered, in 1926, the equation governing quantum mechanics,[1] considered in 1931 the following problem:

"A cloud of independent identical particles may be known to initial and final times. What is the most probable state of the cloud to intermediate times?"

Schrödinger chose as a starting point for his research the *a posteriori* equivalence[2,3] of the Schrödinger equation

$$i\partial_t\psi = -\frac{1}{2}\Delta\psi + V\psi, \quad \psi:[0,T]\times\mathbb{R}^n \to \mathbb{C}$$

to the pair of parabolic diffusion equations

$$\partial_t\phi + \frac{1}{2}\Delta\phi + c\phi = 0, \quad -\partial_t\hat{\phi} + \frac{1}{2}\Delta\hat{\phi} + c\hat{\phi} = 0,$$

where the real-valued functions ϕ, $\hat{\phi}$ and c are defined by

$$\phi = e^{R+S}, \quad \hat{\phi} = e^{R-S}, \quad R,S:[0,T]\times\mathbb{R}^n \to \mathbb{R}, \quad c = -V - 2\partial_t S - (\nabla S)^2,$$

if $\psi = e^{R+iS}$. Schrödinger wanted to transform the complex-valued problem into a "real" space. See also Ref. 4 (or Ref. 5 for a more detailed explanation), where the connection of the heat flow equation to Feynman's path integral is treated.

Irrespective of the detailed words in Schrödinger's problem and irrespective of the equivalence to dual parabolic pairs, we want to give a solution in the framework of a geodesic variational problem. We do research on the problem of "geometry of the Schrödinger equation," i.e.,

We look for solutions of the Schrödinger equation, under an eventually prescribed Riemannian structure, where initial and final time absolute squares of the ψ-function are given at the outset.

We will show that this problem is deeply related to a geodesic problem. The real-valued, Euclidean version will be identified as stochastic mass transportation.

The research on the observer variant, a topologically global defined geodesic variational problem and its symmetries, is of a very historical origin. It stands at the beginning of a theory of formal deduction, and was considered by Euclid in 300 B.C.[6] The idea of the shortest connection between two points of a space is the central point of Euclid's geometry.

In the physical applications the variational formalism appears as a principle of least action. It will be shown that also the Schrödinger equation is determined by a Hamiltonian version of a variational problem, where the Lagrangian version is given by stochastic mass transportation. A remarkable point is that the form of the Hamiltonian problem is identical to the form of the deterministic case given in classical (point) mechanics, what also holds true for the Lagrangian version. Variation of the stochastic mass transportation problem leads to the following nonlinear partial differential equation (PDE):

$$\partial_t v + \nabla_v v - \nabla_u u - \frac{\hbar}{2}\Delta u = -\nabla V,$$

called the stochastic Newton equation, with current velocity v and entropic velocity u (see Sec. II A). The stochastic Newton equation generalizes Newton's law and follows from the Schrödinger equation

$$\hbar i \partial_t \psi = H\psi = -\frac{1}{2}\hbar^2 \Delta\psi + V\psi.$$

The energy conservation law for stochastic mass transportation is ruled by the entropy action law. The quantum mechanical energy $\langle \psi, H\psi\rangle$ of a solution ψ of the Schrödinger equation is a constant of the motion. The entropy action law for $[0,T]$,

$$W_{QM}(\psi) := T\langle \psi, H\psi\rangle = W_{kin}(\psi) + W_{pot}(\psi) - \frac{\hbar}{2}\Delta\mathrm{Entrop}(|\psi_T|^2, |\psi_0|^2),$$

shows that the classical action at time T has an additional dissipative term, the negative Gibbs-Boltzmann entropy difference of ψ_T and ψ_0.

The fact that ψ is complex valued can be explained in the framework of a phase space structure. The real-valued Lagrangian version is imbedded as a tangential space analogously to the deterministic formalism. The Itô diffusion equation

$$dY_t = b(t, Y_t)dt + \sqrt{\hbar} dB_t$$

acts as tangential criteria of $b = DY$ referring to the diffusion Y_t.

Such a Lagrangian phase space structure was introduced by Otto[7] (or Ref. 8 where the idea is presented) for deterministic mass transportation. A density way $t \to \varrho_t$ has the tangent φ if the continuity equation

$$\partial_t \varrho_t + \mathrm{div}(\varrho_t \nabla \varphi) = 0$$

holds true. The relevant metric for this differential geometry is given by

$$\langle \dot{\varrho}_t, \dot{\varrho}_t\rangle := \int (\nabla \varphi_t)^2 \varrho_t \, dx.$$

In Ref. 8 the equivalence of the geodesic distance for this metric to the time-independent formulation of the deterministic mass transportation problem, also known as the Wasserstein distance, is (heuristically) shown.

A further new work in this connection is that by Hall and Reginatto,[9] where the authors add a fluctuation term to the classical variational problem of geometric optics by using certain heuristic conditions, to derive the form of the fluctuation term by a transformation property of the spatial uncertainty, called the "exact uncertainty principle," which finally leads to the Schrödinger equa-

tion. The "exact uncertainty principle" is a special case of the Cramér-Rao inequality, well known in information theory. The explanations in Ref. 9 suggest a proof of Heisenberg's uncertainty relation, which is the characteristic of quantum dynamics, and so an exact proof is given in Sec. VII. Note especially that the entropy action law shows that a main assertion in Ref. 9 is, in general, not true.

In opposite direction to Ref. 9, this paper derives the Schrödinger equation directly from a geodesic problem, given by Lagrangian stochastic mass transportation. The advantage of this derivation is the equivalence to classical variational principles

$$\delta \int L(t,x,\dot{x})dt \overset{!}{=} 0, \quad \text{time marginal values!}$$

In the limit, where "zoomout problems" are considered, such that Planck's constant $\hbar$ is very small and the motion is microscopic, the geometry of the Euclidean space is recovered.

This paper wants to introduce a new connection between differential geometry and stochastics. The main result is to generalize the Euclidean space and to show how the classical geometry is "superficial" to the stochastic case. The primary target is to treat the geometry of the Schrödinger equation problem mathematically. Further physical data, like the magnetic vector potential $\vec{A}$ in the Schrödinger equation

$$i\hbar\partial_t\psi = \left(\sum_k \left(\frac{\hbar}{i}\partial_k - A_k\right)\left(\frac{\hbar}{i}\partial_k - A_k\right) + V\right)\psi$$

is ignored. (But see Ref. 10, where $\vec{A}$ is implemented.)

Main result: The geometry of the Schrödinger equation problem, where we look for solutions in a Euclidean setting, is governed in its Lagrangian version by a "pure" geodesic variational problem. The classical geometry can be obtained by a zoomout formalism.

II. PRELIMINARIES

A. Stochastic preliminaries

The following preliminaries are taken under technical modifications from Refs. 10–12 and can be compared there. Detailed proofs can be found in Ref. 13.

Let $T \in \mathbb{R}^+$ and $(\Omega, \mathcal{T}_t)$, $t \in [0,T]$ be a filtrated sample space. For the whole work we can set $\Omega = C^0([0,T],\mathbb{R}^n)$ and $\mathcal{T}_t := \sigma(X_s, 0 \leqslant s \leqslant t)$, where $X_s(c) = c(s)$, and $c \in \Omega$ is the coordinate mapping, i.e., the common Wiener space setting. Following Ref. 10, expectations referring to a measure on $(\Omega, \mathcal{T}_T)$ are denoted by E if they are not expressed as integrals.

Definition 1: (a) A *diffusion* is a measure P on $\mathcal{T}_T$ and a $\sigma(X_t)$-measurable stochastic process $Y:[0,T]\times\Omega \to \mathbb{R}^n$, i.e., $\sigma(Y_t) \subset \sigma(X_t)$, with continuous path and second moments $\forall t$ such that the differential quotients

$$\lim_{\Delta t \to 0^+} E_t \frac{\Delta Y_t^i}{\Delta t} = b^i(t, Y_t), \quad i = 1, \ldots, n,$$

$$\lim_{\Delta t \to 0^+} E_t \frac{\Delta Y_t^i \Delta Y_t^j}{\Delta t} = \sigma^{ij}(t, Y_t), \quad i,j = 1, \ldots, n, \tag{1}$$

exist $\forall t \in [0,T]$. E_t is the conditioned expectation referring to P under $\mathcal{T}_t$, i.e., $E_t(.) = E(.|\mathcal{T}_t)$. $(\sigma^{ij})_{ij}$ is a measurable function on $[0,T]\times\mathbb{R}^n$ with values in the symmetric, positive definite matrices. $(\sigma^{ij})_{ij}$ is called *diffusion matrix*. b is a measurable function on $[0,T]\times\mathbb{R}^n$ with values in $\mathbb{R}^n$, called the *drift*. The limit is supposed to exist in the $L^2(P)$-sense for the drift and in the $L^1(P)$-sense for the diffusion matrix. Especially $b^i(t,Y_t) \in L^2(P)\,\forall\, t \in [0,T]$ and $\sigma^{ij}(t,Y_t) \in L^1(P)\,\forall\, t \in [0,T]$. This definition shall include the case that the limit for the drift exists only in the L^1-sense, but is in

$L^2(P)$. Only diffusions with diffusion matrix $h\cdot id$, $h\in\mathbb{R}^+$, will play a role within this paper.

A diffusion, referring to the Lebesgue measure absolutely continuous distribution Y_t^P, is called *smooth* if the densities $\varrho_t dx = P[X_t \in dx]$ are smooth and bounded, i.e., $\varrho_t \in C^\infty \cap L^\infty$, and furthermore b^i and σ^{ij}, $i,j=1,\ldots,n$, are given on $\{\varrho(t,x)>0\}$, are C^∞ differentiable, and $\int b^2\varrho\, dx$ $<$const is independent of t. The C^∞ property can be weakened to enough differentiability in the respective situation.

Finally

$$D(Y_t) := \lim_{\Delta t\to 0^+} \frac{1}{\Delta t} E(Y_{t+\Delta t} - Y_t | \mathcal{T}_t) = b(t,Y_t) \tag{2}$$

is the *forward derivative* of a diffusion Y_t.

(b) $C_0^\infty(O;\mathbb{R})$, $O\subset\mathbb{R}^m$, open are the C^∞-differentiable functions $\mathbb{R}^m\to\mathbb{R}$ with compact support in O, i.e., $\varphi\in C_0^\infty \Leftrightarrow \mathrm{supp}(\varphi)\subset O$ compact.

Proposition 2: (Differential Itô formula analog.[12] See Ref. 10.) Let Y_t be a diffusion referring to P. For every real-valued function $\chi(t,x)\in C_0^\infty([0,T]\times\mathbb{R}^n;\mathbb{R})$ we have in the $L^1(P)$-sense

$$D\chi(t,Y_t) = \left(\frac{1}{2}\sigma^{ij}\partial_{i,j}^2 + b^i\partial_i + \partial_t\right)\chi(t,Y_t) \quad \text{(Sum convention !)}. \tag{3}$$

Proof: By Taylor's formula! See Ref. 13.

Proposition 3: (See Ref. 10.) Let Y_t be a diffusion referring to P. Let $\sigma^{ij}(t,x)$, $b^i(t,x):[0,T]\times\mathbb{R}^n\to\mathbb{R}\in L^\infty\cap C^0$, $i,j=1,\ldots,n$, and

$$\int_0^T \int b^2(t,Y_t)\, dP\, dt < \infty. \tag{4}$$

For the distributions Y_t^P we have [in the weak sense of (6)] the *Fokker-Planck equation*

$$\partial_t Y_t^P = \frac{1}{2}\partial_{i,j}^2(\sigma^{ij}Y_t^P) - \mathrm{div}(bY_t^P), \quad Y_0^P \text{ given}. \tag{5}$$

Proof: It can be shown that $t\mapsto\int\chi(t,Y_t)\, dP$ is continuously differentiable and that the Fokker-Planck equation holds true in the following weak sense:

The function $t\mapsto\int\chi(t,Y_t)\, dP$ is absolutely continuous and

$$\int \chi(t,Y_t)dP - \int \chi(0,Y_0)dP = \int_0^t \int \left(\frac{\sigma^{ij}}{2}\partial_{i,j}^2 + b^i\partial_i + \partial_t\right)\chi(t,Y_t)dP\, dt,$$

$$\forall\,\chi\in C_0^\infty([0,T]\times\mathbb{R}^n;\mathbb{R}), \quad \forall\, t\in[0,T], \tag{6}$$

where the continuous differentiability is weakened to absolute continuity. The integrability condition (4) is necessary, such that this definition makes sense. See Ref. 13.

Remark 4: (a) Let Y_t^P be absolutely continuous referring to the Lebesgue measure $\forall t$, with $\varrho_t dx = P[X_t\in dx]$. Let ϱ be continuous and b, σ be continuous on $\{\varrho>0\}$. Then the weak Fokker-Planck equation referring to the test function space $C_0^\infty(\{\varrho>0\};\mathbb{R})$ holds true without boundedness of σ and b. Proof of Proposition 3 still remains correct if the test function class is restricted to $\{\varrho>0\}$.

(b) If Y_t is a smooth diffusion referring to P, then the Fokker-Planck equation holds true in the classical sense on $\{\varrho>0\}$.

The *backward derivative* of a diffusion Y_t is defined by

$$D_*(Y_t) := \lim_{\Delta t \to 0^+} \frac{1}{\Delta t} E(Y_t - Y_{t-\Delta t} | \mathcal{T}_t^*) = \lim_{\Delta t \to 0^+} E_t^* \frac{\Delta^* Y_t}{\Delta t}, \tag{7}$$

where $\mathcal{T}_t^* := \sigma(X_s, t \leqslant s \leqslant T)$ and the topology of the convergence will be explained in the next proposition. The *backward drift* b_* is defined by

$$D_* Y_t =: b_*(t, Y_t). \tag{8}$$

Proposition 5: (Partial integration for stochastic derivatives. See Ref. 10.) Let Y_t be a smooth diffusion referring to P, with diffusion matrix $h \cdot id$, $h \in \mathbb{R}^+$. The integrability conditions

$$\int_0^T \int b^2(t, Y_t)\, dP\, dt < \infty, \quad \text{respectively} \int_0^T \int (\nabla \ln \varrho(t, Y_t))^2\, dP\, dt < \infty, \tag{9}$$

may hold true, where $\nabla \ln \varrho(t,x)$ is defined on $\{\varrho(t,x) > 0\}$ and is equal to zero elsewhere. The backward derivative exists in the following weak sense,

$$\lim_{\Delta t \to 0^+} \int_0^T \int \left(E_t^* \frac{\Delta^* Y_t}{\Delta t} \right)^i f(t, Y_t)\, dP\, dt = \int_0^T \int b_*^i(t, Y_t) f(t, Y_t) dP\, dt,$$

$$\forall i = 1, \ldots, n, \quad \forall f \in C_0^\infty(\{\varrho(t,x) > 0\} \cap (0,T) \times \mathbb{R}^n; \mathbb{R}), \tag{10}$$

where on $\{\varrho(t,x) > 0\}$

$$b_* = b - h \nabla \ln \varrho. \tag{11}$$

The partial integration formula

$$\int_0^T E(Df(t, Y_t) g(t, Y_t))\, dt = -\int_0^T E(f(t, Y_t) D_* g(t, Y_t))\, dt + Ef(T, Y_T) g(T, Y_T) - Ef(0, Y_0) g(0, Y_0) \tag{12}$$

holds true for arbitrary C^∞-differentiable functions $g : [0,T] \times \mathbb{R}^n \to \mathbb{R}$ and $f : [0,T] \times \mathbb{R}^n \to \mathbb{R}$ where g and/or f may have compact support in $\{\varrho(t,x) > 0\}$.

Proof: See Ref. 13.

Remark 6: (a) See also Ref. 14, where the time inversion on the Wiener space is treated.

(b) It is not hard to see that with the smoothness of the diffusion and the fact that the test functions have compact support in $\{\varrho(t,x) > 0\}$, the backward derivative exists in the following stochastic Sobolev-sense

$$\int \int Y_t^i Df(t, Y_t)\, dP\, dt = \int_0^T \int b_*^i(t, Y_t) f(t, Y_t)\, dP\, dt,$$

$$\forall i = 1, \ldots, n, \quad \forall f \in C_0^\infty(\{\varrho(t,x) > 0\} \cap (0,T) \times \mathbb{R}^n; \mathbb{R}). \tag{13}$$

(c) Let Y_t be a smooth diffusion referring to P with diffusion matrix $h \cdot id$, $h \in \mathbb{R}^+$. The forward and backward derivatives of a $C_0^\infty([0,T] \times \mathbb{R}^n; \mathbb{R})$-function $f(t, Y_t)$ are calculated according to

$$Df(t, Y_t) = \left(\frac{h}{2} \Delta + b^j \partial_j + \partial_t \right) f(t, Y_t),$$

$$D_* f(t,Y_t) = \left(-\frac{h}{2}\Delta + b_*^j \partial_j + \partial_t \right) f(t,Y_t), \tag{14}$$

where the Laplace operator is defined by the $\mathbb{R}^n$ in which the diffusion takes on its values.

(d) See Ref. 10 for the transformation of drift vectors and diffusion matrices in coordinates.

(e) The following *backward Fokker-Planck equation* on $\{\varrho(t,x)>0\}$ holds true:

$$\partial_t \varrho = -\frac{h}{2}\Delta\varrho - \operatorname{div}(b_*\varrho). \tag{15}$$

Definition 7: The *entropic velocity* on $\{\varrho(t,x)>0\}$ is defined by

$$u := \frac{1}{2}(b - b_*) \tag{16}$$

and the *current velocity* on $\{\varrho(t,x)>0\}$ by

$$v := \frac{1}{2}(b + b_*). \tag{17}$$

We have $u=(h/2)\nabla \ln \varrho = h\nabla \ln \sqrt{\varrho}$ on $\{\varrho(t,x)>0\}$. Averaging (in $\mathbb{R}$) over forward and backward Fokker-Planck equations leads to the *continuity equation* on $\{\varrho(t,x)>0\}$:

$$\partial_t \varrho = -\operatorname{div}(v\varrho). \tag{18}$$

Proposition 8: (Interpretation of the current velocity.) Let $\xi(t,x):[0,T]\times\mathbb{R}^n\to\mathbb{R}^n$ and $p(t,x):[0,T]\times\mathbb{R}^n\to\mathbb{R}$ be a classically differentiable solution of the continuity equation $\partial_t p + \operatorname{div}(\xi p)=0$, $p(0,x)=p_0(x)$ (ξ and p_0 are given). Then we have for the flow T_t of the vector field ξ [i.e., $(d/dt)T_t=\xi(t,T_t)$] $T_{t\#}p_0=p_t$, where the "push-forward" $T_{t\#}p_0$ of a density function p_0 is defined by

$$\int T_{t\#}p_0(y)f(y)dy = \int p_0(x) f(T_t(x))dx \;\forall\, f \in C_0^0(\mathbb{R}^n). \tag{19}$$

If, conversely, T_t classically differentiable is given and $T_{t\#}p_0=p_t$, then for the vector field $\xi(t,x)=d/dtT_t(x)$ the continuity equation holds true.

Proof: See Ref. 13.

Definition 9: The meaning of the *stochastic acceleration* $\frac{1}{2}(DD_*+D_*D)Y_t$ of a smooth diffusion Y_t referring to P with diffusion matrix $h\cdot id$ will become clear in Sec. III B. It can be calculated in detail by

$$\begin{aligned}
\int_0^T \int \frac{1}{2}(DD_* + D_*D)Y_t \eta(t,Y_t)\, dP\, dt &= \int_0^T \int \frac{1}{2}(Db_* + D_*b)(t,Y_t)\,\eta(t,Y_t)\, dP\, dt \\
&= \int_0^T \int \frac{1}{2}\left(\left(\frac{h}{2}\Delta + b^j\partial_j + \partial_t\right) b_* + \left(-\frac{h}{2}\Delta + b_*^j\partial_j + \partial_t\right) b \right) \\
&\quad (t,Y_t)\,\eta(t,Y_t)\, dP\, dt = \int_0^T \int \left(\partial_t v + \nabla_v v - \nabla_u u - \frac{h}{2}\Delta u \right) \\
&\quad \times (t,Y_t)\,\eta(t,Y_t)\, dP\, dt, \\
&\quad \forall\ \eta \in C_0^\infty(\{\varrho>0\};\mathbb{R}),
\end{aligned}$$

where ∇ denotes the Levy-Civita connection of the Euclidean space, i.e., $(\nabla_v v)^i = v\cdot\nabla v^i$, $i=1,\ldots,n$.

The whole treatment of validity on $\{\varrho(t,x)>0\}$ tries to avoid problems with the, by definition, eventual singularities of b and b_* on $\{\varrho=0\}$.

A further possibility to define diffusions is given by Itô diffusion equations $dY_t=b(t,Y_t)dt+\varkappa(t,X_t)dB_t$, for a Brownian motion B_t. The equation with drift b and diffusion coefficient $\varkappa$ (Ref. 12) is valid by definition, if the integral version holds true:[12]

$$Y_t = Y_0 + \int_0^t b(s,Y_s)\,ds + \int_0^t \varkappa(s,X_s)dB_s. \tag{20}$$

Itô diffusions are Markovian.

Lemma 10: Let $h>0$ and $b:[0,T]\times\mathbb{R}^n\to\mathbb{R}^n$ be measurable. Let $|b(t,x)|\leqslant K(1+|x|)\,\forall\, t\in[0,T]$ with a constant $K\in\mathbb{R}^+$. The Itô diffusion equation $dX_t=b(t,X_t)dt+\sqrt{h}dB_t$, $0\leqslant t\leqslant T$, has a weak solution,[12] with arbitrary initial distribution μ, such that X_t is a Brownian motion referring to a measure $\bar{P}$ and such that the Brownian motion (B_t,P) starts in 0, i.e., for every probability measure μ on $\mathbb{R}^n$ there exist Brownian motions $(\Omega,\mathcal{T}_t,X_t,\bar{P})$ and $(\Omega,\mathcal{T}_t,B_t,P)$ such that the Itô diffusion equation holds true and $P^{X_0}=\mu$.

Proof: See Ref. 13.

Remark 11: (a) Notice that in Lemma 10 a stronger version of a weak solution is constructed. $(\Omega,\mathcal{T}_t,X_t,\bar{P})$ is given at the outset as canonical Brownian motion (with X_t as coordinate mapping)!

(b) Let the drift vector $b(t,x)$ and the Itô diffusion equation $dY_t=b(t,Y_t)\,dt+\sqrt{h}dB_t$, (B_t,P) Brownian motion be given. If

$$\int_0^T \int b^2(t,Y_t)dP\,dt<\infty, \tag{21}$$

then the forward derivative exists in the $L^2(P)$-sense for a.e. t and we have $DY_t=b(t,Y_t)$. Furthermore,

$$\lim_{\Delta t\to 0^+} E_t\frac{\Delta Y_t^i \Delta Y_t^j}{\Delta t}=\begin{Bmatrix} 0 & \text{if } i\neq j \\ h & \text{if } i=j \end{Bmatrix} \text{ in } L^1(P) \text{ for a.e. } t. \tag{22}$$

If $\int b^2(t,Y_t)\,dP<\infty\,\forall\, t$, then the assertions hold true $\forall t$.

Proof: See Ref. 13.

B. Analysis of the Fokker-Planck equation

We state theorems concerning the existence, regularity, and uniqueness of the Fokker-Planck equation, needed for the stochastic mass transportation problem. Detailed proofs are given inspired by Ref. 15 in Ref. 13. Compared to Ref. 15 we adapt premises and do technical modifications. Note especially that Ref. 15 works spatially on the torus. The transfer of the proofs to $\mathbb{R}^n$ is surely not trivial.

A *weak solution* of the Fokker-Planck equation in $[0,T]\times\mathbb{R}^n$ with diffusion $h\cdot id$, given by $\varrho:[0,T]\times\mathbb{R}^n\to\mathbb{R}\in L^1$ [ϱ may $\forall t$ be represented, to the data $b:\{\varrho>0\}\to\mathbb{R}^n\cup\{(\pm\infty,\ldots,\pm\infty)\}$, measurable drift and $\varrho_0:\mathbb{R}^n\to\mathbb{R}\in L^1$], is defined by the following:

The function $t\mapsto\int\chi(t,x)\varrho\,dx$ is absolutely continuous and we have

$$\int \chi(t,x)\varrho\,dx-\int\chi(0,x)\varrho\,dx=\int_0^t\int\left(\frac{h}{2}\Delta+b^i(s,x)\partial_i+\partial_s\right)\chi(s,x)\varrho(s,x)\,dx\,ds,$$

$$\forall\,\chi\in C_0^\infty([0,T]\times\mathbb{R}^n;\mathbb{R}),\quad \forall\, t\in[0,T]. \tag{23}$$

In addition the integrability condition

$$\int_0^T \int b^2 \varrho \, dx \, dt < \infty \tag{24}$$

may hold true, such that this definition is in $\mathbb{R}$.

Theorem 12: (Existence.) Let $b:[0,T]\times\mathbb{R}^n\to\mathbb{R}^n\in L^\infty\cap C^0$ and $\varrho_0:\mathbb{R}^n\to\mathbb{R}^+\in L^1$, $\int\varrho_0\,dx=1$. Then there is a positive weak solution of the Fokker-Planck equation in L^1 with diffusion $h\cdot id$. Especially $\varrho(t,x)\geqslant 0$ is given naturally $\forall t$ and we have $\varrho(0,x)=\varrho_0(x)$, respectively $\int\varrho(t,x)\,dx=1\,\forall t$. If $\varrho_0\in L^\infty(\mathbb{R}^n;\mathbb{R}^+)$, then we have $\varrho\in L^\infty([0,T]\times\mathbb{R}^n;\mathbb{R}^+)$.

Proof: See Ref. 13.

Theorem 13: (Regularity.) Let $\varrho:[0,T]\times\mathbb{R}^n\to\mathbb{R}^+\in L^\infty$ and $b:\{\varrho>0\}\to\mathbb{R}^n\cup\{\pm\infty\}$ (measurable) (explicitly given on $\{\varrho>0\}$) constitute a positive weak solution of the Fokker-Planck equation with diffusion $h\cdot id$. Let $\int b^2\varrho dx<\text{const}$ be independent of t. Then it follows that $\varrho\in W^{(0,1),2}_{loc}([0,T]\times\mathbb{R}^n;\mathbb{R})$, i.e., $\varrho\in L^2_{loc}(\varrho\in L^\infty)$ and there is $\forall i=1,\ldots,n$ a $\partial_i\varrho:[0,T]\times\mathbb{R}^n\to\mathbb{R}\in L^2_{loc}$, such that

$$\int_0^T\int \partial_i\varrho\varphi\,dx\,dt=(-1)\int_0^T\int\varrho\partial_i\varphi\,dx\,dt,\quad \forall\,\varphi\in C_0^\infty([0,T]\times\mathbb{R}^n;\mathbb{R}). \tag{25}$$

If, in addition, $\varrho(t,x)\in L^1(\mathbb{R}^n;\mathbb{R})\,\forall t$ and $\|\varrho\|_{L^1(\mathbb{R}^n;\mathbb{R})}\leqslant\text{const}$ independent of t, then $\partial_i\varrho\in W^{(0,1),2}([0,T]\times\mathbb{R}^n;\mathbb{R})$, $i=1,\ldots,n$.

Proof: See Ref. 13.

See also the regularity result in Ref. 14.

The *relative entropy*

$$\int\varrho_1(x)\ln\frac{\varrho_1(x)}{\varrho_2(x)}\,dx \tag{26}$$

of two densities ϱ_1 and ϱ_2 will be important in the following proof.

Theorem 14: (Uniqueness.) Let $\varrho_{1/2}:[0,T]\times\mathbb{R}^n\to\mathbb{R}^+\in L^\infty$ be positive weak solutions of the Fokker-Planck equation with diffusion $h\cdot id$, and $b_{1/2}:\{\varrho_{1/2}>0\}\to\mathbb{R}^n\cup\{(\pm\infty,\ldots,\pm\infty)\}$ be measurable and $\int b_{1/2}^2\varrho_{1/2}\,dx<\text{const}$ be independent of t. Let $\varrho_{1/2}(t,x)\in L^1(\mathbb{R}^n;\mathbb{R})\,\forall t$ and $\|\varrho_{1/2}\|_{L^1(\mathbb{R}^n;\mathbb{R})}\leqslant\text{const}$ independent of t. If the entropies $\int\varrho_{1/2}\ln\varrho_{1/2}\,dx$ exist in $\mathbb{R}$ at the times 0 and T, then uniqueness at time T holds (in the class with the given premises), i.e., if $b_1=b_2$ and $\varrho_1(0,x)=\varrho_2(0,x)$, then $\varrho_1(T,x)=\varrho_2(T,x)$.

Proof: See Ref. 13.

Corollary 15: For the conditions for a weak solution of the Fokker-Planck equation stated in Theorem 14, we have that the entropic velocity $u=1_{\{\varrho>0\}}(h/2)\nabla\ln\varrho$ is in $L^2(\varrho)$, i.e.,

$$\int_0^T\int u^2\varrho\,dx\,dt<\infty. \tag{27}$$

Furthermore, the existence of the entropy in $\mathbb{R}$ at the times T and 0 implies the existence of the entropy at all times $t\in[0,T]$. It follows that uniqueness at all times holds true (in the class with the given premises).

Proof: See Ref. 13.

C. Existence of diffusions

Smooth diffusions, by definition, can have singularities in the points where the distribution density disappears. Lemma 10 is not applicable to construct a diffusion with diffusion matrix $h\cdot id$, $h\in\mathbb{R}^+$, where a drift with singularities is given. Especially in Sec. IV we will look for diffusions with drift vector $\nabla(A+B)$, where $\psi=e^{A+iB}$ is a differentiable solution of the Schrödinger equation. A zero point of such a solution implies necessarily that $A=-\infty$, respectively there is a singularity

for the drift $\nabla(A+B)$. $A+B$ is bounded from above on compact sets. Nevertheless, it is possible to construct Itô diffusion equations $dY_t=\nabla(A+B)(t,Y_t)\,dt+hdB_t$ whereas the condition $|\nabla(A+B)\times(t,x)|\leqslant K(1+|x|)$ in Lemma 10 is not satisfied.

Remark 16: The literature on the existence of diffusions with singular drift is very extensive. See, e.g., Refs. 2, 3, 10, and 16–19 as reference.

The stationary (time independent) case was first treated by Albeverio and Høegh-Krohn.[17]

The case of a compact manifold as configuration space is considered in Ref. 10.

Carlen[16] shows weak existence of a diffusion measure, in the sense that the Martingale characterization for diffusions holds true, from an analytical viewpoint. Singular drift vectors b, b_* and densities ϱ, fulfilling the Fokker-Planck equation in a weak sense, are given at the outset. The central point is to solve a parabolic equation and to obtain a fundamental solution $p_*(y,t;x,s)$. The integrability condition $\int\int(u^2+v^2)\varrho\,dx\,dt<\infty$ is required, which is naturally given in the framework of the Yasue variational problem introduced in Sec. III. Using p_* a measure on $(\mathbb{R}^n)^{\mathbb{R}_+}$ ($\mathbb{R}^n$ one-point compactification) is constructed. If only this measure is constructed, it is left to show that an honest diffusion with the prescribed data is given.

The existence theory of Carlen's diffusions was extended by Guerra[20] using continuity arguments.

With an analogous integrability condition like Ref. 4, Zheng[18] shows, with technically different methods, by using tightness results, the existence of weak solutions of diffusion measures, in the sense that the Martingale property is fulfilled. Regularity conditions are required and regular ψ functions, fulfilling the Fokker-Planck equation on compact manifolds, are considered. An intrinsic feature of these proofs is that under certain conditions, with probability one, the process never visits the sets $\{\varrho=0\}$.

In Ref. 19 strong solutions, where the Fokker-Planck equation with singular drift (at $\{\varrho=0\}$) is given, are constructed. Stopping time methods are used and unattainability criteria of the nodal sets are given. Further conditions on the integrability of certain derivatives of ϱ and the entropic velocity v are needed.

III. STOCHASTIC MASS TRANSPORTATION

A. Definition of stochastic mass transportation

Let χ_1 and χ_2 be two density functions on $\mathbb{R}^n$, which take values in Ω_1 and Ω_2. The normalization

$$\int_{\Omega_1}\chi_1(x)\,dx=\int_{\Omega_2}\chi_2(y)\,dy=1 \tag{28}$$

may hold true. The *deterministic* (L^2-) *mass transportation problem* (see Refs. 21–23), referring to a quadratic cost function, seeks to transform χ_1 into χ_2 by an L^2-optimal transport mapping D, i.e., if the "push forward" $D_\#\chi:\Omega_2\to\mathbb{R}^+$ of a density function χ by the mapping $D:\Omega_1\to\Omega_2$ is as before defined by

$$\int_{\Omega_2}D_\#\chi(y)f(y)\,dy=\int_{\Omega_1}\chi(x)f(D(x))\,dx\;\forall\,f\in C^0(\Omega_2), \tag{29}$$

then the deterministic mass transportation minimizes the functional

$$\int_{\Omega_1}|x-D(x)|^2\chi_1(x)\,dx\overset{!}{=}\inf_D,\quad\text{where } D_\#\chi_1=\chi_2. \tag{30}$$

The square root of this minimal expression is called the *Wasserstein distance* of χ_1 and χ_2. Necessary for a minimum is the nonlinear Monge-Ampère equation

$$\chi_2(D(x))\det((\partial_jD^i)_{ij}(x))=\chi_1(x). \tag{31}$$

The main result in this connection is that D exists and is the gradient of a convex function[24,25] (see also Refs. 21 and 23 as reference). Hereby the second derivatives in the Monge-Ampère equation are justified.

The connection to geodesics can be seen if the interpolation of χ_1 and χ_2 by D is considered in a time continuous setting. The following result is due to Brenier and Benamou[26] [see Ref. 23 for a precise definition of the space of pairs (v,ϱ)].

Let $\varrho_0,\ \varrho_1 \in \mathbb{R}^n \to \mathbb{R}$ be given with $\int \varrho_0(x)\,dx = \int \varrho_1(x)\,dx = 1$ and $T \in \mathbb{R}^+$. The minimization problem

$$\int_0^T \int v^2 \varrho \, dx \, dt \overset{!}{=} \inf_{v,\varrho};$$

$$v:[0,T] \times \mathbb{R}^n \to \mathbb{R}^n \in C^1,$$

$$\varrho:[0,T] \times \mathbb{R}^n \to \mathbb{R}^+ \in C^1, \quad \int \varrho_t \, dx = 1,$$

$$\varrho(0,\,.\,) = \varrho_0, \quad \varrho(T,\,.\,) = \varrho_T, \quad \partial_t \varrho + \operatorname{div}(\varrho v) = 0 \tag{32}$$

takes on its minimum in the unique pair (v,ϱ) defined by the convex function Φ belonging to the non-time-continuous transport problem by

$$\int f(t,x)\varrho(t,x)\,dt\,dx = \int f\left(t, x + \frac{\nabla\Phi - x}{T}\right)\varrho_0(x)\,dt\,dx,$$

$$\int f(t,x)\varrho(t,x)v(t,x)\,dt\,dx = \int \frac{\nabla\Phi - x}{T} f\left(t, x + \frac{\nabla\Phi - x}{T}\right)\varrho_0(x)\,dt\,dx \;\forall\, f \in C^0. \tag{33}$$

The variational formalism is equal to geometric optics. The time continuous, straight convex connection $x + t(\nabla\Phi - x)/T$, $t \in [0,T]$, constitutes the way of light.

Definition 17: (*Euclidean h-stochastic* (L^2-) *mass transportation*, see also Ref. 27 for a variant.) In analogy, let the stochastic mass transportation to the data $\mu_{0/T}$ probability measures on $\mathbb{R}^n$, T, $h \in \mathbb{R}^+$, be defined as follows:

$$\int_0^T \int b^2(t,Y_t)\,dP\,dt \overset{!}{=} \inf_{b,P,B},$$

$$b:[0,T] \times \mathbb{R}^n \to \mathbb{R}^n,$$

$$dY_t = b(t,Y_t)\,dt + \sqrt{h}\,dB_t, \quad Y^P_{0/T} = \mu_{0/T}. \tag{34}$$

$(\Omega, \mathcal{T}_t, B_t, P)$ is a Brownian motion with start in 0 and $(\Omega, \mathcal{T}_t, Y_t, \bar{P})$ is a Brownian motion with initial distribution $\bar{P}^{Y_0}$. The infimum is taken over all Itô diffusion equations, which satisfy the marginal conditions. $(\Omega, \mathcal{T}_t, Y_t, \bar{P})$ can be given at the outset as canonical Brownian motion on $\mathbb{R}^n$ with initial distribution μ, i.e., as before, $\Omega = C^0([0,T)], \mathbb{R}^n)$, $Y_t = X_t$ is the coordinate mapping $X_t(c) = c(t)$, $\mathcal{T}_t$ is the σ-Algebra constituted by X_s, $s \leqslant t$, and $\bar{P}$ is the usual construction of the Wiener measure with initial distribution. The definition above is a Markovian variant of stochastic mass transportation. The minimization can alternatively take place over all triples (b,P,Y), where Y is a diffusion referring to P with diffusion matrix $h \cdot id$ and drift b. What counts is what the triple produces after an application of the picture measure theorem, namely a picture density and drift which fulfill a Fokker-Planck equation.

Proposition 18: Let $\varrho_{0/T} \in L^\infty \cap L^1$ be positive, $|\varrho_{0/T}|_{L^1}=1$, and the entropies $\int \varrho_{0/T} \ln \varrho_{0/T}\, dx$ may exist in $\mathbb{R}$. Let $(\Omega, \mathcal{T}_t, X_t, \bar{P})$ be the canonical Brownian motion with initial distribution $\bar{P}^{X_0}$. The following variational problems can be reformulated in each other:

(I)

$$\int_0^T \int b^2(t,x)\varrho \, dx \, dt \overset{!}{=} \inf_{b,\varrho},$$

$$b:[0,T] \times \mathbb{R}^n \to \mathbb{R}^n \in L^\infty \cap C^0,$$

$$\varrho:[0,T] \times \mathbb{R}^n \to \mathbb{R}^+ \in L^\infty, \quad \int \varrho_t \, dx = 1,$$

$$\varrho(0,x) = \varrho_0, \quad \varrho(T,x) = \varrho_T,$$

$$\partial_t \varrho + \operatorname{div}(\varrho b) - \frac{1}{2} h \Delta \varrho,$$

weak Fokker-Planck equation!

(II)

$$\int_0^T \int b^2(t,X_t)\, dP\, dt \overset{!}{=} \inf_{b,P,B},$$

$$b:[0,T] \times \mathbb{R}^n \to \mathbb{R} \in L^\infty \cap C^0,$$

$$dX_t = b(t,X_t)\, dt + \sqrt{h} dB_t,$$

$(\Omega, \mathcal{T}_t, B_t, P)$ Brownian motion with start in 0, such that

$$P[X_0 \in dx] = \varrho_0 dx, \quad P[X_T \in dx] = \varrho_T dx.$$

Proof: "(II)$\Rightarrow$(I)" The assertion follows by the picture measure theorem and the fact that because of Proposition 3 and Remark 11(b) (or Theorem 12) the stochastic diffusion equations $dX_t = b(t,X_t)\, dt + \sqrt{h} dB_t$ lead to a weak Fokker-Planck equation $\partial_t \varrho + \operatorname{div}(\varrho b) - \frac{1}{2} h \Delta \varrho = 0$, where $\varrho(t,x)\, dx = P[X_t \in dx]$, such that the conditions in (I) are fulfilled.

"(I)$\Rightarrow$(II)" Let b be given. Because b is bounded, according to Lemma 10 there is a weak solution $(\Omega, \mathcal{T}_t, B_t, P)$ of the diffusion equation with initial distribution density ϱ_0. This weak solution again leads to a weak Fokker-Planck equation according to Proposition 3 and Remark 11(b) (respectively, Theorem 12). Especially because of Theorem 13 the conditions of Theorem 13 are fulfilled. By Corollary 15 we can apply the uniqueness at all times. ϱ is therefore uniquely characterized by ϱ_0. Especially the time marginal condition for T is true. The equality of both functionals again is a conclusion of the picture measure theorem. Q.E.D.

Remark 19: The Brownian motion $(\Omega, \mathcal{T}_t, X_t, \bar{P})$ with initial distribution $\bar{P}^{X_0}$ is given at the outset. $(\Omega, \mathfrak{T}_t, X_t, \bar{P})$ is called the *reality* of the transport problem. Let $(\Omega, \mathcal{T}_t, B_t, P)$ be a minimizing solution. B_t is called the *observer* to the time marginal densities ϱ_0, ϱ_T at time T. P is called the observed *deviation* of the reality.

B. Lagrange formalism

The Lagrangian formalism for a point dynamical system on $\mathbb{R}^n$ possesses a stochastic generalization. For an elementary Lagrangian $L(x(t),\dot{x}(t))=\frac{1}{2}\langle\dot{x}(t),\dot{x}(t)\rangle-V(x(t))$, with a Riemannian metric $\langle .,. \rangle$, this generalization is defined by stochastic mass transportation including a potential term concerning V. The Euler-Lagrange equation of the variational problem is given by the stochastic Newton equation. Hereby Newton's law is generalized.

Definition 20: (Variational problem.) Let a variational functional $F: V \to \mathbb{R}$ be defined on a linear *concurrence space* K, such that constraints for F may hold. Let the problem be *homogeneous*, i.e., there is a subspace $U \subset K$, called *variational space*, such that for $f \in K$ it follows that $f+u \in K \ \forall u \in U$. An element f out of the concurrence space is called *stationary* referring to variation with U exactly if $(d/d\varepsilon)|_{\varepsilon=0} F(f+\varepsilon u)=0 \ \forall u \in U$, where existence of the derivatives may be given without restriction. We denote $\delta F(f) \overset{!}{=} 0$, to underline the search for a stationary solution.

The Lagrangian formalism for a point dynamical system on $\mathbb{R}^n$ with a Lagrangian L is given by

$$\delta\left(\int_0^1 L(t,x(t),\dot{x}(t))\,dt\right)\overset{!}{=}0, \quad \text{time marginal values } x(0),x(1). \tag{35}$$

The variation takes place referring to all differentiable ways with a compact support in $[0,1]$ and over the concurrence space of all differentiable ways which fulfill the time marginal conditions. The Euler-Lagrange equations for this problem are[28]

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}}-\frac{\partial L}{\partial x}=0. \tag{36}$$

The well-known stochastic generalization is given by the *Yasue h-problem:*[10,29,30]

$$J(Y) \coloneqq \int_0^T \int \left(\frac{1}{2}L(t,Y,DY)+\frac{1}{2}L(t,Y,D_*Y)\right)dP\,dt, \tag{37}$$

$\delta J(Y) \overset{!}{=} 0$. Variation takes place over the concurrence space of diffusions (Y,P), such that Y is a diffusion referring to P with drift b, the functional is in $\mathbb{R}$, and, furthermore, $P[Y_0 \in dx]=\varrho_0 dx$, $P[Y_T \in dx]=\varrho_T dx$. We seek a smooth solution (Y,P) with diffusion matrix $h \cdot id$.

Reformulating (and simplifying) the variational formalism compared to Refs. 29, 10, and 30 we do variation in the space of diffusions. A smooth diffusion Y_t with $\varrho(t,x)dx=P[Y_t \in dx]$, such that the time marginal conditions are fulfilled, is stationary if for all probability vectors $\xi=\eta(t,Y_t)$, $\eta:[0,T]\times\mathbb{R}^n \to \mathbb{R}^n$, differentiable with compact support in $\{\varrho>0\}\cap[0,T]\times\mathbb{R}^n$ we have: $(d/d\varepsilon)|_{\varepsilon=0} J(Y+\varepsilon\xi)=0$. As can be seen according to the proof of Proposition 2, $Y+\varepsilon\xi$ is again a diffusion referring to P. Furthermore, the time marginal conditions are true for $Y+\varepsilon\xi$, because of the compactness of the support of η. $Y+\varepsilon\xi$ is therefore an element of the concurrence space of diffusions. We find by variational calculus

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} J(Y+\varepsilon\xi)=\int_0^T\int\left(\frac{1}{2}\partial_{x_i}L(t,Y,DY)\xi^i+\frac{1}{2}\partial_{x_i}L(t,Y,D_*Y)\xi^i+\frac{1}{2}\partial_{q_i}L(t,Y,DY)D\xi^i\right.$$
$$\left.+\frac{1}{2}\partial_{q_i}L(t,Y,D_*Y)D_*\xi^i\right)dP\,dt \quad \text{(Sum convention !)}$$

where we have to justify the commutation of integration and differentiation. A justification can be given by the usual argumentations. See, e.g. Ref. 31, Sec. 11.Satz 2. The proof transfers obviously,

without which it is important that the integration takes place over a probability space Ω instead of $\mathbb{R}^n$. The following criteria must be true if we define

$$g(t,c,\varepsilon) \vdots \frac{1}{2}L(t,(Y+\varepsilon\xi)(t,c),D(Y+\varepsilon\xi)(t,c)) + \frac{1}{2}L(t,(Y+\varepsilon\xi)(t,c),D_*(Y+\varepsilon\xi)(t,c)), \quad c \in \Omega:$$

There is a $\kappa > 0$ such that

(I) $\varepsilon \mapsto g(t,c,\varepsilon)$ is continuously differentiable in ε, $\forall\ \varepsilon \in [-\kappa,\kappa]$ for every $(t,c) \in [0,T] \times \Omega$.

(II) $(t,c) \mapsto g(t,c,\varepsilon)$ is integrable for time and probability space for every $\varepsilon \in [-\kappa,\kappa]$.

(III) There is a (positive) integrable function $F(t,c)$ dominating $|(d/d\varepsilon)(g(t,c,\varepsilon))|\ \forall \varepsilon \in [-\kappa,\kappa]$.

To fulfill (I) the Lagrangian must be differentiable. For (II) the diffusions must allow integration, i.e., the drift has to be in $L^2(P)$ if L is quadratic in the velocity component. For (III) we can use the compactness of the support of η.

With the partial integration of Proposition 5 we have, using the compactness of the support of η,

$$\frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} J(Y+\varepsilon\xi) \overset{!}{=} 0\ \forall\ \xi \Leftrightarrow \int_0^T \int \left(\frac{1}{2}\partial_{x_i}L(t,Y,DY) + \frac{1}{2}\partial_{x_i}L(t,Y,D_*Y) - \frac{1}{2}D_*\partial_{q_i}L(t,Y,DY) - \frac{1}{2}D\partial_{q_i}L(t,Y,D_*Y)\right)\xi^i\, dP\, dt \overset{!}{=} 0, \quad \forall\ \xi = \eta(t,Y_t). \tag{38}$$

Because η can be chosen arbitrarily the integrand is necessarily zero, i.e., the stochastic Euler-Lagrange equations are fulfilled. If the elementary Lagrangian

$$L(x,q) = \frac{1}{2}\langle q,q\rangle_{\text{Eucl}} - V(x) \tag{39}$$

is considered, with the Euclidean metric $\langle .,. \rangle_{\text{Eucl}}$ and a real-valued potential $V: \mathbb{R}^n \to \mathbb{R}$, $V \in C^1$, for which we have

$$\int_0^T \int |V(Y_t)| dP\, dt < \infty \Rightarrow \int_0^T \int |V(Y_t + \varepsilon\,\eta(t,Y_t))| dP\, dt < \infty$$

$$\forall\, \varepsilon \in [-\kappa,\kappa] \text{ for a } \kappa > 0, \quad \forall\ \eta \in C_0^\infty,$$

because $|V|$ is locally bounded, a short calculation with Proposition 5 shows immediately

$$\int_0^T \int \left(-\frac{1}{2}(DD_* + D_*D)Y - \nabla V(Y)\right)\xi\, dP\, dt = 0 \quad \forall\ \xi_t = \eta(t,Y_t). \tag{40}$$

If Y is a smooth stationary solution with diffusion matrix $h \cdot id$, we thereby have, if we calculate the stochastic acceleration $\frac{1}{2}(DD_*+D_*D)$ as in Sec. II A, the stochastic Newton equation[10]

$$\partial_t v + \nabla_v v - \nabla_u u - \frac{h}{2}\Delta u = -\nabla V. \tag{41}$$

The equation is obviously valid in $[0,T] \times \mathbb{R}^n$, at least in the points where the picture density is not zero, i.e., in the points where a validity is of interest.

The *quasi-Euclidean h-stochastic Yasue problem*, with elementary Lagrangian, is defined as follows

$$J_q(Y) := \int_0^T \int \left(\frac{1}{2}b^2(t,Y_t) - V(Y_t)\right) dP\, dt - \frac{1}{2}h\Delta\mathrm{Entrop}(p_T,p_0), \tag{42}$$

$\delta J_q(Y) \overset{!}{=} 0$. Variation takes place over the concurrence space of diffusions (Y,P), such that Y is a diffusion referring to P with drift b, the functional is in $\mathbb{R}$, and, furthermore, $P[Y_0 \in dx] = \varrho_0 dx$, $P[Y_T \in dx] = \varrho_T dx$. We seek a smooth solution (Y,P) with diffusion matrix $h \cdot id$.

The marginal densities ϱ_0 and ϱ_T are given differentiable probability densities such that their entropy is in $\mathbb{R}$. The Gibbs-Boltzman entropy difference

$$\Delta\mathrm{Entrop}(\varrho_T,\varrho_0) = \left(\int \varrho_T \ln \varrho_T\, dx - \int \varrho_0 \ln \varrho_0\, dx\right) \quad \text{(the integral is defined on } \{\varrho_{0/T} > 0\}) \tag{43}$$

of the time marginal densities ϱ_0 and ϱ_T is only introduced because of energy conservation. It is obviously stationarily irrelevant, but note that the gradient flow referring to the entropy functional is the heat flow equation. $\Delta\mathrm{Entrop}(\varrho_T,\varrho_0)$ can be alternatively implemented into the functional, as will be shown in the following.

Proposition 21: (Entropy interpolation.) Let ϱ be a classical differentiable (strong) solution of the Fokker-Planck equation in $[0,T]\times\mathbb{R}^n$ with diffusion $h \cdot id$ and drift b. Let $\varrho > 0$ be in $L^\infty([0,t]\times\mathbb{R}^n;\mathbb{R})$ and $L^1(\mathbb{R}^n;\mathbb{R})$ with $\int \varrho\, dx = 1\ \forall t$. Let $b \in L^2(\varrho)$, i.e., on $\{\varrho > 0\}$ we have

$$\int_0^T \int b^2 \varrho\, dx\, dt < \infty. \tag{44}$$

Furthermore, $\varrho(0,x)$ and $\varrho(T,x)$ may have an entropy in $\mathbb{R}$ and the entropic velocity $u = (h/2)\nabla \ln \varrho$ may also be in $L^2(\varrho)$, i.e., on $\{\varrho > 0\}$

$$\int_0^T \int u^2 \varrho\, dx\, dt < \infty. \tag{45}$$

Then also the current velocity $v = b - u$ is in $L^2(\varrho)$ and we have the entropy interpolation

$$h\Delta\mathrm{Entrop}(\varrho_T,\varrho_0) = 2\int_0^T \int (v \cdot u)\varrho\, dx\, dt. \tag{46}$$

Proof: The strong validity of the Fokker-Planck equation implements the weak validity (referring to C_0^∞ as test functions). Let $B_{1/\varepsilon}(0)$ be the open ball with radius $1/\varepsilon$ at $0 \in \mathbb{R}^n$, for $\varepsilon > 0$. Let $f_\varepsilon : [0,T]\times\mathbb{R}^n \to [0,1] \in C_0^\infty$ be a plateau function, such that $f_\varepsilon|_{[0,T]\times B_{1/\varepsilon}(0)} \equiv 1$ and $\partial_i f_\varepsilon$, $\partial_t f_\varepsilon$ are uniformly bounded in ε for $i = 1,\ldots,n$. Let $\delta > 0$, then $\ln[(f_\varepsilon\varrho + \delta)/(f_\varepsilon + \delta)] \in C_0^\infty$ and we have by the weak Fokker-Planck equation and shifting

$$\int \varrho(T,x) \ln \frac{f_\varepsilon\varrho + \delta}{f_\varepsilon + \delta}(T,x)\, dx - \int \varrho(0,x) \ln \frac{f_\varepsilon\varrho + \delta}{f_\varepsilon + \delta}(0,x) dx = \int_0^T \int \left(\varrho b \nabla \ln \frac{f_\varepsilon\varrho + \delta}{f_\varepsilon + \delta}\right.$$
$$\left. - \nabla \varrho \nabla \ln \frac{f_\varepsilon\varrho + \delta}{f_\varepsilon + \delta} + \varrho\partial_t \ln \frac{f_\varepsilon\varrho + \delta}{f_\varepsilon + \delta}\right) dx\, dt =: \int_0^T \int (\mathrm{I} - \mathrm{II} + \mathrm{III})\, dx\, dt.$$

We see

$$\int_0^T \int \mathrm{I}\, dx\, dt = \int_0^T \int \left(\varrho b \cdot \frac{\nabla(f_\varepsilon\varrho)}{f_\varepsilon\varrho + \delta} - \varrho b \cdot \frac{\nabla f_\varepsilon}{f_\varepsilon + \delta}\right) dx\, dt,$$

$$\int_0^T \int \mathrm{II}\, dx\, dt = \int_0^T \int \left(\nabla \varrho \cdot \frac{\nabla (f_\varepsilon \varrho)}{f_\varepsilon \varrho + \delta} - \nabla \varrho \cdot \frac{\nabla f_\varepsilon}{f_\varepsilon + \delta} \right) dx\, dt,$$

$$\int_0^T \int \mathrm{III}\, dx\, dt = \int_0^T \int \left(\varrho \frac{\partial_t (f_\varepsilon \varrho)}{f_\varepsilon \varrho + \delta} - \varrho \frac{\partial_t f_\varepsilon}{f_\varepsilon + \delta} \right) dx\, dt.$$

The limit $\lim_{\delta \to 0} \lim_{\varepsilon \to 0}$ can be executed and it follows with $\varrho = e^{\ln \varrho} \Rightarrow \nabla \varrho = \varrho \nabla \ln \varrho$ (on $\{\varrho > 0\}$)

$$\Delta \mathrm{Entrop}(\varrho_T, \varrho_0) = \frac{2}{h} \int_0^T \int (v \cdot u) \varrho \, dx\, dt.$$

The limits are obvious, if we use the integrability

$$\int_0^T \int \frac{\nabla \varrho \cdot \nabla \varrho}{\varrho} \, dx\, dt < \infty.$$

Because of $\nabla \varrho \cdot \nabla \varrho \leqslant \max\{1, \|\varrho\|_{L^\infty}\} \nabla \varrho \cdot \nabla \varrho / \varrho$ we have $\varrho \in W^{(0,1),2}([0,T] \times \mathbb{R}^n; \mathbb{R})$, e.g., the limit $\lim_{\delta \to 0}$ in

$$\lim_{\delta \to 0} \lim_{\varepsilon \to 0} \int \varrho(T,x) \ln \frac{f_\varepsilon \varrho + \delta}{f_\varepsilon + \delta}(T,x)\, dx = \int \varrho(T,x) \ln \varrho(T,x)\, dx$$

is obtained by considering positive and negative parts and applying the theorem of monotone convergence. The limit $\lim_{\varepsilon \to 0}$ is clear, because pointwise convergence and domination holds true. Q.E.D.

Corollary 22: For a smooth diffusion (Y_t, P), $\varrho(t,x)\, dx = P[Y_t \in dx]$, with diffusion matrix $h \cdot id$ and with entropies $\int \varrho(0/T, x) \ln \varrho(0/T, x)\, dx$ in $\mathbb{R}$ at the times 0 and T the entropy interpolation of Proposition 21 is valid.

Proof: Smooth diffusions with the given properties fulfill the conditions of Proposition 21, especially the integrability condition referring to the entropic velocity given according to Corollary 15. Q.E.D.

It follows that for a smooth diffusion Y_t, with diffusion matrix $h \cdot id$, we have

$$\int_0^T \int v^2(t, Y_t)\, dP\, dt < \infty, \quad \int_0^T \int u^2(t, Y_t)\, dP\, dt < \infty$$

and

$$\begin{aligned} \int_0^T \int b^2(t, Y_t)\, dP\, dt - h \Delta \mathrm{Entrop}(\varrho_T, \varrho_0) &= \int_0^T \int (v(t, Y_t) + u(t, Y_t))^2\, dP\, dt \\ &\quad - 2 \int_0^T \int (v(x,t) \cdot u(x,t)) \varrho \, dx\, dt \\ &= \int_0^T \int (v^2(t, Y_t) + u^2(t, Y_t))\, dP\, dt. \end{aligned}$$

Theorem 23: For an elementary Lagrangian $L(x,q) = \frac{1}{2} \langle q, q \rangle_{eukl} - V(x)$ and for a smooth diffusion Y_t, with diffusion matrix $h \cdot id$, we have

$$J(Y)=\int_0^T\int\left(\frac{1}{2}L(Y,DY)\,dP\,dt+\frac{1}{2}L(Y,D_*Y)\right)dP\,dt=\int_0^T\int\left(\frac{1}{2}v^2(t,Y_t)+\frac{1}{2}u^2(t,Y_t)\right.$$
$$\left.-V(Y_t)\right)dP\,dt=\int_0^T\int\left(\frac{1}{2}(v(t,Y_t)+u(t,Y_t))^2-\frac{1}{2}2v(t,Y_t)\cdot u(t,Y_t)-V(Y_t)\right)dP\,dt$$
$$=\int_0^T\int L(Y,DY)\,dP\,dt-\frac{1}{2}h\Delta\mathrm{Entrop}(\varrho_T,\varrho_0)=J_q(Y). \tag{47}$$

Proof: $DY=b=u+v$ and $D_*Y=b_*=v-u$. Q.E.D.

Analogously the quasi-Euclidean functional $\int_0^T\int L(Y,DY)\,dP\,dt-\frac{1}{2}h\Delta\mathrm{Entrop}(\varrho_T,\varrho_0)$ can be variated. The same variational calculus shows that for stationary solutions Y we have

$$\int_0^T\int(-D_*DY-\nabla V(Y))\xi\,dP\,dt=0\quad\forall\,\xi_t=\eta(t,Y_t). \tag{48}$$

Corollary 24: The condition for a smooth diffusion Y, with diffusion matrix $h\cdot id$, to be a stationary solution of the problems (37) and (42) (with elemantary Lagrangian) is equivalent to

$$-\frac{h}{2}\Delta v+\nabla_v u-\nabla_u v+\partial_t u=0,\quad DD_*Y=D_*DY=-\nabla V(Y). \tag{49}$$

Proof: We have

$$DD_*Y^i=Db_*^i=\left(\frac{h}{2}\Delta+b^j\partial_j+\partial_t\right)b_*^i=\frac{h}{2}\Delta(v^i-u^i)+v^j\partial_j(v^i-u^i)+u^j\partial_j(v^i-u^i)+\partial_t(v^i-u^i)$$

and

$$D_*DY^i=D_*b^i=\left(-\frac{1}{2}\Delta+b_*^j\partial_j+\partial_t\right)b^i=-\frac{h}{2}\Delta(v^i+u^i)+v^j\partial_j(v^i+u^i)-u^j\partial_j(v^i+u^i)+\partial_t(v^i+u^i).$$

The direct comparison of $\frac{1}{2}(DD_*+D_*D)Y$ and D_*DY leads to

$$\partial_t v+\nabla_v v-\nabla_u u-\frac{h}{2}\Delta u=-\nabla V$$

according to the Yasue problem and

$$-\frac{h}{2}\Delta(v+u)+\nabla_v(v+u)-\nabla_u(v+u)+\partial_t(v+u)=-\nabla V$$

according to the quasi-Euclidean Yasue problem. It follows

$$-\frac{h}{2}\Delta v+\nabla_v u-\nabla_u v+\partial_t u=0$$

for a stationary solution Y of both problems. Furthermore we have $DD_*Y-D_*DY=-2(-(h/2)\Delta v+\nabla_v u-\nabla_u v+\partial_t u)=0$. Q.E.D.

Remark 25: (a) Therefore a stochastic generalization of Newton's law (see Ref. 10)

$$force=mass\times acceleration=mass\times\ddot{x}$$

holds for stationary solutions, where here mass was set identical to one and the two derivatives have to be interpreted as execution of forward and backward derivative, one behind the other respectively.

(b) If the Lagrangian is elementary and $V\equiv 0$, then the *h-stochastic mass transportation* is

defined by minimizing the h-Yasue functional (in the space of general diffusions where we seek for solutions in the space of diffusions with diffusion matrix $h \cdot id$). Analogously let the *quasi-Euclidean h-stochastic mass transportation* be defined by minimizing the quasi-Euclidean h-Yasue functional. A minimizing solution is necessarily stationary.

If in addition we consider a potential $V \leqslant 0$ for the minimization problems, this will be denoted by the expression Lagrangian stochastic mass transportation.

The stochastic mass transportation problem can as well be considered under the constraint that the solution has to be in a certain Riemannian structure, e.g., in the space of diffusions with diffusion matrix $h \cdot id$. Hereby a reachability problem is defined (that of course may not be well posed). Especially the unconstrained transport problem may lead to a general diffusion with contravariant diffusion matrix $(\sigma^{ij})_{ij}$ as an eventual solution. The covariant metric tensor of the problem is given by $(\sigma_{ij})_{ij}$.[10]

The following paragraph will show that solutions of the Schrödinger equation lead to stationary solutions of the Yasue problem. If one has a solution of the Schrödinger equation

$$i\hbar \partial_t \psi = -\frac{\hbar^2}{2m} \Delta \psi + V\psi,$$

with a point mass m, and states the Yasue problem with initial and end density $|\psi_{0/T}|^2$, the m will be a part of the solution of the problem and does not have to be given at the outset!

If one minimizes the stochastic mass transportation problem in the space of diffusions with diffusion matrix $h \cdot id$, then the problem can obviously be restricted to this space. By that a solution of the Euclidean h-stochastic mass transportation problem in Definition 1 is obtained. For a fixed initial density ϱ_0, the reachable end densities ϱ_T, so-constructed solutions of the minimization problem, are called *Euclidean h-stochastic shortest geodesics*.

The hereby demonstrated geodesic theory requires the clarification of the following problems:
(I) existence,
(II) uniqueness,
(III) regularity,
(IV) characterization of reachability, and
(V) an injectivity radius theorem.

IV. GEOMETRY OF THE SCHRÖDINGER EQUATION

A. Hamilton-Jacobi formalism

The Hamilton-Jacobi formalism is characterized by the Hamiltonian action function, which describes the evolution of the action wave of a point dynamical system out of a singular point. Or, equivalently, for a geodesic system where the potential is equal to zero it describes the evolution of the distance spheres. The Hamiltonian action function is determined by the Hamilton-Jacobi equation. Almost analogously to the deterministic case such an action function can be defined for the stochastic scenario, such that this function fulfills almost analogous properties.

The results in this subparagraph are taken from Ref. 10, and so we restrict to a brief sketch of proofs.

Consider the flow $\Phi^w(s;x,T)$ of a time-independent differentiable vector field $w:[0,\mathbb{R}] \times \mathbb{R}^n \to \mathbb{R}^n$, where $\Phi^w(s;x,T)$ is the flow at time s, if the flow is localized to time T in x. Let $L(x,q)=\frac{1}{2}\langle q,q\rangle - V(x)$ be an elementary Lagrangian, with a Riemannian metric $\langle .,. \rangle$. The *Hamiltonian action function* $S^w(T,x)$ of the system is defined by

$$S^w(T,x) := -\int_T^0 L(\Phi^w(s;x,T), w(t,\Phi^w(s;x,T)))\, ds. \tag{50}$$

It describes the evolution of the surfaces of constant action out of a singular point. Application of the total derivative (d/dT) leads to $(d/dT)S^w(T,x)=L(x,w(T,x)) := L^w$. We seek for stationary solutions of the functional $S^w(x,T)$ where we variate w without time marginal constraints. The

execution of the total derivative shows that we have to consider intrinsic dependencies such that $d/dT =: D^w = \partial_t + w^i \partial_i$. Let w be a stationary solution and $\delta w + w = \tilde{w}$. Then

$$D^w(S^w - S^{\tilde{w}}) = D^w S^w - D^{\tilde{w}} S^{\tilde{w}} + (D^w - D^{\tilde{w}}) S^{\tilde{w}} = L^{\tilde{w}} - L^w - \delta w^i \partial_i S^{\tilde{w}} = L^{\tilde{w}} - L^w - \delta w^i \partial_i S^w + o(\delta w).$$

Now $L^{\tilde{w}} - L^w = \Sigma_i w^i \delta w^i + o(\delta w)$ and $S^{\tilde{w}} - S^w = -\int_T^0 (d/ds)(S^{\tilde{w}} - S^w)\, ds$, because $S^{\tilde{w}}$ and S^w are equal to zero at time 0. Therefore

$$S^{\tilde{w}} - S^w = -\int_T^0 \sum_i (w^i - \partial_i S^w)\, \delta w^i\, ds + o(\delta w) \quad \forall\ \delta w.$$

We can conclude the Hamilton-Jacobi condition

$$w = \nabla S, \tag{51}$$

which shows together with $D^w S^w = L^w$, i.e., $\partial_t S^w + v^i \partial_i S^w = \frac{1}{2}\langle w, w\rangle - V$, the Hamilton-Jacobi equation

$$\partial_t S^w + \frac{1}{2}(\nabla S^w)^2 + V = 0. \tag{52}$$

The analogous stochastic formalism was considered by Guerra and Morato[10,32] and will be sketched here, because the following theorem taken from Ref. 10 and especially the stochastic Hamilton-Jacobi condition (62) will have effects on the next subparagraph. Let L_{GM} be the Lagrangian (Guerra-Morato Lagrangian)

$$L_{GM}(x,q) = \frac{1}{2}\langle q, q\rangle_{\text{Eucl}} + \frac{\hbar}{2}\partial_i q^i - V(x) \tag{53}$$

and let the variational functional be given by

$$I(b) = \int_0^T \int L_{GM}(X_t, b(t, X_t))\, dP\, dt. \tag{54}$$

$\hbar$ is *Planck's constant* from quantum mechanics, which later will enter into the validity of the Schrödinger equation. The variation will take place over the drift of the diffusion equation $dX_t = b(t, X_t)\, dt + \sqrt{\hbar} dB_t$; (B_t, P) is a Brownian motion, where the end density at time T is kept fixed. These diffusion equations can be constructed by time inversion on the Wiener space.[14] Especially weak solution methods can be applied and X_t can be chosen as coordinate mapping as usual. I is, following Nelson,[10] critical in the sense of Guerra-Morato in a differentiable b, if for all differentiable δb, with compact support, such that the diffusion, with diffusion matrix $\hbar \cdot id$, belonging to $\tilde{b} := b + \delta b$ has the same end density at time T as the diffusion belonging to b, if

$$I(b) - I(\tilde{b}) = I - \tilde{I} = o(\delta b). \tag{55}$$

Define $P[X_s \in dx] = \varrho dx$ and $R = (\hbar/2) \ln \varrho$, such that $\nabla R = u$. Then we have for $b = u + v = \nabla R + \nabla S$ the Fokker-Planck equation $\partial_t \varrho + \text{div}(b\varrho) - \frac{1}{2}\hbar \Delta \varrho = 0$, respectively the continuity equation $\partial_t \varrho + \text{div}(v\varrho) = 0$. Define, furthermore, the Hamiltonian action function referring to the drift b as follows:

$$S^b(T,x) := -E_T^b\left(\int_T^0 L_{GM}(X_s, b(s, X_s))\, ds | X_T = x\right) \tag{56}$$

with the factorized conditioned expectation associated to the diffusion measure referring to b conditioned under $X_T = x$.[33] We may have[10]

$$D^b S^b(T,X_T) = \lim_{\Delta t \to 0} \frac{1}{\Delta t}\left(E_T^b \int_T^{T+\Delta t} L_{GM}(X_s, b(s,X_s))\, ds \right) = L_{GM}(X_T, b(T,X_T)),$$

and with $D^b S^b(t,X_t) = (\partial_t + b^i \partial_i + (\hbar/2)\Delta) S^b(t,X_t)$

$$\begin{aligned} D^b(S^b - S^{\tilde{b}}) &= D^b S^b - D^{\tilde{b}} S^{\tilde{b}} + (D^b - D^{\tilde{b}}) S^{\tilde{b}} = L_{GM}^{\tilde{b}} - L_{GM}^b - \delta b^i \partial_i S^{\tilde{b}} = L_{GM}^{\tilde{b}} - L_{GM}^b - \delta b^i (\partial_i S^b + O(\delta b)) \\ &= L_{GM}^{\tilde{b}} - L_{GM}^b - \delta b^i \partial_i S^b + o(\delta b). \end{aligned} \tag{57}$$

Now we have $L_{GM}^{\tilde{b}} - L_{GM}^b = \Sigma_i b^i \delta b^i + (\hbar/2)\partial_i \delta b^i + o(\delta b)$ and

$$-E^b \int_T^0 D^b(S^{\tilde{b}} - S^b)\, ds = E^b S^{\tilde{b}}(T,X_T) - E^b S^b(T,X_T) = E^{\tilde{b}} S^{\tilde{b}}(T,X_T) - E^b S^b(T,X_T) = -I^{\tilde{b}} + I^b \tag{58}$$

because $S^{\tilde{v}}$ and S^v disappear identically at time 0 and because X_T has an identical picture distribution density ϱ_T referring to the measures belonging to $\tilde{b}$ and b. Therefore we have by (56)–(58)

$$I^{\tilde{b}} - I^b = E^b \int_T^0 \sum_i \left(b^i - \partial_i S^b + \frac{\hbar}{2}\partial_i \right) \delta b^i\, ds + o(\delta b)\ \forall\ \delta b. \tag{59}$$

But with $P[X_s \in dx] = \varrho dx$ and $R = (\hbar/2)\ln \varrho$, respectively $\nabla R = u$, we obtain by shifting in (59) (δb has compact support)

$$E^b \frac{\hbar}{2}\partial_i \delta b^i(s,X_s) = \int \frac{\hbar}{2}\partial_i \delta b^i \varrho\, dx = \int \sum_i u^i \delta b^i \varrho\, dx. \tag{60}$$

Because of $b^i - u^i = v^i$ we finally have by (59) and (60)

$$I^{\tilde{b}} - I^b = E^b \int_T^0 \sum_i (v^i - \partial_i S^b) \delta b^i\, ds + o(\delta b)\ \forall\ \delta b. \tag{61}$$

Theorem 26:[10] In the sense of Guerra-Morato stationary solutions b fulfills necessarily the Hamilton-Jacobi condition, i.e., with $S^b = S$ we have

$$v = \nabla S. \tag{62}$$

The current velocity is necessarily a gradient of a scalar function. We have the stochastic Hamilton-Jacobi equation

$$\partial_t S + \frac{1}{2}(\nabla S)^2 - \frac{1}{2}(\nabla R)^2 - \frac{\hbar}{2}\Delta R + V = 0, \tag{63}$$

from which we can conclude by differentiation the stochastic Newton equation and which is inclusively the validity of the continuity equation $\partial_t e^{(2/\hbar)R} + \mathrm{div}(v e^{(2/\hbar)R}) = 0$ equivalent to the Schrödinger equation.

Proof: (See Ref. 10.) The Hamilton-Jacobi condition follows from the preceding explanations. The stochastic Hamilton-Jacobi condition together with $D^b S = L^b$, i.e., $(\partial_t + b^i \partial_i + (\hbar/2)\Delta) S^b = \frac{1}{2}\langle b, b\rangle + (\hbar/2)\partial_i b^i - V(x)$, leads to the stochastic Hamilton-Jacobi equation. An application of ∂_i shows

$$\partial_t v^i + \frac{1}{2}\partial_i\left(\sum_j v^j v^j \right) - \frac{1}{2}\partial_i\left(\sum_j u^j u^j \right) - \frac{1}{2}\partial_i \Delta(\hbar R) + \partial_i V = 0,$$

i.e., the stochastic Newton equation from Sec. III B:

$$\partial_t v^i + \sum_j v^j \partial_i v^j - \sum_j u^j \partial_i u^j - \frac{1}{2}\Delta(\hbar u^i) + \partial_i V = 0.$$

An easy calculation shows that the stochastic Hamilton-Jacobi equation together with the equation

$$\partial_t R + \nabla R \cdot \nabla S + \frac{\hbar}{2}\Delta S = 0$$

and the substitution $\psi := e^{(1/\hbar)(R+iS)}$ is just the Schrödinger equation

$$\hbar i \partial_t \psi = -\frac{\hbar^2}{2}\Delta\psi + V\psi$$

in real and imaginary parts, respectively. The equation

$$\partial_t R + \nabla R \cdot \nabla S + \frac{\hbar}{2}\Delta S = 0$$

is concluded from $\varrho = e^{(2/\hbar)R}$ and $\partial_t \varrho + \mathrm{div}(v\varrho) = 0$ by differentiation of ϱ. Q.E.D.

Remark 27: (a) The formula (56) gives a geometric meaning to the Guerra-Morato functional by the phase function S.

(b) By shifting on the other side in (54), what has to be justified appropriately, it can easily be shown that

$$\int_0^T \int \left(\frac{1}{2}v^2(t,x) - \frac{1}{2}u^2(t,x) - V(x)\right)\varrho \, dx \, dt = \int_0^T \int L_{GM}(x, b(t,x))\varrho \, dx \, dt. \tag{64}$$

Therefore the following problem,

$$\delta\left(\int_0^T \int \left(\frac{1}{2}v^2 - \frac{1}{2}u^2 - V\right)\varrho \, dx \, dt\right) \overset{!}{=} 0,$$

$$u = \frac{\hbar}{2}\nabla \ln \varrho, \quad \partial_t \varrho + \mathrm{div}(v\varrho) = 0,$$

probability density time marginal constraints for ϱ, is considered. The given Hamilton-Jacobi problem is sufficient for the stationarity of the Yasue formalism, whereas both problems differ like day and night by the sign in the functional. This fact will be explained by the formalism of stochastic Legendre transformations in Sec. V.

B. Hamilton formalism

In analogy to the Hamiltonian and Lagrangian formalisms of a (point) geodesic variational problem the Schrödinger equation can be thought of as a necessary and sufficient stationary condition for the Hamiltonian formalism of a stochastic geodesic variational problem. The Schrödinger equation can be deduced directly from a Hamiltonian problem that has, compared to the point problem, an almost similar exterior form.

By a Legendre transformation of the Lagrangian formalism

$$H(x,g) = g \cdot \dot{x} - L(x,\dot{x}), \tag{65}$$

where the derivative component is substituted by a new variable g, the Hamilton formalism with Hamiltonian H (Ref. 28) is obtained:

$$\delta\left(\int_0^1 (\dot{x}(t)\cdot g(t) - H(x(t),g(t)))\,dt\right) \overset{!}{=} 0, \tag{66}$$

time marginal values for $x(0), x(1)$, free time marginal values for g.

Variation leads to the canonical equations[28]

$$\dot{x} = \frac{\partial H}{\partial g}, \quad \dot{g} = -\frac{\partial H}{\partial x} \tag{67}$$

as stationarity criteria.

Consider now for $[0,T]$ the time-dependent, complex-valued, and differentiable functions on $\mathbb{R}^n$, which may furthermore be spatially quadratically integrable. These functions constitute in the spatial closure with the canonical Hermitian metric

$$\langle \varphi, \chi \rangle := \int \varphi \bar{\chi}\, dx, \tag{68}$$

a Hilbert space. Well known in quantum mechanics is Planck's constant $\hbar$, the Hamilton operator

$$H = -\frac{1}{2}\hbar^2 \Delta_{\mathbb{C}} + V, \tag{69}$$

with a real-valued potential $V \in C^1$, and the momentum operator

$$-i\hbar\nabla_{\mathbb{C}}. \tag{70}$$

$\nabla_{\mathbb{C}}$ acts as gradient and $\Delta_{\mathbb{C}}$ as Laplace operator on the complex-valued functions of the Euclidean space.

Compared to general dynamical systems of (point) mechanics on symplectic manifolds (M,ω) the quantum mechanical formalism implements the restriction of the motion on a Lagrangian submanifold intrinsically (compare Ref. 34 for that issue). Nevertheless, the quantum mechanical formalism is a model of a phase space.

Remark 28: Well known in quantum mechanics is that for bounded and time-independent observable operators A (Hermitian) and solutions of the Schrödinger equation ψ we have

$$\frac{d}{dt}\langle \psi, A\psi \rangle = \frac{i}{\hbar}\langle \psi, [A,H]\psi \rangle. \tag{71}$$

Especially the quantum mechanical energy $\langle \psi, H\psi \rangle$ is a constant of the motion, because the commutator $[H,H]=HH-HH$ is trivially equal to zero.

Lemma 29: Let $\psi = e^{(1/\hbar)(R+iS)}$ be a differentiable solution of the Schrödinger equation $\hbar i \partial_t \psi = H\psi$. Then we have on $\{|\psi|^2 > 0\}$, with $j := -(i\hbar/2)(\bar{\psi}\nabla\psi - \nabla\bar{\psi}\psi)$,

$$\text{(I)} \quad j = |\psi|^2 \nabla S,$$

$$\text{(II)} \quad \operatorname{div}(j) + \partial_t |\psi|^2 = 0,$$

$$\text{(III)} \quad \partial_t |\psi|^2 + \operatorname{div}(\nabla\phi |\psi|^2) - \frac{1}{2}\hbar\Delta|\psi|^2 = 0,$$

where $\phi = (S+R)$. Note especially that the continuity equation (20) holds true according to (II) and the Fokker-Planck equation (6) according to (III).

Proof: Elementary calculation! The third identity follows, e.g., from the first and the second with

$$\partial_t|\psi|^2 = -\operatorname{div} j = -\operatorname{div}(|\psi|^2 \nabla S)$$
$$= -\operatorname{div}(|\psi|^2 \nabla \phi - |\psi|^2 \nabla R) \overset{|\psi|^2\nabla R = 1/2\hbar\nabla|\psi|^2}{=} -\operatorname{div}\left(\nabla\phi|\psi|^2 - \frac{1}{2}\hbar\,\nabla\,|\psi|^2\right).$$

Q.E.D.

Theorem 30: (Entropy action law.) Let $\psi = e^{(1/\hbar)(R+iS)}: [0,T]\times\mathbb{R}^n \to \mathbb{C} \in L^\infty$ be a differentiable solution of the Schrödinger equation, with $R: [0,T]\times\mathbb{R}^n \to \mathbb{R}\cup\{-\infty\}$. The condition in Proposition 21 for $b = \nabla(R+S)$, $\varrho = |\psi|^2$ and $u = \nabla R$ may hold true. Then we have the entropy action law

$$T\langle\psi, H\psi\rangle = \frac{1}{2}\int_0^T \int b^2|\psi|^2 dx\,dt + \int_0^T \int V|\psi|^2 dx\,dt - \frac{\hbar}{2}\Delta\mathrm{Entrop}(|\psi_T|^2, |\psi_0|^2), \tag{72}$$

where $v = \nabla S$.

Remark 31: If we interpret $b = u + v$ as kinematical active drift, then the common energy conservation has an additional dissipative term, given by the negative Gibbs-Boltzman entropy difference of final and initial absolute square of ψ. Notice that the pair (b, ϱ) is Lagrangian, whereas $\psi = e^{(1/\hbar)(R+iS)}$ is Hamiltonian. The entropy action law is the Lagrangian energy conservation expression.

Proof: $\langle\psi, H\psi\rangle$ is constant $\forall t$ according to the preceding Remark 28. We have

$$\int_0^T \langle\psi, H\psi\rangle\,dt = -\frac{1}{2}\hbar^2\int_0^T \langle\psi, \Delta_{\mathbb{C}}\psi\rangle\,dt + \int_0^T\int V|\psi|^2\,dx\,dt = \frac{1}{2}\hbar^2\int_0^T\int (\nabla_{\mathbb{C}}\psi\cdot\nabla_{\mathbb{C}}\psi)\,dx\,dt$$
$$+ \int_0^T\int V|\psi|^2\,dx\,dt = \frac{1}{2}\hbar^2\int_0^T\int \left(\frac{1}{\hbar}\nabla_{\mathbb{C}}(R+iS)\cdot\frac{1}{\hbar}\nabla_{\mathbb{C}}(R+iS)\right)|\psi|^2\,dx\,dt$$
$$+ \int_0^T\int V|\psi|^2\,dx\,dt = \frac{1}{2}\hbar^2\left(\int_0^T\int \left(\frac{1}{\hbar}\nabla(R+S)\cdot\frac{1}{\hbar}\nabla(R+S)\right)|\psi|^2\,dx\,dt\right.$$
$$\left. - 2\frac{1}{2}\int_0^T\int (\nabla R\cdot\nabla S)|\psi|^2\,dx\,dt\right) + \int_0^T\int V|\psi|^2\,dx\,dt.$$

With Lemma 29 and the calculations in Proposition 21 the assertion follows. Q.E.D.

Definition 32: Let two variational functionals F_1, F_2 on linear concurrence spaces K_1, K_2 be given. Constraints for F_1, F_2 may hold. Let the problems be homogenous, with variational spaces $U_{1/2} \subset K_{1/2}$, such that for elements $f \in K_{1/2}$ fulfilling the constraints $f+u \in K_{1/2}\,\forall\, u \in U_{1/2}$. The functionals are called *stationary equivalent* referring to the respective variational spaces exactly if the stationary solutions are in $K_1 \cap K_2$ and the stationarity conditions

$$F_{1/2}(f) < \infty, \quad \frac{d}{d\varepsilon}F_{1/2}(f+\varepsilon u) \overset{!}{=} 0, \tag{73}$$

for $f \in K_{1/2}$ stationary and $\forall u \in U_{1/2}$ are equivalent.

Theorem 33: Let $\varrho_{0/T}$, $\varrho_{0/T} > 0$, $\int \varrho_{0/T}\,dx = 1$, $\varrho_{0/T}$ differentiable and with compact support be given. Consider the concurrence space $K_1 := \{\varphi: [0,T]\times\mathbb{R}^n \to \mathbb{C} \backslash \varphi$ is differentiable, spatially quadratically integrable, and has compact support$\}$ of the variational problem

$$\delta F_1 \overset{!}{=} 0, \quad \text{with } U_1 = \{\delta\psi\,|\,\delta\psi \in C_0^\infty([0,T]\times\mathbb{R}^n \to \mathbb{C})\},$$

$$\text{where } F_1(\varphi) := \int_0^T \langle\varphi, i\hbar(\nabla_{\mathbb{C}}\cdot\dot{x} - \nabla_{\mathbb{C}}\cdot\dot{x}^T)\varphi - H\varphi\rangle\,dt, \quad \varphi \in K_1,$$

$$\text{with the constraints } |\varphi(0,.)|^2 = \varrho_0, \quad |\varphi(T,.)|^2 = \varrho_T, \tag{74}$$

where the operator $\nabla_C \cdot \dot{x} - \nabla_C \cdot \dot{x}^T$ is defined by

$$\int_0^T \int \overline{f(\nabla_C \cdot \dot{x} - \nabla_C \cdot \dot{x}^T)\varphi}\, dx\, dt := \int_0^T \int \left(\frac{1}{n}\sum_{j=1}^n (\partial_j \overline{f(-x_j \partial_t \varphi)}) + \frac{1}{n}\sum_{j=1}^n (\partial_t \overline{f(x_j \partial_j \varphi)}) \right) dx\, dt \; \forall\, f \in C_0^\infty.$$

Then the Schrödinger equation gives the Eulerian variational expression of the problem.

Remark 34: Notice the formal equivalence of the form of the variational functional (74) and of the functional given in point mechanics (66).

Proof: The problem is homogeneous referring to the variational space U_1. Let $\psi \in K_1$ be a differentiable stationary solution, i.e., the functional may be finite in ψ and the stationarity criteria

$$0 \overset{!}{=} \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} \int_0^T \langle \psi', i\hbar(\nabla_C \cdot \dot{x} - \nabla_C \cdot \dot{x}^T)\psi' - H\psi' \rangle\, dt, \quad \psi' = \psi + \varepsilon\, \delta\psi \; \forall\; \delta\psi \in U_1$$

may hold true. Executing the differentiation $(d/d\varepsilon)|_{\varepsilon=0}$ and shifting $\delta\psi$ (compact support!) free leads together with

$$\left\langle \psi, \frac{1}{n}\sum_{j=1}^n \partial_j(x_j \partial_t \delta\psi) \right\rangle = \langle -\partial_t \psi, \delta\psi \rangle + \left\langle \frac{1}{n}\sum_{j=1}^n \partial_j(x_j \partial_t \psi), \delta\psi \right\rangle$$

to

$$\begin{aligned} 0 &= \int_0^T \langle \psi, i\hbar(\nabla_C \cdot \dot{x} - \nabla_C \cdot \dot{x}^T)\delta\psi - H\delta\psi \rangle\, dt + \int_0^T \langle \delta\psi, i\hbar(\nabla_C \cdot \dot{x} - \nabla_C \cdot \dot{x}^T)\psi - H\psi \rangle\, dt \\ &= \int_0^T \Bigg(-i\hbar(\langle -\partial_t \psi, \delta\psi \rangle + \langle \nabla_C \cdot \dot{x}\psi, \delta\psi \rangle - \langle \nabla_C \cdot \dot{x}\psi, \delta\psi \rangle + \langle \delta\psi, \nabla_C \cdot \dot{x}\psi \rangle - \langle \delta\psi, -\partial_t \psi \rangle \\ &\quad - \langle \delta\psi, \nabla_C \cdot \dot{x}\psi \rangle) + \left(-\left\langle -\frac{1}{2}\hbar^2 \Delta_C \psi + V\psi, \delta\psi \right\rangle - \left\langle \delta\psi, -\frac{1}{2}\hbar^2 \Delta_C \psi + V\psi \right\rangle \right) \Bigg) dt \quad \forall\; \delta\psi, \end{aligned}$$

where time marginal expressions disappear because of $|\delta\psi(0,.)| = |\delta\psi(T,.)| = 0$. Therefore

$$0 = \int_0^T \left\langle i\hbar\partial_t \psi - \left(-\frac{1}{2}\hbar^2 \Delta_C \psi + V\psi \right), \delta\psi \right\rangle dt + \int_0^T \left\langle \delta\psi, i\hbar\partial_t \psi - \left(-\frac{1}{2}\hbar^2 \Delta_C \psi + V\psi \right) \right\rangle dt \quad \forall\; \delta\psi,$$

i.e., the Schrödinger equation $i\hbar\partial_t \psi - \left(-\frac{1}{2}\hbar^2 \Delta_C \psi + V\psi\right) = 0$ as necessary and sufficient stationarity criteria. Q.E.D.

Proposition 35: Let K_1 be given as in Theorem 33. Consider the concurrence space $K_2 = \{(R,S) \backslash R, S : [0,T] \times \mathbb{R}^n \to \mathbb{R}, e^{(1/\hbar)(R+iS)} \in K_1\}$. Then the following variational problems are, under the "up-to-constants-injection" $K_2 \hookrightarrow K_1$ (see remark), stationary equivalent:

(I) The problem (74) (with classical exterior form).

(II) The problem

$$\delta F_2(R,S) \overset{!}{=} 0,$$

$$F_2(R,S) := \int_0^T \int \left(\partial_t S + \frac{1}{2}(\nabla S)^2 + \frac{1}{2}(\nabla R)^2 + V \right) \varrho\, dx\, dt,$$

$$R, S \in V_2, \quad \varrho := e^{(2/\hbar)R},$$

$$\text{with the constraints } \varrho(0,\,.\,)=\varrho_0,\quad \varrho(T,\,.\,)=\varrho_T.$$

(III) And finally the problem [see Remark 27(b)]

$$\delta F_3(R,S)\overset{!}{=}0,$$

$$F_3(R,S) := \int_0^T \int \left(\frac{1}{2}(\nabla S)^2-\frac{1}{2}(\nabla R)^2-V\right)\varrho\, dx\, dt,$$

$$R,S\in V_2,\quad \varrho := e^{(2/\hbar)R},$$

$$\text{with the constraints } \partial_t\varrho+\operatorname{div}(\nabla S\varrho)=0$$

$$\text{and } \varrho(0,\,.\,)=\varrho_0,\quad \varrho(T,\,.\,)=\varrho_T.$$

Remark 36: The transition of an element of K_1 to an element of K_2, i.e., the construction of a representation $\psi=e^{A+iB}$, is done by covering theory. B is a lift for the covering $\exp(i\,.\,):\mathbb{R}\to S^1$, which can be aligned arbitrarily by a constant $\lambda\in S^1$.

A constant $\lambda\in S^1$ is not relevant for the motion. The fundamental group of $\mathbb{R}^n$ is trivial. The lift of the mapping $\psi/|\psi|:\mathbb{R}^n\to S^1$ exists if only $\psi\neq 0$. We can continue the lift up to the boundary of $\mathbb{R}^n\backslash\psi^{-1}(0)$ in connected components, what can be done because of the differentiability in such a way that B is bounded on compact sets. (See Ref. 35 for covering theory.)

Proof: It follows by shifting (compact support)

$$-i\hbar\int_0^T\langle(\nabla_{\mathbb{C}}\cdot\dot{x})\psi,\psi\rangle\,dt=-i\hbar\int_0^T\langle\psi,(\nabla_{\mathbb{C}}\cdot\dot{x})\psi\rangle\,dt-\int_0^T\langle i\hbar\partial_t\psi,\psi\rangle\,dt+\text{marginal term}.$$

So we obtain the problem

$$\delta\left(\int_0^T(\langle i\hbar\partial_t\psi,\psi\rangle-\langle\psi,H\psi\rangle)\,dt\right)\overset{!}{=}0,$$

$$|\psi(0,\,.\,)|^2=\varrho_0,\quad |\psi(T,\,.\,)|^2=\varrho_T$$

because marginal terms are irrelevant for the stationary character of the variational problem. (The inspection of the so-obtained problem leads immediately to the Schrödinger equation as stationarity criteria.) Furthermore, we have with $\psi=e^{(1/\hbar)(R+iS)}$

$$\int_0^T\langle i\hbar\partial_t\psi,\psi\rangle\,dt=+i\hbar\int_0^T\int\frac{1}{\hbar}(\partial_tR+i\partial_tS)|\psi|^2\,dx\,dt\overset{|\psi|^2\partial_tR=1/2\hbar\partial_t|\psi|^2}{=}-\int_0^T\int\partial_tS|\psi|^2\,dx\,dt$$
$$+i\hbar^2\frac{1}{2}\int_0^T\partial_t\int|\psi|^2\,dx\,dt=-\int_0^T\int\partial_tS|\psi|^2\,dx\,dt,$$

whereby we have shown the stationary equivalence of (I) and (II) by ordinary reformulation, if in addition we use that we have, analogously to the proof in Theorem 30,

$$-\frac{1}{2}\hbar^2\int_0^T \langle \psi, \Delta\psi\rangle\, dt = \frac{1}{2}\hbar^2\int_0^T \int (\nabla_{\mathbb{C}}\psi\cdot\nabla_{\mathbb{C}}\psi)\, dx\, dt$$
$$= \frac{1}{2}\hbar^2\int_0^T \int \left(\frac{1}{\hbar}\nabla_{\mathbb{C}}(R+iS)\cdot\frac{1}{\hbar}\nabla_{\mathbb{C}}(R+iS)\right)p\, dx\, dt$$
$$= \frac{1}{2}\int_0^T \int ((\nabla R)^2 + (\nabla S)^2)|\psi|^2\, dx\, dt.$$

If for $\psi = e^{(1/\hbar)(R+iS)}$ the Fokker-Planck equation on $\{|\psi|^2 > 0\}$,

$$\partial_t|\psi|^2 + \mathrm{div}\big(|\psi|^2\,\nabla\,(R+S)\big) - \frac{1}{2}\hbar\Delta|\psi|^2 = 0,$$

holds true, then we have the continuity equation on $\{|\psi|^2 > 0\}$:

$$\partial_t|\psi|^2 + \mathrm{div}(|\psi|^2\,\nabla\,S) = 0.$$

If we add the continuity equation as additional constraint to problem (II), the stationary character will not change. (We can immediately calculate the validity of the continuity equation by variation of S in F_2. See also Proposition 44.) We will obtain a stationary equivalent problem. We have

$$-\int_0^T \int \partial_t S|\psi|^2\, dx\, dt \overset{\text{Shifting}}{=} \text{marginal term} + \int_0^T \int S\partial_t|\psi|^2\, dx\, dt \underset{\text{equation}}{\overset{\text{Continuity}-}{=}} \text{marginal term}$$
$$-\int_0^T \int S\,\mathrm{div}(|\psi|^2\,\nabla\,S)\, dx\, dt = \text{marginal term} + \int_0^T \int (\nabla S)^2|\psi|^2\, dx\, dt$$

such that we can conclude the stationary equivalence of the problems (II) and (III). Q.E.D.

Remark 37: Solutions of the Schrödinger equation ψ are naturally normalized. The unitary operator e^{-tiH}, defined by spectral integration theory, determines for ψ_0 the solution by $\psi_t = e^{-tiH}\psi_0$. The time marginal densities $\varrho_{0/T}$ have necessarily the same norm. In other cases the problem would be ill-posed.

V. TRANSFORMATIONS

A. Stochastic Legendre transformations

The point dynamical Legendre transformation is a pointwise transformation between the Hamiltonian and Lagrangian functions. The dependency of the Lagrangian of the derivative variable is transformed to a dependency of a new variable in the Hamiltonian. In the stochastic case this transformation is obtained by augmenting the tangential structure given by the Fokker-Planck equation into the functional.

The Legendre transformation between Hamiltonian and Lagrangian is given in point dynamics by

$$L(x,\dot{x}) = g\cdot\dot{x} - H(x,g), \tag{75}$$

where g is a new variable.

The stochastic formalism is given, where the case of an elementary Lagrangian $L(x,q) = \frac{1}{2}\langle q,q\rangle - V(x)$ is considered, by variation of the Yasue h-problem (37)

$$\delta F(R,S) = \delta\left(\int_0^T \int \left(\frac{1}{2}(\nabla R(t,x))^2 + \frac{1}{2}(\nabla S(t,x))^2 - V(x)\right)\varrho\, dx\, dt\right) \overset{!}{=} 0,$$

$$v = \nabla S, \quad \varrho = e^{(2/h)R}, \quad \partial_t \varrho + \mathrm{div}(v\varrho) = 0,$$

and time marginal constraints.

Notice that the variation is done referring to general diffusions, but we seek a solution with diffusion matrix $h \cdot id$. Now the goal is to augment the constraints into the functional.

Definition 38: Let $F(R,S) = \int_0^T \int \mathcal{F}(R,S)\, dx\, dt$ be a scalar functional of the real-valued functions S and R, defined on a space-time. We seek stationary solutions, with variation referring to C_0^∞, under the constraint given by a scalar differential equation $G(R,S,\nabla S,\nabla R,(\partial_{ij}S)_{ij},(\partial_{ij}R)_{ij}) = 0$. Then a scalar functional given by $K(R,S) = \int_0^T \int \mathcal{K}(R,S)\, dx\, dt$ is called *functional augmentation* of F and G exactly if for instance $\delta K/\delta S = 0$ is equivalent to the constraint and $\delta K/\delta R = 0$ is sufficient for the stationarity of F under the constraint, where, for instance, $\delta K/\delta R$ is the functional notation for the Eulerian variational expression referring to a variation of R, i.e.,

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \int_0^T \int \mathcal{K}(R + \varepsilon\,\delta R, S)\, dx\, dt = \int_0^T \int \frac{\delta K}{\delta R}(R,S)\,\delta R\, dx\, dt \quad \forall\ \delta R \in C_0^\infty. \tag{76}$$

Theorem 39: (*Stochastic Legendre transformation* and existence of a functional augmentation for stochastic mass transportation.) A functional augmentation for the Yasue h-problem is given by the variational problem Proposition 35 (II):

$$\delta\left(\int_0^T \int \left(\partial_t S(t,x) + \frac{1}{2}(\nabla R(t,x))^2 + \frac{1}{2}(\nabla S(t,x))^2 + V(x) \right) \varrho\, dx\, dt \right) \overset{!}{=} 0,$$

$$\varrho = e^{(2/h)R}, \quad \text{time marginal constraints!}$$

Proof: One finds immediately that variation $\delta/\delta S$ leads to the continuity equation. The rest follows by the argumentations in Secs. IV A and IV B, because the variation $\delta/\delta R$ leads to the stochastic Hamilton-Jacob equation (63) as stationarity criteria, as can be calculated easily by

$$\begin{aligned}
&\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \int_0^T \int \left[\partial_t S + \frac{1}{2}(\nabla(R + \varepsilon\,\delta R))^2 + \frac{1}{2}(\nabla S)^2 + V \right] e^{(2/h)(R+\varepsilon\,\delta R)}\, dx\, dt \\
&= \int_0^T \int \left[(2\partial_t S + (\nabla S)^2 + (\nabla R)^2 + 2V)\frac{1}{h}\varrho - \mathrm{div}(\nabla R\,\varrho) \right] \delta R\, dx\, dt \\
&= \int_0^T \int \left[\left(\frac{2}{h}\partial_t S + \frac{1}{h}(\nabla S)^2 - \frac{1}{h}(\nabla R)^2 - \Delta R + \frac{2}{h}V \right) \right] \varrho\,\delta R\, dx\, dt, \quad \forall\ \delta R,
\end{aligned}$$

i.e., the stochastic Hamilton-Jacobi equation

$$\partial_t S + \frac{1}{2}(\nabla S)^2 - \frac{1}{2}(\nabla R)^2 - \frac{h}{2}\Delta R = -V$$

holds. Q.E.D.

Remark 40: (a) The problem of finding a functional augmentation has, at least directly, nothing to do with the method of Lagrangian multipliers, which is used to solve variational problems under constraints. In this method the variational expression $F + \lambda G$ is considered to be equal to zero. The additional parameter λ and the integration constants are obtained by the constraints and the marginal conditions.

(b) Note that the potential in the Hamiltonian has a positive sign. The transition to the Lagrange problem produces a negative sign. Hereby we can detect, as in the classical case, the transition from the Hamiltonian (kinetic energy + potential energy) to the Lagrangian (kinetic energy − potential energy) formalism.

B. Stochastic symplectic transformations

Symplectic geometry is, for the main example, the research on a cotangential space T^*M of a manifold M with a given nondegenerated two-form ω on T^*M. The topological basis of the here-introduced stochastic symplectic geometry is now the research on the stochastic analysis of pairs of scalar functions on a space-time that are suitably put together to a complex-valued function and such that in addition a Hermitian scalar product is given. This structure is determined by the momentum operator and its Fourier transformation, the operator of multiplication with the identity, i.e., we do research on the stochastic analysis of a Hermitian line bundle on a space-time.

In the case of symplectic topology with the Hamiltonian $H(x,g)$ we have the canonical equations (67)

$$\dot{x} = \frac{\partial H}{\partial g}, \quad \dot{g} = -\frac{\partial H}{\partial x}$$

as in Sec. IV B which can be deduced from $\omega(X_H, .) = dH(.)$, with the Hamiltonian vector field X_H. A symplectomorphism $\Theta: T^*M \to T^*M$ preserves the two-form $\Theta^*\omega = \omega$ and the canonical equations (with the transformed Hamiltonian).

In the framework of stochastic symplectic geometry analogous canonical equations are given by (variation of ϱ instead of R exactly as in Theorem 39)

$$\partial_t \varrho = \frac{\delta H}{\delta S}, \quad \partial_t S = -\frac{\delta H}{\delta \varrho},$$

where the here elementary Hamiltonian functional is defined by

$$H(\varrho, S) = \int_0^T \int \left(\frac{1}{2}(\nabla R(t,x))^2 + \frac{1}{2}(\nabla S(t,x))^2 + V(x) \right) \varrho \, dx \, dt, \quad \varrho = e^{(2/h)R}.$$

The stochastic canonical equations are constituted by the stochastic Hamilton-Jacobi equation (63) and the continuity equation (20).

Definition 41: A *stochastic symplectomorphism*

$$\Theta: (\varrho(t,x), S(t,x)) \to (\varrho'(t',x'), S'(,t',x')) \tag{77}$$

is in analogy a transformation that preserves the form of the stochastic canonical equations (see also Ref. 28, definition of canonical transformations).

Example 42: It is well known that the Fourier transformation $F(\psi(t,x)) = \psi^F(t,p)$ preserves the validity of the Schrödinger equation $i\hbar\partial_t\psi = \frac{1}{2}p^2\psi - V\psi$ also for the momentum representation of the ψ function $\psi^F(t,p)$.

VI. ZOOMOUT GEOMETRIES

A. An elementary zoomout formalism

Consider an observer who measures the Planck constant $\hbar$ to a special value (and therefore has a normalized space-time scale). The geodesic problem defined by stochastic mass transportation, for the marginal densities $\varrho_{0/T}$ and to the data T and $\hbar$, is a viewpoint of an $\hbar$-associated dynamical process. By decreasing $\hbar$ and "compactifying" the time marginal densities a "zoomout" is defined. With this zoomout technique the "absolute" geodesic problem on the Euclidean space can be recovered by the limit $\hbar \to 0$. The Euclidean problem is, so to speak, "superficial" to the stochastic one. Therefore a possibility to establish the continuity of the quantum world is given.

Proposition 43: (Case of constant time marginal densities.) If we solve for

$$u = \nabla R \text{ and } v = \nabla S, \tag{78}$$

the Yasue $\hbar$-problem with a trivial potential, then for

$$\hbar\widetilde{R} = R \text{ and } \hbar\widetilde{S} = S \text{ with } \psi = e^{\widetilde{R}+i\widetilde{S}} = e^{(1/\hbar)(R+iS)} \tag{79}$$

the Schrödinger equation is valid, where we obviously can add a potential. So if we are interested in the Schrödinger equation, we have to consider the problem (for a trivial potential)

$$\int_0^T \int (\hbar^2(\nabla\widetilde{S})^2 + \hbar^2(\nabla\widetilde{R})^2)\varrho\, dx\, dt \overset{!}{=} \text{Min},$$

$$\varrho = e^{2\widetilde{R}}, \quad \partial_t\varrho + \operatorname{div}(\hbar\,\nabla\,\widetilde{S}\varrho) = 0,$$

$$\text{probability time marginal densities for } \varrho. \tag{80}$$

The problem (80) obviously tends formally with $\hbar \to 0$, where the time marginal densities are fixed, to the time-continuous deterministic mass transportation problem (32)

$$\int_0^T \int (\nabla S(t,x))^2\varrho\, dx\, dt \overset{!}{=} \text{Min},$$

$$\partial_t\varrho + \operatorname{div}(\nabla S\varrho) = 0,$$

$$\text{probability time marginal densities for } \varrho,$$

because we can substitute $\hbar v \hat{=} v$ in the space of possible solutions. Especially the minima will not change under such a substitution and will tend to each other for $\hbar \to 0^+$ as can be seen as follows. Let (S,ϱ) and $(S^\hbar,\varrho^\hbar)$ without restriction be differentiable minimizers of the deterministic, respectively the stochastic mass transportation problem. Then we have with $\varrho = e^{2\widetilde{R}}$, respectively $\varrho^\hbar = e^{2\widetilde{R}^\hbar}$,

$$\int_0^T \int (\nabla S)^2\varrho\, dx\, dt \leqslant \int_0^T \int (\nabla S^\hbar)^2\varrho^\hbar\, dx\, dt + \int_0^T \int \hbar^2(\nabla\widetilde{R}^\hbar)^2\varrho^\hbar\, dx\, dt \leqslant \int_0^T \int (\nabla S)^2\varrho\, dx\, dt + \int_0^T \int \hbar^2(\nabla\widetilde{R})^2\varrho\, dx\, dt.$$

The square root of the quantum mechanical action tends to the Wasserstein distance given in Sec. III A.

Proposition 44: (Case of compactified time marginal densities.) Let $0 < \hbar \leqslant 1$ be given. An observer associated to this $\hbar$ solves the problem

$$\int_0^T \int (\hbar^2(v(t,X_t)^2) + \hbar^2(\nabla R(t,X_t))^2)\, dP\, dt \overset{!}{=} \text{Min},$$

$$dX_t = b(t,X_t)dt + \sqrt{\hbar}dB_t,$$

$$(B_t,P) \text{ Brownian motion},$$

$$\text{probability time marginal densities } \varrho_{0/T} \text{ for } \varrho$$

$$(\text{i.e., } \varrho\, dx = P[X_t \in dx] = e^{(2/\hbar)R}dx, \quad \partial_t\varrho + \operatorname{div}(\hbar v\varrho) = 0). \tag{81}$$

If $\hbar$ is very small now, then also the time marginal densities for ϱ are compactified. For $\hbar \to 0$ this will lead to a compactification of the time marginal densities $\varrho_{0/T}^{\hbar}$ of the problem for $\hbar$ at their expectation values, which may exist, i.e., there will be a compactification to the Dirac measures of the expectations. This is modeled by

$$\varrho_{0/T}^{\hbar}(x) := \varrho_{0/T}\left(\frac{1}{h(\hbar)}(x - EX_t) + EX_t\right)\left(\frac{1}{h(\hbar)}\right)^n,$$

with $h(\hbar) \to 0$ for $\hbar \to 0$, which can be chosen appropriately. The by $(1/h(\hbar))^n$ normalized transformed time marginal densities are again probability densities in $\mathbb{R}^n$. For a "zoomed out" $\hbar$ we so obtain the problem

$$\int_0^T \int (\hbar^2(v(t,x)^2) + \hbar^2(\nabla R(t,x))^2)\varrho \, dx \, dt \overset{!}{=} \text{Min},$$

$$\varrho = e^{(2/\hbar)R}, \quad \partial_t \varrho + \operatorname{div}(\hbar v \varrho) = 0,$$

$$\varrho(0,x) = \varrho_0^{\hbar}(x), \quad \varrho(T,x) = \varrho_T^{\hbar}(x). \tag{82}$$

The new time marginal densities define a *zoomout*. The problem (82) tends formally for $\hbar \to 0$ to the deterministic mass transportation with delta distribution time marginal densities, because we can substitute $\hbar v \widehat{=} v$, i.e.,

$$\int_0^T \int (v(t,x)^2)\varrho \, dx \, dt \overset{!}{=} \text{Min},$$

$$\partial_t \varrho + \operatorname{div}(v\varrho) = 0, \quad \varrho(0,x) = \delta_{E_0}(x), \quad \varrho(T,x) = \delta_{E_1}(x),$$

$$E_0 = \int x\varrho_0(x) \, dx, \quad E_1 = \int x\varrho_1(x) \, dx.$$

But this problem is solved by the Euclidean geodesic between the expectation values of ϱ_0 and ϱ_T. A macroscopical observer with a very small $\hbar$, who observes a microscopical motion, will therefore visualize a Euclidean geodesic.

Remark 45: The connection of both cases can be seen by considering a large number of bosonic particles and executing a zoomout according to Proposition 44, whereby a cloud of bosonic particles appears.

B. Interpretation

The following "explanations" cannot be understood as well. But it should be emphasized clearly that to find a model for the quantum mechanical measurement problem is serious, besides the fact that a contradiction to human reason may be the case.

Interpretation 46: The Yasue problem (with elementary Lagrangian)

$$\delta\left(\int E\left(\frac{1}{4}b^2(t,X_t) + \frac{1}{4}b_*^2(t,X_t) - V(X_t)\right) dt\right) \overset{!}{=} 0$$

under certain variational formalisms is known in stochastic mechanics. See e.g., Ref. 30 where in V.5 the variant

$$\delta\left(\int E\left(\frac{1}{2}b(t,X_t)b_*(t,X_t) - V(X_t)\right) dt\right) \overset{!}{=} 0$$

is discussed. Because $b=u+v$ and $b_*=v-u$ this problem is just the Guerra-Marato problem because of Remark 27b). In Ref. 30 it is explained that the Guerra-Morato variation leads to the stochastic Hamilton-Jacobi equation, as demonstrated in sec. IV A. The equation is called the Madelung fluid equation there. New in this paper is that it was discovered that the Guerra-Morato problem, analogously to the deterministic case, is obtained by applying a stochastic Legendre transformation to the Yasue problem. The variation of the so-obtained Hamiltonian problem leads to the Schrödinger equation, which can be understood as suitable complex-valued unition of continuity and stochastic Hamilton-Jacobi equation. The transformation

$$\psi = e^{(1/\hbar)(R+iS)} \rightleftarrows (\varrho, b),$$

Fokker - Plank equation:

$$\partial_t \varrho + \operatorname{div}(b\varrho) - \frac{\hbar}{2}\Delta\varrho = 0$$

shall be called the *Madelung transformation*.

Compared to the Yasue problem, where the backward derivative term has to be interpreted, the Lagrangian quasi-Euclidean Yasue problem

$$\delta\left(\int E\left(\frac{1}{2}b^2(t,X_t) - V(X_t)\right)dt - \Delta\text{Entrop}\right) \overset{!}{=} 0$$

is clearly recognizable as a geometric problem. It has the advantage that it has the "pure" form of a geodesic functional

$$\delta\left(\int \langle \dot{x}_t, \dot{x}_t\rangle \, dt\right) \overset{!}{=} 0.$$

The time derivative in $\dot{x}$ has to be interpreted as validity of an Itô diffusion equation.

By the geodesic problem Schrödinger's basic law of nature can be found by a reasonable formalism.

The transition to the Yasue problem can be understood as time-symmetric variant.

The entropy time marginal term is stationary irrelevant, but it belongs to the "(B_t, P)" in the Itô equation

$$dX_t = b(t,X_t)\, dt + dB_t,$$

because the heat flow equation is the gradient flow for the entropy functional. Furthermore, it enters in the entropy action law, such that energy is preserved. Note that $(X_t, \bar{P})$ induces a natural time orientation by the direction of the entropic expansion.

The here demonstrated zoomout formalism shows how the classical geodesic formalism is "superficial" to the stochastic formalism. Compared to semiclassical analysis,[36–38] where the limit $\hbar \to 0$ is considered, in the transition of stochastic to deterministic mass transportation, the geodesic variational problems transfer. In comparison to semiclassical analysis, where, e.g., the behavior of the spectrum of the Schrödinger operator is analyzed for $\hbar \to 0$, the stochastic geodesic problem shows the direct geometric connection to the classical case, therefore hits the problem much more directly, and casts a new bright light on the quantum mechanical correspondence principle. Especially the theory does not try to model the particle phenomena by single trajectories of the underlying path space; the particle phenomena is obtained by a zoomout projection.

The background field hypothesis in Ref. 10 is replaced allusively by a, compared to set theoretic topology, more difficult treatment of a theory of a topological view. As suggested in Remark 19 an absolute entropic expansion is given at the outset and every observed drift, respectively diffusion movement, is a subjective interpretation of a single one-particle phase. The solu-

tion of the stochastic geodesic problem leads to an observer as defined in Remark 19. Especially we do not have an observer-independent motion within this concept, as, e.g., in set theoretic topology. There is no information of reality without observation. There is an equivalence principle, which states that information and reality are one and the same. We have to note that this concept is just mathematically obvious, especially concerning the fact that the quantum mechanical measurement problematic consists of experimentally proven contradictions to human reason. This general topological concept may not be seen as mathematically ensured and has to be found in detail.

For a more physical treatment of the analytical side of the Hamiltonian problem, see Ref. 39.

For an interesting nonquantum mechanical physical application of stochastic mechanics to the constitution of the system of planets, the morphology of galaxies and the formation of wind zones and the rings of planets study Ref. 40.

VII. EXAMPLES

Example 1: Wave packets. Let the potential V in the Hamilton operator be equal to zero. Then the planar waves $Ae^{i(\vec{k}\cdot\vec{r}-\omega t)}$ are solutions of the Schrödinger equation, where the wave vector $\vec{k}$, $\omega=\frac{1}{2}\hbar^2k^2$, and A a constant normalization factor are given. By superposition we obtain the wave packets

$$\psi(t,\vec{r}) = \frac{1}{(2\pi)^{n/2}} \int \hat{\psi}_0(\vec{k}) e^{i(\vec{k}\cdot\vec{r}-\omega(\vec{k})t)}\, d\vec{k}; \quad \omega(\vec{k}) = \frac{1}{2}\hbar^2k^2 \tag{83}$$

as solutions, as can be easily shown. $\psi_0(\vec{r})$ is the Fourier transformation of $\hat{\psi}_0(\vec{k})$:

$$\psi_0(\vec{r}) = \frac{1}{(2\pi)^{n/2}} \int \hat{\psi}_0(\vec{k}) e^{i(\vec{k}\cdot\vec{r})}\, d\vec{k}.$$

The Schrödinger equation with trivial potential is the necessary and sufficient stationarity condition for the Hamiltonian version of the stochastic mass transportation problem. Therefore, in analogy, the wave packets are stochastic Euclidean geodesics.

Example 2: Hydrogen atom. (See Ref. 41.) The Hamilton operator of the hydrogen atom (in $\mathbb{R}^3$) is defined by $H=-(\hbar^2/2m)\Delta+Ze^2/|x|$, with system constants e, Z and the reduced mass m. We consider the ground state given by

$$\psi(t,x) = Ne^{(-|x|/a-iEt/\hbar)} = e^{(\hbar/m)(R+iS)}, \tag{84}$$

$a=\hbar^2/me^2Z$ is the Bohr radius and $E=-\hbar^2/2ma^2$ is the ground state energy. The normalization constant N can be shown to be equal to $2a$, but is unimportant to calculate the entropic, respectively the current velocity, because

$$Ne^{(-|x|/a-iEt/\hbar)} = e^{\ln N+(-|x|/a-iEt/\hbar)} = e^{(m/\hbar)(R+iS)}$$

Therefore

$$\frac{m}{\hbar}R = \ln N - \frac{|x|}{a}, \text{ respectively } \frac{m}{\hbar}\, S = \frac{Et}{\hbar},$$

and the gradient of a constant term is equal to zero such that we have the drift

$$b = \nabla\,(R+S) = \frac{-\hbar}{am}\,\nabla\,|x| = -\frac{\hbar x}{am|x|}.$$

The ground state diffusion equation fulfills $[(t,x)\mapsto x/|x| \in L^{\infty} \overset{1.1.10}{\Rightarrow} \exists$ of a weak solution$]$

$$dX_t = -\frac{\hbar}{am}\frac{X_t}{|X_t|}dt + \sqrt{\frac{\hbar}{m}}dB_t.$$

Then in this connection the analog of Newton's law holds for the reduced mass of the electron.

Proposition 47: We have on $\{X_t \neq 0\}$

$$mD_*DX_t = mDD_*X_t = \frac{m}{2}(DD_* + D_*D)X_t = -Ze^2\frac{X_t}{|X_t|^3}. \tag{85}$$

Proof: Because of the diffusion equation we see immediately that $DX_t = -(\hbar/am)(X_t/|X_t|)$ and $D_*X_t = +(\hbar/am)(X_t/|X_t|)$.

As in Sec. II A we have

$$D(f(X_t)) = \nabla f(X_t)\cdot DX_t + \frac{\hbar}{2m}\Delta f(X_t),$$

$$D_*(f(X_t)) = \nabla f(X_t)\cdot D_*X_t - \frac{\hbar}{2m}\Delta f(X_t).$$

Especially for $f(x) = x/|x|$ we have $\nabla f\cdot DX_t = \nabla f\cdot D_*X_t = 0$ and $\Delta f(x) = -2x/|x|^3$, such that as in Corollary 24

$$DD_*X_t = D_*DX_t = -\frac{\hbar^2}{m^2 a}\frac{X_t}{|X_t|^3}.$$

Q.E.D.

Remark 48: The notation of mass and the treatment of mass for the transition from Lagrangian to Hamiltonian formalism in general is an open problem. For simplicity we can set $m=1$.

Example 3: Harmonic oscillator. The one-dimensional, normalized harmonic oscillator is given by the Hamilton operator $H = -\frac{1}{2}(\partial^2/\partial x^2) + \frac{1}{2}x^2$. The function

$$\psi(t,x) = \exp\left(-\frac{1}{2}(x - ae^{-it})^2 - \frac{a^2}{4}(1 - e^{-2it}) - \frac{it}{2}\right) = e^{R+iS}, \quad a \in \mathbb{R},$$

solves the one-dimensional Schrödinger equation $i(\partial\psi/\partial t) = -\frac{1}{2}(\partial^2\psi/\partial x^2) + \frac{1}{2}x^2\psi$. We see

$$R = -\frac{1}{2}(x^2 - 2ax\cos t) + \mathrm{Konst}(t),\ S = -\frac{1}{2}(2ax\sin t) + \mathrm{Konst}(t),$$

respectively

$$b = \frac{\partial}{\partial x}(R+S) = (-x + a\cos(t) - a\sin(t)),$$

$$b_* = \frac{\partial}{\partial x}(S-R) = (+x - a\cos(t) - a\sin(t)).$$

The diffusion equation belonging to b [$|b| \leqslant \mathrm{Konst}(1+|x|) \overset{1.1.10}{\Rightarrow} \exists$ of a weak solution] is given by

$$dX_t = (-X_t + a\cos(t) - a\sin(t))dt + dB_t.$$

We calculate

$$DD_*X_t = Db_* = \left(b\partial_x + \partial_t + \frac{1}{2}\frac{\partial^2}{\partial x^2}\right)b_* = +b + a\sin t - a\cos t = -x$$

and

$$D_*DX_t = D_*b = \left(b_*\partial_x + \partial_t - \frac{1}{2}\frac{\partial^2}{\partial x^2}\right)b = -b_* - a\sin t - a\cos t = -x$$

as in Corollary 24.

Example 4: Heisenberg's uncertainty relation. Heisenberg's uncertainty relation is the historic characteristic feature of time continuous quantum mechanical behavior. Expectation of momentum and spatial localization never can be measured sharply at the same time. The focus of one variable immediately implies that the other smears. It can be shown that this inequality follows more or less elementarily from the formalism developed in this paper, as was suggested in Ref. 9 for the case of dimension $n=1$, but was not executed concretely. Especially the entropy action law can be seen as a Lagrangian version of Heisenberg's uncertainty relation. This can be expressed by the fact that to focus we have to work against the entropy functional.

Lemma 49: (Special case of the Cramér-Rao inequality[42] for a probability variable that is the estimator of the parameter constituted by itself.) Let ϱ be a, in ∞, rapidly enough decreasing, differentiable probability density (of a probability variable X with first and second moments) in $\mathbb{R}^n$. Then we have [if $E(\nabla \ln \varrho(X))^2 < \infty$]

$$\text{variance}(\varrho) \geqslant \text{Fisherlength}^2(\varrho) := (E(\nabla \ln \varrho(X))^2)^{-1}.$$

Therefore the quadratic Fisher length is a measure for the minimal variance of a probability variable.

Proof: (1) We have

$$E\nabla \ln \varrho(X) = \int \nabla \ln \varrho(x)\varrho(x)\,\mathrm{dx} \overset{\text{in the i-th component}}{=} \int \partial_i \ln \varrho(x)\varrho(x)\,dx = \int \cdots \int \partial_i \varrho(x)\,dx_1 \cdots dx_n$$

$$= \int \cdots \int \left(\int \partial_i \varrho(x)\,dx_i\right) dx_1\, d\hat{x}_i\, dx_n = 0.$$

It follows that $E[(\nabla \ln \varrho(X) - E\nabla \ln \varrho(X))\cdot(X-EX)] = E[\nabla \ln \varrho(X)\cdot X]$.

(2) According to the Cauchy-Schwarz inequality we have

$$(E[(\nabla \ln \varrho(X) - E\nabla \ln \varrho(X))\cdot(X-EX)])^2 \leqslant E[(\nabla \ln \varrho(X) - E\nabla \ln \varrho(X))^2]E[(X-EX)^2],$$

i.e., with (1),

$$(E[\nabla \ln \varrho(X)\cdot X])^2 \leqslant \text{ variance } (\varrho)(\text{Fisherlength}^2\ (\varrho))^{-1}.$$

It is left to show (where without restriction ϱ decreases rapidly enough, such that we can shift ∂_i without spatial marginal terms)

$$(E[\nabla \ln \varrho(X)\cdot X])^2 = \left(\int \left(\sum_{i=1}^{n} \partial_i \varrho(x) x_i\right) dx\right)^2 = \left(-\int n\varrho(x)\,dx\right)^2 = n^2 \geqslant 1.$$

Q.E.D.

For concluding the uncertainty relation we define for the momentum operator (70) $p = -i\hbar\nabla$ in $\psi = e^{(1/\hbar)(R+iS)}$ (referring to a normalized solution of the Schrödinger equation)

$$\Delta p^2 \overset{\text{Formal}}{=} \langle (p-\langle p\rangle)^2\rangle \overset{\text{Formal}}{=} \langle p^2\rangle - \langle p\rangle^2 \overset{\text{Definition}}{=} \langle \psi, -\hbar^2\Delta_{\mathbb{C}}\psi\rangle - \langle \psi, (-i\hbar\nabla_{\mathbb{C}})\psi\rangle^2 = \langle \psi, -\hbar^2\Delta_{\mathbb{C}}\psi\rangle - \left(\int |\psi|^2(\nabla S - i\nabla R)\, dx\right)^2$$

(The term $\int |\psi|^2 \nabla R\, dx = 0$ according to the lemma .)

$$= \langle \psi, -\hbar^2\Delta_{\mathbb{C}}\psi\rangle - \left(\int |\psi|^2 \nabla S\, dx\right)^2 \overset{\text{As in } 3.2}{=} \int ((\nabla S)^2 + (\nabla R)^2)|\psi|^2\, dx - \left(\int |\psi|\nabla S\, dx\right)^2$$

$$= \int \left((\nabla S)^2 + \left(\frac{\hbar}{2}\nabla \ln|\psi|^2\right)^2\right)|\psi|^2\, dx - \left(\int |\psi|^2 \nabla S\, dx\right)^2 \geqslant \frac{\hbar^2}{4}\int (\nabla \ln|\psi|^2)^2|\psi|^2\, dx$$

$$= \frac{\hbar^2}{4}(\text{Fisherlength}^2(|\psi|^2))^{-1}$$

where the estimation is done by the Schwarz inequality in $L^2(|\psi|^2)$,

$$\left(\int \nabla S|\psi|^2\, dx\right)^2 \leqslant 1\int (\nabla S)^2|\psi|^2\, dx.$$

With Lemma 49 we can conclude Heisenberg's uncertainty relation

$$\Delta p\Delta x \geqslant \frac{\hbar}{2},$$

where $\Delta x^2 = \text{variance}(|\psi|^2)$, i.e., Δx is the standard deviation.

Remark 50: (a) As can be seen in the proof of the lemma the more sharp estimations

$$\text{variance}(\varrho) \geqslant n^2\ \text{Fisherlength}^2(\varrho), \quad \text{respectively } \Delta p\Delta x \geqslant \frac{n\hbar}{2},$$

hold true.

(b) The fact that the expectation of the entropic velocity disappears identically is a corollary of its own interest.

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PT-invariant periodic potentials with a finite number of band gaps

Avinash Khare
Institute of Physics, Sachivalaya Marg, Bhubaneswar 751005, India

Uday Sukhatme
Department of Physics, State University of New York at Buffalo, Buffalo, New York 14260

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We obtain the band edge eigenstates and the midband states for the complex, generalized associated Lamé potentials $V^{PT}(x)=-a(a+1)m\,\mathrm{sn}^2(y,m)-b(b+1)m\,\mathrm{sn}^2(y+K(m),m)-f(f+1)m\,\mathrm{sn}^2(y+K(m)+iK'(m),m)-g(g+1)m\,\mathrm{sn}^2(y+iK'(m),m)$, where $y\equiv ix+\beta$, and there are four parameters a, b, f, g. By construction, this potential is PT-invariant since it is unchanged by the combined parity (P) and time reversal (T) transformations. This work is a substantial generalization of previous work with the associated Lamé potentials $V(x)=a(a+1)m\,\mathrm{sn}^2(x,m)+b(b+1)m\,\mathrm{sn}^2(x+K(m),m)$ and their corresponding PT-invariant counterparts $V^{PT}(x)=-V(ix+\beta)$, both of which involving just two parameters a,b. We show that for many integer values of a,b,f,g, the PT-invariant potentials $V^{PT}(x)$ are periodic problems with a finite number of band gaps. Further, using supersymmetry, we construct several additional, complex, PT-invariant, periodic potentials with a finite number of band gaps. We also point out the intimate connection between the above generalized associated Lamé potential problem and Heun's differential equation. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2000207]

I. INTRODUCTION

In the past few years, Bender and others[1,2] have looked at several complex potentials with PT-symmetry, that is, potentials which remain invariant under the combined parity (P) and time reversal (T) operations. They have shown that the energy eigenvalues are real when PT-symmetry is unbroken, whereas they occur in complex conjugate pairs when PT-symmetry is spontaneously broken. However, there have been relatively few papers discussing periodic potentials with PT-symmetry.[3,4] Recently, we[4] have constructed several classes of analytically solvable, complex, PT-invariant, periodic potentials with the special feature that they possess just a finite number of band gaps. The purpose of this paper is to substantially increase this list of solvable periodic potentials.

A few years ago, we obtained the band edges of the associated Lamé (AL) potentials[5]

$$V(x) = a(a+1)m\,\mathrm{sn}^2(x,m) + b(b+1)m\,\mathrm{sn}^2(x+K(m),m)$$
$$= a(a+1)m\,\mathrm{sn}^2(x,m) + b(b+1)m\frac{\mathrm{cn}^2(x,m)}{\mathrm{dn}^2(x,m)}. \quad (1)$$

Here, $\mathrm{sn}(x,m)$, $\mathrm{cn}(x,m)$, $\mathrm{dn}(x,m)$ are Jacobi elliptic functions with elliptic modulus parameter $m(0\leqslant m\leqslant 1)$. They are doubly periodic functions with periods $[4K(m),i2K'(m)]$, $[4K(m), 2K(m)+i2K'(m)]$, $[2K(m),i4K'(m)]$, respectively (Ref. 13), where $K(m)\equiv\int_0^{\pi/2}\mathrm{d}\theta[1-m\sin^2\theta]^{-1/2}$ denotes the complete elliptic integral of the first kind, and $K'(m)\equiv K(1-m)$. For simplicity, from now on, we will not explicitly display the modulus parameter m as an argument of Jacobi elliptic functions. It was shown that the AL potentials with integral values of a, b are periodic potentials with a finite number of band gaps.[6] We also constructed and studied the

PT-invariant potentials $V^{PT}(x) \equiv -V(ix+\beta)$ obtained from the AL potentials via the anti-isospectral transformation of variables $x \to ix+\beta$.[4]

In this paper, we make a substantial generalization of our previous work. We consider the four parameter family of generalized associated Lamé (GAL) potentials

$$\begin{aligned} V(x) &= a(a+1)m\,\mathrm{sn}^2(x,m) + b(b+1)m\,\mathrm{sn}^2(x+K(m),m) + f(f+1)m\,\mathrm{sn}^2(x+K(m)+iK'(m),m) \\ &\quad + g(g+1)m\,\mathrm{sn}^2(x+iK'(m),m) \\ &= a(a+1)m\,\mathrm{sn}^2(x,m) + b(b+1)m\frac{\mathrm{cn}^2(x,m)}{\mathrm{dn}^2(x,m)} + f(f+1)\frac{\mathrm{dn}^2(x,m)}{\mathrm{cn}^2(x,m)} + g(g+1)\frac{1}{\mathrm{sn}^2(x,m)}. \end{aligned} \tag{2}$$

In contrast to the AL potentials of Eq. (1) where there are two parameters a,b and the two terms correspond to real translations of the independent variable x by 0 and $K(m)$, the GAL potentials of Eq. (2) have four parameters a,b,f,g and the four terms correspond to complex translations of the independent variable x by 0, $K(m)$, $K(m)+iK'(m)$, $iK'(m)$. Although the GAL potentials are real, they do have singularities on the real axis coming from the zeros of the Jacobi elliptic functions $\mathrm{sn}(x)$ and $\mathrm{cn}(x)$ in the last two terms. Consequently, we will focus our attention on the PT-invariant versions of the GAL potentials, which are given by

$$\begin{aligned} V^{PT}(x) &= -a(a+1)m\,\mathrm{sn}^2(y,m) - b(b+1)m\,\mathrm{sn}^2(y+K(m),m) - f(f+1)m\,\mathrm{sn}^2(y+K(m)+iK'(m),m) \\ &\quad - g(g+1)m\,\mathrm{sn}^2(y+iK'(m),m) \\ &= -a(a+1)m\,\mathrm{sn}^2(y,m) - b(b+1)m\frac{\mathrm{cn}^2(y,m)}{\mathrm{dn}^2(y,m)} - f(f+1)\frac{\mathrm{dn}^2(y,m)}{\mathrm{cn}^2(y,m)} - g(g+1)\frac{1}{\mathrm{sn}^2(y,m)} \\ &\equiv [a(a+1),b(b+1),f(f+1),g(g+1)], \end{aligned} \tag{3}$$

where

$$y = ix + \beta, \tag{4}$$

with β being an arbitrary constant. We shall frequently use the notation $[a(a+1),\ b(b+1),\ f(f+1),\ g(g+1)]$ to denote $V^{PT}(x)$. In this notation, PT-invariant ordinary Lamé potentials are denoted by $[a(a+1),\ 0,\ 0,\ 0]$, and PT-invariant AL potentials are denoted by $[a(a+1),\ b(b+1),\ 0,\ 0]$. Here, the arbitrary constant β is chosen so as to avoid the singularities of the Jacobi elliptic functions on the real axis. We show that several of these periodic potentials for specific integer values of a,b,f,g have a finite number of band gaps. Looking at the symmetry of these potentials, we are in fact tempted to conjecture that many (and perhaps all) of these potentials with integral values of the parameters a,b,f,g also have a finite number of band gaps. It would be nice if this conjecture could be proved.

In addition, we also discover a huge class of midband states when at least one of the parameters a,b,f,g is half-integral. As a special case, we find some new midband eigenstates of the associated Lamé potentials. Further, we show that the Schrödinger equation for the generalized AL potential is intimately connected with the celebrated Heun's differential equation.[7] In fact, using the exact solutions obtained in this paper, one can immediately obtain the corresponding solutions of Heun's equation. In another related paper,[8] we use this connection and discover a wide class of new quasiperiodic solutions of Heun's equation.

Finally, using the exact eigenstates of the GAL potentials (3) and the machinery of supersymmetric quantum mechanics,[9] we construct several more potentials with finite band-gaps. There is one important point involved here using which we are in fact able to construct many more supersymmetric partner potentials corresponding to a given potential. The key point to note is that normally, in supersymmetric quantum mechanics,[9] given a potential $V_-(x)$, the ground state wave function $\psi_0(x)$ is used to construct the superpotential $W(x) = -\psi_0'(x)/\psi_0(x)$, which then yields the supersymmetric (SUSY) partner potential $V_+(x) = W^2 + W'$. If one uses any excited state wave function $\psi(x)$ of $V_-(x)$ to construct a superpotential $W(x)$, then the original potential $V_-(x)$ is

recovered correctly (by construction), but the corresponding partner potential $V_+(x)$ turns out to be singular on the real x-axis due to the zeros of the excited state wave function $\psi(x)$. However, as has been noticed recently,[10] if we consider PT-symmetric complex potentials, then the singularity is not on the real axis. Besides, as we have stressed previously,[4,11] in the case of doubly periodic potentials composed of Jacobi elliptic functions, both $V(x)$ and $V^{\mathrm{PT}}(x)$ can be simultaneously periodic even though their periods are different. In this way, by starting from the analytically solvable Lamé and associated Lamé potentials and using the excited state band edges of the corresponding PT-symmetric potentials, we discover a wide range of analytically solvable, complex PT-invariant periodic potentials with a finite number of band gaps. As an illustration, we discuss a few of these potentials in detail.

The plan of the paper is the following. In Sec. II we discuss the PT-invariant GAL potentials (3) in some detail and obtain band edges as well as midband states of several of these potentials. As a byproduct we also obtain some solutions of the AL potentials (which we had missed in earlier work[5,6]). Further, we show that the class of potentials $[a(a+1), 0, 0, g(g+1)]$ have finite number of band gaps in case a,g are integers. In Sec. III we start from the energy eigenstates obtained in Sec. II and using both the ground state as well as excited state wave functions, obtain periodic PT-invariant potentials with a finite number of band gaps. In Sec. IV we briefly discuss the connection between the solutions of the potentials (3) and Heun's differential equation.

II. SOLUTIONS FOR THE GENERALIZED ASSOCIATED LAMÉ (GAL) POTENTIALS

A few years ago, we obtained analytic solutions of the associated Lamé potentials (1)[5,6] and showed that when a,b are integers, then the resulting potentials all had a finite number of band gaps. The purpose of this section is to show that the complex PT-invariant GAL potentials as given by Eq. (3) are also quasiexactly solvable. In particular, we show that the band edges or midband states of these problems can be obtained depending on whether $a+b+f+g$ (or $a-b-f-g$) is an integer or an arbitrary noninteger number. It should be noted that we are considering PT-invariant potentials (3), since the corresponding real potentials (2) are singular on the real axis.

It may be worthwhile explaining the underlying basic idea here, even though it has been well established by us before.[4] Note that if $\psi(x)$ is a solution of the Schrödinger equation for the real potential $V(x)$ with energy E, then $\psi(ix+\beta)$ is a solution of the Schrödinger equation for the complex potential $-V(ix+\beta)$ with energy $-E$, where β is an arbitrary nonzero constant. The potential $-V(ix+\beta)$, generated by the anti-isospectral transformation $x \to ix+\beta$,[12] is clearly PT symmetric and will be denoted by $V^{\mathrm{PT}}(x)$. Further, if $\psi(x)$ and $\psi(ix+\beta)$ satisfy appropriate boundary conditions, they are eigenfunctions of $V(x)$ and $V^{\mathrm{PT}}(x)$, respectively. The ordering of energy levels for $V^{\mathrm{PT}}(x)$ is the opposite of the ordering of energy levels for $V(x)$.

In this paper, our main focus is on the Schrödinger equation ($\hbar=2m=1$)

$$-\frac{d^2}{dx^2}\psi(x) + V^{\mathrm{PT}}(x)\psi(x) = E\psi(x), \tag{5}$$

where $V^{\mathrm{PT}}(x)$ is the potential given by Eq. (3). Equation (5) is called the generalized associated Lamé equation, and we are seeking its eigenstates and midband states.

A. Symmetries

At this stage, it is worth pointing out the symmetries of the PT-invariant GAL potential (3) and hence the corresponding Schrödinger equation (5).

(1) The potential (3) and hence the Schrödinger equation (5) remains unchanged when any one (or more) of the four parameters a,b,f,g change to $-a-1$, $-b-1$, $-f-1$, $-g-1$, respectively.
(2) Under the translation $y \to y+K(m)$, the GAL potential $[a(a+1),b(b+1),f(f+1),g(g+1)]$ goes to the potential $[b(b+1), a(a+1), g(g+1), f(f+1)]$. Hence, both GAL potentials must have the same energy eigenvalues and the corresponding energy eigenfunctions are simply related, $y \to y+K(m)$, i.e.,

$$E^{\mathrm{PT}}(b,a,g,f;m) = E^{\mathrm{PT}}(a,b,f,g;m), \quad \psi(y,b,a,g,f;m) \propto \psi(y+K(m),a,b,f,g;m). \tag{6}$$

(3) Similarly, by considering the translations $y \to y+K(m)+iK'(m)$, and $y \to y+iK'(m)$, it is easy to show that

$$E^{\mathrm{PT}}(f,g,a,b;m) = E^{\mathrm{PT}}(a,b,f,g;m), \quad \psi(y,f,g,a,b;m) \propto \psi(y+K(m)+iK'(m),a,b,f,g;m), \tag{7}$$

$$E^{\mathrm{PT}}(g,f,b,a;m) = E^{\mathrm{PT}}(a,b,f,g;m), \quad \psi(y,g,f,b,a;m) \propto \psi(y+iK'(m),a,b,f,g;m). \tag{8}$$

Thus, once we obtain the eigenvalues and eigenfunctions of a given GAL potential $[a(a+1),b(b+1),f(f+1),g(g+1)]$, then we immediately know the eigenvalues and eigenfunctions of three other potentials, $[b(b+1),a(a+1),g(g+1),f(f+1)]$, $[f(f+1),g(g+1),a(a+1),b(b+1)]$, and $[g(g+1),f(f+1),b(b+1),a(a+1)]$. Therefore, it suffices to present results for only one of the four potentials.

B. Duality relations

We shall now derive some remarkable relations relating the quasiexactly solvable eigenvalues and eigenfunctions (corresponding either to the band edges or midband states) of two GAL potentials at two different values m and $1-m$ of the modulus parameter.

To that purpose we start from the Schrödinger equation (5) for the PT-invariant GAL potential (3). On using the relations[13]

$$\sqrt{m}\,\mathrm{sn}(y,m) = -\,\mathrm{dn}[iy+K'(m)+iK(m),1-m],$$

$$\mathrm{dn}(y,m) = \sqrt{1-m}\,\mathrm{sn}[iy+K'(m)+iK(m),1-m], \tag{9}$$

$$\sqrt{m}\,\mathrm{cn}(y,m) = i\sqrt{1-m}\,\mathrm{cn}[iy+K'(m)+iK(m),1-m],$$

and defining a variable $w=iy+K'(m)+iK(m)$, the Schrödinger equation (5) takes the form

$$\psi''(w) - \left[a(a+1)(1-m)\mathrm{sn}^2(w,1-m) + g(g+1)(1-m)\frac{\mathrm{cn}^2(w,1-m)}{\mathrm{dn}^2(w,1-m)} + f(f+1)\frac{\mathrm{dn}^2(w,1-m)}{\mathrm{cn}^2(w,1-m)} + b(b+1)\frac{1}{\mathrm{sn}^2(w,1-m)} \right]\psi(w) = -[a(a+1)+b(b+1)+f(f+1)+g(g+1)+E]\psi(w). \tag{10}$$

On comparing Eqs. (5) and (10) we then have the remarkable relations

$$E^{\mathrm{PT}}(a,b,f,g,m) = -[a(a+1)+b(b+1)+f(f+1)+g(g+1)] - E^{\mathrm{PT}}(a,g,f,b,1-m),$$
$$\psi(y,m) \propto \psi(iy+K'(m)+iK(m),1-m), \tag{11}$$

which is valid for the QES states corresponding to either the band edges or midband states. Note that here, a,b,f,g can be arbitrary (real) numbers and are not restricted to integer values. This is a very powerful relation which has several interesting consequences. One immediate important consequence of Eq. (11) is that for arbitrary integer values of a,g, the potential $[a(a+1),0,0,g(g+1)]$ has only a finite number of band gaps. This happens because, for $f=g=0$, one has

$$E^{\mathrm{PT}}(a,b,0,0,m) = -[a(a+1)+b(b+1)] - E^{\mathrm{PT}}(a,0,0,g=b,1-m), \tag{12}$$

so that both the potentials must have the same number of band edges and band gaps and we have already proved[6] that the AL potentials have a finite number of band gaps in case a,b are integers.

C. QES solutions

Let us now seek solutions of the Schrödinger Equation (5) for the PT-invariant GAL potential (3). On making the ansatz

$$\psi(x) = \mathrm{dn}^{-b}(y)\mathrm{sn}^{-g}(y)\mathrm{cn}^{-f}(y)\,\phi(y), \quad y = ix + \beta, \tag{13}$$

it is easily shown that ϕ satisfies the equation

$$\phi''(y) + 2\left[mb\frac{\mathrm{sn}(y)\mathrm{cn}(y)}{\mathrm{dn}(y)} - g\frac{\mathrm{cn}(y)\mathrm{dn}(y)}{\mathrm{sn}(y)} + f\frac{\mathrm{dn}(y)\mathrm{sn}(y)}{\mathrm{cn}(y)}\right]\phi'(y) + [Qm\,\mathrm{sn}^2(y) - R]\phi(y) = 0, \tag{14}$$

where

$$Q = (b+g+f)(b+g+f-1) - a(a+1), \quad R = E + (f+g)^2 + m(g+b)^2. \tag{15}$$

It is well known[14] that this is a quasiexactly solvable (QES) problem. We shall now systematically consider solutions of Eq. (14) for several special cases and then finally consider the most general case.

D. $b=f=g=0$

The simplest possibility is when three out of the four parameters a,b,f,g are zero. For example, when $b=f=g=0$, then the problem reduces to the PT-invariant version of the well-studied Lamé potential problem. We might add here that, instead of a, if any one of the other parameters b,f,g is nonzero, one still has a potential which is strictly isospectral to the PT invariant Lamé potential. It may be noted that while the Lamé potential is a periodic potential with (real) period $2K(m)$, the PT-invariant Lamé potential has real period $2K'(m)$. Further, the band-edge eigenvalues, eigenfunctions, and the discriminant Δ of $V^{\mathrm{PT}}(x)$ are related to those of Lamé potential by[4]

$$E_j^{\mathrm{PT}}(m) = -E_{2a-j}(m), \quad \psi_j^{\mathrm{PT}}(x,m) \propto \psi_{2a-j}(ix+\beta,m), \quad j = 0,1,2,\ldots,2a,$$
$$\Delta^{\mathrm{PT}}(E,m) = \Delta[E + a(a+1), 1-m]. \tag{16}$$

From Eq. (11), it follows that the PT-invariant Lamé band-edge eigenvalues and eigenfunctions, for integral a satisfy the remarkable relations ($j=0,1,2,\ldots,2a$)

$$E_j^{\mathrm{PT}}(m) = -a(a+1) - E_{2a-j}^{\mathrm{PT}}(1-m), \quad \psi_j(y,m) \propto \psi_{2a-j}(iy + K'(m) + iK(m), 1-m). \tag{17}$$

We would like to add here that even the midband states satisfy (for half-integral a) relations analogous to (17),

$$E_j(m) = a(a+1) - E_{a-1/2-j}(1-m), \quad \psi_j(y,m) \propto \psi_{a-1/2-j}(iy + K'(m) + iK(m), 1-m), \tag{18}$$

where $j=0,1,2,\ldots,a-1/2$. Note the remarkable fact that for any integer a, all bands and band gaps exchange their role as one goes from the Lamé potential to its PT-invariant version $V^{\mathrm{PT}}(x)$.[4]

The next simple possibility is when two of the four parameters a,b,f,g are zero. Here there are three distinct possibilities which we discuss one by one.

E. $f=g=0$

In this case the problem reduces to the PT-invariant AL potential which we have already discussed at great length.[5,6] Note that if either a or b is zero (or -1), then this potential reduces to the PT-invariant of the Lamé potential. As previously shown by us,[6] for arbitrary integral values of a and b, AL potentials are exactly solvable problems with finite number of band gaps for which one can write down the form of all the band-edge eigenfunctions, as we do below. We note here that when $a>b$ are both integers, then there are precisely a bound bands (some of which are

unusual in that both the band edges are of the same period), same (a) number of band gaps and all the $2a+1$ band edges are analytically known beyond which there is a continuum band extending to $E=\infty$. Note that if $b>a$, then also there are b bound bands and b band gaps and the corresponding eigenfunctions are simply obtained from the $a>b$ case by the transformation $x\to x+K(m)$ while the $a=b$ case essentially corresponds to the Lamé potential $[a(a+1),0,0,0]$. Without any loss of generality, we shall only consider AL potentials with $a>b$.

The form of the $2a+1$ band edge eigenfunctions of the AL potential depends on whether $a-b$ is an odd or an even integer. For example, when $b=a-2p-1$ ($p=0, 1, 2,\ldots$), then there are

$$p \text{ eigenstates of the form } \mathrm{sn}(x)\mathrm{cn}(x)\mathrm{dn}(x)F_{p-1}[\mathrm{sn}^2(x)],$$

$$p+1 \text{ eigenstates of the form } \mathrm{dn}^{a-2p}(x)F_p[\mathrm{sn}^2(x)],$$

$$a-p \text{ eigenstates of the form } \mathrm{cn}(x)\mathrm{dn}^{2p+1-a}(x)F_{a-p-1}[\mathrm{sn}^2(x)],$$

$$a-p \text{ eigenstates of the form } \mathrm{sn}(x)\mathrm{dn}^{2p+1-a}(x)F_{a-p-1}[\mathrm{sn}^2(x)].$$

On the other hand, when $b=a-2p$, there are

$$p \text{ eigenstates of the form } \mathrm{cn}(x)\mathrm{dn}^{a-2p+1}(x)F_{p-1}[\mathrm{sn}^2(x)],$$

$$p \text{ eigenstates of the form } \mathrm{sn}(x)\mathrm{dn}^{a-2p+1}(x)F_{p-1}[\mathrm{sn}^2(x)],$$

$$a-p \text{ eigenstates of the form } \mathrm{sn}(x)\mathrm{cn}(x)\mathrm{dn}^{2p-a}(x)F_{a-p-1}[\mathrm{sn}^2(x)],$$

$$a-p+1 \text{ eigenstates of the form } \mathrm{dn}^{2p-a}(x)F_{a-p}[\mathrm{sn}^2(x)].$$

Here $F_n[\mathrm{sn}^2(x)]$ denotes a polynomial in $\mathrm{sn}^2(x)$ of order n.

We would like to restate here that all the eigenstates of the PT-invariant version of the AL potentials are immediately obtained from the known eigenfunctions of the associated Lamé problem and the ordering of energy levels of these is the opposite of the corresponding AL problem. Hence, this is also an exactly solvable problem with a finite number (a) of band gaps and $2a+1$ known band edges when both a,b are integers.

F. $b=f=0$

Following our discussion for the AL case, without any loss of generality we assume here that $a>g$. In this case, one obtains $n+1$ QES solutions when $a+g=n$ (or $g-a=n+1$) with $n=01,2,\ldots$. The QES solutions for $n=0,1,2,3,4$ are given in Table I. In particular, for any choice of $a(a+1)$, Table I lists the eigenstates for various values of $g(g+1)$. The general form of these eigenfunctions is obtained from the corresponding AL eigenfunctions as given in Table 3 of Ref. 5 by simply interchanging $\mathrm{dn}(y)$ and $\mathrm{sn}(y)$.

A few remarks are in order.

(1) Since we are considering the case ($b=f=0$), the duality relation (11) takes the form

$$E^{\mathrm{PT}}(a,0,0,g;m) = -[a(a+1)+g(g+1)] - E^{\mathrm{PT}}(a,b=g,0,0;1-m),$$
$$\psi(y,a,0,0,g;m) \propto \psi(iy+K'(m)+iK(m),a,b=g,0,0;1-m). \tag{19}$$

Using Table 3 of Ref. 5 and this duality relation, it is straightforward to obtain all the QES eigenstates, thereby providing an independent check on the results given in Table I. Further, it follows that for arbitrary integer values of a and g, $[a(a+1),0,0,g(g+1)]$ is an exactly

TABLE I. Energy eigenstates of PT-invariant GAL potentials with $b=f=0$, $g=n-a$, $n=0, 1, 2,\ldots$;
$\delta_1 \equiv \sqrt{(1+m)^2(a-1)^2-(2a-1)(2a-3)m}$, $\delta_2 \equiv \sqrt{[a-1+m(a-2)]^2-(2a-1)(2a-5)m}$,
$\delta_3 \equiv \sqrt{[a-2+m(a-1)]^2-(2a-1)(2a-5)m}$, $\delta_4 \equiv \sqrt{(1+m)^2(a-2)^2-(2a-1)(2a-7)m}$.

n	$g(g+1)$	E	$\mathrm{sn}^{-a}(y)\psi$
0	$(a-1)a$	$-(1+m)a^2$	1
1	$(a-2)(a-1)$	$-a^2-m(a-1)^2$	$\frac{\mathrm{cn}(y)}{\mathrm{sn}(y)}$
1	$(a-2)(a-1)$	$-(a-1)^2-ma^2$	$\frac{\mathrm{dn}(y)}{\mathrm{sn}(y)}$
2	$(a-3)(a-2)$	$-(1+m)(a-1)^2$	$\frac{\mathrm{cn}(y)\mathrm{dn}(y)}{\mathrm{sn}^2(y)}$
2	$(a-3)(a-2)$	$-(1+m)(a^2-2a+2)\pm 2\delta_1$	$\frac{[E+(1+m)(a-2)^2]\mathrm{sn}^2(y)+2(2a-3)}{\mathrm{sn}^2(y)}$
3	$(a-4)(a-3)$	$-(a^2-2a+2)-(a^2-4a+5)m\pm 2\delta_2$	$\frac{[[E+(a-2)^2+m(a-3)^2]\mathrm{sn}^2(y)+2(2a-5)]\mathrm{cn}(y)}{\mathrm{sn}^3(y)}$
3	$(a-4)(a-3)$	$-(a^2-4a+5)-(a^2-2a+2)m\pm 2\delta_3$	$\frac{[[E+(a-3)^2+m(a-2)^2]\mathrm{sn}^2(y)+2(2a-5)]\mathrm{dn}(y)}{\mathrm{sn}^3(y)}$
4	$(a-5)(a-4)$	$-(1+m)(a^2-4a+5)\pm 2\delta_4$	$\frac{[[E+(1+m)(a-3)^2]\mathrm{sn}^2(y)+2(2a-7)]\mathrm{cn}(y)\mathrm{dn}(y)}{\mathrm{sn}^4(y)}$

solvable potential problem with a finite number (a) of bandgaps. From the duality relation (19), it follows that for integer values of a,g,

$$E_j^{\mathrm{PT}}(a,0,0,g;m) = -[a(a+1)+g(g+1)] + E_j(a,b=g,0,0;1-m), \tag{20}$$

and hence the corresponding discriminants Δ are related by

$$\Delta^{\mathrm{PT}}(E,m;a,0,0,g) = \Delta[E+a(a+1)+g(g+1),1-m;a,b=g,0,0]. \tag{21}$$

(2) Following the structure of the eigenfunctions of the AL potentials as given above, it is now straightforward to write down the general form of the eigenfunctions for arbitrary value of n. However, to obtain the corresponding eigenvalues, one needs to solve cubic and higher order equations.

(3) Under the transformation $y \to y+iK'(m)$ followed by the interchange of a and g (note $b=f=0$), the Schrödinger equation (5) for the GAL potential (3) remains unchanged. Thus it follows that under the interchange of a with g, the eigenvalue spectrum must remain unaltered. Clearly, this is only possible if either the energy eigenvalues remain unchanged under this transformation, or if two of the eigenvalues go into each other. It is easy to verify from Table I that the eigenvalues corresponding to the eigenfunctions of period $2iK'(m)$ remain unaltered under $a \to g$ while the other eigenvalues go into each other under this transformation.

(4) Similarly, From Table 3 of Ref. 5, it is easy to check that for the AL potentials (1), the eigenvalues corresponding to the eigenfunctions of period $2K(m)$ remain unaltered under $a \to b$ while the other eigenvalues go into each other under this transformation. This happens because the AL potentials remain unaltered under the transformation $y \to y+K(m)$ followed by the interchange of a with b.

Summarizing, we have discovered exactly solvable potential problems with a finite number of band gaps when a,g are arbitrary integers. In fact everything about these potentials can be derived from previously known results for AL potentials.

TABLE II. Energy eigenstates of PT-invariant GAL potentials with parameters $b=g=0$, $f=n-a$, $n=0, 1, 2,\ldots$; $\delta_5\equiv\sqrt{(a-1+m)^2-(2a-1)m}$, $\delta_6\equiv\sqrt{(a-1+2m)^2-3(2a-1)m}$, $\delta_7\equiv\sqrt{(a-2+2m)^2-(2a-1)m}$, $\delta_8\equiv\sqrt{(a-2+3m)^2-3(2a-1)m}$.

n	$f(f+1)$	E	$\mathrm{cn}^{-a}(y)\psi$
0	$(a-1)a$	$-a^2$	1
1	$(a-2)(a-1)$	$-a^2-m$	$\frac{\mathrm{sn}(y)}{\mathrm{cn}(y)}$
1	$(a-2)(a-1)$	$-(a-1)^2-m$	$\frac{\mathrm{dn}(y)}{\mathrm{cn}(y)}$
2	$(a-3)(a-2)$	$-(a-1)^2-4m$	$\frac{\mathrm{dn}(y)\mathrm{sn}(y)}{\mathrm{cn}^2(y)}$
2	$(a-3)(a-2)$	$-(a^2+2-2a+2m)\pm 2\delta_5$	$\frac{(E+(a-2)^2)\mathrm{sn}^2(y)+2}{\mathrm{cn}^2(y)}$
3	$(a-4)(a-3)$	$-(a^2+2-2a+5m)\pm 2\delta_6$	$\frac{[(E+(a-2)^2+m)\mathrm{sn}^2(y)+6]\mathrm{sn}(y)}{\mathrm{cn}^3(y)}$
3	$(a-4)(a-3)$	$-(a^2+5-4a+5m)\pm 2\delta_7$	$\frac{[(E+(a-3)^2+m)\mathrm{sn}^2(y)+2]\mathrm{dn}(y)}{\mathrm{cn}^3(y)}$
4	$(a-5)(a-4)$	$-(a^2+5-4a+10m)\pm 2\delta_8$	$\frac{[(E+(a-3)^2+4m)\mathrm{sn}^2(y)+6]\mathrm{dn}(y)\mathrm{sn}(y)}{\mathrm{cn}^4(y)}$

G. $b=g=0$

In this case, one obtains $n+1$ QES solutions when $a+f=n$ with $n=0,1,2,\ldots$. The solutions for $n=0,1,2,3,4$ are given in Table II. In particular, for any choice of $a(a+1)$, Table II lists the eigenstates for various values of $f(f+1)$. The general form of these eigenfunctions is simply obtained from the corresponding AL eigenfunctions as given in Table 2 of Ref. 5 by interchanging $\mathrm{dn}(y)$ and $\mathrm{cn}(y)$.

Some comments are in order at this stage.

(1) The form of eigenfunctions for arbitrary value of n is easily written down following the structure of the AL eigenfunctions given in the preceding section.

(2) From Eq. (11) it follows that the potential (3) with $b=g=0$ is a self-dual potential, satisfying

$$E_{j_1}^{\mathrm{PT}}(a,f,m) = -[a(a+1)+f(f+1)] - E_{j_2}^{\mathrm{PT}}(a,f,1-m). \tag{22}$$

Using Table II, it is easily checked that indeed this is true, for any values of a,f. In particular, whereas δ_5,δ_8 are invariant under $m\to 1-m$, $\delta_6\leftrightarrow\delta_7$ under the same transformation.

(3) Under the transformation $y\to y+K(m)+iK'(m)$ followed by the interchange of a and f (note $b=g=0$), the Schrödinger equation (5) for the GAL potential (3) remains unchanged. Thus it follows that under the interchange of a with f, the eigenvalue spectrum must remain unaltered. Clearly, this is only possible if either the energy eigenvalues remain unchanged under this transformation, or if two of the eigenvalues go into each other. It is easy to verify from Table II that the eigenvalues corresponding to the eigenfunctions of period $2K(m)+2iK'(m)$ remain unaltered under $a\to f$ while the other eigenvalues go into each other under this transformation. In particular, while δ_5,δ_8 are invariant under $a\leftrightarrow f$, $\delta_6\leftrightarrow\delta_7$ under the same transformation.

TABLE III. Energy eigenstates of PT-invariant GAL potentials with $f=0$, $g=n-a-b$, $n=0, 1, 2,\ldots$; $\delta_9 \equiv \sqrt{[(1+m)(a-1)+b]^2-(2a-1)(2a+2b-3)m}$, $\delta_{10} \equiv \sqrt{[a+b-1+m(a-2)]^2-(2a-1)(2a+2b-5)m}$.

n	E	$\mathrm{dn}^b(y)\mathrm{sn}^{-(a+b)}(y)\psi$
0	$-(a+b)^2-ma^2$	1
1	$-(a+b)^2-m(a-1)^2$	$\frac{\mathrm{cn}(y)}{\mathrm{sn}(y)}$
2	$-(1+m)-(a+b-1)^2-m(a-1)^2\pm 2\delta_9$	$\frac{[E+(a+b-2)^2+m(a-2)^2]\mathrm{sn}^2(y)+2(2a+2b-3)}{\mathrm{sn}^2(y)}$
3	$-(1+m)-(a+b-1)^2-m(a-2)^2\pm 2\delta_{10}$	$\frac{[[E+(a+b-2)^2+m(a-3)^2]\mathrm{sn}^2(y)+2(2a+2b-5)]\mathrm{cn}(y)}{\mathrm{sn}^3(y)}$

H. $f=0$

Let us consider the case when only one out of the four parameters a,b,f,g is zero. As an illustration, we discuss the case $f=0$. In fact, as described below, once we know the eigenstates of this problem, the eigenstates of the other three problems corresponding to either b or g or a equal to zero are immediately obtainable, since the four potentials are related by translations of the independent variable.

For the case $f=0$, one obtains $(n+2)/2[(n+1)/2]$ QES solutions when n is even [odd]. Here $a+b+g=n$ with $n=0,1,2,\ldots$. The QES solutions for $n=0,1,2,3$ are given in Table III. In particular, for any choice of $a(a+1)$, Table III lists the eigenstates for various values of $(b+g)(b+g+1)$.

Some remarks are appropriate.

(1) By looking at the structure of the QES eigenfunctions in Table III, it is easy to write down the nature of eigenfunctions for the general case.

(2) From Table III, it is easily checked that the duality relation

$$E^{\mathrm{PT}}(a,b,g,m) = -[a(a+1)+b(b+1)+g(g+1)] - E^{\mathrm{PT}}(a,g,b,1-m) \tag{23}$$

is indeed satisfied. In particular, both δ_9,δ_{10} are invariant under $b \leftrightarrow g$ followed by $m \to 1-m$.

(3) Under the transformation $y \to y+K(m)$ followed by the interchange of a and b, and replacing g by f, the Schrödinger equation (5) for the GAL potential (3) with $f=0$ goes over to the Schrödinger equation for the GAL potential (3) with $g=0$. Hence, under the interchange of a and b and replacing g by f, all the energy eigenvalues of the potential (3) with $f=0$ must go over into those of (3) with $g=0$, while the corresponding eigenfunctions are simply obtained from Table III by replacing y by $y+K(m)$.

(4) Using similar reasoning it also follows that under the interchange of a with g and replacing b by f, all the energy eigenvalues of the GAL potential (3) with $f=0$ go over to those of potential (3) with $b=0$ while the corresponding eigenfunctions are obtained from Table III by replacing y by $y+iK'(m)$. And finally, under the interchange of b with g and replacing a by f, all the energy eigenvalues of the GAL potential (3) with $f=0$ go over to those of potential (3) with $a=0$, while the corresponding eigenfunctions are easily obtained from Table III by replacing y by $y+K(m)+iK'(m)$.

TABLE IV. Energy eigenstates of PT-invariant GAL potentials with $f=2n-a-b-g$, $n=0, 1, 2,\ldots$; $\delta_{11}\equiv\sqrt{[(a+b-1)+m(1-b-g)]^2-(2a-1)(1-2g)m}$.

n	E	$\mathrm{sn}^g(y)\mathrm{dn}^b(y)\mathrm{cn}^{-(a+b+g)}(y)\psi$
0	$-(a+b)^2-m(g+b)^2$	1
1	$-(a+b-1)^2-m(b+g-1)^2-(1+m)\pm 2\delta_{11}$	$\dfrac{[E+(a+b-2)^2+m(b+g)^2]\mathrm{sn}^2(y)-2(2g-1)}{\mathrm{cn}^2(y)}$

I. The general case: *a*,*b*,*f*,*g* all nonzero

Finally, let us discuss the most general case when all four parameters are nonzero. In this case one obtains $n+1$ solutions when $a+b+f+g=2n$ with $n=0,1,2,\ldots$. The QES solutions for $n=0$, 1 are given in Table IV.

(1) It is easy to see that in the general case, the eigenfunction is of the form

$$\psi=\mathrm{sn}^{-g}(y)\mathrm{cn}^{-f}(y)\mathrm{dn}^{-b}(y)\sum_{k=0}^{n}A_k\,\mathrm{sn}^{2k}(y), \tag{24}$$

while the corresponding eigenvalues are solutions of a $n+1$th order equation.

(2) It can be checked from Table IV that δ_{11} is invariant under $b\leftrightarrow g$ followed by $m\rightarrow 1-m$.

(3) The GAL potential (3) and hence the corresponding Schrödinger equation (5) is invariant under the transformation $y\rightarrow y+K(m)$ followed by the interchange of a with b and f with g. Hence, under the interchange of a with b and f with g, all the eigenvalues of the GAL system must either remain invariant or go into each other. In fact it is easily checked from Table IV that all the eigenvalues are invariant under the interchange of a with b and f with g. Extending this argument, in fact one finds that all the eigenvalues are also invariant under $a\leftrightarrow f$, $b\leftrightarrow g$ as well as under $a\leftrightarrow g$, $b\leftrightarrow f$.

J. Midband states

So far we have discussed the results for the PT-invariant GAL potentials, which give eigenvalues and eigenfunctions corresponding to the band edges. It may be noted that in all these cases, while a,b,f,g need not be integers, either $a+b+f+g$ or $a-b-f-g$ is always integral. We now show that when at least one of a, b, f, g is half-integral and either $a+b+f+g$ and/or $a-b-f-g$ is an arbitrary number (being an integer is of course a very special case here), then one can obtain doubly degenerate eigenstates which correspond to midband states. In fact depending on whether we want b or f or g to be half-integral (with the other two parameters being integral), we need to use different trial solutions. Therefore, we shall consider all three cases one by one.

Case 1. b half-integral: We start from Eq. (14) and further substitute the ansatz

$$\phi(y)=[\mathrm{cn}(y)+i\,\mathrm{sn}(y)]^tZ(y), \tag{25}$$

where t is any real number. After lengthy but straightforward algebra, one can show that $Z(y)$ satisfies the equation

$$Z''(y)+\left[2it\,\mathrm{dn}(y)+2mb\frac{\mathrm{sn}(y)\mathrm{cn}(y)}{\mathrm{dn}(y)}-2g\frac{\mathrm{cn}(y)\mathrm{dn}(y)}{\mathrm{sn}(y)}+2f\frac{\mathrm{dn}(y)\mathrm{sn}(y)}{\mathrm{cn}(y)}\right]Z'(y)+\left[-(R+t^2)\right.$$
$$\left.+(Q+t^2)m\,\mathrm{sn}^2(y)-2itg\frac{\mathrm{cn}(y)}{\mathrm{sn}(y)}+2itf(1-m)\frac{\mathrm{sn}(y)}{\mathrm{cn}(y)}+imt(2b+2f+2g-1)\mathrm{sn}(y)\mathrm{cn}(y)\right]Z(y)$$
$$=0, \tag{26}$$

where R and Q are as given by Eq. (15). Not surprisingly, $Z(y)=$constant is a solution with energy $E=-(4t^2+m)/4$ provided $f=g=0$, $b=1/2$, $a=t-1/2$ (i.e., $b+f+g=1/2$).

One can build solutions for higher values of $b+f+g$ from here. In particular, for $b+f+g=2M+1/2$, we consider the ansatz ($M=0,1,2,\ldots$)

$$Z(y)=\sum_{k=0}^{M} A_k\,\mathrm{sn}^{2k}(y)+\mathrm{cn}(y)\mathrm{sn}(y)\sum_{k=0}^{M-1} B_k\,\mathrm{sn}^{2k}(y), \tag{27}$$

while if $b+f+g=2M+3/2$ then we consider the ansatz ($M=0,1,2,\ldots$)

$$Z(y)=\mathrm{cn}(y)\sum_{k=0}^{M} A_k\,\mathrm{sn}^{2k}(y)+\mathrm{sn}(y)\sum_{k=0}^{M} B_k\,\mathrm{sn}^{2k}(y). \tag{28}$$

Substitution into Eq. (26) and simplification yields analytic expressions for the energy eigenvalues and eigenfunctions for arbitrary M for $b=1/2$ and $b=3/2$. In particular, for $b=1/2$, we find that

$$b=1/2,\quad f=p,\quad f+g=N,\quad a=t-1/2,\quad E=-[t^2+m(g+b)^2], \tag{29}$$

where both f,g are non-negative integers satisfying $f+g=N$ with $N=0,1,2,\ldots$.

Similarly, when $b=3/2$, $a=t-1/2$, $f=p$, $f+g=N$ we find that

$$E=m(2g+1)-[1+t^2+m(g+b)^2]\pm\sqrt{(2g+1)^2m^2+4m(N+1)(f-g)+4(1-m)t^2}, \tag{30}$$

where, f and g are again non-negative integers. In all these cases, the corresponding eigenfunctions have the form as given above in Eqs. (27) and (28). For small values of N, the explicit coefficients A_k,B_k appearing in the eigenfunction expressions can be easily written down. For example, for $b=1/2$ and $N=1$, the eigenfunction is $Z(y)=A\,\mathrm{cn}(y)+B\,\mathrm{sn}(y)$ with $A/B=it$ in case $f=1$, $g=0$ while $B/A=-it$ in case $g=1$, $f=0$.

For the special case of $f=g=0$ and $t\neq 1/2$, these results represent the generalization of results obtained by us previously[6] in the case of AL potential. Further, for $f=g=0$, $t=1/2$, the results obtained above match with the energy eigenvalue expressions obtained in Ref. 6 (as they should).

Several comments can be readily made.

(1) Since, in the variable y, the GAL potential (3) has period $2K(m)$ as well as $2iK'(m)$, hence $\psi(y)$ and $\psi(y+2K(m))$ as well as $\psi(y+2iK'(m))$ are all eigenfunctions of the GAL equation with the same eigenvalue. As a consequence, $\phi(y)=[\mathrm{cn}(y)-i\,\mathrm{sn}(y)]^tZ(y)$ is also the eigenfunction with the *same* eigenvalue. Thus for any nonintegral t, each level is doubly degenerate. The same remark also applies to the other two solutions (when f or g is half-integral) discussed below.

(2) There is one remarkable symmetry associated with Eq. (26). In particular, notice that this equation is invariant under $t\to -t$ followed by $i\to -i$ (where $i=\sqrt{-1}$). But under this transformation, the ansatz (25) becomes

$$\phi(y)=[\mathrm{cn}(y,m)-i\,\mathrm{sn}(y,m)]^{-t}. \tag{31}$$

Hence it follows that the energy eigenvalues must be independent of sign of t, i.e., they must be a function of t^2. Similar remarks also apply in the other two cases discussed below (i.e., when f,g are half-integral).

(3) For integral t, both a,b are half-integral and these solutions reduce to those discussed in the preceding section and in that case they correspond to QES band-edge eigenstates.

(4) Here we have obtained solutions $\psi(y)$ in which $a=t-1/2$, $f=p$, $g=N-p$, and $b=1/2$ or $3/2$. In view of the symmetries of the GAL potentials, we then also have solutions $\psi(y+K(m))$ with the same energy in the case $b=t-1/2$, $g=p$, $f=N-p$, and a is either $1/2$ or $3/2$. Similarly we have solutions $\psi(y+K(m)+iK'(m))$ with the same energy in the case $f=t-1/2$, $a=p$, $b=N-p$, and $g=1/2$ or $3/2$. Further, we also have solutions $\psi(y+iK'(m))$ with the same energy in the case $g=t-1/2$, $a=N-p$, $b=p$, and $f=1/2$ or $3/2$.

Case 2. f half-integral: We start from Eq. (14) and further substitute the ansatz

$$\phi(y) = [\mathrm{dn}(y) + ik\,\mathrm{sn}(y)]^t Z(y), \tag{32}$$

where t is any real number and $k=\sqrt{m}$. After some lengthy but straightforward algebra, one finds that $Z(y)$ satisfies the equation

$$Z''(y) + \left[2ikt\,\mathrm{cn}(y) + 2mb\frac{\mathrm{sn}(y)\mathrm{cn}(y)}{\mathrm{dn}(y)} - 2g\frac{\mathrm{cn}(y)\mathrm{dn}(y)}{\mathrm{sn}(y)} + 2f\frac{\mathrm{dn}(y)\mathrm{sn}(y)}{\mathrm{cn}(y)} \right] Z'(y) + \left[-(R+mt^2) + (Q+t^2)m\,\mathrm{sn}^2(y) - 2itkg\frac{\mathrm{dn}(y)}{\mathrm{sn}(y)} - 2iktb(1-m)\frac{\mathrm{sn}(y)}{\mathrm{dn}(y)} + ikt(2b+2f+2g-1)\mathrm{sn}(y)\mathrm{dn}(y) \right] Z(y) = 0, \tag{33}$$

where R and Q are as given by Eq. (15). Not surprisingly, $Z(y)=$constant is a solution with energy $E=-(4mt^2+1)/4$ provided $b=g=0$, $f=1/2$, $a=t-1/2$ (i.e. $b+f+g=1/2$).

One can build solutions for higher values of $b+f+g$ from here. In particular, in the case $b+f+g=2M+1/2$, we consider the ansatz ($M=0,1,2,\ldots$)

$$Z(y) = \sum_{k=0}^{M} A_k\,\mathrm{sn}^{2k}(y) + \mathrm{sn}(y)\mathrm{dn}(y)\sum_{k=0}^{M-1} B_k\,\mathrm{sn}^{2k}(y), \tag{34}$$

while if $b+f+g=2M+3/2$ then we consider the ansatz ($M=0,1,2,\ldots$)

$$Z(y) = \mathrm{dn}(y)\sum_{k=0}^{M} A_k\,\mathrm{sn}^{2k}(y) + \mathrm{sn}(y)\sum_{k=0}^{M} B_k\,\mathrm{sn}^{2k}(y). \tag{35}$$

On substituting this ansatz in Eq. (33) and making algebraic simplifications, we obtain analytic expressions for the energy eigenvalues and eigenfunctions for arbitrary M for $f=1/2$ and $f=3/2$. In particular, for $f=1/2$, we find that

$$f = 1/2, \quad b+g=N, \quad a=t-1/2, \quad E=-[mt^2+(g+f)^2], \tag{36}$$

where both b,g are non-negative integers satisfying $b+g=N$ with $N=0,1,2,\ldots$.

Similarly, when $f=3/2$, $a=t-1/2$, $b+g=N$ we find that

$$E = (2g+1) - [(1+t^2)m + (g+f)^2] \pm \sqrt{(2g+1)^2 + 4m(N+1)(b-g) - 4m(1-m)t^2}, \tag{37}$$

where, b and g are again non-negative integers. In all these cases, the corresponding eigenfunctions have the form as given above in Eqs. (34) and (35). For small values of N, the explicit coefficients A_k, B_k in the eigenfunction expressions can be easily written down. Further, as in the half-integral b case, one can write down three more solutions with the same energy.

Case 3. g half-integral: We start from Eq. (14) and further substitute the ansatz

$$\phi(y) = [\mathrm{dn}(y) + k\,\mathrm{cn}(y)]^t Z(y), \tag{38}$$

where t is any real number. After algebraic simplification, it is easy to show that $Z(y)$ satisfies the equation

$$Z''(y) + \left[-2kt\,\mathrm{sn}(y) + 2mb\frac{\mathrm{sn}(y)\mathrm{cn}(y)}{\mathrm{dn}(y)} - 2g\frac{\mathrm{cn}(y)\mathrm{dn}(y)}{\mathrm{sn}(y)} + 2f\frac{\mathrm{dn}(y)\mathrm{sn}(y)}{\mathrm{cn}(y)} \right] Z'(y) + \left[-R + (Q+t^2)m\,\mathrm{sn}^2(y) - 2ktb\frac{\mathrm{cn}(y)}{\mathrm{dn}(y)} - 2ktf\frac{\mathrm{dn}(y)}{\mathrm{cn}(y)} + kt(2b+2f+2g-1)\mathrm{cn}(y)\mathrm{dn}(y) \right] \times Z(y) = 0, \tag{39}$$

where R and Q are as given by Eq. (15). Not surprisingly, $Z(y)=$constant is a solution with energy $E=-(1+m)/4$ provided $b=f=0$, $g=1/2$, $a=t-1/2$ (i.e., $b+f+g=1/2$).

One can build solutions for higher values of $b+f+g$ from here. In particular, in the case $b+f+g=2M+1/2$, we consider the ansatz ($M=0,1,2,\ldots$)

$$Z(y)=\sum_{k=0}^{M} A_k\,\mathrm{sn}^{2k}(y)+\mathrm{cn}(y)\mathrm{dn}(y)\sum_{k=0}^{M-1} B_k\,\mathrm{sn}^{2k}(y), \tag{40}$$

while if $b+f+g=2M+3/2$ then we consider the ansatz ($M=0,1,2,\ldots$)

$$Z(y)=\mathrm{cn}(y,m)\sum_{k=0}^{M} A_k\,\mathrm{sn}^{2k}(y)+\mathrm{dn}(y)\sum_{k=0}^{M} B_k\,\mathrm{sn}^{2k}(y). \tag{41}$$

Substituting this ansatz in Eq. (39) and simplifying, one gets analytic expressions for the energy eigenvalues and eigenfunctions for arbitrary M for $b=1/2$ and $b=3/2$. In particular, for $b=1/2$, we find that

$$g=1/2,\quad b+f=N,\quad a=t-1/2,\quad E=-[(f+g)^2+m(g+b)^2], \tag{42}$$

where both b,f are non-negative integers satisfying $b+f=N$ with $N=0,1,2,\ldots$.

Similarly, when $g=3/2$, $a=t-1/2$, $b+f=N$ we find that

$$E=1+2f+(2b+1)m-[(f+g)^2+m(g+b)^2]\pm\sqrt{(1-m)[(2f+1)^2-(2b+1)^2m]+4mt^2}, \tag{43}$$

where, b and f are again non-negative integers. In all these cases, the corresponding eigenfunctions have the form as given in Eqs. (40) and (41). For small values of N, the coefficients A_k,B_k appearing in the eigenfunctions can be easily written down. Further, as in the half-integral b case, one can write down three more solutions with the same energy.

III. SUPERSYMMETRY AND POTENTIALS WITH A FINITE NUMBER OF BAND GAPS

We shall now start with the ground state as well as the excited state eigenfunctions of various PT-invariant GAL potentials discussed in the preceding section and using supersymmetry obtain the corresponding SUSY partner potentials. In this manner, we obtain many periodic potentials $V_+(x)$ with a finite number of band gaps. As emphasized in the introduction, unlike real potentials, if we take a complex PT-invariant potential, then even if we start with an excited state wave function and calculate the corresponding superpotential W, the singularities in W and hence $V_+(x)$ are not on the real axis, and do not cause problems.

A. Supersymmetry partners of PT-invariant Lamé potentials

The simplest case is when only one parameter, (say a) is nonzero. This gives the PT-invariant Lamé potential

$$V(x)=-a(a+1)m\,\mathrm{sn}^2(y). \tag{44}$$

For concreteness, take $a=1$, which yields $V(x)=-2m\,\mathrm{sn}^2(y)$. Here, the three band-edge eigenfunctions (in order of increasing energy eigenvalues) are $\mathrm{sn}(y)$, $\mathrm{cn}(y)$, $\mathrm{dn}(y)$. It is easily computed that corresponding to these three eigenstates, the corresponding partner potentials (up to a constant) are $V_+(x)=-2m\,\mathrm{sn}^2(y+K(m))$, $-2m\,\mathrm{sn}^2(y+iK'(m))$, $-2m\,\mathrm{sn}^2(y+K(m)+iK'(m))$ which are all strictly isospectral potentials to the original Lamé potential. Thus, in this case we do not obtain any different solvable potentials by using supersymmetry.

Now consider the case $a=2$. All the five band-edge eigenvalues and eigenfunctions of the PT-invariant Lamé potential $V(x)=-6m\,\mathrm{sn}^2(y)$ have already been given by us in Table 4 of Ref. 11. Starting from any of the five band-edge eigenfunctions and calculating the corresponding

TABLE V. The five supersymmetric partner potentials of the PT-invariant Lamé potential $V_-^{PT}(x)=-6m\,\mathrm{sn}^2(y)$. Here $y=ix+\beta$ and $\delta\equiv\sqrt{1-m+m^2}$. All partner potentials have a period $2K'(m)$.

E	$\psi^{(-)}$	$V_+(x)$
$-2(1+m)-2\delta$	$1+\frac{E}{2}\,\mathrm{sn}^2(y)$	$6m\,\mathrm{sn}^2(y)+E-\frac{2E^2\mathrm{sn}^2(y)\mathrm{cn}^2(y)\mathrm{dn}^2(y)}{\left(1+\frac{E}{2}\mathrm{sn}^2(y)\right)}$
$-4-m$	$\mathrm{sn}(y)\mathrm{cn}(y)$	$-2m[\mathrm{sn}^2(y)+\mathrm{sn}^2(y+K(m)+iK'(m))+\mathrm{sn}^2(y+iK'(m)]-E$
$-1-4m$	$\mathrm{sn}(y)\mathrm{dn}(y)$	$-2m[\mathrm{sn}^2(y)+\mathrm{sn}^2(y+K(m))+\mathrm{sn}^2(y+iK'(m)]-E$
$-1-m$	$\mathrm{cn}(y)\mathrm{dn}(y)$	$-2m[\mathrm{sn}^2(y)+\mathrm{sn}^2(y+K(m))+\mathrm{sn}^2(y+K(m)+iK'(m)]-E$
$-2(1+m)+2\delta$	$1+\frac{E}{2}\,\mathrm{sn}^2(y)$	$6m\,\mathrm{sn}^2(y)+E-\frac{2E^2\,\mathrm{sn}^2(y)\mathrm{cn}^2(y)\mathrm{dn}^2(y)}{\left(1+\frac{E}{2}\mathrm{sn}^2(y)\right)}$

superpotentials, we obtain five different supersymmetric partner potentials all of which have the same band-edge energy eigenvalues as given in Table 4 of Ref. 11. In Table V we have given the expressions for these five different strictly isospectral potentials. It is worth noting that out of these five potentials, three are self-isospectral—they are the PT-invariant GAL potentials [2,2,2,0]. Hence, truly speaking, we only have three genuinely different potentials, all having the same band-edge energies. For each of these cases, using the formalism of supersymmetric quantum mechanics,[9] we can easily obtain expressions for the corresponding five eigenstates. Now, again by starting from these eigenfunctions, we can construct still different partner potentials but with identical band edges. In this way, one could construct a large number of periodic potentials with five band edges and two band gaps, all strictly isospectral to the PT-invariant Lamé potential (44) with $a=2$.

Similarly, if we consider the PT-invariant Lamé potential (44) with $a=3$, then we have seven band-edge eigenfunctions and eigenvalues all of which are analytically known and are given in Table 1 of Ref. 4. Again, using supersymmetry, we can obtain seven different partner potentials V_+ all with the same band-edge eigenvalues. By starting from any one of them and using other eigenfunctions recursively, we can in principle construct a huge class of isospectral potentials. Particular mention may be made of the case when we start from the eigenfunction $\mathrm{sn}(y)\mathrm{cn}(y)\mathrm{dn}(y)$ of the potential $V(x)=-12m\,\mathrm{sn}^2(y)$. It is easily shown that the corresponding partner potential V_+ (up to a constant) is given by

$$V(x)=-m[6\,\mathrm{sn}^2(y)+2\,\mathrm{sn}^2(y+K(m))+2\,\mathrm{sn}^2(y+iK'(m))+2\,\mathrm{sn}^2(y+K(m)+iK'(m))]. \tag{45}$$

Thus, we see that the PT-invariant GAL potential [6,2,2,2] has precisely three bands, three band gaps, and seven band edges, since it is the supersymmetric partner of the PT-invariant Lamé potential (44) with $a=3$. The process described above is readily extended to any Lamé potential with integer a. We can start from any of the $2a+1$ band edges and obtain the corresponding supersymmetric partner potentials all having the same band edges.

We have shown that the SUSY partners of the PT-invariant Lamé potentials [6,0,0,0] and [12,0,0,0] are the potentials [2,2,2,0] and [6,2,2,2], respectively. What about the higher Lamé potentials? In this connection, it is amusing to notice that the band edges of the PT-invariant Lamé potential [20,0,0,0] and the potential [6,6,6,2] (which follow from Table IV) are identical. For example, out of nine band edges, the six band-edge energy eigenvalues of [20,0,0,0] are given by

$$E = -5(m+2) \pm \sqrt{4m^2 - 9m + 9}, \quad E = -5(1+m) \pm 2\sqrt{4m^2 + m + 4},$$
$$E = 5(1+2m) \pm 2\sqrt{9m^2 - 9m + 4}. \tag{46}$$

It is easily seen from Table IV that exactly the same eigenvalues are obtained when a,b,f,g take the values (2,2,−3,1), (2,−3,2,1), (−3,2,2,1). Similarly, one can show that the three remaining eigenvalues of [20,0,0,0] satisfy the same cubic equation as [6,6,6,2] when a, b, f, g take the values (2,2,2,−2).

In fact, one can show that the number (and structure) of band edges of the PT-invariant Lamé potential $[2a(2a+1),0,0,0]$ is the same as the QES states of the potential $[a(a+1), a(a+1), a(a+1), (a-1)a]$. For example, for this PT-invariant Lamé potential it is well known that out of the $4a+1$ band edges of the Lamé potential, a states each are of the form $\mathrm{cn}(y)\mathrm{sn}(y)F_{a-1}(\mathrm{sn}^2(y))$, $\mathrm{cn}(y)\mathrm{dn}(y)F_{a-1}(\mathrm{sn}^2(y))$, $\mathrm{dn}(y)\mathrm{sn}(y)F_{a-1}(\mathrm{sn}^2(y))$, while the remaining $a+1$ states are of the form $F_a(\mathrm{sn}^2(y))$. Using Table IV, it is easily shown that there are again $4a+1$ QES states of the potential $[a(a+1), a(a+1), a(a+1), (a-1)a]$, out of which a QES states each are obtained when a,b,f,g are of the form a, a, $a-1$, $a-1$, or a, $a-1$, a, $a-1$, or $a-1,a,a,a-1$, while $a+1$ QES states are obtained when a, b, f, g are of the form a, a, a, $-a$. In fact we believe that all the band-edge eigenvalues of the potentials $[2a(2a+1),0,0,0]$ and $[a(a+1), a(a+1), a(a+1), (a-1)a]$ are identical. While this is easily shown for low values of a, at the moment, a general proof is still lacking.

Similarly, one can show that the number (as well as the structure) of band edges of the PT-invariant Lamé potential $[(2a-1)2a,0,0,0]$ is the same as the QES states of the potential $[a(a+1), (a-1)a, (a-1)a, (a-1)a]$. For example, it is well known that out of the $4a-1$ band edges of the PT-invariant Lamé potential, a states each are of the form $\mathrm{cn}(y)F_{a-1}(\mathrm{sn}^2(y))$, $\mathrm{dn}(y)F_{a-1}(\mathrm{sn}^2(y))$, $\mathrm{sn}(y)F_{a-1}(\mathrm{sn}^2(y))$, while the remaining $a-1$ states are of the form $\mathrm{sn}(y)\mathrm{cn}(y)\mathrm{dn}(y)F_{a-2}(\mathrm{sn}^2(y))$. Using Table IV, it is easily shown that there are $4a-1$ QES states of the potential $[a(a+1),(a-1)a,(a-1)a,(a-1)a]$, out of which a QES states each are obtained when a,b,f,g are of the form a, $-a$, $a-1$, $a-1$, or a, $a-1$, $-a$, $a-1$, or a, $a-1$, $a-1$, $-a$, while $a-1$ QES states are obtained when a, b, f, g are of the form $-a-1$, $a-1$, $a-1$, $a-1$. In fact we believe that all the band-edge eigenvalues of the potentials $[(2a-1)2a,0,0,0]$ and $[a(a+1),(a-1)a,(a-1)a, (a-1)a]$ are identical. While this is easily shown for low values of a, a general proof is not available.

On the basis of these results, we then conjecture that the potentials $[a(a+1), a(a+1), a(a+1), (a-1)a]$, for integer a, have the same band edges as the Lamé potential $[2a(2a+1), 0, 0, 0]$ and hence these potentials also have precisely $2a$ band gaps and $(4a+1)$ band edges, all of which are known in principle. Further, the potentials $[a(a+1), (a-1)a, (a-1)a, (a-1)a]$ have the same band edges as the Lamé potential $[(2a-1)2a, 0, 0, 0]$ and hence are also potentials with a finite number $(2a-1)$ of band gaps. It would be nice to have a general proof.

B. Supersymmetry partners of PT-invariant associated Lamé potentials

We start our discussion with the $a=2$, $b=1$ associated Lamé potential and its corresponding PT-invariant potential $V^{\mathrm{PT}}(x) = -6m\,\mathrm{sn}^2(y) - 2m\,\mathrm{cn}^2(y)/\mathrm{dn}^2(y)$. All five band-edge eigenvalues and eigenfunctions for this potential have been given by us in Table 3 of Ref. 11. As established previously,[5,11] this is a self-isospectral potential and hence using the band-edge eigenfunction $\mathrm{dn}^2(y)$ does not give any partner potential. However, if instead we use the remaining four band-edge eigenfunctions, then one gets four SUSY partner potentials which are strictly isospectral to the PT-invariant [6,2,0,0] potential.

Let us now consider the PT-invariant AL potential $[a(a+1),(a-2)(a-1),0,0]$, i.e., the potential (3) with $b=a-2$, $f=g=0$. As shown by us,[5] one of its exact band-edge eigenfunctions is $\psi(x) = \mathrm{cn}(y)\mathrm{dn}^{a-1}(y)$. It is easy to see that the corresponding partner potential V_+ (up to a constant) is the potential $[(a-1)a,(a-1)a,2,0]$. Thus we immediately conclude that the PT-invariant potential $[(a-1)a,(a-1)a,2,0]$ is strictly isospectral to the PT-invariant AL potential $[a(a+1),(a-2)(a$

$-1),0,0]$. In the special case when both a,b are integers, in view of our results on AL potentials,[6] it then follows that the GAL potential $[(a-1)a,\ (a-1)a,\ 2,\ 0]$ has a band gaps and a bands, out of which $b=a-2$ bands are rather unusual.

Note that if instead we use $\psi(x)=\mathrm{sn}(y)\mathrm{dn}^{a-1}(y,m)$, which is also one of the exact eigenfunctions of the above AL potential, then nothing different is obtained. In particular, the corresponding partner potential is $[(a-1)a,(a-1)a,0,2]$ which is strictly isospectral to the potential $[(a-1)a,\ (a-1)a,\ 2,\ 0]$.

Let us now consider the PT-invariant AL potential $[a(a+1),(a-3)(a-2),0,0]$, i.e., the potential (3) with $b=a-3$, $f=g=0$. As shown by us,[5] one of its exact band-edge eigenfunctions is $\psi(x)=\mathrm{sn}(y)\mathrm{cn}(y)\mathrm{dn}^{a-2}(y)$. It is easy to see that the corresponding partner potential V_+ (up to a constant) is the potential $[(a-1)a,(a-2)(a-1),2,2]$ in the notation of (3). Thus we immediately conclude that when a, b are integers, then this PT-invariant potential is strictly isospectral to the AL potential $[a(a+1),(a-3)(a-2),0,0]$, has a band gaps and a bands, out of which $b=a-3$ bands are rather unusual.

We can generalize the above arguments. In particular, we find that the number (and even structure) of the potentials $[(a-p)(a-p+1),(a-p-1)(a-p),p(p+1),p(p+1)]$ is the same as the AL potentials $[a(a+1),(a-2p-1)(a-2p),0,0]$. For example, as remarked in the preceding section, if $b=a-2p-1$ $(p=0,1,2,\ldots)$, then there are p eigenstates of the form $\mathrm{sn}(y)\mathrm{cn}(y)\mathrm{dn}(y)F_{p-1}(\mathrm{sn}^2(y))$, $p+1$ eigenstates of the form $\mathrm{dn}^{a-2p}(y)F_p(\mathrm{sn}^2(y))$, $a-p$ eigenstates of the form $\mathrm{cn}(y)\mathrm{dn}^{2p+1-a}(y)F_{a-p-1}(\mathrm{sn}^2(y))$, and also $a-p$ eigenstates of the form $\mathrm{sn}(y)\mathrm{dn}^{2p+1-a}(y)F_{a-p-1}(\mathrm{sn}^2(y))$. Using Table IV it is easy to show that for the GAL potential $[(a-p)(a-p+1),\ (a-p-1)(a-p),p(p+1),p(p+1)]$, there are p eigenstates of the form $\mathrm{sn}^{-p}(y)\mathrm{cn}^{-p}(y)\mathrm{dn}^{1+p-a}(y)F_{p-1}(\mathrm{sn}^2(y))$, $p+1$ eigenstates of the form $\mathrm{dn}^{a-p}(y)\mathrm{cn}^{-p}(y)\mathrm{sn}^{-p}(y)F_p(\mathrm{sn}^2(y))$, $a-p$ eigenstates of the form $\mathrm{cn}^{p+1}(y)\mathrm{sn}^{-p}(y)\mathrm{dn}^{p+1-a}(y)F_{a-p-1}(\mathrm{sn}^2(y))$, and also $a-p$ eigenstates of the form $\mathrm{sn}^{p+1}(y)\mathrm{cn}^{-p}(y)\mathrm{dn}^{p+1-a}(y)F_{a-p-1}(\mathrm{sn}^2(y))$. In fact we believe that all the band-edge eigenvalues of the potentials $[a(a+1),(a-2p)(a-2p+1),0,0]$ and $[(a-p)(a-p+1),(a-p-1)(a-p),\ p(p+1),p(p+1)]$ are identical. While this is easily shown for low values of a and p, a general proof is still lacking.

Similarly, we can show that the number (and even structure) of the potentials $[(a-p)(a-p+1),(a-p)(a-p+1),p(p+1),(p-1)p]$ is the same as the AL potentials $[a(a+1),(a-2p)(a-2p+1),0,0]$. In particular, for the AL potential, as shown in Sec. II, when $b=a-2p$, then there are p eigenstates of the form $\mathrm{cn}(x)\mathrm{dn}^{a-2p+1}(x)F_{p-1}(\mathrm{sn}^2(x))$, p eigenstates of the form $\mathrm{sn}(x)\mathrm{dn}^{a-2p+1}(x)F_{p-1}(\mathrm{sn}^2(x))$, $a-p$ eigenstates of the form $\mathrm{sn}(x)\mathrm{cn}(x)\mathrm{dn}^{2p-a}(x)F_{a-p-1}(\mathrm{sn}^2(x))$, and $a-p+1$ eigenstates of the form $\mathrm{dn}^{2p-a}(x)F_{a-p}(\mathrm{sn}^2(x))$. It is easily shown that for the potential $[(a-p)(a-p+1),(a-p)(a-p+1),p(p+1),(p-1)p]$, there are $4a-1$ QES states of similar form. In particular, there are p eigenstates of the form $\mathrm{sn}^{-p}(y)\mathrm{cn}^{1-p}(y)\mathrm{dn}^{p-a}(y)F_{p-1}(\mathrm{sn}^2(y))$, p eigenstates of the form $\mathrm{dn}^{a+1-p}(y)\mathrm{cn}^{1-p}(y)\mathrm{sn}^{-p}(y)F_{p-1}(\mathrm{sn}^2(y))$, $a-p+1$ eigenstates of the form $\mathrm{cn}^{p}(y)\mathrm{sn}^{-p}(y)\mathrm{dn}^{p-a}(y)F_{a-p}(\mathrm{sn}^2(y))$ and also $a-p$ eigenstates of the form $\mathrm{sn}^{p+1}(y)\mathrm{cn}^{1-p}(y)\mathrm{dn}^{p-a}(y)F_{a-p-1}(\mathrm{sn}^2(y))$. In fact we believe that all the band-edge eigenvalues of the potentials $[a(a+1),(a-2p)(a-2p+1),0,0]$ and $[(a-p)(a-p+1),(a-p)(a-p+1),p(p+1),(p-1)p]$ are identical. While this is easily shown for low values of a and p, we do not yet have a general proof.

C. SUSY partners of potentials with $b=f=0$

Let us now consider the SUSY partners of the potential $[a(a+1),0,0,g(g+1)]$ which for integral values of a,g, is a problem with a finite number of band gaps. By exactly following the above discussion about the PT-invariant AL potential, we can construct a host of potentials with a finite number of band gaps. For example, by starting from the potential $[6,0,0,2]$ and following the procedure as in the AL case, we can easily obtain four SUSY partner potentials, all with two band gaps.

From Table I we observe that for integral a, two of the exact eigenfunctions of the potential $[a(a+1),0,0,(a-2)(a-1)]$ with a band gaps are $\mathrm{cn}(y)\mathrm{sn}^{a-2}(y)$ and $\mathrm{dn}(y)\mathrm{sn}^{a-2}(y)$. It is easily seen

that if we start with either of these eigenfunctions, then the corresponding SUSY partner potential with the same finite (a) number of band gaps is the potential $[(a-1)a,2,0,(a-1)a]$(or its isospectral partner $[(a-1)a,0,2,(a-1)a]$).

From Table I we also observe that one of the exact eigenfunctions of the potential $[a(a+1),0,0,(a-3)(a-2)]$ is $\mathrm{cn}(y,m)\mathrm{dn}(y,m)\mathrm{sn}^{a-3}(y,m)$. On starting with this eigenfunction, it is easily shown that the corresponding SUSY partner potential is $[(a-1)a,2,2,(a-2)(a-1)]$ which therefore must also be a potential with finite (a) number of band gaps when a is an integer.

Similarly, by starting from the finite band-gap potentials $[a(a+1),0,0,(a-2p-1)(a-2p)]$ as well as $[a(a+1),0,0,(a-2p)(a-2p+1)]$, and following the discussion in the case of PT-invariant AL potential, it is easily shown that the corresponding GAL potentials with the same (finite) number of band gaps are $[(a-p)(a-p+1),p(p+1),p(p+1),(a-p-1)(a-p)]$ and $[(a-p)(a-p+1),p(p+1),(p-1)p,(a-p)(a-p+1)]$, respectively, where a and p are positive integers.

D. SUSY partners of potentials with $b=g=0$

Let us now consider the SUSY partners of the PT-invariant potential $[a(a+1),0,f(f+1),0]$. From Table II we observe that two of the exact eigenfunctions of the potential $[a(a+1),0,(a-2)\times(a-1),0]$ are $\mathrm{sn}(y)\mathrm{cn}^{a-2}(y)$ and $\mathrm{dn}(y)\mathrm{cn}^{a-2}(y)$. It is easily seen that if we start with either of these eigenfunctions, then the corresponding GAL potentials turn out to be $[(a-1)a,2,(a-1)a,0]$ or $[(a-1)a,0,(a-1)a,2]$. Since we know that the potentials $[a(a+1),a(a-1),2,0]$ as well as $[a(a+1),2,0,(a-1)a]$ have a finite number of band gaps, we conjecture that maybe the potential $[a(a+1),2,(a-1)a,0]$ also has only a finite number (a) of band gaps when a is an integer.

From Table II we also observe that one of the exact eigenfunctions of the potential $[a(a+1),0,(a-3)(a-2),0]$ is $\mathrm{sn}(y)\mathrm{dn}(y)\mathrm{cn}^{a-3}(y)$. Starting with this eigenfunction, it is easily shown that the corresponding SUSY partner potential is $[(a-1)a,2,(a-2)(a-1),2]$. Again, since for integer a, the potential $[(a-1)a,(a-2)(a-1),2,2]$ has only a finite number of band gaps, it is tempting to conjecture that the same may also be true for the potential $[(a-1)a,2,(a-2)(a-1),2]$.

Similarly, by starting from the finite band-gap potentials $[a(a+1),0,(a-2p-1)(a-2p),0]$ as well as $[a(a+1),0,(a-2p)(a-2p+1),0]$, and following the discussion in the case of PT-invariant AL potentials, it is easily shown that the corresponding SUSY partners with the same number of band gaps are the GAL potentials $[(a-p)(a-p+1),p(p+1),p(p+1),(a-p-1)(a-p)]$ and $[(a-p)\times(a-p+1),p(p+1),(p-1)p,(a-p)(a-p+1)]$, respectively, when a and p are integers.

E. SUSY partners of potentials with $f=0$

Let us now consider the SUSY partners of the potential $[a(a+1),b(b+1),0,g(g+1)]$. From Table III we observe that one of the exact eigenfunctions is $\mathrm{dn}^{-b}(y)\mathrm{sn}^{-g}(y)$ when $a+b+g=0$. If we start with this eigenfunction, then the corresponding SUSY partner potential turns out to be $[(a-1)a,(b-1)b,0,(g-1)g]$.

From Table III we also observe that an exact eigenfunction of the potential $[a(a+1),b(b+1),0,g(g+1)]$ is $\mathrm{cn}(y)\mathrm{dn}^{-b}(y)\mathrm{sn}^{-g}(y)$ when $a+b+g=1$. Starting with this eigenfunction, it is easily shown that the corresponding SUSY partner potential is $[(a-1)a,(b-1)b,2,(g-1)g]$.

In summary, we have discovered a large number of complex PT-invariant periodic potentials with a finite number of band gaps, many occurring when the parameters a,b,c,d have specific integer values. This leads us to make the plausible conjecture that all GAL potentials (3) for integer values of a,b,f,g have a finite number of band gaps, but there is as yet no formal proof.

IV. HEUN'S EQUATION AND THE GENERALIZED ASSOCIATED LAMÉ EQUATION

In this section, we point out an interesting connection between Heun's differential equation[7] and the generalized associated Lamé equation (5). This connection enables us to use the various solutions of Eq. (5) obtained in this paper to write down several solutions of Heun's equation which have apparently not been studied in the mathematics literature.

The canonical form of Heun's equation is given by[7]

$$\left[\frac{d^2}{dx^2}+\left(\frac{\gamma}{x}+\frac{\delta}{x-1}+\frac{\epsilon}{x-c}\right)\frac{d}{dx}+\frac{\alpha\beta x-q}{x(x-1)(x-c)}\right]G(x)=0, \tag{47}$$

where α, β, γ, δ, ϵ, q, c are real parameters, except that $c\neq 0,1$ and the first five parameters are constrained by the relation

$$\gamma+\delta+\epsilon=\alpha+\beta+1. \tag{48}$$

If we make the transformation $x=\mathrm{sn}^2(y,m)$, then Heun's equation takes the form[7]

$$F''(y)+\left[(1-2\epsilon)m\frac{\mathrm{sn}(y)\mathrm{cn}(y)}{\mathrm{dn}(y)}+(1-2\delta)\frac{\mathrm{sn}(y)\mathrm{dn}(y)}{\mathrm{cn}(y)}+(2\gamma-1)\frac{\mathrm{cn}(y)\mathrm{dn}(y)}{\mathrm{sn}(y)}\right]F'(y)$$
$$-[4mq-4\alpha\beta m\,\mathrm{sn}^2(y)]F(y)=0, \tag{49}$$

where $[G(x)\equiv F(y)]$ and $m=1/c$. It is interesting to note that Eq. (49) is very similar to the ϕ equation (14) which we have analyzed in great detail. In particular, with the identification

$$b=\tfrac{1}{2}-\epsilon,\quad f=\tfrac{1}{2}-\delta,\quad g=\tfrac{1}{2}-\gamma,\quad b+f+g=\tfrac{1}{2}-\alpha-\beta,\quad 4\alpha\beta=Q,\quad 4mq=R, \tag{50}$$

all the results discussed above can be immediately used to obtain different solutions of Heun's equation. It turns out that using the midband states obtained in Sec. II, one generates quasiperiodic solutions of Heun's equation (49), which we discuss in a separate presentation.[8]

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Bounds on localizable information via semidefinite programming

Barbara Synak-Radtke
Institute of Theoretical Physics and Astrophysics, University of Gdańsk, Poland

Karol Horodecki
Department of Mathematics, Physics and Computer Science, University of Gdańsk, Poland

Michał Horodecki
Institute of Theoretical Physics and Astrophysics, University of Gdańsk, Poland

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We investigate the so-called localizable information of bipartite states and a parallel notion of information deficit. Localizable information is defined as the amount of information that can be concentrated by means of classical communication and local operations where only maximally mixed states can be added for free. The information deficit is defined as difference between total information contents of the state and localizable information. We consider a larger class of operations, the so-called PPT operations, which in addition preserve maximally mixed state (PPT-PMM operations). We formulate the related optimization problem as a semidefinite program with suitable constraints. We then provide bound for fidelity of transition of a given state into product pure state on Hilbert space of dimension d. This allows to obtain a general upper bound for localizable information (and also for information deficit). We calculated the bounds exactly for Werner states and isotropic states in any dimension. Surprisingly it turns out that related bounds for information deficit are equal to relative entropy of entanglement (in the case of Werner states, regularized one). We compare the upper bounds with lower bounds based on simple protocol of localization of information. © *2005 American Institute of Physics.*
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I. INTRODUCTION

In recent developments[1,2] an idea of localizing (or concentrating) information in paradigm of distant laboratories was devised. It originated from the concept of drawing thermodynamical work from heat bath and an additional physical system used as entropy sink (see, e.g., Refs. 3 and 4). Namely, using one qubit in pure state, one can draw $kT\ln 2$ of work[5] from heat bath of temperature T. More generally, using n qubit state ρ one can draw $n-S(\rho)$ of work. (We neglect the obvious factor $\ln kT$, counting work in bits.) In Ref. 1 this idea was applied to the distant laboratory paradigm. There are distant parties, who share some n qubit quantum state, and have local heat baths of temperature T. If the parties can communicate quantum information, then they can use the shared state to draw $n-S(\rho)$ bits of work. This can be achieved, by sending the whole subsystem to one party. The party can then draw work from local heat bath by use of the total state. However, if they can only use local operations and classical communication (LOCC), then they usually will not be able to draw such amount of work. Indeed, if they try to send all subsystems to one party, the state will be decohered, due to transmission via classical channel. Thus all quantum correlations will disappear, which will result in increase of entropy of the state to some value $S'>S$, so that we will observe a difference between total information $n-S$ and information localizable by LOCC. The difference is called quantum deficit and denoted by Δ.

Since it represents the information that must be destroyed during travel through classical channel, it reports quantumness of correlations of a state. In this way tracing what is local, we can also understand what is nonlocal.

The basic problem arises. *Given a quantum compound state, how much information can be localized by LOCC?* Or, equivalently, *how large is quantum deficit for a given state?* For pure state the answer is known,[2] the amount of information that cannot be localized is precisely the entanglement of formation of the state,[6] given by entropy of the subsystem. However, for mixed states even separable states can have nonzero deficit. Thus the deficit can account for quantumness that is not covered by entanglement. One could also expect that deficit is the measure of all quantumness of correlations, so that reasonable entanglement measures should not exceed it. In any case, it is important to evaluate deficit for different states.

In Ref. 2 the problem of localizing information into a subsystem was translated into a problem of distilling pure local states. In this paper, basing on this concept, we provide general upper bound for the localizable information, which gives in turn lower bound for information deficit. We compute the bound for symmetric states, like Werner states[7] and isotropic states.[8] We use the method of semidefinite programming following Rains approach to the problem of entanglement distillation.[9] Though our problem is quite opposite, instead of singlets, we want to draw pure product states, the technique can be still applied, and the bounds we obtain share some features of Rains bound for distillable entanglement. Even more suprisingly, the bounds for information deficit obtained for Werner and isotropic states are just *equal* to Rains bounds for those states, which in turn are equal to relative entropy of entanglement (regularized in the case of Werner states). We also present lower bounds, obtained by some specific protocols of localizing information.

II. PRELIMINARIES

In this section we will provide some definitions. The set of linear operators on Hilbert space $\mathcal{H}$ will be denoted as $\mathcal{B}(\mathcal{H})$. By $\mathcal{H}$ we will mean finite dimensional Hilbert space with a fixed isomorphism to $\mathcal{C}^d$, where $d=\dim \mathcal{H}$. For a vector $|\psi\rangle \in \mathcal{H}$, the projector $P=|\psi\rangle\langle\psi|$ is a pure state represented by this vector. Any mixed state is a mixture of such projectors, i.e., it is of the form $\rho=\Sigma_i p_i|\psi_i\rangle\langle\psi_i|$, where $\{p_i\}$ is a probability distribution. Equivalently, a state is positive operator on $\mathcal{H}$ with trace one.

We will need the notion of positive and negative parts of the operator. An operator A is Hermitian if $A=A^\dagger$ where $\dagger$ denotes Hermitian conjugation. The set of Hermitian operators acting on $\mathcal{H}$ will be denoted as $\chi(\mathcal{H})$. For Hermitian operator $H \in \mathcal{B}(\mathcal{H})$ positive H_+ and negative H_- parts are defined by $H_+ - H_- = H$ and $H_+ H_- = 0$, i.e., $H_+ = \Sigma_i \lambda_i^+ |\psi_i^+\rangle\langle\psi_i^+|$, $H_- = \Sigma_i \lambda_i^- |\psi_i^-\rangle\langle\psi_i^-|$ where $\lambda_i^+ (\lambda_i^-)$ are non-negative (negative) eigenvalues and $\psi_i^\pm$ are corresponding eigenvectors.

Trace norm and operator norm will be denoted by $\|.\|_{\mathrm{tr}}$ and $\|.\|_{\mathrm{op}}$, respectively, where

$$\|A\|_{\mathrm{tr}} = \mathrm{Tr}|\sqrt{AA^\dagger}|, \tag{1}$$

$$\|A\|_{\mathrm{op}} = \sup_{\|\psi\|=1} \|A|\psi\rangle\|. \tag{2}$$

We shall consider composite quantum systems which are represented by tensor product of Hilbert spaces $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B \simeq C^{d_A} \otimes C^{d_B}$, where $\mathcal{H}_A$ and $\mathcal{H}_B$ are spaces of subsystems A and B. There are two kinds of states, separable and entangled ones. Separable state ϱ_{sep} can be written as a convex combination of products of states

$$\varrho_{\mathrm{sep}} = \sum_k p_k \rho_k^A \otimes \sigma_k^B, \tag{3}$$

where ρ_k^A and ρ_k^B are states acting on Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. Entangled state are those that cannot be written in form (3).

Some of the obtained results will hold for any bipartite states, and some will be shown for specific classes of the states. We shall consider two well known classes of symmetric states, Werner states[7] and isotropic states,[8] which we recall here.

The Werner states are the states acting on Hilbert space $\mathcal{C}^d \otimes \mathcal{C}^d$, which do not change if subjected to the same unitary transformation to both subsystems,

$$\varrho = U \otimes U \varrho U^\dagger \otimes U^\dagger \tag{4}$$

for any unitary U. Such states have the following form:[7]

$$\varrho_W = \frac{1}{d^2 + \mathrm{d}\beta}(I + \beta V), \quad -1 \leqslant \beta \leqslant 1, \tag{5}$$

where V is a unitary flip operator V acting on Hilbert space $\mathcal{C}^d \otimes \mathcal{C}^d$ system defined by $V\phi \otimes \varphi = \varphi \otimes \phi$. Another useful form of ϱ_W is

$$\varrho_W = p\frac{P_A}{N_A} + (1-p)\frac{P_S}{N_S}, \tag{6}$$

where $P_S = (I+V)/2$ and $P_A = I - P_S$ are projectors onto symmetric and antisymmetric subspaces of total space, respectively. $N_A = (d^2-d)/2$ and $N_S = (d^2+d)/2$ are the dimensions of the antisymmetric and symmetric subspaces, respectively.

The isotropic states are those bipartite states which are invariant under $U \otimes \bar{U}$ transformations[8] (where $\bar{U}$ is complex comjugate of U). They are of the following form:

$$\varrho_{\mathrm{iso}} = \lambda P_+ + \frac{1-\lambda}{d^2} I, \qquad \lambda \in \left[-\frac{1}{d}, 1\right], \tag{7}$$

where P_+ is a projector onto maximally entangled state $|\psi\rangle_+ = \Sigma_{k=1}^d (1/\sqrt{d})|kk\rangle$ (which one can call the singlet state) and I/d^2 is the maximally mixed state.

We will consider states that have more than two subsystems, however we will always consider a distinguished cut dividing groups of subsystems into two groups. For example, we can have state $\rho_{AA'B'}$ which is tripartite, though from our point of view it is a bipartite state of two subsystems AA' and B.

In the paper we consider some transformations of the bipartite state. Apart from transformations that have physical meaing it is good, for technical reasons, to consider some purely mathematical transformations as well. For this reason we recall here the operation of partial transposition, and its basic properties. Namely it is a linear map $\Gamma : \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \to \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ which acts on a state with matrix elements ρ_{ijkl},

$$\rho_{AB} = \sum_{i,k=1}^{d_A} \sum_{j,l=1}^{d_B} \rho_{ijkl} |ij\rangle\langle kl| \tag{8}$$

as the following permutation:

$$\rho_{AB}^\Gamma = \sum_{i,k=1}^{d_A} \sum_{j,l=1}^{d_B} \rho_{ijkl} |il\rangle\langle kj|. \tag{9}$$

The state is written in a canonical product basis $\{|ij\rangle\}$. This map has useful properties. For any operators A and B one has

$$(\Gamma_1) \quad \mathrm{Tr}\, A^\Gamma = \mathrm{Tr}\, A,$$

$$(\Gamma_2) \quad \mathrm{Tr}\, A^\Gamma B = \mathrm{Tr}\, A B^\Gamma,$$

$$(\Gamma_3) \quad \mathrm{Tr}(AB) = \mathrm{Tr}\, A^{\Gamma} B^{\Gamma},$$

$$(\Gamma_4) \quad (A^{\Gamma})^{\Gamma} = A,$$

$$(\Gamma_5) \quad \Gamma \text{ preserves Hermiticity}. \tag{10}$$

Note, that (Γ_2) follows from (Γ_1), (Γ_3), and (Γ_4), but we state it separately for clarity. The operator ρ^{Γ} depends on the chosen basis $\{|ij\rangle\}$, however its eigenvalues do not.

In QIT one investigates processing of quantum state by means of different subclasses of all physical operations. In this paper we consider the following classes, given below.

Class of *quantum operations* (QO) is the set of completely positive,[10,11] trace preserving maps (CPTP) i.e. (as it has been shown by Choi and Kraus[10–13]), for Hilbert spaces $\mathcal{H}_1$, $\mathcal{H}_2$, with dimensions d_1 and d_2 respectively,

$$\mathrm{QO} = \left\{ \Lambda : \pi(\mathcal{H}_1) \to \pi(\mathcal{H}_2) \middle| \forall_{B \in \pi(\mathcal{H}_1)} \Lambda(B) = \sum_{i=1}^{d_1 d_2} V_i B V_i^{\dagger}, V_i : \mathcal{H}_1 \to \mathcal{H}_2, \sum_{i=1}^{d_1 d_2} V_i^{\dagger} V_i = I \right\} \tag{11}$$

the operators V_i are often referred to as Kraus operators.

Quantum operation can be composed out of the following operations:

(i) unitary transformations, $\rho \to U \rho U^{\dagger}$;
(ii) adding ancilla, $\rho \to \rho \otimes \sigma$;
(iii) discarding subsystem $\rho_{AB} \to \rho_A = \mathrm{Tr}_B \rho_{AB}$.

Class of *noisy operations* (NO) is a subclass of the QO class. This differs from them by restriction that we allow adding only maximally mixed ancillas, i.e., $\sigma = I/d$ where d is dimension of the added system.

Class of *local quantum operations and classical communication* (LOCC) is defined for states from $\pi(\mathcal{H}_A \otimes \mathcal{H}_B)$. By LOCC operations on the bipartite system of n_{AB} qubits we mean all operations that can be composed out of

(i) local unitary transformations $\rho_{AB} \to U_A \otimes U_B \rho_{AB} U_A^{\dagger} \otimes U_B^{\dagger}$,
(ii) sending subsystem down completely decohering (dephasing) channel $\rho_{AA'B} \to \rho_{AB'B} = I_{AB} \otimes \Lambda$ where $\Lambda : \mathcal{B}(\mathcal{H}_{A'}) \to \mathcal{H}_{B'}$ is a composition of the complete von Neumann measurement performed on subsystem A' given by

$$\Lambda'(\cdot) = \sum_i P_i(\cdot) P_i, \tag{12}$$

where P_i are one-dimensional projectors satisfying $\Sigma_i P_i = I_{A'}$ and an operation that transfers subsystem A' into B' (the spaces $\mathcal{H}_{B'}$ and $\mathcal{H}_{A'}$ must be equal, and we assume some fixed isomorphism between them; then the map of transfer acts simply as identity on AB tensored with the isomorphism),
(iii) adding local ancilla $\rho_{AB} \to \rho_{A'} \otimes \rho_{AB}$,
(iv) discarding local subsystem $\rho_{A'AB} \to \rho_{AB} = \mathrm{Tr}_{A'} \rho_{A'AB}$.

Class of *noisy quantum operations and classical communication* (NLOCC) is a subclass of the LOCC class. The difference is that we allow to add only the maximally mixed state as an ancilla.

By NLOCC operations on the bipartite system of n_{AB} qubits we mean all operations that can be composed out of

(i) local unitary transformations,
(ii) sending subsystem from the down completely decohering (dephasing) channel,
(iii) adding ancilla in the maximally mixed state,
(iv) discarding local subsystem.

Class of *PPT* operations. They have been introduced by Rains in Ref. 14 and are defined as those CPTP maps Λ, which conjugated with partial transposition, $\Gamma\circ\Lambda\circ\Gamma$ are still legitimate CPTP maps.

Class of *PPT maps which preserves maximally mixed state* (PPT-PMM) is given by the intersection of class of PPT operations, and those linear maps $\Lambda:\mathcal{H}_1\to\mathcal{H}_2$ with $d_{\text{in}}=\dim\mathcal{H}_1$ and $d_{\text{out}}=\dim\mathcal{H}_2$, which satisfies

$$\Lambda\left(\frac{\mathrm{I}}{d_{\text{in}}}\right)=\frac{\mathrm{I}}{d_{\text{out}}}. \tag{13}$$

In the context of distant laboratory paradigm, all but the two last classes have operational meaning, while the last two ones are some abstract subclasses of quantum operations. For these classes, the following inclusions holds:

$$\text{NLOCC}\subset\text{PPT-PMM}\subset\text{QO},\quad \text{NLOCC}\subset\text{LOCC}\subset\text{QO},\quad \text{NLOCC}\subset\text{NQ}\subset\text{QO}. \tag{14}$$

Using this, one can study features of operational class NLOCC, considering mathematical, i.e., more easy to deal with, PPT-PMM class.

A. Paradigm of localizing information

In any paradigm of manipulating states by operations the basic notion is *rate of transition*. Given a class of operations, one can ask, at what rate it is possible to transform state ρ into σ, given large amount of n independent copies of ρ, where ρ and σ act on Hilbert space $\mathcal{H}=\mathcal{H}_A\otimes\mathcal{H}_B$,

$$\rho^{\otimes n}\to\sigma^{\otimes m}. \tag{15}$$

In our case the target state σ will be a pure product state $|0\rangle|0\rangle$ on Hilbert space $C^2\otimes C^2$, and the class of allowed operations will be the NLOCC class, since we consider the scenario introduced in Ref. 1. Namely, Alice and Bob are given some bipartite state ρ acting on $\mathcal{C}^d\otimes\mathcal{C}^d$ and their task is to obtain from this state the greatest possible amount of $C^2\otimes C^2$ systems in bipartite pure product state $|0\rangle|0\rangle$ by means of noisy operations and classical communication. Clearly, to achieve this goal they should try to avoid producing much entropy, since any entropy increase would decrease the amount of desired (pure) output systems. The task can be viewed as localizing information, since the bipartite system in the pure product state has the maximal amount of local information contents.

To state it formally we provide here definition of *localizable information* I_l.

Definition 1: For any given state $\rho_{AB}\in\mathcal{C}^d\otimes\mathcal{C}^d$ *let us consider sequence* P_n *of NLOCC operations such that* $P_n(\rho_{AB}^{\otimes n})=\sigma_n$, *where* σ_n *acting on* $(\mathcal{C}^2\otimes\mathcal{C}^2)^{\otimes m_n}$.

Set of operations $\mathcal{P}\equiv\cup_{n=1}^{\infty}\{P_n\}$ *is called a protocol of localizing information if there holds*

$$\lim_{n\to\infty}\|\sigma_n-P_{00}^{\otimes m_n}\|_{\text{Tr}}=0, \tag{16}$$

with $P_{00}=|00\rangle\langle 00|$ *acting on* $\mathcal{C}_2\otimes\mathcal{C}_2$. *For given protocol* $\mathcal{P}$, *its rate is given by*

$$r_{\mathcal{P}}(\rho_{AB})=\lim_{n,d_n\to\infty}\sup\frac{2m_n}{n}. \tag{17}$$

Then the localizable information of state ρ_{AB} *is given by*

$$I_l(\rho_{AB})=\sup_{\mathcal{P}} r_{\mathcal{P}}(\rho_{AB}). \tag{18}$$

We will write $r_{\mathcal{P}}$ omitting the state ρ_{AB} if it will not lead to confusion. Please note, that for any protocol $\mathcal{P}$, its rate $r_{\mathcal{P}}$ gives the lower bound on optimal rate, i.e., on localizable information I_l. It

is then easy to obtain a bound on I_l by considering protocol $\mathcal{P}$ which needs only one-way (say from Alice to Bob) communication. A rate gained by such one-way protocol will be denoted as $r_{\mathcal{P}}^{\rightarrow}$.

Please note, that this definition is nontrivial, due to the choice of class of allowed operations. We can see it when replacing in the above definition NLOCC class with larger class of quantum operations NO.[15,2,16] The information which can be localized is in this case (due to Schumacher compression) equal to the information contents of the state, i.e., $I_{\mathrm{tot}}=n-S(\rho_{AB})$, where n is the number of qubit the state ρ_{AB} occupies. The completely trivial answer is obtained only when one uses operations without the prefix N, i.e., either QO or LOCC. Then the quantity would be always equal to infinity, because within these classes it is possible to add unlimited amount of systems in pure state.

Having defined localizable information we can proceed to recall here the definition of information deficit. The information deficit Δ equals difference between the mentioned total information content of the state I_{tot} and the localizable information I_l

Definition 2: For any bipartite state ρ_{AB} which acts on Hilbert space $\mathcal{H}_A\otimes\mathcal{H}_B$, the information deficit Δ is given by

$$\Delta(\rho_{AB}) = n - S(\rho_{AB}) - I_l(\rho_{AB}), \tag{19}$$

where $n=\log d_A+\log d_B$ is the number of qubits which ρ_{AB} occupies.

This quantity tells us to what extent the optimal process of localizing information is irreversible. In other words, how much of the total information content of the state is of the nonlocal form in a sense that it cannot be transformed into a local form, but gets destroyed during the localization process. For technical reasons, instead of norm condition (16) we will consider condition for fidelity,

$$\lim_{n\to\infty} \widetilde{F}(\sigma_n, P_{00}^{\otimes d_n}) = 1. \tag{20}$$

Those conditions are shown to be equivalent in Ref. 17. Fidelity is defined as

$$\widetilde{F}(\rho,\sigma) = \mathrm{Tr}\sqrt{\sqrt{\sigma}\rho\sqrt{\sigma}}. \tag{21}$$

In our case the state σ is pure so that we have a simpler expression,

$$F(\rho,\sigma) = \sqrt{\mathrm{Tr}\,\rho\sigma}. \tag{22}$$

Now, the monotonicity of the square root, allows for considering the quantity $F(\rho,\sigma)=\mathrm{Tr}\,\rho\sigma$.

Since the information deficit Δ reports some nonlocality of the state, it would be of great interest to compare this quantity with the well-known functions of nonlocal parameters of the state—entanglement measures. Let us here recall the main definitions of the entanglement measures, that we shall refer to when comparing with information deficit Δ. For any states ϱ and σ acting on $\mathcal{C}^d\otimes\mathcal{C}^{d'}$ we have, among others, the following functions:

(1) *Entanglement of distillation E_D* (Ref. 6) is a maximal number of singlets per copy distillable by LOCC operations from the state ϱ in asymptotic regime of $n\to\infty$ copies.
(2) *Entanglement of formation*[6] E_f is defined as

$$E_f(\rho) = \inf_{\{p_i,\rho_i\}} \sum_i p_i S(\rho_{\mathrm{red}}^i), \tag{23}$$

where the infimum is taken over all decompositions of state ρ, i.e., ensembles $\{p_i,\rho_i\}$ satisfying $\rho=\Sigma_i p_i\rho_i$, and $S(\rho_{\mathrm{red}}^i)$ being von Neumann entropy of the subsystem of state ρ^i.
(3) *Entanglement cost E_c* (Refs. 6 and 18) is the minimal number of singlets per copy needed to create a state ϱ by LOCC operations in asymptotic regime of $n\to\infty$ copies.
(4) *Relative entropy of entanglement E_R* (Ref. 19) is defined as follows:

$$E_R(\varrho) = \inf_{\sigma_{\text{sep}}} S(\varrho|\sigma), \tag{24}$$

where $S(\varrho|\sigma) = \text{tr}\,\varrho \log_2 \varrho - \text{tr}\,\varrho \log_2 \sigma$ is relative entropy and the infimum is taken over all separable states σ.

For an entanglement measure E, its regularization is denoted by E^∞ given by $\lim_{n\to\infty}[E(\varrho^{\otimes n})/n]$. In this paper we will consider regularized relative entropy of entanglement E_r^∞. Comparison of work deficit with E_f will also be important, for it has been proven[18] that regularized entanglement of formation E_f^∞ equals entanglement cost of the state E_c.

In this paper we will not use definitions of these entanglement measures. We will only need values of those measures for the mentioned symmetric states, which one can find in the literature.

III. BOUNDS ON THE FIDELITY OF TRANSITIONS

Given a quantum mixed state ρ one may ask how much of the information it contains which can be concentrated to a local form.[1] In other words, how many pairs of pure *product* states P_{00} can one achieve from ρ per copy of ρ in asymptotic regime under noisy local operations and classical communication (NLOCC).[2] The class of NLOCC maps is rather difficult to deal with. Then similarly as in entanglement theory, it is more convenient to consider some larger class that has clear mathematical characterization. In Ref. 14 a class of PPT maps was introduced which is larger than LOCC. In our case, the analogous larger class will be PPT-PMM maps. If we are able to get upper bound for the rate of distillation of pure product states with this class it will be also upper bound for rate achievable by NLOCC maps. Our analysis of the rate under PPT-PMM maps, will be analogous to the analysis of distillation of entanglement in Ref. 9. Having fixed the rate of conversion from ρ to P_{00} we evaluate the fidelity of conversion, i.e., the overlap of the current output with desired output. If the fidelity can approach 1 in limit of many input copies, the rate is attainable.

Let us then fix the rate r which means, that for n input copies of a given state we will obtain $m = \lfloor nr/2 \rfloor$ output copies. The m pairs are in a final joint state $\rho' = \Lambda(\rho^{\otimes n})$, where Λ is an operation of conversion. In the following we will assume, that operations of conversion (operations) are PPT-PMM. Then we will maximize the following quantity:

$$F_n = \text{Tr}[P_{00}^{\otimes m} \Lambda(\rho^{\otimes n})]. \tag{25}$$

The fidelity F is a function of n, since the rate r is fixed. Our general argument will be the following. If for given rate F optimized over such operations is smaller than one, then the rate is not achievable. Infimum over such rates is the upper bound for the optimal achievable rate, hence for I_L.

We will optimize F in two stages. First we will change the problem of optimization over Λ to optimization over set of some positive operators Π, which fulfills some (rather complicated) constraints. We will however not optimize F over those constraints. Rather, in second stage by duality method used in semidefinite programming we will find the bound on F expressed as infimum over Hermitian operators (without any additional constraints). We will then obtain bounds for localizable information for Werner and isotropic states by choosing appropriate Hermitian operator or by optimizing over a class of Hermitian operators.

It is useful to observe, that since Λ is a CPTP map we have

$$\text{Tr}[P_{00}^{\otimes m} \Lambda(\rho^{\otimes n})]\, \text{Tr}\left[P_{00}^{\otimes m} \sum_i V_i \rho^{\otimes n} V_i^\dagger \right] = \text{Tr}\left[\sum_i V_i^\dagger P_{00}^{\otimes m} V_i \rho^{\otimes n} \right], \tag{26}$$

where V_i are Kraus operators of the map. We used here the fact $\text{Tr}\,AB = \text{Tr}\,BA$ for any operators A and B. The map $\Sigma_i V_i^\dagger(\cdot)V_i \equiv \Lambda^\dagger$ is called dual map (with respect to Λ). It is clearly a CP map too (yet it need not be trace preserving). The meaning of dual maps to NLOCC operations is exhibited in Ref. 20. Here we are interested in the following operator:

$$\Pi = \Lambda^{\dagger}(P_{00}^{\otimes m}). \tag{27}$$

We can write fidelity by means of Π as follows:

$$F = \sup_{\Pi} \mathrm{Tr}[\rho^{\otimes n}\Pi], \tag{28}$$

where supremum is taken over all Π of the form (27). Let us now prove the following fact, which amounts to the first stage of optimization.

Fact 1: For given rate r and the number of input copies n of any state $\rho \in \mathcal{B}(C^d \otimes C^d)$, *the optimal fidelity is bounded by*

$$F \leqslant \sup_{\Pi} \mathrm{Tr}[\Pi(\rho^{\otimes n})], \tag{29}$$

where

$$0 \leqslant \Pi \leqslant I, \quad \Pi^{\Gamma} \geqslant 0, \quad \mathrm{Tr}\,\Pi = 2^{n(2\log d - r)} \equiv K. \tag{30}$$

This problem is a particular example of so-called semidefinite program. After proving the above fact we will provide the dual problem, which give bound for fidelity in the original problem (29).

Proof: We need to show that Π satisfies the displayed constraints. To this end we will use previously mentioned properties of partial transposition. Let us first check if the Π defined above operator fulfills the stated constraints. Actually, we will see, that $0 \leqslant \Pi \leqslant I$ is a consequence of the fact that Λ is CPTP map and that $P_{00}^{\otimes m} \leqslant \mathrm{I}$, and positivity of Π^{Γ} is a consequence of Λ being PPT map and the fact that $(P_{00}^{\otimes m})^{\Gamma} \geqslant 0$. We will use P instead of $P_{00}^{\otimes m}$ for convenient notation.

Positivity of Π is rather clear, since—as it came up—$\Lambda^{\dagger}$ is a positive map. Comparing Π with identity is simple, too. For any state σ we have $\sigma \leqslant \mathrm{I}$, which implies that for any positive operator A,

$$\mathrm{Tr}\,[\Lambda(A)\sigma] \leqslant \mathrm{Tr}\,\Lambda(A) = \mathrm{Tr}\,A, \tag{31}$$

where the equality expresses the fact that Λ is trace preserving. This however is equivalent to the

$$\mathrm{Tr}\,[A\Lambda^{\dagger}(\sigma)] \leqslant \mathrm{Tr}[AI] \tag{32}$$

which for $\sigma = P$ gives $\Pi \leqslant I$. To check positivity of partially transposed Π we need to show, that for any state σ,

$$\mathrm{Tr}\,[\sigma[\Lambda^{\dagger}(P)]^{\Gamma}] \geqslant 0. \tag{33}$$

Applying (Γ_2) of Eq. (11) one gets

$$\mathrm{Tr}\,[\sigma^{\Gamma}\Lambda^{\dagger}(P)] \geqslant 0, \tag{34}$$

what by definition of dual map is equivalent to

$$\mathrm{Tr}\,[\Lambda(\sigma^{\Gamma})P] \geqslant 0. \tag{35}$$

Applying subsequently (Γ_1) and (Γ_3) one ends up with

$$\mathrm{Tr}\,[(\Gamma\Lambda\Gamma)(\sigma)P^{\Gamma}] \geqslant 0, \tag{36}$$

which is true, since both $(\Gamma\Lambda\Gamma)(\sigma)$ and P^{Γ} are positive operators. First because Λ is a PPT map and second because P is a product state for which Peres separability criterion guarantees positivity of partial transposition.

To prove the last property of Π we use the fact that Λ is PMM, we then obtain

$$\mathrm{Tr}\,\Pi \equiv \mathrm{Tr}\,\Lambda^{\dagger}(P)\mathrm{I}_{\mathrm{in}} = d_{\mathrm{in}}\,\mathrm{Tr}\,P\Lambda\left(\frac{\mathrm{I}_{\mathrm{in}}}{d_{\mathrm{in}}}\right) = d_{\mathrm{in}}\,\mathrm{Tr}\,P\frac{I}{d_{\mathrm{out}}} = \frac{d_{\mathrm{in}}}{d_{\mathrm{out}}} = K, \tag{37}$$

where $d_{\mathrm{in}}=d^{2n}$ and $d_{\mathrm{out}}=2^{2m}$. This ends the proof. ■

Now, in a second stage of optimization of the fidelity, we can rearrange our task, using the concept of duality in semidefinite programming.

Theorem 1: *For any state* ρ *acting on Hilbert space* $\mathcal{C}^d\otimes\mathcal{C}^d$ *and a fixed rate* r,

$$F \leqslant \inf_{D\in\chi(\mathcal{H})}[\mathrm{Tr}(\rho - D)_+ + K\lambda_{\max}(D^{\Gamma})], \tag{38}$$

where $\lambda_{\max}(D^{\Gamma})$ *is the maximal eigenvalue of Hermitian operator* D^{Γ} *and* $K=2^{n(2\log d-r)}$.

Proof: By just adding and subtracting proper terms which is similar to the Lagrange multipliers method, using (Γ_2) we can state that for any operators A, B, and for any real parameter λ, we have

$$\mathrm{Tr}\,\Pi\rho = \mathrm{Tr}\,A - \mathrm{Tr}(-\rho + A - B^{\Gamma} + \lambda I)\Pi + \lambda K - \mathrm{Tr}\,A(I-\Pi) - \mathrm{Tr}\,B\Pi^{\Gamma} + \lambda(\mathrm{Tr}\,\Pi - K). \tag{39}$$

Now if A and B are positive operators and $A\geqslant\rho+B^{\Gamma}-\lambda\mathrm{I}$ we have

$$\mathrm{Tr}\,\Pi\rho \leqslant \mathrm{Tr}\,A + \lambda K, \tag{40}$$

since absent terms on the right-handside (RHS) are nonpositive according to the constraints on Π. Then

$$\sup_{\Pi}\mathrm{Tr}\,\Pi\rho \leqslant \inf_{A,B,\lambda}\mathrm{Tr}\left[A + \lambda\frac{K}{d^2}I\right], \tag{41}$$

where $A\geqslant 0$, $B\geqslant 0$, $A-B^{\Gamma}+\lambda I\geqslant\rho, \lambda\in R$. By introducing variable $D=\lambda I-B$ it can be changed into the following form:

$$F \leqslant \inf_{\substack{A\geqslant 0, B\geqslant 0\\ A\geqslant\rho-D^{\Gamma}\\ D=\lambda\mathrm{I}-B,\lambda\in R}}\mathrm{Tr}\left[A + \lambda\frac{K}{d^2}I\right]. \tag{42}$$

Taking subsequently infimum over D, A, and B we obtain

$$F \leqslant \inf_{D}\left\{\inf_{\substack{A\geqslant 0\\ A\geqslant\rho-D^{\Gamma}}}[\mathrm{Tr}\,A] + \inf_{\substack{B\geqslant 0\\ \lambda\mathrm{I}=D+B,\lambda\in R}}\mathrm{Tr}\left[\lambda\frac{K}{d^2}I\right]\right\}, \tag{43}$$

where D (as a combination of positive operators) is a Hermitian operator. Having D fixed one can easily minimize two separate terms over A and B, respectively. Concerning the first term, since $A\geqslant 0$ and $A\geqslant\rho-D^{\Gamma}$, the eigenvalues λ_i^A of A must be greater than zero, and greater than the eigenvalues $\lambda_i^{\rho,D}$ of the $\rho-D^{\Gamma}$ operator. Thus we have $\lambda_i^A=\max(\lambda_i^{\rho,D},0)$ which gives

$$\inf_{\substack{A\geqslant 0\\ A\geqslant\rho-D^{\Gamma}}}[\mathrm{Tr}\,A] = \mathrm{Tr}(\rho - D^{\Gamma})_+. \tag{44}$$

Turning now to the second term, one can see, that $\lambda I-D\geqslant 0$, hence λ must be not less than maximal eigenvalue of D, thus we end up with

$$\inf_{\substack{B\geqslant 0\\ \lambda I=D+B\\ \lambda\in R}} \operatorname{Tr}\left[\lambda\frac{K}{d^2}I\right]K\lambda_{\max}(D). \tag{45}$$

This leds to the formula

$$F\leqslant \inf_{D\in\chi(\mathcal{H})}\{\operatorname{Tr}(\rho-D^{\Gamma})_{+}+K\lambda_{\max}(D)\}. \tag{46}$$

By Γ_4 and Γ_5 any Hermitian operator D is of the form $\tilde{D}^{\Gamma}$, where $\tilde{D}$ is also Hermitian operator, hence we can rewrite the formula in the following way:

$$F\leqslant \inf_{D\in\chi(\mathcal{H})}\{\operatorname{Tr}(\rho-D)_{+}+K\lambda_{\max}(D^{\Gamma})\}, \tag{47}$$

which ends the proof. ■

The above result, gives us the condition on F with much simpler constraints—we optimize over a set of Hermitian operators. Analogously, one can prove a similar theorem for the case of not equal dimensions, i.e., for $\rho\in(\mathcal{C}^{d_1}\otimes\mathcal{C}^{d_2})^{\otimes n}$.

IV. BOUND FOR RATE OF CONCENTRATING INFORMATION

In the preceding section we showed that the fidelity of concentrating information by NLOCC is bounded by

$$F\leqslant \inf_{D\in\chi(\mathcal{H})}\operatorname{Tr}(\varrho^{\otimes n}-D)_{+}+2^{n(2\log_2 d-r)}\lambda_{\max}(D^{\Gamma}). \tag{48}$$

Starting from this inequality we can find two bounds for the rate r (by PPT-PMM operations) denoted by B_1 and B_2. The bound B_1 is weaker than B_2, however we derive it separately, as the proof for B_1 is more transparent than that for B_2.

Theorem 2: *For any states ϱ acting on Hilbert space $\mathcal{C}^d\otimes\mathcal{C}^d$*

$$r\leqslant 2\log_2 d+\log_2\lambda_{\max}(|\varrho^{\Gamma}|)\equiv B_1(\varrho), \tag{49}$$

where $\lambda_{\max}(|\varrho^{\Gamma}|)$ is maximal eigenvalue of operator $|\varrho^{\Gamma}|$.

Proof: We will show that inequality (49) must be true to make the fidelity converge to 1. Let us choose in (48) $D=\varrho^{\otimes n}$. Then

$$F\leqslant \limsup_{n\to\infty}2^{n(2\log_2 d-r)}\lambda_{\max}((\varrho^{\otimes n})^{\Gamma}). \tag{50}$$

The requirement $F\to 1$ is equivalent to condition

It implies

$$r\leqslant 2\log_2 d+\limsup_{n\to\infty}\frac{1}{n}\log_2\lambda_{\max}(\varrho^{\Gamma})^{\otimes n}. \tag{52}$$

Notice that

$$\limsup_{n\to\infty}\frac{1}{n}\log_2\lambda_{\max}(\varrho^{\Gamma})^{\otimes n}=\limsup_{n\to\infty}\frac{1}{n}\log_2(\max|\lambda(\varrho^{\Gamma})|)^n=\limsup_{n\to\infty}\log_2\lambda_{\max}(|\varrho^{\Gamma}|)$$
$$=\log_2\lambda_{\max}(|\varrho^{\Gamma}|).$$

Then we have

$$r \leqslant 2\log_2 d + \log_2 \lambda_{\max}(|\varrho^{\Gamma}|). \tag{53}$$

This ends the proof.

Theorem 3: *For any states ϱ and σ acting on Hilbert space $\mathcal{C}^d \otimes \mathcal{C}^d$,*

$$r(\varrho) \leqslant 2\log_2 d + S(\varrho|\sigma) + \log_2 \lambda_{\max}(|\sigma^{\Gamma}|) \equiv B_2(\varrho,\sigma). \tag{54}$$

Remark 1: Notice, that $\lambda_{\max}(|\varrho^{\Gamma}|) = \|\sigma^{\Gamma}\|_{\mathrm{op}}$. Then the bound can be written as

$$B_2(\varrho,\sigma) = 2\log_2 d + S(\varrho|\sigma) + \log_2 \|\sigma^{\Gamma}\|_{\mathrm{op}}. \tag{55}$$

It is interesting to compare this expression this formula with Rains bound for PPT distillable entanglement D:

$$D \leqslant S(\varrho|\sigma) + \log_2 \|\sigma^{\Gamma}\|_{\mathrm{Tr}}. \tag{56}$$

Proof: Let $S = S(\varrho\,|\,\sigma)$ and $L = \log_2 \lambda_{\max}(|\sigma^{\Gamma}|) = \log_2 \|\sigma^{\Gamma}\|_{\mathrm{op}}$. We will show that if

$$r - 2\log_2 d \equiv x > S + L \tag{57}$$

then F cannot converge to 1. We have

$$F \leqslant \mathrm{Tr}(\varrho^{\otimes n} - D)_+ + 2^{-nx}\lambda_{\max}(D^{\Gamma}). \tag{58}$$

Let us take

$$D = 2^{ny}\sigma^{\otimes n}, \tag{59}$$

where $S < y < x - L$. (We can find such y, because $x > S + L$)

Notice that

$$2^{-nx}\lambda_{\max}[(2^{ny}\sigma^{\otimes n})^{\Gamma}] \leqslant 2^{n(y-x+L)}. \tag{60}$$

Then

$$F \leqslant \mathrm{Tr}(\varrho^{\otimes n} - 2^{ny}\sigma^{\otimes n})_+ + 2^{n(y-x+L)}, \tag{61}$$

$2^{n(y-x+L)}$ converges to 0 because

$$y - x + L < 0. \tag{62}$$

The first term in (61) cannot converge to 1 because $y > S(\varrho\,|\,\sigma)$, as shown by Rains.[9] (It follows from quantum Stein lemma, see, e.g., Ref. 21.) This ends the proof.

Remark 2: To obtain the full strength of bound of Theorem 3, one should optimize over the choices of state σ. In what follows, we will say that σ is optimal for ϱ if

$$B_2(\varrho,\sigma) = \min_{\sigma'} B_2(\varrho,\sigma') \overset{\mathrm{d}f}{=} B_2(\varrho), \tag{63}$$

where σ' ranges over all states acting on $C^d \otimes C^d$.

V. RESULTS FOR WERNER AND ISOTROPIC STATES

In this section we will find bounds for the rate of states possessing high symmetry, Werner states, and isotropic ones, as well as compare bounds B_1 and B_2 with each other.

Let us start with the Werner state. We describe our results for the Werner state of the form (5). Using Theorem 2 we obtained the following bound:

$$B_1 = \begin{cases} 2\log_2 d - \log_2(d^2 + \mathrm{d}\beta) & \text{for } -\frac{2}{d} < \beta < 0, \\ 2\log_2 d + \log_2\left|\frac{1+\mathrm{d}\beta}{d^2+\mathrm{d}\beta}\right| & \text{for } 0 \leqslant \beta \leqslant 1 \quad \text{and} \quad -1 \leqslant \beta \leqslant -\frac{2}{d}. \end{cases} \tag{64}$$

If we want to find the bound using Theorem 3 we must optimize $B_2(\varrho,\sigma)$. As in Ref. 9, it boils down to minimizing only over the Werner states. It is due to the following facts. First, any state ϱ if subjected to random transformation of form $U\otimes U$ (called $U\otimes U$ twirling) becomes the Werner state,

$$\int U\otimes U\varrho U^\dagger\otimes U^\dagger \,\mathrm{d}U=\varrho_W. \tag{65}$$

Second, the value of $B_2(\varrho,\sigma)$ is nonincreasing after the twirling operation. Third, $B_2(\varrho,\sigma)$ is a convex function, because the quantities S and L possess these properties. Then for any state σ,

$$\begin{aligned} B_2(\varrho_W,\sigma)&=\int B_2(\varrho_W,\sigma)\mathrm{d}U\int B_2(U\otimes U\varrho_W U^\dagger\otimes U^\dagger, U\otimes U\sigma U^\dagger\otimes U^\dagger)\mathrm{d}U\\ &\geqslant B_2\left(\int U\otimes U\varrho_W U^\dagger\otimes U^\dagger\,\mathrm{d}U,\int U\otimes U\sigma U^\dagger\otimes U^\dagger\,\mathrm{d}U\right)\\ &=B_2\left(\varrho_W,\int U\otimes U\sigma U^\dagger\otimes U^\dagger\,\mathrm{d}U\right)=B_2(\varrho_W,\sigma_W), \end{aligned}$$

where σ_W is a Werner state. Thus, we can see that for any state σ we can find such Werner state σ_W, which gives no greater value of B_2 than σ. This fact simplifies our calculation to optimize $B_2(\varrho_W,\sigma)$ on Werner state. Now, we can find the smallest value of $B_2(\varrho_W,\sigma_W)$, where ϱ_W is given by the formula ((5)) and σ_W is of the following form:

$$\varrho_W=\frac{1}{d^2+\mathrm{d}\alpha}(I+\alpha V),\quad -1\leqslant\alpha\leqslant 1. \tag{66}$$

In this case $B_2(\varrho_W,\sigma)$ is a function of three parameters, d, β, and α, where the first two parameters are fixed. So to optimize $B_2(\varrho_W,\sigma)[\alpha]$ it is enough to find a minimum of this function depending on α. This way we obtain the following value of $B_2(\varrho)$,

$$B_2=\begin{cases} 2\log_2 d-S(\varrho_W)-\frac{d^2+d}{2}\frac{1+\beta}{d^2+\mathrm{d}\beta}\log_2\frac{d-2}{d}-\frac{d^2-d}{2}\frac{1-\beta}{d^2+\mathrm{d}\beta}\log_2\frac{d+2}{d} & \text{for } -1\leqslant\beta<\frac{-3d}{d^2+2},\\ 2\log_2 d-S(\varrho_W)-\frac{d^2+d}{2}\frac{1+\beta}{d^2+\mathrm{d}\beta}\log_2(1+\alpha)-\frac{d^2-d}{2}\frac{1-\beta}{d^2+\mathrm{d}\beta}\log_2(1-\alpha) & \text{for } \frac{-3d}{d^2+2}\leqslant\beta<\frac{-1}{d},\\ 2\log_2 d-S(\varrho_W) & \text{for } \dfrac{-1}{d}\leqslant\beta\leqslant 1, \end{cases} \tag{67}$$

where $\alpha=(1+d\beta)/(d+\beta)$. The entropy $S(\varrho_W)$ is given by

$$S(\varrho_W)=-\frac{d^2-d}{2}\frac{1-\beta}{d^2+\mathrm{d}\beta}\log_2\frac{1-\beta}{d^2+\mathrm{d}\beta}-\frac{d^2+d}{2}\frac{1+\beta}{d^2+\mathrm{d}\beta}\log_2\frac{1+\beta}{d^2+\mathrm{d}\beta}. \tag{68}$$

We have obtained two upper bounds for the amount of information one can localize. Of course B_2 is not always worse than B_1, so we will consider B_1 only to compare with B_2. Now, we would like to find a lower bound for I_l. To this end we shall consider some NLOCC (one-way) protocol $\mathcal{P}$ for concentrating information to the local form. The amount of information we can concentrate using $\mathcal{P}$ is a lower bound for I_l. Our protocol $\mathcal{P}$ is the following: (i) Alice makes an optimal complete von Neumann measurement represented by $P_i=|i\rangle\langle i|$ on her subsystem. (ii) After that she sends her part to Bob. Alice can do this, because after measurement her part of the state is classical-like and classical channel does not destroy it, if she does it adequately, i.e., sometimes before sending she should perform some unitary operation to avoid changing the state by the channel. (iii) Bob upon

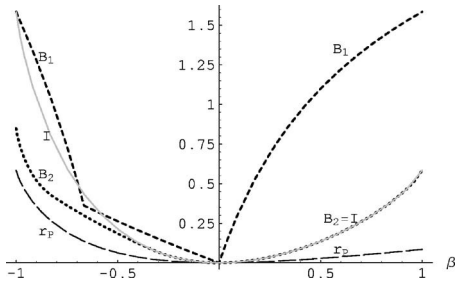

FIG. 1. The dashed lines represent bounds of rate for Werner states $(d=3)(r_{\mathcal{P}}^{\rightarrow} \leqslant B_2 \leqslant B_1)$ and continuous line represents quantity described by $I=2\log_2 d-S(\varrho)$. Note that B_2 is equal to the information content of the state in the whole range of separability $\left(\beta \geqslant -\frac{1}{3}\right)$.

receiving the whole state can extract $2\log_2 d-S(\varrho'_{AB})$ bits of information, where ϱ'_{AB} is obtained from ϱ_{AB} by Alice's operation (i) and (ii).

Lemma V.1: For state ϱ_{AB} acting on Hilbert space $\mathcal{C}^d \otimes \mathcal{C}^d$ with maximally mixed subsystem A by use of the protocol $\mathcal{P}$, we can concentrate to local form $r_{\mathcal{P}}^{\rightarrow}$ information, where $r_{\mathcal{P}}^{\rightarrow}$ is described by

$$r_{\mathcal{P}}^{\rightarrow} = \sup_{P_i}\left(\log_2 d - \sum_i p_i S(\varrho_B^i)\right),$$

$$\text{where } p_i = \mathrm{tr}(\varrho_{AB} P_i \otimes I) \quad \text{and } \varrho_B^i = \frac{1}{p_i}\mathrm{tr}_A(P_i \otimes I \varrho_{AB} P_i \otimes I). \tag{69}$$

Proof: After sending by Alice her part, Bob possesses the whole state and can extract $2\log_2 d-S(\varrho'_{AB})$, where $\varrho'_{AB}=\Sigma_i p_i |i\rangle\langle i| \otimes \varrho_B^i$. The states $|i\rangle$ are orthogonal and it implies that $S(\varrho'_{AB})=H(p_i)+\Sigma_i p_i S(\varrho'^i_B)$. Shannon entropy $H(p_i)$ is the amount to entropy of Alice's part after her measurement. We know, that entropy cannot decrease after measurement but also cannot increase, because it is maximal. It implies that $H(p_i)=\log_2 d$. Then we have

$$r_{\mathcal{P}}^{\rightarrow} = 2\log_2 d - S(\varrho'_{AB}) = 2\log_2 d - \left[\log_2 d + \sup_{P_i}\left(\sum_i p_i S(\varrho'^i_B)\right)\right] = \log_2 d - \sup_{P_i}\left(\sum_i p_i S(\varrho'^i_B)\right).$$

This ends the proof.

For Werner states $r_{\mathcal{P}}^{\rightarrow}$ is achieved by any measurement of Alice. It follows from the fact that ϱ_W is $U \otimes U$ invariant. We obtain

$$r_{\mathcal{P}}^{\rightarrow}(\varrho_W) = \log_2 d + \frac{1+\beta}{d+\beta}\log_2(1+\beta) - \log_2(d+\beta). \tag{70}$$

Let us here compare the bounds for amount of localizable information with each other.

Figure 1 shows lower and upper bounds for rate in comparison to information content of state. For Werner states bound B_2 is much better than B_1. For separable state B_2 is trivial, it coincides with information contents of state $I=2\log_2 d-S(\varrho)$. For entangled states it is better than I.

Looking at Fig. 2 we can see B_2 and $r_{\mathcal{P}}^{\rightarrow}$ for some different dimensions of Hilbert space of the Werner state. Continuous lines represent bounds for $d=3$, the long dashed lines bounds for $d=4$ and the short dashed lines for $d=5$.

Now, let us present results for the isotropic state. For these states the bound B_1 is given by

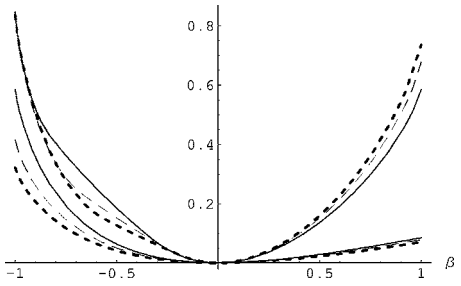

FIG. 2. Upper bound B_2 and lower bound $r_{\vec{\mathcal{P}}}$ of rate for the Werner states ($d=3,4,5$).

$$B_1 = \begin{cases} \log_2[-\lambda(d+1)+1] & \text{for } \lambda < 0, \\ \log_2[\lambda(d-1)+1] & \text{for } \lambda \geqslant 0. \end{cases} \tag{71}$$

Using the same arguments as for the Werner state we can show that if we want to find the value of $B_2(\varrho_{\text{iso}})$ we should optimize $B_2(\varrho_{\text{iso}},\sigma)$ on the isotropic state. Analogously, as in the previous case, we can find out that

$$B_2 = \begin{cases} 2\log_2 d - S(\varrho_{\text{iso}}) & \text{for } \dfrac{-1}{d^2-1} \leqslant \lambda \leqslant \dfrac{1}{d+1}, \\ 2\log_2 d - S(\varrho_{\text{iso}}) + \log_2 \dfrac{1+p(d-1)}{1-p} - \dfrac{1+\lambda(d^2-1)}{d^2}\log_2 \dfrac{1-p}{1+p(d^2-1)} & \text{for } \dfrac{1}{d+1} \leqslant \lambda \leqslant 1. \end{cases} \tag{72}$$

where $p=[(d+1)\lambda-1]/[(1-d^2)(\lambda-1)+d]$. The entropy of the isotropic state is given by

$$S(\varrho_{\text{iso}}) = -\frac{1+\lambda(d^2-1)}{d^2}\log_2\frac{1+\lambda(d^2-1)}{d^2} - \frac{(1-\lambda)(d^2-1)}{d^2}\log_2\frac{1-\lambda}{d^2}. \tag{73}$$

Isotropic state possesses similar properties as the Werner states, so if we want to obtain a value of $r_{\vec{\mathcal{P}}}$ we should proceed similarly for that family of state. Then we have

$$r_{\vec{\mathcal{P}}} = \log_2 d + \left(\lambda + \frac{1-\lambda}{d}\right)\log_2\left(\lambda + \frac{1-\lambda}{d}\right) + (d-1)\frac{1-\lambda}{d}\log_2\left(\frac{1-\lambda}{d}\right). \tag{74}$$

For the isotropic state the bound B_2 is better again than B_1 and also only for entangled isotropic state the upper bound is nontrivial. The upper and lower bounds agree for P_+ and are obviously equal to $\log_2 d$. The bounds and information content are compared in Fig. 3 for $d=3$. The upper dashed line represents B_2, the lower $r_{\vec{\mathcal{P}}}$. The gray continuous line is the information content of state, i.e., $2\log_2 d - S(\varrho_{\text{iso}})$.

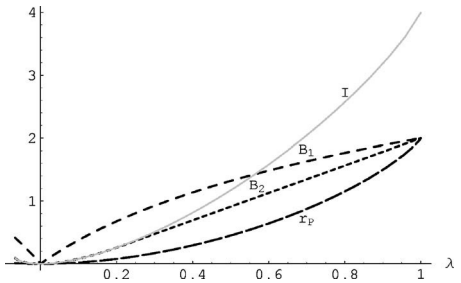

FIG. 3. The dashed lines represent bounds of rate for isotropic states ($d=3$) and continuous line represents information content of state. Note that B_2 is equal to $I=2\log_2 d - S(\varrho)$ for the whole range of separability [$\lambda \leqslant 1/(1+d)$]).

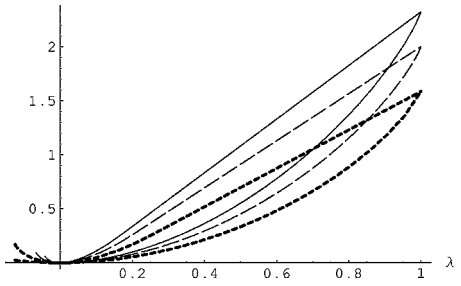

FIG. 4. Upper bound B_2 and lower bound $r_{\mathcal{P}}^{\rightarrow}$ of rate for isotropic states ($d=3,4,5$).

In Fig. 4 quantities B_2 and $r_{\mathcal{P}}^{\rightarrow}$ are compared for some different dimension ($d=3,4,5$).

VI. COMPARING QUANTUM DEFICIT WITH MEASURES OF ENTANGLEMENT

As one knows, quantum deficit Δ can be treated as a measure of quantum correlations.[1] Having bound localizable information we can find bounds for Δ. We can do this, because quantum deficit is defined as a difference between total information and information I_l, which can be localized by NLOCC (19) and we know that I_l is bounded by information localizable by using PPT-PMM operations. That is, by $I_l \leqslant B_2$ we have lower bound δ_B on quantum deficit,

$$\delta_B(\varrho) = 2\log_2 d - S(\varrho) - B_2. \tag{75}$$

On the other hand, we have considered particular NLOCC protocol, namely the one which uses only one-way communication. This gives $I_l \geqslant r_{\mathcal{P}}^{\rightarrow}$, which in turn gives upper bound δ_P on quantum deficit,

$$\delta_P(\varrho) = 2\log_2 d - S(\varrho) - r_{\mathcal{P}}^{\rightarrow}. \tag{76}$$

Quantum deficit is believed to be a more general measure of "quantumness" of state, than measures of entanglement. It is then interesting to compare it with some known entanglement measures.

We now compare bounds on Δ with the relative entropy of entanglement and entanglement of formation of the bipartite state.

The regularized relative entropy of entanglement E_R^{∞} for Werner states is given by[22]

$$E_R^{\infty}\begin{cases} \log_2\frac{d-2}{d} + \frac{(d-1)(1-\beta)}{2(d+\beta)}\log_2\frac{d+2}{d-2} & \text{for } -1 \leqslant \beta \leqslant -\frac{3d}{d^2+2}, \\ 1 - H\left(\frac{(d-1)(1-\beta)}{2(d+\beta)}\right) & \text{for } -\frac{3d}{d^2+2} \leqslant \beta \leqslant -\frac{1}{d}, \\ 0 & \text{for } -\frac{1}{d} \leqslant \beta \leqslant 1. \end{cases} \tag{77}$$

Entanglement of formation is described by the following formula:

$$E_F\begin{cases} H\left(\frac{1}{2}\left(1 - \sqrt{1 - \left(\frac{1+d\beta}{d+\beta}\right)^2}\right)\right) & \text{for } -1 \leqslant \beta \leqslant -\frac{1}{d}, \\ 0 & \text{for } -\frac{1}{d} < \beta \leqslant 1. \end{cases} \tag{78}$$

We can see in Fig. 5 the graphs of δ_B , δ_P, E_F, and E_R^{∞} for the Werner states. We obtain that δ_B and E_R^{∞} are equal. For Werner states with $\beta < 0.42$ we have that quantum deficit is not greater than entanglement of formation, $\Delta \leqslant E_F$.

Let us now pass to isotropic states. For entangled ones with parameter $\lambda \in (1/(d+1), 1)$ the relative entropy of entanglement E_R is given by

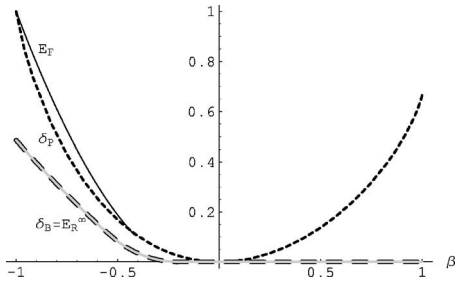

FIG. 5. The dashed lines represent upper and lower bounds of Δ for Werner states ($d=5$), grey continuous regularized relative entropy of entanglement E_R^∞ and black continuous entanglement of formation E_F.

$$E_R = \log_2 d + f \log_2 f + (1-f)\log_2 \frac{1-f}{d-1}, \tag{79}$$

where $f=[(d^2-1)\lambda+1]/d^2$. For another isotropic states it is zero. The formula of entanglement of formation can be found in Ref. 23. For nonseparable states it is in the form of

$$E_F(\varrho) = \mathrm{co}(g(\gamma)), \tag{80}$$

$$g(\gamma) = (H_2(\gamma) + (1-\gamma)\log_2(d-1)), \tag{81}$$

where $\gamma=(1/d^2)(\sqrt{d\lambda+[(1-\lambda)/d]}+\sqrt{(d-1)[(d^2-1)(1-\lambda)/d]})^2$ and co means a convex hull.[23] In Fig. 6 we can see graphs of two measures of entanglement and bounds for Δ.

We can notice that the graphs of δ_B agree with E_R. Similary as for the Werner states we have $\delta_B=E_R$. δ_P is greater than E_F for most isotropic states. (We do not know, if it is true for all isotropic states.) For maximally entangled state P_+ all these quantities are equal.

VII. FIDELITY FOR DISTILLATION OF LOCAL PURE STATES AND SINGLETS

The well-known counterpart of a qubit which represents the unit of local information is ebit—one bit of entanglement, represented by singled state, i.e., unit of nonlocal information. It has been stated in Ref. 24 that these two forms of information are complementary. If one distills maximal possible amount of one type of information, possibility of gaining the second type disappears. The optimal protocol in the case of pure initial state $\psi_{AB}^{\otimes n}$, in which both types are obtained with some ratios, has been also shown there. We will find a bound for the fidelity of such transition, in which both qubits and ebits are drawn in an NLOCC protocol in case of general mixed state $\rho_{AB}^{\otimes n}$. One can view this as a *purity distillation protocol*, because purity in general has two extreme forms, purely local and purely nonlocal. This is due to the fact, that any nonproduct pure state, is asymptotically equivalent to the singlet state under the set of NLOCC operations.[2] To this end—as before—we will consider a broader class than the NLOCC, namely the class PPT-

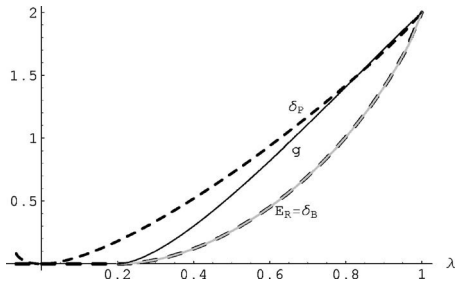

FIG. 6. The dashed lines represent bounds for Δ for isotropic states ($d=3$), grey continuous regularized relative entropy of entanglement E_R, and black continuous $g(\gamma)$ (whose convex hull is entanglement of formation E_F).

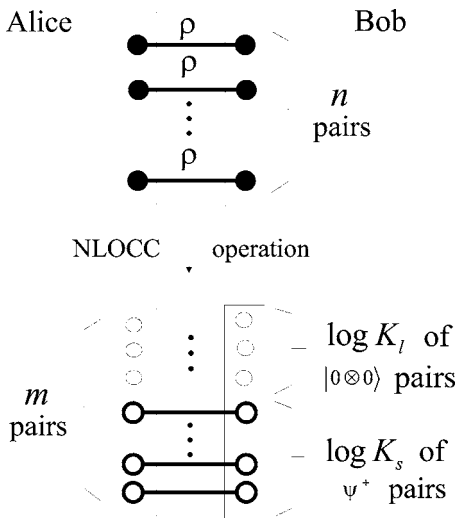

FIG. 7. Scenario of distillation of pure states in their two extremal forms, purely local (product) states and purely nonlocal (maximally entangled) states. The fixed rates of transition gives the proportion of the number of input copies n of state ρ to the numbers of output copies of *local* states ($\log K_l$) and singlet states ($\log K_s$).

PMM. This time we must fix two rates, one which tells us how many pure local qubits we would like to obtain (r_l), but also how many singlet states (r_s) will be acheived per n copies of input state (see Fig. 7).

Namely

$$r_s = \frac{\log K_s}{n}, \quad r_l = \frac{2m - 2\log K_s}{n}, \tag{82}$$

where n is the number of input states, m is the number of qubits that output states occupy (both pure qubits, and singlets together) and $\log K_s$ is the output number of singlet states. We get less than $2m/n$ pure qubits since $\log K_s$ singlets use up $2\log K_s$ qubits out of $2m$ final. We should maximize the fidelity of transition,

$$F = \mathrm{Tr}[P_+^{\otimes \log K_s} \otimes P_{00}^{\otimes (m-\log K_s)} \Lambda(\rho^{\otimes n})], \tag{83}$$

where $P_+^{\otimes \log K_s}$ is the projector onto the singlet state on $\mathcal{C}^{K_s} \otimes \mathcal{C}^{K_s}$. Instead of tensor product of singlets and product states, we can equally well consider the output state as the same singlet state embedded in the larger Hilbert space $\mathcal{C}^m \otimes \mathcal{C}^m$. Thus we shall maximize the following quantity:

$$F = \mathrm{Tr}[P_+^{K_s} \Lambda(\rho^{\otimes n})], \tag{84}$$

where K_s reminds that P_+ is of less dimension than the whole Hilbert space it is embedded in. The rest of the space is occupied by pure local qubits, i.e., the second resource drawn in this process.

Consequently we will first consider the fidelity in terms of the $\Pi = \Lambda^\dagger(P_+^{K_s})$ operator where $\Lambda^\dagger$ is dual (hence CP) to the Λ which is CPTP from assumption.

Analogously as in Sec. III we can obtain the following fact.

Fact 2: For given rates r_l, r_s and the number of input copies n, the optimal fidelity is given by

$$F \leqslant \sup_{\Pi} \mathrm{Tr}[\Pi(\rho^{\otimes n})], \tag{85}$$

where

$$0 \leqslant \Pi \leqslant \mathrm{I}, \quad \frac{-\mathrm{I}}{K_s} \leqslant \Pi^\Gamma \leqslant \frac{\mathrm{I}}{K_s}, \quad \mathrm{Tr}[\Pi] = 2^{n(2\log d - r_l - 2r_s)} \equiv K. \tag{86}$$

Passing to the dual problem, after some algebra we get the following.

Theorem 4: *For any state* ρ *acting on* $C^d \otimes C^d$ *and rates* r_l *and* r_s *we have*

$$F \leqslant \inf_D \left\{ \mathrm{Tr}(\rho - D)_+ + \inf_\lambda \left[\frac{1}{K_s} \mathrm{Tr}|D^\Gamma - \lambda I| + \lambda K \right] \right\}, \tag{87}$$

where infimum are taken over all Hermitian operators D *and all real numbers* λ, *respectively*, $K = 2^{n(2 \log d - r_l - 2r_s)}$ *and* $K_s = 2^{nr_s}$.

It is not easy to obtain nontrivial results. Suppose that we want to apply analogous ideas to those applied in Sec. IV. Let us rewrite fidelity as follows (for some fixed D):

$$F \leqslant \mathrm{Tr}(\rho^{\otimes n} - D) + 2^{-nr_s} \mathrm{Tr}|D^\Gamma - \lambda I| + \lambda 2^{n(2 \log d - r_l)}. \tag{88}$$

The simplest approach would be to force first terms to vanish by choosing $D = \varrho^{\otimes n}$. However, even by this simplification it is very difficult to find any bound for rates.

Yet, there are also "higher level" problems. Namely the main problem within the connection between distillation of entanglement and the paradigm of localizing information, is whether distillation process consumes local information.[25] It seems that our class of operations cannot feel this problem at all. Indeed, it is likely, that any distillation process is a map that preserves a maximally mixed state.[26] Thus one should perhaps improve the approach, by imposing more stringent constraints on class of operations. This is because for initial maximally mixed state, we impose only final maximally mixed state. However generically, the final dimension is smaller than the initial one. This means that some tracing out must take place, and we do not require the state that was traced out to be maximally mixed. Thus in our class, pure ancillas can be added, under the condition that they are finally traced out.

VIII. DISCUSSION

In this paper we have investigated *localizable information* and associated *information deficit* of the quantum bipartite states. We used the fact, that localizable information can be defined as the amount of pure local qubits (per input copy) that can be distilled by means of classical communication and local operations that do not allow adding local ancilla in the nonmaximally mixed state.

We considered a larger class of operations which we called PPT-PMM operations. They are those PPT operations which preserve the maximally mixed state. Then we managed to formulate the problem of distillation of pure product qubits in terms of semidefinite program. Using duality concept in semidefinite programming we have obtained bound for fidelity of transition from given state to pure product ones by PPT-PMM operations. In this way we have found a general upper bound for the amount of localizable information of arbitrary state. The bound was denoted B_2 (we also obtained a simpler, but weaker bound B_1). It gives bound δ_B for information deficit.

We were able to evaluate exactly the value of the bound B_2 for states exhibiting high symmetry—Werner states and isotropic states. Quite surprisingly, the obtained related lower bound δ_B for information deficit turned out to coincide with relative entropy of entanglement in the case of isotropic states, and with regularized relative entropy of entanglement for Werner states. In other words, in those two cases, our bound for information deficit, turned out to be equal to Rains bound for distillable entanglement.

We have also analyzed a simple lower bound r_P for localizable information, and a parallel upper bound δ_P for information deficit. We compared the latter bound with entanglement of formation. In particular we obtained that for Werner states ($d=3$), in entangled region it is strictly smaller than entanglement of formation. If one believes that information deficit is a measure of total quantumness of correlations, the conclusion would be that either E_F is nonadditive for some Werner states, or, which is more likely, it is additive, i.e., equal to entanglement cost E_c, but E_c does not describe the entanglement present in the state in this case. Rather it includes also the entanglement that got dissipated during formation of the state.

We have also discussed possibility of application of our approach to the problem of simultaneous distillation of singlets and pure local states. We provided bound for fidelity in this case. However it is likely, that the chosen class of operations is too large to describe information consumption in the process of distillation of entanglement.

There are a lot of open problems, which we have not addressed in this paper. For example, the question of continuity of the localizable information. For operationally defined quantities such as I_l, this is usually not an easy question. However one can hope that I_l continues to some extent. Namely, in Ref. 27 Vidal has proven some continuity properties of distillable entanglement E_D. Though distillable entanglement is quite an opposite quantity to localizable information (cf. Ref. 24) it is also operationally defined. Moreover I_l and E_D are both based on the notion of distillation.[2] In this context, the techniques used in Ref. 27 may be fruitful for investigations of continuity of localizable information.

An important open question is also the connection between information deficit and entanglement measures. In particular, it is intriguing, how general is the equality of our lower bound for deficit, and the relative entropy of entanglement E_r—upper bound for distillable entanglement.

Another interesting question arises in the context of phenomenon of locking[28–30] where removing a single qubit can result in a big change of a quantity. It is likely that I_l cannot be locked, due to its relations with relative entropy distance (see Ref. 31 in this context). However, we have not been able to prove it.

Finally, we believe that our results will stimulate further research on the properties of localizable information and information deficit, as well as their relations with other quantum informational quantites.

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A constructive algorithm for the Cartan decomposition of SU(2^N)

Henrique N. Sá Earp[a)]
Department of Mathematics, Imperial College London, Prince Consort Road, London, SW7 2BW, United Kingdom

Jiannis K. Pachos
Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, United Kingdom

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We present an explicit numerical method to obtain the Cartan-Khaneja-Glaser decomposition of a general element $G \in \mathrm{SU}(2^N)$ in terms of its "Cartan" and "non-Cartan" components. This effectively factors G in terms of group elements that belong in $\mathrm{SU}(2^n)$ with $n<N$, a procedure that can be iterated down to $n=2$. We show that every step reduces to solving the zeros of a matrix polynomial, obtained by truncation of the Baker-Campbell-Hausdorff formula, numerically. All computational tasks involved are straightforward and the overall truncation errors are well under control. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2008210]

I. INTRODUCTION

In their seminal paper, Khaneja and Glaser[1] presented a generic method to decompose "large" unitary elements in terms of "smaller" ones. The initial unitaries can be viewed as evolution operators of a multipartite system of spin-1/2's or as quantum algorithms acting on qubits. Experimentally it is only possible to control the interactions between a small number of subsystems at a time. Hence, this decomposition is of particular interest. It allows us to address questions such as how to optimize a dynamical evolution in terms of control procedures applied to a small number of spins or how a certain quantum algorithm can be obtained with the smallest possible number of experimentally feasible one and two qubit gates.

In particular, Khaneja and Glaser show that any element of the Lie group $\mathbf{G}=\mathrm{SU}(2^N)$ is, up to local unitaries in $\mathrm{SU}(2)^{\otimes N}$, determined by components generated from certain Abelian subalgebras $\mathfrak{h}_n$ and $\mathfrak{f}_n$, $n=2,\ldots,N$, of the Lie algebra $\mathfrak{su}(2^N)$. This is achieved by employing iteratively the Cartan decomposition

$$G = K' H K'',$$

where H is generated by $\mathfrak{h}_n(\mathfrak{f}_n)$ and the factors K' and K'' belong to the subgroup $\mathbf{K}\subset\mathbf{G}$ generated by a particular subalgebra orthogonal to $\mathfrak{h}_n(\mathfrak{f}_n)$. These relevant substructures are specified in terms of a fortunate choice of basis for $\mathfrak{su}(2^n)$ that can be obtained recurrently for $n=2,\ldots,N$.

The beauty of this result and its promising applications in quantum algorithms,[2,3] control theory, quantum error correction,[4] or the quantification of entanglement in multi-partite systems[5] have motivated the search for a constructive method to perform the decompositions for any given matrix $G \in \mathrm{SU}(2^N)$. Although substantial work has been done on the first non-trivial instance SU(4),[6,7] little seems to be known so far for the higher N case.[8]

Here we address the decomposition problem for the general group $\mathrm{SU}(2^N)$. Employing a convenient truncation of the Baker-Campbell-Hausdorff (BCH) formula, we show that the prob-

[a)]Electronic mail: henrique.saearp@imperial.ac.uk

lem allows for a numerical algorithm to calculate all such **KHK** decompositions with controlled error. Hence, we can perform the full Khaneja-Glaser decomposition of a general element $G \in \mathrm{SU}(2^N)$ with arbitrary computational precision.

This article is organized as follows. In Sec. II we briefly review the Khaneja-Glaser decomposition[1] and establish the formalism for our approach. In Sec. III we reinterpret the problem in terms of the BCH formula; we explain how a truncation of the BCH series renders our problem solvable by straightforward numerical tasks. In Sec. IV we give a user-friendly summary of the essential steps involved and we finally conclude in Sec. V.

II. THE KHANEJA-GLASER DECOMPOSITION

We consider the compact semi-simple Lie group $\mathbf{G}=\mathrm{SU}(2^N)$ and a particular compact closed subgroup $\mathbf{K}\subset\mathbf{G}$; we denote by $\mathfrak{g}=\mathfrak{su}(2^N)$ the Lie algebra of $\mathbf{G}$ and by $\mathfrak{k}\subset\mathfrak{g}$ the Lie algebra of $\mathbf{K}$ understood as a subalgebra of $\mathfrak{g}$. Since $\mathbf{G}$ is semi-simple, the Killing form $\langle .,. \rangle$ is non-degenerate and defines a bi-invariant metric on $\mathbf{G}$. Hence, we can define $\mathfrak{m}=\mathfrak{k}^{\perp}$ to be the orthogonal complement of $\mathfrak{k}$ with respect to the metric. Notice that, in general, the vector space $\mathfrak{m}\subset\mathfrak{g}$ is *not* a subalgebra. Since $\mathfrak{m}$ is determined by $\mathfrak{k}$ and the Killing metric, we shall refer to this structure as the *Lie algebra pair* $(\mathfrak{g},\mathfrak{k})$.

We shall adopt the following typographic conventions in most cases:

$\mathbf{G}$	capital bold	group or subgroup
G	capital italic	element of $\mathbf{G}$
$\mathfrak{g}$	German fraktur	Lie algebra or subspace
g	normal	element of $\mathfrak{g}$

The only exception to the choice of fonts just stated will be the familiar Pauli matrices, seen as elements of $\mathfrak{su}(2)$, which will be denoted by majuscules

$$X=\frac{\mathbf{i}}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad Y=\frac{\mathbf{i}}{2}\begin{pmatrix}0 & -\mathbf{i}\\ \mathbf{i} & 0\end{pmatrix},\quad Z=\frac{\mathbf{i}}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

and the 2×2 identity matrix

$$I=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}.$$

Finally, we shall use an abbreviated normalized notation for their tensor products given by

$$A_1A_2\ldots B_j\ldots A_k \doteq \left(\frac{2}{\mathbf{i}}\right)^{k-1} A_1\otimes A_2\otimes\ldots\otimes B_j\otimes\ldots\otimes A_k,\quad \begin{matrix}A_i=X,Y,Z\\ B_j=I.\end{matrix}$$

For example, $YXI=\frac{\mathbf{i}}{2}\begin{pmatrix}0 & -\mathbf{i}\\ \mathbf{i} & 0\end{pmatrix}\otimes\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\otimes\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$.

A. Cartan decomposition

Definition 1: *A* Cartan decomposition *of* $\mathfrak{g}$ *is an orthogonal split of* $\mathfrak{g}$,

$$\mathfrak{g}=\mathfrak{k}\oplus\mathfrak{m}$$

given by a Lie algebra pair $(\mathfrak{g},\mathfrak{k})$ *satisfying the commutation relations*

$$[\mathfrak{k},\mathfrak{k}]\subset\mathfrak{k},\quad [\mathfrak{m},\mathfrak{k}]\subset\mathfrak{m},\quad [\mathfrak{m},\mathfrak{m}]\subset\mathfrak{k}. \tag{1}$$

In this case $(\mathfrak{g},\mathfrak{k})$ *is called a* symmetric Lie algebra pair.

Remark 2: *The appearently artificial conditions in the above definition have an interpretation in Riemannian geometry:* $\mathfrak{g}=\mathfrak{k}\oplus\mathfrak{m}$ *is a Cartan decomposition if and only if the quotient manifold* $\mathbf{G}/\mathbf{K}=\exp(\mathfrak{m})$ *is a* globally Riemannian symmetric space.[9] *Such a space possesses a canonical*

global involution *(i.e., an automorphism s of the space onto itself such that* $s^2=I$*) which induces naturally a linear involution* s_* *on* $\mathfrak{g}$ *that preserves the Lie algebra structure* $[.,.]$. *Since* s_* *squares to identity, its eigenvalues must be* ± 1, *and the subspaces* $\mathfrak{k}$ *and* $\mathfrak{m}$ *emerge, respectively, as the* $+1$ *and* -1*-eigenspaces of* s_*.

We can start exploring the Cartan decomposition $\mathfrak{g}=\mathfrak{k}\oplus\mathfrak{m}$ by noticing that if $\mathfrak{h}\subset\mathfrak{m}$ is a subalgebra of $\mathfrak{g}$ then, by (1), $\mathfrak{h}$ is automatically Abelian. Since $\mathfrak{m}$ itself is not in general a subalgebra of $\mathfrak{g}$, it is natural to look for a *maximal* (Abelian) subalgebra $\mathfrak{h}\subset\mathfrak{m}$.

Definition 3: *A* Cartan subalgebra *of the pair* $(\mathfrak{g},\mathfrak{k})$ *is a maximal (in* $\mathfrak{m}$*) Abelian subalgebra* $\mathfrak{h}\subset\mathfrak{m}$.

From now on we shall assume that the Cartan subalgebra $\mathfrak{h}$ refers to the pair $(\mathfrak{g},\mathfrak{k})$ unless stated otherwise. The following *Proposition* shows that the whole $\mathfrak{m}$ is obtained from $\mathfrak{h}$ by the adjoint action of $\mathbf{K}$ and that there is only one such $\mathfrak{h}$ up to this action. In the context of the particular application we have in mind, this means $\mathfrak{h}$ carries the "essential" information about $\mathfrak{m}$.

Proposition 4: *Let* $\mathfrak{h}$ *and* $\mathfrak{h}'$ *be two Cartan subalgebras; then*

1. $\mathfrak{m}=\bigcup_{K\in\mathbf{K}}\mathrm{Ad}_K(\mathfrak{h})$;
2. $\mathfrak{h}'=\mathrm{Ad}_K(\mathfrak{h})$ *for some element* $K\in\mathbf{K}$.

Proof: *Please see* Appendix B. ■

Denote $\mathbf{H}=\exp(\mathfrak{h})\subset\mathbf{G}$ the subgroup generated by $\mathfrak{h}$. The Cartan decomposition theorem states that any group element $G\in\mathbf{G}$ can be written as an element $H\in\mathbf{H}$ together with left- and right-multiplications by elements of $\mathbf{K}$:

Theorem 5 (Cartan decomposition): *The Cartan decomposition* $\mathfrak{g}=\mathfrak{k}\oplus\mathfrak{m}$ *induces a* Cartan decomposition *of the group* $\mathbf{G}$,

$$\mathbf{G}=\mathbf{KHK}, \tag{2}$$

where $\mathbf{H}=\exp(\mathfrak{h})$.

The Cartan decomposition of a given element $G\in\mathbf{G}$ *has the form*

$$G=K_0\underbrace{K_1HK_1^\dagger}_{M}=K_0M, \tag{3}$$

where $K_0,K_1\in\mathbf{K}$, $H\in\mathbf{H}$ *and* $M=K_1HK_1^\dagger\in\exp(\mathfrak{m})$.

Proof: *Since* $\mathbf{G}/\mathbf{K}=\exp(\mathfrak{m})$, *there exist* $K_0\in\mathbf{K}$ *and* $M\in\exp(\mathfrak{m})$ *such that* $G=K_0M$. *Let* $m=\log(M)\in\mathfrak{m}$; *from* Proposition 4, *item* 1, *there exists* $K_1\in\mathbf{K}$ *such that* $\mathrm{Ad}_{K_1}m=h\in\mathfrak{h}$, *so*

$$G=K_0\exp(m)=K_0\exp(\mathrm{Ad}_{K_1^\dagger}h)=K_0K_1\underbrace{\exp(h)}_{H}K_1^\dagger.$$

■

B. The Khaneja-Glaser basis

The Khaneja-Glaser basis[1] for arbitrary $\mathfrak{su}(2^n)$ makes explicit all the structures which concern us. In particular, the splitting $\mathfrak{g}=\mathfrak{k}\oplus\mathfrak{m}$ and the Cartan subalgebras $\mathfrak{h}_n$ and $\mathfrak{f}_n$ are manifest.

We start with a familiar example:

Example 6: *For* $n=2$, *we propose basis elements for the Lie algebra* $\mathfrak{su}(4)$ *and organize them into subspaces* $\mathfrak{m}_2$ *and* $\mathfrak{k}_2$ *as follows:*

$\mathfrak{su}(4)$				
$\mathfrak{m}_2$			$\mathfrak{k}_2$	
XX	XY	XZ	XI	IX
YY	YZ	YX	YI	IY
ZZ	ZX	ZY	ZI	IZ
$\cup$				
$\mathfrak{h}_2$				

(4)

$$\mathfrak{h}_2 = \mathrm{span}\{XX, YY, ZZ\}$$

$$\mathfrak{f}_2 = \{0\}$$

Now we obtain the *Khaneja-Glaser basis* for $\mathfrak{su}(2^n)$ by a relatively simple iteration process starting from $\mathfrak{su}(4)$, as summarized in the following:

$\mathfrak{su}(2^n)$			
$\mathfrak{m}_n$		$\mathfrak{k}_n$	
$I^{n-1}\otimes X$	$I^{n-1}\otimes Y$	$I^{n-1}\otimes Z$	
		$\widehat{\mathfrak{k}_n}$	
$\mathfrak{su}(2^{n-1})\otimes X$	$\mathfrak{su}(2^{n-1})\otimes Y$	$\mathfrak{su}(2^{n-1})\otimes Z$	$\mathfrak{su}(2^{n-1})\otimes I$
		$\mathfrak{k}_{n,1}$	$\mathfrak{k}_{n,0}$
$\cup$		$\cup$	
$\mathfrak{h}_n$		$\mathfrak{f}_n$	

$$I^{n-1} = I^{\otimes(n-1)} = \underbrace{I\otimes..\otimes I}_{n-1}$$

NB.: Terms of the form $\mathfrak{su}(2^{n-1})\otimes A$ denote the set obtained by tensoring each element of $\mathfrak{su}(2^{n-1})$ with the matrix $A=X,Y,X,I$; in all cases we consider the span of the basis elements over $\mathbb{R}$.

Notice that for $n>2$ two successive Cartan decompositions can be performed. First, the expected one referring to the pair $(\mathfrak{su}(2^n),\mathfrak{k}_n)$, with Cartan subalgebra $\mathfrak{h}_n$. In the terms of *Theorem 5*, this means we can write $G\in \mathrm{SU}(2^n)$ as $G=K'HK''$ with $H\in \exp(\mathfrak{h}_n)$ and $K',K''\in \exp(\mathfrak{k}_n)$. However, the decomposition of $\mathfrak{k}_n$ given by diagram (4) is

$$\mathfrak{k}_n = \mathfrak{k}_{n,1} \oplus \mathfrak{k}_{n,0} \oplus \mathrm{span}\{I^{n-1}Z\} \simeq \mathfrak{su}(2^{n-1}) \oplus \mathfrak{su}(2^{n-1}) \oplus \mathfrak{u}(1),$$

where both $\mathfrak{k}_{n,1}$ and $\mathfrak{k}_{n,0}$ are canonically isomorphic to $\mathfrak{su}(2^{n-1})$. Since our aim is to iteratively decompose the factors $K^{(j)}$ until they eventually reduce to "local" unitaries in $\mathrm{SU}(2)^{\otimes N}$ and non-local "Cartan" factors, we would expect $\mathfrak{k}_n$ to generate something of the form $\mathrm{SU}(2^{n-1}) \otimes \mathrm{SU}(2)$. Thus, there is a $\mathfrak{su}(2^{n-1})$ component too many in $\mathfrak{k}_n$ that we need to factor away in order to define the complete recurrence step.

A closer look at $\mathfrak{k}_n$ reveals another Lie Algebra pair, thereby clearing the way for a second Cartan decomposition: we just have to leave aside the "complex phase" generated by $I^{n-1}Z$ [see diagram (4)] that can be seen as a "local" transformation under the inclusion $\mathrm{U}(1) \hookrightarrow \mathrm{SU}(2)$. Let $\widehat{\mathfrak{k}_n} = \mathfrak{k}_{n,1} \oplus \mathfrak{k}_{n,0}$ denote the subalgebra obtained from $\mathfrak{k}_n$ in this manner, so that $\mathfrak{k}_n = \widehat{\mathfrak{k}_n} \oplus \mathfrak{u}(1) \hookrightarrow \widehat{\mathfrak{k}_n} \oplus \mathfrak{su}(2)$. Accordingly, given a group element $K = \exp(k) \in \mathbf{K}$, let us write $\hat{K} = \exp(\hat{k})$, where $\hat{k} \in \widehat{\mathfrak{k}_n}$ is obtained from $k \in \mathfrak{k}$ by eliminating the component spanned by $I^{n-1}Z$. This is well defined as $I^{n-1}Z$ commutes with every element in $\mathfrak{k}_n$.

It is now straightforward to check that $(\widehat{\mathfrak{k}_n}, \mathfrak{k}_{n,0})$ is also a Lie algebra pair,[1] whose Cartan subalgebra we call $\mathfrak{f}_n$. Hence, we can apply *Theorem 5* again to decompose the factors $\widehat{K'}$ and $\widehat{K''}$ into elements of $\exp(\mathfrak{f}_n)$ together with left and right multiplication by some new factors generated by $\mathfrak{k}_{n,0}$. This time the orthogonal subalgebra $\mathfrak{k}_{n,0} = \mathfrak{su}(2^{n-1}) \otimes I$ is canonically isomorphic to $\mathfrak{su}(2^{n-1})$, so it generates $\exp(\mathfrak{k}_{n,0} \oplus \mathrm{span}\{I^{n-1}Z\}) \simeq SU(2^{n-1}) \otimes SU(2)$. Thus, we have accomplished the complete nth recurrence step that yields the decomposition

$$G = K^{(1)}F^{(1)}K^{(2)}HK^{(3)}F^{(2)}K^{(4)},$$

with $F^{(j)} \in \exp(\mathfrak{f}_n)$, $H \in \exp(\mathfrak{h}_n)$ and $K^{(j)} \in \mathrm{SU}(2^{n-1}) \otimes \mathrm{SU}(2)$.

Note, finally, that we are particularly interested in the "Cartan" factors, i.e. those generated by the Cartan subalgebras $\mathfrak{h}_n$ of $(\mathfrak{su}(2^n), \mathfrak{k}_n)$ and $\mathfrak{f}_n$ of $(\widehat{\mathfrak{k}_n}, \mathfrak{k}_{n,0})$, that emerge in each step. It is thus convenient to know explicitly a set of basis elements for each of these subalgebras. This can be achieved by the following recurrence formula, starting from $\mathfrak{h}_2 = \mathrm{span}\{XX, YY, ZZ\}$,

$$\left.\begin{array}{l} \mathfrak{h}_n = \mathrm{span}\,\mathfrak{a}(n) \\ \mathfrak{f}_n = \mathrm{span}\,\mathfrak{b}(n) \end{array}\right\}, \; n = 2, ..., N \tag{5}$$

$$\boxed{\begin{array}{l} \mathfrak{a}(2) = \{XX, YY, ZZ\}, \mathfrak{b}(2) = \{0\} \\ \mathfrak{s}(n) = \bigcup_{j=2}^{n} \mathfrak{a}(j) \otimes I^{n-j} \\ \mathfrak{a}(n+1) = \{I^n, \mathfrak{s}(n)\} \otimes X \\ \mathfrak{b}(n+1) = \{\mathfrak{s}(n)\} \otimes Z \end{array}}$$

The *Example* below illustrates all the above constructions for the first non-trivial case $\mathfrak{su}(8)$:

Example 7: $n = 3 : \mathfrak{su}(8)$

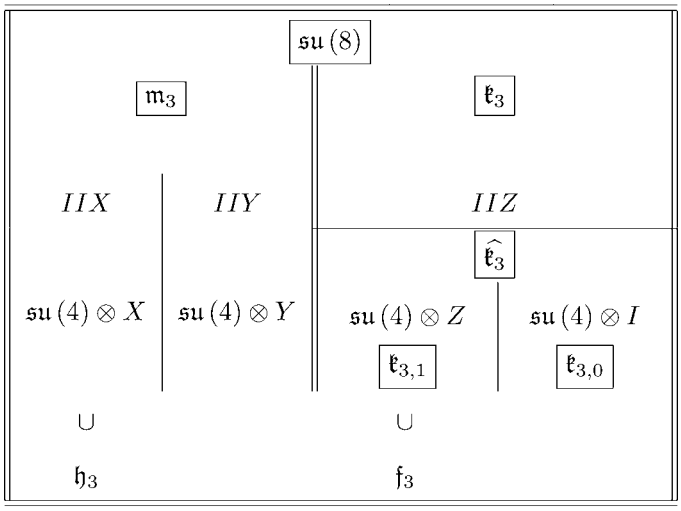

$$\mathfrak{h}_3 = \mathrm{span}\{IIX, XXX, YYX, ZZX\}$$

$$\mathfrak{f}_3 = \mathrm{span}\{XXZ, YYZ, ZZZ\}$$

C. The Baker-Campbell-Hausdorff formula

The matrix Lie algebra $\mathfrak{g}$ is noncommutative and thus, for general elements $a,b\in\mathfrak{g}$, the product of exponentials $e^a e^b$ does not coincide with the exponential of their sum, e^{a+b}. In fact the expression for $\log(e^a e^b)$ has an infinite series of correction terms and is known as the *BCH formula*, after Baker-Campbell-Hausdorff.

Although the original formula was rather complicated and computationally unpractical, a remarkable simplification made by Dynkin[10,11] expresses all the terms as successive commutators of a and b,

$$\log(e^a e^b) = \sum_{i,j=1}^{\infty} T_{i,j}(a,b).$$

Here $T_{i,j}(a,b)$ denotes the homogeneous term of degree i in a and degree j in b; its expression is

$$T_{i,j}(a,b) = \frac{1}{i+j}\sum_{(i_1,j_1,\ldots,i_k,j_k)} \frac{(-1)^{k-1}}{k}\frac{1}{i_1!\,j_1!\ldots i_k!\,j_k!}[a^{i_1}b^{j_1}\ldots a^{i_k}b^{j_k}],$$

where we abbreviate $[a^{i_1}b^{j_1}\ldots a^{i_k}b^{j_k}]=\underbrace{[a,\ldots[a}_{i_1},\underbrace{[b,\ldots[b}_{j_1},[a,\ldots[b,\underbrace{[a,\ldots[a}_{i_k},\underbrace{[b,\ldots,b]\ldots]}_{j_k}$

and the sum ranges over all possible $2k$-uples of non-negative integers $(i_1,j_1,\ldots,i_k,j_k)$ such that

$$\sum_{c=1}^{k} i_c = i,\ \sum_{c=1}^{k} j_c = j \quad \text{and} \quad i_c + j_c > 0.$$

The first few terms are

$$\log(e^a e^b) = a + b + \frac{1}{2}[a,b] + \frac{1}{12}[a,[a,b]] + \frac{1}{12}[b,[b,a]] + \frac{1}{24}[a,[b,[a,b]]] + \frac{1}{120}(\ldots) \qquad (6)$$

and the higher order coefficients after $\frac{1}{120}$ decrease quickly (see, e.g., Ref. 12). This will motivate us later on to perform convenient truncations on this convergent series.

III. NUMERICAL ALGORITHM FOR THE KHK DECOMPOSITION

In this section we will develop a technique that allows the explicit numerical calculation of the components of a general group element $G \in \mathbf{G}$ under Cartan decomposition. The idea is to consider the Cartan decomposition (3) in the light of the BCH expansion (6). Let $g \in \mathfrak{g}$, $m \in \mathfrak{m}$, and $k \in \mathfrak{k}$ be the generators of G, M, and K_0, respectively. Then (3) reads

$$G = e^g = e^k e^m. \tag{7}$$

Since the matrix G is given, (3) shows that k can be obtained from m (and vice-versa) by

$$k = k(m) = \log(Ge^{-m}). \tag{8}$$

Hence, the decomposition problem is reduced to finding m.

A. Determining *m*

First, taking logarithms in (3), we obtain

$$g = \log(e^k e^m). \tag{9}$$

We then apply (6) to expand g in terms of successive brackets of k and m. In light of *Remark 2* we can easily deduce that each of the brackets belongs in either $\mathfrak{k}$ or $\mathfrak{m}$. Hence, the expansion is split into two orthogonal components,

$$\begin{aligned} g &= k + m + \underbrace{\frac{1}{2}[k,m]}_{\in \mathfrak{m}} + \underbrace{\frac{1}{12}[k,[k,m]]}_{\in \mathfrak{m}} + \underbrace{\frac{1}{12}[m,[m,k]]}_{\in \mathfrak{k}} + \underbrace{\frac{1}{24}[k,[m,[k,m]]]}_{\in \mathfrak{k}} + \cdots \\ &= g_{\mathfrak{k}} + g_{\mathfrak{m}}, \end{aligned}$$

where

$$g_{\mathfrak{k}} = k + \tfrac{1}{12}[m,[m,k]] + \tfrac{1}{24}[k,[m,[k,m]]] + \cdots \in \mathfrak{k}, \tag{10}$$

$$g_{\mathfrak{m}} = m + \tfrac{1}{2}[k,m] + \tfrac{1}{12}[k,[k,m]] + \cdots \in \mathfrak{m}. \tag{11}$$

Note that computing $g_{\mathfrak{k}}$ and $g_{\mathfrak{m}}$ from g is a straightforward task since the Khaneja-Glaser basis (4) makes explicit the partition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{m}$.

At this stage we can use (3) to eliminate $k = k(m)$ in either of the equations (10) or (11). Choosing (11) whose first few terms are simpler we obtain

$$g_{\mathfrak{m}} = g_{\mathfrak{m}}(m) = m + \tfrac{1}{2}[k(m),m] + \tfrac{1}{12}[k(m),[k(m),m]] + \cdots, \tag{12}$$

which is an infinite series with rapidly decreasing coefficients. As $g_{\mathfrak{m}}(m)$ is a converging series we can truncate it so that the resulting equation will provide an *approximation* of m with an error that decreases by including higher commutator terms. If we call $\widetilde{P}_p(m)$ the truncation that includes all terms with up to p commutators, i.e.,

$$g_{\mathfrak{m}}(m) = \widetilde{P}_p(m) + \text{further terms}, \tag{13}$$

we can in principle solve

$$P_p(m) \equiv \widetilde{P}_p(m) - g_{\mathfrak{m}} = 0 \tag{14}$$

with respect to the single matrix variable m. However, the expression of $k(m)$ given by (3) is rather complicated. So we propose using again the BCH expansion to obtain

$$k(m) = \log(e^g e^{-m}) = g - m - \tfrac{1}{2}[g,m] - \tfrac{1}{12}[g,[g,m]] + \tfrac{1}{12}[m,[m,g]] \ldots . \tag{15}$$

As before, we can truncate (15) to a term that includes all qth order brackets. This yields a polynomial $Q_q(m)$ that approximates $k(m)$ as well as we desire at the cost of taking extra high-order commutators

$$k(m) = Q_q(m) + \text{further terms}. \tag{16}$$

After both truncations, Eq. (14) is approximated by

$$0 = P_p(m) \simeq -g_{\mathfrak{m}} + m + \tfrac{1}{2}[Q_q(m),m] + \tfrac{1}{12}[Q_q(m),[Q_q(m),m]] + \ldots,$$

where $P_p(m)$ is now a polynomial in one matrix variable with matrix coefficients. Our problem of finding m has thus been reduced to finding the zeros of a polynomial. This can be easily performed with a numerical algorithm.[13] The accuracy of the result can be increased by including more terms in the truncated series P_p and Q_q, i.e., increasing p and q. Specifically, we prove in Appendix A that, in this way, the errors in determining m by the truncation procedure are well under control.

Example 8*: Take the "first order" truncations* $p=1, q=1$*:*

$$P_1(m) = -g_{\mathfrak{m}} + m + \tfrac{1}{2}[k(m),m],$$

$$Q_1(m) = g - m - \tfrac{1}{2}[g,m].$$

Then, approximating $k(m) \simeq Q_1(m)$*, we obtain*

$$P_1(m) \simeq -g_{\mathfrak{m}} + m + \tfrac{1}{2}\left[g - m - \tfrac{1}{2}[g,m],m\right] = -g_{\mathfrak{m}} + m + \tfrac{1}{2}[g,m] - \tfrac{1}{4}[m,[m,g]].$$

B. The $M=K_1HK_1^\dagger$ decomposition

Once m is known, it remains to find the subgroup element $K_1^\dagger \in \mathbf{K}$ whose adjoint action rotates M onto $H=e^h, h \in \mathfrak{h}$.

Lemma 9*: The following properties are associated to* $\mathbf{H}=\exp(\mathfrak{h})$*:*

1. $\mathbf{H}$ *is a torus (compact connected Abelian Lie subgroup) of* $\mathbf{G}$*;*
2. *any vector* $v \in \mathfrak{h}$ *whose 1-parameter subgroup* $\{\exp(tv)\}$ *is dense in* $\mathbf{H}$ *is centralized in* $\mathfrak{m}$ *just by* $\mathfrak{h}$*:*

$$\{u \in \mathfrak{m} | [u,v] = 0\} = \mathfrak{h} \tag{17}$$

Proof: *See, e.g., Spaces of Constant Curvature (Sec. 8.6).*[14] ■

As shown in *Appendix* B, the first necessary ingredient to perform the decomposition $M=K_1HK_1^\dagger$ is some vector $v \in \mathfrak{h}$ that generates a dense 1-parameter subgroup $\exp(tv) \subset \mathfrak{h}$. This may seem abstract, but since we have an explicit basis (5) for $\mathfrak{h}$, it suffices to take any irrational combination of the Cartan generators.

Example 10: *In* $\mathfrak{su}(8)$*, take, e.g.,*

$$v = IIX + \pi\,.\,XXX + \pi^2\,.\,YYX + \pi^3\,.\,ZZX.$$

The reluctant reader may verify that, indeed, the centralizer of such v *in* $\mathfrak{m}$ *is just* $\mathfrak{h}$.

Now, we may define $f_{v,m}$ as in Appendix B to be given by

$$f_{v,m}(K) = \langle v, \mathrm{Ad}_K(m)\rangle = \sum_{a,b,c,d} C_{ad}^c C_{bc}^d v^a (K^\dagger m K)^b \tag{18}$$

and recover K_1 numerically as a minimum of $f_{v,m}$.

We conclude that m can be rotated into $h=\mathrm{Ad}_{K_1}(m)$. Thus we have completed the decomposition

$$G = K_0 K_1 e^h K_1^\dagger.$$

IV. STEP-BY-STEP SUMMARY

What we have described so far consists of the main building blocks necessary to perform the Khaneja-Glaser decomposition. Here, we will summarize all the steps one needs to take when given an arbitrary unitary $G \in \mathrm{SU}(2^n)$.

1. Calculate its (matrix) logarithm $g=\log(G) \in \mathfrak{g}=\mathfrak{su}(2^n)$.
2. Compute the Khaneja-Glaser basis following the recurrence in diagram (4); take $g_\mathfrak{m}$, the component of g on the subspace $\mathfrak{m}_n$.
3. Truncate (12) including pth commutators to get $\tilde{P}_p(m)$; let $P_p(m)=\tilde{P}_p(m)-g_\mathfrak{m}$.
4. Truncate (15) including qth commutator to get $Q_q(m)$, as in (16).
5. Replace $Q_q(m)$ for $k(m)$ in the expression of $P_p(m)$ obtained in 3, so that $P_p(m)$ becomes a polynomial in m.
6. Solve the zeros of $P_p(m)$ to get a solution m to (14).
7. Use m from item 6 above to calculate $K_0=Ge^{-m}$ as in (3).
8. Compute $\mathfrak{h}_n$ following (5); order its elements $\{u_j\}$, e.g., alphabetically and define $v=\Sigma \pi^{j-1} u_j$ to satisfy the density hypothesis of *Lemma 9*.
9. Use m and v to define $f_{v,m}(K)=\Sigma_{a,b,c,d} C_{ad}^c C_{bc}^d v^a (K^\dagger m K)^b$ as in (18); minimize f on $\mathbf{K}=\exp(\mathfrak{k}_n)$ to find K_1.
10. Calculate $h=K_1^\dagger m K_1$, and thus $H=\exp(h)$.
11. Assembling the results from items 7, 9. and 10, obtain

$$G = K_0 K_1 H K_1^\dagger.$$

12. Repeat the above steps for $G=\widehat{K_0 K_1}$ and then for $G=\widehat{K_1^\dagger}$, replacing $\mathfrak{k}_n \to \mathfrak{k}_{n,0}$, $\mathfrak{m}_n \to \mathfrak{k}_{n,1}$ and $\mathfrak{h}_n \to \mathfrak{f}_n$.
13. Items 11 and 12 yield the decomposition

$$G = K^{(1)} F^{(1)} K^{(2)} H K^{(3)} F^{(2)} K^{(4)},$$

with $F^{(j)} \in \exp(\mathfrak{f}_n)$, $H \in \exp(\mathfrak{h}_n)$, and $K^{(j)} \in \mathrm{SU}(2^{n-1}) \otimes \mathrm{SU}(2)$.

14. Decrease $n \to n-1$ and iterate this process to further decompose each factor $K^{(j)} \in \mathrm{SU}(2^{n-1}) \otimes \mathrm{SU}(2)$ until they all reduce to a product of Cartan factors $F_n^{(j)}$ and $H_n^{(l)}$ and local unitaries in $\mathrm{SU}(2)^{\otimes N}$.

NB.: As far as accuracy in step 6 is concerned, tasks 3 to 5 should be performed in light of *Appendix* A. Namely, truncations at higher order should be tried until numerical errors are satisfactory, which will happen after a finite number of attempts.

V. CONCLUSIONS

As the advances in quantum technologies move beyond the control of one or two spins, or qubits, it is important to minimize the overall cost of processing quantum information. The Khaneja-Glaser decomposition of SU(2^N) offers an upper bound for this optimization procedure given by 4^{N-1} multi-local $\mathrm{SU}(2)^{\otimes N}$ rotations together with $4^{N-1}-1$ purely entangling operations. The latter can be reduced, if desired, into bipartite interactions, or two-qubit gates. Moreover, in Ref. 15, Nielsen gives lower bounds for such optimization. Here we exploit the Khaneja-Glaser approach to build a constructive method for decomposing a general unitary in terms of its local unitary components. Abstract as it may seem, the decomposition problem can be cast in such a way that can be easily solved by a numerical algorithm that can be found at *http://cam.qubit.org/users/jiannis/lie_solve[1].tar.gz*.

Finally, one should notice that the solutions we obtained are not necessarily unique. In general, neither the zeros of the matrix polynomials, $P_p(m)$, nor the minima of the functions, f, are

unique. In particular, viewing the minimization procedure from the equivalent point of view of the diagonalization of the matrix m, where K_1 is constructed out of the eigenvectors of m, there are many equivalent solutions depending on the particular ordering of the eigenvectors. Moreover, one should also take into account that the exponential function has a natural 2π periodicity and the adjoint action is $\mathbb{Z}_2$-symmetric.[6,7] While our approach is not concerned with the actual parametrizations of the group elements, this is an important issue which should be addressed in the future.

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APPENDIX A: ACCURACY OF BCH TRUNCATIONS

Here, a generalized version of Rouché's theorem[16] is employed to show that the truncations performed in Sec. III A yield a rigorous approximation for the zeros of (12).

Theorem 11: *Let $\varphi,\psi:\mathbb{C}^r\to\mathbb{C}^r$ be holomorphic functions and $D\subset\mathbb{C}^r$ be an open domain such that neither φ nor ψ have zeros on ∂D; if*

$$|\varphi(m)-\psi(m)|<|\varphi(m)|+|\psi(m)|,\quad \forall\, m\in\partial D, \tag{A1}$$

then φ and ψ have the same number of zeros in D.

NB.: We adopt, e.g., the norm $|\varphi|=\max_{i,j}|\varphi_{ij}|$, but the argument holds for any L^p-norm.

Let $r=2^{2n}$ be the number of entries of a matrix $m\in\mathfrak{su}(2^n)$, seen as a complex vector. Consider then a BCH-type series $\varphi(m)$ and its truncated version $\psi(m)=P_p(m)$ containing all its terms of up to p successive brackets, calling $R_p(m)$ the truncation remainder

$$\varphi(m)=P_p(m)+R_p(m).$$

Suppose $\hat{m}\in\mathfrak{su}(2^n)$ is a zero of $P_p(m)$; then $\varphi(m)$ will also have a zero inside the polydisc $D=\Delta_\delta(\hat{m})\subset\mathbb{C}^r$ of radius $\delta>0$ about $\hat{m}$ if the following (stronger) instance of (A1) holds:

$$|R_p(m)|<|P_p(m)|,\quad \forall\, m\in\partial\Delta_\delta(\hat{m}). \tag{A2}$$

In other words, $\hat{m}$ approximates at least one zero of $\varphi(m)$ with error inferior to an arbitrarily chosen δ.

All we have to show is that condition (A2) holds for suitably large p; this is a relatively straightforward consequence of the uniform convergence of the BCH series $\varphi(m)=\lim_{p\to\infty}P_p(m)$, as we will now see. For any (small) $\varepsilon_0>0$, there is a p_0 such that

$$p>p_0\Rightarrow|P_p(m)-P_{p_0}(m)|<\varepsilon_0,\quad \forall\, m, \tag{A3a}$$

hence

$$|P_p(m)|>|P_{p_0}(m)|-\varepsilon_0,\quad \forall\, m. \tag{A3b}$$

In particular, if m_0 is a zero of $P_{p_0}(m)$, Eq. (A3a) restricted to the boundary $\partial\Delta_\delta(m_0)$ implies that all polynomials $P_p(m)$, $p>p_0$, also have at least one zero inside $\Delta_\delta(m_0)$, by Rouché's theorem.

On the other hand, convergence also implies $\lim_{p\to\infty}|R_p(m)|=0$, hence, for a given $\varepsilon_1>0$, there is p_1 such that

$$p>p_1\Rightarrow|R_p(m)|<\varepsilon_1,\quad \forall\, m. \tag{A4}$$

Set $\varepsilon_1=\min_{m\in\partial\Delta_\delta(m_0)}|P_{p_0}(m)|-\varepsilon_0$; assuming this is positive (if not, take a larger p_0 for a smaller ε_0), take some $p>\max\{p_0,p_1\}$ and find $m_1\in\Delta_\delta(m_0)$ such that $P_p(m_1)=0$. Then consider any smaller polydisc $\Delta_{\delta'}(m_1)\subset\Delta_\delta(m_0)$, and restrict Eqs. (A3b) and (A4) to its boundary. We obtain

$$|R_p(m)| < |P_p(m)|, \quad \forall\, m \in \partial\Delta_{\delta'}(m_1),$$

thus, by Rouché's theorem again, $\varphi(m)=P_p(m)+R_p(m)$ has a zero inside $\Delta_{\delta'}(m_1)\subset\Delta_\delta(m_0)$.

APPENDIX B: PROOF OF PROPOSITION 4

In this *Appendix* we will develop the proof of *Proposition 4*, following Ref. 14 (Sec. 8.3). This argument contains most of the crucial elements to understanding the **KHK** decomposition in detail.

Proof of Proposition 4.

1. Given $m \in \mathfrak{m}$, we want to find $K_1^\dagger \in \mathbf{K}$ whose action rotates m onto some element h of the Cartan subalgebra $\mathfrak{h}$. First, take any $v \in \mathfrak{h}$ that generates a dense 1-parameter subgroup $\exp(tv)\subset\mathbf{H}=\exp(\mathfrak{h})$, as in *Lemma 9* and define the function

$$f_{v,m} = f:\mathbf{K} \to \mathbb{R},$$

$$K \mapsto f(K) = \langle v, \mathrm{Ad}_K(m)\rangle, \tag{B1}$$

where $\langle a,b\rangle=\mathrm{tr}(\mathrm{ad}_a\,\mathrm{ad}_b)$ is the Killing form on $\mathfrak{g}$. Since f is continuous and $\mathbf{K}$ is compact, f admits an absolute minimum $K_1 \in \mathbf{K}$. If we consider a local perturbation of K_1 by e^{tk}, for any $k \in \mathfrak{k}$, we have

$$0 = \left.\frac{d}{dt}\right|_{t=0} f(e^{tk}K_1) = \left.\frac{d}{dt}\right|_{t=0} \langle v,\ \mathrm{Ad}_{e^{tk}}\,\mathrm{Ad}_{K_1}(m)\rangle$$

$$\langle v, [k, \underbrace{\mathrm{Ad}_{K_1}(m)}_{h}]\rangle = \mathrm{tr}(\mathrm{ad}_v \mathrm{ad}_{[k,h]})$$

$$= \mathrm{tr}(\mathrm{ad}_v(\mathrm{ad}_k\,\mathrm{ad}_h - \mathrm{ad}_h\,\mathrm{ad}_k)) \overset{\text{(c.p.t.)}}{=} \mathrm{tr}(\mathrm{ad}_{[h,v]}\mathrm{ad}_k)$$

$$\Leftrightarrow \langle [h,v],k\rangle = 0, \quad \forall\, k \in \mathfrak{k}.$$

But the Killing form is non-degenerate on $\mathfrak{k}$, so we must have $[h,v]=0$ and thus $h \in \mathfrak{h}$, as v is centralized by $\mathfrak{h}$; hence, we have shown that

$$m = \mathrm{Ad}_{K_1^\dagger}(h),\ h \in \mathfrak{h}.$$

2. By 1. there exists $K \in \mathbf{K}$ such that

$$\mathrm{Ad}_K(v) \in \mathfrak{h}'.$$

Now take centralizers on both sides. ■

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Clean positive operator valued measures

Francesco Buscemi[a] and Michael Keyl[b]
Dipartimento di Fisica "A. Volta," QUIT Group, via Bassi 6, I-27100 Pavia, Italy

Giacomo Mauro D'Ariano[c]
Dipartimento di Fisica "A. Volta," QUIT Group, via Bassi 6, I-27100 Pavia, Italy, and Department of Electrical and Computer Engineering, Northwestern University, Evanston, Illinois 60208

Paolo Perinotti[d]
Istituto Nazionale di Fisica della Materia, QUIT Group, Unità di Pavia, Dipartimento di Fisica "A. Volta," via Bassi 6, I-27100 Pavia, Italy

Reinhard F. Werner[e]
Institut für Mathematische Physik, TU Braunschweig, Mendelssohnstrasse 3, 38106 Braunschweig, Germany

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In quantum mechanics the statistics of the outcomes of a measuring apparatus is described by a positive operator valued measure (POVM). A quantum channel transforms POVMs into POVMs, generally irreversibly, thus losing some of the information retrieved from the measurement. This poses the problem of *which POVMs are "undisturbed," i.e., they are not irreversibly connected to another POVM*. We will call such POVMs *clean*. In a sense, the clean POVMs would be "perfect," since they would not have any additional "extrinsical" noise. Quite unexpectedly, it turns out that such a "*cleanness*" property is largely unrelated to the convex structure of POVMs, and there are clean POVMs that are not extremal and vice versa. In this article we solve the cleannes classification problem for number n of outcomes $n \leqslant d$ (d dimension of the Hilbert space), and we provide a set of either necessary or sufficient conditions for $n > d$, along with an iff condition for the case of informationally complete POVMs for $n = d^2$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2008996]

I. INTRODUCTION

The new quantum information technology[1] has resurrected the interest in the theory of quantum measurements[2] and quantum open systems,[3,4] shifting the interest from applications to high-sensitivity and high-precision experiments[5] to its use in quantum information processing.[6] Depending on the particular kind of quantum processing—e.g., teleportation,[7,8] entanglement detection,[9] and distillation[10]—that are used in quantum computation[1,6] and quantum cryptography,[11] various new types of quantum measurements are now needed. The theory for engineering new quantum measurements optimized according to given criteria has been pioneered since the late 1960s by many authors[12] who concurred to the making of the quantum estimation theory,[13] the ancestor of the modern quantum information theory.

The general strategy of quantum estimation theory is to optimize the output statistics of the measuring apparatus according to a given criterion/fidelity, which depends on the specific use of

[a]Electronic mail: buscemi@fisicavolta.unipv.it
[b]Electronic mail: M.Keyl@tu-bs.de
[c]Electronic mail: dariano@unipv.it
[d]Electronic mail: perinotti@fisicavolta.unipv.it
[e]Electronic mail: r.werner@tu-bs.de

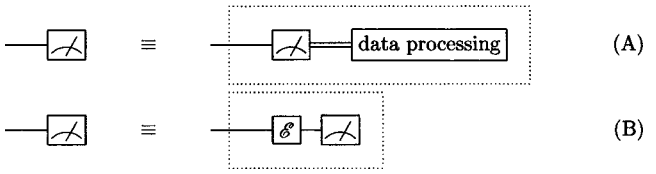

FIG. 1. There are two ways of processing POVMs: (a) the *postprocessing* of the output data and (b) *preprocessing* of the input state by a quantum channel. The postprocessing cannot generally achieve the same result of a *preprocessing:* the postprocessing is purely classical, whereas the preprocessing is quantum.

the measurement, the outcome statistics of the measurement for all possible input states being described by a positive operator valued measure (POVM).[13] POVMs form a convex set, where convex combinations correspond to random choices among different apparatuses. Most optimization problems actually resort to minimize a concave function on such a convex set, thereby optimization can be restricted to its extremal points, where concave functions attain their minimum. Coincidentally, due to the specific form of the optimization function, in many applications the optimal POVMs turn out to have unit rank—e.g., for phase estimation on pure states[13,14]—and this has led to the widespread belief that optimality is synonym of rank-one, whereas for sufficiently large dimension, and typically for optimization with input mixed states, the rank of extremal POVMs can be easily larger than one, as shown in Refs. 15–17.

In a specific application the optimal POVM does not necessarily attain the whole accessible information. At first sight, this assertion may appear contradictory: how a POVM can be optimal, if it wastes accessible information? However, once the measurement is performed, no other possibility for optimization is left apart from the processing of the outcome—*postprocessing* for short—and, being purely classical, the postprocessing cannot generally achieve the same result of a *preprocessing* by a quantum channel. The situation is depicted in Fig. 1. Clearly, the preprocessing can change the POVM irreversibly, reducing the information from the measurement. On the other hand, it is possible that a POVM optimal for a given criterion is obtainable from another *cleaner* one via an irreversible preprocessing as in Fig. 1(b). This means that in some cases we need to give up some *quantity* of information for the *quality* of the information.

The above-mentioned scenario poses the problem of *which POVMs are "undisturbed,"* namely *are not irreversibly connected to another POVM*. We will call such POVMs *clean*—in a sense a clean POVM would be "perfect," since it would not have any additional "extrinsical" noise, or it has lost no information irreversibly. Quite surprisingly, as announced, in this article we will see that the *cleanness* property of the POVM is largely unrelated to its extremality, and there are clean POVMs that are not extremal and vice versa. The problem of classifying clean POVMs turns out to be more difficult than that of classifying extremal ones, and in this article we will give a complete classification of clean POVMs only for a number n of outcomes $n \leqslant d$, whereas for $n > d$ we will give a set of interesting necessary conditions, and an iff condition for the case of informationally complete POVMs for $n = d^2$. Clearly, the need for a number of outcomes $n > d$ can be required by the particular optimization problem (see, e.g., Refs. 18 and 19), however, no more than $n = d^2$ elements are needed, which is the maximum number of outcomes for extremality.[15] Davies[20] proved d^2 to be an upper bound for the maximal cardinality of the POVM needed to attain the accessible information, and still it is debated if d^2 outcomes are actually needed (the cases of Refs. 18 and 19 proved that the lower bound is actually larger than d). This difficulties reflect those in classifying cleanness for $n > d$. In a sense it is clear that d^2 elements are needed to retrieve the accessible information, when the kind of information needs to be decided after the measurement has been performed. Indeed, an extremal POVM with d^2 outcomes is versatile to any kind of information encoding, as it is "informationally complete,"[21] namely it makes it possible to estimate any ensemble average by changing only the data processing of the outcomes (such an extremal measurement with d^2 elements can be proved to exist for any dimension d[15]). Clearly, for an extremal informationally complete measurement, a further optimization step can be achieved at the level of data processing,[22,23] once the kind of information of interest has been decided. Thus,

the postprocessing of the measurement is still a useful tool in retrieving the right information from a measurement.

The article is organized as follows. After introducing some notations and prerequisites in Sec. II, in Sec. III we state some general results about channels and POVMs which will be used throughout the article. In Sec. IV we analyze the convex set of channels connecting two POVMs. Section V is devoted to a complete analysis of the classical postprocessing, and give a complete characterization of "cleanness" under postprocessing. Section VI addresses the problem of the preprocessing ordering of POVMs, namely if a POVM is "cleaner" than another, and when they are "equivalent," which corresponds to the possibility of reversing the action of the channel connecting the two POVMs. Section VIII shows that for dimension $d=2$ equivalence under cleanness is the same as unitary equivalence. Section IX fully solves the case of number of outcomes $n \leqslant d$, and gives some interesting alternative theorems for the case of *effects*, namely the two-outcome POVMs. Section X analyzes the case of informationally complete POVMs, giving also an iff condition characterizing the clean POVMs. Section XI gives some conditions for rank-one measurements. Finally, we conclude the paper in Sec. XII with a list of most relevant results and of the main open problems.

II. NOTATION AND PREREQUISITES

Throughout this article we will consider a quantum system with Hilbert space H with finite dimension $d=\dim(\mathsf{H})$, and denote by S the set of states on H (corresponding to a positive unit-trace operator on H), and by $\mathsf{B}(\mathsf{H})$ the algebra of bounded operators on H. We will use capital script fonts e.g., $\mathcal{A},\mathcal{B},\ldots$, to denote operator algebras in $\mathsf{B}(\mathsf{H})$, and with the symbol $\mathcal{A}'$ we will denote the commutant of $\mathcal{A}$, namely the algebra defined as $\mathcal{A}' \doteq \{Y \in \mathsf{B}(\mathsf{H}) \,|\, [X,Y]=0, X \in \mathcal{A}\}$. Completely positive trace-preserving (CPT) and identity-preserving maps on S and $\mathsf{B}(\mathsf{H})$, respectively—all generally referred to as *channels*—will be denoted by capital calligraphic letters, e.g., $\mathcal{A},\mathcal{B},\ldots$, whereas we will always use capital Roman letters for operators. We will restrict attention to POVMs $\{P_e\}_{e\in\mathsf{E}}$ with finite sampling space E, namely

$$P_e \geqslant 0, \quad \forall\, e \in \mathsf{E}, \quad \sum_{e\in\mathsf{E}} P_e = I. \tag{1}$$

We will extensively use the vector notation $\mathbf{P} \equiv \{P_e\}$, $\mathsf{E}(\mathbf{P})$ denoting the sampling space of $\mathbf{P}$, and $|\mathbf{P}|$ the cardinality of $\mathsf{E}(\mathbf{P})$. The vector notation will be naturally extended to tensor products—e.g., $\mathbf{P}\otimes\mathbf{Q}$ for the POVM $\{P_e \otimes Q_f\}_{e\in\mathsf{E}(\mathbf{P}),f\in\mathsf{E}(\mathbf{Q})}$ on $\mathsf{H}\otimes\mathsf{H}$—and to functionals—e.g., $\mathrm{Tr}[\rho\mathbf{P}]$ for the vector of probabilities $\mathrm{Tr}[\rho P_e]$. By $\mathsf{Span}(\mathbf{P})$ we will denote the linear operator space spanned by the POVM elements $\{P_e\}_{e\in\mathsf{E}(\mathbf{P})}$, and by $\mathsf{Rng}(\mathbf{P})$ the range of the POVM $\mathbf{P}$, which is defined as the following convex subset of $\mathbb{R}_+^{|\mathbf{P}|}$

$$\mathsf{Rng}(\mathbf{P}) \doteq \{\mathbb{R}_+^{|\mathbf{P}|} \ni \boldsymbol{p} = \mathrm{Tr}[\rho\mathbf{P}], \quad \rho \in \mathsf{S}\}. \tag{2}$$

The convex set of POVMs with cardinality N will be denoted by $\mathcal{P}_N$.

Finally, we will use the symbol $|A\rangle\rangle$ to denote the following bipartite vector in $\mathsf{H}\otimes\mathsf{H}$

$$|A\rangle\rangle \doteq \sum_{m,n=1}^{d} A_{m,n}|m\rangle|n\rangle, \tag{3}$$

where $A \in \mathsf{B}(\mathsf{H})$ is the operator corresponding to the $d\times d$ matrix with elements $A_{m,n}$ on the basis $\{|n\rangle\}$. One can easily verify the following useful identities

$$A \otimes B^{\mathsf{T}}|C\rangle\rangle = |ACB\rangle\rangle,$$

$$\mathrm{Tr}_1[|A\rangle\rangle\langle\langle B|] = A^{\mathsf{T}}B^*, \tag{4}$$

$$\mathrm{Tr}_2[|A\rangle\rangle\langle\langle B|] = AB^\dagger,$$

where X^T denotes the transpose in the basis $\{|n\rangle\}$, while X^* is the complex conjugate in the same basis. Tr_i denotes the partial trace on the ith space.

III. USEFUL LEMMAS ABOUT CHANNELS AND POVMs

In the following we will name a map $\mathcal{E}$ *spectrum-width decreasing* when it reduces the "spectral width" of a real symmetric operator X, namely when

$$[\lambda_m(\mathcal{E}(X)), \lambda_M(\mathcal{E}(X))] \subseteq [\lambda_m(X), \lambda_M(X)], \tag{5}$$

$\lambda_M(X)$ and $\lambda_m(X)$ denoting the maximum and minimum eigenvalues of X, respectively.

Lemma III.1: Channels are spectrum-width decreasing.

Proof: Consider the eigenvector $|\psi_j\rangle$ of $\mathcal{E}(X)$ corresponding to the eigenvalue $\lambda_j(\mathcal{E}(X))$. One has

$$\lambda_j(\mathcal{E}(X)) = \mathrm{Tr}[\mathcal{E}(X)|\psi_j\rangle\langle\psi_j|] = \mathrm{Tr}[X\mathcal{E}^\mathsf{T}(|\psi_j\rangle\langle\psi_j|)] \in [\lambda_m(X), \lambda_M(X)], \tag{6}$$

since the dual map $\mathcal{E}^\mathsf{T}$ is CPT. ■

Notice that in the above-mentioned lemma the identity-preserving condition is crucial, since the lemma would not hold for a CPT map $\mathcal{E}$, e.g., $\mathcal{E}(\rho)=|\psi\rangle\langle\psi|$, and the spectral width increases from $[\lambda_m(\rho), \lambda_M(\rho)]$ to $[0, 1]$.

The inverse of a non-unitary invertible channel is necessarily not completely positive.

Theorem III. 2 (Wigner): *Any invertible channel has CP inverse iff it is unitary*.

Proof: Let $\mathcal{E}_1$ and $\mathcal{E}_2$ be two channels such that $\mathcal{E}_2^\mathsf{T} \circ \mathcal{E}_1^\mathsf{T}(\rho)=\rho$. Hence:

$$|\psi\rangle\langle\psi| = \sum_{ij} B_j A_i |\psi\rangle\langle\psi| A_i^\dagger B_j^\dagger, \quad \forall\, |\psi\rangle, \tag{7}$$

where A_i and B_j are canonical Kraus representations for $\mathcal{E}_1$ and $\mathcal{E}_2$, respectively. Since all terms in the sum are positive, this means that $B_j A_i|\psi\rangle = \beta_{ij}^{\psi}|\psi\rangle$, for all $|\psi\rangle$ and all i,j. By linearity, it is clear that β_{ij} cannot depend on $|\psi\rangle$, implying that $B_j A_i = \beta_{ij} I$, for all i,j.

We can now prove that $\beta_{ij} \neq 0$, for all i,j. Otherwise, there exists a couple of operators B_k and A_l for which $B_k A_l = 0$. These two operators must both be noninvertible, since, if one is invertible, the other has to be null, and we can without loss of generality (w.l.o.g.) drop it from the Kraus representation (7). Let us fix the couple k,l for which $B_k A_l = 0$, namely both are not invertible. Now, the only possibility to have $B_j A_i = \beta_{ij} I$ for all i,j is that $B_k A_i = 0$ for all i (since B_k is not invertible, whence necessarily $B_k A_i$ cannot be full rank), and analogously $B_j A_l = 0$ for all j. In this case, all B_j's supports would be forced to be contained in the orthogonal complement to the range of A_l (which is strictly contained in the full Hilbert space), and this would be in contradiction with the normalization condition $\Sigma_j B_j^\dagger B_j = I$. Therefore, $\beta_{ij} \neq 0$ for all i,j, and the operators A_i and B_j are all invertible. This allows us to write

$$\begin{aligned} B_j &= \beta_{ij} A_i^{-1}, \quad \forall\, j, \\ A_i &= \beta_{ij} B_j^{-1}, \quad \forall\, i, \end{aligned} \tag{8}$$

whence all B_j's are proportional to each other, and analogously for the A_i. In other words, the Kraus representations of $\mathcal{E}_1$ and $\mathcal{E}_2$ are made of only one operator. This means that $\mathcal{E}_1$ and $\mathcal{E}_2$ are unitary, one the inverse of the other.

The converse direction is trivial. In Corollary X.4, we will prove that the inverse map of an invertible nonunitary channel is indeed nonpositive. ■

Theorem III.3 (Chefles, Jozsa, Winter): *Consider two sets of pure states on* H *with the same cardinality. There exist two channels mapping the elements of the first set to the corresponding elements of the second set and vice versa, iff the two sets of states are unitarily equivalent*.

Proof: See Ref. 24. ■

Lemma III.4. (Lindblad): A channel $\mathcal{E}$ stabilizes an algebra $\mathcal{S}\subseteq\mathsf{B}(\mathsf{H})$, namely

$$\mathcal{E}(X)=X, \quad \forall\, X\in\mathcal{S}, \tag{9}$$

iff the operators $\{E_k\}$ of any Kraus form $\mathcal{E}(X)=\Sigma_k E_k^\dagger X E_k$ belong to the commutant $\mathcal{S}'$ of the algebra $\mathcal{S}$.

Proof: See Ref. 25. ■

Finally let us state some results about extendiblity of completely positive maps (mostly taken from Ref. 26). To this end let us consider a linear subset $\mathcal{S}$ of $\mathsf{B}(\mathsf{H})$ which contains the identity and is closed under adjoints—each set $\mathcal{S}$ of this type will be called in the following an *operator system*. It is easy to see that $\mathcal{S}$ is generated (as a linear space) by its positive elements. It makes therefore sense to speak about positive maps $\mathcal{E}:\mathcal{S}\to\mathcal{A}$ into an algebra $\mathcal{A}$ and we can define also *complete positivity* in the usual way. Now the question arises whether such an $\mathcal{E}$ can be extended *as a completely positive map* to $\mathsf{B}(\mathsf{H})$. The following theorem gives a positive answer (Ref. 26, Theorems 6.2 and 7.5):

Theorem III.5. (Arveson's extension theorem): *Each completely positive map $\mathcal{E}:\mathcal{S}\to\mathsf{B}(\mathsf{H})$ defined on an operator system $\mathcal{S}\subset\mathsf{B}(\mathsf{H})$ can be extended to a completely positive map on $\mathsf{B}(\mathsf{H})$.*

If $\mathcal{E}$ is only positive (and not necessarily completely positive) a similar result is not available (cf. the corresponding discussion in Sec. VII). An important exception arises however, if the algebra $\mathcal{A}$ is abelian (Ref. 26, Theorem 3.9).

Theorem III.6: *If $\mathcal{E}:\mathcal{S}\to\mathcal{A}$ is positive, $\mathcal{S}$ an operator system and $\mathcal{A}$ an abelian algebra, the map $\mathcal{E}$ is completely positive.*

IV. THE CONVEX SET OF CHANNELS CONNECTING TWO POVMs

We now analyze the convex set of channels connecting two given POVMs **P** and **Q**, in equations

$$\mathcal{C}_{\mathbf{PQ}}=\{\mathcal{E}\ \text{channel}|\mathcal{E}(\mathbf{P})=\mathbf{Q}\}. \tag{10}$$

The extremal elements of $\mathcal{C}_{\mathbf{PQ}}$ can be characterized in terms of the operators $\{E_i\}$ of the canonical Krauss decomposition by the following theorem.

Theorem IV.1: *The map $\mathcal{E}\in\mathcal{C}_{\mathbf{PQ}}$ is extremal iff for some element P_k of the POVM* **P** *the operators $\{E_i^\dagger P_k E_j\}_{ij}$ made with the canonical Kraus operators $\{E_i\}$ of the map are linearly independent.*

Proof: First we show by contradiction that the condition is sufficient. In fact, suppose that $\mathcal{E}$, with $\{E_i^\dagger P_k E_j\}_{ij}$ linearly independent, is not extremal in $\mathcal{C}_{\mathbf{PQ}}$. Then there exist two different channels $\mathcal{E}_\pm\in\mathcal{C}_{\mathbf{PQ}}$ such that

$$\mathcal{E}=\tfrac{1}{2}(\mathcal{E}_+ +\mathcal{E}_-). \tag{11}$$

Upon defining $\mathcal{P}\equiv\mathcal{E}_+-\mathcal{E}$, clearly one has $\mathcal{P}(\mathbf{P})=0$ and $\mathcal{E}\pm\mathcal{P}=\mathcal{E}_\pm$, which are channels. Then $R_{\mathcal{E}_\pm}\equiv R_{\mathcal{E}}\pm R_{\mathcal{P}}\geqslant 0$, where for any channel $\mathcal{E}$ the positive operator $R_{\mathcal{E}}$ in linear correspondence with $\mathcal{E}$ is defined as $R_{\mathcal{E}}=\Sigma_j|E_j\rangle\rangle\langle\langle E_j|$ for $\{E_j\}$ Kraus operators of $\mathcal{E}$.[27] This implies that $\mathsf{Supp}(R_{\mathcal{P}})\subseteq\mathsf{Supp}(R_{\mathcal{E}})$, namely there exists a nonvanishing matrix p_{ij} such that $R_{\mathcal{P}}=\Sigma_{ij}p_{ij}|E_i\rangle\rangle\langle\langle E_j|$. As a consequence we have

$$\mathcal{P}(P_k)=\sum_{ij}p_{ij}E_i^\dagger P_k E_j=0, \quad \forall\, k. \tag{12}$$

This contradicts the hypothesis. The proof that it is also necessary is now straightforward. Suppose indeed that the operators $\{E_i^\dagger P_k E_j\}_{ij}$ are linearly dependent. Then there exists a nonvanishing matrix of coefficients a_{ij} such that $\Sigma_{ij}a_{ij}E_i^\dagger P_k E_j=0$ for all k. If we define $p_{ij}=\kappa(a_{ij}+a_{ij}^*)$, then the map $\mathcal{P}(X)=\Sigma_{ij}p_{ij}E_j^\dagger X E_i$ will annihilate all elements of the POVM **P**, namely $\mathcal{P}(\mathbf{P})=0$. Moreover,

for a sufficiently small $\kappa \neq 0$ both maps $\mathcal{E}_{\pm}=\mathcal{E}\pm\mathcal{P}$ will be channels and will belong to $\mathcal{C}_{\mathbf{PQ}}$. This implies that $\mathcal{E}=\frac{1}{2}(\mathcal{E}_{+}+\mathcal{E}_{-})$, namely $\mathcal{E}$ is not extremal. ■

One can prove that either any element of the border of $\mathcal{C}_{\mathbf{PQ}}$ is also an element of the border of the full convex set of channels, or $\mathcal{C}_{\mathbf{PQ}} \equiv \{\mathcal{E}\}$. This comes from the definition of the border of a convex set

Definition IV.2: For a convex set $\mathcal{C}$, an element $p \in \mathcal{C}$ belongs to its boundary $\partial\mathcal{C}$ if and only if there exists $q \in \mathcal{C}$ such that

$$p + \epsilon(q-p) \in \mathcal{C}, \quad p - \epsilon(q-p) \notin \mathcal{C}, \quad \forall\, \epsilon \in [0,1],. \tag{13}$$

or, equivalently iff there exists $q \in \mathcal{C}$ such that for all $\epsilon > 0$ for which $p+\epsilon q \in \mathcal{C}$ then $p-\epsilon q \notin \mathcal{C}$.

We will now prove the following lemma.

Lemma IV.3: The border of the convex $\mathcal{C}_{\mathbf{PQ}}$ is a subset of the border of the convex of all channels.

Proof: Consider a channel $\mathcal{E} \in \mathcal{C}_{\mathbf{PQ}}$ and a "perturbation" $\mathcal{P}$ such that $\mathcal{E}+\epsilon\mathcal{P} \in \mathcal{C}_{\mathbf{PQ}} \forall\, \epsilon \in [0, 1]$. By definition $\mathcal{P}(P_i)=0$ for all P_i, whence, if $\mathcal{E}-\epsilon\mathcal{P}$ is completely positive, then it necessarily belongs to $\mathcal{C}_{\mathbf{PQ}}$. Therefore, the only way to have $\mathcal{E}$ on the border of $\mathcal{C}_{\mathbf{PQ}}$ is to have $\mathcal{E}-\epsilon\mathcal{P}$ not CP, namely $\mathcal{E}$ lies on the border of the convex of all channels. ■

A "geometrical" proof is also the following. Since the constraint defining $\mathcal{C}_{\mathbf{PQ}}$ is linear, then $\mathcal{C}_{\mathbf{PQ}}$ is a linear section of the convex of all channels, whence its border belongs to the border of the convex of all channels.

Remark: Notice that the convex set $\mathcal{C}_{\mathbf{II}}$ will coincide with that of all channels, $\mathbf{I}=\{I\}$ denoting the trivial POVM.

Remark: From Lemma IV.3 it follows that when two POVMs are connected by a channel they can be always connected by a border channel, apart from the case in which the connecting channel is unique.

V. POSTPROCESSING

The most general postprocessing of a POVM, is a shuffling of the POVM elements with conditional probability $p(i|j)$, corresponding to the mapping

$$Q_i = \sum_j p(i|j) P_j. \tag{14}$$

When two POVMs $\mathbf{P}$ and $\mathbf{Q}$ are connected by a mapping of the form (14) for some conditional probability $p(i|j)$ we will write $\mathbf{P} >_p \mathbf{Q}$, and say that the POVM $\mathbf{P}$ is *cleaner under postprocessing*—for short *postprocessing cleaner*—than the POVM $\mathbf{Q}$. Notice that a relation of the form (14) is meaningful generally for $|\mathbf{P}| \neq |\mathbf{Q}|$, with the number of outcomes changing from input to output.

Relevant examples of post processing are:

(i) identification of two outcomes, e.g., j and k are identified with the same outcome l, corresponding to $p(n|j)=\delta_{ln}$, $p(n|k)=\delta_{ln}$ and

(ii) permutation π of outcomes, corresponding to $p(\pi(j)|k)=\delta_{jk}$.

The relation $>_p$ is a pseudo-ordering, since it is

(i) reflexive, corresponding to

$$\mathbf{P} >_p \mathbf{P}, \quad p(i|j) = \delta_{ij}; \tag{15}$$

(ii) transitive, i.e., $\mathbf{P} >_p \mathbf{Q} >_p \mathbf{R}$, corresponding to

$$R_i = \sum_j p(i|k) Q_k,\ Q_k = \sum_j p'(k|j) P_j, \Rightarrow R_i = \sum_j p''(i|j) P_j,$$

$$p''(i|j) = \sum_k p(i|k)p'(k|j). \tag{16}$$

An equivalence relation under postprocessing can be defined as follows.

Definition V.1: The POVMs $\mathbf{P}$ *and* $\mathbf{Q}$ *are* postprocessing equivalent—*in symbols* $\mathbf{P} \simeq_p \mathbf{Q}$—*iff both relations* $\mathbf{P} \succ_p \mathbf{Q}$ *and* $\mathbf{Q} \succ_p \mathbf{P}$ *hold.*

We are now in position to define *cleanness under postprocessing*, namely

Definition V.2: A POVM $\mathbf{P}$ *is* postprocessing clean *if for any POVM* $\mathbf{Q}$ *such that* $\mathbf{Q} \succ_p \mathbf{P}$, *then also* $\mathbf{P} \succ_p \mathbf{Q}$ *holds, namely* $\mathbf{P} \simeq_p \mathbf{Q}$.

The characterization of cleanness under postprocessing (classical) is much easier than that of cleanness under preprocessing (quantum), and is given by the following theorem.

Theorem V.3: *A POVM* $\mathbf{P}$ *is postprocessing clean iff it is rank-one.*

Proof: First notice that a POVM $\mathbf{P}$ with elements having rank higher than one are not postprocessing clean. In fact, in this case one can diagonalize all the POVM elements and consider the POVM $\mathbf{P}'$ made of rank-one projections over all eigenvectors multiplied by the corresponding eigenvalue. Then, clearly $\mathbf{P}' \succ_p \mathbf{P}$ by identification of outcomes. In equations

$$P_i = \sum_{k_i} |\lambda_{k_i}^{(i)}\rangle\langle\lambda_{k_i}^{(i)}|, \quad P'_{i,k} = |\lambda_k^{(i)}\rangle\langle\lambda_k^{(i)}|, \Rightarrow \mathbf{P}' \succ_p \mathbf{P}, \tag{17}$$

corresponding to the identification of outcomes

$$p(i|j,k_j) = \delta_{ij} \,\forall\, k_j. \tag{18}$$

Reversely, all rank-one POVMs are postprocessing clean, namely if $\mathbf{Q} \succ_p \mathbf{P}$, then also $\mathbf{P} \simeq_p \mathbf{Q}$ must hold. In fact, suppose that $\mathbf{P}$ is rank one and that there exists a POVM $\mathbf{Q}$ such that $\mathbf{Q} \succ_p \mathbf{P}$, namely

$$P_i = \sum_j p(i|j)Q_j. \tag{19}$$

Now, since all elements P_i are rank one, the elements Q_j are necessarily proportional to P_i for all the indices j such that $p(i|j) \neq 0$, namely also $\mathbf{Q}$ is rank one, with

$$p(i|j)Q_j = \alpha_j P_i, \tag{20}$$

with $\Sigma_j \alpha_j = 1$, and $\alpha_j \geqslant 0$. For a fixed j, $p(i|j) = 0$ for at least one i, otherwise all the P_i's would be proportional. For the same reason, for a fixed i, $p(i|j) = 0$ for at least one j. We can then collect the indices i such that $p(i|j) \neq 0$ in the set $I(j)$, and write

$$Q_j = \sum_i p(i|j)Q_j = \sum_{i \in I(j)} p(i|j)Q_j = \sum_{i \in I(j)} \alpha_j P_i. \tag{21}$$

Finally, it is immediately verified that

$$q(j|i) = \begin{cases} \alpha_j, & i \in I(j) \\ 0 & \text{otherwise} \end{cases} \tag{22}$$

is a conditional probability since for all i one has $\Sigma_j q(j|i) = \Sigma_j \alpha_j = 1$. Therefore, from Eq. (21) it follows that we have also $\mathbf{P} \succ_p \mathbf{Q}$, namely $\mathbf{P} \simeq_p \mathbf{Q}$. ■

VI. PREPROCESSING: ORDERING AND EQUIVALENCE OF POVMs

The action of channels allows to define the following pseudo-ordering.

Definition VI.1: Given the POVMs $\mathbf{P}$ *and* $\mathbf{Q}$ *with* $|\mathbf{P}| = |\mathbf{Q}|$ *we define* $\mathbf{P} \succ \mathbf{Q}$ *iff there exists a channel* $\mathcal{E}$ *such that*

$$\mathbf{Q} = \mathcal{E}(\mathbf{P}), \tag{23}$$

and we will say that the POVM $\mathbf{P}$ *is cleaner than the POVM* $\mathbf{Q}$.

Definition VI.2: We call a POVM $\mathbf{P}$ *"clean" iff for any POVM* $\mathbf{Q}$ *such that* $\mathbf{Q}\succ\mathbf{P}$ *one also has* $\mathbf{P}\succ\mathbf{Q}$.

It is easily proved that the relation $\succ$ is transitive and reflexive, namely it is a pseudo-ordering. Let us now define the following relation

Definition VI.3: We say that the two POVMs $\mathbf{P}$ *and* $\mathbf{Q}$ *are equivalent—denoted as* $\mathbf{P}\simeq\mathbf{Q}$*—when one has both* $\mathbf{P}\succ\mathbf{Q}$ *and* $\mathbf{Q}\succ\mathbf{P}$.

Clearly $\simeq$ is an equivalence relation. The pseudo-ordering $\succ$ now defines a partial ordering between equivalence classes. Indeed define the ordering between classes as follows:

$$[\mathbf{P}]\succcurlyeq[\mathbf{Q}] \quad \text{iff} \quad \mathbf{P}'\succ\mathbf{Q}', \quad \forall\,\mathbf{P}'\in[\mathbf{P}], \quad \mathbf{Q}'\in[\mathbf{Q}]. \tag{24}$$

The above-mentioned ordering is consistently defined, since $\mathbf{P}',\mathbf{P}''\in[\mathbf{P}]$ means both $\mathbf{P}'\succ\mathbf{P}''$ and $\mathbf{P}''\succ\mathbf{P}'$, whence, by transitivity $\mathbf{P}''\succ\mathbf{P}'\succ\mathbf{Q}'\succ\mathbf{Q}''$, and the ordering does not depend on the chosen elements of the equivalence classes. This proves the consistency of the definition of $\succcurlyeq$. Therefore, in the following we can consider a single element $\mathbf{P}$ instead of the class $[\mathbf{P}]$. In this way we can easily prove reflexivity $[\mathbf{P}]\succcurlyeq[\mathbf{P}]$, since $\mathbf{P}\succ\mathbf{P}$, and transitivity

$$[\mathbf{P}]\succcurlyeq[\mathbf{Q}], \quad [\mathbf{Q}]\succcurlyeq[\mathbf{R}]\Rightarrow[\mathbf{P}]\succcurlyeq[\mathbf{R}], \tag{25}$$

since $\mathbf{P}\succ\mathbf{Q}$, $\mathbf{Q}\succ\mathbf{R}$ implies $\mathbf{P}\succ\mathbf{R}$ by transitivity of $\succ$. Now let us consider the case when both $[\mathbf{P}]\succcurlyeq[\mathbf{Q}]$ and $[\mathbf{Q}]\succcurlyeq[\mathbf{P}]$. Then we have $\mathbf{P}\succ\mathbf{Q}$ and $\mathbf{Q}\succ\mathbf{P}$, namely $[\mathbf{P}]\equiv[\mathbf{Q}]$. ■

One would be tempted to conjecture that the relation $\simeq$ is equivalent to unitary equivalence, which is defined through

Definition VI.4: The POVMs $\mathbf{P}$ *and* $\mathbf{Q}$ *are unitarily equivalent, for short* $\mathbf{P}\simeq_U\mathbf{Q}$ *iff there exists a unitary operator* U *such that* $\mathbf{Q}=U\mathbf{P}U^\dagger$.

However, as we will see in the following, there exist equivalent POVMs which are not unitarily equivalent.

We have now the following necessary condition for equivalence under preprocessing

Theorem VI.5: *If* $\mathbf{P}\simeq\mathbf{Q}$ *then for each event* $e\in\mathsf{E}(\mathbf{P})$ *we have*

$$\lambda_M(P_e)=\lambda_M(Q_e)\equiv\lambda_M(e), \quad \lambda_m(P_e)=\lambda_m(Q_e)\equiv\lambda_m(e). \tag{26}$$

Proof: By Lemma III.1 we have both $\lambda_M(P_i)\geqslant\lambda_M(Q_i)$ and $\lambda_M(P_i)\leqslant\lambda_M(Q_i)$, and similarly for the minimum eigenvalues. ■

VII. PREPROCESSING: POSITIVE MAPS AND RELATED THEOREMS

There are two interesting variants of the relation $\succ$ just introduced, which help to get a more geometric insight into the structure. The first arises, if we replace the completely positive map $\mathcal{E}$ in Definition VI.1 by positive (but not necessarily *completely* positive) one. Hence we can define for two POVMs $\mathbf{P}$, $\mathbf{Q}$ with $|\mathbf{P}|=|\mathbf{Q}|$

$$\mathbf{P}\gg\mathbf{Q}\Leftrightarrow\mathbf{Q}=\mathcal{E}(\mathbf{P}), \quad \mathcal{E}\ \text{positive}. \tag{27}$$

It is obvious that $\mathbf{P}\succ\mathbf{Q}$ implies $\mathbf{P}\gg\mathbf{Q}$ but the other way round does not hold. This can be seen, if we consider an informationally complete POVM $\mathbf{P}$ and define $\mathbf{Q}=\Theta(\mathbf{P})$, where Θ denotes the transposition map (i.e. $\Theta(A)=A^\mathsf{T}$). Positivity of Θ implies $\mathbf{P}\gg\mathbf{Q}$. But Θ is only positive and not completely positive and it is the only map which connects $\mathbf{P}$ and $\mathbf{Q}$. The latter follows from informational completeness of $\mathbf{P}$, because this implies that the elements of $\mathbf{P}$ are a basis of $\mathsf{B}(\mathsf{H})$. Hence $\mathbf{P}\succ\mathbf{Q}$ *does not hold.*

Now consider the *ranges* $\mathsf{Rng}(\mathbf{P})$, $\mathsf{Rng}(\mathbf{Q})$ of $\mathbf{P}$ and $\mathbf{Q}$, defined in Eq. (2). If $\boldsymbol{p}\in\mathsf{Rng}(\mathbf{Q})$ there is by definition a density operator ρ with $\boldsymbol{p}=\mathrm{Tr}[\mathbf{Q}\rho]$. Hence, $\mathbf{P}\gg\mathbf{Q}$ implies

$$\boldsymbol{p}=\mathrm{Tr}[\mathbf{Q}\rho]=\mathrm{Tr}[\mathcal{E}(\mathbf{P})\rho]=\mathrm{Tr}[\mathbf{P}\mathcal{E}^\mathsf{T}(\rho)] \tag{28}$$

and therefore we get $\boldsymbol{p}\in\mathsf{Rng}(\mathbf{P})$. This observation motivates the definition:

$$\mathbf{P} \supset_r \mathbf{Q} \Leftrightarrow \mathsf{Rng}(\mathbf{Q}) \subset \mathsf{Rng}(\mathbf{P}). \tag{29}$$

According to our previous discussion we get in this way a hierarchy of relations

$$\mathbf{P} \succ \mathbf{Q} \Rightarrow \mathbf{P} \succcurlyeq \mathbf{Q} \Rightarrow \mathbf{P} \supset_r \mathbf{Q}. \tag{30}$$

We have already seen that the direction of the implication between $\succ$ and $\succcurlyeq$ cannot be reversed. For $\succcurlyeq$ and $\supset_r$ this is more difficult. To see that they are (very) closely related, consider the linear hull $\mathsf{Span}(\mathbf{P})$ of the elements of $\mathbf{P}$, which is obviously an *operator system* (cf. Sec. III). Hence we can speak about positive linear maps from $\mathsf{Span}(\mathbf{P})$ to $\mathsf{Span}(\mathbf{Q})$. This fact can be used to characterize the relation $\supset_r$ in the following way.

Proposition VII.1: Consider two POVMs $\mathbf{P}$, $\mathbf{Q}$ *with* $|\mathbf{P}|=|\mathbf{Q}|$. *Then the following statements are equivalent:*

(i) $\mathbf{P} \supset_r \mathbf{Q}$
(ii) *There is a (unique) positive map* $\mathcal{E}$: $\mathsf{Span}(\mathbf{P}) \to \mathsf{Span}(\mathbf{Q})$ *with* $\mathcal{E}(\mathbf{P})=\mathbf{Q}$.

Proof: The implication (ii)$\Rightarrow$(i) is trivial. Hence consider only the other direction. Here, the idea is to define the map $\mathcal{E}$ by

$$\mathcal{E}(P_e) = Q_e, \quad \forall\, e \in \mathsf{E}. \tag{31}$$

This map is well defined because we have (by assumption) for each density operator ρ a second density operator σ such that $\mathrm{Tr}[Q_e\rho]=\mathrm{Tr}[P_e\sigma]$ holds for all $e \in \mathsf{E}$. Hence if $\Sigma_e \lambda_e P_e = 0$ for some real λ_e we get

$$\sum_{e\in\mathsf{E}} \lambda_e \mathrm{Tr}[\rho Q_e] = \sum_{e\in\mathsf{E}} \lambda_e \mathrm{Tr}[\sigma P_e] = \mathrm{Tr}\left[\sigma \sum_{e\in\mathsf{E}} \lambda_e P_e\right] = 0. \tag{32}$$

Since ρ is arbitrary this implies $\Sigma_e \lambda_e Q_e = 0$. Therefore $\mathcal{E}$ defined in (31) is well defined, as stated. Using the same reasoning we can show that $\mathcal{E}$ is positive, which concludes the proof. ■

The difference between condition (ii) of this lemma and the definition of $\succcurlyeq$ in Eq. (27) is the *domain* of the the map $\mathcal{E}$. The following counter example which is taken (in a slightly modified form) from Ref. 26 shows that such a map is in general *not extendible* as a positive map to $\mathsf{B}(\mathsf{H})$.

Consider the diagonal 4×4 matrix $X=\mathrm{diag}(1,i,-1,-i)$ and the operator system $\mathcal{S}$ spanned by $I, X, X^\dagger$. It is easy to see that a general element $A=aI+bX+cX^\dagger$ is Hermitian iff $c=b^*$ and $a=a^*$ hold, and it is positive iff in addition $a \geqslant 2\max(|\Re b|, |\Im b|)$ hence,

$$A \geqslant 0 \Rightarrow c = b^*, \quad a \geqslant \sqrt{2}|b|. \tag{33}$$

Now consider the linear map

$$\mathcal{S} \ni A = aI + bX + cX^\dagger \mapsto \mathcal{E}(A) = \begin{pmatrix} a & \sqrt{2}b \\ \sqrt{2}c & a \end{pmatrix} \otimes I_2, \tag{34}$$

where I_2 denotes the 2×2 unit matrix. Since a 2×2 matrix is positive iff its diagonal elements and its determinant are positive, positivity of $\mathcal{E}$ follows directly from Eq. (33). On the other hand we have $\|\mathcal{E}(I)\|=1$ and $\|\mathcal{E}(X)\|=\sqrt{2}$. Since $\|X\|=1$ this implies $\|\mathcal{E}\| \geqslant \sqrt{2} > \|\mathcal{E}(I)\|$. But a positive map from a C^* algebra $\mathcal{A}$ into a a C^* algebra $\mathcal{B}$ always satisfies (Ref. 26, Corollary 2.9) $\|\mathcal{E}\|=\|\mathcal{E}(I)\|$. Hence the map defined in Eq. (34) can not be extended to $\mathsf{B}(\mathbb{C}^4)$—not even to the abelian algebra generated by $I, X, X^\dagger$. As a consequence of this reasoning we have shown that $\mathbf{P} \supset_r \mathbf{Q}$ *does not imply* $\mathbf{P} \succcurlyeq \mathbf{Q}$.

Hence positive maps can in general not be extended as a *positive* map to a bigger algebra. A very important special case arises, however, if the map $\mathcal{E}$ is *completely* positive. In this case a completely positive extension always exists (cf. Theorem III.5) This fact can be used along with Proposition VII.1 to get an interesting characterisation of $\succ$ in terms of ranges.

Theorem VII.2: *Consider two POVMs* $\mathbf{P}$, $\mathbf{Q}$ *with* $|\mathbf{P}|=|\mathbf{Q}|$. *Then the following statements are equivalent:*

(i) $\mathbf{P}\succ\mathbf{Q}$
(ii) *There is an informationally complete POVM* $\mathbf{M}$ *such that* $\mathbf{P}\otimes\mathbf{M}\supset_r\mathbf{Q}\otimes\mathbf{M}$
(iii) $\mathbf{P}\otimes\mathbf{M}\supset_r\mathbf{Q}\otimes\mathbf{M}$ *holds for all POVMs* $\mathbf{M}$.

Proof: The implication (i)$\Rightarrow$(iii) follows from the fact that (i) implies the existence of a map $\mathcal{E}$ such that $\mathbf{Q}=\mathcal{E}(\mathbf{P})$, and trivially the map $\mathcal{E}\otimes\mathcal{I}$ connects $\mathbf{P}\otimes\mathbf{M}$ with $\mathbf{Q}\otimes\mathbf{M}$, whence the statement via Eq. (29). Implication (i)$\Rightarrow$(ii) is just a special case of the previous one. Implication (iii)$\Rightarrow$(ii) is trivial. Hence only (ii)$\Rightarrow$(i) remains to be shown.

To this end note that informational completeness of $\mathbf{M}$ implies

$$\mathsf{Span}(\mathbf{Q}\otimes\mathbf{M})=\mathsf{Span}(\mathbf{Q})\otimes\mathsf{B}(\mathsf{H}), \tag{35}$$

and similarly for $\mathbf{P}\otimes\mathbf{M}$. Therefore we have [according to (ii) and Proposition VII.1] a unique positive map

$$\mathcal{F}:\mathsf{Span}(\mathbf{P})\otimes\mathsf{B}(\mathsf{H})\rightarrow\mathsf{Span}(\mathbf{Q})\otimes\mathsf{B}(\mathsf{H}) \tag{36}$$

with

$$\mathcal{F}(\mathbf{P}\otimes\mathbf{M})=\mathbf{Q}\otimes\mathbf{M}. \tag{37}$$

If we can show that $\mathcal{F}$ has the form

$$\mathcal{F}=\mathcal{E}\otimes\mathcal{I} \tag{38}$$

with a positive map $\mathcal{E}$: $\mathsf{Span}(\mathbf{P})\rightarrow\mathsf{Span}(\mathbf{Q})$ and the identity $\mathcal{I}$ on $\mathsf{B}(\mathsf{H})$, the theorem is proved because:

- Due to Eq. (38) and positivity of $\mathcal{F}$ the map $\mathcal{E}$ is completely positive as a map on the *operator system* $\mathsf{Span}(\mathbf{P})$. Hence by theorem III.5 it is extendible to a completely positive map on $\mathsf{B}(\mathsf{H})$.
- Eqs. (37) and (38) imply $\mathcal{E}(\mathbf{P})=\mathbf{Q}$ and therefore $\mathbf{P}\succ\mathbf{Q}$.

To prove Eq. (38) firstly note that (ii) implies $\mathbf{P}\supset_r\mathbf{Q}$. This follows from (with $e\in\mathsf{E}(\mathbf{Q})$ and a density matrix ρ on H):

$$\mathrm{Tr}[\rho Q_e]=\mathrm{Tr}\left[\frac{\rho\otimes I}{d}\left(Q_e\otimes\sum_{f\in\mathsf{E}(\mathbf{M})}M_f\right)\right] \tag{39}$$

$$=\sum_{f\in\mathsf{E}(\mathbf{M})}\mathrm{Tr}\left[(Q_e\otimes M_f)\left(\rho\otimes\frac{I}{d}\right)\right] \tag{40}$$

because we have by assumption a density matrix σ on $\mathsf{H}\otimes\mathsf{H}$ such that

$$\mathrm{Tr}\left[(\mathbf{Q}\otimes\mathbf{M})\left(\rho\otimes\frac{I}{d}\right)\right]=\mathrm{Tr}[(\mathbf{P}\otimes\mathbf{M})\sigma] \tag{41}$$

which in turn implies

$$\mathrm{Tr}[\rho Q_e]=\sum_{f\in\mathsf{E}(\mathbf{M})}\mathrm{Tr}[(P_e\otimes M_f)\sigma] \tag{42}$$

$$=\mathrm{Tr}\left[P_e\otimes\left(\sum_{f\in\mathsf{E}(\mathbf{M})}M_f\right)\sigma\right] \tag{43}$$

$$= \mathrm{Tr}[(P_e \otimes I)\sigma] = \mathrm{Tr}[P_e \, \mathrm{Tr}_2 \, \sigma], \tag{44}$$

where Tr_2 denotes the partial trace over the second tensor factor. Hence $\mathrm{Tr}[\rho\mathbf{Q}] = \mathrm{Tr}[(\mathrm{Tr}_2\sigma)\mathbf{P}]$ which implies $\mathbf{P} \supset_r \mathbf{Q}$ as stated.

Now we can apply again Propostion VII.1 and get a positive map $\mathcal{E}$: $\mathsf{Span}(\mathbf{P}) \to \mathsf{Span}(\mathbf{Q})$ satisfying $\mathcal{E}(\mathbf{P}) = \mathbf{Q}$ and therefore $\mathcal{E} \otimes \mathcal{I}(\mathbf{P} \otimes \mathbf{M}) = \mathbf{Q} \otimes \mathbf{M}$. Since $\mathcal{F}$ is uniquely determined by Eq. (37) this implies $\mathcal{F} = \mathcal{E} \otimes \mathcal{I}$, which completes the proof. ■

This theorem gives a clear geometric picture for the relation $\succ$ and it helps to understand the difference between $\succ$ and $\gg$: if $\mathbf{P} \gg \mathbf{Q}$ holds we find for each *separable state* ρ on $\mathsf{H} \otimes \mathsf{H}$ a second separable state σ such that $\mathrm{Tr}[\mathbf{Q} \otimes \mathbf{M}\rho] = \mathrm{Tr}[\mathbf{P} \otimes \mathbf{M}\sigma]$. Hence, if $\mathbf{P} \succ \mathbf{Q}$ does not hold (but $\mathbf{P} \gg \mathbf{Q}$) there must be an *entangled* state ρ such that the probability vector $\mathrm{Tr}[\mathbf{Q} \otimes \mathbf{M}\rho]$ can not be reproduced by any expectation value of $\mathbf{P} \otimes \mathbf{M}$. This can be rephrased as follows: If $\mathbf{P} \gg \mathbf{Q}$ holds but not $\mathbf{P} \succ \mathbf{Q}$ we can reproduce the distribution of outcomes of $\mathbf{Q}$ measurements on *one system* by appropriate $\mathbf{P}$ measurements, but there is information about entangled states which can be gained only by $\mathbf{Q}$ and not by $\mathbf{P}$.

A second special case of Proposition VII.1 arises, when $\mathbf{Q}$ is abelian (i.e., all elements of the POVM commute). In this case the map $\mathcal{E}$ constructed in Proposition VII.1 is a map into an abelian algebra and therefore completely positive. Hence we get

Theorem VII.3: *Consider two POVMs* $\mathbf{P}, \mathbf{Q}$ *with* $|\mathbf{P}| = |\mathbf{Q}|$ *and assume that* $\mathbf{Q}$ *is abelian. Then* $\mathbf{P} \supset_r \mathbf{Q}$ *and* $\mathbf{P} \succ \mathbf{Q}$ *are equivalent*.

Proof: According to Proposition VII.1 there is a positive map $\mathcal{E}$ from $\mathsf{Span}(\mathbf{P})$ into the abelian C^* algebra $\mathcal{A}$ generated by the elements of $\mathbf{Q}$. According to Theorem III.6 this map is completely positive and by Theorem III.5 therefore extendible as a completely positive map to $\mathsf{B}(\mathsf{H})$. Hence $\mathbf{P} \supset_r \mathbf{Q}$ implies $\mathbf{P} \succ \mathbf{Q}$. Since the other implication is trivial the proof is completed. ■

Note that a similar result does not hold if $\mathbf{P}$ is abelian and $\mathbf{Q}$ is not. The counter example given after Proposition VII.1 applies even in this case.

The result from Theorem VII.3 is very useful, in particular because the range $\mathsf{Rng}(\mathbf{P})$ of an abelian POVM has a very simple structure, which is completely characterized by the joint eigenvalues of the elements of $\mathbf{P}$. To see this, consider a joint set of eigenvectors ψ_α, $\alpha = 1, \ldots, d$ and

$$P_e = \sum_{\alpha=1}^{d} \lambda_{e,\alpha} |\psi_\alpha\rangle\langle\psi_\alpha|, \quad \forall \, e \in \mathsf{E}. \tag{45}$$

The joint eigenvalues vectors

$$\boldsymbol{\lambda}_\alpha = (\lambda_{e,\alpha})_{e \in \mathsf{E}} \in \mathbb{R}^{|\mathbf{P}|} \tag{46}$$

form a set of probability vectors (in the case of joint degeneracies of the elements of $\mathbf{P}$ some of them may coincide) and for each convex linear combination

$$\boldsymbol{p} = \sum_{\alpha=1}^{d} p_\alpha \boldsymbol{\lambda}_\alpha, \quad p_\alpha \geqslant 0, \quad \sum_\alpha p_\alpha = 1 \tag{47}$$

we can find a density operator ($\rho = \Sigma_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$ will do) such that $\boldsymbol{p} = \mathrm{Tr}[\rho\mathbf{P}]$ holds. Hence the *convex hull* of the $\boldsymbol{\lambda}_\alpha$ satisfies $\mathrm{conv}(\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_d) \subset \mathsf{Rng}(\mathbf{P})$. On the other hand we have for each density operator ρ:

$$\mathrm{Tr}[\rho\mathbf{P}] = \sum_{\alpha=1}^{d} \langle\psi_\alpha, \rho\psi_\alpha\rangle \boldsymbol{\lambda}_\alpha \tag{48}$$

which implies $\mathrm{Tr}[\rho\mathbf{P}] \in \mathrm{conv}(\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_d)$. Hence we have just shown the following proposition

Proposition VII.4: The range $\mathsf{Rng}(\mathbf{P})$ *of an abelian POVM* $\mathbf{P}$ *coincides with the convex hull of the* $\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_d$.

The most simple example arises in the case of *effects*, i.e., measurements with two outcomes.

Obviously, each effect is abelian and has the form $\mathbf{P}=\{P, I-P\}$ with a positive operator $P \leqslant I$. If $\mu_1, \ldots, \mu_d$ are the eigenvalues of P given in decreasing order we get $\boldsymbol{\lambda}_\alpha=(\mu_\alpha, 1-\mu_\alpha)$. Hence all $\boldsymbol{\lambda}_\alpha \in \mathbb{R}^2$ are located on the graph of the function $\mathbb{R} \ni x \mapsto 1-x \in \mathbb{R}$, and $\boldsymbol{\lambda}_1$ respectively $\boldsymbol{\lambda}_d$ are the outermost points. This leads immediately to the following characterization of the relation $\succ$ for effects:

Theorem VII.5: *The effect* $\mathbf{P}$ *is "cleaner" than the effect* $\mathbf{Q}$, *i.e.* $\mathbf{P} \succ \mathbf{Q}$ *iff*

$$[\lambda_M(P), \lambda_m(P)] \supseteq [\lambda_M(Q), \lambda_m(Q)]. \tag{49}$$

Corollary VII.6: *Given two effects* $\mathbf{P}$ *and* $\mathbf{Q}$, *then* $\mathbf{P} \simeq \mathbf{Q}$ *iff* $\lambda_M(P)=\lambda_M(Q)$ *and* $\lambda_m(P)=\lambda_m(Q)$.

VIII. PREPROCESSING: EQUIVALENCE IN DIMENSION TWO

For dimension two the cleanness equivalence $\simeq$ and the unitary equivalence $\simeq_U$ coincide.

Theorem VIII.1: *For two-level systems* $\mathbf{P} \simeq \mathbf{Q}$ *iff* $\mathbf{P} \simeq_U \mathbf{Q}$.

Proof: If all the elements of both POVM are trivial, i.e., $P_e=\alpha_e I$ and $Q_e=\beta_e I$, $\forall e$, then the thesis follows easily. Therefore, we will focus on the nontrivial case, in which there exists at least one element P_i of $\mathbf{P}$ (or Q_i of $\mathbf{Q}$) that is nontrivial. Then, first, also Q_i (or P_i) is not proportional to the identity, since otherwise $P_i=\mathcal{F}(Q_i)=\alpha_i \mathcal{F}(I)=\alpha_i I$, which contradicts the hypothesis. Second, by Theorem VI.5 one has

$$P_i = \lambda_M(i) |\phi_M^{(i)}\rangle\langle\phi_M^{(i)}| + \lambda_m(i) |\phi_m^{(i)}\rangle\langle\phi_m^{(i)}|, \tag{50}$$

$$Q_i = \lambda_M(i) |\psi_M^{(i)}\rangle\langle\psi_M^{(i)}| + \lambda_m(i) |\psi_m^{(i)}\rangle\langle\psi_m^{(i)}|. \tag{51}$$

Now, by hypothesis, there exist channels $\mathcal{E}$ and $\mathcal{F}$ such that $Q_i=\mathcal{E}(P_i)$ and $P_i=\mathcal{F}(Q_i)$. Then, by linearity,

$$Q_i = \lambda_M(i) \mathcal{E}(|\phi_M^{(i)}\rangle\langle\phi_M^{(i)}|) + \lambda_m(i) \mathcal{E}(|\phi_m^{(i)}\rangle\langle\phi_m^{(i)}|). \tag{52}$$

We will now consider

$$\mathrm{Tr}[Q_i |\psi_M^{(i)}\rangle\langle\psi_M^{(i)}|] = \lambda_M(i) = \mathrm{Tr}[P_i \mathcal{E}^\mathsf{T}(|\psi_M^{(i)}\rangle\langle\psi_M^{(i)}|)], \tag{53}$$

and this clearly implies that $\mathcal{E}^\mathsf{T}(|\psi_M^{(i)}\rangle\langle\psi_M^{(i)}|)=|\phi_M^{(i)}\rangle\langle\phi_M^{(i)}|$. Analogous arguments lead to the conclusion that $\mathcal{E}^\mathsf{T}(|\psi_m^{(i)}\rangle\langle\psi_m^{(i)}|)=|\phi_m^{(i)}\rangle\langle\phi_m^{(i)}|$, and moreover $\mathcal{F}^\mathsf{T}(|\phi_M^{(i)}\rangle\langle\phi_M^{(i)}|)=|\psi_M^{(i)}\rangle\langle\psi_M^{(i)}|$ and $\mathcal{F}^\mathsf{T}(|\phi_m^{(i)}\rangle\langle\phi_m^{(i)}|)=|\psi_m^{(i)}\rangle\langle\psi_m^{(i)}|$. By collecting all the eigenstates of nondegenerate P_i's and Q_i's in two sets, namely,

$$\begin{aligned} \mathcal{E}^\mathsf{T}&:\{|\psi_M^{(i)}\rangle\langle\psi_M^{(i)}|, |\psi_m^{(i)}\rangle\langle\psi_m^{(i)}|\}_i \mapsto \{|\phi_M^{(i)}\rangle\langle\phi_M^{(i)}|, |\phi_m^{(i)}\rangle\langle\phi_m^{(i)}|\}_i \\ \mathcal{F}^\mathsf{T}&:\{|\phi_M^{(i)}\rangle\langle\phi_M^{(i)}|, |\phi_m^{(i)}\rangle\langle\phi_m^{(i)}|\}_i \mapsto \{|\psi_M^{(i)}\rangle\langle\psi_M^{(i)}|, |\psi_m^{(i)}\rangle\langle\psi_m^{(i)}|\}_i, \end{aligned} \tag{54}$$

and applying Theorem III.3 it follows that there exists a unitary U such that $Q_i=UP_iU^\dagger$ for all nontrivial Q_i's. Clearly, the same unitary transformation maps the trivial elements. ■

IX. PREPROCESSING: CLEANNESS FOR NUMBER OF OUTCOMES $n \leqslant d$

Lemma IX.1: For fixed number of elements $n \leqslant d$ *the POVM* $\mathbf{P}$ *is clean iff* $\lambda_M(P_i)=1$ *for all* i. *Such condition is also equivalent to* $\lambda_m(P_i)=0$ *with multiplicity at least* $n-1$, *and each vector which is eigenvector with unit eigenvalue for some element* P_j *must belong to the kernel of all other POVM elements*.

Proof: We first prove that the condition is also equivalent to $\lambda_m(P_i)=0$ for all i. Indeed, consider a normalized eigenvector $|u\rangle$ of P_j with eigenvalue 1, and suppose by absurd that some element P_i has $\lambda_m(P_i)>0$. Then

$$\langle u|u\rangle = \sum_k \langle u|P_k|u\rangle = \langle u|P_j|u\rangle + \langle u|P_i|u\rangle + \sum_{k\neq i,j} \langle u|P_k|u\rangle > 1, \tag{55}$$

and in order to have no contradiction one must have $\langle u|P_i|u\rangle = 0$, namely $\lambda_m(P_i) = 0$. Notice that Eq. (55) also implies that $\langle u|P_k|u\rangle = 0$ for all $k \neq j$, namely the same eigenvector $|u\rangle$ of P_j is eigenvector of all P_k for all $k \neq j$. Moreover, since there must be at least n vectors as $|u\rangle$, each being eigenvector of a different element P_j corresponding to unit eigenvalue, and since any two vectors must be orthogonal (since for some j they are eigenvectors corresponding to different eigenvalues of P_j), this means that the 0 eigenvalue for each POVM element must have multiplicity at least $n-1$, and all the eigenvectors of any element with eigenvalue 1 are in the kernel of the remaining elements.

We now prove that the condition is sufficient. Suppose that a POVM $\mathbf{Q}$ exists such that $\mathbf{Q} > \mathbf{P}$. Then by Lemma III.1 $\{0,1\} \subseteq \mathsf{Sp}(Q_i)$ for all i. We then need to prove that in this case $\mathbf{P} \simeq \mathbf{Q}$. From now on we will denote by $|u\rangle_i^P$ an eigenvector of P_i with eigenvalue 1 and by $|u\rangle_i^Q$ the same for Q_i. The proof is constructive: consider the map with Stinespring form $\mathcal{E}(X) = V^\dagger(I \otimes X)V$, where

$$V = \sum_i \sqrt{P_i} \otimes |u\rangle_i^Q, \tag{56}$$

and the notation $T = O \otimes |u\rangle$ denotes the operator defined as $T|\psi\rangle = O|\psi\rangle \otimes |u\rangle$ for all $|\psi\rangle \in \mathsf{H}$. It is clear that $\mathcal{E}(Q_i) = P_i$. Similarly, consider the map $\mathcal{F}(X) = W^\dagger(I \otimes X)W$, where

$$W = \sum_i \sqrt{Q_i} \otimes |u\rangle_i^P. \tag{57}$$

This is such that $\mathcal{F}(P_i) = Q_i$. We proved that POVMs $\mathbf{P}$ such that $\lambda_M(P_i) = 1$ for all i are clean. We will now prove that it is also a necessary condition. Consider indeed a generic POVM $\mathbf{Q}$ such that at least for one outcome j $\lambda_M(Q_j) < 1$. Then one can consider any POVM $\mathbf{P}$ with $\lambda_M(P_i) = 1$ for all i and construct the isometry

$$W = \sum_i \sqrt{Q_i} \otimes |u\rangle_i^P. \tag{58}$$

It is clear that the Stinespring form $W^\dagger(I \otimes X)W$ defines a channel $\mathcal{E}$ such that $\mathcal{E}(P_i) = Q_i$ for all i. Then $\mathbf{P} > \mathbf{Q}$. Moreover, by hypothesis $\lambda_M(P_j) > \lambda_M(Q_j)$ and then it is impossible that $\mathbf{P} \simeq \mathbf{Q}$. ■

An immediate corollary is the following

Corollary IX.2: The only clean elements with $n = d$ are the observables.

Proof: In Lemma IX.1 for $n = d$ the iff condition is equivalent to have eigenvalue 0 with multiplicity $d-1$ for each POVM element, namely each POVM element is rank one, and they are orthogonal. ■

Allowing mapping between POVMs with different number of outcomes, the situation simplifies:

Theorem IX.3: *For $n \leqslant d$ outcomes the set of clean POVMs coincides with the set of observables.*

Proof: Consider a generic POVM P_i with $i = 1, \ldots, n \leqslant d$. This can be always regarded as the preprocessing of any desired observable $\{|i\rangle\langle i|\}_{i=1,\ldots,d}$. In fact, using the isometry from H to $\mathsf{H}^{\otimes 2}$

$$V = \sum_{i=1}^{n} \sqrt{P_i} \otimes |i\rangle, \tag{59}$$

the following channel expressed in the Stinespring form

$$\mathcal{M}(X) = V^\dagger(I \otimes X)V \tag{60}$$

gives

$$\mathcal{M}(|i\rangle\langle i|) = P_i, \quad i = 1, \dots d. \tag{61}$$

For a POVM with $n < d$ outcomes (strictly), notice that it is equivalent to a POVM with d outcomes and $d-n$ vanishing elements. On the other hand, for $n < d$ there is no channel that can increase the number of outcomes back to d, whence a POVM with $n < d$ outcomes cannot be clean. For $n = d$ Corollary IX.2 asserts that the only clean POVMs are the observables. ■

X. PREPROCESSING: ORDERING OF INFORMATIONALLY COMPLETE POVMs

Lemma X.1: If the POVM $\mathbf{Q}$ *is infocomplete then every* $\mathbf{P}$ *such that* $\mathbf{P} > \mathbf{Q}$ *is infocomplete, too.*

Proof: For d^2 outcomes POVMs, $\mathbf{P}$ and $\mathbf{Q}$ are infocomplete iff their elements are linearly independent. Suppose by absurd that there exists a nonnull vector of d^2 coefficients c_i such that $\sum_{i=1}^{d^2} c_i P_i = 0$, then also

$$\mathcal{E}\left(\sum_{i=1}^{d^2} c_i P_i\right) = 0 = \sum_{i=1}^{d^2} c_i Q_i = 0, \tag{62}$$

which contradicts the hypothesis.

If the number of outcomes is greater than d^2, suppose

$$\mathcal{E}(X) = 0, \tag{63}$$

for some $X \neq 0$, namely $\mathcal{E}$ would have non trivial kernel, in which case $\mathsf{Span}(\mathbf{Q}) \subseteq \mathsf{Rng}(\mathcal{E}) \subset \mathsf{B}(\mathsf{H})$, which contradicts the hypothesis that $\mathbf{Q} = \mathcal{E}(\mathbf{P})$ is infocomplete. Then $\mathcal{E}$ is invertible. Now, $\mathbf{P}$ must be infocomplete, otherwise the inverse of $\mathcal{E}$ would not have full rank, which is absurd. ■

The above theorem is immediately extended to any linearly independent POVM $\mathbf{Q}$. More interestingly, for any infocomplete POVM $\mathbf{P}$ one can prove the following lemma

Lemma X.2: If the POVM $\mathbf{P}$ *is infocomplete then every* $\mathbf{Q}$ *such that* $\mathbf{P} \simeq \mathbf{Q}$ *is infocomplete, too.*

Proof: It follows immediately from definition of $\simeq$ and Lemma X.1. ■

On the other hand, each POVM that is equivalent to an infocomplete one, is also unitarily equivalent to it, namely, more precisely

Theorem X.3: If $\mathbf{P}$ *is an infocomplete POVM, then* $\mathbf{P} \simeq \mathbf{Q}$ *iff* $\mathbf{P} \simeq_U \mathbf{Q}$.

Proof: Since the POVMs $\mathbf{P}$ and $\mathbf{Q}$ must be both infocomplete by the previous lemma, then the maps $\mathcal{E}$ and $\mathcal{F}$ are uniquely defined, and are the inverse of each other. Then, by Theorem III.2 $\mathcal{E}(X) = UXU^\dagger$ for some unitary U. ■

An alternative elegant proof of the above theorem would be the following.

Proof: By hypothesis, there exist $\mathcal{E}$ and $\mathcal{F}$ such that $\mathcal{E}(\mathbf{P}) = \mathbf{Q}$ and $\mathcal{F}(\mathbf{Q}) = \mathbf{P}$. This means that $\mathcal{F} \circ \mathcal{E}$ stabilizes the algebra generated by $\mathbf{P}$, that is $\mathsf{Span}(\mathbf{P}) \equiv \mathsf{B}(\mathsf{H})$. On the other hand, the commutant of an infocomplete POVM is only the identity, since $[P_i, X] = 0$ for all i implies $[A, X] = \sum_i a_i [P_i, X] = 0$ for all $A \in \mathsf{B}(\mathsf{H})$. This fact along with Lemma III.4 implies that $\mathcal{F} \circ \mathcal{E}$ is the identical map. The thesis is then a straightforward consequence of Theorem III.2. ■

Corollary X.4: For each non unitary invertible channel $\mathcal{E}$ *on* $\mathsf{B}(\mathsf{H})$ *there exists at least a pure state* $\psi \in \mathsf{H}$ *such that* $\mathcal{E}^{\mathsf{T}-1}(|\psi\rangle\langle\psi|) \ngeq 0$.

Proof: Let us consider an extremal POVM with d^2 rank-one elements $\{|\alpha_i\rangle\langle\alpha_i|\}$ $i = 1, \dots, d^2$ (according to Ref. 15 such a POVM always exists for any dimension d, and it is necessarily informationally complete). Assuming $\mathcal{E}$ invertible, let's consider $Q_i = \mathcal{E}^{-1}(|\alpha_i\rangle\langle\alpha_i|)$. The POVM $|\alpha_i\rangle\langle\alpha_i|$ is clean since it is rank-one. However, since it is also infocomplete, then Q_i cannot be itself a POVM, otherwise according to Theorem X.3 it would be unitarily equivalent to $|\alpha_i\rangle\langle\alpha_i|$. Moreover, being both $|\alpha_i\rangle\langle\alpha_i|$ and Q_i infocomplete, the map $\mathcal{E}$ would be univocally defined, whence itself unitary, contrarily to the hypothesis. Then, $\{Q_i\}$ is not a POVM. However, since the map $\mathcal{E}$ is a channel, whence $\mathcal{E}^{-1}$ must be identity preserving, one has $\sum_i Q_i = I$, then necessarily at least one element Q_j cannot be positive, namely there exists a vector $\psi \in \mathsf{H}$ for which

$$\langle\psi|Q_j|\psi\rangle < 0. \tag{64}$$

This inequality can be rewritten as follows:

$$\mathrm{Tr}[|\psi\rangle\langle\psi|\mathcal{E}^{-1}(|\alpha_j\rangle\langle\alpha_j|)] = \mathrm{Tr}[\mathcal{E}^{\mathsf{T}-1}(|\psi\rangle\langle\psi|)|\alpha_j\rangle\langle\alpha_j|] < 0, \tag{65}$$

namely $\mathcal{E}^{\mathsf{T}-1}(|\psi\rangle\langle\psi|)$ is not positive. ■

We have also the following interesting theorem.

Theorem X.5: *Every channel $\mathcal{F}$ which maps the set of states S surjectively on itself, i. e. such that $\mathcal{F}(\mathsf{S})\equiv\mathsf{S}$, is necessarily unitary.*

Proof: First, suppose that $\mathcal{F}$ is invertible, then $\mathcal{F}$ must be unitary, otherwise $\mathcal{F}^{-1}(\mathsf{S})=\mathsf{S}$ would not be possible by Lemma X.4. On the other hand, if $\mathcal{F}$ is not invertible, then its range must have dimension strictly smaller than d^2. Now, consider a rank-one infocomplete POVM $\mathbf{P}$ with $|\mathbf{P}|=d^2$. Clearly, some POVM element cannot belong to $\mathcal{F}(\mathsf{S})$, and this proves that $\mathcal{F}(\mathsf{S})\subset\mathsf{S}$ strictly, since such normalized POVM elements are just pure states. ■

For qubits this theorem has the simple geometric interpretation that the Bloch sphere transformed under $\mathcal{F}^{-1}$ for any invertible non unitary $\mathcal{F}$ becomes an ellipsoid which contains elements outside the Bloch sphere.

By definition, and according to Theorem X.3 an infocomplete POVM $\mathbf{P}$ is clean iff $\mathcal{E}^{-1}(\mathbf{P})$ is not a POVM for all invertible non unitary maps $\mathcal{E}$. This means that as soon as the set S of states is transformed by $\mathcal{E}^{-1}$, the POVM is able to detect at least one of the points in $\mathcal{E}^{-1}(\mathsf{S})-\mathsf{S}$, say $\mathcal{E}^{-1}(|\psi\rangle\langle\psi|)$, since the "probability distribution" corresponding to $\mathcal{E}^{-1}(|\psi\rangle\langle\psi|)$ is no longer positive.

XI. PREPROCESSING: ORDERING OF RANK-ONE POVMs

Intuitively one thinks that a rank-one POVM is clean. This is actually true, and it is more precisely stated by theorem XI.2 in this section. In order to prove it, we first need the following

Lemma XI.1: If the POVM $\mathbf{Q}$ is rank-one (i.e. each element Q_i can be written as $Q_i=|w_i\rangle\langle w_i|$), then for any POVM $\mathbf{P}$ such that $\mathbf{P}\succ\mathbf{Q}$, also $\mathbf{P}$ is rank one, and $\mathrm{Tr}[P_i]=\mathrm{Tr}[Q_i]$, $\forall i$.

Proof: Consider the following normalized vectors

$$|\widetilde{w}_i\rangle = \frac{1}{\sqrt{N_i}}|w_i\rangle, \quad Q_i = N_i|\widetilde{w}_i\rangle\langle\widetilde{w}_i|, \tag{66}$$

where $N_i=\mathrm{Tr}[Q_i]=\|w_i\|^2$, whence $\Sigma_i N_i=d$. Suppose $\mathbf{P}\succ\mathbf{Q}$, and $\mathcal{E}(\mathbf{P})=\mathbf{Q}$. Then one can easily verify the following identity:

$$N_i = \mathrm{Tr}[Q_i|\widetilde{w}_i\rangle\langle\widetilde{w}_i|] = \mathrm{Tr}[\mathcal{E}(P_i)|\widetilde{w}_i\rangle\langle\widetilde{w}_i|] = \mathrm{Tr}[P_i\mathcal{E}^{\mathsf{T}}(|\widetilde{w}_i\rangle\langle\widetilde{w}_i|)]. \tag{67}$$

Now, by the CPT property of $\mathcal{E}^{\mathsf{T}}$, $\mathcal{E}^{\mathsf{T}}(|\widetilde{w}_i\rangle\langle\widetilde{w}_i|)$ is a state and clearly the last expression in Eq. (67) is less than or equal to the maximum eigenvalue $\lambda_M(P_i)$ of P_i. We have than the following situation:

$$N_i \leqslant \lambda_M(P_i) \leqslant \mathrm{Tr}[P_i]. \tag{68}$$

By the normalization and positivity of POVMs, we have that $d=\Sigma_i N_i=\Sigma_i\mathrm{Tr}[P_i]$ and $N_i\geqslant 0$, $\mathrm{Tr}[P_i]\geqslant 0$. These conditions along with Eq. (68) imply

$$N_i \equiv \mathrm{Tr}[P_i] \ \ \forall\, i, \tag{69}$$

and this in turn implies $\lambda_M(P_i)=\mathrm{Tr}[P_i]$, namely P_i is rank one. ■

We will now prove the following theorem.

Theorem XI.2: *If $\mathbf{Q}$ is rank one, then $\mathbf{P}\succ\mathbf{Q}$ iff $\mathbf{P}\simeq_U\mathbf{Q}$. Namely, rank-one POVMs are clean.*

Proof: First, notice that by Lemma XI.1, $\mathbf{P}\succ\mathbf{Q}$ implies that $\mathbf{P}$ is rank one with $\mathrm{Tr}[P_i]=\mathrm{Tr}[Q_i]$, for all i. We have then

$$P_i = |v_i\rangle\langle v_i| = M_i|\widetilde{v}_i\rangle\langle\widetilde{v}_i|, \quad \|\widetilde{v}_i\| = 1, \tag{70}$$

$$Q_i = |w_i\rangle\langle w_i| = M_i|\widetilde{w}_i\rangle\langle\widetilde{w}_i|, \quad \|\widetilde{w}_i\| = 1, \tag{71}$$

where $M_i \equiv \mathrm{Tr}[P_i] = \mathrm{Tr}[Q_i]$, consistently with Lemma XI.1. Now, by hypothesis we have

$$M_i = \mathrm{Tr}[\mathcal{E}(P_i)|\widetilde{w}_i\rangle\langle\widetilde{w}_i|] = \mathrm{Tr}[P_i\mathcal{E}^{\mathsf{T}}(|\widetilde{w}_i\rangle\langle\widetilde{w}_i|)] = M_i\,\mathrm{Tr}[|\widetilde{v}_i\rangle\langle\widetilde{v}_i|\mathcal{E}^{\mathsf{T}}(|\widetilde{w}_i\rangle\langle\widetilde{w}_i|)]. \tag{72}$$

As a consequence, necessarily $\mathrm{Tr}[|\widetilde{v}_i\rangle\langle\widetilde{v}_i|\mathcal{E}^{\mathsf{T}}(|\widetilde{w}_i\rangle\langle\widetilde{w}_i|)] = 1$, and by CPT property of $\mathcal{E}^{\mathsf{T}}$ this implies $\mathcal{E}^{\mathsf{T}}(|\widetilde{w}_i\rangle\langle\widetilde{w}_i|) \equiv |\widetilde{v}_i\rangle\langle\widetilde{v}_i|$. Notice that since $\mathcal{E}^{\mathsf{T}}(I) = \Sigma_i M_i \mathcal{E}^{\mathsf{T}}(|\widetilde{w}_i\rangle\langle\widetilde{w}_i|) = \Sigma_i M_i |\widetilde{v}_i\rangle\langle\widetilde{v}_i| = I$, then $\mathcal{E}^{\mathsf{T}}$ and $\mathcal{E}$ are unital, namely both CPT and CPI. Then, by applying Theorem III.3 one has $\mathbf{P} \simeq_U \mathbf{Q}$. The converse is trivial. ■

XII. CONCLUSIONS

In this paper we have introduced the notion of *clean* POVMs, namely which are not irreversibly connected to another POVM via a quantum channel. We used the adjective clean for such POVMs in the sense that they are not affected by extrinsical quantum noise from the action of a channel which is in principle avoidable. We have seen that, quite unexpectedly, the *cleanness* property is largely unrelated to the convex structure of POVMs, and there are clean POVMs that are not extremal and extremal POVMs that are not clean.

The classification problem of POVMs cleanness turned out to be much harder than that of their extremality, and in this paper we gave a complete classification of clean POVMs only for number n of outcomes $n \leqslant d$ (d dimension of the Hilbert space), whereas for $n > d$ we gave a set of either necessary or sufficient conditions, and an iff condition for the case of informationally complete POVMs for $n = d^2$. The difficulty for classifying the case $n > d$ reflects analogous difficulties in the theory of quantum measurements in assessing the maximal POVM cardinality needed to attain the accessible information, cardinality whose lower bound has been shown to be actually larger than d.[18,19]

The novel issue of clean POVMs naturally opens new problems in the theory of quantum information and quantum measurements. Besides the problem of the general classification of cleanness, it raises the problem of characterizing all POVMs achievable from a given one via a quantum channel, or, reversely, of all POVMs which can be evolved toward a given one via a quantum channel. These are only initial steps toward a thorough analysis of the general problem of the partial ordering induced by channels on the convex set of measurements, an issue which is not an academic mathematical problem, but which is relevant for engineering new quantum measurements with minimal available resources.

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The potential $(iz)^m$ generates real eigenvalues only, under symmetric rapid decay boundary conditions

Kwang C. Shin[a)]
Department of Mathematics, University of Missouri, Columbia, Missouri 65211

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We consider the non-Hermitian eigenvalue problems $-u''(z)\pm(iz)^m u(z)=\lambda u(z)$, $m\geqslant 3$, under *every* rapid decay boundary condition that is symmetric with respect to the imaginary axis in the complex z plane. We prove that the eigenvalues λ are all real and positive. © *2005 American Institute of Physics.*
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I. INTRODUCTION

For integers $m\geqslant 3$ fixed and $1\leqslant \ell \leqslant m-1$, we are considering the non-Hermitian eigenvalue problems

$$(H_\ell u)(z) := \left[-\frac{d^2}{dz^2}+(-1)^\ell (iz)^m\right] u(z)=\lambda u(z) \quad \text{for some } \lambda\in\mathbb{C}, \tag{1}$$

with the boundary condition that

$$u(z)\to 0 \text{ exponentially, as } z\to\infty \text{ along the two rays } \arg z=-\frac{\pi}{2}\pm\frac{\ell+1}{m+2}\pi. \tag{2}$$

If a non-constant function u along with a complex number λ solves (1) with the boundary condition (2), then we call λ an *eigenvalue of* H_ℓ and u an *eigenfunction associated with the eigenvalue* λ. It is known that any solution of (1) is entire (analytic on the complex plane). In Section 7.4 of Ref. 1, Hille shows that every solution of (1) is either decaying to zero or blowing up exponentially as z tends to infinity along any ray $\{z\in\mathbb{C}:\arg z=\text{const.}\}$, except along $m+2$ critical rays where the transition between decaying and blowing-up sectors might occur. Along these $m+2$ critical rays, any non-constant solution decays algebraically. We will explain these asymptotic properties of the solution in Sec. II.

Before we state our main theorem, we first introduce some known facts about the eigenvalues λ of H_ℓ, facts due to Hille[1] and Sibuya.[2]

Proposition 1: *For* $1\leqslant\ell\leqslant m-1$, *the eigenvalues* λ *of* H_ℓ *are the zeros of a certain entire function of order* $\frac{1}{2}+1/m\in(\frac{1}{2},1)$. *In particular, the eigenvalues have the following properties.*

(i) *eigenvalues are discrete;*
(ii) *all eigenvalues are simple; and*
(iii) *infinitely many eigenvalues exist.*

For our purposes, we will need to examine the proof of this proposition in some detail. In Lemmas 7 and 8, we prove that the eigenvalues are zeros of certain entire functions of order $\frac{1}{2}+1/m\in(\frac{1}{2},1)$, due to Sibuya.[2] Then claims (i) and (iii) are consequences of the Hadamard factorization theorem, whereas claim (ii) is due to Hille.[1]

[a)]Electronic mail:kcshin@math.missouri.edu

In this paper, we will prove the following main theorem regarding the positivity of the eigenvalues.

Theorem 2. *The eigenvalues* λ *of* H_ℓ *for integers* $1 \leqslant \ell \leqslant m-1$ *are all real and positive*.

One can show that the eigenvalues of H_ℓ are the same as those of $H_{m-\ell}$, by using the reflection $z \mapsto -z$. The case $\ell = 1$ of the theorem is due to Dorey *et al.*[3] Also when m is even and $\ell = m/2$, one can see that H_ℓ in $L^2(\mathbb{R})$ is Hermitian and hence, $\lambda \in \mathbb{R}$. In all other cases, Theorem 2 is new and provides the first result of its kind for boundary conditions that neither cluster near the negative imaginary axis nor lie on the real axis. We will explain how Theorem 2 covers *every* symmetric rapid decay condition when we discuss admissible boundary conditions in Sec. II.

For the rest of the Introduction, we will mention brief history and give some background about our main problem and our method of proof. Then in Sec. II, we will introduce work of Hille[1] and Sibuya[2] about some properties of solutions of (1). In Sec. III, we establish an induction step on ℓ, which is the key element in our proof of Theorem 2. More precisely, we will prove that for $1 \leqslant \ell \leqslant m/2-1$, every eigenvalue λ of $H_{\ell+1}$ is real and positive if all eigenvalues σ of H_ℓ lie in the sector $|\arg \sigma| \leqslant 2\pi/(m+2)$ in the complex plane. In Sec. IV, we will outline a proof of the induction basis $\ell = 1$, that is, the eigenvalues of H_1 lie in the sector $|\arg \lambda| \leqslant 2\pi/(m+2)$ (in fact, $\arg \lambda = 0$; see Refs. 3 and 4). We then prove Theorem 2 by induction on ℓ and the reflection $z \mapsto -z$. In the last section, we mention some open problems.

A. History and overview of the method

In this subsection, we introduce some earlier work related with Theorem 2. Also, we discuss our method of the proof of Theorem 2.

The Hamiltonians with the potential $\pm(iz)^m$ have been studied in many physics and mathematics papers, either under a boundary condition on the real axis,[5–7] $u(\pm\infty + 0i) = 0$, or under the boundary condition (2) with the $\ell = 1$ case.[3,4,8] Also, Bender and Turbiner[9] considered all the boundary conditions (2) with $1 \leqslant \ell \leqslant m-1$.

Caliceti *et al.*[5] and Simon[6] studied the Hamiltonians $-\mathrm{d}^2/\mathrm{d}x^2 + x^2 + \beta x^m$ on the real line, where $\beta \in \mathbb{C} \backslash \mathbb{R}_-$ and integers $m \geqslant 3$, and they proved compactness of the resolvent and discreteness of the spectrum. Regarding the reality of the eigenvalues, Caliceti *et al.*[5] showed that the eigenvalues for $(-\mathrm{d}^2/\mathrm{d}x^2) + x^2 + \beta x^{2n+1}$ are real if β is small enough.

Recently, a conjecture of Bessis and Zinn-Justin has been verified by Dorey *et al.*[3] and extended by Shin.[4] That is, the eigenvalues λ of

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}z^2} - (iz)^3 + \beta z^2 \right] u(z) = \lambda u(z), \quad u(\pm\infty + 0i) = 0 \quad \text{for } \beta \in \mathbb{R}, \tag{3}$$

are all real and positive. Dorey *et al.*[3] verified for the case $\beta = 0$, and later Shin[4] extended it for the case $\beta \in \mathbb{R}$.

In fact, Dorey *et al.*[3] have proved more. They studied the following eigenvalue problem:

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}z^2} - (iz)^{2M} - \alpha(iz)^{M-1} + \frac{l(l+1)}{z^2} \right] u(z) = \lambda u(z), \tag{4}$$

under the boundary condition (2) with $\ell = 1$, and M, α, l being all real. They proved that for $M > 1, \alpha < M + 1 + |2l+1|$, the eigenvalues are all real, and for $M > 1, \alpha < M + 1 - |2l+1|$, they are all positive. A special case of (4) is the potential iz^3 (when $M = \frac{3}{2}, \alpha = l = 0$), which is the $\beta = 0$ version of the Bessis and Zinn-Justin (BZJ) conjecture, but their results do not cover the $\beta \neq 0$ version.

Later, Shin[4] studied the following eigenvalue problem:

$$-\left[\frac{d^2}{dz^2}+(iz)^m+a_1(iz)^{m-1}+a_2(iz)^{m-2}+\cdots+a_{m-1}(iz)\right]u(z)=\lambda u(z),$$

with the boundary condition (2) with $\ell=1$, where $a_k\in\mathbb{R}$ for all k. He proved that if for some $1\leqslant j\leqslant m/2$ we have $(j-k)a_k\geqslant 0$ for all k, then the eigenvalues λ are all real and positive.[4] This covers the full BZJ conjecture.

The proof of our main theorem, Theorem 2, has four parts. The first part follows closely the method of Dorey *et al.*,[3] developing functional equations for spectral determinants, expressing them in factored forms and estimating eigenvalues by Green's transform. The second part establishes an induction step on $1\leqslant\ell\leqslant m/2$ and estimates eigenvalues by Green's transform again. In the third part, we use the result of Dorey *et al.*[3] that says the eigenvalues of H_1 are all real and positive (also, see Theorem 2 in Ref. 4). This induction basis, along with the induction step established in the second part, proves our main theorem for $1\leqslant\ell\leqslant m/2$. Last, we use the reflection $z\mapsto -z$ to cover $m/2<\ell\leqslant m-1$. Of course both this paper, and Dorey *et al.*[3] and Shin[4] are indebted to the work of Sibuya.[2]

B. $\mathcal{PT}$-symmetric oscillators

The above-mentioned Hamiltonians are not Hermitian in general, and hence the reality of eigenvalues is not obviously guaranteed. However, these Hamiltonians share a common symmetry, the so-called $\mathcal{PT}$ symmetry. A $\mathcal{PT}$-symmetric Hamiltonian is a Hamiltonian which is invariant under the combination of the parity operation $\mathcal{P}(:z\mapsto -\bar{z})$ (an over bar denotes the complex conjugate) and the time reversal operation $\mathcal{T}(:i\mapsto -i)$. These $\mathcal{PT}$-symmetric Hamiltonians have arisen in recent years in a number of physics papers[10–20] and other references mentioned previously, which support that some $\mathcal{PT}$-symmetric Hamiltonians have real eigenvalues only. The work of Dorey *et al.*[3] and Shin,[4] and the results in this paper, prove rigorously that some $\mathcal{PT}$-symmetric Hamiltonians indeed have real eigenvalues only.

We also know that if $H=-d^2/dz^2+V(z)$ is $\mathcal{PT}$ symmetric and if $V(z)$ is a polynomial, then $V(z)=Q(iz)$ for some real polynomial Q, because $\overline{V(-\bar{z})}=V(z)$. Thus, Re $V(z)$ is an even function and Im $V(z)$ is an odd function. Certainly, (1) is a $\mathcal{PT}$-symmetric Hamiltonian. Moreover, if $u(z)$ is an eigenfunction of H_ℓ associated with the eigenvalue $\lambda\in\mathbb{C}$, then so is $\overline{u(-\bar{z})}$, associated with the eigenvalue $\bar{\lambda}$.

II. PROPERTIES OF THE SOLUTIONS

In this section we will introduce some definitions and known facts related to Eq. (1). One of our main tasks is to identify the eigenvalues as being zeros of certain entire functions, in Lemmas 7 and 8. But first, we rotate Eq. (1) as follows because some known facts, which are related to our argument throughout, are directly available for this rotated equation.

Fix the integer $m\geqslant 3$. Let u be a solution of (1) and let $v(z)=u(-iz)$. Then v solves

$$-v''(z)+[(-1)^{\ell+1}z^m+\lambda]v(z)=0.$$

The boundary condition (2) of u becomes that $v(z)\to 0$ exponentially as $z\to\infty$ along the two rays

$$\arg z=\pm\frac{\ell+1}{m+2}\pi.$$

Throughout this paper, we will use the complex number

$$\omega=\exp\left[\tfrac{2\pi i}{m+2}\right].$$

When ℓ is even, it will be convenient to rotate it once more, letting $w(z):=v(\omega^{1/2}z)$ so that $w(z)$ solves

$$-w''(z)+[z^m+\omega\lambda]w(z)=0.$$

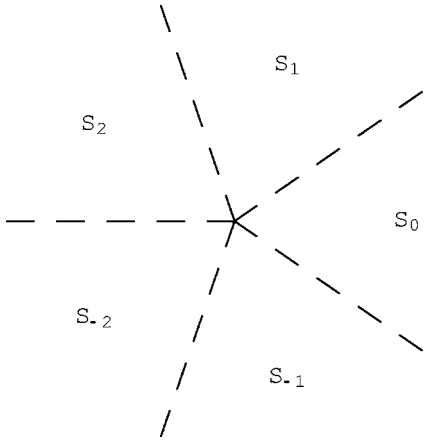

FIG. 1. The Stokes sectors S_j of (5) with $m=3$. The dashed rays are the critical rays: $\arg z = \pm\pi/5, \pm 3\pi/5, \pi$.

We mention that Hille[1] and Sibuya[2] have studied the general equation of the form

$$-v''(z) + [z^m + P(z) + \lambda]v(z) = 0,$$

where $P(z)$ is a polynomial of degree less than m. We proceed now to summarize work of Hille[1] and expand on some work of Sibuya[2] for $P \equiv 0$, that is, for

$$-v''(z) + [z^m + \lambda]v(z) = 0, \quad \text{where } m \geqslant 3. \tag{5}$$

A. Results of Hille

It is known that every solution of (5) has simple asymptotic behavior near infinity.[1] We will explain this asymptotic behavior using the following.

Definition: Consider the equation

$$g''(z) + \left[b_m z^m + b_{m-1} z^{m-1} + \cdots + b_1 z + b_0\right] g(z) = 0, \tag{6}$$

where $b_k \in \mathbb{C}$ for $0 \leqslant k \leqslant m$ with $b_m \neq 0$. Let

$$\theta_j = \frac{2j\pi - \arg b_m}{m+2} \quad \text{for } j \in \mathbb{Z},$$

where we choose $-\pi < \arg b_m \leqslant \pi$. For $j \in \mathbb{Z}$ we call the open sectors

$$S_j = \{z \in \mathbb{C} : \theta_j < \arg z < \theta_{j+1}\} \tag{7}$$

the *Stokes sectors* of (6). Also we call the rays $\{\arg z = \theta_j\}$ the *critical rays*.

In particular, the Stokes sectors of (5) are

$$S_j = \left\{ z \in \mathbb{C} : \frac{(2j-1)\pi}{m+2} < \arg z < \frac{(2j+1)\pi}{m+2} \right\} \quad \text{for } j \in \mathbb{Z}. \tag{8}$$

See Fig. 1.

Now we are ready to introduce some asymptotic behavior of solutions of (5), due to Hille.[1]

Lemma 3: *Let v be a non-constant solution of (5) (with no boundary conditions imposed). Then the following hold.*

(i) *In each Stokes sector S_j, the solution v is asymptotic to*

$$(\text{const.})z^{-m/4}\exp\left[\pm\frac{2}{m+2}z^{(m+2)/2}\right] \tag{9}$$

as $z\to\infty$ *in every closed subsector of* S_j.

(ii) *If* v *decays to zero in* S_j, *for some* $j\in\mathbb{Z}$, *then it must blow up in* S_{j-1} *and* S_{j+1}. *(However, it is possible for* v *to blow up in many adjacent Stokes sectors.) Moreover, the asymptotic expansion (9) is valid with the same constant for the three consecutive Stokes sectors* $S_{j-1}\cup cl(S_j)\cup S_{j+1}$, *where* $cl(S_j)$ *is the closure of* S_j.

(iii) *For each Stokes sector* S_j, *there exists a solution of (5) that decays in* S_j, *and there exists a solution of (5) that blows up in* S_j. *And any solution of (5) can be expressed as a linear combination of these two solutions*.

Proof: See the Section 7.4 in Ref. 1 for a proof. □

Remark: In Lemma 3, we state some asymptotic behavior of solutions of (5). In the general case, the corresponding Stokes sectors of (6) are given by (7). With these Stokes sectors, Lemma 3 holds though the asymptotic expansion (9) becomes more complicated due to more complicated potentials.

Note that Lemma 3 (iii) implies Proposition 1 (ii). More precisely, if an eigenvalue were not simple, then Eq. (1) would have two linearly independent solutions satisfying the boundary condition in (2). Hence, any solution of (1) could be expressed as a linear combination of these solutions. So there would be no solution of (1) that blows up in either of the two Stokes sectors containing the rays in (2). This contradicts Lemma 3 (iii). Therefore, every eigenvalue is simple.

From now on, we denote S_j the Stokes sectors of (5).

B. Admissible boundary conditions

Note, in particular, that the asymptotic expansion (9) implies that for each j, $v(z)$ either decays to zero or blows up exponentially, as z approaches infinity in closed subsectors of S_j. Also, the asymptotic expansion (9) implies that if $v(z)\to 0$ as $z\to\infty$ along one ray in S_j, then $v(z)\to 0$ as $z\to\infty$ along every ray in S_j. Likewise, if $v(z)\to\infty$ as $z\to\infty$ along one ray in S_j, then $v(z)\to\infty$ as $z\to\infty$ along every ray in S_j.

Let u be an eigenfunction of H_ℓ. Then the above-mentioned observation shows that when $\ell=2n-1$ is odd, the boundary condition (2) for H_ℓ is equivalent to having $v(z)=u(-iz)$ decaying to zero as $z\to\infty$ along rays in S_{-n} and S_n. (Note that the rays $\arg z=\pm[(\ell+1)/(m+2)]\pi$ are center rays of S_{-n} and S_n.) Also, when $\ell=2n$ is even, the boundary condition (2) for H_ℓ is equivalent to having $w(z)=u(-i(\omega^{1/2}z))$ decaying to zero as $z\to\infty$ along the rays in S_{-n-1} and S_n.

As we see, one needs not choose the two rays being symmetric, as in (2), so long as they stay in the Stokes sectors that are symmetric with respect to the imaginary axis.

Next, we will show that for each $j\in\mathbb{Z}$, there exist two linearly independent solutions of (5) decaying to zero algebraically as $z\to\infty$ along the critical ray $\arg(z)=\theta_j$. Then, this implies that every solution of (5) decays to zero algebraically as z tends to infinity along the critical ray since the solution can be expressed as a linear combination of two linearly independent solutions of (5). To this end, we will use Lemma 3.

Equation (5) has two solutions f_{j-1} and f_j, decaying in S_{j-1} and in S_j, respectively. Then it is not difficult to see that f_{j-1} blows up in S_j and hence, f_{j-1} and f_j are linearly independent. Moreover, the asymptotic expansions (9) of f_{j-1} and f_j are valid as $z\to\infty$ in $S_{j-2}\cup\text{cl}(S_{j-1})\cup S_j$ and in $S_{j-1}\cup\text{cl}(S_j)\cup S_{j+1}$, respectively. Note that the critical ray $\arg(z)=\theta_j$ is contained in both sectors. Finally, since $\text{Re}(z^{(m+2)/2})=0$ for all z on the critical ray, we see that both f_{j-1} and f_j [and hence all solutions of (5)] decay to zero algebraically as z tends to infinity along the critical ray $\arg(z)=\theta_j$. [Incidently, the Stokes sectors S_j are the sectors where $\text{Re}(z^{(m+2)/2})$ keeps a constant sign.]

One might wonder why we do not consider the eigenvalue problem

$$\left[-\frac{d^2}{dz^2}-(-1)^{\ell}(iz)^m\right]u(z)=\lambda u(z),$$

under the boundary condition (2). [Here we have the opposite sign in front of $(-1)^{\ell}$, compared to (1).] In this case, under the rotation $v(z)=u(-iz)$ and $w(z)=v(\omega^{1/2}z)$ if necessary, the two rays in (2) map to two of the critical rays of (5). So we have algebraic decay of the solution. Thus, if one requires the eigenfunction decay to zero exponentially, there are no eigenvalues, whereas if one requires the eigenfunction decay to zero merely algebraically, then every complex number λ is an eigenvalue. Hence, we have no interest in this case.

Now we are ready to explain how Theorem 2 covers every symmetric rapid decay boundary condition. When ℓ is odd, Eq. (1) becomes $-u''(z)-(iz)^m u(z)=\lambda u(z)$. In this case, the negative imaginary axis is the center of a Stokes sector and the critical rays are $\arg z=-\pi/2\pm(2k-1)\pi/(m+2)$ for integers $1\leqslant k\leqslant(m+3)/2$. The two rays in (2) are not critical rays and they are, in fact, centers of the Stokes sectors. When ℓ is increased by 2, the rays in (2) move, away from the negative imaginary axis, to the centers of adjacent Stokes sectors. So Theorem 2 covers all symmetric rapid decay boundary condition for the potential $-(iz)^m$. Similarly, one can see that when ℓ is even, Theorem 2 covers all symmetric rapid decay boundary condition for the potential $(iz)^m$.

So far in this subsection, we have discussed all possible symmetric decaying boundary conditions, except the "imaginary axis" boundary condition that $u(z)$ decays to zero as $z\to\infty$ along the both ends of the imaginary axis when m is even. In this case, if $u(z)$ is an eigenfunction of $-u''(z)-(iz)^m u(z)=\lambda u(z)$ satisfying this "imaginary axis" boundary condition, then $\lambda\in\mathbb{R}$ since $v(z):=u(-iz)$ is an eigenfunction of the Hermitian equation

$$-v''(z)+z^m v(z)=-\lambda v(z),\quad v(\pm\infty+0i)=0.$$

Next, we briefly mention nonsymmetric decaying boundary conditions. Let us consider, as an example,

$$\left[-\frac{d^2}{dz^2}-(iz)^m\right]u(z)=\lambda u(z),$$

under the boundary condition that $u(z)$ decays to zero exponentially as z tends to infinity along the rays $\arg z=-(\pi/2)+2\pi/(m+2)$ and $\arg z=-(\pi/2)-4\pi/(m+2)$. Set $u_1(z):=u(\omega^{-1/2}z)$. Then $u_1(z)$ solves

$$\left[-\frac{d^2}{dz^2}+(iz)^m\right]u_1(z)=\omega^{-1}\lambda u_1(z),$$

under the boundary condition (2) with $\ell=2$. Theorem 2 shows that $\omega^{-1}\lambda$ is real and positive and hence, λ is not real. In general, if we impose a decaying boundary condition along the two rays in some Stokes sectors that are not symmetric with respect to the imaginary axis, then the eigenvalues are not real and positive.

Finally, we mention that the integer ℓ in (1) and (2) equals to the number of Stokes sectors between the two sectors where we impose the boundary condition (2).

C. Results of Sibuya

We will introduce Sibuya's results, but first we define the order of an entire function g as

$$\text{order}(g)=\limsup_{r\to\infty}\frac{\log\log M(r,g)}{\log r},$$

where $M(r,g)=\max\{|g(re^{i\theta})|:0\leqslant\theta\leqslant 2\pi\}$ for $r>0$. If for some positive real numbers σ,c_1,c_2, we have $M(r,g)\leqslant c_1\exp[c_2 r^{\sigma}]$ for all large r, then the order of g is finite and less than or equal to σ. In this paper, we choose $\arg z^{\alpha}=\alpha\arg z$ for $-\pi<\arg z\leqslant\pi$ and $\alpha\in\mathbb{R}$.

Now we are ready to introduce some existence results and asymptotic estimates of Sibuya.[2] The existence of an entire solution with a specified asymptotic representation for fixed λ, is presented as well as an asymptotic expansion of the value of the solution at $z=0$ as λ tends to infinity. These results are in Theorems 6.1, 7.2, 19.1, and 20.1 of Sibuya's book.[2] The following is a special case of these theorems that is enough for our later argument.

Proposition 4: *Equation (5) admits a solution* $f(z,\lambda)$ *with the following properties.*

(i) $f(z,\lambda)$ *is an entire function of* (z,λ).

(ii) $f(z,\lambda)$ *and* $f'(z,\lambda)=(\mathrm{d}/\mathrm{d}z)f(z,\lambda)$ *admit the following asymptotic expansions. Let* $\varepsilon>0$. *Then*

$$f(z,\lambda) = z^{-m/4}(1+O(z^{-1/2}))\exp\left[-\frac{2}{m+2}z^{(m+2)/2}\right],$$

$$f'(z,\lambda) = -z^{m/4}(1+O(z^{-1/2}))\exp\left[-\frac{2}{m+2}z^{(m+2)/2}\right],$$

as z *tends to infinity in the sector* $|\arg z|\leqslant 3\pi/(m+2)-\varepsilon$, *uniformly on each compact set of the complex* λ*-plane.*

(iii) *Properties* (i) *and* (ii) *uniquely determine the solution* $f(z,\lambda)$ of (5)).

(iv) *For each fixed* $\delta>0$, f *and* f' *also admit the asymptotic expansions,*

$$f(0,\lambda) = [1+o(1)]\lambda^{-1/4}\exp\left[K\lambda^{1/2+1/m}\right], \tag{10}$$

$$f'(0,\lambda) = -[1+o(1)]\lambda^{1/4}\exp\left[K\lambda^{1/2+1/m}\right], \tag{11}$$

as λ *tends to infinity in the sector* $|\arg\lambda|\leqslant\pi-\delta$, *where*

$$K = \int_0^\infty \left(\sqrt{1+t^m}-\sqrt{t^m}\right)\mathrm{d}t. \tag{12}$$

(v) *The entire functions* $\lambda\mapsto f(0,\lambda)$ *and* $\lambda\mapsto f'(0,\lambda)$ *have orders* $\frac{1}{2}+1/m$.

Proof: In Sibuya's book,[2] see Theorem 6.1 for a proof of (i) and (ii); Theorem 7.2 for a proof of (iii); and Theorem 19.1 for a proof of (iv). And (v) is a consequence of (iv) along with Theorem 20.1. Note that properties (i), (ii) and (iv) are summarized on pages 112 and 113 of Sibuya's book.[2] □

The next thing we want to introduce is the Stokes multiplier. Let $f(z,\lambda)$ be the function in Proposition 4. Note that $f(z,\lambda)$ decays to zero exponentially as $z\to\infty$ in S_0, and blows up in $S_{-1}\cup S_1$. Then, the function

$$f_k(z,\lambda) := f(\omega^{-k}z,\omega^{-mk}\lambda), \tag{13}$$

obtained by rotating $f(z,\omega^{-mk}\lambda)$ in the z variable, solves (5). It is clear that $f_0(z,\lambda)=f(z,\lambda)$, and that $f_k(z,\lambda)$ decays in S_k and blows up in $S_{k-1}\cup S_{k+1}$ since $f(z,\omega^{-mk}\lambda)$ decays in S_0. Since no non-constant solution decays in two adjacent Stokes sectors, f_k and f_{k+1} are linearly independent and hence, any solution of (5) can be expressed as a linear combination of these two. Especially, for some coefficients $C_{j,k}(\lambda)$ and $D_{j,k}(\lambda)$,

$$f_j(z,\lambda) = C_{j,k}(\lambda)f_k(z,\lambda)+D_{j,k}(\lambda)f_{k+1}(z,\lambda), \quad j,k\in\mathbb{Z}. \tag{14}$$

These $C_{j,k}(\lambda)$ and $D_{j,k}(\lambda)$ are called the *Stokes multipliers of* f_j *with respect to* f_k *and* f_{k+1}.

Then,

$$C_{j,k}(\lambda) = \frac{W_{j,k+1}(\lambda)}{W_{k,k+1}(\lambda)}, \quad D_{j,k}(\lambda) = -\frac{W_{j,k}(\lambda)}{W_{k,k+1}(\lambda)}, \tag{15}$$

where $W_{j,k}=f_jf_k'-f_j'f_k$ is the Wronskian of f_j and f_k. Since both f_j and f_k are solutions of the same linear equation (5), the Wronskians are constant functions of z. Also, since f_k and f_{k+1} are linearly independent, $W_{k,k+1}\neq 0$ for all $k\in\mathbb{Z}$. In the next lemma, we will show that the Wronskian $W_{k,k+1}(\lambda)$ is constant, which is needed in the proof of our main theorem.

Lemma 5: *For each* $k\in\mathbb{Z}, W_{k,k+1}(\lambda)=-2\omega^{-m/4-k-1}$, *that is independent of* λ.

Proof: Since $f_k(z,\lambda)=f(\omega^{-k}z,\omega^{-mk}\lambda)$, we get

$$f_{k+1}(z,\lambda) = f(\omega^{-(k+1)}z,\omega^{-m(k+1)}\lambda) = f_k(\omega^{-1}z,\omega^{-m}\lambda) = f_k(\omega^{-1}z,\omega^2\lambda), \quad \text{by } \omega^{m+2}=1.$$

This along with $f_{k+1}'(z,\lambda)=\omega^{-1}f_k'(\omega^{-1}z,\omega^2\lambda)$, one can show that

$$W_{j+1,k+1}(\lambda) = \omega^{-1}W_{j,k}(\omega^2\lambda). \tag{16}$$

Using Proposition 4 (ii) and

$$W_{-1,0}(\lambda) = f_{-1}f_0' - f_0f_{-1}' = f(\omega z,\omega^{-2}\lambda)f'(z,\lambda) - f(z,\lambda)\omega f'(\omega z,\omega^{-2}\lambda),$$

one can show that as z tends to infinity in S_0 (for which above-mentioned asymptotics are valid),

$$\begin{aligned} W_{-1,0}(\lambda) &= -(\omega z)^{-m/4}z^{m/4}(1+O(z^{-1/2}))\exp\left[-\frac{2}{m+2}(\omega z)^{(m+2)/2} - \frac{2}{m+2}z^{(m+2)/2}\right] \\ &\quad + z^{-m/4}\omega(\omega z)^{m/4}(1+O(z^{-1/2}))\exp\left[-\frac{2}{m+2}(\omega z)^{(m+2)/2} - \frac{2}{m+2}z^{(m+2)/2}\right] \\ &= -2\omega^{-m/4}(1+O(z^{-1/2})) \quad \text{since } \omega^{(m+2)/2}=-1. \end{aligned}$$

Finally,

$$W_{-1,0}(a,\lambda) = -2\omega^{-m/4}. \tag{17}$$

Thus (16) and (17) complete the proof. □

In the next lemma, we will show that the Wronskians $W_{k,0}(\lambda)$ for $2\leq k\leq m$ have orders $\frac{1}{2}+1/m$, which is needed in establishing the induction step in Theorem 11 and proving existence of the eigenvalues under various boundary conditions. This lemma is due to Sibuya,[2] but we give a full proof here.

Lemma 6: *For each* $2\leq k\leq m$, *the Wronskian* $W_{k,0}(\lambda)$ *has its order* $\frac{1}{2}+\frac{1}{m}\in\left(\frac{1}{2},1\right)$.

Proof: First, we look at

$$W_{k,0}(\lambda) = f_k(z,\lambda)f_0'(z,\lambda) - f_0(z,\lambda)f_k'(z,\lambda) = f(0,\omega^{2k}\lambda)f'(0,\lambda) - f(0,\lambda)\omega^{-k}f'(0,\omega^{2k}\lambda), \tag{18}$$

where we take $z=0$ since the Wronskian is independent of z. Then the Wronskian $W_{k,0}(\lambda)$ has order less than or equal to $\frac{1}{2}+1/m$ because each term in the right hand side of (18) has order $\frac{1}{2}+1/m$ by Lemma 4 (v). So in order to show $W_{k,0}(\lambda)$ has order equal to $\frac{1}{2}+1/m$, it suffices to show that there exist $c_1>0$ and $c_2>0$ such that $|W_{k,0}(\lambda)|\geq c_1\exp[c_2|\lambda|^{1/2+1/m}]$ for all large $|\lambda|$ along some ray.

Next, we examine the right-hand side of (18) along the ray

$$\arg\lambda \equiv \theta = \pi - \frac{4\pi}{m+2},$$

by using the asymptotic expansions (10) and (11). Note that $\theta\in(-\pi+\delta,\pi-\delta)$, for all $0<\delta<\pi/(m+2)$. Recall that the expansions (10) and (11) are valid when $\lambda\to\infty$ in $|\arg\lambda|\leq\pi-\delta$. Since

$$\arg(\omega^{2k}\lambda) \equiv \theta_* = \theta + \frac{4k\pi}{m+2} - 2\pi \quad \text{for } 2 \leqslant k \leqslant \frac{m+2}{2}, \tag{19}$$

we have

$$-\pi < -\frac{m\pi}{m+2} < \theta_* < \theta < \frac{m\pi}{m+2} < \pi \quad \text{for } 2 \leqslant k \leqslant \frac{m+2}{2}. \tag{20}$$

Thus,

$$f(0,\omega^{2k}\lambda) = [1+o(1)]|\lambda|^{-1/4}e^{-i\theta_*/4}\exp\left[K|\lambda|^{1/2+1/m}e^{i[(m+2)/2m]\theta_*}\right],$$

$$f'(0,\omega^{2k}\lambda) = -[1+o(1)]|\lambda|^{-1/4}e^{-i\theta_*/4}\exp\left[K|\lambda|^{1/2+1/m}e^{i[(m+2)/2m]\theta_*}\right].$$

This along with (18) yields

$$\begin{aligned}
W_{k,0}(\lambda) &= -[1+o(1)]|\lambda|^{1/4}e^{i\theta/4}|\lambda|^{-1/4}e^{-i\theta_*/4}\exp\left[K|\lambda|^{1/2+1/m}\left(e^{i(1/2+1/m)\theta}+e^{i(1/2+1/m)\theta_*}\right)\right] \\
&\quad +[1+o(1)]|\lambda|^{-1/4}e^{-i\theta/4}\omega^{-k}|\lambda|^{1/4}e^{i\theta_*/4}\exp\left[K|\lambda|^{1/2+1/m}\left(e^{i(1/2+1/m)\theta}+e^{i(1/2+1/m)\theta_*}\right)\right] \\
&= \left[-e^{i(\theta-\theta_*)/4}+\omega^{-k}e^{i(\theta_*-\theta)/4}\right][1+o(1)]\exp\left[K|\lambda|^{1/2+1/m}\left(e^{i(1/2+1/m)\theta}+e^{i(1/2+1m)\theta_*}\right)\right] \\
&= -2i\omega^{-k/2}[1+o(1)]\exp\left[K|\lambda|^{1/2+1/m}\left(e^{i(1/2+1/m)\theta}+e^{i(1/2+1/m)\theta_*}\right)\right],
\end{aligned}$$

where the last step is by $\theta-\theta_*=2\pi-4k\pi/(m+2)$. So when $\arg\lambda=\pi-4\pi/(m+2)$, we have

$$\mathrm{Re}\left[e^{i(1/2+1/m)\theta}+e^{i(1/2+1/m)\theta_*}\right] = \mathrm{Re}\left[\cos\left(\frac{m+2}{2m}\theta\right)+\cos\left(\frac{m+2}{2m}\theta_*\right)\right] > 0,$$

where the last step is by (20).

So for $2\leqslant k\leqslant(m+2)/2$, since $K>0$, there exists $c_2>0$ such that $|W_{k,0}(\lambda)| \geqslant \exp[c_2|\lambda|^{1/2+1/m}]$ for all large $|\lambda|$ on the ray $\arg\lambda=\pi-4\pi/(m+2)$. Thus the order of $W_{k,0}(\lambda)$ for $2\leqslant k\leqslant(m+2)/2$ is $1/2+1/m$.

Certainly, the Wronskian $W_{k,0}(\lambda)$ for $2\leqslant k\leqslant(m+2)/2$ is blowing up in some other directions as well. If one finds θ and θ_* satisfying (20), the above argument will show that $W_{k,0}(\lambda)$ is blowing up along $\arg\lambda=\theta$.

Next for $(m+2)/2<k\leqslant m$, one can choose $\theta=-\pi+4\pi/(m+2)$ and θ_* by (19), and then follow an argument similar to the above to conclude that the order of $W_{k,0}(\lambda)$ is $1/2+1/m$. Or one uses an index change to reduce to the case already considered. That is,

$$\begin{aligned}
W_{k,0}(\lambda) &= W_{k-(m+2),0}(\lambda) \\
&= \omega^{m+2-k}W_{0,m+2-k}(\omega^{-2(m+2-k)}\lambda) \quad \text{by (16)} \\
&= -\omega^{m+2-k}W_{m+2-k,0}(\omega^{-2(m+2-k)}\lambda).
\end{aligned}$$

Then since $2\leqslant m+2-k<(m+2)/2$, we know the order of $W_{m+2-k,0}(\omega^{2(m+2-k)}\lambda)$ is $1/2+1/m$, and hence so is the order of $W_{k,0}(\lambda)$ for $(m+2)/2<k\leqslant m$. This completes the proof. □

D. Further results of Sibuya; identifying the eigenvalues as zeros of certain entire functions

We can relate the zeros of $C_{-n,n-1}(\lambda)$ and $D_{-n,n}(\lambda)$ with the eigenvalues of H_ℓ. First, we study the case when ℓ is odd, as follows.

Lemma 7: *Let $\ell=2n-1$ be odd, with $1\leqslant\ell\leqslant m-1$. Then the following are equivalent:*

(i) *a complex number λ is an eigenvalue of H_ℓ;*
(ii) *λ is a zero of the entire function $C_{-n,n-1}(\lambda)$; and*
(iii) *λ is a zero of the entire function $D_{-n,n}(\lambda)$.*

Moreover, the orders of the entire functions $C_{-n,n-1}(\lambda)$ and $D_{-n,n}(\lambda)$ are $\frac{1}{2}+1/m \in (\frac{1}{2},1)$.

Hence, the eigenvalues are discrete because they are zeros of a non-constant entire function. Note that the Stokes multipliers $C_{-n,n-1}(\lambda)$ and $D_{-n,n}(\lambda)$ are called *spectral determinants* or *Evans functions*.

Proof: Suppose that λ is an eigenvalue of H_{2n-1} with the corresponding eigenfunction u. We let $v(z)=u(-iz)$. Then v solves

$$-v''(z)+(z^m+\lambda)v(z)=0,$$

and decays in $S_{-n}\cup S_n$. Since $f_{-n}(z,\lambda)$ is another solution of this equation that decays in S_{-n}, we see that $f_{-n}(z,\lambda)$ is a multiple of v. Similarly $f_n(z,\lambda)$ is a multiple of v. Since

$$f_{-n}(z,\lambda)=C_{-n,n-1}(\lambda)f_{n-1}(z,\lambda)+D_{-n,n-1}(\lambda)f_n(z,\lambda), \tag{21}$$

and since $f_{n-1}(z,\lambda)$ blows up in S_n, we conclude that $C_{-n,n-1}(\lambda)=0$.

Conversely, we suppose that $C_{-n,n-1}(\lambda)=0$ for some $\lambda\in\mathbb{C}$. Then from (21) we see that $f_{-n}(z,\lambda)$ is a constant multiple of $f_n(z,\lambda)$. Thus both are decaying in $S_{-n}\cup S_n$, and hence $u(z)\coloneqq f_{-n}(iz,\lambda)$ is an eigenfunction of H_{2n-1} associated with the eigenvalue λ.

Similarly, since

$$f_{-n}(z,\lambda)=C_{-n,n}(\lambda)f_n(z,\lambda)+D_{-n,n}(\lambda)f_{n+1}(z,\lambda),$$

we see that λ is an eigenvalue of H_{2n-1} if and only if $D_{-n,n}(\lambda)=0$.

Finally, since $W_{k,k+1}(\lambda)$ is a constant by Lemma 5 and since $W_{k,0}(\lambda)$ for $2\leqslant k\leqslant m$ has order $\frac{1}{2}+\frac{1}{m}$ by Lemma 6, we see from (15) that $C_{-n,n-1}(\lambda)$ and $D_{-n,n}(\lambda)$ are of order $\frac{1}{2}+\frac{1}{m}\in(\frac{1}{2},1)$. This completes the proof. □

Second, we can relate the zeros of $C_{-n-1,n-1}(\lambda)$ and $D_{-n-1,n}(\lambda)$ with the eigenvalues of H_ℓ, when ℓ is even, as follows.

Lemma 8: *Let $\ell=2n$ be even, with $1\leqslant\ell\leqslant m-1$. Then the following are equivalent:*

(i) *a complex number λ is an eigenvalue of H_ℓ;*
(ii) *λ is a zero of the entire function $\lambda\mapsto C_{-n,n}(\omega^{-1}\lambda)$; and*
(iii) *λ is a zero of the entire function $\lambda\mapsto D_{-n-1,n}(\omega\lambda)$.*

Moreover, the orders of the entire functions $\lambda\mapsto C_{-n,n}(\omega^{-1}\lambda)$ and $\lambda\mapsto D_{-n-1,n}(\omega\lambda)$ are $\frac{1}{2}+\frac{1}{m}\in(\frac{1}{2},1)$.

Note again that the Stokes multipliers $C_{-n,n}(\omega^{-1}\lambda)$ and $D_{-n-1,n}(\omega\lambda)$ are spectral determinants or Evans functions.

Proof: Let u be an eigenfunction of H_{2n} associated with the eigenvalue λ. Then $v(z)\coloneqq u(-iz)$ solves

$$v''(z)+z^m v(z)=\lambda v(z).$$

Next we set $w_1(z)\coloneqq v(\omega^{-1/2}z)$. Then $w_1(z)$ solves

$$-w_1''(z)+[z^m+\omega^{-1}\lambda]w_1(z)=0. \tag{22}$$

One can then check that the boundary condition of H_{2n} becomes that $w_1(z)\to 0$ as $z\to\infty$ in $S_{-n}\cup S_{n+1}$. Then like we did for Lemma 7, since

$$f_{-n}(z,\omega^{-1}\lambda)=C_{-n,n}(\omega^{-1}\lambda)f_n(z,\omega^{-1}\lambda)+D_{-n,n}(\omega^{-1}\lambda)f_{n+1}(z,\omega^{-1}\lambda),$$

λ is an eigenvalue of H_{2n} if and only if $C_{-n,n}(\omega^{-1}\lambda)=0$.

Similarly, we let $w_2(z)\coloneqq v(\omega^{1/2}z)$. Then $w_2(z)$ solves

$$-w_2''(z)+[z^m+\omega\lambda]w_2(z)=0, \tag{23}$$

and the boundary condition of H_{2n} becomes that $w_2(z)\to 0$ as $z\to\infty$ in $S_{-n-1}\cup S_n$. Then since

$$f_{-n-1}(z,\omega\lambda) = C_{-n-1,n}(\omega\lambda) f_n(z,\omega\lambda) + D_{-n-1,n}(\omega\lambda) f_{n+1}(z,\omega\lambda),$$

λ is an eigenvalue of H_{2n} if and only if $D_{-n-1,n}(\omega\lambda)=0$. This completes the proof. □

Next we want infinite product representations of the entire functions $f(0,\lambda)$ and $f'(0,\lambda)$. Recall that the integer $m \geqslant 3$ is fixed.

Lemma 9: *The functions $f(0,\lambda)$ and $f'(0,\lambda)$ have infinitely many zeros $E_j<0$ and $E'_j<0$, respectively. Moreover, they admit the following infinite product representations:*

$$f(0,\lambda) = A_1 \prod_{j=1}^{\infty} \left(1 - \frac{\lambda}{E_j}\right) \quad \textit{for some } A_1 \in \mathbb{C}\setminus\{0\}. \tag{24}$$

$$f'(0,\lambda) = A_2 \prod_{j=1}^{\infty} \left(1 - \frac{\lambda}{E'_j}\right) \quad \textit{for some } A_2 \in \mathbb{C}\setminus\{0\}. \tag{25}$$

Proof: We know that $f(0,\lambda)$ and $f'(0,\lambda)$ have orders $\frac{1}{2}+1/m \in (0,1)$ by Proposition 4 (v), and hence by the Hadamard factorization theorem (see, for example, Theorem 14.2.6 on page 199 of Ref. 21), we know $f(0,\lambda)$ and $f'(0,\lambda)$ have infinite product representations (24) and (25) where $f(0,E_j)=0$ and $f'(0,E'_j)=0$ for all $j \in \mathbb{N}$. So in order to complete the proof, we need to show $E<0$ if $f(0,E)=0$, and $E'<0$ if $f'(0,E')=0$.

Suppose $f(0,E_*)=0$ or $f'(0,E_*)=0$. By the definition, we know that $f(z,E_*)$ solves

$$-f''(z,E_*) + z^m f(z,E_*) = -E_* f(z,E_*),$$

and decays to zero exponentially in S_0. (Note that $-\mathrm{d}^2/\mathrm{d}x^2+x^m$ is Hermitian in $L^2([0,+\infty))$.) In order to show $E_*<0$, we multiply this equation by $\overline{f(z,E_*)}$ and integrate over the positive real axis to get

$$-\int_0^\infty f''(x,E_*)\overline{f(x,E_*)}\mathrm{d}x + \int_0^\infty x^m |f(x,E_*)|^2 \mathrm{d}x = -E_* \int_0^\infty |f(x,E_*)|^2 \mathrm{d}x.$$

Next we integrate the first term by parts, and use $f(0,E_*)=0$ or $f'(0,E_*)=0$. Clearly the left-hand side of the resulting equation is positive, and hence we conclude $E_*<0$. This completes the proof. □

Next, we will introduce a symmetry lemma, regarding $f(z,\lambda)$ and $f(z,\lambda)$.

Lemma 10: *For each $\lambda \in \mathbb{C}$,*

$$\overline{f(\bar{z},\lambda)} = f(z,\bar{\lambda}), \quad \overline{f'(\bar{z},\lambda)} = f'(z,\bar{\lambda}). \tag{26}$$

Proof: This lemma for $z=0$ is contained in Lemma 8 in Ref. 4, and in fact that is all we will need in this paper. A proof of this lemma is essentially the same as that of Lemma 8 in Ref. 4. So we omit the proof here. □

III. THE INDUCTION STEP

In proving Theorem 2, we will use induction on ℓ. The induction step will be provided by the following theorem.

Theorem 11: *If $1 \leqslant \ell \leqslant m/2-1$ and all the eigenvalues of H_ℓ lie in the sector $|\arg\cdot| \leqslant 2\pi/(m+2)$, then every eigenvalue of $H_{\ell+1}$ is real and positive.*

Proof of Theorem 11 (Case I: *$\ell=2n-1$ is odd, with $1 \leqslant n \leqslant \frac{m}{4}$*): Suppose that all the eigenvalues σ_j of H_{2n-1} lie in the sector $|\arg\sigma_j| \leqslant 2\pi/(m+2)$. That is, zeros σ_j of the entire function $\sigma \mapsto D_{-n,n}(\sigma)$ lie in the sector $|\arg\sigma| \leqslant 2\pi/(m+2)$ (see Lemma 7). We will show that every eigenvalue λ of H_{2n} is real and positive.

Suppose $u(z)$ is an eigenfunction of H_{2n} associated with the eigenvalue λ. Then $u(z)$ solves

$$-u''(z)+(iz)^m u(z)=\lambda u(z),$$

and decays to zero as z tends to infinity along the two rays $\arg z=-\pi/2\pm(2n+1)\pi/(m+2)$. Set $v(z)=u(-iz)$. Then $v(z)$ solves

$$v''(z)+z^m v(z)=\lambda v(z), \tag{27}$$

and decays to zero as z tends to infinity along the two rays $\arg z=\pm(2n+1)\pi/(m+2)$.

Next we let $w(z)=v(\omega^{-1/2}z)$ so that $w(z)$ solves

$$-w''(z)+[z^m+\omega^{-1}\lambda]w(z)=0, \tag{28}$$

and decays to zero as z tends to infinity along the two rays $\arg z=(2n+2)\pi/(m+2)$, $-2n\pi/(m+2)$, the center rays of S_{n+1} and S_{-n}.

Then we examine

$$f_{-n}(z,\omega^{-1}\lambda)=C_{-n,n}(\omega^{-1}\lambda)f_n(z,\omega^{-1}\lambda)+D_{-n,n}(\omega^{-1}\lambda)f_{n+1}(z,\omega^{-1}\lambda),$$

or equivalently,

$$f(\omega^n z,\omega^{-2n-1}\lambda)=C_{-n,n}(\omega^{-1}\lambda)f(\omega^{-n}z,\omega^{2n-1}\lambda)+D_{-n,n}(\omega^{-1}\lambda)f(\omega^{-n-1}z,\omega^{2n+1}\lambda). \tag{29}$$

Since $C_{-n,n}(\omega^{-1}\lambda)=0$ by Lemma 8, we get $D_{-n,n}(\omega^{-1}\lambda)\neq 0$.

Next we will show that $|D_{-n,n}(\omega^{-1}\lambda)|\leqslant 1$ when λ is an eigenvalue of H_{2n} with $\operatorname{Im}\lambda\geqslant 0$. To this end, we evaluate the Eq. (29) and its differentiated form at $z=0$ to get

$$f(0,\omega^{-2n-1}\lambda)=D_{-n,n}(\omega^{-1}\lambda)f(0,\omega^{2n+1}\lambda), \tag{30}$$

$$\omega^n f'(0,\omega^{-2n-1}\lambda)=\omega^{-n-1}D_{-n,n}(\omega^{-1}\lambda)f'(0,\omega^{2n+1}\lambda). \tag{31}$$

Since λ is an eigenvalue, so is $\bar{\lambda}$. Thus,

$$f(0,\omega^{-2n-1}\bar{\lambda})=D_{-n,n}(\omega^{-1}\bar{\lambda})f(0,\omega^{2n+1}\bar{\lambda}),$$

$$\omega^n f'(0,\omega^{-2n-1}\bar{\lambda})=\omega^{-n-1}D_{-n,n}(\omega^{-1}\bar{\lambda})f'(0,\omega^{2n+1}\bar{\lambda}).$$

We take the complex conjugates of these, and apply (26) at $z=0$ to get

$$f(0,\omega^{2n+1}\lambda)=\overline{D_{-n,n}(\omega^{-1}\bar{\lambda})}f(0,\omega^{-2n-1}\lambda),$$

$$\omega^{-n}f'(0,\omega^{2n+1}\lambda)=\omega^{n+1}\overline{D_{-n,n}(\omega^{-1}\bar{\lambda})}f'(0,\omega^{-2n-1}\lambda).$$

So these along with (30) and (31) imply

$$D_{-n,n}(\omega^{-1}\lambda)\overline{D_{-n,n}(\omega^{-1}\bar{\lambda})}=1. \tag{32}$$

Clearly the order of the entire function $\sigma\mapsto D_{-n,n}(\sigma)$ is $\frac{1}{2}+1/m\in(0,1)$. So by the Hadamard factorization theorem we have

$$D_{-n,n}(\lambda)=B\prod_{j=1}^{\infty}\left(1-\frac{\lambda}{\sigma_j}\right)\quad\text{for some } B\in\mathbb{C}\setminus\{0\},$$

where the σ_j are the zeros of $D_{-n,n}(\sigma)$, and so $|\arg\sigma_j|\leqslant 2\pi/(m+2)$ for all $j\in\mathbb{N}$, by hypothesis.

Thus,

$$\left|\frac{D_{-n,n}(\omega^{-1}\lambda)}{D_{-n,n}(\omega^{-1}\bar{\lambda})}\right| = \prod_{j=1}^{\infty}\left|\frac{1-\dfrac{\omega^{-1}\lambda}{\sigma_j}}{1-\dfrac{\omega^{-1}\bar{\lambda}}{\sigma_j}}\right| = \prod_{j=1}^{\infty}\left|\frac{\omega\sigma_j-\lambda}{\omega\sigma_j-\bar{\lambda}}\right| \leqslant 1, \quad \text{when } \operatorname{Im}\lambda \geqslant 0, \tag{33}$$

since $\operatorname{Im}(\omega\sigma_j)\geqslant 0$ for all $j\in\mathbb{N}$. This along with (32) implies

$$|D_{-n,n}(\omega^{-1}\lambda)| \leqslant 1 \quad \text{when } \operatorname{Im}\lambda \geqslant 0.$$

Since the non-constant entire function $f(z,\omega^{2n+1}\lambda)$ solves

$$-f''(z,\omega^{2n+1}\lambda)+[z^m+\omega^{2n+1}\lambda]f(z,\omega^{2n+1}\lambda)=0,$$

we know $f(0,\omega^{2n+1}\lambda)$ and $f'(0,\omega^{2n+1}\lambda)$ cannot be zero at the same time. Otherwise, $f(z,\omega^{2n+1}\lambda)=0$ for all $z\in\mathbb{C}$.

Suppose that $f(0,\omega^{2n+1}\lambda)\neq 0$. Then we get

$$1 \geqslant |D_{-n,n}(\omega^{-1}\lambda)| = \prod_{j=1}^{\infty}\left|\frac{1-\dfrac{\omega^{-2n-1}\lambda}{E_j}}{1-\dfrac{\omega^{2n+1}\lambda}{E_j}}\right| = \prod_{j=1}^{\infty}\left|\frac{\omega^{2n+1}E_j-\lambda}{\omega^{2n+1}E_j-\bar{\lambda}}\right| \geqslant 1 \quad \text{when } \operatorname{Im}\lambda\geqslant 0,$$

where the last inequality holds since $\operatorname{Im}(\omega^{2n+1}E_j)\leqslant 0$ if $0\leqslant\arg(\omega^{2n+1})\leqslant\pi$, by Lemma 9 (this is where we use $1\leqslant n\leqslant m/4$). So we obtain

$$|D_{-n,n}(\omega^{-1}\lambda)| = 1 \quad \text{when } \operatorname{Im}\lambda\geqslant 0. \tag{34}$$

Similarly, when $f'(0,\omega^{2n+1}\lambda)\neq 0$,

$$1 \geqslant |D_{-n,n}(\omega^{-1}\lambda)| = \prod_{j=1}^{\infty}\left|\frac{1-\dfrac{\omega^{-2n-1}\lambda}{E'_j}}{1-\dfrac{\omega^{2n+1}\lambda}{E'_j}}\right| = \prod_{j=1}^{\infty}\left|\frac{\omega^{2n+1}E'_j-\lambda}{\omega^{2n+1}E'_j-\bar{\lambda}}\right| \geqslant 1 \quad \text{when } \operatorname{Im}\lambda\geqslant 0,$$

where the E'_j are zeros of $f'(0,E)$. So we again have (34). Hence (33) along with combining (32) and (34) yields

$$\prod_{j=1}^{\infty}\left|\frac{\omega\sigma_j-\lambda}{\omega\sigma_j-\bar{\lambda}}\right| = 1. \tag{35}$$

Since $|\arg\sigma_j|\leqslant 2\pi/(m+2)$ for all $j\in\mathbb{N}$, we know $\operatorname{Im}(\omega\sigma_j)\geqslant 0$ for all $j\in\mathbb{N}$. Moreover, $\operatorname{Im}(\omega\sigma_j)>0$ for some j since both σ_j and $\overline{\sigma_j}$ are eigenvalues of the $\mathcal{PT}$-symmetric oscillator H_{2n-1}. Therefore, from (35) we conclude $\lambda=\bar{\lambda}$, and so λ is real.

We still need to show positivity of the eigenvalues. The function $v(z)$ solves (27) and we know $\lambda\in\mathbb{R}$. Also, one can check that $\overline{v(\bar{z})}$ solves the same equation. Since the eigenvalues are simple, $v(z)$ and $\overline{v(\bar{z})}$ must be linearly dependent, and hence $v(z)=c\overline{v(\bar{z})}$ for some $c\in\mathbb{C}$. Since $|v(z)|$ and $|v(\bar{z})|$ agree on the real line, we see that $|c|=1$ and $|v(z)|=|v(\bar{z})|$ for all $z\in\mathbb{C}$. That is, $|v(x+iy)|$ is even in y. From this we have that

$$0 = \frac{\partial}{\partial y}|v(x+iy)|^2\Big|_{y=0} = -2\operatorname{Im}\big(v'(x)\overline{v(x)}\big) \quad \text{for all } x\in\mathbb{R}. \tag{36}$$

Let $g(r)=v(re^{i\theta})$ for $2n\pi/(m+2)<\theta<(2n+2)\pi/(m+2)$. Then $g(r)$ satisfies

$$e^{-2i\theta}g''(r)+e^{mi\theta}r^m g(r)=\lambda g(r).$$

Multiplying this by $\overline{g(r)}$ and integrating the resulting equation over $r\in[0,\infty)$ yield

$$e^{-2i\theta}\int_0^\infty g''(r)\overline{g(r)}\mathrm{d}r+e^{mi\theta}\int_0^\infty r^m|g(r)|^2\mathrm{d}r=\lambda\int_0^\infty|g(r)|^2\mathrm{d}r.$$

Next we integrate the first term by parts and multiply the resulting equation by $e^{i\theta}$ to have

$$-e^{-i\theta}g'(0)\overline{g(0)}-e^{-i\theta}\int_0^\infty|g'(r)|^2\mathrm{d}r+e^{(m+1)i\theta}\int_0^\infty r^m|g(r)|^2\mathrm{d}r=\lambda e^{i\theta}\int_0^\infty|g(r)|^2\mathrm{d}r.$$

Then we use $e^{-i\theta}g'(0)=v(0)$ and take the imaginary parts to get, for all $2n\pi/(m+2)<\theta<(2n+2)\pi/(m+2)$,

$$\sin\theta\int_0^\infty|g'(r)|^2\mathrm{d}r+\sin[(m+1)\theta]\int_0^\infty r^m|g(r)|^2\mathrm{d}r=\lambda\sin\theta\int_0^\infty|g(r)|^2\mathrm{d}r.$$

We evaluate this at $\theta=(2n+1)\pi/(m+1)$ to have $\lambda>0$. Note that since $1\leqslant n\leqslant(m-2)/4$, we see that $2n\pi/(m+2)<\theta=(2n+1)\pi/(m+1)<(2n+2)\pi/(m+2)$. □

Proof of Theorem 11 (Case II: $\ell=2n$ *is even, with* $1\leqslant n\leqslant(m-2)/4$): Suppose that all the eigenvalues τ_j of H_{2n} lie in the sector $|\arg\tau|\leqslant 2\pi/(m+2)$. Equivalently, zeros of the entire function $\tau\mapsto D_{-n-1,n}(\omega\tau)$ lie in the sector $|\arg\tau|\leqslant 2\pi/(m+2)$. We will show that every eigenvalue λ of H_{2n+1} is real and positive.

First, we examine $D_{-n-1,n}(\tau)$. From Lemma 8 (iii), the zeros of $\tau\mapsto D_{-n-1,n}(\omega\tau)$ are the eigenvalues τ_j of H_{2n}, which lie in the sector $|\arg\tau|\leqslant 2\pi/(m+2)$, by hypothesis. So

$$D_{-n-1,n}(\omega\tau)=B_1\prod_{j=1}^\infty\left(1-\frac{\tau}{\tau_j}\right)\quad\text{for some } B_1\in\mathbb{C}-\{0\},$$

where $\mathrm{Im}(\omega\tau_j)\geqslant 0$ for all $j\in\mathbb{N}$. Hence,

$$D_{-n-1,n}(\lambda)=B_1\prod_{j=1}^\infty\left(1-\frac{\omega^{-1}\lambda}{\tau_j}\right).$$

Thus, since $\mathrm{Im}(\omega\tau_j)\geqslant 0$,

$$\left|\frac{D_{-n-1,n}(\lambda)}{D_{-n-1,n}(\bar\lambda)}\right|=\prod_{j=1}^\infty\left|\frac{1-\dfrac{\omega^{-1}\lambda}{\tau_j}}{1-\dfrac{\omega^{-1}\bar\lambda}{\tau_j}}\right|=\prod_{j=1}^\infty\left|\frac{\omega\tau_j-\lambda}{\omega\tau_j-\bar\lambda}\right|\leqslant 1\quad\text{when Im}\,\lambda\geqslant 0.\tag{37}$$

Next, we suppose that $u(z)$ is an eigenfunction of H_{2n+1} associate with the eigenvalue λ. That is, $u(z)$ solves

$$-u''(z)+(-1)^{2n+1}(iz)^m u(z)=\lambda u(z),$$

and decays to zero as z tends to infinity along the two rays $\arg z=-\pi/2\pm(2n+2)\pi/(m+2)$. Set $v(z)=u(-iz)$. Then $v(z)$ solves

$$-v''(z)+(z^m+\lambda)v(z)=0, \tag{38}$$

and decays to zero as z tends to infinity along the two rays $\arg z=\pm(2n+2)\pi/(m+2)$, the center rays of S_{n+1} and S_{-n-1}.

We take a close look at

$$f_{-n-1}(z,\lambda)=C_{-n-1,n}(\lambda)f_n(z,\lambda)+D_{-n-1,n}(\lambda)f_{n+1}(z,\lambda). \tag{39}$$

Since $C_{-n-1,n}(\lambda)=0$ by Lemma 7, $D_{-n-1,n}(\lambda)\neq 0$. So

$$f(\omega^{n+1}z,\omega^{-2n-2}\lambda)=D_{-n-1,n}(\lambda)f(\omega^{-n-1}z,\omega^{2n+2}\lambda). \tag{40}$$

We will show that $|D_{-n-1,n}(\lambda)|\leqslant 1$ when λ is an eigenvalue of H_{2n+1} with $\operatorname{Im}\lambda\geqslant 0$.

Suppose $f(0,\omega^{-2n-2}\lambda)\neq 0$. Since λ is an eigenvalue, so is $\bar{\lambda}$. We replace λ by $\bar{\lambda}$ in (40), and then evaluate the resulting equation at $z=0$ to get

$$f(0,\omega^{-2n-2}\bar{\lambda})=D_{-n-1,n}(\bar{\lambda})f(0,\omega^{2n+2}\bar{\lambda}).$$

Then we take the complex conjugate of this and apply (26) so that we have

$$f(0,\omega^{2n+2}\lambda)=\overline{D_{-n-1,n}(\bar{\lambda})}f(0,\omega^{-2n-2}\lambda).$$

Combining this with (40) at $z=0$ yields

$$\overline{D_{-n-1,n}(\bar{\lambda})}D_{-n-1,n}(\lambda)=1, \tag{41}$$

where we used $f(0,\omega^{-2n-2}\lambda)\neq 0$.

Similarly, when $f'(0,\omega^{-2n-2}\lambda)\neq 0$, we get (41) again.

Eq. (41) along with the inequality in (37) implies $|D_{-n-1,n}(\lambda)|\leqslant 1$ when λ is an eigenvalue of H_{2n+1} with $\operatorname{Im}\lambda\geqslant 0$. So from (40) at $z=0$ we have

$$1\geqslant|D_{-n-1,n}(\lambda)|=\prod_{j=1}^{\infty}\left|\frac{1-\dfrac{\omega^{-2n-2}\lambda}{E_j}}{1-\dfrac{\omega^{2n+2}\lambda}{E_j}}\right|=\prod_{j=1}^{\infty}\left|\frac{\omega^{2n+2}E_j-\lambda}{\omega^{2n+2}E_j-\bar{\lambda}}\right|\geqslant 1\quad\text{when }\operatorname{Im}\lambda\geqslant 0, \tag{42}$$

where the last inequality holds since $\operatorname{Im}(\omega^{2n+2}E_j)\leqslant 0$ if $0\leqslant\arg(\omega^{2n+2})\leqslant\pi$ (this is where we use $1\leqslant n\leqslant(m-2)/4$). Then like in the proof for the case ℓ odd, we have $|D_{-n-1,n}(\lambda)|=1$, which is also obtained when $f(0,\omega^{-2n-2}\lambda)=0$ (and hence $f'(0,\omega^{-2n-2}\lambda)\neq 0$.) Therefore, we conclude $\lambda=\bar{\lambda}$, and so λ is real, like in the proof of the case ℓ odd.

We still need to show positivity of the eigenvalues λ. Recall that $\lambda\in\mathbb{R}$ and that $v(z)=u(-iz)$ solves (38). Let $g(r)=v(re^{i\theta})$. Then,

$$e^{-2i\theta}g''(r)+e^{mi\theta}r^m g(r)=\lambda g(r).$$

We multiply this by $\overline{g(r)}$ and integrate over $r\in[0,\infty)$ to get

$$e^{-2i\theta}\int_0^{\infty}g''(r)\overline{g(r)}\mathrm{d}r+e^{mi\theta}\int_0^{\infty}r^m|g(r)|^2\mathrm{d}r=\lambda\int_0^{\infty}|g(r)|^2\mathrm{d}r.$$

Since $v(z)$ decays exponentially to zero as z tends to infinity in $S_{n+1}\cup S_{-n-1}$, we have integrability for $(2n+1)\pi/(m+2)<\theta<(2n+3)\pi/(m+2)$.

Note that since $\lambda\in\mathbb{R}$, Eq. (36) is valid for this case as well. We integrate the first term by parts and multiply the resulting equation by $e^{i\theta}$ to get

$$-e^{-i\theta}g'(0)\overline{g(0)}-e^{-i\theta}\int_0^\infty |g'(r)|^2\mathrm{d}r+e^{(m+1)i\theta}\int_0^\infty r^m|g(r)|^2\mathrm{d}r=\lambda e^{i\theta}\int_0^\infty |g(r)|^2\mathrm{d}r.$$

Then we use $e^{-i\theta}g'(0)=v(0)$ and take the imaginary parts with using (36) to get, for all $(2n+1)\pi/(m+2)<\theta<(2n+3)\pi/(m+2)$,

$$\sin\theta\int_0^\infty |g'(r)|^2\mathrm{d}r+\sin[(m+1)\theta]\int_0^\infty r^m|g(r)|^2\mathrm{d}r=\lambda\sin\theta\int_0^\infty |g(r)|^2\mathrm{d}r.$$

Evaluating this at $\theta=(2n+1)\pi/(m+1)$ proves $\lambda>0$. Note that since $1\leqslant n\leqslant(m-2)/4$, we see that $(2n+1)\pi/(m+2)<\theta=(2n+1)\pi/(m+1)<(2n+3)\pi/(m+2)$. □

IV. PROOF OF THEOREM 2

In proving Theorem 2, our induction basis is provided by the following lemma that is due to Dorey *et al.*[3] (also, see Shin[4]).

Lemma 12: *The eigenvalues* λ *of* H_1 *are all real and positive.*

Here we will give an outline of the proof.

Proof: Let λ be an eigenvalue of H_1 with the corresponding eigenfunction $u(z)$. Set $v(z)=u(-iz)$. Then $v(z)$ decays in $S_{-1}\cup S_1$ and solves

$$-v(z)+(z^m+\lambda)v(z)=0.$$

Since

$$f_{-1}(z,\lambda)=C_{-1,0}(\lambda)f_0(z,\lambda)+D_{-1,0}(\lambda)f_1(z,\lambda), \tag{43}$$

$C_{-1,0}(\lambda)=0$. Moreover, we know that from (15) and (16), and Lemma 5,

$$|D_{-1,0}(\lambda)|=\left|\frac{W_{-1,0}(\lambda)}{W_{0,1}(\lambda)}\right|=1.$$

Next, we use infinite product forms of either (43) when $f_{-1}(0,\lambda)\neq 0$, or its differentiated form when $f'_{-1}(0,\lambda)\neq 0$ at $z=0$. Then like in the proof of Theorem 11, one can show that $\lambda>0$. Note that the hypothesis in Theorem 11 is needed for showing $|D_{-1,0}(\lambda)|=1$ only. □

Now we are ready to prove Theorem 2.

Proof of Theorem 2. For integers $1\leqslant\ell\leqslant m/2$, the theorem easily follows from induction on ℓ along with Theorem 11 and Lemma 12.

For $m/2<\ell\leqslant m-1$, suppose that λ is an eigenvalue of H_ℓ with the corresponding eigenfunction $u_1(z)$. Let $u(z):=u_1(-z)$. Then $u(z)$ solves $-u''(z)+(-1)^\ell(-iz)^m u(z)=\lambda u(z)$, that is, $u(z)$ solves

$$-u''(z)+(-1)^{m-\ell}(iz)^m u(z)=\lambda u(z).$$

Next, we examine the boundary condition. It is clear that since $u_1(z)$ decays along the two rays $\arg z=-\pi/2\pm[\ell+1/(m+2)]\pi$, we see that $u(z)$ decays along the two rays

$$\arg z=-\pi-\frac{\pi}{2}+\frac{\ell+1}{m+2}\pi=-\frac{\pi}{2}-\frac{(m-\ell)+1}{m+2}\pi,$$

$$\arg z=\pi-\frac{\pi}{2}-\frac{\ell+1}{m+2}\pi=-\frac{\pi}{2}+\frac{(m-\ell)+1}{m+2}\pi.$$

This is the boundary condition (2) with $m-\ell$ in the place of ℓ. Hence, $u(z)$ is an eigenfunction of $H_{m-\ell}$ associated with the eigenvalue λ. Since $m/2<\ell\leqslant m-1$, we see that $1\leqslant m-\ell<m/2$. So $\lambda>0$. This completes the proof. □

Remark: Our method in this paper closely follows the $\ell=1$ method of Dorey *et al.*[3] and Shin.[4]

One big difference is that if $\ell=1$ then $|D_{-1,0}(\sigma)|=1$ for all $\sigma\in\mathbb{C}$, whereas for $1<\ell<m-1$, the corresponding functions $\sigma\mapsto D_{-n,n}(\omega^{-1}\sigma)$ in (29) and $\sigma\mapsto D_{-n-1,n}(\sigma)$ in (39) are entire functions of order $\frac{1}{2}+1/m$. However, when λ is an eigenvalue of $H_{\ell+1}$, under some hypothesis on the eigenvalues σ of H_ℓ we are able to show that $|D_{-n,n}(\omega^{-1}\lambda)|=1$ for $\ell=2n-1$ odd, and $|D_{-n-1,n}(\lambda)|=1$ for $\ell=2n$ even. This is the new and main idea in proving the induction step, Theorem 11.

V. CONCLUSIONS

In this paper, we proved that for each integer $1\leqslant\ell\leqslant m-1$, the eigenvalues $\lambda\in\mathbb{C}$ of

$$-u''(z)+(-1)^\ell(iz)^m u(z)=\lambda u(z),$$

under the boundary condition that $u(z)\to 0$ exponentially, as $z\to\infty$ along the two rays $\arg z=-\pi/2\pm(\ell+1)/(m+2)$, are all real and positive. And we studied other boundary conditions. Due to asymptotic behavior of the solution $u(z)$ as $z\to\infty$, if the Stokes sectors that contain the two ray where we impose the boundary condition are symmetric with respect to the imaginary axis, then the eigenvalues are all real and positive, except the case when the two Stokes sectors contain the imaginary axis. For all other rapid decaying boundary conditions, either there is no eigenvalue or the eigenvalues are not real.

It will be interesting to consider the eigenvalue problem with more general polynomial potentials $(-1)^\ell(iz)^m+P(iz)$ where $P(z)$ is a real polynomial with degree less than m, under the boundary condition (2).

It is known that some $\mathcal{PT}$-symmetric oscillators with some cubic and quartic polynomial potentials have nonreal eigenvalues.[13,14,16,17] One would like to classify when $\mathcal{PT}$-symmetric oscillators with polynomial potentials have nonreal eigenvalues.

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Monopole-antimonopole and vortex rings

Rosy Teh[a] and Khai-Ming Wong
School of Physics, Universiti Sains Malaysia, 11800 USM Penang, Malaysia

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The SU(2) Yang-Mills-Higgs theory supports the existence of monopoles, antimonopoles, and vortex rings. In this paper, we would like to present new exact static antimonopole-monopole-antimonopole (A-M-A) configurations. The net magnetic charge of these configurations is always −1, while the net magnetic charge at the origin is always +1 for all positive integer values of the solution's parameter m. However, when m increases beyond 1, vortex rings appear coexisting with these AMA configurations. The number of vortex rings increases proportionally with the value of m. They are located in space where the Higgs field vanishes along rings. We also show that a single-point singularity in the Higgs field does not necessarily correspond to a structureless 1-monopole at the origin but to a zero-size monopole-antimonopole-monopole (MAM) structure when the solution's parameter m is odd. This monopole is the Wu-Yang-type monopole and it possesses the Dirac string potential in the Abelian gauge. These exact solutions are a different kind of Bogomol'nyi-Prasad-Sommerfield (BPS) solutions as they satisfy the first-order Bogomol'nyi equation but possess infinite energy due to a point singularity at the origin of the coordinate axes. They are all axially symmetrical about the z-axis. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1996832]

I. INTRODUCTION

The SU(2) Yang-Mills-Higgs (YMH) field theory, with the Higgs field in the adjoint representation, possesses magnetic monopole, multimonopole, antimonopoles, and vortex rings solutions.[1–8] The only spherically symmetric monopole solution is the unit magnetic charge monopole. The 't Hooft–Polyakov monopole solution with nonzero Higgs mass and Higgs self-interaction is numerically and spherically symmetrical.[1,2] Multimonopole solutions possess at most axial symmetry.[3]

The model with nonvanishing Higgs vacuum expectation value but vanishing Higgs potential possesses exact monopole and multimonopole solutions which can be obtained by solving the first-order Bogomol'nyi equations.[9] These solutions satisfying the Bogomol'nyi-Prasad-Sommerfield (BPS) limit possess minimal energies. Exact monopole and multimonopoles solutions exist in the BPS limit,[2,3] while outside the BPS limit, when the Higgs field potential is nonvanishing, only numerical solutions are known. Asymmetric multimonopole solutions with no rotational symmetry are numerical solutions even in the BPS limit.[4]

At present, the different exact configurations of monopoles found are the BPS multimonopole solutions of magnetic charges M greater than unity with all the magnetic charges superimposed into a single point in space.[3] These superimposed multimonopole solutions possess axial and mirror symmetries. Following these works, finitely separated 1-monopoles were also constructed.[4,5]

Numerical axially symmetric non-Bogomol'nyi monopole-antimonopole chain solutions were

[a]Electronic mail: rosyteh@usm.my

also found to exist both in the limit of a vanishing Higgs potential as well as in the presence of a finite Higgs potential. Recently, numerical BPS axially symmetric vortex rings solutions have also been reported.[6]

We have reported on the existence of a different type of BPS static monopole-antimonopole solution in Ref. 7. This solution, which is exact and axially symmetric, represents two separate antimonopoles located at equal distances along the z-axis from a 1-monopole which is located at the origin. We have also shown that the extended ansatz of Ref. 7 possesses more multimonopole-antimonopole configurations, together with their anticonfigurations.[8] These configurations possess either radial, axial, or mirror symmetries about the z-axis, and they represent different combinations of monopoles, multimonopole, and antimonopoles.

In general, configurations of the YMH field theory with a unit magnetic charge are spherically symmetric,[1,2] while multimonopole configurations with magnetic charges greater than unity possess at most axial symmetry.[3] However, we have emphasized in a recent work[10] that unit magnetic charge configurations are not necessarily spherically symmetric. By employing the ansatz of Ref. 7, we have found an exact unit magnetic charge solution that does not even possess axial symmetry but only mirror symmetry about a vertical plane through the z-axis. However, the converse is true, and it has been shown that multimonopole solutions cannot possess spherical symmetry.[11] We would also like to mention that, within the ansatz of Ref. 7, half-monopole solutions have also been reported.[10]

In this paper we would like to present new static axially symmetric antimonopole-monopole-antimonopole (A-M-A) configurations of the SU(2) YMH theory with the Higgs field in the adjoint representation. Here, the Higgs field vanishes either at points corresponding to antimonopoles or at rings corresponding to vortex loops. The net magnetic charge of these configurations is always -1, while the net magnetic charge at the origin, $r=0$, is always $+1$ for all positive integer values of the solution's parameter m. However, when m increases beyond 1, vortex rings appear coexisting with these A-M-A configurations. The number of vortex rings in the configuration is equal to $(m-1)$, where $m \geqslant 1$. They are located horizontally in space where the Higgs field is zero along rings. Hence, this family of solutions all lies in the topologically nontrivial sector with topogical charge -1.

The two antimonopoles of the solutions are located at the two zeros of the Higgs field along the z-axis, while the Wu-Yang-type 1-monopole is located at a point singularity of the Higgs field at the origin. We also show that this single-point singularity in the Higgs field need not correspond to a structureless 1-monopole at the origin but to a zero-size monopole-antimonopole-monopole (MAM) structure when m is odd. These exact solutions are a different kind of BPS solution as they satisfy the first-order Bogomol'nyi equation, but possess infinite energy due to a point singularity at the origin of the coordinate axes.

We briefly review the SU(2) Yang-Mills-Higgs field theory and discuss the boundary conditions of these solutions in Sec. II. We discuss the magnetic ansatz and its formulation in Sec. III and present the solutions in Sec. IV. We end with some comments in Sec. V.

II. THE SU(2) YANG-MILLS-HIGGS THEORY

The SU(2) group admits the triplet Yang-Mills gauge fields potential A_μ^a which when coupled to a scalar Higgs triplets field Φ^a in $3+1$ dimensions gives the SU(2) YMH theory.[12] The index a is the SU(2) internal space index and, for a given a, Φ^a is a scalar whereas A_μ^a is a vector under Lorentz transformation. The SU(2) YMH Lagrangian is given by

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}^a F^{a\mu\nu} + \frac{1}{2}D^\mu \Phi^a D_\mu \Phi^a - \frac{1}{4}\lambda\left(\Phi^a\Phi^a - \frac{\mu^2}{\lambda}\right)^2, \tag{1}$$

where the Higgs field mass, μ, and the strength of the Higgs potential, λ, are constants. The vacuum expectation value of the Higgs field is then $\mu/\sqrt{\lambda}$. The Lagrangian (1) is gauge invariant under the set of independent local SU(2) transformations at each space–time point. The covariant derivative of the Higgs field and the gauge field strength tensor are given, respectively, by

$$D_\mu \Phi^a = \partial_\mu \Phi^a + \epsilon^{abc} A_\mu^b \Phi^c, \tag{2}$$

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + \epsilon^{abc} A_\mu^b A_\nu^c. \tag{3}$$

Since the gauge field coupling constant g can be scaled away, we can set g to 1 without any loss of generality. The metric used is $g_{\mu\nu}=(-+++)$. The SU(2) internal group indices a, b, c run from 1 to 3 and the spatial indices are μ, ν, $\alpha=0$, 1, 2, and 3 in Minkowski space.

The equations of motion that follow from the Lagrangian (1) are

$$D^\mu F_{\mu\nu}^a = \partial^\mu F_{\mu\nu}^a + \epsilon^{abc} A^{b\mu} F_{\mu\nu}^c = \epsilon^{abc} \Phi^b D_\nu \Phi^c,$$

$$D^\mu D_\mu \Phi^a = -\lambda \Phi^a \left(\Phi^b \Phi^b - \frac{\mu^2}{\lambda} \right). \tag{4}$$

The tensor to be identified with the Abelian electromagnetic field, as proposed by 't Hooft,[1,13] is

$$F_{\mu\nu} = \hat{\Phi}^a F_{\mu\nu}^a - \epsilon^{abc} \hat{\Phi}^a D_\mu \hat{\Phi}^b D_\nu \hat{\Phi}^c = \partial_\mu A_\nu - \partial_\nu A_\mu - \epsilon^{abc} \hat{\Phi}^a \partial_\mu \hat{\Phi}^b \partial_\nu \hat{\Phi}^c, \tag{5}$$

where $A_\mu = \hat{\Phi}^a A_\mu^a$, $\hat{\Phi}^a = \Phi^a / |\Phi|$, $|\Phi| = \sqrt{\Phi^a \Phi^a}$. Hence, the Abelian electric field is $E_i = F_{0i}$, and the Abelian magnetic field is $B_i = -\frac{1}{2} \epsilon_{ijk} F_{jk}$, where the indices i, j, $k = 1, 2, 3$. The topological magnetic current, which is also the topological current density of the system, is[13]

$$k_\mu = \frac{1}{8\pi} \epsilon_{\mu\nu\rho\sigma} \epsilon_{abc} \partial^\nu \hat{\Phi}^a \partial^\rho \hat{\Phi}^b \partial^\sigma \hat{\Phi}^c. \tag{6}$$

Therefore, the corresponding conserved topological magnetic charge is

$$M = \int d^3x k_0 = \frac{1}{8\pi} \int \epsilon_{ijk} \epsilon^{abc} \partial_i (\hat{\Phi}^a \partial_j \hat{\Phi}^b \partial_k \hat{\Phi}^c) d^3x = \frac{1}{8\pi} \oint d^2\sigma_i (\epsilon_{ijk} \epsilon^{abc} \hat{\Phi}^a \partial_j \hat{\Phi}^b \partial_k \hat{\Phi}^c) = \frac{1}{4\pi} \oint d^2\sigma_i B_i. \tag{7}$$

Our work is restricted to the static case where $A_0^a = 0$ with massless Higgs field and vanishing self-interaction. The magnitude of the Higgs field vanishes as $1/r$ at large r. However, this does not affect the Abelian magnetic field of the solutions, as this magnetic field depends only on the unit vector of the Higgs field. It is in this limit that the solutions are solved using both the second-order Euler-Lagrange equations and the Bogomol'nyi equations, $B_i^a \pm D_i \Phi^a = 0$. The $\pm$ sign corresponds to monopoles and antimonopoles, respectively, for the usual BPS solutions.[13] In our case, the A-M-A configuration is solved with the $+$ sign, and its anticonfiguration, that is, the M-A-M configuration, is solved with the $-$ sign.[8]

III. THE ANSATZ AND ITS FORMULATION

The static gauge fields and Higgs field which will lead to the axially symmetric vortex rings solutions are given, respectively, by[7]

$$A_\mu^a = \frac{1}{r} \psi(r) (\hat{\theta}^a \hat{\phi}_\mu - \hat{\phi}^a \hat{\theta}_\mu) + \frac{1}{r} R(\theta) (\hat{\phi}^a \hat{r}_\mu - \hat{r}^a \hat{\phi}_\mu),$$

$$\Phi^a = \Phi_1 \hat{r}^a + \Phi_2 \hat{\theta}^a, \tag{8}$$

where $\Phi_1 = (1/r)\psi(r)$, $\Phi_2 = (1/r)R(\theta)$. The spherical coordinate orthonormal unit vectors, $\hat{r}^a$, $\hat{\theta}^a$, and $\hat{\phi}^a$, are defined by

$$\hat{r}^a = \sin\theta \cos\phi \delta_1^a + \sin\theta \sin\phi \delta_2^a + \cos\theta \delta_3^a,$$

$$\hat{\theta}^a = \cos\theta\cos\phi\delta_1^a + \cos\theta\sin\phi\delta_2^a - \sin\theta\delta_3^a,$$

$$\hat{\phi}^a = -\sin\phi\delta_1^a + \cos\phi\delta_2^a, \tag{9}$$

where $r=\sqrt{x^i x_i}$, $\theta=\cos^{-1}(x_3/r)$, and $\phi=\tan^{-1}(x_2/x_1)$. The gauge field strength tensor and the covariant derivative of the Higgs field are given, respectively, by

$$\begin{aligned} F_{\mu\nu}^a = {} & \frac{1}{r^2}\hat{r}^a\{\dot{R} + R\cot\theta + 2\psi - \psi^2\}(\hat{\phi}_\mu\hat{\theta}_\nu - \hat{\phi}_\nu\hat{\theta}_\mu) + \frac{1}{r^2}\hat{\theta}^a\{R(1-\psi)\}(\hat{\phi}_\mu\hat{\theta}_\nu - \hat{\phi}_\nu\hat{\theta}_\mu) \\ & + \frac{1}{r^2}\{\hat{r}^a R(1-\psi) + \hat{\theta}^a(r\psi' + R\cot\theta - R^2)\}(\hat{r}_\mu\hat{\phi}_\nu - \hat{r}_\nu\hat{\phi}_\mu) \\ & + \frac{1}{r^2}\hat{\phi}^a\{-(r\psi' + \dot{R})\}(\hat{r}_\mu\hat{\theta}_\nu - \hat{r}_\nu\hat{\theta}_\mu), \end{aligned} \tag{10}$$

$$\begin{aligned} D_\mu\Phi^a = {} & \frac{1}{r^2}\{\hat{r}^a(r\psi' - \psi - R^2) - \hat{\theta}^a R(1-\psi)\}\hat{r}_\mu + \frac{1}{r^2}\{-\hat{r}^a R(1-\psi) + \hat{\theta}^a(\dot{R} + \psi - \psi^2)\}\hat{\theta}_\mu \\ & + \frac{1}{r^2}\{\hat{\phi}^a(\psi - \psi^2 + R\cot\theta - R^2)\}\hat{\phi}_\mu. \end{aligned} \tag{11}$$

Here, prime means $\partial/\partial r$ and dot means $\partial/\partial\theta$. The gauge-fixing condition that we used here is the radiation or Coulomb gauge, $\partial^i A_i^a = 0$, $A_0^a = 0$.

The ansatz (8) is substituted into the equations of motion (4) as well as the Bogomol'nyi equations with the positive sign, and the resulting equations of motion are just two first-order differential equations

$$r\psi' + \psi - \psi^2 = -p, \tag{12}$$

$$\dot{R} + R\cot\theta - R^2 = p, \tag{13}$$

where p is an arbitary constant. Equation (12) is exactly solvable for all real values of p and the integration constant can be scaled away by letting $r \to r/c$, where c is the arbitrary integration constant. Hence, without any loss in generality, c is set to unity. In order to obtain solutions of ψ with $(2m+1)$ powers of r, we can write $p=m(m+1)$, where m is real. By doing so, the solutions of the Riccati equation (13) can be exactly solved in terms of the Legendre functions of the first and second kind. For the solutions of Eq. (13) to be regular along the z-axis, we require $R(\theta)$ to vanish when $\theta=0$ and $\theta=\pi$. To achieve these boundary conditions, the integration constant of Eq. (13) is set to zero and m is restricted to take integer values. The solutions for ψ and R are then given, respectively, by

$$\psi(r) = \frac{(m+1) - mr^{2m+1}}{1 + r^{2m+1}},$$

$$R(\theta) = (m+1)\left\{\cot\theta - \frac{P_{m+1}(\cos\theta)}{P_m(\cos\theta)}\csc\theta\right\}, \tag{14}$$

where P_m is the Legendre polynomial of degree m, and $m=0,1,2,3,\ldots$. Hence, the boundary conditions of the solutions, Eq. (14), are $\psi(0)=m+1$, $\psi(\infty)=-m$, $R(0)=R(\pi)=0$.

In the BPS limit, the energy can be written in the form

$$E = \mp \int \partial_i (B_i^a \Phi^a) d^3x + \int \frac{1}{2}(B_i^a \pm D_i \Phi^a)^2 d^3x = \mp \int \partial_i (B_i^a \Phi^a) d^3x = 4\pi M \frac{\mu}{\sqrt{\lambda}}, \tag{15}$$

where M is the "topological charge" when the vacuum expectation value of the Higgs field, $\mu/\sqrt{\lambda}$, is nonzero coupled with some nontrivial topological structure of the fields at large r.

The energy density $\partial_i(B_i^a \Phi^a)$ of the non-Abelian system is finite everywhere and vanishes as $1/r^2$ at large r except at the origin $r=0$ due to the presence of a point singularity there and along singular planes where $P_m(\cos\theta)$ vanishes. The two antimonopoles which are regular antimonopoles and the vortex rings are located at points and rings where the Higgs field, $r\Phi^a$, vanishes, respectively. The monopole at the origin is of a different nature and is located where the Higgs field is singular. In the Abelian gauge, this monopole carries a Dirac string singularity.

The topological charge is also related to another gauge invariant quantity of the system as given by Eq. (7)

$$M_\infty = \frac{1}{8\pi} \oint d^2\sigma_i \, (\epsilon_{ijk} \epsilon^{abc} \hat{\Phi}^a \partial_j \hat{\Phi}^b \partial_k \hat{\Phi}^c)|_{r\to\infty}. \tag{16}$$

The magnetic charges enclosed by the sphere at infinity can be associated with the zeros of the Higgs field, $r\Phi^a$, and at points where $\hat{\Phi}^a$ becomes indeterminate. The positions of the two antimonopole do correspond to the two point zeros of the Higgs field in the A-M-A solutions. However, the Wu-Yang-type 1-monopole is not located at the zeros of the Higgs field but at the origin of the coordinate axes where the Higgs field is singular.

From the ansatz (8), $A_\mu = \hat{\Phi}^a A_\mu^a = 0$. Hence, from Eq. (5), the Abelian electric field is zero and the Abelian magnetic field is independent of the gauge fields A_μ^a. To calculate for the 't Hooft Abelian magnetic field B_i, we rewrite the Higgs field of Eq. (8) from the spherical to the Cartesian coordinate system[6–8]

$$\Phi^a = \Phi_1 \hat{r}^a + \Phi_2 \hat{\theta}^a + \Phi_3 \hat{\phi}^a = \tilde{\Phi}_1 \delta^{a1} + \tilde{\Phi}_2 \delta^{a2} + \tilde{\Phi}_3 \delta^{a3}, \tag{17}$$

where

$$\tilde{\Phi}_1 = \sin\theta\cos\phi\Phi_1 + \cos\theta\cos\phi\Phi_2 - \sin\phi\Phi_3 = |\Phi|\cos\alpha\sin\beta,$$

$$\tilde{\Phi}_2 = \sin\theta\sin\phi\Phi_1 + \cos\theta\sin\phi\Phi_2 + \cos\phi\Phi_3 = |\Phi|\cos\alpha\cos\beta,$$

$$\tilde{\Phi}_3 = \cos\theta\Phi_1 - \sin\theta\Phi_2 = |\Phi|\sin\alpha. \tag{18}$$

The Higgs unit vector is then simplified to

$$\hat{\Phi}^a = \cos\alpha\sin\beta\delta^{a1} + \cos\alpha\cos\beta\delta^{a2} + \sin\alpha\delta^{a3}, \tag{19}$$

where

$$\sin\alpha = \frac{\psi\cos\theta - R\sin\theta}{\sqrt{\psi^2 + R^2}}, \quad \beta = \frac{\pi}{2} - \phi,$$

and the Abelian magnetic field is found to reduce to only the $\hat{r}_i$ and $\hat{\theta}_i$ components

$$B_i = \frac{1}{r^2\sin\theta}\left\{\frac{\partial\sin\alpha}{\partial\theta}\frac{\partial\beta}{\partial\phi} - \frac{\partial\sin\alpha}{\partial\phi}\frac{\partial\beta}{\partial\theta}\right\}\hat{r}_i + \frac{1}{r\sin\theta}\left\{\frac{\partial\sin\alpha}{\partial\phi}\frac{\partial\beta}{\partial r} - \frac{\partial\sin\alpha}{\partial r}\frac{\partial\beta}{\partial\phi}\right\}\hat{\theta}_i + \frac{1}{r}\left\{\frac{\partial\sin\alpha}{\partial r}\frac{\partial\beta}{\partial\theta} - \frac{\partial\sin\alpha}{\partial\theta}\frac{\partial\beta}{\partial r}\right\}\hat{\phi}_i,$$

$$=-\frac{1}{r^2\sin\theta}\left\{\frac{\partial\sin\alpha}{\partial\theta}\right\}\hat{r}_i+\frac{1}{r\sin\theta}\left\{\frac{\partial\sin\alpha}{\partial r}\right\}\hat{\theta}_i. \tag{20}$$

Since $\sin\alpha$ is a nonsingular function except at the points where the Higgs field, $r\Phi^a$, vanishes, the 't Hooft magnetic field is regular everywhere except at the locations of the A-M-A and the vortex rings.

By noticing that the magnetic field, Eq. (20), can also be written as

$$B_i=\epsilon_{ijk}\partial^j(\sin\alpha)\partial^k\beta,$$

$$=\epsilon_{ijk}\partial^j(\sin\alpha\partial^k\beta), \tag{21}$$

we found that a suitable Maxwell four-vector gauge potential for this 't Hooft magnetic field is

$$\mathcal{A}_0=0,$$

$$\mathcal{A}_i=(\sin\alpha-1)\partial_i\beta=-\frac{(\sin\alpha-1)}{r\sin\theta}\hat{\phi}_i. \tag{22}$$

This gauge potential also satisfies the Coulomb gauge condition, $\partial^i\mathcal{A}_i=0$. The function $\sin\alpha$ is a bounded function of r and θ, and it is not smooth and discontinuous only when the profile function $R(\theta)$ is singular. When $m=0$, the gauge potential Eq. (22) is just the usual Dirac string potential and it is singular along the negative z-axis. However, when $m>0$, the gauge potential $\mathcal{A}_i$ possesses a broken Dirac string singularity. This Dirac string singularity extends from the origin to $z=-\sqrt[2m+1]{(m+1)/m}$ along the negative z-axis and from $z=\sqrt[2m+1]{(m+1)/m}$ to infinity along the positive z-axis. The gauge potential, $\mathcal{A}_i$, is only discontinuous at values of θ when $R(\theta)$ is singular.

From Eq. (21), it is obvious that the magnetic field is always perpendicular to the gradient of $\sin\alpha$. Hence, the magnetic field lines lie on the line $\sin\alpha=k$, $-1<k<1$, and $\phi=$constant. By plotting $\sin\alpha=k$ on a vertical plane through the origin, we manage to draw the magnetic field lines for the configurations when $m=1$, Fig. 2; $m=2$, Fig. 6; and $m=3$, Fig. 8.

Defining the Abelian field magnetic flux as

$$\Omega=4\pi M=\oint d^2\sigma_i B_i=\int B_i(r^2\sin\theta\,d\theta)\hat{r}_i d\phi, \tag{23}$$

the magnetic charge enclosed by the sphere at infinity, M_∞, is calculated to be

$$M_\infty=-\left.\frac{1}{2}\sin\alpha\right|_{0,r\to\infty}^{\pi}=-1,\quad \text{when } m=1,2,3,\ldots;M_\infty=1,\quad \text{when } m=0. \tag{24}$$

From Eq. (24), we can conclude that the total magnetic charge M of these axially symmetric solutions does not depend on the degree of the Legendre polynomial when $m>0$. Hence, the net magnetic charge of the system when $m>0$ is always -1. By letting M_0 be the net magnetic charge when the radius of the enclosing sphere tends to zero at the origin, we get

$$M_0=-\left.\frac{1}{2}\sin\alpha\right|_{0,r\to0}^{\pi}=1,\quad m=0,1,2,3,\ldots. \tag{25}$$

Similarly, the net magnetic charge, M_0, at the point singularity of the solution is independent of the value of m. In fact, it is true that for positive nonzero m, when $r<\sqrt[2m+1]{(m+1)/m}$, the topological magnetic charge is $+1$, and when $r>\sqrt[2m+1]{(m+1)/m}$, the topological magnetic charge is -1. Hence, there is a 1-monopole located at $r=0$ and two antimonopoles located along the z-axis at $r=\sqrt[2m+1]{(m+1)/m}$.

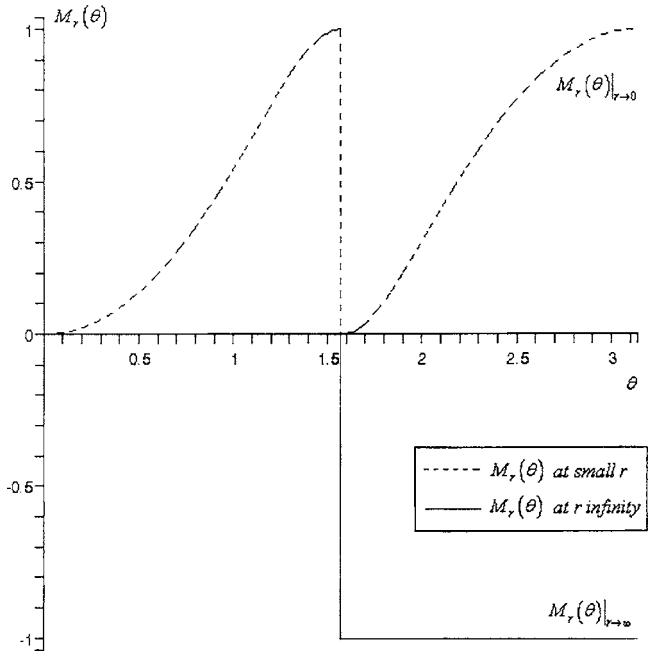

FIG. 1. A plot of $M_r(\theta)$ at small r close to zero and $M_r(\theta)$ at r infinity when $m=1$, versus θ.

We also notice that we can write the net magnetic flux per 4π sterad passing through the spherical surface of a partial enclosing sphere of radius r, sustaining an angle θ at the origin with the positive z-axis as

$$M_r(\theta) = -\left.\frac{(\psi(r)\cos\theta - R(\theta)\sin\theta)}{2\sqrt{\psi^2(r)+R^2(\theta)}}\right|_0^\theta = \frac{1}{2}\left\{\frac{\psi}{|\psi|} - \sin\alpha\right\}. \tag{26}$$

IV. MONOPOLE, ANTIMONOPOLES, AND VORTEX RINGS

The first member of this series of axially symmetric solutions is when $m=0$. As discussed in our previous work,[7] this solution is the Wu-Yang-type monopole located at $r=0$. This radially symmetric monopole with its magnetic field, $B_i=(1/r^2)\hat{r}_i$, has the vector potential $\mathcal{A}_i$ given by Eq. (22). This is just the Dirac string gauge potential, $\mathcal{A}_\mu=(1/r)\tan(\frac{1}{2}\theta)\hat{\phi}_\mu$, which is singular along the negative z-axis.

When $m=1$, the configuration is the second member of the axially symmetric monopole solutions. This configuration is similar to the (A1) solution of Refs. 7 and 8 with gauge potentials and Higgs field given by

$$A^a_\mu = \frac{1}{r}\left\{\frac{2-r^3}{1+r^3}\right\}(\hat{\theta}^a\hat{\phi}_\mu - \hat{\phi}^a\hat{\theta}_\mu) + \frac{1}{r}\tan\theta(\hat{\phi}^a\hat{r}_\mu - \hat{r}^a\hat{\phi}_\mu),$$

$$\Phi^a = \frac{1}{r}\left\{\frac{2-r^3}{1+r^3}\right\}\hat{r}^a + \frac{1}{r}\tan\theta\hat{\theta}^a. \tag{27}$$

It was first thought to consist of a 1-monopole at $r=0$, surrounded by two antimonopoles located at the point zeros of the Higgs field at $z=\pm\sqrt[3]{2}=\pm 1.2599$. However, a closer study of this solution reveals that the 1-monopole actually has a zero-size MAM structure along the z-axis and hence possesses a net unit magnetic charge. The MAM structure can be read from the plots of Eq. (26), $M_r(\theta)$ versus θ for the cases of $r\to 0$ and $r\to\infty$; see Fig. 1. The plot at $r\to\infty$ indicates that there

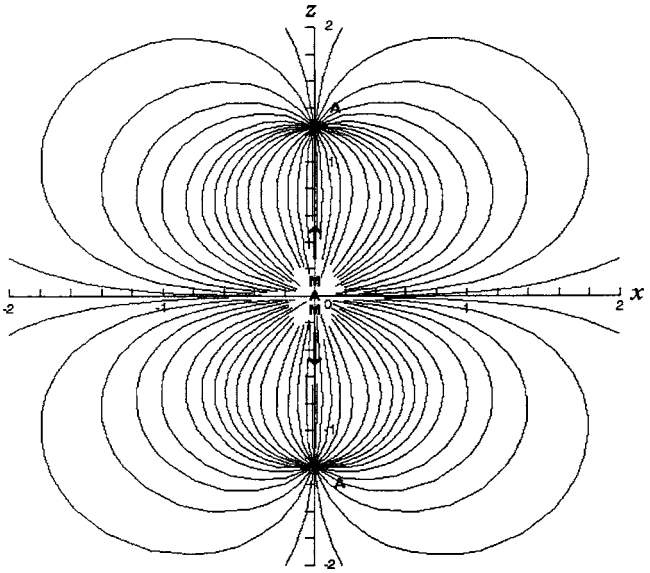

FIG. 2. A plot of the magnetic field lines when $m=1$ along a vertical plane through the z-axis. At large r, all the field lines are concentrated radially inward along the equatorial plane. The two antimonopoles are located along the z-axis at $z=\pm 1.2599$.

is zero flux through the spherical shell at infinity when $\theta \neq \pi/2$ rad. Hence, all the flux at infinity is radially inward along the equatorial plane toward the origin, $r=0$, giving a net topological charge of -1 for the $m=1$ configuration. The radial component of the magnetic field at large r is just a Dirac delta function of θ, given by $B_r=-(2/r^2\sin\theta)\delta[\theta-(\pi/2)]$. Hence, the singularity of the solution $R(\theta)$ at the equatorial plane $\theta=\pi/2$ gives rise to a Dirac delta function singularity in the magnetic field. The antimonopole at the positive z-axis interacts with the nearest MAM 1-monopole at $r=0$ to form a dipole pair; similarly, the antimonopole at the negative z-axis interacts with the other MAM 1-monopole at $r=0$ to form the other dipole pair, leaving behind an antimonopole at the origin; see Fig. 2. At large distances all the magnetic fields above and below the equatorial plane are being screened off by the two dipole pairs along the z-axis, leaving behind a Dirac delta function magnetic field along the plane of singularity, $\theta=\pi/2$.

At finite $r<\sqrt[3]{2}$, the radial component of the magnetic field is a regular function of r and θ but not smooth at $\theta=\pi/2$. In fact, at $\theta=\pi/2$, B_r possesses a negative Dirac delta function singularity, indicating an antimonopole at the center of the composite 1-monopole. Figure 1 shows that at small r, the net flux through the upper $(0<\theta<\pi/2)$ and lower $(\pi/2<\theta<\pi)$ spherical shell is $+4\pi$ each and the flux through the circle at constant r and $\theta=\pi/2$ is -4π, hence indicating a MAM structure for the 1-monopole at the origin.

By plotting the magnetic field lines of this configuration, we can confirm that at large r all the magnetic field lies in the equatorial plane and is pointing radially inward as the net magnetic charge M_∞ is -1. A plot of the magnetic field lines is shown in Fig. 2. Hence, the pole at the center of the composite monopole is an antimonopole surrounded by two 1-monopoles at zero range from each other and yet they do not annihilate each other. The antimonopoles situated at $z=\pm\sqrt[3]{2}$ form dipole pairs with the nearest 1-monopoles of the MAM structure, thus screening off all the magnetic field above and below the equatorial plane at r infinity. There is no vortex ring in this configuration. The Abelian gauge potential, $\mathcal{A}_\mu=-[\sin\alpha-1]/(r\sin\theta)\hat{\phi}_\mu$, possesses a Dirac string singularity along the negative z-axis for $0<r<\sqrt[3]{2}$ and along the positive z-axis for $r>\sqrt[3]{2}$ to infinity.

The vortex ring appears when $m=2$, that is, when the gauge field potentials and Higgs field are, respectively

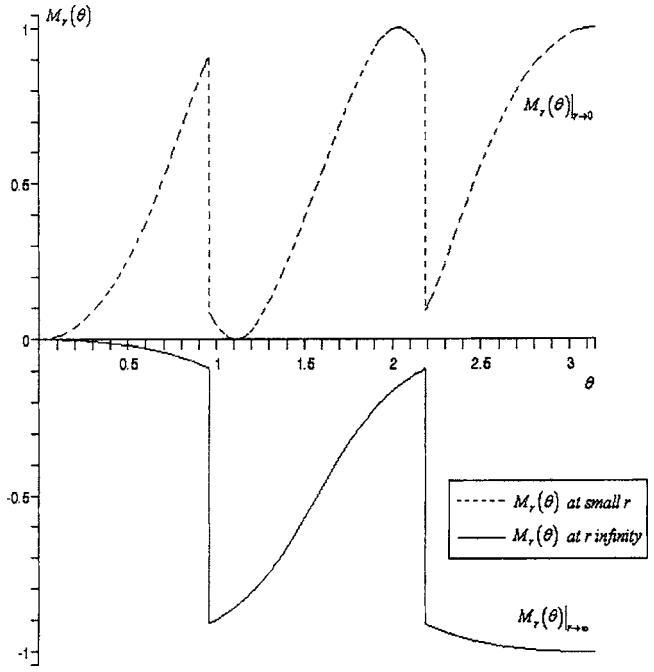

FIG. 3. A plot of $M_r(\theta)$ at r close to zero and $M_r(\theta)$ at r infinity, when $m=2$, versus θ.

$$A^a_\mu = \frac{1}{r}\left\{\frac{3-2r^5}{1+r^5}\right\}(\hat{\theta}^a\hat{\phi}_\mu - \hat{\phi}^a\hat{\theta}_\mu) + \frac{1}{r}\left\{\frac{6\cos\theta\sin\theta}{3\cos^2\theta - 1}\right\}(\hat{\phi}^a\hat{r}_\mu - \hat{r}^a\hat{\phi}_\mu),$$

$$\Phi^a = \frac{1}{r}\left\{\frac{3-2r^5}{1+r^5}\right\}\hat{r}^a + \frac{1}{r}\left\{\frac{6\cos\theta\sin\theta}{3\cos^2\theta - 1}\right\}\hat{\theta}^a. \tag{28}$$

The plots of the magnetic flux, Eq. (26), versus θ, for values of $r\to 0$ and r at infinity, Fig. 3, reveal that the 1-monopole at $r=0$ has an MAMAM structure. However, only the monopole at the center has unit charge. All the other four poles have charge less than unity. Hence, there exist a vortex point both above and below the 1-monopole.

The two outer regular antimonopoles are located at the two point zeros of the Higgs field at $z=\pm\sqrt[5]{3/2}=\pm 1.0845$, Fig. 4, and the vortex ring is located along the ring of radius 1.0845 on the equatorial plane where the Higgs field vanishes, Fig. 5. The magnetic field lines of this one vortex ring solution is shown in Fig. 6.

The two vortex rings solution is the next solution of this series of axially symmetric monopole configurations with parameter $m=3$. The gauge field potentials and Higgs field are, respectively, given by

$$A^a_\mu = \frac{1}{r}\left\{\frac{4-3r^7}{1+r^7}\right\}(\hat{\theta}^a\hat{\phi}_\mu - \hat{\phi}^a\hat{\theta}_\mu) + \frac{3\tan\theta}{r}\left\{\frac{5\cos^2\theta - 1}{5\cos^2\theta - 3}\right\}(\hat{\phi}^a\hat{r}_\mu - \hat{r}^a\hat{\phi}_\mu),$$

$$\Phi^a = \frac{1}{r}\left\{\frac{4-3r^7}{1+r^7}\right\}\hat{r}^a + \frac{3\tan\theta}{r}\left\{\frac{5\cos^2\theta - 1}{5\cos^2\theta - 3}\right\}\hat{\theta}^a. \tag{29}$$

As usual, the two point antimonopoles are situated at the two point zeros, $z=\pm\sqrt[7]{4/3}=\pm 1.0420$, of the Higgs field. The two vortex rings are located horizontally at $r=1.0420$ and $\theta=1.1071$ ($\pi - 1.1071$) rad. Again, from the plots of magnetic flux, $M_r(\theta)|_{r\to 0}$ and $M_r(\theta)|_{r\to\infty}$, Fig. 7, of Eq. (26), together with the plot of the magnetic field lines, Fig. 8, we can conclude that the structure

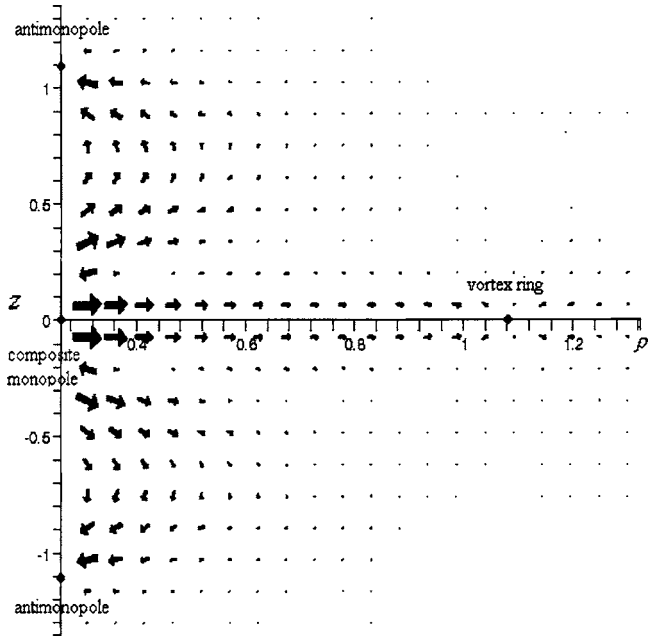

FIG. 4. The Abelian magnetic field of the $m=2$ solution at finite distances showing the presence of the two dipole pairs along the z-axis and the vortex ring at $z=0$, $\rho=1.0845$.

of the composite 1-monopole at the origin is MAMAMAM, with an antimonopole at the center. The three poles in the center, MAM, possess unity charge, whereas the other four poles possess charge less than unity. Hence, there exist a vortex point both above and below the MAM 1-monopole. Hence, by induction, we conclude that the number of A and M "poles" in the composite monopole is equal to $2m+1$, and when m is even, the pole in the center of the structure

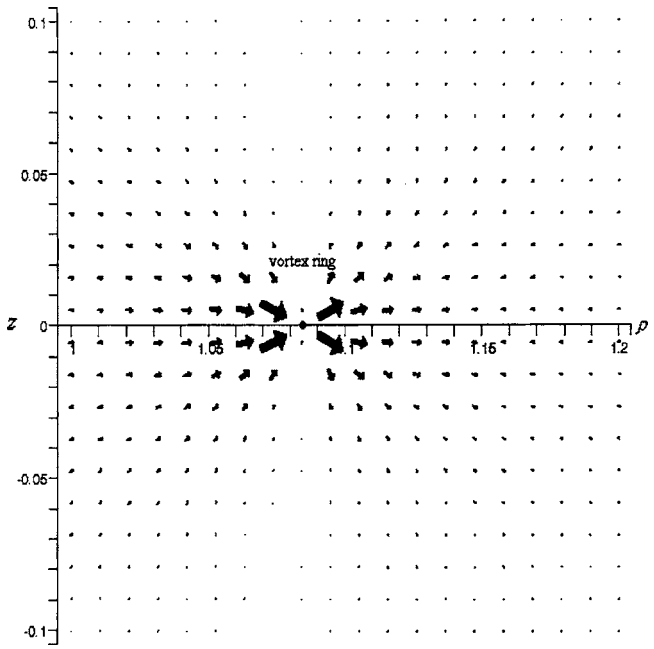

FIG. 5. The Abelian magnetic field of the $m=2$ solution at distances close to $z=0$ and $\rho=1.0845$ showing the presence of the vortex ring.

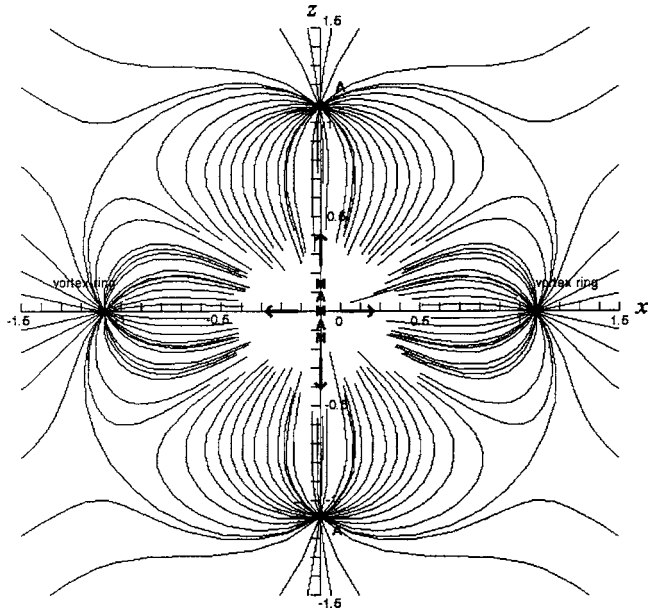

FIG. 6. A plot of the magnetic field lines when $m=2$ along a vertical plane through the z-axis. The vortex ring is situated horizontally at equal distances from the origin as the two antimonopoles at $z=\pm 1.0845$.

is a monopole and when m is odd, we have an antimonopole or a MAM 1-monopole in the center of the structure.[6] The number of vortex rings in the solution increases with m and is equal to $(m-1)$.

V. COMMENTS

We have obtained exact axially symmetric A-M-A configurations of the SU(2) YMH theory which are characterized by a positive integer parameter m. The 1-monopole which is located at the

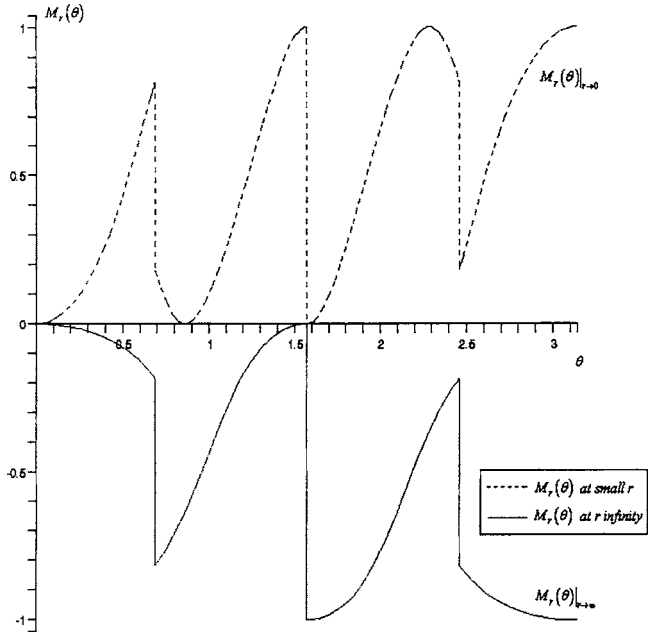

FIG. 7. A plot of $M_r(\theta)$ at r close to zero and $M_r(\theta)$ at r infinity, when $m=3$, versus θ.

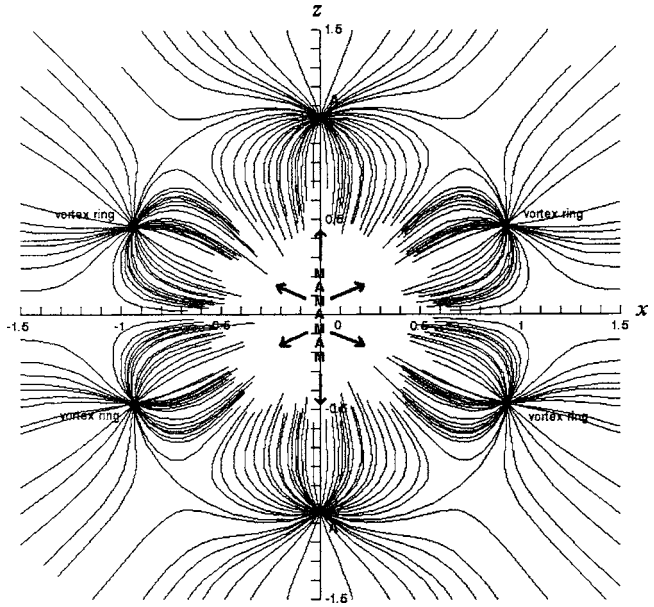

FIG. 8. A plot of the magnetic field lines when $m=3$ along a vertical plane through the z-axis. The two vortex rings are situated horizontally at equal distances from the origin as the two antimonopoles at $z=\pm 1.0420$.

origin, $r=0$, where the Higgs field is singular, is a Wu-Yang-type monopole. The two regular outer antimonopoles are located at the two point zeros of the Higgs field along the z-axis at $z=\pm\sqrt[2m+1]{(m+1)/m}$. When the parameter m exceeds unity, vortex rings start to appear around the z-axis. The number of vortex rings in the solution is equal to $(m-1)$.

Further investigations reveal that the 1-monopole at the origin possesses structure. It corresponds to a zero-size composite monopole with its axis lying along the z-axis. By induction, we conclude that the number of "poles" in the composite monopole is given by $2m+1$. When m is even, the center of the structure corresponds to a 1-monopole M and, when m is odd, it corresponds to an antimonopole or a MAM 1-monopole. We have analyzed the solutions for the cases of $m=0$, 1, 2, and 3, with 1-monopole given by M, MAM, MAMAM, and MAMAMAM, respectively. The MA and AM above and below the 1-monopole when $m=2$ and 3 can be thought of as a vortex point as the magnetic charges of these poles are less than unity.

There are two types of singularities in solutions (14). The point singularity at the origin, $r=0$, gives rise to a Wu-Yang-type monopole, M or MAM. This monopole possesses the usual Dirac string potential in the Abelian gauge when $m=0$. However, when $m=1,2,3,\ldots$, the Dirac string is broken into two parts. The string stretches from $z=0$ to $z=-\sqrt[2m+1]{(m+1)/m}$ along the negative z-axis and from $z=\sqrt[2m+1]{(m+1)/m}$ to positive infinity along the positive z-axis.

The singularities in $R(\theta)$ when $P_m(\cos\theta)=0$ give rise to plane singularities. The number of singular planes in the solution is equal to m. Hence, when $m=1$, the singular plane is the equatorial plane. The Abelian magnetic field possesses a negative Dirac delta function singularity along this plane, $B_r=-2/(r^2\sin\theta)\delta[\theta-(\pi/2)]$. Similarly, when $m=2$, the singular planes are $\theta=0.9553$ and 2.1863 rad, and when $m=3$, the singular planes are $\theta=0.6847$, 0, and 2.4569 rad. In all these solutions, the Abelian magnetic fields possess negative Dirac delta function singularity along these planes as the Abelian gauge potentials are discontinuous at these values of θ.

Numerical static axially symmetric M-A-M-… chain at finite pole separation has also been discussed in Ref. 6. These numerical solutions belong to the topologically trivial sector when the total number of poles and antipoles is even and to the topological unit sector when the total number of poles and antipoles is odd. We have only managed to find odd total number of poles and antipoles in our solutions. Similar to the results of Ref. 6, we have a monopole at the center of the

composite 1-monopole when m is even and an antimonopole in the center when m is odd. Also similar is that our solutions have zero magnetic dipole moment as the number of poles in our solutions is odd.

Unlike the monopole solutions of Ref. 6, our A-M-A poles here are of unit charge only. We did not manage to get monopoles and antimonopoles of charge equal to two units for our axially symmetric monopoles solutions. In fact, we have not found any M-monopoles with finite separations when $|M| \geqslant 2$.

We would also like to mention that, for every monopole, antimonopole, vortex rings solution that we have discussed so far, there always exists an anticonfiguration of the configurations discussed. This can be done by changing the ϕ winding number in the ansatz (8) from +1 to −1 and solving the Bogomol'nyi equation with the negative sign.[8]

We would also like to mention that one-half topological magnetic charge monopole is obtained when the parameter m is set to $-\frac{1}{2}$ in the solution, Eq. (14).[10]

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Extending the Picard-Fuchs system of local mirror symmetry

Brian Forbes[a] and Masao Jinzenji[b]
Division of Mathematics, Graduate School of Science, Hokkaido University, Kita-ku, Sapporo, 060-0810, Japan

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We propose an extended set of differential operators for local mirror symmetry. If X is Calabi-Yau such that $\dim H_4(X,\mathbb{Z})=0$, then we show that our operators fully describe mirror symmetry. In the process, a conjecture for intersection theory for such X is uncovered. We also find operators on several examples of type $X=K_S$ through similar techniques. In addition, open string Picard-Fuchs systems are considered. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1996441]

I. INTRODUCTION

For some time now, mirror symmetry has been successfully used to make enumerative predictions on certain Calabi-Yau manifolds. While mirror symmetry for the compact Calabi-Yau has been extensively studied, local mirror symmetry is relatively new, and a complete formulation does not yet exist.

The first unified treatment of local mirror symmetry was written down in Ref. 3, in the case that the space looks like $X=K_S$, where S is a Fano surface and K_S is its canonical bundle. Very recently,[10] the work of Ref. 3 was formulated more mathematically. With the ideas of Ref. 10, we are able to determine all information relevant for mirror symmetry directly from the Picard-Fuchs equations of the mirror. These techniques are limited to the case that X satisfies $b_2(X)=b_4(X)$.

The aim of this paper is to further the program of local mirror symmetry. We propose a set of differential operators, whose solutions contain the usual local mirror symmetry solutions as a subset. In the event that the space in question contains no 4 cycle, the operators completely solve the problem for an arbitrary number of Kähler parameters. For the more traditional mirror symmetry constructions of Ref. 3, our methods still complete missing data; however, a general formulation here is lacking.

The key point in the construction of the extended Picard-Fuchs system is the determination of triple intersection numbers of Kähler classes for open Calabi-Yau manifolds. Up to now, a natural definition of triple intersection numbers of Kähler classes on open Calabi-Yau manifolds is not known, but in this paper, we search for triple intersection numbers that are "natural" from the point of view of mirror symmetry in the sense of the following conjecture.

Conjecture 1: Consider the A-model on a Calabi-Yau threefold X. Let u_i *be the logarithm of the B-model complex deformation parameter* z_i *obtained from the toric construction of the mirror Calabi-Yau manifold* $\hat{X}$*. Then the B-model Yukawa coupling* $C_{u_iu_ju_k}$ *of* $\hat{X}$ *obtained from the A-model Yukawa coupling of X via the mirror map is a rational function in* $z_i=\exp(u_i)$*. Moreover, its denominator consists of the factors of the defining equation of the discriminant locus of* $\hat{X}$*.*

Since the triple intersection number is just the constant term of the B-model Yukawa coupling $C_{u^iu^ju^k}$, the above conjecture imposes constraints on these triple intersection numbers.

We regard the existence of such intersection theory as an interesting analogue of the physical predictions arising from large N duality, e.g., Ref. 7. Recall that in Ref. 7, the postulated large N

[a]Electronic mail: brian@math.sci.hokudai.ac.jp
[b]Electronic mail: jin@math.sci.hokudai.ac.jp

dual of $X=\mathcal{O}(-1)\oplus\mathcal{O}(-1)\to\mathbb{P}^1$ led to a fractional triple intersection number for $\mathbb{P}^1\hookrightarrow X$. We find a similar fractional intersection theory, and this is done via calculations which are independent of a large N dual. Hence, we may think of this intersection theory as a prediction for what one would find if computations were done on a large N dual theory.

With these intersection numbers in hand, we can construct an extended quantum cohomology ring of X and an associated Gauss-Manin system. In the examples treated in this paper, this quantum cohomology ring satisfies Poincare duality as a compact threefold, even if X is an open Calabi-Yau threefold. Let t_i be coordinates on the complexified Kähler moduli space of X. With this Gauss-Manin system, we can write down differential equations for $\psi_0(t_i)$, the function associated to the identity element of the quantum cohomology ring. Then we can rewrite these differential equations by using the mirror map $t_i=t_i(z_*)$. Our assertion in this paper is that the differential equations so obtained are the extension of the Picard-Fuchs operators obtained from the standard toric construction of $\hat{X}$. Moreover, the extended Picard-Fuchs system has all the properties that the Picard-Fuchs system associated to a compact Calabi-Yau threefold should have a unique triple log solution, B-model Yukawa couplings, etc. These extended Picard-Fuchs systems give us a very simple derivation of B-model Yukawa couplings of local mirror symmetry known in some special cases. In particular, we can compute B-model Yukawa couplings of any K_S case. Therefore, we can see the global behavior of the instanton expansion of local mirror symmetry. We expect that the extended Picard-Fuchs system can be derived from the B-model point of view. The results of this paper gives us some useful guidelines of such a construction, since extended Picard-Fuchs systems have a very elegant form in some cases.

One problem in the construction is that in some cases, the constraints obtained from the above conjecture are not strong enough to determine all the triple intersection numbers. In other words, we have some real moduli parameters in the triple intersection numbers. Yet, we can still construct the extended Picard-Fuchs system for each value of the moduli parameters, and these systems have all the properties desired for a Picard-Fuchs system associated to a compact Calabi-Yau threefold. In the case that $b_4(X)=b_6(X)=0$, we find unique triple intersection numbers compatible with the above conjecture by considering the change of the prepotential under flops. Hence, our construction of an extended Picard-Fuchs system has no ambiguity in this situation.

We should mention that our constructions do not lead to Gromov-Witten invariants on the spaces we consider. Rather, the differential systems we find have the property that all Gromov-Witten invariants can be derived purely as solutions of our differential systems, a feature which was absent in the original work.[3] Moreover, we believe that through the study of such systems, we will come closer to a formulation of local mirror symmetry on all Calabi-Yau purely in terms of the complex geometry of the mirror.

Here is the organization of the paper. Section II spells out the generalities of the Gauss-Manin system and intersection theory for open Calabi-Yau manifolds. In Sec. III, we thoroughly consider $\mathcal{O}(-1)\oplus\mathcal{O}(-1)\to\mathbb{P}^1$, giving a PF operator for mirror symmetry and a geometric view of the meaning of the operator. Section IV is the generalization, which spells out a conjecture on how to deal with all X such that $\dim H_4(X,\mathbb{Z})=0$. This is subsequently applied to several cases and shown to produce the expected results. Section V explores the application of our techniques to open string theory on $\mathcal{O}(-1)\oplus\mathcal{O}(-1)\to\mathbb{P}^1$, while Secs. VI and VII work through examples of type K_S. Some of the results for our more unwieldy examples are collected in the appendixes.

II. THE MAIN STRATEGY: OVERVIEW OF THE GAUSS-MANIN SYSTEM

Let X be a noncompact Calabi-Yau threefold, and choose a basis $\{k_i\}$ for $H^{1,1}(X,\mathbb{C})$. Suppose that we have obtained "natural" classical triple intersection numbers $\langle k_a k_b k_c\rangle\in\mathbb{Q}$ for two cycles on X under the assumption of Conjecture 1. Suppose also that we know the instanton part of the prepotential for X. Recall that the prepotential is the generating function of Gromov-Witten invariants for X; then we denote this instanton part by $\mathcal{F}^{\text{inst}}(t_*)$, where t_a is the Kähler deformation parameter associated to the Kähler form k_a $[a=1,\ldots,h^{1,1}(X)]$. With this data, we can construct an A-model Yukawa coupling for X,

$$Y_{abc}(t_*) = \langle k_a k_b k_c \rangle + \frac{\partial^3 \mathcal{F}^{\text{inst}}(t_*)}{\partial t_a \, \partial t_b \, \partial t_c}. \tag{1}$$

Using the classical intersection numbers $\langle k_a k_b k_c \rangle$, we can construct a virtual basis $m_\alpha [\alpha = 1, \ldots, h^{1,1}(X)]$ of formal 4 cycles with the following property. If $\eta_{a\alpha}$ is the virtual intersection matrix of 2 cycles and formal 4 cycles, then with respect to the basis m_α, we have

$$\eta_{a\alpha} := \delta_{a\alpha}. \tag{2}$$

With this setup, we obtain a (virtually compactified) quantum cohomology ring of X, which is the usual cohomology ring with a deformed product, defined as follows:

$$\begin{gathered} k_a \circ 1 = k_a, \\ k_a \circ k_b = \sum_{c,\gamma} Y_{abc}(t_*) \eta^{c\gamma} m_\gamma = \sum_{\gamma} Y_{ab\gamma}(t_*) m_\gamma, \\ k_a \circ m_\alpha = Y_{a\alpha 0} v = \delta_{a\alpha} v, \\ k_a \circ v = 0. \end{gathered} \tag{3}$$

Above, we have taken advantage of a standard feature of the quantum cohomology ring, namely

$$Y_{a\alpha 0} = \eta_{a\alpha}. \tag{4}$$

Here v is the formal volume form of X and we use the subscript 0 to denote the identity 1 of this quantum cohomology ring. Then we consider a system of partial differential equations,

$$\begin{gathered} \partial_a \psi_0 = \psi_a, \\ \partial_a \psi_b = \sum_{c,\gamma} Y_{abc}(t_*) \eta^{c\gamma} \psi_\gamma = \sum_{\gamma} Y_{ab\gamma}(t_*) \psi_\gamma, \\ \partial_a \psi_\alpha = Y_{a\alpha 0} \psi_v = \delta_{a\alpha} \psi_v, \\ \partial_a \psi_v = 0. \end{gathered} \tag{5}$$

Next, we consider the inverse matrix $(Y_a^{-1}(t_*))^{bc}$ of $(Y_a(t_*))_{bc} := Y_{abc}(t_*)$. From (5), we obtain,

$$\psi_\alpha = \sum_{b,c} \eta_{\alpha c} \cdot (Y_a^{-1}(t_*))^{cb} \partial_a \partial_b \psi_0 = \sum_{b} (Y_a^{-1}(t_*))^{\alpha b} \partial_a \partial_b \psi_0. \tag{6}$$

Since ψ_α is unique for each α, we must impose integrability conditions

$$\sum_{c} (Y_a^{-1}(t_*))^{\alpha c} \partial_a \partial_c \psi_0 = \sum_{c} (Y_b^{-1}(t_*))^{\alpha c} \partial_b \partial_c \psi_0 \quad (a \neq b) \tag{7}$$

for any $a, b \in \{1, 2, \ldots, h^{1,1}(X)\}$. We have another integrability condition from the third line of (5):

$$\partial_a \left(\sum_{c} (Y_a^{-1}(t_*))^{ac} \partial_a \partial_c \psi_0 \right) = \partial_b \left(\sum_{c} (Y_b^{-1}(t_*))^{bc} \partial_b \partial_c \psi_0 \right) \quad (a \neq b),$$

$$\partial_b\left(\sum_c (Y_a^{-1}(t_*))^{ac}\partial_a\partial_c\psi_0\right)=0 \quad (a\neq b), \tag{8}$$

for any $a, b\in\{1,2,\ldots,h^{1,1}(X)\}$. Finally, we can derive differential equations from the fourth line of (5),

$$\partial_a^2\left(\sum_c (Y_a^{-1}(t_*))^{ac}\partial_a\partial_c\psi_0\right)=0. \tag{9}$$

Our strategy in this paper is to translate the equations (7)–(9) in terms of the mirror map

$$t_a=t_a(z_*) \tag{10}$$

into the differential equations of the complex deformation parameters z_a of the mirror manifold $\hat{X}$. Of course, in the one parameter case, the equations (7) and (8) become trivial, and the only nontrivial equation is

$$\partial_t^2\left(\frac{1}{Y_{ttt}}\right)\partial_t^2\psi_0(t)=0, \tag{11}$$

which follows from (9) with the identification $t=t_1$.

In the following, we will explicitly compute (7)–(9) in many examples, and we find that these equations are highly overdetermined. Therefore, in this paper, we will choose the minimal independent set of equations for an extended Picard-Fuchs system.

By construction, the Picard-Fuchs system so obtained has a solution space given by

$$\left(1,t_1,\ldots,t_{h^{1,1}(X)},\frac{\partial\mathcal{F}}{\partial t_1},\ldots,\frac{\partial\mathcal{F}}{\partial t_{h^{1,1}(X)}},2\mathcal{F}-\sum_{a=1}^{h^{1,1}(X)} t_a\frac{\partial\mathcal{F}}{\partial t_a}\right) \tag{12}$$

for some function $\mathcal{F}$ which is smooth in the t_i. Then $\mathcal{F}$ is that relevant for the counting of Gromov-Witten invariants.

III. MIRROR SYMMETRY FOR LOCAL $\mathbb{P}^1$

A. A Picard-Fuchs operator for local $\mathbb{P}^1$

Before diving into the details of Gauss-Manin systems and the like, we will first take a simple-minded look at a familiar example, namely $\mathcal{O}(-1)\oplus\mathcal{O}(-1)\to\mathbb{P}^1$. We will see that in trying to apply the techniques of local mirror symmetry to this basic case, we are inevitably led to introduce the generalized intersection theory explained in the introduction. In fact, this is the example that originally motivated the investigations of this paper.

Recall the symplectic quotient definition of $\mathcal{O}(-1)\oplus\mathcal{O}(-1)\to\mathbb{P}^1$,

$$X=\{(w_1,\ldots,w_4)\in\mathbb{C}^4-Z:|w_1|^2+|w_2|^2-|w_3|^2-|w_4|^2=r\}/S^1. \tag{13}$$

Above, $Z=\{w_1=w_2=0\}$, $r\in\mathbb{R}^+$ and

$$S^1:(w_1,\ldots,w_4)\to(e^{i\theta}w_1,e^{i\theta}w_2,e^{-i\theta}w_3,e^{-i\theta}w_4), \quad \theta\in S^1.$$

We can naively employ the methods of Ref. 10 to produce a Picard-Fuchs operator associated to the mirror Calabi-Yau $\hat{X}$ of X. The family $\hat{X}$ is described as[9]

$$\hat{X}_z=\{(u,v,y_1,y_2)\in\mathbb{C}^2\times(\mathbb{C}^*)^2:uv+1+y_1+y_2+zy_1y_2^{-1}=0\}. \tag{14}$$

Then Ref. 10 provides a recipe for dealing with noncompact period integrals for such an $\hat{X}$. They are defined by

$$\Pi_\Gamma(z) = \int_\Gamma \frac{du\, dv\, dy_1\, dy_2/(y_1 y_2)}{uv + 1 + y_1 + y_2 + z y_1 y_2^{-1}}$$

for $\Gamma \in H_4(\mathbb{C}^2 \times (\mathbb{C}^*)^2 - \hat{X}, \mathbb{Z})$. As usual, we utilize the GKZ formalism in order to exhibit a differential operator which annihilates the Π_Γ. One finds

$$\mathcal{D} = (1-z)\theta^2, \quad \theta = z\frac{d}{dz} \tag{15}$$

as the relevant PF operator.

This is a puzzling situation. Clearly, the solutions of $\mathcal{D}f=0$ are given by $\{1, \log z\}$. This is sensible, because noncompact PF systems always have a constant solution,[3] and the mirror map is trivial for $\mathcal{O}(-1)\oplus\mathcal{O}(-1)\to\mathbb{P}^1$, leading to a $\log z$ solution. However, there is no double-logarithmic solution, because $\mathcal{D}$ is only of order 2. Hence, we have no function $\mathcal{F}$ with which to count holomorphic curves on X! But, since X contains exactly 1 holomorphic curve, we know that the sought after function should be of the form

$$\mathcal{F}(z) = K\frac{(\log z)^3}{6} + \sum_{n>0}\frac{z^n}{n^3}. \tag{16}$$

Here K is a classical triple intersection number for $\mathbb{P}^1 \hookrightarrow X$. Also, notice that the leading factor of $1-z$ in front of $\mathcal{D}$, while naturally appearing through the techniques of the GKZ formalism, is auxiliary to the solution set of $\mathcal{D}$.

At this point, we can gain a bit of insight from the compact case. Recall[4] that in the event of a compact Calabi-Yau X with one Kähler parameter, there is always a flat coordinate t in which the Picard-Fuchs operator for the mirror family is given as

$$\mathcal{D}_{\text{compact}}(t) = \partial_t^2\left(\frac{1}{Y}\right)\partial_t^2, \tag{17}$$

which is the same as formula (11). This is reminiscent of our situation (15), upon making the identification $t=\log z$.

If one surrendered to the impulse of emulating the above compact expression, one would be compelled to work with the following modified differential operator:

$$\mathcal{D} \to \mathcal{D}' = \theta^2\mathcal{D}.$$

Rewrite this as

$$\theta^2(1-z)\theta^2 = \theta^2\left(\frac{1}{1-z}\right)^{-1}\theta^2.$$

By comparison with (17), it is natural to identify the Yukawa coupling Y of $\mathcal{O}(-1)\oplus\mathcal{O}(-1)\to\mathbb{P}^1$ as

$$Y = \frac{1}{1-z}. \tag{18}$$

And indeed, the condition that $Y=\theta^3\mathcal{F}$, which follows from the form of $\mathcal{D}'$, yields the expected function $\mathcal{F}$ (16), if we take $K=1$. Later, we will find that a more natural choice for generalization is $K=1/2$.

The resulting period vector of solutions for $\mathcal{D}'f=0$ is

$$\Pi' = (1, \log z, \theta\mathcal{F}, 2\mathcal{F} - (\log z)\theta\mathcal{F}),$$

which is of the same type as encountered when dealing with the compact Calabi-Yau. Hence, we have found a cure for mirror symmetry on $X = \mathcal{O}(-1) \oplus \mathcal{O}(-1) \to \mathbb{P}^1$; the operator $\theta^2\mathcal{D}$ reproduces all relevant data to describe mirror symmetry for X.

We can also view this $\theta^2\mathcal{D}$ from the vantage of the Frobenius method. The geometry of X is determined by the set of vertices $\{\nu_0, \ldots, \nu_3\} = \{(0,0), (1,0)(0,1), (1,1)\}$, together with a choice of triangulation of the resulting toric graph. These give rise to the lattice vector $l = (1, -1, -1, 1)$, and identify z as the correct variable on the complex moduli space of $\hat{X}$. Then the solutions of our extended PF operator $\theta^2\mathcal{D}$ can be generated, via the Frobenius method, from the function $\omega_0(z, \rho) = \Sigma_{n \geqslant 0} c(n, \rho) z^{n+\rho}$, with $c(n, \rho)^{-1} = \Gamma(1+n+\rho)^2 \Gamma(1-n-\rho)^2$. It is a simple matter to verify that

$$\Pi' = (\omega_0(z,0), \partial_\rho \omega_0(z,\rho)|_{\rho=0}, \partial_\rho^2 \omega_0(z,\rho)|_{\rho=0}, \partial_\rho^3 \omega_0(z,\rho)|_{\rho=0}).$$

Clearly this had to be the case, since the extension of the original $\mathcal{D}$ on the left-hand side by each factor of θ adds one more Frobenius-generated solution.

B. PF extensions and Riemann surfaces

In physics literature,[1,10] a frequently used technique of local mirror symmetry is to consider periods on a Riemann surface $\Sigma \hookrightarrow \hat{X}$, rather than periods of the full mirror geometry $\hat{X}$. In this section, we will review evidence in favor of this approach.

Looking back at the mirror geometry (14), this can be rewritten as

$$\hat{X}_z = \{uv + 1 + y_1 + y_2 + z y_1 y_2^{-1} = uv + f(z, y_1, y_2) = 0\},$$

which is a hypersurface in $\mathbb{C}^2 \times (\mathbb{C}^*)^2$. Notice that there is an imbedded Riemann surface in this space, defined as

$$\Sigma_z = \{(y_1, y_2) \in (\mathbb{C}^*)^2 : f(z, y_1, y_2) = 0\}. \tag{19}$$

In fact, this statement applies not only to the local $\mathbb{P}^1$ case, but to all toric local mirror symmetry constructions.[1] Now take $(a_0, \ldots, a_3)$ as homogeneous coordinates on the moduli spaces of $\hat{X}$ and Σ, i.e.,

$$\hat{X}_a = \{uv + a_0 + a_1 y_1 + a_2 y_2 + a_3 z y_1 y_2^{-1} = uv + f(a, y_1, y_2) = 0\}.$$

Recall that the GKZ operators are differential operators $\{\mathcal{L}_i\}$ in the variables a, such that

$$\mathcal{L}_i \int_\Gamma \frac{du\, dv\, dy_1\, dy_2/(y_1 y_2)}{uv + f(a, y_1, y_2)} = 0, \quad \forall\, i.$$

We can recover the PF operators from the GKZ operators via a canonical reduction on the homogeneous moduli space.

With these things in mind, we note the following.

Proposition 1: The GKZ operators associated to the geometry $\hat{X}$ are the same as those associated to Σ.

Proof: Notice that Σ is a complex dimension 1 noncompact Calabi-Yau manifold. In particular, it makes sense to define the period integrals of Σ as

$$\Pi_\gamma^\Sigma(a) = \int_\gamma \frac{dy_1\, dy_2/(y_1 y_2)}{f(a,y_1,y_2)}$$

with $\gamma \in H_2((\mathbb{C}^*)^2 - \Sigma, \mathbb{Z})$. Let $\mathcal{L}$ be a GKZ operator on the moduli space of Σ_a, so that $\mathcal{L}\Pi_\gamma^\Sigma(a) = 0$. If a_i are homogeneous coordinates on the moduli space of Σ, then $\mathcal{L}$ is a homogeneous polynomial (say, of degree n) in ∂_{a_i}. We obtain

$$\mathcal{L}\frac{1}{f(a,y_1,y_2)} = \frac{P_\mathcal{L}(y_1,y_2)}{f(a,y_1,y_2)^{n+1}}, \tag{20}$$

where $P_\mathcal{L}$ is a polynomial in y_1, y_2 which is identically zero. We now want to apply this $\mathcal{L}$ to period integrals in $\hat{X}_a$. Recall that these are given as

$$\Pi_\Gamma^{\hat{X}}(a) = \int_\Gamma \frac{du\, dv\, dy_1\, dy_2/(y_1 y_2)}{uv + f(a,y_1,y_2)} \tag{21}$$

for $\Gamma \in H_4(\mathbb{C}^2 \times (\mathbb{C}^*)^2 - \hat{X}, \mathbb{Z})$. Then operating on the left-hand side of the integral, we find

$$\mathcal{L}\frac{1}{uv + f(a,y_1,y_2)} = \frac{P_\mathcal{L}(y_1,y_2)}{(uv + f(a,y_1,y_2))^{n+1}}$$

because the additive factor of uv in the period integrals of $\hat{X}$ is independent of a. Since $P_\mathcal{L} \equiv 0$, we have demonstrated that $\mathcal{L}\Pi_\Gamma^{\hat{X}}(a) = 0$. Clearly the converse of this statement is also true, so the proposition follows. □

Note that, as pointed out in Ref. 10, there is a subtlety in terms of the scaling properties of the period integrals on $\hat{X}_a$ and Σ_a; this scaling difference implies that the PF operators we derive from the above $\mathcal{L}$ will be different on Σ_z and $\hat{X}_z$. In the following, we will ignore this point, and carry on as though the period integrals on Σ_z actually reproduce the same PF operators.

As the geometry of Σ is far simpler than that of $\hat{X}$, this proposition will greatly aid the search for a geometric interpretation of our extended Picard-Fuchs operator. We will explore this in the next section.

C. Geometric interpretation through the Riemann surface

First, we will give a brief description of what "adding extra period integrals" means (which we are doing, via the extended PF operator) in the context of the space $\hat{X}$. This follows the lead of, e.g., Refs. 9 and 2.

Recall that mirror symmetry between compact spaces X and $\hat{X}$ means, in particular, that $\dim H^{1,1}(X) = \dim H^{2,1}(\hat{X})$. Hence, for every 2 cycles of X, we can expect a mirror 3 cycle of $\hat{X}$. Let $\dim H_3(\hat{X},\mathbb{Z}) = n$, and take Γ_i, $\Gamma_j \in H_3(\hat{X},\mathbb{Z})$ with Poincaré duals α_i, $\alpha_j \in H^3(\hat{X},\mathbb{Z})$. Then there is a symplectic structure on $H_3(\hat{X},\mathbb{Z})$, defined by the intersection pairing

$$(\Gamma_i,\Gamma_j) = \int_{\hat{X}} \alpha_i \wedge \alpha_j.$$

In the compact case, we can find a basis $\{\Phi_1,\ldots,\Phi_{n/2}, \Psi_1,\ldots,\Psi_{n/2}\}$ for $H_3(\hat{X},\mathbb{Z})$ satisfying

$$(\Phi_i,\Phi_j) = (\Psi_i,\Psi_j) = 0, \quad (\Phi_i,\Psi_j) = \delta_{ij}.$$

Next, consider the case in which X and $\hat{X}$ are noncompact. Here, we find there is no such nice construction. In fact, we can explicitly exhibit this failure in the example we are considering, $\mathcal{O}(-1) \oplus \mathcal{O}(-1) \to \mathbb{P}^1$. First, rewrite the equation for the mirror $\hat{X}$,

$$\hat{X}_z = \{(\tilde{u},v,\tilde{y}_1,\tilde{y}_2) \in \mathbb{C}^2 \times (\mathbb{C}^*)^2 : \tilde{u}v + z + \tilde{y}_1 + \tilde{y}_2 + \tilde{y}_1\tilde{y}_2 = 0\},$$

where we have taken $\tilde{y}_i = y_i^{-1}$ and $\tilde{u} = u/y_1y_2$. Set $z = 1-a$, where $a \in \mathbb{R}^+$. Then

$$\hat{X}_z = \{\tilde{u}v + 1 + \tilde{y}_1 + \tilde{y}_2 + \tilde{y}_1\tilde{y}_2 = a\},$$

and we can identify a 3 cycle,

$$\Gamma_1 = \hat{X}_z \cap \{\tilde{u} = \bar{v}, \tilde{y}_2 = \bar{\tilde{y}}_1\} = \{v\bar{v} + (1+\tilde{y}_1)\overline{(1+\tilde{y}_1)} = a\}.$$

It is easy to verify that this cycle has no symplectic dual in $H_3(\hat{X},\mathbb{Z})$.

We may, however, define a noncompact symplectic dual for Γ_1. This proceeds as follows. Let $p \in \Gamma_1$, and take $\tilde{\Gamma}_1 = (N_{\Gamma_1/\hat{X}})_p$. Then $\tilde{\Gamma}_1$ intersects Γ_1 in a point, and could be thought of as a dual; however, integrals over $\tilde{\Gamma}_1$ may not be well defined. Instead take

$$\tilde{\Gamma}_1^{\lambda} = \{v \in (N_{\Gamma_1/\hat{X}})_p : \|v\| \leqslant \lambda\}, \quad \lambda \in \mathbb{R}^+.$$

The norm $\| \|$ is defined with respect to the metric inherited from $\mathbb{C}^2 \times (\mathbb{C}^*)^2$. Set

$$\Omega_{\hat{X}} = \mathrm{Res}_{\{uv+f(z,y_1,y_2)=0\}}\left(\frac{du\, dv\, dy_1\, dy_2/(y_1y_2)}{uv + f(z,y_1,y_2)}\right).$$

We recall the proposal of Ref. 9 for dealing with the "missing" period integrals for local mirror symmetry. Specifically for the local $\mathbb{P}^1$ case we are considering, Ref. 9 makes the claim that the period integral which is the symplectic dual of the mirror map represents a truncated volume of the (noncompact) 4 cycle which is dual to the $\mathbb{P}^1$. In our notation, this means we should be considering $\int_{\tilde{\Gamma}_1^{\lambda}} \Omega_{\hat{X}}$ as periods of the noncompact geometry $\hat{X}$. Mathematically, this means that the definition of noncompact period integrals of $\hat{X}$ are to be taken as all $\int_{\Gamma} \Omega_{\hat{X}}$ for $\Gamma \in H_3(\hat{X},\mathbb{Z}) \oplus (H_3(\hat{X},\mathbb{Z}))_c$. Here, the subscript c indicates compactly supported homology. In view of Proposition 1, one can then make the following.

Definition 1: Let $\hat{X}$ be the noncompact Calabi-Yau hypersurface,

$$\hat{X} = \{(u,v,y_1,y_2) \in \mathbb{C}^2 \times (\mathbb{C}^*)^2 : uv + f(z,y_1,y_2) = 0\}$$

and Σ the imbedded Riemann surface $\Sigma_z = \hat{X} \cap \{u=v=0\}$. Then the period integrals of $\hat{X}$ are defined to be

$$\Pi_{\gamma}(z) = \int_{\gamma} \mathrm{Res}_{f=0}\left(\frac{dy_1\, dy_2/(y_1y_2)}{f(z,y_1,y_2)}\right)$$

for $\gamma \in H_1(\Sigma,\mathbb{Z}) \oplus (H_1(\Sigma,\mathbb{Z}))_c$.

In the next section, we will apply this definition to $\mathcal{O}(-1) \oplus \mathcal{O}(-1) \to \mathbb{P}^1$, and see that the explicit evaluation of the period integrals on Σ gives the same answer as the extended PF operator of Sec. III A.

D. Period integrals for local $\mathbb{P}^1$

Before describing the cycles of Σ and computing their associated integrals, we will need to make use of the following proposition. This will give a (1, 0) form $\alpha \in H_1(\log(\Sigma),\mathbb{Z})$, which can be integrated over lines in Σ. Some of the arguments below can be found in Ref. 13.

Proposition 2: Let Σ be as above, and choose $\gamma \in H_1(\Sigma,\mathbb{Z}) \oplus (H_1(\Sigma,\mathbb{Z}))_c$. Then

$$\int_{\gamma} \mathrm{Res}_{f=0}\left(\frac{dy_1\, dy_2/(y_1y_2)}{f(z,y_1,y_2)}\right) = -\int_{\gamma} \log y_2 \frac{dy_1}{y_1} = -\int_{\gamma} \log y_1 \frac{dy_2}{y_2}.$$

Proof: Let $T(\gamma)$ be a tubular neighborhood of γ in Σ. We first claim that the same GKZ operators annihilate both of the following types of integrals:

$$\int_{T(\gamma)} \frac{dy_1\, dy_2/(y_1y_2)}{f(z,y_1,y_2)}, \quad \int_{T(\gamma)} \log(f) dy_1\, dy_2/(y_1y_2). \tag{22}$$

In fact, we can see this immediately from the proof of Proposition 1. That is, if $\mathcal{L}$ is a degree n GKZ operator annihilating $\int_{T(\gamma)}(dy_1\, dy_2/(y_1y_2)/f(z,y_1,y_2))$, then as before write

$$\mathcal{L}\frac{1}{f(z,y_1,y_2)} = \frac{P_{\mathcal{L}}(y_1,y_2)}{f(z,y_1,y_2)^{n+1}}, \tag{23}$$

where $P_{\mathcal{L}}(y_1,y_2) \equiv 0$. Then it follows immediately that $\mathcal{L}\log(f) = P_{\mathcal{L}}(y_1,y_2)/f^n \equiv 0$, as claimed.

Now, note that we are only interested in computations of period integrals as they arise as solutions of the GKZ system. Therefore, since they are both annihilated by the same system, we have that

$$\int_{T(\gamma)} \frac{dy_1\, dy_2/(y_1y_2)}{f(z,y_1,y_2)} = \int_{T(\gamma)} \log(f) dy_1\, dy_2/(y_1y_2). \tag{24}$$

The rest of the proof is then straightforward,

$$\int_\gamma \mathrm{Res}_{f=0}\left(\frac{dy_1\, dy_2/(y_1y_2)}{f(z,y_1,y_2)}\right) = \int_\gamma \mathrm{Res}_{f=0}(\log(f) dy_1\, dy_2/(y_1y_2)) = -\int_\gamma \mathrm{Res}_{f=0}\left(d(\log(f))\log y_2 \frac{dy_1}{y_1}\right)$$
$$= -\int_\gamma \mathrm{Res}_{f=0}\left(\frac{df}{f}\log y_2 \frac{dy_1}{y_1}\right) = -\int_\gamma \log y_2 \frac{dy_1}{y_1}.$$

This argument applies equally well upon exchanging y_1 and y_2. □

With this proposition in hand, we can take up the task of working out period integrals on local $\mathbb{P}^1$. Recall that the original, unmodified PF operator for this space was found to be $\mathcal{D} = (1-z)\theta^2$, with solution set $\{1, \log z\}$. We will at first content ourselves with finding cycles $\gamma_0, \gamma_1 \in H_1(\Sigma,\mathbb{Z})$ whose period integrals reproduce these solutions. To this end, note that the defining equation

$$\Sigma = \{(y_1,y_2) \in (\mathbb{C}^*)^2 : 1 + y_1 + y_2 + zy_1y_2^{-1} = 0\} \tag{25}$$

can be solved in two ways,

$$y_1 = \frac{-1-y_2}{1+zy_2^{-1}}, \quad y_2^{\pm} = \frac{-1-y_1 \pm \sqrt{(1+y_1)^2 - 4zy_1}}{2}.$$

Now, since y_1 and y_2 are $\mathbb{C}^*$ variables, we can define three elements of $H_1(\Sigma,\mathbb{Z})$ from these equations,

$$\gamma_0 = \left\{(y_1,y_2) \in (\mathbb{C}^*)^2 : y_1 = \frac{-1-y_2}{1+zy_2^{-1}},\ |y_2| = \epsilon\right\},$$

$$\tau_\pm = \left\{(y_1,y_2) \in (\mathbb{C}^*)^2 : y_2^{\pm} = \frac{-1-y_1 \pm \sqrt{(1+y_1)^2 - 4zy_1}}{2},\ |y_1| = \epsilon\right\}.$$

Then, two of these must be responsible for the solution set $\{1, \log z\}$. To motivate the correct choice of cycles, let us first look closely at the mirror construction that originally provided Eq. (25). Starting with the description

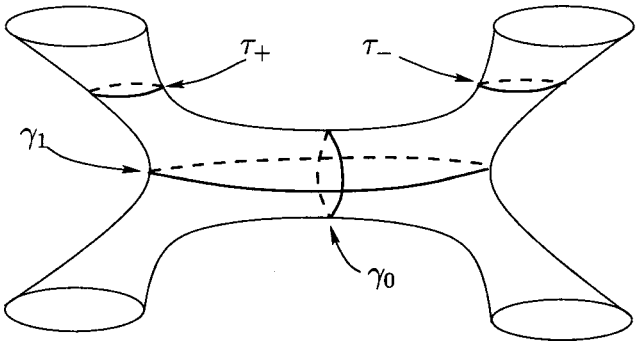

FIG. 1. 1-cycles on Σ. $\{\gamma_0, \tau_+, \tau_-\}$ is a basis for $H_1(\Sigma, \mathbb{Z})$.

$$\mathcal{O}(-1) \oplus \mathcal{O}(-1) \to \mathbb{P}^1 = \{(w_1, \ldots, w_4) \in \mathbb{C}^4 - Z : |w_1|^2 + |w_2|^2 - |w_3|^2 - |w_4|^2 = r\}/S^1,$$

from Ref. 2, the mirror geometry can be characterized as

$$\{uv + x_1 + \cdots + x_4 = 0 : x_1 x_2 x_3^{-1} x_4^{-1} = z, x_i = 1 \text{ for some } i\}.$$

Here u, $v \in \mathbb{C}$ and $x_i \in \mathbb{C}^*$. Also, the x_i obey $|x_i| = \exp(-|w_i|^2)$, and $|z| = e^{-r}$. To arrive at the form (25), we set $x_3 = 1$ and solved for x_1 in the constraint $x_1 x_2 x_3^{-1} x_4^{-1} = z$. Finally, the identification $y_1 = x_4$, $y_2 = x_2$ was made. Note that in choosing $x_3 = 1$, we are working in a specific coordinate patch on the Riemann surface. This coordinate patch is convenient for the problem at hand, as we now explain.

We can motivate the final choice of variables x_2, x_4 on Σ as follows. On $\mathcal{O}(-1) \oplus \mathcal{O}(-1) \to \mathbb{P}^1$, $[w_1, w_2]$ are homogeneous coordinates on the base $\mathbb{P}^1$, while w_3, w_4 are coordinates on each respective $\mathcal{O}(-1)$ factor. In order to study curves which start from the $\mathbb{P}^1$ and move off into a normal direction, we should use a coordinate patch with one base and one fiber variable, i.e., w_2, w_4. The mirror variables are then x_2, x_4, and hence our choice of them as local variables on Σ. To be more precise, the locus where $w_3 = w_4 = 0$, we thus have a bound $0 \leqslant |w_2|^2 \leqslant r$. Then $|y_2| = \exp(-|w_2|^2)$ implies that $1 \geqslant |y_2| \geqslant e^{-r} = |z|$; taking these considerations together, we may accurately label Fig. 1.

Proposition 3: Let γ_0, $\tau_\pm$ be as described above, and set $\gamma_1 = [\tau_+] + [\tau_-]$, with the sum taken in $H_1(\Sigma, \mathbb{Z})$. Then

$$\int_{\gamma_0} \log y_1 \frac{dy_2}{y_2}, \quad \int_{\gamma_1} \log y_2 \frac{dy_1}{y_1}$$

span the space of solutions $\{1, \log(z)\}$ of the PF operator $(1-z)\theta^2$.

Proof: The first integral is trivial,

$$\int_{\gamma_0} \log y_1 \frac{dy_2}{y_2} = \int_{|y_2|=\epsilon} \log\left(\frac{-1-y_2}{1+zy_2^{-1}}\right)\frac{dy_2}{y_2} = \int_{|y_2|=\epsilon} \left(i\pi + \log\left(\frac{1+y_2}{1+zy_2^{-1}}\right)\right)\frac{dy_2}{y_2}$$

and this is a constant. Of course, the branch cut of log must be taken to lie off the negative real axis. For the second,

$$\int_{\gamma_1} \log y_2 \frac{dy_1}{y_1} = \int_{\tau_+} \log y_2^+ \frac{dy_1}{y_1} + \int_{\tau_-} \log y_2^- \frac{dy_1}{y_1} = \int_{|y_1|=\epsilon} \log(y_2^+ y_2^-)\frac{dy_1}{y_1} = \int_{|y_1|=\epsilon} \log(zy_1)\frac{dy_1}{y_1}$$
$$= \text{const} + 2\pi i \log z.$$

□

Next, we turn to locating a period integral based on Definition 1. Since the constraint $1 \geqslant |y_2|$

$\geqslant |z|$ only applies in regions with $w_3=w_4=0$, outside of this locus, it is sensible to define a path on Σ as follows. Let $\lambda<|z|$ be real, and take a smooth increasing function $\sigma:[0,1]:\to\Sigma$ such that $\sigma(0)=\lambda$, $\sigma(1)=z$. Then

$$\gamma_2(\lambda)=\left\{(y_1,y_2)\in(\mathbb{C}^*)^2:y_1=\frac{-1-y_2}{1+zy_2^{-1}},\ y_2=\sigma[0,1],\ y_1\neq 1\right\}$$

defines an element of $(H_1(\Sigma,\mathbb{Z}))_c$.

Proposition 4: Let Σ, γ_2 be defined as above. Then

$$\theta\mathcal{F}=\int_{\gamma_2}\log y_1\frac{dy_2}{y_2},$$

where $\theta=z(d/dz)$ and $\theta\mathcal{F}$ is the double-logarithmic solution of the extended PF operator $\mathcal{D}'=\theta^2(1-z)\theta^2$ associated to the mirror of the local model $\mathcal{O}(-1)\oplus\mathcal{O}(-1)\to\mathbb{P}^1$.

Proof: The computation is straightforward,

$$\int_{\gamma_2}\log y_1\frac{dy_2}{y_2}=\int_\lambda^z\log\left(\frac{-1-y_2}{1+zy_2^{-1}}\right)\frac{dy_2}{y_2}=\int_\lambda^z\left(i\pi+\sum_{n>0}\frac{(-y_2)^n}{n}-\sum_{n>0}\frac{(-zy_2^{-1})^n}{n}\right)\frac{dy_2}{y_2}$$

$$=\text{const}+(\lambda-\text{dependent})+\sum_{n>0}\frac{(-z)^n}{n^2}=(\theta\mathcal{F})(-z).$$

In order to achieve the result, we should have z rather than $-z$ in the above. However, this is accounted for by the fact that $\arg(y_2)$ is not determined in local mirror symmetry, and hence we are free to use the variable $y_2'=e^{i\pi}y_2$ in place of y_2. □

Notice that, with this definition of period integrals, the logarithmic terms of $\theta\mathcal{F}$ are not uniquely determined, as they depend on λ. It is for this reason that λ dependent terms are disregarded in the calculation.

It may seem that the choice of γ_2 is artificial, since we could have equally well chosen an increasing function $\sigma':[0,1]\to\Sigma$ with $\sigma'(0)=1$, $\sigma'(1)=\lambda>1$. However, it is easy to show that this is equivalent; if

$$\gamma_2'(\lambda)=\left\{(y_1,y_2)\in(\mathbb{C}^*)^2:y_1=\frac{-1-y_2}{1+zy_2^{-1}},\ y_2=\sigma'[0,1],\ y_1\neq 1\right\},$$

then

$$\lim_{\lambda\to\infty}\left(\theta\int_{\gamma_2'}\log y_1\frac{dy_2}{y_2}\right)=\sum_{n>0}\frac{(-z)^n}{n},$$

so the two approaches are interchangeable.

Thus, we have demonstrated that the ordinary period integrals obtained by integrating a meromorphic 1-form on Σ over a basis of $H_1(\Sigma,\mathbb{Z})$ is not sufficient to provide all the information we need, from the perspective of mirror symmetry. We must also consider "noncompact cycles" in order to fill in the missing data, which is what we showed in this section.

IV. MIRROR SYMMETRY FOR TORIC TREES

In this section, we will exhibit Picard-Fuchs operators for a broad class of noncompact threefolds X such that $\dim H_4(X,\mathbb{Z})=0$.

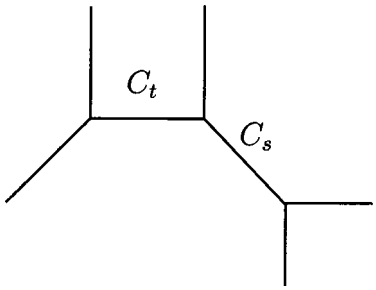

FIG. 2. Toric diagram for X_1.

A. Ordinary Picard-Fuchs systems

Our first interest will be to take a look at the PF systems one would arrive at through use of existing local mirror symmetry techniques. We wish to understand exactly how much information one might recover through these systems alone, in order to determine an appropriate fix.

Let us clarify what we are exploring here. Let $\{l^1,\ldots,l^n\}\subset\mathbb{Z}^m$ be a choice of basis for the secondary fan of a noncompact toric Calabi-Yau threefold X satisfying $\dim H_4(X,\mathbb{Z})=0$. Recall that we can derive all solutions of the Picard-Fuchs system on the mirror $\hat{X}$ to X by taking appropriate linear combinations of derivatives (in ρ) of the generating function $\omega(z,p)=\Sigma_{n>0}c(n,\rho)z^{n+\rho}$. Here z is the complex variable on the complex structure moduli space of $\hat{X}$, which we note is canonically identified by the basis vectors $\{l^1,\ldots,l^n\}$. In the above expression, $c(n,\rho)^{-1}=\Pi_i\Gamma(1+\Sigma_k l_i^k(n_k+\rho_k))$, where we are using the convention that $l^k=(l_1^k,\ldots,l_m^k)$. Then we want to look at the functions

$$\Pi_{ij}=(\partial_{\rho_i}\partial_{\rho_j}\omega(z,\rho))_{\rho=0}. \tag{26}$$

Our interest in this section, then, is to ascertain how much information we can find by looking at the Π_{ij}. In so doing, we will gain a better understanding of what to do in order to remedy mirror symmetry in this situation. Note that if X satisfies $\dim H_4(X,\mathbb{Z})=0$, then there is no linear combination of the Π_{ij}'s that is a solution of the associated PF system. But, we could consider a simple extension of a given PF system $\{\mathcal{D}_1,\mathcal{D}_2,\ldots\}$ of the form $\{\theta_1\mathcal{D}_1,\theta_2\mathcal{D}_2,\ldots\}$ which would have all the Π_{ij} as solutions.

Example 1: Consider the space

$$X_1=\{-2|w_1|^2+|w_2|^2+|w_3|^2=t_R,\ |w_1|^2-|w_2|^2+|w_4|^2-|w_5|^2=s_R\}/(S^1)^2,$$

where $(w_1,\ldots,w_5)\in\mathbb{C}^5-(\{w_2=w_3=0\}\cup\{w_1=w_4=0\}\cup\{w_4=w_5=0\})$, and s_R, t_R are positive real numbers. Choose s, $t\in\mathbb{C}$ satisfying $\mathrm{Re}(s)=s_R$, $\mathrm{Re}(t)=t_R$. Then X_1 contains two curves C_t, C_s with respective normal bundles $\mathcal{O}\oplus\mathcal{O}(-2)$ and $\mathcal{O}(-1)\oplus\mathcal{O}(-1)$ in X_1. Note also that s_R, t_R determine the radius of each respective curve. We have that $b_2=2$ and $b_4=0$.

From Ref. 16 we can draw a planar trivalent graph for X_1 corresponding to the torus weights. Using the rules of that paper, we find the toric skeleton shown in Fig. 2. Through the GKZ formalism, we have the PF operators associated to X_1,

$$\begin{aligned}\mathcal{D}_1&=\theta_1(\theta_1-\theta_2)-z_1(2\theta_1-\theta_2)(2\theta_1-\theta_2+1),\\ \mathcal{D}_2&=(2\theta_1-\theta_2)\theta_2-z_2(\theta_1-\theta_2)\theta_2,\\ \mathcal{D}_3&=\theta_1\theta_2-z_1z_2(2\theta_1-\theta_2)\theta_2.\end{aligned} \tag{27}$$

Let s, t be the logarithmic solutions of this system. From physics[5,11] the instanton part of the prepotential in s, t variables is

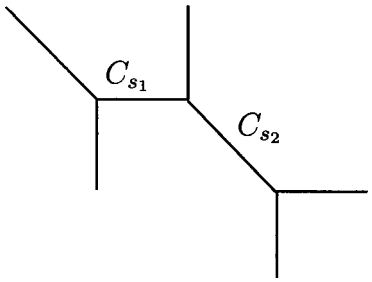

FIG. 3. Toric diagram for X_2.

$$\mathcal{F}_1^{\text{inst}} = \sum_{n>0} \frac{e^{ns}}{n^3} + \frac{e^{n(s+t)}}{n^3} - \frac{e^{nt}}{n^3}. \tag{28}$$

The Frobenius functions are

$$\Pi_{11}(s,t) = 0,$$

$$\Pi_{12}(s,t) = \sum_{n>0} \frac{e^{n(t+s)}}{n^2} - \frac{e^{ns}}{n^2}, \tag{29}$$

$$\Pi_{22}(s,t) = 2\sum_{n>0} \frac{e^{ns}}{n^2}.$$

We have neglected the logarithmic terms of each function. Notice that there is no linear combination of Π_{ij}'s that we can take to reproduce the term $\Sigma_{n>0} e^{nt}/n^2$. Apparently, the PF system cannot see the curve with normal bundle $\mathcal{O}\oplus\mathcal{O}(-2)$.

Example 2: Next, consider the space

$$X_2 = \{|w_1|^2 + |w_2|^2 - |w_3|^2 - |w_4|^2 = s_{1,R}, -|w_1|^2 - |w_3|^2 + |w_4|^2 + |w_5|^2 = s_{2,R}\}/(S^1)^2,$$

with $(w_1,\ldots,w_5) \in \mathbb{C}^5 - (\{w_1=w_2=0\}\cup\{w_4=w_5=0\}\cup\{w_2=w_5=0\})$. Also $s_{i,R} \in \mathbb{R}^+$ and we choose $s_i \in \mathbb{C}$ with $\text{Re}(s_i)=s_{i,R}$. We again have $b_2=2$, $b_4=0$, and now $\mathcal{N}_{C_i/X_2} \cong O(-1)\oplus\mathcal{O}(-1)$ for each i. Notice that we can flop from X_2 to X_1, if $l^1=(1,1,-1,-1,0)$ and $l^2=(-1,0,-1,1,1)$, then the combinations l^1+l^2, $-l^2$ give the secondary fan for X_1. The planar trivalent toric graph for X_2 is given in Fig. 3. We have the PF system from the mirror manifold,

$$\mathcal{D}_1 = (\theta_1 - \theta_2)\theta_1 - z_1(-\theta_1 - \theta_2)(-\theta_1 + \theta_2),$$

$$\mathcal{D}_2 = (\theta_2 - \theta_1)\theta_2 - z_2(-\theta_2 - \theta_1)(-\theta_2 + \theta_1), \tag{30}$$

$$\mathcal{D}_3 = \theta_1\theta_2 - z_1z_2(\theta_1 + \theta_2 + 1)(\theta_1 + \theta_2).$$

Let s_i be the logarithmic solutions. Using the same conventions as example 1, we find

$$\Pi_{11}(s_1,s_2) = \sum_{n>0} \frac{e^{ns_1}}{n^2} - \frac{e^{ns_2}}{n^2},$$

$$\underset{12}{\Pi}(s_1,s_2)=0,$$

with $\Pi_{22}=-\Pi_{11}$. Again, these expressions already include the mirror map. Let us take a look at the prepotential,

$$\mathcal{F}_2^{\text{inst}}=\sum_{n\geqslant 0}\frac{e^{ns_1}}{n^3}+\frac{e^{ns_2}}{n^3}-\frac{e^{n(s_1+s_2)}}{n^3}.$$

Then we see that

$$\underset{11}{\Pi}=\frac{\partial\mathcal{F}_2^{\text{inst}}}{\partial s_1}-\frac{\partial\mathcal{F}_2^{\text{inst}}}{\partial s_2}.$$

However, the cross term corresponding to $C_{s_1+s_2}$ cannot be detected from the Π_{ij}'s. Our work with example 1 suggests the reason for the problem with the $C_{s_1+s_2}$ curve. To exhibit this, recall that the lattice vectors $\{l^1,l^2\}$ for this geometry are

$$\begin{pmatrix} l^1 \\ l^2 \end{pmatrix}=\begin{pmatrix} 1 & 1 & -1 & -1 & 0 \\ 0 & -1 & -1 & 1 & 1 \end{pmatrix}.$$

Each vector represents a curve C_{s_i} in X_2. Then $C_{s_1+s_2}$ is determined by the single vector

$$l^1+l^2=\begin{pmatrix} 1 & 0 & -2 & 0 & 1 \end{pmatrix}.$$

This curve satisfied $\mathcal{N}_{C_{s_1+s_2}/X_2}\cong\mathcal{O}\oplus\mathcal{O}(-2)$. Hence, we do not expect that we can retrieve its information from the PF system.

We have performed similar computations for three and four parameter cases, all of which support this general principle. This leads us to the following.

Conjecture 2: Let X be a noncompact toric Calabi-Yau threefold with $\dim H_4(X,\mathbb{Z})=0$, *and say* $\{l^1,\ldots l^m\}$ *define X via symplectic quotient. Let* $\omega=\Sigma_{n>0}c(n,\rho)z^{n+\rho}$ *be the generating function for*

$$\Pi_{ij}^{\text{inst}}=\sum_n\left(\partial_{\rho_i}\partial_{\rho_j}c(n,\rho)\right)\big|_{\rho=0}z^n \tag{31}$$

with $c(n,\rho)^{-1}=\Pi_i\Gamma(1+\Sigma_k l_i^k(n_k+\rho_k))$. *If* $\mathcal{F}$ *is the prepotential, and* $s_i=\partial_{\rho_i}\omega|_{\rho=0}$ *for each i such that* $l^i=(1\ \ 1\ \ -1\ \ -1\ \ 0\ \ \ldots\ \ 0)$ (*up to a permutation of the columns of* l^i), *then there are rational numbers* $m_{ij}\in\mathbb{Q}$ *such that*

$$\sum_{i,j}m_{ij}\Pi_{ij}^{\text{inst}}=\sum_i(-1)^{i-1}\frac{\partial\mathcal{F}^{\text{inst}}}{\partial s_i}.$$

Here, $\mathcal{F}^{\text{inst}}$ is the instanton part of the prepotential. We use the notation Π_{ij}^{inst} to distinguish these functions from the usual derivatives of ω (i.e., $\Pi_{ij}=\partial_{\rho_i}\partial_{\rho_j}\omega|_{\rho=0}$). We remark that no linear combination of the Π_{ij} is a solution of the associated PF system; yet, since these functions are essential to the counting of Gromov-Witten invariants in usual mirror symmetry constructions, we have tested the limits of the information they carry. This conjecture is equivalent to the statement that although we cannot detect curves with normal bundle $\mathcal{O}\oplus\mathcal{O}(-2)$ via the Π_{ij}, we can exhibit all curves with normal bundle $\mathcal{O}(-1)\oplus\mathcal{O}(-1)$ using these functions.

Let us now briefly recap what we have explored, and what we have learned, in this section. First, from general principles we know that the PF systems have no double-logarithmic solutions, and hence there are no curve-counting functions on these spaces. Second, we looked at the functions Π_{ij} to determine if we could fix the problem by simply considering some basic extended system (e.g, $\{\mathcal{D}_1,\mathcal{D}_2,\ldots\}\to\{\theta_1\mathcal{D}_1,\theta_2\mathcal{D}_2,\ldots\}$). However, the absence of curves with normal bundle

$\mathcal{O}\oplus\mathcal{O}(-2)$ in the functions Π_{ij} means that we must work a little harder to find the right extended systems. We will now turn to this task, by seeking a way to include such curves in the differential systems.

B. Two building blocks of solutions

Assume X is a noncompact Calabi-Yau threefold such that $\dim H_4(X,\mathbb{Z})=0$, and that every two cycle $C\hookrightarrow X$ has normal bundle $\mathcal{O}\oplus\mathcal{O}(-2)$ or $\mathcal{O}(-1)\oplus\mathcal{O}(-1)$. We will refer to these as t and s curves, respectively, in the following. Then, as any such space X is obtained by gluing s and t curves together in some way, it is reasonable to expect that we can solve all these models by extension from the two basic one parameter cases

$$X_s=\mathcal{O}(-1)\oplus\mathcal{O}(-1)\to\mathbb{P}^1,$$

$$X_t=\mathcal{O}\oplus\mathcal{O}(-2)\to\mathbb{P}^1.$$

We have already exhibited the solution on X_s. We will now modify this slightly to allow extension to the general cases, and subsequently demonstrate a similar solution on X_t.

Recall, from Sec. II A, the differential operator for X_s,

$$\widetilde{\mathcal{D}}_1=\theta_s^2(1-z_s)\theta_s^2.$$

As before, $\theta_s=z_s d/\mathrm{d}z_s$, and $\widetilde{Y}_1=1/(1-z_s)$ is the Yukawa coupling. Note that this expression for $\widetilde{Y}_1$ implies a classical triple intersection number 1 for $\mathbb{P}^1\hookrightarrow X_s$.

We will now need to make a slightly different choice of Yukawa coupling on X_s. Recall[17,7] that, in the context of the toric flop $s\to -s$, the natural value for the triple intersection number is $1/2$. There is a simple proof for this, which we give now. From Sec. II A, we had the prepotential on local $\mathbb{P}^1$ with arbitrary triple intersection number [Eq. (16)],

$$\mathcal{F}(z)=K\frac{(\log z)^3}{6}+\sum_{n>0}\frac{z^n}{n^3}. \tag{32}$$

A flop of the $\mathbb{P}^1$ on X_s is the same as a change of variables $z\to 1/z$ in the prepotential

$$\mathcal{F}^{\mathrm{flop}}(z)=K\frac{(-\log z)^3}{6}+\sum_{n>0}\frac{z^{-n}}{n^3}. \tag{33}$$

Taking the difference of these,

$$\mathcal{F}(z)-\mathcal{F}^{\mathrm{flop}}(z)=-\tfrac{1}{3}K(\log z)^3. \tag{34}$$

We have ignored the terms including $\sqrt{-1}$, since the Yukawa coupling is insensitive to them. Then according to Witten,[17] we are supposed to find

$$\mathcal{F}(z)-\mathcal{F}^{\mathrm{flop}}(z)=-\tfrac{1}{6}(\log z)^3, \tag{35}$$

and hence $K=1/2$ is uniquely determined. Recall that the result[17] cited here was derived by considering the analytic continuation of the instanton sum across a flop; the difference in intersection pairings between the geometries X_s and X_{-s} was shown to be -1, which is equivalent to Eq. (35).

This means that we should really be using

$$Y_1 = \frac{1}{2} + \frac{z_s}{1 - z_s}$$

for the Yukawa coupling. We obtain the following differential operator describing mirror symmetry for X_s:

$$\mathcal{D}_1 = \theta_s^2 \left(\frac{2(1 - z_s)}{1 + z_s} \right) \theta_s^2.$$

Next, let us turn to X_t. Note that the naturally occurring PF operator on the mirror to $\mathcal{O} \oplus \mathcal{O}(-2) \to \mathbb{P}^1$, which is $\mathcal{D}_2' = \theta_t^2 - z_t(2\theta_t)(2\theta_t + 1)$, has no curve information, since there is no double-logarithmic solution. Moreover, the second Frobenius derivative of the generating function of solutions has no instanton part. Yet, in view of the solution on X_s, we can easily exhibit a Picard-Fuchs operator for X_t; it is given by

$$\mathcal{D}_2 = \partial_t^2 (1/Y_2) \partial_t^2.$$

Here

$$t(z) = \log(z_t) + 2 \sum_{n>0} \frac{(2n-1)!}{n!^2} z_t^n$$

is the mirror map for X_t, and Y_2 is the Yukawa coupling on X_t, which in these coordinates is

$$Y_2 = - \frac{1 + e^t}{2(1 - e^t)}.$$

Let us briefly discuss the motivation for this choice of Y_2. First of all, we take an overall minus sign on the instanton part of Y_2 relative to the X_s case, because of considerations coming from the topological vertex.[11] Also, the constant term of $-1/2$ is determined from Conjecture 1, i.e., from the requirement of rationality of the B-model Yukawa coupling.

Then, as in the compact case, it follows automatically that the solutions Π_t of $\mathcal{D}_2 \Pi_t = 0$ are given as

$$\Pi_t = \left(1, t, \frac{\partial \mathcal{F}}{\partial t}, t \frac{\partial \mathcal{F}}{\partial t} - 2\mathcal{F} \right),$$

where $\mathcal{F}$ is a holomorphic function in t such that $\partial^3 \mathcal{F} / \partial t^3 = Y_2$. Then it is a simple matter to write down an explicit differential operator on the mirror of X_t, by a change of coordinates for $\mathcal{D}_2$. We find

$$\mathcal{D}_2 = \theta_t^4 - z_t(2\theta_t + 2)(2\theta_t + 1)^2 \theta_t + (z_t)^2 (2\theta_t + 4)(2\theta_t + 3)(2\theta_t + 1) 2\theta_t \quad \left(\theta_t := z_t \frac{d}{\mathrm{d}z_t} \right). \tag{36}$$

The solutions of (36) are generated by the Fröbenius function,

$$w(z_t, \rho) := \sum_{n=0}^{\infty} \frac{1}{\Gamma(1 - 2n - 2\rho)(\Gamma(1 + n + \rho))^2} \left(1 + \sum_{j=1}^{n} \frac{\rho}{j + \rho} \right) z_t^{n+\rho}.$$

We can easily check that the vector space

$$\left\langle 1, t, \frac{\partial \mathcal{F}}{\partial t}, 2\mathcal{F} - t \frac{\partial \mathcal{F}}{\partial t} \right\rangle_{\mathbb{C}},$$

is equal to the vector space

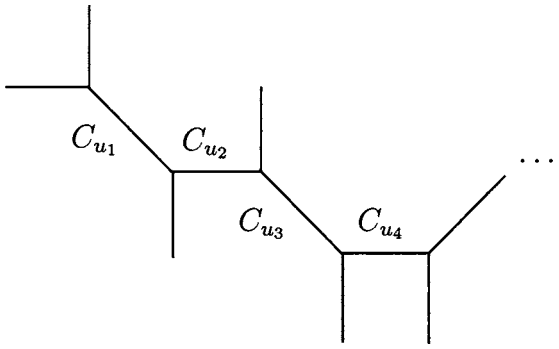

FIG. 4. X containing a string of curves.

$$\langle w(z_t,0), \partial_\rho w(z_t,0), \partial_\rho^2 w(z_t,0), \partial_\rho^3 w(z_t,0)\rangle_{\mathbb{C}}.$$

Hence, we have demonstrated the existence of mirror symmetry for both X_s and X_t, in terms of solutions of differential operators. It should be noted that $\mathcal{D}_1$, $\mathcal{D}_2$ cannot be derived from any GKZ system on these spaces.

We close this section by making a general remark about the constructions here. Note that, on X_t, we have simply taken the known results of Gromov-Witten invariants and translated this into a Picard-Fuchs equation on the mirror. Yet, we view this as an important step towards our ultimate goal, which is a formulation of local mirror symmetry purely in terms of the complex geometry of the mirror $\hat{X}_t$. By a careful study of such operators, we hope to better understand exactly why local mirror symmetry fails on spaces such as X_t.

C. Mirror symmetry when dim $H_4(X,\mathbb{Z})=0$

We can use the results of the preceding section to find a general solution for such spaces, as follows. We are interested in noncompact toric Calabi-Yau threefolds X with dim $H_4(X,\mathbb{Z})=0$ such that for each $C \in H_2(X,\mathbb{Z})$, we have

$$\mathcal{N}_{C/X} \cong \mathcal{O}(-1) \oplus \mathcal{O}(-1)$$

or

$$\mathcal{N}_{C/X} \cong \mathcal{O} \oplus \mathcal{O}(-2).$$

Let $\{C_{s_1},\ldots,C_{s_m},C_{t_1},\ldots,C_{t_n}\}$ is a basis of $H_2(X,\mathbb{Z})$, where $\mathcal{N}_{C_{s_i}/X} \cong \mathcal{O}(-1)\oplus\mathcal{O}(-1)$, $\mathcal{N}_{C_{t_j}/X} \cong \mathcal{O} \oplus \mathcal{O}(-2)\,\forall\, i,j$, and $u=(s_1,\ldots,s_m,t_1,\ldots,t_n)$.

From the topological vertex formalism, the authors of Ref. 11 were able to determine the instanton part of the prepotential for the class of examples we are considering. Explicitly,

$$\mathcal{P}^{\text{inst}} = \sum_{C_s}\sum_{k>0}\frac{e^{ks}}{k^3} - \sum_{C_t}\sum_{k>0}\frac{e^{kt}}{k^3}.$$

Here, the sum over C_s represents the sum over all curves $C_s \hookrightarrow X$ such that $N_{C_s/X} \cong \mathcal{O}(-1)\oplus\mathcal{O}(-1)$, and similarly for the sum over C_t.

As explained in the introduction, our problem reduces to that of defining a consistent (triple) intersection theory on X. Thanks to the simple structure of X, together with our preliminary choice of intersection numbers for $\mathcal{O}(-1)\oplus\mathcal{O}(-1)\to\mathbb{P}^1$ and $\mathcal{O}\oplus\mathcal{O}(-2)\to\mathbb{P}^1$, there is in fact a unique choice. We will first give the general definition, and afterward explain its significance through an example. To give the prescription for intersection theory for the general case, we will only consider X with the toric diagram as shown in Fig. 4. That is, only two curves in X are allowed to

intersect at any point. Hence, we exclude cases where three curves meet at one point in X, etc. With this restriction, we can introduce an ordering on the curves in X,

$$C_{u_1} < C_{u_2} < C_{u_3} < \cdots .$$

Define a function

$$\mathrm{sgn}: H_2(X,\mathbb{Z}) \to \{1,-1\}$$

so that $\mathrm{sgn}(C)=1$ if $\mathcal{N}_{C/X} \cong \mathcal{O}(-1)\oplus\mathcal{O}(-1)$, and $\mathrm{sgn}(C)=-1$ otherwise. With these conventions, we can now state our conjecture on intersection theory.

Definition 2: Let X and u be as above. Then the classical intersection numbers for X are given by

$$K_{abc} = \frac{1}{2}\sum_{C\notin\mathcal{A}} \mathrm{sgn}([C_{abc}]+[C]), \tag{37}$$

where the sum is taken in homology, and

$$[C_{abc}] = [C_{u_a}] + \sum_{C_{u_a}<C_\alpha<C_{u_b}} [C_\alpha] + [C_{u_b}] + \sum_{C_{u_b}<C_\beta<C_{u_c}} [C_\beta] + [C_{u_c}].$$

The sum is taken away from the set $\mathcal{A}=\{[C_{u_a}],[C_{u_b}],\ldots,[C_{u_a}+C_{u_{a+1}}],\ldots\}$.

This formula can be most simply understood as follows. The curve of minimum volume containing all three curves C_{u_a}, C_{u_b}, and C_{u_c} can be represented by the homology class

$$[C_{abc}] = [C_{u_a}] + \sum_{C_{u_a}<C_\alpha<C_{u_b}} [C_\alpha] + [C_{u_b}] + \sum_{c_{u_b}<C_\beta<C_{u_c}} [C_\beta] + [C_{u_c}].$$

Then each term of the sum $[C_{abc}]+[C]$ corresponds to a curve in X containing C_{abc}.

For example, consider the case $a=b=c$. Then both of the sums collapse, we are left with only $\mathrm{sgn}([C_{u_a}]+[C])$. The sum will contribute $\pm 1/2$ for each curve containing C_{u_a}, depending on the normal bundle of that curve.

Let us now apply this definition to a concrete case. Consider again the instanton part of the prepotential from example 1 above, Eq. (28),

$$\mathcal{F}^{\mathrm{inst}} = \sum_{n>0} \frac{e^{ns}}{n^3} + \frac{e^{n(s+t)}}{n^3} - \frac{e^{nt}}{n^3}.$$

Then, e.g.,

$$\frac{\partial^3 \mathcal{F}^{\mathrm{inst}}}{\partial s^3} = \sum_{n>0} (e^{ns} + e^{n(s+t)}).$$

Both the s curve and the $s+t$ curve have normal bundle $\mathcal{O}(-1)\oplus\mathcal{O}(-1)$ (this can be seen from the toric diagram, or directly from the vectors defining the secondary fan). Thus, each curve should have an intersection number equal to $1/2$, which implies

$$K_{sss} = \tfrac{1}{2} + \tfrac{1}{2} = 1.$$

By applying similar reasoning, we obtain the other intersection numbers $K_{tss}=K_{tts}=1/2$, $K_{ttt}=0$.

In fact, we can provide a simple argument as to why this is the correct choice of intersection theory for this class of examples. We must only verify that the intersection numbers are consistent under the analytic continuation of the prepotential through a flop transformation. And indeed, the numbers given above are the unique ones that satisfy this requirement.

D. Extended Picard-Fuchs system for X_1 and X_2

In this section, we derive an extended PF system under the assumption of the conjecture given in the preceding section. The operators $\mathcal{D}_i$ appearing below are the same as in Sec. IV A. First, we look at the example X_1. In this case, we start from four A-model Yukawa couplings,

$$\begin{aligned} Y_{ttt} &:= -\frac{e^t}{1-e^t} + \frac{e^{s+t}}{1-e^{s+t}}, \\ Y_{tts} &:= \frac{1}{2} + \frac{e^{s+t}}{1-e^{s+t}}, \\ Y_{tss} &:= \frac{1}{2} + \frac{e^{s+t}}{1-e^{s+t}}, \\ Y_{sss} &:= 1 + \frac{e^s}{1-e^s} + \frac{e^{s+t}}{1-e^{s+t}}. \end{aligned} \tag{38}$$

The constant part of each Yukawa coupling is given by the conjecture, and the instanton (nonconstant) part was taken from Ref. 11. By solving (27), we obtain mirror maps $s=s(z_1,z_2)$ and $t=t(z_1,z_2)$. In particular, the Jacobian of these mirror maps are written in terms of simple functions, as follows:

$$\frac{\partial t}{\partial u_1} = \frac{1}{\sqrt{1-4z_1}}, \quad \frac{\partial t}{\partial u_2} := 0, \quad \frac{\partial s}{\partial u_1} = \frac{1}{2}\frac{-1+4z_1+\sqrt{1-4z_1}}{-1+4z_1}, \quad \frac{\partial s}{\partial u_2} = 1, \tag{39}$$

where $u_i=\log(z_i)$. With this data, we can compute the B-model Yukawa couplings in u^i coordinates, and they turn out to be rational functions in z_i whose denominators are given by the divisor of the defining equation of discriminant locus of $\hat{X}_1$,

$$\mathrm{dis}(\hat{X}_1) = (1-z_2+z_1z_2^2)(1-4z_1). \tag{40}$$

The explicit results are given as follows:

$$\begin{aligned} Y_{111} &= -\frac{1}{2}\frac{z_1(-4z_1+5-7z_2+12z_1z_2+2z_2^2-5z_1z_2^2+4z_1^2z_2^2)}{(1-z_2+z_1z_2^2)(-1+4z_1)^2}, \\ Y_{112} &= -\frac{1}{2}\frac{(1-2z_1-z_2+4z_1z_2-z_1z_2^2+2z_1^2z_2^2)}{(1-z_2+z_1z_2^2)(-1+4z_1)}, \\ Y_{122} &= -\frac{1}{2}\frac{(-1+z_2+z_1z_2^2)}{(1-z_2+z_1z_2^2)}, \\ Y_{222} &= \frac{1-z_1z_2^2}{1-z_2+z_1z_2^2}. \end{aligned} \tag{41}$$

These results show that the conjecture given in the preceding section is compatible with Conjecture 1 in Sec. I. Therefore, we can construct an extended PF system by using the strategy outlined in Sec. II. For brevity, we introduce here the following notation:

$$M_a^{\alpha}(t_*) := \sum_b (Y_a^{-1}(t_*))^{\alpha b}\partial_a\partial_b\psi_0. \tag{42}$$

In the case of X_1, we have two integrability conditions given in (7),

$$M_1^1(s,t) = M_2^1(s,t), \quad M_1^2(s,t) = M_2^2(s,t), \tag{43}$$

where we use the subscripts 1 and 2 for s and t. By explicit computation, these two conditions turn out to be the same, and translated into a differential equation in z_i variables by using (39) and (41), we obtain

$$((1 + z_2 + z_1z_2^2)\mathcal{D}_1 + \mathcal{D}_2 + z_2\mathcal{D}_3)\psi_0 = 0. \tag{44}$$

Next, we consider the second integrability condition given in (8),

$$\partial_1 M_1^1(s,t) = \partial_2 M_2^2(s,t), \quad \partial_2 M_1^1(s,t) = 0, \quad \partial_1 M_2^2(s,t) = 0. \tag{45}$$

By explicit computation, we found that the second and third conditions are translated into one rational differential equation,

$$\theta_2\mathcal{D}_1\psi_0 = 0. \tag{46}$$

The first condition is also translated into a rational differential equation but the result is very complicated. We do not have to use this equation because we can say that (44) and (46) are a minimal set of extended PF operators for X_1. The reason is the following. Let us consider the large radius limit of (44) and (46),

$$(\theta_1^2 + \theta_1\theta_2 - \theta_2^2)\psi_0 = 0, \quad (\theta_1^2\theta_2 - \theta_1\theta_2^2)\psi_0 = 0. \tag{47}$$

These conditions are equivalent to the relations of the classical cohomology ring of $\bar{X}_1$,

$$k_t^2 + k_tk_s - k_s^2 = 0, \quad k_t^2k_s - k_tk_s^2 = 0, \tag{48}$$

which reproduces the conjectured triple intersection numbers, up to an overall scaling. From this fact, we can see that (44) and (46) give us a complete set of relations for the classical cohomology ring of X_1 at the large radius limit. Since the PF equations are nothing but the noncommutative version of the relations of the quantum cohomology ring of X_1, which reduce to relations of classical cohomology at the large radius limit,[8] we can propose the following set of differential operators as an extended PF system:

$$\begin{aligned}\widetilde{\mathcal{D}}_1 &= (1 + z_2 + z_1z_2^2)\mathcal{D}_1 + \mathcal{D}_2 + z_2\mathcal{D}_3,\\ \widetilde{\mathcal{D}}_2 &= \theta_2\mathcal{D}_1.\end{aligned} \tag{49}$$

We checked that the solution space of (49) is given by

$$\left\langle 1, t, s, \frac{\partial\mathcal{F}}{\partial t}, \frac{\partial\mathcal{F}}{\partial s}, 2\mathcal{F} - t\frac{\partial\mathcal{F}}{\partial t} - s\frac{\partial\mathcal{F}}{\partial s}\right\rangle_{\mathbb{C}}. \tag{50}$$

Of course, we can derive the B-model Yukawa couplings (41) by using (49) as the starting point. An explicit example of this kind of computation will be given in Sec. VI of this paper.

We can also construct an extended PF system of X_2 in the same way as X_1. Here, we briefly present the data of this construction. The starting point is the A-model Yukawa couplings,

$$Y_{111} := \frac{e^{s_1}}{1 - e^{s_1}} - \frac{e^{s_1+s_2}}{1 - e^{s_1+s_2}},$$

$$
\begin{aligned}
Y_{112} &:= -\frac{1}{2} - \frac{e^{s_1+s_2}}{1-e^{s_1+s_2}},\\
Y_{122} &:= -\frac{1}{2} - \frac{e^{s_1+s_2}}{1-e^{s_1+s_2}},\\
Y_{222} &:= \frac{e^{s_2}}{1-e^{s_2}} - \frac{e^{s_1+s_2}}{1-e^{s_1+s_2}}.
\end{aligned}
\tag{51}
$$

Let us introduce the logarithm of the B-model coordinates z_i,

$$
u_1 = \log(z_1), \quad u_2 = \log(z_2). \tag{52}
$$

By solving (30), we obtain the mirror maps $s_1=s_1(z_1,z_2)$ and $s_2=s_2(z_1,z_2)$ and their Jacobian,

$$
\begin{aligned}
&\frac{\partial s_1}{\partial u_1} = \frac{1}{2}\frac{(-\sqrt{1-4z_1z_2}-1+4z_1z_2)}{(4z_1z_2-1)}, \quad \frac{\partial s_1}{\partial u_2} = -\frac{1}{2}\frac{(-1+4z_1z_2+\sqrt{1-4z_1z_2})}{(4z_1z_2-1)},\\
&\frac{\partial s_2}{\partial u_1} = -\frac{1}{2}\frac{(-1+4z_1z_2+\sqrt{1-4z_1z_2})}{(4z_1z_2-1)}, \quad \frac{\partial s_2}{\partial u_2} = \frac{1}{2}\frac{(-\sqrt{1-4z_1z_2}-1+4z_1z_2)}{(4z_1z_2-1)}.
\end{aligned}
\tag{53}
$$

With this data, we can compute the B-model Yukawa couplings in u^i,

$$
\begin{aligned}
Y_{111} &= \frac{1}{2}z_1\frac{(5z_1z_2-2-12z_1z_2^2+7z_2+4z_2^3z_1-5z_2^2-4z_1^2z_2^2)}{(z_2-1+z_1)(4z_1z_2-1)^2},\\
Y_{112} &= \frac{1}{2}\frac{(1-z_1-z_2-z_1z_2-z_2z_1^2+z_1z_2^2+4z_1^2z_2^2+4z_2^2z_1^3-4z_2^3z_1^2)}{(z_2-1+z_1)(4z_1z_2-1)^2},\\
Y_{122} &= \frac{1}{2}\frac{(1-z_2-z_1-z_2z_1-z_1z_2^2+z_2z_1^2+4z_2^2z_1^2+4z_1^2z_2^3-4z_1^3z_2^2)}{(z_1-1+z_2)(4z_2z_1-1)^2},\\
Y_{222} &= \frac{1}{2}z_2\frac{(5z_2z_1-2-12z_2z_1^2+7z_1+4z_1^3z_2-5z_1^2-4z_2^2z_1^2)}{(z_1-1+z_2)(4z_2z_1-1)^2},
\end{aligned}
\tag{54}
$$

and they turn out to be rational functions in z_i whose denominators are divisors of defining equation of discriminant locus of $\hat{X}_2$,

$$
\mathrm{dis}(\hat{X}_2) = (1-z_1-z_2)(1-4z_1z_2). \tag{55}
$$

The derivation of the extended PF system by using the recipe in Sec. II proceeds in the same way as X_1. In this case, we must only consider

$$
M_1^1(s_1,s_2) = M_2^1(s_1,s_2), \quad M_1^2(s_1,s_2) = M_2^2(s_1,s_2) \tag{56}
$$

and

$$
\partial_1 M_1^1(s_1,s_2) = \partial_2 M_2^2(s_1,s_2), \quad \partial_2 M_1^1(s_1,s_2) = 0, \quad \partial_1 M_2^2(s_1,s_2) = 0. \tag{57}
$$

Equation (56) gives us one differential equation for ψ_0 with rational function coefficients in z_i,

$$
(\mathcal{D}_1 + \mathcal{D}_2 + (1+z_1+z_2)\mathcal{D}_3)\psi_0 = 0. \tag{58}
$$

As for (57), the second and the third conditions give us a differential equation for ψ_0,

$$(\theta_1 - \theta_2)\mathcal{D}_3\psi_0 = 0, \tag{59}$$

and the first one gives us a complicated rational differential equation. For the same reasoning as X_1, we can propose an extended PF system for X_2 as follows:

$$\begin{aligned}\widetilde{\mathcal{D}}_1 &:= \mathcal{D}_1 + \mathcal{D}_2 + (1 + z_1 + z_2)\mathcal{D}_3,\\ \widetilde{\mathcal{D}}_2 &:= (\theta_1 - \theta_2)\mathcal{D}_3.\end{aligned} \tag{60}$$

We have also constructed an extended PF system for a three parameter space X_3, in order to further test the conjecture made in the preceding section. Specifically, X_3 satisfies $\dim H_2(X,\mathbb{Z}=3)$, $\dim H_4(X,\mathbb{Z}=0)$, and is defined by the following vectors:

$$\begin{pmatrix} l^1 \\ l^2 \\ l^3 \end{pmatrix} = \begin{pmatrix} 1 & 1 & -1 & -1 & 0 & 0 \\ 0 & -1 & -1 & 1 & 1 & 0 \\ 0 & -1 & 1 & 0 & -1 & 1 \end{pmatrix}. \tag{61}$$

The results are collected in Appendix A.

V. ADDING OPEN STRINGS TO $\dot{\mathcal{O}}(-1)\oplus\mathcal{O}(-1)\to\mathbb{P}^1$

So far, we have been able to demonstrate the existence of differential operators which determine mirror symmetry for noncompact toric Calabi-Yau manifolds which have no 4 cycle. One may also wonder what the applications are to the PF system derived for open string mirror symmetry.[14,6] Briefly, we recall that in Ref. 14, a system of Picard-Fuchs differential operators for open strings was proposed. By considering the toric data arising from a noncompact toric Calabi-Yau threefold X and a Lagrangian submanifold $L\subset X$,[14] gives a method of associated PF differential equations, whose solutions are then shown to reproduce known open string mirror symmetry data,[6] subsequently identified the integrals which correspond to these differential operators. Below, we will see that in some cases, the PF system of Ref. 14 also requires extension.

Recall[1,6] that open string mirror symmetry is a local isomorphism of moduli spaces $(\mathcal{X},\mathcal{L})$ and $(\hat{\mathcal{X}},\mathcal{C})$; X and $\hat{X}$ are Calabi-Yau manifolds which are mirror in the usual sense, and $L\subset X$ is Lagrangian, while $C\subset\hat{X}$ is holomorphic. In the case at hand, $(\mathcal{X},\mathcal{L})$ will be given by

$$X_r = \{(w_1,\ldots,w_4) \in \mathbb{C}^4 - Z : |w_1|^2 + |w_2|^2 - |w_3|^2 - |w_4|^2 = r\}/S^1,$$

together with either

$$L_{r,c} = X_r \cap \left\{ |w_2|^2 - |w_4|^2 = c, \quad |w_3|^2 - |w_4|^2 = 0, \quad \sum_i \arg(w_i) = 0 \right\} \tag{62}$$

or

$$L'_{r,c} = X_r \cap \left\{ |w_2|^2 - |w_4|^2 = 0, \quad |w_3|^2 - |w_4|^2 = c, \quad \sum_i \arg(w_i) = 0 \right\}. \tag{63}$$

There are then local moduli space isomorphisms $(\mathcal{X},\mathcal{L})\cong(\hat{\mathcal{X}},\mathcal{C})$, $(\mathcal{X},\mathcal{L}')\cong(\hat{\mathcal{X}},\mathcal{C}')$, where

$$\hat{X}_{z_1} = \{(u,v,y_1,y_2) \in \mathbb{C}^2 \times (\mathbb{C}^*)^2 : uv + 1 + y_1 + y_2 + z_1 y_1 y_2^{-1} = 0\},$$

$$C_{z_1,z_2} = \hat{X}_{z_1} \cap \{y_2^{-1} y_1 = z_2, \quad y_1 = 1\}, \tag{64}$$

$$C'_{z_1,z_2} = \hat{X}_{z_1} \cap \{y_2^{-1} y_1 = 1, \quad y_1 = z_2\}. \tag{65}$$

The detailed derivation of these spaces is given in Ref. 1. One mathematical implication of open string mirror symmetry is that the geometry of $(\hat{X}, C)$ should determine the genus 0 open Gromov-Witten invariants of (X, L). This means that there should be functions defined on the moduli space $(\hat{\mathcal{X}}, \mathcal{C})$ which count holomorphic maps $f: D = \{z \in \mathbb{C} : |z| \leqslant 1\} \to X$ such that $f(\partial D) \subset L$. Furthermore, in many cases such functions can be derived from an open string Picard-Fuchs system on $(\hat{X}, C)$. However, for the case at hand, it will be shown that the same sort of modification of the PF system, proposed for ordinary closed mirror symmetry, is also necessary in the open string setting.

We turn to the PF system on the moduli spaces $(\hat{\mathcal{X}}, \mathcal{C})$ and $(\hat{\mathcal{X}}, \mathcal{C}')$.

From Ref. 6, we can define "open period integrals" on $(\hat{\mathcal{X}}, \mathcal{C})$ by

$$\Pi_\Gamma(z_1, z_2) = \int_\Gamma \frac{du\, dv\, dy_1\, dy_2/(y_1 y_2)}{(uv + 1 + y_1 + y_2 + z_1 y_1 y_2^{-1})(y_1 - z_2 y_2)(y_1 - 1)}, \tag{66}$$

$\Gamma \in H_4(\mathbb{C}^2 \times (\mathbb{C}^*)^2 - \hat{X}, \hat{X} - C, \mathbb{Z})$. Then the derivations in Ref. 6 lead to a Picard-Fuchs system for $(\hat{\mathcal{X}}, \mathcal{C})$, given as

$$\begin{aligned} \mathcal{D}_1 &= \theta_1(\theta_1 + \theta_2) - z_1 \theta_1(\theta_1 + \theta_2), \\ \mathcal{D}_2 &= \theta_2(\theta_1 + \theta_2) - z_2 \theta_2(\theta_1 + \theta_2), \end{aligned} \tag{67}$$

$\theta_i = z_i(d/dz_i)$. These operators satisfy $\mathcal{D}_i \Pi_\Gamma(z_1, z_2) = 0$. This is exactly the noncompact PF system of the vectors $l^1 = (1, 1, -1, -1, 0, 0)$, $l^2 = (0, 1, 0, -1, 1, -1)$, and agrees with the results of Ref. 14.

As was shown in Ref. 3, the solution space of $\{\mathcal{D}_1, \mathcal{D}_2\}$ can be obtained, using the Frobenius method, from a function $\omega_0(z, \rho) = \Sigma_{n \geqslant 0} c(n, \rho) z_1^{n_1 + \rho_1} z_2^{n_2 + \rho_2}$, where $c(n, \rho)$ is

$$\begin{aligned} &\Gamma(1 + n_1 + \rho_1)\Gamma(1 + n_1 + \rho_1 + n_2 + \rho_2)\Gamma(1 - n_1 - \rho_1)\Gamma(1 - n_1 - \rho_1 - n_2 - \rho_2)\Gamma(1 + n_2 + \rho_2) \\ &\times \Gamma(1 - n_2 - \rho_2). \end{aligned} \tag{68}$$

According to Ref. 15, the solutions are expected to be $(1, t_1, t_2, W_1, W_2, \ldots)$. t_1 and t_2 give the open string mirror map, and this is trivial for the present example, so we have $t_i(z) = \log(z_i)$. Also, the W_i count disks on (X, L).

Upon looking at the equations of (X, L), we can make the following geometric observation about a map $f: D \to X$ with $f(\partial D) \subset L$. In the region where $w_3 = w_4 = 0$, L will intersect the $\mathbb{P}^1$ of X; hence, such an f must obey $f(D) \subset \mathbb{P}^1$. Then the natural interpretation of the variable z_2 is as a parameter controlling the size of a holomorphic disk $f(D)$ in X. It is therefore expected that one of the double-logarithmic solutions of (67) will look like

$$W_1(z_2) = \sum_{n > 0} \frac{z_2^n}{n^2}, \tag{69}$$

where the log terms have been disregarded due to ambiguity.[1] And indeed, it is the case that $W_1(z_2) = (\partial_{\rho_2}^2 \omega_0)|_{\rho = 0}$. The problem, though, is that $(\partial_{\rho_2}^2 \omega_0)|_{\rho = 0}$ is not a solution of (67). The easiest way to see this is to note that W_1 is independent of z_1, and (67) reduces to $\mathcal{D}_2 = (1 - z_2)\theta_2^2$ if $z_1 = 0$. The minimal resolution of this issue, which continues in the spirit of extended operators, is to instead work with the system

$$\{\mathcal{D}_1, \theta_2 \mathcal{D}_2\}. \tag{70}$$

W_1 is indeed a solution of these higher order operators.

Similarly, we can perform calculations on the family $(\hat{X}, C')$. This moduli space is given by vectors $k^1 = l^1$, $k^2 = (0, 0, 1, -1, 1, -1)$, and the open string PF system we arrive at is

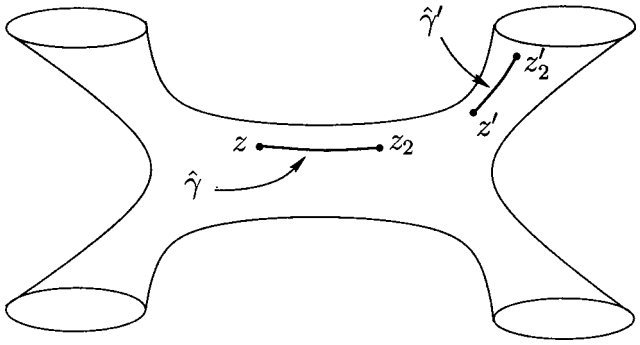

FIG. 5. Real curves defining open string periods on Σ.

$$\mathcal{D}_1' = \theta_1^2 - z_1(\theta_1 - \theta_2)(\theta_1 + \theta_2),$$
$$\mathcal{D}_2' = (\theta_2 - \theta_1)\theta_2 - z_2(\theta_1 + \theta_2)\theta_2. \tag{71}$$

Again, analogously to the above, let ω_0' be the generator of solutions of $\{\mathcal{D}_1', \mathcal{D}_2'\}$. Then there is a disc counting function

$$\partial_{\rho_2}^2 \omega_{0\rho=0}' = W'(z_1, z_2) = \sum_{n_2 > n_1 \geqslant 0} \frac{(-1)^{n_1}(n_1 + n_2 - 1)!}{(n_1\,!)^2(n_2 - n_1)\,!\,n_2} z_1^{n_1} z_2^{n_2} \tag{72}$$

which agrees with the result of Ref. 1. Yet, once again we have the problem of this not being a solution of the given PF system, the same modification gives the system $\{\mathcal{D}_1', \theta_2\mathcal{D}_2'\}$. W' is now among the solutions of this.

Next, we will give an open string period integral definition for these degenerate situations. For motivation, let us review some geometric facts about $(\hat{\mathcal{X}}, \mathcal{C})$. Let y be a local coordinate on Σ. Then following Ref. 1, we can think of the curve C as

$$C_{z_1,z_2} = \hat{X}_{z_1} \cap \{v = 0, y = z_2\} = \mathbb{C} \times \{z_2 \in \Sigma\}.$$

Then the coordinate on $C \cong \mathbb{C}$ is u, and z_2 parametrizes a family of curves in Σ.

Earlier, it was noted that the problem of period integrals was reducible to that of integrals on Σ. Here it is beneficial to make the same simplification. Notice that, when projected to Σ, the family of curves $\{C_{z_1,y} | y \in [z, z_2]\}$ becomes a real curve connecting z to z_2. Hence, the sensible extension of Definition 1 to open strings is the following.

Definition 3: Let $\hat{X}$, Σ be as given in Definition 1, and C as above. Choose z, $z_2 \in \Sigma$ and $\hat{\gamma} \in H_1(\Sigma, \{z, z_2\}, \mathbb{Z})$. Then the open period integrals of $(\hat{\mathcal{X}}, \mathcal{C})$ are defined to be

$$W(z_1, z_2) = \int_{\hat{\gamma}} \mathrm{Res}_{f=0}\left(\frac{dy_1\, dy_2/(y_1 y_2)}{f(z_1, y_1, y_2)} \right).$$

For the purposes of the definition, z is considered to be fixed on Σ, and z_2 is taken as a parameter. In the local $\mathbb{P}^1$ example, the relevant curves $\hat{\gamma}$ are shown in Fig. 5. Note that these are smooth real curves, so that, e.g., $\hat{\gamma}:[0,1] \to \Sigma$ is smooth and such that $\hat{\gamma}(0) = z$, $\hat{\gamma}(1) = z_2$, and similarly for $\hat{\gamma}'$. In Fig. 5, we have abused notation and set $\hat{\gamma} = \hat{\gamma}[0,1]$.

We now move on to the evaluation of these, and show agreement with the solutions of the proposed extended open string PF system of the last section. There are two integrals associated to the curves of the figure, and their calculation proceeds as follows:

$$W(z_1,z_2)=\int_{\hat{\gamma}}\log y_1\frac{dy_2}{y_2}=\int_z^{z_2}\log\left(\frac{-1-y_2}{1+z_1y_2^{-1}}\right)\frac{dy_2}{y_2}=\sum_{n>0}\frac{(-z_2)^n}{n^2}-\sum_{n>0}\frac{(-z_2^{-1}z_1)^n}{n^2}.$$

We also find

$$W'(z_1,z_2)=\int_{\hat{\gamma}'}\log y_2\frac{dy_1}{y_1}=\int_z^{z_2}\log\left(\frac{-1-y_1-\sqrt{(1+y_1)^2-4z_1y_1}}{2}\right)\frac{dy_1}{y_1}.$$

This integral is more difficult to directly evaluate, but as in Ref. 1 we can simply note that

$$z_2\frac{d}{dz_2}W'=\log\left(\frac{-1-z_2-\sqrt{(1+z_2)^2-4z_1z_2}}{2}\right).$$

After Taylor expanding about $z_1=0$ and integrating the result in z_2, this matches (72).

VI. MORE GENERAL LOCAL GEOMETRIES

We have come a long way toward a more complete picture of the differential equations governing local mirror symmetry. However, we have yet to test these ideas in the domain of applicability of Ref. 3; namely, local Calabi-Yau manifolds K_S, where S is a Fano surface and K_S is its canonical bundle. The system of differential operators as given in Ref. 3 is not complete unless

$$\dim H_2(S)=\dim H_4(S). \tag{73}$$

Notice the only surface S satisfying this condition is $\mathbb{P}^2$. We should give some explanation as to what we mean by complete. Assume that there exists a physical definition for a prepotential $\mathcal{F}$ for K_S. Then a double-logarithmic solution W of the Picard-Fuchs system on K_S will satisfy $W=\Sigma_i a_i^W\partial\mathcal{F}/\partial t_i$ for some rational numbers a_i^W, where t_i are logarithmic solutions of the system. Then we cannot integrate the functions W to a single prepotential $\mathcal{F}$ unless there are $\dim H_2(S)$ double-logarithmic solutions; since the set of independent double-logarithmic solutions has the same cardinality as $\dim H_4(S)$, we see that the condition (73) is required. We will now test our techniques on such cases.

A. One one-parameter example

The simplest, though rather trivial, example is $K_{\mathbb{P}^2}=\mathcal{O}(-3)\to\mathbb{P}^2$. This can be defined as a symplectic quotient,

$$K_{\mathbb{P}^2}=\{(w_1,\ldots,w_4)\in\mathbb{C}^4-Z:|w_1|^2+|w_2|^2+|w_3|^2-3|w_4|^2=r\}/S^1,$$

where $Z=\{w_1=w_2=w_3=0\}$, $r\in\mathbb{R}^+$ and the S^1 action is given as $(w_1,\ldots,w_4)\to(e^{i\theta}w_1,e^{i\theta}w_2,e^{i\theta}w_3,e^{-3i\theta}w_4)$. The original paper[3] associates a Picard-Fuchs system here, which is ultimately derivable from the period integrals of the mirror

$$\hat{X}_z=\{(u,v,y_1,y_2)\in\mathbb{C}^2\times(\mathbb{C}^*)^2:uv+1+y_1+y_2+zy_1^{-1}y_2^{-1}=0\}.$$

Again, from Ref. 10,

$$\Pi_\Gamma(z)=\int_\Gamma\frac{du\,dv\,dy_1\,dy_2/(y_1y_2)}{uv+1+y_1+y_2+zy_1^{-1}y_2^{-1}}$$

for $\Gamma\in H_4(\mathbb{C}^2\times(\mathbb{C}^*)^2-\hat{X},\mathbb{Z})$ are the period integrals. Then we immediately recover the well-known PF operator

$$\mathcal{D} = \theta^3 + z(3\theta)(3\theta+1)(3\theta+2), \quad \theta = z\frac{d}{dz},$$

whose solution space is generated by a function $\omega_0(z,\rho)=\Sigma_{n\geqslant 0}c(n,\rho)z^{n+\rho}$. Here, the coefficients can be written $c(n,\rho)^{-1}=\Gamma(1-3n-3\rho)\Gamma(1+n+\rho)^3$. If we write the solutions in the variable $t=\partial_\rho\omega_0|_{\rho=0}$, we get $\Pi=(1,t,\partial\mathcal{F}/\partial t)$. Naturally, this implies that in the t variable, it must be the case that

$$\mathcal{D} = \partial_t\left(\frac{\partial^3\mathcal{F}}{\partial t^3}\right)^{-1}\partial_t^2.$$

Then, we can again give a compactified operator $\partial_t\mathcal{D}$ which possesses a completed set of solutions, i.e., the solution space can be written as

$$\left(1, t, \frac{\partial\mathcal{F}}{\partial t}, 2\mathcal{F} - t\frac{\partial\mathcal{F}}{\partial t}\right). \tag{74}$$

It is actually equivalent to just work with

$$\theta\mathcal{D} = \theta(\theta^3 + z(3\theta)(3\theta+1)(3\theta+2))$$

on account of the invertibility of the Jacobian. This is our extended PF operator.

B. Completing mirror symmetry for Hirzebruch surfaces

One parameter spaces of type K_S have already been exhausted, by the $K_{\mathbb{P}^2}$ case. We will now turn to the two-parameter spaces, namely the canonical bundle over the Hirzebruch surfaces F_0, F_1, F_2. As is well known,[3] the instanton part of the double-log arithmic solution of the standard PF system is given by a linear combination of the $\partial\mathcal{F}_{\text{inst}}/\partial t_a$. This fact tells us that the standard PF system of K_S already includes the information coming from $Y_a^{-1}(t_*)$ in (6). Therefore, we can take a short cut in the process of constructing an extended PF system on K_S. Examples of this explicit construction will be given in the next section.

The symplectic quotient description is given by

$$K_{F_n} = \{-2|w_1|^2 + |w_2|^2 + |w_3|^2 = r_1^n,\ (-2+n)|w_1|^2 - n|w_2| + |w_4|^2 + |w_5|^2 = r_2^n\}/(S^1)^2$$

where $(w_1,\ldots,w_5)\in\mathbb{C}^5 - Z_n$. That is, the vectors in the secondary fan are

$$\begin{pmatrix} l_n^1 \\ l_n^2 \end{pmatrix} = \begin{pmatrix} -2 & 1 & 1 & 0 & 0 \\ -2+n & -n & 0 & 1 & 1 \end{pmatrix}.$$

The methods of Ref. 3 lead to PF operators, K_{F_0},

$$\mathcal{D}_1^0 = \theta_1^2 - z_1(2\theta_1+2\theta_2)(2\theta_1+2\theta_2+1),$$

$$\mathcal{D}_2^0 = \theta_2^2 - z_2(2\theta_1+2\theta_2)(2\theta_1+2\theta_2+1);$$

K_{F_1},

$$\mathcal{D}_1^1 = \theta_1(\theta_1-\theta_2) - z_1(2\theta_1+\theta_2)(2\theta_1+\theta_2+1),$$

$$\mathcal{D}_2^1 = \theta_2^2 - z_2(2\theta_1+\theta_2)(\theta_1-\theta_2);$$

K_{F_2},

$$\mathcal{D}_1^2 = \theta_1(\theta_1-2\theta_2) - z_1 2\theta_1(2\theta_1+1),$$

$$\mathcal{D}_2^2 = \theta_2^2 - z_2(2\theta_2 - \theta_1)(2\theta_2 - \theta_1 + 1).$$

For each respective system, we let t_1^n, t_2^n be the logarithmic solutions. Each case comes equipped with a single double-logarithmic solution W_n. If ω^n is the generating function of solutions on K_{F_n} and $\Pi_{ij}^n = \partial_{\rho_i}\partial_{\rho_j}\omega^n|_{\rho=0}$, then we can write these as

$$W_0 = \Pi_{12}^0, \quad W_1 = \Pi_{11}^1 + 2\Pi_{12}^1, \quad W_2 = \Pi_{11}^2 + \Pi_{12}^2.$$

Taking $\mathcal{F}_n$ for the prepotential on K_{F_n}, we have the following equalities:

$$W_n = 2\frac{\partial \mathcal{F}_n}{\partial t_1^n} + (2-n)\frac{\partial \mathcal{F}_n}{\partial t_2^n}.$$

By a comparison of power series, we can demonstrate that the Π_{ij}^n contain all the information necessary to derive the (instanton part of) the prepotential on K_{F_n}. We find

$$\begin{pmatrix} \Pi_{11}^n \\ \Pi_{12}^n \end{pmatrix} = \begin{pmatrix} 0 & 4 \\ 2 & -3n+2 \end{pmatrix} \begin{pmatrix} \partial \mathcal{F}_n/\partial t_1^n \\ \partial \mathcal{F}_n/\partial t_2^n \end{pmatrix}. \tag{75}$$

The equality above holds at the level of instanton parts of $\mathcal{F}_n$. We will now investigate the classical terms of these prepotentials.

First, we give here the discriminant locus of K_{F_n} where the corresponding mirror hypersurface $\hat{K}_{F_n}$ becomes singular,

$$\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_0}) = 1 - 8(z_1 + z_2) + 16(z_1 - z_2)^2, \tag{76}$$

$$\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_1}) = (1 - 4z_1)^2 - z_2 + 36z_1z_2 - 27z_1z_2^2, \tag{77}$$

$$\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_2}) = (1 - 4z_1)^2 - 64z_1^2z_2. \tag{78}$$

In the K_{F_2} case, there is another component of the discriminant locus defined by $1-4z_2$; we note that this appears in the B-model Yukawa couplings. With these results, Naka determined the B-model Yukawa couplings of K_{F_n} with respect to $u=\log(z_1)$, $v=\log(z_2)$ variables by assuming compatibility with the instanton expansion given by the double-logarithmic solution, and that they should be written in terms of simple rational functions multiplied by $1/\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_n})$,[12] $n=0$,

$$Y_{uuu} = \frac{-4z_1^2 + 4z_2^2 - 4z_1 - 2z_2 + \frac{1}{4}}{\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_0})}, \quad Y_{uuv} = \frac{4z_1^2 - 4z_2^2 + 2z_2 - \frac{1}{4}}{\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_0})},$$

$$Y_{uvv} = \frac{-4z_1^2 + 4z_2^2 + 2z_1 - \frac{1}{4}}{\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_0})}, \quad Y_{vvv} = \frac{4z_1^2 - 4z_2^2 - 2z_1 - 4z_2 + \frac{1}{4}}{\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_0})};$$

$n=1$,

$$Y_{uuu} = -\frac{((-162x+9)z_1z_2^2 + (96x-4)z_1^2 + (216x-14)z_1z_2 + (5-48x)z_1 - 6x(z_2-1))}{\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_1})},$$

$$Y_{uuv} = -\frac{((324x-18)z_1z_2^2 + (8-192x)z_1^2 + (25-432x)z_1z_2 + (96x-6)z_1 + (12x-1)(z_2-1))}{\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_1})},$$

$$Y_{uvv} = -\frac{((36-648x)z_1z_2^2+(384x-16)z_1^2+(864x-44)z_1z_2+(8-192x)z_1-(24x-1)(z_2-1))}{\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_1})},$$

$$Y_{vvv} = -\frac{((1296x-72)z_1z_2^2+(32-768x)z_1^2+(76-1728x)z_1z_2+(384x-16)z_1+(48x-2)(z_2-1)-z_2)}{\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_1})},$$

$n=2$,

$$Y_{uuu} = \frac{-1}{\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_2})}, \quad Y_{uuv} = \frac{2z_1-\frac{1}{2}}{\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_2})},$$

$$Y_{uvv} = \frac{-z_2(8z_1-1)}{\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_2})(1-4z_2)}, \quad Y_{vvv} = \frac{-z_2\left(24z_1z_2+2z_1-2z_2-\frac{1}{2}\right)}{\mathrm{dis}(\hat{\mathbf{K}}_{\mathbf{F}_2})(1-4z_2)^2}. \tag{79}$$

In the $n=1$ case, there exists a moduli parameter x that leaves the instanton part of Y_{ijk} invariant. (In the $n=0$ case, we also have one moduli parameter if we do not assume symmetry between u and v.) In other words, we cannot determine the value of x from the compatibility of the instanton numbers. The aim of this section is to give a derivation of these Yukawa couplings by using an extended set of Picard-Fuchs operators of local F_n as the starting point. First, we notice that (79) tells us of the existence of a natural classical triple intersection theory on K_{F_n} compatible with the instanton expansion, $n=0$,

$$\langle k_uk_uk_u\rangle = \tfrac{1}{4}, \quad \langle k_uk_uk_v\rangle = -\tfrac{1}{4}, \quad \langle k_uk_vk_v\rangle = -\tfrac{1}{4}, \quad \langle k_vk_vk_v\rangle = \tfrac{1}{4};$$

$n=1$,

$$\langle k_uk_uk_u\rangle = -6x, \quad \langle k_uk_uk_v\rangle = -1+12x, \quad \langle k_uk_vk_v\rangle = -24x+1, \quad \langle k_vk_vk_v\rangle = -2+48x;$$

$n=2$,

$$\langle k_uk_uk_u\rangle = -1, \quad \langle k_uk_uk_v\rangle = -\tfrac{1}{2}, \quad \langle k_uk_vk_v\rangle = 0, \quad \langle k_vk_vk_v\rangle = 0. \tag{80}$$

In (80), we denote the classical triple intersection numbers of Kähler forms k_u, k_v by $\langle k_uk_uk_u\rangle$, etc. Therefore, we must reproduce (80) from the information obtained from some extended PF system. The key idea of constructing such an extended system becomes more clear upon looking at the triple log series obtained from the generating hypergeometric series of the solution of the PF system,

$$w(u,v,r_1,r_2) := \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{1}{\prod_{j=0}^{4}\Gamma(1+l_j^1(m+r_1)+l_j^2(n+r_2))}\exp((m+r_1)u+(n+r_2)v). \tag{81}$$

It is well known that $w(u,v,r_1,r_2)|_{(r1,r2)=(0,0)}=1$ is the trivial solution of the PF system, and that the log arithmic solutions $\partial_{r_i}w(u,v,r_1,r_2)|_{(r1,r2)=(0,0)}$ gives us the mirror map t^i. Then we consider the relation between the triple log series $W_{ijk}(u,v) := \partial_{r_i}\partial_{r_j}\partial_{r_k}w(u,v,r_1,r_2)|_{(r1,r2)=(0,0)}$ and the prepotential $\mathcal{F}(t^1,t^2)$ of K_{F_n}. Surprisingly, the classical intersection number (80) is determined from the following assumption:

$$\frac{1}{6}\langle k_u k_u k_u\rangle \cdot W_{111}(u(t_*),v(t_*)) + \frac{1}{2}\langle k_u k_u k_v\rangle \cdot W_{112}(u(t_*),v(t_*)) + \frac{1}{2}\langle k_u k_v k_v\rangle \cdot W_{122}(u(t_*),v(t_*))$$

$$+ \frac{1}{6}\langle k_v k_v k_v\rangle \cdot W_{222}(u(t_*),v(t_*)) = t_1\frac{\partial \mathcal{F}(t_*)}{\partial t_1} + t_2\frac{\partial \mathcal{F}(t_*)}{\partial t_2} - 2\mathcal{F}(t_*), \tag{82}$$

that holds in mirror symmetry of compact Calabi-Yau threefolds if we look at the logarithmic part of the triple log functions. In the $n=0$, 2 cases, we can determine classical intersection number (80) uniquely from the instanton expansion of the right-hand side of (82), but in the $n=1$ case, we have one moduli parameter x that leaves the instanton expansion invariant. Therefore, this situation is the same as in Naka's result. With these intersection numbers, we can construct the set of relations of the classical cohomology ring of K_{F_n} in the sense of Sec. II as follows:
$n=0$,

$$k_u^2 + k_v^2 = 0, \quad k_u k_v^2 - k_u^2 k_v = 0;$$

$n=1$,

$$(24x-1)(k_u^2 - k_u k_v) - (18x-1)k_v^2 = 0, \quad 2k_u k_v^2 + k_v^3 = 0 \quad \left(x \neq \tfrac{1}{24}\right),$$

$$k_v^2 = 0, \quad 2k_u^3 - k_u^2 k_v = 0 \quad \left(x = \tfrac{1}{24}\right);$$

$n=2$,

$$k_v^2 = 0, \quad k_u^3 - 2k_u^2 k_v = 0. \tag{83}$$

With this set up, we can construct an extended Picard-Fuchs system of K_{F_n} that has the same principle part as (83), and is constructed from the linear combination of $\mathcal{D}_i$, $\theta_1\mathcal{D}_i$, $\theta_2\mathcal{D}_i$ ($i=1, 2$), $n=0$,

$$\tilde{\mathcal{D}}_1^0 = \mathcal{D}_1^0 + \mathcal{D}_2^0, \quad \tilde{\mathcal{D}}_2^0 = \theta_1\mathcal{D}_2^0 - \theta_2\mathcal{D}_1^0;$$

$n=1$,

$$\tilde{\mathcal{D}}_1^1 = (24x-1)\mathcal{D}_1^1 - (18x-1)\mathcal{D}_2^1, \quad \tilde{\mathcal{D}}_2^1 = (2\theta_1+\theta_2)\tilde{\mathcal{D}}_2^1 \quad \left(x \neq \tfrac{1}{24}\right),$$

$$\tilde{\mathcal{D}}_1^1 = \mathcal{D}_2^1, \quad \tilde{\mathcal{D}}_2^1 = (2\theta_1+\theta_2)\mathcal{D}_1^1 \quad \left(x = \tfrac{1}{24}\right),$$

$n=2$,

$$\tilde{\mathcal{D}}_1^2 = \mathcal{D}_2^2, \quad \tilde{\mathcal{D}}_2^2 = \theta_1\mathcal{D}_1^2. \tag{84}$$

In the remaining part of this section, we briefly discuss the derivation of the Yukawa coupling of F_0 in (79) by using (84) as the starting point. The other cases can be done in exactly the same way as in this computation. First, we use the standard definition of the B-model Yukawa coupling of mirror symmetry for a compact Calabi-Yau threefold,

$$Y_{ijk} = \int_M \Omega \wedge \partial_i\partial_j\partial_k\Omega. \tag{85}$$

In the case of K_{F_n}, the existence of M and of a global holomomorphic three form Ω are not guaranteed, but we proceed here by assuming the existence of such an M and Ω. We also apply the standard results obtained from Kodaira-Spencer theory on a compact Calabi-Yau threefold to the computation on M. It is easy to show the following formula by application of this machinery:

$$\int_M \Omega \wedge \partial_i\partial_j\partial_k\partial_l\Omega = \frac{1}{2}(\partial_i Y_{jkl} + \partial_j Y_{ikl} + \partial_k Y_{ijl} + \partial_l Y_{ijk}). \tag{86}$$

Next, we derive two relations among different Yukawa couplings obtained from $\theta_1(\mathcal{D}_1^0+\mathcal{D}_2^0)\Omega = \theta_2(\mathcal{D}_1^0+\mathcal{D}_2^0)\Omega=0$,

$$\begin{aligned} Y_{uuu} + Y_{uvv} - 4(z_1+z_2)(Y_{uuu} + 2Y_{uuv} + Y_{uvv}) = 0, \\ Y_{uuv} + Y_{vvv} - 4(z_1+z_2)(Y_{uuv} + 2Y_{uvv} + Y_{vvv}) = 0. \end{aligned} \tag{87}$$

We can also derive another relation from $(\theta_1\mathcal{D}_2^0 - \theta_2\mathcal{D}_1^0)\Omega=0$,

$$Y_{uuv} - 4z_1(Y_{uuv} + 2Y_{uvv} + Y_{vvv}) = Y_{uvv} - 4z_2(Y_{uuu} + 2Y_{uuv} + Y_{uvv}). \tag{88}$$

Since (87) and (88) are linear relations, we can easily solve them and obtain

$$\begin{aligned} Y_{uuu} &= (1 - 16z_1 - 8z_2 - 16z_1^2 + 16z_2^2)S(u,v), \\ Y_{uuv} &= (-1 + 8z_2 + 16z_1^2 - 16z_2^2)S(u,v), \\ Y_{uuv} &= (-1 + 8z_1 + 16z_2^2 - 16z_1^2)S(u,v), \\ Y_{vvv} &= (1 - 16z_2 - 8z_1 - 16z_2^2 + 16z_1^2)S(u,v). \end{aligned} \tag{89}$$

where $S(u,v)$ is an unknown function at this stage. Then we can derive differential equations of $S(u,v)$ from the relations $((\theta_1)^2-(\theta_2)^2)\mathcal{D}_2^0\Omega=((\theta_1)^2-(\theta_2)^2)\mathcal{D}_1^0\Omega=0$ and (86) by substituting the right-handside (rhs) of (89). These operations result in the following differential equations of $S(u,v)$:

$$\begin{aligned} \frac{\partial_u S(u,v)}{S(u,v)} &= \frac{8z_1 - 32z_1^2 + 32z_1z_2}{1 - 8z_1 - 8z_2 + 16z_1^2 - 32z_1z_2 + 16z_2^2}, \\ \frac{\partial_v S(u,v)}{S(u,v)} &= \frac{8z_2 - 32z_2^2 + 32z_1z_2}{1 - 8z_1 - 8z_2 + 16z_1^2 - 32z_1z_2 + 16z_2^2}. \end{aligned} \tag{90}$$

We can immediately solve the above equations and obtain

$$S(u,v) = (\text{const})\frac{1}{1 - 8z_1 - 8z_2 + 16z_1^2 - 32z_1z_2 + 16z_2^2}. \tag{91}$$

Finally, the classical intersection numbers in (80) tell us that $(\text{const})=\frac{1}{4}$.

VII. THE DEL PEZZO SURFACE K_{dP_2}

We can also look to a three-parameter model, in order to determine what we might expect in more general situations (Fig. 6). The examples of the two-parameter case might cause one to hope that, for every local geometry of the form K_S, we can extend the original PF system to give a complete description of mirror symmetry from the B-model geometry alone. Here we will demonstrate that this is indeed the case for K_{dP_2}. However, it is no longer necessary to use a higher order system for three and higher parameter cases; we can find a complete set of solutions by "forgetting" about some of the originally proposed local mirror symmetry operators.

The symplectic quotient description of K_{dP_2} may be written as

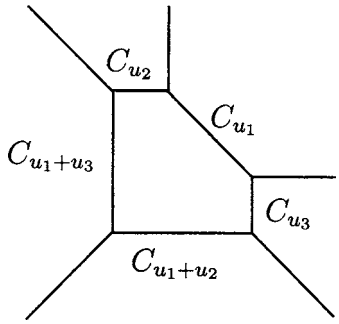

FIG. 6. The del Pezzo dP_2. Each curve C_{u_i} corresponds to a vector l^i.

$$\left\{(w_1,\ldots,w_6)\in\mathbb{C}^6-Z:\sum_{k=1}^{6} l_k^i|w_k|^2=r_i\,,i=1,2,3\right\}/(S^1)^3$$

with the vectors

$$\begin{pmatrix} l^1 \\ l^2 \\ l^3 \end{pmatrix} = \begin{pmatrix} -1 & 1 & -1 & 1 & 0 & 0 \\ -1 & -1 & 1 & 0 & 0 & 1 \\ -1 & 0 & 1 & -1 & 1 & 0 \end{pmatrix}.$$

Note that $b_2=3$ and $b_4=1$. This comes with PF operators

$$\begin{aligned}
\mathcal{D}_1 &= (\theta_1-\theta_2)(\theta_1-\theta_3)-z_1(\theta_1+\theta_2+\theta_3)(\theta_1-\theta_2-\theta_3),\\
\mathcal{D}_2 &= (\theta_2+\theta_3-\theta_1)\theta_2-z_2(\theta_1+\theta_2+\theta_3)(\theta_2-\theta_1),\\
\mathcal{D}_3 &= (\theta_2+\theta_3-\theta_1)\theta_3-z_3(\theta_1+\theta_2+\theta_3)(\theta_3-\theta_1),\\
\mathcal{D}_4 &= \theta_2(\theta_1-\theta_3)-z_1z_2(\theta_1+\theta_2+\theta_3+1)(\theta_1+\theta_2+\theta_3),\\
\mathcal{D}_5 &= \theta_3(\theta_1-\theta_2)-z_1z_3(\theta_1+\theta_2+\theta_3+1)(\theta_1+\theta_2+\theta_3).
\end{aligned} \tag{92}$$

Let $\mathcal{F}$, t_1, t_2, t_3 and the Π_{ij}'s be as before. Then Ref. 3 provides a single double-logarithmic solution W, corresponding to the 4 cycle in the base of the A-model geometry, which satisfies

$$W=\Pi_{11}+\Pi_{12}+\Pi_{13}+\Pi_{23}=\frac{\partial\mathcal{F}}{\partial t_1}+\frac{\partial\mathcal{F}}{\partial t_2}+\frac{\partial\mathcal{F}}{\partial t_3}.$$

The naive approach in this case suggests that we need to add two 4 cycles to the A-model geometry. Using as motivation the notion that each double-logarithmic solution of the system should correspond to a 4 cycle on the mirror, we are led to work with a system consisting of three of the original five PF differential operators. For reasons to be discussed shortly, we will use the set

$$\begin{aligned}
\tilde{\mathcal{D}}_1 &= (6x+2y-1)(\mathcal{D}_1-\mathcal{D}_2-\mathcal{D}_3)-x(\mathcal{D}_2+\mathcal{D}_3),\\
\tilde{\mathcal{D}}_2 &= (5x+y-1)(\mathcal{D}_2+\mathcal{D}_3+\mathcal{D}_4+\mathcal{D}_5)+(x+y)(\mathcal{D}_4+\mathcal{D}_5),
\end{aligned} \tag{93}$$

$$\widetilde{\mathcal{D}}_3 = (x-y-1)(\mathcal{D}_2 - \mathcal{D}_3 + \mathcal{D}_4 - \mathcal{D}_5) + (x-y)(\mathcal{D}_4 - \mathcal{D}_5),$$

where x and y are real free parameters. If we set $(x,y)=(0,0)$, we can easily show that a basis of the solution space with double-logarithmic singularities is three dimensional, and is provided by

$$\Pi_{12} = \frac{\partial \mathcal{F}}{\partial t_2}, \quad \Pi_{13} = \frac{\partial \mathcal{F}}{\partial t_3}, \quad \Pi_{11} + \Pi_{23} = \frac{\partial \mathcal{F}}{\partial t_1}. \tag{94}$$

Hence, we can recover the full prepotential from solutions of the PF system alone. We expect that this phenomenon will continue to hold true in all cases of the type K_S.

The extended PF system of K_{dP_2} (93) is derived in the same way as K_{F_n}. Let us introduce the logarithm of the standard B-model coordinates z_i,

$$u_1 = \log(z_1), \quad u_2 = \log(z_2), \quad u_3 = \log(z_3), \tag{95}$$

and consider the generating function of solutions of the PF system (92),

$$w(u_1,u_2,u_3,r_1,r_2,r_3) := \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{n_3=0}^{\infty} \frac{1}{\prod_{j=0}^{5}\Gamma(1+l_j^1(n_1+r_1)+l_j^2(n_2+r_2)+l_j^3(n_3+r_3))} \times \exp((n_1+r_1)u_1+(n_2+r_2)u_2+(n_3+r_3)u_3). \tag{96}$$

The mirror map of K_{dP_2} is given by

$$t_i(u_*) := \partial_{r_i} w(u_1,u_2,u_3,r_1,r_2,r_3)_{r_i=0}. \tag{97}$$

From the triple-logarithmic function

$$W_{ijk}(u_1,u_2,u_3) := \partial_{r_i}\partial_{r_2}\partial_{r_3} w(u_1,u_2,u_3,r_1,r_2,r_3)_{r_i=0}, \tag{98}$$

obtained from (96), we can find the classical triple intersection number $\langle k_{u_i}k_{u_j}k_{u_m}\rangle$ of Kähler forms k_{u_i} by assuming the following relation:

$$\begin{aligned}
&\frac{1}{6}\langle k_{u_1}k_{u_1}k_{u_1}\rangle W_{111}(u_1(t_*),u_2(t_*),u_3(t_*)) + \frac{1}{6}\langle k_{u_2}k_{u_2}k_{u_2}\rangle W_{222}(u_1(t_*),u_2(t_*),u_3(t_*)) \\
&\quad + \frac{1}{6}\langle k_{u_3}k_{u_3}k_{u_3}\rangle W_{333}(u_1(t_*),u_2(t_*),u_3(t_*)) + \frac{1}{2}\langle k_{u_1}k_{u_1}k_{u_2}\rangle W_{112}(u_1(t_*),u_2(t_*),u_3(t_*)) \\
&\quad + \frac{1}{2}\langle k_{u_1}k_{u_2}k_{u_2}\rangle W_{122}(u_1(t_*),u_2(t_*),u_3(t_*)) + \frac{1}{2}\langle k_{u_2}k_{u_2}k_{u_3}\rangle W_{223}(u_1(t_*),u_2(t_*),u_3(t_*)) \\
&\quad + \frac{1}{2}\langle k_{u_2}k_{u_3}k_{u_3}\rangle W_{233}(u_1(t_*),u_2(t_*),u_3(t_*)) + \frac{1}{2}\langle k_{u_1}k_{u_1}k_{u_3}\rangle W_{113}(u_1(t_*),u_2(t_*),u_3(t_*)) \\
&\quad + \frac{1}{2}\langle k_{u_1}k_{u_3}k_{u_3}\rangle W_{133}(u_1(t_*),u_2(t_*),u_3(t_*)) + \langle k_{u_1}k_{u_2}k_{u_3}\rangle W_{123}(u_1(t_*),u_2(t_*),u_3(t_*)) \\
&= t_1\frac{\partial \mathcal{F}(t_*)}{\partial t_1} + t_2\frac{\partial \mathcal{F}(t_*)}{\partial t_2} + t_3\frac{\partial \mathcal{F}(t_*)}{\partial t_3} - 2\mathcal{F}(t_*),
\end{aligned} \tag{99}$$

where we used instanton expansion part of $\mathcal{F}(t_1,t_2,t_3)$ read off from the double-logarithmic solution of (92). Taking the symmetry between k_{u_2} and k_{u_3} into account, we found the following classical intersection numbers with two free parameters (in this case, we have four moduli parameters unless we assume symmetry between k_{u_2} and k_{u_3}) x and y:

$$\langle k_{u_1}k_{u_1}k_{u_1}\rangle = -1+6x+2y, \quad \langle k_{u_2}k_{u_2}k_{u_2}\rangle = -y, \quad \langle k_{u_3}k_{u_3}k_{u_3}\rangle = -y, \quad \langle k_{u_1}k_{u_1}k_{u_2}\rangle = -3x-y,$$

$$\langle k_{u_1}k_{u_2}k_{u_2}\rangle = x+y, \quad \langle k_{u_2}k_{u_2}k_{u_3}\rangle = -x, \quad \langle k_{u_2}k_{u_3}k_{u_3}\rangle = -x, \quad \langle k_{u_1}k_{u_1}k_{u_3}\rangle = -3x-y,$$

$$\langle k_{u_1}k_{u_3}k_{u_3}\rangle = x+y, \quad \langle k_{u_1}k_{u_2}k_{u_3}\rangle = -1+2x. \tag{100}$$

With this data, we can construct a complete set of relations of k_{u^i} that reproduce (100) as follows:

$$R_1 = (6x+2y-1)(p_1-p_2-p_3) - x(p_2+p_3),$$

$$R_2 = (5x+y-1)(p_2+p_3+p_4+p_5) + (x+y)(p_4+p_5), \tag{101}$$

$$R_3 = (x-y-1)(p_2-p_3+p_4-p_5) + (x-y)(p_4-p_5),$$

where

$$p_1 = (k_{u_1}-k_{u_2})(k_{u_1}-k_{u_3}), \quad p_2 = k_{u_2}(k_{u_2}+k_{u_3}-k_{u_1}), \quad p_3 = k_{u_3}(k_{u_2}+k_{u_3}-k_{u_1}),$$

$$p_4 = k_{u_2}(k_{u_1}-k_{u_3}), \quad p_5 = k_{u_3}(k_{u_1}-k_{u_2}). \tag{102}$$

The extended PF system (93) is obtained from linear combinations of the $\mathcal{D}_i$'s that reduce to (101) at the large radius limit. Of course, we can compute the B-model Yukawa coupling of K_{dP_2} by using (93) as the starting point in the same way as F_0, and we collect the resulting Yukawa couplings in Appendix B.

VIII. CONCLUSION

Through a variety of examples, we have seen the emergence of a set of differential operators for local mirror symmetry. In this sense, we may view this as a next step towards a complete treatment of the program initiated in Ref. 3. There are, however, some outstanding issues. First, our constructions have taken for granted the instanton expansion from the A model. In principle, we would like to be able to canonically associate an extended Picard-Fuchs system to a B-model geometry without reference to the A model. Second, it would be interesting to exhibit a family of Calabi-Yau manifolds parametrized by a complex structure such that the period integrals agreed with the ones we find as solutions to the extended Picard-Fuchs system. We leave these questions for future work.

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APPENDIX A: AN EXTENDED PICARD-FUCHS SYSTEM FOR X_3

Here, we apply our conjecture on intersection theory for X satisfying $\dim H_4(X,\mathbb{Z})=0$ to a three-parameter example, in order to more fully explore its applicability. We will work with

$$X_3 = \{(w_1,\ldots,w_6) \in \mathbb{C}^6 - Z : \sum_{k=1}^{6} l_k^i |w_k|^2 = r_i, \quad i=1,2,3\}/(S^1)^3$$

where

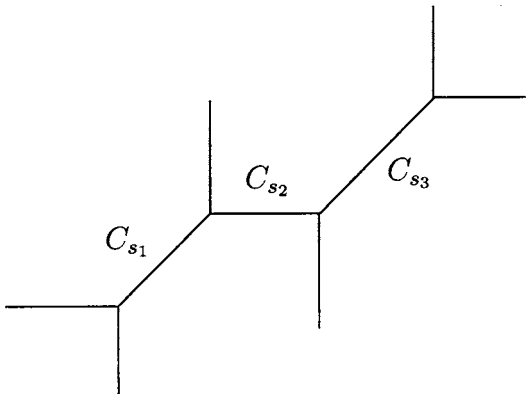

FIG. 7. Toric graph for X_3.

$$\begin{pmatrix} l^1 \\ l^2 \\ l^3 \end{pmatrix} = \begin{pmatrix} 1 & 1 & -1 & -1 & 0 & 0 \\ 0 & -1 & -1 & 1 & 1 & 0 \\ 0 & -1 & 1 & 0 & -1 & 1 \end{pmatrix}. \tag{A1}$$

The toric graph is provided in Fig. 7. Then X_3 has no 4 cycle, and for each curve C_{s_i} corresponding to the secondary fan vector l^i, we have that $\mathcal{N}_{C_{s_i}/X_3} \cong \mathcal{O}(-1) \oplus \mathcal{O}(-1)$.

By making use of the instanton parts given in Ref. 11 and our conjecture, we immediately have the Yukawa couplings.

A-**model Yukawa couplings of** X_3 **(with respect to** s_i**)**,

$$Y_{111} = \frac{1}{2} + \frac{e^{s_1}}{1-e^{s_1}} - \frac{e^{s_1+s_2}}{1-e^{s_1+s_2}} + \frac{e^{s_1+s_2+s_3}}{1-e^{s_1+s_2+s_3}},$$

$$Y_{113} = \frac{1}{2} + \frac{e^{s_1+s_2+s_3}}{1-e^{s_1+s_2+s_3}},$$

$$Y_{113} = \frac{1}{2} + \frac{e^{s_1+s_2+s_3}}{1-e^{s_1+s_2+s_3}},$$

$$Y_{333} = \frac{1}{2} + \frac{e^{s_3}}{1-e^{s_3}} - \frac{e^{s_3+s_2}}{1-e^{s_3+s_2}} + \frac{e^{s_1+s_2+s_3}}{1-e^{s_1+s_2+s_3}},$$

$$Y_{112} = -\frac{e^{s_1+s_2}}{1-e^{s_1+s_2}} + \frac{e^{s_1+s_2+s_3}}{1-e^{s_1+s_2+s_3}},$$

$$Y_{233} = -\frac{e^{s_3+s_2}}{1-e^{s_3+s_2}} + \frac{e^{s_1+s_2+s_3}}{1-e^{s_1+s_2+s_3}},$$

$$Y_{122} = -\frac{e^{s_1+s_2}}{1-e^{s_1+s_2}} + \frac{e^{s_1+s_2+s_3}}{1-e^{s_1+s_2+s_3}},$$

$$Y_{223} = -\frac{e^{s_3+s_2}}{1-e^{s_3+s_2}} + \frac{e^{s_1+s_2+s_3}}{1-e^{s_1+s_2+s_3}},$$

$$Y_{222} = \frac{e^{s_2}}{1-e^{s_2}} - \frac{e^{s_1+s_2}}{1-e^{s_1+s_2}} - \frac{e^{s_3+s_2}}{1-e^{s_3+s_2}} + \frac{e^{s_1+s_2+s_3}}{1-e^{s_1+s_2+s_3}},$$

$$Y_{123} = \frac{1}{2} + \frac{e^{s_1+s_2+s_3}}{1-e^{s_1+s_2+s_3}}, \tag{A2}$$

Once we have these, the rest of the calculations are routine. We list the results here.

Ordinary Picard-Fuchs system of X_3,

$$\begin{aligned}
\mathcal{D}_1 &= \theta_1(\theta_1-\theta_2-\theta_3) - z_1(\theta_1-\theta_2)(\theta_1+\theta_2-\theta_3),\\
\mathcal{D}_2 &= (\theta_2-\theta_1)(\theta_2-\theta_3) - z_2(\theta_2+\theta_3-\theta_1)(\theta_2+\theta_1-\theta_3),\\
\mathcal{D}_3 &= \theta_3(\theta_3-\theta_2-\theta_1) - z_3(\theta_3-\theta_2)(\theta_3+\theta_2-\theta_1),\\
\mathcal{D}_4 &= \theta_1(\theta_1-\theta_3) - z_1z_2(\theta_1+\theta_2-\theta_3+1)(\theta_1+\theta_2-\theta_3),\\
\mathcal{D}_5 &= \theta_1\theta_3 - z_1z_3(\theta_2-\theta_1)(\theta_2-\theta_3),\\
\mathcal{D}_6 &= \theta_3(\theta_3-\theta_1) - z_2z_3(\theta_3+\theta_2-\theta_1+1)(\theta_3+\theta_2-\theta_1).
\end{aligned} \tag{A3}$$

Jacobian of the mirror map,

$$u_1 = \log(z_1), \quad u_2 = \log(z_2), \quad u_3 = \log(z_3),$$

$$\frac{\partial s_1}{\partial u_1} = \frac{1}{2}\frac{-\sqrt{1-4z_1z_2}-1+4z_1z_2}{4z_1z_2-1},$$

$$\frac{\partial s_1}{\partial u_2} = \frac{1}{2}\frac{4z_1z_2\sqrt{1-4z_2z_3}+\sqrt{1-4z_1z_2}-\sqrt{1-4z_2z_3}-4z_2z_3\sqrt{1-4z_1z_2}}{(4z_1z_2-1)(4z_2z_3-1)},$$

$$\frac{\partial s_1}{\partial u_3} = \frac{1}{2}\frac{-1+4z_2z_3+\sqrt{1-4z_2z_3}}{4z_2z_3-1},$$

$$\frac{\partial s_2}{\partial u_1} = -\frac{1}{2}\frac{-1+4z_1z_2+\sqrt{1-4z_1z_2}}{4z_1z_2-1},$$

$$\frac{\partial s_2}{\partial u_2} = -\frac{1}{2}\frac{-\sqrt{1-4z_1z_2}+4z_1z_2\sqrt{1-4z_2z_3}-\sqrt{1-4z_2z_3}+4z_2z_3\sqrt{1-4z_1z_2}}{(4z_1z_2-1)(4z_2z_3-1)},$$

$$\frac{\partial s_2}{\partial u_3} = -\frac{1}{2}\frac{-1+4z_2z_3+\sqrt{1-4z_2z_3}}{4z_2z_3-1},$$

$$\frac{\partial s_3}{\partial u_1} = \frac{1}{2}\frac{-1+4z_1z_2+\sqrt{1-4z_1z_2}}{4z_1z_2-1},$$

$$\frac{\partial s_3}{\partial u_2} = \frac{1}{2}\frac{\sqrt{1-4z_2z_3}+4z_2z_3\sqrt{1-4z_1z_2}-4z_1z_2\sqrt{1-4z_2z_3}-\sqrt{1-4z_1z_2}}{(4z_1z_2-1)(4z_2z_3-1)},$$

$$\frac{\partial s_3}{\partial u_3} = \frac{1}{2}\frac{-\sqrt{1-4z_2z_3}-1+4z_2z_3}{4z_2z_3-1}. \tag{A4}$$

***B*-model Yukawa couplings of X_3 (with respect to u_i),**

$$\begin{aligned}
Y_{111} &= (8z_2^3z_1^4z_3^2 - 10z_3^2z_1^3z_2^2 + 3z_1^2z_2z_3^2 + 8z_3z_1^3z_2^2 - 24z_3z_1^2z_2^2 - 2z_3z_2z_1^2 + 12z_3z_1z_2 - z_3 - z_3z_1 - 8z_1^2z_2^3 \\
&\quad + 16z_1^2z_2^2 + 10z_1z_2^2 - z_2 - 12z_1z_2 + 1 + z_1) \\
&\quad \times/(\Delta(4z_1z_2-1)^2),
\end{aligned}$$

$$\begin{aligned}
Y_{113} &= (2z_3^2z_1^3z_2^2 - z_1^2z_2z_3^2 + 4z_3z_2z_1^2 - 4z_3z_1z_2 - z_3z_1 + z_3 - 2z_1z_2^2 - 2z_2z_1^2 + 2z_1z_2 + z_2 + z_1 - 1) \\
&\quad \times/(\Delta(4z_1z_2-1)),
\end{aligned}$$

$$\begin{aligned}
Y_{133} &= (2z_1^2z_2^2z_3^3 - 2z_3z_2^2 - z_1^2z_2z_3^2 + 4z_3^2z_2z_1 - 4z_3z_1z_2 + z_2 + 2z_2z_3 - 2z_3^2z_2 - z_3z_1 + z_1 + z_3 - 1) \\
&\quad \times/(\Delta(4z_2z_3-1)),
\end{aligned} \tag{A5}$$

$$\begin{aligned}
Y_{333} &= (8z_3^4z_2^3z_1^2 - 8z_3^2z_2^3 - 10z_1^2z_2^2z_3^3 + 8z_3^3z_2^2z_1 - 24z_3^2z_1z_2^2 + 16z_3^2z_2^2 + 10z_3z_2^2 + 3z_1^2z_2z_3^2 - 2z_3^2z_2z_1 \\
&\quad + 12z_3z_1z_2 - z_2 - 12z_2z_3 + 1 + z_3 - z_1 - z_3z_1)/(\Delta(4z_2z_3-1)^2),
\end{aligned}$$

$$\begin{aligned}
Y_{112} &= -2z_2z_1(2z_1^2z_2z_3^2 - z_3^2z_1 - 8z_3z_2z_1^2 + 4z_3z_1z_2 + 4z_3z_1 - 2z_3 + 4z_2 * z_1^2 - 2z_2 - 3z_1 + 2) \\
&\quad \times/(\Delta(4z_1z_2-1)^2),
\end{aligned}$$

$$\begin{aligned}
Y_{233} &= -2z_2z_3(2z_1^2z_2z_3^2 - 8z_3^2z_2z_1 + 4z_3^2z_2 + 4z_3z_1z_2 + 4z_3z_1 - 3z_3 - z_3z_1^2 - 2z_2 - 2z_1 + 2) \\
&\quad \times/(\Delta(4z_2z_3-1)^2),
\end{aligned}$$

$$\begin{aligned}
Y_{122} &= -2(4z_3^3z_2^2z_1^3 - 3z_3^3z_2z_1^2 - 16z_3^2z_1^3z_2^2 + 4z_3^2z_1^4z_2^2 + 12z_1^2z_2z_3^2 - 3z_3^2z_2z_1^3 + z_1^2z_3^2 - z_3^2 - 4z_2^2z_3z_1 \\
&\quad + 16z_3z_1^2z_2^2 - z_2z_3 + 4z_3z_2z_1^3 - 12z_3z_2z_1^2 + 2z_3z_1 + z_3 - 3z_3z_1^2 - 2z_1 + 2z_1^2 + 3z_1z_2 \\
&\quad - 4z_1^2z_2^2)z_2/(\Delta(4z_2z_3-1)(4z_1z_2-1)^2),
\end{aligned}$$

$$\begin{aligned}
Y_{223} &= -2(4z_3^4z_2^2z_1^2 + 4z_3^3z_2^2z_1^3 - 16z_1^2z_2^2z_3^3 - 3z_3^3z_2z_1^2 + 4z_3^3z_2z_1 + 16z_3^2z_1z_2^2 - 4z_3^2z_2^2 - 3z_3^2z_2z_1^3 + 12z_1^2z_2z_3^2 \\
&\quad - 12z_3^2z_2z_1 + z_1^2z_3^2 - 3z_3^2z_1 + 2z_3^2 - 4z_2^2z_3z_1 + 3z_2z_3 + 2z_3z_1 - 2z_3 - z_1z_2 - z_1^2 + z_1)z_2 \\
&\quad \times/(\Delta(4z_2z_3-1)^2(4z_1z_2-1)),
\end{aligned}$$

$$\begin{aligned}
Y_{222} &= 2(1 + 32z_3z_1z_2 - 28z_3z_2z_1^2 - 32z_3z_1^2z_2^2 + 32z_1^2z_2z_3^2 - 32z_3^2z_1^3z_2^2 - 28z_3^2z_2z_1 - 4z_3^2z_2z_1^3 - 32z_3^2z_1z_2^2 \\
&\quad - 4z_3^3z_2z_1^2 - 32z_1^2z_2^2z_3^3 + 8z_3^4z_2^2z_1^2 + 8z_3^2z_1^4z_2^2 + 96z_3^2z_2^2z_1^2 - 2z_1 - 2z_3 + 8z_1^2z_2^2 - 4z_1z_2 + 4z_3z_1 + 8z_3^2z_2^2 \\
&\quad + z_1^2z_3^2 - 2z_3^2z_1 - 4z_2z_3 + z_1^2 + z_3^2 - 2z_3z_1^2 + 4z_1^3z_2 + 4z_3^3z_2)z_2/(\Delta(4z_2z_3-1)^2(4z_1z_2-1)^2),
\end{aligned}$$

$$\begin{aligned}
Y_{123} &= -(2z_1^2z_2^2z_3^3 - 16z_3^2z_2^2z_1^2 + 8z_3^2z_1z_2^2 + 2z_3^2z_1^3z_2^2 + 4z_3^2z_2z_1 - z_1^2z_2z_3^2 - 2z_3^2z_2 - 2z_3z_2^2 + 8z_3z_1^2z_2^2 \\
&\quad - 8z_3z_1z_2 + 4z_3z_2z_1^2 + 2z_2z_3 - z_3z_1 + z_3 - 1 + 2z_1z_2 - 2z_1z_2^2 + z_1 - 2z_2z_1^2z_2) \\
&\quad \times/(\Delta(4z_2z_3-1)(4z_1z_2-1)).
\end{aligned} \tag{A6}$$

Discriminant of X_3,

$$\Delta = 2(-z_1^2 z_2 z_3^2 + 2z_3 z_1 z_2 + z_3 z_1 - z_3 - z_2 - z_1 + 1). \tag{A7}$$

Extended Picard-Fuchs system of X_3,

$$\begin{aligned}
\widetilde{\mathcal{D}}_1 &= a_1(z_1,z_2,z_3)\cdot\mathcal{D}_1 + a_2(z_1,z_2,z_3)\cdot\mathcal{D}_2 + a_3(z_1,z_2,z_3)\cdot\mathcal{D}_3 + a_5(z_1,z_2,z_3)\cdot\mathcal{D}_5 \\
&\quad - 2(1+z_1+z_2+z_3-2z_1z_2z_3+z_1z_3+z_1^2z_2z_3^2)\mathcal{D}_6 \\
&= (-\theta_2^2 - 2\theta_2\theta_3 - \theta_1^2 + 2\theta_2\theta_1 + 3\theta_3^2)z_1^2z_2z_3^2 + (((-4\theta_1^2 + 4\theta_2^2 + 8\theta_1\theta_3 + 4\theta_2\theta_3 - 8\theta_3^2)z_1 \\
&\quad + (4\theta_1\theta_3 - 4\theta_3^2 + 4\theta_2\theta_3)z_1^2)z_2 + (-2\theta_2\theta_3 + 2\theta_2\theta_1 - 2\theta_1\theta_3 - \theta_1^2 - \theta_2^2 + 3\theta_3^2)z_1 - \theta_2^2 \\
&\quad - 2\theta_2\theta_3 - 2\theta_1\theta_3 + 3\theta_3^2 + \theta_1^2)z_3 + ((-4\theta_1^2 + 4\theta_2^2 + 4\theta_1\theta_3 - 4\theta_2\theta_3)z_1 + \theta_1^2 + \theta_3^2 - 2\theta_2\theta_1 \\
&\quad + \theta_2^2 - 2\theta_2\theta_3)z_2 + (-\theta_1^2 + \theta_3^2 + 2\theta_2\theta_1 - \theta_2^2 - 2\theta_1\theta_3)z_1 + \theta_1^2 + \theta_3^2 - \theta_2^2 - 2\theta_1\theta_3 \\
&\quad - 2(1+z_1+z_2+z_3-2z_1z_2z_3+z_1z_3+z_1^2z_2z_3^2)\mathcal{D}_6,
\end{aligned}$$

$$\widetilde{\mathcal{D}}_2 = \text{interchange between } z_1 \text{ and } z_3 \text{ of } \widetilde{\mathcal{D}}_1,$$

$$\widetilde{\mathcal{D}}_3 = (1+z_3)\mathcal{D}_1 + (1+z_1)\mathcal{D}_3 + (1-z_1^2z_3^2)\mathcal{D}_2 + (1-z_1z_3)\mathcal{D}_5, \tag{A8}$$

where $a_j(z_1,z_2,z_3)$ are rational functions in z_i whose denominators are given by Δ.

APPENDIX B: *B*-MODEL YUKAWA COUPLINGS OF $K_{\mathrm{d}P_2}$

In this Appendix, we present the *B*-model Yukawa couplings of $K_{\mathrm{d}P_2}$ computed from the extended PF system (93), and the assumption of the existence of Kodaira-Spencer theory,

$$Y_{ijk} = \int_M \Omega \wedge \frac{\partial^3\Omega}{\partial u_i\,\partial u_j\,\partial u_k}, \tag{B1}$$

$$\begin{aligned}
Y_{222} &= -(16z_3^3yz_1^2 + ((-27y-18)z_1z_2^2 + 16yz_1^3 - 16yz_1^2 + ((-24y-8)z_1^2 + (4+36y)z_1)z_2 - 8z_1y)z_3^2 \\
&\quad + (((-24y-14)z_1^2 + (22+36y)z_1)z_2^2 - 8yz_1^2 + ((64y+12)z_1^2 + (-2-46y)z_1 \\
&\quad + (-32y-8)z_1^3 - y - 1)z_2 + 8z_1y + y)z_3 + (12+16y)z_1^2z_2^3 + ((16y+8)z_1^3 + (-16y-4)z_1^2 \\
&\quad + (-3-8y)z_1)z_2^2 + (y + (2-8y)z_1^2 + 1 + (-3+8y)z_1)z_2 + z_1y - y)/\Delta,
\end{aligned}$$

$$\begin{aligned}
Y_{223} &= -(16z_3^3xz_1^2 + ((-27x+9)z_1z_2^2 + 16xz_1^3 - 16xz_1^2 + ((-24x+8)z_1^2 + (36x-8)z_1)z_2 - 8z_1x)z_3^2 \\
&\quad + (((36x-11)z_1 + (-24x+6)z_1^2)z_2^2 - 8xz_1^2 + ((-16+64x)z_1^2 + (-32x+8)z_1^3 \\
&\quad + (10-46x)z_1 - x)z_2 + 8z_1x + x)z_3 + (16x-8)z_1^2z_2^3 + ((-16x+8)z_1^2 + (16x-8)z_1^3 \\
&\quad + (-8x+2)z_1)z_2^2 + ((8x-2)z_1 + (-8x+2)z_1^2 + x)z_2 + z_1x - x)/\Delta,
\end{aligned}$$

$$\begin{aligned}
Y_{233} &= -((16x-8)z_1^2z_3^3 + ((-27x+9)z_1z_2^2 + (16x-8)z_1^3 + (-16x+8)z_1^2 \\
&\quad + ((36x-11)z_1 + (-24x+6)z_1^2)z_2 + (-8x+2)z_1)z_3^2 + (((-24x+8)z_1^2 \\
&\quad + (36x-8)z_1)z_2^2 + (-8x+2)z_1^2 + ((-16+64x)z_1^2 + (-32x+8)z_1^3 + (10-46x)z_1 - x)z_2 \\
&\quad + (8x-2)z_1 + x)z_3 + 16z_2^3xz_1^2 + (-16xz_1^2 + 16xz_1^3 - 8z_1x)z_2^2 \\
&\quad + (8z_1x - 8xz_1^2 + x)z_2 + z_1x - x)/\Delta,
\end{aligned}$$

$$Y_{333} = -((12+16y)z_1^2z_3^3 + ((-27y-18)z_1z_2^2 + (-16y-4)z_1^2 + ((-24y-14)z_1^2 + (22+36y)z_1)z_2 + (16y+8)z_1^3 + (-3-8y)z_1)z_3^2 + ((2-8y)z_1^2 + ((-24y-8)z_1^2 + (4+36y)z_1)z_2^2 + (-3+8y)z_1 + 1 + ((64y+12)z_1^2 + (-2-46y)z_1 + (-32y-8)z_1^3 - y - 1)z_2 + y)z_3 + 16z_2^3yz_1^2 + (16yz_1^3 - 16yz_1^2 - 8z_1y)z_2^2 + z_1y + (-8yz_1^2 + y + 8z_1y)z_2 - y)/\Delta,$$

$$Y_{122} = ((16x+16y)z_1^2z_3^3 + ((16x+16y)z_1^3 + (-27y-9-27x)z_1z_2^2 + ((-24x-24y)z_1^2 + (8+36y+36x)z_1)z_2 + (-16x-16y)z_1^2 + (-8x-8y)z_1)z_3^2 + ((8y+8x)z_1 + (-8x-8y)z_1^2 + ((-8-24x-24y)z_1^2 + (36y+36x+14)z_1)z_2^2 + ((-32x-32y)z_1^3 + (-46y-46x-12)z_1 - x - y + (64y+8+64x)z_1^2)z_2 + x + y)z_3 + (4+16y+16x)z_1^2z_2^3 + ((16x+16y)z_1^3 + (-16x-16y)z_1^2 + (-8x-8y-5)z_1)z_2^2(y+x)z_1 + ((8y+4+8x)z_1 + x + y + (-8y-8x-4)z_1^2)z_2 - x - y)/\Delta,$$

$$Y_{133} = ((4+16y+16x)z_1^2z_3^3 + ((16x+16y)z_1^3 + (-27y-9-27x)z_1z_2^2 + ((-8-24x-24y)z_1^2 + (36y+36x+14)z_1)z_2 + (-16x-16y)z_1^2 + (-8x-8y-5)z_1)z_3^2 + ((8y+4+8x)z_1 + (-8y-8x-4)z_1^2 + ((-24x-24y)z_1^2 + (8+36y+36x)z_1)z_2^2 + ((-32x-32y)z_1^3 + (-46y-46x-12)z_1 - x - y + (64y+8+64x)z_1^2)z_2 + x + y)z_3 + (16x+16y)z_1^2z_2^3 + ((16x+16y)z_1^3 + (-16x-16y)z_1^2 + (-8x-8y)z_1)z_2^2 + (y+x)z_1 + ((8y+8x)z_1x + y + (-8x-8y)z_1^2)z_2 - x - y)/\Delta,$$

$$Y_{112} = -((48x+16y-8)z_1^2z_3^3 + ((48x+16y-8)z_1^3 + (-27y-81x+9)z_1z_2^2 + ((-24y-72x+14)z_1^2 + (36y+108x-11)z_1)z_2 + (8-16y-48x)z_1^2 + (-8y+2-24x)z_1)z_3^2 + ((8y+24x-2)z_1 + (-8y+2-24x)z_1^2 + ((6-72x-24y)z_1^2 + (36y+108x-14)z_1)z_2^2 + ((-32y-96x+16)z_1^3 + (-138x+16-46y)z_1 - 3x - y + (64y+192x-28)z_1^2)z_2 + 3x + y)z_3 + (48x-4+16y)z_1^2z_2^3 + ((48x+16y-8)z_1^3 + (4-48x-16y)z_1^2 + (-8y+5-24x)z_1)z_2^2 + (y+3x)z_1 + ((24x+8y-5)z_1 + 3x + y + (-24x-8y+6)z_1^2)z_2 - 3x - y)/\Delta,$$

$$Y_{113} = -((48x-4+16y)z_1^2z_3^3 + ((48x+16y-8)z_1^3 + (-27y-81x+9)z_1z_2^2 + ((6-72x-24y)z_1^2 + (36y+108x-14)z_1)z_2 + (4-48x-16y)z_1^2 + (-8y+5-24x)z_1)z_3^2 + ((24x+8y-5)z_1 + (-24x-8y+6)z_1^2 + ((-24y-72x+14)z_1^2 + (36y+108x-11)z_1)z_2^2 + ((-32y-96x+16)z_1^3 + (-138x+16 - 46y)z_1 - 3x - y + (64y+192x-28)z_1^2)z_2 + 3x + y)z_3 + (48x+16y-8)z_1^2z_2^3 + ((48x+16y - 8)z_1^3 + (8-16y-48x)z_1^2 + (-8y+2-24x)z_1)z_2^2 + (y+3x)z_1 + ((8y+24x-2)z_1 + 3x + y + (-8y+2-24x)z_1^2)z_2 - 3x - y)/\Delta,$$

$$
\begin{aligned}
Y_{123} = {} & ((-8+32x)z_1^2z_3^3 + ((-32x+8)z_1^2 + (6-16x)z_1 + ((72x-25)z_1 + (14-48x)z_1^2)z_2 \\
& + (-8+32x)z_1^3 + (18-54x)z_1z_2^2)z_3^2 + ((16x-6)z_1 + (1+(-40+128x)z_1^2 + (16-64x)z_1^3 \\
& - 2x + (33-92x)z_1)z_2 + (6-16x)z_1^2 + 2x - 1 + ((72x-25)z_1 + (14-48x)z_1^2)z_2^2)z_3 \\
& + (-8+32x)z_1^2z_2^3 + ((-32x+8)z_1^2 + (-8+32x)z_1^3 + (6-16x)z_1)z_2^2 + (-1+2x)z_1 \\
& + ((-6-16x)z_1^2 - 1 + 2x + (16x-6)z_1)z_2 + 1 - 2x)/\Delta,
\end{aligned}
$$

$$
\begin{aligned}
Y_{111} = {} & ((-12+96x+32y)z_1^2z_3^3 + ((8-32y-96x)z_1^2 + (-16+96x+32y)z_1^3 \\
& + (-162x+18-54y)z_1z_2^2 + (-48x-16y+3)z_1 + ((20-48y-144x)z_1^2 \\
& + (216x+72y-22)z_1)z_2)z_3^2 + ((-6x+1+(-192x+32-64y)z_1^3 - 2y + (128y-48 \\
& + 384x)z_1^2 \\
& + (-92y+26-276x)z_1)z_2 + (8-16y-48x)z_1^2 + 2y + ((20-48y-144x)z_1^2 + (216x+72y \\
& - 22)z_1)z_2^2 \\
& + 6x + (48x+16y-2)z_1 - 1)z_3 + (-12+96x+32y)z_1^2z_2^3 + ((8-32y-96x)z_1^2 \\
& + (-16+96x+32y)z_1^3 + (-48x-16y+3)z_1)z_2^2 + 1 + (2y-2+6x)z_1 + (6x+2y+(8-16y \\
& - 48x)z_1^2 - 1 \\
& + (48x+16y-2)z_1)z_2 - 6x - 2y)/\Delta,
\end{aligned}
$$

$$
\begin{aligned}
\Delta = {} & -((-16z_2^2 + 32z_3z_2 - 16z_3^2)z_1^3 + (24z_3^2z_2 - 16z_3^3 - 16z_2^3 - 64z_3z_2 + 24z_3z_2^2 + 16z_2^2 + 8z_3 + 16z_3^2 \\
& + 8z_2)z_1^2 + (8z_3^2 - 1 + 27z_2^2z_3^2 - 36z_3z_2^2 - 8z_2 + 8z_2^2 - 8z_3 - 36z_3^2z_2 + 46z_3z_2)z_1 + 1 - z_2 + z_3z_2 - z_3).
\end{aligned}
$$

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Superselection in the presence of constraints

Hellmut Baumgaertel[a)]
Mathematical Institute, University of Potsdam, Am Neuen Palais 10, Postfach 601 553, D-14415 Potsdam, Germany

Hendrik Grundling[b)]
Department of Mathematics, University of New South Wales, Sydney, NSW 2052, Australia

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Superselection and constraints occur together in many gauge theories, and here we begin a study of such systems. Our main focus will be to analyze compatibility questions between constraining and superselection, and we will develop an example modelled on QED in which our framework is realized. We proceed from a generalization of Doplicher-Roberts superselection theory to the case of the nontrivial center, and a set of Dirac quantum constraints and find conditions under which the superselection structures will survive constraining in some form. This involves an analysis of the restriction and factorization of superselection structures. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1985038]

I. INTRODUCTION

In heuristic quantum field theory, there are many examples of systems which contain global charges (hence superselection structure) as well as a local gauge symmetry (hence constraints). Most of these systems cannot currently be written in a consistent mathematical framework, due to the presence of interactions. Nevertheless, the mathematical structure of superselection by itself has been properly developed (cf. Refs. 1–3), as well as the mathematical structure of quantum constraints (Refs. 4–6), hence one can at least abstractly consider systems which contain both. This will be the focus of our investigations in this paper, which is a first step in this direction. We will address the natural intertwining questions for the two structures, as well as compatibility issues. Unfortunately, in spite of our physical motivation the discussion will be unavoidably technical, but we have an interesting model which goes at least part way to illustrating our general setting.

The class of physical systems with both superselection and constraints, is a large one. One of the most important examples in this class, is that of a quantized local gauge field, acting on a fermion field. It has a Gauss law constraint (implementing the local gauge transformations) as well as a set of global charges (leading to superselection). An important feature of it, is that the global gauge transformations preserve the set of constraints, and we will assume this property for the systems we analyze. There are plenty of other examples of systems satisfying this property, e.g., the constraints can be independent of the global gauge group, for instance, they can be equations of motion, or restriction to a submanifold. Or there may be two or more local gauge symmetries which commute (e.g., isospin and electromagnetism), in which case the Gauss law constraint of one symmetry will commute with the global charges of the other.

We will be concerned with the question of under what conditions (and how much of) the

[a)]Electronic mail: baumg@rz.uni-potsdam.de
[b)]Electronic mail: hendrik@maths.unsw.edu.au

superselection structures will survive the constraining procedure. Since charge is a physically measurable quantity, this should survive constraining, which removes nonphysical information from the system.

For superselection, we will use the Doplicher-Roberts theory which originated in the Doplicher-Haag-Roberts concept of admissible representations.[2] In the context of a local net of von Neumann algebras on Minkowski space with a distinguished vacuum representation π_0, a representation π is *admissible* if on the C*-algebra associated to the causal complement of any double cone, π is unitarily equivalent to π_0. In physical terms this means that π and the vacuum π_0 cannot be distinguished at spacelike infinity (e.g., if the only difference is a finite charge in some bounded set). The unitary equivalence classes of admissible representations (e.g., corresponding to different total charges) are in bijection with a class of "canonical endomorphisms" by $\pi \cong \pi_0 \circ \rho$, and this leads to the study of these endomorphisms, and the construction of a *Hilbert system* from them. These concepts will all be defined and discussed in Sec. II, where we include recent results for an observable algebra with nontrivial center (cf. Ref. 7). The Doplicher-Haag-Roberts theory is presently not directly applicable to QED due to the presence of massless particles, however we were able to realize the abstract Doplicher-Roberts version explicitly in our model, using the global charge.

For quantum constraints, we will use the framework developed by Grundling and Hurst[4,8,5] which is based on Dirac's constraint theory, and produced physically correct results on application to QEM and other systems. The basic idea is to select those cyclic representations of the field algebra, where the cyclic vector is annihilated by the constraints. The observables consist of those elements of the field algebra which map a vector annihilated by the constraints to another such vector in any representation. These satisfy a "weak commutativity" condition with the constraints, so can be identified with Dirac's observables. There are quite a number of diverse quantum constraint methods available in the literature at various levels of rigour (cf. Ref. 6). The one we use here is the most congenial from the point of view of C*-algebraic methods, and we summarize it in Sec. III. In fact, in Ref. 5 it was shown that this method can avoid indefinite inner product representations (endemic to gauge theories), yet it produced the same results as those obtained from such representations.

In Sec. IV we collect our main results. The proofs for these are in Sec. VI, and in Sec. V we present our example which is based on the Maxwell equation in (interacting) QED.

II. FUNDAMENTALS OF SUPERSELECTION

In this section we summarize the structures from superselection theory which we need. For proofs, we refer to the literature if possible.

The superselection problem in algebraic quantum field theory, as stated by the Doplicher-Haag-Roberts (DHR) selection criterion, led to a profound body of work, culminating in the general Doplicher-Roberts (DR) duality theory for compact groups. The DHR criterion selects a distinguished class of "admissible" representations of a quasilocal algebra $\mathcal{A}$ of observables, where the center is trivial, i.e., $Z(\mathcal{A}) = \mathbb{C}1$, or even $\mathcal{A}$ is assumed to be simple. This corresponds to the selection of a DR-category $\mathcal{T}$ of "admissible" endomorphisms of $\mathcal{A}$. Furthermore, from this endomorphism category $\mathcal{T}$ the DR-analysis constructs a C*-algebra $\mathcal{F} \supset \mathcal{A}$ together with a compact group action $\alpha: \mathcal{G} \ni g \to \alpha_g \in \mathrm{Aut}\,\mathcal{F}$ such that

(i) $\mathcal{A}$ is the fixed point algebra of this action,
(ii) $\mathcal{T}$ coincides with the category of all "canonical endomorphisms" of $\mathcal{A}$ (cf. Sec. II C).

$\mathcal{F}$ is called a Hilbert extension of $\mathcal{A}$ in Ref. 3. Physically, $\mathcal{F}$ is identified as a field algebra and $\mathcal{G}$ with a global gauge group of the system. $\{\mathcal{F}, \alpha_{\mathcal{G}}\}$ is uniquely determined by $\mathcal{T}$ up to $\mathcal{A}$-module isomorphisms. Conversely, $\{\mathcal{F}, \alpha_{\mathcal{G}}\}$ determines uniquely its category of all canonical endomorphisms. Therefore one can state the equivalence of the "selection principle," given by $\mathcal{T}$ and the "symmetry principle," given by $\mathcal{G}$. This duality is one of the crucial theorems of the Doplicher-Roberts theory.

In contrast to the original theory of Doplicher and Roberts, we allow here a nontrivial center for $\mathcal{A}$. The reason for this is that when there are constraints present, the system contains nonphysical information, so there is no physical reason why $\mathcal{A}$ should be simple. Only after eliminating the constraints should one require the final observable algebra to be simple, hence having trivial center. Now a duality theorem for a C*-algebra with nontrivial center has been proven recently,[7,9] establishing a bijection between distinguished categories of endomorphisms of $\mathcal{A}$ and Hilbert extensions of $\mathcal{A}$ satisfying some additional conditions, of which the most important is $\mathcal{A}' \cap \mathcal{F} = Z(\mathcal{A})$ (i.e., the relative commutant is assumed to be minimal). This will be properly explained below. This condition has already been used by Mack and Schomerus[10] as a "new principle."

A. Basic properties of Hilbert systems

Below $\mathcal{F}$ will always denote a unital C*-algebra. A Hilbert space $\mathcal{H} \subset \mathcal{F}$ is called algebraic if the scalar product $\langle \cdot, \cdot \rangle$ of $\mathcal{H}$ is given by $\langle A, B \rangle \mathbb{1} := A^* B$ for $A, B \in \mathcal{H}$. Henceforth we consider only finite-dimensional algebraic Hilbert spaces. The support $\operatorname{supp} \mathcal{H}$ of $\mathcal{H}$ is defined by $\operatorname{supp} \mathcal{H} := \Sigma_{j=1}^{d} \Phi_j \Phi_j^*$, where $\{\Phi_j | j = 1, \ldots, d\}$ is any orthonormal basis of $\mathcal{H}$. *Unless otherwise specified, we assume below that each algebraic Hilbert space $\mathcal{H}$ considered, satisfies* $\operatorname{supp} \mathcal{H} = \mathbb{1}$.

We also fix a compact C*-dynamical system $\{\mathcal{F}, \mathcal{G}, \alpha\}$, i.e., $\mathcal{G}$ is a compact group and $\alpha: \mathcal{G} \ni g \to \alpha_g \in \operatorname{Aut} \mathcal{F}$ is a pointwise norm-continuous morphism. For $\gamma \in \hat{\mathcal{G}}$ (the dual of $\mathcal{G}$) its spectral projection $\Pi_\gamma \in \mathcal{L}(\mathcal{F})$ is defined by

$$\Pi_\gamma(F) := \int_{\mathcal{G}} \overline{\chi_\gamma(g)} \alpha_g(F) \mathrm{d}g \quad \text{for all } F \in \mathcal{F},$$

where

$$\chi_\gamma(g) := \dim \gamma \cdot \operatorname{Tr} \pi(g), \quad \pi \in \gamma$$

and its spectral subspace $\Pi_\gamma \mathcal{F}$ satisfies $\Pi_\gamma \mathcal{F} = \text{clo-span}\{\mathcal{L} \subset \mathcal{F}\}$ where $\mathcal{L}$ runs through all invariant subspaces of $\mathcal{F}$ which transform under $\alpha_\mathcal{G}$ according to γ (cf. Ref. 11). Define the spectrum of $\alpha_\mathcal{G}$ by

$$\operatorname{spec} \alpha_\mathcal{G} := \{\gamma \in \hat{\mathcal{G}} | \Pi_\gamma \neq 0\}.$$

Our central object of study is the following.

Definition 2.1: The C*-*dynamical system* $\{\mathcal{F}, \mathcal{G}, \alpha\}$ *is called a* Hilbert system *if for each* $\gamma \in \hat{\mathcal{G}}$ *there is an algebraic Hilbert space* $\mathcal{H}_\gamma \subset \mathcal{F}$, *such that* $\alpha_\mathcal{G}$ *acts invariantly on* $\mathcal{H}_\gamma$, *and the unitary representation* $\mathcal{G} \upharpoonright \mathcal{H}_\gamma$ *is in the equivalence class* $\gamma \in \hat{\mathcal{G}}$.

Remark 2.2: Note that for a Hilbert system $\{\mathcal{F}, \mathcal{G}, \alpha\}$ we have necessarily that the algebraic Hilbert spaces satisfy $\mathcal{H}_\gamma \subset \Pi_\gamma \mathcal{F}$ for all γ, and hence that $\operatorname{spec} \alpha_\mathcal{G} = \hat{\mathcal{G}}$, i.e., the spectrum is *full*. The morphism $\alpha: \mathcal{G} \to \operatorname{Aut} \mathcal{F}$ is necessarily faithful. So, since $\mathcal{G}$ is compact and $\operatorname{Aut} \mathcal{F}$ is Hausdorff with respect to the topology of pointwise norm convergence, α is a homeomorphism of $\mathcal{G}$ onto its image. Thus $\mathcal{G}$ and $\alpha_\mathcal{G}$ are isomorphic as topological groups.

We are mainly interested in Hilbert systems whose fixed point algebras coincide such that they appear as extensions of it.

Definition 2.3: A Hilbert system $\{\mathcal{F}, \mathcal{G}, \alpha\}$ *is called a* Hilbert extension *of a C*-algebra* $\mathcal{A} \subset \mathcal{F}$ *if* $\mathcal{A}$ *is the fixed point algebra of* $\mathcal{G}$. *Two Hilbert extensions* $\{\mathcal{F}_i, \mathcal{G}, \alpha^i\}$, $i = 1, 2$ *of* $\mathcal{A}$ *(with respect to the same group* $\mathcal{G}$*) are called* $\mathcal{A}$-module isomorphic *if there is an isomorphism* $\tau: \mathcal{F}_1 \to \mathcal{F}_2$ *such that* $\tau(A) = A$ *for* $A \in \mathcal{A}$, *and* τ *intertwines the group actions, i.e.,* $\tau \circ \alpha_g^1 = \alpha_g^2 \circ \tau$.

Remark 2.4: (i) Group automorphisms of $\mathcal{G}$ lead to $\mathcal{A}$-module isomorphic Hilbert extensions of $\mathcal{A}$, i.e., if $\{\mathcal{F}, \mathcal{G}, \alpha\}$ is a Hilbert extension of $\mathcal{A}$ and ξ an automorphism of $\mathcal{G}$, then the Hilbert extensions $\{\mathcal{F}, \mathcal{G}, \alpha\}$ and $\{\mathcal{F}, \mathcal{G}, \alpha \circ \xi\}$ are $\mathcal{A}$-module isomorphic. So the Hilbert system $\{\mathcal{F}, \mathcal{G}, \alpha\}$ depends, up to $\mathcal{A}$-module isomorphisms, only on $\alpha_\mathcal{G}$, which is isomorphic to $\mathcal{G}$. In other words, up to $\mathcal{A}$-module isomorphism we may identify $\mathcal{G}$ and $\alpha_\mathcal{G} \subset \operatorname{Aut} \mathcal{F}$ neglecting the action α which has

no relevance from this point of view. Therefore in the following, unless it is otherwise specified, we use the notation $\{\mathcal{F},\mathcal{G}\}$ for a Hilbert extension of $\mathcal{A}$, where $\mathcal{G}\subset \mathrm{Aut}\,\mathcal{F}$.

(ii) As mentioned above, examples of Hilbert systems arise in DHR-superselection theory (cf. Refs. 3 and 2). There are also constructions by means of tensor products of Cuntz algebras (cf. Ref. 12). In these examples the relative commutant of the fixed point algebra $\mathcal{A}$, hence also its center, is trivial. Another construction for $\mathcal{G}=\mathbb{T}$, by means of the loop group $C^\infty(S^1,\mathbb{T})$ is in Ref. 13, and for this $Z(\mathcal{A})$ is nontrivial.

Remark 2.5: A Hilbert system $\{\mathcal{F},\mathcal{G}\}$ is a highly structured object; we list some important facts and properties (for details, consult Refs. 2 and 3).

(i) The spectral projections satisfy

$$\Pi_{\gamma_1}\Pi_{\gamma_2}=\Pi_{\gamma_2}\Pi_{\gamma_1}=\delta_{\gamma_1\gamma_2}\Pi_{\gamma_1},$$

$$\|\Pi_\gamma\|\leqslant d(\gamma)^{3/2},\quad d(\gamma):=\dim(\mathcal{H}_\gamma),$$

$$\Pi_\gamma\mathcal{F}=\mathrm{span}(\mathcal{A}\mathcal{H}_\gamma),\quad \Pi_\iota\mathcal{F}=\mathcal{A},$$

where $\iota\in\hat{\mathcal{G}}$ denotes the trivial representation of $\mathcal{G}$.

(ii) Each $F\in\mathcal{F}$ is uniquely determined by its projections $\Pi_\gamma F$, $\gamma\in\hat{\mathcal{G}}$, i.e., $F=0$ iff $\Pi_\gamma F=0$ for all $\gamma\in\hat{\mathcal{G}}$, cf. Corollary 2.6 of Ref. 9.

(iii) A useful *-subalgebra of $\mathcal{F}$ is

$$\mathcal{F}_{\mathrm{fin}}:=\{F\in\mathcal{F}|\Pi_\gamma F\neq 0 \text{ for only finitely many } \gamma\in\hat{\mathcal{G}}\}$$

which is dense in $\mathcal{F}$ with respect to the C*-norm (cf. Ref. 14).

(iv) In $\mathcal{F}$ there is an $\mathcal{A}$-scalar product given by $\langle F,G\rangle_{\mathcal{A}}:=\Pi_\iota FG^*$, with respect to which the spectral projections are symmetric, i.e., $\langle\Pi_\gamma F,G\rangle_{\mathcal{A}}=\langle F,\Pi_\gamma G\rangle_{\mathcal{A}}$ for all $F,G\in\mathcal{F}$, $\gamma\in\hat{\mathcal{G}}$. Using the $\mathcal{A}$-scalar product one can define a norm on $\mathcal{F}$, called the $\mathcal{A}$-norm,

$$|F|_{\mathcal{A}}:=\|\langle F,F\rangle_{\mathcal{A}}\|^{1/2},\quad F\in\mathcal{F}.$$

Note that $|F|_{\mathcal{A}}\leqslant\|F\|$ and that $\mathcal{F}$ in general is not closed with respect to the $\mathcal{A}$-norm. Then for each $F\in\mathcal{F}$ we have that $F=\Sigma_{\gamma\in\hat{\mathcal{G}}}\Pi_\gamma F$ where the sum on the right-hand side is convergent with respect to the $\mathcal{A}$-norm but not necessarily with respect to the C*-norm $\|\cdot\|$. We also have Parseval's equation, $\langle F,F\rangle_{\mathcal{A}}=\Sigma_{\gamma\in\hat{\mathcal{G}}}\langle\Pi_\gamma F,\Pi_\gamma F\rangle_{\mathcal{A}}$, cf. Proposition 2.5 in Ref. 9. Moreover $|\Pi_\gamma|_{\mathcal{A}}=1$ for all $\gamma\in\hat{\mathcal{G}}$, where $|\cdot|_{\mathcal{A}}$ denotes the operator norm of Π_γ with respect to the norm $|\cdot|_{\mathcal{A}}$ in $\mathcal{F}$.

(v) Generally for a Hilbert system, the assignment $\gamma\to\mathcal{H}_\gamma$ is not unique. If $U\in\mathcal{A}$ is unitary then also $U\mathcal{H}_\gamma\subset\Pi_\gamma\mathcal{F}$ is a $\mathcal{G}$-invariant algebraic Hilbert space carrying the representation $\gamma\in\hat{\mathcal{G}}$. Each $\mathcal{G}$-invariant algebraic Hilbert space $\mathcal{K}$ which carries the representation γ is of this form, i.e., there is a unitary $V\in\mathcal{A}$ such that $\mathcal{K}=V\mathcal{H}_\gamma$. For a general $\mathcal{G}$-invariant algebraic Hilbert space $\mathcal{H}\subset\mathcal{F}$, we may have that $\mathcal{G}\restriction\mathcal{H}$ is not irreducible, i.e., it need not be of the form $\mathcal{K}=V\mathcal{H}_\gamma$. Below we will consider further conditions on the Hilbert system to control the structure of these.

(vi) Given two $\mathcal{G}$-invariant algebraic Hilbert spaces $\mathcal{H}$, $\mathcal{K}\subset\mathcal{F}$, then $\mathrm{span}(\mathcal{H}\cdot\mathcal{K})$ is also a $\mathcal{G}$-invariant algebraic Hilbert space which we will briefly denote by $\mathcal{H}\cdot\mathcal{K}$. It is a realization of the tensor product $\mathcal{H}\otimes\mathcal{K}$ within $\mathcal{F}$ and carries the tensor product of the representations of $\mathcal{G}$ carried by $\mathcal{H}$ and $\mathcal{K}$ in the obvious way.

(vii) Let $\mathcal{H}$, $\mathcal{K}$ be two $\mathcal{G}$-invariant algebraic Hilbert spaces, but not necessarily of support 1. Then there is a natural isometric embedding $\mathcal{J}:\mathcal{L}(\mathcal{H},\mathcal{K})\to\mathcal{F}$ given by

$$\mathcal{J}(T) := \sum_{j,k} t_{j,k} \Psi_j \Phi_k^*, \quad t_{j,k} \in \mathbb{C}, \quad T \in \mathcal{L}(\mathcal{H},\mathcal{K}),$$

where $\{\Phi_k\}_k$, $\{\Psi_j\}_j$ are orthonormal bases of $\mathcal{H}$ and $\mathcal{K}$, respectively, and where

$$T(\Phi_k) = \sum_j t_{j,k} \Psi_j,$$

i.e., $(t_{j,k})$ is the matrix of T with respect to these orthonormal bases. One has

$$T(\Phi) = \mathcal{J}(T) \cdot \Phi, \quad \Phi \in \mathcal{H}.$$

This implies the following: if $T_j \in \mathcal{L}(\mathcal{H}_j,\mathcal{K}_j)$, $j=1, 2$, hence $T_1 \otimes T_2 \in \mathcal{L}(\mathcal{H}_1\mathcal{H}_2,\mathcal{K}_1\mathcal{K}_2)$, then $\mathcal{J}(T_1 \otimes T_2)\Phi_1\Phi_2 = \mathcal{J}(T_1)\Phi_1\mathcal{J}(T_2)\Phi_2$ for $\Phi_j \in \mathcal{H}_j$. Moreover $\mathcal{J}(T) \in \mathcal{A}$ iff $T \in \mathcal{L}_\mathcal{G}(\mathcal{H},\mathcal{K})$, where $\mathcal{L}_\mathcal{G}(\mathcal{H},\mathcal{K})$ denotes the linear subspace of $\mathcal{L}(\mathcal{H},\mathcal{K})$ consisting of all intertwining operators of the representations of $\mathcal{G}$ on $\mathcal{H}$ and $\mathcal{K}$ (cf. Ref. 3, p. 222).

B. The category of $\mathcal{G}$-invariant algebraic Hilbert spaces

The $\mathcal{G}$-invariant algebraic Hilbert spaces $\mathcal{H}$ of $\{\mathcal{F},\mathcal{G}\}$ form the objects of a category $\mathcal{T}_\mathcal{G}$ associated to $\{\mathcal{F},\mathcal{G}\}$ whose arrows are given by the elements of $(\mathcal{H},\mathcal{K}) := \mathcal{J}(\mathcal{L}_\mathcal{G}(\mathcal{H},\mathcal{K})) \subset \mathcal{A}$. It is already large enough to carry all tensor products of the representations of $\mathcal{G}$ on its objects by Remark 2.5(vi) (though not necessarily subrepresentations and direct sums). First, let us state some of its rich structure (cf. Refs. 3 and 12).

Proposition 2.6: For $\{\mathcal{F},\mathcal{G}\}$ the category $\mathcal{T}_\mathcal{G}$ is a tensor C*-category, *i.e., the arrow spaces $(\mathcal{H},\mathcal{K})$ are Banach spaces such that*

(i) *with respect to composition of arrows R, S we have $\|R \circ S\| \leqslant \|R\| \, \|S\|$,*
(ii) *there is an antilinear involutive contravariant functor $*: \mathcal{T}_\mathcal{G} \to \mathcal{T}_\mathcal{G}$ such that $\|R^* \circ R\| = \|R\|^2$ for all arrows R with the same range and domain (here the functor * is given by the involution in $\mathcal{F}$).*
(iii) *There is an associative product $\cdot$ on* Ob $\mathcal{T}_\mathcal{G}$ *and an identity object $1 \in$* Ob $\mathcal{T}_\mathcal{G}$ *(i.e., $1 \cdot \mathcal{H} = \mathcal{H} = \mathcal{H} \cdot 1$) and there is an associative bilinear product $\times$ of the arrows, such that if $R \in (\mathcal{H},\mathcal{K})$ and $R' \in (\mathcal{H}',\mathcal{K}')$ then $R \times R' \in (\mathcal{H} \cdot \mathcal{H}', \mathcal{K} \cdot \mathcal{K}')$. Moreover we require that for R, R' as above,*

$$1_\iota \times R = R \times 1_\iota = R, \quad (R \times R')^* = R^* \times R'^*, \tag{1}$$

where $1_\iota \in (1,1)$ is the identity arrow, as well as the interchange law

$$(S \circ R) \times (S' \circ R') = (S \times S') \circ (R \times R'),$$

whenever the left-hand side is defined. Here in $\mathcal{T}_\mathcal{G}$, the product $\cdot$ is given by the product of $\mathcal{F}$, the identity object is $1 := \mathbb{C}\,\mathbb{I}$ and the product $\times$ is defined by

$$R \times R' := \mathcal{J}(T \otimes T'),$$

for $R = \mathcal{J}(T)$, $R' = \mathcal{J}(T')$, where $T \in \mathcal{L}_\mathcal{G}(\mathcal{H},\mathcal{K})$, $T' \in \mathcal{L}_\mathcal{G}(\mathcal{H}',\mathcal{K}')$. Note that $(1,1) = (\mathbb{C}\,\mathbb{I}, \mathbb{C}\,\mathbb{I}) = \mathbb{C}\,\mathbb{I}$, i.e., $1_\iota = \mathbb{I}$.

$\mathcal{T}_\mathcal{G}$ has additional important structures (permutation and conjugation), which we will consider below in Sec. II D.

We need to examine conditions on $\{\mathcal{F},\mathcal{G}\}$ to ensure that $\mathcal{T}_\mathcal{G}$ carries subrepresentations and direct sums.

Definition 2.7: Let $\mathcal{H}$, $\mathcal{K} \in$ Ob $\mathcal{T}_\mathcal{G}$*, and define $\mathcal{H} < \mathcal{K}$ to mean that there is an orthoprojection E on $\mathcal{K}$ such that $E\mathcal{K}$ is invariant with respect to $\mathcal{G}$ and the representation $\mathcal{G}|\mathcal{H}$ is unitarily equivalent to $\mathcal{G}|E\mathcal{K}$. Call $\mathcal{H}$ a* subobject *of $\mathcal{K}$.*

It is easy to see that $<$ is a partial order. Note that $\mathcal{H}<\mathcal{K}$ iff there is an isometry $V \in \mathcal{L}_{\mathcal{G}}(\mathcal{H},\mathcal{K})$ such that $VV^* =: E$ is a projection of $\mathcal{K}$, i.e., $V\mathcal{H}=E\mathcal{K}$. Then $\mathcal{J}(V) \in \mathcal{A}$ and $E\mathcal{K} = \mathcal{J}(V)\cdot\mathcal{H}$.

If $E \in \mathcal{L}_{\mathcal{G}}(\mathcal{K})$ is an orthoprojection $0<E<\mathbb{I}$, i.e., E is a reducing projection for the representation of $\mathcal{G}$ on $\mathcal{K}$, then the question arises whether there is an object $\mathcal{H}$ such that the representations on $\mathcal{H}$ and $E\mathcal{K}$ are unitarily equivalent. This suggests the concept of *closedness* of $\mathcal{T}_{\mathcal{G}}$ with respect to subobjects.

Definition 2.8: The category $\mathcal{T}_{\mathcal{G}}$ is closed with respect to subobjects *if to each $\mathcal{K} \in Ob\ \mathcal{T}_{\mathcal{G}}$ and to each nontrivial orthoprojection $E \in \mathcal{L}_{\mathcal{G}}(\mathcal{K})$ there is an isometry $\hat{V} \in \mathcal{A}$ with $\hat{V}\hat{V}^* = \mathcal{J}(E)$. In this case $\mathcal{H} := \hat{V}^*\cdot\mathcal{K}$ is a subobject $\mathcal{H}<\mathcal{K}$ assigned to E, where $\hat{V}=\mathcal{J}(V)$ for some isometry $V \in \mathcal{L}_{\mathcal{G}}(\mathcal{H},\mathcal{K})$ with $VV^*=E$.*

Next, we consider when an object of $\mathcal{T}_{\mathcal{G}}$ carries the direct sum of the representations of two other objects. If V, $W \in \mathcal{A}$ are isometries with $VV^*+WW^*=\mathbb{I}$ and $\mathcal{H}$, $\mathcal{K} \in \mathrm{Ob}\ \mathcal{T}_{\mathcal{G}}$ then we call the algebraic Hilbert space $V\mathcal{H}+W\mathcal{K}$ of support 1 a direct sum of $\mathcal{H}$ and $\mathcal{K}$. It is $\mathcal{G}$-invariant and carries the direct sum of the representations on $\mathcal{H}$ and $\mathcal{K}$ but in general depends on the choice of isometries V, W. We define the following.

Definition 2.9: (i) The category $\mathcal{T}_{\mathcal{G}}$ is closed with respect to direct sums *if to each $\mathcal{H}_1$, $\mathcal{H}_2 \in \mathrm{Ob}\ \mathcal{T}_{\mathcal{G}}$ there is an object $\mathcal{K} \in \mathrm{Ob}\ \mathcal{T}_{\mathcal{G}}$ and there are isometries V_1, $V_2 \in \mathcal{A}$ with $V_1V_1^*+V_2V_2^*=\mathbb{I}$ such that $\mathcal{K}=V_1\mathcal{H}_1+V_2\mathcal{H}_2$ [then $V_1 \in (\mathcal{H}_1,\mathcal{K})$ and $V_2 \in (\mathcal{H}_2,\mathcal{K})$ follow].*

(ii) A C^*-algebra $\mathcal{A}$ satisfies Property B *if there are isometries V_1, $V_2 \in \mathcal{A}$ such that $V_1V_1^* + V_2V_2^*=\mathbb{I}$. A Hilbert system $\{\mathcal{F},\mathcal{G}\}$ is said to satisfy* Property B *if its fixed point algebra $\mathcal{A} := \Pi_\iota\mathcal{F}$ satisfies Property B.*

Remark 2.10: For a Hilbert system $\{\mathcal{F},\mathcal{G}\}$ we have the following.

(i) It satisfies Property B iff $\mathcal{T}_{\mathcal{G}}$ is closed with respect to direct sums.
(ii) For non-Abelian $\mathcal{G}$, the category $\mathcal{T}_{\mathcal{G}}$ is closed with respect to subobjects iff it is closed with respect to direct sums iff it has Property B, cf. Proposition 3.5 of Ref. 9.
(iii) In the case that $\mathcal{G}$ is Abelian, the theory simplifies. This is because we already have Pontryagin's duality theorem, hence it is not necessary to consider closure under subobjects and direct sums to obtain a duality theory.

C. The category of canonical endomorphisms

The main aim of DR theory is to obtain an intrinsic structure on $\mathcal{A}$ from which we can reconstruct the Hilbert system $\{\mathcal{F},\mathcal{G}\}$ in an essentially unique way. Here we want to transport the rich structure of $\mathcal{T}_{\mathcal{G}}$ to $\mathcal{A}$.

Definition 2.11: To each $\mathcal{G}$-invariant algebraic Hilbert space $\mathcal{H}\subset\mathcal{F}$ there is assigned a corresponding inner endomorphism $\rho_{\mathcal{H}} \in \mathrm{End}\ \mathcal{F}$ *given by*

$$\rho_{\mathcal{H}}(F) := \sum_{j=1}^{d(\mathcal{H})} \Phi_j F \Phi_j^*,$$

where $\{\Phi_j | j=1,\ldots,d(\mathcal{H})\}$ is any orthonormal basis of $\mathcal{H}$. Note that $\rho_{\mathcal{H}}$ preserves $\mathcal{A}$. A canonical endomorphism *is the restriction of an inner endomorphism to $\mathcal{A}$, i.e., it is of the form $\rho_{\mathcal{H}}\restriction\mathcal{A} \in End\ \mathcal{A}$.*

Remark 2.12: (i) The definition of the canonical endomorphisms uses $\mathcal{F}$ explicitly. The question arises whether the canonical endomorphisms can be characterized by intrinsic properties within $\mathcal{A}$. This interplay between the $\rho_{\mathcal{H}}$ and the $\rho_{\mathcal{H}}\restriction\mathcal{A}$ plays an essential role in the DR theory. Below, we omit the restriction symbol and regard the $\rho_{\mathcal{H}}$ also as endomorphisms of $\mathcal{A}$.

(ii) If the emphasis is only on the representation γ and not on its corresponding algebraic Hilbert space $\mathcal{H}_\gamma$, we will write ρ_γ instead of $\rho_{\mathcal{H}_\gamma}$.

(iii) Note that $\Phi A=\rho_{\mathcal{H}}(A)\Phi$ for all $\Phi \in \mathcal{H}$ and $A \in \mathcal{A}$.

(iv) Note that the identity endomorphism ι is assigned to $\mathcal{H}=\mathbb{C}\,\mathbb{I}$, i.e., $\rho_{\mathbb{C}\mathbb{I}} := \iota$.

(v) Let $\mathcal{H}$, $\mathcal{K}$ be as before, then $\rho_{\mathcal{H}}\circ\rho_{\mathcal{K}}=\rho_{\mathcal{H}\cdot\mathcal{K}}$.

(vi) The map ρ from Ob $\mathcal{T}_{\mathcal{G}}$ to the canonical endomorphisms is in general not injective. In fact we have the following: if $\mathcal{H}$, $\mathcal{K}\in$ Ob $\mathcal{T}_{\mathcal{G}}$, then $\rho_{\mathcal{H}}\restriction\mathcal{A}=\rho_{\mathcal{K}}\restriction\mathcal{A}$ iff $\Psi^*\Phi\in\mathcal{A}'\cap\mathcal{F}$ for all $\Phi\in\mathcal{H}$, $\Psi\in\mathcal{K}$, cf. Proposition 3.9 in Ref. 9.

Definition 2.13: Define $\mathcal{T}$ to be the category with objects the canonical endomorphisms, and arrows the intertwiner spaces, where the intertwiner space *of canonical endomorphisms σ, $\tau\in$ End $\mathcal{A}$ is*

$$(\sigma,\tau):=\{X\in\mathcal{A}\,|\,X\sigma(A)=\tau(A)X \text{ for all } A\in\mathcal{A}\},$$

and this is a complex Banach space. For $A\in(\sigma,\sigma')$, $B\in(\tau,\tau')$, we define $A\times B:=A\sigma(B)\in(\sigma\tau,\sigma'\tau')$. We will say that σ, $\tau\in$ End $\mathcal{A}$ are mutually disjoint *if $(\sigma,\tau)=\{0\}$ when $\sigma\neq\tau$.*

Remark 2.14: (i) We have $(\iota,\iota)=Z(\mathcal{A}):=$ center of $\mathcal{A}$.

(ii) The composition of two canonical endomorphisms [which corresponds to products of the generating Hilbert spaces, see Remark 2.13 (v), i.e., to tensor products of representations] satisfies the correct compatibility conditions with the product $\times$ of intertwiners to ensure that $\mathcal{T}$ is a C*-tensor category cf. Proposition 2.6 and Ref. 1. The identity object is ι.

(iii) Recall the isometry $\mathcal{J}:\mathcal{L}_{\mathcal{G}}(\mathcal{H},\mathcal{K})\to\mathcal{A}$ encountered in Remark 2.5 (vii). We claim that its image is in fact contained in $(\rho_{\mathcal{H}},\rho_{\mathcal{K}})$. To see this, let $\Phi\in\mathcal{H}$, $A\in\mathcal{A}$, and $T\in\mathcal{L}_{\mathcal{G}}(\mathcal{H},\mathcal{K})$. Then

$$\mathcal{J}(T)\rho_{\mathcal{H}}(A)\Phi=\mathcal{J}(T)\Phi\cdot A=T(\Phi)\cdot A=\rho_{\mathcal{K}}(A)T(\Phi)=\rho_{\mathcal{K}}(A)\mathcal{J}(T)\cdot\Phi$$

hence

$$\mathcal{J}(T)\rho_{\mathcal{H}}(A)=\rho_{\mathcal{K}}(A)\mathcal{J}(T),$$

i.e., $\mathcal{J}(T)\in(\rho_{\mathcal{H}},\rho_{\mathcal{K}})$ or

$$(\mathcal{H},\mathcal{K})=\mathcal{J}(\mathcal{L}_{\mathcal{G}}(\mathcal{H},\mathcal{K}))\subseteq(\rho_{\mathcal{H}},\rho_{\mathcal{K}}). \tag{2}$$

In general, the inclusion is proper. Note that for $R\in(\mathcal{H},\mathcal{K})$, $R'\in(\mathcal{H}',\mathcal{K}')$ we have $\mathcal{J}(R\otimes R')=R\rho_{\mathcal{H}}(R')$, i.e., $\times$ restricted to the $(\mathcal{H},\mathcal{K})$'s coincides with the definition of $\times$ in Proposition 2.6 of the category $\mathcal{T}_{\mathcal{G}}$.

Next we would like to define the concepts of subobject and direct sums on Ob $\mathcal{T}$ compatibly with those on Ob $\mathcal{T}_{\mathcal{G}}$ under the morphism ρ. Recall that $\mathcal{H}<\mathcal{K}$ iff we have an isometry $V\in\mathcal{L}_{\mathcal{G}}(\mathcal{H},\mathcal{K})$ and a projection $E\in\mathcal{L}_{\mathcal{G}}(\mathcal{K})$ with $V\mathcal{H}=E\mathcal{K}=\mathcal{J}(E)\cdot\mathcal{K}=\mathcal{J}(V)\cdot\mathcal{H}$. Then by (2) we get that $\mathcal{J}(V)\in(\rho_{\mathcal{H}},\rho_{\mathcal{K}})$ and $\mathcal{J}(E)\in(\rho_{\mathcal{K}},\rho_{\mathcal{K}})$.

Note that if $\mathcal{L}=V\mathcal{H}+W\mathcal{K}$ for isometries V, $W\in\mathcal{A}$ with $VV^*+WW^*=\mathbb{1}$, then $V\in(\rho_{\mathcal{H}},\rho_{\mathcal{L}})$ and $W\in(\rho_{\mathcal{K}},\rho_{\mathcal{L}})$.

Definition 2.15: (i) $\tau\in$ Ob $\mathcal{T}$ is a subobject *of $\sigma\in$ Ob $\mathcal{T}$, denoted $\tau<\sigma$, if there is an isometry $V\in(\tau,\sigma)$. In this case $\tau(\cdot)=V^*\sigma(\cdot)V$ and $VV^*=:E\in(\sigma,\sigma)$ follow.*

(ii) $\lambda\in$ Ob $\mathcal{T}$ is a direct sum *of σ, $\tau\in$ Ob $\mathcal{T}$, if there are isometries $V\in(\sigma,\lambda)$, $W\in(\tau,\lambda)$ with $VV^*+WW^*=\mathbb{1}$ such that*

$$\lambda(\cdot)=V\sigma(\cdot)V^*+W\tau(\cdot)W^*.$$

Remark 2.16: (i) The subobject relation $\tau<\sigma$ is again a partial order, because $\tau<\sigma$ and $\sigma<\mu$ imply the existence of isometries $V\in(\tau,\sigma)$, $W\in(\sigma,\mu)$. Then $WV\in(\tau,\mu)$ is also an isometry, i.e., $\tau<\mu$.

(ii) A direct sum as defined above is only unique up to unitary equivalence, i.e., if λ, λ' are direct sums of σ, $\tau\in$ Ob $\mathcal{T}$, then there is a unitary $U\in(\lambda,\lambda')$.

(iii) We have $\rho_{V\mathcal{H}+W\mathcal{K}}(\cdot)=V\rho_{\mathcal{H}}(\cdot)V^*+W\rho_{\mathcal{K}}(\cdot)W^*$ where the isometries V, $W\in\mathcal{A}$ satisfy $VV^*+WW^*=\mathbb{1}$. Also, if $\mathcal{H}<\mathcal{K}$, then $\tau:=\rho_{\mathcal{H}}<\rho_{\mathcal{K}}=:\sigma$. However, this does not mean that the partial order $\tau<\sigma$ can be *defined* by $\mathcal{H}<\mathcal{K}$ because the transitivity can be violated for some choices of $\mathcal{H}$, $\mathcal{K}$, cf. Remark 2.12 (vi).

The closedness of $\mathcal{T}$ with respect to direct sums is defined by the closedness of $\mathcal{T}_\mathcal{G}$ with respect to direct sums. The closedness with respect to subobjects for $\mathcal{T}$ is defined by the closedness with respect to subobjects for $\mathcal{T}_\mathcal{G}$ in the following sense: If

$$\lambda = \rho_\mathcal{H} \in \mathrm{Ob}\,\mathcal{T} \tag{3}$$

is given then for all $\mathcal{H}$ satisfying (3) and to each nontrivial projection $E \in \mathcal{J}(\mathcal{L}_\mathcal{G}(\mathcal{H}))$ there is an isometry $V \in \mathcal{A}$ with $VV^* = E$. Then we have the following.

Proposition 2.17: If $\{\mathcal{F},\mathcal{G}\}$ is non-Abelian and satisfies Property B then $\mathcal{T}$ is closed with respect to direct sums and subobjects.

D. Connection between $\mathcal{T}_\mathcal{G}$ and $\mathcal{T}$ and further structures

In the following we assume that $\{\mathcal{F},\mathcal{G}\}$ satisfies Property B.

There is a very important relation between the two categories $\mathcal{T}_\mathcal{G}$ and $\mathcal{T}$, obtained as follows. The two assignments $\rho: \mathrm{Ob}\,\mathcal{T}_\mathcal{G} \to \mathcal{T}$ (by $\mathcal{H} \to \rho_\mathcal{H}$) and $\mathcal{J}: \mathcal{L}_\mathcal{G}((\mathcal{H},\mathcal{K})) \to (\rho_\mathcal{H},\rho_\mathcal{K})$ combine into a faithful categorial morphism from $\mathcal{T}_\mathcal{G}$ to $\mathcal{T}$ which is compatible with direct sums and subobjects [cf. Remark 2.16 (iii)] but is not full in general, i.e., the inclusion in Eq. (2) is improper for some $\mathcal{H}$ and $\mathcal{K}$. If $\mathcal{A}' \cap \mathcal{F} = \mathbb{C}\,\mathbb{1}$, then this categorial morphism becomes an isomorphism, cf. Proposition 3.12 in Ref. 9.

The category $\mathcal{T}_\mathcal{G}$ has the following additional structures (Refs. 3 and 12).

Proposition 2.18: For $\{\mathcal{F},\mathcal{G}\}$ the category $\mathcal{T}_\mathcal{G}$ satisfies

(1) *it has a* permutation structure, *i.e., a map ϵ from* $\mathrm{Ob}\,\mathcal{T}_\mathcal{G} \times \mathrm{Ob}\,\mathcal{T}_\mathcal{G}$ *into the arrows such that*

- (i) $\epsilon(\mathcal{H},\mathcal{K}) \in (\mathcal{H}\mathcal{K},\mathcal{K}\mathcal{H})$ *is a unitary*,
- (ii) $\epsilon(\mathcal{H},\mathcal{K})\epsilon(\mathcal{K},\mathcal{H}) = \mathbb{1}$,
- (iii) $\epsilon(1,\mathcal{H}) = \epsilon(\mathcal{H},1) = \mathbb{1}$,
- (iv) $\epsilon(\mathcal{H}\mathcal{K},\mathcal{L}) = \epsilon(\mathcal{H},\mathcal{L})\rho_\mathcal{H}(\epsilon(\mathcal{K},\mathcal{L}))$,
- (v) $\epsilon(\mathcal{H}',\mathcal{K}')A \times B = B \times A\epsilon(\mathcal{H},\mathcal{K})$ *for all* $A \in (\mathcal{H},\mathcal{H}')$, $B \in (\mathcal{K},\mathcal{K}')$.

For $\mathcal{T}_\mathcal{G}$ the permutation structure is given by

$$\epsilon(\mathcal{H},\mathcal{K}) := \mathcal{J}(\Theta(\mathcal{H},\mathcal{K})) = \sum_{j,k} \Psi_j \Phi_k \Psi_j^* \Phi_k^*,$$

where Θ is the flip operator $\mathcal{H}\otimes\mathcal{K} \to \mathcal{K}\otimes\mathcal{H}$, and where $\{\Phi_k\}_k$, $\{\Psi_j\}_j$ are orthonormal bases of $\mathcal{H}$ and $\mathcal{K}$, respectively.

(2) *It has a* conjugation structure, *i.e., for each $\mathcal{H} \in \mathrm{Ob}\,\mathcal{T}_\mathcal{G}$ there is a conjugated object $\bar{\mathcal{H}} \in \mathrm{Ob}\,\mathcal{T}_\mathcal{G}$, carrying the conjugated representation of $\mathcal{G}$ and there are conjugate arrows $R_\mathcal{H} \in (1,\bar{\mathcal{H}}\mathcal{H})$, $S_\mathcal{H} = \epsilon(\bar{\mathcal{H}},\mathcal{H})R_\mathcal{H}$ such that*

$$S_\mathcal{H}^* \rho_\mathcal{H}(R_\mathcal{H}) = \mathbb{1}, \quad R_\mathcal{H}^* \rho_{\bar{\mathcal{H}}}(S_\mathcal{H}) = \mathbb{1}.$$

For $\mathcal{T}_\mathcal{G}$ we have $\mathcal{R}_\mathcal{H} := \Sigma_j \bar{\Psi}_j \Psi_j$, where $\{\bar{\Psi}_j\}_j$ is an orthonormal basis of $\bar{\mathcal{H}}$. If $\mathcal{H}$ carries the representation $\oplus_j \gamma_j$, $\gamma_j \in \hat{\mathcal{G}}$, then $\bar{\mathcal{H}}$ is given by a direct sum of $\mathcal{H}_{\overline{\gamma_j}}$, where $\overline{\gamma_j} \in \hat{\mathcal{G}}$ represents the conjugated representation of γ_j.

Remark 2.19: Using the categorial morphism from $\mathcal{T}_\mathcal{G}$ to $\mathcal{T}$ we equip $\mathcal{T}$ with the image permutation and conjugation structures of those on $\mathcal{T}_\mathcal{G}$. Note that for the image permutation structure in $\mathcal{T}$, property (v) need not hold for *all* arrows [cf. Remark 2.14 (iii)].

For the next definition, observe first that from the operations defined for an abstract tensor category (cf. Proposition 2.6), we can define isometries and projections in its arrow spaces, i.e., an arrow $V \in (\lambda,\tau)$ is an isometry if $V^* \circ V = 1_\lambda$, and an arrow $E \in (\lambda,\lambda)$ is a projection if $E = E^* = E \circ E$.

Definition 2.20: An (abstract) DR category *is an (abstract) tensor C^*-category $\mathcal{C}$ with* $(1,1)$

$=\mathbb{C}\,\mathbb{I}$ *which has a permutation and a conjugation structure, and has direct sums and subobjects, i.e., to all objects* λ, σ *there is an object* τ *and isometries* $V\in(\lambda,\tau)$, $W\in(\sigma,\tau)$ *such that* $VV^*+WW^*=1_\tau$, *and to each nontrivial projection* $E\in(\lambda,\lambda)$ *there is an object* σ *and an isometry* $V\in(\sigma,\lambda)$ *such that* $E=VV^*$.

If the Hilbert system $\{\mathcal{F},\mathcal{G}\}$ satisfies Property B then $\mathcal{T}_\mathcal{G}$ is an example of a DR category, but not necessarily $\mathcal{T}$ [since property (v) in Proposition 2.18 need not hold for all arrows]. However, if additionally $\mathcal{A}'\cap\mathcal{F}=\mathbb{C}\,\mathbb{I}$ holds then also $\mathcal{T}$ is a DR category.

E. Duality theorems

Unless otherwise specified, in the following we assume Property B for $\{\mathcal{F},\mathcal{G}\}$ when $\mathcal{G}$ is non-Abelian. The DR theorem produces a bijection between pairs

$$\{\mathcal{A},\mathcal{T}\} \quad \text{and } \{\mathcal{F},\mathcal{G}\},$$

where $\mathcal{T}$ is a DR category of unital endomorphisms of the unital C*-algebra $\mathcal{A}$ with $Z(\mathcal{A})=\mathbb{C}\,\mathbb{I}$, and $\{\mathcal{F},\mathcal{G}\}$ is a Hilbert extension of $\mathcal{A}$ having trivial relative commutant, i.e., $\mathcal{A}'\cap\mathcal{F}=\mathbb{C}\,\mathbb{I}$ (see Refs. 1,15, and 16). The DR theorem says that in the case of Hilbert extensions of $\mathcal{A}$ with trivial relative commutant, the category $\mathcal{T}$ of all canonical endomorphisms can indeed be characterized intrinsically by their abstract algebraic properties as endomorphisms of $\mathcal{A}$ and a corresponding bijection can be established.

In this section we want to state how to obtain such a bijection for C*-algebras $\mathcal{A}$ with nontrivial center $\mathcal{Z}\supset\mathbb{C}\,\mathbb{I}$. A first problem is that the category $\mathcal{T}_\mathcal{G}$ and $\mathcal{T}$ *need not* be isomorphic anymore, cf. Remark 2.14 (iv) and Remark 2.12 (vi), since now we have

$$\mathbb{C}\,\mathbb{I}\neq\mathcal{Z}\subseteq\mathcal{A}'\cap\mathcal{F}.$$

We will investigate in the following the class of Hilbert extensions $\{\mathcal{F},\mathcal{G}\}$ with compact group $\mathcal{G}$ and where the relative commutant satisfies the following *minimality* condition.

Definition 2.21: A Hilbert system $\{\mathcal{F},\mathcal{G}\}$ *is called* minimal *if the condition*

$$\mathcal{A}'\cap\mathcal{F}=Z(\mathcal{A}) \tag{4}$$

is satisfied.

Then we have (cf. Proposition 4.3 of Ref. 9) the following.

Proposition 2.22: Let $\{\mathcal{F},\mathcal{G}\}$ *be a given Hilbert system. Then* $\mathcal{A}'\cap\mathcal{F}=Z(\mathcal{A})$ *iff* $(\rho_\gamma,\rho_{\gamma'})=\{0\}$ *for* $\gamma\neq\gamma'$, *i.e., iff the set* $\{\rho_\gamma|\,\gamma\in\hat{\mathcal{G}}\}$ *is mutually disjoint.*

Observe that in any Hilbert system, for each $\tau\in\mathrm{Ob}\,\mathcal{T}$ the space $\mathfrak{h}_\tau:=\mathcal{H}_\tau Z(\mathcal{A})$ (where $\mathcal{H}_\tau$ is a $\mathcal{G}$-invariant algebraic Hilbert space) is a $\mathcal{G}$-invariant right Hilbert $Z(\mathcal{A})$-module, i.e., there is a nondegenerate inner product taking its values in $Z(\mathcal{A})$ and it is $\langle A,B\rangle=A^*B$. Now we have (cf. Proposition 3.1 of Ref. 17) the following.

Proposition 2.23: Let $\{\mathcal{F},\mathcal{G}\}$ *be a given minimal Hilbert system, then the correspondence* $\tau\leftrightarrow\mathfrak{h}_\tau$ *is a bijection. Thus* $\mathfrak{h}_\tau=\mathcal{H}_\tau Z(\mathcal{A})$ *is independent of the choice of* $\mathcal{H}_\tau$, *providing that* $\tau=\rho_{\mathcal{H}_\tau}$. *This bijection satisfies the conditions*

$$\sigma\circ\tau\leftrightarrow\mathfrak{h}_\sigma\cdot\mathfrak{h}_\tau,$$

$$\lambda=(\mathrm{Ad}\,V)\circ\sigma+(\mathrm{Ad}\,W)\circ\tau\leftrightarrow\mathfrak{h}_\lambda=V\mathfrak{h}_\sigma+W\mathfrak{h}_\tau.$$

Thus for minimal Hilbert systems, the $Z(\mathcal{A})$-modules $\mathfrak{h}_\tau$ are uniquely determined by their canonical endomorphisms τ, even though the choice of $\mathcal{H}_\tau$ is not unique. We are now interested in those choices of $\mathcal{H}_\tau$ which are compatible with products.

Definition 2.24: A Hilbert system $\{\mathcal{F},\mathcal{G}\}$ *is called* regular *if there is an assignment* $\sigma\to\mathcal{H}_\sigma$ *from* Ob $\mathcal{T}$ *to* $\mathcal{G}$*-invariant algebraic Hilbert spaces in* $\mathcal{F}$ *such that*

(i) $\sigma=\rho_{\mathcal{H}_\sigma}$, *i.e.,* σ *is the canonical endomorphism of* $\mathcal{H}_\sigma$,

(ii) $\sigma\circ\tau\to\mathcal{H}_\sigma\cdot\mathcal{H}_\tau$.

In a minimal Hilbert system regularity means that there is a "representing" Hilbert space $\mathcal{H}_\tau\subset\mathfrak{h}_\tau$ for each τ with $\mathfrak{h}_\tau=\mathcal{H}_\tau Z(\mathcal{A})$ such that the compatibility relation (ii) holds.

If a Hilbert system is minimal and $Z(\mathcal{A})=\mathbb{C}1$ then it is necessarily regular. Thus a class of examples which are trivially minimal and regular, is provided by DHR-superselection theory. A nontrivial example of a minimal and regular Hilbert system is constructed in Ref. 9.

Then we obtain, cf. Theorem 4.9 of Ref. 9, the following.

Theorem 2.25: *Let $\{\mathcal{F},\mathcal{G}\}$ be a minimal and regular Hilbert system, then $\mathcal{T}$ contains a* C**-subcategory $\mathcal{T}_\mathbb{C}$ with the same objects*, $\mathrm{Ob}\,\mathcal{T}_\mathbb{C}=\mathrm{Ob}\,\mathcal{T}$, *and arrows* $(\sigma,\tau)_\mathbb{C}:=(\mathcal{H}_\sigma,\mathcal{H}_\tau)=\mathcal{J}(\mathcal{L}_\mathcal{G}(\mathcal{H}_\sigma,\mathcal{H}_\tau))\subset(\sigma,\tau)$ *such that*

P.1, $\mathcal{T}_\mathbb{C}$ *is a DR-category* [*in particular* $(\iota,\iota)_\mathbb{C}=\mathbb{C}1$],

P.2, $(\sigma,\tau)=(\sigma,\tau)_\mathbb{C}\sigma(Z(\mathcal{A}))=\tau(Z(\mathcal{A}))(\sigma,\tau)_\mathbb{C}\sigma(Z(\mathcal{A}))$.

Remark 2.26: (i) The conditions P.1 and P.2 imply that each basis of $(\sigma,\tau)_\mathbb{C}$ is simultaneously a module basis of (σ,τ) modulo $\sigma(\mathcal{Z}(\mathcal{A}))$ as a right module, i.e., the module (σ,τ) is free.

(ii) We will call the DR-subcategory $\mathcal{T}_\mathbb{C}$ in Theorem 2.25 admissible. If "minimality" is omitted from the hypotheses of Theorem 2.25, then property P.1 remains valid, but not P.2. In this case $\mathcal{T}_\mathbb{C}$ is a DR-subcategory only. A construction of an example with admissible subcategory can be found in Ref. 9.

The converse of Theorem 2.25 is also true, and states the main duality result, cf. Ref. 7.

Theorem 2.27: *Let $\mathcal{T}$ be a C*-tensor category of unital endomorphisms of $\mathcal{A}$ and let $\mathcal{T}_\mathbb{C}$ be an admissible (DR-) subcategory. Then there is a minimal and regular Hilbert extension $\{\mathcal{F},\mathcal{G}\}$ of $\mathcal{A}$ such that $\mathcal{T}$ is isomorphic to the category of all canonical endomorphisms of $\{\mathcal{F},\mathcal{G}\}$. Moreover, if $\mathcal{T}_\mathbb{C}$, $\mathcal{T}'_\mathbb{C}$ are two admissible subcategories of $\mathcal{T}$, then the corresponding Hilbert extensions are $\mathcal{A}$-module isomorphic iff $\mathcal{T}_\mathbb{C}$ is* equivalent *to $\mathcal{T}'_\mathbb{C}$, i.e., iff there is a map V from* Ob $\mathcal{T}$ *to the arrows such that*

$$V_\lambda\in(\lambda,\lambda),\quad V_\lambda \text{ is unitary, and } V_{\lambda\circ\sigma}=V_\lambda\times V_\sigma,$$

$$(\lambda,\sigma)'_\mathbb{C}=V_\sigma(\lambda,\sigma)_\mathbb{C}V_\lambda^*\subset(\lambda,\sigma)$$

and we have the following compatibility relations for the corresponding permutators ϵ, ϵ' and conjugates R_λ, R'_λ:

$$\epsilon'(\lambda,\sigma)=(V_\sigma\times V_\lambda)\cdot\epsilon(\lambda,\sigma)\cdot(V_\lambda\times V_\sigma)^*$$

$$R'_\lambda=V_{\bar\lambda\circ\lambda}R_\lambda,\quad S'_\lambda=\epsilon'(\lambda,\bar\lambda)R'_\lambda.$$

Thus, in minimal and regular Hilbert systems there is an intrinsic characterization of the category of all canonical endomorphisms in terms of $\mathcal{A}$ only. Moreover, up to $\mathcal{A}$-module isomorphisms, there is a bijection between minimal and regular Hilbert extensions and C*-tensor categories $\mathcal{T}$ of unital endomorphisms of $\mathcal{A}$ with admissible subcategories.

Note that Theorem 2.27 is a generalization of the DR theorem for the case of nontrivial center $Z(\mathcal{A})\supset\mathbb{C}1$, i.e., it contains the case of the DR theorem, in that if $Z(\mathcal{A})=\mathbb{C}1$ then $\mathcal{T}$ itself is admissible (hence a DR-category) and the corresponding Hilbert extensions have trivial relative commutant.

F. Hilbert systems with Abelian groups

If $\mathcal{G}$ is Abelian the preceding structure simplifies radically. Specifically, $\hat{\mathcal{G}}$ is a discrete Abelian group (the character group), each $\mathcal{H}_\gamma$, $\gamma\in\hat{\mathcal{G}}$ is one-dimensional with a generating unitary U_γ, hence the canonical endomorphisms $\rho_{\mathcal{H}_\gamma}$ (denoted by ρ_γ) are in fact automorphisms, necessarily

outer on $\mathcal{A}$. Since $\rho_{\gamma_1}\circ\rho_{\gamma_2}=\rho_{\gamma_1\gamma_2}$ in this case the set Γ of all canonical endomorphisms $\rho_{\mathcal{H}_\gamma}$ is a group with the property $\hat{\mathcal{G}}\cong\Gamma/\mathrm{int}\,\mathcal{A}$. Hence it is not necessary to consider direct sums, i.e., Property B for $\mathcal{A}$ can be dropped.

In the case $Z(\mathcal{A})=\mathbb{C}\mathbb{1}$ the permutators ϵ (restricted to $\hat{\mathcal{G}}\times\hat{\mathcal{G}}$) are elements of the second cohomology group $H^2(\hat{\mathcal{G}})$ and

$$U_{\gamma_1}\cdot U_{\gamma_2}=\omega(\gamma_1,\gamma_2)U_{\gamma_1\circ\gamma_2},$$

where

$$\epsilon(\gamma_1,\gamma_2)=\frac{\omega(\gamma_1,\gamma_2)}{\omega(\gamma_2,\gamma_1)}$$

and ω is a corresponding 2-cocycle. The field algebra $\mathcal{F}$ is just the ω-twisted discrete crossed product of $\mathcal{A}$ with $\hat{\mathcal{G}}$ (see, e.g., Ref. 2, p. 86ff for details). For the case $Z(\mathcal{A})\supset\mathbb{C}\mathbb{1}$ see Ref. 18 (though the minimal case is not mentioned there).

III. KINEMATICS FOR QUANTUM CONSTRAINTS

In this section we give a brief summary of the method of imposing quantum constraints, developed by Grundling and Hurst.[4,8,5] Our starting point is the following.

Definition 3.1: A quantum system with constraints *is a pair* $(\mathcal{B},\mathcal{C})$ *where the* system algebra $\mathcal{B}$ *is a unital* C^**-algebra containing the* constraint set $\mathcal{C}=\mathcal{C}^*$. *A* constraint condition *on* $(\mathcal{B},\mathcal{C})$ *consists of the selection of the physical state space by*

$$\mathfrak{S}_D:=\{\omega\in\mathfrak{S}(\mathcal{B})\,|\,\pi_\omega(C)\Omega_\omega=0\ \ \forall\ C\in\mathcal{C}\},$$

where $\mathfrak{S}(\mathcal{B})$ *denotes the state space of* $\mathcal{B}$, *and* $(\pi_\omega,\mathcal{H}_\omega,\Omega_\omega)$ *denotes the GNS data of* ω. *The elements of* $\mathfrak{S}_D$ *are called* Dirac states. *The case of* unitary constraints *means that* $\mathcal{C}=\mathcal{U}-\mathbb{I},\mathcal{U}\subset\mathcal{B}_u$, *and for this we will also use the notation* $(\mathcal{B},\mathcal{U})$.

The assumption is that all physical information is contained in the pair $(\mathcal{B},\mathfrak{S}_D)$. Examples of constraint theories as defined here, have been worked out in detail for various forms of electromagnetism cf. Refs. 4,19, and 5.

For the case of unitary constraints we have the following equivalent characterizations of the Dirac states [cf. Ref. 4, Theorem 2.19 (ii)]:

$$\mathfrak{S}_D=\{\omega\in\mathfrak{S}(\mathcal{B})\,|\,\omega(U)=1\ \ \forall\ U\in\mathcal{U}\} \tag{5}$$

$$=\{\omega\in\mathfrak{S}(\mathcal{B})\,|\,\omega(FU)=\omega(F)=\omega(UF)\ \ \forall\ F\in\mathcal{B},U\in\mathcal{U}\}. \tag{6}$$

Moreover, the set $\{\alpha_U:=\mathrm{Ad}(U)\,|\,U\in\mathcal{U}\}$ of automorphisms of $\mathcal{B}$ leaves every Dirac state invariant, i.e., we have $\omega\circ\alpha_U=\omega$ for all $\omega\in\mathfrak{S}_D$, $U\in\mathcal{U}$.

For a general constraint set $\mathcal{C}$, observe that we have

$$\mathfrak{S}_D=\{\omega\in\mathfrak{S}(\mathcal{B})\,|\,\omega(C^*C)=0\ \ \forall\ C\in\mathcal{C}\}=\{\omega\in\mathfrak{S}(\mathcal{B})\,|\,\mathcal{C}\subseteq N_\omega\}=\mathcal{N}^\perp\cap\mathfrak{S}(\mathcal{B}).$$

Here $N_\omega:=\{F\in\mathcal{B}\,|\,\omega(F^*F)=0\}$ is the left kernel of ω and $\mathcal{N}:=\cap\{N_\omega\,|\,\omega\in\mathfrak{S}_D\}$, and $\mathcal{N}^\perp$ denotes the annihilator of $\mathcal{N}$ in the dual of $\mathcal{B}$. Now $\mathcal{N}=\text{clo-span}(\mathcal{B}\mathcal{C})$ because every closed left ideal is the intersection of the left kernels which contains it (cf. 3.13.5 in Ref. 20). Thus $\mathcal{N}$ is the left ideal generated by $\mathcal{C}$. Since $\mathcal{C}$ is self-adjoint and contained in $\mathcal{N}$ we conclude

$$\mathcal{C}\subset\mathrm{C}^*(\mathcal{C})\subset\mathcal{N}\cap\mathcal{N}^*=\text{clo-span}(\mathcal{B}\mathcal{C})\cap\text{clo-span}(\mathcal{C}\mathcal{B}),$$

where $\mathrm{C}^*(\cdot)$ denotes the C^*-algebra in $\mathcal{B}$ generated by its argument. Then we have (cf. Ref. 5) the following.

Theorem 3.2: *For the Dirac states we have*

(i) $\mathfrak{S}_D \neq \emptyset$ *iff* $\mathbb{I} \notin \mathrm{C}^*(\mathcal{C})$ *iff* $\mathbb{I} \notin \mathcal{N} \cap \mathcal{N}^* =: \mathcal{D}$.
(ii) $\omega \in \mathfrak{S}_D$ *iff* $\pi_\omega(\mathcal{D})\Omega_\omega = 0$.
(iii) *An extreme Dirac state is pure*.

We will call a constraint set $\mathcal{C}$ first class if $\mathbb{I} \notin \mathrm{C}^*(\mathcal{C})$, and this is the nontriviality assumption which we henceforth make (Ref. 21, Sec. 3).

Now define

$$\mathcal{O} := \{F \in \mathcal{B} | [F,D] := FD - DF \in \mathcal{D} \ \forall D \in \mathcal{D}\}.$$

Then $\mathcal{O}$ is the C^*-algebraic analog of Dirac's observables (the weak commutant of the constraints).[22] Then (cf. Ref. 5) we have the following.

Theorem 3.3: *With the preceding notation we have*

(i) $\mathcal{D} = \mathcal{N} \cap \mathcal{N}^*$ *is the unique maximal* C^**-algebra in* $\cap\{\mathrm{Ker}\,\omega | \omega \in \mathfrak{S}_D\}$. *Moreover* $\mathcal{D}$ *is a hereditary* C^**-subalgebra of* $\mathcal{B}$.
(ii) $\mathcal{O} = M_{\mathcal{B}}(\mathcal{D}) := \{F \in \mathcal{B} | FD \in \mathcal{D} \ni DF \ \forall D \in \mathcal{D}\}$, *i.e., it is the relative multiplier algebra of* $\mathcal{D}$ *in* $\mathcal{B}$.
(iii) $\mathcal{O} = \{F \in \mathcal{B} | [F,\mathcal{C}] \subset \mathcal{D}\}$, *hence* $\mathcal{C}' \cap \mathcal{B} \subseteq \mathcal{O}$.
(iv) $\mathcal{D} = \text{clo-span}(\mathcal{O}\mathcal{C}) = \text{clo-span}(\mathcal{C}\mathcal{O})$.
(v) *For the case of unitary constraints, i.e.,* $\mathcal{C} = \mathcal{U} - \mathbb{1}$, *we have* $\mathcal{U} \subset \mathcal{O}$ *and* $\mathcal{O} = \{F \in \mathcal{B} | \alpha_U(F) - F \in \mathcal{D} \ \forall U \in \mathcal{U}\}$ *where* $\alpha_U := \mathrm{Ad}\, U$.

Thus $\mathcal{D}$ is a closed two-sided ideal of $\mathcal{O}$ and it is proper when $\mathfrak{S}_D \neq \emptyset$ [which we assume here by $\mathbb{I} \notin \mathrm{C}^*(\mathcal{C})$]. Since the traditional observables are $\mathcal{C}' \cap \mathcal{B}$, by (iii) we see that these are in $\mathcal{O}$. In general $\mathcal{O}$ can be much larger than $\mathcal{C}' \cap \mathcal{B}$.

Define the *maximal* C^**-algebra of physical observables as*

$$\mathcal{R} := \mathcal{O}/\mathcal{D}.$$

The factoring procedure is the actual step of imposing constraints. This method of constructing $\mathcal{R}$ from $(\mathcal{B},\mathcal{C})$ is called the T-procedure in Ref. 4, and it defines a map T from first class constraint pairs $(\mathcal{B},\mathcal{C})$ to unital C^*-algebras by $T(\mathcal{B},\mathcal{C}) := \mathcal{R} = \mathcal{O}/\mathcal{D}$. We require that after the T-procedure all physical information is contained in the pair $(\mathcal{R},\mathfrak{S}(\mathcal{R}))$, where $\mathfrak{S}(\mathcal{R})$ denotes the set of states on $\mathcal{R}$. Now, it is possible that $\mathcal{R}$ may not be simple (Ref. 4, Sec. 2), and this would not be acceptable for a physical algebra. So, using physical arguments, one would in practice choose a C^*-subalgebra $\mathcal{O}_c \subset \mathcal{O}$ containing the traditional observables $\mathcal{C}'$ such that

$$\mathcal{R}_c := \mathcal{O}_c/(\mathcal{D} \cap \mathcal{O}_c) \subset \mathcal{R}$$

is simple. The following result justifies the choice of $\mathcal{R}$ as the algebra of physical observables (cf. Theorem 2.20 in Ref. 4).

Theorem 3.4: *There exists a* w^**-continuous isometric bijection between the Dirac states on* $\mathcal{O}$ *and the states on* $\mathcal{R}$.

Insofar as the physics is now specified by $\mathcal{R}$, this suggests that we call two constraint sets equivalent if they produce the same $\mathcal{R}$. More precisely two constraint sets $\mathcal{C}_1 \subset \mathcal{B} \supset \mathcal{C}_2$ are called equivalent, denoted $\mathcal{C}_1 \sim \mathcal{C}_2$, if they select the same set of Dirac states, cf. Ref. 5. In fact

$$\mathcal{C}_1 \sim \mathcal{C}_2 \quad \text{iff clo-span}(\mathcal{B}\mathcal{C}_1) = \text{clo-span}(\mathcal{B}\mathcal{C}_2) \quad \text{iff } \mathcal{D}_1 = \mathcal{D}_2.$$

The hereditary property of $\mathcal{D}$ can be further analyzed, and we list the main points (the proofs are in Appendix A of Ref. 5).

Denote by π_u the universal representation of $\mathcal{B}$ on the universal Hilbert space $\mathcal{H}_u$ (Ref. 20, Sec. 3.7). $\mathcal{B}''$ is the strong closure of $\pi_u(\mathcal{B})$ and since π_u is faithful we make the usual identification of $\mathcal{B}$ with a subalgebra of $\mathcal{B}''$, i.e., generally omit explicit indication of π_u. If $\omega \in \mathfrak{S}(\mathcal{B})$, we will use the same symbol for the unique extension of ω from $\mathcal{B}$ to $\mathcal{B}''$.

Theorem 3.5: *For a constrained system* $(\mathcal{B},\mathcal{C})$ *there exists a projection* $P \in \mathcal{B}''$ *such that*

(i) $\mathcal{N}=\mathcal{B}''P\cap\mathcal{B}$,
(ii) $\mathcal{D}=P\mathcal{B}''P\cap\mathcal{B}$,
(iii) $\mathcal{S}_D=\{\omega\in\mathcal{S}(\mathcal{B})\,|\,\omega(P)=0\}$,
(iv) $\mathcal{O}=\{A\in\mathcal{B}\,|\,PA(\mathbb{I}-P)=0=(\mathbb{I}-P)AP\}=P'\cap\mathcal{B}$.

A projection satisfying the conditions of Theorem 3.5 is called *open* in Ref. 20.

What this theorem means, is that with respect to the decomposition

$$\mathcal{H}_u=P\mathcal{H}_u\oplus(\mathbb{I}-P)\mathcal{H}_u$$

we may rewrite

$$\mathcal{D}=\left\{F\in\mathcal{B}|F=\begin{pmatrix}D&0\\0&0\end{pmatrix},D\in P\mathcal{B}P\right\}$$

and

$$\mathcal{O}=\left\{F\in\mathcal{B}|F=\begin{pmatrix}A&0\\0&B\end{pmatrix},A\in P\mathcal{B}P,B\in(\mathbb{I}-P)\mathcal{B}(\mathbb{I}-P)\right\}.$$

It is clear that, in general, $\mathcal{O}$ can be much greater than the traditional observables $\mathcal{C}'\cap\mathcal{B}$. Next we show how to identify the final algebra of physical observables $\mathcal{R}$ with a subalgebra of $\mathcal{B}''$.

Theorem 3.6: *For P as above we have*

$$\mathcal{R}\cong\left\{F\in\mathcal{B}|F=\begin{pmatrix}0&0\\0&A\end{pmatrix}\right\}=(\mathbb{I}-P)(P'\cap\mathcal{B})\subset\mathcal{B}''.$$

Below we will need to consider a constraint system contained in a larger algebra, specifically, $\mathcal{C}\subset\mathcal{A}\subset\mathcal{F}$ where $\mathcal{C}$ is a first-class constraint set, and $\mathcal{A}$, $\mathcal{F}$ are unital C*-algebras. Now there are two constrained systems to consider; $(\mathcal{A},\mathcal{C})$ and $(\mathcal{F},\mathcal{C})$. The first one produces the algebras $\mathcal{D}\subset\mathcal{O}\subseteq\mathcal{A}$, and the second produces $\mathcal{D}_\mathcal{F}\subset\mathcal{O}_\mathcal{F}\subseteq\mathcal{F}$, where as usual,

$$\mathcal{N}=\text{clo-span}(\mathcal{AC}),\quad \mathcal{D}=\mathcal{N}\cap\mathcal{N}^*,\quad \mathcal{O}=M_\mathcal{A}(\mathcal{D})$$

and

$$\mathcal{N}_\mathcal{F}=\text{clo-span}(\mathcal{FC}),\quad \mathcal{D}_\mathcal{F}=\mathcal{N}_\mathcal{F}\cap\mathcal{N}_\mathcal{F}^*,\quad \mathcal{O}_\mathcal{F}=M_\mathcal{F}(\mathcal{D}_\mathcal{F}).$$

Then we have (cf. Theorem 3.2 of Ref. 8) the following.

Theorem 3.7: *Given as above* $\mathcal{C}\subset\mathcal{A}\subset\mathcal{F}$ *then*

$$\mathcal{N}_\mathcal{F}\cap\mathcal{A}=\mathcal{N},\quad \mathcal{D}_\mathcal{F}\cap\mathcal{A}=\mathcal{D},\quad \text{and}\quad \mathcal{O}_\mathcal{F}\cap\mathcal{A}=\mathcal{O}.$$

Hence $\mathcal{R}=\mathcal{O}/\mathcal{D}=(\mathcal{O}_\mathcal{F}\cap\mathcal{A})/(\mathcal{D}_\mathcal{F}\cap\mathcal{A})$.

IV. SUPERSELECTION WITH CONSTRAINTS

Next we would like to consider systems containing both constraints and superselection. There is a choice in how to define this problem mathematically, so let us consider the physical background. Perhaps the most important example, is that of a local gauge theory. It usually has a set of global charges (leading to superselection) as well as a Gauss law constraint (implementing the local gauge symmetry), and possibly also other constraints associated with the field equation. Only if the gauge group is Abelian will the Gauss law constraint commute with the global charge, since the Gauss law constraint takes its values in the Lie algebra of the gauge group. Thus, for non-Abelian local gauge theories we do not expect the constraints to be in the algebra of gauge invariant observables $\mathcal{A}$ of the superselection theory of the global charge. This problem is however not as serious as it looks. The reason is that while the global gauge group does not preserve the individual Gauss law constraints, it does preserve the set of these, hence it also preserves the set

of Dirac states selected by them. Thus we can replace the original constraint set by an equivalent constraint (i.e., selecting the same set of Dirac states) which is invariant under the global gauge group. Such an equivalent constraint is given by the projection in Theorem 3.5. It comes at the cost of slightly enlarging the system algebra $\mathcal{B}$, since P is in the universal von Neumann algebra of $\mathcal{B}$. We can avoid this cost if clo-span($\mathcal{C}$) is separable, since then there is an equivalent constraint in $\mathcal{B}$ itself, cf. Theorem 3.4 of Ref. 5.

We therefore will assume below that the constraints are in $\mathcal{A}$. This will include a large class of physical examples, as mentioned in Sec. I.

Let now $(\mathcal{A},\mathcal{C})$ be a first-class constraint system, hence we have the associated algebras $\mathcal{D}\subset\mathcal{O}\subseteq\mathcal{A}$, and $\mathcal{R}=\mathcal{O}/\mathcal{D}$. In addition, let $\mathcal{A}$ have a superselection structure, i.e., there is a given Hilbert extension $\{\mathcal{F},\mathcal{G}\}$ of $\mathcal{A}$. Thus the category $\mathcal{T}$ of canonical endomorphisms of $\mathcal{A}$ defines a selection criterion of unital endomorphisms of $\mathcal{A}$. In the case that the Hilbert extension is minimal and regular, the superselection structure of $\mathcal{T}$ is given within $\mathcal{A}$ without any reference to the Hilbert extension.

Then the following natural questions arise:

(1) what compatibility conditions should be satisfied in order to pass the superselection structure through T, thus obtaining a superselection structure on $T(\mathcal{A},\mathcal{C})=\mathcal{R}$?
(2) what is the relation between $T(\mathcal{A},\mathcal{C})$ and $T(\mathcal{F},\mathcal{C})$ where $\mathcal{F}$ is the field algebra generated from $\mathcal{T}$?

An inverse question also arises, i.e.,

(3) if $\mathcal{R}$ has a superselection structure, what is the weakest structure one can expect on $\mathcal{A}$ which would produce this superselection structure on $\mathcal{R}$ via T? (One should call this a *weak* superselection structure.)

To address (1) and (2), recall that the map T consists of a restriction (of $\mathcal{A}$ to $\mathcal{O}$) followed by a factoring ($\mathcal{O}\to\mathcal{O}/\mathcal{D}$). So, we first work out the compatibility conditions involved with restrictions and factoring maps.

Since $\mathcal{C}\subset\mathcal{A}\subset\mathcal{F}$, there are two constrained systems to consider; $(\mathcal{A},\mathcal{C})$ and $(\mathcal{F},\mathcal{C})$. The first one produces the algebras $\mathcal{D}\subset\mathcal{O}\subseteq\mathcal{A}$, and the second produces $\mathcal{D}_{\mathcal{F}}\subset\mathcal{O}_{\mathcal{F}}\subseteq\mathcal{F}$ (cf. Theorem 3.7). Now since $\mathcal{C}\subset\mathcal{A}$, the $\mathcal{G}$-invariant part of $\mathcal{F}$, it follows that $\mathcal{G}$ preserves the set of Dirac states, hence $\mathcal{G}$ preserves both $\mathcal{D}_{\mathcal{F}}$ and $\mathcal{O}_{\mathcal{F}}$, i.e., $g\mathcal{D}_{\mathcal{F}}=\mathcal{D}_{\mathcal{F}}$ and $g\mathcal{O}_{\mathcal{F}}=\mathcal{O}_{\mathcal{F}}$ for all $g\in\mathcal{G}$.

We denote the restriction of $\mathcal{G}$ to $\mathcal{O}_{\mathcal{F}}$ by $\beta_g:=g\restriction\mathcal{O}_{\mathcal{F}}$. The homomorphism $\beta:\mathcal{G}\ni g\to\beta_g\in\mathrm{Aut}\,\mathcal{O}_{\mathcal{F}}$ is not necessarily injective but β is again pointwise norm-continuous, hence $\mathcal{G}/\mathcal{K}$ is compact where $\mathcal{K}:=\mathrm{Ker}\,\beta$. The isomorphism $\tilde{\beta}:\mathcal{G}/\mathcal{K}\to\beta_{\mathcal{G}}$ by $\tilde{\beta}(g\mathcal{K}):=\beta_g$ is also a topological one (cf. p. 58 of Ref. 23). Note that $\widehat{(\mathcal{G}/\mathcal{K})}=\{\gamma\in\hat{\mathcal{G}}\,|\,\gamma(k)=1 \text{ for all } k\in\mathcal{K}\}\supseteq\mathrm{spec}\,\beta_{\mathcal{G}}$.

The spectral projections Π_γ^β of $\beta_{\mathcal{G}}$ are given by the restriction to $\mathcal{O}_{\mathcal{F}}$ of the spectral projections Π_γ of $\mathcal{G}$, i.e., $\Pi_\gamma^\beta X=\Pi_\gamma X$ for $X\in\mathcal{O}_{\mathcal{F}}$.

We now have the following:

(I) *Restriction problem:* Find conditions to guarantee that the C*-dynamical system $\{\mathcal{O}_{\mathcal{F}},\mathcal{G},\beta\}$ is a Hilbert system $\{\mathcal{O}_{\mathcal{F}},\beta_{\mathcal{G}}\}$. Thus we must find conditions to ensure there are algebraic Hilbert spaces in $\Pi_\gamma^\beta\mathcal{O}_{\mathcal{F}}$ for $\gamma\in\widehat{(\mathcal{G}/\mathcal{K})}$. (Note that this is stronger than what we need; we only need a Hilbert system on $\mathcal{R}_{\mathcal{F}}$ after factoring out by $\mathcal{D}_{\mathcal{F}}$.)
(II) *Factoring problem:* Find conditions to guarantee that under the map $\mathcal{O}_{\mathcal{F}}\to\mathcal{R}_{\mathcal{F}}:=\mathcal{O}_{\mathcal{F}}/\mathcal{D}_{\mathcal{F}}$ the factoring through of the action of $\mathcal{G}$ to $\mathcal{R}_{\mathcal{F}}$ is a Hilbert system corresponding to a DR-category. This is of course a special case of the general problem for homomorphic images of Hilbert systems under factoring by invariant ideals. The reason why we require $Z(\mathcal{A})=\mathbb{C}\mathbb{1}$ for $\mathcal{R}_{\mathcal{F}}$ is because after implementing constraints, the final physical algebra should be simple.

Below we list our major results; since some proofs are lengthy, we defer these to Sec. VI to preserve the main flow of ideas.

A. Restricting a superselection structure

We consider now for the system above the restriction problem (I), i.e., we are given a Hilbert extension $\{\mathcal{F},\mathcal{G}\}$ of $\mathcal{A}$, containing constraints $\mathcal{C}\subset\mathcal{A}$, and we need to examine when $\{\mathcal{O}_\mathcal{F},\beta_\mathcal{G}\}$ is a Hilbert system.

Theorem 4.1: *(i)* $\{\mathcal{O}_\mathcal{F},\mathcal{G},\beta\}$ *has fixed point algebra* $\mathcal{O}$. *Moreover,* $Z(\mathcal{A})\subseteq Z(\mathcal{O})$.

(ii) For any $\mathcal{G}$ *-invariant algebraic Hilbert space* $\mathcal{H}_\gamma\subset\Pi_\gamma\mathcal{F}$ *we have either* $\mathcal{H}_\gamma\cap\mathcal{O}_\mathcal{F}=\{0\}$, *or* $\mathcal{H}_\gamma\subset\mathcal{O}_\mathcal{F}$. *In the latter case we have* $\gamma\in\widehat{\mathcal{G}/\mathcal{K}}$ *where* $\mathcal{K}=\mathrm{Ker}\,\beta$, *and*

$$\mathcal{H}_\gamma\subset\Pi_\gamma\mathcal{O}_\mathcal{F}=\text{clo-span}(\mathcal{O}\mathcal{H}_\gamma).$$

(iii) Let $\sigma\in\mathrm{Ob}\,\mathcal{T}$, *with* $\mathcal{H}_\sigma\subset\mathcal{F}$ *a* $\mathcal{G}$ *-invariant algebraic Hilbert space such that* $\sigma=\rho_{\mathcal{H}_\sigma}$. *If* $\mathcal{H}_\sigma\subset\mathcal{O}_\mathcal{F}$, *then* $\sigma(\mathcal{D})\subseteq\mathcal{D}$ *and* $\sigma(\mathcal{O})\subseteq\mathcal{O}$. *Thus* σ *restricts to* $\mathcal{O}$, $\sigma\restriction\mathcal{O}\in\mathrm{End}\,\mathcal{O}$.

The central condition for $\{\mathcal{O}_\mathcal{F},\mathcal{G},\beta\}$ to be a Hilbert system $\{\mathcal{O}_\mathcal{F},\beta_\mathcal{G}\}$ with respect to the factor group $\mathcal{G}/\mathcal{K}$ is $\mathcal{H}_\gamma\subset\mathcal{O}_\mathcal{F}$, i.e., $\mathcal{H}_\gamma\subset\Pi^\beta_\gamma\mathcal{O}_\mathcal{F}$ for all $\gamma\in\widehat{\mathcal{G}/\mathcal{K}}$.

Next, we develop an internal criterion on $\mathcal{A}$ to guarantee that a given $\mathcal{H}\in\mathrm{Ob}\,\mathcal{T}_\mathcal{G}$ is contained in $\mathcal{O}_\mathcal{F}$.

Theorem 4.2: *(i) Given the Hilbert extension* $\{\mathcal{F},\mathcal{G}\}$ *of the constrained system* $\mathcal{C}\subset\mathcal{A}$ *assumed here, we have for any* $\mathcal{G}$*-invariant algebraic Hilbert space* $\mathcal{H}$ *that*

$$\mathcal{H}\subset\mathcal{O}_\mathcal{F}\quad\text{iff}\quad\mathcal{D}\sim\rho_\mathcal{H}(\mathcal{D}),\quad\text{i.e., }\mathcal{D}=\text{clo-span}(\mathcal{A}\rho_\mathcal{H}(\mathcal{D}))\cap\text{clo-span}(\rho_\mathcal{H}(\mathcal{D})\mathcal{A}).$$

(ii) For all σ, $\tau\in\mathrm{Ob}\,\mathcal{T}$ *with* $\mathcal{H}_\sigma$, $\mathcal{H}_\tau\subset\mathcal{O}_\mathcal{F}$ *we have*

$$(\sigma,\tau)_\mathcal{A}\subseteq(\sigma\restriction\mathcal{O},\tau\restriction\mathcal{O})_\mathcal{O}.$$

Observe that $\mathcal{D}\sim\rho_\mathcal{H}(\mathcal{D})$ implies that $\rho_\mathcal{H}(\mathcal{D})\subseteq\mathcal{D}$.

Corollary 4.3: We have that $\{\mathcal{O}_\mathcal{F},\mathcal{G}/\mathcal{K},\tilde{\beta}\}$ *is a Hilbert system* $\{\mathcal{O}_\mathcal{F},\beta_\mathcal{G}\}$ with respect to $\mathcal{G}/\mathcal{K}$ *iff* $\mathcal{D}\sim\rho_\gamma(\mathcal{D})$ *holds for all* $\gamma\in\widehat{\mathcal{G}/\mathcal{K}}$. *In particular, if* $\mathcal{D}\sim\rho_\gamma(\mathcal{D})$ *holds for all* $\gamma\in\hat{\mathcal{G}}$ *then* $\mathcal{G}/\mathcal{K}\cong\mathcal{G}$ *i.e.,* $\mathcal{K}$ *is trivial.*

While the condition $\mathcal{D}\sim\rho_\gamma(\mathcal{D})$ is exact for $\mathcal{H}_\gamma\subset\mathcal{O}_\mathcal{F}$, it may not be in practice that easy to verify. We therefore consider alternative conditions which will allow the main structures involved with Hilbert extensions to survive the restriction of $\{\mathcal{F},\mathcal{G}\}$ to $\{\mathcal{O}_\mathcal{F},\beta_\mathcal{G}\}$.

Recalling the definition of subobjects, introduce the notation $E\simeq\mathbb{1}(\mathrm{mod}\,\mathcal{A})$ for a projection $E\in\mathcal{A}$ to mean that there is an isometry $V\in\mathcal{A}$, $V^*V=\mathbb{1}$ such that $VV^*=E$ (i.e., Murray-von Neumann equivalence of E and $\mathbb{1}$).

Definition 4.4: We say the constraint set $\mathcal{C}\subset\mathcal{A}$ *is an* E-constraint set *if for each projection* $E\in\mathcal{O}$ *such that* $E\simeq\mathbb{1}(\mathrm{mod}\,\mathcal{A})$, *we have that* $E\simeq\mathbb{1}(\mathrm{mod}\,\mathcal{O})$.

The E-constraint condition will ensure the survival of decomposition relations of restrictable canonical endomorphisms.

Proposition 4.5: Let $\{\mathcal{F},\mathcal{G}\}$ *be a Hilbert system and let* $\mathcal{C}\subset\mathcal{O}$ *be an E-constraint set,* $\sigma\in\mathrm{Ob}\,\mathcal{T}$ *and* $\mathcal{H}_\sigma\subset\mathcal{O}_\mathcal{F}$ *a* $\mathcal{G}$*-invariant algebraic Hilbert space. Then*

(i) *to each decomposition*

$$\sigma(\cdot)=\sum_j V_j\rho_{\gamma_j}(\cdot)V_j^*,\quad V_j\in(\rho_{\gamma_j},\sigma)_\mathcal{A},$$

where $\gamma_j\in\hat{\mathcal{G}}$ *and* $V_j\in\mathcal{A}$ *are isometries, there corresponds a decomposition on* $\mathcal{O}$, *i.e., there are* $\mathcal{G}$*-invariant algebraic Hilbert spaces* $\mathcal{K}_j\subset\mathcal{O}_\mathcal{F}$, *which carry the representation* γ_j *and with canonical endomorphisms* $\tau_j:=\rho_{\mathcal{K}_j}\restriction\mathcal{O}\in\mathrm{End}\,\mathcal{O}$ *such that on* $\mathcal{O}$,

$$\sigma(\cdot)=\sum_j W_j\tau_j(\cdot)W_j^*,\quad W_j\in(\tau_j,\sigma)_\mathcal{O},$$

where $W_j\in\mathcal{O}$ *are isometries.*

(ii) *Let* $\{\mathcal{F},\hat{\mathcal{G}}\}$ *in addition satisfies Property B and let* $\tau<\sigma\in\mathcal{T}$ *in the sense of* $\mathcal{A}$, *i.e., there is*

an isometry $V \in (\tau,\sigma)_{\mathcal{A}}$, *and let* $\mathcal{H}_\sigma \subset \mathcal{O}_{\mathcal{F}}$. *Then there is a corresponding Hilbert space* $\mathcal{H}_\tau \subset \mathcal{O}_{\mathcal{F}}$, *i.e.,* $\tau\restriction\mathcal{O} < \sigma\restriction\mathcal{O} \in \mathrm{End}\,\mathcal{O}$ *also in the sense of* $\mathcal{O}$.

Theorem 4.6: *Let the Hilbert system* $\{\mathcal{F},\mathcal{G}\}$ *satisfy Property B where* $\mathcal{G}$ *is a group with a distinguished irreducible representation* $\gamma_0 \in \hat{\mathcal{G}}$ *such that every irreducible representation of* $\mathcal{G}$ *is contained in a tensor representation of* γ_0. *Let* $\mathcal{C} \subset \mathcal{A}$ *be an E-constraint set then* $\mathcal{H}_{\gamma_0} \subset \mathcal{O}_{\mathcal{F}}$ *implies that* $\{\mathcal{O}_{\mathcal{F}}, \beta_{\mathcal{G}}\}$ *is a Hilbert system.*

Proof: This follows from Proposition 4.5, by making use of the obvious fact that $\mathcal{H}_\tau \subset \mathcal{O}_{\mathcal{F}} \supset \mathcal{H}_\sigma$ implies that $\mathcal{H}_\tau \cdot \mathcal{H}_\sigma \subset \mathcal{O}_{\mathcal{F}}$ for $\sigma,\ \tau \in \mathrm{Ob}\,\mathcal{T}$. □

If the group $\mathcal{G}$ is isomorphic to $U(N)$ then it satisfies the condition of Theorem 4.6.

The property of being an E-constraint set can be characterized in terms of the open projection $P \in \mathcal{A}''$ corresponding to the constraints (cf. Theorem 3.5). Observe that if there is an $E \in \mathcal{O}$ with $E \simeq \mathbb{I}(\mathrm{mod}\,\mathcal{A})$, then the set of isometries

$$\mathcal{V}_E := \{V \in \mathcal{A} \,|\, VV^* = E, V^*V = \mathbb{I}\}$$

is nonempty. We have the following.

Proposition 4.7: Let $E \in \mathcal{O}$ *with* $E \simeq \mathbb{I}(\mathrm{mod}\,\mathcal{A})$, *then* $\mathcal{V}_E \cap \mathcal{O} \neq \emptyset$ *iff for each* $V \in \mathcal{V}_E$ *there is a*

$$U \in \mathcal{U}_E := \{U \in \mathcal{A} \,|\, U^*U = E = UU^*\}$$

such that $VPV^* = UPU^*$.

B. Morphisms of general Hilbert systems

Recall that the second step in the enforcement of constraints, is the factoring $\mathcal{O}_{\mathcal{F}} \to \mathcal{R}_{\mathcal{F}} := \mathcal{O}_{\mathcal{F}}/\mathcal{D}_{\mathcal{F}}$. We now consider problem (II), the factoring problem, first in a general context. Consider a morphism of C*-algebras $\xi: \mathcal{F} \to \mathcal{L} = \xi(\mathcal{F})$. This specifies the subgroup of automorphisms

$$\mathrm{Aut}_\xi\,\mathcal{F} := \{\alpha \in \mathrm{Aut}\,\mathcal{F} \,|\, \alpha(\mathrm{Ker}\,\xi) \subseteq \mathrm{Ker}\,\xi\}$$

and a homomorphism $\mathrm{Aut}_\xi\,\mathcal{F} \to \mathrm{Aut}\,\mathcal{L}$ by $\alpha \to \alpha^\xi$ where $\alpha^\xi(\xi(F)) := \xi(\alpha(F))$ for all $F \in \mathcal{F}$. Henceforth let $\{\mathcal{F},\mathcal{G}\}$ be a Hilbert system with Property B and $\mathcal{G} \subset \mathrm{Aut}_\xi\,\mathcal{F}$. Our task will be to find the best conditions to ensure that $\{\mathcal{L},\mathcal{G}^\xi\}$ is a Hilbert system associated with a category described in Theorem 2.25. We will denote the spectral projections of $\mathcal{G}$ (respectively, $\mathcal{G}^\xi$) by Π_γ (respectively, Π^ξ_γ). (Recall that in the context of the T-procedure, we have that $\mathcal{G}$ preserves $\mathcal{D}_{\mathcal{F}}$ due to the invariance of the constraints under $\mathcal{G}$. So the current analysis applies.)

Theorem 4.8: *Given a Hilbert system* $\{\mathcal{F},\mathcal{G}\}$ *and a unital morphism* $\xi: \mathcal{F} \to \mathcal{L} = \xi(\mathcal{F})$, *such that* $\mathcal{G} \subset \mathrm{Aut}_\xi\,\mathcal{F}$, *then we have*

(i) $\{\mathcal{L},\mathcal{G}^\xi\}$ *is a Hilbert system and* $\mathcal{G} \cong \mathcal{G}^\xi$.
(ii) *If* $\mathcal{H}_\gamma \subset \Pi_\gamma \mathcal{F}$ *is an invariant algebraic Hilbert space for* $\mathcal{G}$, *then so is* $\xi(\mathcal{H}_\gamma) \subset \Pi^\xi_\gamma \mathcal{L}$ *for* $\mathcal{G}^\xi$.
(iii) *Let* $\mathcal{N}_\gamma$ *be any orthonormal basis for* $\xi(\mathcal{H}_\gamma)$, *then* $\cup\{\mathcal{N}_\gamma \,|\, \gamma \in \hat{\mathcal{G}}\}$ *is a left module basis of* $\xi(\mathcal{F}_{\mathrm{fin}})$ with respect to $\xi(\mathcal{A})$, *i.e., the "essential part" of* ξ *is its action on* $\mathcal{A}$.
(iv) *The fixed point algebra of* $\mathcal{L}$ with respect to $\mathcal{G}^\xi$ *is exactly* $\xi(\mathcal{A})$, *and* $\xi(\mathcal{F}_{\mathrm{fin}}) = \mathcal{L}_{\mathrm{fin}}$.
(v) *If* $\{\mathcal{F},\mathcal{G}\}$ *has Property B, so does* $\{\mathcal{L},\mathcal{G}^\xi\}$.

Thus corresponding to the two Hilbert systems $\{\mathcal{F},\mathcal{G}\}$ and $\{\mathcal{L},\mathcal{G}^\xi\}$ we now have the two categories $\mathcal{T}$ and $\mathcal{T}^\xi$, respectively. Moreover we have the following.

Corollary 4.9: Under the conditions of Theorem 4.8 we have that

(i) *for any canonical endomorphism* $\lambda \in \mathrm{Ob}\,\mathcal{T}$,

$$\lambda(\mathrm{Ker}\,\xi \cap \mathcal{A}) \subseteq \mathrm{Ker}\,\xi \cap \mathcal{A}.$$

Hence there is a well-defined map $\mathrm{Ob}\,\mathcal{T} \ni \lambda \to \lambda^\xi \in \mathrm{Ob}\,\mathcal{T}^\xi$, *given by* $\lambda^\xi(\xi(A)) := \xi(\lambda(A))$ *for all* $A \in \mathcal{A}$.

(ii) *The map* $\mathrm{Ob}\,\mathcal{T}\ni\lambda\to\lambda^\xi\in\mathrm{Ob}\,\mathcal{T}^\xi$ *is compatible with products, direct sums and subobjects. It also preserves unitary equivalence.*

We have that $(\mathrm{Ob}\,\mathcal{T})^\xi\subseteq\mathrm{Ob}\,\mathcal{T}^\xi$, and we now claim that up to unitary equivalence, we have in fact equality.

Theorem 4.10: *Under the conditions of Theorem 4.8 we have that*

(i) *if* $\sigma\in\mathrm{Ob}\,\mathcal{T}^\xi$, *then there is always a* $\lambda\in\mathrm{Ob}\,\mathcal{T}$ *such that* λ^ξ *is unitarily equivalent to* σ, *i.e., each unitary equivalence class in* $\mathrm{Ob}\,\mathcal{T}^\xi$ *contains at least one element of the form* λ^ξ.

(ii) *The map* $\mathrm{Ob}\,\mathcal{T}\ni\lambda\to\lambda^\xi\in\mathrm{Ob}\,\mathcal{T}^\xi$ *produces an isomorphism between the sets of unitary equivalence classes of* $\mathrm{Ob}\,\mathcal{T}$ *and* $\mathrm{Ob}\,\mathcal{T}^\xi$ *which is compatible with products direct sums and subobjects.*

The relation between the arrows of the two categories is however less direct.

Lemma 4.11: Under the conditions of Theorem 4.8 we have

$$\xi((\sigma,\tau)_{\mathcal{A}})\subseteq(\sigma^\xi,\tau^\xi)_{\xi(\mathcal{A})}.$$

Next we show that $\mathrm{Ker}\,\xi$ is uniquely determined by $\mathrm{Ker}\,\xi\cap\mathcal{F}_{\mathrm{fin}}$.

Proposition 4.12: Under the conditions of Theorem 4.8 we have that

(i) $\mathrm{Ker}\,\xi\cap\mathcal{F}_{\mathrm{fin}}=\mathrm{Span}\{(\mathrm{Ker}\,\xi\cap\mathcal{A})\mathcal{H}_\gamma|\,\gamma\in\hat{\mathcal{G}}\}$,

(ii) $\mathrm{Ker}\,\xi=\mathrm{clo}_{|\cdot|_{\mathcal{A}}}(\mathrm{Ker}\,\xi\cap\mathcal{F}_{\mathrm{fin}})\cap\mathcal{F}$.

Thus $\mathrm{Ker}\,\xi$ is in fact uniquely determined by $\mathrm{Ker}\,\xi\cap\mathcal{A}$, as is already suggested by Theorem 4.8 (iii). Since $\mathcal{F}$ is in general not complete with respect to $|\cdot|_{\mathcal{A}}$, the intersection with $\mathcal{F}$ in Proposition 4.12 (ii) is necessary.

Theorem 4.8 suggests that we consider the following subcategory of $\mathcal{T}^\xi$.

Definition 4.13: The subcategory $\xi(\mathcal{T})$ *of* $\mathcal{T}^\xi$ *is defined by the objects*

$$\mathrm{Ob}\,\xi(\mathcal{T}):=(\mathrm{Ob}\,\mathcal{T})^\xi$$

and the arrows

$$(\sigma^\xi,\tau^\xi)^{(0)}_{\xi(\mathcal{A})}:=\xi((\sigma,\tau)_{\mathcal{A}}).$$

By Theorem 4.10 the sets of all unitary equivalence classes of $\mathrm{Ob}\,\xi(\mathcal{T})$ and $\mathrm{Ob}\,\mathcal{T}^\xi$ coincide, each equivalence class of $\mathrm{Ob}\,\xi(\mathcal{T})$ is a subset of the corresponding equivalence class of $\mathrm{Ob}\,\mathcal{T}^\xi$, but in general these equivalence classes are much larger.

Lemma 4.11 says that the arrow sets $(\sigma^\xi,\tau^\xi)_{\xi(\mathcal{A})}$ of the objects of $\mathrm{Ob}\,\xi(\mathcal{T})$ considered as objects of $\mathrm{Ob}\,\mathcal{T}^\xi$ are in general larger than the corresponding arrow sets in $\xi(\mathcal{T})$. The reason is that an element $X=\xi(Y)$, $Y\in\mathcal{A}$, belongs to $(\sigma^\xi,\tau^\xi)_{\xi(\mathcal{A})}$ iff $Y\sigma(A)-\tau(A)Y\in\mathrm{Ker}\,\xi$ for all $A\in\mathcal{A}$. The arrow sets coincide only if this relation already implies $Y\sigma(A)-\tau(A)Y=0$.

C. Morphisms of minimal and regular Hilbert systems

Recall now that by Theorems 2.25 and 2.27 we have an equivalence between minimal and regular Hilbert systems with Property B and the endomorphism category $\mathcal{T}$ with an admissible subcategory $\mathcal{T}_{\mathbb{C}}$. We called a subcategory $\mathcal{T}_{\mathbb{C}}$ *admissible* if it satisfies conditions P.1 and P.2 in Theorem 2.25.

As in the last section, we consider a unital morphism $\xi:\mathcal{F}\to\mathcal{L}=\xi(\mathcal{F})$, and recall by Proposition 4.12 that ξ is determined by its action on $\mathcal{A}$. Now while it is obvious that $\xi(Z(\mathcal{A}))\subseteq Z(\xi(\mathcal{A}))$, we require below the stronger condition

$$\xi(Z(\mathcal{A})) = Z(\xi(\mathcal{A})). \tag{7}$$

When $\xi(\mathcal{A})$ is a simple C*-algebra (as we require for the final observables after a T-procedure), the condition (7) will be satisfied.

Theorem 4.14: *Given a minimal and regular Hilbert system* $\{\mathcal{F},\mathcal{G}\}$ *with Property B, and a unital morphism* $\xi:\mathcal{F}\to\mathcal{L}=\xi(\mathcal{F})$ *such that* $\mathcal{G}\subset \mathrm{Aut}_\xi \mathcal{F}$ *and condition (7) holds, then*

(i) *there is a DR-subcategory* $\mathcal{T}^\xi_{\mathbb{C}}$ *of* $\xi(\mathcal{T})$,
(ii) *property P.2 is satisfied for* $\mathcal{T}^\xi_{\mathbb{C}}$ *iff* $\xi(\mathcal{A})'\cap\xi(\mathcal{F})=\xi(Z(\mathcal{A}))$. *In this case the subcategory* $\mathcal{T}^\xi_{\mathbb{C}}$ *is admissible*.
(iii) *If* $\xi(\mathcal{A})'\cap\xi(\mathcal{F})=\xi(Z(\mathcal{A}))$, *then*

$$(\sigma^\xi,\tau^\xi)_{\xi(\mathcal{A})} = \xi((\sigma,\tau)_{\mathcal{A}})$$

for all $\sigma,\ \tau\in \mathrm{Ob}\,\mathcal{T}$, *where we made use of the notation and result in Corollary 4.9.*
(iv) *In this case choose* $\mathcal{H}_\gamma\in \mathrm{Ob}\,\mathcal{T}_{\mathcal{G}}$. *Then*

$$\mathcal{M}^\xi := \{\rho_{\xi(\mathcal{H}_\gamma)} | \gamma\in\hat{\mathcal{G}}\}\subset \mathrm{Ob}\ \xi(\mathcal{T})$$

is a complete system of (irreducible) and mutually disjoint objects of $\mathrm{Ob}\ \xi(\mathcal{T})$.

D. The inverse problem

Theorem 4.15: *Let* $\mathcal{A}$ *be a unital C*-algebra with Property B, and let* $\mathcal{T}$ *be a C*-tensor category of unital endomorphisms of* $\mathcal{A}$. *Let* $\mathcal{T}$ *have an admissible subcategory* $\mathcal{T}_{\mathbb{C}}$ *whose arrow spaces are denoted by* $(\sigma,\tau)_{\mathbb{C}}$. *Furthermore, let* ξ *be a unital morphism of* $\mathcal{A}$ *such that*

(i) $\xi(Z(\mathcal{A}))=Z(\xi(\mathcal{A}))$,
(ii) $\lambda(\mathrm{Ker}\,\xi)\subseteq\mathrm{Ker}\,\xi$ *for all* $\lambda\in\mathrm{Ob}\,\mathcal{T}$. *Thus we can define endomorphisms* $\lambda^\xi\in\mathrm{End}\,\xi(\mathcal{A})$ *by* $\lambda^\xi(\xi(A)):=\xi(\lambda(A))$ *for all* $A\in\mathcal{A}$ *and a category* $\xi(\mathcal{T})$ *with objects*

$$\mathrm{Ob}\ \xi(\mathcal{T}) := \{\lambda^\xi | \lambda\in \mathrm{Ob}\ \mathcal{T}\} \tag{8}$$

and arrows $(\sigma^\xi,\tau^\xi)_{\xi(\mathcal{A})}$, *which is closed with respect to direct sums and products*,
(iii) $\xi((\sigma,\tau)_{\mathcal{A}})=(\sigma^\xi,\tau^\xi)_{\xi(\mathcal{A})}$ *for all* $\sigma,\ \tau\in\mathrm{Ob}\,\mathcal{T}$.

Then there is a subcategory $\mathcal{T}^\xi_{\mathbb{C}}$ *of* $\xi(\mathcal{T})$ *with* $\mathrm{Ob}\,\mathcal{T}^\xi_{\mathbb{C}}=\mathrm{Ob}\,\xi(\mathcal{T})$ *which is admissible for* $\xi(\mathcal{T})$.

Thus by Theorem 2.27 there are Hilbert extensions $\mathcal{F}$ *and* $\mathcal{F}^\xi$ *corresponding to* $\mathcal{T}$ *and* $\xi(\mathcal{T})$, *repectively. Moreover, the Hilbert extension* $\mathcal{F}^\xi$ *of* $\xi(\mathcal{A})$ *can be chosen in such a way that it is the homomorphic image of* $\mathcal{F}$ *under a morphism which is an extension of* ξ. *That is*, $\mathcal{F}^\xi=\tilde{\xi}(\mathcal{F})$ *where* $\tilde{\xi}$ *is a morphism of* $\mathcal{F}$ *such that* $\tilde{\xi}(A)=\xi(A)$ *for all* $A\in\mathcal{A}$.

Remark 4.16: A posteriori, the set of objects $\mathrm{Ob}\,\xi(\mathcal{T})$ defined in (8) could be enlarged by filling up the unitary equivalence classes of each λ^ξ by *all* τ with $\tau=\mathrm{Ad}\,V\circ\xi(\lambda)$, where $V\in\xi(\mathcal{A})$ is unitary. This corresponds to the objects of the category $\mathcal{T}^\xi$ of Definition 4.13. In this case we must also add additional arrows, so if $\tau_i=\mathrm{Ad}\,V_i\circ\xi(\lambda_i)$, $i=1,2$, then we also need

$$(\tau_1,\tau_2)_{\xi(\mathcal{A})} := V_2(\tau_1^\xi,\tau_2^\xi)_{\xi(\mathcal{A})}V_1^{-1}.$$

However, for the application of Theorem 2.27 this is not necessary.

E. Superselection structures left after constraining

Recall that the enforcement of constraints by T-procedure produces a final physical algebra $\mathcal{R}$. This algebra is usually assumed to be simple; if it is not, then the physics is not fully defined, and one should extend the constraint set $\mathcal{C}\subset\mathcal{A}$ to make $\mathcal{R}$ simple (the choice of the extension needs to be physically motivated).

In the preceding sections we examined which conditions need to be satisfied by a Hilbert extension $\{\mathcal{F},\mathcal{G}\}$ of $\mathcal{A}$ for its structure to pass through the two parts of the T-procedure. Here we combine these to produce conditions on the initial system which will ensure that we obtain a Hilbert extension of $\mathcal{R}$. We will also examine when this final Hilbert extension is regular (and this produces then a DR-category via simplicity of $\mathcal{R}$).

Theorem 4.17: *Let $\{\mathcal{F},\mathcal{G}\}$ be a Hilbert extension of $\mathcal{A}$, and let $\mathcal{C}\subset\mathcal{A}$ be a first-class constraint set such that $\mathcal{D}\sim\rho_\gamma(\mathcal{D})$ holds for all $\gamma\in\widehat{\mathcal{G}/\mathcal{K}}$. Then $\{\mathcal{R}_\mathcal{F},\beta_\mathcal{G}\}$ is a Hilbert extension of $\mathcal{R}$, where $\mathcal{R}_\mathcal{F}=\xi(\mathcal{O}_\mathcal{F})$, and ξ is the factor map $\mathcal{O}_\mathcal{F}\to\mathcal{O}_\mathcal{F}/\mathcal{D}_\mathcal{F}$.*

Proof: By Corollary 4.3 it follows from the hypotheses that $\{\mathcal{O}_\mathcal{F},\beta_\mathcal{G}\}$ is a Hilbert extension of $\mathcal{O}$. Since the constraint set $\mathcal{C}\subset\mathcal{A}$ is $\mathcal{G}$-invariant, we have that $\alpha(\mathcal{D}_\mathcal{F})=\mathcal{D}_\mathcal{F}$ for all $\alpha\in\beta_\mathcal{G}\subset\mathrm{Aut}\,\mathcal{O}_\mathcal{F}$, i.e., $\beta_\mathcal{G}\subset\mathrm{Aut}_\xi\,\mathcal{O}_\mathcal{F}$. (Recall the discussion in the introductory part of Sec. IV.) Thus by Theorem 4.8 it follows that $(\beta_\mathcal{G})^\xi\cong\beta_\mathcal{G}$, and that

$$\{\xi(\mathcal{O}_\mathcal{F}),(\beta_\mathcal{G})^\xi\}=\{\mathcal{R}_\mathcal{F},\beta_\mathcal{G}\}$$

is a Hilbert extension of $\mathcal{R}=\xi(\mathcal{O})$. ■

Next, we would like to examine when a Hilbert extension as in Theorem 4.17 will produce a minimal and regular Hilbert extension of $\mathcal{R}$ (with Property B).

First recall the requirement for a Hilbert system $\{\mathcal{F},\mathcal{G}\}$ to be regular, there is an assignment $\sigma\to\mathcal{H}_\sigma$ from $\mathrm{Ob}\,\mathcal{T}$ to $\mathcal{G}$-invariant algebraic Hilbert spaces in $\mathcal{F}$ such that

(i) $\sigma=\rho_{\mathcal{H}_\sigma}$, i.e., σ is the canonical endomorphism of $\mathcal{H}_\sigma$,
(ii) $\sigma\circ\tau\to\mathcal{H}_\sigma\cdot\mathcal{H}_\tau$,

that is, the assignment is compatible with products.

We now want to check whether this property also survives the map $T:\{\mathcal{F},\mathcal{G}\}\to\{\mathcal{R}_\mathcal{F},\beta_\mathcal{G}\}$.

Proposition 4.18: Let $\mathcal{T}$ satisfy regularity. Let $\mathcal{D}\sim\rho_\gamma(\mathcal{D})$ for all $\gamma\in\widehat{\mathcal{G}/\mathcal{K}}$, then $\{\mathcal{R}_\mathcal{F},\beta_\mathcal{G}\}$ satisfies regularity, i.e., there is an assignment $\sigma\to\mathcal{H}_\sigma$ such that

(i) $\sigma=\rho_{\mathcal{H}_\sigma}$, *i.e., σ is the canonical endomorphism of $\mathcal{H}_\sigma$*,
(ii) $\sigma\circ\tau\to\mathcal{H}_\sigma\cdot\mathcal{H}_\tau$.

Proof: Given the assignment $\sigma\to\mathcal{H}_\sigma$ in $\mathcal{F}$, then whenever $\sigma=\rho_\gamma$, $\gamma\in\widehat{\beta_\mathcal{G}}$ we have

$$\sigma\to\mathcal{H}_\sigma\subset\mathcal{O}_\mathcal{F}\to\mathcal{R}_\mathcal{F},$$

where the last map is ξ, so the assignment which we take for this proposition is $\sigma\to\xi(\mathcal{H}_\sigma)$. Then (i) and (ii) are automatic. □

Second, we consider Property B.

Proposition 4.19: Let $\{\mathcal{F},\mathcal{G}\}$ satisfy Property B, let $\mathcal{G}$ be non-Abelian and $\mathcal{C}\subset\mathcal{A}$ be an E-constraint set. If $\mathcal{D}\sim\rho_\gamma(\mathcal{D})$ for all $\gamma\in(\widehat{\mathcal{G}/\mathcal{K}})$, then $\{\mathcal{O}_\mathcal{F},\beta_\mathcal{G}\}$ satisfies Property B.

Proof: First $\{\mathcal{O}_\mathcal{F},\beta_\mathcal{G}\}$ is a Hilbert extension of $\mathcal{O}$ with respect to $\mathcal{G}/\mathcal{K}$ because of Corollary 4.3. Choose a $\mathcal{G}$-invariant Hilbert space $\mathcal{H}\subset\mathcal{O}_\mathcal{F}\subset\mathcal{F}$ which is not irreducible, i.e., there is a projection $E\in\mathcal{J}(\mathcal{L}_\mathcal{G}(\mathcal{H}))$, $0<E<\mathbb{1}$. Then one has $E\in(\rho_\mathcal{H},\rho_\mathcal{H})_\mathcal{A}\subset(\rho_\mathcal{H}\restriction\mathcal{O},\rho_\mathcal{H}\restriction\mathcal{O})_\mathcal{O}\subset\mathcal{O}$ by Theorem 4.2 (ii). By Property B we get closure under subobjects, so there is a $V\in\mathcal{A}$, $V^*V=\mathbb{1}$, $VV^*=E$. In other words, $E\cong\mathbb{1}(\mathrm{mod}\,\mathcal{A})$. Similarly we obtain $\mathbb{1}-E\cong\mathbb{1}(\mathrm{mod}\,\mathcal{A})$. Since $\mathcal{C}$ is an E-constraint set and $E\in\mathcal{O}$ we get that $E\cong\mathbb{1}(\mathrm{mod}\,\mathcal{O})$ and $\mathbb{1}-E\cong\mathbb{1}(\mathrm{mod}\,\mathcal{O})$ and this is the assertion. ■

Finally, we need to consider whether the requirement

$$\mathcal{A}'\cap\mathcal{F}=Z(\mathcal{A})$$

passes through the T-procedure. In full generality, this is a very hard problem, because both stages of the T-procedure can eliminate or create elements of $\mathcal{A}'$. In fact, since $\mathcal{A}'\cap\mathcal{F}\subset\mathcal{D}'\cap\mathcal{F}\subset\mathcal{O}_\mathcal{F}$ and $Z(\mathcal{A})\subset Z(\mathcal{O})$, we can only deduce from $\mathcal{A}'\cap\mathcal{F}=Z(\mathcal{A})$ that $\xi(\mathcal{A}'\cap\mathcal{F})=\xi(Z(\mathcal{A}))$. On the other hand, $\mathcal{R}'\cap\mathcal{R}_\mathcal{F}=Z(\mathcal{R})$ iff

$$A \in \mathcal{O}_{\mathcal{F}} \quad \text{and } [A,\mathcal{O}] \subset \mathcal{D}_{\mathcal{F}} \text{ implies } A \in \mathcal{O} + \mathcal{D}_{\mathcal{F}}$$

which can be true in general for more elements than those in $\xi(\mathcal{A}' \cap \mathcal{F})$.

We do have from Theorem 4.2 and Proposition 2.22 the following condition.

Proposition 4.20: Let $\{\mathcal{F},\mathcal{G}\}$ be a minimal Hilbert extension of $\mathcal{A}$, and let $\mathcal{C} \subset \mathcal{A}$ be a first-class constraint set such that $\mathcal{D} \sim \rho_\gamma(\mathcal{D})$ holds for all $\gamma \in \widehat{\mathcal{G}/\mathcal{K}}$. If the disjointness of canonical endomorphisms survives the restriction to $\mathcal{O}$ then the Hilbert system $\{\mathcal{O}_{\mathcal{F}}, \beta_{\mathcal{G}}\}$ is minimal, i.e., $\mathcal{O}' \cap \mathcal{O}_{\mathcal{F}} = \mathcal{Z}(\mathcal{O})$.

V. EXAMPLE

It is difficult to produce interesting worked examples in the current state of the theory. The problem is that in almost all theories of physical significance, the canonical endomorphisms ρ_γ are not known explicitly, and so one cannot check the compatibility conditions with the constraints explicitly (cf. Corollary 4.3). Here we give an example which is extracted from QED, so it may have some physical interest. It consists of a fermion in an Abelian gauge potential. Since the global gauge group $\mathcal{G}$ is Abelian, the superselection theory simplifies radically. However, we have explicit endomorphisms ρ_γ and can check the compatibility conditions with the constraints. Nevertheless, even at this simple level, it is not possible to verify all the conditions of regularity. We will not treat the issue of dynamics.

A. Constraint structure of QED

We start with a discussion of the setup of QED in order to motivate our subsequent example. The starting point for QED, is a fermion field ψ in $\mathbb{R}^4$ satisfying the free CARs, and a U(1)-gauge potential A in $\mathbb{R}^4$ satisfying free CCRs, and initially these are assumed to commute. So the appropriate C*-algebraic framework at this initial level is

$$\mathcal{B} := \mathrm{CAR}(\mathcal{H}) \otimes \mathrm{CCR}(S,B),$$

where $\mathcal{H} = L^2(\mathbb{R}^4,\mathbb{C}^4)$, $S = \mathcal{S}(\mathbb{R}^4,\mathbb{R}^4)/\mathrm{Ker}\, B$, and B denotes the symplectic form for QEM, coming from the Jordan-Wigner distribution, cf. Sec. 5 of Ref. 5. [Note that the tensor product $\mathcal{B}$ is unique because $\mathrm{CAR}(\mathcal{H})$ is a nuclear algebra.] There is a global charge Q acting on $\mathrm{CAR}(\mathcal{H})$ and there are constraints in the heuristic theory,

$$A_\mu{}^{,\mu}(x) := 0 \quad \text{(Lorentz condition)}$$

and

$$\Box A_\mu := j_\mu \quad \text{(Maxwell equation)},$$

where $j_\mu := -e\tilde{\psi}\gamma_\mu\psi$ is the electron current, and we denote $\tilde{\psi} := \psi^*\gamma_0$. The Lorentz condition has been treated in the C*-algebra context (cf. Ref. 5) and it needs special treatment, e.g., indefinite metric or nonregular states, but it is not very interesting for us, since it only affects the electromagnetic field $\mathrm{CCR}(S,B)$, hence is independent of the charge Q. The Maxwell equation is more interesting, since it involves both factors of $\mathcal{B}$ and it expresses part of the interaction between the two fields. It is however very difficult to enforce in the C*-algebra context (and ultimately leads to the conclusion that $\mathcal{B}$ is too small an algebra to do this in). Naively, it seems that we can easily realize both sides of the Maxwell equation in the present C*-setting, smear the left-hand side over $\mathcal{S}(\mathbb{R}^4,\mathbb{R}^4)$,

$$\int \Box A_\mu(x) f^\mu(x)\mathrm{d}x = \int A_\mu \Box f^\mu \,\mathrm{d}x = A(\Box f)$$

then this is realized in $\mathrm{CCR}(S,B)$ through the identification of the generating Weyl unitaries δ_h with the heuristic $\exp iA(h)$ where $h = \Box f$. If we smear the right-hand side of the Maxwell equation

$$j(f) = -e \int \tilde{\psi}(x)\gamma_\mu \psi(x) f^\mu(x) \mathrm{d}x,$$

then $j(f)$ generates a Bogoliubov transformation T_f on $L^2(\mathbb{R}^4, \mathbb{C}^4)$ by

$$\mathrm{Ad}(\exp ij(f))\psi(g) := (\exp i \,\mathrm{ad}\, j(f))(\psi(g)) = \psi(T_f g) =: \alpha_{T_f}(\psi(g)),$$

where α_{T_f} is its associated automorphism on CAR($\mathcal{H}$) (we will calculate T_f explicitly in a simplified setting below). Let $G \subset \mathrm{Aut}\,\mathcal{B}$ be the discrete group generated in Aut $\mathcal{B}$ by

$$\{\beta_f := \alpha_{T_f} \otimes \iota | f \in \mathcal{S}(\mathbb{R}^4, \mathbb{R}^4)\}$$

and let ν denote its action on $\mathcal{B}$. Define the crossed product

$$\mathcal{E} := \mathcal{G} \underset{\nu}{\times} \mathcal{B} = \mathrm{C}^*\{\mathcal{B}, U_g | U_g^* = U_g^{-1}, \nu_g = \mathrm{Ad}\, U_g, U_g U_h = U_{gh}, g, h \in G\}$$

then we identify the heuristic objects $\exp ij(f)$ with the implementing unitaries U_{β_f}. So each side of the Maxwell equation has a C*-realization, and we only need to decide how to impose the constraint equation. Heuristically, the Maxwell equations are imposed as state conditions, $A(\Box f)\phi = j(f)\phi$ for vectors ϕ in the representing Hilbert (or Krein) space. If we take instead the stronger condition $A(\Box f)^n \phi = j(f)^n \phi$ for $n \in \mathbb{N}$, then we can rewrite the constraint conditions in the form $e^{iA(\Box f)}\phi = e^{if(f)}\phi$. This suggests that we choose constraint unitaries $V_f := U_{-\beta_f} \cdot \delta_{\Box f}$ in $\mathcal{E}$ and thus select our Dirac states ω on $\mathcal{E}$ by

$$\omega(V_f) = 1 \quad \forall f \in \mathcal{S}(\mathbb{R}^4, \mathbb{R}^4).$$

As one expects from the interaction, this program encounters problems.

(1) We always have that $\Box f \in \mathrm{Ker}\, B$, hence $\Box f$ corresponds to zero in S (since we factor out by Ker B). This can be remedied by changing S to $\mathcal{S}(\mathbb{R}^4, \mathbb{R}^4)$, in which case (S, B) is a degenerate symplectic space. This problem is connected to the fact that the heuristic smearing formula

$$A(f) = \int_{C_+} (a_\mu(\mathbf{p})\hat{f}^\mu(p) + a_\mu^+(\mathbf{p})\bar{\hat{f}}^\mu(p)) \frac{d^3p}{p_0}$$

cannot be correct for the interacting theory, since it implies that $A(\Box f) = 0$, in contradiction with the Maxwell equation.

(2) Interaction mixes the fermions and bosons, so it is unrealistic to expect that the interacting fermion and boson fields will commute (as in the tensor product structure of $\mathcal{B}$). In fact, if one assumes that the bosons and fermions commute, then the Maxwell equation forces the local charges to become central, in which case only neutral local fields are allowed, which is too restrictive for QED. Even worse, perturbation theory suggests that the interacting fields need not be canonical, so the assumption of the CCR and CAR relations for the interacting bosons and fermions is problematic.

B. Model for the interacting Maxwell constraint

Inspired by the observations above, we now propose an example which is a simplified version of the Maxwell constraint. Heuristically, we want to impose a constraint of the form

$$a^*(x)a(x) = LA(x),$$

where $a(x)$ is a fermion field on $\mathbb{R}^4$, A is a boson field and L is a linear differential operator on $\mathcal{S}(\mathbb{R}^4)$. To realize this, together with a superselection structure in a suitable C*-algebra setting, we present our construction in six steps.

Step 1: For the fermion field, let $\mathcal{H}=L^2(\mathbb{R}^4)$ and define $\mathrm{CAR}(\mathcal{H})$ in Araki's self-dual form (cf. Ref. 24) as follows. On $\mathcal{K}:=\mathcal{H}\oplus\mathcal{H}$ define an antiunitary involution Γ by $\Gamma(h_1\oplus h_2):=\bar{h}_2\oplus\bar{h}_1$. Then $\mathrm{CAR}(\mathcal{H})$ is the unique simple C^*-algebra with generators $\{\Phi(k)\,|\,k\in\mathcal{K}\}$ such that $k\to\Phi(k)$ is antilinear, $\Phi(k)^*=\Phi(\Gamma k)$, and

$$\{\Phi(k_1),\Phi(k_2)^*\}=(k_1,k_2)\mathbb{1},\quad k_i\in\mathcal{K}.$$

The correspondence with the heuristic creators and annihilators of fermions is given by $\Phi(h_1\oplus h_2)=a(h_1)+a^*(\bar{h}_2)$, where

$$a(h)=\int a(x)\overline{h(x)}d^4x,\quad a^*(h)=\int a^*(x)h(x)d^4x.$$

Step 2: For the boson field, let $S=\mathcal{S}(\mathbb{R}^4,\mathbb{R})$, and let $K:S\to L^2(M,\mu)$ be a linear map, where (M,μ) is a fixed measure space. Define a symplectic form on S by $B(f,g):=\mathrm{Im}(Kf,Kg)$, where $(\cdot,\cdot)$ is the inner product of $L^2(M,\mu)$. Note that B is degenerate if $\mathrm{Ker}\,K$ is nonzero. Define then $\mathrm{CCR}(S,B)=C^*\{\delta_f|f\in S\}$ where the δ_f are unitaries satisfying the Weyl relations

$$\delta_f\cdot\delta_g=\delta_{f+g}\exp[iB(f,g)/2],$$

i.e., $\mathrm{CCR}(S,B)$ is the σ-twisted discrete group algebra of S with respect to the two-cocycle $\sigma(f,g):=\exp[iB(f,g)/2]$.

Step 3: To combine the bosons and fermions in one C^*-algebra, we want to allow for the possibility that they may not commute with each other, hence we will not take the tensor algebra $\mathrm{CAR}(\mathcal{H})\otimes\mathrm{CCR}(S,B)$. However, we do not know what form their commutators should take, so we start with the free C^*-algebra $\mathcal{E}$ generated by $\mathrm{CAR}(\mathcal{H})$ and $\mathrm{CCR}(S,B)$. The free C^*-algebra $\mathcal{E}$ seems to be big enough to allow for possible interactions, but it is also likely to contain redundant elements.

To be explicit, let $\mathcal{L}$ be the linear space spanned by all monomials of the form $A_0B_0A_1B_1\cdots A_nB_n$ where $A_i\in\mathrm{CAR}(\mathcal{H})$ and $B_i\in\mathrm{CCR}(S,B)$. Note that $\mathcal{L}$ is an algebra with respect to concatenation. Factor out by the ideal generated by $\mathbb{1}_{\mathrm{CAR}}-\mathbb{1}_{\mathrm{CCR}}$ and replace concatenation by multiplication for any two elements in a monomial which are in the same algebra (either CAR or CCR) after the factorization. Note that this will now produce all possible monomials of elements in $\mathrm{CAR}(\mathcal{H})$ and $\mathrm{CCR}(S,B)$, just consider those monomials in $\mathcal{L}$ with A_0 or B_n the identity to obtain all other monomials. Now the resultant algebra $\mathcal{N}$ is a *-algebra with the involution given by

$$(A_0B_0\cdots A_nB_n)^*=B_n^*A_n^*\cdots B_0^*A_0^*.$$

Form the enveloping C^*-algebra $\mathcal{E}$ of $\mathcal{N}$, i.e., let

$$\mathcal{I}_0:=\cap\{\mathrm{Ker}\,\pi|\pi\in\text{Hilbert space representations of }\mathcal{N}\}$$

and set $\mathcal{E}:=\overline{\mathcal{N}/\mathcal{I}_0}$ where the closure is with respect to the enveloping C^*-norm, i.e.,

$$\|A\|:=\sup\{\|\pi(A)\|\,|\,\pi\in\text{Hilbert space representations of }\mathcal{N}\}.$$

That $\mathcal{E}$ is nontrivial, follows from the fact that any tensor product representation of $\mathrm{CAR}(\mathcal{H})\otimes\mathrm{CCR}(S,B)$ defines a Hilbert space representation of $\mathcal{N}$, hence it follows that $\mathcal{E}$ is nonzero and that $\mathrm{CAR}(\mathcal{H})$ and $\mathrm{CCR}(S,B)$ are faithfully embedded in $\mathcal{E}$ (as the images under the factorization maps of the original generating algebras in the construction). Note that we have a surjective homomorphism $\zeta:\mathcal{E}\to\mathrm{CAR}(\mathcal{H})\otimes\mathrm{CCR}(S,B)$ given by

$$\zeta(A_0B_0\cdots A_nB_n) \coloneqq (A_0\cdots A_n)\otimes(B_0\cdots B_n), \quad A_i\in \mathrm{CAR}(\mathcal{H}), \quad B_i\in \mathrm{CCR}(S,B).$$

Clearly the ideal $\mathcal{I}_T$ of $\mathcal{E}$ generated by the commutators $[\mathrm{CAR}(\mathcal{H}), \mathrm{CCR}(S,B)]$ is in Ker ζ. Since $\mathcal{E}$ probably contains redundant elements, we do not require it to be simple. ζ will be important in proofs below.

Step 4: Next, we would like to model in the curent C*-setting, the global and local heuristic charges,

$$Q=\int a^*(x)a(x)d^4x, \quad Q(f)=\int a^*(x)a(x)f(x)d^4x, \quad f\in\mathcal{S}(\mathbb{R}^4,\mathbb{R}).$$

Let us calculate the Bogoliubov transformations which they induce,

$$\begin{aligned}
[Q(f),\Phi(h_1\oplus h_2)] &= \int\int [a^*(x)a(x)f(x),a(y)\overline{h_1(y)}+a^*(y)\overline{h_2(y)}]d^4x\,d^4y\\
&= \int\int f(x)\{(a^*(x)a(x)a(y)-a(y)a^*(x)a(x))\overline{h_1(y)}\\
&\quad +(a^*(x)a(x)a^*(y)-a^*(y)a^*(x)a(x))\overline{h_2(y)}\}d^4x\,d^4y\\
&= \int\int f(x)\{-\{a^*(x),a(y)\}a(x)\overline{h_1(y)}+(a^*(x)(\delta(x-y)-a^*(y)a(x))\\
&\quad -a^*(y)a^*(x)a(x))\overline{h_2(y)}\}d^4x\,d^4y\\
&= \int\int f(x)\{-\delta(x-y)\overline{h_1(y)}a(x)+\delta(x-y)a^*(x)\overline{h_2(y)}\}d^4x\,d^4y\\
&= -a(\overline{f}\cdot h_1)+a^*(f\cdot\overline{h_2})=\Phi(-\overline{f}\cdot h_1\oplus\overline{f}\cdot h_2)=\Phi(f(-h_1\oplus h_2))
\end{aligned}$$

since f is real. For the global charge Q, just set $f=1$ in the last calculation. Thus

$$(\mathrm{ad}\,Q(f))^n(\Phi(h_1\oplus h_2))=\Phi(f^n\cdot((-1)^nh_1\oplus h_2)),$$

hence,

$$\begin{aligned}
(\mathrm{Ad}(\exp iQ(f)))(\Phi(h_1\oplus h_2)) &= (\exp i\,\mathrm{ad}\,Q(f))(\Phi(h_1\oplus h_2))\\
&= \sum_{n=0}^{\infty}\frac{(i\,\mathrm{ad}\,Q(f))^n}{n!}(\Phi(h_1\oplus h_2))\\
&= \sum_{n=0}^{\infty}\frac{i^n}{n!}\Phi(f^n((-1)^nh_1\oplus h_2))=\Phi(e^{-if}h_1\oplus e^{if}h_2)\eqqcolon\Phi(T_f(h_1\oplus h_2)).
\end{aligned}$$

Now T_f is unitary on $\mathcal{K}$, and satisfies $[T_f,\Gamma]=0$, hence it is a Bogoliubov transformation (cf. p. 43 in Ref. 24), and so we can define automorphisms on $\mathrm{CAR}(\mathcal{H})$ by

$$\tilde{\gamma}_f(\Phi(k))\coloneqq\Phi(T_fk).$$

It is clear that $T_fT_g=T_{f+g}$, hence that $\tilde{\gamma}:\mathcal{S}(\mathbb{R}^4)+\mathbb{R}\to\mathrm{Aut}(\mathrm{CAR}(\mathcal{H}))$ is a homomorphism. We extend these automorphisms to maps γ_f on $\mathcal{E}$ by setting

$$\gamma_f\restriction\mathrm{CAR}(\mathcal{H})=\tilde{\gamma}_f, \quad \text{and} \quad \gamma_f\restriction\mathrm{CCR}(S,B)=\iota,$$

where ι is the identity map. The only relations between $\mathrm{CAR}(\mathcal{H})$ and $\mathrm{CCR}(S,B)$ in the free construction of $\mathcal{E}$, is $\mathbb{1}_{\mathrm{CAR}}=\mathbb{1}_{\mathrm{CCR}}$, so since the definition of γ_f preserves this relation, it will extend to a well-defined map on the free *-algebra $\mathcal{N}$. In fact, since γ_f replaces $\mathrm{CAR}(\mathcal{H})$ by an isomor-

phic one in a free construction, it will be an automorphism on $\mathcal{N}$, and so will define an automorphism on the enveloping algebra $\mathcal{E}$.

Let G denote the Abelian group generated in Aut $\mathcal{E}$ by $\{\gamma_f | f \in \mathcal{S}(\mathbb{R}^4) \cup \mathbb{R}\}$ and equip it with the discrete topology. Denote its action by $\beta: G \to \text{Aut}\,\mathcal{E}$, and define the algebra

$$\mathcal{A} := \mathcal{G} \underset{\beta}{\times} \mathcal{E},$$

then we identify the implementing unitaries $U_{\gamma_f} \in \mathcal{A}$ of $\gamma_f \in \text{Aut}\,\mathcal{E}$ with the heuristic objects $\exp iQ(f)$, $f \in \mathcal{S}(\mathbb{R}^4) \cup \mathbb{R}$ [in the case that $f = t \in \mathbb{R}$, we denote $Q(t) = tQ$]. Now γ is a surjective homomorphism $\gamma: \mathcal{S}(\mathbb{R}^4) + \mathbb{R} \to G$ and from the definitions above, it is clear that its kernel is $2\pi\mathbb{Z} \subset \mathbb{R}$, hence the discrete group G is isomorphic to $\mathcal{S}(\mathbb{R}^4) \times \mathbb{T}$. Of course $\mathbb{T}$ will be our global gauge group below.

Step 5: Next, we would like to realize in $\mathcal{E}$ the heuristic constraints

$$Q(f)^n \psi = A(Lf)^n \psi \quad \forall\, f \in \mathcal{S}(\mathbb{R}^4), \quad n \in \mathbb{N},$$

where $L: S \to \text{Ker}\, K \subseteq \text{Ker}\, B$ is a given linear map. First write the heuristic constraints in bounded form

$$e^{iQ(f)}\psi = e^{iA(Lf)}\psi, \quad \text{i.e.,}\ e^{-iA(Lf)}e^{iQ(f)}\psi = \psi.$$

So, given the identifications with heuristic objects above, we define our constraint unitaries to be

$$\mathcal{U} := \{\delta_{-Lf} \cdot U_{\gamma_f} =: V_f | f \in \mathcal{S}(\mathbb{R}^4, \mathbb{R})\} \subset \mathcal{A}.$$

Proposition 5.1: $\mathcal{U}$ is first class.

The proof is in the next section. The heuristic constraint conditions now correspond to the application of the T-procedure to $\mathcal{U}$.

Step 6: Now we will specify the superselection structure associated with the global charge Q using the fact that Q must take integer values on the vacuum state. Recall that the global gauge transformations γ_t, $t \in \mathbb{R}$ are implemented by the unitaries $U_{\gamma_t} \in \mathcal{A}$ which we identify with the heuristic objects $\exp itQ$ (cf. Step 3). For the superselection sectors we need to find cyclic representations (π, Ω) such that

$$\pi(U_{\gamma_t})\Omega = e^{itn}\Omega \quad \forall\, t \in \mathbb{R}$$

and some $n \in \mathbb{Z}$ (the heuristic corresponding conditions are $Q\Omega = n\Omega$). We recognize these as constraint conditions for Dirac states of the constraint unitaries,

$$\mathcal{V}_n := \{V_t^{(n)} := e^{-itn} U_{\gamma_t} | t \in \mathbb{R}\}.$$

Denote the sets of these Dirac states by

$$\mathfrak{S}_D^{(n)} := \{\omega \in \mathfrak{S}(\mathcal{A}) | \omega(V_t^{(n)}) = 1 \ \ \forall\, t \in \mathbb{R}\}.$$

These folia of states will be our superselection sectors.

Lemma 5.2: With notation as above, we have

(i) $\mathfrak{S}_D^{(n)} \cap \mathfrak{S}_D^{(m)} = \emptyset$ *if* $n \neq m$,

(ii) $\mathfrak{S}_D^{(0)} \neq \emptyset$.

Proof: (i) If there is a $\omega \in \mathfrak{S}_D^{(n)} \cap \mathfrak{S}_D^{(m)}$ for $n \neq m$, then

$$\omega(e^{-itn}U_{\gamma_t}) = 1 = \omega(e^{-itm}U_{\gamma_t}),$$

so

$$\omega(U_{\gamma_t}) = e^{itn} = e^{itm} \quad \forall\, t$$

which contradicts $n \neq m$.

(ii) In the proof of Lemma 5.1 we constructed a state $\omega_3 \in \mathfrak{S}(\mathcal{A})$ satisfying $\omega_3(U_g) = 1$ for all $g \in G$. If we take $g = \gamma_t$, then this implies that $\omega_3 \in \mathfrak{S}_D^{(0)}$. ■

To connect with the usual machinery for superselection used above, we need to exhibit the canonical endomorphisms (automorphisms in the Abelian case). We construct an action $\rho: \mathbb{Z} \to \mathrm{Aut}\,\mathcal{A}$ such that its dual action on $\mathcal{A}^*$ satisfies $\rho_k^*(\mathfrak{S}_D^{(n)}) = \mathfrak{S}_D^{(n+k)}$.

Definition 5.3: For each $k \in \mathbb{Z}$ define a $*$-automorphism ρ_k of $\mathcal{A}$ by

$$\rho_k(A) = A \quad \forall\, A \in \mathcal{E}, \quad \rho_k(U_{\gamma_t}) = e^{itk} U_{\gamma_t} \quad \forall\, t \in \mathbb{R},$$

$$\rho_k(U_{\gamma_f}) = U_{\gamma_f} \quad \forall\, f \in \mathcal{S}(\mathbb{R}^4).$$

Lemma 5.4: ρ_k is well-defined, and $\rho_k \in \mathrm{Aut}\,\mathcal{A}$.

The proof is in the next section. Recall that for any $\alpha \in \mathrm{Aut}\,\mathcal{A}$ we define its dual $\alpha^*: \mathcal{A}^* \to \mathcal{A}^*$ by $\alpha^*(f) := f \circ \alpha$ for all functionals $f \in \mathcal{A}^*$.

Proposition 5.5: With notation as above, we have $\rho_k^*(\mathfrak{S}_D^{(n)}) = \mathfrak{S}_D^{(n+k)}$ and $\mathfrak{S}_D^{(n)} \neq \emptyset$ for all $n \in \mathbb{Z}$.

Proof: Let $\omega \in \rho_k^*(\mathfrak{S}_D^{(n)})$, i.e., $\omega = \omega_n \circ \rho_k$ for some $\omega_n \in \mathfrak{S}_D^{(n)}$. Thus

$$\omega(e^{-it(n+k)} U_{\gamma_t}) = \omega_n(e^{-it(n+k)} \rho_k(U_{\gamma_t})) = \omega_n(e^{-itn} U_{\gamma_t}) = 1,$$

i.e., $\omega \in \mathfrak{S}_D^{(n+k)}$. Conversely, for any $\omega \in \mathfrak{S}_D^{(n+k)}$ there is a $\omega_n \in \mathfrak{S}_D^{(n)}$ for which $\omega = \omega_n \circ \rho_k$ and it is obviously $\omega_n = \omega \circ \rho_{-k}$. Thus $\rho_k^*(\mathfrak{S}_D^{(n)}) = \mathfrak{S}_D^{(n+k)}$. Since we have that $\mathfrak{S}_D^{(0)} \neq \emptyset$, it is now immediate that $\mathfrak{S}_D^{(n)} = \rho_k^*(\mathfrak{S}_D^{(0)}) \neq \emptyset$. ■

Recall from our earlier discussions that the canonical automorphisms (Abelian case) must necessarily be outer on $\mathcal{A}$.

Proposition 5.6: With notation as above, $\rho_k \in \mathrm{Out}\,\mathcal{A}$ if $k \neq 0$.

The proof of this is long, and is in the next section.

From the action $\rho: \mathbb{Z} \to \mathrm{Out}\,\mathcal{A}$ we construct a Hilbert extension (cf. Sec. II F). First set

$$\Lambda := \{\mathrm{Ad}\, U \circ \rho_k | U \in \mathcal{A} \text{ unitary}, k \in \mathbb{Z}\}$$

so $\mathbb{Z} \cong \Lambda / \mathrm{Inn}\,\mathcal{A}$. So the class of $k \in \mathbb{Z}$ in $\Lambda / \mathrm{Inn}\,\mathcal{A}$ is $\chi_k := \{\mathrm{Ad}\, U \circ \rho_k \,|\, U \in \mathcal{A}_u\}$. Take the monomorphic section $\chi_k \to k$, then it has a trivial cocycle $\sigma(n,m) = 1$ for all $n, m \in \mathbb{Z}$. Define $\mathcal{F} := \mathbb{Z} \times_{\rho} \mathcal{A}$, then it has the dense $*$-algebra

$$\mathcal{F}_0 := \left\{ \sum_{n \in F} A_n U^n | A_n \in \mathcal{A}, F \subset \mathbb{Z} \text{ finite} \right\},$$

where $U \in \mathcal{F}$ is the unitary which implements ρ_1, i.e., $\rho_1 = \mathrm{Ad}\, U \restriction \mathcal{A}$. Fix $t \in \mathbb{T} = \hat{\mathbb{Z}}$ and define an action $\alpha: \mathbb{T} \to \mathrm{Aut}\,\mathcal{F}$ by

$$\alpha_t\left(\sum_{n \in F} A_n U^n \right) := \sum_{n \in F} A_n t^n U^n \quad \text{on } \mathcal{F}_0.$$

Then the fixed point algebra of α is $\mathcal{A}$. We verify the compatibility condition in Corollary 4.3.

Proposition 5.7: $\rho_k(\mathcal{D}) \sim \mathcal{D}$ for all $k \in \mathbb{Z}$.

Proof: The constraint unitaries from which we define $\mathcal{D}$ are $V_f := \delta_{-Lf} \cdot U_{\gamma_f}$, $f \in \mathcal{S}(\mathbb{R}^4)$. By Definition 5.3 we have $\rho_k \restriction \mathcal{E} = \iota$, hence $\rho_k(\delta_{-Lf}) = \delta_{-Lf}$. Also $\rho_k(U_{\gamma_f}) = U_{\gamma_f}$ for all $f \in \mathcal{S}(\mathbb{R}^4)$, hence $\rho_k(V_f) = V_f$ for all $f \in \mathcal{S}(\mathbb{R}^4)$. Thus ρ_k preserves the Dirac states $\mathfrak{S}_D$ and hence $\rho_k(\mathcal{D}) = \mathcal{D}$ for all $k \in \mathbb{Z}$. ■

It remains to show that this Hilbert system is regular and minimal. However, at this stage we do not have a proof because little is known about the ideal $\mathcal{I}_0$ factored out in Step 3.

VI. PROOFS

Proof of Theorem 4.1: (i) We have that $\beta_g := g \restriction \mathcal{O}_\mathcal{F}$. The pointwise norm-continuity of $\beta_\mathcal{G}$ follows from the pointwise norm-convergence topology of $\mathcal{G}$. So $\{\mathcal{O}_\mathcal{F}, \mathcal{G}, \beta\}$ is a C*-dynamical system. Since $\mathcal{A}$ is the fixed point algebra of $\mathcal{G}$, the fixed point algebra of $\beta_\mathcal{G}$ is $\mathcal{O}_\mathcal{F} \cap \mathcal{A}$. By Theorem 3.7 we have that $\mathcal{O}_\mathcal{F} \cap \mathcal{A} = \mathcal{O}$.

If $A \in Z(\mathcal{A})$, then $[A, \mathcal{C}] = 0$, hence $A \in \mathcal{O}$ by Theorem 3.3 (iii), and from this it follows that $Z(\mathcal{A}) \subseteq Z(\mathcal{O})$.

(ii) Now let $\mathcal{H}_\gamma \subset \Pi_\gamma \mathcal{F}$. If there is a unit vector $\Phi \in \mathcal{H}_\gamma \cap \mathcal{O}_\mathcal{F}$, then by invariance of $\mathcal{H}_\gamma \cap \mathcal{O}_\mathcal{F}$ under $\mathcal{G}$, we also have $\mathcal{H}_\gamma \cap \mathcal{O}_\mathcal{F} \supset$ span $(\mathcal{G}\Phi) = \mathcal{H}_\gamma$, where the last equality follows from irreducibility of the action of $\mathcal{G}$ on $\mathcal{H}_\gamma$. Thus $\mathcal{H}_\gamma \cap \mathcal{O}_\mathcal{F} \neq \{0\}$ implies that $\mathcal{H}_\gamma \subset \mathcal{O}_\mathcal{F}$, hence $\mathcal{H}_\gamma \subset \Pi_\gamma \mathcal{O}_\mathcal{F}$.

To prove that $\Pi_\gamma \mathcal{O}_\mathcal{F} = \text{clo-span}(\mathcal{O}\mathcal{H}_\gamma)$ we follow the proof of Lemma 10.1.3 in Ref. 3. First, since $\mathcal{O} = \Pi_\iota \mathcal{O}_\mathcal{F}$, it follows that $\mathcal{O}\mathcal{H}_\gamma \subseteq \Pi_\gamma \mathcal{O}_\mathcal{F}$ by Remark 2.5 (v).

By Evans and Sund,[11] $\Pi_\gamma \mathcal{O}_\mathcal{F}$ is the closed span of all the $\mathcal{G}$-invariant subspaces $\mathcal{E} \subset \mathcal{O}_\mathcal{F}$ such that $\beta_\mathcal{G}$ acts on $\mathcal{E}$ as an element of $\gamma \in \widehat{\mathcal{G}/\mathcal{K}}$. So for the reverse inclusion, $\Pi_\gamma \mathcal{O}_\mathcal{F} \subseteq$ clo-span$\{\mathcal{O}\mathcal{H}_\gamma\}$, it suffices to show that span $\{\mathcal{O}\mathcal{H}_\gamma\}$ contains all $\mathcal{G}$-invariant subspaces $\mathcal{E} \subset \mathcal{O}_\mathcal{F}$ such that $\mathcal{G}$ acts on $\mathcal{E}$ as an element of γ. Let $\{\Psi_1, \ldots, \Psi_d\}$, $d = \dim \gamma$ be a basis of such an $\mathcal{E}$ under which the matrix representation of the action of $\mathcal{G}$ is an element of γ, i.e.,

$$g\Psi_i = \sum_j \lambda_{ji}(g)\Psi_j,$$

where the matrix $(\lambda_{ji}(g))$ is a unitary matrix representation of $\mathcal{G}$ of the type γ. Choose an orthonormal basis $\{\Phi_1, \ldots, \Phi_d\}$ of $\mathcal{H}_\gamma$ which also transforms under $\mathcal{G}$ according to $(\lambda_{ji}(g))$. Consider now the element $A := \Sigma_j \Psi_j \Phi_j^* \in \mathcal{O}_\mathcal{F}$. Then

$$g(A) = \sum_j g(\Psi_j \Phi_j^*) = \sum_{i,k} \left(\sum_j \lambda_{ij}(g)\overline{\lambda_{kj}(g)} \right) \Psi_i \Phi_k^* = \sum_{i,k} \delta_{ik} \Psi_i \Phi_k^* = \sum_j \Psi_j \Phi_j^* = A.$$

Thus $A \in \mathcal{O}$, and hence all $\Psi_i = A\Phi_i \in \mathcal{O}\mathcal{H}_\gamma$, i.e., $\mathcal{E} \subset$ span $(\mathcal{O}\mathcal{H}_\gamma)$.

(iii) Let $\mathcal{H}_\sigma$ have an orthonormal basis $\{\Phi_1, \ldots, \Phi_d\}$ hence $\rho_\sigma(F) = \Sigma_{j=1}^d \Phi_j F \Phi_j^*$ for $F \in \mathcal{F}$, $\rho_\sigma \restriction \mathcal{A} = \sigma$. Since $\{\Phi_j\} \subset \mathcal{O}_\mathcal{F} = M(\mathcal{D}_\mathcal{F})$ it is clear that ρ_σ preserves both $\mathcal{D}_\mathcal{F}$ and $\mathcal{O}_\mathcal{F}$. Since ρ_σ also preserves $\mathcal{A}$, it preserves $\mathcal{D} = \mathcal{D}_\mathcal{F} \cap \mathcal{A}$ and $\mathcal{O} = \mathcal{O}_\mathcal{F} \cap \mathcal{A}$, where these equalities come from Theorem 3.7.

Proof of Theorem 4.2: (i) Let $\mathcal{H} \subset \mathcal{O}_\mathcal{F}$ have an orthonormal basis $\{\Phi_j\}$. By the same proof as for Theorem 4.1 (iii) we have that $\rho_\mathcal{H}(\mathcal{D}) \subseteq \mathcal{D}$.

Since $\mathcal{O}_\mathcal{F}$ is a *-algebra and the relative multiplier algebra of $\mathcal{D}_\mathcal{F} \supset \mathcal{D}$, we have that

$$[\Phi_j^*, D] \in \mathcal{D}_\mathcal{F} \quad \text{for all } D \in \mathcal{D}, j.$$

Thus

$$\Phi_j[\Phi_j^*, D] \in \Phi_j \mathcal{D}_\mathcal{F} = \rho_\mathcal{H}(\mathcal{D}_\mathcal{F})\Phi_j \subset \text{clo-span}(\rho_\mathcal{H}(\mathcal{D}_\mathcal{F})\mathcal{F}),$$

i.e.,

$$D - \rho_\mathcal{H}(D) = \sum_j (\Phi_j \Phi_j^* D - \Phi_j D \Phi_j^*) \in \text{clo-span}(\rho_\mathcal{H}(\mathcal{D}_\mathcal{F})\mathcal{F}).$$

So

$$D \in \text{clo-span}(\rho_\mathcal{H}(\mathcal{D}_\mathcal{F})\mathcal{F}) \quad \text{for all } D \in \mathcal{D}.$$

Thus we have shown that $\mathcal{D} \subset \text{clo-span}(\rho_\mathcal{H}(\mathcal{D}_\mathcal{F})\mathcal{F})$, and now we would like to show that clo-span$(\rho_\mathcal{H}(\mathcal{D}_\mathcal{F})\mathcal{F}) = \text{clo-span}(\rho_\mathcal{H}(\mathcal{D})\mathcal{F})$. We have that

$$\text{clo-span}(\mathcal{C}\mathcal{F}) = \text{clo-span}(\mathcal{D}\mathcal{F}) = \text{clo-span}(\mathcal{D}_{\mathcal{F}}\mathcal{F}),$$

so if we apply $\rho_{\mathcal{H}}$ to both sides of the last equation, multiply by $\mathcal{F}$ on the right and take closed span, we get

$$\text{clo-span}(\rho_{\mathcal{H}}(\mathcal{D})\rho_{\mathcal{H}}(\mathcal{F})\mathcal{F}) = \text{clo-span}(\rho_{\mathcal{H}}(\mathcal{D}_{\mathcal{F}})\rho_{\mathcal{H}}(\mathcal{F})\mathcal{F}),$$

i.e.,

$$\text{clo-span}(\rho_{\mathcal{H}}(\mathcal{D}_{\mathcal{F}})\mathcal{F}) = \text{clo-span}(\rho_{\mathcal{H}}(\mathcal{D})\mathcal{F}).$$

Thus

$$\mathcal{D} \subset \text{clo-span}(\rho_{\mathcal{H}}(\mathcal{D})\mathcal{F}) \quad \text{and since } \mathcal{D} \text{ is a * -algebra in } \mathcal{A},$$

$$\mathcal{D} \subseteq \text{clo-span}(\rho_{\mathcal{H}}(\mathcal{D})\mathcal{F}) \cap \text{clo-span}(\mathcal{F}\rho_{\mathcal{H}}(\mathcal{D})) \cap \mathcal{A} \subseteq \text{clo-span}(\mathcal{D}\mathcal{F}) \cap \text{clo-span}(\mathcal{F}\mathcal{D}) \cap \mathcal{A} = \mathcal{D},$$

where we used $\mathcal{D}_{\mathcal{F}} \cap \mathcal{A} = \mathcal{D}$. Thus,

$$\mathcal{D} = \text{clo-span}(\rho_{\mathcal{H}}(\mathcal{D})\mathcal{F}) \cap \text{clo-span}(\mathcal{F}\rho_{\mathcal{H}}(\mathcal{D})) \cap \mathcal{A} = \text{clo-span}(\rho_{\mathcal{H}}(\mathcal{D})\mathcal{A}) \cap \text{clo-span}(\mathcal{A}\rho_{\mathcal{H}}(\mathcal{D}))$$

which also follows from Theorem 3.7, treating $\rho_{\mathcal{H}}(\mathcal{D}) \subseteq \mathcal{D}$ as a second constraint set. Thus $\mathcal{D} \sim \rho_{\mathcal{H}}(\mathcal{D})$ in $\mathcal{A}$.

For the converse, let $\mathcal{D} \sim \rho_{\mathcal{H}}(\mathcal{D})$ and take $\Phi \in \mathcal{H}$. From the equation $\Phi D = \rho_{\mathcal{H}}(D)\Phi$ for all $D \in \mathcal{D}$, we conclude that

$$\Phi \cdot \text{clo-span}(\mathcal{D}\mathcal{F}) \subset \text{clo-span}(\rho_{\mathcal{H}}(\mathcal{D})\mathcal{F}) = \text{clo-span}(\mathcal{D}\mathcal{F})$$

using $\mathcal{D} \sim \rho_{\mathcal{H}}(\mathcal{D})$. Since we have trivially that $\Phi \cdot \text{clo-span}(\mathcal{F}\mathcal{D}) \subset \text{clo-span}(\mathcal{F}\mathcal{D})$, it follows that

$$\Phi\mathcal{D}_{\mathcal{F}} = \Phi(\text{clo-span}(\mathcal{F}\mathcal{D}) \cap \text{clo-span}(\mathcal{D}\mathcal{F})) \subset \mathcal{D}_{\mathcal{F}}$$

so Φ is in the left multiplier of $\mathcal{D}_{\mathcal{F}}$. We also have that

$$\text{clo-span}(\mathcal{F}\mathcal{D})\Phi = \text{clo-span}(\mathcal{F}\rho_{\mathcal{H}}(\mathcal{D}))\Phi = \text{clo-span}(\mathcal{F}\Phi\mathcal{D}) \subseteq \text{clo-span}(\mathcal{F}\mathcal{D}).$$

Since trivially $\text{clo-span}(\mathcal{D}\mathcal{F})\Phi \subseteq \text{clo-span}(\mathcal{D}\mathcal{F})$, it follows that

$$\mathcal{D}_{\mathcal{F}}\Phi = (\text{clo-span}(\mathcal{F}\mathcal{D}) \cap \text{clo-span}(\mathcal{D}\mathcal{F}))\Phi \subset \mathcal{D}_{\mathcal{F}}$$

and hence Φ is in the relative multiplier algebra of $\mathcal{D}_{\mathcal{F}}$, i.e., $\Phi \in \mathcal{O}_{\mathcal{F}}$ by Theorem 3.3 (ii).

(ii) Let $\mathcal{H}_\sigma \subset \mathcal{O}_{\mathcal{F}} \supset \mathcal{H}_\tau$, hence by (i) $\mathcal{D} \sim \sigma(\mathcal{D}) \sim \tau(\mathcal{D})$.

First let $X \in (\sigma, \tau)_{\mathcal{A}} \cap \mathcal{O}$, i.e., $X \in \mathcal{O}$ and $X\sigma(A) = \tau(A)X$ for all $A \in \mathcal{A}$. By letting A range over only $\mathcal{O} \subset \mathcal{A}$, we immediately get that $X \in (\sigma\restriction\mathcal{O}, \tau\restriction\mathcal{O})_{\mathcal{O}}$, making use of Theorem 4.1 (iii). Therefore, it suffices to prove that $(\sigma, \tau)_{\mathcal{A}} \subset \mathcal{O}$.

Let $X \in (\sigma, \tau)_{\mathcal{A}}$, i.e., $X \in \mathcal{A}$ and $X\sigma(A) = \tau(A)X$ for all $A \in \mathcal{A}$. Thus

$$X \cdot \text{clo-span}(\mathcal{D}\mathcal{A}) = X \cdot \text{clo-span}(\sigma(\mathcal{D})\mathcal{A}) = \text{clo-span}(X\sigma(\mathcal{D})\mathcal{A}) \subseteq \text{clo-span}(\tau(\mathcal{D})X\mathcal{A})$$

$$\subseteq \text{clo-span}(\tau(\mathcal{D})\mathcal{A}) = \text{clo-span}(\mathcal{D}\mathcal{A}).$$

Since we have trivially that $X \cdot \text{clo-span}(\mathcal{A}\mathcal{D}) \subseteq \text{clo-span}(\mathcal{A}\mathcal{D})$, it follows that

$$X\mathcal{D} \subseteq \text{clo-span}(\mathcal{A}\mathcal{D}) \cap \text{clo-span}(\mathcal{D}\mathcal{A}) = \mathcal{D},$$

i.e., X is in the left multiplier of $\mathcal{D}$. Likewise,

$$\text{clo-span}(\mathcal{AD})\cdot X=\text{clo-span}(\mathcal{A}\tau(\mathcal{D}))\cdot X=\text{clo-span}(\mathcal{A}\tau(\mathcal{D})X)$$
$$\subseteq \text{clo-span}(\mathcal{A}X\sigma(\mathcal{D}))\subseteq \text{clo-span}(\mathcal{A}\sigma(\mathcal{D}))=\text{clo-span}(\mathcal{AD}).$$

Since trivially $\text{clo-span}(\mathcal{DA})\cdot X\subseteq\text{clo-span}(\mathcal{DA})$, we have

$$\mathcal{D}\cdot X\subseteq \text{clo-span}(\mathcal{AD})\cap\text{clo-span}(\mathcal{DA})=\mathcal{D},$$

and hence X is in the relative multiplier of $\mathcal{D}$, i.e., $X\in\mathcal{O}$.

Proof of Proposition 4.5: (i) According to the decomposition

$$\sigma(\cdot)=\sum_j V_j\rho_{\gamma_j}(\cdot)V_j^*,\quad V_j\in(\rho_{\gamma_j},\sigma)_{\mathcal{A}},$$

we have $\mathcal{H}_\sigma=\Sigma_j V_j\mathcal{K}_j'$ where $\rho_{\gamma_j}=\rho_{\mathcal{K}_j'}$ and the $\mathcal{K}_j'$ are irreducible with respect to $\mathcal{G}$ carrying the representation $\gamma_j\in\hat{\mathcal{G}}$. Moreover supp $\mathcal{K}_j'=1$.

Set $E_j:=V_jV_j^*$. Then $\Sigma_jE_j=1$. Since $V_j\mathcal{K}_j'\subset\mathcal{H}_\sigma\subset\mathcal{O}_\mathcal{F}$ it follows that

$$E_j=\text{supp}\ V_j\mathcal{K}_j'\in\mathcal{O}$$

for all j. Therefore, by assumption, there are isometries $W_j\in\mathcal{O}$ with $E_j=W_jW_j^*$. Now we set

$$\mathcal{K}_j:=W_j^*V_j\mathcal{K}_j'\subset\mathcal{O}_\mathcal{F}.$$

Then $\mathcal{K}_j$ is an algebraic Hilbert space with supp $\mathcal{K}_j=1$, carrying the representation γ_j and we have $V_j\mathcal{K}_j'=W_j\mathcal{K}_j$. Hence $\mathcal{H}_\sigma=\Sigma_jW_j\mathcal{K}_j$ and

$$\sigma(\cdot)=\sum_j W_j\rho_{\mathcal{K}_j}(\cdot)W_j^*,\quad W_j\in(\rho_{\mathcal{K}_j},\sigma)_{\mathcal{O}}$$

follows.

(ii) This follows from (i) using the existence of subobjects.

Proof of Theorem 4.8: Let $\mathcal{H}\subset\mathcal{F}$ be an arbitrary algebraic Hilbert space. Then $\xi(\mathcal{H})\subset\mathcal{L}$ is also an algebraic Hilbert space, with support 1. To see this, let $\{\Phi_j\}_j$ be an orthonormal basis of $\mathcal{H}$, i.e., $\Phi_j^*\Phi_k=\delta_{j,k}1$ and $\Sigma_j\Phi_j\Phi_j^*=1$ then the same relations are true for the system $\{\xi(\Phi_j)\}_j$. In particular ξ is injective on $\mathcal{H}$. Moreover, if $\mathcal{H}$ is $\mathcal{G}$-invariant and $g(\Phi_j)=\Sigma_ku_{k,j}(g)\Phi_k$ then $g^\xi(\xi(\Phi_j))=\Sigma_ku_{k,j}(g)\xi(\Phi_k)$, i.e., $\xi(\mathcal{H})$ carries the same representation as $\mathcal{H}$. In particular, if $\mathcal{H}_\gamma$ carries γ, i.e., $\mathcal{H}_\gamma\subset\Pi_\gamma\mathcal{F}$ then $\xi(\mathcal{H}_\gamma)\subset\Pi_\gamma^\xi\mathcal{L}$. This proves (ii) and (i).

Let $\mathcal{N}_\gamma$ be an orthonormal basis for $\xi(\mathcal{H}_\gamma)$, then by the first part it is the image under ξ of an orthonormal basis $\{\Phi_{\gamma,j}\}_j$ of $\mathcal{H}_\gamma$. Let $F=\Sigma A_{\gamma,j}\Phi_{\gamma,j}\in\mathcal{F}_{\text{fin}}$ such that $\xi(F)=0=\Sigma\xi(A_{\gamma,j})\xi(\Phi_{\gamma,j})$. By applying $\mathcal{G}^\xi$ to this equality, and using the relation $g^\xi(\xi(\Phi_{\gamma,j}))=\Sigma_ku_{k,j}(g)\xi(\Phi_{\gamma,k})$ we get $\Sigma_{\gamma,j,k}u_{k,j}^\gamma(g)\xi(A_{\gamma,j})\xi(\Phi_{\gamma,k})=0$ for all $g\in\mathcal{G}$. Now the orthogonality relations for the matrix elements of the irreducible representations of $\mathcal{G}$ imply $\xi(A_{\gamma,j})\xi(\Phi_{\gamma,k})=0$ for all $\gamma\in\hat{\mathcal{G}},j,k$. Hence $\xi(A_{\gamma,j})=0$ follows. This proves (iii). From $\xi\circ\Pi_\gamma=\Pi_\gamma^\xi\circ\xi$ (iv) follows.

For (v) observe that the homomorphic images of isometries $V_i\in\mathcal{A}$ with $V_1V_1^*+V_2V_2^*=1$ produces a pair of isometries in $\xi(\mathcal{A})$ satisfying the same relation. So Property B for $\mathcal{A}$ implies Property B for $\xi(\mathcal{A})$.

Proof of Corollary 4.9: (i) Let λ be generated by $\mathcal{H}$, i.e., let $\lambda=\rho_\mathcal{H}$ such that $\lambda(A)=\Sigma_j\Phi_jA\Phi_j^*$ where $\{\Phi_j\}_j$ is an orthonormal basis of $\mathcal{H}$. Then $\xi(\lambda(A))=\Sigma_j\xi(\Phi_j)\xi(A)\xi(\Phi_j)^*$ and $\xi(A)=0$ implies $\xi(\lambda(A))=0$. Furthermore, $\lambda^\xi(\xi(A))=\rho_{\xi(\mathcal{H})}(\xi(A))$.

(ii) $\lambda(\cdot)=\Sigma_jW_j\lambda_j(\cdot)W_j^*$ implies $\lambda^\xi(\cdot)=\Sigma_j\xi(W_j)\lambda_j^\xi(\cdot)\xi(W_j)^*$ and $(\lambda\circ\sigma)^\xi=\lambda^\xi\circ\sigma^\xi$. Further, if $\sigma(\cdot)=V^*\lambda(\cdot)V$ where $V\in(\sigma,\lambda)$, i.e., $V\sigma(\cdot)=\lambda(\cdot)V$ then $\xi(V)\sigma^\xi(\cdot)=\lambda^\xi(\cdot)\xi(V)$ and $\sigma^\xi(\cdot)=\xi(V)^*\lambda^\xi(\cdot)\xi(V)$.

In particular, if $\lambda\cong\sigma$ then $\lambda^\xi\cong\sigma^\xi$.

Proof of Theorem 4.10: (i) Let $\sigma\in\text{Ob}\,\mathcal{T}^\xi$. Then there is a $\mathcal{G}$-invariant algebraic Hilbert space $\mathcal{H}\subset\mathcal{L}$ such that $\sigma(X)=\Sigma_j\Psi_jX\Psi_j^*$, $X\in\xi(\mathcal{A})$, where $\{\Psi_j\}_j$ denotes an orthonormal basis of $\mathcal{H}$. On

the other hand, there is a corresponding $\mathcal{G}$-invariant Hilbert space $\mathcal{K}\subset\mathcal{F}$ such that $\mathcal{H}$ and $\mathcal{K}$ carry unitarily equivalent representations of $\mathcal{G}$. In $\mathcal{K}$ we choose an orthonormal basis $\{\Phi_j\}_j$ such that the representation matrix of $\mathcal{G}$ in $\mathcal{H}$ with respect to $\{\Psi_j\}_j$ coincides with that in $\mathcal{K}$ with respect to $\{\Phi_j\}_j$. Then $\xi(\mathcal{K})$ transforms under $\mathcal{G}$ with respect to $\{\xi(\Phi_j)\}_j$ with the same representation matrix. Now we set

$$V := \sum_j \Psi_j \xi(\Phi_j)^* \in \mathcal{L}.$$

Obviously, V is unitary and $g^\xi(V)=V$ for all $g\in\mathcal{G}$, i.e., $V\in\xi(\mathcal{A})$. Then $V\xi(\Phi_j)=\Psi_j$ or $\mathcal{H}=V\xi(\mathcal{K})$ and $\sigma=\mathrm{Ad}\,V\circ\rho_{\mathcal{K}}^\xi$.

(ii) According to Corollary 4.9 and $(\mathrm{Ob}\,\mathcal{T})^\xi\subseteq\mathrm{Ob}\,\mathcal{T}^\xi$ the image $\mathcal{C}^\xi$ of an equivalence class $\mathcal{C}\subset\mathrm{Ob}\,\mathcal{T}$ is contained in a unique equivalence class of $\mathrm{Ob}\,\mathcal{T}^\xi$. But (i) says that every equivalence class $\mathcal{E}$ of $\mathrm{Ob}\,\mathcal{T}^\xi$ is an image $\mathcal{E}=\mathcal{C}^\xi$.

Proof of Lemma 4.11: Let $A\in(\sigma,\tau)_{\mathcal{A}}$, then it follows immediately from $A\sigma(B)=\tau(B)A$, $B\in\mathcal{A}$ that $\xi(A)\sigma^\xi(\xi(B))=\tau^\xi(\xi(B))\xi(A)$ for all $B\in\mathcal{A}$. Recall that $\xi(\mathcal{A})$ is the fixed point algebra of $\mathcal{G}^\xi$.

Proof of Proposition 4.12: (i) This is obvious because the union $\cup_\gamma\mathcal{N}_\gamma$ of orthonormal bases $\mathcal{N}_\gamma$ of $\mathcal{H}_\gamma$ is an $\mathcal{A}$-left module basis of $\mathcal{F}_{\mathrm{fin}}$.

(ii) By a straightforward calculation one obtains for all $F\in\mathcal{F}$ that

$$\langle\xi(F),\xi(F)\rangle_{\xi(\mathcal{A})}=\xi(\langle F,F\rangle_{\mathcal{A}})$$

and

$$|\xi(F)|_{\xi(\mathcal{A})}=\|\xi(\langle F,F\rangle_{\mathcal{A}})\|^{1/2}\leqslant\|\langle F,F\rangle_{\mathcal{A}}\|^{1/2}=|F|_{\mathcal{A}},$$

i.e., ξ is continuous with respect to the norm $|\cdot|_{\mathcal{A}}$. Now let $F\in\mathrm{clo}_{|\cdot|_{\mathcal{A}}}(\mathrm{Ker}\,\xi\cap\mathcal{F}_{\mathrm{fin}})$, hence there is a sequence $\{F_n\}\subset\mathrm{Ker}\,\xi\cap\mathcal{F}_{\mathrm{fin}}$ such that $|F_n-F|_{\mathcal{A}}\to 0$. Then $\xi(F)=0$ follows. Conversely, let $F\in\mathrm{Ker}\,\xi$. Recall $\xi\circ\Pi_\gamma=\Pi_\gamma^\xi\circ\xi$ which implies $\Pi_\gamma F\in\mathrm{Ker}\,\xi$. Now, according to Remark 2.5 (iv) we have $F=\Sigma_\gamma\Pi_\gamma F$ with respect to the $|\cdot|_{\mathcal{A}}$-norm convergence. This implies

$$F\in\mathrm{clo}_{|\cdot|_{\mathcal{A}}}(\mathrm{Ker}\,\xi\cap\mathcal{F}_{\mathrm{fin}}).$$

Proof of Theorem 4.14: (i) Since $\{\mathcal{F},\mathcal{G}\}$ is minimal and regular, there exists an assignment $\sigma\to\mathcal{H}_\sigma$ such that an admissible (DR-) subcategory $\mathcal{T}_{\mathbb{C}}$ can be defined by

$$(\sigma,\tau)_{\mathcal{A},\mathbb{C}} := (\mathcal{H}_\sigma,\mathcal{H}_\tau),$$

cf. Theorem 2.25. Now we use the morphism ξ to define a corresponding subcategory $\mathcal{T}_{\mathbb{C}}^\xi$ for $\xi(\mathcal{T})$. Recall $\mathrm{Ob}\,\xi(\mathcal{T})=(\mathrm{Ob}\,\mathcal{T})^\xi\subset\mathrm{Ob}\,\mathcal{T}^\xi$. We set

$$\mathrm{Ob}\,\mathcal{T}_{\mathbb{C}}^\xi := \mathrm{Ob}\,\xi(\mathcal{T}).$$

Let $\lambda,\sigma\in\mathrm{Ob}\,\mathcal{T}$. Then λ^ξ, $\sigma^\xi\in\mathrm{Ob}\,\xi(\mathcal{T})$ and the arrows are defined by

$$(\sigma^\xi,\tau^\xi)_{\xi(\mathcal{A}),\mathbb{C}} := \xi((\sigma,\tau)_{\mathcal{A},\mathbb{C}})=(\xi(\mathcal{H}_\sigma),\xi(\mathcal{H}_\tau)).$$

Then

$$(\iota^\xi,\iota^\xi)_{\xi(\mathcal{A}),\mathbb{C}}=\xi((\iota,\iota)_{\mathcal{A},\mathbb{C}})=\xi(\mathbb{C}\,\mathbb{I})=\mathbb{C}\xi(\mathbb{I}).$$

It is straightforward to show that $\mathcal{T}_{\mathbb{C}}^\xi$ has direct sums and subobjects [in the latter case note that if F is a nontrivial projection from $(\sigma^\xi,\sigma^\xi)_{\xi(\mathcal{A}),\mathbb{C}}$ then there is a nontrivial projection $E\in(\sigma,\sigma)_{\mathcal{A},\mathbb{C}}$ such that $F=\xi(E)$ because the ($\mathcal{G}$ -invariant) matrix $\{p_{j,k}\}_{j,k}$ of F with respect to $\{\xi(\Phi_{\sigma,j})\}_j$, where the $\Phi_{\sigma,j}$ form an orthonormal basis of $\mathcal{H}_\sigma$, can be used to define a corresponding E in $(\sigma,\sigma)_{\mathcal{A},\mathbb{C}}$]. Furthermore, the permutation and conjugation structures of $\mathcal{T}_{\mathbb{C}}$ survive the morphism ξ. Thus $\mathcal{T}_{\mathbb{C}}^\xi$ is

a DR-category. We use the notation $\mathcal{T}^{\xi}_{\mathbb{C}}=\xi(\mathcal{T}_{\mathbb{C}})$. [This result means, the Hilbert system $\{\xi(\mathcal{F}),\mathcal{G}\}$ is regular.]

(ii) First let $\xi(\mathcal{A})'\cap\xi(\mathcal{F})=\xi(Z(\mathcal{A}))$. Then, according to Theorem 2.25, property P.2 can be fulfilled by an appropriate subcategory of the form described before. Second, let property P.2 be satisfied. Then $\xi(\mathcal{T}_{\mathbb{C}})$ is an admissible (DR-) subcategory of $\xi(\mathcal{T})$. Therefore, according to Theorem 2.27 there is a corresponding minimal and regular Hilbert extension $\widetilde{\mathcal{F}}$ of $\xi(\mathcal{A})$. The uniqueness part of Theorem 2.27 gives that $\widetilde{\mathcal{F}}$ and $\xi(\mathcal{F})$ are $\mathcal{A}$-module isomorphic, hence $\xi(\mathcal{A})'\cap\xi(\mathcal{F})=Z(\xi(\mathcal{A}))$ is also true.

(iii) The inclusion $\supseteq$ is obvious (see Lemma 4.11). The assertion is

$$(\sigma^{\xi},\tau^{\xi})_{\xi(\mathcal{A})}\subseteq\xi((\sigma,\tau)_{\mathcal{A}}). \tag{9}$$

First we prove this inclusion for the admissible subcategory, i.e., we assert

$$(\sigma^{\xi},\tau^{\xi})_{\xi(\mathcal{A}),\mathbb{C}}\subseteq\xi((\sigma,\tau)_{\mathcal{A}}).$$

This is obvious by

$$(\sigma^{\xi},\tau^{\xi})_{\xi(\mathcal{A}),\mathbb{C}}=\xi((\sigma,\tau)_{\mathbb{C}})\subset\xi((\sigma,\tau)_{\mathcal{A}}).$$

Second, recall that $\xi((\sigma,\tau)_{\mathcal{A}})$ is a right module with respect to $\sigma^{\xi}(\xi(Z(\mathcal{A})))$ and a left module with respect to $\tau^{\xi}(\xi(Z(\mathcal{A})))$. On the other hand, $(\sigma^{\xi},\tau^{\xi})_{\xi(\mathcal{A})}$ is a right module with respect to $\sigma^{\xi}(Z(\xi(\mathcal{A})))$ and a left module with respect to $\tau^{\xi}(Z(\xi(\mathcal{A})))$. Further, according to P.2. $(\sigma^{\xi},\tau^{\xi})_{\xi(\mathcal{A}),\mathbb{C}}$ is a generating subset for this module. Since, by assumption, $Z(\xi(\mathcal{A}))$ and $\xi(Z(\mathcal{A}))$ coincide, the inclusion (9) follows.

(iv) This follows directly from $\xi(\mathcal{A})'\cap\xi(\mathcal{F})=Z(\xi(\mathcal{A}))$ and the fact that the unitary equivalence classes of $\mathcal{T}^{\xi}$ and $\xi(\mathcal{T})$ coincide.

Proof of Theorem 4.15: Since $\mathcal{T}_{\mathbb{C}}$ is an admissible (DR-) subcategory of $\mathcal{T}$ we can apply Theorem 2.27, i.e., there is a corresponding minimal and regular Hilbert extension $\{\mathcal{F},\mathcal{G}\}$ of $\mathcal{A}$. Therefore the arrows of the category $\mathcal{T}_{\mathbb{C}}$ are given by

$$(\sigma,\tau)_{\mathcal{A},\mathbb{C}}=(\mathcal{H}_{\sigma},\mathcal{H}_{\tau}), \tag{10}$$

where the Hilbert spaces $\mathcal{H}_{\sigma}$, $\mathcal{H}_{\tau}$ generate the endomorphisms σ, τ, respectively.

Now it is not hard to show that the morphism ξ can be extended to a morphism of $\mathcal{F}$ by setting

$$\xi(\Phi_{\lambda,j}):=\Phi_{\lambda,j}, \tag{11}$$

where λ runs through a complete system of irreducible and mutually disjoint endomorphisms and $\{\Phi_{\lambda,j}\}$ denotes an orthonormal basis of the Hilbert space $\mathcal{H}_{\lambda}$ which generates λ (recall and use Proposition 4.12). This morphism satisfies the assumptions of Theorem 4.8. The corresponding Hilbert system is denoted by $\{\mathcal{F}^{\xi},\mathcal{G}\}$ (recall that $\mathcal{G}^{\xi}\cong\mathcal{G}$). Equations (10) and (11) imply

$$\sigma^{\xi}(\xi(\mathcal{A}))=\sum_{j}\Phi_{\lambda,j}\xi(A)\Phi^{*}_{\lambda,j}\quad\text{and}\quad\xi((\sigma,\tau)_{\mathcal{A},\mathbb{C}})=(\sigma,\tau)_{\mathcal{A},\mathbb{C}}.$$

By assumption (iii) we have $\xi((\sigma,\tau)_{\mathcal{A}})=(\sigma^{\xi},\tau^{\xi})_{\xi(\mathcal{A})}$. Since $(\sigma,\tau)_{\mathcal{A},\mathbb{C}}\subset(\sigma,\tau)_{\mathcal{A}}$ we have $\xi((\sigma,\tau)_{\mathcal{A},\mathbb{C}})\subset(\sigma^{\xi},\tau^{\xi})_{\xi(\mathcal{A})}$. Therefore the subcategory $\mathcal{T}^{\xi}_{\mathbb{C}}$ of $\xi(\mathcal{T})$ defined by

$$(\sigma^{\xi},\tau^{\xi})_{\xi(\mathcal{A}),\mathbb{C}}:=\xi((\sigma,\tau)_{\mathcal{A},\mathbb{C}}=(\sigma,\tau)_{\mathcal{A},\mathbb{C}}$$

is a DR-category.

Now we prove property P.2 for $\mathcal{T}^{\xi}_{\mathbb{C}}$. We must show

$$\sigma^{\xi}(Z(\xi(\mathcal{A})))(\lambda^{\xi},\sigma^{\xi})_{\xi(\mathcal{A}),\mathbb{C}}\lambda^{\xi}(Z(\xi(\mathcal{A})))=(\lambda^{\xi},\sigma^{\xi})_{\xi(\mathcal{A})}.$$

The left-hand side equals

$$\sigma^{\xi}\xi(Z(\mathcal{A}))(\lambda^{\xi},\sigma^{\xi})_{\xi(\mathcal{A}),\mathbb{C}}\lambda^{\xi}(\xi(Z(\mathcal{A}))) = \xi(\sigma(Z(\mathcal{A})))(\lambda^{\xi},\sigma^{\xi})_{\xi(\mathcal{A}),\mathbb{C}}\xi(\lambda(Z(\mathcal{A})))$$
$$= \xi(\sigma(Z(\mathcal{A})))\xi((\lambda,\sigma)_{\mathcal{A},\mathbb{C}})\xi(\lambda(Z(\mathcal{A})))$$
$$= \xi(\sigma(Z(\mathcal{A}))(\lambda,\sigma)_{\mathcal{A},\mathbb{C}}\lambda(Z(\mathcal{A}))) = \xi((\lambda,\sigma)_{\mathcal{A}})$$

and this coincides, by assumption, with the right-hand side.

Now we can apply Theorem 2.27 to obtain a further Hilbert extension $\{\tilde{\mathcal{F}}^{\xi},\mathcal{G}^{\xi}\}$ where again $\mathcal{G}^{\xi}\cong\mathcal{G}$. Using the uniqueness part of Theorem 2.27 we obtain that both Hilbert extensions are $\xi(\mathcal{A})$-module isomorphic.

Proof of Proposition 5.1: It suffices to show that there is one Dirac state, i.e., a state $\omega \in \mathfrak{S}(\mathcal{A})$ with $\omega(\mathcal{U})=1$. Recall the homomorphism $\zeta:\mathcal{E}\to\mathrm{CAR}(\mathcal{H})\otimes\mathrm{CCR}(S,B)$. Let $\omega_0 \in \mathfrak{S}(\mathrm{CAR}(\mathcal{H}))$ be that quasifree state which is zero on any normal-ordered monomial of $a(f)$ and $a^*(h)$ of degree greater or equal to 1. Then ω_0 is invariant with respect to $\tilde{\gamma}_f$ for all $f \in \mathcal{S}(\mathbb{R}^4)\cup\mathbb{R}$. Moreover, since $L(S)\subset\mathrm{Ker}\,B$, there is a state $\omega_1\in\mathfrak{S}(\mathrm{CCR}(S,B))$ such that $\omega_1(\delta_{Lf})=1$ for all $f\in S$. Then $\omega_2 := \omega_0\otimes\omega_1 \in \mathfrak{S}(\mathrm{CAR}(\mathcal{H})\otimes\mathrm{CCR}(S,B))$ is a $\tilde{\gamma}_f\otimes\iota$-invariant state on $\mathrm{CAR}(\mathcal{H})\otimes\mathrm{CCR}(S,B)$ such that $\omega_2(\mathbb{I}\otimes\delta_{Lf})=1$ for all $f\in S$. From this we define a state on $\mathcal{E}$ by $\tilde{\omega}_2 := \omega_2\circ\zeta$ and since $\zeta\circ\beta_{\gamma_f}=\tilde{\gamma}_f\otimes\iota$, it follows that $\tilde{\omega}_2$ is β_G-invariant on $\mathcal{E}$. Thus $\tilde{\omega}_2$ extends to a state ω_3 on $\mathcal{A}=G\times_{\beta}\mathcal{E}$ by $\omega_3(U_g)=1$ for all $g\in G$, where U_g denotes the unitary implementer for β_g. So $\omega_3\in\mathfrak{S}(\mathcal{A})$ is a Dirac state with respect to the unitaries $U_G\cup\delta_{LS}$. Since the maximal set of constraint unitaries for a Dirac state is a group, it follows that for the products $V_f=\delta_{-Lf}\cdot U_{\gamma_f}$ we have $\omega_3(V_f)=1$ for all f, i.e., ω_3 is a Dirac state with respect to $\mathcal{U}$, hence $\mathcal{U}$ is first class.

Proof of Lemma 5.4: Note that ρ_k on the unitary implementers $\rho_k:U_G\to\mathcal{A}$ is a faithful group homomorphism. This is because it is the pointwise product of the identity map ι with the character $\chi_k:U_G\to\mathbb{C}$ given by $\chi_k(U_{\gamma_{f+t}}) := e^{itk}$, $t\in\mathbb{R}$, $f\in\mathcal{S}(\mathbb{R}^4)$. Furthermore, $\mathcal{A}=C^*(\rho_k(U_G)\cup\mathcal{E})$. Thus the pair $\{\rho_k(U_G),\mathcal{E}\}$ is also a covariant system for the action $\beta:G\to\mathrm{Aut}\,\mathcal{E}$ (cf. Step 3), hence by the universal property of cross products (cf. Ref. 25) there is a *-homomorphism $\theta:\mathcal{A}\to\mathcal{A}$ such that $\theta(A)=A$ for $A\in\mathcal{A}$, and $\theta(U_g)=\rho_k(U_g)\equiv$ implementing unitary of the second system. Then θ coincides with the definition of ρ_k on the generating elements, so it follows that ρ_k extends uniquely to a homomorphism. Since it is clear that ρ_k is bijective (its inverse is ρ_{-k}) it follows that ρ_k is an automorphism of $\mathcal{A}$.

Proof of Proposition 5.6: Proof by contradiction. Let $k\neq 0$ and assume $\rho_k\in\mathrm{Inn}\,\mathcal{A}$, i.e., $\rho_k=\mathrm{Ad}\,V$ for some unitary $V\in\mathcal{A}$. Recall the homomorphism

$$\zeta:\mathcal{E}\to\mathrm{CAR}(\mathcal{H})\otimes\mathrm{CCR}(S,B)$$

encountered in Step 3. Since (S,B) is degenerate, $\zeta(\mathcal{E})$ is not simple which will be inconvenient in the proof below. Choose therefore a maximal ideal $\mathcal{I}$ of $\mathrm{CCR}(S,B)$ [necessarily associated with a character of the center $Z(\mathrm{CCR}(S,B))$], and let

$$\eta:\mathrm{CAR}(\mathcal{H})\otimes\mathrm{CCR}(S,B)\to\mathrm{CAR}(\mathcal{H})\otimes\mathrm{CCR}(S,B)/\mathcal{I}$$

be the factorization by the ideal $\mathbb{I}\otimes\mathcal{I}$. Then the composition

$$\xi := \eta\circ\zeta:\mathcal{E}\to\mathrm{CAR}(\mathcal{H})\otimes\mathrm{CCR}(S,B)/\mathcal{I}$$

is a homomorphism of which the image is a simple algebra.

Now the action $\beta:G\to\mathrm{Aut}\,\mathcal{E}$ (Step 4) only affects $\mathrm{CAR}(\mathcal{H})$ in $\mathcal{E}$, so preserves the ideal generated by the commutators $[\mathrm{CAR}(\mathcal{H}),\mathrm{CCR}(S,B)]$ in $\mathcal{E}$ as well as the ideal $\mathbb{I}\otimes\mathcal{I}$. Thus each β_g can be taken through the homomorphism ξ to define an action $\beta^{\xi}:G\to\mathrm{Aut}(\mathrm{CAR}(\mathcal{H})\otimes\mathrm{CCR}(S,B)/\mathcal{I})$ and it is just $\beta^{\xi}_{\gamma_f}=\tilde{\gamma}_f\otimes\iota$. Thus we can extend ξ from $\mathcal{E}$ to $\mathcal{A}=G\overset{\times}{_{\beta}}\mathcal{E}$ to get a surjective homomorphism

$$\xi:\mathcal{A}\to \underset{\beta^{\xi}}{G\times}(\mathrm{CAR}(\mathcal{H})\otimes \mathrm{CCR}(S,B)/\mathcal{I}).$$

Now $\rho_k\in \mathrm{Aut}\,\mathcal{A}$ only affects U_G, leaving $\mathcal{E}$ invariant, hence it preserves $\mathrm{Ker}\,\xi\subset\mathcal{A}$. Thus ρ_k can be factored through ξ to obtain the automorphisms $\rho_k^{\xi}\in \mathrm{Aut}\,\xi(\mathcal{A})$ by

$$\rho_k^{\xi}(\xi(A)) := \xi(\rho_k(A)) \quad \forall\, A\in\mathcal{A}, \quad \text{and so } \rho_k^{\xi}=\mathrm{Ad}\,\xi(V). \tag{12}$$

Recall now that each element of the discrete crossed product $\xi(\mathcal{A})=G\underset{\beta^{\xi}}{\times}\xi(\mathcal{E})$ [with $\xi(\mathcal{E})=\mathrm{CAR}(\mathcal{H})\otimes\mathrm{CCR}(S,R)/\mathcal{I}$] can be written as a C*-norm convergent series $\Sigma_{n=1}^{\infty}B_nU_{g_n}$ where $B_n\in\xi(\mathcal{E})$ and $g_n\in G$ (with g_n distinct for different n) and that the unitaries U_G form a left $\xi(\mathcal{E})$-module basis. In particular, for the implementing unitaries $\xi(V)$ of ρ_k^{ξ} we have a series $\xi(V)=\Sigma_{n=1}^{\infty}B_nU_{g_n}$, $B_n\in\xi(\mathcal{E})\backslash 0$. Since $\rho_k\restriction\mathcal{E}=\iota$, it follows from Eq. (12) that $\xi(V)A=A\xi(V)$ for all $A\in\xi(\mathcal{E})$, i.e.,

$$A\xi(V)=\sum_{n=1}^{\infty}AB_nU_{g_n}=\xi(V)A=\sum_{n=1}^{\infty}B_nU_{g_n}A=\sum_{n=1}^{\infty}B_n\beta_{g_n}^{\xi}(A)U_{g_n}$$

for all $A\in\xi(\mathcal{E})$. So by the basis property of U_G we have

$$AB_n=B_n\beta_{g_n}^{\xi}(A) \quad \forall\, A\in\xi(\mathcal{E})=\mathrm{CAR}(\mathcal{H})\otimes\mathrm{CCR}(S,B)/\mathcal{I}. \tag{13}$$

Since $\beta_{g_n}^{\xi}\restriction\mathrm{CCR}(S,B)/\mathcal{I}=\iota$, this implies that $B_n\in(\mathrm{CCR}(S,B)/\mathcal{I})'$. From the fact that $\mathrm{CCR}(S,B)/\mathcal{I}$ is simple (hence has trivial center) this means that $B_n\in\mathrm{CAR}(\mathcal{H})\otimes\mathbb{1}$, and hence Eq. (13) claims that B_n is a nonzero intertwiner between ι and $\beta_{g_n}^{\xi}$ in $\mathrm{CAR}(\mathcal{H})$. We next prove that B_n is invertible, in which case $\beta_{g_n}^{\xi}$ becomes inner on $\mathrm{CAR}(\mathcal{H})$.

Let $\pi:\mathrm{CAR}(\mathcal{H})\to\mathcal{B}(\mathcal{L})$ be any faithful irreducible representation of $\mathrm{CAR}(\mathcal{H})$ on a Hilbert space $\mathcal{L}$, e.g., the Fock representation, and let $\psi\in\mathrm{Ker}\,\pi(B_n)$. Then by (13),

$$\pi(B_nA)\psi=\pi(\beta_{g_n^{-1}}(A))\pi(B_n)\psi=0 \quad \forall\, A\in\mathrm{CAR}(\mathcal{H}).$$

Thus $\pi(\mathrm{CAR}(\mathcal{H}))\psi\subseteq\mathrm{Ker}\,\pi(B_n)$. However, in an irreducible representation every nonzero vector is cyclic, so either $\psi=0$ or $\pi(B_n)=0$, and the latter case is excluded by $B_n\neq 0$, π faithful. Thus $\psi=0$, i.e., we have shown that $\mathrm{Ker}\,\pi(B_n)=\{0\}$. Moreover by Eq. (13) we have

$$\pi(A)\pi(B_n)\varphi=\pi(B_n)\pi(\beta_{g_n}(A))\varphi \quad \forall\,\varphi\in\mathcal{L}\backslash 0, \quad A\in\mathrm{CAR}(\mathcal{H}),$$

hence $\pi(\mathrm{CAR}(\mathcal{H}))(\pi(B_n)\varphi)\subseteq\mathrm{Ran}\,\pi(B_n)$ for all $\varphi\in\mathcal{L}\backslash 0$. Now $\pi(B_n)\varphi\neq 0$ [by $\mathrm{Ker}\,\pi(B_n)=\{0\}$] and so by Dixmier 2.8.4 (Ref. 26) we have that $\pi(\mathrm{CAR}(\mathcal{H}))(\pi(B_n)\varphi)=\mathcal{L}$ (no closure is necessary). Thus $\mathrm{Ran}\,\pi(B_n)=\mathcal{L}$, i.e., $\pi(B_n)$ is invertible, and so since π is faithful (hence preserves the spectrum of an element) it follows that B_n is also invertible in $\mathrm{CAR}(\mathcal{H})$.

Using the fact that B_n is invertible, Eq. (13) becomes $\beta_{g_n}(A)=B_n^{-1}AB_n$ for all $A\in\mathrm{CAR}(\mathcal{H})$. Since β_{g_n} is a *-homomorphism, this implies that $B_n^{-1}A^*B_n=B_n^*A^*(B_n^{-1})^*$, i.e., $B_nB_n^*A^*=A^*B_nB_n^*$ for all $A\in\mathrm{CAR}(\mathcal{H})$, and since $\mathrm{CAR}(\mathcal{H})$ has trivial center, this means $B_nB_n^*\in\mathbb{C}\,\mathbb{1}$. Set $B_nB_n^*=:t_n$ (necessarily $t_n>0$) then $U_n:=B_n/\sqrt{t_n}$ satisfies $U_nU_n^*=\mathbb{1}$. By substituting A by $\beta_{g_n^{-1}}(A)$ in (13) we also obtain $B_n^*B_n\in\mathbb{C}\,\mathbb{1}$ by the above argument, then using $t_n=\|B_nB_n^*\|=\|B_n\|^2=\|B_n^*B_n\|=B_n^*B_n$ we get also $U_n^*U_n=\mathbb{1}$. Thus

$$\beta_{g_n}(A)=B_n^{-1}AB_n=\left(\frac{B_n}{\sqrt{t_n}}\right)^{-1}A\left(\frac{B_n}{\sqrt{t_n}}\right)=U_n^*AU_n$$

for $A\in\mathrm{CAR}(\mathcal{H})$, i.e., β_{g_n} is inner on $\mathrm{CAR}(\mathcal{H})$. Recall however, that on $\mathrm{CAR}(\mathcal{H})$, β_{g_n} is just an automorphism $\tilde{\gamma}_{f_n}$ for some $f_n\in\mathcal{S}(\mathbb{R}^4)+\mathbb{R}$, coming from a Bogoliubov transformation, $\tilde{\gamma}_{f_n}(\Phi(k)):=\Phi(T_{f_n}k)$ (cf. Step 4). So for β_{g_n} to be inner on $\mathrm{CAR}(\mathcal{H})$, this means that either of

$I \pm T_{f_n}$ must be trace-class (cf. Theorem 4.1, p. 48 of Ref. 24 or Theorem 4.1.4 in Ref. 27). However,

$$T_{f_n}(h_1 \oplus h_2) := e^{-if_n} h_1 \oplus e^{if_n} h_2 \quad \forall\, h_i \in \mathcal{H} = L^2(\mathbb{R}^4).$$

Now for any f_n such that $T_{f_n} \neq I$, it is clear that the multiplication operators on $L^2(\mathbb{R}^4)$ by $(I \pm e^{\pm if_n})$ cannot be trace-class. This contradicts our finding that β_{g_n} is inner if $g_n \neq e$, hence only $g_n = e$ is possible in the series $\xi(V) = \Sigma_{n=1}^{\infty} B_n U_{g_n}$, i.e., $\xi(V) = B \cdot U_e$, $B \in \xi(\mathcal{E}) \backslash 0$. But in this case, Eq. (13) becomes $AB = BA$ for all $A \in \xi(\mathcal{E})$ and so since $\xi(\mathcal{E})$ is simple, $B \in \mathbb{C}\,\mathbb{I}$. This however implies that $\iota = \mathrm{Ad}\ \xi(V) = \rho_k^{\xi}$ which cannot be because $\rho_k(U_{\gamma_t}) = e^{ikt} U_{\gamma_t}$ factors unchanged through ξ. From this contradiction, it follows that our initial assumption $\rho_k \in \mathrm{Inn}\ \mathcal{A}$ is false.

VII. CONCLUSIONS

In this paper, we studied the question of under what conditions, and how much of the superselection structures will survive the constraining procedure. We did this in the context of DR theory (extended to the case of nontrivial center of the observable algebra), and the method of the T-procedure for enforcing constraints.

Since the T-procedure involves a restriction and a factoring, this meant that we had to analyze for Hilbert systems their behavior first, with respect to restriction, and then with respect to general morphisms (this seems to be of independent interest). Finally, in Sec. IV E we combined these to obtain conditions for a Hilbert system to pass through a constraining. We also obtained conditions for the preservation of the regularity property, and partial conditions for the preservation of the minimality property as well as Property B.

In Sec. V we developed an example based on the Maxwell constraint of interacting QED. In this setting the superselection structure came explicitly from the usual global electromagnetic charge, and we could verify the basic compatibility conditions on the endomorphisms, but not the additional conditions of regularity, minimality and Property B.

Our results suggest the following further directions: to solve the compatibility problem of minimality and Property B with respect to constraining; to obtain a physically convincing example with a non-Abelian global gauge group where supersymmetry passes through the constraining.

There is also another possible line of analysis; since the initial constraint system contains nonphysical information, the supersymmetry structures need not be precisely defined as in the DR theory, indeed one can ask for a "weak" supersymmetry structure, with the only requirement on it, that after constraining it produces the usual DR structures on the physical algebra. (This line of thought is parallel to the development of "weak" Haag-Kastler axioms in Ref. 5.) This will enlarge the set of examples of systems with both supersymmetry and constraints.

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Operator product expansions as a consequence of phase space properties

Henning Bostelmann[a)]
Institut für Theoretische Physik, Universität Göttingen, 37077 Göttingen, Germany

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The paper presents a model-independent, nonperturbative proof of operator product expansions in quantum field theory. As an input, a recently proposed phase space condition is used that allows a precise description of point field structures. Based on the product expansions, we also define and analyze normal products (in the sense of Zimmermann). © *2005 American Institute of Physics.* [DOI: 10.1063/1.2007567]

I. INTRODUCTION

Quantum fields, representing observables sharply localized in space–time, generally are quite singular objects.[1] In particular, their products at coinciding space–time points are ill-defined and lead to divergences. Since such products play a vital role in the definition and classification of models (by means of path integrals or field equations), a thorough understanding and precise description of their singularities is of considerable interest.

A step toward this goal was taken by Wilson,[2] who proposed that a product of two fields $\phi(x)$ and $\phi'(y)$ should be expandable into a series,

$$\phi(x)\cdot\phi'(y)=\sum_j c_j(x-y)\phi_j\left(\frac{x+y}{2}\right), \tag{1.1}$$

where $\phi_j(\cdot)$ are local fields as well, and $c_j(\cdot)$ are (generalized) functions which show singularities at the origin. This operator product expansion should then be valid at short distances, i.e., in the limit $x\to y$.

The operator product expansion provides a detailed description of the product's singular behavior. It may furthermore serve to define "normal products" of fields, in generalization of the Wick product. Any field ϕ_j in Eq. (1.1) whose coefficient $c_j(\cdot)$ does not vanish in the limit may be taken as a candidate for such a normal product.[3]

However, it remains to clear up in which sense and under which conditions Eq. (1.1) holds precisely. The expansion has originally been proposed in perturbation theory[2,3] and has widely been used as a tool in Lagrangian field theory.[4] Investigations in the framework of axiomatic field theory[5] aimed at a rigorous proof; it seems that the Wightman axioms are too weak to ensure existence of the expansion structure, and that additional conditions are needed. Unfortunately, these conditions could not be connected directly to physical properties of the theory. More detailed results are available in conformal field theory,[6] especially in $1+1$-dimensional models.[7] Here the expansion is a consequence of conformal symmetry. These methods cannot be carried over to physically more realistic situations, though.

This paper presents an approach that explains operator product expansions in a model-independent way, based on physically motivated assumptions. We make use of the theory's phase space behavior, which has recently been shown to have a strong impact on the field content.[8,9] A phase space condition proposed in Ref. 9 can be taken as a physically natural assumption to ensure

[a)]Electronic mail: bostelm@theorie.physik.uni-goettingen.de

a regular short distance behavior. On these grounds, we will establish operator product expansions rigorously in the sense of an asymptotic series. Furthermore, we will define normal products of fields and investigate their properties.

In Sec. II, we recall the relevant facts and results on the point field structure established in Ref. 9, which lie at the root of our investigation. Section III defines products of pointlike fields and gives a proof of their product expansion. Normal products and their properties are discussed in Sec. IV. We end with a brief outlook on the classification of models in Sec. V.

The present work is based on the author's thesis;[10] it presents an abbreviated and partially improved version of material developed there. The reader is referred to the original text for a more detailed exposition, especially regarding mathematical aspects and the development of proofs.

II. POINTLIKE FIELDS AND PHASE SPACE PROPERTIES

It has been outlined in Refs. 8 and 11 that a strong connection exists between the phase space properties of a quantum field theory and its point field structure. A natural phase space condition, similar but not identical to the usual compactness or nuclearity conditions,[12] was proposed in Ref. 9 and shown to allow a precise description of the theory's field content. We will give a brief review of the results established in Ref. 9, mainly to fix our notation.

We start from a quantum field theory in the framework of local quantum physics[13] in the vacuum sector, i.e., given by a net of observable algebras $\mathcal{O}\mapsto\mathfrak{A}(\mathcal{O})$, where $\mathcal{O}\subset\mathcal{M}:=\mathbb{R}^{s+1}$ are open bounded regions in Minkowski space of $s+1$ space–time dimensions, and $\mathfrak{A}(\mathcal{O})$ are W^*-algebras acting on some common Hilbert space $\mathcal{H}$. We assume the standard axioms: isotony, locality, covariance with respect to some strongly continuous unitary representation $U(x,\Lambda)$ of the connected Poincaré group $\mathfrak{P}_+^\uparrow$, and the spectrum condition (positivity of energy). We will denote the elements of the translation subgroup of $\mathfrak{P}_+^\uparrow$ as $U(x)=\exp(iP_\mu x^\mu)$, where $H:=P_0$ is the Hamiltonian; its spectral projections will be written as $P_H(E)$. Σ stands for the predual space of $\mathfrak{B}(\mathcal{H})$, i.e. the space of weak-$*$-continuous linear functionals on $\mathfrak{B}(\mathcal{H})$, the positive normed elements of which represent the physical states of the system.

As we restrict our attention to point fields fulfilling polynomial H-bounds (cf. Ref. 1), we consider the space

$$\mathcal{C}^\infty(\Sigma):=\bigcap_{\ell>0} R^\ell\Sigma R^\ell, \quad \text{where } R=(1+H)^{-1}, \tag{2.1}$$

equipped with the topology of simultaneous convergence in the norms $\|\sigma\|^{(\ell)}:=\|R^{-\ell}\sigma R^{-\ell}\|$, $\ell>0$. We also make use of its dual space $\mathcal{C}^\infty(\Sigma)^*$, equipped with the weak topology; its elements are linear forms ϕ which fulfill

$$\|\phi\|^{(\ell)}:=\|R^\ell\phi R^\ell\|<\infty \quad \text{for some } \ell>0. \tag{2.2}$$

For linear maps $\alpha:\mathcal{C}^\infty(\Sigma)^*\to\mathcal{C}^\infty(\Sigma)^*$, we sometimes consider

$$\|\alpha\|^{(\ell,\ell')}:=\|R^{\ell'}\alpha(R^{-\ell}\cdot R^{-\ell})R^{\ell'}\| \quad (\ell,\ell'>0) \tag{2.3}$$

in case this expression is finite.

Let Ψ be the space of linear continuous maps from $\mathcal{C}^\infty(\Sigma)$ to Σ, where Σ is equipped with the norm topology. For our setup, the inclusion map $\Xi\in\Psi$ plays a central role,

$$\Xi:\mathcal{C}^\infty(\Sigma)\to\Sigma, \quad \sigma\mapsto\sigma. \tag{2.4}$$

In order to analyze this map in the short distance limit, we refer to the algebras $\mathfrak{A}(r):=\mathfrak{A}(\mathcal{O}_r)$, where $\mathcal{O}_r$ is the standard double cone of radius $r>0$ centered at the origin, then define for $\psi\in\Psi$,

$$\|\psi\|_r^{(\ell)}:=\|\psi\lceil\mathfrak{A}(r)\|^{(\ell)}=\sup_{\sigma\in\Sigma}\sup_{A\in\mathfrak{A}(r)}\frac{|\psi(R^\ell\sigma R^\ell)(A)|}{\|\sigma\|\,\|A\|}, \tag{2.5}$$

which is finite for sufficiently large $\ell>0$, and for $\gamma\geqslant 0$ consider the pseudometrics,

$$\delta_\gamma(\psi) := \begin{cases} 0 & \text{if } r^{-\gamma}\|\psi\|_r^{(\ell)} \underset{r\to 0}{\to} 0 \quad \text{for some } \ell > 0, \\ 1 & \text{otherwise.} \end{cases} \tag{2.6}$$

We say that the net $\mathfrak{A}$ fulfills the *microscopic phase space condition* if for every $\gamma \geqslant 0$, there exists a map $\psi \in \Psi$ of finite rank such that

$$\delta_\gamma(\Xi - \psi) = 0. \tag{2.7}$$

It is not overly difficult to see that this condition holds for a wide range of free theories (see the Appendix of Ref. 9), and it seems plausible that the same condition is fulfilled in any model with a sufficiently regular short distance behavior. Its consequences are the following: There exists an increasing sequence of finite-dimensional vector spaces $\Phi_\gamma \subset \mathcal{C}^\infty(\Sigma)^*$, $\gamma \geqslant 0$, the elements of which are Wightman fields located at $x=0$. Their union $\cup_\gamma \Phi_\gamma =: \Phi_{\mathrm{FH}}$ exhausts the field content of the theory as investigated by Fredenhagen and Hertel.[1] Given $\phi \in \Phi_{\mathrm{FH}}$, we can find a sequence $A_r \in \mathfrak{A}(r)$ $(r>0)$ such that

$$\|\phi - A_r\|^{(\ell)} = O(r), \quad \|A_r\| = O(r^{-k}) \tag{2.8}$$

as $r \to 0$, where $k, \ell > 0$ can be chosen uniformly for all $\phi \in \Phi_\gamma$, with γ being fixed. If $p_\gamma : C^\infty(\Sigma)^* \to C^\infty(\Sigma)^*$ is any continuous projection onto Φ_γ, and $p_{\gamma *}$ its predual, then we find

$$\delta_\gamma(\Xi - \Xi \circ p_{\gamma *}) = 0. \tag{2.9}$$

[Note that a continuous projection can be found for any given finite-dimensional subspace $V \subset \mathcal{C}^\infty(\Sigma)^*$. We will require all such projections considered in the following to be continuous and refrain from noting this fact repeatedly.]

Every Φ_γ is invariant under a certain class of symmetry transformations, including Lorentz transformations, dilations and inner symmetries, provided that they exist as symmetries of the underlying net $\mathfrak{A}$. Linear differential operators act as maps $\Phi_{\mathrm{FH}} \to \Phi_{\mathrm{FH}}$ as well, but typically map Φ_γ into some larger space $\Phi_{\gamma'}$.

III. PRODUCT EXPANSIONS

Our task will now be to establish operator product expansions, assuming that the theory under discussion fulfills the microscopic phase space condition. We will prove the expansion in the form

$$\phi(x) \cdot \phi'(y) = \sum_j c_j(x,y)\phi_j(0) \quad (x,y \to 0), \tag{3.1}$$

which can easily be transformed into the more familiar form (1.1) and vice versa.

The proof is based on the following heuristic idea: Let $A, A' \in \mathfrak{A}(r)$ be two bounded localized observables, and $A(x) := U(x)AU(x)^*$, etc. Choosing a projector p_γ onto Φ_γ, the phase space property (2.9) can roughly be expressed as $\Xi \approx \Xi \circ p_{\gamma *}$ at small distances. This means

$$A(x)A'(y) \approx p_\gamma(A(x)A'(y)) \tag{3.2}$$

if x, y, and r are small enough. Expanding $p_\gamma = \Sigma_j \sigma_j(\cdot)\phi_j$ in a finite basis, this reads

$$A(x)A'(y) \approx \sum_j \sigma_j(A(x)A'(y))\phi_j \tag{3.3}$$

in the limit $x,y,r \to 0$. If now $A \approx \phi$ and $A' \approx \phi'$ in this limit, we can define $c_j(x,y) := \sigma_j(A(x)A'(y))$ and arrive at the expansion (3.1).

In order to transfer this heuristic idea into a rigorous expression for the product of pointlike fields, we will first define the product of two fields [the left-hand side of Eq. (3.1)] for spacelike-separated x and y, namely by means of approximating them with bounded observables; this is

done in Sec. III A. On these grounds, we will then establish the product expansion in Sec. III B. Some generalizations, such as products of more than two factors and products for non-spacelike-separated arguments, will be discussed in Sec. III C.

A. Spacelike products

In the following, let $\phi, \phi' \in \Phi_{\mathrm{FH}}$ be fixed. As a first step towards the expansion (3.1), we will give meaning to the *a priori* ill-defined product $\phi(x)\cdot\phi'(y)$. This is certainly possible in a distributive sense (as a product of smeared Wightman fields); however, we shall use a more direct approach here. For $(x-y)^2<0$, we will define $\phi(x)\cdot\phi'(y)$ as an element of $\mathcal{C}^\infty(\Sigma)^*$, i.e., as a sesquilinear form.

This will be achieved by an approximation with bounded operators. We choose sequences $A_r \to \phi$, $A'_r \to \phi'$ as specified in Eq. (2.8). Then it seems natural to define

$$\phi(x)\cdot\phi'(y) := \lim_{r\to 0} A_r(x)A'_r(y), \quad (x-y)^2<0. \tag{3.4}$$

We will use methods from complex analysis to establish the existence of this limit and to control the convergence dependent on x and y.

To this end, let $\sigma=(\xi|\cdot|\xi')$ be an energy-bounded functional, i.e., $\xi^{(\prime)}\in P_H(E)\mathcal{H}$ for some $E>0$. We assume $\|\sigma\|=1$. Leaving x fixed for the moment, we consider the function

$$f_r(z) = \sigma(U(x)A_rU(z)A'_rU(-x-z)), \quad z\in\mathcal{M}. \tag{3.5}$$

f is the boundary value of a function analytic on $\mathcal{M}+i\mathcal{V}_+$, where $\mathcal{V}_+$ denotes the open forward light cone. This is seen from

$$f_r(z) = \sigma(U(x)A_r\exp(iP_\mu z^\mu)A'_rU(x)^*\exp(-iP_\mu z^\mu)), \tag{3.6}$$

using the spectrum condition and the strong continuity of translations. [Note that the factor $\exp(-iP_\mu z^\mu)$ does not disturb analyticity here, since σ is energy bounded.] We can estimate the modulus of f_r on $\mathcal{M}+i\mathcal{V}_+$ as

$$|f_r(z)| \leqslant \|P_H(E)R^{-\ell}\|\,\|R^\ell A_r R^\ell\|\,\|R^{-\ell}\exp(iP_\mu z^\mu)R^{-\ell}\|\,\|R^\ell A'_r R^\ell\|\,\|R^{-\ell}P_H(E)\|\,\|P_H(E)\exp(-iP_\mu z^\mu)\|. \tag{3.7}$$

Here $\|R^\ell A_r^{[\prime]} R^\ell\|$ stays bounded in the limit $r\to 0$ if ℓ is sufficiently large. A straightforward calculation shows that

$$\|R^{-2\ell}\exp(iP_\mu z^\mu)\| \leqslant \|\mathrm{Im}\, z\|^{-2\ell}\cdot c_1, \quad \|P_H(E)\exp(-iP_\mu z^\mu)\| \leqslant e^{c_2 E\|\mathrm{Im}\, z\|} \quad \text{for } \|\mathrm{Im}\, z\|\leqslant 1, \tag{3.8}$$

where $c_1, c_2>0$ can be chosen constant if $\mathrm{Im}\, z$ varies over some open convex cone $\mathcal{C}$ with $\bar{\mathcal{C}}\subset\mathcal{V}_+$, which we keep fixed in the following. (All c_i will be positive constants in what follows.) Thus we have

$$|f_r(z)| \leqslant (1+E)^{2\ell}e^{c_2E\|\mathrm{Im}\, z\|}\|\mathrm{Im}\, z\|^{-2\ell}\cdot c_3 \quad \text{for } r\leqslant 1, \quad \mathrm{Im}\, z\in\mathcal{C}, \quad \|\mathrm{Im}\, z\|\leqslant 1. \tag{3.9}$$

By these and similar arguments, it follows in particular that $\{f_r\}_{r\leqslant 1}$ is a normal family of analytic functions on $\mathcal{M}+i\mathcal{V}_+$, i.e., uniformly bounded on compact subsets.

In just the same way, we may represent

$$\hat{f}_r(z) = \sigma(U(x+z)A'_rU(-z)A_rU(-x)) \tag{3.10}$$

as a boundary value of functions analytic on $\mathcal{M}-i\mathcal{V}_+$; similar bounds as in Eq. (3.9) can be established. If we choose z real and spacelike, the operators A_r and $A'_r(z)$ will commute for small r, hence we find

$$f_r(z) = \hat{f}_r(z) \quad \text{for } z \text{ real}, \quad z^2 < 0, \quad \text{and small } r. \tag{3.11}$$

This allows us to apply the edge of the wedge theorem to f_r and $\hat{f}_r$: They are parts of a single function f_r analytic on $\mathcal{M} \pm i\mathcal{V}_+$ and on some complex neighborhood of those real points where (3.11) holds.

Let us investigate this common analytic continuation more closely. We choose some fixed $v \in \mathcal{M}$, $u \in \mathcal{C}$ with $v^2 < 0$, $\|u\| = 1$. For r small enough, the function

$$f_{r,v,u}(t) = \begin{cases} f_r(v + tu) & \text{if } \operatorname{Im} t \geqslant 0, \\ \hat{f}_r(v + tu) & \text{if } \operatorname{Im} t < 0 \end{cases} \tag{3.12}$$

is analytic on $\mathbb{C}\backslash\mathbb{R}$ and continuous on some real neighborhood of $t=0$, which is, e.g., given by

$$|t| < \tfrac{1}{2} d(v), \quad \text{where } d(v) := \min\{1, \operatorname{dist}(v, \partial\mathcal{V}_+ \cup -\partial\mathcal{V}_+)\}, \tag{3.13}$$

assuming $r < \frac{1}{4} d(v)$. Applying Painlevé's theorem,[14] we see that $f_{r,v,u}$ is indeed analytic on $\mathbb{C}\backslash\{t \,|\, \operatorname{Im} t = 0, |t| \geqslant \frac{1}{2} d(v)\}$. From Eq. (3.9), we can derive the estimate

$$|f_{r,v,u}(t)| \leqslant c_4 (1+E)^{2\ell} e^{c_2 E |\operatorname{Im} t|} |\operatorname{Im} t|^{-2\ell} \quad \text{if } |t| < \tfrac{1}{2} d(v), \quad r \leqslant 1. \tag{3.14}$$

A Phragmén-Lindelöf-type of argument (cf. Lemma 5.7 of Ref. 10) then leads us to

$$|f_{r,v,u}(t)| \leqslant c_5 (1+E)^{2\ell} e^{\lambda c_2 E} \lambda^{-2\ell} \quad \text{for } r < \tfrac{1}{4} d(v), \quad |t| < \lambda, \quad \text{and any } \lambda \leqslant \tfrac{1}{4} d(v), \tag{3.15}$$

where c_5 depends neither on v nor on u. Choosing t to be purely imaginary, this means

$$|f_r(v + iu)| \leqslant c_5 (1+E)^{2\ell} e^{\lambda c_2 E} \lambda^{-2\ell} \quad \text{for } v^2 < 0, \quad u \in \mathcal{C}, \quad \|u\| < \lambda, \quad \lambda \leqslant \tfrac{1}{4} d(v), \quad r < \tfrac{1}{4} d(v). \tag{3.16}$$

The same estimate holds at the real points ($u=0$), setting $t=0$ in Eq. (3.15).

As mentioned above, f_r possesses an analytic continuation to a complex neighborhood of any real spacelike z, provided that r is sufficiently small for z. This continuation is known very explicitly (see the proof of the edge of the wedge theorem in Ref. 14 for details); in fact, the domain of holomorphy depends only on the geometry of $\mathcal{C}$, and the estimate (3.16) can be carried over to the continued function, showing that $\{f_r\}_{r \leqslant 1}$ is a normal family throughout its domain.

We are now in the position to control the limit $r \to 0$. Since $\|R^{-2\ell} \exp(iP_\mu z^\mu)\| < \infty$ for $\operatorname{Im} z \in \mathcal{V}_+$, the expression

$$f(z) := \sigma(U(x) \phi U(z) \phi' U(-x-z)) \tag{3.17}$$

is well-defined for $z \in M + i\mathcal{V}_+$. Using the approximation properties (2.8) of A_r and A_r', and applying the same methods that lead to Eq. (3.14), we can establish the estimate

$$\begin{gathered} |f(z) - f_r(z)| \leqslant c_6 (1+E)^{2\ell} e^{c_2 E |\operatorname{Im} t|} |\operatorname{Im} t|^{-2\ell} \cdot r \\ \text{for } z = v + itu, \quad v \in \mathcal{M}, \quad u \in \mathcal{C}, \quad \|u\| = 1, |t| < \tfrac{1}{2} d(v), \quad r \leqslant 1. \end{gathered} \tag{3.18}$$

Combined with similar estimates for $\|\operatorname{Im} z\| > 1$, we see in particular that $f_r(z) \to f(z)$ for $z \in \mathcal{M} + i\mathcal{V}_+$. In analogy to (3.10), we may define $f(z)$ on $\mathcal{M} - i\mathcal{V}_+$; pointwise convergence $f_r \to f$ and estimates of the form (3.18) hold there, too. Now, since $\{f_r\}_{r \leqslant 1}$ is a normal family, we know that f_r converges to some analytic limit throughout its domain, where the convergence is uniform on compact subsets; so f has an analytic continuation to that region, and $f_r \to f$ holds in particular at the real points. Thus the limit

$$\sigma(\phi(x)\cdot\phi'(y)) := \lim_{r\to 0} f_r(y-x) \tag{3.19}$$

is well-defined and—cf. Eq. (3.17)—independent of the choice of sequences A_r, A'_r. This definition obviously is linear in σ; so $\phi(x)\cdot\phi'(y)$ is a well-defined linear form on $P_H(E)\Sigma P_H(E)$ for any E. In view of Eq. (3.16), the following estimate holds:

$$\|P_H(E)\phi(x)\cdot\phi'(y)P_H(E)\| \leqslant c_5(1+E)^{2\ell}e^{\lambda c_2 E}\lambda^{-2\ell} \quad \text{for } (x-y)^2<0, \quad \lambda \leqslant \tfrac{1}{4}d(x-y). \tag{3.20}$$

Applying this result with $\lambda=(c_2E)^{-1}$ for $(c_2E)^{-1}<\frac{1}{4}d(x-y)$, and with $\lambda=\frac{1}{4}d(x-y)$ otherwise, we obtain a $c_7>0$ such that

$$\|P_H(E)\phi(x)\cdot\phi'(y)P_H(E)\| \leqslant c_7(1+E)^{4\ell}d(x-y)^{-2\ell} \quad \text{for any } E>0. \tag{3.21}$$

Using the spectral representation of R, one can show on these grounds that $\phi(x)\cdot\phi'(y)\in\mathcal{C}^\infty(\Sigma)^*$, and

$$\|\phi(x)\cdot\phi'(y)\|^{(4\ell+1)} \leqslant c_8 d(x-y)^{-2\ell}. \tag{3.22}$$

The same methods can be applied to quantify the convergence $A_r(x)A'_r(y)\to\phi(x)\cdot\phi'(y)$. Starting from Eq. (3.18) and using the arguments that lead to Eqs. (3.16) and (3.21), we arrive at the estimate

$$\|\phi(x)\cdot\phi'(y)-A_r(x)A'_r(y)\|^{(4\ell+1)} \leqslant c_9 d(x-y)^{-2\ell}r \quad \text{for } r<\tfrac{1}{4}d(x-y). \tag{3.23}$$

To summarize, we have established the following result:

Theorem 3.1: *For $\phi,\phi'\in\Phi_{\mathrm{FH}}$, there exist linear forms*

$$\phi(x)\cdot\phi'(y)\in\mathcal{C}^\infty(\Sigma)^* \quad \text{for } x,y\in\mathcal{M}, \quad (x-y)^2<0,$$

with the following properties: Given γ, we can choose constants $\ell,m>0$, and for any fixed ϕ, $\phi'\in\Phi_\gamma$ another constant $c>0$ such that

$$\|\phi(x)\cdot\phi'(y)\|^{(m)} \leqslant c d(x-y)^{-2\ell}.$$

If A_r, $A'_r\in\mathfrak{A}(r)$ are sequences of operators with $\|\phi^{[r]}-A_r^{[r]}\|^{(\ell)}=O(r)$, then

$$\|\phi(x)\cdot\phi'(y)-A_r(x)A'_r(y)\|^{(m)} \leqslant O(r)d(x-y)^{-2\ell},$$

where the estimate $O(r)$ is uniform in x,y, given that $r<\frac{1}{4}d(x-y)$.

Note that the spacelike product usually diverges as $x\to y$, say, on a straight line, but that the singularity is bounded by an inverse power of $d(x-y)$.

B. Proof of the expansion

Based on the detailed results established for the spacelike product $\phi(x)\cdot\phi'(y)$, we are now going to prove the operator product expansion for this case, making use of the phase space approximation

$$\delta_\gamma(\Xi-\Xi\circ p_{\gamma*})=0. \tag{3.24}$$

We follow the heuristic motivation given at the beginning of this section. To be precise, let $\gamma\geqslant 0$ be given, and let $\phi,\phi'\in\Phi_\gamma$. As before, we choose approximating sequences A_r, $A'_r\in\mathfrak{A}(r)$ with

$$\|\phi^{[r]}-A_r^{[r]}\|^{(\ell)}=O(r), \quad \|A_r^{[r]}\|=O(r^{-k}), \tag{3.25}$$

where $k,\ell>0$ are suitably chosen; note that we can choose them dependent on γ only.

First of all, we will approximate the bounded product $A_r(x)A_r'(y)$. Let $\gamma'>0$ (its value will be specified later), and fix a projector $p_{\gamma'}$ onto $\Phi_{\gamma'}$. Since $A_r(x)A_r'(y)\in\mathfrak{A}(r+2\|x\|+2\|y\|)$, it follows from Eqs. (3.24) and (3.25) that for some $m>0$ (dependent on γ),

$$\|p_{\gamma'}(A_r(x)A_r'(y))-A_r(x)A_r'(y)\|^{(m)}\leqslant(r+2\|x\|+2\|y\|)^{\gamma'}O(r^{-2k}). \tag{3.26}$$

Since $\Phi_{\gamma'}$ is finite dimensional, we can find $m'\geqslant m$ such that $\|p_{\gamma'}\|^{(m,m')}<\infty$; in fact, this choice depends on γ' only. Now on the left-hand side of Eq. (3.26), $A_r(x)A_r'(y)$ converges to $\phi(x)\cdot\phi'(y)$ in the limit $r\to 0$: In view of Theorem 3.1, one sees that

$$\|p_{\gamma'}(\phi(x)\cdot\phi'(y))-\phi(x)\cdot\phi'(y)\|^{(m')}\leqslant(r+2\|x\|+2\|y\|)^{\gamma'}O(r^{-2k})+d(x-y)^{-2\ell}O(r), \tag{3.27}$$

given that $r<\frac{1}{4}d(x-y)$.

We will now consider the limit $x,\ y\to 0$, where we assume that

$$d(x-y)\geqslant(\|x\|+\|y\|)\cdot\text{const}, \tag{3.28}$$

i.e., we demand that $x-y$ does not approach the light cone too fast. We will refer to this approximation as the *spacelike limit* and denote it by $\to^{\text{sp}}$. Now given some $\beta>0$, we set

$$r(x,y):=(\|x\|+\|y\|)^{1+\beta+2\ell}, \tag{3.29}$$

which fulfills $r<\frac{1}{4}d(x-y)$ for small x,y due to Eq. (3.28). If now γ' was chosen sufficiently large (dependent on β), we see that (3.27) vanishes faster than $(\|x\|+\|y\|)^{\beta}$ in the spacelike limit. Thus, we have achieved the following.

Theorem 3.2: *Let $\gamma>0$, $\beta>0$ be given. We can find constants $\gamma'>0$ and $\ell>0$ such that for any ϕ, $\phi'\in\Phi_\gamma$ and any projection $p_{\gamma'}$ onto $\Phi_{\gamma'}$:*

$$(\|x\|+\|y\|)^{-\beta}\|\phi(x)\cdot\phi'(y)-p_{\gamma'}(\phi(x)\cdot\phi'(y))\|^{(\ell)}\overset{\text{sp}}{\to}0.$$

This establishes the operator product expansion—as explained at the beginning of this section, we may expand $p_{\gamma'}$ in a basis in order to pass to the more explicit form (3.1). In mathematical terms, product expansions are asymptotic series; while with increasing β we will usually have to increase γ', to any finite approximation order β a finite "number of approximation terms" will suffice. Note that the approximation terms are not unique (since $p_{\gamma'}$ is not); however, the ambiguities are restricted to terms that vanish rapidly in the limit, so at least the singular structure of an operator product expansion can be understood as an intrinsic property of the theory. It is also worth noting that the approximation is not only valid in the weak sense, as originally proposed in Ref. 2, but holds uniformly for all states of sufficiently regular high energy behavior.

Furthermore, the coefficients of the product expansion are simply matrix elements of the spacelike product $\phi(x)\cdot\phi'(y)$; thus, we can apply Theorem 3.1 directly, which shows that their divergences at $x=y=0$ are bounded by an inverse power of $d(x-y)$.

C. Further directions

The results established in Secs. III A and III B can be generalized in many ways. For the sake of brevity, we will just sketch these findings; the reader is referred to Chap. 5 of Ref. 10 for details of the construction.

First, we may consider products of arbitrary many factors; though we restricted ourselves to the case of two factors in the above, our methods carry over quite directly. In the following, let $n\in\mathbb{N}$ and $\gamma\geqslant 0$ be given. It seems natural not only to consider n-fold products, but also their linear combinations; by the same methods as outlined in Sec. III A, we may define spacelike products

$$\Pi(x) = \sum_k c_k \phi_k^{(1)}(x^{(1)}) \cdot \cdots \cdot \phi_k^{(n)}(x^{(n)}) \in \mathcal{C}^\infty(\Sigma)^*, \quad \text{where } c_k \in \mathbb{C}, \quad \phi_k^{(j)} \in \Phi_\gamma. \tag{3.30}$$

This expression is multilinear in the fields $\phi_k^{(j)}$ [note that the products $\phi(x)\cdot\phi'(y)$ were bilinear in ϕ,ϕ' by definition], so we can formally obtain the products from a map $\Pi \mapsto \Pi(x)$ which is well-defined on the tensor product space $\Phi_\gamma^{\otimes n}$. In Eq. (3.30), we must demand that the components of $x=(x^{(1)},\ldots,x^{(n)}) \in \mathcal{M}^n$ are (pairwise) spacelike separated. More abstractly, let

$$\mathcal{M}^n_{\mathrm{sp}} := \{x \in \mathcal{M}^n | (x^{(i)} - x^{(j)})^2 < 0 \ \forall\ 1 \leqslant i < j \leqslant n\}, \tag{3.31}$$

and define

$$d(x) := \min\{1, \mathrm{dist}(x, \partial\mathcal{M}^n_{\mathrm{sp}})\}; \tag{3.32}$$

we then demand of the spacelike limit $x \to^{\mathrm{sp}} 0$ that

$$x \in \mathcal{M}^n_{\mathrm{sp}}, \quad \|x\| \leqslant d(x) \cdot \mathrm{const}, \quad x \to 0, \tag{3.33}$$

where $\|x\|$ stands for the Euclidean norm of x in $\mathcal{M}^n = \mathbb{R}^{n(s+1)}$. Following the line of arguments given in Sec. III A, the divergence of the spacelike products can be estimated as

$$\|\Pi(x)\|^{(n\cdot m)} = O(d(x)^{-n\cdot\ell}) \quad (x \overset{\mathrm{sp}}{\to} 0), \tag{3.34}$$

where m,ℓ depend on γ only. Finally, we may obtain the following analog of Theorem 3.2.

Theorem 3.3: *Let $\gamma>0$, $\beta>0$, $n\in\mathbb{N}$ be given. We can find constants $\gamma'>0$ and $\ell>0$ such that for any $\Pi\in\Phi_\gamma^{\otimes n}$ and any projection $p_{\gamma'}$ onto $\Phi_{\gamma'}$,*

$$\|x\|^{-\beta} \|\Pi(x) - p_{\gamma'}\Pi(x)\|^{(\ell)} \overset{\mathrm{sp}}{\to} 0.$$

Hence product expansions exist for products of an arbitrary (finite) number of fields.

Moreover, similar expansions can be established for arbitrary (not necessarily spacelike) distances of arguments. Here the field products are defined in the sense of distributions only, i.e., we replace $\Pi(x)$ with $\Pi(f)\in\mathcal{C}^\infty(\Sigma)^*$, where $f\in\mathcal{S}(\mathcal{M}^n)$ is a test function with compact support. Theorem 3.3 holds in an analogous way, where $\|x\|$ is substituted with

$$d(f) := \sup\{\|x\| \mid x \in \mathrm{supp}\, f\}; \tag{3.35}$$

instead of the spacelike limit, we consider the limit $d(f)\to 0$, and we must require that for every multi-index μ, a constant c_μ exists such that

$$\|\partial^\mu f\|_{L_1} \leqslant d(f)^{-|\mu|} c_\mu \quad \text{as } d(f) \to 0. \tag{3.36}$$

So the product expansions can be extended to the non-space-like region, where their coefficients are no longer functions, but rather tempered distributions.

Furthermore, one may investigate the action of symmetry transformations on the products and their expansions, demanding that these transformations are compatible with translations and with the product structure on $\mathfrak{B}(\mathcal{H})$ (in a suitably defined way—see Chap. 5.4 of Ref. 10; these conditions are, e.g., fulfilled for Lorentz transforms, dilations and inner symmetries). The results are compatible with what is expected from perturbation theory.[15]

IV. ZIMMERMANN'S NORMAL PRODUCTS

In the preceding section, we have defined and analyzed products of fields at different (spacelike separated) space–time points, and investigated their divergences at small distances. However, with possible applications in mind, one would like to develop some substitute for the ill-defined product at coinciding points in the sense of a local field (i.e., an element of Φ_{FH}). In free field

theory, such a substitute is given by means of the Wick product, e.g., the normal ordered square $:\phi^2:(x)$ of a real scalar field. According to Wick's theorem,[16] it can be constructed from spacelike products by subtraction of divergent terms,

$$:\phi^2:(0) = \lim_{x,y\to 0} (\phi(x)\cdot\phi(y) - (\Omega|\phi(x)\cdot\phi(y)|\Omega)\mathbb{1}). \tag{4.1}$$

In interacting theories, one would not expect such a limit to exist; nevertheless, similar "subtraction methods" combined with a suitable "renormalization factor" can be used at least in a perturbative context to justify the existence of local field equations.[17,18] Zimmermann[3] used operator product expansions to derive these constructions more generally: For any field ϕ_k occuring in the expansion (1.1), one obtains heuristically

$$\phi_k(0) = \lim_{x,y\to 0} \frac{1}{c_k(x-y)}\left(\phi(x)\cdot\phi'(y) - \sum_{j\neq k} c_j(x-y)\,\phi_j\left(\frac{x+y}{2}\right)\right), \tag{4.2}$$

provided that the coefficient c_k does not vanish in the limit. So every "composite field operator" ϕ_k that appears in the expansion can serve as a candidate for a normal product.

Let us see how this can be formalized in our context. We fix a product $\Pi\in\Phi_{\mathrm{FH}}^{\otimes n}$ and try to collect all "relevant" terms in its product expansion. To this end, we make the following definition: We say that a finite-dimensional subspace $V\subset\mathcal{C}^\infty(\Sigma)^*$ is spacelike approximating for Π if for some projection p_V onto V and some $\ell>0$,

$$\|\Pi(x) - p_V\Pi(x)\|^{(\ell)} \overset{\mathrm{sp}}{\to} 0. \tag{4.3}$$

It can easily be seen, using the triangle inequality, that then the same is true for any projection p_V onto V. In view of Theorem 3.3, Φ_γ always is spacelike approximating (sp-app) for Π if γ is chosen sufficiently large. Moreover, a short calculation shows that if V and W are two spaces which are sp-app for Π, then the same holds for $V\cap W$; this is easily extended to the intersection $\cap_{i\in I}V_i$ of an arbitrary family $\{V_i\}_{i\in I}$ of sp-app spaces, even if I is infinite. (Note that all spaces in question are finite dimensional.) That justifies the following definition.

Definition 4.1: *Let* $\Pi\in\Phi_{\mathrm{FH}}^{\otimes n}$. *The finite-dimensional space*

$$N[\Pi] := \bigcap_{V\text{sp-app for }\Pi} V \subset \Phi_{\mathrm{FH}}$$

is called the normal product space *of* Π. *It is the smallest space that is spacelike approximating for* Π.

Let p be a projection onto $N[\Pi]$, and choose a basis $\{\phi_j\}_{j=1}^J$ of $N[\Pi]$. Since $N[\Pi]\subset\Phi_{\mathrm{FH}}$, the basis elements ϕ_j are local Wightman fields. Expanding p in this basis, we find functions $c_j(x)$ such that

$$p\Pi(x) = \sum_{j=1}^{J} c_j(x)\,\phi_j. \tag{4.4}$$

Due to the minimality of $N[\Pi]$, none of the coefficients $c_j(x)$ vanishes in the spacelike limit. Thus for every $k\in\{1,\ldots,J\}$, we can find a sequence (x_n) with $x_n\to^{\mathrm{sp}} 0$ such that

$$\phi_k = \lim_{n\to\infty} \frac{1}{c_k(x_n)}\left(\Pi(x_n) - \sum_{j\neq k} c_j(x_n)\,\phi_j\right) \tag{4.5}$$

with respect to some norm $\|\cdot\|^{(\ell)}$; we have recovered Zimmermann's approximation formula.

$N[\Pi]$ is a normal product not in the sense of a single field, but as a vector space containing all possible candidates for such a normal product field. In the case of a real scalar free field $\phi(x)$, one obtains the result (cf. Chap. 5.7 of Ref. 10)

$$N[\phi \otimes \phi] = \mathrm{span}\{\mathbb{1}, :\phi^2:\}, \tag{4.6}$$

so the normal product space gives us some generalization of the Wick product. In free field theory, it is possible to choose a distinct element $:\phi^2: \in N[\phi \otimes \phi]$ by virtue of "normal ordering" or of Eq. (4.1). This structure is lost in the general case, as is suggested by perturbation theory and low-dimensional integrable models. Certainly, for specific applications, there may be additional restrictions on the choice of a normal product field. One can try to isolate a "most divergent term" in the product expansion, seek for specific representations of the Lorentz group[19] (see also below), or use field equations as selection criteria.[18] Still, some ambiguities may remain;[20] in our general setting, it does not seem possible to establish a full substitute for the Wick product.

We can slightly modify the methods developed above in order to define "extended" normal product spaces $N[\Pi]_\beta$ for $\beta \geqslant 0$, requiring that the left-hand side of Eq. (4.3) vanishes faster than $\|x\|^\beta$ in the limit. That provides us with an increasing sequence of vector spaces $N[\Pi]_0 \subset N[\Pi]_1 \subset \cdots$ containing higher and higher order composite field operators of some fixed product Π. This construction has recently found application in a characterization of nonequilibrum thermodynamical states.[21]

We shall now investigate the behavior of $N[\Pi]$ under Lorentz transformations or other symmetries and under differential operators. All these cases will be treated within a single concept. We consider a transformation α which acts in three different ways (denoted by the same symbol for simplicity),

(i) a linear, continuous map $\alpha: \mathcal{C}^\infty(\Sigma)^* \to \mathcal{C}^\infty(\Sigma)^*$,
(ii) linear maps $\alpha: \Phi_{\mathrm{FH}}^{\otimes n} \to \Phi_{\mathrm{FH}}^{\otimes n}$ (for every n),
(iii) an invertible action $x \mapsto \alpha.x$ on $\mathcal{M}^n$ (for every n)

with the following properties:

(1) $\alpha(\Pi(x)) = (\alpha\Pi)(\alpha.x)\ \forall \Pi \in \Phi_{\mathrm{FH}}^{\otimes n}, \quad n \in \mathbb{N}, \quad x \in \mathcal{M}^n$,
(2) $\alpha.x \to^{\mathrm{sp}} 0 \Leftrightarrow x \to^{\mathrm{sp}} 0$,
(3) $\|\alpha\|^{(\ell,\ell')} < \infty$ for any $\ell > 0$ and appropriate $\ell' > 0$ (dependent on ℓ).

We shall show that under these conditions, one has $\alpha N[\Pi] = N[\alpha\Pi]$; applications of this "covariance property" will be discussed below. As a first step, we shall prove the following lemma:

Lemma 4.2: *Let $V \subset \mathcal{C}^\infty(\Sigma)^*$ be a finite-dimensional subspace. There exist projections p onto V and p' onto αV such that*

$$\alpha \circ p = p' \circ \alpha.$$

Proof: Let $K := \ker \alpha \cap V$. Choose a space $\hat{V}$ such that $V = K \oplus \hat{V}$. Furthermore, choose projections p_K onto K such that $p_K \restriction \hat{V} = 0$, and p' onto $\alpha V = \alpha\hat{V}$. (This is certainly possible, since V is finite dimensional.) Denote the inverse of $\alpha: \hat{V} \to \alpha V$ by $\hat{\alpha}^{-1}$. We define

$$p := p_K + \hat{\alpha}^{-1} \circ p' \circ \alpha. \tag{4.7}$$

A short calculation shows $p^2 = p$, $\mathrm{img}\, p = V$, $\alpha \circ p = p' \circ \alpha$, so p has the properties desired. ■

Now we are in the position to prove the "covariance" of $N[\Pi]$.

Theorem 4.3: *Let α fulfill the conditions (1) to (3) listed above. Then*

$$N[\alpha\Pi] = \alpha N[\Pi] \quad \forall\, \Pi \in \Phi_{\mathrm{FH}}^{\otimes n}, \quad n \in \mathbb{N}.$$

Proof: Let $V \subset \mathcal{C}^\infty(\Sigma)^*$ be sp-app for Π, and p, p' projections as in Lemma 4.2. Then for sufficiently large ℓ, ℓ', we have

$$\|(\alpha\Pi)(\alpha\,.\,x)-p'(\alpha\Pi)(\alpha\,.\,x)\|^{(\ell)}=\|\alpha(\Pi(x)-p\Pi(x))\|^{(\ell)}\leqslant\|\alpha\|^{(\ell,\ell')}\|\Pi(x)-p\Pi(x)\|^{(\ell')}\overset{\text{sp}}{\to}0; \tag{4.8}$$

due to property (2), this means that αV is sp-app for $\alpha\Pi$. Hence $N[\alpha\Pi]\subset\alpha N[\Pi]$.

To show the opposite inclusion, split $V:=N[\Pi]$ into a direct sum

$$N[\Pi]=V=V_0\oplus V_1\oplus V_2, \tag{4.9}$$

where

$$V_0=\ker\alpha\cap V,\quad \alpha V_1=N[\alpha\Pi],\quad \alpha V_2\cap N[\alpha\Pi]=\{0\}.$$

Let $p_i: V\to V_i$ $(i=0,1,2)$ denote the projection operators with respect to that direct sum, and let $p_i': \alpha V\to\alpha V_i$ $(i=1,2)$ be the projections with regard to the direct sum $\alpha V=\alpha V_1\oplus\alpha V_2$. We then have $p_i'\alpha=\alpha p_i$ for $i=1,2$. We choose projections p,p' as in Lemma 4.2; then $p_i\circ p:\mathcal{C}^\infty(\Sigma)\to V_i$ are projections onto V_i, and $p_i'\circ p':\mathcal{C}^\infty(\Sigma)\to\alpha V_i$ are projections onto αV_i. Now, since both αV and $\alpha V_1=N[\alpha\Pi]$ are sp-app for $\alpha\Pi$, we see that for sufficiently large ℓ,

$$\|(\alpha\Pi)(x)-(p_1'+p_2')p'(\alpha\Pi)(x)\|^{(\ell)}\overset{\text{sp}}{\to}0\quad\text{and}\quad\|(\alpha\Pi)(x)-p_1'p'(\alpha\Pi)(x)\|^{(\ell)}\overset{\text{sp}}{\to}0, \tag{4.10}$$

which means that

$$\|p_2'p'(\alpha\Pi)(x)\|^{(\ell)}\overset{\text{sp}}{\to}0. \tag{4.11}$$

Using the relation $p_2'p'\alpha=\alpha p_2p$ together with properties (1) and (2), and noting that α is invertible on αV_2, it follows that

$$\|p_2p\Pi(x)\|^{(\ell)}\overset{\text{sp}}{\to}0\ \Rightarrow\ \|\Pi(x)-(p_0+p_1)p\Pi(x)\|^{(\ell)}\overset{\text{sp}}{\to}0; \tag{4.12}$$

thus $V_0\oplus V_1$ is sp-app for Π. Due to the minimality of $N[\Pi]$, this is only possible if $V_2=\{0\}$; hence $\alpha N[\Pi]=\alpha V_1=N[\alpha\Pi]$. ■

The properties (1)–(3) requested for α are fulfilled by a number of relevant transformations.

Lorentz transformations: A Lorentz transformation $\alpha=\alpha(\Lambda)$ acts on $\mathcal{C}^\infty(\Sigma)^*$ "as usual" [i.e. through ad $U(\Lambda)$], on $\Phi_{\text{FH}}^{\otimes n}$ in the same way on every tensor factor, and on $\mathcal{M}$ by $\alpha\,.\,x=\Lambda x$, which is extended to $\mathcal{M}^n$ componentwise. The properties (2) and (3) are obvious. Applying ad $U(\Lambda)$ to the approximating sequences in Eq. (3.4), it is also easy to see that $\alpha(\Pi(x))=(\alpha\Pi)(\alpha\,.\,x)$. So Theorem 4.3 tells us that $N[\alpha(\Lambda)\Pi]=\alpha(\Lambda)N[\Pi]$; the normal product spaces are Lorentz covariant *as vector spaces*. Note that $N[\Pi]$ is not necessarily stable under $\alpha(\Lambda)$, since possibly $\Pi\neq\alpha(\Lambda)\Pi$; we would have to pass to a closure $\hat{N}[\Pi]=\text{span}\cup_\Lambda N[\alpha(\Lambda)\Pi]$ if we aim at a decomposition of $\Lambda\mapsto\alpha(\Lambda)$ into irreducible subrepresentations.

Other symmetries with "geometric action," such as dilations $[\alpha(\lambda)\,.\,x=\lambda x]$ and inner symmetries $(\alpha\,.\,x=x)$, show the same behavior as Lorentz transformations, as long as they are unitary implemented and fulfill certain regularity properties (cf. Lemma 5.5 of Ref. 10). Since for our construction, it suffices to use a local unitary implementation rather than a global one, it does not matter whether the symmetries are broken or unbroken.[22]

Derivatives: To treat linear differential operators in our context, it suffices to consider first order operators D_μ, which act on $\mathcal{C}^\infty(\Sigma)^*$ through $i[P_\mu,\cdot]$. Since they leave Φ_{FH} invariant,[9] they also act on $\Phi_{\text{FH}}^{\otimes n}$ by a formal product rule. As D_μ satisfies the product rule on $\mathfrak{B}(\mathcal{H})$, one may establish

$$D_\mu(\Pi(x))=(D_\mu\Pi)(x). \tag{4.13}$$

[To see this, note that the approximating sequences "$A_r\to\phi$" can be chosen to be "smeared" with some test function f_r—compare the remark after the proof of Lemma 3.5 in Ref. 9—such that

$D_\mu A_r = D_\mu(\hat{A}_r(f_r)) = \hat{A}_r(-\partial_\mu f_r)$, so D_μ preserves the localization of the operator sequence.] Again, property (3) is obvious, so the differential operators D_μ fulfill properties (1)–(3), with D_μ acting trivially on $\mathcal{M}^n$. By concatenation and linear combination, the same is then true for linear differential operators D of arbitrary order. Hence we have

$$N[D\Pi] = DN[\Pi]. \tag{4.14}$$

The perturbative analog to this relation is known as *Lowenstein's rule*.[23]

V. CONCLUSIONS AND OUTLOOK

In the course of the present paper, we have given a rigorous model-independent proof of operator product expansions, based on a physically motivated assumption that was formulated as a phase space condition. In this context, product expansions are asymptotic series in the short distance limit; their singular behavior is bounded by an inverse power. We have introduced normal products in the sense of vector spaces that consist of all fields contributing to the product expansion (up to a given level of accuracy). These vector spaces show the expected properties, such as Lorentz covariance and Lowenstein's rule.

Originally, Wilson[2] proposed operator product expansions as a substitute for the Lagrangian, as a method of defining field theoretic models. Though it would seem exaggerated to aim at constructive approaches from our results, they might indeed serve as a basis for the classification of models. For example, they could give a well-defined sense to the concept of local field equations: The famous ϕ^4 equation

$$(\Box + m^2)\phi = \lambda{:}\phi^3{:}, \quad \lambda \neq 0, \tag{5.1}$$

well known in perturbation theory,[18] can be introduced in our context as

$$(\Box + m^2)\phi \in N[\phi^{\otimes 3}] \setminus \mathbb{C}\phi. \tag{5.2}$$

At present, it is unknown whether such a relation is stringent enough to define a field theory (nor, in fact, whether it is compatible with any field theory at all). There is strong evidence[24] that in physical space–time, the standard lattice approximation approach does not lead to a theory that fulfills Eq. (5.2); however, other methods have been proposed that might result in such a solution.[25] Equation (5.2) at least allows us to pose the existence problem of ϕ_4^4 independent of specific construction schemes.

More generally, it seems interesting to what extent field equations—or other properties of product expansions—can define a field theory uniquely. One encounters some obvious obstructions here, since there exist nontrivial theories with a trivial field content[26] $\Phi_{\mathrm{FH}} = \mathbb{C}\mathbb{1}$, which might always occur as a tensor factor. We can exclude these components, however, by defining the following subnet $\mathfrak{A}_F$ of $\mathfrak{A}$ which may be regarded as the "point field part" of the theory (as remarked in Ref. 9):

$$\mathfrak{A}_F(\mathcal{O}) := \mathcal{P}(\mathcal{O})'', \tag{5.3}$$

where $\mathcal{P}(\mathcal{O})$ is the polynomial algebra generated by all $\phi(f)$ with $\phi \in \Phi_{\mathrm{FH}}$, $\operatorname{supp} f \subset \mathcal{O}$.

In models which are generated by observable point fields (such as the free-field examples in Ref. 9), we have $\mathfrak{A} = \mathfrak{A}_F$, and one would hope to find a description of $\mathfrak{A}$ in terms of field equations or similar relations. In the presence of gauge fields, on the other hand, it might happen that $\mathfrak{A}_F \subsetneq \mathfrak{A}$, since $\mathfrak{A}$ may include inherently non-point-like observables like Wilson loops or Mandelstam strings. In this case, it is possible that the dynamics of the system cannot be described in terms of Φ_{FH} alone, but that field equations need to involve the extended objects mentioned. Still, it would be worthwhile to ask what physical properties (such as cross sections) are determined by $\mathfrak{A}_F$ only. However, the details of such an analysis remain vague at the present stage.

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[26] M. Lutz, Diplomarbeit (diploma thesis), Universität Hamburg, 1997. Compare also the appendix of Ref. 9.

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Stability of Landau-Ginzburg branes

Johannes Walcher
School of Natural Sciences, Institute for Advanced Study, Princeton, New Jersey 08540

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We evaluate the ideas of Π-stability at the Landau-Ginzburg (LG) point in moduli space of compact Calabi-Yau manifolds, using matrix factorizations to *B*-model the topological *D*-brane category. The standard requirement of unitarity at the IR fixed point is argued to lead to a notion of "*R*-stability" for matrix factorizations of quasihomogeneous LG potentials. The *D*0-brane on the quintic at the Landau-Ginzburg point is not obviously unstable. Aiming to relate *R*-stability to a moduli space problem, we then study the action of the gauge group of similarity transformations on matrix factorizations. We define a naive moment maplike flow on the gauge orbits and use it to study boundary flows in several examples. Gauge transformations of nonzero degree play an interesting role for brane-antibrane annihilation. We also give a careful exposition of the grading of the Landau-Ginzburg category of *B*-branes, and prove an index theorem for matrix factorizations. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2007590]

I. INTRODUCTION

The main purpose of this work is to develop a stability condition, to be called "*R*-stability," on the triangulated category of matrix factorizations describing *D*-branes at the Landau-Ginzburg point p_{LG} in the Kähler moduli space $\mathcal{M}_k$ of a compact Calabi-Yau manifold *X*. The proposal is motivated by physical considerations similar to the ones leading to the notion of Π-stability on the derived category of coherent sheaves $\mathbf{D}(X)$, which describes the variation of the spectrum of *B*-type BPS branes over $\mathcal{M}_k$. In fact, the notion of *R*-stability can be thought of as the specialization of Π-stability to p_{LG}. It is expected, however, that *R*-stability should be intrinsic to the Landau-Ginzburg model and does in principle not depend on knowledge of the stable spectrum elsewhere in $\mathcal{M}_k$.

In this paper, Sec. II is a brief review of the relevant aspects of Π-stability that we want to abstract to the Landau-Ginzburg model. Section III contains the basic definitions related to matrix factorizations. Section IV explains how quasihomogeneous matrix factorizations can be, first $\mathbb{Q}$-, then $\mathbb{Z}$-graded. Section V is a somewhat independent unit concerned with the (RR) Ramond-Ramond charges of matrix factorizations in string theory and an index theorem. Section VI gives a preliminary definition of *R*-stability and partial answers to the difficulties in relating it to the action of the gauge group on matrix factorizations. This general discussion is then applied in Sec. VII and the proposal shown to work well in several relevant examples. Section VIII gives a summary.

II. REVIEW OF Π-STABILITY

Π-stability was introduced in Refs. 1 and 2, and further sharpened and tested in Refs. 3 and 4. It was subsequently abstracted into a precise mathematical definition of stability condition on triangulated categories in Ref. 5. We refer to these works for the categorical aspects of Π-stability, as well as to Aspinwall's review[6] for more extensive background material. Instead, we begin with a slightly personal review of the worldsheet origin of Π-stability, following Douglas.[2]

The basic physical intuition is quite simple. Consider a fixed two-dimensional conformally invariant string worldsheet quantum field theory $\mathcal{C}$ defining a closed string background. By definition, a *D*-brane in this background is a conformally invariant boundary condition, $\mathcal{B}$, for $\mathcal{C}$. A

popular way to define $\mathcal{C}$'s and $\mathcal{B}$'s is as IR fixed points of bulk or boundary RG flows, induced by turning on a relevant operator $\mathcal{O}$ in a known bulk or boundary theory. Such a UV description is "stable" if it flows to a theory in the infrared which is "acceptable" in the sense of, e.g., having the right central charge, being unitary, etc. Finding necessary and/or sufficient stability conditions on $\mathcal{O}$ is in general a very hard question.

A situation in which more can be said is when one requires bulk and boundary theories to preserve $\mathcal{N}=2$ supersymmetry with a nonanomalous U (1) R-symmetry, so that the chiral algebra underlying $\mathcal{C}$ and $\mathcal{B}$ will contain the $\mathcal{N}=2$ superconformal algebra. A necessary condition on acceptable $\mathcal{B}$'s is that the R-charges of all open string NS chiral primary operators satisfy the unitarity constraint[7]

$$0 \leqslant q \leqslant \hat{c}, \tag{2.1}$$

where $\hat{c}$ is the central charge of the superconformal algebra. Often, $\hat{c}$ and q can be determined in the UV and the Eq. (2.1) therefore provides a stability condition in the above sense.

The ideas of Π-stability in fact go further than (2.1). Assume that $\hat{c}$ and the R-charges of $\mathcal{C}$ are all integral. The chiral algebra of $\mathcal{C}$ then contains, in addition to the $\mathcal{N}=2$ superconformal algebra, the (square of the) spectral flow operator $\mathcal{S}$. One can then contemplate imposing a boundary condition of the form

$$\mathcal{S}_L = e^{i\pi\varphi}\mathcal{S}_R, \tag{2.2}$$

involving an arbitrary phase, φ. Standard conformal field theory arguments [using the doubling trick, one transports $\mathcal{S}^2$ around an open string vertex operator inserted at the boundary of the worldsheet, and notes that the total monodromy of $\mathcal{S}^2$, which evaluates to the difference of phases, measures the U (1) charge of the operator up to an integer] then show that the R-charges of an open string spanning between two branes $\mathcal{B}$ and $\mathcal{B}'$ (with phase φ and φ') satisfy

$$q = \varphi' - \varphi \bmod \mathbb{Z}. \tag{2.3}$$

If we bosonize the left- and right-moving U (1) currents in terms of two canonically normalized chiral bosons ϕ_L and ϕ_R, the spectral flow operators are $\mathcal{S}_{L,R}=e^{i(\sqrt{\hat{c}}/2)\phi_{L,R}}$, and we can visualize the boundary condition (2.2) as Dirichlet or Neumann boundary condition on the compact boson $\phi = \phi_L \pm \phi_R$ with radius $\sqrt{\hat{c}}$. [The sign depending on which side (A or B) of the mirror one chooses to present the conformal field theory.] Of course, the equation $e^{i(\sqrt{\hat{c}}/2)\phi_L}=e^{i\pi\varphi}e^{i(\sqrt{\hat{c}}/2)\phi_R}$ leaves a $\hat{c}$-fold ambiguity on the position/Wilson line of the boundary condition on ϕ. In such a picture,[2] the strings stretching between the different images correspond to the different values of q in (2.3).

We emphasize that, in conformal field theory, φ is defined as a real number modulo even integers. We should also like to stress that φ is, in general, independent of the phases appearing in the boundary condition on the $\mathcal{N}=2$ currents, as in, $G_L^{\pm}=e^{\pm i\alpha}G_R^{\pm}$, $G_L^{\pm}=e^{\pm i\beta}G_R^{\mp}$ for A- and B-type, respectively. (See, e.g., Ref. 8 for a BCFT discussion of this.) φ determines which $\mathcal{N}=1$ space–time supersymmetry is preserved by the brane, and can be different for different branes. On the other hand, the phases appearing in the boundary condition on the $\mathcal{N}=2$ currents determine which $\mathcal{N}=1$ worldsheet supersymmetry is preserved. This is a gauge symmetry and must be the same for all branes.

Now recall that an $\mathcal{N}=2$ field theory (conformal or not) with a conserved U (1) R-current can be twisted to a topological theory. As anticipated in Ref. 9, and by now well appreciated in the physics literature, the set of branes in the topological theory together with open strings between them carries the algebraic structure of a "triangulated category" (plus more). Two important pieces of structure are, first, the so-called "distinguished triangles," such as

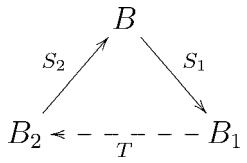

(2.4)

which expresses the fact that the topological brane B can be obtained as a topological bound state of the two branes B_1 and B_2 by condensing the "topological tachyon" T on the base of the triangle. Second, a triangulated category has a so-called shift functor, which in physics terms sends a brane B to a copy of its antibrane $\bar{B}$.[1]

In relating the physical to the topological theory, one chooses a lift of the phase φ to a real number called "grade" and identifies the ghost number n of open strings as the integer appearing in (2.3), i.e.,

$$n = q + \varphi - \varphi' . \tag{2.5}$$

Consequently, for every physical brane $\mathcal{B}$ there are in fact an infinite number of topological branes $B[m]$ whose grade differs by an integers. Shifting the grade shifts the ghost number by integers, and hence modifies the topological theory. On the other hand, the topological theory is unaware of the unitarity constraint (2.1). In particular, the topological theory is independent of changes of q and φ. This decoupling of the topological theory from the variation of q with (part of) the moduli is one of the central ideas underlying Π-stability.

Π-stability, then, is designed to decide when the bound state formation described in the topological theory by triangles such as (2.4) is stable in the physical theory, and thereby provides a picture of the spectrum of BPS branes in some given closed string background. Let us, for concreteness, focus on the case of B-type D-branes on a Calabi-Yau manifold X. In that case, the topological branes are objects of the derived category of coherent sheaves, $\mathbf{D}(X)$, of the algebraic variety underlying X. $\mathbf{D}(X)$ depends only on the complex structure of X, and is independent of the Kähler moduli. Within this category of topological branes, the set of stable branes, conjectured to flow to BPS branes in the physical theory, varies over the stringy Kähler moduli space $\mathcal{M}_k$ of X. Essentially, one follows the continuous variation of the phases φ, and hence of U (1) R-charges of open strings, over $\mathcal{M}_k$. Charges leaving and/or entering the unitarity bound (2.1) signal loss and/or gain of stable branes, with decay and bound state formation described by the triangles (2.4).

For the details of this construction, consistency with monodromies in $\mathcal{M}_k$, and a lot of examples, see Ref. 6 One peculiar aspect of the story is that Π-stability really only describes the changes of the BPS spectrum as one moves around in $\mathcal{M}_k$. To determine the spectrum at any given point p of $\mathcal{M}(X)$, one must know the spectrum at some distinguished point p_0 and then follow it to p using Π-stability.

One natural choice for basepoint is large volume, p_{LV}, in the compactification of $\mathcal{M}_k$. At p_{LV}, Π-stability reduces to μ-stability for the Abelian category of coherent sheaves on X.[1] Although μ-stability does not extend over an open neighborhood of p_{LV} (and hence does not allow determining the complete BPS spectrum there), it is at present the only useful handle on the spectrum elsewhere in $\mathcal{M}_k$.

Another special point, which one expects exists when X is a noncompact Calabi-Yau manifold, is the so-called "orbifold point" p_{O} in $\mathcal{M}$. Even if X is not the resolution of an actual orbifold singularity, one may define p_{O} as a point in $\mathcal{M}_k$ at which the phases of all branes are aligned. In such a situation, determining the BPS spectrum is a problem of solving F- and D-flatness conditions in a supersymmetric quiver gauge theory, as argued in Ref. 1. More rigorously, Aspinwall shows in Ref. 10 that in an open neighborhood of such an orbifold point, Π-stability reduces to θ-stability for the Abelian category of quiver representations in the sense of King.[11]

Such a point at which all phases align is expected not to exist in the moduli space of a generic compact Calabi-Yau model. The closest one can get seems to be the Landau-Ginzburg point, which resembles ordinary orbifolds in the appearance of a discrete quantum symmetry, but with the important difference that not all phases of branes are aligned. The purpose of the present paper,

pursuing a suggestion made in Refs. 12 and 13, is to investigate the ideas underlying Π-stability at the Landau-Ginzburg orbifold point in the Kähler moduli space of compact Calabi-Yau manifolds, using the recently introduced description of the topological category using matrix factorizations. We now turn to explaining various (old and new) aspects of matrix factorizations, and pick up the stability discussion in Sec. VI.

III. MATRIX FACTORIZATIONS

Let $W \in \mathcal{R} = \mathbb{C}[x_1, \ldots, x_r]$ be a polynomial. To keep things simple, we will assume throughout that W has an isolated critical point at the origin $x_i = 0$. A matrix factorization (of dimension N) of W is a pair of square matrices $f, g \in \mathrm{Mat}(N \times N, \mathcal{R})$ with polynomial entries satisfying

$$fg = gf = W \cdot \mathrm{id}_{N \times N}. \tag{3.1}$$

A matrix factorization is called reduced if all entries of f and g have no constant term, i.e., $f(0) = g(0) = 0$.

Matrix factorizations (f, g) and (f', g') are called equivalent if they are related by a similarity transformation

$$U_1 f = f' U_2, \quad U_2 g = g' U_1, \tag{3.2}$$

where $U_1, U_2 \in \mathrm{GL}(N, \mathcal{R})$ are invertible matrices with polynomial entries.

A. Maximal Cohen-Macaulay modules

Matrix factorizations originated in Eisenbud's work[14] in the context of so-called maximal Cohen-Macaulay modules over local rings of hypersurface singularities. See Refs. 15 and 16 for some background. An example of such a ring is given by $\widetilde{\mathcal{R}}_{\mathfrak{m}} = \mathcal{R}_{\mathfrak{m}}/(W)$, where $\mathcal{R}_{\mathfrak{m}} = \mathbb{C}[[x_1, \ldots, x_r]]$ is the complete local ring of power series, with maximal ideal $\mathfrak{m} = (x_1, \ldots, x_r)$, and W is a polynomial, as above. If (f, g) is a matrix factorization of W, consider the $\mathcal{R}_{\mathfrak{m}}$-module $M = \mathrm{Coker}\, f$ with the $\mathcal{R}_{\mathfrak{m}}$-free resolution

$$0 \to G \xrightarrow{f} F \to M \to 0, \tag{3.3}$$

where $F \cong G \cong (\mathcal{R}_{\mathfrak{m}})^N$ are rank N free modules. Since multiplication by W on ((3.3)) is homotopic to zero, M descends to a $\widetilde{\mathcal{R}}_{\mathfrak{m}}$-module, with the infinite free resolution

$$\cdots \to \widetilde{G} \xrightarrow{f} \widetilde{F} \xrightarrow{g} \widetilde{G} \xrightarrow{f} \widetilde{F} \to M \to 0 \tag{3.4}$$

with $\widetilde{F} \cong \widetilde{G} \cong (\widetilde{\mathcal{R}}_{\mathfrak{m}})^N$.

The resolution (3.3) being of length one, which is the codimension of a hypersurface, makes M into a so-called maximal Cohen-Macaulay module (MCM) over $\widetilde{\mathcal{R}}_{\mathfrak{m}}$ (see Refs. 15 and 16 for the definitions). Eisenbud's theorem[14] essentially says that all MCMs over hypersurface rings come from matrix factorizations.

The category of Cohen-Macaulay modules[15] will be denoted by $\mathrm{MCM}(W)$. Objects of $\mathrm{MCM}(W)$ are matrix factorizations of W and morphism are morphisms of Cohen-Macaulay modules. In other words, a morphism from (f, g) to (f', g') in $\mathrm{MCM}(W)$ is a pair of $N' \times N$-dimensional matrices a, b, with polynomial entries, satisfying

$$bg = g'a, \quad af = f'b, \tag{3.5}$$

so that the diagram

$$\begin{array}{ccccc} F & \xrightarrow{g} & G & \xrightarrow{f} & F \\ {\scriptstyle a}\downarrow & & {\scriptstyle b}\downarrow & & {\scriptstyle a}\downarrow \\ F' & \xrightarrow{g'} & G' & \xrightarrow{f'} & F' \end{array} \tag{3.6}$$

commutes. We will make no direct use of the category MCM(W), but have included its definition here since it might play a role in a precise formulation of R-stability.

B. Triangulated category

A different category's construction based on matrix factorization was observed by Kontsevich.[17] The construction starts from triples (M,σ,Q), where M is a free $\mathcal{R}=\mathbb{C}[x_1,\ldots,x_r]$-module with a $\mathbb{Z}_2$-grading σ, and Q is an odd ($\sigma Q+Q\sigma=0$) endomorphism of M satisfying

$$Q^2 = W\cdot \mathrm{id}_M. \tag{3.7}$$

Decomposing $M=M_0\oplus M_1$ into homogeneous components, with equal rank N,Q can be represented as the matrix

$$Q=\begin{pmatrix} 0 & f \\ g & 0 \end{pmatrix}, \tag{3.8}$$

making the relation of (3.7) to (3.1) obvious. The grading is then given by the matrix

$$\sigma=\begin{pmatrix} \mathrm{id}_{N\times N} & 0 \\ 0 & -\mathrm{id}_{N\times N} \end{pmatrix}. \tag{3.9}$$

Let us denote by DG(W) the category which has such triples as objects and as morphisms the (even) morphisms of free modules (forgetting the Q's). The gauge transformations in DG(W) are the even automorphisms of M as an $\mathcal{R}$-module, $\mathrm{GL}^+(2N,\mathcal{R})$, acting as

$$\mathrm{GL}^+(2N,\mathcal{R}) \ni U=\begin{pmatrix} U_1 & 0 \\ 0 & U_2 \end{pmatrix}: Q\mapsto UQU^{-1} \tag{3.10}$$

with $U_1,U_2\in \mathrm{GL}(N,\mathcal{R})$, as in (3.2).

The point of the construction (Refs. 30 and 19) is that the category DG(W) has the structure of a differential graded category. This means that morphism spaces $\mathrm{Hom}_{\mathcal{R}}(M,M')$ are equipped with an odd differential D acting as a supercommutator

$$D\Phi = Q'\Phi-\sigma'\Phi\sigma\ \Phi Q=\begin{pmatrix} 0 & f' \\ g' & 0 \end{pmatrix}\begin{pmatrix} A & B \\ C & D \end{pmatrix}-\begin{pmatrix} A & -B \\ -C & D \end{pmatrix}\begin{pmatrix} 0 & f \\ g & 0 \end{pmatrix}, \tag{3.11}$$

on morphisms

$$\Phi=\begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{3.12}$$

in DG(W). One easily checks that $D^2=0$ by the super-Jacobi identity. By a general construction,[18,19] one can then associate a triangulated category, MF(W) to DG(W), which has the same objects as DG(W) [i.e., triples (M,σ,Q)], but in which morphisms are given by the $\mathbb{Z}_2$-graded cohomology of Q. Thus $\mathrm{Hom}_{\mathrm{MF}(W)}(M,M')=H^*(D)=\mathrm{Ker}\,D/\mathrm{Im}\,D$. We shall usually embezzle M and σ, and simply write $\mathrm{Hom}_{\mathrm{MF}(W)}(Q,Q')=H^0(Q,Q')\oplus H^1(Q,Q')$ for the morphisms in MF(W). We also write $H^0(Q),H^1(Q)$ for the morphisms from Q to itself.

For future reference, let us spell out a few triangulated constructions in the language of matrix factorizations. First, the shift functor[1] is nothing but the reversal of the $\mathbb{Z}_2$-grading $\sigma \to -\sigma$, or, equivalently, the exchange of f and g, i.e.,

$$Q[1] = \begin{pmatrix} 0 & f \\ g & 0 \end{pmatrix}[1] = \begin{pmatrix} 0 & g \\ f & 0 \end{pmatrix}, \tag{3.13}$$

with M and σ fixed. This operation obviously exchanges H^0 with H^1. Second, given two matrix factorizations Q_1 and Q_2 and an odd morphism $T \in H^1(Q_1, Q_2)$, we obtain a third factorization simply as

$$Q = \begin{pmatrix} Q_1 & 0 \\ T & Q_2 \end{pmatrix}, \tag{3.14}$$

fitting into the triangle

$$\begin{array}{ccc} & Q & \\ {\scriptstyle S_2}\nearrow & & \searrow{\scriptstyle S_1} \\ Q_2 & \xleftarrow[T]{} & Q_1 \end{array} \tag{3.15}$$

where

$$S_1 = \begin{pmatrix} 1 & 0 \end{pmatrix}, \quad S_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{3.16}$$

The construction (3.14) is referred to as the "cone" over the map $T[1] \in H^0(Q_1, Q_2[1])$.

Let us also note explicitly that the construction of MF(W) implies in particular that we identify matrix factorizations which differ by the direct addition of the trivial factorization $f=1$, $g=W$,

$$Q \equiv Q \oplus \begin{pmatrix} 0 & 1 \\ W & 0 \end{pmatrix} \equiv Q \oplus \begin{pmatrix} 0 & W \\ 1 & 0 \end{pmatrix}. \tag{3.17}$$

This identification occurs because adding the trivial factorization does not affect the cohomology of D between Q and any other factorization Q'.

C. Relation to $\mathcal{N}=2$ Landau-Ginzburg model

Orbifoldized $\mathcal{N}=2$ Landau-Ginzburg models[20] are known[21,22] to describe the small-volume continuation of Calabi-Yau sigma models, see Ref. 23 for the background. (LG also describe, in particular, the mirrors of CY sigma models, as well as the mirrors of toric Fano and noncompact Calabi-Yau manifolds, but this will not be important here. We will stay on the B side throughout.)

In the bulk, LG models are characterized by the worldsheet superpotential W, such as the polynomial we have been studying in this section. The x_i are $\mathcal{N}=2$ chiral field variables, whose interaction is described by W. The kinetic term for the x_i is described by a Kähler potential $K(x_i, \overline{x_i})$, and is usually ignored in the discussion of LG models because it does not affect topological quantities such as the chiral ring. What is more, in the quasihomogeneous case, it is actually conjectured that there is a Kähler potential, uniquely determined by the superpotential, such that the associated model is conformal. This Kähler potential can be reached by RG flow along which W is unchanged by nonrenormalization theorems.

When adding boundaries to the worldsheet of an $\mathcal{N}=2$ *LG* model, the supersymmetry variation of the superpotential exhibits a peculiar boundary term, whose nonvanishing is known as the Warner problem.[24–28] Following a proposal of Kontsevich, it was shown in Refs. 29–31 that matrix factorizations of W provide a solution of the Warner problem. More precisely, it was argued

there that the category of topological *B*-branes in a Landau-Ginzburg model is equivalent to the category MF(W) we have described in the preceding section. The extent to which MF(W) also describes "physical" branes in the untwisted Landau-Ginzburg model will be the subject of the present paper.

In the LG application, the space M is the Chan-Paton space of a (target space–time filling) DDbar-system, with equal number of branes and antibranes, and f and g describe a tachyon configuration. The shift functor[1] is nothing but the exchange of branes with antibranes. The matrix Q is part of the BRST charge, and the matrix factorization equation $Q^2=W$ is the condition that the tachyon configuration be BRST invariant (or preserve $\mathcal{N}=2$ supersymmetry in the untwisted model). Open string states between two such brane systems are given by the cohomology of D, i.e., are elements of $H^*(Q,Q')$. (H^0 being referred to as bosonic, and H^1 as fermionic.) The cone (3.14) describes the formation of a "topological bound state" between two such configurations. Finally, (3.17) simply corresponds to the addition of a brane-antibrane pair which is canceled by an identical tachyon.

For other recent work on matrix factorizations in their relation to *D*-branes in Landau-Ginzburg models, see Refs. 32–43 and 12.

IV. GRADED MATRIX FACTORIZATIONS

By construction so far, our *D*-brane category MF(W) is $\mathbb{Z}_2$-graded. In particular, the shift functor squares to the identity. On the other hand, the prime example of a triangulated category, namely the derived category of coherent sheaves on an algebraic variety $\mathbf{D}(X)$, is $\mathbb{Z}$-graded (and has shifts by arbitrary integers). As pointed out in Ref. 12, there is a simple way to improve MF(W) to a $\mathbb{Z}$-graded category in the special case that W is quasihomogeneous.

A. *R*-symmetry

W being quasihomogeneous is the condition that there exists an assignment of degrees to the variables x_i such that W has definite degree. In the physical model, this grading is worldsheet *R*-charge, and W having *R*-charge 2 is the conventional normalization. Thus, we assume that there exist *R*-charges $q_i \in \mathbb{Q}$ such that

$$W(e^{i\lambda q_i}x_i) = e^{2i\lambda}W(x_i) \quad \text{for all } \lambda \in \mathbb{R}. \tag{4.1}$$

One can think of *R*-charge as a U(1) (or $\mathbb{C}^\times$) action on the space of polynomials with respect to which W is equivariant. The U(1) action closes for $\lambda=\pi H$, where H is the smallest integer such that $Hq_i \in 2\mathbb{Z}$ for all i.

When considering matrix factorizations of W, it is natural to require that this U(1) action can be extended to (M,σ,Q). This condition that the boundary interactions preserve the U(1) *R*-symmetry is a necessary condition for the existence of a conformal IR fixed point. We will call such matrix factorizations quasihomogeneous. For compatibility with (3.7), we must require that Q has *R*-charge 1. We will, at first, assume that this U(1) acts on M as an $\mathcal{R}=\mathbb{C}[x_1,\ldots,x_r]$-module (instead of as a $\mathbb{C}$-vector space). We will, however, assume that the action is even, i.e., commutes with σ. Explicitly, we assume that there exists a map

$$\rho:\mathbb{R} \to \mathrm{GL}^+(2N,\mathcal{R}) = \mathrm{GL}(N,\mathcal{R}) \times \mathrm{GL}(N,\mathcal{R}), \tag{4.2}$$

such that

$$\rho(0,x_i) = \rho(\pi H,x_i) = \mathrm{id}_{2N\times 2N}, \tag{4.3}$$

$$\rho(\lambda,x_i)Q(e^{i\lambda q_i}x_i) = e^{i\lambda}Q(x_i)\rho(\lambda,x_i). \tag{4.4}$$

Note that this implies the slightly nonstandard group law

$$\rho(\lambda,x_i)\rho(\lambda',e^{i\lambda q_i}x_i)=\rho(\lambda+\lambda',x_i). \tag{4.5}$$

In (4.2), $\mathrm{GL}(N,\mathcal{R})$ is the group of invertible $N\times N$ matrices with polynomial entries. Under gauge transformations, $Q(x_i)\to U(x_i)Q(x_i)U(x_i)^{-1}$ with $U\in \mathrm{GL}^+(2N,\mathcal{R})$, ρ transforms as

$$\rho^U(\lambda,x_i)=U(x_i)\rho(\lambda,x_i)U(e^{i\lambda q_i}x_i)^{-1}. \tag{4.6}$$

Note that if we can find a gauge transformation such that ρ^U is diagonal, then by (4.3), ρ^U must be independent of the x_i. Hence ρ^U is an ordinary U(1) representation on M as a $\mathbb{C}$-vector space. On general grounds, one expects that one can always find such gauge transformation that makes ρ diagonal. We will assume that this is true. But, as will become clear later, we do not want to exclude altogether gauge transformations of nonzero degree which might make ρ nondiagonal (and x_i dependent).

B. Gradability is a topological condition

Consider the vector field generating the U(1) action (4.2)

$$R(\lambda,x_i)=-i\partial_\lambda\rho(\lambda,x_i)\rho(\lambda,x_i)^{-1}. \tag{4.7}$$

In general, this will depend on λ, but it is easy to see that $R(\lambda,x_i)$ is actually determined for all λ by (4.5) and $R(0,x_i)$. At $\lambda=0$, the condition (4.4) becomes

$$EQ+[R,Q]=Q, \tag{4.8}$$

where

$$E=\sum_i q_i x_i\frac{\partial}{\partial x_i} \tag{4.9}$$

is the "Euler vector field." Note that W being quasihomogeneous means $EW=2W$, and therefore, if $Q^2=W$,

$$\{Q,EQ-Q\}=0, \tag{4.10}$$

where $\{\cdot,\cdot\}$ is the anticommutator. In other words, $EQ-Q$ defines a class in $H^1(Q)$. The existence of R is the statement that this class is trivial.

The quasihomogeneity condition on matrix factorizations is therefore a topological condition that is roughly analogous, by mirror symmetry, to the vanishing of the Maslov class of Lagrangian cycles. Recall[44] that the vanishing of the Maslov class ensures that Floer cohomology can be $\mathbb{Z}$-graded. Here, requiring (4.8) will immediately only give a $\mathbb{Q}$-grading, which commutes with the $\mathbb{Z}_2$ grading. In Sec. IV F, we will combine the two gradings into a single $\mathbb{Z}$-grading.

Actually, requiring the infinitesimal version (4.8) is somewhat weaker than the integrated version (4.3) and (4.4), because it does not guarantee that R generates a compact U(1) action. Equivalently, we might not be able to diagonalize R by a gauge transformation. Deferring a discussion of this point to Sec. IV D, let us assume that R is diagonalized (and hence its entries are in $\mathbb{Q}$). We then obtain an induced (diagonalizable) U(1) action on the morphism spaces in the DG-category $\mathrm{DG}(W)$. $\mathbb{Q}$-homogeneous elements of $\mathrm{Hom}_{\mathrm{DG}(W)}(Q,Q')$ satisfy

$$E\Phi+R'\Phi-\Phi R=q_\Phi\Phi. \tag{4.11}$$

By (4.8), this descends to a $\mathbb{Q}$-grading of D-cohomology, and hence, of $\mathrm{MF}(W)$. To avoid confusion, we will use $\mathfrak{H}^*(Q,Q')=\oplus_{q\in\mathbb{Q}}\mathfrak{H}^q(Q,Q')$ to denote this $\mathbb{Q}$-graded cohomology, and also use the split

$$\mathfrak{H}^q(Q,Q')=\mathfrak{H}^{q,0}(Q,Q')\oplus\mathfrak{H}^{q,1}(Q,Q') \tag{4.12}$$

into $\mathbb{Z}_2$ even and odd pieces.

C. Serre duality

If the boundary tachyon configuration described by Q and Q' flows to a conformal theory in the IR, one expects the spectrum of Ramond ground states to be charge conjugation symmetric. As usual,[7] by spectral flow, this means for the chiral primaries, which are given by D-cohomology,

$$\begin{aligned} H^*(Q,Q') &= H^{*+r}(Q',Q), \\ \mathfrak{H}^q(Q,Q') &= \mathfrak{H}^{\hat{c}-q}(Q',Q), \end{aligned} \tag{4.13}$$

for the $\mathbb{Z}_2$- and $\mathbb{Q}$-graded cohomologies, respectively. Here $\hat{c}=\Sigma_{i=1}^{r}(1-q_i)$ is the central charge of the bulk CFT associated with W. In mathematical terms, (4.13) expresses "Serre duality" for the category MF(W), with trivial Serre functor given purely by a shift in rational degree by $\hat{c}$, and reversal of $\mathbb{Z}_2$ degree if the number of variables is odd.

Serre duality is equivalent to nondegeneracy of the boundary topological metric, which was computed in Refs. 32 and 39. If $\Phi \in \mathrm{Hom}_{\mathrm{MF}(W)}(Q,Q')$ and $\Psi \in \mathrm{Hom}_{\mathrm{MF}(W)}(Q',Q)$, this Serre pairing is given by

$$\langle \Psi\Phi \rangle = \oint \frac{\mathrm{Str}_M\left[(\partial Q)^{\wedge r}\Psi\Phi\right]}{\partial_1 W \cdots \partial_r W}, \tag{4.14}$$

where the integral is a multidimensional residue. It is easy to see that this pairing has $\mathbb{Q}$-degree $\hat{c}$, i.e., $\langle \Psi\Phi \rangle = 0$ unless $q_\Phi + q_\Psi = \hat{c}$. It also has $\mathbb{Z}_2$ grading given by r, the number of variables in the model. Thus, proving nondegeneracy of (4.14) is equivalent to (4.13). It would be interesting to show this.

D. Ambiguities of *R*

As we have mentioned, the condition (4.8) does not guarantee that R generates a compact U(1) action that closes for $\lambda = \pi H$. On the other hand, it determines R only up to an even matrix that commutes with Q, i.e., a representative of $H^0(Q)$. The author is not aware of any example in which (4.8) has a solution, but no solution which does not generate a compact U(1) action, or which is not diagonalizable.

For example, if all entries of $Q=\begin{pmatrix} 0 & f \\ g & 0 \end{pmatrix}$ are in fact homogeneous polynomials, then one expects that (4.8) generically has a solution $R=\mathrm{diag}(R_1,\ldots,R_{2N})$ which is diagonal. Indeed, denoting polynomial degree by deg, Eq. (4.8) becomes

$$\begin{aligned} R_j - R_{k+N} &= 1 - \deg(f_{jk}) \\ & \qquad \text{for } j,k = 1,\ldots,N, \\ R_{k+N} - R_j &= 1 - \deg(g_{kj}) \end{aligned} \tag{4.15}$$

which is a system of $2N^2$ equations for $2N$ unknowns. The nontrivial relations on the left-hand side of (4.15) are given by permutations $\pi \in \Sigma_N$ on N indices,

$$\sum_j \left(R_j - R_{\pi(j)+N}\right), \tag{4.16}$$

being independent of π. On the right-hand side, these relations become

$$N - \sum_j \deg(f_{j\pi(j)}). \tag{4.17}$$

On the other hand, on taking determinant of (3.1), we see that

$$\det(f)\det(g) = W^N, \tag{4.18}$$

which, assuming that W is irreducible, implies $\det(f) = W^k$ for some $0 \leqslant k \leqslant N$. Since $\Sigma \deg(f_{j\pi(j)})$ is the degree of a summand of $\det(f)$, we see that if there are no exceptional cancellations, (4.17) is independent of π. Similarly, $gf = W$ generically implies $\deg(f_{jk}) + \deg(g_{kj}) = 2$.

Thus if all entries of Q are homogeneous, we expect that there is a diagonal solution of (4.8) (this is true in all examples the author has studied). It is easy to see that the converse is also true, R is diagonal, then all entries of Q must be homogeneous. (But there are factorizations that are not quasihomogeneous, see Sec. VIII F.)

We will generally assume that there is a solution of (4.8) that is diagonalizable, keeping in mind that this assumption can conceivably fail at singular loci in the moduli space of matrix factorizations. Let us then analyze the ambiguities of R.

The proposal for fixing the ambiguity of R is motivated by the examples of Sec. VII and the general considerations of Sec. VI. (It is also reminiscent of the "a-maximization" procedure used to find the R-charge of $\mathcal{N}=1$ superconformal gauge theories in four dimensions.[45]) The essential idea is that R defines a character on the gauge group of similarity transformations. Infinitesimally, such gauge transformations are given by even endomorphisms of M as a $\mathcal{R}$-module, i.e., block-diagonal matrices $V \in \mathrm{Mat}^+(2N \times 2N, \mathcal{R})$, with $\mathrm{Tr}\, V \in \mathbb{C}$. They act on Q by $\delta Q = [V, Q]$, and the character induced by R is given by

$$\chi_R(V) = \mathrm{Tr}_M(RV). \tag{4.19}$$

The condition we would like to impose on R is that this character be trivial on the part of the gauge group acting trivially,

$$\mathrm{Tr}(RV) = 0 \quad \text{whenever} \quad [V, Q] = 0. \tag{4.20}$$

Note that under such infinitesimal gauge transformations, R transforms according to

$$\delta R = -EV - [R, V] \tag{4.21}$$

which leaves (4.8) invariant to first order. By all we have said, it might then seem natural to fix a diagonal R and restrict to gauge transformation of degree 0, i.e., those which satisfy $EV + [R, V] = 0$ leave R invariant. As we will see in Sec. VII, however, this would be too restrictive, as we would not be able to describe brane-antibrane annihilation.

To fix the ambiguity, and impose (4.20), one may proceed as follows. Start with a reference solution R_0, assumed to be diagonal. The ambiguities of (4.8), which are parametrized by even cycles of Q, can be decomposed according to the degree with respect to R_0,

$$C^0(Q) = \oplus_q \mathfrak{C}^{q,0}(Q), \tag{4.22}$$

where

$$\mathfrak{C}^{q,0} = \left\{ V \in \mathrm{Mat}(2N \times 2N, \mathcal{R}); [Q, V] = 0, [\sigma, V] = 0, EV + [R_0, V] = qV \right\}. \tag{4.23}$$

To see what can happen if we modify R_0 by an element of $C^0(Q)$, it is instructive to consider the following example. Let

$$R_0 = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \tag{4.24}$$

with a and b rational. Then (we are neglecting Q and σ in this discussion—R_0 and V could be submatrices in a larger problem),

$$V = \begin{pmatrix} 0 & x \\ 0 & 0 \end{pmatrix} \tag{4.25}$$

is of (total) degree $q(V)=\deg(x)+a-b$ with respect to R_0. Clearly, R_0 generates a compact U(1) by $\rho_0(\lambda)=e^{i\lambda R_0}$, but R_0+V not necessarily so. Indeed, it is easy to see that the solution of (4.5) generated by R_0+V at $\lambda=0$ is

$$\rho(\lambda,x) = \begin{pmatrix} e^{i\lambda a} & x\dfrac{e^{i\lambda(a+\deg(x))}-e^{i\lambda b}}{a+\deg(x)-b} \\ 0 & e^{i\lambda b} \end{pmatrix}, \tag{4.26}$$

which for $b=a+\deg(x)$ goes over into

$$\rho(\lambda,x) = \begin{pmatrix} e^{i\lambda a} & ix\lambda e^{i\lambda b} \\ 0 & e^{i\lambda b} \end{pmatrix}. \tag{4.27}$$

We see that as long as $q(V)=\deg(x)+a-b\neq 0$, $R=R_0+V$ generates a compact U(1) and can be diagonalized. This fails when $q(V)=0$.

Thus, by rediagonalizing R if necessary, we can neglect the modifications of R_0 by elements of $\mathfrak{C}^{q,0}(Q)$ for $q\neq 0$. And clearly, χ_{R_0} vanishes automatically on $V\in\mathfrak{C}^{q,0}(Q)$, because such V does not have diagonal entries.

What about the ambiguities parametrized by $\mathfrak{C}^{0,0}(Q)$? As we have just seen, we cannot add V's without diagonal entries. Among those with diagonal entries, we choose a maximal commuting subalgebra, with basis $\{V_i\}_{i=1,\ldots,s}$, and impose (4.20) on the ansatz

$$R = R_0 + \sum_{i=1}^{s} a_i V_i. \tag{4.28}$$

In all examples the author has studied, this procedure leads to an unambiguously determined R which is diagonalizable and satisfies (4.20).

E. Cone construction

We next show that the grading we just introduced is compatible with the triangulated structure. In particular, we show that the cone (3.14) over a map $T[1]\in H^0(Q_1,Q_2[1])$ between two quasihomogeneous matrix factorizations is again quasihomogeneous.

Indeed,

$$\begin{aligned} EQ-Q &= \begin{pmatrix} EQ_1-Q_1 & 0 \\ ET-T & EQ_2-Q_2 \end{pmatrix} = \begin{pmatrix} [Q_1,R_1] & 0 \\ (q_T-1)T-R_2T+TR_1 & [Q_2,R_2] \end{pmatrix} \\ &= \left[Q, \begin{pmatrix} R_1+(q_T-1)\mathrm{id}_1 & 0 \\ 0 & R_2 \end{pmatrix} \right] \end{aligned} \tag{4.29}$$

is exact. More properly, we could choose

$$R = \begin{pmatrix} R_1+(q_T-1)\dfrac{N_2}{N_1+N_2}\mathrm{id}_1 & 0 \\ 0 & R_2-(q_T-1)\dfrac{N_1}{N_1+N_2}\mathrm{id}_2 \end{pmatrix} \tag{4.30}$$

so as to satisfy $\mathrm{Tr}(R)=0$ as well as $EQ-Q=[Q,R]$. But in the generic case, $C^0(Q)$ will contain more elements than just the identity so that we will not satisfy (4.20) in general.

F. Orbifolding and the phase of matrix factorizations

Recall that the Calabi-Yau/Landau-Ginzburg correspondence relates Calabi-Yau manifolds given as complete intersections in toric varieties to Landau-Ginzburg orbifold models.[22] In the simplest case, the Calabi-Yau is a hypersurface X given as the vanishing locus of a polynomial P of total degree H in weighted projective space $\mathbb{P}^{r-1}_{w_1,\ldots,w_r}$ such that $\Sigma_{i=1}^r w_i = H$. Such an X corresponds, via CY/LG correspondence, to the Landau-Ginzburg orbifold model with superpotential $W=P$ and orbifold group $\Gamma=\mathbb{Z}_H$, with central charge $\hat{c}=r-2$. The x_i have R-charge $q_i=2w_i/H$ and Γ is generated by $x_i \mapsto \omega_i x_i$ with $\omega_i = e^{i\pi q_i}$. The R-charges of the invariant part of the bulk chiral ring $\mathcal{J}=(\mathcal{R}/\partial W)^\Gamma$ are then all even integers.

Now let Q be a quasihomogeneous matrix factorization of W with R-matrix R uniquely determined as in Sec. IV D, and diagonal. Obviously, we would like to extend the Γ action to Q, and we require that it commutes with the rational and the $\mathbb{Z}_2$-grading. In other words, we are looking for a representation of Γ on (the associated $\mathbb{Z}_2$-graded $\mathcal{R}$-module of CP factors) M such that

$$\gamma Q(\omega_i x_i)\gamma^{-1} = Q(x_i). \tag{4.31}$$

It is easy to see that such a representation must be related to R in a simple manner. Indeed, we see that

$$\tilde{\gamma} = \sigma e^{-i\pi R}\gamma \tag{4.32}$$

commutes with Q. It is no restriction to assume that it is diagonal. If Q is reduced (i.e., contains not entries with a constant term), then all diagonal degree 0 elements of $C^0(Q)$ are actually nontrivial in $\mathfrak{H}^{0,0}(Q)$. We conclude that if Q is reduced and irreducible (i.e., $\mathfrak{H}^{0,0}(Q)$ is one dimensional), then $\tilde{\gamma}$ is a multiple of the identity, $\tilde{\gamma}=e^{i\pi\varphi}$. In other words, we find

$$\gamma = \sigma e^{i\pi R} e^{-i\pi\varphi}. \tag{4.33}$$

Imposing $\gamma^H=1$ fixes $\varphi \in \mathbb{R} \bmod 2/H$. Lifting to $\varphi \in \mathbb{R} \bmod 2$ gives H different equivariant factorizations for each factorization of W. (To be sure, if H is even, these correspond to $H/2$ branes together with their antibranes.)

A Γ-action on the objects induces an action on the morphism spaces $\mathfrak{H}^*(Q,Q')$, and we can project onto invariant morphisms by requiring

$$\gamma' \Phi(\omega_i x_i)\gamma^{-1} = \Phi. \tag{4.34}$$

By combining the definitions, it is easy to see that invariant morphisms satisfy the condition

$$e^{i\pi q_\Phi}(-1)^\Phi e^{\pi i(\varphi-\varphi')} = 1. \tag{4.35}$$

In other words, $q_\Phi = \varphi' - \varphi + n$, where n has the same parity as Φ. This constraint on the U(1) charges is the same as (2.3), and leads to the identification of φ as the phase of the matrix factorization.

Let us then define the category $\mathfrak{MF}(W)$, in which objects are quasihomogeneous matrix factorizations Q together with a lift of the phase φ to a real "grade," and morphism spaces are

$$\mathrm{Hom}^n((Q,\varphi),(Q',\varphi')) = \mathfrak{H}^{q=n+\varphi'-\varphi}(Q,Q'). \tag{4.36}$$

This is the promised $\mathbb{Z}$-graded category of matrix factorizations. Note in particular that the shift functor, which, because of (4.32), must be accompanied by $\varphi \to \varphi+1$, does not square to the identity in $\mathfrak{MF}(W)$.

G. Conjecture

The general decoupling statements of Ref. 2, the result that B-branes are described at large volume by the derived category of coherent sheaves, together with the assumption that all topo-

logical *B*-branes of the Landau-Ginzburg model have a description using matrix factorizations, naturally lead to the statement that—in appropriate cases—there should be an equivalence of categories

$$\mathfrak{MF}(W) \cong \mathbf{D}(X), \tag{4.37}$$

where $\mathfrak{MF}(W)$ is the category of quasihomogeneous Γ-equivariant matrix factorizations of W and $\mathbf{D}(X)$ is the derived category of coherent sheaves on the Calabi–Yau manifold X related to W/Γ by Witten's gauged linear sigma model construction.[22] Cases in which one expects such a correspondence include those GLSM's in which both large volume and Landau-Ginzburg points exist and are unique, such as the quintic in $\mathbb{P}^4$, or hypersurfaces in weighted projective spaces.

The author hopes that such a correspondence appears well-motivated from the physics point of view. It has essentially already been stated by Ashok, Dell'Aquila, and Diaconescu in Ref. 35 (for the quintic case and without the homogeneity condition). The author should, however, add that the correspondence is somewhat different from existing (and mathematically proven) equivalences between categories of matrix factorizations and other structures. Besides Eisenbud's canonical correspondence[14] with maximal Cohen-Macaulay modules, there is also an equivalence between matrix factorizations and a so-called "triangulated category of singularities" which was proven by Orlov.[19] Moreover, there is the classical correspondence of Grothendieck and Serre between graded modules over graded rings and vector bundles over the associated projective variety. This correspondence was exploited by Laza, Pfister, and Popescu in Ref. 46 for the case of the elliptic curve. If (4.37) is true, it is likely that the equivalence favored by physics is different from those just mentioned. For the elliptic curve, for instance, the methods of Ref. 46 on the one hand and Refs. 47 and 42 on the other hand yield quite different bundles corresponding to some given matrix factorization.

H. Landau-Ginzburg monodromy

We can make one further check that our conjecture makes sense. The Landau-Ginzburg point p_{LG} is an orbifold point in the Kähler moduli space $\mathcal{M}_k$. The action of the monodromy around p_{LG} acts on matrix factorizations in $\mathfrak{MF}(W)$ simply by rotating the choice of lift of φ in (4.33),

$$\varphi \to \varphi + 2/H. \tag{4.38}$$

As a consequence, the Hth power of the Landau-Ginzburg monodromy operator acts by $\varphi \to \varphi + 2$. This does nothing on the physical brane associated with Q, but is a shift by 2 in the triangulated category. This solves a problem posed in Ref. 6, in which the fifth power of the Landau-Ginzburg monodromy on the quintic Calabi-Yau was computed and found to correspond to a shift by 2 on the derived category. We can simply confirm this result using matrix factorizations, and in fact extend it to all Calabi-Yau manifolds with a Landau-Ginzburg description.

V. RR CHARGES AND INDEX THEOREM

If matrix factorizations represent *D*-branes in string theory, they must carry Ramond-Ramond (RR) charge. This charge takes value in the dual of the appropriate space $\mathcal{H}^B_{\mathrm{RR}}$ of closed string RR ground states. Because of the boundary condition on the worldsheet U(1) current, *B*-branes couple to those RR ground states with opposite left and right-moving *R*-charge, $q_L = -q_R$. The purpose of this section is to determine these RR charges of matrix factorizations. We first describe $\mathcal{H}^{\mathrm{B}}_{\mathrm{RR}}$.

The space of Ramond-Ramond ground states in Landau-Ginzburg orbifolds and their left-right *R*-charges was computed in Ref. 20. For simplicity, we will restrict here to a cyclic orbifold group $\Gamma = \mathbb{Z}_H$, as well as to integer central charge (we mostly have in mind, of course, $\hat{c}=3$). The generalization of at least some of the formulas to the more general case should be obvious. In general, those RR ground states with $q_L \neq q_R$ arise purely from the twisted sector, and if $\hat{c}$ is integer, the $\mathbb{Z}_H$ projection on twisted sectors implies that the RR ground states have $q_L \equiv q_R \equiv \hat{c}/2 \bmod \mathbb{Z}$.

Consider the lth twisted sector, and divide the field variables of the LG model into two classes, according to whether $lq_i \in 2\mathbb{Z}$ or $lq_i \notin 2\mathbb{Z}$. Those fields, $\{x_j^t\}$, with $lq_i \notin 2\mathbb{Z}$ satisfy twisted boundary condition in this sector, and must be set to zero in the semiclassical analysis used to determine the RR ground states. The contribution of those fields to the R-charges is (what we have called q_i is the sum of left- and right-moving charges of the variables x_i in the normalization of Ref. 20)

$$q_L^t = -q_R^t = \sum_{lq_i \notin \mathbb{Z}} \left(l\frac{q_i}{2} - \left[l\frac{q_i}{2} \right] - \frac{1}{2} \right). \tag{5.1}$$

On the other hand, those fields, $\{x_i^u\}_{i=1,\ldots,r_l}$, with $lq_i \in 2\mathbb{Z}$ satisfy untwisted boundary conditions in the lth twisted sector. Their quantization leads to a spectrum of RR ground states which is that corresponding to the effective potential $W_l(x_i^u) = W(x_i^u, x_i^t = 0)$. In particular, they contribute, $q_L^u = q_R^u$, equal amounts to left and right charge.

What is important for us, the ground states with $q_L = q_L^u + q_L^t = -q_R = q_R^u + q_R^t$ from the lth twisted sector correspond precisely to the neutral ground states of the effective potential $W_l(x_i^u)$ obtained by setting those fields with $lq_i \notin 2\mathbb{Z}$ to zero. These ground states have $q_L \equiv q_R \equiv \hat{c}/2 \bmod \mathbb{Z}$ if the number, r_l, of fields with $lq_i \in 2\mathbb{Z}$ is even. A basis of these ground states can be labeled as $|l;\alpha\rangle$, where l ranges between 0 and $H-1$, and α ranges over a basis $\phi_l^\alpha = (x^u)^\alpha = \prod_{i=1}^{r_l} (x_i^u)^{\alpha_i}$ of the subspace, $\mathcal{J}_l^0$, of the untwisted chiral ring $\mathcal{J}_l = \mathbb{C}[x_i^u]/\partial W_l$ with R-charge $q_L^u = q_R^u = \sum_{lq_i \in 2\mathbb{Z}} \alpha_i q_i/2 = \hat{c}^u/2$. Here, $\hat{c}^u = \sum_{lq_i \in 2\mathbb{Z}} (1-q_i)$ is the central charge corresponding to W_l. The states $|l;\alpha\rangle$ can be thought of as being obtained by acting with ϕ_α^l on the unique state $|l;0\rangle$, which has R-charge $-\hat{c}^u/2$.

Now by definition, the RR charge is the correlation function on the disk with the RR ground state inserted in the bulk. We propose that for a matrix factorization $Q \in \mathfrak{MF}(W)$, this is given by

$$\mathrm{ch}(Q): \mathcal{H}_{\mathrm{RR}}^{\mathrm{B}} \to \mathbb{C},$$

$$\mathrm{ch}(Q)(|l;\alpha\rangle) = \langle l;\alpha| Q_{\mathrm{disk}} = \frac{1}{r_l!} \mathrm{Res}_{W_l}(\phi_l^\alpha \, \mathrm{Str}[\gamma^l (\partial Q_l)^{\wedge r_l}]) = \frac{1}{r_l!} \oint \frac{\phi_l^\alpha \, \mathrm{Str}[\gamma^l (\partial Q_l)^{\wedge r_l}]}{\partial_1 W_l \cdots \partial_{r_l} W_l}, \tag{5.2}$$

where γ is the representation of the generator of $\mathbb{Z}_H$ on the matrix factorization, and $\mathrm{Str}(\cdot) = \mathrm{Tr}_M(\sigma \cdot)$ is the supertrace over the $\mathbb{Z}_2$-graded module M. The residue is the same as the one appearing in the Serre pairing (4.14). It is normalized[48] such that the determinant of the Hessian of the superpotential W_l has residue equal to the dimension of the chiral ring,

$$\mathrm{Res}_l(\det \partial_i \partial_j W_l) = \oint \frac{\det \partial_i \partial_j W_l}{\partial_1 W_l \cdots \partial_{r_l} W_l} = \dim \mathcal{J}_l = \mu_l = \prod_{lq_i \in 2\mathbb{Z}} \frac{2-q_i}{q_i}. \tag{5.3}$$

Moreover, in (5.2), $Q_l(x_i^u) = Q(x_i^u, x_i^t = 0)$ is the restriction of Q to the untwisted fields in the lth sector. It satisfies $Q_l^2 = W_l$.

Formula (5.2) makes sense since by (4.31),

$$\gamma^l Q^l(x_i^u) = Q^l(x_i^u) \gamma^l, \tag{5.4}$$

so γ^l represents a cohomology class of the matrix factorization Q_l, and (5.2) computes the disk correlation function[32,39] of $\gamma^l \phi_l^\alpha$ in this model. Moreover, since Res_l has $\mathbb{Q}$ degree $\hat{c}^u$ and $\mathbb{Z}_2$ degree r_l, we see that (5.2) would vanish if r_l were odd or if we tried to insert an element of $\mathcal{J}_l$ with charge not equal to $\hat{c}^u$.

In those twisted sectors with $r_l = 0$, i.e., $lq_i \notin 2\mathbb{Z}$ for all i, (5.2) reduces to

$$\mathrm{ch}(Q)(|l;0\rangle) = \mathrm{Str}\, \gamma^l. \tag{5.5}$$

One can check that (5.2) gives the correct value for the RR charges in those cases where an alternate computation exists, namely minimal models and their tensor products. Also, we see immediately that $\mathrm{ch}(Q[1])=-\mathrm{ch}(Q)$. The main evidence, however, that (5.2) is the correct expression for the RR charge is the index theorem for matrix factorizations, i.e., the fact that the Witten index for open strings between two matrix factorization Q and Q' can be computed via $\mathrm{ch}(Q)$ and $\mathrm{ch}(Q')$ as

$$\mathrm{Tr}(-1)^F=\sum_{n\in\mathbb{Z}}(-1)^n\dim \mathrm{Hom}^n_{\mathfrak{MF}(W)}(Q,Q')=\langle \mathrm{ch}(Q'),\mathrm{ch}(Q)\rangle, \tag{5.6}$$

where $(-1)^F$ is the $\mathbb{Z}_2$ grading (fermion number) of matrix factorizations. The Chern pairing is given by

$$\langle \mathrm{ch}(Q'),\mathrm{ch}(Q)\rangle=\frac{1}{H}\sum_{l=0}^{H-1}\sum_{\alpha,\beta}\mathrm{ch}(Q')(|l;\alpha\rangle)\frac{1}{\prod_{lq_i\notin 2\mathbb{Z}}(1-\omega_i^l)}\eta_l^{\alpha\beta}\,\mathrm{ch}(Q)(|l;\beta\rangle)^*. \tag{5.7}$$

For fixed l, $\Sigma_{\alpha,\beta}$ is a sum over the chosen basis of $\mathcal{J}_l^0$ of elements of the chiral ring $\mathcal{J}_l$ with charge $\hat{c}^u/2$, and $\eta_l^{\alpha\beta}$ is the inverse of the closed string topological metric in this sector,

$$\eta^l_{\alpha\beta}=\mathrm{Res}_l(\phi_l^\alpha\phi_l^\beta). \tag{5.8}$$

We will now prove (5.6) in the case that $r_l=0$ in all twisted sectors. The index of interest is the equivariant index of the operator D acting as in (3.11) on the complex given by the morphism space in $\mathrm{DG}(W)$, i.e.,

$$\mathrm{Tr}(-1)^F=\frac{1}{H}\sum_{l=0}^{H-1}\mathrm{Tr}(-1)^F\tilde{\gamma}^l, \tag{5.9}$$

where $\tilde{\gamma}$ is the action of the generator of $\mathbb{Z}_H$ on the cohomology spaces. We can regularize the computation of $\mathrm{Tr}(-1)^F\tilde{\gamma}=\lim_{t\to 1}Z_l(t)$ by using the $\mathbb{Q}$-grading by U(1) charge

$$Z_l(t)=\mathrm{Tr}(-1)^F t^q\tilde{\gamma}^l. \tag{5.10}$$

[More precisely, we should use an appropriate covering of this U(1) to make the charges integer.] By a standard argument, we can then replace the trace over the space of ground states by the trace over $\mathrm{Hom}_{\mathrm{DG}(W)}(Q,Q')=\mathrm{Hom}_{\mathcal{R}}(M,M')$, effectively reducing the computation to the setting $Q=Q'=0$. We decompose

$$\mathrm{Hom}_{\mathcal{R}}(M,M')=\bigoplus_{j,k=1}^{2N}\bigoplus_{\alpha}\mathcal{V}_{j,k,\alpha} \tag{5.11}$$

into one-dimensional pieces indexed by matrix entries (j,k) and monomials $x^\alpha=\Pi x_i^{\alpha_i}$ with multi-index $\alpha=(\alpha_1,\ldots,\alpha_r)$. Note that the combination of fermion number and $\mathbb{Z}_H$-action restricts on $\mathcal{V}_{j,k,\alpha}$ to

$$((-1)^F\tilde{\gamma})_{\mathcal{V}_{j,k,\alpha}}=\sigma'_j\gamma'_j\left(\prod_{i=1}^r\omega_i^{\alpha_i}\right)\sigma_k\gamma_k^{-1}, \tag{5.12}$$

where $\omega_i=e^{\pi i q_i}$, and we are using that both σ and γ are diagonal matrices. Therefore,

$$Z_l(t) = \sum_{j,k=1}^{2N} \sum_{\alpha} \sigma'_j(\gamma'_j)^l t^{R'_j} \left(\prod_{i=1}^{r} \omega_i^{l\alpha_i} t^{q_i \alpha_i} \right) \sigma_k(\gamma_k)^{-l} t^{-R_k} = \mathrm{Str}((\gamma')^l t^{R'}) \frac{1}{\prod_i (1 - t^{q_i} \omega_i^l)} \mathrm{Str}(\gamma^{-l} t^{-R}). \tag{5.13}$$

Since $\mathrm{Str}(\mathrm{id}) = 0$, and we are assuming that $lq_i \notin \mathbb{Z}$ for all other l and i, we can smoothly take $t \to 1$, and obtain

$$\mathrm{Tr}(-1)^F = \frac{1}{H} \sum_{l=1}^{H-1} \mathrm{Str}(\gamma')^l \frac{1}{\prod_i (1 - \omega_i^l)} \mathrm{Str}\ \gamma^{-l}, \tag{5.14}$$

as was to be shown.

To establish (5.6) and (5.7) in general, one should combine the proof we just gave with the formula

$$\frac{1}{(r_l!)^2} \mathrm{Res}_l(\mathrm{Str}[(\partial Q'_l)^{\wedge r_l}] \mathrm{Str}[(\partial Q_l)^{\wedge r_l}]) = \sum_{\alpha,\beta} \frac{1}{r_l!} \mathrm{Res}_l(\phi_l^\alpha \mathrm{Str}[(\partial Q'_l)^{\wedge r_l}]) \eta_l^{\alpha\beta} \frac{1}{r_l!} \mathrm{Res}_l(\phi_l^\beta \mathrm{Str}[(\partial Q_l)^{\wedge r_l}]). \tag{5.15}$$

This formula expresses the factorization rule for the topological annulus correlator[32] with no boundary insertions via two disk amplitudes and (the inverse of) the closed string topological metric $\eta^l_{\alpha,\beta}$ (5.8) given by the sphere amplitude.[48] [Note that in (5.15), the sum over α, β can be extended to the full chiral ring $\mathcal{J}_l$ because the disk correlators vanish outside of $\mathcal{J}_l^0$.] In the general axioms of open-closed topological field theory,[49,50] this factorization is known as the "Cardy condition." By the same axioms, the annulus correlator (5.15) computes the open string Witten index $\mathrm{Tr}(-1)^F$ between the matrix factorizations Q_l, Q'_l in the untwisted Landau-Ginzburg model corresponding to W_l. The author has checked the equality of the two sides of (5.15), and that they compute the open string Witten index, in all known examples, but the author does not know a proof based directly on the residue formula.

We close this section with a few comments.

First, we note that there is an obvious analogy between (5.6) and (5.7) and the well-known Hirzebruch-Riemann-Roch theorem which computes the Witten index for open strings coupled to two vector bundles E and F on the Calabi-Yau manifold X,

$$\mathrm{Tr}(-1)^F = \int \mathrm{ch}(E^*)\mathrm{ch}(F)\mathrm{Td}(X). \tag{5.16}$$

Our formula is simply the small volume version of this. In particular, the factor $\eta_l^{\alpha\beta}/\Pi(1-\omega_i^l)$ can be viewed as the analog of the Todd class of X. From this perspective, the normalization in which the square root of this factor is included in the charge might seem more natural.

Second, we return to the split of the Ramond ground states into those from twisted sectors with $r_l = 0$ and those from twisted sectors with $r_l \neq 0$ and even. In the RCFT description of LG models as Gepner models,[51] the ground states with $r_l \neq 0$ are not left-right symmetric in each individual $\mathcal{N}=2$ minimal model. (Geometrically, they correspond to nontoric blowups of X. For this reason, most models that have been studied geometrically in any depth do not have such states.) As a consequence, the BCFT constructions of boundary states in Gepner models[52] did not produce boundary states with charge under those RR ground states with $r_l \neq 0$, the only exception being related to the so-called fixed point resolution phenomenon discussed in Refs. 53 and 54 (see also Refs. 55 and 32). On the other hand, it is easy to find matrix factorizations for which charges with $r_l \neq 0$ do not vanish. (The two-variable factorizations of Sec. VII D, when embedded in the appropriate Calabi-Yau model, provide useful examples.) It seems likely that matrix factorizations span the free part of K-theory that is expected from cohomology. What the Chern classes (5.2)

miss, of course, is the torsion part of the *K*-theory. Unorbifolded minimal models, for example, have *K*-theory that is purely torsion. One might expect that some of this will survive the orbifold procedure, conceivably in the twisted sectors with r_l odd. It would be interesting to determine the full *K*-theory of these Landau-Ginzburg orbifolds and compare with their geometric computation. This would be a zeroth order check of (4.37).

VI. A STABILITY CONDITION

In mathematical models of *D*-branes similar to the one we are studying, such as Lagrangian submanifolds of symplectic manifolds, holomorphic vector bundles on complex manifolds, or representations of a quiver algebra, a stability condition is introduced with the purpose of identifying a subset of objects whose orbits under the group of appropriate automorphisms fit together into "nice" moduli spaces. Often, the stable orbits admit a distinct (unique) representative at the zero of a "moment map" associated with the stability condition (for instance, the special condition for Lagrangians or the Hermitian Yang-Mills equation for the connection on the holomorphic vector bundle). (See, e.g., Chap. 38 of Ref. 23 for a recount of these stories.)

In physics, the zeroes of the moment map are associated with the solution of the condition that the *D*-brane preserve supersymmetry in the uncompactified part of space–time. Stability is the condition that such a supersymmetric configuration can be reached by boundary renormalization group (RG) flow on the string worldsheet. In the unstable (including semistable) case, the theory is expected to split at singular points along RG flow into the direct sum of several decoupled theories. The endpoint of the flow is the decomposition into the stable pieces.

For a general Landau-Ginzburg model (orbifolded or not, with arbitrary central charge), the interpretation involving spacetime supersymmetry is not necessarily available, and we will factor it out accordingly. What remains is the unitarity constraint (2.1) and the assertion that if this condition is satisfied, worldsheet RG flow should lead to a single unitary boundary CFT in the IR (i.e., a theory with a unique open string vacuum). This is a stability condition that can be imposed on the triangulated category of any quasihomogeneous Landau-Ginzburg model.

If the model has a geometric interpretation, then in view of the expected equivalence (4.37), this is a particular stability condition on $\mathbf{D}(X)$. It is distinguished by the fact that it arises only from data involving the unorbifolded model (or equivalently, the orbifolded model divided by the quantum symmetry). In the general framework of Ref. 5, the space of (numerical) stability conditions is locally modeled on the free part of the *K*-theory. As we have seen in Sec. V, most of the *K*-theory (all of it for an odd number of variables) appears during orbifolding. Therefore, the stability condition in the Landau-Ginzburg model should be more rigid than the ones on $\mathbf{D}(X)$.

A. A notion of stability

As we have reviewed in Sec. II, the basic idea underlying Π-stability is that open strings between physical branes should satisfy the unitarity constraint $0 \leqslant q \leqslant \hat{c}$. It is hard, however, to impose such a constraint directly on individual objects to determine whether they are stable, essentially because this would involve an infinite number of checks, and moreover because a stable object does not only have strings satisfying (2.1) ending on it. Physically,[2] one should not try to impose the condition (2.1) on configurations described as (topological) bound states containing both branes and antibranes. One expects that in certain regimes,[2,4] or even at all points in the space of stability conditions,[5] integrating out all canceling brane-antibrane pairs will reduce the problem to a stability condition on an Abelian category, which involves only a finite number of checks. Still, these discussions leave open the question whether Π-stability is sufficient or just a self-consistent "bootstrap" condition. Our point of view is that the Landau-Ginzburg model should posses an intrinsic (rigid) stability condition that does not depend on what is going on in the rest of the moduli space. It is this notion of stability that we are after.

In the Landau-Ginzburg context, "integrating out brane-antibrane pairs" simply corresponds to restricting to reduced matrix factorizations, i.e., those without scalar entries. It is not unreasonable to expect, therefore, that by going to reduced matrix factorizations, one obtains the Abelian

category of interest for the discussion of Ref. 5. This Abelian category could be simply related to the category of Cohen-Macaulay module of Sec. III A. In any case, we now make the following tentative definition.

Let $W(x_1,\ldots,x_r)$ be a quasihomogeneous Landau-Ginzburg polynomial, $EW=2W$, where $E=\Sigma q_i x_i \partial_i$. Let Q be a reduced quasihomogeneous matrix factorization of W. Q is called R-semistable if in all triangles

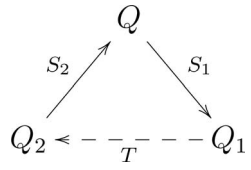

(6.1)

in which Q participates opposite to the fermionic morphism T, we have

$$q_T \leqslant 1 \Leftrightarrow q_{S_1} \geqslant 0 \Leftrightarrow q_{S_2} \geqslant 0. \tag{6.2}$$

Q is stable if the only triangles for which $q_T=1$ are those with Q_1 or Q_2 equal to Q (and the other equivalent to 0).

Here q_T is defined by the condition

$$ET + R_2T - TR_1 = q_T T, \tag{6.3}$$

where R_1 and R_2 are the R-matrices of Q_1 and Q_2, respectively.

We can give one simple check that relates R-stability to a stability condition in the sense of Bridgeland.[5] Recall that in the orbifolded case (Sec. IV F), we have defined morphism between objects in $\mathfrak{MF}(W)$ by $\mathrm{Hom}^0(Q,Q')=\mathfrak{H}^{q=\varphi'-\varphi}(Q,Q')$. Therefore, our condition (6.2) directly implies

$$\varphi > \varphi' \Rightarrow \mathrm{Hom}^0(Q,Q') = 0, \tag{6.4}$$

which is one of the axioms of Ref. 5.

We also note that our formulation is similar to those of a stability condition for Lagrangian submanifolds proposed by Thomas[56] and further studied in Ref. 57.

B. A moment map problem?

The stability condition we have proposed is physically well motivated. It only deserves its name, however, if it can be related to the moduli space problem for matrix factorizations. In other words, one would like to show that stable matrix factorizations have nicely behaved orbits under the group of gauge equivalences. As we have mentioned before, this group is the group of similarity transformations

$$G \cong \mathrm{GL}^+(2N,\mathcal{R}) \cong \mathrm{GL}(N,\mathcal{R}) \times \mathrm{GL}(N,\mathcal{R}) \tag{6.5}$$

acting as in (3.2). Thus we have an algebraic group acting on a linear space with a constraint. This problem is quite similar to the one studied by King.[11]

In Ref. 11, the general setup of geometric invariant theory (GIT)[58] is used to define moduli spaces for representations of finite-dimensional algebras, which can be equivalently described as the representations of quiver diagrams. Quivers arise naturally as world-volume theories for D-branes at singularities, and the theory of quivers has played an important role in the development of Π-stability.[1,10] In the quiver case, the gauge group $\mathcal{G}$ is the product of general linear groups acting on the vector spaces at each node of the quiver. King uses GIT to give a geometric description of the algebraic quotient of the representation space Y with respect to a character $\chi:\mathcal{G}\to\mathbb{C}^\times$ via "Mumford's numerical criterion:" A representation $y\in Y$ is χ-semistable iff χ is

trivial on the stabilizer of y and if every one-parameter subgroup $g(\lambda)=e^{\lambda a}$ of $\mathcal{G}$, for which $\lim_{\lambda\to\infty} y$ exists, satisfies $\langle d\chi, a\rangle \geqslant 0$, where $d\chi$ is the infinitesimal version of χ evaluated on the generator a of $g(\lambda)$.

Our stability condition is precisely equivalent to such a "numerical criterion." To see this, note that all triangles in MF(W) are isomorphic to the standard cone (4.29), namely

$$Q = Q_1 \oplus Q_2 + T, \quad R = R_1 \oplus R_2 + (q_t - 1)\left[\frac{N_2}{N_1+N_2}S_1 - \frac{N_1}{N_1+N_2}S_2\right], \tag{6.6}$$

where $S_i=\mathrm{id}_i$. Under the one-parameter group of gauge transformations generated by $V=S_1$, this cone transforms as

$$Q_\lambda = e^{\lambda V} Q e^{-\lambda V} = Q_1 \otimes Q_2 + e^{-\lambda} T \underset{\lambda\to\infty}{\to} Q_1 \otimes Q_2. \tag{6.7}$$

The limit $\lambda \to \infty$ simply splits the cone back into its constituents. The condition $q_T \leqslant 1$ is equivalent to

$$-\mathrm{Tr}(RV) = -(q_t - 1)\frac{2N_2N_1}{N_2+N_1} \geqslant 0, \tag{6.8}$$

thus identifying $\mathrm{Tr}(R\cdot)$ as the character of G with respect to which we are defining stability. The condition (4.20) we are imposing to fix the ambiguities of R is precisely the condition that $\mathrm{Tr}(R\cdot)$ should vanish on the trivially acting gauge transformations. Similarly as in Ref. 11, we can then formulate a "numerical criterion" that a matrix factorization Q is R-semistable if all one-parameter subgroups $e^{\lambda V}$ of the gauge group, for which the limit $\lim_{\lambda\to\infty} e^{\lambda V} Q e^{-\lambda V}$ exists, satisfy $\mathrm{Tr}(RV) \leqslant 0$.

In Ref. 11, King then goes on to describing a symplectic quotient construction of the moduli space, which is the basis for the relation to quiver gauge theories.

We can at present see two difficulties in making such a relation in our situation more precise, both of which due to the fact that G is not as simple a gauge group as the one acting on quiver representations. First of all, as a complex Lie group, G is infinite-dimensional. This is similar to the situation with vector bundles or Lagrangian submanifolds, giving reason for hope. The second difficulty appears if, as might seem natural, we would restrict to the degree 0 gauge transformations, i.e., those generated by

$$\mathfrak{g}^0 = \{V \in \mathfrak{g}; EV + [R,V] = 0\}. \tag{6.9}$$

The problem with $\mathfrak{g}^0$ is that it is nonreductive. Indeed, since both polynomial and total degree are preserved in matrix multiplication, $\mathfrak{g}^0$ has a maximal solvable subalgebra consisting of those matrices without constant term. In other words, we can decompose $\mathfrak{g}^0$ into its maximal reductive subalgebra consisting of those elements annihilated by E, and the nilpotent part. This nonreductiveness of $\mathfrak{g}^0$ makes it more difficult to apply the general results of GIT and to find a relation with a moment map problem. In any case, however, restricting to gauge transformations of degree 0 makes the description of brane-antibrane annihilation somewhat unnatural, see Sec. VII B.

Setting aside these difficulties for the moment, we will naively follow the usual steps to write down a moment maplike flow equation on the gauge orbits. As we will see in Sec. VII, this naive flow works quite well in a number of examples. Imitating,[11] we introduce a metric on the space of matrix factorizations,

$$\langle Q, Q'\rangle = \sum_\alpha \mathrm{Tr}(Q_\alpha^\dagger Q'_\alpha), \tag{6.10}$$

where

$$Q = \sum_\alpha Q_\alpha x^\alpha, \quad Q' = \sum_\alpha Q'_\alpha x^\alpha \tag{6.11}$$

is the decomposition of Q and Q' into a sum over monomials $x^\alpha = \Pi_i x_i^{\alpha_i}$. In any given case, we restrict to a finite-dimensional subgroup of G and choose a basis of generators, $\{V_i\}$. The flow equation then is

$$\frac{dQ}{dt} = -(\langle Q, [V^i, Q]\rangle - \mathrm{Tr}\, RV^i)[V_i, Q]. \tag{6.12}$$

Note that by construction, (6.12) is indeed a moment map for the maximal reductive subgroup of the degree 0 gauge group.

Moreover, one can see that the flow (6.12) indeed reproduces the correct splitting (6.7) of the standard cone (4.29) in the case that $q_T \geqslant 1$. A simple calculation gives

$$\frac{d\lambda}{dt} = (e^{-2\lambda}\|T\|^2 + (q_T - 1)\beta) \tag{6.13}$$

where $\beta = 2N_2N_2/(N_2+N_1)$. Evidently, this has a solution at finite λ if $q_T < 1$, whereas for $q_T \geqslant 1$, the flow drives us to $\lambda \to \infty$. The form of Eq. (6.13) is of course familiar in the context of solving D-flatness conditions in four-dimensional $\mathcal{N}=1$ supersymmetric gauge theories.

VII. EXAMPLES

We conclude the paper with several concrete examples of matrix factorizations and flows on their gauge orbits defined by (6.12). As alluded to before, one can view these flows as toy models for boundary flows in Landau-Ginzburg models. (Landau-Ginzburg descriptions of boundary flows have also recently been discussed in Ref. 59.)

A. Minimal models

Matrix factorizations of A-type minimal models with type 0A GSO projection, corresponding to the LG superpotential $W = x^h$ were discussed in detail in Refs. 31, 33, 36, and 41. They are given by

$$Q_n = \begin{pmatrix} 0 & x^n \\ x^{h-n} & 0 \end{pmatrix} \quad \text{for } n = 1, \ldots, h-1. \tag{7.1}$$

The R-matrix is

$$R = \begin{pmatrix} \frac{1}{2} - \frac{n}{h} & 0 \\ 0 & -\frac{1}{2} + \frac{n}{h} \end{pmatrix}. \tag{7.2}$$

It is easy to see that there is only one nontrivial element of the degree 0 gauge algebra,

$$V = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}. \tag{7.3}$$

The orbit generated by V looks like

$$Q_n(\lambda) = e^{\lambda V} Q_n e^{-\lambda V} = \begin{pmatrix} 0 & e^{\lambda} x^n \\ e^{-\lambda} x^{h-n} & \end{pmatrix}, \tag{7.4}$$

so that the flow (6.12) becomes

$$\frac{d\lambda}{dt} = -(\langle Q_n(\lambda),[V,Q_n(\lambda)]\rangle - \mathrm{Tr}\, RV) = -\left(e^{2\,\mathrm{Re}\,\lambda} - e^{-2\,\mathrm{Re}\,\lambda} - \frac{1}{2} + \frac{n}{h}\right). \tag{7.5}$$

Obviously, this flow has just one stationary point, which is stable. This is as expected. Indeed, one can check explicitly that all open strings between different minimal model factorizations satisfy $0 \leqslant q \leqslant \hat{c} = 1 - (2/h) < 1$.

B. Brane-antibrane annihilation

We have been tempted several times in this paper to restrict attention to the gauge transformations of degree 0 only. In this section, we show that in fact, the description of brane-antibrane annihilation in the context of matrix factorizations requires the inclusion of gauge transformation of nonzero degree.

Let (f,g) be a matrix factorization of W with R-matrix $R=(R_+,R_-)$, and consider the cone over the identity id, $(f,g)\to(f,g)$,

$$Q_0 = \begin{pmatrix} 0 & 0 & f & 0 \\ 0 & 0 & 1 & g \\ g & 0 & 0 & 0 \\ -1 & f & 0 & 0 \end{pmatrix}. \tag{7.6}$$

This is gauge equivalent to direct sums of the trivial factorization $W=1\cdot W$ via the gauge transformation

$$U_\lambda = \begin{pmatrix} 1 & -\lambda f & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & \lambda g \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{7.7}$$

Namely,

$$Q_\lambda = U_\lambda Q_0 U_\lambda^{-1} = \begin{pmatrix} 0 & 0 & (1-\lambda)f & (\lambda^2-2\lambda)W \\ 0 & 0 & 1 & (1-\lambda)g \\ (1-\lambda)g & (2\lambda-\lambda^2)W & 0 & 0 \\ -1 & (1-\lambda)f & 0 & 0 \end{pmatrix} \tag{7.8}$$

which for $\lambda=1$ becomes

$$Q_1 = \begin{pmatrix} 0 & 0 & 0 & -W \\ 0 & 0 & 1 & 0 \\ 0 & W & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}. \tag{7.9}$$

What is the R-matrix associated with Q_0? The cone construction of Sec. IV E gives one possible solution (4.30)

$$R^{\mathrm{cone}} = \begin{pmatrix} R_+ - \frac{1}{2} & 0 & 0 & 0 \\ 0 & R_- + \frac{1}{2} & 0 & 0 \\ 0 & 0 & R_- - \frac{1}{2} & 0 \\ 0 & 0 & 0 & R_+ + \frac{1}{2} \end{pmatrix}. \tag{7.10}$$

However, this R-matrix does not satisfy (4.20). By using the equivalence with Q_1, one finds that the generators of $C^0(Q_0)$ with nonvanishing diagonal entries and degree 0 with respect to R^{cone} are

$$V_i = \begin{pmatrix} e_i & -f_i & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -g^i \\ 0 & 0 & 0 & e_i \end{pmatrix} \quad \text{and} \quad V^i = \begin{pmatrix} 0 & f^i & 0 & 0 \\ 0 & e_i & 0 & 0 \\ 0 & 0 & e_i & g_i \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{7.11}$$

where e_i is the $N \times N$ matrix with a 1 at the ith position on the diagonal, and zeroes elsewhere, and $f_i = e_i f$ and $f^i = f e_i$ are the ith row and column of f, respectively.

Then the combination of R^{cone}, V_i, and V^i satisfying (4.20) is

$$R_0 = \begin{pmatrix} -\frac{1}{2} & R_+ f - f R_- & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & gR_+ - R_- g \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & -Ef + f & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & Eg - g \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}. \tag{7.12}$$

Under the similarity transformation (7.8), R_0 transforms into the diagonal matrix $R_1 = \text{diag}(-1/2, 1/2, -1/2, 1/2)$. This R_1 is the R-matrix one would naturally assign to a sum of copies of the trivial branes described by Q_1.

Note that while the gauge transformation relating Q_0 and Q_1 has degree zero with respect to R^{cone}, it does not have definite degree with respect to R_0. We conclude that either we are forced to work with gauge transformations of nonzero degree or we should be using R^{cone} as R-matrix for the cone. We cannot completely exclude the second possibility since (by definition) the factorization $(1, W)$ does not have any nontrivial morphism ending on it, so there are no R-charges to check. But the symmetric end result, R_1, is good justification for the procedure we have proposed. And the moment map equation only makes sense if we use R_0. One can also check that the flow defined by (6.12) on the gauge orbit (7.8) flows to $\lambda = 1$.

C. Boundary flows in minimal models

Having argued for the general relevance of gauge transformations of nonzero degree, we now return to minimal models and study boundary flows associated with perturbations by a boundary condition changing operator. General aspects of such boundary flows in $\mathcal{N}=2$ minimal models were discussed recently in Ref. 36 and in Ref. 41. In particular, these works discuss the similarity transformations relating the different minimal model branes at the topological level, as well as the operators inducing these relations. Our flow equation (6.12) gives a handle on the complete flow in the physical theory.

We will consider as an example the starting point

$$Q_0 = \begin{pmatrix} 0 & 0 & x^2 & 0 \\ 0 & 0 & -x & x^3 \\ x^{h-2} & 0 & 0 & 0 \\ x^{h-4} & x^{h-3} & 0 & 0 \end{pmatrix}. \tag{7.13}$$

The R-matrix, obtained by the methods above is

$$\begin{pmatrix} \frac{1}{2} - \frac{4}{h} & -\frac{x}{h} & 0 & 0 \\ 0 & \frac{1}{2} - \frac{1}{h} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} + \frac{1}{h} & -\frac{x^2}{h} \\ 0 & 0 & 0 & -\frac{1}{2} + \frac{4}{h} \end{pmatrix}. \tag{7.14}$$

We have studied the flow induced by (6.12) on the orbit of Q_0 under the gauge transformations generated by

$$V=\begin{pmatrix} \lambda_1 & \lambda_3 x & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & -\lambda_2 & \lambda_4 x^2 \\ 0 & 0 & 0 & -\lambda_1 \end{pmatrix} \tag{7.15}$$

and find that it does converge to the diagonal

$$\begin{pmatrix} 0 & 0 & 0 & \alpha x^4 \\ 0 & 0 & -\beta x & 0 \\ 0 & -\beta^{-1}x^{h-1} & 0 & 0 \\ \alpha^{-1}x^{h-4} & 0 & 0 & 0 \end{pmatrix} \cong Q_1 \oplus Q_4, \tag{7.16}$$

where α and β are the appropriate solutions of (7.5). The R-matrix becomes diag$(1/2-4/h, 1/2-1/h, -1/2+1/h, -1/2+4/h)$, which is certainly the correct result for this factorization.

We should note that the perturbation we have turned on in (7.13) is not the most relevant between the two minimal model branes Q_2 and Q_3. We have chosen this one to illustrate that there are various possible flow patterns in $\mathcal{N}=2$ minimal models. In this simple case the range of possibilities is essentially governed by the K-theory, isomorphic to $\mathbb{Z}_H$. One can create a free K-theory [and make the perturbation in (7.13) the most relevant one] by considering an appropriate orbifold.

In any case, the end result of the flow is consistent with the predictions made, for instance, in Refs. 36 and 59.

D. *D*0-brane in quintic Gepner model

In Ref. 35, matrix factorizations were constructed which describe (at the topological level) $D0$-branes at the Landau-Ginzburg orbifold point in the Kähler moduli space of the quintic Calabi-Yau. We here want to address the issue whether these factorizations can be stable by checking that the open strings stretched between this $D0$-brane and the rational tensor products of minimal model branes satisfy the unitarity bound. While this does of course not settle the question whether the $D0$-brane can become unstable far away from the large volume limit, it is certainly a nontrivial check.

The superpotential of interest is $W=\Sigma_{i=1}^5 x_i^5$. The factorizations of Ref. 35 are tensor products of minimal model factorizations in three of the five minimal factors together with a nonfactorizable factorization in the remaining two factors. Since taking tensor products simply adds U(1) charges, but does not affect the unitarity bound, it will suffice to consider this two-variable factorization. We can factorize

$$x^5-y^5=(x-y)(x^4+x^3y+x^2y^2+xy^3+y^4). \tag{7.17}$$

One can see that the R-matrix associated with this factorization is diag$(3/10,-3/10)$. We want to compute the charges of open strings between this factorization and the tensor product of minimal model branes

$$f=\begin{pmatrix} x & -y \\ -y^4 & x^4 \end{pmatrix}, \quad g=\begin{pmatrix} x^4 & y \\ y^4 & x \end{pmatrix}, \quad R=\mathrm{diag}(3/5,-3/5,0,0). \tag{7.18}$$

As computed in Ref. 35, there is one bosonic and one fermionic cohomology class between (7.17) and (7.18), represented by

$$\Phi^0=\begin{pmatrix} y^3 & 1 & 0 & 0 \\ 0 & 0 & y^3 & x^3+x^2y+xy^2+y^3 \end{pmatrix},$$

$$\Phi^1 = \begin{pmatrix} 0 & 0 & -1 & 1 \\ x^3+x^2y+xy^2+y^3 & -1 & 0 & 0 \end{pmatrix}, \tag{7.19}$$

respectively. We easily find

$$q(\Phi^0) = \tfrac{9}{10}, \quad q(\Phi^1) = \tfrac{3}{10} \tag{7.20}$$

satisfying the unitarity bound $0 \leqslant q \leqslant \hat{c} = \frac{6}{5}$. We have also checked the open strings between the $D0$-brane factorization and the other minimal model branes. They all satisfy the bound.

E. Decay of an unstable factorization

In this section, we give an example of a matrix factorization that is unstable and investigate to what extent our flow (6.12) can detect this without having to check the charges of open strings. The superpotential is $W=x^5+y^5$, and the factorization given by

$$f_{\text{unst}} = \begin{pmatrix} x & y & 0 \\ 0 & x^3 & y \\ y^3 & 0 & x \end{pmatrix}, \quad g_{\text{unst}} = \begin{pmatrix} x^4 & -xy & y^2 \\ y^4 & x^2 & -xy \\ -x^3y^3 & y^4 & x^4 \end{pmatrix},$$

$$R = \text{diag}(7/10, -1/10, -1/10, 1/10, 1/10, -7/10), \tag{7.21}$$

A morphism between this factorization and the tensor product of minimal model branes (7.18) is given by

$$T = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & x & -y & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \tag{7.22}$$

and one can easily check that this field has R-charge $-\frac{1}{10}$, violating the unitarity bound. (Note that since T has scalar entries, it cannot be exact.) The cone over T is another copy of the tensor product of minimal branes, thus exhibiting (7.21) as an unstable bound state, obtained by "condensing" a field with $q>1$ between two such objects. Namely, $(f_{\text{unst}}, g_{\text{unst}})$ is stably equivalent to

$$F_{\text{unst}} = \begin{pmatrix} x & y & 0 & 0 \\ -y^4 & x^4 & 0 & 0 \\ 0 & -x^3 & x^4 & -y \\ y^3 & 0 & y^4 & x \end{pmatrix}, \quad \text{with corresponding } G_{\text{unst}}. \tag{7.23}$$

To be precise, we should note that $(F_{\text{unst}}, G_{\text{unst}})$ is really a cone over a brane and its own antibrane, but via a field that is not the identity. As a consequence, $(f_{\text{unst}}, g_{\text{unst}})$ has a unitarity violating field in the spectrum with itself. But since this field can easily be projected out by going to an appropriate orbifold, it should not be viewed as the cause of the instability.

In discussing the flow, it is useful to contrast the unstable factorization with a very similarly structured stable (with the same caveat as before) bound state of two minimal model tensor products, namely

$$F_{\text{stab}} = \begin{pmatrix} x & y^2 & 0 & 0 \\ -y^3 & x^4 & 0 & 0 \\ 0 & -x^3 & x^4 & -y^2 \\ y & 0 & y^3 & x \end{pmatrix}, \quad G_{\text{stab}}, \tag{7.24}$$

which can be reduced to

$$f_{\text{stab}} = \begin{pmatrix} x & y^2 & 0 \\ 0 & x^3 & y^2 \\ y & 0 & x \end{pmatrix}, \quad g_{\text{stab}} = \text{adj}(f_{\text{stab}}). \tag{7.25}$$

We have studied numerically the flow defined by (6.12) on the 12-parameter gauge orbit of $(F_{\text{unst}}, F_{\text{unst}})$ and $(F_{\text{stab}}, G_{\text{stab}})$ generated by

$$\begin{pmatrix} \lambda_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda_2 & x\lambda_3 & y\lambda_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda_5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda_6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \lambda_7 & 0 & y\lambda_8 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda_9 & x\lambda_{10} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \lambda_{11} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \lambda_{12} \end{pmatrix} \tag{7.26}$$

and

$$\begin{pmatrix} \lambda_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda_2 & x\lambda_3 & y^2\lambda_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda_5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda_6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \lambda_7 & 0 & y^2\lambda_8 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda_9 & x\lambda_{10} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \lambda_{11} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \lambda_{12} \end{pmatrix}, \tag{7.27}$$

respectively. We find that starting from quite general initial conditions, (6.12) indeed drives $(F_{\text{unst}}, G_{\text{unst}})$ to the split into the direct sum of two copies of the tensor product brane. On the other hand $(F_{\text{stab}}, G_{\text{stab}})$ flows to the direct sum of $(f_{\text{stab}}, g_{\text{stab}})$ and a copy of the trivial factorization $(1, W)$.

It is worthwhile emphasizing that this statement does not hold for all initial conditions. One of the consequence of nonreductiveness is that the flow defined by (6.12) is not convex. Taking a second derivative on the right-hand side does not produce something positive definite because $\langle Q, [V, Q'] \rangle \neq \langle [V^\dagger, Q], Q' \rangle$ in general. If the flow is not convex, there is no guarantee that stationary points will be unique. In the present case, there does exist a stationary point for the flow close to $f_{\text{unst}}, g_{\text{unst}} \oplus (1, W)$. But this point is a saddle point of the flow, i.e., it is unstable in the sense of dynamical systems. One must account for this possibility if one wants to make sense of (6.12) in general.

Another example of the same character as the one we have been discussing in this section arises in the series of models $W = x^h + y^3$, with factorizations given by

$$f = \begin{pmatrix} x^n & y & 0 \\ 0 & x^n & y \\ y & 0 & x^{h-2n} \end{pmatrix} \tag{7.28}$$

[and, as by now familiar, $g = \text{adj}(f)$]. By considerations similar to those we have given above, one finds that the factorizations (7.28) are stable when $n < h/6$ and (apparently) stable otherwise. (In particular, for $h < 6$, where W describes an E-type minimal model, these factorizations are all stable.)

F. A nonhomogeneous factorization

Lest we leave the impression that all matrix factorizations of quasihomogeneous polynomials are quasihomogeneous, here is a counter-example.

The superpotential $W=x^3+y^7$ is one of the simplest superpotentials that is not a simple singularity. In fact, it is unimodular. Torsion free rank one modules over local rings of unimodular singularities were classified in Ref. 60. It is a simple exercise to determine the associated matrix factorizations. On the list for $W=x^3+y^7$, one finds the following one-parameter family of factorizations:

$$f=\begin{pmatrix} x^2-\lambda y^5 & xy \\ xy+\lambda^2 y^4 & -\lambda x+y^2 \end{pmatrix},$$

$$g=\begin{pmatrix} x-\frac{y^2}{\lambda} & \frac{xy}{\lambda} \\ \frac{xy}{\lambda}+\lambda y^4 & -\frac{x^2}{\lambda}+y^5 \end{pmatrix}. \tag{7.29}$$

For $\lambda\neq 0$, this is stably equivalent to the following factorization:

$$\tilde{f}=\begin{pmatrix} -xy^5 & \lambda xy^4+y^6 & -x^2 \\ y^6 & x^2-\lambda y^5 & xy \\ -x^2-\lambda y^5 & yx+\lambda^2 y^4 & -\lambda x+y^2 \end{pmatrix},$$

$$\tilde{g}=\begin{pmatrix} \lambda & y & -x \\ y & x & 0 \\ -x & \lambda y^4 & y^5 \end{pmatrix}, \tag{7.30}$$

which is nonreduced, but has a limit as $\lambda\to 0$. While W is quasihomogeneous with $q_x=2/3$, $q_y=2/7$, we see that

$$Ef-f+R_+f-fR_-=\frac{2}{21}\lambda\begin{pmatrix} -y^5 & 0 \\ 2\lambda y^4 & -x \end{pmatrix}=\frac{2}{21}\lambda\partial_\lambda f, \tag{7.31}$$

where

$$R=\begin{pmatrix} R_+ & 0 \\ 0 & R_- \end{pmatrix}=\begin{pmatrix} -\frac{7}{42} & 0 & 0 & 0 \\ 0 & \frac{9}{42} & 0 & 0 \\ 0 & 0 & \frac{7}{42} & 0 \\ 0 & 0 & 0 & -\frac{9}{42} \end{pmatrix}. \tag{7.32}$$

Since this $\partial_\lambda f$ is the marginal deformation of the family (7.29), it is a nontrivial cohomology class (this can also be checked directly). As a consequence, the matrix factorization (f,g) is not quasihomogeneous.

It is interesting to ask for a geometric interpretation of this example. For example, one could embed $W=x^3+y^7$ into the appropriate Calabi-Yau Landau-Ginzburg model, and try to identify a mirror Lagrangian cycle. Nonhomogeneity of (f,g) should be mirror to nonvanishing of the Maslov class. Of course, it is not clear to what extent Lagrangians with nonvanishing Maslov anomaly participate in mirror symmetry. The intriguing point is that the limit of (7.29) for $\lambda\to 0$ is actually quasihomogeneous and therefore might have a good mirror. One way to avoid the paradox conclusion that the deformation of a nonanomalous Lagrangian is anomalous would be to show that the brane described by this factorization is never stable on the moduli space. (It is unstable in the Landau-Ginzburg model, as the examples in Sec. VII E.)

VIII. SUMMARY

For convenience and definiteness, we shall here give a summary of the main ingredients that are proposed to enter into a stability condition for matrix factorizations.

As explained in Sec. II, the physical origin of stability conditions in string theory is the grading by worldsheet R-charge. In the context of matrix factorizations, which originate in local commutative algebra, it is also quite natural to consider the graded situation, so it would not seem that physics has much input to give. Before repeating the claim that it does, it is worthwhile to fix the convenient normalization of the grading: Physics suggests a normalization in which W has charge 2, giving the field variables fractional charge, whereas a more standard mathematical choice is to make all degrees integer.

With this in mind, we have associated to any matrix factorization

$$Q^2 = W$$

of a Landau-Ginzburg potential W, satisfying the anomaly free condition that $EQ-Q$ is cohomologically trivial, a matrix R, defined by the conditions (4.8) and (4.20),

$$EQ - Q = [Q,R] \text{ and } \mathrm{Tr}(RV) = 0 \quad \text{whenever} \quad [V,Q] = 0,$$

where we have argued that the latter condition would fix R uniquely. Via (4.11), this induces a grading, q, of the morphism spaces.

The choice of normalization of the grading is important because we intend to compare the grading of morphisms with another natural quantity that can be associated to a Landau-Ginzburg potential, namely the central charge

$$\hat{c}.$$

A mathematical quantity that is closely related to $\hat{c}$ is the so-called "singular index" that appears in singularity theory (see Ref. 61), but it does not seem to have played a crucial role in the purely algebraic context so far.

The basic idea, motivated by Π-stability as we have explained, is to impose the unitarity constraint (2.1)

$$0 \leqslant q \leqslant \hat{c}$$

as a stability condition on the category of topological D-branes.

The problem at this point, which is inherited from Π-stability, is that it is not *a priori* clear exactly *how* to impose this condition. For example, should it be imposed on *all* morphisms, or only on all morphisms involving stable objects? Or should one rather attempt to define the stable branes as a "maximal set" of objects satisfying this (and maybe some other) condition? Although the latter option would seem to depend on too many arbitrary choices, such ambiguities might not be unnecessary. The set of stable objects is expected to be unique only up to autoequivalences of the topological category or monodromies in the moduli space.[2,6]

In the mathematical approach of Ref. 5, the problem is circumvented by postulating the existence of Abelian subcategories at each point in moduli space, on which a stability condition can be imposed in a more standard well-defined form.

We have argued here that there should be a way to identify uniquely a set of stable objects at the Landau-Ginzburg point, essentially because our definition of the grading *does not depend* on the rest of moduli space, and is hence insensitive to monodromies. *A posteriori*, this should also provide an Abelian subcategory.

To gain further confidence that such an approach is possible, we have then proposed a relation to a moduli space problem via a "moment maplike" flow equation (6.12)

$$\frac{dQ}{dt} = -(\langle Q,[V^i,Q]\rangle - \mathrm{Tr}\, RV^i)[V_i,Q],$$

which is expected to provide the split of any given object into its stable constituents. We have implemented this flow in various relevant examples, with reasonable results.

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Homogeneous cosmologies from the quasi-Maxwell formalism

João Costa
Departmento de Métodos Quantitativos, Instituto Superior das Ciências do Trabalho e da Empresa, Portugal

José Natário[a)]
Department of Mathematics, Instituto Superior Técnico, Portugal

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We show how to use the quasi-Maxwell formalism to obtain solutions of Einstein's field equations corresponding to homogeneous cosmologies—namely Einstein's universe, Gödel's universe, and the Ozsvath-Farnsworth-Kerr class I solutions—written in frames for which the associated observers are stationary. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2009587]

I. INTRODUCTION

A particularly intuitive framework for obtaining and interpreting stationary solutions of Einstein's field equations is the so-called *quasi-Maxwell formalism*.[2,5] Although such solutions have been extensively treated in the past,[1,7] this approach has been successfully used in recent times.[3,4] In this paper we apply the quasi-Maxwell formalism in the case when the space manifold is a Lie group with left-invariant metric and fields, and rediscover Einstein's universe, Gödel's universe and the Ozsvath-Farnsworth-Kerr class I solutions, sometimes written in unconventional frames.

The organization of the paper is as follows: In the first section we briefly review the quasi-Maxwell formalism for stationary spacetimes. In the second section we analyze the form taken by the quasi-Maxwell equations when the space manifold is a Lie group. In the third section we further specialize to Lie groups with class A Lie algebras. Finally, solutions of the quasi-Maxwell equations for these space manifold are obtained and identified in the last section.

We use Einstein summation convention, irrespective of the position of the indices (which will often be irrelevant as we will be leading with orthonormal frames on Riemannian manifolds). We will take Latin indices $i, j, \ldots$ to run from 1 to 3.

II. QUASI-MAXWELL FORMALISM

In this section we briefly review the quasi-Maxwell formalism for stationary spacetimes. For more details, see Ref. 5.

Recall that a *stationary spacetime* (M, g) is a Lorentzian four-manifold with a global timelike Killing vector field T. We assume that there exists a global time function $t: M \to \mathbb{R}$ such that $T = \partial/\partial t$. The quotient of M by the integral curves of T is a three-dimensional manifold Σ to which we refer as the *space manifold*. If $\{x^i\}$ are local coordinates in Σ, we can write the line element of (M, g) as

$$ds^2 = -e^{2\phi}(dt + A_i dx^i)^2 + \gamma_{ij} dx^i dx^j$$

where ϕ, A_i, and γ_{ij} do not depend on t. This allows us to interpret ϕ, $A = A_i dx^i$ and $\gamma = \gamma_{ij} dx^i \otimes dx^j$ as tensor fields on the space manifold. It turns out that γ is a Riemannian metric in Σ, independent of the choice of the global time function t. The differential forms $G = -d\phi$ and H

a)Electronic mail: jnatar@math.ist.utl.pt

$=-e^{\phi}\mathrm{d}A$ are also independent of this choice, and play a central role in the so-called *quasi-Maxwell formalism*. We define the *gravitational* and *gravitomagnetic* (vector) fields **G** and **H** through

$$G = \gamma(\mathbf{G}, \cdot\,), \tag{1}$$

$$H = \epsilon(\mathbf{H}, \cdot\,, \cdot\,) \tag{2}$$

where ϵ is a Riemannian volume form in (Σ, γ) (which we assume to be orientable).

We identify a vector $\mathbf{v} \in T_p\Sigma$ with the unique vector field v along the integral curve of T through p which is orthogonal to T and satisfies $\pi_* v = \mathbf{v}$ ($\pi: M \to \Sigma$ being the quotient map). Let $\{X_0, X_i\}$ be a local orthonormal frame on M, where $X_0 = (-g(T,T))^{-1/2}T$. If

$$u = u^0 X_0 + u^i X_i = u^0 X_0 + \mathbf{u}$$

represents the unit tangent vector to a timelike geodesic, the motion equation

$$\tilde{\nabla}_u u = 0$$

is equivalent to

$$\nabla_{\mathbf{u}}\mathbf{u} = u^0(u^0\mathbf{G} + \mathbf{u} \times \mathbf{H})$$

with $u^0 = (1+\mathbf{u}^2)^{1/2}$ (where $\tilde{\nabla}$ is the Levi-Civita connection of (M, g), ∇ is the Levi-Civita connection of (Σ, γ), and $\mathbf{u}^2 = \gamma(\mathbf{u}, \mathbf{u})$).

If we let R_{ij} and $\nabla_i G_j$ represent the components of the Ricci tensor of ∇ and of the covariant derivative of G, Einstein's equations for a perfect fluid with density ρ, pressure p and 4-velocity u reduce to the *quasi-Maxwell equations* (QM)

$$\operatorname{div} \mathbf{G} = \mathbf{G}^2 + \tfrac{1}{2}\mathbf{H}^2 - 8\pi(\rho + p)\mathbf{u}^2 - 4\pi(\rho + 3p), \tag{QM.1}$$

$$\operatorname{curl} \mathbf{H} = 2\mathbf{G} \times \mathbf{H} - 16\pi(\rho + p)u^0\mathbf{u}, \tag{QM.2}$$

$$R_{ij} + \nabla_i G_j = G_i G_j + \tfrac{1}{2}H_i H_j - \tfrac{1}{2}\mathbf{H}^2\gamma_{ij} + 8\pi\left((\rho + p)u_i u_j + \tfrac{1}{2}(\rho - p)\gamma_{ij}\right). \tag{QM.3.ij}$$

We can use QM to solve Einstein's equations by writing down a Riemannian metric for the space manifold (eventually depending on unknown functions), and solving for the fields (see Refs. 2–5). For instance, the Schwarzchild solution is the static solution (i.e., $\mathbf{H}=0$) obtained when we consider a spherically symmetric space manifold with radial **G**.

A word of caution must be issued here: the quasi-Maxwell decomposition does depend on the choice of the timelike Killing vector field T. Therefore when one solves the QM equations, one is really solving for (M, g, T). If a given space-time has a large enough isometry group, it can yield many different solutions of QM.

The goal of this paper is the classification of solutions whose space manifolds are Lie groups with left-invariant metrics, and whose vector fields **G** and **H** are left invariant.

III. QUASI-MAXWELL EQUATIONS FOR A LIE GROUP

Let the space manifold Σ be a three-dimensional Lie group. To choose a left-invariant metric we fix a frame $\{X_i\}$ of left-invariant vector fields and declare it to be orthonormal. All the information about the geometry of the space manifold will then be encoded in the structure constants, defined by

$$[X_i,X_j]=C_{ij}^kX_k=C_{kij}X_k.$$

The last equality emphasizes that there is no need to worry about the vertical position of the indices, as we're working with an orthonormal frame. The Christoffel symbols of the Levi-Civita connection are then given by

$$\Gamma_{jk}^i=\tfrac{1}{2}(C_{ijk}+C_{kij}-C_{jki}).$$

Letting $G=G_i\omega^i$, where $\{\omega^i\}$ is the dual basis of $\{X_i\}$, we have

$$\nabla_iG_j=-\Gamma_{ij}^kG_k.$$

Consequently,

$$\operatorname{div}\mathbf{G}=\nabla_iG_i=-\Gamma_{ii}^kG_k.$$

The Maurer-Cartan formula

$$d\omega^i=-\tfrac{1}{2}C_{jk}^i\omega^j\wedge\omega^k$$

assures us that the exterior derivative is a linear transformation between the spaces $\Omega_L^1(\Sigma)$ and $\Omega_L^2(\Sigma)$ of the left-invariant 1 and 2 forms, whose matrix for the bases $\{\omega^1,\omega^2,\omega^3\}$ of $\Omega_L^1(\Sigma)$ and $\{\omega^2\wedge\omega^3,\omega^3\wedge\omega^1,\omega^1\wedge\omega^2\}$ of $\Omega_L^2(\Sigma)$ is

$$D=\begin{pmatrix}C_{132} & C_{232} & C_{332}\\ C_{113} & C_{213} & C_{313}\\ C_{121} & C_{221} & C_{321}\end{pmatrix}.$$

By definition, curl $\mathbf{H}$ is the only vector field satisfying

$$\epsilon(\operatorname{curl}\mathbf{H},\cdot\,,\cdot\,)=d(\gamma(\mathbf{H},\cdot\,)).$$

Since vectors, 1 and 2 forms are related by the isomorphisms given by the metric and the volume element of Σ, we obtain

$$\operatorname{curl}\mathbf{H}=(X_1X_2X_3)\cdot D\cdot\begin{pmatrix}H_1\\ H_2\\ H_3\end{pmatrix}.$$

The fact that γ, $\mathbf{G}$, and $\mathbf{H}$ are left-invariant imposes restrictions on the fluid generating the gravitational field:

Proposition 2.1: *The density and pressure are constant and* $\mathbf{u}$ *is left invariant.*

Proof: QM.3.*ii* gives us

$$(\rho+p)u_i^2=-\tfrac{1}{2}(\rho-p)+\text{constant}.$$

Adding these three equations we obtain

$$(\rho+p)\mathbf{u}^2=-\tfrac{3}{2}(\rho-p)+\text{constant},$$

which substituted in Eq. QM.1 yields

$$-3(\rho-p)+\rho+3p=\text{constant}\Leftrightarrow 3p-\rho=\text{constant}.$$

From Eq. QM.2 we see that

$$(\rho+p)u^0u_i=\text{constant}\Rightarrow(\rho+p)^2(u^0)^2u_i^2=\text{constant}$$

$$\Leftrightarrow (\rho+p)(\mathbf{u}^2+1)(\rho+p)u_i^2 = \text{constant}$$

$$\Leftrightarrow \left[-\tfrac{3}{2}(\rho-p)+\text{constant}+(\rho+p)\right]\cdot\left[-\tfrac{1}{2}(\rho-p)+\text{constant}\right] = \text{constant}$$

$$\Leftrightarrow \tfrac{1}{4}\rho^2+\tfrac{5}{4}p^2-\tfrac{3}{2}\rho p+\text{first order terms} = \text{constant}.$$

But since $\rho=3p+\text{constant}$, we get

$$-p^2+\text{first order terms} = \text{constant}.$$

We conclude that ρ and p can take at most two distinct values in Σ, and, being so, the result follows from their continuity.

Its now clear that for $\rho+p\neq 0$ the components of $\mathbf{u}$ are constant, which suffices to insure that it is left invariant. For $\rho+p=0$, $\mathbf{u}$ becomes undefined and we can take it to be left invariant (e.g., zero) without loss of generality. □

Corollary 2.2. *The vector field u has the following proprieties*:

$$\widetilde{\operatorname{div}}\, u = 0$$

and

$$\tilde{\nabla}_u u = 0.$$

Proof: We have seen that we only have to consider the case $\rho+p\neq 0$. Euler's equation for a perfect fluid is

$$\widetilde{\operatorname{div}}\, T = 0 \Leftrightarrow \begin{cases} \widetilde{\operatorname{div}}(\rho u) + p\,\widetilde{\operatorname{div}}\, u = 0 \\ (\rho+p)\tilde{\nabla}_u u = -(\widetilde{\operatorname{grad}}\, p)^{\perp} \end{cases}$$

where $(\widetilde{\operatorname{grad}}\, p)^{\perp}$ designates the component of $\widetilde{\operatorname{grad}}\, p$ orthogonal to u. Since ρ and p are constant with $\rho+p\neq 0$, it follows that

$$\begin{cases} (\rho+p)\widetilde{\operatorname{div}}\, u = 0 \\ (\rho+p)\tilde{\nabla}_u u = 0 \end{cases} \Leftrightarrow \begin{cases} \widetilde{\operatorname{div}}\, u = 0 \\ \tilde{\nabla}_u u = 0. \end{cases}$$

□

Corollary 2.3: *The vector fields* $\mathbf{u}$ *and* $\mathbf{G}$ *are orthogonal.*

Proof: The motion equation yields

$$\tilde{\nabla}_u u = 0 \Rightarrow \nabla_{\mathbf{u}}\mathbf{u} = u^0(u^0\mathbf{G}+\mathbf{u}\times\mathbf{H}).$$

Since $\mathbf{u}$ is left invariant and u^0 is a nonzero constant,

$$0 = \frac{\mathrm{d}}{\mathrm{d}\tau}\gamma(\mathbf{u},\mathbf{u}) = 2\gamma(\nabla_{\mathbf{u}}\mathbf{u},\mathbf{u}) = 2(u^0)^2\gamma(\mathbf{G},\mathbf{u}) \Rightarrow \gamma(\mathbf{G},\mathbf{u}) = 0.$$

□

The following result relates solutions corresponding to conformally related left-invariant metrics.

Proposition 2.4. (Rescaling Lemma): *From a solution* (G_i,H_j,u_k,ρ,p) *of QM, where the left-invariant metric is associated to the frame* $\{X_i\}$, *we can construct a solution* $(\hat{G}_i,\hat{H}_j,\hat{u}_k,\hat{\rho},\hat{p})$ *for the left-invariant metric associated to the frame* $\{\hat{X}_i=\lambda X_i\}$, *by setting*

$$\hat{G}_i = \lambda G_i,$$

$$\hat{H}_j = \lambda H_j,$$

$$\hat{u}_k = u_k,$$

$$\hat{\rho} = \lambda^2 \rho,$$

$$\hat{p} = \lambda^2 p.$$

Proof: Since

$$[\hat{X}_i, \hat{X}_j] = \lambda^2 [X_i, X_j] = \lambda^2 C_{kij} X_k = \lambda C_{kij} \hat{X}_k,$$

we obtain

$$\hat{C}_{kij} = \lambda C_{kij},$$

from which follows

$$\hat{\Gamma}^i_{jk} = \lambda \Gamma^i_{jk} \quad \text{and} \quad \hat{D} = \lambda D$$

and consequently

$$\hat{R}_{ij} = \lambda^2 R_{ij}, \quad \widehat{\operatorname{div}}\, \hat{G} = \lambda^2 \operatorname{div} G, \quad \widehat{\operatorname{curl}}\, \hat{H} = \lambda^2 \operatorname{curl} H.$$

Since that, by construction, $\hat{\gamma}_{ij} = \gamma_{ij} = \delta_{ij}$, the result follows. □

It is easy to see that this rescaling corresponds to rescaling the full space-time metric by $1/\lambda^2$.

IV. CLASS A LIE ALGEBRAS

If we take Σ to be connected and simply connected, Lie's theorem[9] guarantees that the space manifold will be uniquely determined, up to isomorphism, by its Lie algebra. Therefore, the consideration of all possible space manifolds becomes the classification of three-dimensional Lie algebras—a much simpler task!

Following Ref. 8, we learn that this classification may be realized by means of a (2/0) symmetric tensor M and a covector $\nu \in \ker M$, whose components in a given basis for the Lie algebra are $\nu_i = C^k_{ki}$. It becomes natural to divide the classification in two classes: class A for Lie algebras with $\nu = 0$, and class B for Lie algebras with $\nu \neq 0$.

We shall restrict ourselves to class A algebras. These are classified by the rank and signature of the symmetric tensor M, and are six in total: the abelian algebra (corresponding to rank $M = 0$), the Heisenberg algebra (corresponding to rank $M = 1$), the semidirect products $\mathfrak{so}(1,1) \ltimes \mathbb{R}^2$ and $\mathfrak{so}(2) \ltimes \mathbb{R}^2$ (corresponding to the two possible signatures for rank $M = 2$) and the simple algebras $\mathfrak{sl}(2)$ and $\mathfrak{so}(3)$ (corresponding to the two possible signatures for rank $M = 3$). In terms of the more usual Bianchi classification, these are Bianchi types I, II, VI with parameter $h = -1$, VII with parameter $h = 0$, VIII and IX, respectively (see Refs. 6 and 7).

Since $C^k_{ki} = 0$, M can be identified, using the left-invariant metric on which the Lie algebra basis is orthonormal, with minus the linear operator yielding the exterior derivative restricted to Ω^1_L. Therefore, class A Lie algebras are classified by the rank and signature of the matrix D of the previous section. This matrix is also useful for computing the Ricci tensor:

Proposition 3.1: *In a Lie group with class A Lie algebra and left-invariant metric, the matrix of components of the Ricci tensor in the basis* $\{\omega^i \otimes \omega^j\}$, *where* $\{\omega^i\}$ *is an orthonormal left-invariant co-frame, is given by*

$$(R_{ij}) = D^2 - \tfrac{1}{2}\mathrm{tr}(D^2)I + \mathrm{cof}(D).$$

The proof of this result is straightforward but lengthy and will be omitted.

Since D is symmetric, we are guaranteed the existence of a left-invariant orthonormal coframe $\{\omega_i\}$ for which

$$D = \mathrm{diag}(C_{132}, C_{213}, C_{321}).$$

Consequently, we can eliminate two unknowns in QM:

Proposition 3.2: *There exists a left-invariant orthonormal frame* $\{\hat{X}_i\}$ *for which the exterior derivative matrix in the basis* $\{\gamma(\hat{X}_k, \cdot)\}$ *and* $\{\epsilon(\hat{X}_k, \cdot, \cdot)\}$ *is diagonal and* $\mathbf{G} = G\hat{X}_1$.

Proof: Choose $\{X_i\}$ such that $D = \mathrm{diag}(a,b,c)$ and let $\mathbf{G} = G_i X_i$. Since G is a closed 1 form, we get

$$\mathrm{d}G = \mathrm{d}(\gamma(\mathbf{G}, \cdot)) = 0 \Leftrightarrow aG_1X_1 + bG_2X_2 + cG_3X_3 = 0.$$

Rearranging the indices if necessary, the last equation tells us that:

(1) $\mathrm{rank}(D) = 3 \Rightarrow a,b,c \neq 0 \Rightarrow \mathbf{G} = \mathbf{0}$;
(2) $\mathrm{rank}(D) = 2 \Rightarrow a = 0, b, c \neq 0 \Rightarrow G_2 = G_3 = 0$;
(3) $\mathrm{rank}(D) = 1 \Rightarrow a, b = 0, c \neq 0 \Rightarrow G_3 = 0 \Rightarrow \mathbf{G} \perp X_3$. For the nontrivial case (i.e., $\mathbf{G} \neq \mathbf{0}$) it suffices to choose $\hat{X}_1 = \frac{1}{\|\mathbf{G}\|}\mathbf{G}$, $\hat{X}_3 = X_3$ and $\hat{X}_2$ in such a way as to complete the basis as an orthonormal basis;
(4) $\mathrm{rank}(D) = 0$: identical to (3).

□

We end this section with three useful results easily proved from the diagonalization of the exterior derivative matrix.

Proposition 3.3: *Left-invariant vector fields have vanishing divergence*.

Proof: If we choose a basis for which D is diagonal, we conclude that the only structure constants not necessarily zero are those with no repeated indices, and consequently

$$\Gamma^i_{jk} \neq 0 \Rightarrow (i,j,k) \text{ is a permutation of } (1,2,3).$$

The result then follows from the equation

$$\mathrm{div}\,\mathbf{G} = -\Gamma^k_{ii} G_k.$$

□

Equivalently, we have

Proposition 3.4: $d(\Omega_L^2) = 0$.

Corollary 3.5: $\mathbf{G}$ *and* $\mathbf{H}$ *are orthogonal*.

Proof: Since H is a left-invariant 2 form, the last result tells us that

$$\mathrm{d}H = 0 \Leftrightarrow d(-e^{\phi}\mathrm{d}A) = 0$$

$$\Leftrightarrow -e^{\phi} d\phi \wedge \mathrm{d}A - e^{\phi}\mathrm{d}(\mathrm{d}A) = 0$$

$$\Leftrightarrow G \wedge H = 0.$$

Using Proposition 3.2, we get

$$G_1\omega^1 \wedge (H_1\omega^2 \wedge \omega^3 + H_2\omega^3 \wedge \omega^1 + H_3\omega^1 \wedge \omega^2) = 0$$

$$\Leftrightarrow G_1H_1\omega^1 \wedge \omega^2 \wedge \omega^3 = 0 \Leftrightarrow G_1H_1 = 0 \Leftrightarrow \gamma(\mathbf{G},\mathbf{H}) = 0.$$

□

V. CLASSIFICATION

For now on we will consider only orthonormal bases $\{X_i\}$ of left-invariant vector fields for the class A Lie algebras of the space manifold such that $D=\mathrm{diag}(a,b,c)$. From Proposition 3.1 we have

$$(R_{ij})=\mathrm{diag}\left(\tfrac{1}{2}a^2-\tfrac{1}{2}b^2-\tfrac{1}{2}c^2+bc,-\tfrac{1}{2}a^2+\tfrac{1}{2}b^2-\tfrac{1}{2}c^2+ac,-\tfrac{1}{2}a^2-\tfrac{1}{2}b^2+\tfrac{1}{2}c^2+ab\right)$$

A. Vacuum solutions with cosmological constant

For convenience, we begin with the computation of QM solutions such that $\rho+p=0$. These correspond to vacuum solutions with cosmological constant.

Proposition 4.1. *The only QM vacuum solution with cosmological constant ($\rho+p=0$) is Minkowski spacetime, i.e.*, $\mathbf{G}=\mathbf{H}=0$ *and* $\rho=p=0$. *The space manifold is then Ricci-flat (Ricci* $=0$*), and hence we necessarily have* $D=\mathrm{diag}(0,b,b)$ *for some* $b\in\mathbb{R}$ *in an appropriate basis of the space manifold's Lie algebra.*

Proof: Let $\rho+p=0$. The indefiniteness of $\mathbf{u}$ allows us to assume, without loss of generality (wlg), that $\mathbf{u}=0$. From the motion equation we get

$$0=(u^0)^2\mathbf{G}=0\Leftrightarrow\mathbf{G}=0.$$

Therefore,

$$\mathrm{QM}.1\Leftrightarrow 0=\tfrac{1}{2}\mathbf{H}^2-4\pi(\rho+3p)\Leftrightarrow\mathbf{H}^2=16\pi p.$$

Since (R_{ij}) is diagonal,

$$\mathrm{QM}.3\,.\,ij(i\neq j)\Leftrightarrow 0=H_iH_j.$$

Therefore, two of the components of $\mathbf{H}$ must vanish. Taking, wlg, $\mathbf{H}=HX_1$ and writing $D=\mathrm{diag}(a,b,c)$, we get

$$QM.2\Leftrightarrow D\cdot\mathbf{H}=0\Leftrightarrow aH=0.$$

If $H=0$, we obtain $p=0\Rightarrow\rho=0$.

If $a=0$,

$$\mathrm{QM}.3\,.\,ii(i\neq 1)\Leftrightarrow R_{22}=R_{33}=-\tfrac{1}{2}\mathbf{H}^2+4\pi(\rho-p)=4\pi(\rho-3p).$$

But

$$R_{22}=R_{33}\Leftrightarrow\tfrac{1}{2}b^2-\tfrac{1}{2}c^2=-\tfrac{1}{2}b^2+\tfrac{1}{2}c^2\Leftrightarrow b^2=c^2\Rightarrow R_{22}=R_{33}=0,$$

yielding $\rho-3p=0$, and therefore $\rho=p=0$ (hence $H=0$).

Thus the only solution with $\rho+p=0$ is Minkowski spacetime, and verifies Ricci$=0$. From the diagonalization of D, it is easily seen that a space manifold is Ricci-flat if and only if there is a basis for its Lie algebra such that $D=\mathrm{diag}(0,b,b),b\in\mathbb{R}$. □

For the remaining computations we will therefore assume that $\rho+p\neq 0$.

B. Solutions with a flat space manifold

In this section we will compute all solutions of QM with flat space manifold (Σ,γ). Since this is a three-dimensional manifold, the curvature tensor is completely determined by the Ricci tensor, and therefore flatness is equivalent to Ricci-flatness.

Theorem 4.2: *The QM solutions with flat space manifold (i.e., with Ricci*$=0$*) correspond to Lie algebras with a basis for which* $D=\mathrm{diag}(0,b,b),b\in\mathbb{R}$, *and such that*:

(1) *(Gödel's universe)* $b=0$, $\mathbf{G}=\sqrt{16\pi p}X_1$, $\mathbf{H}=\sqrt{32\pi p}X_2$, $\mathbf{u}=X_3$ *and* $\rho=p\in\mathbb{R}^+$;
(2) *(Minkowski spacetime)* $\mathbf{G}=\mathbf{H}=\mathbf{0}$, $p=\rho=0$ *is a solution, for all* $b\in\mathbb{R}$ *(cf. Proposition 4.1).*

Proof: We already saw that Ricci-flatness implies that we can choose $D=\mathrm{diag}(0,b,b), b\in\mathbb{R}$. Arguing as in the demonstration of proposition 3.2, we can take $\mathbf{G}=GX_1$ and $\mathbf{H}=H_1X_1+H_2X_2$.

Suppose first that $\mathbf{G}=\mathbf{0}$. In this case,

$$\mathrm{QM.2}\Leftrightarrow\begin{cases}0=16\pi(\rho+p)u^0u_1\\ bH_2=-16\pi(\rho+p)u^0u_2\\ 0=16\pi(\rho+p)u^0u_3\end{cases}\Rightarrow u_1=u_3=0\Leftrightarrow\mathbf{u}=uX_2.$$

We then have as the only nontrivial equation Eq. QM.3.ij ($i\neq j$)

$$\mathrm{QM.3.12}\Leftrightarrow H_1H_2=0.$$

If $H_1=0$, then $\mathbf{H}=HX_2$. Therefore

$$\mathrm{QM.3}\,.\,ii\Leftrightarrow\begin{cases}0=-\frac{1}{2}H^2+4\pi(\rho-p)\\ 0=\frac{1}{2}H^2-\frac{1}{2}H^2+8\pi(\rho+p)u^2+4\pi(\rho-p)\\ 0=-\frac{1}{2}H^2+4\pi(\rho-p)\end{cases}$$

$$\Leftrightarrow\begin{cases}H^2=8\pi(\rho-p)\\ 8\pi(\rho+p)u^2=-4\pi(\rho-p)=-\frac{1}{2}H^2\end{cases}$$

and

$$\mathrm{QM.1}\Leftrightarrow 0=\tfrac{1}{2}H^2-8\pi(\rho+p)u^2-4\pi(\rho+3p)\Leftrightarrow H^2=4\pi(\rho+3p).$$

Consequently,

$$4\pi(\rho+3p)=8\pi(\rho-p)\Leftrightarrow\rho=5p,$$

and therefore

$$\mathrm{QM.3.22}\Leftrightarrow 8\pi(\rho+p)u^2=-4\pi(\rho-p)\Leftrightarrow 12pu^2=-4p\Rightarrow p=0\Rightarrow\rho=0.$$

If $H_2=0(\Rightarrow\mathbf{H}=HX_1)$, we get

$$\mathrm{QM.3}\,.\,ii\Leftrightarrow\begin{cases}0=4\pi(\rho-p)\\ 0=-\frac{1}{2}H^2+8\pi(\rho+p)u^2+4\pi(\rho-p)\\ 0=-\frac{1}{2}H^2+4\pi(\rho-p)\end{cases}$$

$$\Leftrightarrow\begin{cases}\rho=p\\ \mathbf{u}=\mathbf{H}=\mathbf{0}\end{cases}$$

and

$$\mathrm{QM.1}\Leftrightarrow 0=4\pi(\rho+3p).$$

But since $\rho=p$, we obtain $\rho=p=0$.

Let us now consider the case $\mathbf{G}\neq\mathbf{0}$. From Corollary 3.5 we have

$$\gamma(\mathbf{G},\mathbf{H}) = 0 \Leftrightarrow H_1 = 0 \Leftrightarrow \mathbf{H} = HX_2.$$

If $b=0$,

$$\text{QM.2} \Leftrightarrow \begin{cases} 0 = u_1 \\ 0 = u_2 \\ 0 = 2GH - 16\pi(\rho + p)u^0 u_3 \end{cases} \Leftrightarrow \begin{cases} \mathbf{u} = uX_3 \\ GH = 8\pi(\rho + p)u^0 u \end{cases},$$

and since

$$\begin{aligned} \nabla G &= \nabla_i G_j \omega^i \otimes \omega^j = -\Gamma^k_{ij} G_k \omega^i \otimes \omega^j = -\Gamma^1_{23} G_1 \omega^2 \otimes \omega^3 - \Gamma^1_{32} G_1 \omega^3 \otimes \omega^2 \\ &= -\tfrac{1}{2}(C_{123} + C_{312} - C_{231}) G\omega^2 \otimes \omega^3 - \tfrac{1}{2}(C_{132} + C_{213} - C_{321}) G\omega^3 \otimes \omega^2 \\ &= -\tfrac{1}{2}(0 - b + b) G\omega^2 \otimes \omega^3 - \tfrac{1}{2}(0 + b - b) G\omega^3 \otimes \omega^2 = 0, \end{aligned}$$

equations QM.3ij($i \neq j$) are trivial.

On the other hand,

$$\text{QM.3 . } ii \Leftrightarrow \begin{cases} 0 = G^2 - \dfrac{1}{2}H^2 + 4\pi(\rho - p) \\ 0 = 4\pi(\rho - p) \\ 0 = -\dfrac{1}{2}H^2 + 8\pi(\rho + p)u^2 + 4\pi(\rho - p) \end{cases}$$

$$\Leftrightarrow \begin{cases} G^2 = \dfrac{1}{2}H^2 \Rightarrow H \neq 0 \\ \rho = p \\ 16\pi p u^2 = \dfrac{1}{2}H^2 \end{cases}$$

from which

$$\text{QM.1} \Leftrightarrow 0 = G^2 + \tfrac{1}{2}H^2 - 8\pi(\rho + p)u^2 - 4\pi(\rho + 3p)$$

$$\Leftrightarrow G^2 = 4\pi(\rho + 3p) = 16\pi p \Rightarrow H^2 = 32\pi p \quad \text{and} \quad p > 0.$$

Consequently,

$$16\pi p u^2 = \tfrac{1}{2}H^2 = 16\pi p \Leftrightarrow u^2 = 1.$$

Equation QM.2.3 is immediately satisfied if we respect its only imposition: $GHu > 0$. It can be shown that this solution is in fact Gödel's universe (see Sec. V F).

We are now left with the case $\mathbf{G} \neq \mathbf{0}$, $b \neq 0$. We have

$$\text{QM.2} \Leftrightarrow \begin{cases} 0 = u_1 \\ bH = -16\pi(\rho + p)u^0 u_2 \\ 0 = 2GH - 16\pi(\rho + p)u^0 u_3 \end{cases}$$

Since $\nabla G=0$, $\mathbf{H}=HX_2$ and $u_1=0$, all of the QM.3 . ij ($i \neq j$) are trivial with the exception of

$$\text{QM.3.23} \Leftrightarrow \text{QM.3.32} \Leftrightarrow 0 = 8\pi(\rho + p)u_2 u_3 \Leftrightarrow 0 = u_2 u_3.$$

But since the components of $\mathbf{u}$ are constant,

$$\nabla_{\mathbf{u}}\mathbf{u} = u_i u_j \nabla_{X_i} X_j = u_2 u_3 (\nabla_{X_2} X_3 + \nabla_{X_3} X_2) = 0.$$

If $u_3 = 0$ we obtain $\mathbf{u}$ parallel to $\mathbf{H}$ and hence

$$\text{motion equation} \Leftrightarrow 0 = (u^0)^2 G \Leftrightarrow G = 0,$$

yielding a contradiction.

If $u_2 = 0$, $QM.2.2 \Rightarrow H = 0$ and again the motion equation will lead us to $G = 0$. Therefore we must have $b = 0$ whenever $\mathbf{G} \neq \mathbf{0}$. □

C. Solutions for Lie algebras with rank $D = 3$

It is easily seen that a change of basis from $\{X_1, X_2, X_3\}$ to $\{-X_1, X_2, X_3\}$ changes the exterior derivative matrix from $D = \text{diag}(a, b, c)$ to $D = \text{diag}(-a, -b, -c)$. Therefore we can assume wlg that $a > 0$.

Theorem 4.3: *The QM solutions with* rank $D = 3$ *correspond to Lie algebras with a basis such that* $a > 0$ *and*:

(1) *(Einstein's universe)* $D = \text{diag}(a, b, b)$, *with* $b > 0$, $a \geqslant b$, $\mathbf{G} = \mathbf{0}$, $\mathbf{H} = \sqrt{a(a-b)}X_1$, $\mathbf{u} = -\sqrt{(a-b)/b}X_1$ *and* $\rho = -3p = 3ab/32\pi$;

(2) *(Gödel's universe)* $D = \text{diag}(a, b, b)$, *with* $b < 0$, $\mathbf{G} = 0$, $\mathbf{H} = \sqrt{a(a-2b)}X_1$, $\mathbf{u} = -\sqrt{-a/2b}X_1$ *and* $\rho = p = -ab/16\pi$;

(3) *(Ozsvath-Farnsworth-Kerr class I)* $D = \text{diag}(a, b, a-b)$, *with* $16b(a-b) > 3a^2 \Leftrightarrow \frac{1}{4}a < b < \frac{3}{4}a$, $\mathbf{G} = 0$, $\mathbf{H} = \sqrt{4b(a-b) - \frac{1}{2}a^2}X_1$, $\mathbf{u} = -a/\sqrt{16b(a-b) - 3a^2}X_1$, $p = -a^2/64\pi$ *and* $\rho = 32b(a-b) - 5a^2/64\pi$.

Proof: Let $D = \text{diag}(d_1, d_2, d_3)$, with $\Pi_i d_i \neq 0$. Then $\mathbf{G} = 0$, and consequently

$$\text{QM.2} \Leftrightarrow d_i H_i = -16\pi(\rho + p)u^0 u_i \Leftrightarrow H_i = -\frac{16\pi(\rho + p)}{d_i} u^0 u_i$$

(the Einstein summation convention will not apply for the duration of this proof). Therefore,

$$QM.3\,.\,ij(i \neq j) \Leftrightarrow 0 = H_i H_j + 16\pi(\rho + p)u_i u_j$$

$$\Leftrightarrow 0 = \frac{[16\pi(\rho + p)]^2}{d_i d_j}(u^0)^2 u_i u_j + 16\pi(\rho + p)u_i u_j$$

$$\Leftrightarrow 0 = 16\pi(\rho + p)u_i u_j \left(\frac{16\pi(\rho + p)}{d_i d_j}(u^0)^2 + 1 \right)$$

$$\Leftrightarrow 0 = u_i u_j \text{ or } (u^0)^2 = -\frac{d_i d_j}{16\pi(\rho + p)}.$$

We have to consider the following cases.

(1) $u_{i_1} = 0$ and:

(a) $u_{i_2} = 0$;

(b) $(u^0)^2 = -d_{i_2} d_{i_3}/16\pi(\rho + p)$ (where (i_1, i_2, i_3) is an arbitrary permutation of (1, 2, 3));

(2) $(u^0)^2 = -d_i d_j/16\pi(\rho + p)$, for all $i, j \in \{1, 2, 3\}$ with $i \neq j$.

Let us do so:

(1) (a) Suppose, wlg, that $u_2=u_3=0\Rightarrow \mathbf{u}=uX_1$. Then $QM.2\Rightarrow \mathbf{H}=HX_1$, and therefore

$$\text{QM.3 . } ii(i\neq 1)\Leftrightarrow R_{22}=R_{33}=-\tfrac{1}{2}H^2+4\pi(\rho-p).$$

However,

$$R_{22}=R_{33}\Leftrightarrow -\tfrac{1}{2}a^2+\tfrac{1}{2}b^2-\tfrac{1}{2}c^2+ac=-\tfrac{1}{2}a^2-\tfrac{1}{2}b^2+\tfrac{1}{2}c^2+ab$$

$$\Leftrightarrow b^2-c^2+ac-ab=0$$

$$\Leftrightarrow (b-c)(b+c)-a(b-c)=0$$

$$\Leftrightarrow (b-c)(b+c-a)=0$$

$$\Leftrightarrow c=b \text{ or } c=a-b,$$

which leads us to the consideration of two subcases:

(i) $c=b$;
(ii) $c=a-b$.

Let us do so:

(i) We have $D=\mathrm{diag}(a,b,b)$. The Rescaling Lemma (Proposition 2.4) allows us to choose $a=1$. Let $\Omega=8\pi(\rho+p)\neq 0$. The QM equations are:

$$\text{QM.1}\Leftrightarrow \tfrac{1}{2}H^2=\Omega\, u^2+\tfrac{1}{2}\Omega+8\pi p;$$

$$\text{QM.2}\Leftrightarrow H=-2\Omega\, u^0 u;$$

$$\text{QM.3 . } ij\ (i\neq j) \text{ are already satisfied;}$$

$$\text{QM.3 . } ii\Leftrightarrow \begin{cases} R_{11}=\tfrac{1}{2}=\Omega\, u^2+4\pi(\rho-p) \\ R_{22}=R_{33}=b-\tfrac{1}{2}=-\tfrac{1}{2}H^2+4\pi(\rho-p) \end{cases}$$

We then have

$$\text{QM.3.11 + QM.3.22}\Leftrightarrow b=-\tfrac{1}{2}H^2+\Omega u^2+8\pi(\rho-p).$$

Inserting QM.1 in the last equation yields

$$b=-\Omega\, u^2-\tfrac{1}{2}\Omega-8\pi p+\Omega\, u^2+8\pi(\rho-p)$$

$$\Leftrightarrow b=-\tfrac{1}{2}\Omega-8\pi p+8\pi(\rho+p)-16\pi p=\tfrac{1}{2}\Omega-24\pi p$$

$$\Leftrightarrow p=\frac{1}{24\pi}\left(\tfrac{1}{2}\Omega-b\right).$$

On the other hand,

$$\text{QM.3.11}\Leftrightarrow \Omega\, u^2=\tfrac{1}{2}-4\pi(\rho-p)=\tfrac{1}{2}-4\pi(\rho+p)+8\pi p=\tfrac{1}{2}-\tfrac{1}{3}\Omega-\tfrac{1}{3}b.$$

Therefore,

$$u^2 = \frac{3-2b}{6\Omega} - \frac{1}{3}.$$

Similarly,

$$\mathrm{QM}.1 \Leftrightarrow H^2 = \frac{2}{3}(\Omega - 2b) + 1.$$

Now

$$\mathrm{QM}.2 \Leftrightarrow H = -2\,\Omega\,u^0 u$$

$$\Rightarrow H^2 = 4\,\Omega^2 (u^0)^2 u^2 \Leftrightarrow \frac{1}{4\,\Omega^2} H^2 = u^4 + u^2$$

$$\Leftrightarrow \frac{1}{4\,\Omega^2}\left(\frac{2}{3}(\Omega - 2b) + 1\right) - \left(\frac{3-2b}{6\Omega} - \frac{1}{3}\right)^2 - \left(\frac{3-2b}{6\Omega} - \frac{1}{3}\right) = 0$$

$$\Leftrightarrow \left(-\frac{b}{3} + \frac{1}{4} - \frac{(3-2b)^2}{36}\right)\frac{1}{\Omega^2} + \left(\frac{1}{6} + \frac{6-4b}{18} + \frac{2b-3}{6}\right)\frac{1}{\Omega} + \frac{2}{9} = 0$$

$$\Leftrightarrow -b^2 \frac{1}{\Omega^2} + b\frac{1}{\Omega} + 2 = 0 \Leftrightarrow \frac{1}{\Omega} = \frac{-b \pm 3b}{-2b^2}$$

$$\Leftrightarrow \Omega = \frac{b}{2} \text{ or } \Omega = -b.$$

Let $\Omega = b/2$. We easily obtain

$$H^2 = 1 - b;$$

$$u^2 = \frac{1-b}{b};$$

$$p = -\frac{b}{32\pi};$$

$$\rho = -3p.$$

To obtain the general solution, i.e., for $D = \mathrm{diag}(a,b,b)$, we have to use the Rescaling Lemma. We have

$$H^2(a,b,b) = a^2 H^2\left(1, \frac{b}{a}, \frac{b}{a}\right) = a^2\left(1 - \frac{b}{a}\right) = a(a-b)$$

yielding the condition $a \geqslant b$. Similarly,

$$u^2(a,b,b) = u^2\left(1, \frac{b}{a}, \frac{b}{a}\right) = \frac{1 - b/a}{b/a} = \frac{a-b}{b},$$

yielding the condition $b > 0$. *QM*.2 requires only that H and u satisfy $Hu \leqslant 0$. Finally,

$$p(a,b,b) = a^2\left(-\frac{b/a}{32\pi}\right) = -\frac{ab}{32\pi}.$$

It can be shown that all these solutions of QM are in fact Einstein's universe in different frames (see Sec. V F).

If $\Omega=-b$, the procedure above yields the second family of solutions, corresponding to Gödel's universe.

(ii) We have $D=\mathrm{diag}(a,b,a-b)$. Let us set $a=1$. The only changes with respect to the previous case occur in

$$\mathrm{QM.3}\,.\,ii \Leftrightarrow \begin{cases} R_{11} = 2b(1-b) = 8\pi(\rho+p)u^2 + 4\pi(\rho-p) \\ R_{22} = R_{33} = 0 = -\frac{1}{2}H^2 + 4\pi(\rho-p) \Leftrightarrow H^2 = 8\pi(\rho-p) \end{cases}.$$

From the last equation we obtain

$$\mathrm{QM.1} \Leftrightarrow 4\pi(\rho-p) = 8\pi(\rho+p)u^2 + 4\pi(\rho+3p)$$

$$\Leftrightarrow 8\pi(\rho+p)u^2 = -16\pi p$$

$$\Leftrightarrow u^2 = -\frac{2p}{\rho+p}$$

$$\Rightarrow (p \leqslant 0 \quad \text{and} \quad \rho+p>0) \text{ or } (p \geqslant 0 \quad \text{and} \quad \rho+p<0).$$

The second condition implies $\rho-p<-2p\leqslant 0$, contradicting $H^2=8\pi(\rho-p)$. Since $\rho+p>0$, H and u must have opposite signs and

$$\mathrm{QM.2} \Leftrightarrow \sqrt{8\pi(\rho-p)} = 16\pi(\rho+p)\sqrt{1-\frac{2p}{\rho+p}}\sqrt{\frac{-2p}{\rho+p}}$$

$$\Leftrightarrow \rho - p = 64\pi p(p-\rho).$$

But $\rho-p=0 \Rightarrow H=0 \overset{QM.2}{\Rightarrow} u=0 \overset{QM.3.11}{\Rightarrow} R_{11}=0 \Leftrightarrow bc=0$, which is absurd. We then have

$$p = -\frac{1}{64\pi}$$

and

$$\mathrm{QM.3.11} \Leftrightarrow \rho = \frac{32b(1-b)-5}{64\pi}.$$

From the above-mentioned equations we can then obtain the expression for H^2 and u^2, in the special case $a=1$. To obtain the general solution and the restrictions over a and b, we proceed as in the previous case. This third family of solutions can be shown to be the Ozsvath-Farnsworth-Kerr class I family of solutions.

(b) Let $u_1=0(\Rightarrow H_1=0)$ and $(u^0)^2=-bc/16\pi(\rho+p)$. We will prove that there are no solutions satisfying these hypotheses. We start by checking that

$\mathbf{u}^2+1=-bc/16\pi(\rho+p) \Leftrightarrow 8\pi(\rho+p)\mathbf{u}^2=-1/2bc-8\pi(\rho+p)$, and hence

$$\mathrm{QM.1} \Leftrightarrow \mathbf{H}^2 = -bc - 8\pi(\rho-p).$$

On the other hand,

$$\text{QM.3.11} \Leftrightarrow 8\pi(\rho - p) = R_{11} - \tfrac{1}{2}bc$$

and so

$$\text{QM.3.22} + \text{QM.3.33} \Leftrightarrow R_{22} + R_{33} = 4\pi(\rho - p) - 16\pi p$$

$$\Leftrightarrow p = \frac{2R_{11} - 4R_{22} - 4R_{33} - bc}{64\pi}.$$

It is now immediate that

$$\rho = \frac{10R_{11} - 4R_{22} - 4R_{33} - 5bc}{64\pi}.$$

On the other hand,

$$QM.2 \Leftrightarrow \begin{cases} bH_2 = -16\pi(\rho + p)u^0 u_2 \\ cH_3 = -16\pi(\rho + p)u^0 u_3 \end{cases} \Rightarrow \begin{cases} b^2(H_2)^2 = [16\pi(\rho + p)]^2 (u^0)^2 (u_2)^2 \\ c^2(H_3)^2 = [16\pi(\rho + p)]^2 (u^0)^2 (u_3)^2 \end{cases}$$

$$\Leftrightarrow \begin{cases} (H_2)^2 = -16\pi(\rho + p)\dfrac{c}{b}(u_2)^2 \\ (H_3)^2 = -16\pi(\rho + p)\dfrac{b}{c}(u_3)^2 \end{cases}.$$

Using $(\text{QM.2.2})^2$, we get

$$\text{QM.3.22} \Leftrightarrow R_{22} = \frac{1}{2}(H_2)^2 - \frac{1}{2}\mathbf{H}^2 + 8\pi(\rho + p)(u_2)^2 + 4\pi(\rho - p)$$

$$\Leftrightarrow \left(1 - \frac{c}{b}\right) 8\pi(\rho + p)(u_2)^2 = R_{22} - R_{11}.$$

It is easily checked that there are no solutions with $b = c$, and hence

$$8\pi(\rho + p)(u_2)^2 = \frac{b}{b - c}(R_{22} - R_{11}).$$

As a consequence of $(\text{QM.2.2})^2$, we have

$$(H_2)^2 = \frac{2c}{c - b}(R_{22} - R_{11}).$$

A similar procedure will give us

$$8\pi(\rho + p)(u_3)^2 = \frac{c}{c - b}(R_{33} - R_{11});$$

$$(H_3)^2 = \frac{2b}{b - c}(R_{33} - R_{11}).$$

From equation

$$(H_2)^2 + (H_3)^2 = -bc - 8\pi(\rho - p)$$

we obtain the restriction

$$-3a^2b + 3a^2c + 4ab^2 - 4ac^2 - b^3 - 4b^2c + 4bc^2 + c^3 = 0.$$

To simplify this last expression we use the Rescaling lemma to set $a=1$ and divide the resulting polynomial equation by $b-c$, thus obtaining

$$b^2 + c^2 + 5bc - 4b - 4c + 3 = 0.$$

We have

$$(u^0)^2 = -\frac{bc}{16\pi(\rho + p)} \Rightarrow bc(\rho + p) < 0.$$

The expression for $(H_3)^2$ implies that $[b/(b-c)](R_{33}-R_{11}) \geqslant 0$, and since $8\pi(\rho+p)(u_2)^2=[b/(b-c)](R_{22}-R_{11}) \Leftrightarrow 8\pi bc(\rho+p)(u_2)^2=[b^2c/(b-c)](R_{22}-R_{11})$, the restriction implied by the expression for $(u^0)^2$ gives us

$$\frac{c}{c-b}(R_{22} - R_{11}) \geqslant 0.$$

If we proceed in a similar fashion using the expressions for $(H_2)^2$ and $8\pi(\rho+p)(u_3)^2$, and then compute the components of the Ricci tensor in terms of a and b, we will obtain the following restrictions:

(i) $b^2+c^2+5bc-4b-4c+3=0$;
(ii) $c(c-b)(b-1)(b-c+1) \geqslant 0$;
(iii) $b(b-c)(c-1)(c-b+1) \geqslant 0$;
(iv) $bc(\rho+p)<0 \Rightarrow 64\pi bc(\rho+p)<0 \Rightarrow bc[3(b^2+c^2-3bc+4(b+c)-7]>0$.

From (i) we obtain $b^2+c^2=-5bc+4b+4c-3$, which when used in (iv) yields

(iv') $bc(-9bc+8b+8c-8)>0$.

It is now easy to use a geometrical argument to determine the incompatibility of restrictions (ii), (iii) and (iv'): we just have to check that the regions determined in the bc-plane by these restrictions do not intersect.

(2) It is obvious that

$$ab = bc = ac \Leftrightarrow a = b = c.$$

Symmetry allows us to consider $u_2=u_3=0$, and thus we are back to the very first case we analyzed. □

D. Solutions with G=0

The next two results complete the classification of QM class *A* solutions with zero gravitational field.

Proposition 4.4: *There are no class A QM solutions with zero gravitational field corresponding to Lie algebras with rank D*=1.

Proof: Let $D=\mathrm{diag}(0,0,1)$. Symmetry allows us to take $\mathbf{H}=H_2X_2+H_3X_3 \overset{\text{QM.2}}{\Rightarrow} \mathbf{u}=uX_3$. Therefore, QM.3.23 $\Leftrightarrow 0=H_2H_3$.

If $H_3=0 \overset{\text{QM.2}}{\Rightarrow} \mathbf{u}=0$, we have

$$\text{QM.3 . } ii \Leftrightarrow \mathbf{H}^2 = -1.$$

If $H_2=0$, we have

$$\text{QM.3 . } ii \Leftrightarrow \begin{cases} H^2 = 8\pi(\rho - p) + 1 \\ 8\pi(\rho + p)u^2 = \dfrac{1}{2} - 4\pi(\rho - p) \end{cases}$$

and

$$QM.1 \Leftrightarrow \rho = 5p \Rightarrow p \neq 0.$$

Using all this in QM.2.2 leads to $p=0$. □

Proposition 4.5: *The only class A solution of QM with zero gravitational field corresponding to a Lie algebra with* rank $D=2$ *is Minkowski spacetime*.

Proof: We can assume $a=0$. Thus $QM.2 \Rightarrow u_1=0$, and therefore

$$\begin{aligned} \nabla_{\mathbf{u}}\mathbf{u} &= u_2u_3(\Gamma^1_{23} + \Gamma^1_{32})X_1 = \tfrac{1}{2}u_2u_3(C_{123} + C_{312} - C_{231} + C_{132} + C_{213} - C_{321})X_1 \\ &= \tfrac{1}{2}u_2u_3(0 - c + b + 0 + b - c)X_1 = (b-c)u_2u_3X_1. \end{aligned}$$

We then have

$$\text{Motion equation} \Leftrightarrow \begin{cases} (b-c)u_2u_3 = u^0(u_2H_3 - u_3H_2) \\ u_3H_1 = 0 \\ u_2H_1 = 0 \end{cases} \Rightarrow H_1 = 0 \text{ or } \mathbf{u} = \mathbf{0}.$$

It can be easily seen that no solutions exist for $\mathbf{u}=\mathbf{0}$, and that solutions featuring $H_1=0$ and $u_2u_3=0$ must verify $b=c$, and hence are Minkowski spacetime (cf. Theorem 4.2).

We are left with the case $H_1=0$ and $u_2u_3 \neq 0$. Using QM.2 we obtain

$$\text{Motion equation} \Leftrightarrow \text{QM.3 . } ij(i \neq j) \Leftrightarrow (u^0)^2 = -\frac{bc}{16\pi(\rho + p)}.$$

The situation is now quite similar to the one in the demonstration of case 1b of Theorem 4.3. Using the same procedure we obtain

$$u_2 = \pm\frac{2\sqrt{3}}{3}\sqrt{\frac{b^2}{-b^2 - c^2 + bc}} \Rightarrow -b^2 - c^2 + bc > 0$$

and

$$H_2 = \pm\sqrt{-2bc} \Rightarrow bc < 0.$$

But

$$1 + (u_2)^2 + (u_3)^2 = -\frac{bc}{16\pi(\rho + p)} \Leftrightarrow b^2 + c^2 + 5bc = 0$$

and, therefore,

$$-b^2 - c^2 + bc > 0 \Leftrightarrow b^2 + c^2 + 5bc - 6bc < 0 \Leftrightarrow bc > 0,$$

yielding a contradiction. □

E. Solutions with G≠0

For solutions with $\mathbf{G} \neq 0$ we can assume $\mathbf{G}=GX_1$ with $G \neq 0$, which implies $H_1=u_1=0$ and $D=\text{diag}(0,b,c)$. It is then easy to see that QM.1+QM.3.22+QM.3.33 yields

$$G^2 + 4\pi(\rho - 5p) = 0.$$

These solutions must of course include the two-parameter family given by

$$H_2 = \sqrt{2}G\cos\theta;$$
$$H_3 = \sqrt{2}G\sin\theta;$$
$$u_2 = -\sin\theta;$$
$$u_3 = \cos\theta;$$
$$p = \rho = \frac{G^2}{16\pi};$$
$$b = c = 0,$$

corresponding to the Gödel universe. Apart from these, one can show that there exist further solutions, belonging to the category 2 of Ozsvath classification (see Sec. V F). Unfortunately, it is not possible to obtain simple expressions for these solutions.

F. Identifying the solutions

Recall that a solution of Einstein's field equations is said to be spacetime homogeneous if it admits a transitive action by isometries. This will happen if, for instance, the solution is a left-invariant metric on a (four-dimensional) Lie group.

The solutions we have been considering have in fact a Lie group structure, as $M = \mathbb{R} \times \Sigma$ and Σ is a three-dimensional Lie group.

Proposition 4.6: *A stationary spacetime* (M, g) *corresponding to a solution of QM for which the space manifold* (Σ, γ) *is a Lie group with a left-invariant Riemannian metric and whose fields* **G** *and* **H** *are left-invariant is a Lie group with a left-invariant Lorentzian metric*.

Proof: One just has to check that

$$\{X_0, X_i\}$$

is a left-invariant orthonormal frame, where $\{X_i\}$ are the vector fields in M associated to a left-invariant orthonormal frame on the space manifold. □

Since all spacetime homogeneous perfect fluid solutions which are left-invariant Lorentzian metrics on a Lie group have been classified (see Refs. 6 and 7), we can use this classification to identify the solutions we have obtained. One must be careful to use frame-independent quantities when comparing solutions; in most cases it suffices to compare the equations of state.

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The recollapse problem of closed Friedmann–Robertson–Walker models in higher-order gravity theories

John Miritzis[a)]
Department of Marine Sciences, University of the Aegean, University Hill, Mytilene, 81100 Greece

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We study the closed universe recollapse conjecture for positively curved Friedmann–Robertson–Walker models with a perfect fluid matter source and a scalar field which arises in the conformal frame of the $R+\alpha R^2$ theory. By including ordinary matter, we extend the analysis of a previous work. We analyze the structure of the resulted four-dimensional dynamical system with the methods of the center manifold theory and the normal form theory. It is shown that an initially expanding closed FRW universe, starting close to the Minkowski space-time, cannot avoid recollapse. We discuss the possibility that potentials with a positive minimum may prevent the recollapse of closed universes. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2009648]

I. INTRODUCTION

A closed Friedmann–Robertson–Walker (FRW) universe is often considered almost synonymous to a recollapsing universe. This is mainly due to our experience with the dust and radiation filled FRW models usually treated in textbooks. That this picture is misleading follows clearly from an example found by Barrow *et al.*[1] according to which an expanding homogeneous and isotropic model with spatial topology S^3 satisfying the weak, the strong, the dominant energy conditions and the generic condition may not recollapse. Thus the problem of recollapse of a closed universe to a second singularity is delicate already in the FRW case.

The *closed-universe recollapse conjecture* states roughly that a closed universe cannot expand forever, provided that the matter content satisfies some energy condition and has nonnegative pressures. The conjecture was found true in certain spatially homogeneous cosmologies,[2] in certain spherically symmetric space-times[3] and in space-times admitting a constant mean-curvature foliation that possesses a maximal hypersurface.[4] In these investigations it has proved useful to demand that the dominant energy condition and the positive pressure criterion hold (see also Ref. 5 for a dynamical system approach).

In this paper we investigate the evolution of positively curved FRW models with a scalar field having the potential which arises in the conformal frame of the $R+\alpha R^2$ theory[6–8] and ordinary matter described by a perfect fluid with energy density ρ and pressure p. The motivation for this choice was presented in Ref. 9. The purpose of the present article is to generalize the results in Ref. 9 by including ordinary matter and to correct the mistake found therein. {In Ref. 9, inequality (11) has the wrong direction [compare with (12) in this paper]. This mistake and a different rescaling [compare with (8)] were the sources of the erroneous conclusion that an initially expanding universe avoids recollapse. In fact, inequality (11) must be reversed and as a consequence, the admissible trajectories of the system (16) start below the line $H=\sqrt{2}r$ in Fig. 1. This implies that an initially expanded closed universe cannot avoid recollapse. Nevertheless, the calculations and the mathematical analysis of the system (12) near the equilibrium (0,0,0) remain correct. Moreover, the above-mentioned mistake does not essentially affect the rest of the paper.}

[a)]Electronic mail: imyr@aegean.gr

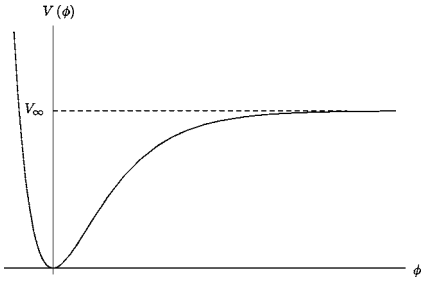

FIG. 1. The potential (5).

The plan of the paper is as follows. In the next section we write down the field equations, as a constrained five-dimensional dynamical system. We use the constraint equation to reduce the dimension of the system to four and after a suitable change of variables the system becomes quadratic. In Sec. III we analyze the structure of the equilibrium corresponding to the de Sitter solution using the methods of the center manifold theory. Further, we find the so-called normal form of the dynamical system describing a large, slowly expanding universe with low total energy density; we show that such a universe cannot avoid recollapse. In the last section, we consider potentials having a strict positive minimum and argue that this class of potentials prevent a closed universe from recollapse.

II. REDUCTION TO A FOUR-DIMENSIONAL QUADRATIC SYSTEM

In General Relativity the evolution of FRW models with a scalar field (ordinary matter is described by a perfect fluid with energy density ρ and pressure p) are governed by the Friedmann equation,

$$\left(\frac{\dot{a}}{a}\right)^2+\frac{k}{a^2}=\frac{1}{3}\left[\rho+\frac{1}{2}\dot{\phi}^2+V(\phi)\right], \tag{1}$$

the Raychaudhuri equation,

$$\frac{\ddot{\alpha}}{a}=-\frac{1}{6}(\rho+3p+2\dot{\phi}^2-2V), \tag{2}$$

the equation of motion of the scalar field,

$$\ddot{\phi}+3\frac{\dot{a}}{a}\dot{\phi}+V'(\phi)=0, \tag{3}$$

and the conservation equation,

$$\dot{\rho}+3(\rho+p)\frac{\dot{a}}{a}=0. \tag{4}$$

We adopt the metric and curvature conventions of Ref. 10. $a(t)$ is the scale factor, an overdot denotes differentiation with respect to time t, and units have been chosen so that $c=1=8\pi G$. Here $V(\phi)$ is the potential energy of the scalar field and $V'=\mathrm{d}V/\mathrm{d}\phi$. We assume an equation of state of the form $p=(\gamma-1)\rho$, with $2/3<\gamma\leqslant 2$.

In what follows we assume that the potential function of the scalar field is

$$V(\phi)=V_\infty(1-e^{-\sqrt{2/3}\phi})^2 \tag{5}$$

which arises in the conformal frame of the $R+\alpha R^2$ theory.[7] The conformal equivalence of $f(R)$ theories to general relativity raises several conceptual problems, for example, does conformal

equivalence imply physical equivalence between the two theories? For an extensive discussion of related issues see Ref. 8 and references therein. For our purposes the conformal transformation is well behaved as far as $f'(R)$ does not vanish.

The flat plateau of this potential is responsible for an early inflationary period of the universe and, for homogeneous spacetimes provides a mechanism of isotropization.[7,11] From the field equations it is easy to see that in an expanding universe the energy density of the scalar field, namely

$$E = \tfrac{1}{2}\dot{\phi}^2 + V(\phi)$$

is a decreasing function of time. Since the energy density, ρ, of ordinary matter also decreases, it may happen that in a future time, E be comparable to ρ. In particular, for closed, $k=1$, models, once the scale factor reaches its maximum value and recollapse commences i.e., $H<0$, the term $3H\dot{\phi}$ in (3) is no longer a damping factor, but acts as a driving force which forces the field ϕ to oscillate with larger and larger amplitude. If this be the case, the repulsive effect of the cosmological term may drastically change the evolution of a classical FRW model.

Setting $\dot{\phi} =: y$, $\dot{a}/a =: H$, we obtain from (1) the constraint equation

$$3H^2 + 3k/a^2 = \rho + \tfrac{1}{2}y^2 + V(\phi), \tag{6}$$

which we use to eliminate a from the evolution equations (2)–(4). As a consequence, the dimension of the dynamical system is reduced to four and we obtain

$$\begin{aligned} \dot{\phi} &= y, \\ \dot{y} &= -3Hy - V'(\phi), \\ \dot{\rho} &= -3\gamma\rho H, \\ \dot{H} &= \frac{1}{3}V(\phi) - \frac{1}{3}y^2 - \frac{3\gamma-2}{6}\rho - H^2. \end{aligned} \tag{7}$$

We remind the reader that the exponential potential which is popular in the literature of scalar-field cosmologies has the nice property that $V' \propto V$, which allows the introduction of normalized variables according to the formalism of Wainwright and Ellis.[10] For an exponential potential the dimension of the dynamical system for a closed FRW model reduces to three.[12]

We simplify the system by rescaling the variables by the equations

$$\phi \to \sqrt{3/2}\phi, \quad y \to \sqrt{2V_\infty}y, \quad \rho \to \frac{4V_\infty}{3}\rho, \quad H \to \sqrt{\frac{4V_\infty}{3}}H, \quad t \to \sqrt{\frac{3}{4V_\infty}}t. \tag{8}$$

Further, in order to take into account the equilibrium point corresponding to the point at "infinity" and to remove the transcendental functions, it is convenient to introduce the variable u defined by

$$u := e^{-\phi}, \tag{9}$$

and system (7) finally becomes

$$\begin{aligned} \dot{u} &= -uy, \\ \dot{y} &= -u + u^2 - 3Hy, \\ \dot{\rho} &= -3\gamma\rho H, \end{aligned}$$

$$\dot{H} = \frac{1}{4}(1-u)^2 - \frac{1}{2}y^2 - \frac{3\gamma - 2}{6}\rho - H^2. \tag{10}$$

Note that under the transformation (9), the resulted four-dimensional dynamical system (10) is quadratic.

Remark: The system (10) is not an arbitrary "free" four-dimensional system. In view of (6) the initial conditions have to satisfy the condition $3H_0^2 - \rho - \frac{1}{2}y_0^2 - V(\phi_0) < 0$, or, in terms of the new variables,

$$H_0^2 - \frac{1}{3}\rho - \frac{1}{4}y_0^2 - \frac{1}{4}(1-u_0)^2 < 0. \tag{11}$$

With a little manipulation of the equations (10) it can be shown that, once we start with initial conditions satisfying at time t_0 the inequality (11), the solutions of the system satisfy

$$H(t)^2 - \tfrac{1}{3}\rho(t) - \tfrac{1}{4}y(t)^2 - \tfrac{1}{4}(1-u(t))^2 < 0$$

for all $t > t_0$. This is a general property of the Einstein equations, namely that the subsequent evolution of the system is such that the solutions respect the constraint. We conclude that the phase space of the system (10) is the set

$$\Sigma := \left\{(u,y,\rho,H) \in \mathbb{R}^4 : H^2 - \tfrac{1}{3}\rho - \tfrac{1}{4}y^2 - \tfrac{1}{4}(1-u)^2 < 0\right\}. \tag{12}$$

III. STABILITY ANALYSIS

There are several equilibrium points of (10). Some of them correspond to static universes with a cosmological constant equal to $\sqrt{V_\infty}$. In the study of the equilibrium points we note that $u=1$ corresponds to $\phi=0$, i.e., to the minimum of the potential and $u=0$ corresponds to $\phi=\infty$, i.e., to the flat plateau of the potential. In the following we pay attention to the most interesting equilibrium solutions which are as follows.

EQ1: $(u=0, y=0, \rho=0, H=1/2)$. This corresponds to the de Sitter universe with a cosmological constant equal to $\sqrt{V_\infty}$. We analyze the flow of (10) near EQ1 in the next subsection.

EQ2: $(u=1, y=0, \rho=0, H=0)$. This corresponds to the limiting state of an ever-expanding universe with $H \to 0$ while the scalar field approaches the minimum of the potential and the scale factor goes to infinity. Equality in (12) which arises from the flat, $k=0$, case defines a set on the boundary of Σ. We conclude that the point EQ2 which corresponds to the Minkowski solution, is located on this boundary. The detailed structure of this equilibrium will be analyzed in Sec. III B.

As we shall see, both equilibria are non-hyperbolic, i.e., some or all of the eigenvalues of the Jacobian have zero real parts. That means that the linearization theorem does not yield any information about the stability of the equilibria and therefore, more powerful methods are needed. The study of the qualitative behaviour of a dynamical system near a nonhyperbolic equilibrium point is difficult even in two dimensions. There are two general methods for simplifying a dynamical system having a nonhyperbolic equilibrium. The first is the center manifold theory. According to the center manifold theorem, the qualitative behavior in a neighborhood of a nonhyperbolic equilibrium point $\mathbf{q}$ is determined by its behavior on the center manifold near $\mathbf{q}$. Since the dimension of the center manifold is generally smaller than the dimension of the dynamical system, this greatly simplifies the problem (cf. Refs. 13 and also 14 for cosmological applications). The second method is the normal form theory, which consists in a nonlinear coordinate transformation that allows to simplify the nonlinear part of the system (cf. Ref. 13 for a brief introduction). Both methods are used in the next two subsections.

A. Center manifold for the system at EQ1

It is easy to see that at the equilibrium point $\mathbf{q}=(u=0, y=0, \rho=0, H=1/2)$, the Jacobian matrix of (10) has one zero and three negative eigenvalues and, consequently the Hartman-Grobman

theorem does not apply. The center manifold theorem implies that there exists a local three-dimensional stable manifold through $\mathbf{q}$ (see, e.g., Ref. 13). That means that all trajectories asymptotically approaching $\mathbf{q}$ as $t\to\infty$, lie on a three-dimensional invariant manifold. Since $\mathbf{q}$ is a nonhyperbolic fixed point, the topology of the flow near $\mathbf{q}$ is nontrivial and is characterized by a one-dimensional local center manifold containing $\mathbf{q}$. We prove the following result.

Proposition: The equilibrium point $\mathbf{q}=(0,0,0,1/2)$ *of* (10) *is locally asymptotically unstable*.

In order to determine the local center manifold of (10) at $\mathbf{q}$, we have to transform the system into a form suitable for the application of the center manifold theorem. The procedure is fairly systematic and will be accomplished in the following steps.

1. The Jacobian of (10) at $\mathbf{q}=(0,0,0,1/2)$ has eigenvalues 0, -1, $-3/2$, and $-3\gamma/2$ with corresponding eigenvectors $(-2,4/3,0,1)^T$, $(0,0,0,1)^T$, $(0,1,0,0)^T$, and $(0,0,3,1)^T$. Let T be the matrix having as columns these eigenvectors. We shift the fixed point to (0, 0, 0, 0) by setting $\tilde{H}=H-1/2$ and write (10) in vector notation as

$$\dot{\mathbf{z}}=A\mathbf{z}+\mathbf{F}(\mathbf{z}), \tag{13}$$

where A is the linear part of the vector field and $\mathbf{F}(\mathbf{0})=\mathbf{0}$.

2. Using the matrix T which transforms the linear part of the vector field into Jordan canonical form, we define new variables, $(x,y_1,y_2,y_3)\equiv\mathbf{x}$, by the equations

$$u=-2x,$$

$$y=\tfrac{4}{3}x+y_2,$$

$$\rho=3y_3,$$

$$\tilde{H}=x+y_1+y_3,$$

or in vector notation $\mathbf{z}=T\mathbf{x}$, so that (13) becomes

$$\dot{\mathbf{x}}=T^{-1}AT\mathbf{x}+T^{-1}\mathbf{F}(T\mathbf{x}).$$

Denoting the canonical form of A by B we finally obtain the system

$$\dot{\mathbf{x}}=B\mathbf{x}+\mathbf{f}(\mathbf{x}), \tag{14}$$

where $\mathbf{f}(\mathbf{x}):=T^{-1}\mathbf{F}(T\mathbf{x})$. In components system (14) is

$$\begin{bmatrix}\dot{x}\\ \dot{y}_1\\ \dot{y}_2\\ \dot{y}_3\end{bmatrix}=\begin{bmatrix}0&0&0&0\\ 0&-1&0&0\\ 0&0&-3/2&0\\ 0&0&0&-3\gamma/2\end{bmatrix}\begin{bmatrix}x\\ y_1\\ y_2\\ y_3\end{bmatrix}+\begin{bmatrix}-\frac{4}{3}x^2-xy_2\\ \frac{4}{9}x^2-y_1^2-\frac{1}{2}y_2^2+(3\gamma-1)y_3^2-2xy_1-\frac{1}{3}xy_2+(3\gamma-2)xy_3+(3\gamma-2)y_1y_3\\ \frac{16}{9}x^2-\frac{3}{2}y_2^2-4xy_1-\frac{5}{3}xy_2-4xy_3-3y_1y_2-3y_2y_3\\ -3\gamma(xy_3+y_1y_3+y_3^2)\end{bmatrix}. \tag{15}$$

3. The system (15) is written in diagonal form

$$\dot{x} = Cx + f(x,\mathbf{y}),$$
$$\dot{\mathbf{y}} = P\mathbf{y} + \mathbf{g}(x,\mathbf{y}), \tag{16}$$

where $(x,\mathbf{y}) \in \mathbb{R}\times\mathbb{R}^3$, C is the zero 1×1 matrix, P is a 3×3 matrix with negative eigenvalues and $f,\mathbf{g}$ vanish at $\mathbf{0}$ and have vanishing derivatives at $\mathbf{0}$. The center manifold theorem asserts that there exists a one-dimensional invariant local center manifold $W^c(\mathbf{0})$ of (16) tangent to the center subspace (the $\mathbf{y}=\mathbf{0}$ space) at $\mathbf{0}$. Moreover, $W^c(\mathbf{0})$ can be represented as

$$W^c(\mathbf{0}) = \{(x,\mathbf{y}) \in \mathbb{R}\times\mathbb{R}^3 : \mathbf{y} = \mathbf{h}(x),\ |x| < \delta\};\quad \mathbf{h}(0) = \mathbf{0},\quad D\mathbf{h}(0) = \mathbf{0},$$

for δ sufficiently small (cf. Ref. 13, p. 155). The restriction of (16) to the center manifold is

$$\dot{x} = f(x,\mathbf{h}(x)). \tag{17}$$

According to Theorem 3.2.2 in Ref. 15, if the origin $x=0$ of (17) is stable (respectively, unstable) then the origin of (16) is also stable (respectively, unstable). Therefore, we have to find the local center manifold, i.e., the problem reduces to the computation of $\mathbf{h}(x)$.

4. Substituting $\mathbf{y}=\mathbf{h}(x)$ in the second component of (16) and using the chain rule, $\dot{\mathbf{y}} = D\mathbf{h}(x)\dot{x}$, one can show that the function $\mathbf{h}(x)$ that defines the local center manifold satisfies

$$D\mathbf{h}(x)[f(x,\mathbf{h}(x))] - P\mathbf{h}(x) - \mathbf{g}(x,\mathbf{h}(x)) = 0. \tag{18}$$

This condition allows for an approximation of $\mathbf{h}(x)$ by a Taylor series at $x=0$. Since $\mathbf{h}(0)=\mathbf{0}$ and $D\mathbf{h}(0)=\mathbf{0}$, it is obvious that $\mathbf{h}(x)$ commences with quadratic terms. We substitute

$$\mathbf{h}(x) =: \begin{bmatrix} h_1(x) \\ h_2(x) \\ h_3(x) \end{bmatrix} = \begin{bmatrix} a_1x^2 + a_2x^3 + O(x^4) \\ b_1x^2 + b_2x^3 + O(x^4) \\ c_1x^2 + c_2x^3 + O(x^4) \end{bmatrix}$$

into (18) and set the coefficients of like powers of x equal to zero to find the unknowns $a_1, b_1, c_1, \ldots$.

5. Since y_1 and y_3 are absent from the first of (15), we give only the result for $h_2(x)$. We find $b_1=32/27$, $b_2=-32/81$. Therefore, (17) yields

$$\dot{x} = -\tfrac{4}{3}x^2 - \tfrac{32}{27}x^3 + \tfrac{32}{81}x^4 + O(x^5). \tag{19}$$

It is obvious that the origin $x=0$ of (19) is asymptotically unstable (saddle point). The theorem mentioned after (17) implies that the origin $\mathbf{x}=\mathbf{0}$ of the full four-dimensional system is unstable. This completes the proof.

B. Normal form of the system near EQ2

Regarding the stability of this equilibrium, it is easy to see that the eigenvalues of the Jacobian of (10) are, $\pm i, 0, 0$, i.e., it is totally degenerate. Nevertheless, it is the most interesting case because in other equilibria the scalar field reaches the flat plateau, which is impossible if we restrict ourselves to initial values of H smaller than $\sqrt{V_\infty}$. We find the normal form of the system (10) near the equilibrium point $(u=1, y=0, \rho=0, H=0)$. The idea of the normal form theory is the following: Given a dynamical system with equilibrium point at the origin, $\dot{\mathbf{x}}=A\mathbf{x}+\mathbf{f}(\mathbf{x})$, where A is the Jordan form of the linear part and $\mathbf{f}(\mathbf{0})=\mathbf{0}$, perform a nonlinear transformation $\mathbf{x}\to\mathbf{x}+\mathbf{h}(\mathbf{x})$, where $\mathbf{h}(\mathbf{x})=O(|\mathbf{x}|^2)$ as $|\mathbf{x}|\to 0$, such that the system becomes "as simple as possible."

To write the system in a form suitable for the application of the normal form theory, we shift the fixed point to (0, 0, 0, 0) by setting $x=u-1$ and the system becomes

$$\dot{x} = -y - xy,$$

$$\dot{y} = x + x^2 - 3Hy,$$
$$\dot{\rho} = -3\gamma\rho H, \tag{20}$$
$$\dot{H} = \frac{1}{4}x^2 - \frac{1}{2}y^2 - \frac{3\gamma - 2}{6}\rho - H^2.$$

Now we make the nonlinear change of variables

$$x \to x - y^2 - \frac{3\gamma - 2}{16}\rho x + \frac{3}{4}Hy,$$

$$y \to y + xy + \frac{3\gamma - 2}{16}\rho y + \frac{3}{4}Hx,$$

$$\rho \to \rho,$$

$$H \to H + \frac{3}{8}xy,$$

and keeping only terms up to second order, we obtain the normal form of the system, viz.,

$$\dot{x} = -y - \frac{3}{2}Hx,$$

$$\dot{y} = x - \frac{3}{2}Hy,$$

$$\dot{\rho} = -3\gamma\rho H,$$

$$\dot{H} = -\frac{3\gamma - 2}{6}\rho - \frac{1}{8}(x^2 + y^2) - H^2. \tag{21}$$

Note that the results are valid only near the origin.

Passing to cylindrical coordinates ($x = r\cos\theta, y = r\sin\theta, \rho = \rho, H = H$), we have

$$\dot{r} = -\frac{3}{2}rH,$$
$$\dot{\theta} = 1,$$
$$\dot{\rho} = -3\gamma\rho H, \tag{22}$$
$$\dot{H} = -\frac{1}{8}r^2 - H^2 - \frac{3\gamma - 2}{6}\rho.$$

We note that the θ dependence of the vector field has been eliminated, so that we can study the system in the (r, ρ, H) space. The equation $\dot{\theta} = 1$ means that the trajectory in the x–y plane spirals with angular velocity 1. The constraint [cf. (12)]

$$H^2 < \tfrac{1}{3}\rho + \tfrac{1}{4}y^2 + \tfrac{1}{4}x^2$$

becomes

$$H^2 < \tfrac{1}{4}r^2 + \tfrac{1}{3}\rho. \tag{23}$$

We observe that the first and third of (22) can be written as a differential equation

$$\frac{\mathrm{d}\rho}{\mathrm{d}r} = 2\gamma\frac{\rho}{r},$$

which has the general solution

$$\rho = Cr^{2\gamma}, \quad C > 0. \tag{24}$$

Therefore, for $\gamma=1$, we obtain from (22)

$$\dot{r} = -\tfrac{3}{2}rH,$$

$$\dot{H} = -\tfrac{1}{8}r^2 - \tfrac{1}{6}Cr^2 - H^2.$$

It is convenient to rescale r by

$$r \to \sqrt{\frac{24}{4C+3}}r, \tag{25}$$

so that the projection of (22) on the r–H plane is

$$\begin{aligned} \dot{r} &= -\tfrac{3}{2}rH, \\ \dot{H} &= -r^2 - H^2. \end{aligned} \tag{26}$$

This system belongs to a family of systems studied in 1974 by Takens.[16] Note that the constraint (23) becomes in the new variables

$$H^2 < 2r^2$$

and we conclude that the phase space of (26) is given by

$$-\sqrt{2}r \leqslant H \leqslant \sqrt{2}r. \tag{27}$$

The phase portrait of (26) is shown in Fig. 2 (see Ref. 9 for a detailed analysis). The system (26) has invariant lines $H=cr$ with $c=\pm\sqrt{2}$. Since no trajectory can cross the line $H=cr$, on any trajectory starting in the first quadrant below the line $H=cr$, H becomes zero at some time and the trajectory crosses vertically the r axis. Once the trajectory enters the second quadrant, r increases and H decreases. At first sight, it seems probable that an initially expanding universe may avoid recollapse; in fact all trajectories starting above the line $H=\sqrt{2}r$, asymptotically approaches the origin and the corresponding universes would be ever-expanding. But, (27) implies that all trajectories with $H>0$ must start below the line $H=\sqrt{2}r$. In conclusion, inequality (27) leaves no room for an ever-expanding closed universe, contrary to what was claimed in Ref. 9.

We conclude that for an initially expanding universe H continuously decreases while x and y oscillate with decreasing amplitude. H becomes zero at some time and the scale factor reaches a maximum value. Subsequently the universe begins to recollapse, i.e., H continuously decreases below zero while x and y oscillate with increasing amplitude. A typical trajectory of (21) is shown in Fig. 3, where the variable ρ was suppressed. One obtains qualitatively the same picture for all $\gamma \in [2/3, 2]$.

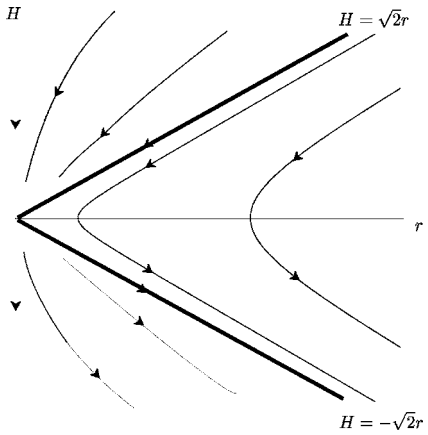

FIG. 2. The phase portrait of (26).

IV. FURTHER COMMENTS

We have analyzed the qualitative behavior of a positively curved FRW model filled with ordinary matter and containing a scalar field with the potential (5). This model is conformally equivalent to the positively curved FRW space-time in the simplest higher order gravity theory, namely the $R+\alpha R^2$ theory. We have shown that even for large initial values of H, near the flat plateau of the potential, the corresponding de Sitter equilibrium is asymptotically unstable. Further, an initially expanding closed universe in the neighborhood of EQ2 cannot avoid recollapse. This is in accordance to the well known global result concerning the closed universe recollapse conjecture, namely that a closed universe recollapses provided that the strong energy condition (SEC) is satisfied and there exists a maximal spacelike hypersurface Σ, i.e., the expansion is zero on Σ (cf. Ref. 17). In fact, it can be shown that for ϕ oscillating around the minimum of the potential, $V(0)=0$, the energy density, E, of the scalar field varies as $E\sim a^{-3}$.[18] Comparing this with the time dependence of the density $\rho\sim a^{-3\gamma}$ we arrive at the conclusion that for $\gamma\leqslant 1$, if at some time $t=t_0$

$$E<\rho, \quad 2\dot{\phi}^2-2V<\rho+3p,$$

then the SEC on the total stress-energy tensor is satisfied for all $t\geqslant t_0$. Hence the universe follows the classical Friedmannian evolution and has a time of maximum expansion. The above mentioned global theorem implies that this universe recollapses.

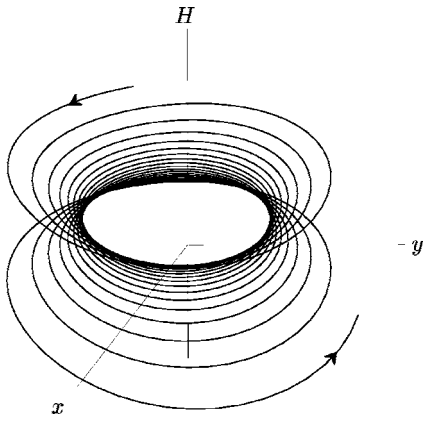

FIG. 3. A trajectory of (21).

For open and flat models having potentials with a unique minimum, $V(0)=0$, we have shown elsewhere,[18] that in an expanding universe, the energy density ρ of ordinary matter, the Hubble function H and the scalar field ϕ asymptotically approach zero. This theorem was proved without referring to the precise form of the potential. Putting all these results together, we may conjecture that potentials with a minimum equal to zero, cannot provide a mechanism of late accelerating expansion of the universe. On the other hand, in expanding universes with a potential having a positive minimum, the scalar field rolls down to the minimum of the potential and this residual cosmological term may explain the late accelerating expansion of the universe.[19]

We illustrate this idea by the example of the more general quadratic theory, derived from the Lagrangian density $R+\alpha R^2-2\Lambda$. The corresponding potential in the Einstein frame is

$$V_\Lambda(\phi) = V_\infty(1 - e^{-\sqrt{2/3}\phi})^2 + \Lambda e^{-2\sqrt{2/3}\phi}. \tag{28}$$

For every $\Lambda>0$, the functions $V_\Lambda(\phi)$ have the same qualitative behavior as (5) but, have a positive minimum, say $V_{\min}$ at some $\phi_m>0$. Both $V_{\min}$ and ϕ_m increase with increasing Λ.

We consider again expanding closed FRW models. It is easy to see that when $V_\Lambda(\phi)=V_{\min}$, the system (7) has an equilibrium $(\phi=\phi_m, y=0, \rho=0, H=\sqrt{V_{\min}/3})$ representing the de Sitter solution. It can be shown simply by the linearization theorem that this equilibrium is stable. To avoid complicating expressions for the eigenvalues we proceed as in Sec. II and obtain the following system [compare to (10)]:

$$\begin{aligned} \dot{u} &= -uy, \\ \dot{y} &= -u(1-u) + \lambda u^2 - 3Hy, \\ \dot{\rho} &= -3\gamma\rho H, \\ \dot{H} &= \frac{1}{4}(1-u)^2 + \frac{\lambda}{4}u^2 - \frac{1}{2}y^2 - \frac{3y-2}{6}\rho - H^2, \end{aligned} \tag{29}$$

with $\lambda=\Lambda/V_\infty$. The equilibrium point

$$\mathbf{p} = \left(\phi = \frac{1}{1+\lambda}, \quad y=0, \quad \rho=0, \quad H=\frac{1}{2}\sqrt{\frac{\lambda}{1+\lambda}}\right)$$

corresponds to the de Sitter solution with a cosmological term equal to $V_{\min}$. Linearization of (29) near $\mathbf{p}$ is sufficient to show that this point is a sink [all eigenvalues of the Jacobian matrix of (29) have negative real parts]. Therefore $\mathbf{p}$ attracts all nearby solutions and initially expanding closed universes enter a phase of accelerating expansion. This attracting property of the de Sitter solution for expanding models is well known from the cosmic no-hair conjecture and is not restricted only to isotropic cosmology. We conclude that $\Lambda=0$ in (28) is a bifurcation value for closed models that recollapse or not.

However, de Sitter universe is not a global attractor for (29). Numerical experiments show that for highly curved models, or models filled with an excess of ordinary matter, there are solutions of (29) which recollapse. Conditions to prevent the premature recollapse of closed models were given in Ref. 20.

Our results are based on the analysis of the behavior of the dynamical system (10) near the equilibrium solutions. A rigorous proof of the closed universe recollapse conjecture may come from the investigation of the global structure of the solutions of (2)–(4) with $k=+1$. The study of the same question for Bianchi-IX models is an interesting challenge for mathematical relativity.

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Instabilities of multiphase wave trains in coupled nonlinear Schrödinger equations: A bisymplectic framework

F. E. Laine-Pearson[a)]
Department of Mathematics and Statistics, University of Surrey, Guildford, Surrey, GU2 7XH, United Kingdom

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Hamiltonian systems, with bisymplectic structure, are known to model a wide range of interesting phenomena occurring in optics, oceanography, biochemistry, geology, and materials science. Examples of such systems are nonlinear Schrödinger (NLS) equations and Klein-Gordon (KG) equations. The paper focuses on a general class of the former and presents a linear stability theory for the interaction of a basic class of periodic traveling wave solutions, which exploits the geometric structure of the system. A criterion for linear instability is derived. Additionally, for the qualitatively tractable cases, criteria for linear instability are given explicitly in terms of: the amplitudes of the modes; the parameters of the system that characterize the medium as well as the interaction between component modes; and, when the solutions of the system are both time-and space dependent, the wave numbers. An extension to the coupled NLS equations case study is introduced, namely the consideration of a related class of coupled KG equations, which has the potential to lead to further development for the underlying bisymplectic systems theory. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1996831]

I. INTRODUCTION

Bisymplectic systems[1] appear in many areas of the physical sciences. Formally, they are dynamical systems, describable by a Hamiltonian function, with bisymplectic structure. To put such systems into context, recall that classical symplecticity considers a system of Hamiltonian partial differential equations (PDEs) based on a single symplectic operator and a Hamiltonian function. Bisymplecticity naturally extends this concept by requiring that a distinct symplectic operator is associated with each of two coordinates (in this paper, these coordinates will be a single spatial direction and time). Consequentially, bisymplecticity will contain more geometric information than its classical (symplectic) counterpart.

There is a plethora of PDEs that can be cast into a bisymplectic framework. Examples include the semilinear wave equation,[2] the water wave equations[3,4] and classes of coupled nonlinear Schrödinger (CNLS) equations[5] as well as classes of coupled Klein-Gordon (CKG) equations.[2] Therefore, since there are numerous members of the bisymplectic systems family and bisymplecticity has more to offer than classical symplecticity, it is highly motivational to acquire the additional detail revealed by the bisymplectic structure.

The objective of this paper is to present a theory for the instability of multiphase wave-train solutions of a general class of CNLS equations by casting the system into a bisymplectic framework. The purpose is to demonstrate what can be achieved through exploiting the structure of bisymplectic systems.

The specific class of CNLS equations considered are those that can be expressed as

[a)]Electronic mail: f.laine-pearson@surrey.ac.uk

$$i\epsilon_j M_{j,T} + id_j M_{j,X} + \gamma_j M_{j,XX} + \sum_{\ell=1}^{N} \beta_{j\ell} |M_\ell|^2 M_j = 0, \quad \text{for } j = 1, \ldots, N,$$

where subscripts in T and X (after the comma) denote partial derivatives, $M_j = M_j(X,T)$ are the modes, and $\epsilon_j \neq 0$, d_j, $\gamma_j \neq 0$, $\beta_{j\ell}$, for j, $\ell = 1, \ldots, N$, are real-valued scalars with the usual hypothesis that $\beta_{j\ell} = \beta_{\ell j}$. From now on, these equations will be referred to as the "N CNLS equations." Roskes[6] remarked that similar equations can be derived from multiphase envelope equations for weakly nonlinear conservative physical systems. Moreover, these types of systems are known to appear in optics applications.[7] They are also associated with CKG equations, which have been used to model, and subsequently analyze, a wide variety of physical phenomena such as dislocations in metals, processes in DNA double helices, and wave processes in bilayers as well as crack propagation in composites (see the literature, Refs. 8–12, for further details). In particular, CNLS equations can be constructed to govern the modes of weakly nonlinear solutions of CKG equations; for recent interest see Khusnutdinova *et al.*[13,14]

It is well known that CNLS equations can be formulated as an infinite-dimensional Hamiltonian system (illustrated by Bridges and Laine-Pearson[5] for $N=2$). However, there are two disadvantages of the Hamiltonian formulation, namely

(1) the symplectic structure is on an infinite-dimensional phase space;
(2) a function space is required for the X-dependence.

In contrast, the bisymplectic formulation is advantageous as it is posed on a phase space of finite dimension. In this paper, it will be shown that N CNLS equations can be re-expressed using such a formulation.

The theory presented will indicate that in systems with N-phase wave trains and a bisymplectic structure, there are natural $2N$-parameter families of wave trains with a variational principle and a geometric instability condition. These results are presented for the N CNLS equations when accompanied by the class of solutions

$$M_j(X,T) = M_{0j} e^{i\phi_j(X,T)}, \quad \text{for } j = 1, \ldots, N,$$

with complex-valued scalars M_{0j} and where $\phi_j(X,T)$ depends linearly on X and T; that is, say, $\phi_j(X,T) = \omega_j T + k_j X$, where $(\omega_1, \ldots, \omega_N, k_1, \ldots, k_N)$ are linked with the $2N$-parameter family. Moreover, since these exact solutions are associated with a generalized toral symmetry of the N CNLS equations,[5] their linear stability equation can be analyzed explicitly. It will be shown that obtaining instability results for the N CNLS case study rests on the analysis of a $2N$th-order polynomial equation, which also can be analyzed explicitly. Inevitably, a complete investigation into such an equation will increase in difficulty as N increases.

Incidentally, the $2N$th-order stability polynomial equation can be thoroughly investigated given N small enough. Furthermore, only considering X-independent solutions will remove the odd coefficients of the polynomial equation, making the sufficient conditions for instability fully obtainable for $N \leqslant 4$ (deduced in Sec. IV). Some of these tractable cases have already been considered in the literature: the case $N=1$ is a standard result[6] and the case $N=2$ has been completely discussed.[5] In this exposition, the cases $N=3,4$ are qualitatively explored in full (motivated by the belief that these cases have previously only been partially investigated); in addition, remarks are made regarding partial results for arbitrary N. Additionally, $k_j \neq 0$ is considered for the tractable cases $N=1,2$, which are fully explored, resulting in criteria for linear instability of (X,T)-dependent solutions.

The paper is organized as follows. In Sec. II a general system of N CNLS equations is re-expressed as a bisymplectic system. A generalization of the instability theory for two-phase solutions (given in Bridges and Laine-Pearson[5]) to multiphase solutions is presented and applied in Sec. III so that the associated stability polynomial is obtained. In Sec. IV, the stability polynomial equation is analyzed in full for the tractable cases. For $k_j \neq 0$, instability criteria are determined by evaluating the polynomial equation and are found to be based on the parameters of the

governing equations, the amplitudes $|M_{0j}|$, and the wave numbers k_j. (For brevity, the instability results when $k_j=0$, for all j, are relegated to Appendix A.) A particular case for $N=2$ when $k_j \neq 0$ is presented (primarily for illustration of how the conditions for linear instability may simplify when more qualitative information is known, or can be deduced, about the modes and associated parmaeters) for the reduction of the arbitrary superposition of two traveling wave trains with quasiperiodic motion to synchronized counterpropagating waves, determining that the interaction of a pair of stable component periodic traveling waves can be stable and also that an unstable component periodic traveling wave may stabilize under the influence of a stable one. The paper concludes (Sec. V) with a short discussion on the case study as well as an introduction to a more challenging system related to the N CNLS equations that also has a bisymplectic structure (a class of CKG equations) but does not have the luxury of exact solutions associated with a symmetry of the governing equations.

II. A BISYMPLECTIC FRAMEWORK FOR CNLS EQUATIONS

Consider N CNLS equations expressed in the following form:

$$i\epsilon_j M_{j,T} + id_j M_{j,X} + \gamma_j M_{j,XX} + r_j M_j = 0, \quad \text{for } j = 1, \ldots, N, \tag{2.1}$$

where subscripts in T and X (after the comma) denote partial derivatives, and

$$\mathbf{r} = \boldsymbol{\beta}\mathbf{a}, \quad \text{where } \mathbf{r} = \begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_N \end{pmatrix}, \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_{11} & \beta_{12} & \cdots & \beta_{1N} \\ \beta_{21} & \beta_{22} & \cdots & \beta_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{N1} & \beta_{N2} & \cdots & \beta_{NN} \end{pmatrix} \quad \text{and } \mathbf{a} = \begin{pmatrix} |M_1|^2 \\ |M_2|^2 \\ \vdots \\ |M_N|^2 \end{pmatrix},$$

with real-valued scalars $\epsilon_j \neq 0$, $\gamma_j \neq 0$, d_j, and $\beta_{j\ell}$, for $j, \ell = 1, \ldots, N$, which characterize the medium and the interaction between component modes $M_j = M_j(X,T)$. To cast system (2.1) into a bisymplectic framework, it is necessary that $\mathbf{r}$ is associated with a symmetric matrix (otherwise a suitable functional cannot be constructed, which is a necessary requirement so that system (2.1) can be rewritten as a bisymplectic system; this will be elaborated on in due course). Therefore, assume that $\beta_{j\ell} = \beta_{\ell j}$ for all j, ℓ. It is also beneficial to scale away the d_j. This is accomplished by calling on the substitution

$$M_j = e^{i(\xi_j T + \eta_j X)} \hat{M}_j, \quad \text{where } \xi_j = \frac{d_j^2}{4\gamma_j \epsilon_j} \text{ and } \eta_j = -\frac{d_j}{2\gamma_j}.$$

So, the interest now lies with the following set of N CNLS equations:

$$i\epsilon_j \hat{M}_{j,T} + \gamma_j \hat{M}_{j,XX} + \sum_{\ell=1}^{N} \beta_{j\ell} |\hat{M}_\ell|^2 \hat{M}_j = 0, \quad \text{for } j = 1, \ldots, N. \tag{2.2}$$

It is this transformed system that will be cast into a bisymplectic framework. [Incidentally, system (2.1) can also be directly manipulated into a bisymplectic framework, but the formulation is unnecessarily complicated—this matter will be readdressed in Sec. V].

To cast system (2.2) into a bisymplectic framework, introduce real variables q_{2j-1} and q_{2j} such that

$$\hat{M}_j = q_{2j-1} + iq_{2j}, \quad \text{for } j = 1, \ldots, N.$$

Furthermore, introduce the associated real variables p_{2j-1} and p_{2j}, satisfying the following expressions:

$$\gamma_j \hat{M}_{j,X} = \gamma_j \frac{\partial}{\partial X}(q_{2j-1} + iq_{2j}) = p_{2j-1} + ip_{2j}.$$

By using the q_{2j-1}, q_{2j}, p_{2j-1}, and p_{2j} coordinates to construct the vector

$$Z(X,T) = [q(X,T), p(X,T)]^{\mathrm{T}} \in \mathbb{R}^{4N},$$

where

$$q = (q_1, q_2, \ldots, q_{2N-1}, q_{2N})^{\mathrm{T}} \text{ and } p = (p_1, p_2, \ldots, p_{2N-1}, p_{2N})^{\mathrm{T}},$$

system (2.2) can be re-expressed as

$$\mathbf{M}Z_T + \mathbf{K}Z_X = \nabla S(Z), \tag{2.3}$$

where

$$\mathbf{M} = \begin{pmatrix} -\epsilon_1 \mathbf{J} & \mathbf{0}_2 & \cdots & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \cdots & \mathbf{0}_2 \\ \mathbf{0}_2 & -\epsilon_2 \mathbf{J} & \cdots & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \cdots & \mathbf{0}_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_2 & \mathbf{0}_2 & \cdots & -\epsilon_N \mathbf{J} & \mathbf{0}_2 & \mathbf{0}_2 & \cdots & \mathbf{0}_2 \\ \mathbf{0}_2 & \mathbf{0}_2 & \cdots & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \cdots & \mathbf{0}_2 \\ \mathbf{0}_2 & \mathbf{0}_2 & \cdots & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \cdots & \mathbf{0}_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_2 & \mathbf{0}_2 & \cdots & \mathbf{0}_2 & \mathbf{0}_2 & \mathbf{0}_2 & \cdots & \mathbf{0}_2 \end{pmatrix},$$

$$\mathbf{K} = \begin{pmatrix} \mathbf{0}_{2N} & -\mathbf{I}_{2N} \\ \mathbf{I}_{2N} & \mathbf{0}_{2N} \end{pmatrix}, \quad \mathbf{J} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

$\mathbf{0}_j$ and $\mathbf{I}_j$ are the $j \times j$ zero matrix and identity matrix, respectively. A fundamental underpinning of Eq. (2.3) is that both matrices $\mathbf{M}$ and $\mathbf{K}$ are skew-symmetric. The symmetry requirement $\beta_{j\ell} = \beta_{\ell j}$ permits the construction of the functional

$$S(Z) = \sum_{j=1}^{N} \frac{1}{2\gamma_j}(p_{2j-1}^2 + p_{2j}^2) + \frac{1}{4}\sum_{\ell=1}^{N}\sum_{j=1}^{N} \beta_{j\ell}(q_{2j-1}^2 + q_{2j}^2)(q_{2\ell-1}^2 + q_{2\ell}^2).$$

The gradient of this functional is taken with respect to the standard (Euclidean) inner product on $\mathbb{R}^{4N}$, resulting in the vector $\nabla S(Z) = (S_q, S_p)^T$, where

$$S_q = (\hat{r}_1 q_1, \hat{r}_1 q_2, \ldots, \hat{r}_N q_{2N-1}, \hat{r}_N q_{2N})^{\mathrm{T}},$$

$$S_p = \left(\frac{1}{\gamma_1}p_1, \frac{1}{\gamma_1}p_2, \ldots, \frac{1}{\gamma_N}p_{2N-1}, \frac{1}{\gamma_N}p_{2N}\right)^{\mathrm{T}},$$

with

$$\hat{r}_j = \sum_{\ell=1}^{N} \beta_{j\ell}(q_{2\ell-1}^2 + q_{2\ell}^2).$$

We conclude that system (2.2) has a "bisymplectic system" form, as it can be re-expressed as system (2.3), namely a system that has two distinct symplectic operators ($\mathbf{M}$ and $\mathbf{K}$) associated with each of two coordinates (T and X, respectively). Additionally, it is noted that system (2.2) cast as system (2.3) is a generalization of a result deduced by Bridges and Laine-Pearson.[5]

III. DETERMINING THE STABILITY POLYNOMIAL FOR A CLASS OF SOLUTIONS

A basic class of solutions of system (2.2) take the form

$$\hat{M}_j(X,T) = \hat{M}_{0j} e^{i\theta_j(X,T)}, \quad \text{where } \theta_j(X,T) = \omega_j T + k_j X, \tag{3.1}$$

for $j=1,\ldots,N$, with complex-valued scalars $\hat{M}_{0j}$. Assume such solutions are 2π-periodic in θ_j for each j. Substituting the coupled-wave solution (3.1) into system (2.2) results in a set of relations for the parameters ω_j, k_j, ϵ_j, γ_j, $\beta_{j\ell}$ and the amplitudes $\hat{M}_{0j}$, namely

$$\boldsymbol{\beta}\mathbf{a}_0 = \mathbf{b}, \quad \mathbf{a}_0 = \begin{pmatrix} |\hat{M}_{01}|^2 \\ |\hat{M}_{02}|^2 \\ \vdots \\ |\hat{M}_{0N}|^2 \end{pmatrix} \text{ and } \mathbf{b} = \begin{pmatrix} \epsilon_1\omega_1 + \gamma_1 k_1^2 \\ \epsilon_2\omega_2 + \gamma_2 k_2^2 \\ \vdots \\ \epsilon_N\omega_N + \gamma_N k_N^2 \end{pmatrix}. \tag{3.2}$$

The approach that follows is a generalization (from $N=2$ to arbitrary N) of results contained in a sister paper.[5] The family of solutions (3.1) can be re-expressed in bisymplectic coordinates by introducing $Z(X,T)=\hat{Z}(\boldsymbol{\theta})$, where $\boldsymbol{\theta}=(\theta_1,\theta_2,\ldots,\theta_N)$, such that

$$\hat{Z}(\boldsymbol{\theta}) = \mathbf{G}(\boldsymbol{\theta}(X,T))\mathcal{U}, \tag{3.3}$$

with a starting point

$$\mathcal{U} = (\mathcal{U}_1,\ldots,\mathcal{U}_{4N})^{\mathrm{T}} \in \mathbb{R}^{4N},$$

where

$$\hat{M}_{0j} = \mathcal{U}_{2j-1} + i\mathcal{U}_{2j} \text{ and } \gamma_j k_j \hat{M}_{0j} = \mathcal{U}_{2N+2j} - i\mathcal{U}_{2N+2j-1}, \tag{3.4}$$

and an orthogonal matrix

$$\mathbf{G}(\boldsymbol{\theta}) = \mathbf{R}(\theta_1) \oplus \cdots \oplus \mathbf{R}(\theta_N) \oplus \mathbf{R}(\theta_1) \cdots \oplus \mathbf{R}(\theta_N) \in \mathbb{R}^{4N\times 4N},$$

where

$$\mathbf{R}(\theta_j) = \begin{pmatrix} \cos\theta_j & -\sin\theta_j \\ \sin\theta_j & \cos\theta_j \end{pmatrix} \quad \text{for } j=1,\ldots,N.$$

It is emphasized that the approach embeds the family of solutions $Z(X,T)=\hat{Z}(\boldsymbol{\theta})$ in $(X,T,\omega_1,\ldots,\omega_N,k_1,\ldots,k_N)$-space, and so the introduction of $\boldsymbol{\theta}$ has reduced $2+2N$ variables to N independent variables θ_j. For then the geometry of Eq. (2.3)—reformulated from system (2.2)—and the character of solutions (3.1) suggests the association of $2N$ functionals $P_j:\mathbb{R}^{4N}\to\mathbb{R}$ and $Q_j:\mathbb{R}^{4N}\to\mathbb{R}$ such that

$$P_j(\hat{Z}) = \tfrac{1}{2}\langle \mathbf{M}\hat{Z}_{\theta_j}, \hat{Z}\rangle \quad \text{and} \quad Q_j(\hat{Z}) = \tfrac{1}{2}\langle \mathbf{K}\hat{Z}_{\theta_j}, \hat{Z}\rangle$$

(where the subscript θ_j denotes partial differentiation with respect to θ_j), which satisfy $\mathbf{M}\mathbf{G}_{\theta_j}\mathcal{U} = \nabla P_j(\hat{Z})$ and $\mathbf{K}\mathbf{G}_{\theta_j}\mathcal{U} = \nabla Q_j(\hat{Z})$. Then, Eq. (2.3), with the substitution $Z(X,T)=\hat{Z}(\boldsymbol{\theta})$, can be re-expressed as

$$\sum_{j=1}^{N} [\omega_j \nabla P_j(\hat{Z}) + k_j \nabla Q_j(\hat{Z})] = \nabla S(\hat{Z}),$$

and as such characterizes $\hat{Z}$ as a critical point of $S(\hat{Z})$ restricted to level sets of the P_j and Q_j, with the components ω_j and k_j cast as Lagrange multipliers; in other words, the expression can be

interpreted as the necessary condition for a constrained variational principle. The nondegeneracy condition for the basic state $\hat{Z}$ is given by the following expression:

$$\det\begin{pmatrix} \dfrac{\delta P}{\delta \omega} & \dfrac{\delta P}{\delta k} \\ \dfrac{\delta Q}{\delta \omega} & \dfrac{\delta Q}{\delta k} \end{pmatrix} \neq 0, \tag{3.5}$$

where

$$\frac{\delta P}{\delta \omega} = \begin{pmatrix} \dfrac{\partial P_1}{\partial \omega_1} & \cdots & \dfrac{\partial P_1}{\partial \omega_N} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial P_N}{\partial \omega_1} & \cdots & \dfrac{\partial P_N}{\partial \omega_N} \end{pmatrix} \text{ and } \frac{\delta P}{\delta k} = \begin{pmatrix} \dfrac{\partial P_1}{\partial k_1} & \cdots & \dfrac{\partial P_1}{\partial k_N} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial P_N}{\partial k_1} & \cdots & \dfrac{\partial P_N}{\partial k_N} \end{pmatrix};$$

similarly,

$$\frac{\delta Q}{\delta \omega} = \begin{pmatrix} \dfrac{\partial Q_1}{\partial \omega_1} & \cdots & \dfrac{\partial Q_1}{\partial \omega_N} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial Q_N}{\partial \omega_1} & \cdots & \dfrac{\partial Q_N}{\partial \omega_N} \end{pmatrix} \text{ and } \frac{\delta Q}{\delta k} = \begin{pmatrix} \dfrac{\partial Q_1}{\partial k_1} & \cdots & \dfrac{\partial Q_1}{\partial k_N} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial Q_N}{\partial k_1} & \cdots & \dfrac{\partial Q_N}{\partial k_N} \end{pmatrix}.$$

The entries of the matrix presented in expression (3.5) encode information regarding the linear stability problem for the basic state $\hat{Z}=\mathbf{G}\mathcal{U}$. The linear stability problem associated with basic state (3.3) and governing equation (2.3) is formulated by letting

$$Z(X,T) = \mathbf{G}(\boldsymbol{\theta}(X,T))[\mathcal{U} + \hat{V}(\boldsymbol{\theta},X,T)],$$

where $\hat{V}(\boldsymbol{\theta},X,T)$ is a perturbation considered for fixed ω_j and k_j and is assumed to be 2π-periodic in each θ_j. Substituting into system (2.3) and linearizing about $\hat{Z}$ gives

$$\mathbf{M}\hat{V}_T + \mathbf{K}\hat{V}_X = \mathbf{L}\hat{V}, \quad \text{where } \mathbf{L} = \mathrm{D}^2 S(\mathcal{U}) - \sum_{j=1}^{N} [\omega_j \mathrm{D}^2 P_j(\mathcal{U}) + k_j \mathrm{D}^2 Q_j(\mathcal{U})],$$

due to $P_j(\hat{Z})=P_j(\mathcal{U})$ and $Q_j(\hat{Z})=Q_j(\mathcal{U})$. The spectral problem associated with this equation, obtained by letting $\hat{V}(\boldsymbol{\theta},X,T)=\mathrm{Re}[e^{\lambda T+i\alpha X}V(\boldsymbol{\theta};\lambda,\alpha)]$, is

$$\mathbf{L}V = \lambda \mathbf{M}V + i\alpha \mathbf{K}V, \quad V \in \mathbb{C}^{4N}.$$

The entries of condition (3.5) will now be calculated. First, note that P_j and Q_j evaluate to the following:

$$P_j(\mathcal{U}) = \tfrac{1}{2}\epsilon_j(\mathcal{U}_{2j-1}^2 + \mathcal{U}_{2j}^2) \quad \text{and} \quad Q_j(\mathcal{U}) = \mathcal{U}_{2j-1}\mathcal{U}_{2N+2j} - \mathcal{U}_{2j}\mathcal{U}_{2N+2j-1}.$$

Therefore, under the assumption that $\boldsymbol{\beta}$ is invertible

$$[P_1(\mathcal{U}), P_2(\mathcal{U}), \ldots, P_N(\mathcal{U})]^{\mathrm{T}} = \tfrac{1}{2}\boldsymbol{\Upsilon}\,\boldsymbol{\beta}^{-1}\mathbf{b}$$

and

$$[Q_1(\mathcal{U}), Q_2(\mathcal{U}), \ldots, Q_N(\mathcal{U})]^{\mathrm{T}} = \mathbf{\Gamma}\,\boldsymbol{\beta}^{-1}\mathbf{b},$$

with

$$\mathbf{\Upsilon} = \begin{pmatrix} \epsilon_1 & 0 & \cdots & 0 \\ 0 & \epsilon_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \epsilon_N \end{pmatrix}, \quad \mathbf{\Gamma} = \begin{pmatrix} \gamma_1 k_1 & 0 & \cdots & 0 \\ 0 & \gamma_2 k_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \gamma_N k_N \end{pmatrix},$$

which is determined by noting the first set of expressions (3.4), consequently, relation (3.2) can be used. Hence

$$\frac{\delta P}{\delta \omega} = \frac{1}{2}\mathbf{\Upsilon}\,\boldsymbol{\beta}^{-1}\mathbf{\Upsilon}, \quad \frac{\delta P}{\delta k} = \mathbf{\Upsilon}\,\boldsymbol{\beta}^{-1}\mathbf{\Gamma}, \quad \frac{\delta Q}{\delta \omega} = \mathbf{\Gamma}\,\boldsymbol{\beta}^{-1}\mathbf{\Upsilon},$$

and

$$\frac{\delta Q}{\delta k} = 2\mathbf{\Gamma}\,\boldsymbol{\beta}^{-1}\mathbf{\Gamma} + \mathrm{diag}(\gamma_1|\hat{M}_{01}|^2, \ldots, \gamma_N|\hat{M}_{0N}|^2),$$

with the last evaluation simplified by noting relation (3.2). A definition for linear instability now follows.

Given

$$\hat{\Delta}(\Lambda, \alpha) := \det\left[\Lambda^2\frac{\delta P}{\delta \omega} + \alpha\Lambda\left(\frac{\delta P}{\delta k} + \frac{\delta Q}{\delta \omega}\right) + \alpha^2\frac{\delta Q}{\delta k}\right], \quad \text{where } \Lambda = -i\lambda.$$

If $\hat{\Delta}(\Lambda, \alpha) = 0$ for some $\alpha \in \mathbb{R}$ and $\Lambda \in \mathbb{C}$ with $\mathrm{Im}(\Lambda) \neq 0$ and $|\Lambda|^2 + |\alpha|^2$ sufficiently small, then the basic state $\hat{Z}(\boldsymbol{\theta}) = \mathbf{G}(\boldsymbol{\theta})\mathcal{U}$ is "linearly unstable." (The above definition is similar to the one used for two-phase solutions[5] and is consistent with the theory developed by Bridges.[3]) For the N CNLS system, the introduction of $\lambda = i\Lambda$ into the spectral problem results in $\hat{\Delta}(\Lambda, \alpha) = 0$, which is a polynomial equation with real coefficients.

Therefore, to determine sufficient conditions for linear instability, it is enough to study the qualitative aspect of the roots of the $2N$th-order polynomial equation $\hat{\Delta}(\Lambda, \alpha) = 0$. This deduction agrees with the expected outcome from implementing a classical approach to the linear stability problem, which usually consists of taking a solution of interest plus a (suitable) perturbation and then substituting the perturbed solution directly into the particular system (in this case, N CNLS equations). Such a classical approach is illustrated, for instance, by Roskes[6] when $N = 2$ and $k_j = 0$.

IV. EVALUATING THE STABILITY POLYNOMIAL

Returning to $\hat{\Delta}(\Lambda, \alpha) = 0$, determining when

$$\text{at least one } \Lambda \text{ exists such that } \mathrm{Im}(\Lambda) \neq 0, \tag{4.1}$$

will encapsulate sufficient conditions for linear instability. Fortunately, the task is less demanding when $k_j = 0$ for all $j = 1, \ldots, N$, i.e., X-independent basic solutions. In particular, determining a complete description of the parameter space where requirement (4.1) occurs is tractable for $N \leqslant 4$.

Under the assumption that $k_j = 0$ for all $j = 1, \ldots, N$, the components of the matrix given in expression (3.5) simplify to

$$\frac{\delta P}{\delta \omega} = \frac{1}{2}\mathbf{\Upsilon}\boldsymbol{\beta}^{-1}\mathbf{\Upsilon}, \quad \frac{\delta P}{\delta k} = \frac{\delta Q}{\delta \omega} = \mathbf{0}, \quad \frac{\delta Q}{\delta k} = \mathrm{diag}(\gamma_1|\hat{M}_{01}|^2, \ldots, \gamma_N|\hat{M}_{0N}|^2).$$

Therefore, obtaining stability information relies on the analysis of the roots of the even polynomial equation of order $2N$

$$a_{2N}\hat{\Lambda}^{2N} + a_{2(N-1)}\hat{\Lambda}^{2(N-1)} + \cdots + a_2\hat{\Lambda}^2 + a_0 = 0, \quad \text{with } \hat{\Lambda} = \frac{\Lambda}{\alpha}, \tag{4.2}$$

where the coefficients $a_{2\ell}$, for $\ell = 0, 1, \ldots, N$, follow a predictable pattern—this is detailed in Appendix B; additionally, the rescaling of Λ to $\hat{\Lambda}$ has removed the parameter α from the assignments of the coefficients $a_{2\ell}$. Furthermore, a complete qualitative description of the parameter space satisfying requirement (4.1), when Λ is governed by Eq. (4.2), can be given for $N \leqslant 4$. For completeness, these analyses are presented in Appendix A; some remarks are also made regarding partial descriptions of the parameter space satisfying requirement (4.1) for arbitrary N.

Now, consider $k_j \neq 0$. For $N \leqslant 2$, a full qualitative description of the parameter space satisfying requirement (4.1) can be given for the one-phase and two-phase solutions with nonzero k_j. These cases will be presented, followed by remarks regarding arbitrary N as well as an application of the case $N=2$ for a family of synchronized counterpropagating wave trains.

A. A single wave

The single wave basic state $\hat{M}_1(X,T) = \hat{M}_{01}e^{i(\omega_1 T + k_1 X)}$, where (ω_1, k_1) satisfy $\beta_{11}|\hat{M}_{01}|^2 = \epsilon_1\omega_1 + \gamma_1 k_1^2$, determined from relation (3.2), has a quadratic stability equation

$$a_2\hat{\Lambda}^2 + a_1\hat{\Lambda} + a_0 = 0,$$

where $a_2 = \epsilon_1^2$, $a_1 = 4\gamma_1\epsilon_1 k_1$ and $a_0 = 2\gamma_1(2\gamma_1 k_1^2 + \beta_{11}|\hat{M}_{01}|^2)$. For a general quadratic equation, the existence of at least one $\hat{\Lambda}$ with nonzero imaginary part [requirement (4.1)] is confirmed whenever $a_1^2 - 4a_2a_0 < 0$ holds. Since a_2, a_1, a_0 are known, the condition evaluates to $\gamma_1\beta_{11} > 0$, which is the same for when $k=0$ (confirmed in Appendix A).

B. Two coupled waves

Consider two coupled waves (3.1) with $k_j \neq 0$. Instability criteria for the arbitrary superposition of two traveling wave trains with quasiperiodic motion will now be deduced from the associated quartic stability equation

$$a_4\hat{\Lambda}^4 + a_3\hat{\Lambda}^3 + a_2\hat{\Lambda}^2 + a_1\hat{\Lambda} + a_0 = 0,$$

where

$$a_4 = \frac{1}{4}\epsilon_1^2\epsilon_2^2,$$

$$a_3 = \epsilon_1\epsilon_2(\epsilon_2\gamma_1 k_1 + \epsilon_1\gamma_2 k_2),$$

$$a_2 = (\epsilon_2\gamma_1 k_1 + \epsilon_1\gamma_2 k_2)^2 + 2\epsilon_1\epsilon_2\gamma_1\gamma_2 k_1 k_2 + \tfrac{1}{2}(\epsilon_2^2\gamma_1\beta_{11}|\hat{M}_{01}|^2 + \epsilon_1^2\gamma_2\beta_{22}|\hat{M}_{02}|^2),$$

$$a_1 = 2\gamma_1\gamma_2[\epsilon_1\beta_{22}|\hat{M}_{02}|^2 k_1 + \epsilon_2\beta_{11}|\hat{M}_{01}|^2 k_2 + 2(\epsilon_2\gamma_1 k_1 + \epsilon_1\gamma_2 k_2)k_1 k_2],$$

$$a_0 = \gamma_1\gamma_2[2(2\gamma_1\gamma_2 k_1^2 k_2^2 + \gamma_1\beta_{22}|\hat{M}_{02}|^2 k_1^2 + \gamma_2\beta_{11}|\hat{M}_{01}|^2 k_2^2) + \det(\boldsymbol{\beta})|\hat{M}_{01}|^2|\hat{M}_{02}|^2],$$

with

$$\beta_{11}|\hat{M}_{01}|^2 + \beta_{12}|\hat{M}_{02}|^2 = \epsilon_1\omega_1 + \gamma_1 k_1^2 \quad \text{and} \quad \beta_{21}|\hat{M}_{01}|^2 + \beta_{22}|\hat{M}_{02}|^2 = \epsilon_2\omega_2 + \gamma_2 k_2^2,$$

where $\beta_{12}=\beta_{21}$. Divide through by a_4 and transform the cubic term away by introducing $Y=\hat{\Lambda} + a_3/4a_4$, resulting in

$$Y^4 + \tau_1 Y^2 + \tau_2 Y + \tau_3 = 0, \tag{4.3}$$

where

$$\tau_1 = \frac{1}{a_4^2}\left(-\frac{3}{8}a_3^2 + a_4 a_2\right),$$

$$\tau_2 = \frac{1}{a_4^3}\left(\frac{1}{8}a_3^3 - \frac{1}{2}a_4 a_3 a_2 + a_4^2 a_1\right),$$

$$\tau_3 = \frac{1}{a_4^4}\left(-\frac{3}{256}a_3^4 + \frac{1}{16}a_4 a_3^2 a_2 - \frac{1}{4}a_4^2 a_3 a_1 + a_4^3 a_0\right).$$

There are three diagnostic functions associated with the general reduced quartic equation (4.3)

$$D_1 = \tau_1, \quad D_2 = \text{DISCRIMINANT}, \quad D_3 = \tau_1^2 - 4\tau_3,$$

where

$$\text{DISCRIMINANT} = 16\tau_3\tau_1^4 - 4\tau_2^2\tau_1^3 - 128\tau_3^2\tau_1^2 + 144\tau_2^2\tau_3\tau_1 - 27\tau_2^4 + 256\tau_3^3.$$

Note that, since a_4 and a_3 are real, $\text{Im}(\hat{\Lambda}) \neq 0$ if and only if $\text{Im}(Y) \neq 0$. Therefore, the conditions for instability (the existence of at least one root $\hat{\Lambda}$ with nonzero imaginary part) are

$$[D_1 > 0] \text{ or } [D_1 = 0 \text{ and } (\tau_2 \neq 0 \text{ or } \tau_3 \neq 0)]$$

$$\text{or } [D_1 < 0 \text{ and } D_2 < 0] \text{ or } [D_1 < 0, D_2 \geqslant 0 \text{ and } D_3 < 0].$$

The discriminant surface, plotted in τ-space, is illustrated in Fig. 1. If $\tau_1 > 0$, then it is immediate that there is at least one unstable eigenvalue. When $\tau_1 \leqslant 0$, then additional diagnostics require checking. A section through the discriminant surface for $\tau_1 < 0$ is shown in Fig. 2. Unless τ_2 and τ_3 are in the enclosed central region (marked with "4" in the figure) there will be a root which is unstable (having a nonzero imaginary part). Therefore, given a basic state, the problem of instability for the two-wave interaction reduces to checking the above conditions for the quartic equation. So, for a particular application, sufficient conditions for instability can be deduced by substituting the values of parameters into the diagnostic functions.

C. Remarks on *N*-coupled waves

Determining conditions for linear instability of N-interacting wave trains boils down to analyzing a $2N$th order polynomial equation. This task becomes increasingly difficult to do in full as N increases. This is clearly demonstrated by the complexity of conditions for the case of $N=2$. If further qualitative information is known about the wave type, then evaluation can become a more straightforward task. To illustrate this fact, consider the example that follows for a particular instance of the interaction of two counterpropagating waves.

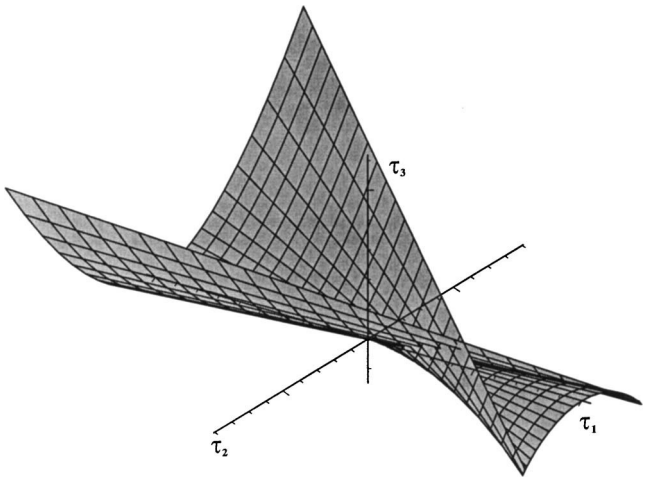

FIG. 1. The discriminant surface for the quartic equation.

D. An application: Synchronized counterpropagating waves

Consider a special case of $N=2$ where the waves are counterpropagating. Set $k_1=-k_2=k$ with $\hat{M}_{01}=\hat{M}_{02}=\hat{M}_0\neq 0$, $\epsilon_1=\epsilon_2=\epsilon$, and $\gamma_1=\gamma_2=\gamma$. Then, since $a_3=0$ (the special case $Y=\hat{\Lambda}$)

$$D_1=\frac{4\gamma}{\epsilon^2}\left[-2\gamma k^2+\frac{1}{2}(\beta_{11}+\beta_{22})|\hat{M}_0|^2\right];$$

the other diagnostic functions can be determined similarly.

For simplicity, set $\omega_1=\omega_2=\omega$. Then, $\beta_{11}=\beta_{22}$ [determined using relations (3.2)] and $a_1=0$, which means that $\tau_2=0$ too and $D_2=16\tau_3 D_3^2$. The quartic equation (4.3) simplifies to $Y^4+\tau_1 Y^2+\tau_3=0$, which is a bi-quadratic equation. Therefore, for at least one Y^2 with $\mathrm{Im}(Y^2)\neq 0$ to occur then $\tau_1^2-4\tau_3<0$ must hold—this is sufficient but not necessary for at least one Y such that $\mathrm{Im}(Y)\neq 0$. The region of (τ_1,τ_3)-space represented by the shaded region in Fig. 3 (in the diagram $y=Y$, $c_1=\tau_1$, and $c_2=\tau_3$) depicts the qualitative nature of the roots Y—for instance, the third and fourth quadrants show that two real roots and one complex pair of roots occur whenever $\tau_3<0$. For the linear instability conditions, at least one Y with $\mathrm{Im}(Y)\neq 0$ is required and so the shaded

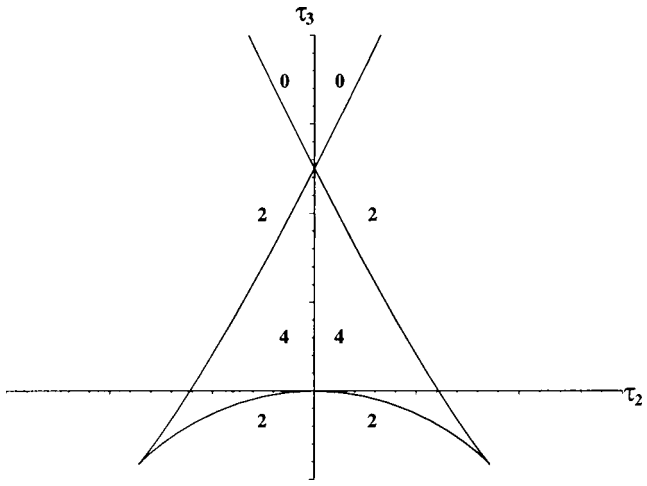

FIG. 2. A constant τ_1 section through the discriminant surface with $\tau_1<0$. The number of real roots of the quartic equation in each region of parameter space is labeled 0, 2, or 4.

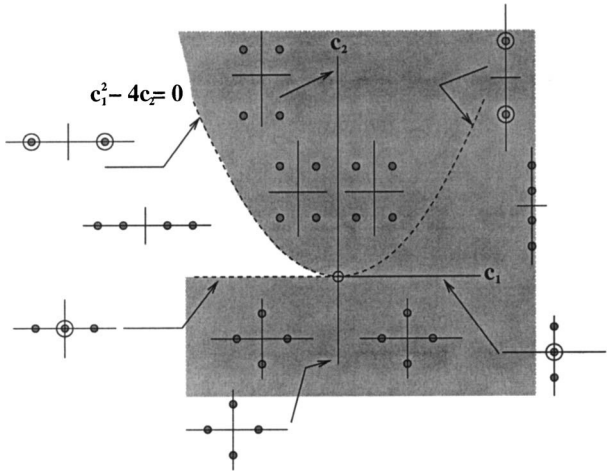

FIG. 3. The qualitative nature of the roots y satisfying $y^4+c_1y^2+c_2=0$. The shaded region indicates where at least one root y exists with $\mathrm{Im}(y)\neq 0$. Four real roots, y, occur in the unshaded region.

region includes these two quadrants. To describe this whole region in (τ_1,τ_3)-space, break it up into smaller, easily expressible, parts. (Note that this is not a unique process.) Since $Y=\hat{\Lambda}$, instability (the existence of at least one root $\hat{\Lambda}$ with nonzero imaginary part) can occur whenever any of the following conditions are satisfied:

(i) $\tau_3<0$;
(ii) $\tau_3\geqslant 0$ and $\tau_1>0$;
(iii) $\tau_1\leqslant 0$ and $\tau_1^2-4\tau_3<0$;

which evaluates to the following:

(i) $C<0$;
(ii) $C\geqslant 0$ and $\gamma(\beta_{11}|\hat{M}_0|^2-2\gamma k^2)>0$;
(iii) $\gamma(\beta_{11}|\hat{M}_0|^2-2\gamma k^2)\leqslant 0$ and $\beta_{12}^2|\hat{M}_0|^2-8\gamma\beta_{11}k^2<0$;

where $C=(\beta_{11}^2-\beta_{12}^2)|\hat{M}_0|^4+4\gamma\beta_{11}k^2|\hat{M}_0|^2+4\gamma^2k^4$ and, due to the relations (3.2), with $(\beta_{11}+\beta_{12})|\hat{M}_0|^2=\epsilon\omega+\gamma k^2$. It should be noted that these three conditions reduce to the three conditions given in Appendix A when $k=0$, $\gamma_1=\gamma_2=\gamma$, $\epsilon_1=\epsilon_2=\epsilon$, $|\hat{M}_{01}|=|\hat{M}_{02}|=|\hat{M}_0|$, $\beta_{11}=\beta_{22}$, and $\beta_{12}=\beta_{21}$, which is consistent.

In application, ϵ and γ may be given. For ease of calculation, set $\gamma=1/2$ and $\epsilon=1$. Then $(\beta_{11}+\beta_{12})|\hat{M}_0|^2=\omega+k^2/2$. Considering the interaction of both waves (see above and Sec. IV B), the criteria for linear instability simplify to the following:

(i) $C_0<0$;
(ii) $C_0\geqslant 0$ and $\beta_{11}|\hat{M}_0|^2-k^2>0$;
(iii) $\beta_{11}|\hat{M}_0|^2-k^2\leqslant 0$ and $\beta_{12}^2|\hat{M}_0|^2-4\beta_{11}k^2<0$;

where $C_0=(\beta_{11}^2-\beta_{12}^2)|\hat{M}_0|^4+2\beta_{11}k^2|\hat{M}_0|^2+k^4$. Note that the instability condition for the wave solutions $\hat{M}_1(X,T)=\hat{M}_0e^{i(\omega T+kX)}$ and $\hat{M}_2(X,T)=\hat{M}_0e^{i(\omega T-kX)}$ considered separately is $\beta_{1j}>0$ (see Sec. IV A). Therefore, the instability of the synchronized counterpropagating waves is determined by a much more complex mechanism than that for single waves.

Conversely, consider a criterion for stability, namely $\mathrm{Im}(\hat{\Lambda})=0$ for all $\hat{\Lambda}$. For the single-wave

case, the required condition is $a_1^2-4a_2a_0\geqslant 0$, which, for the example, simplifies to $\beta_{11}<0$ (noting, by construction, $\beta_{11}\neq 0$). For two coupled waves, the unshaded area in Fig. 3 (in the diagram $y=Y$, $c_1=\tau_1$, and $c_2=\tau_3$) will give the condition for stability, namely

$$\tau_3\geqslant 0, \quad \tau_1\leqslant 0, \quad \text{and } \tau_1^2-4\tau_3\geqslant 0,$$

which, for the example, simplifies to

$$C_0\geqslant 0, \quad \beta_{11}|\hat{M}_0|^2-k^2\leqslant 0, \quad \text{and} \quad \beta_{12}^2|\hat{M}_0|^2-4\beta_{11}k^2\geqslant 0.$$

Therefore the condition for stability is also more complex for the interaction of synchronized counterpropagating waves, and the region of stability is much smaller, when comparing to the component traveling waves.

A little more can be deduced. Let $D_0=\beta_{11}|\hat{M}_0|^2-k^2$. Consider two unstable component waves, for then $\beta_{11}>0$ and $\beta_{12}>0$. Assume that $\beta_{11}>\beta_{12}$. Recall that by viewing each of conditions (i) to (iii) separately, they are each a sufficient condition for instability. Instability condition

(i) is not valid, whereas
(ii) $\beta_{11}>k^2/|\hat{M}_0|^2$, is a possibility, and
(iii) $\beta_{11}\leqslant k^2/|\hat{M}_0|^2$ and $\beta_{12}^2<4k^4/|\hat{M}_0|^4$ is also a possibility.

Therefore it is possible that either condition (ii) or condition (iii) may be satisfied. The stability condition is not valid, that is, when $\beta_{11}>\beta_{12}$ the interaction of the two component waves cannot be stable. We conclude that when two component waves are unstable such that $\beta_{11}>\beta_{12}>0$, then the two-wave interaction is unstable. Now, consider when one component wave is unstable and the other is stable such that $\beta_{11}>0$ and $\beta_{12}<0$. Assume further that $|\beta_{11}|>|\beta_{12}|$. The conditions mimic those of two unstable component waves previously discussed. Consequently, when one of the component waves is unstable and the other stable such that $\beta_{11}>0$, $\beta_{12}<0$ and $|\beta_{11}|>|\beta_{12}|$, then the two-wave interaction is also unstable. Although these two situations conclude with such straightforward results, the interplay of component modes is generally a delicate issue. For instance, this may be seen when the behavior of the previous two component waves is swapped or when both component waves are stable, which could occur through $\beta_{11}<0$ (and possibly when $|\beta_{12}|>|\beta_{11}|$), then allowing the possibility of any of the three instability conditions or the stability condition to hold for a particular application (for it is the relative magnitudes of β_{11}, β_{12}, $|\hat{M}_0|$, and k that open up the possibilities further). Now there may be the potential that two stable component modes may interact in a stable manner and, perhaps, it is plausible that an unstable component mode may stabilize by interacting with a stable component mode.

These speculations can be made concrete. Note that $C_0=D_0^2+E_0$, where $E_0=(4\beta_{11}k^2-\beta_{12}^2|\hat{M}_0|^2)|\hat{M}_0|^2$. Therefore, the two-wave interaction is unstable if any of the following conditions hold:

$$(C_0<0) \text{ or } (C_0\geqslant 0 \text{ and } D_0>0) \text{ or } (D_0\leqslant 0 \text{ and } E_0>0).$$

Conversely, the interaction is stable if

$$C_0\geqslant 0, \quad D_0\leqslant 0, \quad \text{and } E_0\leqslant 0.$$

Figure 4 shows the intersection of surface C_0 in (E_0,D_0,C_0)-space. The regions of instability/stability are shown for a constant E_0 section through C_0 with $E_0<0$ in Fig. 5 and for a constant D_0 section through C_0 with $D_0<0$ in Fig. 6. The second and third quadrants of Fig. 5 and Fig. 6 show that stability can occur when $D_0\leqslant 0$ and $E_0\leqslant 0$, which automatically happens when β_{11} is negative, but must be sufficiently negative, relative to $-|\beta_{12}|$, especially as $C_0\geqslant 0$ is also required for stability; additionally, note that a component mode with $\beta_{11}<0$ is stable. Since β_{12} appears only through β_{12}^2 in the instability/stability conditions, the relevancy of whether the corresponding component mode is stable ($\beta_{12}<0$) or unstable ($\beta_{12}>0$) is of no importance for the form of the conditions derived; it is only the magnitude, $|\beta_{12}|$, that is crucial. We conclude, for this particular

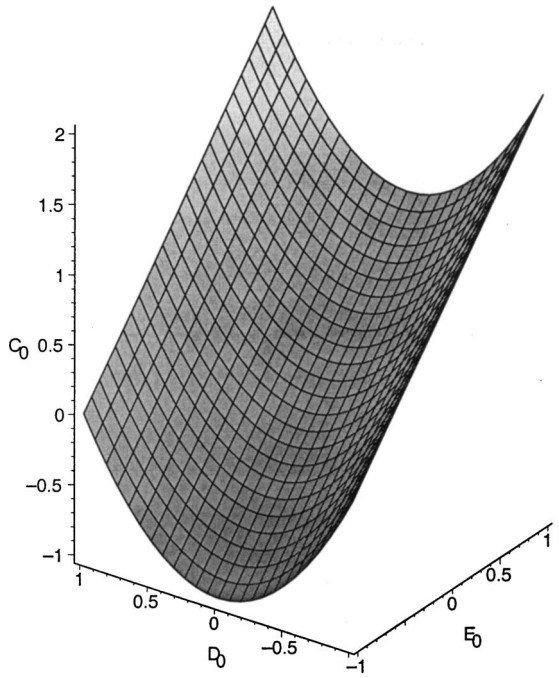

FIG. 4. The surface $C_0=D_0^2+E_0$.

application, that it is possible that two component stable modes can interact in a stable manner and an unstable component mode ($\beta_{12}>0$) can be stabilized by a stable component mode ($\beta_{11}<0$).

Last, briefly consider a specific application with the same parameters as above but with the exception that $\gamma=1$ and $\beta_{11}=\beta_{12}=\beta_{21}=\beta_{22}=\sigma/2$, where $\sigma=\pm 1$. It is noted that the $\beta_{j\ell}$ values imply that individual component modes are either both unstable ($\sigma=+1$) or both stable ($\sigma=-1$). For focusing behavior ($\sigma=+1$), the two-wave interaction is unstable. However, for defocusing behavior ($\sigma=-1$), the two-wave interaction is stable if $2k^2 \geqslant |\hat{M}_0|^2$ and unstable if $2k^2<|\hat{M}_0|^2$; in other words, at small amplitudes, the plane waves are stable to long-wave disturbances, whereas at larger amplitudes the two CNLS equations can exhibit long-wave instabilities. These deductions agree with those of Forest *et al.*[15]

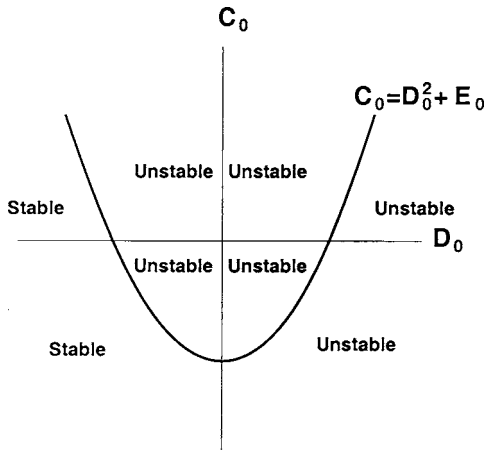

FIG. 5. A constant E_0 section through the surface $C_0=D_0^2+E_0$ with $E_0<0$. The regions of instability/stability are indicated.

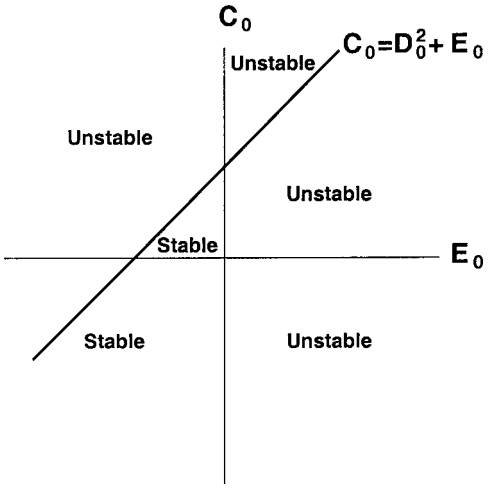

FIG. 6. A constant D_0 section through the surface $C_0=D_0^2+E_0$ with $D_0<0$. The regions of instability/stability are indicated.

V. DISCUSSION

Although it was mentioned, in Sec. II, that Eq. (2.1) can be cast into a bisymplectic framework, it is not required for directly relating the instability conditions for the modes $\hat{M}_j$ to the modes M_j. Recall that

$$M_j = e^{i(\xi_j T+\eta_j X)}\hat{M}_j = \hat{M}_{0j}e^{i[(\xi_j+\omega_j)T+(\eta_j+k_j)X]},$$

and let

$$M_j = \hat{M}_{0j}e^{i(\hat{\omega}_j T+\hat{k}_j X)},$$

where $\hat{\omega}_j=\xi_j+\omega_j$ and $\hat{k}_j=\eta_j+k_j$. Substitute $\omega_j=\hat{\omega}_j-\xi_j$ and $k_j=\hat{k}_j-\eta_j$, where

$$\xi_j = \frac{d_j^2}{4\gamma_j\epsilon_j} \quad \text{and} \quad \eta_j = -\frac{d_j}{2\gamma_j},$$

into the instability conditions: they will now be expressed in terms of the basic solution $M_j=\hat{M}_{0j}e^{i\hat{\theta}(X,T)}$, where $\hat{\theta}(X,T)=\hat{\omega}_j T+\hat{k}_j X$, of governing equations (2.1).

Returning to the transformed governing equations (2.2), in Sec. II, it was shown that this general class of N CNLS equations can be re-expressed as a bisymplectic system. The successful application of the theory to these CNLS equations is due to a very special feature of the multiphase wave trains considered, namely the basic class of N-phase wave trains can be characterized as (bisymplectic) relative equilibria.[5,16] "Relative equilibria" are solutions associated with some symmetry of the system of governing equations; for the N CNLS equations (2.2) it is a generalized toral symmetry (the symmetry group is $\mathbb{T}^N$ with action $\mathbf{G}$, a generalized rotational matrix). For the stability analysis, it is the parameter structure naturally associated with relative equilibria that is required.[16] The geometric structure is such that for the CNLS system with a basic class of multiphase wave trains with N-components, and a bisymplectic structure, there are natural $2N$-parameter families $(P_1,\ldots,P_N,Q_1,\ldots,Q_N)$ with a variational principle and a geometric instability condition. Moreover, since these parameters do not appear explicitly in the equations—although they are an intrinsic part of the structure of the system—they are not obvious. Furthermore, when treated as functions of the wave numbers and frequencies, the partial derivatives of these parameters encode stability information. Specifically, sufficient conditions for linear instability can be offered through these partial derivatives. This remarkable feature does not depend on explicit properties of N CNLS equations; it only depends on their structure.

A potentially interesting case study would be to consider the CKG equations

$$u_{tt} - u_{xx} = f_u(u,w),$$

$$w_{tt} - c^2 w_{xx} = f_w(u,w),$$

where $f(u,w)$ is a potential function of the nonlinear coupling and c is a real-valued scalar. These type of equations can also be re-expressed as a bisymplectic system.[2] Particular interest lies with weakly nonlinear solutions, which are not associated with a symmetry of the system. These weakly nonlinear solutions can be expanded in Fourier series—with the first term resembling the basic class of solution—and the linear stability problem could be investigated within a geometric framework. Although there is a potential small divisor problem,[2] the beauty of this investigation is that CNLS equations can be constructed to govern the modes of weakly nonlinear solutions of the CKG equations.[13,14] Therefore, the analysis of associated systems of CNLS equations ($N=2$,[13] and $N=4$,[14] have been proposed)—with the basic class of solution identified with the toral symmetry of the equations—may provide some insight into the stability problem for weakly nonlinear solutions of the connected CKG equations. Further details of this investigation will be presented elsewhere.

ACKNOWLEDGMENTS

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APPENDIX A: SUFFICIENT CONDITIONS FOR LINEAR INSTABILITY

The analyses for solutions (3.1) with $k_j=0$, for all j, governed by system (2.2), that lead to determining a complete description of the parameter space satisfying requirement (4.1) for $N \leqslant 4$ are presented. A partial description of the required region of parameter space for arbitrary N is also mentioned.

1. A single wave

The one-wave basic state

$$\hat{M}_1(X,T) = \hat{M}_{01} e^{i\omega_1 T}, \quad \text{where} \quad \omega_1 = \frac{1}{\epsilon_1}\beta_{11}|\hat{M}_{01}|^2,$$

determined from relation (3.2), has a quadratic (or bilinear) stability equation $a_2\hat{\Lambda}^2 + a_0 = 0$. Clearly, $\hat{\Lambda} = \pm\sqrt{-a_0/a_2}$. Thus, the existence of at least one root $\hat{\Lambda}$ with nonzero imaginary part is confirmed whenever $a_0 a_2 > 0$. Referring to Appendix B, this inequality evaluates to $\gamma_1\beta_{11} > 0$. According to Roskes,[6] this is exactly the necessary and sufficient condition for the single mode $\hat{M}_1$ to be unstable.

2. Two coupled waves

Consider two coupled waves (3.1) with $k_j=0$. The associated bi-quadratic stability equation is $a_4\hat{\Lambda}^4 + a_2\hat{\Lambda}^2 + a_0 = 0$. For a general bi-quadratic equation with $a_4 \neq 0$, the existence of at least one $\hat{\Lambda}$ with nonzero imaginary part is confirmed whenever any of the following criteria are satisfied:

(i) $a_0 a_4 < 0$;
(ii) $a_0 a_4 \geqslant 0$ and $a_2 a_4 > 0$;
(iii) $a_2 a_4 \leqslant 0$ and $a_2^2 - 4a_4 a_0 < 0$.

It should be noted that this description is not unique—see Fig. 3 (in the diagram $y=\hat{\Lambda}$, $c_1=\hat{a}_2$, and

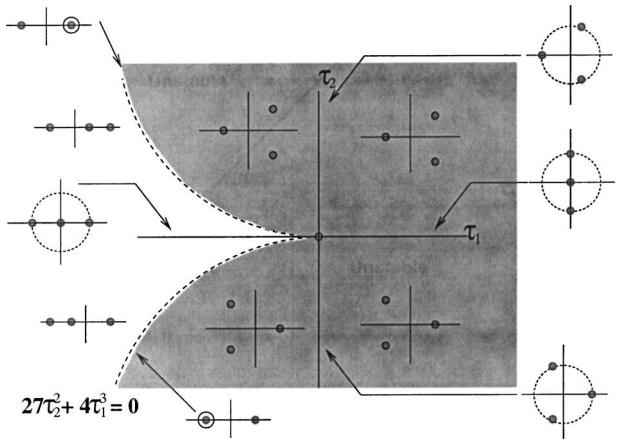

FIG. 7. The qualitative nature of the roots Y^2 satisfying $Y^6+\tau_1 Y^2+\tau_2=0$. The shaded region indicates where at least one root Y^2 exists with $\mathrm{Im}(Y^2)\neq 0$. Three real roots, Y^2, occur in the unshaded region.

$c_2=\hat{a}_0$, where $\hat{a}_{2\ell}=a_{2\ell}/a_4$). This figure highlights (shaded region) where at least one root $\hat{\Lambda}$ exists with $\mathrm{Im}(\hat{\Lambda})\neq 0$. It completely describes the region of parameter space satisfying requirement (4.1). For instance, when $a_0/a_4<0$ [exactly condition (i) given above] the root sketches show that two real roots $\hat{\Lambda}$ exist (denoted by the circles on the horizontal axes) and a pair of complex roots $\hat{\Lambda}$ exists (denoted by the circles on the vertical axes). Hence, at least one $\hat{\Lambda}$ with $\mathrm{Im}(\hat{\Lambda})\neq 0$ occurs in this part of the (a_0,a_2,a_4)-space. Referring to Appendix B, the conditions evaluate to the following:

(i) $\gamma_1\gamma_2\det(\boldsymbol{\beta})<0$;
(ii) $\gamma_1\gamma_2\det(\boldsymbol{\beta})\geqslant 0$ and $\tilde{a}_2>0$;
(iii) $\tilde{a}_2\leqslant 0$ and $\tilde{a}_2^2<4\epsilon_1^2\epsilon_2^2|\hat{M}_{01}|^2|\hat{M}_{02}|^2\gamma_1\gamma_2\det(\boldsymbol{\beta})$;

where $\tilde{a}_2=\gamma_1\epsilon_2^2\beta_{11}|\hat{M}_{01}|^2+\epsilon_1^2\gamma_2\beta_{22}|\hat{M}_{02}|^2$. The first condition was originally presented by Roskes,[6] while the other two conditions are additions presented by Bridges and Laine-Pearson.[5]

3. Three coupled waves

Consider three coupled waves (3.1) with $k_j=0$. The associated bicubic stability equation is

$$a_6\hat{\Lambda}^6+a_4\hat{\Lambda}^4+a_2\hat{\Lambda}^2+a_0=0. \tag{A1}$$

Assuming $a_6\neq 0$, the simplest way of retrieving qualitative information from this equation is to transform the fourth-order term away, obtaining

$$Y^6+\tau_1 Y^2+\tau_2=0, \quad \text{where } Y^2=\hat{\Lambda}^2+\frac{a_4}{3a_6}, \tag{A2}$$

with

$$\tau_1=\frac{1}{a_6^2}\left(-\frac{1}{3}a_4^2+a_2a_6\right) \quad \text{and} \quad \tau_2=\frac{1}{a_6^3}\left(\frac{2}{27}a_4^3-\frac{1}{3}a_2a_4a_6+a_0a_6^2\right).$$

The qualitative nature of the roots Y^2 for the reduced cubic equation (A2) is illustrated in Fig. 7. The shaded region indicates where there exists at least one Y^2 satisfying $\mathrm{Im}(Y^2)\neq 0$, which comes from one real root Y^2 (denoted by a circle on each horizontal axis of the root sketches in the shaded region) and one pair of complex roots Y^2. These roots will directly relate back to the roots $\hat{\Lambda}$—see the remarks that follow. The details for the construction of the split (τ_1,τ_2)-plane are

given, for instance, by Bruce and Giblin.[17] To describe the region where requirement (4.1) holds, note the following remarks:

(1) $\mathrm{Im}(\hat{\Lambda}^2) \neq 0$ if and only if $\mathrm{Im}(Y^2) \neq 0$;
(2) $\mathrm{Im}(\hat{\Lambda}) \neq 0$ whenever $\mathrm{Im}(\hat{\Lambda}^2) \neq 0$;
(3) all real roots Y^2 relate back to all real roots $\hat{\Lambda}^2$ but there is the possibility that at least one of these roots will be negative; hence, $\mathrm{Im}(\hat{\Lambda}) \neq 0$ for at least one $\hat{\Lambda}$.

Therefore, the existence of at least one root $\hat{\Lambda}$ with nonzero imaginary part is confirmed whenever any of the following criteria are satisfied:

(i) $27\tau_2^2+4\tau_1^3>0$;
(ii) $27\tau_2^2+4\tau_1^3\leqslant 0$, $Y^2-(a_4/3a_6)<0$, and $\tau_1\tau_2\neq 0$.

It should be noted that, for N CNLS equations, substituting the appropriate coefficient expressions from Appendix B will result in a particularly complicated pair of criteria (one of which will only be obtainable after solving the reduced cubic equation). Fortunately, condition (i) can be split into a number of smaller disjoint areas; for example, it can be represented as the union of the following:

(i)
  (a) $\tau_1>0$;
  (b) $\tau_1<0$ and $27\tau_2^2+4\tau_1^3>0$;

which is just another way of describing the shaded region in Fig. 7. Indeed, condition (i)(a) is a lot more pleasant to evaluate. Although it does not give the complete picture, it does give a relatively simpler sufficient condition for instability. On evaluating condition (i)(a), under the convenient assumption that $\epsilon_j^2=1$ for all j, the following is obtained:

$$3\textsc{Mixed} > (\gamma_1\beta_{11}|\hat{M}_{01}|^2 + \gamma_2\beta_{22}|\hat{M}_{02}|^2 + \gamma_3\beta_{33}|\hat{M}_{03}|^2)^2,$$

where

$$\begin{aligned}\textsc{Mixed} = {} & \gamma_1\gamma_2(\beta_{11}\beta_{22}-\beta_{12}\beta_{21})|\hat{M}_{01}|^2|\hat{M}_{02}|^2 + \gamma_1\gamma_3(\beta_{11}\beta_{33}-\beta_{13}\beta_{31})|\hat{M}_{01}|^2|\hat{M}_{03}|^2 \\ & + \gamma_2\gamma_3(\beta_{22}\beta_{33}-\beta_{23}\beta_{32})|\hat{M}_{02}|^2|\hat{M}_{03}|^2.\end{aligned}$$

It is noted that condition (ii) can be simplified for the nontrivial case (all roots nonzero) whenever Eq. (A1) has an odd number of negative real roots. This can be determined by considering $\mathrm{sign}(a_0/a_6)$. Therefore, a partial—but, in practice, useful—alternative to condition (ii) is the following:

$$27\tau_2^2+4\tau_1^3\leqslant 0, \quad \frac{a_0}{a_6}>0, \quad \text{and} \quad \tau_1\tau_2\neq 0.$$

It should also be noted that there is no obvious way to distinguish between two negative real roots (from three nontrivial real roots) using $\mathrm{sign}(a_0/a_6)$, as one positive and two negative real roots share the same sign as three positive real roots.

4. Four coupled waves

Consider four coupled waves (3.1) with $k_j=0$. The associated biquartic stability equation is

$$a_8\hat{\Lambda}^8 + a_6\hat{\Lambda}^6 + a_4\hat{\Lambda}^4 + a_2\hat{\Lambda}^2 + a_0 = 0. \tag{A3}$$

The retrieve qualitative information regarding the roots of Eq. (A3), first divide through by a_8 (assuming $a_8\neq 0$) and reduce Eq. (A3) to the following form:

$$Y^8 + \tau_1 Y^4 + \tau_2 Y^2 + \tau_3 = 0, \quad \text{where} \quad Y^2 = \hat{\Lambda}^2 + \frac{a_6}{4a_8}, \tag{A4}$$

with

$$\tau_1 = \frac{1}{a_8^2}\left(-\frac{3}{8}a_6^2 + a_8 a_4\right),$$

$$\tau_2 = \frac{1}{a_8^3}\left(\frac{1}{8}a_6^3 - \frac{1}{2}a_8 a_6 a_4 + a_8^2 a_2\right),$$

$$\tau_3 = \frac{1}{a_8^4}\left(-\frac{3}{256}a_6^4 + \frac{1}{16}a_8 a_6^2 a_4 - \frac{1}{4}a_8^2 a_6 a_2 + a_8^3 a_0\right).$$

Therefore, the transformation has reduced the four-parameter set $\{\hat{a}_6, \hat{a}_4, \hat{a}_2, \hat{a}_0\}$ where $\hat{a}_{2\ell} = a_{2\ell}/a_8$ to a related three-parameter set $\{\tau_1, \tau_2, \tau_3\}$, which greatly aids realizing the division of parameter space. The envelope surface for a general quartic equation, plotted in (τ_1, τ_2, τ_3)-space, is commonly known as a dovetail or swallowtail surface.[17] (See also Fig. 1.) There are three diagnostic functions associated with the general reduced quartic equation (A4), namely

$$D_1 = \tau_1, \quad D_2 = \text{DISCRIMINANT}, \quad D_3 = \tau_1^2 - 4\tau_3,$$

where

$$\text{DISCRIMINANT} = 16\tau_3\tau_1^4 - 4\tau_2^2\tau_1^3 - 128\tau_3^2\tau_1^2 + 144\tau_2^2\tau_3\tau_1 - 27\tau_2^4 + 256\tau_3^3.$$

These diagnostics will allow the region where requirement (4.1) holds to be completely described. Taking into account remarks (1)–(3), the existence of at least one $\hat{\Lambda}$ with nonzero imaginary part is confirmed whenever any of the following criteria are satisfied:

(i) $D_1 > 0$;
(ii) $D_1 = 0$ and ($\tau_2 \neq 0$ or $\tau_3 \neq 0$);
(iii) $D_1 < 0$ and $D_2 < 0$;
(iv) $D_1 < 0$, $D_2 \geqslant 0$, and $D_3 < 0$;
(v) $D_1 < 0$, $D_2 \geqslant 0$, $D_3 \geqslant 0$, and $Y^2 - (a_6/4a_8) < 0$.

Criteria (i)–(iv) result from directly analyzing the quartic equation in Y^2, while criterion (v) is an additional possibility due to investigating the roots $\hat{\Lambda}$ and can be verified for each particular application as both a_6 and a_8 will be known and Y^2 can be calculated [by solving the quartic equation (A4) for Y^2 by hand[18] or by using computer algebra software such as MAPLE[19]). Calling on Appendix B, supposing $\epsilon_j^2 = 1$ for all j, condition (i) evaluates to

$$3(\gamma_1^2\beta_{11}^2|\hat{M}_{01}|^4 + \gamma_2^2\beta_{22}^2|\hat{M}_{02}|^4 + \gamma_3^2\beta_{33}^2|\hat{M}_{03}|^4 + \gamma_4^2\beta_{44}^2|\hat{M}_{04}|^4) - 2\text{MIXED} < 0,$$

where

$$\begin{aligned}\text{MIXED} = {} & \gamma_1\gamma_2(\beta_{11}\beta_{22} - 4\beta_{12}\beta_{21})|\hat{M}_{01}|^2|\hat{M}_{02}|^2 + \gamma_1\gamma_3(\beta_{11}\beta_{33} - 4\beta_{13}\beta_{31})|\hat{M}_{01}|^2|\hat{M}_{03}|^2 + \gamma_1\gamma_4(\beta_{11}\beta_{44} \\ & - 4\beta_{14}\beta_{41})|\hat{M}_{01}|^2|\hat{M}_{04}|^2 + \gamma_2\gamma_3(\beta_{22}\beta_{33} - 4\beta_{23}\beta_{32})|\hat{M}_{02}|^2|\hat{M}_{03}|^2 + \gamma_2\gamma_4(\beta_{22}\beta_{44} - 4\beta_{24}\beta_{42}) \\ & \times|\hat{M}_{02}|^2|\hat{M}_{04}|^2 + \gamma_3\gamma_4(\beta_{33}\beta_{44} - 4\beta_{34}\beta_{43})|\hat{M}_{03}|^2|\hat{M}_{04}|^2.\end{aligned}$$

Conditions (ii)–(v) can be evaluated likewise. Similar to the analysis for the bicubic equation (A1), if Eq. (A3) has an odd number of negative real roots (for the nontrivial four real roots case), then condition (v) can be partially substituted for the simpler condition

$$D_1 < 0, \quad D_2 \geqslant 0, \quad D_3 \geqslant 0, \quad \text{and } \frac{a_0}{a_8} < 0.$$

Just as for the bicubic analysis, no simplified expression is offered for (v) with two or four negative real roots as they cannot be distinguished from an even number of positive real roots by using $\text{sign}(a_0/a_8)$.

A simpler set of criteria can be offered for the special case when $\tau_2=0$. Under this assumption, Y is governed by $Y^8+\tau_1 Y^4+\tau_3=0$. So, Y^4 satisfies a quadratic equation and, therefore, by noting remarks (1)–(3), the existence of at least one root $\hat{\Lambda}$ with nonzero imaginary part is confirmed whenever any of the following criteria are satisfied:

(I) $\tau_1 > 0$;
(II) $\tau_1 < 0$ and $\tau_3 \leqslant 0$;
(III) $\tau_1 \leqslant 0$ and $\tau_1^2 - 4\tau_3 < 0$;
(IV)

$$\tau_1 \leqslant 0, \quad \gamma_1^2 - 4\tau_3 \geqslant 0, \quad \text{and} \quad \pm\left(\frac{-\tau_1 \pm \sqrt{\tau_1^2 - 4\tau_3}}{2}\right)^{1/2} - \frac{a_6}{4a_8} < 0.$$

To emphasize the nonuniqueness for a complete description of requirement (4.1), the region encapsulated by criteria (I) and (II) could equally well be given as the following pair of criteria:

(I) $\tau_3 < 0$;
(II) $\tau_3 \geqslant 0$ and $\tau_1 > 0$.

See Fig. 3 for a graphical representation of where at least one root Y^2 exists with $\text{Im}(Y^2) \neq 0$—the shaded parts denote the relevant region (in the diagram $y=Y^2$, $c_1=\tau_1$ and $c_2=\tau_3$).

5. Remarks on *N* coupled waves

Consider N coupled waves (3.1) with $k_j=0$. It has already been illustrated that sufficient conditions for linear instability can be offered from criteria that only partially describe the parameter space satisfying requirement (4.1). These criteria must be used with care as they do not tell the whole story.

Determining sufficient conditions for instability pivots on how one attempts to analyze the stability polynomial equation (4.2). After all, other assumptions can be made, which will result in a reduced parameter space. For example, Roskes[6] noted that a generalization to N modes may be obtained by recalling there will be a suitable root of Eq. (4.2), whenever $\text{POLY}(0) < 0$, where

$$\text{POLY}(\hat{\Lambda}) = \hat{\Lambda}^{2N} + \frac{a_{2(N-1)}}{a_{2N}}\hat{\Lambda}^{2(N-1)} + \cdots + \frac{a_2}{a_{2N}}\hat{\Lambda}^2 + \frac{a_0}{a_{2N}},$$

occurring for α small, if

$$(-1)^N \det(\boldsymbol{\beta}) \prod_{j=1}^{N} \gamma_j < 0.$$

Roskes also remarked that, although this criterion conveniently generalizes the necessary and sufficient condition for instability of one mode ($\gamma_1\beta_{11}>0$), by no means is it necessary for instability of more than one mode. This was illustrated by Roskes[6] for $N=2$, which is recapped (by fixing ϵ_1 and ϵ_2) as follows. An unstable system for which $\gamma_1\gamma_2 \det(\boldsymbol{\beta}) < 0$ does not hold may be constructed by setting $\epsilon_1=\epsilon_2=1$, $\gamma_1=\gamma_2>0$, $\beta_{11}=\beta_{22}=2\beta_{12}=2\beta_{21}>0$ and, if one sets $\hat{M}_1=\hat{M}_2 \neq 0$, this returns the problem to the unstable single-mode case. Although Roskes' criterion[6] does not hold, the criterion

$$\gamma_1\gamma_2 \det(\boldsymbol{\beta}) \geqslant 0 \quad \text{and} \quad \gamma_1\epsilon_2^2\beta_{11}|\hat{M}_{01}|^2 + \epsilon_1^2\gamma_2\beta_{22}|\hat{M}_{02}|^2 > 0$$

presented by Bridges and Laine-Pearson[5]—and recalled in this paper—does.

APPENDIX B: COEFFICIENTS FOR THE *N* CNLS EQUATIONS

The coefficients that follow relate to the system of N CNLS equations (2.2) governing the solution family (3.1) with $k_j=0$, for all j.

1. One wave

For $N=1$ the stability equation is $a_2\hat{\Lambda}^2+a_0=0$, where

$$a_2 = \frac{\epsilon_1^2}{2\det(\boldsymbol{\beta})} \quad \text{and} \quad a_0 = \gamma_1|\hat{M}_{01}|^2.$$

2. Two waves

For $N=2$ the stability equation is $a_4\hat{\Lambda}^4+a_2\hat{\Lambda}^2+a_0=0$, where

$$a_4 = \frac{\epsilon_1^2\epsilon_2^2}{4\det(\boldsymbol{\beta})},$$

$$a_2 = \frac{1}{2\det(\boldsymbol{\beta})}(\gamma_1\epsilon_2^2\beta_{11}|\hat{M}_{01}|^2 + \epsilon_1^2\gamma_2\beta_{22}|\hat{M}_{02}|^2),$$

$$a_0 = \gamma_1\gamma_2|\hat{M}_{01}|^2|\hat{M}_{02}|^2.$$

3. Three waves

For $N=3$ the stability equation is $a_6\hat{\Lambda}^6+a_4\hat{\Lambda}^4+a_2\hat{\Lambda}^2+a_0=0$, where

$$a_6 = \frac{\epsilon_1^2\epsilon_2^2\epsilon_3^2}{8\det(\boldsymbol{\beta})},$$

$$a_4 = \frac{1}{4\det(\boldsymbol{\beta})}(\gamma_1\epsilon_2^2\epsilon_3^2\beta_{11}|\hat{M}_{01}|^2 + \epsilon_1^2\gamma_2\epsilon_3^2\beta_{22}|\hat{M}_{02}|^2 + \epsilon_1^2\epsilon_2^2\gamma_3\beta_{33}|\hat{M}_{03}|^2),$$

$$a_2 = \frac{1}{2\det(\boldsymbol{\beta})}\left(\gamma_1\gamma_2\epsilon_3^2\begin{vmatrix}\beta_{11} & \beta_{12}\\ \beta_{21} & \beta_{22}\end{vmatrix}|\hat{M}_{01}|^2|\hat{M}_{02}|^2 + \gamma_1\epsilon_2^2\gamma_3\begin{vmatrix}\beta_{11} & \beta_{13}\\ \beta_{31} & \beta_{33}\end{vmatrix}|\hat{M}_{01}|^2|\hat{M}_{03}|^2\epsilon_1^2\gamma_2\gamma_3\begin{vmatrix}\beta_{22} & \beta_{23}\\ \beta_{32} & \beta_{33}\end{vmatrix}\right)$$
$$\times|\hat{M}_{02}|^2|\hat{M}_{03}|^2,$$

$$a_0 = \gamma_1\gamma_2\gamma_3|\hat{M}_{01}|^2|\hat{M}_{02}|^2|\hat{M}_{03}|^2.$$

4. Four waves

For $N=4$ the stability equation is $a_8\hat{\Lambda}^8+a_6\hat{\Lambda}^6+a_4\hat{\Lambda}^4+a_2\hat{\Lambda}^2+a_0=0$, where

$$a_8 = \frac{\epsilon_1^2\epsilon_2^2\epsilon_3^3\epsilon_4^2}{16\det(\boldsymbol{\beta})},$$

$$a_6 = \frac{1}{8\,\det(\boldsymbol{\beta})}(\gamma_1\epsilon_2^2\epsilon_3^2\epsilon_4^2\beta_{11}|\hat{M}_{01}|^2 + \epsilon_1^2\gamma_2\epsilon_3^3\epsilon_4^2\beta_{22}|\hat{M}_{02}|^2 + \epsilon_1^2\epsilon_2^2\gamma_3\epsilon_4^2\beta_{33}|\hat{M}_{03}|^2 + \epsilon_1^2\epsilon_2^2\epsilon_3^3\gamma_4\beta_{44}|\hat{M}_{04}|^2),$$

$$\begin{aligned} a_4 = \frac{1}{4\,\det(\boldsymbol{\beta})}\Bigg(& \gamma_1\gamma_2\epsilon_3^2\epsilon_4^2\begin{vmatrix}\beta_{11} & \beta_{12}\\ \beta_{21} & \beta_{22}\end{vmatrix}|\hat{M}_{01}|^2|\hat{M}_{02}|^2 + \gamma_1\epsilon_2^2\gamma_3\epsilon_4^2\begin{vmatrix}\beta_{11} & \beta_{13}\\ \beta_{31} & \beta_{33}\end{vmatrix}|\hat{M}_{01}|^2|\hat{M}_{03}|^2 \\ & + \gamma_1\epsilon_2^2\epsilon_3^2\gamma_4\begin{vmatrix}\beta_{11} & \beta_{14}\\ \beta_{41} & \beta_{44}\end{vmatrix}|\hat{M}_{01}|^2|\hat{M}_{04}|^2 + \epsilon_1^2\gamma_2\gamma_3\epsilon_4^2\begin{vmatrix}\beta_{22} & \beta_{23}\\ \beta_{32} & \beta_{33}\end{vmatrix}|\hat{M}_{02}|^2|\hat{M}_{03}|^2 + \epsilon_1^2\gamma_2\epsilon_3^2\gamma_4\begin{vmatrix}\beta_{22} & \beta_{24}\\ \beta_{42} & \beta_{44}\end{vmatrix} \\ & \times|\hat{M}_{02}|^2|\hat{M}_{04}|^2 + \epsilon_1^2\epsilon_2^2\gamma_3\gamma_4\begin{vmatrix}\beta_{33} & \beta_{34}\\ \beta_{43} & \beta_{44}\end{vmatrix}|\hat{M}_{03}|^2|\hat{M}_{04}|^2\Bigg), \end{aligned}$$

$$\begin{aligned} a_2 = \frac{1}{2\,\det(\boldsymbol{\beta})}\Bigg(& \gamma_1\gamma_2\gamma_3\epsilon_4^2\begin{vmatrix}\beta_{11} & \beta_{12} & \beta_{13}\\ \beta_{21} & \beta_{22} & \beta_{23}\\ \beta_{31} & \beta_{32} & \beta_{33}\end{vmatrix}|\hat{M}_{01}|^2|\hat{M}_{02}|^2|\hat{M}_{03}|^2 + \gamma_1\gamma_2\epsilon_3^2\gamma_4\begin{vmatrix}\beta_{11} & \beta_{12} & \beta_{14}\\ \beta_{21} & \beta_{22} & \beta_{24}\\ \beta_{41} & \beta_{42} & \beta_{44}\end{vmatrix} \\ & \times|\hat{M}_{01}|^2|\hat{M}_{02}|^2|\hat{M}_{04}|^2 + \gamma_1\epsilon_2^2\gamma_3\gamma_4\begin{vmatrix}\beta_{11} & \beta_{13} & \beta_{14}\\ \beta_{31} & \beta_{33} & \beta_{34}\\ \beta_{41} & \beta_{43} & \beta_{44}\end{vmatrix}|\hat{M}_{01}|^2|\hat{M}_{03}|^2|\hat{M}_{04}|^2 \\ & + \epsilon_1^2\gamma_2\gamma_3\gamma_4\begin{vmatrix}\beta_{22} & \beta_{23} & \beta_{24}\\ \beta_{32} & \beta_{33} & \beta_{34}\\ \beta_{42} & \beta_{43} & \beta_{44}\end{vmatrix}|\hat{M}_{02}|^2|\hat{M}_{03}|^2|\hat{M}_{04}|^2\Bigg), \end{aligned}$$

$$a_0 = \gamma_1\gamma_2\gamma_3\gamma_4|\hat{M}_{01}|^2|\hat{M}_{02}|^2|\hat{M}_{03}|^2|\hat{M}_{04}|^2.$$

5. *N* waves

For arbitrary N waves the stability equation is

$$a_{2N}\hat{\Lambda}^{2N} + a_{2(N-1)}\hat{\Lambda}^{2(N-1)} + \cdots + a_2\hat{\Lambda}^2 + a_0 = 0,$$

where

$$a_{2N} = \frac{1}{2^N\,\det(\boldsymbol{\beta})}\prod_{j=1}^{N}\epsilon_j^2,$$

$$a_{2(N-1)} = \frac{1}{2^{N-1}\,\det(\boldsymbol{\beta})}\sum_{j=1}^{N}\left(\prod_{\substack{\ell=1\\ \ell\neq j}}^{N}\epsilon_\ell^2\right)\gamma_j\beta_{jj}|\hat{M}_{0j}|^2,$$

$$\vdots$$

$$a_0 = \prod_{j=1}^{N}\gamma_j|\hat{M}_{0j}|^2.$$

[1] Note that the notion of a 'bisymplectic system' is not the same as a 'bi-Hamiltonian system' (see Olver Ref. 20, for details regarding the latter).
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Supersymmetric nonlocal gas equation

Ashok Das
Department of Physics and Astronomy, University of Rochester, Rochester, New York 14627-0171

Z. Popowicz[a)]
Institute of Theoretical Physics, University of Wrocław, pl. M. Borna 9, 50-205 Wrocław, Poland

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In this paper we study systematically the question of supersymmetrization of the nonlocal gas equation. We obtain both the $N=1$ and the $N=2$ supersymmetric generalizations of the system which are integrable. We show that both the systems are bi-Hamiltonian. While the $N=1$ supersymmetrization allows the hierarchy of equations to be extended to negative orders (local equations), we argue that this is not the case for the $N=2$ supersymmetrization. In the bosonic limit, however, the $N=2$ system of equations lead to a new coupled integrable system of equations. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1993547]

I. INTRODUCTION

The classical isentropic gas equations[1]

$$u_t + uu_x + \frac{1}{v}P_x = 0,$$

$$v_t + (vu)_x = 0, \tag{1}$$

where u, v denote, respectively, the velocity and the density of the gas, are known to constitute an interesting class of dispersionless integrable systems when the pressure is a monomial function of the density. For example, $P=v^\gamma$, $\gamma \neq 0$, 1 corresponds to the polytropic gas, while $P=-1/v$ describes the Chaplygin gas.[2,3] Both these systems are of hydrodynamic type,[4] integrable, and a lot is known about the properties of these systems. Recently, it was shown that the gas equation for the case $P=-\frac{1}{2}(\partial^{-1}v)^2$ (called the nonlocal gas equation) is also integrable and has a very rich algebraic structure.[5,6] This system of equations arises in astrophysical models of dark matter.[7] In this paper, we will study the supersymmetrization of this system maintaining integrability of the model.

It is worth recalling that supersymmetrization of dispersionless systems is at best poorly understood at the present.[8,9] For example, in the case of polytropic gas, an integrable supersymmetric hierarchy has been obtained only for $N=1$ supersymmetrization besides the "trivial" susy-B supersymmetrization[10,11] and the supersymmetrization of the Chaplygin gas[12] resembles a susy-B symmetrization.[9] Even in the case of the $N=1$ supersymmetric polytropic gas (which is integrable), it is not known if it is a bi-Hamiltonian system. In contrast, we will show that integrable $N=1$ and $N=2$ supersymmetrizations are possible for the system of nonlocal gas dynamics. Furthermore, the $N=1$ supersymmetric system possesses two Hamiltonian structures which are com-

a)Electronic mail: ziemek@ift.uni.wroc.pl

patible so that it is truly a bi-Hamiltonian system and possesses all the rich algebraic structures of its bosonic counterpart. The $N=2$ supersymmetrization, on the other hand, leads to a new system of coupled integrable equations in the bosonic limit.

The paper is organized as follows. In Sec. II, we briefly recapitulate the essential features of the bosonic system and present results on the $N=1$ supersymmetric generalization that is integrable. We obtain the bi-Hamiltonian structure, the Casimir functionals as well as the conserved charges (local and nonlocal) of the system. In Sec. III, we present the essential results on the $N=2$ supersymmetrization of the system preserving integrability. We obtain the bi-Hamiltonian structure and argue that the second structure has no Casimir functional so that the system of equations cannot be extended to the negative orders. We present a brief summary of our results in Sec. IV.

II. $N=1$ SUPERSYMMETRIZATION

The nonlocal gas equation is described by the system of equations

$$u_t = -uu_x + (\partial^{-1}v),$$

$$v_t = -(uv)_x. \tag{2}$$

This system of equations is known to be integrable and alot of the algebraic properties for the system are well known. For example, it is known[5] that the system of Eqs. (2) is a bi-Hamiltonian system with the two compatible Hamiltonian structures described by

$$\mathcal{D}_1 = \begin{pmatrix} 0 & -\partial \\ -\partial & 0 \end{pmatrix}, \quad \mathcal{D}_2 = \begin{pmatrix} \partial^{-1} & -u_x \\ u_x & -(v\,\partial + \partial v) \end{pmatrix}. \tag{3}$$

The conserved charges satisfying the recursion relation can be constructed recursively and these charges are in involution by construction making the system integrable. Furthermore, the Hamiltonian structure $\mathcal{D}_1$ has three Casimir functionals (conserved charges whose gradients are annihilated by the Hamiltonian structures)

$$H_1 = \int \mathrm{d}x\, v,$$

$$H_1^{(1)} = -\int \mathrm{d}x\, u_x \to 0,$$

$$H_1^{(2)} = \int \mathrm{d}x\, u, \tag{4}$$

while the second Hamiltonian structure has a single Casimir functional

$$H_{-1} = 2\int \mathrm{d}x\left(v - \tfrac{1}{2}u_x^2\right)^{1/2}. \tag{5}$$

The existence of the Casimir functionals allows the hierarchy of flows to be extended to the negative order using the recursion relation and these are local equations unlike (2). In addition to the charges that are recursively constructed, the model also possesses two series of conserved charges whose gradients are not related by the recursion operator (and, therefore, are not in involution with the infinitely many charges which are in involution)

$$G_n = \int \mathrm{d}x\, u_x(\partial^{-1}v)^n, \quad \tilde{G}_n = \int \mathrm{d}x\left[u^2v + \frac{2}{2+n}(\partial^{-1}v)^2\right](\partial^{-1}v)^n. \tag{6}$$

However, a scalar Lax representation for the system is not known which leads to difficulties in applying the standard techniques of supersymmetrizing the system. Therefore, we construct the $N=1$ supersymmetric extension of the non-local gas equation which is integrable as follows.

Let us introduce the two fermionic superfields

$$U = \psi + \theta u, \quad V = \chi + \theta v, \tag{7}$$

where θ represents the Grassmann coordinate of the supermanifold and we assume the canonical dimensions

$$[x] = -1, \quad [t] = 2, \quad [U] = \tfrac{1}{2}, \quad [V] = \tfrac{7}{2}. \tag{8}$$

Writing out the most general equation of dimension $\left[\frac{5}{2}\right]$, the one that leads to the correct bosonic limit is given by

$$U_t = -U_x(DU) + (D^{-2}V), \tag{9}$$

$$V_t = -((DU)V)_x, \tag{10}$$

where

$$D = \frac{\partial}{\partial\theta} + \theta\frac{\partial}{\partial x}, \quad D^2 = \partial_x, \tag{11}$$

represents the supercovariant derivative on the superspace. In components, the equations take the forms

$$u_t = -uu_x + (\partial^{-1}v),$$

$$v_t = -(uv + \psi_x\chi)_x,$$

$$\psi_t = -\psi_x u + (\partial^{-1}\chi),$$

$$\chi_t = -(u\chi)_x. \tag{12}$$

Clearly, this represents a nontrivial $N=1$ supersymmetrization (and not a B-supersymmetrization) of (2). However, it is not obvious immediately if this is integrable.

We note that the system of Eqs. (10) is a Hamiltonian system of equations. In fact, the Hamiltonian

$$H_3 = \tfrac{1}{2}\int \mathrm{d}Z(V(DU)^2 + (D^{-2}V)(D^{-1}V)), \tag{13}$$

where $\mathrm{d}Z = \mathrm{d}x\mathrm{d}\theta$, together with the Hamiltonian structure

$$\mathcal{D}_1 = \begin{pmatrix} 0 & -D \\ -D & 0 \end{pmatrix}, \tag{14}$$

leads to (10) as

$$\begin{pmatrix} U_t \\ V_t \end{pmatrix} = \mathcal{D}_1 \begin{pmatrix} \dfrac{\delta H_3}{\delta U} \\ \dfrac{\delta H_3}{\delta V} \end{pmatrix}. \tag{15}$$

Similarly, it can also be checked that (10) can also be written as Hamiltonian equations with the Hamiltonian

$$H_2 = \int \mathrm{d}Z\, U(DV), \tag{16}$$

and the Hamiltonian structure

$$\mathcal{D}_2 = \begin{pmatrix} D^{-3} & -\frac{1}{2}(U_x + D^{-1}(DU_x)) \\ \frac{1}{2}(U_x + (DU_x)D^{-1}) & -\left(D(DV) + (DV)D - \frac{3}{2}DVD\right) \end{pmatrix}, \tag{17}$$

as

$$\begin{pmatrix} U_t \\ V_t \end{pmatrix} = \mathcal{D}_2 \begin{pmatrix} \dfrac{\delta H_2}{\delta U} \\ \dfrac{\delta H_2}{\delta V} \end{pmatrix}. \tag{18}$$

The Hamiltonian structures (14) and (17) have the necessary symmetry properties and it can be checked through the method of prolongation[13] that they satisfy Jacobi identity as well. Therefore, both $\mathcal{D}_1$ as well as $\mathcal{D}_2$ define genuine Hamiltonian structures. In fact, it is obvious that $\mathcal{D}_1$ satisfies Jacobi identity trivially. It can also be checked that the change of variables

$$\widetilde{U} = U_x, \quad \widetilde{V} = V - \tfrac{1}{2}(DU_x)U_x = V - \tfrac{1}{2}(D\widetilde{U})\widetilde{U}, \tag{19}$$

diagonalizes the second Hamiltonian structure which coincides with the supersymmetric $SL(2) \otimes U(1)$ algebra and thereby satisfies the Jacobi identity. More importantly, it can also be checked through the method of prolongation that an arbitrary linear combination

$$\mathcal{D} = \mathcal{D}_2 + \alpha\mathcal{D}_1, \tag{20}$$

also defines a Hamiltonian structure (satisfies Jacobi identity) so that we conclude that the system of Eqs. (10) is truly a bi-Hamiltonian system. It follows now from Magri's theorem that the supersymmetric system of equations is integrable.

From the two Hamiltonian structures in (14) and (17), we can obtain the recursion operator associated with the system defined as

$$\mathcal{R} = \mathcal{D}_2\mathcal{D}_1^{-1} \tag{21}$$

$$= \begin{pmatrix} \frac{1}{2}(U_x + D^{-1}(DU_x))D^{-1} & -D^{-4} \\ (D^2V)D^{-1} + \frac{1}{2}(DV) + \frac{3}{2}VD & -\frac{1}{2}(U_x + D^{-1}(DU_x)D^{-1} \end{pmatrix}. \tag{22}$$

This helps us determine the conserved quantities associated with the system recursively and the first few take the forms

$$H_1 = \int \mathrm{d}Z\, V,$$

$$H_2 = \int \mathrm{d}Z\, U(DV),$$

$$H_3 = \tfrac{1}{2} \int \mathrm{d}Z[(DU)^2 V + (D^{-1}V)(D^{-2}V)],$$

$$H_4 = \int \mathrm{d}Z[(DU)^3 V - 3U(D^{-1}V)^2 - 6(DU)V(D^{-3}V)],$$

$$\vdots \tag{23}$$

These charges are all conserved and are in involution with one another by construction reflecting the integrability of the system.

It is worth noting that all the charges in the series (23) are bosonic. In addition, we have found a charge that is fermionic and is conserved under the flow. It has the form

$$\widetilde{H} = \int \mathrm{d}Z\, UV(D^{-2}V). \tag{24}$$

Furthermore, much like the bosonic system, we have also found two series of bosonic conserved charges that are not related recursively

$$G_n = \int \mathrm{d}Z\, U(DV)(D^{-1}V)^n,$$

$$\widetilde{G}_n = \int \mathrm{d}Z(\partial^{-1}V)(D^{-1}V)^n[(n+2)(D^{-1}V)^2 + (n+1)(n+3)U_x V(DU) - (n+3)(D^{-1}U)(DU)(DU_x)]. \tag{25}$$

Much like the bosonic system, the $N=1$ supersymmetric system also has Casimir functionals whose gradients are annihilated by the two Hamiltonian structures of the system. It is easy to check that the three conserved quantities

$$H_1 = \int \mathrm{d}Z\, V,$$

$$H_1^{(1)} = -\int \mathrm{d}Z\, U_x \to 0,$$

$$H_1^{(2)} = \int \mathrm{d}Z\, U, \tag{26}$$

are conserved and are Casimir functionals of the first Hamiltonian structure (14), namely,

$$\mathcal{D}_1 \begin{pmatrix} \dfrac{\delta H_1}{\delta U} \\ \dfrac{\delta H_1}{\delta V} \end{pmatrix} = \mathcal{D}_1 \begin{pmatrix} \dfrac{\delta H_1^{(1)}}{\delta U} \\ \dfrac{\delta H_1^{(1)}}{\delta V} \end{pmatrix} = \mathcal{D}_1 \begin{pmatrix} \dfrac{\delta H_1^{(2)}}{\delta U} \\ \dfrac{\delta H_1^{(2)}}{\delta V} \end{pmatrix} = 0. \tag{27}$$

This is very much like in the bosonic model. Furthermore, the second Hamiltonian structure (17) also has a Casimir functional

$$H_{-1} = \int \mathrm{d}Z \frac{V - \frac{1}{2}(DU_x)U_x}{\sqrt{(DV) - \frac{1}{2}(DU_x)^2 - \frac{1}{2}U_{xx}U_x}}, \tag{28}$$

which is conserved and satisfies

$$\mathcal{D}_2 \begin{pmatrix} \dfrac{\delta H_{-1}}{\delta U} \\ \dfrac{\delta H_{-1}}{\delta V} \end{pmatrix} = 0. \tag{29}$$

The existence of Casimir functionals suggests that the hierarchy of equations generated by H_n, $n>0$ can be extended to the negative orders through the inverse of the recursion operator (22). Formally, the inverse can be defined as

$$\mathcal{R}^{-1} = \mathcal{D}_1 \mathcal{D}_2^{-1}. \tag{30}$$

However, it is worth noting here that unlike in the bosonic case where a closed form expression for the inverse exists, here we have not found such a form. However, one can easily construct the conserved charges associated with the negative order of the hierarchy using the recursion relation

$$\mathcal{D}_1 \begin{pmatrix} \dfrac{\delta H_{-n}}{\delta U} \\ \dfrac{\delta H_{-n}}{\delta V} \end{pmatrix} = \mathcal{D}_2 \begin{pmatrix} \dfrac{\delta H_{-n-1}}{\delta U} \\ \dfrac{\delta H_{-n-1}}{\delta V} \end{pmatrix}. \tag{31}$$

For example, this leads to the first few conserved local charges of the forms

$$H_{-1} = 2\int \mathrm{d}Z \frac{\tilde{V}}{\sqrt{(D\tilde{V})}},$$

$$H_{-2} = -\int \mathrm{d}Z \left[\frac{2U_{xx}}{\sqrt{(D\tilde{V})}} - \frac{(DU_{xx})\tilde{V}}{(D\tilde{V})^{3/2}} \right],$$

$$H_{-3} = \frac{1}{12}\int \mathrm{d}Z \left[\frac{\left(12U_{xx}(DU_{xx}) + 10\tilde{V}_{xx}\right)}{(D\tilde{V})^{3/2}} - \frac{9\tilde{V}\left((D\tilde{V}_{xx}) + (DU_{xx})^2\right)}{(D\tilde{V})^{5/2}} \right],$$

$$H_{-4} = \frac{1}{8}\int \mathrm{d}Z \left[\frac{10U_{xxx}(D\tilde{V}_x) - 6U_{xx}(D\tilde{V}_{xx}) - 6U_{xx}(DU_{xx})^2 - 10\tilde{V}_{xx}(DU_{xx}) - 6\tilde{V}(DU_{xxxx})}{(D\tilde{V})^{5/2}} + \frac{15\tilde{V}(D\tilde{V}_{xx})(DU_{xx}) + 5\tilde{V}(DU_{xx})^3}{(D\tilde{V})^{7/2}} \right],$$

$$\vdots \tag{32}$$

where $\tilde{V}$ is defined in (19). These charges, of course, satisfy the recursion relation (and, therefore, are in involution) and reduce to the known charges in the bosonic limit, but it is interesting to note that in the bosonic limit, the last two terms in H_{-4} vanish.

Given the Hamiltonians in the negative hierarchy, we can obtain the equations through the known Hamiltonian structures. We simply note that the lowest order equation in the negative hierarchy has the form

$$U_{t_{-1}} = -D\left(\frac{1}{(D\tilde{V})^{1/2}} - D\frac{\tilde{V}}{2\tilde{V}_x^{3/2}} \right), \tag{33}$$

$$V_{t_{-1}} = -D\,\partial\left((DU_x - (\mathrm{DU}_X))\frac{1}{(D\tilde{V})^{1/2}} - (2(\mathrm{DU}_X)D - U_X\,\partial)\frac{\tilde{V}}{2(D\tilde{V})^{3/2}} \right)$$

The bosonic limit of these equations can be easily checked to be the local equations of the negative hierarchy of the nonlocal gas equation.[5]

III. *N*=2 SUPERSYMMETRIZATION

The $N=2$ supersymmetrization of the nonlocal gas equation can now be obtained in a simple manner. Let us define bosonic superfields $\bar{U}$, $\bar{V}$ in the $N=2$ extended superspace as

$$\bar{U} = U_1 + \theta_2 U, \quad \bar{V} = V_1 + \theta_2 V, \tag{34}$$

where U, V are the $N=1$ superfields defined in the last section while U_1, V_1 represent two new $N=1$ bosonic superfields. In this extended superspace, we can define two covariant derivatives as

$$D_1 = \frac{\partial}{\partial\theta_1} + \theta_1\frac{\partial}{\partial x},$$

$$D_2 = \frac{\partial}{\partial\theta_2} + \theta_2\frac{\partial}{\partial x},$$

$$D_1^2 = D_2^2 = \frac{\partial}{\partial x}, \quad D_1 D_2 + D_2 D_1 = 0. \tag{35}$$

With these, the $N=2$ supersymmetric nonlocal gas equation which reduces to the $N=1$ system (10) and is integrable takes the form

$$\bar{U}_t = -(D_1 D_2 \bar{U})\bar{U}_x + (\partial^{-1}\bar{V}),$$

$$\bar{V}_t = -(\bar{V}(D_1 D_2 \bar{U}))_x + D_1 D_2[\bar{V}\bar{U}_x + (D_2\bar{U}_x)(D_1\bar{U}_x)\bar{U}_x - (D_1 D_2 \bar{U}_x)\bar{U}_x^2]. \tag{36}$$

The system of Eqs. (36) can be written as a Hamiltonian system with

$$\mathcal{D}_1 = \begin{pmatrix} 0 & D_1 D_2 \partial^{-1} \\ D_1 D_2 \partial^{-1} & 0 \end{pmatrix},$$

$$H = \tfrac{1}{6}\int d\bar{Z}[(D_1 D_2 \bar{U}_x)\bar{U}_x^3 - 3(D_1 D_2 \partial^{-1}\bar{V})(2(D_1 D_2 \bar{U})\bar{U}_x - (\partial^{-1}\bar{V}))], \tag{37}$$

(where $d\bar{Z} = dx\, d\theta_1 d\theta_2$) so that

$$\begin{pmatrix} \bar{U}_t \\ \bar{V}_t \end{pmatrix} = \mathcal{D}_1 \begin{pmatrix} \dfrac{\delta H}{\delta \bar{U}} \\ \dfrac{\delta H}{\delta \bar{V}} \end{pmatrix}. \tag{38}$$

The Hamiltonian structure clearly has the necessary antisymmetry properties and trivially satisfies the Jacobi identity.

The system of Eqs. (36) has a second Hamiltonian description as well. It can be checked that the equations can be written in the Hamiltonian form

$$\begin{pmatrix} \bar{U}_t \\ \bar{V}_t \end{pmatrix} = \mathcal{D}_2 \begin{pmatrix} \dfrac{\delta \bar{H}}{\delta \bar{U}} \\ \dfrac{\delta \bar{H}}{\delta \bar{V}} \end{pmatrix} \tag{39}$$

with the Hamiltonian

$$\bar{H} = \int d\bar{Z}(D_1 D_2 \bar{U})\left[\bar{V} - \tfrac{1}{2}D_1(\bar{U}_x(D_2\bar{U}_x))\right], \tag{40}$$

and the second Hamiltonian structure $\mathcal{D}_2$ with the elements

$$(\mathcal{D}_2)_{11} = -\partial^{-1}D_1^{-1}D_2^{-1},$$

$$(\mathcal{D}_2)_{12} = \tfrac{1}{2}(-2\bar{U}_x + D_1^{-1}(D_1\bar{U}_x) + D_2^{-1}(D_2\bar{U}_x) + 2D_1^{-1}D_2^{-1}(D_1 D_2\bar{U}_x)),$$

$$(\mathcal{D}_2)_{21} = \tfrac{1}{2}(2\bar{U}_x + (D_1\bar{U}_x)D_1^{-1} + (D_2\bar{U}_x)D_2^{-1} - 2(D_1 D_2\bar{U}_x)D_1^{-1}D_2^{-1}),$$

$$(\mathcal{D}_2)_{22} = \tfrac{1}{2}(-2\,\partial\bar{V} - 2\bar{V}\,\partial + D_1\bar{V}D_1 + D_2\bar{V}D_2 - \partial\bar{U}_x^2 D_1D_2 + \bar{U}_x^2\,\partial D_1D_2 + D_2\bar{U}_x^2\,\partial D_1 - D_1\bar{U}_x^2\,\partial D_2)$$
$$+ (D_1D_2\bar{U}_x)\partial^{-1}D_1D_2\bar{U}_xD_1D_2. \tag{41}$$

The second Hamiltonian structure is quite complicated and one can check the Jacobi identity through the method of prolongation. However, it is much easier to check this through a change of variables

$$\tilde{\bar{U}} = \bar{U}_x, \quad \tilde{\bar{V}} = \bar{V} - (D_1D_2\tilde{\bar{U}})\tilde{\bar{U}} - \tfrac{1}{2}(D_1\tilde{\bar{U}})(D_2\tilde{\bar{U}}), \tag{42}$$

the second Hamiltonian structure coincides with the $N=2$ supersymmetric generalization of the $SL(2)\otimes U(1)$ algebra and thereby satisfies the Jacobi identity. Furthermore, the compatibility of the two structures $\mathcal{D}_1$ and $\mathcal{D}_2$ can also be checked in a straightforward manner through prolongation. Therefore, it follows that the system of $N=2$ supersymmetric Eqs. (36) are integrable. The infinite set of conserved charges in involution can be constructed using the recursion relation. However, their forms are extremely complicated and are not very enlightening. So, we do not list them here.

The bosonic limit of (36) leads to a new and interesting coupled equation that is integrable. Introducing the notation that u_0, u_1 represent the bosonic variables of the superfield $\bar{U}$ and v_0, v_1 represent the bosonic variables of the superfield $\bar{V}$, the equations can be written as

$$u_{0,t} = -u_1u_{0,x} + (\partial^{-1}v_0),$$

$$u_{1,t} = u_{0,xx}u_{0,x} - u_{1,x}u_1 + (\partial^{-1}v_1),$$

$$v_{0,t} = u_{0,xxx}u_{0,x}^2 + u_{0,xx}^2u_{0,x} - u_{1,x}^2u_{0,x} - v_{0,x}u_1 + v_1u_{0,x},$$

$$v_{1,t} = (u_{1,xx}u_{0,x}^2 + 2u_{1,x}u_{0,xx}u_{0,x} - v_{0,x}u_{0,x} - v_1u_1)_x. \tag{43}$$

This is a new integrable system of equations and has the interesting feature that the second Hamiltonian structure for this system does not have any Casimir functional. As a result, the second Hamiltonian structure for the $N=2$ supersymmetric system in (41) does not also possess any Casimir functional (although the first structure does) and the system of Eqs. (36) cannot be extended to the negative hierarchy.

IV. SUMMARY

In this paper we have systematically studied the supersymmetrization of the nonlocal gas equation preserving integrability. We obtain the $N=1$ supersymmetric system of equations and show that it has two compatible Hamiltonian structures making it a bi-Hamiltonian system. We construct the conserved charges of the system and show that the two Hamiltonian structures possess Casimir functionals. As a result, the system of supersymmetric equations can be extended to negative orders and these give rise to local equations of motion. We also construct the $N=2$ supersymmetric generalization of the nonlocal gas equation and show that it is a bi-Hamiltonian system. In the bosonic limit, this equation leads to a new coupled integrable system of equations. Furthermore, we argue that in the $N=2$ supersymmetric case, while the first Hamiltonian structure possesses Casimir functionals, the second does not. As a result, these equations cannot be extended to negative orders.

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Existence theorems for two-fluid magnetohydrodynamics

Manuel Núñez[a)]
Departamento de Análisis Matemático, Universidad de Valladolid, 47005 Valladolid, Spain

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The description of a plasma as composed by two types of fluids, formed by ions and electrons, is more complete than the classical one-fluid magnetohydrodynamics (MHD) model and it has proved necessary to explain the phenomena of fast magnetic reconnection. We prove a finite-time theorem of existence and uniqueness of solutions for this system for either Dirichlet or periodic boundary conditions in dimension three. It turns out that the regularity estimates for the magnetic field are finer than the MHD ones. © *2005 American Institute of Physics.*
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I. INTRODUCTION AND MATHEMATICAL SETTING

The evolution of a collection of charged particles can often be modeled as the motion of several fluid species linked by electromagnetic forces. The most important instance is probably the two-fluid case, where positive ions and electrons form a quasineutral plasma. The equations of motion of both species, under reasonable approximations[1–3] may be combined to yield

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t}+\mathbf{v}\cdot\nabla\mathbf{v}\right)=\nu\Delta\mathbf{v}+\mathbf{J}\times\mathbf{B}-\nabla p+\mathbf{f}$$
$$\mathbf{E}+\mathbf{v}\times\mathbf{B}=\eta\mathbf{J}+\frac{1}{en}\mathbf{J}\times\mathbf{B}-\frac{1}{en}\nabla p_e+\frac{m}{e^2n}\frac{\partial\mathbf{J}}{\partial t}, \tag{1}$$

where the variables are explained as follows:

(1) $\mathbf{v}$ is the mass velocity

$$\mathbf{v}=\frac{M\mathbf{v}_i+m\mathbf{v}_e}{M+m},$$

where $\mathbf{v}_i$ is the ions velocity, M is its mass, $\mathbf{v}_e$ is the electrons velocity, and m is its mass. Since $M\gg m$, $\mathbf{v}\approx\mathbf{v}_i$.

(2) e is the electron charge.

(3) n is the electrons number density, approximately equal to the ions one, $\rho=n(M+m)$ the mass density. We will assume the fluid incompressible and will scale ρ to 1.

(4) ν is the kinematic viscosity and η is the resistivity. Both are taken as constant (positive) scalars, meaning that these plasma properties are homogeneous and isotropic.

(5) $p=p_i+p_e$ is the total pressure, sum of the ion and electron ones.

(6) $\mathbf{E}$ is the electric field, $\mathbf{B}$ is the magnetic one, and $\mathbf{J}=\nabla\times\mathbf{B}$ is the current density. This is also equal to $(\mathbf{v}_i-\mathbf{v}_e)en$.

(7) $\mathbf{f}$ is an arbitrary forcing on the momentum equation, given, e.g., by gravitational forces.

a)Electronic mail: mnjmhd@am.uva.es

It is apparent that the coefficient $m/(e^2n)$ is very small. Neglecting it we are left with the Hall magnetohydrodynamics (MHD) system. By neglecting also the current displacement in Maxwell's equations, an admissible procedure in low-frequency phenomena, and using Faraday's law

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E},$$

we are left with the Hall induction equation

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times (\eta \mathbf{J}) + \nabla \times (\mathbf{v} \times \mathbf{B}) - \frac{1}{en} \nabla \times (\mathbf{J} \times \mathbf{B}). \tag{2}$$

The Hall current term $(1/en)\nabla \times (\mathbf{J} \times \mathbf{B})$ is small in dense plasmas, and in general at large scales its effect is less important than the one of the velocity. Omitting it and using certain vector analysis identities, we obtain the classical incompressible MHD equations

$$\frac{\partial \mathbf{v}}{\partial t} = \nu \Delta \mathbf{v} - \mathbf{v} \cdot \nabla \mathbf{v} + \mathbf{B} \cdot \nabla \mathbf{B} - \nabla \left(p + \frac{1}{2} B^2 \right) + \mathbf{f},$$

$$\frac{\partial \mathbf{B}}{\partial t} = \eta \Delta \mathbf{B} + \nabla \times (\mathbf{v} \times \mathbf{B}), \tag{3}$$

$$\nabla \cdot \mathbf{v} = \nabla \cdot \mathbf{B} = 0.$$

Its study is well known and similar in many aspects to the one of the Navier–Stokes equation.[4] However, it has become apparent that in certain important physical phenomena, in particular those involving magnetic reconnection, the one-fluid description given by (3) is not appropriate. The extremely rapid conversion rate from magnetic to kinetic energy present in such spectacular phenomena as solar flares could not be adequately explained by any MHD model, and there was no lack of effort in this sense. There exists an enormous literature on this problem: see, e.g., Refs. 5–7, and references therein. It is generally accepted now that near the current sheets where reconnection occurs, electrons and ions cease to move together: it is the high electron velocity which prevents the throttling of MHD reconnection schemes and allows fast energy conversion. It is clear that a two-fluid description is necessary and therefore it seems natural to ask for some existence theorem for the relevant equation. Although admittedly the electron inertia term $m/(e^2n)$ is small, its presence is necessary to obtain a mathematically consistent model. By taking the curl of (1) and using Faraday's law, we obtain the two-fluid MHD system

$$\frac{\partial \mathbf{v}}{\partial t} = \nu \Delta \mathbf{v} - \mathbf{v} \cdot \nabla \mathbf{v} + \mathbf{B} \cdot \nabla \mathbf{B} - \nabla \left(p + \frac{1}{2} B^2 \right) + \mathbf{f}, \tag{4}$$

$$\frac{m}{e^2 n} \frac{\partial \nabla \times \mathbf{J}}{\partial t} + \frac{\partial \mathbf{B}}{\partial t} = \eta \Delta \mathbf{B} + \nabla \times (\mathbf{v} \times \mathbf{B}) - \frac{1}{en} \nabla \times (\mathbf{J} \times \mathbf{B}), \tag{5}$$

which will be our object of study. We will abbreviate the electron inertia term $m/(e^2n)$ to α, the Hall coefficient $1/(en)$ to h. In addition to these equations, both $\mathbf{v}$ and $\mathbf{B}$ must be solenoidal. This follows automatically for $\mathbf{B}$ for all time if it happens for the initial condition at time zero, because the divergence of the induction equation yields

$$\frac{\partial(\nabla \cdot \mathbf{B})}{\partial t} = 0.$$

As for the momentum one, the task of keeping $\mathbf{v}$ solenoidal is given to the pressure: p satisfies an elliptic equation to this end. Indeed, physically the pressure compensates for the tensions created by the fluid incompressibility.

Finally, boundary conditions must be added. Although other possibilities exist, we will concentrate for simplicity on two cases:

(1) The domain Ω is smooth, and both $\mathbf{v}$ and $\mathbf{B}$ satisfy homogeneous Dirichlet conditions at its boundary $\partial\Omega$.
(2) Ω is a box $(0,L_1)\times(0,L_2)\times(0,L_3)$, and both $\mathbf{v}$ and $\mathbf{B}$ are periodic at opposite faces. Moreover, in this case the mean of both in Ω is zero.

Incidently, notice that, in contrast to the MHD and Navier–Stokes cases, there is no possibility here of studying two-dimensional problems, because even when both velocity and magnetic field are horizontal, the current density and the Hall term are not.

We first recall the definitions of the classical Lebesgue and Sobolev spaces: $L^p(\Omega)$ is the space of measurable functions f defined in Ω whose L^p-norm

$$\|f\|_p = \left(\int_\Omega |f|^p \mathrm{d}V \right)^{1/p}$$

is bounded. $L^\infty(\Omega)$ is the space of measurable functions defined in Ω such that they are bounded outside a set of zero measure E, and $\|f\|_\infty$ is the maximum of $|f(\mathbf{x})|$ when $\mathbf{x} \notin E$. $H^p(\Omega)$ is the space of functions whose differentials up to the order p are square integrable [i.e., they belong to $L^2(\Omega)$]. The norm $\|f\|_{H^p(\Omega)}$ is the sum of the L^2-norms of all the partial derivatives of f up to the order p. We will only use $H^1(\Omega)$ and $H^2(\Omega)$. $H_0^1(\Omega)$ is the subspace of $H^1(\Omega)$ formed (roughly) by the functions vanishing in the boundary $\partial\Omega$. (The correct definition is somewhat more involved, but essentially amounts to this). We will use a number of standard notations:[4,8]

In the Dirichlet case,

$$H = \{\mathbf{B} \in L^2(\Omega)^3 : \nabla \cdot \mathbf{B} = 0, \mathbf{B} \cdot \mathbf{n}|_{\partial\Omega} = 0\}. \tag{6}$$

Although this divergence and trace term must be understood in the sense of distributions, it is known that H is a closed subspace of $L^2(\Omega)^3$.

$$V = H_0^1(\Omega)^3 \cap H,$$

$$D(A) = H^2(\Omega)^3 \cap V, \tag{7}$$

$$A : D(A) \to H, \quad A = P_H \Delta,$$

where P_H is the orthogonal projection on H. In the periodic case,

$$H = \left\{ \mathbf{u} \in L^2(\Omega)^3 : \int_\Omega \mathbf{u}\, \mathrm{d}V = \mathbf{0}, \quad \nabla \cdot \mathbf{u} = 0,\ \mathbf{u} \cdot \mathbf{n} \text{ antiperiodic at opposite sides of } \Omega \right\}. \tag{8}$$

Again H is a closed subspace of $L^2(\Omega)^3$

$$V = H^1(\Omega)^3 \cap H,$$

$$D(A) = H^2(\Omega)^3 \cap V, \tag{9}$$

$$A:D(A) \to H, \quad A = \Delta.$$

In connection with these spaces, we will use the following inequality (see Ref. 8): For all $\mathbf{f} \in V, \mathbf{g} \in D(A), \mathbf{h} \in H$,

$$\left| \int_\Omega \mathbf{f} \cdot \nabla \mathbf{g} \cdot \mathbf{h} \, dV \right| \leqslant c \|\mathbf{f}\|_{H^1} \|\mathbf{g}\|_{H^1}^{1/2} \|A\mathbf{g}\|_2^{1/2} \|h\|_2. \tag{10}$$

c is a constant depending only on Ω. To avoid an unmanageable proliferation of constants, we will always denote such parameters by c: thus, e.g., $3c + c^{1/2} = c$. Constants not depending on Ω, such as the diffusivity terms or bounds depending on specific functions will be given different names.

We intend to prove local existence and uniqueness of the solution to the problem (4) and (5) with initial condition $\mathbf{v}(0) \in V, \mathbf{B}(0) \in D(A)$. We will consider first the induction equation, which in the MHD case models the so-called kinematic dynamo, where the velocity is taken as a datum. The momentum equation in a classical Navier–Stokes one with a forcing given by the Lorentz force, for which well-known estimates are available. Combining the bounds for both equations we will obtain a contractive operator whose fixed point is the unique solution. Finally we will obtain some energy inequalities emphasizing the difference with the single-fluid MHD model. All these results will hold even in infinitely conducting plasmas ($\eta = 0$), in contrast with classical MHD.

II. INDUCTION EQUATION

Definition 2.1: For $\mathbf{B} \in D(A)$ we will denote by $\mathbf{w}$ the function

$$\mathbf{w} = -\alpha \Delta \mathbf{B} + \mathbf{B}. \tag{11}$$

Notice that the properties of elliptic systems guarantee that $\mathbf{w} \in H$ and $\|\mathbf{B}\|_{H^2} \leqslant c\|\mathbf{w}\|_2$.

Lemma 2.2: *Consider the term* $\eta \Delta \mathbf{B} + \nabla \times (\mathbf{v} \times \mathbf{B}) - h \nabla \times (\mathbf{J} \times \mathbf{B})$ *as a (nonlocal) function* $F(\mathbf{w}, \mathbf{v})$. *Then, for every* $\mathbf{v} \in V, F$ *is a continuous function from* H *into* H. *Moreover, for any* $\mathbf{v} \in V, \mathbf{w} \in H$,

$$\|F(\mathbf{w}, \mathbf{v})\|_2 \leqslant c(\eta + \|\mathbf{v}\|_{H^1} + \|\mathbf{w}\|_2)\|\mathbf{w}\|_2, \tag{12}$$

and for any $\mathbf{v}_1, \mathbf{v}_2 \in V, \mathbf{w}_1, \mathbf{w}_2 \in H$,

$$\begin{aligned} &\|F(\mathbf{w}_1, \mathbf{v}_1) - F(\mathbf{w}_2, \mathbf{v}_2)\|_2 \\ &\quad \leqslant c(\eta + \|\mathbf{v}_1\|_{H^1} + \|\mathbf{v}_2\|_{H^1} + \|\mathbf{w}_1\|_2 + \|\mathbf{w}_2\|_2)\|\mathbf{w}_1 - \mathbf{w}_2\|_2 + c(\|\mathbf{w}_1\|_2 + \|\mathbf{w}_2\|)\|\mathbf{v}_1 - \mathbf{v}_2\|_{H^1}. \end{aligned} \tag{13}$$

Proof: Recall that

$$\nabla \times (\mathbf{v} \times \mathbf{B}) = -\mathbf{v} \cdot \nabla \mathbf{B} + \mathbf{B} \cdot \nabla \mathbf{v},$$

$$\nabla \times (\mathbf{J} \times \mathbf{B}) = -\mathbf{J} \cdot \nabla \mathbf{B} + \mathbf{B} \cdot \nabla \mathbf{J}.$$

By standard Sobolev inequalities:

$$\eta \|\Delta \mathbf{B}_1 - \Delta \mathbf{B}_2\|_2 \leqslant c\eta \|\mathbf{B}_1 - \mathbf{B}_2\|_{H^2} \leqslant c\eta \|\mathbf{w}_1 - \mathbf{w}_2\|_2,$$

and

$$\begin{aligned} &\|\nabla \times (\mathbf{v}_1 \times \mathbf{B}_1) - \nabla \times (\mathbf{v}_2 \times \mathbf{B}_2)\|_2 \\ &\quad = \|-\mathbf{v}_1 \cdot \nabla (\mathbf{B}_1 - \mathbf{B}_2) - (\mathbf{v}_1 - \mathbf{v}_2) \cdot \nabla \mathbf{B}_2 + \mathbf{B}_1 \cdot \nabla (\mathbf{v}_1 - \mathbf{v}_2) + (\mathbf{B}_1 - \mathbf{B}_2) \cdot \nabla \mathbf{v}_2\|_2 \\ &\quad \leqslant \|\mathbf{v}_1\|_4 \|\nabla (\mathbf{B}_1 - \mathbf{B}_2)\|_4 + \|\mathbf{v}_1 - \mathbf{v}_2\|_4 \|\nabla \mathbf{B}_2\|_4 + \|\mathbf{B}_1\|_\infty \|\nabla (\mathbf{v}_1 - \mathbf{v}_2)\|_2 + \|\mathbf{B}_1 - \mathbf{B}_2\|_\infty \|\nabla \mathbf{v}_2\|_2. \end{aligned}$$

Since for dimension 3, $V \subset L^4(\Omega)$, $D(A) \subset L^\infty(\Omega)$, this amount may be bounded by

$$c(\|\mathbf{v}_1\|_{H^1}\|\mathbf{B}_1-\mathbf{B}_2\|_{H^2}+\|\mathbf{B}_2\|_{H^2}\|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}+\|\mathbf{B}_1\|_{H^2}\|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}+\|\mathbf{v}_2\|_{H^1}\|\mathbf{B}_1-\mathbf{B}_2\|_{H^2}$$
$$\leqslant c(\|\mathbf{v}_1\|_{H^1}+\|\mathbf{v}_2\|_{H^1})\|\mathbf{w}_1-\mathbf{w}_2\|_2+c(\|\mathbf{w}_1\|_2+\|\mathbf{w}\|_2)\|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}.$$

Finally, by changing in the previous inequalities $\mathbf{v}_i$ to $\mathbf{J}_i$ we find

$$\|\nabla\times(\mathbf{J}_1\times\mathbf{B}_1)-\nabla\times(\mathbf{J}_2\times\mathbf{B}_2)\|_2$$
$$\leqslant\|\mathbf{J}_1\|_4\|\nabla(\mathbf{B}_1-\mathbf{B}_2)\|_4+\|\mathbf{J}_1-\mathbf{J}_2\|_4\|\nabla\mathbf{B}_2\|_4+\|\mathbf{B}_1\|_\infty\|\nabla(\mathbf{J}_1-\mathbf{J}_2)\|_2+\|\mathbf{B}_1-\mathbf{B}_2\|_\infty\|\nabla\mathbf{J}_2\|_2$$
$$\leqslant c(\|\mathbf{J}_1\|_{H^1}+\|\mathbf{B}_2\|_{H^2}+\|\mathbf{B}_1\|_{H^2}+\|\mathbf{J}_2\|_{H^1})\|\mathbf{B}_1-\mathbf{B}_2\|_{H^2}\leqslant c(\|\mathbf{w}_1\|_2+\|\mathbf{w}_2\|_2)\|\mathbf{w}_1-\mathbf{w}_2\|_2.$$

The inequality (12) is a simplified version of the previous calculation, with only a single $\mathbf{v}$ and $\mathbf{w}$. This concludes the proof. ■

Theorem 2.3: *For fixed* $\mathbf{v}\in L^2((0,S),V)$, *Eq. (5), which may be written in the form*

$$\frac{d\mathbf{w}}{dt}=F(\mathbf{w},\mathbf{v}),\qquad \mathbf{w}(0)\in H, \tag{14}$$

admits a unique a.e. differentiable solution $\mathbf{w}:(0,T)\to H$, *for some* $T\leqslant S$, $T>0$. *We may take T so that this solution satisfies* $\|\mathbf{w}(t)\|_2\leqslant\|\mathbf{w}(0)\|_2+1$ *for all* $t\in(0,T)$. *Moreover, the interval* $(0,T)$ *depends only on* $\|\mathbf{w}(0)\|_2$ *and* $\|\mathbf{v}\|_{L^2((0,T),V)}$.

Proof: Let us prove that the integral operator, defined in the closed ball of $\mathcal{C}((0,T),H)$ of center $\mathbf{0}$ and radius $\|\mathbf{w}(0)\|_2+1$ given by

$$\mathbf{w}\to\mathbf{w}(0)+\int_0^t F(\mathbf{w}(s),\mathbf{v}(s))ds,$$

takes the ball to itself and is contractive for T small enough. Using (12), for any $\mathbf{w}$ bounded by $\|\mathbf{w}(0)\|_2+1$,

$$\int_0^t\|F(\mathbf{w},\mathbf{v})\|_2ds\leqslant c\int_0^t(\eta+\|\mathbf{v}\|_{H^1}+\|\mathbf{w}\|_2)\|\mathbf{w}\|_2ds$$
$$\leqslant c\left(\sqrt{T}\left(\int_0^T\|\mathbf{v}\|_{H^1}^2ds\right)^{1/2}+T(\eta+\|\mathbf{w}(0)\|_2+1)\right)(\|\mathbf{w}(0)\|_2+1).$$

Clearly we can take T so that this amount is less than 1 for all $t\in(0,T)$. Taking now (13),

$$\int_0^t\|F(\mathbf{w}_1,\mathbf{v})-F(\mathbf{w}_2,\mathbf{v})\|_2ds\leqslant c\int_0^t(\eta+2\|\mathbf{v}\|_{H^1}+\|\mathbf{w}_1\|_2+\|\mathbf{w}_2\|_2)\|\mathbf{w}_1-\mathbf{w}_2\|_2ds,$$

so that

$$\|\mathbf{w}_1-\mathbf{w}_2\|_{\mathcal{C}(0,T),H}\leqslant c\left(\int_0^T2\|v\|_{H^1}+\|\mathbf{w}_1\|_2+\|\mathbf{w}_2\|_2ds\right)\|\mathbf{w}_1-\mathbf{w}_2\|_{\mathcal{C}(0,T),H}$$
$$\leqslant c\left(2\sqrt{T}\left(\int_0^T\|\mathbf{v}\|_{H^1}^2ds\right)^{1/2}+2T(\|\mathbf{w}(0)\|_2+1)\right)\|\mathbf{w}_1-\mathbf{w}_2\|_{\mathcal{C}(0,T),H}.$$

Obviously by taking T small enough we can make this functional to take the ball of radius $\|\mathbf{w}(0)\|_2+1$ in itself in a contractive manner. The classical proof follows. ■

Let us study now the dependence of the solutions upon the velocity:

Theorem 2.4: *Let* $\mathbf{w}_1$, $\mathbf{w}_2$ *be the respective solutions of*

$$\frac{d\mathbf{w}_i}{dt} = F(\mathbf{w}_i, \mathbf{v}_i)$$
$$\mathbf{w}_i(0) = \mathbf{w}(0), \tag{15}$$

for $\mathbf{v}_i \in L^2((0,S),V)$, *and let* $(0,T)$ *be a common interval of existence of* $\mathbf{w}_1$, $\mathbf{w}_2$. *Then there exists* $T_1 \leqslant T$, *depending only on* $\|\mathbf{w}(0)\|_2$, $\|\mathbf{v}_i\|_{L^2((0,T),V)}$, *such that*

$$\|\mathbf{w}_1 - \mathbf{w}_2\|_{C((0,T_1),H)} \leqslant \tfrac{1}{2}\|\mathbf{v}_1 - \mathbf{v}_2\|_{L^2((0,T_1),V)}. \tag{16}$$

Proof: Using inequality (13), and taking an interval short enough for Therom 2.3 to hold for both $\mathbf{w}_i$,

$$\|\mathbf{w}_1(t) - \mathbf{w}_2(t)\|_2 = \left\| \int_0^t F(\mathbf{w}_1,\mathbf{v}_1) - F(\mathbf{w}_2,\mathbf{v}_2)ds \right\|_2 \leqslant c\int_0^t (\eta + \|\mathbf{v}_1\|_{H^1} + \|\mathbf{v}_2\|_{H^1} + \|\mathbf{w}_1\|_2 + \|\mathbf{w}_2\|_2)\|\mathbf{w}_1 - \mathbf{w}_2\|_2 + (\|\mathbf{w}_1\|_2 + \|\mathbf{w}_2\|_2)\|\mathbf{v}_1 - \mathbf{v}_2\|_{H^1}ds \leqslant c[\sqrt{T}(\|\mathbf{v}_1\|_{L^2((0,T),V)} + \|\mathbf{v}_2\|_{L^2((0,T),V)}) + T\eta + 2T(\|\mathbf{w}(0)\|_2 + 1)]\|\mathbf{w}_1 - \mathbf{w}_2\|_{C((0,T),H)} + 2\sqrt{T}(\|\mathbf{w}(0)\|_2 + 1)\|\mathbf{v}_1 - \mathbf{v}_2\|_{L^2((0,T),V)}.$$

Hence it is enough to take T_1 small enough for

$$c[\sqrt{T_1}(\|\mathbf{v}_1\|_{L^2((0,T_1),V)} + \|\mathbf{v}_2\|_{L^2((0,T_1),V)}) + T_1\eta + 2T_1(\|\mathbf{w}(0)\|_2 + 1)] < \tfrac{1}{2}, 2\sqrt{T_1}(\|\mathbf{w}(0)\|_2 + 1) < \tfrac{1}{4}.$$

III. MOMENTUM EQUATION

This is the Navier–Stokes one with two forcings: the independent one $\mathbf{f}$ and the Lorentz force $\mathbf{J}\times\mathbf{B}$. We will denote the last one by $G(\mathbf{w})$. Notice that

$$\|\mathbf{J}\times\mathbf{B}\|_2 \leqslant \|\mathbf{J}\|_4\|\mathbf{B}\|_4 \leqslant c\|\mathbf{w}\|_2^2. \tag{17}$$

We may apply the classical results (see, e.g., Ref. 8) and conclude the following.

(a) For every initial condition $\mathbf{v}(0) \in V$, there exists a unique solution for an interval $(0,T)$ satisfying

$$\|\mathbf{v}(t)\|_{H^1} \leqslant 2(\|\mathbf{v}(0)\|_{H^1} + 1), \tag{18}$$

where T depends only on $\|\mathbf{v}(0)\|_{H^1}$, $\|G(\mathbf{w})\|_{C((0,T),H)}$, $\sup_{(0,T)}\|\mathbf{f}\|_2$.

(b) $\mathbf{v} \in L^2((0,T),D(A))$, and the norm of $\mathbf{v}$ in this space is bounded by a constant depending only on the same quantities given in (a). We will first estimate the norm of $\mathbf{v}$ in the space $L^2((0,T),V)$. To emphasize its value, it is convenient to single out (only in this instance) the Poincaré constant in V, $\|\mathbf{v}\|_{H^1}^2 \leqslant k_p\|\nabla\mathbf{v}\|_2^2$.

Proposition 3.1.: If $\mathbf{v}$ is the solution of (4) in the interval $(0,T)$,

$$\|\mathbf{v}\|_{L^2((0,T),V)}^2 \leqslant \frac{k_p}{\nu}\|\mathbf{v}(0)\|_2^2 + c\frac{T}{\nu^2}\|\mathbf{w}\|_{C((0,T),H)}^4 + c\frac{T}{\nu^2}\sup_{(0,T)}\|\mathbf{f}\|_2^2. \tag{19}$$

Proof: By making the scalar product of (4) with $\mathbf{v}$, and using standard inequalities (Cauchy–Schwarz, Poincaré, and Young's),

$$\frac{1}{2}\frac{d\|\mathbf{v}\|_2^2}{dt} \leqslant -\nu\|\nabla\mathbf{v}\|_2^2 + \|G(\mathbf{w})\|_2\|\mathbf{v}\|_2 + \|\mathbf{f}\|_2\|\mathbf{v}\|_2 \leqslant -\nu\|\nabla\mathbf{v}\|_2^2 + c\|G(\mathbf{w})\|_2\|\nabla\mathbf{v}\|_2 + c\|\mathbf{f}\|_2\|\nabla\mathbf{v}\|_2$$

$$\leqslant -\nu\|\nabla\mathbf{v}\|_2^2 + \frac{c^2}{\nu}\|G(\mathbf{w})\|_2^2 + \frac{\nu}{4}\|\nabla\mathbf{v}\|_2^2 + \frac{c^2}{\nu}\|\mathbf{f}\|_2^2 + \frac{\nu}{4}\|\nabla\mathbf{v}\|_2^2.$$

Integrating in $(0,T)$ and omitting the term in $\|\mathbf{v}(t)\|_2$,

$$\frac{\nu}{2}\int_0^T \|\nabla\mathbf{v}\|_2^2 ds \leqslant \frac{1}{2}\|\mathbf{v}(0)\|_2^2 + \frac{c^2}{\nu}\int_0^T \|G(\mathbf{w})\|_2^2 ds + \frac{c^2}{\nu}\int_0^T \|\mathbf{f}\|_2^2 ds,$$

from which, in view of (17), the result follows. ■

Corollary 3.2.: There exists a time $T_1 \leqslant T$, depending only on $\|\mathbf{w}\|_{\mathcal{C}((0,T_1),H)}$, such that

$$\|\mathbf{v}\|_{L^2((0,T_1),V)} \leqslant \frac{k_p}{\sqrt{\nu}}\|\mathbf{v}(0)\|_2 + 1 \leqslant \frac{k_p}{\sqrt{\nu}}\|\mathbf{v}(0)\|_{H^1} + 1. \tag{20}$$

We will consider now the difference between two solutions corresponding to different $\mathbf{w}_i$ and the same initial condition:

Theorem 3.2: *Let* $\mathbf{v}_1, \mathbf{v}_2$ *be the respective solutions of Eq. (4) in* $(0,T)$ *corresponding to Lorentz forces* $\mathbf{w}_1, \mathbf{w}_2 \in \mathcal{C}((0,T),H)$ *and the same initial condition. Then there exists* $T_2 \leqslant T$, *depending only on* $\|\mathbf{w}_i\|_{\mathcal{C}((0,T),H)}$, *such that*

$$\|\mathbf{v}_1 - \mathbf{v}_2\|_{L^2((0,T_2),V)} \leqslant \frac{1}{2}\|\mathbf{w}_1 - \mathbf{w}_2\|_{\mathcal{C}((0,T_2),H)}. \tag{21}$$

Proof: The scalar product of $(\partial(\mathbf{v}_1 - \mathbf{v}_2))/(\partial t)$ with $\mathbf{v}_1 - \mathbf{v}_2$ yields

$$\frac{1}{2}\frac{\partial}{\partial t}\|\mathbf{v}_1 - \mathbf{v}_2\|_2^2 + \nu\|\nabla(\mathbf{v}_1 - \mathbf{v}_2)\|_2^2 = (-\mathbf{v}_1 \cdot \nabla\mathbf{v}_1 + \mathbf{v}_2 \cdot \nabla\mathbf{v}_2, \mathbf{v}_1 - \mathbf{v}_2) + (G(\mathbf{w}_1) - G(\mathbf{w}_2), \mathbf{v}_1 - \mathbf{v}_2)$$

$$-(\nabla(p_1 - p_2), \mathbf{v}_1 - \mathbf{v}_2).$$

The last term is zero. We have

$$(-\mathbf{v}_1 \cdot \nabla\mathbf{v}_1 + \mathbf{v}_2 \cdot \nabla\mathbf{v}_2, \mathbf{v}_1 - \mathbf{v}_2) = (-\mathbf{v}_1 \cdot \nabla(\mathbf{v}_1 - \mathbf{v}_2) + (-\mathbf{v}_1 + \mathbf{v}_2) \cdot \nabla\mathbf{v}_2, \mathbf{v}_1 - \mathbf{v}_2),$$

and $(-\mathbf{v}_1 \cdot \nabla(\mathbf{v}_1 - \mathbf{v}_2), \mathbf{v}_1 - \mathbf{v}_2) = 0$. By using inequality (10), we find

$$|(-\mathbf{v}_1 \cdot \nabla\mathbf{v}_1 + \mathbf{v}_2 \cdot \nabla\mathbf{v}_2, \mathbf{v}_1 - \mathbf{v}_2)| \leqslant \|\mathbf{v}_1 - \mathbf{v}_2\|_{H^1}\|\mathbf{v}_1 - \mathbf{v}_2\|_2\|\mathbf{v}_2\|_{H^1}^{1/2}\|A\mathbf{v}_2\|_2^{1/2}.$$

Finally

$$|(G(\mathbf{w}_1) - G(\mathbf{w}_2), \mathbf{v}_1 - \mathbf{v}_2)| \leqslant \|G(\mathbf{w}_1) - G(\mathbf{w}_2)\|_2\|\mathbf{v}_1 - \mathbf{v}_2\|_2.$$

In order to abbreviate the notation, let us denote by $\|g\|_{2,\infty}$ the supremum of $\|g\|_2$ when $t \in (0,T)$. Property (a) of the solutions of the Navier–Stokes equations guarantees that $\|\mathbf{v}_2\|_{H^1}$ is bounded in $(0,T)$ by an amount depending only on $\|\mathbf{v}_2(0)\|_{H^1}$, $\|G(\mathbf{w}_2)\|_{2,\infty}$, and $\|\mathbf{f}\|_{2,\infty}$. Let M be an upper bound of $\|\mathbf{v}_2\|_{H^1}^{1/2}$ in $(0,T)$. Integrating the resulting inequality in time,

$$\frac{1}{2}\|(\mathbf{v}_1-\mathbf{v}_2)(t)\|_2^2+\nu\int_0^t\|\nabla(\mathbf{v}_1-\mathbf{v}_2)\|_2^2\mathrm{d}s$$

$$\leqslant cM\int_0^t\|\mathbf{v}_1-\mathbf{v}_2\|_2\|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}\|\mathbf{v}_2\|_{H^2}^{1/2}\mathrm{d}s+c\int_0^t\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_2\|\mathbf{v}_1-\mathbf{v}_2\|_2\mathrm{d}s$$

$$\leqslant cM\|\mathbf{v}_1-\mathbf{v}_2\|_{2,\infty}\left(\int_0^T\|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2\mathrm{d}s\right)^{1/2}\left(\int_0^T\|\mathbf{v}_2\|_{H^2}\mathrm{d}s\right)^{1/2}$$

$$+cT\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_{2,\infty}\|\mathbf{v}_1-\mathbf{v}_2\|_{2,\infty}. \tag{22}$$

Since this is valid for any $t\in(0,T)$, by considering only the first term in the left-hand side of (22) and using Young's inequality,

$$\frac{1}{2}\|\mathbf{v}_1-\mathbf{v}_2\|_{2,\infty}^2\leqslant\frac{c^2M^2}{2}\left(\int_0^T\|\mathbf{v}_2\|_{H^2}\mathrm{d}s\right)\|\mathbf{v}_1-\mathbf{v}_2\|_{2,\infty}^2+\frac{1}{2}\int_0^T\|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2\mathrm{d}s+\frac{T}{2}\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_{2,\infty}^2$$

$$+\frac{c^2}{2}T\|\mathbf{v}_1-\mathbf{v}_2\|_{2,\infty}^2.$$

Since by property (b)

$$\int_0^T\|\mathbf{v}_2\|_{H^2}\mathrm{d}s\leqslant\sqrt{T}\left(\int_0^T\|\mathbf{v}_2\|_{H^2}^2\mathrm{d}s\right)^{1/2}\leqslant N\sqrt{T},$$

where N is a constant depending on the same functions stated before for $\|\mathbf{v}_2\|_{H^1}$, we find

$$(1-c^2M^2N\sqrt{T}-c^2T)\|\mathbf{v}_1-\mathbf{v}_2\|_{2,\infty}^2\leqslant\int_0^T\|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2\mathrm{d}s+T\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_{2,\infty}^2.$$

Taking T small enough for the constant before $\|\mathbf{v}_1-\mathbf{v}_2\|_{2,\infty}^2$ to be at least $1/2$, we find

$$\|\mathbf{v}_1-\mathbf{v}_2\|_{2,\infty}^2\leqslant 2\int_0^T\|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2\mathrm{d}s+2T\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_{2,\infty}^2,$$

which implies

$$\|\mathbf{v}_1-\mathbf{v}_2\|_{2,\infty}\leqslant\sqrt{2}\left(\int_0^T\|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2\mathrm{d}s\right)^{1/2}+\sqrt{2}T\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_{2,\infty}. \tag{23}$$

Let us now return to (22) omitting now the term $\|(\mathbf{v}_1-\mathbf{v}_2)(t)\|_{2,\infty}^2$, and bounding the last term in a slightly different form:

$$\int_0^T\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_2\|\mathbf{v}_1-\mathbf{v}_2\|\mathrm{d}s\leqslant\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_{2,\infty}\int_0^T\|\mathbf{v}_1-\mathbf{v}_2\|_2\mathrm{d}s$$

$$\leqslant\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_{2,\infty}\int_0^T\|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}\mathrm{d}s.$$

By using again Poincaré's inequality on $\mathbf{v}_1-\mathbf{v}_2$, we get

$$\nu\int_0^T \|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2 \mathrm{d}s$$
$$\leqslant cM\|\mathbf{v}_1-\mathbf{v}_2\|_{2,\infty}\left(\int_0^T \|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2 \mathrm{d}s\right)^{1/2}\left(\int_0^T \|\mathbf{v}_2\|_{H^2}\mathrm{d}s\right)^{1/2}$$
$$+ c\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_{2,\infty}\int_0^T \|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}\mathrm{d}s. \tag{24}$$

This, jointly with (23), yields

$$\nu\int_0^T \|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2 \mathrm{d}s \leqslant cM\left(\int_0^T \|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2 \mathrm{d}s\right)\left(\int_0^T \|\mathbf{v}_2\|_{H^2}\mathrm{d}s\right)^{1/2}$$
$$+ cM\sqrt{T}\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_{2,\infty}\left(\int_0^T \|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2 \mathrm{d}s\right)^{1/2}\left(\int_0^T \|\mathbf{v}_2\|_{H^2}\mathrm{d}s\right)^{1/2}$$
$$+ c\sqrt{T}\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_{2,\infty}\left(\int_0^T \|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2 \mathrm{d}s\right)^{1/2}.$$

Our previous bound on the H^2 norm of $\mathbf{v}_2$ and Young's inequality yield

$$\nu\int_0^T \|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2 \mathrm{d}s \leqslant cMN^{1/2}T^{1/4}\int_0^T \|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2 \mathrm{d}s$$
$$+ cMN^{1/2}T^{3/4}\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_{2,\infty}\left(\int_0^T \|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2 \mathrm{d}s\right)^{1/2}$$
$$+ c\sqrt{T}\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_{2,\infty}\left(\int_0^T \|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2 \mathrm{d}s\right)^{1/2}$$
$$\leqslant \left(cMN^{1/2}T^{1/4}+\frac{c^2M^2N}{2}T^{3/4}+\frac{c^2}{2}T^{1/2}\right)\int_0^T \|\mathbf{v}_1-\mathbf{v}_2\|_{H^1}^2 \mathrm{d}s$$
$$+ \frac{1}{2}(T^{3/4}+T^{1/2})\|G(\mathbf{w}_1)-G(\mathbf{w}_2)\|_{2,\infty}^2.$$

It is therefore to take $T_2 \leqslant T$ small enough for

$$cMN^{1/2}T_2^{1/4}+c^2M^2NT_2^{3/4}+c^2T_2^{1/2} \leqslant \frac{\nu}{2},\ T_2^{3/4}+T_2^{1/2} \leqslant \frac{\nu}{2},$$

for the theorem to hold. Notice that if we know an *a priori* bound on

$$\|\mathbf{w}_i\|_{2,\infty} = \|\mathbf{w}_i\|_{C((0,T),H)}$$

(say $\|\mathbf{w}(0)\|_2+1$), then M and N may also be bounded *a priori* and T_2 does not depend on any unknown quantity. ■

IV. EXISTENCE AND UNIQUENESS OF THE SOLUTIONS

We now state the main theorem of the paper. For the benefit of readers unwilling to spend time mastering all the previous mathematical notations, perhaps it is appropriate to state the result, at least approximately, in words: *When the velocity at time $t=0$ is differentiable, and the magnetic field is twice differentiable, there exists a solution of the two-fluid magnetohydrodynamics equations up to some time T. This solution is such that the velocity and its differential (with respect to*

the space variables) are continuous in time, and the magnetic field, plus its first and second differentials, are also continous in time. The rigorous form is as follows.

Theorem 4.1: *Take initial conditions* $\mathbf{v}(0)=\mathbf{v}_0 \in V$, $\mathbf{B}(0)=\mathbf{B}_0 \in D(A)$. *Then there exists an interval* $[0,T]$ *such that the two-fluid MHD Eqs. (4) and (5) have a unique solution. Moreover*

$$\mathbf{v} \in \mathcal{C}((0,T),V) \cap L^2((0,T),D(A)),$$
$$\mathbf{B} \in \mathcal{C}((0,T),D(A)). \tag{25}$$

Proof: Take $T>0$ small enough for:

(a) For $\mathbf{v}^* \in L^2((0,T),V)$, with

$$\|\mathbf{v}^*\|_{L^2((0,T),V)} \leqslant \frac{k_p}{\sqrt{\nu}}\|\mathbf{v}_0\|_{H^1} + 1, \tag{26}$$

the solution of

$$\frac{d\mathbf{w}}{dt} = F(\mathbf{w},\mathbf{v}^*), \tag{27}$$

$$\mathbf{w}(0) = \mathbf{w}_0 = -\alpha\Delta\mathbf{B}_0 + \mathbf{B}_0, \tag{28}$$

satisfies

$$\|\mathbf{w}\|_{\mathcal{C}((0,T),H)} \leqslant \|\mathbf{w}(0)\|_2 + 1, \tag{29}$$

and, for two functions $\mathbf{v}_1^*, \mathbf{v}_2^*$ satisfying (26), the solutions of

$$\frac{d\mathbf{w}_i}{dt} = F(\mathbf{w}_i,\mathbf{v}_i^*), \tag{30}$$

$$\mathbf{w}_i(0) = -\alpha\Delta\mathbf{B}_0 + \mathbf{B}_0, \tag{31}$$

satisfy

$$\|\mathbf{w}_1 - \mathbf{w}_2\|_{\mathcal{C}((0,T),H)} \leqslant \tfrac{1}{2}\|\mathbf{v}_1^* - \mathbf{v}_2^*\|_{L^2((0,T),V)}. \tag{32}$$

(b) For $\mathbf{w}^* \in \mathcal{C}((0,T),H)$, with

$$\|\mathbf{w}^*\|_{\mathcal{C}((0,T),H)} \leqslant \|\mathbf{w}(0)\|_2 + 1, \tag{33}$$

the solution of

$$\frac{\partial\mathbf{v}}{\partial t} = \nu\Delta\mathbf{v} - \mathbf{v}\cdot\nabla\mathbf{v} + G(\mathbf{w}^*) - \nabla p + \mathbf{f},$$
$$\mathbf{v}(0) = \mathbf{v}_0, \tag{34}$$

satisfies

$$\|\mathbf{v}\|_{L^2((0,T),V)} \leqslant \frac{k_p}{\sqrt{\nu}}\|\mathbf{v}_0\|_{H^1} + 1, \tag{35}$$

and, for two functions $\mathbf{w}_1^*, \mathbf{w}_2^*$ satisfying (33), the solutions of (34) with parameters $\mathbf{w}_1^*$ and $\mathbf{w}_2^*$ satisfy

$$\|\mathbf{v}_1-\mathbf{v}_2\|_{L^2((0,T),V)}\leqslant\tfrac{1}{2}\|\mathbf{w}_1^*-\mathbf{w}_2^*\|_{\mathcal{C}((0,T),H)}. \tag{36}$$

That T may be found satisfying (a) follows from Theorems 2.3 and 2.4, whereas proposition 3.1 and Theorem 3.2 guarantee that for T small enough, it also satisfies (b). Then the mapping defined in the product

$$\bar{B}_{L^2((0,T),V)}\left(\frac{k_p}{\sqrt{\nu}}\|\mathbf{v}_0\|_{H^1}+1\right)\times\bar{B}_{\mathcal{C}((0,T),H)}(\|\mathbf{w}_0\|_2+1) \tag{37}$$

and given by $(\mathbf{v}^*,\mathbf{w}^*)\to(\mathbf{v},\mathbf{w})$, takes this product of balls into itself in a contractive manner. Therefore it has a unique fixed point. This is a solution of the equation, and conversely every solution is a fixed point, which guarantees uniqueness. Although in principle we only know that $\mathbf{v}\in L^2((0,T),V)$, since $\mathbf{w}$ and therefore $G(\mathbf{w})$ are uniformly bounded in H for all $t\in(0,T)$, implies that $\mathbf{v}$, as the solution to a Navier–Stokes equation with a bounded forcing, belongs to $\mathcal{C}((0,T),V)\cap L^2((0,T),D(A))$. On the other hand, since $\|\mathbf{B}\|_{H^2}\leqslant c\|\mathbf{w}\|_2$, we find $\mathbf{B}\in\mathcal{C}((0,T),D(A))$.

V. FINAL CONSIDERATIONS

The key difference with classical MHD is that the induction equation is actually simpler in our case, since the advective and diffusive terms are actually continuous functions of the new variable $\mathbf{w}=\alpha\boldsymbol{\nabla}\times\mathbf{J}+\mathbf{B}$. However, this will not help us to prove global existence. For one thing, the induction equation remains nonlinear in $\mathbf{w}$; and second, no matter how regular the magnetic field is, the momentum equation is a Navier–Stokes one, where global existence of solutions is a celebrated unsolved question. Still, it is apparent from our proofs that the difussive term $\eta\Delta\mathbf{B}$ does not play any role and can be dispensed with. This is in sharp contrast with one-fluid MHD, and it is a welcome feature, since most of the reconnection models where two-fluid MHD becomes necessary are actually infinitely conducting, i.e., the resistivity is taken as zero. That the two-fluid MHD equations yield more regularity than the classical MHD ones is apparent from the following energy inequality: it does not involve the L^2-norm of $\mathbf{w}$, whose evolution is complex, but rather the current density norm.

Theorem 5.1: *Let k_p be the Poincaré constant $\|\mathbf{v}\|_2^2\leqslant k_p\|\nabla\mathbf{v}\|_2^2$. The solutions to systems (4) and (5) satisfy, for as long as they are defined*,

$$\begin{aligned}&\alpha\|\mathbf{J}(t)\|_2^2+\|\mathbf{B}(t)\|_2^2+\|\mathbf{v}(t)\|_2^2+2\eta\int_0^t\|\nabla\mathbf{B}\|_2^2+\nu\int_0^t\|\nabla\mathbf{v}\|_2^2\mathrm{d}s\\&\leqslant\alpha\|\mathbf{J}(0)\|_2^2+\|\mathbf{B}(0)\|_2^2+\|\mathbf{v}(0)\|_2^2+\frac{k_p}{\nu}\int_0^t\|\mathbf{f}\|_2^2\mathrm{d}s.\end{aligned} \tag{38}$$

Proof: With our boundary conditions

$$\int_\Omega J^2\mathrm{d}V=\int_\Omega\mathbf{J}\cdot(\nabla\times\mathbf{B})\mathrm{d}V=\int_\Omega(\nabla\times\mathbf{J})\cdot\mathbf{B}\,\mathrm{d}V=-\int_\Omega\Delta\mathbf{B}\cdot\mathbf{B}\,\mathrm{d}V=\int_\Omega|\nabla\mathbf{B}|^2\mathrm{d}V.$$

Therefore

$$\frac{\partial}{\partial t}\int_\Omega J^2\mathrm{d}V=2\int_\Omega\frac{\partial\nabla\mathbf{B}}{\partial t}\cdot\nabla\mathbf{B}\,\mathrm{d}V=-2\int_\Omega\frac{\partial\Delta\mathbf{B}}{\partial t}\cdot\mathbf{B}\,\mathrm{d}V=2\int_\Omega\frac{\partial(\nabla\times\mathbf{J})}{\partial t}\cdot\mathbf{B}\,\mathrm{d}V.$$

Let us multiply the momentum equation by $\mathbf{v}$, the induction one by $\mathbf{B}$, and add both. As in classical MHD, the advective terms add to zero, as well as

$$\int_\Omega \nabla\left(\frac{1}{2}B^2+p\right)\cdot\mathbf{v}\,\mathrm{d}V=\int_{\partial\Omega}\left(\frac{1}{2}B^2+p\right)\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}\sigma=0.$$

As for the Hall term,

$$\int_\Omega(\nabla\times(\mathbf{J}\times\mathbf{B}))\cdot\mathbf{B}\,\mathrm{d}V=\int_\Omega(\mathbf{J}\times\mathbf{B})\cdot\mathbf{J}\,\mathrm{d}V=0.$$

Writing as usual

$$\left|\int_\Omega \mathbf{f}\cdot\mathbf{v}\,\mathrm{d}V\right|\leqslant\sqrt{k_p}\|\mathbf{f}\|_2\|\nabla\mathbf{v}\|_2\leqslant\frac{\nu}{2}\|\nabla\mathbf{v}\|_2^2+\frac{k_p}{2\nu}\|\mathbf{f}\|_2^2,$$

we obtain the stated inequality. ■

Thus, although the main existence theorem proved a finite-time bound for the maximum of $\|\mathbf{v}\|_{H^1}$ and $\|\mathbf{B}\|_{H^2}$, the present one remains valid for as long as the integrals make sense and is therefore more robust than the previous one. It plays the role of the energy inequality for MHD, but supplies more information about the smoothness of the field. Whereas in one-fluid MHD it was the total (kinetic plus magnetic) energy $\|\mathbf{v}\|_2^2+\|\mathbf{B}\|_2^2$ which remained bounded, here also the current density energy $\|\mathbf{J}\|_2^2$ does: hence the H^1-norm of the magnetic field is kept by the flow, which precludes any sharp gradients.

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A relaxation method for constructing a Beltrami flow in a bounded domain

Takahiro Nishiyama[a)]
Department of Applied Science, Faculty of Engineering, Yamaguchi University, Ube 755-8611, Japan

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It is shown that a time-dependent equation generates a Beltrami flow (or a force-free field) at time $t=\infty$ from non-Beltrami initial data in an arbitrary bounded domain in three dimensions. The generated Beltrami flow has a zero normal component on the boundary and its helicity is equal to a prescribed value. The existence and uniqueness of a solution to the equation are guaranteed globally in time and no finite-time singularity occurs. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The three-dimensional function $\mathbf{u}$ which satisfies

$$(\nabla \times \mathbf{u}) \times \mathbf{u} = \mathbf{0}, \quad \nabla \cdot \mathbf{u} = 0 \tag{1}$$

is called a Beltrami flow or a force-free field. It is known to play an important role in fluid mechanics, magnetohydrodynamics, astrophysics, etc., and has been studied by many authors (see Refs. 4–7, 9, 13, 17, 21, and 28, and references therein). One of its properties is that its streamlines (field lines of $\mathbf{u}$) can be complex. In fact, Dombre *et al.*[10] showed that the Arnold–Beltrami–Childress (ABC) flow, which is a spatially periodic solution of $\nabla \times \mathbf{u} = \mathbf{u}$, has chaotic streamlines (see also Refs. 12 and 29). Moreover, it was shown in Refs. 23 and 30 that some Beltrami flows in a sphere have chaotic streamlines, too.

It is obvious that every Beltrami flow is a solution to the stationary Euler equations. Moffatt[19,20] pointed out that some nonstationary systems of equations for a viscous and perfectly conductive magnetofluid generate stationary Euler flows, at time $t=\infty$, whose streamline topology is complex if the topology of initial magnetic force lines is complex. Vallis *et al.*[27] obtained stationary Euler flows as equilibria of the nonstationary Euler equations with an artificial term added.

Using these ideas of Moffatt and Vallis *et al.*, the author[22] proposed the equation

$$\mathbf{w}_t = \nabla \times \{[(\nabla \times \mathbf{w}) \times \mathbf{w}] \times \mathbf{w}\} \tag{2}$$

with periodic boundary conditions. He deduced that its solution $\mathbf{w}$ converges to a Beltrami flow, as $t \to \infty$, by noting that $(\nabla \cdot \mathbf{w})_t = 0$,

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathrm{cube}} |\mathbf{w}|^2 \mathrm{d}^3\mathbf{x} = -\int_{\mathrm{cube}} |(\nabla \times \mathbf{w}) \times \mathbf{w}|^2 \mathrm{d}^3\mathbf{x},$$

[a)]Electronic mail: t-nishi@yamaguchi-u.ac.jp

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathrm{cube}} \boldsymbol{\phi}\cdot\mathbf{w}\,\mathrm{d}^3\mathbf{x}=0.$$

Here "cube" means a cube in which periodic boundary conditions are applied and $\boldsymbol{\phi}$ is a vector potential of $\mathbf{w}$. Furthermore, noting that (2) is similar to the vorticity equation of a compressible perfect fluid, we can rewrite it as

$$\left(\frac{\mathbf{w}}{\rho}\right)_t+(\mathbf{U}\cdot\boldsymbol{\nabla})\frac{\mathbf{w}}{\rho}=\left(\frac{\mathbf{w}}{\rho}\cdot\boldsymbol{\nabla}\right)\mathbf{U}\quad\text{with}\quad\rho_t+\boldsymbol{\nabla}\cdot(\rho\mathbf{U})=0,$$

where $\mathbf{U}=(\boldsymbol{\nabla}\times\mathbf{w})\times\mathbf{w}$. This implies that field lines of $\mathbf{w}/\rho$ are "frozen" in the fluid which moves with the pseudo-velocity $\mathbf{U}$. Therefore, we can obtain a Beltrami flow $\mathbf{w}|_{t=\infty}$ with complex streamline topology if topologically complex initial data $\mathbf{w}|_{t=0}$ are given. However, from a practical point of view, (2) has some problems. The integrability of $|\boldsymbol{\nabla}\times\mathbf{w}|^2$ over the cube at $t=\infty$ is not guaranteed and some singularities may occur at finite time. Besides, the applicability of (2) to a nonperiodic case has not been known.

The aim of this paper is to propose a time-dependent equation, (11) below, which generates a Beltrami flow at $t=\infty$ from non-Beltrami initial data in a bounded domain Ω in three dimensions. Here Ω is simply or multiply connected and its shape is arbitrary but its boundary $\partial\Omega$ is sufficiently smooth. The Beltrami flow obtained in this way has a zero normal component on $\partial\Omega$. Its helicity, which measures the degree of knottedness of vortex lines, is equal to a prescribed value, although (11) does not have frozen-field structure unlike (2). These facts are shown in Sec. III, after introducing some inequalities of function analysis and an operator P_X in Sec. II.

In addition to the applicability to a nonperiodic case, another advantage of (11) over (2) is that the existence and uniqueness of a solution to our initial-boundary value problem for (11) can be proved globally in time. Moreover, this solution at any $t<\infty$ is as smooth as initial data, that is, no finite-time singularity occurs. These are studied in Sec. IV. In Sec. V, our results are summarized.

We can rewrite (1) as $\boldsymbol{\nabla}\times\mathbf{u}=\lambda\mathbf{u}$ with a scalar function λ satisfying $\mathbf{u}\cdot\boldsymbol{\nabla}\lambda=0$. The existence of solutions $\mathbf{u}$ to boundary value problems for this equation was rigorously proved for constant λ in Refs. 7, 17, and 28, and for nonconstant λ in Refs. 5 and 13. Our method is completely different from the approaches in these references, although it is open whether λ is constant or nonconstant for our Beltrami flow.

The time evolution of solutions to (11) does not seem difficult to investigate numerically. This approach to numerical construction of a Beltrami flow is completely different from the algorithms in Refs. 4 and 6.

II. PRELIMINARIES

First, we define the norms $\|\cdot\|_{L^p}$, $\langle\langle\cdot\rangle\rangle_{n,L^p}$, and $\|\cdot\|_{n,L^p}$ $(n=1,2,3,\ldots;\ p\geqslant 1)$ by

$$\|\mathbf{f}\|_{L^p}=\left(\int_\Omega|\mathbf{f}|^p\mathrm{d}^3\mathbf{x}\right)^{1/p},$$

$$\langle\langle\mathbf{f}\rangle\rangle_{n,L^p}=\left(\sum_{k+l+m=n}\left\|\frac{\partial^n\mathbf{f}}{\partial x_1^k\,\partial x_2^l\,\partial x_3^m}\right\|_{L^p}^p\right)^{1/p},$$

$$\|\mathbf{f}\|_{n,L^p}=\left(\|\mathbf{f}\|_{L^p}^p+\sum_{k=1}^{n}\langle\langle\mathbf{f}\rangle\rangle_{k,L^p}^p\right)^{1/p}.$$

Particularly, in the case $p=2$, they are simply written as $\|\cdot\|$, $\langle\langle\cdot\rangle\rangle_n$, and $\|\cdot\|_n$, respectively.

The inequalities

$$\|\mathbf{f}\|_{L^q} \leqslant C\|\mathbf{f}\|_{1,L^p}, \quad 1 \leqslant p < 3, \quad 1 \leqslant q \leqslant \frac{3p}{3-p}, \tag{3}$$

$$\sup_{\mathbf{x}\in\Omega}|\mathbf{f}(\mathbf{x})| + \sup_{\mathbf{x},\mathbf{x}'\in\Omega}\frac{|\mathbf{f}(\mathbf{x})-\mathbf{f}(\mathbf{x}')|}{|\mathbf{x}-\mathbf{x}'|^{1-3/p}} \leqslant C\|\mathbf{f}\|_{1,L^p}, \quad p > 3 \tag{4}$$

are derived from the embedding theorem (see Ref. 16). Here, and from now on, we use C to denote positive constants independent of estimated functions. Its value depends on each individual equality or inequality. In the same way, C' will be also used.

It is well known that Hölder's inequality

$$\int_\Omega \prod_{k=1}^{n} |\mathbf{f}_k| \mathrm{d}^3\mathbf{x} \leqslant \|\mathbf{f}_1\|_{L^p}\|\mathbf{f}_2\|_{L^q}\cdots\|\mathbf{f}_n\|_{L^r} \tag{5}$$

is valid when $p^{-1}+q^{-1}+\cdots+r^{-1}=1$. Its combination with Young's inequality leads to

$$\int_\Omega \prod_{k=1}^{n} |\mathbf{f}_k| \mathrm{d}^3\mathbf{x} \leqslant \|\mathbf{f}_1\|_{L^p}^p + \|\mathbf{f}_2\|_{L^q}^q + \cdots + \|\mathbf{f}_n\|_{L^r}^r. \tag{6}$$

If $(\mathrm{d}/\mathrm{d}t)y(t) \leqslant c_1(t)y(t)+c_2(t)$ for non-negative functions y, c_1, and c_2, then Gronwall's inequality

$$y(t) \leqslant \left[y(0) + \int_0^t c_2(t')\mathrm{d}t' \right] \exp\left[\int_0^t c_1(t')\mathrm{d}t' \right] \tag{7}$$

is valid (an extension of Lemma 5.5 of Ref. 16).

It was shown in Refs. 11 and 24 that the space $\mathbf{L}^p(\Omega)=\{\mathbf{f}:\Omega\to\mathbf{R}^3 \,|\, \|\mathbf{f}\|_{L^p}<\infty\}$ with $p>1$ is decomposed into the two subspaces

$$L^p_\sigma = \{\mathbf{f}\in\mathbf{L}^p(\Omega) \,|\, \nabla\cdot\mathbf{f}=0,\ \mathbf{f}\cdot\hat{\mathbf{n}}|_{\partial\Omega}=0\}, \quad G_p = \{\mathbf{f}|\mathbf{f}=\nabla Q,\ \|Q\|_{1,L^p}<\infty\},$$

where $\hat{\mathbf{n}}$ is the unit outward normal vector on $\partial\Omega$. Moreover, if Ω is $(N+1)$-ply connected and the N cuts $\Sigma_1,\Sigma_2,\ldots,\Sigma_N$ ($\Sigma_j\cap\Sigma_k=\emptyset$ for $j\neq k$) make $\Omega-\cup_{j=1}^N\Sigma_j$ simply connected, then L^p_σ is decomposed into

$$X_p = \left\{ \mathbf{f}\in L^p_\sigma \,\middle|\, \int_{\Sigma_j}\mathbf{f}\cdot\hat{\mathbf{n}}_j\mathrm{d}S = 0 \text{ for } j=1,2,\cdots,N \right\}$$

and the N-dimensional irrotational subspace F_N spanned by $\{\nabla Q_1, \nabla Q_2, \ldots, \nabla Q_N\}$. Here $\hat{\mathbf{n}}_j$ is a unit normal vector on Σ_j and Q_j is a solution to

$$\Delta Q_j = 0 \quad \text{in } \Omega - \cup_{k=1}^N\Sigma_k,$$

$$\nabla Q_j\cdot\hat{\mathbf{n}}|_{\partial\Omega}=0, \quad [\nabla Q_j\cdot\hat{\mathbf{n}}_k]_k = 0 \text{ for } k=1,2,\ldots,N,$$

$$[Q_j]_k = \begin{cases} 1 \text{ for } k=j \\ 0 \text{ for } k\neq j, \end{cases}$$

$[\cdot]_k$ denotes the jump of value in passing through Σ_k in the opposite direction to $\hat{\mathbf{n}}_k$ (see Ref. 26). For example, when Ω is the interior of a torus ($N=1$) which is symmetrical with respect to the x_3-axis, $\Sigma_1=\Omega\cap\{\theta=0\}$ and $Q_1=\theta/(2\pi)$ in the cylindrical coordinate system (R,θ,x_3). Another equivalent definition of F_N was introduced in Refs. 3 and 8. If Ω is simply connected, then we set $X_p=L^p_\sigma$.

Let us introduce the projection operator P_X from $\mathbf{L}^p(\Omega)$, $p>1$, onto X_p such that

$$\nabla\cdot(P_X\mathbf{f})=0,\quad (P_X\mathbf{f})\cdot\hat{\mathbf{n}}|_{\partial\Omega}=0\quad \text{for any } \mathbf{f}\in\mathbf{L}^p(\Omega),$$

and in addition,

$$\int_{\Sigma_j}(P_X\mathbf{f})\cdot\hat{\mathbf{n}}_j\mathrm{d}S=0 \text{ for } j=1,2,\ldots,N \text{ if } \Omega \text{ is } (N+1)\text{-ply connected.}$$

When Ω is simply connected, we define P_X by $P_X\mathbf{f}=\mathbf{f}-\nabla Q_0$ with Q_0 satisfying

$$\Delta Q_0=\nabla\cdot\mathbf{f},\quad \nabla Q_0\cdot\hat{\mathbf{n}}|_{\partial\Omega}=\mathbf{f}\cdot\hat{\mathbf{n}}|_{\partial\Omega}. \tag{8}$$

In general, it is not easy to write Q_0 explicitly by using $\mathbf{f}$. For example, however, if Ω is the interior of a unit sphere, then

$$Q_0(\mathbf{x})=\int_\Omega G(\mathbf{x},\mathbf{x}')\nabla\cdot\mathbf{f}(\mathbf{x}')\mathrm{d}^3\mathbf{x}'-\int_{\partial\Omega}G(\mathbf{x},\mathbf{x}')\mathbf{f}(\mathbf{x}')\cdot\hat{\mathbf{n}}(\mathbf{x}')\mathrm{d}S'+\text{const},$$

where

$$G(\mathbf{x},\mathbf{x}')=-\frac{1}{4\pi}\left(\frac{1}{|\mathbf{x}-\mathbf{x}'|}+\frac{1}{|\mathbf{x}'||\mathbf{x}-\mathbf{x}^*|}+\ln\frac{1}{1-\mathbf{x}\cdot\mathbf{x}'+|\mathbf{x}'||\mathbf{x}-\mathbf{x}^*|}\right)$$

and $\mathbf{x}^*=\mathbf{x}'/|\mathbf{x}'|^2$ (see Eq. (2.6.62) in Ref. 14).

When Ω is $(N+1)$-ply connected, we define P_X by

$$P_X\mathbf{f}=\mathbf{f}-\nabla Q_0-\sum_{j=1}^N a_j\nabla Q_j.$$

Here Q_0 is determined by (8) with $\int_{\Sigma_j}\nabla Q_0\cdot\hat{\mathbf{n}}_j\mathrm{d}S=0$ $(j=1,2,\ldots,N)$ and a_j is given by the system of N linear equations

$$\sum_{k=1}^N\left(\int_{\Sigma_j}\nabla Q_k\cdot\hat{\mathbf{n}}_j\mathrm{d}S\right)a_k=\int_{\Sigma_j}\mathbf{f}\cdot\hat{\mathbf{n}}_j\mathrm{d}S,$$

which is uniquely solvable [Eq. (1.18) in Ref. 26].

The inequality

$$\|P_X\mathbf{f}\|_{L^p}\leqslant C\|\mathbf{f}\|_{L^p},\quad p>1 \tag{9}$$

was proved in Refs. 11 and 24. Moreover, using Lemma 2.14 of Ref. 15 in Ω (or $\Omega-\cup_{j=1}^N\Sigma_j$ if Ω is $(N+1)$-ply connected) and noting that $\nabla\times P_X\mathbf{f}=\nabla\times\mathbf{f}$, we have

$$\left.\begin{aligned}\|P_X\mathbf{f}\|_{1,L^p}&\leqslant C\|\nabla\times\mathbf{f}\|_{L^p},\quad p\geqslant 2,\\ \|P_X\mathbf{f}\|_{n+1,L^q}&\leqslant C\|\nabla\times\mathbf{f}\|_{n,L^q},\quad n=1,2,3,\ldots;q>1.\end{aligned}\right\} \tag{10}$$

III. MAIN EQUATION AND BELTRAMI FLOW

The following is our main equation:

$$\boldsymbol{\omega}_t=P_X\left[\frac{(\boldsymbol{\omega}\times\mathbf{v})\times\mathbf{v}}{\sqrt{1+|\boldsymbol{\omega}|^2}(1+|\mathbf{v}|^2)}\right] \tag{11}$$

with $\mathbf{v}$ defined by $\mathbf{v}=P_X\mathbf{V}$, where

$$\mathbf{V} = \nabla \times \boldsymbol{\Psi} = \nabla \times \int_\Omega \frac{\boldsymbol{\omega}(\mathbf{x}',t)}{4\pi|\mathbf{x}-\mathbf{x}'|}\mathrm{d}^3\mathbf{x}' = \int_\Omega \frac{\boldsymbol{\omega}(\mathbf{x}',t)\times(\mathbf{x}-\mathbf{x}')}{4\pi|\mathbf{x}-\mathbf{x}'|^3}\mathrm{d}^3\mathbf{x}'.$$

As an initial condition,

$$\boldsymbol{\omega}|_{t=0} = \boldsymbol{\omega}_0(\mathbf{x}) \tag{12}$$

is imposed, where $\boldsymbol{\omega}_0 \in X_2$, that is,

$$\left.\begin{array}{c} \nabla\cdot\boldsymbol{\omega}_0 = 0, \quad \boldsymbol{\omega}_0\cdot\hat{\mathbf{n}}\big|_{\partial\Omega} = 0, \quad \|\boldsymbol{\omega}_0\| < \infty \\ \left(\text{and}\int_{\Sigma_j}\boldsymbol{\omega}_0\cdot\hat{\mathbf{n}}_j\mathrm{d}S = 0 \text{ for } j = 1,2,\ldots,N \text{ if } \Omega \text{ is } (N+1)\text{-ply connected}\right). \end{array}\right\} \tag{13}$$

We denote $\mathbf{v}|_{t=0}$ by $\mathbf{v}_0$ and assume that it is non-Beltrami, that is,

$$(\nabla\times\mathbf{v}_0)\times\mathbf{v}_0 \not\equiv \mathbf{0}. \tag{14}$$

In this section, let us consider the evolution of $\boldsymbol{\omega}$ (and $\mathbf{v}$) for $t>0$ and show that $\mathbf{v}|_{t=\infty}$ is a Beltrami flow whose normal component on $\partial\Omega$ vanishes and helicity is equal to $\int_\Omega \mathbf{v}_0\cdot\boldsymbol{\omega}_0\mathrm{d}^3\mathbf{x}$.

First, it should be noted that $P_X\boldsymbol{\omega}=\boldsymbol{\omega}$, that is, $\nabla\cdot\boldsymbol{\omega}=0$ and $\boldsymbol{\omega}\cdot\hat{\mathbf{n}}|_{\partial\Omega}=0$ for every $t>0$ because of (13) and $P_X\boldsymbol{\omega}_t=\boldsymbol{\omega}_t$. This fact yields that $\nabla\cdot\boldsymbol{\Psi}=0$ (see Ref. 1) and we get

$$\nabla\times\mathbf{v} = \nabla\times\mathbf{V} = -\Delta\boldsymbol{\Psi} = \boldsymbol{\omega}.$$

It is clear that $\nabla\cdot\mathbf{v}=\nabla\cdot\mathbf{V}=0$. The difference between $\mathbf{v}$ and $\mathbf{V}$ is that $\mathbf{v}\cdot\hat{\mathbf{n}}|_{\partial\Omega}=0$ for all $t\in[0,\infty]$, while $\mathbf{V}\cdot\hat{\mathbf{n}}|_{\partial\Omega}$ does not always vanish.

Note that

$$\int_\Omega (P_X\mathbf{f})\cdot\mathbf{g}\,\mathrm{d}^3\mathbf{x} = \int_\Omega \mathbf{f}\cdot(P_X\mathbf{g})\mathrm{d}^3\mathbf{x} = \int_\Omega (P_X\mathbf{f})\cdot(P_X\mathbf{g})\mathrm{d}^3\mathbf{x}$$

is valid for any $\mathbf{f}$ and $\mathbf{g}$ if the integrals have a finite value. Particularly, if $\mathbf{f}$ is the gradient of some function, then the integrals are equal to zero. Then, from (11), $\boldsymbol{\omega}=P_X\boldsymbol{\omega}$, and

$$\begin{aligned}\int_\Omega \mathbf{v}_t\cdot\boldsymbol{\omega}\,\mathrm{d}^3\mathbf{x} &= \int_\Omega \mathbf{V}_t(\mathbf{x},t)\cdot\boldsymbol{\omega}(\mathbf{x},t)\mathrm{d}^3\mathbf{x} = \int_\Omega\int_\Omega \frac{\boldsymbol{\omega}(\mathbf{x},t)\cdot[\boldsymbol{\omega}_t(\mathbf{x}',t)\times(\mathbf{x}-\mathbf{x}')]}{4\pi|\mathbf{x}-\mathbf{x}'|^3}\mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}' \\ &= \int_\Omega \mathbf{V}(\mathbf{x}',t)\cdot\boldsymbol{\omega}_t(\mathbf{x}',t)\mathrm{d}^3\mathbf{x}' = \int_\Omega \mathbf{v}\cdot\boldsymbol{\omega}_t\mathrm{d}^3\mathbf{x},\end{aligned}$$

we calculate

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\omega}\|^2 = -\int_\Omega \frac{|\boldsymbol{\omega}\times\mathbf{v}|^2}{\sqrt{1+|\boldsymbol{\omega}|^2}(1+|\mathbf{v}|^2)}\mathrm{d}^3\mathbf{x}, \tag{15}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \mathbf{v}\cdot\boldsymbol{\omega}\,\mathrm{d}^3\mathbf{x} = 0. \tag{16}$$

It follows from (15) that $\|\boldsymbol{\omega}\|^2$ keeps decreasing with t as long as $|\boldsymbol{\omega}\times\mathbf{v}|\not\equiv 0$, and $\|\boldsymbol{\omega}\|\lneqq\|\boldsymbol{\omega}_0\|$ is valid because of (14). Moreover, (15) gives

$$\int_0^\infty\left[\int_\Omega \frac{|\boldsymbol{\omega}\times\mathbf{v}|^2}{\sqrt{1+|\boldsymbol{\omega}|^2}(1+|\mathbf{v}|^2)}\mathrm{d}^3\mathbf{x}\right]\mathrm{d}t \leqslant \frac{1}{2}\|\boldsymbol{\omega}_0\|^2.$$

Making use of (5) and noting that

$$\|\mathbf{v}\|_{L^4} \leqslant C\|\mathbf{v}\|_1 \leqslant C'\|\boldsymbol{\omega}\| < C'\|\boldsymbol{\omega}_0\| \tag{17}$$

follows from (3) and (10), we derive

$$\left(\int_\Omega |\boldsymbol{\omega}\times\mathbf{v}|\mathrm{d}^3\mathbf{x}\right)^2 \leqslant \int_\Omega \frac{|\boldsymbol{\omega}\times\mathbf{v}|^2}{\sqrt{1+|\boldsymbol{\omega}|^2}(1+|\mathbf{v}|^2)}\mathrm{d}^3\mathbf{x}\left[\int_\Omega (1+|\boldsymbol{\omega}|^2)\mathrm{d}^3\mathbf{x}\int_\Omega (1+|\mathbf{v}|^2)^2\mathrm{d}^3\mathbf{x}\right]^{1/2}$$
$$\leqslant C(\|\boldsymbol{\omega}_0\|^3+1)\int_\Omega \frac{|\boldsymbol{\omega}\times\mathbf{v}|^2}{\sqrt{1+|\boldsymbol{\omega}|^2}(1+|\mathbf{v}|^2)}\mathrm{d}^3\mathbf{x}.$$

Therefore,

$$\int_0^\infty \left(\int_\Omega |\boldsymbol{\omega}\times\mathbf{v}|\mathrm{d}^3\mathbf{x}\right)^2 \mathrm{d}t < \infty,$$

which means that

$$\int_\Omega |\boldsymbol{\omega}\times\mathbf{v}|\mathrm{d}^3\mathbf{x} = \int_\Omega |(\boldsymbol{\nabla}\times\mathbf{v})\times\mathbf{v}|\mathrm{d}^3\mathbf{x} = 0 \quad \text{at } t=\infty.$$

Furthermore, by (9), we obtainF

$$\|\boldsymbol{\omega}_t\|^2 \leqslant C\left\|\frac{(\boldsymbol{\omega}\times\mathbf{v})\times\mathbf{v}}{\sqrt{1+|\boldsymbol{\omega}|^2}(1+|\mathbf{v}|^2)}\right\|^2 \leqslant C\int_\Omega |\boldsymbol{\omega}\times\mathbf{v}|\mathrm{d}^3\mathbf{x} = 0 \quad \text{at } t=\infty.$$

These facts imply that $\boldsymbol{\omega}$ reaches a steady state at $t=\infty$ and $\mathbf{v}|_{t=\infty}$ is a Beltrami flow whose enstrophy ($\frac{1}{2}\|\boldsymbol{\omega}\|^2$ at $t=\infty$) is less than $\frac{1}{2}\|\boldsymbol{\omega}_0\|^2$ and helicity ($\int_\Omega \mathbf{v}\cdot\boldsymbol{\omega}\,\mathrm{d}^3\mathbf{x}$ at $t=\infty$) is equal to the prescribed value $\int_\Omega \mathbf{v}_0\cdot\boldsymbol{\omega}_0\mathrm{d}^3\mathbf{x}$. Particularly, if $\int_\Omega \mathbf{v}_0\cdot\boldsymbol{\omega}_0\mathrm{d}^3\mathbf{x}\neq 0$, then it is easy to see that $\|\boldsymbol{\omega}\|$ at $t=\infty$ is nonzero. Indeed, (16) with (5) and (10) yields

$$0 < \left|\int_\Omega \mathbf{v}_0\cdot\boldsymbol{\omega}_0\mathrm{d}^3\mathbf{x}\right| = \left|\int_\Omega \mathbf{v}\cdot\boldsymbol{\omega}\,\mathrm{d}^3\mathbf{x}\right| \leqslant \|\mathbf{v}\|\|\boldsymbol{\omega}\| \leqslant C\|\boldsymbol{\omega}\|^2. \tag{18}$$

The quantity $\int_\Omega \mathbf{v}\cdot\boldsymbol{\omega}\,\mathrm{d}^3\mathbf{x}$ is known to measure the degree of knottedness of $\boldsymbol{\omega}$-lines (Refs. 2 and 18). Thus we can expect that streamlines of the Beltrami flow $\mathbf{v}|_{t=\infty}$ (parallel to lines of vortex $\boldsymbol{\omega}|_{t=\infty}$) are complex if field lines of $\boldsymbol{\omega}_0$ are topologically complex, although (11) does not have frozen-field structure unlike (2).

IV. UNIQUE SOLVABILITY OF MAIN EQUATION

In this section, we discuss the existence and uniqueness of a solution $\boldsymbol{\omega}$ to our initial-boundary value problem (11) and (12), and $\boldsymbol{\omega}\cdot\hat{\mathbf{n}}|_{\partial\Omega}=0$. For this, we first calculate some estimates of $\boldsymbol{\omega}$ assuming its existence in a sufficiently smooth class.

In addition to (13), let us assume that $\|\boldsymbol{\omega}_0\|_{2,L^\alpha}<\infty$ with $\alpha>3$. Then, by (5), (9), and (11), we derive, for $\beta>2$

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\omega}\|_{L^\beta}^\beta = \beta\int_\Omega |\boldsymbol{\omega}|^{\beta-2}\boldsymbol{\omega}\cdot\boldsymbol{\omega}_t\mathrm{d}^3\mathbf{x} \leqslant \beta\|\boldsymbol{\omega}\|_{L^\beta}^{\beta-1}\|\boldsymbol{\omega}_t\|_{L^\beta},$$

$$\|\boldsymbol{\omega}_t\|_{L^\beta} \leqslant C\left\|\frac{(\boldsymbol{\omega}\times\mathbf{v})\times\mathbf{v}}{\sqrt{1+|\boldsymbol{\omega}|^2}(1+|\mathbf{v}|^2)}\right\|_{L^\beta} \leqslant C\left(\int_\Omega \mathrm{d}^3\mathbf{x}\right)^{1/\beta},$$

which mean $(\mathrm{d}/\mathrm{d}t)\|\boldsymbol{\omega}\|_{L^\beta}\leqslant C$. This and (10) give

$$\|\mathbf{v}\|_{1,L^\beta} \leqslant C\|\boldsymbol{\omega}\|_{L^\beta} \leqslant C\|\boldsymbol{\omega}_0\|_{L^\beta} + C't, \quad \beta > 2. \tag{19}$$

Next, verifying that

$$\left| \frac{\partial}{\partial x_j} \frac{(\boldsymbol{\omega} \times \mathbf{v}) \times \mathbf{v}}{\sqrt{1+|\boldsymbol{\omega}|^2}(1+|\mathbf{v}|^2)} \right| \leqslant C(|\boldsymbol{\omega}_{x_j}| + |\mathbf{v}_{x_j}|)$$

and making use of (6), (10), (17), and (19), we get, for $\beta \geqslant 2$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle\boldsymbol{\omega}\rangle\rangle^\beta_{1,L^\beta} = \beta\sum_{j=1}^{3}\int_\Omega |\boldsymbol{\omega}_{x_j}|^{\beta-2}\boldsymbol{\omega}_{x_j}\cdot\boldsymbol{\omega}_{tx_j}\mathrm{d}^3\mathbf{x} \leqslant \beta(\langle\langle\boldsymbol{\omega}\rangle\rangle^\beta_{1,L^\beta} + \langle\langle\boldsymbol{\omega}_t\rangle\rangle^\beta_{1,L^\beta}),$$

$$\langle\langle\boldsymbol{\omega}_t\rangle\rangle^\beta_{1,L^\beta} \leqslant C\left\|\nabla\times\frac{(\boldsymbol{\omega}\times\mathbf{v})\times\mathbf{v}}{\sqrt{1+|\boldsymbol{\omega}|^2}(1+|\mathbf{v}|^2)}\right\|^\beta_{L^\beta} \leqslant C'(\langle\langle\boldsymbol{\omega}\rangle\rangle^\beta_{1,L^\beta} + \langle\langle\mathbf{v}\rangle\rangle^\beta_{1,L^\beta}) \leqslant C'\langle\langle\boldsymbol{\omega}\rangle\rangle^\beta_{1,L^\beta} + c(t,\|\boldsymbol{\omega}_0\|_{L^\beta}).$$

Here, and from now on, $c(t,s)$ is used without distinction in order to denote positive functions which are monotonically increasing in each of t and s, finite for any $t<\infty$ and $s<\infty$, and independent of estimated functions. From (7) and (10),

$$\|\mathbf{v}\|_{2,L^\beta} \leqslant C\|\boldsymbol{\omega}\|_{1,L^\beta} \leqslant c(t,\|\boldsymbol{\omega}_0\|_{1,L^\beta}), \quad \beta \geqslant 2 \tag{20}$$

follows. In the same way, noting that

$$\left|\frac{\partial^2}{\partial x_j\,\partial x_k}\frac{(\boldsymbol{\omega}\times\mathbf{v})\times\mathbf{v}}{\sqrt{1+|\boldsymbol{\omega}|^2}(1+|\mathbf{v}|^2)}\right| \leqslant C[|\boldsymbol{\omega}_{x_jx_k}| + |\mathbf{v}_{x_jx_k}| + (|\boldsymbol{\omega}_{x_j}| + |\mathbf{v}_{x_j}|)(|\boldsymbol{\omega}_{x_k}| + |\mathbf{v}_{x_k}|)],$$

we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle\boldsymbol{\omega}\rangle\rangle^{\beta/2}_{2,L^{\beta/2}} \leqslant \frac{\beta}{2}(\langle\langle\boldsymbol{\omega}\rangle\rangle^{\beta/2}_{2,L^{\beta/2}} + \langle\langle\boldsymbol{\omega}_t\rangle\rangle^{\beta/2}_{2,L^{\beta/2}}),$$

$$\langle\langle\boldsymbol{\omega}_t\rangle\rangle^{\beta/2}_{2,L^{\beta/2}} \leqslant C\left\|\nabla\times\frac{(\boldsymbol{\omega}\times\mathbf{v})\times\mathbf{v}}{\sqrt{1+|\boldsymbol{\omega}|^2}(1+|\mathbf{v}|^2)}\right\|^{\beta/2}_{1,L^{\beta/2}} \leqslant C'\langle\langle\boldsymbol{\omega}\rangle\rangle^{\beta/2}_{2,L^{\beta/2}} + c(t,\|\boldsymbol{\omega}_0\|_{1,L^\beta})$$

for $\beta>2$. They lead to

$$\|\mathbf{v}\|_{3,L^{\beta/2}} \leqslant C\|\boldsymbol{\omega}\|_{2,L^{\beta/2}} \leqslant c(t,\|\boldsymbol{\omega}_0\|_{2,L^{\beta/2}} + \|\boldsymbol{\omega}_0\|_{1,L^\beta}), \quad \beta > 2. \tag{21}$$

For $\beta/2=\alpha>3$,

$$\sup_{\substack{\mathbf{x}\in\Omega\\ j=1,2,3}}|\boldsymbol{\omega}_{x_j}(\mathbf{x},t)| + \sup_{\substack{\mathbf{x},\mathbf{x}'\in\Omega\\ j=1,2,3}}\frac{|\boldsymbol{\omega}_{x_j}(\mathbf{x},t)-\boldsymbol{\omega}_{x_j}(\mathbf{x}',t)|}{|\mathbf{x}-\mathbf{x}'|^{1-3/\alpha}} \leqslant C\|\boldsymbol{\omega}\|_{2,L^\alpha} \leqslant c(t,\|\boldsymbol{\omega}_0\|_{2,L^\alpha}) \tag{22}$$

follows from (4). This means that $\boldsymbol{\omega}$ at any $t<\infty$ is as smooth in $\mathbf{x}$ as $\boldsymbol{\omega}_0$, if it exists. Furthermore, since

$$\|\boldsymbol{\omega}_t\|_{2,L^\alpha} \leqslant c(t,\|\boldsymbol{\omega}_0\|_{2,L^\alpha}) \tag{23}$$

is derived from the above calculations, $\boldsymbol{\omega}$ is also smooth in t.

Using the Galerkin method in Ref. 25 and (20) for $\beta=2$ with $\|\boldsymbol{\omega}_t\|\leqslant C$, we can prove the temporally global existence of $\boldsymbol{\omega}$ such that $\boldsymbol{\omega}(\cdot,t)\in X_2$ is continuous in t. Then the differentiability of $\boldsymbol{\omega}$ is raised so that (19)–(23) hold.

This smoothness of $\boldsymbol{\omega}$ enables us to prove that the initial data $\boldsymbol{\omega}_0$ cannot generate two different solutions. Indeed, supposing that $\boldsymbol{\omega}=\boldsymbol{\omega}_1,\boldsymbol{\omega}_2$ (correspondingly, $\mathbf{v}=\mathbf{v}_1,\mathbf{v}_2$) are generated by (11) from the same initial condition and noting that $\sup_\Omega|\mathbf{v}|$ and $\sup_\Omega|\boldsymbol{\omega}|$ are bounded by $c(t,\|\boldsymbol{\omega}_0\|_{1,L^\alpha})$ with $\alpha>3$, we can obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\omega}_1-\boldsymbol{\omega}_2\|^2 \leqslant c(t,\|\boldsymbol{\omega}_0\|_{1,L^\alpha})\|\boldsymbol{\omega}_1-\boldsymbol{\omega}_2\|^2.$$

From this,

$$\|\mathbf{v}_1-\mathbf{v}_2\| \leqslant C\|\boldsymbol{\omega}_1-\boldsymbol{\omega}_2\|=0$$

is deduced by virtue of (7) and (10). By contrast we do not know whether or not two different initial data reach the same steady state $\boldsymbol{\omega}|_{t=\infty}$.

V. CONCLUSIONS

It was shown that each solution $\boldsymbol{\omega}$ to (11) with (12) reaches a steady state at $t=\infty$ and $\mathbf{u}=\mathbf{v}|_{t=\infty}$ is a solution to (1), that is, a Beltrami flow such that $\mathbf{u}\cdot\hat{\mathbf{n}}|_{\partial\Omega}=0$,

$$\|\mathbf{u}\|_1 \leqslant C\|\boldsymbol{\nabla}\times\mathbf{u}\| < C\|\boldsymbol{\omega}_0\|, \quad \int_\Omega \mathbf{u}\cdot(\boldsymbol{\nabla}\times\mathbf{u})\mathrm{d}^3\mathbf{x}=\int_\Omega \mathbf{v}_0\cdot\boldsymbol{\omega}_0\mathrm{d}^3\mathbf{x}.$$

Unlike (17) and (18), which remain valid at $t=\infty$, the estimates (19)–(23) hold only for $t<\infty$ and $\boldsymbol{\omega}$ may be nonsmooth at $t=\infty$. Nevertheless, (19)–(23) guarantee that (11) is really solvable globally in time, $\boldsymbol{\omega}$ is unique for $\boldsymbol{\omega}_0$ (not for $\boldsymbol{\omega}|_{t=\infty}$), and no finite-time singularity occurs. This fact seems convenient for numerical construction of a Beltrami flow.

It should be noted that $\mathbf{v}|_{t=\infty}$ generated by

$$\boldsymbol{\omega}_t = P_X[(\boldsymbol{\omega}\times\mathbf{v})\times\mathbf{v}] \tag{24}$$

is a Beltrami flow, too. Indeed, instead of (15)

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\omega}\|^2=-\|\boldsymbol{\omega}\times\mathbf{v}\|^2$$

is derived and (16) is also valid for (24). However, we do not know whether (19)–(23) are deduced from (24) or not. The denominator $\sqrt{1+|\boldsymbol{\omega}|^2}(1+|\mathbf{v}|^2)$ in (11) helps to obtain (19)–(23). Thus (11) seems more suitable to numerical construction of a Beltrami flow than (24).

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On nonhomogeneous Bose condensation

Joseph V. Pulé[a)]
Department of Mathematical Physics, University College Dublin, Belfield, Dublin 4, Ireland

André F. Verbeure[b)]
Instituut voor Theoretische Fysika, Katholieke Universiteit Leuven, Celestijnenlaan 200D, 3001 Leuven, Belgium

Valentin A. Zagrebnov[c)]
Université de la Méditerranée and Centre de Physique Théorique Luminy-Case 907, 13288 Marseille, Cedex 09, France

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We prove, in great generality, that in a system of bosons, whenever Bose condensation in a nonzero mode occurs then there is also spontaneous breaking of translation symmetry. In particular the proof holds for realistic Bose systems with two-body superstable interaction. This generalizes an old result proving that the occurrence of Bose-Einstein condensation in the zero mode implies spontaneous breaking of gauge invariance. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1985025]

I. INTRODUCTION

For homogenous systems of bosons, the phenomenon of Bose-Einstein condensation into the *ground state* is very well known and intensively studied. In this situation, the ground state density ρ_0 is nonzero, that is we have

$$\rho_0 = \lim_{\Lambda} \omega\left(\frac{a_0^* a_0}{V}\right) > 0, \tag{1.1}$$

where $\lim_\Lambda$ stands for $\lim_{\Lambda \nearrow \mathbb{R}^\nu}$, $\omega(\cdot)$ denotes the expectation with respect to the equilibrium state and

$$a_k^{\#} = \frac{1}{\sqrt{V}} \int_\Lambda \mathrm{d}x \, a^{\#}(x) e^{ik\cdot x}$$

are the usual creation and annihilation operators for momentum k for the system in a (cubic) domain $\Lambda \subset \mathbb{R}^\nu$ of volume V. Another manifestation of this phenomenon is breaking of gauge symmetry as expressed by the formula

$$\lim_{\Lambda} \omega\left(\frac{a_0}{\sqrt{V}}\right) \neq 0. \tag{1.2}$$

In this case we also have that

[a)]Research Associate, School of Theoretical Physics, Dublin Institute for Advanced Studies. Electronic mail: joe.pule@ucd.ie
[b)]Electronic mail: andre.verbeure@fys.kuleuven.be
[c)]Electronic mail: zagrebnov@cpt.univ-mrs.fr

$$\rho_0 = \lim_{\Lambda} \omega\left(\frac{a_0^* a_0}{V}\right) = \lim_{\Lambda} \left|\omega\left(\frac{a_0}{\sqrt{V}}\right)\right|^2. \tag{1.3}$$

It is easy to deduce from the Cauchy-Schwarz inequality that spontaneous breaking of gauge symmetry in the sense of (1.2) implies the existence of condensation. However in the literature on Bose condensation of homogenous systems, one notices that many authors seem to take for granted or consider trivially true the converse of this statement, that is, the fact that the existence of condensation ($\rho_0 > 0$) implies spontaneous breaking of gauge symmetry. This result (1.3), which is far from trivial, indeed holds true and was first proved in a very general setting in Ref. 1, where one finds the following proposition.

Proposition 1.1: If in the state ω, *the ground state condensate density* $\rho_0 > 0$, *then there exists a family of equilibrium states* $\{\omega_\alpha | \alpha \in [0, 2\pi)\}$ *such that*

(a) $\omega = (1/2\pi)\int_0^{2\pi} \mathrm{d}\alpha\, \omega_\alpha$,
(b) $\lim_\Lambda \omega_\alpha(a_0/\sqrt{V}) \neq 0$ *for all* $\alpha \in [0, 2\pi)$.

Through the recent activity in the domain of condensation in traps (see, for example, Ref. 2), the possibility of condensation in a mode corresponding to a nonzero momentum q has arisen. This requires a generalization of above theorem to the case $q \neq 0$. In this paper we shall prove the following proposition.

Proposition 1.2: Suppose that for the equilibrium state ω, *for some* $q \neq 0$ *the condensate density* $\rho_q > 0$ *and let* $q = (2\pi/\gamma)e$ *where* e *is a unit vector in* $\mathbb{R}^\nu$ *and* $\gamma > 0$. *Then there exists a family of periodic equilibrium states* $\{\tilde{\omega}_{te} | t \in [0, \gamma)\}$, *with period* γ *such that*

(a) $\omega = (1/\gamma)\int_0^\gamma \mathrm{d}t\, \tilde{\omega}_{te}$,
(b) $\lim_\Lambda \tilde{\omega}_{te}(a_q/\sqrt{V}) \neq 0$ *for all* $t \in [0, \gamma)$.

We give the exact formulation and proof of this result in Sec. II (see Theorems 2.1 and 2.2). The statement in (b) means that now, not only the gauge symmetry is spontaneously broken, but also the space translation invariance since under translation by y, for example, the operator a_q is transformed into $e^{-iq\cdot y}a_q$. For an explicit application of this result see Ref. 3. The main practical result is that for homogenous gauge invariant systems, a thermodynamic limit Gibbs states, showing condensation in a mode $q \neq 0$, can be decomposed with respect to periodic equilibrium states also showing gauge symmetry breaking. This decomposition of the state ω in the direction of q can straightforwardly be generalized to more dimensions by constructing from ω states which are periodic in any dimension at the same time.

II. CONDENSATION AND SPONTANEOUS SYMMETRY BREAKING

The models we have in mind in this note are realistic Bose systems, with two-body interactions in dimension $\nu \geqslant 1$. The two-body potential v is supposed to be *well-behaved* and in particular *superstable*.[4]

The algebra of observables $\mathcal{A}$ (Ref. 5) is as usual generated by the Weyl operators,

$$W(h) = \exp i\{a(h) + a^*(h)\} h \in \mathcal{H} = L^2(\mathbb{R}^\nu),$$

where $a^\#(h)$ are the boson annihilation and creation operators in the symmetric Fock space $\mathcal{F}(\mathcal{H})$ satisfying the canonical commutation relations

$$[a(f), a^*(g)] = \langle f, g\rangle_{\mathcal{H}}, \tag{2.1}$$

with $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ denoting the scalar product in the Hilbert space $\mathcal{H}$.

For a cubic region Λ in $\mathbb{R}^\nu$ centered at the origin let $\mathcal{H}_\Lambda = L^2(\Lambda)$. Then the algebra $\mathcal{A}_\Lambda$ generated by $\{W(h) | h \in \mathcal{H}_\Lambda\}$ is embedded in $\mathcal{A}$ in the natural way.

On the n-particle subspaces of $\mathcal{F}(\mathcal{H}_\Lambda)$, the local Hamiltonians H_Λ are given by

$$H_\Lambda^n = T_\Lambda^n + U_\Lambda^n, \tag{2.2}$$

where $T_\Lambda^n = -\Sigma_{i=1}^n \Delta_i/2$, Δ being the self-adjoint extension of the Laplacian on $\mathcal{H}_\Lambda$ corresponding to *periodic* boundary conditions, and U_Λ^n the multiplication operator by $\Sigma_{1\leqslant i<j\leqslant n} v(|x_i - x_j|)$, $x_i, x_j \in \Lambda$. The superstability condition ensures the existence of local Gibbs states and all n-point correlation functions for any number of creation and annihilation functions, see, e.g., Refs. 4 and 5, Chap. 6.3.4. We denote the number operator for the volume Λ by N_Λ.

We are interested in the properties of the equilibrium states corresponding to the system (2.2). In what follows the most convenient way to define these states is by means of the correlation inequalities.[6] In particular a state ω on $\mathcal{A}$ is an equilibrium state at inverse temperature β and chemical potential $\mu \in \mathbb{R}$ if it satisfies the following *energy-entropy balance conditions:*

$$\beta\omega(X^*[H_\Lambda - \mu N_\Lambda, X]) \geqslant \omega(X^*X)\ln \frac{\omega(X^*X)}{\omega(XX^*)} \tag{2.3}$$

for all Λ and for any observable $X \in \mathcal{A}_\Lambda$ in the domain $\mathcal{D}([H_\Lambda - \mu N_\Lambda, \cdot])$. Our aim is to find solutions ω satisfying (2.3). The thermodynamic limit Gibbs states are solutions of (2.3) and because of the homogeneity and gauge invariance of the Hamiltonian (2.2), they are translation and gauge invariant solutions. With this in mind, we consider the class of states ω satisfying (2.3), and the following conditions which are satisfied in realistic Bose systems with superstable interaction:

(A) The state ω is translation and gauge invariant.
(B) The state ω is *analytic* in the sense of Ref. 5, Chap. 5.2.3, this means that the state can be completely described in terms of all n-point correlation functions of the creation and annihilation operators.

Denote the volume of Λ by V and let

$$\Lambda^* = \{2\pi n/V^{1/\nu} | n \in \mathbb{Z}^\nu\}$$

be the *dual momentum set* for the cubic region Λ with periodic boundary conditions. As above for any $k \in \Lambda^*$, we define the creation and annihilation operators of a particle with momentum k,

$$a_k^\# = a^\#(\phi_{\Lambda,k}) \quad \text{where } \phi_{\Lambda,k}(x) = \frac{1}{\sqrt{V}} e^{ik\cdot x}\mathbb{I}_\Lambda(x),$$

$\mathbb{I}_\Lambda$ being the characteristic function of region Λ.

We say that the state ω shows *condensation* in the mode $q \in \Lambda^*$ if

$$\rho_q = \lim_\Lambda \omega\left(\frac{a_q^* a_q}{V}\right) > 0 \tag{2.4}$$

and then ρ_q is called the *condensate density* in the q mode.

We consider the system $(\mathcal{A}, \omega)$ and its *GNS construction*[5] on the Hilbert space $\mathfrak{H}$ with cyclic and separating vector $\Omega \in \mathfrak{H}$, i.e., for all $X \in \mathcal{A}$, one has

$$\omega(X) = \langle \Omega, X\Omega \rangle, \tag{2.5}$$

where for notational convenience, we denote by the *same symbol* the element X of $\mathcal{A}$ and its image under the GNS representation, an operator on $\mathfrak{H}$. We denote by $\mathcal{A}''$ the von Neumann algebra generated by the representation of $\mathcal{A}$, and by $\mathcal{A}'$ its commutant. Take $q \in \Lambda^*$ with $q \neq 0$ and let

$$\alpha_{q,\Lambda} := a(\phi_{\Lambda,q}/\sqrt{V}) = \frac{1}{V}\int_\Lambda \mathrm{d}x\, e^{iq\cdot x} a(x). \tag{2.6}$$

This operator converges strongly to an operator α_q in the representation space $\mathfrak{H}$.[5] So, we define

$$\alpha_q = \lim_{\Lambda} \alpha_{q,\Lambda} \quad \text{and} \quad \alpha_q^* = \lim_{\Lambda} \alpha_{q,\Lambda}^*. \tag{2.7}$$

Because the operators $\alpha_{q,\Lambda}$ are local averages (2.6), α_q is a limit average operator, also called *observable at infinity*, and therefore affiliated to the *center* $\mathcal{C}=\mathcal{A}''\cap\mathcal{A}'$ of the algebra $\mathcal{A}''$, see, e.g., Ref. 5.

For $y\in\mathbb{R}^\nu$ let τ_y be the translation $*$-automorphism of $\mathcal{A}$ over the distance y, that is,

$$(\tau_y a^\#)(x) = a^\#(x+y). \tag{2.8}$$

Then from (2.6)–(2.8) we obtain

$$\tau_y \alpha_q = e^{-iq\cdot y}\alpha_q, \tag{2.9}$$

$$\tau_y(\alpha_q^*\alpha_q) = \alpha_q^*\alpha_q. \tag{2.10}$$

From (2.10) we see that the particle density operator in the mode q, $n_q := \alpha_q^*\alpha_q$, is translation invariant.

For the rest of this section we make the assumption that in the state ω there is condensation in the *nonzero* mode $q\neq 0$, i.e., we shall assume that

$$\rho_q = \omega(\alpha_q^*\alpha_q) = \omega(n_q) > 0. \tag{2.11}$$

This implies that $n_q>0$ and therefore also that

$$\omega(n_q^{1/2}) \neq 0, \tag{2.12}$$

since $\omega(n_q^{1/2})$ cannot be zero because of the *separating* character of the equilibrium state.[5] Consider the *polar decomposition* of the operator α_q,

$$\alpha_q = U_q n_q^{1/2}. \tag{2.13}$$

As α_q belongs to the center $\mathcal{C}$, it is a *normal* operator. By Ref. 7, Chap. X.9, operator U_q can be taken as the unitary extension of the partial isometry defined by the polar decomposition. Since

$$0 \neq \omega(n_q^{1/2}) = \omega(U_q^*\alpha_q) = \lim_{\Lambda} \omega(U_q^*\alpha_{q,\Lambda}),$$

we can find $h\in\mathcal{H}$ such that

$$\omega(U_q^* a(h)) \neq 0. \tag{2.14}$$

Now we define a representation of $\mathcal{A}$ on $\mathfrak{H}$. For any $h\in\mathcal{H}$, define the boson field

$$\tilde{\phi}(h) := \{U_q^* a(h) + U_q a^*(h)\}^*. \tag{2.15}$$

By definition (2.15), the operator $\tilde{\phi}(h)$ is essentially self-adjoint in $\mathfrak{H}$, and we can define Weyl operators $\tilde{W}$, $\mathcal{H}\to\mathcal{B}(\mathfrak{H})$,

$$\tilde{W}(h) := e^{i\tilde{\phi}(h)}, \quad h\in\mathcal{H}. \tag{2.16}$$

Using the fact that U_q is a unitary belonging to the center, it is trivial to check that $\tilde{W}$ is a representation of $\mathcal{A}$ on $\mathfrak{H}$. Denote by η the $*$-isomorphic map of $\mathcal{A}$ into $\mathcal{B}(\mathfrak{H})$,

$$\eta(W(h)) = \tilde{W}(h). \tag{2.17}$$

Then one can easily derive the following identities for the annihilation and creation operators:

$$\tilde{a}(h) := \eta(a(h)) = U_q^* a(h),$$

$$\tilde{a}^*(h) := \eta(a^*(h)) = U_q a^*(h).$$

For any $x \in \mathbb{R}^\nu$, we define the functional $\tilde{\omega}_x$ on $\mathcal{A}$ by

$$\tilde{\omega}_x(W(h)) := \langle \Omega, \tilde{W}(h_x)\Omega \rangle = \omega(\eta \circ \tau_x(W(h))), \tag{2.18}$$

where $h_x(y)=h(x+y)$ is the translate of h over x. It is clear from (2.18) that $\tilde{\omega}_x$ is again a state on algebra $\mathcal{A}$.

It follows immediately from (2.14) and (2.18) that the states $\tilde{\omega}_x$ are *not* gauge invariant, in particular $\tilde{\omega}_x(a(h))=\omega(U_q^*\tau_x a(h)) \neq 0$ for some $h \in \mathcal{H}$. Also directly from the definition (2.18) one sees that the states $\tilde{\omega}_x$, $x \in \mathbb{R}^\nu$, have the property that for all $y \in \mathbb{R}^\nu$,

$$\tilde{\omega}_x \circ \tau_y = \tilde{\omega}_{x+y}. \tag{2.19}$$

Now we concentrate on the direction of the translation. Let $q=(2\pi/\gamma)e$ where $e \in \mathbb{R}^\nu$ is the unit vector in the direction of q and let γ be the period or wavelength of the mode q, i.e., $\gamma = 2\pi/\|q\|$. We have the following.

Theorem 2.1 *(existence of periodic states):*

(a) *Each state $\tilde{\omega}_x$ is translation invariant in any direction orthogonal to q: for all $y \in \mathbb{R}^\nu$ such that $y \cdot q = 0$,*

$$\tilde{\omega}_{x+y} = \tilde{\omega}_x.$$

(b) *Each state $\tilde{\omega}_x$ is periodic with period γ in the direction of q:*

$$\tilde{\omega}_{x+\gamma e} = \tilde{\omega}_x.$$

Proof: From (2.15), (2.16), and (2.18) we obtain

$$\tilde{\omega}_{x+y}(W(h)) = \langle \Omega, e^{i\tilde{\phi}(h_{x+y})}\Omega \rangle. \tag{2.20}$$

Now we have

$$\tilde{\phi}(h_{x+y}) = \{U_q^* \tau_y a(h_x) + U_q \tau_y a^*(h_x)\}^* = \tau_y\{\tau_{-y}(U_q^*)a(h_x) + \tau_{-y}(U_q)a^*(h_x)\}^* \tag{2.21}$$

and from (2.9), (2.10), and (2.13) it follows that

$$\tau_y(U_q) = U_q e^{-iq\cdot y}.$$

Therefore, if $y \cdot q = 0$ or $y = \gamma e$ (since then $q \cdot y = 2\pi$), one gets $\tau_y(U_q) = U_q$. Thus for both cases we get

$$\tilde{\phi}(h_{x+y}) = \tau_y \tilde{\phi}(h_x). \tag{2.22}$$

Then inserting (2.22) into (2.20) and using the translation invariance of the state ω (2.5) one gets the proof of (a) and (b). □

Now we come to the analysis of the states and their translates in the direction of the vector q.

Theorem 2.2 *(decomposition into periodic states):*

(c) *The states $\tilde{\omega}_{te}$ are all distinct, that is, for any $t, t' \in [0, \gamma)$ such that $t \neq t'$ one has*

$$\tilde{\omega}_{te} \neq \tilde{\omega}_{t'e}.$$

(d) *The original state ω is the convex combination of the family of states $\{\tilde{\omega}_{te} | t \in [0, \gamma)\}$:*

$$\omega = \frac{1}{\gamma}\int_0^\gamma \mathrm{d}t\, \tilde{\omega}_{te}.$$

(e) *All the states $\{\tilde{\omega}_{te} | t \in [0, \gamma)\}$ are equilibrium states.*

Proof: Since the state ω is analytic [condition (B)], it follows from definition (2.18) that the

states $\tilde{\omega}_x$ are also analytic. Therefore, it is sufficient to check the statements of the theorem only for *all monomials* in the field operators (Ref. 5, Chap. 5.2.3.).

Recall that by (2.18) we have

$$\tilde{\omega}_{te}(a(h)) = \omega(U_q^* \tau_{te} a(h)).$$

Using (2.9) and the translation invariance of the state ω [condition (A)], we obtain

$$\tilde{\omega}_{te}(a(h)) = e^{-iq\cdot te}\omega(U_q^* a(h)) = e^{-i(2\pi/\gamma)t}\omega(U_q^* a(h)).$$

By (2.14), there exists an element $h \in \mathcal{H}$ such that $\omega(U_q^* a(h)) \neq 0$. Then for any $t, t' \in [0, \gamma)$, $t \neq t'$ one gets

$$(\tilde{\omega}_{te} - \tilde{\omega}_{t'e})(a(h)) = (e^{-it(2\pi/\gamma)} - e^{-it'(2\pi/\gamma)})\omega(U_q^* a(h)) \neq 0,$$

proving (c).

We now prove (d). Let $m, n \in \mathbb{N}$ and $f \in \mathcal{H}$. Then we have

$$\frac{1}{\gamma}\int_0^\gamma \mathrm{d}t\ \tilde{\omega}_{te}(a^*(f)^n a(f)^m) = \frac{1}{\gamma}\int_0^\gamma \mathrm{d}t\ \omega(\tau_{te}(a^*(f)^n)\tau_{te}(a_{te}(f)^m)U_q^n U_q^{-m}).$$

By virtue of (2.9) and by translation and gauge invariance of the state ω [condition (A)] we get

$$\begin{aligned}\frac{1}{\gamma}\int_0^\gamma \mathrm{d}t\ \tilde{\omega}_{te}(a^*(f)^n a(f)^m) &= \frac{1}{\gamma}\int_0^\gamma \mathrm{d}t\ e^{i(2\pi/\gamma)t(m-n)}\omega(a^*(f)^n a(f)^m U_q^{n-m}) \\ &= \delta_{n,m}\omega(a^*(f)^n a(f)^m) = \omega(a^*(f)^n a(f)^n),\end{aligned}$$

which proves (d).

Finally we prove that for any $t \in [0, \gamma)$ the state $\tilde{\omega}_{te}$ is an equilibrium state, by showing that these states satisfy the equilibrium conditions (2.3). Let X be an arbitrary monomial in the creation and annihilation operators. Then using condition (A) for the state ω together with the translation and gauge invariance of the local Hamiltonians (2.2), one gets

$$\begin{aligned}\lim_\Lambda \tilde{\omega}_{te}(X^*[H_\Lambda - \mu N_\Lambda, X]) &= \lim_\Lambda \omega(\eta \circ \tau_{te}(X^*[H_\Lambda - \mu N_\Lambda, X])) \\ &= \lim_\Lambda \omega((\eta \circ \tau_{te}(X))^*[H_\Lambda - \mu N_\Lambda, \eta \circ \tau_{te}(X)]) \geqslant \omega((\eta \circ \tau_{te}(X))^*(\eta \\ &\circ \tau_{te}(X))) \\ &\times \ln \frac{\omega((\eta \circ \tau_{te}(X))^* \eta \circ \tau_{te}(X))}{\omega(\eta \circ \tau_{te}(X)(\eta \circ \tau_{te}(X))^*)} = \tilde{\omega}_{te}(X^*X)\ln \frac{\tilde{\omega}_{te}(X^*X)}{\tilde{\omega}_{te}(XX^*)}.\end{aligned}$$

This yields (e) concluding the proof of the theorem. □

Theorems 2.1 and 2.2 prove that if one has an equilibrium state ω showing condensation in the *non zero q* mode (2.4) then there exists a set of periodic equilibrium states $\{\tilde{\omega}_{te} | t \in [0, \gamma)\}$ in the q direction with period γ. In directions orthogonal to q, these states remain *homogenous*. Note that these states simultaneously break the gauge symmetry and that they live in the same representation space $\mathfrak{H}$ of the CCR algebra $\mathcal{A}$ determined by the original state ω. We have proved that spontaneous translation and gauge symmetry breaking occur *simultaneously*.

The *converse* statement is clearly not true in general. For example, bosonic atoms may crystallize without undergoing Bose condensation as in the case of ^{4}He at sufficiently high pressure, see also the discussion in Sec. III. However, if we assume a *stronger* form of translation invariance symmetry breaking of the state $\tilde{\omega}_x$, namely,

$$\tilde{\omega}_x(\alpha_q) = \lim_{\Lambda} \tilde{\omega}_x(\alpha_{q,\Lambda}) \neq 0, \tag{2.23}$$

then the existence of Bose condensation in the q mode follows immediately from the Cauchy-Schwarz inequality as it does for the zero mode.

Remark 2.1: Theorems 2.1 and 2.2 are in fact valid under weaker assumptions. In particular the second condition (B) *can be dispensed with. But then one must work almost entirely with the Weyl operators as observables and not the creation/annihilation operators. Also one must replace the equilibrium conditions* (2.3) *by the KMS-state definition of equilibrium.*[5]

Remark 2.2: Above we analyzed the situation for one direction q. It is a simple exercise to generalize the analysis to an arbitrary number of dimensions. In particular, suppose that one has condensation in ν *independent directions* $q_1, \ldots, q_\nu$, *i.e., that* $\rho_{q_i} > 0$ *for* $i = 1, \ldots \nu$, *and*

$$q_i \cdot q_j = \delta_{ij} |q_i|^2.$$

Then we can perform the above constructions in each direction independently because the corresponding α*-operators commute with each other and with their adjoints. One obtains equilibrium states* $\tilde{\omega}_x$, *with* $x = t_1 e_1 + \cdots + t_\nu e_\nu$, *periodic in all directions creating a* ν*-dimensional lattice.*

III. CONCLUSION

As we mentioned in the Introduction there are situations when there is condensation in a nonzero mode. In fact in Ref. 3 we considered a model that exhibits condensation in the *zero* mode and a *nonzero* mode simultaneously. For this model Theorems 2.1 and 2.2 can be used to show the existence of *periodic* interference fringes (*condensate grating*), which is observed experimentally, see discussion in Ref. 3. Here we give a brief account of this argument.

In the limiting equilibrium state ω, which is translation invariant, clearly the average local particle density is constant. However in this model when condensation occurs in the mode $q \neq 0$ also, by Theorem 2.1 the translation invariance of equilibrium states will be broken in the direction of e simultaneously with the gauge symmetry. This implies that

$$\eta_0(t) := \lim_{\Lambda} \tilde{\omega}_{te}(\alpha_{0,\Lambda}) \neq 0 \quad \text{and} \quad \eta_q(t) := \lim_{\Lambda} \tilde{\omega}_{te}(\alpha_{q,\Lambda}) \neq 0 \tag{3.1}$$

for any of the states $\{\tilde{\omega}_{te} | t \in [0, \gamma)\}$, see Proposition 1.2 (b). Recall that the local particle density operator is given by

$$\rho_\Lambda(x) := \sum_{k \in \Lambda^*} \hat{\rho}_{k,\Lambda} e^{ik \cdot x}, \tag{3.2}$$

where

$$\hat{\rho}_{k,\Lambda} := \sum_{p \in \Lambda^*} \alpha^*_{p+k,\Lambda} \alpha_{p,\Lambda}. \tag{3.3}$$

The conservation laws for this model imply that

$$\tilde{\omega}_{te}(\alpha^*_{p+k,\Lambda} \alpha_{p,\Lambda}) = \delta_{k,q} \delta_{p,0} \tilde{\omega}_{te}(\alpha^*_{k,\Lambda} \alpha_{0,\Lambda}) + \delta_{k,0} \tilde{\omega}_{te}(\alpha^*_{p,\Lambda} \alpha_{p,\Lambda}) \tag{3.4}$$

and one also has (see Ref. 3, Sec. 4)

$$\lim_{\Lambda} \tilde{\omega}_{te}(\alpha^*_{q,\Lambda} \alpha_{0,\Lambda}) = \lim_{\Lambda} \tilde{\omega}_{te}(\alpha^*_{q,\Lambda}) \lim_{\Lambda} \tilde{\omega}_{te}(\alpha_{0,\Lambda}) = \overline{\eta_q(t)}\, \eta_0(t). \tag{3.5}$$

Then by definition (3.2) and (3.3) and by virtue of (3.1), (3.4), and (3.5) we obtain

$$\lim_{\Lambda} \tilde{\omega}_{te}(\rho_\Lambda(x)) = 2\, \mathrm{Re}\{e^{iq \cdot x} \overline{\eta_q(t)}\, \eta_0(t)\} + \lim_{\Lambda} \tilde{\omega}_{te}(\rho_\Lambda(0)). \tag{3.6}$$

This means that one gets a nonhomogeneity (*grating*) of the equilibrium total particle density, as

observed experimentally (see Refs. 2 and 3), if and only if there is simultaneous condensation in some nonzero mode and in the zero mode.

Another possible application of our general results is motivated by Remark 2. This is related to the theory of a hypothetic *coherent* boson crystals,[8,9] proposed to explain some unusual properties of ^{4}He in the solid phase. The main ingredients of this approach are the Hartree or the Gross-Pitaevskii variational calculations based on the hypothesis of the existence of the condensate in the zero mode as well as in several other *nonzero* modes to imitate an elementary cell of the solid helium. In this case the Helium atoms are *not localized* and the corresponding periodic state implies the occurrence of space variation in the particle density by virtue of (2.23) and by the arguments (3.1) and (3.6) in this section. Note that the coherent crystallization is drastically different from the standard one, where the atoms on the lattice sites are completely localized, thus do not obey many-body quantum statistics and the assumption (2.23) cannot be valid. This point of view on the crystal state, in which delocalized particles still satisfy Bose statistics, has led in turn to the hypothesis of *superfluidity* of quantum crystals, see, e.g., Ref. 10.

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Energy levels of a nonlocal functional

G. Bellettini[a)]
Dipartimento di Matematica, Università di Roma "Tor Vergata," via della Ricerca Scientifica 00133 Roma, Italy

A. De Masi[b)]
Dipartimento di Matematica, Università di L'Aquila, via Vetoio, loc. Coppito, 67100 L'Aquila, Italy

E. Presutti[c)]
Dipartimento di Matematica, Università di Roma "Tor Vergata," via della Ricerca Scientifica 00133 Roma, Italy

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We study the critical points of a nonlocal free energy functional. The functional has two minimizers (ground states) $m^{(\pm)}$ with zero energy. We prove that there is a first excited state identified as the instanton $\hat{m}_L$, and that above the energy of the instanton there is a gap. We also characterize parts of the basin of attraction of $m^{(\pm)}$ and $\hat{m}_L$ under a dynamics associated to the free energy functional. The result completes the analysis of tunneling from $m^{(-)}$ to $m^{(+)}$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1990107]

I. INTRODUCTION

In this paper we consider a nonlocal free energy functional $\mathcal{F}_L$ on $L^\infty([-L,L];[-1,1])$ defined by

$$\mathcal{F}_L(m)=\int_{-L}^{L}\phi_\beta(m)\mathrm{d}x+\frac{1}{4}\int_{-L}^{L}\int_{-L}^{L}J^{\mathrm{neum}}(x,x')[m(x)-m(x')]^2\mathrm{d}x\,\mathrm{d}x', \tag{1.1}$$

where $\beta>1$,

$$\phi_\beta(m)=\tilde{\phi}_\beta(m)-\min_{|s|\leqslant 1}\tilde{\phi}_\beta(s),\quad \tilde{\phi}_\beta(m)=-\frac{m^2}{2}-\frac{1}{\beta}\mathcal{S}(m),$$

$$\mathcal{S}(m)=-\frac{1-m}{2}\log\frac{1-m}{2}-\frac{1+m}{2}\log\frac{1+m}{2},$$

and

$$J^{\mathrm{neum}}(x,y)=J(x,y)+J(x,R_L(y))+J(x,R_{-L}(y))$$

with $R_\xi(y)=\xi-(y-\xi)$ the reflection of y around ξ and $J(x,y)$, $(x,y)\in\mathbb{R}\times\mathbb{R}$, a smooth, symmetric, translational invariant probability kernel supported in $|y-x|\leqslant 1$. We also assume that $J(0,x)$ is a nonincreasing function whenever restricted to $x\geqslant 0$. The functional (1.1) arises in statistical mechanics in the analysis of Ising systems with Kac potentials,[9] and it has been extensively studied in the recent years.

[a)]Electronic mail: belletti@mat.uniroma2.it
[b)]Electronic mail: demasi@univaq.it
[c)]Electronic mail: presutti@mat.uniroma2.it

The critical points of $\mathcal{F}_L$ are defined as the functions $m \in L^\infty([-L,L];[-1,1])$ which solve in the whole of $[-L,L]$ the "nonlocal mean field equation"

$$m = \tanh\{\beta J^{\text{neum}} * m\}. \tag{1.2}$$

(1.2) also has a dynamical interpretation as the equation for the stationary points of the evolution equation

$$u_t = g_L(u) := -u + \tanh\{\beta J^{\text{neum}} * u\} \tag{1.3}$$

which is derived from Glauber dynamics in the Ising systems with Kac potentials mentioned previously.[9]

We call "energy levels" of $\mathcal{F}_L$ its values at the critical points and borrowing from the terminology on linear operators, we call "spectrum" of $\mathcal{F}_L$ the set of all its energy levels. Many physical properties are determined by the structure of the spectrum at its bottom and its investigation is the main aim of this article. We start by observing that the spectrum of $\mathcal{F}_L$ is contained in the positive axis, as both terms on the right-hand side (r.h.s.) of (1.1) are nonnegative. The spectrum actually starts at 0. Indeed, since J^{neum} is a probability kernel, the solutions of (1.2) which are spatially homogeneous, namely $m(x)=u\in[-1,1]$ for all $x\in[-L,L]$, satisfy the "mean field equation" $u=\tanh\{\beta u\}$. As $\beta>1$, there are three solutions $u=\pm m_\beta$, $m_\beta\in(0,1)$, and $u=0$. The two critical points $m^{(\pm)}(x)=\pm m_\beta$, $x\in[-L,L]$, have zero energy, $\mathcal{F}_L(m^{(\pm)})=0$, and are called "ground states," while $\mathcal{F}_L(0)=2\phi_\beta(0)L>0$.

Thus the spectrum starts at 0 and 0 has degeneracy 2 as there is no other m besides $m^{(\pm)}$ with 0 energy. In fact the second term on the r.h.s. of (1.1) forces a minimizer to be spatially homogeneous and we have already seen that, among the spatially homogeneous functions, $m^{(\pm)}$ are the only ground states. We also know from the literature that the state $m\equiv 0$ is not the first excited state (i.e., with minimal positive energy), at least for L large enough. In fact its energy $2\phi_\beta(0)L$ becomes, as L increases, larger than the energy of the instanton $\hat{m}_L$ (a spatially nonhomogeneous critical point), which instead remains bounded as $L\to\infty$.[5–7] In this article we will prove the following.

Theorem 1.1: *For all L large enough, $\mathcal{F}_L(\hat{m}_L)$ is the first energy level above 0, it is not degenerate and above $\mathcal{F}_L(\hat{m}_L)$ there is a spectral gap, namely there is $\epsilon>0$ so that if m is a critical point and $\mathcal{F}_L(m)\leqslant\mathcal{F}_L(\hat{m}_L)+\epsilon$, then $m\in\{m^{(-)},m^{(+)},\hat{m}_L\}$.*

Such a characterization of the spectrum was the missing element in Ref. 3 in the analysis of tunnelling from $m^{(-)}$ to $m^{(+)}$, which therefore with the help of Theorem 1.1 is now complete. We can also use Theorem 1.1 to determine partially the basin of attraction of $m^{(\pm)}$ and $\hat{m}_L$.

Theorem 1.2: *For all L large enough, there is $\epsilon>0$ so that for any m such that $\mathcal{F}_L(m)\leqslant\mathcal{F}_L(\hat{m}_L)+\epsilon$*

$$\lim_{t\to\infty} S_t(m) \in \{m^{(-)},m^{(+)},\hat{m}_L\}, \tag{1.4}$$

where $S_t(m)$ is the solution of (1.3) *starting from m at time* 0.

Theorem 1.2 is a corollary of Theorem 1.1 (but the converse is also true and indeed we will prove Theorem 1.1 as a consequence of Theorem 1.2). In fact, the semigroup $S_t(m)$ decreases the energy, in the sense that $\mathcal{F}_L(S_t(m))$ is a strictly decreasing function of t, unless m is a critical point. Moreover, by compactness and continuity the limit points of an orbit $S_t(m)$ are critical points and by lower semicontinuity of $\mathcal{F}_L$ their energy is smaller than $\mathcal{F}_L(m)$, hence (1.4).

The information on the basin of attraction of $\{m^{(-)},m^{(+)},\hat{m}_L\}$ contained in Theorem 1.2 is sufficient for the analysis of tunneling, because the control parameter is the energy, but in many applications in statistical physics natural neighborhoods are in the L^∞ topology. In such neighborhoods the energy may grow proportionally to L (the domain size) and new criteria for being attracted to $\{m^{(-)},m^{(+)},\hat{m}_L\}$ are needed. To formulate the results we need some more notation and definition and we postpone the issue to the next section at the end of which we give an outline on the content of the paper. A preliminary version of the present paper is in Ref. 4.

II. DEFINITIONS AND RESULTS

For ease of notation it is sometimes convenient to work in the whole line rather than in $[-L,L]$, this is possible provided we suitably restrict the space of functions. $m \in L^\infty(\mathbb{R};[-1,1])$ is symmetric around ξ if $m(\xi+x)=m(\xi-x)$, $x \in \mathbb{R}$; it is called L-symmetric if it is symmetric around all points $(2n+1)L$, $n \in \mathbb{Z}$. The symmetric extension of $m \in L^\infty([-L,L];[-1,1])$ is then the L-symmetric function on $\mathbb{R}$ which agrees with m in $[-L,L]$ and

$$\int_{-L}^{L} \phi_\beta(m)\mathrm{d}x + \frac{1}{4}\int_{-L}^{L}\int_{\mathbb{R}} J(x,x')(m(x)-m(x'))^2\mathrm{d}x\ \mathrm{d}x' \tag{2.1}$$

is equal to $\mathcal{F}_L(m\mathbf{1}_{|x|\leqslant L})$. Moreover if m is L-symmetric and $S_t(m)$ solves

$$u_t = g(u) := -u + \tanh\{\beta J * u\}, \quad u(\cdot,0)=m, \tag{2.2}$$

then $S_t(m)$ is L-symmetric and its restriction to $[-L,L]$ solves (1.3). It is therefore equivalent to consider (2.1) and (2.2) on the space of L-symmetric functions or to work in the context of Sec. I, and we take advantage of this equivalence by setting each problem in the one of the two contexts which is more convenient for the specific purpose. To have more compact notation we sometimes use the same symbol for a function and its L-symmetric extension. Natural neighborhoods in statistical mechanics are defined in terms of "closeness in the average" and of "coarse graining" transformations. We briefly recall the main notion adapted to the present context.

Definition 2.1. (Coarse graining): Let $\mathcal{D}^{(\ell)}$, $\ell>0$, be the partition of $\mathbb{R}$ into the intervals $[n\ell, (n+1)\ell)$, $n \in \mathbb{Z}$, and $I_x^{(\ell)}$ the interval in $\mathcal{D}^{(\ell)}$ which contains the point x. Then the ℓ-coarse grained image of a L^∞ function m is

$$m^{(\ell)}(x) := \fint_{I_x^{(\ell)}} m(y)\mathrm{d}y, \quad \fint_\Lambda m(y)\mathrm{d}y := \frac{1}{|\Lambda|}\int_\Lambda m(y)\mathrm{d}y. \tag{2.3}$$

Definition 2.2. (Phase indicators): Given an "accuracy parameter" $\zeta>0$, let

$$\eta^{(\zeta,\ell)}(m;x) = \begin{cases} \pm 1 & \text{if } |m^{(\ell)}(x) \mp m_\beta| \leqslant \zeta \\ 0 & \text{otherwise.} \end{cases}$$

Denoting ℓ_- and ℓ_+ two values of the parameter ℓ, with ℓ_+ an integer multiple of ℓ_-, we then define the "phase indicator"

$$\Theta^{(\zeta,\ell_-,\ell_+)}(m;x) = \begin{cases} \pm 1 & \text{if } \eta^{(\zeta,\ell_-)}(m;\cdot) = \pm 1 \text{ in } [-L,L] \cap (I^{(\ell_+)}_{x-\ell_+} \cup I^{(\ell_+)}_x \cup I^{(\ell_+)}_{x+\ell_+}) \\ 0 & \text{otherwise.} \end{cases}$$

Definition 2.3. (Contours): The contours of a function $m \in L^\infty$ are defined as the connected components of the set $\{x:\Theta^{(\zeta,\ell_-,\ell_+)}(m;x)=0\}$. $\Gamma=[x_-,x_+)$ is a plus contour if $\eta^{(\zeta,\ell_-)}(m;x_\pm)=1$, a minus contour if $\eta^{(\zeta,\ell_-)}(m;x_\pm)=-1$, otherwise it is called mixed. The parameters (ζ,ℓ_-,ℓ_+,L) are called compatible with $(\zeta_0,c_1,\kappa) \in \mathbb{R}^3_+$ if $\zeta \in (0,\zeta_0)$, $\ell_- \leqslant \kappa\zeta$, $1/\ell_- \leqslant \ell_+$; L is a multiple integer of ℓ_+ and ℓ_+ a multiple integer of ℓ_-.

Definition 2.4. (Good choice of parameters): In the sequel we take $\zeta \leqslant \zeta_0$, $\zeta_0>0$ suitably small, $L>\zeta^{-8}$ and $\ell_\pm$ determined by L and ζ as follows. ℓ_+ is the smallest number $\geqslant \zeta^{-4}$ such that $L=n\ell_+$, $n \in \mathbb{N}$; ℓ_- is the largest number $\leqslant \zeta^2$ such that $\ell_+=p\ell_-$, $p \in \mathbb{N}$, $p>1$. To have more compact notation we will omit the dependence on (ζ,ℓ_-,ℓ_+), unless ambiguities may arise.

The regions where $\Theta^{(\zeta,\ell_-,\ell_+)}(m;x)=1$ are said to be in plus equilibrium (or in the plus phase), those where $\Theta^{(\zeta,\ell_-,\ell_+)}=-1$ are in the minus equilibrium and the mixed contours which separate plus and minus regions represent an interface. The equilibrium interface (defined by an optimization problem, see Refs. 1 and 2) is represented, when the minus phase is to the left, by the instanton $\bar{m}(x)$ which is a stationary solution of (2.2)

$$\bar{m}(x) = \tanh\{\beta(J * \bar{m})(x)\}, \quad x \in \mathbb{R}, \tag{2.4}$$

with asymptotic behavior

$$\lim_{x\to\pm\infty} \bar{m}(x) = \pm m_\beta. \tag{2.5}$$

As recalled in Sec III, $\bar{m}(x)$ is unique (modulo translations) and it is a $\mathcal{C}^\infty$, strictly increasing, antisymmetric function. We denote by $\bar{m}_\xi$ a translation of the instanton, namely

$$\bar{m}_\xi(x) = \bar{m}(x-\xi), \quad \xi \in \mathbb{R} \tag{2.6}$$

which is interpreted as the equilibrium interface located at ξ.

Definition 2.5. (Neighborhoods of pure phases and interfaces): Given $k \in \mathbb{N}$ and $(\zeta, \ell_-, \ell_+, L)$ as in Definition 2.4, setting $\Theta = \Theta^{(\zeta,\ell_-,\ell_+)}$, we define

$U_- = \{m \in L^\infty([-L,L];[-1,1]) : \Theta(m,\cdot) < 1, |\{\Theta(m,\cdot)=0\}| \le k\ell_+\}$,

$U_+ = \{m : -m \in U_-\}$,

$U_{-,+} = \{m \in L^\infty([-L,L];[-1,1]) : m$ has a unique mixed contour $\Gamma, |\Gamma| \le k\ell_+$, and there exists $\xi \in \Gamma$ such that $\mathrm{dist}(\xi, [-L,L]\setminus\Gamma) \ge \ell_+/2$, and $|m^{(\ell_-)} - \bar{m}_\xi^{(\ell_-)}| \le 2\zeta$ on $[-L,L]\}$,

$U_{+,-} = \{m : -m \in U_{-,+}\}$.

Observing that U_-, U_+, $U_{-,+}$, $U_{+,-}$ are pairwise disjoint, we finally define

$$U = U_- \cup U_{-,+} \cup U_{+,-} \cup U_+.$$

A first step in the proof of Theorem 1.2 is the following result, proved in Sec. VI.

Theorem 2.6: *If $\zeta > 0$ is small enough, there is $k \in \mathbb{N}$ such that, for L large enough*

$$\{m \in L^\infty([-L,L];[-1,1]) : \mathcal{F}_L(m) < \mathcal{F}_L(\hat{m}_L) + \zeta^{100}\} \subset U$$

(recall that U depends on k and ζ).

Of course, the number 100 in the previous statement can be replaced by any number sufficiently large. The profiles in $U_- \cup U_+$ are attracted by $m^{(\pm)}$, more precisely in Sec. VII we prove the following theorem.

Theorem 2.7: *If $\zeta > 0$ is small enough, there is $k \in \mathbb{N}$ such that, for L large enough*

$$\lim_{t\to\infty} \|S_t(m) - m^{(\pm)}\|_\infty = 0 \quad \text{for all } m \in U_\pm$$

so that if $m \in U_\pm$ is stationary then $m = m^{(\pm)}$.

If $m \in U \setminus (U_- \cup U_+)$, then m may either be attracted by $m^{(\pm)}$ as in Theorem 2.7 but it could also be attracted by $\hat{m}_L$.

Theorem 2.8: *Given any $r \in (0,1)$, for all L large enough the set $\{m \in U_{-,+} : \Gamma \cap (-L, -rL] \neq \emptyset\}$ (Γ the contour of $m \in U_{-,+}$) is attracted by $m^{(+)}$; the set $\{m \in U_{-,+} : \Gamma \cap [rL, L) \neq \emptyset\}$ by $m^{(-)}$; any other $m \in U_{-,+}$ is attracted either by $m^{(\pm)}$ or by $\hat{m}_L$.*

By symmetry under sign change, Theorem 2.8 extends to its analog in $U_{+,-}$, we do not state explicitly the result. Theorem 2.8 is proved in two steps. We show that any element in $U_{-,+}$ evolves after a finite time to a function which is in sup norm close to an instanton (restricted to $[-L,L]$); we then prove that functions close to an instanton in sup norm are attracted to $m^{(\pm)}$ if the center of the instanton is not too close to the origin, otherwise they may as well converge to $\hat{m}_L$.

Outline of the paper: In Sec. III we recall results known in the literature and which are used later in the proofs. Therefore in a first reading Sec. III may be skipped: specific references to the results stated in Sec. III will be given when needed. In Sec. IV we prove lower bounds on $\mathcal{F}_L$ analogous to the Peierls bounds in statistical mechanics. In Sec. V we prove lower bounds on the infinite volume version $\mathcal{F}$ of the free energy functional. With such a background, in Sec. VI we then prove the localization statement in Theorem 2.6. The second part of this article contains the analysis of the critical points in U: in Sec. VII we prove Theorem 2.7. In Sec. VIII we prove that

functions close to an instanton in sup norm are attracted to $m^{(\pm)}$ if the center of the instanton is not too close to the origin. This proof exploits the existence of a traveling subsolution that converges to $m^{(\pm)}$ as proved in Sec. IX and the Appendix . Finally in Sec. X we complete the proof of Theorem 2.8.

III. GENERAL BACKGROUND

In this section we collect some results in the literature which will be useful in the sequel. Some statements are not really explicit in the literature, in particular those about the finite volume instantons (see Sec. III C) which often have been proved in the presence of an external magnetic field, but they are all close enough to omit their proofs. The assumption that $J(0,x)$ is a nonincreasing function of $x \geqslant 0$ is used only in Sec. III C, all the other statements hold without such an assumption and in more generality.

In Sec. III A we state results on the spirit of the Peierls estimates for the free energy functional. To this end we need some definitions.

If Λ is a finite union of intervals contained in $[-L,L]$, we write $\Lambda^c := [-L,L] \setminus \Lambda$ for its complement in $[-L,L]$ and m_Λ for the restriction of m to Λ. We define

$$\mathcal{F}_{L;\Lambda}(m_\Lambda) = \int_\Lambda \phi_\beta(m_\Lambda)\mathrm{d}x + \frac{1}{4}\int_\Lambda \int_\Lambda J^{\mathrm{neum}}(x,x')(m_\Lambda(x) - m_\Lambda(x'))^2 \mathrm{d}x\, \mathrm{d}x',$$

$$\mathcal{F}_{L;\Lambda}(m_\Lambda | m_{\Lambda^c}) = \mathcal{F}_{L;\Lambda}(m_\Lambda) + \frac{1}{2}\int_\Lambda \int_{\Lambda^c} J^{\mathrm{neum}}(x,x')(m_\Lambda(x) - m_{\Lambda^c}(x'))^2 \mathrm{d}x\, \mathrm{d}x'. \tag{3.1}$$

We let $\mathcal{F}(m)$ be the functional on $L^\infty(\mathbb{R};[-1,1])$ with values in $[0,\infty]$ defined by (1.1) with $L = \infty$ and J in place of J^{neum}.

A. Properties of the free energy functional (Ref. 11)

We suppose that ζ_0, c_1, and $0 < \kappa < 1$ are small enough and that the parameters $(\zeta, \ell_-, \ell_+, L)$ are compatible with ζ_0, c_1, and κ.

- There is $\omega > 0$ so that for any interval $\Lambda = [x', x'') \subset [-L,L]$, union of intervals belonging to $\mathcal{D}^{(\ell_+)}$, and for any m such that $\eta^{(\zeta,\ell_-)}(m;\cdot) = 1$ on Λ, there is ψ with the following properties. $\mathcal{F}_L(m) \geqslant \mathcal{F}_L(\psi)$; $\psi = m$ on $[x'+1, x''-1]^c$; $\eta^{(\zeta,\ell_-)}(\psi;\cdot) = 1$ on Λ;

$$\psi = \tanh\{\beta J^{\mathrm{neum}} * \psi\}, \quad \text{on } [x'+1, x''-1], \tag{3.2}$$

$$|\psi(x) - m_\beta| \leqslant c_2 e^{-\omega\ \mathrm{dist}(x,\Lambda^c)}, \quad x \in [x'+1, x''-1]. \tag{3.3}$$

  Equation (3.2) supplemented by the condition $\psi = m$ outside $[x'+1, x''-1]$, has a unique solution. The analogous result holds for $\Theta^{(\zeta,\ell_-,\ell_+)}(m;\cdot) = -1$ on Λ and $-m_\beta$ replaced by m_β and when $L = \infty$ (in which case $[x', x'')$ may also be unbounded).
- Let $\Gamma = [x', x'')$ be a contour for $m \in L^\infty([-L,L];[-1,1])$. Then

$$\mathcal{F}_{L;\Gamma}(m_\Gamma | m_{\Gamma^c}) \geqslant 2c_1\zeta^2\frac{\ell_-}{\ell_+}. \tag{3.4}$$

- The functional $\mathcal{F}_L(m)$ is continuous both in L^2 and L^∞. Then (lower semicontinuity) if m_n converges to m in $L^2_{\mathrm{loc}}(\mathbb{R})$,

$$\liminf_{n\to\infty} \mathcal{F}(m_n) \geqslant \mathcal{F}(m).$$

We now state results on the dynamics (2.2) which will be used in the sequel. We start with the following theorem that summarizes general properties of the evolution whose proof can be found for instance in Ref. 11.

Theorem 3.1: *The following holds.*

(1) *Super and subsolutions.* $z(x,t)$, $x\in\mathbb{R}$, $t\geqslant 0$, *is a subsolution (respectively, a supersolution) of* (1.3) *if* $z_t - g_L(z) \leqslant 0$ *[respectively* $\geqslant 0$*]. Then* $z(\cdot,t)\leqslant S_t(m)$, *if* $z(\cdot,0)\leqslant m$ *[respectively* $z(\cdot,t)\geqslant S_t(m)$, *if* $z(\cdot,0)\geqslant m$*].*

(2) *Barrier Lemma. There is a constant* $C>0$ *so that, setting* $m_i(\cdot,t)=S_t(m_i)$, $i=1$, *2, for any* $V\geqslant e^2\beta$ *and for any* $t>0$,

$$\sup_{s\leqslant t}|m_1(0,s)-m_2(0,s)| \leqslant e^{(\beta-1)t}\sup_{|r|\leqslant Vt}|m_1(r,0)-m_2(r,0)| + Ce^{-tV\log(V/(e\beta))}. \tag{3.5}$$

(3) *Basin of attraction of* $m^{\pm}$. *The sets* $\{m\in L^\infty(\mathbb{R};[-1,1]):\lim_{t\to\infty}\|S_t(m)-m^{\pm}\|_\infty=0\}$ *are open both in* L^2 *and* L^∞ *and they contain the functions which are strictly positive, respectively negative.*

We call instantons stationary solutions of (1.3) and (2.2) which are increasing, antisymmetric, and bounded in modulus by m_β. In particular we denote by $\bar m:\mathbb{R}\to(-m_\beta,m_\beta)$ an instanton on the whole of $\mathbb{R}$ and by $\hat m_L:[-L,L]\to(-m_\beta,m_\beta)$ a finite volume instanton, thus

$$\bar m(x)=\tanh\{\beta J*\bar m(x)\},\quad x\in\mathbb{R};\qquad \hat m_L(x)=\tanh\{\beta J^{\mathrm{neum}}*\hat m_L(x)\},\quad x\in[-L,L].$$

Properties like existence, uniqueness, and stability of instantons have been widely studied and, in the next two subsections, we summarize those needed in the sequel.

B. Properties of the instanton (see Refs. 8 and 11)

There is a unique antisymmetric $\bar m(x)$ solution of (2.4) and (2.5). Further, $\bar m(x)$ is a $\mathcal{C}^\infty$, strictly increasing and antisymmetric function.

(1) *Asymptotic behavior of the instanton*. For $\beta>1$, let $\alpha>0$ be such that

$$\beta(1-m_\beta^2)\int_{\mathbb{R}} J(0,y)e^{\alpha y}\mathrm{d}y = 1. \tag{3.6}$$

Then there are $a>0$, $\alpha_0>\alpha$ and $c>0$ so that for all $x\geqslant 0$

$$|\bar m(x)-(m_\beta-ae^{-\alpha x})|+|\bar m'(x)-a\alpha e^{-\alpha x}|+|\bar m''(x)+a\alpha^2e^{-\alpha x}|\leqslant ce^{-\alpha_0 x}, \tag{3.7}$$

where $\bar m'$ and $\bar m''$ are, respectively, the first and second derivatives of $\bar m$.

(2) *Basin of attraction of the instantons manifold*. All the translations of $\bar m$ are solutions of (2.4) and, recalling (2.6), we have that the set $\{\bar m_\xi:\xi\in\mathbb{R}\}$ attracts the set

$$\mathcal{N}:=\{m\in L^\infty(\mathbb{R};[-1,1]):\limsup_{x\to-\infty}m(x)<0,\quad \liminf_{x\to\infty}m(x)>0\}. \tag{3.8}$$

Namely, if $m\in\mathcal{N}$, then there is $\xi\in\mathbb{R}$ so that

$$\lim_{t\to\infty}\|S_t(m)-\bar m_\xi\|_\infty=0. \tag{3.9}$$

(3) ξ is a center of m if

$$(m-\bar m_\xi,\bar m_\xi')_\xi=0, \tag{3.10}$$

where $(\cdot,\cdot)_\xi$ denotes the scalar product in $L^2(\mathbb{R},d\nu_\xi)$, and

$$\frac{\mathrm{d}\nu_\xi(x)}{\mathrm{d}x} = p_\xi(x)^{-1}, \quad p_\xi(x) = \beta[1 - \bar{m}_\xi(x)^2]. \tag{3.11}$$

(4) Any $m \in \mathcal{N}$ has a center. Moreover, there are positive constants c and δ so that if $v = m - \bar{m}_{\xi_0}$, $\|v\|_\infty < \delta$ then m has a unique center ξ and letting

$$N_{v,\xi} = \frac{(v, \bar{m}')_\xi}{(\bar{m}', \bar{m}')_\xi}, \quad N_{v,0} = N_v$$

we have

$$|\xi - (\xi_0 - N_{v,\xi_0})| \leq c\|v\|_\infty^2, \quad |N_{v,\xi_0}| \leq c\|v\|_\infty.$$

(5) Let Ω_ξ be the linear operator on $L^\infty(\mathbb{R})$ or $L^2(\mathbb{R}, \mathrm{d}\nu_\xi)$

$$\Omega_\xi \psi = -\psi + p_\xi J * \psi \tag{3.12}$$

obtained by linearizing (2.2) around $\bar{m}_\xi$. Ω_ξ has eigenvalue 0 with eigenvector $\bar{m}_\xi'$ and a strictly positive spectral gap both as an operator in $L^\infty(\mathbb{R})$ and in $L^2(\mathbb{R}, d\nu_\xi)$. Thus, there is $B > 0$ so that

$$(v, \Omega_\xi v)_\xi \leq -B(v,v)_\xi, \quad (v, \bar{m}_\xi')_\xi = 0. \tag{3.13}$$

C. Properties of finite volume instantons (see Refs. 5–8)

(1) The instanton $\hat{m}_L$ is an antisymmetric function, and there are $\mathfrak{s}$ and C so that

$$|\hat{m}_L(x) - m_\beta| \leq Ce^{-\mathfrak{s}(L-x)}, \quad 0 < x < L. \tag{3.14}$$

Moreover, given any $\epsilon > 0$, if L is large enough

$$\sup_{|x| \leq L} |\hat{m}_L(x) - \bar{m}(x)| \leq \epsilon.$$

(2) Let $\hat{\mathcal{L}}$ be the operator on $L^2([-L, L], \mathrm{d}\hat{\nu}_L)$, $\mathrm{d}\hat{\nu}_L/\mathrm{d}x = [\beta(1 - \hat{m}_L^2)]^{-1}$,

$$\hat{\mathcal{L}}\psi = -\psi + \beta(1 - \hat{m}_L^2) J * \psi$$

obtained by linearizing (1.3) around $\hat{m}_L$. If L is large enough, $\hat{\mathcal{L}}$ has a positive eigenvalue λ, $c_- e^{-2L} \leq \lambda \leq c_+ e^{-2L}$, $c_\pm$ positive constants, with eigenvector $e_{\hat{m}_L}(x)$, $|x| \leq L$, which is a strictly positive, regular symmetric function. Moreover, there is $B' > 0$ so that for all L large enough

$$(v, \hat{\mathcal{L}} v)_{\hat{m}_L} \leq -B'(v,v)_{\hat{m}_L}, \quad (v, e_{\hat{m}_L})_{\hat{m}_L} = 0,$$

where $(\cdot, \cdot)_{\hat{m}_L}$ is the scalar product on $L^2([-L, L], d\hat{\nu}_L)$.

(3) Given any $\epsilon > 0$ small enough and $r \in (0, 1)$, define

$$B_{\epsilon,r} := \{m \in L^\infty([-L, L]; [-1, 1]) : \exists\, \xi \in [-rL, rL] : \|m - \bar{m}_\xi \mathbf{1}_{|x| \leq L}\|_\infty \leq \epsilon\} \tag{3.15}$$

$$\Sigma_{\epsilon,r}^\pm := \{m \in L^\infty([-L, L]; [-1, 1]) : \|m - \bar{m}_\xi \mathbf{1}_{|x| \leq L}\|_\infty \leq \epsilon \quad \text{for } \xi = \pm rL\}.$$

Then, for L large enough, if m is in $B_{\epsilon,r}$ either $\lim_{t \to \infty} \|S_t(m) - \hat{m}_L\|_\infty = 0$ or else there is a time t when $S_t(m) \in \Sigma_{2\epsilon,r}^- \cup \Sigma_{2\epsilon,r}^+$ while $S_s(m) \in B_{2\epsilon,r}$ for all $s \leq t$.

(4) There exist two manifolds, $w^{(\pm)}(x, s)$, $x \in [-L, L]$, $s \in \mathbb{R}$, such that $\mathcal{F}_L(w^\pm(\cdot, s)) < \mathcal{F}_L(\hat{m}_L)$,

$$S_t(w^{(\pm)}(\cdot, s)) = w^{(\pm)}(\cdot, s + t)$$

$w^{(\pm)}(\cdot, \cdot) \in (-m_\beta, m_\beta)$ and

$$\lim_{s\to-\infty} w^{(\pm)}(\cdot,s)=\hat{m}_L,\quad \lim_{s\to\infty} w^{(\pm)}(\cdot,s)=m^{(\pm)}$$

(the limits can be taken both in L^∞ and in L^2). Moreover, for any $s\in\mathbb{R}$, $w^{(+)}(x,s)$ is a non decreasing function of $x\in[-L,L]$, $w^{(-)}(x,s)=-w^{(+)}(-x,s)$ and $w^{(+)}(x,s)>w^{(-)}(x,s)$.

IV. LOWER BOUNDS FOR $\mathcal{F}_L$

The main result of this section is Theorem 4.2 where we estimate the cost in energy of the contours. This result extends (3.4) and its proof is mainly taken from Ref. 12.

We first prove the following preliminary proposition.

Proposition 4.1: There are $c>0$ and $\omega>0$ so that for all L large enough

$$|\mathcal{F}(\bar{m})-\mathcal{F}_L(\hat{m}_L)|\leqslant ce^{-\omega L}. \tag{4.1}$$

Proof: The orbit $S_t(\bar{m}(x)\mathbf{1}_{|x|\leqslant L})$ is made of antisymmetric functions since antisymmetry is preserved by the dynamics. Thus any limit point of the orbit is antisymmetric and it is a stationary solution because $\mathcal{F}_L$ is strictly decreasing at points which are not stationary solutions. Then by item 3 of Sec. III C, $S_t(\bar{m}(x)\mathbf{1}_{|x|\leqslant L})$ converges to $\hat{m}_L$ so that

$$\mathcal{F}_L(\bar{m}\mathbf{1}_{|x|\leqslant L})\geqslant\mathcal{F}_L(\hat{m}_L). \tag{4.2}$$

On the other hand,

$$\mathcal{F}_L(\bar{m}\mathbf{1}_{|x|\leqslant L})\leqslant\mathcal{F}(\bar{m})+\frac{1}{2}\int_{[-L,L]}\int_{[-L,L]^c}J(x,y)\{(\bar{m}(x)-\bar{m}(R(y))^2-(\bar{m}(x)-\bar{m}(y))^2\}\mathrm{d}y\,\mathrm{d}x, \tag{4.3}$$

where $R(y)$ denotes the point obtained by reflecting y around $-L$ or L, respectively, when $y>L$ and $y<-L$. By (3.7), (4.2), and (4.3) we get $\mathcal{F}_L(\hat{m}_L)\leqslant\mathcal{F}(\bar{m})+ce^{-\omega L}$ for L large enough.

To prove the lower bound, we denote by $\tilde{m}(x)$ the function equal to $\hat{m}_L$ for $|x|\leqslant L$ and to $\pm m_\beta$, for $x>L$ and, respectively, $x<-L$. Then

$$\mathcal{F}_L(\hat{m}_L)=\mathcal{F}(\tilde{m})+\frac{1}{2}\int_{[-L,L]}\int_{[-L,L]^c}J(x,y)\{(\hat{m}_L(x)-\hat{m}_L(R(y))^2-(\hat{m}_L(x)\mp m_\beta)^2\}\mathrm{d}y\,\mathrm{d}x,$$

where $\mp$ is minus if $x>0$ and plus if $x<0$. By (3.9), $\lim_{t\to\infty}S_t(\tilde{m})=\bar{m}$ and since $\mathcal{F}$ is lower semicontinuous, $\mathcal{F}(\tilde{m})\geqslant\mathcal{F}(\bar{m})$. Then, by (3.14), we conclude the proof. □

Theorem 4.2: *There are positive constants ζ_0, c_1, κ, c_2, and ω so that if (ζ,ℓ_-,ℓ_+,L) is compatible with (ζ_0,c_1,κ), then*

$$\mathcal{F}_L(m)\geqslant\sum_{\Gamma\text{ contour of }m}w_{\zeta,\ell_-,\ell_+}(\Gamma)\quad\forall\, m\in L^\infty([-L,L];[-1,1]), \tag{4.4}$$

where

$$w_{\zeta,\ell_-,\ell_+}(\Gamma)=\begin{cases}2c_1\zeta^2\dfrac{\ell_-}{\ell_+}|\Gamma| & \text{if }\Gamma\text{ is a plus or a minus contour}\\ \max\left\{2c_1\zeta^2\dfrac{\ell_-}{\ell_+}|\Gamma|;\mathcal{F}(\bar{m})-c_2e^{-\omega\ell_+}\right\} & \text{if }\Gamma\text{ is a mixed contour.}\end{cases}$$

Proof: Let G_+, respectively G_-, be the collection of all plus, minus, contours for m. By (3.1) and (3.4), for any $\Gamma\in G_+\cup G_-$,

$$\mathcal{F}_L(m) = \mathcal{F}_{L;\Gamma^c}(m_{\Gamma^c}) + \mathcal{F}_{L;\Gamma}(m_\Gamma|m_{\Gamma^c}) \geqslant \mathcal{F}_{L;\Gamma^c}(m_{\Gamma^c}) + 2c_1\zeta^2\frac{\ell_-}{\ell_+}|\Gamma|.$$

Denoting by Δ the complement in $[-L,L]$ of $G_+\cup G_-$, iterating we deduce

$$\mathcal{F}_L(m) \geqslant \mathcal{F}_{L;\Delta}(m_\Delta) + 2c_1\zeta^2\frac{\ell_-}{\ell_+}\sum_{\Gamma\in G_+\cup G_-}|\Gamma|.$$

Let $\Gamma=[x',x'')$ be a mixed contour possibly still present in Δ. We could bound it using the previous procedure, but we could also use the following alternative, which will be adopted when it gives a better bound. We have $\eta^{(\zeta,\ell_-)}(m;\cdot)=-1$ on $[x'-\ell_+,x'+\ell_+)$ and $\eta^{(\zeta,\ell_-)}(m;\cdot)=1$ on $[x''-\ell_+,x''+\ell_+)$ or viceversa. Suppose for instance that the former holds. By (3.2) and (3.3), there is ψ equal to m_Δ outside $[x'-\ell_++1,x'+\ell_+-1]$ such that $\eta^{(\zeta,\ell_-)}(\psi;\cdot)=-1$ on $[x'-\ell_+,x'+\ell_+)$, $\psi=-m_\beta$ on $[x'-1,x']$ and

$$\mathcal{F}_{L;\Delta}(m_\Delta) \geqslant \mathcal{F}_{L;\Delta}(\psi) - c'e^{-\omega\ell_+}.$$

By repeating the argument relative to the interval $[x''-\ell_++1,x''+\ell_+-1]$, we conclude that there is ϕ equal to ψ outside $[x''-\ell_++1,x''+\ell_+-1]$ such that $\eta^{(\zeta,\ell_-)}(\phi;\cdot)=1$ on $[x''-\ell_+,x''+\ell_+)$, $\phi=m_\beta$ on $[x''-1,x''+1]$ and

$$\mathcal{F}_{L;\Delta}(m_\Delta) \geqslant \mathcal{F}_{L;\Delta}(\phi) - 2c'e^{-\omega\ell_+}.$$

We then have

$$\mathcal{F}_{L;\Delta}(m_\Delta) \geqslant \mathcal{F}_{L;\Delta\setminus\Gamma}(m_{\Delta\setminus\Gamma}) + \mathcal{F}_\Gamma(\phi_\Gamma|m_\beta\mathbf{1}_{x>x''} - m_\beta\mathbf{1}_{x<x'}) - 2c'e^{-\omega\ell_+}.$$

Let $u(x)$, $x\in\mathbb{R}$, be equal to ϕ on Γ and $=\pm m_\beta$ to the right and left of Γ, then

$$\mathcal{F}_\Gamma(\phi_\Gamma|m_\beta\mathbf{1}_{x>x''} - m_\beta\mathbf{1}_{x<x'}) = \mathcal{F}(u) \geqslant \mathcal{F}(\bar{m})$$

by (3.9) and because $\mathcal{F}(S_t(u))$ is decreasing and lower semicontinuous. Thus

$$\mathcal{F}_{L;\Delta}(m_\Delta) \geqslant \mathcal{F}_{L;\Delta\setminus\Gamma}(m_{\Delta\setminus\Gamma}) + \max\left\{\mathcal{F}(\bar{m}) - 2c'e^{-\omega\ell_+}; 2c_1\zeta^2\frac{\ell_-}{\ell_+}|\Gamma|\right\}.$$

By iterating the argument over all the other, possibly still present, mixed contours, we conclude the proof. □

V. LOWER BOUNDS FOR $\mathcal{F}$

In this section we prove that the free energy of a profile $m\in L^\infty(\mathbb{R};[-1,1])$ which is asymptotically strictly positive as $x\to\infty$ and negative as $x\to-\infty$ increases quadratically with the distance of m from $\bar{m}$, the precise statement is given in Proposition 5.2. We need preliminarily a regularization result.

Proposition 5.1: There is $c>0$ and for all ℓ small enough and such that $L=n\ell$, $n\in\mathbb{N}$, there is a (regularizing) map $\mathcal{R}$ from $L^\infty([-L,L];[-1,1])$ into itself, continuous in the L^∞ norm, such that $\mathcal{F}_L(m)\geqslant\mathcal{F}_L(\mathcal{R}(m))$,

$$(\mathcal{R}(m))^{(\ell)} = m^{(\ell)},$$

where $\mathcal{R}(m)$ is differentiable at all points of $[-L,L]\setminus\ell\mathbb{Z}$, and

$$\left|\frac{d\mathcal{R}(m)(x)}{dx}\right| \leqslant \beta\|J'\|_\infty, \quad x\in[-L,L]\setminus\ell\mathbb{Z}. \tag{5.1}$$

Proof: Given m we denote by

$$M_i := \fint_{I_i} m(y)\mathrm{d}y,$$

where $I_i \in \mathcal{D}^{(\ell)}$ is the ith element of the partition of $[-L,L]$.

We want to prove that there is a unique function ψ_i which verifies the following properties:

(1) $\psi_i(x)=m(x)$ for all $x \in I_i^c$,
(2) $\fint_{I_i}\psi_i(y)dy=M_i$, and
(3) if φ verifies (1) and (2), then $\mathcal{F}_L(\varphi|m_{I_i^c}) \geqslant \mathcal{F}_L(\psi_i|m_{I_i^c})$.

To prove the above-mentioned properties we introduce a Lagrange multiplier h and define

$$\mathcal{F}_{L,h}(\varphi|m_{I_i^c}) := \mathcal{F}_L(\varphi|m_{I_i^c}) - h\int_{I_i}\varphi(y)\mathrm{d}y.$$

The inf of $\mathcal{F}_{L,h}(\cdot|m_{I_i^c})$ over $L^\infty([-L,L];[-1,1])$ is reached on functions u such that $A_h(u)=u$, where

$$A_h(u) = \begin{cases} \tanh\{\beta[J*u+h]\} & \text{on } I_i \\ m_{I_i^c} & \text{on } I_i^c \end{cases}$$

(see for instance Ref. 11). For ℓ such that $\beta\|J\|_\infty\ell<1/2$, A_h is a contraction:

$$\|A_h(\phi)-A_h(\psi)\|_\infty \leqslant \beta\|J\|_\infty\ell\|\phi-\psi\|_\infty.$$

Denote by $\phi^{(h)}$ its unique fixed point: $\phi^{(h)}=A_h(\phi^{(h)})$, $\phi^{(h)}=\lim_{n\to\infty}A_h^n(u)$, where, for instance $u \equiv 0$. From such a representation we deduce that, for each x, $\phi^{(h)}(x)$ is differentiable in h. By differentiating the fixed point equation, we find for $x \in I_i$,

$$\frac{d\phi^{(h)}}{dh} = p_h\left\{J*\frac{d\phi^{(h)}}{dh}+1\right\}, \quad p_h = \frac{\beta}{\cosh^2\left\{\beta\left[J*\frac{\mathrm{d}\phi^{(h)}}{\mathrm{d}h}+h\right]\right\}}$$

with $\mathrm{d}\phi^{(h)}(x)/\mathrm{d}h=0$ when $x \notin I_i$. For the above-mentioned ℓ, this identifies uniquely $\mathrm{d}\phi^{(h)}/\mathrm{d}h$ and shows that when $x \in I_i$, the derivative is strictly positive. Then

$$a(h) := \fint_{I_i}\phi^{(h)}(x)\mathrm{d}x$$

is a strictly increasing, continuous function of h; since $a(h)\to\pm1$ as $h\to\pm\infty$, there is h^* such that, $a(h^*)=M_i$ and h^* depends continuously on M_i and since M_i is a continuous function of m, $\phi^{(h^*)}$ is a continuous function of m.

The function $\psi_i := \phi^{(h^*)}$ verifies the previous (1) and (2). Let φ be any other function which verifies (1) and (2). Then, unless $\varphi=\psi_i$ almost everywhere,

$$\mathcal{F}_L(\varphi|m_{I_i^c}) = \mathcal{F}_{L,h^*}(\varphi|m_{I_i^c}) + h^*\ell M_i > \mathcal{F}_{L,h^*}(\psi_i|m_{I_i^c}) + h^*\ell M_i = \mathcal{F}_L(\psi_i|m_{I_i^c}).$$

Finally $\phi^{(h^*)}(x)$ is differentiable with respect to (w.r.t.) x in the interior of I_i and its derivative is bounded as in (5.1), as it follows by differentiating the fixed point equation and integrating by parts using regularity of J.

By repeating the argument for the other intervals I_j's we conclude the proof of the proposition. □

Since the proof is local, Proposition 5.1 holds also when $[-L,L]$ is replaced by $\mathbb{R}$.

Proposition 5.2: There is $c>0$ so that for all ℓ small enough,

$$\mathcal{F}(m) \geqslant \mathcal{F}(\bar m) + c\,\ell\left(\inf_{\xi\in\mathbb{R}}\|m^{(\ell)}-\bar m_\xi^{(\ell)}\|_\infty\right)^2, \quad m \in \mathcal{N} \tag{5.2}$$

with $\mathcal{N}$ defined in (3.8).

Proof: Set

$$w_\ell(m) = \inf_{\xi\in\mathbb{R}} \|m^{(\ell)} - \bar{m}_\xi^{(\ell)}\|_\infty. \tag{5.3}$$

We start with an outline of the proof. By expanding $\mathcal{F}(m)$ around $\bar{m}_\xi$, and calling $v=m-\bar{m}_\xi$,

$$\mathcal{F}(m) = \mathcal{F}(\bar{m}_\xi) - (v,\Omega_\xi v)_\xi + \text{remainder terms} \tag{5.4}$$

with Ω_ξ defined in (3.12) and the scalar product right after (3.10). By (3.13), there is $B>0$ so that if $(v,\bar{m}'_\xi)_\xi=0$ then $(v,\Omega_\xi v)_\xi \leqslant -B(v,v)_\xi$. To prove (5.2) we thus have to take care of the remainder terms in (5.4), fit in the condition $(v,\bar{m}'_\xi)_\xi=0$ and finally relate the bound $(v,v)_\xi$ to the quantity $w_\ell(m)$.

We will prove that there are $\delta_0\in(0,1/2)$ and $c'>0$ so that

$$\inf_{\delta\leqslant\delta_0} \delta^{-2} \inf_{m\in\mathcal{N}:w_\ell(m)\geqslant\delta} [\mathcal{F}(m)-\mathcal{F}(\bar{m})] \geqslant c'\ell. \tag{5.5}$$

We claim that (5.2) will then hold with $c=c'\delta_0^2/4$. We first prove the claim for a function $m^*\in\mathcal{N}$ such that $\delta^* := w_\ell(m^*)\leqslant\delta_0$. Then, the inf on the left-hand side (l.h.s.) of (5.5) is not larger than the value at $\delta=\delta^*$, so that it is $\leqslant\delta^{*-2}[\mathcal{F}(m^*)-\mathcal{F}(\bar{m})]$, hence $c'\ell w_\ell(m^*)^2\leqslant[\mathcal{F}(m^*)-\mathcal{F}(\bar{m})]$, which yields (5.2) with c replaced by c'. Finally, $c'>c'\delta_0^2/4$ because $\delta_0<1/2$.

If instead $w_\ell(m^*)>\delta_0$, then (5.5) yields $\delta_0^{-2}[\mathcal{F}(m^*)-\mathcal{F}(\bar{m})]\geqslant c'\ell$ hence

$$\mathcal{F}(m^*)-\mathcal{F}(\bar{m}) \geqslant c'\ell w_\ell(m^*)^2 \frac{\delta_0^2}{w_\ell(m^*)^2}$$

which concludes the proof of the claim because $w_\ell(m^*)\leqslant 2$.

Thus (5.2) will be proved, once we show that if $\tilde{m}\in\mathcal{N}$ and $w_\ell(\tilde{m})\geqslant\delta$, then

$$\mathcal{F}(\tilde{m}) \geqslant \mathcal{F}(\bar{m}) + c'\ell\delta^2. \tag{5.6}$$

We first suppose that $w_\ell(\tilde{m})\leqslant\delta_0$. By Proposition 5.1, there is m in $\mathcal{N}$ such that

$$\mathcal{F}(\tilde{m})\geqslant\mathcal{F}(m), \quad \tilde{m}^{(\ell)}=m^{(\ell)}, \quad w_\ell(m)=w_\ell(\tilde{m})\geqslant\delta \tag{5.7}$$

with the derivative m' of m, almost everywhere well defined and such that

$$\|m'\|_\infty \leqslant \beta\|J'\|_\infty.$$

Then, given any ξ,

$$\|m^{(\ell)}-\bar{m}_\xi^{(\ell)}\|_\infty \leqslant \|m-\bar{m}_\xi\|_\infty \leqslant \|m^{(\ell)}-\bar{m}_\xi^{(\ell)}\|_\infty + \beta\|J'\|_\infty\ell.$$

Since $\|m^{(\ell)}-\bar{m}_\xi^{(\ell)}\|_\infty=\|\tilde{m}^{(\ell)}-\bar{m}_\xi^{(\ell)}\|_\infty$, if δ_0 and ℓ are small enough, by (3.12), m has a unique center ξ and

$$\delta_0+\beta\|J'\|_\infty\ell =: \epsilon \geqslant \|m-\bar{m}_\xi\|_\infty. \tag{5.8}$$

There is $a>0$ so that $\phi_\beta(m)\geqslant a(|m|-m_\beta)^2$ and, since $\phi_\beta(m)\in L^1(\mathbb{R})$ (because $\mathcal{F}(m)<\infty$), $m\mp m_\beta\in L^2(\mathbb{R}_\pm)$. Then, with ξ the center of m,

$$\mathcal{F}(m)-\mathcal{F}(\bar{m}_\xi) = -\frac{1}{\beta}\int \mathcal{S}(m(x))-\mathcal{S}(\bar{m}_\xi(x))\mathrm{d}x - \frac{1}{2}\int\int J(x,y)\{m(x)m(y)-\bar{m}_\xi(x)\bar{m}_\xi(y)\}\mathrm{d}x\,\mathrm{d}y.$$

Calling $v=m-\bar{m}_\xi$ and $\rho=\max(|m|,|\bar{m}_\xi|)$,

$$-\big(\mathcal{S}(m)-\mathcal{S}(\bar m_\xi)\big)\geqslant -\mathcal{S}'(\bar m_\xi)v+\frac{1}{1-\bar m_\xi^2}v^2-\frac{2}{1-\rho^2}|v|^3.$$

By (5.8), $\rho\leqslant m_\beta+\epsilon$ and by letting δ and ℓ small enough, $1-\rho^2\geqslant(1-m_\beta^2)/2$ so that

$$-\big(\mathcal{S}(m)-\mathcal{S}(\bar m_\xi)\big)\geqslant -\mathcal{S}'(\bar m_\xi)v+\frac{1}{1-\bar m_\xi^2}v^2-\frac{8}{1-m_\beta^2}|v|^3. \tag{5.9}$$

By (5.9) and since $-\beta^{-1}\mathcal{S}'(\bar m_\xi)-J*\bar m_\xi=0$,

$$\mathcal{F}(m)-\mathcal{F}(\bar m_\xi)\geqslant -(v,\Omega_\xi v)_\xi-\frac{8\|v\|_\infty}{1-m_\beta^2}(v,v)_\xi. \tag{5.10}$$

Since $(v,\bar m_\xi')_\xi=0$, because ξ is the center of m, by (3.13),

$$\mathcal{F}(m)-\mathcal{F}(\bar m_\xi)\geqslant (v,v)_\xi\left(B-\frac{8\|v\|_\infty}{1-m_\beta^2}\right). \tag{5.11}$$

By letting δ small enough we conclude that there is $c'>0$ so that, recalling (5.7),

$$\mathcal{F}(\tilde m)-\mathcal{F}(\bar m_\xi)\geqslant c'(v,v)_\xi\geqslant c'\ell\,\delta^2. \tag{5.12}$$

The last inequality is proved as follows. Since $w_\ell(m)=\delta$, there is an interval of $\mathcal{D}^{(\ell)}$ where $|m^{(\ell)}-\bar m_\xi^{(\ell)}|\geqslant\delta$. By using Cauchy–Schwartz in such an interval we then get (5.12).

This proves (5.6) when $w_\ell(\tilde m)\leqslant\delta_0$. This is what needed in the text and we omit, for brevity, the proof of the full statement in the theorem, which uses that if $m\in\mathcal{N}$, then $S_t(m)\to\bar m_\xi$ as $t\to\infty$, while $\mathcal{F}(S_t(m))\leqslant\mathcal{F}(m)$. The result then follows by showing that $w_\ell(S_t(m))$ is a continuous function of t, so that there is $s>0$ so that $w_\ell(S_s(m))=\delta$ with $\delta\leqslant\delta_0$. The proposition is proved.□

VI. LOCALIZATION OF THE ENERGY SUBLEVELS

In this section we prove the localization property of the free energy sublevels stated in Theorem 2.6, indeed the proof of Theorem 2.6 follows directly from Lemma 6.1 and Lemma 6.2.

Recalling Definitions 2.3 and 2.4, we choose L and $\ell_\pm$ as functions of ζ so that (ζ,ℓ_-,ℓ_+) is a good choice of the parameters. We also fix the positive constants ζ_0, c_1, κ, and c_2 of Theorem 4.2 and we write $\Theta(m;\cdot)$ for $\Theta^{(\zeta,\ell_-,\ell_+)}(m;\cdot)$. The following preliminary Lemmas are in fact corollaries of Theorem 4.2.

Lemma 6.1: There is $\zeta<\zeta_0$ so that if $m\in L^\infty([-L,L];[-1,1])$ is such that $\mathcal{F}_L(m)\leqslant\mathcal{F}_L(\hat m_L)+\zeta^{100}$, then the following holds:

$$|\{\Theta(m;\cdot)=0\}|\leqslant k\ell_+,\quad k=\text{smallest integer}\geqslant\frac{1}{c_1\zeta^2\ell_-}[\mathcal{F}_L(\hat m_L)+\zeta^{100}]. \tag{6.1}$$

Further, if there are two points $x_\pm\in[-L,L]$, $x_+>x_-$, where $\Theta(m;x_+)\Theta(m;x_-)=-1$, then there is a unique contour Γ and $|\Gamma|\leqslant k\ell_+$, k as in (6.1).

Proof: By (4.4) we have

$$c_1\zeta^2\frac{\ell_-}{\ell_+}\sum_\Gamma|\Gamma|\leqslant\mathcal{F}_L(\hat m_L)+\zeta^{100}$$

so that

$$|\{\Theta(m;\cdot)=0\}|\leqslant\frac{\ell_+}{c_1\zeta^2\ell_-}[\mathcal{F}_L(\hat m_L)+\zeta^{100}]$$

hence (6.1).

Assume now that there are $x_\pm$ as in the statement. Then there is at least one mixed contour that we denote by Γ. Suppose by contradiction that there is another contour Γ'. By using Theorem 4.2, the inequality (4.1) and the fact that $|\Gamma'|>\ell_+$ we get

$$\mathcal{F}_L(m) \geqslant \mathcal{F}(\bar{m}) - c_2 e^{-\omega\ell_+} + c_1\zeta^2\ell_- \geqslant \mathcal{F}_L(\hat{m}_L) - ce^{-\omega L} - c_2 e^{-\omega\ell_+} + c_1\zeta^2\ell_-. \tag{6.2}$$

Since $L>\zeta^{-8}$, if ζ is small enough, then the r.h.s. of (6.2) is larger than $\mathcal{F}_L(\hat{m}_L)+\zeta^{100}$, hence the desired contradiction, which shows that there is a unique contour Γ with (6.1) holding. □

Lemma 6.2: Let m, x_-, x_+ be as in Lemma 6.1 and let $\Gamma=[x_-,x_+)$ be the unique contour of m. Suppose $\Theta(m;x)=\pm 1$ for $x>x_+$, respectively $x<x_-$. Then there is $\xi\in[x_-+\ell_+/2, x_+-\ell_+/2]$, so that, for all ζ small enough,

$$\|m^{(\ell_-)} - \bar{m}_\xi^{(\ell_-)}\|_\infty \leqslant 2\zeta.$$

Proof: If $x>x_+$ then $\Theta(m;x)=1$ and for any $\xi\in\Gamma$, $\mathrm{dist}(\xi,\Gamma^c)\geqslant\ell_+/2$ from (3.7) we get

$$|m^{(\ell_-)}(x) - \bar{m}_\xi^{(\ell_-)}(x)| \leqslant |m^{(\ell_-)}(x) - m_\beta| + ce^{-\alpha\ell_+/2}.$$

Since $\eta(m;x)=1$ by taking ζ small enough we then get

$$|m^{(\ell_-)}(x) - \bar{m}_\xi^{(\ell_-)}(x)| \leqslant \zeta + ce^{-\alpha\ell_+/2} \leqslant 2\zeta \quad \text{for all } x > x_+.$$

An analogous argument applies in the case $x<x_-$ for which $\Theta(m;x)=-1$. Thus we only need to prove that there is $\xi\in[\xi_-,\xi_+]$, where $\xi_\pm=x_\pm\mp\ell_+/2$, so that,

$$\sup_{x\in\Gamma}|m^{(\ell_-)}(x) - \bar{m}_\xi^{(\ell_-)}(x)| \leqslant 2\zeta. \tag{6.3}$$

We suppose by contradiction that (6.3) is not verified by any $\xi\in[\xi_-,\xi_+]$ and want to deduce that $\mathcal{F}_L(m)>\mathcal{F}_L(\hat{m}_L)+\zeta^{100}$. The strategy for the proof is to reduce to a similar problem on the whole line where we can use Proposition 5.2.

By item 1 in Sec. III A, there is ψ which is equal to m on Γ, $\mathcal{F}_L(\psi)\leqslant\mathcal{F}_L(m)$ and

$$\sup_{x\in[-L,-L+1]}|\psi(x)+m_\beta| \leqslant c_2 e^{-\omega\ell_+}, \qquad \sup_{x\in[L-1,L]}|\psi(x)-m_\beta| \leqslant c_2 e^{-\omega\ell_+}. \tag{6.4}$$

We denote by ϕ the function on $\mathbb{R}$, equal to ψ on $[-L,L]$ and to m_β on $x>L$ and to $-m_\beta$ in $x<-L$. Then from (6.4) it follows that $\mathcal{F}_L(\phi)\geqslant\mathcal{F}(\phi)-ce^{-\omega\ell_+}$ that implies

$$\mathcal{F}_L(m) \geqslant \mathcal{F}(\phi) - c'e^{-\omega\ell_+}.$$

Since $\phi^{(\ell_-)}(x)=m^{(\ell_-)}(x)$, for all $x\in\Gamma$ and all $\xi\in[\xi_-,\xi_+]$, by the contradiction assumption

$$\sup_{x\in\Gamma}|\phi^{(\ell_-)}(x) - \bar{m}_\xi^{(\ell_-)}(x)| > 2\zeta \quad \text{for all } \xi\in[\xi_-,\xi_+].$$

Note now that if $\xi\leqslant\xi_-$ and $x=\xi_-+\ell_+/4$, then $|\phi^{(\ell_-)}(x)-\bar{m}_\xi^{(\ell_-)}(x)|\geqslant 2m_\beta-2c_2e^{-\omega\ell_+/4}-ce^{-\alpha\ell_+/8}>2\zeta$. An analogous argument applies for $\xi\geqslant\xi_+$, so that

$$\inf_{\xi\in\mathbb{R}}\|\phi^{(\ell_-)} - \bar{m}_\xi^{(\ell_-)}\|_\infty > 2\zeta.$$

Then, by Proposition 5.2, $\mathcal{F}(\phi)\geqslant\mathcal{F}(\bar{m})+c\ell_-(2\zeta)^2$. Moreover, by (4.1), $\mathcal{F}(\bar{m})\geqslant\mathcal{F}_L(\hat{m}_L)-ce^{-\omega L}$, so that $\mathcal{F}_L(m)>\mathcal{F}_L(\hat{m}_L)+2\zeta$ for ζ small enough, hence the desired contradiction. □

VII. ON THE BASIN OF ATTRACTION OF THE PURE PHASES

In this section we will prove Theorem 2.7. By symmetry it suffices to prove the statements relative to U_+. We start with the following preliminary proposition whose proof is taken from Ref. 12. Given $b>0$, $R>0$ let

$$\mathcal{M}_{b,R}=\{m\in L^\infty(\mathbb{R};[-1,1]):m(x)\geqslant b,|x|\geqslant R\}.$$

Proposition 7.1: For any ϵ, b, R *positive there is* $\tau_{\epsilon,b,R}$ *so that*

$$S_t(m)\geqslant m_\beta-\epsilon \quad \text{for all } m\in\mathcal{M}_{b,R} \quad \text{and } t\geqslant\tau_{\epsilon,b,R}. \tag{7.1}$$

Further

$$\lim_{t\to\infty}\|S_t(m)-m^{(+)}\|_\infty=0 \quad \text{for all } m\in\mathcal{M}_{b,R}. \tag{7.2}$$

Proof: By item 3 of Theorem 3.1, $\lim_{t\to\infty}S_t(-1)=-m_\beta$, where we shorthand by $S_t(a)$, $a\in\mathbb{R}$, the function $S_t(m)$ with $m\equiv a$. By item 1 of Theorem 3.1, for any $\epsilon_-<0$ there is $t_-<0$ so that for all m, $S_{t_-}(m)\geqslant S_{t_-}(-1)\geqslant -m_\beta-\epsilon_-$.

Since $\lim_{t\to\infty}S_t(b)=m_\beta$ by the Barrier Lemma (see item 2 of Theorem 3.1), for any $\epsilon'>0$, there are $t_0=t_0(b,\epsilon')$ and $a=a(b,R,\epsilon')$, $a>R$, so that, for any $m\in\mathcal{M}_{b,R}$,

$$S_{t_0}(m)\geqslant S_{t_0}(b)-\frac{\epsilon'}{2}\geqslant m_\beta-\epsilon',\quad |x|\geqslant a.$$

Thus

$$S_{t_0}(m)\geqslant\psi,\quad \psi(x)=\begin{cases}m_\beta-\epsilon' & \text{for } |x|\geqslant a\\ -m_\beta-\epsilon' & \text{otherwise.}\end{cases} \tag{7.3}$$

Let $d>0$ be such that $\bar m(x)\leqslant -m_\beta+\epsilon'$ for all $x\leqslant -d$. Then

$$\bar m_{d+a}(x)\leqslant -m_\beta+\epsilon' \quad \text{for all } x\leqslant a \tag{7.4}$$

so that, by (7.3), $\psi(x)\geqslant\bar m_{d+a}(x)-2\epsilon'$ for all $x\leqslant a$ and $\psi\geqslant\bar m_{d+a}-\epsilon'$ for all $x\geqslant a$. Hence

$$\psi\geqslant\bar m_{d+a}-2\epsilon' \quad \text{for all } x. \tag{7.5}$$

By item 2 of Sec. III B, if $\epsilon'>0$ is small enough, there is ξ so that

$$\lim_{s\to\infty}\|S_s(\bar m_{d+a}-2\epsilon')-\bar m_\xi\|_\infty=0.$$

Then any limit point ψ^* of $S_s(\psi)$ (under uniform convergence on the compacts) verifies $\psi^*\geqslant\bar m_\xi$. The set $A:=\{\xi'\in\mathbb{R}:\psi^*\geqslant\bar m_{\xi'}\}$ is thus nonempty and closed. In Sec. 5 of Ref. 11 it is proved that if m^* is stationary, $m^*\geqslant\bar m_\xi$ and $m^*\neq\bar m_\xi$ then there is $\xi'>\xi$ such that $m^*\geqslant\bar m_{\xi'}$. It then follows that either $A=\mathbb{R}$ or there is ξ'' so that $\psi^*=\bar m_{\xi''}$. The second alternative cannot be verified: denoting by $\mathcal{R}$ the reflection operator around 0, $\mathcal{R}\psi=\psi$, $S_t(\psi)=S_t(\mathcal{R}\psi)=\mathcal{R}S_t(\psi)$ and by $\{t_n\}$ the time sequence defining ψ^*,

$$\psi^*=\lim_{t_n\to\infty}S_{t_n}(\psi)=\mathcal{R}\lim_{t_n\to\infty}S_{t_n}(\psi)=\mathcal{R}\psi^*\geqslant-\bar m_{-\xi}$$

hence $\psi^*\geqslant\bar m_{\xi'}$ for all ξ'. Then ψ^* is strictly positive, and since ψ^* is stationary, $\psi^*=m_\beta$. Thus there is t_1 so that $S_{t_1}(\psi)\geqslant m_\beta-\epsilon$ and $S_{t_0+t_1}(m)\geqslant m_\beta-\epsilon$ for any $m\in\mathcal{M}_{b,R}$. From item 1 of Theorem 3.1 and from (7.1) it follows that

$$S_t(m_\beta-\epsilon)\leqslant S_{t+\tau_{\epsilon,b,R}}(m)\leqslant S_t(1). \tag{7.6}$$

Since $S_t(1)$ and $S_t(m_\beta-\epsilon)$ converge exponentially fast to m_β as $t\to\infty$, there are c and ω positive so that, for any $m\in\mathcal{M}_{b,R}$,

$$\|S_{t+\tau_{\epsilon,b,R}}(m) - m_\beta\|_\infty \leqslant ce^{-\omega t}. \tag{7.7}$$

□

By the Barrier Lemma (item 2 of Theorem 3.1) it is possible to weaken the condition $m(x) \geqslant b$ for all $|x| \geqslant R$ in Proposition 7.1. The extension is needed for applications to L-symmetric functions, which cannot be in $\mathcal{M}_{b,R}$ unless $m(x) \geqslant b$ for all x.

Let C and $V = e^2\beta$ be as in the Barrier Lemma, ζ, $\zeta' > \zeta$ and R all positive with ζ' small enough. Let

$$\tau^+_{\zeta, m_\beta - \zeta', R} = \max\{\tau_{\zeta, m_\beta - \zeta', R}, t^*\}, \quad Ce^{-t^* V} = \zeta. \tag{7.8}$$

Notice that

$$Ce^{-\tau^+ V \log\{V/(e\beta)\}} \leqslant \zeta, \quad \tau^+ = \tau^+_{\zeta, m_\beta - \zeta', R}. \tag{7.9}$$

By Proposition 7.1 we have $S_{\tau^+}(m) \geqslant m_\beta - \zeta$ for all $m \in \mathcal{M}_{m_\beta - \zeta', R}$. Moreover by items 1 and 2 of Theorem 3.1,

$$S_t(m) \geqslant m_\beta - \zeta' - \zeta \quad \text{for } |x| \geqslant R + V\tau^+ \quad \text{and } t \leqslant \tau^+. \tag{7.10}$$

Lemma 7.2: For any $\zeta' > \zeta > 0$ small enough, any $R > 0$ and ψ such that $\psi(x) > m_\beta - \zeta'$ for all $R \leqslant |x| \leqslant R + 2V\tau^+ + 1$, $\tau^+ = \tau^+_{\zeta, m_\beta - \zeta', R}$, we have

$$S_{\tau^+}(\psi) > m_\beta - 2\zeta \quad \text{for all } |x| \leqslant R + V\tau^+ + 1, \tag{7.11}$$

$$S_t(\psi) > m_\beta - \zeta' - \zeta \quad \text{for all } t \leqslant \tau^+ \text{ and all } |x| \in [R + V\tau^+, R + V\tau^+ + 1]. \tag{7.12}$$

Proof: We define

$$\psi^*(x) = \begin{cases} \psi(x) & \text{if } |x| \leqslant R + 2V\tau^+ + 1 \\ m_\beta - \zeta' & \text{otherwise.} \end{cases}$$

By (3.5) and (7.9),

$$S_t(\psi) \geqslant S_t(\psi^*) - \zeta \quad \text{for all } |x| \leqslant R + V\tau^+ + 1 \text{ and } t \leqslant \tau^+ \tag{7.13}$$

and by (7.1)

$$S_{\tau^+}(\psi^*)(x) \geqslant m_\beta - \zeta \quad \text{for all } x \in \mathbb{R}$$

and (7.11) follows. Set

$$\tilde{\psi}(x) = \begin{cases} \psi(x) & \text{for } |x| \in [R, R + 2V\tau^+ + 1] \\ m_\beta - \zeta' & \text{elsewhere} \end{cases}$$

so that $\tilde{\psi} \geqslant m_\beta - \zeta'$ everywhere. By the Barrier Lemma, $S_t(\psi) \geqslant S_t(\tilde{\psi}) - \zeta$ for all $|x| \in [R + V\tau^+, R + V\tau^+ + 1]$ and all $t \leqslant \tau^+$. Then (7.12) follows from the inequality $S_t(\tilde{\psi}) \geqslant m_\beta - \zeta'$. □

In the next lemma we will require ζ so small that

$$\beta\|J'\|_\infty \ell_- < \frac{\zeta}{2}, \quad Ce^{-\ell_+} < \zeta, \quad C \text{ as in the Barrier Lemma} \tag{7.14}$$

(recall that ℓ_- and ℓ_+ are determined by ζ, see Definition 2.4).

Lemma 7.3: Let $\zeta > 0$ be small enough and such that (7.14) *holds. Then for all $t \leqslant \ell_+/V$, $V = e^2\beta$, and all $m \in L^\infty(\mathbb{R}, [-1, 1])$,*

$$|S_t(m) - m_\beta| \leqslant 3\zeta \quad \text{for all } x \text{ such that } \Theta(m; x) = 1, \tag{7.15}$$

where $\Theta \equiv \Theta^{(\zeta,\ell_-,\ell_+)}$.

Proof: Calling $\psi(x,t)=S_t(m)-e^{-t}m$, by differentiating w.r.t. x the integral version of (1.3),

$$\left|\frac{\mathrm{d}}{\mathrm{d}x}\psi(x,t)\right| \leqslant \beta\|J'\|_\infty.$$

Let $I_x^{(\ell_-)}$ be the interval $[n\ell_-,(n+1)\ell_-)$ which contains x; we have

$$\left|\psi(x,t)-\fint_{I_x^{(\ell_-)}}\psi\right| \leqslant \beta\|J'\|_\infty\ell_- \leqslant \frac{\zeta}{2}.$$

In [Ref. 12] it is proved that for ζ small enough, $\Theta(S_t(m);\cdot)\equiv 1$ for all $t>0$ if it holds at $t=0$. Suppose $\Theta(m;\cdot)\equiv 1$, then, taking $t=\log(4\zeta)$,

$$|S_t(m)(x)-m_\beta| \leqslant 2e^{-t}+\left|\psi(x,t)-\fint_{I_x^{(\ell_-)}}\psi\right|+\left|\fint_{I_x^{(\ell_-)}}S_t(m)-m_\beta\right| \leqslant 2\zeta.$$

We will next use the Barrier Lemma to drop the assumption $\Theta(m;\cdot)\equiv 1$. Let $[a,b)$ be a maximal connected component of $\{x:\Theta(m;x)=1\}$ and $G=[a-\ell_+,b+\ell_+)$. By definition of Θ, $\eta(m;x)=1$ for all $x\in G$. Set $m^*=m$ in G and $m^*=m_\beta$ in G^c and $t^*=\ell_+/V$. Then, if $x\in[a,b)$ and $t\leqslant t^*$,

$$|S_t(m)(x)-m_\beta| \leqslant |S_t(m^*)(x)-m_\beta|+Ce^{-t^*V} \leqslant 3\zeta.$$

□

Lemma 7.4: For all $\zeta'>0$ small enough the following holds. Suppose there are m, an interval $[a,b)$ and $T>0$ such that $m\geqslant m_\beta-\zeta'$ in $[a,b)$ and $S_t(m)\geqslant m_\beta-\zeta'$ in $\{[a-1,a)\cup[b,b+1)\}\times[0,T]$. Then

$$S_t(m) \geqslant m_\beta-\zeta' \quad \text{for all } x\in[a,b) \text{ and all } t\leqslant T. \tag{7.16}$$

Proof: Denote by ψ the restriction of $S_t(m)$ to $[a,b)$, so that ψ is a function on $[a,b)\times[0,T]$. It then solves the equation

$$\frac{\mathrm{d}\psi(x,t)}{\mathrm{d}t} = -\psi(x,t)+\tanh\left\{h(x,t)+\int_{[a,b)}J(x,y)\psi(y,t)\right\}, \quad x\in[a,b), t\in[0,T]$$

with

$$h(x,t)=\int_{[a,b)^c}J(x,y)m(y,t).$$

Notice that in the previous integral $m(y,t)\geqslant m_\beta-\zeta'$ because J has range 1.

By the comparison theorem (whose validity extends to the present situation) $\psi(x,t)\geqslant\psi^*(x,t)$ for any ψ^* which solves the above equation with $h^*\leqslant h$ and $\psi(x,0)\geqslant\psi^*(x,0)$, hence (7.16). □

As a corollary of the above lemmas we have the following result.

Proposition 7.5: For ζ small enough and L large enough, there is $\tau>0$ such that if $m\in U^+$ then $S_\tau(m)(x)\geqslant m_\beta-4\zeta$ for all $x\in[-L,L]$.

Proof: We need some preliminary definitions. Recalling (7.8) we shorthand

$$\tau_R^+=\tau^+_{\zeta,m_\beta-3\zeta,R}. \tag{7.17}$$

For any interval $I=[a,b)$, denote

$$I^* = [a', b'), \quad b' = b + 2\tau^+_{(b-a)/2} + 1; \quad a' = a - 2\tau^+_{(b-a)/2} - 1. \tag{7.18}$$

Call connected two intervals I_1 and I_2 if $I_1^* \cap I_2^* \neq \emptyset$. Given a sequence $\{I_i\}$ of disjoint intervals, let $\{I_i'\}$ be the sequence of intervals obtained as follows. For any maximal connected component $\{I_{i_k}\}$ of $\{I_i\}$, let $[a,b)$ be the minimal interval which contains all I_{i_k}; the set of all such intervals defines $\{I_i'\}$.

We apply the previous to the set of contours of m. By an abuse of notation, we still denote by m its L-symmetric extension, see the notation at the beginning of Sec. II. Since $m \in U^+$, the contours $\{\Gamma_i\}$ of the L-symmetric extension of m are such that

$$\sum_{\Gamma_i} |\Gamma_i \cap [-L, L]| \leqslant \kappa \ell_+. \tag{7.19}$$

We then define iteratively $\{I_{i;n}\}$ by setting $\{I_{i;1}\} = \{\Gamma_i\}$ and, for $n > 1$, $\{I_{i;n}\} = \{I'_{i;n-1}\}$. Since m is L-symmetric, there is N so that $\{I_{i;n}\} = \{I_{i;N}\}$ for all $n \geqslant N$. Moreover by (7.19), for L large enough all $I_{i;N}$ are bounded and mutually disconnected, in particular they do not cover $\mathbb{R}$. We still need a few notations. Recalling (7.17), given an interval I we call $I^+ = \{x : \mathrm{dist}(x, I) \leqslant \tau^+_{|I|/2}\}$, and $\partial I^+ = \{x \notin I^+ : \mathrm{dist}(x, I^+) \leqslant 1\}$. Denote by $\{t_1, t_2, \dots, t_k\}$ the set $\{\tau^+_{|I_{i;N}|/2}\}$, where t_i are in increasing order, $t_1 < t_2 \cdots < t_k$. Let $\mathcal{I}_j = \{I_{i,N} : \tau^+_{|I_{i;N}|/2} = t_j\}$ and

$$\Lambda_j = \bigcup_{I \in \mathcal{I}_j} I_j^+, \quad \Lambda = \cup \Lambda_j, \tag{7.20}$$

$$\partial \Lambda_j = \bigcup_{I \in \mathcal{I}_j} \partial I_j^+. \tag{7.21}$$

By Lemma 7.3, for ζ small enough there is s_0 so that

$$|S_{s_0}(m)(x) - m_\beta| \leqslant 3\zeta \quad \text{for all } x \in G := \{x : \Theta(m; x) = 1\}. \tag{7.22}$$

Define $\zeta' := 3\zeta$ and $\psi := S_{s_0}(m)$. By (7.22) we have $\psi(x) \geqslant m_\beta - \zeta'$ for all $x \in \Lambda^c$. By Lemma 7.2 $S_{t_j}(\psi) \geqslant m_\beta - 2\zeta$ on Λ_j and $S_t(\psi) \geqslant m_\beta - \zeta - \zeta'$ on $\partial \Lambda_j$ for $t \leqslant t_j$. By Lemma 7.4, $S_{t_1}(\psi) \geqslant m_\beta - \zeta - \zeta'$ on $\Lambda^c \cup \Lambda_1$; $S_{t_2}(\psi) \geqslant m_\beta - \zeta - \zeta'$ on $\Lambda^c \cup [\Lambda_1 \cup \Lambda_2]$ and, by iteration, $S_{t_k}(\psi) \geqslant m_\beta - \zeta - \zeta'$ everywhere. □

Proof of Theorem 2.7: From Proposition 7.5 it follows that for any $m \in U_+$ and any $t \geqslant 0$,

$$S_{t+\tau}(m_\beta - 3\zeta) \leqslant S_{t+\tau}(m) \leqslant S_{t+\tau}(1).$$

Both $S_t(m_\beta - 3\zeta)$ and $S_t(1)$ converge exponentially to $m^{(+)}$ as $t \to \infty$, hence Theorem 2.7 is proved. □

VIII. INTERFACE MOTION

In this section we prove the following result. For any $\epsilon > 0$ and $r \in (0,1)$, define $\Lambda_r^+ := (-L, -rL]$, $\Lambda_r^- := [rL, L)$ and

$$\mathcal{M}^\pm_{\epsilon,r} = \{m \in L^\infty([-L,L];[-1,1]) : \exists\, \xi \in \Lambda_r^\pm : \|m - \bar{m}_\xi\|_\infty \leqslant \epsilon\}.$$

Theorem 8.1: *For any $\epsilon > 0$ and $r \in (0,1)$ there is $L(\epsilon, r)$ so that for $L > L(\epsilon, r)$,*

$$\lim_{t \to \infty} \|S_t(m) - m^{(\pm)}\|_\infty = 0 \quad \text{for all } m \in \mathcal{M}^\pm_{\epsilon,r}. \tag{8.1}$$

It is enough to prove (8.1) when $m \in \mathcal{M}^+_{\epsilon,r}$, because, by symmetry, the result extends to $m \in \mathcal{M}^-_{\epsilon,r}$. The scheme of the proof is the following.

We will prove that at the end of an initial time layer, $S_t(m)$ is above a function "much closer" than ϵ to an instanton which is "only slightly" shifted to the right of the original one (to which m is close as an element of $\mathcal{M}^+_{\epsilon,r}$). We will then complete the proof by showing that this is above a travelling subsolution of (1.3) which converges to $m^{(+)}$.

For any m close to an instanton we will construct a subsolution which starts below m and which, after a suitably long time, is much closer to a new instanton than the original m. We introduce below the parameters which will be used in the construction of the subsolution, their justification lies in the proof of Proposition 8.2 below.

Let

$$b^+_\xi = ce^{-\alpha(L-\xi)}, \quad \xi \leqslant 0; \quad c = \sup_{L\geqslant 1, \xi\leqslant 0} \max_{x\in[L-1,L], y\in[L,L+1]} |\bar m_\xi(x) - \bar m_\xi(y)| \tag{8.2}$$

with c being finite by (3.7). Let p_ξ be as in (3.11). Since $\lim_{|x|\to\infty} p_\xi(x) = \beta(1-m^2_\beta) < 1$, if L is large enough there is $N>0$ (large enough) so that, for all $|\xi - x| > N$,

$$p_\xi(x) + Cb^+_0 \leqslant p < 1, \quad C = \beta^2 \sup_{x\in\mathbb{R}} |\tanh''(x)|. \tag{8.3}$$

We finally define the positive parameters ω and T_ξ as

$$\omega = \frac{1-p}{2}, \quad \frac{1-p}{4} 2\epsilon e^{-\omega T_\xi} = b^+_\xi + Cb^{+2}_\xi \tag{8.4}$$

with T_ξ being well defined for L large enough, as the r.h.s. in the second equality vanishes as $L \to \infty$.

Proposition 8.2: With ω, N as above and $\epsilon>0$ sufficiently small, let ξ_0 be such that

$$\xi_0 \leqslant -\eta, \quad \eta = \frac{2(\omega+1)\epsilon}{\omega[\min_{|x|\leqslant N} \bar m'(x)]}. \tag{8.5}$$

Then, for all L large enough and any $t \in [0, T_{\xi_0}]$ the function

$$u(x,t) := \bar m_{\xi(t)}(x) 1_{|x|\leqslant L} - \delta(t), \quad \delta(t) = 2\epsilon e^{-\omega t}, \tag{8.6}$$

$$\xi(t) = \xi_0 + \eta[1 - e^{-\omega t}] \tag{8.7}$$

is a subsolution of (1.3)*, namely*

$$u_t - g_L(u) \leqslant 0. \tag{8.8}$$

Proof: The time derivative of $u(x,t)$ is

$$u_t = -\xi_t \mathbf{1}_{|x|\leqslant L} \bar m'_{\xi(t)} + \omega\delta(t). \tag{8.9}$$

We will see that for $x \approx \xi(t)$, $|g_L(u)| \leqslant c\delta(t)$, $c>0$ a suitable constant. Since $\bar m'$ has the order of unity and, by (8.7), ξ_t is larger than $(\omega+c)\delta(t)$, (8.8) will hold for $x \approx \xi(t)$. For $|x-\xi(t)|$ large, instead, $\omega\delta(t)$, which is dangerously positive, becomes dominant in (8.9), but, as we will see, $g_L(u)$ will contrast it.

For $|x| \leqslant L-1$, $J^{\text{neum}}(x,\cdot) = J(x,\cdot)$, so that

$$g_L(u) = \delta + \tanh\{\beta[J * \bar m_\xi - \delta(t)]\} - \tanh\{\beta J * \bar m_\xi\} \tag{8.10}$$

and, by a Taylor expansion,

$$g_L(u) \geqslant -[p_{\xi(t)} - 1]\delta(t) - \frac{C}{2}\delta(t)^2 \tag{8.11}$$

with C as in (8.3) and p_ξ as in (3.11).

Define $b_\xi(x) := J^{\text{neum}} * \bar{m}_\xi - J * \bar{m}_\xi$ and notice that $b_\xi(x) = 0$ for $|x| \leqslant L-1$. Since $\bar{m}_\xi(x)$ is an increasing function of x, for $x \in [-L, -L+1]$, $b_\xi(x) \geqslant 0$, and we get the same bound as in (8.11):

$$g_L(u) = \delta + \tanh\{\beta[J * \bar{m}_\xi + b_\xi - \delta]\} - \tanh\{\beta J * \bar{m}_\xi\} \geqslant -[p_\xi - 1]\delta - \frac{C}{2}\delta(t)^2.$$

For $x \in [L-1, L]$, instead, $b_\xi(x) \leqslant 0$ and the previous inequality fails. Recalling (8.2), for $\xi \leqslant 0$, $b_\xi^+ \geqslant \max_{x\in[L-1,L]}|b_\xi(x)|$, and, since $\xi(t) \leqslant \xi_0 + \eta \leqslant 0$,

$$g_L(u) \geqslant -[p_\xi - 1 + Cb_0^+]\delta + p_\xi b_\xi - \frac{C}{2}(\delta(t)^2 + b_\xi^{+2}).$$

For $|x - \xi(t)| \leqslant N$, we bound $g_L(u) \geqslant \delta(t)$ (see (8.10)) while, for $|x - \xi(t)| > N$, we use (8.3) and (8.4) getting

$$u_t - g_L(u) \leqslant \begin{cases} -\xi_t[\min_{|x|\leqslant N} \bar{m}'(x)] + \omega\delta(t) + \delta(t), & |x - \xi(t)| \leqslant N \\ \dfrac{p-1}{2}\delta(t) + b_\xi^+ + \dfrac{C}{2}(\delta(t)^2 + b_\xi^{+2}), & |x - \xi(t)| \geqslant N. \end{cases} \tag{8.12}$$

By (8.7) the first line in (8.12) is non positive. By the second inequality in (8.4), for $|x - \xi(t)| \geqslant N$ and $t \leqslant T_{\xi_0}$,

$$u_t - g_L(u) \leqslant -\frac{1-p}{4}\delta(t) + \frac{C}{2}\delta(t)^2 \leqslant 0$$

having supposed ϵ so small that $(1-p)/4 \geqslant (C/2)2\epsilon$. □

Let $m \in \mathcal{M}_{\epsilon,r}^+$; then there is $\xi_0 \in (-L, -rL]$ such that $\|m - \bar{m}_{\xi_0}\|_{L^\infty([-L,L])} \leqslant \epsilon$. Given any $r \in (0,1)$ for L large enough we have that $-rL < -\eta$ so that by (8.6), $m \geqslant u(\cdot, 0)$. Then, by Proposition 8.2,

$$S_{T_{\xi_0}}(m) \geqslant \bar{m}_{\xi(T_{\xi_0})} - 2\epsilon e^{-\omega T_{\xi_0}}.$$

Since $\bar{m}_\xi$ is a decreasing function of ξ, there is a positive constant c' so that

$$S_{T_{\xi_0}}(m) \geqslant \bar{m}_{\xi_0+\eta} - c' e^{-\alpha(L-\xi_0)}, \tag{8.13}$$

with η as in (8.5). We will prove (see (8.17)) that the r.h.s. of (8.13) is bounded from below by a function $z_{\xi'}$, $\xi' > \xi_0 + \eta$, where z_ξ has the following structure:

$$z_\xi(x) = \bar{m}_\xi(x) - ae^{-\alpha(2L-\xi-x)} + ae^{-\alpha(2L+\xi+x)} + \Psi_\xi(x) \tag{8.14}$$

with α and a positive constants defined in (3.7), whereas the function Ψ_ξ is small (see (8.16)) at least when ξ is away from the boundaries. The important point is that there is a decreasing function $\xi(t)$ so that $z_{\xi(t)}$ is a traveling subsolution of (1.3).

Theorem 8.3: *For any $r \in (0,1)$ and $\delta > 0$, there is $L_0(r, \delta)$ such that, for any $L > L_0(r, \delta)$, $z_{\xi(t)}$ is a subsolution of* (1.3) *for all t such that $\xi(t) \in [-(1-r)L, -rL]$ and provided*

$$\frac{d\xi(t)}{dt} = -\sqrt{\mu}K(1 - \delta)e^{-2\alpha\xi(t)} \tag{8.15}$$

with $\sqrt{\mu}$ defined in (9.13), *K in* (9.23). *Moreover $|z_\xi(x)| < m_\beta$ for all $|x| \leqslant L$ and*

$$|\Psi_\xi(x)| \leqslant \delta e^{-\alpha|\xi-x|}. \tag{8.16}$$

Theorem 8.3 will be proved in Sec. IX, where we will see that δ can be chosen exponentially small in L.

Proposition 8.4: Given any $r \in (0,\bar r)$, for all L large enough and any $\xi_0 \in (-L,-\bar r L]$ there is $\xi' \in [-(1-r)L,-rL]$ so that

$$\bar m_{\xi_0+\eta}(x) - c' e^{-\alpha(L-\xi_0)} \geqslant z_{\xi'}(x), \quad |x| \leqslant L. \tag{8.17}$$

Proof: Since $\bar m_{\xi_0+\eta}(x) - c' e^{-\alpha(L-\xi_0)}$ is a decreasing function of ξ_0, without loss of generality we may suppose $\xi_0 \in [-(1-\bar r)L,-\bar r L]$. To simplify notation, we let $\xi=\xi_0+\eta$ and will prove (8.17) with $\xi'=\xi+R$, R being a "large" constant independent of L. We will do that by deriving a lower bound for $\bar m_\xi(x)-\bar m_{\xi+R}(x)$, an upper bound for $z_{\xi+R}(x)-\bar m_{\xi+R}(x)$, with the former larger than the latter. Recalling (8.14)–(8.16),

$$z_{\xi+R}(x) - \bar m_{\xi+R}(x) \leqslant a e^{-\alpha(2L+\xi+R+x)} + \delta e^{-\alpha|\xi+R-x|}. \tag{8.18}$$

Let $N>0$ be such that $c e^{-\alpha_0 N}=(a/2)e^{-\alpha N}$, where a, α, α_0, and c are as in (3.7) (without loss of generality we may and will suppose that $c>a$). Call $m'=\bar m(N)$, choose arbitrarily $m'' \in (m', m_\beta)$, define R_0 so that $\bar m(R_0)=m''$ and require $R \geqslant 2R_0$. Then,

$$\bar m_\xi(x) - \bar m_{\xi+R}(x) \geqslant m'', \quad x \in [\xi, \xi+R]$$

as it follows by bounding $\bar m_\xi(x) \geqslant 0$, $\bar m_{\xi+R}(x) \leqslant -m''$ for $x \in [\xi, \xi+R/2]$ and using an analogous bound for $x \in [\xi+R/2, \xi+R]$. Moreover

$$\bar m_\xi(x) - \bar m_{\xi+R}(x) \geqslant m'' - m', \quad x \in [\xi - N, \xi]$$

because $\bar m_\xi(x) \geqslant -m'$ and $\bar m_{\xi+R}(x) \leqslant -m''$. For $x \leqslant \xi - N$, using that $\bar m$ is antisymmetric and (3.7), we write

$$\begin{aligned}\bar m_\xi(x) - \bar m_{\xi+R}(x) &= [\bar m(x-\xi) + m_\beta] + [\bar m(\xi+R-x) - m_\beta] \\ &\geqslant a e^{-\alpha(\xi-x)} - c e^{-\alpha_0(\xi-x)} - a e^{-\alpha(\xi+R-x)} - c e^{-\alpha_0(\xi+R-x)}.\end{aligned}$$

Using the definition of N we then get

$$\bar m_\xi(x) - \bar m_{\xi+R}(x) \geqslant \frac{a}{2} e^{-\alpha(\xi-x)} - \frac{3a}{2} e^{-\alpha(\xi+R-x)}, \quad x \leqslant \xi - N.$$

Similarly

$$\bar m_\xi(x) - \bar m_{\xi+R}(x) \geqslant m'' - m', \quad x \in [\xi+R, \xi+R+N],$$

$$\bar m_\xi(x) - \bar m_{\xi+R}(x) \geqslant -\frac{3a}{2} e^{-\alpha(x-\xi)} + \frac{a}{2} e^{-\alpha(x-[\xi+R])}, \quad x \geqslant \xi+R+N.$$

Using the above-mentioned upper bounds and by taking $\delta \leqslant a/4$ in Theorem 8.3 it is not difficult to check that for L and R sufficiently large,

$$\bar m_\xi(x) - \bar m_{\xi+R}(x) - c' e^{-\alpha(L-\xi)} \geqslant a e^{-\alpha(2L+\xi+R+x)} + \delta e^{-\alpha|\xi+R-x|}.$$

This, together with (8.18) concludes the proof of the proposition. □

By (8.13) and (8.17), pointwise,

$$S_{T_\xi}(m) \geqslant z_{\xi'}. \tag{8.19}$$

We will prove convergence of $S_t(z_{\xi+\eta+R})$ to $m^{(+)}$ in L^∞ and this will prove that any limit point ϕ of $S_t(m)$ is not smaller than $m^{(+)}$. Since any limit point is stationary, $\phi=\tanh\{\beta J^{\text{neum}} * \phi\}$; then b

$:=\max_{|x|\leq L}\phi(x)$ must be such that $b\geq\tanh\{\beta b\}$, hence $\phi(x)\leq m_\beta$ for all x, which will then conclude the proof of (8.1) of Proposition 8.1.

Proposition 8.5: For any positive $r<\bar{r}$ there is a constant $L_2(r,\epsilon)$ so that for any $L\geq L_2(r,\epsilon)$, if $m\in\mathcal{M}^+_{\epsilon,\bar{r}}$ then there is a time t^* such that

$$S_{t^*}(m)\geq z_{-(1-r)L}. \tag{8.20}$$

Proof: For L large enough, (8.19) (recalling from Proposition 8.4 that $\xi'\in[-(1-r)L,-rL]$) and Theorem 8.3 yield (8.20). □

Let $N>0$ be such that $\bar{m}(x)>m_\beta-\epsilon$ for all $x\geq N$ (ϵ as in $\mathcal{M}^+_{\epsilon,\bar{r}}$). Let

$$w(x)=\begin{cases}-m_\beta, & x<-(1-r)L-N\\ z_{-(1-r)L}, & |x+(1-r)L|\leq N\\ m_\beta-2\epsilon, & x>-(1-r)L+N.\end{cases}$$

Then, for L large enough, $z_{-(1-r)L}(x)\geq w(x)$, $|x|\leq L$ and $|w(x)-\bar{m}_{-(1-r)L}(x)|\leq 2\epsilon$ for all $|x|\leq L$.

We will prove that there is a time T such that

$$S_T(w)(x)\geq\delta>0 \quad \text{for all } |x|\leq L \tag{8.21}$$

so that also $S_T(z_{-(1-r)L})>\delta$. Since the strictly positive functions are in the basin of attraction of $m^{(+)}$ (because a strictly positive function is bounded in between two positive constants, and all constant, positive functions are attracted by $m^{(+)}$), it then follows that the limit points of $S_t(z_{-(1-r)L})$ are above $m^{(+)}$ which is what we wanted to prove.

Thus we are left with the proof of (8.21). It is now convenient to regard (1.3) as an equation on the whole line, with $J^{\text{neum}}(x,y)$ replaced by $J(x,y)$, namely we will consider Eq. (2.2). We thus need to show that there are δ and T positive such that

$$u(x,T)>\delta \quad \text{for all } |x|\leq L,\ u(\cdot,t) \text{ solving (2.2) with } u(\cdot,0)=w(\cdot),$$

where, by an abuse of notation, we have denoted by w the symmetric extension of w.

Let

$$k=-(1-r)L-N-(-L)=rL-N$$

so that $w(x)=-m_\beta$ when x is in the interval $[-L-k,-L+k]$, as well as in all its translates by $4nL$, $n\in\mathbb{Z}$. We then introduce a function w^* as follows. Let $k'=11k$ and define $w^*(x)=-m_\beta$ for all $x\in[-L-k',-L+k]$. Let then $w^*(x)=w(x+10k)$ for $x\in[-L-k'-2N,-L-k']$. We then set $w^*(x+4nL)=w^*(x)$, for all $x\in[-L-k'-2N,-L+k]$ and all $n\in\mathbb{Z}$. We complete the definition of w^* by setting $w^*(x)=w(x)$ at all other points $x\in\mathbb{R}$. It follows from this construction that $w^*(x)\leq w(x)$ for all $x\in\mathbb{R}$ and that $w^*(x)$ is invariant under reflections around the points $(-L-5k)+4nL$, $n\in\mathbb{Z}$, so that, modulo a translation, we are still in the context of (1.3).

By applying the analysis in Proposition 8.2, Theorem 8.3, and Proposition 8.4 to the evolution starting from w^*, we conclude that there is a time T so that, denoting by z_ξ the symmetric extension of the function defined in (8.14), then

$$S_T(w^*)(x)\geq z_{-(1-r)L}(x+5k)$$

which shows that for L large enough, $S_T(w^*)(x)>0$ for $x\in[-L,L]$. This concludes the proof. □

IX. A TRAVELING SUBSOLUTION

In this section we will prove Theorem 8.3. As the analysis will focus on what happens around the left end of the spatial domain, it is convenient to change coordinates, considering the interval $[0,2L]$ instead of $[-L,L]$. By an abuse of notation, we will not change symbols, thus writing

$$u_t(x,t) = g_L(u(x,t)), \quad x \in [0,2L], \quad g_L(u) = -u + \tanh\{\beta J^{\text{neum}} * u\} \tag{9.1}$$

with J^{neum} now defined with reflections at 0 and $2L$; $S_{t;L}(m)$ is here the flow solution of (9.1) with initial datum m.

As discussed in Sec. I we may regard (9.1) as an equation on the whole of $\mathbb{R}$, writing

$$u_t(x,t) = g(u(x,t)), \quad x \in \mathbb{R}, \quad g(u) = -u + \tanh\{\beta J * u\}. \tag{9.2}$$

Call "symmetric" the functions invariant under all reflections R_{n2L}, $n \in \mathbb{Z}$, then the solution of (9.2) starting from a symmetric function, is symmetric and its restriction to $x \in [0,2L]$ solves (9.1). Thus (9.2) restricted to the space of symmetric functions is equivalent to our (9.1) and we will shift back and forth in the sequel between the two representations.

The construction of a subsolution is done by adding "corrections" to the instanton like function $\bar{m}_\xi(x)$, $x \in [0,2L]$. $\bar{m}_{\xi(t)}(x)$ alone, in fact, does not do the job: indeed, $g(\bar{m}_{\xi(t)})=0$ for $x \in [1,2L-1]$ while

$$\frac{\mathrm{d}}{\mathrm{d}t}\bar{m}_{\xi(t)}(x) = -\bar{m}'_{\xi(t)}(x)\xi_t(t) > 0, \quad \xi_t(t) < 0.$$

The instanton however must have an important role, as it solves the stationary equation in the limit $L \to \infty$ and it is natural to expect that, when L is finite, the boundary effects are responsible for the motion of the "instanton." To catch the effect, we "correct" the instanton into a function $m^0_\xi(x)$, which is the symmetric extension of

$$m^0_\xi(x) = \bar{m}_\xi(x) + A_\xi(x), \quad x \in [0,2L]; \quad A_\xi(x) = -ae^{-\alpha(4L-\xi-x)} + ae^{-\alpha(\xi+x)}. \tag{9.3}$$

Recalling (3.7), we have the following nice interpretation of A_ξ, by remarking that the terms $ae^{-\alpha(x+\xi)}$ and $-ae^{-\alpha(4L-\xi-x)}$ are the corrections to the asymptotic behavior of $\bar{m}(\xi-x)$, which is the reflection of the original instanton through the origin, and, respectively, to $-\bar{m}(2L-\xi-x)$, which is the reflection through the point $2L$.

In the end, we will show that the true subsolution, denoted by $z_{\xi(t)}(x)$, differs from $m^0_{\xi(t)}$ by higher order terms, for L large. These are however necessary to have $g(z_\xi)(x)>0$ for all x, and all $\xi \in [rL,(1-r)L]$; then since $\mathrm{d}z_\xi/\mathrm{d}\xi$ is uniformly bounded, $z_t - g(z_{\xi(t)}) < 0$ if $\mathrm{d}\xi(t)/\mathrm{d}t$ is negative, but sufficiently small, hence $z_{\xi(t)}$ is a sub-solution. By a more careful analysis we will also find the right speed.

We will write

$$z_\xi = m^0_\xi + \psi_\xi + \psi^*_\xi,$$

where ψ_ξ and ψ^*_ξ are two symmetric functions to be determined. To this end, we write, for $x \in [0,2L]$,

$$g(z_\xi) = -[\bar{m}_\xi + A_\xi + \psi_\xi + \psi^*_\xi] + \tanh\{\beta J * [\bar{m}_\xi + A_\xi + B_\xi + \psi_\xi + \psi^*_\xi]\}, \tag{9.4}$$

where

$$B_\xi(x) = m^0_\xi(x) - \{\bar{m}_\xi(x) + A_\xi(x)\}, \tag{9.5}$$

namely B_ξ denotes the difference between the symmetric function $m^0_\xi(x)$ and the non symmetric one, $\bar{m}_\xi + A_\xi$. Thus $B_\xi(x)=0$ for $x \in [0,2L]$ and $\neq 0$ elsewhere and for this reason its contribution appears only in the convolution term and it is different from zero except for some $x \in [0,1]$ and $x \in [2L-1,2L]$.

Recalling that $\bar{m}_\xi = \tanh\{\beta J * \bar{m}_\xi\}$, we will next rewrite (9.4) via a Taylor expansion to second order around $\bar{m}_\xi$. Let

$$\Omega_\xi m = -m + p_\xi J * m,$$

where $p_\xi(x)$ is here the symmetric function equal to $\beta(1-\bar{m}_\xi(x)^2)$ when $x \in [0,2L]$. We regard Ω_ξ as an operator on $L^\infty(\mathbb{R})$, noticing that it maps symmetric functions into symmetric ones. We then get from (9.4) the following equality, valid for all x in $[0,2L]$:

$$g(m_\xi^0 + \psi_\xi + \psi_\xi^*) = \Omega_\xi[A_\xi + \psi_\xi + \psi_\xi^*] + p_\xi J * B_\xi + \rho_\xi[J * (A_\xi + B_\xi + \psi_\xi + \psi_\xi^*)]^2 + 0_3, \tag{9.6}$$

where

$$\rho_\xi = \frac{\beta^2}{2}\tanh''\{\beta J * \bar{m}_\xi\} \tag{9.7}$$

and 0_3 is the remainder term in the expansion: there is a constant c (proportional to β^3) so that

$$|0_3(\psi_\xi, \psi_\xi^\star, A_\xi, B_\xi)| \leqslant c \sum_{i_1+i_2+i_3=3} |J * \psi_\xi|^{i_1} |J * \psi_\xi^\star|^{i_2} |J * (A_\xi + B_\xi)|^{i_3}.$$

In the sequel we will denote by the same symbol the symmetric extension of each term on the r.h.s of (9.6), so that equality holds on the whole of $\mathbb{R}$. Thus, for instance, by $\rho_\xi(x)$ we mean the expression (9.7) if $x \in [0,2L]$, and its symmetric extension elsewhere. The same applies to all the other terms of (9.6).

By an explicit computation which uses (3.6), we get for $x \in [0,2L]$,

$$a_\xi = \Omega_\xi A_\xi = -e^{-2\alpha(2L-\xi)} k_\xi^+ + e^{-2\alpha\xi} k_\xi^-, \quad k_\xi^\pm(x) := a e^{\pm\alpha(x-\xi)} \frac{m_\beta^2 - \bar{m}_\xi(x)^2}{1-m_\beta^2} > 0 \tag{9.8}$$

which, as said previously, is then regarded as a function on the whole of $\mathbb{R}$ by symmetric extension. To specify ψ_ξ and ψ_ξ^*, we introduce the operator

$$\mathcal{T}_\xi = \sum_{n=0}^{N} (1+\Omega_\xi)^n, \quad N = \text{integer part of } L^2$$

and define

$$\psi_\xi = \mathcal{T}_\xi(a_\xi + p_\xi J * B_\xi + \rho_\xi[J * (A_\xi + B_\xi)]^2), \tag{9.9}$$

$$\psi_\xi^\star = \mathcal{T}_\xi(2\rho_\xi[J * \psi_\xi][J * (A_\xi + B_\xi)] + \rho_\xi[J * \psi_\xi]^2), \tag{9.10}$$

where, according to the previous convention, all terms on which $\mathcal{T}_\xi$ acts are symmetric functions.

Lemma 9.1: Ω_ξ *as an operator on the* L^∞ *symmetric functions is invertible and*

$$\Omega_\xi \mathcal{T}_\xi m = -m + (1+\Omega_\xi)^{N+1} m. \tag{9.11}$$

Proof: The invertibility statement is proved in Ref. 8, the remaining statements are well known algebraic identities. □

With the choice (9.9) and (9.10) and using (9.11), we get from (9.6)

$$g(m_\xi^0 + \psi_\xi + \psi_\xi^*) = (1+\Omega_\xi)^{N+1}(a_\xi + p_\xi J * B_\xi + \rho_\xi[J * (A_\xi + B_\xi)]^2) + (1+\Omega_\xi)^{N+1}(2\rho_\xi[J * \psi_\xi][J * (A_\xi + B_\xi)] + \rho_\xi[J * \psi_\xi]^2) + \rho_\xi([J * \psi_\xi^*]^2 + 2[J * \psi_\xi^*]\{[J * \psi_\xi] + [J * (A_\xi + B_\xi)]\}) + 0_3$$

so that all terms, except those that multiply ρ_ξ, which we will prove to be suitably small, are in the range of the operator $(1+\Omega_\xi)^{N+1}$ which, as we are going to see, has a nice behavior. In Ref. 8 it has been proved that there is $s^\star > 0$ so that for all $\xi \in [s^\star, 2L-s^\star]$, a Perron–Frobenius theorem holds for $1+\Omega_\xi$ (with domain the space of symmetric L^∞ functions). It is shown that Ω_ξ has a strictly positive eigenvalue λ_ξ with strictly positive eigenvector v_ξ; $\|\Omega_\xi\|_\infty = \lambda_\xi$ and the remaining part of

the spectrum is made by complex numbers whose real part is not larger than $-\omega$, $\omega>0$. Let then π_ξ be the linear functional on $L^\infty(\mathbb{R})$, defined by

$$\pi_\xi(m) := \int_0^{2L} m(x) v_\xi(x) \frac{\mathrm{d}x}{p_\xi(x)} \tag{9.12}$$

and normalize v_ξ so that

$$\pi_\xi(v_\xi) = 1$$

while we call $\mu>0$ the normalizing constant when $L=\infty$, i.e.,

$$\mu \int_{\mathbb{R}} \bar{m}'_\xi(x)^2 \frac{\mathrm{d}x}{1-\bar{m}_\xi(x)^2} \mathrm{d}x = 1. \tag{9.13}$$

We recall some results we need in the sequel, see (Ref. 8, Theorems 2.1, 2.3, 2.4), and also (Ref. 7, Theorem 3.2). There are constants $c_\pm>0$, $c'>0$ and $\delta>0$ so that for $\xi\in[s^\star, 2L-s^\star]$

$$c_-[e^{-2\alpha\xi}+e^{-2\alpha(2L-\xi)}] \leqslant \lambda_\xi \leqslant c_+[e^{-2\alpha\xi}+e^{-2\alpha(2L-\xi)}], \tag{9.14}$$

$$|v_\xi(x) - \sqrt{\mu}\bar{m}'_\xi(x)| \leqslant c_+[e^{-2\alpha\xi}+e^{-2\alpha(2L-\xi)}]e^{\alpha|\xi-x|}\xi^4 \quad \text{for } |\xi-x| \leqslant \frac{\xi}{2}, \tag{9.15}$$

$$|v_\xi(x) - \sqrt{\mu}a\alpha e^{-\alpha\xi}(e^{-\alpha x}+e^{\alpha x})| \leqslant c_+ e^{-(\alpha+\delta)(\xi-x)} \quad \text{for } x\in\left[0,\frac{\xi}{2}\right], \tag{9.16}$$

$$|v_\xi(x) - \sqrt{\mu}a\alpha e^{-\alpha(2L-\xi)}(e^{-\alpha x}+e^{\alpha x})| \leqslant c_+ e^{-(\alpha+\delta)(x-\xi)} \quad \text{for } x\in\left[\frac{3\xi}{2},2L\right]. \tag{9.17}$$

Lemma 9.2: There are c and ω positive so that for any L^∞ symmetric function m,

$$\|(1+\Omega_\xi)^{N+1}m - (1+\lambda_\xi)^{N+1}\pi_\xi(m)v_\xi\|_\infty \leqslant ce^{-\omega N}\|m\|_\infty.$$

Proof: It follows from Theorem 2.4 in Ref. 8. □

Notice that $e^{-\omega N}\leqslant e^{-\omega(L^2-1)}$, which will be a negligible error. Moreover, by (9.14), for ξ large enough, $(1+\lambda_\xi)^{N+1}\sim 1+\lambda_\xi(N+1)$ and to leading order ~ 1, so that we may think that $(1+\Omega_\xi)^{N+1}m$ is essentially given by $\pi_\xi(m)v_\xi$. We then rewrite (9.6) as

$$g(m^0_\xi+\psi_\xi+\psi^*_\xi) = d_\xi v_\xi + E_\xi + 0_3 + 0_{\exp}, \tag{9.18}$$

where

$$d_\xi = (1+\lambda_\xi)^{N+1}\pi_\xi(a_\xi + p_\xi J*B_\xi + \rho_\xi[[J*(A_\xi+B_\xi)]^2 + 2\{J*\psi_\xi\}\{J*(A_\xi+B_\xi)\} + [J*\psi_\xi]^2]), \tag{9.19}$$

$$E_\xi = \rho_\xi\{[J*\psi^\star_\xi]^2 + 2[J*\psi^\star_\xi][J*\psi_\xi + J*(A_\xi+B_\xi)]\}, \tag{9.20}$$

and $0_{\exp}$ is the error term, for replacing $(1+\Omega_\xi)^{N+1}(\cdot)$ by $(1+\lambda_\xi)^{N+1}\pi_\xi(\cdot)v_\xi$.

Lemma 9.3: There is a constant c' so that

$$|0_{\exp}| \leqslant c'N^2e^{-\omega N}. \tag{9.21}$$

Proof: Since $\|a_\xi\|_\infty\leqslant c''$, $\|A_\xi\|_\infty\leqslant c''$ and $\|B_\xi\|_\infty\leqslant c''$, $\|\mathcal{T}_\xi\|_\infty\leqslant N+1$, then $\|\psi_\xi\|_\infty\leqslant C(N+1)$ and $\|\psi^*_\xi\|_\infty\leqslant C'(N+1)^2$ and (9.21) follows. □

Lemma 9.4: There is $c_1>0$ such that $\|k^\pm_\xi\|_\infty\leqslant c_1$ and moreover

$$|\pi_\xi(a_\xi) - \sqrt{\mu}K\{e^{-2\alpha\xi} - e^{-2\alpha(2L-\xi)}\}| \leqslant c_1[e^{-5\alpha/2(2L-\xi)} + e^{-5\alpha/2\xi}], \tag{9.22}$$

where

$$K = \frac{a}{\beta(1-m_\beta^2)}\int_{\mathbb{R}} \mathrm{d}x \frac{e^{\alpha x}\bar{m}'(x)(m_\beta^2 - \bar{m}^2(x))}{1-\bar{m}^2(x)} > 0. \tag{9.23}$$

Proof: By (3.7),

$$0 \leqslant k_\xi^\pm(y) \leqslant \frac{2m_\beta}{1-m_\beta^2}[1 + e^{-(\alpha_0-\alpha)|y-\xi|}], \quad y \in [0,2L].$$

Then

$$\pi_\xi(k_\xi^\pm) = \int_{|x-\xi|\leqslant \xi/2} \frac{v_\xi(x)}{p_\xi(x)} k_\xi^\pm(x) + O(e^{-\alpha\xi/2}).$$

From (9.15) we then get that for a suitable constant $c>0$,

$$\left| \pi_\xi(k_\xi^\pm) - \int_{|y|\leqslant\xi/2} \frac{\sqrt{\mu}\bar{m}'(y)}{p(y)} k_0^\pm(y) \right| \leqslant c e^{-2\alpha\xi} e^{\alpha\xi/2}\xi^4.$$

On the other hand, using (3.7) and recalling the definition (9.23) of K we have

$$\sqrt{\mu}K = \sqrt{\mu}\int \mathrm{d}x \frac{\bar{m}'(x)}{p_{\bar{m}}(x)} k^\pm(x) = \int_{|y|\leqslant\xi/2} \frac{\sqrt{\mu}\bar{m}'(y)}{p(y)} k_0^\pm(y) + O(e^{-\alpha\xi/2})$$

so that

$$|\pi_\xi(k_\xi^\pm) - \sqrt{\mu}K| \leqslant Ce^{-\alpha\xi/2}.$$

Hence (9.22) follows. □

By using Lemma 9.4 on the r.h.s. of (9.19), we then get from (9.18)

$$g(m_\xi^0 + \psi_\xi + \psi_\xi^\star) = (1+\lambda_\xi)^{N+1}\sqrt{\mu}K\{e^{-2\alpha\xi} - e^{-2\alpha(2L-\xi)}\}v_\xi + D_\xi v_\xi + E_\xi + 0_3 + 0_{\exp}, \tag{9.24}$$

where

$$D_\xi = (1+\lambda_\xi)^{N+1}[\pi_\xi(a_\xi) - \sqrt{\mu}K\{e^{-2\alpha\xi} - e^{-2\alpha(2L-\xi)}\}] + (1+\lambda_\xi)^{N+1}\pi_\xi(p_\xi J * B_\xi + \rho_\xi[J*(A_\xi + B_\xi)]^2$$
$$+ 2\{J*\psi_\xi\}\{J*(A_\xi + B_\xi)\} + \rho_\xi[J*\psi_\xi]^2). \tag{9.25}$$

The analysis proceeds by showing that $|D_\xi|$ is negligible w.r.t. the coefficient multiplying v_ξ in the first term on the r.h.s. of (9.24). We will then show that $|E_\xi| \leqslant \epsilon e^{-2\alpha\xi - \alpha|\xi - x|}$ with $\epsilon \to 0$ as $L \to \infty$, while $\|0_3\|_\infty < ce^{-2\alpha L}$ and $0_{\exp}$ can be also bounded in the same way. The proof of such statements requires a careful bound of each one of the terms which appear in the previous expressions and uses essentially the following estimate proved by Eqs. (6.28) and (6.29) of Ref. 8: for any $\zeta \in (0,\alpha)$ there is a constant c so that, denoting by $\mathcal{T}_\xi(x,y) + \delta(x-y)$ the kernel of $\mathcal{T}_\xi$ (the δ function coming from $n=0$),

$$|\mathcal{T}_\xi(x,y)| \leqslant cN^2 e^{-\zeta|x-y|}, \quad x \neq y.$$

We will thus bound

$$|\mathcal{T}_\xi m(x)| \leqslant cN^2\left\{ |m(x)| + \int_0^{2L} e^{-\zeta|x-y|}|m(y)|\mathrm{d}y \right\}. \tag{9.26}$$

To use (9.26) we need bounds on $|m(y)|$, which, in the case of B_ξ, are proved below.

Lemma 9.5: There are positive constants c_1 and c_2 so that

$$|p_\xi J * B_\xi(x)| \leqslant c_1[(e^{-\alpha_0\xi} + e^{-\alpha(4L-\xi)})\mathbf{1}_{x\in[0,1]} + (e^{-\alpha_0(2L-\xi)} + e^{-\alpha(2L+\xi)})\mathbf{1}_{x\in[2L-1,2L]}], \quad (9.27)$$

$$|\pi_\xi(p_\xi J * B_\xi)| \leqslant c_2[e^{-(\alpha_0+\alpha)\xi} + e^{-(\alpha_0+\alpha)(2L-\xi)} + e^{-\alpha 4L}] \quad (9.28)$$

with α_0 as in (3.7).

Proof: By (9.5), $B_\xi(x)=0$ for $x\in[0,2L]$ and we just need to specify its values in the two intervals $[-1,0]$ and $[2L,2L+1]$. We write $B^0_\xi(x)=B_\xi(x)\mathbf{1}_{x\in[-1,0]}$ and $B^+_\xi(x)=B_\xi(x)\mathbf{1}_{x\in[2L,2L+1]}$. Explicitly

$$\begin{aligned} B^0_\xi(x) &= [\{\bar m(-x-\xi) - ae^{-\alpha(4L+x-\xi)} + ae^{-\alpha(-x+\xi)}\} - \{\bar m(x-\xi) - ae^{-\alpha(4L-x-\xi)} + ae^{-\alpha(x+\xi)}\}]\mathbf{1}_{x\in[-1,0]} \\ &= (ae^{-\alpha(4L-\xi)}[e^{\alpha x} - e^{-\alpha x}] + \{\bar m(-x-\xi) - [-m_\beta + ae^{-\alpha(x+\xi)}]\} \\ &\quad - \{\bar m(x-\xi) - [-m_\beta + ae^{-\alpha(\xi-x)}]\})\mathbf{1}_{x\in[-1,0]}. \end{aligned}$$

Since J has support equal to one, by using (3.7), we get

$$|p_\xi J * B^0_\xi(x)| \leqslant c(e^{-\alpha(4L-\xi)} + e^{-\alpha_0\xi})\mathbf{1}_{x\in[0,1]}.$$

Analogously we write

$$\begin{aligned} B^+_\xi(x) &= [\{\bar m(4L-x-\xi) - ae^{-\alpha(x-\xi)} + ae^{-\alpha(4L-x+\xi)}\} - \{\bar m(x-\xi) - ae^{-\alpha(4L-x-\xi)} + ae^{-\alpha(x+\xi)}\}]\mathbf{1}_{x\in[2L,2L+1]} \\ &= (ae^{-\alpha(2L+\xi)}[e^{\alpha(2L-x)} - e^{-\alpha(2L-x)}] + \{\bar m(4L-x-\xi) - m_\beta + ae^{-\alpha(4L-x-\xi)}]\} - \{\bar m(x-\xi) - m_\beta \\ &\quad + ae^{-\alpha(x-\xi)}\})\mathbf{1}_{x\in[2L,2L+1]}. \end{aligned}$$

By using again (3.7), we then get

$$|p_\xi J * B^+_\xi(x)| \leqslant c(e^{-\alpha_0(2L-\xi)} + e^{-\alpha(2L+\xi)})\mathbf{1}_{x\in[2L-1,2L]}$$

hence (9.27) follows. Applying the definition (9.12) of π_ξ, we bound $|\pi_\xi(p_\xi J * B_\xi)|$ using the l.h.s. of (9.27). We then get (9.28). □

The remaining part of the proof of Theorem 8.3 is just computational, we thus outline the way computations are performed and state the results, a few details are reported in the Appendix . The result holds for L large enough: given r we need to choose ζ (ζ as in (9.26)) sufficiently close to α, in a way which depends on r, and which then determines how large L should be. Recall that $\xi\in[(1-r)L, rL]$.

We need first to estimate $\psi_\xi(x)$, which is given by (9.9). We use (9.26), expressing a_ξ as in (9.8); bound $p_\xi J * B_\xi$ using (9.27); we are then left with integrals of functions which are piecewise pure exponentials. The result is then bounded proportionally to the value of the integrand computed at the endpoints of the intervals where it is a pure exponential. The bound is reported in (A1). The same strategy is used for $\psi^\star_\xi$, the result is (A4).

The next step is to prove that for any $\epsilon>0$, if L is large enough, then $|D_\xi|e^{2\alpha\xi}\leqslant\epsilon$, so that the first term on the r.h.s. of (9.24) dominates the second one, with D_ξ. Expression (9.25) for D_ξ involves the action of the linear functional π_ξ, namely an integral with the function v_ξ. We then take (9.15)–(9.17) and reduce them to integrals which are like those for ψ_ξ and ψ^*_ξ.

By direct inspection, given any $\epsilon>0$ and L large enough, $e^{2\alpha\xi}e^{\alpha|\xi-x|}|E_\xi(x)|\leqslant\epsilon$. Also $e^{-2\alpha(2L-\xi)}\leqslant e^{-2\alpha\xi}\epsilon$, because $2L-\xi\geqslant Lr$, it then follows from (9.24) that

$$g(m_\xi^0 + \psi_\xi + \psi_\xi^\star) \geqslant \sqrt{\mu} K e^{-2\alpha\xi}(1-\epsilon) v_\xi.$$

We then have

$$z_t(x,t) - g(z(x,t)) \leqslant -\left[\bar{m}_\xi'(x) + a\alpha e^{-\alpha(x+\xi)} - \frac{\partial \psi_\xi(x)}{\partial \xi} - \frac{\partial \psi_\xi^\star(x)}{\partial \xi}\right]\xi_t - \sqrt{\mu} K e^{-2\alpha\xi}(1-\epsilon) v_\xi(x).$$

Since the square bracket which multiplies ξ_t is bounded, the whole expression is negative with ξ_t negative but sufficiently small, hence z_ξ is a subsolution. A further analysis shows that for any $\epsilon > 0$ if L is large enough, then

$$e^{\alpha|\xi - x|}\left|\frac{\partial \psi_\xi(x)}{\partial \xi}\right| \leqslant \epsilon; \quad e^{\alpha|\xi-x|}\left|\frac{\partial \psi_\xi^\star(x)}{\partial \xi}\right| \leqslant \epsilon$$

which proves (8.15) since we can take ξ_t arbitrarily close to $-\sqrt{\mu} K e^{-2\alpha\xi}$. The proof of (8.16) is given in the Appendix , see (A6) and (A7). The proof of Theorem 8.3 is completed.

X. PROOF OF THEOREM 2.8

By Definition 2.5, for any $m \in U_{-,+}$ there exists ξ such that $L - |\xi| \geqslant \ell_+/2$ and $\sup_{|x|\leqslant L}|m^{(\ell_-)} - \bar{m}_\xi^{(\ell_-)}| \leqslant 2\zeta$.

Lemma 10.1: There is $c > 0$ so that for all L large enough, the following holds. For any $m \in U_{-,+}$ and any $t \geqslant 0$,

$$\sup_{|x|\leqslant L}|S_t(m) - \bar{m}_\xi| \leqslant e^{\beta t}(2\zeta + c\ell_-) + 2e^{-t}. \tag{10.1}$$

Proof: Let $u(\cdot,t) = S_t(m) - \bar{m}_\xi$, then, with $u^{(\ell_-)}$ as in (2.3),

$$\frac{\mathrm{d}}{\mathrm{d}t}u^{(\ell_-)} = -u^{(\ell_-)} + \tanh\{\beta J^{(\ell_-)} * m^{(\ell_-)}\} - \tanh\{\beta J^{(\ell_-)} * \bar{m}_\xi^{(\ell_-)}\} + R, \tag{10.2}$$

where, calling I_x the interval in $\mathcal{D}^{(\ell_-)}$ which contains x,

$$J^{(\ell_-)}(x,y) = \int_{I_x}\int_{I_y} J^{\mathrm{neum}}(x',y')\mathrm{d}x'\mathrm{d}y'$$

whereas the remainder R such that $\sup_{|x|\leqslant L}|R| \leqslant c'(\ell_- + e^{-\alpha\ell_+/2})$, for a suitable constant c'. The term $e^{-\alpha\ell_+/2}$ takes into account the fact that $\bar{m}_\xi \neq \tanh\{J^{\mathrm{neum}} * \bar{m}_\xi\}$ when $|x| \geqslant L-1$, but the error is exponentially small by (3.9). From (10.2) we then get

$$\sup_{|x|\leqslant L}|u^{(\ell_-)}(x,t)| \leqslant e^{(\beta-1)t}2\zeta + \frac{\|R\|_\infty}{\beta - 1}e^{(\beta-1)t}.$$

(10.1) is then a consequence of the inequality $\|\bar{m}'\|_\infty \leqslant \beta\|J'\|_\infty$ and

$$\left|\frac{\mathrm{d}}{\mathrm{d}x}\{m(x,t) - e^{-t}m(x,0)\}\right| \leqslant \beta\|J'\|_\infty$$

which follows straightly from the integral version of (2.2). Then $|u(x,t)| \leqslant |u^{(\ell_-)}(x,t)| + 2e^{-t} + c''\ell_-$ and Lemma 10.1 is proved. □

Proof of Theorem 2.8: Given $\epsilon > 0$ let t_0 be such that $2e^{-t_0} = \epsilon/2$ and ζ so small that $e^{\beta t_0}(2\zeta + c\ell_-) = \epsilon/2$. Then by (10.1)

$$\sup_{|x|\leqslant L}|S_{t_0}(m)-\bar m_\xi|\leqslant\epsilon\quad\text{for some }\xi\equiv\xi(m)\in(-L,L).$$

We fix $r\in(0,1)$ as in Proposition 8.1 and we consider the set $B_{\epsilon,r}$ defined in (3.16). It then follows that either $S_{t_0}(m)\in\mathcal{M}^+_{\epsilon,r}\cup\mathcal{M}^-_{\epsilon,r}$ or $S_{t_0}(m)\in B_{\epsilon,r}$. In the first case, from Proposition 8.1 it follows that $S_{t_0+s}(m)$ converges to $m^{(+)}$ or to $m^{(-)}$ as $s\to\infty$. In the second case, using Ref. 5, we have that either $S_{t_0+s}(m)$ converges to $\hat m_L$ as $s\to\infty$, or else, at some time s_1, $S_{t_0+s_1}(m)\in\{\Sigma^-_{2\epsilon,r}\cup\Sigma^+_{2\epsilon,r}\}$, see (3.16) for the definition of the latter. Since $\{\Sigma^-_{2\epsilon,r}\cup\Sigma^+_{2\epsilon,r}\}$ is a subset of $\mathcal{M}^+_{2\epsilon,r}\cup\mathcal{M}^-_{2\epsilon,r}$, from Proposition 8.1 it follows that $S_{t_0+s_1+s}(m)$ converges to $m^{(+)}$ or to $m^{(-)}$ as $s\to\infty$, concluding the proof of Theorem 2.8.

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APPENDIX: SOME DETAILS ON THE TRAVELING SUBSOLUTION

1. Analysis of $\psi_\xi(x)$

We have

$$|\psi_\xi(x)|\leqslant n_-(x)\mathbf{1}_{x\leqslant\xi}+n_+(x)\mathbf{1}_{x\geqslant\xi},\tag{A1}$$

where

$$n_-(x)=cL^4\{e^{-2\alpha\xi}+e^{-\alpha_0\xi-\zeta x}\},$$

$$n_+(x)=cL^4\{e^{-2\alpha(2L-\xi)}+e^{-2\alpha\xi-\zeta|x-\xi|}+(e^{-\alpha_0(2L-\xi)}+e^{-\alpha(2L+\xi)})e^{-\zeta(2L-x)}\}.$$

Recalling its definition (9.9) we start by examining $\mathcal{T}_\xi a_\xi$, with a_ξ given by (9.8). We have

$$|k^+_\xi(y)|\leqslant c\{\mathbf{1}_{y\geqslant\xi}+\mathbf{1}_{y<\xi}e^{-2\alpha(\xi-y)}\},\quad |k^-_\xi(y)|\leqslant c\{e^{-2\alpha(y-\xi)}\mathbf{1}_{y\geqslant\xi}+\mathbf{1}_{y<\xi}\}.$$

We will use (9.26), so that, calling $a^\pm_\xi$ the contributions to a_ξ with $k^\pm_\xi$, and recalling that $\zeta<\alpha$,

$$|\mathcal{T}_\xi a^+_\xi|\leqslant cN^2e^{-2\alpha(2L-\xi)}\begin{cases}e^{-\zeta|\xi-x|},&x\leqslant\xi\\1,&x>\xi,\end{cases}$$

$$|\mathcal{T}_\xi a^-_\xi|\leqslant cN^2e^{-2\alpha\xi}\begin{cases}1,&x\leqslant\xi\\e^{-\zeta|x-\xi|},&x>\xi.\end{cases}$$

Since $\xi\leqslant L$,

$$|\mathcal{T}_\xi a_\xi|\leqslant cL^4\begin{cases}e^{-2\alpha\xi},&x\leqslant\xi\\e^{-2\alpha(2L-\xi)}+e^{-2\alpha\xi}e^{-\zeta|x-\xi|},&x>\xi.\end{cases}$$

Recalling (9.27), and since $\alpha_0<2\alpha$,

$$|\mathcal{T}_\xi(p_\xi J*B_\xi)|\leqslant cL^4(e^{-\alpha_0\xi}e^{-\zeta x}+(e^{-\alpha_0(2L-\xi)}+e^{-\alpha(2L+\xi)})e^{-\zeta(2L-x)})$$

and same bounds (even better) holds for $|\mathcal{T}_\xi(\rho_\xi[J*B_\xi]^2)|$.

Recalling definition (9.3) of A_ξ, we have

$$|\mathcal{T}_\xi\rho_\xi[J*A_\xi]^2|\leqslant cL^4(e^{-2\alpha(2L-\xi)}e^{-\zeta(2L-x)}+e^{-\zeta x}e^{-2\alpha\xi}).\tag{A2}$$

(A1) is thus proved. □

2. Analysis of $\psi^{\star}_{\xi}(x)$

We have

$$|\mathcal{T}_{\xi}(\rho_{\xi}[J*\psi_{\xi}]^2)| \leqslant V_1^-(x)\mathbf{1}_{x\leqslant\xi} + V_1^+(x)\mathbf{1}_{x\geqslant\xi} = V_1(x),$$

$$|\mathcal{T}_{\xi}(\rho_{\xi}[J*\psi_{\xi}][J*A_{\xi}])| \leqslant V_2^-(x)\mathbf{1}_{x\leqslant\xi} + V_2^+(x)\mathbf{1}_{x\geqslant\xi} = V_2(x),$$

$$|\mathcal{T}_{\xi}(\rho_{\xi}[J*\psi_{\xi}][J*B_{\xi}])| \leqslant V_3(x) \tag{A3}$$

so that

$$|\psi^{*}_{\xi}(x)| \leqslant V_1(x) + V_2(x) + V_3(x) \tag{A4}$$

where (bounding $e^{-(2L-\xi)(\alpha-\zeta)} \leqslant 1$)

$$V_1^- = cL^4(e^{-4\alpha\xi} + e^{-2\alpha_0\xi-\zeta x}),$$

$$V_1^+ = cL^4(e^{-\zeta(2L-x)}n_+(2L)^2 + n_+(x)^2 + e^{-\zeta(x-\xi)}[n_+(\xi)^2 + n_-(\xi)^2] + e^{-\zeta x}n_-(0)^2),$$

$$V_2^- = cL^4(e^{-\zeta x-(\alpha_0+\alpha)\xi} + e^{-\zeta(2L-x)-\alpha(2L-\xi)}),$$

$$V_2^+ = cL^4(e^{-\zeta(2L-x)}n_+(2L)A_{\xi}(2L) + n_+(x)A_{\xi}(x) + e^{-\zeta|x-\xi|}[n_+(\xi) + n_-(\xi)]A_{\xi}(\xi) + e^{-\zeta x}n_-(0)A_{\xi}(0)),$$

$$V_3 = cL^4(e^{-\zeta x}n_-(0)(e^{-\alpha_0\xi} + e^{-\alpha(4L-\xi)}) + e^{-\zeta(2L-x)}n_+(2L)(e^{-\alpha_0(2L-\xi)} + e^{-\alpha(2L+\xi)})).$$

3. Bounds on D_{ξ}

We will prove that for any $\epsilon > 0$ there is L_{ϵ} so that for any $L \geqslant L_{\epsilon}$

$$e^{2\alpha\xi}|D_{\xi}| \leqslant \epsilon.$$

Since $(1+\lambda_{\xi})^{N+1} \leqslant 2$, using (9.22), the contribution of the first term on the r.h.s. of (9.25) is bounded by

$$2c_1e^{2\alpha\xi}[e^{-(5/2)\alpha})(2L-\xi) + e^{-(5/2)\alpha\xi}$$

which, for $\xi \geqslant rL$ is exponentially small in L.

By (9.28), the contribution of the second term on the r.h.s. of (9.25) is bounded by

$$2e^{2\alpha\xi}c_2[e^{-(\alpha_0+\alpha)\xi} + e^{-(\alpha_0+\alpha)(2L-\xi)} + e^{-\alpha 4L}]$$

which is again exponentially small. Moreover

$$e^{2\alpha\xi}\pi_{\xi}(\rho_{\xi}(J*B_{\xi})^2) \leqslant ce^{2\alpha\xi}[e^{-2\alpha_0\xi}e^{-\alpha\xi} + \{e^{-2\alpha_0(2L-\xi)} + e^{-2\alpha(2L+\xi)}\}e^{-\alpha(2L-\xi)}].$$

Observe that the next bounds can be recovered from the corresponding ones with $\mathcal{T}_{\xi}(\cdot)$, provided the latter are computed at $x=\xi$ and with ζ replaced by α, the term L^4 being dropped. Thus, from (A2),

$$e^{2\alpha\xi}\pi_{\xi}(\rho_{\xi}(J*A_{\xi})^2) \leqslant ce^{2\alpha\xi}[e^{-2\alpha\xi}e^{-\alpha\xi} + e^{-2\alpha(2L-\xi)}e^{-\alpha(2L-\xi)}] \leqslant e^{-\alpha\xi} + e^{-\alpha(2L-\xi)}.$$

The same strategy applies to the terms

$$e^{2\alpha\xi}\pi_\xi(\rho_\xi(J*\psi_\xi)(J*A_\xi)),\quad e^{2\alpha\xi}|\pi_\xi(\rho_\xi[J*\psi_\xi][J*B_\xi])|,\quad e^{2\alpha\xi}|\pi_\xi(\rho_\xi[J*\psi_\xi]^2)|$$

which are estimated in terms of (A3). They also vanish as $L\to\infty$. In particular, the first one is bounded by $e^{-(\alpha+\alpha')(2L-\xi)+2\alpha\xi}$ which vanishes by the assumption that $\xi>rL$, $r>0$.

4. Bounds on E_ξ

We will prove that for any $\epsilon>0$ there is L_ϵ so that for any $L\geqslant L_\epsilon$

$$\sup_{x\in[0,2L]} e^{2\alpha\xi}e^{\alpha|\xi-x|}|E_\xi(x)|\leqslant\epsilon. \tag{A5}$$

We bound the terms in (9.20), using the bounds on ψ_ξ, ψ^*_ξ, A_ξ, and B_ξ already obtained. We distinguish the intervals $x\leqslant\xi$ and $x>\xi$. In each of them the dependence on x is of the form e^{bx}, with b depending on the term under consideration. Thus the max of the function to bound will be achieved at one of the endpoints. The bound at $x=0$ is

$$e^{3\alpha\xi}\rho_\xi[J*\psi^\star_\xi]^2|_0\leqslant cL^8e^{3\alpha\xi}\{e^{-2\alpha_0\xi}+[e^{-(\alpha_0+\alpha)\xi}+e^{-\zeta 2L-\alpha(2L-\xi)}]+[n_-(0)(e^{-\alpha_0\xi}+e^{-\alpha(4L-\xi)})+e^{-\zeta 2L}n_+(2L)(e^{-\alpha_0(2L-\xi)}+e^{-\alpha(2L+\xi)})]\}^2,$$

$$e^{3\alpha\xi}2\rho_\xi[J*\psi^\star_\xi][J*\psi_\xi]|_0\leqslant cL^8e^{3\alpha\xi}\{e^{-2\alpha_0\xi}+[e^{-(\alpha_0+\alpha)\xi}+e^{-\zeta 2L-\alpha(2L-\xi)}]+[n_-(0)(e^{-\alpha_0\xi}+e^{-\alpha(4L-\xi)})+e^{-\zeta 2L}n_+(2L)(e^{-\alpha_0(2L-\xi)}+e^{-\alpha(2L+\xi)})]\}n_-(0),$$

$$e^{3\alpha\xi}2\rho_\xi[J*\psi^\star_\xi][J*A_\xi]|_0\leqslant cL^8e^{3\alpha\xi}\{e^{-2\alpha_0\xi}+[e^{-(\alpha_0+\alpha)\xi}+e^{-\zeta 2L-\alpha(2L-\xi)}]+[n_-(0)(e^{-\alpha_0\xi}+e^{-\alpha(4L-\xi)})+e^{-\zeta 2L}n_+(2L)(e^{-\alpha_0(2L-\xi)}+e^{-\alpha(2L+\xi)})]\}[e^{-\alpha(4L-\xi)}+e^{-\alpha\xi}],$$

$$e^{3\alpha\xi}2\rho_\xi[J*\psi^\star_\xi][J*B_\xi]|_0\leqslant cL^8e^{3\alpha\xi}\{e^{-2\alpha_0\xi}+[e^{-(\alpha_0+\alpha)\xi}+e^{-\zeta 2L-\alpha(2L-\xi)}]+[n_-(0)(e^{-\alpha_0\xi}+e^{-\alpha(4L-\xi)})+e^{-\zeta 2L}n_+(2L)(e^{-\alpha_0(2L-\xi)}+e^{-\alpha(2L+\xi)})]\}e^{-\alpha_0\xi}.$$

All these terms, with $\xi<L$, are bounded by ϵ for L large enough.

When $x=\xi$, we have from (A5),

$$e^{2\alpha\xi}\rho_\xi[J*\psi^\star_\xi]|_\xi\leqslant cL^8e^{2\alpha\xi}(e^{-\alpha 4\xi}+e^{-(2\alpha_0+\zeta)\xi}+e^{-(\zeta+\alpha+\alpha_0)\xi}+e^{-(\alpha+\zeta)(2L-\xi)})$$

which vanishes as $L\to\infty$ and $(1-r)L>\xi>rL$. It then follows that the contribution in (A5) of $x=\xi$ can be made as small as desired, by taking L large. When $x=2L$,

$$e^{2\alpha\xi+\alpha(2L-\xi)}\rho_\xi[J*\psi^\star_\xi]|_{2L}\leqslant cL^8e^{2\alpha\xi+\alpha(2L-\xi)}\{e^{-(\alpha+\alpha_0)(2L-\xi)}\}.$$

This term alone does not vanish as $L\to\infty$, but once multiplied by $J*\psi_\xi$, $J*A_\xi$, $J*B_\xi$ the contribution to (A5) becomes as small as desired, for L large.

5. Asymptotic behavior of the subsolution

We will first prove that for any $\epsilon>0$ there is L_ϵ so that for $L>L_\epsilon$ and $\xi\in[rL,(1-r)L]$,

$$\sup_{x\in[0,2L]} e^{\alpha|\xi-x|}|\psi_\xi(x)|\leqslant\epsilon. \tag{A6}$$

For $x\leqslant\xi$, $e^{\alpha|\xi-x|}|\psi_\xi(x)|$ is bounded by cL^4 times

$$e^{\alpha|\xi-x|}n_-(x)\leqslant e^{\alpha(\xi-x)-2\alpha\xi}+e^{\alpha(\xi-x)-\alpha_0\xi-\zeta x}\leqslant e^{-\alpha(\xi+x)}+e^{-(\alpha+\zeta)x-(\alpha_0-\alpha)\xi}$$

which vanishes as $L\to\infty$. For $x\geqslant\xi$, $|\psi_\xi(x)|\leqslant n_+(x)$ which is the sum of three terms, thus $e^{\alpha|\xi-x|}|\psi_\xi(x)|$ is bounded by cL^4 times the sum of the following three terms.

$$e^{\alpha|x-\xi|}e^{-2\alpha(2L-\xi)} \leqslant e^{-\alpha(2L-\xi)},$$

$$e^{\alpha(x-\xi)}e^{-2\alpha\xi-\zeta(x-\xi)} \leqslant e^{(\alpha-\zeta)(2L-\xi)-2\alpha\xi},$$

$$e^{\alpha(x-\xi)}e^{-\zeta(2L-x)}\left[e^{-\alpha_0(2L-\xi)} + e^{-\alpha(2L+\xi)}\right] \leqslant e^{-(\alpha_0-\alpha)(2L-\xi)} + e^{-2\alpha\xi}.$$

We will next prove that for any $\epsilon>0$ there is L_ϵ so that for $L>L_\epsilon$ and $\xi\in[rL,(1-r)L]$,

$$\sup_{x\in[0,2L]} e^{\alpha|\xi-x|}\left|\psi^*_\xi(x)\right| \leqslant \epsilon. \tag{A7}$$

Recalling (A4), we have, with $x\leqslant\xi$,

$$e^{\alpha(\xi-x)}(V_1^- + V_2^-) \leqslant cL^4(\{e^{-2\alpha\xi} + e^{-(2\alpha_0-\alpha)\xi}\} + \{e^{-\alpha_0\xi} + e^{2\alpha\xi-(\alpha+\zeta)2L}\})$$

$$e^{\alpha(\xi-x)}V_3(x) \leqslant cL^4e^{\alpha\xi}V_3(0)$$

which vanish as $L\to\infty$.

For $x\geqslant\xi$,

$$e^{\alpha(x-\xi)}[V_1^+(x) + V_2^+(x) + V_3^+(x)] \leqslant e^{\alpha(2L-\xi)}[V_1^+(2L) + V_2^+(2L) + V_3^+(2L)]$$

which vanishes as $L\to\infty$.

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Dynamical symmetry group and quantum splittings for a free particle on the group manifold AdS_3

A. Chenaghlou[a)]
Physics Department, Faculty of Science, Sahand University of Technology, P.O. Box 51335-1996, Tabriz, Iran and Department of Mathematical Sciences, University of Durham, Durham DH1 3LE, United Kingdom

H. Fakhri[b)]
Institute for Studies in Theoretical Physics and Mathematics (IPM), P.O. Box 19395-5531, Tehran, Iran and Department of Theoretical Physics and Astrophysics, Physics Faculty, Tabriz University, P.O. Box 51664, Tabriz, Iran

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It is shown that the set of all quantum states corresponding to the motion of a free particle on the group manifold AdS_3 as the bases with two different labels, constitute a Hilbert space. The second label is bounded by the first one however, the first label is semibounded. The Casimir operator corresponding to the simultaneous and agreeable shifting generators of both labels along with the Cartan subalgebra generator describe the Hamiltonian of a free particle on AdS_3 with dynamical symmetry group U(1,1) and infinite-fold degeneracy for the energy spectrum. The Hilbert space for the Lie algebra of the dynamical symmetry group is a reducible representation space. But the Hilbert subspaces constructed by all the bases which have a given constant value for the difference of two their labels, constitute an irreducible representation for it. It is also shown that the irreducible representation subspaces of the Lie algebras u(1,1) and u(2) are separately spanned by the bases which have the same value for the second and first labels, respectively. These two bunches of Hilbert subspaces present two different types of quantum splittings on the Hilbert space. © *2005 American Institute of Physics.*
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I. INTRODUCTION AND MOTIVATION

After introducing nonrelativistic supersymmetric quantum mechanics,[1–3] the study of solvable problems has attracted a considerable attention. In the beginning of the theory, a lot of fundamental results were obtained (for further review see Refs. 4–7). Based on supersymmetry, if we know the wave function of the ground state with the zero energy for a given potential then we will obtain a hierarchy of partner potentials and their wave functions as well as energy eigenvalues. During that time, Gendenshtein remarkably developed supersymmetric quantum mechanics by defining the shape invariance concept for the potentials.[8] On this basis, most of the potentials obtained by the supersymmetry and shape invariance methods had the same functional of spatial coordinates, however, they had different parameters with respect to each other. Thus, the shape invariant potentials were identified with the known potentials which had analytic solutions. At first, it was supposed that all of the solvable potentials are shape invariant. Afterwards, it was realized that the shape invariance is a sufficient and not a necessary condition for the solvability.[9] Much work has been done to investigate shape invariance in the framework of supersymmetry (for example, see Refs. 10–18).

[a)]Electronic mail: a.chenaghlou@sut.ac.ir
[b)]Electronic mail: hfakhri@ipm.ir

Simultaneous shape invariance with respect to two different parameters whose formulation was first performed for the associated hypergeometric and Jacobi functions,[19,20] and then for the associated Laguerre functions,[21] provides a rich algebraic structure for the special functions and their corresponding differential equations. However, for the special functions (polynomials) of Hermite, simultaneous shape invariance with respect to two parameters has not been propounded. Due to this fact, the harmonic oscillator as the simplest problem of quantum mechanics is derived from the Hermite differential equation and occurred as the base and foundation of much studies in physics. Since, first, the factorization and consequently the shape invariance of the Hermite differential equation take place with respect to only one parameter. Second, the corresponding raising and lowering operators are not functions from the shape invariance parameter. On the other hand, in contrast with this simple case, the complication of the hypergeometric, Jacobi (which is from the same hypergeometric type) and Laguerre (which is from the confluent hypergeometric type) differential equations supplies the simultaneous shape invariance with respect to two different parameters and also the corresponding operators are functions from the shape invariance parameters.

It seems that introducing the simultaneous shape invariance with respect to two different parameters in the equations leads to the simplification of them like the Hermite differential equation however, their applications become rich. For example, the simultaneous shape invariance with respect to two different parameters of the associated Gegenbauer differential equation has played an important role in connection with investigating dynamical symmetry groups SU(2) and SU(1,1) and realizing the representation of parasupersymmetry algebra by the quantum states corresponding to the motion of a free particle on the sphere S^2 and the two-dimensional manifold AdS_2, respectively.[22] Further, for a free particle on the sphere, Barut–Girardello coherent states have been constructed by the spherical harmonics.[23] As another two-dimensional example, applying the simultaneous shape invariance with respect to two parameters in the associated Laguerre functions, we obtained the realization of new quantum splittings for the Landau levels, and consequently construction of the corresponding coherent states.[24,25] Besides, the simultaneous shape invariance with respect to two parameters leads to a deep and extended understanding of supersymmetry for the one-dimensional solvable models like the Morse, three-dimensional harmonic oscillator, and generalized radial Hulthén potentials, and radial potential of hydrogen-like atoms.[26–28] In Ref. 29, it has been emphasized that most of the shape invariant models are classified in two different classes so that in the first and second classes, the shape invariance parameters are n (degree of polynomial) and m (the dependence index of the special functions), respectively.

In this article, by using the associated Gegenbuer functions, we construct the Hilbert space $\mathcal{H}=\mathrm{span}\{|n,m\rangle\}_{0\leqslant m\leqslant n<\infty}$ spanned by the orthonormal bases $|n,m\rangle$, with two labels and restrictions $n\geqslant 0$ and $0\leqslant m\leqslant n$ for two integers n and m, which in fact are the solutions of the eigenvalue equation associated with the Hamiltonian of a free particle on the group manifold $AdS_3 \cong \mathrm{SU}(1,1)\cong \mathrm{SL}(2,R)$. We introduce four generators of the noncompact Lie algebra u(1,1) in such a manner that their corresponding laddering generators shift both the indices n and m of quantum states $|n,m\rangle$ simultaneously and agreeably. The Casimir operator of these generators is basically the Hamiltonian that describes the dynamical symmetry group U(1,1) for the free particle moving on AdS_3. It is shown that the Hilbert space $\mathcal{H}$ as the set of all quantum states of this problem represents reducibly the Lie algebra of the dynamical symmetry group U(1,1) which has an infinite-fold degeneracy for the energy spectrum. However, the infinite dimensional Hilbert subspaces $\mathcal{H}_i=\mathrm{span}\{|m+i,m\rangle\}_{m\geqslant 0}$, $i\geqslant 0$, which divide the whole Hilbert space $\mathcal{H}$ (as $\mathcal{H}=\cup_{i=0}^{\infty}\mathcal{H}_i$ and $\mathcal{H}_i\cap\mathcal{H}_{i'}=\emptyset$ for $i\neq i'$), represent the Lie algebra irreducibly. Moreover, the Hilbert space $\mathcal{H}$ is divided by two other different ways through infinite dimensional Hilbert subspaces $\mathcal{H}_m=\mathrm{span}\{|n,m\rangle\}_{n\geqslant m}$ (as $\mathcal{H}=\cup_{m=0}^{\infty}\mathcal{H}_m$ and $\mathcal{H}_m\cap\mathcal{H}_{m'}=\emptyset$ for $m\neq m'$) and finite dimensional ones $\mathcal{H}_n=\mathrm{span}\{|n,m\rangle\}_{m\leqslant n}$ (as $\mathcal{H}=\cup_{n=0}^{\infty}\mathcal{H}_n$ and $\mathcal{H}_n\cap\mathcal{H}_{n'}=\emptyset$ for $n\neq n'$). We show that the Hilbert subspaces $\mathcal{H}_m$ as positive discrete series, and $\mathcal{H}_n$ represent the noncompact Lie algebra u(1,1), and the compact Lie algebra u(2), respectively. These representations automatically propose infinite-u(1,1)- and finite-u(2)-quantum splittings on the whole space of quantum states. Realization of the

dynamical symmetry group U(1,1) by simultaneous shift operators of both quantum states labels and also u(1,1)- and u(2)-quantum splittings is a direct consequence of the simultaneous shape invariance idea with respect to two different parameters. The discussions performed in this article may be compared with the classical and quantum mechanical investigations done in Ref. 30 for a massive particle on the group manifold AdS_3 in the framework of the Klein–Gordon equation.

II. MATHEMATICAL FOUNDATION

In Ref. 20 it has been shown that if the normalization coefficients of the associated Gegenbauer functions $P_{n,m}^{(\alpha)}(x)$ in the Rodrigues representation are chosen as

$$P_{n,m}^{(\alpha)}(x)=\frac{(-1)^m}{2^n\Gamma(\alpha+n+1)}\sqrt{\frac{\Gamma(2\alpha+n+m+1)}{\Gamma(n-m+1)}}\frac{1}{(1-x^2)^{\alpha+m/2}}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^{n-m}(1-x^2)^{\alpha+n}, \tag{1}$$

then the following laddering relations are simultaneously realized with respect to the parameters n and m, respectively:

$$A_+(n;x)P_{n-1,m}^{(\alpha)}(x)=\sqrt{(n-m)(2\alpha+n+m)}P_{n,m}^{(\alpha)}(x), \tag{2a}$$

$$A_-(n;x)P_{n,m}^{(\alpha)}(x)=\sqrt{(n-m)(2\alpha+n+m)}P_{n-1,m}^{(\alpha)}(x), \tag{2b}$$

and

$$A_+(m;x)P_{n,m-1}^{(\alpha)}(x)=\sqrt{(n-m+1)(2\alpha+n+m)}P_{n,m}^{(\alpha)}(x), \tag{3a}$$

$$A_-(m;x)P_{n,m}^{(\alpha)}(x)=\sqrt{(n-m+1)(2\alpha+n+m)}P_{n,m-1}^{(\alpha)}(x), \tag{3b}$$

where the parameters n and m take nonnegative integer values. The explicit forms of the laddering operators $A_\pm(n;x)$ and $A_\pm(m;x)$ are calculated as

$$A_\pm(n,x)=\pm(1-x^2)\frac{d}{dx}-(n+\alpha\pm\alpha)x, \tag{4}$$

$$A_\pm(m,x)=\pm\sqrt{1-x^2}\frac{d}{dx}+\frac{\left(m+\alpha\mp\alpha-\frac{1}{2}\mp\frac{1}{2}\right)x}{\sqrt{1-x^2}}. \tag{5}$$

For a given m the number of the laddering equations with respect to n is infinite. However, for a given m, the number of the laddering equations with respect to m is finite. Combination of Eqs. (2a) and (2b) by two different ways leads to the shape invariance equations with respect to the parameter n. Similarly, combination of Eqs. (3a) and (3b) by the same procedure gives rise to the shape invariance equations with respect to the parameter n.

It is also shown that if the real parameter α is chosen as $\alpha>-1$ then, the associated Gegenbauer functions $P_{n,m}^{(\alpha)}(x)$ for a given m but with different n's are orthogonal with respect to an inner product with the weight function $(1-x^2)^\alpha$ in the interval $(-1,+1)$ so that their norms are given by the following relation:

$$\int_{-1}^{+1}P_{n,m}^{(\alpha)}(x)P_{n',m}^{(\alpha)}(x)(1-x^2)^\alpha\mathrm{d}x=\delta_{nn'}h_n^2(\alpha),\quad n,n'\geqslant m \tag{6}$$

with

$$h_n(\alpha) = \frac{2^{\alpha+1/2}}{\sqrt{2\alpha+2n+1}}.$$

Now by using the Rodrigues representation (1), let us rewrite relation (6) as

$$\int_0^1 P_{n,m}^{(\alpha)}(x) P_{n',m}^{(\alpha)}(x)(1-x^2)^{\alpha} \mathrm{d}x = \delta_{n\,n'} \frac{h_n^2(\alpha)}{2}, \quad n,n' \geqslant m. \tag{7}$$

It should be pointed out that the special case $\alpha=0$ yields the associated Legendre functions $P_{n,m}^{(0)}(x)=P_{n,m}(x)$. In this case by using just the laddering equations (3) and by replacing n with l, it is well-known that representation of Lie algebra su(2) on the space of spherical harmonics $|l,m\rangle = Y_{l\,m}(\theta,\phi)$ via shifting just m, is realized. In trigonometric harmonics $Y_{l\,m}(\theta,\phi)$, θ and ϕ are local coordinate patch on the two-dimensional sphere S^2. Realization of irreducible representation su(2) via (deformed) spherical harmonics is a problem which arises in the many many contents in mathematical physics (for example, see Refs. 31–34). In a similar approach, we shall show that simultaneous formulation of Eqs. (2) and (3) gives rise to the derivation of the hyperbolic harmonics $|n,m\rangle$ as functions of three coordinates corresponding to the parametrization of the group manifold $\mathrm{AdS}_3 \cong \mathrm{SL}(2,R)$.

III. REALIZATION OF REDUCIBLE REPRESENTATIONS OF THE LIE ALGEBRAS u(1,1) AND u(2) BY A HILBERT SPACE

In this section a Hilbert space is constructed to represent the noncompact Lie algebra u(1,1) as well as the compact Lie algebra u(2) reducibly. We also obtain the irreducible Hilbert subspaces corresponding to the representations of the Lie algebras so that each of them divides the Hilbert space separately. First of all we define the kets $|n,m\rangle$ as functions of the variables $0<r<\infty$, $0 \leqslant \phi < 2\pi$ and $-\pi \leqslant \psi < \pi$:

$$|n,m\rangle := \frac{e^{in\phi+im\psi} P_{n,m}^{(\alpha)}\left(\frac{1}{\cosh r}\right)}{\pi\sqrt{2h_n(\alpha)}}. \tag{8}$$

It is easily shown that the kets $|n,m\rangle$ form an orthonormal set with respect to both the indices, and with an inner product whose measure is $(\tanh^{2\alpha+1} r/\cosh r)\mathrm{d}r\mathrm{d}\phi\mathrm{d}\psi$:

$$\langle n,m|n',m'\rangle = \int_{r=0}^{\infty}\int_{\phi=0}^{2\pi}\int_{\psi=-\pi}^{\pi} \left(\frac{e^{in\phi+im\psi} P_{n,m}^{(\alpha)}\left(\frac{1}{\cosh r}\right)}{\pi\sqrt{2h_n(\alpha)}}\right)^* \times \left(\frac{e^{in'\phi+im'\psi} P_{n',m'}^{(\alpha)}\left(\frac{1}{\cosh r}\right)}{\pi\sqrt{2h_{n'}(\alpha)}}\right) \frac{\tanh^{2\alpha+1} r}{\cosh r} \mathrm{d}r\mathrm{d}\phi\mathrm{d}\psi = \delta_{n\,n'}\delta_{m\,m'}. \tag{9}$$

Note that by using $x=1/\cosh r$, the relation (9) converts to the relation (7). Consequently, we can introduce infinite dimensional Hilbert space $\mathcal{H}$ which is spanned by the bases $|n,m\rangle$, i.e., $\mathcal{H} := \mathrm{span}\{|n,m\rangle\}_{0\leqslant m\leqslant n<\infty}$.

Now if we define the operators L_+ and L_- as

$$L_{\pm} = e^{\pm i\phi}\left(\mp \sinh r \frac{\partial}{\partial r} + \frac{i}{\cosh r}\frac{\partial}{\partial\phi} - \frac{\alpha+\frac{1}{2} \pm \left(\alpha+\frac{1}{2}\right)}{\cosh r}\right), \tag{10}$$

then by using Eq. (2) we may show that they satisfy the raising and lowering relations of the index n for a given m as

$$L_+|n-1,m\rangle = \sqrt{\frac{(n-m)(2\alpha+n+m)(2\alpha+2n-1)}{2\alpha+2n+1}}|n,m\rangle, \tag{11a}$$

$$L_-|n,m\rangle = \sqrt{\frac{(n-m)(2\alpha+n+m)(2\alpha+2n+1)}{2\alpha+2n-1}}|n-1,m\rangle, \tag{11b}$$

respectively. Meanwhile by defining $L_3=-i\,\partial/\partial\phi$, we have

$$L_3|n,m\rangle = n|n,m\rangle. \tag{12}$$

Using the explicit forms of the operators or Eqs. (11) and (12) which represent these operators in the Hilbert space $\mathcal{H}$, it is easily seen that four generators L_+, L_-, L_3, and $I:=1$ satisfy the commutation relations of the noncompact Lie algebra u(1,1) as follows

$$[L_+,L_-] = -2L_3 - (2\alpha+1)I,$$

$$[L_3,L_\pm] = \pm L_\pm,$$

$$[\mathbf{L},I] = 0. \tag{13}$$

It is evident that for $\alpha=-\frac{1}{2}$ (the associated Chebyshev functions of the first type), the Lie algebra u(1, 1) is decomposed into $\mathrm{su}(1,1)\oplus\mathrm{u}(1)$. The representation of the noncompact Lie algebra u(1,1), i.e., (13) in the Hilbert space $\mathcal{H}$ is reducibly realized by Eqs. (11) and (12) as well as the following relation:

$$I|n,m\rangle = |n,m\rangle. \tag{14}$$

In fact for every given m, we obtain a positive discrete irreducible representation $\mathcal{D}_m^+=\{m,m+1,m+2,\ldots\}$ for the Lie algebra u(1,1). The infinite dimensional Hilbert subspaces $\mathcal{H}_m$ which are defined as $\mathcal{H}_m := \mathrm{span}\{|n,m\rangle\}_{n\geqslant m}$ represent irreducibly the Lie algebra u(1,1) again as Eqs. (11), (12), and (14). They divide the Hilbert space $\mathcal{H}$ (as $\mathcal{H}=\cup_{m=0}^{\infty}\mathcal{H}_m$ and $\mathcal{H}_m\cap\mathcal{H}_{m'}=\varnothing$ for $m\neq m'$). All bases of the irreducible subspaces $\mathcal{H}_m$ are algebraically generated by the representation relations. For this purpose by solving the differential equation $L_-|m,m\rangle=0$ which is obtained by (11b), we get the lowest base $|m,m\rangle$ as

$$|m,m\rangle = \frac{e^{im\phi+im\psi}(-1)^m}{\pi 2^{\alpha+m+1}}\frac{\sqrt{\Gamma(2\alpha+2m+2)}}{\Gamma(\alpha+m+1)}\tanh^m r, \tag{15}$$

which is consistent with (8). Equation (11a) gives all other bases of $\mathcal{H}_m$ as

$$|n,m\rangle = \sqrt{\frac{(2\alpha+2n+1)\Gamma(2\alpha+2m+1)}{(2\alpha+2m+1)\Gamma(n-m+1)\Gamma(2\alpha+n+m+1)}}L_+^{n-m}|m,m\rangle, \quad n\geqslant m. \tag{16}$$

Also, if we define operators K_+ and K_+ as

$$K_\pm := e^{\pm i\psi}\left(\mp\cosh r\frac{\partial}{\partial r} - \frac{i}{\sinh r}\frac{\partial}{\partial\psi} + \frac{\alpha\mp\alpha}{\sinh r}\right), \tag{17}$$

then by using relations (3) for a given n, we derive the raising and lowering relation of the label m, that is,

$$K_+|n,m-1\rangle = \sqrt{(n-m+1)(2\alpha+n+m)}|n,m\rangle, \tag{18a}$$

$$K_-|n,m\rangle = \sqrt{(n-m+1)(2\alpha+n+m)}|n,m-1\rangle. \tag{18b}$$

For $K_3 := -i\partial/\partial\psi$ we have

$$K_3|n,m\rangle = m|n,m\rangle. \tag{19}$$

Using the explicit forms of the operators K_+, K_-, K_3, and I or equations which are related to the operation of these operators on the Hilbert space $\mathcal{H}$, one may deduce

$$[K_+,K_-] = 2K_3 + 2\alpha I,$$

$$[K_3,K_\pm] = \pm K_\pm,$$

$$[\mathbf{K},I] = 0. \tag{20}$$

Therefore, the four generators K_+, K_-, K_3, and I satisfy the commutation relations of the compact Lie algebra u(2). The Hilbert space $\mathcal{H}$ represents this Lie algebra reducibly through Eqs. (18), (19), and (14). It is clear that for $\alpha=0$ (the associated Legendre functions), the Lie algebra u(2) i.e., (20) is decomposed into $\mathrm{su}(2)\oplus\mathrm{u}(1)$. The $(n+1)$-dimensional Hilbert subspaces $\mathcal{H}_n := \mathrm{span}\{|n,m\rangle\}_{m\leqslant n}$, which divide the Hilbert space $\mathcal{H}$ (as $\mathcal{H}=\cup_{n=0}^{\infty}\mathcal{H}_n$ and $\mathcal{H}_n\cap\mathcal{H}_{n'}=\varnothing$ for $n\neq n'$), represent the compact Lie algebra u(2) reducibly via the relations (18), (19), and (14) once again. In other words for a given n, all bases of $\mathcal{H}_n$ are calculated by an algebraic method. The highest base $|n,n\rangle$ is computed by (18a) as (15) except that m is replaced by n. Using (18b), all other bases are obtained as

$$|n,m\rangle = \sqrt{\frac{\Gamma(2\alpha+n+m+1)}{\Gamma(n-m+1)\Gamma(2\alpha+2n+1)}}K_-^{n-m}|n,n\rangle, \quad m\leqslant n. \tag{21}$$

In the next section we shall show that the bases $|n,m\rangle$ of the Hilbert space $\mathcal{H}$ are the eigensolutions of the Schrödinger operator corresponding to the motion of a free particle on the group manifold AdS_3. In addition, $\mathcal{H}$ will also represent the noncompact Lie algebra u(1,1) in a manner that is different from Eqs. (11) and (12).

IV. REALIZATION OF DYNAMICAL SYMMETRY GROUP U(1,1) FOR A FREE PARTICLE ON THE AdS_3 BY THE HILBERT SPACE $\mathcal{H}$

Simultaneous realization of representations of the noncompact Lie algebra u(1,1) and compact Lie algebra u(2) by the Hilbert space $\mathcal{H}$ via equations (11), (12), and (14), and (18), (19), and (14) respectively, gives us the possibility to define new differential generators for the Lie algebra u(1,1) (this time, they are functions from three coordinates r, ϕ, and ψ of the group manifold AdS_3) by a different method. So in addition to obtain a different representation for the Lie algebra u(1,1) by the Hilbert space $\mathcal{H}$, we can show that the Casimir operator of these new generators is basically the Schrödinger operator corresponding to the motion of a free particle on the group manifold AdS_3. First of all let us define

$$J_\pm := \pm[K_\pm,L_\pm] = e^{\pm i\phi\pm i\psi}\left[\pm\frac{\partial}{\partial r} + i\tanh r\frac{\partial}{\partial\phi} + i\coth r\frac{\partial}{\partial\psi} - \left[\left(\alpha+\frac{1}{2}\right)\pm\left(\alpha+\frac{1}{2}\right)\right]\tanh r - (\alpha\mp\alpha)\coth r\right]$$

$$J_3 := L_3 + K_3 = -i\left(\frac{\partial}{\partial\phi}+\frac{\partial}{\partial\psi}\right). \tag{22}$$

Using equations (11), (12), (18), and (19) it is easily shown that

$$J_+|n-1,m-1\rangle = \sqrt{\frac{(2\alpha+n+m)(2\alpha+n+m-1)(2\alpha+2n-1)}{2\alpha+2n+1}}|n,m\rangle, \tag{23a}$$

$$J_-|n,m\rangle = \sqrt{\frac{(2\alpha+n+m)(2\alpha+n+m-1)(2\alpha+2n+1)}{2\alpha+2n-1}}|n-1,m-1\rangle, \tag{23b}$$

$$J_3|n,m\rangle = (n+m)|n,m\rangle. \tag{23c}$$

Applying the recent result and also by using the explicit form of the generators, one can derive the commutation relations of the noncompact Lie algebra u(1,1) as

$$[J_+,J_-] = -4J_3 - 2(4\alpha+1),$$

$$[J_3,J_\pm] = \pm 2J_\pm,$$

$$[\mathbf{J},I] = 0. \tag{24}$$

Obviously, the representation of the Lie algebra u(1,1) in the Hilbert space $\mathcal{H}$ via Eqs. (23) and (14) is reducible. If we divide $\mathcal{H}$ in terms of the Hilbert subspaces $\mathcal{H}_i = \text{span}\{|m+i,m\rangle\}_{m\geqslant 0}$, $i \geqslant 0$, (as $\mathcal{H} = \cup_{i=0}^{\infty}\mathcal{H}_i$ and $\mathcal{H}_i \cap \mathcal{H}_{i'} = \varnothing$ for $i \neq i'$) then the representation of the Lie algebra u(1,1) by $\mathcal{H}_i$'s through the four generators J_+, J_-, J_3, and I will be irreducible.

The Casimir operator of the generators J_+, J_-, and J_3 has the following explicit form:

$$H = \frac{1}{2}[J_+J_- - J_3^2 - (4\alpha-1)J_3] = \frac{1}{2}\Bigg[-\frac{\partial^2}{\partial r^2} + \frac{1}{\cosh^2 r}\frac{\partial^2}{\partial\phi^2} - \frac{1}{\sinh^2 r}\frac{\partial^2}{\partial\psi^2} + [2\alpha\tanh r - (2\alpha+1)\coth r]\frac{\partial}{\partial r} + i\frac{(2\alpha+1)}{\cosh^2 r}\frac{\partial}{\partial\phi} - i\frac{2\alpha}{\sinh^2 r}\frac{\partial}{\partial\psi} + 2\alpha(2\alpha-1)\Bigg]. \tag{25}$$

The general form of the Schrödinger operator is $\mathcal{L} = -\frac{1}{2}D_i^{\mathbf{A}}D^{\mathbf{A}i} + V$ in which the index i takes the values r, ϕ, and ψ, respectively. Further, $D_i^{\mathbf{A}}$ is the covariant derivative and $\mathbf{A}$ stands for the connection associated with the presence of an external magnetic field. If we equalize the Casimir operator given in (25) with $\mathcal{L}$ then by comparing the coefficients of the second-order derivatives, the metric tensor will be calculated to yield

$$g_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\cosh^2 r & 0 \\ 0 & 0 & \sinh^2 r \end{pmatrix}. \tag{26}$$

The nonzero components of the Christoffel symbols related to the metric (26) are computed as

$$\Gamma^r_{\phi\phi} = \tfrac{1}{2}\sinh 2r, \quad \Gamma^r_{\psi\psi} = -\tfrac{1}{2}\sinh 2r, \quad \Gamma^{\phi}_{r\phi} = \tanh r, \quad \Gamma^{\psi}_{r\psi} = \coth r. \tag{27}$$

Thus, the nonzero component of the Ricci tensor are given by

$$R_{rr} = -2, \quad R_{\phi\phi} = 2\cosh^2 r, \quad R_{\psi\psi} = -2\sinh^2 r. \tag{28}$$

Consequently, Ricci scalar curvature becomes $R = g^{ij}R_{ij} = -6$. So, the parameters r, ϕ, and ψ describe the coordinates of a three-dimensional manifold with constant negative curvature. It is well-known that[35,36] r, ϕ, and ψ can show an appropriate parametrization for the elements of the group manifold $\text{AdS}_3 \cong \text{SL}(2,R) \cong \text{SU}(1,1)$. Therefore, by using suitable matrix generators for the Lie algebra su(1,1), one can construct left and right invariant differential forms of these generators which may be compared with (22). Note that AdS_3 is not globally a hyperbolic space.

Comparing the coefficients of the first-order derivative and the terms without derivative in the Casimir and Schrödinger operators, then the components of the gauge and scalar potentials are obtained as

$$A_r = \frac{-i}{2}(2\alpha+1)\tanh r, \quad A_\phi = -\frac{1}{2}(2\alpha+1), \quad A_\psi = -\alpha, \quad V = \alpha(2\alpha-1) - \frac{3}{8}. \tag{29}$$

Hence, the two-form magnetic field and the electric field vector become zero:

$$\mathbf{B} = \frac{\partial A_j}{\partial x_i}\mathbf{dx_i} \wedge \mathbf{dx_j} = 0, \quad \mathbf{E} = -\nabla V = 0. \tag{30}$$

Thus, the Casimir operator H describes the Hamiltonian corresponding to a particle moving on the group manifold $\mathrm{SL}(2,R)$ in the absence of magnetic and electric fields. Equations (23a)–(23c) immediately give the following eigenvalue equation on the reducible representation space $\mathcal{H}$ with infinite-fold degeneracy for the energy spectrum:

$$H|n,m\rangle = \alpha(2\alpha-1)|n,m\rangle, \quad 0 \leqslant m \leqslant n < \infty. \tag{31}$$

It is clear that if we restrict the eigenvalue equation (31) on the Hilbert subspaces $\mathcal{H}_i$ which represent the Lie algebra u(1,1), i.e., (24) irreducibly, then it will have infinite-fold degeneracy for the spectrum once again. So, the bases of the Hilbert space, i.e., the kets $|n,m\rangle$ are the quantum states associated to the motion of a free particle on the group manifold AdS_3. Besides, the dynamical symmetry group U(1,1) with infinite-fold degeneracy for the spectrum is described by means of the Casimir operator H. At the same time, as has been shown in the previous section, two other symmetry are exhibited by the space $\mathcal{H}$ of quantum states. In these symmetries we introduce the generators of the non-compact Lie algebra u(1,1) and compact Lie algebra u(2) such that their irreducible representation subspaces are irrelevant with respect to the functional behavior of the variables ψ and ϕ, respectively.

V. CONCLUSION

In this article, in addition to obtaining a dynamical symmetry group U(1,1) via simultaneous shift operators of two parameters n and m, we obtained two different quantum splittings for all the quantum states of a free particle on AdS_3. These two types of quantum splittings are realized by the raising and lowering generators of the noncompact Lie algebra u(1,1) and compact Lie algebra u(2) corresponding to the shift of just the index n for a given m, and the shift of just the index m for a given n, respectively. In other words, there exist two different types of quantum splitting with u(1,1)- and u(2)-irreducible representations on the space of all quantum states. They are infinite- and finite-dimensional Hilbert subspaces with the same functionalities of variables ψ and ϕ for the bases, respectively. Further, the functionalities of both variables ψ and ϕ are changed in the irreducible representations of dynamical symmetry group U(1,1).

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Construction of Parseval wavelets from redundant filter systems

L. W. Baggett[a)]
Department of Mathematics, Campus Box 395, University of Colorado, Boulder, Colorado 80309-0395

P. E. T. Jorgensen[b)]
Department of Mathematics, University of Iowa, 14 MacLean Hall, Iowa City, Iowa 52242-1419

K. D. Merrill[c)]
Department of Mathematics, Colorado College, Colorado Springs, Colorado 80903-3294

J. A. Packer[d)]
Department of Mathematics, Campus Box 395, University of Colorado, Boulder, Colorado 80309-0395

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We consider wavelets in $L^2(\mathbb{R}^d)$ which have generalized multiresolutions. This means that the initial resolution subspace V_0 in $L^2(\mathbb{R}^d)$ is not singly generated. As a result, the representation of the integer lattice $\mathbb{Z}^d$ restricted to V_0 has a nontrivial multiplicity function. We show how the corresponding analysis and synthesis for these wavelets can be understood in terms of unitary-matrix-valued functions on a torus acting on a certain vector bundle. Specifically, we show how the wavelet functions on $\mathbb{R}^d$ can be constructed directly from the generalized wavelet filters. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1982768]

I. INTRODUCTION

The theory of wavelets is concerned with the Hilbert space $L^2(\mathbb{R}^d)$. The problem is to find "good" orthonormal bases (ONB), where "good" makes reference to several conflicting requirements:

(1) These bases must be constructed from a small number of model functions, called wavelets, and two discrete operations, translation, and scaling. In this article, we are concerned with translation by the standard integer lattice $\mathbb{Z}^d$, and scaling by some prescribed integral matrix A which is assumed expansive.
(2) In passing from function to expansion coefficients, referring to a wavelet basis, and back again (this is called analysis/synthesis), the steps must be algorithmic, ideally avoiding direct reference to integration over $\mathbb{R}^d$.
(3) The wavelet functions should have compact support, and should have some prescribed number of derivatives.

The algorithms that have been popular since the mid-1980s are based on what is called multiresolution analysis (MRA). This was pioneered by Daubechies,[1] Mallat,[2] and Meyer,[3,4] and the idea, although simple, has been extremely powerful. The idea itself is much like that of the

[a)]Electronic mail: baggett@euclid.colorado.edu
[b)]Electronic mail: jorgen@math.uiowa.edu
[c)]Electronic mail: kmerrill@coloradocollege.edu
[d)]Electronic mail: packer@euclid.colorado.edu

Gram–Schmidt algorithm from Hilbert space, in that it is based on a scale of closed subspaces, resolutions V_n, and relative orthogonal complements, detail subspaces W_n. The scale of subspaces V_n play the role of martingales from probability theory.

Daubechies's book[1] stresses how Requirements (1)–(3) can be met with the MRA approach, and all starting with a fixed cleverly chosen function φ in the subspace V_0 from the resolution. The function φ, the father function, is the solution in L^2 to a scaling, or refinement, equation; a solution which results from a cascade approximation. The wavelet functions, mother functions, can then be constructed from the subspace W_0 which is the relative orthocomplement of V_0 in V_1. One drawback of this approach is that if $N=|\det A|$, then $N-1$ wavelet generators from W_0 are needed. In the dyadic case, $d=1$, $N=2$, that makes one function, but in general, N can be large. Now the spaces V_0 and W_0 are invariant under translation by $\mathbb{Z}^d$, and there is a corresponding pair of multiplicity functions which dictate a minimal choice of generators for V_0 and W_0.

In fact, for the general case of $L^2(\mathbb{R}^d)$ and a fixed scaling matrix A, it is possible to get W_0 singly generated, i.e., to find a single generator ψ. In some cases ψ may be taken to be the inverse Fourier transform of a subset E of $\mathbb{R}^d$. Such subsets E are called wavelet sets, see Refs. 5–10. But there are other choices of sets of generating functions ψ, with the number of generators between 1 and $N-1$. What emerges is that these constructions force frequency localization, and the compact support in the x variable is typically lost, i.e., we must relax Requirement (3). As it turns out, the kind of frequency localization we obtain is well suited for effective sampling algorithms. A second issue enters: The wavelet algorithm may lead to bases which only satisfy a certain Parseval property (also called "normalized tight frames"). Although we still have the resolution structure V_n, the number of generators in V_0 may increase, but they are not directly part of the wavelet basis. This setup is referred to as a generalized multiresolution analysis (GMRA); see Refs. 8–10.

The GMRA theory was in fact introduced (in an operator-theoretic/operator-algebraic framework) in a pioneering paper by Baggett, *et al.*[11] By now there is a rich journal literature which reflects wavelet constructions with some degree of multiplicity; see, e.g., Refs. 12–24. In addition our multiplicity analysis has recently been used in papers by Dutkay and Jorgensen[25–28] in the study of nonlinear dynamical models.

A recent and interesting paper of Papadakis[29] offers a global and natural approach to generalized multiresolution analyses (GMRAs) based on a geometric frame construction which has the advantage of including all GMRA constructions in $L^2(\mathbb{R})$. Some of the differences between the approach in Ref. 29 and the present one lie in our use here of operator algebraic tools deriving from the Cuntz algebras[30] in operator theory. Further, our use of vector bundles in Sec. IV offers a rather explicit and concrete representation of the matrix functions which in turn describe the filters for GMRA normalized tight frame wavelets, alias, for Parseval wavelet frames.

Our article and other recent articles on wavelet frames may be said to generalize a celebrated theorem first proved by Lawton in this journal.[31] Lawton's pioneering result states that a trigonometric low-pass filter which satisfies a certain conjugate-mirror filter condition must give rise to a wavelet frame. However, the resulting wavelet frame may not be associated with a classical MRA. We generalize Lawton's theorem in several directions to a much broader class of subband wavelet filters. Our matrix-valued low-pass filters are still associated with GMRA wavelets. These in turn are the most general types of multiresolution structures.

Finally, we emphasize that the use of wavelet filters derives historically from signal processing in communications engineering, see e.g., Ref. 32.

In the standard case of MRAs, it is well known how the subband filters from signal processing allow us to construct the wavelet functions by an elegant algorithm. The function φ is a solution to a certain refinement equation. The subband filters may be thought of as functions on a torus $\mathbb{T}$, frequency response functions. But in the case of multiplicity and multiple generators, the corresponding functions on $\mathbb{T}$ are matrix valued, and the refinement equation is a matrix equation.

In this article we show that the generalized setup admits solutions in $L^2(\mathbb{R}^d)$ starting with this matrix/vector version of the refinement equation. Starting with a matrix system of subband filter functions on a torus, we show that our corresponding wavelet solutions are in $L^2(\mathbb{R}^d)$, and that they will be Parseval frames for the Hilbert space $L^2(\mathbb{R}^d)$.

Although this is a weakening of the stricter ONB in Requirement (2), the Parseval frame property still allows the same recursive analysis/synthesis algorithms popular in the MRA case. The now classical method of Mallat and Meyer for constructing an orthonormal wavelet in $L^2(\mathbb{R})$ [relative to translation by integers and dilation by 2 (Refs. 2 and 3)] proceeds as follows: Let h be a periodic function on $\mathbb{R}$ that satisfies the "conjugate mirror filter condition" (the so-called Smith–Barnwell condition)

$$|h(x)|^2 + \left|h\left(x+\tfrac{1}{2}\right)\right|^2 = 2. \tag{1.1}$$

The function h is the conjugate mirror filter, referred to previously, and in our context is called a *low-pass filter*. Consider the infinite product

$$P(x) = \prod_{j=1}^{\infty} \frac{1}{\sqrt{2}} h\left(\frac{x}{2^j}\right),$$

and suppose that there exists a nonzero L^2 function ϕ whose Fourier transform $\hat{\phi}$ coincides with P. Under not too strenuous assumptions on h, this does in fact hold. For instance, if we take h to be smooth, and satisfying Cohen's orthogonality conditions and the *low-pass condition* $|h(0)| = \sqrt{2}$, the set of integer translates of ϕ turn out to be orthonormal functions in L^2, and in fact ϕ is a scaling function for a multiresolution analysis $\{V_j\}$.

Given such a low-pass filter function h, there exists an associated periodic function g, which also satisfies the filter equation (1.1), and such that h and g satisfy the following orthogonality condition:

$$h(x)\overline{g(x)} + h\left(x+\tfrac{1}{2}\right)\overline{g\left(x+\tfrac{1}{2}\right)} = 0. \tag{1.2}$$

Any such function g, called a *high-pass filter*, can be obtained from the low-pass filter function via the standard technique of constructing a unitary matrix whose first row is given by $((h(x)/\sqrt{2}), (h(x+1/2)/\sqrt{2})$ Finally, the function ψ, defined by

$$\hat{\psi}(x) = \frac{1}{\sqrt{2}} g\left(\frac{x}{2}\right)\hat{\phi}\left(\frac{x}{2}\right)$$

is an orthonormal wavelet. That is, the collection $\{\psi_{j,n}\} \equiv \{\sqrt{2}^j \psi(2^j x - n)\}$, for j and n in $\mathbb{Z}$, forms an orthonormal basis for $L^2(\mathbb{R})$.

A famous example of Cohen[33] shows that eliminating the nonvanishing condition can cause the Mallat–Meyer method to go wrong in an interesting but not disastrous way. Cohen exhibited a low-pass filter function h, for which the infinite product P exists, is the Fourier transform of a nonzero L^2 function ϕ, but for which the integer translates of ϕ are not orthonormal. Further, the translates and dilates $\{\psi_{j,n}\}$ of the corresponding function ψ, defined just as in the classical method, is not an orthonormal basis. So, for this choice of filter h, the Mallat–Meyer procedure fails to produce a scaling function, and the resulting function ψ is not an orthonormal wavelet. Nevertheless, its translates and dilates do form what is called a *Parseval frame*. By definition, this means that for each $f \in L^2(\mathbb{R})$ we have

$$\|f\|^2 = \sum_j \sum_n |\langle f|\psi_{j,n}\rangle|^2.$$

In Refs. 31 and 34, the Mallat–Meyer phenomenon was generalized to incorporate the Cohen example in the following way. Suppose h is a low-pass filter for dilation by a positive integer N, i.e., satisfies the filter equation

$$\sum_{l=0}^{N-1} \left| h\left(x+\frac{l}{N}\right)\right|^2 = N$$

and the low-pass condition $|h(0)| = \sqrt{N}$, and suppose $g_1, \ldots, g_{N-1}$ are corresponding high-pass filters, i.e., are periodic functions for which the N functions $h, g_1, \ldots, g_{N-1}$ satisfy the following orthogonality conditions:

$$\sum_{l=0}^{N-1} h\left(x+\frac{l}{N}\right)\overline{g_i}\left(x+\frac{l}{N}\right) = 0$$

for all $1 \leqslant i \leqslant N-1$, and

$$\sum_{l=0}^{N-1} g_i\left(x+\frac{l}{N}\right)\overline{g_j\left(x+\frac{l}{N}\right)} = \begin{cases} N, & i=j \\ 0, & i \neq j, \end{cases}$$

for all i, j between 1 and $N-1$. Again, these $N-1$ high-pass filters can be constructed from the low-pass filter h by the matrix completion technique.

Let P be the infinite product

$$P = \prod_{j=1}^{\infty} \frac{1}{\sqrt{N}} h\left(\frac{x}{N^j}\right).$$

Then, if the functions $h, g_1, \ldots, g_{N-1}$ are Lipschitz continuous, it is shown in Ref. 34 that there exists a nonzero L^2 function ϕ whose Fourier transform coincides with P, and the $N-1$ functions $\{\psi_k\}$, defined by

$$\widehat{\psi_k}(x) = \frac{1}{\sqrt{N}} g_k\left(\frac{x}{N}\right)\hat{\phi}\left(\frac{x}{N}\right),$$

form a Parseval frame multiwavelet. That is, the collection

$$\{\psi_{j,n,k} \equiv \sqrt{N}^j \psi_k(N^j x - n)\},$$

$j, n \in \mathbb{Z}$ and $1 \leqslant k \leqslant N-1$, forms a Parseval frame for $L^2(\mathbb{R})$.

Just as in the Cohen phenomenon in the Mallat–Meyer constructions, the integer translates of the function ϕ may or may not be orthonormal, even though their closed linear span V_0 does form the core subspace of a (generalized) multiresolution analysis. Also, the wavelets ψ_k may or may not have orthonormal translates and dilates, and may or may not belong to the subspace $V_1 \ominus V_0$ of this associated GMRA.

The arguments in the proof of this result introduce some ideas from operator theory, specifically in the form of the Ruelle operator and partial isometries that satisfy relations similar to the Cuntz relations.[30] In the case of dilation by 2, Lawton[31] used a cascade algorithm in the time domain to independently derive the same result (in the special case of trigonometric polynomials, i.e., the case corresponding to a single compactly supported scaling function).

Although the constructions of Refs. 31 and 34 start with filters associated with a classical multiresolution analysis, they build a frame wavelet that may be obtained from only a generalized multiresolution analysis. The purpose of the present article is to extend and clarify this kind of result to filters defined in higher dimensional and non MRA contexts. That is, we suppose that A is an expansive, integral, $d \times d$ matrix, and we investigate frame wavelets constructed from filter systems associated to generalized multiresolution analyses in $L^2(\mathbb{R}^d)$ relative to dilation by A and translation by lattice points in $\mathbb{Z}^d$.

The theory of generalized conjugate mirror filters relative to a generalized multiresolution analysis was first developed in Refs. 35 and 36. In Sec. II we briefly review that subject, and in particular we recall the analogs to Eqs. (1.1) and (1.2), i.e., generalized filter and orthogonality

equations. These generalized equations are considerably different from the original ones, because the right-hand side now involves an integer-valued multiplicity function on the d-dimensional torus $\mathbb{T}^d \equiv [-\frac{1}{2}, \frac{1}{2})^d$. In general, the low-pass filter becomes a square matrix $H=[h_{i,j}]$ of periodic functions, and the high-pass filter becomes a not necessarily square matrix $G=[g_{k,j}]$ of periodic functions. Because the filters in this generalized context are matrices of periodic functions, we refer to them as redundant systems of filters.

By generalizing the arguments in Ref. 34, we are able here to build wavelets from generalized filters more simply and with fewer restrictions than in Ref. 36. In Sec. III, under smoothness and low-pass conditions analogous to those in Ref. 34, we prove that the infinite matrix product

$$P = \prod_{j=1}^{\infty} \frac{1}{\sqrt{|\det(A)|}} H(A^{t^{-j}}(x))$$

converges pointwise, and the first column Φ of P is the Fourier transform of a set $\phi_1, \phi_2, \ldots$ of L^2 functions that together generate a generalized multiresolution analysis. We then prove that the functions $\{\psi_k\}$ given by

$$\widehat{\psi_k}(x) = \frac{1}{\sqrt{|\det(A)|}} \sum_j g_{k,j}(A^{t^{-1}}(x)) \widehat{\phi_j}(A^{t^{-1}}(x))$$

form a Parseval wavelet frame for $L^2(\mathbb{R}^d)$.

In engineering, the various classes of multiresolution analyses are motivated by filters from signal and image processing. Although these are practical concerns, our present aim is theoretical. In most of the engineering MRA constructions, the multiplicity function is equal to 1 on the entire fundamental domain $[-1/2, 1/2)$, so this only produces classical MRA quadrature-mirror filters. One must choose the multiplicity function to be mixed, i.e., equal to the characteristic function of delicately selected configurations of subsets of $[-1/2, 1/2)$, to get genuinely generalized filters, i.e., GMRA filters. If the multiplicity function is not constant, the filters can never all be continuous in the frequency domain, which can be a problem for engineers. The reason that all the filters for a GMRA cannot be continuous is that they must satisfy the filter equations (2.4) and (2.5), both of which involve noncontinuous characteristic functions for nonconstant multiplicity functions. This particular feature of our theory becomes evident in our example in Sec. III, Example 3.6. Yet, this example is surprising in two ways. First, it is related to a nonclassical MRA wavelet, the Journé wavelet. Second, we construct two low-pass filters which have discontinuities in the frequency domain, but the resulting scaling functions are C^∞ in the frequency domain! This prompts the following question: can the scaling functions and wavelets associated to GMRAs be constructed to have nice properties in both the time and the frequency domains? From the viewpoint of engineering, this is an important question, and it is addressed in a sequel paper[37] in much more detail. We have established this in the affirmative in Ref. 37, where we construct a frame wavelet that is C^r in the time domain and C^∞ in the frequency domain. More importantly, it would be interesting to know whether or not scaling functions and frame wavelets that have nice properties in both the time and frequency domains can be constructed for every choice of a multiplicity function.

In Ref. 34 the set of functions $h, g_1, \ldots, g_{N-1}$ is called an *M system*. It is shown in Ref. 34 that there is a group that acts freely and transitively on the set of M systems, thus suggesting a natural structure on these systems and therefore on the corresponding frame wavelet systems. In Sec. IV of this article, we describe an analogous action on the generalized filter systems we have introduced. This time, it is a group bundle that acts freely and transitively.

II. GENERALIZED FILTERS

We collect here the relevant definitions concerning wavelets and multiresolution analyses in $L^2(\mathbb{R}^d)$, relative to translation by lattice points and dilation by an expansive integer matrix A; i.e., a matrix each of whose eigenvalues has modulus greater than 1.

Recall that a *frame* in $L^2(\mathbb{R}^d)$ is a sequence $\{f_n\}$ for which there exist positive numbers a and b such that

$$a\|f\|_2^2 \leqslant \sum_n |\langle f|f_n\rangle|^2 \leqslant b\|f\|_2^2$$

for every $f \in L^2(\mathbb{R}^d)$. It is called a *Parseval frame* or a *normalized tight frame* if $a=b=1$ in the inequalities above. That is, $\{f_n\}$ is a Parseval frame if $\|f\|_2^2=\Sigma_n|\langle f|f_n\rangle|^2$ for every $f \in L^2(\mathbb{R}^d)$.

For each $z \in \mathbb{Z}^d$, we write τ_z for the unitary *translation operator* on $L^2(\mathbb{R}^d)$ given by $[\tau_z(f)](t)=f(t+z)$. Fix an expansive, $d\times d$, integer matrix A and let $B=A^t$ and $N=|\det(A)|$. We write δ for the unitary *dilation operator* given by $[\delta(f)](t)=\sqrt{N}f(A(t))$. For each element $\omega \in \mathbb{T}^d$, there exist exactly N distinct points $\zeta \in \mathbb{T}^d$ such that $\alpha(\zeta)=\omega$, where α denotes the endomorphism on $\mathbb{T}^d$ induced by the action of B on $\mathbb{R}^d$. We denote these points ζ in a Borel manner as $\omega_0, \omega_1, \ldots, \omega_{N-1}$. Note also that, because A is an expansive matrix, the endomorphism α is ergodic.

Definition 2.1: A MRA in $L^2(\mathbb{R}^d)$, relative to the group $\{\tau_z\}$ of translation operators and the dilation operator δ, is a sequence $\{V_j\}_{-\infty}^{\infty}$ of closed subspaces of $L^2(\mathbb{R}^d)$ for which:

(1) $V_j \subseteq V_{j+1}$;
(2) $V_{j+1}=\delta(V_j)$;
(3) $\cup V_j$ is dense in $L^2(\mathbb{R}^d)$, and $\cap V_j=\{0\}$; and
(4) There exists an element $\phi \in V_0$ whose translates $\{\tau_z(\phi)\}$ form an orthonormal basis for V_0. Such an element ϕ is called a *scaling function* for the multiresolution analysis.

A GMRA is a sequence $\{V_j\}$ of closed subspaces of $L^2(\mathbb{R}^d)$ that satisfies Conditions (1), (2), and (3) mentioned above, but satisfies the weaker fourth condition

(4′) V_0 is invariant under all the translation operators τ_z.

In both cases, the subspace V_0 is called the *core subspace* of the GMRA.

The theory of GMRAs is developed in Refs. 9–11 (see also Ref. 20). In particular, it is shown there that by Stone's theorem for unitary representations of the group $\mathbb{Z}^d$, or more generally by spectral multiplicity theory for a set of commuting unitary operators, the invariance under translation of the core subspace V_0 implies the existence of a *multiplicity function* $m:\mathbb{T}^d \mapsto \{0,1,2,\ldots,\infty\}$. The multiplicity function m counts the number of times each exponential function is represented as a subrepresentation of translation by $\mathbb{Z}^d$ on V_0. We will assume in this paper that m is bounded, with maximum value c. We let $S_i=\{\omega \in \mathbb{T}^d: m(\omega) \geqslant i\}$, and recall from Ref. 10 that there exist *generalized scaling functions* $\{\phi_i\}_{1\leqslant i\leqslant c}$ such that the collection $\{\tau_z(\phi_i)\}$ for $z \in \mathbb{Z}^d$ and $1 \leqslant i \leqslant c$ forms a Parseval frame for V_0, and such that $\Sigma_{z\in\mathbb{Z}^d}|\hat{\phi}_i(\omega+z)|^2=\chi_{S_i}(\omega)$. Note that these results translate to the classical conditions in an MRA, which is the special case of a GMRA in which the multiplicity function is identically 1.

If V_0 is the core subspace of a generalized multiresolution analysis $\{V_j\}$, then the subspace $W_0=V_1 \cap V_0^{\perp}$ of a GMRA $\{V_j\}$ also is invariant under all the translation operators τ_z. Hence, again by Stone's theorem, there exists a *complementary multiplicity function* $\tilde{m}:\mathbb{T}^d \mapsto \{0,1,2,\ldots,\infty\}$ that characterizes the representation of $\mathbb{Z}^d$ on W_0. As a direct result of the fact that $V_1=V_0 \oplus W_0$, the multiplicity functions m and $\tilde{m}$ must satisfy the following *consistency equation* (see Ref. 9):

$$m(\omega)+\tilde{m}(\omega)=\sum_{l=0}^{N-1} m(\omega_l). \tag{2.1}$$

By the consistency equation, the assumption that m is bounded implies that $\tilde{m}$ is bounded as well. We write $\tilde{c}$ for the maximum value of $\tilde{m}$, and $\tilde{S}_k$ for $\{\omega \in \mathbb{T}^d: \tilde{m}(\omega) \geqslant k\}$.

Generalized multiresolution analyses are useful because of their relationship to wavelets. In particular, in Ref. 9 it is shown that every orthonormal multiwavelet is associated to a GMRA with $\tilde{m}$=the number of wavelets. We recall the relevant definitions here:

Definition 2.2: An *orthonormal wavelet*, or more generally an *orthonormal multiwavelet*, in

$L^2(\mathbb{R}^d)$, relative to the group $\{\tau_z\}$ of translation operators and the dilation operator δ, is a finite set $\psi_1,\ldots,\psi_m$ of functions in $L^2(\mathbb{R}^d)$ for which the collection $\{\psi_{j,z,k}\}\equiv\{\delta^j(\tau_z(\psi_k))\}$ forms an orthonormal basis for $L^2(\mathbb{R}^d)$. A set of functions $\psi_1,\ldots,\psi_m$ forms a *frame multiwavelet* if the collection $\{\psi_{j,z,k}\}$ forms a frame for $L^2(\mathbb{R}^d)$, and the set is called a *Parseval frame multiwavelet* if the collection $\{\psi_{j,z,k}\}$ forms a Parseval frame for $L^2(\mathbb{R}^d)$.

We now are ready to develop the definition of generalized filters. The classical filter equation [Eq. (1.1)], which is the basis for the Mallat–Meyer construction of scaling functions and wavelets, emerges naturally from the study of classical multiresolution analyses. For, if ϕ is a function, for which the closure of the linear span of the translates of ϕ is invariant under the dilation $f(x)\to f(x/2)$, e.g., if ϕ is a scaling function for a MRA, then it follows from elementary Fourier analysis that $\hat{\phi}$ satisfies the following classical *refinement equation*:

$$\sqrt{2}\hat{\phi}(2x)=h(x)\hat{\phi}(x), \tag{2.2}$$

where h is a periodic function that satisfies the filter equation (1.1). As described in Sec. I, the Mallat–Meyer construction[2,3] reverses this procedure, by beginning with a sufficiently well behaved function h that satisfies filter equation (1.1), and producing a corresponding scaling function and multiresolution analysis by iterating Eq. (2.2) to get an infinite product expression for $\hat{\phi}$.

In an analogous way, the theory of generalized filters emerges naturally from the study of generalized multiresolution analyses (see Refs. 35 and 36). Because $V_{-1}=\delta^{-1}(V_0)$ is contained in V_0, it follows that, for each i, there exists a sequence $\{h_{i,j}\}$ of functions on the torus $\mathbb{T}^d$ such that

$$\sqrt{N}\hat{\phi}_i(B(x))=\sum_j h_{i,j}(x)\widehat{\phi_j}(x). \tag{2.3}$$

As is shown in Ref. 36, these generalized filters satisfy the *generalized filter equation*:

$$\sum_j\sum_{l=0}^{N-1} h_{i,j}(\omega_l)\overline{h_{i',j}(\omega_l)}=\delta_{i,i'}N\chi_{S_i}(\omega), \tag{2.4}$$

and also have $h_{i,j}$ supported on S_j. In analogy with the classical case, we make the following definition.

Definition 2.3: A *generalized low-pass filter* relative to a GMRA with multiplicity functions m and $\tilde{m}$ is a matrix of functions $H=[h_{i,j}]$ on $\mathbb{T}^d$ (or equivalently $\mathbb{Z}^d$ periodic functions on $\mathbb{R}^d$), with $h_{i,j}$ supported on S_j (or the periodization of S_j), that satisfy both the generalized filter equation (2.4) and the generalized low-pass condition $h_{i,j}(0)=\delta_{i,1}\delta_{j,1}\sqrt{N}$.

Just as in the classical case, we can sometimes reverse the procedure of producing filters from wavelets. In particular, generalized low-pass filters give rise to generalized high-pass filters. The relevant result is contained in the following theorem, again from Ref. 36.

Theorem 2.4: *Let $H=[h_{i,j}]$ be a generalized low-pass filter relative to a GMRA with multiplicity functions m and $\tilde{m}$. Then there exists a matrix $G=[g_{k,j}]$ of functions on $\mathbb{T}^d$ satisfying*

$$\sum_j\sum_{l=0}^{N-1} g_{k,j}(\omega_l)\overline{g_{k',j}(\omega_l)}=\delta_{k,k'}N\chi_{\tilde{S}_k}(\omega), \tag{2.5}$$

and

$$\sum_j\sum_{l=0}^{N-1} h_{i,j}(\omega_l)\overline{g_{k,j}(\omega_l)}=0 \tag{2.6}$$

for all i and k. The matrix of functions $G=[g_{k,j}]$ is called a generalized high-pass filter.

Under conditions which allow the production of generalized scaling functions from generalized low-pass filters, these high-pass filters can be used to build frame multiwavelets. Some narrow conditions that allow this are described in Ref. 36. In Sec. III, we show that more general conditions allow the same construction.

There is one final property of a generalized low-pass and high-pass filter that we will need in Sec. III, which was not presented in Ref. 36.

Theorem 2.5: *Let H and G be a generalized low-pass and high-pass filter relative to multiplicity and complementary multiplicity functions m and $\tilde{m}$. Assume that the maximum value of m is c and the maximum value of $\tilde{m}$ is $\tilde{c}$. Then*

$$\sum_{i=1}^{c} h_{i,j}(\omega_l)\overline{h_{i,j'}(\omega_{l'})} + \sum_{k=1}^{\tilde{c}} g_{k,j}(\omega_l)\overline{g_{k,j'}(\omega_{l'})} = \delta_{j,j'}\delta_{l,l'}N\chi_{S_j}(\omega_l). \tag{2.7}$$

Proof: For each $\omega \in \mathbb{T}^d$, we define a matrix $K(\omega)$ having $c+\tilde{c}$ rows and $c\times N$ columns as follows: We index the $c\times N$ columns of $K(\omega)$ by pairs (j,l), where $1\leqslant j\leqslant c$ and $0\leqslant l\leqslant N-1$. Then the entry $k_{i,(j,l)}(\omega)$ is defined to be $(1/\sqrt{N})h_{i,j}(\omega_l)$ if $1\leqslant i\leqslant c$, and $k_{i,(j,l)}(\omega) = (1/\sqrt{N})g_{i-c,j}(\omega_l)$ if $c<i\leqslant\tilde{c}$. We see directly from Eq. (2.4) that, for $1\leqslant i\leqslant c$, the ith row of the matrix $K(\omega)$ contains a nonzero entry if and only if $\omega\in S_i$, i.e., if and only if $i\leqslant m(\omega)$. And, from Eq. (2.5), for $c<i\leqslant c+\tilde{c}$, the ith row of $K(\omega)$ contains a nonzero entry if and only if $\omega\in\tilde{S}_{(i-c)}$, i.e., if and only if $i-c\leqslant\tilde{m}(\omega)$. Therefore, there are exactly $m(\omega)+\tilde{m}(\omega)$ nonzero rows in $K(\omega)$.

Next, we note that the column indexed by the pair (j,l) has a nonzero entry only when some $h_{i,j}(\omega_l)$ or $g_{i,j}(\omega_l)$ is nonzero. That is, the (j,l)th column has a nonzero entry only when $\omega_l\in S_j$, i.e., only when $j\leqslant m(\omega_l)$. So, the maximum number of columns having a nonzero entry in them is equal to $\Sigma_{l=0}^{N-1}m(\omega_l)$, which, by the consistency equation (2.1), equals $m(\omega)+\tilde{m}(\omega)$, and this is exactly the number of rows of $K(\omega)$ that have a nonzero entry.

Therefore, the set of nonzero entries in the matrix $K(\omega)$ are contained in a square submatrix $L(\omega)$ of size $(m(\omega)+\tilde{m}(\omega))\times(m(\omega)+\tilde{m}(\omega))$.

Finally, from Eqs. (2.4)–(2.6), we see that the rows of this square matrix $L(\omega)$ are orthonormal. Hence, the columns of $L(\omega)$ are also orthonormal, and this implies the orthogonality equations of the theorem. □

III. CONSTRUCTION OF FRAME WAVELETS FROM GENERALIZED FILTERS

We are now ready to use the generalized filters from Sec. II to extend the construction procedure for frame wavelets described in Ref. 34. Just as in the classical case, the first step of the construction is to take an infinite product of dilations of the low-pass filters.

Proposition 3.1: Let $H=[h_{i,j}]$ be a generalized low-pass filter as in Definition 2.3 Assume that the components of H are Lipschitz continuous functions in a neighborhood of 0.

(1) *The infinite product*

$$P = \prod_{q=1}^{\infty} \frac{1}{\sqrt{N}} H(B^{-q}(x))$$

converges almost everywhere on $\mathbb{R}^d$, and the entries $P_{i,j}$ of P are square-integrable functions on $\mathbb{R}^d$, with $P_{i,j}=0$ for $j>1$.

(2) *For $1\leqslant i\leqslant c$, let ϕ_i be the inverse Fourier transform of the function $P_{i,1}$. Then the $\hat{\phi}_i$'s are continuous at 0, satisfy $\hat{\phi}_{i,1}(0)=\delta_{i,1}$, and also satisfy the following generalized refinement equation.*

$$\hat{\phi}_i(B(x)) = \frac{1}{\sqrt{N}}\sum_{j=1}^{c} h_{i,j}(x)\hat{\phi}_j(x).$$

Proof: Throughout the proof, we will use the following result from linear algebra. If C is a

$c \times c$ matrix all of whose eigenvalues have modulus less than 1, then $\Sigma_{k=0}^{\infty}\|C^k(x)\|$ converges, for every $x \in \mathbb{R}^c$. This result follows by using the Jordan canonical form for the matrix C to show that $\Sigma\|C^k(x)\|$ is dominated by a convergent geometric series.

We prove the convergence of the infinite product first. If β is the Lipschitz constant, note that by the low-pass condition we have $\|h_{i,j}(x)\| \leq \beta\|x\|$ for $\{i,j\} \neq \{1,1\}$, and $\|h_{1,1}(x) - \sqrt{N}\| \leq \beta\|x\|$, both for $\|x\|$ sufficiently small. Write P^k for the partial product $\Pi_{q=1}^{k}\left(1/\sqrt{N}\right)H(B^{-q}(x))$, where as before $N=|\det(A)|$. We first show by induction that for each fixed x, there is a bound K such that $|P_{i,j}^k(x)| \leq K$ for all $1 \leq i,j \leq c$, and $k \geq 1$. To see this, write

$$|P_{i,j}^k(x)| = \sum_{l=1}^{c} P_{i,l}^{k-1}(x)\frac{1}{\sqrt{N}}h_{l,j}(B^{-k}(x)) \leq |P_{i,1}^{k-1}(x)| + \left|\sum_{l=2}^{c} P_{i,l}^{k-1}(x)\right|\frac{\beta}{\sqrt{N}}\|B^{-k}(x)\|,$$

for k sufficiently large (where in the first term we use the fact that the orthogonality conditions give $|h_{i,1}| \leq \sqrt{N}$). Using induction on k, and the linear algebra result mentioned above, we get the bound we seek.

Now, using this bound, we see that for fixed x and for $j \geq 2$, $|P_{i,j}^k(x)| \leq |\Sigma_{l=1}^{c} P_{i,l}^{k-1}(x)|\left(\beta/\sqrt{N}\right)\|B^{-k}(x)\| \to 0$ as $k \to \infty$. For the remaining case of $j=1$, we have

$$\begin{aligned}
|P_{i,1}^k(x) - P_{i,1}^{k-1}(x)| &= \left|\sum_{l=1}^{c} P_{i,l}^{k-1}(x)\frac{1}{\sqrt{N}}h_{l,1}(B^{-k}x) - P_{i,1}^{k-1}(x)\right| \\
&= \left|P_{i,1}^{k-1}(x)\left(\frac{1}{\sqrt{N}}h_{1,1}(B^{-k}x) - 1\right) + \sum_{l=2}^{c} P_{i,l}^{k-1}(x)\left(\frac{1}{\sqrt{N}}h_{l,1}(B^{-k}x)\right)\right| \\
&\leq \sum_{l=1}^{c} |P_{i,l}^{k-1}(x)|\frac{\beta}{\sqrt{N}}\|B^{-k}x\| < \frac{\beta}{\sqrt{N}}cK\|B^{-k}x\|.
\end{aligned}$$

We then see that $\{P_{i,1}^k(x)\}$ is Cauchy and thus convergent, again by using the linear algebra result mentioned at the beginning of the proof.

To complete the proof of (1), it remains to show that the limiting functions $P_{i,1}$ are in $L^2(\mathbb{R}^d)$. To do this, we will first use induction to prove that

$$\sum_{j=1}^{c}\int_{B^k(Q)} |P_{i,j}^k(x)|^2 \mathrm{d}x \leq 1.$$

We note that because the $h_{k,j}$ are periodic modulo $\mathbb{Z}^d$, the $P_{i,j}^k$ are periodic modulo $B^k(\mathbb{Z}^d)$, and thus the domain of integration can be replaced by any set that is congruent to $B^k(Q)$ modulo $B^k(\mathbb{Z}^d)$. To select the replacement set, we first choose coset representatives $\omega_1=0, \omega_2, \cdots, \omega_N$ of $\mathbb{Z}^d/B(\mathbb{Z}^d)$. Since

$$\sqcup_{n=1}^{N}(Q+\omega_n) \equiv B(Q) \quad \text{modulo } B(\mathbb{Z}^d),$$

we can take as our domain of integration the set $B^{k-1}(\sqcup_{n=1}^{N}(Q+\omega_n))$ Using this, we have

$$\begin{aligned}
\sum_{j=1}^{c}\int_{B^k(Q)} |P_{i,j}^k(x)|^2 \mathrm{d}x &= \sum_{j=1}^{c}\int_{B^{k-1}\sqcup_{n=1}^{N}(Q+\omega_n)} \left(\sum_{l=1}^{c} P_{i,l}^{k-1}(x)\frac{1}{\sqrt{N}}h_{l,j}(B^{-k}x)\right)\overline{\left(\sum_{m=1}^{c} P_{i,m}^{k-1}(x)\frac{1}{\sqrt{N}}h_{m,j}(B^{-l}x)\right)}\mathrm{d}x \\
&= N^{k-1}\int_{\sqcup_{n=1}^{N}(Q+\omega_n)} \sum_{j,l,m} P_{i,l}^{k-1}(B^{k-1}x)\overline{P_{i,m}^{k-1}(B^{k-1}x)}\frac{1}{\sqrt{N}}h_{l,j}(B^{-1}x)\overline{\frac{1}{\sqrt{N}}h_{m,j}(B^{-1}x)}\mathrm{d}x \\
&= N^{k-1}\int_{Q} \sum_{l,m} P_{i,l}^{k-1}(B^{k-1}x)\overline{P_{i,m}^{k-1}(B^{k-1}x)}\sum_{j=1}^{c}\sum_{n=1}^{N}\frac{1}{\sqrt{N}}h_{l,j}(B^{-1}x - B^{-1}\omega_n)\overline{\frac{1}{\sqrt{N}}h_{m,j}(B^{-1}x - B^{-1}\omega_n)}\mathrm{d}x.
\end{aligned}$$

We note now that modulo $\mathbb{Z}^d$, the set $\{B^{-1}\omega_1, B^{-1}\omega_2, \ldots, B^{-1}\omega_N\}$ parameterize the distinct N elements of $Q=\left[-\frac{1}{2},\frac{1}{2}\right)^d$ that map to (0, 0, …, 0) under the endomorphism $\alpha:\mathbb{T}^d\to\mathbb{T}^d$, where here we are identifying $\mathbb{T}^d$ and $\left[-\frac{1}{2},\frac{1}{2}\right)^d$. Using the orthogonality relations satisfied by the $h_{l,j}$, the last equation simplifies to

$$N^{k-1}\int_Q \sum_{l=1}^{c} P_{i,l}^{k-1}(B^{k-1}x)\overline{P_{i,l}^{k-1}(B^{k-1}x)}\chi_{S_l}(x)\mathrm{d}x \leqslant \sum_{l=1}^{c}\int_{B^{k-1}(Q)} |P_{i,l}^{k-1}(x)|^2\mathrm{d}x \leqslant 1.$$

It follows that

$$\sum_{j=1}^{c}\int_{B^k(Q)} |P_{i,j}^{k}(x)|^2\mathrm{d}x \leqslant 1$$

for all $k\in\mathbb{N}$, and since $\cup_{k=0}^{\infty}B^k(Q)=\mathbb{R}^d$, by Fatou's Lemma we have

$$\sum_{j=1}^{c}\int_{\mathbb{R}^d} |P_{i,j}(x)|^2\mathrm{d}x \leqslant 1.$$

In particular we get $P_{i,j}\in L^2(\mathbb{R}^d)$, which completes the proof of Part (1).

The refinement equation in Part (2) is immediate. It also follows from the proof above that the infinite product P converges uniformly on neighborhoods of 0, and thus that the $\hat{\phi}_i$'s are continuous at 0. Finally, $\hat{\phi}_i(0)=\delta_{i,1}$ is a consequence of the low-pass condition. □

We will now use the results of Proposition 3.1 to build a frame wavelet. We begin by generalizing the computational ideas in Ref. 34. Define two Hilbert spaces $\mathcal{H}$ and $\widetilde{\mathcal{H}}$ by $\mathcal{H}=\oplus_{j=1}^{c}L^2(S_i)$ and $\widetilde{\mathcal{H}}=\oplus_{k=1}^{\tilde{c}}L^2(\widetilde{S}_k)$; and two operators $S_H:\mathcal{H}\to\mathcal{H}$ and $S_G:\widetilde{\mathcal{H}}\to\mathcal{H}$ by

$$[S_H(f)](\omega)=H^t(\omega)f(\alpha(\omega))$$

and

$$[S_G(\widetilde{f})](\omega)=G^t(\omega)\widetilde{f}(\alpha(\omega)),$$

where $f\equiv\oplus f_j\in\mathcal{H}$, H^t and G^t denote the transposes of the matrix functions H and G, respectively, and as α denotes the map on the torus $\mathbb{T}^d$ induced by the action of the transpose B of A acting on $\mathbb{R}^d$. Note that $f_j(\alpha(\omega))$ and $\widetilde{f}_k(\alpha(\omega))$ are necessarily only defined when $\alpha(\omega)$ belongs to S_j for the first case and $\widetilde{S}_k$ for the second. We define these functions to be 0 outside of these domains. We record here the formulas for the adjoints of the two operators:

$$[S_H^*(f)](\omega)=\frac{1}{N}\sum_{l=0}^{N-1}\bar{H}(\omega_l)f(\omega_l),$$

$$[S_G^*(f)](\omega)=\frac{1}{N}\sum_{l=0}^{N-1}\bar{G}(\omega_l)f(\omega_l). \tag{3.1}$$

It will also be convenient to have explicit formulas for the powers of both S_H and S_H^*:

$$[S_H^n(f)](\omega)=\prod_{k=0}^{n-1}H^t(\alpha^k(\omega))f(\alpha^n(\omega)), \tag{3.2}$$

$$[S_H^{*n}(f)](\omega) = \frac{1}{N^n} \sum_{l=0}^{N^n-1} \prod_{k=n-1}^{0} \bar{H}(\alpha^k(\omega_{l,n}))f(\omega_{l,n}),$$

where the $\omega_{l,n}$'s are the N^n points $\zeta \in \mathbb{T}^d$ for which $\omega = \alpha^n(\zeta)$.

We also include here an estimate involving these operators that we will need later,

$$\sum_{i=1}^{c}\sum_{j=1}^{c}\sum_{l=0}^{N^n-1} \left| \left[\prod_{k=0}^{n-1} H^t(\alpha^k(\omega_{l,n})) \right]_{i,j} \right|^2 \leqslant cN^n, \tag{3.3}$$

which we prove using induction. The case $n=1$,

$$\sum_{i=1}^{c}\sum_{j=1}^{c}\sum_{l=0}^{N-1} |h_{j,i}(\omega_l)|^2 \leqslant cN,$$

follows from Eq. (2.4) together with the fact that $\Sigma_{j=1}^{c}\chi_{S_j}(\omega) = m(\omega) \leqslant c$. For the induction step, note that the $\omega_{l,n+1}$ can be labeled in such a way that $\alpha^n(\omega_{sN+q,n+1}) = \omega_q$, so that $\omega_{sN+q,n+1} = (\omega_q)_{s,N}$. Thus, writing $l = sN+q$ and using the Cauchy–Schwarz inequality, we obtain:

$$\begin{aligned}
\sum_{i=1}^{c}\sum_{j=1}^{c}\sum_{l=0}^{N^{n+1}-1} \left| \left[\prod_{k=0}^{n} H^t(\alpha^k(\omega_{l,n+1})) \right]_{i,j} \right|^2 &= \sum_{i=1}^{c}\sum_{j=1}^{c}\sum_{l=0}^{N^{n+1}-1} \left| \sum_{r=1}^{c} \left[\prod_{k=0}^{n-1} H^t(\alpha^k(\omega_{l,n+1})) \right]_{i,r} \left[H^t(\omega_q) \right]_{r,j} \right|^2 \\
&\leqslant \sum_{i=1}^{c}\sum_{j=1}^{c}\sum_{s=0}^{N^n-1}\sum_{q=0}^{N-1} \left(\sum_{r=1}^{c} \left| \prod_{k=0}^{n-1} h_{r,i}(\alpha^k(\omega_{sN+q,n+1})) \right|^2 \right) \\
&\quad \times \left(\sum_{r'=1}^{c} |h_{j,r'}(\omega_q)|^2 \right) \leqslant cN^nN
\end{aligned}$$

Lemma 3.2: The operators S_H and S_G satisfy the following relations:

(1) $S_H^* S_H = I$, *the identity operator on* $\mathcal{H}$;
(2) $S_G^* S_G = \tilde{I}$, *the identity operator on* $\tilde{\mathcal{H}}$;
(3) $S_H^* S_G = 0$ *and* $S_G^* S_H = \tilde{0}$, *the* 0 *operators on the appropriate Hilbert spaces*; and
(4) $S_H S_H^* + S_G S_G^* = I$, *the identity operator on* $\mathcal{H}$.

Proof: These are direct consequences of the orthogonality relations satisfied by generalized filter systems relative to m and $\tilde{m}$. For example, to prove relation (1), in Lemma 3.2 for $f \in \mathcal{H}$, we write

$$S_H^* S_H f(\omega) = \frac{1}{N}\sum_{l=0}^{N-1} \overline{H(\omega_l} S_H f(\omega_l) = \frac{1}{N}\sum_{l=0}^{N-1} \overline{H(\omega_l)} H^t(\omega_l) f(\omega) = f(\omega),$$

where the last equality follows from (2.4). The other parts of the lemma follow similarly from (2.5), (2.6), and (2.7), respectively. □

We note that both S_H and S_G are partial isometries, and that the relations in the lemma are similar to the famous relations defining the Cuntz algebra $\mathcal{O}_2$. We now use these operators to decompose the Hilbert space $\mathcal{H}$ in a convenient way.

Lemma 3.3: Let R_0 denote the range of S_G, and let $R_n = S_H^n(R_0)$. Then $\mathcal{H} = \oplus_{n=0}^{\infty} R_n$. Moreover, if z is any element in $\mathbb{Z}^d$, and $\tilde{f}_{k,z}$ is the element of $\tilde{\mathcal{H}}$ whose kth component is the exponential function $e^{2\pi i\langle\omega|z\rangle}$ and whose other components are 0, then the collection $\{S_H^n(S_G(\tilde{f}_{k,z}))\}$, for k running from 1 to $\tilde{c}$ and each z running through $\mathbb{Z}^d$, forms a Parseval frame for the subspace R_n. Consequently, the collection $\{S_H^n(S_G(\tilde{f}_{k,z}))\}$, $1 \leqslant k \leqslant \tilde{c}$, $z \in \mathbb{Z}^d$, and $0 \leqslant n < \infty$, forms a Parseval frame for $\mathcal{H}$.

Proof: That the subspaces $\{R_n\}$ are orthogonal follows directly from the relations in Lemma 3.2. That the elements $\{S_H^n(S_g(\tilde{f}_{k,z}))\}$ form a Parseval frame for R_n follows from the fact that S_H and S_G are partial isometries, together with the fact that the elements $\{\tilde{f}_{k,z}\}$, as k runs from 1 to $\tilde{c}$ and z runs over $\mathbb{Z}^d$, form a Parseval frame for $\tilde{\mathcal{H}}$.

Write R_∞ for the orthogonal complement in $\mathcal{H}$ of the direct sum $\oplus R_n$. We must show that $R_\infty=\{0\}$. Note that R_∞ is invariant under both S_H and S_H^*, and therefore that the restriction of both these operators to R_∞ are unitary operators.

By way of contradiction, suppose that f_0 is a unit vector in R_∞. For each natural number n, write $f_n=S_H^{*n}(f_0)$. Note that $f_{n+m}=S_H^{*m}(f_n)$. We make two observations about f_n. First of all, for almost all $\omega\in\mathbb{T}^d$, we have

$$\begin{aligned}\|f_n(\omega)\|^2=\|S_H^{*n}(f_0(\omega))\|^2&=\frac{1}{N^{2n}}\sum_{i=1}^{c}\left|\sum_{p=1}^{c}\sum_{l=0}^{N^n-1}\left[\prod_{k=n-1}^{0}\bar{H}(\alpha^k(\omega_{l,n}))\right]_{i,p}[f_0]_p(\omega_{l,n})\right|^2\\&\leqslant\frac{1}{N^n}\sum_{i=1}^{c}\sum_{p=1}^{c}\sum_{l=0}^{N^n-1}\left|\left[\prod_{k=n-1}^{0}\bar{H}(\alpha^k(\omega_{l,n}))\right]_{i,p}\right|^2\times\frac{1}{N^m}\sum_{p'=1}^{c}\sum_{l'=0}^{N^n-1}|[f_0]_{p'}(\omega_{l',n})|^2\\&\leqslant c\times\frac{1}{N^m}\sum_{p'=1}^{c}\sum_{l'=0}^{N^n-1}|[f_0]_{p'}(\omega_{l',n})|^2,\end{aligned}$$

where the last inequality follows from the transpose of Eq. (3.3). By the pointwise ergodic theorem this then implies that

$$\limsup\|f_n(\omega)\|^2\leqslant c\int_0^1\|f_0(\omega)\|^2\mathrm{d}\omega=c.$$

Second, since S_H is unitary on R_∞, we have

$$\begin{aligned}\frac{1}{N^n}\sum_{l=0}^{N^n-1}\|f_0(\omega_{l,n})\|^2&=\frac{1}{N^n}\sum_{l=0}^{N^n-1}\|S_H^nS_H^{*n}(f_0)(\omega_{l,n})\|^2\\&=\frac{1}{N^n}\sum_{l=0}^{N^n-1}\sum_{i=1}^{c}\left|\sum_{p=1}^{c}\left[\prod_{k=0}^{n-1}H^t(\alpha^k(\omega_{l,n}))\right]_{i,p}[S_H^{*n}(f_0)]_p(\omega)\right|^2\\&\leqslant\frac{1}{N^n}\sum_{i=1}^{c}\sum_{l=0}^{N^n-1}\sum_{p=1}^{c}\left|\left[\prod_{k=0}^{n-1}H^t(\alpha^k(\omega_{l,n}))\right]_{i,p}\right|^2\times\sum_{p'=1}^{c}|[f_n]_{p'}(\omega)|^2\leqslant c\|f_n(\omega)\|^2,\end{aligned}$$

implying (again by the pointwise ergodic theorem) that

$$\liminf\|f_n(\omega)\|^2\geqslant\frac{1}{c}.$$

Consequently, by Egorov's Theorem, for any $\epsilon>0$, there exists an M_0 and a set $E\subseteq\mathbb{T}^d$ such that the measure of the complement of E is less than ϵ, and $1/c-\epsilon<\|f_n(\omega)\|^2<c+\epsilon$ for all $\omega\in E$ and all $n\geqslant M_0$. Before we apply this theorem, we will establish some other estimates needed in our choice of ϵ.

First, we pick an integer $K_0\geqslant 3\log_2 c+9$, so that we then have

$$\sqrt{N}^{K_0+1}>32c^{3/2}. \tag{3.4}$$

(This follows since $N=|\det A|\geqslant 2$.)

Next, we choose a $\delta>0$ so that

$$\delta < \frac{1}{4c^{K_0+3}\sqrt{N}^{K_0}} \tag{3.5}$$

and

$$\sqrt{N}(1-\delta)^{K_0+1} - \delta c^{K_0} > \frac{\sqrt{N}}{2}. \tag{3.6}$$

Note the second condition is possible since the function on the left-hand side approaches $\sqrt{N}$ as δ goes to 0.

From the low-pass condition and the requirement of Lipschitz near 0, we know that for any $\delta>0$ there exists a neighborhood U of $0\in\mathbb{T}^d$ such that $|h_{i,j}(\omega)|<\delta$ for all $\omega\in U$ and all pairs $(i,j)\neq(1,1)$, and $|h_{1,1}(\omega)|>\sqrt{N}(1-\delta)$ for all $\omega\in U$. Let U be the neighborhood corresponding to our choice of δ satisfying (1) and (2). By continuity of α, there further exists a neighborhood $V\subseteq U$ such that for every $\omega\in V$ we have $\alpha^k(\omega)\in U$ for all $0\leqslant k\leqslant 2(K_0+1)$. Hence, if $\widetilde{P}(\omega)$ is the matrix given by $\widetilde{P}(\omega)=\Pi_{k=0}^{5}H^t(\alpha^k(\omega))$, then for $(i,j)\neq(1,1)$, $0\leqslant l\leqslant K_0+1$ and $\omega\in V$,

$$|\widetilde{P}_{i,j}(\alpha^l(\omega))| \leqslant \delta(c\sqrt{N})^{K_0}.$$

(There are c^{K_0} summands, each having K_0 factors, and in each, one factor is bounded by δ, and the other factors [by (2.4)] are bounded by $\sqrt{N}$.) For $(i,j)=(1,1)$, we have

$$(\sqrt{N}(1-\delta))^{K_0+1} - \delta(c\sqrt{N})^{K_0} \leqslant |\widetilde{P}_{1,1}(\alpha^l(\omega))| \leqslant \sqrt{N}^{K_0+1} + \delta(c\sqrt{N})^{K_0}.$$

(Again, there are c^{K_0} summands, each having K_0+1 factors. One of these summands is bounded below by $(\sqrt{N}(1-\delta))^{K_0+1}$ and above by $\sqrt{N}^{K_0+1}$, and the other $(c^{K_0}-1)$ summands are bounded by $\delta\sqrt{N}^{K_0}$.)

Now choose an ϵ smaller than the measure of V, and also smaller than $1/(4c)$, so that we are assured that the corresponding set E will satisfy $\lambda(E\cap V)>0$. In fact, we may even assume that the set of $\omega\in V$ for which $\alpha^k(\omega)\in E\cap U$ for all $0\leqslant k\leqslant 2(K_0+1)$ has positive measure.

Fix an $\omega\in E\cap V$ for which $\alpha^k(\omega)\in E\cap U$ for $0\leqslant k\leqslant 2(K_0+1)$. If M_0 is the natural number corresponding to this choice of ϵ as mentioned above, and $n\geqslant M_0$, we have the following estimates on the components of $f_n(\omega)$. First, for $i\neq 1$ and $0\leqslant l\leqslant K_0+1$,

$$|f_{n_i}(\alpha^l(\omega))| = |[S_H^{K_0+1}(f_{n+K_0+1})]_i(\alpha^l(\omega))| = \left|\sum_{j=1}^{c}\widetilde{P}_{i,j}(\alpha^l(\omega))[f_{n+K_0+1}]_j(\alpha^{l+K_0+1}(\omega))\right| \leqslant \sum_{j=1}^{c}|\widetilde{P}_{i,j}(\alpha^l(\omega))|$$
$$\times |[f_{n+K_0+1}]_j(\alpha^{l+K_0+1}(\omega))| \leqslant c\,\delta(c\sqrt{N})^{K_0}\sqrt{c+\epsilon} \leqslant 2\,\delta c^{K_0+2}\sqrt{N}^{K_0},$$

so that by condition (3.5) on δ,

$$\sum_{i=2}^{c}|[f_n]_i(\alpha^l(\omega))|^2 \leqslant 4c\,\delta^2 c^{2(K_0+2)}N^{K_0} < \frac{1}{2c}.$$

Therefore, because $\omega\in E$, for all $n\geqslant N_0$ we must have, for $0\leqslant l\leqslant K_0+1$,

$$|[f_n]_1(\alpha^l(\omega))|^2 > \frac{1}{2c} - \epsilon > \frac{1}{4c}.$$

On the other hand,

$$[f_n]_1(\omega) = \sum_{j=1}^{c} \widetilde{P}_{1,j}(\omega)[f_{n+K_0+1}]_j(\alpha^{K_0+1}(\omega)) = \widetilde{P}_{1,1}(\omega)[f_{n+K_0+1}]_1(\alpha^{K_0+1}(\omega)) + \sum_{j=2}^{c} \widetilde{P}_{1,j}(\omega) \times [f_{n+K_0+1}]_j(\alpha^{K_0+1}(\omega)),$$

implying that

$$|[f_{n+K_0+1}]_1(\alpha^{K_0+1}(\omega))| \leqslant \frac{|[f_n]_1(\omega)| + \sum_{j=2}^{c} |\widetilde{P}_{1,j}(\omega)| \times |[f_{n+K_0+1}]_j(\alpha^{K_0+1}(\omega))|}{|\widetilde{P}_{1,1}(\omega)|}$$
$$\leqslant \frac{\sqrt{c+\epsilon} + c\delta(c\sqrt{N})^{K_0}\sqrt{c+\epsilon}}{(\sqrt{N}(1-\delta))^{K_0+1} - \delta(c\sqrt{N})^{K_0}} \leqslant \frac{4\sqrt{c+\epsilon}}{\sqrt{N}^{K_0+1}} \leqslant \frac{8\sqrt{c}}{\sqrt{N}^{K_0+1}} \leqslant \frac{1}{4c},$$

where in the third step we use conditions (3.5) and (3.6) to simplify the numerator and denominator, respectively, and in the final step, we use condition (3.4). Hence, the point $\alpha^{K_0+1}(\omega)$ satisfies

$$\frac{1}{4c} \leqslant |[f_{n+K_0+1}]_1(\alpha^{K_0+1}(\omega))|^2 < \frac{1}{4c},$$

which is a contradiction. □

We now state our main result.

Theorem 3.4: *Let ϕ_i be defined from the infinite product of the low-pass filter system H as in Proposition 3.1, and let $G=[g_{k,j}]$ be the corresponding high-pass filter system. Then, if we define a function $\psi_k \in L^2(\mathbb{R}^d)$, for $1 \leqslant k \leqslant \widetilde{c}$, by*

$$\widehat{\psi_k}(x) = \frac{1}{\sqrt{N}} \sum_{j=1}^{c} g_{k,j}(B^{-1}(x))\widehat{\phi_j}(B^{-1}(x)),$$

the collection $\{\psi_k\}$ is a Parseval frame wavelet for $L^2(\mathbb{R}^d)$ relative to dilation by A and translation by lattice points $z \in \mathbb{Z}^d$. Further, if V_0 is the closed linear span of the translates of the ϕ_i's by lattice elements $z \in \mathbb{Z}^d$, then $\{V_j\} \equiv \{\delta^j(V_0)\}_{j\in\mathbb{Z}}$ is a generalized multiresolution analysis for $L^2(\mathbb{R}^d)$.

Proof: We prove first that the $\{\psi_k\}$ form a frame wavelet. For convenience in what follows, we introduce the following notation. For each $1 \leqslant k \leqslant \widetilde{c}$ and each $z \in \mathbb{Z}^d$, write $\gamma^{k,z}$ for the element $S_G(\widetilde{f}_{k,z})$ of $R_0 \subseteq \mathcal{H}$, where as in the previous lemma, $\widetilde{f}_{k,z}$ is the element of $\widetilde{\mathcal{H}}$ whose kth component is the exponential function $e^{2\pi i\langle\omega|z\rangle}$ and whose other components are 0. Note that $\gamma^{k,z} = \oplus_{j=1}^{c} \gamma_j^{k,z}$, where

$$\gamma_j^{k,z}(\omega) = g_{k,j}(\omega)e^{2\pi i\langle\alpha(\omega)|z\rangle}.$$

It then follows from Lemma 3.3 that for each $F \in \mathcal{H}$ we have

$$\|F\|^2 = \sum_{n=0}^{\infty} \sum_{k=1}^{\widetilde{c}} \sum_{z\in\mathbb{Z}^d} |\langle F|S_H^n(\gamma^{k,z})\rangle|^2.$$

For each integer n, each $1 \leqslant k \leqslant \widetilde{c}$, and each $z \in \mathbb{Z}^d$, define the function $\psi_{n,k,z}$ by

$$\psi_{n,k,z}(t) = \sqrt{N^n}\psi_k(A^n(t) + z),$$

and note that the Fourier transform of $\psi_{n,k,z}$ is given by

$$\widehat{\psi_{n,k,z}}(x) = N^{(-n-1)/2} e^{2\pi i \langle B^{-n}(x)|z\rangle} \sum_{j=1}^{c} g_{k,j}(B^{-n-1}(x))\, \widehat{\phi_j}(B^{-n-1}(x)).$$

We wish to prove that the collection $\{\psi_{n,k,z}\}$ is a Parseval frame for $L^2(\mathbb{R}^d)$.

Now, let f be an element of $L^2(\mathbb{R}^d)$ whose Fourier transform $\hat{f}$ has compact support. For a fixed integer $J \geqslant 0$, we have

$$\begin{aligned}
&\sum_{n=-\infty}^{J} \sum_{k=1}^{\tilde{c}} \sum_{z\in\mathbb{Z}^d} |\langle f|\psi_{n,k,z}\rangle|^2 \\
&\quad = \sum_{n=-\infty}^{J} \sum_{k=1}^{\tilde{c}} \sum_{z\in\mathbb{Z}^d} |\langle \hat{f}|\widehat{\psi_{n,k,z}}\rangle|^2 \\
&\quad = \sum_{n=-\infty}^{J} \sum_{k=1}^{\tilde{c}} \sum_{z\in\mathbb{Z}^d} \left| \int_{\mathbb{R}^d} \hat{f}(x) N^{\frac{-n-1}{2}} \overline{\sum_{j=1}^{c} e^{2\pi i \langle B^{-n}(x)|z\rangle} g_{k,j}(B^{-n-1}(x))\, \widehat{\phi_j}(B^{-n-1}(x))}\, \mathrm{d}x \right|^2 \\
&\quad = \sum_{n=-\infty}^{J} \sum_{k=1}^{\tilde{c}} \sum_{z\in\mathbb{Z}^d} N^{-n+2J+1} \left| \int_{\mathbb{R}^d} \hat{f}(B^{J+1}(x)) \overline{e^{2\pi i \langle B^{-n+J+1}(x)|z\rangle}} \times \overline{\sum_{j=1}^{c} g_{k,j}(B^{-n+J}(x))\, \widehat{\phi_j}(B^{-n+J}(x))}\, \mathrm{d}x \right|^2 \\
&\quad = \sum_{n=0}^{\infty} \sum_{k=1}^{\tilde{c}} \sum_{z\in\mathbb{Z}^d} N^{n+1+J} \left| \int_{\mathbb{R}^d} \hat{f}(B^{J+1}(x)) \overline{e^{2\pi i \langle B^{n+1}(x)|z\rangle} \sum_{j=1}^{c} g_{k,j}(B^{n}(x))\, \widehat{\phi_j}(B^{n}(x))}\, dx \right|^2 \\
&\quad = \sum_{n=0}^{\infty} \sum_{k=1}^{\tilde{c}} \sum_{z\in\mathbb{Z}^d} N^{1+J} \left| \int_{\mathbb{R}^d} \hat{f}(B^{J+1}(x) e^{2\pi i \langle B^{n+1}(x)|z\rangle} \overline{\sum_{j=1}^{c} g_{k,j}(B^{n}(x))} \times \overline{\left[\prod_{p=n-1}^{0} H(B^p(x))\Phi(x)\right]_j} dx \right|^2 \\
&\quad = \sum_{n=0}^{\infty} \sum_{k=1}^{\tilde{c}} \sum_{z\in\mathbb{Z}^d} N^{1+J} \left| \int_{\mathbb{T}^d} \sum_{j=1}^{c} \sum_{\zeta\in\mathbb{Z}^d} \hat{f}(B^{J+1}(x+\zeta))\, \overline{\widehat{\phi_j}(x+\zeta)} \overline{\prod_{p=0}^{n-1} H^t(B^p(x))}\, \overline{\gamma^{k,z}}(B^n(x)) dx \right|^2 \\
&\quad = \sum_{n=0}^{\infty} \sum_{k=1}^{\tilde{c}} \sum_{z\in\mathbb{Z}^d} |\langle F^J|S_H^n(\gamma^{k,z})\rangle_{\mathcal{H}}|^2 = \|F^J\|_{\mathcal{H}}^2,
\end{aligned}$$

where $F^J = \oplus F^J_j$ is the element of $\mathcal{H}$ given by

$$F^J_j(\omega) = \sqrt{N}^{1+J} \sum_{\zeta\in\mathbb{Z}^d} \hat{f}(B^{1+J}(x+\zeta))\, \overline{\widehat{\phi_j}}(x+\zeta).$$

Hence,

$$\begin{aligned}
\sum_{n=-\infty}^{J} \sum_{k=1}^{\tilde{c}} \sum_{z\in\mathbb{Z}^d} |\langle f|\psi_{n,k,z}\rangle|^2 &= \sum_{j=1}^{c} \int_{\mathbb{T}^d} |F^J_j(\omega)|^2 \mathrm{d}\omega \\
&= \sum_{j=1}^{c} \int_{B^{1+J}(\mathbb{T}^d)} \left| \sum_{\zeta\in\mathbb{Z}^d} \hat{f}(x + B^{1+J}(\zeta))\, \overline{\widehat{\phi_j}}(B^{-1-J}(x)+\zeta) \right|^2 \mathrm{d}x \\
&= \sum_{j=1}^{c} \int_{\mathbb{R}^d} \chi_{B^{1+J}(\mathbb{T}^d)}(x) \left| \sum_{\zeta\in\mathbb{Z}^d} \hat{f}(x + B^{1+J}(\zeta))\, \overline{\phi_j}(B^{-1-J}(x)+\zeta) \right|^2 \mathrm{d}x.
\end{aligned}$$

Now, because $\hat{f}$ has compact support, and the matrix B is expansive, there exists a J' such that the support of $\hat{f}$ is contained in $B^{1+J'}(Q)$. There must also exist, by the compactness of $B^{1+J'}(\overline{Q})$, a J_0

such that $B^{1+J}(Q)$ contains $B^{1+J'}(Q)$ for all $J \geqslant J_0$. Now, for $J \geqslant J_0$, the product $\chi_{B^{1+J}(Q)}(x)\hat{f}(x+B^{1+J}(\zeta))$ is nonzero only if $x=B^{1+J}(y)$ for some $y \in Q$, and also $x+B^{1+J}(\zeta) = B^{1+J}(y+\zeta) \in B^{1+J}(Q)$. Consequently, for any $J>J_0$, and any $\zeta \neq 0$, we must have $\chi_{B^{1+J}(Q)}(x)\hat{f}(x+B^{1+J}(\zeta))=0$ for all $x \neq 0$. Hence, for $J>J_0$ we have

$$\sum_{n=-\infty}^{J} \sum_{k=1}^{\tilde{c}} \sum_{z \in \mathbb{Z}^d} |\langle f|\psi_{n,k,z}\rangle|^2 = \sum_{j=1}^{c} \int_{\mathbb{R}^d} |\hat{f}(x)|^2 |\widehat{\phi_j}(B^{-1-J}(x))|^2 \mathrm{d}x,$$

so that, by the Dominated Convergence Theorem, we obtain

$$\sum_{n=-\infty}^{\infty} \sum_{k=1}^{\tilde{c}} \sum_{z \in \mathbb{Z}^d} |\langle f|\psi_{n,k,z}\rangle|^2 = \int_{\mathbb{R}^d} |\hat{f}(x)|^2 \sum_{j=1}^{c} |\widehat{\phi_j}(0)|^2 \mathrm{d}x = \|f\|^2.$$

This demonstrates the Parseval frame property for elements f whose Fourier transforms have compact support. For general $f \in L^2(\mathbb{R}^d)$, the Parseval equality follows from the density of these functions.

It remains to show that $\{V_j\}$ form a GMRA. Properties (2) and (4′) of Definition 2.1 are direct consequences of the definition of the V_j, and property (1) follows immediately from Proposition 3.1 (2). The density required in Property (3) is a consequence of the fact that the $\{\psi_{n,k,z}\}$ form a Parseval frame for $L^2(\mathbb{R}^d)$.

To finish the proof, we now show that $\cap V_j=\{0\}$. Write $\{\phi_i'\}$ for a sequence of elements whose translates form a Parseval frame for V_0 (such a sequence must exist since V_0 is closed under translation), and P_j for the orthogonal projection operator onto the subspace V_j. To prove that $\cap V_j=\{0\}$, it will suffice to show that $\lim_{j\to\infty}\|P_{-j}(f)\|=0$ for each $f \in L^2(\mathbb{R}^d)$. By a standard approximation argument, it will suffice to show this holds on a dense subset of $L^2(\mathbb{R}^d)$. Thus, let f be a Schwartz function for which $\hat{f}$ vanishes in some neighborhood N_f of 0, and write C_f for the (finite) number $\Sigma_k|f*f^*(k)|$. Such f's are dense in $L^2(\mathbb{R}^d)$. The Poisson summation formula holds for such an f, and we will use it in the following form:

$$\frac{1}{N^j}\sum_l |\hat{f}(B^{-j}(\xi+l))|^2 = \sum_k f*f^*(A^j(k))e^{-2\pi i\langle k|\xi\rangle}.$$

Now, for each $\xi \in \mathbb{T}^d$, let $l_j(\xi)$ be the largest number for which $B^{-j}(\xi+l) \in N_f$ for all $\|l\|<l_j(\xi)$. Because A (and thus $B=A^t$) is expansive, we must have that $l_j(\xi)$ tends to infinity for almost every ξ. Finally, we use the fact that the function

$$m(\omega) = \sum_i \chi_{S_i}(\omega) = \sum_i \sum_l |\widehat{\phi_i'}(\omega+l)|^2$$

is integrable on the cube. Hence, we have

$$\begin{aligned}
\|P_{-j}(f)\|^2 &= N^j \sum_i \sum_z \left| \int_{\mathbb{R}^d} \widehat{\phi_i'}(B^j(\xi))\bar{\hat{f}}(\xi)e^{-2\pi i\langle B^j(\xi)|z\rangle}\mathrm{d}\xi \right|^2 \\
&= \frac{1}{N^j}\sum_i \sum_z \left| \int_{\mathbb{R}^d} \widehat{\phi_i'}(\xi)\bar{\hat{f}}(B^{-j}(\xi))e^{-2\pi i\langle z|\xi\rangle}\mathrm{d}\xi \right|^2 = \frac{1}{N^j}\sum_i \int_{\mathbb{T}^d} \left| \sum_l \widehat{\phi_i'}(\xi+l)\bar{\hat{f}}(B^{-j}(\xi+l)) \right|^2 \mathrm{d}\xi \\
&= \frac{1}{N^j}\sum_i \int_{\mathbb{T}^d} \left| \sum_{\|l\|\geqslant l_j(\xi)} \widehat{\phi_i'}(\xi+l)\bar{\hat{f}}(B^{-j}(\xi+l)) \right|^2 \mathrm{d}\xi \leqslant \frac{1}{N^j}\sum_i \int_{\mathbb{T}^d} \sum_{|l|\geqslant l_j(\xi)} |\widehat{\phi_i'}(\xi+l)|^2 \\
&\quad \times \sum_{|l|\geqslant l_j(\xi)} |\hat{f}(B^{-j}(\xi+l))|^2 \mathrm{d}\xi = \int_{\mathbb{T}^d} \left[\sum_i \sum_{|l|\geqslant l_j(\xi)} |\widehat{\phi_i'}(\xi+l)|^2 \right] \left[\frac{1}{N^j}\sum_l |\hat{f}(B^{-j}(\xi+l))|^2 \right] \mathrm{d}\xi
\end{aligned}$$

$$= \int_{\mathbb{T}^d} \left[\sum_i \sum_{|l| \geqslant l_j(\xi)} |\widehat{\phi_i'}(\xi + l)|^2 \right] \left[\sum_k f * f^*(A^j(k)) e^{-2\pi i \langle k|\xi \rangle} \right] \mathrm{d}\xi \leqslant \int_{\mathbb{T}^d} \left[\sum_i \sum_{|l| \geqslant l_j(\xi)} |\widehat{\phi_i'}(\xi + l)|^2 \right]$$

$$\times \left[\times \sum_k |f * f^*(A^j(k))| \right] \mathrm{d}\xi \leqslant C_f \int_{\mathbb{T}^d} \sum_i \sum_{|l| \geqslant l_j(\xi)} |\widehat{\phi_i'}(\xi + l)|^2 \mathrm{d}\xi,$$

which approaches 0 as j goes to infinity by the dominated convergence theorem, the integrand here being bounded by m. □

Theorem 3.4 shows that the functions ψ_k are in the set V_1, so that the Parseval frame wavelet $\{\psi_k\}$ that we have constructed is *obtained from* the GMRA $\{V_j\}$, in the sense defined by Zalik.[38] It is an open question whether the wavelet is *associated with* the GMRA $\{V_j\}$ in the sense that V_j is the closure of the span of $\{\delta'(\tau_z(\psi_k))\}_{l<j}$ (see e.g., Ref. 39). Moreover, the multiplicity function of the GMRA produced by the theorem may not coincide with the multiplicity function used in the construction of the filters, as the first of the examples shows.

Example 3.5: Let $d=1$, $A=2$, and the multiplicity functions m and $\tilde{m}$ both be identically 1, so that we start in the classical setting. For our filters, we take

$$h = \sqrt{2}[\chi_{-1/8,1/8)} + \chi_{\pm[1/4,3/8)}],$$

and

$$g = \sqrt{2}[\chi_{\pm 1/8,1/4)} + \chi_{\pm[3/8,1/2)}].$$

Note that h and g satisfy the definitions of generalized low- and high-pass filters, and are Lipschitz in a neighborhood of 0. The infinite product $P = \prod_{j=1}^{\infty} \frac{1}{\sqrt{2}} h(x/2^j)$ equals $\chi_{[-1/4,1/4)}$. The integer translates of the function ϕ whose Fourier transform is this infinite product P, are not orthonormal, and do not determine the core subspace of any classical multiresolution analysis. On the other hand, as predicted by Theorem 3.4, the standard construction in this case does produce a generalized multiresolution analysis $\{V_j\}$, with multiplicity function $m = \chi_{[-1/4,1/4)}$. As guaranteed by Theorem 3.4, the construction also produces a Parseval frame wavelet ψ, here given by

$$\hat{\psi}(x) = \chi_{[-1/2,-1/4)} + \chi_{[1/4,1/2)}.$$

In this case the function ϕ is easily constructed out of negative dilates of ψ, so the wavelet is necessarily associated with as well as obtained by the GMRA.

We end this section with an another example for dilation by 2 in $L^2(\mathbb{R})$. This one begins with filters for the multiplicity function of the well-known Journé wavelet, whose Fourier transform is the characteristic function of the set

$$\left[-\frac{16}{7}, -2 \right) \cup \left[-\frac{1}{2}, -\frac{2}{7} \right) \cup \left[\frac{2}{7}, \frac{1}{2} \right] \cup \left[2, \frac{16}{7} \right).$$

We use Theorem 3.4 to build a Parseval wavelet with a C^∞ Fourier transform that is associated with the Journé multiplicity function.

Example 3.6: The Journé multiplicity function m takes on the values 0, 1, and 2, with $S_1 = [-\frac{1}{2}, -\frac{3}{7}) \cup [-\frac{2}{7}, \frac{2}{7}) \cup [\frac{3}{7}, \frac{1}{2})$ and $S_2 = [-\frac{1}{7}, \frac{1}{7})$. The complementary multiplicity function $\tilde{m}(x) \equiv 1$, since the Journé wavelet is a single orthonormal wavelet.

To build the filters, we let p_0 be a C^∞ classical (MRA) low-pass filter for dilation by 2 [i.e., that satisfies the classical filter equation (1.1)], that in addition satisfies $p_0(x) = 0$ for $x \in \pm(\frac{1}{7} - \epsilon, \frac{3}{14} + \epsilon) \cup (\frac{3}{7} - \epsilon, \frac{4}{7} + \epsilon)$. Note that by (1.1), we then have $p_0(x) = \sqrt{2}$ for $x \in \pm(\frac{2}{7} - \epsilon, \frac{5}{14} + \epsilon) \cup (-\frac{1}{14} - \epsilon, \frac{1}{14} + \epsilon)$. Let p_1 be the standard choice of C^∞ high-pass filter associated to p_0, given by $p_1(x) = e^{2\pi i x} \overline{p_0(x + \frac{1}{2})}$. Then it is easily checked that the following functions satisfy (2.4)–(2.6), and thus are generalized low- and high-pass filters by our definitions in Sec. II.

$$h_{1,1}(x)=\begin{cases}p_0(x), & x\in\left[-\frac{2}{7},\frac{2}{7}\right)\\ 0 & \text{otherwise},\end{cases}$$

$$h_{1,2}(x)=\begin{cases}p_0\left(x+\frac{1}{2}\right), & x\in\left[-\frac{1}{7},\frac{1}{7}\right)\\ 0 & \text{otherwise},\end{cases}$$

$$h_{2,1}(x)=\begin{cases}\sqrt{2}, & x\in\pm\left[\frac{3}{7},\frac{1}{2}\right)\\ 0 & \text{otherwise},\end{cases}$$

$$h_{2,2}(x)=0,$$

$$g_1(x)=\begin{cases}p_1(x), & x\in\left[-\frac{2}{7},\frac{2}{7}\right)\\ 0 & \text{otherwise},\end{cases}$$

$$g_2(x)=\begin{cases}p_1\left(x+\frac{1}{2}\right), & x\in\left[\frac{-1}{7},\frac{1}{7}\right)\\ 0 & \text{otherwise}.\end{cases}$$

Now we check that the resulting wavelet does in fact have a C^∞ transform. We first fix an x and show that $\hat{\phi}_1$ and $\hat{\phi}_2$ are C^∞ in a neighborhood of x. Recall that these functions form the first column of the infinite product matrix

$$\prod_{j=1}^{\infty}\frac{1}{\sqrt{2}}\begin{pmatrix}h_{1,1}\left(\frac{x}{2^j}\right) & h_{1,2}\left(\frac{x}{2^j}\right)\\ h_{2,1}\left(\frac{x}{2^j}\right) & 0\end{pmatrix}.$$

Because $h_{2,1}$ is 0 on $\left(-\frac{3}{7},\frac{3}{7}\right)$, all but a finite number of the matrix factors are upper triangular. Thus, each of the entries in the first column of the infinite product contains only a finite number of terms. Since $h_{1,1}=\sqrt{2}$ in a neighborhood of 0, each of the terms has only a finite number of factors not equal to 1. Thus, it will suffice to show that each of the factors in each of the terms is C^∞.

By construction, we have that the $h_{i,j}$ are all C^∞ everywhere except for $h_{1,1}$ at $n\pm\frac{2}{7}$, $h_{1,2}$ at $n\pm\frac{1}{7}$, and $h_{2,1}$ at $n\pm\frac{3}{7}$ for $n\in\mathbb{Z}$. We will show that whenever one of these discontinuities occurs as a factor in the infinite product, it is cancelled by a following factor that is 0 in a neighborhood of the point of discontinuity. Note that the product of two adjacent factors in the infinite matrix product has the form

$$\begin{pmatrix}h_{1,1}(y)h_{1,1}\left(\frac{y}{2}\right)+h_{1,2}(y)h_{2,1}\left(\frac{y}{2}\right) & h_{1,1}(y)h_{1,2}\left(\frac{y}{2}\right)\\ h_{2,1}(y)h_{1,1}\left(\frac{y}{2}\right) & h_{2,1}(y)h_{1,2}\left(\frac{y}{2}\right)\end{pmatrix}.$$

Thus any term in the infinite product that contains a factor of $h_{2,1}\left(n\pm\frac{3}{7}\right)$ must also contain a factor of one of the forms $h_{1,1}\left(n\pm\frac{2}{7}\right)$, $h_{1,1}\left(n\pm\frac{3}{14}\right)$, $h_{1,2}\left(n\pm\frac{3}{14}\right)$, and $h_{1,2}\left(n\pm\frac{2}{7}\right)$. The first three possibilities are 0 in a neighborhood of the point in question, so if we have a discontinuous factor of $h_{2,1}$, it is

either cancelled out by a 0 factor, or we also have a factor of $h_{1,1}\left(n\pm\frac{2}{7}\right)$ with a smaller n. Similarly, any term in the infinite product that contains a factor of $h_{1,1}\left(n\pm\frac{2}{7}\right)$ must also contain a factor of one of the forms $h_{1,1}\left(n\pm\frac{5}{14}\right)$, $h_{1,1}\left(n\pm\frac{1}{7}\right)$, $h_{1,2}\left(n\pm\frac{5}{14}\right)$, or $h_{1,2}\left(n\pm\frac{1}{7}\right)$. The first three of these possibilities are 0 in a neighborhood of the points in question, so any discontinuous factor of $h_{1,1}$ is either cancelled out by a 0 factor, or is followed by a factor of $h_{1,2}\left(n\pm\frac{1}{7}\right)$ with an equal or smaller n. Finally, any term in the infinite product that contains a factor of $h_{1,2}\left(n\pm\frac{1}{7}\right)$ must also contain a factor of either the form $h_{2,1}\left(n\pm\frac{1}{14}\right)$ or the form $h_{2,1}\left(n\pm\frac{3}{7}\right)$. The first of these possibilities is 0 in again 0 in a neighborhood of the point in question; the second possibility throws us back into the first type of discontinuity we considered above, but with a smaller n. We can repeat the above sequence of arguments if necessary, noting that each succeeding factor is evaluated at a point half the distance from the origin as its predecessor, so that the chain above must eventually end with a factor of 0.

This argument shows that $\hat{\phi}_1$ and $\hat{\phi}_2$ are C^∞. To see that $\hat{\psi}$ is C^∞ as well, it suffices to note that g_1 and g_2 are.

Remark 3.7: With some more work it is possible to slightly improve the previous arguments and to show that in fact the Fourier transform vanishes rapidly at infinity.

IV. A GENERALIZED LOOP GROUPOID ACTION ON THE BUNDLE OF GENERALIZED FILTER SYSTEMS

Let $\{h_{i,j}\}_{1\leqslant i,j\leqslant c}$ and $\{g_{k,j}\}_{1\leqslant k\leqslant\tilde{c},1\leqslant j\leqslant c}$ be generalized low-pass and high-pass filter functions defined as in Sec. II. Since $\oplus_{i=1}^{c}L^2(S_i)\cong L^2(\sqcup_{i=1}^{c}S_i)$, we can suppress the second index of the filter functions and view generalized filter functions as a vector ($c+\tilde{c}$-tuple) of functions:

$$(h_1,h_2,\ldots,h_c,g_1,g_2,\ldots,g_{\tilde{c}})\in\left[L^2\left(\bigsqcup_{i=1}^{c}S_i\right)\right]^{c+\tilde{c}}.$$

Further, we note that for any fixed $\omega\in\mathbb{T}^d$, all the information in the output of the vector of functions $(h_1,h_2,\ldots,h_c,g_1,g_2,\ldots,g_{\tilde{c}})$ is actually in $\mathbb{C}^{m(\alpha(\omega))+\tilde{m}(\alpha(\omega))}$, where as in Sec. II, α is the endomorphism of $\mathbb{T}^d$ defined by the matrix $B=A^t$, since by the orthogonality relations, $h_i(\omega)=0$ if $i>m(\alpha(\omega))$ and $g_k(x)=0$ if $k>\tilde{m}(\alpha(\omega))$.

We want to generalize the discussion given by Bratteli and Jorgensen in Ref. 40, and construct a loop groupoid which acts on the class of filter systems with bounded multiplicity functions corresponding to a fixed dilation matrix A acting on $\mathbb{R}^n$. We will also impose the condition the filter systems satisfy some "initial conditions" that are in some sense canonical.

We first remind readers of the notion of a vector bundle over a topological space X; more details can be found in Ref. 41.

Definition 4.1: Let X be a topological space. A (finite dimensional) vector bundle over the space X, denoted by (E,p,X), is a topological space E, together with a continuous open surjection $p:E\to X$, and operations and norms making each fiber $E_x=p^{-1}(X)$ into a (finite dimensional) vector space, which in addition satisfies the following conditions:

(i) $y\mapsto\|y\|$ is continuous from E to $\mathbb{R}$.
(ii) The operation + is continuous as a function from $\{(y,z)\in E\times E:p(y)=p(z)\}$ to E.
(iii) For each $\lambda\in\mathbb{C}$, the map $y\mapsto\lambda\cdot y$ is continuous from E to E.
(iv) If $x\in X$ and $\{y_i\}$ is any net of elements of E such that $\|y_i\|\to 0$ and $p(y_i)\to x$ in X, then $y_i\to\vec{0}\in E_x$ in E.

A Borel map $s:X\to E$ is called a Borel cross section if $p\circ s(x)=x,\ \forall x\in X$.

We review the notion of essentially bounded multiplicity functions m associated to a dilation matrix A that can give rise to GMRAs, as described in Refs. 10 and 36. We first recall that m must satisfy the consistency inequality

$$m(\omega) \leqslant \sum_{l=0}^{N-1} m(\omega_l), \tag{4.1}$$

where we recall from Sec. II that $\{\omega_l: 0 \leqslant l \leqslant N-1\}$ is the set of N distinct preimages of $\omega \in \mathbb{T}^d$ under the endomorphism α given by $\alpha(\omega)=B(\omega)$, for $\omega \in \mathbb{T}^d=\mathbb{R}^d/\mathbb{Z}^d$ and $B=A^t$. This inequality leads to the consistency equality Equation (2.1) discussed in Sec. II. Moreover, we can enumerate the ω_l as follows. Enumerate a set of coset representatives $\{\xi_0=\vec{0}, \xi_1, \ldots, \xi_{N-1}\}$ for $B^{-1}(\mathbb{Z}^d)/\mathbb{Z}^d$ including $\vec{0} \in B^{-1}(\mathbb{Z}^d)$. For each $l, 0 \leqslant l \leqslant N-1\}$ let ζ_l be the image of ξ_l under the natural projection from $\mathbb{R}^d$ onto $\mathbb{T}^d=\mathbb{R}^d/\mathbb{Z}^d$. Note that the ζ_l are distinct elements of $\mathbb{T}^d$ and that $\alpha(\zeta_l)=\vec{0}$, $0 \leqslant l \leqslant N-1$. Find a Borel cross section $\sigma: \mathbb{T}^n=\mathbb{R}^d/\mathbb{Z}^d \to \mathbb{T}^n=\mathbb{R}^d/B^{-1}(\mathbb{Z}^d) \cong [\mathbb{R}^d/\mathbb{Z}^d]/[B^{-1}(\mathbb{Z}^d)/\mathbb{Z}^d]$, with $\sigma(\vec{0})=\vec{0}$. This Borel map satisfies $\alpha \circ \sigma(\omega)=\omega$ for all $\omega \in \mathbb{T}^d$. Then define

$$\omega_l = \sigma(\omega)\zeta_l, \quad 0 \leqslant l \leqslant N-1;$$

one easily verifies that the $\{\omega_l: 0 \leqslant l \leqslant N-1\}$ are the N distinct preimages of $\omega \in \mathbb{T}^d$ under α.

Let $\Delta=\cup_{k=0}^{\infty} B^k(S_1+\mathbb{Z}^d)$. Recall from Refs. 10 and 42 that in order for m to be the multiplicity function for a GMRA, Δ must satisfy

$$\sum_{n \in \mathbb{Z}^d} \chi_\Delta(\omega+n) \geqslant m(\omega). \tag{4.2}$$

Finally, Δ should satisfy

$$\cup_{p \in \mathbb{Z}} B^p(\Delta) = \mathbb{R}^n. \tag{4.3}$$

If conditions (4.1)–(4.3) are satisfied we say that m is an (essentially) bounded multiplicity function with respect to the dilation matrix A. Given such an m, we construct the conjugate multiplicity function $\tilde{m}$ by defining

$$\tilde{m}(\omega) = \sum_{l=0}^{N-1} m(\omega_l) - m(\omega), \omega \in \mathbb{T}^d; \tag{4.4}$$

by definition, m and $\tilde{m}$ will satisfy Eq. (2.1).

Given an (essentially) bounded multiplicity function m on $\mathbb{T}^d$, let $c=\operatorname{ess\,sup} m$, and $\tilde{c}=\operatorname{ess\,sup} \tilde{m}$. We recall from Baggett *et al.* that to such an m we can explicitly construct a canonical system of low-pass filters, or "generalized conjugate mirror filters" $\{h_{i,j}^{\mathcal{C}}: 1 \leqslant i,j \leqslant c\}$, by using the method of Theorem 3.6 of Ref. 36. Given this system $\{h_{i,j}^{\mathcal{C}}: 1 \leqslant i,j \leqslant c\}$, Theorem 2.5 item (1) of Ref. 36 gives us a way of explicitly constructing an associated system of high-pass filters, or "complementary conjugate mirror filters," $\{g_{k,j}^{\mathcal{C}}: 1 \leqslant k \leqslant \tilde{c}, 1 \leqslant j \leqslant c\}$. We call this family of filters $\{h_{i,j}^{\mathcal{C}}: 1 \leqslant i,j \leqslant c\} \cup \{g_{k,j}^{\mathcal{C}}: 1 \leqslant k \leqslant \tilde{c}, 1 \leqslant j \leqslant c\}$ the **canonical filter system** associated to the multiplicity function m.

Now let $T_j=\{\omega \in \mathbb{T}^d: m(\alpha(\omega))+\tilde{m}(\alpha(\omega))=j\}$, $0 \leqslant j \leqslant c+\tilde{c}$. Set $T_{i,j}=S_i \cap T_j$, $0 \leqslant j \leqslant c+\tilde{c}$; then each $T_{i,j}$ is Borel and $S_i=\sqcup_{j=0}^{c+\tilde{c}} T_{i,j}$.

Definition 4.2: Fix a bounded multiplicity function m associated to the dilation matrix A. Let E_m be the Borel space given by

$$E_m = \bigsqcup_{i=1}^{c} \bigsqcup_{j=0}^{c+\tilde{c}} [T_{i,j} \times \mathbb{C}^j].$$

Let $(E_m, p, \sqcup_{i=1}^c S_i)$ be the Borel vector bundle where the map $p: E_m \to \sqcup_{i=1}^c S_i$ is defined by $p(x,\vec{v})=x$, $(x,\vec{v}) \in T_{i,j} \times \mathbb{C}^j$. By definition, $(E_m, p, \sqcup_{i=1}^c S_i)$ is a vector bundle over $\sqcup_{i=1}^c S_i$ whose fiber over $\omega \in S_i$ is a complex vector space of dimension $m(\alpha(\omega))+\tilde{m}(\alpha(\omega))$. An M **system associated to the multiplicity function** m is a Borel cross section $M: \sqcup_{j=1}^c S_j \to E_m$ of this bundle whose values, $(M_1(\omega), M_2(\omega), \ldots, M_{m(\alpha(\omega))+\tilde{m}(\alpha(\omega))})$, are the output of a vector of generalized low-

and high-pass filters. That is, for fixed $\omega \in \sqcup_{j=1}^{c} S_j$, the first $m(\alpha(\omega))$ components of the vector $M(\omega)$ correspond exactly to the generalized low-pass filter function values $h_1(\omega)$, $h_2(\omega)$, …, $h_{m((\alpha(\omega))}(\omega)$, and the last $\tilde{m}(\alpha(\omega))$ components of $M(\omega)$ correspond to the generalized high-pass filter function values $g_1(\omega)$, $g_2(\omega)$, …, $g_{\tilde{m}(\alpha(\omega))}(\omega)$, where the filters involved satisfy the low-pass and Lipschitz conditions defined in Sec. II, and where in addition the filters $\{h_i\} \cup \{g_k\}$ satisfy the initial conditions $h_i(\zeta_l) = h_i^C(\zeta_l)$, $1 \leqslant i \leqslant c$, $0 \leqslant l \leqslant N-1$, and $g_k(\zeta_l) = g_k^C(\zeta_l)$, $1 \leqslant k \leqslant \tilde{c}$, $0 \leqslant l \leqslant N-1$, where the h_i^C and the g_k^C are the canonical filters associated to m in the previous paragraph. Denote by $\mathcal{M}_m$ the set of M systems associated to the bounded multiplicity function m. We remark that $\mathcal{M}_m$ can be given the structure of a topological space if its elements are viewed as elements of the Hilbert space $\oplus_{i=0}^{c} \oplus_{j=0}^{c+\tilde{c}} L^2(T_{i,j}) \otimes \mathbb{C}^j$.

Remark 4.3: The above-mentioned definition is essentially the same as Definition 4.2 of Ref. 8 except for the additional assumption that the M system have the appropriate canonical values at the preimages of $\vec{0}$ under the endomorphism α, which was missing from Ref. 8. Note all the information about the generalized filters $\{h_{i,j}\}$ and $\{g_{k,j}\}$ is encoded in the M system. In particular, for any fixed multiplicity function m, such that both m and $\tilde{m}$ are constant in a neighborhood of the origin, we have a one-to-one correspondence between M systems and collections of generalized filter functions as defined in Section II which satisfy the canonical initial conditions. These generalized filters will in turn give rise to an orthonormal frame wavelet family and its associated GMRA $\{V_j\}$ by Theorem 3.4 from Sec. III. However, as shown by one of the examples given in Sec. III, the multiplicity function m' for the GMRA $\{V_j\}$ **need not** be equal to m. So, there is no correspondence in general, between the class of M-systems associated to a given multiplicity function m and the class of GMRAs associated to m.

To develop the loop group action on these M systems, we first define an endomorphism $\Pi_\alpha : \sqcup_{i=1}^{c} S_i \to \mathbb{T}^d$ by $\Pi_\alpha(\omega) = \alpha(\omega)$. Each $\omega \in \mathbb{T}^d$ has $\Sigma_{l=0}^{N-1} m(\omega_l) = m(\omega) + \tilde{m}(\omega)$ preimages in $\sqcup_{i=1}^{c} S_i$, where the $\{\omega_l : 0 \leqslant l \leqslant N-1\}$ are the N distinct preimages of ω in $\mathbb{T}^d$ under the endomorphism α, parametrized as discussed earlier. For convenience of notation, we label these preimage maps $r_{(l,j)}$, where $r_{(l,j)}(\omega) = \omega_l \in S_j \subseteq \sqcup_{i=1}^{c} S_i$ for $1 \leqslant j \leqslant m(\omega_l)$. (Note that this range on j, as l varies from 0 to $N-1$, gives all the preimages, since if $j > m(\omega_l)$, by definition ω_l is not an element of S_j.) For each fixed ω, we give the pairs (l,j) the lexicographical order, so that $(l_1, j_1) \leqslant (l_2, j_2)$ if $l_1 < l_2$ or if $l_1 = l_2$ and $j_1 \leqslant j_2$. We thus implicitly define a 1-1 map λ_ω taking the pairs (l,j) onto the integers from 1 to $m(\omega) + \tilde{m}(\omega)$.

We now construct a unitary group bundle $(F, q, \mathbb{T}^d)$ as follows. For each $j \in \{1, \ldots, c+\tilde{c}, \}$, let $Z_j = \{\omega \in \mathbb{T}^d : m(\omega) + m(\tilde{\omega}) = j\}$. Let

$$F_m = \sqcup_{j=0}^{c+\tilde{c}} [Z_j \times U(j, \mathbb{C})],$$

where $U(j, \mathbb{C})$ is viewed as a the topological group of unitary $j \times j$ matrices: it inherits its topology from being a subset of C^*-algebra of complex $j \times j$ matrices given the operator norm. Define $q : F_m \to \mathbb{T}^d$ by $q(\omega, T) = \omega$, for $(\omega, T) \in F_m$, and note that $q : F_m \to \mathbb{T}^d$ is a continuous open surjection, and the fiber $q^{-1}(\omega)$ of the bundle consists of the group of complex unitary matrices $U(m(\omega) + \tilde{m}(\omega), \mathbb{C})$. Borel cross sections to this group bundle consist of Borel maps $L : \mathbb{T}^d \to F_m$ such that $q \circ L(\omega) = \omega$. Note also that $(F_m, q, \mathbb{T}^d)$ is a subset of a Borel vector bundle over $\mathbb{T}^d$ in the sense of Definition 4.1, whose fibers over particular values of $\omega \in \mathbb{T}^d$ are made up of algebras of finite-dimensional matrices of varying dimension. We denote the set of sections of this bundle by $\Gamma_m(F_m, q)$. Note $\Gamma_m(F_m, q)$ is a group under pointwise operations on $\mathbb{T}^d$, where the identity element of the group is given by that section whose value at ω is equal to $Id_{m(\omega)+\tilde{m}(\omega)}$.

Also, it is possible to define a groupoid corresponding to a dilation matrix A as follows. Let Ω_A consist of the set of all bounded multiplicity functions corresponding to the dilation matrix A, that is, $\Omega_A = \{m : \mathbb{T}^d \to \mathbb{N} \cup \{0\} : m$ is essentially bounded and satisties (4.1)–(4.3)$\}$, where two multiplicity functions for A are identified if they are equal almost everywhere on $\mathbb{T}^d$. There are a variety of topologies we can put on Ω_A; for the moment the Hilbert space topology of L^2 functions on $\mathbb{T}^d$ will do. We call Ω_A **the multiplicity function space associated to** A. Now set

$$\mathcal{L}_A = \bigsqcup_{m \in \Omega_A} \Gamma_m(F_m, q).$$

Then $\mathcal{L}_A$ is a groupoid, with range map r equal to the source map s defined from $\mathcal{L}_A$ to Ω_A by $r(\gamma)=s(\gamma)=m$ for $\gamma \in \Gamma_m(F_m,q)$. Hence two elements γ_1 and γ_2 of $\mathcal{L}_A$ can be multiplied together if and only if $\gamma_1, \gamma_2 \in \Gamma_m(F_m,q)$ for a fixed bounded multiplicity function m.

We are now state a theorem about M-systems that can be derived in a fairly straightforward fashion from the orthogonality relations. This theorem is a generalization of Theorem 4.3 of Ref. 8, and thus we merely sketch the proof and refer the reader to Ref. 8 for details.

Theorem 4.4: *Let $\Gamma_m(F_m,q)$ be the group of cross sections of the group bundle associated to a fixed bounded multiplicity function m defined above. Let $M: \sqcup_{j=1}^{c} S_j \to E$ be an M-system associated to m. Then $\omega \mapsto (L_{i,\lambda_\omega(l,j)}(\omega))$, where*

$$L_{i,\lambda_\omega(l,j)}(\omega) = \sqrt{\frac{1}{N}} M_i(r_{(l,j)}(\omega))$$

is an element of $\Gamma_m(F_m,q)$.

Proof: As noted previously, $1 \leq \lambda_\omega(l,j) \leq m(\omega)+\tilde{m}(\omega)$, so for each $\omega \in \mathbb{T}$, the matrix $(L_{i,\lambda_\omega(l,j)}(\omega))$ is a square matrix of the correct dimension.

We shall show that for all $\omega \in \mathbb{T}^d$, the rows of $(L_{i,\lambda_\omega(l,j)}(\omega))$ are orthonormal, by means of the orthogonality relations for generalized filter functions given in Eq. (2.7) in the statement of Theorem 2.5.

Write L_i for the ith row of $(L_{i,\lambda_\omega(l,j)}(\omega))$. If $1 \leq i \leq i' \leq m(\omega)$,

$$\langle L_i, L_{i'} \rangle = \sum_{\lambda_\omega(l,j)=1}^{m(\omega)+\tilde{m}(\omega)} L_{i,\lambda_\omega(l,j)}(\omega)\overline{L_{i,\lambda_\omega(l,j)}(\omega)} = \sum_{l=0}^{N-1} \sum_{j=1}^{m(\omega_l)} \sqrt{\frac{1}{N}} M_i(r_{(l,j)}(\omega)) \overline{\sqrt{\frac{1}{N}} M_{i'}(r_{(l,j)}(x))}$$

$$= \sum_{l=0}^{N-1} \sum_{j=1}^{m(\omega_l)} \frac{1}{N} h_{i,j}(\omega_l)\overline{h_{i',j}(\omega_l)} = \frac{1}{N} \sum_{j=1}^{c} \sum_{l=0}^{N-1} h_{i,j}(\omega_l)\overline{h_{i',j}(\omega_l)}$$

(as $h_{i,j}(\omega_l)=0$ for $j > \mu(\omega_l)$, since $\omega_l \notin S_j$ in that case)

$$= [\text{by Eq. 2.2}] N \tfrac{1}{N} \delta_{i,i'} \chi_{S_i}(\omega) = \delta_{i,i'}$$

[we note that $\chi_{S_i}(\omega)=1$ since we have $i \leq m(\omega)$ and for those values of i, $\omega \in S_i$ by definition of $m(\omega)$].

The cases $m(\omega) < i \leq i' \leq m(\omega)+\tilde{m}(\omega)$ and $1 \leq i \leq m(\omega) < i' \leq m(\omega)+\tilde{m}(\omega)$ follow from similar arguments using Eqs. (2.4) and (2.5). Thus we have that in all cases, the rows of $(L_{i,\lambda_\omega(l,j)} \times(\omega))$ are orthonormal, and we have the desired unitary matrix. □

Remark 4.5: We note that for $\omega \in \mathbb{T}^d$, the $(m(\omega)+\tilde{m}(\omega)) \times (m(\omega)+\tilde{m}(\omega))$ matrix $L(\omega)$ is exactly the submatrix $L(\omega)$ of the matrix $K(\omega)$ defined in Theorem 2.5. Thus in some sense the proof given above is redundant. We have added in the extra detail because we want to exercise care in enumerating the rows and columns of $L(\omega)$ for future use. We also note that the "initial condition" on M systems given in Definition 4.2 can be rephrased as follows. Let $L^{\mathcal{C}}_{i,\lambda_\omega(l,j)}(\omega))$ be the element of $\Gamma_m(F_m,q)$ corresponding to the "canonical" filter system associated to the multiplicity function m, and let $L_{\mathcal{C}}$ be the $[m(\vec{0})+\tilde{m}(\vec{0})] \times [m(\vec{0})+\tilde{m}(\vec{0})]$ unitary matrix $L^{\mathcal{C}}_{i,\lambda_\omega(l,j)}(\vec{0})$. Then for any M system M associated to m, we have $\sqrt{1/N} M_i(r_{(l,j)}(\vec{0})) = L_{\mathcal{C}}$. This follows from the initial conditions satisfied by any M system outlined in Definition 4.2.

The results of Theorem 4.4 imply that the columns of $(L_{i,\lambda_\omega(l,j)}(\omega))$ are orthonormal as well, and allow us to obtain the following corollary, which is a generalization of Corollary 4.4 of Ref. 8.

Corollary 4.6: Let m and $\tilde{m}$ be bounded multiplicity and conjugate multiplicity functions associated to a dilation matrix A that are constant in a neighborhood of the origin, with related

sequences of sets $\{S_i | 1 \leqslant i \leqslant c\}$ *and* $\{\widetilde{S}_k | 1 \leqslant k \leqslant \tilde{c}\}$. *Suppose* $\{h_{i,j}\}_{1 \leqslant i,j \leqslant c}$ *and* $\{g_{k,j}\}_{1 \leqslant k \leqslant \tilde{c}, 1 \leqslant j \leqslant c}$ *are generalized low-pass and high-pass filter functions associated to the multiplicity function m. Then for all* $\omega \in \mathbb{T}^d$, *and for all* l, $l' \in \{0,1,\ldots,N-1\}$ *and* j, $j' \in \{1,\ldots,c)\}$, *we have*

$$\sum_{i=1}^{c+\tilde{c}} \frac{1}{N} M_i(r_{(l,j)}(\omega))\overline{M_i(r_{(l',j')}(\omega))} = \sum_{i=1}^{c} \frac{1}{N} h_{i,j}(\omega_l)\overline{h_{i,j'}(\omega_l)} + \sum_{k=1}^{\tilde{c}} \frac{1}{N} g_{k,j}(\omega_l)\overline{g_{k,j'}(\omega_l)} = \delta_{j,j'}\delta_{l,l'},$$

where here the M_i *correspond to the generalized filter functions* $h_{i,j}$ *and* $g_{k,j}$ *as given in Definition 4.2.*

Proof: This result follows fairly directly from Theorems 2.5 and 4.4, and we omit the details of the proof. □

We are ready to define the generalized loop group and its associated action on the set of M systems associated to a multiplicity function m.

Definition 4.7: The **loop group** associated to the multiplicity function m is defined to be the subgroup $\mathrm{Loop}_m(F_m,q)$ of the group of Borel sections $\Gamma_m(F_m,q)$ whose elements K satisfy $L(\vec{0}) = Id_{m(\vec{0})+\tilde{m}(\vec{0})}$, and $L_{i,\lambda_\omega(j,l)}$ are Lip_1 in a neighborhood of the origin.

We now prove that the generalized loop group $\mathrm{Loop}_m(F,q)$ acts freely and transitively on the set of M-systems associated to the multiplicity function m. The following theorem generalizes Theorem 4.7 of Ref. 8.

Theorem 4.8: *There is a free and transitive action of* $\mathrm{Loop}_m(F,q)$ *on the set of M-systems associated to an essentially bounded multiplicity function m such that m is constant in neighborhoods of* 0_l, $0 \leqslant l \leqslant N-1$, *where the set* $\{0_l : 0 \leqslant l \leqslant N-1\}$ *consists of the preimages of* 0 *under the endomorphism* $\alpha : \mathbb{T}^d \to \mathbb{T}^d$. *This action is given by*

$$L \cdot M(\omega) = L(\Pi_\alpha(\omega))[(M_1(\omega), M_2(\omega), \ldots, M_{m(\alpha(\omega))+\tilde{m}(\alpha(\omega))}(\omega))]^t.$$

Proof: We first prove the transitivity. Suppose we are given two different M-systems, labeled $M=(M_i)$ and $\widetilde{M}=(\widetilde{M}_i)$. Define an element L of the group bundle associated to m, that is, an element of $\Gamma_m(F,q)$, where $L(\omega)$ has dimension $m(\omega)+\tilde{m}(\omega)$, as follows:

$$L_{i,i'}(\omega) = \frac{1}{N} \sum_{\lambda_\omega(l,j)=1}^{m(\omega)+\tilde{m}(\omega)} \overline{M_{i'}(r_{(l,j)}(\omega))}\widetilde{M}_i(r_{(l,j)}(\omega)). \tag{4.5}$$

Since the M systems M and $\widetilde{M}$ have the same values at $\vec{0}$ and at the preimages ζ_l of $\vec{0}$ under the automorphism α, one easily verifies that $L(\vec{0}) = Id_{m(\vec{0})+\tilde{m}(\vec{0})}$. Also, one sees by inspection that if L_M and $L_{\widetilde{M}}$ are the elements of $\Gamma_m(F_m,q)$ corresponding to the M-systems M and $\widetilde{M}$ as in Theorem 4.4, then the proposed element L of $\mathrm{Loop}_m(F,q)$ given in Eq. (4.5) is exactly $L(\omega) = L_{\widetilde{M}}(\omega) \times [L_M(\omega)]^*$.

In addition, as shown by Bratteli and Jorgensen in the classical case, we have

$$\begin{aligned}
[L \cdot M]_i(\omega) &= \sum_{i'=1}^{m(\alpha(\omega))+\tilde{m}(\alpha(\omega))} L_{i,i'}(\Pi_\alpha(\omega))M_{i'}(\omega) \\
&= \sum_{i'=1}^{m(\alpha(\omega))+\tilde{m}(\alpha(\omega))} \left(\frac{1}{N} \sum_{\lambda_{\alpha(\omega)}(l,j)=1}^{m(\alpha(\omega))+\tilde{m}(\alpha(\omega))} \overline{M_{i'}(r_{(l,j)}(\alpha(\omega)))}\widetilde{M}_i(r_{(l,j)}(\alpha(\omega))) \right) M_{i'}(\omega) \\
&= \sum_{\lambda_{\alpha(\omega)}(l,j)=1}^{m(\alpha(\omega))+\tilde{m}(\alpha(\omega))} \widetilde{M}_i(r_{(l,j)}(\alpha(\omega))) \left(\sum_{i'=1}^{m(\alpha(\omega))+\tilde{m}(\alpha(\omega))} \overline{M_{i'}(r_{(l,j)}(\alpha(\omega)))}M_{i'}(\omega) \right) = \widetilde{M}_i(\omega),
\end{aligned}$$

where the last equality follows from the orthogonality of the columns of M as established in Corollary 2.7, so that the inside sum is 0 except for the single values of l and j where $r_{l,j}(\alpha(\omega)) = \omega$.

To prove that the action is free, suppose $M=(M_i)$ is a M system associated to m and $L \in \mathrm{Loop}_m(F,q)$ satisfies

$$L(\Pi_\alpha(\omega))[(M_1(\omega),M_2(\omega),\ldots,M_{m(\alpha(\omega))+\tilde{m}(\alpha(\omega))}(\omega))]^t=[(M_1(\omega),M_2(\omega),\ldots,M_{m(\alpha(\omega))+\tilde{m}(\alpha(\omega))}(\omega))]^t.$$

Using Theorem 4.4, for each $\omega \in \mathbb{T}^d$ we define a $(m(\alpha(\omega))+\tilde{m}(\alpha(\omega)))\times(m(\alpha(\omega))+\tilde{m}(\alpha(\omega)))$ unitary matrix $\mathcal{M}$ by

$$\mathcal{M}_{i,\lambda_{\alpha(\omega)}(l,j)}(\omega)=\sqrt{\frac{1}{N}}M_i(r_{(l,j)}(\alpha(\omega))),$$

$$1 \leqslant i \leqslant m(\alpha(\omega))+\tilde{m}(\alpha(\omega)),\ 0 \leqslant l \leqslant N-1,\ 1 \leqslant j \leqslant m(\alpha(\omega)_l).$$

We then see that $L(\alpha(\omega))\mathcal{M}(\omega)=\mathcal{M}(\omega)$ for all $\omega \in \mathbb{T}^d$. By unitarity of $\mathcal{M}(\omega)$, this shows that $L(\alpha(\omega))$ is the $(m(\alpha(\omega))+\tilde{m}(\alpha(\omega)))\times(m(\alpha(\omega))+\tilde{m}(\alpha(\omega)))$ identity matrix for all $\omega \in \mathbb{T}^d$, which implies that L is the identity element of $\mathrm{Loop}_m(F,q)$, as desired. □

Similarly, we can define the generalized loop groupoid assigned to a dilation matrix A.

Definition 4.9: Let A be a $d\times d$ integer dilation matrix. Let Ω_A be the multiplicity function space associated to A. The **loop groupoid** associated to A consists of the set

$$\mathcal{LOOP}_A=\bigsqcup_{m\in\Omega_A}\mathrm{Loop}_m(F_m,q),$$

where $r=s:\mathcal{LOOP}_A\to\Omega_A$ is defined by $r(L)=s(L)=m$ for $L \in \mathrm{Loop}_m(F_m,q)$.

We can also define a fiber bundle of M systems over Ω_A as follows.

Definition 4.10: Let Ω_A be the multiplicity function space associated to A. Define $\mathbb{M}_A=\cup_{m\in\Omega_A}\{m\}\times\mathbb{M}_m$, where $\mathbb{M}_m$ consists of the set of M systems associated to a fixed multiplicity function m, where two M systems are identified if they are equal almost everywhere. Give elements of $\mathbb{M}_m$ the Hilbert space topology mentioned in Definition 4.2. The topology on $\mathbb{M}_A$ is obtained from viewing an element $(m,\mathcal{M}) \in \mathbb{M}_A$ as a tuple $(m,\mathcal{M})$ of functions defined on the Cartesian product space $\mathbb{T}^d\times\sqcup_{i=1}^{\infty}[\mathbb{T}^d]_i$, taking on values in $[\mathbb{N}\cup\{0\}]\oplus l_2(\mathbb{N})$, where

$$(m,\mathcal{M})(\omega,z)=(m(\omega),\mathcal{M}_1(z),\mathcal{M}_2(z),\ldots,\mathcal{M}_{m(\alpha(z))+\tilde{m}(\alpha(z))}(z),0,0,0,\cdots),$$

and where $\mathcal{M}_j(z)=M_j(z)$ if $z \in \sqcup_{i=1}^{c}S_i$ and $1\leqslant j\leqslant m(\alpha(z))+\tilde{m}(\alpha(z))$, and $\mathcal{M}_j(z)=0$ if $z \notin \sqcup_{i=1}^{c}S_i$, for $\{S_i\}$ the standard subsets of $\mathbb{T}^d$ associated to the multiplicity function m. Then $\mathbb{M}_A$ is a topological space, if we view elements of $\mathbb{M}_A$ as elements in the Hilbert space $L^2(\mathbb{T}^d)\oplus L^2(\sqcup_{i=1}^{\infty}[\mathbb{T}^d]_i)\otimes[l_2(\mathbb{N})]$. Define a map $\Pi:\mathbb{M}_A\to\Omega_A$ by $\Pi((m,\mathcal{M}))=m$. Then Π is a continuous surjection, since it is a restriction of the Hilbert space projection from $L^2(\mathbb{T}^d)\oplus L^2(\sqcup_{i=1}^{\infty}[\mathbb{T}^d]_i)\otimes[l_2(\mathbb{N})]$ onto $L^2(\mathbb{T}^d)\oplus[\{\vec{0}\}]\cong L^2(\mathbb{T}^d)$, and $\Pi^{-1}(m)=\mathbb{M}_m$, so that $\mathbb{M}_A$ is a fiber bundle over Ω_A, called the **fiber bundle of M systems associated to A**.

Using these definitions, we obtain the following corollary to Theorem 4.8.

Corollary 4.11: Let A be a $d\times d$ integer dilation matrix, and let $\mathcal{LOOP}_A$ and $\mathbb{M}_A$ the loop groupoid and fiber bundle of M systems associated to A, respectively. Then there is a groupoid action of $\mathcal{LOOP}_A$ on $\mathbb{M}_A$, where $L \in \mathcal{LOOP}_A$ is allowed to act on $\mathcal{M} \in \mathbb{M}_A$ if and only if $r(L)=\Pi(\mathcal{M})=m$. This action is fiber-wise transitive.

Proof: This is just a restatement of part of Theorem 4.8. □

We now modify Example 4.5 of Ref. 8, in order to show how we can use the loop group action to transform the canonical filter functions for the Journé wavelet into the filter functions discussed in Example 3.6. The construction of the canonical filter functions for the Journé wavelet was first done in the thesis of Courter.[35]

Example 4.12: The Journé wavelet in the frequency domain is the characteristic function of the set

$$\left[-\frac{16}{7},-2\right)\cup\left[-\frac{1}{2},-\frac{2}{7}\right)\cup\left[\frac{2}{7},\frac{1}{2}\right]\cup\left[2,\frac{16}{7}\right).$$

Here the multiplicity function m takes on the values 0, 1, and 2, and $\tilde{m}(x)\equiv 1$, since the Journé wavelet is a single orthonormal wavelet. If we identify $\mathbb{T}$ with $\left[-\frac{1}{2},\frac{1}{2}\right)$, we can write $S_1=\left[-\frac{1}{2},-\frac{3}{7}\right)\cup\left[-\frac{2}{7},\frac{2}{7}\right)\cup\left[\frac{3}{7},\frac{1}{2}\right)$, $S_2=\left[-\frac{1}{7},\frac{1}{7}\right)$, and $\widetilde{S_1}=\left[-\frac{1}{2},\frac{1}{2}\right]$. The canonical generalized filter functions then are:

$$h_{1,1}^{\mathcal{C}}(x)=\sqrt{2}\chi_{\left[-\frac{2}{7},-\frac{1}{4}\right)\cup\left[-\frac{1}{7},\frac{1}{7}\right)\cup\left[\frac{1}{4},\frac{2}{7}\right)}(x),$$

$$h_{2,1}^{\mathcal{C}}=\sqrt{2}\chi_{\left[-\frac{1}{2},-\frac{3}{7}\right)\cup\left[\frac{3}{7},\frac{1}{2}\right)}(x),$$

$$g_1^{\mathcal{C}}(x)=\sqrt{2}\chi_{\left[-\frac{1}{4},-\frac{1}{7}\right)\cup\left[\frac{1}{7},\frac{1}{4}\right)}(x);$$

$$h_{1,2}^{\mathcal{C}}(x)=0,$$

$$h_{2,2}^{\mathcal{C}}(x)=0,$$

$$g_2^{\mathcal{C}}(x)=\sqrt{2}\chi_{\left[-\frac{1}{7},\frac{1}{7}\right)}(x).$$

One calculates that the "initial condition" matrix $L_{\mathcal{C}}$ discussed in Remark 4.5 corresponding to this canonical filter system is the 3×3 matrix

$$L_{\mathcal{C}}=\begin{pmatrix}1&0&0\\0&0&1\\0&1&0\end{pmatrix}.$$

We now construct an element of the loop group L_p such that if M_J is the M-system corresponding to the above output of generalized low- and high-pass filters, the M-system $L_p\cdot M_J$ has as its output the filter functions corresponding to those given in the example in Section III. Consider the decomposition of the disjoint union $S_1\sqcup S_2$ (identified with a subset of $\left[-\frac{1}{2},\frac{1}{2}\right)\sqcup\left[-\frac{1}{2},\frac{1}{2}\right)$) given by

$$T_{1,1}=\pm\left[\frac{1}{7},\frac{3}{14}\right)(\text{here } m(x)\geqslant 1, m(2x)+\tilde{m}(2x)=1),$$

$$T_{1,2}=\pm\left[\frac{1}{14},\frac{1}{7}\right)\cup\pm\left[\frac{3}{14},\frac{2}{7}\right)(\text{here } m(x)\geqslant 1, m(2x)+\tilde{m}(2x)=2),$$

$$T_{1,3}=\left[-\frac{1}{14},\frac{1}{14}\right)\cup\pm\left[\frac{3}{7},\frac{1}{2}\right)(\text{here } m(x)\geqslant 1, m(2x)+\tilde{m}(2x)=3),$$

$$T_{2,2}=\pm\left[\frac{1}{14},\frac{1}{7}\right)(\text{here } m(x)=2, m(2x)+\tilde{m}(2x)=2),$$

$$T_{2,3}=\left[-\frac{1}{14},\frac{1}{14}\right)(\text{here } m(x)=2, m(2x)+\tilde{m}(2x)=3).$$

Then as in the general case, $S_j=\sqcup_{k=0}^{3}T_{j,k}$, $j=1,2$.

We now describe the M system $M_J: \sqcup_{i=1}^{2} S_i \to E_m$ associated to the filter functions above. We describe M_J as a cross section separately on both of the (disjoint) sets S_1 and S_2.

On S_1, M_J is given by

$$[M_J(x)] = \begin{cases} [\sqrt{2}] & \text{if } x \in T_{1,1} \\ [\sqrt{2},0] & \text{if } x \in \pm\left[\frac{1}{14},\frac{1}{7}\right) \cup \pm\left[\frac{1}{4},\frac{2}{7}\right) \subseteq T_{1,2} \\ [0,\sqrt{2}] & \text{if } x \in \pm\left[\frac{3}{14},\frac{1}{4}\right) \subseteq T_{1,2} \\ [0,\sqrt{2},0] & \text{if } x \in T_{1,3} \setminus T_{2,3} \\ [\sqrt{2},0,0] & \text{if } x \in [T_{1,3} \cap T_{2,3}]. \end{cases}$$

On S_2, M_J is given by

$$[M_J(x)] = \begin{cases} [0,\sqrt{2}] & \text{if } x \in T_{2,2} \\ [0,0,\sqrt{2}] & \text{if } x \in T_{2,3}. \end{cases}$$

Consider the decomposition of the circle $\mathbb{T}$ (identified with $[-\frac{1}{2}, \frac{1}{2})$) given by

$$P_1 = \left[-\frac{1}{7},\frac{1}{7}\right)\left(\text{here } m(x)=2, m\left(\frac{x}{2}\right)=2, m\left(\frac{x+1}{2}\right)=1\right),$$

$$P_2 = \pm\left[\frac{1}{7},\frac{2}{7}\right)\left(\text{here } m(x)=1, m\left(\frac{x}{2}\right)=2, m\left(\frac{x+1}{2}\right)=0\right),$$

$$P_3 = \pm\left[\frac{2}{7},\frac{3}{7}\right), \left(\text{here } m(x)=0, m\left(\frac{x}{2}\right)=1, m\left(\frac{x+1}{2}\right)=0\right),$$

$$P_4 = \pm\left[\frac{3}{7},\frac{1}{2}\right)\left(\text{here } m(x)=1, m\left(\frac{x}{2}\right)=1, m\left(\frac{x+1}{2}\right)=1\right).$$

We note the following, which will be useful in our calculations: $2T_{1,1}=P_3$, $2\left(\pm\left[\frac{3}{14},\frac{1}{4}\right)\right) = 2\left(\pm\left[\frac{1}{4},\frac{2}{7}\right)\right)=P_4$, $2T_{1,3}=P_1$, $2\left(\pm\left[\frac{1}{14},\frac{1}{7}\right)\right)=2T_{2,2}=P_2$, and $2T_{2,3}=P_1$.

Now as in Example 3.5, let p_0 be any classical (MRA) low-pass filter for dilation by 2, [i.e., one that satisfies the classical filter equation (1.1)], that also satisfies $p_0(x)=0$ for $x \in \pm\left(\frac{1}{7}-\epsilon, \frac{3}{14}+\epsilon\right) \cup \left(\frac{3}{7}-\epsilon, \frac{4}{7}+\epsilon\right)$. Note that by Eq. (1.1), we then have $p_0(x)=\sqrt{2}$ for $x \in \pm\left(\frac{2}{7}-\epsilon, \frac{5}{14}+\epsilon\right) \cup \left(-\frac{1}{14}-\epsilon, \frac{1}{14}+\epsilon\right)$. Let $\widetilde{p_0}=p_0/\sqrt{2}$ be the normalization of p_0, so that $\widetilde{p_0}(0)=1$. Let p_1 be the standard choice of associated high-pass filter, so that $p_1(x)=e^{2\pi i x}\overline{p_0\left(x+\frac{1}{2}\right)}$, and let $\widetilde{p_1}=p_1/\sqrt{2}$ be the normalization of p_1. Again, by Eq. (1.1), $\widetilde{p_1}$ must have modulus 1 for $x \in \pm\left(\frac{1}{7}-\epsilon, \frac{3}{14}+\epsilon\right) \cup \left(\frac{3}{7}-\epsilon, \frac{4}{7}+\epsilon\right)$.

The associated element of the loop group L_p that we want to choose is:

$$L_p(x)=\begin{cases}\begin{pmatrix}\widetilde{p_0}\left(\frac{x}{2}\right) & 0 & \widetilde{p_0}\left(\frac{x+1}{2}\right)\\ 0 & 1 & 0\\ \widetilde{p_1}\left(\frac{x}{2}\right) & 0 & \widetilde{p_1}\left(\frac{x+1}{2}\right)\end{pmatrix} & \text{if } x\in P_1\\ \begin{pmatrix}\widetilde{p_0}\left(\frac{x}{2}\right) & \widetilde{p_0}\left(\frac{x+1}{2}\right)\\ \widetilde{p_1}\left(\frac{x}{2}\right) & \widetilde{p_1}\left(\frac{x+1}{2}\right)\end{pmatrix} & \text{if } x\in P_2\\ \widetilde{p_1}\left(\frac{x}{2}\right) & \text{if } x\in P_3\\ \begin{pmatrix}\widetilde{p_0}\left(\frac{x+1}{2}\right) & \widetilde{p_0}\left(\frac{x}{2}\right)\\ \widetilde{p_1}\left(\frac{x+1}{2}\right) & \widetilde{p_1}\left(\frac{x}{2}\right)\end{pmatrix} & \text{if } x\in P_4.\end{cases}$$

On S_1, our new M system $[M_{p,J}(x)]=[L_p(2x)[M_J(x)]^t]^t$ is the M system $M_{p,J}$ defined by

$$[M_{p,J}](x)=\begin{cases}[p_1(x)] & \text{if } x\in T_{1,1}\\ [p_0(x),p_1(x)] & \text{if } x\in \pm\left[\frac{1}{14},\frac{1}{7}\right)\cup\pm\left[\frac{3}{14},\frac{1}{4}\right)\subseteq T_{1,2}\\ [p_0(x),p_1(x)] & \text{if } x\in \pm\left[\frac{1}{4},\frac{2}{7}\right)\subseteq T_{1,2}\\ [0,\sqrt{2},0] & \text{if } x\in \pm\left[\frac{3}{7},\frac{1}{2}\right)=T_{1,3}\setminus T_{2,3}\\ [p_0(x),0,p_1(x)] & \text{if } x\in \left[-\frac{1}{14},\frac{1}{14}\right)=T_{1,3}\cap T_{2,3}\\ \left[p_0\left(x+\frac{1}{2}\right),p_1\left(x+\frac{1}{2}\right)\right] & \text{if } x\in T_{2,2}\\ \left[p_0\left(x+\frac{1}{2}\right),0,p_1\left(x+\frac{1}{2}\right)\right] & \text{if } x\in T_{2,3}.\end{cases}$$

We thus obtain the generalized filter functions coming from $M_{p,J}$:

$$h^p_{1,1}(x)=p_0(x)\chi_{[-2/7,2/7)}(x),$$

$$h^p_{2,1}(x)=\sqrt{2}\chi_{[-1/2,-3/7)\cup[3/7,1/2)}(x),$$

$$g^p_1(x)=p_1(x)\chi_{[-2/7,1/7)\cup[1/7,2/7)}(x),$$

$$h^p_{1,2}(x)=p_0\left(x+\tfrac{1}{2}\right)\chi_{[-1/7,1/7)}(x),$$

$$h^p_{2,2}(x)=0,$$

$$g^p_2(x)=p_1\left(x+\tfrac{1}{2}\right)\chi_{[-1/7,1/7)}(x).$$

Note that these are exactly the filter functions obtained in Example 3.6.

One could no doubt adapt the previous example to obtain generalized filters similar to those given in Examples 4.2 and 4.3 of Ref. 36.

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A new derivation of the CPT and spin-statistics theorems in noncommutative field theories

Daniel H. T. Franco[a)]
Departamento de Física, Campus Universitário de Goiabeiras, Universidade Federal do Espírito Santo (UFES), CEP:29060-900, Vitória, ES, Brasil

Caio M. M. Polito
Centro Brasileiro de Pesquisas Físicas, (CBPF), Coordenação de Campos e Partículas, (CCP), Rua Dr. Xavier Sigaud 150, Urca, CEP:22290-180, Rio de Janeiro, RJ, Brasil

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We propose an alternative axiomatic description for noncommutative field theories (NCFT) based on some ideas by Soloviev to nonlocal quantum fields. The local commutativity axiom is replaced by the weaker condition that the fields commute at sufficiently large spatial separations, called asymptotic commutativity, formulated in terms of the theory of analytic functionals. The question of a possible violation of the CPT and spin-statistics theorems caused by nonlocality of the commutation relations $[\hat{x}_\mu,\hat{x}_\nu]=i\theta_{\mu\nu}$ is investigated. In spite of this inherent nonlocality, we show that the modification aforementioned is sufficient to ensure the validity of these theorems for NCFT. We restrict ourselves to the simplest model of a scalar field in the case of only space–space noncommutativity. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1982769]

I. INTRODUCTION

In recent years a considerable effort has been made to clarify the structural aspects of noncommutative field theories (NCFT). The first paper on quantum field theory by exploring the noncommutativity of a space–time manifold was published by Snyder, in 1947,[1] who used this idea to give a solution for the problem of ultraviolet divergences which had plagued quantum field theories from the very beginning. Since then, due to the success of the renormalization theory, this subject was abandoned. Only recently the plan of investigating field theories on noncommutative space–times has been revived. In a fundamental paper Doplicher–Fredenhagen–Roberts[2] have shown that a model quantum space–time can be described by a noncommutative algebra whose commutation relations do imply uncertainty relations motivated by Heisenberg's uncertainty principle and by Einstein's theory. Later, in a different context, NCFT appear directly related with the string theory:[3] the noncommutative Yang–Mills theory can be seen as a vestige, in the low-energy limit, of open strings in the presence of a constant magnetic field, $B_{\mu\nu}$ (for a review see Refs. 4 and 5).

From an axiomatic standpoint, a language has been developed which, in principle, ought to enable one to extend the Wightman axioms to this context. Álvarez-Gaumé and Vásquez-Mozo[6] have recently taken the first step to examine general properties of NCFT within the axiomatic framework by modifying the standard Wightman axioms. By using as guiding principles the breaking of Lorentz symmetry down to the subgroup $\mathrm{O}(1,1)\times\mathrm{SO}(2)$, which leaves invariant the commutation relations for the coordinate operators $[\hat{x}_\mu,\hat{x}_\nu]=i\theta_{\mu\nu}$, and the relaxation of local commutativity to make it compatible with the causal structure of the theory, described by the light wedge associated with the O(1, 1) factor of the kinematical symmetry group, they have demonstrated the validity of the CPT theorem for NCFT. As it was stressed in Ref. 6, a source of

[a)]On leave from the Centro de Estudos de Física Teórica, Belo Horizonte, MG, Brasil. Electronic mail: dhtf@terra.com.br

difficulty in formulating NCFT which satisfy the adapted axioms has been the very harmful UV/IR mixing, which is probably the most surprising feature of these theories. The existence of hard infrared singularities in the nonplanar sector of the theory, induced by uncancelled quadratic ultraviolet divergences, can result in two kinds of problems: they can destroy the *tempered* nature of the Wightman functions and/or they can introduce tachyonic states in the spectrum, so the modified postulate of local commutativity is not preserved. This can be a signal that the NCFT must be analyzed from another set of principles, whose mathematical basis may shed new light on the existence (or not) of many of the desirable properties of fields, in particular the CPT operator and the connection between spin-statistics.

Clearly, in order to formulate a NCFT, a different type of generalized function space has to be used. First, we must to keep in mind that NCFT are *nonlocal* due to the commutation relations $[\hat{x}_\mu,\hat{x}_\nu]=i\theta_{\mu\nu}$. Second, this nonlocality can have implications on highly physical properties. For example, in the formulation of general properties of a field theory the localization plays a fundamental role in the concrete realization of the locality of field operators in coordinate space and the spectral condition in energy–momentum space, which are achieved through the *localization of test functions*—the fields are considered tempered functionals on the test function space $\mathcal{S}(\mathbb{R}^n)$, the Schwartz space of rapidly decreasing functions. However, the nonlocal character of the interactions in NCFT seems to suggest that there are good reasons to expect that fields are not tempered. Therefore, from a mathematical point of view, we must to have serious attention with the decision about the choice of the test function space to be used. This means that the extension of Wightman axioms to the context of NCFT has deeper roots in the mathematical structure and must first start with the replacement of the standard space $\mathcal{S}(\mathbb{R}^n)$ by another suitable space. As a matter of fact, since Wightman and Gårding formulated the quantum field theory in an axiomatic way, by regarding fields as operator-valued tempered distributions, many authors have attempted to generalize the theory to take in more fields represented by more singular generalized functions by restricting the class of test functions. We would like to mention the work by Jaffe,[7] on the strictly localizable field theory, and the work by Nagamachi–Mugibayashi[8] and Brüning–Nagamachi[9] on the field theory in terms of Fourier hyperfunctions. Wightman himself suggested that physically relevant interacting fields do not seem to be tempered.[10]

The class of distributions on which a NCFT should be built has been explored some time by Lücke[11–13] and Soloviev.[14–17] These authors have shown that one adequate solution to treat field theories with nonlocal interactions, it is to take the fields to be averaged with test functions belonging to the space $\mathcal{S}^0(\mathbb{R}^n)$ consisting of the restrictions to $\mathbb{R}^n$ of entire analytic functions on $\mathbb{C}^n$, whose Fourier transform is just the Schwartz space $\mathcal{D}(\mathbb{R}^n)$ of C^∞ functions of compact support. The space $\mathcal{S}^0(\mathbb{R}^n)$ is the smallest space among the Gelfand–Shilov spaces,[18] $\mathcal{S}^\beta(\mathbb{R}^n)$, where $0 \leqslant \beta < 1$, which naturally allows us to treat a theory of *nonlocalizable fields*. Elements in the dual space $\mathcal{S}'^0$ of the space of entire functions are called analytic functionals. Because the elements in $\mathcal{S}^0$ are entire functions, the locality axiom cannot be formulated in the usual way, i.e., there is no sensible notion of support for distributions in $\mathcal{S}'^0$. For this reason, in principle, expressing physical requirements such as the causality in clear way become problematic. Consequently, structural results of quantum field theories (QFT) usually seen to be firmly dependent on the locality, and that are supposed to be universally valid, do not *a priori* hold to the NCFT case. These structural results of QFT we have in mind here are (i) the existence of the fundamental symmetry CPT, and (ii) the spin-statistics connection.

The main purpose of this work is to show that, from a distributional-theoretical framework, the analysis of Álvarez-Gaumé and Vásquez-Mozo[6] on the extension of the Wightman axioms to the context of NCFT can be reformulated by adoption immediate of some ideas introduced by Soloviev,[14–17] which are applicable to noncommutative quantum field models. Then, we examine how essential are the locality of interactions and the microcausality axiom in order to reach a conclusion about the validity of the CPT and spin-statistics theorems in NCFT, in the case of only spatial noncommutativity—this choice preserves the unitarity[19] and the causality.[20] We show that both theorems hold within this environment if the postulate of microcausality suggested by

Álvarez-Gaumé and Vásquez-Mozo[6] is replaced with a condition implying the macrocausality as suggested by Soloviev.[14–17] This makes our proofs stronger than ones given byÁlvarez-Gaumé and Vásquez-Mozo,[6] in the sense that our hypotheses are weaker.

The article is organized as follows. Section II contains a brief sketch of some results by Soloviev about modern functional analysis that make it possible to extend the basic results of axiomatic approach[21,22] to nonlocal interactions. In Sec. III, the necessary modifications of the Wightman axioms to include the case of NCFT are explained. In Sec. IV, we outline the arguments that guarantee the validity of the CPT theorem and the spin-statistics relation for NCFT. Section V contains concluding remarks. We conclude with the Appendix which contains the sketch of proof of Proposition 4.1.

II. ANALYTIC FUNCTIONALS AND ANGULAR LOCALIZABILITY

In this section, we are going to introduce the basic facts which allow handling the analytic functionals of class $\mathcal{S}'^0$, in most cases, as easily as tempered distributions. As mentioned previously, the elements of $\mathcal{S}'^0$ are analytic functionals in the coordinate representation for which the notion of support is inapplicable. Nevertheless, Soloviev has shown that the functionals of this class retain a kind of *angular localizability*, which ensures the existence of minimal carrier cones of the distributions in $\mathcal{S}'^0$. This replaces the notion of support for nonlocalizable distributions and leads to a natural generalization of the local commutativity in NCFT with singular short distance behavior, since the latter theories are nonlocal. For sake of completeness, we recall this property here *mutatis mutandis*—the reader is referred to Refs. 14–17, and references therein for details.

We start recalling that the space of test functions composed by entire analytic functions is such that the following estimate holds:

$$|f(z)| \leqslant C_N(1+|x|)^{-N}e^{b|y|} \quad (z=x+iy), \quad N=0,1,\ldots,$$

where b and C_N are positive constants depending on f. The space of functions satisfying the previous estimate, with fixed b, is denoted as $\mathcal{S}^{0,b}$, whereas in nonlocal field theory the union $\cup_{b>0}\mathcal{S}^{0,b}$ is denoted as $\mathcal{S}^0$. Together with space $\mathcal{S}^0(\mathbb{R}^n)$, we introduce a space associated with closed cones $K\subset\mathbb{R}^n$. One recalls that K is called a cone if $x\in K$ implies $\lambda x\in K$ for all $\lambda>0$. Let U be an open cone in $\mathbb{R}^n$. For each U, one assigns a space $\mathcal{S}^0(U)$ consisting of those entire analytic functions on $\mathbb{C}^n$, that satisfy the inequalities

$$|f(z)| \leqslant C_N(1+|x|)^{-N}e^{b|y|+bd(x,U)}, \quad N=0,1,\ldots, \tag{2.1}$$

with $d(x,U)$ being the distance from the point x to the cone U (the norm in $\mathbb{R}^n$ is assumed to be Euclidean). This space can naturally be given a topology by regarding it as the inductive limit of the family of countably normed spaces $\mathcal{S}^{0,b}(U)$ whose norms are defined in accordance with inequalities (2.1), i.e.,

$$\|f\|_{U,b,N}=\sup_z|f(z)|(1+|x|)^N e^{-b|y|-bd(x,U)}.$$

For each closed cone $K\subset\mathbb{R}^n$, one also defines a space $\mathcal{S}^0(K)$ by taking another inductive limit through those open cones U that contain the set $K\backslash\{0\}$ and shrink to it. Clearly, $\mathcal{S}^0(\mathbb{R}^n)=\mathcal{S}^0$. As usual, we use a prime to denote the continuous dual of a space under consideration. A closed cone $K\subset\mathbb{R}^n$ is said to be a *carrier* of a functional $v\in\mathcal{S}'^0$ if v has a continuous extension to the space $\mathcal{S}^0(K)$, i.e., belongs to $\mathcal{S}'^0(K)$. As is seen from estimate (2.1), this property may be thought of as a fast decrease—no worse than an exponential decrease of order 1 and maximum type—of v in the complement of K. It should also be emphasized that if v is a tempered distribution with support in K, then the restriction $v|_{\mathcal{S}^0}$ is carried by K.

We now list some results proved by Soloviev, which formalize the property of angular localizability:

R.1: The spaces $\mathcal{S}^0(U)$ are Hausdorff and complete. A set $B\subset\mathcal{S}^0(U)$ is bounded if, and only if, it is contained in some space $\mathcal{S}^{0,b}(U)$ and is bounded in each of its norms.

R.2: The space $\mathcal{S}^0$ *is dense in every* $\mathcal{S}^0(U)$ *and in every* $\mathcal{S}^0(K)$.

R.3: If a functional $v \in \mathcal{S}'^0$ *is carried by each of closed cones* K_1 *and* K_2, *then it is carried by their intersection*.

R.4: If $v \in \mathcal{S}'^0(K_1 \cup K_2)$, *then* $v = v_1 + v_2$, *where* $v_j \in \mathcal{S}'^0(U_j)$ *and* U_j *are any open cones such that* $U_j \supset K_j \backslash \{0\}$, $j = 1, 2$.

III. ALTERNATIVE AXIOMATIC DESCRIPTION FOR NCFT

The axiomatic approach proposed by Gårding and Wightman for QFT consists of studying the consequences of a set of a few fundamental postulates on the theory such as the relativistic invariance, the locality, the existence and stability of the vacuum, in order to verify whether are logically consistent the basic principles suggested by the two pillars of the modern physics: the relativity theory and the quantum mechanics. The Wightman axioms can be summarized as follows: (i) States are described by vectors of a Hilbert space with positive definite metric. (ii) There is a *vacuum state* $|\Omega_0\rangle$ with the properties of being the state of lowest energy and invariant by all the unitary operators $\mathcal{U}(\Lambda, a)$ of the Poincaré group, where a is a space–time translation and Λ is a Lorentz transformation. (iii) The local fields are tempered distribution valued field operators. (iv) The spectrum of the energy–momentum operator is contained in the closed forward light cone. This condition is equivalent to the condition that the operators p_0 and p^2 are both positive. (v) Cyclicity of the vacuum. This means that one can construct a dense set of states in Hilbert space by application of products of field operators on this state. This condition ensures that the Hilbert space is not too large.

It turns out that these properties can be fully re-expressed in terms of an equivalent set of properties of the vacuum expectation values of their ordinary field products, called *Wightman functions* (or correlation functions of the theory):

$$\mathcal{W}_n(x_1, \ldots, x_n) \overset{\text{def}}{=} \langle \Omega_0 | \Phi(x_1) \cdots \Phi(x_n) | \Omega_0 \rangle. \tag{3.1}$$

For most purposes, the basis of the formulation of a QFT starts from a given set of Wightman functions which are assumed to satisfy the following properties:

P.1: Wightman functions are tempered distributions.

P.2: Wightman functions are invariant under the inhomogeneous Lorentz group.

P.3: Spectral condition: the Fourier transforms of the Wightman functions have support in the region

$$\left\{ (p_1, \ldots, p_n) \in \mathbb{R}^{4n} \Big| \sum_{j=1}^{n} p_j = 0, \sum_{j=1}^{k} p_j \in \bar{V}_+, k = 1, \ldots, n-1 \right\}, \tag{SC}$$

where $\bar{V}_+ = \{(p^0, \mathbf{p}) \in \mathbb{R}^4 | p^2 \geqslant 0, p^0 \geqslant 0\}$ is the closed forward light cone.

P.4: Local commutativity

$$\mathcal{W}_n(x_1, \ldots, x_i, x_{i+1}, \ldots, x_n) = \mathcal{W}_n(x_1, \ldots, x_{i+1}, x_i, \ldots, x_n) \quad \text{if } (x_i - x_{i+1})^2 < 0.$$

P.5: Condition of positive definiteness.

It can be shown on general grounds that a quantum field theory which satisfies all these conditions respect the CPT and spin-statistics theorems.[21,22]

As indicated in Sec. I, in NCFT the contact with the axiomatic formalism is made by modifying some of the Wightman axioms. In effect, most of the properties can be taken over in parallel with Wightman approach for tempered fields, except by following modifications:

Modification 1: We replace the test function space $\mathcal{S}(\mathbb{R}^n)$ by $\mathcal{S}^0(\mathbb{R}^n)$.

Modification 2: We replace the axiom of local commutativity, which cannot be formulated in terms of the analytic test functions, by asymptotic commutativity in the sense of Soloviev.

The main purpose of the present article is to show that NCFT subject to these modifications respect the CPT and spin-statistics theorems, within the same framework along the lines sketched in Refs. 14–17.

A. Fields are operator-valued distributions

As already mentioned, for NCFT we will assume that all fields are operator-valued generalized functions (throughout this paper, the term generalized functions is used synonymously with distributions) living in an appropriate space of functions $f(x) \in \mathcal{S}^0(\mathbb{R}^{4n})$, the space of entire analytic test functions. In particular, we will consider only one scalar field $\Phi(x)$. We shall denote by D_0 the minimal common invariant domain, which is assumed to be dense, of the field operators in the Hilbert space $\mathcal{H}$ of states, i.e., the vector subspace of $\mathcal{H}$ that is spanned by the vacuum state $|\Omega_0\rangle$ and by various vectors of the form $\Phi(f_1)\ldots\Phi(f_n)|\Omega_0\rangle$—with $(n=1,2,\ldots)$–where $f_i(x) \in \mathcal{S}^0(\mathbb{R}^4)$. It should be noted that, the space $\mathcal{S}^0$, being Fourier isomorphic to $\mathfrak{D}$, is *nuclear*. The property of nuclearity enables us to define in addition the expressions

$$\Phi^n(f) = \int \mathrm{d}x_1 \cdots \mathrm{d}x_n \Phi(x_1) \cdots \Phi(x_n) f(x_1,\ldots,x_n)|\Omega_0\rangle \quad (n=1,2,\ldots), \tag{3.2}$$

and to verify that every operator $\Phi(f)$ can be extended to the subspace $D_1 \supset D_0$ spanned by vectors (3.2).

Vacuum Expectation Values of Fields: The Wightman generalized functions $\mathcal{W}_n \in \mathcal{S}'^0(\mathbb{R}^{4n})$, i.e., the vacuum expectation values of fields (3.1) define analytic distributions on space $\mathcal{S}^0(\mathbb{R}^{4n})$. In Ref. 23, Chaichian *et al.* propose new Wightman functions as vacuum expectation values of field operators which involve the ★ products

$$\mathcal{W}_\star(x_1,\ldots,x_n) \overset{\text{def}}{=} \langle\Omega_0|\Phi(x_1) \star \Phi(x_2) \star \cdots \star \Phi(x_n)|\Omega_0\rangle, \tag{3.3}$$

where

$$\Phi(x_1) \star \Phi(x_2) = \exp\left(\frac{i}{2}\theta^{\mu\nu}\frac{\partial}{\partial x_1^\mu}\frac{\partial}{\partial x_2^\nu}\right)\Phi(x_1)\Phi(x_2),$$

represents a generalization of the ★ product for noncoinciding points, with the relation between the ordinary Wightman functions $\mathcal{W}_n(x_1,\ldots,x_n)$ and the new functions $\mathcal{W}_\star(x_1,\ldots,x_n)$ being defined by

$$\mathcal{W}_\star(x_1,\ldots,x_n) = \exp\left(\frac{i}{2}\theta^{\mu\nu}\sum_{i<j}\frac{\partial}{\partial x_i^\mu}\frac{\partial}{\partial x_j^\nu}\right)\mathcal{W}_n(x_1,\ldots,x_n),$$

which is a consequence of

$$\Phi(x_1) \star \cdots \star \Phi(x_n) = \exp\left(\frac{i}{2}\theta^{\mu\nu}\sum_{i<j}\frac{\partial}{\partial x_i^\mu}\frac{\partial}{\partial x_j^\nu}\right)\Phi(x_1)\cdots\Phi(x_n).$$

The new formulation of the Wightman functions has the advantage of including explicitly noncommutativity effects. In Ref. 6 the deformation parameter θ appears only to indicate that the Lorentz invariance is "broken" to a lower symmetry. However, in Ref. 23 the fields are still assumed to be *tempered* fields. In our opinion, same within the framework proposed in Ref. 23 the fields must be considered as generalized functions on space $\mathcal{S}^0(\mathbb{R}^{4n})$.

In what follows, by Wightman distributions we shall understand the vacuum expectation values of fields given by (3.1). It is very clear that the proofs of the CPT and spin-statistics theorems in Sec. V hold without modifications for the distributions (3.3), since the ★-products

introduced in the new Wightman functions no affect the analytic continuation of these functions to the complex plane with respect the "electrical" coordinates $x_e=(x^0,x^1)$. (The coordinates $\vec{x}_m=(x^2,x^3)$ are called "magnetic" coordinates in Ref. 6.)

B. Asymptotic commutativity

In extending the usual Wightman framework of the axiomatic quantum field theory our greatest concern is how to formulate the locality axiom for NCFT. The strict localizability of fields is connected, mathematically, with the fact that the test function space contains C^∞ functions of compact support. This requirement is satisfied by Wightman fields, because these fields were originally constructed on the basis of the space $\mathcal{S}$. But, this is not the case for fields constructed on the basis of the space $\mathcal{S}^0$.

In order to adapt the postulate of microcausality for NCFT, Álvarez-Gaumé and Vázquez-Mozo[6] (see also Ref. 24) have relaxed the condition that field (anti)commutators vanish outside the light cone, by replacing the light cone by the light *wedge* $V_{lw}=\{(x_e,\vec{x}_m)\in\mathbb{R}^4 \,|\, x_e^2=0\}$ so that

$$[\Phi(x_e,\vec{x}_m),\Phi(x'_e,\vec{x}'_m)]_\pm=0 \quad \text{if } (x_e-x'_e)^2=(x^0-x'^0)^2-(x^1-x'^1)^2<0. \tag{3.4}$$

Here, following Soloviev,[14–17] we relax the condition (3.4) and introduce, as a substitute for the axiom of locality, the following axiom:

Definition 3.1 (axiom of asymptotic (anti)commutativity): (It should be mentioned that the term "asymptotic commutativity" was introduced within the context which we have followed in Ref. 25 and with some other meaning in Ref. 11.) *The field components* $\Phi(x_e,\vec{x}_m)$ *and* $\Phi(x'_e,\vec{x}'_m)$ *are said to (anti)commute asymptotically for sufficiently large space-like separation of their arguments, if the functional*

$$f=\langle\Theta,[\Phi(x_e,\vec{x}_m),\Phi(x'_e,\vec{x}'_m)]_\pm\Psi\rangle, \tag{3.5}$$

is carried by the closed light wedge $\bar{V}_e^{(2)}\times\mathbb{R}^4=\{(x_e,\vec{x}_m);(x'_e,\vec{x}'_m)\in\mathbb{R}^{4\cdot2} \,|\, (x_e-x'_e)^2\geqslant 0\}$ *for any vectors* Θ, $\Psi\in D_0$.

A few comments about our requirement that the functional (3.5) is carried by the closed wedge $\bar{V}_e^{(2)}\times\mathbb{R}^4$ are now in order. In Ref. 6 this condition has been supported by the $\mathrm{SO}(1,1)\times\mathrm{SO}(2)$ symmetry, which is the feature arising when one has only spatial noncommutativity.[26] This fact leads the authors of Ref. 6 to argue that the notion of a light cone is generally modified to that of a light wedge. More recently, Chu *et al.*[29] have shown that the reduction from light cone to light wedge is a generic effect for noncommutative geometry and it is independent of the type of Lorentz symmetry breaking interaction.

A key point of the our argument is the equality $\mathcal{S}^0(\mathbb{R}^4\times\mathbb{R}^4)=\mathcal{S}^0(\mathbb{R}^4)\hat{\otimes}_i\mathcal{S}^0(\mathbb{R}^4)$, where the index i indicates that the tensor product is endowed with the inductive topology and the hat means the corresponding completion. By definition of the inductive topology, the dual space of $\mathcal{S}^0(\mathbb{R}^4)\hat{\otimes}_i\mathcal{S}^0(\mathbb{R}^4)$ is isomorphic to the space of separately continuous functionals on $\mathcal{S}^0(\mathbb{R}^4)\times\mathcal{S}^0(\mathbb{R}^4)$ (see Refs. 16 and 17). By result *R.2* in Sec. II, the space $\mathcal{S}^0(\mathbb{R}^4)$ is dense in $\mathcal{S}^0(U)$, where U is any open cone in $\mathbb{R}^4$ such that $\bar{V}_e^{(2)}\backslash\{0\}\subset U$. Hence, the functional f is carried by the closed cone $\bar{V}_e^{(2)}\times\mathbb{R}^4$. Moreover, a consideration analogous to that of Lemma 3 in Ref. 16 shows that if we introduce, for $0\leqslant j\leqslant n$ and $n=0,1,2,\ldots$, Wightman functions $\mathcal{W}_{n,j}\in\mathcal{S}'^0(\mathbb{R}^{4(n+2)})$ defined by

$$\mathcal{W}_{n,j}(x_1,\ldots,x_j,x,y,x_{j+1},\ldots,x_n)=\mathcal{W}_{n+2}(x_1,\ldots,x_j,x,y,x_{j+1},\ldots,x_n)\pm\mathcal{W}_{n+2}(x_1,\ldots,x_j,y,x,x_{j+1},\ldots,x_n),$$

it follows from the asymptotic commutativity condition that $\mathcal{W}_{n,j}$ defined on $\mathcal{S}^0(\mathbb{R}^{4(n+2)})$ has a continuous extension to the space $\mathcal{S}^0(\mathbb{R}^{4j}\times(U\times\mathbb{R}^4)\times\mathbb{R}^{4(n-j)})$. Then, $\mathcal{W}_{n,j}$ is carried by the closed cone $\mathbb{R}^{4j}\times(\bar{V}_e^{(2)}\times\mathbb{R}^4)\times\mathbb{R}^{4(n-j)}$.

IV. PROOF OF THE CPT AND SPIN-STATISTICS THEOREMS

In this section, we want to show that the above-mentioned arguments allow us to deduce some structural results of NCFT. We have in mind here the existence of the CPT symmetry[6,30] and the connection between spin and statistics.[30] The proof of these results as given in the literature[21,22] usually seem to rely on the tempered character of the distributions in an essential way. In the approach which we follow the main sources of difficulties in proving these results are: the absence of test functions of compact support and the fact that for functionals belonging to $\mathcal{S}'^0$ the notion of support breaks down. In Refs. 12 and 13, Lücke overcame this problem using the analyticity properties of vacuum expectation values in the momentum space and analyzed the relevant envelopes of holomorphy. More recently, an alternative and elegant solution has been given by Soloviev[14–16] using the notion of the analytic wavefront set and a type of uniqueness theorem for distributions. For simplicity, we are going to discuss the CPT and spin-statistics theorems only for the scalar field $\Phi(x)$. Ours results are corollaries of the Soloviev's theorems generalizing the CPT invariance and spin-statistics connection for nonlocal field theories, and our proofs follow directly from the chain of reasoning of Refs. 14–17.

A. CPT invariance

Let $\Phi(x)$ be a Hermitian scalar field. For this field, it is well known that in terms of the Wightman functions, a necessary and sufficient condition for the existence of CPT theorem is given by

$$\mathcal{W}_n(x_1,\ldots,x_n)=\mathcal{W}_n(-x_n,\ldots,-x_1). \tag{4.1}$$

Under the usual temperedness assumption, the proof of the equality (4.1) as given by Jost[31] starts from the weak local commutativity (WLC) condition, namely under the condition that the vacuum expectation value of the commutator of n scalar fields vanishes outside the light cone, which in terms of Wightman functions takes the form

$$\mathcal{W}_n(x_1,\ldots,x_n)-\mathcal{W}_n(x_n,\ldots,x_1)=0 \quad \text{for } (x_1,\ldots,x_n)\in\mathcal{J}_n, \tag{4.2}$$

where $\mathcal{J}_n$ represents the set of Jost points, which are real points lying outside the light cone. This implies that $(x_k-x_{k+1})^2<0$ for $k=1,\ldots,n-1$. Jost's proof that the WLC condition (4.2) is equivalent to the CPT symmetry (4.1) one relies on the fact that the proper complex Lorentz group contains the total space–time inversion. Therefore, by the Bargmann-Hall-Wightman (BHW) theorem, the equality $\mathcal{W}_n(x_n,\ldots,x_1)=\mathcal{W}_n(-x_n,\ldots,-x_1)$ holds taking into account the symmetry property $\mathcal{J}_n=-\mathcal{J}_n$ in whole extended analyticity domain.

In order to prove that equality (4.1) holds in NCFT, the following auxiliary proposition (proved in the Appendix) will be fundamental.

Proposition 4.1: The functional $F(x)=\mathcal{W}_n(x_1,\ldots,x_n)-\mathcal{W}_n(-x_1,\ldots,-x_n)$, *is carried by the complement of the Jost points*

$$\mathcal{J}_n=\left\{(x_1,\ldots,x_n)\in\mathbb{R}^{4n}\Big|\left(\sum_{i=1}^{n-1}\lambda_i(x_{e_i}-x_{e_{i+1}})\right)^2<0,\lambda_i\geqslant 0,\sum_{i=1}^{n-1}\lambda_i>0\right\}. \tag{JP}$$

Remark 1: It is worthwhile to emphasize that, according to Ref. 6, for $n>2$ the Jost points are formed by $(x_{e_i}-x_{e_{i+1}})^2<0$ with the condition that $x_i^1-x_{i+1}^1>0$.

We also formulate an analogous of the WLC condition:

Definition 4.2: The noncommutative quantum field $\Phi(x)$ *defined on the test function space* $\mathcal{S}^0(\mathbb{R}^{4n})$ *is said to satisfy the weak asymptotic commutativity (WAC) condition if the functional on left-hand side of Eq. (4.2) is carried by the set* $\complement\mathcal{J}_n$ *complementary to the Jost points (JP).*

Theorem 4.3 (Modified CPT Theorem): *In a noncommutative scalar field theory in which the modified Wightman axioms hold, the weak asymptotic commutativity condition is equivalent to the CPT invariance.*

Proof: We start assuming that the CPT invariance is fulfilled. This implies the equality

$$\mathcal{W}_n(x_1,\ldots,x_n) = \mathcal{W}_n(-x_n,\ldots,-x_1). \tag{4.3}$$

Then, one subtracts the functional $\mathcal{W}_n(-x_1,\ldots,-x_n)$ from the left-hand and right-hand sides of (4.3) in order to obtain the expression:

$$[\mathcal{W}_n(x_1,\ldots,x_n) - \mathcal{W}_n(-x_1,\ldots,-x_n)] = [\mathcal{W}_n(-x_n,\ldots,-x_1) - \mathcal{W}_n(-x_1,\ldots,-x_n)].$$

By Proposition 4.1, the difference functional on the left-hand side, denoted by $F(x)$, is carried by set $\complement\mathcal{J}_n$. Hence, from the previous functional equality, we conclude that the weak asymptotic commutativity condition is fulfilled. The reverse is also easily proved. If the WAC is satisfied, then the difference $\mathcal{W}_n(x_1,\ldots,x_n)-\mathcal{W}_n(-x_n,\ldots,-x_1)$ is carried by the set $\complement\mathcal{J}_n \neq \mathbb{R}^{4n}$. On the other hand, by virtue of the spectral condition,[32] the Fourier transform of this difference has support in the properly convex cone (SC), defined by Property P.3, in Sec. III. Therefore, the CPT invariance holds identically by Theorem 4 in Ref. 15, which asserts that $\mathcal{W}_n(x_1,\ldots,x_n)-\mathcal{W}_n(-x_n,\ldots,-x_1) \equiv 0$, since the property of this functional of having its Fourier transform supported by the aforementioned properly convex cone requires that each carrier of $\mathcal{W}_n(x_1,\ldots,x_n)-\mathcal{W}_n(-x_n,\ldots,-x_1)$ cannot be different from the whole space $\mathbb{R}^{4n}$. ■

B. Spin-statistics connection

Here, let us state the theorem for a scalar field only. The general case, mainly when gauge fields are present, deserves careful study once we have to admit an indefinite metric, which invalidates the connection of spin with statistics due the existence of "scalar fermions" as the Faddeev–Popov ghosts.[33]

Theorem 4.4 (Spin-Statistics Theorem): *Suppose that* Φ *and its Hermitian conjugate* Φ^* *satisfy the weak asymptotic condition with the "wrong" connection of spin and statistics. Then* $\Phi(x)\Omega_0=\Phi^*(x)\Omega_0=0$.

Proof: Under the hypothesis of the anomalous connection between spin and statistics, the weak asymptotic condition implies that

$$W_2(\xi) + W_2^{\mathrm{tr}}(-\xi) \in \mathcal{S}'^0(\bar{V}_e \times \mathbb{R}^2), \quad \xi = x_1 - x_2, \tag{4.4}$$

with $W_2(x_1-x_2)=\langle\Omega_0,\Phi(x_1)\Phi^*(x_2)\Omega_0\rangle$ and $W_2^{\mathrm{tr}}(x_2-x_1)=\langle\Omega_0,\Phi^*(x_2)\Phi(x_1)\Omega_0\rangle$. Using the same arguments as in the proof of the Proposition 4.1, we conclude that for the regularized function $W_2^{(\Lambda)}(\xi)$, the equality $W_2^{(\Lambda)}(\xi)=W_2^{(\Lambda)}(-\xi)$ takes place for the complement of the closed light wedge $\bar{V}_e\times\mathbb{R}^2$, according to BHW theorem. This implies that the difference $W_2^{(\Lambda)}(\xi)-W_2^{(\Lambda)}(-\xi)$ is carried by $\bar{V}_e\times\mathbb{R}^2$. Since the unregularized difference $W_2(\xi)-W_2(-\xi)$ admits a continuous extension to the space $\mathcal{S}^0(\bar{V}_e\times\mathbb{R}^2)$ as $\Lambda\to\infty$, it is possible to rewrite the condition (4.4) as $W_2(\xi)+W_2^{\mathrm{tr}}(\xi) \in \mathcal{S}'^0(\bar{V}_e\times\mathbb{R}^2)$. On the other hand, because of the spectral condition, in momentum space, $\tilde{W}_2 + \tilde{W}_2^{\mathrm{tr}}$ has support in the convex cone $\{(p_1,p_2)\in\mathbb{R}^8 \,|\, p_1+p_2=0, p_1\in\bar{V}_+\}$. Hence, again by Theorem 4 in Ref. 15 we get $W_2(\xi)+W_2^{\mathrm{tr}}(\xi)\equiv 0$. Finally, after averaging the fields with a test function, we obtain $\|\Phi^*(f)\Omega_0\|^2+\|\Phi(\bar{f})\Omega_0\|^2=0$, which yields $\Phi(x)\Omega_0=\Phi^*(x)\Omega_0=0$. ■

V. CONCLUDING REMARKS

In the present paper, we reexamine the recent work byÁlvarez-Gaumé and Vásquez-Mozo[6] on the extension of the Wightman axioms to the context of NCFT under another outlook. Our results are similar to those published in Ref. 6, but are obtained under mildly more general assumptions. We assume a weaker version of Wightman's axioms, where (a) fields are operator-valued generalized functions living in an appropriate space of functions $f(x)\in\mathcal{S}^0(\mathbb{R}^{4n})$, the space of entire analytic test functions, (b) the local (anti)commutativity is replaced by the asymptotic variant in the sense of Soloviev. Two profound results of the ordinary QFT, the existence of the symmetry

CPT and the spin-statistics connection were proved to hold for the case of a theory with space–space noncommutativity. Here, we restrict ourselves to the simplest case, that of a single, scalar, Hermitian field $\Phi(x)$ associated with spinless particles of mass $m>0$.

We would like to conclude mentioning a number of questions for future research based on the ideas of this paper:

(1) The arguments that we have used evidently may provide new insights which will allow us to study others structural results of QFT within the axiomatic description of NCFT, such as the existence of the Borchers class of quantum fields, a representation of the Jost–Lehmann–Dyson type, the Haag's theorem and so on.

(2) As it was pointed out in Ref. 6, for gauge theories, in particular the noncommutative QED (NCQED), the questions associated to the Wightman axioms and their consequences are more involved due to the UV/IR mixing. As already mentioned, the existence of hard infrared singularities in the nonplanar sector of the theory, induced by uncanceled quadratic ultraviolet divergences, can result in two kinds of problems: they can destroy the *tempered* nature of the Wightman functions and/or they can introduce tachyonic states in the spectrum, so the modified postulate of local commutativity *is not preserved*. Nevertheless, it is worthwhile to call attention to the fact that the nontemperedness arising from hard infrared singularities in NCFT is not a newness. Actually, in the case of the local and covariant formulation of standard gauge quantum field theories the necessary lack of positivity allows the occurrence of hard infrared singularities which recall those related to the UV/IR mixing in NCFT. These results appear to reinforce the hypothesis that the infrared issue in NCFT must be dealt with another approach which enables the simultaneous control of infrared singularities. This problem could be attacked with the Gelfand–Shilov spaces $\mathcal{S}^0_\alpha(\mathbb{R}^n)$, with $\alpha>1$—in order to obtain the nontriviality of $\mathcal{S}^0_\alpha$—being a multi-index which control the infrared behavior of the Wightman functions.[16,34] In this case the fields under consideration are ultradistributions, not distributions, in variables of the momentum space. This may be an interesting step in the proof of absence of the UV/IR mixing in NCFT and of the spin-statistics theorem for NCQED.

These topics are under investigation. We intend to report our conclusions on these issues in forthcoming papers.

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APPENDIX: SKETCH OF PROOF OF THE PROPOSITION 4.1

Due to the nuclearity property for $\mathcal{S}^0(\mathbb{R}^{4n})$,[36] $\mathcal{W}_n$ is a multilinear functional which can be uniquely identified with a functional $\mathcal{W}_n(f,g)$ in $\mathcal{S}'^0(\mathbb{R}^{2n}\times\mathbb{R}^{2n})$, continuous separately over $f \in \mathcal{S}^0(\mathbb{R}^{2n})$ and $g \in \mathcal{S}^0(\mathbb{R}^{2n})$, defined by

$$\int \prod_{i=1}^{n} \mathrm{d}^2x_{e_i}\mathrm{d}^2\vec{x}_{m_i}\mathcal{W}_n((x_{e_1},\vec{x}_{m_1}),\ldots,(x_{e_n},\vec{x}_{m_n}))f(x_{e_1},\ldots,x_{e_n})g(\vec{x}_{m_1},\ldots,\vec{x}_{m_n}).$$

Taking into account the invariance under translations, we pass to the difference variables ξ_k, in order to obtain a generalized function

$$\mathcal{W}_n((x_{e_1},\vec{x}_{m_1}),\ldots,(x_{e_n},\vec{x}_{m_n})) = W_n((\xi_{e_1},\vec{\xi}_{m_1}),\ldots,(\xi_{e_{n-1}},\vec{\xi}_{m_{n-1}})),$$

in $\mathcal{S}'^0(\mathbb{R}^{2(n-1)}\times\mathbb{R}^{2(n-1)})$, which depends on the variables $\xi_{e_i}\in\mathbb{R}^{2(n-1)}$ and $\vec{\xi}_{m_i}\in\mathbb{R}^{2(n-1)}$. Following Soloviev,[16] we regularize the ultraviolet behavior of W_n by multiplying its Fourier transform $\widetilde{W}_n$ with a cutoff function. Then, with the "magnetic" coordinates being held fixed, we regularize the Fourier transform of $W_n((\xi_{e_1},\vec{\xi}_{m_1}),\ldots,(\xi_{e_{n-1}},\vec{\xi}_{m_{n-1}}))$ with an invariant cutoff function of form $\omega_\Lambda(p_e)=\omega((p_e\cdot p_e)/\Lambda^2)\in C_0^\infty(\mathbb{R})$, where $p_e\cdot p_e=p_0^2-p_1^2$ and such that $\omega_\Lambda(p_e)=1$ for $|(p_e\cdot p_e)/\Lambda^2|\leqslant 1$. The regularized distribution $W_n^{(\Lambda)}$ turns into a tempered distribution, in the "electrical" coordinates. Thus, $\widetilde{W}_n^{(\Lambda)}$ has an inverse Fourier–Laplace transform $\mathbf{W}_n^{(\Lambda)}$. The generalized function $\mathbf{W}_n^{(\Lambda)}((\zeta_{e_1},\vec{\xi}_{m_1}),\ldots,(\zeta_{e_{n-1}},\vec{\xi}_{m_{n-1}}))$, with $\zeta_{e_j}=\xi_{e_j}-i\eta_{e_j}$, is an analytic function of $2(n-1)$ complex variables on the "subtube" $T_{n-1}=\mathbb{R}^{2(n-1)}-iV_{e_+}^{(n-1)}$, where V_{e_+} is a subcone of the forward light cone V_+:

$$V_{e_+}=\{(\eta_e,\vec{\eta}_m)\in V_+|\,\eta_e^2>0,\eta^0>0,\vec{\eta}_m=0\}.$$

Under temperedness assumption, the function $\mathbf{W}_n^{(\Lambda)}$ can be analytically continued into the extended subtube $T_{n-1}^{\text{ext.}}$ by the BHW theorem, with the continued function being covariant under the Lorentz group $\mathcal{L}_+(\mathbb{C})$—the complexification of O(1,1) is made of similar way with that of the Lorentz group O(1,3). In particular, the transformations of $\mathcal{L}_+(\mathbb{C})$ leave the magnetic coordinates invariant (see Ref. 6 for details). Moreover, $\mathbf{W}_n^{(\Lambda)}$ has $W_n^{(\Lambda)}((\xi_{e_1},\vec{\xi}_{m_1}),\ldots,(\xi_{e_{n-1}},\vec{\xi}_{m_{n-1}}))=\mathcal{W}_n^{(\Lambda)}((x_{e_1},\vec{x}_{m_1}),\ldots,(x_{e_n},\vec{x}_{m_n}))$ as boundary value as $\eta_{e_j}\to 0$. Hence, the equality $\mathcal{W}_n^{(\Lambda)}(x_1,\ldots,x_n)=\mathcal{W}_n^{(\Lambda)}(-x_1,\ldots,-x_n)$ takes place in the corresponding analyticity domain, keeping in mind that the inversion of the four space-time coordinates is the product of the transformations $I_{\text{st}}\in\mathcal{L}_+(\mathbb{C})$ [see Eq. (3.5) in Ref. 6] and a SO(2) rotation of 180°. Since $T_{n-1}^{\text{ext.}}$ contains the Jost points, the tempered distribution $F^\Lambda(x)=\mathcal{W}_n^{(\Lambda)}(x_1,\ldots,x_n)-\mathcal{W}_n^{(\Lambda)}(-x_1,\ldots,-x_n)$ vanishes for the Jost points and its restriction to $\mathcal{S}^0$ is carried by $\complement\mathcal{J}_n$. By construction, $\widetilde{F}^\Lambda(p)$ coincides with $\widetilde{F}(p)$ in a neighborhood of the origin, which enlarges indefinitely as $\Lambda\to\infty$, and given that the space $\mathcal{S}^0(\mathbb{R}^{4n})$ is dense in $\mathcal{S}^0(\complement\mathcal{J}_n)$, the unregularized generalized function $F(x)\in\mathcal{S}'^0(\mathbb{R}^{4n})$ admits a continuous extension to the space $\mathcal{S}^0(\complement\mathcal{J}_n)$. This completes the outline of the proof.

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Nonlinear Schrödinger Equation with Inhomogeneous Dirichlet Boundary Data

Charles Bu[a)]
Department of Mathematics, Wellesley College, Wellesley, Massachusetts 02481

Kimitoshi Tsutaya
Department of Mathematics, Hokkaido University, Sapporo 060-0810, Japan

Chenying Zhang
Department of Mathematics, Wellesley College, Wellesley, Massachusetts 02481

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In this article we study the following nonlinear Schrödinger equation $iu_t=\Delta u - g|u|^{p-1}u$ in a domain $\Omega\subset\mathbb{R}^n$ with initial condition $u(x,0)=\phi(x)$ and the Dirichlet boundary condition $u(x,t)=Q(x,t)$ on $\partial\Omega$, where ϕ, Q are given smooth functions. The nonlinear term contributes a negative term to the energy (i.e., $g<0$). We present the existence theorem for a global solution of finite energy when $p\leqslant 1+2/n$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1914730]

I. PRELIMINARIES

In this paper we are concerned with a Dirichlet inhomogeneous boundary value problem for a nonlinear Schrödinger equation in n space dimensions:

$$\begin{aligned} &i\,\partial_t u = \Delta u - g|u|^{p-1}u, \quad \text{for } x\in\Omega\subset\mathbb{R}^n,\\ &u(x,0)=\phi(x), \quad u(x,t)=Q(x,t), \quad \text{for } x\in\partial\Omega, \end{aligned} \tag{1.1}$$

where $g\in\mathrm{R}$ is a constant.

Inhomogeneous boundary value problems for nonlinear PDEs such as the NLS have physical implications. For example, in one space dimension, such problems are often called forced problems when an external force is applied to the time evolution of systems governed by nonlinear partial differential equations. Frequently the forcing is put in as a boundary condition. For instance, in ionospheric modification experiments of one space dimension, one directs a radio frequency wave at the ionosphere. At the reflection point of the wave, a sufficient level of electron plasma waves is excited to make the nonlinear behavior important. This may be described by the NLS equation with the cubic nonlinear term and a Dirichlet type of boundary condition.

It is well known that there is a very large literature on nonlinear Schrödinger equations in $\mathbb{R}^n$. However, for boundary value problems in a domain Ω, results are rare. Tsutsumi[1] and Tsutsumi[2] obtained well-posedness for the homogeneous problem in an exterior domain with sufficiently small and smooth initial data. Brezis and Gallouet[3] and Tsutsumi[4] studied the case of large initial data in two dimensions.

For inhomogeneous boundary conditions there were certain results in one space dimension. Bu[5] proved the well-posedness of smooth solutions with arbitrarily large data for $n=1$ and a nonlinear term of positive energy. Carroll and Bu[6] proved the same for $n=1$ and a nonlinear cubic term of either sign. There are also some results in one dimension using inverse scattering techniques.

[a)]Corresponding author. Electronic mail: cbu@wellesley.edu; fax (781) 283-3642.

When space dimension $n>1$, Strauss and Bu[7] obtained the global existence of an H^1 solution if the nonlinear term contributes a positive term to the energy, i.e., $g>0$.

Our main objective is to prove a similar theorem when $g<0$.

II. *A PRIORI* ESTIMATES

Write $P=\nabla u|_{\partial\Omega}$, $\eta=\Sigma_j \partial_j \xi_j=\nabla\cdot\xi$, and $\mathbf{n}=(n_1,n_2,\ldots,n_n)$ standard unit outer normal vector for $\partial\Omega$. Since $\partial\Omega$ is smooth, there exists a smooth function $\xi=(\xi_1,\xi_2,\ldots,\xi_n)$ independent of t from $\mathbb{R}^n$ to $\mathbb{R}^n$, such that $\xi|_{\partial\Omega}=(n_1,n_2,\ldots,n_n)=\mathbf{n}$. In case $\partial\Omega$ is unbounded, we assume that (a) the derivatives up to third order of ξ are bounded and (b) there exists $R>0$ such that $Q(x,t)=0$ for $|x|>R$. We sometimes denote $\partial_j u=\partial u/\partial x_j$ for $j=1,2,\ldots,n$.

The following lemma was proved in Ref. 7.

Lemma 2.1: For the nonlinear Schrödinger equation in n space dimensions with Dirichlet inhomogeneous boundary condition (1.1), four a priori identities are available: First,

$$\partial_t \int_\Omega |u|^2\,\mathrm{d}x = 2\,\mathrm{Im}\int_{\partial\Omega}(\mathbf{n}\cdot P)\bar{Q}\,\mathrm{d}S. \tag{2.1}$$

Second,

$$\partial_t \int_\Omega \left(|\nabla u|^2+\frac{2g}{p+1}|u|^{p+1}\right)\mathrm{d}x = 2\,\mathrm{Re}\int_{\partial\Omega}(\mathbf{n}\cdot P)\bar{Q}_t\,\mathrm{d}S. \tag{2.2}$$

Third,

$$\begin{aligned}\partial_t \int_\Omega u(\xi\cdot\nabla u)\mathrm{d}x - \int_{\partial\Omega} Q\bar{Q}_t\,\mathrm{d}S + \int_\Omega \eta u\bar{u}_t\,\mathrm{d}x = &-2i\int_{\partial\Omega}|\mathbf{n}\cdot P|^2\,\mathrm{d}S - \sum_{m,j}\int_\Omega \partial_m\xi_j\,\partial_m u\,\partial_j\bar{u}\,\mathrm{d}x\\ &+ i\int_{\partial\Omega}|P|^2\,\mathrm{d}S - i\int_\Omega \eta|\nabla u|^2\,\mathrm{d}x\\ &+ i\frac{2g}{p+1}\int_{\partial\Omega}|Q|^{p+1}\,\mathrm{d}S - i\frac{2g}{p+1}\int_\Omega \eta|u|^{p+1}\,\mathrm{d}x.\end{aligned} \tag{2.3}$$

Fourth,

$$\begin{aligned}i\int_{\partial\Omega}[2|\mathbf{n}\cdot P|^2-|P|^2+(\mathbf{n}\cdot\bar{P})Q\eta]\mathrm{d}S = &\int_{\partial\Omega}\left[Q\bar{Q}_t+i\frac{2g}{p+1}|Q|^{p+1}\right]\mathrm{d}S - \partial_t\int_\Omega u(\xi\cdot\nabla u)\mathrm{d}x\\ &- i\int_\Omega\left\{\eta\left[+\frac{2g}{p+1}|u|^{p+1}\right]-(\nabla\eta\cdot\nabla\bar{u})u\right\}\mathrm{d}x\\ &-\int_\Omega\left\{\sum_{j,m}\partial_m\xi_j\,\partial_m u\,\partial_j\bar{u}-\mathrm{i}\,\eta|u|^{p+1}\right\}\mathrm{d}x.\end{aligned} \tag{2.4}$$

To prove global existence, consider $[0,T]$ for any $T>0$. We define

$$|P|^2=|\mathbf{n}\cdot P|^2+|A\cdot P|^2=|\mathbf{n}\cdot P|^2+|A\cdot\nabla\tilde{Q}|^2 \tag{2.5}$$

and

$$J^2 = \int_0^t \int_{\partial\Omega} |\mathbf{n} \cdot P|^2 \, \mathrm{d}S \, \mathrm{d}\tau, \tag{2.6}$$

where $A \cdot P$ denotes the tangential component of P. Integrating (2.1) and (2.2) over $[0,t]$, we obtain

$$\|u\|_2^2 \leqslant c + cJ \quad \text{and} \quad \|\nabla u\|_2^2 + \frac{2g}{p+1}\|u\|_{p+1}^{p+1} \leqslant c + cJ, \tag{2.7}$$

where c is treated as a generic constant (see Ref. 7, for example).

From Gagliardo-Nirenburg estimate:[10]

$$\|u\|_{p+1} \leqslant m(\|\nabla u\|_2^a \|u\|_2^{1-a} + \|u\|_2), \tag{2.8}$$

where

$$\frac{1}{p+1} = a\left(\frac{1}{2} - \frac{1}{n}\right) + \frac{1-a}{2}. \tag{2.9}$$

We find

$$a = \frac{n}{2} - \frac{n}{p+1}, \tag{2.10}$$

$$a(p+1) = \frac{n}{2}(p-1), \tag{2.11}$$

and

$$(1-a)(p+1) = \left(1 - \frac{n}{2}\right)(p+1) + n. \tag{2.12}$$

Case (i): $p < 1 + 2/n$. From (2.11) and (2.12) one has

$$a(p+1) = \beta < \frac{n}{2}\left(1 + \frac{2}{n} - 1\right) = 1 \tag{2.13}$$

and

$$(1-a)(p+1) \leqslant \left(1 - \frac{n}{2}\right)\left(2 + \frac{2}{n}\right) + n = 1 + \frac{2}{n} \leqslant 2; \tag{2.14}$$

here we assume that $n \geqslant 2$.

Therefore (2.8), (2.13), and (2.14) imply that (noting that $p+1 \leqslant 2 + \frac{2}{h} \leqslant 3$)

$$\|u\|_{p+1}^{p+1} \leqslant (\|\nabla u\|_2^\beta (\|u\|_2^2 + 1) + \|u\|_2^3 + 1) \leqslant \epsilon \|\nabla u\|_2^2 + \epsilon \|u\|_2^4 + c \leqslant c + cJ + c\epsilon J^2, \tag{2.15}$$

for any $\epsilon > 0$ and some c depending on m, ϵ and initial data.

Combining (2.6), (2.7), and (2.15) one has (again we treat c as a generic constant)

$$\|u\|_2^2 + \|\nabla u\|_2^2 \leqslant c + cJ + c\epsilon J^2. \tag{2.16}$$

Substituting (2.5) into (2.4), integrating over $[0,t]$, where $t < T$ and using the assumption that up to three derivatives of ξ are bounded, we obtain

$$J^2 \leqslant \left| \int_\Omega u(\xi \cdot \nabla u)\mathrm{d}x \right| + \left| \int_\Omega \phi(\xi \cdot \nabla \phi)\mathrm{d}x \right| + \int_0^t \int_{\partial\Omega} |A \cdot \nabla \tilde{Q}|^2 \,\mathrm{d}S\,\mathrm{d}\tau + \int_0^t \int_{\partial\Omega} |Q\bar{Q}_t|\mathrm{d}S\,\mathrm{d}\tau$$
$$+ c\int_0^t \int_{\partial\Omega} |(\mathbf{n}\cdot\bar{P})Q|\mathrm{d}S\,\mathrm{d}\tau + c\int_0^t \int_\Omega |\nabla u||u|\mathrm{d}x\,\mathrm{d}\tau + c\int_0^t \int_\Omega |\nabla u|^2\,\mathrm{d}x\,\mathrm{d}\tau$$
$$- \frac{2g}{p+1}\int_0^t \int_{\partial\Omega} |Q|^{p+1}\,\mathrm{d}S\,\mathrm{d}\tau - \frac{2g}{p+1}\int_0^t \int_\Omega |u|^{p+1}\,\mathrm{d}x\,\mathrm{d}\tau. \tag{2.17}$$

Since $\phi \in H^1(\Omega)$, Q is C^3 with compact support in x, each term in (2.17) involving ϕ and Q is bounded. Therefore (2.17) is estimated as

$$J^2 \leqslant c' + c'J + c'\int_\Omega (|u|^2 + |\nabla u|^2)\mathrm{d}x + c'\int_0^t \int_\Omega (|u|^2 + |\nabla u|^2)\mathrm{d}x\,\mathrm{d}\tau + c'\int_0^t \int_\Omega |u|^{p+1}\,\mathrm{d}x\,\mathrm{d}\tau. \tag{2.18}$$

It is important to note that all the constants denoted by c and c' only depend on n, p, Q, T, ϕ, and $\partial\Omega$, but not on u. Let ϵ be sufficiently small such that $\epsilon c c' = \frac{1}{4}$. Substituting (2.15) and (2.16) into (2.18) we obtain

$$\begin{aligned} J^2 &\leqslant c' + c'J + c'(c + cJ + c\epsilon J^2) + 2c'\int_0^t (c + cJ + c\epsilon J^2)\mathrm{d}\tau \\ &\leqslant c' + \frac{1}{2}\left((2c')^2 + \left(\frac{J}{2}\right)^2\right) + c'c + \frac{1}{2}\left((2c'c)^2 + \left(\frac{J}{2}\right)^2\right) + \frac{J^2}{4} + 2c'\int_0^t \left(c + \frac{1}{2}(c^2 + J^2) + c\epsilon J^2\right)\mathrm{d}\tau \\ &\leqslant c' + 2(c')^2 + \frac{J^2}{8} + c'c + 2(c'c)^2 + \frac{J^2}{8} + \frac{J^2}{4} + 2c'cT + c'c^2T + \left(c' + \frac{1}{2}\right)\int_0^t J^2\,\mathrm{d}\tau \\ &\leqslant c_0 + \frac{J^2}{2} + c_0\int_0^t J^2\,\mathrm{d}\tau. \end{aligned} \tag{2.19}$$

Then (2.19) implies that

$$J^2 \leqslant 2c_0 + 2c_0\int_0^t J^2\,\mathrm{d}\tau. \tag{2.20}$$

By Gronwall's lemma there exists $M > 0$ depending on n, p, Q, T, ϕ, and $\partial\Omega$, such that

$$J^2 \leqslant M, \tag{2.21}$$

for any $t \in [0, T]$.

By (2.16) we deduce that $\|u\|_{H^1}$ is bounded for bounded T.

Case (ii) $p = 1 + 2/n$. For any $\epsilon > 0$, let t_1 be sufficiently small, such that

$$\int_0^{t_1} \int_{\partial\Omega} (|Q|^2 + |Q_t|^2)\mathrm{d}S\,\mathrm{d}\tau < \epsilon. \tag{2.22}$$

Thus (2.6) and (2.7) are modified as

$$\|u\|_2^2 \leqslant c + \epsilon J \tag{2.23}$$

and

$$\|\nabla u\|_2^2 + \frac{2g}{p+1}\|u\|_{p+1}^{p+1} \leqslant c + \epsilon J, \tag{2.24}$$

for $t \in [0,t_1]$. Since

$$a(p+1) = \frac{n}{2}\left(1 + \frac{2}{n} - 1\right) = 1 \tag{2.25}$$

and

$$(1-a)(p+1) = \left(1 - \frac{n}{2}\right)\left(2 + \frac{2}{n}\right) + n = 1 + \frac{2}{n} \leqslant 2, \tag{2.26}$$

(2.15) becomes (for any $t \in [0,t_1]$)

$$\|u\|_{p+1}^{p+1} \leqslant (\|\nabla u\|_2(\|u\|_2^2 + 1) + \|u\|_2^3 + 1) \leqslant \delta\|\nabla u\|_2^2 + c'\|u\|_2^4 + c', \tag{2.27}$$

for any sufficiently small δ.

Substituting (2.23) and (2.27) into (2.24) we obtain

$$\|\nabla u\|_2^2 \leqslant \tilde{c}(c + \epsilon J + \|u\|_2^4) \leqslant \tilde{c}(c + \epsilon J + (c + \epsilon J)^2) \leqslant \hat{c} + \hat{c}\epsilon J^2. \tag{2.28}$$

By combining (2.23), (2.27), and (2.28), and choosing ϵ, δ sufficiently small, we estimate (2.17) as

$$J^2 \leqslant c + c\epsilon J^2 + \int_0^t (c + c\epsilon J^2)\mathrm{d}\tau, \tag{2.29}$$

where c only depends on ϵ, δ, n, p, Q, t_1, ϕ, and $\partial\Omega$. This proves that u is bounded in H^1 space on $[0,t_1]$.

Since $Q \in C^3$ has compact support, for any $\epsilon > 0$, $T > 0$ there exists a finite partition $0 \leqslant t_1 \leqslant t_2, \cdots \leqslant t_N = T$, such that

$$\int_{t_i}^{t_{i+1}} (|Q|^2 + |Q_t|^2)\mathrm{d}\tau \leqslant \epsilon, \tag{2.30}$$

for $i = 1,2,\ldots,N-1$. By mathematical induction we conclude that u is bounded in H^1 space on $[0,T]$. Since T is arbitrary, this solution is a global solution in H^1.

The existence and uniqueness theorem can be obtained in the similar manner as in Refs. 7–9 by truncating the nonlinear term, converting the original problem into a problem with a homogeneous boundary condition, and applying Aubin's compactness theorem and Cantor diagonalization. For uniqueness, we notice that $p < 1 + 4/(n-2)$ is required in case of $g > 0$ for a Dirichlet inhomogeneous boundary value problem for the NLS.[7] However, $p \leqslant 1 + 2/n$ would ensure that. Therefore, we have the following result.

Global existence-uniqueness theorem: *For $n > 1$, $g < 0$, assume that $p \leqslant 1 + 2/n$. Let $\phi \in H^1(\Omega)$ and Ω be a (bounded or unbounded) open subset of $\mathbb{R}^n$ with a C^∞ boundary. Suppose that $Q \in C^3(\partial\Omega \times (-\infty,\infty))$ has compact support and satisfies the compatibility condition $\phi(x) \equiv Q(x,0)$ on $\partial\Omega$ in the sense of traces. Then there exists a solution $u \in L^\infty_{\mathrm{loc}}((-\infty,\infty); H^1(\Omega) \cap L^{p+1}(\Omega))$ to the problem (1.1) for $-\infty < t < \infty$. The PDE is understood in the sense of distributions while the boundary condition is understood as $u(\cdot,t) - Q(\cdot,t) \in H_0^1(\Omega)$ for a.e. t. Further, if $\|e^{i\Delta t}\|_{\mathcal{L}(L^1(\Omega),L^\infty(\Omega))} \leqslant c/t^{n/2}$, where $e^{i\,\Delta t}$ denotes the evolution operator for the free Schrödinger equation with a homogeneous boundary condition on $\partial\Omega$, then this solution is unique.*

We state the following remark as the conclusion of this paper.

Remark: In the case of $n = 1$, we note that global existence was found if $p < 3$ (see Ref. 6), which is consistent with our criteria for global existence in general n space dimensions $p < 1 + 2/n$. We also did some numerical calculations using the FLEXPDE *program when $n = 2,3$. We are*

particularly interested in the situation $p>1+2/n$ *when* $n=2$ *and* $1+2/n<p<1+4/(n-2)$ *when* $n=3$ *with assorted initial and boundary data. However, the results do not seem to be conclusive and therefore further study is needed.*

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Existence and regularity for an energy maximization problem in two dimensions

Spyridon Kamvissis
Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany

Evguenii A. Rakhmanov
Department of Mathematics, University of South Florida, Tampa, Florida 33620

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We consider the variational problem of maximizing the weighted equilibrium Green's energy of a distribution of charges free to move in a subset of the upper half-plane, under a particular external field. We show that this problem admits a solution and that, under some conditions, this solution is an S-curve (in the sense of Gonchar-Rakhmanov). The above problem appears in the theory of the semiclassical limit of the integrable focusing nonlinear Schrödinger equation. In particular, its solution provides a justification of a crucial step in the asymptotic theory of nonlinear steepest descent for the inverse scattering problem of the associated linear non-self-adjoint Zakharov-Shabat operator and the equivalent Riemann-Hilbert factorization problem. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Let $\mathbb{H}=\{z:\operatorname{Im} z>0\}$ be the complex upper-half plane and $\overline{\mathbb{H}}=\{z:\operatorname{Im} z\geqslant 0\}\cup\{\infty\}$ be the closure of $\mathbb{H}$. Let also $\mathbb{K}=\{z:\operatorname{Im} z>0\}\backslash\{z:\operatorname{Re} z=0, 0<\operatorname{Im} z\leqslant A\}$, where A is a positive constant. In the closure of this space, $\overline{\mathbb{K}}$, we consider the points ix_+ and ix_-, where $0\leqslant x<A$ as distinct. In other words, we cut a slit in the upper half-plane along the segment $(0,iA)$ and distinguish between the two sides of the slit. The point infinity belongs to $\overline{\mathbb{K}}$, but not $\mathbb{K}$. We define $\mathbb{F}$ to be the set of all "continua" F in $\overline{\mathbb{K}}$ (i.e., connected compact sets) containing the distinguished points $0_+,0_-$.

Next, let $\rho^0(z)$ be a given complex-valued function on $\overline{\mathbb{H}}$ satisfying

$$\begin{gathered}\rho^0(z)\ \textit{is holomorphic in}\ \mathbb{H},\\ \rho^0(z)\ \textit{is continuous in}\ \overline{\mathbb{H}},\\ \operatorname{Re}[\rho^0(z)]=0,\quad \textit{for}\ z\in[0,iA],\\ \operatorname{Im}[\rho^0(z)]>0,\quad \textit{for}\ z\in(0,iA]\cup\mathbb{R}.\end{gathered}\tag{1}$$

Define $G(z;\eta)$ to be the Green's function for the upper half-plane

$$G(z;\eta)=\log\frac{|z-\eta^*|}{|z-\eta|}\tag{2}$$

and let $\mathrm{d}\mu^0(\eta)$ be the non-negative measure $-\rho^0(\eta)\mathrm{d}\eta$ on the segment $[0,iA]$ oriented from 0 to iA. The star denotes complex conjugation. Let the "external field" ϕ be defined by

$$\phi(z) = -\int G(z;\eta)\mathrm{d}\mu^0(\eta) - \mathrm{Re}\left(i\pi J \int_z^{iA} \rho^0(\eta)\mathrm{d}\eta + 2iJ(zx+z^2t)\right), \tag{3}$$

where x,t are real parameters with $t\geqslant 0$ and $J=1$, *for* $x\geqslant 0$, while $J=-1$, *for* $x<0$. Re denotes the real part.

The particular form of this field is dictated by the particular application to the dynamical system we are interested in. The conditions (1) are natural in view of this application. But many of our results in this paper are valid if the term $zx+z^2t$ is replaced by any polynomial in z. Here x,t are in fact the space and time variables for the associated partial differential equation (PDE) problem [see (9) and (10) below].

Let $\mathbb{M}$ be the set of all positive Borel measures on $\overline{\mathbb{K}}$, such that both the free energy

$$E(\mu) = \int\int G(x,y)\mathrm{d}\mu(x)\mathrm{d}\mu(y), \quad \mu \in \mathbb{M} \tag{4}$$

and $\int \phi\, \mathrm{d}\mu$ are finite. Also, let

$$V^{\mu}(z) = \int G(z,x)\mathrm{d}\mu(x), \quad \mu \in \mathbb{M} \tag{5}$$

be the Green's potential of the measure μ.

The weighted energy of the field ϕ is

$$E_{\phi}(\mu) = E(\mu) + 2\int \phi\, \mathrm{d}\mu, \quad \mu \in \mathbb{M}. \tag{6}$$

Now, given any continuum $F \in \mathbb{F}$, the equilibrium measure λ^F supported in F is defined by

$$E_{\phi}(\lambda^F) = \min_{\mu \in M(F)} E_{\phi}(\mu), \tag{7}$$

where $M(F)$ is the set of measures in $\mathbb{M}$ which are supported in F, provided such a measure exists. $E_{\phi}(\lambda^F)$ is the equilibrium energy of F.

The aim of this paper is to prove the existence of a so-called S-curve (Ref. 1) joining the points 0_+ and 0_- and lying entirely in $\overline{\mathbb{K}}$, at least under some extra assumptions. By S-curve we mean an oriented curve F such that the equilibrium measure λ^F exists, its support consists of a finite union of analytic arcs and at any interior point of supp μ,

$$\frac{d}{\mathrm{d}n_+}(\phi + V^{\lambda^F}) = \frac{d}{\mathrm{d}n_-}(\phi + V^{\lambda^F}), \tag{8}$$

where the two derivatives above denote the normal (to supp μ) derivatives.

To prove the existence of the S-curve we will first need to prove the existence of a continuum F maximizing the equilibrium energy over $\mathbb{F}$. Then we will show that the maximizer is in fact an S-curve.

It is not always true that an equilibrium measure exists for a given continuum. The Gauss-Frostman theorem (Ref. 2, p.135) guarantees the existence of the equilibrium measure when F does not touch the boundary of the domain $\mathbb{H}$. This is not the case here. Still, as we show in the next section, in the particular case of our special external field, for any given x,t and for a large class of continua F not containing infinity, the weighted energy is bounded below and λ^F exists. So, in particular, we do know that the supremum of the equilibrium weighted energies over all continua is greater than $-\infty$.

S-curves were first defined in Ref. 1, where the concept first arose in connection with the problem of rational approximation of analytic functions. Our own motivation comes from a seem-

ingly completely different problem, which is the analysis of the so-called semiclassical asymptotics for the focusing nonlinear Schrödinger equation. More precisely, we are interested in studying the behavior of solutions of

$$i\hbar\partial_t\psi + \frac{\hbar^2}{2}\partial_x^2\psi + |\psi|^2\psi = 0,$$
$$\text{under } \psi(x,0) = \psi_0(x), \tag{9}$$

in the so-called semiclassical limit, i.e., as $\hbar \to 0$. For a concrete discussion, let us here assume that $\psi_0(x)$ is a positive "bell-shaped" function; in other words assume that

$$\psi_0(x) > 0, \quad x \in \mathbb{R},$$
$$\psi_0(-x) = \psi_0(x),$$
$$\psi_0 \text{ has one single local maximum at } 0, \quad \psi_0(0) = A, \tag{10}$$
$$\psi_0''(0) < 0,$$
$$\psi_0 \text{ is Schwartz}.$$

This is a completely integrable PDE and can be solved via the method of inverse scattering. The semiclassical limit is analyzed in the recent research monograph.[3] In Chap. 8 of Ref. 3 it is noted that the semiclassical problem is related and can be reduced to a particular "electrostatic" variational problem of maximizing the equilibrium energy of a distribution of charges that are free to move under a given external electrostatic field (assuming that the WKB-approximated density of the eigenvalues admits a holomorphic extension in the upper half-plane). In fact, it is pointed out that the existence and regularity of an S-curve implies the existence of the so-called "g-function" necessary to justify the otherwise rigorous methods employed in Ref. 3.

We would like to point out that the problem of the existence of the "g function" for the semiclassical nonlinear Schrödinger problem is not a mere technicality of isolated interest. Rather, it is an instance of a crucial element in the asymptotic theory of Riemann-Hilbert problem factorizations associated to integrable systems. This asymptotic method has been made rigorous and systematic in Ref. 4 where in fact the term "nonlinear steepest descent method" was first employed to stress the relation with the classical "steepest descent method" initiated by Riemann in the study of exponential integrals with a large phase parameter. Such exponential integrals appear in the solution of Cauchy problems for linear evolution equations, when one employs the method of Fourier transforms. In the case of nonlinear integrable equations, on the other hand, the nonlinear analog of the Fourier transform is the scattering transform and the inverse problem is now a Riemann-Hilbert factorization problem. While in the "linear steepest descent method" the contour of integration must be deformed to a union of contours of "steepest descent" which will make the explicit integration of the integral possible, in the case of the "nonlinear steepest descent method" one deforms the original Riemann-Hilbert factorization contour to appropriate steepest descent contours where the resulting Riemann-Hilbert problems are explicitly solvable.

In the linear case, if the phase and the critical points of the phase are real it may not be necessary to deform the integration contour. One has rather a Laplace integral problem on the contour given. For Riemann-Hilbert problems the analog is the self-adjointness of the underlying Lax operator. In this case the spectrum of the associated linear Lax operator is real and the original Riemann-Hilbert contour is real. The "deformation contour" must then stay near the real line. One novelty of the semiclassical problem for (9) and (10) studied in Ref. 3 however is that, due to the non-self-adjointness of the underlying Lax operator, the "target contour" is very specific (if not

unique) and by no means obvious. It is best characterized via the solution of a maximin energy problem, in fact it is an S-curve. The term "nonlinear steepest descent method" thus acquires full meaning in the non-self-adjoint case.

Given the importance and the recent popularity of the "steepest descent method" and the various different applications to such topics as soliton theory, orthogonal polynomials, solvable models in statistical mechanics, random matrices, combinatorics and representation theory, we believe that the present work offers an important contribution. In particular we expect that the results of this paper may be useful in the treatment of Riemann-Hilbert problems arising in the analysis of general complex or normal random matrices.

On the other hand, we believe that the main results of this paper, Theorems 3, 4, 5, 7, 8 are interesting on their own. This paper can be read without the applications to dynamical systems in mind. It concerns existence and regularity of a solution to an energy variational maximin problem in the complex plane.

The method used to prove the existence of the S-curves arising in the solution of the "max-min" energy problem was first outlined in Ref. 1 and further developed in Ref. 5, at least for logarithmic potentials. But, the concrete particular problem addressed in this paper involves additional technical issues.

The main points of the proof of our results are as follows:

(i) Appropriate definition of the underlying space of continua (connected compact sets) and its topology. This ensures the compactness of our space of continua which is crucial in proving the existence of an energy maximizing element.
(ii) Proof of the semicontinuity of the energy functional that takes a continuum to the energy of its associated equilibrium measure (Theorem 3).
(iii) Proof of existence of an energy maximizing continuum (Theorem 4).
(iv) A discussion of how some assumptions ensure that the maximizing continuum does not touch the boundary of the underlying space except at a finite number of points. This ensures that variations of continua can be taken.
(v) Proof of formula (22) involving the support of the equilibrium measure on the maximizing continuum and the external field (Theorem 5).
(vi) Proof that the support of the equilibrium measure on the maximizing continuum consists of a union of finitely many analytic arcs.
(vii) Proof that the maximizing continuum is an S-curve (Theorems 7 and 8).

The paper is organized as follows. In the rest of Sec. I, we introduce the appropriate topology for our set of continua that will provide the necessary compactness. In Sec. II, we prove a "Gauss-Frostman" type theorem which shows that the variational problem that we wish to solve is not vacuous. In Sec. III, we present the proof of upper semicontinuity of a particularly defined "energy functional." In Sec. IV, we present a proof of existence of a solution of the variational problem. Existence is thus derived from the semicontinuity and the compactness results acquired earlier. In Sec. V, we show that, at least under a simplifying assumption, the "max-min" solution of the variational problem does not touch the boundary of the underlying domain, except possibly at some special points. This enables us to eventually take variations and show that the max-min property implies regularity of the support of the solution and the S-property in Secs. VI and VII. By regularity, we mean that the support of the maximizing measure is a finite union of analytic arcs. In Sec. VIII, we conclude by stating the consequence of the above results in regard to the semiclassical limit of the nonlinear Schödinger equation.

We also include three appendixes. The first one discusses in detail some topological facts regarding the set of closed subsets of a compact space, equipped with the so-called Hausdorff distance. The fact that such a space is compact is vital for proving existence of a solution for the variational problem. The second appendix presents the semiclassical asymptotics for the initial value problem (9) and (10) in terms of theta functions, under the S-curve assumption (as in Ref. 3). It is included so that the connection with the original motivating problem of semiclassical NLS is made more explicit. The third appendix sketches an argument on how to get rid of the simpli-

fying assumption introduced in Sec. V. We feel that the argument leading to Theorem 9 is quite transparent, although an absolutely rigorous proof would require a thorough revisiting of the discussion and results in Ref. 3.

Following Ref. 6 (see Appendix A) we introduce an appropriate topology on $\mathbb{F}$. We think of the closed upper half-plane $\overline{\mathbb{H}}$ as a compact space in the Riemann sphere. We thus choose to equip $\overline{\mathbb{H}}$ with the "chordal" distance, denoted by d_0, that is the distance between the images of z and ζ under the stereographic projection. This induces naturally a distance in $\overline{\mathbb{K}}$ [so $d_0(0_+,0_-)\neq 0$]. We also denote by d_0 the induced distance between compact sets E,F in $\overline{\mathbb{K}}$, $d_0(E,F)=\max_{z\in E}\min_{\zeta\in F} d_0(z,\zeta)$. Then, we define the so-called Hausdorff metric on the set $I(\overline{\mathbb{K}})$ of closed nonempty subsets of $\overline{\mathbb{K}}$ as follows:

$$d_{\mathbb{K}}(A,B)=\sup(d_0(A,B),d_0(B,A)). \tag{11}$$

In Appendix A, we prove the following.

Lemma A.1: The Hausdorff metric defined by (11) is indeed a metric. The set $I(\overline{\mathbb{K}})$ is compact and complete.

Now, it is easy to see that $\mathbb{F}$ is a closed subset of $I(\overline{\mathbb{K}})$. Hence $\mathbb{F}$ is also compact and complete.

Remarks: (1) Because of the particular symmetry $\psi(x)=\psi(-x)$ of the solution to the Cauchy problem (9) and (10) we will restrict ourselves to the case $x\geqslant 0$ from now on. We then set $J=1$ and the external field is

$$\phi(z)=-\int G(z;\eta)\mathrm{d}\mu^0(\eta)-\mathrm{Re}\left(i\pi\int_z^{iA}\rho^0(\eta)\mathrm{d}\eta+2i(zx+z^2t)\right). \tag{3'}$$

(2) The function ρ^0 expresses the density of eigenvalues of the Lax operator associated to (9), in the limit as $h\to 0$. WKB theory can be used to derive an expression for ρ^0 in terms of the initial data $\psi^0(x)$ via an Abel transform (see Ref. 3), from which it follows that

$$\mathrm{Re}[\rho^0(z)]=0 \quad \text{for } z\in[0,iA],$$

$$\mathrm{Im}[\rho^0(z)]>0 \quad \text{for } z\in(0,iA].$$

The rest of the conditions (1) are not a necessary consequence of WKB theory. In particular, it is not *a priori* clear what the analyticity properties of ρ^0 are. In this paper, we *assume*, for simplicity, that ρ^0 admits a continuous extension in the closed upper complex plane which is holomorphic in the open upper complex plane. We also assume that $\mathrm{Im}\,\rho^0$ is positive in the real axis. This will be used later to show that the maximizing continuum does not touch the real line, except at $0_+,0_-,\infty$. It is a simplifying but not essential assumption. All conditions (1) are satisfied in the simple case where the initial data are given by $\psi(x,0)=A\,\mathrm{sech}\,x$, where A is a positive constant.

(3) It follows that ϕ is a subharmonic function in $\mathbb{H}$ which is actually harmonic in $\mathbb{K}$; it also follows that it is upper semicontinuous in $\mathbb{H}$. It is then subharmonic and upper semicontinuous in $\overline{\mathbb{H}}$ except at infinity.

(4) Even though in the end we wish that the maximum of $E_\phi(\lambda^F)$ over "continua" F is a regular curve, we will begin by studying the variational problem over the set of continua $\mathbb{F}$ and only later (in Sec. VI) we will show that the maximizing continuum is in fact a nice curve. The reason is that the set $\mathbb{F}$ is compact, so once we prove in Sec. III the upper semicontinuity of the energy functional, existence of a maximizing continuum will follow immediately.

II. A GAUSS-FROSTMAN THEOREM

We claim that for any continuum $F \in \mathbb{F}$, not containing the point ∞ and approaching 0_+, 0_- nontangentially to the real line, the weighted energy is bounded below and the equilibrium measure λ^F exists. This is not true for any external field, but it is true for the field given by (3′) because of the particular behavior of the function ρ^0 near zero.

We begin by considering the equilibrium measure on the particular contour F_0 that wraps itself around the straight line segment $[0, iA]$, say λ_0^F. We have

Proposition 1: Consider the contour $F_0 \in \mathbb{F}$ consisting of the straight line segments joining 0_+ to $iA_+ = iA$ and $iA = iA_-$ to 0_-. The equilibrium measure λ_0^F exists. Its support is the imaginary segment $[0, ib_0(x)]$, for some $0 < b_0(x) \leqslant A$, lying on the right-hand side of the slit $[0, iA]$. It can be written as $\rho(z)\mathrm{d}z$ where $\rho(z)$ is a differentiable function in $[0, ib(x)]$, such that $\rho - \rho^0$ belongs in the Hölder class with exponent $1/2$.

Proof: See section 6.2.1 of Ref. 3; $\rho(z)$ can be expressed explicitly. The Hölder condition follows from 5.14 of Ref. 3. Note that the field ϕ is independent of time on F_0, so λ_0^F is also independent of time.

From Proposition 1, it follows that the maximum equilibrium energy over continua is bounded below,

$$\max_{F \in \mathbb{F}} E_\phi(\lambda^F) = \max_{F \in \mathbb{F}} \min_{\mu \in M(F)} E_\phi(\mu) > -\infty. \tag{12}$$

The following formula is easy to verify:

$$E_\phi(\mu) - E_\phi(\lambda^F) = E(\mu - \lambda^F) + 2 \int (V^{\lambda^F} + \phi) d(\mu - \lambda^F), \tag{13}$$

for any μ which is a positive measure on the continuum F. Here

$$V^{\lambda^F}(u) = \int G(u,v)\mathrm{d}\lambda^F(v),$$

where again $G(u,v)$ is the Green function for the upper half-plane.

To show that $E_\phi(\mu)$ is bounded below, all we need to show is that the difference $E_\phi(\mu) - E_\phi(\lambda^F)$ is bounded below.

Note that since $V^{\lambda^F} + \phi = 0$, *on* $\mathrm{supp}(\lambda^F)$, the integral in (13) can be written as $\int (V^{\lambda^F} + \phi)\mathrm{d}\mu$.

We have

$$\begin{aligned} V^{\lambda^F}(z) + \phi(z) &= \int_0^{b_0(x)} \log \frac{|z+iu|}{|z-iu|} (-\rho)_{t=0}\, \mathrm{d}u + \phi \\ &= -\mathrm{Re}\left(\int_0^{b_0(x)} \log \frac{|z+iu|}{|z-iu|} u^{1/2}\, \mathrm{d}u \right) + O(|z|) = O(|z|) \ \textit{near}\ z = 0. \end{aligned}$$

So we can write $V^{\lambda^F} + \phi \geqslant c(A,x)|z|$ in a neighborhood of $z=0$, where $c(A,x)$ will be some negative constant independent of z. Note that the dependence on t is not suppressed, but it is of order $O(|z^2|)$.

It is now not hard to see that the $O(|z|)$ decay implies our result.

Write $\mu = M\sigma$, where $M > 0$ is the total mass of μ and σ is a probability measure (on F). Choose ϵ such that for $|u| < \epsilon$ we have $V^{\lambda^F} + \phi \geqslant c(A,x)|u|$. Then

$$\begin{aligned} E_\phi(\mu) - E_\phi(\lambda^F) \geqslant & \int G(u,v) d(\mu - \lambda^F)(u) d(\mu - \lambda^F)(v) + 2 \int_{|v| \geqslant \epsilon} (V^{\lambda^F} + \phi)(v) \mathrm{d}\mu(v) \\ & + \int_{|v| < \epsilon} 2c(A,x)|v| d(\mu - \lambda^F)(v). \end{aligned} \tag{14}$$

The first integral of the right-hand side (RHS) can be written as $\int_{|u|\geqslant\epsilon,|v|\geqslant\epsilon}+2\int_{|u|<\epsilon,|v|\geqslant\epsilon}+\int_{|u|,|v|<\epsilon}$. The sum of the first integral plus the second term on the RHS of (14) is bounded below, by the standard Gauss-Frostman theorem (Ref. 6, p. 135). It remains to consider

$$\left(\int_F+\int_{|v|\geqslant\epsilon}\right)\left(\int_{|u|<\epsilon}G(u,v)d(\mu-\lambda^F)(u)\right)d(\mu-\lambda^F)(v)+\int_{|v|<\epsilon}2c(A,x)|v|d(\mu-\lambda^F)(v)$$
$$\geqslant\left(\int_F+\int_{|v|\geqslant\epsilon}\right)\left(\int_{|u|<\epsilon}G(u,v)d(M\sigma-\lambda^F)(u)+2c(A,x)|v|\right)d(M\sigma-\lambda^F)(v). \tag{15}$$

Now, it is easy to see that for M large, and since F is nontangential to the real line,

$$\int_{|u|<\epsilon}G(u,v)d(M\sigma-\lambda^F)(u)+2c(A,x)|v|\geqslant|v\log v|+2c(A,x)|v|. \tag{16}$$

By adjusting ϵ if necessary, we have $|v\log v|>2|c(A,x)||v|$, and hence the integral in (16) is positive. Integrating again with respect to $M\,\mathrm{d}\sigma-\mathrm{d}\lambda^F$, again for M large, we see that the integral of (15) is positive.

Since when M is bounded above we have our estimates trivially, we get boundedness below over all positive M.

We have thus proved one part of our (generalized) Gauss-Frostman theorem.

Theorem 1: Let ϕ be given by (3′). Let F be a continuum in $\overline{\mathbb{K}}\backslash\infty$ and suppose that F is contained in some sector $\pi<\alpha<\arg(\lambda)<\beta<0$ as $\lambda\to0$. Let $M(F)$ be the set of measures $\in\mathbb{M}$ which are supported in F. [So, in particular their free energy is finite and $\phi\in L_1(\mu)$.] We have

$$\inf_{\mu\in M(F)}E_\phi(\mu)>-\infty. \tag{17}$$

Furthermore the equilibrium measure on F exists, that is there is a measure $\lambda^F\in M(F)$ such that $E_\phi[F]=E_\phi(\lambda^F)=\inf_{\mu\in M(F)}E_\phi(\mu)$.

Proof: The proof that (17) implies the existence of an equilibrium measure is a well-known theorem. For our particular field ϕ given by (3) it is easy to prove. Indeed, the identity

$$E(\mu-\nu)=2E_\phi(\mu)+2E_\phi(\nu)-4E_\phi\left(\frac{\mu+\nu}{2}\right)$$

implies that any sequence μ_n minimizing $E_\phi(\mu)$ is a Cauchy sequence in (unweighted) energy. Since the space of positive measures is complete (see, for example, Ref. 7, Theorem 1.18, p. 90), there is a measure μ_0 such that $E(\mu_n-\mu_0)\to0$. We then have $E(\mu_n)\to E(\mu_0)<+\infty$ and hence $\mu_n\to\mu_0$ weakly (see, e.g., Ref. 7, pp. 82–88; this is a standard result).

The fact that $\phi\in L_1(\mu_0)$ is trivial for our particular field.

III. SEMICONTINUITY OF THE ENERGY FUNCTIONAL

We consider the functional that takes a given continuum F to the equilibrium energy on this continuum,

$$\mathbb{E}:F\to E_\psi[F]=E_\psi(\lambda^F)=\inf_{\mu\in M(F)}\left(E(\mu)+2\int\psi\,\mathrm{d}\mu\right) \tag{18}$$

and we want to show that it is continuous, if ψ is continuous in $\overline{\mathbb{H}}$. Note that this is not the case for the field ϕ given by (3′), since it has a singularity at ∞; that field is only upper semicontinuous. We will see how to circumvent this difficulty later. For the moment, ψ is simply assumed to be a continuous function in $\overline{\mathbb{H}}$.

Theorem 2: If ψ is a continuous function in $\overline{\mathbb{H}}\backslash\infty$ then the energy functional defined by (18) is continuous at any given continuum F not containing the point ∞.

Proof: Suppose $G \in \mathbb{F}$, also not containing ∞, with $d_{\mathbb{K}}(F,G) < d$, a small positive constant. Let $\lambda = \lambda_\psi^F$ be the equilibrium measure on F and $\mu = \lambda_\psi^G$ be the equilibrium measure on G.

We consider the Green's balayage of μ on F, say $\hat{\mu}$. Then supp $\hat{\mu} \in F$ and

$$V^{\hat{\mu}} = V^{\mu} \quad \text{on } F,$$

$$\int u \, \mathrm{d}\hat{\mu} = \int u \, \mathrm{d}\mu,$$

for any function u that is harmonic in $\mathbb{H}\backslash F$ and continuous in $\overline{\mathbb{H}}$.

Similarly consider $\hat{\lambda}$, the balayage of λ to G. We trivially have

$$E_\psi[G] \leqslant E_\psi(\hat{\lambda}),$$

$$E_\psi[F] \leqslant E_\psi(\hat{\mu}).$$

Lemma 1: Suppose $Q \in \mathbb{F}$, μ some positive measure supported in $\mathbb{K}$ and $\hat{\mu}$ is the Green's balayage to Q. Then

$$V^{\hat{\mu}} = V^{\mu} - V^{\mu}_{Q^c},$$

$$E(\hat{\mu}) = E(\mu) - E_{Q^c}(\mu),$$

where $E_{Q^c}(\mu)$ is the unweighted Green energy with respect to $Q^c = \mathbb{K}\backslash Q$. In particular, since unweighted energies are non-negative,

$$E(\hat{\mu}) \leqslant E(\mu).$$

Proof: The first identity follows from the fact that $V^{\hat{\mu}} - V^{\mu}$ vanishes on Q and the real line, and is harmonic in Q^c and superharmonic in $\mathbb{K}$.

Integrating $E(\hat{\mu}) = \int V^{\hat{\mu}} \, \mathrm{d}\hat{\mu} = \int V^{\mu} \, \mathrm{d}\hat{\mu} - \int V^{\mu}_{Q^c} \, \mathrm{d}\hat{\mu} = \int (V^{\mu} - V^{\mu}_{Q^c}) \mathrm{d}\mu = E(\mu) - E_{Q^c}(\mu)$. The proof of the Lemma follows.

So, let u_ψ be a function harmonic in $\mathbb{H}\backslash F$ such that $u_\psi = \psi$ on F and $u_\psi = 0$ on $\partial\mathbb{H}\backslash F$. By the definition of balayage one has $\int \psi \, \mathrm{d}\hat{\mu} = \int u_\psi \, \mathrm{d}\mu$.

We have $E_\psi[F] \leqslant E_\psi(\hat{\mu}) = E(\hat{\mu}) + 2\int \psi \, \mathrm{d}\hat{\mu} \leqslant E(\mu) + 2\int \psi \, \mathrm{d}\mu + 2\int (u_\psi - \psi) \mathrm{d}\mu = E_\psi(\mu) + 2\int (u_\psi - \psi) \mathrm{d}\mu = E_\psi[G] + 2\int (u_\psi - \psi) \mathrm{d}\mu$.

In a small neighborhood of F, $\overline{F_d} = \{z : d(z,F) \leqslant d\}$, we have

$$\left| 2 \int (u_\psi - \psi)(y) \mathrm{d}\mu(y) \right| \leqslant C \max_{y \in \overline{F_d}} |u_\psi(y) - \psi(y)|. \tag{19}$$

We assumed here that the equilibrium measures on continua near F are bounded above. This is easy to see. Suppose, first, that the point ∞ is not in F. Indeed, on the support of the equilibrium measure λ, we have

$$V^{\lambda} + \psi = 0.$$

If the equilibrium measures on continua near F were unbounded, then so would be the potentials V^{λ}. But ψ is definitely bounded near F. This contradicts the above equality.

Now given $y \in \overline{F_d}$, choose $z \in F$ such that $|z - y| = d$. The above expression (19) is less or equal than

$$C \max_{y \in \overline{F_d}} |u_\psi(y) - \psi(y) - u_\psi(z) + \psi(z)| \leqslant o(1) + C \max_{y \in \overline{F_d}} |u_\psi(y) - u_\psi(z)|.$$

It remains to bound $|u_\psi(y) - u_\psi(z)|$ by an $o(1)$ quantity.

The next Lemma is due to Milloux and can be found in Ref. 8.

Lemma 2: Suppose D is an open disc of radius R, with center z_0; let y be a point in D, F a continuum in $\mathbb{C}$, containing z_0, and Ω be the connected component of $D\backslash F$ containing y. Let $w(z)$ be a function harmonic in Ω such that

$$w(z)=0, \quad z \in F \cap \partial\Omega,$$

$$w(z)=1, \quad z \in \partial\Omega \setminus F.$$

Then $w(y) \leqslant C(|y-z_0|/R)^{1/2}$.

Proof: See Ref. 8, p. 347.

Now, select a disc of radius $d^{1/2}$, centered on z. We have $|u_\psi(y)-u_\psi(z)|=o(1)$ on the part of F lying in the disc, while $|u_\psi(y)-u_\psi(z)|$ is bounded by some positive constant M on the disc boundary.

Lemma 3: Let Ω be a domain, $\partial\Omega=F_1\cup F_2$ and

$$w_1=0, \quad z \in F_1=1, \quad z \in F_2,$$

$$w_2=1, \quad z \in F_1=0, \quad z \in F_2.$$

Suppose u is harmonic in Ω and

$$u(z) \leqslant \epsilon, \quad z \in F_1,$$

$$u(z) \leqslant M, \quad z \in F_2.$$

Then $u(z) \leqslant \epsilon w_2(z)+Mw_1(z)$.

Proof: Maximum principle.

Now, using Milloux's lemma, we get $|u_\psi(y)-u_\psi(z)| \leqslant o(1)w_2(z)+Mw_1(z) \leqslant o(1)+MC(|y-z|/d)^{1/2} \leqslant o(1)+MCd^{1/2}$. This concludes the proof of Theorem 2.

We now recall that the energy continuity proof was based on the continuity of ψ. In our case, ϕ is upper semicontinuous and discontinuous at ∞. Still we can prove that the energy is upper semicontinuous and that will be enough.

Theorem 3: For the external field given by (3′), the energy functional defined in (18) is upper semicontinuous.

Proof: We first note that if the external field ϕ' is upper semicontinuous away from infinity then so is the energy functional that takes a given continuum F to the equilibrium energy of F. Indeed, if ϕ' is upper semicontinuous away from infinity, then there exists a sequence of continuous functions (away from infinity) such that $\phi_n \downarrow \phi'$. Each functional $E_{\phi_n}[F]$ is continuous, away from infinity, and $E_{\phi_n}[F] \downarrow E_{\phi'}[F]$. So, $E_{\phi'}[F]$ is upper semicontinuous, away from infinity.

Now consider the field ϕ given by (3′). Let F be a continuum. If ∞ is not in F, then we are done. If $\infty \in F$, let $\lambda=\lambda^F$ be the equilibrium measure. We can assume that on the equilibrium measure ϕ is bounded by 0. Indeed, on the support of the equilibrium measure λ, we have

$$V^\lambda + \phi = 0.$$

But $V^\lambda \geqslant 0$, so $\phi \leqslant 0$.

This means that we can change ϕ to $\phi'=\min(\phi,0)$, which *is* an upper semicontinuous function. Theorem 3 is proved.

Remark: If we naively consider the functional taking a measure to its weighted energy we will see that it is not continuous even if the external field is continuous. It is essential that the energy functional is defined on equilibrium measures.

IV. PROOF OF EXISTENCE OF A MAXIMIZING CONTINUUM

Theorem 4: For the external field given by $(3')$, there exists a continuum $F \in \mathbb{F}$ such that the equilibrium measure λ^F exists and

$$E_\phi[F](=E_\phi(\lambda^F)) = \max_{F\in\mathbb{F}} \min_{\mu\in M(F)} E_\phi(\mu).$$

Proof: We know (see, for example, Sec. II) that there is at least one continuum F for which the equilibrium measure exists and $E_\phi(\lambda^F) > -\infty$, for all time. On the other hand, clearly $E_\phi(\lambda^F) \leqslant 0$ for any F. Hence the supremum over continua in $\mathbb{F}$ is finite (and trivially nonpositive), since $\mathbb{F}$ is compact. Call it L.

We can now take a sequence F_n such that $E_\phi[F_n] \to L$. Choose a convergent subsequence of continua $F_n \to F$, say. By upper semicontinuity of the weighted energy functional,

$$\limsup E_\phi[F_n] \leqslant E_\phi[F] \leqslant L = \lim E_\phi[F_n].$$

So $L = E_\phi[F]$. The theorem is proved.

V. ACCEPTABILITY OF THE CONTINUUM

We have thus shown that a solution of the maximum-minimum problem exists. We do not know yet that the maximizing continuum is a contour. Clearly the pieces of the continuum lying in the region where the external field is positive do not support the equilibrium measure and by the continuity of the external field they can be perturbed to a finite union of analytic arcs. The real problem is to show that the support of the equilibrium measure is a finite union of analytic arcs. This will follow from the analyticity properties of the external field.

Note that the maximizing continuum cannot be unique, since the subset where the equilibrium measure is zero can be perturbed without changing the energy. A more interesting question is whether the support of the equilibrium measure of the maximizing contour is unique. We do not know the answer to this question but it is not important as far as the application to the semiclassical limit of NLS is concerned. (See Appendix B.)

It is important however, that the maximizing continuum does not touch the boundary of the space $\mathbb{K}$ except of course at the points 0^-, 0^+, and perhaps at ∞. This is to guarantee that variations with respect to the maximizing contour can be properly taken.

The proof of the acceptability of the continuum requires two things.

(i) The continuum does not touch the real negative axis.
(ii) The continuum does not touch the real positive axis.

We will also make the following assumption.

Assumption (A): The continuum maximizing the equilibrium energy does not touch the linear segment $(0, iA]$.

Remark: Assumption (A) is not satisfied at $t=0$, where in fact the continuum is a contour F_0 wrapping around the linear segment $[0, iA]$. However, the case $t=0$ is well understood. The equilibrium measure for F_0 exists and its support is connected. On the other hand, assumption (A) *is* satisfied for small $t>0$. (See Chap. 6 of Ref. 3.)

Remark: It is conceivable that at some positive t_0 there is an x for which assumption (A) is not satisfied. It can in fact be dropped but the analysis of the semiclassical limit of the nonlinear Schrödinger equation will get more tedious; see Appendix C.

Proposition 2: The continuum maximizing the equilibrium energy does not touch the real axis except at the points zero and possibly infinity.

Proof: (i) If $z<0$, then $\phi(z) = \pi \int_z^0 |\rho^0(\eta)| \mathrm{d}\eta > 0$.

This follows from an easy calculation, using the conditions defining ρ^0. But we can always delete the strictly positive measure lying in a region where the field is positive and make the energy smaller. So even the solution of the "inner" minimizing problem must lie away from the real negative axis.

(ii) If $z>0$, then again a short calculation shows that $\mathrm{d}\phi/d\,\mathrm{Im}\,z>0$, *for* $t>0$.

It is crucial here that if $u\in\mathbb{R}$ then $G(u,v)=0$, while if both u, v are off the real line $G(u,v)>0$. Hence, for any configuration that involves a continuum including points on the real line, we can find a configuration with no points on the real line, by pushing measures up away from the real axis, which has greater (unweighted *and* weighted) energy. So, suppose the maximizing continuum touches the axis. We can always push the measures up away from the real axis and end up with a continuum that has greater minimal energy, thus arriving at a contradiction.

The proposition is now proved.

Remark: It is also important to consider the point at infinity. We cannot prove that the continuum does not hit this point. [In fact, our numerics (Ref. 3, Chap. 6) show that it may well do so.] In connection with the semiclassical problem (9) and (10) as analyzed in Ref. 3, it might seem at first that the maximizing continuum should not pass through infinity. Indeed, the transformations (2.17) and (4.1) of Ref. 3 implicitly assume that the continuum C lies in $\mathbb{C}$. Otherwise, one would lose the appropriate normalization for M at infinity. However, one must simply notice that infinity is just an arbitrary choice of normalizing point, once we view our Riemann-Hilbert problems in the compact Riemann sphere. The important observation is that the composition of transformations (2.17) and (4.1) (which are purely formal, i.e., no estimates are required and no approximation is needed) does not introduce any bad (essential) singularities. In the end, the asymptotic behavior of $\widetilde{N}^{\sigma}$ is still the identity as $z\to\infty$ in the lower half-plane and nonsingular as $z\to\infty$ in the upper half-plane. So, in the end it *is* acceptable for a continuum to go through the point infinity.

VI. TAKING SMALL VARIATIONS

We now complexify the external field and extend it to a function in the whole complex plane, by turning a Green's potential to a logarithmic potential. We will thus be able to make direct use of the results of Ref. 5.

We let, for any complex z,

$$V(z)=-\int_{-iA}^{iA}\log(z-\eta)\rho^{0}(\eta)\mathrm{d}\eta-\left(2ixz+2itz^{2}+i\pi\int_{z}^{iA}\rho^{0}(\eta)\mathrm{d}\eta\right) \tag{20}$$

and $V_R=\mathrm{Re}\,V$ be the real part of V. In the lower half-plane the function ρ^0 is extended simply by

$$\rho^{0}(\eta^{*})=(\rho^{0}(\eta))^{*}. \tag{20'}$$

Note right away that the field ϕ defined in (3′) is the restriction of $V_R=\mathrm{Re}\,V$ to the closed upper half-plane.

The actual contour of the logarithmic integral is chosen to be the linear segment χ joining the points $-iA,0,iA$. The branch of the logarithm function $\log(z-\eta)$ is then defined to agree with the principal branch as $z\to\infty$, and with jump across the very contour χ.

The unweighted Green's energy (4) can be written as

$$E_{V_R}(\mu)=\int_{\mathrm{supp}\,\mu}\int_{\mathrm{supp}\,\mu}\log\frac{1}{|u-v|}\mathrm{d}\mu(u)\mathrm{d}\mu(v)+2\int_{\mathrm{supp}\,\mu}V_{R}(u)\mathrm{d}\mu(u), \tag{21}$$

where the measures μ are extended to the lower half complex plane by

$$\mu(z^{*})=-\mu(z). \tag{21'}$$

(So they are "signed" measures.)

Having established in Sec. V that the contour solving the variational problem does not touch the real line we can take small variations of measures and contours, never intersecting the real line, and keeping the points 0_-, 0_+ fixed. In view of (21′) we can think of them as variations of measures symmetric under (21′) in the full complex plane, never intersecting the real line, and

keeping the points 0_-, 0_+ fixed. The perturbed measures do not change sign. The fact that ∞ can belong to the contour is not a problem. Our variations will keep it automatically fixed.

The first step is to show that the solution of the variational problem satisfies a crucial relation.

Remark: It is not hard to see that the variational problem of Theorem 4 is actually *equivalent* to the variational problem of maximizing equilibrium measures on continua in the whole complex plane, under the symmetry (21′) and the condition that measures are to positive in the upper half-plane and negative in the lower half-plane.

Theorem 5: Let F be the maximizing continuum of Theorem 4 and λ^F be the equilibrium measure minimizing the weighted logarithmic energy (6) under the external field $V_R=\mathrm{Re}\, V$ where V is given by (20). Let μ be the extension of λ^F to the lower complex plane via $\mu(z^*)=-\mu(z)$. Then

$$\mathrm{Re}\left(\int \frac{\mathrm{d}\mu(u)}{u-z}+V'(z)\right)^2=\mathrm{Re}(V'(z))^2-2\,\mathrm{Re}\int\frac{V'(z)-V'(u)}{z-u}\mathrm{d}\mu(u)+\mathrm{Re}\left(\frac{1}{z^2}\int 2(u+z)V'(u)\mathrm{d}\mu(u)\right). \tag{22}$$

Proof: We first need to prove the following.

Theorem 6: Let Γ be a critical point of the functional taking a continuum $\Gamma\in\mathbb{F}$ to $E_{V_R}(\lambda^\Gamma)$, and assume that Γ is not tangent to $\mathbb{R}$. Also assume that Γ does not touch the segment $[0,iA]$ except at zero. Let μ be the extension of λ^Γ via $\mu(z^*)=-\mu(z)$, O_Γ be an open set containing the interior of $\Gamma\cup\Gamma^*$ and $h\in C^1(O_\Gamma)$ such that $h(0)=0$. We have

$$\mathrm{Re}\left(\int\int\frac{h(u)-h(v)}{u-v}\mathrm{d}\mu(u)\mathrm{d}\mu(v)\right)=2\,\mathrm{Re}\left(\int V'(u)h(u)\mathrm{d}\mu(u)\right). \tag{23}$$

Proof: Consider the family of (signed) measures $\{\mu^\tau,\tau\in\mathbb{C},|\tau|<\tau_0\}$ defined by $\mathrm{d}\mu^\tau(z^\tau)=\mathrm{d}\mu(z)$ where $z^\tau=z+\tau h(z)$, or equivalently, $\int f(z)\mathrm{d}\mu^\tau(z)=\int f(z^\tau)\mathrm{d}\mu(z)$, $f\in L_1(O_\Gamma)$. Assume that τ is small enough so that the support of the deformed continuum does not hit the linear segment $(0,iA]$ or a nonzero point in the real line.

With $\hat{h}=\hat{h}(u,v)=[h(u)-h(v)]/(u-v)$, we have $(u^\tau-v^\tau)/(u-v)=1+\tau\hat{h}$, so that $\log(1/|u^\tau-v^\tau|)-\log(1/|u-v|)=-\log|1+\tau\hat{h}|=-\mathrm{Re}(\tau\hat{h})+O(\tau^2)$.

Integrating with respect to $\mathrm{d}\mu(u)\mathrm{d}\mu(v)$ we arrive at

$$E(\mu^\tau)-E(\mu)=-\mathrm{Re}\left(\tau\int\hat{h}\,\mathrm{d}\mu(u)\mathrm{d}\mu(v)\right)+O(\tau^2), \tag{24}$$

where $E(\mu)$ denotes the free logarithmic energy of the measure μ. Also,

$$\int V_R\,\mathrm{d}\mu^\tau-\int V_R\,\mathrm{d}\mu=2\int(V_R(u^\tau)-V_R(u))\mathrm{d}\mu(u)=2\,\mathrm{Re}\left(\tau\int V'(u)h(u)\mathrm{d}\mu(u)\right)+O(\tau^2).$$

Combining with the above,

$$E_{V_R}(\mu^\tau)-E_{V_R}(\mu)=\mathrm{Re}\left(-\tau\int\hat{h}\,\mathrm{d}\mu(u)\mathrm{d}\mu(v)+2\tau\int V'h\,\mathrm{d}\mu\right)+O(\tau^2). \tag{25}$$

So, if μ is (the symmetric extension of) a critical point of the map $\mu\to E_{V_R}(\mu)$ the linear part of the increment is zero. In other words given a C^1 function h and a measure μ the function $E_{V_R}(\mu^\tau)$ of τ is differentiable at $\tau=0$ and the derivative is

$$\mathrm{Re}(-H(\mu)),\quad \textit{where } H(\mu)=\int\int\hat{h}\,\mathrm{d}\mu^2-2\int V'h\,\mathrm{d}\mu. \tag{26}$$

But what we really want is the derivative of the energy as a function of the equilibrium measure. This function can be shown to be differentiable and its derivative can be set to zero at a critical continuum.

Indeed, we need to show the following.

Lemma 4:

$$\frac{d}{d\tau}E_{V_R}((\lambda^\Gamma)^\tau)\big|_{\tau=0} = \frac{d}{d\tau}E_{V_R}(\lambda^{\Gamma_\tau})\big|_{\tau=0} = 0.$$

In the relation above $\Gamma_\tau = \mathrm{supp}(\lambda^\Gamma)^\tau$. The first derivative is of a function of general measures. The second derivative is of a function of equilibrium measures.

Proof: Define the measure σ_τ with support Γ and such that $(\sigma_\tau)^\tau = \lambda^{\Gamma_\tau}$.

LEMMA 5: With H defined by (26), we have

$$\mathrm{Re}\, H(\sigma_\tau) \to \mathrm{Re}\, H(\lambda^\Gamma),$$

as $\tau \to 0$.

Proof: By (25) and (26), we have

$$E_{V_R}((\lambda^\Gamma)^\tau) - E_{V_R}(\lambda^\Gamma) = -\mathrm{Re}(\tau H(\lambda^\Gamma) + O(\tau^2)),$$

$$E_{V_R}(\lambda^{\Gamma_\tau}) - E_{V_R}(\sigma_\tau) = -\mathrm{Re}(\tau H(\sigma_\tau) + O(\tau^2)).$$

On the other hand, $E_{V_R}(\sigma_\tau) \geqslant E_{V_R}(\lambda^\Gamma)$, and $E_{V_R}((\lambda^\Gamma)^\tau) \geqslant E_{V_R}(\lambda^{\Gamma_\tau})$. It follows that

$$E_{V_R}(\sigma_\tau) - \mathrm{Re}(\tau H(\sigma_\tau)) + O(\tau^2) = E_{V_R}(\lambda^{\Gamma_\tau}) \leqslant E_{V_R}((\lambda^\Gamma)^\tau) = E_{V_R}(\lambda^\Gamma) - \mathrm{Re}(\tau H(\lambda^\Gamma)) + O(\tau^2).$$

Hence $E_{V_R}(\sigma_\tau) \to E_{V_R}(\lambda^\Gamma)$.

As in the proof of Theorem 1, it follows that $\sigma_\tau \to \lambda^\Gamma$ weakly; see Ref. 7, pp. 82–88. It then follows immediately that $H(\sigma_\tau) \to H(\lambda^\Gamma)$. This proves Lemma 5.

To complete the proof of Lemma 4, we note that $0 \geqslant E_{V_R}((\lambda^\Gamma)^\tau) - E_{V_R}(\lambda^\Gamma) \geqslant E_{V_R}(\lambda^{\Gamma_\tau}) - E_{V_R}(\sigma_\tau) = -\mathrm{Re}(\tau H(\sigma_\tau)) + O(\tau^2)$. Hence the derivative of $E_{V_R}((\lambda^\Gamma)^\tau)$ at $\tau = 0$ is equal to the derivative of $E_{V_R}(\lambda^{\Gamma_\tau})$ at $\tau = 0$ which is equal to $\mathrm{Re}\, H(\lambda^\Gamma)$. This proves Lemma 4 and Theorem 6.

Proof of Theorem 5: Consider the Schiffer variation, i.e., take $h(u) = u^2/(u-z)$ where z is some fixed point not in Γ. Note that $h(0) = 0$ so that the deformation $z^\tau = z + \tau h(z)$ keeps the points $0_+, 0_-$ fixed. Also assume that τ is small enough so that the support of the deformed continuum does not hit the linear segment $(0, iA]$ or a nonzero point in the real line. We have

$$\hat{h} = \hat{h}(u,v) = \frac{h(u) - h(v)}{u - v} = 1 - \frac{z^2}{(u-z)(v-z)},$$

and therefore

$$\mathrm{Re}\left(\int \int \hat{h}(u,v)\, d\mu(u)\, d\mu(v) \right) = \mathrm{Re}\left[\int \int du(u)\, d\mu(v) - z^2 \left(\int_{\mathrm{supp}\ \mu} \frac{d\mu(u)}{u - z} \right)^2 \right].$$

Next

$$\mathrm{Re}\left(\int 2V'(u)h(u)\mathrm{d}\mu(u)\right) = 2\,\mathrm{Re}\left(\int (u+z)V'(u)\mathrm{d}\mu(u) + z^2\int \frac{V'(u)\mathrm{d}\mu(u)}{u-z}\right)$$
$$= \mathrm{Re}\left(\int 2V'(u)(u+z)\mathrm{d}\mu(u) + 2z^2\int \frac{V'(u)-V'(z)}{u-z}\mathrm{d}\mu(u)\right.$$
$$\left. + 2z^2V'(z)\int \frac{\mathrm{d}\mu(u)}{u-z}\right).$$

Theorem 5 now follows from Theorem 6.

Remark: If our continuum is allowed to touch the point iA [so we slightly weaken assumption (A)] then we may need to keep points $\pm iA$ fixed under a small variation. We can then choose the Schiffer variation $h(u)=u^2(u^2+A^2)/(u-z)$. We will arrive at a similar and equally useful formula.

In general if one wants to keep points $a_1,\ldots,a_s$ fixed, the appropriate Schiffer variation is $h(u)=\Pi_{i=1}^{i=s}(u-a_i)/(u-z)$.

Proposition 3: The support of the equilibrium measure consists of a finite number of analytic arcs.

Proof: Theorem 5 above implies that the support of μ is the level set of the real part of a function that is analytic except at countably many branch points. In fact, supp μ is characterized by $\int\log(1/|u-z|)\mathrm{d}\mu(u)+V_R(z)=0$. From Theorem 5 we get

$$\mathrm{Re}\left(\int \frac{\mathrm{d}\mu(u)}{u-z} + V'(z)\right) = \mathrm{Re}[(R_\mu(z))^{1/2}], \tag{27}$$

where

$$R_\mu(z) = (V'(z))^2 - 2\int_{\mathrm{supp}\ \mu} \frac{V'(z)-V'(u)}{z-u}\mathrm{d}\mu(u) + \frac{1}{z^2}\left(\int_{\mathrm{supp}\ \mu} 2(u+z)V'(u)\mathrm{d}\mu(u)\right). \tag{28}$$

This is a function analytic in K, with possibly a pole at zero. By integrating, we have that supp(μ) is characterized by

$$\mathrm{Re}\int^z (R_\mu)^{1/2}\,\mathrm{d}z = 0. \tag{29}$$

The locus defined by (29) is a union of arcs with endpoints at zeros of R_μ. To see this, consider (29) as an equation of two real variables $f(u,v)=0$ and try to solve for u as an analytic expression of v. One can only do this if the derivative of f is nonzero, which means (via the Cauchy-Riemann equations) that $R_\mu\neq 0$. The points where $R_\mu=0$ are exactly the points where the analytic arcs cannot be continued.

Note that

$$R_\mu(z) \sim -[16t^2z^2 + \pi^2(\rho^0(z))^2], \quad \text{as } z\to\infty,$$
$$R_\mu(z) \sim \frac{1}{z^2}\int 2uV'(u)\mathrm{d}\mu(u), \quad \text{as } z\to 0. \tag{30}$$

By conditions (1) for ρ^0, R_μ is blowing up at the point ∞ (at least for $t>0$; but the case $t=0$ is well understood: the equilibrium measure consists of a single analytic arc; see Sec. V). Hence it can only have finitely many zeros near infinity, otherwise they would have to accumulate near ∞ and then R_μ would be 0 there. On the other hand, R_μ cannot have an accumulation point of zeros at $z=0$, because even if the pole at 0 were removed (the coefficients of $1/z^2$, $1/z$ being zero), R_μ would be holomorphically extended across $z=0$. So, R_μ can only have a finite number of zeros in $\mathbb{K}$. It follows that the support of the maximizing equilibrium measure consists of only finitely many arcs.

REMARK: Of course, conditions (1) can be weakened. We could allow ρ^0 to have a pole at infinity of order other than two. But our aim here is not to prove the most general theorem possible, but instead illustrate a method that can be applied in the most general settings under appropriate amendments.

Remark: The assumption that ρ^0 is continuous and hence bounded at infinity is only needed to prove the finiteness of the components of the support of the equilibrium measure of the maximizing continuum. If it is dropped then we may have an infinite number of components for isolated values of x,t. This will result in infinite genus representations of the semiclassical asymptotics. Of course infinite genus solutions of the focusing NLS equation are known and well understood. So the analysis of Ref. 3 is expected to also apply in that case, although it will be more tedious.

For a justification of the "finite gap ansatz," concerning the semiclassical limit of focusing NLS, it only remains to verify the "S-property."

VII. THE S-PROPERTY

Theorem 7: (The S-property.)

Let C be the contour maximizing the equilibrium energy, for the field given by (3′) with conditions (1). Let μ be the extension of its equilibrium measure to the full complex plane via (21′). Assume for simplicity that assumption (A) holds. Let $X(z)=\int_{\mathrm{supp}\,\mu}\log[1/(u-z)]\mathrm{d}\mu(u)$, $X_R(z)=\mathrm{Re}\,X(z)=\int_{\mathrm{supp}\,\mu}\log(1/|u-z|)\mathrm{d}\mu(u)$, $W_\mu=X'$. Then, at any interior point of supp μ other than zero,

$$\frac{d}{\mathrm{d}n_+}(V_R+X_R)=\frac{d}{\mathrm{d}n_-}(V_R+X_R), \tag{8′}$$

where the two derivatives above denote the normal derivatives, on the + and − sides, respectively.

Proof: From Theorem 5, we have

$$|\mathrm{Re}(W_\mu(z)+V'(z))|=|\mathrm{Re}(R_\mu)|^{1/2}.$$

Using the definition for X, the above relation becomes

$$\left|\frac{d}{\mathrm{d}z}\,\mathrm{Re}(X+V)\right|=|\mathrm{Re}(R_\mu)|^{1/2}.$$

Now, $\mathrm{Re}(X+V)=0$ on the support of the equilibrium measure. So, in particular $\mathrm{Re}(X+V)$ is constant along the equilibrium measure. Hence $|(d/\mathrm{d}z)\mathrm{Re}(X+V)|$ must be equal to the modulus of *each* normal derivative across the equilibrium measure. So,

$$\left|\frac{d}{\mathrm{d}n_\pm}(V_R+\mathrm{Re}\,X)\right|=\left|\frac{d}{\mathrm{d}z}\,\mathrm{Re}(X+V)\right|=|\mathrm{Re}(R_\mu)|^{1/2}.$$

Hence,

$$\left|\frac{d}{\mathrm{d}n_+}(V_R+\mathrm{Re}\,X)\right|=\left|\frac{d}{\mathrm{d}n_-}(V_R+\mathrm{Re}\,X)\right|.$$

But it is easy to see that both LHS and RHS quantities inside the modulus sign are negative. This is because $V_R+\mathrm{Re}\,X=0$ on supp μ and negative on each side of supp μ. Hence result.

Remark: Once Theorem 7 is proved it follows by the Cauchy-Riemann equations that $(V_I+\mathrm{Im}\,X)_+-(V_I+\mathrm{Im}\,X)_-$ is constant on each connected component of supp μ, which means that $\mathrm{Im}\,\tilde{\phi}$ is constant on connected components of the contour, where $\tilde{\phi}$ is as defined in formula (4.13) of Ref. 3. This proves the existence of the appropriate "g functions" in Ref. 3.

We recapitulate our results in the following theorem, set in the upper complex half-plane. Note that (8′) is the "doubled up" version of (8).

Theorem 8: Let ϕ be given by (3′), where ρ^0 satisfies conditions (1). Under assumption (A), there is a piecewise smooth contour $C \in \mathbb{F}$, containing points $0_+, 0_-$ and otherwise lying in the cut upper half-plane $\mathbb{K}$, with equilibrium measure λ^C, such that $\mathrm{supp}(\lambda^C)$ consists of a union of finitely many analytic arcs and

$$E_\phi(\lambda^C) = \max_{C' \in \mathbb{F}} E_\phi(\lambda^{C'}) = \max_{C' \in \mathbb{F}} [\inf_{\mu \in M(F)} E_\phi(\mu)].$$

On each interior point of $\mathrm{supp}(\lambda^C)$ we have

$$\frac{d}{dn_+}(\phi + V^{\lambda^C}) = \frac{d}{dn_-}(\phi + V^{\lambda^C}), \tag{8''}$$

where V^{λ^C} is the Green's potential of the equilibrium measure λ^C [see (5)] and the two derivatives above are the normal derivatives.

A curve satisfying (8) such that the support of its equilibrium measure consists of a union of finitely many analytic arcs is called an S-curve.

Proof: The fact that the maximizing continuum C is actually a contour is proved as follows. If this were not the case, then we could choose a subset of C, say F, which *is* a contour, starting at 0_+ and ending at 0_-, and going around the point iA. Clearly, by definition, the equilibrium energy of C is less than the equilibrium energy of F, i.e., $E_\phi(\lambda^C) \leqslant E_\phi(\lambda^F)$. On the other hand, since C maximizes the equilibrium energy, we have $E_\phi(\lambda^F) \leqslant E_\phi(\lambda^C)$. So $E_\phi(\lambda^F) = E_\phi(\lambda^C)$.

VIII. CONCLUSION

In view of the interpretation of the variational problem in terms of the semiclassical NLS problem, we have the following result.

Consider the semiclassical limit ($\hbar \to 0$) of the solution of (9) and (10) with bell-shaped initial data. Replace the initial data by the so-called soliton ensembles data (as introduced in Ref. 3) defined by replacing the scattering data for $\psi(x,0) = \psi_0(x)$ by their WKB approximation, so that the spectral density of eigenvalues is

$$d\mu_0^{\mathrm{WKB}}(\eta) := \rho^0(\eta)\chi_{[0,iA]}(\eta)d\eta + \rho^0(\eta^*)\chi_{[-iA,0]}(\eta)d\eta,$$

$$\text{with } \rho^0(\eta) := \frac{\eta}{\pi}\int_{x_-(\eta)}^{x_+(\eta)} \frac{dx}{\sqrt{A(x)^2 + \eta^2}} = \frac{1}{\pi}\frac{d}{d\eta}\int_{x_-(\eta)}^{x_+(\eta)} \sqrt{A(x)^2 + \eta^2}\, d\mu,$$

for $\eta \in (0, iA)$, where $x_-(\eta) < x_+(\eta)$ are the two real turning points, i.e., $(A(x_\pm))^2 + \eta^2 = 0$, the square root is positive and the imaginary segments $(-iA, 0)$ and $(0, iA)$ are both considered to be oriented from bottom to top to define the differential $d\eta$.

Assume that ρ^0 satisfies conditions (1). Then, under assumption (A), asymptotically as $\hbar \to 0$, the solution $\psi(x,t)$ admits a "finite genus description." (For a more precise explanation, see Appendix B.)

The proof of this is the main result of Ref. 3, *assuming* that the variational problem of Sec. I has an S-curve as a solution. But this is now guaranteed by Theorem 8.

Remark: For conditions weaker than the above, the particular spectral density ρ^0 arising in the semiclassical NLS problem can conceivably admit branch singularities in the upper complex plane and condition (1) will not be satisfied. We claim that even in such a case the finite gap genus can be justified, at least generically. The proof of this fact will require setting the variational problem on a Riemann surface with moduli at the branch singularities of ρ^0.

Remark: Consider the semiclassical problem (9) and (10) in the case of initial data $\psi_0(x) = A \operatorname{sech} x$, where $A > 0$. Then the WKB density is given by $\rho^0 = i$ [see (3.1) and (3.2) of Ref. 3; note that condition (1) is satisfied]. So the finite genus ansatz holds for any x, t, as long as the assumption (A) of Sec. V holds. But then assumption (A) can be eventually dropped; see Appendix C.

Remark: The behavior of a solution of (9) in general depends not only on the eigenvalues of the Lax operator, but also on the associated norming constants and the reflection coefficient. In the special case of the soliton ensembles data the norming constants alternate between -1 and 1 while the reflection coefficient is by definition zero. More generally, for real analytic data decaying at infinity the reflection coefficient is exponentially small everywhere except at zero and can be neglected (although the rigorous proof of this is not trivial).

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APPENDIX A: COMPACTNESS OF THE SET OF CONTINUA

In this section we prove that the sets $I(\overline{\mathbb{K}})$ and hence $\mathbb{F}$ defined in Sec. I are compact and complete.

As stated in Sec. I, the space we must work with is the upper half-plane: $\mathbb{H}=\{z:\mathrm{Im}\, z>0\}$. The closure of this space is $\overline{\mathbb{H}}=\{z:\mathrm{Im}\ z\geqslant 0\}\cup\{\infty\}$. Also $\mathbb{K}=\{z:\mathrm{Im}\, z>0\}\backslash\{z:\mathrm{Re}\, z=0, 0<\mathrm{Im}\, z\leqslant A\}$. In the closure of this space, $\overline{\mathbb{K}}$, we consider the points ix_+ and ix_-, where $0\leqslant x<A$ as distinct.

Even though we eventually wish to consider only smooth contours, we are forced to *a priori* work with general closed sets. The reason is that the set of contours is not compact in any reasonable way, so it seems impossible to prove any existence theorem for a variational problem defined only on contours. Instead, we define $\mathbb{F}$ to be the set of all "continua" F in $\overline{\mathbb{K}}$ (i.e., connected compact sets, containing the points $0_+, 0_-$).

Furthermore, we need to introduce an appropriate topology on $\mathbb{F}$, that will make it a compact set. In this we follow the discussion of Dieudonné (Ref. 6, Chap. III.16).

We think of the closed upper half-plane $\overline{\mathbb{H}}$ as a compact space in the Riemann sphere. We thus choose to equip $\overline{\mathbb{H}}$ with the "chordal" distance, denoted by $d_0(z,\zeta)$, that is the distance between the images of z and ζ under the stereographic projection. This induces naturally a distance in $\overline{\mathbb{K}}$ [so, for example, $d_0(0_+,0_-)\neq 0$]. We also denote by d_0 the induced distance between compact sets E,F in $\overline{\mathbb{K}}$: $d_0(E,F)=\max_{z\in E}\min_{\zeta\in F} d_0(z,\zeta)$. Then, we define the so-called Hausdorff metric on the set $I(\overline{\mathbb{K}})$ of closed nonempty subsets of $\overline{\mathbb{K}}$ as follows:

$$d_{\mathbb{K}}(A,B)=\sup(d_0(A,B),d_0(B,A)). \tag{A1}$$

Lemma A.1: The Hausdorff metric defined by (A1) is indeed a metric. The set $I(\overline{\mathbb{K}})$ is compact and complete.

Proof: It is clear that $d_{\mathbb{K}}(A,B)$ is non-negative and symmetric by definition. Also if $d_{\mathbb{K}}(A,B)=0$, then $d_0(A,B)=0$, hence $\max_{z\in A}\min_{\zeta\in B} d_0(z,\zeta)=0$ and thus for all $z\in A$, we have $\min_{\zeta\in B} d_0(z,\zeta)=0$. In other words, $z\in B$. By symmetry, $A=B$.

The triangle inequality follows from the triangle inequality for d_0. Indeed, suppose $A,B,C\in I(\overline{\mathbb{K}})$. Then $d_{\mathbb{K}}(A,B)=\sup(d_0(A,B),d_0(B,A))=d_0(A,B)$, without loss of generality. Now,

$$d_0(A,B)=\max_{z\in A}\min_{\zeta\in B} d_0(z,\zeta)\leqslant \max_{z\in A}\min_{\zeta\in B}\min_{\zeta_0\in C}(d_0(z,\zeta_0)+d_0(\zeta_0,\zeta)),$$

by the triangle inequality for d_0. Let $z=z_0\in A$ be the value of z that maximizes $\min_{\zeta\in B}\min_{\zeta_0\in C}(d_0(z,\zeta_0)+d_0(\zeta_0,\zeta))$. This is then

$$\min_{\zeta\in B}\min_{\zeta_0\in C}(d_0(z_0,\zeta_0)+d_0(\zeta_0,\zeta)) \leqslant \min_{\zeta_0\in C} d_0(z_0,\zeta_0)+\min_{\zeta\in B}\min_{\zeta_0\in C} d_0(\zeta_0,\zeta)$$
$$\leqslant \max_{z\in A}\min_{\zeta_0\in C} d_0(z,\zeta_0)+\max_{\zeta\in B}\min_{\zeta_0\in C} d_0(\zeta_0,\zeta)$$
$$\leqslant d_0(A,C)+d_0(B,C)\leqslant d_{\mathbb{K}}(A,C)+d_{\mathbb{K}}(B,C).$$

The result follows from symmetry.

We will next show that $I(\overline{\mathbb{K}})$ is complete and precompact. Since a precompact, complete metric space is compact [Ref. 6, proposition (3.16.1)] the proof of Lemma A.1 follows.

Lemma A.2: If the metric space $\mathbb{E}$ equipped with a distance d_0 is complete, then so is $I(\mathbb{E})$, the set of closed nonempty subsets of $\mathbb{E}$, equipped with the Hausdorff distance

$$d_{\mathbb{E}}(A,B)=\sup(d_0(A,B),d_0(B,A)),$$

for any closed nonempty subsets A,B, where $d_0(A,B)=\max_{a\in A}\min_{b\in B} d_0(a,b)$.

Furthermore, if $\mathbb{E}$ is precompact, then so is $I(\mathbb{E})$.

Proof: Suppose $\mathbb{E}$ is complete. Let X_n be a Cauchy sequence in $I(\mathbb{E})$. We will show that X_n converges to $X=\cap_{n\geqslant 0}\overline{\cup}_{p\geqslant 0}X_{n+p}$. (Overbar denotes closure.)

Indeed, given any $\epsilon>0$,

$$d_0(X_n,X)=\max_{x\in X_n}\min_{y\in X} d_0(x,y)\leqslant \max_{x\in X_n}\max_{y\in \bar{\cup}_{p\geqslant 0}X_{n+p}} d_0(x,y)<\varepsilon,$$

for large n, by the completeness of $\mathbb{E}$. Similarly,

$$d_0(X,X_n)=\max_{x\in X}\min_{y\in X_n} d_0(x,y)\leqslant \max_{x\in \bar{\cup}_{p\geqslant 0}X_{n+p}}\min_{y\in X_n} d_0(x,y)<\varepsilon.$$

Next, suppose $\mathbb{E}$ is precompact. Then, by definition, given any $\epsilon>0$, there is a finite set, say $S=\{s_1,s_2,\ldots,s_n\}$, where n is a finite integer, such that any point x of $\mathbb{E}$ is at a distance d_0 less than ϵ to the set S. Now, consider the set of subsets of S, which is of course finite. Clearly every closed set is at a distance less than ϵ to a member of that set,

$$d_0(A,S)=\max_{a\in A}\min_{s\in S} d_0(a,s)<\varepsilon,$$

$$d_0(S,A)=\max_{s\in S}\min_{a\in A} d_0(a,s)<\varepsilon,$$

for any closed nonempty set A. Hence $d_{\mathbb{E}}(A,S)<\epsilon$.

So, any closed nonempty set A is at a distance less than ϵ to the finite power set of S. So $I(\mathbb{E})$ is precompact.

APPENDIX B: THE DESCRIPTION OF THE SEMICLASSICAL LIMIT OF THE FOCUSING NLS EQUATION UNDER THE FINITE GENUS ANSATZ

We present one of the main results of Ref. 3 on the semiclassical asymptotics for problem (9) and (10), in view of the fact that the finite genus ansatz holds. In particular, we fix x,t and use the result that the support of the maximizing measure of Theorems 4 and 8 consists of a finite union of analytic arcs.

First, we define the so-called g function. Let C be the maximizing contour of Theorem 4. *A priori* we seek a function satisfying

$$g(\lambda) \textit{ is independent of } \hbar,$$

$$g(\lambda) \textit{ is analytic for } \lambda\in\mathbb{C}\setminus(C\cup C^*),$$

$$g(\lambda)\to 0 \textit{ as } \lambda\to\infty,$$

$$g(\lambda) \textit{ assumes continuous boundary values from both sides of } C\cup C^*,$$

denoted by $g_+(g_-)$ on the left (right) of $C \cup C^*$,

$$g(\lambda^*) + g(\lambda)^* = 0 \quad \textit{for all } \lambda \in \mathbb{C} \setminus (C \cup C^*).$$

The assumptions above are satisfied if we write g in terms of the maximizing equilibrium measure of Theorem 8, $\mathrm{d}\mu = \mathrm{d}\lambda^C = \rho(\eta)\mathrm{d}\eta$, doubled up according to (21′). Indeed,

$$g(\lambda) = \int_{C \cup C^*} \log(\lambda - \eta)\rho(\eta)\mathrm{d}\eta,$$

for an appropriate definition of the logarithm branch (see Ref. 3).

For $\lambda \in C$, define the functions

$$\theta(\lambda) := i(g_+(\lambda) - g_-(\lambda)),$$

$$\Phi(\lambda) := \int_0^{iA} \log(\lambda - \eta)\rho^0(\eta)\mathrm{d}\eta + \int_{-iA}^0 \log(\lambda - \eta)\rho^0(\eta^*)^*\mathrm{d}\eta$$

$$+ 2i\lambda x + 2i\lambda^2 t + i\pi \int_\lambda^{iA} \rho^0(\eta)\mathrm{d}\eta - g_+(\lambda) - g_-(\lambda),$$

where $\rho^0(\eta)$ is the holomorphic function (WKB density of eigenvalues) introduced in Sec. I [see conditions (1)].

The finite genus ansatz implies that for each x,t there is a finite positive integer G such that the contour C can be divided into "bands" [the support of $\rho(\eta)\mathrm{d}\eta$] and "gaps" (where $\rho=0$). We denote these bands by I_j. More precisely, we define the analytic arcs $I_j, I_j^*, j=1,\ldots,G/2$ as follows (they come in conjugate pairs). Let the points λ_j, $j=0,\ldots,G$, in the open upper half-plane be the branch points of the function g. All such points lie on the contour C and we order them as $\lambda_0,\lambda_1,\ldots,\lambda_G$, according to the direction given to C. The points $\lambda_0^*,\lambda_1^*,\ldots,\lambda_G^*$ are their complex conjugates. Then let $I_0=[0,\lambda_0]$ be the subarc of C joining points 0 and λ_0. Similarly, $I_j = [\lambda_{2j-1},\lambda_{2j}]$, $j=1,\ldots,G/2$. The connected components of the set $\mathbb{C}\setminus\cup_j(I_j \cup I_j^*)$ are the so-called "gaps," for example, the gap Γ_1 joins λ_0 to λ_1, etc.

It actually follows from the properties of g, ρ that the function $\theta(\lambda)$ defined on C is constant on each of the gaps Γ_j, taking a value which we will denote by θ_j, while the function Φ is constant on each of the bands, taking the value denoted by α_j on the band I_j.

The finite genus ansatz for the given fixed x,t implies that the asymptotics of the solution of (9) and (10) as $\hbar \to 0$ can be given by the next theorem.

Theorem A.1: Let x_0, t_0 be given. The solution $\psi(x,t)$ of (9) and (10) is asymptotically described (locally) as a slowly modulated $G+1$ phase wavetrain. Setting $x=x_0+\hbar\hat{x}$ and $t=t_0+\hbar\hat{t}$, so that x_0,t_0 are "slow" variables while $\hat{x},\hat{t}$ are "fast" variables, there exist parameters

$a, U=(U_0,U_1,\ldots,U_G)^T$, $k=(k_0,k_1,\ldots,k_G)^T$, $w=(w_0,w_1,\ldots,w_G)^T$, $Y=(Y_0,Y_1,\ldots,Y_G)^T$, $Z=(Z_0,Z_1,\ldots,Z_G)^T$ [depending on the slow variables x_0 and t_0 (but not $\hat{x}\hat{t}$) such that

$$\psi(x,t) = \psi(x_0+\hbar\hat{x}, t_0+\hbar t) \sim a(x_0,t_0)e^{iU_0(x_0,t_0)/\hbar}e^{i(k_0(x_0,t_0)\hat{x} - w_0(x_0,t_0)t)} \times \frac{\Theta(Y(x_0,t_0) + iU(x_0,t_0)/\hbar + i(k(x_0,t_0)\hat{x} - w(x_0,t_0)t))}{\Theta(Z(x_0,t_0) + iU(x_0,t_0)/\hbar + i(k(x_0,t_0)\hat{x} - w(x_0,t_0)t))}. \tag{B1}$$

All parameters can be defined in terms of an underlying Riemann surface X. The moduli of X are given by λ_j, $j=0,\ldots,G$ and their complex conjugates λ_j^*, $j=0,\ldots,G$. The genus of X is G. The moduli of X vary slowly with x,t, i.e., they depend on x_0,t_0 but not $\hat{x},\hat{t}$. For the exact formulas for the parameters as well as the definition of the theta functions we present the following construction.

The Riemann surface X is constructed by cutting two copies of the complex sphere along the slits $I_0 \cup I_0^*, I_j, I_j^*, j=1,\dots,G$, and pasting the "top" copy to the "bottom" copy along these very slits.

We define the homology cycles a_j, b_j, $j=1,\dots,G$ as follows. Cycle a_1 goes around the slit $I_0 \cup I_0^*$ joining λ_0 to λ_0^*, remaining on the top sheet, oriented counterclockwise, a_2 goes through the slits I_{-1} and I_1 starting from the top sheet, also oriented counterclockwise, a_3 goes around the slits $I_{-1}, I_0 \cup I_0^*, I_1$ remaining on the top sheet, oriented counterclockwise, etc. Cycle b_1 goes through I_0 and I_1 oriented counterclockwise, cycle b_2 goes through I_{-1} and I_1, also oriented counterclockwise, cycle b_3 goes through I_{-1} and I_2, and around the slits $I_{-1}, I_0 \cup I_0^*, I_1$, oriented counterclockwise, etc.

On X there is a complex G-dimensional linear space of holomorphic differentials, with basis elements $\nu_k(P)$ for $k=1,\dots,G$ that can be written in the form

$$\nu_k(P) = \frac{\sum_{j=0}^{G-1} c_{kj} \lambda(P)^j}{R_X(P)} \mathrm{d}\lambda(P),$$

where $R_X(P)$ is a "lifting" of the function $R(\lambda)$ from the cut plane to X, if P is on the first sheet of X then $R_X(P)=R(\lambda(P))$ and if P is on the second sheet of X then $R_X(P)=-R(\lambda(P))$. The coefficients c_{kj} are uniquely determined by the constraint that the differentials satisfy the normalization conditions

$$\oint_{a_j} \nu_k(P) = 2\pi i \delta_{jk}.$$

From the normalized differentials, one defines a $G \times G$ matrix H (the period matrix) by the formula

$$H_{jk} = \oint_{b_j} \nu_k(P).$$

It is a consequence of the standard theory of Riemann surfaces that H is a symmetric matrix whose real part is negative definite.

In particular, we can define the theta function

$$\Theta(w) := \sum_{n \in \mathbb{Z}^G} \exp\left(\frac{1}{2} n^T H n + n^T w\right),$$

where H is the period matrix associated to X. Since the real part of H is negative definite, the series converges.

We arbitrarily fix a base point P_0 on X. The Abel map $A: X \to \mathrm{Jac}(X)$ is then defined componentwise as follows:

$$A_k(P; P_0) := \int_{P_0}^{P} \nu_k(P'), \quad k = 1, \dots, G,$$

where P' is an integration variable.

A particularly important element of the Jacobian is the Riemann constant vector K which is defined, modulo the lattice Λ, componentwise by

$$K_k := \pi i + \frac{H_{kk}}{2} - \frac{1}{2\pi i} \sum_{\substack{j=1 \\ j \neq k}}^{G} \oint_{a_j} \left(\nu_j(P) \int_{P_0}^{P} \nu_k(P') \right),$$

where the index k varies between 1 and G.

Next, we will need to define a certain meromorphic differential on X. Let $\Omega(P)$ be holomorphic away from the points ∞_1 and ∞_2, where it has the behavior

$$\Omega(P) = \mathrm{d}p(\lambda(P)) + \left(\frac{\mathrm{d}\lambda(P)}{\lambda(P)^2}\right), \quad P \to \infty_1,$$

$$\Omega(P) = -\mathrm{d}p(\lambda(P)) + O\left(\frac{\mathrm{d}\lambda(P)}{\lambda(P)^2}\right), \quad P \to \infty_2,$$

and made unique by the normalization conditions

$$\oint_{a_j} \Omega(P) = 0, \quad j = 1, \ldots, G.$$

Here p is a polynomial, defined as follows.

First, let us introduce the function $R(\lambda)$ defined by

$$R(\lambda)^2 = \prod_{k=0}^{G} (\lambda - \lambda_k)(\lambda - \lambda_k^*),$$

choosing the particular branch that is cut along the bands I_k^+ and I_k^- and satisfies

$$\lim_{x\to\infty} \frac{R(\lambda)}{\lambda^{G+1}} = -1.$$

This defines a real function, i.e., one that satisfies $R(\lambda^*) = R(\lambda)^*$. At the bands, we have $R_+(\lambda) = -R_-(\lambda)$, while $R(\lambda)$ is analytic in the gaps. Next, let us introduce the function $k(\lambda)$ defined by

$$k(\lambda) = \frac{1}{2\pi i}\sum_{n=1}^{G/2} \theta_n \int_{\Gamma_n^+\cup\Gamma_n^-} \frac{\mathrm{d}\eta}{(\lambda - \eta)R(\eta)} + \frac{1}{2\pi i}\sum_{n=0}^{G/2} \int_{I_n^+\cup I_n^-} \frac{\alpha_n \,\mathrm{d}\eta}{(\lambda - \eta)R_+(\eta)}.$$

Next let

$$H(\lambda) = k(\lambda)R(\lambda).$$

The function k satisfies the jump relations

$$k_+(\lambda) - k_-(\lambda) = -\frac{\theta_n}{R(\lambda)}, \quad \lambda \in \Gamma_n^+ \cup \Gamma_n^-,$$

$$k_+(\lambda) - k_-(\lambda) = -\frac{\alpha_n}{R_+(\lambda)}, \quad \lambda \in I_n^+ \cup I_n^-,$$

and is otherwise analytic. It blows up like $(\lambda - \lambda_n)^{-1/2}$ near each endpoint, has continuous boundary values in between the endpoints, and vanishes like $1/\lambda$ for large λ. It is the only such solution of the jump relations. The factor of $R(\lambda)$ renormalizes the singularities at the endpoints, so that, as desired, the boundary values of $H(\lambda)$ are bounded continuous functions. Near infinity, there is the asymptotic expansion

$$H(\lambda) = H_G\lambda^G + H_{G-1}\lambda^{G-1} + \cdots + H_1\lambda + H_0 + O(\lambda^{-1}) = p(\lambda) + O(\lambda^{-1}), \tag{B2}$$

where all coefficients H_j of the polynomial $p(\lambda)$ can be found explicitly by expanding $R(\lambda)$ and the Cauchy integral $k(\lambda)$ for large λ. It is easy to see from the reality of θ_j and α_j that $p(\lambda)$ is a polynomial with real coefficients.

Thus the polynomial $p(\lambda)$ is defined and hence the meromorphic differential $\Omega(P)$ is defined.

Let the vector $U \in \mathbb{C}^G$ be defined componentwise by

$$U_j := \oint_{b_j} \Omega(P).$$

Note that $\Omega(P)$ has no residues.

Let the vectors V_1, V_2 be defined componentwise by

$$V_{1,k} = (A_k(\lambda_{1+}^*) + A_k(\lambda_{2+}) + A_k(\lambda_{3+}^*) + \cdots + A_k(\lambda_{G+})) + A_k(\infty) + \pi i + \frac{H_{kk}}{2},$$

$$V_{2,k} = (A_k(\lambda_{1+}^*) + A_k(\lambda_{2+}) + A_k(\lambda_{3+}^*) + \cdots + A_k(\lambda_{G+})) - A_k(\infty) + \pi i + \frac{H_{kk}}{2},$$

where $k=1,\ldots,G$, and the $+$ index means that the integral for A is to be taken on the first sheet of X, with base point λ_+^0.

Finally, let

$$a = \frac{\Theta(Z)}{\Theta(Y)} \sum_{k=0}^{G} (-1)^k \mathfrak{J}(\lambda_k),$$

$$k_n = \partial_x U_n, \quad w_n = -\partial_t U_n, \quad n = 0, \ldots, G,$$

where

$$Y = -A(\infty) - V_1, \quad Z = A(\infty) - V_1,$$

and $U_0 = -(\theta_1 + \alpha_0)$ where θ_1 is the (constant in λ) value of the function θ in the gap Γ_1 and α_0 is the (constant) value of the function ϕ in the band I_0.

Now, the parameters appearing in formula (B1) are completely described.

We simply note here that the U_i and hence the k_i and w_i are real. We also note that the denominator in (B1) never vanishes (for any $x_0, t_0, \hat{x}, \hat{t}$).

Remark: Theorem A.1 presents pointwise asymptotics in x,t. In Ref. 3, these are extended to uniform asymptotics in certain compact sets covering the x,t plane. Error estimates are also given in Ref. 3.

Remark: As mentioned above, we do not know if the support of the equilibrium measure of the maximizing continuum is unique. But the asymptotic formula (B1) depends only on the endpoints λ_j of the analytic subarcs of the support. Since the asymptotic expression (B1) must be unique, it is easy to see that the endpoints also must be unique. Different Riemann surfaces give different formulas (except of course in degenerate cases, a degenerate genus 2 surface can be a pinched genus 0 surface and so on).

APPENDIX C: DROPPING ASSUMPTION (A) OF SEC. V

In Sec. V, we have assumed that the solution of the problem of the maximization of the equilibrium energy is a continuum, say F, which does not intersect the linear segment $[0, iA]$ except of course at $0_+, 0_-$. We also prove that F does not touch the real line, except of course at 0 and possibly ∞. This enables us to take variations in Sec. VI, keeping fixed a finite number of points, and thus arrive at the identity of Theorem 5, from which we derive the regularity of F and the fact that F is, after all, an S-curve.

In general, it is conceivable that F intersects the linear segment $[0, iA]$ at points other than $0_+, 0_-$. If the set of such points is finite, there is no problem, since we can always consider variations keeping fixed a finite number of points, and arrive at the same result (see the remark after the proof of Theorem 5).

If, on the other hand, this is not the case, we have a different kind of problem, because the function V introduced in Sec. VI (the complexification of the field) is not analytic across the segment $[-iA, iA]$.

What is true, however, is that V is analytic in a Riemann surface consisting of infinitely many sheets, cut along the line segment $[-iA, iA]$. So, the appropriate, underlying space for the (doubled up) variational problem should now be a noncompact Riemann surface, say $\mathbb{L}$.

Compactness is crucial in the proof of a maximizing continuum. But we can compactify the Riemann surface $\mathbb{L}$ by compactifying the complex plane. Let the map $\mathbb{C} \to \mathbb{L}$ be defined by

$$y = \log(z - iA) - \log(z + iA).$$

The point $z = iA$ corresponds to infinitely many y points, i.e., $y = -\infty + i\theta$, $\theta \in \mathbb{R}$, which will be identified. Similarly, the point $z = -iA$ corresponds to infinitely many points $y = +\infty + i\theta$, $\theta \in \mathbb{R}$, which will also be identified. The point $0 \in \mathbb{C}$ corresponds to the points $k\pi i$, k odd.

By compactifying the plane we then compactify the Riemann surface $\mathbb{L}$. The distance between two points in the Riemann surface $\mathbb{L}$ is defined to be the corresponding stereographic distance between the images of these points in the compactified $\mathbb{C}$.

With these changes, the proof of the existence of the maximizing continuum in Secs. I, III, and IV goes through virtually unaltered. In Sec. VI, we would have to consider the complex field V as a function defined in the Riemann surface $\mathbb{L}$ and all proofs go through. The corresponding result of Sec. VII will give us an S-curve C in the Riemann surface $\mathbb{L}$. We then have the following facts.

Consider the image $\mathbb{D}$ of the closed upper half-plane under

$$y = \log(z - iA) - \log(z + iA).$$

Consider continua in $\mathbb{D}$ containing the points $y = \pi i$ and $y = -\pi i$. Define the Green's potential and Green's energy of a Borel measure by (4)–(6) and the equilibrium measure by (7). Then there exists a continuum C maximizing the equilibrium energy, for the field given by (3) with conditions (1). C does not touch $\partial\mathbb{D}$ except at a finite number of points. By taking variations as in Sec. VI, one sees that C is a S-curve. In particular, the support of the equilibrium measure on C is a union of analytic arcs and at any interior point of supp μ,

$$\frac{d}{dn_+}(\phi + V^{\lambda^C}) = \frac{d}{dn_-}(\phi + V^{\lambda^C}), \tag{8'''}$$

where the two derivatives above denote the normal derivatives.

As far as the consequences of the above facts regarding the semiclassical limit of NLS, some more work on the details is necessary. Indeed, the analysis of the dynamics of the semiclassical problem (9) and (10) presented in Ref. 3 assumes that the S-curve C lies entirely in $\mathbb{K} \cup \{0_+, 0_-\}$. However, the explicit computation of the equilibrium measure on the S-curve and the derivation of the equations implicitly defining the endpoints of the components of the support of the equilibrium measure also make sense when extended to the Riemann surface $\mathbb{L}$. As a result the statement of Theorem A.1 is correct, when interpreted correctly, i.e., allowing for all contours involved in the definition of the line integrals appearing in formula (B1) as well as the bands $I_0 \cup I_0^*, I_j, I_j^*, j = 1, \ldots, G$ and the gaps Γ_j to lie in $\mathbb{L}$.

We plan to describe the details of the evolution of the S-curve in the Riemann surface $\mathbb{L}$ in a later publication. In particular, one must check that all the deformations described in Ref. 3 are valid; this is indeed true, as one can see by the analysis of Ref. 3 transferred to the Riemann surface $\mathbb{L}$.

Remark: The "discrete-to-continuous" passage.

The following caveat has to be addressed here. One of the problems dealt with in Ref. 3 was to transform the so-called "discrete" Riemann-Hilbert problem (problem 4.1.1 of Ref. 3) to a "continuous" Riemann-Hilbert problem (problem 4.2.1 of Ref. 3). The initial (discrete) problem posed is to construct a (matrix) meromorphic function from the information on its poles. These poles indeed accumulate (as $\hbar$ goes to 0) along the segment $(-iA, iA)$. Then one transforms the

problem to a properly speaking (continuous) holomorphic Riemann-Hilbert problem with jumps, by constructing two contours, one encircling the poles with positive imaginary part and the other encircling the poles with negative imaginary part, and redefining the matrix functions inside the contours so that the singularities are removed. Naturally the information concerning the poles appears in the arising jump along the two loops.

One then (formally at first) approximates the jump on the loops in an obvious way (it is a Riemann sum approximated by an integral). This jump involves a logarithmic function with a cut along the linear segment $[-iA, iA]$.

Now, to rigorously show that the approximation is valid one needs a very careful analysis of what happens near 0, because the "Riemann sum" approximation breaks down there. Indeed this is done in Sec. 4.4.3 of Ref. 3, where, however, it is assumed that the loop (the jump contour) is located exactly at the S-curve (which solves the variational problem), and that this S-curve emanates from 0+ at an acute, nonright, angle to the horizontal axis.

Even though in Ref. 3 the S-curve is assumed not to touch the linear segment $[-iA, iA]$, this condition is actually only necessary *locally* near 0. There is no problem in allowing the S-curve to intersect the spike, as long as it emanates from 0_+ at an acute, nonright, angle to the horizontal axis. Now it is *proved* in Ref. 3 that the S-curve solving the variational problem must emanate from 0+ at an acute, nonright, angle to the horizontal axis. [This in fact follows immediately from the measure reality condition (4.18) applied at the origin.] So the proof of Theorem A.1 will go through even if the S-curve intersects the linear segment $[-iA, iA]$.

We then have the following.

Theorem 9: Consider the semiclassical limit ($\hbar \to 0$) of the solution of (9) and (10) with bell-shaped initial data. Replace the initial data by the so-called soliton ensembles data (as introduced in Ref. 3) defined by replacing the scattering data for $\psi(x,0)=\psi_0(x)$ by their WKB approximation. Assume, for simplicity, that the spectral density of eigenvalues satisfies conditions (1).

Then, asymptotically as $\hbar \to 0$, the solution $\psi(x,t)$ admits a "finite genus description," in the sense of Theorem A.1.

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Nonlinear fractional diffusion equation: Exact results

E. K. Lenzi, R. S. Mendes, and Kwok Sau Fa
Departamento de Física, Universidade Estadual de Maringá, Av. Colombo 5790, 87020-900 Maringá-PR, Brazil

L. S. Moraes
Departamento de Engenharia Química, Universidade Estadual de Maringá, Av. Colombo 5790, 87020-900 Maringá-PR, Brazil

L. R. da Silva and L. S. Lucena
International Center for Complex Systems and Departamento de Física, Universidade Federal do Rio Grande do Norte, 59078-970 Natal-RN, Brazil

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The nonlinear fractional diffusion equation $\partial_t\rho=r^{1-d}\partial_r^{\mu'}\{r^{d-1}\mathcal{D}(r,t;\rho)\partial_r^{\mu}\rho^{\nu}\}-r^{1-d}\partial_r\{r^{d-1}F(r,t)\rho\}+\overline{\alpha}(t)\rho$ is studied by considering the diffusion coefficient $\mathcal{D}(r,t;\rho)=\mathcal{D}(t)r^{-\theta}\rho^{\gamma}$ and the external force $F(r,t)=-k_1(t)r+k_\alpha r^{\alpha}$. In addition, a rich class of diffusive processes, including normal and anomalous ones, is obtained from the study present in this work. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1993527]

I. INTRODUCTION

Due to the broadness of physical applications covering almost every field, the diffusion equations have been widely investigated. In this direction, we have, for instance, the nonlinear diffusion equations, the fractional diffusion equations, and the diffusion equations that contain a mix of nonlinear terms and fractional derivatives. These equations extend the usual diffusion equation by considering the presence of nonlinear terms and fractional derivatives. They have been applied to several scenarios such as percolation of gases through porous media,[1] thin saturated regions in porous media,[2] a standard solid-on-solid model for surface growth, thin liquid films spreading under gravity,[3] modeling of non-Markovian dynamical processes in protein folding,[4] relaxation to equilibrium in system (such as polymer chains and membranes) with long temporal memory,[5] and in anomalous transport in disordered systems.[6] A representative nonlinear diffusion equation usually employed in the above context is the *porous medium equation*.[7,8] We may also have the high order diffusion-like equation such as the thin film equation,[9] which contains a fourth order derivative. This kind of diffusion equation can be applied to describe the lubrication models for thin viscous films, spreading droplets, and Hele–Shaw cells.[10] In addition to the above context, the fractional equations[11] have also been employed to investigate the situations related to the anomalous diffusion and, in particular, the diffusion equations that accomplish nonlinear terms and fractional derivatives.[12,13]

From the previous discussion, we note the importance of these equations not only due to the various types of scenarios which can be described, but also due to the growing interest on the feasibility of covering new situations. In this direction, we have, for example, the displacement of a viscous fluid by a less viscous one in a petroleum reservoir requires a more general approach in order to take the nonlinear behavior of the interface into account, and also the fractal or multifractal characteristics of porous rocks in which the oil is immersed. In particular, the geostatistics of these reservoirs are well described by a fractional Brownian motion and fractional Levy motion.[14] Thus, the present work intends to establish some classes of solutions of a general nonlinear fractional diffusion equation with absorption and investigate the classes of diffusive processes described by this equation. More precisely, we focus our attention on the following generalized equation:

$$\frac{\partial}{\partial t}\rho(r,t)=\frac{1}{r^{d-1}}\frac{\partial^{\mu'}}{\partial r^{\mu'}}\left\{r^{d-1}\mathcal{D}(r,t;\rho)\frac{\partial^{\mu}}{\partial r^{\mu}}[\rho(r,t)]^{\nu}\right\}-\frac{1}{r^{d-1}}\frac{\partial}{\partial r}\{r^{d-1}F(r,t)\rho(r,t)\}+\overline{\alpha}(t)\rho(r,t), \tag{1}$$

where ρ is a density function, d is a spatial dimension of the system under consideration, r is nonnegative, the parameters $\nu,\mu',\mu\in\mathcal{R}$, $\mathcal{D}(r,t;\rho)=\mathcal{D}(t)r^{-\theta}[\rho(r,t)]^{\gamma}$ is the diffusion coefficient, $F(r,t)$ is an external force (*drift*), and $\overline{\alpha}(t)$ plays the role of an absorbent (or source) rate related to a reaction-diffusion process. The presence of the reaction term like the one given in the above equation has been studied in several situations. Here, for example, we may recall the catalytic processes in regular, heterogeneous, or disordered systems.[15] Another example is an irreversible first-order reaction of transported substance so that the rate of removal is $\overline{\alpha}\rho$.[16] This extra term may also appear when a tracer undergoing radioactive decay is transported through a porous medium,[17] in heat flow involving heat production.[18] Equation (1) applies in these situations and in solute transport through adsorbent samples that are usually proportional to the concentration in the solution. It is also interesting to note that Eq. (1) may be related to several physical situations such as the axisymmetric flow of a very viscous fluid,[19] turbulent diffusion,[20] adsorption-desorption equilibrium locally maintained through a permeable solid,[21] and nonlinear diffusion in hard and soft superconductors.[22]

For $\overline{\alpha}(t)=0$, one can verify that $\int_0^{\infty}drr^{d-1}\rho(r,t)$ is time independent (hence, if ρ is normalized at $t=0$, it will remain so forever). Indeed, if Eq. (1) is written as $\partial_t\rho=-r^{1-d}\partial_r\mathcal{J}$ and the boundary condition $\mathcal{J}(r\to\infty,t)\to 0$ is assumed, it can be shown that $\int_0^{\infty}drr^{d-1}\rho(r,t)$ is a constant of motion. According to Refs. 12 and 13, we use the Riemann–Liouville operator[11,23] for the spatial fractional derivatives. Also, we employ the boundary condition $\rho(r\to\infty,t)\to 0$. Note that Eq. (1) recovers, for $(\mu',\mu,\gamma,\nu)=(1,1,0,1)$, the standard Fokker–Planck equation[24] in the presence of a drift with an adsorbent (source) term for a d-dimensional case within radial symmetry. The particular case $F(r,t)=0$ (no drift), $\mathcal{D}(r,t)=$*constant*, and $(\mu',\mu,\gamma,d)=(1,1,0,1)$ has been considered by Spohn.[8] Other features of Eq. (1) with $(\mu',\mu,\theta,\gamma,d)=(1,1,0,0,1)$ have also been considered in Refs. 25 and 26. The case $(\mu',\theta,\gamma,d)=(0,0,0,1)$ with $\mathcal{D}(t)=$*constant* without external force has been investigated in Ref. 12. In Ref. 13 the presence of external forces and a spatial time dependence on the diffusion coefficient has been considered for $(d,\mu')=(1,1)$. Therefore, our present discussion involves extensions of these cases by taking a wide variety of situations into account; employing the nonlinear, fractional, and the mixing of these cases. Moreover, we develop, in a unified approach, extending the results presented in Refs. 8, 12, 25, and 26 for a d-dimensional case by considering the presence of fractional derivatives, external forces and a spatial time dependent diffusion coefficient. The remainder of this paper goes as follows. In Sec. II, we consider several situations for Eq. (1) as well as the connection of the solutions with the ones obtained within the maximum entropy principle. In Sec. III, we present our conclusions.

II. DIFFUSION EQUATION: SOLUTIONS

This section considers the solutions for Eq. (1) expressed as a scaled function of the type

$$\overline{\rho}(r,t)=\frac{1}{\Phi(t)}\tilde{\rho}\left[\frac{r}{\Phi(t)}\right], \tag{2}$$

where $\Phi(t)$ is a positive time dependent function. These solutions may satisfy the initial and the boundary condition. Before substituting Eq. (2) in Eq. (1), some changes in Eq. (1) are carried out in order to simplify the analysis. Supposing the solution of Eq. (1) can be given by $\rho(r,t)=\exp[\int_0^t d\tilde{t}\overline{\alpha}(\tilde{t})]\overline{\rho}(r,t)/r^{d-1}$, where $\overline{\rho}(r,t)$ is a function to be determined, yields

$$\frac{\partial}{\partial t}\overline{\rho}(r,t)=\overline{\mathcal{D}}(t)\frac{\partial^{\mu'}}{\partial r^{\mu'}}\left\{r^{(1-\gamma)(d-1)-\theta}[\overline{\rho}(r,t)]^{\gamma}\frac{\partial^{\mu}}{\partial r^{\mu}}\{r^{-\nu(d-1)}[\overline{\rho}(r,t)]^{\nu}\}\right\}-\frac{\partial}{\partial r}\{F(r,t)\overline{\rho}(r,t)\}, \tag{3}$$

with $\overline{\mathcal{D}}(t)=\mathcal{D}(t)\exp[(\nu+\gamma-1)\int_0^t d\tilde{t}\overline{\alpha}(\tilde{t})]$.

Applying Eq. (2) in Eq. (3) by taking the drift term, specifically, $F(r,t)=-k_1(t)r$ into account and following the procedure employed in Refs. 12 and 13, Eq. (3) can be reduced to

$$\frac{d^{\mu'}}{dz^{\mu'}}\left\{z^{(1-\gamma)(d-1)-\theta}[\tilde{\rho}(z)]^{\gamma}\frac{d^{\mu}}{dz^{\mu}}\{z^{-\nu(d-1)}[\tilde{\rho}(z)]^{\nu}\}\right\}=\overline{k}\frac{d}{dz}[z\tilde{\rho}(z)] \tag{4}$$

and

$$[\Phi(t)]^{\xi-2}\frac{d}{dt}\Phi(t)+k_1(t)[\Phi(t)]^{\xi-1}=-\overline{kD}(t), \tag{5}$$

where $\xi=d(\gamma+\nu)-(d-1)+\mu+\mu'+\theta$, $z=r/\Phi(t)$ and $\overline{k}$ is an arbitrary constant. Note that we have used the generic property

$$\frac{d^{\delta}}{dx^{\delta}}\mathcal{G}(ax)=a^{\delta}\frac{d^{\delta}}{d\overline{z}^{\delta}}\mathcal{G}(\overline{z})\quad(\delta\in\mathcal{R}), \tag{6}$$

where $\overline{z}=ax$. This basic property holds not only for the ordinary derivative but also for all fractional operators which are considered in this analysis. By solving Eq. (5), results

$$\Phi(t)=\left[(\Phi(0))^{\xi-1}+k'\int_0^t d\tilde{t}\mathcal{D}(\tilde{t})e^{(\nu+\gamma-1)\int_0^{\tilde{t}}dt'\overline{\alpha}(t')+(\xi-1)\int_0^{\tilde{t}}dt'k_1(t')}\right]^{1/(\xi-1)}e^{-\int_0^t dt'k_1(t')}, \tag{7}$$

with $k'=(1-\xi)\overline{k}$. Performing an integration in Eq. (4), we have that

$$\frac{d^{\mu'-1}}{dz^{\mu'-1}}\left\{z^{(1-\gamma)(d-1)-\theta}[\tilde{\rho}(z)]^{\gamma}\frac{d^{\mu}}{dz^{\mu}}\{z^{-\nu(d-1)}[\tilde{\rho}(z)]^{\nu}\}\right\}=\overline{k}z\tilde{\rho}(z)+\mathcal{C}, \tag{8}$$

where $\mathcal{C}$ is an integration constant (see Refs. 12 and 13 for details).

The next step is the analysis of the solutions of Eq. (8) by considering several situations of the parameters μ', μ, θ, γ, and d. Starting our study by the solutions of Eq. (8) with the following case, $\mu'=1$, $\mathcal{C}=0$ and (μ,θ,γ,d) being arbitraries, it is feasible to propose the following *ansatz*: $\tilde{\rho}(z)=\mathcal{N}z^{\alpha/\nu}(a+bz)^{\beta/\nu}$, as a solution for Eq. (8). To verify the last statement, the following result is considered:

$$\frac{d^{\delta}}{dz^{\delta}}\left[z^{\alpha}(a+bz)^{\beta}\right]=a^{\delta}\frac{\Gamma[\alpha+1]}{\Gamma[\alpha+1-\delta]}z^{\alpha-\delta}(a+bz)^{\beta-\delta}, \tag{9}$$

when $\delta=\alpha+\beta+1$ ($\Gamma[\ldots]$ is the Gamma function). By applying the ansatz and the above equation in Eq. (8), we find

$$\frac{\alpha}{\nu}=\frac{(1+\mu+\theta)(2+\mu+\theta)}{(1+2\mu+\theta)(\gamma-1)}+d-1,$$

$$\frac{\beta}{\nu}=\frac{\mu(2+\mu+\theta)}{(1+2\mu+\theta)(\gamma-1)},$$

$$\nu=\frac{(\mu-1)(\gamma-1)}{2+\mu+\theta}. \tag{10}$$

Note that the above results recover those obtained in Ref. 12 for $(\theta,\gamma,d)=(0,0,1)$ and contain the results obtained in Ref. 13 for $d=1$ by replacing μ with $\mu-1$ as a consequence. These results allow us to write the solution in the form

$$\tilde{\rho}(z) = \mathcal{N} z^{d-1}\left[z^{1+\mu+\theta}(1+bz)^{\mu}\right]^{(2+\mu+\theta)/[(1+2\mu+\theta)(\gamma-1)]}, \tag{11}$$

with

$$\mathcal{N} = \left[\frac{\overline{k\Gamma}(-\beta)}{\Gamma(1+\alpha-\nu(d-1))}\right]^{1/(\nu+\gamma-1)}, \tag{12}$$

where b is an arbitrary constant to be taken as ± 1 according to the specific solutions to be studied in order that the solution satisfies the boundary condition (consequently normalization condition) and $\mathcal{N}$ can be determined be the normalization condition. For $b=-1$, we have a cutoff distribution and for $b=1$ we have classical solutions which are nonvanishing on the whole positive axis. In addition, the requirement of normalization for $\mathcal{N}$ implies that $\rho(r,t)$ is normalized to unity at least for the initial time $t=0$. Note that the explicit form of $\mathcal{N}$ and b depend on the behavior of the density function which is defined by the parameters μ, θ, γ, and d, see the cases worked below.

In order to analyze the behavior of the solution $\rho(r,t)$ several range values for the parameters μ, d, θ, and γ may be considered. For simplicity, taking $\alpha(t)=0$ we illustrate three of them: (i) $\mu>0$ with $\mu+\theta \geqslant 0$ and $\gamma>1$, (ii) $-1<\mu+\theta<0$ with $\mu>1$ and $\gamma=1-1/d$, and (iii) $d(1-\gamma)-(2+\theta)<\mu<-(1+\theta)/2$, $d>2$, $1/d<\gamma<1-1/d$, $\mu<0$ and $\theta>2d(1-\gamma)-3$. Starting by case (i), without loss of generality, $b=-1$ can be chosen. The normalization condition

$$\mathcal{N}\int_0^1 z^{d-1}\left[z^{1+\mu+\theta}(1-z)^{\mu}\right]^{(2+\mu+\theta)/[(1+2\mu+\theta)(\gamma-1)]}dz = 1 \tag{13}$$

implies that

$$\mathcal{N} = \frac{\Gamma\left(1+d+\dfrac{2+\mu+\theta}{\gamma-1}\right)}{\Gamma\left(1+\dfrac{\mu(2+\mu+\theta)}{(1+2\mu+\theta)(\gamma-1)}\right)\Gamma\left(d+\dfrac{(1+\mu+\theta)(2+\mu+\theta)}{(1+2\mu+\theta)(\gamma-1)}\right)}, \tag{14}$$

(see Fig. 1). The second moment obtained from the above equation is $\langle r^2\rangle \propto [\Phi(t)]^2$. For cases (ii) and (iii), $b=1$ is taken. The normalization factor yields

$$\mathcal{N} = \frac{\Gamma\left(\dfrac{\mu(2+\mu+\theta)}{(1+2\mu+\theta)(1-\gamma)}\right)}{\Gamma\left(d-\dfrac{(1+\mu+\theta)(2+\mu+\theta)}{(1+2\mu+\theta)(1-\gamma)}\right)\Gamma\left(\dfrac{2+\mu+\theta}{1-\gamma}-d\right)} \tag{15}$$

(see Fig. 2). It is interesting to note that this case has a divergent behavior at the origin for the normalized density probability. Case (iii), in contrast to case (ii), presents a defined behavior at the origin as shown in Fig. 3 and it has a long tail behavior.

Following the previous procedure, the above result can be extended by considering $\mu' \neq 1$, leading to the solution for this case given by

$$\tilde{\rho}(z) = \overline{\mathcal{N}} z^{d-1}\left[z^{\mu+\theta+\mu'}(1+bz)^{\mu+\mu'-1}\right]^{(\mu+2\mu'+\theta)/[(1-2(\mu+\mu')-\theta)(1-\gamma)]}, \tag{16}$$

where

$$\overline{\mathcal{N}} = \left[\frac{\Gamma(1+\alpha-\nu(d-1))}{\overline{k\Gamma}(1+\alpha-\nu(d-1)-\mu)}\frac{\Gamma\left(\alpha\left(1+\dfrac{\gamma}{\nu}\right)+(1-\gamma-\nu)(d-1)-\theta-\mu+1\right)}{\Gamma\left(\alpha\left(1+\dfrac{\gamma}{\nu}\right)+(1-\gamma-\nu)(d-1)-\theta-\mu-\mu'+2\right)}\right]^{1/(1-\nu-\gamma)}$$

and

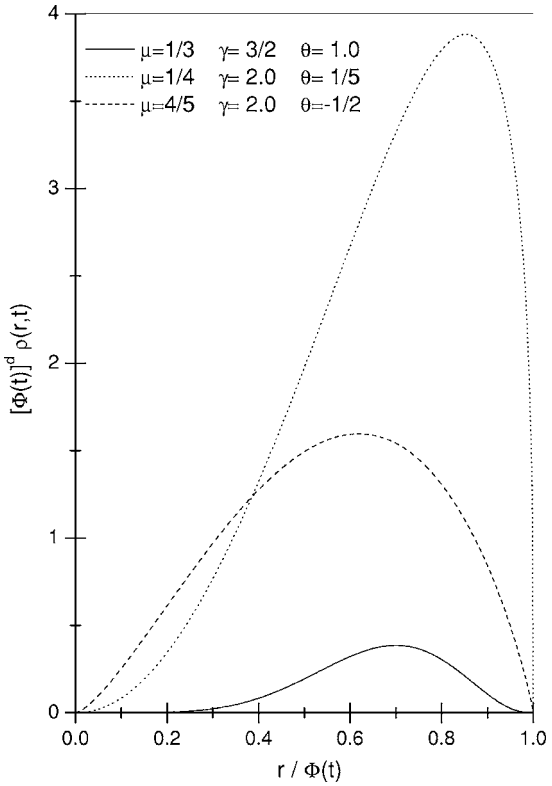

FIG. 1. Behavior of $[\Phi(t)]^d\rho(r,t)$ vs $r/\Phi(t)$ which illustrates the solution with typical values for $\mu>0$ with $\mu+\theta \geqslant 0$, $d=3$, $\gamma>1$ and $\overline{\alpha}(t)=0$. We notice that the distribution vanishes at the abcissa equal to 1, and remains zero outside this interval.

$$\frac{\beta}{\nu}=\frac{(\mu+\mu'-1)(\mu+2\mu'+\theta)}{(1-2(\mu+\mu')-\theta)(1-\gamma)},$$

$$\frac{\alpha}{\nu}=\frac{(\mu+\mu'+\theta)(\mu+2\mu'+\theta)}{(1-2(\mu+\mu')-\theta)(1-\gamma)}+d-1,$$

$$\nu=\frac{(1-\mu)(1-\gamma)}{\mu+2\mu'+\theta},$$

$$\gamma=-\frac{\mu+\theta-d}{\mu'+d}. \tag{17}$$

Note that Eq. (16) presents a similar structure of Eq. (11), however, the conditions on the parameters γ, β, μ, μ', ν, and θ are different.

Now, particular cases of Eq. (8) are discussed by considering special values of μ and μ', with $\mathcal{C}=0$ and (θ,γ,d) arbitraries. Considering $\mu=0$, $\mu'=2$, and $\overline{k}=-k''$, Eq. (8) turns out to be

$$\frac{d}{dz}\left\{z^{(1-\gamma-\nu)(d-1)-\theta}[\tilde{\rho}(z)]^{\gamma+\nu}\right\}=-k''z\tilde{\rho}(z). \tag{18}$$

Solving Eq. (18), we obtain

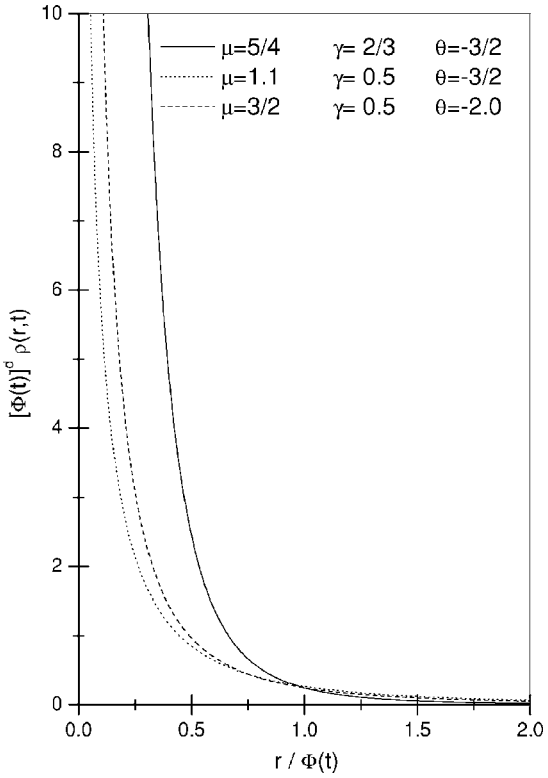

FIG. 2. Behavior of $[\Phi(t)]^d\rho(r,t)$ vs $r/\Phi(t)$ which illustrates the solution with typical values for $-1<\mu+\theta<0$ with $\mu>1$, $\gamma=1-1/d$, and $\overline{\alpha}(t)=0$.

$$\tilde{\rho}(z) = z^{d-1+(1+\theta-d)/(\nu+\gamma)}\exp_q\left[-\mathcal{K}z^{1+d+1+\theta-d/\gamma+\nu}\right] \tag{19}$$

with $\mathcal{K}=k''/[1-d+\theta+(\gamma+\nu)(d+1)]$, $q=2-\nu-\gamma$, where $\exp_q(r)\equiv[1+(1-q)r]^{1/1-q}$ is the q-exponential function that arises within the nonextensive thermostatistical formalism by optimizing, under appropriate constraints, the entropic form[27]

$$S_q = \frac{1-\int dr' r'^{d-1}[p(r')]^q}{q-1}. \tag{20}$$

The constant k'' can be obtained from the normalization condition. By using Eq. (19), $\rho(r,t)$ is illustrated in Fig. 4 by considering the absence of source (absorbent) term. Note that $d(\nu+\gamma)-d+\theta>0$, $d(\nu+\gamma)-d+\theta=0$, and $d(\nu+\gamma)-d+\theta<0$, respectively, correspond to the subdiffusive, normal, and superdiffusive regimes for $(k_1(t),\overline{\alpha}(t))=(0,0)$, since $\langle r^2\rangle\propto t^{2/(2+d(\nu+\gamma)-d+\theta)}$. Note that the above equation leads to an explicit dependence on the dimension d in $\rho(r,t)$, differently from Eqs. (11) and (16).

The solution (19) can also be extended by assuming the external force as $F(r,t)=-k_1(t)r+k_\alpha r^\alpha$ and $\overline{\mathcal{D}}(t)=constant$. It is still not known what happens in the general case for $(\alpha,\theta,\nu,\gamma)$, but there is a special case for which the scaled solution of the type indicated in Eq. (2) can be used. This special case corresponds to $\alpha=d(1-\gamma-\nu)-1-\theta$, i.e., $\alpha+\theta+(2-q)d=d-1$. If this condition is satisfied, we obtain

$$\tilde{\rho}(z') = z'^{d-1}z'^{(1+\theta-d)/(\nu+\gamma)}\exp_q\left[-\frac{\mathcal{K}}{\overline{\mathcal{D}}}z'^{1+d+(1+\theta-d)/(\gamma+\nu)}+\frac{k_\alpha}{(\nu+\gamma)\overline{\mathcal{D}}}\ln_{\bar{q}}(z')\right],$$

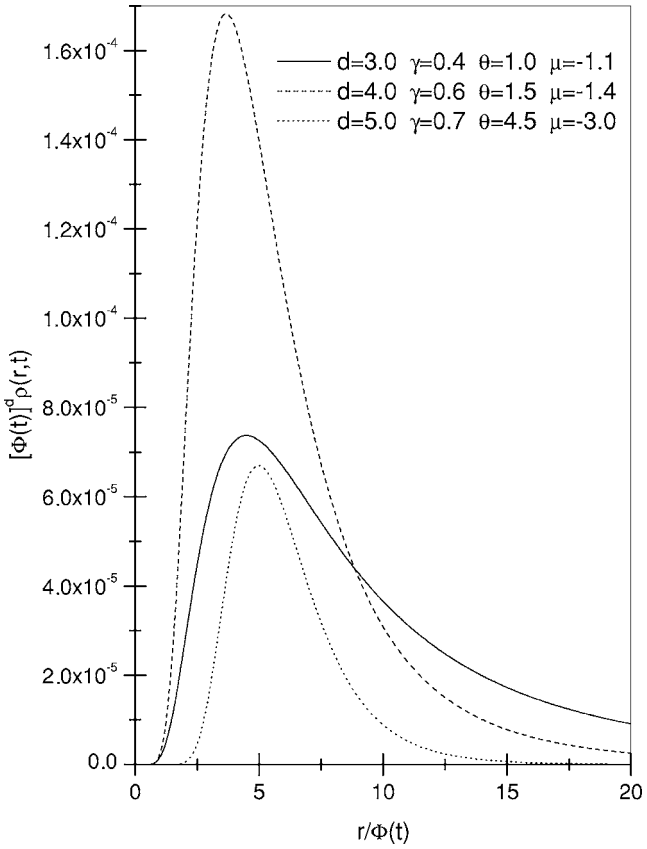

FIG. 3. Behavior of $[\Phi(t)]^d\rho(r,t)$ vs $r/\Phi(t)$, which illustrates the solution with typical values for $d(1-\gamma)-(2+\theta)<\mu<-(1+\theta)/2$, $d>2$, $1/d<\gamma<1-1/d$, $\mu<0$, $\theta>2d(1-\gamma)-3$, and $\overline{\alpha}(t)=0$.

$$\overline{\Phi}(t)=\left[(\overline{\Phi}(0))^{\overline{\xi}+1}+\mathcal{C}_1\int_0^t d\tilde{t}e^{(\overline{\xi}+1)\int_0^{\tilde{t}}dt'k_1(t')}\right]^{1/\overline{\xi}+1}e^{-\int_0^t dt'k_1(t')} \text{ and } z'=\frac{r}{\overline{\Phi}(t)}, \tag{21}$$

where $\overline{q}=1+\overline{\xi}-d-(1+\theta-d)/(\nu+\gamma)$, $\overline{\xi}=1-d+\theta+d(\nu+\gamma)$, $\mathcal{C}_1=(\overline{\xi}+1)k''$, and $\ln_q x\equiv(x^{1-q}-1)/(1-q)$ is the q-logarithm function (that is, the inverse function of the q-exponential). Eq. (21) exhibits an explicit dependence on the dimension d in $\rho(r,t)$ as well as Eq. (19).

Now we focus our attention on the case $\mu=1$, $\mu'=1$ and $\overline{k}=-\tilde{k}$. By substituting these values in Eq. (8), we obtain

$$z^{(1-\gamma)(d-1)-\theta}[\tilde{\rho}(z)]^{\gamma}\frac{d}{dz}\{z^{-\nu(d-1)}[\tilde{\rho}(z)]^{\nu}\}=\tilde{k}z\tilde{\rho}(z). \tag{22}$$

The solution for the above equation is also given in terms of the q-exponential functions as well as the solutions found for Eq. (18). In particular, the solution for Eq. (22) is given by

$$\tilde{\rho}(z)=z^{d-1}\exp_q\left[-\frac{\tilde{k}}{\nu(2+\theta)}z^{2+\theta}\right], \tag{23}$$

with $q=2-(\nu+\gamma)$.

Another interesting case is given by $\mu'=1$ and $\mu=-1$. For this case Eq. (8) reads

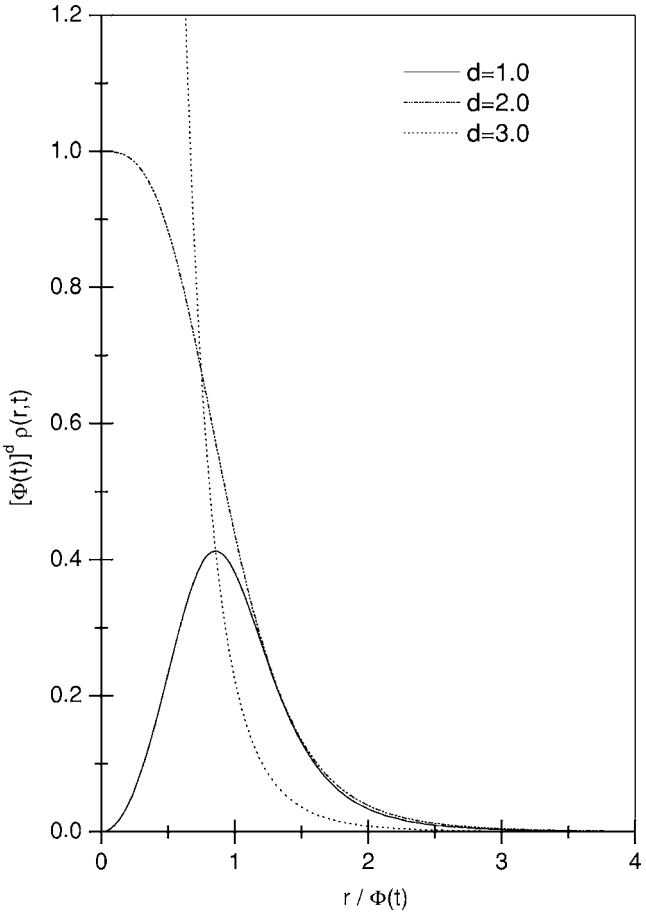

FIG. 4. We show the behavior of $[\Phi(t)]^d\rho(r,t)$ vs $r/\Phi(t)$ for a typical value of d with $\theta=1$, $\nu+\gamma=1/2$ and $\overline{\alpha}(t)=0$. It is interesting to note that depending on the value of d we can have a divergent behavior for $\rho(r,t)$, since in these cases $\rho(r,t)$ is normalized.

$$z^{(1-\gamma)(d-1)-\theta}[\tilde{\rho}(\overline{z})]^{\gamma}\int_0^z d\overline{z}\,\overline{z}^{\nu(d-1)}[\tilde{\rho}(\overline{z})]^{\nu}=\overline{k}z\tilde{\rho}(z). \tag{24}$$

After some calculations, it is possible to show that a solution for Eq. (24) is

$$\tilde{\rho}(z)=z^{d-1-(1+\theta)/(1-\gamma)}\left[1+\overline{\mathcal{C}}z^{1-\nu(1+\theta)/1-\gamma}\right]^{1/(1-\nu-\gamma)}, \tag{25}$$

where $\overline{\mathcal{C}}$ is a constant.

The case $\mu'=0$ and $\mu=0$ leads to

$$\int_0^z d\overline{z}\,\overline{z}^{(d-1)(1-\gamma-\nu)-\theta}[\tilde{\rho}(\overline{z})]^{\gamma+\nu}=\overline{k}z\tilde{\rho}(z). \tag{26}$$

The corresponding solution is given by

$$\tilde{\rho}(z)=\frac{1}{z}\left[1+\mathcal{K}'z^{\alpha'}\right]^{1/(1-\gamma-\nu)}, \tag{27}$$

where $\mathcal{K}'=(1-\gamma-\nu)/[1-\theta+(d-1)(1-2(\nu+\gamma))\overline{k}]$ and $\alpha'=1-\theta+(d-1)[1-2(\nu+\gamma)]$.

To analyze the case $\mu=0$, $\mu'=1$, and $\mathcal{C}\neq 0$ it is convenient to go back to Eq. (4) in order to obtain its solution. Thus, it follows that:

$$\overline{kz}\tilde{\rho}(z) = z^{(1-\nu-\gamma)(d-1)-\theta}[\tilde{\rho}(z)]^{\gamma+\nu} + \overline{\mathcal{C}}, \tag{28}$$

which implicitly determines $\tilde{\rho}(z)$. The solution corresponding to $\mathcal{C}=0$ is $\tilde{\rho}(z)\propto z^{d-1+(1+\theta)/(\gamma+\nu-1)}$.

Considering $\mu'=1$, $\mu=2$, and $\overline{k}=-\tilde{k}'$ Eq. (1) can be reduced to a thin-film-like equation. By applying these assumptions into Eq. (1) and using the above procedure the equation for $\tilde{\rho}(z)$ obtained from Eq. (8) is given by

$$z^{(1-\gamma)(d-1)-\theta}[\tilde{\rho}(z)]^{\gamma}\frac{d^2}{dz^2}\{z^{-\nu(d-1)}[\tilde{\rho}(z)]^{\nu}\} = -\tilde{k}'z\tilde{\rho}(z), \tag{29}$$

and for the time function, by using Eq. (7), we obtain

$$\Phi(t) = \left[(\Phi(0))^{\varepsilon-1} + k'\int_0^t d\tilde{t}\mathcal{D}(\tilde{t})e^{(\nu+\gamma-1)\int_0^{\tilde{t}}dt'\overline{\alpha}(t')+(\varepsilon-1)\int_0^{\tilde{t}}dt'k_1(t')}\right]^{1/(\varepsilon-1)} e^{-\int_0^t dt'k_1(t')}, \tag{30}$$

with $k'=(\varepsilon-1)\tilde{k}'$ where $\varepsilon=4+d(\gamma+\nu)-d+\theta$. The solution for Eq. (29) may be obtained by considering the *ansatz*: $\tilde{\rho}(z)=\mathcal{N}'z^{d-1}(1+\alpha'z^{\lambda})^{\eta/\nu}$. Applying the proposed *ansatz* in Eq. (29) we obtain the following conditions on the parameters η, λ, and ν:

$$\lambda = 3+\theta; \quad \eta = \frac{1}{3+\theta}; \quad \nu = \frac{\gamma-1}{5+2\theta}, \tag{31}$$

with $\alpha'=-\tilde{k}'/(2+\theta)$ where $\gamma>1$ and $\theta>-2$. By substituting the above parameters in Eq. (19), $\tilde{\rho}(z)$ is given by

$$\tilde{\rho}(z) = \mathcal{N}'z^{d-1}(1+\alpha'z^{3+\theta})^{(5+2\theta)/[(\gamma-1)(3+\theta)]}. \tag{32}$$

III. CONCLUSIONS

In summary, a generalized diffusion equation (Eq. (1)) has been worked out for several situations by incorporating some space and time dependent classes of drifts and diffusion coefficients. We have shown that it admits exact solutions where the space scales with a function of time. For Eqs. (19) and (21), we have discussed the explicit dependence on the dimension d in the solution $\rho(r,t)$. This result is very interesting since it shows that, depending on the parameters θ, γ, and ν, we may have an anomalous diffusion (i.e., $\langle r^2\rangle\propto t^{\alpha}$) for a given dimension and a usual diffusion (i.e., $\langle r^2\rangle\propto t$) for other dimensions. Another interesting point is the presence of the q-exponential and the q-logarithm functions of the nonextensive formalism in some solutions, suggesting that these solutions may also be obtained by using the maximum principle of entropy and the nonextensive entropy with adequate constraints. The results obtained in Refs. 12, 13, 25, and 26 have been extended. Finally, we hope that the results obtained here may be useful to discuss the physical situations where the anomalous diffusion is present.

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Threshold properties of matrix-valued Schrödinger operators

Michael Melgaard[a)]
Department of Mathematics, Uppsala University, Box 480, S-751 06 Uppsala, Sweden

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We present some results on the perturbation of eigenvalues embedded at a threshold for a two-channel Hamiltonian with three-dimensional Schrödinger operators as entries and with a small off-diagonal perturbation. In particular, we show how the threshold eigenvalue gives rise to discrete eigenvalues below the threshold and, moreover, we establish a criterion on existence of half-bound states associated with embedded pseudo eigenvalues. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Consider matrix-valued Schrödinger operators of the form

$$H=\widetilde{H}_0+V=\begin{pmatrix}-\Delta & 0\\ 0 & -\Delta+\lambda_0\end{pmatrix}+V(x),\quad x\in\mathbb{R}^3, \tag{1.1}$$

in $\mathcal{H}=L^2(\mathbb{R}^3)\oplus L^2(\mathbb{R}^3)$, where $0<\lambda_0\in\mathbb{R}$ and $V(x)$ is a 2×2 operator-valued matrix

$$V(x)=\begin{pmatrix}V_a & V_{ab}\\ V_{ba} & V_b\end{pmatrix},\quad V(x)^*=V(x), \tag{1.2}$$

which is $\widetilde{H}_0$ compact. We may introduce

$$H_0=\begin{pmatrix}H_a & 0\\ 0 & H_b\end{pmatrix}=\begin{pmatrix}-\Delta+V_a & 0\\ 0 & -\Delta+\lambda_0+V_b\end{pmatrix} \tag{1.3}$$

and write, with g being a real off-diagonal coupling constant

$$H(g):=H_0+g\begin{pmatrix}0 & V_{ab}\\ V_{ba} & 0\end{pmatrix}. \tag{1.4}$$

In particular, $H=H(1)$. The direct sum structure of H_0 means that one can easily give examples of eigenvalues embedded at the threshold λ_0.

A particular case of interest is the following. Under appropriate conditions on V_a we have $\sigma_{\mathrm{ac}}(H_a)=[0,\infty)$ and H_a has discrete spectrum in $(-\infty,0)$. Similarly, $\sigma_{\mathrm{ac}}(H_b)=[\lambda_0,\infty)$ and H_b has discrete spectrum in $(-\infty,\lambda_0)$. Furthermore, we assume that 0 is an (isolated) eigenvalue of H_b (well-defined under suitable decay conditions on V_b) with, say, multiplicity $\varkappa$. Thus $H(0)=H_0$ has an eigenvalue embedded at the threshold 0. To obtain information on what happens when the off-diagonal interaction is switched on, we assume that 0 is a regular point of H_a (see Sec. IV for the terminology). It turns out that the spectral properties of $H(g)$ in the vicinity of 0 are determined by a matrix

a)Electronic mail: melgaard@math.uu.se

$$M_{ab} = (\langle R_a(0) V_{ab} \psi_j, V_{ab} \psi_k \rangle)_{1 \leqslant j,k \leqslant \varkappa}, \tag{1.5}$$

where $R_a(\zeta) = (H_a - \zeta)^{-1}$ is the resolvent of H_a and ψ_k, $k = 1, \ldots, \varkappa$, are the normalized eigenfunctions corresponding to the zero eigenvalue of H_b. Assuming that M_{ab} has strictly positive (real) eigenvalues, the following result holds (see Theorem 4.2). There exist $\eta_0 > 0$ and $\delta_0 > 0$ such that

$$(-\delta_0, 0) \cap \sigma_{\mathrm{pp}}(H(g)) \text{ is discrete and nonempty} \tag{1.6}$$

for all g with $g \in (0, \eta_0]$. This result should be compared with the one in Ref. 7, where the same situation (and several other cases) is considered. Under the hypothesis that a certain (effective interaction of off-diagonal part) operator is strictly positive and invertible, it is shown in Ref. 7 that there are no eigenvalues of $H(g)$ contained in an interval of the form $(-cg^2, \delta_0)$, some $c > 0$. It is worth it to mention that the methods used in the present work are quite different from the ones used in Ref. 7.

In some cases one would expect that embedded eigenvalues become resonances under perturbation. In this paper we are not imposing assumptions on the Hamiltonians, which makes it possible to give a reasonable definition of a resonance, hence, we have no results in this direction here; for two-channel Hamiltonians with one-dimensional Schrödinger operators as components, some results were established in Ref. 11 by a different method.

The proof of Theorem 4.2 can easily be seen to give a necessary and sufficient criterion (see Theorem 5.2) on the existence of half-bound states associated with embedded pseudo eigenvalues of $H(g)$; see Definition 5.1 for this notion. Within this context Theorem 5.4 asserts that if $\lambda \in (0, \lambda_0)$ is an eigenvalue of H_b and $M_{ab}(\lambda + i0)$ (see (1.5)) has no real eigenvalues, then there exist $\eta_0 > 0$ and $\delta_0 > 0$ such that

$$[\lambda - \delta_0, \lambda + \delta_0] \cap \sigma_{\mathrm{pp}}(H(g)) = \emptyset. \tag{1.7}$$

The results obtained herein give rise to two open problems: under suitable hypotheses on V, can one prove that

- negative eigenvalues of M_{ab} (cf. Theorem 4.2) give rise to resonances?
- Theorem 5.2 holds if, in its formulation, pseudo eigenvalues are replaced by eigenvalues in the usual sense?

These problems will be pursued elsewhere.

Except for the work in Ref. 7, there seems to be few results on this problem. A general result on absorption of eigenvalues in the continuum is given in Ref. 16. In Ref. 1 a result is obtained concerning the survival of the ground state of a Pauli–Fierz Hamiltonian. In Ref. 2 the possibility of having a modified Fermi Golden Rule at a threshold is considered. In a time-dependent framework the perturbation of threshold eigenvalues has been discussed in Ref. 17. Another closely related issue is the derivation of asymptotic expansions of the resolvent as the spectral parameter tends to a threshold. Results on two-channel Hamiltonians are given in Ref. 9, based on resolvent expansions for three-dimensional and one-dimensional Schrödinger operators found in Refs. 6 and 12. The latter results are applied to scattering theory for pairs of two-channel Hamiltonians in Ref. 10 and also to scattering theory near the lowest Landau threshold for the three-dimensional Schrödinger operator with a constant magnetic field.[13,14] There is a vast literature on 2×2 operator-valued matrices, e.g., in system theory (see, e.g., Ref. 3) and in semigroup theory (see, e.g., Ref. 5). Most notably in this context is the substantial number of questions of a general nature which have been answered on spectral theory in recent years, see, e.g., Ref. 18. However, the methods therein are not related to ours although some of the questions addressed clearly are, e.g. the appearance of resonances discussed in Ref. 15.

II. PRELIMINARIES

Let us fix some basic notation. Let $\mathcal{H}$ be a separable complex Hilbert space. We denote its scalar product and norm by $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ and $\| \cdot \|_{\mathcal{H}}$, respectively. If $\mathcal{K}$ is another Hilbert space, then we

write $\mathcal{K}\subset\mathcal{H}$ if $\mathcal{K}$ is embedded in $\mathcal{H}$. Let T be a self-adjoint operator on a Hilbert space $\mathcal{H}$ with domain $\mathfrak{D}(T)$. The spectrum and resolvent set are denoted by $\sigma(T)$ and $\rho(T)$, respectively. We use standard terminology for the various parts of the spectrum, see for example, Ref. 8. The resolvent is $R(\zeta)=(T-\zeta)^{-1}$. The spaces of bounded and compact operators from a Hilbert space $\mathcal{H}_1$ into a Hilbert space $\mathcal{H}_2$ are denoted by $\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)$ and $\mathcal{K}(\mathcal{H}_1,\mathcal{H}_2)$, respectively. If $\mathcal{H}:=\mathcal{H}_1=\mathcal{H}_2$ we use the notation $\mathcal{B}(\mathcal{H})$ and $\mathcal{K}(\mathcal{H})$, respectively.

We adopt the usual notation for function spaces: C_0^∞, L^2, etc. The Schwartz space of rapidly decreasing functions and its adjoint space of tempered distributions are denoted by $\mathcal{L}$ and $\mathcal{L}'$, respectively. The Fourier transformation is denoted by $\mathcal{F}$. The weighted Sobolev spaces on $\mathbb{R}^3$ are defined by

$$H^{t,s}(\mathbb{R}^3)=\{\psi\in\mathcal{L}'(\mathbb{R}^3):\langle p\rangle^s\langle x\rangle^t\psi\in L^2(\mathbb{R}^3)\}.$$

Here $\langle x\rangle$ denotes the operator of multiplication by the function $(1+|x|^2)^{1/2}$ and $\langle p\rangle=\mathcal{F}^*\langle x\rangle\mathcal{F}$. In particular, the weighted L^2 spaces are defined by $L^{2,s}(\mathbb{R}^3):=H^{0,s}(\mathbb{R}^3)$ and the standard Sobolev spaces are defined by $H^t(\mathbb{R}^3)=H^{t,0}(\mathbb{R}^3)$.

It is convenient to introduce the following short-hand notation: $\mathcal{L}^{2,s}(\mathbb{R}^3):=L^{2,s}(\mathbb{R}^3)\oplus L^{2,s}(\mathbb{R}^3)$, $\mathcal{L}^2(\mathbb{R}^3):=\mathcal{L}^{2,0}(\mathbb{R}^3)$, $\mathcal{H}^t(\mathbb{R}^3):=H^t(\mathbb{R}^3)\oplus H^t(\mathbb{R}^3)$ and also $\mathcal{H}^{t,s}(\mathbb{R}^3):=H^{t,s}(\mathbb{R}^3)\oplus H^{t,s}(\mathbb{R}^3)$.

The Feshbach formula gives a convenient explicit representation of the resolvent $R(g;\zeta)$ of $H(g)$. There are two variants. We give only one of them. The other version is just an interchange of indices. Define

$$R_a(\zeta):=(H_a-\zeta)^{-1},\quad R_b(\zeta):=(H_b-\zeta)^{-1},\tag{2.1}$$

$$W_b(\zeta):=V_{ab}R_b(\zeta)V_{ba},\tag{2.2}$$

and

$$T_a(g;\zeta):=R_a(\zeta)(1-g^2W_b(\zeta)R_a(\zeta))^{-1}.\tag{2.3}$$

Then, for $\operatorname{Im}\zeta\neq 0$, we have

$$R(g;\zeta)=\begin{pmatrix} T_a(g;\zeta) & -gT_a(g;\zeta)V_{ab}R_b(\zeta)\\ -gR_b(\zeta)V_{ba}T_a(g;\zeta) & R_b(\zeta)(1+g^2V_{ba}T_a(g;\zeta)V_{ab}R_b(\zeta))\end{pmatrix}.\tag{2.4}$$

In this way we have solved the (Feshbach) problem $(H(g)-\zeta)\Psi=\Phi$, $\operatorname{Im}\zeta\neq 0$.

We impose the following hypotheses on V_a, V_b, and V_{ab}:

Assumption 2.1:

(i) $V_\#\in\mathcal{K}(H^2(\mathbb{R}^3),L^2(\mathbb{R}^3))$ for $\#=a,b$.

(ii) $x\nabla V\in\mathcal{K}(H^2(\mathbb{R}^3),H^{-2}(\mathbb{R}^3))$ for $\#=a,b$.

(iii) For $\#=a,b$ and some $\beta_\#>0$,

$$|V_\#(x)|\leq C\langle x\rangle^{-\beta_\#}$$

for $|x|$ large.

(iv) $V_{ab}\in\mathcal{K}(H^2(\mathbb{R}^3),L^2(\mathbb{R}^3))$, $x\nabla V_{ab}\in\mathcal{K}(H^2(\mathbb{R}^3),H^{-2}(\mathbb{R}^3))$ and, for some $\beta>0$,

$$|V_{ab}(x)|\leq C\langle x\rangle^{-\beta},$$

for large $|x|$.

Assumption 2.1, in conjunction with the Kato–Rellich theorem, ensures that H_a and H_b are well-defined as self-adjoint operators in $L^2(\mathbb{R}^3)$, with domain $\mathfrak{D}(H_a)=\mathfrak{D}(H_b)=H^2(\mathbb{R}^3)$, and the basic spectral properties are as described in the Introduction. Moreover, V is $\widetilde{H}_0$ compact, which implies that H is a well-defined self-adjoint operator in $\mathcal{L}^2(\mathbb{R}^3)$, with domain $\mathcal{H}^2(\mathbb{R}^3)$.

We begin by considering the resolvent of $H(g)$. For this purpose we define the following set. Let $0<l<r<\lambda_0$ and set $\Lambda=[l,r]$. For some $\delta_0>0$ define

$$\Omega=\{\zeta=\mu+i\epsilon\in\mathbb{C}:\mu\in\Lambda,\operatorname{dist}(\mu,\sigma(H_b))\geqslant\delta_0 \text{ and } \epsilon\in(0,1]\}. \tag{2.5}$$

Lemma 2.2: *Let Assumption 2.1 hold with $\beta>1/2$. Then there exists $\eta_0>0$ such that, for $g\in(0,\eta_0]$, $\zeta\mapsto R(g;\zeta)$ has a norm-continuous extension to $\bar{\Omega}$, uniformly bounded in g, with values in $\mathcal{B}(L^{2,s}(\mathbb{R}^3)\oplus L^2(\mathbb{R}^3),H^{2,-s}(\mathbb{R}^3)\oplus H^2(\mathbb{R}^3))$, $s>1/2$.*

Proof: Under the hypotheses, the limiting absorption principle is valid for H_a (see, e.g., Ref. 4). It asserts that $R_a(\zeta)$, defined initially on $\operatorname{Im}\zeta>0$, extends continuously to $\zeta\in\bar{\Omega}$ as an operator in $\mathcal{B}(L^{2,s}(\mathbb{R}^3),L^{2,-s}(\mathbb{R}^3))$, $s>1/2$. Taking $\beta>1/2$ and $1/2<s<\beta$ ensure that $g^2W_b(\zeta)R_a(\zeta)$ maps $L^{2,s}(\mathbb{R}^3)$ into $L^{2,2\beta-s}(\mathbb{R}^3)\subset L^{2,s}(\mathbb{R}^3)$ and it is uniformly bounded by g^2 (up to a multiplicative constant). Hence, choosing η_0 sufficiently small,

$$1-g^2W_b(\zeta)R_a(\zeta):L^{2,s}(\mathbb{R}^3)\to L^{2,s}(\mathbb{R}^3)$$

is invertible and it has a uniformly bounded inverse. It follows that:

$$T_a(g;\zeta)=R_a(\zeta)(1-g^2W_b(\zeta)R_a(\zeta))^{-1}:L^{2,s}(\mathbb{R}^3)\to H^{2,-s}(\mathbb{R}^3)$$

is uniformly bounded and it extends continuously to $\bar{\Omega}$. □

III. A FACTORIZATION OF THE RESOLVENT

Throughout this section we consider the following situation.

Assumption 3.1: Let $\lambda\in\sigma(H_b)$

(i) Assume $\lambda\in(0,\lambda_0)$ is an eigenvalue of H_b having multiplicity $\varkappa$, with normalized eigenfunctions ψ_k, $k=1,\ldots,\varkappa$.
(ii) Assume that $\delta_0>0$ is chosen such that $\operatorname{dist}(\lambda,\sigma(H_b)\backslash\{\lambda\})\geqslant 2\delta_0$.

Corresponding to the eigenvalue λ of H_b we use the notation P_b for the eigenprojection and, moreover, we set $Q_b:=1-P_b$.

Define $\tilde{H}_b:=Q_bH_bQ_b$, $\tilde{R}_b(\zeta):=(\tilde{H}_b-\zeta)^{-1}Q_b$,

$$\tilde{W}_b(\zeta):=V_{ab}\tilde{R}_b(\zeta)V_{ba}, \tag{3.1}$$

$$\tilde{T}_a(g;\zeta):=R_a(\zeta)(1-g^2\tilde{W}_b(\zeta)R_a(\zeta))^{-1}, \tag{3.2}$$

and

$$\tilde{R}(g;\zeta):=\begin{pmatrix}\tilde{T}_a(g;\zeta) & -g\tilde{T}_a(g;\zeta)V_{ab}\tilde{R}_b(\zeta)\\ -g\tilde{R}_b(\zeta)V_{ba}\tilde{T}_a(g;\zeta) & \tilde{R}_b(\zeta)(1+g^2V_{ba}\tilde{T}_a(g;\zeta)V_{ab}\tilde{R}_b(\zeta))\end{pmatrix}. \tag{3.3}$$

Define

$$\Omega_+(\delta_0;\lambda):=\{\zeta=\mu+i\epsilon\in\mathbb{C}:\mu\in(\lambda-\delta_0,\lambda+\delta_0)\text{and }\epsilon\in(0,1]\}.$$

Then, for $\zeta\in\Omega_+(\delta_0;\lambda)$, we have that

$$(H(g)-\zeta)\tilde{R}(g;\zeta)=\begin{pmatrix}1 & 0\\ gP_bV_{ba}\tilde{T}_a(g;\zeta) & Q_b-g^2P_bV_{ba}\tilde{T}_a(g;\zeta)V_{ab}\tilde{R}_b(\zeta)\end{pmatrix}. \tag{3.4}$$

Consider the equation $(H(g)-\zeta)\Psi=\Phi$ on $\Omega_+(\delta_0;\lambda)$. We wish to derive a formula for the resolvent which solves this problem. For this purpose we define

$$\tilde{X}_r:\mathbb{C}^\varkappa \ni (z_1,\ldots,z_\varkappa) \mapsto \left(0,\sum_{k=1}^{\varkappa} z_k\psi_k\right) \in \mathcal{H}^2(\mathbb{R}^3), \tag{3.5}$$

$$\tilde{X}_l:\mathcal{L}^2(\mathbb{R}^3) \ni (\phi,\psi) \mapsto (\langle\psi_1,\psi\rangle,\ldots,\langle\psi_\varkappa,\psi\rangle) \in \mathbb{C}^\varkappa, \tag{3.6}$$

and consider an analogous equation related to the operator

$$\mathbf{H}(g;\zeta) = \begin{pmatrix} H(g)-\zeta & \tilde{X}_r \\ \tilde{X}_l & 0 \end{pmatrix}:\mathcal{H}^2(\mathbb{R}^3)\oplus\mathbb{C}^\varkappa \to \mathcal{L}^2(\mathbb{R}^3)\oplus\mathbb{C}^\varkappa. \tag{3.7}$$

The structure of (3.4) motivates the introduction of

$$Y(g;\zeta) := \begin{pmatrix} 0 & 0 \\ gP_bV_{ba}\tilde{T}_a(g;\zeta) & -g^2P_bV_{ba}\tilde{T}_a(g;\zeta)V_{ab}\tilde{R}_b(\zeta) \end{pmatrix}, \tag{3.8}$$

$$Z(g;\zeta) := (H(g)-\zeta)\tilde{X}_r. \tag{3.9}$$

Then the inverse of $\mathbf{H}(g;\zeta)$, denoted by $\mathbf{R}(g;\zeta)$, is given by

$$\mathbf{R}(g;\zeta) = \begin{pmatrix} \tilde{R}(g;\zeta)(1-Y(g;\zeta)) & \tilde{X}_r-\tilde{R}(g;\zeta)(1-Y(g;\zeta))Z(g;\zeta) \\ \tilde{X}_l(1-Y(g;\zeta)) & -\tilde{X}_l(1-Y(g;\zeta))Z(g;\zeta) \end{pmatrix} =: \begin{pmatrix} X(g;\zeta) & X_r(g;\zeta) \\ X_l(g;\zeta) & X_{rl}(g;\zeta) \end{pmatrix}. \tag{3.10}$$

By introducing

$$\tilde{X}_r':\mathbb{C}^\varkappa \ni (z_1,\ldots,z_\varkappa) \mapsto \psi = \sum_{k=1}^{\varkappa} z_k\psi_k$$

and its adjoint, denoted by $\tilde{X}_l'$, we may write

$$X_{rl}(g;\zeta) = \tilde{X}_l'(\zeta-\lambda+g^2V_{ba}\tilde{T}_a(g;\zeta)V_{ab})\tilde{X}_r'. \tag{3.11}$$

Then it follows from the latter that, for $\zeta\in\mathbb{C}_+$,

$$R(g;\zeta) = X(g;\zeta) - X_r(g;\zeta)X_{rl}(g;\zeta)^{-1}X_l(g;\zeta). \tag{3.12}$$

To determine the mapping properties of the operator-valued functions X, X_r, etc., we begin by taking a closer look at $\tilde{T}_a(g;\mu+i0)$.

Lemma 3.2: *Let Assumption 2.1 hold with $\beta>1/2$. Moreover, let Assumption 3.1 be satisfied. Then there exists $\eta_0>0$ such that, for $g\in(0,\eta_0]$, $\tilde{T}_a(g;\mu+i0)$ exists in $\mathcal{B}(L^{2,s}(\mathbb{R}^3),L^{2,-s}(\mathbb{R}^3))$, $s>1/2$, and it is Hölder continuous in μ provided $|\mu-\lambda|\leqslant\delta_0$; uniformly in $g\in(0,\eta_0]$.*

Proof: As an operator from $L^2(\mathbb{R}^3)$ into $L^{2,2\beta}(\mathbb{R}^3)$, $\tilde{W}_b(\zeta)=V_{ab}\tilde{R}_b(\zeta)V_{ba}$ is continuous in $\zeta\in\overline{\Omega_+(\delta_0;\lambda)}$. Since $R_a(\mu+i0):L^{2,s}\to L^{2,-s}$ exists (due, once again, to the limiting absorption principle) and is Hölder continuous in $\mu>0$ (provided $s>1/2$), we infer that

$$\zeta\mapsto\tilde{W}_b(\zeta)R_a(\zeta)\in\mathcal{B}(L^{2,s}(\mathbb{R}^3),L^{2,s}(\mathbb{R}^3))$$

is uniformly bounded and the limiting value $\tilde{W}_b(\mu)R_a(\mu+i0)$ exists in $\mathcal{B}(L^{2,s}(\mathbb{R}^3),L^{2,-s}(\mathbb{R}^3))$ provided $1/2<s<\beta$ and $|\mu-\lambda|\leqslant\delta_0$. In particular, for $g\in(0,\eta_0]$ with η_0 sufficiently small, the operator $1-g^2\tilde{W}_b(\mu)R_a(\mu+i0):L^{2,s}(\mathbb{R}^3)\to L^{2,s}(\mathbb{R}^3)$ is invertible and

$$\widetilde{T}_a(g;\mu+i0) = R_a(\mu+i0)(1-g^2\widetilde{W}_b(\mu)R_a(\mu+i0))^{-1}: L^{2,s}(\mathbb{R}^3) \to L^{2,-s}(\mathbb{R}^3)$$

exists and it is Hölder continuous in μ on $|\mu-\lambda| \leqslant \delta_0$; uniformly in g. □

We immediately obtain the next result.

Proposition 3.3: *Let Assumption 2.1 hold with $\beta > 1/2$. Moreover, let Assumption 3.1 be satisfied. Then there exists $\eta_0 > 0$ such that, for $g \in (0, \eta_0]$ and $s > 1/2$, the operator-valued functions*

$$\zeta \mapsto X(g;\zeta) \in \mathcal{B}(L^{2,s}(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3), H^{2,-s}(\mathbb{R}^3) \oplus H^2(\mathbb{R}^3)),$$

$$\zeta \mapsto X_r(g;\zeta) \in \mathcal{B}(\mathbb{C}^\varkappa, H^{2,-s}(\mathbb{R}^3) \oplus H^2(\mathbb{R}^3)),$$

$$\zeta \mapsto X_l(g;\zeta) \in \mathcal{B}(L^{2,s}(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3), \mathbb{C}^\varkappa),$$

$$\zeta \mapsto X_{rl}(g;\zeta) \in \mathcal{B}(\mathbb{C}^\varkappa)$$

are analytic in ζ on $\zeta \in \mathbb{C}_+$ and they extend continuously to $\zeta \in \overline{\Omega_+(\delta_0,\lambda)}$; uniformly in $g \in (0, \eta_0]$.

IV. PERTURBATION OF AN EIGENVALUE AT A THRESHOLD

A priori zero can be an eigenvalue of H_a or a zero resonance for H_a, or both. We have a zero resonance (or half-bound state) if $H_a\psi = 0$ has a solution ψ in a space slightly larger than $L^2(\mathbb{R}^3)$. It turns out that essentially three cases may occur: H_a has no eigenvalue zero and no zero resonance (*zero is a regular point*), H_a has no eigenvalue zero but has a zero resonance (*zero is an exceptional point of first kind*), H_a has eigenvalue zero but has no zero resonance (*zero is an exceptional point of second kind*), or H_a has both eigenvalue zero and a zero resonance (*zero is an exceptional point of the third kind*).

When zero is a regular point, say, of H_a, then $\zeta \mapsto R_a(\zeta) \in \mathcal{B}(L^{2,s}(\mathbb{R}^3), L^{2,-s}(\mathbb{R}^3))$, $s > 1/2$, defined on $\zeta \in \mathbb{C}_+$, extends continuously up to the real axis in a neighborhood of zero.

We first consider the case, which we discussed in the Introduction.

Assumption 4.1:

(i) Assume that zero is a regular point of H_a.

(ii) Assume that zero is an eigenvalue of H_b having multiplicity $\varkappa$, with normalized eigenfunctions ψ_k, $k = 1, \ldots, \varkappa$.

To ensure that a zero eigenvalue of H_b is well-defined, we require that Assumption 2.1(iii) holds with $\beta_b > 2$; see Ref. 6, Sec. 2 for an explanation.

Theorem 4.2: *Let Assumption 2.1 hold with $\beta_b > 2$ and $\beta > 1/2$. Moreover, let Assumption 4.1 hold. If*

$$M_{ab} = (\langle R_a(0)V_{ab}\psi_j, V_{ab}\psi_k\rangle)_{1 \leqslant j,k \leqslant \varkappa}$$

has ϑ strictly positive eigenvalues ν_l, $1 \leqslant l \leqslant \vartheta$ (taking into account multiplicity), then there exist $\eta_0 > 0$ and $\delta_0 > 0$ such that, for $g \in (0, \eta_0]$, the operator $H(g)$ has at least ϑ eigenvalues (again counting multiplicity) $\nu_l(g)$ in $(-\delta_0, 0)$ obeying

$$\nu_l(g) = -\nu_l g^2 + o(g^2), \quad 1 \leqslant l \leqslant \vartheta. \tag{4.1}$$

If, in particular, M_{ab} is positive definite, then $H(g)$ has exactly $\varkappa$ eigenvalues in $(-\delta_0, 0)$ given by (4.1) *with $\varkappa = \vartheta$.*

Proof: We divide the proof into two steps.

Step 1. In this step we prove that, for $\mu \in (-\delta_0, \delta_0)$, the equation $H(g)\Phi = \mu\Phi$ has a solution $\Phi \in \mathcal{H}^{2,-s}(\mathbb{R}^3)$ for any $s > 1/2$ if and only if $\det X_{rl}(g;\mu+i0) = 0$; see (3.10) for the definition of $X_{rl}(g;\zeta)$.

We first observe that Proposition 3.3 asserts that the identities $\mathbf{H}(g;\zeta)\mathbf{R}(g;\zeta)=1$ on $\mathcal{L}^2(\mathbb{R}^3)$ and $\mathbf{R}(g;\zeta)\mathbf{H}(g;\zeta)=1$ on $\mathcal{H}^2(\mathbb{R}^3)$ extend continuously to $[-\delta_0,\delta_0]$ in the setting of weighted spaces. In particular

$$(H(g)-\zeta)X_r(g;\zeta)+\widetilde{X}_rX_{rl}(g;\zeta)=0, \tag{4.2}$$

$$X_l(g;\zeta)(H(g)-\zeta)+X_{rl}(g;\zeta)\widetilde{X}_l=0 \tag{4.3}$$

are valid for $\zeta\in\overline{\Omega_+(\delta_0;0)}$.

Now if $\mu\in[-\delta_0,\delta_0]$ fulfills $H(g)\Phi=\mu\Phi$ with $\Phi=(\varphi_a,\varphi_b)\neq 0$ as above, then (4.3) implies that

$$X_{rl}(g;\mu+i0)\widetilde{X}_l\Phi=0.$$

Since, as an operator from $H^{2,-s}(\mathbb{R}^3)\oplus H^2(\mathbb{R}^3)$ into itself

$$X(g;\mu+i0)(H(g)-\mu)+X_r(g;\mu+i0)\widetilde{X}_l=1,$$

we deduce that

$$X_r(g;\mu+i0)\widetilde{X}_l\Phi=\Phi,$$

and $\widetilde{X}_l\Phi=(\langle\varphi_b,\psi_1\rangle,\ldots,\langle\varphi_b,\psi_\varkappa\rangle)\neq 0$. Hence, $\det X_{rl}(g;\mu+i0)=0$. On the other hand, if $\det X_{rl}(g;\mu+i0)=0$ and $z\in\mathbb{C}^\varkappa\backslash\{0\}$ belongs to $\operatorname{Ker}X_{rl}(g;\mu+i0)$, then, by setting $\Phi=X_r(g;\mu+i0)z\in H^{2,-s}(\mathbb{R}^3)\oplus H^2(\mathbb{R}^3)$ for any $s>1/2$, (4.2) implies that $(H(g)-\mu)\Phi=0$ and $\Phi\neq 0$ because $\widetilde{X}_r\Phi=\widetilde{X}_lX_r(g;\mu+i0)z=z\neq 0$. This proves the assertion.

Step 2. For $\delta_0>0$ we bear in mind that $(-\delta_0,0)\cap\sigma(H_a)=\varnothing$ and that $R_a(\mu+i0)=R_a(\mu)$ is symmetric for $\mu\in(-\delta_0,0]$. In view of (3.11) with $\lambda=0$, we have that, for $\mu\in(-\delta_0,0]$,

$$X_{rl}(g;\mu+i0)=\mu+g^2M(\mu)+g^4N(g;\mu),$$

where the matrices $M(\mu)$ and $N(g;\mu)$ are given by

$$M(\mu)=(R_a(\mu)V_{ab}\psi_j,V_{ab}\psi_k\rangle_{1\leqslant j,k\leqslant\varkappa},$$

$$N(g;\mu)=(\langle R_a(\mu)\widetilde{W}_b(\mu)\widetilde{T}_a(g;\mu)V_{ab}\psi_j,V_{ab}\psi_k\rangle)_{1\leqslant j,k\leqslant\varkappa}.$$

Let $\nu_0>0$ be an eigenvalue of M_{ab} having multiplicity $\varkappa_0$. The continuity of $N(g;\mu)$ in μ and its analyticity with respect to g^2 in a neighborhood of 0 in conjunction with standard (finite-dimensional) perturbation theory imply that, for every $\mu\in(-\delta_0,0]$, there exist $\varkappa_0$ eigenvalues $\xi_k(g;\mu)$ of $M(\mu)+g^2N(g;\mu)$ (taking into counting multiplicity). The eigenvalues are analytic in g^2 in a neighborhood of 0 and they satisfy

$$\xi_k(g;\mu)=\xi_k(\mu)+\sum_{l=1}^{\infty}g^{2l}\xi_{kl}(\mu),\quad k=1,\ldots,\varkappa_0, \tag{4.4}$$

where $\xi_k(\mu)$ are eigenvalues of $M(\mu)$ which converge to ν_0 as $\mu\to 0$. Provided η_0 is sufficiently small, the function $h_k(g;\mu)=\mu+g^2\xi_k(g;\mu)$ obeys $h_k(g;-\delta_0)<0$ and $h_k(g;0)=\nu_0+O(g^2)>0$. The continuity and real valuedness of h_k imply that h_k has at least one zero in $(-\delta_0,0)$, $\mu=\nu_k(g)$, which fulfills

$$\nu_k(g)=-g^2\xi_k(g;\nu_k(g)).$$

Then (4.4) yields that

$$\nu_k(g) = -g^2(\nu_0 + o(1)) \text{ as } g \downarrow 0.$$

Now let $w_k(g;\mu)$ be normalized eigenfunctions of $M(\mu)+g^2N(g;\mu)$ corresponding to the eigenvalues $\xi_k(g;\mu)$, $k=1,\ldots,\varkappa_0$. Evidently $v_k(g)=w_k(g;\nu_k(g)) \in \operatorname{Ker} X_{rl}(g;\nu_k(g)+i0)$, $k=1,\ldots,\varkappa_0$. If $\nu_j(g)=\nu_k(g)$, then $v_j(g)$ and $v_k(g)$ are orthogonal. Following the reasoning in Step 1, we deduce that $v_k(g)$ generates $\varkappa_0$ linearly independent functions, namely $\Phi_k(g)=X(g;\nu_k(g)+i0)v_k(g) \in H^{2,-s}(\mathbb{R}^3)\oplus H^2(\mathbb{R}^3)$, which satisfy $H(g)\Phi_k(g)=\nu_k(g)\Phi_k(g)$. We note that, in fact, $\nu_k(g)<0$ implies that $\Phi_k(g) \in \mathcal{H}^2(\mathbb{R}^3)$ is an eigenfunction of $H(g)$ in the usual sense. Consequently, from a positive eigenvalue of multiplicity $\varkappa_0$ of M_{ab}, we can construct $\varkappa_0$ independent eigenfunctions of $H(g)$. This proves the first assertion. Invoking (3.12) we infer that $H(g)$ has at most $\varkappa$ eigenvalues in $(-\delta_0,\delta_0)$ (counting multiplicity). Therefore, if M_{ab} is positive definite, then each of these eigenvalues is given by (4.1) with $\varkappa=\vartheta$. □

Next we investigate another situation.

Assumption 4.3:

(i) Assume that 0 is an eigenvalue of H_a, but not a zero resonance, having multiplicity $\varkappa$, with normalized eigenfunctions ψ_k, $k=1,\ldots,\varkappa$.
(ii) Assume that $0 \notin \sigma_d(H_b)$.

Bear in mind that $G_0=\lim_{\zeta\to 0,\operatorname{Im}\zeta>0}(-\Delta-\zeta)^{-1}$ exists as an operator from $H^{-1,s}(\mathbb{R}^3)$ to $H^{1,-s}(\mathbb{R}^3)$ provided $s>1$, and $\operatorname{Ker}(1+G_0V_a)$ in $H^{1,-s}(\mathbb{R}^3)$ coincides with the eigenspace of H_a corresponding to the zero eigenvalue provided and $s>1/2$ and $\beta_a>2\beta_a>2$.[9] As usual we use the notation P_a for the eigenprojection corresponding to the zero eigenvalue of H_a. Its complement is denoted by Q_a. The operator

$$\widetilde{R}_a(\zeta) := (Q_aH_aQ_a-\zeta)^{-1}Q_a,$$

defined initially on $\operatorname{Im}\zeta>0$ is bounded as a map from $L^{2,s}(\mathbb{R}^3)$ to $L^{2,-s}(\mathbb{R}^3)$ and it extends continuously up to the real axis in a neighborhood of 0. Define

$$\widetilde{R}(g;\zeta) := \begin{pmatrix} \widetilde{R}_a(\zeta)+g^2\widetilde{R}_a(\zeta)V_{ab}\widetilde{T}_b(g;\zeta)V_{ba}\widetilde{R}_a(\zeta) & -g\widetilde{R}_a(\zeta)V_{ab}\widetilde{T}_b(g;\zeta) \\ -g\widetilde{T}_b(g;\zeta)V_{ba}\widetilde{R}_a(\zeta) & \widetilde{T}_b(g;\zeta) \end{pmatrix}$$

with

$$\widetilde{W}_a(\zeta) := V_{ba}\widetilde{R}_a(\zeta)V_{ab} \tag{4.5}$$

and

$$\widetilde{T}_b(g;\zeta) := (H_b-\zeta-g^2\widetilde{W}_a(\zeta))^{-1}. \tag{4.6}$$

Introduce

$$\widetilde{Y}_r:\mathbb{C}^\varkappa \ni (z_1,\ldots,z_\varkappa) \mapsto \left(\sum_{k=1}^{\varkappa} z_k\psi_k,0\right) \in \mathcal{H}^2(\mathbb{R}^3), \tag{4.7}$$

$$\widetilde{Y}_l:\mathcal{L}^2(\mathbb{R}^3) \ni (\phi,\psi) \mapsto (\langle\psi_1,\phi\rangle,\ldots,\langle\psi_\varkappa,\phi\rangle) \in \mathbb{C}^\varkappa. \tag{4.8}$$

We shall investigate the Feshbach problem related to the operator

$$\mathbf{H}(g;\zeta) = \begin{pmatrix} H(g)-\zeta & \widetilde{Y}_r \\ \widetilde{Y}_l & 0 \end{pmatrix}:\mathcal{H}^2(\mathbb{R}^3)\oplus\mathbb{C}^\varkappa \to \mathcal{L}^2(\mathbb{R}^3)\oplus\mathbb{C}^\varkappa. \tag{4.9}$$

Similar to (3.10), the inverse

$$\mathbf{R}(g;\zeta)=\begin{pmatrix} Y(g;\zeta) & Y_r(g;\zeta) \\ Y_l(g;\zeta) & Y_{rl}(g;\zeta) \end{pmatrix} \tag{4.10}$$

is computed explicitly for $\zeta\in\mathbb{C}_+$ and, in suitable function spaces, it extends continuously up to a small interval containing 0. In analogy with (3.11), we find that

$$Y_{rl}(g;\zeta)=\widetilde{Y}_l'(\zeta-\lambda+g^2V_{ba}\widetilde{T}_b(g;\zeta)V_{ab})\widetilde{Y}_r',$$

where

$$\widetilde{Y}_{r,2}:\mathbb{C}^\varkappa\ni(z_1,\ldots,z_\varkappa)\to\phi=\sum_{k=1}^{\varkappa}z_k\psi_k$$

and its adjoint is denoted by $\widetilde{Y}_{l,2}$.

In analogy with Theorem 4.2 we obtain the following result.

Theorem 4.4: *Let Assumption 2.1 hold with $\beta_a>2$ and $\beta>1/2$. Moreover, let Assumption 4.3 hold. If*

$$M_{ba}=(\langle R_b(0)V_{ba}\psi_j,V_{ba}\psi_k\rangle)_{1\leqslant j,k\leqslant\varkappa}$$

has ϑ strictly positive eigenvalues ν_l, $1\leqslant l\leqslant\vartheta$ (taking into account multiplicity). Then there exist $\eta_0>0$ and $\delta_0>0$ such that, for $g\in(0,\eta_0]$, the operator $H(g)$ has at least ϑ eigenvalues (again counting multiplicity) $\nu_l(g)$ in $(-\delta_0,0)$ obeying

$$\nu_l(g)=-\nu_lg^2+o(g^2),\quad 1\leqslant l\leqslant\vartheta. \tag{4.11}$$

If, in particular, M_{ab} is positive definite, then $H(g)$ has exactly $\varkappa$ eigenvalues in $(-\delta_0,\delta_0)$ given by (4.11) with $\vartheta=\varkappa$.

Proof: Follows the same reasoning as in the proof of Theorem 4.2. □

The results in Theorems 4.2 and 4.4 should be compared with the results in Ref. 7. We have already discussed this issue in the Introduction.

Our approach allows us to treat also the case where zero is an eigenvalue of both H_a and H_b, provided H_a does not have a zero resonance. The situation where H_a has a zero resonance seems to be more difficult to handle.

V. EXISTENCE OF HALF-BOUND STATES

Now we return to the situation characterized in Assumption 3.1. We begin with a definition.

Definition 5.1: A real number μ is said to be a pseudo eigenvalue of $H(g)$ if there exists a nonzero function $\Phi\in\mathcal{L}^{2,-s}(\mathbb{R}^3)$ satisfying

$$H(g)\Phi=\mu\Phi$$

with $s>1$ if $\mu=0$ or $\mu=\lambda_0$, and with $s>1/2$ if $\mu\neq0,\lambda_0$.
The function Φ is called a half-bound state.

From Step 1 in the proof of Theorem 4.2 we immediately obtain the following result.

Theorem 5.2: *Let Assumption 2.1 hold with $\beta>1/2$. Moreover, let Assumption 3.1 be satisfied and let $\mu\in[\lambda-\delta_0,\lambda+\delta_0]$. Then there exists η_0 such that, for $g\in(0,\eta_0]$, μ is a pseudo eigenvalue of $H(g)$ if and only if*

$$\det X_{rl}(g;\mu+i0)=0.$$

Remark 5.3: Theorem 5.2 also holds when Assumption 3.1 is replaced by Assumption 4.1; see the proof of Theorem 4.2, Step 1.

To formulate the next result, we define

$$M(\zeta)=(\langle R_a(\zeta)V_{ab}\psi_j,V_{ab}\psi_k\rangle)_{1\leqslant j,k\leqslant\varkappa},\quad \zeta\in\overline{\Omega_+(\delta_0;\lambda)}.$$

Theorem 5.4: *Let Assumption 2.1 hold with* $\beta > 1/2$. *Moreover, let Assumption 3.1 be satisfied. If* $M(\lambda + i0)$ *has no real eigenvalues, then there exists* η_0 *such that* $[\lambda - \delta_0, \lambda + \delta_0] \cap \sigma_{\mathrm{pp}}(H(g)) = \emptyset$ *for any* $g \in (0, \eta_0]$.

Proof: As $g \to 0$, the definition of $\widetilde{T}_a(g;\zeta)$ and Lemma 3.2 imply that

$$\widetilde{T}_a(g;\zeta) = R_a(\zeta) + O(g^2)$$

holds in $\mathcal{B}(L^{2,s}(\mathbb{R}^3), L^{2,-s}(\mathbb{R}^3))$, $1/2 < s < \beta$, uniformly in $\zeta = \mu + i\epsilon \in \Omega_+(\delta_0;\lambda)$. In addition, we have that

$$X_{rl}(g;\mu + i0) = \mu - \lambda + g^2(M(\mu + i0) + O(g^2)) \tag{5.1}$$

$$= \mu - \lambda + g^2(M(\lambda + i0) + o(1) + O(g^2)), \tag{5.2}$$

which holds uniformly in μ in the vicinity of λ. By hypothesis, $M(\lambda + i0)$ has no real eigenvalues, i.e., there exists C_0 such that, for all $\nu \in \mathbb{R}$,

$$\|(\nu + M(\lambda + i0))^{-1}\|_{\mathcal{B}(\mathbb{C}^\varkappa)} \leq C_0.$$

We next let $\mu = \lambda + g^2\tilde{\mu}(g)$ for a real $\tilde{\mu}(g)$. Choosing $|\mu - \lambda| \geq \delta_0$ and $\eta_0 > 0$ sufficiently small ensures invertibility of the matrix

$$X_{rl}(\mu + i0) = g^2(\tilde{\mu}(g) + M(\lambda + i0)) \times \{1 + (\tilde{\mu}(g) + M(\lambda + i0))^{-1}(o(1) + O(g^2)\}. \tag{5.3}$$

This verifies that $\det X_{rl}(g;\mu + i0) \neq 0$. In view of Theorem 5.2, $H(g)$ has no pseudo eigenvalues and thus no usual eigenvalues in $(-\lambda - \delta_0, \lambda + \delta_0)$. □

Remark 5.5: Theorem 5.4 also holds when Assumption 3.1 is replaced by Assumption 4.1.

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Description of surfaces associated with Grassmannian sigma models on Minkowski space

A. M. Grundland[a)]
Centre de Recherches Mathématiques, Université de Montréal, C. P. 6128, Succ. Centre-ville, Montréal, Quebec H3C 3J7, Canada and Université du Québec, Trois-Rivières CP500, Quebec G9A 5H7, Canada

L. Šnobl[b)]
Centre de Recherches Mathématiques, Université de Montréal, C. P. 6128, Succ. Centre-ville, Montréal, Quebec H3C 3J7, Canada and Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University, Břehová 7, 115 19 Prague 1, Czech Republic

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We construct and investigate smooth orientable surfaces in $\mathfrak{su}(N)$ algebras. The structural equations of surfaces associated with Grassmannian sigma models on Minkowski space are studied using moving frames adapted to the surfaces. The first and second fundamental forms of these surfaces as well as the relations between them as expressed in the Gauss–Weingarten and Gauss–Codazzi–Ricci equations are found. The scalar curvature and the mean curvature vector expressed in terms of a solution of Grassmanian sigma model are obtained. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1996369]

I. INTRODUCTION

Sigma models are of great interest in mathematical physics because a significant number of physical systems can be reduced to these relatively simple models, either on Euclidean or Minkowski space. One such example is the string theory in which sigma models on spacetime and their supersymmetric extensions play a crucial role. Other relevant applications of recent interest are in the areas of statistical physics (for example, reduction of self-dual Yang–Mills equations to the Ernst model[1,2]), phase transitions,[3,4] and the theory of fluid membranes.[5,6]

The objective of this paper is to study geometric properties of surfaces in Lie algebras associated with sigma models on Minkowski space. Recently, we investigated surfaces in $\mathfrak{su}(N)$ associated with $\mathbb{C}P^{N-1}$ sigma models[7] and found a few examples.[8] In this paper we extend this approach to more general models based on Grassmannian manifolds, i.e., the homogeneous spaces

$$G(m,n)=\frac{SU(N)}{S(U(m)\times U(n))},\quad N=m+n.$$

Grassmannian sigma models are a generalization of $\mathbb{C}P^{N-1}$ sigma models. Their important common feature is that the Euler–Lagrange equations can be written in terms of projectors only.[9] They share a lot of properties like an infinite number of local and/or nonlocal conserved quantities, Hamiltonian structure, complete integrability, infinite-dimensional symmetry algebra, existence of multisoliton solutions, etc. The $N\times N$ projector matrix P for the complex Grassmannian sigma models has, in general, rank lower than the corresponding one for the $\mathbb{C}P^{N-1}$ sigma model and consequently some new phenomena can arise.

The generalization of our previous results[7,8] to Grassmannian sigma models seemed to be rather natural—in fact, it was in a sense more straightforward than the generalization from $\mathbb{C}P^1$ to

[a)]Electronic mail: grundlan@crm.umontreal.ca
[b)]Electronic mail: libor.snobl@fjfi.cvut.cz

$\mathbb{C}P^{N-1}$, provided one expressed the corresponding formulas in terms of the projector (2.8). On the other hand, a different perspective obtained in more general case allowed us to write some of the results in a more compact and presumably more natural way.

The results can be of interest in the area of relativistic classical and quantum field theory[10,11] and in string theory in which sigma models on space-time and their supersymmetric extensions play a crucial role.[12] Other relevant applications of recent interest are in the areas of nonlinear interactions in particle physics.[13] The explicit forms of the surfaces can serve to illuminate the role of the Kac–Moody algebras in integrable models associated with the Grassmannian sigma models.[14,15]

The paper is organized as follows. In Sec. II we recall some basic notions and definitions dealing with the complex Grassmannian sigma models and their Euler–Lagrange equations. In Sec. III we perform the analysis of two-dimensional surfaces immersed in the $\mathfrak{su}(N)$ algebra, associated with these models. The geometric properties of surfaces and the construction of moving frames are discussed in detail in Sec. IV and V. Finally, we summarize our results.

II. GRASSMANNIAN SIGMA MODELS AND THEIR EULER–LAGRANGE EQUATIONS

As a starting point let us present some basic formulas and notation for complex Grassmannian sigma models defined on Minkowski space. We adapt to our signature the notation introduced in Ref. 9 for Euclidean Grassmannian sigma models.

The Grassmannian manifold is defined as a homogeneous space

$$G(m,n)=\frac{SU(N)}{S(U(m)\times U(n))},\quad N=m+n. \tag{2.1}$$

We express the elements of $G(m,n)$ using the equivalence classes of elements $g\in SU(N)$ as

$$[g]=\{g\,.\,\psi|\psi=\begin{pmatrix}U_m & 0\\ 0 & U_n\end{pmatrix},\quad U_m\in U(m),\quad U_n\in U(n),\quad \det\psi=1\}\,. \tag{2.2}$$

We decompose $g\in SU(N)$ into the submatrices X,Y,

$$g=(\phi_1,\ldots,\phi_N)=(X,Y),\quad X=(\phi_1,\ldots,\phi_m),\quad Y=(\phi_{m+1},\ldots,\phi_N), \tag{2.3}$$

and from $g^\dagger g=\mathbf{1}$, i.e., $\phi_j^\dagger\phi_k=\delta_{jk}$, we find

$$X^\dagger X=\mathbf{1}_{m\times m},\quad X^\dagger Y=0,\quad Y^\dagger X=0,\quad Y^\dagger Y=\mathbf{1}_{n\times n}.$$

From these orthogonality relations and (2.2) we realize that on the subset of $G(m,n)$ such that the lower square $n\times n$ submatrix of Y is nonsingular, X itself is sufficient to determine $[g]$ (since U_n can be used to bring the lower square part of Y to $\mathbf{1}_{n\times n}$ and the remaining entries in Y are fully determined by the orthogonality properties). In the following we shall assume that we are working in such a chart. Evidently it covers the whole $G(m,n)$ up to lower dimensional submanifolds. We shall denote the equivalence classes either $[X]$ or $[g]$ depending on circumstances. Note that there is still some freedom in the choice of X, namely X and $X.h, h\in\begin{pmatrix}SU(m) & 0\\ 0 & \mathbf{1}\end{pmatrix}$ give rise to the same equivalence class $[X]=[Xh]$. Therefore, one cannot identify $X=[X]$.

Let ξ^0, ξ^1 be the standard Minkowski coordinates in $\mathbb{R}^2$, with the metric

$$(\mathrm{d}s)^2=(\mathrm{d}\xi^0)^2-(\mathrm{d}\xi^1)^2.$$

In what follows we suppose that $\xi_L=\xi^0+\xi^1$, $\xi_R=\xi^0-\xi^1$ are the light-cone coordinates in $\mathbb{R}^2$, i.e.,

$$(\mathrm{d}s)^2=\mathrm{d}\xi_L\mathrm{d}\xi_R. \tag{2.4}$$

We shall denote by ∂_L and ∂_R the derivatives with respect to ξ_L and ξ_R, respectively.

Let us assume that Ω is an open, connected, and simply connected subset in $\mathbb{R}^2$ with Minkowski metric (2.4). We define covariant derivatives D_μ acting on maps $X:\Omega\to G(m,n)$ by

$$D_\mu X = \partial_\mu X - XX^\dagger \partial_\mu X, \quad \partial_\mu \equiv \partial_{\xi^\mu}, \quad \mu = 0,1. \tag{2.5}$$

In the study of Grassmannian sigma models we are interested in maps $X:\Omega\to G(m,n)$ which are stationary points of the action functional

$$\mathcal{S} = \int_\Omega \mathrm{tr}\{(D_\mu X)^\dagger (D^\mu X)\} \mathrm{d}\xi^0 \mathrm{d}\xi^1. \tag{2.6}$$

The Lagrangian density can be further developed to get

$$\mathcal{L} = \mathrm{tr}\{(D_\mu X)^\dagger (D^\mu X)\} = \mathrm{tr}\{\partial^\mu X (\partial_\mu X)^\dagger P\}, \tag{2.7}$$

where

$$P = \mathbf{1} - XX^\dagger \tag{2.8}$$

is an orthogonal projector, i.e., $P^2=P$, $P^\dagger=P$ satisfying $PX=0$, $X^\dagger P=0$.

The action (2.6) has the local (gauge) $SU(m)$ symmetry

$$X(\xi_L,\xi_R) \to X(\xi_L,\xi_R)\,.\,h(\xi_L,\xi_R), \quad h(\xi_L,\xi_R) \in \begin{pmatrix} SU(m) & 0 \\ 0 & \mathbf{1} \end{pmatrix} \tag{2.9}$$

proving that the model does not depend on the choice of representatives X of elements $[X]$ of $G(m,n)$; and the $SU(N)$ global symmetry

$$X(\xi_L,\xi_R) \to g\,.\,X(\xi_L,\xi_R), \quad g \in SU(N). \tag{2.10}$$

It is also invariant under the conformal transformations

$$\xi_L \to \alpha(\xi_L), \quad \xi_R \to \beta(\xi_R), \tag{2.11}$$

where $\alpha,\beta:\mathbb{R}\to\mathbb{R}$ are arbitrary 1-to-1 maps such that $\partial_L\alpha(\xi_L)\neq 0$, $\partial_R\beta(\xi_R)\neq 0$, as well as under the parity transformation

$$\xi_L \to \xi_R, \quad \xi_R \to \xi_L. \tag{2.12}$$

Let us note that the invariance properties (2.9)–(2.12) are naturally reproduced on the level of the Euler–Lagrange equations.

By variation of the action (2.6) respecting the constraint

$$X^\dagger X = \mathbf{1},$$

i.e.,

$$\delta X^\dagger X + X^\dagger \delta X = 0, \quad \partial_\mu X^\dagger X + X\partial_\mu \delta X = 0, \tag{2.13}$$

and assuming that due to suitable boundary conditions the boundary terms vanish we find the Euler–Lagrange equations

$$P(\partial_L\partial_R X - \partial_L XX^\dagger \partial_R X - \partial_R XX^\dagger \partial_L X) = 0. \tag{2.14}$$

They can be also expressed in the matrix form

$$[\partial_L\partial_R P, P] = 0 \tag{2.15}$$

or in the form of a conservation law

$$\partial_L[\partial_R P, P] + \partial_R[\partial_L P, P] = 0. \tag{2.16}$$

Methods for finding special solutions of (2.14), e.g., soliton solutions, are known.[16,17]

By explicit calculation one can check that the real-valued functions

$$J_L = \mathrm{tr}(\partial_L X \partial_L X^\dagger P), \quad J_R = \mathrm{tr}(\partial_R X \partial_R X^\dagger P) \tag{2.17}$$

satisfy

$$\partial_L J_R = \partial_R J_L = 0 \tag{2.18}$$

for any solution X of the Euler–Lagrange equations (2.14). The functions J_L, J_R are invariant under local $SU(m)$ and global $SU(N)$ transformations (2.9) and (2.10).

III. SURFACES OBTAINED FROM THE GRASSMANNIAN SIGMA MODEL

Let us now discuss the analytical description of a two-dimensional smooth orientable surface $\mathcal{F}$ immersed in the $\mathfrak{su}(N)$ algebra, associated with the Grassmannian sigma model (2.14). We shall construct an exact $\mathfrak{su}(N)$-valued one-form whose "potential" zero-form defines the surface $\mathcal{F}$. Next, we shall investigate the geometric characteristics of the surface $\mathcal{F}$.

Let us introduce a scalar product

$$(A,B) = -\tfrac{1}{2}\mathrm{tr}\, AB$$

on $\mathfrak{su}(N)$ and identify the (N^2-1)-dimensional Euclidean space with the $\mathfrak{su}(N)$ algebra

$$\mathbb{R}^{N^2-1} \simeq \mathfrak{su}(N).$$

We denote

$$M_L = [\partial_L P, P], \quad M_R = [\partial_R P, P]. \tag{3.1}$$

It follows from (2.16) that if X is a solution of the Euler–Lagrange equations (2.14) then

$$\partial_L M_R + \partial_R M_L = 0. \tag{3.2}$$

We identify tangent vectors to the surface $\mathcal{F}$ with the matrices M_L and M_R, as follows:

$$\mathcal{Z}_L = M_L, \quad \mathcal{Z}_R = -M_R. \tag{3.3}$$

Equation (3.2) implies there exists a closed $\mathfrak{su}(N)$-valued one-form on Ω,

$$\mathcal{Z} = \mathcal{Z}_L \mathrm{d}\xi_L + \mathcal{Z}_R \mathrm{d}\xi_R, \quad \mathrm{d}\mathcal{Z} = 0.$$

Because $\mathcal{Z}$ is closed and Ω is connected and simply connected, $\mathcal{Z}$ is also exact. In other words, there exists a well-defined $\mathfrak{su}(N)$-valued function Z on Ω such that $\mathcal{Z}=\mathrm{d}Z$. The matrix function Z is unique up to addition of any constant element of $\mathfrak{su}(N)$ and we identify the components of Z with the coordinates of the sought-after surface $\mathcal{F}$ in $\mathbb{R}^{N^2-1}$. Consequently, we get

$$\partial_L Z = \mathcal{Z}_L, \quad \partial_R Z = \mathcal{Z}_R. \tag{3.4}$$

The map Z is called the Weierstrass formula for immersion. In practice, the surface $\mathcal{F}$ is found by integration

$$\mathcal{F}{:}Z\,(\xi_L,\xi_R) = \int_{\gamma(\xi_L,\xi_R)} \mathcal{Z} \tag{3.5}$$

along any curve $\gamma(\xi_L,\xi_R)$ in Ω connecting the point $(\xi_L,\xi_R) \in \Omega$ with an arbitrary chosen point $(\xi_L^0,\xi_R^0) \in \Omega$.

By computation of the traces of $\mathcal{Z}_B.\mathcal{Z}_D$, $B,D=L,R$ we find the components of the induced metric on the surface $\mathcal{F}$,

$$G=\begin{pmatrix} G_{LL}, & G_{LR} \\ G_{LR}, & G_{RR} \end{pmatrix}=\begin{pmatrix} J_L & -\mathrm{tr}\left(\frac{\partial_L X\partial_R X^\dagger+\partial_R X\partial_L X^\dagger}{2}P\right) \\ -\mathrm{tr}\left(\frac{\partial_L X\partial_R X^\dagger+\partial_R X\partial_L X^\dagger}{2}P\right) & J_R \end{pmatrix}. \tag{3.6}$$

The first fundamental form of the surface $\mathcal{F}$ takes surprisingly compact form

$$I=J_L(\mathrm{d}\xi_L)^2-2G_{LR}\mathrm{d}\xi_L\mathrm{d}\xi_R+J_R(\mathrm{d}\xi_R)^2$$

$$=(2\delta_{B,D}-1)\mathrm{tr}(\partial_B X\partial_D X^\dagger P)\mathrm{d}\xi_B\mathrm{d}\xi_D, \tag{3.7}$$

where summation over repeated indices $B,D=L,R$ applies and $\delta_{B,D}=1$ if $B=D$ and 0 otherwise.

In order to establish conditions on a solution X of the Euler–Lagrange equations (2.14) under which the surface exists, we check explicitly whether the induced first fundamental form (3.7) is positive (as it must be by construction even when the surface degenerates to a curve) and when it is positively definite, i.e., we really have a surface.

We introduce a scalar product on the space of $N\times m$ matrices X,

$$\langle a,b\rangle=\mathrm{tr}(a^\dagger\cdot b), a,b\in\mathbb{C}^{N\times m}.$$

Due to the positivity of the projector P we may write

$$J_D=\langle P\partial_D X,\partial_D X\rangle\geqslant 0,\quad D=L,R. \tag{3.8}$$

Further, using the Schwarz inequality

$$|\langle Ab,a\rangle|^2\leqslant\langle Aa,a\rangle\langle Ab,b\rangle \tag{3.9}$$

valid for any positive Hermitian operator A, namely for $P:P(a)=P\cdot a$ we find

$$\langle P\partial_L X,\partial_L X\rangle\langle P\partial_R X,\partial_R X\rangle\geqslant|\langle P\partial_L X,\partial_R X\rangle|^2\geqslant(\Re\langle P\partial_L X,\partial_R X\rangle)^2,$$

i.e.,

$$\det G=\langle P\partial_L X,\partial_L X\rangle\langle P\partial_R X,\partial_R X\rangle-(\Re\langle P\partial_L X,\partial_R X\rangle)^2\geqslant 0. \tag{3.10}$$

Therefore, the 2×2 Hermitian matrix of the metric (3.6) has non-negative diagonal elements and determinant, and consequently, as one may easily show, its eigenvalues are non-negative. This means that the first fundamental form I defined by (3.7) is positive for any solution X of the Euler–Lagrange equations (2.14).

Investigating when sharp inequalities hold we find that I is positive definite in the point (ξ_L^0,ξ_R^0) either if the inequality

$$\Im\,\mathrm{tr}(\partial_L X\partial_R X^\dagger P)\neq 0 \tag{3.11}$$

holds in (ξ_L^0,ξ_R^0) or if the matrices

$$\partial_L X(\xi_L^0,\xi_R^0),\quad \partial_R X(\xi_L^0,\xi_R^0),\quad X(\xi_L^0,\xi_R^0) \tag{3.12}$$

are linearly independent. Therefore any of the conditions (3.11) and (3.12) is a sufficient condition for the existence of the surface $\mathcal{F}$ associated with the solution X of the Euler–Lagrange equations (2.14) in the vicinity of the point (ξ_L^0,ξ_R^0).

Using (3.6) we can write the formula for scalar curvature[18] as

$$K=\frac{1}{\sqrt{J_L J_R-G_{LR}^2}}\partial_R\left(\frac{\partial_L G_{LR}-\frac{1}{2}G_{LR}\partial_L(\ln J_L)}{\sqrt{J_L J_R-G_{LR}^2}}\right). \tag{3.13}$$

IV. THE GAUSS–WEINGARTEN EQUATIONS

Now we may formally determine a moving frame on the surface $\mathcal{F}$ and write the Gauss–Weingarten equations. Let X be a solution of the Euler–Lagrange equations (2.14) such that $\det(G)$ is not zero in a neighborhood of a regular point (ξ_L^0, ξ_R^0) in Ω. Assume also that the surface $\mathcal{F}$ (3.5), associated with these equations is described by the moving frame

$$\vec{\tau} = (\partial_L Z, \partial_R Z, n_3, \ldots, n_{N^2-1})^T,$$

where the vectors $\partial_L Z, \partial_R Z, n_3, \ldots, n_{N^2-1}$ satisfy the normalization conditions

$$(\partial_L Z, n_k) = (\partial_R Z, n_k) = 0, \quad (n_j, n_k) = \delta_{jk}. \tag{4.1}$$

We now show that the moving frame satisfies the Gauss–Weingarten equations

$$\begin{aligned}
\partial_L \partial_L Z &= A_L^L \partial_L Z + A_R^L \partial_R Z + Q_j^L n_j, \\
\partial_L \partial_R Z &= H_j n_j, \\
\partial_L n_j &= \alpha_j^L \partial_L Z + \beta_j^L \partial_R Z + s_{jk}^L n_k, \\
\partial_R \partial_L Z &= H_j n_j, \\
\partial_R \partial_R Z &= A_L^R \partial_L Z + A_R^R \partial_R Z + Q_j^R n_j, \\
\partial_R n_j &= \alpha_j^R \partial_L Z + \beta_j^R \partial_R Z + s_{jk}^R n_k,
\end{aligned} \tag{4.2}$$

where $s_{jk}^L + s_{kj}^L = 0$, $s_{jk}^R + s_{kj}^R = 0$, $j,k = 3, \ldots, N^2 - 1$,

$$\alpha_j^L = \frac{H_j G_{LR} - Q_j^L J_R}{\det G}, \quad \beta_j^L = \frac{Q_j^L G_{LR} - H_j J_L}{\det G},$$

$$\alpha_j^R = \frac{Q_j^R G_{LR} - H_j J_R}{\det G}, \quad \beta_j^R = \frac{H_j G_{LR} - Q_j^R J_L}{\det G},$$

and A_L^L, A_R^L (A_L^R, A_R^R have similar form which can be obtained by exchanging $L \leftrightarrow R$) are written as

$$\begin{aligned}
A_L^L &= \frac{1}{\det G}(J_R(\partial_L \partial_L Z, \partial_L Z) - G_{LR}(\partial_L \partial_L Z, \partial_R Z)), \\
A_R^L &= \frac{1}{\det G}(J_L(\partial_L \partial_L Z, \partial_R Z) - G_{LR}(\partial_L \partial_L Z, \partial_L Z)),
\end{aligned} \tag{4.3}$$

where

$$\begin{aligned}
(\partial_L \partial_L Z, \partial_L Z) &= \tfrac{1}{2}\mathrm{tr}((\partial_L \partial_L X \partial_L X^\dagger + \partial_L X \partial_L \partial_L X^\dagger) P), \\
(\partial_L \partial_L Z, \partial_R Z) &= -\tfrac{1}{2}\mathrm{tr}((\partial_L \partial_L X \partial_R X^\dagger + \partial_R X \partial_L \partial_L X^\dagger) P + 2 \partial_L X \partial_L X^\dagger (X \partial_R X^\dagger + \partial_R X X^\dagger)).
\end{aligned} \tag{4.4}$$

Note that in fact we can write it in a compact way

$$(\partial_B \partial_B Z, \partial_D Z) = \left(\delta_{B,D} - \tfrac{1}{2}\right)\mathrm{tr}((\partial_B \partial_B X \partial_D X^\dagger + \partial_D X \partial_B \partial_B X^\dagger) P + 2 \partial_B X \partial_B X^\dagger (X \partial_D X^\dagger + \partial_D X X^\dagger)). \tag{4.5}$$

The explicit form of the coefficients H_j, Q_j^D (where $D=L,R$; $j=3,\ldots,N^2-1$) depends on the chosen orthonormal basis $\{n_3,\ldots,n_{N^2-1}\}$ of the normal space to the surface $\mathcal{F}$ at the point $X(\xi_L^0,\xi_R^0)$. Partial information about them will be obtained in (5.6).

Indeed, if $\partial_L Z, \partial_R Z$ are defined by (3.4) for an arbitrary solution X of the Euler–Lagrange equations (2.14), then by straightforward calculation using (2.15) one finds that

$$\partial_L\partial_R Z = \partial_R\partial_L Z = [\partial_L P, \partial_R P] = \lambda - \lambda XX^\dagger - XX^\dagger\lambda + X(\partial_L X^\dagger \partial_R X - \partial_R X^\dagger \partial_L X)X^\dagger,$$

where

$$\lambda = \partial_L X \partial_R X^\dagger - \partial_R X \partial_L X^\dagger.$$

By computing

$$\mathrm{tr}(\partial_L\partial_R Z \,.\, \partial_D Z) = \pm\,\mathrm{tr}([\partial_L P, \partial_R P] \,.\, [\partial_D P, P]) = 0, \quad D = L,R \tag{4.6}$$

we conclude that $\partial_L\partial_R Z$ is perpendicular to the surface $\mathcal{F}$ and consequently it has the form given in (4.2).

The remaining relations in (4.2) and (4.3) follow as differential consequences from the assumed normalizations of the normals (4.1), e.g.,

$$(n_j, n_k) = 0, \quad j \neq k,$$

which gives

$$0 = (\partial_L n_j, n_k) + (\partial_L n_k, n_j) = s_{jk}^L + s_{kj}^L.$$

Similarly

$$(n_j, \partial_L Z) = 0, \quad (n_j, \partial_R Z) = 0$$

by differentiation leads to

$$(\partial_R n_j, \partial_L Z) + (n_j, \partial_L\partial_R Z) = 0, \quad (\partial_R n_j, \partial_R Z) + (n_j, \partial_R\partial_R Z) = 0$$

implying

$$J_L \alpha_j^R + G_{LR}\beta_j^R + H_j = 0, \quad G_{LR}\alpha_j^R + J_R\beta_j^R + Q_j^R = 0.$$

Consequently, α_j^R, β_j^R can be determined in terms of H_j, Q_j^R and of the components of the induced metric G. The remaining coefficients α_j^L, β_j^L are derived in an analogous way by exchanging indices $L \leftrightarrow R$ in the successive differentiations.

The coefficients $A_L^L,\ldots,A_R^R$ are obtained by the requirement that $(\partial_D\partial_D Z - A_L^D\partial_L Z - A_R^D\partial_R Z)$ is normal to the surface, i.e.,

$$\mathrm{tr}(\partial_B Z \,.\, (\partial_D\partial_D Z - A_L^D\partial_L Z - A_R^D\partial_R Z)) = 0, \quad B,D = L,R. \tag{4.7}$$

From (3.1) and (3.4) we find

$$\begin{aligned}\partial_L\partial_L Z = [\partial_L\partial_L P, P] &= \partial_L\partial_L XX^\dagger - XX^\dagger\partial_L\partial_L XX^\dagger + X\partial_L\partial_L X^\dagger XX^\dagger - X\partial_L\partial_L X^\dagger + 2X\partial_L X^\dagger X\partial_L X^\dagger \\ &\quad - 2\partial_L XX^\dagger\partial_L XX^\dagger.\end{aligned} \tag{4.8}$$

The expression for $\partial_R\partial_R Z$ is obtained by the change of the overall sign and $L \leftrightarrow R$. After substituting the above expressions into (4.7) we solve the resulting linear equations for A_B^D.

Let us note that the Gauss–Weingarten equations (4.2) can be written equivalently in the $N \times N$ matrix form

$$\partial_L\vec{\tau} = U\vec{\tau}, \quad \partial_R\vec{\tau} = V\vec{\tau}, \tag{4.9}$$

where

$$U=\begin{pmatrix} A_L^L & A_R^L & Q_3^L & \cdots & Q_{N^2-1}^L \\ 0 & 0 & H_3 & \cdots & H_{N^2-1} \\ \alpha_3^L & \beta_3^L & s_{33}^L & \cdots & s_{3(N^2-1)}^L \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \alpha_{(N^2-1)}^L & \beta_{(N^2-1)}^L & s_{(N^2-1)3}^L & \cdots & s_{(N^2-1)(N^2-1)}^L \end{pmatrix},$$

$$V=\begin{pmatrix} 0 & 0 & H_3 & \cdots & H_{N^2-1} \\ A_L^R & A_R^R & Q_3^R & \cdots & Q_{N^2-1}^R \\ \alpha_3^R & \beta_3^R & s_{33}^R & \cdots & s_{3(N^2-1)}^R \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \alpha_{(N^2-1)}^R & \beta_{(N^2-1)}^R & s_{(N^2-1)3}^R & \cdots & s_{(N^2-1)(N^2-1)}^R \end{pmatrix}. \tag{4.10}$$

The Gauss–Codazzi–Ricci equations

$$\partial_R U-\partial_L V+[U,V]=0 \tag{4.11}$$

are the compatibility conditions for the Gauss–Weingarten equations (4.2). They are the necessary and sufficient conditions for the local existence of the corresponding surface $\mathcal{F}$. They are satisfied for any solution X of the Euler–Lagrange equations (2.14), provided that explicit forms of Q_j^D, H_j are inserted (they can be found, for example, by the method developed in Sec V.). On the other hand, the Gauss–Codazzi–Ricci equations (4.11) can be used to derive differential constraints that Q_j^D, H_j must satisfy for any possible choice of normals n_j.

The second fundamental form and the mean curvature vector of the surface $\mathcal{F}$ at the regular point p can be expressed, according to Refs. 19 and 20, as

$$\begin{aligned} \mathbf{II}&=(\partial_L\partial_L Z)^{\perp}\mathrm{d}\xi_L\mathrm{d}\xi_L+2(\partial_L\partial_R Z)^{\perp}\mathrm{d}\xi_L\mathrm{d}\xi_R+(\partial_R\partial_R Z)^{\perp}\mathrm{d}\xi_R\mathrm{d}\xi_R,\\ \mathbf{H}&=\frac{1}{\det G}(J_R(\partial_L\partial_L Z)^{\perp}-2G_{LR}(\partial_L\partial_R Z)^{\perp}+J_L(\partial_R\partial_R Z)^{\perp}), \end{aligned} \tag{4.12}$$

where $(\ )^{\perp}$ denotes the normal part of the vector. In our case the expressions (4.12) take the form

$$\begin{aligned} \mathbf{II}&=\left(Q_j^L\mathrm{d}\xi_L\mathrm{d}\xi_L+2H_j\mathrm{d}\xi_L\mathrm{d}\xi_R+Q_j^R\mathrm{d}\xi_R\mathrm{d}\xi_R\right)n_j=(\partial_L\partial_L Z-A_L^L\partial_L Z-A_R^L\partial_R Z)\mathrm{d}\xi_L\mathrm{d}\xi_L+2(\partial_L\partial_R Z)\mathrm{d}\xi_L\mathrm{d}\xi_R\\ &\quad+(\partial_R\partial_R Z-A_L^R\partial_L Z-A_R^R\partial_R Z)\mathrm{d}\xi_R\mathrm{d}\xi_R,\\ \mathbf{H}&=\frac{1}{\det G}(J_RQ_j^L-2G_{LR}H_j+J_LQ_j^R)n_j=\frac{1}{\det G}(J_R(\partial_L\partial_L Z-A_L^L\partial_L Z-A_R^L\partial_R Z)-2G_{LR}(\partial_L\partial_R Z)\\ &\quad+J_L(\partial_R\partial_R Z-A_L^R\partial_L Z-A_R^R\partial_R Z)). \end{aligned} \tag{4.13}$$

The derivatives $\partial_D\partial_B Z$ are expressed explicitly in terms of X in Eqs. (4.6) and (4.8) but after substitution of them into (4.13) the expressions get rather complicated, therefore we do not present them here.

V. THE MOVING FRAME OF A SURFACE IN THE ALGEBRA (N)

Now we proceed to construct the moving frame of the surface $\mathcal{F}$ immersed in the $\mathfrak{su}(N)$ algebra, i.e., matrices $\partial_L Z, \partial_R Z, n_a$, $a=3,\ldots,N^2-1$ satisfying (4.1).

Let X be a solution of the Euler–Lagrange equations (2.14) and let (ξ_L^0,ξ_R^0) be a regular point in Ω, i.e., such that $\det G(X(\xi_L^0,\xi_R^0))\neq 0$. Let us denote $X^0=X(\xi_L^0,\xi_R^0)$, $Z^0=Z(\xi_L^0,\xi_R^0)$. Taking into account that

$$\mathrm{tr}(A) = \mathrm{tr}(\Phi A \Phi^{\dagger}), \quad A \in \mathfrak{su}(N), \quad \Phi \in SU(N),$$

we employ the adjoint representation of the group $SU(N)$ in order to bring $\partial_L Z, \partial_R Z, n_a$ to the simplest form possible. We shall request in the neighborhood of (ξ_L^0, ξ_R^0) that

$$X(\xi_L, \xi_R) = \Phi(\xi_L, \xi_R) \begin{pmatrix} \mathbf{1}_{m\times m} \\ \mathbf{0}_{n\times m} \end{pmatrix}. \tag{5.1}$$

The existence of such a matrix function $\Phi(\xi_L, \xi_R)$ follows from the fact that $G(m,n)$ is a homogeneous space (2.1). In fact $\Phi(\xi_L, \xi_R)$ is just any representative in $SU(N)$ of the equivalence class $[X(\xi_L, \xi_R)]$ such that

$$X(\xi_L, \xi_R) = \begin{pmatrix} \Phi_{11}(\xi_L, \xi_R) & \cdots & \Phi_{1m}(\xi_L, \xi_R) \\ & \cdots & \\ \Phi_{N1}(\xi_L, \xi_R) & \cdots & \Phi_{Nm}(\xi_L, \xi_R) \end{pmatrix},$$

$$[X(\xi_L, \xi_R)] = [\Phi(\xi_L, \xi_R)]$$

and consequently $\Phi(\xi_L, \xi_R)$ is not unique. An explicit (local) construction of $\Phi(\xi_L, \xi_R)$ can be performed algorithmically in such a way that Φ depends smoothly on ξ_L, ξ_R (for a detailed explanation in the case $G(m,1) = \mathbb{C}P^m$ see Ref. 7).

Let us choose an orthonormal basis in $\mathfrak{su}(N)$ of the following form:

$$\begin{aligned} (A_{jk})_{ab} &= i(\delta_{ja}\delta_{kb} + \delta_{jb}\delta_{ka}), \quad 1 \leqslant j < k \leqslant N, \\ (B_{jk})_{ab} &= (\delta_{ja}\delta_{kb} - \delta_{jb}\delta_{ka}), \quad 1 \leqslant j < k \leqslant N, \end{aligned} \tag{5.2}$$

$$(C_p)_{ab} = i\sqrt{\frac{2}{p(p+1)}} \left(\sum_{d=1}^{p} \delta_{da}\delta_{db} - p\,\delta_{p+1,a}\delta_{p+1,b} \right), \quad 1 \leqslant p \leqslant N-1.$$

Using the definition of $\partial_D Z$ (3.1)–(3.4) in terms of the projector P and its derivatives, we find that $\partial_D^{\Phi} Z \equiv \Phi^{\dagger} \partial_D Z(\xi_L, \xi_R) \Phi$ has a simple block off-diagonal structure

$$\partial_D^{\Phi} Z = \Phi^{\dagger} \partial_D Z(\xi_L, \xi_R) \Phi = \begin{pmatrix} \mathbf{0}_{m\times m} & -(Z_D^{\Phi})^{\dagger} \\ Z_D^{\Phi} & \mathbf{0}_{n\times n} \end{pmatrix}, \tag{5.3}$$

where the nontrivial blocks Z_D^{Φ} are defined by the relation (5.3).

When the matrix function Φ satisfying (5.1) is found, the construction of the moving frame can proceed as follows. Assume that one finds, using a variant of Gramm–Schmidt orthogonalization procedure, for each ξ_L, ξ_R, the orthonormal vectors

$$\widetilde{A}_{aj}, \widetilde{B}_{aj}, \quad a = 1, \ldots, m, \quad j = m+1, \ldots, N, \quad a + j > m + 2$$

satisfying

$$(\partial_D^{\Phi} Z, \widetilde{A}_{aj}) = 0, \quad (\partial_D^{\Phi} Z, \widetilde{B}_{bj}) = 0$$

and

$$\mathrm{span}(\partial_D^{\Phi} Z, \widetilde{A}_{aj}, \widetilde{B}_{aj})_{D=L,R,a=1,\ldots,m,j=m+2,\ldots,N,a+j>m+2} = \mathrm{span}(A_{aj}, B_{aj})_{a=1,\ldots,m,j=m+1,\ldots,N}. \tag{5.4}$$

[The vectors $\widetilde{A}_{aj}, \widetilde{B}_{aj}$ as well as $\partial_D^{\Phi} Z$ are functions of ξ_L, ξ_R, the arguments are not written out in order to save space. The relations hold for each pair of values of ξ_L, ξ_R in the considered neighborhood of (ξ_L^0, ξ_R^0)]. We identify the remaining tilded and untilded matrices

$$\tilde{A}_{jk} = A_{jk}, \quad \tilde{B}_{jk} = B_{jk}, \quad \tilde{C}_p = C_p,$$

where $a,j=1,\ldots,m$ or $a,j=m+1,\ldots,N$, $1 \leqslant p \leqslant N-1$. As a result, from Gramm–Schmidt orthogonalization and (5.3) we get

$$(\partial_D^\Phi Z, \tilde{A}_{ak}) = (\partial_D^\Phi Z, \tilde{B}_{ak}) = (\partial_D^\Phi Z, \tilde{C}_p) = 0$$

and

$$(\tilde{A}_{ai}, \tilde{A}_{bk}) = (\tilde{B}_{ai}, \tilde{A}_{bk}) = \delta_{ab}\delta_{ik}, \quad (\tilde{C}_p, \tilde{C}_q) = \delta_{pq},$$

$$(\tilde{A}_{1i}, \tilde{B}_{jk}) = (\tilde{A}_{1i}, \tilde{C}_p) = (\tilde{B}_{1i}, \tilde{C}_p) = 0,$$

where indices run through all the values for which the respective tilded matrices are defined.

Therefore, under the above-given assumptions and notation, we can state the following

Proposition 1: Let the moving frame of the surface $\mathcal{F}$ in the neighborhood Υ of point $Z^0 = Z(\xi_L^0, \xi_R^0)$ be

$$\partial_L Z = \Phi \partial_L^\Phi Z \Phi^\dagger,$$

$$\partial_R Z = \Phi \partial_R^\Phi Z \Phi^\dagger,$$

$$n_{jk}^A = \Phi \tilde{A}_{jk} \Phi^\dagger, \tag{5.5}$$

$$n_{jk}^B = \Phi \tilde{B}_{jk} \Phi^\dagger,$$

$$n_p^C = \Phi \tilde{C}_p \Phi^\dagger,$$

where indices run through the values for which $\tilde{A}, \tilde{B}, \tilde{C}$ are defined and $\Phi(\xi_L, \xi_R)$ on Υ satisfies

$$X(\xi_L, \xi_R) = \Phi(\xi_L, \xi_R) \begin{pmatrix} \mathbf{1}_{m\times m} \\ \mathbf{0}_{n\times m} \end{pmatrix}.$$

Then (5.5) satisfies the normalization conditions (4.1) and consequently the Gauss–Weingarten equations (4.2).

Note that the first two lines of (5.5) are equivalent to (5.3). The remaining lines of (5.5) give a rather explicit description of the normals to the surface $\mathcal{F}$. Since the construction is local, we do not have an *a priori* control of the orientation of the normals. Of course, in the neighborhood where the procedure is applied the normals have the same orientation.

The explicit form of the moving frame (5.5) might be quite complicated because of the orthogonalization process involved in the construction of

$$n_{aj}^A, n_{aj}^B, \quad a = 1,\ldots,m, \quad j = m+1,\ldots,N, \quad a + j > m + 2$$

(i.e., in the construction of $\tilde{A}_{1j}, \tilde{B}_{1j}$). On the other hand, the remaining normals

$$n_{ak}^A, n_{ak}^B, n_p^C$$

where $a,j=1,\ldots,m$ or $a,j=m+1,\ldots,N$, $1 \leqslant p \leqslant N-1$ can be constructed immediately after finding Φ. In fact, one particular combination of normals n_p^C of the form

$$n_P = i\sqrt{2}\left(\sqrt{\frac{N-m}{mN}}\mathbf{1} - \sqrt{\frac{N-m}{m(N-m)}}P\right)$$

can be constructed from X, i.e., P, alone, without the knowledge of corresponding Φ.

If we choose another matrix Φ satisfying (5.1), the constructed normals would have been rotated by a local (gauge) transformation from the subgroup of $SU(N)$ leaving $\partial_L Z, \partial_R Z$ invariant.

It is worth noting that from Eqs. (4.6) and (4.8) it immediately follows that

$$\begin{aligned}(\partial_L\partial_L Z)^\perp, (\partial_R\partial_R Z)^\perp &\in \operatorname{span}(n^A_{1j}, n^B_{1j})_{a=1,\ldots,m, j=m+1,\ldots,N},\\ (\partial_L\partial_R Z)^\perp = \partial_L\partial_R Z &\in \operatorname{span}(n^A_{jk}, n^B_{jk}, n^C_p)_{a,j=1,\ldots,m, \text{ or } a,j=m+1,\ldots,N, p<N},\end{aligned} \tag{5.6}$$

i.e., $\partial_L\partial_R Z$ is orthogonal to $\partial_L\partial_L Z, \partial_R\partial_R Z$ [and also to the surface, see (4.2)].

VI. FINAL REMARKS

The above presented technique for finding surfaces associated with complex Grassmannian sigma models defined on Minkowski space can be seen to give a rather detailed analytical description of the surfaces in question. This description provides effective tools for constructing surfaces without reference to additional considerations, proceeding directly from the given complex Grassmannian sigma model equations (2.14). Through the use of Cartan's language of moving frames we derived via this sigma model, the structural equations of two-dimensional smooth surfaces immersed in $\mathfrak{su}(N)$ algebra. It allows one to find the first and second fundamental forms of the surfaces as well as the relations between them as expressed in the Gauss–Weingarten and Gauss–Codazzi–Ricci equations. An extension of the classical Enneper–Weierstrass representation of surfaces in multidimensional spaces, expressed in terms of any nonsingular solution of (2.14), was presented in an explicit form.

Explicit examples of surfaces constructed by the presented method were given in Ref. 8 in the $\mathbb{C}P^1$ case. In the more complicated $\mathbb{C}P^N$ and truly Grassmannian cases the construction of examples relies on the knowledge of explicit solutions in closed form of the corresponding sigma models on Minkowski space (numerical solutions are not good enough, since the numerical computation of derivatives in the construction of the tangent vectors $\mathcal{Z}$ would lead to unreliable results). Finding such solutions is by itself a nontrivial task which we plan to investigate in the future. (For example, the solutions obtained by the method presented in Ref. 21 are becoming computationally too complicated to allow even numerical computation of the surface in feasible time.)

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Neumann series and lattice sums

R. C. McPhedran
School of Physics, University of Sydney, NSW 2006, Australia

N. A. Nicorovici and L. C. Botten
Department of Mathematical Sciences, University of Technology, Sydney, NSW 2007, Australia

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We consider sums over the square lattice which depend only on radial distance, and provide formulas which enable sums of functions with Neumann series to be reexpressed as combinations of hypergeometric series. We illustrate the procedure using trigonometric sums previously studied by Borwein and Borwein, sums combining logarithms, Bessel functions J_λ, and powers of distance, and sums of Neumann functions. We also exhibit sums which may be evaluated analytically and recurrence formulas linking sums. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Many problems involving wave propagation through periodic structures can be dealt with through the construction of Green's functions built up from lattice sums which incorporate the periodicity required of the solution. The long history of lattice sums was reviewed by Glasser and Zucker[1] in 1980, but there have been a number of recent papers dealing with new methods to evaluate efficiently and accurately these slowly converging or conditionally converging series.[2–8] Many of these papers deal with techniques well adapted to particular sums, but difficult to adapt to variants on the form of the summand. Here we will deal with more general methods and will concentrate on sums over the square lattice which depend only on the radial distance to the lattice point. While similar methods may be applied to sums depending on the angle of the lattice point as well as its distance,[9] there are considerable advantages of simplicity to be gained by considering sums over distance alone.

We commence by studying a Schlömilch series of general form over the square lattice and treat this using the Poisson summation formula, expressing it as a series of hypergeometric type in which the sums over the square lattice have been evaluated analytically. We illustrate particular cases where the Schlömilch series can be summed analytically, as well as integral and differential recurrence relations for them.

We next apply these results to Neumann series involving Bessel functions of even order, for which simple results can be obtained. We illustrate this by considering a cosine double sum previously evaluated by Borwein and Borwein.[10] For sums over Bessel functions of odd order, the results are more complicated, but once again we show the results agree with those previously established for a sine double sum.

We show next that, by taking an appropriate partial derivative of the Schlömilch series, we can generate a general formula for a sum involving the logarithm of distance, as well as Bessel functions and powers of it. We then consider double sums over Neumann functions, Y_n, where another partial derivative of the Schlömilch series is required. We obtain highly accurate and efficient expressions for the sums of Y_0 and Y_2 over the square lattice, and show for the former how the range of convergence of these expressions may be increased if required.

II. ANALYTIC EXPRESSIONS FOR NONANGULAR ARRAY SUMS

Many interesting results have been derived for lattice sums using Schlömilch series.[1,11,12] We wish to consider here a general sum $\mathcal{S}$ which depends on distance from the origin to a general point $K_h=2\pi\sqrt{h_1^2+h_2^2}$ in the reciprocal lattice of a square lattice with unit period:

$$\mathcal{S}_{\lambda,0,\nu}(\xi)=\sum_{h\neq 0}\frac{J_\lambda(K_h\xi)}{K_h^\nu}, \tag{1}$$

where the indices λ and μ are integral, real, or complex, and h is a pair of subscripts (h_1,h_2). The parameter ξ is taken to be real and positive. We generalize the argument in Ref. 3 to allow for these (possibly) complex indices. We use the Poisson summation formula

$$\sum_h f(\mathbf{K}_h)=\frac{1}{(2\pi)^2}\sum_p F(\mathbf{R}_p), \tag{2}$$

where

$$F(\mathbf{R}_p)=\int\int_{\mathbb{R}^2} f(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{R}_p}\,d\mathbf{k}, \quad f(\mathbf{K}_h)=\frac{1}{(2\pi)^2}\int\int_{\mathbb{R}^2} F(\mathbf{r})e^{i\mathbf{K}_h\cdot\mathbf{r}}\,d\mathbf{r}, \tag{3}$$

R_p are direct lattice vectors, and $p=(p_1,p_2)$. We assume $\mathrm{Re}(\lambda)>\mathrm{Re}(\nu)$, so the term $h=(0,0)$ can be included in $\mathcal{S}$ without changing its value. From (3), with

$$f(\mathbf{k})=\frac{J_\lambda(k\xi)}{k^\nu}, \tag{4}$$

we arrive at an integral of the Weber-Schafheitlin form:[13,14]

$$F(\mathbf{R}_p)=2\pi\int_0^\infty \frac{J_\lambda(k\xi)J_0(kR_p)}{k^{\nu-1}}\,dk. \tag{5}$$

If $\xi<R_p$ and $\mathrm{Re}(\nu)>0$, or $\xi\leqslant R_p$ and $\mathrm{Re}(\nu)>1$, the integral converges for $\mathrm{Re}(\lambda-\nu+2)>0$ and may be expressed as a hypergeometric function:

$$F(\mathbf{R}_p)=\frac{\xi^\lambda\pi\Gamma((\lambda-\nu+2)2)}{2^{\nu-2}R_p^{\lambda-\nu+2}\Gamma(\lambda+1)\Gamma((\nu-\lambda)/2)}\,{}_2F_1\left(\frac{\lambda-\nu+2}{2},\frac{\lambda-\nu+2}{2};\lambda+1;\left(\frac{\xi}{R_p}\right)^2\right). \tag{6}$$

For $p=0$, we have $R_0=0$, and the integral in (5) is

$$F(\mathbf{0})=2\pi\int_0^\infty \frac{J_\lambda(k\xi)}{k^{\nu-1}}\,dk=2\pi\xi^{\nu-2}\frac{2^{-\nu+1}\Gamma((\lambda-\nu+2)/2)}{\Gamma((\lambda+\nu)/2)}, \tag{7}$$

provided that $\mathrm{Re}(\lambda-\nu)>-2$, $\mathrm{Re}(\nu)>\frac{1}{2}$.[13,14] Consequently,

$$\mathcal{S}_{\lambda,0,\nu}(\xi)=\xi^{\nu-2}\frac{\Gamma((\lambda-\nu+2)/2)}{2^\nu\pi\Gamma((\lambda+\nu)/2)}+\sum_{p\neq 0}\frac{\xi^\lambda\Gamma((\lambda-\nu+2)/2)}{2^\nu\pi R_p^{\lambda-\nu+2}\Gamma(\lambda+1)\Gamma((\nu-\lambda)/2)}$$
$$\times\,{}_2F_1\left(\frac{\lambda-\nu+2}{2},\frac{\lambda-\nu+2}{2};\lambda+1;\left(\frac{\xi}{R_p}\right)^2\right). \tag{8}$$

We complete this derivation using the series expansion for the hypergeometric function:

$$ {}_2F_1(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{k=0}^{\infty} \frac{\Gamma(a+k)\Gamma(b+k)}{\Gamma(c+k)} \frac{z^k}{k!}, \tag{9} $$

which converges absolutely in $|z|<1$, and absolutely on $|z|=1$ provided that $\mathrm{Re}(c-a-b)>0$.[14] In our case, this translates to $\mathrm{Re}(\nu)>1$, and (9) gives

$$ \mathcal{S}_{\lambda,0,\nu}(\xi) = \xi^{\nu-2} \frac{\Gamma((\lambda-\nu+2)/2)}{2^\nu \pi \Gamma((\lambda+\nu)/2)} + \frac{\xi^\lambda \sin(\pi(\nu-\lambda)/2)}{2^\nu \pi^2} \sum_{k=0}^{\infty} \frac{[\Gamma((\lambda-\nu)/2+1+k)]^2}{\Gamma(\lambda+k+1)k!} \xi^{2k} \sigma^0_{2k+2+\lambda-\nu}. \tag{10} $$

Here[1]

$$ \sigma^0_{2s} = \sum_{p_1,p_2}{}' \frac{1}{(p_1^2+p_2^2)^s} = 4\zeta(s)\beta(s), \tag{11} $$

where the sum over $(p_1,p_2)\in\mathbb{Z}^2$ excludes $p_1=p_2=0$, as denoted by the prime, with $\beta(s)$ denoting the Catalan β function

$$ \beta(s) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^s}. \tag{12} $$

A useful summary of the properties of $\beta(s)$ has been given by Glasser.[15] The quantities σ^0_{2s} satisfy the reflection formula

$$ \sigma^0_{2s} = \sigma^0_{2-2s} \left[\frac{\pi^{2s-1}\Gamma(1-s)}{\Gamma(s)} \right], \tag{13} $$

which follows from the reflection formulae for the β function[15]

$$ 2^s \Gamma(s) \sin(s\pi/2)\beta(s) = \pi^s \beta(1-s), $$

and for the ζ function[14]

$$ \zeta(s) = 2^s \pi^{s-1} \sin(s\pi/2)\Gamma(1-s)\zeta(1-s). $$

The expression (10) was derived under the conditions $\mathrm{Re}(\lambda)>\mathrm{Re}(\nu)$, $\mathrm{Re}(\nu)>\frac{1}{2}$ and $|\xi|<1$. However, wherever the right-hand side is convergent, it provides, by analytic continuation, the definition of the left-hand side. The sum in (10) is cancelled out by its prefactor when $\lambda-\nu=2p$, for p a positive integer, in which case

$$ \mathcal{S}_{\nu+2p,0,\nu}(\xi) = \xi^{\nu-2} \frac{\Gamma(p+1)}{2^\nu \pi \Gamma(\nu+p)}. \tag{14} $$

This expression may be verified by direct numerical summation when $\mathrm{Re}(\nu)>2$. Regarded as a function of ν, $\mathcal{S}_{\nu+2p,0,\nu}(\xi)$ is analytic, with simple zeros at $\nu=-p-n$, for $n=0,1,2,\ldots$, for fixed $\xi\neq 0$.

We can derive the result for $\lambda=\nu$ from (10) letting $\lambda\to\nu$, and noting that the pole of σ^0_s at $s=1$ cancels the zero of $\sin\pi(\nu-\lambda)/2$. Alternatively, we can use (13) in (10), to give

$$ \mathcal{S}_{\lambda,0,\nu}(\xi) = \xi^{\nu-2} \frac{\Gamma((\lambda-\nu+2)/2)}{2^\nu \pi \Gamma((\lambda+\nu)/2)} + \frac{\xi^\lambda \pi^{\lambda-\nu}}{2^{\nu-2}} \sum_{k=0}^{\infty} \frac{\pi^{2k}(-1)^k \xi^{2k}}{\Gamma(\lambda+k+1)k!} \beta(-k+(\nu-\lambda)/2)\zeta(-k+(\nu-\lambda)/2), \tag{15} $$

where we note that the product $\zeta(s)\beta(s)$ is zero whenever s is a negative integer. The result is

$$\mathcal{S}_{\nu,0,\nu}(\xi) = \frac{\xi^{\nu-2}}{2^\nu \pi \Gamma(\nu)} - \frac{\xi^\nu}{2^\nu \Gamma(\nu+1)} = \frac{\xi^{\nu-2}}{2^\nu \Gamma(\nu+1)}\left(\frac{\nu}{\pi} - \xi^2\right), \tag{16}$$

which is a generalization of the result

$$\mathcal{S}_{n,0,n}(\xi) = \frac{1}{(2n)!!}\left(\frac{n}{\pi}\xi^{n-2} - \xi^n\right), \quad n \in \mathbb{N},$$

derived in Ref. 5 in a different fashion. It is interesting to take $\nu=0$ in (16), with the result $\mathcal{S}_{0,0,0}(\xi)=-1$. The result from Ref. 5 is

$$\mathcal{S}_{0,0,0}(\xi) = \frac{\delta(\xi)}{2\pi\xi} - 1, \tag{17}$$

which agrees with (16) apart from the distributive term, which one would not expect to exist in an analytic continuation. Indeed, in the definition of sums (1) we have assumed that ξ is real and positive so that the two results are equivalent. For fixed $\xi \neq 0$, the expression (16) is an analytic function of ν, with zeros at $\nu=-1,-2,\ldots$, and also at $\nu=\pi\xi^2$. Once again, the expression (16) may be exemplified numerically by choosing $\mathrm{Re}(\nu)>2$.

Another special case of (10) is the formula (43) from Ref. 3, valid for $\lambda-\nu=2p+1$, where λ and ν are non-negative integers, and p is a positive integer. We repeat it here, with an error in a sign factor corrected:

$$\mathcal{S}_{\lambda,0,\nu}(\xi) = \xi^{\nu-2}\frac{\Gamma((\lambda-\nu+2)/2)}{2^\nu \pi \Gamma((\lambda+\nu)/2)} + \frac{(-1)^{(\lambda-\nu+1)/2}\xi^\lambda}{2^\nu \pi^2}\sum_{k=0}^{\infty}\frac{[\Gamma((\lambda-\nu)/2+1+k)]^2}{k!(k+\lambda)!}\xi^{2k}\sigma^0_{2k+2+\lambda-\nu}.$$

The lattice sums $\mathcal{S}$ obey four recurrence relations based on certain integral and differential relations, satisfied by the Bessel functions[3] (see also the Appendix). The forms

$$\mathcal{S}_{\lambda+1,0,\nu+1}(\xi) = \frac{1}{\xi^{\lambda+1}}\int_0^\xi \eta^{\lambda+1}\mathcal{S}_{\lambda,0,\nu}(\eta)\,d\eta, \quad \text{for } \mathrm{Re}(\lambda) > -1, \tag{18}$$

and

$$\mathcal{S}_{\lambda-1,0,\nu+1}(\xi) = \frac{\xi^{\lambda-1}}{2^{\lambda-1}(2\pi)^{\nu-\lambda+2}\Gamma(\lambda)}\sigma^0_{\nu-\lambda+2} - \frac{1}{\xi^{-\lambda+1}}\int_0^\xi \eta^{-\lambda+1}\mathcal{S}_{\lambda,0,\nu}(\eta)\,d\eta \tag{19}$$

act by integration to increment the third subscript. The two differential relations are

$$\mathcal{S}_{\lambda-1,0,\nu-1}(\xi) = \xi^{-\lambda}[\xi^\lambda \mathcal{S}_{\lambda,0,\nu}(\xi)]', \tag{20}$$

and

$$\mathcal{S}_{\lambda+1,0,\nu-1}(\xi) = -\xi^\lambda[\xi^{-\lambda}\mathcal{S}_{\lambda,0,\nu}(\xi)]', \tag{21}$$

which both decrement the third subscript. Appropriate pairwise combinations of these act on either the first or the third subscript alone:

$$\mathcal{S}_{\lambda+2,0,\nu}(\xi) = \frac{2(\lambda+1)}{\xi^{\lambda+2}}\int_0^\xi \eta^{\lambda+1}\mathcal{S}_{\lambda,0,\nu}(\eta)\,d\eta - \mathcal{S}_{\lambda,0,\nu}(\xi), \tag{22}$$

$$\mathcal{S}_{\lambda,0,\nu}(\xi) = \frac{\xi^{\lambda}}{2^{\lambda}(2\pi)^{\nu-\lambda}\Gamma(\lambda+1)}\sigma^{0}_{\nu-\lambda} - \frac{2(\lambda+1)}{\xi^{-\lambda}}\int_{0}^{\xi}\eta^{-\lambda-1}\mathcal{S}_{\lambda+2,0,\nu}(\eta)d\eta - \mathcal{S}_{\lambda+2,0,\nu}(\xi) \tag{23}$$

are inverse operations on the first subscript. The lowering and raising relations for the third subscript are

$$\mathcal{S}_{\lambda,0,\nu-2}(\xi) = \frac{\lambda^2}{\xi^2}\mathcal{S}_{\lambda,0,\nu}(\xi) - \frac{1}{\xi}\mathcal{S}'_{\lambda,0,\nu}(\xi) - \mathcal{S}''_{\lambda-0,\nu}(\xi) \tag{24}$$

and

$$\mathcal{S}_{\lambda,0,\nu+2}(\xi) = \frac{\xi^{\lambda}}{2^{\lambda}(2\pi)^{\nu-\lambda+2}\Gamma(\lambda+1)}\sigma^{0}_{\nu-\lambda+2} - \frac{1}{\xi^{-\lambda}}\int_{0}^{\xi}\left[\frac{1}{\eta^{2\lambda+1}}\int_{0}^{\eta}\tau^{\lambda+1}\mathcal{S}_{\lambda,0,\nu}(\tau)d\tau\right]d\eta. \tag{25}$$

We can verify that the expression (10) satisfies each of the recurrence relations (18)–(21). The algebra is elementary, with the exception of (19), where (13) needs to be used to transform $\sigma^{0}_{\nu-\lambda+2}$ into $\sigma^{0}_{\lambda-\nu}$, before this term is combined with the hypergeometric series. We can thus use either the recurrence relations or the hypergeometric expression (10) in order to extend the calculation of the $\mathcal{S}_{\lambda,0,\nu}(\xi)$ from the region of derivation $\mathrm{Re}(\lambda-\nu)>-2$, $\mathrm{Re}(\nu)>1$ over the whole range of the two complex variables λ and ν. Note the structure of (10); the first term will have simple poles at $\lambda-\nu=-2m$, where m is a positive integer, whereas in the hypergeometric sum the poles of $[\Gamma((\lambda-\nu)/2+1+k)]^2$ are exactly compensated for by the zeros of $\sin(\pi(\nu-\lambda)/2)$ and $\sigma^{0}_{2k+2+\lambda-\nu}$ at the same locations. This is also evident from (15). The hypergeometric sum gives a simple pole at $\nu-\lambda=2k+2$, due to the pole of σ^{0}.

III. NEUMANN SERIES WITH BESSEL FUNCTIONS OF EVEN ORDER

Neumann series express general functions as a combination of Bessel functions J_l of constant argument and varying integer order l.[13,14] The expansion coefficients are given by contour integral of the product of the function and the Neumann polynomials, or can be deduced from the Maclaurin series coefficients of the function.

We start with sums over the square array of Bessel functions of even order:[5]

$$\sum_{h} J_0(K_h\xi) = \sum_{h_1,h_2=-\infty}^{\infty} J_0(2\pi\xi\sqrt{h_1^2+h_2^2}) = \frac{\delta(\xi)}{2\pi\xi} \tag{26}$$

and

$$\sum_{h} J_{2l}(K_h\xi) = \sum_{h_1,h_2=-\infty}^{\infty} J_{2l}(2\pi\xi\sqrt{h_1^2+h_2^2}) = \frac{1}{\pi\xi^2}, \tag{27}$$

for $l\neq 0$. These results can be used to evaluate sums over the square array of functions of distance whose Neumann expansions only involve Bessel functions of even order. As an example, we consider one of the sums evaluated using Abel summation by Borwein and Borwein:[10]

$$\sum_{h_1,h_2}{}' \frac{\sin(\theta\sqrt{h_1^2+h_2^2})}{\sqrt{h_1^2+h_2^2}} = \frac{2\pi}{\theta} - \theta, \quad 0<|\theta|<2\pi. \tag{28}$$

Firstly, we use a Neumann series from Prudnikov *et al.*:[16]

$$\frac{\sin z}{z} = J_0(z) - 2\sum_{l=1}^{\infty}\frac{(-1)^l J_{2l}(z)}{(4l^2-1)}. \tag{29}$$

Then, substituting (26) and (27) into (29) we have

$$\sum_{h_1,h_2}{}' \frac{\sin(2\pi\xi\sqrt{h_1^2+h_2^2})}{\sqrt{h_1^2+h_2^2}} = \delta(\xi) - 2\pi\xi - \frac{4}{\xi}\sum_{l=1}^{\infty}\frac{(-1)^l}{4l^2-1}, \tag{30}$$

where the sum over h_1 and h_2 excludes $h_1=h_2=0$, as denoted by the prime. The sum on the right-hand side of (30) has the value $\left(-\frac{1}{4}\right)$, so that we obtain

$$\sum_{h_1,h_2}{}' \frac{\sin(2\pi\xi\sqrt{h_1^2+h_2^2})}{\sqrt{h_1^2+h_2^2}} = \delta(\xi) - 2\pi\xi + \frac{1}{\xi}. \tag{31}$$

This can be compared with the result of Borwein and Borwein (28). Evidently the two results agree, except that (31), having been obtained using the theory of distributions, includes a delta function term missing from (28).

We next consider the Neumann series:

$$\cos z = J_0(z) + 2\sum_{l=1}^{\infty}(-1)^l J_{2l}(z). \tag{32}$$

Hence,

$$\sum_{h_1,h_2}{}' \cos(2\pi\xi\sqrt{h_1^2+h_2^2}) = \frac{\delta(\xi)}{2\pi\xi} - 1 + \frac{2}{\pi\xi^2}\sum_{l=1}^{\infty}(-1)^l l. \tag{33}$$

The sum is evaluated using the binomial series for $-1/(1+z)^2$ at $z=1$, with the result

$$\mathcal{C}(\xi) = \sum_{h_1,h_2}{}' \cos(2\pi\xi\sqrt{h_1^2+h_2^2}) = \frac{\delta(\xi)}{2\pi\xi} - 1 - \frac{1}{2\pi\xi^2}. \tag{34}$$

Note that, if we differentiate (31) with respect to ξ, we obtain the nondistributive terms in (34).

IV. NEUMANN SERIES WITH BESSEL FUNCTIONS OF ODD ORDER

Results for odd orders corresponding to (26) and (27) were not given in Ref. 5. They may be derived from (10). Hence, we have

$$\sum_h J_{2l+1}(K_h\xi) = \sum_{h_1,h_2=-\infty}^{\infty} J_{2l+1}(2\pi\xi\sqrt{h_1^2+h_2^2}) = \frac{1}{\pi\xi^2}\left(l+\frac{1}{2}\right) - \frac{4}{\pi^2}(-1)^l\sum_{k=0}^{\infty}\frac{[\Gamma(k+l+3/2)]^2}{k!(k+2l+1)!}\zeta(k+l+3/2)\beta(k+l+3/2)\xi^{2k+2l+1}. \tag{35}$$

We apply (35) to the evaluation of

$$\mathcal{S}(\xi) = \sum_{h_1,h_2}{}' \sin(2\pi\xi\sqrt{h_1^2+h_2^2}) = 2\sum_{h_1,h_2}{}'\sum_{l=0}^{\infty}(-1)^l J_{2l+1}\left(2\pi\xi\sqrt{h_1^2+h_2^2}\right). \tag{36}$$

We note that there is no contribution from the $1/\xi^2$ term which arises from using (35) in (36). The evaluation of this contribution is somewhat delicate, since conditionally convergent sums arise. It may be approached using binomial series of the functions $1/(1+z)$ and $-1/(1+z)^2$, and analytic continuation for $z=1$. More rapidly, we may note[15] that

$$\sum_{l=0}^{\infty}(-1)^l\left(l+\frac{1}{2}\right) = \frac{1}{2}\sum_{l=0}^{\infty}\frac{(-1)^l}{(2l+1)^{-1}} = \frac{1}{2}\beta(-1) = 0. \tag{37}$$

Hence,

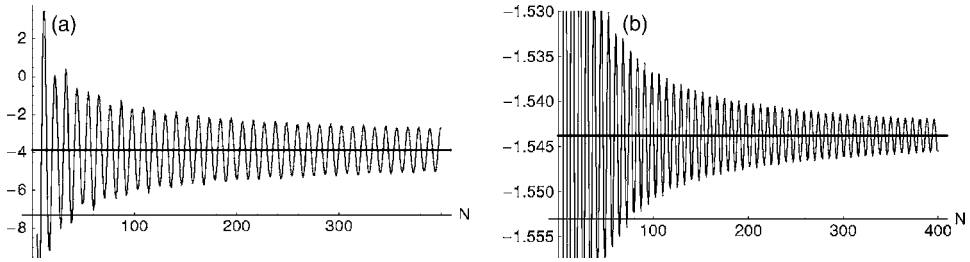

FIG. 1. Partial sums for the left-hand sides of (42) (left) and (43) (right) obtained by summation over a square region, centered on the origin and having side length of $2N+1$, for N up to 400. These are compared with the right-hand sides (solid line) of these equations for $\theta=0.583$.

$$\mathcal{S}(\xi) = -\frac{8}{\pi^2}\sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\frac{[\Gamma(k+l+3/2)]^2}{k!(k+2l+1)!}\zeta(k+l+3/2)\beta(k+l+3/2)\xi^{2k+2l+1}. \tag{38}$$

We can transform the double sum to a single sum, by replacing $k+l$ by n, and using the result

$$\sum_{k,l\geqslant 0,k+l=n}\frac{(2n+1)!}{k!(k+2l+1)!} = \frac{1}{2}\sum_{k=0}^{2n+1}\binom{2n+1}{k} = 2^{2n}. \tag{39}$$

We find

$$\mathcal{S}(\xi) = -\frac{8}{\pi^2}\sum_{n=0}^{\infty}\frac{[\Gamma(n+3/2)]^2}{(2n+1)!}2^{2n}\zeta(n+3/2)\beta(n+3/2)\xi^{2n+1}. \tag{40}$$

After some manipulation of the Γ function term, this becomes

$$\mathcal{S}(\xi) = {\sum_{h_1,h_2}}'\sin(2\pi\xi\sqrt{h_1^2+h_2^2}) = -\frac{4}{\pi}\sum_{n=0}^{\infty}\frac{(2n+1)!}{(n!)^2}\zeta(n+3/2)\beta(n+3/2)\left(\frac{\xi}{2}\right)^{2n+1}. \tag{41}$$

This will be recognized as being identical to the derivative of the result from Borwein and Borwein,[10]

$${\sum_{h_1,h_2}}'\frac{\cos(\theta\sqrt{h_1^2+h_2^2})}{\sqrt{h_1^2+h_2^2}} = 4\sum_{n=0}^{\infty}\frac{(2n)!}{(n!)^2}\zeta(n+1/2)\beta(n+1/2)\left(\frac{\theta}{4\pi}\right)^{2n}, \quad 0<|\theta|<2\pi. \tag{42}$$

Borwein and Borwein[10] also consider the series on the left of (42) with an alternating sign included:

$${\sum_{h_1,h_2}}'(-1)^{h_1+h_2}\frac{\cos(\theta\sqrt{h_1^2+h_2^2})}{\sqrt{h_1^2+h_2^2}} = 4\sum_{n=0}^{\infty}\frac{(2n)!}{(n!)^2}\zeta(n+1/2)\beta(n+1/2)(2^{n+1/2}-1)\left(\frac{\theta}{4\pi}\right)^{2n},$$
$$0<|\theta|<\sqrt{2}\pi. \tag{43}$$

Numerical examples of the convergence of (42) (left) and (43) (right) by direct summation are presented in Fig. 1, together with the results of the rapidly convergent series on their right-hand sides.

V. SERIES COMBINING BESSEL FUNCTIONS AND LOGARITHMS

From the definition (1) we can construct a general formula for sums combining a logarithm with a Bessel function and a power of the distance:

$$\mathcal{L}_{\lambda,0,\nu}(\xi) = -\frac{\partial}{\partial\nu}\mathcal{S}_{\lambda,0,\nu}(\xi) = \sum_{h\neq 0} \log(K_h)\frac{J_\lambda(K_h\xi)}{K_h^\nu}. \tag{44}$$

Using the sum (11) and the expansion (15), we find

$$\mathcal{L}_{\lambda,0,\nu}(\xi) = \left[-\log\left(\frac{\xi}{2}\right) + \frac{1}{2}\psi\left(\frac{\lambda-\nu+2}{2}\right) + \frac{1}{2}\psi\left(\frac{\lambda+\nu}{2}\right)\right]\xi^{\nu-2}\frac{\Gamma((\lambda-\nu+2)/2)}{2^\nu\pi\Gamma((\lambda+\nu)/2)}$$
$$+ \frac{\xi^\lambda\pi^{\lambda-\nu}\log(2\pi)}{2^\nu}\sum_{k=0}^{\infty}\frac{\pi^{2k}(-1)^k\xi^{2k}}{\Gamma(\lambda+k+1)k!}\sigma^0_{\nu-\lambda-2k} - \frac{\xi^\lambda\pi^{\lambda-\nu}}{2^\nu}\sum_{k=0}^{\infty}\frac{\pi^{2k}(-1)^k\xi^{2k}}{\Gamma(\lambda+k+1)k!}\sigma^{0\prime}_{\nu-\lambda-2k}. \tag{45}$$

We now evaluate $\mathcal{L}_{0,0,0}(\xi)$:

$$\mathcal{L}_{0,0,0}(\xi) = \left[-\log\left(\frac{\xi}{2}\right) + \frac{1}{2}\psi(1) + \frac{1}{2}\psi(0)\right]\xi^{-2}\frac{1}{\pi\Gamma(0)} + \log(2\pi)\sum_{k=0}^{\infty}\frac{(-1)^k(\pi\xi)^{2k}}{(k!)^2}\sigma^0_{-2k}$$
$$- \sum_{k=0}^{\infty}\frac{(-1)^k(\pi\xi)^{2k}}{(k!)^2}\sigma^{0\prime}_{-2k}. \tag{46}$$

The factor $1/\Gamma(0)$ makes zero the first term on the right-hand side of (46), apart from the term involving $\psi(0)$. Taking the appropriate limit from (45), we find that we should make the identification $\psi(0)/\Gamma(0)=-1$. The first infinite series reduces just to the term $k=0$, since $\sigma^0_{-2k}=0$ for $k \geqslant 1$, while $\sigma^0_0=-1$. The second series involves the derivative

$$\sigma^{0\prime}_{-2k} = \left.\frac{\partial\sigma^0_{\nu-\lambda-2k}}{\partial\nu}\right|_{\nu=\lambda=0}$$

for negative even order subscripts. Separating out $k=0$ first of all, we use the expansion

$$\sigma^0_{2+\delta\lambda} = \frac{2\pi}{\delta\lambda} + D, \tag{47}$$

where $D=\pi(2\gamma+\log(\pi/2)-C)$, and $C=\log[\Gamma(1/4)^4/(8\pi^2)]\approx 0.783\,188\,785\,414$.[17] We may also write $D=\pi\mathsf{S}\approx 2.584\,981\,759\,5$, where S is the Sierpinski constant.[18] We then obtain

$$\sigma^{0\prime}_0 = \frac{D}{2\pi} - \gamma - \log(\pi). \tag{48}$$

For general $\sigma^{0\prime}_{-2k}$, we take the derivative of the reflection equation (13), and obtain for positive integral k

$$\sigma^{0\prime}_{-2k} = \frac{(-1)^k(k!)^2}{2\pi^{2k+1}}\sigma^0_{2+2k}. \tag{49}$$

Using (48) and (49) in (46), we find

$$\mathcal{L}_{0,0,0}(\xi) = -\frac{1}{2\pi\xi^2} - \frac{D}{2\pi} + \gamma - \log(2) - \frac{1}{2\pi}\sum_{k=1}^{\infty}\xi^{2k}\sigma^0_{2+2k}. \tag{50}$$

A numerical example of this is given in Fig. 2. Note how the envelopes of the results of direct summation separate slowly, due to the extra logarithmic factor in the definition of $\mathcal{L}$. However, the mean of the numerical results (−1.800 32) is in reasonable accord with the analytic result (−1.837 134).

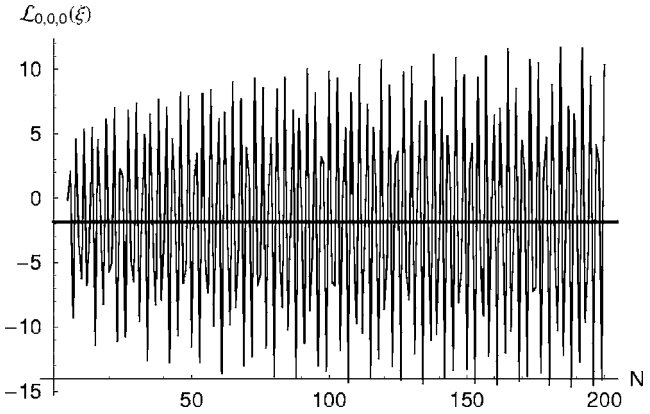

FIG. 2. Partial sums for $\mathcal{L}_{0,0,0}(\xi)$, with $\xi=0.37$, obtained by summation over a square region, centered on the origin and having side length of $2N+1$, for N up to 200. The analytical result (50) is indicated by the horizontal line.

Consider next the form of $\mathcal{L}_{2,0,0}(\xi)$. This is more straightforward than $\mathcal{L}_{0,0,0}(\xi)$, in that the first series in (45) vanishes, and only (49) is needed in the second series. We obtain

$$\mathcal{L}_{2,0,0}(\xi) = -\frac{1}{\pi\xi^2}\log\left(\frac{\xi}{2}\right) + \frac{1-2\gamma}{2\pi\xi^2} + \frac{\xi^2}{2\pi}\sum_{k=0}^{\infty}\frac{k+1}{k+2}\xi^{2k}\sigma^0_{4+2k}. \tag{51}$$

A numerical example of this is given in Fig. 3. The mean of the numerical results is 3.781 26, while the result of (51) is 3.820 33.

VI. SERIES OF NEUMANN FUNCTIONS

These series are of particular interest in the construction of Green's functions for the Helmholtz equation.[2,3,5–8] We start with a particular case of (10):

$$\mathcal{S}_{\lambda,0,0}(\xi) = \frac{\lambda}{2\pi\xi^2} - \frac{\sin(\pi\lambda/2)[\Gamma(1+\lambda/2)]^2}{\pi^2\Gamma(1+\lambda)}\xi^{\lambda}\sigma^0_{2+\lambda} - \frac{\sin(\pi\lambda/2)}{\pi^2}\sum_{k=1}^{\infty}\frac{[\Gamma(\lambda/2+1+k)]^2}{\Gamma(\lambda+k+1)k!}\xi^{2k+\lambda}\sigma^0_{2k+2+\lambda}. \tag{52}$$

We will replace λ by $\delta\lambda$, and expand this to first order in $\delta\lambda$. We use (47) to give

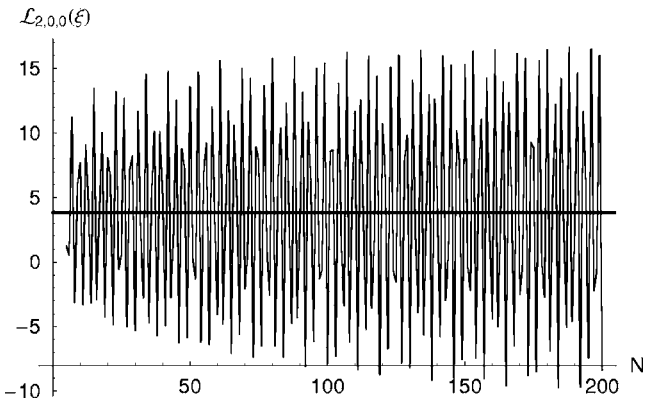

FIG. 3. Partial sums for $\mathcal{L}_{2,0,0}(\xi)$, with $\xi=0.37$, obtained by summation over a square region, centered on the origin and having side length of $2N+1$, for N up to 200. The analytical result (51) is indicated by the horizontal line.

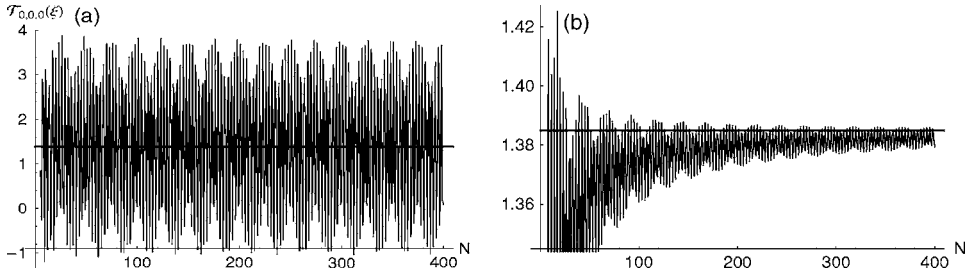

FIG. 4. On the left: partial sums for $\mathcal{T}_{0,0,0}(\xi)$ obtained by summation over a square region, centered on the origin and having side length of $2N+1$, for N up to 400. On the right: the growing mean of the data in the graph on the left. We used $\xi=0.32$, with the analytic result (56) being given by the horizontal line.

$$\mathcal{S}_{\delta\lambda,0,0}(\xi) = \frac{\delta\lambda}{2\pi\xi^2} - 1 - \delta\lambda\left[\log\xi + \frac{D}{2\pi} + \frac{2}{\pi}\sum_{k=1}^{\infty}\xi^{2k}\zeta(k+1)\beta(k+1)\right]. \tag{53}$$

Now, the Neumann functions of zeroth order are defined[13,14] as

$$Y_0(z) = \lim_{\lambda\to 0}\frac{J_\lambda(z)\cos(\lambda\pi) - J_{-\lambda}(z)}{\sin(\lambda\pi)} = \lim_{\lambda\to 0}\frac{J_\lambda(z) - J_{-\lambda}(z)}{\lambda\pi}$$

and, if we denote by

$$\mathcal{T}_{0,0,0}(\xi) = \sum_{h\neq 0} Y_0(K_h\xi), \tag{54}$$

then

$$\mathcal{T}_{0,0,0}(\xi) = \lim_{\delta\lambda\to 0}\frac{\mathcal{S}_{\delta\lambda,0,0}(\xi) - \mathcal{S}_{-\delta\lambda,0,0}(\xi)}{\pi\delta\lambda}. \tag{55}$$

Using (53) in (55), we obtain

$$\mathcal{T}_{0,0,0}(\xi) = \frac{1}{\pi^2\xi^2} - \frac{2}{\pi}\log\xi - \frac{D}{\pi^2} - \frac{4}{\pi^2}\sum_{k=1}^{\infty}\xi^{2k}\zeta(k+1)\beta(k+1). \tag{56}$$

In Fig. 4 we show a comparison of direct summation of (54), and running averages, with the result of (56). Such comparisons are useful in detecting possible algebraic errors in formulas such as (56), but do not provide precise validation because of the slowness of convergence of direct summation. However, rapidly convergent representations of Bessel function series have been found which give $\mathcal{T}_{0,0,0}(\xi)$.[2,4] In the example of Fig. 4, both (56) and accelerated summation[4] give the value 1.384 941 001 791 97. Of course, the computational burden in using Bessel function summation as in Ref. 4 is much larger than that involved in using (56) (for which 15 terms in a Mathematica[19] evaluation of the series gave the 14 decimal places quoted).

An alternative derivation of (56) uses the result (50) and the Neumann expansion:[13,14]

$$Y_0(z) = \frac{2}{\pi}\left[\log\left(\frac{z}{2}\right) + \gamma\right]J_0(z) - \frac{4}{\pi}\sum_{k=1}^{\infty}\frac{(-1)^k J_{2k}(z)}{k}. \tag{57}$$

This procedure also uses (27) to arrive at (56).

The radius of convergence of the series on the right-hand side of (56) is unity. This may be increased by subtracting terms from the product $\zeta\beta$ and adding them analytically. The product

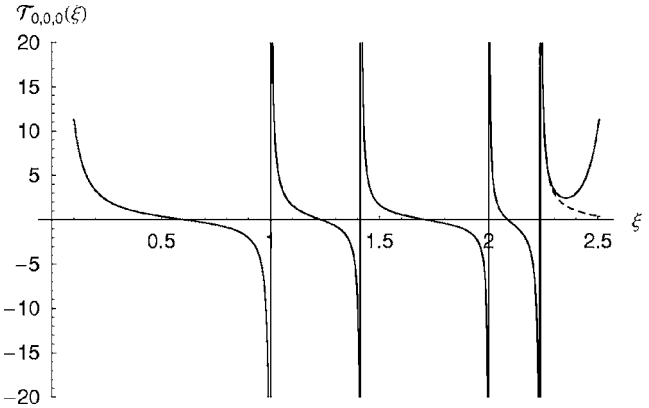

FIG. 5. $\mathcal{T}_{0,0,0}(\xi)$ from Eq. (60) with $N=5$ is compared for summation over k with 10 and 20 terms.

$$\zeta(s)\beta(s) = 1 + \frac{1}{2^s} + \frac{1}{4^s} + \frac{2}{5^s} + \frac{1}{8^s} + \frac{1}{9^s} + \frac{2}{10^s} + \frac{2}{13^s} + \frac{1}{16^s} + \frac{2}{17^s} + \cdots \tag{58}$$

may be written as

$$\zeta(s)\beta(s) = \frac{1}{4}\sum_{n=1}^{\infty} \frac{r_2(n)}{n^s}, \tag{59}$$

where the multiplicities $r_2(n)$ are equal to the number of representations of n by a sum of two squares of integers, allowing zeros and distinguishing signs and order.[20] We substitute (59) into (56), change the order of summation in the double sum, and split the sum over n at $n=N$ to obtain

$$\mathcal{T}_{0,0,0}(\xi) = \frac{1}{\pi^2\xi^2} - \frac{2}{\pi}\log\xi - \frac{D}{\pi^2} - \frac{1}{\pi^2}\sum_{k=1}^{\infty} \xi^{2k}\sigma_N^{\infty}(2k+2) - \frac{1}{\pi^2}\sum_{n=1}^{N} r_2(n)\left[\frac{1}{n-\xi^2} - \frac{1}{n}\right], \tag{60}$$

where the symbol $\sigma_N^{\infty}(2k+2)$ denotes the lattice sum obtained by including only n values in excess of N:

$$\sigma_N^{\infty}(2k+2) = \sum_{n=N+1}^{\infty} \frac{r_2(n)}{n^{k+1}}.$$

This procedure extends the ξ range over which the expression (56) is valid, and the expansion (60) works up until $\xi=\sqrt{N}$.

As an example of the use of (60), we show in Fig. 5 a comparison of the results for summation over k with 10 and 20 terms for $N=5$. The two curves lie on top of each other for ξ up to the last singularity taken into account at an abscissa of $\sqrt{5}$, but then start to separate.

Note that in (60), the only transcendental quantities which require evaluation are the $\sigma_N^{\infty}(2k+2)$. N may be chosen taking into account the upper limit desired for the frequency (say), given by the limit on ξ, and then the $\sigma_N^{\infty}(2k+2)$ may be evaluated once and for all and stored, since they do not depend on ξ. This makes the numerical evaluation of $\mathcal{T}_{0,0,0}(\xi)$ from (60) particularly rapid.

The differential recurrence relations (20) and (21) apply equally to the Neumann sums

$$\mathcal{T}_{\lambda,0,\nu}(\xi) = \sum_{h\neq 0} \frac{Y_\lambda(K_h\xi)}{K_h^\nu}. \tag{61}$$

However, due to the different behaviors between J_λ and Y_λ at the origin, the integral relations (18) and (19) must be altered and become (see the Appendix)

$$\mathcal{T}_{\lambda+1,0,\nu+1}(\xi) = -\frac{\Gamma(1+\lambda)}{2^{\nu+1}\pi^{\lambda+\nu+3}\xi^{\lambda+1}}\sigma^0_{\nu+\lambda+2} + \frac{1}{\xi^{\lambda+1}}\int_0^\xi \eta^{\lambda+1}\mathcal{T}_{\lambda,0,\nu}(\eta)d\eta, \tag{62}$$

and

$$\mathcal{T}_{\lambda-1,0,\nu+1}(\xi) = \frac{\Gamma(1-\lambda)\cos(\lambda\pi)}{2^{\nu+1}\pi^{\nu-\lambda+3}\xi^{-\lambda+1}}\sigma^0_{\nu-\lambda+2} - \frac{1}{\xi^{-\lambda+1}}\int_0^\xi \eta^{-\lambda+1}\mathcal{T}_{\lambda,0,\nu}(\eta)d\eta, \quad \text{for } \mathrm{Re}(\lambda) < 1. \tag{63}$$

The recurrence relation which increments the first subscript alone follows from (62) and the recurrence relations satisfied by Bessel functions

$$\frac{2(\lambda+1)}{z}Y_{\lambda+1}(z) = Y_\lambda(z) + Y_{\lambda+2}(z),$$

and has the form

$$\mathcal{T}_{\lambda+2,0,\nu}(\xi) = -\frac{\Gamma(2+\lambda)}{2^{\nu}\pi^{\nu+\lambda+3}\xi^{\lambda+2}}\sigma^0_{\nu+\lambda+2} + \frac{2(\lambda+1)}{\xi^{\lambda+2}}\int_0^\xi \eta^{\lambda+1}\mathcal{T}_{\lambda,0,\nu}(\eta)d\eta - \mathcal{T}_{\lambda,0,\nu}(\xi). \tag{64}$$

That which decrements the first subscript alone is

$$\mathcal{T}_{\lambda-2,0,\nu}(\xi) = -\frac{\Gamma(2-\lambda)\cos(\lambda\pi)}{2^{\nu}\pi^{\nu-\lambda+3}\xi^{-\lambda+2}}\sigma^0_{\nu-\lambda+2} - \frac{2(\lambda-1)}{\xi^{-\lambda+2}}\int_0^\xi \eta^{-\lambda+1}\mathcal{T}_{\lambda,0,\nu}(\eta)d\eta - \mathcal{T}_{\lambda,0,\nu}(\xi), \tag{65}$$

and holds for $\mathrm{Re}(\lambda) < 1$.

Note that we cannot apply (64) directly to (56), since we would encounter the divergent quantity σ^0_2. Instead, to find $\mathcal{T}_{2,0,0}(\xi)$, we use the same limiting argument as we used to derive (56). We use

$$\mathcal{S}_{2+\delta\lambda,0,0}(\xi) = \frac{1}{\pi\xi^2} + \frac{\delta\lambda}{2\pi\xi^2} + \frac{\delta\lambda}{2\pi}\sum_{k=0}^{\infty}\frac{k+1}{k+2}\xi^{2k+2}\sigma^0_{2k+4}. \tag{66}$$

The calculation for $\mathcal{S}_{-2-\delta\lambda,0,0}(\xi)$ is more involved, since in the sum over k the first two terms are best treated using the form of summand found in (15) rather than (10). The result is

$$\mathcal{S}_{-2-\delta\lambda,0,0}(\xi) = \frac{1}{\pi\xi^2} - \frac{\delta\lambda}{2\pi\xi^2} - \frac{\delta\lambda}{2\pi}\sum_{k=0}^{\infty}\frac{k+1}{k+2}\xi^{2k+2}\sigma^0_{2k+4} - \delta\lambda + \frac{\delta\lambda}{\pi^2\xi^2}[D - 2\pi\log(\pi\xi) + 2\pi(1-\gamma)]. \tag{67}$$

Combining (66) and (67), we obtain

$$\mathcal{T}_{2,0,0}(\xi) = \lim_{\delta\lambda\to 0}\frac{\mathcal{S}_{2+\delta\lambda,0,0}(\xi) - \mathcal{S}_{-2-\delta\lambda,0,0}(\xi)}{\pi\delta\lambda} = \frac{1}{\pi^2\xi^2}\left[-1 + 2\gamma - \frac{D}{\pi} + 2\log(\pi\xi)\right] + \frac{1}{\pi} + \frac{1}{\pi^2}\sum_{k=0}^{\infty}\frac{k+1}{k+2}\xi^{2k+2}\sigma^0_{2k+4}. \tag{68}$$

In the numerical example shown in Fig. 6 the mean of the results from direct summation is −0.285 082, while the result of (68) is −0.297 607.

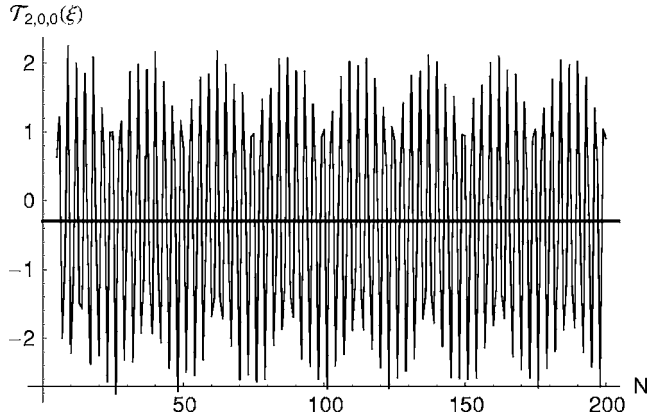

FIG. 6. Partial sums for $\mathcal{T}_{2,0,0}(\xi)$, with $\xi=0.32$, obtained by summation over a square region, centered on the origin and having side length of $2N+1$, for N up to 200. The analytical result (68) is indicated by the horizontal line.

VII. CONCLUSIONS

The results we have given here by no means exhaust those which may be derived using the basic sums (26) and (27) in the Neumann series, or the Schlömilch series (10) and (15). We have also obtained similar results for sums over positive integers rather than the square lattice, which we will submit for publication.

ACKNOWLEDGMENTS

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APPENDIX: RAISING AND LOWERING OPERATORS FOR BESSEL FUNCTIONS

The derivation of recurrence relations for the sums (1) and (61) are based on two differential and two integral relations, satisfied by the Bessel functions. The differential relations are the same for both kinds of Bessel functions,[13,14]

$$\left[\frac{1}{b}x^{\lambda+1}Z_{\lambda+1}(bx)\right]' = x^{\lambda+1}Z_{\lambda}(bx),$$

$$\left[\frac{1}{b}x^{-\lambda+1}Z_{\lambda-1}(bx)\right]' = -x^{-\lambda+1}Z_{\lambda}(bx), \tag{A1}$$

where Z represents one of the Bessel functions J or Y, and the prime denotes a differentiation with respect to x. Due to the different behaviors between J_λ and Y_λ at the origin, the corresponding integral relations are[13,14]

$$\int_0^a x^{\lambda+1}J_{\lambda}(bx)dx = a^{\lambda+1}\frac{J_{\lambda+1}(ba)}{b}, \quad \text{for } \mathrm{Re}(\lambda) > -1 \text{ and } a,b \geqslant 0,$$

$$\int_0^a x^{-\lambda+1}J_{\lambda}(bx)dx = \frac{b^{\lambda-2}}{2^{\lambda-1}\Gamma(\lambda)} - a^{-\lambda+1}\frac{J_{\lambda-1}(ba)}{b}, \quad \text{for } a,b \geqslant 0, \tag{A2}$$

for Bessel functions of the first kind, and

$$\int_0^a x^{\lambda+1} Y_\lambda(bx)dx = \frac{2^{\lambda+1}\Gamma(1+\lambda)}{\pi b^{\lambda+2}} + a^{\lambda+1}\frac{Y_{\lambda+1}(ba)}{b}, \quad \text{for } a,b \geqslant 0,$$

$$\int_0^a x^{-\lambda+1} Y_\lambda(bx)dx = \frac{b^{\lambda-2}\Gamma(1-\lambda)\cos(\lambda\pi)}{2^{\lambda-1}\pi} - a^{-\lambda+1}\frac{Y_{\lambda-1}(ba)}{b}, \quad \text{for } \mathrm{Re}(\lambda) < 1 \text{ and } a,b \geqslant 0, \tag{A3}$$

for Bessel functions of the second kind.

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The relationship between the Wigner-Weyl kinetic formalism and the complex geometrical optics method

Omar Maj[a)]
Physics Department "A. Volta," University of Pavia, I-27100 Pavia, Italy

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The relationship between two different asymptotic techniques, namely, the Wigner-Weyl kinetic formalism and the complex geometrical optics method, is addressed within the framework of semiclassical theory of wave propagation. More specifically, in correspondence to appropriate boundary conditions, the solution of the wave kinetic equation, relevant to the Wigner-Weyl formalism, is obtained in terms of the corresponding solution of the complex geometrical optics equations. In particular, this implies that the two considered techniques yield the same wavefield intensity. Such a result is also discussed on the basis of the analytical solution of the wave kinetic equation specific to Gaussian beams of electromagnetic waves propagating in a "lens-like" medium for which the complex geometrical optics solution is already available. © *2005 American Institute of Physics.*
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I. INTRODUCTION

In the framework of the semiclassical theory of waves,[1–5] i.e., short wavelength asymptotics, the uniform (global) description of the wavefield is complicated by the formation of caustic singularities.[1,2,6–8] Although a complete and deep understanding of the wavefield structure near caustic regions is obtained on the basis of catastrophe theory[2,6,8] and the unfolding of the corresponding singularities can be treated by means of symplectic techniques,[1,2,9] the application of such methods to realistic cases, e.g., to waves in magnetically confined plasmas,[10] appears rather difficult. Therefore, with specific regard to physical applications, several asymptotic methods have been developed which yield numerically tractable equations, though being limited concerning the global properties of the asymptotic solutions.

Such asymptotic techniques can be classified into two different families, depending on whether the relevant wave equation is described in the phase space, *microlocal techniques*, or directly in the configuration space where the wavefield is defined, *quasi-optical methods*.

This work aims to give a detailed comparative analysis of two such techniques, namely, the Wigner-Weyl kinetic formalism[11–13] and the complex geometrical optics (CGO) method,[14–17] which can be considered as benchmarks for microlocal and quasi-optical methods, respectively.

Specifically, in Sec. II, the Wigner-Weyl formalism and the complex geometrical optics method are reviewed and compared. In particular, it is pointed out that, within the Wigner-Weyl formalism, physically meaningful solutions should have a specific form, referred to as momentum distribution, which is characterized in Sec. III.

On the basis of the mathematical properties of momentum distributions, our main result is obtained in Sec. IV. In particular, it is shown that, in correspondence to appropriate boundary conditions, there exists a specific asymptotic solution of the wave kinetic equation relevant to the Wigner-Weyl formalism that can be written in terms of the corresponding solution of the complex geometrical optics equations. This allows us to relate the two considered methods as well as to

[a)]Electronic mail: maj@fisicavolta.unipv.it

determine the specific class of boundary conditions for which they are equivalent. In Sec. V, this general result is illustrated by means of an analytically tractable example, i.e., the propagation of a Gaussian beam of electromagnetic waves in an isotropic "lens-like" medium. In conclusion, a summary of the main results is given in Sec. VI.

II. THE WIGNER-WEYL FORMALISM VERSUS THE CGO METHOD

In order to set up the framework, let us discuss the relevant boundary value problem for a generic *scalar* pseudodifferential wave equation, together with the required mathematical definitions.

Specifically, we will consider the case of a scalar (real or complex) wavefield $\psi(x)$ propagating in the N-dimensional linear space $\mathbb{R}^N$ with $x=(x^1,\ldots,x^N)$ a generic set of Cartesian coordinates and denote by $k=(k_1,\ldots,k_N)$ the corresponding coordinates in the dual space $(\mathbb{R}^N)' \cong \mathbb{R}^N$. Time-dependent wavefields are included as one of the coordinates can play the role of time, e.g., $x^N=ct$, c being a reference speed, and the corresponding dual coordinate is related to frequency, e.g., $k_N=-\omega/c$. To some extent, the results for a scalar wave equation are valid also for a multicomponent wave equation as the latter can be reduced to a set of *independent* scalar equations far from mode conversion regions.[5]

Thereafter, the Wigner-Weyl formalism will be formulated entirely in the space $\mathbb{R}^N \times (\mathbb{R}^N)' \cong \mathbb{R}^{2N}$, with coordinates (x,k), which is viewed as the trivial cotangent bundle[21] over the configuration space $\mathbb{R}^N$ where the wavefield is defined. No explicit reference to the propagation direction is made, differently from the classical derivations.[13] As for the CGO method, it has been originally developed for solving the second-order partial differential equation relevant to the propagation of electromagnetic wave beams in stationary spatially nondispersive media. Hence, we will need to discuss its application to generic pseudodifferential equations. In particular, it is shown that the CGO method yields an approximation of the wavefield directly in the configuration space, provided that the wave equation satisfies an appropriate condition.

First, let us define the class of wave equations undergone to solution. A pseudodifferential wave equation is an equation of the form

$$(\hat{D}\psi)(x) = \frac{1}{(2\pi)^N} \int e^{ik\cdot(x-x')} d(x,x',k)\psi(x')\, d^N x'\, d^N k = 0, \tag{1}$$

which admits propagating wave solutions. The operator $\hat{D}$ is a pseudodifferential operator[3,18–20] acting on the wavefield as a Fourier integral operator[20] characterized by the bilinear phase function $k\cdot(x-x')$. Here, $d(x,x',k)$ belongs to a particular class of smooth functions, referred to as *symbols*, which, roughly speaking, behave like a polynomial in k for $|k|$ large enough. Specifically, a smooth function $a(z,k)$ with $z \in \mathbb{R}^M$ and $k \in (\mathbb{R}^N)'$ is a symbol of order $m \in \mathbb{R}$ if for every multiindices α, β there is a constant $C_{\alpha,\beta} > 0$ such that

$$|\partial_z^\alpha \partial_k^\beta a(z,k)| \leqslant \frac{C_{\alpha,\beta}}{L^{|\alpha|-|\beta|}} (1+|kL|)^{m-|\beta|}, \quad \text{uniformly in } (z,k) \in \mathbb{R}^M \times (\mathbb{R}^N)', \tag{2}$$

and one writes $a \in S^m(\mathbb{R}^M \times (\mathbb{R}^N)')$. In virtue of the symbol estimate (2) the integral in (1) makes sense for $\psi \in \mathcal{S}'(\mathbb{R}^N)$, the space of tempered distribution.[18,21] Moreover, the scale length L characterizes the variations of symbols with respect to the spatial coordinate z and it can be eliminated by the rescaling $z \to z/L$ and $k \to kL$. It is worth noting that any linear differential operator with smooth and bounded coefficients is a pseudodifferential operator.[19]

Boundary conditions of Cauchy type are given on an $(N-1)$-dimensional hypersurface Σ: for simplicity, one can assume Σ to be the hyperplane $\{x: x^N=0\}$ where the wavefield $\psi_0(\mathbf{x})$, $\mathbf{x}=(x^1,\ldots,x^{N-1})$, is assigned together with as many derivatives $\psi_n(\mathbf{x}) = \partial^n \psi / \partial (x^N)^n$ as appropriate. We are interested in semiclassical solutions for which only the covectors k with

$$\kappa = |kL| \gg 1$$

are significant, in the integral in (1). As a consequence, the wavefield should be a highly oscillating function on the (large) scale length L and it should correspond to a specific set of highly oscillating boundary conditions of the form

$$\psi_0(\mathbf{x}) = A_0(\mathbf{x}) e^{iS_0(\mathbf{x})}, \quad \partial_{\mathbf{x}} S_0(\mathbf{x}) L \sim \kappa \gg 1, \tag{3}$$

the amplitude A being slowly varying, that is, $|\partial_x A| \sim |A|/L$.

A. The Wigner-Weyl formalism

In the Wigner-Weyl formalism, the Weyl-symbol map σ^W is applied in order to represent the wave equation (1) in $\mathbb{R}^N \times (\mathbb{R}^N)'$ which is naturally endowed with a phase-space structure. The Weyl-symbol map transforms an operator $\hat{A}: \mathcal{S}(\mathbb{R}^N) \to \mathcal{S}'(\mathbb{R}^N)$, $\mathcal{S}(\mathbb{R}^N)$ being the space of Schwartz's functions,[21] into a tempered distribution by acting on the Schwartz kernel $\mathcal{A}(x_1, x_2) \in \mathcal{S}'(\mathbb{R}^{2N})$ of the operator $\hat{A}$ according to[13]

$$\mathcal{A}(x_1, x_2) \mapsto \sigma^W(\hat{A})(x,k) = \int \mathcal{A}\left(x + \frac{1}{2}s, x - \frac{1}{2}s\right) e^{-ik\cdot s} d^N s. \tag{4}$$

It is worth noting that for the pseudodifferential operator in (1) the Schwartz kernel is

$$\mathcal{D}(x_1, x_2) = \frac{1}{(2\pi)^N} \int e^{ik\cdot(x_1 - x_2)} d(x_1, x_2, k)\, d^N k,$$

thus, the image of $\hat{D}$ under the Weyl-symbol map amounts to the formal series of decreasing order symbols

$$\sigma^W(\hat{D})(x,k) = \sum_\alpha \frac{i^{|\alpha|}}{\alpha!} \partial_s^\alpha \partial_k^\alpha d \left(x + \frac{1}{2}s, x - \frac{1}{2}s, k\right)\Big|_{s=0},$$

where Taylor expansion has been used and $\partial_s^\alpha \partial_k^\alpha d \in S^{m-|\alpha|}$. Series of that kind admit always an asymptotic resummation[3,19] to a symbol of order m,

$$D(x,k) \sim \sigma^W(\hat{D})(x,k) \in S^m, \tag{5}$$

which is referred to as *Weyl symbol* of $\hat{D}$. In (5) the $\sim$ denotes the asymptotic equivalence of symbols.[3,19] On the other hand, one can consider the correlation operator[13] $\hat{S}$ whose Schwartz kernel is given by the tensor product $\psi(x_1)\psi^*(x_2)$. Then the Weyl-symbol map yields the *Wigner function*

$$W(x,k) = \sigma^W(\hat{S})(x,k) = \int \psi\left(x + \frac{1}{2}s\right) \psi^*\left(x - \frac{1}{2}s\right) e^{-ik\cdot s}\, d^N s. \tag{6}$$

The wave equation (1) can be written in the equivalent form $\hat{D}\hat{S}=0$ and, on applying the Weyl-symbol map, one gets[3,13]

$$\sigma^W(\hat{D}\hat{S})(x,k) \sim \sum_{\alpha,\beta} \frac{(-1)^{|\alpha|}}{(2i)^{|\alpha+\beta|}\alpha!\beta!} (\partial_x^\alpha \partial_k^\beta D(x,k))(\partial_x^\beta \partial_k^\alpha W(x,k)) = 0. \tag{7}$$

In the semiclassical limit one has $\partial_x^\alpha \partial_k^\beta D = O(\kappa^{m-|\beta|})$ so that, on assuming the same ordering for the Wigner function,[13] the foregoing equation separates into

$$D'(x,k) W(x,k) = 0, \tag{8a}$$

$$\{W(x,k),D'(x,k)\} = 2D''(x,k)W(x,k), \tag{8b}$$

where $D' \in S^m$ and $D'' \in S^{m-1}$ are the real and imaginary parts of the Weyl symbol; in particular, one has $D''/D' = O(\kappa^{-1})$ which is the condition for weak absorption and/or instabilities.[13] Equation (8a) is a constraint to Eq. (8b) which, on the other hand, has the form of a kinetic equation in the x-k phase space, $\{\cdot,\cdot\}$ being the corresponding Poisson brackets. We will refer to the whole system (8) as the *wave kinetic equation*.

In general, a solution of the wave kinetic equation is a tempered distribution, however, one usually restricts the class of solutions to semiclassical measures. This allows us to make sense of the integrals of the form[3,13]

$$\langle \hat{A} \rangle_\psi = \frac{1}{(2\pi)^N} \int A(x,k)W(x,k)\, d^N x\, d^N k,$$

which expresses the expectation value of a physical quantity represented by the pseudodifferential operator $\hat{A}$ with Weyl symbol $A(x,k)$. In the following we will assume further regularity with respect to x so that the expectation values of physical quantities can be defined *locally*, that is,

$$A(x) = \int \frac{d^N k}{(2\pi)^N} A(x,k)W(x,k) \tag{9a}$$

makes sense as a smooth function in $x \in \mathbb{R}^N$. In particular, the wavefield intensity amounts to

$$|\psi(x)|^2 = \int \frac{d^N k}{(2\pi)^N} W(x,k). \tag{9b}$$

Such a restriction of the class of solutions is justified as, in general wave propagation problems, one needs a description of the space and time profiles of physical quantities.

Let us now discuss the appropriate boundary conditions for (8). On the hyperplane $\Sigma = \{x : x^N = 0\}$ the wavefield $\psi_0(\mathbf{x})$ has been assigned and one can compute the corresponding Wigner function $W_0(\mathbf{x},\mathbf{k}) = \sigma^W(\hat{S}_0)(\mathbf{x},\mathbf{k})$, $\hat{S}_0$ being the correlation operator associated to ψ_0 and $\mathbf{k} = (k_1, \ldots, k_{N-1})$ the coordinates dual to $\mathbf{x}$; then a solution $W(x,k)$ should match $W_0(\mathbf{x},\mathbf{k})$ in some appropriate sense. Specifically, one should impose that the local value $A(x)$ of any physical quantity evaluated on Σ is the same whether it is evaluated by $W(x,k)$ or by $W_0(\mathbf{x},\mathbf{k})$. Within this formulation, the Weyl symbol $A(x,k)$ should be restricted to $\mathbb{R}^{2N-2}$ where W_0 is defined. One can note that the suitable embeddings Γ of $\mathbb{R}^{2N-2}$ into $\mathbb{R}^{2N}$ such that Γ lies over Σ, i.e., $\pi\Gamma = \Sigma$ with $\pi : (x,k) \mapsto x$ the canonical projection,[21] are of the form $\Gamma = \{(x,k) : x^N = 0, k_N = H(\mathbf{x},\mathbf{k})\}$ with $H(\mathbf{x},\mathbf{k})$ a generic smooth function; correspondingly, the restriction of a symbol is readily defined as $A|_\Gamma(\mathbf{x},\mathbf{k}) = A(\mathbf{x},0,\mathbf{k},H(\mathbf{x},\mathbf{k}))$. Then the boundary value conditions read

$$\int \frac{d^N k}{(2\pi)^N} W(x,k)A(x,k)\bigg|_\Sigma = \int \frac{d^{N-1}\mathbf{k}}{(2\pi)^{N-1}} W_0(\mathbf{x},\mathbf{k})A|_\Gamma(\mathbf{x},\mathbf{k}), \tag{10a}$$

which is equivalent to

$$W|_\Sigma(\mathbf{x},\mathbf{k},k_N) = 2\pi W_0(\mathbf{x},\mathbf{k})\,\delta(k_N - H(\mathbf{x},\mathbf{k})). \tag{10b}$$

The function H cannot be arbitrary as (10b) should satisfy the constraint (8a) which reads

$$D'(\mathbf{x},0,\mathbf{k},H(\mathbf{x},\mathbf{k})) = 0, \tag{11}$$

hence, the appropriate functions H are obtained on solving the so-called *local dispersion relation* evaluated on Σ. Since Σ has been assumed to be noncharacteristic, i.e., $\partial D'/\partial k_N \neq 0$ on Γ, the function H is well defined and smooth at least locally, in view of the implicit function theorem. On the other hand, it is not unique since (11) may have multiple solutions, each one corresponding to a specific branch of the dispersion relation. In virtue of the superposition principle for linear wave

equations, the total wavefield is a linear superposition of the contributions from each branch of the dispersion relation, the coefficients being determined by the Cauchy boundary values of the normal derivatives $\partial^n\psi/\partial(x^N)^n|_\Sigma$. Therefore, one has a specific Cauchy boundary value problem for the Wigner function of each branch and the sum over all branches yields the total Wigner function. Since one has

$$|\psi|^2 = \sum_{b,b'} \psi_{b'}^* \psi_b = \sum_b |\psi_b|^2 + \sum_{b\neq b'} \psi_{b'}^* \psi_b,$$

where the indices b and b' run over all branches, and, on noting that the average $\langle\cdot\rangle$ over short-scale oscillations cancels out the mixed terms, $\langle\psi_{b'}^*\psi_b\rangle=0$ for $b'\neq b$, whereas $\langle|\psi_b|^2\rangle=|\psi_b|^2$, one gets

$$\langle|\psi(x)|^2\rangle = \sum_b \int \frac{d^N k}{(2\pi)^N} W_b(x,k) = \int \frac{d^N k}{(2\pi)^N} W(x,k), \tag{12}$$

that is, the projection of the total Wigner function yields the *averaged wavefield intensity* and, thus, it does not account for, e.g., the formation of short-scale diffraction patterns.

B. The complex geometrical optics method

Let us now turn to the complex geometrical optics (CGO) method and, in particular, let us discuss its application to pseudodifferential wave equations. This is based on approximating the solution of (1) by a smooth wave function of the form

$$\psi(x) = u(x)e^{i\bar{S}(x)} = u(x)e^{-\phi(x)}e^{iS(x)}, \tag{13}$$

where, according to the semiclassical limit, $|\partial_x S(x)L|\sim\kappa$ and $\partial_x u(x)|\sim|u(x)|/L$. In addition to the standard oscillating exponential $e^{iS(x)}$, the wave object (13) exhibits a novel scale length $w\sim|\partial_x\phi(x)|^{-1}$ which accounts for intermediate-scales variations of the amplitude profile $A(x)=u(x)e^{-\phi(x)}$ with $\kappa\gg|kw|\gg 1$. In general, such an intermediate scale length w can be determined by both (strong) absorption[16] and diffraction;[17] however, in this paper, it is assumed that the medium is weakly nondissipative [cf. comments after Eqs. (8)] so that only diffraction effects are significant. The total short- and intermediate-scale variations of the wavefield are accounted for by the *complex eikonal function* $\bar{S}(x)=S(x)+i\phi(x)$.

The relevant equations for the three unknown functions u, ϕ, and S are determined on substituting the ansatz (13) into the wave equation (1). For the specific case for which $\hat{D}$ is a differential operator this is straightforward. On the other hand, for the general case, one should deal with the nonlocal response of the operator.[22] With this aim it is convenient writing (1) in the configuration space in terms of the Schwartz kernel, namely,

$$\int \mathcal{D}(x,x')\psi(x')d^N x' \sim \int \mathcal{D}^{(s)}\left(\frac{x+x'}{2}, x-x'\right)\psi(x')\,d^N x' = 0,$$

where the exact kernel has been replaced by the $\mathcal{D}^{(s)}=\sigma^{W-1}(D)$ where D is the Weyl symbol. Actually, one could make use of other symbol maps,[3] yielding asymptotically equivalent results; here the Weyl-symbol maps has been chosen for direct comparison with the Wigner-Weyl approach.

Let us further assume that the kernel $\mathcal{D}^{(s)}(x_1,x_2)$ amounts to a distribution smoothly dependent on x_1 and with compact support in x_2. In virtue of the Paley-Wiener-Schwartz theorem,[21] this is equivalent to assume that the corresponding Weyl symbol $D(x,k)$ extends to an *entire* function of the complex-valued dual vector $\bar{k}=k+ik''$, smoothly dependent on $x\in\mathbb{R}^N$. From a physical standpoint, the foregoing assumption implies that nonlocal effects have a finite range: the response $(\hat{D}\psi)(x)$ of the operator $\hat{D}$ depends only on the value of the wavefield ψ in a compact set.

Within this condition, one can substitute the complex eikonal ansatz (13) into (1) and expand in Taylor series with respect to $s=x-x'$. As a result one has[22]

$$D(x,\bar{k}(x))u(x) - i\frac{\partial D(x,\bar{k}(x))}{\partial k_i}\frac{\partial u(x)}{\partial x^i} - \frac{i}{2}\frac{\partial^2 D(x,\bar{k}(x))}{\partial x^i \partial k_i}u(x) - \frac{i}{2}\frac{\partial^2 \bar{S}(x)}{\partial x^i \partial x^j}\frac{\partial^2 D(x,\bar{k}(x))}{\partial k_i \partial k_j}u(x) = O(\kappa^{-2}),$$

where $\bar{k}(x)=\partial_x S(x)+i\partial_x \phi(x)$ and, for the Paley-Wiener-Schwartz theorem, the estimate $|\partial_x^\alpha \partial_k^\beta D| = O(\kappa^{m-|\beta|})$ is still valid for complex-extended symbols. To leading orders in κ, and for a weakly dissipative media, i.e., $D''/D' = O(\kappa^{-1})$, one gets

$$D'(x,\partial_x \bar{S}(x)) = 0, \tag{14a}$$

$$\frac{\partial D'(x,\partial_x \bar{S}(x))}{\partial k_i}\frac{\partial u(x)}{\partial x^i} = \left[D''(x,\partial_x \bar{S}(x)) - \frac{1}{2}\frac{\partial}{\partial x^i}\left[\frac{\partial D'(x,\partial_x \bar{S}(x))}{\partial k_i} \right] \right] u(x), \tag{14b}$$

$D'(x,\bar{k})$ and $D''(x,\bar{k})$ being the real and imaginary parts of D extended in the complex $\bar{k}$ space and, in general, are complex valued. It is worth noting that the foregoing equations can be formally obtained from the standard geometrical optics equations, e.g., in the form given by Littlejohn and Flynn,[5] by replacing $k(x)$ with $\bar{k}(x)$.

The CGO equations (14) have been dealt with both by means of the characteristics method in the complex domain[15] and on expanding the equations with respect to $\epsilon \equiv |k''(x)|/|k(x)| \sim |k(x)w|^{-1} \ll 1$.[17] In particular, on referring to the latter approach, in the weak-diffraction regime $\epsilon \sim \kappa^{-1/2}$, terms up to order $\epsilon^2 \sim \kappa^{-1}$ should be considered in the CGO equation for the complex eikonal $\bar{S}(x)$, which, after separating the real and imaginary parts, amounts to

$$D'(x,k(x)) - \frac{1}{2}k_i''(x)k_j''(x)\frac{\partial^2 D'(x,k(x))}{\partial k_i \partial k_j} = 0, \tag{15a}$$

$$k_i''(x)\frac{\partial D'(x,k(x))}{\partial k_i} = 0. \tag{15b}$$

Equations (15a) and (15b) constitute a set of coupled first-order partial differential equations for $S(x)$ and $\phi(x)$ with $k(x)=\partial_x S(x)$ and $k''(x)=\partial_x \phi(x)$. As for the complex amplitude $u(x)$, only the lowest order approximation with respect to ϵ is significant, so that the real amplitude $|u(x)|$ is decoupled from the phase $\arg[u(x)]$ (not considered hereafter) and determined by means of the transport equation

$$\frac{\partial}{\partial x^i}\left[\frac{\partial D'(x,k(x))}{\partial k_i}|u(x)|^2 \right] = 2D''(x,k(x))|u(x)|^2. \tag{15c}$$

This is formally the same equation as the geometrical optics transport equation,[5] but diffraction effects are accounted for through the wavevector-field $k(x)$ which differs from that obtained in the geometrical optics. The approximated form (15) of the CGO equations is the one used in physical applications. Moreover, in the zero-diffraction regime ($w \gtrsim L$), one has $\epsilon \sim \kappa^{-1}$, thus terms up to first order only should be considered, with the result that equations (15a) and (15b) are decoupled and the whole set of CGO equations (15) reduces to the standard geometrical optics equations, ϕ being effectively zero.

Equations (15a) and (15b) are usually solved by computing the characteristic curves[18,21] of (15a) with (15b) regarded as a constraint with the result that the characteristics curves thus obtained resemble the geometrical optics rays.[4,5] Therefore, the appropriate boundary conditions should be enough to determine the initial values of the complex vector $\bar{k}|_\Sigma(\mathbf{x})$ evaluated on the boundary surface Σ.

Such conditions are obtained from the Cauchy data (3) on writing

$$\psi_0(\mathbf{x}) = A_0(\mathbf{x})e^{iS_0(\mathbf{x})} = u_0(\mathbf{x})e^{-\phi_0(\mathbf{x})}e^{iS_0(\mathbf{x})} + O(\epsilon), \tag{16}$$

for some functions u_0 and ϕ_0 such that $|\partial_{\mathbf{x}}u_0| \sim |u_0|/L$ and $|\partial_{\mathbf{x}}\phi_0| \sim \phi_0/w$. From (16) one readily gets the value of the component of the complex vector $\bar{k}=k+ik''$ tangent to Σ, namely, $\mathbf{k}(\mathbf{x}) = \partial_{\mathbf{x}}S_0(\mathbf{x})$ and $\mathbf{k}''(\mathbf{x})=\partial_{\mathbf{x}}\phi_0(\mathbf{x})$. The remaining normal component is obtained on imposing that the CGO equations (15) are satisfied on Σ; this yields two equations for k_N and k_N'', viz.,

$$D'(\mathbf{x},0,\mathbf{k}(\mathbf{x}),k_N) - \frac{1}{2}\sum_{i,j<N} A_{ij}(\mathbf{x},0,\mathbf{k}(\mathbf{x}),k_N)k_i''(\mathbf{x})k_j''(\mathbf{x}) = 0, \tag{17a}$$

$$k_N''(\mathbf{x}) = -\sum_{i<N} k_i''(\mathbf{x})X_i(\mathbf{x},0,\mathbf{k}(\mathbf{x}),k_N), \tag{17b}$$

where $A_{ij}(x,k) \in S^{m-2}$ and $X_i(x,k) \in S^0$ are obtained in terms of the first- and second-order k derivatives of D' and evaluated at $x^N=0$. Equation (17a) is an $O(\epsilon^2)$ perturbation of the local dispersion relation (11), hence, it can be solved by

$$k_N(\mathbf{x}) = H(\mathbf{x},\mathbf{k}(\mathbf{x})) + O(\epsilon^2), \tag{18}$$

and, in correspondence of (18), Eq. (17b) yields $k_N''(\mathbf{x})$. As in the Wigner-Weyl formalism, if multiple solutions are found, one should write the wavefield as a sum of contributions from each branch of the local dispersion relation.

From the foregoing discussion, one should note that the CGO method yields the solution directly in the configuration space, but one should deal with the set of partial differential equations (15), the numerical solution of which can be rather cumbersome. Although the characteristics technique can be used for Eq. (15a), the constraint (15b) should be solved in parallel, thus increasing the computational complexity of the problem. As for the global properties of the CGO solution, to our knowledge no general result is still available, though numerical solutions[17] show that the CGO solution is regular even near focal points where the standard geometrical optics solution exhibits a caustic singularity.

In contrast, the Wigner-Weyl formalism appears better suited for numerical solutions. In particular, the wave kinetic equation can be solved along the corresponding Hamiltonian orbits in the phase space so that it is reduced to a set of ordinary differential equations that require limited computational efforts and the solution thus obtained has a global validity in the phase space since the Hamiltonian orbits do not cross each other. In this respect, the constraint (8a) does not constitute a limitation as D' is a constant of motion. Moreover, there is no limitation on the nonlocal response of pseudodifferential operators to which the Wigner-Weyl formalism applies. On the other hand, the solution in the phase space should be projected into the configuration space and, thus, an integral with respect to the momentum k should be carried out numerically.

Notwithstanding these differences, the Wigner-Weyl kinetic formalism and the complex geometrical optics method share a number of features, e.g., the solution of the local dispersion relation (18) relevant to the CGO method is obtained, to the lowest significant order in ϵ, on evaluating the corresponding solution (11) for $\mathbf{k}=\mathbf{k}(\mathbf{x})$. In the following sections, it will be proved that one can project the wave kinetic equation from the phase space into the configuration space in such a way that the CGO equations (15) are recovered.

III. A NOVEL CLASS OF SOLUTIONS TO THE WAVE KINETIC EQUATION

As discussed in Sec. II, the solutions of the wave kinetic equation are usually sought in the space $\mathcal{S}'(\mathbb{R}^N)$ of tempered distributions,[24] or in the space of semiclassical measures.[3] The first formulation is the more general, whereas the second follows from the physical requirement that expectation values (9a) are well defined. Moreover, we have pointed out that, for general wave propagation problems, physics requires a stronger condition on the Wigner function, namely, the

expectation values of physical quantities should be locally defined according to (9b). For instance, if one deals with a time-dependent wavefield for which $x^N=ct$ and $k_N=-\omega/c$, the integral

$$J(\mathbf{x},t)=\int \frac{d^{N-1}\mathbf{k}}{(2\pi)^{N-1}}\int \frac{d\omega}{2\pi}\frac{\partial D'}{\partial \omega}W$$

yields the wave action density $J(\mathbf{x},t)$ in the space-time.[13]

In this section, a mathematical characterization of such novel solutions is given and the corresponding differential calculus is put forward.

First, let us note that for any Schwartz function $\varphi(k)\in\mathcal{S}(\mathbb{R}^N)$ and for any tempered distribution $f\in\mathcal{S}'(\mathbb{R}^{2N})$ one can define a tempered distribution $f_\varphi\in\mathcal{S}'(\mathbb{R}^N)$ over the configuration space only, given by

$$\langle f_\varphi,\chi\rangle=\langle f,\chi\varphi\rangle=\int f(x,k)\chi(x)\varphi(k)\,d^Nx\,d^Nk,\quad \chi\in\mathcal{S}(\mathbb{R}^N),\tag{19}$$

where, in general, angle brackets and the integral are alternative ways to denote the action of a distribution on the corresponding test function. The distribution f is smooth with respect to $x\in\mathbb{R}^N$ if and only if f_φ amounts to a smooth function $f_\varphi(x)$. In this case the map $\varphi\mapsto f_\varphi(x)$ for $\varphi\in\mathcal{S}(\mathbb{R}^N)$ defines at every point location $x\in\mathbb{R}^N$ a tempered distribution $f_x\in\mathcal{S}'(\mathbb{R}^N)$ with

$$\langle f_x,\varphi\rangle=f_\varphi(x)\quad \text{for } \varphi\in\mathcal{S}(\mathbb{R}^N).\tag{20}$$

This is a consequence of the completeness of $\mathcal{S}'(\mathbb{R}^N)$ along with the identity $f_\varphi(x)=\lim_{\delta\to 0}\langle f,\chi_\delta(\cdot-x)\varphi\rangle$ where χ_δ is a compact-supported function that approximates the Dirac's δ function for $\delta\to 0$.

Let us now consider a symbol $A\in S^{-\infty}=\cap_m S^m$, that is, A fulfills the symbol estimate (2) for every order m. It follows that $A_x=A(x,\cdot)\in\mathcal{S}(\mathbb{R}^N)$ and for any $f\in\mathcal{S}'(\mathbb{R}^{2N})$ which is smooth with respect to x one can define

$$\int f(x,k)A(x,k)\,d^Nk=\langle f_x,A_x\rangle,\tag{21}$$

and this is a smooth function on $\mathbb{R}^N$ as required in (9b). The definition (21) should be extended for any symbol $A\in S^m$ with arbitrary order. With this aim, the class of physically admissible solutions [in the sense of (9b)] is restricted. In particular, it is appropriate considering the tempered distributions $f\in\mathcal{S}'(\mathbb{R}^{2N})$ that satisfy the following conditions:

(1) f is smooth with respect to x and
(2) the restriction f_x amounts to a distribution with compact support, i.e., $f_x\in\mathcal{E}'(\mathbb{R}^N)$, where $\mathcal{E}'(\mathbb{R}^N)$ is continuously embedded in $\mathcal{S}'(\mathbb{R}^N)$ in the weak topology.

Such a distribution f will be called *momentum distribution* since for every x its restriction f_x represents the distribution of momentum k over x. For short let us write $f\in\mathcal{M}$ for the space of momentum distributions.

Within this formulation for every $f\in\mathcal{M}$ and for every $A\in S^m$ Eq. (21) is well posed and defines a smooth function on $\mathbb{R}^N$. Let us note that the foregoing definition of the space $\mathcal{M}$ is not the optimal one as functions rapidly decreasing in k are also admissible momentum distributions. However, in the semiclassical limit these functions can be ignored and only compact-supported distributions are significant.

Let us now address the derivatives of a momentum distribution $f\in\mathcal{M}$. First, the derivatives with respect to the momentum k are defined throughout every order. Specifically, since

$$\langle(\partial_k^\alpha f)_\varphi,\chi\rangle=\langle\partial_k^\alpha f,\chi\varphi\rangle=(-1)^{|\alpha|}\langle f,\chi\partial_k^\alpha\phi\rangle=(-1)^{|\alpha|}\langle f_{\partial_k^\alpha\varphi},\chi\rangle,$$

$\partial_k^\alpha f$ is smooth with respect to x; moreover, for every $\varphi\in\mathcal{S}(\mathbb{R}^N)$,

$$\langle(\partial_k^\alpha f)_x,\varphi\rangle=(-1)^{|\alpha|}f_{\partial_k^\alpha\varphi}(x)=(-1)^{|\alpha|}\langle f_x,\partial_k^\alpha\varphi\rangle=\langle\partial_k^\alpha f_x,\varphi\rangle,$$

hence, $(\partial_k^\alpha f)_x$ is compactly supported, and, thus, $\partial_k^\alpha f\in\mathcal{M}$. In terms of the integral notation the latter result evaluated for symbols reads

$$\int\partial_k^\alpha f(x,k)A(x,k)\,d^Nk=(-1)^{|\alpha|}\int f(x,k)\partial_k^\alpha A(x,k)\,d^Nk, \tag{22}$$

which is the "integration-by-parts" formula. On the other hand, the derivatives with respect to x should be dealt with more carefully. For simplicity, let us consider first-order derivative $\partial f/\partial x^i$ for $f\in\mathcal{M}$. One has that

$$(\partial f/\partial x^i)_\varphi=\partial f_\varphi/\partial x^i,$$

in virtue of (19), so that $\partial f/\partial x^i$ is smooth with respect to x. Furthermore,

$$\langle(\partial f/\partial x^i)_x,\varphi\rangle=\frac{\partial}{\partial x^i}\langle f_x,\varphi\rangle,$$

hence $(\partial f/\partial x^i)_x$ is compactly supported and $\partial f/\partial x^i\in\mathcal{M}$. The explicit formula for the derivative is obtained on noting that for every symbol $A\in S^m$, $Af\in\mathcal{M}$ and

$$\langle(\partial Af/\partial x^i)_x,1\rangle=\langle(f\partial A/\partial x^i+A\partial f/\partial x^i)_x,1\rangle=\langle f_x,(\partial A/\partial x^i)_x\rangle+\langle(\partial f/\partial x^i)_x,A_x\rangle,$$

which in the integral notation takes the form

$$\int\frac{\partial f(x,k)}{\partial x^i}A(x,k)\,d^Nk=\frac{\partial}{\partial x^i}\int f(x,k)A(x,k)\,d^Nk-\int f(x,k)\frac{\partial A(x,k)}{\partial x^i}\,d^Nk. \tag{23}$$

The same result would be obtained from the definition $\lim_{\delta\to0}\langle\partial f/\partial x^i,\chi_\delta(\cdot-x)A_x\rangle$ through straightforward but longer calculations. Higher-order derivatives can be defined by recurrence, but they are not explicitly needed in the following.

Searching for solutions of the wave kinetic equations (8) in the space of momentum distributions leads to the weak formulation

$$\int D'(x,k)W(x,k)A(x,k)d^Nk=0, \tag{24a}$$

$$\frac{1}{(2\pi)^N}\int[\{W(x,k),D'(x,k)\}-2D''(x,k)W(x,k)]A(x,k)d^Nk=0, \tag{24b}$$

with $W\in\mathcal{M}$. Furthermore, we are interested in semiclassical solutions for which only large-enough momenta are significant. On recalling that $\langle W_x,1\rangle=(2\pi)^N|\psi(x)|^2$, we will search for solution of (24) in the form

$$W(x,k)=(2\pi)^Nf(x,k-\partial_xS(x))|\psi(x)|^2 \tag{25}$$

where $S(x)$ and $|\psi(x)|^2$ are smooth functions to be determined; in particular, $S(x)$ defines a Lagrangian manifold $k=\partial_xS(x)$ in the x-k phase space. Moreover, $f\in\mathcal{M}$ is normalized, i.e., $\int f\,d^Nk=\langle f_x,1\rangle=1$, and such that

$$K_\alpha(x)\equiv\int f(x,\tilde{k})\tilde{k}^\alpha\,d^N\tilde{k}=O(\tilde{w}^{-|\alpha|}), \tag{26}$$

for any multi-index α. The integrals in (26) are well posed since $\tilde{k}^\alpha=(k-\partial_xS(x))^\alpha$ are symbols of order $|\alpha|$, and the corresponding quantities $K_\alpha(x)$ express the statistical moments of the distribu-

tion f, i.e., they express how important are the *deviations* $\tilde{k}$ of the momentum from the Lagrangian manifold $k=\partial_x S(x)$. In particular, $K_0(x)=1$ in view of the normalization condition. In the semiclassical limit it is assumed that the scale length $\tilde{w}$ characterizing the range of the momentum deviations is large enough as compared to $|\partial_x S(x)|^{-1}=|k(x)|^{-1}$, namely, $|k(x)\tilde{w}| \gg 1$.

In the Appendix, it is proved that, within the weak formulation (24), the momentum distribution f, satisfying the foregoing conditions, can be represented by the asymptotic series, cf. Eq. (A4),

$$f(x,k-\partial_x S(x)) \sim \sum_{\beta} \frac{(-1)^{|\beta|}}{\beta!} K_\beta(x) \partial_k^\beta \delta(k-\partial_x S(x)), \tag{27}$$

controlled by the small parameter $\tilde{\epsilon} \equiv |k(x)\tilde{w}|^{-1} \ll 1$. It is worth noting that $f(x,k-\partial_x S(x))$ is thus represented by a distribution which is point supported on the Lagrangian manifold $k=\partial_x S(x)$ and completely determined by its statistical moments $K_\beta(x)$.

In correspondence of the asymptotic expansion (27), Eq. (24a) reduces to

$$\sum_{\alpha} \frac{1}{\alpha!} \partial_k^\alpha D'(x,\partial_x S(x)) K_{\alpha+\beta}(x) = 0, \tag{28}$$

as shown in details in the Appendix, cf., in particular, Eq. (A5). Formally, Eq. (28) constitutes an infinite set of algebraic equations for the statistical moments $K_\alpha(x)$ characterizing the momentum distribution, where each equation, labelled by β, is expressed as an asymptotic series in $\tilde{\epsilon}$; the function $S(x)$ is determined by imposing that the system (28) admits nontrivial solutions. Equations (28) are valid for a general momentum distribution f which satisfies (24a). In particular, on setting $K_\alpha(x)=0$ for $\alpha \neq 0$, Eq. (27) reduces to

$$f(x,k-\partial_x S(x)) = (2\pi)^N \delta(k-\partial_x S(x)),$$

which is the geometrical-optics-like solution obtained by Bornatici and Kravtsov[23] and by Sparber, Markowich and Mauser,[24] whereas in (28) the only nontrivial equation reduces to the geometrical optics eikonal equation[5] for $S(x)$, namely, $D'(x,\partial_x S(x))=0$.

IV. THE CGO-LIKE SOLUTION OF THE WAVE KINETIC EQUATION

On the basis of the asymptotic expansion (27) for a momentum distribution, one can prove the main result of this paper, that is, relating the wave kinetic equation to the CGO equations for suitable boundary conditions.

First let us consider the specific momentum distribution for which

$$K_\alpha(x) = \begin{cases} 0, & \text{for } |\alpha| = 2n+1 (\text{odd}), \\ (-1)^n (k''(x))^\alpha, & \text{for } |\alpha| = 2n \text{ (even)}, \end{cases} \tag{29}$$

that is, odd-order moments have been set to zero, whereas even-order moments have been related to a single vector field $k''(x)=\partial_x \phi(x)$, with ϕ an unknown smooth function. Correspondingly, the momentum distribution (27) takes the form

$$f(x,k-\partial_x S(x)) \sim \sum_{|\beta|=\text{even}} \frac{(-1)^{|\beta|/2}}{\beta!} (k''(x))^\beta \partial_k^\beta \delta(k-\partial_x S(x)) = \sum_{n=0}^{+\infty} \frac{(-1)^n}{(2n)!} \left[k_i''(x) \frac{\partial}{\partial k_i} \right]^{2n} \delta(k-\partial_x S(x)), \tag{30}$$

the second identity being obtained by means of the multinomial formula

$$\sum_{|\beta|=n} \frac{1}{\beta!} a_1^{\beta_1} \cdots a_N^{\beta_N} = \frac{1}{n!}(a_1 + \cdots + a_N)^n, \tag{31}$$

with $a_i = k_i'' \partial / \partial k_i$ (no sum over i). Let us note that the momentum distribution (30) is symmetric with respect to the Lagrangian manifold $k = \partial_x S(x)$, as even-order moments only appear; in particular, the second order moment $-k_i''(x)k_j''(x)$ for $i=j$ is negative, so that such a distribution cannot be interpreted as a probability measure.

The momentum distribution (30) should be multiplied by $|\psi(x)|^2$ to get the whole Wigner function (25). Let us consider the case for which

$$|\psi(x)|^2 = |u(x)|^2 e^{-2\phi(x)}, \tag{32}$$

$\phi(x)$ being defined in (29) and $|u(x)|^2$ is ordered according to $|\partial_x u| \sim |u|/L$ with $L \gg \tilde{w} \sim |\partial_x \phi|^{-1}$. As a consequence, $\tilde{w}$ is the shortest scale length characterizing the wavefield intensity $|\psi(x)|^2$, hence it can be identified with the scale length w defined after Eq. (13), namely, $\tilde{w} \sim w$ and $\tilde{\epsilon} \sim \epsilon$.

Then one has the following:

The Wigner function $W(x,k) = (2\pi)^N f(x, k - \partial_x S(x))|\psi(x)|^2$, *with* f *given by (30) and* $|\psi(x)|^2$ *expressed in the form (32), satisfies asymptotically the wave kinetic equation in the weak formulation (24) with an* $O(\epsilon)$ *remainder if and only if*

(i) *the smooth functions* $S(x)$ *and* $\phi(x)$ *satisfy the complex geometrical optics equations (15a) and (15b), and*

(ii) the smooth slowly varying function $|u(x)|^2$ *satisfies the transport equation (15c).*

First, let us prove the statement (*i*). In view of the ansatz (29), all the equations obtained from (28) with β such that $|\beta|$ is an even integer reduce to the same equation which reads

$$\sum_{|\alpha|=\text{even}} \frac{(-1)^{|\alpha|/2}}{\alpha!} \partial_k^\alpha D'(x,k(x))(k''(x))^\alpha = \sum_{n=0}^{+\infty} \frac{(-1)^n}{(2n)!} \left[k_i''(x) \frac{\partial}{\partial k_i} \right]^{2n} D'(x,k(x)) = 0, \tag{33a}$$

and, analogously, all the equations obtained from (28) with β such that $|\beta|$ is an odd integer reduce to

$$\sum_{|\alpha|=\text{odd}} \frac{(-1)^{(|\alpha|+1)/2}}{\alpha!} \partial_k^\alpha D'(x,k(x))(k''(x))^\alpha = \sum_{n=0}^{+\infty} \frac{(-1)^{n+1}}{(2n+1)!} \left[k_i''(x) \frac{\partial}{\partial k_i} \right]^{2n+1} D'(x,k(x)) = 0, \tag{33b}$$

where the second identity in both equations (33) follows on using the multinomial formula (31). Equations (33) constitute a set of two coupled equations for the real functions $S(x)$ and $\phi(x)$, and, to lowest significant orders in ϵ, they are the same as the CGO equations (15a) and (15b); this completes the proof of (*i*).

As for (*ii*), on account of the differential calculus for momentum distributions put forward in Sec. III, the term connected with the Poisson brackets in Eq. (24b) should be written in the form, cf. Eq. (23),

$$\int \frac{d^N k}{(2\pi)^N} \{W, D'\} A = \frac{\partial}{\partial x^i} \int \frac{d^N k}{(2\pi)^N} W \frac{\partial D'}{\partial k_i} A - \int \frac{d^N k}{(2\pi)^N} W \frac{\partial}{\partial x^i} \left(\frac{\partial D'}{\partial k_i} A \right) - \int \frac{d^N k}{(2\pi)^N} \frac{\partial W}{\partial k_i} \frac{\partial D'}{\partial x^i} A. \tag{34}$$

Using the specific momentum distribution (30) for which

$$W(x,k) = (2\pi)^N \delta(k - \partial_x S(x))|\psi(x)|^2 + O(\epsilon^2) \tag{35}$$

yields

$$\int \frac{d^N k}{(2\pi)^N}\{W,D'\}A = \frac{\partial}{\partial x^i}\left[\frac{\partial D'(x,k(x))}{\partial k_i}|\psi(x)|^2 A(x,k(x))\right] - \left[\frac{\partial D'(x,k(x))}{\partial k_i}\frac{\partial A(x,k(x))}{\partial x^i} - \frac{\partial D'(x,k(x))}{\partial x^i}\frac{\partial A(x,k(x))}{\partial k_i}\right]|\psi(x)|^2 + O(\epsilon^2)$$
$$= \frac{\partial}{\partial x^i}\left[\frac{\partial D'(x,k(x))}{\partial k_i}|\psi(x)|^2\right]A(x,k(x)) + O(\epsilon). \tag{36}$$

The last identity follows on noting that taking the derivative of (33a) with respect to x^j yields

$$\frac{\partial D'(x,\,k(x))}{\partial k_i}\frac{\partial k_j(x)}{\partial x^i} = \frac{\partial D'(x,\,k(x))}{\partial k_i}\frac{\partial k_i(x)}{\partial x^j} = -\frac{\partial D'(x,\,k(x))}{\partial x^j} + O(\epsilon)$$

with $k_j(x) = \partial S(x)/\partial x^j$. Equation (36) implies that

$$\{W,D'\} = (2\pi)^N \frac{\partial}{\partial x^i}\left[\frac{\partial D'(x,k(x))}{\partial k_i}|\psi(x)|^2\right]\delta(k - \partial_x S(x)) + O(\epsilon)$$

in the weak sense. Hence, from the wave kinetic equation, to lowest order in ϵ, one gets the transport equation

$$\frac{\partial}{\partial x^i}\left[\frac{\partial D'(x,k(x))}{\partial k_i}|\psi(x)|^2\right] = 2D''(x,k(x))|\psi(x)|^2,$$

which reduces to the CGO transport equation (15c) for $|u(x)|^2$, cf. Eq. (32), on noting that, to lowest significant order,

$$\frac{\partial}{\partial x^i}\left[\frac{\partial D'(x,k(x))}{\partial k_i}|u(x)|^2 e^{-2\phi(x)}\right] = e^{-2\phi(x)}\frac{\partial}{\partial x^i}\left[\frac{\partial D'(x,k(x))}{\partial k_i}|u(x)|^2\right],$$

in view of Eq. (33b). This concludes the proof.

The foregoing result shows that there exists a specific form of the Wigner function for which the wave kinetic equation is reduced to the CGO equations.

In order to compare the wavefield intensities predicted by the wave kinetic description with that obtained on solving the CGO equations, one should complete the foregoing argument by discussing Cauchy boundary conditions. With reference to (10) and (11) one has the following:

Let $W(x,k)$ be the weak solution of the wave kinetic equation (8) corresponding to the Cauchy boundary conditions

$$W|_\Sigma(\mathbf{x},\mathbf{k},k_N) = (2\pi)^N \delta(\mathbf{k} - \mathbf{k}(\mathbf{x}))\,\delta(k_N - H(\mathbf{x},\mathbf{k}(\mathbf{x})))|u_0(\mathbf{x})|^2 e^{-2\phi_0(\mathbf{x})} + O(\epsilon), \tag{37}$$

for some smooth functions $S_0(\mathbf{x})$, $\phi_0(\mathbf{x}) \geqslant 0$, and $|u_0(\mathbf{x})|^2$ with $\mathbf{k}(\mathbf{x}) = \partial_{\mathbf{x}} S_0(\mathbf{x})$ satisfying the CGO ordering defined after (16), and let $S(x)$, $\phi(x)$, and $|u(x)|^2$ be solution of the CGO equations (15) with Cauchy boundary conditions given by the same function S_0, ϕ_0, and $|u_0|^2$. Then $W(x,k)$ can be approximated according to

$$W(x,k) = (2\pi)^N \delta(k - \partial_x S(x))|u(x)|^2 e^{-2\phi(x)} + O(\epsilon) \tag{38}$$

in the weak sense of Sec. III.

First, let us note that the Cauchy data (37) is a particular case of (10b) which corresponds to

$$W_0(\mathbf{x},\mathbf{k}) = (2\pi)^{N-1}\delta(\mathbf{k} - \partial_{\mathbf{x}}S_0(\mathbf{x}))|u_0(\mathbf{x})|^2 e^{-2\phi_0(\mathbf{x})} + O(\epsilon); \tag{39}$$

in particular, the Wigner function corresponding to the complex-eikonal wave object (16) can be written in the form (39).

In order to prove the foregoing statement, we will make use of the previous result of this section. Specifically, we have proved that the Wigner function

$$\tilde{W}(x,k) = (2\pi)^N f(x,k - \partial_x S(x))|u(x)|^2 e^{-2\phi(x)},$$

f being the momentum distribution (30), solves asymptotically the wave kinetic equation in the weak sense within an $O(\epsilon)$ accuracy. Moreover,

$$\tilde{W}(x,k) = (2\pi)^N \delta(k - \partial_x S(x))|u(x)|^2 e^{-2\phi(x)} + O(\epsilon^2),$$

in view of (35). As for the boundary condition (37) one gets

$$\begin{aligned}\tilde{W}|_{\Sigma}(\mathbf{x},\mathbf{k},k_N) &= (2\pi)^N \delta(\mathbf{k} - \partial_{\mathbf{x}}S(\mathbf{x},0))\,\delta(k_N - \partial_{x^N}S(\mathbf{x},0))|u(\mathbf{x},0)|^2 e^{-2\phi(\mathbf{x},0)} + O(\epsilon^2)\\ &= (2\pi)^N \delta(\mathbf{k} - \partial_{\mathbf{x}}S_0(\mathbf{x}))\,\delta(k_N - k_N(\mathbf{x}))|u_0(\mathbf{x})|^2 e^{-2\phi_0(\mathbf{x})} + O(\epsilon^2),\end{aligned}$$

where $k_N(\mathbf{x}) = \partial_{\mathbf{x}}S(\mathbf{x},0)$. According to (18), $k_N(\mathbf{x}) = H(\mathbf{x},\mathbf{k}(\mathbf{x})) + O(\epsilon^2)$, and, thus, $\delta(k_N - k_N(\mathbf{x})) = \delta(k_N - H(\mathbf{x},\mathbf{k}(\mathbf{x}))) + O(\epsilon^2)$ in the weak sense, so that $\tilde{W}(x,k)$ matches the boundary conditions (37). Since the solution of the wave kinetic equation along with the Cauchy boundary condition (37) is unique and since $\tilde{W}$ is an $O(\epsilon)$ solution, it follows that

$$W(x,k) = \tilde{W}(x,k) + O(\epsilon),$$

which concludes the proof of (38).

This implies that, whenever the solutions of both the wave kinetic equation and the CGO equations exist, thus, in particular, the Cauchy boundary conditions are of the form (39), the Wigner-Weyl formalism and the complex geometrical optics method are equivalent within an $O(\epsilon)$ accuracy. In particular, the wavefield intensity predicted by the Wigner-Weyl kinetic formalism is the same as that predicted by the CGO method, namely,

$$|\psi(x)|^2 = \int \frac{d^N k}{(2\pi)^N} W(x,k) = |u(x)|^2 e^{-2\phi(x)} + O(\epsilon), \tag{40}$$

the second identity following from (38). In the next section, an analytically tractable case is considered as an example. Specifically, the solution of the wave kinetic equation relevant to the paraxial propagation of a Gaussian wave beam in a "lens-like" medium is obtained and shown to be the same as the corresponding CGO solution.

V. THE KINETIC DESCRIPTION OF DIFFRACTION EFFECTS FOR A "LENS-LIKE" MEDIUM AND ITS ANALOGY WITH THE QUANTUM HARMONIC OSCILLATOR

Let us address the case of a monochromatic ($e^{-i\omega t}$) beam of electromagnetic waves propagating in a *lossless* "lens-like" medium[25] with *real* refractive index $n(\mathbf{r},\omega) \equiv n(x) = n_0[1 - (x/L)]^{1/2}$. It is assumed that the wavefield is localized near the axis $x=0$ of the medium, that is, $(x/L) \ll 1$; moreover, the wave electric field is written in the form $\mathbf{E}(\mathbf{r},\omega) = \hat{\mathbf{y}}E(x,z;\omega)$, i.e., it is polarized along the y axis and propagates in the x-z plane. The relevant wave equation for the wavefield real amplitude $E(x,z;\omega)$ is thus the Helmholtz equation. The corresponding Weyl symbol is real valued and given by

$$D(x,k_x,k_z) = -(k_x^2+k_z^2) + \frac{\omega^2}{c^2}n^2(x) = -(k_x^2+k_z^2) + \frac{\omega^2}{c^2}n_0^2[1-(x/L)^2], \tag{41}$$

thus, the dispersion relation $D=0$ yields two branches, to be referred to as the progressive and the regressive waves. As for the Cauchy boundary conditions, let us assume that the wavefield is purely Gaussian at $z=0$, i.e., $E(x,0;\omega)=u_0\exp[-(x-x_0)^2/w_0^2]$, w_0 being the initial width, and the propagation occurs along the z axis, so that one should solve the dispersion relation $D=0$ for k_z. On assuming that each branch of the dispersion relation carries half of the wavefield intensity, one can consider the progressive wave only which reads

$$\frac{k_z}{k_0} = \sqrt{1-\left(\frac{x}{L}\right)^2 - \left(\frac{k_x}{k_0}\right)^2} \simeq 1 - \frac{1}{2}\left(\frac{x}{L}\right)^2 - \frac{1}{2}\left(\frac{k_x}{k_0}\right)^2 \tag{42}$$

where $k_0=\omega n_0/c$ is the wavevector at $x=0$ and the paraxial approximation $(k_x/k_0)^2 \sim (x/L)^2 \sim (w/L)^2 \sim \lambda/L \ll 1$ has been exploited as relevant to the weak-diffraction regime.[25] It is convenient noting that the dispersion relation corresponding to the second form of (42) can be written as

$$\frac{1}{k_0}(k_0-k_z) - \frac{1}{2}\left(\frac{k_x}{k_0}\right)^2 - \frac{1}{2}\left(\frac{x}{L}\right)^2 = 0, \tag{43}$$

which is formally analogous to the dispersion relation relevant to a quantum harmonic oscillator[13] with unit mass and $1/k_0 \to \hbar$, $1/L \to \omega_0$, ω_0 being the characteristic frequency of the oscillator, $z \to t$, and $k_0-k_z(>0) \to \omega$. In particular, the frequency ω corresponds to the shifted wavevector k_0-k_z along the propagation direction z. The shift occurs because of the oscillations of the wavefield along the propagation direction z.

This analogy allows to make use of the well-known solution of the wave kinetic equation for the quantum harmonic oscillator[13] to describe the paraxial propagation of a Gaussian beam in the "lens-like" medium. More specifically, the solution of the wave kinetic equation for the harmonic oscillator corresponding to an initially Gaussian wave packet $\psi(x,0)=(w_0\sqrt{\pi/2})^{-1/2}\exp[-(x-x_0)^2/w_0^2]$ is[13]

$$|\psi(x,t)|^2 = \sqrt{\frac{2}{\pi w(t)^2}}\exp\left(-2\frac{(x-x_0\cos(\omega_0 t))^2}{w(t)^2}\right), \tag{44a}$$

$$w^2(t) = [\cos^2(\omega_0 t) + \varepsilon^2\sin^2(\omega_0 t)]w_0^2, \tag{44b}$$

where $w(t)$ is the width of the wave packet as a function of time and $\varepsilon=2\hbar/m\omega_0 w_0^2$, m being the mass of the oscillator and x_0 the initial displacement of the Gaussian from the center of the elastic force acting on the oscillator.

Correspondingly, the solution for the wave electric field intensity in the "lens-like" medium, with the considered launching conditions, is

$$\langle|\mathbf{E}(x,z;\omega)|^2\rangle = u_0^2\frac{w_0}{w(z)}\exp\left(-2\frac{(x-x_0\cos(z/L))^2}{w(z)^2}\right), \tag{45a}$$

$$w^2(z) = \left[\cos^2(z/L) + \left(\frac{2L}{k_0 w_0^2}\right)^2\sin^2(z/L)\right]w_0^2 = \left[1+\left(\left(\frac{L}{z_R}\right)^2-1\right)\sin^2(z/L)\right]w_0^2, \tag{45b}$$

with $z_R=k_0w_0^2/2$ the Rayleigh range in the medium. In Eq. (45b), it has been explicitly indicated that the solution obtained from the wave kinetic equation amounts to the averaged intensity $\langle|\mathbf{E}(x,z;\omega)^2\rangle$, rather than to the exact value $|\mathbf{E}(x,z;\omega)|^2$ since two branches of the dispersion relation exist, each one carrying half of the wavefield intensity, cf. comments after Eqs. (12). The intensity (45a) and the beam width (45b) are the same as the corresponding quantities obtained

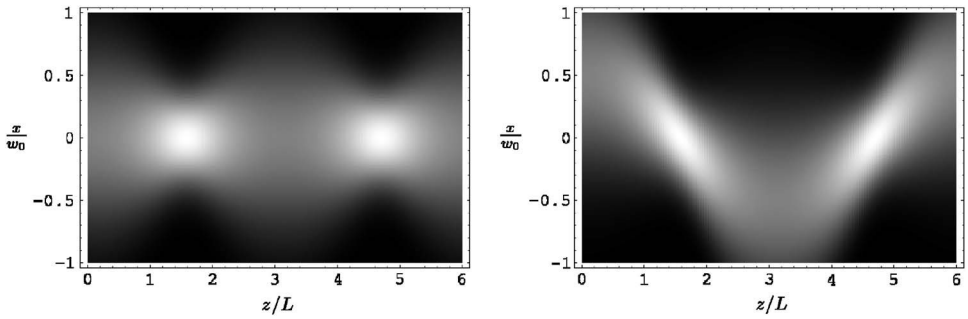

FIG. 1. The wavefield intensity (45) in the (x,z)-plane as obtained from the wave kinetic equations (8) (bright regions correspond to high intensity), for the case $L/z_R=0.5$ [cf. Eq. (45b)] with $x_0=0$ and $x_0=\frac{1}{2}w_0$, respectively. One should note that the wave beam exhibits a finite width even near focal points (characterized by bright spots) where the geometrical optics solution exhibits caustic singularities.

from the CGO solution.[25] As a consequence the intensity profile (45) accounts for diffraction effects as shown in Fig. 1.

One can conclude that, according to results of Sec. IV, the *kinetic formalism can be used to describe the effects of diffraction on the propagation of wave beams*, and, for the case under consideration, it yields the same result as the CGO method. Nevertheless, the detailed structure of the wavefield, i.e., the oscillations along the propagation direction z, the effects of the curvature of phase fronts and the Gouy shift, which are available from the CGO solution,[25] *cannot be resolved by means of the wave kinetic equation*, which instead gives the averaged intensity distribution.

VI. CONCLUSIONS

Within the framework of semiclassical wave propagation, two specific asymptotic techniques have been considered, namely, the Wigner-Weyl kinetic formalism and the complex geometrical optics (CGO) method. A detailed comparative analysis of these techniques has been given in Sec. II, for the case of scalar pseudodifferential wave equations, with Cauchy boundary conditions.

In particular, in the Wigner-Weyl formalism, the wavefield is represented in the phase space by the Wigner function which is a solution to the wave kinetic equation. In the most general case the Wigner function amounts to a tempered distribution. However, physical considerations lead to the definition of a novel class of weak solutions which have been characterized in Sec. III. Such specific weak solutions are referred to as *momentum distributions* since, for every point location x in the configuration space, they give the distribution of momentum k over x, in the x-k phase space.

On the other hand, the CGO method yields an asymptotics solution of a pseudodifferential wave equation directly in the configuration space, in terms of three smoothly varying functions representing, the phase, the wavefield envelope, and the amplitude, respectively.

In Sec. IV, on the basis of the mathematical framework developed in Sec. III, we have proved that, whenever both the solutions of the wave kinetic equation and of the CGO equations exist, thus, in particular, the Cauchy data are of the form (39), the former can be approximated by a momentum distribution, cf. Eq. (38), written in terms of the three smoothly varying functions that solve the CGO equations (15). As a consequence, the two considered techniques are asymptotically equivalent and, in particular, to lowest significant order, the wavefield intensity predicted by the Wigner-Weyl formalism is the same as that predicted by the CGO method, cf. Eq. (40).

In addition, one can conclude that the Wigner-Weyl kinetic formalism properly describes the wavefield near focal points. This is also shown by comparing the solution of the kinetic equation to that of the CGO equations for a specific case, namely, the propagation of electromagnetic Gaussian wave beams in an isotropic "lens-like" medium, cf. Sec. V. In particular, the relevant solution of the wave kinetic equation has been obtained on the basis of the analogy between the "lens-like" medium and the quantum harmonic oscillator.

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APPENDIX: THE ASYMPTOTIC SERIES EXPANSION OF THE MOMENTUM DISTRIBUTION

In this appendix the asymptotic series expansion (27) of the momentum distribution is proved and the corresponding equations (28) are derived from the weak form (24a) of the dispersion relationship (8a).

Since both $D'(x,k)$ and $A(x,k)$ are symbols, they are, in particular, smooth functions, and one can apply the Taylor's formula

$$\begin{bmatrix} D' \\ A \end{bmatrix}(x,k(x)+\tilde{k}) = \sum_{|\alpha|\leqslant n-1} \frac{1}{\alpha!}\begin{bmatrix} \partial_k^\alpha D' \\ \partial_k^\alpha A \end{bmatrix}(x,k(x))\tilde{k}^\alpha + \sum_{|\alpha|=n}\begin{bmatrix} d_\alpha(x,\tilde{k}) \\ a_\alpha(x,\tilde{k}) \end{bmatrix}\tilde{k}^\alpha, \tag{A1}$$

$\alpha=(\alpha_1,\ldots,\alpha_N)$ being an N-dimensional multi-index and

$$\begin{bmatrix} d_\alpha(x,\tilde{k}) \\ a_\alpha(x,\tilde{k}) \end{bmatrix} = \frac{|\alpha|}{\alpha!}\int_0^1 dt(1-t)^{n-1}\begin{bmatrix} \partial_k^\alpha D' \\ \partial_k^\alpha A \end{bmatrix}(x,(1-t)k(x)+t\tilde{k})$$

the remainder of order n relevant to the expansions of D' and A, respectively. More specifically, on making use of (A1) to evaluate the left-hand side of (24a), one gets

$$\int f(x,\tilde{k})D'(x,k(x)+\tilde{k})A(x,k(x)+\tilde{k})d^N\tilde{k} \sim \sum_{\alpha,\beta}\frac{1}{\alpha!\beta!}\partial_k^\alpha D'(x,k(x))\partial_k^\beta A(x,k(x))K_{\alpha+\beta}(x), \tag{A2}$$

where $K_\alpha(x)=O(\tilde{w}^{-|\alpha|})$ are the statistical moments of the momentum distribution $f(x,\tilde{k})$, cf. Eq. (26). By virtue of the symbol estimate (2), symbols are such that, e.g., $|\partial_k^\alpha A(x,k)|=O(|k|^{m-|\alpha|})$ in the semiclassical limit $|k|\to+\infty$ uniformly in x, hence, the asymptotic series expansion (A2) is controlled by the (small) parameter $\tilde{\epsilon}\equiv|k(x)\tilde{w}|^{-1}$. Moreover, on noting that

$$\partial_k^\beta A(x,k(x)) = (-1)^{|\beta|}\int \partial_k^\beta\delta(k-k(x))A(x,k)d^Nk,$$

Eq. (A2) takes the form

$$\int D'(x,k)f(x,k-k(x))A(x,k)d^Nk \sim \int\left[\sum_{\alpha,\beta}\frac{(-1)^{|\beta|}}{\alpha!\beta!}\partial_k^\alpha D'(x,k(x))K_{\alpha+\beta}(x)\partial_k^\beta\delta(k-k(x))\right]A(x,k)d^Nk$$

and, in view of the arbitrariness of $A(x,k)$, one gets

$$D'(x,k)f(x,k-k(x)) \sim \sum_{\alpha,\beta}\frac{(-1)^{|\beta|}}{\alpha!\beta!}\partial_k^\alpha D'(x,k(x))K_{\alpha+\beta}(x)\partial_k^\beta\delta(k-k(x)), \tag{A3}$$

in the weak sense. It is worth noting that the derivation of (A3) does not depend on the explicit form of the symbol $D'(x,k)$, thus, on setting $D'(x,k)=1$, Eq. (A3) reduces to

$$f(x,k-k(x)) \sim \sum_{\beta} \frac{(-1)^{|\beta|}}{\beta!} K_{\beta}(x) \partial_k^{\beta} \delta(k-k(x)), \tag{A4}$$

which is just the general asymptotic expansion (27) of the momentum distribution.

Going back to Eq. (24a), its solution is obtained on setting the expansion (A3) to zero and exploiting the linear independence of the derivatives of the Dirac's δ function, thus yielding a set of equations for the statistical moments, namely,

$$\sum_{\alpha} \frac{1}{\alpha!} \partial_k^{\alpha} D'(x,k(x)) K_{\alpha+\beta}(x) = 0, \tag{A5}$$

which is just Eq. (28). It is worth noting that Eq. (A5) can be also obtained on substituting (A4) into (24a) and exploiting the Leibniz's formula

$$\partial_k^{\beta}(D'A) = \sum_{\alpha+\gamma=\beta} \frac{\beta!}{\alpha!\gamma!} \partial_k^{\alpha} D' \partial_k^{\gamma} A,$$

which expresses the derivative of a product to any orders.

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Combinatorial approach to generalized Bell and Stirling numbers and boson normal ordering problem

M. A. Méndez[a)]
IVIC, Lab. Anal. Mat.-Matemáticas, Carretera Panamericana, Km.11, Caracas, Venezuela and UCV, Dpto. de Matemáticas, Facultad de Ciencias, Caracas, Venezuela

P. Blasiak[b)]
Laboratoire de Physique Théorique de la Matière Condensée, Université Pierre et Marie Curie, CNRS UMR 7600, Tour 24 - 2ème ét., 4 pl. Jussieu, F 75252 Paris Cedex 05, France and H. Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences, ul. Eliasza-Radzikowskiego 152, PL 31342 Kraków, Poland

K. A. Penson[c)]
Laboratoire de Physique Théorique de la Matière Condensée, Université Pierre et Marie Curie, CNRS UMR 7600, Tour 24 - 2ème ét., 4 pl. Jussieu, F 75252 Paris Cedex 05, France

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We consider the numbers arising in the problem of normal ordering of expressions in boson creation $a^\dagger$ and annihilation a operators ($[a,a^\dagger]=1$). We treat a general form of a boson string $(a^\dagger)^{r_n}a^{s_n}\ldots(a^\dagger)^{r_2}a^{s_2}(a^\dagger)^{r_1}a^{s_1}$ which is shown to be associated with generalizations of Stirling and Bell numbers. The recurrence relations and closed-form expressions (Dobiński-type formulas) are obtained for these quantities by both algebraic and combinatorial methods. By extensive use of methods of combinatorial analysis we prove the equivalence of the aforementioned problem to the enumeration of special families of graphs. This link provides a combinatorial interpretation of the numbers arising in this normal ordering problem. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1990120]

I. INTRODUCTION

In this article we consider a pair of boson creation $a^\dagger$ and annihilation a operators satisfying the commutation relation

$$[a,a^\dagger]=1. \tag{1}$$

These operators play a fundamental role in the formalism of second quantization in quantum mechanics and quantum field theory (QFT).[1–3] Because the creation and annihilation operators do not commute there are certain problems with their ordering. A very convenient and well defined form of the operators depending on a and $a^\dagger$ is the so-called normally ordered form.[4] An operator is said to be in a normally ordered form if all creation operators stand to the left of the annihilation operators. The most important application field of the normal order is the QFT.[3] For a recent study of the interplay of the QFT, normal order, and combinatorics see Ref. 5. Procedure of normal ordering of the operator, i.e., moving all the creation operators to the left with the use of relation (1), is in general a nontrivial task. A first example is ordering of the power of the number operator:[6,7]

[a)]Electronic mail: mmendez@cauchy.ivic.ve
[b)]Electronic mail: Pawel.Blasiak@ifj.edu.pl
[c)]Electronic mail: penson@lptl.jussieu.fr

$$(a^\dagger a)^n = \sum_{k=1}^{n} S(n,k)(a^\dagger)^k a^k, \tag{2}$$

where $S(n,k)$ are the Stirling numbers of the second kind[8] enumerating partitions of the set of n elements into k nonempty subsets, and satisfying the following recurrence relation: $S(n+1,k) = S(n,k-1)+kS(n,k)$ with initial values $S(n,n)=S(n,1)=1$.

As the extension of this result we have considered operators in the form $(a^\dagger)^r a^s$ (r, s positive integers, $r \geqslant s$), for which a normally ordered form is given by

$$[(a^\dagger)^r a^s]^n = (a^\dagger)^{n(r-s)} \sum_{k=s}^{ns} S_{r,s}(n,k)(a^\dagger)^k a^k, \tag{3}$$

where $S_{r,s}(n,k)$ are generalized Stirling numbers.[9–14] These kinds of formulas allow one to write the exponentials $e^{\lambda(a^\dagger)^r a^s}$ in the normally ordered form and then easily calculate the coherent state expectation values which are of importance, e.g., in quantum optics.[4] The clue to these calculations is the knowledge of the properties of the numbers $S_{r,s}(n,k)$. As they are of a combinatorial origin, the recurrence relations, Dobiński-type formulas, closed-form expresions and generating functions were extensively studied.[10] In the following we further extend these results to normal ordering of a general *boson string* in the form $(a^\dagger)^{r_n} a^{s_n} \ldots (a^\dagger)^{r_2} a^{s_2} (a^\dagger)^{r_1} a^{s_1}$, by establishing a link to special structures in enumerative combinatorics. This in turn gives us the rigorous demonstration of the properties of the generalized Stirling and Bell numbers arising in this problem. The construction of the graphs (the so called "bugs") associated with these numbers provides a graphical interpretation of the normal ordering procedure.

II. GENERALIZED BELL AND STIRLING NUMBERS

In this section we define the generalization of ordinary Bell and Stirling numbers which arise in the solution of the normal ordering problem for a boson string. Given two sequences of positive integers $\mathbf{r}=(r_1, r_2, \ldots, r_n)$ and $\mathbf{s}=(s_1, s_2, \ldots, s_n)$ we let $S_{\mathbf{r},\mathbf{s}}(k)$ be the positive integers appearing in

$$(a^\dagger)^{r_n} a^{s_n} \ldots (a^\dagger)^{r_2} a^{s_2} (a^\dagger)^{r_1} a^{s_1} = (a^\dagger)^{d_n} \sum_{k=s_1}^{s_1+s_2+\ldots+s_n} S_{\mathbf{r},\mathbf{s}}(k)(a^\dagger)^k a^k, \tag{4}$$

where $d_n = \sum_{i=1}^{n}(r_i - s_i)$, which we assume here to be nonnegative. We observe that the whole theory can be carried through for d_n negative, at the cost of minor adaptations, which however do not change the numbers involved. Note that the r.h.s. of Eq. (4) is already normally ordered.

We call $S_{\mathbf{r},\mathbf{s}}(k)$ the generalized Stirling numbers of the second kind. The generalized Bell number is defined as the sum

$$B_{\mathbf{r},\mathbf{s}} = \sum_{k=s_1}^{s_1+s_2+\ldots+s_n} S_{\mathbf{r},\mathbf{s}}(k). \tag{5}$$

In this notation the generalized Stirling numbers defined in Eq. (3) correspond to a *uniform* case

$$\mathbf{r} = \overbrace{(r, r, \ldots, r)}^{n} \text{ and } \mathbf{s} = \overbrace{(s, s, \ldots, s)}^{n}.$$

We introduce the notation $\mathbf{r} \uplus r_{n+1} = (r_1, r_2, \ldots, r_n, r_{n+1})$ and $\mathbf{s} \uplus s_{n+1} = (s_1, s_2, \ldots, s_n, s_{n+1})$ and state the recurrence relation satisfied by generalized Stirling numbers $S_{\mathbf{r},\mathbf{s}}(k)$

$$S_{\mathbf{r}\uplus r_{n+1},\mathbf{s}\uplus s_{n+1}}(k) = \sum_{j=0}^{s_{n+1}} \binom{s_{n+1}}{j} (d_n + k - j)_{s_{n+1}-j} S_{\mathbf{r},\mathbf{s}}(k-j), \tag{6}$$

where $(l)_p = l\cdot(l-1)\cdot \ldots \cdot(l-p+1)$ is the falling factorial.

One can give the derivation of Eq. (6) by induction using the following consequence of Eq. (1) (see the proof in Ref. 2):

$$a^k(a^\dagger)^l = \sum_{p=0}^{k} \binom{k}{p} (l)_p (a^\dagger)^{l-p} a^{k-p}. \tag{7}$$

The full details of this approach can be consulted in Ref. 14.

Observe that the problem stated previously can also be formulated in terms of the multiplication X and derivative D operators as they satisfy $[D,X]=1$. The representation of boson commutation relation with the D and X operators resembles the Bargmann representation,[4] used in connection with coherent states. (Here we do not enter into that framework, with all the intricacies of the scalar product, hermiticity, etc., as in our context only the algebraic properties matter.) Then Eq. (4) can be rewritten as

$$X^{r_n} D^{s_n} \ldots X^{r_2} D^{s_2} X^{r_1} D^{s_1} = X^{d_n} \sum_{k=s_1}^{s_1+s_2+\ldots+s_n} S_{\mathbf{r},\mathbf{s}}(k) X^k D^k. \tag{8}$$

Acting with both sides of Eq. (8) on the exponential function e^x we get the identity

$$X^{r_n} D^{s_n} \ldots X^{r_2} D^{s_2} X^{r_1} D^{s_1} e^x = x^{d_n} e^x B_{\mathbf{r},\mathbf{s}}(x), \tag{9}$$

where

$$B_{\mathbf{r},\mathbf{s}}(x) = \sum_{k=s_1}^{s_1+s_2+\ldots+s_n} S_{\mathbf{r},\mathbf{s}}(k) x^k \tag{10}$$

is the so-called generalized Bell polynomial. Observe that the order of the so-defined generalized Bell polynomial does not depend on $\mathbf{r}$. Equation (9) gives the formula

$$X^{d_{n+1}} e^x B_{\mathbf{r} \uplus r_{n+1}, \mathbf{s} \uplus s_{n+1}}(x) = X^{r_{n+1}} D^{s_{n+1}} e^x x^{d_n} B_{\mathbf{r},\mathbf{s}}(x). \tag{11}$$

Using the well known commutation rule (equivalent to the Leibniz rule) $D^n e^x f(x) = e^x (D+I)^n f(x)$ we get the recursive formula

$$B_{\mathbf{r} \uplus r_{n+1}, \mathbf{s} \uplus s_{n+1}}(x) = X^{s_{n+1}-d_n} (D+I)^{s_{n+1}} X^{d_n} B_{\mathbf{r},\mathbf{s}}(x). \tag{12}$$

By taking coefficients of x^k on both sides of Eq. (12) we obtain the recurrence relation for the generalized Stirling numbers of Eq. (6).

Observe that the action of the left-hand-side (l.h.s.) of Eq. (8) on e^x may be calculated explicitly. To this end one first evaluates it on the monomial x^n yielding $[\Pi_{j=1}^{n} (d_{j-1}+n)_{s_j}] x^{n+d_n}$ which in turn easily gives the result of the action on the exponential function e^x.

With this observation, together with Eq. (9) we arrive at the extended Dobiński-type relation for generalized Bell polynomials

$$B_{\mathbf{r},\mathbf{s}}(x) = e^{-x} \sum_{m=s_1}^{\infty} \left[\prod_{j=1}^{n} (m + d_{j-1})_{s_j} \right] \frac{x^m}{m!}, \tag{13}$$

which by Cauchy's multiplication of series yields the expression for $S_{\mathbf{r},\mathbf{s}}(k)$:

$$S_{\mathbf{r},\mathbf{s}}(k) = \frac{1}{k!} \sum_{m=0}^{k} \binom{k}{m} (-1)^{k-m} \cdot \prod_{j=1}^{n} (m + d_{j-1})_{s_j}. \tag{14}$$

An alternative, very similar demonstration of the previous results can be carried through with the use of coherent states. These are defined for complex z, as $|z\rangle = e^{-|z|^2/2} \Sigma_{n=0}^{\infty} (z^n / \sqrt{n!}) |n\rangle$, where

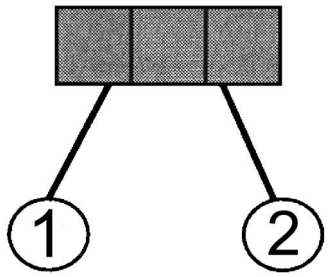

FIG. 1. A (3, 2)-bug.

$a^\dagger a|n\rangle = n|n\rangle$, $a|z\rangle = z|z\rangle$, and $\langle n|n'\rangle = \delta_{n,n'}$.[4] The $|n\rangle$'s are called the number states. The coherent state matrix element of Eq. (4) establishes a link to generalized Bell polynomials of Eq. (10):

$$\langle z|(a^\dagger)^{r_n}a^{s_n}\ldots(a^\dagger)^{r_2}a^{s_2}(a^\dagger)^{r_1}a^{s_1}|z\rangle = (z^*)^{d_n}B_{\mathbf{r},\mathbf{s}}(|z|^2), \tag{15}$$

which after some algebra, provides an equivalent derivation of Eqs. (13) and (14). The first instance where the relation between the coherent state matrix elements and the Bell polynomials appears is Ref. 7, again for the generic case of Eq. (2), for which conventional Bell polynomials are obtained.

We shall proceed now to give a combinatorial interpretation of the previous results. The essence of subsequent paragraphs will be a graph-theoretical description of the problem. We define the structures (graphs) that are counted by the generalized Bell and Stirling numbers and then give a thorough combinatorial derivation of the recurrence relations, Dobiński-type formulas and other closed-form expressions. The Eqs. (6), (13), and (14) will emerge from purely combinatorial considerations and this will permit the bijective identification of algebraic and combinatorial structures.

III. BUGS, COLONIES, SETTLEMENTS, AND RECURRENCE RELATIONS

We introduce now a number of tools needed to describe the problem in the graph-theoretical language.

Definition 3.1: A *bug* of *type* (r,s) consists of a body and s legs. The body is formed by r linearly ordered empty cells. Each foot of the s legs is labeled with one number from an integer segment $(m,m+s] := \{m+1,m+2,\ldots,m+s\}$, see Fig. 1.

Definition 3.2: Consider a set of n bugs, the first one of type (r_1,s_1) and feet labeled with labels in $(0,s_1]$, the second of type (r_2,s_2) with labels in $(s_1,s_1+s_2]$ and so on. A *colony* is one of the possible ways of organizing the bugs using the following procedure. The first bug has to stand over the ground. Once the $(j-1)$th bug is placed, the jth is placed by putting some (or none) of its s_j feet in the ground and each one of the rest in one of the empty cells of the bodies of the preceding bugs, see Fig. 2. The pair of sequences $(\mathbf{r},\mathbf{s})$, $\mathbf{r}=(r_1,r_2,\ldots,r_n)$, $\mathbf{s}=(s_1,s_2,\ldots,s_n)$, carrying the information about the types of the bugs is called the *type* of the colony. The legs of the colony standing on the ground are called *free*.

Assume now that there is a set of m empty cells in the ground. An *m-settlement* is a colony

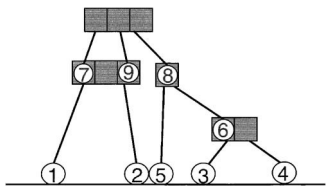

FIG. 2. A colony of type (3,2,1,3;2,2,2,3) and 5 free legs.

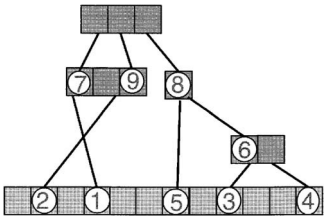

FIG. 3. A 12-settlement of the colony in Fig. 2.

where each one of the feet corresponding to the free legs is placed in one of the ground cells. A *surjective settlement* is one where all the ground cells are occupied. The type of a settlement is defined to be the type of the subjacent colony.

The main theorem of interest for us is as follows.

Theorem 3.1: *The Stirling number* $S_{\mathbf{r},\mathbf{s}}(k)$, $s_1 \leqslant k \leqslant s_1+s_2+\ldots+s_n$, *counts the number of colonies of type* $(\mathbf{r},\mathbf{s})$ *having exactly k free legs. The Bell number* $B_{\mathbf{r},\mathbf{s}}$ *counts the number of colonies of type* $(\mathbf{r},\mathbf{s})$.

Before proving it, we state the following.

Lemma 3.1: A colony of type $(\mathbf{r},\mathbf{s})$ and with k free legs has exactly d_n+k empty cells.

Proof: The total number of cells of the colony is equal to $\Sigma_{i=1}^{n} r_i$. The number of occupied cells is equal to the total number of legs minus the number of free legs $(\Sigma_{i=1}^{n} s_i - k)$. □

Now we are ready to prove the Theorem 3.1.

Proof: Denote by $C_{\mathbf{r},\mathbf{s}}(k)$ the number of colonies of type $(\mathbf{r},\mathbf{s})$ with exactly k free legs. Since $C_{(r_1;s_1)}(k)=S_{(r_1;s_1)}(k)=\delta(s_1,k)$ it is enough to prove that the numbers $C_{\mathbf{r},\mathbf{s}}(k)$ satisfy the same recursion as the generalized Stirling numbers of Eq. (6)

$$C_{\mathbf{r}\uplus r_{n+1},\mathbf{s}\uplus s_{n+1}}(k) = \sum_{j=0}^{s_{n+1}} \binom{s_{n+1}}{j} (d_n + k - j)_{s_{n+1-j}} C_{\mathbf{r},\mathbf{s}}(k-j). \tag{16}$$

The l.h.s. is the number of colonies of type $(\mathbf{r}\uplus r_{n+1},\mathbf{s}\uplus s_{n+1})$ having exactly k free legs. We claim that on the right-hand side (r.h.s.), the expression

$$\binom{s_{n+1}}{j} (d_n + k - j)_{s_{n+1-j}} C_{\mathbf{r},\mathbf{s}}(k-j)$$

gives the number of such colonies where the $(n+1)$th bug has exactly j free legs. Obviously, this would prove the identity. We now prove our claim. In order to get a colony with k free legs the $(n+1)$th bug has to be placed in a colony of type $(\mathbf{r},\mathbf{s})$ and $k-j$ free legs. $C_{\mathbf{r},\mathbf{s}}(k-j)$ is the number of such colonies. We choose the free legs of the $(n+1)$th bug in $\binom{s_{n+1}}{j}$ ways. Since by Lemma (3.1) there are d_n+k-j empty cells in the n bugs colony, $(d_n+k-j)_{s_{n+1-j}}$ gives the number of ways of distributing the rest of the feet of the $(n+1)$th bug into the empty cells. □

In the next section will follow a number of propositions clarifying the properties of structures in question.

IV. COUNTING SETTLEMENTS AND DOBIŃSKI-TYPE RELATIONS

We shall count now the number of m-settlements which will provide the link with Eqs. (13) and (14) viewed from the combinatorial perspective (see Fig. 3).

Theorem 4.1: *Let* $p(m,\mathbf{r},\mathbf{s})$ *be the number of m-settlements of type* $(\mathbf{r},\mathbf{s})$. *We have*

$$p(m,\mathbf{r},\mathbf{s}) = \prod_{j=1}^{n} (m + d_{j-1})_{s_j}. \tag{17}$$

Proof: There are $(m)_{s_1}$ ways of placing the feet of the first bug into the m ground cells. After placing the $(j-1)$th bug there are $m+d_{j-1}$ empty cells available (the previously placed bugs have provided $\Sigma_{i=1}^{j-1} r_i$ empty cells and occupied $\Sigma_{i=1}^{j-1} s_i$ cells). Then, there are $(m+d_{j-1})_{s_j}$ ways of placing the s_j feet of the jth bug. □

Corollary 4.1: We have the polynomial identity

$$\prod_{j=1}^{n} (x+d_{j-1})_{s_j} = \sum_{k=s_1}^{s_1+s_2+\ldots+s_n} S_{\mathbf{r},\mathbf{s}}(k)(x)_k. \tag{18}$$

Proof: By the previous theorem, for an integer value of x the l.h.s. counts the number of x settlements of type $(\mathbf{r},\mathbf{s})$. $S_{\mathbf{r},\mathbf{s}}(k)(x)_k$ counts the number of ways of settling a colony of type $(\mathbf{r},\mathbf{s})$ with k free legs in x ground cells. Then, the r.h.s. is another way of counting x-settlements. □
The exponential generating function of the surjective settlements is equal to the polynomials

$$B_{\mathbf{r},\mathbf{s}}(x) = \sum_{k=s_1}^{s_1+s_2+\ldots+s_n} S_{\mathbf{r},\mathbf{s}}(k) k! \frac{x^k}{k!} = \sum_{k=s_1}^{s_1+s_2+\ldots+s_n} S_{\mathbf{r},\mathbf{s}}(k) x^k.$$

Corollary 4.2 (Extended Dobiński-type relations):
We have the identity

$$B_{\mathbf{r},\mathbf{s}}(x) e^x = \sum_{m=s_1}^{\infty} \prod_{j=1}^{n} (m+d_{j-1})_{s_j} \frac{x^m}{m!}. \tag{19}$$

Proof: Taking the coefficient of $x^m/m!$ on the l.h.s. we obtain

$$\sum_{k=0}^{m} \binom{m}{k} S_{\mathbf{r},\mathbf{s}}(k) k! = \sum_{k=0}^{m} S_{\mathbf{r},\mathbf{s}}(k)(m)_k.$$

By the previous corollary it is equal to the coefficient of $x^m/m!$ on the r.h.s. □
From Eq. (19) we obtain

$$B_{\mathbf{r},\mathbf{s}}(x) = e^{-x} \sum_{m=s_1}^{\infty} \prod_{j=1}^{n} (m+d_{j-1})_{s_j} \frac{x^m}{m!} \tag{20}$$

and

$$B_{\mathbf{r},\mathbf{s}} \equiv B_{\mathbf{r},\mathbf{s}}(1) = e^{-1} \sum_{m=s_1}^{\infty} \frac{1}{m!} \prod_{j=1}^{n} (m+d_{j-1})_{s_j}. \tag{21}$$

Taking the coefficient of $x^k/k!$ on both sides of Eq. (20) we obtain the formula for the generalized Stirling numbers

$$S_{\mathbf{r},\mathbf{s}}(k) = \frac{1}{k!} \sum_{m=0}^{k} \binom{k}{m} (-1)^{k-m} \prod_{j=1}^{n} (m+d_{j-1})_{s_j}. \tag{22}$$

Evidently Eq. (20) is identical to Eq. (13) and so are Eqs. (22) and (14). This emphasizes again the already stated bijective correspondence between algebraic and combinatorial structures.

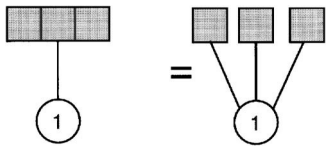

FIG. 4. A (3, 1)-bug and corresponding small planar tree.

V. UNIFORM COLONIES AND SETTLEMENTS

A colony or a settlement with all the bugs of the same type is called *uniform*. A uniform colony with n bugs of type (r,s) is called a colony of type $(r,s)^n$. Following the notation of Ref. 10 the corresponding Stirling and Bell numbers, enumerating uniform colonies of type $(r,s)^n$, are denoted respectively by $S_{r,s}(n,k)$ and $B_{r,s}(n)$. Clearly, for $\mathbf{r}=(\overbrace{r,r,\ldots,r}^{n})$ and $\mathbf{s}=(\overbrace{s,s,\ldots,s}^{k})$, $S_{r,s}(n,k)=S_{\mathbf{r},\mathbf{s}}(k)$ and $B_{r,s}(n)=B_{\mathbf{r},\mathbf{s}}$. The recursive formula, Dobiński-type relations and its consequences appearing here are natural extensions of those investigated in Ref. 10.

The case $s=1$ can be mapped into trees and forests. An $(r,1)$ bug can be identified with a planar tree, i.e., a tree where the leaves are all connected to the root and linearly ordered (see Fig. 4). An increasing tree is one where the internal vertices are labeled with labels in a totally ordered set and the labels increase on any path from the root to any internal vertex. The uniform colonies with $s=1$ corresponds to forests of increasing r-ary planar trees. The free legs are the roots of the trees (see Fig. 5). For $r=1$, there is only one 1-ary increasing tree for each n. Then $B_{1,1}(n)=B(n)$ is the ordinary Bell number.

The exponential generating function of the r-ary planar increasing trees $T_r(x)$ satisfy the differential equation (see Ref. 15, Chap. 5) $y'=(y)^r$. From this we obtain $T_r(x)=\sqrt[1-r]{1-(r-1)x}$, for $r>1$. The generalized Bell number $B_{r,1}(n)$ counts the number of r-forests with n internal vertices. By the exponential formula we obtain

$$\sum_{n=0}^{\infty} B_{r,1}(n)\frac{x^n}{n!}=\exp\{\sqrt[1-r]{1-(r-1)x}-1\}. \tag{23}$$

We quote the explicit expression:[10]

$$B_{r,1}(n)=\frac{(r-1)^{n-1}}{e}\sum_{k=1}^{\infty}\frac{\Gamma\left(n+\frac{k}{r-1}\right)}{\Gamma\left(1+\frac{k}{r-1}\right)(k-1)!}. \tag{24}$$

In a subsequent publication we shall demonstrate that the summation formulas of the type Eq. (24) can be also obtained for many other strings describing the uniform case.

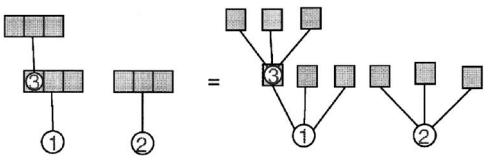

FIG. 5. A uniform colony of type $(3,1)^3$ and the corresponding forest of increasing trees.

VI. CONCLUSIONS

We have obtained analytic expressions and combinatorial interpretation of the integers generalizing conventional Bell and Stirling numbers, arising in the normal ordering of a boson string. All of their properties can be interpreted in terms of graph-theoretical language. The proof of the main result may also be obtained with the use of combinatorial theory of species.[15–17] The results constitute an application of combinatorial analysis which produces the solution of quantum mechanical problem of normal ordering. For alternative interpretations of the numbers investigated in this work see Refs. 18 and 19. It is an outstanding problem how to extend the key results of this work to the boson q-analogs. In this respect the Refs. 20–22 will be of essential help.

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Euler angles for G_2

Sergio L. Cacciatori[a)]
Dipartimento di Matematica dell'Università di Milano, Via Saldini 50, I-20133 Milano, Italy and INFN, Sezione di Milano, Via Celoria 16, I-20133 Milano, Italy

Bianca L. Cerchiai[b)]
Lawrence Berkeley National Laboratory Theory Group, Bldg. 50A5104, 1 Cyclotron Road, Berkeley, California 94720-8162 and Department of Physics, University of California, Berkeley, California 94720

Alberto Della Vedova[c)] and Giovanni Ortenzi[d)]
Dipartimento di Matematica ed Applicazioni, Università Milano Bicocca, via R. Cozzi, 53- I-20126 Milano, Italy

Antonio Scotti[e)]
Dipartimento di Matematica dell' Università di Milano, Via Saldini 50, I-20133 Milano, Italy

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We provide a simple coordinatization for the group G_2, which is analogous to the Euler coordinatization for SU(2). We show how to obtain the general element of the group in a form emphasizing the structure of the fibration of G_2 with fiber SO(4) and base $\mathcal{H}$, the variety of quaternionic subalgebras of octonions. In particular this allows us to obtain a simple expression for the Haar measure on G_2. Moreover, as a by-product it yields a concrete realization and an Einstein metric for $\mathcal{H}$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1993549]

I. INTRODUCTION

The relevance of Lie groups in physics is a well established fact: They appear both in classical and in quantum problems. In this context an important role is played by the Haar measure, needed, e.g., for the construction of a consistent path integral in lattice gauge theories.[1] The canonical 1-form θ of the compact Lie group G is the fundamental structure customarily used to find this measure. In fact the components of θ with respect to a basis of Lie(G) are everywhere linear independent, smooth, left-invariant 1-form on G.[2] So their wedge product gives us a left-invariant volume form. In order to perform explicit calculations we have to choose a suitable local chart and the related local expression for the Haar measure. The logarithmic coordinates[3] are the most obvious choice for a coordinatization of G. In this case the canonical 1-form becomes

$$\theta(X) = \int_0^1 e^{s\ \mathrm{ad}X} ds.$$

The related volume form is

[a)]Electronic mail: cacciatori@mi.infn.it
[b)]Electronic mail: blcerchiai@lbl.gov
[c)]Electronic mail: alberto.dellavedova@unimib.it
[d)]Electronic mail: giovanni.ortenzi@unimib.it
[e)]Graduate visitor (visitatore laureato); electronic mail: ascotti@mindspring.com

$$\omega = \prod_{\lambda \in \sigma(\mathrm{ad}X)} \frac{1-e^{-\lambda}}{\lambda} d\alpha_1 \wedge \cdots \wedge d\alpha_n,$$

where $\sigma(\mathrm{ad}X)$ denotes the spectrum of ad$X$ and α_i are a basis of Lie$(G)^*$. However, these coordinates do not display generally the subgroup structure of G which usually is relevant in the physical applications. The difficulties of such a kind of coordinatization arise when one needs to explicitly determine the global range of the coordinates. A coordinatization which yields a simple form for the Haar measure and at the same time allows a simple determination of the range for the angles can become crucial for numerical computations, e.g., in lattice gauge theories or in random matrix models. For unitary groups such a coordinatization has been constructed in Ref. 4, generalizing the "Euler angle parameterization" for SU(2).

In this paper we provide an analogous simple coordinatization for the exceptional Lie group G_2. We start by showing how a simple matrix realization of the algebra can be obtained starting from the octonions. Then a proposal for a representation of the group elements, based on the previous construction and emphasizing the $SO(4)$ subgroup embedded in G_2, is given and it is proven to cover the whole group.

After computing the left-invariant currents in a way that respects the structure of the fibration, the infinitesimal invariant measure is determined with a suitable normalization. We then use topological tools and symmetry arguments to determine the correct range of the coordinates. As a by-product we obtain a coordinatization and an Einstein metric for the eight-dimensional variety of quaternionic subalgebras of octonions.

Motivations for considering models with G_2 symmetries are provided by different physical systems, for example they arise in the study of deconfinement phase transitions,[5] in random matrix models,[6] or in the new matrix models related to D-brane physics.[7]

II. THE G_2 ALGEBRA

The octonions $\mathbb{O}$ are an eight-dimensional real algebra whose generic element a is a pair of quaternions (α_1, α_2) with the following multiplication rules:

$$(\alpha_1, \alpha_2) \cdot (\beta_1, \beta_2) = (\alpha_1\beta_1 - \overline{\beta_2}\alpha_2, \beta_2\alpha_1 + \alpha_2\overline{\beta_1}). \tag{2.1}$$

Here (α_1, α_2), (β_1, β_2) are generic octonions. This algebra comes naturally equipped with an involution called conjugation

$$\overline{(\alpha_1, \alpha_2)} = (\overline{\alpha_1}, -\alpha_2).$$

Denoting by 1, i, j, k the usual basis of the quaternions yields the following canonical basis for the algebra $\mathbb{O}$

$$e_0 = (1,0), \quad e_1 = (i,0), \quad e_2 = (j,0), \quad e_3 = (k,0), \quad e_4 = (0,1), \quad e_5 = (0,i), \quad e_6 = (0,j),$$
$$e_7 = (0,k).$$

Using this basis it follows easily that the subspace $\mathbb{H}$ spanned by $\{1, e_1, e_2, e_3\}$ is in fact a quaternionic subalgebra that we call the canonical quaternionic subalgebra. Moreover we can consider $\mathbb{O}$ as a two-dimensional module over $\mathbb{H}$, i.e., every octonion z can be decomposed as $z=x+ye_4$, where x, y are suitable quaternions.

The octonions, together with $\mathbb{R}$, $\mathbb{C}$, and $\mathbb{H}$, are the only normed division algebras. The norm is induced by the standard Euclidean structure of the underlying real vector space. They are neither commutative nor associative, but they are alternative, i.e., any subalgebra generated by two octonions is associative. This weak form of associativity implies the Moufang identities,[8] which are multiplication laws among octonions and will prove very useful in the following:

$$(ax)(ya) = a(xy)a,$$

$$a(x(ay)) = (axa)y,$$

$$y(a(xa)) = y(axa). \tag{2.2}$$

The relevance of the octonions in mathematics is due to their deep connection with the exceptional Lie groups (Ref. 9, and references therein). We are interested in the group G_2. In this case the link is easy to understand: G_2 is the automorphism group of the octonions. For every octonion a we denote by l_a the left multiplication $l_a(x)=ax$. Under suitable hypothesis the composition of left multiplications generates elements of G_2. In fact it holds

Proposition 1: *Let* $g=l_{a_1}\ldots l_{a_n}$, *where* $a_1,\ldots,a_n$ *are unitary purely imaginary octonions. If* $g(1)=1$, *then* $g\in G_2$.

Proof: We have to show that $g(x)g(y)=g(xy)$ for all $x,y\in\mathbb{O}$. To this end we prove by induction on n that

$$g(x)g(y) = g((xb)y), \tag{2.3}$$

where $b=(\ldots(a_1a_2)\ldots)a_n$.

For the moment we avoid the hypothesis $g(1)=1$.

If $n=1$ we have

$$(ax)(ay) = -a^2((ax)(ay)) = -a((a(ax)a)y) = a((xa)y),$$

where the first equality holds because a is purely imaginary and the others by the Moufang identities.

Now we suppose the statement is true for n. So we have

$$g(ax)g(ay) = g(((ax)b)(ay)) = -g(a^2(((ax)b)(ay))) = g(a((x(ba))y)),$$

which is Eq. (2.3), if we replace g by gl_a and b by ba.

Finally, to complete the proof we have to show that $b=(\ldots(a_1a_2)\ldots)a_n=1$. So, applying the operator $l_{a_n}\ldots l_{a_1}$ to both members of the equation $1=g(1)=a_1(\ldots(a_{n-1}a_n)\ldots)$ gives us $a_n(a_{n-1}(\ldots(a_2a_1)\ldots))=(-1)^n$, and then by conjugation we obtain $(-1)^n(\ldots(a_1a_2)\ldots)a_n=(-1)^n$ which implies $b=1$. □

We can get some interesting subgroups of G_2 by imposing additional conditions on g. If we add the hypothesis $g(e_1)=e_1$ we obtain a SU(3) subgroup denoted in the following by P. Moreover, imposing also $g(e_2)=e_2$, the resulting subgroup is a copy of SU(2), which we call S.

In order to write down generalized Eulerian coordinates we need to describe the embedding of SO(4) in G_2.[10]

To this end we identify as usual SU(2) with the 3–sphere of unitary quaternions and we consider the following homomorphism:

$$\gamma:\mathrm{SU}(2)\times\mathrm{SU}(2)\to G_2,$$

$$(a,b)\mapsto\gamma_{ab}, \tag{2.4}$$

where $\gamma_{ab}(x+ye_4)=ax\overline{a}+(by\overline{a})e_4$. Using the Moufang identities it is not hard to check that γ_{ab} is truly an octonion automorphism. Fixing $a=1$ provides us with the embedding γ_{1b} of SU(2) in G_2, whose image is the subgroup S. On the other hand the image of the embedding γ_{a1} is a SU(2), which we denote by Σ and which is not conjugate to S.

The map γ is not injective and its kernel is the subgroup $\mathbb{Z}_2=\{(1,1),(-1,-1)\}$. By the homomorphism theorem the image of the map γ in G_2 is isomorphic to $(\mathrm{SU}(2)\times\mathrm{SU}(2))/\mathbb{Z}_2$, which is SO(4) as well known. In the following sections we will refer to the image of γ simply as SO(4).

The homogeneous space $\mathcal{H}=G_2/\mathrm{SO}(4)$ is the eight-dimensional variety of the quaternionic subalgebras of $\mathbb{O}$. So $\mathbb{H}$ can be thought as a point of $\mathcal{H}$. G_2 acts transitively on $\mathcal{H}$ and the stabilizer of $\mathbb{H}$ is the image of γ.[10]
Then we have the fibration

$$\begin{array}{c} \mathrm{SO}(4) \hookrightarrow G_2 \\ \downarrow \\ \mathcal{H}. \end{array}$$

The G_2 generators provided in proposition 1 are useful in particular to find a basis of the Lie algebra $\mathrm{Lie}(G_2)$. Actually, let us take an element of G_2 of the form $g_{abc}=-l_{(cb)a}l_a l_b l_c$, where $(cb)a$, a, b, c are unitary and purely imaginary (i.e., $a+\bar{a}=0$). Notice that the choice of $-(cb)a$ guarantees $g_{abc}1=1$. The condition that $(cb)a$ be purely imaginary amounts to $(cb)\perp a$.

Consider now a path $g_{a_t bc}=-l_{(cb)a_t}l_{a_t}l_b l_c$ where $a_t=c\cos(t)+a\sin(t)$ and with the additional requirements $b\perp c$, $b\perp a$, and $a\perp c$.

By definition $C_{abc}=d/dt|_{t=0}g_{abc}(t)$ is an element of $\mathrm{Lie}(G_2)$. With suitable choices of the elements a, b, and c among the elements of the canonical basis of $\mathbb{O}$ we can find a basis of this algebra. The representative matrices, written below with respect to the canonical basis, are normalized with the condition $\mathrm{Tr}(C_I C_J)=-4\delta_{IJ}$. We remark that they are seven-dimensional because of the trivial action on the real unity.

$$C_1=\begin{pmatrix} 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&-1\\ 0&0&0&0&0&-1&0\\ 0&0&0&0&1&0&0\\ 0&0&0&1&0&0&0 \end{pmatrix} \quad C_2=\begin{pmatrix} 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&1&0\\ 0&0&0&0&0&0&-1\\ 0&0&0&-1&0&0&0\\ 0&0&0&0&1&0&0 \end{pmatrix}$$

$$C_3=\begin{pmatrix} 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&-1&0&0\\ 0&0&0&1&0&0&0\\ 0&0&0&0&0&0&-1\\ 0&0&0&0&0&1&0 \end{pmatrix} \quad C_4=\begin{pmatrix} 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&1\\ 0&0&0&0&0&1&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&-1&0&0&0&0\\ 0&-1&0&0&0&0&0 \end{pmatrix}$$

$$C_5=\begin{pmatrix} 0&0&0&0&0&0&0\\ 0&0&0&0&0&-1&0\\ 0&0&0&0&0&0&1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&1&0&0&0&0&0\\ 0&0&-1&0&0&0&0 \end{pmatrix} \quad C_6=\begin{pmatrix} 0&0&0&0&0&0&0\\ 0&0&0&0&1&0&0\\ 0&0&0&-1&0&0&0\\ 0&0&1&0&0&0&0\\ 0&-1&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0 \end{pmatrix}$$

$$C_7=\begin{pmatrix}0&0&0&0&0&0&0\\0&0&0&-1&0&0&0\\0&0&0&0&-1&0&0\\0&1&0&0&0&0&0\\0&0&1&0&0&0&0\\0&0&0&0&0&0&0\\0&0&0&0&0&0&0\end{pmatrix}\quad C_8=\frac{1}{\sqrt{3}}\begin{pmatrix}0&0&0&0&0&0&0\\0&0&-2&0&0&0&0\\0&2&0&0&0&0&0\\0&0&0&0&1&0&0\\0&0&0&-1&0&0&0\\0&0&0&0&0&0&-1\\0&0&0&0&0&1&0\end{pmatrix}$$

$$C_9=\frac{1}{\sqrt{3}}\begin{pmatrix}0&-2&0&0&0&0&0\\2&0&0&0&0&0&0\\0&0&0&0&0&0&0\\0&0&0&0&0&0&1\\0&0&0&0&0&-1&0\\0&0&0&0&1&0&0\\0&0&0&-1&0&0&0\end{pmatrix}\quad C_{10}=\frac{1}{\sqrt{3}}\begin{pmatrix}0&0&-2&0&0&0&0\\0&0&0&0&0&0&0\\2&0&0&0&0&0&0\\0&0&0&0&0&-1&0\\0&0&0&0&0&0&-1\\0&0&0&1&0&0&0\\0&0&0&0&1&0&0\end{pmatrix}$$

$$C_{11}=\frac{1}{\sqrt{3}}\begin{pmatrix}0&0&0&-2&0&0&0\\0&0&0&0&0&0&-1\\0&0&0&0&0&1&0\\2&0&0&0&0&0&0\\0&0&0&0&0&0&0\\0&0&-1&0&0&0&0\\0&1&0&0&0&0&0\end{pmatrix}\quad C_{12}=\frac{1}{\sqrt{3}}\begin{pmatrix}0&0&0&0&-2&0&0\\0&0&0&0&0&1&0\\0&0&0&0&0&0&1\\0&0&0&0&0&0&0\\2&0&0&0&0&0&0\\0&-1&0&0&0&0&0\\0&0&-1&0&0&0&0\end{pmatrix}$$

$$C_{13}=\frac{1}{\sqrt{3}}\begin{pmatrix}0&0&0&0&0&-2&0\\0&0&0&0&-1&0&0\\0&0&0&-1&0&0&0\\0&0&1&0&0&0&0\\0&1&0&0&0&0&0\\2&0&0&0&0&0&0\\0&0&0&0&0&0&0\end{pmatrix}\quad C_{14}=\frac{1}{\sqrt{3}}\begin{pmatrix}0&0&0&0&0&0&-2\\0&0&0&1&0&0&0\\0&0&0&0&-1&0&0\\0&-1&0&0&0&0&0\\0&0&1&0&0&0&0\\0&0&0&0&0&0&0\\2&0&0&0&0&0&0\end{pmatrix}$$

This basis satisfies the commutation rules summarized in the antisymmetric matrix $B_{IJ}=[C_I,C_J]$ given in Appendix A.

Among that matrices we can recognize the Lie algebras corresponding to the subgroups of G_2 mentioned above. The first eight matrices generate Lie(P) and they are reminiscent of the Gell–Mann matrices. Moreover, the matrices $\{C_1,C_2,C_3\}$ generate Lie(S) and finally $\{C_8,C_9,C_{10}\}$ generate Lie(Σ).

Since the elements C_5 and C_{11} commute, they generate a Cartan subalgebra of Lie(G_2) which is the Lie algebra of the maximal torus T of G_2. Notice that the commutators among the basis of Lie(S), Lie(Σ), and Lie(T) generate the whole basis of Lie(G_2). Our previous observations lead us to the conjecture that a good coordinatization for the generic element $g\in G_2$ can be defined by

$$g=\sigma(a_1,a_2,a_3)s(a_4,a_5,a_6)e^{\sqrt{3}a_7C_{11}}e^{a_8C_5}u(a_9,a_{10},a_{11};a_{12},a_{13},a_{14}),\tag{2.5}$$

where

$$s(x,y,z)=e^{xC_3}e^{yC_2}e^{zC_3},\tag{2.6}$$

$$\sigma(x',y',z') = e^{\sqrt{3}x'C_8} e^{\sqrt{3}y'C_9} e^{\sqrt{3}z'C_8}, \tag{2.7}$$

$$u(x,y,z;x',y',z') = s(x,y,z)\sigma(x',y',z') \tag{2.8}$$

are elements, respectively, of S, Σ, and SO(4).

In this paper we prove that this is in fact a good coordinatization for G_2, which could be used to determine a simple form for the Haar measure on the group. In order to achieve this we will first determine the corresponding invariant metric and then compute the range of the coordinates $a_1, a_2, \ldots, a_{14}$.

III. THE INVARIANT METRIC FOR G_2

In order to compute the invariant metric over the Lie group G_2 we will first show how our coordinatization (2.5) is related to the fibration described in the previous section.

It is well known that for a simple group, and therefore in particular for G_2, the invariant metric is uniquely defined (up to a normalization constant) by the Killing form over the algebra. More precisely, the Killing form defines a metric (and a Lebesgue measure) over the tangent space to the identity, which can be pulled back via the left (or right) multiplication. If $f_{IJ}{}^K$ are the structure constants of the algebra, then the Killing metric has components

$$K_{IJ} = (C_I, C_J) = -k f_{IL}{}^M f_{JM}{}^L, \tag{3.1}$$

where k is a normalization constant. In our case we find $K_{IJ} = 16k\delta_{IJ}$, which suggests to choose $k = 1/16$ conveniently in such a way that the generators $\{C_I\}_{I=1}^{14}$ are orthonormal: $(C_I, C_J) = \delta_{IJ}$. By right multiplication we can associate to every matrix C_I a vector field in the tangent bundle. Its dual (defined using the pullback of the Killing form) is a left-invariant 1-form and the collection of those 1-forms provides a trivialization of the cotangent bundle. In a coordinate patch $\{w^I\}$ the canonical 1-form J becomes

$$J = J^I C_I = g^{-1} \frac{\partial g}{\partial w^J} dw^J, \tag{3.2}$$

so that the invariant metric is

$$ds^2 = g_{IJ} dw^I \otimes dw^J = J^L \otimes J^M (C_L, C_M). \tag{3.3}$$

Therefore, if we define the matrix $\underline{J} = \{J^I{}_K\}$ with components $J^I = J^I{}_K dw^K$ and remember our normalization, we find for the components of the metric

$$g_{IJ} = \delta_{LM} J^L{}_I J^M{}_J. \tag{3.4}$$

This means that the right currents define a 14–bein over the Lie group G_2. In particular the invariant volume form is

$$\omega = J^1 \wedge \ldots \wedge J^{14} = \det(\underline{J}) dx^1 \wedge \ldots \wedge dx^{14} \tag{3.5}$$

and the associated Haar measure is

$$d\mu = \det(\underline{J}) \prod_{I=1}^{14} dw^I. \tag{3.6}$$

Now we use our coordinatization (2.5), which we rewrite in the form

$$g = h(a_1,a_2,a_3,a_4,a_5,a_6,a_7,a_8)u(a_9,a_{10},a_{11};a_{12},a_{13},a_{14}). \tag{3.7}$$

Note that u is the generic element of the subgroup SO(4), while h is an element of $S\Sigma T$ which is not a subgroup of G_2. We can express the currents associated to the elements u and h, respectively, as

$$J_u = duu^{-1} = \sum_{i\in A} J_u^i C_i, \quad J_h = h^{-1}dh = \sum_{i=1}^{14} J_h^i C_i, \tag{3.8}$$

where $A=\{1,2,3,8,9,10\}$. Note that for J_u we have chosen the left currents. This is because from the orthonormality condition it follows that:

$$ds^2 = \sum_{i\in A} (J_u^i + J_h^i)^2 + \sum_{i\notin A} (J_h^i)^2. \tag{3.9}$$

This particular form of the metric stresses the relation with the fibration of G_2 over the variety $\mathcal{H}$. In fact it shows explicitly the separation between the base and the fiber and if we fix the coordinates $(a_1,a_2,a_3,a_4,a_5,a_6,a_7,a_8)$, it reduces to the metric on the fiber SO(4). On the other hand the term $\Sigma_{i\notin A}(J_h^i)^2$ corresponds to the acht-bein $\tilde{J}_h$ obtained after projecting the currents J_h orthogonally to the fiber, and therefore it has to coincide with the metric on the base.

This decomposition greatly simplifies the explicit computation of the metric, the main task being the computation of J_h.

In order to determine J_u remember that $u(x,y,z;x',y',z')=s(x,y,z)\sigma(x',y',z')$ and that s and σ commute, so that in terms of $J_s=dss^{-1}$ and $J_\sigma=d\sigma\sigma^{-1}$, we get $J_u=J_s+J_\sigma$ with

$$\begin{aligned} J_S(x,y,z) &= [-\sin(2x)dy + \cos(2x)\sin(2y)dz]C_1 + [\cos(2x)dy + \sin(2x)\sin(2y)dz]C_2 \\ &\quad + [dx + \cos(2y)dz]C_3, \end{aligned}$$

$$\begin{aligned} J_\Sigma(x,y,z) &= \sqrt{3}[dx + \cos(2y)dz]C_8 + \sqrt{3}[\cos(2x)dy + \sin(2x)\sin(2y)dz]C_9 \\ &\quad + \sqrt{3}[\sin(2x)dy - \cos(2x)\sin(2y)dz]C_{10}. \end{aligned} \tag{3.10}$$

Using Mathematica we have found for the currents J_h the expressions written in Appendix B.

We are now able to compute the Haar measure in our coordinates. In fact, if $\underline{\tilde{J}_h}$ is the 8×8 matrix given by the acht-bein $\tilde{J}_h$ and $\underline{J_s}$, $\underline{J_\sigma}$ are the 3×3 matrices associated to the drei-bein J_s and J_σ, respectively, then $\det(\underline{J})=\det(\underline{\tilde{J}_h})\det(\underline{J_s})\det(\underline{J_\sigma})$ so that

$$d\mu = 27\sqrt{3}f(2a_7,2a_8)\sin(2a_2)\sin(2a_5)\sin(2a_{10})\sin(2a_{13})\prod_{i=1}^{14} da_i, \tag{3.11}$$

where

$$\begin{aligned} f(\alpha,\beta) &= \sin\left(\frac{\beta-\alpha}{2}\right)\sin\left(\frac{\beta+\alpha}{2}\right)\sin\left(\frac{\beta-3\alpha}{2}\right)\sin\left(\frac{\beta+3\alpha}{2}\right)\sin(\alpha)\sin(\beta) \\ &= \tfrac{1}{4}(\cos(\alpha)+\cos(\beta))(\cos(3\alpha)+\cos(\beta))\sin(\alpha)\sin(\beta). \end{aligned} \tag{3.12}$$

This, however, is not the end of the story. We need in fact to determine the range of the coordinates which covers the whole group G_2, apart from a subset of zero measure. To this end we will use a topological argument.

IV. THE RANGE OF THE COORDINATES

Before entering into more details, let us explain our strategy.

Looking at the measure (3.11) one immediately sees that for some values of the coordinates it vanishes. This happens for certain values of the angles a_2, a_5 , a_7 , a_8 , a_{10} , a_{13}. Let us suppose we choose the range for these coordinates in such a way that it delimits a region where $d\mu$ is vanishing only on the boundary. For the other coordinates the range is fixed in such a way that each of them goes around a closed orbit exactly once.

This describes a 14-dimensional closed cycle V which represents an element of the homology group $[V] \in H_{14}(G_2, \mathbb{Z})$. (However, for our purposes it would be enough to consider the homology with rational or real coefficients.) Using the pairing $B: H^k \times H_k \to \mathbb{R}$ given by

$$B([\xi],[W]) = \int_W \xi, \tag{4.1}$$

we define the normalized form

$$\tau = B([\omega],[G_2])^{-1}\omega. \tag{4.2}$$

It is clear that the function $B([\tau], \cdot)$ takes only integer values. In particular $B([\tau],[W])$ counts the number of times the cycle W wraps G_2. Once this is known all we need to do is to find how to restrict the range of coordinates until we obtain a cycle V which wraps G_2 once. We are now going to enter into more details and compute τ in three steps.

A. The evaluation of $B([\omega],[G_2])$

There is a simple way to compute the total volume of a connected simple Lie group, described by Macdonald in Ref. 11. It works as follows.

If G is the group, $t \subset \mathrm{Lie}(G)$ a Cartan subalgebra, and $t_{\mathbb{Z}}$ the integer lattice generated in t by the simple roots, then $T = t/t_{\mathbb{Z}}$ is a torus with the same dimension as t. Let $\alpha > 0$ denote the positive roots and $|\alpha|$ their length.

Then from Hopf theorem, the rational homology of G is equal to the rational homology of a product of odd-dimensional spheres: $H_*(G, \mathbb{Q}) \sim H_*(\Pi_{i=1}^k (S^{2i+1})^{n_i}, \mathbb{Q})$, where n_i is the number of times the given sphere appears. Let $Vol(S^{2i+1}) = 2\pi^{i+1}/i!$ be the volume of the $(2i+1)$-dimensional unit sphere and $Vol(T)$ be the volume of the torus computed using the measure induced by the Lebesgue measure on the algebra. Then the whole volume determined via the pullback of the Lebesgue measure on the algebra is

$$Vol(G) = Vol(T) \cdot \prod_{i=1}^{k} Vol(S^{2i+1})^{n_i} \cdot \prod_{\alpha>0} \frac{4}{|\alpha|^2}. \tag{4.3}$$

The roots of G_2 computed with our choice for the algebra and the normalization, are shown in Appendix C. From the figure we see that there are three positive roots of length 2 and three of length $2/\sqrt{3}$. The torus associated to the simple roots α_1 and α_2 is generated by the coroots H_1 and H_2. Remembering the relations $|H| = 2/|\alpha|$, we find $Vol(T) = \sqrt{3}/2$. Since S^3 and S^{11} are the odd spheres which generate the rational homology of G_2, we obtain the desired result

$$B(\mu, G_2) = Vol(G_2) = 9\sqrt{3}\frac{\pi^8}{20}. \tag{4.4}$$

We are now ready for the next step.

B. The construction of the cycle V

Let us look at (2.5): to determine a closed cycle we first observe that for each one of the two SU(2) subgroups S and Σ it is possible to choose the range of the coordinates in such a way as to cover the whole 3-sphere. The method to do this is well-known (Euler angles) and here we give only the final result

$$0 \leqslant a_1 \leqslant 2\pi, \quad 0 \leqslant a_2 \leqslant \frac{\pi}{2}, \quad 0 \leqslant a_3 \leqslant \pi,$$

$$0 \leqslant a_4 \leqslant 2\pi, \quad 0 \leqslant a_5 \leqslant \frac{\pi}{2}, \quad 0 \leqslant a_6 \leqslant \pi,$$

$$0 \leqslant a_9 \leqslant 2\pi, \quad 0 \leqslant a_{10} \leqslant \frac{\pi}{2}, \quad 0 \leqslant a_{11} \leqslant \pi,$$

$$0 \leqslant a_{12} \leqslant 2\pi, \quad 0 \leqslant a_{13} \leqslant \frac{\pi}{2}, \quad 0 \leqslant a_{14} \leqslant \pi. \tag{4.5}$$

To complete the cycle we need to determine the range for a_7 and a_8 in such a way that $d\mu$ does not vanish. To this end we solve the inequality $f(x,y)>0$ and obtain a tiling of the fundamental region

$$(2a_7, 2a_8) \in [0,2\pi] \times [0,2\pi], \tag{4.6}$$

as we show in Appendix D. There, we also prove that every region of the tiling gives the same (absolute value) contribution to the measure.

The cycle V is then obtained by choosing any one of these regions, for example the one denoted by B in the figure.

C. The evaluation of τ and the range of the Euler angles for G_2

We can now evaluate the degree of the map $V \to G_2$. Using (4.5) for the range of the coordinates, (3.11) for $d\mu$ and (4.4) for $Vol(G_2)$, we easily find $B(\tau,V)=16$. Therefore, our next task is to understand the origin of this factor.

A factor of 4 can be easily accounted for in the following way. We have built the cycle V starting from the closed submanifolds S and Σ corresponding to the two SU(2) embeddings. Thus, naively, we would expect to find a $\mathrm{SU}(2)\times\mathrm{SU}(2)$ submanifold embedded in G_2. But a direct inspection shows that this is not exactly true. In fact, varying for example $a_1 \in [0,2\pi]$ provides a double covering of the six-dimensional submanifold obtained by taking $a_1 \in [0,\pi]$ and $a_2,\ldots,a_6$ as in (4.5). This is because the image of $\mathrm{SU}(2)\times\mathrm{SU}(2)$ in G_2 is $\mathrm{SO}(4)=(\mathrm{SU}(2)\times\mathrm{SU}(2))/\mathbb{Z}_2$, as previously remarked in Sec. II.

Similarly, we must reduce the range of a_{12} to $a_{12} \in [0,\pi]$. The new cycle we obtain in this way wraps G_2 four times.

Now, let us consider the torus $T(a_7,a_8) := e^{\sqrt{3}a_7 C_{11}} e^{a_8 C_5}$. We need to determine the subgroup of 7×7 orthogonal matrices A of SO(4), which leaves each element $T(a_7,a_8)$ invariant under the adjoint action

$$AT(a_7,a_8)A^t = T(a_7,a_8). \tag{4.7}$$

It turns out that it is a finite group generated by the idempotent matrices $\sigma(\sigma=\sigma^{-1})$ and $\eta\ (\eta=\eta^{-1})$

$$\sigma=\begin{pmatrix}1&0&0&0&0&0&0\\0&-1&0&0&0&0&0\\0&0&-1&0&0&0&0\\0&0&0&1&0&0&0\\0&0&0&0&1&0&0\\0&0&0&0&0&-1&0\\0&0&0&0&0&0&-1\end{pmatrix}\quad \eta=\begin{pmatrix}-1&0&0&0&0&0&0\\0&0&1&0&0&0&0\\0&1&0&0&0&0&0\\0&0&0&-1&0&0&0\\0&0&0&0&1&0&0\\0&0&0&0&0&0&-1\\0&0&0&0&0&-1&0\end{pmatrix}. \tag{4.8}$$

Considering the action of σ one finds

$$\begin{aligned}g&=U(a_4,a_5,a_6;a_1,a_2,a_3)T(a_7,a_8)U(a_9,a_{10},a_{11};a_{12},a_{13},a_{14})\\&=U(a_4,a_5,a_6;a_1,a_2,a_3)\sigma T(a_7,a_8)\sigma U(a_9,a_{10},a_{11};a_{12},a_{13},a_{14})\\&=U\left(a_4,a_5,a_6+\frac{\pi}{2};a_1,a_2,a_3+\frac{\pi}{2}\right)T(a_7,a_8)U\left(a_9+\frac{\pi}{2},a_{10},a_{11};a_{12}+\frac{\pi}{2},a_{13},a_{14}\right).\end{aligned} \tag{4.9}$$

Therefore, we can restrict $0\leqslant a_3<\pi/2$.

Analogously, let us now look at the symmetry generated by η:

$$\begin{aligned}g&=U(a_4,a_5,a_6;a_1,a_2,a_3)T(a_7,a_8)U(a_9,a_{10},a_{11};a_{12},a_{13},a_{14})\\&=U(a_4,a_5,a_6;a_1,a_2,a_3)\,\eta T(a_7,a_8)\,\eta U(a_9,a_{10},a_{11};a_{12},a_{13},a_{14}),\end{aligned} \tag{4.10}$$

and restrict our attention to the factor ηU on the right. (Similar relations are true for the factor on the left.) A direct computation using the explicit expression of the matrices shows that the left action of η on U is equivalent to the shift

$$a_9\mapsto\frac{\pi}{4}-a_9,\quad a_{10}\mapsto a_{10}+\frac{\pi}{2},\quad a_{11}\mapsto a_{11},$$

$$a_{12}\mapsto-\frac{\pi}{4}-a_{12},\quad a_{13}\mapsto a_{13}+\frac{\pi}{2},\quad a_{14}\mapsto a_{14}. \tag{4.11}$$

The analysis is more complicated than for the action of σ, because now some of the angles are mapped to values which are outside of the range (4.5) we have fixed. For example, $a_{10}+\pi/2\in[\pi/2,\pi]$, when $a_{10}\in[0,\pi/2]$. Therefore, we need to use other equivalence relations to map the angles back to the original region (4.5).

In fact, the following symmetries hold for S and Σ:

$$S[a_9,a_{10},a_{11}]\sim S\left[a_9+\frac{\pi}{2},\pi-a_{10},a_{11}+\frac{\pi}{2}\right]$$

$$\Sigma[a_{12},a_{13},a_{14}]\sim\Sigma\left[a_{12}+\frac{\pi}{2},\pi-a_{13},a_{14}+\frac{\pi}{2}\right]. \tag{4.12}$$

These are the known symmetries which have been used to determine (4.5) in the first place. Thus the action (4.11) of η is equivalent to

$$a_9\mapsto\frac{3}{4}\pi-a_9,\quad a_{10}\mapsto\frac{\pi}{2}-a_{10},\quad a_{11}\mapsto a_{11}+\frac{\pi}{2},$$

$$a_{12} \mapsto \frac{\pi}{4} - a_{12}, \quad a_{13} \mapsto \frac{\pi}{2} - a_{13}, \quad a_{14} \mapsto a_{14} + \frac{\pi}{2}, \tag{4.13}$$

where now a_{10} and a_{13} stay inside the allowed intervals. The next point to notice is that for the remaining coordinates it is possible to use similarity relations which does not involve a_{10} and a_{13}, e.g.,

$$S[a_9,a_{10},a_{11}]\Sigma[a_{12},a_{13},a_{14}] \sim S[a_9+\pi,a_{10},a_{11}]\Sigma[a_{12}+\pi,a_{13},a_{14}] \tag{4.14}$$

and similar symmetries. Moreover, η is a linear transformation, so that it is enough to restrict the range of one of the angles. Therefore, luckily, we actually do not need to know the action of η on the whole set of coordinates. The solution of our problem simply consists in restricting the range of either a_{10} or a_{13} in the SO(4) factor $U(a_9,a_{10},a_{11};a_{12},a_{13},a_{14})$ on the right. Alternatively, the same result can be achieved by restricting the range of either a_2 or a_5 in the factor $U(a_4,a_5,a_6;a_1,a_2,a_3)$ on the left. Since we prefer a coordinatization which respects the fibration described in Sec. II and we want the angles $a_9,\ldots,a_{14}$ to span the whole fiber $U(a_9,\ldots,a_{14})$, we choose the second option and restrict the range of a_5.

Finally, we can summarize our results for the range of the angles describing G_2:

$$0 \leqslant a_1 \leqslant \pi, \quad 0 \leqslant a_2 \leqslant \frac{\pi}{2}, \quad 0 \leqslant a_3 \leqslant \frac{\pi}{2},$$

$$0 \leqslant a_4 \leqslant 2\pi, \quad 0 \leqslant a_5 \leqslant \frac{\pi}{4}, \quad 0 \leqslant a_6 \leqslant \pi,$$

$$0 \leqslant a_9 \leqslant 2\pi, \quad 0 \leqslant a_{10} \leqslant \frac{\pi}{2}, \quad 0 \leqslant a_{11} \leqslant \pi,$$

$$0 \leqslant a_{12} \leqslant \pi, \quad 0 \leqslant a_{13} \leqslant \frac{\pi}{2}, \quad 0 \leqslant a_{14} \leqslant \pi,$$

$$0 \leqslant a_7 \leqslant \frac{\pi}{6}, \quad 3a_7 \leqslant a_8 \leqslant \frac{\pi}{2}. \tag{4.15}$$

V. CONCLUSIONS

We have found a coordinatization of the G_2 group with a one to one correspondence between the range of coordinates and a full measure subset of the group. In particular, this has allowed us to obtain a quite simple expression for the Haar measure, which should make numerical computations involving the geometry of G_2 much easier, for example in lattice gauge theories or in random matrix models.

However, note that to find an Haar measure on the group we would not have actually needed the last step of the work, i.e., the determination of the correct range of the coordinates which yields an injective map.

In fact, if $d\mu$ indicates the measure over the cycle V, it is possible to simply get an Haar measure $d\tilde{\mu}$ over the Lie group G_2 by just taking

$$d\tilde{\mu} := \frac{1}{16} d\mu, \tag{5.1}$$

16 being the degree of the map $V \to G_2$.

On the other hand the determination of the correct range of coordinates, which covers the whole G_2 wrapping it exactly once except for a subset of vanishing measure, provides a new result, since it determines also a coordinatization of the homogeneous space $\mathcal{H}=G_2/\mathrm{SO}(4)$ of quaternionic subalgebras of octonions.

Moreover, we have also computed the induced metric of $\mathcal{H}$

$$ds^2_{\mathcal{H}} = \delta_{ab} \tilde{J}^a_h \otimes \tilde{J}^b_h, \tag{5.2}$$

and shown that it is an Einstein metric. This result is proven in Appendix E.

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APPENDIX A: COMMUTATORS

$$B = \begin{pmatrix}
0 & 2C_3 & -2C_2 & C_7 & C_6 & -C_5 & -C_4 & 0 & 0 & 0 & C_{14} & C_{13} & -C_{12} & -C_{11} \\
* & 0 & 2C_1 & -C_6 & C_7 & C_4 & -C_5 & 0 & 0 & 0 & -C_{13} & C_{14} & C_{11} & -C_{12} \\
* & * & 0 & C_5 & -C_4 & C_7 & -C_6 & 0 & 0 & 0 & C_{12} & -C_{11} & C_{14} & -C_{13} \\
* & * & * & 0 & C_3+\sqrt{3}C_8 & -C_2 & C_1 & -\sqrt{3}C_5 & -C_{14} & -C_{13} & 0 & 0 & C_{10} & C_9 \\
* & * & * & * & 0 & C_1 & C_2 & \sqrt{3}C_4 & C_{13} & -C_{14} & 0 & 0 & -C_9 & C_{10} \\
* & * & * & * & * & 0 & C_3-\sqrt{3}C_8 & \sqrt{3}C_7 & -C_{12} & C_{11} & -C_{10} & C_9 & 0 & 0 \\
* & * & * & * & * & * & 0 & -\sqrt{3}C_6 & C_{11} & C_{12} & -C_9 & -C_{10} & 0 & 0 \\
* & * & * & * & * & * & * & 0 & \frac{2}{\sqrt{3}}C_{10} & -\frac{2}{\sqrt{3}}C_9 & -\frac{1}{\sqrt{3}}C_{12} & \frac{1}{\sqrt{3}}C_{11} & \frac{1}{\sqrt{3}}C_{14} & -\frac{1}{\sqrt{3}}C_{13} \\
* & * & * & * & * & * & * & * & 0 & \frac{2}{\sqrt{3}}C_8 & C_7-\frac{2}{\sqrt{3}}C_{14} & \frac{2}{\sqrt{3}}C_{13}-C_6 & C_5-\frac{2}{\sqrt{3}}C_{12} & \frac{2}{\sqrt{3}}C_{11}-C_4 \\
* & * & * & * & * & * & * & * & * & 0 & \frac{2}{\sqrt{3}}C_{13}+C_6 & \frac{2}{\sqrt{3}}C_{14}+C_7 & -\frac{2}{\sqrt{3}}C_{11}-C_4 & -\frac{2}{\sqrt{3}}C_{12}+C_5 \\
* & * & * & * & * & * & * & * & * & * & 0 & -\frac{1}{\sqrt{3}}C_8+C_3 & \frac{2}{\sqrt{3}}C_{10}-C_2 & -\frac{2}{\sqrt{3}}C_9+C_1 \\
* & * & * & * & * & * & * & * & * & * & * & 0 & \frac{2}{\sqrt{3}}C_9+C_1 & \frac{2}{\sqrt{3}}C_{10}+C_2 \\
* & * & * & * & * & * & * & * & * & * & * & * & 0 & \frac{1}{\sqrt{3}}C_8+C_3 \\
* & * & * & * & * & * & * & * & * & * & * & * & * & 0
\end{pmatrix}$$

APPENDIX B: THE LEFT-INVARIANT 1-FORMS J_h

$$
\begin{aligned}
J_h^1 = {} & [\cos^3(a_7)\sin(2a_6)\cos(a_8) - \sin^3(a_7)\cos(2a_6)\sin(a_8)]da_5 \\
& - \sin(2a_5)[\cos^3(a_7)\cos(2a_6)\cos(a_8) + \sin^3(a_7)\sin(2a_6)\sin(a_8)]da_4 \\
& + \tfrac{3}{2}\sin(2a_7)[\cos(2a_3)\sin(a_7)\cos(a_8) + \sin(2a_3)\cos(a_7)\sin(a_8)]da_2 + \tfrac{3}{2}\sin(2a_7)\sin(2a_2) \\
& \times[\sin(2a_3)\sin(a_7)\cos(a_8) - \cos(2a_3)\cos(a_7)\sin(a_8)]da_1, \qquad \text{(B1)}
\end{aligned}
$$

$$
\begin{aligned}
J_h^2 = {} & [\cos^3(a_7)\cos(2a_6)\cos(a_8) - \sin^3(a_7)\sin(2a_6)\sin(a_8)]da_5 \\
& + \sin(2a_5)[\cos^3(a_7)\sin(2a_6)\cos(a_8) + \sin^3(a_7)\cos(2a_6)\sin(a_8)]da_4 \\
& - \tfrac{3}{2}\sin(2a_7)[\sin(2a_3)\sin(a_7)\cos(a_8) + \cos(2a_3)\cos(a_7)\sin(a_8)]da_2 + \tfrac{3}{2}\sin(2a_7)\sin(2a_2) \\
& \times[\cos(2a_3)\sin(a_7)\cos(a_8) - \sin(2a_3)\cos(a_7)\sin(a_8)]da_1, \qquad \text{(B2)}
\end{aligned}
$$

$$
J_h^3 = \tfrac{1}{4}(3\cos(2a_7) + \cos(2a_8))(da_6 + \cos(2a_5)da_4) - \sqrt{3}/4(\cos(2a_7) - \cos(2a_8))(da_3 + \cos(2a_2)da_1), \qquad \text{(B3)}
$$

$$
J_h^4 = -\tfrac{1}{2}\sin(2a_8)da_6 - \tfrac{1}{2}\cos(2a_5)\sin(2a_8)da_4 - \tfrac{3}{2}\sin(2a_8)da_3 - \tfrac{3}{2}\sin(2a_8)\cos(2a_2)da_1, \qquad \text{(B4)}
$$

$$
J_h^5 = da_8, \qquad \text{(B5)}
$$

$$
\begin{aligned}
J_h^6 = {} & [\sin^3(a_7)\cos(2a_6)\cos(a_8) + \cos^3(a_7)\sin(2a_6)\sin(a_8)]da_5 \\
& + \sin(2a_5)[\sin^3(a_7)\sin(2a_6)\cos(a_8) - \cos^3(a_7)\cos(2a_6)\sin(a_8)]da_4 \\
& + \tfrac{3}{2}\sin(2a_7)[-\sin(2a_3)\cos(a_7)\cos(a_8) + \cos(2a_3)\sin(a_7)\sin(a_8)]da_2 + \tfrac{3}{2}\sin(2a_7)\sin(2a_2) \\
& \times[\cos(2a_3)\cos(a_7)\cos(a_8) + \sin(2a_3)\sin(a_7)\sin(a_8)]da_1, \qquad \text{(B6)}
\end{aligned}
$$

$$
\begin{aligned}
J_h^7 = {} & [\sin^3(a_7)\sin(2a_6)\cos(a_8) + \cos^3(a_7)\cos(2a_6)\sin(a_8)]da_5 \\
& - \sin(2a_5)[\sin^3(a_7)\cos(2a_6)\cos(a_8) - \cos^3(a_7)\sin(2a_6)\sin(a_8)]da_4 \\
& + \tfrac{3}{2}\sin(2a_7)[\cos(2a_3)\cos(a_7)\cos(a_8) - \sin(2a_3)\sin(a_7)\sin(a_8)]da_2 + \tfrac{3}{2}\sin(2a_7)\sin(2a_2) \\
& \times[\sin(2a_3)\cos(a_7)\cos(a_8) + \cos(2a_3)\sin(a_7)\sin(a_8)]da_1, \qquad \text{(B7)}
\end{aligned}
$$

$$
J_h^{11} = da_7, \qquad \text{(B8)}
$$

$$J_h^{12} = (\sqrt{3}/2)\sin(2a_7)da_6 + (\sqrt{3}/2)\cos(2a_5)\sin(2a_7)da_4 - (\sqrt{3}/2)\sin(2a_7)da_3 - (\sqrt{3}/2)\sin(2a_7)\cos(2a_2)da_1, \tag{B9}$$

$$\begin{aligned} J_h^{13} = &- (\sqrt{3}/2)\sin(2a_7)[\cos(a_7)\cos(2a_6)\cos(a_8) + \sin(a_7)\sin(2a_6)\sin(a_8)]da_5 \\ &+ (\sqrt{3}/2)\sin(2a_7)\sin(2a_5)[-\cos(a_7)\sin(2a_6)\cos(a_8) + \sin(a_7)\cos(2a_6)\sin(a_8)]da_4 \\ &+ \sqrt{3}[\sin(2a_3)\sin(a_7)(3\sin^2(a_7) - 2)\cos(a_8) - \cos(2a_3)\cos(a_7)(3\cos^2(a_7) - 2)\sin(a_8)]da_2 \\ &- \sqrt{3}\sin(2a_2)[\cos(2a_3)\sin(a_7)(3\sin^2(a_7) - 2)\cos(a_8) \\ &+ \sin(2a_3)\cos(a_7)(3\cos^2(a_7) - 2)\sin(a_8)]da_1, \end{aligned} \tag{B10}$$

$$\begin{aligned} J_h^{14} = &(\sqrt{3}/2)\sin(2a_7)[\cos(a_7)\sin(2a_6)\cos(a_8) + \sin(a_7)\cos(2a_6)\sin(a_8)]da_5 \\ &- (\sqrt{3}/2)\sin(2a_7)\sin(2a_5)[\cos(a_7)\cos(2a_6)\cos(a_8) - \sin(a_7)\sin(2a_6)\sin(a_8)]da_4 \\ &+ \sqrt{3}[\cos(2a_3)\sin(a_7)(3\sin^2(a_7) - 2)\cos(a_8) - \sin(2a_3)\cos(a_7)(3\cos^2(a_7) - 2)\sin(a_8)]da_2 \\ &+ \sqrt{3}\sin(2a_2)[\sin(2a_3)\sin(a_7)(3\sin^2(a_7) - 2)\cos(a_8) + \cos(2a_3)\cos(a_7)(3\cos^2(a_7) \\ &- 2)\sin(a_8)]da_1. \end{aligned} \tag{B11}$$

APPENDIX C: THE ROOT SYSTEM

Here we show the roots computed using C_5 and C_{11} normalized to 1. The long roots have length 2 and the short ones have length $2/\sqrt{3}$.

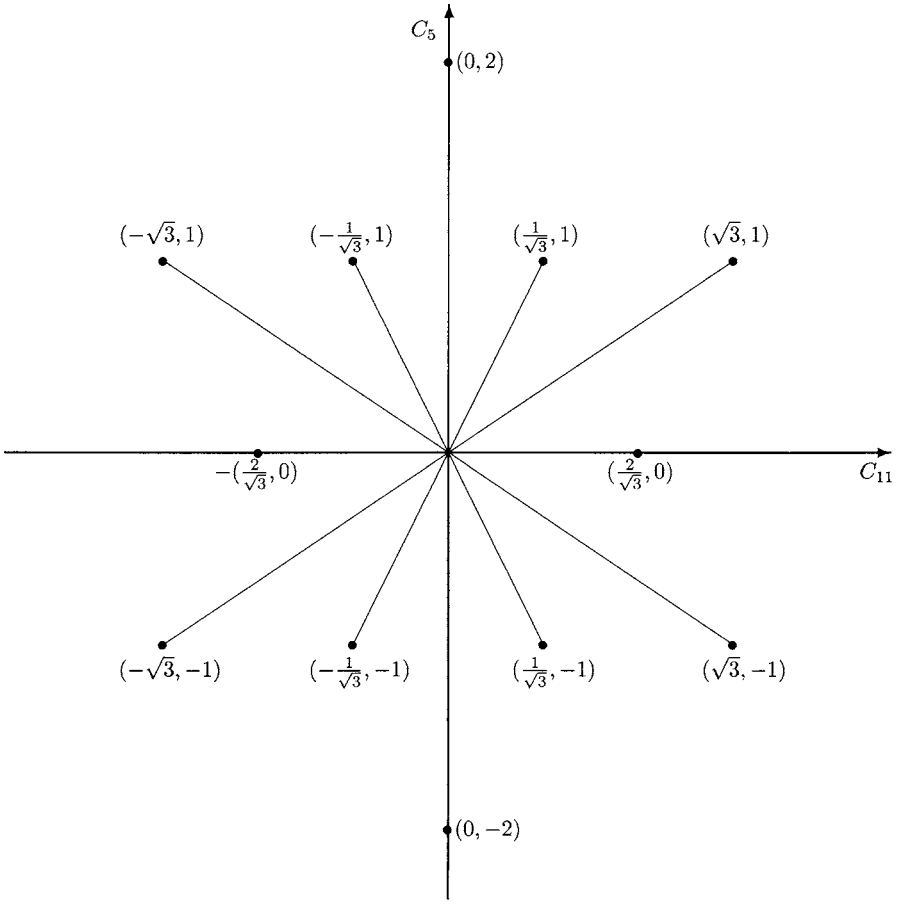

APPENDIX D: THE RANGE FOR a_7 AND a_8

Here we show a plot of the fundamental region for the variables a_7 and a_8, which is determined by the condition $f(\alpha,\beta)>0$ where f is given in (3.12). We obtain a tiling of the torus in 24 triangles, over which the sign of the measure alternates, starting with a positive sign in the region B. In the edges the measure vanishes.

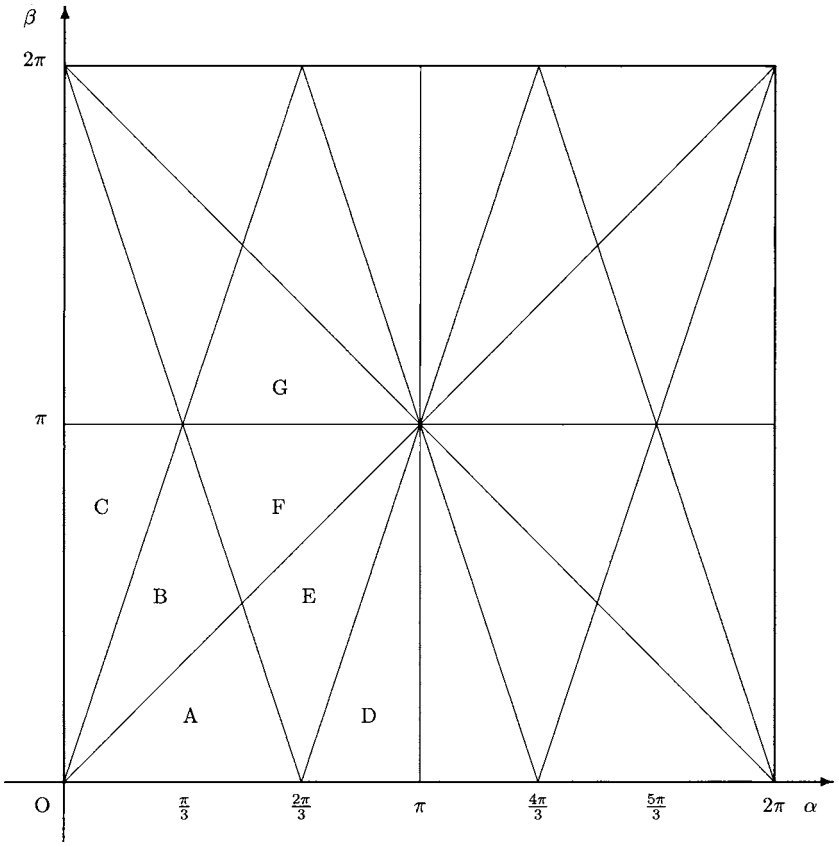

We now show that any sector of this tiling gives exactly the same contribution (obviously up to a sign) to the volume of G_2. To this end we describe some symmetry property of the function $f(\alpha,\beta)$. The translation symmetries $f(\alpha,\beta)=f(\alpha+\pi,\beta+\pi)=f(\alpha-\pi,\beta+\pi)$ and the reflection symmetries $-f(\alpha,\beta)=f(-\alpha,\beta)=f(\alpha,-\beta)$ allows to restrict us to the square $[0,\pi]\times[0,\pi]$. Moreover, the translations gives the equivalence of the triangles A, B, and D with F, E, and C, respectively.

At this point we are left with only three different kinds of triangles: A, B, and D. The symmetry $f(\alpha,\beta)=f((\alpha+\beta)/2,(3\alpha-\beta)/2)$ maps A to B, B to A, and D to G. This proves that we can choose whatever triangle, for example A, as the fundamental region.

APPENDIX E: A METRIC FOR $\mathcal{H}$

Here we give the expression for the metric on $\mathcal{H}$ induced by the metric on G_2, and show that it is an Einstein metric. Let us introduce the 1-forms

$$I_1(x,y,z) := \sin(2y)\cos(2z)dx - \sin(2z)dy,$$

$$I_2(x,y,z) := \sin(2y)\sin(2z)dx + \cos(2z)dy,$$

$$I_3(x,y,z) := dz + \cos(2y)dx. \tag{E1}$$

Thus we can write

$$
\begin{aligned}
ds^2_{\mathcal{H}} = {} & da_8^2 + da_7^2 + [\sin^2 a_8 \cos^2 a_7 + \cos^2 a_8 \sin^2 a_7] \\
& \times (da_5^2 + \sin^2(2a_5) da_4^2 + 3da_2^2 + 3 \sin^2 2a_2 da_1^2) \tfrac{1}{2} \cos(2a_8) \cos 2a_7 \sin^2 2a_7 \\
& \times \{[I_1(a_4,a_5,a_6) + 3I_2(a_1,a_2,a_3)]^2 + [I_2(a_4,a_5,a_6) - 3I_1(a_1,a_2,a_3)]^2\} \\
& + \tfrac{3}{4} \sin^2 2a_7 [I_3(a_4,a_5,a_6) - I_3(a_1,a_2,a_3)]^2 + \tfrac{1}{4} \sin^2(2a_8) [I_3(a_4,a_5,a_6) + 3I_3(a_1,a_2,a_3)]^2 .
\end{aligned}
\tag{E2}
$$

We will now compute the curvature of such a metric. Let us use capital indices for the full algebra, $I=1, \ldots, 14$, Latin indices for the SO(4) subalgebra, $i \in \{1,2,3,8,9,10\}$, and Greek indices for the complementary elements, $\alpha \in \{4,5,6,7,11,12,13,14\}$. Let f_{IJK} be the structure constants with one index lowered through the identity matrix. It is then clear that the nonvanishing structure constants are those with either none or two Greek indices: f_{ijk}, $f_{\alpha\beta k}$ and permutations. Using this fact and the Maurer-Cartan equations (we use the following notations: The spin connection is uniquely defined by $d\tilde{J}_h^\alpha = -\omega^\alpha{}_\beta \tilde{J}_h^\beta$ and $\omega_{\alpha\beta} = -\omega_{\beta\alpha}$; the Riemann tensor field is then $\mathrm{R}^\alpha{}_\beta = d\omega^\alpha{}_\beta + \omega^\alpha{}_\gamma \wedge \omega^\gamma{}_\beta$ with components $R_{\alpha\beta}{}^\gamma{}_\delta$ such that $\mathrm{R}^\gamma{}_\delta = (1/2) R_{\alpha\beta}{}^\gamma{}_\delta J_h^\alpha \wedge J_h^\beta$), the components of the Riemann tensor with respect to the acht-bein are found using only the algebra.

In fact by construction we have that (E2) takes the form $ds^2_{\mathcal{H}} = g_{\alpha\beta} da^\alpha \otimes da^\beta$, with

$$
g_{\alpha\beta} = \tilde{J}^\gamma_\alpha \tilde{J}^\delta_\beta \delta_{\gamma\delta}. \tag{E3}
$$

Let us note that, using notations as in Sec. III, we have

$$
J_h = \tilde{J}_h + J_h^i C_i. \tag{E4}
$$

On the other hand, using $J_h = h^{-1} dh$ one finds

$$
dJ_h = -J_h \wedge J_h = -\tfrac{1}{2} J^I \wedge J^J f_{IJ}{}^K C_K. \tag{E5}
$$

The spin connection can be determined computing $d\tilde{J}_h$ from (E4). Being $\tilde{J}_h^\alpha = J_h^\alpha$ we can omit the tilde in what follows and write:

$$
dJ_h^\alpha = -\tfrac{1}{2} J^I J^J f_{IJ}{}^\alpha = -\tfrac{1}{2} J^\beta J^\gamma f_{\beta\gamma}{}^\alpha - J^i J^\beta f_{i\beta}{}^\alpha, \tag{E6}
$$

where we used the properties of the structure constants. From this we can read the expression for the spin connection one-form, which can be written in the form

$$
\omega^\alpha{}_\beta = J_h^I f_{I\beta}{}^\alpha - \tfrac{1}{2} J_h^\gamma f_{\gamma\beta}{}^\alpha. \tag{E7}
$$

The curvature tensor can then be computed directly

$$
\mathrm{R}^\alpha{}_\beta = J_h^\lambda J_h^\mu \Big[-f_{\lambda i}{}^\alpha f_{\mu\beta}{}^i + \tfrac{1}{4} f_{\lambda\mu}{}^\nu f_{\nu\beta}{}^\alpha - \tfrac{1}{4} f_{\mu\nu}{}^\alpha f_{\lambda\beta}{}^\nu - f_{\lambda\nu}{}^\alpha f_{\mu\beta}{}^\nu \Big], \tag{E8}
$$

or in components

$$
R_{\alpha\beta}{}^\gamma{}_\delta = -f_{\alpha I}{}^\gamma f_{\beta\delta}{}^I + f_{\beta I}{}^\gamma f_{\alpha\delta}{}^I + \tfrac{1}{2} f_{\alpha\beta}{}^I f_{I\delta}{}^\gamma - \tfrac{1}{4} f_{\beta\delta}{}^I f_{I\alpha}{}^\gamma + \tfrac{1}{4} f_{\alpha\delta}{}^I f_{I\beta}{}^\gamma. \tag{E9}
$$

The Ricci tensor $\rho_{\alpha\beta} := R_{\gamma\alpha}{}^\gamma{}_\beta$ is then

$$
\rho_{\alpha\beta} = \tfrac{1}{4} f_\alpha{}^{IJ} f_{\beta IJ} + \tfrac{1}{2} f_\alpha{}^{\gamma i} f_{\beta\gamma i} + \tfrac{1}{2} f_\beta{}^{\gamma i} f_{\alpha\gamma i}. \tag{E10}
$$

The explicit form of the structure constants in our base then yields

$$
\rho_{\alpha\beta} = 8 \delta_{\alpha\beta}, \tag{E11}
$$

or in curvilinear coordinates $\rho_{\mu\nu} dx^\mu \otimes dx^\nu = 8 ds^2_{\mathcal{H}}$.

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L^p estimates on a time-inhomogeneous diffusion process

Litan Yan[a)]
Department of Mathematics, College of Science, Donghua University, Shanghai 200051, People's Republic of China

Ligang Lu and Zhiqiang Xu
Basic College, Zhejiang Wanli University, Qiuai, Ningbo 315101, People's Republic of China

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In this paper we consider the diffusion process X determined by the one-variable time-dependent Fokker-Planck equation, $(\partial/\partial t)P(y,t)=-g(t)(\partial/\partial y)yP(y,t)+\frac{1}{2}f(t)^2(\partial^2/\partial y^2)P(y,t)$, where $f,g:\mathbb{R}_+\to\mathbb{R}_+$ are two continuous functions, i.e., X satisfies Itô stochastic differential equation, $\mathrm{d}X_t=f(t)\mathrm{d}B_t-g(t)X_t\,\mathrm{d}t$, where B is a standard Brownian motion starting at zero. We obtain L^p estimates on the process, and we show that $\|\sqrt{\log(1+J_\tau)}\|_p$ and $\|\sup_{0\leqslant t\leqslant\tau}|a(t)X_t|\|_p$ are equivalent for all stopping times τ of B, where $J_t=\int_0^t a^2(s)f^2(s)\mathrm{d}s$ and $a:\mathbb{R}_+\to\mathbb{R}_+$ the solution to the equation $(\mathrm{d}a/\mathrm{d}t)-g(t)a=-a^3f^2(t)$, $a(0)=1$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2000208]

I. INTRODUCTION

The Fokker-Planck equation (see, for example, Refs. 4, 19, and 22) is one of the most celebrated equations in Physics, since it has been very useful for studying dynamic behavior of stochastic differential equations driven by Gaussian noises. It is a special type of master equation, which is often used as an approximation to the actual equation or as a model for more general Markov processes. We have known that the linear Fokker-Planck equation

$$\frac{\partial}{\partial t}P(y,t)=-\lambda\frac{\partial}{\partial y}yP(y,t)+\frac{1}{2}\nu\frac{\partial^2}{\partial y^2}P(y,t), \tag{1.1}$$

arises in many fields of applied sciences such that statistical mechanics, chemistry, mathematical finance (see Refs. 4, 19, and 22). Such that a drift-diffusion equation can be derived from the Langevin equation

$$\mathrm{d}V_t=-\lambda V_t\,\mathrm{d}t+\nu^{1/2}\,\mathrm{d}B_t,\quad V_0=x, \tag{1.2}$$

where B is a standard Brownian motion starting at 0, to model the Brownian motion of particles in thermodynamical equilibrium. In this case, the parameters λ and ν are two positive constants which represent, respectively, the friction term and the temperature of the system. The stationary Markov process determined by the linear Fokker-Planck equation (1.1) with $\lambda,\nu>0$ is the Ornstein-Uhlenbeck process. The Ornstein-Uhlenbeck process has a notable history in physics, and it is a better model to make the velocity of the particle diffusion process, and it is the solution of the Langevin equation (1.2). Clearly, we have

[a)]Electronic mail: litanyan@dhu.edu.cn

$$V_t = e^{-\lambda t}\left(x + \nu \int_0^t e^{\lambda s}\, \mathrm{d}B_s\right),$$

and furthermore, one can also write

$$V_t = xe^{-\lambda t} + \frac{\nu}{\sqrt{2\lambda}} B_{1-e^{-2\lambda t}}$$

in the sense of the same finite dimensional distributions. For more information on the Ornstein-Uhlenbeck process, see Refs. 4, 16, 18, 20, and 22.

Recently, for the Ornstein-Uhlenbeck process V with $V_0=0$, Graversen and Peskir[9] showed that there exist two universal constants $b_1, b_2 > 0$ such that the inequalities

$$\frac{b_1}{\sqrt{\beta}} E[\sqrt{\log(1+\beta\tau)}] \leqslant E \sup_{0\leqslant t\leqslant \tau} |V_t| \leqslant \frac{b_1}{\sqrt{\beta}} E[\sqrt{\log(1+\beta\tau)}] \tag{1.3}$$

hold for all stopping times τ of B, where $\beta=\lambda/\nu$. This result shows that the maximal velocity of the Brownian particle, taken up to a stopping time τ, in average behaves as $\sqrt{\log(1+\tau)}$. The main objective of this paper is to generalize this result allowing the friction term λ and the temperature ν to fluctuate with time. In this case, the Fokker-Planck equation (1.1) reads

$$\frac{\partial}{\partial t} P(y,t) = -\, g(t) \frac{\partial}{\partial y} y P(y,t) + \frac{1}{2} f(t)^2 \frac{\partial^2}{\partial y^2} P(y,t), \tag{1.4}$$

where $f, g : \mathbb{R}_+ \to \mathbb{R}_+$ are two continuous functions. Nonautonomous Fokker-Planck equations arise for instance in the study of a periodically driven Brownian rotor[1] and in this case $g(t)$ and $f(t)$ are periodic functions of time. In statistical mechanics, Eq. (1.4) arises as a natural generalization of Eq. (1.1) in the context of nonequilibrium thermodynamics.[15] Among other models, Eq. (1.4) appears in the study of the tagged particle dynamics of a heavy particle in a gas of much lighter inelastic particles. As observed by Brey, Dufty, and Santos,[3] the large particles exhibit Brownian motion and the Boltzmann-Lorentz kinetic equation satisfied by the distribution function of large particles can be reduced to a Fokker-Planck equation whose coefficients depend on the temperature of the surrounding gas. Granular gases being nonequilibrium systems, this temperature turns out to be time dependent and the Fokker-Planck equation derived in Ref. 3 is of the shape (1.4). Furthermore, in Ref. 14, Lods and Toscani analyzed the asymptotic behavior of the time-dependent Fokker-Planck equation (1.1).

Clearly, the time-inhomogeneous diffusion processes X determined by Eq. (1.4) is the unique strong solution to the stochastic differential equation

$$\mathrm{d}X_t = f(t)\mathrm{d}B_t - g(t)X_t\, \mathrm{d}t, \quad X_0 = y. \tag{1.5}$$

According to Ref. 12, the process X is called the *Ornstein-Uhlenbeck type process*. Our starting point is Theorem 2.1, where, we show that for all stopping times τ and all $0<p<\infty$, the inequalities

$$\frac{1}{b_p} \left\| \sqrt{\log(1+J_\tau)} \right\|_p \leqslant \left\| \sup_{0\leqslant t\leqslant \tau} |a(t)X_t| \right\|_p \leqslant \sqrt{2} b_p \left\| \sqrt{\log(1+J_\tau)} \right\|_p \tag{1.6}$$

hold with $b_p = 3(e+ep)^{(1+p)/p}$, where $J_t = \int_0^t a^2(s) f^2(s) \mathrm{d}s$ and $a : \mathbb{R}_+ \to \mathbb{R}_+$ the solution to the equation

$$\frac{\mathrm{d}a}{\mathrm{d}t} - g(t)a = -\, a^3 f^2(t), \quad a(0) = 1.$$

As an interesting related problem, we consider the process X given by the equation

$$dX_t = 2f(t)\sqrt{X_t}\,dB_t + \delta g(t)dt, \quad X_0 = 0 \tag{1.7}$$

with $\delta > 0$. Clearly, If $f \equiv 1$ and $g \equiv 1$, then the squares of the solution is a Bessel process of dimension $\delta > 0$ starting at $\sqrt{x_0}$ (see Refs. 6, 7, and 18 for Bessel processes). For the process X given by (1.7) we show that the inequalities

$$\frac{\delta}{C_p}\left\|\int_0^\tau g(t)dt\right\|_p \leqslant \left\|\sup_{0\leqslant t\leqslant\tau} X_t\right\|_p \leqslant \delta C_p\left\|\int_0^\tau g(t)dt\right\|_p$$

hold for all stopping times τ and all $0 < p < \infty$, where $C_p = 9(e+2ep)^{(1+2p)/p}$. This extends the inequalities with $\delta \geqslant 1$ obtained by Graversen and Peskir[8] (see also DeBlassie,[5] Dubins *et al.*,[6] Rosenkrantz and Sawyer[21]). (Also see Ref. 10.)

II. RESULTS AND PROOFS

In this section we give L^p estimates on the time-inhomogeneous diffusion process determined by Eq. (1.4) and some related results. In order to obtain these inequalities we need some preliminaries.

Let $a: \mathbb{R}_+ \to \mathbb{R}_+$ be the solution to the equation

$$\frac{da}{dt} - g(t)a = -a^3 f^2(t), \quad a(0) = 1 \tag{2.1}$$

and let for $x \in \mathbb{R}$,

$$h(x) = 2\int_0^x e^{z^2}\,dz \int_0^z e^{-s^2}\,ds. \tag{2.2}$$

For $x \in \mathbb{R}, t \geqslant 0$ we set $F(t,x) = h(a(t)x)$. Then F satisfies

$$\frac{\partial F}{\partial t} - g(t)x\frac{\partial F}{\partial x} + \frac{1}{2}f^2(t)\frac{\partial^2 F}{\partial x^2} = a^2(t)f^2(t) \tag{2.3}$$

and $F(t,0) = (\partial F/\partial x)(t,0) = 0$ for all $t \geqslant 0$.

On the other hand, it is not difficult to show that

$$e^{x^2/2} - 1 \leqslant h(x) \leqslant e^{x^2} - 1 \quad (x \geqslant 0) \tag{2.4}$$

hold. For $x \geqslant 0$ we define the function $H_p: \mathbb{R}_+ \to \mathbb{R}_+$ by

$$H_p(h(x)) = x^p \quad (p > 0).$$

Then H_p is an increasing continuous function on $\mathbb{R}_+$ with $H_p(0) = 0$. For $x \geqslant 0$ we set

$$\tilde{H}_p(x) = x\int_x^\infty \frac{1}{s}dH_p(s) + 2H_p(x).$$

Lemma 2.1: Let H_p and $\tilde{H}_p$ be defined as above. Then for all $p > 0$ we have

$$\log^{p/2}(1+x) \leqslant H_p(x) \leqslant 2^{p/2}\log^{p/2}(1+x) \quad (x \geqslant 0), \tag{2.5}$$

and for $0 < p < 2$ we have

$$\tilde{H}_p(x) \leqslant \frac{4-p}{2-p}H_p(x) \quad (x \geqslant 0). \tag{2.6}$$

Proof: The inequalities (2.5) follows from (2.4). To prove (2.6), it now is enough to assume that

$$H_p(x) = A_p \log^{p/2}(1+x) \quad (p > 0)$$

for some constant $A_p > 0$ depending only on p. For $x \geqslant 0$ we set $G_p(x) \equiv [x/H_p(x)] \int_x^\infty (1/s) \mathrm{d}H_p(s)$. An elementary calculation can show that for all $x \geqslant 0$ and all $0 < p < 2$,

$$\lim_{x \downarrow 0} G_p(x) = \frac{p}{2-p}, \quad \lim_{x \to +\infty} G(x) = 0$$

and

$$0 \leqslant G_p(x) \leqslant \frac{p}{2-p}.$$

It follows that

$$\widetilde{H}_p(x) = x \int_x^\infty \frac{1}{s} \mathrm{d}H_p(s) + 2H_p(x) \leqslant \frac{4-p}{2-p} H_p(x)$$

for all $x \geqslant 0$ and all $0 < p < 2$. This completes the proof. □

Lemma 2.2: Let $D = (D_t)_{t \geqslant 0}$ be a non-negative right-continuous process, and let $A = (A_t)_{t \geqslant 0}$ be an increasing continuous process with $A_0 = 0$. Assume that $H : \mathbb{R}_+ \to \mathbb{R}_+$ is an increasing continuous function with $H(0) = 0$. If for all bounded stopping times τ

$$E[D_\tau] \leqslant E[A_\tau],$$

then

$$E(\sup_{0 \leqslant t \leqslant \tau} H(D_t)) \leqslant E[\widetilde{H}(A_\tau)]$$

holds for all stopping times τ, where $\widetilde{H} : \mathbb{R}_+ \to \mathbb{R}_+$ is defined by

$$\widetilde{H}(x) = x \int_x^\infty \frac{1}{s} \mathrm{d}H(s) + 2H(x), \quad x \geqslant 0.$$

The proof of the lemma above can be found in (Ref. 18, pp. 162–163) (also see Lemma 2.1 in Ref. 17), and the following lemma is a modification of Lemma 1.1 in Ref. 13, and it is a useful technique to obtain L^p estimates of random variables, which is proved in Ref. 11 (see also Ref. 2).

Lemma 2.3 (Ref. 11): Let A and B be two continuous, $(\mathcal{F}_t)$-adapted, increasing processes, with $A_0 = 0$ and $B_0 = 0$. If there exist some constants $\alpha, \beta > 0$ such that

$$E[(A_T^\beta - A_S^\beta)^\alpha] \leqslant \|B_T\|_\infty^{\alpha\beta} P(S < T)$$

holds for all couples (S, T) of stopping times S, T with $S \leqslant T$. Then, for any $0 < p < \infty$, we have

$$E[A_\infty^p] \leqslant (e + ep/\alpha\beta)^{1+p/\beta} E[B_\infty^p].$$

Theorem 2.1: *Let the diffusion process X be given by the equation*

$$\mathrm{d}X_t = f(t)\mathrm{d}B_t - g(t)X_t \, \mathrm{d}t \tag{2.7}$$

with $X_0 = 0$, where $f, g : \mathbb{R}_+ \to \mathbb{R}_+$ are two continuous functions, and let $a : \mathbb{R}_+ \to \mathbb{R}_+$ be the solution to Eq. (2.1). *For $t \geqslant 0$ we define*

$$J_t = \int_0^t a^2(s) f^2(s) \mathrm{d}s.$$

Then for all $0<p<\infty$ *and all stopping times* τ, *we have*

$$b_p^{-1}\|\sqrt{\log(1+J_\tau)}\|_p \leqslant \|\sup_{0\leqslant t\leqslant\tau}|a(t)X_t|\|_p \leqslant \sqrt{2}b_p\|\sqrt{\log(1+J_\tau)}\|_p, \tag{2.8}$$

where $b_p=3(e+ep)^{(1+p)/p}$, *in particular, for* $0<p<2$ *we have*

$$\frac{2-p}{4-p}E[\log^{p/2}(1+J_\tau)] \leqslant E[\sup_{0\leqslant t\leqslant\tau}|a(t)X_t|^p] \leqslant 2^{p/2}\frac{4-p}{2-p}E[\log^{p/2}(1+J_\tau)].$$

Proof: Let a and h be given by (2.1) and (2.2), respectively, and let $F(t,x)=h(a(t)x)$ for $t\geqslant 0$, $x\in\mathbb{R}$. Noting that h is even, we get by the Itô formula and Eq. (2.3),

$$h(|a(t)X_t|)=h(a(t)X_t)=F(t,X_t)=\int_0^t\frac{\partial}{\partial s}F(s,X_s)\mathrm{d}s+\int_0^t f(s)\frac{\partial}{\partial x}F(s,X_s)\mathrm{d}B_s-\int_0^t g(s)X_s\frac{\partial}{\partial x}F(s,X_s)\mathrm{d}s$$
$$+\frac{1}{2}\int_0^t f^2(s)\frac{\partial^2}{\partial x^2}F(s,X_s)\mathrm{d}s=\int_0^t f(s)\frac{\partial}{\partial x}F(s,X_s)\mathrm{d}B_s+\int_0^t a^2(s)f^2(s)\mathrm{d}s.$$

It follows that for all bounded stopping times τ

$$E[F(\tau,X_\tau)]=E[J_\tau]. \tag{2.9}$$

Now, for these processes $D=(F(t,X_t);t\geqslant 0)$ and $A=(J_t;t\geqslant 0)$, by using Lemma 2.1 and Lemma 2.2, we get

$$E[\sup_{0\leqslant t\leqslant\tau}|a(t)X_t|]=E[\sup_{0\leqslant t\leqslant\tau}H_p(F(t,X_t))]\leqslant E[\tilde{H}_p(J_\tau)]\leqslant\frac{4-p}{2-p}E[H_p(J_\tau)]$$
$$\leqslant 2^{p/2}\frac{4-p}{2-p}E[\log^{p/2}(1+J_\tau)]$$

for all stopping times τ and $0<p<2$. On the other hand, we see that (2.9) implies

$$E[J_\tau]\leqslant E[\sup_{0\leqslant t\leqslant\tau}F(t,X_t)]$$

for all bounded stopping times τ. Consequently, by using Lemma 2.1 and Lemma 2.2 to these processes $D=(J_t;t\geqslant 0)$ and $A=(\sup_{0\leqslant s\leqslant t}F(s,X_s);t\geqslant 0)$, we get

$$E[H_p(J_\tau)]\leqslant E[\tilde{H}_p(\sup_{0\leqslant t\leqslant\tau}F(t,X_t))]\leqslant\frac{4-p}{2-p}E[H_p(\sup_{0\leqslant t\leqslant\tau}F(t,X_t))]=\frac{4-p}{2-p}E[\sup_{0\leqslant t\leqslant\tau}|a(t)X_t|^p]$$

for all stopping times τ and all $0<p<2$. Thus, we obtain the following inequalities:

$$\frac{2-p}{4-p}E[\log^{p/2}(1+J_\tau)]\leqslant E[\sup_{0\leqslant t\leqslant\tau}|a(t)X_t|^p]\leqslant 2^{p/2}\frac{4-p}{2-p}E[\log^{p/2}(1+J_\tau)] \tag{2.10}$$

for all stopping times τ and all $0<p<2$.

Next, we extend (2.10) to all $0<p<\infty$ by using Lemma 2.3. Consider any couple (S,T) of stopping times S, T with $S\leqslant T$. Then, from the left inequality in (2.10) with $p=1$ and the inequality

$$\log(1+x)-\log(1+y)\leqslant\log(1+x-y)\quad(x\geqslant y\geqslant 0),$$

we find

$$E[\sqrt{\log(1+J_T)}-\sqrt{\log(1+J_S)}] \leqslant E[\sqrt{\log(1+J_T-J_S)}] \leqslant E[\sqrt{\log(1+J_{T1_{\{T>S\}}})}]$$
$$\leqslant 3E[\sup_{0\leqslant t\leqslant T1_{\{T>S\}}}|a(t)X_t|] \leqslant \|3\sup_{0\leqslant t\leqslant T}|a(t)X_t|\|_\infty P(T>S),$$

where 1_A stands for the indicate function of set A, which shows for all stopping times T and all $0<p<\infty$,

$$\|\sqrt{\log(1+J_T)}\|_p \leqslant 3(e+ep)^{(1+p)/p}\|\sup_{0\leqslant t\leqslant T}|a(t)X_t|\|_p$$

by Lemma 2.3 with $\alpha=\beta=1$.

To prove the right inequality in (2.8), for any couple (S,T) of stopping times S, T with $S \leqslant T$, we have by the right inequality in (2.10) with $p=1$,

$$E[\sup_{0\leqslant t\leqslant T}|a(t)X_t|-\sup_{0\leqslant t\leqslant S}|a(t)X_t|] \leqslant E[\sup_{S\leqslant t\leqslant T}\|a(t)X_t|-|a(S)X_S\|1_{\{S<T\}}]$$
$$\leqslant E[\sup_{0\leqslant t\leqslant (T-S)1_{\{T>S\}}}|a(t+S)X_{t+S}|]$$
$$\leqslant 3\sqrt{2}E[\sqrt{\log(1+J_T)}1_{\{T>S\}}] \leqslant \|3\sqrt{2}\sqrt{\log(1+J_T)}\|_\infty P(S<T),$$

which shows for all stopping times T and all $0<p<\infty$,

$$\|\sup_{0\leqslant t\leqslant T}|a(t)X_t|\|_p \leqslant 3\sqrt{2}(e+ep)^{(1+p)/p}\|\sqrt{\log(1+J_T)}\|_p$$

by Lemma 2.3 with $\alpha=\beta=1$. This completes the proof. □

We now consider some very interesting examples. Let $t\mapsto K(t)$ be a differentiable function on $\mathbb{R}_+$ with $K(t)>0$ for all $t\geqslant 0$ and let $X_t=B_t/K(t)$, $t\geqslant 0$, where B is a standard Brownian motion starting at zero. Then we have by Itô's formula

$$\mathrm{d}X_t=\frac{1}{K(t)}\mathrm{d}B_t-\frac{K'(t)}{K(t)}X_t\,\mathrm{d}t$$

with $X_0=0$. On the other hand, from (2.1) we have for all $t\geqslant 0$,

$$a(t)^{-2}=e^{-2\int_0^t g(s)\mathrm{d}s}\left(2\int_0^t f^2(s)e^{2\int_0^s g(z)\mathrm{d}z}\,\mathrm{d}s+1\right)=\frac{1}{K(t)^2}(2t+K(0)),$$

since $f(t)=1/K(t)$ and $g(t)=K'(t)/K(t)$.

Without loss of generality, one may assume $K(0)=2$. It follows that

$$J_t=\int_0^t a^2(s)f^2(s)\mathrm{d}s=\frac{1}{2}\log(1+t)$$

for all $t\geqslant 0$. Thus, the following corollary follows from Theorem 2.1.

Corollary 2.1 *(Ref. 9): Let B be a standard Brownian motion starting at zero. Then we have*

$$c_p\|\log^{1/2}(1+\log(1+\tau))\|_p \leqslant \left\|\sup_{0\leqslant t\leqslant \tau}\frac{|B_t|}{\sqrt{1+t}}\right\|_p \leqslant C_p\|\log^{1/2}(1+\log(1+\tau))\|_p$$

for all $0<p<\infty$ and all stopping times τ of B, where c_p and C_p are some positive constants depending only on p.

From the above we can conjecture that the following inequalities hold:

$$c_p\|\sqrt{\log(1+L_{m+1}(\tau))}\|_p \leqslant \left\| \sup_{0\leqslant t\leqslant \tau} \frac{|B_t|}{\prod_{i=0}^{m}(1+L_i(t))^{1/2}} \right\|_p \leqslant C_p\|\sqrt{\log(1+L_{m+1}(\tau))}\|_p$$

for all stopping times τ of B, where c_p and C_p are some positive constants depending only on p, and the function $t\mapsto L_{m+1}(t)$ inductively by

$$L_{m+1}(t)=\log(1+L_m(t)) \quad (m=0,1,2,\ldots)$$

with $L_0(t)=t$.

At the end of this paper, we consider the equation

$$\mathrm{d}X_t = 2f(t)\sqrt{X_t}\,\mathrm{d}B_t + \delta g(t)\mathrm{d}t, \quad X_0 = x_0 \geqslant 0, \tag{2.11}$$

where $\delta>0$ and f, g two positive, bounded continuous functions defined on $\mathbb{R}_+$. Then we have the following.

Theorem 2.2: *Let X be a process given by* (2.16) *with $x_0=0$. Then the inequalities*

$$\frac{\delta}{C_p}\left\|\int_0^\tau g(t)\mathrm{d}t\right\|_p \leqslant \|\sup_{0\leqslant t\leqslant\tau} X_t\|_p \leqslant \delta C_p\left\|\int_0^\tau g(t)\mathrm{d}t\right\|_p \tag{2.12}$$

hold with $0<p<\infty$ for all stopping times τ, where $C_p=9(e+2ep)^{(1+2p)/p}$.

It is easy to see that Eq. (2.11) admits a unique solution and the solution is strong, and furthermore the solution $X_t\geqslant 0$ for all $x_0\geqslant 0$. If $f\equiv 1$ and $g\equiv 1$, then the solution is called the squares of a Bessel process of dimension $\delta>0$ starting at $\sqrt{x_0}$ (see Refs. 6, 7, and 18 for Bessel processes). Thus, the theorem above extends the inequalities with $\delta\geqslant 1$ obtained by Graversen and Peskir[8] (see also DeBlassie,[5] Dubins *et al.*,[6] Rosenkrantz and Sawyer[21]).

Proof of Theorem 2.2: Let X be a process given by (2.16) with $x_0=0$. It follows that for all bounded stopping times τ,

$$E[X_\tau] = \delta E\left[\int_0^\tau g(t)\mathrm{d}t\right]. \tag{2.13}$$

Consequently, from Lemma 2.2 we get for all stopping times τ,

$$E[(\sup_{0\leqslant t\leqslant\tau} X_t)^p] \leqslant \delta^p \frac{2-p}{1-p} E\left[\left(\int_0^\tau g(t)\mathrm{d}t\right)^p\right] \tag{2.14}$$

by assuming $H_p(x)=x^p$ for $x\geqslant 0$ and $0<p<1$. On the other hand, we see that (2.13) implies

$$\delta E\left[\int_0^\tau g(t)\mathrm{d}t\right] \leqslant E[\sup_{0\leqslant t\leqslant\tau} X_t]$$

for all bounded stopping times τ. From Lemma 2.2 with $H_p(x)=x^p(0<p<1)$ it follows that

$$\delta^p E\left[\left(\int_0^\tau g(t)\mathrm{d}t\right)^p\right] \leqslant \frac{2-p}{1-p} E[(\sup_{0\leqslant t\leqslant\tau} X_t)^p] \tag{2.15}$$

for all stopping times τ. Thus, we obtain the following inequalities:

$$\delta^p \frac{1-p}{2-p} E\left[\left(\int_0^t g(t)\mathrm{d}t\right)^p\right] \leqslant E[(\sup_{0\leqslant t\leqslant T} X_t)^p] \leqslant \delta^p \frac{2-p}{1-p} E\left[\left(\int_0^\tau g(t)\mathrm{d}t\right)^p\right] \tag{2.16}$$

for all stopping times τ and all $0<p<1$.

Now, it is not difficult to extend (2.16) to all $0<p<\infty$ by using Lemma 2.3. Indeed, for any couple (S,T) of stopping times S, T with $S\leqslant T$ we have from (2.16) with $p=\frac{1}{2}$,

$$E\left[\sqrt{\int_0^T g(t)\mathrm{d}t}-\sqrt{\int_0^S g(t)\mathrm{d}t}\right]\leqslant E\left[\sqrt{\int_0^{T1_{\{T>S\}}} g(t)\mathrm{d}t}\right]\leqslant \frac{3}{\sqrt{\delta}}E\left[\sqrt{\sup_{0\leqslant t\leqslant T1_{\{T>S\}}} X_t}\right]$$
$$\leqslant \frac{3}{\sqrt{\delta}}E\left[\sqrt{\sup_{0\leqslant t\leqslant T} X_t}1_{\{T>S\}}\right]\leqslant \left\|\frac{9}{\delta}X_T^*\right\|_\infty^{1/2} P(T>S)$$

and

$$E\left[\sqrt{\sup_{0\leqslant t\leqslant T} X_t}-\sqrt{\sup_{0\leqslant t\leqslant T} X_s}\right]\leqslant E\left[\sqrt{\sup_{S\leqslant t\leqslant T}|X_t-X_S|1_{\{S<T\}}}\right]=E\left[\sqrt{\sup_{0\leqslant t\leqslant (T-S)1_{\{S<T\}}}|X_{t+S}-X_S|}\right]$$
$$\leqslant 3\sqrt{\delta}E\left[\sqrt{\int_0^{T1_{\{T>S\}}} g(t)\mathrm{d}t}\right]\leqslant \left\|9\delta\int_0^T g(t)\mathrm{d}t\right\|_\infty^{1/2} P(S<T).$$

Combining these with Lemma 2.3, we obtain the inequalities (2.12).

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The Perron-Frobenius operators, invariant measures and representations of the Cuntz-Krieger algebras

Katsunori Kawamura[a)]
Research Institute for Mathematical Sciences, Kyoto University, Kyoto 606-8502, Japan

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For a transformation F on a measure space (X,μ), we show that the Perron-Frobenius operator of F can be written by a representation $(L_2(X,\mu),\pi)$ of the Cuntz-Krieger algebra $\mathcal{O}_A$ associated with F when F satisfies some assumption. Especially, when $\mathcal{O}_A$ is the Cuntz algebra $\mathcal{O}_N$ and $(L_2(X,\mu),\pi)$ in the above is some irreducible representation of $\mathcal{O}_N$, then there is an F-invariant measure on X which is absolutely continuous with respect to μ. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2000209]

I. INTRODUCTION

The representation theory of groups is an important tool for modern physics. For a family of invertible transformations, such method is useful. On the other hand, transformations in dynamical systems are not always invertible. We show a relation between the theory of dynamical systems and the representation theory of operator algebras by the Perron-Frobenius operator. Invariant measures (especially, Haar measures) play an important role in the representation theory of Lie groups and harmonic analysis. On the other hand, invariant measures of noninvertible transformations are studied in Refs. 7–9 by the Perron-Frobenius operators of dynamical systems. By using the Perron-Frobenius operators, the characterization of a given dynamical system and the construction of invariant measure are obtained. We show their roles in representation theory of operator algebras in this paper.

Let $L_p(X,\mu)$ be the set of all complex-valued measurable functions ϕ on a measure space (X,μ) satisfying $\|\phi\|_{L_p}<\infty$ and let $L_p(X,\mu;\mathbf{R})$ be the subset of all real-valued functions in $L_p(X,\mu)$ for $p=1,2,\infty$. For a nonsingular transformation F on X, that is, $\mu(F^{-1}(A))=0$ if $\mu(A)=0$ for $A\subset X$, P_F is the *Perron-Frobenius operator* of F if P_F is the operator on $L_1(X,\mu)$ which satisfies

$$\int_A (P_F\psi)(x)\mathrm{d}\mu(x)=\int_{F^{-1}(A)}\psi(x)\mathrm{d}\mu(x)\quad(\forall\,\psi\in L_1(X,\mu)) \tag{1.1}$$

for each measurable subset A of X.[7] By (1.1), $P_F\psi$ is uniquely determined as an element in $L_1(X,\mu)$ for each $\psi\in L_1(X,\mu)$. For $\psi\in L_1(X,\mu)$ and $\theta\in L_\infty(X,\mu)$, we obtain $\int_X\theta(F(x))\psi(x)\mathrm{d}\mu(x)=\int_X\theta(x)(P_F\psi)(x)\mathrm{d}\mu(x)$. From this, P_F is a bounded linear operator on $L_1(X,\mu)$ and $\|P_F\psi\|_{L_1}\leqslant\|\psi\|_{L_1}$ for each $\psi\in L_1(X,\mu;\mathbf{R})$. Further, a positive function $\rho\in L_1(X,\mu)$ satisfies $P_F\rho=\rho$ if and only if ρ is the density of an *F-invariant measure*, that is, the following holds for any $\psi\in L_1(X,\mu)$:

$$\int_X\psi(F(x))\rho(x)\mathrm{d}\mu(x)=\int_X\psi(x)\rho(x)\mathrm{d}\mu(x). \tag{1.2}$$

a)Electronic mail: kawamura@kurims.kyoto-u.ac.jp

In order to describe both the Perron-Frobenius operators and representations of the Cuntz-Krieger algebras simultaneously, we introduce branching function systems on a measure space (X,μ). A family $f=\{f_i\}_{i=1}^N$ of maps on X is a *semibranching function system* if there is a finite family $\{D_i\}_{i=1}^N$ of measurable subsets of X such that f_i is a measurable map from D_i to $R_i \equiv f_i(D_i)$, $\mu(X\backslash R_1\cup\cdots\cup R_N)=0$, $\mu(R_i\cap R_j)=0$ when $i\neq j$ and there is the Radon-Nikodým derivative Φ_{f_i} of $\mu\circ f_i$ with respect to μ and $\Phi_{f_i}>0$ almost everywhere in D_i for $i=1,\ldots,N$. A map F on X is called the *coding map* of a semibranching function system $f=\{f_i\}_{i=1}^N$ if $F\circ f_i=id_{D_i}$ for $i=1,\ldots,N$.

For a semibranching function system $f=\{f_i\}_{i=1}^N$ with the coding map F, define a family $\{S(f_i)\}_{i=1}^N$ of operators on $L_2(X,\mu)$ by

$$(S(f_i)\phi)(x)\equiv\chi_{R_i}(x)\cdot\{\Phi_F(x)\}^{1/2}\cdot\phi(F(x))\quad(\phi\in L_2(X,\mu)),\tag{1.3}$$

where χ_{R_i} is the characteristic function of R_i. Then $S(f_i)$ is a partial isometry and $S(f_i)S(f_j)=S(f_i\circ f_j)$ when $D_j\subset R_i$. For $N\geqslant 2$, let A be an $N\times N$ matrix which consists of elements 0 or 1 and any column and row are not 0. A semibranching function system $f=\{f_i\}_{i=1}^N$ is an *A-branching function system* if $\mu(D_i\backslash\cup_{j;a_{ij}=1}R_j)=0$ for each $i=1,\ldots,N$. For an A-branching function system $f=\{f_i\}_{i=1}^N$,

$$\pi_f(s_i)\equiv S(f_i)\quad(i=1,\ldots,N),\tag{1.4}$$

defines a representation $(L_2(X,\mu),\pi_f)$ of the Cuntz-Krieger algebra $\mathcal{O}_A$.[5]

Mori computed eigenvalues of the Perron-Frobenius operator by algebraic method for a concrete example in Ref. 10. On the other hand, we were interested in construction of representations of the Cuntz algebra by using interval dynamical systems in order to find new examples.[4,5] He pointed out the similarity among his study and ours. Hence we obtain Theorem 1.1 and Theorem 1.2.

Theorem 1.1: *For an A-branching function system $f=\{f_i\}_{i=1}^N$ with the coding map F, the following holds:*

$$(P_F\psi)(x)=\{(\pi_f(s_1^*)\sqrt{\psi})(x)\}^2+\cdots+\{(\pi_f(s_N^*)\sqrt{\psi})(x)\}^2$$

for any positive function $\psi\in L_1(X,\mu)$ where $\sqrt{\psi}(x)\equiv\sqrt{\psi(x)}$.

Theorem 1.2: *Assume that F is the coding map of an A-branching function system $f=\{f_i\}_{i=1}^N$ on a measure space (X,μ) and $b_i\equiv\Phi_{f_i}$ is constant for $i=1,\ldots,N$ and $\mu(X)<\infty$. Then the following holds:*

(i) *Define a subspace $V\equiv\mathrm{Lin}\langle\{\chi_{R_1},\ldots,\chi_{R_N}\}\rangle$ of $L_2(X,\mu)$. Then $P_FV\subset V$ where R_i is the image of f_i.*

(ii) *For a diagonal matrix $B\equiv\mathrm{diag}(b_1,\ldots,b_N)\in M_N(\mathbf{R})$, the following identity of matrices holds:*

$$P_{F|V}=BA,$$

where $P_{F|V}$ is the matrix representation over the basis $\chi_{R_1},\ldots,\chi_{R_N}$ of V and the rhs is the product of matrices.

In Theorem 1.2 (ii), the eigenvalues of the Perron-Frobenius operator associated with F depend on not only A but also B. In this sense, eigenvalues of the Perron-Frobenius operator have the information of a representation of the Cuntz-Krieger algebra.

It is an important problem to construct the invariant measure for a given dynamical system. For example, Lasota-York theorem shows a construction of invariant measure by using the Perron-Frobenius operator of a dynamical system.[8] We show the condition of existence of invariant measure from the viewpoint of representation theory of the Cuntz algebra.

$f=\{f_i\}_{i=1}^N$ is a *branching function system* if $f=\{f_i\}_{i=1}^N$ is an A-branching function system for a matrix $A=(a_{ij})$, $a_{ij}=1$ for each $i,j=1,\ldots,N$. In this case, $(L_2(X,\mu),\pi_f)$ is a representation of the

Cuntz algebra $\mathcal{O}_N$. For $z=(z_i)_{i=1}^N \in S^{N-1} \equiv \{y \in \mathbf{R}^N : \|y\|=1\}$, $(\mathcal{H}, \pi)$ is $GP(z)$ of $\mathcal{O}_N$ (Ref. 6) if there is a unit cyclic vector $\Omega \in \mathcal{H}$ such that

$$\pi(z_1 s_1 + \cdots + z_N s_N)\Omega = \Omega. \tag{1.5}$$

We call Ω by the *GP vector* of $(\mathcal{H}, \pi)$. In this case, there is $g \in O(N) \subset U(N)$ such that $(\pi \circ \alpha_g)(s_1)\Omega = \Omega$ where α is the canonical action of $U(N)$ on $\mathcal{O}_N$. This implies that $(\mathcal{H}, \pi \circ \alpha_g)$ is an irreducible permutative representation of $\mathcal{O}_N$.[1] Hence $GP(z)$ of $\mathcal{O}_N$ exists uniquely up to unitary equivalence and it is irreducible. Further we see that $GP(z) \sim GP(y)$ if and only if $z=y$ where $\sim$ means the unitary equivalence.

Theorem 1.3: *Let F be the coding map of a branching function system f on a measure space (X, μ). If there is $z \in S^{N-1}$ such that $(L_2(X, \mu), \pi_f)$ is $GP(z)$ with the GP vector $\Omega \in L_2(X, \mu; \mathbf{R})$, then there is a probabilistic F-invariant measure ν on X which is absolutely continuous with respect to μ and it is given as follows:*

$$\mathrm{d}\nu(x) \equiv \{\Omega(x)\}^2 \mathrm{d}\mu(x) \quad (x \in X).$$

In Sec. II, we show the main theorems. It is explained that (1.5) implies the eigenequation of the Perron-Frobenius operator. In Sec. III, we show concrete examples.

II. PROOFS OF THE MAIN THEOREMS

For $N \geqslant 2$, let $M_N(\{0,1\})$ be the set of all $N \times N$ matrices such that each element is 0 or 1 and any row and column is not 0. For $A=(a_{ij}) \in M_N(\{0,1\})$, $\mathcal{O}_A$ is the *Cuntz-Krieger algebra by A* if $\mathcal{O}_A$ is a C*-algebra which is universally generated by partial isometries $s_1, \ldots, s_N$ and they satisfy $s_i^* s_i = \Sigma_{j=1}^N a_{ij} s_j s_j^*$ for $i=1, \ldots, N$ and $\Sigma_{i=1}^N s_i s_i^* = I$.[3] Especially, when $a_{ij}=1$ for each $i, j=1, \ldots, N$, $\mathcal{O}_A$ is the *Cuntz algebra* $\mathcal{O}_N$.[2] In this paper, any representation is unital and $*$-preserving.

Proof of Theorem 1.1: By (1.3), the adjoint operator $S(f_i)^*$ of $S(f_i)$ on $L_2(X, \mu)$ is as follows:

$$(S(f_i)^* \phi)(x) = \chi_{D_i}(x) \cdot \{\Phi_{f_i}(x)\}^{1/2} \cdot \phi(f_i(x)) \quad (\phi \in L_2(X, \mu)). \tag{2.1}$$

For the coding map F of a semibranching function system $f=\{f_i\}_{i=1}^N$, we have

$$(P_F \psi)(x) = \sum_{i=1}^N \chi_{D_i}(x) \cdot \Phi_{f_i}(x) \cdot \psi(f_i(x)) \quad (\psi \in L_1(X, \mu)). \tag{2.2}$$

(2.2) is obtained by (1.1).[7] By (2.1), (2.2), and (1.4), the statement holds. ■

Proof of Theorem 1.2: Define $v_i \equiv \chi_{R_i}$ for $i=1, \ldots, N$. By (2.1), $S(f_i)^* v_j = \Sigma_{k=1}^N b_i^{-1/2} c_{ik}^{(j)} v_k$ for $i=1, \ldots, N$ where $c_{ik}^{(j)} = \delta_{ij} b_i a_{ik}$. This implies that $S(f_i)^*|_V = (b_i^{-1/2} c_{jk}^{(i)})$ as a matrix with respect to $v_1, \ldots, v_N$ and $S(f_i)^* V \subset V$. By (2.2), $P_F = b_1^{1/2} S(f_1)^* + \cdots + b_N^{1/2} S(f_N)^*$. Hence the statements hold. ■

Corollary 2.1: Let X be a bounded closed interval of $\mathbf{R}$ and $A \in M_N(\{0,1\})$. Assume that $f=\{f_i\}_{i=1}^N$ is an A-branching function system on X and $b_i \equiv \Phi_{f_i}$ is constant for each $i=1, \ldots, N$. Then the eigenvalue of BA becomes that of P_F for the coding map F of f where $B \equiv \mathrm{diag}(b_1, \ldots, b_N)$.

Proof of Theorem 1.3: Assume that $\Omega \in L_2(X, \mu; \mathbf{R})$ satisfies $\pi_f(z_1 s_1 + \cdots + z_N s_N)\Omega = \Omega$. Define $\rho(x) \equiv \{\Omega(x)\}^2$ for $x \in X$. By Theorem 1.1 and $\pi_f(s_i)^* \Omega = z_i \Omega$, we have $P_F \rho = \rho$. Hence the statement holds. ■

Corollary 2.2: Let X be a measurable subset of $\mathbf{R}$. Assume that a piecewise C^1-class map F on X is the coding map of a branching function system $\{f_i\}_{i=1}^N$ on the measure space $(X, \mathrm{d}x)$ where $\mathrm{d}x$ is the Lebesgue measure. If $\phi_0 \in L_2(X, \mathrm{d}x; \mathbf{R})$ satisfies that

$$\sqrt{|F'(x)|}\,\phi_0(F(x)) = \sqrt{N}\phi_0(x) \quad (a.e.\ x \in X), \tag{2.3}$$

then $\mathrm{d}\mu(x) \equiv \{\phi_0(x)\}^2 \mathrm{d}x$ is an invariant measure on X with respect to F.

Proof: By (1.3) and (1.4), we see that $(\pi_f(s_1 + \cdots + s_N)\phi)(x) = \sqrt{|F'(x)|}\,\phi(F(x))$ for each $\phi \in L_2(X, \mathrm{d}x)$. From this and (2.3), $N^{-1/2} \pi_f(s_1 + \cdots + s_N)\phi_0 = \phi_0$. By Theorem 1.3 for $z=(N^{-1/2}, \ldots, N^{-1/2}) \in S^{N-1}$, the statement holds. ■

In Sec. 6.5 of Ref. 7, it is explained that intertwiners among dynamical systems bring new invariant measures from known ones. We show its unitary version as follows:

Proposition 2.3: Let F be the coding map of a branching function system $f=\{f_i\}_{i=1}^N$ on a measure space (X,μ). Assume that $(L_2(X,\mu),\pi_f)$ is $GP(z)$ for $z\in S^{N-1}$ with the GP vector $\Omega\in L_2(X,\mu;\mathbf{R})$. If ζ is a measure space isomorphism from (X,μ) to other (Y,ν) and $G\equiv\zeta\circ F\circ\zeta^{-1}$, then $\rho\equiv\{S(\zeta)\Omega\}^2$ is the density of a probabilistic G-invariant measure on Y which is absolutely continuous with respect to ν where $S(\zeta)$ is a unitary operator from $L_2(X,\mu)$ to $L_2(Y,\nu)$ defined by $(S(\zeta)\phi)(y)\equiv\{\Phi_{\zeta^{-1}}(y)\}^{1/2}\phi(\zeta^{-1}(y))$.

Proof: Define $g=\{g_i\}_{i=1}^N$ by $g_i\equiv\zeta\circ f_i\circ\zeta^{-1}$. Then G is the coding map of g. We see that $S(\zeta)\pi_f(\cdot)S(\zeta)^*=\pi_g(\cdot)$ and $\pi_g(z_1s_1+\cdots+z_Ns_N)\Omega'=\Omega'$ for $\Omega'\equiv S(\zeta)\Omega\in L_2(Y,\nu;\mathbf{R})$. Hence $(L_2(Y,\nu),\pi_g)$ is $GP(z)$ with the GP vector Ω'. By Theorem 1.3, we have the statement. ■

III. EXAMPLES

Example 3.1: Let $0<a<1$ and $X\equiv[0,1]$. Define a map F on X by $F(x)\equiv x/a$ on $R_1\equiv[0,a]$ and $F(x)\equiv-(x-1)/(1-a)$ on $R_2\equiv[a,1]$.

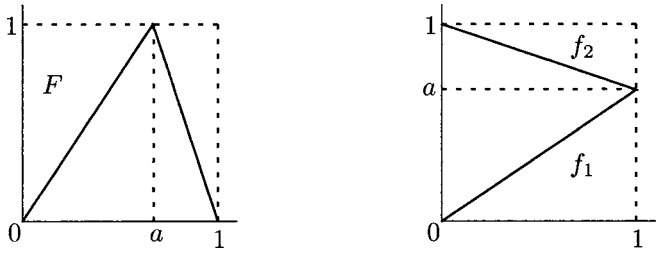

Then F is the coding map of a branching function system $f\equiv\{f_1,f_2\}$ defined by $f_i\equiv(F|_{R_i})^{-1}$ for $i=1,2$. Then $(\pi_f(s_1)\phi)(x)=a^{-1/2}\chi_{R_1}(x)\phi(x/a)$, $(\pi_f(s_2)\phi)(x)=(1-a)^{-1/2}\chi_{R_2}(x)\phi(-(x-1)/(1-a))$ for $\phi\in L_2(X,\mathrm{d}x)$.

$$(P_F\psi)(x)=a\psi(ax)+(1-a)\psi(-(1-a)x+1)\quad(\psi\in L_1(X,\mathrm{d}x)).$$

We see that Theorem 1.1 holds. The Lebesgue measure $\mathrm{d}x$ is the probabilistic invariant measure of X with respect to F. $(L_2(X,\mathrm{d}x),\pi_f)$ is $GP(\sqrt{a},\sqrt{1-a})$ of $\mathcal{O}_2$ with the GP vector 1. The invariant measure is independent in the parameter a.

Example 3.2: For $a,b\in\mathbf{R}$, $a\neq0$, define $F(x)\equiv(x-b)^2/a+b-2a$ on $X\equiv[-2|a|+b,2|a|+b]$. Define a branching function system $f=\{f_1,f_2\}$ on X by $f_i\equiv(F|_{R_i})^{-1}$, $i=1,2$ for $R_1\equiv[-2|a|+b,b]$ and $R_2\equiv[b,2|a|+b]$. Then $\pi_f(s_1+s_2)\Omega=\sqrt{2}\Omega$ for $\Omega(x)\equiv\pi^{-1/2}\{4a^2-(x-b)^2\}^{-1/4}$. We see that $(L_2(X),\pi_f)$ is $GP(2^{-1/2},2^{-1/2})$ of $\mathcal{O}_2$ with the GP vector Ω.[4] By Theorem 1.3,

$$p(x)\equiv\frac{1}{\pi}\frac{1}{\sqrt{4a^2-(x-b)^2}}$$

is the density of a probabilistic invariant measure on X with respect to F. When $a=-1/4$ and $b=1/2$, we have $F(x)=4x(1-x)$ and $\rho(x)=1/(\pi\sqrt{x(1-x)})$. This was first obtained by Ulam and von Neumann.[11]

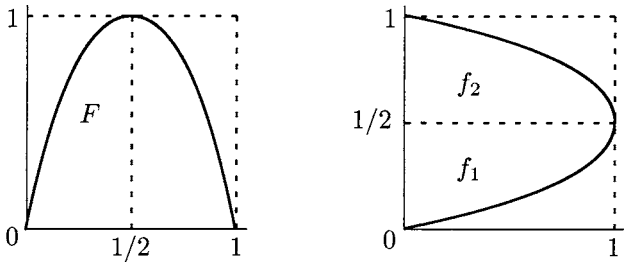

Example 3.3: For $0<a<1$, define a map $F:[0,1]\to[0,1]$ as follows:

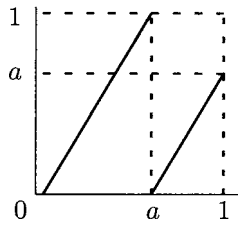

Define $R_1\equiv[0,a]$, $R_2\equiv[a,1]$, $D_1\equiv[0,1]$, $D_2\equiv[0,a]$. Then F is the coding map of the following $A=\left(\begin{smallmatrix}1&1\\1&0\end{smallmatrix}\right)$-branching function system on $X=[0,1]$: $f_i:D_i\to R_i$, $f_1(x)=ax$ for $x\in[0,1]$ and $f_2(x)=(1-a)x/a+a$ for $x\in[0,a]$. Define $v_1\equiv\chi_{[0,a]}$, $v_2\equiv\chi_{[a,1]}$, $V\equiv\mathrm{Lin}\langle\{v_1,v_2\}\rangle$. By Theorem 1.2, the matrix representation of P_F with respect to v_1, v_2 is given as follows:

$$P_{F|V}=\begin{pmatrix}a & (1-a)/a\\ a & 0\end{pmatrix}.$$

Hence its eigenvalues are $a-1$ and 1. Their normalized eigenvectors are given as follows:

$$w_1=\sqrt{\frac{1-a}{a}}\chi_{[0,a]}-\sqrt{\frac{a}{1-a}}\chi_{[a,1]},\quad w_2=\frac{1}{\sqrt{a(1+a-a^2)}}(\chi_{[0,a]}+a\chi_{[a,1]}).$$

Especially $(w_2)^2$ is the density of the invariant measure on [0,1] with respect to F.

Example 3.4: Let F be a map defined by the following graph:

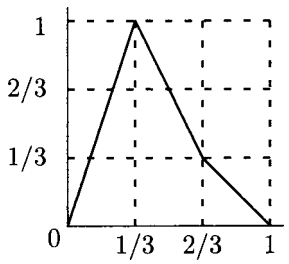

Define

$$A\equiv\begin{pmatrix}1&1&1\\0&1&1\\1&0&0\end{pmatrix},$$

$B\equiv\mathrm{diag}(1/3,1/2,1)$, $R_1\equiv[0,1/3]$, $R_2\equiv[1/3,2/3]$, $R_3\equiv[2/3,1]$, $D_1\equiv[0,1]$, $D_2\equiv[1/3,1]$, $D_3\equiv[0,1/3]$. The A-branching function system $f=\{f_1,f_2,f_3\}$, $f_i:D_i\to R_i$, $i=1,2,3$, with the coding map F is given by $f_1(x)=x/3$, $f_2(x)=-(x-1)/2+1/3$, $f_3(x)=-x+1$. From this and Theorem 1.2 (ii), $P_F|_W=BA$ where $W\equiv\mathrm{Lin}\langle\{\chi_{R_1},\chi_{R_2},\chi_{R_3}\}\rangle$. We see that 0, $-1/6$, 1 are eigenvalues of $P_F|_W$. Hence they are eigenvalues of P_F.

Example 3.5: For $A\in M_N(\{0,1\})$ and an A-branching function system $f=\{f_i\}_{i=1}^N$ on a measure

space (X,μ), $\mu(X)<\infty$, assume that $b_i \equiv \Phi_{f_i}$ is constant for each $i=1,\ldots,N$. Then $b_i = r_i/(\Sigma_{j=1}^{N} a_{ij} r_j)$ where $r_i \equiv \mu(R_i)$. When

$$A \equiv \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix},$$

we have

$$B = (b_1, b_2, b_3) = \mathrm{diag}\left(\frac{r_1}{r_2 + r_3}, \frac{r_2}{r_1 + r_3}, \frac{r_3}{r_1 + r_2 + r_3} \right).$$

For $0<a<b<1$, consider the case F on $X=[0,1]$ which graph is given as follows:

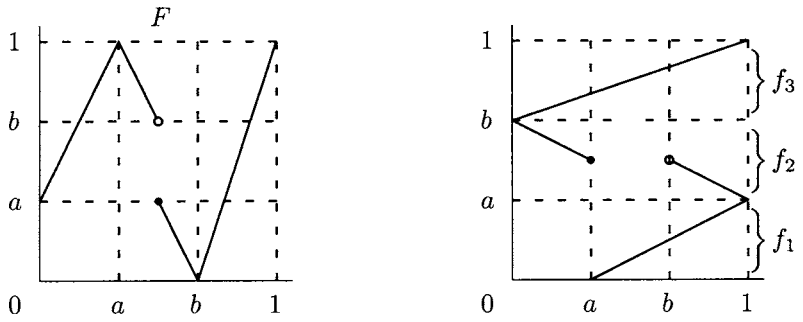

F is the coding map of an A-branching function system given as follows: $f_i : D_i \to R_i$, $i=1,2,3$,

$$\begin{cases} f_1(x) = \dfrac{a}{1-a}(x-a) \quad (x \in D_1), \\ f_2(x) = \begin{cases} -\dfrac{b-a}{1-b+a}x + b, & (x \in R_1), \\ -\dfrac{b-a}{1-b+a}(x-1) + a & (x \in R_3), \end{cases} \\ f_3(x) = (1-b)x + b \quad (x \in [0,1]), \end{cases}$$

where $R_1 \equiv [0,a]$, $R_2 \equiv [a,b]$, $R_3 \equiv [b,1]$, $D_1 \equiv [a,1]$, $D_2 \equiv [0,a] \cup (b,1]$, $D_3 \equiv [0,1]$. From these, we have $B = \mathrm{diag}(a/(1-a), (b-a)/(1-b+a), 1-b)$.

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Darboux transformations for Schrödinger equations in two variables

Mayer Humi
Department of Mathematical Sciences, Worcester Polytechnic Institute, Worcester, Massachusetts 01609

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Darboux transformations in one variable form the basis for the factorization methods and have numerous applications to geometry, nonlinear equations and SUSY quantum mechanics. In spite of this wide range of applications the theory of Darboux transformations in two variables and its elegant relationship to analytic complex functions has not been recognized in the literature. To close this gap we develop in this paper the theory of Darboux transformation in the context of Schrödinger equations in two variables. This yields a constructive algorithm to determine the relationship between potential functions which are related by Darboux transformations. © *2005 American Institute of Physics.*
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I. INTRODUCTION

For over half a century Darboux transformations in one independent variable have found numerous application in various field of mathematics and physics.[1–4] (References 1 and 2 contain an extensive list of references.) In particular the factorization method[5,6] and its generalizations[7–11] which have been instrumental in many physical applications [including SUSY quantum mechanics (QM)[12]] has its roots based on these transformations. Recently however these transformations were generalized and applied to systems of nonlinear equations such as the KdV hierarchy and others.[13] In addition various applications of this method in geometry were worked out and form an important ongoing research area.[2] Extensions of the method to multidimensional oriented Riemann manifolds,[14] time dependent potentials[15] and shape invariant potentials[16] have appeared in the literature.

It is surprising that in spite of this extensive research effort the theory of these transformations in two variables and its elegant relationship to complex analytic function theory has not been worked out (as far as we could ascertain). An exception is the recent paper by Demircioglu *et al.*[17] which considered these transformations under some additional constraints using real variables and polar coordinates. However under these additional constraints only partial results were obtained and the relationship between these transformations and analytic complex functions was lost.

We now give a short overview of Darboux transformations for Schrödinger equation in one variable.

We say that the solutions of two Schrödinger equations with different potentials $u(x)$, $v(x)$, i.e.,

$$\phi'' = (u(x) + \lambda)\phi, \tag{1.1}$$

$$\psi'' = (v(x) + \lambda)\psi, \tag{1.2}$$

are related by a Darboux transformation if there exist $A(x)$, $B(x)$ so that

$$\psi = \left[A(x) + B(x)\frac{\partial}{\partial x} \right] \phi(x). \tag{1.3}$$

Letting $B(x)=1$ one can easily show that in order for Eqs (1.1) and (1.2) to be related by the transformation (1.3) $A(x)$, $u(x)$, $v(x)$ must satisfy

$$A'' + u' + A(u - v) = 0, \tag{1.4}$$

$$2A' + u - v = 0. \tag{1.5}$$

Eliminating $(u-v)$ between these equations and integration yields

$$A' - A^2 + u = -\nu, \tag{1.6}$$

where ν is an integration constant. Equation (1.6) is a Riccati equation which can be linearized by the transformation $A=-\zeta'/\zeta$ which leads to

$$\zeta'' = (u(x) + \nu)\zeta. \tag{1.7}$$

Thus ζ is an eigenfunction of the original Eq. (1.2) with $\lambda=\nu$. From (1.5) we now infer that

$$v = u - 2(\ln \zeta)'', \tag{1.8}$$

i.e., a Darboux transformation changes the potential function $u(x)$ by $\Delta u=-2(\ln \zeta)''$ where ζ is an arbitrary eigenfunction of (1.1).

Our objective in this paper is to generalize these transformations to Schrödinger equations in two independent variables and determine the relationship between their potentials. From a broader point of view the goal of this project is to derive for two dimensional nonseparable potentials results similar to those that followed from the application of Darboux transformations and the factorization method in one dimension. That is an enumeration of physically important potentials which can be treated and solved by these transformations. This program includes the exploration of the Lie algebraic structure underlying these potentials and may lead to the definition of generic families of "special functions" in two variables. (That is, functions which cannot be expressed as a finite sum of products of functions in one variable.) The present paper represents the first step towards achieving these objectives.

The plan of the paper is as follows: In Sec. II we derive the basic equations that constrain Darboux transformations in two variables and their solutions. In Secs. III and IV we construct explicitly some Darboux transformations and their related potentials. In Sec. V we consider potential cascades whose functional form is preserved under these transformations. We end up in Sec VI with summary and conclusions.

II. DARBOUX TRANSFORMATIONS IN TWO VARIABLES

We shall say that two Schrödinger equations in two independent variables

$$\nabla^2 \phi = u(x,y,\lambda)\phi, \tag{2.1}$$

$$\nabla^2 \psi = v(x,y,\lambda)\psi, \tag{2.2}$$

are related by a Darboux transformation if there exist (smooth functions) $A(x,y)$, $B(x,y)$, $C(x,y)$ so that their solutions satisfy

$$\psi(x,y) = \left[A(x,y) + B(x,y)\frac{\partial}{\partial x} + C(x,y)\frac{\partial}{\partial y} \right] \phi(x,y). \tag{2.3}$$

For brevity we drop in the following the dependence of the various functions on the independent variables.

Using Eq. (2.3) to substitute for ψ in Eq. (2.2) and eliminating the higher order derivatives of ϕ and $\partial^2\phi/\partial y^2$ using Eq. (2.1) we obtain

$$\left[-2\frac{\partial C}{\partial y}+2\frac{\partial B}{\partial x}\right]\frac{\partial^2\phi}{\partial x^2}+\left[2\frac{\partial B}{\partial y}+2\frac{\partial C}{\partial x}\right]\frac{\partial^2\phi}{\partial x\,\partial y}+\left\{\nabla^2 C+2\frac{\partial A}{\partial y}+C[u-v]\right\}\frac{\partial\phi}{\partial y}$$
$$+\left\{\nabla^2 B+2\frac{\partial A}{\partial x}+B[u-v]\right\}\frac{\partial\phi}{\partial x}+\left\{\nabla^2 A+2\frac{\partial C}{\partial y}u+A[u-v]+B\frac{\partial u}{\partial x}+C\frac{\partial u}{\partial y}\right\}\phi=0. \tag{2.4}$$

To satisfy this equation we treat ϕ and its derivatives as independent variables and let their coefficients be zero. This leads then to the following system of equations:

$$\frac{\partial B}{\partial x}-\frac{\partial C}{\partial y}=0, \tag{2.5}$$

$$\frac{\partial B}{\partial y}+\frac{\partial C}{\partial x}=0, \tag{2.6}$$

$$\nabla^2 B+2\frac{\partial A}{\partial x}+B[u-v]=0, \tag{2.7}$$

$$\nabla^2 C+2\frac{\partial A}{\partial y}+C[u-v]=0, \tag{2.8}$$

$$\nabla^2 A+A[u-v]+2\frac{\partial C}{\partial y}u+B\frac{\partial u}{\partial x}+C\frac{\partial u}{\partial y}=0. \tag{2.9}$$

We observe that Eq. (2.9) can be rewritten in a symmetric form in B, C in view of Eq. (2.5).

Equations (2.5) and (2.6) are Cauchy-Riemann equations for B, C. Hence these functions must be harmonic conjugates and

$$\Phi=B+iC \tag{2.10}$$

is analytic. In view of this fact $\nabla^2 C=\nabla^2 B=0$ and Eqs. (2.7) and (2.8) simplify to

$$2\frac{\partial A}{\partial x}+B[u-v]=0,\quad 2\frac{\partial A}{\partial y}+C[u-v]=0. \tag{2.11}$$

By eliminating $u-v$ we then get the following equation for A:

$$C\frac{\partial A}{\partial x}-B\frac{\partial A}{\partial y}=0. \tag{2.12}$$

This leads us to consider the following equation:

$$B\,\mathrm{d}x+C\,\mathrm{d}y=0. \tag{2.13}$$

Although this equation is not exact an integrating factor is given by $1/(B^2+C^2)$. (This fact follows from Cauchy-Riemann equations for B, C.) The general solution of this equation can be expressed therefore by the standard formula

$$w(x,y)=\int_{x_0}^{x}\frac{B(x,y)}{B(x,y)^2+C(x,y)^2}\mathrm{d}x+\int_{y_0}^{y}\frac{C(x_0,y)}{B(x_0,y)^2+C(x_0,y)^2}\mathrm{d}y. \tag{2.14}$$

It follows then that the general solution for A is of the form $A=f(w)$ where f is any smooth function of w.

To treat Eq. (2.9) we use Eq. (2.7) to eliminate $u-v$. This leads to

$$B\frac{\partial u}{\partial x}+C\frac{\partial u}{\partial y}+2\frac{\partial C}{\partial y}u=-\nabla^2 A+\frac{2A\dfrac{\partial A}{\partial x}}{B}. \tag{2.15}$$

This equation can be used now to determine u for a proper choice of the function $f(w)$. To proceed we now note that [using Eq. (2.14)]

$$-\nabla^2 A+\frac{2A\dfrac{\partial A}{\partial x}}{B}=\frac{1}{B^2+C^2}[-f'+f^2]'. \tag{2.16}$$

Hence we set

$$[-f'+f^2]'=g'(w), \tag{2.17}$$

where $g(w)$ is some smooth function. As a result we are led to the following equation for $f(w)$:

$$f'-f^2+g(w)=0. \tag{2.18}$$

[We are not adding a constant of integration since $g(w)$ is arbitrary.] This is a Riccati equation which can be linearized by the transformation $f=-q'/q$ and this leads to

$$q''-g(w)q=0. \tag{2.19}$$

Since we want to consider only analytic solutions to this equation which can be expressed in terms of known functions the function $g(w)$ must be chosen appropriately. In particular $g(w)$ can be chosen so that Eq. (2.19) is factorizable.[5] Here we consider only three possible choices for $g(w)$,

(1) $g(w)=\text{constant}=c$. If c is negative $c=-\alpha^2$ then $q=D\cos(\alpha w+\eta)$ where D, η are constants. Hence $f=\alpha\tan(\alpha w+\eta)$. If on the other hand $c=0$ then $q=Dw+E$ (E is a constant) and hence $f=-D/(Dw+E)$. Finally if c is positive $c=\alpha^2$ then $q=D\cosh(\alpha w+\eta)$ and $f=-\alpha\tanh(\alpha w+\eta)$.

(2) $g(w)=w^2-(2n+1)$, $n=0, 1,\ldots$. (This is the kernel of the differential equation for the harmonic oscillator.) For $n=0$ this leads to $f=w$ while for $n>0$ we obtain $f=w-[2nH_{n-1(w)}/H_n(w)]$, where $H_n(w)$ are Hermite functions.

(3) $g(w)=n(n-1)/w^2$, $n=2, 3,\ldots$. In this case Eq. (2.19) is a Euler equation and $q=w^n$ or $q=w^{-(n-1)}$. In either case this leads to $f\sim 1/w$.

We observe that different choices of $g(w)$ can lead to the same $f(w)$.

Having made a choice for $g(w)$ Eq. (2.15) becomes

$$B\frac{\partial u}{\partial x}+C\frac{\partial u}{\partial y}+2\frac{\partial C}{\partial y}u=\frac{g'}{B^2+C^2}. \tag{2.20}$$

To find the general solution to this equation we must find two independent solutions to the system,

$$\frac{dx}{B} = \frac{dy}{C} = \frac{-du}{2u\dfrac{\partial C}{\partial y} - \dfrac{g'}{B^2 + C^2}}. \tag{2.21}$$

The first equality in this equation leads to

$$C\,dx - B\,dy = 0. \tag{2.22}$$

Once again this equation is not exact but an integrating factor is given by $1/(B^2+C^2)$ and the solution of the equation $w_1(x,y)$ can be expressed then by a standard formula similar to Eq. (2.14). Using w_1 we can eliminate x or y from the second equation in (2.21) and find a solution $w_2(u,y)$. The function u is given then implicitly by any smooth function $F(w_1,w_2)=0$. Once u has been determined v can be computed from Eq. (2.7) or (2.8).

To summarize the procedure, one starts by choosing an analytic function $\Phi=B+iC$ then computes w using Eq. (2.14). For a proper choice of $g(w)$ one computes $A=f(w)$ from Eq. (2.19). The determination of u (and hence v) requires then the solution of Eqs. (2.20) and (2.21). We note however that instead of choosing the function g one can choose u so that the left-hand side of Eq. (2.20) multiplied by B^2+C^2 is a function of w only. This will determine g' and hence A from Eq. (2.18).

In the following section we work out this procedure for the (complex) functions $\Phi=z^n$ and $\Phi=iz^n$.

III. DARBOUX TRANSFORMATIONS WITH $\Phi=z^n$

A. $n\neq 1$

In this case $B=r^n\cos(n\theta)$ and $C=r^n\sin(n\theta)$ hence it is expedient to work in polar coordinates. Equation (2.12) becomes

$$(C\cos\theta - B\sin\theta)\frac{\partial A}{\partial r} - \frac{1}{r}(C\sin\theta + B\cos\theta)\frac{\partial A}{\partial \theta} = 0. \tag{3.1}$$

For the present choice of B, C this yields

$$\sin[(n-1)\theta]\frac{\partial A}{\partial r} - \frac{1}{r}\cos[(n-1)\theta]\frac{\partial A}{\partial \theta} = 0. \tag{3.2}$$

From Eq. (2.14) we then find that

$$w = -\frac{\cos[(n-1)\theta]}{(n-1)r^{(n-1)}}. \tag{3.3}$$

Choosing $g(w)=0$ in Eq. (2.17) we find that $A=f(w)=-D/(Dw+E)$. (In the following we let $D=1$, $E=0$.) Equation (2.20) for u becomes

$$r\frac{\partial u}{\partial r} + \tan[(n-1)\theta]\frac{\partial u}{\partial \theta} + 2nu = 0. \tag{3.4}$$

The general solution of this equation is given implicitly by

$$F\left(r^{2n}u, \frac{r^{(n-1)}}{\sin[(n-1)\theta]}\right) = 0$$

where F is a smooth function. For example, if $F(w_1,w_2)=w_1-w_2$ then

$$u = \frac{1}{r^{(n+1)} \sin[(n-1)\theta]}. \tag{3.5}$$

Using Eq. (2.7) to compute $u-v=-2f'(w)/(B^2+C^2)$ we find for the present choice of f,

$$u - v = -\frac{2(n-1)^2}{r^2 \cos^2[(n-1)\theta]}. \tag{3.6}$$

B. $n=1$

In this case $B=x$ and $C=y$. Hence from Eq. (2.14) we deduce that $w=\ln r$ and $A=f(w)$. [Since f is arbitrary we could have written this relation as $A=f(r)$ but this will change the expression for $\nabla^2 A$ in Eq. (2.15)]. Equation (2.15) with the left-hand side reexpressed in polar coordinates becomes

$$r\frac{\partial u}{\partial r} + 2u = \frac{g'(w)}{r^2}. \tag{3.7}$$

We conclude then that in this case u is given by

$$u = \frac{G(\theta)}{r^2} + \frac{1}{r^2}\int \frac{g'(w)}{r} \mathrm{d}r, \tag{3.8}$$

where $G(\theta)$ is a smooth function and $u-v=-2[f'(w)/r^2]$.

IV. DARBOUX TRANSFORMATIONS WITH $\Phi=iz^n$

A. $n\neq 1$

For this choice of Φ we have $B=-r^n \sin(n\theta)$, $C=r^n \cos(n\theta)$ and the roles of B, C have been (essentially) exchanged. In this case w is given by

$$w = \frac{\sin[(n-1)\theta]}{(n-1)r^{(n-1)}} \tag{4.1}$$

and $A=f(w)$. The equation for u with $g'(w)=0$ becomes

$$r\frac{\partial u}{\partial r} - \cot[(n-1)\theta]\frac{\partial u}{\partial \theta} + 2nu = 0 \tag{4.2}$$

whose general solution is of the form

$$F\left(r^{2n}u, \frac{r^{(n-1)}}{\cos[(n-1)\theta]}\right) = 0, \tag{4.3}$$

where $F(w_1, w_2)$ is a smooth function. If we let $f(w)=-1/w$ then

$$u - v = -\frac{2(n-1)^2}{r^2 \sin^2[(n-1)\theta]}. \tag{4.4}$$

B. $n=1$

In this case $B=-y$ and $C=x$. Hence $w=\theta$, $A=f(\theta)$ and the equation for u in polar coordinate is

$$\frac{\partial u}{\partial \theta} = \frac{g'(w)}{r^2}. \tag{4.5}$$

Hence

$$u = \frac{g(\theta)}{r^2} + G(r) \tag{4.6}$$

and $u-v=-2f'(\theta)/r^2$.

V. CASCADES

One of the important (and interesting) features of the factorization method in one independent variable is that the application of the ladder operator (or equivalently a Darboux transformation) on a potential $u(x)$ leads to potentials with the same dependence on x but with different parameters. As a result one can apply these operators on "essentially the same potential" a finite or infinite number of times creating a cascade of potentials whose solutions are interrelated by Darboux transformations.

To explore the existence of such cascades in two independent variables we shall assume that $\beta(u-v)=u$. Using this relation to substitute in Eq. (2.7) we obtain

$$u = -\frac{2\beta\dfrac{\partial A}{\partial x}}{B}. \tag{5.1}$$

Substituting this expression for u in Eq. (2.9) and using Eqs. (2.5) and (2.12) to simplify we infer that A must satisfy

$$(2\beta-1)\nabla^2 A + \frac{2A\dfrac{\partial A}{\partial x}}{B} = 0 \tag{5.2}$$

and therefore [since $A=f(w)$]

$$[(2\beta-1)f'(w) + f^2(w)]' = 0. \tag{5.3}$$

Hence

$$(2\beta-1)f'(w) + f^2(w) = c, \tag{5.4}$$

where c is a constant. We deduce then (following the discussion in Sec. II of a similar equation) that $f(w)$ can take any of the following forms:

(1) $c=0$ then $f(w)=(2\beta-1)/(w+c_1)$,
(2) $c=\gamma^2$ then $f(w)=\gamma\tanh[(\gamma w+c_2)/(2\beta-1)]$,
(3) $c=-\gamma^2$ then $f(w)=-\gamma\tan[(\gamma w+c_3)/(2\beta-1)]$.

[We assumed that $2\beta\neq 1$ since otherwise $f(w)=$constant.] Here c_1, c_2, c_3 are arbitrary constants and the corresponding potential u can be computed from Eq. (5.1).

For $c=c_1=0$ and $\Phi=z^n(n\neq 1)$ this leads to

$$u = \frac{2\beta(2\beta-1)(n-1)^2}{r^2\cos^2[(n-1)\theta]}. \tag{5.5}$$

Similarly for $\Phi=iz^n$ it follows that

$$u = \frac{2\beta(2\beta-1)(n-1)^2}{r^2 \sin^2[(n-1)\theta]}. \tag{5.6}$$

Similar but more complicated expressions can be obtained for the other choices of c.

For $n=1$ we infer from Eqs. (3.8) and (4.6) that cascades exist but the corresponding potentials are essentially in one variable. In particular for $\Phi=iz$ Eq. (4.6) implies that a cascade exists when $G(r)=0$ and

$$g(\theta) = -2\beta f'(\theta). \tag{5.7}$$

Substituting this relation in eq. (2.18) it follows that

$$(1-2\beta)f'(\theta) - f^2(\theta) = 0 \tag{5.8}$$

and therefore $f(\theta)=-[(1-2\beta)/(\theta+c_4)]$ where c_4 is a constant.

VI. SUMMARY AND CONCLUSIONS

In this paper we showed that Darboux transformations in two independent variables have strong affinity to the theory of analytic complex functions. This relationship enabled us to analyze these transformations in full. It allowed us also to give a constructive algorithm for the application of these transformations. This algorithm was used to make a partial classification of Darboux transformations for two classes of analytic functions and their related potentials. Further (exhaustive) enumeration of other potential functions especially those that related to the factorization method through Eq. (2.19) [by the choice of the function $g(w)$] is needed. Moreover it will be important to identify classes of physically interesting nonseparable potentials in two variables and find out if they are amenable to treatment by Darboux transformations through the application of Eq. (2.20). We discussed also the existence of potential cascades whose form is preserved under these transformations. However there are other possible definitions of this property, e.g., $u-v$ =constant. The differential equations that correspond to these cascades are the exact analogs of factorizable equations in one dimension and their algebraic structure from group theoretical point of view remains an important open question.

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Commuting quantum traces for quadratic algebras

Zoltán Nagy[a] and Jean Avan[b]
Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise (CNRS UMR 8089), 2 avenue Adolphe Chauvin, Pontoise, 95031 Cergy-Pontoise Cedex, France

Anastasia Doikou[c]
Laboratoire d'Annecy-Le-Vieux de Physique Théorique, LAPTH (CNRS UMR 5108), B.P. 110, Annecy-Le-Vieux, F-74941, France

Geneviève Rollet[d]
Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise (CNRS UMR 8089), 2 avenue Adolphe Chauvin, Pontoise, 95031 Cergy-Pontoise Cedex, France

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Consistent tensor products on auxiliary spaces, hereafter denoted "fusion procedures," and commuting transfer matrices are defined for general quadratic algebras, nondynamical and dynamical, inspired by results on reflection algebras. Applications of these procedures then yield integer-indexed families of commuting Hamiltonians. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2007587]

I. INTRODUCTION

A procedure to construct commuting quantum traces for a particular form of quadratic exchange algebras, known as reflection algebra,[1] was recently developed in Ref. 2, building on the pioneering work in Ref. 3. We recall that it entails three different steps, construction of the quadratic exchange algebra itself, and its so-called "dual" (this notion will be clarified soon); construction of realizations of the exchange algebra and its dual on consistent tensor products of the initial auxiliary space (which we will denote here as "fusion" procedure) while keeping a single "quantum" Hilbert space on which all operators are assumed to act; combination of these realizations into traces over the tensorized auxiliary spaces, yielding commuting operators acting on the original quantum space, labeled by the integer set of tensorial powers of the auxiliary space.

We immediately insist that this procedure is distinct of, and in a sense complements, the familiar construction of transfer matrices by tensoring over distinct quantum spaces (using an appropriate comodule structure of the quantum algebra) while keeping a single common auxiliary space; the trace is then taken over the auxiliary space to yield a generating functional of commuting operators.[4] In the case when there exists a universal formulation of the algebra as a bialgebra with a coproduct structure, both constructions stem from two separate applications of this coproduct. However, the resulting operators are quite distinct, the trace of the monodromy matrix yields commuting operators acting on a tensor product of Hilbert spaces (as in, e.g., the case of spin chains); the trace of the fused auxiliary matrix yields operators acting on one single Hilbert space. These can be shown in some particular cases to realize the quantum analog of the classical Poisson-commuting traces of powers of the classical Lax-matrix $\mathrm{Tr}(L^n)$ (see Refs. 2, 5, and 6). This is the reason for our phrasing of "quantum traces" actually borrowed from Ref. 7. In addition it must be emphasized that the procedure itself, combining a construction of a "dual" algebra and

[a]Electronic mail: nagy@ptm.u-cergy.fr
[b]Electronic mail: avan@ptm.u-cergy.fr
[c]Electronic mail: doikou@lapp.in2p3.fr
[d]Electronic mail: rollet@ptm.u-cergy.fr

the establishing of exact fusion formulas, yields very interesting results on the quadratic exchange algebra itself, and its possible identification as a coalgebra (e.g., Hopf or quasi-Hopf). As we will later comment, it also plays a central role in the (similarly named) Mezincescu-Nepomechie fusion constructions for spin chains.[8,9]

A word of caution is in order. Throughout the paper, we use the term "fusion" in a restrictive sense, insofar as we only consider the possibility of acting on auxiliary spaces. The general fusion procedure itself has been applied also to the quantum spaces, yielding, e.g., higher spin interactions[10] or multiparticle bound states S matrices.

Our purpose here is to fully describe the quantum trace procedure for three types of general quadratic algebras. The first one is the quantum nondynamical quadratic exchange algebra introduced in Ref. 3. The second one was formulated in Ref. 11 as a dynamical version of the quadratic exchange algebras in Ref. 3 with particular zero-weight conditions. It will be denoted "semidynamical" here, for reasons to be explained later. The third one (similarly denoted here as "fully dynamical") was first built in Ref. 12 for the $\mathfrak{sl}(2)$ case, and extended to the $\mathfrak{sl}_n$ case in Ref. 13, albeit with particular restrictions on the coefficient matrices. The zero-weight conditions are different; the algebra structure itself mimicks the reflection algebra introduced by Cherednik and Sklyanin in Ref. 1; a comodule structure was identified and a universal structure was proposed in Ref. 14. We will here briefly comment on the differences between the quantum traces built in both dynamical cases.

II. NONDYNAMICAL QUADRATIC ALGEBRAS

These algebras were recognized[1,7] as generalizations of the usual R-matrix and quantum group structure, leading to non skewsymmetrical r-matrices in the quasiclassical limit.

They are characterized by the following exchange relations:

$$A_{12}T_1B_{12}T_2 = T_2C_{12}T_1D_{12}, \tag{1}$$

where, as usual, the quantum generators sit in the matrix entries of T. Let us recall some examples of this structure.

(i) The Yangian and quantum group structures where $A=D$, $B=C=\mathbf{1}$.
(ii) Donin-Kulish-Mudrov (DKM) reflection algebra without spectral parameters.[15] $A=C$, $B=D=A^{\pi}$, where $(\,)^{\pi}$ denotes the permutation of auxiliary spaces, $(A^{\pi})_{12}=A_{21}$.
(iii) Kulish-Sklyanin-type reflection algebra containing spectral parameters,[2,16] $A=R^{-}_{12}$, $B=R^{+}_{21}$, $C=R^{+}_{12}$, $D=R^{-}_{21}$ ($\pm$ signs refer to the relative signs of spectral parameters in the R-matrix).

In Refs. 3 and 17 consistency relations involving the structure matrices were derived and it was found that they had the form of cubic relations on the matrices A,B,C,D,

$$A_{12}A_{13}A_{23} = A_{23}A_{13}A_{12}, \tag{2}$$

$$A_{12}C_{13}C_{23} = C_{23}C_{13}A_{12}, \tag{3}$$

$$D_{12}D_{13}D_{23} = D_{23}D_{13}D_{12}, \tag{4}$$

$$D_{12}B_{13}B_{23} = B_{23}B_{13}D_{12}. \tag{5}$$

We can see that A and D obey the usual YB equations whereas C and B are their respective representations.

Furthermore, generalized unitarity conditions can be derived from self-consistency of (1) under exchange of spaces 1 and 2 which imposes

$$A_{12} = \alpha A_{21}^{-1}, \quad D_{12} = \beta D_{21}^{-1}, \quad B_{12} = \gamma C_{21} \quad (\alpha, \beta, \gamma \in \mathbb{C}). \tag{6}$$

The constants of proportionality must obey an additional constraint, $\alpha\gamma = \beta\gamma^{-1}$. In the sequel, we will restrict ourselves to the simplest choice of $\alpha = \beta = \gamma = 1$.

Let us also note that although $B_{12} = C_{21}$, for aesthetical and mnemotechnical reasons we continue to use C whenever it allows for the more familiar and significant (12, 13, 23) display of indices.

In Ref. 3 the authors had already introduced an algebra which they called "dual" to (1). This "dual" structure is characterized by the following exchange relation,

$$(A_{12}^{-1})^{t_1 t_2} K_1 ((B_{12}^{t_1})^{-1})^{t_2} K_2 = K_2 ((C_{12}^{t_2})^{-1})^{t_1} K_1 (D_{12}^{t_1 t_2})^{-1}. \tag{7}$$

Two respective representations of (1) and (7) (assumed to act on different quantum spaces) can be combined by means of a trace[3,8,16] on the common auxiliary space to generate commuting quantum operators. It is with respect to this trace that Eq. (7) can be characterized as the dual of Eq. (1). We formulate the conjecture that this is the trace of a $*$-algebra structure on some underlying universal algebra. Some freedom remains as to the actual form of the trace and in the sequel we will stick to the choice of H as $\mathrm{Tr}_V(K^t T)$. Here the superscript t stands for any antimorphism on the auxiliary space V, which satisfies also the trace invariance property $\mathrm{Tr}(KT) = \mathrm{Tr}(K^t T^t)$, for all matrices K and T. The actual antimorphism may differ from the usual transposition (e.g., by additional conjugation, crossing operation) since the proof of commutation uses only (see theorems 5, 6, and 14) the antimorphism and trace invariance properties (see, e.g., the supertransposition in superalgebras, or the crossing operation in R-matrices). Let us also remark here that it is possible to choose a trace formula where the antimorphism acts on the quantum space, as it is the case in Ref. 2, but we prefer not to do so here. Our particular choice is motivated by the fact that transposition on the auxiliary space is always defined whereas on the quantum space it is not necessarily straightforward and could require a supplementary hypothesis on this quantum representation which may not be easily implemented.

The quantum trace formulation for such a nondynamical algebra stems from the results in Refs. 2 and 3; it is however interesting to give a rather detailed derivation of it in the general case, since both dynamical algebras will present similar features, albeit with crucial modifications in the fusion and trace formulas induced by the dynamical dependence.

We will describe two fusions (consistent tensor product of auxiliary spaces) of Eq. (1), respectively, inspired by Refs. 2 (itself relying on Ref. 1) and 15. While the fusion of the structure matrices is uniquely defined in each case, the solutions of the fused exchange relations are not. In particular, they can be dressed, i.e., multiplied by suitable "coupling" factors. This dressing procedure turns out to be crucial, indeed, when the simplest solutions of the fused exchange relation are combined in a quantum trace, they decouple, giving rise to products of lower order Hamiltonians. To obtain nontrivial commuting quantities these fused T-matrices must be dressed.

We will finally show that the two fusion procedures identified in Refs. 2 and 15 are related by a coupling matrix L_M and that they generate the same commuting quantities.

A. First fusion procedure

Let us first start by introducing some convenient notations (see Ref. 2) for fused matrices,

$$A_{MN'} = \prod_{i \in M}^{\rightarrow} \prod_{j \in N'}^{\rightarrow} A_{ij} = A_{11'} A_{12'} \cdots A_{1n'} \times A_{21'} A_{22'} \cdots A_{2n'} \cdots \times A_{m1'} \cdots A_{mn'}, \tag{8}$$

where $M = \langle 1, 2, \ldots, m \rangle$ and $N' = \langle 1', 2', \ldots, n' \rangle$ are ordered sets of labels. The same sets with reversed ordering are denoted by $\bar{M}$ and $\bar{N}'$. A set M deprived of its lowest (highest) element is denoted by $M_0 (M^0)$.

Remark: In many explicit examples we would have to deal only with one single exchange formula (1) with two isomorphic auxiliary spaces. However our derivation also applies to a

situation where more general coupled sets of exchange relations would occur as $A_{ij}T_iB_{ij}T_j = T_jC_{ij}T_iD_{ij}$ with $\{i,j\}\subset\{1,\ldots,m_0<\infty\}$ and generically $V_i\neq V_j$. Such situations will occur whenever a universal structure is identifiable and the auxiliary spaces V_i carry different representations of the algebra, as in, e.g., Ref. 15. It is therefore crucial that the order in the index set be stipulated.

Similar notations are used for the fusion of the other structure matrices. The next lemma states that the structure matrices in (1) can be fused in a way that respects the YB equations (2)–(5).

Lemma 1: Let A,B,C,D be solutions of the Yang-Baxter equations (2)–(5).

Then the following fused Yang-Baxter equations hold:

$$A_{M\bar{N}'}A_{M\bar{L}''}A_{N'\bar{L}''} = A_{N'\bar{L}''}A_{M\bar{L}''}A_{M\bar{N}'}, \tag{9}$$

$$A_{M\bar{N}'}C_{ML''}C_{N'L''} = C_{N'L''}C_{ML''}A_{M\bar{N}'}, \tag{10}$$

$$D_{M\bar{N}'}D_{M\bar{L}''}D_{N'\bar{L}''} = D_{N'\bar{L}''}D_{M\bar{L}''}D_{M\bar{N}'}, \tag{11}$$

$$D_{M\bar{N}'}B_{ML''}B_{N'L''} = B_{N'L''}B_{ML''}D_{M\bar{N}'}. \tag{12}$$

Proof: Simple induction on $\#M+\#N'$. ■

We now describe a fusion procedure for the algebra characterized by (1), generalizing the one introduced in Ref. 2.

Theorem 1: *If T is a solution of*

$$A_{12}T_1B_{12}T_2 = T_2C_{12}T_1D_{12} \tag{13}$$

then

$$T_M = \prod_{i\in M}^{\rightarrow}\left(T_i\left(\prod_{\substack{i<j\\ j\in M}}^{\rightarrow}B_{ij}\right)\right) \tag{14}$$

verifies the following fused equation:

$$A_{M\bar{N}'}T_MB_{MN'}T_{N'} = T_{N'}C_{MN'}T_MD_{M\bar{N}'}. \tag{15}$$

Proof: Induction on the cardinality n of the index sets, $n=\#M+\#N'$ which repeats and generalizes the steps in Ref. 2. ■

The solution T_M obtained above can be dressed, i.e., can be multiplied from the left and the right by suitable factors.

Proposition 1: Let T_M be a solution of the fused exchange relation. Then $Q_MT_MS_M$ is also a solution of the fused exchange relation provided Q_M and S_M verify

$$\begin{aligned}&[Q_M,A_{M\bar{N}'}] = [Q_{N'},A_{M\bar{N}'}] = [Q_{N'},B_{MN'}] = [Q_M,C_{MN'}] = 0,\\ &[S_M,D_{M\bar{N}'}] = [S_{N'},D_{M\bar{N}'}] = [S_{N'},C_{MN'}] = [S_M,B_{MN'}] = 0.\end{aligned} \tag{16}$$

A particular solution of these constraints is provided by

$$\begin{aligned}Q_M &= \check{A}_{12}\check{A}_{23}\ldots\check{A}_{m-1,m},\\ S_M &= \check{D}_{12}\check{D}_{23}\ldots\check{D}_{m-1,m},\end{aligned} \tag{17}$$

where $\check{A}_{12}=P_{12}A_{12},\ldots P_{12}$ being the permutation exchanging two auxiliary spaces.

Proof: Again by induction on the cardinality of the index sets. In the induction step we use the decomposition $Q_{N'}B_{MN'}=\check{A}_{12}\cdots\check{A}_{n'-1,n'}B_{M,N'00}B_{M,n'-1}B_{M,n'}$, for example. ■

The fusion procedure can be repeated for the dual exchange relation as follows.

Theorem 2: *If K is a solution of the dual exchange relation,*

$$(A_{12}^{-1})^{t_1t_2}K_1((B_{12}^{t_1})^{-1})^{t_2}K_2 = K_2((C_{12}^{t_2})^{-1})^{t_1}K_1(D_{12}^{t_1t_2})^{-1} \tag{18}$$

then

$$K_M = \prod_{i\in M}^{\rightarrow}\left(K_i\left(\prod_{\substack{i<j\\ j\in M}}^{\rightarrow}((B_{ij}^{t_1})^{-1})^{t_2}\right)\right) \tag{19}$$

is a solution of the dual fused equation

$$(A_{M\bar{N}'}^{-1})^{t_Mt_{N'}}K_M((B_{MN'}^{t_M})^{-1})^{t_{N'}}K_{N'} = K_{N'}((C_{MN'}^{t_{N'}})^{-1})^{t_M}K_M(D_{M\bar{N}'}^{t_Mt_{N'}})^{-1}. \tag{20}$$

Proof: Similar to that of Theorem 1. Note that the dual structure matrices obey a set of appropriate YB equations, isomorphic to (9)–(12), for instance,

$$(A_{M\bar{N}'}^{-1})^{t_Mt_{N'}}(A_{M\bar{L}''}^{-1})^{t_Mt_{L''}}(A_{N\bar{L}''}^{-1})^{t_Nt_{L''}} = (A_{N\bar{L}''}^{-1})^{t_Nt_{L''}}(A_{M\bar{L}''}^{-1})^{t_Mt_{L''}}(A_{M\bar{N}'}^{-1})^{t_Mt_{N'}}. \tag{21}$$

■

A similar dual dressing procedure exists: Any dressing of a solution of (18) should obey the commutativity constraints

$$\begin{aligned}[Q'_M,(A_{M\bar{N}'}^{-1})^{t_Mt_{N'}}] = [Q'_{N'},(A_{M\bar{N}'}^{-1})^{t_Mt_{N'}}] = [Q'_{N'},((B_{MN'}^{t_M})^{-1}\ ] = [Q'_M,((C_{MN'}^{t_{N'}})^{-1}\ ] = [S'_M,(D_{M\bar{N}'}^{t_Mt_{N'}})^{-1}]\\ = [S'_{N'},(D_{M\bar{N}'}^{t_Mt_{N'}})^{-1}] = [S'_{N'},((C_{MN'}^{t_{N'}})^{-1}\ ] = [S'_M,((B_{MN'}^{t_M})^{-1}\ ] = 0\end{aligned} \tag{22}$$

involving fused dual structure matrices. It is easy to check that if Q_M and S_M dress solutions of (15) then $Q'_M=Q_M^{t_M}$ and $S'_M=S_M^{t_M}$ dress solutions of (18).

B. Second fusion procedure

Results in Ref. 15 hint that relation (1) admits another fusion procedure. We will explicitely link the fusion described in the preceding section to the one inspired by Ref. 15.

The DKM type fusion is characterized by the following fused exchange relation for fused matrices $\tilde{T}$ to be described in the following:

$$A_{\bar{M}N'}\tilde{T}_MB_{M\bar{N}'}\tilde{T}_{N'} = \tilde{T}_{N'}C_{\bar{M}N'}\tilde{T}_MD_{M\bar{N}'}. \tag{23}$$

This equation can actually be obtained from a multiplication of the KS exchange relation (15) by suitable factors reversing the ordering of indices where it is needed. The next lemma specifies this statement.

Lemma 2: Let T_M be a solution of the fused exchange relation (15). If L_M verifies the following commutation rules:

$$\begin{aligned}L_MA_{M\bar{N}'} = A_{\bar{M}\bar{N}'}L_M,\quad L_{N'}A_{M\bar{N}'} = A_{MN'}L_{N'},\\ L_{N'}B_{MN'} = B_{M\bar{N}'}L_{N'},\quad L_MC_{MN'} = C_{\bar{M}N'}L_M\end{aligned} \tag{24}$$

then $\tilde{T}_M=L_MT_M$ is a solution of the exchange relation

$$A_{\bar{M}N'}\tilde{T}_MB_{M\bar{N}'}\tilde{T}_{N'} = \tilde{T}_{N'}C_{\bar{M}N'}\tilde{T}_MD_{M\bar{N}'}. \tag{25}$$

An example of such an L_M is given by

$$L_M = A_{12}\cdots A_{1m}A_{23}\cdots A_{2m}\cdots A_{m-1,m} = \overrightarrow{\prod_{1\leqslant i<j\leqslant m}} A_{ij}. \tag{26}$$

Proof: The first part is straightforward. Example (26) is verified by induction using $L_M = A_{1M_0}L_{M_0}$. For instance, the first relation of (24) is proved as

$$L_M A_{M\bar{N}'} = A_{1M_0}L_{M_0}A_{1\bar{N}'}A_{M_0\bar{N}'} = A_{1M_0}A_{1\bar{N}'}L_{M_0}A_{M_0\bar{N}'} = A_{1M_0}A_{1\bar{N}'}A_{\bar{M}_0\bar{N}'}L_{M_0} = A_{\bar{M}_0\bar{N}'}A_{1\bar{N}'}A_{1M_0}$$
$$= A_{\bar{M}\bar{N}'}L_M,$$

where fused YB equations are used. ■

Combined with Theorem 1, this lemma leads to the following.

Theorem 3: *If $\tilde{T}$ is a solution of*

$$A_{12}\tilde{T}_1B_{12}\tilde{T}_2 = \tilde{T}_2C_{12}\tilde{T}_1D_{12} \tag{27}$$

then

$$\tilde{T}_M = \overrightarrow{\prod_{i\in M}}\left(\overrightarrow{\prod_{\substack{j>i\\ j\in M}}} A_{ij}\tilde{T}_i \overleftarrow{\prod_{\substack{j>i\\ j\in M}}} B_{ij}\right) \tag{28}$$

is a solution of

$$A_{\bar{M}N'}\tilde{T}_MB_{M\bar{N}'}\tilde{T}_{N'} = \tilde{T}_{N'}C_{\bar{M}N'}\tilde{T}_MD_{M\bar{N}'}. \tag{29}$$

Proof: The only property left to check is that the solution $\tilde{T}_M$ in (28) is obtained from T_M in (14) by a multiplication by L_M in (26). It is enough to show that $\tilde{T}_M = A_{1M_0}\tilde{T}_1B_{1\bar{M}_0}\tilde{T}_{M_0}$. We only develop the induction step,

$$L_MT_M = A_{1M_0}L_{M_0}T_1B_{1M_0}T_{M_0} = A_{1M_0}T_1L_{M_0}B_{1M_0}T_{M_0} = A_{1M_0}T_1B_{1\bar{M}_0}L_{M_0}T_{M_0} = A_{1M_0}\tilde{T}_1B_{1\bar{M}_0}\tilde{T}_{M_0}. \tag{30}$$

■

The next proposition describes the dressing of the solutions.

Proposition 2: Let $\tilde{T}_M$ be a solution of the DKM-type fused exchange relations. Then $\tilde{Q}_M\tilde{T}_M\tilde{S}_M$ is also a solution provided $\tilde{Q}_M$ and $\tilde{S}_M$ verify

$$[\tilde{Q}_M, A_{\bar{M}N'}] = [\tilde{Q}_{N'}, A_{\bar{M}N'}] = [\tilde{Q}_{N'}, B_{M\bar{N}'}] = [\tilde{Q}_M, C_{\bar{M}N'}] = 0,$$
$$[\tilde{S}_M, D_{M\bar{N}'}] = [\tilde{S}_{N'}, D_{M\bar{N}'}] = [\tilde{S}_{N'}, C_{\bar{M}N'}] = [\tilde{S}_M, B_{M\bar{N}'}] = 0. \tag{31}$$

These equations are solved by

$$\tilde{Q}_M = L_MQ_ML_M^{-1}, \quad \tilde{S}_M = S_M,$$

where Q_M and *S_M dress the solutions of the fused exchange relation (15) and L_M is a solution of (24).*

Proof: Straightforward. ■

We saw that T_M and $\tilde{T}_M$ were linked by a factor L_M. The question arises whether there is a similar relation between the corresponding dual exchange algebras and their solutions. The relation is established in the following.

Theorem 4: *Let K_M be a solution of the first fused exchange relation (15) and L_M be a solution of (24). Then $\tilde{K}_M = (L_M^{t_M})^{-1}K_M$ is a solution of the KDM-type dual fused exchange relation:*

$$(A^{-1}_{\bar{M}N'})^{t_M t_{N'}}\widetilde{K}_M((B^{t_M}_{M\bar{N}'})^{-1})^{t_{N'}}\widetilde{K}_{N'} = \widetilde{K}_{N'}((C^{t_{N'}}_{\bar{M}N'})^{-1})^{t_M}\widetilde{K}_M(D^{t_M t_{N'}}_{M\bar{N}'})^{-1}. \tag{32}$$

Proof: We first see that (32) is indeed the dual exchange relation associated with (25). The next step is to check that $(L^{t_M}_M)^{-1}$ obeys the appropriate commutation relations that enable it to transform the fused dual AD type algebra (18) into the fused dual DKM-type one (32). It is obvious since these equations are the inverse transpose of (24). ■

Dressings of these dual fused solutions are obtained from dressings of (25) by the same operation as for the AD type fusion, i.e., by transposing.

C. Commuting traces

In the preceding sections we have derived two distinct fusion procedures both of which allow for building commuting quantities. In this section we will describe this construction, and show the two different quantum traces are identified once the dressing is used.

We first establish the following.

Theorem 5: *Let $\mathcal{T}_M$ be a solution of the fused AD-type exchange relation (15). $\mathcal{T}_M$ acts on the tensor product of the auxiliary spaces labeled by M and on the quantum space V_q.*

Let $\mathcal{K}_M$ be a solution of the dual fused AD-type exchange relation (18). $\mathcal{K}_M$ acts on the tensor product of the auxiliary spaces labeled by M and on the quantum space $V_{q'}$.

The following operators,

$$H_M = \mathrm{Tr}_M(\mathcal{K}^{t_M}_M \mathcal{T}_M), \tag{33}$$

constitute a family of mutually commuting quantum operators acting on $V_q \otimes V_{q'}$:

$$[H_M, H_{N'}] = 0. \tag{34}$$

Proof: It repeats the steps of Refs. 2 and 16. ■

The proof is independent of the particular fusion procedure so it remains valid for the DKM case too. Thus we have the following.

Theorem 6: *Let $\widetilde{\mathcal{T}}_M$ be a solution of the fused DKM-type exchange relation (25). $\widetilde{\mathcal{T}}_M$ acts on the tensor product of the auxiliary spaces labeled by M and on the quantum space V_q.*

Let $\widetilde{\mathcal{K}}_M$ be a solution of the dual fused DKM-type exchange relation (32). $\widetilde{\mathcal{K}}_M$ acts on the tensor product of the auxiliary spaces labeled by M and on the quantum space $V_{q'}$.

The following operators:

$$\widetilde{H}_M = \mathrm{Tr}_M(\widetilde{\mathcal{K}}^{t_M}_M \widetilde{\mathcal{T}}_M) \tag{35}$$

constitute a family of mutually commuting quantum operators acting on $V_q \otimes V_{q'}$:

$$[\widetilde{H}_M, \widetilde{H}_{N'}] = 0. \tag{36}$$

So far we have two seemingly different sets of commuting quantities obtained from the same defining relations (1) via two distinct fusion procedures. However we will show that the operation consisting in dressing and taking the trace smears out this difference and one is left with only one set of commuting Hamiltonians. This is summarized in.

Proposition 3: The quantum commuting Hamiltonians obtained from any set of solutions T_M, K_M of (15) and (20) are identified with the quantum commuting Hamiltonians obtained from a suitable set of solutions $\widetilde{T}_M, \widetilde{K}_M$ of (25) and (32). This identification is implemented by a coupling matrix L_M.

Proof: Let $\mathcal{T}_M$ be the solution (14) and $\mathcal{K}_M$ the corresponding dual solution (19). The results of the multiplication by L_M and $(L^{t_M}_M)^{-1}$ are denoted by $\widetilde{\mathcal{T}}M$ and $\widetilde{\mathcal{K}}M$. We calculate the tilded Hamiltonians after dressing and we find that they are equal to the dressed untilded ones,

$$\mathrm{Tr}_M(\widetilde{\mathcal{K}}_M^{t_M}\widetilde{Q}_M\widetilde{\mathcal{T}}_M\widetilde{S}_M)=\mathrm{Tr}_M(\mathcal{K}_M^{t_M}L_M^{-1}L_MQ_ML_M^{-1}L_M\mathcal{T}_MS_M)=\mathrm{Tr}_M(\mathcal{K}_M^{t_M}Q_M\mathcal{T}_MS_M). \tag{37}$$

■

The following proposition justifies the technical relevance of dressings.

Proposition 4: Operators built from the solution (14) decouple as $H_N=\mathrm{Tr}_N(K_N^{t_N}T_N)=\mathrm{Tr}(K^tT)^{\#N}$.

Proof: By induction using the property $T_N=T_1B_{1N_0}T_{N_0}$. Let us detail the induction step,

$$H_N=\mathrm{Tr}_N(K_N^{t_N}T_N)=\mathrm{Tr}((K_1(B_{1N_0}^{t_1})^{-1t_{N_0}}K_{N_0})^{t_N}T_1B_{1N_0}T_{N_0})=\mathrm{Tr}((K_1(B_{1N_0}^{t_1})^{-1t_{N_0}}K_{N_0})^{t_{N_0}}(T_1B_{1N_0}T_{N_0})^{t_1})$$
$$=\mathrm{Tr}(K_1K_{N_0}^{t_{N_0}}(B_{1N_0}^{t_1})^{-1}B_{1N_0}^{t_1}T_1^{t_1}T_{N_0})=\mathrm{Tr}(K_1T_1^{t_1})\mathrm{Tr}(K_{N_0}^{t_{N_0}}T_{N_0}).$$

■

Note that the result in Proposition 3 implies that the same goes for the operators built using the second fusion. Three important remarks are in order here.

The use of dressed quantum traces: Dressed quantum traces yield *a priori* independent operators. Indeed, the classical limit of a quantum trace computed with the particular dressing (17) in Proposition 1 will yield $\mathrm{Tr}\,T^n$ instead of $(\mathrm{Tr}\,T)^n$ (since $A,B,C,D\to\mathbf{1}\otimes\mathbf{1}$ but $P_{12}\to P_{12}$!). Quantum traces are directly, in this particular case, (as was already known in the context of quantum group structures[6]) quantum analogs of the classical Poisson-commuting power traces $\mathrm{Tr}\,T^n$.

The use of undressed quantum traces: It must on the other hand, be emphasized that the decoupling of the undressed fused quantities plays an essential role in the formulation of the analytical Bethe ansatz solution of $\mathfrak{sl}(n)$ spin chains (as is seen in Ref. 9) and more generally in the formulation of a generalized Mezincescu-Nepomechie procedure for fusion of transfer matrices,[8] in that it gives a natural construction of products of monodromy matrices such as are required by this formulation.

Explicit computation of the dressings: From a more theoretical point of view, it must be noticed that Eq. (24), as already discussed for the particular example treated in Ref. 2, would appear as a condition obeyed by coproducts of the central elements of a (hypothetical) universal algebra, thereby promoting the dressing matrices Q and S from "technical auxiliaries" to get nontrivial traces, to representations of Casimir elements of the algebra itself (this was pointed out to us by Arnaudon).

A second more technical remark is required here regarding the actual computation of the quantum traces with the particular explicit dressing determined in Proposition 1. Difficulties in applying (35) with the explicit dressings (17) may occur when the auxiliary space V is a loop space $V^{(n)}\otimes\mathbb{C}(z)$ (n=finite dimension of the vector space). Indeed, the permutation of spectral parameters required in formula (17) is only achieved at a formal level by the singular distribution $\delta(z_i/z_j)$ (see Ref. 2 for discussions). Hence the actual explicit computations of such quantum traces may entail delicate regularization procedures. However, if one only focuses on the practical purpose of the quantum trace procedure, which is to build a set of commuting operators, use of higher-power fused objects as in (14) and (19) is mostly required when no spectral parameter is present in the represented exchange algebra (1). Otherwise one needs to consider only the first order trace $\mathrm{Tr}_1\,\widetilde{K}_1(z_1)T_1(z_1)$ and expand it in formal series in z_1. If no spectral parameter is available, one can then use (14), (19), (17), and (35) to build explicitly without difficulties *a priori* independent commuting quantum operators. (For an application to a different algebraic structure see Ref. 5.)

D. Further example, "soliton nonpreserving" boundary conditions: Twisted Yangians

We have mentioned in the Introduction several examples of nondynamical quadratic exchange algebras. Another interesting example to which we plan to apply this scheme is related to the so-called "soliton nonpreserving" boundary conditions in integrable lattice models (see Ref. 18). To characterize it we will focus on the $\mathfrak{su}(n)$ invariant R-matrix given by

$$R_{12}(\lambda) = \lambda I + i\mathcal{P}_{12}, \tag{38}$$

where $\mathcal{P}$ is the permutation operator on the tensor product $V_1 \otimes V_2$. The R matrix is a solution of the Yang-Baxter equation[19–22] and also satisfies the following.

(i) *Unitarity*,

$$R_{12}(\lambda)R_{21}(-\lambda) = \zeta(\lambda), \tag{39}$$

where $R_{21}(\lambda)=\mathcal{P}_{12}R_{12}(\lambda)\mathcal{P}_{12}=R^{t12}_{12}(\lambda)$ and $\mathcal{P}$ is the permutation operator.

(ii) *Crossing unitarity*,

$$R^{t_1}_{12}(\lambda)M_1R^{t_2}_{12}(-\lambda - 2i\rho)M_1^{-1} = \zeta'(\lambda + i\rho), \tag{40}$$

$M=V^tV$ [$M=1$ for the $\mathfrak{su}(n)$ case], $\rho=n/2$ and also

$$[M_1M_2, R_{12}(\lambda)] = 0, \tag{41}$$

$$\zeta(\lambda) = (\lambda + i)(-\lambda + i), \quad \zeta'(\lambda) = (-\lambda + i\rho)(\lambda + i\rho). \tag{42}$$

It is interpreted as the scattering matrix[23,22,24] describing the interaction between two solitons—objects that correspond to the fundamental representation of $\mathfrak{su}(n)$.

One may also derive the scattering matrix that describes the interaction between a soliton and an antisoliton, which corresponds to the conjugate representation of $\mathfrak{su}(n)$. It reads

$$R_{\bar{1}\bar{2}}(\lambda) = R_{1\bar{2}}(\lambda) = \bar{R}_{12}(\lambda) = U_1R^{t_2}_{12}(-\lambda - i\rho)U_1, \tag{43}$$

and it can also be written as

$$\bar{R}_{12}(\lambda) = (-\lambda - i\rho)I + iQ, \tag{44}$$

where Q is a projector onto a one-dimensional space, and where U is a matrix of square 1. Note that for the su(2) case

$$\bar{R}_{12}(\lambda) = R_{12}(\lambda), \tag{45}$$

which is expected because su(2) is self-conjugate. The $\bar{R}$-matrix also satisfies the Yang-Baxter equation and

(i) *Unitarity*,

$$\bar{R}_{12}(\lambda)\bar{R}_{21}(-\lambda) = \zeta'(\lambda). \tag{46}$$

(ii) *Crossing unitarity*

$$\bar{R}^{t_1}_{12}(\lambda)M_1\bar{R}^{t_2}_{12}(-\lambda - 2i\rho)M_1^{-1} = \zeta(\lambda). \tag{47}$$

The reflection equation: The usual reflection equation[1] describes physically the reflection of a soliton [fundamental representation of $\mathfrak{su}(n)$] as a soliton. The associated quadratic algebra was considered, e.g., in Ref. 2,

$$R_{12}(\lambda_1 - \lambda_2)T_1(\lambda_1)R_{21}(\lambda_1 + \lambda_2)T_2(\lambda_2) = T_2(\lambda_2)R_{12}(\lambda_1 + \lambda_2)T_1(\lambda_1)R_{21}(\lambda_1 - \lambda_2). \tag{48}$$

Considering now the reflection of a soliton as antisoliton one is similarly lead to the formulation of another quadratic algebra,

$$R_{12}(\lambda_1-\lambda_2)T_1(\lambda_1)\bar{R}_{21}(\lambda_1+\lambda_2)T_2(\lambda_2)=T_2(\lambda_2)\bar{R}_{12}(\lambda_1+\lambda_2)T_1(\lambda_1)R_{21}(\lambda_1-\lambda_2). \tag{49}$$

More specifically Eq. (49) is the definition of the so-called twisted Yangian. Its dual reflection equation is obtained essentially by taking its formal transposition

$$\begin{aligned}&R_{12}(-\lambda_1+\lambda_2)K_1^{t_1}(\lambda_1)M_1^{-1}\bar{R}_{21}(-\lambda_1-\lambda_2-2i\rho)M_1K_2^{t_2}(\lambda_2)\\&\quad=K_2^{t_2}(\lambda_2)M_1\bar{R}_{12}(-\lambda_1-\lambda_2-2i\rho)M_1^{-1}K_1^{t_1}(\lambda_1)R_{21}(-\lambda_1+\lambda_2).\end{aligned} \tag{50}$$

This indeed realizes the general quadratic exchange relation (1) and (7), with the following identifications (using unitarity and crossing symmetries of the R-matrix):

$$A_{12}=R_{12}(\lambda_1-\lambda_2),\quad B_{12}=\bar{R}_{21}(\lambda_1+\lambda_2),\quad C_{12}=\bar{R}_{12}(\lambda_1+\lambda_2),\quad D_{12}=R_{21}(\lambda_1-\lambda_2),$$

$$(A_{12}^{-1})^{t_1t_2}=R_{12}(-\lambda_1+\lambda_2),\quad ((B_{12}^{t_1})^{-1})^{t_2}=M_1\bar{R}_{12}(-\lambda_1-\lambda_2-2i\rho)M_1^{-1},$$

$$((C_{12}^{t_2})^{-1})^{t_1}=M_1^{-1}\bar{R}_{21}(-\lambda_1-\lambda_2-2i\rho)M_1,\quad (D_{12}^{-1})^{t_1t_2}=R_{21}(-\lambda_1+\lambda_2).$$

Explicit application of the quantum trace procedure to this particular algebra will be left for further studies.

III. QUANTUM TRACES FOR SEMIDYNAMICAL QUADRATIC ALGEBRAS

The second type of quadratic exchange relations considered here consists of the dynamical quadratic algebras generically described and studied in Ref. 11 which were first exemplified in the context of scalar Ruijsenaars-Schneider models in Ref. 26. Fusion procedures and commuting traces can be built up for these dynamical quadratic algebras following the same overall procedure as in the nondynamical case, albeit with crucial, nontrivial differences.

A. The semidynamical quadratic algebra

Let us recall here the basic definitions. Our starting point is the dynamical quadratic exchange relation

$$A_{12}(\lambda)T_1(\lambda)B_{12}(\lambda)T_2(\lambda+\gamma h_1)=T_2(\lambda)C_{12}(\lambda)T_1(\lambda+\gamma h_2)D_{12}. \tag{51}$$

This describes an algebra generated by the matrix entries of T. A,B,C,D are matrices in End($V\otimes V$) depending on $\lambda\in\mathfrak{h}^*$ where $\mathfrak{h}$ is a commutative Lie algebra, of dimension n, making V a diagonalizable $\mathfrak{h}$-module. Introducing coordinates λ_i on $\mathfrak{h}^*$ and the dual base h_i on $\mathfrak{h}$ the shift $\lambda+\gamma h$ can be defined in the following way. For any differentiable function $f(\lambda)=f(\{\lambda_i\})$,

$$f(\lambda+\gamma h)=e^{\gamma\mathcal{D}}f(\lambda)e^{-\gamma\mathcal{D}}, \tag{52}$$

where

$$\mathcal{D}=\sum_i h_i\partial_{\lambda_i}. \tag{53}$$

In the forthcoming calculations γ is set to 1 for simplification. Zero weight conditions are imposed on the first space of B and the second one of C; D is of total weight zero,

$$[B_{12},h\otimes\mathbf{1}]=[C_{12},\mathbf{1}\otimes h]=[D_{12},h\otimes\mathbf{1}+\mathbf{1}\otimes h]=0\quad(h\in\mathfrak{h}). \tag{54}$$

These particular conditions, together with the absence of dynamical shift in two out of four T matrices in (51), lead us to denote this structure as "semidynamical." We will restrict ourselves from now on to the case where V is of dimension n, the basis of V and the generators of $\mathfrak{h}$, can then be chosen so that one identifies $h_i=E_{ii}$ [diagonal basis elements of $\mathfrak{gl}(n)$, see, e.g., Ref. 25 for

introduction of this condition]. These conditions mean in particular that B and C are diagonal on the corresponding spaces, respectively, V_1 and V_2. In addition, D has components on basis elements $E_{ij}\otimes E_{kl}$ of $\mathfrak{gl}(n)\otimes\mathfrak{gl}(n)$ only when the sets $\{i,k\}$ and $\{j,l\}$ are equal (property ZW). In other words nonzero elements have identical unordered multiplets of line and column indices.

For the consistency of the exchange relations the following set of coupled "dynamical" YB equations is imposed,

$$A_{12}A_{13}A_{23} = A_{23}A_{13}A_{12}, \tag{55}$$

$$D_{12}(\lambda + \gamma h_3)D_{13}D_{23}(\lambda + \gamma h_1) = D_{23}D_{13}(\lambda + \gamma h_2)D_{12}, \tag{56}$$

$$D_{12}B_{13}B_{23}(\lambda + \gamma h_1) = B_{23}B_{13}(\lambda + \gamma h_2)D_{12}, \tag{57}$$

$$A_{12}C_{13}C_{23} = C_{23}C_{13}A_{12}(\lambda + \gamma h_3). \tag{58}$$

The simplest example of this algebra is related to the elliptic scalar $\mathfrak{gl}(n)$ Ruijsenaars-Schneider model and was first written in Ref. 26. We only write down its rational limit here,

$$A(\lambda) = 1 + \sum_{i\neq j}\frac{\gamma}{\lambda_{ij}}(E_{ii} - E_{ij})\otimes(E_{jj} - E_{ji}), \tag{59}$$

$$B(\lambda) = C(\lambda)^{\pi} = 1 + \sum_{i\neq j}\frac{\gamma}{\lambda_{ij} - \gamma}E_{jj}\otimes(E_{ii} - E_{ij}), \tag{60}$$

$$D(\lambda) = 1 - \sum_{i\neq j}\frac{\gamma}{\lambda_{ij}}E_{ii}\otimes E_{jj} + \sum_{i\neq j}\frac{\gamma}{\lambda_{ij}}E_{ij}\otimes E_{ji}, \tag{61}$$

where E_{ij} is the elementary matrix whose entries are $(E_{ij})_{kl}=\delta_{ik}\delta_{jl}$ and $\lambda_{ij}=\lambda_i-\lambda_j$. These matrices verify the consistency conditions (55)–(58). A scalar representation of the exchange algebra defined with these structure matrices is then provided by

$$T(\lambda) = \sum_{ij}\frac{\prod_{a\neq i}(\lambda_{aj} + \tilde{\gamma})}{\prod_{a\neq j}\lambda_{aj}}E_{ij}\otimes\mathbf{1}. \tag{62}$$

The word "scalar" is used here in the sense that $T(\lambda)$ acts on a one-dimensional (trivial) quantum space. The exchange relation (51) is just a c-number equality. Representation of (51) on nontrivial quantum spaces is provided in this context by the comodule structure in Ref. 11.

Let us note here that the condition $AB=CD$ found in Ref. 26 means in this context that the identity matrix is also a solution of (51). This is not a trivial statement; in fact it does not hold in general, and is not preserved by fusion procedures.

B. Fusion procedures and the "dual" algebra

Let A,B,C,D be solutions of the dynamical exchange relation. We will define their fusion by induction as follows. We omit the dependence on λ and simplify the notations of the shifts as $(h_{(\ldots)})$; otherwise we use the notations introduced in Sec. II A, defining the multiple-index matrices by induction as

$$A_{M\bar{N}'} = A_{1\bar{N}'}A_{M_0\bar{N}'} = A_{Mn'}A_{M\bar{N}'_0},$$

$$B_{MN'} = B_{M1'}B_{MN'_0} = B_{1N'}[B_{M_0N'}(h_1)],$$

$$C_{MN'} = C_{1N'} C_{M_0 N'} = C_{M1'}[C_{MN'_0}(h_{1'})],$$

$$D_{M\bar{N}'} = D_{1\bar{N}'}[D_{M_0\bar{N}'}(h_1)] = [D_{Mn'}(h_{(1',n'-1)})] D_{M\bar{N}'_0}.$$

It is clear that there is no change in the fusion of A, cf. Eq. (8). As for the three other matrices, their fusion is written in a more explicit form as

$$B_{MN'} = B_{11'} B_{12'} \cdots B_{1n'} \times B_{21'}(h_1) B_{22'}(h_1) \cdots B_{2n'}(h_1) \cdots \times B_{m1'}(h_1 + \cdots + h_{m-1}) \cdots \times B_{mn'}(h_1 + \cdots + h_{m-1}), \tag{63}$$

$$C_{MN'} = C_{11'} C_{12'}(h_{1'}) \cdots C_{1n'}(h_{(1',n'-1)}) \times C_{21'} C_{22'}(h_{1'}) \cdots C_{2n'}(h_{(1',n'-1)}) \cdots \times C_{m1'} C_{m2'}(h_{1'}) \cdots C_{mn'}(h_{(1',n'-1)}), \tag{64}$$

$$D_{M\bar{N}'} = D_{1n'}(h_{(1',n'-1)}) D_{1,n'-1}(h_{(1',n'-2)}) \cdots D_{11'} \times D_{2n'}(h_1 + h_{(1',n'-1)}) D_{2,n'-1}(h_1 + h_{(1',n'-2)}) \cdots \times D_{21'}(h_1) \cdots \times D_{mn'}(h_{(1,m-1)} + h_{(1',n'-1)}) D_{m,n'-1}(h_{(1,m-1)} + h_{(1',n'-2)}) \cdots D_{m1'}(h_{(1,m-1)}), \tag{65}$$

where $h_{(i,j)} := \sum_{k=i}^{j} h_k$. These fused structure matrices verify the fused dynamical YB equations which are gathered together in the next proposition.

Proposition 5. Let A, B, C, D be solutions of the dynamical Yang-Baxter equations (55)–(58). Then the following fused dynamical Yang-Baxter equations hold

$$A_{M\bar{N}'} A_{M\bar{L}''} A_{N'\bar{L}''} = A_{N'\bar{L}''} A_{M\bar{L}''} A_{M\bar{N}'},$$

$$A_{M\bar{N}'} C_{ML''} C_{N'L''} = C_{N'L''} C_{ML''} A_{M\bar{N}'}(h_{L''}),$$

$$D_{M\bar{N}'}(h_{L''}) D_{M\bar{L}''} D_{N'\bar{L}''}(h_M) = D_{N'\bar{L}''} D_{M\bar{L}'}(h_{N'}) D_{M\bar{N}'},$$

$$D_{M\bar{N}'} B_{ML''} B_{N'L''}(h_M) = B_{N'L''} B_{ML''}(h_{N'}) D_{M\bar{N}'}.$$

Proof: By induction, using at crucial stages the zero weight properties. The fusion procedure respects the property ZW for D and the diagonality of B. It is also clear from the fusion procedure that the fused shift matrix h_M is identified with $h_{(1,m)}$. ■

Theorem 7: *Let T be a solution of the dynamical quadratic exchange relation*,

$$A_{12} T_1 B_{12} T_2(h_1) = T_2 C_{12} T_1(h_2) D_{12}, \tag{66}$$

then

$$T_M = \prod_{i \in M}^{\rightarrow} \left(T_i \left(\sum_{\substack{k<i \\ k \in M}} h_k \right) \left(\prod_{\substack{j>i \\ j \in M}}^{\rightarrow} B_{ij} \right) \right) \tag{67}$$

verifies the fused dynamical exchange relation

$$A_{M\bar{N}'} T_M B_{MN'} T_{N'}(h_M) = T_{N'} C_{MN'} T_M(h_{N'}) D_{M\bar{N}'}. \tag{68}$$

Proof: Similar to that of Theorem 1 but the induction step uses the fact that $T_M = T_1 B_{1M_0} T_{M_0}(h_1)$ and uses the fused dynamical YB equations. ■

The dual exchange relation and an associated fusion procedure are described in the next theorem.

Theorem 8: *Let K be a solution of the dynamical quadratic exchange relation*,

$$(A_{12}^{-1})^{t_1t_2}K_1(B_{12}^{t_2})^{-1}K_2(h_1) = K_2(C_{12}^{t_1})^{-1}K_1(h_2)(D_{12}^{-1})^{t_1t_2} \tag{69}$$

then

$$K_M = \overrightarrow{\prod_{i\in M}} \left(K_i\left(\sum_{\substack{k<i \\ k\in M}} h_k \right) \left(\overrightarrow{\prod_{\substack{j>i \\ j\in M}}} (B_{ij}^{t_j})^{-1} \right) \right) \tag{70}$$

verifies the fused dynamical exchange relation

$$(A_{M\bar{N}'}^{-1})^{t_Mt_N}K_M(B_{MN'}^{t_{N'}})^{-1}K_{N'}(h_M) = K_{N'}(C_{MN'}^{t_M})^{-1}K_M(h_{N'})(D_{M\bar{N}'}^{-1})^{t_Mt_{N'}}. \tag{71}$$

Proof: Similar to the nondynamical case. ■

Note that the structure matrices of this dual relation are related to original ones in the same way as in the nondynamical case once we take into account the partial zero weight property of B and C which implies diagonality on the corresponding spaces, respectively, V_1 and V_2.

C. Second fusion

As in the nondynamical case, one can define another KDM-type fusion with the appropriate shifts. This fusion is characterized by the following exchange relation:

$$A_{\bar{M}N'}T_MB_{M\bar{N}'}T_{N'}(h_M) = T_{N'}C_{\bar{M}N'}T_M(h_{N'})D_{M\bar{N}'}. \tag{72}$$

The analogy with the nondynamical case can be pushed further, i.e., there exists an object L_M linking the fusions in Theorems 7 and 9. This allows us to use directly the proofs of Theorems 3 and 4.

Lemma 3: Let T_M be a solution of the fused equation (68). If L_M verifies the following commutation rules:

$$\begin{gathered} L_MA_{M\bar{N}'} = A_{\bar{M}\bar{N}'}L_M, \\ L_{N'}A_{M\bar{N}'} = A_{MN'}L_{N'}, \\ L_{N'}B_{MN'} = B_{M\bar{N}'}L_{N'}(h_M), \\ L_MC_{MN'} = C_{\bar{M}N'}L_M(h_{N'}) \end{gathered} \tag{73}$$

then L_MT_M is a solution of the exchange relation

$$A_{\bar{M}N'}T_MB_{\bar{M}N'}T_{N'}(h_M) = T_{N'}C_{M\bar{N}'}T_M(h_{N'})D_{M\bar{N}'}. \tag{74}$$

An example of such an L_M is given by

$$L_M = A_{12}\cdots A_{1m}A_{23}\cdots A_{2m}\cdots A_{m-1,m} = \overrightarrow{\prod_{1\leqslant i<j\leqslant m}} A_{ij}. \tag{75}$$

Proof: Straightforward, using the dynamical YB equations (55)–(57). ■

Now we state the dynamical versions of Theorems 3 and 4.

Theorem 9: *Let T be a solution of the dynamical quadratic exchange relation*

$$A_{12}T_1B_{12}T_2(h_1) = T_2C_{12}T_1(h_2)D_{12} \tag{76}$$

then

$$T_M = \prod_{i\in M}^{\rightarrow} \left(\prod_{\substack{j>i \\ j\in M}}^{\rightarrow} A_{ij} T_i \left(\sum_{\substack{k<i \\ k\in M}} h_k \right) \prod_{\substack{j>i \\ j\in M}}^{\leftarrow} B_{ij} \right) \tag{77}$$

verifies the fused dynamical exchange relation

$$A_{\bar{M}N'} T_M B_{M\bar{N}'} T_{N'}(h_M) = T_{N'} C_{\bar{M}N'} T_M(h_{N'}) D_{M\bar{N}'}. \tag{78}$$

Proof: Reproduces the proof of Theorem 3, with suitable dynamical shifts. ■

The dual exchange relation and an associated fusion procedure are described in the next theorem.

Theorem 10: *Let K_M be a solution of the first fused exchange relation (69) and L_M be a solution of (73). Then $\tilde{K}_M = (L_M^{t_M})^{-1} K_M$ is a solution of the KDM-type dual fused exchange relation*

$$(A^{-1}_{\bar{M}N'})^{t_M t_{N'}} \tilde{K}_M ((B^{t_M}_{M\bar{N}'})^{-1})^{t_{N'}} \tilde{K}_{N'}(h_M) = \tilde{K}_{N'}((C^{t_{N'}}_{\bar{M}N'})^{-1})^{t_M} \tilde{K}_M(h_{N'}) (D^{t_M t_{N'}}_{M\bar{N}'})^{-1}. \tag{79}$$

Proof: Reproduces the proof of Theorem 4, with suitable dynamical shifts. ■

D. Dressing

Solutions T_M of the fused dynamical exchange relations also admit dressing procedures. However, because of the dynamical nature of the exchange relations some of the equations that the dressings Q_M and S_M obey exhibit shifts, too. Specifically we have the following.

Proposition 6: Let T_M be a solution of the fused dynamical exchange relation. Then $Q_M T_M S_M$ is also a solution of the fused exchange relation provided Q_M and S_M verify

$$[Q_M, A_{M\bar{N}'}] = [Q_{N'}, A_{M\bar{N}'}] = 0, \tag{80}$$

$$Q_{N'} B_{MN'} = B_{MN'} Q_{N'}(h_M), \quad Q_M C_{MN'} = C_{MN'} Q_M(h_{N'}),$$

$$[S_{N'}, C_{MN'}] = [S_M, B_{MN'}] = 0, \tag{81}$$

$$S_M(h_{N'}) D_{M\bar{N}'} = D_{M\bar{N}'} S_M, \quad S_{N'} D_{M\bar{N}'} = D_{M\bar{N}'} S_{N'}(h_M).$$

A particular solution of these constraints is given by

$$Q_M = \check{A}_{12} \check{A}_{23} \cdots \check{A}_{m-1,m},$$

$$S_M = \check{D}_{12} \check{D}_{23}(h_1) \cdots \check{D}_{m-1,m}(h_{(1,m-2)}).$$

Proof: By induction, similar to the nondynamical dressings. ■

An interesting comparison can be drawn between this formula for S_M and the formula used in Ref. 5 to dress the quantum traces for dynamical quantum groups. The formula for S_M is exactly the "mirror image" of the formula $S_M^{ABB} = \check{R}_{12}(h_{(3,m)}) \cdots \check{R}_{m,m-1}$.

E. Three lemmas: dynamical and cyclic properties of *D*

Three easy technical lemmas are required to proceed with the construction.

Lemma 4 (dynamical transposition): Let $R(q)$ and $S(q)$ be two matrices with mutually commuting entries depending on a set of commuting coordinates $\{q_k\}_{k=1}^n$. We then have

$$(R(q) e^{\mathcal{D}} S(q))^t = [S^{SL}(q)]^t e^{\mathcal{D}} [R^{SC}(q)]^t, \tag{82}$$

where $S^{SL}(q)_{ij}=e^{\partial_i}S(q)_{ij}e^{-\partial_i}=S_{ij}((q_1,\ldots,q_{\{i\}}+1,\ldots,q_n))$ *(shift on line index) and* $R^{SC}(q)_{ij}=e^{-\partial_j}R(q)_{ij}e^{\partial_j}$ *(shift on column index).*

Proof: We compare the ijth entry on both sides using the fact that entries of S^{SL} and R^{SC} do not contain explicit shift quantities e^{∂} and therefore commute with each other. If (in the case of k-tensor products) "i" denotes a k-uple of indices $(i_1,\ldots,i_k)$, the notation $q_{\{i\}}+1$ must be interpreted as $q_{i_1}+1,\ldots,q_{i_k}+1$. ■

Remark: Later we will use this lemma in the special case when $R(q)$ is diagonal. This implies $R^{SC}(q)=e^{-\mathcal{D}}R(q)e^{\mathcal{D}}$.

Lemma 5 (matrix dynamical shift): Let $D(q)$ be a matrix obeying the zero weight condition

$$[D_{12},h\otimes\mathbf{1}+\mathbf{1}\otimes h]=0\quad(h\in\mathfrak{h}). \tag{83}$$

Then the exponentials can be "pushed through" D, that is we have

$$e^{-\mathcal{D}_1-\mathcal{D}_2}D_{12}=\bar{D}_{12}e^{-\mathcal{D}_1-\mathcal{D}_2}, \tag{84}$$

where $\bar{D}_{12}=D_{12}^{-SL_{12}}$.

Proof: What this lemma means is that one can write $e^{-\mathcal{D}_1-\mathcal{D}_2}D_{12}e^{\mathcal{D}_1+\mathcal{D}_2}$ in a *matrix form* where the exponentials of derivatives cancel out. The proof is straightforward because the zero weight condition implies the identification of incoming and outgoing indices of D. One then verifies easily the equality of the two sides. ■

Lemma 6: Let $D(q)$ be a matrix obeying the zero weight condition:

$$[D_{12},h\otimes\mathbf{1}+\mathbf{1}\otimes h]=0\quad(h\in\mathfrak{h}). \tag{85}$$

Then D is cyclic with respect to the trace operation over $V_1\otimes V_2$ as follows:

$$\mathrm{Tr}_{12}(D_{12}X_{12}D_{12}^{-1}e^{\mathcal{D}_1}e^{\mathcal{D}_2})=\mathrm{Tr}_{12}(X_{12}e^{\mathcal{D}_1}e^{\mathcal{D}_2}), \tag{86}$$

where X is an arbitrary matrix the entries of which commute with the entries of D.

Proof: Consequence of the ZW property of D, which allows to reinterpret the matrix indices of $e^{\mathcal{D}_1+\mathcal{D}_2}$ as line instead of column indices of D_{12}^{-1}, allowing then to independently sum over the now decoupled column indices of D_{12}^{-1} with line indices of D_{12} to altogether eliminate the matrix D from the trace. Labels 1 and 2 formally denote here tensored auxiliary spaces. ■

F. Commuting Hamiltonians

We can now state the fundamental result of this section.

Theorem 11: *Let $\mathcal{T}_M$ be a solution of the fused dynamical exchange relations (68). $\mathcal{T}_M$ acts on the tensor product of the auxiliary spaces labeled by M and on the quantum space V_q.*

Let $\mathcal{K}_M$ be a solution of the dual fused dynamical exchange relation (71). $\mathcal{K}_M$ acts on the tensor product of the auxiliary spaces labeled by M and on the quantum space $V_{q'}$.

The following operators,

$$H_M=\mathrm{Tr}_M(T_Me^{\mathcal{D}_M}(K_M^{SC})^{t_M}), \tag{87}$$

constitute a family of mutually commuting quantum operators acting on $V_q\otimes V_{q'}$,

$$[H_M,H_{N'}]=0. \tag{88}$$

Proof: Similar to the preceding one, but extra care must be taken because of the shift operators that enter the expression. Using the dynamical transposition lemma for $K_{N'}$ one has

$$H_MH_{N'}=\mathrm{Tr}(T_Me^{\mathcal{D}_M}(K_M^{SC})^{t_M}T_{N'}e^{\mathcal{D}_{N'}}(K_{N'}^{SC})^{t_{N'}})=\mathrm{Tr}(T_Me^{\mathcal{D}_M}(K_M^{SC})^{t_M}T_{N'}^{t_{N'}}K_{N'}e^{\mathcal{D}_{N'}}), \tag{89}$$

since the invariance of the trace with respect to transposition is preserved in the dynamical case. One then writes

$$\mathrm{Tr}(T_M T_{N'}^{t_{N'}}(h_M) e^{\mathcal{D}_M} (K_M^{SC})^{t_M} K_{N'} e^{\mathcal{D}_{N'}}) = \mathrm{Tr}(T_M T_{N'}^{t_{N'}}(h_M) B_{MN'}^{t_{N'}} (B_{MN'}^{t_{N'}})^{-1} e^{\mathcal{D}_M} (K_M^{SC})^{t_M} K_{N'} e^{\mathcal{D}_{N'}})$$
$$= \mathrm{Tr}((T_M B_{MN'} T_{N'}(h_M))^{t_M t_{N'}} ((B_{MN'}^{t_{N'}})^{-1} e^{\mathcal{D}_M} (K_M^{SC})^{t_M})^{t_M} K_{N'} e^{\mathcal{D}_{N'}}).$$

In the last equality the identification $T_{N'}^{t_{N'}}(h_M) B_{MN'}^{t_{N'}} = (B_{MN'} T_{N'}(h_M))^{t_{N'}}$ uses the zero-weight condition $[B_{MN'}, h_M] = 0$. Using once again the dynamical transposition lemma and the zero-weight condition on B which guarantees $e^{\mathcal{D}_M}((B_{MN'}^{t_{N'}})^{-1})^{SCt_M} = (B_{MN'}^{t_{N'}})^{-1} e^{\mathcal{D}_M}$ as commented above, one gets

$$\mathrm{Tr}((T_M B_{MN'} T_{N'}(h_M))^{t_M t_{N'}} A_{MN'}^{t_M t_{N'}} (A_{MN'}^{t_M t_{N'}})^{-1} K_M (B_{MN'}^{t_{N'}})^{-1} e^{\mathcal{D}_M} K_{N'} e^{\mathcal{D}_{N'}})$$
$$= \mathrm{Tr}((A_{MN'} T_M B_{MN'} T_{N'}(h_M))^{t_M t_{N'}} (A_{MN'}^{t_M t_{N'}})^{-1} K_M (B_{MN'}^{t_{N'}})^{-1} K_{N'}(h_M) e^{\mathcal{D}_M} e^{\mathcal{D}_{N'}}).$$

One here identifies the direct and dual exchange relation, to yield

$$\mathrm{Tr}((T_{N'} C_{MN'} T_M(h_{N'}) D_{MN'})^{t_M t_{N'}} K_{N'} (C_{MN'}^{t_M})^{-1} K_M(h_{N'}) (D_{MN'}^{t_M t_{N'}})^{-1} e^{\mathcal{D}_M} e^{\mathcal{D}_{N'}})$$
$$= \mathrm{Tr}(D_{MN'}^{t_M t_{N'}} (T_{N'} C_{MN'} T_M(h_{N'}))^{t_M t_{N'}} K_{N'} (C_{MN'}^{t_M})^{-1} K_M(h_{N'}) (D_{MN'}^{t_M t_{N'}})^{-1} e^{\mathcal{D}_M} e^{\mathcal{D}_{N'}}).$$

Here Lemma 6 is at work,

$$\mathrm{Tr}((T_{N'} C_{MN'} T_M(h_{N'}))^{t_M t_{N'}} K_{N'} (C_{MN'}^{t_M})^{-1} K_M(h_{N'}) e^{\mathcal{D}_M} e^{\mathcal{D}_{N'}})$$
$$= \mathrm{Tr}(T_{N'} (C_{MN'} T_M(h_{N'}))^{t_M} (K_{N'} (C_{MN'}^{t_M})^{-1} e^{\mathcal{D}_{N'}})^{t_{N'}} K_M e^{\mathcal{D}_M})$$
$$= \mathrm{Tr}(T_{N'} T_M^{t_M}(h_{N'}) C_{MN'}^{t_M} (C_{MN'}^{t_M})^{-1} e^{\mathcal{D}_{N'}} K_{N'}^{SCt_{N'}} K_M e^{\mathcal{D}_M}).$$

Once again we have used the dynamical transposition lemma and the partial weight zero property of $C_{MN'}$,

$$\mathrm{Tr}(T_{N'} T_M^{t_M}(h_{N'}) e^{\mathcal{D}_{N'}} (K_{N'}^{SC})^{t_{N'}} K_M e^{\mathcal{D}_M}) = \mathrm{Tr}(T_{N'} e^{\mathcal{D}_{N'}} (K_{N'}^{SC})^{t_{N'}} T_M^{t_M} K_M e^{\mathcal{D}_M})$$
$$= \mathrm{Tr}(T_{N'} e^{\mathcal{D}_{N'}} K_{N'} T_M e^{\mathcal{D}_M} (K_M^{SC})^{t_M}).$$

■

Without the dressing described by Proposition 6 the traces constructed in (67) decouple just as in the nondynamical case. Indeed we have the following.

Proposition 7: Operators built from the solution (67) decouple as

$$\mathrm{Tr}_M(T_M e^{\mathcal{D}_M} (K_M^{SC}(\ {}^{t_M}) \quad = \mathrm{Tr}(T e^{\mathcal{D}} (K^{SC})^t)^{\#M}.$$

Proof: We will prove the proposition for M with two elements. The statement remains valid for higher powers by induction. We also need to set the trace under a more amenable form. In fact, $\mathrm{Tr}(T_M e^{\mathcal{D}_M} (K_M^{SC})^{t_M}) = \mathrm{Tr}(T_M^{t_M} K_M e^{\mathcal{D}_M})$. By virtue of Lemma 4,

$$\mathrm{Tr}([T_1 B_{12} T_2(h_1)]^{t_1 t_2} K_1 (B_{12}^{t_2})^{-1} K_2(h_1) e^{\mathcal{D}_1 + \mathcal{D}_2}) = \mathrm{Tr}(T_1 [B_{12} T_2(h_1)]^{t_2} [K_1 e^{\mathcal{D}_1} ((B_{12}^{t_2})^{-1})^{SC_1}]^{t_1} K_2 e^{\mathcal{D}_2}),$$

where $(\ )^{SC_1}$ means $(\ )^{SC}$ operation applied on the first space,

$$\mathrm{Tr}(T_1 T_2^{t_2}(h_1) B_{12}^{t_2} (B_{12}^{t_2})^{-1} e^{\mathcal{D}_1} K_1^{SCt_1} K_2 e^{\mathcal{D}_2}) = \mathrm{Tr}(T_1 e^{\mathcal{D}_1} T_2^{t_2} K_1^{SCt_1} K_2 e^{\mathcal{D}_2}) = \mathrm{Tr}(T_1 e^{\mathcal{D}_1} K_1^{SCt_1} T_2^{t_2} K_2 e^{\mathcal{D}_2})$$
$$= \mathrm{Tr}(T e^{\mathcal{D}} K^{SCt})^2.$$

■

Of course, the three comments made after Proposition 4 in the nondynamical case remain valid, although we do not know yet of explicit examples for Mezincescu-Nepomechie procedure in a dynamical context.

IV. THE FULLY DYNAMICAL ALGEBRA

The third type of quadratic algebra considered here is the extension to general structure matrices A,B,C,D of the "boundary dynamical algebra" (BDA) considered in Refs. 13 and 27. Fusion and trace formulas were defined in Ref. 13 for the particular case of BDA where $A=D=R(u_1-u_2)$, $B=C=R(u_1+u_2)$, R being the IRF $\mathbb{Z}_n$ R-matrix. The most general "fully dynamical" (denomination to be justified presently) exchange algebra reads

$$A_{12}(\lambda)T_1(\lambda+\gamma h_2)B_{12}(\lambda)T_2(\lambda+\gamma h_1)=T_2(\lambda+\gamma h_1)C_{12}(\lambda)T_1(\lambda+\gamma h_2)D_{12}(\lambda). \tag{90}$$

Once again we assume $\dim \mathfrak{h}=\dim V$.[25] The following conditions are imposed on the structure matrices ($R=A$, B, C or D) unitarity;

$$R_{12}(u_1,u_2;\lambda)R_{21}(u_2,u_1;\lambda)=\mathbf{1}. \tag{91}$$

Zero weight property,

$$[h\otimes\mathbf{1}+\mathbf{1}\otimes h,R_{12}(u_1,u_2;\lambda)]=0 \quad (h\in\mathfrak{h}). \tag{92}$$

R then verifies the same ZW property as in the semidynamical case. By contrast with the previous case all four matrices in (90) exhibit a dynamical shift and all four structure matrices have (1+2) zero weight, hence the denomination "fully dynamical." In some specific examples[27,28] the structure matrices also obey the dynamical zero weight property,

$$[\mathcal{D}\otimes\mathbf{1}+\mathbf{1}\otimes\mathcal{D},R_{12}(u_1,u_2;\lambda)]=0. \tag{93}$$

Structure matrices all obey Gervais-Neveu-Felder-type equations,

$$\begin{aligned}
&A_{12}(\lambda)A_{13}(\lambda+\gamma h_2)A_{23}(\lambda)=A_{23}(\lambda+\gamma h_1)A_{13}(\lambda)A_{12}(\lambda+\gamma h_3),\\
&A_{12}(\lambda)C_{13}(\lambda+\gamma h_2)C_{23}(\lambda)=C_{23}(\lambda+\gamma h_1)C_{13}(\lambda)A_{12}(\lambda+\gamma h_3),\\
&D_{12}(\lambda+\gamma h_3)D_{13}(\lambda)D_{23}(\lambda+\gamma h_1)=D_{23}(\lambda)D_{13}(\lambda+\gamma h_2)D_{12}(\lambda),\\
&D_{12}(\lambda+\gamma h_3)B_{13}(\lambda)B_{23}(\lambda+\gamma h_1)=B_{23}(\lambda)B_{13}(\lambda+\gamma h_2)D_{12}(\lambda).
\end{aligned} \tag{94}$$

If the dynamical zero weight property is verified then all equations can be rewritten under the more familiar alternating shift form,

$$R_{12}(\lambda-\gamma h_3)R_{13}(\lambda+\gamma h_2)R_{23}(\lambda-\gamma h_1)=R_{23}(\lambda+\gamma h_1)R_{13}(\lambda-\gamma h_2)R_{12}(\lambda+\gamma h_3).$$

As in the previous situation, these equations ensure the compatibility of the algebra in the following sense. Let us take the left-hand side of exchange relation (90), embed it in a triple tensor product and shift it on the third space. Then let us multiply it with $B_{13}(u_1,u_3;\lambda)B_{23}(u_2,u_3;\lambda+\gamma h_1)T_3(u_3;\lambda+\gamma h_1+\gamma h_2)$. One can reverse the order of the T's in two different ways which yield the same result if Eqs. (94) are obeyed.

A. Fusion procedure and the "dual" algebra

The fusion of the structure matrices is again defined by induction as follows:

$$A_{M\bar{N}'}=A_{1\bar{N}'}(h_{(2,m)})A_{M_0\bar{N}'}=A_{Mn'}A_{M\bar{N}'_0}(h_{n'}),$$

$$B_{MN'}=B_{1N'}B_{M_0N'}(h_1)=B_{M1'}(h_{(2',n')})B_{MN'_0},$$

$$C_{MN'}=C_{1N'}(h_{(2,m)})C_{M_0N'}=C_{M1'}C_{MN'_0}(h_1),$$

$$D_{M\bar{N}'} = D_{1\bar{N}'} D_{M_0\bar{N}'}(h_1) = D_{Mn'}(h_{(1',n'-1)}) D_{M\bar{N}'_0}.$$

A and C are fused in the same way which is written more explicitly as

$$A_{M\bar{N}'} = A_{1n'}(h_{(2,m)}) A_{1,n'-1}(h_{n'} + h_{(2,m)}) \cdots A_{11'}(h_{(2',n')} + h_{(2,m)}) A_{2n'}(h_{(3,m)}) A_{2,n'-1}(h_{n'} + h_{(3,m)}) \cdots$$
$$\times A_{21'}(h_{(2',n')} + h_{(3,m)}) \cdots \times A_{mn'} A_{m,n'-1}(h_{n'}) \cdots A_{m1'}(h_{(2',n')}). \tag{95}$$

B and D are otherwise fused in the same way as in Eq. (65).

These fused matrices verify the corresponding fused YB equations and the ZW property.

Proposition 8: Let A,B,C,D be solutions of the dynamical Yang-Baxter equations (94). Then the following fused dynamical Yang-Baxter equations hold:

$$A_{M\bar{N}'} A_{M\bar{L}''}(h_{N'}) A_{N'\bar{L}''} = A_{N'\bar{L}''}(h_M) A_{M\bar{L}''} A_{M\bar{N}'}(h_{L''}),$$

$$A_{M\bar{N}'} C_{ML''}(h_{N'}) C_{N'L''} = C_{N'L''}(h_M) C_{ML''} A_{M\bar{N}'}(h_{L''}),$$

$$D_{M\bar{N}'}(h_{L''}) D_{M\bar{L}''} D_{N'\bar{L}''}(h_M) = D_{N'\bar{L}''} D_{M\bar{L}''}(h_{N'}) D_{M\bar{N}'},$$

$$D_{M\bar{N}'}(h_{L''}) B_{ML''} B_{N'L''}(h_M) = B_{N'L''} B_{ML''}(h_{N'}) D_{M\bar{N}'}.$$

Proof. Straightforward by induction. ∎

Note that the dynamical zero weight property does not survive fusion, but algebraic zero weight does. In this sense this dynamical zero weight property is not relevant for the construction of commuting traces, and is not (generically) a feature of the universal algebra. We will from now on disregard it. In addition, we will concentrate here on the most relevant features of quantum trace building, ignoring for instance the possibility of a "second fusion."

Theorem 12: *Let T be a solution of the dynamical quadratic exchange relation*

$$A_{12} T_1(h_2) B_{12} T_2(h_1) = T_2 C_{12} T_1(h_2) D_{12}, \tag{96}$$

then

$$T_M = \overrightarrow{\prod_{i \in M}} \left(T_i \left(\sum_{\substack{k \neq i \\ k \in M}} h_k \right) \left(\overrightarrow{\prod_{\substack{j > i \\ j \in M}}} B_{ij} \left(\sum_{\substack{k < i \\ k \in M}} h_k + \sum_{\substack{k > j \\ k \in M}} h_k \right) \right) \right) \tag{97}$$

verifies the fused dynamical exchange relation

$$A_{M\bar{N}'} T_M(h_{N'}) B_{MN'} T_{N'}(h_M) = T_{N'}(h_M) C_{MN'} T_M(h_{N'}) D_{M\bar{N}'}. \tag{98}$$

Proof: Similar to that of Theorem 1 but the induction step uses the fact that $T_M = T_1(h_{M_0}) B_{1M_0} T_{M_0}(h_1)$ and uses the fused dynamical YB equations. ∎

The dual exchange relation and the associated fusion procedure are described in the next theorem.

Theorem 13: *Let K be a solution of the dynamical quadratic exchange relation*

$$A^d_{12}(\lambda) K_1\ (\lambda + \gamma h_2) B^d_{12}(\lambda)) K_2(\lambda + \gamma h_1) = K_2(\lambda + \gamma h_1) C^d_{12}(\lambda) K_1(\lambda + \gamma h_2) D^d_{12}(\lambda),$$

where

$$A^d_{12} = ((A_{12}^{-SL_{12}})^{-1})^{-SC_{12}t_{12}}\ B^d_{12} = (((B_{12}^{-SL_{12}})^{-SC_2 t_2})^{-1})^{SL_1 t_1},$$

$$C^d_{12} = (((C_{12}^{-SL_{12}})^{-SC_1 t_1})^{-1})^{SL_2 t_2}\ D^d_{12} = ((D_{12}^{-SL_{12}})^{-1})^{SL_{12} t_{12}},$$

then

$$K_M = \overrightarrow{\prod_{i\in M}} \left(K_i\left(\sum_{\substack{k\neq i\\ k\in M}} h_k \right) \left(\overrightarrow{\prod_{\substack{j>i\\ j\in M}}} B^d_{ij}\left(\sum_{\substack{k<i\\ k\in M}} h_k + \sum_{\substack{k>j\\ k\in M}} h_k \right) \right) \right) \tag{99}$$

verifies the fused dynamical exchange relation

$$A^d_{M\bar{N}'} K_M(h_{N'}) B^d_{MN'} K_{N'}(h_M) = K_{N'}(h_M) C^d_{MN'} K_M(h_{N'}) D^d_{M\bar{N}'}. \tag{100}$$

Proof: Straightforward once one has established that the fused dual structure matrix is equal to the dual of the fused structure matrix and that the YB equations obeyed by the dual structure matrices derive from the equations (94). ■

B. Dressing

Proposition 9: Let T_M be a solution of the fused fully dynamical exchange relation. Then $Q_M T_M S_M$ is also a solution of the fused exchange relation provided Q_M and S_M verify

$$\begin{aligned} &Q_M A_{M\bar{N}'} = A_{M\bar{N}'} Q_M(h_{N'}), \quad Q_{N'}(h_M) A_{M\bar{N}'} = A_{M\bar{N}'} Q_{N'}, \\ &Q_{N'} B_{MN'} = B_{MN'} Q_{N'}(h_M), \quad Q_M C_{MN'} = C_{MN'} Q_M(h_{N'}), \end{aligned} \tag{101}$$

$$\begin{aligned} &S_{N'}(h_M) C_{MN'} = C_{MN'} S_{N'}, \quad S_M(h_{N'}) B_{MN'} = B_{MN'} S_M, \\ &S_M(h_{N'}) D_{M\bar{N}'} = D_{M\bar{N}'} S_M, \quad S_{N'} D_{M\bar{N}'} = D_{M\bar{N}'} S_{N'}(h_M). \end{aligned} \tag{102}$$

A particular solution of these constraints is given by

$$Q_M = \check{A}_{12}(h_{(3,m)}) \check{A}_{23}(h_{(4,m)}) \cdots \check{A}_{m-1,m},$$

$$S_M = \check{D}_{12} \check{D}_{23}(h_1) \cdots \check{D}_{m-1,m}(h_{(1,m-2)}).$$

Proof: By induction. ■

C. Commuting traces

We use the following properties inferred from Lemma 5:

$$e^{-\mathcal{D}_1-\mathcal{D}_2} A_{12} = A_{12}^{-SL_{12}} e^{-\mathcal{D}_1-\mathcal{D}_2} = \bar{A}_{12} e^{-\mathcal{D}_1-\mathcal{D}_2},$$

$$e^{-\mathcal{D}_2} A_{12} e^{\mathcal{D}_1} = e^{\mathcal{D}_1} \bar{A}_{12} e^{-\mathcal{D}_2},$$

and their transposed variants

$$e^{\mathcal{D}_1} (\bar{A}_{12}^{-SC_2 t_2})^{-1} e^{\mathcal{D}_2} = e^{\mathcal{D}_2} (A_{12}^{-SL_2 t_2})^{-1} e^{\mathcal{D}_1} \tag{103}$$

and so on. Since these relations are immediately derived from the ZW property on the structure matrices, they remain valid for fused structure matrices, too, since the fusion respects the zero weight property as opposed to the dynamical zero weight property (cf. remark above). In this case labels 1 and 2 formally denote tensored auxiliary spaces.

Theorem 14: *Let $\mathcal{T}_M$ be a solution of the fused dynamical exchange relations (68). $\mathcal{T}_M$ acts on the tensor product of the auxiliary spaces labeled by M and on the quantum space V_q.*

Let $\mathcal{K}_M$ be a solution of the dual fused dynamical exchange relation (72). $\mathcal{K}_M$ acts on the

tensor product of the auxiliary spaces labeled by M and on the quantum space $V_{q'}$.

The following operators:

$$H_M = \mathrm{Tr}_M e^{-\mathcal{D}_M} T_M e^{\mathcal{D}_M} K_M^{SCt_M} \tag{104}$$

constitute a family of commuting operators acting on $V_q \otimes V_{q'}$

$$[H_M, H_{N'}] = 0. \tag{105}$$

Proof: It is worth to give a detailed description of the proof as in Theorem 11 since the occurence of derivative objects $\sim e^{\mathcal{D}_M}$ considerably modifies it in comparison to the standard Sklyanin-type proof for nondynamical algebras. Once again the dynamical transposition lemma plays an essential role,

$$\begin{aligned}
H_M H_{N'} &= \mathrm{Tr}\, e^{-\mathcal{D}_M} T_M e^{\mathcal{D}_M} K_M^{SC_M t_M} e^{-\mathcal{D}_{N'}} T_{N'} e^{\mathcal{D}_{N'}} K_{N'}^{SC_{N'} t_{N'}} \\
&= \mathrm{Tr}\, e^{-\mathcal{D}_M} T_M e^{\mathcal{D}_M} K_M^{SC_M t_M} (e^{-\mathcal{D}_{N'}} T_{N'})^{t_{N'}} (e^{\mathcal{D}_{N'}} K_{N'}^{SC_{N'} t_{N'}})^{t_{N'}} \\
&= \mathrm{Tr}\, e^{-\mathcal{D}_M} T_M e^{\mathcal{D}_M} K_M^{SC_M t_M} T_{N'}^{-SL_{N'} t_{N'}} e^{-\mathcal{D}_{N'}} K_{N'} e^{\mathcal{D}_{N'}} \\
&= \mathrm{Tr}\, e^{-\mathcal{D}_M} T_M e^{\mathcal{D}_M} T_{N'}^{-SL_{N'} t_{N'}} K_M^{SC_M t_M} e^{-\mathcal{D}_{N'}} K_{N'} e^{\mathcal{D}_{N'}} \\
&= \mathrm{Tr}\, e^{-\mathcal{D}_M} [e^{-\mathcal{D}_{N'}} A_{MN'}^{-1} T_{N'}(h_M) C_{MN'} T_M(h_{N'}) D_{MN'} e^{\mathcal{D}_M}]^{t_{N'}} \\
&\quad \times (\bar{B}_{MN'}^{-SC_{N'} t_{N'}})^{-1} e^{\mathcal{D}_{N'}} K_M^{SC_M t_M} e^{-\mathcal{D}_{N'}} K_{N'} e^{\mathcal{D}_{N'}} \\
&= \mathrm{Tr} [e^{-\mathcal{D}_M - \mathcal{D}_{N'}} A_{MN'}^{-1} T_{N'}(h_M) C_{MN'} T_M(h_{N'}) D_{MN'}]^{t_{MN'}} \\
&\quad \times [e^{\mathcal{D}_M} (\bar{B}_{MN'}^{-SC_{N'} t_{N'}})^{-1} e^{\mathcal{D}_{N'}} K_M^{SC_M t_M}]^{t_M} e^{-\mathcal{D}_{N'}} K_{N'} e^{\mathcal{D}_{N'}}.
\end{aligned}$$

Pushing exponentials through B,

$$\begin{aligned}
&\mathrm{Tr}[e^{-\mathcal{D}_M - \mathcal{D}_{N'}} A_{MN'}^{-1} T_{N'}(h_M) C_{MN'} T_M(h_{N'}) D_{MN'}]^{t_{MN'}} e^{\mathcal{D}_{N'}} [(B_{MN'}^{-SL_{N'} t_{N'}})^{-1} e^{\mathcal{D}_M} K_M^{SC_M t_M}]^{t_M} e^{-\mathcal{D}_{N'}} K_{N'} e^{\mathcal{D}_{N'}} \\
&= \mathrm{Tr}[\bar{A}_{MN'}^{-1} e^{-\mathcal{D}_M - \mathcal{D}_{N'}} T_{N'}(h_M) C_{MN'} T_M(h_{N'}) D_{MN'}]^{t_{MN'}} e^{\mathcal{D}_{N'}} K_M e^{\mathcal{D}_M} ((B_{MN'}^{-SL_{N'} t_{N'}})^{-1})^{SC_M t_M} e^{-\mathcal{D}_{N'}} K_{N'} e^{\mathcal{D}_{N'}}.
\end{aligned}$$

Using zero weight of A and B transposed,

$$\begin{aligned}
&\mathrm{Tr}[T_{N'}(h_M) C_{MN'} T_M(h_{N'}) D_{MN'}]^{-SL_{MN'} t_{MN'}} \\
&\quad \times e^{-\mathcal{D}_M - \mathcal{D}_{N'}} (\bar{A}_{MN'}^{-1})^{-SC_{MN'} t_{MN'}} e^{\mathcal{D}_{N'}} K_M e^{-\mathcal{D}_{N'}} ((\bar{B}_{MN'}^{-SC_{N'} t_{N'}})^{-1})^{SL_1 t_M} e^{\mathcal{D}_M} K_{N'} e^{-\mathcal{D}_M} e^{\mathcal{D}_M + \mathcal{D}_{N'}} \\
&= \mathrm{Tr}[T_{N'}(h_M) C_{MN'} T_M(h_{N'}) D_{MN'}]^{-SL_{MN'} t_{MN'}} \\
&\quad \times e^{-\mathcal{D}_M - \mathcal{D}_{N'}} \{(\bar{A}_{MN'}^{-1})^{-SC_{MN'} t_{MN'}} K_M(h_{N'}) ((B_{MN'}^{-SC_{N'} t_{N'}})^{-1})^{SL_1 t_M} K_{N'}(h_M)\} e^{\mathcal{D}_M + \mathcal{D}_{N'}} \\
&= \mathrm{Tr}[T_{N'}(h_M) C_{MN'} T_M(h_{N'}) D_{MN'}]^{-SL_{MN'} t_{MN'}} e^{-\mathcal{D}_M - \mathcal{D}_{N'}} K_{N'}(h_M) ((\bar{C}_{MN'}^{-SC_M t_M})^{-1})^{SL_{N'} t_{N'}} \\
&\quad \times K_M(h_{N'}) (\bar{D}_{MN'}^{-1})^{SL_{MN'} t_{MN'}} e^{\mathcal{D}_M + \mathcal{D}_{N'}} \\
&= \mathrm{Tr}[e^{-\mathcal{D}_M - \mathcal{D}_{N'}} T_{N'}(h_M) C_{MN'} T_M(h_{N'}) D_{MN'}][K_{N'}(h_M) ((\bar{C}_{MN'}^{-SC_M t_M})^{-1})^{SL_{N'} t_{N'}} \\
&\quad \times K_M(h_{N'}) e^{\mathcal{D}_M + \mathcal{D}_{N'}} (D_{MN'}^{-1})^{SC_{MN'} t_{MN'}}]^{t_{MN'}} \\
&= \mathrm{Tr}\, e^{-\mathcal{D}_M - \mathcal{D}_{N'}} T_{N'}(h_M) C_{MN'} T_M(h_{N'}) D_{MN'} D_{MN'}^{-1} e^{\mathcal{D}_M + \mathcal{D}_{N'}} \\
&\quad \times [K_{N'}(h_M) ((\bar{C}_{MN'}^{-SC_M t_M})^{-1})^{SL_{N'} t_{N'}} K_M(h_{N'})]^{SL_{MN'} t_{MN'}}
\end{aligned}$$

$$= \mathrm{Tr}\, e^{-\mathcal{D}_{N'}} T_{N'} [e^{-\mathcal{D}_M} C_{MN'} e^{\mathcal{D}_{N'}} T_M]^{t_M} e^{\mathcal{D}_M - \mathcal{D}_{N'}}$$

$$\times [K_{N'} e^{-\mathcal{D}_M} ((\bar{C}_{MN'}^{-SC_M t_M})^{-1})^{SL_{N't_{N'}}} e^{\mathcal{D}_{N'}}]^{t_{N'}} K_M e^{\mathcal{D}_M}$$

$$= \mathrm{Tr}\, e^{-\mathcal{D}_{N'}} T_{N'} e^{\mathcal{D}_{N'}} [\bar{C}_{MN'} e^{-\mathcal{D}_M} T_M]^{t_M} e^{\mathcal{D}_M - \mathcal{D}_{N'}} [K_{N'} e^{\mathcal{D}_{N'}} \ (C_{MN'}^{-SL_1 t_M})^{-1})^{SC_{N't_{N'}}}]^{t_{N'}} e^{-\mathcal{D}_M} K_M e^{\mathcal{D}_M}$$

$$= \mathrm{Tr}\, e^{-\mathcal{D}_{N'}} T_{N'} e^{\mathcal{D}_{N'}} T_M^{-SL_1 t_M} e^{-\mathcal{D}_M} \bar{C}_{MN'}^{-SC_M t_M} e^{\mathcal{D}_M - \mathcal{D}_{N'}} (C_{MN'}^{-SL_1 t_M})^{-1} e^{\mathcal{D}_{N'}} K_{N'}^{SC_{N't_{N'}}} e^{-\mathcal{D}_M} K_M e^{\mathcal{D}_M}.$$

Using zero weight of C,

$$\mathrm{Tr}\, e^{-\mathcal{D}_{N'}} T_{N'} e^{\mathcal{D}_{N'}} T_M^{-SL_1 t_M} e^{-\mathcal{D}_{N'}} C_{MN'}^{-SL_1 t_M} (C_{MN'}^{-SL_1 t_M})^{-1} e^{\mathcal{D}_{N'}} K_{N'}^{SC_{N't_{N'}}} e^{-\mathcal{D}_M} K_M e^{\mathcal{D}_M}$$

$$= \mathrm{Tr}\, e^{-\mathcal{D}_{N'}} T_{N'} e^{\mathcal{D}_{N'}} T_M^{-SL_1 t_M} K_{N'}^{SC_{N't_{N'}}} e^{-\mathcal{D}_M} K_M e^{\mathcal{D}_M}$$

$$= \mathrm{Tr}\, e^{-\mathcal{D}_{N'}} T_{N'} e^{\mathcal{D}_{N'}} K_{N'}^{SC_{N't_{N'}}} T_M^{-SL_1 t_M} e^{-\mathcal{D}_M} K_M e^{\mathcal{D}_M}$$

$$= \mathrm{Tr}\, e^{-\mathcal{D}_{N'}} T_{N'} e^{\mathcal{D}_{N'}} K_{N'}^{SC_{N't_{N'}}} [T_M^{-SL_1 t_M} e^{-\mathcal{D}_M}]^{t_M} [K_M e^{\mathcal{D}_M}]^{t_M}$$

$$= \mathrm{Tr}\, e^{-\mathcal{D}_{N'}} T_{N'} e^{\mathcal{D}_{N'}} y K_{N'}^{SC_{N't_{N'}}} e^{-\mathcal{D}_M} T_M e^{\mathcal{D}_M} K_M^{SC_M t_M} = H_{N'} H_M.$$

■

V. CONCLUSION

We have now defined fusion and trace procedures in view of obtaining commuting Hamiltonians of "quantum trace type," for the nondynamical general quadratic algebra (1), for the semidynamical quadratic algebra (51) and for the fully dynamical quadratic algebra (90). Our immediate interest is now to apply this procedure to some particularly interesting examples of such quadratic algebras, the most relevant being at this time the scalar Ruijsenaars-Schneider quantum Lax formulation (semidynamical type).[29]

Note in this respect that previous application of an order-one trace formulation (i.e., without auxiliary space tensor products) to the specific case of "boundary dynamical $\mathfrak{sl}(2)$ algebras" considered in Ref. 12 yielded models described in Ref. 27 as generalizations of the Gaudin models. Positions of the sites were associated with values of the spectral parameters (in a spin-chain-type construction), not with the dynamical variable itself whose interpretation is unclear.

As already emphasized, our elucidation of tensor product structure for quadratic algebras is also very important in formulating generalizations of the Mezincescu-Nepomechie fusion procedure in general open spin chains.[9]

Our constructions moreover also shed light on some characteristic properties of the quadratic algebra. The building of commuting traces requires first of all the introduction of a dual exchange relation. It seems possible that this notion reflects the existence of antiautomorphisms of the underlying hypothetical algebra structure, of which the transposition and crossing relations used in the nondynamical cases (see Ref. 2) would be realizations.

The explicit formulation of consistent fusion relations should also help in understanding the meaning of quantum algebra (QA) structures and characterizing in particular their coalgebra properties. As pointed out, the DKM-type fusions do stem in at least one case from a universal structure,[15] and so does the fusion for boundary dynamical algebra (case when A,B,C,D stem from one single dynamical R-matrix[14]). Regarding the semidynamical QA it was already known[11] that one could extend the quantum space on which entries of T act, by auxiliary spaces of A and B or C and D matrices, thereby obtaining spin-chain-type construction of a monodromy matrix (comodule structure). We have now defined the complementary procedure, extending the auxiliary space by a "fusion" procedure. This yields the full "coproduct" or rather comodule structure of the DQA (51).

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The global strong solutions of Hasegawa-Mima-Charney-Obukhov equation

Hongjun Gao[a] and Anyou Zhu
School of Mathematics and Computer Sciences, Nanjing Normal University, Nanjing, 210097, People's Republic of China

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The quasigeostrophic model is a simplified geophysical fluid model at asymptotically high rotation rate or at small Rossby number. We consider the quasigeostrophic equation with no dissipation term which was obtained as an asymptotic model from the Euler equations with free surface under a quasigeostrophic velocity field assumption. It is called the Hasegawa-Mima-Charney-Obukhov equation, which also arises from plasmas theory. We use *a priori* estimates to get the global existence of strong solutions for an Hasegawa-Mima-Charney-Obukhov equation. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2008208]

I. INTRODUCTION

This paper is devoted to study of the Cauchy problem on R^2 and to the existence of strong solutions for a general class of equations arising in plasma theory and geophysics. The quasigeostrophic equations describe large scale motion in the atmosphere and oceans at middle latitudes. Being considerably simper than the primitive equations, they have been widely used for modeling atmospheric and oceanic circulation, and for studies of stability, frontogenesis, and turbulence. A number of assertions have been made about these equations. Charney[4] and Obukhov[16] have derived a shallow water model from the Euler equation with free surface under a quasigeostrophic velocity field assumption. The reader could find some additional details on the formal derivation in Ref. 18. As in Ref. 17, by an asymptotic multiscale development with respect to δ (Aspect ratio) and ϵ (Rossby number) and using the β-plane approximation, the following quasigeostrophic equation was obtained:

$$(\Delta\eta_0 - F\eta_0)_t + J(\eta_0, \Delta\eta_0) + J(\eta_0, \eta_B + \beta y) = 0,$$

where η_0 is the amplitude of the surface perturbation at the lowest order in ϵ, $\eta_B(x,y)$ is the equation of the bottom and J is the Poisson bracket $J(u,v)=u_x v_y - u_y v_x$, F is Froude number. In this context, η_0 is a wave function of the velocity field. Moreover, for sake of simplicity we consider a flat bottom that is η_B is taken to be zero:

$$(\Delta\eta_0 - F\eta_0)_t + J(\eta_0, \Delta\eta_0) + \beta\eta_{0_x} = 0. \tag{1.1}$$

In plasma theory, these models describe drift waves in a nonuniform, β-low plasma in magnetic field and Eq. (1.1) was first derived in this setting by Hasegawa and Mima (see Refs. 8 and 9).

In Ref. 1, based on the results of Refs. 10 and 11, the authors obtained an existence and uniqueness theorem for a simplified quasigeostrophic equation in a bounded open annular cylinder. In Ref. 2, a coupled system of a second-order elliptic equation for a stream function, first-order hyperbolic equations for relative potential vorticity, and surface potential temperatures on a three-dimensional domain which is periodic in both horizontal spatial coordinates had been stud-

[a]Electronic mail: gaohj@njnu.edu.cn

ied. The authors of Ref. 2 used Schauder estimates and a Schauder fixed-point theorem to prove the existence and uniqueness of strong solution of the model in a finite interval of time, which is inversely proportional to the sum of the norms for the initial vorticity and surface temperatures.

In Refs. 5, 6, 15, and 19, the authors considered the initial value problem for two-dimensional critical dissipative quasigeostrophic equation:

$$\partial_t\theta + u\cdot\nabla\theta + \kappa(-\Delta)^\alpha\theta = f, \quad x\in\Omega, \quad t>0, \tag{1.2}$$

where $\kappa>0$, $\alpha\in[0,1]$, θ is a scalar function of x and t, and $u=(u_1,u_2)$ is the velocity field determined from θ by a stream function ψ via the auxiliary relations:

$$u=(u_1,u_2)=\left(-\frac{\partial\psi}{\partial x_2},\frac{\partial\psi}{\partial x_1}\right) \text{ and } (-\Delta)^{1/2}\psi=-\theta.$$

The authors have obtained many results for (1.2).

Let us remark that, (1.1) with $F=\beta=0$ could be treated as the two-dimensional Euler equation by setting $u=(-\eta_{0_y},\eta_{0_x})$. About the Euler equations for incompressible fluid motion in R^n for $n\geqslant 2$, it is proved by Kato and Lai,[12] Kato and Ponce[13] that there exists a $W^{s,p}(s>n/p+1)$ solution on the interval $[0,T)$. The time interval T of existence of the solution depends only on initial value in $W^{s,p}$-norm. It is an interesting question whether the solution is global one.

In this paper, for the simplicity, letting $F=1$, then we could rewrite the Cauchy problem for (1.1) as

$$(\Delta-I)u_t+u_x+J(u,\Delta u)=0, \quad u(0,x,y)=u_0(x,y)\in H^2(R^2). \tag{1.3}$$

The existence and uniqueness of local strong solution for (1.3) was obtained in Ref. 17. In this paper, our major goal is to get a global strong solution with H^4 initial data for (1.3). So, our result gives a partial answer in R^2. First, let us recall the results from Ref. 17.

Theorem 1.1: Let u_0 in $H^s(R^2)$ for an integer $s\geqslant 4$, then there exist $T^*=T^*(\|u_0\|_s)$ and a unique $u=u(t,x,y)$ satisfying

$$u\in L^\infty([0,T^*],H^s(R^2))\cap C^0([0,T^*],H^1(R^2)),$$

$$u_t\in L^\infty([0,T^*],H^{s-1}(R^2))\cap C^0([0,T^*],L^2(R^2))$$

and

$$(\Delta-I)u_t+u_x+J(u,\Delta u)=0, \quad u(0,x,y)=u_0(x,y)$$

with

$$J(u,\Delta u)\in L^\infty([0,T^*],H^{s-3}(R^2)).$$

The proof of this theorem can be found in Ref. 17. In Sec. II, we will use *a priori* estimates to prove the existence and uniqueness of global strong solution of (1.3).

II. GLOBAL THEORY IN $H^4(R^2)$

Hereafter C will denote possibly different constants. Let $\|\cdot\|_{H^s}$ and $|\cdot|_{L^2}$ denote the norm in the standard Sobolev space H^s (s is an integer) and L^2, respectively. And $\int_{R^2}u$ denote $\int_{R^2}u\mathrm{d}x\mathrm{d}y$.

Lemma 2.1: For any solution u from Theorem 1.1, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}(|\nabla u|_{L^2}^2+|u|_{L^2}^2)=0, \tag{2.1}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(|\Delta u|_{L^2}^2+|\nabla u|_{L^2}^2)=0. \tag{2.2}$$

Proof: Multiplying (1.3) by u and Δu, respectively, and integrating over R^2, we will obtain (2.1) and (2.2) immediately.

Lemma 2.2: For any solution u from Theorem 1.1, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}(|\nabla^3 u|_{L^2}^2 + |\Delta u|_{L^2}^2) \leqslant C(1+\log(1+\|u\|_{H^4}))\|u\|_{H^4}^2. \tag{2.3}$$

Proof: Multiplying (1.3) by $\Delta^2 u$ and integrating over R^2, we obtain

$$-\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}(|\nabla^3 u|_{L^2}^2 + |\Delta u|_{L^2}^2) + \int_{R^2} u_x \Delta^2 u + \int_{R^2} J(u,\Delta u)\Delta^2 u = 0.$$

Since $\int_{R^2} u_x \Delta^2 u = 0$, we get

$$-\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}(|\nabla^3 u|_{L^2}^2 + |\Delta u|_{L^2}^2) + \int_{R^2} J(u,\Delta u)\Delta^2 u = 0. \tag{2.4}$$

Furthermore, we have

$$\begin{aligned}
\left|\int_{R^2} J(u,\Delta u)\Delta^2 u\right| &= \left|\int_{R^2} (u_x \Delta u_y \Delta^2 u - u_y \Delta u_x \Delta^2 u)\right| \leqslant \left|\int_{R^2} u_x \Delta u_y \Delta^2 u\right| + \left|\int_{R^2} u_y \Delta u_x \Delta^2 u\right| \\
&\leqslant |u_x|_{L^\infty}\int_{R^2} |\Delta u_y||\Delta^2 u| + |u_y|_{L^\infty}\int_{R^2} |\Delta u_x||\Delta^2 u| \leqslant |u_x|_{L^\infty}|\Delta u_y|_{L^2}|\Delta^2 u|_{L^2} \\
&\quad + |u_y|_{L^\infty}|\Delta u_x|_{L^2}|\Delta^2 u|_{L^2} \leqslant C(1+\log(1+\|u\|_{H^3}))(\|u\|_{H^3}\|u\|_{H^4} + \|u\|_{H^3}\|u\|_{H^4}) \\
&\leqslant C(1+\log(1+\|u\|_{H^3}))\|u\|_{H^4}^2 \leqslant C(1+\log(1+\|u\|_{H^4}))\|u\|_{H^4}^2,
\end{aligned} \tag{2.5}$$

where the Brezis-Gallouet's inequality[3] has been used. Combining (2.4) and (2.5), the proof of Lemma 2.2 is completed.

Lemma 2.3: For any solution u from Theorem 1.1, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}(|\Delta^2 u|_{L^2}^2 + |\nabla^3 u|_{L^2}^2) \leqslant C(1+\log(1+\|u\|_{H^4}))\|u\|_{H^4}^2. \tag{2.6}$$

Proof: Multiplying Eq. (1.3) by $\Delta^3 u$, and integrating over R^2, we get

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}(|\Delta^2 u|_{L^2}^2 + |\nabla^3 u|_{L^2}^2) + \int_{R^2} u_x \Delta^3 u + \int_{R^2} J(u,\Delta u)\Delta^3 u = 0.$$

Since $\int_{R^2} u_x \Delta^3 u = 0$, we obtain,

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}(|\Delta^2 u|_{L^2}^2 + |\nabla^3 u|_{L^2}^2) + \int_{R^2} J(u,\Delta u)\Delta^3 u = 0. \tag{2.7}$$

Since,

$$\begin{aligned}
\left|\int_{R^2} J(u,\Delta u)\Delta^3 u\right| &= \left|\int_{R^2} u_x \Delta u_y \Delta^3 u - \int_{R^2} u_y \Delta u_x \Delta^3 u\right| = \left|\int_{R^2} \Delta(u_x \Delta u_y)\Delta^2 u - \int_{R^2} \Delta(u_y \Delta u_x)\Delta^2 u\right| \\
&= \left|\int_{R^2} \mathrm{div}(\nabla u_x \Delta u_y + u_x \nabla \Delta u_y)\Delta^2 u - \int_{R^2} \mathrm{div}(\nabla u_y \Delta u_x + u_y \nabla \Delta u_x)\Delta^2 u\right| \\
&= \left|\int_{R^2} (\Delta u_x \Delta u_y + \nabla u_x \nabla \Delta u_y + \nabla u_x \nabla \Delta u_y + u_x \Delta^2 u_y)\Delta^2 u - \int_{R^2} (\Delta u_y \Delta u_x\right.
\end{aligned}$$

$$+ \nabla u_y \nabla \Delta u_x + \nabla u_y \nabla \Delta u_x + u_y \Delta^2 u_x) \Delta^2 u \Big| = \Big| 2 \int_{R^2} (\nabla u_x \nabla \Delta u_y \Delta^2 u$$

$$- \nabla u_y \nabla \Delta u_x \Delta^2 u) + \int_{R^2} (u_x \Delta^2 u_y \Delta^2 u - u_y \Delta^2 u_x) \Delta^2 u) \Big|$$

$$= \Big| 2 \int_{R^2} (\nabla u_x \nabla \Delta u_y \Delta^2 u - \nabla u_y \nabla \Delta u_x \Delta^2 u) + \int_{R^2} J(u, \Delta^2 u) \Delta^2 u \Big|$$

$$= \Big| 2 \int_{R^2} (\nabla u_x \nabla \Delta u_y \Delta^2 u - \nabla u_y \nabla \Delta u_x \Delta^2 u) \Big| \leqslant 2 |\nabla u_x|_{L^\infty} |\nabla \Delta u_y|_{L^2} |\Delta^2 u|_{L^2}$$

$$+ 2 |\nabla u_y|_{L^\infty} |\nabla \Delta u_x|_{L^2} |\Delta^2 u|_{L^2} \leqslant C(1 + \log(1 + \|u\|_{H^4}))(\|u\|_{H^4} \|u\|_{H^4} + \|u\|_{H^4} \|u\|_{H^4})$$

$$= C(1 + \log(1 + \|u\|_{H^4})) \|u\|_{H^4}^2, \tag{2.8}$$

where we have used the property $\int_{R^2} J(u, \Delta^2 u) \Delta^2 u = 0$ (which we obtain by integrating by parts) and Brezis-Gallouet's inequality. Combining (2.7) and (2.8), the proof of Lemma 2.3 is completed.

Lemma 2.4: There exist constant C, C' and constant $C''(\|u_0\|_{H^4})$ such that, for every $T > 0$:

$$\|u\|_{H^4} \leqslant C' e^{1/2 e^{CT + C''(\|u_0\|_{H^4})}}.$$

Proof: From (2.1), (2.3), and (2.6), we deduce

$$\frac{\mathrm{d}}{\mathrm{d}t} (|\Delta^2 u|_{L^2}^2 + |\nabla^3 u|_{L^2}^2 + |\nabla^3 u|_{L^2}^2 + |\Delta u|_{L^2}^2 + |\nabla u|_{L^2}^2 + |u|_{L^2}^2) \leqslant C(1 + \log(1 + \|u\|_{H^4}))\|u\|_{H^4}^2.$$

Let

$$|\Delta^2 u|_{L^2}^2 + 2|\nabla^3 u|_{L^2}^2 + |\Delta u|_{L^2}^2 + |\nabla u|_{L^2}^2 + |u|_{L^2}^2 = [u]_{H^4}^2.$$

It is well known that the norm $\|\cdot\|_{H^s}$ is equivalent to

$$\sqrt{\sum_{|\alpha| \leqslant s} |\partial^\alpha|_{L^2}}$$

(s is an integer), so $\|\cdot\|_{H^4}$ and $[\cdot]_{H^4}$ are equivalent norms,[14] and there exists one constant C_1, such that, $\|u\|_{H^4} \leqslant C_1 [u]_{H^4}$, and

$$\frac{\mathrm{d}}{\mathrm{d}t} [u]_{H^4}^2 \leqslant C(1 + \log(1 + C_1 [u]_{H^4}))[u]_{H^4}^2 \leqslant C(1 + \log(1 + [u]_{H^4}^2))[u]_{H^4}^2,$$

where the Cauchy's inequality has been used. Then, we can choose one suitable constant $N(C, C_1)$, if $[u]_{H^4} \leqslant N(C, C_1)$, for every $T > 0$, the conclusion will be obtained. Otherwise, for suitable C, we have

$$\frac{\mathrm{d}}{\mathrm{d}t} [u]_{H^4}^2 \leqslant C[u]_{H^4}^2 \log [u]_{H^4}^2.$$

So, for every $T > 0$, we have

$$\log \log [u]_{H^4}^2 \leqslant CT + \log \log [u]_{H^4}^2(0) \leqslant CT + C''(\|u_0\|_{H^4}),$$

$$[u]_{H^4}^2 \leqslant e^{e^{CT + C''(\|u_0\|_{H^4})}},$$

$$[u]_{H^4} \leqslant e^{(1/2)e^{CT+C''(\|u_0\|_{H^4})}},$$

so, by the equivalence of $\|\cdot\|_{H^4}$ and $[\cdot]_{H^4}$, we have

$$\|u\|_{H^4} \leqslant C' e^{(1/2)e^{CT+C''(\|u_0\|_{H^4})}}.$$

Theorem 2.1: Let $u_0 \in H^4$, then problem (1.3) has a global unique solution in H^4.

Proof: From Theorem 1.1, we know problem (1.3) has a unique local strong solution $u(t,x,y) \in L^\infty([0,T^*],H^4(R^2)) \cap C^0([0,T^*],H^1(R^2))$, where T^* depends on $\|u_0\|_{H^4}$. By Lemma 2.4, for any given $T>0$, $\|u\|_{H^4}$ is bounded. We have global existence for (1.3) using the standard discussion (for example, Ref. 7).

Remark 2.1: Results of Theorem 2.1 remain true in $H^s(s \geqslant 4)$ for any $u_0 \in H^s$. To prove this, we multiply (1.3) by $\Delta^s u$ and integrate by parts over R^2, and then we use the property[1]

$$\begin{aligned}\left| \int_{R^2} \Delta^{s/2-1}(u_x \Delta u_y - u_y \Delta u_x)\Delta^{s/2} u \right| &= \left| \int_{R^2} \sum_{|\alpha| \leqslant s-2, |\beta| \leqslant s} C_{\alpha,\beta} \partial_\alpha u \partial_\beta u \Delta^{s/2} u \right| \\ &\leqslant C \sum_{|\alpha| \leqslant s-2, |\beta| \leqslant s} |\partial_\alpha u|_{L^\infty} |\partial_\beta u|_{L^2} |\Delta^{s/2} u|_{L^2} \\ &\leqslant C(1 + \log(1 + \|u\|_{H^s}))\|u\|_{H^s}^2\end{aligned}$$

and the equivalence of the norms (similar to lemma 2.4).

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Analytical solution of the time evolution of an entangled electron spin pair in a double quantum dot nanostructure

M. Blaauboer
Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands

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Using master equations, we present an analytical solution of the time evolution of an entangled electron spin pair which can occupy 36 different quantum states in a double quantum dot nanostructure. This solution is exact, given a few realistic assumptions, and takes into account relaxation and decoherence rates of the electron spins as phenomenological parameters. Our systematic method of solving a large set of coupled differential equations is straightforward and can be used to obtain analytical predictions of the quantum evolution of a large class of complex quantum systems, for which until now commonly numerical solutions have been sought. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2007629]

I. INTRODUCTION

Master equations are used to describe the quantum evolution of a physical system interacting with some "reservoir,"[1] and have been applied to a wide variety of physical systems, ranging from two-level atoms in the presence of light fields[2] to solid-state nanostructures such as quantum dots and Josephson junction devices.[3] For simple systems, such as a two-level atom damped by a reservoir consisting of simple harmonic oscillators[4] or an electron in a single or double quantum dot coupled to external leads,[5] the set of master equations that describes the quantum dynamics of the system is small and its solution can be obtained analytically in a straightforward way. If the system is more involved, however, due to the presence of quite a few atomic levels or because the nanostructure is composed of various coherent parts, its quantum state space consists of a large number of quantum states with various coherent and incoherent couplings between them, and the analytical solution of the corresponding large set of coupled master equations does not spring to the eye. Hence, often a numerical solution is sought.[6] Understanding the quantum evolution of such "complex" quantum systems—where complex refers to a system which is described by a large number of coupled quantum states—has recently become increasingly important, in particular in fundamental research aimed at investigating the dynamic behavior of qubits, the basic building blocks for quantum computation.[7] A large theoretical and experimental effort in various fields, e.g., quantum optics, atomic physics, and condensed-matter physics, is presently directed toward investigating possibilities to use two-level systems such as polarized photons, cold atoms, electron spins, and superconducting circuits as qubits, and finding ways to couple these qubits together. In the latter three systems, one of the major questions involved is how the desired coherent evolution of the system will be affected by coupling to the environment, which is necessary to manipulate and measure the states of the qubits but invariably introduces undesired decoherence of their quantum states. A master equation model of the quantum evolution of one or more qubits interacting with their environment allows one to construct transparent general formulas and is therefore very suitable to give both qualitative and quantitative insight into the dynamics of these complex quantum systems.

In this paper we present an analytical solution of a large set of coupled master equations that describes the quantum evolution of a particular condensed-matter system, namely the time evolution of an entangled electron spin pair in a double quantum dot nanostructure. Even though our

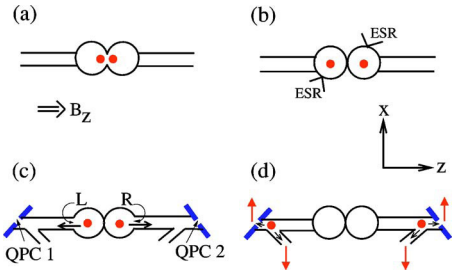

FIG. 1. Schematic top view of the double quantum dot nanostructure as discussed in Sec. II.

model applies to this specific quantum system, the presented method of solving the master equations is general and can be applied to study the dynamics of many other complex quantum systems. The time evolution of the electron spins is governed by several coherent and incoherent processes, each of which depends on time in a simple way as either oscillatory (cosine) or exponential functions. The solution we obtain shows how these simple ingredients combine to describe the evolution of the entangled spins in a complex nanostructure which consists of several coherent parts. It can be used to predict the occupation probability of all quantum states at any given time and to provide analytical estimates of the important time scales in the problem, such as the time at which decoherence of the entangled pair becomes substantial.[8]

The paper is organized as follows. In Sec. II the quantum nanostructure and the assumptions made are described. Section III contains the master equations and their solution, with technical details given in Appendixes A and B. A summary of the results and their range of applicability is presented in Sec. IV.

II. THE DOUBLE QUANTUM DOT NANOSTRUCTURE

The system we consider consists of a double quantum dot nanostructure, which is occupied by two entangled electron spins and operated as a turnstile. We studied this system in an earlier paper as a suitable setup for the detection of entanglement between electron spins.[9] Here, we focus on the dynamic evolution of the electron pair in the system, which is depicted in Fig. 1.

In detail, the structure consists of two adjacent quantum dots in a parallel magnetic field $B_z\hat{z}$, which are connected to two quantum point contacts (QPCs) via empty quantum channels. A quantum dot is a small metallic or semiconducting island, confined by gates and connected to electron reservoirs (leads) through quantum point contacts. If the gates are nearly closed and form tunnel barriers, the dot is occupied by a finite and controllable number of electrons which occupy discrete quantum levels, similar to atomic orbitals in atoms.[10] In our system, the gate between the two dots is assumed to be initially open and the dots are occupied by two electrons[11] [Fig. 1(a)] in their lowest energy state, the singlet state.[12] The gate between the two dots is then adiabatically closed, so that the electrons become separated and one dot is occupied by an electron with spin-up and the other by one with spin-down. The two spins do not interact anymore and are independently rotated by electron spin resonance (ESR) fields [Fig. 1(b)]. The latter are oscillating magnetic fields which, if the frequency of oscillation matches the energy difference between the two spin-split single-electron energy levels, cause coherent rotations of a spin between these levels, analogous to Rabi oscillations in a two-level atom. After spin rotation, the electrons are emitted into empty quantum channels by opening gates L and R [Fig. 1(c)] and scattered at quantum point contacts QPC 1 and QPC 2. In a parallel magnetic field and for conductances $G_{\mathrm{QPC1(QPC2)}} \leqslant e^2/h$ these QPCs are spin selective,[13] transmitting electrons with spin-up and reflecting those with spin-down [Fig. 1(d)]. The transmitted and reflected electrons are separately detected in the four exits.

In the next section we analyze the dynamics of the two spins from the moment they are separated and each occupies one of the two dots, until both have been detected in one of the four

exits. We use a master equation approach in which the effects of relaxation and decoherence are included as phenomenological decay rates.[1] The solution presented is exact under three assumptions:

(i) The time evolution during ESR in the dots is decoupled from the time evolution in the channels and exits. Physically, this means that the gates between the dots and channels are closed during the ESR rotations, so no tunneling occurs out of the dots during that time.
(ii) Once the electrons are in a channel they cannot tunnel back into the dots, i.e., backreflection of the electrons to the dots during their journey to the detectors is neglected. This corresponds to ballistic transport through the channels.
(iii) Once the electrons are in one of the exits they cannot return to the channels, i.e., the electrons are immediately detected and absorbed into the detectors.

III. THE MASTER EQUATIONS AND THEIR SOLUTION

In the setup as depicted in Fig. 1, each electron is assumed to be either in a dot, in a channel, or detected. This leads to a set of 36 possible quantum states represented by a 36×36 density matrix $\rho(t)$. This set consists of all possible combinations $A\sigma B\sigma'$, with $A\in\{D,C,X\}$ and $\sigma\in\{\uparrow,\downarrow\}$ indicating, respectively, the position (D=dot, C=channel, and X=exit) and the spin direction along $\hat{z}$ of the electron which started out in the left dot, and $B\in\{D,C,X\}$ and $\sigma'\in\{\uparrow,\downarrow\}$ representing the position and spin direction of the electron which started out in the right dot. The set is given by

$$\begin{aligned}\{&D\uparrow D\uparrow, D\uparrow D\downarrow, D\downarrow D\uparrow, D\downarrow D\downarrow, C\uparrow D\uparrow, C\uparrow D\downarrow, C\downarrow D\uparrow, C\downarrow D\downarrow, D\uparrow C\uparrow, D\uparrow C\downarrow, D\downarrow C\uparrow, D\downarrow C\downarrow, C\uparrow C\uparrow,\\ &C\uparrow C\downarrow, C\downarrow C\uparrow, C\downarrow C\downarrow, X\uparrow D\uparrow, X\uparrow D\downarrow, X\downarrow D\uparrow, X\downarrow D\downarrow, D\uparrow X\uparrow, D\uparrow X\downarrow, D\downarrow X\uparrow, D\downarrow X\downarrow, X\uparrow C\uparrow, X\uparrow C\downarrow,\\ &X\downarrow C\uparrow, X\downarrow C\downarrow, C\uparrow X\uparrow, C\uparrow X\downarrow, C\downarrow X\uparrow, C\downarrow X\downarrow, X\uparrow X\uparrow, X\uparrow X\downarrow, X\downarrow X\uparrow, X\downarrow X\downarrow\}.\end{aligned} \tag{1}$$

We number the states in set (1) by the numbers 1 to 36, so $1=D\uparrow D\uparrow$, $2=D\uparrow D\downarrow$, etc. The states labeled by C and X do not refer to *individual* quantum states in the channels and detectors, since in a channel many longitudinal modes exist and the detectors consist of many quantum states which together form a macroscopic state. What is meant by the states C and X is the *set* of all channel modes, respectively, all quantum states in the detectors. These states thus describe the probability of an electron to occupy any one of these channel modes or detector states. We come back to why this definition is useful and appropriate in the paragraph below Eq. (9). For long times, the only states that are occupied are 33–36, in which both electrons have entered into an exit and the channels and dots are empty.

The time evolution of the density matrix elements $\rho_{nm}(t)$ is given by the master equations[1]

$$\dot{\rho}_n(t) = -\frac{i}{\hbar}[\mathcal{H}(t),\rho(t)]_{nn} + \sum_{m\neq n}[W_{nm}\rho_m(t) - W_{mn}\rho_n(t)], \tag{2a}$$

$$\dot{\rho}_{n,m}(t) = -\frac{i}{\hbar}[\mathcal{H}(t),\rho(t)]_{nm} - V_{nm}\rho_{n,m}(t) \quad n\neq m, \tag{2b}$$

for $n,m\in\{1,\ldots,36\}$. The Hamiltonian $\mathcal{H}(t)$ describes the coherent evolution of the spins in the quantum dots due to the ESR fields and is given by, for two oscillating magnetic fields $B_{xL}\cos(\omega t)\hat{x}$ and $B_{xR}\cos(\omega t)\hat{x}$ applied to the left and right dots, respectively,

$$\mathcal{H}(t) = \mathcal{H}_0 - \tfrac{1}{2}g^*\mu_B\cos(\omega t)\sum_{\substack{M,N\in\{L,R\}\\ M\neq N}}(B_{xM}+\epsilon B_{xN})\bar{\sigma}_{xM}. \tag{3}$$

Here, $\mathcal{H}_0$ is a diagonal matrix containing the energies $E_n(n=1,\ldots,36)$ of each state, g^* the electron g factor, μ_B the Bohr magneton, and $\bar{\sigma}_{xL(R)}$ a 36×36 matrix with elements $(\bar{\sigma}_{xL(R)})_{ij}=1$

for each pair of states (i,j) that is coupled by the oscillating field $B_{xL(R)}$ and zero otherwise. For $g^*<0$ the 4×4 upper-left corner $\mathcal{H}_{\text{dots}}(t)$ of $\mathcal{H}(t)$ is then given explicitly as

$$\mathcal{H}_{\text{dots}}(t)=\begin{pmatrix} E_1 & \hbar\Delta_{RL}\cos(\omega t) & \hbar\Delta_{LR}\cos(\omega t) & 0 \\ \hbar\Delta_{RL}\cos(\omega t) & E_2 & 0 & \hbar\Delta_{LR}\cos(\omega t) \\ \hbar\Delta_{LR}\cos(\omega t) & 0 & E_3 & \hbar\Delta_{RL}\cos(\omega t) \\ 0 & \hbar\Delta_{LR}\cos(\omega t) & \hbar\Delta_{RL}\cos(\omega t) & E_4 \end{pmatrix},$$

with $E_1=2E_\uparrow+E_C$, $E_2=E_3=E_\uparrow+E_\downarrow+E_C$, and $E_4=2E_\downarrow+E_C$ in terms of the single-particle energies $E_\uparrow$ and $E_\downarrow$ and the charging energy $E_C=e^2/C$, where C is the total capacitance of the quantum dot (assumed to be equal for both dots), $\Delta_{RL}\equiv\Delta_R+\delta_L$ and $\Delta_{LR}\equiv\Delta_L+\delta_R$, with $\Delta_{R(L)}\equiv[|g^*|\mu_B B_{xR(L)}]/2\hbar$ and $\delta_{R(L)}\equiv[\epsilon|g^*|\mu_B B_{xR(L)}]/2\hbar$. The parameter ϵ, with $0\leqslant\epsilon<1$, represents the relative reduction of the field which is applied to one dot at the position of the spin in the other dot.[9] The remaining 32×32 part of the matrix $\mathcal{H}(t)$ is diagonal and equal to $\mathcal{H}_0$, since the ESR fields are applied when both electrons are located in a dot and the quantum channels do not contain any electrons whose spin might otherwise also be rotated by these fields.

Turning to the transition rates W_{nm} (from state m to n) in Eq. (2a), we distinguish between two kinds of transitions: (1) spin-flip transitions between two quantum states that differ by the direction of one spin only and (2) tunneling (without spin-flip) between quantum states that involve adjacent parts of the system, i.e., from dot to channel and from channel to exit. The latter are externally controlled by opening and closing the gates between the dots and channels. The former are modeled by the phenomenological rate $1/T_{1,\alpha}\equiv W_{\alpha\uparrow\downarrow}+W_{\alpha\downarrow\uparrow}$, with $\alpha\in\{D,C\}$ for spin flips in a dot or channel. Here, the W's depend on the Zeeman energy $\Delta E_Z\equiv|g^*|\mu_B B_z$ and temperature T via detailed balance $W_{\alpha\uparrow\downarrow}/W_{\alpha\downarrow\uparrow}=e^{\Delta E_Z/k_BT}$, so that

$$W_{\alpha\uparrow\downarrow(\downarrow\uparrow)}=\frac{1}{T_{1,\alpha}}\frac{1}{1+e^{-(+)\Delta E_Z/k_BT}},\quad \alpha\in\{D,C\}. \tag{4}$$

The spin decoherence rates V_{nm} in Eqs. (2b) for states n and m with $n,m\in\{1,\ldots,4\}$, i.e., the decoherence rate between states in which both electrons are located in a quantum dot, is given by

$$V_{nm}=\frac{1}{T_{2,D}}+\frac{1}{2}\sum_{j\neq n,m}(W_{jn}+W_{jm})\quad n,m\in\{1,\ldots,4\}, \tag{5}$$

where the W's refer to tunnel rates out of a dot. The coherence between state n and m thus not only depends on the intrinsic spin decoherence time $T_{2,D}$ which is caused by, e.g., spin-orbit or hyperfine interactions in the dots,[14] but is also reduced by the (incoherent) tunneling processes from dot to channel.[15] Similarly, V_{nm} for all other states n and m is given by

$$V_{nm}=\begin{cases}\dfrac{1}{T_{2,C}}+\dfrac{1}{2}\displaystyle\sum_{j\neq n,m}(W_{jn}+W_{jm}) & n,m\in\{1,\ldots,16\},\ \text{but not both } n,m\in\{1,\ldots,4\} \\ \infty & n\in\{17,\ldots,36\}\ \text{and/or}\ m\in\{17,\ldots,36\},\end{cases} \tag{6}$$

with the W's tunnel rates from a channel to an exit. Note that energy relaxation processes between different modes in the channels, i.e., between modes that contribute to the same set of channel states C, do not affect the transition rates W_{nm} and decoherence rates V_{nm} for the states where either n or m or both refer to a channel state. The reason for this is that these rates refer to, respectively, *spin* flip and *spin* decoherence processes, which are not affected by *orbital* (energy) relaxation and decoherence.[16] Hence, our definition of the channel states as sets of all modes with the same spin does not interfere with the definition of spin relaxation and decoherence of the quantum states.

With the above ingredients, the coupled equations (2) can be solved analytically. We proceed in three steps: ESR applied to the left dot, ESR applied to the right dot, and the time evolution

after the gates to the quantum channels have been opened. During each step only part of the quantum states are evolving in time, while the others remain unchanged. This simplifies the procedure to obtain an analytical solution.

A. Step 1: ESR applied to the left dot

Initially, at time $t=0$, both spins are assumed to be in the singlet state in the quantum dots, so

$$\rho_2(0)=\rho_3(0)=1/2;\quad \rho_j(0)=0\quad \forall\, j\in\{1,4,5,\ldots,36\}, \tag{7a}$$

$$\rho_{2,3}(0)=\rho_{3,2}(0)=-1/2;\quad \rho_{i,j}(0)=0 \text{ otherwise}. \tag{7b}$$

During ESR applied to the left dot, quantum states $\rho_5(t)-\rho_{36}(t)$ remain unchanged, since the gates between the dots and channels are closed. The coherent evolution of $\rho_1(t)-\rho_4(t)$ is then governed by the Hamiltonian

$$\mathcal{H}_{\mathrm{ESR}}(t)=\begin{pmatrix} E_1 & \hbar\delta_L\cos(\omega t) & \hbar\Delta_L\cos(\omega t) & 0\\ \hbar\delta_L\cos(\omega t) & E_2 & 0 & \hbar\Delta_L\cos(\omega t)\\ \hbar\Delta_L\cos(\omega t) & 0 & E_2 & \hbar\delta_L\cos(\omega t)\\ 0 & \hbar\Delta_L\cos(\omega t) & \hbar\delta_L\cos(\omega t) & E_4 \end{pmatrix}.$$

Including spin-flip rates $W_{D\uparrow\downarrow}$ and $W_{D\downarrow\uparrow}$ and the decoherence rate $\Gamma\equiv 1/T_{2,D}$ for both dots,[17] we then obtain from Eqs. (2) the master equations

$$\dot\rho_1=-\delta_L\,\mathrm{Im}\,\tilde\rho_{1,2}-\Delta_L\,\mathrm{Im}\,\tilde\rho_{1,3}-2W_{D\downarrow\uparrow}\rho_1+W_{D\uparrow\downarrow}(\rho_2+\rho_3), \tag{8a}$$

$$\dot\rho_2=\delta_L\,\mathrm{Im}\,\tilde\rho_{1,2}-\Delta_L\,\mathrm{Im}\,\tilde\rho_{2,4}+W_{D\uparrow\downarrow}+(W_{D\downarrow\uparrow}-W_{D\uparrow\downarrow})\rho_1-(2W_{D\uparrow\downarrow}+W_{D\downarrow\uparrow})\rho_2-W_{D\uparrow\downarrow}\rho_3, \tag{8b}$$

$$\dot\rho_3=-\delta_L\,\mathrm{Im}\,\tilde\rho_{3,4}+\Delta_L\,\mathrm{Im}\,\tilde\rho_{1,3}+W_{D\uparrow\downarrow}+(W_{D\downarrow\uparrow}-W_{D\uparrow\downarrow})\rho_1-W_{D\uparrow\downarrow}\rho_2-(2W_{D\uparrow\downarrow}+W_{D\downarrow\uparrow})\rho_3, \tag{8c}$$

$$\mathrm{Im}\,\dot{\tilde\rho}_{1,2}=-\frac{\delta_L}{2}(\rho_2-\rho_1)+\frac{\Delta_L}{2}(\mathrm{Re}\,\tilde\rho_{1,4}-\mathrm{Re}\,\tilde\rho_{2,3})-\Gamma\,\mathrm{Im}\,\tilde\rho_{1,2}, \tag{8d}$$

$$\mathrm{Im}\,\dot{\tilde\rho}_{1,3}=-\frac{\Delta_L}{2}(\rho_3-\rho_1)+\frac{\delta_L}{2}(\mathrm{Re}\,\tilde\rho_{1,4}-\mathrm{Re}\,\tilde\rho_{2,3})-\Gamma\,\mathrm{Im}\,\tilde\rho_{1,3}, \tag{8e}$$

$$\mathrm{Im}\,\dot{\tilde\rho}_{2,4}=-\frac{\Delta_L}{2}(\rho_4-\rho_2)-\frac{\delta_L}{2}(\mathrm{Re}\,\tilde\rho_{1,4}-\mathrm{Re}\,\tilde\rho_{2,3})-\Gamma\,\mathrm{Im}\,\tilde\rho_{2,4}, \tag{8f}$$

$$\mathrm{Im}\,\dot{\tilde\rho}_{3,4}=-\frac{\delta_L}{2}(\rho_4-\rho_3)-\frac{\Delta_L}{2}(\mathrm{Re}\,\tilde\rho_{1,4}-\mathrm{Re}\,\tilde\rho_{2,3})-\Gamma\,\mathrm{Im}\,\tilde\rho_{3,4}, \tag{8g}$$

$$\mathrm{Re}\,\dot{\tilde\rho}_{1,4}=-\frac{\delta_L}{2}(\mathrm{Im}\,\tilde\rho_{1,3}-\mathrm{Im}\,\tilde\rho_{2,4})-\frac{\Delta_L}{2}(\mathrm{Im}\,\tilde\rho_{1,2}-\mathrm{Im}\,\tilde\rho_{3,4})-\Gamma\,\mathrm{Re}\,\tilde\rho_{1,4}, \tag{8h}$$

$$\mathrm{Re}\,\dot{\tilde\rho}_{2,3}=\frac{\delta_L}{2}(\mathrm{Im}\,\tilde\rho_{1,3}-\mathrm{Im}\,\tilde\rho_{2,4})+\frac{\Delta_L}{2}(\mathrm{Im}\,\tilde\rho_{1,2}-\mathrm{Im}\,\tilde\rho_{3,4})-\Gamma\,\mathrm{Re}\,\tilde\rho_{2,3}, \tag{8i}$$

$$\mathrm{Re}\,\dot{\tilde{\rho}}_{1,2} = -\frac{\Delta_L}{2}(\mathrm{Im}\,\tilde{\rho}_{1,4} + \mathrm{Im}\,\tilde{\rho}_{2,3}) - \Gamma\,\mathrm{Re}\,\tilde{\rho}_{1,2}, \tag{8j}$$

$$\mathrm{Re}\,\dot{\tilde{\rho}}_{1,3} = -\frac{\delta_L}{2}(\mathrm{Im}\,\tilde{\rho}_{1,4} - \mathrm{Im}\,\tilde{\rho}_{2,3}) - \Gamma\,\mathrm{Re}\,\tilde{\rho}_{1,3} \tag{8k}$$

$$\mathrm{Re}\,\dot{\tilde{\rho}}_{2,4} = \frac{\delta_L}{2}(\mathrm{Im}\,\tilde{\rho}_{1,4} - \mathrm{Im}\,\tilde{\rho}_{2,3}) - \Gamma\,\mathrm{Re}\,\tilde{\rho}_{2,4}, \tag{8l}$$

$$\mathrm{Re}\,\dot{\tilde{\rho}}_{3,4} = \frac{\Delta_L}{2}(\mathrm{Im}\,\tilde{\rho}_{1,4} + \mathrm{Im}\,\tilde{\rho}_{2,3}) - \Gamma\,\mathrm{Re}\,\tilde{\rho}_{3,4}, \tag{8m}$$

$$\mathrm{Im}\,\dot{\tilde{\rho}}_{1,4} = \frac{\delta_L}{2}(\mathrm{Re}\,\tilde{\rho}_{1,3} - \mathrm{Re}\,\tilde{\rho}_{2,4}) + \frac{\Delta_L}{2}(\mathrm{Re}\,\tilde{\rho}_{1,2} - \mathrm{Re}\,\tilde{\rho}_{3,4}) - \Gamma\,\mathrm{Im}\,\tilde{\rho}_{1,4}, \tag{8n}$$

$$\mathrm{Im}\,\dot{\tilde{\rho}}_{2,3} = -\frac{\delta_L}{2}(\mathrm{Re}\,\tilde{\rho}_{1,3} - \mathrm{Re}\,\tilde{\rho}_{2,4}) + \frac{\Delta_L}{2}(\mathrm{Re}\,\tilde{\rho}_{1,2} - \mathrm{Re}\,\dot{\tilde{\rho}}_{3,4}) - \Gamma\,\mathrm{Im}\,\tilde{\rho}_{2,3}, \tag{8o}$$

with $\tilde{\rho}_{i,j}(t) \equiv \rho_{i,j}(t)e^{-i\omega t}$ for $(ij) \in \{(12), (13), (24), (34)\}$, $\tilde{\rho}_{1,4}(t) \equiv \rho_{1,4}(t)e^{-2i\omega t}$ and $\tilde{\rho}_{2,3}(t) \equiv \rho_{2,3}(t)$. Equations (8) are valid on resonance, so $\hbar\omega \equiv E_2 - E_1 = E_4 - E_2 = \Delta E_Z$ and within the rotating wave approximation (RWA).[18] Here, $\rho_4(t)$ is given by $\rho_4(t) = 1 - \rho_1(t) - \rho_2(t) - \rho_3(t)$.

Equations (8) can be split into two sets of coupled equations: Eqs. (8a)–(8i) and Eqs. (8j)–(8o). The solution of the second set is straightforwardly obtained and given by

$$\begin{aligned}\mathrm{Re}\,\tilde{\rho}_{1,2}(t) = \tfrac{1}{2}(&\mathrm{Re}[\tilde{\rho}_{1,2}(0) - \tilde{\rho}_{3,4}(0)]\cos(\Delta_L t) - \mathrm{Im}[\tilde{\rho}_{1,4}(0) + \tilde{\rho}_{2,3}(0)]\sin(\Delta_L t)\\ &+ \mathrm{Re}[\tilde{\rho}_{1,2}(0) + \tilde{\rho}_{3,4}(0)])e^{-\Gamma t},\end{aligned} \tag{9a}$$

$$\begin{aligned}\mathrm{Re}\,\tilde{\rho}_{1,3}(t) = \tfrac{1}{2}(&\mathrm{Re}[\tilde{\rho}_{1,3}(0) - \tilde{\rho}_{2,4}(0)]\cos(\delta_L t) - \mathrm{Im}[\tilde{\rho}_{1,4}(0) - \tilde{\rho}_{2,3}(0)]\sin(\delta_L t)\\ &+ \mathrm{Re}[\tilde{\rho}_{1,3}(0) + \tilde{\rho}_{2,4}(0)])e^{-\Gamma t},\end{aligned} \tag{9b}$$

$$\begin{aligned}\mathrm{Re}\,\tilde{\rho}_{2,4}(t) = \tfrac{1}{2}(&-\mathrm{Re}[\tilde{\rho}_{1,3}(0) - \tilde{\rho}_{2,4}(0)]\cos(\delta_L t) + \mathrm{Im}[\tilde{\rho}_{1,4}(0) - \tilde{\rho}_{2,3}(0)]\sin(\delta_L t)\\ &+ \mathrm{Re}[\tilde{\rho}_{1,3}(0) + \tilde{\rho}_{2,4}(0)])e^{-\Gamma t},\end{aligned} \tag{9c}$$

$$\begin{aligned}\mathrm{Re}\,\tilde{\rho}_{3,4}(t) = \tfrac{1}{2}(&-\mathrm{Re}[\tilde{\rho}_{1,2}(0) - \tilde{\rho}_{3,4}(0)]\cos(\Delta_L t) + \mathrm{Im}[\tilde{\rho}_{1,4}(0) + \tilde{\rho}_{2,3}(0)]\sin(\Delta_L t)\\ &+ \mathrm{Re}[\tilde{\rho}_{1,2}(0) + \tilde{\rho}_{3,4}(0)])e^{-\Gamma t},\end{aligned} \tag{9d}$$

$$\begin{aligned}\mathrm{Im}\,\tilde{\rho}_{1,4}(t) = \tfrac{1}{2}(&\mathrm{Im}[\tilde{\rho}_{1,4}(0) + \tilde{\rho}_{2,3}(0)]\cos(\Delta_L t) + \mathrm{Im}[\tilde{\rho}_{1,4}(0) - \tilde{\rho}_{2,3}(0)]\cos(\delta_L t)\\ &+ \mathrm{Re}[\tilde{\rho}_{1,2}(0) - \tilde{\rho}_{3,4}(0)]\sin(\Delta_L t) + \mathrm{Re}[\tilde{\rho}_{1,3}(0) - \tilde{\rho}_{2,4}(0)]\sin(\delta_L t))e^{-\Gamma t},\end{aligned} \tag{9e}$$

$$\begin{aligned}\mathrm{Im}\,\tilde{\rho}_{2,3}(t) = \tfrac{1}{2}(&\mathrm{Im}[\tilde{\rho}_{1,4}(0) + \tilde{\rho}_{2,3}(0)]\cos(\Delta_L t) - \mathrm{Im}[\tilde{\rho}_{1,4}(0) - \tilde{\rho}_{2,3}(0)]\cos(\delta_L t)\\ &+ \mathrm{Re}[\tilde{\rho}_{1,2}(0) - \tilde{\rho}_{3,4}(0)]\sin(\Delta_L t) - \mathrm{Re}[\tilde{\rho}_{1,3}(0) - \tilde{\rho}_{2,4}(0)]\sin(\delta_L t))e^{-\Gamma t}.\end{aligned} \tag{9f}$$

In order to solve the set of equations (8a)–(8i) we express $\rho_1 - \rho_3$, $\mathrm{Im}\,\tilde{\rho}_{1,2}$, $\mathrm{Im}\,\tilde{\rho}_{1,3}$, $\mathrm{Im}\,\tilde{\rho}_{2,4}$, $\mathrm{Im}\,\tilde{\rho}_{3,4}$, $\mathrm{Re}\,\tilde{\rho}_{1,4}$, and $\mathrm{Re}\,\tilde{\rho}_{2,3}$ in terms of new variables $x_1 - x_8$ as follows:

$$\rho_1(t) = \tfrac{1}{2}(x_1(t) + x_2(t) - x_3(t))e^{-\Gamma t},$$

$$\rho_2(t) = \tfrac{1}{2}(x_1(t) - x_2(t) + x_3(t))e^{-\Gamma t},$$

$$\rho_3(t) = \tfrac{1}{2}(-x_1(t) + x_2(t) + x_3(t))e^{-\Gamma t},$$

$$\mathrm{Im}\ \tilde{\rho}_{1,2}(t) = \tfrac{1}{2}(x_4(t) + x_6(t))e^{-\Gamma t},$$

$$\mathrm{Im}\ \tilde{\rho}_{1,3}(t) = \tfrac{1}{2}(x_5(t) + x_7(t))e^{-\Gamma t},$$

$$\mathrm{Im}\ \tilde{\rho}_{2,4}(t) = \tfrac{1}{2}(x_5(t) - x_7(t))e^{-\Gamma t},$$

$$\mathrm{Im}\ \tilde{\rho}_{3,4}(t) = \tfrac{1}{2}(x_4(t) - x_6(t))e^{-\Gamma t},$$

$$\mathrm{Re}\ \tilde{\rho}_{1,4}(t) = x_8(t)e^{-\Gamma t},$$

$$\mathrm{Re}\ \tilde{\rho}_{2,3}(t) = (-x_8(t) + Z)e^{-\Gamma t}, \tag{10}$$

with $Z \equiv \mathrm{Re}[\tilde{\rho}_{1,4}(0) + \tilde{\rho}_{2,3}(0)]$. The transformation (10) originates from pairwise adding and subtracting those equations among (8d)–(8i) which share a common term on the right-hand side, e.g., the equations for $\mathrm{Im}\ \dot{\tilde{\rho}}_{1,2}$ and $\mathrm{Im}\ \dot{\tilde{\rho}}_{3,4}$. The definition of $x_1 - x_8$ then naturally arises. Physically, the new variables x_1, x_2, and x_3 can be interpreted as $x_{1(2)}$ = the probability for the spin in the left (right) dot to be up, and x_3 = the probability for the two spins to be antiparallel, each modulated by the exponential dependence on the decoherence rate Γ. Using (10), Eqs. (8a)–(8i) are rewritten in terms of $x_1(t) - x_8(t)$, which leads to three sets of coupled equations. These equations and their solution are given in Appendix A. Equations (10) at time $t = t_1$, where t_1 is the time during which the ESR field is switched on, thus represent the density matrix elements for the double-dot states after the ESR rotation applied to the left dot.

B. Step 2: ESR applied to the right dot

Equations (10) can also be used directly to obtain the solution after the second ESR rotation applied to the right dot, by substituting $\Delta_L \to \delta_R$ and $\delta_L \to \Delta_R$ in Eqs. (9) and (A2), and by exchanging $x_6 \leftrightarrow x_7$ in Eqs. (A4), using $\rho_1(t_1)$ instead of $\rho_1(0)$, etc., as initial conditions. In order to illustrate this solution, let us consider the initial condition of a singlet in the double dot [Eq. (7)], and let t_2 be the duration of the second ESR rotation. In the case of no dissipation (all W's = 0) and no influence of ESR applied to one dot on the spin in the other dot, we then obtain from Eqs. (10), (A2), and (A4), e.g., the occupation probability $\rho_2(t_1 + t_2)$ the expression

$$\rho_2(t_1 + t_2) = \frac{1}{4}\left[1 + \left\{\left[\cos(\tilde{\Omega}_\Delta t_1) + \frac{\Gamma}{2\tilde{\Omega}_\Delta}\sin(\tilde{\Omega}_\Delta t_1)\right]\left[\cos(\tilde{\Omega}_\Delta t_2) + \frac{\Gamma}{2\tilde{\Omega}_\Delta}\sin(\tilde{\Omega}_\Delta t_2)\right] + \frac{\Delta}{\tilde{\Omega}_\Delta}\sin(\Delta\, t_1)\sin(\tilde{\Omega}_\Delta t_2)e^{-(\Gamma/2)t_1}\right\}e^{-(\Gamma/2)(t_1+t_2)}\right], \tag{11}$$

with $\tilde{\Omega}_\Delta \equiv \frac{1}{2}\sqrt{4\Delta^2 - \Gamma^2}$ and $\Delta \equiv \Delta_L = \Delta_R$. In the absence of decoherence ($\Gamma = 0$) the expressions for $\rho_2(t_1 + t_2)$ and the other density matrix elements simplify to

$$\rho_1(t_1 + t_2) = \rho_4(t_1 + t_2) = \tfrac{1}{4}(1 - \cos\,\theta_1 \cos\,\theta_2 - \sin\,\theta_1 \sin\,\theta_2), \tag{12a}$$

$$\rho_2(t_1 + t_2) = \rho_3(t_1 + t_2) = \tfrac{1}{4}(1 + \cos\,\theta_1 \cos\,\theta_2 + \sin\,\theta_1 \sin\,\theta_2), \tag{12b}$$

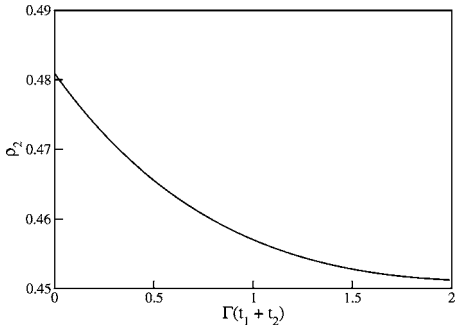

FIG. 2. The occupation probability $\rho_2(t_1+t_2)$ [Eq. (11)] of the quantum state $D\uparrow D\downarrow$ as a function of the amount of decoherence [in units of $1/(t_1+t_2)$]. For $\Gamma=0$ ρ_2 is given by Eq. (12b). Parameters used are $\Delta t_1=\pi/4$, $\Delta t_2=\pi/8$, and all W's=0.

$$\rho_{1,2}(t_1+t_2)=\rho_{2,4}(t_1+t_2)=-\frac{i}{4}(\cos\theta_1\sin\theta_2-\sin\theta_1\cos\theta_2), \tag{12c}$$

$$\rho_{1,3}(t_1+t_2)=\rho_{3,4}(t_1+t_2)=\frac{i}{4}(\cos\theta_1\sin\theta_2-\sin\theta_1\cos\theta_2), \tag{12d}$$

$$\rho_{1,4}(t_1+t_2)=-\tfrac{1}{4}(1-\cos\theta_1\cos\theta_2-\sin\theta_1\sin\theta_2), \tag{12e}$$

$$\rho_{2,3}(t_1+t_2)=-\tfrac{1}{4}(1+\cos\theta_1\cos\theta_2+\sin\theta_1\sin\theta_2), \tag{12f}$$

with $\theta_1\equiv\tilde{\Omega}_\Delta t_1$ and $\theta_2\equiv\tilde{\Omega}_\Delta t_2$. Equation (11) is plotted in Fig. 2 as a function of the amount of decoherence Γ.

Already for moderate amounts of decoherence $\Gamma(t_1+t_2)=0.001$, the occupation probability has become 0.01% less than its value in the absence of decoherence $\rho_2^{\Gamma=0}(t_1+t_2)=0.481$, for the set of parameters chosen in Fig. 2. This increases to 0.1% for $\Gamma(t_1+t_2)=0.01$.

C. Step 3: Time evolution after the gates to the channels have been opened

We now turn to the next step in the evolution of the entangled pair in Fig. 1, namely the time evolution of the density matrix elements after the ESR rotations are completed and the gates to the quantum channels are opened; see Fig. 1(c). From this moment onward the coherent evolution due to the first term on the right-hand side of Eqs. (2) stops and the time evolution of the matrix elements is solely determined by decay and decoherence rates represented by the second terms on the right-hand side of Eqs. (2). The off-diagonal elements $\rho_{i,j}(t)$ then rotate with $(E_i-E_j)/\hbar$ and decay with rate V_{ij}

$$\rho_{i,j}(t)=\rho_{i,j}(t_{\mathrm{ESR}})e^{i(E_i-E_j)(t-t_{\mathrm{ESR}})/\hbar}e^{-V_{ij}(t-t_{\mathrm{ESR}})}\quad\text{for } t\geqslant t_{\mathrm{ESR}}, \tag{13}$$

where $t_{\mathrm{ESR}}\equiv t_1+t_2$ and V_{ij} is given by Eq. (5) for $i,j\in\{1,\ldots,4\}$ and Eq. (6) otherwise. The initial values $\rho_{i,j}(t_{\mathrm{ESR}})$ for $i,j\in\{1,\ldots,16\}$ are given by $\rho_{m,n}(t_{\mathrm{ESR}})$ for $m,n\in\{1,\ldots,4\}$ [Eqs. (10)] with the correspondence in indices

$$i(j)\in\{1,5,9,13\}\leftrightarrow m(n)=1,$$

$$i(j)\in\{2,6,10,14\}\leftrightarrow m(n)=2,$$

$$i(j)\in\{3,7,11,15\}\leftrightarrow m(n)=3,$$

$$i(j) \in \{4,8,12,16\} \leftrightarrow m(n) = 4.$$

In this way the coherence at time t_{ESR} between any pair of states $i,j \in \{1,\ldots,16\}$ is given by the coherence at t_{ESR} between those dot states $m,n \in \{1,\ldots,4\}$ which can (eventually) coherently evolve into i and j, i.e., the dot states m and n which have the same spin states as i and j, respectively. So, for example, $\rho_{C\uparrow C\uparrow,D\downarrow C\downarrow}(t_{\mathrm{ESR}}) = \rho_{D\uparrow D\uparrow,D\downarrow D\downarrow}(t_{\mathrm{ESR}}) \equiv \rho_{1,4}(t_{\mathrm{ESR}})$. Note that $\rho_{i,j}(t)=0$ for those states in which at least one electron has reached a detector ($i \in \{17,\ldots,36\}$ and/or $j \in \{17,\ldots,36\}$), since for those states $V_{ij}=\infty$. This corresponds to the assumption of immediate detection.

In the remaining part of this paper we focus on the evolution of the populations $\rho_1(t)-\rho_{36}(t)$ for times $t \geqslant t_{\mathrm{ESR}}$ under the following conditions:

(i) We neglect the possibility of spin flips in the dots, i.e., we set $W_{D\uparrow\downarrow}=W_{D\downarrow\uparrow}=0$. This is based on the fact that $T_{1,D}$ is known to be much longer (0.85 ms at magnetic fields $B_z=8T$) (Ref. 19) than the time required to travel through the channels to the exits. This assumption is not essential to obtain an analytical solution; it only simplifies the resulting equations.

(ii) We assume that the tunnel rate W_T out of the dots into the channels is equal for spin-up and spin-down electrons, i.e., the two electrons tunnel out of the singlet state with a negligible time delay t_{delay} in between, and that spin is conserved during this tunneling process. Typically[20] $t_{\mathrm{delay}} \approx 10^{-13}$ s, which is much less than the travel time through a channel, $\sim 10^{-10}$ s.

(iii) The tunnel rate W_E through the QPCs is taken to be constant and equal for spin-up and spin-down electrons, i.e., the setup is assumed to be constructed in such a way that the detection time for spin-up and spin-down electrons once they have reached the QPCs is the same.

(iv) Spin flips in the exits are neglected, i.e., detection is assumed to be faster (with typical times $\sim 10^{-11}$ s) (Ref. 21) than the spin-flip rate ($\geqslant 10^{-11}$ s) (Ref. 9) in the detectors.

The evolution equations for $\rho_1(t)-\rho_{36}(t)$ for times $t \geqslant t_{\mathrm{ESR}}$ are then given by the master equations

$$\dot{\rho}_i = -2W_T\rho_i \text{ for } i \in \{1,\ldots,4\}. \tag{14}$$

$$\dot{\rho}_i = W_T\rho_{i-4} + W_{C\uparrow\downarrow}\rho_{i+2} - (W_E + W_T + W_{C\downarrow\uparrow})\rho_i, \quad i \in \{5,6\}, \tag{15a}$$

$$\dot{\rho}_i = W_T\rho_{i-4} + W_{C\downarrow\uparrow}\rho_{i-2} - (W_E + W_T + W_{C\uparrow\downarrow})\rho_i, \quad i \in \{7,8\}, \tag{15b}$$

$$\dot{\rho}_i = W_T\rho_{i-8} + W_{C\uparrow\downarrow}\rho_{i+1} - (W_E + W_T + W_{C\downarrow\uparrow})\rho_i, \quad i \in \{9,11\}, \tag{15c}$$

$$\dot{\rho}_i = W_T\rho_{i-8} + W_{C\downarrow\uparrow}\rho_{i-1} - (W_E + W_T + W_{C\uparrow\downarrow})\rho_i, \quad i \in \{10,12\}. \tag{15d}$$

$$\dot{\rho}_{13} = W_T(\rho_5 + \rho_9) + W_{C\uparrow\downarrow}(\rho_{14} + \rho_{15}) - 2(W_E + W_{C\downarrow\uparrow})\rho_{13}, \tag{16a}$$

$$\dot{\rho}_{14} = W_T(\rho_6 + \rho_{10}) + W_{C\downarrow\uparrow}\rho_{13} + W_{C\uparrow\downarrow}\rho_{16} - (2W_E + W_{C\uparrow\downarrow} + W_{C\downarrow\uparrow})\rho_{14}, \tag{16b}$$

$$\dot{\rho}_{15} = W_T(\rho_7 + \rho_{11}) + W_{C\downarrow\uparrow}\rho_{13} + W_{C\uparrow\downarrow}\rho_{16} - (2W_E + W_{C\uparrow\downarrow} + W_{C\downarrow\uparrow})\rho_{15}, \tag{16c}$$

$$\dot{\rho}_{16} = W_T(\rho_8 + \rho_{12}) + W_{C\downarrow\uparrow}(\rho_{14} + \rho_{15}) - 2(W_E + W_{C\uparrow\downarrow})\rho_{16}. \tag{16d}$$

$$\dot{\rho}_i(t) = W_E\rho_{i-12}(t - t_{\mathrm{travel}} + t_{\mathrm{ESR}}) - W_T\rho_i(t), \quad i \in \{17,\ldots,24\}. \tag{17}$$

$$\dot{\rho}_i(t) = W_T\rho_{i-8}(t) + W_E\rho_{i-12}(t - t_{\text{travel}} + t_{\text{ESR}}) + W_{C\uparrow\downarrow}\rho_{i+1}(t) - (W_E + W_{C\downarrow\uparrow})\rho_i(t) \quad \text{for } i \in \{25,27\}, \tag{18a}$$

$$\dot{\rho}_i(t) = W_T\rho_{i-8}(t) + W_E\rho_{i-12}(t - t_{\text{travel}} + t_{\text{ESR}}) + W_{C\downarrow\uparrow}\rho_{i-1}(t) - (W_E + W_{C\uparrow\downarrow})\rho_i(t) \quad \text{for } i \in \{26,28\}, \tag{18b}$$

$$\dot{\rho}_i(t) = W_T\rho_{i-8}(t) + W_E\rho_{i-16}(t - t_{\text{travel}} + t_{\text{ESR}}) + W_{C\uparrow\downarrow}\rho_{i+2}(t) - (W_E + W_{C\downarrow\uparrow})\rho_i(t) \quad \text{for } i \in \{29,30\}, \tag{18c}$$

$$\dot{\rho}_i(t) = W_T\rho_{i-8}(t) + W_E\rho_{i-16}(t - t_{\text{travel}} + t_{\text{ESR}}) + W_{C\downarrow\uparrow}\rho_{i-2}(t) - (W_E + W_{C\uparrow\downarrow})\rho_i(t) \quad \text{for } i \in \{31,32\}. \tag{18d}$$

$$\dot{\rho}_i = W_E(\rho_{i-8} + \rho_{i-4}) \quad i \in \{33, \ldots, 36\}. \tag{19}$$

Here, $t_{\text{travel}} > t_{\text{ESR}}$ denotes the earliest time at which an electron has traveled through the channels and reached an exit. For times $t \leqslant t_{\text{travel}}$, $\rho_1(t) - \rho_{36}(t)$ is thus given by Eqs. (14)–(19) for $W_E = 0$, since at those times no electron can have arrived at a detector yet. The above sets of coupled equations can be solved one by one: first those for $\rho_1(t) - \rho_4(t)$, then once the latter are known those for $\rho_5(t) - \rho_{12}(t)$ [in the pairs (5,7), (6,8), (9,10), and (11,12)], then $\rho_{13}(t) - \rho_{16}(t)$ and $\rho_{17}(t) - \rho_{24}(t)$, subsequently $\rho_{25}(t) - \rho_{32}(t)$ [in the pairs (25,26), (27,28), (29,31), and (30,32)] and finally $\rho_{33}(t) - \rho_{36}(t)$. Proceeding in this order and using initial conditions

$$\rho_i(t_{\text{ESR}}) = \begin{cases} \text{Eqs. (10)} & \text{for } i = 1, \ldots, 4, \\ 0 & \text{for } i = 5, \ldots, 36, \end{cases} \tag{20}$$

we obtain for $\rho_1(t) - \rho_4(t)$, the states in which both electrons are located in a dot,

$$\rho_i(t) = \rho_i(t_{\text{ESR}})e^{-2W_T(t - t_{\text{ESR}})} \quad i \in \{1, \ldots, 4\},\ t \geqslant t_{\text{ESR}}. \tag{21}$$

Next, we find for $\rho_5(t) - \rho_{12}(t)$, which correspond to the quantum states in which one electron is located in a dot and the other in a channel, from Eqs. (15)

$$\rho_5(t) = A_{5,7,1,3}e^{-W_{ETC}(t - t_{\text{ESR}})} + B_{5,7,1,3}e^{-(W_E + W_T)(t - t_{\text{ESR}})} + C_{1,3}e^{-2W_T(t - t_{\text{ESR}})}, \tag{22a}$$

$$\rho_6(t) = A_{6,8,2,4}e^{-W_{ETC}(t - t_{\text{ESR}})} + B_{6,8,2,4}e^{-(W_E + W_T)(t - t_{\text{ESR}})} + C_{2,4}e^{-2W_T(t - t_{\text{ESR}})}, \tag{22b}$$

$$\rho_7(t) = -A_{5,7,1,3}e^{-W_{ETC}(t - t_{\text{ESR}})} + \frac{W_{C\downarrow\uparrow}}{W_{C\uparrow\downarrow}}B_{5,7,1,3}e^{-(W_E + W_T)(t - t_{\text{ESR}})} + D_{1,3}e^{-2W_T(t - t_{\text{ESR}})}, \tag{22c}$$

$$\rho_8(t) = -A_{6,8,2,4}e^{-W_{ETC}(t - t_{\text{ESR}})} + \frac{W_{C\downarrow\uparrow}}{W_{C\uparrow\downarrow}}B_{6,8,2,4}e^{-(W_E + W_T)(t - t_{\text{ESR}})} + D_{2,4}e^{-2W_T(t - t_{\text{ESR}})}, \tag{22d}$$

$$\rho_9(t) = A_{9,10,1,2}e^{-W_{ETC}(t - t_{\text{ESR}})} + B_{9,10,1,2}e^{-(W_E + W_T)(t - t_{\text{ESR}})} + C_{1,2}e^{-2W_T(t - t_{\text{ESR}})}, \tag{22e}$$

$$\rho_{10}(t) = -A_{9,10,1,2}e^{-W_{ETC}(t - t_{\text{ESR}})} + \frac{W_{C\downarrow\uparrow}}{W_{C\uparrow\downarrow}}B_{9,10,1,2}e^{-(W_E + W_T)(t - t_{\text{ESR}})} + D_{1,2}e^{-2W_T(t - t_{\text{ESR}})}, \tag{22f}$$

$$\rho_{11}(t) = A_{11,12,3,4}e^{-W_{ETC}(t - t_{\text{ESR}})} + B_{11,12,3,4}e^{-(W_E + W_T)(t - t_{\text{ESR}})} + C_{3,4}e^{-2W_T(t - t_{\text{ESR}})}, \tag{22g}$$

$$\rho_{12}(t) = -A_{11,12,3,4}e^{-W_{ETC}(t-t_{\mathrm{ESR}})} + \frac{W_{C\downarrow\uparrow}}{W_{C\uparrow\downarrow}}B_{11,12,3,4}e^{-(W_E+W_T)(t-t_{\mathrm{ESR}})} + D_{3,4}e^{-2W_T(t-t_{\mathrm{ESR}})}, \quad (22h)$$

where

$$W_{ETC} \equiv W_E + W_T + W_{C\uparrow\downarrow} + W_{C\downarrow\uparrow}, \quad (23a)$$

$$A_{i,j,k,l} \equiv \frac{W_{C\downarrow\uparrow}\rho_i(t_{\mathrm{ESR}}) - W_{C\uparrow\downarrow}\rho_j(t_{\mathrm{ESR}})}{W_{C\uparrow\downarrow} + W_{C\downarrow\uparrow}} + \frac{W_T(-W_{C\downarrow\uparrow}\rho_k(t_{\mathrm{ESR}}) + W_{C\uparrow\downarrow}\rho_l(t_{\mathrm{ESR}}))}{(W_{C\uparrow\downarrow} + W_{C\downarrow\uparrow})(W_E - W_T + W_{C\uparrow\downarrow} + W_{C\downarrow\uparrow})}, \quad (23b)$$

$$B_{i,j,k,l} \equiv \frac{W_{C\uparrow\downarrow}}{W_{C\uparrow\downarrow} + W_{C\downarrow\uparrow}}\left[\rho_i(t_{\mathrm{ESR}}) + \rho_j(t_{\mathrm{ESR}}) - \frac{W_T}{W_E - W_T}(\rho_k(t_{\mathrm{ESR}}) + \rho_l(t_{\mathrm{ESR}}))\right], \quad (23c)$$

$$C_{i,j} = \frac{W_T}{W_E - W_T}\frac{(W_E - W_T + W_{C\uparrow\downarrow})\rho_i(t_{\mathrm{ESR}}) + W_{C\uparrow\downarrow}\rho_j(t_{\mathrm{ESR}})}{W_E - W_T + W_{C\uparrow\downarrow} + W_{C\downarrow\uparrow}}, \quad (23d)$$

$$D_{i,j} = \frac{W_T}{W_E - W_T}\frac{W_{C\downarrow\uparrow}\rho_i(t_{\mathrm{ESR}}) + (W_E - W_T + W_{C\downarrow\uparrow})\rho_j(t_{\mathrm{ESR}})}{W_E - W_T + W_{C\uparrow\downarrow} + W_{C\downarrow\uparrow}}. \quad (23e)$$

For times $t \leqslant t_{\mathrm{travel}}$, the evolution of $\rho_5(t)-\rho_{12}(t)$ is given by Eqs. (22) with $W_E=0$. For times $t \geqslant t_{\mathrm{travel}}$, these populations are given by Eqs. (22) with $t_{\mathrm{ESR}} \to t_{\mathrm{travel}}$.

In order to obtain the solution for $\rho_{13}(t)-\rho_{16}(t)$, which corrresponds to the situation in which both electrons are located in a channel, we rewrite the equations for $\rho_{13}-\rho_{16}$ as

$$\dot{\rho}_{13} = W_T(\rho_5 + \rho_9) + W_{C\uparrow\downarrow}(\rho_{14} + \rho_{15}) - 2(W_E + W_{C\downarrow\uparrow})\rho_{13}, \quad (24a)$$

$$\dot{\rho}_{14} + \dot{\rho}_{15} = W_T(\rho_6 + \rho_7 + \rho_{10} + \rho_{11}) + 2W_{C\downarrow\uparrow}\rho_{13} - (2W_E + W_{C\uparrow\downarrow} + W_{C\downarrow\uparrow})(\rho_{14} + \rho_{15}) + 2W_{C\uparrow\downarrow}\rho_{16}, \quad (24b)$$

$$\dot{\rho}_{16} = W_T(\rho_8 + \rho_{12}) + W_{C\downarrow\uparrow}(\rho_{14} + \rho_{15}) - 2(W_E + W_{C\uparrow\downarrow})\rho_{16}, \quad (24c)$$

$$\dot{\rho}_{14} - \dot{\rho}_{15} = W_T(\rho_6 - \rho_7 + \rho_{10} - \rho_{11}) - (2W_E + W_{C\uparrow\downarrow} + W_{C\downarrow\uparrow})(\rho_{14} - \rho_{15}). \quad (24d)$$

Equations (24) consist of three coupled equations (24a)–(24c) and a separate one, Eq. (24d). We first solve the latter and then the first three. In each case the solution is a combination of a homogeneous and a particular solution. Taking from now on $W_{C\uparrow\downarrow}=W_{C\downarrow\uparrow}\equiv W_C$,[22] we obtain

$$\rho_{13}(t) = -Ee^{-2(W_E+W_C)(t-t_{\mathrm{ESR}})} + \tfrac{1}{2}Fe^{-2W_E(t-t_{\mathrm{ESR}})} - \tfrac{1}{2}\widetilde{F}e^{-2(W_E+2W_C)(t-t_{\mathrm{ESR}})} + H_{13}e^{-(W_E+W_T+2W_C)(t-t_{\mathrm{ESR}})} + K_{13}e^{-(W_E+W_T)(t-t_{\mathrm{ESR}})} + L_{13}e^{-2W_T(t-t_{\mathrm{ESR}})}, \quad (25a)$$

$$\rho_{14}(t) = \widetilde{E}e^{-2(W_E+W_C)(t-t_{\mathrm{ESR}})} + \tfrac{1}{2}Fe^{-2W_E(t-t_{\mathrm{ESR}})} + \tfrac{1}{2}\widetilde{F}e^{-2(W_E+2W_C)(t-t_{\mathrm{ESR}})} + H_{14}e^{-(W_E+W_T+2W_C)(t-t_{\mathrm{ESR}})} + K_{14}e^{-(W_E+W_T)(t-t_{\mathrm{ESR}})} + L_{14}e^{-2W_T(t-t_{\mathrm{ESR}})}, \quad (25b)$$

$$\rho_{15}(t) = -\widetilde{E}e^{-2(W_E+W_C)(t-t_{\mathrm{ESR}})} + \tfrac{1}{2}Fe^{-2W_E(t-t_{\mathrm{ESR}})} + \tfrac{1}{2}\widetilde{F}e^{-2(W_E+2W_C)(t-t_{\mathrm{ESR}})} + H_{15}e^{-(W_E+W_T+2W_C)(t-t_{\mathrm{ESR}})} + K_{15}e^{-(W_E+W_T)(t-t_{\mathrm{ESR}})} + L_{15}e^{-2W_T(t-t_{\mathrm{ESR}})}, \quad (25c)$$

TABLE I. Coefficients A_i, B_i, and C_i in Eqs. (26).

i	A_i	B_i	C_i
17	$-W_E A_{5,7,1,3}/(W_E+2W_C)$	$B_{5,7,1,3}$	$W_E/W_T C_{1,3}$
18	$-W_E A_{6,8,2,4}/(W_E+2W_C)$	$B_{6,8,2,4}$	$W_E/W_T C_{2,4}$
19	$W_E A_{5,7,1,3}/(W_E+2W_C)$	$B_{5,7,1,3}$	$W_E/W_T D_{1,3}$
20	$W_E A_{6,8,2,4}/(W_E+2W_C)$	$B_{6,8,2,4}$	$W_E/W_T D_{2,4}$
21	$-W_E A_{9,10,1,2}/(W_E+2W_C)$	$B_{9,10,1,2}$	$W_E/W_T C_{1,2}$
22	$W_E A_{9,10,1,2}/(W_E+2W_C)$	$B_{9,10,1,2}$	$W_E/W_T D_{1,2}$
23	$-W_E A_{11,12,3,4}/(W_E+2W_C)$	$B_{11,12,3,4}$	$W_E/W_T C_{3,4}$
24	$W_E A_{11,12,3,4}/(W_E+2W_C)$	$B_{11,12,3,4}$	$W_E/W_T D_{3,4}$

$$\rho_{16}(t) = Ee^{-2(W_E+W_C)(t-t_{\mathrm{ESR}})} + \tfrac{1}{2}Fe^{-2W_E(t-t_{\mathrm{ESR}})} - \tfrac{1}{2}\tilde{F}e^{-2(W_E+2W_C)(t-t_{\mathrm{ESR}})} + H_{16}e^{-(W_E+W_T+2W_C)(t-t_{\mathrm{ESR}})} + K_{16}e^{-(W_E+W_T)(t-t_{\mathrm{ESR}})} + L_{16}e^{-2W_T(t-t_{\mathrm{ESR}})}. \tag{25d}$$

The coefficients in Eqs. (25) are given in Appendix B. Also here, $\rho_{13}(t)-\rho_{16}(t)$ for times $t \leqslant t_{\mathrm{travel}}$ are given by Eqs. (25) with $W_E=0$, and for times $t \geqslant t_{\mathrm{travel}}$ these populations are given by Eqs. (25) with $t_{\mathrm{ESR}} \to t_{\mathrm{travel}}$.

The solution of the next set, $\rho_{17}(t)-\rho_{24}(t)$, corresponding to the states in which one electron is located in a dot while the other has reached a detector, is given by

$$\rho_i(t) = A_i e^{-(W_E+W_T+2W_C)(t-t_{\mathrm{travel}})} - B_i e^{-(W_E+W_T)(t-t_{\mathrm{travel}})} - C_i e^{-2W_T(t-t_{\mathrm{travel}})} + [\rho_i(t_{\mathrm{travel}}) - A_i + B_i + C_i]e^{-W_T(t-t_{\mathrm{travel}})} \quad \text{for } i \in \{17, \ldots, 24\},\ t \geqslant t_{\mathrm{travel}}, \tag{26}$$

and $\rho_i(t)=0$ for $t \leqslant t_{\mathrm{travel}}$. The coefficients A_i, B_i, and C_i in Eqs. (26) are given in Table I. Next, we solve for $\rho_{25}(t)-\rho_{32}(t)$, the states in which one spin has reached a detector, while the other is still in a channel, in the pairs $\rho_i(t)\&\rho_j(t) \in \{\rho_{25}(t)\&\rho_{26}(t), \rho_{27}(t)\&\rho_{28}(t), \rho_{29}(t)\&\rho_{31}(t),$ and $\rho_{30}(t)\&\rho_{32}(t)\}$; see Eqs. (18). For each pair the solution is given by, for times $t \geqslant t_{\mathrm{travel}}$

$$\rho_i(t) = P_{i,j}e^{-W_E(t-t_{\mathrm{travel}})} + Q_{i,j}e^{-(W_E+2W_C)(t-t_{\mathrm{travel}})} + M_{i,1}e^{-2(W_E+W_C)(t-t_{\mathrm{travel}})} + M_{i,2}e^{-2W_E(t-t_{\mathrm{travel}})} + M_{i,3}e^{-2(W_E+2W_C)(t-t_{\mathrm{travel}})} + M_{i,4}e^{-(W_E+W_T+2W_C)(t-t_{\mathrm{travel}})} + M_{i,5}e^{-(W_E+W_T)(t-t_{\mathrm{travel}})} + M_{i,6}e^{-2W_T(t-t_{\mathrm{travel}})} + M_{i,7}e^{-W_T(t-t_{\mathrm{travel}})}, \tag{27a}$$

$$\rho_j(t) = P_{j,i}e^{-W_E(t-t_{\mathrm{travel}})} + Q_{j,i}e^{-(W_E+2W_C)(t-t_{\mathrm{travel}})} + M_{j,1}e^{-2(W_E+W_C)(t-t_{\mathrm{travel}})} + M_{j,2}e^{-2W_E(t-t_{\mathrm{travel}})} + M_{j,3}e^{-2(W_E+2W_C)(t-t_{\mathrm{travel}})} + M_{j,4}e^{-(W_E+W_T+2W_C)(t-t_{\mathrm{travel}})} + M_{j,5}e^{-(W_E+W_T)(t-t_{\mathrm{travel}})} + M_{j,6}e^{-2W_T(t-t_{\mathrm{travel}})} + M_{j,7}e^{-W_T(t-t_{\mathrm{travel}})}, \tag{27b}$$

and $\rho_i(t)=\rho_j(t)=0$ for $t \leqslant t_{\mathrm{travel}}$. The coefficients $P_{i,j}$, $Q_{i,j}$, and $M_{i,1}, \ldots, M_{i,7}$ for $i,j \in \{25, \ldots, 32\}$ are given in Appendix B.

Finally, we obtain the time evolution of the states $\rho_{33}(t)-\rho_{36}(t)$ in which both electrons have reached an exit. This is given by, for times $t \geqslant t_{\mathrm{travel}}$

$$\rho_j(t) = -W_E\left\{\frac{P_{m,p}+P_{n,q}}{W_E}e^{-W_E(t-t_{\mathrm{travel}})} + \frac{Q_{m,p}+Q_{n,q}}{W_E+2W_C}e^{-(W_E+2W_C)(t-t_{\mathrm{travel}})} + \frac{M_{m,1}+M_{n,1}}{2(W_E+W_C)}e^{-2(W_E+W_C)(t-t_{\mathrm{travel}})} + \frac{M_{m,2}+M_{n,2}}{2W_E}e^{-2W_E(t-t_{\mathrm{travel}})} + \frac{M_{m,3}+M_{n,3}}{2(W_E+2W_C)}e^{-2(W_E+2W_C)(t-t_{\mathrm{travel}})} + \frac{M_{m,4}+M_{n,4}}{W_E+W_T+2W_C}e^{-(W_E+W_T+2W_C)(t-t_{\mathrm{travel}})}\right.$$

$$+\frac{M_{m,5}+M_{n,5}}{W_E+W_T}e^{-(W_E+W_T)(t-t_{\text{travel}})}+\frac{M_{m,6}+M_{n,6}}{2W_T}e^{-2W_T(t-t_{\text{travel}})}+\frac{M_{m,7}+M_{n,7}}{W_T}e^{-W_T(t-t_{\text{travel}})}\Bigg\}$$
$$+W_E\left(\text{sum of all previous coefficients, so }\frac{P_{m,p}+P_{n,q}}{W_E}+\frac{Q_{m,p}+Q_{n,q}}{W_E+2W_C}+\cdots\right), \tag{28}$$

for

$$(j,m,n,p,q)\in\{(33,25,29,26,31),(34,26,30,25,32),(35,27,31,28,29),(36,28,32,27,30)\}.$$

Special case. In order to illustrate the solution (28), we now derive explicit expressions for $\rho_{33}(t)$ and $\rho_{34}(t)$, the probabilities that a spin-up is detected in the left detector and, respectively, a spin-up or a spin-down in the right detector, for the special case of $\Gamma=0$ (no decoherence in the dots) and $W_{C\uparrow\downarrow}=W_{C\downarrow\uparrow}=0$ (no relaxation in the channel). This corresponds to the situation in which the time evolution occurs in the absence of any decoherence and dissipation mechanisms in the dots and channels and only depends on W_T, the tunnel rate from dot to channel, and W_E, the tunnel rate from channel to exit.

We are interested in finding $\rho_{33}(t)$ and $\rho_{34}(t)$ for times $t\geqslant t_{\text{travel}}$ [since $\rho_{33}(t)=\rho_{34}(t)=0\ \forall t\leqslant t_{\text{travel}}$]. To that end, we first calculate $\rho_j(t_{\text{travel}})$ for $j\leqslant 16$ from Eqs. (21), (22), and (25) and then all coefficients entering the expressions for $\rho_{33}(t)$ and $\rho_{34}(t)$ in Eqs. (28). For $\rho_1(t_{\text{travel}})$ -$\rho_{16}(t_{\text{travel}})$ we then obtain

$$\rho_1(t_{\text{travel}})=\rho_4(t_{\text{travel}})=\rho_1(t_{\text{ESR}})e^{-2W_T(t_{\text{travel}}-t_{\text{ESR}})}, \tag{29a}$$

$$\rho_2(t_{\text{travel}})=\rho_3(t_{\text{travel}})=\rho_2(t_{\text{ESR}})e^{-2W_T(t_{\text{travel}}-t_{\text{ESR}})}, \tag{29b}$$

$$\rho_i(t_{\text{travel}})=\rho_1(t_{\text{ESR}})e^{-W_T(t_{\text{travel}}-t_{\text{ESR}})}(1-e^{-W_T(t_{\text{travel}}-t_{\text{ESR}})}),\quad i\in\{5,8,9,12\}, \tag{29c}$$

$$\rho_i(t_{\text{travel}})=\rho_2(t_{\text{ESR}})e^{-W_T(t_{\text{travel}}-t_{\text{ESR}})}(1-e^{-W_T(t_{\text{travel}}-t_{\text{ESR}})}),\quad i\in\{6,7,10,11\}, \tag{29d}$$

$$\rho_{13}(t_{\text{travel}})=\rho_{16}(t_{\text{travel}})=\rho_1(t_{\text{ESR}})(1-e^{-W_T(t_{\text{travel}}-t_{\text{ESR}})})^2, \tag{29e}$$

$$\rho_{14}(t_{\text{travel}})=\rho_{15}(t_{\text{travel}})=\rho_2(t_{\text{ESR}})(1-e^{-W_T(t_{\text{travel}}-t_{\text{ESR}})})^2. \tag{29f}$$

Equation (29) form the initial conditions that appear in the expressions for $\rho_{33}(t)-\rho_{36}(t)$ [Eqs. (28)]. We then find $\forall t\geqslant t_{\text{travel}}$

$$\rho_{33}(t)=\left(\rho_{13}(t_{\text{travel}})-\frac{2W_T}{W_E-W_T}\rho_5(t_{\text{travel}})+\frac{W_T^2}{(W_E-W_T)^2}\rho_1(t_{\text{travel}})\right)e^{-2W_E(t-t_{\text{travel}})}+\Bigg(-2\rho_{13}(t_{\text{travel}})$$
$$-\frac{2(W_E-2W_T)}{W_E-W_T}\rho_5(t_{\text{travel}})+\frac{2W_T}{W_E-W_T}\rho_1(t_{\text{travel}})\Bigg)e^{-W_E(t-t_{\text{travel}})}+\frac{2W_E}{W_E-W_T}\Bigg(\rho_5(t_{\text{travel}})$$
$$-\frac{W_T}{W_E-W_T}\rho_1(t_{\text{travel}})\Bigg)e^{-(W_E+W_T)(t-t_{\text{travel}})}-\frac{2W_E}{W_E-W_T}(\rho_5(t_{\text{travel}})+\rho_1(t_{\text{travel}}))e^{-W_T(t-t_{\text{travel}})}$$
$$+\frac{W_E^2}{(W_E-W_T)^2}\rho_1(t_{\text{travel}})e^{-2W_T(t-t_{\text{travel}})}+\rho_{13}(t_{\text{travel}})+2\rho_5(t_{\text{travel}})+\rho_1(t_{\text{travel}}), \tag{30a}$$

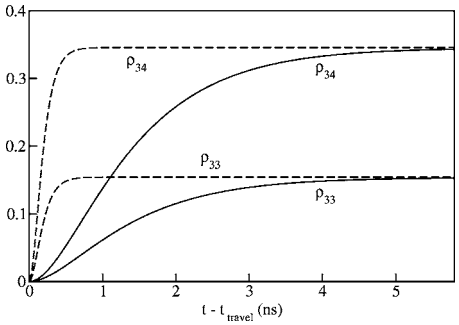

FIG. 3. The probabilities ρ_{33} to measure two spin-up electrons and ρ_{34} to measure a spin-up and a spin-down electron in the left and right exits, respectively, for times $t \geqslant t_{\text{travel}}$. Parameters used are $\theta_1 = \pi/2$, $\theta_2 = \pi/8$ [so that $\rho_1(t_{\text{ESR}}) = 0.154$ and $\rho_2(t_{\text{ESR}}) = 0.346$], $t_{\text{travel}} - t_{\text{ESR}} = 0.1$ ns, $W_E = 10^{10}$ s^{-1} and $W_T = 10^9$ s^{-1} (9.9×10^9 s^{-1}) for the solid (dashed) curves.

$$\rho_{34}(t) = \left(\rho_{14}(t_{\text{travel}}) - \frac{2W_T}{W_E - W_T}\rho_6(t_{\text{travel}}) + \frac{W_T^2}{(W_E - W_T)^2}\rho_2(t_{\text{travel}})\right)e^{-2W_E(t-t_{\text{travel}})} + \left(-2\rho_{14}(t_{\text{travel}})\right.$$
$$\left. - \frac{2(W_E - 2W_T)}{W_E - W_T}\rho_6(t_{\text{travel}}) + \frac{2W_T}{W_E - W_T}\rho_2(t_{\text{travel}})\right)e^{-W_E(t-t_{\text{travel}})} + \frac{2W_E}{W_E - W_T}\left(\rho_6(t_{\text{travel}})\right.$$
$$\left. - \frac{W_T}{W_E - W_T}\rho_2(t_{\text{travel}})\right)e^{-(W_E+W_T)(t-t_{\text{travel}})} - \frac{2W_E}{W_E - W_T}(\rho_6(t_{\text{travel}}) + \rho_2(t_{\text{travel}}))e^{-W_T(t-t_{\text{travel}})}$$
$$+ \frac{W_E^2}{(W_E - W_T)^2}\rho_2(t_{\text{travel}})e^{-2W_T(t-t_{\text{travel}})} + \rho_{14}(t_{\text{travel}}) + 2\rho_6(t_{\text{travel}}) + \rho_2(t_{\text{travel}}). \tag{30b}$$

One can see directly from Eqs. (30) that the time dependence of ρ_{33} and ρ_{34} is determined by five exponential functions, whose relative magnitude depends on the ratio between W_E and W_T. This is illustrated in Fig. 3, which shows Eqs. (30) as a function of $t - t_{\text{travel}}$ for various rates W_E and W_T. For $W_T \ll W_E$ the time needed to reach the stationary state (the average detection time) is dominated by the term $\sim e^{-W_T(t-t_{\text{travel}})}$, whereas for $W_T \approx W_E$ the terms $\sim e^{-2W_E(t-t_{\text{travel}})}$, $e^{-(W_E+W_T)(t-t_{\text{travel}})}$, and $e^{-2W_T(t-t_{\text{travel}})}$ dominate.

IV. CONCLUSION

In summary, we have presented an analytical solution of a set of coupled master equations that describes the time evolution of an entangled electron spin pair which can occupy 36 different quantum states in a double quantum dot nanostructure. Our method of solving these equations is based on separating the time evolution in three parts, namely two coherent rotations of the electron spins in the isolated quantum dots and the subsequent travel of the electrons through two quantum channels. As a result of this separation, the total number of master equations is split into various closed subsets of coupled equations. Our analytical solution is the first of its kind for a large set of coupled master equations, and the same method can be used to study and predict the quantum evolution of other quantum systems which are described by a large set of quantum states. This type of analysis complements numerical approaches to study the dynamic evolution of complex quantum systems and allows one to obtain qualitative insight in the competition between time scales in these systems.

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APPENDIX A: SOLUTION OF EQS. (8a)–(8i)

Using the substitution Eqs. (10), Eqs. (8a)–(8i) transform into

$$\dot{x}_1 = -(W_{D\downarrow\uparrow} + W_{D\uparrow\downarrow} - \Gamma)x_1 - \Delta_L x_5 + W_{D\uparrow\downarrow}e^{\Gamma t}, \tag{A1a}$$

$$\dot{x}_5 = \Delta_L x_1 - \frac{\Delta_L}{2}e^{\Gamma t}, \tag{A1b}$$

$$\dot{x}_2 = -(W_{D\downarrow\uparrow} + W_{D\uparrow\downarrow} - \Gamma)x_2 - \delta_L x_4 + W_{D\uparrow\downarrow}e^{\Gamma t}, \tag{A1c}$$

$$\dot{x}_4 = \delta_L x_2 - \frac{\delta_L}{2}e^{\Gamma t}, \tag{A1d}$$

$$\dot{x}_3 = -(2W_{D\downarrow\uparrow} + 2W_{D\uparrow\downarrow} - \Gamma)x_3 + \delta_L x_6 + \Delta_L x_7 + 2W_{D\uparrow\downarrow}e^{\Gamma t} + (W_{D\downarrow\uparrow} - W_{D\uparrow\downarrow})(x_1 + x_2), \tag{A1e}$$

$$\dot{x}_6 = -\delta_L x_3 + 2\Delta_L x_8 + \frac{\delta_L}{2}e^{\Gamma t} - \Delta_L Z, \tag{A1f}$$

$$\dot{x}_7 = -\Delta_L x_3 + 2\delta_L x_8 + \frac{\Delta_L}{2}e^{\Gamma t} - \delta_L Z, \tag{A1g}$$

$$\dot{x}_8 = -\frac{\Delta_L}{2}x_6 - \frac{\delta_L}{2}x_7, \tag{A1h}$$

with $Z \equiv \mathrm{Re}[\tilde{\rho}_{1,4}(0) + \tilde{\rho}_{2,3}(0)]$. In deriving Eqs. (A1), we have used that

$$\rho_4 = 1 - \rho_1 - \rho_2 - \rho_3,$$

$$\mathrm{Re}\,\tilde{\rho}_{2,3} = -\mathrm{Re}\,\tilde{\rho}_{1,4} + Ze^{-\Gamma t}.$$

Equations (A1) consist of three sets of coupled equations: (A1a)–(A1b), (A1c)–(A1d), and (A1e)–(A1h). The solution of the first two sets is given by

$$x_1(t) = \left[-\left(\frac{(W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow} - \Gamma)(x_1(0) - A_1) + 2\Delta_L(x_5(0) - A_2)}{2\Omega_\Delta} \right) \sin \Omega_\Delta t + (x_1(0) - A_1)\cos \Omega_\Delta t \right] e^{-(1/2)(W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow} - \Gamma)t} + A_1 e^{\Gamma t}, \tag{A2a}$$

$$x_5(t) = \left[\left(\frac{2\Delta_L(x_1(0) - A_1) + (W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow} - \Gamma)(x_5(0) - A_2)}{2\Omega_\Delta} \right) \sin \Omega_\Delta t + (x_5(0) - A_2)\cos \Omega_\Delta t \right] e^{-(1/2)(W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow} - \Gamma)t} + A_2 e^{\Gamma t}, \tag{A2b}$$

$$x_2(t) = \left[-\left(\frac{(W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow} - \Gamma)(x_2(0) - A_3) + 2\delta_L(x_4(0) - A_4)}{2\Omega_\delta} \right) \sin \Omega_\delta t \right.$$
$$\left. + (x_2(0) - A_3)\cos \Omega_\delta t \right] e^{-(1/2)(W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow} - \Gamma)t} + A_3 e^{\Gamma t}, \tag{A2c}$$

$$x_4(t) = \left[\left(\frac{2\delta_L(x_2(0) - A_3) + (W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow} - \Gamma)(x_4(0) - A_4)}{2\Omega_\delta} \right) \sin \Omega_\delta t \right.$$
$$\left. + (x_4(0) - A_4)\cos \Omega_\delta t \right] e^{-(1/2)(W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow} - \Gamma)t} + A_4 e^{\Gamma t}, \tag{A2d}$$

with

$$\Omega_\Delta = \frac{1}{2}\sqrt{4\Delta_L^2 - (W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow} - \Gamma)^2}, \tag{A3a}$$

$$\Omega_\delta = \frac{1}{2}\sqrt{4\delta_L^2 - (W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow} - \Gamma)^2}, \tag{A3b}$$

$$A_1 = \frac{\Delta_L^2 + 2\Gamma W_{D\uparrow\downarrow}}{2(\Delta_L^2 + \Gamma(W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow}))}, \tag{A3c}$$

$$A_2 = \frac{\Delta_L(W_{D\uparrow\downarrow} - W_{D\downarrow\uparrow})}{2(\Delta_L^2 + \Gamma(W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow}))}, \tag{A3d}$$

$$A_3 = \frac{\delta_L^2 + 2\Gamma W_{D\uparrow\downarrow}}{2(\delta_L^2 + \Gamma(W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow}))}, \tag{A3e}$$

$$A_4 = \frac{\delta_L(W_{D\uparrow\downarrow} - W_{D\downarrow\uparrow})}{2(\delta_L^2 + \Gamma(W_{D\uparrow\downarrow} + W_{D\downarrow\uparrow}))}. \tag{A3f}$$

So far no approximations have been made, apart from assuming the decoherence rate Γ to be equal for all off-diagonal terms of the density matrix ρ [Eqs. (8)]. In order to obtain the solution of the remaining equations (A1e)–(A1h), we assume $\delta_L = 0$ (no influence of the ESR field on the spin in the right dot) and $W_{D\uparrow\downarrow} = W_{D\downarrow\uparrow} = 0$,[23] and find[24]

$$x_3(t) = \left[\frac{\Gamma\left(x_3(0) - \frac{1}{2}\right) + 2\Delta_L x_7(0)}{2\tilde{\Omega}_\Delta} \sin \tilde{\Omega}_\Delta t + \left(x_3(0) - \frac{1}{2}\right)\cos \tilde{\Omega}_\Delta t \right] e^{(\Gamma/2)t} + \frac{1}{2}e^{\Gamma t}, \tag{A4a}$$

$$x_6(t) = x_6(0)\cos \Delta_L t + (2x_8(0) - Z)\sin \Delta_L t, \tag{A4b}$$

$$x_7(t) = \left[\frac{-2\Delta_L\left(x_3(0) - \frac{1}{2}\right) - \Gamma x_7(0)}{2\tilde{\Omega}_\Delta} \sin \tilde{\Omega}_\Delta t + x_7(0)\cos \tilde{\Omega}_\Delta t \right] e^{(\Gamma/2)t}, \tag{A4c}$$

$$x_8(t) = \tfrac{1}{2}[-x_6(0)\sin\Delta_L t + (2x_8(0) - Z)\cos\Delta_L t + Z], \tag{A4d}$$

with $\tilde{\Omega}_\Delta = \frac{1}{2}\sqrt{4\Delta_L^2 - \Gamma^2}$.

APPENDIX B: COEFFICIENTS OF EQS. (25) and (27)

The coefficients in Eqs. (25) are given by

$$E = \frac{-\rho_{13}(t_{\mathrm{ESR}}) + \rho_{16}(t_{\mathrm{ESR}}) + H_{13} - H_{16} + K_{13} - K_{16} + L_{13} - L_{16}}{2},$$

$$\tilde{E} = \frac{\rho_{14}(t_{\mathrm{ESR}}) - \rho_{15}(t_{\mathrm{ESR}}) - H_{14} + H_{15} - K_{14} + K_{15} - L_{14} + L_{15}}{2},$$

$$F = \frac{\rho_{13}(t_{\mathrm{ESR}}) + \rho_{14}(t_{\mathrm{ESR}}) + \rho_{15}(t_{\mathrm{ESR}}) + \rho_{16}(t_{\mathrm{ESR}}) - 2(K_{14} + K_{15}) - L_{13} - L_{14} - L_{15} - L_{16}}{2},$$

$$\tilde{F} = \frac{-\rho_{13}(t_{\mathrm{ESR}}) + \rho_{14}(t_{\mathrm{ESR}}) + \rho_{15}(t_{\mathrm{ESR}}) - \rho_{16}(t_{\mathrm{ESR}}) - 2(H_{14} + H_{15}) + L_{13} - L_{14} - L_{15} + L_{16}}{2},$$

$$H_{13} = \frac{W_T[(W_E - W_T + W_C)(A_{5,7,1,3} + A_{9,10,1,2}) + W_C(A_{6,8,2,4} + A_{11,12,3,4})]}{(W_E - W_T)(W_E - W_T + 2W_C)},$$

$$H_{14} = \frac{W_T[W_C(A_{5,7,1,3} - A_{11,12,3,4}) + (W_E - W_T + W_C)(A_{6,8,2,4} - A_{9,10,1,2})]}{(W_E - W_T)(W_E - W_T + 2W_C)},$$

$$H_{15} = -H_{14}[(5,7,1,3) \leftrightarrow (6,8,2,4), (9,10,1,2) \leftrightarrow (11,12,3,4)],$$

$$H_{16} = -H_{13}[(5,7,1,3) \leftrightarrow (6,8,2,4), (9,10,1,2) \leftrightarrow (11,12,3,4)],$$

$$K_{13} = H_{13}(A \to B),$$

$$K_{14} = \frac{W_T[W_C(B_{5,7,1,3} + B_{11,12,3,4}) + (W_E - W_T + W_C)(B_{6,8,2,4} + B_{9,10,1,2})]}{(W_E - W_T)(W_E - W_T + 2W_C)},$$

$$K_{15} = K_{14}[(5,7,1,3) \leftrightarrow (6,8,2,4), (9,10,1,2) \leftrightarrow (11,12,3,4)],$$

$$K_{16} = H_{16}(A \to -B),$$

$$\begin{aligned} L_{13} = W_T[&(2(W_E - W_T + W_C)^2 - W_C^2)(C_{1,2} + C_{1,3}) + W_C^2(D_{2,4} + D_{3,4}) + W_C(W_E - W_T + W_C) \\ &\times (C_{2,4} + C_{3,4} + D_{1,2} + D_{1,3})]/[4(W_E - W_T)(W_E - W_T + 2W_C)(W_E - W_T + W_C)], \end{aligned}$$

$$\begin{aligned} L_{14} = W_T[&W_C(W_E - W_T + W_C)(C_{1,2} + C_{1,3} + D_{2,4} + D_{3,4}) + 2(W_E - W_T + W_C)^2(C_{2,4} + D_{1,2}) \\ &+ W_C^2(C_{3,4} - C_{2,4} - D_{1,2} + D_{1,3})]/[4(W_E - W_T)(W_E - W_T + 2W_C)(W_E - W_T + W_C)], \end{aligned}$$

$$L_{15} = L_{14}(C_{2,4} \leftrightarrow C_{3,4}, D_{1,2} \leftrightarrow D_{1,3}),$$

$$L_{16} = L_{13}(C_{1,2} \leftrightarrow D_{2,4}, C_{1,3} \leftrightarrow D_{3,4}). \tag{B1}$$

For $(i,j)=(25,26)$ the coefficients in Eqs. (27) are given by

$$P_{25,26} = P_{26,25} = -\frac{1}{2}\sum_{k=1}^{7}(M_{25,k} + M_{26,k}),$$

$$Q_{25,26} = -Q_{26,25} = -\frac{1}{2}\sum_{k=1}^{7}(M_{25,k} - M_{26,k}),$$

$$M_{25,1} = \frac{(W_E + W_C)E + W_C\tilde{E}}{W_E + 2W_C},$$

$$M_{26,1} = M_{25,1}(E \leftrightarrow -\tilde{E}),$$

$$M_{25,2} = M_{26,2} = -\frac{1}{2}F,$$

$$M_{25,3} = -M_{26,3} = \frac{W_E}{2(W_E + 2W_C)}\tilde{F},$$

$$M_{25,4} = \frac{W_E[-(W_T + W_C)((W_E + 2W_C)H_{13} - W_T A_{5,7,1,3}) + W_C((W_E + 2W_C)H_{14} - W_T A_{6,8,2,4})]}{W_T(W_E + 2W_C)(W_T + 2W_C)},$$

$$M_{26,4} = M_{25,4}(H_{13} \leftrightarrow H_{14}, A_{5,7,1,3} \leftrightarrow A_{6,8,2,4}),$$

$$M_{25,5} = \frac{(W_C - W_T)(W_E K_{13} - W_T B_{5,7,1,3}) + W_C(W_E K_{14} - W_T B_{6,8,2,4})}{W_T(W_T - 2W_C)},$$

$$M_{26,5} = M_{25,5}(K_{13} \leftrightarrow K_{14}, B_{5,7,1,3} \leftrightarrow B_{6,8,2,4}),$$

$$M_{25,6} = \frac{W_E[(W_E - 2W_T + W_C)(L_{13} - C_{1,3}) + W_C(L_{14} - C_{2,4})]}{(W_E - 2W_T + 2W_C)(W_E - 2W_T)},$$

$$M_{26,6} = M_{25,6}(L_{13} \leftrightarrow L_{14}, C_{1,3} \leftrightarrow C_{2,4}),$$

$$M_{25,7} = W_T[(W_E - W_T + W_C)[-A_{17} + B_{17} + C_{17}] + W_C[-A_{18} + B_{18} + C_{18}]]/[(W_E - W_T + 2W_C) \times (W_E - W_T)],$$

$$M_{26,7} = M_{25,7}(17 \leftrightarrow 18). \tag{B2}$$

TABLE II. Required substitution of indices and coefficients in Eqs. (27) in order to obtain the corresponding coefficients for $\rho_i(t)\&\rho_j(t)$ with $(i,j) \in \{(27,28),(29,31),(30,32)\}$.

(27,28)	(29,31)	(30,32)
$25\rightarrow 28$	$25\rightarrow 29$	$25\rightarrow 32$
$26\rightarrow 27$	$26\rightarrow 31$	$26\rightarrow 30$
$13\rightarrow 16$		$13\rightarrow 16$
$14\rightarrow 15$	$14\rightarrow 15$	
$17\rightarrow 20$	$17\rightarrow 21$	$17\rightarrow 24$
$18\rightarrow 19$	$18\rightarrow 23$	$18\rightarrow 22$
$E\leftrightarrow -E$		$E\leftrightarrow -E$
$\tilde{E}\leftrightarrow -\tilde{E}$	$\tilde{E}\leftrightarrow -\tilde{E}$	
$A_{5,7,1,3}\leftrightarrow -A_{6,8,2,4}$	$(5,7,1,3)\rightarrow(9,10,1,2)$	$A_{5,7,1,3}\rightarrow -A_{11,12,3,4}$
$B_{5,7,1,3}\leftrightarrow B_{6,8,2,4}$		$B_{5,7,1,3}\rightarrow B_{11,12,3,4}$
	$(6,8,2,4)\rightarrow(11,12,3,4)$	$A_{6,8,2,4}\rightarrow -A_{9,10,1,2}$
		$B_{6,8,2,4}\rightarrow B_{9,10,1,2}$
$C_{1,3}\rightarrow D_{2,4}$	$C_{1,3}\rightarrow C_{1,2}$	$C_{1,3}\rightarrow D_{3,4}$
$C_{2,4}\rightarrow D_{1,3}$	$C_{2,4}\rightarrow C_{3,4}$	$C_{2,4}\rightarrow D_{1,2}$

The coefficients in Eqs. (27) for $(i,j)=(27,28)$, (29,31), and (30,32) are obtained from Eqs. (B2) by replacing indices as given in Table II.

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Semilattice graded weak Hopf algebra and its related quantum G-double

Fang Li[a] and Haijun Cao[b]
Department of Mathematics, Zhejiang University, Hangzhou, Zhejiang 310028, China

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The major purpose of this paper is to construct a weak Hopf algebra with grading from a family of Hopf algebras, and then to gain a related quantum G-double with regular R-matrix. First, over a field k, we introduce a so-called semilattice graded weak Hopf algebra $H=\oplus_{\alpha\in Y}H_\alpha$. Then the quantum G-double $D'(H)$ of H is obtained in case that H is commutative. Moreover, it is shown that $D'(H)$ is semisimple (respectively, von Neumann regular) if and only if H is a semisimple (respectively, von Neumann regular) Hopf algebra. At last, a nontrivial example of semilattice graded weak Hopf algebras is obtained. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2000687]

I. INTRODUCTION

Because of the important role of Hopf algebra in the theory of quantum group and related mathematical physics, along with the deepening of researches, the meaning of some weaker concepts of Hopf algebra is understood and is paid close attention more and more. A well-known example is weak Hopf algebra, which is introduced in Ref. 6 for studying the noninvertible solution of the Yang-Baxter equation based on this class of bialgebras (in Refs. 6 and 12). Due to the importance of the Yang-Baxter equation in theoretical physics, its solution is the keystone in research. The theory of singular solutions extends largely the scope of the research field. On the other aspect, there is a tight relation between weak Hopf algebra and regular monoid, for example, a semigroup algebra is a weak Hopf algebra if and only if the semigroup is a regular monoid. Obviously, it is necessary to find more nontrivial weak Hopf algebras in order to study these two aspects deeply. In this paper, we construct a so-called semilattice graded weak Hopf algebra from a family of Hopf algebras. An example of semilattice graded weak Hopf algebra is just Clifford moniod algebra. And, based on Ref. 13, a regular solution of the Yang-Baxter equation and its decomposition can be obtained. Moreover, similar to the corresponding results in Ref. 10, we will finish the decomposition and semisimplicity of G-quantum doubles of semilattice graded weak Hopf algebras under the condition of commutativity.

First, we introduce some useful concepts.

H is called an *almost bialgebra* if H is an algebra and also a coalgebra and the comultiplication of H is an algebra morphism.

A bialgebra H over k is called a *weak Hopf algebra*[6] if there exists $T\in \mathrm{Hom}_k(H,H)$ (the convolution algebra) satisfying $\mathrm{id}*T*\mathrm{id}=\mathrm{id}$ and $T*\mathrm{id}*T=T$, where T is called a *weak antipode* of H. A weak Hopf algebra H is called (1) a *perfect weak Hopf algebra*[7] if its weak antipode T is an antibialgebra morphism satisfying $(\mathrm{id}*T)(H)\subseteq C(H)$ (the center of H); (2) a *coperfect weak Hopf algebra*[9] if its weak antipode is an antibialgebra morphism satisfying $\Sigma_{(x)}x'T(x'')\otimes x'''=\Sigma_{(x)}x''T(x''')\otimes x'$ for any $x\in H$; (3) a *biperfect weak Hopf algebra* if it is perfect and also coperfect.

[a]Electronic mail: fangli@zju.edu.cn
[b]Electronic mail: hjcao99@163.com

Since the concept of weak Hopf algebra was introduced in Ref. 6, and more early, in an unpublished report,[11] one has only two ways to give examples, that is, through semigroup algebras of regular monoids (in particular, Clifford monoids) and the weak quantum algebras $wsl_q(2)$ and $vsl_q(2)$ (see Ref. 12).

The same name "weak Hopf algebra" was also used as another kind of generalization of Hopf algebra in Refs. 2, 20, and 16 which comultiplication is no longer required to preserve the unit (equivalently, the counit is not required to be an algebra homomorphism). We must point out that these two kinds of weak Hopf algebra are completely different generalizations of each other in various directions, since the only common subclass just consists of Hopf algebras (see Ref. 8). The initial motivation of the latter was its connection with the theory of algebra extension.

In this paper, we always assume H denotes a weak Hopf algebra under Li's meaning over a field k and $G(H)$ the monoid of all grouplike elements in H. A semigroup with identity is called a *monoid*.

A semigroup S is called a *Clifford semigroup*[17] if it is a regular semigroup and all of its idempotents lie in its center $C(S)$. An equivalent definition is that a Clifford semigroup S is a semilattice of groups, which means the set of maximal subgroups $\{G_\alpha : \alpha \in Y\}$ of S can be indexed by elements of a semilattice (i.e., a commutative semigroup of idempotents) Y such that $S = \cup_{\alpha \in Y} G_\alpha$ and $G_\alpha G_\beta \subseteq G_{\alpha\beta}$ for each $\alpha, \beta \in Y$. For each $\alpha, \beta \in Y$ with $\alpha\beta = \beta$ there exists a homomorphism $\varphi_{\alpha,\beta} : G_\alpha \to G_\beta$. The homomorphisms are such that $\varphi_{\alpha,\alpha}$ is the identity map on G_α, and if $\alpha\beta = \beta$, $\beta\gamma = \gamma$, then $\varphi_{\beta,\gamma}\varphi_{\alpha,\beta} = \varphi_{\alpha,\gamma}$. For any $\alpha, \beta \in Y$ and $a \in G_\alpha$, $b \in G_\beta$, the multiplication in S is given by $ab = \varphi_{\alpha,\alpha\beta}(a)\varphi_{\beta,\alpha\beta}(b)$. In a semilattice Y, a partial order $\leqslant$ is defined satisfying $\alpha \leqslant \beta$ if $\alpha\beta = \alpha$ for $\alpha, \beta \in Y$, which is called the *natural partial order* in Y.

It is easy to see for every Clifford monoid S, the semigroup algebra kS is a weak Hopf algebra and $kS = \oplus_{\alpha \in Y} kG_\alpha$ is a semilattice grading sum. As its natural generalization, we will define the following concept, which provides a way to obtain a class of weak Hopf algebras through some given Hopf algebras.

Definition I.1: A weak Hopf algebra H with weak antipode T is called a semilattice graded weak Hopf algebra *if $H = \oplus_{\alpha \in Y} H_\alpha$ is a semilattice grading sum where H_α is a weak sub-Hopf algebras of H which is a Hopf algebra with antipodes $T|_{H_\alpha}$ for each $\alpha \in Y$ and there homomorphisms of Hopf algebras $\varphi_{\alpha,\beta}$ from H_α to H_β if $\alpha\beta = \beta$, such that for $a \in H_\alpha$ and $b \in H_\beta$, the multiplication $a * b$ in H can be given by $a * b = \varphi_{\alpha,\alpha\beta}(a)\varphi_{\beta,\alpha\beta}(b)$.*

Thus the set of grouplike elements of H is the Clifford monoid $G(H) = [Y; G(H_\alpha), \varphi_{\alpha,\beta}]$.

In Sec. II, for a semilattice graded weak Hopf algebra $H = \oplus_{\alpha \in Y} H_\alpha$, we define a kind of product, the quantum G-double $D'(H) = H^{op^*} \infty' H$ which give a nontrivial solution for the Yang-Baxter equation in case H is commutative. In Sec. III, we discuss the structure of $D'(H)$ depending upon $D'(H_\alpha)(\alpha \in Y)$ and then obtain the structure theorem Theorem III.4. Moreover, in Sec. IV, by using this structure theorem, we will verify that the quantum G-double $D'(H)$ of H cannot be semisimple unless H is a Hopf algebra. In the special case for a commutative Clifford monoid, our result in Sec. IV is similar to that in Ref. 10. At last, we will construct an example of this kind of weak Hopf algebras through Ore extension as the construction producing pointed Hopf algebras from a group algebra in Ref. 1.

II. QUANTUM G-DOUBLE OF A COMMUTATIVE WEAK HOPF ALGEBRA

In this section, we suppose a semilattice graded weak Hopf algebra $H = \oplus_{\alpha \in Y} H_\alpha$ is commutative with finite dimension.

Let B_α be a basis of H_α for every $\alpha \in Y$, then $B = \cup_{\alpha \in Y} B_\alpha$ is a basis of H. For any $a \in B_\alpha$, let ϕ_a be the dual morphism of a in H_α^*, that is,

$$\phi_a(x) = \begin{cases} 1 & \text{if } a = x \in H_\alpha, \\ 0 & \text{if } a \neq x \in H_\alpha. \end{cases}$$

Then, $\{\phi_a | a \in B_\alpha\}$ is a basis of H_α^* for any $\alpha \in Y$.

At k-linear spaces, we have $H^*\otimes H=H^*\otimes(\oplus_{\alpha\in Y}H_\alpha)$. Moreover, $H^*=(\oplus_{\alpha\in Y}H_\alpha)^*=\Pi_{\alpha\in Y}(H_\alpha)^*$. Y is finite since H is finite dimensional. As is known, the direct product and the direct sum are equivalent for a finite number of linear spaces. So, $\Pi_{\alpha\in Y}(H_\alpha)^*=\oplus_{\alpha\in Y}(H_\alpha)^*$.

Since for any $f\in H^*=\oplus_{\alpha\in Y}H_\alpha^*$, it can be decomposed to $f=\Sigma_{\alpha\in Y}f_\alpha$ with $f_\alpha\in H_\alpha^*$. So we can introduce a kind of product as follows.

Definition II.1: For a semilattice graded weak Hopf algebra $H=\oplus_{\alpha\in Y}H_\alpha$, we define a product $D'(H)=H^{op^*}\infty' H$ *from H which can be constructed by*

$$(f\infty' a)(g\infty' b)=fg(1_{H_\alpha}?)\infty' ab$$

for $f\in H_{\alpha_1}^{op^*}$, $g\in H_{\alpha_2}^{op^*}$, $a\in H_{\beta_1}$, $b\in H_{\beta_2}$, *where* $fg(1_{H_\alpha}?)$ *means the morphism,* $x\mapsto\Sigma_{(x)}f(x')g(1_{H_\alpha}x'')$ *for* $x\in H_{\alpha_1}$. *We call* $D'(H)$ *the* quantum G-double *of H. (Note that all "?" in this paper are under the same meaning.)*

Thus, we get $D'(H)=\oplus_{\alpha,\beta\in Y}(H_\alpha^*\otimes H_\beta)$ as linear spaces. Denote $D'(H_\alpha,H_\beta)=H_\alpha^{op^*}\otimes H_\beta$ and $Q_H(H_\alpha)=H_\alpha^{op^*}\otimes H=\oplus_{\beta\in Y}D'(H_\alpha,H_\beta)$. Then, as linear spaces,

$$D'(H)=\bigoplus_{\alpha\in Y}Q_H(H_\alpha)=\bigoplus_{\alpha,\beta\in Y}D'(H_\alpha,H_\beta). \tag{2.1}$$

Theorem II.2: *For a commutative semilattice graded weak Hopf algebra $H=\oplus_{\alpha\in Y}H_\alpha$, the quantum G-double $D'(H)$ defined above is a noncommutative and noncocommutative almost bialgebra with regular R-matrix $R=\Sigma_{\alpha\in Y}\Sigma_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})$, but it is usually not quasitriangular although $(\Delta\otimes\mathrm{id}_H)(R)=R_{13}R_{23}$ and $(\mathrm{id}_H\otimes\Delta)(R)=R_{13}R_{12}$ hold.*

Proof: (1) First we can prove that $D'(H)$ is an almost bialgebra.

For any $\alpha_1,\alpha_2,\beta_1,\beta_2\in Y$, $x\in B_{\beta_1}$, $y\in B_{\beta_2}$, $a\in B_{\alpha_1}$ and its duality ϕ_a in $H_{\alpha_1}^{op^*}$, $b\in B_{\alpha_2}$ and its duality ϕ_b in $H_{\alpha_2}^{op^*}$, we have

$$(\phi_a\infty' x)(\phi_b\infty' y)=(\phi_a\infty' x)(\phi_b\infty' y)=\phi_a\phi_b(1_{H_{\beta_1}}?)\infty' xy,$$

where

$$\phi_a\phi_b(1_{H_{\beta_1}}?)=\begin{cases}0 & \text{if } \alpha_1\beta_1\neq\alpha_2,\\ \phi_a\phi_b(1_{H_\beta}?) & \text{if } \alpha_1\beta_1=\alpha_2.\end{cases}$$

Then, for any $x\in B_{\alpha_1}$, $y\in B_{\alpha_2}$, $z\in B_{\alpha_3}$, $a\in B_{\beta_1}$ and its duality ϕ_a in $H_{\beta_1}^{op^*}$, $b\in B_{\beta_2}$ and its duality ϕ_b in $H_{\beta_2}^{op^*}$, $c\in B_{\beta_3}$ and its duality ϕ_c in $H_{\beta_3}^{op^*}$, we have

$$\begin{aligned}((\phi_a\infty' x)(\phi_b\infty' y))(\phi_c\infty' z)&=(\phi_a\phi_b(1_{H_{\alpha_1}}?)\infty' xy)(\phi_c\infty' z)\\&=\begin{cases}0 & \text{if } \beta_1\alpha_1\neq\beta_2\\ (\phi_a\phi_b(1_{H_{\alpha_1}}?)\infty' xy)(\phi_c\infty' z) & \text{if } \alpha_1\beta_1=\alpha_2\end{cases}\\&=\begin{cases}0 & \text{if } \beta_1\alpha_1\neq\beta_2 \quad\text{or } \beta_1\alpha_1\alpha_2\neq\beta_3\\ \phi_a\phi_b(1_{H_{\alpha_1}}?)\phi_c(1_{H_{\alpha_1\alpha_2}})\infty' xyz & \text{if } \beta_1\alpha_1=\beta_2 \quad\text{and } \beta_1\alpha_1\alpha_2=\beta_3,\end{cases}\end{aligned}$$

$$\begin{aligned}(\phi_a\infty' x)((\phi_b\infty' y)(\phi_c\infty' z))&=(\phi_a\infty' x)(\phi_b\phi_c(1_{H_{\alpha_2}}?)\infty' yz)\\&=\begin{cases}0 & \text{if } \alpha_2\beta_2\neq\beta_3\\ ((\phi_a\infty' x)(\phi_b\phi_c(1_{H_{\alpha_2}}?)\infty' yz) & \text{if } \alpha_2\beta_2=\beta_3\end{cases}\\&=\begin{cases}0 & \text{if } \alpha_2\beta_2\neq\beta_3 \quad\text{or } \alpha_1\beta_1\neq\beta_2\\ \phi_a(\phi_b\phi_c(1_{H_{\alpha_2}}?)(1_{H_{\alpha_1}}?))\infty' xyz & \text{if } \alpha_2\beta_2=\beta_3 \quad\text{and } \alpha_1\beta_1=\beta_2.\end{cases}\end{aligned}$$

If $\beta_1\alpha_1=\beta_2$ and $\beta_1\alpha_1\alpha_2=\beta_3$, then $\alpha_2\beta_2=\alpha_2\beta_1\alpha_1=\beta_1\alpha_1\alpha_2=\beta_3$; conversely, if $\alpha_1\beta_1=\beta_2$ and $\alpha_2\beta_2=\beta_3$, then $\beta_1\alpha_1\alpha_2=\beta_2\alpha_2=\beta_3$. Hence, $\beta_1\alpha_1=\beta_2$ and $\beta_1\alpha_1\alpha_2=\beta_3\Leftrightarrow\alpha_1\beta_1=\beta_2$ and $\alpha_2\beta_2=\beta_3$. So, for some $d\in H_{\beta_1}$ and $u\in H^*$, then

$$(\phi_a\phi_b(1_{H_{\alpha_1}}?)\phi_c(1_{H_{\alpha_1\alpha_2}}?)\infty' xyz)(d\otimes u)=\sum_{(d)}\phi_a(d')\phi_b(1_{H_{\alpha_1}}d'')\phi_c(1_{H_{\alpha_1\alpha_2}}d''')u(xyz),$$

$$\begin{aligned}(\phi_a(\phi_b\phi_c(1_{H_{\alpha_2}}?))(1_{H_{\alpha_1}}?)\infty' xyz)(d\otimes u)&=\sum_{(d)}\phi_a(d')\phi_b\phi_c(1_{H_{\alpha_2}}?)(1_{H_{\alpha_1}}d'')u(xyz)\\&=\sum_{(d)}\phi_a(d')\phi_b((1_{H_{\alpha_1}}d'')')\phi_c(1_{H_{\alpha_2}}(1_{H_{\alpha_1}}d'')'')u(xyz)\\&=\sum_{(d)}\phi_a(d')\phi_b(1_{H_{\alpha_1}}d'')\phi_c(1_{H_{\alpha_2}}1_{H_{\alpha_1}}d''')u(xyz)\\&=\sum_{(d)}\phi_a(d')\phi_b(1_{H_{\alpha_1}}d'')\phi_c(1_{H_{\alpha_1\alpha_2}}d''')u(xyz).\end{aligned}$$

That is $((\phi_a\infty' x)(\phi_b\infty' y))(\phi_c\infty' z)=(\phi_a\infty' x)((\phi_b\infty' y)(\phi_c\infty' z))$.

Moreover, $1_{D(H)}=\varepsilon_H\infty' 1_H=\Sigma_{\alpha\in Y}\varepsilon_{H_\alpha}\infty' 1_H$ is the identity of $D'(H)$. Since for any $\phi_a\in H_\alpha^*$, $x\in H_\beta$,

$$(\varepsilon_H\infty' 1_H)(\phi_a\infty' x)=\varepsilon_H\phi_a(1_H?)\infty' 1_H x=\varepsilon_{H_\alpha}\phi_a\infty' x,$$

$$(\phi_a\infty' x)(\varepsilon_H\infty' 1_H)=\phi_a\varepsilon_H(1_{H_\beta}?)\infty' x1_H=\phi_a\varepsilon_H(1_{H_\beta})\varepsilon_H(?)\infty' x=\phi_a\varepsilon_H\infty' x,$$

and for any $z\in H_\alpha$, $\phi_a\varepsilon_H(z)=\Sigma_{(z)}\phi_a(z')\varepsilon_H(z'')=\Sigma_{(z)}\phi_a(z')\varepsilon_{H_\alpha}(z'')=\phi_a(x)$, that is $(\varepsilon_H\infty' 1_H)\times(\phi_a\infty' x)=(\phi_a\infty' x)(\varepsilon_H\infty' 1_H)=\phi_a\infty x'$.

Therefore $D'(H)$ is an algebra.

The comultiplication Δ in $D'(H)$ is trivial, that is, for $f\in H^{op*}$ and $x\in B$,

$$\Delta(f\infty' x)=\sum_{(f)(x)}(f'\infty' x')\otimes(f''\infty' x''),$$

where $\Delta(f)=\Sigma_{(f)}f'\otimes f''$ according to the comultiplication in H^{op*}.

The counit ε of $D'(H)$ is given as $\varepsilon(\phi_a\infty' x)=\varepsilon_{H_\alpha^{op*}}(\phi_a)\varepsilon_{H_\beta}(x)$ for $a\in B_\alpha$, $x\in B_\beta$. But, $\varepsilon_{H_\alpha^{op*}}(\phi_a)=\eta_{H_\alpha^*}(\phi_a)(1_k)=\phi_a\eta_{H_\alpha}(1_k)=\phi_a(1_{H_\alpha})=\delta_{a,1_{H_\alpha}}$. Therefore, we get

$$\varepsilon(\phi_a\infty' x)=\delta_{a,1H\alpha}\varepsilon_{H_\beta}(x).$$

Obviously, $(\Delta\otimes 1)\Delta=(1\otimes\Delta)\Delta$.

For any $f\in H_\alpha^*$, $x\in H_\beta$, $(\varepsilon\otimes 1)\Delta(f\infty' x)=(\varepsilon\otimes 1)\Sigma_{(f),(x)}(f'\infty' x')\otimes(f''\infty' x'')=\Sigma_{(f),(x)}\varepsilon(f'\infty' x')\times(f''\infty' x'')=\Sigma_{(f),(x)}\varepsilon_{H_\alpha^{op*}}(f')\varepsilon_{H_\beta}(x')f''\infty' x''=\Sigma_{(f),(x)}\varepsilon_{H_\alpha^{op*}}(f')f''\infty'\varepsilon_{H_\beta}(x')x''=f\infty' x$. Similarly, $(1\otimes\varepsilon)\Delta(f\infty' x)=f\infty' x$. Hence, $(\varepsilon\otimes 1)\Delta=(1\otimes\varepsilon)\Delta=\mathrm{id}$. Therefore, $D'(H)$ becomes a coalgebra on Δ and ε.

For any $a\in B_{\alpha_1}$, $b\in B_{\alpha_2}$, $x\in B_{\beta_1}$, $y\in B_{\beta_2}$,

(a) Δ is an algebra homomorphism,

$$\Delta((\phi_a\infty' x)(\phi_b\infty' y))=\Delta(\phi_a\phi_b(1_{H_{\beta_1}}?)\infty' xy)=\begin{cases}0 & \text{if } \beta_1\alpha_1\neq\alpha_2\\ \Delta(\phi_a\phi_b(1_{H_{\beta_1}}?)\infty' xy) & \text{if } \beta_1\alpha_1=\alpha_2\end{cases}$$

$$=\begin{cases}0 & \text{if } \beta_1\alpha_1\neq\alpha_2\\ \sum((\phi_a\phi_b(1_{H_{\beta_1}}?))'\infty' x'y')\otimes((\phi_a\phi_b(1_{H_{\beta_1}}?))''\infty' x''y'') & \text{if } \beta_1\alpha_1=\alpha_2,\end{cases}$$

$$\Delta(\phi_a\infty' x)\Delta(\phi_b\infty' y)=\Big(\sum_{(\phi_a),(x)}(\phi_a'\infty' x')\otimes(\phi_a''\infty' x'')\Big)\Big(\sum_{(\phi_b),(y)}(\phi_b'\infty' y')\otimes(\phi_b''\infty' y'')\Big)$$
$$=\sum_{(\phi_a),(\phi_b),(x),(y)}(\phi_a'\infty' x')(\phi_b'\infty' y')\otimes(\phi_a''\infty' x'')(\phi_b''\infty' y'')$$
$$=\sum_{(\phi_a),(\phi_b),(x),(y)}(\phi_a'\phi_b'(1_{H_{\beta_1}}?)\infty' x'y')\otimes(\phi_a''\phi_b''(1_{H_{\beta_1}}?)\infty' x''y'')$$
$$=\begin{cases}0 & \text{if } \beta_1\alpha_1\neq\alpha_2\\ \displaystyle\sum_{(\phi_a),(\phi_b),(x),(y)}(\phi_a'\phi_b'(1_{H_{\beta_1}}?)\infty' x'y')\otimes(\phi_a''\phi_b''(1_{H_{\beta_1}}?)\infty' x''y'') & \text{if } \beta_1\alpha_1=\alpha_2.\end{cases}$$

For any $u, v\in H^*$, $s, t\in B_{\alpha_1}$,

$$\Delta((\phi_a\infty' x)(\phi_b\infty' y))(s\otimes u\otimes t\otimes v)$$
$$=\begin{cases}0 & \text{if } \beta_1\alpha_1\neq\alpha_2\\ \sum(\phi_a\phi_b(1_{H_{\beta_1}}?))'(s)u(x'y')(\phi_a\phi_b(1_{H_{\beta_1}}?))''(t)v(x''y'') & \text{if } \beta_1\alpha_1=\alpha_2\end{cases}$$
$$=\begin{cases}0 & \text{if } \beta_1\alpha_1\neq\alpha_2\\ \sum(\phi_a\phi_b(1_{H_{\beta_1}}?))(st)u(x'y')v(x''y'') & \text{if } \beta_1\alpha_1=\alpha_2\end{cases}$$

$$=\begin{cases}0 & \text{if } \beta_1\alpha_1\neq\alpha_2\\ \displaystyle\sum_{(st)}\phi_a(s't')\phi_b(1_{H_{\beta_1}}s''t'')u(x'y')v(x''y'') & \text{if } \beta_1\alpha_1=\alpha_2,\end{cases}$$

$$\Delta(\phi_a\infty' x)\Delta(\phi_b\infty' y)(s\otimes u\otimes t\otimes v)$$
$$=\begin{cases}0 & \text{if } \beta_1\alpha_1\neq\alpha_2\\ \displaystyle\sum_{(s),(t)}\phi_a'(s')\phi_b'(1_{H_{\beta_1}}s'')u(x'y')\phi_a''(t')\phi_b''(1_{H_{\beta_1}}t'')v(x''y'') & \text{if } \beta_1\alpha_1=\alpha_2\end{cases}$$
$$=\begin{cases}0 & \text{if } \beta_1\alpha_1\neq\alpha_2\\ \displaystyle\sum_{(s),(t)}\phi_a(s't')\phi_b(1_{H_{\beta_1}}s''1_{H_{\beta_1}}t'')u(x'y')v(x''y'') & \text{if } \beta_1\alpha_1=\alpha_2\end{cases}$$
$$=\begin{cases}0 & \text{if } \beta_1\alpha_1\neq\alpha_2\\ \displaystyle\sum_{(s),(t)}\phi_a(s't')\phi_b(1_{H_{\beta_1}}s''t'')u(x'y')v(x''y'') & \text{if } \beta_1\alpha_1=\alpha_2.\end{cases}$$

Thus, we have $\Delta((\phi_a\infty' x)(\phi_b\infty' y))(s\otimes u\otimes t\otimes v)=\Delta(\phi_a\infty' x)\Delta(\phi_b\infty' y)(s\otimes u\otimes t\otimes v)$ for any $u, v\in H^*$, $s, t\in B_{\alpha_1}$. It implies

$$\Delta((\phi_a\infty' x)(\phi_b\infty' y))=\Delta(\phi_a\infty' x)\Delta(\phi_b\infty' y).$$

(b) ε is not an algebra homomorphism,

$$\varepsilon((\phi_a\infty' x)(\phi_b\infty' y))=\varepsilon(\phi_a\phi_b(1_{H_{\beta_1}}?)\infty' xy)$$
$$=\begin{cases}0 & \text{if } \beta_1\alpha_1\neq\alpha_2\\ \varepsilon_{H^*_{\alpha_1}}(\phi_a)\varepsilon_{H^*_{\alpha_1}}(\phi_b(1_{H_{\beta_1}}?))\varepsilon_{H_{\beta_1\beta_2}}(xy) & \text{if } \beta_1\alpha_1=\alpha_2\end{cases}$$
$$=\begin{cases}0 & \text{if } \beta_1\alpha_1\neq\alpha_2\\ \phi_a(1_{H_{\alpha_1}})\phi_b(1_{H_{\beta_1}}1_{H_{\alpha_1}})\varepsilon_{H_{\beta_1\beta_2}}(xy) & \text{if } \beta_1\alpha_1=\alpha_2\end{cases}$$

$$= \begin{cases} 0 & \text{if } \beta_1\alpha_1 \neq \alpha_2 \\ \delta_{a,1_{H_{\alpha_1}}}\delta_{b,1_{H_{\alpha_2}}}\varepsilon_{H_{\beta_1\beta_2}}(xy) & \text{if } \beta_1\alpha_1 = \alpha_2, \end{cases}$$

$$\varepsilon(\phi_a \infty' x)\varepsilon(\phi_b \infty' y) = \varepsilon_{H^*_{\alpha_1}}(\phi_a)\varepsilon_{H_{\beta_1}}(x)\varepsilon_{H^*_{\alpha_2}}(\phi_b)\varepsilon_{H_{\beta_2}}(y) = \delta_{a,1_{H_{\alpha_1}}}\delta_{b,1_{H_{\alpha_2}}}\varepsilon_{H_{\beta_1}}(x)\varepsilon_{H_{\beta_2}}(y).$$

So, in the usual, $\varepsilon((\phi_a \infty' x)(\phi_b \infty' y)) \neq \varepsilon(\phi_a \infty' x)\varepsilon(\phi_b \infty' y)$, hence the counit ε is not an algebra homomorphism.

It implies, in general, $D'(H)$ is only an almost bialgebra but not a bialgebra.

(2) Next, we can find a regular R-matrix $R=\Sigma_{\alpha\in Y}\Sigma_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})$ (i.e., there exists a $\bar{R}$ such that $\bar{R}R\bar{R}=\bar{R}$ and $R\bar{R}R=R$) which is a nontrival solution of the Yang-Baxter equation [i.e., not the identity of $(H^{op^*}\infty' H)\otimes(H^{op^*}\infty' H)$]. This is the reason we say $D'(H)$ directly as the so-called quantum G-double.

Since

$$R_{12} = \sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})\otimes(\varepsilon_H\infty' 1_H),$$

$$R_{13} = \sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\varepsilon_H\infty' 1_H)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha}),$$

$$R_{23} = \sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_H\infty' 1_H)\otimes(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha}),$$

and

$$\begin{aligned} R_{12}R_{13} &= \Big(\sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})\otimes(\varepsilon_H\infty' 1_H)\Big)\Big(\sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha) \\ &\quad \otimes(\varepsilon_H\infty' 1_H)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})\Big) \\ &= \sum_{\alpha,\beta\in Y}\sum_{a_\alpha\in B_\alpha, b_\beta\in B_\beta}(\varepsilon_{H_\alpha}\infty' a_\alpha)(\varepsilon_{H_\beta}\infty' b\beta)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})(\varepsilon_H\infty' 1_H)\otimes(\varepsilon_H\infty' 1_H)(\phi_{b_\beta}\infty' 1_{H_\beta}) \\ &= \sum_{\alpha,\beta\in Y}\sum_{a_\alpha\in B_\alpha, b_\beta\in B_\beta}(\varepsilon_{H_\alpha}\varepsilon_{H_\beta}(1_{H_\alpha}?)\infty' a_\alpha b_\beta) \\ &\quad \otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})\otimes(\phi_{b_\beta}\infty' 1_{H_\beta}). \end{aligned}$$

From the definition we know that $\varepsilon_{H_\alpha}\varepsilon_{H_\beta}(1_{H_\alpha}?)=0$ if $\alpha\neq\beta$, hence

$$\varepsilon_{H_\alpha}\varepsilon_{H_\beta}(1_{H_\alpha}?)\infty' a_\alpha b_\beta = \begin{cases} 0 & \text{if } \alpha\neq\beta, \\ \varepsilon_{H_\alpha}\infty' a_\alpha b_\alpha & \text{if } \alpha=\beta. \end{cases}$$

Then

$$R_{12}R_{13} = \sum_{\alpha\in Y}\sum_{a_\alpha, b_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha b_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})\otimes(\phi_{b_\alpha}\infty' 1_{H_\alpha}),$$

$$
\begin{aligned}
R_{12}R_{13}R_{23} &= \Bigg(\sum_{\alpha\in Y}\sum_{a_\alpha,b_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha b_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})\otimes(\phi_{b_\alpha}\infty' 1_{H_\alpha})\Bigg)\Bigg(\sum_{\alpha\in Y}\sum_{c_\alpha\in B_\alpha}(\varepsilon_H\infty' 1_H)\\
&\quad\otimes(\varepsilon_{H_\alpha}\infty' c_\alpha)\otimes(\phi_{c_\alpha}\infty' 1_{H_\alpha})\Bigg)\\
&= \sum_{\alpha,\beta\in Y}\sum_{a_\alpha,b_\alpha\in B_\alpha,c_\beta\in B_\beta}(\varepsilon_{H_\alpha}\infty' a_\alpha b_\alpha)(\varepsilon_H\infty' 1_H)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})(\varepsilon_{H_\beta}\infty' c_\beta)\\
&\quad\otimes(\phi_{b_\alpha}\infty' 1_{H_\alpha})(\phi_{c_\beta}\infty' 1_{H_\beta})\\
&= \sum_{\alpha,\beta\in Y}\sum_{a_\alpha,b_\alpha\in B_\alpha,c_\beta\in B_\beta}(\varepsilon_{H_\alpha}\infty' a_\alpha b_\alpha)\otimes(\phi_{a_\alpha}\varepsilon_{H_\beta}(1_{H_\alpha}?)\infty' c_\beta)\\
&\quad\otimes(\phi_{b_\alpha}\phi_{c_\beta}(1_{H_\alpha}?)\infty' 1_{H_\alpha}1_{H_\beta})\\
&= \sum_{\alpha\in Y}\sum_{a_\alpha,b_\alpha,c_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha b_\alpha)\otimes(\phi_{a_\alpha}\infty' c_\alpha)\otimes(\phi_{b_\alpha}\phi_{c_\alpha}\infty' 1_{H_\alpha}).
\end{aligned}
$$

Similarly, we can get

$$
R_{23}R_{13}R_{12} = \sum_{\alpha\in Y}\sum_{c_\alpha,b_\alpha,a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' b_\alpha a_\alpha)\otimes(\phi_{a_\alpha}\infty' c_\alpha)\otimes(\phi_{c_\alpha}\phi_{b_\alpha}\infty' 1_{H_\alpha}).
$$

Since H is commutative and the random choosing of a_α, b_α, c_α, we can conclude that $R_{12}R_{13}R_{23}=R_{23}R_{13}R_{12}$. This shows that R is a nontrivial solution of Yang-Baxter equation.

It can be proved that R is regular with the regular inverse $\bar{R}=\Sigma_{\alpha\in Y}\Sigma_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes((\phi_{a_\alpha}\circ T)\otimes 1_{H_\alpha})$. In fact, since

$$
\begin{aligned}
R\bar{R} &= \Bigg(\sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})\Bigg)\Bigg(\sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes((\phi_{a_\alpha}\circ T)\infty' 1_{H_\alpha})\Bigg)\\
&= \sum_{\alpha,\beta\in Y}\sum_{a_\alpha\in B_\alpha,b_\beta\in B_\beta}(\varepsilon_{H_\alpha}\infty' a_\alpha)(\varepsilon_{H_\beta}\infty' b_\beta)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})((\phi_{b_\beta}\circ T)\infty' 1_{H_\beta})\\
&= \sum_{\alpha,\beta\in Y}\sum_{a_\alpha\in B_\alpha,b_\beta\in B_\beta}(\varepsilon_{H_\alpha}\varepsilon_{H_\beta}(1_{H_\alpha}?)\infty' a_\alpha b_\beta)\otimes(\phi_{a_\alpha}(\phi_{b_\beta}\circ T)(1_{H_\alpha}?)\infty' 1_{H_\alpha}1_{H_\beta})\\
&= \sum_{\alpha\in Y}\sum_{a_\alpha,b_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha b_\alpha)\otimes(\phi_{a_\alpha}(\phi_{b_\alpha}\circ T)\infty' 1_{H_\alpha}).
\end{aligned}
$$

Consider an element $\xi=b\otimes u\otimes c\otimes v$ with b, $c\in H$ and u, $v\in H^*$. Since $\varepsilon_{H_\alpha}(H_\beta)=0$ if $\alpha\neq\beta$, we can suppose that b, $c\in H_\alpha$ for some $\alpha\in Y$. So,

$$
\begin{aligned}
\langle R\bar{R},\xi\rangle &= \sum_{\alpha\in Y}\sum_{a_\alpha,b_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha b_\alpha)\otimes(\phi_{a_\alpha}(\phi_{b_\alpha}\circ T)\infty' 1_{H_\alpha})(b\otimes u\otimes c\otimes v)\\
&= \sum_{\alpha\in Y}\sum_{a_\alpha,b_\alpha\in B_\alpha}\varepsilon_{H_\alpha}(b)u(a_\alpha b_\alpha)\sum_{(c)}\phi_{a_\alpha}(c')(\phi_{b_\alpha}\circ T)(c'')v(1_{H_\alpha})\\
&= \varepsilon_{H_\alpha}(b)v(1_{H_\alpha})\sum_{\alpha\in Y}\sum_{a_\alpha,b_\alpha\in B_\alpha}\sum_{(c)}u(a_\alpha b_\alpha)\phi_{a_\alpha}(c')\phi_{b_\alpha}(T(c''))\\
&= \varepsilon_{H_\alpha}(b)v(1_{H_\alpha})\sum_{(c)}u\Bigg(\sum_{a_\alpha\in B_\alpha}\phi_{a_\alpha}(c')a_\alpha\Bigg)u\Bigg(\sum_{b_\alpha\in B_\alpha}\phi_{b_\alpha}(T(c''))b_\alpha\Bigg)\Bigg(\sum_{a_\alpha\in B_\alpha}\phi_{a_\alpha}(x)a_\alpha = x\Bigg)\\
&= \varepsilon_{H_\alpha}(b)v(1_{H_\alpha})\sum_{(c)}u(c')u(T(c'')) = \varepsilon_{H_\alpha}(b)v(1_{H_\alpha})u(c'T(c'')) = \varepsilon_{H_\alpha}(b)v(1_{H_\alpha})u(\varepsilon_{H_\alpha}(c)1_{H_\alpha})\\
&= \varepsilon_{H_\alpha}(b)v(1_{H_\alpha})\varepsilon_{H_\alpha}(c)u(1_{H_\alpha}) = ((\varepsilon_{H_\alpha}\infty' 1_{H_\alpha})\otimes(\varepsilon_{H_\alpha}\infty' 1_{H_\alpha}))(b\otimes u\otimes c\otimes v).
\end{aligned}
$$

From random of choice of α, we can get $R\bar{R}=\Sigma_{\alpha\in Y}(\varepsilon_{H_\alpha}\infty' 1_{H_\alpha})\otimes(\varepsilon_{H_\alpha}\infty' 1_{H_\alpha})$. Hence,

$$
\begin{aligned}
R\bar{R}R &= \left(\sum_{\alpha\in Y}(\varepsilon_{H_\alpha}\infty' 1_{H_\alpha})\otimes(\varepsilon_{H_\alpha}\infty' 1_{H_\alpha})\right)\left(\sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})\right)\\
&= \sum_{\alpha,\beta\in Y}\sum_{a_\beta\in B_\beta}(\varepsilon_{H_\alpha}\infty' 1_{H_\alpha})(\varepsilon_{H_\beta}\otimes a_\beta)\otimes(\varepsilon_{H_\alpha}\infty' 1_{H_\alpha})(\phi_{a_\beta}\infty' 1_{H_\beta})\\
&= \sum_{\alpha,\beta\in Y}\sum_{a_\beta\in B_\beta}(\varepsilon_{H_\alpha}\varepsilon_{H_\beta}(1_{H_\alpha}?)\infty' 1_{H_\alpha}a_\beta)\otimes(\varepsilon_{H_\alpha}\phi_{a_\beta}(1_{H_\alpha}?)\infty' 1_{H_\alpha}1_{H_\beta})\\
&= \sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\infty'(\varepsilon_{H_\alpha}\phi_{a_\alpha}\infty' 1_{H_\alpha}) = \sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha}) = R.
\end{aligned}
$$

Similarly, we can prove that $\bar{R}R\bar{R}=\bar{R}$. So $\bar{R}$ is a regular inverse of R.

It can be proved that R satisfies $(\Delta\otimes \mathrm{id}_H)(R)=R_{13}R_{23}$ and $(\mathrm{id}_H\otimes\Delta)(R)=R_{13}R_{12}$ as follows:

$$
\begin{aligned}
(\Delta\otimes \mathrm{id}_H)(R) &= (\Delta\otimes \mathrm{id}_H)\left(\sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})\right)\\
&= \sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}\sum_{(a_\alpha)}(\varepsilon_{H_\alpha}\infty' a'_\alpha)\otimes(\varepsilon_{H_\alpha}\infty' a''_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha}),
\end{aligned}
$$

$$
\begin{aligned}
R_{13}R_{23} &= \left(\sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\varepsilon_H\infty' 1_H)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})\right)\\
&\quad\times\left(\sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_H\infty' 1_H)\otimes(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})\right)\\
&= \sum_{\alpha,\beta\in Y}\sum_{a_\alpha\in B_\alpha, b_\beta\in B_\beta}(\varepsilon_{H_\alpha}\infty' a_\alpha)(\varepsilon_H\infty' 1_H)\otimes(\varepsilon_H\infty' 1_H)(\varepsilon_{H_\beta}\infty' b_\beta)\otimes(\phi_{a_\alpha}\infty 1_{H_\alpha})(\phi_{b_\beta}\infty' 1_{H_\beta})\\
&= \sum_{\alpha,\beta\in Y}\sum_{a_\alpha\in B_\alpha, b_\beta\in B_\beta}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\varepsilon_{H_\beta}\infty' b_\beta)\otimes(\phi_{a_\alpha}\phi_{b_\beta}(1_{H_\alpha}?)\infty' 1_{H_\alpha}1_{H_\beta})\\
&= \sum_{\alpha\in Y}\sum_{a_\alpha, b_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\varepsilon_{H_\alpha}\infty' b_\alpha)\otimes(\phi_{a_\alpha}\phi_{b_\alpha}\infty' 1_{H_\alpha})
\end{aligned}
$$

since $\phi_{a_\alpha}\phi_{b_\beta}(1_{H_\alpha}?)=0$ if $\alpha\neq\beta$.

For some $a\otimes t\otimes b\otimes u\otimes c\otimes v=\theta$, if $a\notin H_\alpha$, then $\varepsilon_{H_\alpha}(a)=0$, similarly discussed we can suppose that there exists a $a\in Y$ such that a, b, $c\in H_\alpha$, and t, u, $v\in H^*$. Then

$$
\begin{aligned}
\langle(\Delta\otimes \mathrm{id}_H)(R),\theta\rangle &= \sum_{a_\alpha\in B_\alpha}\sum_{(a_\alpha)}\varepsilon_{H_\alpha}(a)\varepsilon_{H_\alpha}(b)\phi_{a_\alpha}(c)t(a'_\alpha)u(a''_\alpha)v(1_{H_\alpha})\\
&= \varepsilon_{H_\alpha}(a)\varepsilon_{H_\alpha}(b)v(1_{H_\alpha})\sum_{a_\alpha\in B_\alpha}\sum_{(a_\alpha)}\phi_{a_\alpha}(c)t(a'_\alpha)u(a''_\alpha)\\
&\quad\left(\text{since } a=\sum_{a_\alpha\in B_\alpha}\phi_{a_\alpha}(a)a_\alpha,\ \Delta(a)=\sum_{(a)}a'\otimes a''=\sum_{a_\alpha\in B_\alpha}\phi_{a_\alpha}(a)a'_\alpha\otimes a''_\alpha\right)\\
&= \varepsilon_{H_\alpha}(a)\varepsilon_{H_\alpha}(b)v(1_{H_\alpha})\sum_{(c)}t(c')u(c'') = \varepsilon_{H_\alpha}(a)\varepsilon_{H_\alpha}(b)v(1_{H_\alpha})uv(c),
\end{aligned}
$$

$$
\begin{aligned}
\langle R_{13}R_{23},\theta\rangle &= \sum_{a_\alpha, b_\alpha\in B_\alpha}\varepsilon_{H_\alpha}(a)\varepsilon_{H_\alpha}(b)v(1_{H_\alpha})t(a_\alpha)u_{b_\alpha}\phi_{a_\alpha}\phi_{b_\alpha}(c)\\
&= \varepsilon_{H_\alpha}(a)\varepsilon_{H_\alpha}(b)v(1_{H_\alpha})\sum_{(c)}t\left(\sum_{a_\alpha\in B_\alpha}\phi_{a_\alpha}(c')a_\alpha\right)u\left(\sum_{b_\alpha\in B_\alpha}\phi_{b_\alpha}(c'')b_\alpha\right)\\
&= \varepsilon_{H_\alpha}(a)\varepsilon_{H_\alpha}(b)v(1_{H_\alpha})\sum_{(c)}t(c')u(c'') = \varepsilon_{H_\alpha}(a)\varepsilon_{H_\alpha}(b)v(1_{H_\alpha})uv(c).
\end{aligned}
$$

From the random choice of α, we can conclude that $(\Delta\otimes \mathrm{id}_H)(R)=R_{13}R_{23}$. Similarly, we can prove that $(\mathrm{id}_H\otimes\Delta(R))=R_{13}R_{12}$.

Now, we explain that R usually does not satisfy $\Delta^{op}(h)R=R\Delta(h)$ for any $h\in D'(H)$, that is, $D'(H)$ is not almost cocommutative in general.

For any $a\in B_\beta$, $x\in B_\gamma$, we have

$$\begin{aligned}\Delta^{op}(\phi_a\infty' x)R &= \left(\sum_{(\phi_a),(x)}(\phi_a''\infty' x'')\otimes(\phi_a'\infty x')\right)\left(\sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})\right)\\ &= \sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}\sum_{(\phi_a),(x)}(\phi_a''\infty' x'')(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_a'\infty' x')(\phi_{a_\alpha}\infty' 1_{H_\alpha})\\ &= \sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}\sum_{(\phi_a),(x)}(\phi_a''\varepsilon_{H_\alpha}(1_{H_\gamma}?)\infty' x''a_\alpha)\otimes(\phi_a'\phi_{a_\alpha}(1_{H_\gamma}?)\infty' x'1_{H_\alpha})\\ &= \sum_{a_\alpha\in B_\alpha}\sum_{(\phi_a),(x)}(\phi_a''\varepsilon_{H_\alpha}(1_{H_\gamma}?)\infty' x''a_\alpha)\otimes(\phi_a'\phi_{a_\alpha}(1_{H_\gamma}?)\infty' x'1_{H_\alpha})\quad(\text{when }\alpha=\beta\gamma),\end{aligned}$$

$$\begin{aligned}R\Delta(\phi_a\infty' x) &= \left(\sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})\right)\left(\sum_{(\phi_a),(x)}(\phi_a'\infty' x')\otimes(\phi_a''\infty x'')\right)\\ &= \sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}\sum_{(\phi_a),(x)}(\varepsilon_{H_\alpha}\infty' a_\alpha)(\phi_a'\infty' x')\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})(\phi_a''\infty' x'')\\ &= \sum_{\alpha\in Y}\sum_{a_\alpha\in B_\alpha}\sum_{(\phi_a),(x)}(\varepsilon_{H_\alpha}\phi_a'(1_{H_\alpha}?)\infty' a_\alpha x')\otimes(\phi_{a_\alpha}\phi_a''(1_{H_\alpha}?)\infty' 1_{H_\alpha}x'')\\ &= \sum_{a_\alpha\in B_\alpha}\sum_{(\phi_a),(x)}(\phi_a'\infty' a_\alpha x')\otimes(\phi_{a_\alpha}\phi_a''\infty' 1_{H_\alpha}x'')\quad(\text{when }\alpha=\beta).\end{aligned}$$

Then, for some $\xi=b\otimes u\otimes c\otimes v$, with b, $c\in H_\beta$ and u, $v\in H^*$, we can get

$$\begin{aligned}\langle\Delta^{op}(\phi_a\infty' x)R,\xi\rangle &= \sum_{a_\alpha\in B_\alpha}\sum_{(\phi_a),(x)}\sum_{(b),(c)}\phi_a''(b')\varepsilon_{H_\alpha}(1_{H_\gamma}b'')u(x''a_\alpha)\phi_a'(c')\phi_{a_\alpha}(c'')v(x'1_{H_\alpha})\\ &= \sum_{a_\alpha\in B_\alpha}\sum_{(x)}\sum_{(b),(c)}\phi_a(b'c')\varepsilon_{H_\alpha}(b''\varphi_{\beta,\alpha}1_{H_\gamma}\varphi_{\gamma,\alpha})u(x''a_\alpha)\phi_{a_\alpha}(1_{H_\gamma}c'')v(x'1_{H_\alpha})\\ &= \sum_{a_\alpha\in B_\alpha}\sum_{(x)}\sum_{(b),(c)}\phi_a(b'c')\varepsilon_{H_\beta}(b'')\varepsilon_{H_\gamma}(1_{H_\gamma})u(x''a_\alpha)\phi_{a_\alpha}(1_{H_\gamma}c'')v(x'1_{H_\alpha})\\ &= \sum_{(x)}\sum_{(b),(c)}\phi_a(b'\varepsilon_{H_\beta}(b'')c')u\left(x''\sum_{a_\alpha\in B_\alpha}\phi_{a_\alpha}(1_{H_\gamma}c'')a_\alpha\right)v(x'1_{H_\alpha})\\ &= \sum_{(x)}\sum_{(c)}\phi_a(bc')u(x''1_{H_\gamma}c'')v(x'1_{H_\alpha})=\sum_{(x)}\sum_{(c)}\phi_a(bc')u(x''c'')v(x'1_{H_\alpha}),\end{aligned}$$

$$\begin{aligned}\langle R\Delta(\phi_a\infty' x),\xi\rangle &= \sum_{a_\alpha\in B_\alpha}\sum_{(\phi_a),(x)}\sum_{(c)}\phi_a'(b)u(a_\alpha x')\phi_{a_\alpha}(c')\phi_a''(c'')v(x''1_{H_\alpha})\\ &= \sum_{(x)}\sum_{(c)}\phi_a(bc')u\left(\sum_{a_\alpha\in B_\alpha}\phi_{a_\alpha}(c')a_\alpha x'\right)v(x''1_{H_\alpha})=\sum_{(x)}\sum_{(c)}\phi_a(bc')u(c'x')v(x''1_{H_\alpha}).\end{aligned}$$

From the above equation, we can see that in general $\Delta^{op}(\phi_a\infty' x)R\neq R\Delta(\phi_a\infty' x)$ unless H is cocommutative.

Remark: The R-matrix can be decomposed as $R=\Sigma_{\alpha\in Y}\Sigma_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})=\Sigma_{\alpha\in Y}R_\alpha$, where $R_\alpha=\Sigma_{a_\alpha\in B_\alpha}(\varepsilon_{H_\alpha}\infty' a_\alpha)\otimes(\phi_{a_\alpha}\infty' 1_{H_\alpha})$ is the R-matrix for the classical quantum double $D(H_\alpha)$ for every $\alpha\in Y$. Moreover, for any α, $\beta\in Y$,

$$
\begin{aligned}
R_\alpha R_\beta &= \left(\sum_{a_\alpha \in B_\alpha} (\varepsilon_{H_\alpha} \infty' a_\alpha) \otimes (\phi_{a_\alpha} \infty' 1_{H_\alpha})\right)\left(\sum_{a_\beta \in B_\beta} (\varepsilon_{H_\beta} \infty' a_\beta) \otimes (\phi_{a_\beta} \infty' 1_{H_\beta})\right) \\
&= \sum_{a_\alpha \in B_\alpha, b_\beta \in B_\beta} ((\varepsilon_{H_\alpha} \infty' a_\alpha)(\varepsilon_{H_\beta} \infty' b_\beta)) \otimes ((\phi_{a_\alpha} \infty' 1_{H_\alpha})(\phi_{b_\beta} \infty' 1_{H_\beta})) \\
&= \sum_{a_\alpha \in B_\alpha, b_\beta \in B_\beta} (\varepsilon_{H_\alpha} \varepsilon_{H_\beta} (1_{H_\alpha} ?) \infty' a_\alpha b_\beta) \otimes (\phi_{a_\alpha} \phi_{b_\beta} (1_{H_\alpha} ?) \infty' 1_{H_\alpha} 1_{H_\beta}) \\
&= \begin{cases} 0 & \text{if } \alpha \neq \beta, \\ \displaystyle\sum_{a_\alpha, b_\alpha \in B_\alpha} (\varepsilon_{H_\alpha} \infty' a_\alpha b_\alpha) \otimes (\phi_{a_\alpha} \phi_{b_\alpha} \infty' 1_{H_\alpha}) & \text{if } \alpha = \beta, \end{cases}
\end{aligned}
$$

which usually is not equal to $R_{\alpha\beta}$.

This implies that $R = \Sigma_{\alpha \in Y} R_\alpha$ does not have the graded structure.

III. STRUCTURE OF QUANTUM G-DOUBLE

In this section, we discuss the structure of $D'(H)$ depending upon $D'(H_\alpha)(\alpha \in Y)$ and then obtain the structure theorem.

First, for α_1, α_2, β_1, $\beta_2 \in Y$, we consider the multiplication between $D'(H_{\alpha_1}, H_{\beta_1})$ and $D'(H_{\alpha_2}, H_{\beta_2})$. For $x \in B_{\beta_1}$, $y \in B_{\beta_2}$, $a \in B_{\alpha_1}$ and its duality ϕ_a in $H_{\alpha_1}^{op^*}$, $b \in B_{\alpha_2}$ and its duality ϕ_b in $H_{\alpha_2}^{op^*}$, from definition we have

$$
(\phi_a \infty x)(\phi_b \infty y) = \phi_a \phi_b (1_{H_{\beta_1}} ?) \infty xy = \begin{cases} 0 & \text{if } \beta_1 \alpha_1 \neq \alpha_2, \\ \phi_a \phi_b (1_{H_{\beta_1}} ?) & \text{if } \beta_1 \alpha_1 = \alpha_2, \end{cases}
$$

hence, $\phi_a \phi_b (1_{H_{B_1}} ?)$ is always in $H_{\alpha_1}^{op^*}$. And, $xy \in H_{\beta_1 \beta_2}$. Therefore, $(\phi_a \infty' x) \times (\phi_b \infty' y) \in H_{\alpha_1}^{op^*} \infty' H_{\beta_1 \beta_2}$. Since $\{\phi_a : a \in B_{\alpha_1}\}$ and $\{\phi_b : b \in B_{\alpha_2}\}$ are, respectively, a basis of $H_{\alpha_1}^{op^*}$ and $H_{\alpha_2}^{op^*}$, we get that

$$
(H_{\alpha_1}^{op^*} \infty' H_{\beta_1})(H_{\alpha_2}^{op^*} \infty' H_{\beta_2}) \subseteq H_{\alpha_1}^{op^*} \infty' H_{\beta_1 \beta_2},
$$

that is,

$$
D'(H_{\alpha_1}, H_{\beta_1}) D'(H_{\alpha_2}, H_{\beta_2}) \subseteq D'(H_{\alpha_1}, H_{\beta_1 \beta_2}); \tag{3.1}
$$

and, if and only if $\alpha_2 \not\leq \alpha_1$ or $\alpha_2 \not\leq \beta_1$, the following holds:

$$
D'(H_{\alpha_1}, H_{\beta_1}) D'(H_{\alpha_2}, H_{\beta_2}) = 0, \tag{3.2}
$$

since in this case, $1_{H_{\beta_1}} a \notin H_{\alpha_2}$; then always $1_{H_{\beta_1}} a \neq b$.

In (3.1), let $\alpha_1 = \alpha_2 = \alpha$, then

$$
D'(H_\alpha, H_{\beta_1}) D'(H_\alpha, H_{\beta_2}) \subseteq D'(H_\alpha, H_{\beta_1 \beta_2}). \tag{3.3}
$$

We call $D'(H_\alpha, H_\beta)$ the *bicrossed G-product* of two subweak Hopf algebras H_α and H_β which are included in $H = \oplus_{\alpha \in Y} H_\alpha$; $Q_H(H_\alpha)$ the *bicrossed G-product* of H and its subweak Hopf algebra H_α. Denote $D'(H_\alpha, H_\beta) = H_\alpha^{op^*} \infty' H_\beta$; $Q_H(H_\alpha) = H_\alpha^{op^*} \infty' H$.

First, we need the following lemmas on $D'(H_\alpha, H_\beta)$ and $Q_H(H_\alpha)$.

Lemma III.1: For all α, $\beta \in Y$, $D'(H_\alpha, H_\beta)$ are coalgebras and subrings of $D'(H)$. For any $\alpha \not\leq \beta$, $D'(H_\alpha, H_\beta)$ is a null subring. For any $\alpha \leqslant \beta$, $D'(H_\alpha, H_\beta)$ is a bialgebra under the same multiplication.

Proof: For $f \in H_\alpha^{op^*}$ and $x \in H_\beta$,

(i) define Δ, $D'(H_\alpha, H_\beta) \to D'(H_\alpha, H_\beta) \otimes D'(H_\alpha, H_\beta)$ satisfying $\Delta(f \infty' x) = \Sigma_{(f)(x)} (f' \infty' x') \otimes (f'' \infty' x'')$, where $\Delta(f) = \Sigma_{(f)} f' \otimes f''$ according to the comultiplication of $H_\alpha^{op^*}$.

(ii) Define ε, $D'(H_\alpha,H_\beta)\to k$ satisfying $\varepsilon(f\infty' x)=\varepsilon_{H_\alpha^{op*}}(f)\varepsilon_{H_\beta}(x)$.

From the discussion of Theorem II.2 we know $D'(H_\alpha,H_\beta)$ becomes a coalgebra on Δ and ε.

The multiplication of $D'(H_\alpha,H_\beta)$ is given as that of $D'(H)$, that is, for $\alpha,\beta\in Y$, $a,b\in B_\alpha$, and $x,y\in B_\beta$,

$$(\phi_a\infty' x)(\phi_b\infty' y)=\phi_a\phi_b(1_{H_\beta}{}^?)\infty' xy=\begin{cases}0 & \text{if } \beta\alpha\neq\alpha,\\ \phi_a\phi_b(1_{H_\beta}{}^?)\infty' xy & \text{if } \beta\alpha=\alpha.\end{cases}$$

In (3.3), let $\beta_1=\beta_2=\beta$, then $D'(H_\alpha,H_\beta)D'(H_\alpha,H_\beta)\subseteq D'(H_\alpha,H_\beta)$ since $\beta\beta=\beta$. Then, every $D'(H_\alpha,H_\beta)$ is a subring of $D'(H)$.

By (3.2), when and only when $\alpha\not\leqslant\beta$, $D'(H_\alpha,H_\beta)D'(H_\alpha,H_\beta)=0$. Hence, in this case, $D'(H_\alpha,H_\beta)$ is a null subring.

Now, suppose that $\alpha\leqslant\beta$. $D'(H_\alpha,H_\beta)$ possesses the identity $\varepsilon_{H_\alpha}\infty' 1_{H_\beta}$ since for any $a\in B_\alpha$, $x\in B_\beta$, $(\phi_a\infty' x)(\varepsilon_{H_\alpha}\infty' 1_{H_\beta})=\phi_a\varepsilon_{H_\alpha}(1_{H_\beta}{}^?)\infty' x1_{H_\beta}=\phi_a\varepsilon_{H_\alpha}(1_{H_\beta}{}^?)\infty' x$, and $(\varepsilon_{H_\alpha}\infty' 1_{H_\beta})(\phi_a\infty' x)=\varepsilon_{H_\alpha}\phi_a(1_{H_\beta}{}^?)\infty' x$ since $\alpha\leqslant\beta$, that is $\beta\alpha=\alpha$, hence, for any $b\in H_\alpha$, $u\in H^*$, we have

$$\begin{aligned}((\phi_a\infty' x)(\varepsilon_{H_\alpha}\infty' 1_{H_\beta}))(b\otimes u)&=\sum_{(b)}\phi_a(b')\varepsilon_{H_\alpha}(1_{H_\beta}b'')u(x)=\sum_{(b)}\phi_a(b')\varepsilon_{H_\alpha}(\varphi_{\beta,\alpha}(1_{H_\beta})\varphi_{\alpha,\alpha}(b''))u(x)\\&=\sum_{(b)}\phi_a(b')\varepsilon_{H_\alpha}\varphi_{\beta,\alpha}(1_{H_\beta})\varepsilon_{H_\alpha}(b'')u(x)\\&=\sum_{(b)}\phi_a(b'\varepsilon_{H_\alpha}(b''))\varepsilon_{H_\beta}(1_{H_\beta})u(x)=\phi_a(b)u(x)=(\phi_a\infty' x)(b\otimes u)\end{aligned}$$

and

$$\begin{aligned}((\varepsilon_{H_\alpha}\infty' 1_{H_\beta})(\phi_a\infty' x))(b\otimes u)&=\sum_{(b)}\varepsilon_{H_\alpha}(b')\phi_a(1_{H_\beta}b'')u(x)=\sum_{(b)}\phi_a(1_{H_\beta}\varepsilon_{H_\alpha}(b')b'')u(x)\\&=\phi_a(1_{H_\beta}b)u(x)=\phi_a(\varphi_{\beta,\alpha}(1_{H_\beta})\varphi_{\alpha,\alpha}(b))u(x)=\phi_a(1_{H_\alpha}b)u(x)\\&=\phi_a(b)u(x)=(\phi_a\infty' x)(b\otimes u).\end{aligned}$$

That is $(\phi_a\infty' x)(\varepsilon_{H_\alpha}\infty' 1_{H_\beta})=(\varepsilon_{H_\alpha}\infty' 1_{H_\beta})(\phi_a\infty' x)=\phi_a\infty' x$.

Therefore $D'(H_\alpha,H_\beta)$ itself is an algebra.

For any $a,b\in B_\alpha$, $x,y\in B_\beta$, as discussed in Theorem II.2, in the case of $\alpha_1=\alpha_2$, $\beta_1=\beta_2$, we can have

$$\Delta((\phi_a\infty' x)(\phi_b\infty' y))=\Delta(\phi_a\infty' x)\Delta(\phi_b\infty' y).$$

Obviously,

$$\Delta(1_{D'(H_\alpha,H_\beta)})=\Delta(\varepsilon_{H_\alpha}\infty' 1_{H_\beta})=(\varepsilon_{H_\alpha}\infty' 1_{H_\beta})\otimes(\varepsilon_{H_\alpha}\infty' 1_{H_\beta})=1_{D'(H_\alpha,H_\beta)}\otimes 1_{D'(H_\alpha,H_\beta)}.$$

Since $\alpha\leqslant\beta$, then from Theorem II.2, in the case of $\beta_1=\beta_2$, $\alpha_1=\alpha_2$ we have $\varepsilon((\phi_a\infty' x)\times(\phi_b\infty' y))=\varepsilon(\phi_a\infty' x)\varepsilon(\phi_b\infty' y)$. And, $\varepsilon(1_{D'(H_\alpha,H_\beta)})=\varepsilon(\varepsilon_{H_\alpha}\infty' 1_{H_\beta})=\varepsilon_{H_\alpha^{op*}}(\varepsilon_{H_\alpha})\varepsilon_{H_\beta}(1_{H_\beta})=\varepsilon_{H_\alpha}(1_{H_\alpha})1=1$. Therefore, ε is an algebra morphism.

From the discussion above, we know that $D'(H_\alpha,H_\beta)$ becomes a bialgebra.

Lemma III.2: *For any $\alpha\in Y$, $Q_H(H_\alpha)$ is a right ideal of $D'(H)$ and itself is a coalgebra with comultiplication Δ satisfying $\Delta((\phi_a\infty' x)(\phi_b\infty' y))=\Delta(\phi_a\infty' x)\Delta(\phi_b\infty' y)$ for any $x,y\in B$ and $a,b\in B_\alpha$. Moreover, $Q_H(H_\alpha)=N_H(H_\alpha)\oplus B_H(H_\alpha)$ where $N_H(H_\alpha)=\Sigma_{\beta\in Y,\beta\not\geqslant\alpha}D'(H_\alpha,H_\beta)$ is a null right ideal of $D'(H)$ and is a subcoalgebra and ideal of $Q_H(H_\alpha)$, $B_H(H_\alpha)=\Sigma_{\beta\in Y,\beta\geqslant\alpha}D'(H_\alpha,H_\beta)$ is a sub-bialgebra of $Q_H(H_\alpha)$ with $N_H(H_\alpha)B_H(H_\alpha)=0$ and $B_H(H_\alpha)N_H(H_\alpha)\subseteq N_H(H_\alpha)$.*

Proof: From (3.1) and (3.3), we get $Q_H(H_\alpha)D'(H)\subseteq Q_H(H_\alpha)$ for any $\alpha\in Y$, which means that $Q_H(H_\alpha)$ is a right ideal of $D'(H)$, and thus $D'(H)$ can be decomposed into a direct sum of these ideals.

For $f\in H_\alpha^{op^*}$ and $x\in B$,

(1) Define $Q_H(H_\alpha)\to Q_H(H_\alpha)\otimes Q_H(H_\alpha)$ satisfying $\Delta(f\infty' x)=\Sigma_{(f),(x)}(f'\infty' x')\otimes(f''\infty' x'')$, where $\Delta(f)=\Sigma_{(f)}f'\otimes f''$ according to the comultiplication of $H_\alpha^{op^*}$.
(2) Define ε, $Q_H(H_\alpha)\to k$ satisfying $\varepsilon(f\infty' x)=\varepsilon_{H_\alpha^{op^*}}(f)\varepsilon_H(x)$.

As for $D'(H_\alpha,H_\beta)$ in Lemma III.1, $Q_H(H_\alpha)$ is a coalgebra on Δ and ε. And as discussed in Theorem II.2, in the case of $\alpha_1=\alpha_2$. That is, for any a, $b\in B_\alpha$, $x\in B_{\beta_1}\subset B$, $y\in B_{\beta_2}\subset B$, we have

$$\Delta((\phi_a\infty' x)(\phi_b\infty' y))=\Delta(\phi_a\infty' x)\Delta(\phi_b\infty' y).$$

By the definition of Δ, $N_H(H_\alpha)$ and $B_H(H_\alpha)$ are both subcoalgebras of $Q_H(H_\alpha)$.

Let $\beta\not\geqslant\alpha$ and $\gamma\in Y$. From (3.3), $D'(H_\alpha,H_\beta)D'(H_\alpha,H_\gamma)=0$. It means that $N_H(H_\alpha)Q_H(H_\alpha)=0$. Specially for $N_H(H_\alpha)N_H(H_\alpha)=0$ [i.e., $N_H(H_\alpha)$ is null] and $N_H(H_\alpha)B_H(H_\alpha)=0$.

For any $D'(H_\gamma,H_\xi)$ in $D'(H)$, $D'(H_\alpha,H_\beta)D'(H_\gamma,H_\xi)\subseteq D'(H_\alpha,H_{\beta\xi})$. But, $\alpha\not\leqslant\beta$. So, $\alpha\not\leqslant\beta\xi$. Then, $D'(H_\alpha,H_{\beta\xi})\subseteq N_H(H_\alpha)$. Thus, $N_H(H_\alpha)$ is a right ideal of $D'(H)$.

If $\alpha\leqslant\gamma$, then $\alpha\not\leqslant\gamma\beta$ since $\alpha\not\leqslant\beta$, thus $D'(H_\alpha,H_\gamma)D'(H_\alpha,H_\beta)\subseteq D'(H_\alpha,H_{\gamma\beta})\subseteq N_H(H_\alpha)$. It follows that $B_H(H_\alpha)N_H(H_\alpha)\subseteq N_H(H_\alpha)$ and $N_H(H_\alpha)$ is an ideal of $Q_H(H_\alpha)$.

It is easy to see that $B_H(H_\alpha)$ possesses the identity $1_{B_H(H_\alpha)}=\varepsilon_{H_\alpha}\infty' 1_H$ and $B_H(H_\alpha)B_H(H_\alpha)\subseteq B_H(H_\alpha)$. So, $B_H(H_\alpha)$ is an algebra and a subring of $Q_H(H_\alpha)$. Since $B_H(H_\alpha)$ is a subcoalgebra of $Q_H(H_\alpha)$, $\Delta((\phi_a\infty' x)(\phi_b\infty' y))=\Delta(\phi_a\infty' x)\Delta(\phi_b\infty' y)$ for any a, $b\in B_\alpha$, x, $y\in B_\beta$, where $\alpha\leqslant\beta$. As like in Lemma III.1, we also have $\varepsilon((\phi_a\infty' x)(\phi_b\infty' y))=\varepsilon(\phi_a\infty' x)\varepsilon(\phi_b\infty' y)$, $\varepsilon(1_{B_H(H_\alpha)})=1$. Therefore, we know that $B_H(H_\alpha)$ is a bialgebra.

Note that the comultiplication, the unit and the counit of $D'(H)$ are not correspondent with those of $D'(H_\alpha,H_\beta)$ and $B_H(H_\alpha)$. And, let $\alpha=\beta$ in $D'(H_\alpha,H_\beta)$, then $D'(H_\alpha,H_\alpha)=H_\alpha^{op^*}\infty' H_\alpha$. Since the multiplication is given by $(\phi_a\infty' x)(\phi_b\infty' y)=\phi_a\phi_b(1_{H_\alpha}?)\infty' xy$, which is the same as the quantum double $D'(H_\alpha)$ of H_α the condition commutative and H satisfies $\Sigma_{(a)}T(a''')a'\otimes a''=\Sigma_{(a)}T(a'')a'''\otimes a'$ for any $a\in H$. Since for $x\in B_{\beta_1}$, $y\in B_{\beta_2}$, $a\in B_{\alpha_1}$ and its duality ϕ_a in $H_{\alpha_1}^{op^*}$, $b\in B_{\alpha_2}$ and its duality ϕ_b in $H_{\alpha_2}^{op^*}$, we have

$$\begin{aligned}(\phi_a\infty x)(\phi_b\infty y)&=\sum_{(x)}\phi_a\phi_b(T^{-1}(x''')?x')\infty x''y=\sum_{(x)}\phi_a\phi_b(T^{-1}(x''')x'?)\infty x''y\\&=\sum_{(x)}\phi_a\phi_b(T^{-1}(x'')x'''?)\infty x'y=\sum_{(x)}\phi_a\phi_b(\varepsilon_{\beta_1}(x'')1_{H_{\beta_1}}?)\infty x'y\\&=\sum_{(x)}\phi_a\phi_b(1_{H_{\beta_1}}?)\infty\varepsilon_{\beta_1}(x'')x'y=\phi_a\phi_b(1_{H_{\beta_1}}?)\infty xy.\end{aligned}$$

Hence $D'(H_\alpha,H_\beta)$ is iust $D'(H_\alpha)$, as a sub-bialgebra of $D'(H)$.

Definition III.3 (Ref. 21):

(1) *A ring R is a* semilattice sum of subrings R_α, $\alpha\in\Omega$, *if* Ω *is a semilattice*, $R=\Sigma_{\alpha\in\Omega}R_\alpha$ *and* $R_\alpha R_\beta\subseteq R_{\alpha\beta}$.
(2) *A ring R is a* supplementary semilattice sum of subrings R_α, $\alpha\in\Omega$, *if R is a semilattice sum of subrings* R_a, $\alpha\in\Omega$, *and if for every* $\alpha\in\Omega$, $R_\alpha\cap\Sigma_{\beta\neq\alpha}R_\beta=\{0\}$; *i.e., if the sum is direct*.

By (3.3) and Definition III.3, every $Q_H(H_\alpha)$ is a supplementary semilattice sum of $D'(H_\alpha,H_\beta)$ for $\beta\in Y$.

From the discussion above, we get the following main result.

Theorem III.4 ***(structure theorem)***: *For a finite dimensional commutative semilattice graded weak Hopf algebra* $H=\oplus_{\alpha\in Y}H_\alpha$ *with weak antipode T, where Y is a semilattice and* H_α *a subweak Hopf algebra of H which is a Hopf algebra with antipode* $T|_{H_\alpha}$ *for each* $\alpha\in Y$, *suppose there exists a basis* B_α *of* H_α *for every* $\alpha\in Y$, *such that* $B=\cup_{\alpha\in Y}B_\alpha$ *a basis of H. Then the quantum G-double* $D'(H)$ *is a direct sum of right ideals* $Q_H(H_\alpha)$, $\alpha\in Y$, *where*

(1) *every* $Q_H(H_\alpha)$ *is a supplementary semilattice sum of subrings* $D'(H_\alpha,H_\beta)$ *for* $\beta\in Y$ *and is a coalgebra with comultiplication* Δ *satisfying* $\Delta((\phi_a\infty' x)(\phi_b\infty' y))=\Delta(\phi_a\infty' x)\Delta(\phi_b\infty' y)$ *for any* $x, y\in B$ *and* $a, b\in B_\alpha$;

(2) $Q_H(H_\alpha)=N_H(H_\alpha)\oplus B_H(H_\alpha)$ *where* $N_H(H_\alpha)=\Sigma_{\beta\in Y,\beta\not\geqslant\alpha}D'(H_\alpha,H_\beta)$ *is a null right ideal of* $D'(H)$ *and is a subcoalgebra and ideal of* $Q_H(H_\alpha)$, $B_H(H_\alpha)=\Sigma_{\beta\in Y,\beta\geqslant\alpha}D'(H_\alpha,H_\beta)$ *is a subbialgebra of* $Q_H(H_\alpha)$ *with* $N_H(H_\alpha)B_H(H_\alpha)=0$ *and* $B_H(H_\alpha)N_H(H_\alpha)\subseteq N_H(H_\alpha)$;

(3) $D'(H_\alpha,H_\beta)$ *are subcoalgebras of* $Q_H(H_\alpha)$. *If* $\alpha\not\leqslant\beta$, $D'(H_\alpha,H_\beta)$ *is a null subring. If* $\alpha\leqslant\beta$, $D'(H_\alpha,H_\beta)$ *is a bialgebra. If* $\alpha=\beta$, *then* $D'(H_\alpha,H_\alpha)=D'(H_\alpha)$, *which means that every quantum G-double* $D'(H_\alpha)$ *is a direct sum component of* $D'(H)$.

In fact, Theorem III.4 is similar to the main conclusion in Ref. 10 for noncommutative Clifford monoid algebras.

IV. SEMISIMPLICITY OF QUANTUM G-DOUBLE

In this section, as an application to Theorem III.4, we discuss the semisimplicity of quantum G-doubles.

In Ref. 22, it is shown that for a finite group G, the quantum double $D(G)$ is semisimple as an algebra if and only if the characteristic p of k does not divide the order $|G|$ of G. Here, we will consider the similar question for a semilattice grading weak Hopf algebra as above, i.e., under what conditions, the quantum G-double $D'(H)$ is semisimple as an algebra.

On the other hand, we know[3] that an algebra is semisimple if and only if it is regular and Noetherian. But, for a finite-dimensional weak Hopf algebra H, $D'(H)$ is finite dimensional, then it is Noetherian. Hence, in fact, $D'(H)$ is regular if and only if it is semisimple. So, in the sequel, we will only study the regularity of $D'(H)$.

Suppose $D'(H)$ is a semisimple algebra for H is commutative. A k-algebra is semisimple if it is a semisimple right module over itself, and any submodule of a semisimple module is semisimple. Then, $D'(H)$ is semisimple as a right $D'(H)$ module. From Theorem III.4, every $Q_H(H_\alpha)$ is a right ideal of $D'(H)$, then is a right $D'(H)$ submodule of the right $D'(H)$ module $D'(H)$. Hence $Q_H(H_\alpha)$ must be semisimple as a right $D'(H)$ module.

Suppose $N_H(H_\alpha)\neq 0$ for an arbitrary fixed $\alpha\in Y$. Then there exists $\beta\in Y$ such that $\alpha\not\leqslant\beta$. From the semisimplicity of $Q_H(H_\alpha)$, we know that $N_S(H_\alpha)$ is also semisimple as right $D'(H)$ module since it is a right submodule of $Q_H(H_\alpha)$. Then, $N_H(H_\alpha)$ can be decomposed as a direct sum of some simple right $D'(H)$ submodules.

Let $\theta=\Pi_{\lambda\in Y}\lambda$. Then $\theta\leqslant\lambda$ for all $\lambda\in Y$ and $\alpha\not\leqslant\theta$ [otherwise, $N_H(H_\alpha)=0$]. Thus, $D'(H_\alpha,H_\theta)\subseteq N_H(H_\alpha)$. It is easy to see that $D'(H_\alpha,H_\theta)$ is a right $D'(H)$ submodule of $N_H(H_\alpha)$.

We will make our discussion through two steps.

Lemma IV.1: $N_H(H_\alpha)=D'(H_\alpha,H_\theta)$.

Proof: Assume M is a simple right $D'(H)$ submodule of $N_H(H_\alpha)$. Let $0\neq z\in M$. Then $zD'(H)=M$. Write $z=\Sigma_{i=1}^m k_i(\phi_{a_i}\infty' x_i)$ where $0\neq k_i\in k$, $a_i\in B_\alpha$, $x_i\in B_{\gamma_i}(\alpha\not\leqslant\gamma_i)$ and $\phi_{a_i}\infty' x_i\neq\phi_{a_j}\infty' x_j$ for $i\neq j$, i.e., $x_i\neq x_j$ or $a_i\neq a_j$.

Set $b\in B_{\gamma_1\alpha}$ ($\notin H_\alpha$ since $\alpha\not\leqslant\gamma_1$) and $x\in B_\theta$. Consider

$$z(\phi_b\infty' x)=\sum_{i=1}^m k_i(\phi_{a_i}\phi_b(1H_{\gamma_i}?)\infty' x_i x). \tag{4.1}$$

Since $b\in B_{\gamma_1\alpha}$ we get $\phi_{a_1}\phi_b(1_{H_{\gamma_1}}?)\neq 0$ and $\phi_{a_1}\phi_b(1_{H_{\gamma_1}}?)\in H_\alpha^*$. In other terms for $i=1$, if $x_i=x_1$ then $a_i\neq a_1$ thus $\phi_{a_i}\phi_b(1_{H_{\gamma_i}}?)\infty' x_i x=\phi_{a_i}\phi_b(1_{H_{\gamma_1}}?)\neq 0$ since $\gamma_1=\gamma_i$; if $x_i\neq x_1$, then $\phi_{a_i}\phi_b(1_{H_{\gamma_i}}?)\infty' x_i x=0$ since $\alpha\not\leqslant\gamma_i$.

Hence on the right-hand side of (4.1), every term is 0 or $\phi_{a_i}\phi_b(1_{H_{\gamma_1}}?)\infty' x_i x$. Note the these nonzero terms are all in $Q_H(H_\alpha)$ and at least one of them [i.e., $\phi_{a_1}\phi_b(1_{H_{\gamma_1}}?)\infty' x_1 x$] is not equal to 0. It implies this sum is not equal to 0. Then $z(\phi_b\infty' x)\neq 0$.

And, $x_i x \in H_{\gamma_i \theta} = H_\theta$. So, every nonzero term $\phi_{a_1}\phi_b(1_{H_{\gamma_1}}?)\infty' x_i x \in D'(H_\alpha, H_\theta)$. Thus, $z(\phi_b \infty' x) \in D'(H_\alpha, H_\theta)$. It follows that $0 \neq z(\phi_b \infty' x) \in M \cap D'(H_\alpha, H_\theta)$. Then, we get a nonzero right $D'(H)$ submodule $M \cap D'(H_\alpha, H_\theta)$ of M. But M is simple, it means $M \cap D'(H_\alpha, H_\theta) = M$. Thus, $M \subseteq D'(H_\alpha, H_\theta)$. Since M is an arbitrary simple submodule in the semisimple module $N_H(H_\alpha)$. Therefore, it must get $N_H(H_\alpha) \subseteq D'(H_\alpha, H_\theta)$. Finally, we have $N_H(H_\alpha) = D'(H_\alpha, H_\theta)$.

Lemma IV.2: $Q_H(H_\alpha) = N_H(H_\alpha)$.

Proof: Assume W is a simple right $D'(H)$ submodule of $Q_H(H_\alpha)$. Let $0 \neq w \in W$. Then $wD'(H) = W$. Write $w = u + v$ where $u \in N_H(H_\alpha)$ and $v \in B_H(H_\alpha)$. $N_H(H_\alpha)$ is null, so $uN_H(H_\alpha) = 0$. By Theorem III.4, $vN_H(H_\alpha) \subseteq N_H(H_\alpha)$.

Write $v = \Sigma_{i=1}^m k_i(\phi_{\alpha_i} \infty' x_i)$ where $0 \neq k_i \in k$, $a_i \in B_\alpha$, $x_i \in B_{\beta_i}(\beta_i \geqslant \alpha)$, and $\phi_{a_i} \infty' x_i \neq \phi_{a_j} \infty' x_j$ for $i \neq j$, i.e., $x_i \neq x_j$ or $a_i \neq a_j$.

Set $b \in B_{\beta_1 \alpha}$ ($\in B_\alpha$ since $\alpha \leqslant \beta_1$) and $x \in B_\theta$. Consider $z(\phi_b \infty' x) = \Sigma_{i=1}^m k_i(\phi_{a_i}\phi_b(1_{H_{\gamma_i}}?)\infty' x_i x)$. By the similar method in (i), we can get $v(\phi_b \infty' x) \neq 0$.

And, $x_i x \in H_{\beta_i \theta} = H_\theta$. So, every nonzero term $\phi_{a_i}\phi_b(1_{H_{\beta_i}}?)\infty' x_i x \in D'(H_\alpha, H_\theta)$. Thus, $v(\phi_b \infty' x) \in D'(H_\alpha, H_\theta) = N_H(H_\alpha)$. It follows that $0 \neq v(\phi_b \infty' x) \in W \cap N_H(H_\alpha)$. Then, we get a nonzero right $D'(H)$ submodule $W \cap N_H(H_\alpha)$ of M. But W is simple, it means $W \cap N_H(H_\alpha) = W$. Thus, $W \subseteq N_H(H_\alpha)$ where W is an arbitrary simple submodule in the semisimple module $Q_H(H_\alpha)$.

From this, we get $Q_H(H_\alpha) \subseteq N_H(H_\alpha)$. Thus, $Q_H(H_\alpha) = N_H(H_\alpha)$.

From Lemma IV.2, we get $B_H(H_\alpha) = 0$. But it is impossible in fact, since $0 \neq D'(H_\alpha) \subseteq B_H(H_\alpha)$ by Theorem III.4. From this contradiction, we know that the supposition $N_H(H_\alpha) \neq 0$ is not true. Therefore $N_H(H_\alpha) = 0$. It means $\alpha \leqslant \beta$ for any $\beta \in Y$, i.e., $\alpha = \theta$. Note that α is arbitrary in Y. Hence, we know θ is the unique element of Y, i.e., $H = H_\theta$ is a Hopf algebra, whose quantum G-double is semisimple if and only if H_θ is semisimple by Ref. 15.

So, we get the following.

Theorem IV.3: *For a finite-dimensional commutative weak Hopf algebra H satisfying the same conditions in Theorem III.4, its quantum G-double $D'(H)$ over a field k is semisimple (respectively, regular) if and only if H is a semisimple Hopf algebra (respectively, regular).*

The similar result of this theorem for classical quantum groups holds in the case of $H = kS$ with S a noncommutative Clifford monoid (see Ref. 10).

V. EXAMPLES

The concept of semilattice graded weak Hopf algebra, introduced in this paper, is important for our research. Of course, Clifford monoid algebras are examples for this concept. However, we hope to give more nontrivial examples.

In Ref. 1, there is a general construction producing pointed Hopf algebras through Ore extension from a group algebra. This gives an idea to construct semilattice graded weak Hopf algebras through the Ore extension.

First, we need some preparation works.

Recall, that for a k-algebra A, an algebra endomorphism φ of A, and a φ derivation δ of A [i.e., a linear map $\delta : A \to A$ such that $\delta(ab) = \delta(a)b + \varphi(a)\delta(b)$ for all $a, b \in A$], the Ore extension $A[X, \varphi, \delta]$ is $A[X]$ as an Abelian group, with multiplication induced by $Xa = \delta(a) + \varphi(a)X$ for all $a \in A$.

The following is an obvious extension of the universal property for polynomial rings.

Lemma V.1 (Ref. 1): *Let $A[X, \varphi, \delta]$ be an Ore extension of A and $i : A \to A[X, \varphi, \delta]$ the inclusion morphism. Then for any algebra B, any algebra morphism $f : A \to B$ and every element $b \in B$ such that $bf(a) = f(\delta(a)) + f(\varphi(a))b$ for all $a \in A$, there exists a unique algebra morphism $\overline{f} : A[X, \varphi, \delta] \to B$ such that $\overline{f}(X) = b$ and $\overline{f}i = f$.*

Let S be a finite semigroup, an element a of a semigroup is called *regular* if there exists $x \in S$ such that $axa = a$. The semigroup S is called *regular* if all its elements are regular. We write $a \mathcal{J} b$ if there exist x, y, u, v in $S^1 = S \cup \{1\}$ for which $xay = b$ and $ubv = a$. Obviously, $\mathcal{J}$ is an equivalent relation on S. This equivalent relation is one of the important five kinds of equivalent relations on a semigroup S. A $\mathcal{J}$ class of some element $x \in S$ is the set $\{y \in S | x \mathcal{J} y\}$, i.e., the equivalent class

including x under the relation $\mathcal{J}$. A $\mathcal{J}$ class is called regular $\mathcal{J}$ class if all its elements are regular (see Ref. 17).

If $\Gamma: S \to \mathrm{Hom}(A,A)$ is a representation of S, by linear transformations of a finite-dimensional vector space A over the complex field $\mathbf{C}$, then the *character* χ_Γ of Γ is the function $S \to \mathbf{C}$ defined by

$$\chi_\Gamma(x) = \mathrm{Tr}\,\Gamma(x) \quad \textit{for each } x \in S,$$

where $\mathrm{Tr}\,\Gamma(x)$ denotes the sum of the diagonal entries in any matrix expression of $\Gamma(x)$. Let $a \in S$ and let $\bar{a}=ae$, where e is the unique idempotent in the cyclic subsemigroup $\langle a\rangle$ generated by a, we shall say that two elements $a, b \in S$, are *conjugate* if and only if $\bar{b}=x'\bar{a}x$, $\bar{a}=x\bar{b}x'$ for some regular element x with inverse x', i.e., $xx'x=x$, $x'xx'=x'$. Then a function $S \to \mathbf{C}$ is called a *class function* if it is constant on each conjugacy class of S, and all the class functions form an algebra over $\mathbf{C}$ under pointwise addition and multiplication, we denote this algebra by *cfS*. The *character ring* of S, which is denoted by *chS*, is a subring of the class function algebra which is spanned by the irreducible characters of S (see Ref. 14).

Lemma V.2 (Ref. 14): Let S be a finite semigroup, let $J_1,\ldots,J_r$, be the regular $\mathcal{J}$ classes of S, and let $H_1,\ldots,H_r$ be the maximal subgroups of $J_1,\ldots,J_r$, respectively. Then, $chS \cong chH_1 \times \cdots \times chH_r$.

For a Clifford semigroup S, we can see that J_i, $i=1,2,\ldots,r$ are the maximal subgroups G_α, $\alpha \in Y$ of S. Hence, $chS \cong \Pi_{\alpha\in Y} chG_\alpha$.

Second, we will construct a pointed weak Hopf algebra by starting with the coradical, forming Ore extensions.

Let $A=kS=\oplus_{\alpha\in Y} kG_\alpha$ be the algebra of a finite commutative Clifford monoid $S=[Y;G_\alpha,\varphi_{\alpha,\beta}]$ (the method for constructing some concrete Clifford monoids can be seen in Ref. 13.) Let G_α^* be the character group of G_α for each $\alpha \in Y$, then the character semigroup of S is $\Pi_{\alpha\in Y} G_\alpha^*$. Since S is a monoid, we can assume that the maximal subgroup which contains 1 is G_i, where i is the identity element in Y.

Let $c \in G_i$ and $c^* \in G_i^*$. According to Lemma V.2, for each $\alpha \in Y$, chG_α is embeded into *chS* such that for any $c^* \in chG_i$ is mapped to $\chi=(c^*,1,\ldots,1) \in chS \cong \Pi_{\alpha\in Y} chG_\alpha$.

Let φ be an algebra automorphism of A defined by $\varphi(x)=\langle \chi,x\rangle x$ for all $x \in S$, then it is clear that if $x \in G_i$, then $\langle \chi,x\rangle=\langle c^*,x\rangle$; if $x \in G_\alpha$ with $\alpha \neq i$, then $\langle \chi,x\rangle=\langle 1,x\rangle=1$. Consider the Ore extension $A_1=A[X,\varphi,\delta]=A[X,\varphi,0]$, where $\delta=0$. Apply Lemma V.I first with $B=A_1\otimes A_1$, $f=(i\otimes i)\cdot\Delta_A$, $b=c\otimes X+X\otimes 1$ and then with $B=k$, $f=\epsilon_A$, $b=0$, to define algebra homomorphism $\Delta: A_1 \to A_1\otimes A_1$ and $\epsilon: A_1 \to k$ by

$$\Delta(X) = c\otimes X + X\otimes 1 \quad \textit{and } \epsilon(X)=0.$$

It is easily checked that Δ and ϵ defined a bialgebra structure on A_1. The weak antipode T of A extends to a weak antipode on A_1 by $T(X)=-c^{-1}X$ and $T(Xe_\alpha)=-(ce_\alpha)^{-1}X=-c^{-1}e_\alpha X$.

If we let $A_1^\alpha=kG_\alpha[Xe_\alpha,\varphi^\alpha,\delta^\alpha]=kG_\alpha[Xe_\alpha,\varphi^\alpha,0]$, where $\delta^\alpha=0$ and $\varphi^\alpha(g_\alpha)=\langle \chi|_{chG_\alpha}, g_\alpha\rangle g_\alpha$. Then A_1^α is a subweak Hopf algebra of A_1 which is a Hopf algebra for each $\alpha \in Y$ under the defined Δ, ϵ and antipode T. We have

$$Xe_\alpha g_\alpha = Xg_\alpha = \langle \chi, g_\alpha\rangle g_\alpha = g_\alpha X,$$

$$\Delta(Xe_\alpha) = (c\otimes X + X\otimes 1)(e_\alpha\otimes e_\alpha) = ce_\alpha\otimes Xe_\alpha + Xe_\alpha\otimes 1e_\alpha = ce_\alpha\otimes Xe_\alpha + Xe_\alpha\otimes e_\alpha$$

[i.e., Xe_α is (e_α, ce_α)-primitive], and

$$\epsilon(Xe_\alpha) = \epsilon(X)\epsilon(e_\alpha) = 0.$$

At the same time, $m(\mathrm{id}*T)\Delta(Xe_\alpha)=ce_\alpha S(Xe_\alpha)+Xe_\alpha S(e_\alpha)=ce_\alpha(-c^{-1})e_\alpha X+Xe_\alpha e_\alpha=-1e_\alpha X+Xe_\alpha=-Xe_\alpha+Xe_\alpha=0=\epsilon(Xe_\alpha)$.

Thus, we can get the following proposition.

Proposition V.3: The Ore extension $A_1=A[X,\varphi,0]=\oplus_{\alpha\in Y}A_1^\alpha$ *and* $A_1^\alpha=kG_\alpha[Xe_\alpha,\varphi^\alpha,0]$ *as defined above is a subweak Hopf algebra of* A_1 *which is a Hopf algebra for each* $\alpha\in Y$. *Define a Hopf algebra homomorphism* $\phi_{\alpha,\beta}$ *from* A_1^α *to* A_1^β *if* $\alpha\beta=\beta$ *satisfying* $\phi_{\alpha,\beta}(a_\alpha)=\varphi_{\alpha,\beta}(a_\alpha)$ *for any* $a_\alpha\in G_\alpha$ *and* $\phi_{\alpha,\beta}(Xe_\alpha)=Xe_\beta$. *Then* A_1 *is a semilattice graded weak Hopf algebra.*

Proof: The above construction shows that A_1 has a basis $\{gX^n|g\in S,n\in N\}$ and A_1^α has a basis $B_\alpha=\{g_\alpha(Xe_\alpha)^n|g_\alpha\in G_\alpha,n\in N\}$ for each $\alpha\in Y$.

We have known that $Xe_\alpha=e_\alpha X$ for any $\alpha\in Y$ and $Xg_\alpha=g_\alpha X$ for any $g_\alpha\in G_\alpha$ with $\alpha\neq i$, therefore for any $g_\alpha(Xe_\alpha)^{n_1}\in B_\alpha$, $g_\beta(Xe_\beta)^{n_2}\in B_\beta$, it follows that

$$\begin{aligned}
g_\alpha(Xe_\alpha)^{n_1}g_\beta(Xe_\beta)^{n_2} &= g_\alpha X^{n_1}e_\alpha g_\beta X^{n_2}e_\beta\\
&= g_\alpha X^{n_1}\varphi_{\alpha,\alpha\beta}(e_\alpha)\varphi_{\beta,\alpha\beta}(g_\beta)X^{n_2}e_\beta\\
&= g_\alpha X^{n_1}e_{\alpha\beta}\varphi_{\beta,\alpha\beta}(g_\beta)X^{n_2}e_\beta = g_\alpha X^{n_1}\varphi_{\beta,\alpha\beta}(g_\beta)e_\beta X^{n_2}\\
&= \langle\chi,\varphi_{\beta,\alpha\beta}(g_\beta)\rangle^{n_1}g_\alpha\varphi_{\beta,\alpha\beta}(g_\beta)e_\beta X^{n_1}X^{n_2}\\
&= \langle\chi,\varphi_{\beta,\alpha\beta}(g_\beta)\rangle^{n_1}\varphi_{\alpha,\alpha\beta}(g_\alpha)\varphi_{\beta,\alpha\beta}(g_\beta)\varphi_{\beta,\alpha\beta}(e_\beta)X^{n_1+n_2}\\
&= \langle\chi,\varphi_{\beta,\alpha\beta}(g_\beta)\rangle^{n_1}(g_\alpha g_\beta)(e_{\alpha\beta}X^{n_1+n_2}\\
&= \langle\chi,\varphi_{\beta,\alpha\beta}(g_\beta)\rangle^{n_1}(g_\alpha g_\beta)(Xe_{\alpha\beta})^{n_1+n_2}\in A_1^{\alpha\beta}.
\end{aligned}$$

It means $A_1^\alpha A_1^\beta\subseteq A_1^{\alpha\beta}$ for any α, $\beta\in Y$. And,

$$\begin{aligned}
\phi_{\alpha,\alpha\beta}(g_\alpha(Xe_\alpha)^{n_1})\phi_{\beta,\alpha\beta}(g_\beta(Xe_\beta)^{n_2}) &= \varphi_{\alpha,\alpha\beta}(g_\alpha)(\phi_{\alpha,\alpha\beta}(Xe_\alpha)^{n_1})\varphi_{\beta,\alpha\beta}(g_\beta)(\phi_{\beta,\alpha\beta}(Xe_\beta)^{n_2})\\
&= \varphi_{\alpha,\alpha\beta}(g_\alpha)(\phi_{\alpha,\alpha\beta}(Xe_\alpha))^{n_1}\varphi_{\beta,\alpha\beta}(g_\beta)(\phi_{\beta,\alpha\beta}(Xe_\beta))^{n_2}\\
&= \varphi_{\alpha,\alpha\beta}(g_\alpha)(Xe_{\alpha\beta})^{n_1}\varphi_{\beta,\alpha\beta}(g_\beta)(Xe_{\alpha\beta})^{n_2}\\
&= \varphi_{\alpha,\alpha\beta}(g_\alpha)(X^{n_1}e_{\alpha\beta})\varphi_{\beta,\alpha\beta}(g_\beta)(X^{n_2}e_{\alpha\beta})\\
&= \langle\chi,\varphi_{\beta,\alpha\beta}(g_\beta)\rangle^{n_1}\varphi_{\alpha,\alpha\beta}(g_\alpha)\varphi_{\beta,\alpha\beta}(g_\beta)X^{n_1}X^{n_2}e_{\alpha\beta}\\
&= \langle\chi,\varphi_{\beta,\alpha\beta}(g_\beta)\rangle^{n_1}(g_\alpha g_\beta)(Xe_{\alpha\beta})^{n_1+n_2}.
\end{aligned}$$

So, $g_\alpha(Xe_\alpha)^{n_1}g_\beta(Xe_\beta)^{n_2}=(g_\alpha(Xe_\alpha)^{n_1})\phi_{\alpha,\alpha\beta}(g_\beta(Xe_\beta)^{n_2})\phi_{\beta,\alpha\beta}$. Hence, A_1 is a semilattice graded weak Hopf algebra. (See also Refs. 4, 5, 18, and 19.)

If we choose $c^*\neq 1\in G_i^*$, $Xg_\alpha=\langle\chi,g_\alpha\rangle g_\alpha X\neq g_\alpha X$ for $\alpha=i$, hence A_1 is noncommutative and noncocommutative. Otherwise, let $c^*=1\in G_i^*$, $\chi=(1,\ldots,1)$, $Xg_\alpha=\langle\chi,g_\alpha\rangle g_\alpha X=g_\alpha X$ for any $\alpha\in Y$, hence A_1 is commutative. In this case, by Proposition V.3, one can see that A_1 is a nontrivial example satisfying the condition in Theorem III.4.

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A simple parametrization for G_2

Sergio L. Cacciatori[a)]
Dipartimento di Matematica, Università di Milano, Via Saldini 50, I-20133 Milano, Italy and INFN, Sezione di Milano, Via Celoria 16, I-20133 Milano, Italy

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We give a simple parametrization of the G_2 group, which is consistent with the structure of G_2 as a SU(3) fibration. We also explicitly compute the (bi)invariant measure, which turns out to have a simple expression. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2009627]

I. INTRODUCTION

Group theory plays an important role in physics. When a group describes a symmetry of the system, invariant quantities are often obtained by integrating over the group. For example, to have an unbroken symmetry in a path-integral formulation of gauge field theory, the integration measure must be invariant under the group action.

Every semisimple group has a unique invariant measure (up to normalization constants), obtained by pulling back the Killing form on its Lie algebra via the group left action. However, it is generally difficult to find an explicit parametrization of the group elements by which the invariant measure acquires a reasonably simple expression while also allowing for a full specification of the range of parameters. This is indeed what is needed in performing practical computations.

In Ref. 1, a solution of this problem was found for the group G_2. The group parametrization given there, emphasizes the structure of G_2 as a fibration over the base space $\mathcal{H}$ of quaternionic linear subalgebras of octonions and fiber SO(4). Here we give another parametrization of the same group based on the well-known fact that G_2 can be seen as an SU(3) fibration over the six sphere S^6. (See, for example, Ref. 2.) The resulting measure turns out to have a very simple expression, with all the parameters varying in a 14-dimensional hypercube.

The motivation for G_2 comes from nonperturbative gauge theory used to test confinement in lattice chromodynamics. It is believed that confinement should be due to excitation modes belonging to the center of the gauge group so that a group with no center, preventing the existence of these modes, should not produce confinement. So if one observes no confinement in a toy model gauge theory with group G_2 which is center free, this belief is proved to be consistent. Having a global explicit parametrization of the group renders nonperturbative computations easier to work out and implement.

II. THE REPRESENTATION ALGEBRA AND THE GROUP ANSATZ

For the algebra, we choose the fundamental representation (**7**) as done in Ref. 1. All the notations employed here will agree with those used in that reference. Since from that paper, we will only use the commutators matrix $B_{IJ}:=[C_I,C_J]$ we have transcribed it and set it in Appendix C. Now note that the $\{C_i\}_{i=1}^8$ generates an su(3) algebra. Thus we want to use this fact to produce a parametrization for the G_2 elements capable of highlighting the SU(3) subgroup.

With this purpose, let us note that the C_9 commutator with su(3) suffices to reproduce all the remaining generators of the g_2 algebra. Then we can hope to find a parametrization of the group resembling the Euler parametrization for SU(n). Let us write the generic element of G_2 as

a)Electronic mail: sergio.cacciatori@mi.infn.it

$$g = \mathrm{SU}(3)[\alpha_1,\ldots,\alpha_8]e^{\beta C_9}\,\mathrm{SU}(3)[\gamma_1,\ldots,\gamma_8], \tag{2.1}$$

where $\mathrm{SU}(3)[\alpha_1,\ldots,\alpha_8]$ is the general Euler parametrization of SU(3) shown in Appendix A. Note that here we have three redundant parameters, the dimension of G_2 being 14. We can easily cancel them out as follows. In (2.1) the left-hand side SU(3) term has the expansion

$$\mathrm{SU}(3)[\alpha_1,\ldots,\alpha_8] = h[\alpha_1,\ldots,\alpha_5]e^{\alpha_6 C_3}e^{\alpha_7 C_2}e^{\alpha_8 C_3}. \tag{2.2}$$

But C_1, C_2, C_3 commute with C_9 so that $\alpha_1, \alpha_2, \alpha_3$ can be reabsorbed in the right-hand side SU(3) in (2.1). Thus, it seems clear we should make the ansatz

$$g[\alpha_1,\ldots,\alpha_6;\gamma_1,\ldots,\gamma_8] = \Sigma[\alpha_1,\ldots,\alpha_6]\mathrm{SU}(3)[\gamma_1,\ldots,\gamma_8] \tag{2.3}$$

with

$$\Sigma[\alpha_1,\ldots,\alpha_6] = e^{\alpha_1 C_3}e^{\alpha_2 C_2}e^{\alpha_3 C_3}e^{(\sqrt{3}/2)\alpha_4 C_8}e^{\alpha_5 C_5}e^{(\sqrt{3}/2)\alpha_6 C_9}. \tag{2.4}$$

To prove that this ansatz is the right one, we show that it allows to fix the range of parameters so as to cover (up to a a subset of vanishing measure) all of G_2 only once.

A. Fibration and computation of the metric

We have said that the quotient of G_2 by its SU(3) subgroup is a sphere S^6. We will use this information to compute the range of parameters. For brevity we will call $S := \mathrm{SU}(3)[\gamma_1,\ldots,\gamma_8]$. The group metric can be deduced from the left-hand side invariant currents

$$Jg = g^{-1}\,\mathrm{d}g = \sum_{I=1}^{14} Jg^I C_I \tag{2.5}$$

via

$$\mathrm{d}s^2_{G_2} = -\tfrac{1}{4}\mathrm{Trace}\{Jg \otimes Jg\}. \tag{2.6}$$

[The factor $-\frac{1}{4}$ is due to the normalization $\mathrm{Trace}\{C_I C_J\} = -4\delta_{IJ}$. Choosing a metric $(C_I|C_J) = \delta_{IJ}$ on the algebra is equivalent to fixing normalizations such that long and short roots of g_2 have length 2 and $2/\sqrt{3}$, respectively.[1]]

If we now write

$$J_\Sigma = \Sigma^{-1}\,\mathrm{d}\Sigma = \sum_{I=1}^{14} J^I_\Sigma C_I, \tag{2.7}$$

$$J_S = \mathrm{d}S\,S = \sum_{I=1}^{8} J^I_S C_I, \tag{2.8}$$

it is straightforward to show that

$$\mathrm{d}s^2_{G_2} = \sum_{I=1}^{8}(J^I_S + J^I_\Sigma)^2 + \sum_{I=9}^{14}(J^I_\Sigma)^2. \tag{2.9}$$

Now Σ parametrizes the quotient space between G_2 and the SU(3) orbits generated by S. Fixing the base point Σ we recover the SU(3) invariant metric as

$$ds^2_{SU(3)} = \sum_{I=1}^{8} (J^I_S)^2. \tag{2.10}$$

To find the induced metric on the base one should compute the current $\Sigma^{-1}\,d\Sigma$ and project out the components that are tangent to the su(3) directions. Doing so we find

$$ds^2_{BASE} = \sum_{I=9}^{14} (J^I_\Sigma)^2. \tag{2.11}$$

This term should represent the metric of a six sphere. We now show that this is exactly the case. Using the results obtained in Appendix B for the currents, one finds

$$\frac{4}{3} ds^2_{BASE} = d\alpha_6^2 + \sin^2\alpha_6 \left\{ d\alpha_5^2 + \cos^2\alpha_5\, d\alpha_4^2 + \sin^2\alpha_5 \left[s_1^2 + s_2^2 + \left(s_3 + \tfrac{1}{2} d\alpha_4 \right)^2 \right] \right\}, \tag{2.12}$$

where

$$\begin{aligned} s_1 &= -\sin(2\alpha_2)\cos(2\alpha_3) d\alpha_1 + \sin(2\alpha_3) d\alpha_2, \\ s_2 &= \sin(2\alpha_2)\sin(2\alpha_3) d\alpha_1 + \cos(2\alpha_3) d\alpha_2, \\ s_3 &= \cos(2\alpha_2) d\alpha_1 + d\alpha_3. \end{aligned} \tag{2.13}$$

We can now recognize the metric of a six sphere S^6 with coordinates $(\alpha_6, \vec{X})$, where α_6 is the azimuthal coordinate, $\alpha_6 \in [0, \pi]$, and $\vec{X}$ covers a five sphere. We can look at this sphere as immersed in $\mathbb{C}^3$ via

$$\vec{X} = (z_1, z_2, z_3) = (\cos\alpha_5 e^{i\alpha_4}, \sin\alpha_5 \cos\alpha_2 e^{i[\alpha_1+\alpha_3+(\alpha_4/2)]}, \sin\alpha_5 \sin\alpha_2 e^{i[\alpha_1-\alpha_3-(\alpha_4/2)]}),$$

$$\alpha_1 \in [0,\pi], \quad \alpha_2 \in \left[0, \frac{\pi}{2}\right], \quad \alpha_3 \in [0, 2\pi], \quad \alpha_4 \in [0, 2\pi], \quad \alpha_5 \in \left[0, \frac{\pi}{2}\right].$$

Computing the metric $ds^2_{S^5} = |dz_1|^2 + |dz_2|^2 + |dz_3|^2$ in these coordinates we find

$$\tfrac{4}{3} ds^2_{BASE} = d\alpha_6^2 + \sin^2\alpha_6 \{ ds^2_{S^5} \}. \tag{2.14}$$

which completes our identification.

III. CONCLUSIONS

We have shown that the elements of the group G_2 can be parametrized as

$$g = e^{\alpha_1 C_3} e^{\alpha_2 C_2} e^{\alpha_3 C_3} e^{(\sqrt{3}/2)\alpha_4 C_8} e^{\alpha_5 C_5} e^{(\sqrt{3}/2)\alpha_6 C_9} \mathrm{SU}(3)[\gamma_1, \ldots, \gamma_8] \tag{3.1}$$

with

$$\alpha_1 \in [0,\pi], \quad \alpha_2 \in \left[0, \frac{\pi}{2}\right], \quad \alpha_3 \in [0, 2\pi], \quad \alpha_4 \in [0, 2\pi], \quad \alpha_5 \in \left[0, \frac{\pi}{2}\right], \quad \alpha_6 \in [0, \pi], \tag{3.2}$$

$$\gamma_1 \in [0, 2\pi], \quad \gamma_2 \in \left[0, \frac{\pi}{2}\right], \quad \gamma_3 \in [0, \pi], \quad \gamma_4 \in \left[0, \frac{\pi}{2}\right], \quad \gamma_5 \in [0, 2\pi], \quad \gamma_6 \in [0, \pi],$$

$$\gamma_7 \in \left[0, \frac{\pi}{2}\right], \quad \gamma_8 \in [0, \pi].$$

From (2.9) one could easily find the (bi)invariant metric. The corresponding invariant measure is

$$d\mu_{G_2} = \tfrac{27}{32}\sin^5\alpha_6 \cos\alpha_5 \sin^3\alpha_5 \sin(2\alpha_2) d\mu_{SU(3)} d\alpha_6\, d\alpha_5\, d\alpha_4\, d\alpha_3\, d\alpha_2\, d\alpha_1. \tag{3.3}$$

$d\mu_{SU(3)}$ being the invariant measure over SU(3) as given in Appendix A.

This is a quite simple parametrization for G_2, which evidences the SU(3) subgroup, as a fiber over S^6. It should be useful for implementing analytical or numerical computations in lattice gauge theory and in random matrix models.

The approach employed here to determine the range of parameters, is mainly a geometrical one. The same results could also be obtained by means of topological arguments of the type developed in Ref. 1.

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APPENDIX A: EULER PARAMETRIZATION FOR SU(3)

The Euler parametrization for SU(3) can be easily obtained as (again the ranges could be found using the topological method, however we simply rearranged the results shown in Appendix B of Ref. 3 to our case)

$$SU(3)[\gamma_1,\ldots,\gamma_8] = e^{\gamma_1 C_3} e^{\gamma_2 C_2} e^{\gamma_3 C_3} e^{\gamma_4 C_5} e^{\sqrt{3}\gamma_5 C_8} e^{\gamma_6 C_3} e^{\gamma_7 C_2} e^{\gamma_8 C_3}, \tag{A1}$$

with range

$$\gamma_1 \in [0,2\pi], \quad \gamma_2 \in \left[0,\frac{\pi}{2}\right], \quad \gamma_3 \in [0,\pi], \quad \gamma_4 \in \left[0,\frac{\pi}{2}\right], \tag{A2}$$

$$\gamma_5 \in [0,2\pi], \quad \gamma_6 \in [0,\pi], \quad \gamma_7 \in \left[0,\frac{\pi}{2}\right], \quad \gamma_8 \in [0,\pi].$$

In this way $\gamma_1, \gamma_2, \gamma_3$ cover an SU(2) subgroup, the γ_5 covers an U (1) and $\gamma_6, \gamma_7, \gamma_8$ cover SO (3). The resulting invariant measure is

$$d\mu_{SU(3)} = \sqrt{3}\sin(2\gamma_2)\sin^3\gamma_4 \cos\gamma_4 \sin(2\gamma_7) \prod_{i=1}^{8} d\gamma_i. \tag{A3}$$

APPENDIX B: J_h CURRENTS

Here we give the currents J_h used to generate the metric on the base manifold. The required relations follow from the commutators matrix given in Appendix C and are given by

$$e^{-xC_3} C_2 e^{xC_3} = \cos(2x) C_2 + \sin(2x) C_1,$$

$$e^{-xC_3} C_1 e^{xC_3} = \cos(2x) C_1 - \sin(2x) C_2,$$

$$e^{-xC_2} C_3 e^{xC_2} = \cos(2x) C_3 + \sin(2x) C_1,$$

$$e^{-xC_5} C_1 e^{xC_5} = \cos x C_1 + \sin x C_6,$$

$$e^{-xC_5}C_2e^{xC_5} = \cos xC_2 + \sin xC_7,$$

$$e^{-xC_5}C_3e^{xC_5} = \frac{1}{4}(3+\cos(2x))C_3 - \frac{1}{2}\sin(2x)C_4 - \frac{\sqrt{3}}{2}\sin^2 xC_8,$$

$$e^{-xC_5}C_8e^{xC_5} = \frac{1}{4}(1+3\cos(2x))C_3 - \frac{\sqrt{3}}{2}\sin(2x)C_4 - \frac{\sqrt{3}}{2}\sin^2 xC_3,$$

$$e^{-\sqrt{3}xC_9}C_4e^{\sqrt{3}xC_9} = \cos^3 xC_4 - \sin^3 xC_7 + \sqrt{3}\cos x\sin^2 xC_{11} - \sqrt{3}\sin x\cos^2 xC_{14},$$

$$e^{-\sqrt{3}xC_9}C_5e^{\sqrt{3}xC_9} = \cos^3 xC_5 + \sin^3 xC_6 + \sqrt{3}\cos x\sin^2 xC_{12} + \sqrt{3}\sin x\cos^2 xC_{13},$$

$$e^{-\sqrt{3}xC_9}C_6e^{\sqrt{3}xC_9} = \cos^3 xC_6 - \sin^3 xC_5 + \sqrt{3}\cos x\sin^2 xC_{13} - \sqrt{3}\sin x\cos^2 xC_{12},$$

$$e^{-\sqrt{3}xC_9}C_7e^{\sqrt{3}xC_9} = \cos^3 xC_7 + \sin^3 xC_4 + \sqrt{3}\cos x\sin^2 xC_{14} + \sqrt{3}\sin x\cos^2 xC_{11},$$

$$e^{-\sqrt{3}xC_9}C_8e^{\sqrt{3}xC_9} = \cos(2x)C_8 + \sin(2x)C_{10}, \tag{B1}$$

along with the fact that C_9 commutes with C_1, C_2, and C_3.

If we set

$$s_1 = -\sin(2\alpha_2)\cos(2\alpha_3)\mathrm{d}\alpha_1 + \sin(2\alpha_3)\mathrm{d}\alpha_2,$$

$$s_2 = \sin(2\alpha_2)\sin(2\alpha_3)\mathrm{d}\alpha_1 + \cos(2\alpha_3)\mathrm{d}\alpha_2,$$

$$s_3 = \cos(2\alpha_2)\mathrm{d}\alpha_1 + \mathrm{d}\alpha_3, \tag{B2}$$

the resulting currents are shown to be

$$J_h^1 = \cos\alpha_5 s_1,$$

$$J_h^2 = \cos\alpha_5 s_2,$$

$$J_h^3 = \tfrac{1}{4}(3+\cos(2\alpha_5))s_3 - \tfrac{3}{4}\sin^2\alpha_5\,\mathrm{d}\alpha_4,$$

$$J_h^4 = -\frac{1}{2}\sin(2\alpha_5)\cos^3\frac{\alpha_6}{2}\left[s_3 + \frac{3}{2}d\alpha_4\right] + \sin a_5\sin^3\frac{\alpha_6}{2}s_2,$$

$$J_h^5 = -\sin\alpha_5\sin^3\frac{\alpha_6}{2}s_1 + \cos^3\frac{\alpha_6}{2}\mathrm{d}\alpha_5,$$

$$J_h^6 = \cos\alpha_5\sin^3\frac{\alpha_6}{2}s_1 + \sin^3\frac{\alpha_6}{2}\mathrm{d}\alpha_5,$$

$$J_h^7 = \frac{1}{2}\sin(2\alpha_5)\sin^3\frac{\alpha_6}{2}\left[s_3 + \frac{3}{2}\mathrm{d}\alpha_4\right] + \sin\alpha_5\cos^3\frac{\alpha_6}{2}s_2,$$

$$J_h^8 = \cos\alpha_6\left[\frac{1}{4}(1+3\cos(2\alpha_5)) - \frac{\sqrt{3}}{2}\sin^2\alpha_5 s_3\right],$$

$$J_h^9 = \frac{\sqrt{3}}{2} \mathrm{d}\alpha_6,$$

$$J_h^{10} = \frac{\sqrt{3}}{2} \sin\alpha_6 \left[\frac{1}{4}(1 + 3\cos(2\alpha_5))\mathrm{d}\alpha_4 - \sin^2\alpha_5 s_3 \right],$$

$$J_h^{11} = -\frac{\sqrt{3}}{2} \sin(2\alpha_5)\cos\frac{\alpha_6}{2}\sin^2\frac{\alpha_6}{2}\left[s_3 + \frac{3}{2}\mathrm{d}\alpha_4 \right] + \sqrt{3}\sin\alpha_5 \sin\frac{\alpha_6}{2}\cos^2\frac{\alpha_6}{2} s_2,$$

$$J_h^{12} = -\sqrt{3}\sin\alpha_5 \sin\frac{\alpha_6}{2}\cos^2\frac{\alpha_6}{2} s_1 + \sqrt{3}\cos\frac{\alpha_6}{2}\sin^2\frac{\alpha_6}{2}\mathrm{d}\alpha_5,$$

$$J_h^{13} = \sqrt{3}\sin\alpha_5 \cos\frac{\alpha_6}{2}\sin^2\frac{\alpha_6}{2} s_1 + \sqrt{3}\sin\frac{\alpha_6}{2}\cos^2\frac{\alpha_6}{2}\mathrm{d}\alpha_5,$$

$$J_h^{14} = \frac{\sqrt{3}}{2}\sin(2\alpha_5)\sin\frac{\alpha_6}{2}\cos^2\frac{\alpha_6}{2}\left[s_3 + \frac{3}{2} d\alpha_4 \right] + \sqrt{3}\sin\alpha_5 \cos\frac{\alpha_6}{2}\sin^2\frac{\alpha_6}{2} s_2. \tag{B3}$$

These currents, together with the SU(3) currents (as given in Ref. 3 can be used in (2.9) to compute the full (bi-)invariant metric of G_2.

APPENDIX C: THE COMMUTATORS MATRIX

We find

$$B = \begin{pmatrix}
0 & 2C_3 & -2C_2 & C_7 & C_6 & -C_5 & -C_4 & 0 & 0 & 0 & C_{14} & C_{13} & -C_{12} & -C_{11} \\
* & 0 & 2C_1 & -C_6 & C_7 & C_4 & -C_5 & 0 & 0 & 0 & -C_{13} & C_{14} & C_{11} & -C_{12} \\
* & * & 0 & C_5 & -C_4 & C_7 & -C_6 & 0 & 0 & 0 & C_{12} & -C_{11} & C_{14} & -C_{13} \\
* & * & * & 0 & C_3+\sqrt{3}C_8 & -C_2 & C_1 & -\sqrt{3}C_5 & -C_{14} & -C_{13} & 0 & 0 & C_{10} & C_9 \\
* & * & * & * & 0 & C_1 & C_2 & \sqrt{3}C_4 & C_{13} & -C_{14} & 0 & 0 & -C_9 & C_{10} \\
* & * & * & * & * & 0 & C_3-\sqrt{3}C_8 & \sqrt{3}C_7 & -C_{12} & C_{11} & -C_{10} & C_9 & 0 & 0 \\
* & * & * & * & * & * & 0 & -\sqrt{3}C_6 & C_{11} & C_{12} & -C_9 & -C_{10} & 0 & 0 \\
* & * & * & * & * & * & * & 0 & \frac{2}{\sqrt{3}}C_{10} & -\frac{2}{\sqrt{3}}C_9 & -\frac{1}{\sqrt{3}}C_{12} & \frac{1}{\sqrt{3}}C_{11} & \frac{1}{\sqrt{3}}C_{14} & -\frac{1}{\sqrt{3}}C_{13} \\
* & * & * & * & * & * & * & * & 0 & \frac{2}{\sqrt{3}}C_8 & C_7-\frac{2}{\sqrt{3}}C_{14} & \frac{2}{\sqrt{3}}C_{13}-C_6 & C_5-\frac{2}{\sqrt{3}}C_{12} & \frac{2}{\sqrt{3}}C_{11}-C_4 \\
* & * & * & * & * & * & * & * & * & 0 & \frac{2}{\sqrt{3}}C_{13}+C_6 & \frac{2}{\sqrt{3}}C_{14}+C_7 & -\frac{2}{\sqrt{3}}C_{11}-C_4 & -\frac{2}{\sqrt{3}}C_{12}+C_5 \\
* & * & * & * & * & * & * & * & * & * & 0 & -\frac{1}{\sqrt{3}}C_8+C_3 & \frac{2}{\sqrt{3}}C_{10}-C_2 & -\frac{2}{\sqrt{3}}C_9+C_1 \\
* & * & * & * & * & * & * & * & * & * & * & 0 & \frac{2}{\sqrt{3}}C_9+C_1 & \frac{2}{\sqrt{3}}C_{10}+C_2 \\
* & * & * & * & * & * & * & * & * & * & * & * & 0 & \frac{1}{\sqrt{3}}C_8+C_3 \\
* & * & * & * & * & * & * & * & * & * & * & * & * & 0
\end{pmatrix}.$$

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Discrete vakonomic mechanics

Roberto Benito[a] and David Martín de Diego[b]
Instituto de Matemáticas y Física Fundamental, CSIC, Serrano 123, 28006 Madrid, Spain

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Discretizations of vakonomic mechanics are developed by using the methodology of variational integrators. The resulting algorithms are symplectic (in some sense that we will explain) and preserve the momentum map associated with a Lie group of symmetries. A specific example illustrating the theory is tested numerically. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2008214]

I. INTRODUCTION

This paper is devoted to the so-called vakonomic mechanics, a terminology coined by Arnold and Kozlov (see Ref. 1). Vakonomic mechanics are obtained from a Lagrangian function subject to nonholonomic constraints, but instead of using Lagrange-d'Alembert principle as in nonholonomic mechanical systems, one uses a variational principle, that is, one looks for extremals of the integral functional determined by the Lagrangian among all the curves satisfying the constraints (see Refs. 3, 7, and 19). As we will briefly discuss, vakonomic mechanics describe interesting and applied problems such as optimal control theory, mathematical economics (for instance, economic growth theory), sub-Riemannian geometry, motion of microorganisms, etc.

In this paper, we will develop variational integrators for this kind of problem. Variational integrators are symplectic integrators,[26] preserving momentum and they are known to have near-energy preservation behavior. These integrators have their roots in the optimal control literature in the 1960s and 1970s (see Ref. 4) and recently, they were studied by many authors from a more geometrical point of view (Refs. 13, 20, 8, 9, and 29, and references therein).

Throughtout the paper, Einstein convention will be used without explicit mention.

A. Vakonomic mechanics

Vakonomic mechanics were introduced by V. V. Kozlov in Ref. 16, see also Ref. 1. Such systems are defined by a regular Lagrangian $\mathbb{L}:TQ\to\mathbb{R}$ on the tangent bundle TQ of the configuration space Q subject to nonholonomic constraints $\phi^\alpha(q,\dot{q})=0$, $1\leqslant\alpha\leqslant m$, determining a $2n-m$ dimensional submanifold M of TQ. We will take fibered coordinates $(q^A,\dot{q}^A)$ in TQ.

These systems are usually described by the extended Lagrangian $\mathcal{L}=\mathbb{L}+\lambda_\alpha\phi^\alpha$, which includes the Lagrange multipliers λ_α as new extra variables. The equations of motion for the vakonomic problem are the Euler-Lagrange equations for $\mathcal{L}$; that is

$$\begin{cases}\dfrac{\mathrm{d}}{\mathrm{d}t}\left(\dfrac{\partial\mathbb{L}}{\partial\dot{q}}\right)-\dfrac{\partial\mathbb{L}}{\partial q}=-\dot{\lambda}_\alpha\dfrac{\partial\phi^\alpha}{\partial\dot{q}}-\lambda_\alpha\left[\dfrac{\mathrm{d}}{\mathrm{d}t}\left(\dfrac{\partial\phi^\alpha}{\partial\dot{q}}\right)-\dfrac{\partial\phi^\alpha}{\partial q}\right],\\ \phi^\alpha(q,\dot{q})=0,1\leqslant\alpha\leqslant m,\end{cases}\tag{1}$$

Observe that the Lagrangian $\mathcal{L}:T(Q\times\mathbb{R}^m)\to\mathbb{R}$ is degenerate, since the extra velocities $\dot{\lambda}^\alpha$ do not appear. Therefore, it is necessary to apply the Dirac-Bergmann-Gotay-Nester constraint procedure developed in Ref. 12 in order to find, if it exists, a final constraint submanifold where the

[a]Electronic mail: rbenito@imaff.cfmac.csic.es
[b]Electronic mail: d.martin@imaff.cfmac.csic.es

dynamics of the vakonomic problem are well defined (see Refs. 21 and 5). Thus, Eq. (1) has solution on the final constraint submanifold (see Ref. 21 for more details).

Moreover, solutions to Eq. (1) are exactly the same as the solutions obtained extremizing the functional $\mathcal{J}=\int_0^1 \mathbb{L}(\dot{c}(t))\mathrm{d}t$, among the curves satisfying the constraints. Precisely, for this type of system it was coined the name *vakonomic* (mechanics of variational axiomatic kind) in Ref. 1.

An interesting remark is that Eq. (1) is expressed in terms of the ambient Lagrangian $\mathbb{L}:TQ \to \mathbb{R}$, but, from the above description, these equations only depend on $\widetilde{\mathbb{L}}=\mathbb{L}_{|M}:M\to\mathbb{R}$, the restriction of $\mathbb{L}$ to M (see Ref. 6, and references therein).

Recently, the second author and collaborators[6] proposed an intrinsic version of vakonomic mechanics. First, they consider the Whitney sum of T^*Q and TQ: $T^*Q\oplus TQ$ and its submanifold $W_0=T^*Q\times_Q M$. Let $\pi_1:T^*Q\times_Q M\to T^*Q$ and $\pi_2:T^*Q\times_Q M\to M$ be the canonical projections. Define in $T^*Q\times_Q M$ the presymplectic two-form $\omega=\pi_1^*\omega_Q$, where ω_Q is the canonical symplectic form in T^*Q, and the Hamiltonian function $H=\langle\pi_1,\pi_2\rangle-\pi_2^*\widetilde{\mathbb{L}}$ where $\widetilde{\mathbb{L}}:M\to\mathbb{R}$ is the restriction of $\mathbb{L}$ to M. Therefore, vakonomic dynamics are intrinsically described by the equation $i_X\omega=dH$ of the presymplectic system $(T^*Q\times_Q M,\omega,H)$.

B. Vakonomic mechanics: Applications

The main goal of the following is to illustrate from different points of view the importance of developing geometric integrators, showing different applications of vakonomic mechanics.

1. Optimal control theory

It is well known that the dynamics of a large class of engineering and economic systems can be expressed as a set of differential equations

$$\dot{q}^A=\Gamma^A(q(t),u(t)),\quad 1\leqslant A\leqslant n, \tag{2}$$

where t is the time, q^A, $1\leqslant A\leqslant n$, denote the state variables, and u^a, $1\leqslant a\leqslant m$, the control inputs to the system that must be specified. Given an initial condition of the state variables and given control inputs, we completely know the trajectory of the state variables $q(t)$ (all the functions are assumed to be at least C^2).

With a fixed initial condition, usually $q_0=q(t_0)$, our aim is to find a C^2-piecewise smooth curve $\gamma(t)=(q(t),u(t))$, satisfying the control equations (2) and minimizing the functional

$$\mathcal{J}(\gamma)=\int_{t_0}^{T} L(q(t),u(t))\mathrm{d}t, \tag{3}$$

for some fixed and given final time $T\in\mathbb{R}^+$. The integral $\int_{t_0}^{T}L(q(t),u(t))\mathrm{d}t$ depends on the time history (from t_0 to T) of the state variables and the control inputs.

A necessary condition for the solutions of such problem is provided by Pontryaguin's maximum principle. If we construct the pseudo-Hamiltonian function:

$$H(q,p,u)=p_A\Gamma^A(q,u)-L(q,u) \tag{4}$$

where p_A, $1\leqslant A\leqslant n$, are now considered as Lagrange's multipliers, then a curve $\gamma:[t_0,T]\to C$, $\gamma(t)=(q(t),u(t))$, is an optimal trajectory if there exist functions $p_A(t)$, $1\leqslant A\leqslant n$, such that

$$\begin{cases} \dot{q}^A(t) = \dfrac{\partial H}{\partial p_A}(q(t),p(t),u(t)), \\ \dot{p}_A(t) = -\dfrac{\partial H}{\partial q^A}(q(t),p(t),u(t)), \\ 0 = \dfrac{\partial H}{\partial u^a} \end{cases} \tag{5}$$

jointly with transversality conditions: $q(t_0)=q_0$ and $p(T)=0$.

In a global description, one assumes a fiber bundle structure $\pi: C \to Q$, where Q is the configuration manifold with local coordinates (q^A) and C is the bundle of controls, with coordinates (q^A, u^a), $1 \leqslant A \leqslant n$, $1 \leqslant a \leqslant m$.

The ordinary differential equations (2) on Q depending on the parameters u can be seen as a vector field Γ along the projection map π, that is, Γ is a smooth map $\Gamma: C \to TQ$ such that the diagram

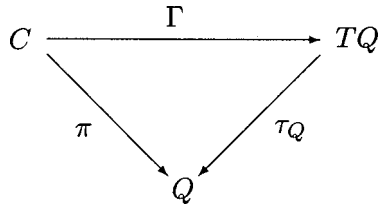

is commutative, where $\tau_Q: TQ \to \mathbb{R}$ is the canonical projection. This vector field is locally written as $\Gamma = \Gamma^A(q,u)(\partial/\partial q^A)$.

Next, we will show that optimal control problems, under adequate regularity assumptions, can be reformulated in terms of vakonomic dynamics (see Ref. 21 for an alternative approach).

Proposition 1.1: Suppose that $\Gamma: C \to TQ$ is an embedding, then if we denote by $G: \Gamma(C) \to C$ the diffeomorphism such that $\Gamma \circ G = \mathrm{id}_C$, we have that the solutions of the optimal control problem

$$extremize \int_{t_0}^{T} L(q(t),u(t))\mathrm{d}t$$

subject to $\dot{q} = \Gamma(q,u)$ are solutions of the vakonomic problem determined by the function $\bar{L}: \Gamma(C) \to \mathbb{R}$, where $\bar{L} = L \circ G$, and the constraint submanifold $\Gamma(C)$.

Conversely, if we have a vakonomic problem given by (i) a submanifold M of TQ, verifying that $\tau_Q: M \to Q$ is a surjective submersion, (ii) the Lagrangian $\mathbb{L}: TQ \to \mathbb{R}$; then the solutions of the vakonomic problem are the solutions of the optimal control problem determined by $C = M$ and $L = \mathbb{L}_{|M}$.

Proof: Using Pontryaguin's maximum principle, an optimal trajectory $(q(t),u(t))$ of the optimal control problem satisfies

$$\begin{cases} \dot{q}^A = \Gamma^A(q,u), \\ \dot{p}_A = \dfrac{\partial L}{\partial q^A} - p_B \dfrac{\partial \Gamma^B}{\partial q^A}, \\ 0 = -\dfrac{\partial L}{\partial u^a} + p_B \dfrac{\partial \Gamma^B}{\partial u^a}. \end{cases} \tag{6}$$

Since Γ is an embedding we can consider local coordinates $(\tilde{q}^A, \tilde{u}^a)$ such that

$$\Gamma: (\tilde{q}^A, \tilde{u}^a) \to (\tilde{q}^A, \tilde{u}^a, \Psi^\alpha(\tilde{q},\tilde{u})), \quad 1 \leqslant A \leqslant N, \quad 1 \leqslant a \leqslant m, \quad 1 \leqslant \alpha \leqslant n-m.$$

Observe that $\dot{\tilde{q}}^a = \tilde{u}^a$ and $\dot{\tilde{q}}^\alpha = \Psi^\alpha(\tilde{q}^A, \tilde{u}^a)$.

Rewriting Eq. (6) in terms of these coordinates:

$$\begin{cases} \dot{\tilde{q}}^{\alpha} = \Psi^{\alpha}(\tilde{q},\tilde{u}), \\ \dot{\tilde{q}}^{a} = \tilde{u}^{a}, \\ \dot{p}_A = \dfrac{\partial \bar{L}}{\partial \tilde{q}^A} - p_{\alpha}\dfrac{\partial \Psi^{\alpha}}{\partial \tilde{q}^A}, \\ 0 = -\dfrac{\partial \bar{L}}{\partial \tilde{q}^a} + p_a + p_{\alpha}\dfrac{\partial \Psi^{\alpha}}{\partial \tilde{q}^a}, \end{cases} \tag{7}$$

which are the vakonomic equations obtained in Ref. 6 (see also Ref. 14). The converse is trivial.■

Example 1.2 Optimal control and a particle in a magnetic field: (See Ref. 2, p. 353 for a detailed exposition)

Consider the optimal control problem

$$\min \int (u^2 + v^2)\mathrm{d}t$$

subject to equations $\dot{x}=u$, $\dot{y}=v$, $\dot{z}=A_1(x,y)u+A_2(x,y)v$. Obviously it is equivalent to the vakonomic problem given by $\mathbb{L}=\frac{1}{2}(\dot{x}^2+\dot{y}^2)$ and the nonholonomic constraint $\dot{z}=A_1(x,y)\dot{x}+A_2(x,y)\dot{y}$.

2. SubRiemannian geometry

A subRiemannian structure on a manifold is a generalization of a Riemannian structure where the metric is only defined on a vector subbundle of the tangent bundle to the manifold. In such case, the notion of length is only assigned to a subclass of curves, namely curves with tangent vectors belonging to the vector subbundle for each point.[18,23,28] More precisely, consider an n-dimensional manifold equipped with a smooth distribution D of constant rank $n-m$. A *subRiemannian metric* on D consists of giving a positive definite quadratic form g_q on $\mathcal{D}_q$ smoothly varying in q. We will say that a piecewise smooth curve γ in Q is *admissible* if $\dot{\gamma}(t) \in D_{\gamma(t)}$ for all t. Using g, it is possible to define the length

$$\mathrm{length}(\gamma) = \int_0^h \sqrt{g(\dot{\gamma}(t),\dot{\gamma}(t))}\mathrm{d}t$$

for admissible curves $\gamma:[0,h]\to Q$. From this definition, we define the distance between two points $x,y \in Q$ as

$$\mathrm{d}(x,y) = \inf_{\gamma}(\mathrm{length}(\gamma)),$$

if there exists admissible curves γ connecting x and y; in other case, the distance is considered infinite. A curve which realizes the distance between two points is called a *minimizing subRiemannian geodesic*. Let $\mu_1,\ldots,\mu_m$ be a basis of one-forms for the annihilator D^o. Then, an admissible path must verify the nonholonomic constraints

$$\mu_i(\dot{\gamma}) = 0, \quad 1 \leqslant i \leqslant m. \tag{8}$$

Therefore, it is clear that the problem of finding minimizing subRiemannian geodesics is exactly the same as the vakonomic problem determined by the restricted Lagrangian $\widetilde{L}=\frac{1}{2}g$ and the nonholonomic constraints (8).

3. Economic growth theory

Optimization is a crucial topic in dynamic economic analysis. Therefore, variational calculus (free or constrained) and optimal control theory play an important role as fundamental tools.[15,27] A typical optimization problem in modern economics deals with extremizing the functional

$$\int_0^T \rho(t)U[f(t,k,\dot{k})]\mathrm{d}t$$

subject or not to constraints. Here, $\rho(t)$ is a discount rate factor, U an utility function, f a consumption function, and k the capital-labor ratio.

For instance, a classical example is the closed von Neumann system,[25] given by a transformation function $F(K_1,\ldots,K_n,\dot{K}_1,\ldots,\dot{K}_n)$ which relates n capital goods $K_1,K_2,\ldots,K_n$ and the net capital formations $\dot{K}_1,\dot{K}_2,\ldots,\dot{K}_n$. The von Neumann problem consists of maximizing the functional $\int_0^T \dot{K}_n \mathrm{d}t$ subject to $F(K_1,\ldots,K_n,\dot{K}_1,\ldots,\dot{K}_n)=0$.

C. Discrete variational calculus

Now, we will briefly describe discrete variational calculus, following the approach in Refs. 29 and 20. A discrete Lagrangian is a map $\mathbb{L}_d: Q\times Q\to\mathbb{R}$ (this discrete Lagrangian may be considered as an approximation of the continuous Lagrangian $\mathbb{L}: TQ\to\mathbb{R}$). Define the action sum $S_d: Q^{N+1}\to\mathbb{R}$ corresponding to the Lagrangian $\mathbb{L}_d$ by

$$S_d=\sum_{k=1}^{N}\mathbb{L}_d(q_{k-1},q_k),$$

where $q_k\in Q$ for $0\leqslant k\leqslant N$.

Observe that for any covector $\alpha\in T^*_{(x_1,x_2)}(Q\times Q)$, we have the decomposition $\alpha=\alpha_1+\alpha_2$ where $\alpha_i\in T^*_{x_i}Q$, thus,

$$\mathrm{d}\mathbb{L}_d(q_0,q_1)=D_1\mathbb{L}_d(q_0,q_1)+D_2\mathbb{L}_d(q_0,q_1).$$

The discrete variational principle states that the solutions of the discrete system determined by $\mathbb{L}_d$ must extremize the action sum given fixed points q_0 and q_N. Extremizing S_d over q_k, we obtain the following system of difference equations:

$$D_1\mathbb{L}_d(q_k,q_{k+1})+D_2\mathbb{L}_d(q_{k-1},q_k)=0,\quad 1\leqslant k\leqslant N-1. \tag{9}$$

These equations are usually called the *Discrete Euler-Lagrange equations*. Under some regularity hypothesis (the matrix $(D_{12}\mathbb{L}_d(q_k,q_{k+1}))$ is regular), it is possible to define a discrete flow $\Upsilon: Q\times Q\to Q\times Q$, by $\Upsilon(q_{k-1},q_k)=(q_k,q_{k+1})$ from Eq. (9).

Define the discrete Legendre transformation associated with $\mathbb{L}_d$ by

$$\mathbb{FL}_d: Q\times Q\to T^*Q$$

$$(q_0,q_1)\mapsto(q_0,-D_1\mathbb{L}_d(q_0,q_1)),$$

and the two-form $\omega_d=F\mathbb{L}_d^*\omega_Q$, where ω_Q is the canonical symplectic form on T^*Q. The discrete algorithm determined by Υ preserves the symplectic form ω_d, i.e., $\Upsilon^*\omega_d=\omega_d$. Moreover, if the discrete Lagrangian is invariant under the diagonal action of a Lie group G, then the discrete momentum map $J_d: Q\times Q\to\ ^*$ defined by $\langle J_d(q_k,q_{k+1}),\xi\rangle=\langle D_2\mathbb{L}_d(q_k,q_{k+1}),\xi_Q(q_{k+1})\rangle$ is preserved by the discrete flow. Therefore, these integrators are symplectic-momentum preserving. Here, ξ_Q is the fundamental vector field determined by $\xi\in\ $, the Lie algebra of G.

II. A GEOMETRIC APPROACH TO VAKONOMIC MECHANICS

In this section we obtain the equations of motion for vakonomic mechanics from a different point of view which, in Sec. III, will be useful in the construction of variational integrators.

Let Q be the configuration manifold of dimension n and TQ its tangent bundle with $\mathbb{L}$ the Lagrangian function $\mathbb{L}:TQ\to\mathbb{R}$. Consider the constraints $\phi^\alpha:TQ\to\mathbb{R}$, $1\leqslant\alpha\leqslant m$, and the augmented Lagrangian

$$\widetilde{\mathbb{L}}:TQ\times\mathbb{R}^m\to\mathbb{R}$$

$$(v_q,\lambda)\mapsto(\mathbb{L}+\lambda_\alpha\phi^\alpha)(v_q)$$

where summation over the repeated indexes α is understood.

Consider also the fiber derivative:

$$\mathbb{F}\widetilde{\mathbb{L}}:TQ\times\mathbb{R}^m\to T^*Q$$

$$(v_q,\lambda)\mapsto \mathrm{d}(\widetilde{\mathbb{L}}|_{T_qQ\times\{\lambda\}})(v_q)$$

which in local coordinates is

$$\mathbb{F}\widetilde{\mathbb{L}}(q^A,\dot{q}^A,\lambda_\alpha)=\left(q^A,\frac{\partial\widetilde{\mathbb{L}}}{\partial\dot{q}^A}(q^A,\dot{q}^A,\lambda_\alpha)\right). \tag{10}$$

Now, we can define a two-form ω in $TQ\times\mathbb{R}^m$ by pulling back by $\mathbb{F}\widetilde{\mathbb{L}}$ the canonical symplectic two-form ω_Q on T^*Q; that is, $\omega=\mathbb{F}\widetilde{\mathbb{L}}^*(\omega_Q)$. In local coordinates we have

$$\omega=\mathbb{F}\widetilde{\mathbb{L}}^*(\mathrm{d}q^A\wedge\mathrm{d}p_A)=\mathrm{d}q^A\wedge d\left(\frac{\partial\widetilde{\mathbb{L}}}{\partial\dot{q}^A}\right)=\frac{\partial^2\widetilde{\mathbb{L}}}{\partial\dot{q}^A\partial q^B}\mathrm{d}q^A\wedge\mathrm{d}q^B+\frac{\partial^2\widetilde{\mathbb{L}}}{\partial\dot{q}^A\partial\dot{q}^B}\mathrm{d}q^A\wedge\mathrm{d}\dot{q}^B+\frac{\partial^2\widetilde{\mathbb{L}}}{\partial\lambda_\alpha\partial\dot{q}^A}\mathrm{d}q^A\wedge\mathrm{d}\lambda_\alpha.$$

The energy function associated with the augmented Lagrangian $\widetilde{\mathbb{L}}$ is: $E_{\widetilde{\mathbb{L}}}=\Delta\widetilde{\mathbb{L}}-\widetilde{\mathbb{L}}$ where Δ stands for the Liouville vector field on TQ. Locally, $\Delta=\dot{q}^A(\partial/\partial\dot{q}^A)$ and $E_{\widetilde{\mathbb{L}}}=\dot{q}^A(\partial\widetilde{\mathbb{L}}/\partial\dot{q}^A)-\widetilde{\mathbb{L}}$.

Next, we will see how the dynamics of the vakonomic system determined by $(\mathbb{L},\phi^\alpha)$ is determined by the solutions of

$$i_X\omega=dE_{\widetilde{\mathbb{L}}}. \tag{11}$$

Observe that the system $(TQ\times\mathbb{R}^m,\omega,E_{\widetilde{\mathbb{L}}})$ is a presymplectic system (see Ref. 12).

In what follows, we will assume that

$$\widetilde{\mathcal{W}}=\left(\frac{\partial^2\widetilde{\mathbb{L}}}{\partial\dot{q}^A\partial\dot{q}^B}\right)=\left(\frac{\partial^2\mathbb{L}}{\partial\dot{q}^A\partial\dot{q}^B}+\lambda_\alpha\frac{\partial^2\phi_\alpha}{\partial\dot{q}^A\partial\dot{q}^B}\right)$$

is regular (see Ref. 1).

First, note that

$$\mathrm{d}E_{\widetilde{\mathbb{L}}}=\dot{q}^A\frac{\partial^2\widetilde{\mathbb{L}}}{\partial\dot{q}^A\partial q^B}\mathrm{d}q^B+\dot{q}^A\frac{\partial^2\widetilde{\mathbb{L}}}{\partial\dot{q}^A\partial\dot{q}^B}\mathrm{d}\dot{q}^B+\dot{q}^A\frac{\partial\phi^\alpha}{\partial\dot{q}^A}\mathrm{d}\lambda_\alpha-\frac{\partial\widetilde{\mathbb{L}}}{\partial q^A}\mathrm{d}q^A-\frac{\partial\widetilde{\mathbb{L}}}{\partial\lambda_\alpha}\mathrm{d}\lambda_\alpha.$$

Now let

$$\xi = X^A \frac{\partial}{\partial q^A} + Y^A \frac{\partial}{\partial \dot{q}^A} + Z_\alpha \frac{\partial}{\partial \lambda_\alpha}$$

be a generic vector field on $TQ \times \mathbb{R}^m$, a direct computation shows that $i_\xi \omega = \mathrm{d}E_{\tilde{\mathbb{L}}}$ if and only if X^A, Y^A, and Z_α satisfy the following conditions:

$$\begin{cases} X^A = \dot{q}^A, \\ \dfrac{\partial \tilde{\mathbb{L}}}{\partial \lambda_\alpha} = 0, \\ \dfrac{\partial \tilde{\mathbb{L}}}{\partial q^A} = X^B \dfrac{\partial^2 \tilde{\mathbb{L}}}{\partial \dot{q}^A \partial q^B} + Y^B \dfrac{\partial^2 \tilde{\mathbb{L}}}{\partial \dot{q}^A \partial \dot{q}^B} + Z_\alpha \dfrac{\partial^2 \tilde{\mathbb{L}}}{\partial \lambda_\alpha \partial \dot{q}^A}. \end{cases}$$

The first of these conditions implies the SODE character of the equations on q's, the second one is just the statement $\phi^\alpha = 0$ (the constraint conditions). Therefore, $M_1 = \{(v_q, \lambda) \in TQ \times \mathbb{R}^m / \phi^\alpha(v_q) = 0\}$ is the first constraint submanifold after applying the Dirac-Bergmann-Gotay-Nester algorithm[11,12] to the presymplectic system $(TQ \times \mathbb{R}^m, \omega, E_{\tilde{\mathbb{L}}})$.

If we suppose that $\gamma(t) = (q(t), \dot{q}(t), \lambda(t))$ is an integral curve for ξ, the following equations must hold along γ:

$$\begin{cases} \dfrac{\partial \tilde{\mathbb{L}}}{\partial q^A} = \dot{q}^B \dfrac{\partial^2 \tilde{\mathbb{L}}}{\partial \dot{q}^A \partial q^B} + \ddot{q}^B \dfrac{\partial^2 \tilde{\mathbb{L}}}{\partial \dot{q}^A \partial \dot{q}^B} + \dot{\lambda}_\alpha \dfrac{\partial^2 \tilde{\mathbb{L}}}{\partial \lambda_\alpha \partial \dot{q}^A}, \\ \phi^\alpha = 0. \end{cases}$$

Since

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \tilde{\mathbb{L}}}{\partial \dot{q}^A} \right) = \dot{q}^B \frac{\partial^2 \tilde{\mathbb{L}}}{\partial \dot{q}^A \partial q^B} + \ddot{q}^B \frac{\partial^2 \tilde{\mathbb{L}}}{\partial \dot{q}^A \partial \dot{q}^B} + \dot{\lambda}_\alpha \frac{\partial^2 \tilde{\mathbb{L}}}{\partial \lambda_\alpha \partial \dot{q}^A},$$

if we expand $\tilde{\mathbb{L}} = \mathbb{L} + \lambda_\alpha \phi^\alpha$ then we obtain (1), which are exactly the vakonomic equations of motion for the constrained system given by $(\mathbb{L}, \phi^\alpha)$, $\alpha = 1, \ldots, m$.

The solutions on M_1 may not be tangent to M_1. In such case, we have to restrict M_1 to the submanifold M_2 where there exists a solution tangent to M_1. Proceeding further, we obtain a sequence of submanifolds (assuming that all the subsets generated by the algorithm are submanifolds, in other case see Ref. 17)

$$\cdots \hookrightarrow M_k \hookrightarrow \cdots \hookrightarrow M_2 \hookrightarrow M_1 \hookrightarrow M_0 = TQ \times \mathbb{R}^m.$$

If this constraint algorithm stabilizes, i.e., if there exists a positive integer $k \in \mathbb{N}$ such that $M_{k+1} = M_k$ and $\dim M_k \neq 0$, then we would have a final constraint submanifold $M_f = M_k$ on which a vector field X exists such that

$$(i_X \omega = dE_{\tilde{\mathbb{L}}})_{|M_f}.$$

An interesting case is when the final constraint submanifold is just M_1, say $M_f = M_1$. Additionally, observe that $\dim M_1 = 2n$. Denote by ω_{M_1} the restriction of the presymplectic two-form ω to W_1 and by $\tilde{\mathcal{C}}_2 = (\tilde{C}_{A\alpha})$ the $n \times m$ matrix with entries $\tilde{C}_{A\alpha} = \partial \phi^\alpha / \partial \dot{q}^A$.

Proposition 2.1: (M_1, ω_{M_1}) *is a symplectic manifold if and only if, for any choice of coordinates* $(q^A, \dot{q}^A, \lambda_\alpha)$ *on* $TQ \times \mathbb{R}^m$ *and every point in* M_1,

$$\begin{pmatrix} \tilde{\mathcal{W}} & \tilde{\mathcal{C}}_2 \\ \tilde{\mathcal{C}}_2^T & \mathbf{0}_{m \times m} \end{pmatrix}$$

is invertible.

Proof: It is proved following the same arguments as in Theorem 4.2. ■

Observe that if (M_1,ω_{M_1}) is a symplectic manifold then $(\mathbb{F}\widetilde{\mathbb{L}})_1=\mathbb{F}\widetilde{\mathbb{L}}\circ i_{M_1}:M_1\to T^*Q$ is a symplectomorphism (see Ref. 1, p. 34, for more details), where $i_{M_1}:M_1\hookrightarrow TQ\times\mathbb{R}^m$ is the canonical inclusion.

III. A DISCRETE ALGORITHM FOR VARIATIONAL CONSTRAINED OPTIMIZATION

In this section, inspired by our last geometric approach to vakonomic mechanics, we develop a numerical integrator that preserves, as we shall discuss later, certain structures naturally associated with this system.

Given an n-dimensional configuration space Q, a Lagrangian function $\mathbb{L}:TQ\to\mathbb{R}$, and constraints $\phi^\alpha:TQ\to\mathbb{R}$, $1\leqslant\alpha\leqslant m$, let $\mathbb{L}_d:Q\times Q\to\mathbb{R}$ and $\phi_d^\alpha:Q\times Q\to\mathbb{R}$ be discrete versions of these Lagrangian and constraints, respectively.[29]

Thus we can consider the following problem of static constrained optimization which will be called the discrete version of constrained variational calculus (or discrete vakonomic mechanics):

$$\begin{cases}\min \mathbb{S}(q_0,q_1,\ldots,q_N) & \text{with fixed } q_0 \text{ and } q_N\\ \text{subject to } \phi_d^\alpha(q_k,q_{k+1})=0, & 1\leqslant\alpha\leqslant m,\ 0\leqslant k\leqslant N-1,\end{cases}\tag{12}$$

where $\mathbb{S}(q_0,q_1,\ldots,q_N)=\Sigma_{k=0}^{N-1}\mathbb{L}_d(q_k,q_{k+1})$ stands for the discrete action. Observe that the system is subjected to $N\cdot m$ constraint functions.

Considering (12) as a typical constrained optimization problem, we define a discrete augmented Lagrangian $\widetilde{\mathbb{L}}_d(x,y,\lambda)=\mathbb{L}_d(x,y)+\lambda_\alpha\phi_d^\alpha(x,y)$ on $Q\times Q\times\mathbb{R}^m$ and the associated unconstrained discrete variational problem:

$$\begin{cases}\min \widetilde{\mathbb{S}}(q_0,q_1,\ldots,q_N,\lambda^0,\lambda^1,\ldots,\lambda^{N-1}) & \text{with fixed } q_0 \text{ and } q_N\\ q_k\in Q, \quad \lambda_k\in\mathbb{R}^m \quad k=0,\ldots,N-1, & q_N\in Q,\end{cases}\tag{13}$$

where $\widetilde{\mathbb{S}}(q_0,q_1,\ldots,q_N,\lambda^0,\lambda^1,\ldots,\lambda^{N-1})=\Sigma_{k=0}^{N-1}\widetilde{\mathbb{L}}_d(q_k,q_{k+1},\lambda^k)=\Sigma_{k=0}^{N-1}[\mathbb{L}_d(q_k,q_{k+1})+\lambda_\alpha^k\phi_d^\alpha(q_k,q_{k+1})]$ where λ^k is an m-vector with components $\lambda_\alpha^k, 1\leqslant\alpha\leqslant m$.

The critical points of problem (13), will be those annihilating $\partial\widetilde{\mathbb{S}}/\partial q_k$, $k=1,\ldots,N-1$ (q_0 and q_N are fixed) and the constraints equations ($\partial\widetilde{\mathbb{S}}/\partial\lambda^k=0, k=0,\ldots,N-1$). Thus, the *discrete vakonomic equations* are:

$$\begin{cases}D_1\mathbb{L}_d(q_k,q_{k+1})+D_2\mathbb{L}_d(q_{k-1},q_k)+\lambda_\alpha^k D_1\phi_d^\alpha(q_k,q_{k+1})+\lambda_\alpha^{k-1}D_2\phi_d^\alpha(q_{k-1},q_k)=0, \quad 1\leqslant k\leqslant N-1,\\ \phi_d^\alpha(q_k,q_{k+1})=0, \quad 1\leqslant\alpha\leqslant m, \quad 0\leqslant k\leqslant N-1\end{cases}.\tag{14}$$

In the sequel, we will use the notation $D_{12}F$ to denote the $n\times n$ matrix $(\partial^2F/\partial x^A\partial y^B)$ for any C^2-function $F:Q\times Q\to\mathbb{R}$. Now, if the matrix

$$\begin{pmatrix} D_{12}\mathbb{L}_d+\lambda_\alpha D_{12}\phi_d^\alpha & \dfrac{\partial\phi_d^\alpha}{\partial x}\\ \left(\dfrac{\partial\phi_d^\alpha}{\partial y}\right)^T & \mathbf{0}_{m\times m}\end{pmatrix}\in\mathcal{M}_{(n+m)\times(n+m)}(\mathbb{R})$$

is invertible, then there exists a local discrete map:

$$\Phi:Q\times Q\times\mathbb{R}^m\to Q\times Q\times\mathbb{R}^m$$

$$(x,y,\lambda)\mapsto(y,v,\Lambda)$$

such that along solutions $(q_0,q_1,\ldots,q_N,\lambda^0,\lambda^1,\ldots,\lambda^{N-1})$ of Eq. (14) we have that

$$\Phi(q_{k-1},q_k,\lambda^{k-1}) = (q_k,q_{k+1},\lambda^k),$$

which is our integrator for the vakonomic problem.

Remark 3.1: In the case where the constraints are holonomic (i.e., $\phi^\alpha: Q \to \mathbb{R}$), we can choose (between many others) the discretization:

$$\phi_d^\alpha: Q \times Q \to \mathbb{R}$$

$$(q_0,q_1) \mapsto \phi^\alpha(q_0)$$

and then our procedure leads to the same equations as those proposed in Ref. 20 just for the holonomic case.

IV. SYMPLECTIC-MOMENTUM INTEGRATOR

In Sec. III, we have constructed a variational integrator for vakonomic mechanics. In what follows, we want to study the symplectic and momentum preserving character of this algorithm. First, it is necessary to make precise the sense in which Φ is symplectic and also to define a suitable discrete momentum map related obviously to the original continuous case.

A. Symplectic behavior

Consider the discrete fiber derivative

$$\mathbb{F}_d: Q \times Q \times \mathbb{R}^m \to T^*Q$$

$$(x,y,\lambda) \mapsto -D_1\tilde{\mathbb{L}}_d(x,y,\lambda) = -D_1\mathbb{L}_d(x,y) - \lambda_\alpha D_1\phi_d^\alpha(x,y) \in T_x^*Q.$$

Following the lines developed in Sec. II, we now define the two-form ω_d on $Q\times Q\times\mathbb{R}^m$ by pulling back the canonical symplectic two-form $\omega_Q = \mathrm{d}q^A \wedge \mathrm{d}p_A = -\mathrm{d}(p_A \mathrm{d}q^A)$ on T^*Q via $\mathbb{F}_d$; that is

$$\omega_d = \mathbb{F}_d^*(\omega_Q) = \mathrm{d}[D_1\mathbb{L}_d + \lambda_\alpha D_1\phi_d^\alpha]. \tag{15}$$

Thus, the coordinate expression for ω_d is

$$\omega_d(x,y,\lambda) = -\left[\frac{\partial^2\mathbb{L}_d}{\partial x^A \partial y^B}(x,y) + \lambda_\alpha \frac{\partial^2\phi_d^\alpha}{\partial x^A \partial y^B}(x,y)\right]\mathrm{d}x^A \wedge \mathrm{d}y^B + \frac{\partial\phi_d^\alpha}{\partial x^A}(x,y)\mathrm{d}\lambda_\alpha \wedge \mathrm{d}x^A. \tag{16}$$

Next, consider the constraint submanifold $\tilde{M}_d \subset Q\times Q$ determined by the vanishing of the constraints $\phi_d^\alpha = 0$, $1 \leqslant \alpha \leqslant m$, with canonical inclusion $j: \tilde{M}_d \times \mathbb{R}^m \hookrightarrow Q\times Q\times\mathbb{R}^m$, and the two-form $\omega_{\tilde{M}_d} = j^*\omega_d$. From the definition of Φ it is obvious that it applies $\tilde{M}_d \times \mathbb{R}^m$ onto itself. Our aim now is to prove that $(\Phi_{|\tilde{M}_d\times\mathbb{R}^m})^*\omega_{\tilde{M}_d} = \omega_{\tilde{M}_d}$.

Lemma 4.1:

$$\omega_d = \mathrm{d}(D_1\mathbb{L}_d + \lambda_\alpha D_1\phi_d^\alpha) = -\mathrm{d}(D_2\mathbb{L}_d + \lambda_\alpha D_2\phi_d^\alpha) - \mathrm{d}\phi_d^\alpha \wedge \mathrm{d}\lambda_\alpha$$

Proof:

$$\begin{aligned} 0 &= \mathrm{d}(d\mathbb{L}_d + \mathrm{d}(\lambda_\alpha\phi_d^\alpha)) = \mathrm{d}(D_1\mathbb{L}_d + D_2\mathbb{L}_d + \lambda_\alpha D_1\phi_d^\alpha + \lambda_\alpha D_2\phi_d^\alpha + \phi_d^\alpha d\lambda_\alpha) \\ &= \mathrm{d}(D_1\mathbb{L}_d + \lambda_\alpha D_1\phi_d^\alpha) + \mathrm{d}(D_2\mathbb{L}_d + \lambda_\alpha D_2\phi_d^\alpha) + d\phi_d^\alpha \wedge d\lambda_\alpha \end{aligned}$$

■

Now, properties of the pull-back, Eq. (14), and the above lemma imply that

$$\Phi^*\omega_d = \Phi^*[\mathrm{d}(D_1\mathbb{L}_d + \lambda_\alpha D_1\phi_d^\alpha)] = \mathrm{d}[\Phi^*(D_1\mathbb{L}_d + \lambda_\alpha D_1\phi_d^\alpha)] = \mathrm{d}[-(D_2\mathbb{L}_d + \lambda_\alpha D_2\phi_d^\alpha)]$$
$$= \mathrm{d}\,(D_1\mathbb{L}_d + \lambda_\alpha D_1\phi_d^\alpha)] + \mathrm{d}\phi_d^\alpha \wedge \mathrm{d}\lambda_\alpha = \omega_d + d\phi_d^\alpha \wedge d\lambda_\alpha$$

and then $(\Phi|_{\tilde{M}_d\times\mathbb{R}^m})^*\omega_{\tilde{M}_d} = \omega_{\tilde{M}_d}$ since $d\phi_d^\alpha$ vanishes on tangent vectors to $\tilde{M}_d$.

Observe now that $\tilde{M}_d \times \mathbb{R}^m$ is a $2n$-dimensional manifold. Therefore, it is a natural question to ask about conditions that ensure the symplectic character of the two-form $\omega_{\tilde{M}_d}$.

Theorem 4.2: *Suppose that the $n\times n$ matrix $\mathcal{A}=(D_{12}\mathbb{L}_d+\lambda_\alpha D_{12}\phi_d^\alpha)$ is invertible. Then $\omega_{\tilde{M}_d}$ is symplectic if and only if the matrix*

$$\begin{pmatrix} (D_{12}\mathbb{L}_d + \lambda_\alpha D_{12}\phi_d^\alpha) & \mathcal{C}_1 \\ \mathcal{C}_2^T & \mathbf{0}_{m\times m} \end{pmatrix}$$

is invertible. Here, $\mathcal{C}_1$ and $\mathcal{C}_2$ denote the $n\times m$ matrices:

$$\mathcal{C}_1 = ((\mathcal{C}_1)_{A\alpha}) = \left(\frac{\partial\phi_d^\alpha}{\partial x^A}\right) \text{ and } \mathcal{C}_2 = ((\mathcal{C}_2)_{A\alpha}) = \left(\frac{\partial\phi_d^\alpha}{\partial y^A}\right).$$

Proof: Let $\mathcal{C}$ be the $(2n+m)\times m$ matrix defined by

$$\mathcal{C} = \begin{pmatrix} \mathcal{C}_1 \\ \mathcal{C}_2 \\ \mathbf{0}_{m\times m} \end{pmatrix}.$$

Moreover, $\mathcal{B}$ is the $(2n+m)\times(2n+m)$ matrix defined by

$$\mathcal{B} = \begin{pmatrix} 0 & -\mathcal{A} & -\mathcal{C}_1 \\ \mathcal{A}^T & \mathbf{0}_{n\times n} & \mathbf{0}_{n\times m} \\ \mathcal{C}_1^T & \mathbf{0}_{m\times n} & \mathbf{0}_{m\times m} \end{pmatrix}.$$

The matrix $\mathcal{B}$ represents the two-form ω_d [see Eq. (16)] and then, the two-form $\omega_{\tilde{M}_d}$ is symplectic if and only if the following system of equations admits as unique solution $(X^A, Y^A, C^\alpha) = \mathbf{0}_{1\times(2n+m)}$:

$$\left.\begin{aligned} &(\tilde{X}^A, \tilde{Y}^A, \tilde{C}^\alpha)\cdot\mathcal{B}\cdot(X^A, Y^A, C^\alpha)^T = 0 \\ &(X^A, Y^A, C^\alpha)\cdot\mathcal{C} = \mathbf{0}_{1\times m} \end{aligned}\right\} \text{ for all } (\tilde{X}^A, \tilde{Y}^A, \tilde{C}^\alpha) \text{ verifying } (\tilde{X}^A, \tilde{Y}^A, \tilde{C}^\alpha)\cdot\mathcal{C} = \mathbf{0}_{1\times m}.$$

This problem is equivalent to the regularity of the $(2n+2m)\times(2n+2m)$ matrix:

$$\mathcal{D} = \begin{pmatrix} 0 & -\mathcal{A} & -\mathcal{C}_1 & -\mathcal{C}_1 \\ \mathcal{A}^T & \mathbf{0}_{n\times n} & \mathbf{0}_{n\times m} & -\mathcal{C}_2 \\ \mathcal{C}_1^T & \mathbf{0}_{m\times n} & \mathbf{0}_{m\times m} & \mathbf{0}_{m\times m} \\ \mathcal{C}_1^T & \mathcal{C}_2^T & \mathbf{0}_{m\times m} & \mathbf{0}_{m\times m} \end{pmatrix}.$$

Since the $n\times n$ matrix $\mathcal{A}$ is invertible, then so is the matrix in the upper left quarter part of $\mathcal{D}$ and, taking its Schur complement in $\mathcal{D}$ (see Ref. 24), the regularity of $\mathcal{D}$ is equivalent to

$$0 \neq \left| \begin{pmatrix} \mathcal{C}_1^T & \mathbf{0}_{m\times n} \\ \mathcal{C}_1^T & \mathcal{C}_2^T \end{pmatrix} \cdot \begin{pmatrix} \mathbf{0}_{n\times n} & (\mathcal{A}^T)^{-1} \\ (-\mathcal{A})^{-1} & \mathbf{0}_{n\times n} \end{pmatrix} \cdot \begin{pmatrix} -\mathcal{C}_1 & -\mathcal{C}_1 \\ \mathbf{0}_{n\times m} & -\mathcal{C}_2 \end{pmatrix} \right| = \begin{vmatrix} \mathbf{0}_{m\times m} & -\mathcal{C}_1^T(\mathcal{A}^T)^{-1}\mathcal{C}_2 \\ \mathcal{C}_2^T\mathcal{A}^{-1}\mathcal{C}_1 & \mathcal{C}_2^T\mathcal{A}^{-1}\mathcal{C}_1 - \mathcal{C}_1^T(\mathcal{A}^T)^{-1}\mathcal{C}_2 \end{vmatrix}$$

$$= \begin{vmatrix} \mathbf{0}_{m\times m} & -(\mathcal{C}_2^T\mathcal{A}^{-1}\mathcal{C}_1)^T \\ \mathcal{C}_2^T\mathcal{A}^{-1}\mathcal{C}_1 & \mathbf{0}_{m\times m} \end{vmatrix},$$

which is equivalent to the regularity of the matrix $\mathcal{C}_2^T\mathcal{A}^{-1}\mathcal{C}_1$, the Schur complement of $\mathcal{A}$ in the matrix:

$$\begin{pmatrix} \mathcal{A} & \mathcal{C}_1 \\ \mathcal{C}_2^T & \mathbf{0}_{m\times m} \end{pmatrix}$$

Therefore, this last matrix is invertible if and only $\omega_{\tilde{M}_d}$ is symplectic. ■

In the conditions of Theorem 4.2, the variational algorithm is symplectic.

Remark 4.3: The classical approach to constrained variational calculus is developed by using the extended Lagrangian $\mathcal{L}: T(Q\times\mathbb{R}^m)\to\mathbb{R}$ defined by $\mathcal{L}=L+\lambda_\alpha\phi_d^\alpha$. A natural discretization of this extended Lagrangian is

$$\mathcal{L}_d = \mathbb{L}_d + \lambda_\alpha\phi_d^\alpha,$$

where $\mathcal{L}_d: Q\times\mathbb{R}^m\times Q\times\mathbb{R}^m\to\mathbb{R}$. The action sum is

$$\widetilde{\mathbb{S}} = \sum_{k=0}^{N-1} \mathcal{L}_d(q_k,\lambda^k,q_{k+1},\lambda^{k+1}) = \sum_{k=0}^{N-1} (\mathbb{L}_d(q_k,q_{k+1}) + \lambda_\alpha^k\phi_d^\alpha(q_k,q_{k+1})),$$

where $q_k\in Q$ and $\lambda^k=(\lambda_\alpha^k)\in\mathbb{R}^m$.

The discrete Euler-Lagrange equations (DEL) are

$$D_1\mathcal{L}_d(q_k,\lambda^k,q_{k+1},\lambda^{k+1}) + D_2\mathcal{L}_d(q_{k-1},\lambda^{k-1},q_k,\lambda^k) = 0, \quad 1\leqslant k\leqslant N-1, \tag{17}$$

which are equivalent to

$$\begin{cases} D_1\mathbb{L}_d(q_k,q_{k+1}) + \lambda_\alpha^k D_1\phi_d^\alpha(q_k,q_{k+1}) + D_2\mathbb{L}_d(q_{k-1},q_k) + \lambda_\alpha^{k-1}D_2\phi_d^\alpha(q_{k-1},q_k) = 0, \\ \phi_d^\alpha(q_k,q_{k+1}) = 0. \end{cases}$$

Now, (17) are exactly (14). Observe that our procedure is more direct and, moreover, the analysis of the geometric properties is easier with the approach that we follow. For instance, observe that using the extended approach the final constraint submanifold,

$$\bar{M}_d = \{\phi_d^\alpha = 0\} \subset Q\times\mathbb{R}^m\times Q\times\mathbb{R}^m,$$

is *presymplectic* instead of symplectic.

B. Momentum preservation

Let $\mathbb{L}_d$ be the discrete Lagrangian and ϕ_d^α, $1\leqslant\alpha\leqslant m$ the discrete constraints. Suppose that $\mathbb{L}_d$ and ϕ_d^α are invariant under the diagonal action of a Lie group G on Q. Therefore, for any $\xi\in$ (where is the Lie algebra of G) we have:

$$\mathbb{L}_d(\exp(s\xi)q_k,\exp(s\xi)q_{k+1}) = \mathbb{L}_d(q_k,q_{k+1}), \tag{18}$$

$$\phi_d^\alpha(\exp(s\xi)q_k,\exp(s\xi)q_{k+1}) = \phi_d^\alpha(q_k,q_{k+1}),\ 1\leqslant\alpha\leqslant m \tag{19}$$

Consider the discrete momentum map

$$J_d: Q\times Q\times\mathbb{R}^m\to\ ^*$$

$$(x,y,\lambda) \mapsto J_d(x,y,\lambda): \quad \to \mathbb{R}$$

$$\xi \mapsto \langle D_2\mathbb{L}_d(x,y) + \lambda_\alpha D_2\phi_d^\alpha(x,y), \xi_Q(y)\rangle,$$

where ξ_Q is the infinitesimal generator of ξ.

Proposition 4.4: The flow $\Phi: Q\times Q\times\mathbb{R}^m \to Q\times Q\times\mathbb{R}^m$ *preserves the momentum map.*

Proof: Differentiating Eqs. (18) and (19) and taking $s=0$ we obtain the following two equations:

$$D_1\mathbb{L}_d(q_k,q_{k+1})\xi_Q(q_k) + D_2\mathbb{L}_d(q_k,q_{k+1})\xi_Q(q_{k+1}) = 0,$$

$$D_1\phi_d^\alpha(q_k,q_{k+1})\xi_Q(q_k) + D_2\phi_d^\alpha(q_k,q_{k+1})\xi_Q(q_{k+1}) = 0.$$

Multiplying the latter equation by λ_α^k, adding then the former equation, and using Eq. (14) then we have

$$\begin{aligned} &D_2\mathbb{L}_d(q_k,q_{k+1})\xi_Q(q_{k+1}) + \lambda_\alpha^k D_2\phi_d^\alpha(q_k,q_{k+1})\xi_Q(q_{k+1}) \\ &\quad = D_2\mathbb{L}_d(q_{k-1},q_k)\xi_Q(q_k) + \lambda_\alpha^{k-1} D_2\phi_d^\alpha(q_{k-1},q_k)\xi_Q(q_k) \end{aligned}$$

or

$$J_d[\Phi(q_{k-1},q_k,\lambda^{k-1})] = J_d(q_{k-1},q_k,\lambda^{k-1}).$$

■

Remark 4.5: Observe that, more generally, we may impose the condition of invariance of $\widetilde{\mathbb{L}}_d=\mathbb{L}_d+\lambda_\alpha\phi_d^\alpha$ instead of the stronger condition of invariance of $\mathbb{L}_d$ and ϕ_d^α, independently.

V. EXAMPLE: THE HEISENBERG SYSTEM

Define the differential one-form Θ in $Q=\mathbb{R}^3$ by

$$\Theta = \mathrm{d}z - y\mathrm{d}x + x\mathrm{d}y$$

and its associated distribution:

$$\mathcal{H}_{(x,y,z)} = \{\Theta(x,y,z)\}^0 = \{(v_1,v_2,v_3) \in \mathbb{R}^3 : v_3 - yv_1 + xv_2 = 0\},$$

which can be alternatively expressed as

$$\mathcal{H}_{(x,y,z)} = \mathrm{Span}\{(1,0,y),(0,-1,x)\}.$$

We can then compute the Lie bracket of both generators: $[(1,0,y),(0,-1,x)]=(0,0,2)$, which is not in $\mathcal{H}_{\{(x,y,z)\}}$, therefore the distribution is not integrable. In fact,

$$\mathbb{R}^3 = \mathrm{Span}\{(1,0,y),(0,-1,x),(0,0,2)\}$$

and, considered as a Lie algebra, it is just the Heisenberg algebra that one meets in quantum mechanics: $(1,0,y)$ and $(0,-1,x)$ corresponding to position and momentum operators and (0,0,2) to a multiple of the identity. Anyway, we have chosen the Heisenberg system just as an example of vakonomic dynamics[2,23] when we take the kinematic Lagrangian: $\mathbb{L}=\frac{1}{2}(\dot{x}^2+\dot{y}^2+\dot{z}^2)$ and force the velocity vectors of admissible curves to lie in the distribution $\mathcal{H}$; that is, we require that the solutions satisfy the nonholonomic constraint: $\phi=\dot{z}-y\dot{x}+x\dot{y}=0$. The equations for this vakonomic problem turn out to be

$$\begin{cases} \ddot{x} = 2\lambda\dot{y} + \dot{\lambda}y, \\ \ddot{y} = -2\lambda\dot{x} - \dot{\lambda}x, \\ \ddot{z} = \dot{\lambda}, \\ \dot{z} = y\dot{x} - x\dot{y}(\text{the constraint}), \end{cases} \tag{20}$$

supplied with initial conditions in positions and velocities or, alternatively, initial and final conditions in positions.

Let us now consider the action of the group

$$G = S^1 = \{e^{i\alpha}, \alpha \in [0,2\pi]\} = \left\{ \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 & 0 \\ \sin\alpha & \cos\alpha & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} : \alpha \in [0,2\pi] \right\}$$

over $\mathbb{R}^3 \times \mathbb{R}$:

$$\Phi^Q : G \times \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}^3 \times \mathbb{R}$$

$$(e^{i\alpha}, (x,y,z,\lambda)) \mapsto (x\cos\alpha - y\sin\alpha, x\sin\alpha + y\cos\alpha, z, \lambda),$$

which induces an action of G over $T(\mathbb{R}^3 \times \mathbb{R}) \simeq \mathbb{R}^3 \times \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}$:

$$\Phi^{TQ}(e^{i\alpha}, (x,y,z,\lambda), (v_1,v_2,v_3,v_4)) = (\Phi^Q(e^{i\alpha}, (x,y,z,\lambda)), (v_1\cos\alpha - v_2\sin\alpha, v_1\sin\alpha + v_2\cos\alpha, v_3, v_4))$$

and, due to the fact that G leaves invariant the augmented Lagrangian $\tilde{L}$, the momentum map $J_{\tilde{L}}$ provide us a *conserved quantity:*

$$J_{\tilde{L}}((x,y,z,\lambda),(v_1,v_2,v_3,v_4)): \quad \to \mathbb{R}$$

$$\xi \mapsto (xv_2 - v_1 y + \lambda(x^2 + y^2))\xi$$

Therefore, along solution curves, the function:

$$f : T(\mathbb{R}^3 \times \mathbb{R}) \to \mathbb{R}$$

$$(x,y,z,\lambda,\dot{x},\dot{y},\dot{z},\dot{\lambda}) \mapsto x\dot{y} - \dot{x}y + \lambda(x^2 + y^2)$$

remains constant.

Vakonomic integrator. We turn now to our discrete scheme. First, we select the usual discretization of variables when we are on vector spaces (as is the case): $x = (x_0 + x_1)/2$; $\dot{x} = (x_1 - x_0)/h$; and the analogue for $y, \dot{y}, z, \dot{z}$. Then the discretization of the Lagrangian and constraint function results on

$$\mathbb{L} = \frac{1}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2), \quad \mathbb{L}_d = \frac{1}{2h^2}[(x_1 - x_0)^2 + (y_1 - y_0)^2 + (z_1 - z_0)^2],$$

$$\phi = \dot{z} - y\dot{x} + x\dot{y}, \quad \phi_d = \frac{1}{h}(z_1 - z_0 + x_0 y_1 - x_1 y_0).$$

After some computing, we find that

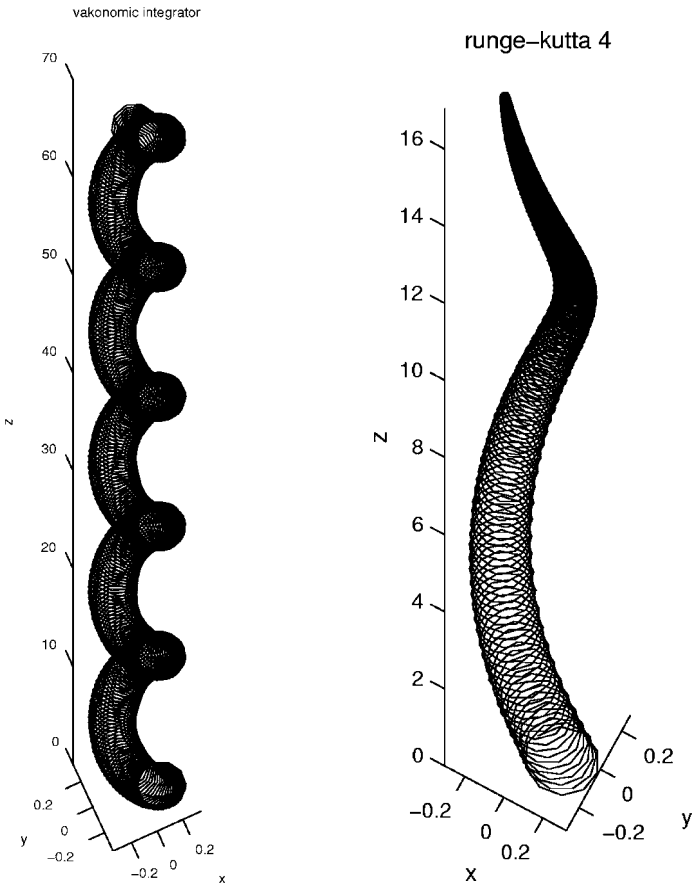

FIG. 1. Vakonomic integrator and Runge-Kutta.

$$\begin{pmatrix} (D_{12}\mathbb{L}_d + \lambda_\alpha D_{12}\phi_d^\alpha) & D_1\phi_d^\alpha \\ (D_2\phi_d^\alpha)^T & 0 \end{pmatrix}_{|(x_0,y_0,z_0,x_1,y_1,z_1,\lambda^0)} = \frac{1}{h^2}\begin{pmatrix} -1 & -\lambda^0 h & 0 & hy_1 \\ \lambda^0 h & -1 & 0 & -hx_1 \\ 0 & 0 & -1 & -h \\ -hy_0 & hx_0 & h & 0 \end{pmatrix}$$

whose determinant is equal to $(1+(\lambda^0)^2h^2)(1+y_1y_0+x_1x_0)=1+O(h^2)$. We can run our method for h enough small such that the discrete vakonomic equations become

$$\begin{cases} 0 = -x_2 + 2x_1 - x_0 + h(\lambda^1 y_2 - \lambda^0 y_0), \\ 0 = -y_2 + 2y_1 - y_0 + h(\lambda^0 x_0 - \lambda^1 x_2), \\ 0 = -z_2 + 2z_1 - z_0 + h(\lambda^0 - \lambda^1), \\ 0 = z_2 - z_1 + x_1 y_2 - x_2 y_1, \end{cases}$$

which are a discrete version of the continuous equations at the end of the last paragraph and can be solved with initial conditions (x_0,y_0,z_0,λ^0) and (x_1,y_1,z_1) or initial and final conditions (x_0,y_0,z_0,λ^0) and (x_N,y_N,z_N), all them satisfying the constraint $\phi_d=0$. In the first case, resolution of the vakonomic equations gives us (x_2,y_2,z_2,λ^1), and from it and (x_1,y_1,z_1) we obtain (x_3,y_3,z_3,λ^2) and so on. To compare our method with the classical four-order Runge-Kutta method (RK4), we write Eq. (20) as follows:

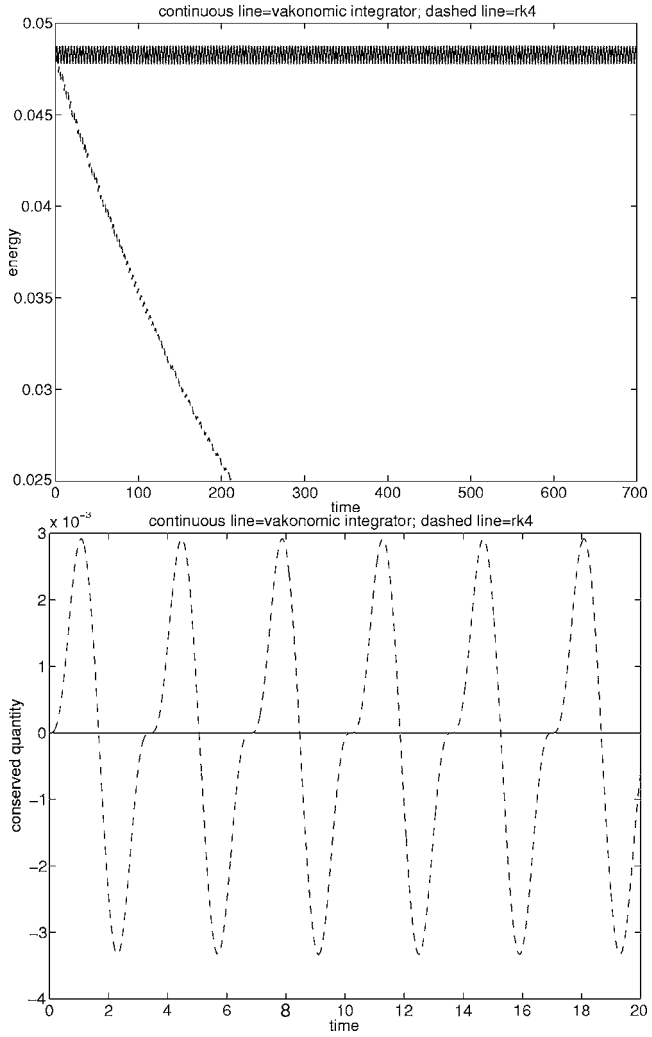

FIG. 2. Energy behavior and preservation of the discrete momentum map.

$$\begin{cases} \dot{x} = u, \\ \dot{y} = v, \\ \dot{z} = yu - xv, \\ \dot{\lambda} = \dfrac{-2\lambda(xu+yv)}{1+x^2+y^2}, \\ \dot{u} = 2\lambda v + y\left(\dfrac{-2\lambda(xu+yv)}{1+x^2+y^2}\right), \\ \dot{v} = -2\lambda u - x\left(\dfrac{-2\lambda(xu+yv)}{1+x^2+y^2}\right). \end{cases} \tag{21}$$

Then, we apply RK4 to Eq. (21) with $h=0.35$, $N=4000$ and initial conditions: $x_0=y_0=z_0=0$; $u_0=0.1$; $v_0=0.3$; $\lambda^0=1$. We also use these initial conditions, together with the (x_1,y_1,z_1) calculated by RK4, to start the vakonomic integrator (Fig. 1). Results and comparison of energies are shown in Fig. 2 (left). They show that the variational integrator behavior is much better in the long time running.

Observe that Φ^Q induces an action on $\mathbb{R}^3\times\mathbb{R}^3$:

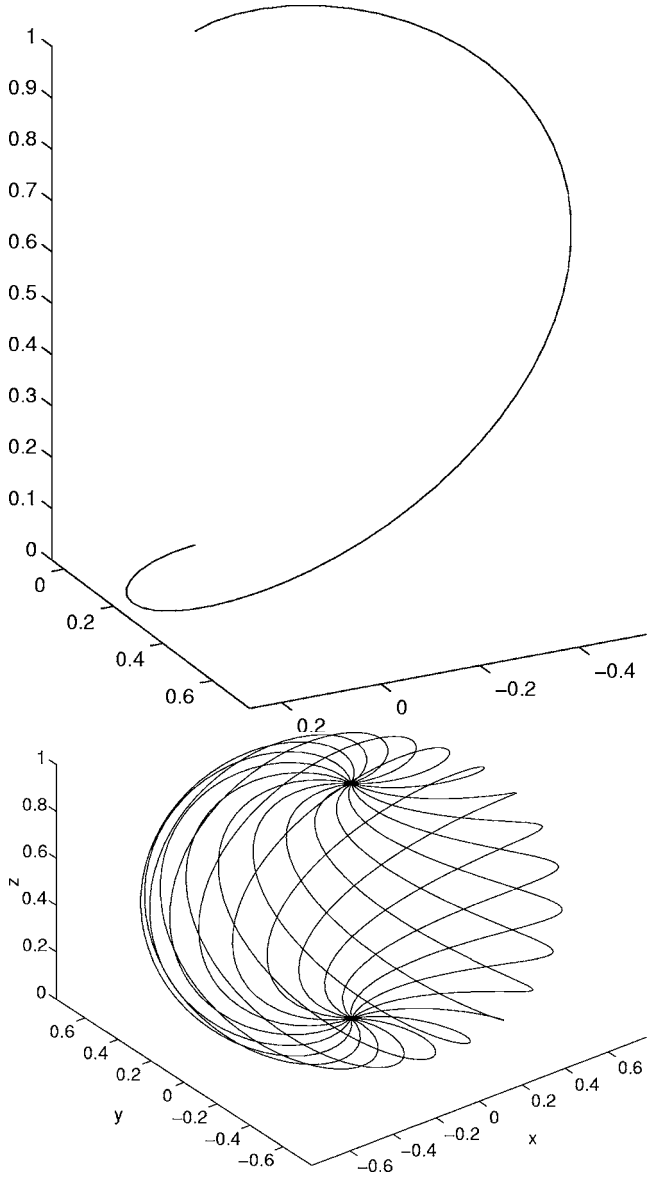

FIG. 3. Initial and final conditions.

$$\Phi_d : G \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3 \times \mathbb{R}^3$$

and, being ϕ_d and L_d invariants under the action of G, the discrete momentum map J_d:

$$J_d(x_0, y_0, z_0, x_1, y_1, z_1, \lambda): \quad \to \mathbb{R}$$

$$\xi \mapsto (y_1 x_0 - x_1 y_0 + \lambda h(x_0 x_1 + y_0 y_1))\xi$$

gives us the following conserved quantity:

$$f_d = y_1 x_0 - x_1 y_0 + \lambda^0 h(x_0 x_1 + y_0 y_1).$$

Figure 2 (on the right) shows the behavior of f_d for the variational integrator and RK4, respectively. Initial conditions are the same as those for Fig. 1 while the step has been reduced to $h=0.01$ and the number of steps has been reduced to $N=2000$. It is shown that RK4 does not preserve f_d even in better conditions for its implementation.

In the case, where initial and final conditions (x_0,y_0,z_0) and (x_N,y_N,z_N) are given, we set a system of $4(N-1)$ equations taking $h=T/N$ where T is the time in which the final position is reached. Then, we solve that system by using Newton's method. Figure 3 (on the left) shows the result for the problem of connecting the origin with the point (0,0,1) with $N=50$, $T=10$. In Fig. 3 (on the right) we show some solutions after rotation using the symmetry of the problem (Refs. 10 and 22).

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Omar Maj[a)]
Physics Department "A. Volta," University of Pavia, I-27100 Pavia, Italy

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[a)]Electronic mail: maj@fisicavolta.unipv.it.

Introduction: Superconductivity and the Ginzburg–Landau model

Jacob Rubinstein
Department of Mathematics, Indiana University Bloomington, IN 47405, USA

Peter Sternberg
Department of Mathematics, Indiana University Bloomington, IN 47405, USA

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The Ginzburg–Landau model has met with phenomenal success in capturing the behavior of superconductors in a wide variety of settings. In particular, it has been used for many years to interpret experiments and to predict new results related to phase transitions, vortex creation and dynamics, Josephson junctions, etc. The papers in this volume cover a wide spectrum of topics of current interest in research on the Ginzburg–Landau model.

- The volume contains one review paper by Du on the numerical approximation of the Ginzburg–Landau model. In addition to finding special explicit solutions and asymptotic limits for the equations, it is useful to have solutions in general domains with general parameters. Additionally, efficient and accurate computations on the model allow one to conduct extensive numerical experimentation. Du reviews several numerical methods including finite elements, finite differences, and finite volumes.
  The rest of the volume consists of ten research papers covering a wide range of current topics in Ginzburg–Landau research.
- Alama and Bronsard study the effect of impurities on vortex formation and location for samples with large Ginzburg–Landau parameters. The impurities are modeled through a pinning term in the quartic potential appearing in the energy.
- It is well known that vortices exhibit a lattice structure in bulk samples. On the other hand, in finite samples, superconductivity concentrates near the boundary for magnetic fields just below the critical value H_{c3}. Almog's paper bridges the gap between these two regimes.
- Two of the papers in the volume deal with the time-dependent Ginzburg–Landau system. Baumann *et al.* close an important gap in the existence, uniqueness, and regularity theory for the three-dimensional time-dependent Ginzburg–Landau system by considering the interior problem coupled to the Maxwell equations on the exterior. Another intriguing problem in modeling the time-dependent problem is the nature of the boundary condition on the sample's surface. Most authors assume the supercurrent has only a tangential component at the boundary. However, a more appropriate condition seems to be that the total current (super plus normal) would have no normal component at the boundary. Berger examines this issue and derives conditions under which the supercurrent itself is indeed tangential to the boundary.
- There is considerable recent activity, both theoretical and experimental on mesoscopic superconducting samples. Because the domain size is of the same scale as the coherence length, the shape of the boundary plays a major role in the observed patterns and dynamics. One important topic is the formation and motion of vortices in such samples. Berdiyorov *et al.* study this problem in the London limit. Chibotaru *et al.* consider the phase transition curve $T(H)$ in small samples. It is known that singularites on the boundary, such as vertices in polygons, affect this curve. The authors numerically compute these phase transition curves in triangles, rectangles, and discs, and compare their results to their experimental observations.
- The Ginzburg–Landau model serves as a prototypical energy functional in several physical disciplines, in particular in liquid crystals. Berlyand and Khruslov study a variant of the Ginzburg–Landau model that incorporates small inclusions with very strong anchoring conditions. They find a canonical scaling for the model and homogenize it. Kim *et al.* exploit the

analogy between nematic liquid crystals and superconductors to predict the existence of topologically driven patterns in nematic liquid crystals. These patterns are reminiscent of persistent currents in superconductivity.

- The richness of the Ginzburg–Landau model is evidenced by an elaborate bifurcation picture controlled by several parameters in the problem. Kosugi *et al.* consider bifurcation diagrams for a one-dimensional Ginzburg–Landau model on a circle. This model serves as a paradigm for Little-Parks oscillations. The existence of a stable bifurcating branch from the normal state means that the phase transition is second order, i.e., smooth. Physically, a strong Meissner effect destabilizes the bifurcation branch and favors first-order phase transitions. Ma and Wang study the stability question and derive a general formula to determine whether or not the bifurcating branch is stable.

Pinning effects and their breakdown for a Ginzburg–Landau model with normal inclusions

Stan Alama[a] and Lia Bronsard[b]
Department of Mathematics and Statistics, McMaster University, Hamilton, Ontario, Canada L8S 4K1

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We study a Ginzburg–Landau model for an inhomogeneous superconductor in the singular limit as the Ginzburg–Landau parameter $\kappa=1/\epsilon\to\infty$. The inhomogeneity is represented by a potential term $V(\psi)=\frac{1}{4}(a(x)-|\psi|^2)^2$, with a given smooth function $a(x)$ which is assumed to become negative in finitely many smooth subdomains, the "normally included" regions. For bounded applied fields (independent of the Ginzburg–Landau parameter $\kappa=1/\epsilon\to\infty$) we show that the normal regions act as "giant vortices," acquiring large vorticity for large (fixed) applied field h_{ex}. For $h_{ex}=O(|\ln\epsilon|)$ we show that this pinning effect eventually breaks down, and free vortices begin to appear in the superconducting region where $a(x)>0$, at a point set which is determined by solving an elliptic boundary-value problem. The associated operators are strictly but not uniformly elliptic, leading to some regularity questions to be resolved near the boundaries of the normal regions. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2010354]

I. INTRODUCTION

In this article we study a two-dimensional Ginzburg–Landau model for an inhomogeneous superconductor with finitely many "normal" regions in the interior. Inhomogeneous Ginzburg–Landau models have been introduced in order to understand vortex pinning (see, e.g., Ref. 8). Typically, the inhomogeneity is introduced via a potential term

$$V(\psi)=\tfrac{1}{4}(a(x)-|\psi|^2)^2,$$

with real-valued function $a(x)$. Since $a(x)\sim(T_c-T)$, its spatial variation indicates that the critical temperature may vary within the sample. One expects that vortices will be drawn to the least strongly superconducting regions, at local minima of $a(x)$, and this phenomenon is called pinning. In most studies of pinning the coefficient $a(x)$ is assumed to be strictly positive in the sample (see, e.g., Refs. 5, 2, and 11), but a recent article by André *et al.*[4] considers the interesting case where $a(x)=0$ at finitely many isolated points. These pinning points represent defects where the material assumes normal conductivity. In this paper we consider the case where $a(x)<0$ in the pinning sites, and thus model "normal inclusions," open regions of normally conducting material in the interior of the superconducting sample.

Let $\mathcal{D}\subset\mathbf{R}^2$ be a smooth simply connected domain, $\psi\in H^1(\mathcal{D};\mathbf{C})$ the complex-valued order parameter, $A\in H^1(\mathcal{D};\mathbf{R}^2)$ the vector potential, $h=\operatorname{curl}A=\partial_x A_y-\partial_y A_x$, and h_{ex} a constant applied field. We define the energy:

[a]Electronic mail: alama@mcmaster.ca
[b]Electronic mail: bronsard@mcmaster.ca

$$E_\epsilon(\psi,A) := \int_{\mathcal{D}} \left\{ \frac{1}{2}|(\nabla - iA)\psi|^2 + \frac{1}{4\epsilon^2}[(|\psi|^2 - a(x))^2 - (a^-)^2] + \frac{1}{2}(h - h_{ex})^2 \right\} \mathrm{d}x. \tag{1.1}$$

Note that subtracting $(a^-)^2$ alters the usual inhomogeneous Ginzburg–Landau energy by a constant, which would give the highest order term $O(\epsilon^{-2})$ as $\epsilon \to 0$. Note that the energy density is still nonnegative everywhere in the sample $\mathcal{D}$. We assume the following conditions on $a(x)$;

(H1) $a(x) \in C^2(\bar{\mathcal{D}})$.

(H2) $\{x \in \bar{\mathcal{D}} : a(x) \leqslant 0\} = \overline{\cup_{j=1}^n \omega_j}$, with finitely many smooth, simply connected domains $\omega_j \subset\subset \mathcal{D}$.

(H3) $\nabla a(x) \neq 0$ for all $x \in \partial\omega_j$, $j = 1, \ldots, n$.

We define

$$\Omega = \mathcal{D} \setminus \{x : a(x) \leqslant 0\} = \mathcal{D} \setminus \left(\cup_{j=1}^n \overline{\omega_j} \right).$$

Note that it follows from the above-mentioned hypotheses that $a(x)$ is bounded away from zero on the exterior boundary $\partial\mathcal{D}$. In addition, we do not allow any isolated pinning points $a(x_0) = 0$: unlike the case studied in Ref. 4, we admit only normal inclusions with nonempty interior.

It is intuitively clear that (as long as the energy of minimizers remains small compared with $1/\epsilon^2$,) in the limit the order parameter's modulus $|\psi|$ will tend to $\sqrt{a^+(x)}$ in the bulk of the sample. In other words, the sets on which $a(x) < 0$ strongly penalize superconducting order and essentially act as holes punched in the domain. Thus the situation closely resembles the problem studied in our previous article,[3] in which a uniform superconductor (i.e., $a(x) \equiv 1$) occupied a multiply connected domain $\Omega = \mathcal{D} \setminus \cup_{j=1}^n \omega_j$, with finitely many holes ω_j. In Ref. 3 we present two results for different regimes of the applied field h_{ex}. First, we show that when the applied field is fixed (independent of ϵ) there are no interior vortices in Ω but the holes ω_j act as "giant vortices," with nonzero winding of the phase of ψ for large enough h_{ex}. There is an associated limiting problem which governs the distribution of vorticity among the holes, and these degrees are directly calculable from h_{ex}.

Next we pose the question: for which h_{ex} do vortices first appear in the bulk Ω, and at which locations? We show that interior vortices appear at $h_{ex} = O(|\ln \epsilon|)$. The appearance of interior vortices for the Ginzburg–Landau model in simply connected domains for fields of order $|\ln \epsilon|$ is well-known to physicists, and the mathematics of this phenomenon has been thoroughly and elegantly studied in works by Serfaty,[18,19] Sandier and Serfaty.[15,17] In our setting (as in the multiply connected case[3]) these "free" vortices coexist with giant vortices of high degree in each hole, and the location of the free vortices is precisely determined by maximizing an auxilliary function depending only on the geometry of the multiply connected domain Ω. We show that the vortices do not cluster near the holes ω_j, but choose to accumulate on one of a finite number of points or closed curves strictly contained within the bulk Ω.

Another related problem, arising in the context of Bose–Einstein condensates (BEC) is presented in Ref. 1. In the BEC problem, the condensate is assumed to be subjected to a uniform rotation ω which plays the role of the applied field in (1.1), but the vector potential $A = \omega(-x_2, x_1)$ is predetermined. In Ref. 1 the domain $\mathcal{D}$ is a disk, and $a(x)$ is chosen to be radial with a positive in a symmetric circular annulus Ω and negative in the hole. The negativity of a forces the order parameter to zero in the hole, and the situation is qualitatively very similar to having a doubly connected domain. The results of Ref. 1 are parallel to those in Ref. 3: one concerning pinning for bounded rotations, and one concerning the breakdown of pinning when the rotation $\omega = O(|\ln \epsilon|)$. In the second result, the vortices again appear far from the hole, and accumulate along a finite number of concentric circles with radii explicitly determined by the function

$a(x)$. Some care must be taken due to the vanishing of $a(x)$ near the boundary of the hole, and in Ref. 1 the radial symmetry of the domain was used to circumvent some technical points and focus on the qualitative nature of the results.

Our results in this article combine many aspects of both papers. The general scheme to find interior vortices will be along the same lines as in the multiply connected case,[3] and the vanishing (and negativity) of $a(x)$ will play a role much as in the BEC setting.[1] However, in Ref. 1 radial symmetry was used in an essential way to deal with many difficult technical problems arising due to the vanishing of $a(x)$ near the hole. In the general nonsymmetric setting many of these arguments rely on sharp estimates for solutions to boundary-value problems for elliptic operators which are strictly elliptic, but lose uniform ellipticity at each $\partial\omega_j$. (See, e.g., (1.4) in Sec. I A). In the radial case of [Ref. 1] these are obtained explicitly by integration; here we provide some regularity results near the boundary of the holes (see Sec. III). Even with these estimates the nonsymmetric setting requires substantial refinement of the analysis of vortices near the holes from Refs. 1 and 3, and so we provide full details of this analysis in Sec. V.

Our results can also be applied to the BEC context, and we make some remarks on this connection at the end of the Introduction.

We now give some more detailed description of the content of the paper. As mentioned above, the presence of the inhomogeneity $a(x)$ creates problems near the boundaries of the pinning sites. For starters, under our hypotheses, $\sqrt{a^+(x)} \notin H^1(\Omega)$, and this results in a singular boundary layer as $\epsilon \to 0$. Fortunately, a remarkable identity (see Lassoued and Mironescu[12]) allows us to split this singular part from the rest of the energy. Define a functional,

$$J_\epsilon(\eta) := \int_{\mathcal{D}} \left\{ \frac{1}{2}|\nabla \eta|^2 + \frac{1}{4\epsilon^2}[(\eta^2 - a(x))^2 - (a^-)^2] \right\} dx,$$

and let $\eta_\epsilon \in H^1(\mathcal{D};\mathbf{R})$ be the (unique) minimizer. With $u = \psi/\eta_\epsilon$ we have

$$E_\epsilon(\psi,A) = J_\epsilon(\eta_\epsilon) + \int_{\mathcal{D}} \left\{ \frac{\eta_\epsilon^2}{2}|\nabla_A u|^2 + \frac{\eta_\epsilon^4}{4\epsilon^2}(|u|^2 - 1)^2 + \frac{1}{2}(h - h_{ex})^2 \right\} dx =: J_\epsilon(\eta_\epsilon) + F_\epsilon(u,A),$$

and the object of interest becomes the reduced energy F_ϵ. We now consider various aspects of the problem separately.

A. A limiting energy

The most important consequence of the presence of holes is that there is a rich class of "vortexless" configurations. These are obtained as critical points of the limiting energy:

$$F_\infty(u,A) := \frac{1}{2}\int_\Omega a(x)|\nabla_A u|^2 dx + \frac{1}{2}\int_{\mathcal{D}} (h - h_{ex})^2,$$

for

$$u \in H^1_a(\Omega;S^1) := \left\{ u \in W^1(\Omega;S^1) : \|u\|^2_{H^1_a} := \int_\Omega a(x)|\nabla u|^2 dx < \infty \right\}, \tag{1.2}$$

and $A \in H^1(\mathcal{D};\mathbf{R}^2)$. Although these configurations cannot have any vortices in the sense of zeros of u in Ω, nevertheless they do exhibit vorticity around the holes ω_j due to the nontrivial topology of Ω. In Sec. III we study this minimization problem as a function of the applied field h_{ex}. We show that minimizers of the limit problem are completely characterized by the magnetic field $h = \operatorname{curl} A$, much in the same way that the harmonic conjugate function is used by Bethuel *et al.*[6] to solve the S^1-harmonic map problem. We have:

Theorem 1.1: *There exists a constant E_0 (independent of h_{ex}) such that*

$$\min_{(u,A)\in\mathcal{H}_\infty} F_\infty(u,A) = h_{ex}^2 E_0 + g(D_*;h_{ex}), \tag{1.3}$$

where $D_*=[D_1,\ldots,D_n]\in\mathbf{Z}^n$ minimizes

$$g(D;h_{ex}) := \pi(\vec{D}\cdot C\vec{D} - 2h_{ex}\vec{X}\cdot\vec{D}) = \pi\sum_{i,k=1}^{n} c_{i,k}D_iD_k - 2\pi h_{ex}\sum_{i=1}^{n} c_{0,i}D_i,$$

for a uniquely determined constant matrix $C=(C_{i,k})$ and constant vector $\vec{X}=(c_{0,1},\ldots,c_{0,n})$. The minimizers (u_*,A_*) of F_∞ satisfy $|u_*|=1$ almost everywhere in Ω, and $\deg(u_*;\partial\omega_j)=D_j$ for each $j=1,\ldots,n$.

The constants $C=(c_{i,j})$ and $\vec{X}$ are explicitly calculated from solutions to elliptic boundary-value problems in $\mathcal{D}$ (see Eq. (3.14)).

The optimal magnetic field $h_*=\operatorname{curl} A_*$ is given approximately by $h_*(x)\simeq h_{ex}(1-\zeta(x))$, where $\zeta(x)$ solves

$$-\nabla\left(\frac{1}{a(x)}\nabla\zeta\right)+\zeta=1 \text{ in } \Omega,$$

$$\zeta=0 \text{ on } \partial\Omega. \tag{1.4}$$

(Lemma 3.4 gives precise statement of this fact.) An analogous function was used in Ref. 3, and has been instrumental in the study, by Serfaty,[18] of vortices in simply connected domains, where it describes the vortexless Meissner phase. In a multiply connected domain there are many such phases, and ζ chooses the one which minimizes the energy of the limit problem. In particular, we will show in Sec. III that the degrees of the holes ω_j will be determined by h_{ex} and the boundary value of $\partial\zeta/\partial\nu$ on each ω_j, giving an explicit formula for each degree.

B. Vortex pinning in bounded fields

When h_{ex} is independent of ϵ we prove the convergence result below for minimizers of E_ϵ. Since our functionals E_ϵ, F_∞ are gauge invariant we must choose spaces $\mathcal{H}$, $\mathcal{H}_\infty$ (respectively) which fix a gauge. These are defined in Sec. II.

Theorem 1.2: *Let h_{ex} be fixed, $\vec{D}_*$ as in Theorem 1.1, and let $(\psi_\epsilon,A_\epsilon)$ be minimizers of E_ϵ in $\mathcal{H}$.*

(i) $E_\epsilon(\psi_\epsilon,A_\epsilon)-J_\epsilon(\eta_\epsilon)\to\min_{\mathcal{H}_\infty}F_\infty=h_{ex}^2E_0+g(D_*;h_{ex})$ *as* $\epsilon\to 0$.

(ii) $(\psi_\epsilon/\eta_\epsilon,A_\epsilon)\to(u_*,A_*)$ *strongly in* $H^1_{loc}(\Omega)\times H^1(\mathcal{D};\mathbf{R}^2)$, *with* (u_*,A_*) *minimizers of* F_∞.

According to Theorem 1.2 we can expect minimizers to have nontrivial winding for sufficiently large but bounded (in ϵ) fields h_{ex}. This is in contrast to the simply connected case where the solution exhibits no winding until the appearance of the first vortex, at applied fields of order $|\ln\epsilon|$. In our model, the minimizers undergo a sequence of transitions to higher and higher winding number as h_{ex} increases, although the ratios of the degrees among the holes ω_j remains fixed, modulo the discontinuous constraint that the degrees must be integers. The limit functional F_∞ completely describes the system for ϵ small, and minimization of F_∞ itself is completely characterized by the finite dimensional function g.

We note that Ginzburg–Landau solutions with nontrivial winding numbers in nonsimply connected domains have been studied by several authors; see for instance Refs. 10 and 13. In these cases there was no applied field, and the solutions obtained were local minimizers of the energy within a fixed homotopy class, representing the phenomenon of "permanent currents." Here our solutions will be the *global* minimizers, and the applied field and the topology of the domain work together to choose the homotopy class of the minimizers.

C. The breakdown of pinning in stronger fields

When the applied field attains $O(|\ln \epsilon|)$ the pinning effect breaks down, and vortices are nucleated in Ω, at a field strength and location determined by ζ. For this part of the paper, we impose an additional condition on $a(x)$:

(H4) $a(x)$ is real analytic in $\mathcal{D}$.

Under (H4), the function ζ is real-analytic in Ω, and hence also ζ/a, and consequently ζ/a attains its maximum on a set Γ with finitely many connected components. Those components could consist of *isolated points* inside Ω together with *closed curves* which may wind around one or more of the pinning sites ω_j. We will show that the vortices of any minimizer must be localized to the set Γ as $\epsilon \to 0$. We distinguish two possibilities:

Case A: Γ is a finite point set.

Case B: Γ contains at least one closed curve γ.

The nature of minimizers will be different in the two cases. In Case A, the situation is analogous to that of Ref. 17, in which it is shown that if vortices can only accumulate at a finite number of points in Ω then the total degree of all vortices is uniformly bounded in ϵ. In Case B, we have shown for a similar problem in the circular annulus[1] that the number of vortices accumulating on a circle diverges as $\ln|\ln \epsilon|$. In both cases, there is coexistence of large vorticity in the pinning sites with point vortices along Γ inside Ω. We expect to see similar phenomena in our setting.

As in Refs. 1 and 3, we express our minimizers $(\psi_\epsilon, A_\epsilon)$ as perturbations of the minimizers (u_*, A_*) of the limit energy F_∞ (with the given, ϵ-dependent applied field h_{ex}.) There is a technical problem to overcome, as minimization of the limit energy defines u_* in Ω, while ψ_ϵ is defined in the entire bulk $\mathcal{D}$. This difficulty affects mostly the upper bound on the energy; for the lower bound we merely neglect the condensation energy in each pinning site, which is expected to be very small. The ansatz $\psi_\epsilon = \eta_\epsilon u_* v_\epsilon$ in Ω, $A_\epsilon = A_* + A_v$ then leads to a further splitting of the energy, giving a new functional for (v_ϵ, A_v) which measures the internal energy of vortices in Ω and their interaction with the pinning sites (see Lemma 5.1).

Let us explain here what we mean by "vortices" in this paper. We locate the vortices by means of energy concentration, using the method of "vortex balls" of Sandier and Serfaty[16] to derive sharp lower bounds on the energy. Using the result of Ref. 16 we show (see Proposition 5.2) that minimizers have $|u| \simeq 1$ except in a finite number of balls $B_i = B_{s_i}(p_i)$ with vanishingly small total radii, $\Sigma s_i \leqslant |\ln \epsilon|^{-12}$. We associate a degree $d_i = \deg(u/|u|; \partial B_i) = \deg(\psi/|\psi|; \partial B_i)$ to each ball. We say that ψ has an *essential vortex* at $p_i \in \mathcal{A}_\rho$ if there is a vortex ball B_i centered at p_i with degree $d_i \neq 0$.

As in Ref. 1, the vanishing of a near $\partial\omega_j$ blurs the distinction between vortices close to the pinning sites and the pinning sites themselves. The energy cost and benefit of having vortices very close to a pinning site ω_j is very small, and may be too small to capture with our methods. Therefore, we excise a vanishingly small neighborhood of each ω_j, and speak only of vortices which lie outside that slightly enlarged hole. Let ρ_ϵ be chosen with $(\ln|\ln \epsilon|)^2/|\ln \epsilon|^{1/2} \ll \rho_\epsilon \ll 1$, and

$$\Omega_{\rho_\epsilon} := \{x \in \Omega : \mathrm{dist}(x, \cup_{j=1}^n \partial\omega_j) > \rho_\epsilon\}.$$

We then prove the following results for global minimizers:

Theorem 1.3: *Assume hypotheses (H1)–(H4), and* $h_{ex} = \lambda|\ln \epsilon| + \mu \ln|\ln \epsilon|$. *Let* $(\psi_\epsilon, A_\epsilon)$ *be minimizers of* E_ϵ. *Then*:

(i) *if either* $\lambda < \lambda_*$ *or both* $\lambda = \lambda_*$ *and* $\mu < \mu_*$, *then for all* ϵ *sufficiently small* ψ_ϵ *has no essential vortices in* Ω_{ρ_ϵ}: $\mathbf{D}_\epsilon := \Sigma_{p_i \in \Omega_{\rho_\epsilon}} |d_i| = 0$.

(ii) *if* $\lambda = \lambda_*$ *and* $\mu > \mu_*$ *then for all* ϵ *sufficiently small, any essential vortex in* Ω_{ρ_ϵ} *has positive degree and is localized on the set* Γ *in the following sense: there exists an* $M \in \mathbf{N}$ *such that if* p_i *are the centers of the vortex balls* B_i,

$$\sum_{\substack{d_i<0\\ p_i\in\Omega_{\rho_\epsilon}}} |d_i| + \sum_{\substack{\mathrm{dist}(p_i,\mathcal{C})>\\ [\ln\epsilon]^{-1/4M}\\ p_i\in\Omega_{\rho_\epsilon}}} |d_i| = 0$$

for all ϵ sufficiently small. Moreover, the total degree in Ω,

$$\mathbf{D}_\epsilon = \sum_{p_i\in\Omega_{\rho_\epsilon}} |d_i| = \sum_{\substack{\mathrm{dist}(p_i,\mathcal{C})<\\ [\ln\epsilon]^{-1/4M}\\ p_i\in\Omega_{\rho_\epsilon}}} d_i \leqslant \begin{cases} C & \text{in Case A,} \\ C\ln|\ln\epsilon| & \text{in Case B.} \end{cases}$$

for $C=C(\mu)$ independent of ϵ.

(iii) *in Case B, there exists $\mu_\#>0$ so that whenever $\mu\geqslant\mu_\#$ and $\lambda=\lambda_*$, then $\mathbf{D}_\epsilon\geqslant c\ln|\ln\epsilon|$ for c independent of ϵ.*

(iv) *if γ is any simple closed curve in Ω, homotopic to $\partial\omega_j$ for some $j\in\{1,\ldots,n\}$, which does not wind around any subset of Γ, then for all ϵ sufficiently small* $\deg(\psi/|\psi|;\gamma)=D_j+O(\ln|\ln\epsilon|)$, *where D_j is as in Theorem 1.1.*

We emphasize that, as in Ref. 1, these vortices will *not* cluster around the holes, but rather choose fixed optimal locations strictly inside the superconducting bulk Ω. This is why we call this phenomenon the "breakdown of pinning." The key to proving this property is a boundary estimate on the function ζ at each pinning site: in a neighborhood of each ω_j, we prove $0<\zeta(x)\leqslant C\rho^2(x)\ln|\ln\rho(x)|$ where $\rho(x):=\min_j\mathrm{dist}(x,\partial\omega_j)$. Since (by (H3)) $a(x)$ is linear near each $\partial\omega_j$, the maximum of $2\zeta/a$ must therefore occur away from ω_j.

D. Bose–Einstein condensates

As was mentioned previously, we may also apply our analysis to study Bose–Einstein condensates with anharmonic traps which favor multiply connected regions. The variational problem takes the form

$$H_\epsilon(u)=\int_{\mathcal{D}}\left\{\frac{1}{2}|\nabla u|^2-\tau x^\perp\cdot\mathrm{Im}\,(\bar{u}\,\nabla\,u)+\frac{1}{4\epsilon^2}[(|u|^2-a(x))^2-(a^-(x))^2]\right\}\mathrm{d}x, \tag{1.5}$$

for a complex-valued wave function $u\in H_0^1(\mathcal{D})$, where $\epsilon>0$ and τ represents an imposed angular speed of rotation. A discussion of the origins of this model is presented in Ref. 1. The function $a(x)$ now represents the trapping potential, modeling the laser confinement of BEC in laboratory conditions. In early experiments on BEC the trapping was assumed to be harmonic, giving an ellipsoidal form to the condensate domain, $\{x:a(x)>0\}$. In more recent experiments other confinement geometries have been considered, including the annular shape studied in Ref. 1. If we impose hypotheses on $a(x)$,

(H1′) $a(x)\in C^\infty(\mathcal{D})$, and $a(x)=0$ on $\partial\mathcal{D}$;

(H2′) $\{x\in\mathcal{D}:a(x)\leqslant 0\}$
$=\overline{\cup_{j=1}^n\omega_j}$, with finitely many smooth, simply connected domains $\omega_j\subset\subset\mathcal{D}$;

(H3′) $\nabla a(x) \neq 0$ for all $x \in \partial\omega_j, j = 1,\ldots,n$ and for all $x \in \partial\mathcal{D}$;

(H4′) $\int_{\mathcal{D}} a^+(x)dx = 1$;

we may obtain results for H_ϵ which are analogous to those above, but with the imposed rotation τ playing the role of the applied field h_{ex}. Aside from the difference in boundary condition on $\partial\mathcal{D}$, the major difference is that the magnetic field is replaced by the fixed vector field, $\tau x^\perp$ which models the rotation. The consequence of this is that the limiting problem is slightly different, although it is still of a similar type and susceptible to the same solution method. (See the end of Sec. III.) The results for BEC will be the same as those of superconductivity, but with the presence of an additional boundary layer near the exterior boundary $\partial\mathcal{D}$, where we also lose control of the number and location of individual vortices due to the vanishing of $a(x)$.

II. PRELIMINARIES

In this section, we present some preliminary results which we will require throughout the paper.

A. Spaces, gauges, and equations

We define here the appropriate spaces and write down the Euler–Lagrange equations for minimizers.

The energy functional E_ϵ is gauge-invariant: if $\varphi \in H^2(\mathcal{D};\mathbf{R})$ is any scalar potential, then $E_\epsilon(\psi\exp[i\varphi], A+\nabla\varphi) = E_\epsilon(\psi, A)$. As usual we restrict our spaces to eliminate this degeneracy by fixing the Coulomb gauge. We say $(\psi, A) \in \mathcal{H}$ if $\psi \in H^1(\mathcal{D};\mathbf{C})$ and $A \in H^1(\mathcal{D};\mathbf{R}^2)$ with

$$\operatorname{div} A = 0 \text{ in } \mathcal{D}, \quad A \cdot \nu = 0 \text{ on } \partial\mathcal{D}. \tag{2.1}$$

This choice is made with no loss of generality, as to any arbitrary configuration $(\psi, A) \in H^1(\Omega;\mathbf{C}) \times H^1(\mathcal{D};\mathbf{R}^2)$ we may find a function φ so that the gauge-equivalent configuration $(\psi\exp[i\varphi], A+\nabla\varphi) \in \mathcal{H}$ with the same energy. Indeed, we can choose φ to be a solution (unique up to an additive constant) of

$$\Delta\varphi = -\operatorname{div} A \text{ in } \mathcal{D}, \qquad \left.\frac{\partial\varphi}{\partial\nu}\right|_{\partial\mathcal{D}} = A \cdot \nu|_{\partial\mathcal{D}}.$$

We also recall that the magnetic field $h(x) \in L^2(\mathcal{D})$ uniquely determines its vector potential A in the Coulomb gauge. To see this, we solve the Dirichlet problem,

$$\Delta b = h \text{ in } \mathcal{D}, \quad b|_{\partial\mathcal{D}} = 0, \tag{2.2}$$

and then $A = \nabla^\perp b = (-\partial_y b, \partial_x b)$ gives the desired potential. We obtain from this the main analytical advantage of the Coulomb gauge, control of the potential by the L^2 norm of its field: there exists a constant $C_\mathcal{D}$ (depending only on $\mathcal{D}$) such that

$$\|A\|_{H^1(\mathcal{D})} \leqslant C_\mathcal{D}\|h\|_{L^2(\mathcal{D})}. \tag{2.3}$$

The estimate (2.3) follows from the regularity theory for the Dirichlet problem mentioned previously.

Minimizers of E_ϵ satisfy the Ginzburg–Landau system in Ω,

$$-\nabla_A^2\psi + \frac{1}{\epsilon^2}(|\psi|^2 - a(x))\psi = 0 \text{ in } \mathcal{D}, \tag{2.4}$$

$$-\nabla^\perp h = \vec{j} := \operatorname{Im}\{\bar{\psi}(\nabla - iA)\psi\} \text{ in } \mathcal{D}, \tag{2.5}$$

$$h = h_{ex} \text{ on } \partial\mathcal{D}. \tag{2.6}$$

Here we denote $\nabla_A\psi := \nabla\psi - iA\psi$. There is also a boundary condition $\nabla_A\psi\cdot\nu = 0$ on $\partial\mathcal{D}$. From Lemma 1.1 of [4] we have the basic estimate

$$|\psi(x)| \leqslant \sup_{\mathcal{D}}\sqrt{a^+(x)}, \quad \forall\ x \in \Omega, \tag{2.7}$$

where $a^+(x) = \max\{a(x), 0\}$. This is a consequence of the maximum principle applied to the equation for $|\psi|^2$.

B. Decoupling the density profile

As $\epsilon \to 0$ we expect that the potential term in the energy E_ϵ will force $|\psi|^2 \to a^+(x)$. The hypotheses on $a(x)$ do not allow $\sqrt{a^+} \in H^1(\mathcal{D})$, and so this creates a singular boundary layer near the zero set of a. Here we study this boundary layer, so that it can be effectively removed from our energy calculations in the following sections.

Define a functional,

$$J_\epsilon(\eta) := \int_{\mathcal{D}} \left\{ \frac{1}{2}|\nabla\eta|^2 + \frac{1}{4\epsilon^2}[(\eta^2 - a(x))^2 - (a^-)^2] \right\} dx, \tag{2.8}$$

for real-valued functions $\eta \in H^1(\mathcal{D}; \mathbf{R})$. Critical points of J_ϵ solve the boundary-value problem

$$-\Delta\eta + \frac{1}{\epsilon^2}(\eta^2 - a(x))\eta = 0, \text{ in } \mathcal{D}, \quad \frac{\partial\eta}{\partial\nu} = 0, \text{ on } \partial\mathcal{D}. \tag{2.9}$$

Proposition 2.1: Problem (2.9) *admits a unique positive solution* η_ϵ*, which is the unique minimizer of* J_ϵ *in* $H_0^1(\mathcal{D})$ *up to a complex multiplier of modulus one. In addition,*

(i) $0 < \eta_\epsilon(x) \leqslant \max_{\mathcal{D}} a$, *and* $|\nabla\eta_\epsilon| \leqslant C/\epsilon$;

(ii) $J_\epsilon(\eta_\epsilon) \leqslant C|\ln\epsilon|$ *and* η_ϵ *is bounded in* $L^\infty(\Omega)$;

(iii) *There exists a constant* C *independent of* ϵ *so that*

$$|\eta_\epsilon(x) - \sqrt{a^+(x)}| \leqslant C\epsilon^{1/3}\sqrt{a^+(x)} \text{ for every } x \in \Omega \text{ with } \operatorname{dist}(x, \partial\Omega) \geqslant \epsilon^{1/3}; \tag{2.10}$$

(iv) *For every* $j = 1, \ldots, n$ *and* $x \in \omega_j$ *with* $\operatorname{dist}(x, \partial\omega_j) \geqslant \epsilon^{1/3}$,

$$0 < \eta_\epsilon(x) \leqslant C\epsilon^{1/6}\exp[-\operatorname{dist}(x, \partial\omega_j)/\epsilon^{2/3}], \tag{2.11}$$

where $C > 0$ *is a constant independent of* ϵ.

In particular, (iv) implies that $\eta_\epsilon \to 0$ locally uniformly in the holes ω_j. The assertion (iv) implies that $|\eta_\epsilon^2(x) - a^+(x)|$ is small with respect to $a^+(x)$ itself provided we remain at a small distance ($\epsilon^{1/3}$) from the boundary of each $\partial\omega_j$.

The proof of Proposition 2.1 is identical to that of Proposition 2.1 of Ref. 1. In addition we have the result of Proposition 2.3 of Ref. 1 which implies that the negativity of $a(x)$ in the normal regions ω_j acts more or less like an imposed Dirichlet condition:

Proposition 2.2: Assume $h_{ex} \leqslant C_0|\ln\epsilon|$ *for some constant* $C_0 > 0$. *Then, for any minimizer* (ψ, A) *of* E_ϵ *in* $\mathbf{H}$,

$$\int_\Omega (|\psi|^2 - a)^2 + \int_{\cup\omega_j} |\psi|^4 \leqslant C_1\epsilon^2|\ln\epsilon|^2, \tag{2.12}$$

with constant C_1 *depending on* C_0. *Moreover,* $|\psi(x)| \to 0$ *locally uniformly in* $\cup_j \omega_j$ *and*

$$|\psi(x)| \leqslant C\epsilon^{1/6}\exp[-\operatorname{dist}(x,\partial\omega_j)/\epsilon^{2/3}] \tag{2.13}$$

for all $x \in \omega_j$ *with* $\operatorname{dist}(x,\partial\omega_j) \geqslant \epsilon^{1/3}$ *and* $j=1,\ldots,n$.

Again the proof is identical to that in Ref. 1 and is omitted.

We now apply the remarkable observation (see Ref. 12) that the energy of the profile η_ϵ and the remaining complex order parameter $v=u/\eta_\epsilon$ decouple exactly into two independent pieces.

Lemma 2.3: Let $(\psi,A) \in \mathbf{H}$. *Then,* $u=\psi/\eta_\epsilon$ *is well defined, belongs to* $H^1_{\eta_\epsilon^2}$ *(defined in (1.2),) and*

$$E_\epsilon(\psi,A) = J_\epsilon(\eta_\epsilon) + F_\epsilon(u,A) \tag{2.14}$$

where

$$F_\epsilon(u,A) = \int_{\mathcal{D}} \left\{ \frac{\eta_\epsilon^2}{2}|\nabla_A u|^2 + \frac{\eta_\epsilon^4}{4\epsilon^2}(|u|^2-1)^2 + \frac{1}{2}(h-h_{ex})^2 \right\} \mathrm{d}x. \tag{2.15}$$

Proof: Note that v is well defined in $\mathcal{D}$, since $\eta_\epsilon > 0$. The decomposition and the fact that $v \in H^1_{\eta_\epsilon}(\mathcal{D})$ follow exactly as in Serfaty.[20] □

III. THE LIMIT PROBLEM

In this section we consider a limiting energy F_∞, which represents in a formal sense the limit of F_ϵ as $\epsilon \to 0$. Indeed, heuristically we expect that in this limit, $|u| \to 1$ in Ω, but $\eta_\epsilon \to 0$ exponentially fast in each ω_j (by Lemma 2.2), and thus the contribution of the order parameter to the energy from the pinning sites is negligible. Thus, we define:

$$F_\infty(u,A) := \frac{1}{2}\int_\Omega a(x)|\nabla_A u|^2 dx + \frac{1}{2}\int_{\mathcal{D}} (h-h_{ex})^2, \tag{3.1}$$

for

$$u \in H^1_a(\Omega;S^1) := \left\{ u \in W^1(\Omega;S^1) : \|u\|^2_{H^1_a} := \int_\Omega a(x)|\nabla u|^2 dx < \infty \right\},$$

and $A \in H^1(\mathcal{D};\mathbf{R}^2)$. As in the previous part, we refine our space to fix a gauge, and denote by $\mathcal{H}_\infty$ the subspace of $H^1_a(\Omega;S^1)\times H^1(\mathcal{D};\mathbf{R}^2)$ such that A satisfies (2.1). The same remarks concerning the gauges and spaces as above then apply, since the gauge changes affect only the complex phase of u and not its magnitude.

Note the essential differences with the original problem: now the order parameter is only defined in the region $\Omega=\mathcal{D}\backslash\{x : a(x) \leqslant 0\}$, although the magnetic field is calculated everywhere in $\mathcal{D}$. Thus the limit problem strongly resembles the problem in multiply connected domains studied in Ref. 3, although we must now deal with some delicate regularity issues near $\partial\omega_j$, where $a(x)$ vanishes.

The Euler–Langrange equations for the limit problem are

$$-\nabla_A \cdot (a(x)\nabla_A u) = |\nabla_A u|^2 u, \text{ in } \Omega; \tag{3.2}$$

$$-\nabla^\perp h = \vec{j} := a(x)\operatorname{Im}\{\bar{u}\nabla_A u\} \text{ in } \Omega; \tag{3.3}$$

$$h = H_j \text{ (constant) in each } \omega_j, \quad j = 1, \ldots, n; \tag{3.4}$$

$$h = h_{ex} \text{ on } \partial\mathcal{D}. \tag{3.5}$$

There is also a boundary condition, $a(x)\nabla_A u \cdot \nu = 0$, on the exterior boundary $\partial\mathcal{D}$. Note that the constants $H_j = h|_{\omega_j}$ are not prescribed, but are determined by the solution h itself.

Since $|u| = 1$ we may then write locally $u = e^{i\phi}$ for real phase ϕ, and it is then easy to derive from (3.3) the following London equation for $h = \operatorname{curl} A$,

$$-\operatorname{div}\left(\frac{1}{a(x)}\nabla h\right) + h = 0 \text{ in } \Omega. \tag{3.6}$$

This equation is then supplemented by the boundary conditions (3.4) and (3.5). There is an important additional condition on each $\partial\omega_j$, obtained from integrating equation (3.3) around each $\partial\omega_j$ separately:

$$\begin{aligned}\int_{\partial\omega_j} \frac{1}{a}\frac{\partial h}{\partial \nu}\mathrm{d}s &= \int_{\partial\omega_j} \frac{1}{a}\nabla^{\perp} h \cdot \tau \,\mathrm{d}s = -\int_{\partial\omega_j} \mathrm{Im}\{\bar{u}\,\nabla u\} \cdot \tau \, ds + \int_{\partial\omega_j} A \cdot \tau \,\mathrm{d}s \\ &= -2\pi \deg(u, \partial\omega_j) + \int_{\omega_j} h \,\mathrm{d}x = -2\pi \deg(u, \partial\omega_j) + H_j|\omega_j|. \end{aligned} \tag{3.7}$$

Because $|u| = 1$ we may express $|\nabla_A u|^2 = |\nabla\phi - A|^2 = |\vec{j}|^2$ and thus the limiting energy of a minimizer (u, A) may be expressed entirely in terms of the field $h = \operatorname{curl} A$,

$$\min F_\infty(u, A) = \frac{1}{2}\int_\Omega \frac{1}{a(x)}|\nabla h|^2 \mathrm{d}x + \frac{1}{2}\int_{\mathcal{D}} (h - h_{ex})^2 \mathrm{d}x =: E_*(h). \tag{3.8}$$

This characterization of the minimum energy will be especially useful, as it will allow us later on to evaluate the energy explicitly in terms of the degrees around each pinning site.

Our analysis of the limit problem follows[3] in the large. The main difference is that the equations here involve the operator,

$$\mathcal{L}h = -\operatorname{div}\left(\frac{1}{a(x)}\nabla h\right) + h,$$

which is strictly, but not uniformly, elliptic, due to the vanishing of $a(x)$ at the boundary of each pinning site ω_j. As in Ref. 3, we may decompose the magnetic field in order to calculate the contribution from each giant vortex in each pinning site, as well as the contribution to h from the external field. Let $\xi_i(x)$, $i = 0, \ldots, n$ solve

$$\mathcal{L}\xi_i = \delta_{i,0} \text{ in } \Omega,$$

$$\xi_i = 0 \text{ on } \partial\mathcal{D},$$

$$\xi_i = c_{i,j} \text{ on } \omega_j, \quad j = 1, \ldots, n,$$

$$\int_{\partial\omega_j} \frac{1}{a}\frac{\partial \xi_i}{\partial \nu} = -2\pi\delta_{i,j} + c_{i,j}|\omega_j|, \quad j = 1, \ldots, n. \tag{3.9}$$

Here, $c_{i,j}$, $i = 0, \ldots, n$, $j = 1, \ldots, n$ are *constants* determined by the solutions $\xi_i(x)$, and we emphasize that $\delta_{i,j}$ denotes the Kronecker (and not the Dirac) delta. Then the desired field h is given in terms of these via:

$$h = h_{ex}(1 - \xi_0) + \sum_{i=1}^{n} D_i \xi_i, \tag{3.10}$$

where $D_i = \deg(u, \partial\omega_i)$ for the order parameter u associated to h via (3.3). The existence and uniqueness of the components ξ_i follows from a variational problem as in Ref. 6. The regularity is complicated by the fact that uniform ellipticity is lost at the inner boundaries $\partial\omega_j$, but the necessary estimates follow by constructing barriers, blowing up near the boundary, and a modification of the method of Trudinger.[21]

Lemma 3.1: There exist unique constants $\{c_{i,j}\}_{j=1,\ldots,n}^{i=0,\ldots,n}$, *and unique weak solutions* $\xi_0, \ldots, \xi_n$ *to* (3.9). *Moreover*,

(i) *each* $\xi_i \in C^\infty(\mathcal{D}\backslash\overline{\cup_j \omega_j}) \cap C^1(\overline{\mathcal{D}\backslash\cup_j \omega_j})$, $i = 1, \ldots, n$;
(ii) *each* $\xi_i(x) > 0$ *for all* $x \in \Omega$, $i = 0, \ldots, n$;
(iii) *for all* $i = 0, \ldots, n$ *there exists constants* $C > 0$, $\delta_0 > 0$ *so that for every* $j = 1, \ldots, n$ *and for all* x *with* $\rho(x) := \operatorname{dist}(x, \cup_j \partial\omega_j) < \delta_0$,

$$|\xi_i(x) - c_{i,j}| \leqslant C(\rho(x))^2 \ln|\ln \rho(x)| \tag{3.11}$$

$$|\nabla \xi_i(x)| \leqslant C\rho(x) \ln|\ln \rho(x)|. \tag{3.12}$$

Note in particular that (ii) implies that the constant values $c_{i,j} = \xi_i|_{\omega_j} \geqslant 0$. To maintain continuity of presentation we defer the proof of Lemma 3.1 to the end of this section.

As in Lemma 2.2 of Ref. 3, the minimum energy is then expressed in terms of the degrees D_j at each pinning site ω_j and the external field (see also Theorem 3.4 of Ref. 4):

Lemma 3.2: *Let* (u_*, A_*) *minimize* F_∞ *in* $\mathcal{H}$ *and* $h_* = \operatorname{curl} A_*$. *Then*,

$$\min F_\infty = E_*(h_*) = h_{ex}^2 \epsilon_0 + \pi \sum_{i,k=1}^{n} c_{i,k} D_i D_k - 2\pi h_{ex} \sum_{i=1}^{n} c_{0,i} D_i, \tag{3.13}$$

where

$$\epsilon_0 := \frac{1}{2} \int_\Omega \frac{1}{a} |\nabla \xi_0|^2 + \frac{1}{2} \int_{\mathcal{D}} \xi_0^2.$$

Proof: The proof is identical to that of Ref. 3, but we sketch it for completeness. We write $h_* - h_{ex} = -h_{ex}\xi_0 + \Sigma_{i=1}^n D_i \xi_i$ and expand the squares. The constants are obtained by integration by parts, together with (3.9):

$$\int_\Omega \frac{1}{a} \nabla \xi_i \cdot \nabla \xi_k + \int_{\mathcal{D}} \xi_i \xi_k = -\sum_{j=1}^{n} \int_{\partial\omega_j} \frac{1}{a} \frac{\partial \xi_i}{\partial \nu} \xi_k ds + \int_{\cup_j \omega_j} \xi_i \xi_k = 2\pi c_{i,k}. \tag{3.14}$$

□

As in Lemma 2.4 of Ref. 3 (see also Lemma 3.3 of Ref. 4), we have the following.

Lemma 3.3: The matrix $C = (c_{i,k})_{i,k=1,\ldots,n}$ *is positive definite. In particular, it is invertible and its inverse* C^{-1} *is a symmetric positive definite matrix.*

The proof is identical to that of Lemma 2.4 of Ref. 3 and is omitted.

The importance of the preceding analysis is that it enables us to write down *explicitly* the map from the applied field h_{ex} to the degrees $\vec{D}$ of minimizers, just by solving a finite dimensional minimization problem for the quadratic expression given in Lemma 3.2. Indeed, the critical point equation for $\vec{D}$ is easily calculated,

$$\vec{D} = h_{ex} C^{-1} X,$$

$$\text{where } X = (c_{0,1}, \ldots, c_{0,n}). \tag{3.15}$$

Here (as in Ref. 3) we raise a subtle point: in order to represent the magnetic field of actual minimizers of F_∞ it is necessary that the degrees D_j be *integers*. Therefore we must restrict our minimization of the quadratic expression in Lemma 3.2 to $\vec{D} \in \mathbf{Z}^n$, and then the minimizer is given by

$$D_i = \left[\!\!\left[h_{ex} \sum_{k=1}^{n} c_{i,k}^{-1} c_{0,k} \right]\!\!\right], \tag{3.16}$$

the nearest integer to what would normally be the minimizing vector. Here we denote $C^{-1} = (c_{i,k}^{-1})$.

We now present the *proof of Theorem 1.1*. Let $\vec{D}$ be chosen as in (3.16), to minimize (3.13). By the representation (3.10) we then recover a magnetic field h_*, which satisfies (3.7) at each boundary component. We then obtain A_* from h_* with the usual Coulomb gauge by solving the Dirichlet problem (2.2) described in Sec. II. To recover the order parameter u_*, we use the Maxwell equation, (3.3). Since the vector field $A_* - (1/a)\nabla^\perp h_*$ is irrotational in Ω by (3.6), we may define locally a real phase ϕ_* via

$$\nabla \phi_* = A_* - \frac{1}{a} \nabla^\perp h_*. \tag{3.17}$$

In fact, $u_* = \exp(i\phi_*)$ is a well-defined, single-valued function in Ω, since (3.7) implies:

$$\int_{\partial \omega_j} \nabla \phi_* \cdot \tau \, ds = \int_{\partial \omega_j} \left(A_* \cdot \tau - \frac{1}{a} \nabla h_* \cdot \nu \right) ds = 2\pi D_j \in \mathbf{Z}.$$

We thus obtain a configuration $(u_*, A_*) \in \mathcal{H}_\infty$ with $F_\infty(u_*, A_*) = E_*(h_*) = \min_{\vec{D} \in \mathbf{Z}^n} g(\vec{D}; h_{ex})$. By Lemma 3.2, this identifies the minimizer of F_∞, and Theorem 1.1 is proven. □

Despite the above-mentioned remarks concerning the degrees, it will nevertheless be convenient in the following analysis to permit the optimal degrees to be real valued, that is to use (3.15) to define a real vector $\vec{T} \in \mathbf{R}^n$, and to replace $\vec{D} \to \vec{T}$ in (3.10). In this case, the minimizer scales exactly linearly with h_{ex}, and so we define $\vec{T} = (t_1, \ldots, t_n)$ with

$$t_i = \sum_{k=1}^{n} c_{i,k}^{-1} c_{0,k} = (C^{-1} X)_i,$$

which exactly solves the minimization problem of Lemma 3.2 for $\vec{T} \in \mathbf{R}^n$, when $h_{ex} = 1$. The associated applied field $h_1(x) = 1 - \zeta(x)$, with ζ defined by

$$\zeta(x) = \xi_0(x) - \sum_{i=1}^{n} t_i \xi_i(x).$$

Using the equations for ξ_i and for $\vec{T}$ mentioned previously, we observe that $\zeta(x)$ solves:

$$\mathcal{L}\zeta = 1 \text{ in } \Omega,$$

$$\zeta = 0 \text{ on } \partial\mathcal{D} \cup (\overline{\cup_j \omega_j}),$$

$$\int_{\partial\omega_j} \frac{1}{a}\frac{\partial\zeta}{\partial\nu} = 2\pi t_j - |\omega_j|. \tag{3.18}$$

Of course, the first two conditions of (3.18) suffice to determine ζ exactly, and so the third line can be seen as an equivalent definition of the coefficients t_j.

In the case that the solution of the vector equation $C\vec{D}=X$ happens to be a vector of integers (an unlikely coincidence), then the energy minimizing field $h_*=h_{ex}h_1=h_{ex}(1-\zeta)$ exactly. Generically, the two do not differ by much:

Lemma 3.4: There exists a constant C_1 independent of h_{ex} such that if h_* is the magnetic field associated to the minimizers (u_*,A_*) of F_∞ with $h=h_{ex}$, then

$$\max_{\bar{\mathcal{D}}} |h_* - h_{ex}(1-\zeta)| \leqslant C_1.$$

Proof:

$$|h_* - h_{ex}(1-\zeta)| = \left| \sum_{i=1}^{n} (D_i - h_{ex}t_i)\xi_i \right| \leqslant \sum_{i=1}^{N} |D_i - h_{ex}t_i|\xi_i,$$

which is uniformly bounded (independent of h_{ex}) since $D_i=[\![h_{ex}t_i]\!]$ implies $|D_i-h_{ex}t_i|\leqslant 1$, and the ξ_i are uniformly bounded. □

Remark 3.5: Notice that the result of Lemma 3.4 could have been stated in any "reasonable" norm, that is in any norm for which each ξ_i is bounded.

Proof of Lemma 3.1: First we define an appropriate space of functions which take constant values on each ω_j. Adapting the definition in Ref. 21 to our setting, we define $\mathbf{H}$ to be the closure in the norm

$$\|f\|_{\mathbf{H}}^2 := \int_\Omega \frac{1}{a(x)}|\nabla f|^2,$$

of the linear subspace of $C_0^\infty(\mathcal{D})$ consisting of all functions which are constant in a neighborhood of ω_j for each $j=1,\ldots,n$. Since $1/a(x)$ is locally integrable in Ω, this definition is well-defined and $\mathbf{H}$ defines a Hilbert Space. As $a(x)$ is bounded above in Ω, the $\mathbf{H}$-norm dominates the usual H_0^1-norm on $\mathcal{D}$, and so the Poincaré, trace, and Sobolev inequalities hold for functions in $\mathbf{H}$.

To obtain the desired solutions we minimize the energy

$$F_i(\varphi) = \frac{1}{2}\int_\Omega \left[\frac{1}{a}|\nabla\varphi|^2 - \delta_{i0}\varphi\right] + \frac{1}{2}\int_{\mathcal{D}} \varphi^2 - 2\pi(1-\delta_{i0})\varphi\big|_{\omega_i},$$

$i=0,\ldots,n$, for $\varphi\in\mathbf{H}$. By the Poincaré inequality and the trace inequalities, F_i is bounded below on $\mathbf{H}$, and by convexity it attains a unique minimizer ξ_i. A simple computation shows that minimizers give weak solutions to the boundary-value problem (3.9). Indeed, the first variation yields,

$$0 = DF_i(\xi_i)u = \int_\Omega \left[\frac{1}{a} \nabla \xi_i \cdot \nabla u - \delta_{i0} u \right] + \int_{\mathcal{D}} \xi_i u - 2\pi(1-\delta_{i0})u\big|_{\omega_i}$$

$$= \int_\Omega \left[\frac{1}{a} \nabla \xi_i \cdot \nabla u + \xi_i u - \delta_{i0} u \right] + \sum_{j=1}^{n} \left(|\omega_j| \xi_i\big|_{\omega_j} - 2\pi\delta_{ij} \right) u\big|_{\omega_j}, \tag{3.19}$$

for all $u \in \mathbf{H}$. The equation and boundary conditions then follow from choosing u with values either zero or one in the appropriate domains ω_j. Since the coeffient $1/a$ is smooth away from $\cup_j \omega_j$ we have each ξ_i smooth in the interior by standard regularity theory.

As in Ref. 21, the weak maximum principle holds for this equation, since it is nevertheless strictly elliptic in Ω. Taking $u(x) = \xi_i^-(x) = \min\{0, \xi_i(x)\} \leqslant 0$, we have $u \in \mathbf{H}$ and inserting in (3.19) we obtain $\|\xi_i^-\|_{\mathbf{H}} = 0$, that is $\xi_i \geqslant 0$.

Finally, for the global and boundary regularity we require some results from Ref. 21. By Case I of Theorem 4.1 of Ref. 21 the solutions are uniformly bounded. To obtain the boundary behavior (3.11) and (3.12) near $\partial\omega_j$, we construct barriers. Let $\xi(x) = a(x)^2 \ln|\ln a(x)|$. We calculate:

$$\mathcal{L}\xi = \left(\frac{2}{|\ln a(x)|} + \frac{1}{(\ln a(x))^2} \right) \frac{|\nabla a|^2}{a} - \left(2\ln|\ln a| + \frac{1}{\ln a} \right) \Delta a + a(x)^2 \ln|\ln a(x)|.$$

By hypothesis (H3), $a(x) \simeq \alpha_0 \rho(x)$ for x in a neighborhood of $\partial\omega_j$, for each $j = 1, \ldots, n$. In particular, $|\nabla a|$ is bounded away from zero in a neighborhood of each $\partial\omega_j$, and hence the first term on the right-hand side is dominant and tends to $+\infty$ as $\delta(x) \to 0$. Therefore, there exists $\delta_0 > 0$ such that $\mathcal{L}\xi > 1$ for all x with $\rho(x) < \delta_0$.

Now let $\bar{\xi}_{i,j}(x) := c_{i,j} + b_{i,j} a(x)^2 \ln|\ln a(x)|$, with positive constants $b_{i,j} \geqslant 1$. Then $\mathcal{L}\bar{\xi}_{i,j}(x) > c_{i,j} + b_{i,j} \geqslant \delta_{i,j}$ for $\rho(x) < \delta_0$, and so $\bar{\xi}_{i,j}$ is a supersolution in each connected component of $\mathcal{N}_{\delta_0} := \{x \in \Omega : \rho(x) < \delta_0\}$. Note that $\bar{\xi}_{i,j}|_{\partial\omega_j} = c_{i,j} = \xi_i|_{\partial\omega_j}$. Since each $\xi_i(x)$ is uniformly bounded in Ω, we can choose the constants $b_{i,j}$ large enough such that $\bar{\xi}_{i,j} \geqslant \xi_i$ on $\partial\mathcal{N}_{\delta_0} \cap \Omega$. Applying the weak maximum principle in each component of $\mathcal{N}_{\delta_0}$ we conclude that $\xi_i(x) \leqslant \bar{\xi}_{i,j}(x)$ in each component of $\mathcal{N}_{\delta_0}$. The complementary lower bound may be obtained using the subsolution $\underline{\xi}_{i,j} = c_{i,j} - \tilde{b}_{i,j} a(x)^2 \ln|\ln a(x)|$ for constants $\tilde{b}_{i,j}$ appropriately large. This proves (3.11).

To prove (3.12), we use a blow-up argument. Let $x_0 \in \Omega$, and $\delta > 0$ with dist $(x_0, \partial\omega_j) = 2\delta$ for some $j = 1, \ldots, n$. We then blow up the disk $B_\delta(x_0)$: let $x = x_0 + \delta y$ with $y \in B_1(0)$, and define

$$v(y) = \xi_i(x) - c_{i,j} = \xi_i(x_0 + \delta y) - c_{i,j}, \quad y \in B_1(0).$$

By rotating the y plane if necessary, we may assume that the shortest segment joining x_0 to $\partial\omega_j$ is mapped to the y_1 axis, and hence the image $\tilde{\omega}_j = (1/\delta)(\omega_j - \{x_0\})$ of the hole ω_j lies in the half plane $y_1 < -2$ and the distance $\tilde{\rho}(y) := \text{dist}(y, \partial\tilde{\omega}_j) \geqslant y_1 + 2 \geqslant 1$ for $y \in B_1(0)$.

Since $\rho(x)/a(x)$ is smooth and nonzero in a neighborhood of $\partial\omega_j$ in Ω, there exists $b(x)$, smooth and $b(x) > 0$ in a neighborhood of $\partial\omega_j$ with

$$\frac{1}{a(x)} = \frac{b(x)}{\rho(x)}.$$

By homogeneity, $\rho(x) = \delta\tilde{\rho}(y)$, and hence

$$\frac{1}{a(x)} = \frac{1}{\delta} \left(\frac{b(x_0 + \delta y)}{\tilde{\rho}(y)} \right) =: \frac{1}{\delta} \beta_{\delta, x_0}(y).$$

Therefore, the equation for ξ_i implies,

$$-\nabla_y \cdot (\beta_{\delta,x_0}(y)\nabla_y v) = \delta^3(v + \delta_{i,0} + c_{i,j}) =: F_{\delta,x_0}(y).$$

By the above-mentioned remarks, the coefficient β_{δ,x_0} is smooth in $B_1(0)$, and there exist constants $0<\lambda_1<\lambda_2$, $C>0$ (independent of δ,x_0) so that

$$\lambda_1 \leqslant \beta_{\delta,x_0}(y) \leqslant \lambda_2, \quad |\nabla\beta_{\delta,x_0}(y)| \leqslant C,$$

for all $y \in B_1(0)$. Hence Theorem 9.11 of Ref. 9 holds, uniformly in δ,x_0, and for every $p \geqslant 2$ there exists a constant (independent of δ,x_0) $K>0$ with

$$\|v\|_{W^{2,p}(B_{1/2}(0))} \leqslant K(\|v\|_{L^p(B_1(0))} + \|\tilde{F}_{\delta,x_0}\|_{L^p(B_1(0))}) \leqslant K'(\|v\|_{L^\infty(B_1(0))} + \delta^3\|\tilde{f}\|_{L^\infty(B_1(0))}) \leqslant K''\delta^2|\ln|\ln\delta||,$$

using the estimate (3.11) in the last line. By the Sobolev embedding, taking $p>2$ we conclude that v is uniformly bounded in $C^{1,\alpha}(B_{1/2}(0))$, and in particular $|\nabla v(0)| \leqslant C\delta^2|\ln|\ln\delta||$ with constant C independent of x_0, δ. Rescaling, we obtain $|\nabla\xi_i(x_0)| \leqslant C\delta|\ln|\ln\delta|| \leqslant C'\rho(x_0)|\ln|\ln\rho(x_0)||$, which is the desired conclusion (3.12). □

Remark 3.6: We note that in case $\Delta a(x)>0$ on $\partial\omega_j$ we would be able to use $\xi(x)=a(x)^2$ as a supersolution in the above calculation and obtain a slightly better estimate $|\xi_i(x)-c_{i,j}| \leqslant C(\rho(x))^2$ (and similarly for $|\nabla\xi_i|$), on the boundary behavior of solutions. We also remark that in case $\mathcal{D}$ is a disk and $a(x)$ radially symmetric, then the functions ξ_i are radial and the sharper estimate $\xi_i - c_{i,j} = O(\rho(x)^2)$ holds in this case as well.

Finally, the following estimates follow easily from Lemma 3.1, but are stated in a form which will be useful in studying the breakdown of pinning:

Lemma 3.7: For any $\delta>0$, *let* $\Omega_\delta := \{x \in \Omega : \mathrm{dist}(x,\omega_j) > \delta$, *for some* $j \in \{1,\ldots,n\}\}$. *Then, there exists a constant* $C>0$ *so that*

$$\sup_{x\in\Omega_\delta}\left|\frac{\nabla h_*}{a}\right| \leqslant Ch_{ex}|\ln|\ln\delta||, \tag{3.20}$$

$$\int_{\Omega\setminus\Omega_\delta}\frac{1}{a}|\nabla h_*|^2 dx \leqslant Ch_{ex}^2\delta^2[|\ln|\ln\delta||]^2. \tag{3.21}$$

Bose–Einstein Condensates: For the problem of a Bose–Einstein condensate described by the functional H_ϵ of Sec. I, after the reduction via Ref. 12 and formal passage to the $\epsilon\to 0$ limit, we arrive at a similar limit problem,

$$I_\infty(v) = \int_\Omega \left\{\frac{a}{2}|\nabla v|^2 - a(x)\pi x^\perp \cdot \mathrm{Im}[\bar{v}\nabla v]\right\} dx,$$

for $v \in H^1_a(\Omega;S^1)$ with $|v|=1$. There is no associated magnetic field, but minimizers satisfy the conservation of momentum, $\mathrm{div}\,\vec{j} = \mathrm{div}(a(x)[\mathrm{Im}\{\bar{v}\nabla v\} - \pi x^\perp]) = 0$, and hence there is a conjugate function (in the sense of harmonic maps[6]), $h \in H^1_{1/a}(\Omega)$ with

$$\nabla^\perp h = -\vec{j}.$$

It is easy to verify that h satisfies

$$-\mathrm{div}\left(\frac{1}{a(x)}\nabla h\right) = 2\pi \quad \text{in } \Omega,$$

with $h=H_j$ constant on each ω_j, and we may choose $h=0$ on $\partial\mathcal{D}$. By following the same calculations as (3.7) we obtain the flux conditions,

$$\int_{\partial\omega_j} \frac{1}{a}\frac{\partial h}{\partial \nu} ds = -2\pi \deg(v, \partial\omega_j) + 2|\omega_j|, \quad j = 1, \ldots, n.$$

Decomposing $h = \tau\xi_0 - \Sigma d_j \xi_j$ as before, we must solve for

$$-\operatorname{div}\left(\frac{1}{a(x)} \nabla \xi_i\right) = 2\delta_{i,0} \text{ in } \Omega,$$

$$\xi_i = 0 \text{ on } \partial\mathcal{D},$$

$$\xi_i = c_{i,j} \text{ on } \omega_j, \quad j = 1, \ldots, n,$$

$$\int_{\partial\omega_j} \frac{1}{a}\partial_\nu \xi_i = -2\pi\delta_{i,j} + 2|\omega_j|\delta_{i,0}, \quad j = 1, \ldots, n.$$

These may be found by minimizing the functionals

$$I_i(\varphi) = \frac{1}{2}\int_\Omega |\nabla\varphi|^2 dx - \delta_{i,0}\int_{\mathcal{D}} 2\varphi \, dx - \pi(1-\delta_{i,0})\varphi\big|_{\omega_i},$$

over the space **H** defined previously, with φ=constant on each ω_j. The existence and boundary regularity (including now the exterior boundary $\partial\mathcal{D}$) of these solutions follow exactly as in Lemma 3.1, and the expression of the limiting energy in terms of the degrees D_j at each of the holes ω_j is also the same. We leave the details to the interested reader.

IV. PINNING IN BOUNDED FIELDS

In this section we prove Theorem 1.2, with h_{ex} fixed, independent of $\epsilon \to 0$. We begin with an upper bound on the energy, stated in a form which will be useful also in our analysis of the breakdown of pinning for larger h_{ex}. For each given value of h_{ex}, we first take the minimizer (u_*, A_*) of the limiting energy F_∞, as described in the previous section. The degrees $\vec{D}_* = (D_1, \ldots, D_n) = [\![h_{ex} C^{-1} X]\!]$ determined by minimizing (3.13), and the limit energy is given as in Lemma 3.2,

$$F_\infty(u_*, A_*) = h_{ex}^2 \epsilon_0 + g(D; h_{ex}), \tag{4.1}$$

where we denote

$$g(D; h_{ex}) := \pi(\vec{D} \cdot C\vec{D} - 2h_{ex}\vec{X} \cdot \vec{D}) = \pi \sum_{i,k=1}^{n} c_{i,k} D_i D_k - 2\pi h_{ex} \sum_{i=1}^{n} c_{0,i} D_i.$$

Note that this energy is of the order h_{ex}^2. We would like to use (u_*, A_*) as a test function in the energy, but u_* is only defined in Ω and hence we must extend it to the entire domain $\mathcal{D}$. We obtain the following:

Proposition 4.1: Assume $h_{ex} \leqslant C|\ln \epsilon|$. *Then*,

$$\inf E_\epsilon(u, A) \leqslant J_\epsilon(\eta_\epsilon) + F_\infty(u_*, A_*) + o(1) = J_\epsilon(\eta_\epsilon) + h_{ex}^2 \epsilon_0 + g(D_*; h_{ex}) + o(1), \tag{4.2}$$

where (u_*, A_*), $g(D_*; h_{ex})$ *and* D_* *are as mentioned above.*

Proof: Let $\rho(x) := \operatorname{dist}(x, \cup_j \partial\omega_j)$ denote signed distance, with positive values in Ω and negative values in each ω_j. Define a one-sided neighborhood of the holes, $\Delta'_\epsilon := \{x \in \Omega : 0 < \rho(x) < 2\epsilon^{1/6}\}$. By the estimate (3.21) we have

$$\int_{\Delta'_\epsilon} a|\nabla_{A_*} u_*|^2 = \int_{\Delta'_\epsilon} \frac{1}{a}|\nabla h_*|^2 \leqslant C\epsilon^{1/3}(\ln|\ln \epsilon^{1/6}|)^2|\ln \epsilon|^2 = o(1). \tag{4.3}$$

We may therefore excise a portion of the neighborhood Δ'_ϵ with negligible energy cost.

By the energy estimate and Hölder's inequality,

$$\int_{\Delta'_\epsilon} a(x)A_*^2 \leqslant \|A_*\|_{L^4}^2 \left(\int_{\Delta'_\epsilon} a(x)^2 \right)^{1/2} \leqslant \epsilon^{1/4}|\ln \epsilon|^2 = o(1), \tag{4.4}$$

and hence (4.3) implies that

$$\int_{\Delta'_\epsilon} a|\nabla u_*|^2 \leqslant C\epsilon^{1/6}(\ln|\ln \epsilon^{1/6}|)^2|\ln \epsilon|^2.$$

From the previous estimate and Fubini's theorem, there exists a constant C' and $\delta_\epsilon \in (\epsilon^{1/6}, 2\epsilon^{1/6})$ such that

$$\int_{\{\rho(x)=\delta_\epsilon\}} a(x)|\nabla u_*|^2 \leqslant C'(\ln|\ln \epsilon^{1/6}|)^2|\ln \epsilon|^2.$$

Using hypothesis (H3) we then have

$$\int_{\{\rho(x)=\delta_\epsilon\}} |\nabla u_*|^2 \leqslant C''\epsilon^{-1/6}(\ln|\ln \epsilon^{1/6}|)^2|\ln \epsilon|^2, \tag{4.5}$$

for appropriate constant C''.

Define the two-sided neighborhood,

$$\mathcal{N}_\epsilon := \{x \in \mathcal{D} : -\delta_\epsilon < \rho(x) < \delta_\epsilon\}.$$

We claim the following:

Lemma 4.2: There exists a constant $C>0$, independent of ϵ, so that

$$\eta_\epsilon^2(x) \leqslant C\delta_\epsilon \quad \textit{for } x \in \mathcal{N}_\epsilon. \tag{4.6}$$

We defer the proof of Lemma 4.2 until the end.

We now extend the order parameter u_* as $\hat{u}_* = \exp(i\hat{\phi}_*)$ to $\mathcal{N}_\epsilon$ by extending the real phase function $\hat{\phi}_*$ from $\{x : \rho(x) = \delta_\epsilon\}$ to $\mathcal{N}_\epsilon$ as a constant along the normal lines to each $\partial\omega_j$. Note that in $\mathcal{N}_\epsilon$, $|\hat{u}_*| = 1$ and

$$|\nabla \hat{u}_*(x)| = |\nabla \hat{\phi}_*(x)| = |\partial_\tau \hat{\phi}_*(x)| \leqslant C[|\nabla \phi_*|]_{\rho(x)=\delta_\epsilon}. \tag{4.7}$$

In particular, integrating along curves equidistant to $\partial\omega_j$, we then have

$$\begin{aligned} \int_{\mathcal{N}_\epsilon} \eta_\epsilon^2|\nabla_{A_*}\hat{u}_*|^2 &\leqslant 2\int_{\mathcal{N}_\epsilon} \eta_\epsilon^2|\nabla \hat{\phi}_*|^2 + 2\int_{\mathcal{N}_\epsilon} \eta_\epsilon^2 A_*^2 \leqslant C\int_{-\delta_\epsilon}^{\delta_\epsilon} \int_{\rho(x)=t} \eta_\epsilon^2|\nabla \hat{\phi}_*|^2 \mathrm{d}s_t \mathrm{d}t + o(1) \\ &\leqslant C\delta_\epsilon^2\epsilon^{-1/6}(\ln|\ln \epsilon^{1/6}|)^2|\ln \epsilon|^2 = o(1), \end{aligned} \tag{4.8}$$

where we have used (4.4), (4.5), and (4.7), and the estimate (4.6). In summary, we have shown that there exists an extension $\hat{u}_*$ of u_* to $\mathcal{N}_\epsilon$, a small distance into the pinning sites ω_j, with small energy in this neighborhood.

To conclude, we introduce a smooth cut-off, $\chi_\epsilon(x)$ with $0 \leqslant \chi_\epsilon(x) \leqslant 1$,

$$\chi_\epsilon(x) = \begin{cases} 1 & \text{if } \rho(x) > -\dfrac{\delta_\epsilon}{2}, \\ 0 & \text{if } \rho(x) < -\delta_\epsilon, \end{cases}$$

and $|\nabla\chi_\epsilon(x)| \leq C/\delta_\epsilon$. Our test function for the energy F_ϵ is then $u = \chi_\epsilon \hat{u}_*$, $A = A_*$, and we have

$$\begin{aligned} \int_{\mathcal{D}} \eta_\epsilon^2 |\nabla_{A_*} u|^2 &\leq \int_{\Omega \setminus \mathcal{N}_\epsilon} \eta_\epsilon^2 |\nabla_{A_*} u_*|^2 + 2\int_{\mathcal{N}_\epsilon} \eta_\epsilon^2 |\nabla\chi_\epsilon|^2 + 2\int_{\mathcal{N}_\epsilon} \eta_\epsilon^2 |\nabla_{A_*}\hat{u}_*|^2 \\ &= \int_\Omega a(x)|\nabla_{A_*} u_*|^2 + \frac{C}{\delta_\epsilon^2}\int_{\{-\delta_\epsilon < \rho < -\delta_\epsilon/2\}} \eta_\epsilon^2 + o(1) = \int_\Omega a(x)|\nabla_{A_*} u_*|^2 + o(1), \end{aligned}$$

where we have used (2.10), (2.11), (4.3), and (4.8) in the second line. Finally, by (iv) of Proposition 2.1 we have

$$\int_{\mathcal{D}} \frac{\eta_\epsilon^4}{4\epsilon^2}(|\chi_\epsilon \hat{u}_*|^2 - 1)^2 \leq \int_{\left\{-\delta_\epsilon < \rho(x) < -\frac{\delta_\epsilon}{2}\right\}} \frac{\eta_\epsilon^4}{4\epsilon^2} \leq C\frac{\exp[-4\epsilon^{-1/2}]}{\epsilon^{4/3}} = o(1).$$

In conclusion, we have the upper bound:

$$\inf E_\epsilon \leq J_\epsilon(\eta_\epsilon) + F_\epsilon(\chi_\epsilon \hat{u}_*, A_*) \leq J_\epsilon(\eta_\epsilon) + F_\infty(u_*, A_*) + o(1),$$

which concludes the proof of Proposition 4.1. □

Proof of Lemma 4.2: By the choice of δ_ϵ and (2.10) we have $\eta_\epsilon^2(x) \leq 2a(x)$ on $\Gamma = \{x \in \Omega : \rho(x) = \delta_\epsilon\}$. Let $D_\epsilon := \{x \in \mathcal{D} : \rho(x) < \delta_\epsilon\}$, with boundary Γ (including the pinning sites, since we define ρ as the signed distance). Set

$$\bar{u} = \sqrt{2\max_{x\in\Gamma} a(x)} \leq C\sqrt{\delta_\epsilon},$$

with constant $C > 0$ independent of ϵ. Then $\bar{u}$ is a supersolution for the Dirichlet problem,

$$-\Delta u + \frac{1}{\epsilon^2}(u^2 - a(x))u = 0, \quad x \in D_\epsilon,$$

$$u(x) = \eta_\epsilon(x), \quad x \in \Gamma. \tag{4.9}$$

Since $\underline{u} = 0$ is a subsolution, we obtain a solution $0 \leq u(x) \leq \bar{u}$ in D_ϵ. By the result of Brezis and Oswald,[7] the Dirichlet problem (4.9) admits a unique solution for any given boundary condition. Since η_ϵ also solves (4.9) we conclude that the estimate holds for η_ϵ. □

The proof of Theorem 1.2 then follows the same lines as that of Theorem 1.1 of Ref. 1. We sketch the steps here.

Let h_{ex} be fixed, and $(\psi_\epsilon, A_\epsilon)$ minimizers of E_ϵ. From Lemma 2.3 we then have

$$F_\epsilon(u_\epsilon, A_\epsilon) \leq F_\infty(u_*, A_*) + o(1),$$

with $u_\epsilon = \psi_\epsilon/\eta_\epsilon$. It immediately follows that $\|h_\epsilon\|_{L^2(\mathcal{D})}$ and $\|\eta_\epsilon \nabla_{A_\epsilon} u_\epsilon\|_{L^2(\mathcal{D})}$ are uniformly bounded, and

$$\eta_\epsilon^2(|u_\epsilon|^2 - 1) \to 0 \quad \text{strongly in } L^2(\mathcal{D}). \tag{4.10}$$

Extracting a subsequence, $h_\epsilon \rightharpoonup h_0$ in $L^2(\mathcal{D})$ and $A_\epsilon \rightharpoonup A_0$ in $H^1(\mathcal{D})$, with

$$\liminf_{\epsilon\to 0}\int_{\mathcal{D}}(h_\epsilon - h_{ex})^2 \geqslant \int_{\mathcal{D}}(h_0 - h_{ex})^2.$$

Then $\eta_\epsilon \nabla u_\epsilon$ is also bounded in $L^2(\mathcal{D})$, and hence there exists w_0 with $\eta_\epsilon \nabla u_\epsilon \rightharpoonup w_0$ in $L^2(\mathcal{D})$.

Fix $\delta > 0$ and consider $\Omega_\delta = \{x \in \Omega : \rho(x) > \delta\}$. Then

$$\int_{\Omega_\delta} |\nabla u_\epsilon|^2 \leqslant \frac{C}{\delta}\int_{\Omega_\delta} a|\nabla u_\epsilon|^2 \leqslant \frac{2C}{\delta}\int_{\Omega_\delta} \eta_\epsilon |\nabla u_\epsilon|^2 \leqslant C.$$

By a diagonal argument we may extract a further subsequence and $u_0 \in H^1_{loc}(\Omega)$ such that $u_\epsilon \rightharpoonup u_0$ in $H^1(\Omega_\delta)$ for each $\delta > 0$. By lower semicontinuity,

$$\liminf_{\epsilon\to 0}\int_{\Omega} \eta_\epsilon^2 |\nabla u_\epsilon|^2 \geqslant \liminf_{\epsilon\to 0}\int_{\Omega_\delta} \eta_\epsilon^2 |\nabla u_\epsilon|^2 \geqslant \int_{\Omega_\delta} a|\nabla u_0|^2.$$

Again, this is true for all $\delta > 0$, and hence we have $\int_\Omega a|\nabla u_0|^2 \leqslant C$, so $u_0 \in H^1_a(\Omega)$. By (4.10) we conclude that $|u_0| = 1$ almost everywhere in Ω. In addition, we identify the limit $w_0 = \sqrt{a}\nabla u_0$, that is $\eta_\epsilon \nabla u_\epsilon \rightharpoonup \sqrt{a}\nabla u_0$ in $L^2(\Omega)$. By the weak H^1 convergence and uniform convergence $\eta_\epsilon^2 \to a$ in Ω_δ, we also have $\eta_\epsilon A_\epsilon u_\epsilon \to \sqrt{a}A_0 u_0$ in $L^2(\Omega_\delta)$, and hence $\eta_\epsilon \nabla_{A_\epsilon} u_\epsilon \rightharpoonup \sqrt{a}\nabla_{A_0} u_0$ in $L^2(\Omega_\delta)$. Then, by semicontinuity,

$$\liminf_{\epsilon\to 0}\int_{\Omega_\delta} \eta_\epsilon^2 |\nabla_{A_\epsilon} u_\epsilon|^2 \geqslant \int_{\Omega_\delta} a|\nabla_{A_0} u_0|^2.$$

The left-hand side is bounded, independent of δ and so we have

$$F_\infty(u_0, A_0) = \int_\Omega \frac{a}{2}|\nabla_{A_0} u_0|^2 + \frac{1}{2}\int_{\mathcal{D}} (h_0 - h_{ex})^2 \leqslant F_\infty(u_*, A_*).$$

In other words, (u_0, A_0) is a minimizer of E_ϵ, and hence the inequalities above are actually equalities. In particular, we conclude $\eta_\epsilon \nabla u_\epsilon \to \sqrt{a}\nabla u_0$ strongly in $L^2(\Omega)$, and hence $u_\epsilon \to u_0$ strongly in $H^1_{loc}(\Omega)$. Note that in the (generic) case that $\vec{D}$ is the unique minimizer in Lemma 3.2, the limit exists without subsequences.

This concludes the proof of Theorem 1.2.

V. THE BREAKDOWN OF PINNING

In this section we consider external fields of the order $|\ln \epsilon|$, where we expect vortices to nucleate in the superconducting bulk. We assume throughout that the dependence of h_{ex} on ϵ is given by

$$h_{ex} = \lambda|\ln \epsilon| + \mu \ln|\ln \epsilon|, \tag{5.1}$$

for λ, μ constants independent of ϵ.

A. Decoupling the pinning sites

We refine our decomposition of Lemma 2.3 to incorporate the effect of the pinning sites ω_j. It will be necessary to excise not only the pinning sites ω_j, but also a very small neighborhood of each, since the accounting of the energy of vortices near these "holes" is too delicate for our methods. To this end, we define

$$\delta_\epsilon := \frac{1}{|\ln \epsilon|^2},$$

and

$$\Omega_{\delta_\epsilon} := \{x \in \Omega : \mathrm{dist}(x, \partial\omega_j) > \delta_\epsilon, \quad \forall\, j = 1, \ldots, n\}.$$

We then define (v, A_v) via:

$$\psi = \eta_\epsilon u_* v, \text{ for } x \in \Omega, \quad A = A_* + A_v, \text{ for } x \in \mathcal{D}, \tag{5.2}$$

where as usual (u_*, A_*) denote the minimizers of F_∞ with h_{ex} as given, described in the previous section. The energy then decomposes as follows:

Lemma 5.1: Let (ψ, A) *be minimizers of* E_ϵ, *and* (v, A_v) *be defined as in* (5.2). *Then*, $v \in H^1_a(\Omega_{\delta_\epsilon}; \mathbf{C})$, $A_v \in H^1(\mathcal{D}; \mathbf{R}^2)$, *and*

$$E_\epsilon(\psi, A) \geqslant J_\epsilon(\eta_\epsilon) + E_*(h_*) + G_\epsilon(v, A_v) - \int_{\Omega_{\delta_\epsilon}} \nabla^\perp h_* \cdot \mathrm{Im}\{\bar{v} \nabla v\} \mathrm{d}x - o(1), \tag{5.3}$$

where $E_*(h_*) = \min F_\infty$ *(as in Lemma 3.2) and*

$$G_\epsilon(v, A_v) := \int_{\Omega_{\delta_\epsilon}} \left\{ \frac{a}{2} |(\nabla - iA_v)v|^2 + \frac{a^2}{4\epsilon^2}(|v|^2 - 1)^2 \right\} \mathrm{d}x + \frac{1}{2} \int_{\mathcal{D}} |\mathrm{curl}\, A_v|^2 \mathrm{d}x.$$

Proof: As in Lemma 2.3 we write $\psi = \eta_\epsilon u$. Since $|u_*| = 1$ we have $|v| = |u|$. From the upper bound (4.2) and the expansion of Lemma 2.3 we have:

$$C|\ln \epsilon|^2 \geqslant F_\epsilon(u_* v, A_* + A_v) \geqslant \int_{\Omega_{\delta_\epsilon}} \left\{ \frac{\eta_\epsilon^2}{2} |\nabla_A u|^2 + \frac{\eta_\epsilon^4}{4\epsilon^2}(|v|^2 - 1)^2 \right\} \mathrm{d}x + \frac{1}{2} \int_{\mathcal{D}} (h_* - h_{ex} + \mathrm{curl}\, A_v)^2. \tag{5.4}$$

Since $|u_*| = 1$ we have $(|u|^2 - 1)^2 = (|v|^2 - 1)^2$. We immediately conclude that

$$\int_{\Omega_{\delta_\epsilon}} [a(x)]^2 (|v|^2 - 1)^2 \leqslant C\epsilon^2 |\ln \epsilon|^2, \tag{5.5}$$

and that

$$\|A_v\|^2_{H^1(\mathcal{D}; \mathbf{R}^2)} \leqslant C \int_{\mathcal{D}} (\mathrm{curl}\, A_v)^2 \mathrm{d}x \leqslant C |\ln \epsilon|^2. \tag{5.6}$$

We also require a basic estimate on v. Using $v = \bar{u}_* u$,

$$\begin{aligned} \int_{\Omega_{\delta_\epsilon}} a|\nabla v|^2 &\leqslant 2 \int_{\Omega_{\delta_\epsilon}} a(|\nabla u|^2 + |v|^2 |\nabla u_*|^2) \\ &= 2 \int_{\Omega_{\delta_\epsilon}} (\eta_\epsilon^2 |\nabla u|^2 + (a - \eta_\epsilon^2)|\nabla u|^2 + a|\nabla u_*|^2 + (|v|^2 - 1)a|\nabla u_*|^2). \end{aligned} \tag{5.7}$$

We now estimate each term separately. From the energy estimate we estimate the first term by:

$$\int_{\Omega_{\delta_\epsilon}} \eta_\epsilon^2 |\nabla u|^2 \leqslant 2\int_{\Omega_{\delta_\epsilon}} \eta_\epsilon^2 |v|^2 |A_v|^2 dx + C|\ln \epsilon|^2 = 2\int_{\Omega_{\delta_\epsilon}} \eta_\epsilon^2 [(|v|^2-1)|A_v|^2 + |A_v|^2] + C|\ln \epsilon|^2$$
$$\leqslant C\left[\int_{\Omega_{\delta_\epsilon}} \eta_\epsilon^4 (|v|^2-1)^2 \int_{\Omega_{\delta_\epsilon}} |A_v|^4\right]^{1/2} + \|A_v\|_{H^1}^2 + C|\ln \epsilon|^2 \leqslant C|\ln \epsilon|^2.$$

Using (2.10), the second term of (5.7) is small compared to the first. The third term of (5.7) is of order $|\ln \epsilon|^2$ by the choice of degrees in the previous section. For the last term, we again use (2.10) to replace $a(x)$ by $\eta_\epsilon^2(x)$, making an error small compared to the integral itself. Thus,

$$\left|\int_{\Omega_{\delta_\epsilon}} (|v|^2-1)a|\nabla u_*|^2\right| \leqslant \left|\int_{\Omega_{\delta_\epsilon}} 2\eta_\epsilon^2 (|v|^2-1) 2\left(\frac{1}{a^2}|\nabla h_*|^2 + |A_*|^2\right)\right|$$
$$\leqslant C\left\{\sup_{x\in\Omega_{\delta_\epsilon}}\left[\frac{|\nabla h_*|}{a}\right]^2 + \|A_*\|_{H^1}^2\right\}\left[\int_{\Omega_{\delta_\epsilon}} \eta_\epsilon^4 (|v|^2-1)^2\right]^{1/2}$$
$$\leqslant C\epsilon(\ln|\ln \delta_\epsilon|)^2 |\ln \epsilon|^3 = o(1),$$

using (3.21) and the same argument as in the previous calculation. Substituting into (5.7), we obtain

$$\int_{\Omega_{\delta_\epsilon}} a(x)|\nabla v|^2 \leqslant C|\ln \epsilon|^2. \tag{5.8}$$

We now expand the gradient term in (5.4):

$$\eta_\epsilon^2 |(\nabla - iA)u|^2 = \eta_\epsilon^2 [|v|^2 |(\nabla - iA_*)u_*|^2 + |(\nabla - iA_v)v|^2 + 2\,\mathrm{Re}\{(u_*\overline{\nabla u_*} + iA_*)(\bar v\,\nabla\, v - iA_v|v|^2)\}] \tag{5.9}$$

$$= \eta_\epsilon^2 \left[|v|^2 \frac{1}{a^2}|\nabla h_*|^2 + |(\nabla - iA_v)v|^2 - 2\frac{1}{a}\nabla^\perp h_* \cdot \mathrm{Im}\{\bar v\,\nabla\, v\} + 2A_v|v|^2 \cdot \frac{1}{a}\nabla^\perp h_*\right], \tag{5.10}$$

using the definition (3.17) of $u_* = e^{i\phi_*}$ in terms of the field h_*. We simplify each term in turn. First,

$$\left|\int_{\Omega_{\delta_\epsilon}} \frac{\eta_\epsilon^2}{a^2}|v|^2|\nabla h_*|^2 - \int_{\Omega_{\delta_\epsilon}} \frac{1}{a}|\nabla h_*|^2\right| \leqslant \left|\int_{\Omega_{\delta_\epsilon}} \eta_\epsilon^2 (|v|^2-1)\frac{1}{a^2}|\nabla h_*|^2\right| + \left|\int_{\Omega_{\delta_\epsilon}} (\eta_\epsilon^2 - a)\frac{1}{a^2}|\nabla h_*|^2\right|$$
$$\leqslant C\sup_{\Omega_{\delta_\epsilon}}\left|\frac{\nabla h_*}{a}\right|^2 \{\|\eta_\epsilon^2(|v|^2-1)\|_{L^2(\Omega_{\delta_\epsilon})} + \|\eta_\epsilon^2 - a\|_{L^2(\Omega_{\delta_\epsilon})}\}$$
$$\leqslant C(\ln|\ln \delta_\epsilon|)^2 |\ln \epsilon|^3 \epsilon = o(1). \tag{5.11}$$

By (3.21) we have

$$\int_{\Omega\setminus\Omega_{\delta_\epsilon}} \frac{1}{a}|\nabla h_*|^2 \leqslant C{\delta_\epsilon}^2 (\ln|\ln \delta_\epsilon|)^2 |\ln \epsilon|^2 = o(1).$$

Therefore, the first term of (5.10) may be expressed as

$$\int_{\Omega_{\delta_\epsilon}} \frac{\eta_\epsilon^2}{a^2}|v|^2|\nabla h_*|^2 = \int_\Omega \frac{1}{a}|\nabla h_*|^2 + o(1). \tag{5.12}$$

For the second term, we use (2.10), (5.6), and (5.8) to obtain,

$$\int_{\Omega_{\delta_\epsilon}} \eta_\epsilon^2 |(\nabla - iA_v)v|^2 = \int_{\Omega_{\delta_\epsilon}} a|(\nabla - iA_v)v|^2 + \int_{\Omega_{\delta_\epsilon}} (\eta_\epsilon^2 - a)|(\nabla - iA_v)v|^2$$
$$= \int_{\Omega_{\delta_\epsilon}} a|(\nabla - iA_v)v|^2(1 + O(\epsilon^{1/3})) = \int_{\Omega_{\delta_\epsilon}} a|(\nabla - iA_v)v|^2 + o(1). \tag{5.13}$$

The third term may be treated as follows:

$$\left| \int_{\Omega_{\delta_\epsilon}} 2\frac{\eta_\epsilon^2}{a} \nabla^\perp h_* \cdot \mathrm{Im}\{\bar{v}\,\nabla\, v\} - \int_{\Omega_{\delta_\epsilon}} 2\nabla^\perp h_* \cdot \mathrm{Im}\{\bar{v}\,\nabla\, v\} \right| \tag{5.14}$$

$$\leqslant \sup_{\Omega_{\delta_\epsilon}} \left| \frac{\eta_\epsilon^2}{a} - 1 \right| \left| \int_{\Omega_{\delta_\epsilon}} 2\nabla^\perp h_* \cdot \mathrm{Im}\,\{\bar{v}\,\nabla\, v\} \right|$$
$$\leqslant C\epsilon^{1/3} \sup_{\Omega_{\delta_\epsilon}} \left| \frac{\nabla h_*}{a} \right| \int_{\Omega_{\delta_\epsilon}} a(x)((|v|^2 - 1) + 1 + |\nabla v|^2)$$
$$\leqslant C\epsilon^{1/3} \ln|\ln\, \delta_\epsilon| |\ln\, \epsilon|^3 = o(1), \tag{5.15}$$

using (5.5) and (5.8).

For the last term in (5.10), we proceed in two steps. First, using (2.10), (3.21), and (5.6),

$$\left| \int_{\Omega_{\delta_\epsilon}} \eta_\epsilon^2 A_v |v|^2 \cdot \frac{1}{a} \nabla^\perp h_* - \int_{\Omega_{\delta_\epsilon}} A_v \cdot \nabla^\perp h_* \right|$$
$$\leqslant \int_{\Omega_{\delta_\epsilon}} |A_v| \eta_\epsilon^2 ||v|^2 - 1| \frac{1}{a} |\nabla h_*| + \int_{\Omega_{\delta_\epsilon}} |A_v| |\nabla h_*| \left| \frac{\eta_\epsilon^2}{a} - 1 \right|$$
$$\leqslant \sup_{\Omega_{\delta_\epsilon}} \left| \frac{\nabla h_*}{a} \right| \| \eta_\epsilon^2 (|v|^2 - 1)\|_{L^2} \|A_v\|_{L^2(\Omega_{\delta_\epsilon})} + C\|A_v\|_{L^2} \|\nabla h_*\|_{L^\infty(\Omega_{\delta_\epsilon})} \sup_{\Omega_{\delta_\epsilon}} \left| \frac{\eta_\epsilon^2}{a} - 1 \right|$$
$$\leqslant C\epsilon \ln|\ln\, \delta_\epsilon| |\ln\, \epsilon|^2 + C\epsilon^{1/3} |\ln\, \epsilon|^2 = o(1).$$

Next, we compare with the value in all of Ω:

$$\left| \int_{\Omega \setminus \Omega_{\delta_\epsilon}} A_v \cdot \nabla^\perp h_* \right| \leqslant \|A_v\|_{L^2} \left(\int_{\Omega \setminus \Omega_{\delta_\epsilon}} |\nabla h_*|^2 \right)^{1/2} \leqslant C|\ln\, \epsilon|^2 \delta_\epsilon^{3/2} \ln|\ln\, \delta_\epsilon| = o(1). \tag{5.16}$$

Putting these estimates together and using (3.21), we obtain:

$$\int_{\Omega_{\delta_\epsilon}} \eta_\epsilon^2 |(\nabla - iA)u|^2 = \int_{\Omega_{\delta_\epsilon}} \{a(x)|(\nabla - iA_v)v|^2 - 2\nabla^\perp h_* \cdot \mathrm{Im}\{\bar{v}\,\nabla\, v\}\} + \int_\Omega \left\{ \frac{1}{a} |\nabla h_*|^2 + 2A_v \cdot \nabla^\perp h_* \right\}$$
$$+ o(1). \tag{5.17}$$

What's more, we may integrate the last term in (5.17) by parts, recalling that h_* is constant in each pinning site ω_j,

$$\int_\Omega 2A_v \cdot \nabla^\perp h_* = 2\int_\Omega A_v \cdot \nabla^\perp (h_* - h_{ex}) = 2\int_{\partial\Omega} (h_* - h_{ex}) A_v \cdot \tau - 2\int_\Omega (h_* - h_{ex}) \nabla^\perp \cdot A_v$$

$$= -2\left(\sum_{j=1}^{n} (h_* - h_{ex}) \,\Big|_{\omega_j} \int_{\omega_j} \operatorname{curl} A_v + \int_\Omega (h_* - h_{ex}) \operatorname{curl} A_v \right)$$

$$= -2\int_{\mathcal{D}} (h_* - h_{ex}) \operatorname{curl} A_v .$$

On the other hand, we have

$$\int_{\mathcal{D}} (h - h_{ex})^2 = \int_{\mathcal{D}} (h_* - h_{ex})^2 + \int_{\mathcal{D}} (\operatorname{curl} A_v)^2 + \int_{\mathcal{D}} 2(h_* - h_{ex}) \operatorname{curl} A_v ,$$

and so the last term from (5.17) in fact cancels leaving us with the desired conclusion. □

We now define

$$\mathcal{E}_\epsilon(v, A_v) = G_\epsilon(v, A_v) - \int_{\Omega_{\delta_\epsilon}} \nabla^\perp h_* \cdot \operatorname{Im}\{\bar{v} \nabla v\} dx$$

$$= \int_{\Omega_{\delta_\epsilon}} \left\{ \frac{a}{2} |(\nabla - iA_v)v|^2 + \frac{a^2}{4\epsilon^2} (|v|^2 - 1)^2 - \nabla^\perp h_* \cdot \operatorname{Im}\{\bar{v} \nabla v\} \right\} dx + \frac{1}{2}\int_{\mathcal{D}} |\operatorname{curl} A_v|^2 dx .$$

The upper bound (4.2) then implies that for global minimizers, the associated (v, A_v) satisfy the upper bound,

$$\mathcal{E}_\epsilon(v, A_v) \leq o(1). \tag{5.18}$$

B. Vortex balls

Now in Ω_{δ_ϵ}, we may isolate the vortices using the method of Sandier[14] and Sandier and Serfaty.[16] We have the following result.

Proposition 5.2: Assume $h_{ex} \leq C|\ln \epsilon|$. *For any* $C > 0$ *there exist positive constants* ϵ_0, C_0 *so that for any* (v, A_v) *satisfying* (5.18) *there exists a finite collection* $\{B_i = B(p_i, s_i)\}_{i=1,\ldots,m}$ *of disjoint balls such that:*

$$\{x \in \Omega_{\delta_\epsilon} : |v| < 1 - |\ln \epsilon|^{-4}\} \subset \cup_{i=1}^m B_i ; \tag{5.19}$$

$$\sum_{i=1}^{m} s_i < |\ln \epsilon|^{-12} ; \tag{5.20}$$

$$\deg_{\partial B_i}\left(\frac{v}{|v|} \right) := d_i \quad \textit{for all } i ; \tag{5.21}$$

$$\int_{B_i} \left[\frac{a}{2} |(\nabla - iA_v)v|^2 + (\operatorname{curl} A_v)^2 \right] \geq \pi a(p_i) |d_i| (|\ln \epsilon| - C_0 \ln|\ln \epsilon|) \quad \textit{for all } i. \tag{5.22}$$

Sketch of Proof: We sketch the proof, as the details are minor modifications of the analogous results in Refs. 15 and 16. First, from (5.5), (5.6), and (5.8) we have $G_\epsilon(v, A_v) \leq C|\ln \epsilon|^2$. Since $a(x) \geq C\delta_\epsilon$ for $x \in \Omega_{\delta_\epsilon}$, setting $f := |v|$ we have

$$\delta_\epsilon{}^2 \int_{\Omega_{\delta_\epsilon}} \left(\frac{1}{2}|\nabla f|^2 + \frac{1}{4\epsilon^2}(f^2-1)^2 \right) \leqslant C|\ln \epsilon|^2,$$

and hence

$$\int_{\Omega_{\delta_\epsilon}} \left(\frac{1}{2}|\nabla f|^2 + \frac{1}{4\epsilon^2}(f^2-1)^2 \right) \leqslant C|\ln \epsilon|^6.$$

Let $U_{\delta_\epsilon,t} := \{x \in \Omega_{\delta_\epsilon} : f(x) < 1-t\}$, and $\gamma_t = \partial U_{\delta_\epsilon,t}$. Using the co-area formula as in Ref. 16, there exists $t_0 \in (0, |\ln \epsilon|^{-4})$ and a finite set of balls $B_1, \ldots, B_k$ with radii $s_1, \ldots, s_k$ which cover γ_{t_0}, satisfying $\Sigma_i s_i \leqslant C\epsilon|\ln \epsilon|^8$. In $\Omega_{\delta_\epsilon} \setminus U_{\delta_\epsilon,t_0}$ we have $f = |v| \geqslant 1-t$, and we may write $v = fe^{i\phi}$ for a (possibly multivalued) H^1_{loc} function $\phi(x)$.

We then let the balls grow continuously, using the process described in Refs. 14 and 16, to obtain a lower bound in the expanding balls,

$$\int_{B_i \setminus U_{\delta_\epsilon,t_0}} \left[\frac{a}{2}|\nabla \phi - A_v|^2 + (\operatorname{curl} A_v)^2 \right] \geqslant \pi(\min_{B_i} a)|d_i|(\ln \epsilon - \bar{C}_0 \ln|\ln \epsilon|),$$

with constant $\bar{C}_0$ independent of ϵ. Note that the minimum of $a(x)$ over B_i is nonincreasing as the radii increase and as balls are merged (when they touch in the expansion process). We terminate the process when the sum of the radii of the balls equals $|\ln \epsilon|^{-12}$. By continuity of $a(x)$ we may then replace the minimum of a on each ball by the value at its center p_i, making an error which is small compared to $a(p_i)$ itself. This error can then be absorbed into the coefficient of $\ln|\ln \epsilon|$.

Finally,

$$\begin{aligned}
\int_{B_i} \left[\frac{a}{2}|(\nabla - iA_v)v|^2 + (\operatorname{curl} A_v)^2 \right] &\geqslant \int_{B_j \setminus U_{\delta'_\epsilon,t_0}} \left[\frac{a}{2}(1+f^2-1)|\nabla \phi - A_v|^2 + (\operatorname{curl} A_v)^2 \right] \\
&\geqslant (1 - C|\ln \epsilon|^{-4}) \int_{B_j \setminus U_{\delta_\epsilon,t_0}} \frac{a}{2}[|\nabla \phi - A_v|^2 + (\operatorname{curl} A_v)^2] \\
&\geqslant (1 - C|\ln \epsilon|^{-4})(\pi a(p_i)|d_i|(|\ln \epsilon| - \bar{C}_0 \ln|\ln \epsilon|)) \\
&\geqslant \pi a(p_i)|d_i|(|\ln \epsilon| - C_0 \ln|\ln \epsilon|),
\end{aligned}$$

for constant C_0 independent of ϵ, which completes the sketch of the proof of the proposition. □

We recall from Sec. I the following definition: We say ψ has an *essential vortex* at $p_i \in \Omega_{\delta_\epsilon}$ if there is a vortex ball B_i centered at p_i with degree $d_i \neq 0$. Note that $\psi/|\psi| = u/|u| = v/|v|$ in Ω_{δ_ϵ}, and so each has the same essential vortices.

C. A lower bound

To prove Theorem 1.3 we match the upper bound (5.18) with a sharp lower bound for the energy in terms of the vortex balls. We define $\rho_j(x) := \operatorname{dist}(x, \partial\omega_j)$, $j = 1, \ldots, n$, and sets

$$\gamma_{t,j} := \{x \in \Omega : \rho_j(x) = t\}, \quad \gamma_t = \cup_{j=1}^n \gamma_{t,j}.$$

We now choose

$$\sigma_\epsilon \in \left[\frac{[\ln|\ln \epsilon|]^{1/4}}{|\ln \epsilon|}, 2\frac{[\ln|\ln \epsilon|]^{1/4}}{|\ln \epsilon|} \right], \tag{5.23}$$

with the property that $\gamma_{\sigma_\epsilon} \cap (\cup_i B_i) = \emptyset$. This is possible by (5.20). We may then define degrees,

$$\Delta_j := \deg\left(\frac{v}{|v|}; \gamma_{\sigma_\epsilon, j}\right), \quad j = 1, \ldots, n,$$

associated to each interior boundary curve of the domain

$$\Omega_{\sigma_\epsilon} := \{x \in \Omega : \rho(x) > \sigma_\epsilon\}.$$

Then, we prove the following lower bound in Ω_{σ_ϵ}:

Lemma 5.3: There exist bounded constants, $\beta_{\epsilon,j}$, $j=1,\ldots,n$, such that:

$$\mathcal{E}_\epsilon(v, A_v) \geqslant \pi \sum_{\rho(p_i)>\sigma_\epsilon} a(p_i)|d_i|(|\ln \epsilon| - C_0 \ln|\ln \epsilon|) + 2\pi \sum_{\rho(p_i)>\sigma_\epsilon} (h_*(p_i) - h_{ex})d_i + 2\pi \sum_{j=1}^{n} \beta_{\epsilon,j}\Delta_j + \int_{\Omega_{\sigma_\epsilon} \setminus \cup B_i} \left\{ \frac{a}{2}|(\nabla - iA_v)v|^2 + (\operatorname{curl} A_v)^2 \right\} + O([\ln|\ln \epsilon|]^{1/2}).$$

Proof:

Step 1: The first step is to modify δ_ϵ. We claim that there exists $\delta_\epsilon' \in [\delta_\epsilon, 2\delta_\epsilon]$ and a constant $C>0$ (independent of ϵ) so that

$$|v| \geqslant 1 - |\ln \epsilon|^{-5} \quad \text{for all } x \in \gamma_{\delta_\epsilon'}, \tag{5.24}$$

$$\int_{\gamma_{\delta_\epsilon'}} |\nabla v|^2 \mathrm{d}s \leqslant C\frac{|\ln \epsilon|^2}{\delta_\epsilon^2}. \tag{5.25}$$

Indeed, let

$$I_\epsilon = \{t \in [\delta_\epsilon, 2\delta_\epsilon] : \gamma_t \cap (\cup_i B_i) = \emptyset\}.$$

By (5.20), the measure $|I_\epsilon| \geqslant \frac{1}{2}\delta_\epsilon$, and for all $t \in I_\epsilon$ and $x \in \gamma_t$, $|u(x)| \geqslant 1 - |\ln \epsilon|^{-5}$. Define

$$\mathcal{N}_{2\delta_\epsilon} := \{x \in \Omega : \rho(x) \leqslant 2\delta_\epsilon\}.$$

Since

$$\int_{\mathcal{N}_{2\delta_\epsilon}} |\nabla v|^2 \leqslant \delta_\epsilon^{-1} \int_{\mathcal{N}_{2\delta_\epsilon}} a|\nabla v|^2 \leqslant \delta_\epsilon^{-1}|\ln \epsilon|^2,$$

we have

$$\delta_\epsilon^{-1}|\ln \epsilon|^2 \geqslant C\int_{\delta_\epsilon}^{2\delta_\epsilon} \int_{\gamma_t} |\nabla v|^2 \mathrm{d}s_t \mathrm{d}t \geqslant C\int_{I_\epsilon} \int_{\gamma_t} |\nabla v|^2 \mathrm{d}s_t \mathrm{d}t,$$

where ds_t denotes arclength measure on γ_t. Therefore, there exists $C>0$ and $\delta_\epsilon' \in I_\epsilon$ such that

$$\int_{\gamma_{\delta_\epsilon'}} |\nabla v|^2 \mathrm{d}s \leqslant \frac{C|\ln \epsilon|^2}{|I_\epsilon|\delta_\epsilon} \leqslant \frac{2C|\ln \epsilon|^2}{\delta_\epsilon^2}.$$

This proves (5.24) and (5.25).

Step 2: Next, we claim that replacing Ω_{δ_ϵ} with $\Omega_{\delta_\epsilon'}$ in the definition of $\mathcal{E}_\epsilon$ results in an error which is very small.

Indeed, we estimate as in the proof of Lemma 5.1:

$$\left| \int_{\Omega_{\delta'_\epsilon}\setminus\Omega_{\delta_\epsilon}} \nabla^\perp h_* \cdot \mathrm{Im}\{\bar{v}\,\nabla\, v\} \right| \leqslant \int_{\Omega_{\delta'_\epsilon}\setminus\Omega_{\delta_\epsilon}} |\nabla h_*||v||\nabla_{A_v} v| + |\nabla h_*||A_v||v|^2$$
$$\leqslant \int_{\Omega_{\delta'_\epsilon}\setminus\Omega_{\delta_\epsilon}} \left[\frac{1}{2}|\nabla_{A_v} v|^2 + \frac{1}{2}|v|^2|\nabla h_*|^2 + (|v|^2-1)|\nabla h_*||A_v| + |\nabla h_*||A_v| \right]. \tag{5.26}$$

The first term on the right-hand side appears in the integrand in $\mathcal{E}_\epsilon$. The second term estimates as:

$$\int_{\Omega_{\delta'_\epsilon}\setminus\Omega_{\delta_\epsilon}} |v|^2|\nabla h_*|^2 = \int_{\Omega_{\delta_\epsilon{}'}\setminus\Omega_{\delta_\epsilon}} |\nabla h_*|^2[(|v|^2-1)+1]$$
$$\leqslant C \max_{x\in\Omega_{\delta'_\epsilon}} \frac{|\nabla h_*|^2}{a^2} |\Omega_{\delta'_\epsilon}\setminus\Omega_{\delta_\epsilon}|^{1/2} \left(\int_{\Omega_{\delta'_\epsilon}\setminus\Omega_{\delta_\epsilon}} a^2(|v|^2-1)^2 \right)^{1/2} + \int_{\Omega_{\delta'_\epsilon}\setminus\Omega_{\delta_\epsilon}} |\nabla h_*|^2$$
$$\leqslant \frac{C \ln\ln|\ln\epsilon|}{|\ln\epsilon|^4},$$

using (3.21). The third term is done in a similar way,

$$\int_{\Omega_{\delta'_\epsilon}\setminus\Omega_{\delta_\epsilon}} (|v|^2-1)|\nabla h_*|^2|A_v| \leqslant \max_{\Omega_{\delta'_\epsilon}\setminus\Omega_{\delta_\epsilon}} \frac{|\nabla h_*|}{a(x)} \left(\int_{\Omega_{\delta'_\epsilon}\setminus\Omega_{\delta_\epsilon}} a^2(|v|^2-1)^2 \right)^{1/2} \left(\int_{\Omega_{\delta'_\epsilon}\setminus\Omega_{\delta_\epsilon}} A_v^2 \right)^{1/2}$$
$$\leqslant C\,\epsilon\delta_\epsilon |\ln\ln\delta_\epsilon| |\ln\epsilon|^3.$$

Finally, the last term in (5.26) is estimated already in (5.16), so we conclude that the difference in energies in (5.26) is vanishingly small, which completes the claim.

Step 3: Integration by parts:

$$\int_{\Omega_{\delta'_\epsilon}} \nabla^\perp h_* \cdot \mathrm{Im}\{\bar{v}\,\nabla\, v\} = -2\pi \sum_{i=1}^m (h_*(p_i) - h_{ex}) d_i - \int_{\gamma_{\delta'_\epsilon}} (h_* - h_{ex}) \mathrm{Im}\{\bar{w}\,\nabla\, w\} \cdot \tau \,\mathrm{d}s$$
$$+ o(1) \left[1 + \sum_{i=1}^m a(p_i)|d_i| \right], \tag{5.27}$$

where $w = v/|v|$ and τ is the unit tangent vector to each $\gamma_{\delta'_\epsilon,j}$. This step follows exactly as in Lemma II.3 of Ref. 15, with some attention payed to relating the error to the weighted sum of the degrees. We leave the details to the interested reader.

Step 4: We claim

$$\int_{\gamma_{\delta'_\epsilon}} (h_* - h_{ex}) \mathrm{Im}\{\bar{w}\,\nabla\, w\} \cdot \tau \,\mathrm{d}s = 2\pi \sum_{j=1}^n \beta_{\epsilon,j} \deg(w; \gamma_{\delta'_\epsilon,j}) + O(\ln(\ln|\ln\epsilon|)), \tag{5.28}$$

with constants

$$\beta_{\epsilon,j} := (h_*(x) - h_{ex})\big|_{x\in\omega_j}. \tag{5.29}$$

Recall from the previous section that $h_*(x)$ is constant in each ω_j, and $\beta_{\epsilon,j}$ are uniformly bounded, independent of ϵ by Lemma 3.4 and (3.18).

To prove Step 4 we recall the boundary estimate (3.11): when applied to h_* we have

$$|h_*(x) - h_{ex} - \beta_{\epsilon,j}| \leq C(\delta'_\epsilon)^2 \ln|\ln \delta_\epsilon'||\ln \epsilon|, \quad x \in \gamma_{\delta'_\epsilon,j}, \quad j = 1,\ldots,n, \tag{5.30}$$

with constant C independent of ϵ. Hence,

$$\begin{aligned}\left| \int_{\gamma_{\delta'_\epsilon}} (h_* - h_{ex} - \beta_{\epsilon,j}) \mathrm{Im}\{\bar{w} \nabla w\} \cdot \tau \, ds \right| &\leq C(\delta'_\epsilon)^2 \ln|\ln \delta_\epsilon'||\ln \epsilon| \left[\int_{\gamma_{\delta'_\epsilon,j}} |\nabla w|^2 \mathrm{d}s \right]^{1/2} \\ &\leq 2C(\delta'_\epsilon)^2 \ln|\ln \delta_\epsilon'||\ln \epsilon| \left[\int_{\gamma_{\delta'_\epsilon,j}} |\nabla v|^2 \mathrm{d}s \right]^{1/2} \\ &\leq C' \delta'_\epsilon \ln|\ln \delta_\epsilon'||\ln \epsilon|^2 \leq C'' \ln(\ln|\ln \epsilon|),\end{aligned}$$

using (5.24) to replace $|\nabla w|^2 = |\nabla v|^2/|v|^2 \leq 2|\nabla v|^2$, and (5.25) for the next-to-last line above. Then, we calculate,

$$\begin{aligned}\int_{\gamma_{\delta'_\epsilon}} (h_* - h_{ex}) \mathrm{Im}\{\bar{w} \nabla w\} \cdot \tau \, \mathrm{d}s &= \int_{\gamma_{\delta'_\epsilon}} \beta_{\epsilon,j} \mathrm{Im}\{\bar{w} \nabla w\} \cdot \tau \, \mathrm{d}s + \int_{\gamma_{\delta'_\epsilon}} (h_* - h_{ex} - \beta_{\epsilon,j}) \mathrm{Im}\{\bar{w} \nabla w\} \cdot \tau \, \mathrm{d}s \\ &= 2\pi \beta_{\epsilon,j} \deg(w; \gamma_{\delta'_\epsilon,j}) + O(\ln(\ln|\ln \epsilon|)),\end{aligned}$$

which establishes Step 4.

Step 5: Conclusion. By (5.30) and the linear growth of a (hypothesis (H3)) if $\rho_j(p_i) = \mathrm{dist}(p_i, \partial\omega_j) \in [\delta'_\epsilon, \sigma_\epsilon]$, (with σ_ϵ as in (5.23)),

$$|h_*(p_i) - h_{ex} - \beta_{\epsilon,j}| \leq C[\rho_j(p_i)]^2 \ln|\ln \rho(p_i)||\ln \epsilon| \leq C\rho_j(p_i)\sigma_\epsilon \ln|\ln \sigma_\epsilon||\ln \epsilon| \leq Ca(p_i)(\ln|\ln \epsilon|)^{1/2}.$$

Combining Steps 2, 3, and 4, we have,

$$\begin{aligned}\int_{\Omega_{\delta'_\epsilon}} \nabla^\perp h_* \cdot \mathrm{Im}\{\bar{v} \nabla v\} = &-2\pi \sum_{\rho(p_i) > \sigma_\epsilon} (h_*(p_i) - h_{ex}) d_i - 2\pi \sum_{j=1}^n \beta_{\epsilon,j} \deg(w; \gamma_{\delta'_\epsilon,j}) \\ &- 2\pi \sum_{j=1}^n \left[\sum_{\delta'_\epsilon < \rho_j(p_i) \leq \sigma_\epsilon} \beta_{\epsilon,j} d_i \right] + O((\ln|\ln \epsilon|)^{1/2}) \left[1 + \sum_{\rho_j(p_i) > \delta'_\epsilon} a(p_i)|d_i| \right].\end{aligned}$$

Since

$$\deg(w; \gamma_{\sigma_\epsilon,j}) = \deg(w; \gamma_{\delta'_\epsilon,j}) + \sum_{\delta'_\epsilon < \rho_j(p_i) \leq \sigma_\epsilon} d_i,$$

we obtain

$$\begin{aligned}\int_{\Omega_{\delta'_\epsilon}} \nabla^\perp h_* \cdot \mathrm{Im}\{\bar{v} \nabla v\} = &-2\pi \sum_{\rho(p_i) > \sigma_\epsilon} (h_*(p_i) - h_{ex}) d_i - 2\pi \sum_{j=1}^n \beta_{\epsilon,j} \deg(w; \gamma_{\sigma_\epsilon,j}) \\ &+ O((\ln|\ln \epsilon|)^{1/2}) \left[1 + \sum_{\rho(p_i) > \delta'_\epsilon} a(p_i)|d_i| \right].\end{aligned}$$

This last error term may be absorbed into the first term in the lower bound expansion in the balls, (5.22), by adjusting the constant C_0. The conclusion of the Lemma then follows by combining the above with (5.22) in the definition of $\mathcal{E}_\epsilon$. □

D. Analysis of vortices

We now proceed to the proof of Theorem 1.3 using the lower bound established in Lemma 5.3. From the upper bound (5.18) and Lemma 5.3 we have the estimate,

$$O([\ln|\ln \epsilon|]^{1/2}) \geq \pi \sum_{\rho(p_i)>\sigma_\epsilon} a(p_i)|d_i|(|\ln \epsilon| - C_0 \ln|\ln \epsilon|) + 2\pi \sum_{\rho(p_i)>\sigma_\epsilon} (h_*(p_i) - h_{ex})d_i + 2\pi \sum_{j=1}^{n} \beta_{\epsilon,j}\Delta_j + \int_{\Omega_{\sigma_\epsilon}\setminus \cup B_i} \left\{ \frac{a}{2}|(\nabla - iA_v)v|^2 + \frac{a^2}{4\epsilon^2}(|v|^2-1)^2 + (\operatorname{curl} A_v)^2 \right\}, \tag{5.31}$$

in terms of the vortex balls defined in Proposition 5.2. If we consider only the net contribution of interior vortices to (5.31), we see that adding vortex at location p_i becomes economical when $2(h_{ex} - h_*(p_i)) \simeq 2h_{ex}\zeta(p_i)$ exceeds $a(p_i)|\ln \epsilon|$. This rough observation leads us to choose a candidate for a critical value λ_*, defined by

$$\frac{1}{\lambda_*} := \max_{x\in\Omega} \frac{2\zeta(x)}{a(x)}. \tag{5.32}$$

We note that the boundary estimate (3.11), when applied to ζ, shows that

$$0 < \zeta(x)/a(x) \leq C\rho(x)\ln|\ln \rho(x)|$$

for x near each $\partial\omega_j$, and hence the maximum is attained on a set

$$\Gamma := \{x \in \Omega : 2\lambda_*\zeta(x) = a(x)\}$$

which lies strictly *inside* Ω. We note as in the Introduction, the optimal set Γ can be of two different forms:

Case A: Γ is a finite point set.

Case B: Γ contains at least one closed curve γ. In either case we have the following.

Lemma 5.4: There exist constants $K_1 > 0$ and $M \geq 1$ such that

$$\frac{2\zeta(x)}{a(x)} \leq \frac{1}{\lambda_*} - \frac{K_1}{\sqrt{|\ln \epsilon|}} \tag{5.33}$$

whenever $\operatorname{dist}(x,\Gamma) \geq |\ln \epsilon|^{-1/4M}$.

The proof, based on the real analyticity of ζ and a, is exactly as in Ref. 3, and is omitted.

We now proceed as in Refs. 1 and 3 and treat the vortices in different cases, depending on whether they lie close to the optimal set Γ or the boundaries of ω_j. Let $\gamma > 0$ to be chosen so that

$$\frac{\zeta(x)}{a(x)} < \frac{1}{8\lambda_*} \quad \text{for all } x \in \Omega \text{ with } \rho(x) < \gamma. \tag{5.34}$$

Then we define index sets,

$$Z_\gamma := \{i : \sigma_\epsilon < \operatorname{dist}(p_i, \cup_{j=1}^n \partial\omega_j) \leq \gamma\},$$

$$Z_* := \{i : \operatorname{dist}(p_i,\Gamma) < |\ln \epsilon|^{-1/2M} \quad \text{and} \quad d_i \geq 0\},$$

$$Z_- := \{i : \operatorname{dist}(p_i,\Gamma) < |\ln \epsilon|^{-1/2M} \quad \text{and} \quad d_i < 0\},$$

$$Z_0 := (Z_* \cup Z_- \cup Z_\gamma)^C,$$

and set

$$N_x := \sum_{Z_x} a(p_i)|d_i|, \quad x = \gamma, *, -, 0; \quad \mathbf{N}_\epsilon = \sum a(p_i)|d_i| = N_* + N_\gamma + N_- + N_0.$$

The estimate of the interaction term in (5.31) is then different depending on which category the vortex ball belongs to.

Consider first vortex balls with $i \in Z_\gamma$. For such vortex balls, $a(p_i)|\ln \epsilon| \geqslant C\sigma_\epsilon|\ln \epsilon| \geqslant C[\ln|\ln \epsilon|]^{1/4}$. Therefore, using Lemma 3.4 we have:

$$\begin{aligned}|h_{ex} - h_*(p_i)| &\leqslant h_{ex}\zeta(p_i) + |h_{ex}(1-\zeta(p_i)) - h_*(p_i)| \leqslant \frac{1}{8\lambda_*}a(p_i)h_{ex} + C \\ &\leqslant \frac{1}{8\lambda_*}a(p_i)h_{ex} + \frac{C'}{[\ln|\ln \epsilon|]^{1/4}}a(p_i)|\ln \epsilon| \leqslant \frac{1}{6\lambda_*}a(p_i)h_{ex}.\end{aligned}$$

Therefore, recalling that $h_{ex} = \lambda|\ln \epsilon| + \mu \ln|\ln \epsilon|$, we estimate the first two terms in (5.31) corresponding to vortex balls counted by Z_γ by

$$\begin{aligned}&\pi\sum_{Z_\gamma} a(p_i)|d_i|(|\ln \epsilon| - C_0\ln|\ln \epsilon|) + 2\pi\sum_{Z_\gamma}(h_*(p_i) - h_{ex})d_i \\ &\quad \geqslant \pi N_\gamma\left[\left(1 - \frac{\lambda}{3\lambda_*}\right)|\ln \epsilon| - \left(C_0 + \frac{\mu}{3\lambda_*}\right)\ln|\ln \epsilon|\right] \geqslant \pi N_\gamma\left(1 - \frac{\lambda}{2\lambda_*}\right)|\ln \epsilon|. \qquad (5.35)\end{aligned}$$

When $\mathrm{dist}(p_i, \partial\omega_j) \geqslant \gamma$, we use Lemma 3.4 to obtain:

$$|h_*(p_i) - h_{ex} + h_{ex}\zeta(p_i)| \leqslant C \leqslant \frac{C}{a_0}a(p_i),$$

where $a_0 = \min\{a(x) : \mathrm{dist}(x, \cup_j \partial\omega_j) \geqslant \gamma\}$. Hence,

$$\begin{aligned}&\pi\sum_{i \in Z_* \cup Z_- \cup Z_0} \{a(p_i)|d_i|(|\ln \epsilon| - C_0\ln|\ln \epsilon|) + 2(h_*(p_i) - h_{ex})d_i\} \\ &\quad \geqslant \pi\sum_{i \in Z_* \cup Z_- \cup Z_0} \{a(p_i)|d_i|(|\ln \epsilon| - C_0'\ln|\ln \epsilon|) - 2h_{ex}\zeta(p_i)d_i\},\end{aligned}$$

with constant $C_0' \geqslant C_0$, absorbing the $O(1)$ term above. For vortices counted by Z_* and by Z_- we are content to estimate $0 < \zeta(p_i)/a(p_i) \leqslant 1/2\lambda_*$. For Z_*, this results in a lower bound,

$$\pi\sum_{Z_*} a(p_i)|d_i|(|\ln \epsilon| - C_0'\ln|\ln \epsilon|) - 2\pi h_{ex}\sum_{Z_*}\zeta(p_i)d_i \geqslant \pi N_*\left[\left(1 - \frac{\lambda}{\lambda_*}\right)|\ln \epsilon| - \left(C_0' + \frac{\mu}{\lambda_*}\right)\ln|\ln \epsilon|\right]. \qquad (5.36)$$

For vortices counted by Z_- we note in addition that the contribution to the energy is positive. Hence, the first two terms in (5.31) coming from these vortex balls may be estimated by

$$\pi\sum_{Z_-} a(p_i)|d_i|(|\ln \epsilon| - C_0'\ln|\ln \epsilon|) - 2\pi h_{ex}\sum_{Z_-}\zeta(p_i)d_i \geqslant \frac{\pi}{2}N_-|\ln \epsilon|. \qquad (5.37)$$

Finally, when the vortices are counted by Z_0 we use (5.33). This leads to the lower bound,

$$\begin{aligned}
&\pi\sum_{Z_0} a(p_i)|d_i|(|\ln\epsilon| - C_0'\ln|\ln\epsilon|) - 2\pi h_{ex}\sum_{Z_0}\zeta(p_i)d_i \\
&\quad\geqslant \pi N_0\left[\left(1-\frac{\lambda}{\lambda_*}+\frac{K_1}{\sqrt{|\ln\epsilon|}}\right)|\ln\epsilon| - \left(C_0'+\frac{\mu}{\lambda_*}\right)\ln|\ln\epsilon| + o(1)\right] \\
&\quad\geqslant \pi N_0\left(1-\frac{\lambda}{\lambda_*}+\frac{K_2}{\sqrt{|\ln\epsilon|}}\right)|\ln\epsilon|. \qquad (5.38)
\end{aligned}$$

Substituting (5.35)–(5.38) into (5.31) we obtain:

$$\begin{aligned}
O([\ln|\ln\epsilon|]^{1/2}) &\geqslant \pi N_\gamma\left(1-\frac{\lambda}{2\lambda_*}\right)|\ln\epsilon| + \frac{1}{2}\pi N_-|\ln\epsilon| + \pi N_*\left[\left(1-\frac{\lambda}{\lambda_*}\right)|\ln\epsilon| - \left(C_0'+\frac{\mu}{\lambda_*}\right)\ln|\ln\epsilon|\right] \\
&\quad + \pi N_0\left(1-\frac{\lambda}{\lambda_*}+\frac{K_2}{\sqrt{|\ln\epsilon|}}\right)|\ln\epsilon| + 2\pi\sum_{j=1}^{n}\beta_{\epsilon,j}\Delta_j \\
&\quad + \int_{\Omega_{\sigma_\epsilon}\setminus\cup B_i}\left\{\frac{a}{2}|(\nabla - iA_v)v|^2 + (\operatorname{curl} A_v)^2\right\}. \qquad (5.39)
\end{aligned}$$

One difficulty in dealing with this lower bound expansion is the presence of the boundary terms coming from each $\partial\omega_j$, since we have no *a priori* bound on the degrees Δ_j around each curve $\gamma_{j,\sigma_\epsilon}$ surrounding the pinning sites. As in Refs. 1 and 3 we must consider two cases separately.

Case I: $\max_{j=1,\ldots,n}|\Delta_j| \leqslant 2\Sigma_{i=1}^{m}|d_i|$.

Since each $\beta_{\epsilon,j}$ is uniformly bounded (independent of ϵ),

$$\begin{aligned}
|\beta_{\epsilon,j}\Delta_j| &\leqslant C\sum_{i=1}^{m}|d_i| \leqslant \left[\frac{C}{[\ln|\ln\epsilon|]^{1/4}}\sum_{Z_\gamma}a(p_i)|d_i||\ln\epsilon| + \frac{C}{a_\gamma}\sum_{Z_*\cup Z_0\cup Z_-}a(p_i)|d_i|\right] \\
&\leqslant \frac{\pi}{8}N_\gamma|\ln\epsilon| + C'(N_* + N_0 + N_-),
\end{aligned}$$

with $a_\gamma = \min\{a(x):\rho(x)\geqslant\gamma\}$. In particular, we may absorb these terms into (5.39) without affecting the sign of each term for $\lambda\leqslant\lambda_*$:

$$\begin{aligned}
O([\ln|\ln\epsilon|]^{1/2}) &\geqslant \pi N_\gamma\left(\frac{3}{4}-\frac{\lambda}{2\lambda_*}\right)|\ln\epsilon| + \pi N_-\left(\frac{1}{4}+\frac{\lambda}{\lambda_*}\right)|\ln\epsilon| + \pi N_*\left[\left(1-\frac{\lambda}{\lambda_*}\right)|\ln\epsilon|\right. \\
&\quad \left. - \left(C_0''+\frac{\mu}{\lambda_*}\right)\ln|\ln\epsilon|\right] + \pi N_0\left(1-\frac{\lambda}{\lambda_*}+\frac{K_3}{\sqrt{|\ln\epsilon|}}\right)|\ln\epsilon| \\
&\quad + \int_{\Omega_{\sigma_\epsilon}\setminus\cup B_i}\left\{\frac{a}{2}|(\nabla - iA_v)v|^2 + (\operatorname{curl} A_v)^2\right\}, \qquad (5.40)
\end{aligned}$$

with C_0'', K_3 constant.

Consider first the subcritical case $\lambda<\lambda_*$ in (5.1). Then all coefficients of $|\ln\epsilon|$ are positive, and we have

$$\mathbf{N}_\epsilon = N_* + N_- + N_0 + N_\gamma \leqslant O\left(\frac{[\ln|\ln\epsilon|]^{1/2}}{|\ln\epsilon|}\right).$$

Because of the vanishing of $a(x)$ near each $\partial\omega_j$, we cannot directly conclude that there are no vortex balls in Ω_{σ_ϵ}; however, we can restrict our attention to a smaller set to obtain the desired conclusion. Let σ'_ϵ be chosen with

$$\frac{[\ln|\ln\epsilon|]^{1/2}}{|\ln\epsilon|} \ll \sigma'_\epsilon \ll 1.$$

Then for any such choice, by the linearity of $a(x)$ near $\partial\omega_j$, we have

$$\sum_{\Omega_{\sigma'_\epsilon}} |d_i| \leqslant \frac{1}{\sigma'_\epsilon}\sum_{\Omega_{\sigma'_\epsilon}} a(p_i)|d_i| = o(1),$$

and hence there are no essential vortices in $\Omega_{\sigma'_\epsilon}$ for $\lambda < \lambda_*$.

Now consider the critical case, $\lambda = \lambda_*$. Now there is cancellation of the terms multiplying $|\ln\epsilon|$, and (5.40) implies:

$$O([\ln|\ln\epsilon|]^{1/2}) \geqslant \frac{\pi}{4}N_\gamma|\ln\epsilon| + \pi N_-|\ln\epsilon| + CN_0\sqrt{|\ln\epsilon|} - \pi N_*\left(C_0'' + \frac{\mu}{\lambda_*}\right)\ln|\ln\epsilon| + G_\epsilon(v,A_v;\Omega_\epsilon \setminus \cup B_i), \tag{5.41}$$

where we define for $U \subset \Omega$,

$$G_\epsilon(v,A_v;U) := \int_U \left\{\frac{a}{2}|\nabla_{A_v}v|^2 + \frac{a^2}{4\epsilon^2}(|v|^2-1)^2 + \frac{1}{2}(\operatorname{curl} A_v)^2\right\}. \tag{5.42}$$

When $\mu < -C_0''\lambda_*$ all terms on the right-hand side have positive coefficients, and so we conclude that:

$$\sum_{\sigma_\epsilon < \operatorname{dist}(p_i,\cup\omega_j) < \sigma'_\epsilon} |d_i| < o(|\ln\epsilon|[\ln|\ln\epsilon|]^{-1/2})\sum_{Z_\gamma} a(p_i)|d_i| = o(1),$$

$$\sum_{Z_*} |d_i| \leqslant CN_* = O([\ln|\ln\epsilon|]^{-1/2}) = o(1),$$

$$\sum_{Z_-} |d_i| \leqslant CN_- = O([\ln|\ln\epsilon|]^{1/2}|\ln\epsilon|^{-1}) = o(1),$$

$$\sum_{Z_0} |d_i| \leqslant CN_0 = O([\ln|\ln\epsilon|]^{1/2}|\ln\epsilon|^{-1/2}) = o(1).$$

Each of these being integer valued, we conclude that there are no essential vortices in $\Omega_{\sigma'_\epsilon}$ for small ϵ when $\lambda = \lambda_*$ but $\mu < \mu_*$. This proves part (i) of Theorem 1.3, in Case I.

If the applied field is larger at the scale $\ln|\ln\epsilon|$, $\mu > \mu_* = -C_0''\lambda_*$, we may rearrange the terms of (5.41) and divide by $\sqrt{|\ln\epsilon|}$ to arrive at an inequality,

$$N_\gamma + N_0 + N_- \leqslant CN_*\frac{\ln|\ln\epsilon|}{\sqrt{|\ln\epsilon|}} + O\left(\frac{[\ln|\ln\epsilon|]^{1/2}}{\sqrt{|\ln\epsilon|}}\right), \tag{5.43}$$

with C independent of ϵ. Already this implies that a negligable fraction of the essential vortices are outside of a vanishingly small neighborhood of Γ or have negative degrees. We will use the

remaining term (the energy of (v,A_v) outside the balls) to bound N_* and eliminate these undesirable vortices (counted by N_γ, N_-, N_0) completely. We follow the argument of Ref. 3.

By hypothesis, each of the $(n+1)$ boundary curves (one for each $\partial\omega_j$, and the exterior boundary $\partial\mathcal{D}$) is smooth, and hence the distance functions

$$\rho_j(x) = \begin{cases} \operatorname{dist}(x,\partial\omega_j) & \text{for } j=1,\dots,n; \\ \operatorname{dist}(x,\partial\mathcal{D}) & \text{for } j=0, \end{cases}$$

are smooth in some neighborhood of each boundary curve. Let $z_0>0$ be chosen small enough that each ρ_j is smooth in the set $\widetilde{\Omega}_{z_0}=\{x\in\Omega:\operatorname{dist}(x,\partial\Omega)<z_0\}$. Then for all $0<z<z_0$, $|\nabla\rho_j|=1$ and $\partial\widetilde{\Omega}_z$ consists of exactly $(n+1)$ smooth curves $\gamma_{j,z}$, $j=0,\dots,n$, each homotopic to a component of $\partial\Omega$. Denote also $\widetilde{\Omega}_{j,z}$ the component of $\widetilde{\Omega}_z$ bounded by $\gamma_{j,z}$ and $\widetilde{\Omega}_{j,z_1,z_2}=\widetilde{\Omega}_{j,z_2}\setminus\widetilde{\Omega}_{j,z_1}$, an annular domain for each $j=0,\dots,n$.

Define $I_0:=(0,z_0)$ and

$$J_{j,\epsilon} := \left\{ z\in(0,z_0): \gamma_{j,z}\cap \cup B_{s_i}(p_i)=\emptyset \right\}.$$

In other words, $z\in J_{j,\epsilon}$ if the curve $\gamma_{j,z}$ intersects none of the vortex balls. By Proposition 5.2 the set $J_{j,\epsilon}$ is a finite union of intervals whose complement $|(0,z_0)\setminus J_{j,\epsilon}|<|\ln\epsilon|^{-12}$ has very small measure. For each $z\in J_\epsilon$, it follows that $|v|\geqslant 1-|\ln\epsilon|^{-4}$ and hence we may define

$$\Delta_j(z) := \deg\left(\frac{v}{|v|},\gamma_{j,z}\right), \quad j=0,\dots,n.$$

For $j\in\{0,\dots,n\}$ fixed, choose $0<z_1<z_2<z_0$ so that both $z_1,z_2\in J_{j,\epsilon}$. Let

$$a_0 := \min\left\{a(x): x\in \cup_{j=0}^n \widetilde{\Omega}_{j,z_1,z_2}\right\} > 0.$$

Using (5.43), we have

$$|\Delta_j(z_1)-\Delta_j(z_2)| = \left|\sum_{p_i\in\Omega_{j,z_1,z_2}} d_i\right| \leqslant \frac{1}{a_0}\sum_{p_i\in\Omega_{j,z_1,z_2}} a(p_i)|d_i| \leqslant N_0 \leqslant o(1)N_*. \tag{5.44}$$

Now, γ_{0,z_2} encloses all the inner curves γ_{j,z_2}, $j=1,\dots,n$, as well as the optimal set Γ, and therefore

$$\left|\Delta_0(z_2)-\sum_{j=1}^n \Delta_j(z_2)\right| = \left|\sum_{\operatorname{dist}(p_i,\partial\Omega)\geqslant z_2} d_i\right| \geqslant \sum_{\substack{\operatorname{dist}(p_i,\partial\Omega)\geqslant z_2 \\ d_i\geqslant 0}} d_i - \sum_{\substack{\operatorname{dist}(p_i\partial\Omega)\geqslant z_2 \\ d_i<0}} d_i$$

$$\geqslant \frac{1}{a_0}(N_*-(N_-+N_0+N_\gamma)) \geqslant \frac{1}{a_0}N_*(1-o(1)).$$

In particular, it follows that there exists at least one $j_0\in\{0,\dots,n\}$ such that

$$|\Delta_{j_0}(z_2)| \geqslant \frac{1}{a_0(n+1)}N_*.$$

By (5.44) we have

$$|\Delta_{j_0}(z)| \geqslant \frac{1}{2a_0(n+1)}N_* \quad \text{for every } z\in[z_1,z_2]. \tag{5.45}$$

Writing $v=|v|e^{i\phi}$ we estimate the remaining term in the energy using the coarea formula,

$$\int_{\widetilde{\Omega}_{j_0,z_1,z_2}\setminus\cup B_i} a|(\nabla - iA_v)v|^2 dx \geqslant a_0 \int_{\widetilde{\Omega}_{j_0,z_1,z_2}\setminus\cup B_i} \frac{|(\nabla - iA_v)v|^2}{|\nabla \rho_{j_0}|} |\nabla \rho_{j_0}| \mathrm{d}x$$

$$\geqslant a_0 \int_{J_{j_0,\epsilon}} \int_{\gamma_{j_0,z}} |(\nabla - iA_v)v|^2 \mathrm{d}\mathcal{H}^1 \mathrm{d}z$$

$$= a_0 \int_{J_{j_0,\epsilon}} \int_{\gamma_{j_0,z}} |v|^2 |\nabla\phi - A_v|^2 \mathrm{d}\mathcal{H}^1 \mathrm{d}z$$

$$\geqslant \frac{a_0}{2} \int_{J_{j_0,\epsilon}} \int_{\gamma_{j_0,z}} |\nabla\phi - A_v|^2 \mathrm{d}\mathcal{H}^1 \mathrm{d}z, \tag{5.46}$$

since $|v(x)| \geqslant 1 - |\ln \epsilon|^{-4}$ for $z \in J_{j_0,\epsilon}$.

To estimate the last term in (5.46) we use the definition of the degrees and Stokes' Theorem: for $z \in J_{j_0,\epsilon}$,

$$2\pi\Delta_{j_0}(z) - \int_{\widetilde{\Omega}_{j_0,z}} \operatorname{curl} A_v \mathrm{d}x = \int_{\gamma_{j_0,z}} (\nabla\phi - A_v)\cdot\tau \,\mathrm{d}\mathcal{H}^1 \leqslant \left[\mathcal{H}^1(\gamma_{j_0,z}) \int_{\gamma_{j_0,z}} |\nabla\phi - A_v|^2\right]^{1/2},$$

by Cauchy–Schwartz. Rearranging and squaring,

$$4\pi^2[\Delta_{j_0}(z)]^2 \leqslant 2\mathcal{H}^1(\gamma_{j_0,z}) \int_{\gamma_{j_0,z}} |\nabla\phi - A_v|^2 + 2\left[\int_{\widetilde{\Omega}_{j_0,z}\setminus\cup B_i} \operatorname{curl} A_v \mathrm{d}x + \int_{\widetilde{\Omega}_{j_0,z}\cap(\cup B_i)} \operatorname{curl} A_v \mathrm{d}x\right]^2$$

$$\leqslant C\left[\int_{\gamma_{j_0,z}} |\nabla\phi - A_v|^2 + \int_{\widetilde{\Omega}_{j_0,z}\setminus\cup B_i} (\operatorname{curl} A_v)^2 \mathrm{d}x\right] + o(1). \tag{5.47}$$

We now integrate for $z \in (z_1, z_2)$, use (5.45) and (5.46), and substitute into $G_\epsilon(v, A_v; \widetilde{\Omega}_{j_0,z_1,z_2}\setminus\cup B_i)$:

$$G_\epsilon(v, A_v; \widetilde{\Omega}_{j_0,z_1,z_2}\setminus\cup B_i) \geqslant C\int_{J_{j_0,\epsilon}} [\Delta_{j_0}(z)]^2 \mathrm{d}z \geqslant C\mathcal{L}(J_{j_0,\epsilon})N_*^2(1 - o(1)) \geqslant C_1 N_*^2. \tag{5.48}$$

Returning to the estimate (5.41) we see

$$O([\ln|\ln\epsilon|]^{1/2}) \geqslant C_1 N_*^2 - C_2 N_* \ln|\ln\epsilon|,$$

with constants C_1, C_2 independent of ϵ. We conclude that

$$N_* \leqslant C \ln|\ln\epsilon|. \tag{5.49}$$

Since $a(x)$ is bounded below in a neighborhood of the optimal set Γ, we also conclude that the total degree of interior vortices,

$$\sum_{\operatorname{dist}(p_i,\Gamma)<[|\ln\epsilon|]^{-1/4M}} |d_i| \leqslant C \ln|\ln\epsilon|.$$

With (5.43) and (5.49) we have

$$\max\{N_\gamma, N_-, N_0\} \leqslant C\frac{(\ln|\ln\epsilon|)^2}{|\ln\epsilon|^{1/2}} - o(1).$$

Again we are faced with the problem that $a(x)$ vanishes at each pinning site, and so we again need to further restrict the domain to reach a conclusion concerning the nonexistence of interior vortices. Choose any ρ_ϵ with

$$\frac{(\ln|\ln\epsilon|)^2}{|\ln\epsilon|^{1/2}} \ll \rho_\epsilon \ll 1.$$

Then, hypothesis (H3) again implies that

$$\sum_{\substack{i\in Z_\gamma\cup Z_0\cup Z_- \\ \mathrm{dist}(p_i,\cup\omega_j)>\rho_\epsilon}} |d_i| = o(1).$$

Since the degrees are integers, this implies that they are all zero for ϵ sufficiently small, and hence all vortices which lie at least a distance ρ_ϵ from the pinning sites must have nonnegative degree and lie nearby Γ. This, together with (5.49), proves the first part of (ii) of Theorem 1.3 in Case I. To verify (iv) in Case I, we return to the estimate (5.48): choose z_1, z_2 so that each $\widetilde{\Omega}_{j,z_1,z_2}$ lies strictly between the set Γ and the boundary components ω_j, $j=1,\ldots,n$. Recall that we have already shown that there are no essential vortex balls (that is, balls with $d_i\neq 0$) inside $\widetilde{\Omega}_{j,z_1,z_2}$, so $\Delta_j(z)=\Delta_j(z_1)$ is constant in each of these regions. We then re-do estimate (5.48) to obtain a lower bound in terms of $\Delta_j(z_1)$, for each $j=1,\ldots,n$:

$$G_\epsilon(v,A_v;\widetilde{\Omega}_{j_0,z_1,z_2}\setminus\cup B_i) \geqslant C\int_{J_{j,\epsilon}} [\Delta_j(z)]^2 dz \geqslant C\mathcal{L}(J_{j,\epsilon})[\Delta_j(z_1)^2] \geqslant C[\Delta_j(z_1)]^2.$$

Substituting all we know into (5.41) we then have

$$C\sum_{j=1}^{n}[\Delta_j(z_1)]^2 \leqslant G_\epsilon(v,A_v;\widetilde{\Omega}_{j,z_1,z_2}) \leqslant N_*\ln|\ln\epsilon| + O([\ln|\ln\epsilon|]^{1/2}) \leqslant C[\ln|\ln\epsilon|]^2.$$

Hence we conclude $|\Delta_j(z_1)|=|\deg(v/|v|\gamma_{z_1,j})|\leqslant C\ln|\ln\epsilon|$. Since there are no essential vortices between a neighborhood of Γ and a neighborhood of $\cup_j\omega_j$, for any fixed simple closed curve γ homotopic to $\partial\omega_j$ (for some j) which does not wind around any subset of Γ we obtain $|\deg(v/|v|;\gamma)|\leqslant C\ln|\ln\epsilon|$, proving (iv) in Case I.

It remains to prove the upper bound on the total degree stated in parts (ii) and (iii). First we consider Case A, when Γ is a set of isolated points. We return to (5.41) and estimate from below the term $G_\epsilon(v,A_v;\widetilde{\Omega}_\epsilon)$ as in Step 3 of Ref. 17. For any isolated point $P\in\Gamma$ there exists $R>0$ so that $B_R(P)$ remains disjoint from all other points of Γ and from $\partial\Omega$. Let $a_P=\min_{x\in B_R(P)}a(x)>0$. Define $\tau_\epsilon:=|\ln\epsilon|^{-1/4M}$, and

$$D_P = \sum_{\mathrm{dist}(p_i,P)<\tau_\epsilon} d_i.$$

By the analysis above, $\deg(v/|v|;\partial B_r(P))=D_P$ is constant for all $r\in(\rho,R)$, since we have shown already that there are no vortex balls with nonzero degree in the annular region surrounding P. Step 3 of Ref. 17 then applies without modification to obtain the lower bound,

$$\begin{aligned}
&\frac{1}{2}\int_{B_R(P)\setminus B_{\tau_\epsilon}(P)}\left(a(x)|(\nabla-iA_v)v|^2+\frac{a^2(x)}{2\epsilon^2}(|v|^2-1)^2\right)+\frac{1}{2}\int_{B_R(P)}(\mathrm{curl}\,A)^2\\
&\quad\geqslant \min\{a_P,1\}\frac{1}{2}\int_{B_R(P)\setminus B_{\tau_\epsilon}(P)}\left(|(\nabla-iA_v)v|^2+\frac{1}{2\epsilon^2}(|v|^2-1)^2\right)+\frac{1}{2}\int_{B_R(P)}(\mathrm{curl}\,A)^2\\
&\quad\geqslant CD_P^2\ln|\ln\epsilon|+o(1),
\end{aligned}$$

with constant C independent of ϵ. Since the facts $N_0=N_-=0$ imply $N_*=\Sigma_{P\in\Gamma}a(P)D_P$ we have the lower bound

$$G_\epsilon(v,A_v;\cup_{P\in\Gamma}(B_R(P)\setminus B_{\tau_\epsilon}(P))) \geq C' N_*^2 \ln|\ln\epsilon| + o(1),$$

with constant C' independent of ϵ. Replacing this estimate in (5.41) we have

$$O(\sqrt{\ln|\ln\epsilon|}) \geq C' N_*^2 \ln|\ln\epsilon| - \pi N_* \left(C_0'' + \frac{\mu}{\lambda_*}\right)\ln|\ln\epsilon|,$$

and hence N_* is uniformly bounded.

The upper bound on N_* for Case B requires a sharper energy estimate; we will present this proof in the final section. This concludes the analysis for Case I.

Case II: $|\Delta_j| > 2\Sigma_{\rho(p_i)\geq\sigma_\epsilon}|d_i|$ **for at least one** $j\in\{1,\ldots,n\}$.

Let $|\Delta_{j_0}| = \max|\Delta_j|$. Let z_0, $\widetilde{\Omega}_{j,z}$, $\widetilde{\Omega}_{j,z_1,z_2}$, $\Delta_j(r)$, J_ϵ be as in the previous case. By hypothesis,

$$|\Delta_{j_0}(z)| = \left|\Delta_{j_0} + \sum_{p_i\in\Omega_{j_0,z}} d_i\right| \geq \frac{1}{2}|\Delta_{j_0}| \quad \text{for all } z\in J_{j_0,\epsilon}.$$

We then estimate as in (5.46) and (5.47) to obtain:

$$G_\epsilon(v,A_v;\widetilde{\Omega}_{j_0,z_2}\setminus\cup B_i) \geq C\int_{J_{j_0,\epsilon}} (\Delta_{j_0}(z))^2 dz \geq C\frac{1}{4}\mathcal{L}(J_{j_0,\epsilon})\Delta_{j_0}^2 \geq C_1\Delta_{j_0}^2. \tag{5.50}$$

The boundary terms are estimated simply, as $|\beta_j|$ are uniformly bounded,

$$\left|2\pi\sum_{j=1}^{n}\Delta_j\beta_j\right| \leq C_2|\Delta_{j_0}|.$$

The lower bound (5.31) then gives,

$$\begin{aligned} O(\sqrt{\ln|\ln\epsilon|}) \geq{}& C_1\Delta_{j_0}^2 - C_2|\Delta_{j_0}| + \pi\sum_{\rho(p_i)\geq\sigma_\epsilon} a(p_i)|d_i|(|\ln\epsilon| - C_0\ln|\ln\epsilon|) + 2\pi\sum_{\rho(p_i)\geq\sigma_\epsilon} d_i(h_*(p_i)-h_{ex}) \\ &+ G_\epsilon(v,A_v;\Omega\setminus[\widetilde{\Omega}_{j_0,z_2}\cup(\cup B_i)]). \end{aligned}$$

We may now repeat the same steps as in Case I to derive (as in (5.40)),

$$\begin{aligned} O(\sqrt{\ln|\ln\epsilon|}) \geq{}& C_1\Delta_{j_0}^2 - C_2|\Delta_{j_0}| + \pi N_\gamma\left(\frac{3}{4}-\frac{\lambda}{2\lambda_*}\right)|\ln\epsilon| + \pi(N_*+N_0)|\ln\epsilon|\left(1-\frac{\lambda}{\lambda_*}\right) \\ &+ \pi N_-|\ln\epsilon|\left(\frac{1}{4}+\frac{\lambda}{\lambda_*}\right)(1+o(1)) - \pi N_*\left(C_0''+\frac{\mu}{\lambda_*}\right)\ln|\ln\epsilon| + CN_0\sqrt{|\ln\epsilon|}. \end{aligned} \tag{5.51}$$

Since $C_1\Delta_{j_0}^2 - C_2|\Delta_{j_0}| \geq -C_2/2C_1$ is uniformly bounded below, we may repeat the arguments from Case I to conclude that $\mathbf{N}_\epsilon = 0$ for $\lambda<\lambda_*$ or for $\lambda=\lambda_*$ and $\mu<-C_0\lambda_*$. In case $\lambda=\lambda_*$ and $\mu > -C_0\lambda_*$ we obtain (5.43) exactly as in Case I. Using the hypothesis of Case II we obtain from (5.51) that,

$$O(\sqrt{\ln|\ln\epsilon|}) \geq C_1\Delta_{j_0}^2 - C_2|\Delta_{j_0}| - C_3N_*\ln|\ln\epsilon| \geq C_1\Delta_{j_0}^2 - C_4(1+\ln|\ln\epsilon|)|\Delta_{j_0}|.$$

From this we obtain $|\Delta_{j_0}| \leq C\ln|\ln\epsilon|$ for constant C independent of ϵ, and by the Case II hypothesis then $N_* \leq \frac{1}{2}|\Delta_{j_0}| \leq C\ln|\ln\epsilon|$, and the remaining conclusions follow as in Case I.

This completes the proof of parts (i) and (ii) of Theorem 1.3.

E. Case B: Γ contains a closed curve

Now we consider the case that the optimal set Γ contains one or more closed curves γ, in which case Theorem 1.3 asserts that the total degree inside Ω is at least of the order $O(\ln|\ln \epsilon|)$. This part is very similar to the analogous parts of Refs. 1 and 3, and we only provide a sketch here for completeness. The main idea is to derive a stronger upper bound on the energy, with n_ϵ simple vortices regularly placed along γ. The construction uses a modified Green's function to construct a trial configuraton, which we expect well approximates the actual minimizer.

To avoid some technical difficulties associated with the vanishing of a at $\partial\Omega$ we fix t with $0<t<\max_{x\in\Gamma} a(x)$, and consider the truncation

$$a_t(x) := \max\{a(x),t\}.$$

Following Refs. 16, 20, and 2 we use a Green's function to construct our trial function.

Lemma 5.5: *For every fixed $y\in\Omega$ there exist $G(x,y)$ and constants $g_j=g_j(y)$, $j=1,\ldots,n$, such that*

$$-\operatorname{div}_x\left(\frac{1}{a_t}\nabla_x G(x,y)\right)+G(x,y)=\delta_y(x) \quad \text{in } \mathcal{D}'(\mathcal{D}), \tag{5.52}$$

$$G(x,y)\big|_{x\in\partial\mathcal{D}}=0, \tag{5.53}$$

$$G(x,y)\big|_{x\in\partial\omega_j}=g_j, \tag{5.54}$$

$$\int_{\partial\omega_j}\frac{1}{a_t}\frac{\partial G}{\partial \nu_x}=g_j|\omega|. \tag{5.55}$$

Moreover:

(i) $G(x,y)\geqslant 0$ *in* $x\in\bar{\Omega}\backslash\{y\}$ *for each* $y\in\Omega$.

(ii) *For any compact set* $K\subset\subset\Omega$ *there exists a constant* C_K *such that*

$$\left|G(x,y)+\frac{a_t(x)}{2\pi}\ln|x-y|\right|\leqslant C(K) \tag{5.56}$$

for all $y\in K$ *and* $x\in\bar{\Omega}$.

The proof is a combination of the analogous results in Refs. 1 and 3, and is omitted.

To construct the upper bound, we adapt a construction from Ref. 16. (See also Refs. 20 and 2.) Choose n_ϵ points $\{p_i\}_{i=1,\ldots,n_\epsilon}$ which are equidistributed on γ. In particular, we have $|p_i-p_j|\geqslant C/n_\epsilon$ for some $C>0$. Define

$$f_\epsilon^i(x)=\frac{2}{\epsilon^2}\chi_{B_\epsilon(p_i)},$$

the characteristic function of the ball $B_\epsilon(p_i)$, normalized to have total integral 2π. Let

$$f_\epsilon(x)=\frac{1}{n_\epsilon}\sum_{i=1}^{n_\epsilon} f_\epsilon^i(x).$$

The f_ϵ converge weak-$*$ in the sense of measures, $f_\epsilon\rightharpoonup\mu_*=[2\pi/\mathrm{per}_\Omega(\gamma)]\delta_\gamma$, the arclength measure on γ normalized to have mass 2π.

We define the trial function via its magnetic field,

$$h_\epsilon(x) = n_\epsilon \int_\Omega G(x,y) f_\epsilon(y) \mathrm{d}y, \quad x \in \Omega.$$

Then h_ϵ solves the boundary-value problem,

$$-\nabla \cdot \left(\frac{1}{a_t} \nabla h_\epsilon \right) + h_\epsilon = n_\epsilon f_\epsilon \quad \text{in } \Omega,$$

$$h|_{\partial \mathcal{D}} = 0,$$

$$h|_{\partial \omega_j} = n_\epsilon \int_\Omega g_j(y) f_\epsilon(y) \mathrm{d}y := H_{\epsilon,j}(\text{constant}),$$

$$\int_{\partial \omega_j} \frac{1}{a_t} \frac{\partial h_\epsilon}{\partial \nu} = H_{\epsilon,j} |\omega_j|, \quad j = 1, \ldots, n.$$

We then extend $h_\epsilon(x)$ to all of $\mathcal{D}$ by defining h_ϵ to be constant $h_\epsilon(x) = H_{\epsilon,j}$ in each ω_j. Finally, we define A_ϵ to be the associated vector potential in the Coulomb gauge, defined as in (2.3).

Next, we define an order parameter V associated to h_ϵ. Since

$$\operatorname{curl}\left(\frac{1}{a_t} \nabla^\perp h_\epsilon - A_\epsilon \right) = \nabla \cdot \left(\frac{1}{a_t} \nabla h_\epsilon \right) - h_\epsilon = n_\epsilon f_\epsilon$$

has support in $\cup B_\epsilon(p_i)$, we may define a phase ϕ locally in $\Omega \setminus \cup_i B_\epsilon(p_i)$ by

$$\nabla \phi(x) = -\frac{1}{a_t} \nabla^\perp h_\epsilon(x) + A_\epsilon(x), \quad x \in \Omega \setminus \cup B_\epsilon(p_i).$$

We now show that ϕ is single-valued modulo 2π. Let σ be any Jordan curve in $\Omega \setminus \cup B_\epsilon(p_i)$ which encloses a region $\Sigma \subset \mathcal{D}$. The region Σ could enclose some collection $\{\omega_j\}_{j \in J}$ of the holes. Then,

$$\begin{aligned}
\int_\sigma \nabla \phi \cdot \tau \, ds &= -\int_\sigma \frac{1}{a_t} \nabla h_\epsilon \cdot \nu \, \mathrm{d}s + \int_\sigma A_\epsilon \cdot \tau \, \mathrm{d}s \\
&= -\int_{\Sigma \setminus \cup_{j \in J} \omega_j} \nabla \cdot \frac{1}{a_t} \nabla h_\epsilon \mathrm{d}x - \sum_{j \in J} \int_{\partial \omega_j} \frac{1}{a_t} \frac{\partial h_\epsilon}{\partial \nu} + \int_\Sigma h_\epsilon \mathrm{d}x \\
&= \int_{\Sigma \setminus \cup_{j \in J} \omega_j} \left(-\nabla \cdot \frac{1}{a_t} \nabla h_\epsilon + h_\epsilon \right) \mathrm{d}x + \sum_{j \in J} \left[-H_{\epsilon,j} |\omega_j| + \int_{\omega_j} h_\epsilon \right] \\
&= \int_{\Sigma \setminus \cup_{j \in J} \omega_j} n_\epsilon f_\epsilon \mathrm{d}x = 2\pi z_\epsilon,
\end{aligned}$$

for some integer $z_\epsilon \in \mathbf{Z}$, by the quantization of f_ϵ. Therefore $\exp(i\phi(x))$ is well-defined in $\Omega \setminus \cup B_\epsilon(p_i)$.

To complete the definition of V for $x \in \Omega$, take a smooth function $\rho_0(x)$ such that $0 \leqslant \rho_0(x) \leqslant 1$, $\rho_0(x) \equiv 1$ in $|x| \geqslant 2$, and $\rho_0(x) \equiv 0$ when $|x| \leqslant 1$. Define

$$\rho(x) = \rho_\epsilon(x) = \begin{cases} \rho_0\left(\dfrac{x - p_i}{\epsilon} \right) & \text{when } x \in B_{2\epsilon}(p_i), \quad i = 1, \ldots, n_\epsilon, \\ 1 & \text{when } x \in \Omega \setminus \cup B_{2\epsilon}(p_i). \end{cases}$$

Then define

$$V(x) := \rho(x)e^{i\phi(x)},$$

where we interpret this to mean that $V(x) \equiv 0$ in $\cup B_\epsilon(p_i)$. Finally, we extend V to the pinning sites ω_j by the same procedure as in Proposition 4.1.

Following the calculations of Refs. 1 and 3, we then expand the energy: after some computation we obtain the upper bound,

$$\mathcal{E}_\epsilon(V,A_\epsilon) \leqslant \frac{1}{2}n_\epsilon^2 A_* - \pi\frac{\mu}{\lambda_*}n_\epsilon \ln|\ln \epsilon| + O(n_\epsilon \ln n_\epsilon),$$

with constant

$$A_* = \int\int_{\Omega\times\Omega} G(x,y)\mathrm{d}\mu_*(x)\mathrm{d}\mu_*(y).$$

We now choose $n_\epsilon = [\ln|\ln \epsilon|]$, and hence

$$\mathcal{E}_\epsilon(V) \leqslant [\bar{A}(\mu) + o(1)](\ln|\ln \epsilon|)^2,$$

with $\bar{A}(\mu) = \frac{1}{2}A_* - \pi\mu/\lambda_*$. Returning to (5.41), and inserting $N_\gamma, N_0, N_- = 0$ (which we know from our previous analysis), we have

$$\inf \mathcal{E}_\epsilon \geqslant N_*(\underline{A}(\mu) - o(1))\ln|\ln \epsilon|,$$

with $\underline{A}(\mu) = \pi C_0 - \pi\mu/\lambda_*$. When ω_1 is large enough both $\underline{A}, \bar{A} < 0$, and so we have

$$(-\underline{A} + o(1))N_* \geqslant (-\bar{A} - o(1))\ln|\ln \epsilon|,$$

and hence we have $N_* \geqslant C \ln|\ln \epsilon|$. Since a is bounded above we obtain the lower bound for Σd_i claimed in (iii) of Theorem 1.3. This completes the proof of Theorem 1.3 □

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Emergence of the triangular lattice near a flat wall

Y. Almog[a)]
Faculty of Mathematics, Technion–Israel Institute of Technology, Haifa 32000, Israel

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The bifurcation of periodic solutions near a flat wall for applied magnetic fields which are slightly weaker than H_{C_2} is considered for a reduced Ginzburg–Landau model obtained in the large κ limit. We formally demonstrate that following the bifurcation of the first mode, when the applied magnetic field is further decreased, there is a second bifurcation, after which the solution develops continuously into the well-known triangular lattice. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Consider a planar superconducting body at a sufficiently low temperature (below the critical one) under the action of an applied magnetic field. Its energy is given by the Ginzburg–Landau energy functional which can be represented in the dimensionless form[1]

$$E=\int_{\Omega}\left(-|\Psi|^2+\frac{|\Psi|^4}{2}+|h-h_{\mathrm{ex}}|^2+\left|\frac{i}{\kappa}\nabla\Psi+A\Psi\right|^2\right)\mathrm{d}x_1\mathrm{d}x_2, \tag{1.1}$$

in which Ψ is the (complex) superconducting order parameter, such that $|\Psi|$ varies from $|\Psi|=0$ (when the material is at a normal state) to $|\Psi|=1$ (for the purely superconducting state). The magnetic vector potential is denoted by A (the magnetic field is thus $h=\nabla\times A$), h_{ex} is the constant applied magnetic field, and κ denotes the Ginzburg–Landau parameter which is a material property. The superconductor lies in Ω, which is a connected domain. Its Gibbs free energy is given by E, which is invariant under the gauge transformation

$$\Psi\to e^{i\kappa\eta}\Psi;\quad A\to A+\nabla\eta. \tag{1.2}$$

wherein η is any smooth function.

For sufficiently large magnetic fields it is well known, from both experimental observations[2] and theoretical predictions,[3] that superconductivity is destroyed and the material must be at the normal state. If the applied magnetic field is then decreased there exists a critical field where the material enters the superconducting phase. This field is called "the onset field" and is denoted by H_{C_3}.

It is well-known that at the bifurcation from the normal state, superconductivity is concentrated near the boundary. Alternatively we can say that Ψ decays exponentially fast away from the boundaries as either κ or the size of Ω tend to infinity, which is why the phenomenon has been termed surface superconductivity. This result has first been established for a half-plane,[4] then for disks,[5] and for general smooth bounded domains in $\mathbb{R}^2$.[6–9] It has later been extended to weakly nonlinear cases in the large κ limit.[10]

In the absence of boundaries the critical field at which superconductivity nucleates is denoted by H_{C_2} and is smaller than H_{C_3} ($H_{C_3}\approx 1.7\kappa$ whereas $H_{C_2}=\kappa$). Further, the bifurcating modes are periodic Abrikosov lattices[11–13] which have been observed experimentally.[14] Rubinstein[15] has

[a)]Present address: Department of Mathematics, Louisiana State University, Baton Rouge, LA 70803, USA

therefore conjectured that superconductivity remains concentrated near the boundary for $H_{C_2}<h_{\mathrm{ex}}<H_{C_3}$; when $h_{\mathrm{ex}}\approx H_{C_2}$ (either for κ large or for large domains) Abrikosov's lattices bifurcate away from the wall.

Recently, it has been proved both in the large κ limit,[16,17] and in the large domain limit[18] that as long as $H_{C_2}<h_{\mathrm{ex}}<H_{C_3}$ superconductivity remains concentrated near the boundaries. Further, Pan[16] proved that when $\kappa\gg 1$, the solution near the boundary is close to the solution of the problem

$$(i\nabla + x_1\hat{i}_2)^2\psi=\lambda\psi(1-|\psi|^2) \quad \text{in } \mathbb{R}^2_+, \tag{1.3a}$$

$$\left.\frac{\partial\psi}{\partial x_1}\right|_{x_1=0}=0, \tag{1.3b}$$

where $\lambda=\kappa/h_{\mathrm{ex}}$. In addition, it is conjectured in Ref. 16, that the unique bounded solution when $\lambda<1$ is essentially one-dimensional, i.e.,

$$\psi=f(x_1,\lambda)e^{i\omega_0 x_2}, \tag{1.4}$$

for some $\omega_0\in\mathbb{R}$ and $f(x_1,\lambda)$ which satisfies

$$-f''+(x-\omega_0)^2 f=\lambda f(1-f^2); \quad f'(0)=0.$$

Nontrivial positive solutions exist for all $\lambda>\beta(\omega_0)$, where

$$\beta(z)=\inf_{\phi\in H^1(z,\infty)}\frac{\displaystyle\int_z^\infty |\phi'|^2+x^2|\phi|^2}{\displaystyle\int_z^\infty |\phi|^2}. \tag{1.5}$$

Further, $f<1$, and[16]

$$f(x)\sim x^{-(1-\lambda)/2}e^{-(1/2)x^2} \quad \text{as } x\to\infty, \tag{1.6}$$

(cf. Ref. 19 for the definition of $\sim$). In a previous contribution,[20] we studied (1.3), after applying the transformation

$$x_1\to x_1-\omega_0,$$

in the space

$$\mathcal{P}_L^{\omega_0}=\{\phi\in H^1_{\mathrm{mag}}([-\omega_0,\infty)\times\mathbb{R})\,|\,\phi(x_1,x_2+L)=\phi(x_1,x_2)\}. \tag{1.7}$$

In this setting the solutions of (1.3a) a may be treated as critical points of the functional

$$\mathcal{E}(\psi)=\int_0^\infty\int_0^{2\pi/\omega}|(i\nabla+x_1\hat{i}_2)\psi|^2+\lambda\left(\frac{1}{2}|\psi|^4-|\psi|^2\right)\mathrm{d}x_2\mathrm{d}x_1. \tag{1.8}$$

We proved in Ref. 20 that (1.4) must undergo a bifurcation for λ slightly greater than unity, i.e., we proved the existence of a sequence of critical values $\{\lambda_n\}_{n=1}^\infty$ such that $\lambda_n\to 1$ as $n\to\infty$ where a bifurcation from (1.4) can take place. Further, we proved that near the bifurcation, the bifurcating branch is given in the form

$$\lambda\cong\lambda_n+\epsilon^2\left(\frac{\omega}{2\pi}\right)^{3/2}+O(\epsilon^3) \tag{1.9a}$$

$$\psi \cong e^{i\omega_0 x_2}\{f(x_1,\lambda) + \epsilon[\phi_n(x_1)e^{in\omega x_2} + \phi_{-n}(x_1)e^{-in\omega x_2}]\} + O(\epsilon^2), \tag{1.9b}$$

where $\epsilon \ll 1$, $\omega = 2\pi/L$, and $\phi_{\pm n}$ satisfy a system of ordinary differential equations which is described in the next section. Finally, we proved that near the bifurcation, the energy of the bifurcating branch is lower than the energy of (1.4). Hence, for $\lambda > 1$ (1.4) must lose its stability.

While the results in Ref. 20 prove the bifurcation of a single Fourier mode, they do not address the behavior of the bifurcating branch with increasing λ. It was expected in Ref. 20 that with growing λ the solution tends to become periodic in the x_1 direction as well. In other words, the solution should approach an Abrikosov lattice.[12,13] The manner by which (1.9) develops into a periodic solution is not clear: it may either result from a sequence of bifurcations, or it may evolve continuously, or else undergo some combination of the above.

The present contribution focuses on the evolution of (1.9) with increasing λ. We assume that the first bifurcation takes place at $\lambda = \lambda_N$, where $N \gg 1$ (we discuss this choice in Sec. V). Then, by using a combination of formal and rigorous arguments, we find

(1) The value of λ at which the next bifurcation (hereafter referred to as the "second" bifurcation) should take place.
(2) The bifurcating mode.
(3) The behavior of the solution with increasing λ following the second bifurcation. We find that if no other bifurcation occurs after the second bifurcation, then, as $N \to \infty$, for $\lambda > \lambda_{N-l}$ where $1 \ll l \ll N$, the solution tends pointwise to the triangular lattice[21] for

$$\left(N - \frac{5}{8}l\right)\omega < x_1 < \left(N - \frac{3}{8}l\right)\omega.$$

We note that there are many indications, both theoretical[12,13,21] and experimental,[14] that the minimizer of (1.1) is indeed the triangular lattice. It is thus plausible that the transition from (1.9) to a periodic solution in the x_1 direction is indeed described by the results in this work, despite a number of gaps that must be addressed in order to prove these results rigorously.

The rest of this contribution is arranged as follows: In the next section we prove the exact asymptotic behavior of λ_n and $\phi_{\pm n}$ as $n \to \infty$ and conjecture that $\lambda_n > 1$ for all n. In Sec. III we make use of the asymptotic formulas and the above-mentioned conjecture to analyze the second bifurcation. In Sec. IV we formally analyze the behaviour of the solution with increasing λ after the second bifurcation. Finally, in Sec. V, we briefly summarize the main results of this work, emphasize some additional key points, and list the gaps that must be bridged in order to rigorously prove the main results.

II. PRELIMINARIES

Consider the problem

$$(i\nabla + x_1\hat{i}_2)^2\psi = \lambda\psi(1 - |\psi|^2) \text{ in } \mathbb{R}^2_+, \tag{2.1a}$$

$$\left.\frac{\partial\psi}{\partial x_1}\right|_{x_1=0} = 0 \quad \psi(x_1, x_2 + L) = e^{i\theta}\psi(x_1, x_2), \tag{2.1b}$$

where θ is constant. Pan[16] conjectured that for $\lambda < 1$ the unique solution of (2.1) is given by (1.4). In Ref. 20 we prove that there exists a sequence of critical values $\{\lambda_n\}_{n=n_0}^{\infty}$ where solutions of (2.1) can bifurcate from (1.4) such that $\lambda_n \downarrow 1$. Further, near the bifurcation,

$$\psi \approx f(x_1)e^{i\omega_0 x_2} + C(\lambda)[\phi_n(x_1)e^{in\omega x_2} + \phi_{-n}(x_1)e^{-in\omega x_2}],$$

where upon applying the transformation $x \to x - \omega_0$, ϕ_n, ϕ_{-n} satisfy

$$-\phi_n'' + [(x_1 - n\omega)^2 - \lambda]\phi_n + \lambda f^2(2\phi_n + \overline{\phi_{-n}}) = 0 \quad x_1 > -\omega_0, \tag{2.2a}$$

$$-\phi''_{-n}+[(x_1+n\omega)^2-\lambda]\phi_{-n}+\lambda f^2(2\phi_{-n}+\overline{\phi_n})=0 \quad x_1>-\omega_0, \tag{2.2b}$$

$$\phi'_n(-\omega_0)=\phi'_{-n}(-\omega_0)=0, \tag{2.2c}$$

and $C(\lambda)\sim O(|\lambda-\lambda_n|^{1/2})$. The asymptotic behavior of λ_n has been studied as well. In particular, it is proved in Ref. 20, that

$$1+C_1e^{-(1/2)(n\omega+\omega_0)^2}<\lambda_n<1+C_2e^{-(1/2)(n\omega+\omega_0)^2}. \tag{2.3}$$

We now prove the exact asymptotic behavior of λ_n.

Lemma 2.1: Let λ_n be the lowest critical value of (2.2). *Then*

$$\lambda_n\sim 1+2a^2e^{-(n\omega+\omega_0)^2/2}+O(e^{-2(n\omega+\omega_0)^2/3}) \quad \text{as } n\to\infty, \tag{2.4a}$$

where

$$a=\lim_{x\to\infty}e^{x^2/2}f(x,1). \tag{2.4b}$$

Further, let ϕ_n,ϕ_{-n} be the corresponding eigenmodes. Then, for sufficiently large n we have

$$\|\phi_n-e^{-(x-n\omega)^2/2}\|_2^2+\|\phi_{-n}\|_2^2\leqslant e^{-2(n\omega+\omega_0)^2/3}, \tag{2.5}$$

where $\|\cdot\|_2$ denotes the L^2 norm on $(-\omega_0,\infty)$.

Proof: Let

$$\mathcal{H}=\{\phi\in H^2(-\omega_0,\infty)|x\phi\in L^2(-\omega_0,\infty);\phi'(-\omega_0)=0\},$$

and $\mathcal{P}_n:\mathcal{H}\times\mathcal{H}\to L^2\times L^2$ denote the operator

$$\mathcal{P}_n=\begin{bmatrix}-\dfrac{d^2}{dx_1^2}+(x_1-n\omega)^2 & 0\\ 0 & -\dfrac{d^2}{dx_1^2}+(x_1+n\omega)^2\end{bmatrix}+\lambda_n f^2(x_1,\lambda_n)\begin{bmatrix}2&1\\1&2\end{bmatrix}.$$

Clearly,

$$(\mathcal{P}_n-\lambda_n)\begin{bmatrix}\phi_n\\ \bar{\phi}_{-n}\end{bmatrix}=0.$$

We now choose the quasimode

$$v_n=C_n\begin{bmatrix}\chi(x+\omega_0)e^{(-x-n\omega)^2/2}\\ 0\end{bmatrix},$$

where C_n is chosen such that $||v_n||^2=1$ and χ is a smooth cutoff function satisfying

$$\chi(x)=\begin{cases}0 & x\leqslant\dfrac{1}{2},\\ 1 & x\geqslant 1.\end{cases}$$

Let

$$\alpha_n=1+2\lambda_n\int f^2(x,\lambda_n)|v_n|^2.$$

Then

$$|\langle v_n,(\mathcal{P}_n-\alpha_n)v_n\rangle| \leqslant \int |-\chi''+2(x-n\omega)\chi'|e^{-(x-n\omega)^2} \leqslant Ce^{-(n\omega+\omega_0)^2}. \tag{2.6}$$

We now represent the quasimode v_n as

$$v_n = a_n\Phi_n + \tilde{v}_n,$$

where

$$\Phi_n = \begin{bmatrix} \phi_n \\ \phi_{-n} \end{bmatrix},$$

and

$$a_n = \langle v_n, \Phi_n\rangle.$$

From (2.6) we have

$$a_n^2|\lambda_n-\alpha_n| \leqslant |\langle v_n,(\mathcal{P}_n-\alpha_n)v_n\rangle| + |\langle \tilde{v}_n,(\mathcal{P}_n-\alpha_n)\tilde{v}_n\rangle| \leqslant \|\tilde{v}_n\|_2\|(\mathcal{P}_n-\alpha_n)v_n\|_2 + Ce^{-(n\omega+\omega_0)^2}. \tag{2.7}$$

Let

$$\mu_n = \inf_{\substack{u\in\tilde{\mathcal{H}}_n \\ \|u\|_2=1}} \langle \mathcal{P}_n u,u\rangle,$$

where $\tilde{\mathcal{H}}_n$ is the orthogonal complement of span $\{\Phi_n\}$ in $\mathcal{H}\times\mathcal{H}$.

Then,

$$\|\tilde{v}_n\|_2^2 \leqslant \frac{\|(\mathcal{P}_n-\alpha_n)\tilde{v}_n\|_2^2}{|\mu_n-\alpha_n|^2} \leqslant \frac{\|(\mathcal{P}_n-\alpha_n)v_n\|_2^2}{|\mu_n-\alpha_n|^2}. \tag{2.8}$$

We claim that

$$\liminf_{n\to\infty} \mu_n-\alpha_n = 2. \tag{2.9}$$

To prove (2.9) we define the operator

$$Q_n = \begin{bmatrix} -\dfrac{\mathrm{d}^2}{\mathrm{d}x_1^2}+(x_1-n\omega)^2 & 0 \\ 0 & -\dfrac{\mathrm{d}^2}{\mathrm{d}x_1^2}+(x_1+n\omega)^2 \end{bmatrix}. \tag{2.10}$$

Clearly,

$$\nu_n = \inf_{\substack{u\in\tilde{\mathcal{H}}_n \\ \|u\|_2=1}} \langle \mathcal{Q}_n u,u\rangle \leqslant \mu_n. \tag{2.11}$$

We now prove that

$$\liminf_{n\to\infty} \nu_n \geqslant 3. \tag{2.12}$$

Denote by U_n the minimizer of $\langle Q_n u,u\rangle$ in $\mathcal{H}\times\mathcal{H}$. For sufficiently large n we have

$$U_n = \begin{bmatrix} u_n \\ 0 \end{bmatrix},$$

where u_n satisfies

$$-u_n'' + (x - n\omega)^2 u_n = \beta_n u_n, \quad u_n'(-\omega_0) = 0,$$

in which $\beta_n = \beta(-n\omega - \omega_0)$ is given by (1.5) and $\|u_n\|_2 = 1$. Let w denote a unit vector in $\widetilde{\mathcal{H}}_n$. Then,

$$\langle w, U_n \rangle = \langle w, -\Phi_n + \langle \Phi_n, U_n \rangle U_n \rangle + (1 - \langle \Phi_n, U_n \rangle)\langle w, U_n \rangle.$$

We seek to estimate the norm of $\Phi_n - \langle \Phi_n, U_n \rangle U_n$. To this end we apply to it first $Q_n - \beta_n$ and then estimate the norm of the outcome. We have

$$\int |(\mathcal{Q}_n - \beta_n)(\Phi_n - \langle \Phi_n, U_n \rangle U_n)|^2 \leqslant (\lambda_n - \beta_n)^2 + 4\lambda_n^2 \int f^2(|\phi_n|^2 + |\phi_{-n}|^2).$$

To estimate the second term on the right-hand-side, we recall from[20] that

$$\lambda_n \int f^2(|\phi_n|^2 + |\phi_{-n}|^2 + |\phi_n + \overline{\phi}_{-n}|^2) = -\int [|\phi_n'|^2 + |\phi_{-n}'|^2 + (x - n\omega)^2|\phi_n|^2 + (x + n\omega)^2|\phi_{-n}|^2] + \lambda_n$$
$$\leqslant (\lambda_n - \beta_n).$$

From Refs. 7 and 22 we know that

$$\beta_n \sim 1 - O(e^{-(n\omega + \omega_0)^2}).$$

Hence, in view of (2.3) we obtain

$$\int |(\mathcal{Q}_n - \beta_n)(\Phi_n - \langle \Phi_n, U_n \rangle U_n)|^2 \leqslant Ce^{-(n\omega + \omega_0)^2/2}. \tag{2.13}$$

Since $\Phi_n - \langle \Phi_n, U_n \rangle U_n$ is orthogonal to U_n we have

$$\int |(\mathcal{Q}_n - \beta_n)(\Phi_n - \langle \Phi_n, U_n \rangle U_n)|^2 \geqslant (\sigma_n - \beta_n)^2 \|\Phi_n - \langle \Phi_n, U_n \rangle U_n\|_2^2,$$

where

$$\sigma_n = \inf_{\substack{u \in span\{U_n\}^\perp \\ \|u\|_2 = 1}} \langle \mathcal{Q}_n u, u \rangle.$$

Semi-classical analysis[22,23] shows that

$$\sigma_n \xrightarrow[n \to \infty]{} 3. \tag{2.14}$$

Combining the above with (2.13) yields

$$\|\Phi_n - \langle \Phi_n, U_n \rangle U_n\|_2^2 \leqslant Ce^{-(n\omega + \omega_0)^2/2},$$

and consequently

$$|\langle w, U_n \rangle| \leqslant Ce^{-(n\omega + \omega_0)^2/4}, \tag{2.15}$$

where C is independent of w and n.

We now present w in the form

$$w = \langle w, U_n\rangle U_n + w_n.$$

Clearly, $w_n \perp U_n$, and hence

$$\langle \mathcal{Q}_n w, w\rangle = \beta_n \langle w, U_n\rangle^2 + \langle \mathcal{Q}_n w_n, w_n\rangle \geqslant \sigma_n \|w_n\|_2^2 \geqslant \sigma_n (1 - e^{-(n\omega + \omega_0)^2/2}),$$

which proves (2.12). In view of (2.11), we have proved (2.9) too.

We now substitute (2.9) into (2.8) and then into (2.7) to obtain

$$a_n^2 |\lambda_n - \alpha_n| \leqslant \|(\mathcal{P}_n - \alpha_n) v_n\|_2^2 + C e^{-(n\omega + \omega_0)^2},$$

or, equivalently

$$a_n^2 |\lambda_n - \alpha_n| \leqslant 2(\alpha_n - 1)^2 + 5 \int f^4 |v_n|^2 + C e^{-(n\omega + \omega_0)^2} \leqslant C e^{-2(n\omega + \omega_0)^2/3}.$$

Further,

$$a_n^2 = 1 - \|v_n\|_2^2 \geqslant 1 - \|(\mathcal{P}_n - \alpha_n) v_n\|_2^2 \geqslant 1 - C e^{-2(n\omega + \omega_0)^2/3}.$$

Hence,

$$\lambda_n \sim 1 + 2\lambda_n \int f^2(x, \lambda_n) |v_n|^2 + O(e^{-2(n\omega + \omega_0)^2/3}) \quad \text{as } n \to \infty. \tag{2.16}$$

In Ref. 20 we proved that $|\partial f / \partial \lambda| \leqslant C$ for all x in some neighborhood of $\lambda = 1$. Utilizing this result together with (2.3) we obtain

$$\lambda_n \sim 1 + 2 \int f^2(x, 1) e^{-(x - n\omega)^2} + O(e^{-2(n\omega + \omega_0)^2/3}) \quad \text{as } n \to \infty,$$

from which (2.4) readily follows. Similarly, from (2.8) we obtain (2.5). □

We conclude this section by stating the following conjecture, and by making a simple observation.

Conjecture 1: Let

$$\gamma_n(\lambda) = \inf_{\substack{(\chi_n, \chi_{-n}) \in \mathcal{H} \times \mathcal{H} \\ \|\chi_n\|_2^2 + \|\chi_{-n}\|_2^2 = 1}} \mathcal{J}_n(\chi_n, \chi_{-n}), \tag{2.17a}$$

where

$$\begin{aligned} \mathcal{J}_n(\chi_n, \chi_{-n}) := \int_{-\omega_0}^{\infty} & |\chi_n'|^2 + (x - n\omega)^2 |\chi_n|^2 + |\chi_{-n}'|^2 + (x + n\omega)^2 |\chi_{-n}|^2 \\ & - \lambda [|\chi_n|^2 + |\chi_{-n}|^2 - f^2(|\chi_n|^2 + |\chi_n + \bar{\chi}_{-n}|^2 + |\chi_{-n}|^2)]. \end{aligned} \tag{2.17b}$$

Then,

$$\forall n \in \mathbb{N}, \exists\, \delta_n > 0 \colon \lambda < 1 + \delta_n \Rightarrow \gamma_n(\lambda) > 0. \tag{2.18}$$

Note that by (2.4) the above-mentioned conjecture is correct for sufficiently large n, since $\gamma_n(\lambda) > 0$ for all $\lambda < \lambda_n$. For n which is not necessarily large, it is still expected that (2.18) remains valid since otherwise the surface superconductivity solution (1.4) would lose its stability for $\lambda \leqslant 1$ for some $n \in \mathbb{N}$. This would contradict the physical intuition suggesting that (1.4) must be stable for $\lambda \leqslant 1$.

Finally, we prove the leading asymptotic behavior for $\gamma_n(\lambda)$ as $n \to \infty$.

Lemma 2.2: Let $\lambda < 2$. *Then*,

$$\gamma_n(\lambda) \sim (\lambda_n - \lambda)(1 + Ce^{-(1/3)(n\omega + \omega_0)^2}). \tag{2.19}$$

Proof: It is easy to show that

$$-\phi_n'' + [(x_1 - n\omega)^2 - \lambda - \gamma_n]\phi_n + \lambda f^2(2\phi_n + \overline{\phi_{-n}}) = 0, \quad x_1 > -\omega_0$$

$$-\phi_{-n}'' + [(x_1 + n\omega)^2 - \lambda - \gamma_n]\phi_{-n} + \lambda f^2(2\phi_{-n} + \overline{\phi_n}) = 0, \quad x_1 > -\omega_0$$

$$\phi_n'(-\omega_0) = \phi_{-n}'(-\omega_0) = 0.$$

Consequently, in the same manner used to derive (2.16) we can obtain that

$$\gamma_n(\lambda) \sim 1 + 2\lambda \int f^2(x,\lambda)|v_n|^2 + O(e^{-2(n\omega + \omega_0)^2/3}) - \lambda \quad \text{as } n \to \infty.$$

Utilizing (2.16) we have

$$\gamma_n(\lambda) \sim (\lambda_n - \lambda)\left(1 + 2\int f^2(x,\lambda_n)|v_n|^2\right) + 2\lambda \int [f^2(x,\lambda) - f^2(x,\lambda_n)]|v_n|^2$$

and since $|\partial f/\partial\lambda| \leqslant C$ (cf. Ref. 20) we readily obtain (2.19).

III. THE SECOND BIFURCATION

In the preceding section we have considered the bifurcation from the one-dimensional solution (1.4). In this section we study the linear bifurcation from the bifurcating branch, i.e., the second bifurcation. Let then

$$\psi = \psi_0 + u \tag{3.1}$$

where $\psi_0(\lambda)$ denotes the solution which bifurcates from (1.4) at $\lambda = \lambda_N$ for $N \gg 1$. It is convenient to present ψ_0 using the parametric form

$$\psi_0 \cong f_0 + \epsilon V_0 + O(\epsilon^2, e^{-(N\omega + \omega_0)^2/2}), \tag{3.2a}$$

$$\lambda \cong \lambda_N + \epsilon^2\lambda_N^{(2)} + O(\epsilon^2), \tag{3.2b}$$

in which

$$V_n = \phi_{n+N}(x_1)e^{i(n+N)\omega x_2} + \phi_{-n-N}(x_1)e^{-i(n+N)\omega x_2}, \tag{3.2c}$$

$$f_0(x_1) = f(x_1, 1), \tag{3.2d}$$

$$\lambda_N^{(2)} \cong \left(\frac{\omega}{2\pi}\right)^{3/2} + O(e^{-(\omega N + \omega_0)^2/2}). \tag{3.2e}$$

We shall consider in the sequel positive ϵ values which are of $O(e^{-[(N-N_0)\omega + \omega_0]^2/4})$ for $N_0 \ll N$. In view of (3.2c) we have

$$(i\nabla + x_1\hat{i}_2)^2 v_n - \lambda_{N+n}[v_n - f^2|_{\lambda=\lambda_{N+n}}(2v_n + \bar{v}_n)] = 0. \tag{3.3}$$

Consider now the bifurcation from the branch which bifurcated at $\lambda=\lambda_{\tilde{N}}$ from the surface superconductivity solution (1.4) for $\tilde{N}\neq N$ which is still much greater than 1. In this case we obtain from (2.5) that apart from an exponentially small error

$$\tilde{\psi}_0 - f_0|_{(x_1,x_2)} \cong \tilde{\psi}_0 - f_0|_{(x_1+\omega(\tilde{N}-N),x_2}\,,$$

where $\tilde{\psi}_0$ is the mode bifurcating from f at $\lambda=\lambda_{\tilde{N}}$. Thus, the choice of N has little impact on the results obtained in this section. We shall return to this problem in the last section.

Substituting (3.1) into (2.1) while keeping in mind that ψ_0 is a solution of (2.1), we obtain

$$(i\nabla + x_1\hat{i}_2)^2 u - \lambda[u - (2|\psi_0|^2 u + \psi_0^2\bar{u} + 2|u|^2\psi_0 + u^2\bar{\psi}_0 + |u|^2 u)] = 0 \quad x \in \mathbb{R}^2_{\omega_0}, \tag{3.4a}$$

$$u_{x_1}(-\omega_0, x_2) = 0; \tag{3.4b}$$

$$u(x_1, x_2 + L) = u(x_1, x_2), \tag{3.4c}$$

where $L=2\pi/\omega$, and $\mathbb{R}^2_{\omega_0}=\{(x_1,x_2)\,|-\omega_0<x_1,x_2\in\mathbb{R}\}$. We look for solutions in $\mathcal{P}^{\omega_0}_L$ which bifurcate from $u\equiv 0$. We thus assume that such a bifurcation takes place at $\lambda=\mu$ and linearize (3.4) by introducing the expansion

$$\lambda \cong \mu + \delta\mu^{(1)} + \delta^2\mu^{(2)} + O(\delta^3), \tag{3.5a}$$

$$u \cong \delta u^{(0)} + \delta^2 u^{(1)} + \delta^3 u^{(2)} + O(\delta^4), \tag{3.5b}$$

to obtain

$$(i\nabla + x_1\hat{i}_2)^2 u^{(0)} - \mu[u^{(0)} - (2|\psi_0|^2 u^{(0)} + \psi_0^2\bar{u}^{(0)})] = 0, \tag{3.6}$$

together with (3.4b) and (3.4c).

We shall now obtain a necessary condition for the existence of nontrivial solutions of (3.6) involving V_n with $N+n\gg 1$.

Lemma 3.1: Let

$$\mu = \lambda_N + \epsilon^2\lambda_N^{(2)},$$

where $\lambda_N^{(2)}$ *is given by (3.2e). Let further* ψ_0 *be given by (3.2) and* $u^{(0)}$ *satisfy (3.6). Denote by* $\hat{u}_n$ *the Fourier coefficient*

$$\hat{u}_n = \int_0^{2\pi/\omega} e^{-i\omega n x_2}\mathrm{d}x_2.$$

Then, if there exist $\epsilon\leqslant\exp\{-\frac{1}{4}[(N-l)\omega+\omega_0]^2\}$ *(where* $l\ll N$*) such that a nontrivial* $u^{(0)}$ *satisfying*

$$\int_{-\omega_0}^{\infty} |\hat{u}_{N+n}|^2 + |\hat{u}_{N-n}|^2 dx_1 \geqslant \frac{1}{2} \tag{3.7}$$

exists for some $0\leqslant n\leqslant l$*, we must have*

$$\epsilon^2 \cong \eta_{-n}^2 \frac{1-2q^{n^2}}{(1-2q^{n^2})^2 - q^{4n^2}} \tag{3.8a}$$

and

$$\frac{2}{\omega}\pi^{3/2}u^{(0)} \cong \frac{1-2q^{n^2}}{\sqrt{(1-2q^{n^2})^2+q^{4n^2}}}\exp\left\{-\frac{1}{2}[x_1-(N-n)\omega]^2+i\omega(N-n)x_2\right\}$$
$$+\frac{q^{2n^2}}{\sqrt{(1-2q^{n^2})^2+q^{4n^2}}}\exp\left\{-\frac{1}{2}[x_1-(N+n)\omega]^2+i\omega(N+n)x_2\right\}, \tag{3.8b}$$

where

$$\eta_n^2=\left(\frac{2\pi}{\omega}\right)^{3/2}(\lambda_N-\lambda_{N+n}); \quad \eta_{-n}^2=\left(\frac{2\pi}{\omega}\right)^{3/2}(\lambda_N-\lambda_{N+n}), \tag{3.8c}$$

and

$$q=e^{-w^2/2}. \tag{3.8d}$$

Proof: Multiplying (3.6) by $\bar{V}_n$ and integrating by parts over $D=(-\omega_0,\infty)\times(0,L)$ we obtain

$$(\mu-\lambda_{N+n})\int u^{(0)}\bar{V}_n=(\mu-\lambda_{N+n})\int \bar{V}_n[2|\psi_0|^2u^{(0)}+\psi_0^2\bar{u}^{(0)}]+\lambda_{N+n}\int f^2(u^{(0)}\bar{V}_n-\bar{u}^{(0)}V_n)$$
$$+\lambda_{N+n}\int \bar{V}_n[2(|\psi_0|^2-f^2)u^{(0)}+(\psi_0^2-f^2)\bar{u}^{(0)}]. \tag{3.9}$$

We need first an estimate for the first two integrals on the right-hand side of (3.9). Without loss of generality we assume that $\|u^{(0)}\|_{L^2(D)}=1$ (which may always be achieved through appropriately adjusting δ). By (3.6) we also have

$$\int |(i\nabla+x_1\hat{i}_2)u^{(0)}|^2 \leqslant C\int |u^{(0)}|^2 \leqslant C. \tag{3.10}$$

For the first integral on the right-hand side of (3.9) we obtain by using (3.2)

$$\int \bar{V}_n|\psi_0|^2u^{(0)} \cong \int \bar{V}_nf_0^2u^{(0)}+2\epsilon\int \bar{V}_nf_0\Re(V_0)u^{(0)}+O(\epsilon^2).$$

Then, utilizing (2.5) we have

$$\left|\int \bar{V}_nf_0^2u^{(0)}\right|^2 \leqslant \int f_0^4|V_n|^2 \leqslant Ce^{-2[(N+n)\omega+\omega_0]^2/3},$$

$$\left|\int \bar{V}_nf_0V_0u^{(0)}\right|^2 \leqslant \int f_0^2|V_n|^2|V_0|^2 \leqslant Ce^{-2[(N+n/2)\omega+\omega_0]^2/3}.$$

To estimate the second integral on the right-hand side of (3.9) we multiply (3.6) once by $e^{-i(N+n)x_2}$ and once by $e^{i(N+n)x_2}$ and integrate by parts to obtain the system

$$-\hat{u}''_{N+n}+[(x-n\omega)^2-\mu]\hat{u}_{N+n}+\mu f^2(2\hat{u}_{N+n}+\overline{\hat{u}_{-N-n}})$$
$$=-\int_0^{2\pi/\omega}[(|\psi_0|^2-f^2)2u^{(0)}+(\psi_0^2-f^2)\bar{u}^{(0)}]e^{-i\omega(N+n)x_2}\mathrm{d}x_2 \tag{3.11a}$$

$$-\hat{u}''_{-N-n}+[(x+n\omega)^2-\mu]\hat{u}_{-N-n}+\mu f^2(2\hat{u}_{-N-n}+\overline{\hat{u}_{N+n}})$$
$$=-\int_0^{2\pi/\omega}[(|\psi_0|^2-f^2)2u^{(0)}+(\psi_0^2-f^2)\bar{u}^{(0)}]e^{i\omega(N+n)x_2}\mathrm{d}x_2 \tag{3.11b}$$

$$\hat{u}'_{N+n}(-\omega_0) = \hat{u}'_{-N-n}(-\omega_0) = 0. \tag{3.11c}$$

Multiplying (3.11a) by $\bar{\hat{u}}_{N+n}$ and (3.11b) by $\bar{\hat{u}}_{-N-n}$, summing the resulting equations, and integrating with respect to x_1 we obtain

$$\mathcal{J}_{N+n}(\hat{u}_{N+n}, \hat{u}_{-N-n}, \mu) = \int [\overline{e^{-i\omega(N+n)x_2}\hat{u}_{N+n} + e^{i\omega(N+n)x_2}\hat{u}_{-N-n}}] \cdot [(|\psi_0|^2 - f^2)2u^{(0)} + (\psi_0^2 - f^2)\bar{u}^{(0)}],$$

where $\mathcal{J}$ is defined in (2.17). Since $\hat{u}_n e^{i\omega n x_2}$ is the projection of $u^{(0)}$ on the subspace of the n'th Fourier harmonic, it is easy to show that its H^1_{mag} norm is uniformly bounded for all N and n. Consequently,

$$\|u^{(0)}\|_{L^4} \leqslant C; \quad \|\hat{u}_n e^{i\omega n x_2}\|_{L^4} \leqslant C.$$

Therefore, it is not difficult to show that for sufficiently large $N+n$

$$\int |\hat{u}_{-N-n}|^2 + f^2|\hat{u}_{N+n}|^2 - (\mu - \beta|_{z=\omega(N+n)+\omega_0}) \leqslant \mathcal{J}_{N+n}(\hat{u}_{N+n}, \hat{u}_{-N-n}, \mu) \leqslant C(\epsilon + e^{-(N\omega+\omega_0)^2/4})^2. \tag{3.12}$$

where $\beta(z)$ is defined in (1.5). It is thus easy to show from (3.12) that

$$\int |\hat{u}_{-N-n}|^2 + f^2|\hat{u}_{N+n}|^2 \leqslant C(\epsilon + e^{-(N\omega+\omega_0)^2/4})^2.$$

Let U_n be the minimizer of $\langle \mathcal{Q}_n u, u\rangle$ in $\mathcal{H}\times\mathcal{H}$ where $\mathcal{Q}_n$ is defined in (2.10). Let further

$$\hat{u}_{N+n} = \langle \hat{u}_{N+n}, U_{N+n}\rangle U_{N+n} + \tilde{u}_{N+n}. \tag{3.13}$$

Then, by (3.12) and (2.14) we also have

$$\int |\tilde{u}_{N+n}|^2 \leqslant C(\epsilon + e^{-(N\omega+\omega_0)^2/4})^2. \tag{3.14}$$

We now return to the second integral on the right-hand side of (3.9). Obviously,

$$\int f^2 \bar{u}^{(0)} \bar{V}_n = \int_{-\omega_0}^{\infty} f^2[\bar{\phi}_{N+n}\bar{\hat{u}}_{-N-n} + \bar{\phi}_{-N-n}\bar{\hat{u}}_{N+n}]\mathrm{d}x_1. \tag{3.15}$$

From (3.12) and (2.5) and (2.4a) and (2.4b) we obtain

$$\left|\int_{-\omega_0}^{\infty} f^2\bar{\phi}_{N+n}\bar{\hat{u}}_{-N-n}\right|^2 \leqslant \int_{-\omega_0}^{\infty} f^4|\phi_{N+n}|^2 \int_{-\omega_0}^{\infty} |\hat{u}_{-N-n}|^2 \leqslant C(\epsilon + e^{-[\omega(N+n)+\omega_0]^2/4})^2 e^{-2[\omega(N+n)+\omega_0]^2/3}, \tag{3.16}$$

and

$$\left|\int_{-\omega_0}^{\infty} f^2\bar{\phi}_{-N-n}\bar{\hat{u}}_{N+n}\right|^2 \leqslant \int_{-\omega_0}^{\infty} f^4|\hat{u}_{N+n}|^2 \int_{-\omega_0}^{\infty} |\phi_{-N-n}|^2 \leqslant C(\epsilon + e^{-[\omega(N+n)+\omega_0]^2/4})^2 e^{-2[\omega(N+n)+\omega_0]^2/3}. \tag{3.17}$$

Consequently,

$$(\mu-\lambda_{N+n})\int u^{(0)}\bar{V}_n=\lambda_{N+n}\int \bar{V}_n[2(|\psi_0|^2-f^2)u^{(0)}+(\psi_0^2-f^2)\bar{u}^{(0)}]+\tilde{\epsilon}, \tag{3.18a}$$

where

$$|\tilde{\epsilon}|\leqslant C\{\epsilon^2(\epsilon+e^{-[\omega(N+n)+\omega_0]^2/3})^2+(\epsilon+e^{-[\omega(N+n)+\omega_0]^2/4})^2e^{-[\omega(N+n)+\omega_0]^2/3}\}. \tag{3.18b}$$

We now estimate the remaining terms on the right-hand side of (3.9). Evidently,

$$\int \bar{V}_n(|\psi_0|^2-f^2)u^{(0)}\cong\int \bar{V}_n(f_0^2-f^2)u^{(0)}+2\epsilon\int f_0\Re\{V_0u^{(0)}\bar{V}_n\}+\epsilon^2\int |V_0|^2u^{(0)}\bar{V}_n+O(\epsilon^3). \tag{3.19}$$

For the first term on the right-hand side we have

$$\left|\int \bar{V}_n(f_0^2-f^2)u^{(0)}\right|^2\leqslant\left\|\frac{\partial f}{\partial\lambda}\right\|^2_{L^\infty(-\omega_0,\infty)}|\lambda_n-1|^2\int (f_0+f)^2|V_n|^2.$$

In view of (2.4) and since $\partial f/\partial\lambda$ is uniformly bounded,[20] we have

$$\left|\int \bar{V}_n(f_0^2-f^2)u^{(0)}\right|^2\leqslant Ce^{-3[\omega(N+n)+\omega_0]^2/2}. \tag{3.20}$$

For the second term on the right-hand side of (3.19) we have

$$\left|\int f_0\Re\{V_0u^{(0)}\bar{V}_n\}\right|^2\leqslant\int f_0^2|V_0V_n|^2\leqslant Ce^{-2[\omega(N+n)+\omega_0]^2/3}. \tag{3.21}$$

Combining (3.19)–(3.21) we obtain

$$\int \bar{V}_n(|\psi_0|^2-f^2)u^{(0)}\cong\epsilon^2\int |V_0|^2u^{(0)}\bar{V}_n+O(\epsilon^2e^{-[\omega(N+n)+\omega_0]^2/12}).$$

In a similar manner we can obtain a similar estimate for the second term on the right-hand side of (3.18a). Thus,

$$(\mu-\lambda_{N+n})\int u^{(0)}\bar{V}_n=\epsilon^2\int \bar{V}_n[2|V_0|^2u^{(0)}+V_0^2\bar{u}^{(0)}]+\epsilon^2\tilde{\epsilon}_n, \tag{3.22a}$$

where

$$|\tilde{\epsilon}_n|\leqslant e^{-[\omega(N+n)+\omega_0]^2/12}. \tag{3.22b}$$

Let

$$\tilde{d}_n=\int u^{(0)}\bar{V}_n.$$

Then, we can write (3.22) in the form

$$(\epsilon^2+\eta_n^2)\tilde{d}_n=\epsilon^2q^{n^2}[2\tilde{d}_n+\bar{\tilde{d}}_{-n}q^{n^2}]+C\epsilon^2\tilde{\epsilon}_n, \tag{3.23a}$$

$$(\epsilon^2-\eta_{-n}^2)\tilde{d}_{-n}=\epsilon^2q^{n^2}[2\tilde{d}_{-n}+\bar{\tilde{d}}_nq^{n^2}]+C\epsilon^2\tilde{\epsilon}_{-n}. \tag{3.23b}$$

Let $[d_n,d_{-n}]^T$ denote a nontrivial solution and $\epsilon_n^{(0)}$ be a critical value of

$$(\epsilon^2 - \eta_{-n}^2)d_{-n} = \epsilon^2 q^{n^2}[2d_{-n} + \bar{d}_n q^{n^2}] \tag{3.24a}$$

$$(\epsilon^2 - \eta_{-n}^2)d_{-n} = \epsilon^2 q^{n^2}[2d_{-n} + \bar{d}_n q^{n^2}]. \tag{3.24b}$$

Let further μ_{N-n} denote a critical value of μ for which a nontrivial solution of (3.6) satisfying (3.7) exists. Let ϵ_n be given by

$$\epsilon_n^2 = \frac{\mu_{N-n} - \lambda_N}{\lambda_N^{(2)}}.$$

By (3.7) we have to look for a solution of (3.23) which satisfies

$$|\tilde{d}_n|^2 + |\tilde{d}_{-n}|^2 \geqslant \frac{1}{2}.$$

It is not difficult to show that

$$|\epsilon_n - \epsilon_n^{(0)}| + |\tilde{d}_n - d_n| + |\tilde{d}_{-n} - d_{-n}| \leqslant C\tilde{\epsilon}_n, \tag{3.25}$$

where C is independent of n and N. Further, one can easily show that whenever $1 \leqslant k \leqslant 2l$ and $k \neq n$, the solutions of (3.23) with $\epsilon = \epsilon_k$ must satisfy

$$|\tilde{d}_n| + |\tilde{d}_{-n}| \leqslant C\tilde{\epsilon}_n. \tag{3.26}$$

To solve (3.24) we multiply (3.24a) by $\bar{d}_{-n}$ and (3.24b) by $\bar{d}_n$ to obtain

$$[\epsilon^2(1 - 2q^{n^2}) - \eta_{-n}^2]|d_{-n}|^2 = \epsilon^2 q^{2n^2}\bar{d}_n\bar{d}_{-n}, \tag{3.27a}$$

$$[\epsilon^2(1 - 2q^{n^2}) + \eta_n^2]|d_n|^2 = \epsilon^2 q^{2n^2}\bar{d}_n\bar{d}_{-n}. \tag{3.27b}$$

We confine the subsequent discussion to the case $q < 1/2$, (and later also to $q < \sqrt{2} - 1$). This is done because most of the analysis in the next section will be devoted to the limit $q \to 0$. Further, the periodic solution with the minimal energy in $\mathbb{R}^2$ is the triangular lattice[11–13] for which q is either $e^{-\pi\sqrt{3}}$ or $e^{-\pi/\sqrt{3}}$ which are both smaller than $1/2$.

For $q < 1/2$ we must have by (3.27b)

$$\bar{d}_n\bar{d}_{-n} = |d_n||d_{-n}|.$$

Hence,

$$\det\begin{bmatrix} (\epsilon_n^{(0)})^2(1 - 2q^{n^2}) - \eta_{-n}^2 & -(\epsilon_n^{(0)})^2 q^{2n^2} \\ -(\epsilon_n^{(0)})^2 q^{2n^2} & (\epsilon_n^{(0)})^2(1 - 2q^{n^2}) + \eta_n^2 \end{bmatrix} = 0.$$

We now observe that by (2.4)

$$\frac{\eta_n^2}{\eta_{-n}^2} \leqslant Ce^{-\omega nN}.$$

Hence, we can approximate $\epsilon_n^{(0)}$ by

$$(\epsilon_n^{(0)})^2 \cong \eta_{-n}^2 \frac{1 - 2q^{n^2}}{(1 - 2q^{n^2})^2 - q^{4n^2}}.$$

Using (3.2b) the critical values of λ are accordingly

$$\mu_{N-n} = \lambda_N + \frac{1-2q^{n^2}}{(1-2q^{n^2})^2 - q^{4n^2}}(\lambda_{N-n} - \lambda_N).$$

As long as $q < \sqrt{2}-1$ we have

$$\lambda_{N-n} < \mu_{N-n} < \lambda_{N-n-1},$$

and

$$\frac{\mu_{N-n} - \lambda_{N-n}}{\lambda_{N-n-1} - \lambda_{N-n}} \leqslant Ce^{-\omega N}.$$

Consequently, we can assert that the next bifurcation takes place at $\lambda = \mu_{N-1}$ where

$$\mu_{N-1} \cong \lambda_N + \frac{1-2q}{(1-2q)^2 - q^4}(\lambda_{N-1} - \lambda_N). \tag{3.28}$$

The corresponding eigenmode is

$$\frac{2}{\omega}\pi^{3/2}\begin{bmatrix} d_{-1} \\ d_1 \end{bmatrix} = \frac{1}{\sqrt{(1-2q)^2 + q^4}}\begin{bmatrix} 1-2q \\ q^2 \end{bmatrix}. \tag{3.29}$$

Combining (3.13), (3.14), (3.25), and (3.26) we obtain

$$\begin{aligned}\frac{2}{\omega}\pi^{3/2}u^{(0)} \cong{}& \frac{1-2q}{\sqrt{(1-2q)^2+q^4}} \exp\left\{-\frac{1}{2}[x_1 - (N-1)\omega]^2 + i\omega(N-1)x_2\right\} \\ &+ \frac{q^2}{\sqrt{(1-2q)^2+q^4}} \exp\left\{-\frac{1}{2}[x_1 - (N+1)\omega]^2 + i\omega(N+1)x_2\right\} + \tilde{v}_l,\end{aligned} \tag{3.30}$$

where $\tilde{v}_l$ satisfies

$$\int_0^{2\pi/\omega} e^{-i\omega n x_2}\tilde{v}_l dx_2 = 0, \quad \forall\, x_1 \in (-\omega_0, \infty), \quad N - 2l \leqslant |n| \leqslant N + 2l.$$

We first consider the case $|n| \leqslant N-l-1$. By (3.12) and (2.17) we have

$$\gamma_n(\mu)[\|\hat{u}_n\|_2^2 + \|\hat{u}_{-n}\|_2^2] \leqslant C(\epsilon + e^{-(N\omega + \omega_0)^2/4})^2.$$

By (2.19) and (2.18) there exists n_0 such that

$$n > n_0 \Rightarrow \gamma_n(\mu) \geqslant \tfrac{1}{2}(\lambda_n - \mu).$$

Let first $n_0 < n \leqslant N-l-1$. Then

$$\|\hat{u}_n\|_2^2 + \|\hat{u}_{-n}\|_2^2 \leqslant C\frac{\epsilon^2}{\lambda_n - \mu} \leqslant C\frac{\mu - \lambda_N}{\lambda_n - \mu} \leqslant C\frac{\mu - \lambda_N}{\lambda_n - \mu} \leqslant C\frac{\lambda_{N-l} - \lambda_N}{\lambda_{N-2l} - \lambda_{N-l}} \leqslant Ce^{-(1/2)lN\omega}.$$

Consider now the case $n \leqslant n_0$. Let

$$\tilde{\gamma} = \min_{\substack{1 \leqslant n \leqslant n_0 \\ 1 \leqslant \mu \leqslant \lambda_{N-l}}} \gamma_n(\mu).$$

By (2.18) $\tilde{\gamma}$ must be positive for sufficiently large N. Consequently,

$$\|\hat{u}_n\|_2^2 + \|\hat{u}_{-n}\|_2^2 \leqslant C\frac{\epsilon^2}{\tilde{\gamma}}.$$

Finally, we consider the case $n \geqslant N+2l+1$. In this case we can write instead of (3.23a)

$$(\epsilon^2 + \eta_n^2)\tilde{d}_n = 2\epsilon^2 q^{n^2}\tilde{d}_n + C\epsilon^2\tilde{\epsilon}_n,$$

wherein

$$\tilde{\epsilon}_n \leqslant e^{-(1/4)lN\omega}.$$

Hence, $\tilde{d}_n \leqslant C\tilde{\epsilon}_n$. Since (3.14) is still valid we have

$$\|\tilde{v}_l\| \leqslant Ce^{-(1/4)lN\omega},$$

which completes the proof of (3.8). □

Note that as $q \to 0$

$$\mu \to \lambda_{N-1}; \quad \begin{bmatrix} d_{-1} \\ d_1 \end{bmatrix} \to \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

This is the limit of weak interaction between the modes: As $q \to 0$, ω tends to ∞ and hence, since $\phi_n \sim \exp\{-(x-n\omega)^2/2\}$, we obtain exponentially small interaction between the V_0 and its adjacent modes V_1 and V_{-1}. Consequently, as $q \to 0$, the next bifurcation is almost identical in nature with the first bifurcation: It takes place at, $\mu = \lambda_{N-1}$ and the bifurcating mode is V_{N-1}.

The fact that by (3.30) $u^{(0)}$ depends only on a finite number of modes is surprising: One expects that the bifurcating branch would include infinitely many modes since the term $|\psi|^2\psi$ on the right-hand side of (2.1) does not allow us to separate a finite number of modes from the others. It is thus expected that if we consider additional terms in the expansion (3.5), we shall obtain additional modes, so that u, the solution of (3.4) would consist of an infinite number of modes.

Upon multiplying (3.4) by $\bar{V}_n$ and integrating by parts we obtain

$$(\lambda - \lambda_{N+n}) \int u\bar{V}_n = (\lambda - \lambda_{N+n}) \int \bar{V}_n[2|\psi_0|^2 u + \psi_0^2\bar{u}] + \lambda_{N+n} \int f^2(u\bar{V}_n - \bar{u}V_n) + \lambda_{N+n}$$
$$\times \int \bar{V}_n[2(|\psi_0|^2 - f^2)u + (\psi_0^2 - f^2)\bar{u}] + \lambda \int \bar{V}_n[2|u|^2\psi_0 + u^2\bar{\psi}_0] + \lambda \int \bar{V}_n|u|^2 u.$$

We now substitute (3.5) into the above and obtain for the $O(\delta^2)$ balance for $n = \pm 1$, making the same approximations as before

$$\left(\frac{\omega}{2\pi}\right)^{3/2}[\epsilon_1^2 \pm \eta_{\pm 1}^2) \int u^{(0)}\bar{V}_n + \mu_{N-1}^{(1)} \int u^{(0)}\bar{V}_n = \epsilon_1^2 \int \bar{V}_n[2|V_0|^2 u^{(1)} + V_0^2\bar{u}^{(1)}] + \epsilon_1 \int \bar{V}_n[2|u^{(0)}|^2 V_0$$
$$+ V_0(u^{(0)})^2] + \mu_{N-1}^{(1)}\left(\frac{2\pi}{\omega}\right)^{3/2} \int \bar{V}_n[2|V_0|^2 u^{(0)}$$
$$+ V_0^2\bar{u}^{(0)}] + \epsilon_1^2\hat{\epsilon}_n. \tag{3.31}$$

It is possible to show that $\hat{\epsilon}_n$ is exponentially small as $N \to \infty$, since it results from interactions between "distant" modes, e.g., f_0 and V_n. We skip the details here and proceed by formally obtaining the next-order term.

To find $\mu_{N-1}^{(1)}$ we write the equations for $n = \pm 1$ neglecting the exponentially small terms

$$(\epsilon_1^2 - \eta_{-1}^2)d_{-1}^{(1)} = \epsilon_1^2 q[2d_{-1}^{(1)} + \overline{d^{(1)}}_1 q] + \mu_{N-1}^{(1)}[(1-2q)^2 - q^4], \tag{3.32}$$

$$(\epsilon_1^2 + \eta_1^2)d_1^{(1)} = \epsilon_1^2 q[2d_1^{(1)} + \overline{d^{(1)}}_{-1} q], \tag{3.33}$$

where

$$d_n^{(1)} = \int u^{(1)} \bar{V}_n. \tag{3.34}$$

It is easy to show that (3.32) can have solutions only if

$$\mu_{N-1}^{(1)} = 0. \tag{3.35}$$

In this case the solutions are proportional to (3.29) and are therefore of no interest. For $n=0$ we have

$$d_0^{(1)} = 2d_0^{(1)} + \bar{d}_0^{(1)} + \frac{2q}{\epsilon_1}[(1-2q)^2 + q^3 - q^4].$$

Hence,

$$d_0^{(1)} = -\frac{q}{\epsilon_1}[(1-2q)^2 + q^3 - q^4] + iC, \tag{3.36}$$

where the last term can be eliminated using the gauge transformation (1.2). For $n=\pm 2$ we obtain

$$(\epsilon_1^2 - \eta_{-2}^2) d_{-2}^{(1)} = \epsilon_1^2 q^4 [2d_{-2}^{(1)} + \overline{d^{(1)}}_2 q^4] + \epsilon_1 q^2 (1-2q)[2q^5 + 1 - 2q],$$

$$(\epsilon_1^2 + \eta_2^2) d_2^{(1)} = \epsilon_1^2 q^4 [2d_2^{(1)} + \overline{d^{(1)}}_{-2} q^4] + \epsilon_1 q^6 [2q(1-2q) + 1].$$

Since $\epsilon_1^2 / \eta_{-2}^2 \sim O(e^{-\omega N})$, we obtain

$$|d_{-2}^{(1)}| \sim O(e^{-\omega N}).$$

One can then obtain

$$d_2^{(1)} \cong \frac{q^6}{\epsilon_1}[2q(1-2q) + 1] + (e^{-\omega N}).$$

For $n \geqslant 3$ it is easy to show that $d_{\pm n}^{(1)} = 0$.

We can proceed in the same manner to obtain the next order term in the expansion (3.5). However, this solution will not provide any significant information except for the fact that

$$\mu^{(2)} \cong \left(\frac{\omega}{2\pi}\right)^{3/2} [\epsilon_1 (4d_{-1}^{(0)} d_0^{(1)} q + 2d_1^{(0)} d_0^{(1)} q^2 + 2d_1^{(0)} d_2^{(1)} q^5) + (|d_{-1}^{(0)}|^2 + 2q^4 |d_1^{(0)}|^2) d_{-1}^{(0)}] \frac{1 + O(e^{-\omega N})}{(1-2q)^2 - q^4}$$
$$\cong 1 - 2q + O(q^2, e^{-\omega N}) \quad \text{as } q \to 0. \tag{3.37}$$

We see that while $u^{(0)}$ contains the modes V_1 and V_{-1}, $u^{(1)}$ contains V_2 and V_{-2} as well. It can be shown that $u^{(n-1)}$ contains V_n and V_{-n} and hence by (3.5) u contains infinitely many modes. However, the coefficients of V_{-n} for $n \geqslant 2$ are exponentially small.

If we increase δ in (3.5) such that $\delta \gg \epsilon_1$, then the series (3.5) does not seem to converge: It is possible to show from (3.31) that $u^{(n)} \sim O(q^n / \epsilon_1^n)$. Therefore, convergence of (3.5) can be guaranteed only when $\delta \ll \epsilon_1 / q$. We are interested, however, in the behavior of the bifurcating branch when $\delta \gg \epsilon_1$ as well and therefore need to apply a different approach to obtain this behavior, which is what we do in the next section.

To this end we discuss here the behavior of u near the bifurcation in the limit $q \to 0$. Let then,

$$a_n = \lim_{q \to 0} \int u \bar{V}_n.$$

Formally, we have

$$a_n = \sum_{k=1}^{\infty} a_n^{(k)} \delta^k,$$

where

$$a_n^{(k)} = \lim_{q \to 0} \int u^{(k-1)} \bar{V}_n.$$

By (3.8b) we have

$$a_n^{(1)} = \begin{cases} 1 & n = -1, \\ 0 & n \neq -1. \end{cases}$$

Further, since

$$u^{(n)} \sim O(q^n) \quad \text{as } q \to 0,$$

we must have $a_n^{(k)} = 0$ for all n and $k \geqslant 2$. Consequently,

$$\psi \sim f_0 + \epsilon V_0 + \delta V_{-1} + O(q) \quad \text{as } q \to 0. \tag{3.38}$$

IV. POSTBIFURCATION BEHAVIOR

Consider again (2.1). We multiply the equation by $\bar{V}_n$ and integrate by parts to obtain

$$\lambda \int \psi(1 - |\psi|^2)\bar{V}_n = \lambda_{N+n} \int \psi[\bar{V}_n - f^2(2\bar{V}_n + V_n)],$$

or

$$(\lambda - \lambda_{N+n}) \int \psi \bar{V}_n = (\lambda - \lambda_{N+n}) \int \psi|\psi|^2 \bar{V}_n + \lambda_{N+n} \int \psi|\psi - f|^2 \bar{V}_n - \lambda_{N+n} \int f^2[(\bar{\psi} - f)\bar{V}_n - (\psi - f)V_n]. \tag{4.1}$$

We look for solutions of (2.1) for

$$0 < \lambda - \mu_{N-1} \ll 1,$$

which are close to (1.4), i.e.,

$$\lambda = \lambda_N + \left(\frac{\omega}{2\pi}\right)^{3/2} \epsilon^2 \tag{4.2a}$$

and

$$\psi \cong f_0 + \epsilon \psi^{(1)} + \epsilon^2 \psi^{(2)}, \tag{4.2b}$$

where

$$\psi^{(1)} = \sum_{n=-N+1} C_n V_n, \tag{4.2c}$$

$\epsilon_1 < \epsilon \ll 1$, and $\|\psi^{(2)}\|$ is bounded as $\epsilon \to \epsilon_1$ and $N \to \infty$. [Note that (4.2) is an extrapolation of the results in the preceding section.]

We now estimate the various terms on the right-hand side of (4.1). For the first term we have

$$\int \psi|\psi|^2\bar{V}_n = \epsilon \int f^2[2\psi^{(1)} + \bar{\psi}^{(1)}]\bar{V}_n + \epsilon^2 \int f^2[2\psi^{(2)} + \bar{\psi}^{(2)}]\bar{V}_n + \epsilon^2 \int f[2|\psi^{(1)}|^2 + (\psi^{(1)})^2]\bar{V}_n,$$

in which we have the estimates

$$\left| \int f^2[2\psi^{(1)} + \bar{\psi}^{(1)}]\bar{V}_n \right|^2 \leqslant C \int f^4|V_n|^2 \int |\psi^{(1)}|^2 \leqslant Ce^{-2[(N+n)\omega + \omega_0]^2/3},$$

$$\left| \int f[2|\psi^{(1)}|^2 + (\psi^{(1)})^2]\bar{V}_n \right|^2 \leqslant e^{-[(N+n)\omega + \omega_0]^2/2}.$$

Hence,

$$\left| (\lambda - \lambda_{N+n}) \int \psi|\psi|^2\bar{V}_n \right| \leqslant C|\lambda - \lambda_{N+n}|[\epsilon e^{-[(N+n)\omega + \omega_0]^2/3} + \epsilon^2 e^{-[(N+n)\omega + \omega_0]^2/4} + \epsilon^3]. \quad (4.3)$$

For the last term on the right-hand side of (4.1) we have

$$\int f^2[(\bar{\psi} - f)\bar{V}_n - (\psi - f)V_n] = \epsilon \int f^2[\bar{\psi}^{(1)}\bar{V}_n - \psi^{(1)}V_n] + \epsilon^2 \int f^2[\overline{\psi^{(2)}}\bar{V}_n - \psi^{(2)}V_n],$$

in which we have the estimates

$$\left| \int f^2[\bar{\psi}^{(1)}\bar{V}_n - \psi^{(1)}V_n] \right| \leqslant C \left| \int_{-\omega_0}^{\infty} f^2\phi_n\phi_{-n}dx_1 \right| \leqslant Ce^{-2[(N+n)\omega + \omega_0]^2/3},$$

$$\left| \int f^2\psi^{(2)}V_n \right| \leqslant Ce^{-[(N+n)\omega + \omega_0]^2/3}.$$

For the second term on the right-hand side of (4.1) we have

$$\int \psi|\psi - f|^2\bar{V}_n = \epsilon^2 \int f|\psi^{(1)}|^2\bar{V}_n + 2\epsilon^3 \int f\Re\{\bar{\psi}^{(1)}\psi^{(2)}\}\bar{V}_n + \epsilon^3 \int \psi^{(1)}|\psi^{(1)}|^2\bar{V}_n + O(\epsilon^4),$$

in which

$$\left| \int f|\psi^{(1)}|^2\bar{V}_n \right| \leqslant C \sup_{k<n} \left| \int fV_kV_{n-k-N}\bar{V}_n \right| \leqslant Ce^{-[(N+n)\omega + \omega_0]^2/2},$$

and

$$\left| \int f\Re\{\bar{\psi}^{(1)}\psi^{(2)}\}\bar{V}_n \right| \leqslant Ce^{-[(N+n)\omega + \omega_0]^2/4}.$$

Combining the above estimates and (4.1) we obtain

$$(\lambda - \lambda_{N+n}) \int \psi^{(1)}\bar{V}_n = \epsilon^2 \int \psi^{(1)}|\psi^{(1)}|^2\bar{V}_n + \epsilon^2\tilde{\epsilon}_n, \quad (4.4)$$

where $\tilde{\epsilon}_n$ satisfies (3.22b).

Substituting (4.2) into (4.4) and neglecting the exponentially small terms yields

$$\sum_{r,m=n-N+1}^{\infty} C_{n+r}\bar{C}_{n+r+m}C_{n+m}q^{m^2+r^2} - \nu_n C_n = 0, \tag{4.5a}$$

where

$$\nu_n^2 = \frac{\lambda - \lambda_{N+n}}{\lambda - \lambda_N} \tag{4.5b}$$

which is formally valid only when $(N+n) \gg 1$. Let $l \in \mathbb{N}$ and

$$\tfrac{1}{2}(\lambda_{N-l+1} + \lambda_{N-l}) < \lambda \leqslant \tfrac{1}{2}(\lambda_{N-l} + \lambda_{N-l-1}).$$

Then, by (2.4), we have

$$\nu_n \sim \begin{cases} 1 + O(e^{-\omega N}), & n \geqslant -l+1, \\ -O(e^{\omega N}), & n \leqslant -l-1. \end{cases} \tag{4.6}$$

For $n=-l$ the above ratio varies from a negative $O(e^{\omega N})$ value for $\lambda=(\lambda_{N-l+1}+\lambda_{N-l})/2$ to a value close to unity for $\lambda=\frac{1}{2}(\lambda_{N-l}+\lambda_{N-l-1})$. An immediate consequence of (4.6) is that

$$C_n \sim O(e^{-\omega N}), \quad \forall\, n \leqslant -l-1. \tag{4.7}$$

Equation (4.5) possesses infinitely many solutions. We first consider solutions which are analytic functions of q, i.e.,

$$C_n = \sum_{k=0}^{\infty} a_{nk} q^k. \tag{4.8}$$

We first look at $\lambda(q)$ such that ν_{-l} is independent of q. Note that by (4.6) ν_n remains too independent of q except for an $O(e^{-\omega N})$ term, which is negligible for $\omega \ll N$. For $q=0$ (4.5) has the form

$$a_{n0} = |a_{n0}|^2 a_{n0}, \quad -l+1 \leqslant n, \tag{4.9a}$$

$$\nu_{-l} a_{-l,0} = |a_{-l,0}|^2 a_{-l,0}. \tag{4.9b}$$

Note that the real roots of (4.9) are all simple provided that $\lambda \neq \lambda_{N-l}$. Consequently, all real solutions of (4.5) are holomorphic in q in some neighborhood of $q=0$ for $\lambda \neq \lambda_{N-l}$. We later show that the converse statement is also true, i.e., every solution of the form (4.8) is essentially real.

Consider first the case $l=-1$. We shall assume that (3.5) and (4.2) should match $\delta \sim o(\epsilon_1)$. If we continue (3.5) into the region where $\delta \gg \epsilon_1$ [where (3.5) does not necessarily converge], we obtain via the superposition $\psi=\psi_0+u$ a solution in the form (4.2). Near the bifurcation we have by (3.38)

$$a_{n0} = 0, \quad \forall\, n \neq 0, -1. \tag{4.10}$$

By (3.38) we have

$$a_{00} = 1; \quad a_{-1,0} = \lim_{\substack{q \to 0 \\ \nu_{-1}=\text{const.}}} \frac{\delta}{\epsilon}, \tag{4.11}$$

or, equivalently, that near the bifurcation

$$|a_{-1,0}|^2 = \nu_{-1},$$

which is in accordance with (4.9).

We now make the following claim

Lemma 4.1: Let $\{C_n\}_{n=-N+1}^{\infty}$ *satisfy (4.5) and (4.8). Then*,

$$C_n = e^{i[\theta_0(q)+n\theta_1(q)]}C_n', \tag{4.12}$$

where $C_n' \in \mathbb{R}$ *for all* $n \geqslant -N+1$, *and* $\theta_0(q)$ *and* $\theta_1(q)$ *are holomorphic in* q *in some neighborhood of* $q=0$. *Further, let* $\{a_{n0}\}_{n=-N+1}^{\infty}$ *be real solutions of* (4.9). *Then, there exists a unique solution of* (4.5) *which satisfies* (4.8) *in some neighborhood of* $q=0$.

We bring the proof in the Appendix.

In view of (4.12) we can replace $\{C_n\}_{n=-N+1}^{\infty}$ by $\{C_n'\}_{n=-N+1}^{\infty}$ by applying the transformation

$$\psi \to e^{i\theta_0(q)}\psi(x_1, x_2 + \theta_1(q)/\omega).$$

We may thus assume that the C_n's are all real [all other solutions will be gauge equivalent by (4.12)].

Consequently, using (4.12), we can set

$$a_{-1,0} = (\nu_{-1})^{1/2}.$$

When $\lambda - \lambda_{N-1} \gg \lambda_{N-1} - 1$ we obtain $a_{-1,0}=1$.

We now set $l=-2$ to examine the behavior of C_{-2} with increasing λ. As stated earlier C_{-2} is exponentially small when $\lambda - 1 \ll \lambda_{N-2} - 1$. However, we expect C_{-2} to become $O(1)$ for $\lambda > \lambda_{N-2}$.

Substituting (4.8) into (4.5) we obtain for the $O(q)$ balance

$$\nu_n a_{n1} = 3a_{n0}^2 a_{n1} + 2[a_{n+1,0}^2 + a_{n-1,0}^2]a_{n0}. \tag{4.13}$$

For $n \neq 0, -1$ we have $a_{n1}=0$. For $n=0, -1$ we have

$$a_{01} = -\nu_{-1}; \quad a_{-1,1} = -\frac{1}{\nu_{-1}^{1/2}}.$$

The $O(q^2)$ balance is

$$\begin{aligned}\nu_n a_{n2} = {} & 3a_{n0}^2 a_{n2} + 3a_{n1}^2 a_{n0} + 4(a_{n+1,0}a_{n+1,1} + a_{n-1,0}a_{n-1,1})a_{n0} + 2[a_{n+1,0}^2 + a_{n-1,0}^2]a_{n1} \\ & + [a_{n+1,0}^2 a_{n+2,0} + 2a_{n+1,0}a_{n0}a_{n-1,0} + a_{n-1,0}^2 a_{n-2,0}].\end{aligned} \tag{4.14}$$

Since we are interested in the behavior of C_{-2} with increasing λ we solve (4.14) for $n=-2$

$$\nu_{-2}a_{-2,2} = a_{-1,0}^2 a_{00}.$$

Consequently,

$$C_{-2} \sim \frac{\nu_{-1}}{\nu_{-2}}q^2. \tag{4.15}$$

As was expected in (4.7), C_{-2} is exponentially small provided that $\lambda - 1 \ll \lambda_{N-2} - 1$. If, however, $\lambda \uparrow \lambda_{N+2}$, then $a_{-2,2} \to -\infty$ and (4.15) ceases to be valid. To obtain the leading behaviour of C_{-2} in the limit $q \to 0$ when $\nu_{-2} \ll 1$ we consider first the case where $\nu_{-2} \sim O(q)$. Let then

$$\nu_{-2} = \rho q.$$

Substituting into (4.9), (4.13), and (4.14) (recalling that $\nu_{-1} \cong 1$ up to an exponentially small error) we obtain

$$a_{-2,0} = 0,$$

$$\rho a_{-2,1} = 2.$$

Consequently,

$$C_{-2} \cong \frac{1}{\rho - 2} q. \tag{4.16}$$

It is not difficult to show that in the overlap range where $\nu_{-2} \sim O(q^{\alpha})$ for $0 < \alpha < 1$ (4.15) and (4.16) match. We thus formally conclude that (4.15) develops into (4.16), which is valid as long as $\rho < 2$.

When $\rho \uparrow 2$, $a_{-2,1} \to -\infty$ and hence we must consider separately the case $|\rho - 2| \ll 1$. We thus consider ν_{-2} values satisfying

$$\nu_{-2} = 2q + \tau q^{4/3}.$$

In this case (4.8) is no longer valid. We therefore use the more general ansatz

$$C_n = \sum_{k=0}^{\infty} b_{nk} q^{k/3}.$$

Substituting in (4.5) and applying an appropriate gauge transformation we obtain

$$b_{00} = 1; \quad b_{-1,0} = 1; \quad b_{-2,0} = 0,$$

$$b_{-2,1} = 0,$$

and

$$(|b_{-2,2}|^2 - \tau) b_{-2,2} = - b_{-1,0}^2 b_{00} = -1. \tag{4.17}$$

Since our goal is to follow C_{-2} with increasing λ we look for the solution of (4.17) which matches (4.16) as $\tau \to -\infty$. Consequently, we must have

$$b_{-2,2} \sim \frac{1}{\tau} \quad \text{as } \tau \to -\infty.$$

Using the theory of cubic equations, it is easy to show that (4.17) has only one solution for

$$\tau < \tau_c = \frac{3}{2\sqrt[3]{2}},$$

since (4.17) admits only real solutions. We now follow this solution with increasing value of τ in order to find its behaviour as $\tau \to \infty$.

When $\tau = \tau_c$, (4.17) possesses two distinct solutions

$$b_{-2,2} = \frac{1}{\sqrt[3]{2}} \quad \text{with double multiplicity} \tag{4.18a}$$

and

$$b_{-2,2} = \sqrt[3]{4} \quad \text{with single multiplicity}. \tag{4.18b}$$

The former solution does not exist for $\tau < \tau_c$, and therefore, the latter solution is the one we follow. Since $|b_{-2,2}(\tau_c)|^2 > \tau_c$, we must have $|b_{-2,2}(\tau)|^2 > \tau$ for all $\tau \geqslant \tau_c$. Consequently, as $\tau \to \infty$,

$$C_{-2} \sim - \tau^{1/2} q^{2/3} C_{-1}^2 C_0 \sim - \tau^{1/2} q^{2/3}. \tag{4.19}$$

Consider now the case $\nu_{-2} = \rho q$ when $\rho > 2$. In this case we use the ansatz

$$C_n = \sum_{k=0}^{\infty} B_{nk} q^{k/2}.$$

Substituting into (4.5) yields, upon applying an appropriate gauge transformation,

$$B_{00} = 1; \quad B_{-1,0} = 1; \quad B_{-2,0} = 0,$$

$$|B_{-2,1}| = \sqrt{\rho - 2}. \tag{4.20a}$$

To find the phase of $B_{-2,1}$ we match (4.20) with (4.19) to obtain

$$C_{-2} \sim -\sqrt{\rho - 2} q^{1/2} C_{-1}^2 C_0 \sim -\sqrt{\rho - 2} q^{1/2}. \tag{4.21}$$

Finally, we consider positive $\nu_{-2} \sim O(1)$. Here we assume (4.8) once again. By (4.9) we have

$$|a_{-2,0}| = \sqrt{\nu_{-2}}.$$

The sign of $a_{-2,0}$ is determined from matching with (4.21). We obtain

$$C_{-2} \sim -\nu_{-2}^{1/2} C_{-1}^2 C_0 \sim -\nu_{-2}^{1/2}. \tag{4.22}$$

If λ further increases so that $\lambda_{N-2} - 1 \ll \lambda - 1 \ll \lambda_{N-3} - 1$, then $\nu_{-2} \sim 1$ and $C_{-2} \sim -1$.

To summarize: we have followed the $C_{-2}(\lambda)$ and found that it varies from a small negative value when $\lambda - 1 \ll \lambda_{N-2} - 1$ to approximately -1 for $\lambda - 1 \gg \lambda_{N-2} - 1$. This procedure can be applied recursively to obtain

$$C_{-l} \sim -C_{-l+1}^2 C_{l+2}, \tag{4.23}$$

from which we obtain

$$C_n \sim \begin{cases} (-1)^{[(n+1)/2]}, & -l \leqslant n \leqslant 0 \\ 0 & \text{otherwise} \end{cases} + O(q), \tag{4.24}$$

wherein $[\cdot]$ denotes the integer value.

We have thus formally obtained the behavior of the C_n's in the limit $q \to 0$. We now claim that for $l \gg 1$ and $N - l \gg 1$, when substituting (4.24) into (4.2c), ψ becomes close to the well-known triangular lattice.[11–13,21] The following lemma proves a stronger result: If a_{n0} satisfy (4.24), then any solution of the form (4.8) is close to the triangular lattice, for all q where (4.8) converges and not only when $q \to 0$. We should, however, emphasize that the foregoing discussion demonstrates (4.24) only formally and in the limit $q \to 0$. No such result has been proved for a_{n0}.

Lemma 4.2: Let

$$\phi = \epsilon D(q) \sum_{n=-\infty}^{\infty} (-1)^{[(n+1)/2]} \exp\left\{ -\frac{1}{2}(x_1 - n\omega)^2 + in\omega x_2 \right\}, \tag{4.25a}$$

where

$$\frac{1}{D^2} = \sum_{(m,r) \in \mathbb{Z}^2} (-1)^{mr} q^{m^2 + r^2}. \tag{4.25b}$$

Let ψ be given by (4.2) *and* $\{C_n\}_{n=-N+1}^{\infty}$ *satisfy* (4.5). *Then*,

$$\|\phi - \psi\|_{\infty} \leqslant C\epsilon \left[q^{l^2/64} + \epsilon^{1/2} + e^{Cl^2 - \omega N l/4} \right], \tag{4.26a}$$

where

$$\|\cdot\|_{\infty} = \|\cdot\|_{L^{\infty}\{[(N-5l/8)\omega, (N-3l/8)\omega] \times [0, 2\pi/\omega]\}}. \tag{4.26b}$$

Proof: Let

$$\tilde{\psi} = \epsilon \sum_{n=-\infty}^{\infty} e_n \exp\left\{ -\frac{1}{2}(x_1 - n\omega)^2 + in\omega x_2 \right\}, \tag{4.27}$$

where $\{e_n\}_{n=-\infty}^{\infty}$ denotes the solution of

$$\sum_{(r,m)\in\mathbb{Z}^2} e_r \bar{e}_{m-n+r} e_m q^{(r-n)^2+(m-n)^2} - e_n = 0, \tag{4.28}$$

which is holomorphic in q, or

$$e_n = \sum_{k=0}^{\infty} e_{nk} q^k,$$

such that

$$e_{n0} = \begin{cases} (-1)^{[(n+1)/2]}, & -l \leqslant n \leqslant 0 \\ 0 & \text{otherwise} \end{cases}. \tag{4.29}$$

We first prove that there exists $A>0$ which is independent of k, l, ω, q, and N such that

$$|e_{nk} - a_{nk}| \leqslant A^k e^{-\omega Nl/4}, \tag{4.30}$$

for all $0\leqslant k\leqslant l^2/16$ and $-3l/4\leqslant n\leqslant -l/4$. This can be done by using the recurrence relation obtained by substituting (4.8) into (4.5):

$$\nu_n a_{nk} = \sum_{r^2+s^2\leqslant k} \sum_{\substack{m,j\geqslant 0 \\ m+j\leqslant M}} a_{(n+r)j} a_{(n+r+s)(M-m-j)} a_{(n+s)m}, \tag{4.31}$$

where $M(r,s)=k-r^2-s^2$. Note that the C_n's were assumed all real in view of (4.12). By (4.28), e_{nk} satisfy the same recurrence relation with $\nu_n=1$. We can thus proceed by induction: We assume (4.30) for $0\leqslant k\leqslant K-1$. Substituting in (4.31) we obtain

$$\nu_n a_{nK} = \sum_{r^2+s^2\leqslant K} \sum_{\substack{m,j\geqslant 0 \\ m+j\leqslant M(K)}} e_{(n+r)j} e_{(n+r+s)(M-m-j)} e_{(n+s)m} + \Delta_{nK},$$

where

$$\Delta_{nK} \leqslant \sum_{j=1}^{K} 3A^{K-j} j^2 e^{-\omega Nl/4}.$$

Any $A>0$ satisfying

$$\sum_{n=1}^{\infty} A^{-n} n^2 \leqslant \frac{1}{3}$$

would then satisfy (4.30).

Using (4.27) and (4.2) we now have

$$\|\psi - \tilde{\psi}\|_\infty \leqslant \|f_0\|_\infty + \epsilon \sum_{n=-\infty}^{\infty} |C_n - e_n| \| e^{-(1/2)(x_1 - n\omega)^2} \|_\infty.$$

For the first term we have, since $l \ll N$,

$$\|f_0\|_\infty \leqslant C \exp\left\{-\frac{1}{2}\left(N-\frac{5}{8}l\right)^2\omega^2\right\} \leqslant C \exp\left\{-\frac{3}{8}N^2\omega^2\right\} \leqslant C\epsilon^{3/2}.$$

For the second term we have the bound

$$\epsilon \sum_{n=-\infty}^{\infty} |C_n - e_n| \left\| e^{-1/2(x_1 - n\omega)^2} \right\|_\infty \leqslant \epsilon \sum_{n=-3l/4}^{-l/4} |C_n - e_n| + Ce^{-l^2\omega^2/128} \leqslant \epsilon \frac{l}{2} \sum_{k=0}^{l^2/64} (Aq)^k e^{-\omega Nl/4} + Cq^{l^2/64},$$

from which we obtain

$$\|\psi - \tilde{\psi}\|_\infty \leqslant C\epsilon(q^{l^2/64} + \epsilon^{1/2} + e^{Cl^2 - \omega Nl/4}). \tag{4.32}$$

To complete the proof we need to obtain a similar estimate for $\|\phi - \tilde{\psi}\|_\infty$. By (4.25) we can write

$$\phi = \epsilon \sum_{n=-\infty}^{\infty} g_n \exp\left\{-\frac{1}{2}(x_1 - n\omega)^2 + in\omega x_2\right\},$$

where $\{g_n\}_{n=-\infty}^{\infty}$ satisfies (4.28) and

$$g_n = \sum_{k=0}^{\infty} g_{nk} q^k,$$

but in contrast with $\{e_n\}_{n=-\infty}^{\infty}$

$$g_{n0} = (-1)^{[(n+1)/2]}.$$

Substituting the above into (4.28) yields

$$g_{nk} = e_{nk}$$

for all $0 \leqslant k \leqslant l^2/16$ and $-3l/4 \leqslant n \leqslant -l/4$. The proof of the lemma then easily follows. □

V. CONCLUDING REMARKS

In Sec. II we prove the exact asymptotic behaviour of the critical values $\{\lambda_n\}_{n=1}^{\infty}$ of (2.2) and their corresponding modes. We proved that

$$\lambda_n \sim 1 + 2a^2 e^{-(n\omega + \omega_0)^2/2} + O(e^{-2(n\omega + \omega_0)^2/3}) \quad \text{as } n \to \infty,$$

where

$$a = \lim_{x \to \infty} e^{x^2/2} f(x, 1),$$

and that

$$\|\phi_n - e^{-(x_1 - n\omega)^2/2}\|_2^2 + \|\phi_{-n}\|_2^2 \leqslant e^{-2(n\omega + \omega_0)^2/3}.$$

Consequently, immediately after the first bifurcation we have

$$\lambda \cong \lambda_n + \epsilon^2 \left(\frac{\omega}{2\pi}\right)^{3/2},$$

$$\psi \cong e^{i\omega_0 x_2}\{f(x_1,\lambda) + \epsilon e^{-(x_1 - n\omega)^2/2} e^{in\omega x_2}\} + O(e^{-(n\omega + \omega_0)^2/3}),$$

Where f is given in (1.4).

At the conclusion of Sec. II we conjecture that $\lambda_n > 1$ for all $n \in \mathbb{N}$. This appears plausible since we expect that (1.4) would serve as the global minimizer of (1.8) in $\mathcal{P}_L^{\omega_0}$ when $\lambda \leqslant 1$. In Ref. 20 it was shown that any bifurcating branch has lower energy than (1.4) independently of n and λ. Thus, no bifurcation should take place for $\lambda \leqslant 1$ if (1.4) is indeed the global minimizer.

In Sec. III we consider the second bifurcation, while assuming that the first bifurcation takes place at $\lambda = \lambda_N$. We can explain this choice by considering (1.3a) not in $\mathbb{R}_2^+$ but in $[0,d] \times \mathbb{R}$ in the limit $d \to \infty$. In this case we have to add to (2.2) the boundary conditions

$$\phi_n'(d - \omega_0) = \phi_{-n}'(d - \omega_0) = 0.$$

As a result of the introduction of the additional boundary we have

$$\lambda_n(d) \sim n^2\omega^2 \quad \text{when } n\omega \gg d. \tag{5.1}$$

However, because of continuity,[24] one expects that

$$\lambda_n(d) \xrightarrow[d\to\infty]{} \lambda_n(\infty).$$

Although the above convergence is clearly not uniform in n, it still implies that for sufficiently large d there is a large number of critical values $\lambda_n(d)$ which can be approximated by (2.4). Let then,

$$\lambda_N = \min_{n\in\mathbb{N}} \lambda_n(d).$$

In view of (5.1) such a minimum must exist. Further, if (2.18) is correct then λ_N must be very close to 1. Since with increasing λ the first bifurcation from (1.4) must take place at $\lambda = \lambda_N$ we see that the assumption that the bifurcation takes place at $\lambda = \lambda_N$ is in accordance in principle with the situation in finite domains.

We show in Sec. III that, if the second bifurcation exists and if (2.18) is correct, then the second bifurcation must take place at

$$\mu_{N-1} \cong \lambda_N + \frac{1-2q}{(1-2q)^2 - q^4}(\lambda_{N-1} - \lambda_N),$$

where $q = e^{-\omega^2/2}$, and the bifurcating mode must have the form

$$\frac{2}{\omega}\pi^{3/2}u^{(0)} \cong \frac{1-2q}{\sqrt{(1-2q)^2+q^4}} \exp\left\{-\frac{1}{2}[x_1 - (N-n)\omega]^2 + i\omega(N-n)x_2\right\} + \frac{q^2}{\sqrt{(1-2q)^2+q^4}} \exp\left\{-\frac{1}{2}[x_1 - (N+n)\omega]^2 + i\omega(N+n)x_2\right\}.$$

By formally evaluating the next order terms in (3.5) we obtain that each term provides two additional Fourier modes to ψ. Thus, $u^{(1)}$ adds the modes V_{-2} and V_2, etc. However, the coefficients of V_{-k} have been shown to be exponentially small for all $k \geqslant 2$.

In Sec. IV we extrapolate the behaviour of ψ near the bifurcation into the region where

$$\lambda - \mu_{N-1} \sim O(\lambda - \lambda_N).$$

To this end we assume that

$$\psi \cong f + \epsilon \sum_{n=-N+1}^{\infty} C_n V_n, \tag{5.2}$$

and

$$\lambda \cong \lambda_N + \epsilon^2 \left(\frac{\omega}{2\pi} \right)^{3/2}.$$

Based upon this assumption we find that as $N \to \infty$ the C_n's must satisfy the system

$$\sum_{r,m=n-N+1}^{\infty} C_{n+r} \bar{C}_{n+r+m} C_{n+m} q^{m^2+r^2} - \nu_n^2 C_n = 0,$$

where

$$\nu_n^2 = \frac{\lambda - \lambda_{N+n}}{\lambda - \lambda_N}.$$

This system of polynomial equations is very similar to the one obtained by Abrikosov[1] in the absence of boundaries where

$$\sum_{r,m=-\infty}^{\infty} C_{n+r} \bar{C}_{n+r+m} C_{n+m} q^{m^2+r^2} - \nu C_n = 0,$$

in which ν is proportional to $\lambda - 1$.

To investigate the solution of the above-mentioned system with increasing λ we first match (5.2) with the solution obtained in Sec. III. We obtain that near $\lambda = \mu_{N-1}$ as $q \to 0$ with fixed ν_{-1} we have

$$C_0 \sim 1 \quad C_{-1} \sim \sqrt{\nu_{-1}}.$$

By following the leading order of C_{-2} as $q \to 0$ (with fixed ν_{-2}) with increasing λ, we obtain that when $\nu_{-2} \sim 1$

$$C_{-2} \sim -C_0^2 C_{-1} = -1.$$

Since the same procedure can be applied again to derive the behavior of C_{-n} when $\nu_{-n} \sim 1$, we obtain that

$$C_n \sim \begin{cases} (-1)^{[(n+1)/2]}, & -l \leqslant n \leqslant 0 \\ 0 & \text{otherwise.} \end{cases} + O(q)$$

Finally, we show that if C_n is holomorphic in q for all n, then the above-mentioned asymptotic relation implies that (5.2) is closed to the triangular lattice, which is given by

$$\phi = \epsilon D(q) \sum_{n=-\infty}^{\infty} (-1)^{[(n+1)/2]} \exp\left\{ -\frac{1}{2}(x_1 - n\omega)^2 + in\omega x_2 \right\},$$

where

$$\frac{1}{D^2} = \sum_{(m,r) \in \mathbb{Z}^2} (-1)^{mr} q^{m^2+r^2}.$$

We prove that

$$\|\phi - \psi\|_\infty \leqslant C\epsilon[q^{l^2/64} + \epsilon^{1/2} + e^{Cl^2-\omega Nl/4}],$$

where $1 \ll l \ll N$ and

$$\|\cdot\|_\infty = \|\cdot\|_{L^\infty\{[(N-5l/8)\omega,(N-3l/8)\omega]\times[0,2\pi/\omega]\}}.$$

We conclude this section by listing the main gaps which need to be addressed in order to establish a rigorous proof of the main result of this work

(1) Proof of (2.18).
(2) Existence proof of the second bifurcation.
(3) Proving that (5.2) is indeed a continuation of (3.1).
(4) Proving that C_n must be holomorphic in q when $\nu_n \sim 1$ for $n \geqslant -l$ and $\nu_n \sim -O(e^{\omega N})$ for $n \leqslant -l-1$ (here l is any integer smaller than $N/2$).
(5) Proof that either no other bifurcation exists after the second one or, if another bifurcation does exist, then (5.2) has lower energy than the supposed bifurcating branch.

APPENDIX: PROOF OF LEMMA 4.1

We prove here an equivalent statement to (4.12), i.e., that

$$C_{n-1}\bar{C}_n^2 C_{n+1} \in \mathbb{R}. \tag{A1}$$

We prove (A1) by invoking inductive arguments. We first prove that

$$\mathfrak{I}(C_{n-1}\bar{C}_n^2 C_{n+1}) \sim O(q), \quad \forall\, n, \tag{A2}$$

and then that

$$\mathfrak{I}(C_{n-1}\bar{C}_n^2 C_{n+1}) \sim O(q^k) \Rightarrow \mathfrak{I}(C_{n-1}\bar{C}_n^2 C_{n+1}) \sim O(q^{k+1}), \quad \forall\, n. \tag{A3}$$

Substituting (4.8) into (4.5) we obtain from the $O(q^2)$ balance that[13]

$$\mathfrak{I}\{\bar{a}_{(n+2)0}a_{(n+1)0}^2\bar{a}_{n0} + 2a_{(n+1)0}(\bar{a}_{n0})^2 a_{(n-1)0} + \bar{a}_{(n-2)0}a_{(n-1)0}^2\bar{a}_{n0}\} = 0, \quad \forall\, n.$$

From this we easily conclude that

$$\mathfrak{I}\{a_{(n+1)0}(\bar{a}_{n0})^2 a_{(n-1)0}\} = 0, \quad \forall\, n,$$

which is exactly (A2).

To prove (A3) we assume by induction that

$$\mathfrak{I}(C_{n-1}\bar{C}_n^2 C_{n+1}) \sim O(q^k).$$

Equivalently we may assume the existence of θ_0, θ_1, holomorphic in q, such that

$$\mathfrak{I}\{C_n e^{i[\theta_0(q)+n\theta_1(q)]}\} \sim O(q^k).$$

Let

$$C_n' = e^{i[\theta_0(q)+n\theta_1(q)]}C_n.$$

Then,

$$c_n' = \sum_{j=0}^{\infty} a_{nj}' q^j,$$

where

$$a'_{nj} \in \mathbb{R}, \quad \forall\, 0 \leqslant j \leqslant k-1.$$

Let further

$$a'_{nk} = [a'_n + b_n^k]a'_{n0}, \quad -l \leqslant n \leqslant 0.$$

It is easy to show that when $a'_{n0}=0$, then $a'_{nk} \in \mathbb{R}$. Thus, it remains necessary to show that $b_n^k=0$ for all $-l \leqslant n \leqslant 0$. The recurrence relation (4.31) for complex a_{nj} becomes

$$\nu_n a'_{nj} = \sum_{r^2+s^2 \leqslant j} \sum_{\substack{m,j \geqslant 0 \\ m+j \leqslant M}} a'_{(n+r)j} \bar{a}'_{(n+r+s)(M-m-j)} a'_{(n+s)m}, \tag{A4}$$

where $M(r,s)=j-r^2-s^2$. It is easy to show that (A4) is satisfied for $j=k$ and $j=k+1$ independently of the values of the b_n^k's. For $j=k+2$ we obtain after a tedious calculation that (A4) is solvable if and only if

$$Pb = 0 \tag{A5a}$$

where b is the vector

$$b = \begin{bmatrix} b_{0k} \\ \vdots \\ b_{-l,k} \end{bmatrix}, \tag{A5b}$$

and p is the matrix

$$P = \begin{bmatrix} -p_{-l+1} & 2p_{-l+1} & -p_{-l+1} & 0 & \cdots & 0 \\ 2p_{-l+1} & -4p_{-l+1}-p_{-l+2} & 2(p_{-l+1}+p_{-l+2}) & -p_{-l+2} & 0 & \cdots \\ -p_{-l+1} & 2(p_{-l+1}+p_{-l+2}) & -p_{-l+1}-4p_{-l+2}-p_{-l+3} & 2(p_{-l+2}+p_{-l+3}) & -p_{-l+3} & \cdots \\ \vdots & \vdots & \cdots & \cdots & \cdots & \vdots \\ 0 & \cdots & 0 & -p_{-1} & 2p_{-1} & -p_{-1} \end{bmatrix}, \tag{A5c}$$

in which,

$$p_n = a'_{n-1,0}(a'_{n0})^2 a'_{n+1,0}. \tag{A5d}$$

The matrix P can conveniently be decomposed into the product

$$P = P^{(1)}P^{(2)}, \tag{A6a}$$

where

$$P^{(1)} = \begin{bmatrix} 0 & -p_{-l+1} & 0 & 0 & \cdots & 0 & 0 \\ 0 & 2p_{-l+1} & -p_{-l+2} & 0 & \cdots & 0 & 0 \\ 0 & -p_{-l+1} & 2p_{-l+2} & -p_{-l+3} & \cdots & 0 & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -p_{-1} & 0 \end{bmatrix}, \tag{A6b}$$

and

$$P^{(2)} = \begin{bmatrix} -2 & 1 & 0 & \cdots & & 0 & 1 \\ 1 & -2 & 1 & 0 & \cdots & & 0 \\ \vdots & & & & & & \vdots \\ 0 & \cdots & & & 0 & 1 & -2 & 1 \end{bmatrix}. \tag{A6c}$$

The matrix $P^{(2)}$ is circulant. Its kernel is spanned by $[1,\ldots,1]^T$. For $P^{(1)}$ we have

$$\ker P^{(1)} = \operatorname{span}\left\{\begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}; \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}\right\}.$$

Obviously $[1,\ldots,1]^T \in \ker P$. Further, any vector $b \in \mathbb{R}^{l+1}$ for which $P^{(2)}b \in \ker P^{(1)}$ belongs to $\ker P$ as well. Consequently, $r(P)=2$ and

$$\ker P = \operatorname{span}\left\{\begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}; \begin{bmatrix} 0 \\ 1 \\ \vdots \\ l \end{bmatrix}\right\}.$$

and hence

$$b_n^k = b^k + n\tilde{b}^k,$$

which proves (A3). □

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Classical solutions to the time-dependent Ginzburg–Landau equations for a bounded superconducting body in a vacuum

Patricia Bauman
Department of Mathematics, Purdue University, West Lafayette, Indiana 47907-1395

Hala Jadallah
Department of Mathematics, New Mexico Institute of Mining and Technology, Socorro, New Mexico 87801

Daniel Phillips
Department of Mathematics, Purdue University, West Lafayette, Indiana 47907-1395

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I. INTRODUCTION

In this article we study an initial value problem for the time dependent Ginzburg–Landau (TDGL) equations used to model the electrodynamics of a nonmagnetic superconducting body $\Omega \subset \mathbb{R}^3$ placed in a vacuum.[11] We prove existence, uniqueness, and regularity results for solutions $(\psi, \mathbf{A}, \phi)$ where $\psi(\cdot,t):\Omega \to \mathbb{C}$ is the Ginzburg–Landau order parameter, $\mathbf{A}(\cdot,t):\mathbb{R}^3 \to \mathbb{R}^3$ is the magnetic vector potential, and $\phi(\cdot,t):\mathbb{R}^3 \to \mathbb{R}$ is the scalar electric potential. We use the notation $(a,b)=\mathcal{R}_e(a^*b)=(a^*b+ab^*)/2$ for $a,b \in \mathbb{C}$ to denote the real inner product on $\mathbb{C}\times\mathbb{C}$, $\nabla_{\mathbf{A}}=\nabla-i\mathbf{A}$ for the covariant derivative, $D_T=\Omega\times(0,T)$, and $E_T=\mathbb{R}^3\times(0,T)$. The TDGL equations, also known as the Gorkov-Eliashberg equations[5] are

$$\partial_t\psi + i\phi\psi - \nabla_{\mathbf{A}}^2\psi + \kappa^2(|\psi|^2-1)\psi = 0 \quad \text{in } D_T, \tag{1.1}$$

$$\sigma\chi_\Omega(\partial_t\mathbf{A}+\nabla\phi) + \operatorname{curl}^2\mathbf{A} = \chi_\Omega(i\psi,\nabla_{\mathbf{A}}\psi) \quad \text{in } E_T. \tag{1.2}$$

The term $|\psi|^2$ represents the density of superconducting electron pairs in Ω, and $\mathbf{j}_s=(i\psi,\nabla_{\mathbf{A}}\psi)$ denotes the supercurrent density in the body. The quantity $\mathbf{E}=-\partial_t\mathbf{A}-\nabla\phi$ is the electric field. The normal current density is characterized by Ohm's law, $\mathbf{j}_n=\sigma\mathbf{E}$ in Ω. The constants κ and σ are positive and fixed determined by the material, κ is the Ginzburg–Landau constant and σ is the normal conductivity. Writing the total current density as $\mathbf{j}=\mathbf{j}_s+\mathbf{j}_n$ we see that (1.2) can be written as

$$\operatorname{curl}^2\mathbf{A} = \chi_\Omega(\mathbf{j}_s+\mathbf{j}_n) = \chi_\Omega\mathbf{j}. \tag{1.3}$$

This is the quasistatic approximation to Ampere's law for a nonmagnetic, conducting body surrounded by a vacuum.

The domain Ω is an open bounded connected set in $\mathbb{R}^3$ where $\partial\Omega$ will be as smooth as needed (at least $C^{3+\alpha}$). We assume that

$$\nabla_{\mathbf{A}}\psi\cdot\boldsymbol{\nu}=0 \quad \text{on } \partial\Omega, \tag{1.4}$$

where $\boldsymbol{\nu}$ is the exterior normal to the boundary. Since $\mathbb{R}^3\backslash\bar{\Omega}$ is a vacuum neither super or normal current crosses $\partial\Omega$. To see that this property is implied by the system note from (1.4) that

$$0=(i\psi,\nabla_{\mathbf{A}}\psi)\cdot\boldsymbol{\nu}=\mathbf{j}_s\cdot\boldsymbol{\nu} \quad \text{on } \partial\Omega.$$

Further, from (1.3), assuming that $\mathbf{j}$ is sufficiently regular, we have

$$0=\operatorname{div}(\chi_\Omega\mathbf{j})=\chi_\Omega \operatorname{div}\mathbf{j}+\mathbf{j}\cdot\boldsymbol{\nu}dH^2_{\llcorner\partial\Omega} \quad \text{in } \mathcal{D}'(\mathbb{R}^3).$$

Thus $0=\mathbf{j}\cdot\boldsymbol{\nu}$ on $\partial\Omega$, and it follows that $\mathbf{j}_n\cdot\boldsymbol{\nu}=-\mathbf{j}_s\cdot\boldsymbol{\nu}=0$ on $\partial\Omega$ as well.

The electrodynamics are driven by a constant applied magnetic field $\mathbf{H}=h\mathbf{e}_3$ and initial values. These are reflected in the conditions

$$(\operatorname{curl}\mathbf{A}-h\mathbf{e}_3)\in\mathbf{L}_2(\mathbb{R}^3) \quad \text{for } 0\leqslant t<T,$$

$$\psi(x,0)=\psi_0(x) \quad \text{in } \Omega$$

with $|\psi_0|\leqslant 1$,

$$\mathbf{A}(x,0)=\mathbf{A}_0(x) \quad \text{in } \mathbb{R}^3,$$

where $\operatorname{curl}^2\mathbf{A}_0=0$ in $\mathcal{D}'(\mathbb{R}^3\backslash\bar{\Omega})$. The last condition is to be expected since by (1.3) we have $\operatorname{curl}^2\mathbf{A}=0$ in $\mathbb{R}^3\backslash\bar{\Omega}$ for $t>0$.

A specific magnetic potential for the applied field is $h\mathbf{a}(x)=(0,hx_1,0)$, and in this article we view $\mathbf{A}$ as a perturbation of this field, $\mathbf{A}=\tilde{\mathbf{A}}+h\mathbf{a}$. We consider $\tilde{\mathbf{A}}\in\check{\mathbf{H}}(\mathbb{R}^3)$ where $\check{\mathbf{H}}$ is the Hilbert space defined on the closure of $\mathbf{C}_c^\infty(\mathbb{R}^3;\mathbb{R}^3)$ in the norm $\|\tilde{\mathbf{A}}\|_{\check{\mathbf{H}}}=(\int_{\mathbb{R}^3}|\nabla\tilde{\mathbf{A}}|^2\mathrm{d}x)^{1/2}$. Thus $(\psi,\tilde{\mathbf{A}},\phi)$ is a solution to the system,

$$\partial_t\psi+i\phi\psi-\nabla^2_{(\tilde{\mathbf{A}}+h\mathbf{a})}\psi+\kappa^2(|\psi|^2-1)\psi=0 \quad \text{in } D_T, \tag{1.5}$$

$$\sigma\chi_\Omega(\partial_t\tilde{\mathbf{A}}+\nabla\phi)+\operatorname{curl}^2\tilde{\mathbf{A}}=\chi_\Omega\cdot(i\psi,\nabla_{(\tilde{\mathbf{A}}+h\mathbf{a})}\psi) \quad \text{in } E_T, \tag{1.6}$$

$$\nabla_{(\tilde{\mathbf{A}}+h\mathbf{a})}\psi\cdot\boldsymbol{\nu}=0 \quad \text{on } \partial\bar{\Omega}\times(0,T), \tag{1.7}$$

$$\tilde{\mathbf{A}}\in\check{\mathbf{H}}(\mathbb{R}^3) \quad \text{for } 0\leqslant t<T, \tag{1.8}$$

$$\int_\Omega\phi\mathrm{d}x=0 \quad \text{for } 0\leqslant t<T, \tag{1.9}$$

$$\psi=\psi_0, \quad \tilde{\mathbf{A}}=\mathbf{A}_0-h\mathbf{a} \quad \text{at } t=0. \tag{1.10}$$

For $p\in[1,\infty]$ and integer $m\geqslant 1$, $W_p^m(\Omega)$ is the space of functions having all weak derivatives of order up to m in $L_p(\Omega)$, for $p\in[1,\infty)$, $\mathring{W}_p^m(\Omega)$ denotes the closure of $C_c^\infty(\Omega)$ in the $W_p^m(\Omega)$ norm, and $W_p^{2,1}(D_T)$ is the space of functions where weak derivatives $u_{x_i}=\partial_{x_i}u$, $u_{x_ix_j}=\partial_{x_i}\partial_{x_j}u$, $\partial_t u$ belong to $L_p(\Omega)$. Furthermore if W denotes a space of real valued functions then we use $\mathbf{W}$ for the corresponding space of vector valued functions, and $\mathcal{W}$ if the functions are complex valued.

A. The spaces $\check{\mathbf{H}}(\mathbb{R}^3)$ and $\check{\mathbf{G}}(\mathbb{R}^3)$

Elements $\mathbf{B} \in \check{\mathbf{H}}(\mathbb{R}^3)$ satisfy

$$\|\mathbf{B}\|_{\mathbf{L}_6(\mathbb{R}^3)} \leqslant C\|\nabla \mathbf{B}\|_{\mathbf{L}_2(\mathbb{R}^3)}, \tag{1.11}$$

$$\int_{\mathbb{R}^3} |\nabla \mathbf{B}|^2 \mathrm{d}x = \int_{\mathbb{R}^3} [(\operatorname{div} \mathbf{B})^2 + |\operatorname{curl} \mathbf{B}|^2] \mathrm{d}x. \tag{1.12}$$

These are proved first for $\mathbf{B} \in \mathbf{C}_c^\infty(\mathbb{R}^3;\mathbb{R}^3)$ and then follow by density. Inequality (1.11) is a Sobolev inequality where C is a universal constant. Equation (1.12) follows from the identity, $-\Delta \mathbf{B} = -\nabla(\operatorname{div} \mathbf{B}) + \operatorname{curl}^2 \mathbf{B}$ and integration by parts. The space $\check{\mathbf{H}}(\mathbb{R}^3)$ can be written as the direct sum of orthogonal subspaces, $\check{\mathbf{H}}(\mathbb{R}^3) = \mathbb{V}_1 \oplus \mathbb{V}_2$, where

$$\mathbb{V}_1 = \{\mathbf{B} \in \check{\mathbf{H}}(\mathbb{R}^3) : \operatorname{curl} \mathbf{B} = 0\} = \{\mathbf{B} \in \check{\mathbf{H}}(\mathbb{R}^3) : \mathbf{B} = \nabla f \text{ for some } f \in W^2_{2,loc}(\mathbb{R}^3)\},$$

$$\mathbb{V}_2 = \{\mathbf{B} \in \check{\mathbf{H}}(\mathbb{R}^3) : \operatorname{div} \mathbf{B} = 0\}.$$

See the appendix.

Let $(\psi, \widetilde{\mathbf{A}}, \phi)$ be a solution to (1.5)–(1.10). For each t we decompose $\widetilde{\mathbf{A}}(\cdot, t)$ uniquely as $\widetilde{\mathbf{A}} = \nabla f + \mathbf{g}$ where $\nabla f \in \mathbb{V}_1$ and $\mathbf{g} \in \mathbb{V}_2$. The equations (1.5) and (1.6) only require that ∇f and ϕ be specified on Ω. As such we adopt the convention of giving particular extensions of these functions to $\mathbb{R}^3 \backslash \Omega$. Recall $\partial\Omega \in C^{3+\alpha}$, fix $R > 0$ such that $\bar{\Omega} \subset B_R(0)$. Let $\mathcal{E}: W_2^3(\Omega) \to \mathring{W}_2^3(B_R)$ be the bounded extension operator given in Ref. 6 (p. 170). For $0 \leqslant k \leqslant 2, \mathcal{E}(\cdot)$ has a unique continuous extension

$$\mathcal{E}: W_2^k(\Omega) \to \mathring{W}_2^k(B_R),$$

so that for $0 \leqslant k \leqslant 3$ there is a constant C for which

$$\|\mathcal{E}(u)\|_{\mathring{W}_2^k(B_R)} \leqslant C\|u\|_{W_2^k(\Omega)}$$

for all $u \in W_2^k(\Omega)$.

The space $\check{\mathbf{G}}(\mathbb{R}^3)$ is defined as the subspace of $\check{\mathbf{H}}(\mathbb{R}^3)$ given by

$$\check{\mathbf{G}}(\mathbb{R}^3) = \{\mathbf{B} \in \check{\mathbf{H}}(\mathbb{R}^3) : \mathbf{B} = \nabla \mathcal{E}(f) + \mathbf{g}$$

for some $f \in W_2^2(\Omega)$ with $\int_\Omega f \mathrm{d}x = 0$ and $\mathbf{g} \in \mathbb{V}_2\}$.

In this article $\widetilde{\mathbf{A}}(\cdot, t)$ will be constructed so that $\widetilde{\mathbf{A}} \in \check{\mathbf{G}}(\mathbb{R}^3)$ and ϕ will be understood equaling $\mathcal{E}(\phi) = \mathcal{E}(\phi_{\llcorner \Omega})$.

B. Gauge invariance

The evolution problem (1.5)–(1.10) has multiple solutions, even with the extension convention given above. Indeed, the TDGL equations are *gauge invariant* with respect to the transformation $T_q(\psi, \mathbf{A}, \phi) = (\upsilon, \mathbf{B}, \zeta)$ defined by:

$$\upsilon = \psi e^{iq}, \quad \mathbf{B} = \mathbf{A} + \nabla q, \quad \zeta = \phi - \partial_t q \tag{1.13}$$

for some function q. By this, it is meant that $(\upsilon, \mathbf{B}, \zeta)$ is a solution to (1.5)–(1.7) if $(\psi, \mathbf{A}, \phi)$ is one as well, provided q is sufficiently regular. The two solutions are called *gauge equivalent*. Some quantities that are invariant under a change of gauge are the density $|\psi|^2$, the currents $\mathbf{j}_s = (i\psi, \nabla_{\mathbf{A}}\psi)$ and $\mathbf{j}_n = \sigma(\partial_t \mathbf{A} + \nabla\phi)$, and the magnetic intensity curl $\mathbf{A}$. The function q can be chosen so that $(\upsilon, \mathbb{B}, \zeta)$ satisfies prescribed conditions for the equations, boundary, or initial values. The gauge choices used here are listed below:

(i) The Coulomb gauge,

$$\operatorname{div} \mathbf{B} = 0 \quad \text{in } E_T,$$

here q is chosen to satisfy $\Delta q = -\operatorname{div} \mathbf{A}$ in E_T, and $\int_\Omega q \, dx = 0$ for each t.

(ii) The temporal gauge,

$$\zeta = 0 \quad \text{in } E_T,$$

where q is chosen so that $\partial_t q = \phi$ in E_T, and $q(x,0)$ is such that $\operatorname{div}(\chi_\Omega(\nabla q(x,0) + \mathbf{A}_0(x)) = 0$ in $\mathbb{R}^3$. In this case it will follow that we also have

$$\mathbf{B} \cdot \boldsymbol{\nu} = 0 \quad \text{on } \partial\Omega \times (0,T), \tag{1.14}$$

and

$$\operatorname{div}(\chi_\Omega \mathbf{B}(x,0)) = 0 \quad \text{in } \mathbb{R}^3. \tag{1.15}$$

(iii) The Lorentz gauge,

$$\operatorname{div} \mathbf{B} + \sigma\xi = 0 \quad \text{in } D_T,$$

here q is defined on E_T so that

$$\sigma \partial_t q - \Delta q = \operatorname{div} \mathbf{A} + \sigma\phi \quad \text{in } D_T,$$

$$\partial_\nu q = -\mathbf{A} \cdot \boldsymbol{\nu} \quad \text{on } \partial\Omega \times [0,T),$$

$$-\Delta q(x,0) = \operatorname{div} \mathbf{A}(x,0) \quad \text{on } \Omega,$$

and $q = \mathcal{E}(q)$. Moreover $\mathbf{B}$ satisfies (1.14) and (1.15) as well.

C. Results

The TDGL equations are a gradient flow in the $\phi = 0$ gauge, (ii). Using this feature, in Sec. II we prove that the initial value problem has a unique solution. The hypotheses for initial values, $(\psi_0, \mathbf{A}_0)$ in this gauge are as follows:

$\mathfrak{H}$: $\psi_0 \in \mathcal{W}_2^1(\Omega)$ such that $|\psi_0| \leqslant 1$, $(\mathbf{A}_0 - h\mathbf{a}) \in \check{\mathbf{G}}(\mathbb{R}^3)$ such that $\operatorname{curl}^2 \mathbf{A}_0 = 0$ in $\mathbb{R}^3 \backslash \bar{\Omega}$, and $\operatorname{div}(\chi_\Omega \mathbf{A}_0) = 0$ in $\mathbb{R}^3$.

Define the admissible class,

$$\mathfrak{A} = \{(\psi, \mathbf{A}) : |\partial_t \psi|, \quad |\partial_t \mathbf{A}| \in L_2(D_T), \quad \psi \in L_\infty((0,T); \mathcal{W}_2^1(\Omega)),$$

$$(\mathbf{A} - h\mathbf{a}) \in L_\infty((0,T); \dot{\check{\mathbf{G}}}(\mathbb{R}^3)), \quad \psi(0) = \psi_0, \quad \mathbf{A}(0) = \mathbf{A}_0 \quad \text{in } \Omega\}.$$

Using (ii) the problem becomes

$$\partial_t \psi - \nabla_{\mathbf{A}}^2 \psi + \kappa^2(|\psi|^2 - 1)\psi = 0 \quad \text{in } D_T, \tag{1.16}$$

$$\sigma \chi_\Omega \partial_t \mathbf{A} + \operatorname{curl}^2 \mathbf{A} = \chi_\Omega (i\psi, \nabla_{\mathbf{A}} \psi) \quad \text{in } E_T, \tag{1.17}$$

$$(\mathbf{A} - h\mathbf{a}) \in \check{\mathbf{G}}(\mathbb{R}^3) \quad \text{for } 0 \leqslant t < T, \tag{1.18}$$

$$\partial_{\boldsymbol{\nu}} \psi = 0, \ \mathbf{A} \cdot \boldsymbol{\nu} = 0 \quad \text{on } \partial\Omega \times (0,T), \tag{1.19}$$

$$\psi(x,0) = \psi_0(x) \quad \text{in } \Omega, \quad \mathbf{A}(x,0) = \mathbf{A}_0(x) \quad \text{in } \mathbb{R}^3. \tag{1.20}$$

We say that $(\psi,\mathbf{A})\in\mathfrak{A}$ is a *weak solution* to (1.16)–(1.20) if $(\psi,\mathbf{A}-\mathbf{ha})$ satisfies (2.12) and (2.13).

Theorem 1: *Let* $(\psi_0,\mathbf{A}_0)$ *satisfy* $\mathfrak{H}$. *Then there exists a unique weak solution to (1.16)–(1.20) in* $\mathfrak{A}$. *Moreover* $(\psi,\mathbf{A})$ *satisfies*

$$(\psi(t),\mathbf{A}(t)-h\mathbf{a})\to(\psi_0,\mathbf{A}_0-h\mathbf{a})\quad \text{as } t\downarrow 0\quad \text{in } \mathcal{W}_2^1(\Omega)\times\check{\mathbf{G}}(\mathbb{R}^3). \tag{1.21}$$

In Sec. III, this solution is transformed to the $\operatorname{div}\mathbf{A}=-\sigma\phi$ gauge, (iii) where the equations have a parabolic structure in D_T,

$$\partial_t\psi-\frac{i}{\sigma}(\operatorname{div}\mathbf{A})\psi-\nabla_{\mathbf{A}}^2\psi+\kappa^2(|\psi|^2-1)\psi=0\quad \text{in } D_T \tag{1.22}$$

$$\sigma\chi_\Omega\left(\partial_t\mathbf{A}-\frac{1}{\sigma}\nabla(\operatorname{div}\mathbf{A})\right)+\operatorname{curl}^2\mathbf{A}=\chi_\Omega(i\psi,\nabla_{\mathbf{A}}\psi)\quad \text{in } E_T, \tag{1.23}$$

$$(\mathbf{A}(t)-h\mathbf{a})\in\check{\mathbf{G}}(\mathbb{R}^3)\quad \text{for } 0\leqslant t<T, \tag{1.24}$$

$$\partial_{\boldsymbol{\nu}}\psi=0,\quad \mathbf{A}\cdot\boldsymbol{\nu}=0\quad \text{on } \partial\Omega\times(0,T), \tag{1.25}$$

$$\psi(x,0)=\psi_0(x)\quad \text{in } \Omega,\quad \mathbf{A}(x,0)=\mathbf{A}_0(x)\quad \text{in } \mathbb{R}^3. \tag{1.26}$$

Theorem 2: *Assume* $\partial\Omega\in C^{k+\alpha}$ *where k is an integer,* $k\geqslant 3$. *If* $(\psi_0,\mathbf{A}_0)$ *satisfies* $\mathfrak{H}$ *then there exists a unique solution to (1.22)–(1.26) among functions satisfying* $(\psi,\mathbf{A})\in\mathfrak{A}$ *and* $\nabla(\operatorname{div}\mathbf{A})\in\mathbf{L}_2(D_T)$. *The solution is such that*

$$\psi\in C^\infty((0,T);\mathcal{C}^{k+\alpha}(\bar{\Omega})), \tag{1.27}$$

for any $r>0$ *and* $0<\gamma<1$

$$(\mathbf{A}-h\mathbf{a})\in C^\infty((0,T);\mathbf{C}^{1+\gamma}(\bar{B}_r)),$$

and writing $\mathbf{A}=\nabla f+\mathbf{g}$ *where* $\int_\Omega f\,dx=0$, *with* $\nabla f\in\mathbb{V}_1$ *and* $\mathbf{g}=(g_1,g_2,g_3)\in\mathbb{V}_2$, *it holds that*

$$f,g_j\in C^\infty((0,T);C^{k+\alpha}(\bar{\Omega}))\cap C^\infty((0,T);C^{k+\alpha}(\bar{B}_r\setminus\Omega)). \tag{1.28}$$

In addition $(\psi,\mathbf{A})$ *satisfies (1.21).*

Note, it follows that

$$\mathbf{A}\in C^\infty((0,T);\mathbf{C}^{k-1+\alpha}(\bar{\Omega}))\cap C^\infty((0,T);\mathbf{C}^{k-1+\alpha}(\bar{B}_r\setminus\Omega)).$$

Solutions that are regular up to the boundary in the sense of (1.27) and (1.28) are called *classical*. Thus the solution found in Theorem 2 is classical for $t>0$ and the transmission condition at the material-vacuum boundary, $\mathbf{j}_n\cdot\boldsymbol{\nu}=\mathbf{j}_s\cdot\boldsymbol{\nu}=0$ holds pointwise. Further, the gauge invariant terms $|\psi|^2$, $\mathbf{j}_s$, $\mathbf{j}_n$, and $\operatorname{curl}\mathbf{A}$ are regular up to $\partial\Omega$ as well.

In Sec. IV, we describe the solution in the $\phi=0$ gauge in more detail and discuss the case of the $\operatorname{div}\mathbf{A}=0$ gauge. We prove

Theorem 3: *Let* $(\psi,\mathbf{A})$ *be the solution from Theorem 1. Then there is a classical solution to (1.16)–(1.19),* $(v,\mathbf{B})$ *and a function* $q\in\mathring{W}_2^2(B_R)$ *so that* $(\psi,\mathbf{A})=(ve^{iq},\mathbf{B}+\nabla q)$.

Thus solutions in the $\phi=0$ gauge are classical for $t>0$ up to a steady state gauge transformation. For the $\operatorname{div}\mathbf{A}=0$ gauge, we have

Theorem 4: *Let* $\psi_0\in\mathcal{W}_2^1(\Omega)$, $|\psi_0|\leqslant 1$, *and* $(\mathbf{A}_0-h\mathbf{a})\in\mathbb{V}_2$ *such that*

$$\operatorname{curl}^2 \mathbf{A}_0 = 0 \quad \text{in } \mathbb{R}^3 \setminus \bar{\Omega}.$$

Assume $\partial\Omega \in C^{k+\alpha}$ *for some integer* $k \geqslant 3$. *Then there is a unique solution* $(\psi, \mathbf{A}, \phi)$ *to (1.5)–(1.10) among functions that are classical for* $t > 0$, *for which* $\operatorname{div} \mathbf{A} = 0$ *in* E_T, $\phi = \mathcal{E}(\phi)$ *in* $\mathbb{R}^3 \setminus \Omega$, *and such that*

$$(\psi(t), \mathbf{A}(t) - h\mathbf{a}) \to (\psi_0, \mathbf{A}_0 - h\mathbf{a}) \quad \text{in } \mathcal{W}_2^1(\Omega) \times \mathbb{V}_2 \quad \text{as } t \downarrow 0.$$

D. Earlier work

Prior work proving existence, uniqueness, and regularity results for the TDGL equations, modeling a superconducting body in a vacuum, has been done in two dimensions. In this case Ω represents the cross section of an infinitely long cylinder with its generator parallel to the applied magnetic field $h\mathbf{e}_3$. The equations reduce to an evolution problem on the domain Ω with prescribed boundary conditions. See Refs. 1–4 and 9. The main difference between dimensions $d = 2$ and 3 is that for $d = 2$ the magnetic field is constant in the vacuum. Indeed, the interface condition at $\partial\Omega$ implied by Maxwell's equation (1.3) is the transmission condition

$$[\operatorname{curl} \mathbf{A}] \wedge \boldsymbol{\nu} = 0, \tag{1.29}$$

here $[f] := f_{\text{vac}} - f_\Omega$. For $d = 2$ one has $\operatorname{curl} \mathbf{A} = h\mathbf{e}_3$ in $\mathbb{R}^2 \setminus \Omega$ and furthermore (1.29) reduces to $[\operatorname{curl} \mathbf{A}] = 0$. Thus for two dimensions (1.29) is equivalent to the prescribed boundary condition

$$\operatorname{curl} \mathbf{A} = h\mathbf{e}_3 \quad \text{on } \partial\Omega. \tag{1.30}$$

In Refs. 1, 4, and 9 the same methods are applied to a problem for $d = 3$ where (1.29) is formally replaced with the boundary condition

$$\operatorname{curl} \mathbf{A} \wedge \boldsymbol{\nu} = h\mathbf{e}_3 \wedge \boldsymbol{\nu} \quad \text{on } \partial\Omega. \tag{1.31}$$

This can be viewed as a combined approximation to (1.29) and (1.30), and leads to a well posed evolution problem for the TDGL equations on Ω with prescribed boundary conditions. We treat the full problem here and this is the main contribution of the article.

II. THE TEMPORAL GAUGE

We begin by constructing a discrete (in t) version of (1.1) and (1.2) for the $\phi = 0$ gauge, (i). This is known as Rothe's method (see Ref. 8) and is used in Ref. 3 to prove existence of solutions to discrete TDGL equations in two dimensions. Here however the problem is defined on all space and requires a different proof. Fix $\tau > 0$, $\hat{\upsilon} \in \mathcal{W}_2^1(\Omega)$ such that $|\hat{\upsilon}| \leqslant 1$, $\hat{\mathcal{S}} \in \check{\mathbf{H}}(\mathbb{R}^2)$ and consider the energy

$$I(\upsilon, \mathbf{S}) := I(\upsilon, \mathbf{S}; \hat{\upsilon}, \hat{\mathbf{S}}) = \frac{1}{\tau}\int_\Omega (|\upsilon - \hat{\upsilon}|^2 + \sigma|\mathbf{S} - \hat{\mathbf{S}}|^2)\mathrm{d}x + \int_\Omega \left(|\nabla_{(\mathbf{S}+h\mathbf{a})}\upsilon|^2 + \frac{\kappa^2}{2}(|\upsilon|^2 - 1)^2 \right)\mathrm{d}x$$
$$+ \int_{\mathbb{R}^3} |\operatorname{curl} \mathbf{S}|^2 \mathrm{d}x.$$

Set $\mathbb{B} = \mathcal{W}_2^1(\Omega) \times \check{\mathbf{H}}(\mathbb{R}^3)$.

Proposition 1: The energy I has a minimizer $(\upsilon, \mathbf{S}) \in \mathbb{B}$ *such that* $|\upsilon| \leqslant 1$ *and* $\mathbf{S} \in \check{\mathbf{G}}(\mathbb{R}^3)$.

Proof: Let $\{(\upsilon_n, \mathbf{S}_n)\} \subset \mathbb{B}$ be a minimizing sequence for I. Set

$$\bar{v}_n = \begin{cases} v_n & \text{if } |v_n| \leqslant 1 \\ v_n/|v_n| & \text{if } |v_n| > 1 \end{cases}.$$

Then $I(\bar{v}_n, \mathbf{S}_n) \leqslant I(v_n, \mathbf{S}_n)$ with a strict inequality if $|\{x \in \Omega : |v_n(x)| > 1\}| > 0$. Indeed, fix $x_0 \in \Omega$ and assume without loss of generality that $v_n(x_0) \in \mathbb{R}$. Writing $\hat{v}(x_0) = \hat{v}_1 + i\hat{v}_2$ then

$$|v_n(x_0) - \hat{v}(x_0)|^2 = (v_n(x_0) - \hat{v}_1)^2 + (\hat{v}_2)^2.$$

Using $|\hat{v}| \leqslant 1$ it follows directly that

$$(\bar{v}_n(x_0) - \hat{v}_1)^2 \leqslant (v_n(x_0) - \hat{v}_1)^2$$

with equality if and only if $|v_n(x_0)| \leqslant 1$. The other terms in the integrand for I are nonincreasing when v is replaced by $\bar{v}_n$ as well. To see this for the first term we write $v_n = |v_n| v_n'$ then

$$|\nabla_{(\mathbf{S}_n + h\mathbf{a})} v_n|^2 = |\nabla |v_n||^2 + |v_n|^2 |\nabla v_n' - A|^2$$

and it follows that $|\nabla_{(\mathbf{S}_n + h\mathbf{a}_n)} \bar{v}_n|^2 \leqslant |\nabla_{(\mathbf{S}_n + h\mathbf{a})} v_n|^2$. Thus we may assume that $|v_n| \leqslant 1$ in Ω.

We next write $\mathbf{S}_n = \nabla f_n + \mathbf{g}_n$ where $\mathbf{g}_n \in \mathbb{V}_2$ and $\nabla f_n \in \mathbb{V}_1$ with $\int_\Omega f_n \mathrm{d}x = 0$. Passing to a subsequence, we can assume that $v_n \rightharpoonup v_0$ in $\mathcal{W}_2^1(\Omega)$, $f_n \rightharpoonup f_0$ in $\mathcal{W}_2^1(\Omega)$, and $\mathbf{g}_n \rightharpoonup \mathbf{g}_0 \in \check{\mathbf{H}}(\mathbb{R}^3)$. Since $|v_n| \leqslant 1$ it follows that $\nabla_{(\mathbf{S}_n + h\mathbf{a})} v_n \rightharpoonup \nabla_{(\mathbf{S}_0 + h\mathbf{a})} v_0$ in $\mathcal{L}_2(\Omega)$. Note that the energy $I(v, \nabla f + \mathbf{g})$ is well defined for $v \in \mathcal{W}_2^1(\Omega) \cap \mathcal{L}_\infty(\Omega)$, $f \in W_2^1(\Omega)$, and $\mathbf{g} \in \mathbb{V}_2$. We have by weak lower semi-continuity that

$$I(v_0, \nabla f_0 + \mathbf{g}_0) \leqslant \lim_{n \to \infty} I(v_n, \mathbf{S}_n) = \inf_{(v, \mathbf{S}) \in \mathbb{B}} I(v, \mathbf{S}).$$

We in fact have

$$I(v_0, \nabla f_0 + \mathbf{g}_0) \leqslant I(v_0, \nabla (f_0 + k) + \mathbf{g}_0) \tag{2.1}$$

and

$$I(v_0, \nabla f_0 + \mathbf{g}_0) \leqslant I(v_0 e^{ik}, \nabla f_0 + \mathbf{g}_0) \tag{2.2}$$

for any $k(x) \in C^2(\bar{\Omega})$. To prove (2.1), we assume that it is false for some k. Then since the integrand is a polynomial, we expand it to write

$$I(v, \nabla (f + k) + \mathbf{g}) = I(v, \nabla f + \mathbf{g}) + \mathcal{I}(v, \nabla f, \mathbf{g}, k),$$

where $\lim_{n \to \infty} \mathcal{I}(v_n, \nabla f_n, \mathbf{g}_n, k) = \mathcal{I}(v_0, \nabla f_0, \mathbf{g}_0, k)$. Our assumption is that $\mathcal{I}(v_0, \nabla f_0, \mathbf{g}_0, k) = \beta < 0$, so for n sufficiently large we have $\mathcal{I}(v_n, \nabla f_n, \mathbf{g}_n, k) \leqslant \beta/2$. This implies that

$$I(v_n, \nabla \mathcal{E}(f_n + k) + \mathbf{g}_n) \leqslant I(v_n, \nabla f_n + \mathbf{g}_n) + \frac{\beta}{2},$$

and contradicts the assumption that $\{(v_n, \mathbf{S}_n)\}$ is a minimizing sequence. The inequality (2.2) is proved in the same way.

We will show that $f_0 \in W_2^2(\Omega)$. The proof will then be complete since this implies that

$$I(v_0, \nabla \mathcal{E}(f_0) + \mathbf{g}_0) = I(v_0, \nabla f_0 + \mathbf{g}_0) \leqslant \inf_{(v, \mathbf{S}) \in \mathbb{B}} I(v, \mathbf{S})$$

with $\nabla \mathcal{E}(f_0) + \mathbf{g}_0 \in \check{\mathbf{G}}(\mathbb{R}^3)$.

From (2.1) and (2.2) we have

$$0 = \partial_\varepsilon I(v_0, \nabla f_0 + \varepsilon \nabla k + \mathbf{g}_0)|_{\varepsilon = 0},$$

and

$$0 = \partial_\varepsilon I(v_0 e^{i\epsilon k}, \nabla f_0 + \mathbf{g}_0)|_{\varepsilon=0}.$$

These lead to

$$\frac{\sigma}{\tau}(\Delta f_0 - \operatorname{div} \hat{\mathbf{S}}) = \operatorname{div}(iv_0, \nabla v_0 - i(\nabla f_0 + \mathbf{g}_0)v_0) = \frac{1}{\tau}(iv_0, v_0 - \hat{v}) \quad \text{in } \Omega,$$

$$\partial_{\boldsymbol{\nu}} f_0 - (\hat{\mathbf{S}} - \mathbf{g}_0) \cdot \boldsymbol{\nu} = (iv_0, \nabla v_0 - i(\nabla f_0 + \mathbf{g}_0)v_0) \cdot \boldsymbol{\nu} = 0 \quad \text{on } \partial\Omega.$$

Since $(iv_0, v_0 - \hat{v}) \in L_2(\Omega)$ and $\hat{\mathbf{S}}, \mathbf{g}_0 \in \mathbf{W}_2^1(\Omega)$ it follows from elliptic estimates that $f_0 \in W_2^2(\Omega)$.□

Let $(v_0, \mathbf{S}_0 + h\mathbf{a})$ satisfy $\mathfrak{H}$. Fix an integer M and set $\tau = T/M$. For $1 \leqslant m \leqslant M$ we let $\{(v_m, \mathbf{S}_m)\} \subset \mathcal{W}_2^1(\Omega) \times \check{\mathbf{G}}(\mathbb{R}^3)$ be a family of minimizers for

$$I_m(v, \mathbf{S}) = I(v, \mathbf{S}; v_{m-1}, \mathbf{S}_{m-1}).$$

We write

$$\delta_\tau v_m(x) = \frac{v_m - v_{m-1}}{\tau}$$

and a similar definition for $\delta_\tau \mathbf{S}_m$. Next we derive

$$0 = \frac{1}{2}\partial_\varepsilon I_m\,(v_m + \varepsilon\zeta, \mathbf{S}_m)|_{\varepsilon=0} = \int_\Omega (\delta_\tau v_m + \kappa^2 v_m(|v_m|^2 - 1), \zeta)\mathrm{d}x + \int_\Omega (\nabla_{(\mathbf{S}_m + h\mathbf{a})} v_m, \nabla_{(\mathbf{S}_m + h\mathbf{a})}\zeta)\mathrm{d}x \tag{2.3}$$

$$0 = \frac{1}{2}\partial_\varepsilon I_m\,(v_m, \mathbf{S}_m + \varepsilon\mathbf{B})|_{\varepsilon=0} = \int_\Omega \sigma\delta_\tau \mathbf{S}_m \cdot \mathbf{B}\mathrm{d}x + \int_{\mathbb{R}^3} \operatorname{curl} \mathbf{S}_m \cdot \operatorname{curl} \mathbf{B}\mathrm{d}x - \int_\Omega (iv_m, \nabla_{(\mathbf{S}_m + h\mathbf{a})} v_m) \cdot \mathbf{B}\mathrm{d}x \tag{2.4}$$

for $\zeta \in \mathcal{W}_2^1(\Omega)$, $\mathbf{B} \in \check{\mathbf{H}}(\mathbb{R}^3)$, and $1 \leqslant m \leqslant M$.

Thus we have weak solutions to the iterative system:

$$\delta_\tau v_m - \nabla^2_{(\mathbf{S}_m + h\mathbf{a})} v_m + \kappa^2 v_m(|v_m|^2 - 1) = 0 \quad \text{in } \Omega \tag{2.5}$$

$$\sigma\chi_\Omega \delta_\tau \mathbf{S}_m + \operatorname{curl}^2 \mathbf{S}_m = \chi_\Omega \mathbf{J}_m \quad \text{in } \mathbb{R}^3, \tag{2.6}$$

$$\nabla_{(\mathbf{S}_m + h\mathbf{a})} v_m \cdot \boldsymbol{\nu} = 0 \quad \text{on } \partial\Omega, \tag{2.7}$$

$$\mathbf{S}_m \in \check{\mathbf{G}}(\mathbb{R}^3), \tag{2.8}$$

where $\mathbf{J}_m = (iv_m, \nabla_{(\mathbf{S}_m + h\mathbf{a})} v_m)$.

We set

$$G(v, \mathbf{S}) = \int_\Omega \left[|\nabla_{(\mathbf{S} + h\mathbf{a})} v|^2 + \frac{\kappa^2}{2}(|v|^2 - 1)^2 \right] \mathrm{d}x + \int_{\mathbb{R}^3} |\operatorname{curl} \mathbf{S}|^2 \mathrm{d}x \tag{2.9}$$

where G is the Ginzburg–Landau free energy. Thus

$$I_m(\upsilon,\mathbf{S}) = \frac{1}{\tau}\int_\Omega [|\upsilon-\upsilon_{m-1}|^2 + \sigma|\mathbf{S}-\mathbf{S}_{m-1}|^2]\mathrm{d}x + G(\upsilon,\mathbf{S}).$$

The next lemma characterizes energy dissipation along the sequence of minimizers.

Lemma 1: For $1\leqslant m\leqslant M$

$$\sum_{n=1}^{m} \tau\{\|\delta_\tau\upsilon_n\|^2_{\mathcal{L}^2(\Omega)} + \sigma\|\delta_\tau\mathbf{S}_n\|^2_{\mathbf{L}_2(\Omega)}\} + G(\upsilon_m,\mathbf{S}_m) \leqslant G(\upsilon_0,\mathbf{S}_0). \tag{2.10}$$

Proof: Since $(\upsilon_m,\mathbf{S}_m)$ is a minimizer for I_m we find

$$G(\upsilon_m,\mathbf{S}_m) \leqslant I_m(\upsilon_m,\mathbf{S}_m) \leqslant I_m(\upsilon_{m-1},\mathbf{S}_{m-1}) = G(\upsilon_{m-1}\mathbf{S}_{m-1}).$$

Next we add the $(m-1)$st difference quotient to the second and fourth terms mentioned above. We have

$$\sum_{n=m-1}^{m} \tau\{\|\delta_\tau\upsilon_n\|^2_{\mathcal{L}_2(\Omega)} + \sigma\|\delta_\tau\mathbf{S}_n\|^2_{\mathbf{L}_2(\Omega)}\} + G(\upsilon_m,\mathbf{S}_m) \leqslant \tau\{\|\delta_\tau\upsilon_{m-1}\|^2_{\mathcal{L}_2(\Omega)} + \sigma\|\delta_\tau\mathbf{S}_{m-1}\|^2_{\mathbf{L}_2(\Omega)}\} + G(\upsilon_{m-1},\mathbf{S}_{m-1})$$

$$= I_{m-1}(\upsilon_{m-1},\mathbf{S}_{m-1}).$$

Our assertion follows after repeating this argument $m-2$ times. □

Corollary 1:

$$\max_{1\leqslant m\leqslant M} \{\|\mathbf{S}_m\|^2_{\mathbf{L}_2(\Omega)} + \|\nabla\upsilon_m\|^2_{\mathcal{L}_2(\Omega)} + \|\mathrm{curl}\ \mathbf{S}_m\|^2_{\mathbf{L}_2(\mathbb{R}^3)}\} \leqslant C \tag{2.11}$$

where C *depends on* $\|\mathbf{S}_0\|^2_{\check{\mathbf{H}}(\mathbb{R}^3)}$, $\|\nabla\upsilon_0\|^2_{\mathcal{L}_2(\Omega)}$, h, and T.

Proof: For $1\leqslant m\leqslant M$

$$\|\mathbf{S}_m\|^2_{\mathbf{L}_2(\Omega)} - \|\mathbf{S}_0\|^2_{\mathbf{L}_2(\Omega)} = \sum_{n=1}^{m}\tau\int_\Omega \delta_\tau|\mathbf{S}_n|^2\mathrm{d}x \leqslant \sum_{n=1}^{m}\tau\|(\mathbf{S}_n+\mathbf{S}_{n-1})\cdot\delta_\tau\mathbf{S}_n\|_{\mathbf{L}_1(\Omega)}$$

$$\leqslant \frac{1}{2}\max_{1\leqslant n\leqslant m}\|\mathbf{S}_n\|^2_{\mathbf{L}_2(\Omega)} + 4T\sum_{n=1}^{m}\tau\|\delta_\tau\mathbf{S}_n\|^2_{\mathbf{L}_2(\Omega)}.$$

We take the maximum of the left side over $1\leqslant m\leqslant M$ and use (2.10).

Next note that

$$\frac{1}{2}\|\nabla\upsilon_m\|^2_{\mathcal{L}_2(\Omega)} + \|\mathrm{curl}\ \mathbf{S}_m\|^2_{\mathbf{L}_2(\mathbb{R}^3)} \leqslant G(\upsilon_m,\mathbf{S}_m) + 2\|\mathbf{S}_m\|^2_{\mathbf{L}_2(\Omega)} + h^2C$$

for some constant $C(\Omega)$. The assertion follows from these estimates and Lemma 1. □

Lemma 2:

$$\max_{1\leqslant m\leqslant M}\|\mathbf{S}_m\|^2_{\check{\mathbf{H}}(\mathbb{R}^3)} \leqslant C$$

where C *depends on* $\|\mathbf{S}_0\|^2_{\check{\mathbf{H}}(\mathbb{R}^3)}$, $\|\nabla\upsilon_0\|^2_{\mathcal{L}_2(\Omega)}$, h, *and* T.

Proof: From (1.12) we have

$$\|\mathbf{S}_m\|^2_{\check{\mathbf{H}}(\mathbb{R}^3)} = \|\mathrm{div}\ \mathbf{S}_m\|^2_{L_2(\mathbb{R}^3)} + \|\mathrm{curl}\ \mathbf{S}_m\|^2_{\mathbf{L}_2(\mathbb{R}^3)}$$

and from (2.11) we see that it suffices to bound $\|\mathrm{div}\ \mathbf{S}_m\|^2_{L_2(\mathbb{R}^3)}$. Since $\mathbf{S}_m\in\check{\mathbf{G}}(\mathbb{R}^3)$, we have $\mathbf{S}_m = \nabla f_m + \mathbf{g}_m$ where $\mathbf{g}_m\in\mathbb{V}_2$ and $f_m = \mathcal{E}(f_{m\llcorner\Omega})\in\mathring{W}^2_2(B_R)$. Thus

$$\|\operatorname{div} \mathbf{S}_m\|^2_{L_2(\mathbb{R}^3)} = \|\Delta f_m\|^2_{L_2(\mathbb{R}^3)} \leqslant C\|f_m\|^2_{W_2^2(\Omega)}.$$

To estimate the right-hand side we use $\zeta = i\upsilon_m k$, with $k \in C^2(\bar{\Omega})$, as a test function in (2.3). We get

$$\chi_\Omega(i\upsilon_m, \delta_\tau \upsilon_m) = \operatorname{div}(\chi_\Omega \mathbf{J}_m) \quad \text{in } \mathcal{D}'(\mathbb{R}^3).$$

Taking the divergence of (2.6) then gives

$$\sigma \operatorname{div}(\chi_\Omega \delta_\tau \mathbf{S}_m) = \operatorname{div}(\chi_\Omega \mathbf{J}_m) \quad \text{in } \mathcal{D}'(\mathbb{R}^3).$$

Comparing these equalities we see

$$\|\operatorname{div}(\delta_\tau \mathbf{S}_m)\|^2_{L_2(\Omega)} \leqslant \sigma^{-2}\|\delta_\tau \upsilon_m\|^2_{\mathcal{L}_2(\Omega)}$$

and

$$\delta_\tau \mathbf{S}_m \cdot \boldsymbol{\nu} = 0 \quad \text{on } \partial\Omega.$$

Now $\mathbf{S}_m = \Sigma_{n=1}^m \tau \delta_\tau \mathbf{S}_n + \mathbf{S}_0$. Since $\mathbf{S}_0 + h\mathbf{a}$ satisfies $\mathfrak{H}$ we find

$$\|\Delta f_m\|^2_{L_2(\Omega)} = \|\operatorname{div} \mathbf{S}_m\|^2_{L_2(\Omega)} \leqslant \frac{T}{\sigma^2}\sum_{n=1}^m \tau\|\delta_\tau \upsilon_n\|^2_{\mathcal{L}_2(\Omega)},$$

and

$$\partial_\nu f_m = -\mathbf{g}_m \cdot \boldsymbol{\nu} + \mathbf{S}_0 \cdot \boldsymbol{\nu} \quad \text{on } \partial\Omega.$$

Since f_m has mean zero it follows from elliptic estimates that

$$\|f_m\|^2_{W_2^2(\Omega)} \leqslant \Lambda(\|\Delta f_m\|^2_{L_2(\Omega)} + \|\mathbf{g}_m\|^2_{\mathbf{W}_2^1(\Omega)} + \|\mathbf{S}_0\|^2_{\mathbf{W}_2^1(\Omega)}).$$

Using (2.10) and the fact that $\|\mathbf{g}_m\|^2_{\mathbf{W}_2^1(\Omega)} \leqslant C\|\mathbf{g}_m\|^2_{\check{\mathbf{H}}(\mathbb{R}^3)}$ we see that $\|f_m\|^2_{W_2^2(\Omega)} \leqslant C$ where C depends on $\|\mathbf{S}_0\|_{\check{\mathbf{H}}(\mathbb{R}^3)}$, $\|\nabla \upsilon_0\|_{\mathcal{L}_2(\Omega)}$, h and T. □

We now consider a limit as $\tau \to 0$ and pass to the continuous problem. Set

$$\upsilon_\tau(x,t) = \frac{(t-(m-1)\tau)}{\tau}\upsilon_m(x) + \frac{(m\tau - t)}{\tau}\upsilon_{m-1}(x)$$

for $t \in [(m-1)\tau, m\tau]$, and a corresponding interpolate $\mathbf{S}_\tau$. We have $|\upsilon_m| \leqslant 1$, uniform bounds on $\{\upsilon_\tau\}$ in $\mathcal{L}_\infty((0,T);\mathcal{W}_2^1(\Omega)) \cap \mathcal{W}_2^{0,1}(D_T)$. Thus a subsequence $\{\upsilon_{\tau_j}\}$ converges weakly to $\upsilon \in \mathcal{W}_2^{1,1}(D_T)$. Similarly $\{\mathbf{S}_\tau\}$ is uniformly bounded in

$$L_\infty((0,T);\check{\mathbf{G}}(\mathbb{R}^3)) \cap \mathbf{W}_2^{0,1}(D_T) \text{ and for a}$$

further a subsequence $\mathbf{S}_{\tau_j} \rightharpoonup \mathbf{S} \in L^2((0,T);\check{\mathbf{G}}(\mathbb{R}^3)) \cap \mathbf{W}_2^{1,1}(D_T)$.

We now pass to the limit as $\tau_j \to 0$ in the variational forms (2.3) and (2.4), assuming initially that the test functions are smooth, multiplying each equation by τ_j, summing over m, and estimating the difference between the functions that are piecewise constant in t and the interpolates.

We find in weak form, $(\upsilon, \mathbf{S})$ is a solution to

$$\int_{D_T} [(\partial_t \upsilon, \zeta) + (\nabla_{(\mathbf{S}+h\mathbf{a})}\upsilon, \nabla_{(\mathbf{S}+h\mathbf{a})}\zeta) + \kappa^2(\upsilon(|\upsilon|^2 - 1), \zeta)]\mathrm{d}x\mathrm{d}t = 0, \tag{2.12}$$

$$\int_{D_T} [\sigma \partial_t \mathbf{S} \cdot \mathbf{B} - \mathbf{j}_s \cdot \mathbf{B}] \mathrm{d}x\mathrm{d}t + \int_{E_T} \operatorname{curl} \mathbf{S} \cdot \operatorname{curl} \mathbf{B}\, \mathrm{d}x\mathrm{d}t = 0 \tag{2.13}$$

for every $\zeta \in L^2((0,T);\mathcal{W}_2^1(\Omega))$ and $\mathbf{B} \in L^2((0,T);\check{\mathbf{H}}(\mathbb{R}^3))$, such that $\mathbf{S}(x,0)=\mathbf{S}_0(x)$ and $\upsilon(x,0)=\upsilon_0(x)$ in Ω. The estimates from Lemmas 1 and 2 extend to the limit $(\upsilon,\mathbf{S})$. We have

$$|\upsilon| \leqslant 1 \quad \text{in } D_T,$$

$$\sup_{0\leqslant t\leqslant T} \{\|\nabla \upsilon\|_{\mathcal{L}_2(\Omega)} + \|\mathbf{S}\|_{\check{\mathbf{H}}(\mathbb{R}^3)}\} \leqslant C, \tag{2.14}$$

and

$$(\|\partial_t \upsilon\|^2_{\mathcal{L}_2(D_T)} + \sigma \|\partial_t \mathbf{S}\|^2_{\mathbf{L}_2(D_T)}) + \sup_{0\leqslant t\leqslant T} G(\upsilon(t),\mathbf{S}(t)) \leqslant G(\upsilon_0,\mathbf{S}_0), \tag{2.15}$$

where C depends on $\|\nabla \upsilon_0\|_{\mathcal{L}_2(\Omega)}$, $\|\mathbf{S}_0\|_{\check{\mathbf{H}}(\mathbb{R}^3)}$, h, and T.

We next analyze div $\mathbf{S}$.

Lemma 3: div $\mathbf{S} \in W_2^{0,1}(D_T)$ *with*

$$\|\operatorname{div}(\partial_t \mathbf{S})\|_{L_2(D_T)} \leqslant C$$

where C *depends on* $\|\nabla \upsilon_0\|_{\mathcal{L}_2(\Omega)}\|$, $\|\mathbf{S}_0\|_{\check{\mathbf{H}}(\mathbb{R}^3)}$, T, *and* h. *Moreover* $(\mathbf{S}+h\mathbf{a})\cdot\boldsymbol{\nu}=0$ *on* $\partial\Omega$ *for* $0\leqslant t<T$.

Proof: Let $k \in C_c^2(\bar{E}_T)$. Take $\zeta = i\upsilon k$ and $\mathbf{B}=\nabla k$ in (2.12) and (2.13), respectively. We obtain

$$\chi_\Omega(\partial_t \upsilon, i\upsilon) = \operatorname{div}(\chi_\Omega \mathbf{j}_s) = \sigma \operatorname{div}(\chi_\Omega \partial_t \mathbf{S}) \quad \text{in } \mathcal{D}'(\bar{E}_T).$$

Using (2.15) we see

$$\|(\partial_t \upsilon, i\upsilon)\|_{L_2(D_T)} \leqslant C$$

and it follows that div $\partial_t \mathbf{S} \in L_2(D_T)$ with $\|\operatorname{div} \partial_t \mathbf{S}\|_{L_2(D_T)} \leqslant C$ depending on the initial data, T and h. Finally letting $k=k(x)$ and integrating over E_t for $0<t<T$ we find

$$\operatorname{div}(\chi_\Omega(\mathbf{S}(t)-\mathbf{S}(0))) \in L_2(\mathbb{R}^3).$$

This implies that $(\mathbf{S}(t)-\mathbf{S}(0))\cdot\boldsymbol{\nu}=0$ on $\partial\Omega$. Thus $(\mathbf{S}(t)+h\mathbf{a})\cdot\boldsymbol{\nu}=(\mathbf{S}(0)+h\mathbf{a})\cdot\boldsymbol{\nu}=0$ on $\partial\Omega$. □

From (2.12) we obtain the boundary condition (1.4). Combining these results gives

$$\partial_{\boldsymbol{\nu}} \upsilon = 0 \quad \text{on } \partial\Omega \text{ for } 0<t<T.$$

We next examine $\mathbf{S}(\cdot,t)$ in $\mathbb{R}^3\backslash\bar{\Omega}$. We have that $\operatorname{curl}^2 \mathbf{S}(\cdot,t)=0$ in $\mathbb{R}^3\backslash\bar{\Omega}$ for almost every t. We next show that this extension from Ω is done in a unique way.

Lemma 4: Let $\mathbf{B} \in \mathbf{W}_2^1(\Omega;\mathbb{R}^3)$. *Then there is a unique* $\bar{\mathbf{B}} \in \check{\mathbf{G}}(\mathbb{R}^3)$ *so that* $\bar{\mathbf{B}}=\mathbf{B}$ *in* Ω and $\operatorname{curl}^2 \bar{\mathbf{B}}=0$ *in* $\mathbb{R}^3\backslash\Omega$.

Proof: Set $C(\mathbf{K})=\int_{\mathbb{R}^3}|\operatorname{curl} \mathbf{K}|^2 \mathrm{d}x$ for $\mathbf{K} \in \{\mathbf{F} \in \check{\mathbf{H}}(\mathbb{R}^3) : \mathbf{F}=\mathbf{B} \text{ in } \Omega\}$ and let $\{\mathbf{K}_n\}$ be a minimizing sequence. We write $\mathbf{K}_n=\nabla f_n+\mathbf{g}_n$ with $\nabla f_n \in \mathbb{V}_1$ such that $\int_\Omega f_n \mathrm{d}x=0$, and $\mathbf{g}_n \in \mathbb{V}_2$. We can replace f_n by $\mathcal{E}(f_{n\llcorner\Omega}) \in W_2^2(B_R)$ and not change the value of $C(\mathbf{K}_n)$. Thus it is without loss of generality to assume that $\{\mathbf{K}_n\} \subset \check{\mathbf{G}}(\mathbb{R}^3)$. Using Mazur's theorem we can assume that $\mathbf{g}_n \to \mathbf{g}$ in $\mathbb{V}_2$ as $n\to\infty$. Since $\mathbf{K}_n=\mathbf{B}$ in Ω we see that $\{\nabla f_n\}$ is a Cauchy sequence in $W_2^1(\Omega)$ and by the construction of $\check{\mathbf{G}}(\mathbb{R}^3)$ it follows that there is an f so that $f_n \to f$ in $\mathring{W}_2^2(B_R)$ as $n\to\infty$. Thus $\mathbf{K}_0 \equiv \nabla f+g \in \check{\mathbf{G}}(\mathbb{R}^3)$ and minimizes $C(\cdot)$.

Clearly $\operatorname{curl}^2 \mathbf{K}_0=0$ in $\mathbb{R}^3\backslash\bar{\Omega}$, so we can set $\bar{\mathbf{B}}=\mathbf{K}_0$.

If there is another extension of $\mathbf{B}$, $\mathbf{K}_1 \in \check{\mathbf{G}}(\mathbb{R}^3)$ such that $\operatorname{curl}^2 \mathbf{K}_1=0$ in $\mathbb{R}^3\backslash\bar{\Omega}$ then

$$\int_{\mathbb{R}^3} |\mathrm{curl}(\mathbf{K}_1 - \mathbf{K}_0)|^2 \mathrm{d}x = \int_{\mathbb{R}^3\setminus\bar{\Omega}} \mathrm{curl}\,\mathbf{K}_1 \cdot \mathrm{curl}(\mathbf{K}_1 - \mathbf{K}_0)\mathrm{d}x - \int_{\mathbb{R}^3\setminus\bar{\Omega}} \mathrm{curl}\,\mathbf{K}_0 \cdot \mathrm{curl}(\mathbf{K}_1 - \mathbf{K}_0)\mathrm{d}x.$$

Since $\mathbf{K}_0 = \mathbf{K}_1$ in Ω and $\mathrm{curl}^2\,\mathbf{K}_1 = \mathrm{curl}^2\,\mathbf{K}_0 = 0$ in $\mathbb{R}^3\setminus\bar{\Omega}$ we see that both integrals on the right-hand side vanish. Thus $\mathrm{curl}\,\mathbf{K}_1 = \mathrm{curl}\,\mathbf{K}_0$. Writing $\mathbf{K}_0 = \nabla f + \mathbf{g}$ and $\mathbf{K}_1 = \nabla f_1 + \mathbf{g}_1$ we have $\mathbf{g}_1 = \mathbf{g}$. This implies that $\nabla f_1 = \nabla f$ in Ω. By the construction of $\check{\mathbf{G}}$ this implies that $f_1 = f$ in $\mathbb{R}^3$ and thus $\mathbf{K}_1 = \mathbf{K}_0$. □

We have $\mathbf{S}(t) \in C([0,T];\mathbf{L}_2(\Omega)) \cap L_\infty((0,T);\check{\mathbf{G}}(\mathbb{R}^3))$. The lemma above implies that the condition $\mathrm{curl}^2\,\mathbf{S}(t) = 0$ in $\mathbb{R}^3\setminus\bar{\Omega}$ uniquely determines $\mathbf{S}(t)$ in $\mathbb{R}^3\setminus\bar{\Omega}$. With this we can give a more specific description of the trace of $(\upsilon, \mathbf{S})$ as $t \downarrow 0$.

Lemma 5:

$$(\upsilon(t), \mathbf{S}(t)) \to (\upsilon_0, \mathbf{S}_0) \quad \textit{in } \mathcal{W}_2^1(\Omega) \times \check{\mathbf{G}}(\mathbb{R}^3) \quad \textit{as } t \downarrow 0. \tag{2.16}$$

Proof: From our construction of $(\upsilon, \mathbf{S})$ and the previous lemma we have $(\upsilon(t), \mathbf{S}(t)) \rightharpoonup (\upsilon_0, \mathbf{S}_0)$ as $t \downarrow 0$ in $\mathcal{W}_2^1(\Omega) \times \check{\mathbf{G}}(\mathbb{R}^3)$. Expanding the integrand of the Ginzburg–Landau energy (2.9) we have

$$G(\upsilon(t), \mathbf{S}(t)) = \int_\Omega |\nabla \upsilon(t)|^2 \mathrm{d}x + \int_{\mathbb{R}^3} |\mathrm{curl}\,\mathbf{S}(t)|^2 \mathrm{d}x + \mathcal{G}(\upsilon(t), \mathbf{S}(t))$$

where $\lim_{t\to 0} \mathcal{G}(\upsilon(t), \mathbf{S}(t)) = \mathcal{G}(\upsilon_0, \mathbf{S}_0)$. From (2.15) we have $\limsup_{t\to 0} G(\upsilon(t), \mathbf{S}(t)) \leqslant G(\upsilon_0, \mathbf{S}_0)$, and from weak lower semicontinuity we have

$$G(\upsilon_0, \mathbf{S}_0) \leqslant \liminf_{t\to 0} G(\upsilon(t), \mathbf{S}(t)).$$

Thus

$$\lim_{t\to 0} \left\{ \int_\Omega |\nabla \upsilon(t)|^2 \mathrm{d}x + \int_{\mathbb{R}^3} |\mathrm{curl}\,\mathbf{S}(t)|^2 \mathrm{d}x \right\} = \int_\Omega |\nabla \upsilon_0|^2 \mathrm{d}x + \int_{\mathbb{R}^3} |\mathrm{curl}\,\mathbf{S}_0|^2 \mathrm{d}x.$$

Writing $\mathbf{S}(t) = \nabla \tilde{f}(t) + \mathbf{g}(t)$ with $\tilde{f}(t) \in \mathring{W}_2^2(B_R)$ and $\mathbf{g}(t) \in \mathbb{V}_2$ we have

$$(\upsilon(t), \mathbf{g}(t)) \to (\upsilon_0, \mathbf{g}_0) \quad \text{in } \mathcal{W}_2^1(\Omega) \times \mathbb{V}_2 \quad \text{as } t \downarrow 0.$$

We write

$$\Delta f(t) = \mathrm{div}\,\mathbf{S}(t) \quad \text{in } \Omega,$$

$$\partial_\nu f(t) = -\mathbf{g}(t) \cdot \boldsymbol{\nu} - h\mathbf{a} \cdot \boldsymbol{\nu} \quad \text{on } \partial\Omega.$$

From Lemma 3 we have $\mathrm{div}\,\mathbf{S}(t) \to \mathrm{div}\,\mathbf{S}_0 = 0$ in $L^2(\Omega)$ and from the preceding argument $\mathbf{g}(t) \to \mathbf{g}_0$ in $\mathbf{W}_2^1(\Omega)$ as $t \to 0$. Thus from elliptic estimates we have $f(t) \to f_0$ in $\mathcal{W}_2^2(\Omega)$ as $t \to 0$. From the definition of $\check{\mathbf{G}}(\mathbb{R}^3)$ we then have $f(t) \to f_0$ in $\mathring{W}_2^2(B_R)$.

Thus

$$(\upsilon(t), \mathbf{S}(t)) \to (\upsilon_0, \mathbf{S}_0) \quad \text{in } \mathcal{W}_2^1(\Omega) \times \check{\mathbf{G}}(\mathbb{R}^3) \quad \text{as } t \downarrow 0.$$

□

We have $(\upsilon, \mathbf{S} + h\mathbf{a}) \in \mathfrak{A}$ with $|\upsilon| \leqslant 1$, satisfying (2.12) and (2.13), and such that (2.16) holds at $t = 0$. It follows that $(\upsilon, \mathbf{S})$ is a weak solution to

$$\partial_t \upsilon - \Delta \upsilon = -2i\nabla \upsilon \cdot (\mathbf{S} + h\mathbf{a}) - i\upsilon\,\mathrm{div}\,\mathbf{S} - |\mathbf{S} + h\mathbf{a}|^2 \upsilon - \kappa^2 \upsilon(|\upsilon|^2 - 1) \quad \text{in } D_T, \tag{2.17}$$

$$\sigma\chi_\Omega\partial_t\mathbf{S}+\operatorname{curl}^2\mathbf{S}=\chi_\Omega\mathbf{j}_s \quad \text{in } E_T, \tag{2.18}$$

$$(\mathbf{S}+h\mathbf{a})\cdot\boldsymbol{\nu}=0 \text{ and } \partial_{\boldsymbol{\nu}}\upsilon=0 \quad \text{on } \partial\Omega\times(0,T), \tag{2.19}$$

$$\upsilon(x,0)=\upsilon_0(x) \quad \text{in } \Omega, \quad \mathbf{S}(x,0)=\mathbf{S}_0(x) \quad \text{in } \mathbb{R}^3. \tag{2.20}$$

Lemma 6: Let $(\upsilon,\mathbf{S}+h\mathbf{a})\in\mathfrak{A}$ *be a weak solution to (2.12) and (2.13), then* $\upsilon\in\mathcal{W}_2^{2,1}(D_T)$.

Proof: Weak solutions to (1.16) with $|\upsilon_0|\leqslant 1$ satisfy $|\upsilon|\leqslant 1$. See Ref. 2. Furthermore we have $\upsilon\in\mathcal{W}_2^{1,1}(D_T)$, and thus (2.17) can be written as

$$\int_{D_T}(\nabla\upsilon,\nabla\zeta)\mathrm{d}x\mathrm{d}t=-\int_{\delta_\tau}(2i\nabla\upsilon\cdot\mathbf{S},\zeta)\mathrm{d}x\mathrm{d}t+\int_{\delta_\tau}(f,\zeta)\mathrm{d}x\mathrm{d}t$$

for $\zeta\in L_2((0,T);\mathcal{W}_2^1(\Omega))$ where $f\in\mathcal{L}_2(D_T)$. We have using (2.14) and (1.11) that

$$\int_{D_T}|\nabla\upsilon\cdot\mathbf{S}|^{3/2}\mathrm{d}x\mathrm{d}t\leqslant\int_{D_T}(|\nabla\upsilon|^2+|\mathbf{S}|^6)\mathrm{d}x\mathrm{d}t<\infty.$$

Setting $f'=-2i\nabla\upsilon\cdot\mathbf{S}+f$ we have $f'\in\mathcal{L}_{3/2}(D_T)$. It follows from elliptic estimates then that $\upsilon(t)\in\mathcal{W}_{3/2}^2(\Omega)$ for almost every $0<t<T$, and satisfies

$$-\Delta\upsilon=f' \quad \text{in } \Omega,$$

$$\partial_{\boldsymbol{\nu}}\upsilon=0 \quad \text{on } \partial\Omega. \tag{2.21}$$

From elliptic estimates then we have

$$\|\upsilon(t)\|_{\mathcal{W}_{3/2}^2(\Omega)}\leqslant C(\|f'(t)\|_{\mathcal{L}_{3/2}(\Omega)}+1).$$

It follows that

$$\|\upsilon\|_{\mathcal{W}_{3/2}^{2,0}(D_T)}\leqslant C(\|f'\|_{\mathcal{L}_{3/2}(D_T)}+1).$$

For almost every $0<t<T$ we apply the Gagliardo-Nirenberg inequality,[10]

$$\|\nabla\upsilon\|_{\mathcal{L}_3(\Omega)}^3\leqslant C\|\upsilon\|_{\mathcal{W}_{3/2}^2(\Omega)}^{3/2}\cdot\|\upsilon\|_{\mathcal{L}_\infty(\Omega)}^{3/2}.$$

Since $|\upsilon|\leqslant 1$ this implies that $\nabla\upsilon\in\mathcal{L}_3(D_T)$. From (1.11) we have $\mathbf{S}\in\mathbf{L}_6(D_T)$ and it follows that $|\nabla\upsilon\cdot\mathbf{S}|\in L_2(D_T)$. Returning to (2.21) then we see $\upsilon\in\mathcal{W}_2^{2,1}(D_T)$. □

We next prove that weak solutions are unique.

Lemma 7: Let $(\upsilon_0,\mathbf{S}_0+h\mathbf{a})$ *satisfy* $\mathfrak{H}$. *Then there is at most one* $(\upsilon,\mathbf{S}+h\mathbf{a})\in\mathfrak{A}$ *that is a weak solution to* (2.12) and (2.13) *with* $(\upsilon(0),\mathbf{S}(0))=(\upsilon_0,\mathbf{S}_0)$.

Proof: Let $(\upsilon_1,\mathbf{S}_1)$ and $(\upsilon_2,\mathbf{S}_2)$ be two solutions to (2.12) and (2.13) and set $(\upsilon_d,\mathbf{S}_d)$ to be their difference. Equations (2.12) and (2.13) imply the existence of weak equations for almost every $0<t<T$. For each such t we take the differences evaluated at the two solutions and use $\upsilon_d(t)$ and $\mathbf{S}_d(t)$ as test functions. We can then estimate

$$\int_\Omega(\partial_t|\upsilon_d|^2+\partial_t|\mathbf{S}_d|^2+|\nabla\upsilon_d|^2)\mathrm{d}x+\int_{\mathbb{R}^3}|\operatorname{curl}\mathbf{S}_d|^2\mathrm{d}x.$$

This is bounded above by the following sum, where we have integrated by parts in the terms containing div $\mathbf{S}_d$, div$(\mathbf{S}_1+h\mathbf{a})$, or div$(\mathbf{S}_2+h\mathbf{a})$ and used (2.19),

$$C_1\Bigg\{\sum_{m=1}^{2}\Bigg(\int_\Omega|\nabla v_d||\mathbf{S}_m||v_d|\mathrm{d}x+\int_\Omega|\nabla v_m||\mathbf{S}_d||v_d|\mathrm{d}x+\int_\Omega|\mathbf{S}_d||\nabla v_d|\mathrm{d}x+\int_\Omega|\mathbf{S}_m||\mathbf{S}_d||v_d|\mathrm{d}x$$
$$+\int_\Omega|\mathbf{S}_m|^2|v_d|^2\mathrm{d}x+\int_\Omega|\nabla v_d||v_d|\mathrm{d}x+\int_\Omega|\nabla v_m||v_d|^2\mathrm{d}x\Bigg)+\int_\Omega|\mathbf{S}_d|^2\mathrm{d}x+\int_\Omega|v_d|^2\mathrm{d}x\Bigg\}.$$

We label the first integrals $I,\ldots,VII$ and estimate each. We repeatedly use that $\|\mathbf{S}_m(t)\|_{\mathbf{L}_6(\Omega)}\leqslant C$ uniformly in t, the Gagliardo-Nirenberg inequality,

$$\|v\|_{\mathcal{L}_3(\Omega)}\leqslant C\|v\|^{1/2}_{\mathcal{W}^1_2(\Omega)}\|v\|^{1/2}_{\mathcal{L}_2(\Omega)},\tag{2.22}$$

and from Lemma 6 that both $v_1,\ v_2\in\mathcal{W}_2^{2,1}(D_T)$. We have

$$I\leqslant\|\mathbf{S}_m\|_{\mathbf{L}_6(\Omega)}\|\nabla v_d\|_{\mathcal{L}_2(\Omega)}\|v_d\|_{\mathcal{L}_3(\Omega)}\leqslant C\|v_d\|^{3/2}_{\mathcal{W}^1_2(\Omega)}\|v_d\|^{1/2}_{\mathcal{L}_2(\Omega)}\leqslant\epsilon\|\nabla v_d\|^2_{\mathcal{L}_2(\Omega)}+C\|v_d\|^2_{\mathcal{L}_2(\Omega)}.$$

$$II\leqslant\|\mathbf{S}_d\|_{\mathbf{L}_2(\Omega)}\|\nabla v_m\|_{\mathcal{L}_6(\Omega)}\|v_d\|_{\mathcal{L}_3(\Omega)}\leqslant\|\mathbf{S}_d\|_{\mathbf{L}_2(\Omega)}\|v_m\|_{\mathcal{W}^2_2(\Omega)}\|v_d\|_{\mathcal{L}_3(\Omega)}\leqslant\|\mathbf{S}_d\|^2_{\mathbf{L}_2(\Omega)}\|v_m\|^2_{\mathcal{W}^2_2(\Omega)}+\varepsilon\|\nabla v_d\|^2_{\mathcal{L}_2(\Omega)}$$
$$+C\|v_d\|^2_{\mathcal{L}_2(\Omega)}.$$

$$III\leqslant\varepsilon\|\nabla v_d\|^2_{\mathcal{L}_2(\Omega)}+C\|\mathbf{S}_d\|^2_{\mathbf{L}_2(\Omega)}.$$

$$IV\leqslant\|\mathbf{S}_m\|_{\mathbf{L}_6(\Omega)}\|\mathbf{S}_d\|_{\mathbf{L}_2(\Omega)}\|v_d\|_{\mathcal{L}_3(\Omega)}\leqslant\|\mathbf{S}_d\|^2_{\mathbf{L}_2(\Omega)}+\varepsilon\|\nabla v_d\|^2_{\mathcal{L}_2(\Omega)}+C\|v_d\|^2_{\mathcal{L}_2(\Omega)}.$$

$$V\leqslant\|\mathbf{S}_m\|^2_{\mathbf{L}_6(\Omega)}\|v_d\|^2_{\mathcal{L}_3(\Omega)}\leqslant\varepsilon\|\nabla v_d\|^2_{\mathcal{L}_2(\Omega)}+C\|v_d\|^2_{\mathcal{L}_2(\Omega)}.$$

$$VI\leqslant\varepsilon\|\nabla v_d\|^2_{\mathcal{L}_2(\Omega)}+C\|v_d\|^2_{\mathcal{L}_2(\Omega)}.$$

$$VII\leqslant\|\nabla v_m\|_{\mathcal{L}_3(\Omega)}\|v_d\|^2_{\mathcal{L}_3(\Omega)}\leqslant C(1+\|v_m\|^2_{\mathcal{W}^2_2(\Omega)})\|v_d\|^2_{\mathcal{L}_2(a)}+\varepsilon\|\nabla v_d\|^2_{\mathcal{L}_2(\Omega)}.$$

Set $r(t)=Mt+\int_0^t(\|v_1(\tau)\|^2_{\mathcal{W}^2_2(\Omega)}+\|v_2(\tau)\|^2_{\mathcal{W}^2_2(\Omega)})\mathrm{d}\tau$. From Lemma 6 we see that $r(t)$ is bounded. Then for ε small and M large, depending on C and C_1 we have

$$C_1(I+\cdots+IX)\leqslant\frac{\mathrm{d}r}{\mathrm{d}t}(\|v_d\|^2_{\mathcal{L}_2(\Omega)}+\|\mathbf{S}_d\|^2_{\mathbf{L}_2(\Omega)})+\frac{1}{2}\|\nabla v_d\|^2_{\mathcal{L}_2(\Omega)}.$$

Thus

$$\frac{\mathrm{d}}{\mathrm{d}t}(e^{-r(t)}(\|v_d\|^2_{\mathcal{L}_2(\Omega)}+\|\mathbf{S}_d\|^2_{\mathbf{L}_2(\Omega)}))+e^{-r(t)}\|\mathrm{curl}\,\mathbf{S}_d\|^2_{\mathbf{L}_2(\mathbb{R}^3)}\leqslant 0.$$

This leads to

$$e^{-r(t)}(\|v_d(t)\|^2_{\mathcal{L}_2(\Omega)}+\|\mathbf{S}_d(t)\|^2_{\mathbf{L}_2(\Omega)})+\int_0^t e^{-r(\tau)}\|\mathrm{curl}\,\mathbf{S}_d(\tau)\|^2_{\mathbf{L}_2(\mathbb{R}^3)}\mathrm{d}\tau\leqslant\|v_d(0)\|^2_{\mathcal{L}_2(\Omega)}+\|\mathbf{S}_d(0)\|^2_{\mathbf{L}_2(\Omega)}=0.$$

Thus $v_1=v_2$, $\mathbf{S}_1=\mathbf{S}_2$ in D_T, and curl $\mathbf{S}_1=$curl $\mathbf{S}_2$ in E_T. From Lemma 4 we see that this implies $\mathbf{S}_1=\mathbf{S}_2$ in E_T as well. □

Proof of Theorem 1: Since $(\psi_0,\mathbf{A}_0)$ satisfies $\mathfrak{H}$ we see that $(v,\mathbf{S}+h\mathbf{a})=(\psi,\mathbf{A})$ is a solution to

(2.17)–(2.20). Using Lemmas 5 and 7 we see that $(\psi,\mathbf{A})$ is the unique weak solution and that it converges strongly to the initial trace as $t\downarrow 0$. □

Weak solutions in the $\phi=0$ gauge are not classical for $t>0$ in general. The gauge invariant quantities such as $\mathbf{j}_s$, $\mathbf{j}_n$, curl $\mathbf{A}$, and $|\psi|$ are classical however. We prove this by transforming $(v,\mathbf{S}+h\mathbf{a},0)$ to the div $\mathbf{A}+\sigma\phi=0$ gauge where we show that weak solutions are regular for $t>0$.

III. THE LORENTZ GAUGE

We begin by preforming a gauge transformation to $(v,\mathbf{S}+h\mathbf{a},0)$. Let q solve

$$\sigma\partial_t q-\Delta q=\operatorname{div}\mathbf{S}\quad \text{in } D_T,$$

$$\partial_\nu q=0\quad \text{on } \partial\Omega\times[0,T),$$

$$q(x,0)=0\quad \text{in } \Omega. \tag{3.1}$$

Since $\operatorname{div}\mathbf{S}\in W_2^1((0,T);L_2(\Omega))$ and $\operatorname{div}\mathbf{S}(x,0)=0$ in Ω we have that q, $\partial_t q\in W_2^{2,1}(D_T)$, $q\in L_\infty(D_T)$, and $\partial_t q(x,0)=0$. Furthermore since $\int_\Omega \operatorname{div}\mathbf{S}(t)\mathrm{d}x=0$ we have $\int_\Omega q(t)\mathrm{d}x=\int_{\partial\Omega}\partial_t q(t)\mathrm{d}x=0$. As such we can extend q and $\partial_t q$ to $\mathbb{R}^3\backslash\Omega\times[0,T]$ by $\mathcal{E}(q)$ and $\mathcal{E}(\partial_t q)=\partial_t\mathcal{E}(q)$ where these are in $W_2^{2,1}(E_T)$ with support in $\bar{B}_R\times[0,T]$. We use the gauge transformation $T_q(v,\mathbf{S}+h\mathbf{a},0)=(\omega,\mathbf{Q}+h\mathbf{a},p)$. Where $\mathbf{Q}=\mathbf{S}+\nabla q$ and $p=-\partial_t q$ satisfy

$$\operatorname{div}\mathbf{Q}=-\sigma p\quad \text{in } \Omega.$$

The regularity of q and $(v,\mathbf{S})$ imply that

$$\omega\in L_\infty((0,T);\mathcal{W}_2^1(\Omega))\cap\mathcal{W}_2^{1,2}(D_T)\cap\mathcal{L}_\infty(D_T),$$

$$\mathbf{Q}\in L_\infty((0,T);\check{\mathbf{G}}(\mathbb{R}^3))\cap\mathbf{W}_2^{1,1}(D_T),$$

and $p\in W_2^{2,1}(E_T)$.

The system (2.17)–(2.20) becomes

$$\partial_t\omega-\Delta\omega=-2i(\mathbf{Q}+h\mathbf{a})\cdot\nabla\omega+i\left(\frac{1}{\sigma}-1\right)\omega\operatorname{div}\mathbf{Q}-|\mathbf{Q}+h\mathbf{a}|^2\omega-\kappa^2(|\omega|^2-1)\omega\quad \text{in } D_T, \tag{3.2}$$

$$\sigma\chi_\Omega\left(\partial_t\mathbf{Q}-\frac{1}{\sigma}\nabla\ \operatorname{div}\mathbf{Q}\right)+\operatorname{curl}^2\mathbf{Q}=\chi_\Omega\mathbf{j}_s\ \text{in } E_T \tag{3.3}$$

$$\partial_\nu\omega=0\quad \text{on } \partial\Omega\times(0,T), \tag{3.4}$$

$$(\mathbf{Q}+h\mathbf{a})\cdot\boldsymbol{\nu}=0\quad \text{on } \partial\Omega\times[0,T), \tag{3.5}$$

$$\omega(x,0)=\omega_0(x)\quad \text{in } \Omega, \tag{3.6}$$

$$\mathbf{Q}(x,0)=\mathbf{Q}_0(x)\quad \text{in } \mathbb{R}^3, \tag{3.7}$$

where since $q(x,0)=0$ we have $(\omega_0,\mathbf{Q}_0)=(v_0,\mathbf{S}_0)$. The estimates and uniqueness results in the $\phi=0$ gauge carry over to corresponding statements in the present gauge.

Lemma 8: The function $(\omega,\mathbf{Q}+h\mathbf{a})$ *is the unique solution to* (3.2)–(3.7) *among functions*

satisfying $(\omega, \mathbf{Q}+h\mathbf{a}) \in \mathfrak{A}$ *and* $\nabla(\operatorname{div} \mathbf{Q}) \in \mathbf{L}_2(D_T)$. *Moreover it is such that*

$$|\omega| \leqslant 1,$$

$$\|\partial_t \omega\|_{\mathcal{L}_2(D_T)} + \|\partial_t \mathbf{Q}\|_{\mathbf{L}_2(D_T)} + \sup_{0\leqslant t\leqslant T}\{\|\nabla \omega(t)\|_{\mathcal{L}^2(\Omega)} + \|\mathbf{Q}(t)\|_{\check{\mathbf{H}}(\mathbb{R}^3)}\} \leqslant C \tag{3.8}$$

where C *depends on* h, T, $\|\nabla \omega_0\|_{\mathcal{L}_2(\Omega)}$, *and* $\|\mathbf{Q}_0\|_{\check{\mathbf{H}}(\mathbb{R}^3)}$,

$$G(\omega(t), \mathbf{Q}(t)) \leqslant G(\omega_0, \mathbf{Q}_0) \tag{3.9}$$

for $0 \leqslant t \leqslant T$.

Lemma 9: The function $\operatorname{div} \mathbf{Q} \in W_2^{2,1}(D_T)$ *and satisfies*

$$\sigma \partial_t \operatorname{div} \mathbf{Q} - \Delta \operatorname{div} \mathbf{Q} = \operatorname{div} \mathbf{j}_s \quad \text{in } D_T,$$

$$\partial_\nu \operatorname{div} \mathbf{Q} = 0 \quad \text{on } \partial\Omega \times (0,T),$$

$$\operatorname{div} \mathbf{Q}(x,0) = 0 \quad \text{in } \Omega. \tag{3.10}$$

Furthermore

$$\sup_{0\leqslant t\leqslant T} \|\operatorname{div} \mathbf{Q}(t)\|_{W_2^1(\Omega)} \leqslant C, \tag{3.11}$$

where C *depends on* ω_0, $\mathbf{Q}_0$, σ *and* h.

Proof: Since $\operatorname{div} \mathbf{Q} = \sigma \partial_t q$ in Ω we see that (3.10) follows from (3.3). From (3.10) we have $\int_\Omega \operatorname{div} \mathbf{Q}(t) \mathbf{d}s = 0$ and

$$\sup_{0<t<T} \|\nabla \operatorname{div} \mathbf{Q}(t)\|_{\mathbf{L}_2(\Omega)} \leqslant C_1 \|\operatorname{div} \mathbf{j}_s\|_{L_2(D_T)}.$$

Thus

$$\sup_{0<t<T} \|\operatorname{div} \mathbf{Q}(t)\|_{W_2^1(\Omega)} \leqslant C_2 \sup_{0\leqslant t\leqslant T} \|\operatorname{div} \mathbf{j}_s\|_{L_2(D_T)} \leqslant C_3 \|\partial_t \upsilon\|_{\mathcal{L}_2(D_T)} \leqslant C_4,$$

where C_4 depends on $(\upsilon_0, \mathbf{S}_0) = (\omega_0, \mathbf{Q}_0)$, h, and T. □

We now develop higher regularity properties of solutions for $0 < t_0 < t < T$.

Define

$$D_{t_0,T} = \Omega \times (t_0, T) \text{ and } E_{t_0,T} = \mathbb{R}^3 \times (t_0, T).$$

Let $k(t) \in C^\infty(\mathbb{R})$ be a cut off function such that $k(t) = 0$ for $t \leqslant t_0/2$ and $k(t) = 1$ for $t_0 \leqslant t$.

Lemma 10: $\nabla \partial_t \omega \in \mathcal{L}_2(D_{t_0,T})$ *for each* $t_0 > 0$ *and*

$$\sup_{t_0<t<T} \|\partial_t \omega(t)\|_{\mathcal{L}_2(D_{t_0,T})} + \|\nabla \partial_t \omega\|_{\mathcal{L}_2(D_{t_0,T})} \leqslant C,$$

where C *depends on* $\|\omega_0\|_{\mathcal{W}_2^1(\Omega)}$, $\|\mathbf{Q}_0\|_{\check{\mathbf{H}}(\mathbb{R}^3)}$, h, t_0, and T.

Proof: Set

$$D_\tau \omega(x,t) = \frac{\omega(x, t+\tau) - \omega(x,t)}{\tau} \quad \text{for } \tau > 0,$$

and $\eta = k D_\tau \omega$. Using (3.2) we write

$$\partial_t \eta - \Delta \eta = -2i(\mathbf{Q}(t) + ha) \cdot \nabla \eta + i\left(\frac{1}{\sigma} - 1\right) \operatorname{div} \mathbf{Q}(t)\, \eta - |\mathbf{Q}(t) + ha|^2 \eta - 2i \nabla\, \omega(t+\tau) k D_\tau \mathbf{Q}$$

$$+ i\left(\frac{1}{\sigma} - 1\right) \omega(t+\tau) k D_\tau (\operatorname{div} \mathbf{Q}) + \omega(t+\tau) k(t) D_\tau |\mathbf{Q} + \mathbf{a}h|^2 + f_1 \eta + f_2 \quad \text{in } D_T,$$

$$\partial_\nu \eta = 0 \quad \text{on } \partial\Omega \times (0,T),$$

$$\eta(x,0) = 0 \quad \text{in } \Omega, \tag{3.12}$$

where $\|f_1\|_{\mathcal{L}_\infty(D_T)} + \|f_2\|_{\mathcal{L}2}(D_T) \leqslant C(t_0)$ uniformly in τ, $0 < \tau < 1$. We take the inner product of (3.12) with η and integrate over Ω. We further integrate by parts in the fourth term on the right side, using (3.5). The left-hand side becomes

$$\frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \left(\int_\Omega |\eta|^2 \mathrm{d}x + \int_\Omega |\nabla \eta|^2 \mathrm{d}x \right). \tag{3.13}$$

This is bounded by

$$C\left(\int_\Omega |\operatorname{div} \mathbf{Q}(t)||\eta|^2 \mathrm{d}x + \int_\Omega |\mathbf{Q}(t)|^2 |\eta|^2 \mathrm{d}x + \int_\Omega |D_\tau \operatorname{div} \mathbf{Q}||\eta| \mathrm{d}x + \int_\Omega |D_\tau \mathbf{Q}||\nabla \eta| \mathrm{d}x + \int_\Omega (|\mathbf{Q}(t)| \right.$$

$$\left. + |\mathbf{Q}(t+\tau)|) |D_\tau \mathbf{Q}||\eta| \mathrm{d}x \int_\Omega |\eta|^2 \mathrm{d}x + 1 \right) + \frac{1}{2} \int_\Omega (\nabla \eta)^2 \mathrm{d}x. \tag{3.14}$$

We label the first five integrals $I, \ldots, V$ and estimate each.

$$I \leqslant \|\operatorname{div} \mathbf{Q}(t)\|_{L_3(\Omega)} \|\eta\|^2_{\mathcal{L}_3(\Omega)} \leqslant \varepsilon \|\nabla \eta\|^2_{\mathcal{L}_2(\Omega)} + C \|\eta\|^2_{\mathcal{L}_2(\Omega)}$$

for any $\varepsilon > 0$ and $C(\varepsilon)$ independent of t. Here we used (2.22) and (3.11).

$$II \leqslant \|\mathbf{Q}(t)\|^2_{\mathbf{L}_6(\Omega)} \|\eta\|^2_{\mathcal{L}_3(\Omega)} \leqslant \varepsilon \|\nabla \eta\|^2_{\mathcal{L}_2(\Omega)} + C \|\eta\|^2_{\mathcal{L}_2(\Omega)},$$

where we use (1.11). Next we estimate

$$III \leqslant \|\operatorname{div} D_\tau \mathbf{Q}(t)\|^2_{L_2(\Omega)} + \|\eta\|^2_{\mathcal{L}_2(\Omega)},$$

$$IV \leqslant \varepsilon \|\nabla \eta\|^2_{\mathcal{L}_2(\Omega)} + C \|D_\tau \mathbf{Q}(t)\|^2_{\mathbf{L}_2(\Omega)}$$

and

$$V \leqslant \Big(\sup_{0 \leqslant t \leqslant T+1} \|\mathbf{Q}(t)\|_{\mathbf{L}_6(\Omega)} \Big) \|\eta\|_{\mathcal{L}_3(\Omega)} \|D_\tau \mathbf{Q}(t)\|_{\mathbf{L}_2(\Omega)} \leqslant \varepsilon \|\nabla \eta\|^2_{\mathcal{L}_2(\Omega)} + C_1 \|\eta\|^2_{\mathcal{L}_2(\Omega)} + C_2 \|D_\tau \mathbf{Q}(t)\|^2_{\mathbf{L}_2(\Omega)}.$$

Combining these estimates with (3.13) and (3.14) we find

$$\sup_{t_0 \leqslant t \leqslant T} \|D_\tau \omega(t)\|^2_{\mathcal{L}_2(\Omega)} + \|\nabla D_\tau \omega\|^2_{\mathcal{L}_2(D_{t_0,T})} \leqslant C,$$

where C depends on the initial data, h, t_0, and T but independent of $\tau, 0 < \tau < 1$. Letting $\tau \downarrow 0$ we have our assertion. □

Lemma 11: $\omega \in \mathcal{W}^{2,1}_3(D_{t_0,T})$.

Proof: Set $\rho = k\omega$. Then $\rho \in \mathcal{W}^{1,2}_2(D_T)$, $|\rho| \leqslant 1$, and from (3.2)

$$\partial_t \rho - \Delta \rho = \mathbf{F} \cdot \nabla \rho + f \quad \text{in } D_T,$$

$$\partial_\nu \rho = 0 \quad \text{on } \partial\Omega \times (0,T),$$

$$\rho(x,0) = 0 \quad \text{in } \Omega,$$

where $\mathbf{F} = -2i(\mathbf{Q} + h\mathbf{a}) \in L_\infty((0,T);\mathcal{L}_6(\Omega))$ and $f \in \mathcal{L}_3(D_T)$. Set $s = \sup\{m \leqslant 3 : \rho \in \mathcal{W}_m^{2,1}(D_T)\}$. We have the Gagliardo–Nirenberg inequality

$$\|\nabla\rho\|_{\mathcal{L}_{2m}(\Omega)} \leqslant C\|\rho\|^{1/2}_{\mathcal{W}^2_m(\Omega)}\|\rho\|^{1/2}_{\mathcal{L}_\infty(\Omega)}, \tag{3.15}$$

where C is uniformly bounded for $2 \leqslant m \leqslant 3$. From parabolic estimates we have

$$\|\rho\|_{\mathcal{W}_m^{2,1}(D_T)} \leqslant \Lambda(\|\mathbf{F}\|^2_{\mathcal{L}_{2m}(D_T)} + \|f\|_{\mathcal{L}_3(D_T)} + 1)$$

where Λ is independent of m for $2 \leqslant m \leqslant 3$. It follows that

$$\|\rho\|_{\mathcal{W}_m^{2,1}(D_T)} \leqslant \Lambda(\|\mathbf{F}\|^2_{\mathcal{L}_6(D_T)} + \|f\|_{\mathcal{L}_3(D_T)} + 1)$$

for all $m < s$. This implies $\|\rho\|_{\mathcal{W}_s^{2,1}(D_T)}$ is finite and satisfies the same bound.

We claim that $s = 3$. If this is not the case let $s < s' \leqslant 3$. Then

$$\|\mathbf{F}\cdot\nabla\rho\|_{\mathcal{L}_{s'}(D_T)} \leqslant \|\mathbf{F}\|_{\mathcal{L}_6(D_T)}\|\nabla\rho\|_{\mathcal{L}_{6s'/(6-s')}(D_T)} \leqslant C\|\rho\|^{1/2}_{\mathcal{W}^{2,0}_{3s'/(6-s')}(D_T)}. \tag{3.16}$$

Note $3s/(6-s) < s$ if $s < 3$. Thus if $s < s'$, with $s' - s$ sufficiently small we have $3s'/(6-s') < s$ and it follows from (3.16), and parabolic estimates that $\|\rho\|_{\mathcal{W}^{2,1}_{s'}(D_T)} < \infty$. This contradicts the definition of s. □

We can now estimate $\partial_t \mathbf{j}_s$.

Lemma 12: $\partial_t \mathbf{j}_s \in L^2(D_{t_0,T})$.

Proof: We can estimate

$$\|D_\tau \mathbf{j}_s\|^2_{\mathbf{L}_2(D_{t_0,T})} \leqslant \|\nabla D_\tau\omega\|^2_{\mathcal{L}_2(D_{t_0,T})} + \|(\nabla\omega)D_\tau\omega\|^2_{\mathcal{L}_2(D_{t_0,T})} + \|(D_\tau\omega)\mathbf{Q}\|^2_{\mathcal{L}_2(D_{t,T})} + \|D_\tau\mathbf{Q}\|^2_{\mathbf{L}^2(D_{t,T})}.$$

Each term on the right-hand side is bounded by a constant depending only on the data, t_0, and T. Indeed this holds for the first term by Lemma 10. The second term is estimated by

$$\|(\nabla\omega)D_\tau\omega\|^2_{\mathcal{L}_2(D_{t_0,T})} \leqslant \|\nabla\omega\|^2_{\mathcal{L}_6(D_{t_0,T})}\|D_\tau\omega\|^2_{\mathcal{L}_3(D_{t_0,T})} \leqslant C\|\omega\|^3_{\mathcal{W}^{2,1}_3(D_{t_0,T+1})},$$

and this is bounded using Lemma 11. The third term is bounded using Lemma 11 and (3.8), and the fourth term is estimated using (3.8). □

We can now differentiate (3.3) to get further estimates on $\mathbf{Q}$. We use the notation $(\partial_t)^\ell f = f^{(\ell)}$.

Lemma 13: $\mathbf{Q}(t) \in W_2^2(\Omega)$ *for* $t > 0$ *and* $\|\mathbf{Q}\|_{\mathbf{W}_2^2(\Omega)} \leqslant C$ *for* $t_0 \leqslant t < T$ *where* C *depends on the data*, t_0, *and* T.

Proof: Set $\mathbf{V} = k(t)D_\tau\mathbf{Q}$. Then we have

$$\sigma\chi_\Omega\partial_t\mathbf{V} - \chi_\Omega\nabla\ \mathrm{div}\,\mathbf{V} + \mathrm{curl}^2\,\mathbf{V} = \chi_\Omega(kD_\tau\mathbf{j}_s + \sigma\partial_t\mathbf{k}D_\tau Q)$$

Dotting this equation with $\mathbf{V}$, integrating over E_T, and letting $\tau \to 0$ we get $\mathbf{Q}^{(1)} \in L_2(t_0, T; \check{\mathbf{G}}(\mathbb{R}^3))$ for any $t_0 > 0$. Next dotting the equation with $\partial_t\mathbf{V}$, integrating on E_T, and letting $\tau \to 0$ we find that $\mathbf{Q}^{(1)} \in \mathbf{W}_2^{1,1}(D_{t_0,T}) \cap L_\infty((t_0,T);\check{\mathbf{G}}(\mathbb{R}^3))$ and satisfies the estimate

$$\|\mathbf{Q}^{(2)}\|^2_{\mathbf{L}^2(D_{t_0,T})} + \sup_{t_0 \leqslant t \leqslant T}\|\mathbf{Q}^{(1)}(t)\|^2_{\check{\mathbf{G}}(\mathbb{R}^3)} \leqslant C \tag{3.17}$$

where C depends on the data, t_0, and T. The only step in the preceding argument that needs comment is the inequality

$$\|\mathbf{V}\|^2_{\check{\mathbf{H}}(\mathbb{R}^3)} \leqslant C(\|\text{div } \mathbf{V}\|^2_{L_2(\Omega)} + \|\text{curl } \mathbf{V}\|^2_{\mathbf{L}_2(\mathbb{R}^3)}).$$

To see this recall that $\mathbf{V}\cdot\boldsymbol{\nu}=0$ on $\partial\Omega$,

$$\|\mathbf{V}\|^2_{\check{\mathbf{H}}(\mathbb{R})} = \|\text{div } \mathbf{V}\|^2_{L_2(\mathbb{R}^3)} + \|\text{curl } \mathbf{V}\|^2_{\mathbf{L}_2(\mathbb{R}^3)},$$

and by the construction of $\check{\mathbf{G}}(\mathbb{R}^3)$ that

$$\|\text{div } \mathbf{V}\|^2_{L_2(\mathbb{R}^3)} \leqslant C(\|\text{div } \mathbf{V}\|^2_{L_2(\Omega)} + \|\text{curl } \mathbf{V}\|^2_{\mathbf{L}_2(\mathbb{R}^3)} + \|\mathbf{V}\cdot\boldsymbol{\nu}\|^2_{W_2^{1/2}(\partial\Omega)}).$$

From (3.11) and (3.17), and Lemma 12, we have,

$$\|\mathbf{Q}^{(1)}(t)\|_{\mathbf{L}_2(\Omega)} + \|\nabla \text{ div } \mathbf{Q}(t)\|_{\mathbf{L}_2(\Omega)} + \|\mathbf{j}_s(t)\|_{\mathbf{L}_2(\Omega)} \leqslant C \tag{3.18}$$

for $t_0 \leqslant t \leqslant T$. It follows from (3.3) that curl $\mathbf{Q}(t) \in \check{\mathbf{H}}(\mathbb{R}^3)$ and

$$\|\text{curl } \mathbf{Q}(t)\|_{\check{\mathbf{H}}(\mathbb{R}^3)} = \|\text{curl}^2 \mathbf{Q}(t)\|_{\mathbf{L}_2(\mathbb{R}^3)} \leqslant C \tag{3.19}$$

for $t_0 \leqslant t \leqslant T$. We now apply Theorem 3.4 from Ref. 1, which is valid since $(\mathbf{Q}+h\mathbf{a})\cdot\boldsymbol{\nu}=0$ on $\partial\Omega$, to obtain the estimate

$$\|\mathbf{Q}(t)\|_{\mathbf{W}_2^2(\Omega)} \leqslant C(\|\text{curl } \mathbf{Q}(t)\|_{\mathbf{W}_2^1(\Omega)} + \|\mathbf{Q}(t)\|_{\mathbf{L}_2(\Omega)} + \|\Delta\mathbf{Q}(t)\|_{\mathbf{L}_2(\Omega)} + h).$$

Using (3.18) and (3.19) we see

$$\sup_{t_0\leqslant t\leqslant T} \|\mathbf{Q}(t)\|_{\mathbf{W}_2^2(\Omega)} \leqslant C.$$

□

Note, it follows that

$$\|\mathbf{Q}(t)\|_{\mathbf{L}_\infty(\Omega)} \leqslant C \tag{3.20}$$

uniformly for $t_0 \leqslant t \leqslant T$.

We return to (3.2) and (3.4) which we write as

$$\partial_t\omega - \Delta\omega = f \quad \text{in } D_T,$$

$$\partial_\nu\omega = 0 \quad \text{on } \partial\Omega\times(0,T).$$

Using Lemma 11, (3.11), (3.15), and (3.20) we obtain $f \in \mathcal{L}_6(D_{t_0,T})$ for any $0<t_0<T$. As such $\omega \in \mathcal{W}_6^{2,1}(D_{t_0,T})$. It then follows that

$$\text{div } \mathbf{j}_s = \left(i\omega, \partial_t\omega - \frac{i}{\sigma}\omega \text{ div } \mathbf{Q}\right) \in L_6(D_{t_0,T}),$$

and then from (3.10) that div $\mathbf{Q} \in W_6^{2,1}(D_{t_0,T})$ where the $W_6^{2,1}$ estimates depend only on the initial data, h, t_0, and T. These estimates establish the initial step to the induction argument for the next lemma where higher regularity properties for $\omega^{(j)}$ and $\mathbf{Q}^{(j)}$ are proved. The idea behind their proof is to carry enough information forward from the jth step so that $\omega^{(j+1)}$ and $\mathbf{Q}^{(j+1)}$ will be weak solutions to equations with bounded coefficients and thereby easy to analyze.

Lemma 14: $\omega \in C^\infty((0,T);\mathcal{W}_6^2(\Omega))$ *and* $\mathbf{Q} \in C^\infty((0,T);\mathbf{W}_2^2(\Omega)) \cap C^\infty((0,T);\check{\mathbf{G}}(\mathbb{R}^3))$.

Proof: It suffices to prove that $\omega^{(j)} \in \mathcal{W}_6^{2,1}(D_{t_0,T})$ and

$$\mathbf{Q}^{(j)} \in L_\infty((t_0,T); \quad \mathbf{W}_2^2(\Omega)) \cap L_\infty((t_0,T); \quad \check{\mathbf{G}}(\mathbb{R}^3))$$

for each integer $j \geqslant 0$ and $T>t_0>0$.

We will prove:

If $\omega^{(k)} \in \mathcal{W}_6^{2,1}(D_{t_0,T})$, $\operatorname{div} \mathbf{Q}^{(k)} \in W_6^{2,1}(D_{t_0,T})$, $\mathbf{Q}^{(k)} \in \mathbf{L}_2(D_{t_0,T})$, and $\mathbf{Q}^{(m)} \in L_\infty((t_0,T);\mathbf{W}_2^2(\Omega)) \cap L_\infty((t_0,T);\check{\mathbf{G}}(\mathbb{R}^3))$ where $0 \leqslant k \leqslant j$ and $m \leqslant \max(0,j-1)$ for each $0 < t_0 < T$ then $\omega^{(j+1)} \in \mathcal{W}_6^{2,1}(D_{t_0,T})$, $\operatorname{div} \mathbf{Q}^{(j+1)} \in W_6^{2,1}(D_{t_0,T})$, $\mathbf{Q}^{(j+1)} \in \mathbf{L}_2(D_{t_0,T})$, and $\mathbf{Q}^{(j)} \in L_\infty((t_0,T);\mathbf{W}_2^2(\Omega)) \cap L_\infty((t_0,T);\check{\mathbf{G}}(\mathbb{R}^3))$ for each $0 < t_0 < T$.

The induction hypotheses for $j=0$ have been established previously. Assuming these for j, we then have from standard embedding theorems that $\omega^{(k)}$, $\operatorname{div} \mathbf{Q}^{(k)} \in C^{1+1/6,7/12}(\bar{D}_{t_0,T})$, $\mathbf{Q}^{(k)} \in \mathbf{L}_2(D_{t_0,T})$, and $\mathbf{Q}^{(m)} \in \mathbf{L}_\infty(D_{t_0,T})$ for $k \leqslant j$ and $m \leqslant \max(0,j-1)$. It follows that $\mathbf{j}_s^{(j)} \in \mathbf{L}_2(D_{t_0,T})$. Then as in the proof of Lemma 13 we have $\mathbf{Q}^{(j+1)} \in \mathbf{L}_2(D_{t_0,T})$ and $\mathbf{Q}^{(j)} \in L_\infty((t_0,T);\check{\mathbf{G}}(\mathbb{R}^3))$.

We next prove that $\omega^{(j+1)} \in \mathcal{W}_2^{2,1}(D_{t_0,T})$. From the hypotheses we can differentiate (3.2) with respect to t,j times. We then form an equation for $\eta = k(t) D_\tau \omega^{(j)}$ for $\tau > 0$, in D_T. For $j=0$ this is (3.12); we see that η satisfies

$$\partial_t \eta - \Delta \eta = a_1 \cdot \nabla \eta + a_2 \eta + a_3 \quad \text{in } D_T,$$

$$\partial_\nu \eta = 0 \quad \text{on } \partial\Omega \times (0,T),$$

$$\eta(x,0) = 0 \quad \text{in } \Omega,$$

where from the hypotheses and (3.17) we have a_1, $a_2 \in \mathcal{L}_\infty(D_T)$ and $a_3 \in \mathcal{L}_6(D_T)$. Thus $\omega^{(1)} \in \mathcal{W}_2^{2,1}(D)$.

For $j \geqslant 1$ the equation for η is more complex. We write

$$\begin{aligned} L(\eta) :&= \partial_t \eta - \Delta \eta + 2i(\mathbf{Q} + h\mathbf{a}) \cdot \nabla \eta + i\left(\frac{1}{\sigma} - 1\right) \eta \operatorname{div} \mathbf{Q} + |\mathbf{Q} + h\mathbf{a}|^2 \eta + \kappa^2 (|\omega|^2 - 1)\eta + \kappa^2 \omega(\omega \eta^* \\ &\quad + \omega^* \eta) = a_1 \mathbf{Q}^{(j)} + a_2 D_\tau \mathbf{Q}^{(j-1)} + a_3 D_\tau \mathbf{Q}^{(j)} + a_4 D_\tau (\operatorname{div} \mathbf{Q}^{(j)}) + a_5 \mathbf{Q}^{(1)} D_\tau \mathbf{Q} + a_6 \mathbf{Q}^{(1)}(t+\tau) D_\tau \mathbf{Q} \\ &\quad + a_7 \end{aligned}$$

where the a_i are bounded for $1 \leqslant i \leqslant 6$ and $a_7 \in \mathcal{L}_6(D_T)$. Note that the coefficients of $L(\cdot)$ are bounded in $D_{t',T}$ for each $0 < t'$. The first four terms on the right are in $\mathcal{L}_2(D_T)$ and the fifth and sixth terms are the product of functions in $\mathcal{L}_6(D_T)$. It follows that $\eta \in \mathcal{W}_2^{2,1}(D_T)$ uniformly in $\tau, 0 < \tau < 1$. Thus

$$\omega^{(j+1)} \in \mathcal{W}_2^{2,1}(D_{t_0,T}). \tag{3.21}$$

It follows that $\mathbf{j}_s^{(j+1)} \in \mathbf{L}_2(D_{t_0,T})$, and using (3.3) as before

$$\mathbf{Q}^{(j+1)} \in L_\infty((t_0,T); \quad \check{\mathbf{G}}(\mathbb{R}^3)) \cap \mathbf{W}_2^{0,1}(D_{t_0,T}). \tag{3.22}$$

Whence $\mathbf{j}_s^{(j)}, \mathbf{Q}^{(j+1)} \in L_\infty((t_0,T);\mathbf{L}_2(\Omega))$. Using the identity

$$\operatorname{div} \mathbf{j}_s = \left(i\omega, \partial_t \omega - \frac{i}{\sigma} \omega \operatorname{div} \mathbf{Q} \right), \tag{3.23}$$

together with (3.10) and the hypotheses it follows that $\nabla \operatorname{div} \mathbf{Q}^{(j)} \in L_\infty(t_0,T;\mathbf{L}_2(\Omega))$ as well.

From (3.3) then we have $\operatorname{curl}^2 \mathbf{Q}^{(j)} \in L_\infty((t_0,T);\mathbf{L}_2(\mathbb{R}^3))$. Since $\operatorname{curl} \mathbf{Q}^{(j)}(t) \in \mathbf{L}_2(\mathbb{R}^3)$ we have $\operatorname{curl} \mathbf{Q}^{(j)}(t) \in \check{\mathbf{H}}(\mathbb{R}^3)$ and as such

$$\operatorname{curl} \mathbf{Q}^{(j)} \in L_\infty((t_0,T);\mathbf{W}_2^1(\Omega)).$$

Arguing as in Lemma 13, we apply Ref. 1, Theorem 3.4 to obtain

$$\mathbf{Q}^{(j)} \in L_\infty((t_0,T);\mathbf{W}_2^2(\Omega)).$$

It remains to prove $\omega^{(j+1)} \in \mathcal{W}_6^{2,1}(D_{t_0,T})$ and $\operatorname{div} \mathbf{Q}^{(j+1)} \in W_6^{2,1}(D_{t_0,T})$. From (3.21)–(3.23) we have that $\operatorname{div} \mathbf{j}_s^{(j+1)} \in L_2(D_{t_0,T})$. Thus from (3.10) we obtain

$$\operatorname{div} \mathbf{Q}^{(j+1)} \in W_2^{2,1}(D_{t_0,T}) \cap L_\infty((t_0,T);L_6(\Omega)). \tag{3.24}$$

It follows from this and (3.22) that $L(\omega^{(j+1)}) \in \mathcal{L}_6(D_{t',T})$ for any $0<t'<T$, implying that $\omega^{(j+1)} \in \mathcal{W}_6^{2,1}(D_{t_0,T})$. Using this, (3.23) and (3.24) we have $\operatorname{div} \mathbf{j}_s^{(j+1)} \in L_6(D_{t',T})$ for $0<t'<T$. It follows from (3.10) that $\operatorname{div} \mathbf{Q}^{(j+1)} \in W_6^{2,1}(D_{t_0,T})$. □

Lemma 15: $\omega \in C^\infty((0,T);\mathcal{C}^{3+\alpha}(\bar{\Omega}))$, $\operatorname{div} \mathbf{Q} \in C^\infty((0,T);C^{3+\alpha}(\bar{\Omega}))$ *and* $\mathbf{Q} \in C^\infty((0,T);\mathbf{C}^{1+\gamma}(K))$ *for any compact* $K \subset \mathbb{R}^3$ *and* $0<\gamma<1$.

Proof: We have $\mathbf{Q}^{(j)} = \nabla f^{(j)} + \mathbf{g}^{(j)}$ where $\mathbf{g}^{(j)} \in \mathbb{V}_2$ and $f^{(j)} \in \mathring{W}_2^2(B_R)$. Furthermore, from Lemma 14 we have

$$\mathbf{j}_s^{(j)} + \nabla \operatorname{div} \mathbf{Q}^{(j)} - \mathbf{Q}^{(j+1)} \in L_\infty((t_0,T);\mathbf{L}_6(\Omega)).$$

Thus $\Delta \mathbf{g}^{(j)} = -\operatorname{curl}^2 \mathbf{g}^{(j)} \in L_\infty((t_0,T);\mathbf{L}_6(\mathbb{R}^3))$. Since $\mathbf{g}^{(j)} \in L_\infty((t_0,T);\mathbf{L}_6(\mathbb{R}^3))$ and $\operatorname{supp} \Delta \mathbf{g}^{(j)} \subset \bar{\Omega}$ it follows that $\mathbf{g}^{(j)} \in L_\infty((t_0,T);\mathbf{W}_6^2(\mathbb{R}^3))$ for any $t_0>0$, implying that

$$\mathbf{g} \in C^\infty((0,T);\mathbf{W}_6^2(\mathbb{R}^3)). \tag{3.25}$$

We now analyze $\nabla f^{(j)}$. We have

$$\Delta f^{(j)} = \operatorname{div} \mathbf{Q}^{(j)} \quad \text{in } \Omega,$$

$$\partial_{\boldsymbol{\nu}} f^{(j)} = -\mathbf{g}^{(j)} \cdot \boldsymbol{\nu} - h\mathbf{a}^{(j)} \cdot \boldsymbol{\nu} \quad \text{on } \partial\Omega. \tag{3.26}$$

Since $\partial\Omega \in C^{3+\alpha}$ and $\int_\Omega f^{(j)} dx = 0$ we have from elliptic estimates that

$$\|f^{(j)}\|_{W_6^3(\Omega)} \leqslant C(\|\operatorname{div} \mathbf{Q}^{(j)}\|_{W_6^1(\Omega)} + \|\mathbf{g}^{(j)}\|_{\mathbf{W}_6^2(\Omega)} + 1).$$

It follows that $f \in C^\infty((0,T);W_6^3(\Omega))$. From the definition of $\mathcal{E}(f)$ we have $f = \mathcal{E}(f) \in C^\infty((0,T);\mathring{W}_6^3(B_R))$. With this and (3.25) we see that

$$\mathbf{Q} \in C^\infty((0,T);\mathbf{C}^{1+1/2}(K)) \tag{3.27}$$

for any compact set $K \subset \mathbb{R}^3$. We next write

$$\Delta \omega(t) = F(t) \quad \text{in } \Omega,$$

$$\partial_{\boldsymbol{\nu}} \omega(t) = 0 \quad \text{on } \partial\Omega \tag{3.28}$$

where F is a polynomial in the components of ω, $\nabla\omega$, $\partial_t\omega$, $\mathbf{Q}$, and $\operatorname{div} \mathbf{Q}$. Using (3.27) and the estimates from Lemma 14, together with elliptic estimates applied to (3.28) we find that $\omega \in C^\infty((0,T);\mathcal{C}^{3+\beta}(\bar{\Omega}))$ where $\beta = \min(\alpha, \frac{1}{2})$. We get the corresponding result for $\operatorname{div} \mathbf{Q}$ using (3.10).

Our next step is to write $\mathbf{Q} = \nabla f + \mathbf{g}$ with $\mathbf{g} \in \mathbb{V}_2$ for each t where $\mathbf{g}$ satisfies

$$\Delta \mathbf{g} = \chi_\Omega(\sigma \partial_t \mathbf{Q} - \nabla(\operatorname{div} \mathbf{Q}) - \mathbf{j}_s) \equiv \chi_\Omega \ell. \tag{3.29}$$

We have $\ell \in C^\infty((0,T);\mathbf{C}^{1+\beta}(\bar{\Omega}))$ and it follows that $\mathbf{g} \in C^\infty((0,T);\mathbf{W}_p^2(\mathbb{R}^3))$ for any $3<p<\infty$. We can now argue as above, using (3.26), to get $f \in C^\infty((0,T);\mathring{W}_p^3(B_R))$. As a result we get

$$\mathbf{Q} \in C^\infty((0,T);\mathbf{C}^{1+\gamma}(K))$$

for any $0<\gamma<1$ and compact $K \subset \mathbb{R}^3$.

We return to (3.28) and are now able to assert that $F \in C^\infty((0,T);\mathcal{C}^{1+\alpha}(\bar{\Omega}))$. It follows that $\omega \in C^\infty((0,T);\mathcal{C}^{3+\alpha}(\bar{\Omega}))$ and a similar argument proves that $\operatorname{div} \mathbf{Q} \in C^\infty((0,T);C^{3+\alpha}(\bar{\Omega}))$ as well. □

We view equation (3.29) as a diffraction problem. Let k be an integer $k \geqslant 2$. The classical regularity result for a solution $\mathbf{g} \in \mathbf{W}^2_{2,loc}(\mathbb{R}^3)$, provided $\ell \in \mathbf{C}^{k+\alpha-2}(\bar{\Omega})$ and $\partial\Omega \in C^{k+\alpha}$ is that $\mathbf{g} \in \mathbf{C}^1(\mathbb{R}^3) \cap \mathbf{C}^{k+\alpha}(\bar{\Omega}) \cap \mathbf{C}^{k+\alpha}(\mathbb{R}^3 \setminus \Omega)$, satisfying

$$\|\mathbf{g}\|_{\mathbf{C}^{k+\alpha}(\bar{\Omega})} + \|\mathbf{g}\|_{\mathbf{C}^{k+\alpha}(\overline{B_R}\setminus\Omega)} \leqslant \Lambda(\|\ell\|_{\mathbf{C}^{k+\alpha-2}(\bar{\Omega})} + \|\mathbf{g}\|_{\mathbf{C}^0(\bar{B}_{2R})}) \tag{3.30}$$

for any B_R such that $\bar{\Omega} \subset B_R$. This is given in Ref. 7 (p. 198), for the case $k=2$. To prove it for integers $k>2$ one can locally flatten $\partial\Omega$ and establish an estimate analogous to (3.30) with $k=2$, and $\mathbf{g}$ and ℓ replaced by derivatives tangent to the flattened interface. Estimates for the remaining derivatives of $\mathbf{g}$, on either side of the interface, are found in terms of the tangential derivatives using the equation's ellipticity.

We use (3.30) to prove higher regularity properties for ω and $\mathbf{Q}$.

Lemma 16: Assume that $\partial\Omega \in C^{k+\alpha}$ where k is an integer with $k \geqslant 3$, and $\bar{\Omega} \subset B_R$. Then writing $\mathbf{Q} = \nabla f + \mathbf{g}$ we have

$$g_j,\ f \in C^\infty((0,T); C^{k+\alpha}(\bar{\Omega})) \cap C^\infty((0,T); C^{k+\alpha}(\bar{B}_R \setminus \Omega)), \tag{3.31}$$

$$\operatorname{div} \mathbf{Q} \in C^\infty((0,T); C^{k+\alpha}(\bar{\Omega})), \tag{3.32}$$

and

$$\omega \in C^\infty((0,T); \mathcal{C}^{k+\alpha}(\bar{\Omega})). \tag{3.33}$$

Proof: We begin with the case $k=3$. From the proof of Lemma 15, we find that $\ell \in C^\infty(t_0, T; \mathbf{C}^{1+\alpha}(\bar{\Omega}))$. Then using (3.30) for the equations $\Delta \mathbf{g}^{(j)} = \chi_\Omega \ell^{(j)}$ we see that (3.31) holds for $\mathbf{g}$. It remains to establish (3.31) for f. Using (3.26) and Lemma 15 we have $\Delta f \in C^\infty((0,T); C^{3+\alpha}(\bar{\Omega}))$. Using (3.31) for $\mathbf{g}$ with $k=3$, we have $\partial_\nu f \in C^\infty((0,T); C^{2+\alpha}(\partial\Omega))$. It follows from elliptic estimates applied to (3.26) that $f \in C^\infty((0,T); C^{3+\alpha}(\bar{\Omega}))$.

We next assume that $3 < k$ and that (3.31)–(3.33) hold for $3 \leqslant m < k$. These imply that $\Delta\omega$, $\mathbf{Q}$, $\ell \in C^\infty((0,T); C^{m-1+\alpha}(\bar{\Omega}))$. Then using (3.10), (3.23), and (3.28) we get ω, $\operatorname{div} \mathbf{Q} \in C^\infty((0,T); C^{m+1+\alpha}(\bar{\Omega}))$ and using (3.30) we get

$$\mathbf{g} \in C^\infty((0,T); \mathbf{C}^{m+1+\alpha}(\bar{\Omega})) \cap C^\infty((0,T); \mathbf{C}^{m+1+\alpha}(\bar{B}_R \setminus \Omega)).$$

We have $\Delta f \in C^\infty((0,T); C^{m+1+\alpha}(\bar{\Omega}))$, $\partial_\nu f \in C^\infty((0,T); C^{m+\alpha}(\partial\Omega))$, and $\partial\Omega \in C^{m+1+\alpha}$ (since $m+1 \leqslant k$). It follows that $f \in C^\infty((0,T); C^{m+1+\alpha}(\bar{\Omega}))$. By the construction of the extension $\mathcal{E}(f)$, if $f \in C^{m+1+\alpha}(\bar{\Omega})$ then

$$\mathcal{E}(f)_{\llcorner B_R \setminus \Omega} \in C_c^{m+1+\alpha}(B_R \setminus \Omega)$$

and there is a constant C so that

$$\|\mathcal{E}(f)\|_{C^{m+1+\alpha}(\bar{B}_R \setminus \Omega)} \leqslant C \|f\|_{C^{m+1+\alpha}(\bar{\Omega})}.$$

Thus we see that $f \in C^\infty((0,T); C^{m+1+\gamma}(\bar{B}_R \setminus \Omega))$ as well. This proves (3.31)–(3.33). □

Proof of Theorem 2: Let $(\psi_0, \mathbf{A}_0)$ satisfy $\mathfrak{H}$. Then $(\psi, \mathbf{A}) = (\omega, \mathbf{Q} + h\mathbf{a})$ is a solution to (3.2)–(3.7), with the required regularity for $t>0$, and such that $(\psi(t), \mathbf{A}(t)) \rightharpoonup (\psi_0, \mathbf{A}_0)$ in $\mathcal{W}^1_2(\Omega) \times \mathbf{W}^1_2(\Omega)$ as $t \downarrow 0$. Furthermore, since (3.9) holds it follows that the proof of Lemma 5 carries over in this gauge. Thus $(\psi(t), \mathbf{A}(t))$ converges strongly to (ψ_0, A_0) in $\mathbf{W}^1_2(\Omega) \times \check{\mathbf{G}}(\mathbb{R}^3)$ as $t \downarrow 0$. Finally the proof of uniqueness from Lemma 7 carries over as well. □

IV. THE COULOMB GAUGE

We next transform $(\omega,\mathbf{Q})$ to other gauges and examine solutions there. We first consider the $\phi=0$ gauge.

Proof of Theorem 3: Let $q(x,t)$ satisfy

$$\partial_t q = \frac{1}{\sigma}\,\mathrm{div}\,\mathbf{Q} \quad \text{in } D_T,$$

$$q\left(x,\frac{T}{2}\right)=0 \quad \text{for } x\in\Omega,$$

$$q=\mathcal{E}(q) \quad \text{in } E_T.$$

From Sec. III that we have

$$\mathcal{E}(\mathrm{div}\,\mathbf{Q})\in C^\infty((0,T);C_c^{2+\alpha}(B_R))\cap W_2^{2,1}(E_T)$$

and $\partial_{\boldsymbol{\nu}}\,\mathrm{div}\,\mathbf{Q}=0$ on $\partial\Omega\times(0,T)$. Moreover if $\partial\Omega\in C^{k+\alpha}$ for $k\geqslant 3$ then

$$\mathcal{E}(\mathrm{div}\,\mathbf{Q})\in C^\infty((0,T);C^{k+\alpha}(\bar{\Omega}))\cap C^\infty((0,T);C_c^{k+\alpha}(B_R\setminus\Omega)).$$

It follows that

$$(\upsilon,\mathbf{B})\equiv(\upsilon,\mathbf{S}+h\mathbf{a})\equiv(\omega e^{-iq},\mathbf{Q}-\nabla q+h\mathbf{a})$$

is a solution to (2.17)–(2.19) in $\mathfrak{A}$, that is classical for $t>0$ with $(\upsilon(x,0),\mathbf{B}(x,0))=(\psi_0 e^{-iq(x,0)},\mathbf{A}_0-\nabla q(x,0))$. Thus the weak solution $(\psi,\mathbf{A})$ to (2.17)–(2.20) is represented as

$$(\psi,\mathbf{A})=(\upsilon e^{iq(x,0)},\mathbf{B}+\nabla q(x,0)). \tag{4.1}$$

□

We next solve the initial value problem in the $\mathrm{div}\,\mathbf{A}=0$ gauge.

Proof of Theorem 4: Given $(\psi_0,\mathbf{A}_0)$ we write $\mathbf{A}_0=\tilde{\mathbf{A}}_0+h\mathbf{a}$ with $\tilde{\mathbf{A}}_0\in\mathbb{V}_2$. Let f_0 satisfy

$$\Delta f_0=0 \quad \text{in } \Omega,$$

$$\partial_{\boldsymbol{\nu}} f_0=-\mathbf{A}_0\cdot\boldsymbol{\nu} \quad \text{on } \partial\Omega, \tag{4.2}$$

such that $\int_\Omega f_0\,dx=0$ and $f_0=\mathcal{E}(f_0)$ in $\mathbb{R}^3$. Then $f_0\in\mathring{W}_2^2(B_R)$ and $(\psi_0(x)e^{if_0(x)},\nabla f_0(x)+\mathbf{A}_0)\in\mathfrak{H}$. Let $(\omega,\mathbf{Q}+h\mathbf{a})$ be the solution from Theorem 2 with $(\omega(x,0),\mathbf{Q}(x,0))=(\psi_0 e^{if_0},\nabla f_0+\tilde{\mathbf{A}}_0)$. We decompose $\mathbf{Q}=\nabla f+\mathbf{g}$ with $\nabla f\in\mathbb{V}_1$, and $\mathbf{g}\in\mathbb{V}_2$. Set $q=-f$, $(\psi,\tilde{\mathbf{A}})=(\omega e^{-if},\mathbf{Q}-\nabla f)$, and $\phi=\mathcal{E}((-(1/\sigma)\mathrm{div}\,\mathbf{Q})_{\llcorner\Omega})+\partial_t f$. From the properties for f established in the proof of Theorem 2 we have that $(\psi_1,\mathbf{A}_1,\phi_1)\equiv(\psi,\tilde{\mathbf{A}}+h\mathbf{a},\phi)$ is a classical solution to (1.1) and (1.2) for $t>0$ such that $(\psi_1(t),\mathbf{A}_1(t)-h\mathbf{a})\to(\psi_0,\tilde{\mathbf{A}}_0)$ in $\mathbf{W}_2^1(\Omega)\times\mathbb{V}_2$ as $t\downarrow 0$.

Suppose that there is a second solution $(\psi_2,\mathbf{A}_2,\phi_2)$. Since it is classical as well for $t>0$ we can take the inner product of (1.1) with $\partial_t\psi_m+i\phi_m\psi_m$, the dot product of (1.2) with $\partial_t\mathbf{A}_m+\nabla\phi_m$ for $m=1,2$, and integrate over $\mathbb{R}^3\times(t_0,T)$ for $0<t_0<T$. To get

$$2\int_{t_0}^{T}[\|\partial_t\psi_m+i\phi_m\psi_m\|_{\mathcal{L}_2(\Omega)}^2+\sigma\|\partial_t\mathbf{A}_m+\nabla\phi_m\|_{\mathbf{L}_2(\Omega)}^2]\,dt+G(\psi_m,\mathbf{A}_m)(T)=G(\psi_m,\mathbf{A}_0)(t_0). \tag{4.3}$$

Since $(\psi_m(t),\mathbf{A}_m(t))\to(\psi_0,\mathbf{A}_0)$ as $t\downarrow 0$ for $m=1,2$ we can let $t_0\downarrow 0$ and conclude that (4.3) is valid with $t_0=0$ such that all terms are finite.

Next we set $u_{m,n}(x,t)=\int_{1/n}^{t}\phi_m(x,\tau)\mathrm{d}\tau$ for $m=1,2$ and $n\in\mathbb{N}$. Then we have

$$\sigma\Delta u_{m,n}=\int_{1/n}^{t}\operatorname{div}\mathbf{j}_{s,m}\mathrm{d}\tau \quad \text{in } \Omega,$$

$$\partial_{\boldsymbol{\nu}}u_{m,n}=(\mathbf{A}_m(x,1/n)-\mathbf{A}_m(x,t))\cdot\boldsymbol{\nu} \quad \text{on } \partial\Omega$$

for each $t>0$. It follows from this, that $\lim_{n\to\infty}u_{m,n}=\int_0^t\phi_m\mathrm{d}\tau$ exists in $C([0,T);W_2^2(\Omega))$. We set $q_m=\int_0^t\phi_m\mathrm{d}\tau+f_0$ where f_0 satisfies (4.2). Using this and (4.3) it follows that

$$(\upsilon_m,\mathbf{S}_m)\equiv(\psi_m e^{iq_m},\mathbf{A}_m+\nabla q_m)\in\mathfrak{A}$$

for each m with the same initial data at $t=0$ on Ω. Moreover both are solutions to (2.12) and (2.13). It follows from Lemma 7 that $(\upsilon_1,\mathbf{S}_1)=(\upsilon_2,\mathbf{S}_2)$. This implies, by gauge invariance that curl $\mathbf{A}_1=$curl $\mathbf{A}_2$. Since div $\mathbf{A}_1=$div $\mathbf{A}_2=0$ we have $\mathbf{A}_1=\mathbf{A}_2$. Furthermore $\mathbf{j}_{1,s}=\mathbf{j}_{2,s}$. Since ϕ_m satisfy

$$\Delta\phi_m=\sigma\operatorname{div}\mathbf{j}_{m,s} \quad \text{in } \Omega,$$

$$\partial_{\boldsymbol{\nu}}\phi_m=-\partial_t\mathbf{A}_m\cdot\boldsymbol{\nu} \quad \text{on } \partial\Omega,$$

and $\int_\Omega\phi_m\mathrm{d}x=0$ for each $t>0$ we have $\phi_1=\phi_2$. This implies that

$$\psi_1=\upsilon_1e^{-iq_1}=\upsilon_2e^{-iq_2}=\psi_2.$$

Thus the solution is unique. □

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APPENDIX

Lemma A.1: Let $k\in L_2(\mathbb{R}^3)$. *Then there exists a function* $f\in W^2_{2,loc}(\mathbb{R}^3)$ *such that* $\nabla f\in\check{\mathbf{H}}(\mathbb{R}^3)$, $\int_\Omega f\mathrm{d}x=0$, *and* $\Delta f=k$ *in* $\mathbb{R}^3$.

Proof: Let $\{k_\varepsilon\}\subset C_c^\infty(\mathbb{R}^3)$ such that $k_\varepsilon\to k$ in $L_2(\mathbb{R}^3)$ as $\varepsilon\to0$. Set $w_\varepsilon=\Gamma*k_\varepsilon\in C^\infty(\mathbb{R}^3)$ where Γ is the fundamental solution for Δ, $\Gamma(x)=C/|x|$. Then $\nabla w_\varepsilon=0(|x|^{-2})$ and $\nabla^2w_\varepsilon=O(|x|^{-3})$ as $|x|\to\infty$. For r large we have

$$\int_{B_r}|\nabla^2w_\varepsilon|^2\mathrm{d}x=\int_{B_r}|\Delta w_\varepsilon|^2\mathrm{d}x-\int_{\partial B_r}\Delta w_\varepsilon\partial_{\boldsymbol{\nu}}w_\varepsilon\mathrm{d}H^2+\int_{\partial B_r}\partial_{x_i}w_\varepsilon\partial_{\boldsymbol{\nu}}(\partial_{x_i}w_\varepsilon)\mathrm{d}H^2$$

Thus

$$\int_{B_r}|\nabla^2w_\varepsilon|^2\mathrm{d}x=\int_{B_r}|\Delta w_\varepsilon|^2\mathrm{d}x+O(r^{-3}),$$

implying

$$\int_{\mathbb{R}^3}|\nabla^2w_\varepsilon|\mathrm{d}x=\int_{\mathbb{R}^3}|k_\varepsilon|^2\mathrm{d}x.$$

Next we let φ_m be a C^∞ cut off function such that $\varphi_m=1$ on B_m and $\varphi_m=0$ on B_{m+1}^c. Set $\mathbf{Z}_m=\varphi_m\nabla w_\varepsilon\in\mathbf{C}_c^\infty(\mathbb{R}^3;\mathbb{R}^3)$. We see for $n,m\geqslant n_0$ and $\varepsilon>0$ fixed that

$$\|\mathbf{Z}_n - \mathbf{Z}_m\|_{\check{\mathbf{H}}(\mathbb{R}^3)} = O(n_0^{-2}).$$

This implies that $\{\mathbf{Z}_m\}$ is a Cauchy sequence in $\check{\mathbf{H}}(\mathbb{R}^3)$ such that $\mathbf{Z}_m \to \nabla w_\varepsilon$ pointwise.

It follows that $\nabla w_\varepsilon \check{\mathbf{H}}(\mathbb{R}^3)$ for each $\varepsilon > 0$.

Let d_ε be a constant so that $\int_\Omega (d_\varepsilon + w_\varepsilon) dx = 0$ and set $f_\varepsilon = d_\varepsilon + w_\varepsilon$. Let R be such that $\Omega \subset\subset B_R$. Then there exists constants $m_j(R)$, $j = 1, 2$ so that

$$\|f_\varepsilon\|_{L_2(B_R)} \leq m_1 \|\nabla f_\varepsilon\|_{\mathbf{L}_2(B_R)} \leq m_2 \|\nabla f_\varepsilon\|_{\mathbf{L}_6(\mathbb{R}^3)} \leq C m_2 \|\nabla f_\varepsilon\|_{\check{\mathbf{H}}(\mathbb{R}^3)} = C m_2 \|k_\varepsilon\|_{L_2(\mathbb{R}^3)}$$

where C is from (1.11).

Since $k_\varepsilon \to k$ in $L_2(\mathbb{R}^3)$ as $\varepsilon \to 0$ we see there exists $f \in W^2_{2,loc}(\mathbb{R}^3)$ with $\int_\Omega f dx = 0$ so that $f_\varepsilon \to f$ in $W_2^2(B_R)$ for each $R < \infty$, $\nabla f_\varepsilon \to \nabla f$ in $\check{\mathbf{H}}(\mathbb{R}^3)$, and $\Delta f = k$. □

Proposition A.1. $\check{\mathbf{V}}(\mathbb{R}^3) = \mathbb{V}_1 \oplus \mathbb{V}_2$ where

$$\mathbb{V}_1 = \{\mathbf{V} \in \check{\mathbf{H}}(\mathbb{R}^3) : \operatorname{curl} \mathbf{V} = 0\},$$

$$\mathbb{V}_2 = \{\mathbf{W} \in \check{\mathbf{H}}(\mathbb{R}^3) : \operatorname{div} \mathbf{W} = 0\},$$

and $\mathbb{V}_1 \perp \mathbb{V}_2$.

Proof: Let $\mathbf{Z} \in \check{\mathbf{H}}(\mathbb{R}^3)$ and take f as in Lemma A.1 so that $\Delta f = \operatorname{div} \mathbf{Z}$ and $\nabla f \in \check{\mathbf{H}}(\mathbb{R}^3)$. Then $\nabla f \in \mathbb{V}_1$. Set $\mathbf{W} = \mathbf{Z} - \nabla f \in \check{\mathbf{H}}(\mathbb{R}^3)$, then $\operatorname{div} \mathbf{W} = 0$ so that $\mathbf{W} \in \mathbb{V}_2$. The decomposition is unique, since if not there would exist $\mathbb{U} \neq 0$ such that $\mathbf{U} \in \mathbb{V}_1 \cap \mathbb{V}_2$. We see from (1.12) that this is impossible.

Finally since we have

$$\|\mathbf{Z}\|^2_{\check{\mathbf{H}}(\mathbb{R}^3)} = \int_{\mathbb{R}^3} [(\operatorname{div} \mathbf{Z})^2 + |\operatorname{curl} \mathbf{Z}|^2] dx$$

we see the inner product on $\check{\mathbf{H}}(\mathbb{R}^3)$ can be represented as

$$\langle \mathbf{Z}, \mathbf{U} \rangle = \int_{\mathbb{R}^3} [\operatorname{div} \mathbf{Z} \operatorname{div} \mathbf{U} + \operatorname{curl} \mathbf{Z} \cdot \operatorname{curl} \mathbf{U}] dx.$$

From this it is clear that $\mathbb{V}_1 \perp \mathbb{V}_2$. □

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Surface barrier for flux entry and exit in mesoscopic superconducting systems

G. R. Berdiyorov, L. R. E. Cabral,[a] and F. M. Peeters[b]
Departement Fysica, Universiteit Antwerpen (Campus Groenenborger), Groenenborgerlaan 171, B-2020 Antwerpen, Belgium

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The energy barrier which has to be overcome for a single vortex to enter or exit the sample is studied for thin superconducting disks, rings, and squares using the nonlinear Ginzburg–Landau theory. The shape and the height of the nucleation barrier is investigated for different sample radii and thicknesses and for different values of the Ginzburg–Landau parameter κ. It is shown that the London theory considerably overestimates (underestimates) the energy barrier for vortex expulsion (penetration). © *2005 American Institute of Physics.* [DOI: 10.1063/1.2010351]

I. INTRODUCTION

Vortex matter in superconducting samples with sizes on the scale of the coherence and penetration lengths has attracted much attention in recent years.[1,2] In such small confined systems the interaction between the vortices and the sample surface, which tries to impose the symmetry of the sample boundary on the vortex configurations, becomes important. This interaction of vortices with the surface manifests itself through the existence of hysteresis behavior and different phase transitions.[1,3–8] The hysteresis effect is a consequence of the presence of an energy barrier between the states with vorticity L and $L+1$, known as the Bean-Livingston energy barrier,[9] (see also Ref. 10) which increases the first-vortex entry field H_s beyond the first critical field H_{c1}. According to this model the surface barrier appears due to a competition between the vortex attraction to the sample walls by its mirror image and its repulsion by screening currents. This model was further developed for cylindrical samples,[11–13] thin disks,[14–16] rings,[17–20] and strips.[21–25] Most of these barrier models are based on the London theory and do not account for the process of vortex formation (vortices are treated as point particles) and describe only the vortex motion far from the sample boundary. In this limit it is possible to find an analytical expression for the energy and forces for an arbitrary arrangement of vortices inside the superconductor.

The origin of barriers for flux penetration and expulsion has been considered recently through a numerical study of the Ginzburg–Landau (GL) equations.[26–30] Within the GL theory vortices are extended objects where the superconducting condensate vanishes over a length scale ξ, which is very different from the London theory where vortices are point particles, i.e., $\xi \to 0$. The allowed vortex configurations correspond to different minima of the free energy in configurational space and the lowest barrier between those two minima is a saddle point which corresponds to the flux penetration and expulsion state. Schweigert and Peeters[27,28] presented an approach for finding the saddle point states in thin disks and calculated numerically the heights of the free energy barriers separating the stable states with a different number of vortices. Their approach was later extended to the case of superconducting rings.[29]

In this article we study the surface barrier in mesoscopic disks, rings, and squares for different values of the GL parameter κ though a numerical solution of the GL equations using analytical expressions for the phase of the order parameter as obtained from the London approach. Previous

[a]Present address: Departamento de Fisica, Universidade Federal de Pernambuco, 50670-901, Recife-PE, Brazil.
[b]Electronic mail: francois.peeters@ua.ac.be

studies were limited to the London theory or assumed the limit of very thin disks such that only the first GL equation had to be solved. In our approach, both GL equations are solved self-consistently and by fixing the phase of the order parameter locally we are able to move the vortex through the sample. We compare our results with those obtained from the London theory.

The article is organized as follows. The theoretical formulation of the problem is given in Sec. II. The Bean-Livingston barrier for a single vortex entry/exit in a small radius disk is studied in Sec. III for different thickness of the disk and for different values of the GL parameter. In Sec. IV we compare our calculations with the results obtained from the London theory. The $L=2$ giant vortex state in a superconducting disk is considered in Sec. V, and the break up into a multivortex state is investigated. The surface barrier for vortices in a superconducting ring and in a square sample is investigated in Secs. VI and VII, respectively. The results of the present paper are summarized in Sec. VIII.

II. THEORETICAL FORMALISM

A. Ginzburg–Landau theory

We consider a thin superconducting disk or ring with thickness $d<\xi,\lambda$ immersed in an insulating medium in the presence of a perpendicular uniform magnetic field H_0. Measuring the distance in units of the coherence length ξ, the vector potential $\vec{A}$ in $c\hbar/2e\xi$, the magnetic field in $H_{c2}=c\hbar/2e\xi^2=\kappa\sqrt{2}H_c$, and the order parameter Ψ in $\sqrt{-\alpha/\beta}$ with α,β being the GL coefficients, the system of GL equations can be written in the following form:[5]

$$(-i\vec{\nabla}_{2\mathrm{D}}-\vec{A})^2\Psi=\Psi(1-|\Psi|^2), \tag{1a}$$

$$-\Delta_{3\mathrm{D}}\vec{A}=\frac{d}{\kappa^2}\delta(z)\vec{j}_{2\mathrm{D}}, \tag{1b}$$

$$\vec{j}_{2\mathrm{D}}=\frac{1}{2i}(\Psi^*\vec{\nabla}_{2\mathrm{D}}\Psi-\Psi\vec{\nabla}_{2\mathrm{D}}\Psi^*)-|\Psi|^2\vec{A}, \tag{1c}$$

where the indices 2D, 3D refer to two- and three-dimensional operators, respectively, and $\vec{j}_{2D}$ is the density of the superconducting current. The boundary conditions to Eqs. (1a) and (1b) correspond to zero superconducting current at the sample boundaries and an uniform external magnetic field far from the sample $\vec{A}_{|\vec{r}|\to\infty}=\frac{1}{2}[\vec{r}\times\vec{H}_0]$, respectively. To solve the coupled set of nonlinear Eqs. (1a) and (1b) we follow the numerical approach of Schweigert and Peeters.[4,5]

The Gibbs free energy, in units of $F_0=H_c^2V/8\pi$, for the given vortex states is calculated from

$$F=V^{-1}\int_V[2(\vec{A}-\vec{A}_0)\cdot\vec{j}_{2D}-|\Psi|^4]\mathrm{d}\vec{r}, \tag{2}$$

where integration is performed over the sample volume V, and $\vec{A}_0$ is the vector potential of the uniform magnetic field. For Al disks with 1.3 μm (0.2 μm) radius and 0.13 μm (0.01 μm) thickness the unit F_0 is of the order $\sim 10^3$ eV (2 eV) (see, e.g., Ref. 1). The dimensionless magnetization is defined as

$$M=\frac{\langle H\rangle-H_0}{4\pi}, \tag{3}$$

where $\langle H\rangle$ is the magnetic field averaged over the sample.

B. London approach and phase of the order parameter

In thin films, within the limits $S\gg\xi$ (where S are the transverse dimensions of the film) and $H\ll H_{c2}$, $|\Psi|^2$ is practically constant throughout the specimen, except at distances $\sim\xi$ from the vortex cores or the interface. These conditions are satisfied in the London limit, and one may

consider $|\Psi|^2=$const. with singularities in the phase of Ψ at the vortex core positions. Considering the magnetic field pointing in the z direction, the second G-L equation reduces to the London equation,

$$H_z + \frac{4\pi\Lambda}{c}(\nabla \times \vec{J})_z = \Phi_0 \sum_{k=1}^{L} \delta(\vec{r} - \vec{r}_k), \tag{4}$$

where $\vec{J}=\int_0^d \vec{j}\mathrm{d}z \approx \vec{j}d$, $\Lambda=\lambda^2/d$, and $\vec{r}_k$ is the position of vortex k, d is the film thickness.

In order to solve the London equation one may consider taking $\vec{J}=\nabla\times\hat{z}g$, where $g(\vec{r})$ is the streamline function.[31] This function has the property that $g_\Gamma=$constant, where g_Γ represents the value of $g(\vec{r})$ at the specimen edges. For samples without holes, one may consider $g_\Gamma=0$. Otherwise, $g(\vec{r})$ may take different constant values at each hole and at the edges.[20,32] In addition, in thin films where $\Lambda \gg S$, demagnetization effects can be disregarded, and $H_z \approx H_0$ in Eq. (4). This makes the London equation of the Poisson type

$$-\frac{4\pi\Lambda}{c}\nabla^2 g = \Phi_0 \sum_{k=1}^{L} \delta(\vec{r} - \vec{r}_k) - H_0, \tag{5}$$

which can be solved by standard techniques. Analytical solutions, for example, of the problem of a vortex in a thin disk[14,15] or in a ring,[20] have been found. Such analytical expressions—from which the energy of the system can be calculated—are suitable for simulations of systems containing a large number of vortices.[16]

As pointed out by Fetter[14] g_v, which is the streamline function for a vortex inside the mesoscopic superconductor with zero external magnetic field, and θ (in two-dimensional systems) are related by the real and imaginary parts of a complex function, $\Omega(z)$, since both g_v and θ satisfy Laplace equation (except at the vortex core positions). This allows one to obtain analytic expressions for the phase of the order parameter, θ. For a disk, the phase of the order parameter is given by the imaginary part of[14,16] (see also Ref. 33)

$$\Omega = \sum_{j=1}^{L} \ln\left[\left(\frac{z-(R/z_j)^2 z_j}{z-z_j}\right)\frac{r_j}{R}\right], \tag{6}$$

where $z=r\exp(i\phi)=x+iy$, $z_j=r_j\exp(i\phi_j)$ is the position of vortex j, and R is the disk radius. For the case of rings with inner (outer) radius $a(b)$, θ–for one vortex at $(x,0)$–is the imaginary part of

$$\Omega = \ln\left[\frac{A(z,x))}{B(x)}\right] - \left[N + \frac{\ln(b/x)}{\ln(b/a)}\right]\ln(z/a),$$

$$A(z,x) = \frac{\mathrm{cn}[2\gamma\ln(x/a),m]}{\mathrm{sn}[2\gamma\ln(x/a),m]} - \frac{\mathrm{cn}[\gamma\ln(x/z),m]}{\mathrm{sn}[\gamma\ln(x/z),m]},$$

$$B(x) = \frac{\mathrm{cn}[2\gamma\ln(x/a),m]}{\mathrm{sn}[2\gamma\ln(x/a),m]} - \frac{\mathrm{cn}[\gamma\ln(x/a),m]}{\mathrm{sn}[\gamma\ln(x/a),m]}, \tag{7}$$

where N is the number of vortices inside the hole, $(a\leqslant x\leqslant b,0)$ is the vortex position, cn and sn are the Jacobi elliptic functions, $\gamma=K(m)/\ln(b/a)$, $K(m)$ is the complete elliptic integral and the parameter m is determined by the relation $K(1-m)\ln(b/a)=\pi K(m)$ according to Ref. 20.

For a rectangle with dimensions $0\leqslant x\leqslant a$ and $0\leqslant y\leqslant b$, the complex function which is a solution of Eq. (5) (for $H_0=0$) is given by

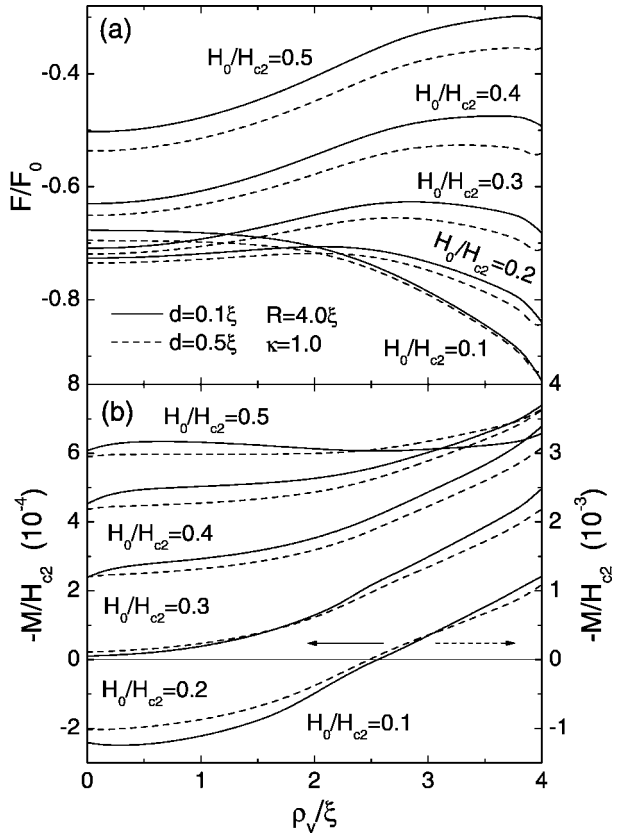

FIG. 1. (a) The free energy and (b) the magnetization of the $L=1$ state as a function of the radial position of the vortex for different values of the applied magnetic field. The radius of the disk is $R=4.0\xi$, the thickness is $d=0.1\xi$ (solid curves) and $d=0.5\xi$ (dashed curves referred to the right axis). The Ginzburg–Landau parameter is $\kappa=1.0$.

$$\Omega=\sum_{j=1}^{L}\ln\left[\frac{\mathrm{sn}^2(K(m)z/a,m)-\mathrm{sn}^2(K(m)z_j^*/a,m)}{\mathrm{sn}^2(K(m)z/a,m)-\mathrm{sn}^2(K(m)z_j/a,m)}\right], \tag{8}$$

which is the same as for the problem of an electric charge inside a rectangle held at zero potential (see Ref. 34). The value of m is now chosen to satisfy $K(1-m)=(b/a)K(m)$ and $z_j^*=r_j\exp(-i\phi_j)$ is the conjugate of the position of vortex j.

III. A SUPERCONDUCTING DISK WITH A SINGLE VORTEX

In earlier works (see, e.g., Refs. 3–5) which were devoted to the study of the properties of superconducting disks, vortex configurations were obtained through a minimization of the energy. In this work we investigate the energy and magnetization of a superconducting disk, by fixing vortices in an arbitrary position for different applied magnetic field. In general, such vortex configurations are not stable. In experiments this can be realized, e.g., by pinning vortices through a pinning potential. First, we consider in Fig. 1 a superconducting disk with radius $R=4.0\xi$ and different thickness d and GL parameter $\kappa=1.0$. For the given parameters of the disk, the $L=1$ state is stable in the magnetic field range $H_0/H_{c2}=0.125-0.71$.[35] As for the bulk case,[9] an energy barrier to flux penetration and expulsion in the disk exists in some magnetic field range. Below this magnetic field range the function $F(\rho_v)$, where ρ_v is the radial position of the vortex, has only one extremum which is a maximum at $\rho_v=0$, i.e., the vortex will leave the sample. At low fields vortices are unstable inside the sample and there is an energy cost associated with vortex entrance. For higher fields it is energetically favorable for the vortex to sit inside the sample and $F(\rho_v)$ is a

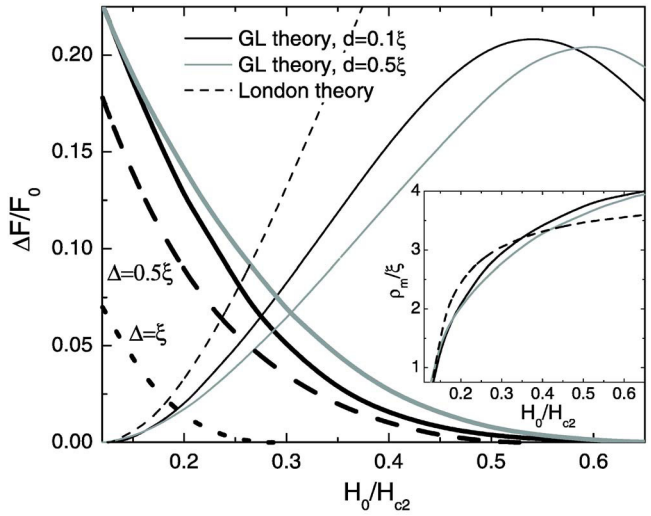

FIG. 2. Energy barrier for the vortex penetration (thick curves) and escape (thin curves) as a function of the applied field for a disk with $R=4.0\xi$, $d=0.1\xi$ (solid black curves), and $d=0.5\xi$ (solid gray curves) and for $\kappa=1.0$. The inset shows the position of the barrier maximum ρ_m as a function of the applied field. The results of the London theory are given by the dashed curves for two different values of the cutoff parameter Δ.

function with a single minimum at $\rho_v=0$. The increase of the disk thickness does not change the qualitative behavior of the free energy but shifts the free energy to lower energy. For small fields the magnetization curves show paramagnetic response (i.e., $M>0$) when the vortex is located close to the center and $-M$ increases with shifting the vortex from the center of the sample. This paramagnetic behavior for the total magnetization results from the existence of the energy barrier. Increasing the disk thickness leads to more flux expulsion from the sample.

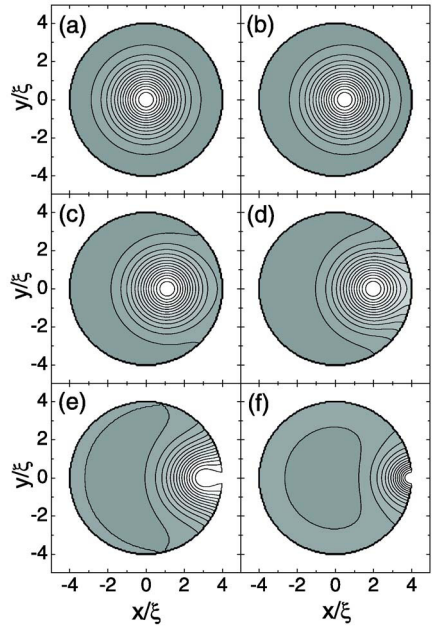

FIG. 3. Contour plots of the Cooper pair density distribution in the disk with radius $R=4.0\xi$, thickness $d=0.1\xi$, $\kappa=1.0$ at $H_0/H_{c2}=0.2$ for different values of the vortex position: (a) $\rho=0\xi$, (b) $\rho=0.5\xi$, (c) $\rho=1.0\xi$, (d) $\rho=2.0\xi$, (e) $\rho=3.0\xi$, and (f) $\rho=3.85\xi$.

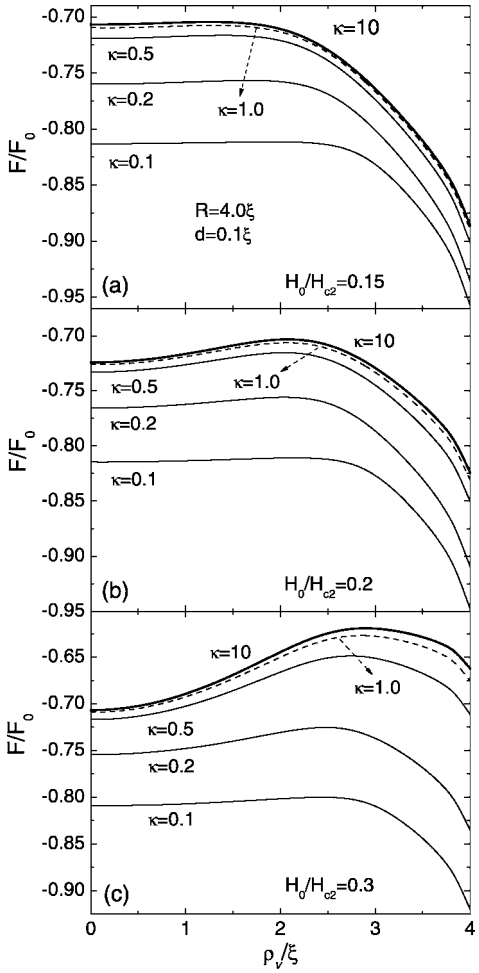

FIG. 4. The free energy as a function of the radial position of the vortex ρ_v for different values of the GL parameter κ and for the applied fields (a) $H_0/H_{c2}=0.15$, (b) $H_0/H_{c2}=0.2$, and (c) $H_0/H_{c2}=0.3$. The radius of the disk is $R=4.0\xi$ and the thickness is $d=0.1\xi$.

Figure 2 presents the energy barrier for vortex penetration (thick curves), $\Delta F_{\text{penetration}}=F_{\max}-F_{\rho_v=R}$, and expulsion (thin curves), $\Delta F_{\text{expulsion}}=F_{\max}-F_{\rho_v=0}$, as a function of the applied field for $d=0.1\xi$ (solid black curves) and $d=0.5\xi$ (solid gray curves). As seen from this figure, the barrier for flux escape disappears at low fields, whereas the barrier for vortex entry increases. Increasing the external field leads to an increase of the barrier for vortex expulsion and to a decrease of the barrier for vortex penetration. The first critical field H_{c1} is the field at which the energy for a vortex inside the superconductor is the same as the energy of the vortex at the sample edge, i.e., $\Delta F_{\text{penetration}}=\Delta F_{\text{expulsion}}$. Therefore, the crossing point of the two barriers determines the first critical field H_{c1}. This barrier is influenced by the sample thickness: the expulsion barrier decreases and the penetration barrier and critical field H_{c1} increases by increasing the thickness. The latter indicates the larger repulsion of the vortex from the surface of the sample with larger thickness. The London theory (dashed curves in Fig. 2) predicts a much larger energy barrier for vortex expulsion (near H_{c1} it is almost a factor of 2 larger). Because the London theory fails close to the sample boundary (i.e., $F\to-\infty$ when $r\to R$), we need to introduce a cutoff distance Δ in order to find finite value for $\Delta F_{\text{penetration}}$. Therefore, within the London theory, we defined $\Delta F_{\text{penetration}}=F_{\max}-F_{\rho_v=R-\Delta}$. The results for two different choices, i.e., $\Delta=\xi$ (dotted curve) and $\Delta=0.5\xi$ (dashed curve), are shown in Fig. 2. For both choices we find that the penetration barrier and the magnetic field range over which this barrier exists, is much smaller within the London approach as

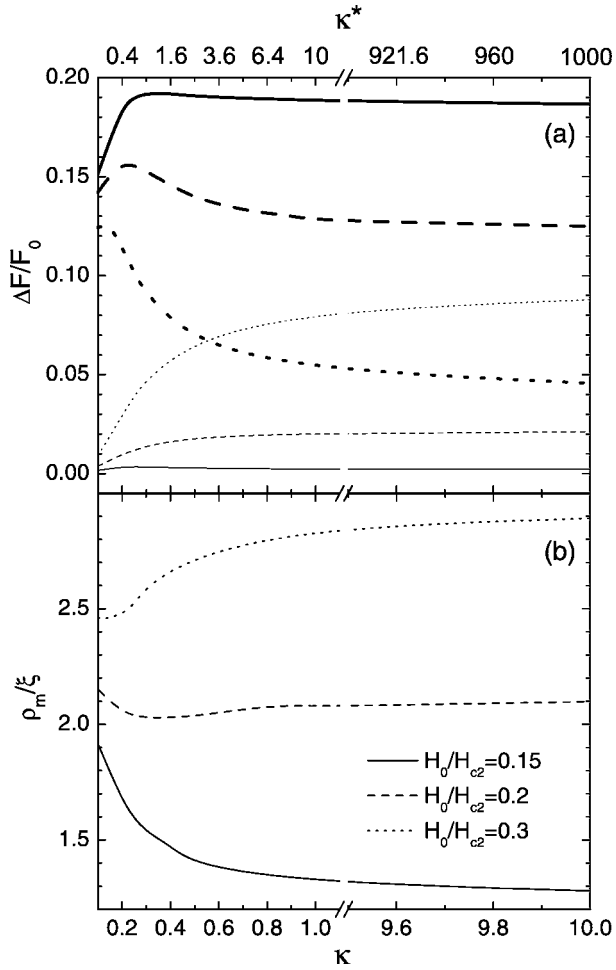

FIG. 5. (a) Energy barrier for flux penetration (thick curves) and escape (thin curves) and (b) the position of the barrier maximum ρ_m as a function of the GL parameter κ for the applied fields $H_0/H_{c2}=0.15$ (solid lines), $H_0/H_{c2}=0.2$ (dashed lines), and $H_0/H_{c2}=0.3$ (dotted lines), with a break at $\kappa=1.1$.

compared to the one in the GL theory. These results show clearly the limited applicability of the surface barrier when obtained from the London theory in case of finite values of the GL-parameter. When calculating the saddle point states, Schweigert and Peeters[27] found a better agreement with the London theory, and a small difference was found only beyond H_{c1}. The position of the barrier maximum ρ_m (see the inset of Fig. 2) is shifted from the center of the sample to the sample boundary with increasing applied field. For small fields ρ_m calculated from the London theory is larger compared to the one obtained from the GL theory and for larger fields the reverse is found.

We found that there is no energy barrier when we place an antivortex inside the disk for any radius of the sample and any positive applied field. The energy minimum is at the edge of the disk and consequently the antivortex will leave the sample.

The spatial distribution of the Cooper-pair density $|\Psi|^2$ calculated for different vortex positions ρ_v is plotted in Fig. 3 for $H_0/H_{c2}=0.2$ and for disk thickness $d=0.1\xi$. Notice the noncircular shape of the contour lines, when the vortex is close to the sample boundary.

The dependence of the surface barrier on the GL parameter κ is shown in Fig. 4. This figure gives the free energy of the disk with radius $R=4.0\xi$ and thickness $d=0.1\xi$, as a function of the vortex position ρ_v for different values of κ, at (a) $H_0/H_{c2}=0.15$, (b) $H_0/H_{c2}=0.2$, and (c) $H_0/H_{c2}=0.3$. Note that the free energy strongly depends on κ: with increasing GL parameter from $\kappa=0.1$ (corresponding to an effective GL parameter $\kappa^*=\kappa^2\xi/d=0.1$) to $\kappa=1.0$ ($\kappa^*=10.0$) (dashed

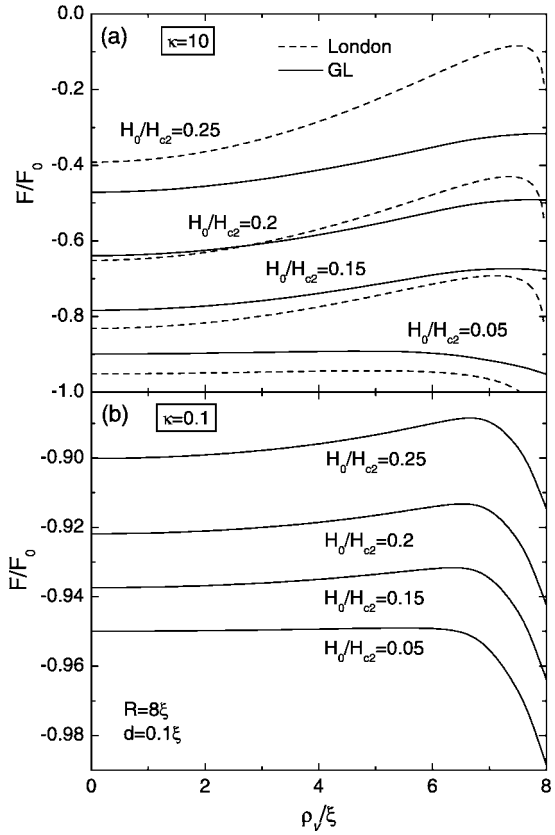

FIG. 6. The free energy of the disk with radius $R=8.0\xi$ and thickness $d=0.1\xi$ as a function of the radial position of the vortex ρ_v for different values of the applied magnetic field. The results from the London theory are given by dashed curves and the results of the GL theory are given by solid curves for (a) $\kappa=10$ and (b) $\kappa=0.1$.

line) the free energy increases considerably, which is due to the larger penetration of the field inside the sample; further increase of κ (thick solid line) leads only to a minor increase of the free energy. We found that the results for $\kappa=10$ ($\kappa^*=1000$) is identical to the results for $\kappa\geqslant 100$.

Figures 5(a) and 5(b) show the height of the barrier for vortex penetration (thick curves) and expulsion (thin curves) and the position of the barrier maximum as a function of κ. At low fields (solid line) the maximum in the expulsion barrier (thin curves) is found for small values of κ and the barrier decreases with further increase of κ. For higher fields (dashed and dotted curves) the expulsion barrier increases with increasing κ and we see the crossing of the curves for penetration and expulsion barrier. At small fields the position of the barrier maximum [Fig. 5(b)] decreases with increasing κ and for higher fields a minimum appears in the plot of the barrier position.

IV. COMPARISON WITH LONDON THEORY FOR LARGE DISKS

The London theory fails close to the sample boundaries at distances of order ξ and for small inter-vortex distances. As a consequence the applicability of the London theory for very small mesoscopic samples is questionable. Therefore, we will consider larger disks and compare the results of the London theory with our GL calculations. In this case the London approach, in which the superconducting density is assumed to be a constant, gives rather accurate results. This model was extended to arbitrary radius of the disk by taking into account the spatial nonuniformity of the modulus of the order parameter in Refs. 16 and 27. This improved version of the London theory was shown to be in good agreement with the GL theory below the nucleation field $H=H_n$ and breaks down for higher fields.

Figure 6 shows the free energy of the superconducting disk with radius $R=8.0\xi$ as a function

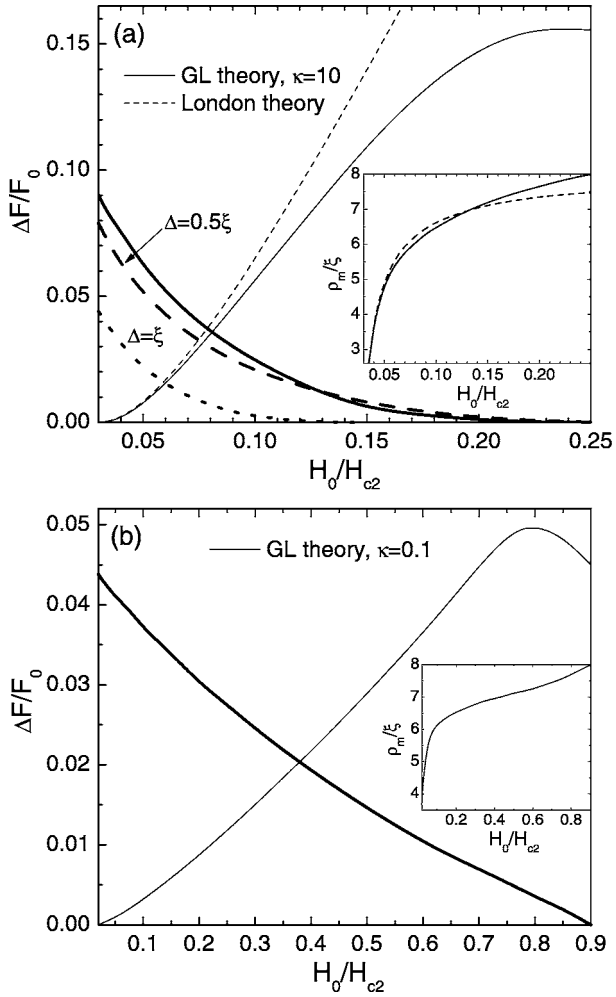

FIG. 7. Energy barrier for vortex penetration (thick curves) and escape (thin curves) as a function of the applied magnetic field for the disk of Fig. 6. Dashed curves are the results of the London theory and solid curves are the one of the GL theory for (a) $\kappa=10$ and (b) $\kappa=0.1$. The insets show the position of the barrier maximum ρ_m as a function of the applied field.

of the vortex position ρ_v, calculated from the London theory (dashed curves) and the GL theory (solid curves) for (a) $\kappa=10$ and (b) $\kappa=0.1$ at different applied fields. The disk thickness is $d=0.1\xi$ whose value is less important in the GL theory [see Eq. (1b)] for larger κ. The free energy shows a similar qualitative behavior in both cases: the appearance of the energy barrier at high fields and its disappearance at lower fields. But the value of the free energy is not the same: at low fields the free energy from the London theory is lower than the free energy of the GL theory which is opposite at higher fields. For small κ the free energy calculated within the GL theory is lower than in the corresponding case of $\kappa=10$, which is the reason why the results of the London theory are not shown in Fig. 6(b).

The height of the energy barrier for the vortex penetration (thick curves) and expulsion (thin curves) is given in Fig. 7 as a function of the applied field. It is seen from this figure that for larger value of κ (a) and at small fields ($H_0<H_{c1}$) our results for the expulsion barrier show good agreement with the one from the London approach. At higher fields the London theory gives a larger expulsion barrier. The penetration barrier within the London limit is calculated for two different values of the cutoff parameter $\Delta=0.5\xi$ (tick dotted curve) and $\Delta=\xi$ (thick dashed curve). For $\Delta=\xi$ a reasonable good agreement with the GL-approach is found for $H_0>H_{c1}$. For small κ [Fig. 7(b)] a surface barrier is found over a larger range of magnetic field, whereas the barrier itself

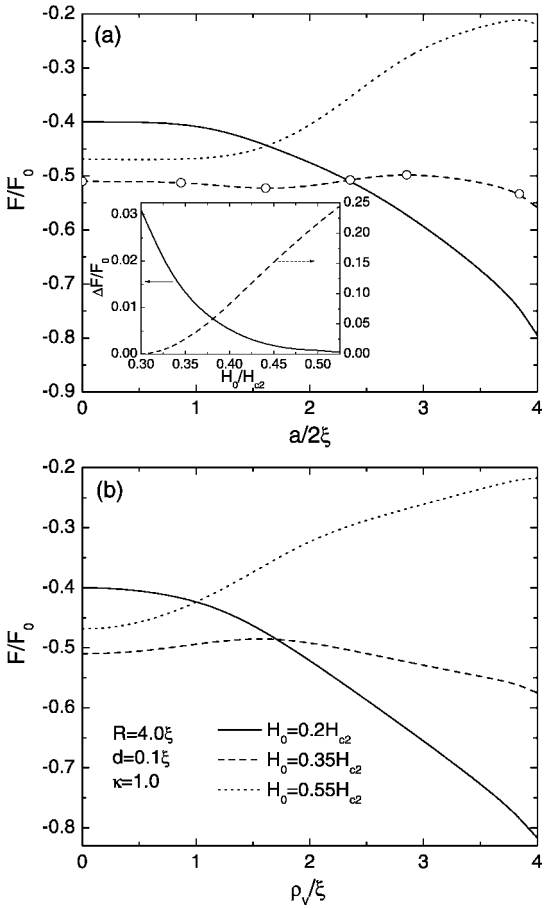

FIG. 8. (a) The free energy of the multivortex ($L=2$) state as a function of the inter-vortex distance a, and (b) the free energy of the giant vortex ($L=2$) state as a function of the radial position of the giant vortex ρ_v for different magnetic fields. The inset shows the height of the energy barrier for the transition from the multivortex $L=2$ state to the giant vortex $L=2$ state (solid curve) and for the transition from multivortex $L=2$ state to the $L=0$ state (dashed curve, referred to the right axis) as a function of the applied field. The radius of the disk is $R=4.0\xi$, the thickness is $d=0.1\xi$, and $\kappa=1.0$.

is smaller than for the larger κ case. If we compare these results with the one for a smaller disk radius (Fig. 2) we see that the barrier height and the magnetic field range, where this barrier exists, decreases with increasing R for fixed κ.

V. THE $L=2$ STATE IN A DISK

A. Giant vortex versus multivortex state

For larger disk radius (i.e., $R \geqslant 3.0\xi$), several vortices can enter the sample at once (see for example Ref. 28), indicating that at the entrance field the energy barriers separating the different vortex states become very small. In such samples many different superconducting states can exist at a given magnetic field. Our approach allows us to study the transitions between these states and calculate the energy barrier as a function of the vortex position for any number of vortices L.

We start with the most simple case—the $L=2$ state, which was studied in Ref. 28 within the modified London approach. Figure 8(a) shows the free energy for a disk with $R=4.0\xi$ and $d=0.1\xi$ as a function of the inter-vortex distance a for different applied fields. It is seen that, at larger magnetic fields (dotted curve, $H_0=0.55H_{c2}$), the free energy has a minimum when both vortices are located in the center implying that the giant vortex state is preferred. With decreasing magnetic field (dashed curve, $H_0=0.35H_{c2}$) the free energy has a minimum when the vortices are separated at a distance $a=3.22\xi$ and has a maximum for $a=5.7\xi$, which shows that at this mag-

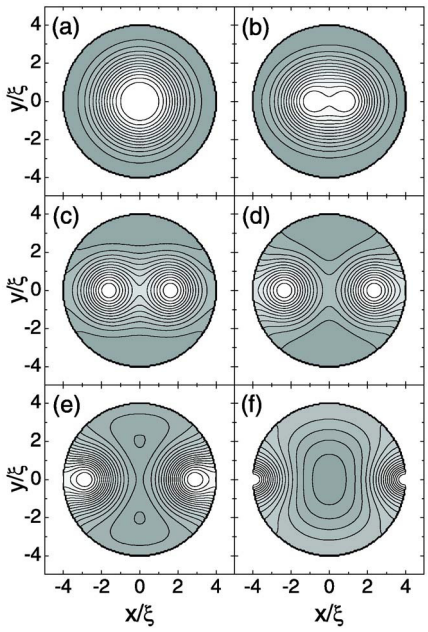

FIG. 9. Contour-plot of the Cooper pair density for a disk with $R=4.0\xi$, $d=0.1\xi$, $\kappa=1.0\xi$ at $H_0/H_{c2}=0.35$ and the distance between vortices is: (a) $a/2=0\xi$, (b) $a/2=0.87\xi$, (c) $a/2=1.61\xi$, (d) $a/2=2.36\xi$, (e) $a/2=2.85\xi$, and (f) $a/2=3.85\xi$.

netic field the multivortex state is energetically favorable. The inset of Fig. 8 shows the height of the energy barrier for the transition from this multivortex state to the giant vortex state (solid curve) and for the transition from the multivortex state to the $L=0$ state (dashed curve, referred to the right axis). Further decreasing the field (solid line, $H_0=0.2H_{c2}$) there is no energy barrier for vortex expulsion and vortices leave the sample. To compare with the multi-vortex state, we plotted in Fig. 8(b) the free energy of the giant vortex state with $L=2$ as a function of the radial position of the giant vortex. It is seen from this figure that the giant vortex behaves similar to what we found for a single vortex: at small fields there is a barrier for the giant vortex to enter the sample which disappears with increasing applied field. The distribution of the Cooper-pair density for different values of a, which are indicated by open circles in Fig. 8, is shown in Fig. 9.

B. Entrance and exit of the second vortex

Contrary to macroscopic samples, where vortices can be located far from the edge of the sample, in mesoscopic samples vortices are confined by the potential well generated by the sample surface, and even a vortex fixed in the center of the sample is still influenced by the edge, generating a contribution to the barrier for the next vortex entry and exit. Now, we fix the first vortex at a given point and change the position of the second vortex. Although the presence of a second vortex influences the first vortex position, a pinning center can fix the first vortex position, i.e., one can study the energy landscape for the second vortex when the first is pinned at ρ_0.

Figures 10(a)–10(c) show the free energy of the superconducting disk for $R=4.0\xi$ and $d=0.1\xi$ as a function of the second vortex position ρ_v, when the first vortex is fixed in the same radial line with the second one (see Fig. 11) at $\rho_0=0$ (solid curve), $\rho_0=R/2$ (dashed curve), and $\rho_0=R$ (dotted curve). At $H_0/H_{c2}=0.2$ (a) and $\rho_0=0$ the second vortex prefers to leave the sample, because there is no barrier for the exit of this vortex (solid line). The barrier for the second vortex exit appears when we shift the first vortex to the sample boundary (dotted line). Notice that for this value of the applied field a single vortex feels a largest energy barrier (compare with Fig. 2). For higher fields [Figs. 10(b) and 10(c)] a giant vortex state in the center of the sample becomes energetically favorable. Figure 11 shows the contour plot for the Cooper pair density for different positions of the first and second vortex at $H_0/H_{c2}=0.35$.

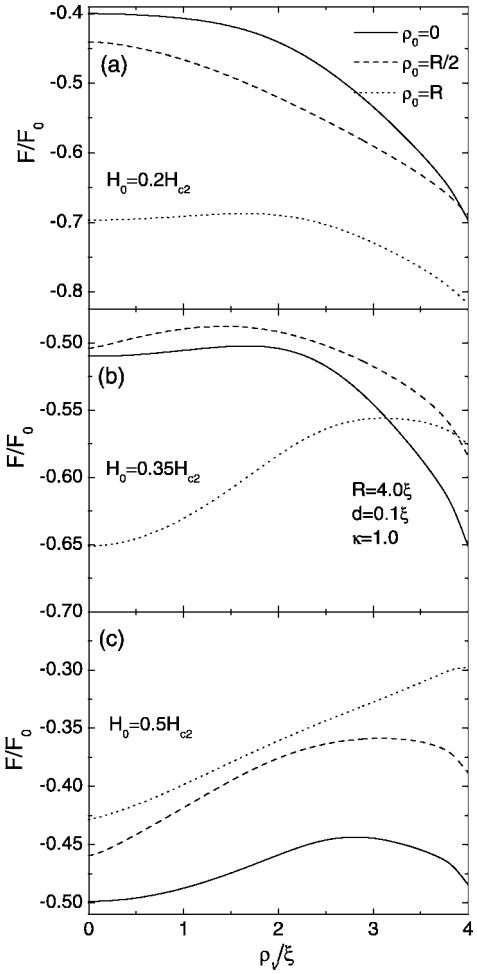

FIG. 10. The free energy of the $L=2$ state as a function of the second vortex position ρ_v, when the first vortex is fixed at $\rho_0=0$ (solid curve), $\rho_0=R/2$ (dashed curve), and $\rho_0=R$ (dotted curve), at different magnetic fields (a) $H_0=0.2H_{c2}$, (b) $H_0=0.35H_{c2}$, and (c) $H_0=0.5H_{c2}$. The radius is $R=4.0\xi$, thickness is $d=0.1\xi$ and $\kappa=1.0$.

VI. SUPERCONDUCTING RING

Although the problem of flux quantization in large superconducting rings was shown experimentally a long time ago,[36] recently there was renewed interest for fluxoid dynamics in such a geometry (see, e.g., Ref. 19), where jumps in the magnetization curve corresponding to changes of the vorticity larger than unity[17] were observed. These jumps appear due to the presence of several metastable states with different vorticity L at a given field and strongly depends on the stability condition for those metastable states.[18] Transitions between these states were investigated within the GL theory in Ref. 29 through the saddle point, i.e., the lowest barrier between two different energy minima. The time for flux penetration and expulsion is determined by the height of the energy barrier. In this section we consider superconducting rings with different inner and outer radii and calculate the energy barrier for flux penetration/exit. This problem was recently considered in Ref. 20 in the London limit.

As an example, we consider a superconducting ring with outer radius $R=15\xi$, inner radius $R_i=5\xi$, thickness $d=0.1\xi$, and $\kappa=1.0$. Figures 12(a)–12(c) show the free energy of the ring as a function of the radial position of the vortex ρ_v for different values of the applied field. At low fields (a) and when there is no vortex trapped inside the ring ($L_0=0$) the maximum of the barrier is in the center of the superconducting region of the ring and the free energy is lowest at the outer

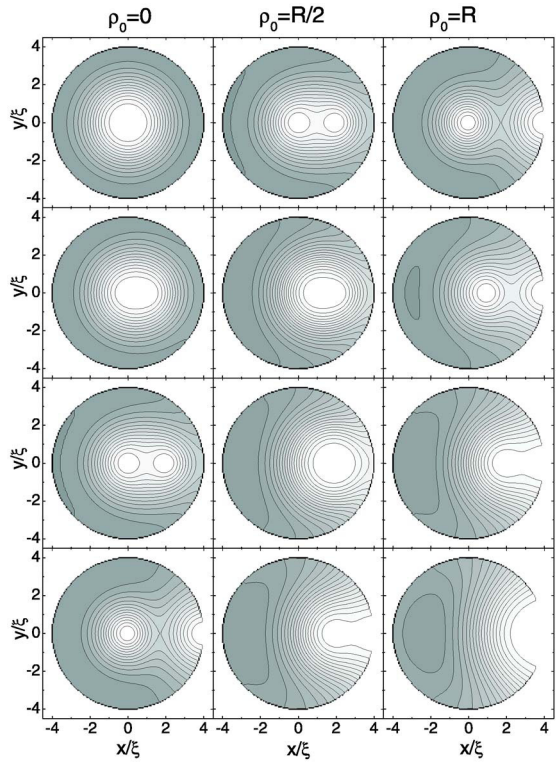

FIG. 11. The Cooper pair density of the $L=2$ state in the disk with $R=4.0\xi$ and $d=0.1\xi$ at $H_0/H_{c2}=0.35$. The first vortex is fixed at $\rho_0=0$ (first column), $\rho_0=R/2$ (second column), and $\rho_0=R$ (third column). From top to bottom figures we positioned the second vortex at $\rho_1=0$ (first row), $\rho_1=1.0\xi$ (second row), $\rho_1=2.0\xi$ (third row), and $\rho_1=4.0\xi$ (fourth row).

ring edge indicating that it costs energy to add an additional vortex inside the ring. When increasing the field the barrier maximum shifts to the outer boundary of the sample [Figs. 12(b) and 12(c)]. The inset of Fig. 12 shows the height of the energy barrier for flux penetration (thick curve) and escape (thin curve) as a function of the applied field. It is seen from this figure that even for zero applied field there is a barrier for vortex expulsion and we have to apply negative field to transit to the $L=0$ state. If there are one or more vortices inside the ring the energy barrier shifts to the inner boundary of the sample and the vortex prefers to leave the sample. For some critical value of the applied field and for a given number of vortices inside the ring the energy has a local minimum in the superconducting region of the ring [dotted and thick solid curves in Fig. 12(c)] indicating that a vortex can be trapped in a metastable state in the superconducting region of the ring. This is more pronounced when there are more vortices inside the ring and the field is higher [thick solid curve in Fig. 12(c)]. For $H_0/H_{c2}=0.05$ it is clear from Fig. 12(c) that energetically it is more favorable to add one extra vortex inside the sample when $L_0 \leqslant 3$. Figure 13 shows contour plots of the phase of the order parameter (left column) and Cooper pair density (right column) for $L_0=1$ and different position of the vortex. Notice that a closed path within $\rho < rho_v$, we correctly have a change in the phase of 2π (i.e., one flux is trapped inside the ring). If, otherwise, we choose a closed path including the vortex position, ρ_v, the phase changes by 4π. The contour lines of the Cooper pair density are nearly circular close to the vortex core, but are distorted farther away due to the geometry of the sample.

VII. SQUARE SAMPLE

The energy barrier for flux penetration and exit in mesoscopic superconductors is partly due to a geometric barrier, which depends on the shape of the sample, and is even more pronounced for superconductors with rectangular cross section. In such samples the edge barrier is caused by a

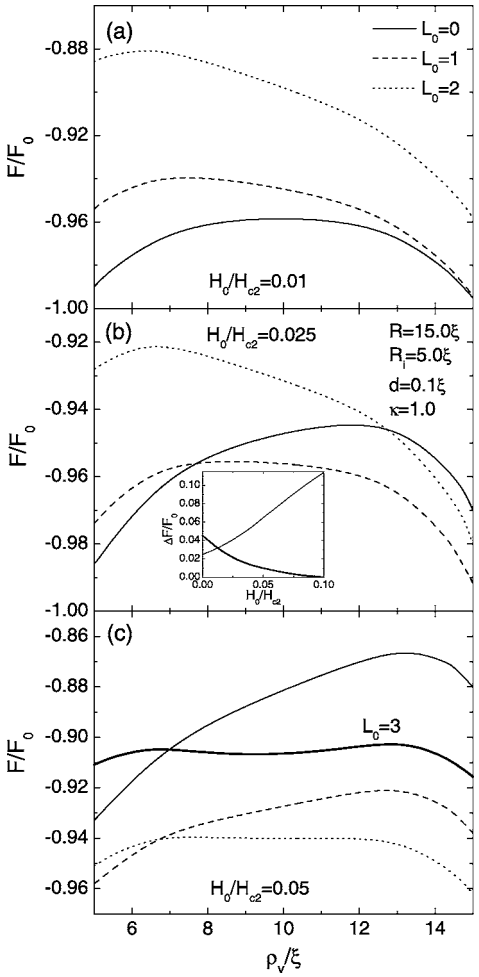

FIG. 12. The free energy of the superconducting ring with outer radius $R=15\xi$, inner radius $R_i=5\xi$, thickness $d=0.1\xi$, and $\kappa=1.0$ as a function of the radial position of the vortex ρ_v for three values of the applied field (a) $H_0=0.01H_{c2}$, (b) $H_0=0.025H_{c2}$, and (c) $H_0=0.05H_{c2}$. The number of vortices inside the hole is $L_0=0$ (solid curves), $L_0=1$ (dashed curves), and $L_0=2$ (dotted curves). Thick solid curve (c) corresponds to $L_0=3$ and $H_0=0.075H_{c2}$. The inset in (b) shows the height of the energy barrier for flux penetration (thick curve) and expulsion (thin curve) for $L_0=0$ as a function of the applied field.

delayed penetration of flux lines at the four corners and exhibits hysteretic behavior even if the sample is free of pinning centers.[22–24] Therefore, in this section we consider a square superconducting sample to study the influence of its edges to the surface barrier. Superconducting cylinders with rectangular cross section were recently considered in Ref. 37 within the London theory in the presence of an axial magnetic field. Calculations show that the energy barrier is higher in the corners and the first vortex tends to enter the sample through the middle of the edges.[38]

Figure 14 shows the contour plot of the free energy of the square superconductor with size $a=8.0\xi$, thickness $d=0.1\xi$, and $\kappa=1.0$ for four different values of the applied field, where dark gray regions correspond to higher energy. At small fields (a) the energy is maximum when the vortex is at the center of the sample and decreases when the vortex approaches to the boundary. The plot of the cross sections (right column) shows that the energy is lower in the corners. An increase of the magnetic field leads to the appearance of an energy barrier (b,c) which is higher near the corners of the sample. By further increasing the applied field (d) the position of the barrier shifts to the sample boundary. It is seen from the plot of the cross sections of the barrier energy that the barrier disappears first near the edges of the sample, which means that the vortex penetrates the sample through the center of the edges and not through the corners of the sample.

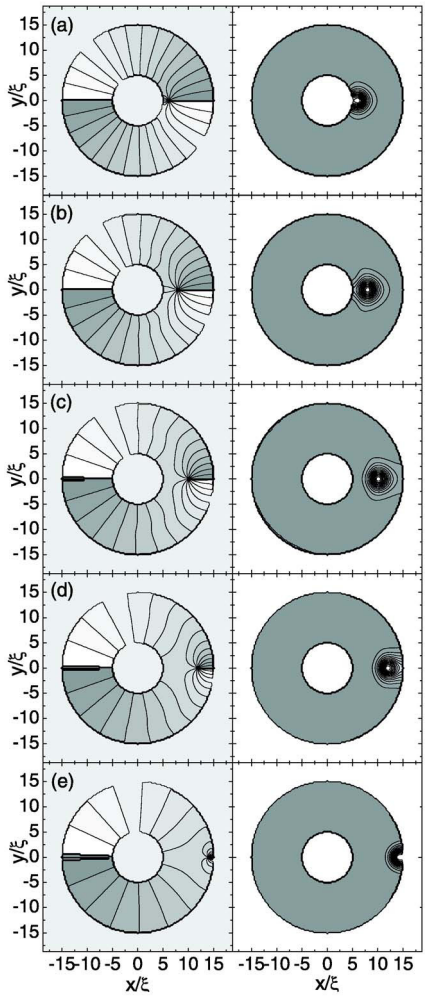

FIG. 13. Contour plots of the phase of the order parameter (left column) and Cooper pair density (right column) at $H_0/H_{c2}=0.01$ for $L_0=1$ for the ring of Fig. 12. Phases near zero are given by white regions and phases near 2π by gray regions. The position of the vortex is (a) $\rho_v=6.0\xi$, (b) $\rho_v=8.0\xi$, (c) $\rho_v=10.0\xi$, (d) $\rho_v=12.0\xi$, and (e) $\rho_v=14.0\xi$.

Figure 15 shows the energy barrier for vortex penetration (thick curves) and expulsion (thin curves) along the diagonal (dashed curves) and side (solid curves) of the square. It is seen from this figure that the vortex feels the largest barrier along the diagonal of the sample. This also means that a vortex placed in the square center has more freedom to wander laterally towards the edges than along the diagonals of the square.

VIII. CONCLUSIONS

We have presented an approach to calculate the energy barrier when a single vortex enters or exits superconducting mesoscopic finite size sample. Our approach is based on a numerical solution of the coupled nonlinear GL equations using analytical expressions for the phase of the order parameter obtained from the London theory.

First we calculated the energy barrier in superconducting disks with small radius and for different values of the disk thickness and GL parameter κ. These results for the energy barrier show clearly the limitations of the London theory which considerably overestimates (underestimates) the barrier for vortex expulsion (penetration). The discrepancy between the results from the GL approach and the one from the London theory decreases with increasing size of the disk. The

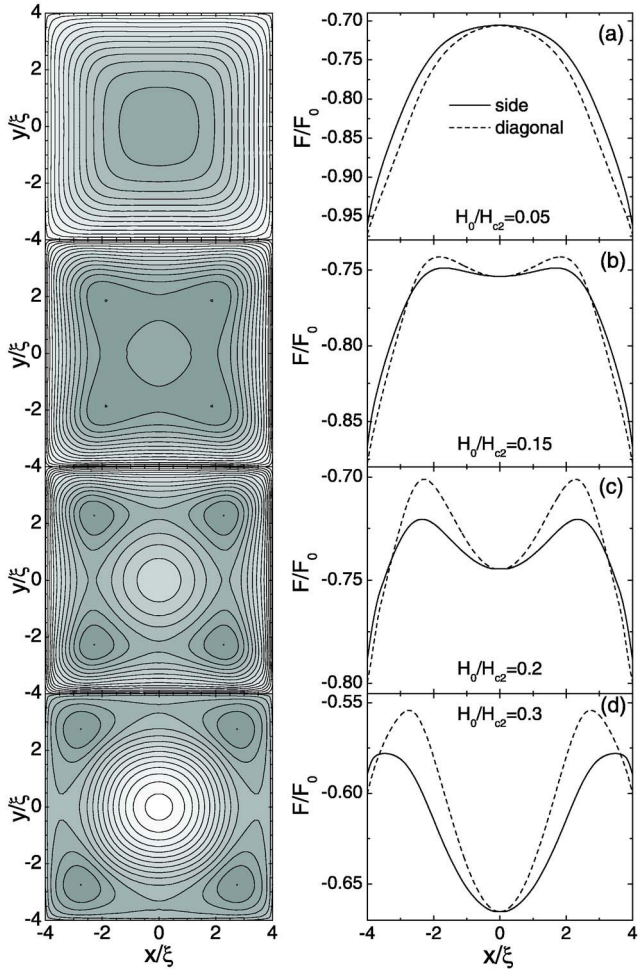

FIG. 14. Contour plots of the dependence of the free energy (left column) on the position of the vortex and cross sections (right column) for $y=0$ (solid curves) and for $x=y$ (dashed curves) in a square sample with side $a=8.0\xi$ and thickness $d=0.1\xi$ and $\kappa=1.0$ for four values of the applied field: (a) $H_0/H_{c2}=0.05$, (b) $H_0/H_{c2}=0.15$, (c) $H_0/H_{c2}=0.2$, and (d) $H_0/H_{c2}=0.3$.

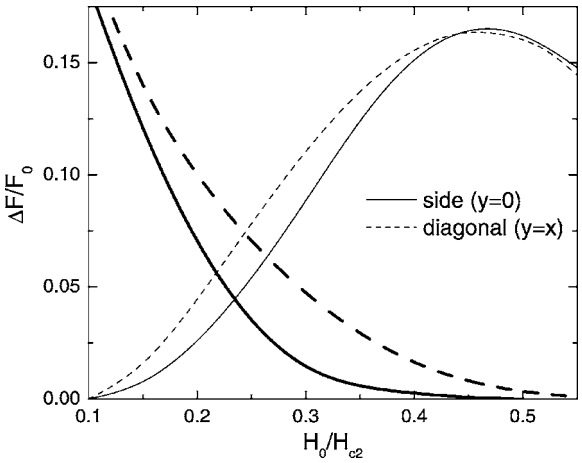

FIG. 15. The energy barrier for vortex penetration (thick curves) and expulsion (thin curves) along the side (solid curves) and diagonal (dashed curves) of the sample as a function of the external field for the sample of Fig. 14.

energy barrier strongly depends on the GL parameter κ: the magnetic field range over which the barrier exists is larger (consequently, the first critical field H_{c1}) for small values of κ, for which the sample behaves like a type-I superconductor.

We also studied the $L=2$ state in the disk and found for some values of the field an energy barrier between the multivortex and the giant vortex state. We also considered a superconducting ring and a square disk. For a superconducting ring we found a minimum in the free energy in the superconducting region of the sample for some range of magnetic field values when there are a number of vortices inside the hole, indicating that a vortex can be trapped in a metastable state in this region. For a superconducting square the vortex feels a larger barrier along the diagonal of the sample, while the lowest barrier is found along the middle of the sides of the square. The results for the square confirm the vortex entry laterally, through the sample edge.

ACKNOWLEDGMENTS

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Time-dependent Ginzburg–Landau equations with charged boundaries

Jorge Berger[a)]
Physics Unit, Ort Braude College, P. O. Box 78, 21982 Karmiel, Israel and Department of Physics, Technion, 32000 Haifa, Israel

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We build a discrete form for the Ginzburg–Landau thermodynamic potential for an infinite film and find how the TDGL equations are related to it. We discuss why the usual superconductor-insulator boundary condition, which prohibits the passage of superconducting current, should be questioned in dynamic problems; nevertheless, we conclude that this condition remains valid. The formalism we develop enables us to deal with situations in which surface charge is present at the boundaries. These situations include the Hall configuration when the influence of the normal electrons is not negligible and the case of an electromagnetic wave parallel to the film. In the case of the electromagnetic wave, we evaluate the electromagnetic field inside the superconductor and follow the motion of the vortices. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2010352]

I. INTRODUCTION

A widely used system of equations for the evolution of physical quantities in a superconductor is a simplified version of the time-dependent Ginzburg–Landau equations:[1]

$$\partial_t \psi = -\frac{1}{\eta}[(-i\nabla - \mathbf{A})^2\psi + (1-T)(|\psi|^2 - 1)\psi] + \tilde{f}, \tag{1}$$

$$\partial_t \mathbf{A} = (1-T)\mathrm{Re}[\overline{\psi}(-i\nabla - \mathbf{A})\psi] - \kappa^2 \nabla \times \nabla \times \mathbf{A}. \tag{2}$$

Here ψ is the order parameter, t is time, $\mathbf{A}$ is the electromagnetic vector potential, η is the ratio between the relaxation times of ψ and $\mathbf{A}$, κ is the Ginzburg-Landau parameter, T is the temperature and $\tilde{f}$ a random "force" that simulates thermal fluctuations. ψ has been normalized so that in the absence of electromagnetic field its absolute value would be 1, the unit of time is $4\pi\kappa^2\xi^2(0)\sigma/c^2$, where $\xi(0)$ is the coherence length at zero temperature and σ is the conductivity, the unit of length is $\xi(0)$, the unit of temperature is the critical temperature, and the the unit of $\mathbf{A}$ is $\Phi_0/2\pi\xi(0)$, where $\Phi_0 = hc/2e$ is the quantum of flux. We have chosen a gauge such that the scalar potential is zero.

We will regard η as a material-dependent parameter, although for given microscopic models its value is prescribed by the model. As a general policy for this article, the parameter values that we will consider are not necessarily those of typical materials, but rather those that easily exhibit the effects that I would like to present.

When the exterior of the sample is insulating, these equations are usually supplemented by the boundary conditions

a)Electronic mail: phr76jb@tx.technion.ac.il

$$\hat{\nu} \cdot (-i\nabla - \mathbf{A})\psi = 0, \tag{3}$$

where $\hat{\nu}$ is a vector perpendicular to the interface, and

$$\nabla \times \mathbf{A} = \nabla \times \mathbf{A}_e, \tag{4}$$

where $\mathbf{A}_e$ is the vector potential at the external part of the interface and in general is obtained by solving Maxwell's equations in the exterior. The main purpose of this article is the revision of these boundary conditions.

This set of equations is usually integrated by a finite-differences method. As a few examples, see Refs. 2–5.

In this study we will limit ourselves to a very simple geometry: an infinite superconducting film with boundaries at the planes $y=0$ and $y=d$, with magnetic field in the z direction. We will assume that the quantities in the problem do not depend on z. In this situation, $\mathbf{A}$ can be taken perpendicular to the z axis.

II. USEFUL EQUALITIES

A. Gauge factor

We define the unitary fields

$$\mathcal{U}^x(x,y,t) = \exp\left(-i\int_0^x A_x(x',y,t)\mathrm{d}x'\right), \tag{5}$$

and similarly we define $\mathcal{U}^y$. We follow a notation in which A_x denotes the component of $\mathbf{A}$ in the x direction. An inherent problem when using A_x is that it grows indefinitely with time if the average electric field in the x direction does not vanish; use of $\mathcal{U}^x$ avoids this problem.

By direct derivation and using the notation $\mathcal{J}^x = \partial_x(\mathcal{U}^x\psi)$ we obtain

$$\overline{\mathcal{U}^x}\mathcal{J}^x = \overline{\mathcal{U}^x}\partial_x(\mathcal{U}^x\psi) = (\partial_x - iA_x)\psi \tag{6}$$

and

$$\overline{\mathcal{U}^x}\partial_x\mathcal{J}^x = \overline{\mathcal{U}^x}\partial_{xx}^2(\mathcal{U}^x\psi) = (\partial_x - iA_x)^2\psi, \tag{7}$$

where the bar denotes complex conjugation.

B. Discretization

Having in view a numeric treatment of the problem by means of a finite difference technique, we introduce a rectangular grid for the coordinates of the position in the sample. Figure 1 shows a miscellaneous portion of the grid. It contains N_y rectangular cells in the y direction. Since we consider an infinite sample, we shall take a reasonably large number N_x of cells in the x direction, that cover a length L, and assume periodic boundary conditions in that direction, with periodicity L. Our discretization scheme will take $\psi(x,y)$ as constant in rectangles centered at the vertices of the grid, as the rectangle "I." The value of $\psi(x,y)$ in the rectangle will be denoted by $\psi_{i,j}$, where (i,j) are the integer coordinates of the vertex at which the rectangle is centered. The sides of the rectangle are $a_x = L/N_x$ and $a_y = d/N_y$. On the other hand, $\partial_x\psi(x,y)$ and $A_x(x,y)$ will be taken as constant in rectangles such as II, which have their vertical sides centered at neighboring vertices. The size of these rectangles is also $a_x \times a_y$.

Special care is required when dealing with quantities at the boundaries $y=0$ and $y=d$, which are marked as thick lines in Fig. 1. $\psi_{5,0}$ is the value of ψ in rectangle III, and the subscript $(3,N_y)$ will be used for $\partial_x\psi$ and A_x in rectangle IV. Both these rectangles have size $a_x \times a_y/2$. On the other hand $\partial_y\psi$ and A_y will have a constant value in rectangles like V, which have size $a_x \times a_y$, even if they touch the boundary.

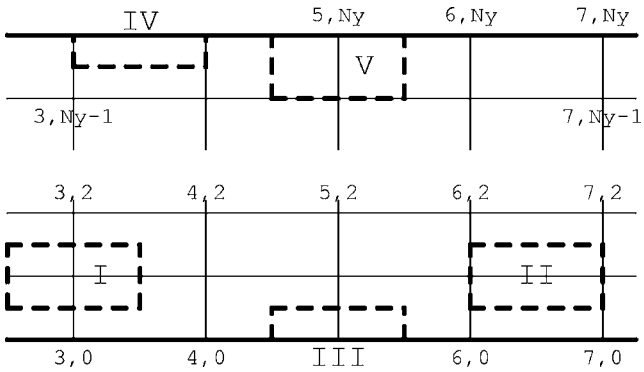

FIG. 1. The dashed rectangles enclose areas over which the fields of the model are approximated by constants. The thick lines are the boundaries of the superconductor.

We define now the link variable $U^x_{i,j}=\exp(-iA_x a_x)$ [respectively, $U^y_{i,j}=\exp(-iA_y a_y)$] where A_x is taken at the rectangle between the vertices (i,j) and $(i+1,j)$ [respectively, between (i,j) and $(i,j+1)$]. In the discrete approximation we have

$$\mathcal{U}^x(x_i,y_j)=\prod_{k=0}^{i-1} U^x_{k,j}, \tag{8}$$

where $x_i=ia_x$ and $y_j=ja_y$, and similarly for $\mathcal{U}^y$. Using Eqs. (7) and (8) and discretizing the second derivative we obtain

$$(\partial_x - iA_x)^2\psi\big|_{x_i,y_j}=(U^x_{i,j}\psi_{i+1,j}-2\psi_{i,j}+\overline{U}^x_{i-1,j}\psi_{i-1,j})/a_x^2 \tag{9}$$

so that the discrete approximation for Eq. (1), excluding the noise, can be written as

$$\eta\partial_t\psi_{i,j}=\frac{U^x_{i,j}\psi_{i+1,j}-2\psi_{i,j}+\overline{U}^x_{i-1,j}\psi_{i-1,j}}{a_x^2}+\frac{U^y_{i,j}\psi_{i,j+1}-2\psi_{i,j}+\overline{U}^y_{i,j-1}\psi_{i,j-1}}{a_y^2}-(1-T)(|\psi_{i,j}|^2-1)\psi_{i,j}. \tag{10}$$

We build now a discrete free energy. The Ginzburg–Landau free energy can be written as

$$G=G^v+G^x+G^y+G^A \tag{11}$$

where G^v is the contribution of the vertices, G^x is the contribution of the links in the x direction and G^y in the y direction, and G^A does not depend on ψ. Explicitly,

$$G^v=(1-T)\int(|\psi|^4/2-|\psi|^2)\mathrm{d}x\,\mathrm{d}y, \tag{12}$$

$$G^x=\int|(-i\partial_x-A_x)\psi|^2\mathrm{d}x\,\mathrm{d}y=\int|\partial_x(\mathcal{U}^x\psi)|^2\mathrm{d}x\,\mathrm{d}y \tag{13}$$

and similarly for G^y. The integrals are over the volume of a period.

We now replace the integrals over volume by sums over rectangles. For G^v we obtain

$$G^v = (1-T)\sum ((\overline{\psi}_{i,j}\psi_{i,j})^2/2 - \overline{\psi}_{i,j}\psi_{i,j})V^v_{i,j}, \tag{14}$$

where $V^v_{i,j}$ is the volume of a rectangle of the type I or III in Fig. 1, which is appropriate for the vertex at (i,j). The sum is over a set of rectangles that cover a period. For G^x we discretize the derivative, make use of Eq. (8) and obtain

$$G^x = \frac{1}{a_x^2}\sum (\overline{U^x_{i,j}\psi}_{i+1,j} - \overline{\psi}_{i,j})(U^x_{i,j}\psi_{i+1,j} - \psi_{i,j})V^x_{i,j}, \tag{15}$$

where $V^x_{i,j}$ is the volume of the appropriate rectangle between the vertices at (i,j) and at $(i+1,j)$. For G^y we have a similar expression, but this time the rectangles are between the vertices at (i,j) and at $(i,j+1)$.

For a vertex (i,j) in the interior of the sample, all the four neighbors $(i\pm1,j)$ and $(i,j\pm1)$ are present in the sums and $V^v_{i,j}=V^x_{i,j}=V^y_{i,j}=a_xa_y$, so that

$$-\frac{1}{V^v_{i,j}}\frac{\partial G}{\partial\overline{\psi}_{i,j}} = -(1-T)(|\psi_{i,j}|^2-1)\psi_{i,j} + \frac{U^x_{i,j}\psi_{i+1,j} - 2\psi_{i,j} + \overline{U^x_{i-1,j}\psi}_{i-1,j}}{a_x^2} + \frac{U^y_{i,j}\psi_{i,j+1} - 2\psi_{i,j} + \overline{U^y_{i,j-1}\psi}_{i,j-1}}{a_y^2} \tag{16}$$

and comparison with Eq. (10) gives

$$\eta\partial_t\psi_{i,j} = -\frac{1}{V^v_{i,j}}\frac{\partial G}{\partial\overline{\psi}_{i,j}} \tag{17}$$

for every vertex in the interior of the sample.

III. BOUNDARY CONDITION FOR THE MAGNETIC FIELD

Assuming that the superconductor and the insulator are not magnetic (i.e., have the same permeability as in vacuum), which is the usual situation in superconductivity, there is no need to distinguish between the magnetic field and the magnetic induction (except for a possible universal factor that depends on the units) and this field is given by $\nabla\times\mathbf{A}$. Since the divergence of $\nabla\times\mathbf{A}$ vanishes identically and since its rotor is proportional to the current density, that is finite, $\nabla\times\mathbf{A}$ is continuous everywhere and Eq. (4) follows.

In some articles it is claimed that only some of the components of $\nabla\times\mathbf{A}$ are continuous at the interface. This would be the case if the permeability were discontinuous, but in practically any situation this is an unnecessary complication.

In most articles that deal with numeric solutions, the implementation of Eq. (4) is not shown explicitly. Perhaps the only exception is Ref. 4. In Ref. 4 Eq. (4) is not enforced at the boundary itself, but rather at the cells that touch the boundary. Although both requirements become equivalent in the limit of a dense grid, Eq. (4) can be substituted by a condition at the boundary itself by requiring an adapted form of Eq. (2):

$$\partial_t(A_x)_{i,0} = \frac{1-T}{a_x}\mathrm{Im}(\overline{\psi}_{i,0}U^x_{i,0}\psi_{i+1,0}) + \frac{2\kappa^2}{a_xa_y^2}\mathrm{Im}(\exp(ia_xa_yH_e)U^x_{i,0}U^y_{i+1,0}\overline{U^x_{i,1}}\,\overline{U^y_{i,0}}), \tag{18}$$

where $H_e=\nabla\times\mathbf{A}_e\cdot\hat{z}$, and similarly for $\partial_t(A_x)_{i,N_y}$. The left-hand side of this equality stands for minus the normal current density, the first term at the right-hand side for the supercurrent density and the last term for minus the total current density. The terms at the right are worked out in Ref. 4. The first term is based on Eq. (6) and the last term approximates the argument of the product of unitary numbers by its imaginary part. The factor 2 in the last term comes from the fact that the magnetic field changes from its value at the rectangle $[(i,0),(i+1,0),(i+1,1),(i,1)]$ to H_e over a

length $a_y/2$. Since the usual computational variable is U^x rather than A_x, one can replace $\partial_t(A_x)_{i,0}=i\overline{U}^x_{i,0}\partial_t U^x_{i,0}/a_x$.

Although Eq. (18) is equivalent to Eq. (4) in the appropriate limit, one might say that it has a different "numerical philosophy," in the sense that Eq. (4) has the form of a constraint, whereas Eq. (18) has the form of an evolution equation.

IV. BOUNDARY CONDITION FOR THE ORDER PARAMETER

A. A "natural" condition

The mathematical inclination toward condition (3) in static problems is that it is a "natural" boundary condition, i.e., when we solve the variational problem $\delta G/\delta\overline{\psi}=0$ without requirements at the boundary, Eq. (3) is automatically obtained. In other words, Eq. (3) causes $\delta G/\delta\overline{\psi}=0$ to have the same form at the boundary as in the interior of the superconductor.

The physical justification for Eq. (3) in static problems is that charge cannot leak into the insulating material. Therefore, the component of the current in the ν direction has to vanish and this is proportional to the real part of the product of expression (3) times $\overline{\psi}$. In order to eliminate the imaginary part too, the De Gennes criterion[6] has to be invoked.

In a dynamic situation, none of these arguments is valid. $\delta G/\delta\overline{\psi}\neq 0$, the De Gennes criterion is not intended to be valid, and it is only the total current that has to be tangential to the interface. *A priori*, there is no physical restriction to the possibility of a supercurrent bringing electrons from the interior to the boundary, and a normal current bringing the electrons back to the interior. Moreover, if the supercurrent is indeed tangential, then the normal current and thus the electric field have to be tangential too. Since there are several problems in which the electric field does have a component perpendicular to the interface, the requirement that this component vanish at the boundary seems quite artificial. Examples in which a perpendicular component of the electric field is expected to exist include the Hall effect,[7,8] anisotropic superconductors[9] and cases in which an electric field is externally applied.[10] We should therefore refrain from accepting condition (3) for time-dependent situations, unless we can extend the justification for it.

We suggest that the natural boundary condition for a time-dependent problem be such that it results in an evolution equation of the same form at the boundary and in the interior. In our case, we will require Eq. (1) to remain valid at the boundaries. But Eq. (1) (without noise) can be written as $\eta\partial_t\psi=-\delta G/\delta\overline{\psi}$. Therefore, since it is Eq. (3) that renders $\delta G/\delta\overline{\psi}$ insensitive to the presence of the boundary, Eq. (3) should remain the natural boundary condition for the time-dependent problem. As a matter of taste, I find it more convincing to show this feature for the discretized problem: we will require that the same evolution equation (17) be obeyed at the vertices located at the boundary. Explicitly, let us consider the vertex $(i,0)$. In this case $\overline{V}^v_{i,0}=a_xa_y/2$ and there are four rectangles that contribute a term to the free energy that includes $\overline{\psi}_{i,0}$. The sum of these terms is

$$G_{i,0}=\frac{a_xa_y}{2}\left((1-T)\left(\frac{(\overline{\psi}_{i,0}\psi_{i,0})^2}{2}-\overline{\psi}_{i,0}\psi_{i,0}\right)+\frac{(\overline{U}^x_{i,0}\overline{\psi}_{i+1,0}-\overline{\psi}_{i,0})(U^x_{i,0}\psi_{i+1,0}-\psi_{i,0})}{a_x^2}\right.$$
$$\left.+\frac{(\overline{U}^x_{i-1,0}\overline{\psi}_{i,0}-\overline{\psi}_{i-1,0})(U^x_{i-1,0}\psi_{i,0}-\psi_{i-1,0})}{a_x^2}\right)+a_xa_y\frac{(\overline{U}^y_{i,0}\overline{\psi}_{i,1}-\overline{\psi}_{i,0})(U^y_{i,0}\psi_{i,1}-\psi_{i,0})}{a_y^2} \quad (19)$$

and Eq. (17) gives

$$\eta\partial_t\psi_{i,0} = -(1-T)(|\psi_{i,0}|^2-1)\psi_{i,0} + \frac{2(U^y_{i,0}\psi_{i,1}-\psi_{i,0})}{a_y^2} + \frac{U^x_{i,0}\psi_{i+1,0} - 2\psi_{i,0} + \overline{U}^x_{i-1,0}\psi_{i-1,0}}{a_x^2} \quad (20)$$

and a similar expression is obtained for the evolution of ψ_{i,N_y}. This equation was also suggested in Ref. 4, using a different line of argument. As in the case of Eq. (18), Eq. (20) replaces a constraint by an evolution equation.

We will now see that in the limit of a dense grid Eq. (20) is equivalent to Eq. (3). We define

$$\mathcal{F}_{i,j} = \mathcal{U}^y_{i,j}\left(\eta\partial_t\psi_{i,j} + (1-T)(|\psi_{i,j}|^2-1)\psi_{i,j} - \frac{U^x_{i,j}\psi_{i+1,j} - 2\psi_{i,j} + \overline{U}^x_{i-1,j}\psi_{i-1,j}}{a_x^2}\right) \quad (21)$$

and note that $\mathcal{F}_{i,j}$ remains finite in the limit of a dense grid. From Eq. (20) and discretization of $\mathcal{J}^y = \partial_y(\mathcal{U}^y\psi)$ we have

$$\mathcal{J}^y\big|_{x_i,a_y/2} = a_y\mathcal{F}_{i,0}/2 + O(a_y^2); \quad (22)$$

likewise, from Eq. (10),

$$\partial_y\mathcal{J}^y\big|_{x_i,a_y} = \mathcal{F}_{i,1} + O(a_y) \quad (23)$$

so that

$$\mathcal{J}^y\big|_{x_i,0} = a_y(\mathcal{F}_{i,0} - \mathcal{F}_{i,1})/2 + O(a_y^2) = 0 + O(a_y^2). \quad (24)$$

But due to Eq. (6), this is the same as condition (3).

The outcome of this subsection is thus that, instead of finding an alternative to Eq. (3), we have found a justification for it.

B. An alternative implementation

If we accept that the boundary condition is Eq. (3), it follows from identity (6) that $\mathcal{J}^y|_{x,0} = 0$ and therefore $\mathcal{U}^y(x,2a_y)\psi(x,2a_y) - \mathcal{U}^y(x,0)\psi(x,0) \approx 4(\mathcal{U}^y(x,a_y)\psi(x,a_y) - \mathcal{U}^y(x,0)\psi(x,0))$. From here we can isolate the order parameter at the boundary and obtain

$$\psi_{i,0} = \tfrac{1}{3}U^y_{i,0}(4\psi_{i,1} - U^y_{i,1}\psi_{i,2}) + O(a_y^3). \quad (25)$$

Since that $U^y_{i,1}\psi_{i,2} - \psi_{i,1}$ is of order $O(a_y^2)$, we can also write $\psi_{i,0} = U^y_{i,0}\psi_{i,1} + O(a_y^2)$. Similarly, at the other boundary, $\psi_{i,N_y} = (1/3)\overline{U}^y_{i,N_y-1}(4\psi_{i,N_y-1} - \overline{U}^y_{i,N_y-2}\psi_{i,N_y-2}) + O(a_y^3)$.

C. Example

We consider a situation in which external sources create a constant magnetic field $0.5\hat{z}$ [in units $\Phi_0/2\pi\xi^2(0)$], while a current I along the film induces an additional field. In appropriate units, the magnetic field will be $(0.5-I)\hat{z}$ for $y<0$ and $(0.5+I)\hat{z}$ for $y>d$. The reason for studying this situation is that we know[8] that for appropriate parameters the transverse electric field does not vanish.

Figure 2 shows the volume average of the component of the electric field in the y-direction, as a function of the current. The same quantity was once evaluated using Eq. (20) for the order parameter at the boundaries, and also using Eq. (25) without the $O(a_y^2)$-correction term. There is practically full agreement between these two methods. When the entire Eq. (25) is used, the evaluation algorithm seems to be unstable for the chosen parameters.

As reported in Ref. 8, this example exhibits chaotic behavior: minute changes in the initial values of ψ and $\mathbf{A}$ can reverse the sign of E_y. For the purpose of comparison, all the results in Fig. 2 are presented with the same sign.

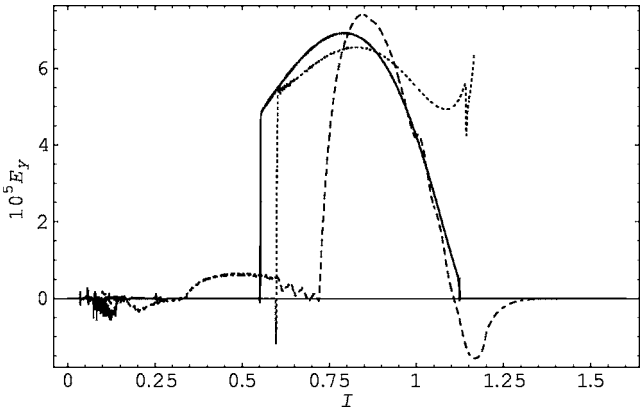

FIG. 2. Volume average of the transverse electric field as a function of the current. There are two solid lines that coalesce within the scale of this graph; these were obtained using Eq. (20) and the $O(a_y^2)$ approximation for Eq. (25). The dotted line was obtained using the entire Eq. (25) and the dashed line was obtained using the method developed in Sec. V, which permits accumulation of volume and surface charge. The unit of current is $c\Phi_0/[2\pi\xi(0)]^2$ per cm of length in the z direction; the electric field unit is $c\Phi_0/[8\pi^2\kappa^2\sigma\xi^3(0)]$. Parameters used: $\eta=0.03$, $\kappa=2$, $d=8$, $dI/dt=3.3\times10^{-4}$ (see Ref. 8 for further details).

V. INTRODUCTION OF A SURFACE CHARGE

The robustness of Eq. (3) when dealing with the Hall effect is somehow surprising, since in the case of a classical normal conductor the Hall field is generated by charges that accumulate at the surface of the conductor, and this field is uniform. However, a model based on Eq. (2) is unable to create a surface charge. Equation (2) can be written as

$$\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{A}\propto\mathbf{j}_T, \tag{26}$$

where $\mathbf{j}_T$ is the total (superconducting plus normal) current density. From here it follows that $\boldsymbol{\nabla}\cdot\mathbf{j}_T=0$ and therefore there cannot be any charge redistribution.

In order to enable the creation of volume and surface charges, we introduce the displacement current and replace Eq. (2) by the entire Maxwell equation:

$$\kappa^2\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{A}+\gamma\partial_{tt}^2\mathbf{A}+\partial_t\mathbf{A}=(1-T)\mathrm{Re}[\overline{\psi}(-i\boldsymbol{\nabla}-\mathbf{A})\psi], \tag{27}$$

where $\gamma=(\kappa/c)^2$ or, dividing the denominator by the unit of velocity, $\gamma=(c/4\pi\kappa\sigma\xi(0))^2$. This reduces to Eq. (2) if we set $\gamma=0$. As in the case of η, we will assume that γ depends on the material and can take a wide range of values.

Since Eq. (27) contains a second derivative with respect to t, Euler integration requires two steps. We define

$$\mathcal{E}_{i,j}^y=-a_y\partial_t A_y\big|_{x_i,(j+1/2)a_y}=-i\overline{U}_{i,j}^y\partial_t U_{i,j}^y, \tag{28}$$

and similarly for the x direction. The y-component of the electric field is $\mathcal{E}_{i,j}^y/ca_y$. From Eq. (27), $\mathcal{E}_{i,j}^y$ obeys

$$\frac{\mathcal{E}_{i,j}^y(t+\Delta t)-\mathcal{E}_{i,j}^y(t)}{\Delta t}=\frac{\mathcal{C}-\mathcal{E}_{i,j}^y(t)}{\gamma}, \tag{29}$$

where Δt is the time step and we have used as shorthand

$$\mathcal{C} = a_y(\kappa^2(\nabla \times \nabla \times \mathbf{A})_y - (1-T)\mathrm{Re}[\overline{\psi}(-i\partial_y - A_y)\psi])|_{x_i,(j+1/2)a_y} =$$

$$-\frac{\kappa^2}{a_x^2}\mathrm{Im}(\overline{U}^x_{i,j}\overline{U}^y_{i+1,j}U^x_{i,j+1}(U^y_{i,j})^2U^x_{i-1,j}\overline{U}^x_{i-1,j+1}\overline{U}^y_{i-1,j}) - (1-T)\mathrm{Im}(\overline{\psi}_{i,j}U^y_{i,j}\psi_{i,j+1}). \tag{30}$$

The algorithm (29) may lead to numerical difficulties for small γ. Therefore, keeping the same order in Δt, we substitute $\mathcal{E}^y_{i,j}(t)$ by $\mathcal{E}^y_{i,j}(t+\Delta t)$ at the right-hand side of Eq. (29) and isolate $\mathcal{E}^y_{i,j}(t+\Delta t)$. This gives

$$\mathcal{E}^y_{i,j}(t+\Delta t) = \frac{\gamma\mathcal{E}^y_{i,j}(t) + \Delta t\mathcal{C}}{\gamma + \Delta t}. \tag{31}$$

After $\mathcal{E}^y_{i,j}(t+\Delta t)$ is evaluated, $U^y_{i,j}(t+\Delta t)$ is evaluated using Eq. (28), i.e.,

$$U^y_{i,j}(t+\Delta t) = U^y_{i,j}(t)(1 + i\Delta t\mathcal{E}^y_{i,j}(t+\Delta t)). \tag{32}$$

The same procedure is followed for $U^x_{i,j}(t+\Delta t)$.

The volume density of charge (per unit length in the z-direction) at an internal vertex (i,j) is given by Gauss law:

$$\rho_{i,j} = \frac{1}{4\pi c}\left(\frac{\mathcal{E}^x_{i,j} - \mathcal{E}^x_{i-1,j}}{a_x^2} + \frac{\mathcal{E}^y_{i,j} - \mathcal{E}^y_{i,j-1}}{a_y^2}\right); \tag{33}$$

for a vertex at the boundary $y=0$

$$\rho_{i,0} = \frac{1}{4\pi c}\left(\frac{\mathcal{E}^x_{i,0} - \mathcal{E}^x_{i-1,0}}{a_x^2} + \frac{2\left(\mathcal{E}^y_{i,0} + a_y\partial_t A_y\big|_{x_i,0}\right)}{a_y^2}\right), \tag{34}$$

and similarly for $y=d$.

A. The Hall field

The same problem treated in Sec. IV C was considered again, using Eq. (27) with $\gamma \neq 0$. The magnetic field is independent of time outside the superconducting film (assuming that the current varies slowly), implying that the electric field has to be uniform in the exterior regions. The easiest way to achieve this condition is by requiring that the electric field vanish outside the film. The result for the average value of the transverse field for $\gamma=100$ is shown in Fig. 2. The curve is rounded, suggesting a sort of capacitive behavior, but the average transverse field is not always smaller than in the case $\gamma=0$.

Figure 3 shows the profile of the transverse field (averaged over t and x only) across the film, for a current close to the maximum in Fig. 2. From the slope of the curve we see that (on the average) there is volume charge in the region between $y=0$ and $y\approx 5.5$; the sign of the charge changes roughly in the middle of this range. At the boundaries, we obtain $E_y(0^+)=E_y(d^-)=0$. In Fig. 4 we investigate whether $E_y(0^+)$ vanishes for the entire range of currents. For this purpose we plot E_y in the closest and next to closest links to the boundary, which correspond to the positions $y=1/2$ and $y=3/2$. If $E_y(0^+)=0$, then in the linear approximation we should have $E_y(1/2)=E_y(3/2)/3$ and Fig. 4 indicates that this is indeed the case.

As a conclusion of this subsection we might state that the behavior of the Hall effect for a superconductor is opposite to that for a classical normal conductor: volume charges are present and surface charges are absent. The absence of surface charge is not surprising if we note that we have entirely neglected the influence of the normal electrons; this influence will be added in the following subsection.

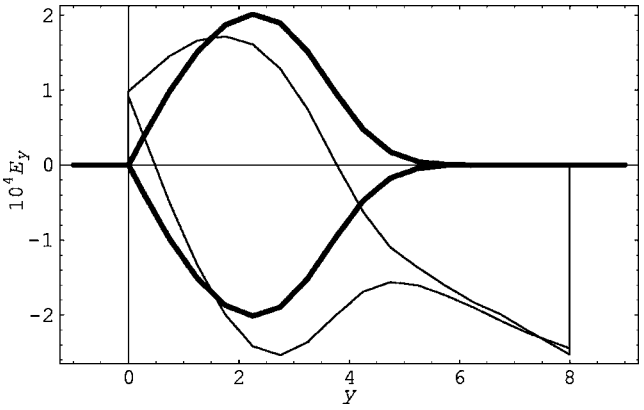

FIG. 3. Transverse component of the electric field as a function of position for $I=0.85$ and $\gamma=100$. The superconducting film occupies the region $0\leqslant y\leqslant 8$. Minute changes in the initial fields may reverse the sign of the contribution of the superconducting electrons to E_y;[8] both cases are presented. Thick lines: $\chi=0$ (Sec. V A); thin lines: $\chi=-5\times10^{-4}$ and $n=2$ (Sec. V B).

B. Influence of the magnetic force

The last term in the left-hand side of Eq. (27) stands for the normal current density. On doing this identification, we are assuming that the normal current density is proportional to the electric field **E**. This assumption is inaccurate; the normal current density is actually proportional to the force exerted on every charge carrier, which equals the charge times $\mathbf{E}+\mathbf{v}\times\mathbf{B}/c$, where **v** is the velocity of the carrier and $\mathbf{B}=\boldsymbol{\nabla}\times\mathbf{A}$ is the magnetic field. This means that Eq. (27) becomes

$$\kappa^2\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{A}+\gamma\partial_{tt}^2\mathbf{A}+\partial_t\mathbf{A}-\mathbf{v}\times(\boldsymbol{\nabla}\times\mathbf{A})=(1-T)\mathrm{Re}[\overline{\psi}(-i\boldsymbol{\nabla}-\mathbf{A})\psi], \tag{35}$$

where **v** is the drift velocity of the normal electrons.

Translated into the variables we are using, substitution of **E** by $\mathbf{E}+\mathbf{v}\times\mathbf{B}/c$ amounts to the replacement of $\mathcal{E}_{i,j}$ at the right-hand side of Eq. (29):

$$\mathcal{E}^x_{i,j}\to\mathcal{E}^x_{i,j}+\frac{v_y}{2a_y}\mathrm{Im}(\overline{U}^x_{i,j-1}\overline{U}^y_{i+1,j-1}\overline{U}^y_{i+1,j}U^y_{i,j-1}U^y_{i,j}U^x_{i,j+1}), \tag{36}$$

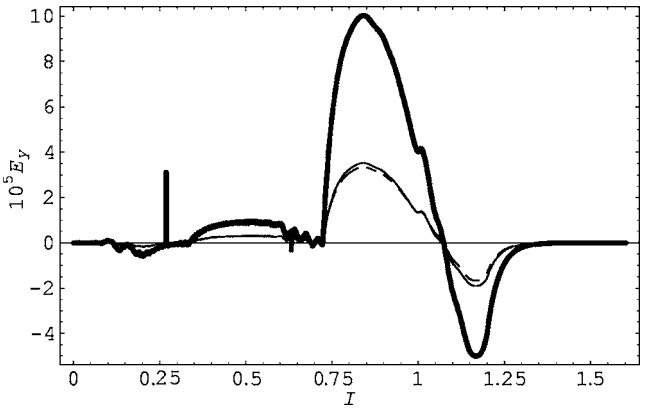

FIG. 4. Transverse component of the electric field at the links close to the boundary at $y=0$. The thick line stands for links centered at $y=3a_y/2$, the thin line for $y=a_y/2$, and the dashed line was obtained by dividing $E_y(3a_y/2)$ by 3. The feature at $I\sim0.25$ corresponds to a short range of currents where E_y is chaotic.

$$\mathcal{E}^y_{i,j} \to \mathcal{E}^y_{i,j} + \frac{v_x}{2a_x}\mathrm{Im}(\overline{U^y_{i-1,j}}\,\overline{U^x_{i-1,j+1}}\,\overline{U^x_{i,j+1}}U^x_{i-1,j}U^x_{i,j}U^y_{i+1,j}). \tag{37}$$

If $j=0$ or $j=N_y$, the term added to $\mathcal{E}^x_{i,j}$ in Eq. (36) should be substituted by $a_x v_y H_e$, where H_e is the magnetic field at the appropriate boundary (and in the present example is affected by the current along the film).

Let us now adopt a model for the drift velocity. Denoting by $-e$ the charge of an electron and by n the total density of electrons relative to the maximal density of condensed electrons, then, in appropriate units, the normal current density is $-e(n-|\psi|^2)\mathbf{v}$. By Ohm's law, this current density equals $\sigma(\mathbf{E}+\mathbf{v}\times\mathbf{B}/c)$, but assuming that the magnetic force is much smaller than the electric force it can be approximated by $\sigma\mathbf{E}$. The conductivity σ might depend on $|\psi|$, but since it is conventionally absorbed within the time unit, we will stick to the assumption that σ is constant. These assumptions lead to the form

$$\mathbf{v} = \frac{\chi\mathbf{E}}{n-|\psi|^2}, \tag{38}$$

where χ and n are "material constants." Operationally, $|\psi|^2$ is conveniently approximated by taking the geometric average of $|\psi_{i,j}|^2$ at both extremes of the appropriate link.

A comparison between this model and the case in which the magnetic force is disregarded is presented in Fig. 3. For the present model E_y is discontinuous at the boundaries, showing that there is indeed a surface charge. E_y has opposite signs at both boundaries; this is due to the fact that in the considered situation the total magnetic field has opposite signs at both boundaries. Also, the size of the magnetic field at $y=8$ is almost four times larger than that at $y=0$, and this has an influence on the respective sizes of E_y. The curves for $\chi=-5\times10^{-4}$ are above the curves for $\chi=0$ for y below ~1.5 and then the situation is reversed; we have verified that this is where the average magnetic field changes sign.

C. Effect of a parallel electromagnetic wave

Let us finally consider a situation in which a time dependent transverse electric field is applied. We consider the case in which outside the superconducting film there is a plane monochromatic electromagnetic wave moving in the x direction, with electric field in the y direction. In order to fit the periodicity that was imposed in the previous sections, we take a wavelength $L'=39.5$. (L' is a bit shorter than L, since a row of links has to overlap in order to implement periodicity.) Let us take $\kappa=2$ and $\gamma=1$, implying that $c=2$. In order to have a concrete problem let us take, outside the film, an electromagnetic potential in the y-direction with

$$A_y = 0.5x - 0.1\frac{L'}{2\pi}\cos\left(\frac{2\pi}{L'}[x-2t]\right) + C, \tag{39}$$

where C is a constant that might be different for $y>d$ and $y<0$. This potential satisfies the Maxwell equation outside the film [Eq. (27) without the right hand side and without the term $\partial_t\mathbf{A}$] and is therefore an acceptable external condition. Equation (39) describes the total external electromagnetic potential; we will not analyze what its sources are. On the average, this potential describes an external magnetic field $0.5\hat{z}$, as in the previous problem. Superimposed to this static field, there is an electromagnetic wave that produces an electric field

$$-\frac{1}{c}\partial_t\mathbf{A} = 0.1\,\sin\left(\frac{2\pi}{L'}[x-2t]\right)\hat{y} \tag{40}$$

outside the film. This time we assume that no net current flows along the film. We will also neglect the magnetic force considered in Sec. V B.

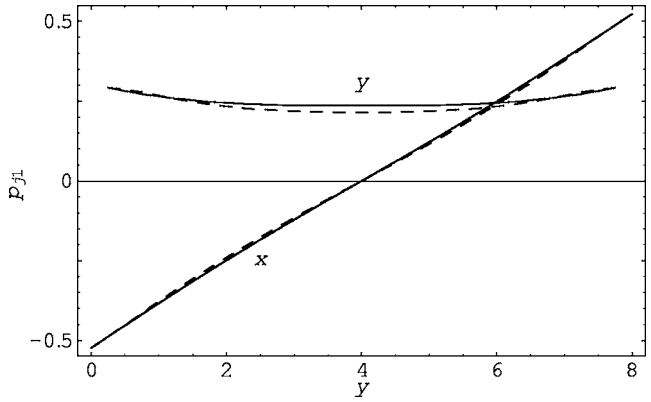

FIG. 5. Size of the first harmonic of the components of the electric field, $p^x_{j,1}$ and $p^y_{j,1}$. The line that refers to $p^x_{j,1}$ (respectively, $p^y_{j,1}$) is marked with the letter "x" (respectively, "y"). The abscissa y is related to the discrete index j through $y=ja_y$ (resp. $y=(j+1/2)a_y$). The dashed lines were evaluated using surface charge only.

Introducing the appropriate expression for the external field H_e into the program, we can find the fields inside the sample. After a transient stage, the electric field, the charge distribution, and the magnetic field take the form of a wave that moves together with the external wave and may be approximated by

$$E_x(x,ja_y,t) \approx 0.1\sum_{m=1}^{\infty} p^x_{j,m}\sin\left(\frac{2m\pi}{L'}[x-2t]+\varphi^x_{j,m}\right),$$

$$E_y(x,(j+1/2)a_y,t) \approx 0.1\sum_{m=1}^{\infty} p^y_{j,m}\sin\left(\frac{2m\pi}{L'}[x-2t]+\varphi^y_{j,m}\right),$$

$$\rho(x,ja_y,t) \approx 0.1\sum_{m=1}^{\infty} p^\rho_{j,m}\sin\left(\frac{2m\pi}{L'}[x-2t]+\varphi^\rho_{j,m}\right),$$

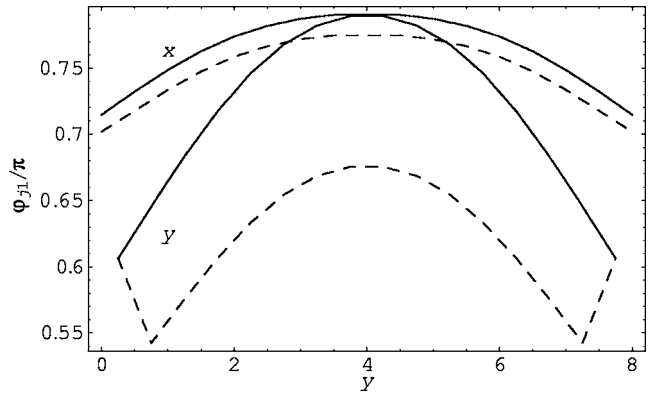

FIG. 6. Phase lag of the first harmonic of the components of the electric field inside the superconducting film. The conventions are the same as in Fig. 5.

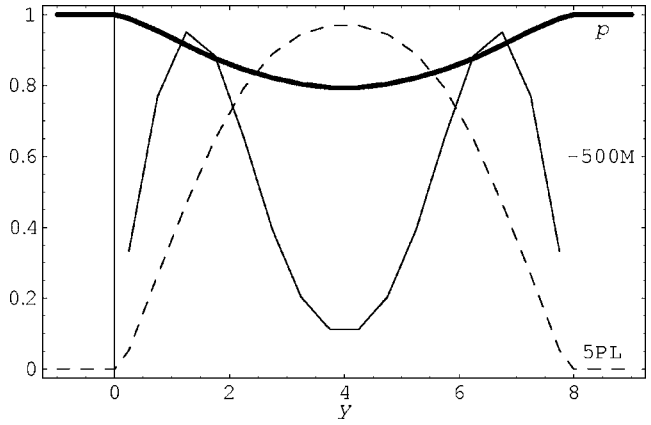

FIG. 7. y dependence of the main contributions to the magnetic field. The thick line ("p") stands for the size of the first harmonic, $p^B_{j,1}$; the dashed line ("5PL") stands for the phase lag and equals $5\varphi^B_{j,1}/\pi$; the thin line ("$-500M$") is the contribution that can be related to the vortex pattern and equals $-500M$, where the magnetization $M\hat{z}$ is the time average of $\nabla\times(\mathbf{A}-\mathbf{A}_e)/4\pi$. The abscissa y is related to the discrete index j through $y=(j+1/2)a_y$.

$$B_z(x,(j+1/2)a_y,t)-0.5\approx 0.1\sum_{m=1}^{\infty} p^B_{j,m}\sin\left(\frac{2m\pi}{L'}[x-2t]+\varphi^B_{j,m}\right), \tag{41}$$

where the $p_{j,m}$ and $\varphi_{j,m}$ sets are constants that can be found by performing a Fourier analysis. The factor 0.1 has been kept for the purpose of comparison with the external field. The main results of this analysis are shown in Figs. 5–7. The coefficients $p_{j,m}$ decrease by an order of magnitude for every unit added to m, and we present the first harmonic only.

We see from Figs. 5 and 6 that the electric field is not continuous at the boundaries, i.e., $p^y_{j,1}$ does not tend to 1 and $p^x_{j,1}$ and $\varphi^y_{j,1}$ do not tend to 0. This discontinuity requires a surface charge. Indeed, evaluation of $p^\rho_{j,1}$ shows that the values of $p^\rho_{0,1}$ and $p^\rho_{N_y,1}$ are more than 600 times larger than the average value of $p^\rho_{j,1}$ in the interior, so that these may be regarded as surface charges. We also checked what happens if only these surface charges are considered and the volume charges are neglected, i.e., we used Eq. (27) only for the links that touch the boundaries and Eq. (2) for the interior links. The results are shown by dashed lines in Figs. 5 and 6 and differ just slightly from those obtained when Eq. (27) is used everywhere.

Figure 7 shows [in agreement with Eq. (4)] that the magnetic field is continuous at the boundaries, implying that there is no surface current. This result may seem surprising, since there

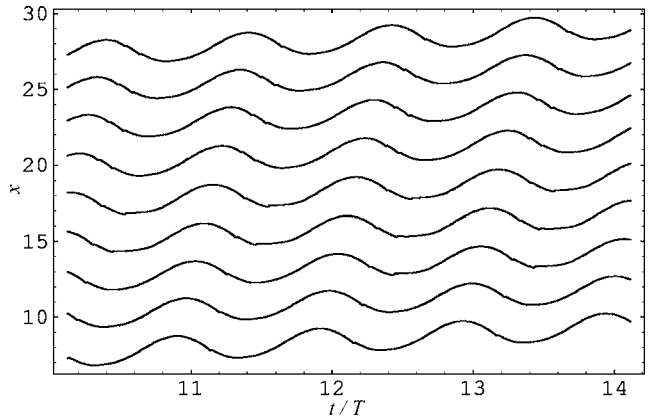

FIG. 8. Positions of several vortices as functions of the number of elapsed periods. $T=L'/2$.

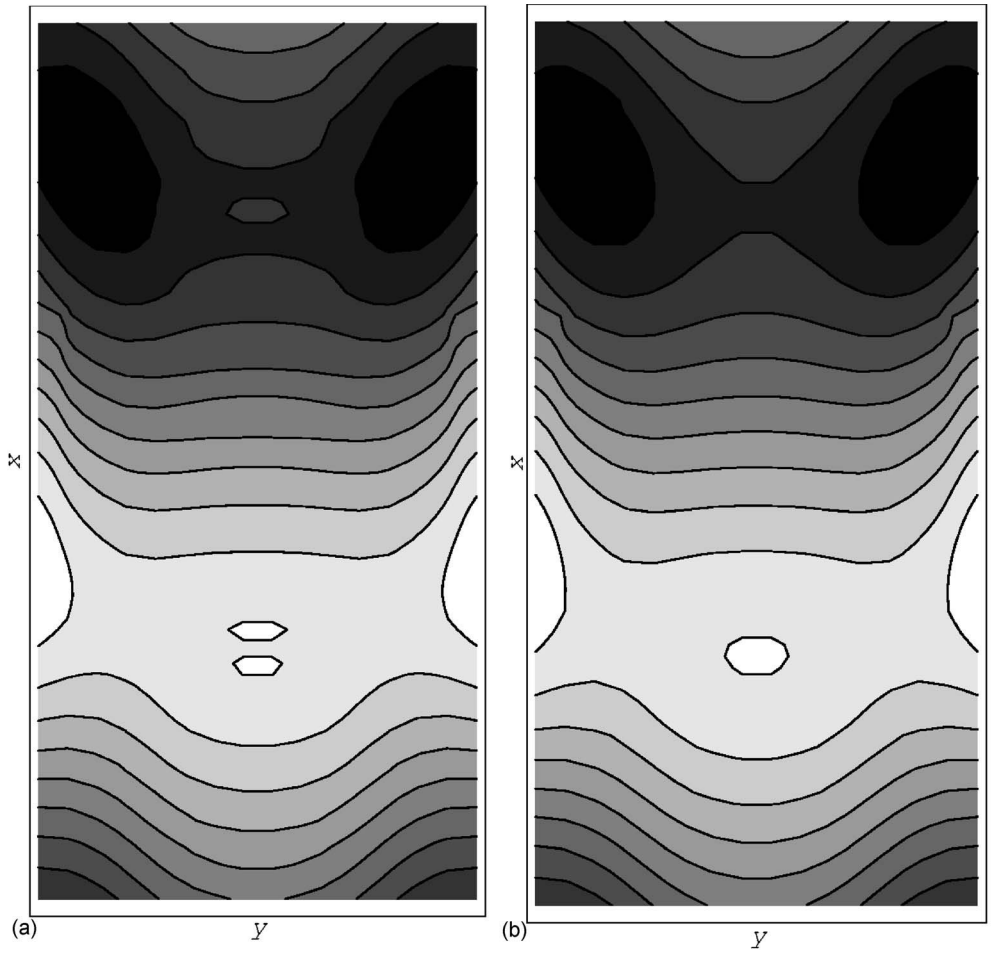

FIG. 9. Contour plots of the magnetic field at time $t=230$. (a) Direct evaluation and (b) approximaton that takes the first harmonic in Eq. (41) and the time average of the magnetization. The plots cover the region $0.25 \leqslant x \leqslant 39.25$, $0.25 \leqslant y \leqslant 7.75$.

are surface charges and the charge distribution advances together with the wave; in order to preserve the continuity of the magnetic field, the motion of these charges has to be compensated by Maxwell's displacement current.

Besides the electromagnetic field, the position of the vortices is usually of interest. We evaluate these positions as follows. We first locate a vertex (i_0, j_0) where the absolute value of the order parameter $\psi_{i,j}$ has a discrete local minimum; we then obtain a fit of ψ as a linear function of x and y in the region that contains nine vertices with corners at $(i_0 \pm 1, j_0 \pm 1)$, and finally solve for the position at which $\psi(x,y)=0$. For the particular example we are considering, when only the static magnetic field is applied and the wave is absent, there is a line of vortices along $y=d/2$. When the wave is applied, we find that the vortices scarcely move in the y direction; the x values for the vortices along a region of half a wavelength are shown in Fig. 8.

We see that the positions of the vortices oscillate in response to the wave, but they are also dragged with a velocity $1.24 \times 10^{-2} c$. Due to this drag, the period of the oscillatory part of a vortex motion is not the same as that of the wave, but is slightly Doppler-shifted.

Since the vortices are arranged in a nearly periodic pattern, with a periodicity and drag velocity that differ from those of the wave, we might also expect contributions to the electromagnetic field that exhibit this periodicity. However, for the parameters chosen in this example, this contribution is smaller by three orders of magnitude than that of the first harmonic that follows the

wave. What happens is that the distance between consecutive vortices is of the order of the magnetic penetration depth and the line of vortices behaves approximately as a continuum. As a consequence, their contribution is approximately independent of x and may be fairly described by the average magnetization $M(y)$. Figure 9 describes the magnetic field for a given instant and compares it to the approximation $B_z(x,(j+1/2)a_y)=0.5+0.1p^B_{j,1}\sin\left(\frac{2\pi}{L'}[x-2t]+\varphi^B_{j,1}\right)+4\pi M(y)$.

VI. DISCUSSION

For a time-independent situation there are good reasons to assume that the supercurrent has to be tangential to the superconductor-insulator boundaries. For time-dependent situations these reasons are no longer valid, but we find new reasons to preserve this assumption. Since the total current cannot cross the boundary, it follows that the normal current has to be tangential too.

Taking into account the displacement current enables the accumulation of charge at the boundary and the total current is not necessarily tangential. However, for a stationary situation, the amount of charge at the boundary achieves a final value and from then on the total and the normal currents become tangential. In the case of a superconducting film in the Hall configuration, when the magnetic force on the normal electrons is not neglected, the electric field is not tangential. This does not imply that the normal current is not tangential, since in this case the normal current is not proportional to the electric force on the electrons.

In the presence of an oscillating electric field perpendicular to the boundary, as may be encountered when a polarized grazing electromagnetic wave propagates parallel to a film, the surface charge also oscillates and does not attain a final value. Accordingly, the total and the normal currents are not tangential.

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Ginzburg–Landau model of a liquid crystal with random inclusions

L. Berlyand[a)]
Department of Mathematics and Materials Research Institute, Pennsylvania State University, University Park, Pennsylvania 16802

E. Khruslov[b)]
Mathematical Division, Institute for Low Temperature Physics and Engineering, 47 Lenin Ave., 61164 Kharkov, Ukraine

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We consider a Ginzburg–Landau three-dimensional functional with a surface energy term to model a nematic liquid crystal with inclusions. The locations and radii of the inclusions are randomly distributed and described by a set of finite dimensional distribution functions. We show that the presence of inclusions can be accounted for by an effective potential. Our main objectives are (a) to derive the sufficient conditions on the distribution functions such that the solutions converge in probability to a solution of a homogenized deterministic problem and (b) to compute the effective potential. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Intermediate between ordered solids and amorphous liquids, liquid crystals possess both special structure and unique optical properties. The simplest kind of a liquid crystal, known as a nematic, is composed of rodlike molecules exhibiting *local orientational order*. That is, the molecules locally orient themselves along some preferred direction, while maintaining the ability to move around freely. The preferred direction can vary from point to point and coincides locally with the direction of the optic axis. As for any heterogeneous, optically uniaxial medium, the overall optical properties of a nematic material are determined by the spatial distribution of the direction of the optic axis.

Because positions of their molecules are not constrained, nematic liquid crystals can flow like liquids. At the same time, spatially nonuniform orientational order can produce elastic interactions that lead to complex nematic structures with elaborate patterns and topological defects. These structures can be subsequently manipulated by influencing molecular orientations with external electromagnetic forces. The corresponding changes in optical characteristics drive most of the current practical uses of liquid crystal materials.

Although in their "pure" form liquid crystals have been widely used in a variety of important applications, most notably liquid crystal displays, a significant research effort has been concentrated recently on liquid crystal-based composites. These materials are of considerable interest for display technologies based upon changing the light scattering properties of composite systems via external fields. Such systems can have distorted or multiply connected random geometries,[14] such as those produced by the polymer-dispersed liquid crystals (PDLC),[13] or dispersions of agglomerations of silica spheres in a nematic host.[17]

A structure of a liquid crystal-based composite depends strongly on whether or not a liquid crystal is used as its host material. For example, in a *direct nematic emulsion*[14] a nematic dispersed

[a)]Electronic mail: berlyand@math.psu.edu
[b)]Electronic mail: khruslov@ilt.kharkov.ua

in water separates into distinct, nearly spherical drops. The drops have simple structures dependent on the boundary conditions at the nematic-water interface. For this reason, direct liquid crystal emulsions have been used as a model medium to study topological defects.[14]

An inverse nematic emulsion[19] differs from a direct emulsion in that isotropic water droplets are dispersed in a nematic host. Structures of inverse emulsions are significantly more complex than direct emulsions. In inverse nematic emulsions and, more generally, in *colloid suspensions* in nematic liquid crystals, the interactions between foreign inclusions in a nematic host lead to formation of a variety of ordered and disordered structures. A defining impact on formation of structures is made by both anchoring conditions on the surfaces of inclusions and the global geometry of a liquid crystalline matrix.

The rheological effects in liquid crystals with inclusions depend crucially on the volume fraction of inclusions (see, e.g., Ref. 26). For example, a soft *solid* with a significant storage modulus was obtained in Ref. 20 by mixing model colloidal particles with a thermotropic nematic liquid crystal. The suspended particles with very small radii, behaving as nearly perfect hard spheres, constituted up to 20% of the mixture. The colloid-liquid-crystal composite described in Ref. 20 is a switchable electro-optical solid material, giving it significant advantages in handling and processing over the conventional, free-flowing liquid crystals.

In this paper we consider a mathematical model for a class of nematic liquid crystal composites with low volume fraction of small *randomly* distributed inclusions. Within this model, a nematic liquid crystal is described by the Ginzburg–Landau functional (2.2) with a (positive or negative) surface energy term. We assume that both the surface energy density and sizes of inclusions are controlled by the same small parameter ϵ. Randomness in the particle's sizes and locations is the main issue of our consideration and the main two objectives of this work are (a) to derive the conditions on the distribution functions such that the solutions converge in probability measure to a solution of a homogenized deterministic problem and (b) to compute the effective potential.

A similar problem for a *deterministic* geometry characterized by a small volume fraction of inclusions was considered in Refs. 4 and 6 (see also Refs. 16 and 25 for physical problems). It was shown that the presence of inclusions can be accounted for by an effective potential that was computed explicitly as a function of material parameters and geometric characteristics of inclusions. Two main control parameters were introduced—the average size of inclusions and the inverse intensity of the surface energy. The asymptotic limits when both parameters tend to zero were considered and all possible relationships between these two parameters that lead to nontrivial homogenization limits were identified and studied. We emphasize that these relationships were not deduced from a specific physical problem—on the contrary, they arose in the course of the homogenization analysis of the model. The relevance of these relationships to liquid crystal composites is an interesting open question suggested by our analysis. In the present paper we show that in the random setting the same scaling relationships lead to a nontrivial deterministic limit.

In Ref. 6, the effective potential was represented as a sum of two terms responsible for the surface and the bulk energy of a thin boundary layer around inclusions, respectively. The analytic formulas for the effective potential that were obtained in Ref. 6 do not require the solution of a cell problem. (Cell problems for linear elliptic problems are defined in Ref. 3.) An additional geometric condition under which the homogenization procedure was carried out in Refs. 4 and 6 was that the inclusions cannot form clusters.

The presence of the surface energy term in a variational formulation of our problem implies that the minimizer (which solves the nonlinear Ginzburg–Landau equation) is subject to Robin boundary conditions on surfaces of inclusions. For linear scalar problems (Laplace operator) a homogenization problem for perforated domains with Robin boundary condition on boundaries of holes has been studied by several authors. In Refs. 8 and 9 the case of large holes, where the homogenized operator becomes anisotropic, has been considered by using the method of mesocharacteristics. In Refs. 11 and 12 several possible relations between a parameter in Robin boundary condition and sizes of periodically arranged holes have been thoroughly studied and classified.

In the same work, a version of the two-scale approach (Refs. 1, 3, 15, and 21) suitable for the analysis of the Robin boundary condition on surfaces of holes, has been developed.

The case of deterministic inclusion that remains sufficiently far apart (the ratio of the size of an inclusion to the distance between it and other inclusions is bounded) was treated in Ref. 5. The domains were not required to have periodic geometry, and the surface energy term in (2.2) was not assumed to be negative. The main consequence of the lack of non-negativity is that there is no *a priori* lower bound on the energy, and this bound must be established independently.

Under these assumptions on the functional and the geometry of the domain, it was shown in Ref. 5 that one can account for inclusions by an anisotropy of the homogenized differential operator and an effective potential. The potential can be viewed as an effective external field. Furthermore, it was established that a "cross-term" of the form $c_{ikj}(\partial u_k/\partial x_j)u_i$ is not present in the homogenized energy. However, such a cross term may appear for more general domains, where distances between inclusions can be much smaller than their sizes. At present this is an interesting open question.

Finally we note that in recent works[22,2] homogenization problems for liquid crystals with a periodic array of polymeric inclusions in the presence of an applied magnetic field were considered.

II. FORMULATION OF THE PROBLEM AND THE MAIN RESULT

An idealized mathematical model for a liquid crystal with spherical inclusions can be formulated as follows.

Let G be a bounded domain in $\mathbf{R}^3$ with a piecewise smooth boundary ∂G and $B^i_\epsilon = B(x^i_\epsilon, a_{i\epsilon})$ be the balls of small radii $a_{i\epsilon}$ centered at the points x^i_ϵ $(i=1,\ldots,N_\epsilon)$.

The small parameter ϵ is of order of the average distance between the nearest balls and also characterizes the sizes of the balls B^i_ϵ. We assume that $N_\epsilon \sim \epsilon^{-3}$ and $a_{i\epsilon} = O(\epsilon^\alpha)$. Here $\alpha > 2$, that is the balls are small with respect to the average distance to the nearest neighbor.

Let

$$G_\epsilon = G \setminus \bigcup_{i=1}^{N_\epsilon} B^i_\epsilon$$

be the perforated domain occupied by a liquid crystal. We introduce the class $H^1_U(G_\epsilon) \subset H^1(G_\epsilon)$ of vector functions $u: G_\epsilon \to \mathbf{R}^3$ with the trace $u = U$ on ∂G, where $U: G \to \mathbf{R}^3$. For simplicity we assume that $U \in C^1(\bar{G})$.

Consider the variational problem

$$E_\epsilon[u] \to \min, \quad u \in H^1_U(G_\epsilon) \tag{2.1}$$

for the Ginzburg–Landau functional with a surface energy contribution on S^i_ϵ,

$$E_\epsilon[u] \equiv k \int_{G_\epsilon} |\nabla u|^2 + \int_{G_\epsilon} (|u|^2 - 1)^2 + q \sum_i \int_{S^i_\epsilon} (1 + \kappa_\epsilon(\nu, u)^2). \tag{2.2}$$

Here $S^i_\epsilon = \partial B^i_\epsilon$ and ν is the unit normal vector to S^i_ϵ (for the sake of definiteness we assume that ν is directed into the domain G_ϵ). The quantity $(\nu, u) = \Sigma_{i=1}^3 \nu_i u_i$ is the scalar product in $\mathbf{R}^3$ and k, q, and κ_ϵ are given parameters.

It follows from standard analysis[18] that there exists at least one global minimizer $u_\epsilon \in H^1_U(G_\epsilon)$ of the problem (2.1) and (2.2). One can show that under certain conditions on the parameters k, q, κ_ϵ, the sizes of the domain G, and the balls B^i_ϵ, the minimizer is unique. However, generally, there could be more than one minimizer. Further, the minimizers of problem (2.1) and (2.2) exist even if the balls intersect, i.e., when the surface term in (2.2) is not defined at the points of intersection of the spheres S^i_ϵ (the surface measure of the set of such points is zero).

The minimizers of the problem (2.1) and (2.2) describe the equilibrium state of a liquid crystalline medium occupying the domain G_ϵ.

The direction of the vector-valued minimizer u_ϵ determines the average direction of the liquid crystal molecules in the neighborhood of the point x and its magnitude determines, roughly speaking, the fraction of the molecules in a neighborhood of a point x oriented along the preferred direction of u (the orientational rate). The parameters k, q, κ_ϵ characterize the materials properties of the liquid crystal and interfacial effects between the liquid crystal and the inclusions. These parameters satisfy the following conditions: $0<k<\infty$, $0\leqslant q<\infty$, and $-1\leqslant\kappa_\epsilon<\infty$.

In this paper we study the asymptotic behavior of the minimizers of problem (2.1) and (2.2) as $\epsilon\to 0$, when the number of the balls N_ϵ tends to infinity, their radii tend to zero, and the locations of the balls in G and their radii are random.

More precisely we assume that the centers x^i_ϵ of the balls B^i_ϵ and their radii $a_{i\epsilon}$ are defined by the set of s-partial distribution functions

$$f^\epsilon_s(x^1,\ldots,x^s;a_1,\ldots,a_s):\quad (G)^s\times[0,\infty)^s\to[0,\infty)\quad (s=1,2,\ldots,N_\epsilon).$$

The probability of finding the location of the centers and the radii of a group of s balls in $(x^i,x^i+\mathrm{d}x^i)$, $(a_i,a_i+\mathrm{d}a_i)$, where $i=1,\ldots,s$ is

$$f^\epsilon_s(x^1,\ldots,x^s;a_1,\ldots,a_s)\mathrm{d}x^1\cdots\mathrm{d}x^s\,\mathrm{d}a_1\cdots\mathrm{d}a_s.$$

These functions satisfy the conditions of symmetry, normalization, and concordance which follow from their probabilistic interpertation (see, e.g., Ref. 10)

$$f^\epsilon_s(x^1,\ldots,x^k,\ldots,x^l,\ldots,x^s;a_1,\ldots,a_k,\ldots,a_l,\ldots,a_s)=f^\epsilon_s(x^1,\ldots,x^l,\ldots,x^k,\ldots,x^s;a_1,\ldots,a_l,\ldots,a_k,\ldots,a_s),$$

$$\int_G\int_0^\infty\cdots\int_G\int_0^\infty f^\epsilon_s(x^1,\cdots,x^s;a_1,\cdots,a_s)\mathrm{d}a_1\,\mathrm{d}x^1\cdots\mathrm{d}a_s\,\mathrm{d}x^s=1,\quad s=1,\ldots,N_\epsilon,$$

$$\int_G\int_0^\infty f^\epsilon_s(x^1,\ldots,x^s;a_1,\ldots,a_s)\mathrm{d}a_s\,\mathrm{d}x^s=f^\epsilon_{s-1}(x^1,\ldots,x^{s-1};a_1,\ldots,a_{s-1}),\quad s=2,\ldots,N_\epsilon.$$

The distribution functions generate the probability measure P_ϵ in the probability space Ω_ϵ. The points ω_ϵ of this space are in one-to-one correspondence with the random sets $B(\omega_\epsilon)=\cup_i B^i_\epsilon$ in G.[23] For any realization of the set $B(\omega_\epsilon)$ there exists at least one minimizer $u_\epsilon(x,\omega_\epsilon)$ of problem (2.1) and (2.2) in the domain $G(\omega_\epsilon)=G\backslash B(\omega_\epsilon)$. Let us denote by $M(\omega_\epsilon)$ the set of the minimizers which correspond to $\omega_\epsilon\in\Omega_\epsilon$ and consider in the space Ω_ϵ the random variable

$$\rho(\omega_\epsilon)=\max_{M(\omega_\epsilon)}\int_{G(\omega_\epsilon)}|u_\epsilon(x,\omega_\epsilon)-u(x)\chi(x,\omega_\epsilon)|^2\,\mathrm{d}x,\tag{2.3}$$

where u is a vector-valued function $u\in H^1(G)$ and $\chi(x,\omega_\epsilon)$ is the characterisic function of the subdomain $G(\omega_\epsilon)\subset G$.

We will show that under some conditions on the distribution functions $f^\epsilon_1(x;a)$ and $f^\epsilon_2(x^1,x^2;a_1,a_2)$ and with the appropriate choice of the vector function u the random variable (2.3) converges to zero in probability P_ϵ as $\epsilon\to 0$, i.e.,

$$\lim_{\epsilon\to 0}P_\epsilon\{\omega_\epsilon\in\Omega_\epsilon:\rho(\omega_\epsilon)<\delta\}=1\tag{2.4}$$

for any $\delta>0$.

We now introduce the limiting (homogenized) vector function u and the conditions on the one-point and two-point distribution functions f^ϵ_1 and f^ϵ_2 for which the convergence takes place.

First, we assume that these functions have the form

(1) $f^\epsilon_1(x;a)=\epsilon^{-\alpha}f(x;\epsilon^{-\alpha}a)$,

(2) $f_2^\epsilon(x^1,x^2;a_1,a_2)=f_1^\epsilon(x^1;a_1)f_1^\epsilon(x^2;a_2)$,
where $f(x;r)\in L^\infty(G\times[0,\infty))$ is some non-negative function normalized by 1 in $L^\infty(G\times[0,\infty))$ with a compact support $G'\times[a_0,A_0]$ in $G\times[0,\infty)$ $(G'\subset G, 0<a_0<A_0<\infty)$.
We also assume that the parameter κ_ϵ which characterizes the properties of the surfaces S_ϵ^i of the balls B_ϵ^i has the form

(3) $\kappa_\epsilon=\kappa_0\epsilon^\beta$, where $\kappa_0\in[-\epsilon^\beta,\infty)$, $\beta\in(-\infty,\infty)$. We set $g_\epsilon=q\kappa_\epsilon\equiv g\epsilon^\beta$, then $g\in(-\infty,\infty)$. Moreover, if $g<0$ we assume that

$$A_0<k|g|^{-1}, \tag{2.5}$$

where A_0 is a number which defines the diameter of the support of the function $f(x;r)$ [see condition (1)], k and $g=q\kappa_0$ are the parameters of the functional (2.2).

This choice of scaling (3) and the condition (2.5) were introduced in Ref. 6 for a deterministic model (see the introduction).

Next we define the limiting vector function u, which appears in the definition (2.3).

We set

$$p(x)=\int_0^\infty p_{\alpha\beta}(a)f(x;a)\mathrm{d}a, \tag{2.6}$$

where $f(x;a)$ is the function from the condition (1) and the functions $p_{\alpha\beta}(a)$ are defined as follows:

$$p_{\alpha\beta}(a)=\begin{cases}\dfrac{4\pi}{3}ga^2 & \text{for } 2<\alpha<3,\ \beta=3-2\alpha,\\ \dfrac{12\pi(22g^2a^3+45k^2ga^2)}{5(9k+5ga)^2} & \text{for } \alpha=3,\ \beta=-3,\\ \dfrac{264}{125}\pi ka & \text{for } \alpha=3,\ \beta<-3,\\ 0 & \text{for } \alpha,\ \beta\in\Lambda_g.\end{cases} \tag{2.7}$$

The sets Λ_g in (2.7) are defined as follows:

$$\Lambda_g=\{2<\alpha\leqslant 3,\beta>3-2\alpha\}\cup\{\alpha>3,-\infty<\beta<\infty\}$$

if $g\geqslant 0$,

$$\Lambda_g=\{2<\alpha\leqslant 3,\beta>3-2\alpha\}\cup\{\alpha>3,\beta\geqslant-\alpha\}$$

if $g<0$.

Also the potential $p(x)$ satisfies the following condition:

$$p(x)\geqslant\min\left\{1,\frac{1}{\lambda_0}-k\right\}, \tag{2.8}$$

where $\lambda_0=\lambda_0(G)$ is the minimal eigenvalue of the operator $-\Delta$ in G with the homogeneous boundary condition on ∂G. Both conditions (2.7) and (2.8) were introduced in an analogous deterministic problem in Ref. 7 and we refer the reader to Ref. 7 for further details.

Consider a variational problem

$$E_p[u]\to\min,\quad u\in H_U^1(G) \tag{2.9}$$

for the functional

$$E_p[u] \equiv k\int_G |\nabla u|^2\,\mathrm{d}x + \int_G (|u|^2-1)^2 + \int_G p(x)|u|^2\,\mathrm{d}x, \tag{2.10}$$

where the function $p(x)$ is defined by (2.6) and (2.7) and satisfies the inequality (2.8).

As it had been pointed out previously, there exists the unique global minimizer u of the problem (2.9) and (2.10). The function u enters into the definition of the random variable (2.3).

The main result of the paper is the following.

Theorem 2.1: *Let the conditions (1)–(3), and the inequalities (2.5) (for $g<0$) and (2.8) hold. Then the random variable $\rho(\omega_\epsilon)$ defined in (2.3) using the minimizers $u_\epsilon(x,\omega_\epsilon)$ and $u(x)$ of problems (2.1), (2.2), (2.9), and (2.10), respectively, converges to zero in probability [i.e., in the sense of (2.4)] as $\epsilon\to 0$.*

Remark 2.1: Theorem 2.1 states the conditions under which all random minimizers of a stochastic problem (2.1) and (2.2) converge in probability in the space $L^2(G_\epsilon)$ to a nonrandom vector function $u(x)$ and this function is the unique minimizer of a deterministic problem (2.9) and (2.10).

Remark 2.2: Condition (1) (scaling) defines the characteristic dimensions of the balls (inclusions) $B^i_\epsilon(\omega_\epsilon)$ in the probabilistic sense. The assumption that the function $f(x;r)$ has a compact support $G'\times[a_0,A_0]$ in $G\times[0,\infty]$ is made for the sake of simplicity only. It can be dropped, but then the proof of Theorem 2.1 becomes much more technical.

Condition (2) means that the balls $B^i_\epsilon(\omega_\epsilon)$ are "pairwise independent." While this condition admits a possibility of their intersection, i.e., $B^i_\epsilon(\omega_\epsilon)\cap B^j_\epsilon(\omega_\epsilon)\neq\emptyset$ (which is not physical), it follows from Lemma 4.1 that the probability of realizations with intersections tends to zero as $\epsilon\to 0$. This condition can be relaxed to a weaker condition of "pairwise almost independence."

Condition (3) defines the character and the strength of the orientation of liquid crystal molecules on the surfaces of the inclusions. They "prefer" to be orientated along the normal vector when $g<0$ and along the tangent vector when $g>0$.

Finally, the inequality (2.8) guarantees the uniqueness of the solution of the problem (2.9) and (2.10) (see Ref. 6).

The proof of Theorem 2.1 is based on the main theorem from Ref. 6, where an analogous deterministic problem was considered. The theorem from Ref. 6 is proved under deterministic conditions on the distribution of the balls B^i_ϵ and their radii. These conditions are presented below (see Theorem 3.1 in Sec. II). In Sec. III we show that if the distribution functions satisfy the conditions stated above, then the conditions of Theorem 3.1 hold "in probabilistic sense" (and for $\alpha>2$). In Sec. IV we use this fact and Theorem 3.1 to prove Theorem 2.1.

III. DETERMINISTIC DISTRIBUTION OF THE BALLS

For convenience of the reader we now present an outline of the results of the paper[6] which will be used below. Let us consider problem (2.1) and (2.2) in a deterministic domain $G_\epsilon = G\setminus\cup_{i=1}^{N_\epsilon} B^i_\epsilon$, where $B^i_\epsilon\,(i=1,\ldots,N_\epsilon)$ are the balls centered at given points $x^i_\epsilon (i=1,\ldots,N_\epsilon)$ of radii $a_{i\epsilon}$. We assume that the following dependences of the parameters of the problem on ϵ hold:

$$(a_1)\quad g_\epsilon = q\kappa_\epsilon \equiv g\epsilon^\beta, \quad \text{where } \beta, g\in(-\infty,\infty).$$

$$(a_2)\quad a_0\epsilon^\alpha \leqslant a_{i\epsilon} \leqslant A_0\epsilon^\alpha, \quad \alpha>1, 0<a_0<A_0<\infty, \text{ also, if } g<0 \text{ then } A_0<k|g|^{-1}.$$

Next, we introduce the following notations:

$$R_{i\epsilon} = \operatorname{dist}\Big(x^i_\epsilon, \cup_{j\neq i} x^j_\epsilon \cup \partial G\Big) = \min\{\min_{j\neq i}|x^j_\epsilon - x^i_\epsilon|, \operatorname{dist}(x^i_\epsilon, \partial G)\} \tag{3.1}$$

and

$$b_{i\epsilon} = b_{i\epsilon}(\alpha,\beta) = \begin{cases} |g_\epsilon| a^2_{i\epsilon} & \text{for } 1<\alpha\leqslant 3,\ \beta\geqslant 3-2\alpha \text{ and } \alpha\geqslant 3,\ \beta\geqslant -\alpha, \\ a_{i\epsilon} & \text{for } \alpha\geqslant 3,\ \beta<-\alpha. \end{cases} \tag{3.2}$$

We assume that the balls B_ϵ^i are located in the domain G and cannot form clusters so that the following conditions hold:

$$(a_3) \quad R_{i\epsilon} \geqslant a_{i\epsilon}^{\kappa} \text{ for some } \kappa\,(2/\alpha < \kappa < 1),$$

$$(a_4) \quad \text{for some } \sigma\,(3/2 < \sigma \leqslant 2), \text{ we have}$$

$$\sum_{i=1}^{N_\epsilon} \frac{b_{i\epsilon}^{\sigma}}{R_{i\epsilon}^{3(\sigma-1)}} < C_\sigma,$$

where C_σ is a constant independent of ϵ.

Introduce a generalized function

$$p_\epsilon(x) = \sum_{i=1}^{N_\epsilon} (p_{si}^{\epsilon} + p_{vi}^{\epsilon})\,\delta(x - x_\epsilon^i), \tag{3.3}$$

where p_{si}^{ϵ} and p_{vi}^{ϵ} are the specific surface and boundary layer energies, respectively, for the ith ball, defined as follows:

$$p_{si}^{\epsilon} = \begin{cases} \dfrac{4\pi}{3} g_\epsilon a_{i\epsilon}^2 & \text{for } 1 < \alpha < 3,\ \beta = 3 - 2\alpha, \\ \dfrac{4\pi}{3} g_\epsilon a_{i\epsilon}^2 \dfrac{(9k)^2}{(9k + 5g_\epsilon a_{i\epsilon})^2} & \text{for } \alpha = 3,\ \beta = -3, \\ 0 & \text{for } (\alpha,\beta) \in \Lambda^+ \setminus (1 < \alpha \leqslant 3, \beta = 3 - 2\alpha), \end{cases} \tag{3.4}$$

and

$$p_{vi}^{\epsilon} = \begin{cases} \dfrac{264\pi}{5(9k + 5g_\epsilon a_{i\epsilon})^2} k (g_\epsilon a_{i\epsilon})^2 a_{i\epsilon} & \text{for } \alpha = 3,\ \beta = -3, \\ \dfrac{264}{125} \pi k a_{i\epsilon} & \text{for } \alpha = 3,\ \beta < -3, \\ 0 & \text{for } (\alpha,\beta) \in \Lambda^+ \setminus (\alpha = 3, \beta \leqslant -3), \end{cases} \tag{3.5}$$

where

$$\Lambda^+ = \{1 < \alpha \leqslant 3, \beta \geqslant 3 - 2\alpha\} \cup \{\alpha \geqslant 3, -\infty < \beta < \infty\}.$$

Suppose that there exists a limit in a weak topology $\mathcal{D}'(G)$,

$$(b) \quad w - \lim_{\epsilon \to 0} p_\epsilon(x) = p(x), \quad \text{where } p \in L^\infty(G) \text{ satisfies inequality (2.8).}$$

The following theorem is proved in Ref. 6.

Theorem 3.1: *If the conditions* (a_1)–(a_4), (b) *and (2.8) hold, then all minimizers of the problem (2.1) and (2.2)* $(u_\epsilon(x) \in M_\epsilon)$ *converge to the unique minimizer* $u(x)$ *of the problem (2.9) and (2.10) in the following sense;*

$$\max_{u_\epsilon(x) \in M_\epsilon} \int_{G_\epsilon} |u_\epsilon(x) - u(x)\chi_\epsilon(x)|^2\, dx \to 0,$$

as $\epsilon \to 0$, *where the function* $p(x)$ *is defined in the condition* (b). *This convergence takes place in the following range of parameters* α, *and* β *:*

$$\Lambda^+ = \{1 < \alpha \leqslant 3,\ \beta \geqslant 3 - 2\alpha\} \cup \{\alpha \geqslant 3,\ -\infty < \beta < \infty\}$$

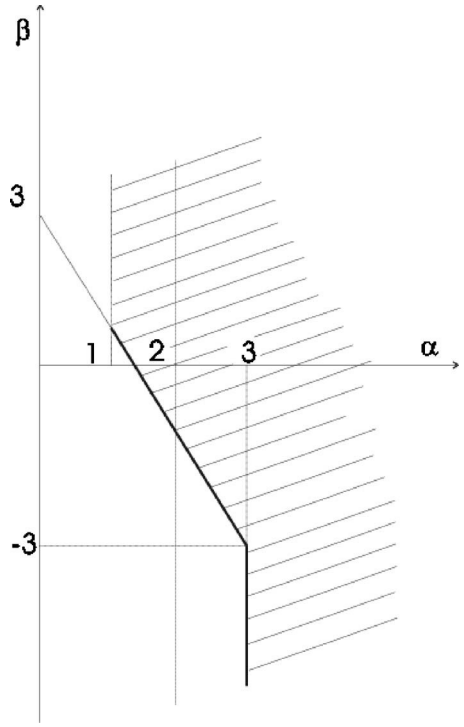

FIG. 1. $g>0$.

when $g_\epsilon>0$ *and*

$$\Lambda^- = \{1 < \alpha \leqslant 3,\ \beta \geqslant 3 - 2\alpha\} \cup \{\alpha \geqslant 3,\ \beta \geqslant -\alpha\}$$

when $g_\epsilon<0$.

The domains Λ^+ and Λ^- are presented (shaded) in Figs. 1 and 2. Notice that the function $p(x)\neq 0$ only on the bold lines. Also, note that we are able to prove a probabilistic analog of this theorem only for the subdomains located in $\Lambda^\pm$ to the right of the vertical line passing through the point $\alpha=2$.

IV. PROBABILISTIC ANALOG OF THE CONDITIONS OF THEOREM 3.1

First, note that the conditions (a_1) and (a_2) are satisfied with probability (1) [this follows from conditions (1) and (3) of Sec. II].

We now show that condition (a_3) holds "in probability." Let μ be a number such that $2/\alpha < \mu < 1$ and let $T^i_{r_\epsilon}$ be the balls centered at the points x^i_ϵ and of radii $r_\epsilon=\epsilon^{\alpha\mu}$. It is clear that $B^i_\epsilon \subset T^i_{r_\epsilon}$. Since the support G' of the function $f(x;a)$ with respect to x is a compact set in G, then (for a sufficiently small ϵ), the balls $T^i_{r_\epsilon}$ do not intersect the boundary ∂G. Consider the event A^μ_ϵ from Ω_ϵ such that the balls $T^i_{r_\epsilon}$ do not have pairwise intersection, i.e.,

$$A^\mu_\epsilon = \{\omega_\epsilon \in \Omega_\epsilon : T^i_{r_\epsilon} \cap T^j_{r_\epsilon} = \emptyset, i,j = 1,\ldots,N_\epsilon, i \neq j\}.$$

Lemma 4.1: If the conditions (1) and (2) of Theorem 2.1 hold, then

$$\lim_{\epsilon\to 0} P_\epsilon\{A^\mu_\epsilon\} = 1.$$

.

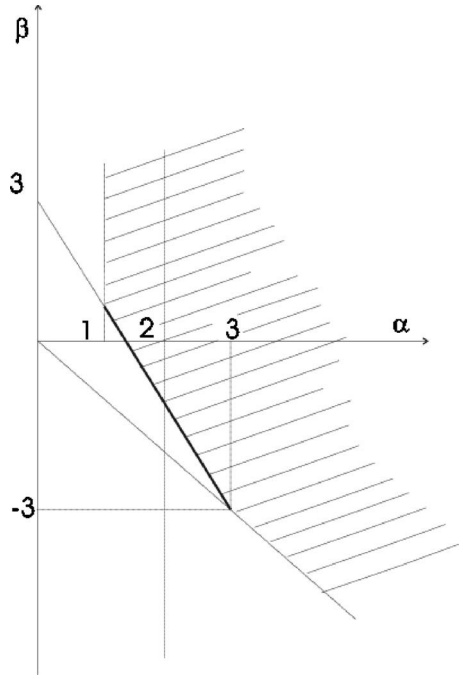

FIG. 2. $g<0$.

Proof: Let $\bar{A}_\epsilon^\mu=\Omega_\epsilon\backslash A_\epsilon^\mu$ be the event that at least one pair of balls $T_{r_\epsilon}^i$ and $T_{r_\epsilon}^j$ intersect, i.e., $\bar{A}_\epsilon^\mu$ is a complement to A_ϵ^μ. Then

$$P_\epsilon\{A_\epsilon^\mu\}=1-P_\epsilon\{\bar{A}_\epsilon^\mu\} \tag{4.1}$$

and

$$\begin{aligned}P_\epsilon\{\bar{A}_\epsilon^\mu\}&=\sum_{\substack{j,i=1\\ j>i}}^{N_\epsilon}\int_G\int_0^\infty\int_{T_{2r_\epsilon}^i}\int_0^\infty f_2^\epsilon(x^i,x^j;a_i,a_j)\mathrm{d}a_j\,\mathrm{d}x^j\,\mathrm{d}a_i\,\mathrm{d}x^i\\&=\frac{N_\epsilon(N_\epsilon-1)}{2}\int_G\int_0^\infty\int_{T_{2r_\epsilon}^1}\int_0^\infty f_2^\epsilon(x^1,x^2;a_1,a_2)\mathrm{d}a_2\,\mathrm{d}x^2\,\mathrm{d}a_1\,\mathrm{d}x^1.\end{aligned}$$

Since $N_\epsilon=\epsilon^{-3}$ and meas $(T_{2r_\epsilon}^1)=(32\pi/3)\epsilon^{3\mu\alpha}$, from conditions (2), (1) and this equality we get

$$\begin{aligned}P_\epsilon\{\bar{A}_\epsilon^\mu\}&\leqslant\frac{\epsilon^{-6}}{2}\int_G\int_0^\infty\int_{T_{2r_\epsilon}^1}\int_0^\infty f_1^\epsilon(x^1;a_1)f_1^\epsilon(x^2;a_2)\mathrm{d}a_2\,\mathrm{d}x^2\,\mathrm{d}a_1\,\mathrm{d}x^1\\&\leqslant\frac{\epsilon^{-6}}{2}\int_G\int_0^\infty f^\epsilon(x^1;a_1)\left(\int_{T_{2r_\epsilon}^1}\int_0^\infty f^\epsilon(x^2;a_2)\mathrm{d}a_2\,\mathrm{d}x^2\right)\mathrm{d}a_1\,\mathrm{d}x^1\leqslant C\epsilon^{3\mu\alpha-6}.\end{aligned}$$

Since $\mu\alpha>2$, the statement of the lemma follows from (4.1). □

Corollary 4.2: It follows from Lemma 4.1 that, if we choose κ *in condition* (a_3) *such that* $2/\alpha<\mu<\kappa<1$, *then for any i* $(i=1,\ldots,N_\epsilon)$ *the inequalities* $R_{i\epsilon}\geqslant a_{i\epsilon}^\kappa$ *hold in probability, i.e.,*

$$\lim_{\epsilon\to0}P_\epsilon\{\omega_\epsilon\in\Omega_\epsilon:R_{i\epsilon}\geqslant a_{i\epsilon}^\kappa,i=1,\ldots,N_\epsilon\}=1.$$

Let us consider now the condition (a_4). To this end we introduce a random variable

$$\zeta_\sigma^\epsilon(\omega_\epsilon)=\sum_{i=1}^{N_\epsilon}\frac{b_{i\epsilon}^\sigma}{R_{i\epsilon}^{3(\sigma-1)}},$$

where $b_{i\epsilon}=b_{i\epsilon}(\omega_\epsilon)$ and $R_{i\epsilon}=R_{i\epsilon}(\omega_\epsilon)$ are random variables defined by (3.2) and (3.1).

Lemma 4.3: If $3/2<\sigma<2$, *then*

$$\overline{\lim_{\epsilon\to 0}}\,P_\epsilon\{\omega_\epsilon\in\Omega_\epsilon:\zeta_\sigma^\epsilon(\omega_\epsilon)\leqslant N\}\geqslant 1-\frac{C(\sigma)}{N}$$

for any $N>0$, *where* $C(\sigma)$ *is independent of* N.

Proof: It follows from the definition of $R_{i\epsilon}$ that

$$\zeta_\sigma^\epsilon(\omega_\epsilon)\leqslant\zeta_{1\sigma}^\epsilon(\omega_\epsilon)+\zeta_{2\sigma}^\epsilon(\omega_\epsilon),$$

where $\zeta_{1\sigma}^\epsilon(\omega_\epsilon)$ and $\zeta_{2\sigma}^\epsilon(\omega_\epsilon)$ are random variables, which are defined as follows:

$$\zeta_{1\sigma}^\epsilon(\omega_\epsilon)=\sum_{i=1}^{N_\epsilon}b_{i\epsilon}^\sigma\max_{j\neq i}\frac{1}{|x_\epsilon^j-x_\epsilon^i|^{3(\sigma-1)}},$$

$$\zeta_{2\sigma}^\epsilon(\omega_\epsilon)=\sum_{i=1}^{N_\epsilon}\frac{b_{i\epsilon}^\sigma}{[\rho(x_\epsilon^i,\partial G)]^{3(\sigma-1)}}.$$

Therefore, it follows from the Chebyshev's inequality that

$$P_\epsilon\{\omega_\epsilon\in\Omega_\epsilon:\zeta_\sigma^\epsilon(\omega_\epsilon)\leqslant N\}\geqslant P_\epsilon\left\{\omega_\epsilon\in\Omega_\epsilon:\sum_{i=1}^{2}\zeta_{i\sigma}^\epsilon(\omega_\epsilon)\leqslant N\right\}\geqslant 1-\frac{\mathbf{M}\left(\sum_{i=1}^{2}\zeta_{i\sigma}^\epsilon\right)}{N}$$
$$=1-\frac{\mathbf{M}(\zeta_{1\sigma}^\epsilon)}{N}-\frac{\mathbf{M}(\zeta_{2\sigma}^\epsilon)}{N}\tag{4.2}$$

for any $N>0$. Here $\mathbf{M}(\cdot)$ is the expectation and in the second inequality it is taken into account that the random variable $\Sigma_{i=1}^2\zeta_{i\sigma}^\epsilon(\omega_\epsilon)$ is positive.

It follows from the properties of the distribution functions (see conditions of Theorem 2.1) that

$$\mathbf{M}(\zeta_{2\sigma}^\epsilon(\omega_\epsilon))=N_\epsilon\int_G\int_0^\infty\frac{b_\epsilon^\sigma(a)f_1^\epsilon(x;a)}{[\rho(x,\partial G)]^{3(\sigma-1)}}\mathrm{d}a\,\mathrm{d}x\leqslant Cb_\epsilon^\sigma(\epsilon^\alpha)N_\epsilon\int_{G'}\frac{\mathrm{d}x}{[\rho(x,\partial G)]^{3(\sigma-1)}},\tag{4.3}$$

where G' is the support of the function $f(x;a)$ with respect to the variable $x\in G$ and the functions $b_\epsilon(a)$ are defined as follows:

$$b_\epsilon(a)=\begin{cases}|g_\epsilon|a^2\equiv|g|\epsilon^\beta a^2 & \text{for } 2<\alpha\leqslant 3,\beta\geqslant 3-2\alpha \text{ and } \alpha\geqslant 3,\beta\geqslant-\alpha,\\ a & \text{for } \alpha\geqslant 3,\beta<-\alpha.\end{cases}$$

Notice that $b_\epsilon(\epsilon^\alpha)\leqslant C\epsilon^\alpha$ for any α, $\beta\in\Lambda^+$. Since $G'\subset G$, then $\rho(x,\partial G)\geqslant\rho_0>0$ for $x\in G'$. Therefore, it follows from (4.3) that

$$\mathbf{M}(\zeta_{2\sigma}^\epsilon)\leqslant C\epsilon^{\sigma\alpha-3},$$

where C is a constant independent of ϵ.

Since $\sigma>3/2$ and $\alpha>2$, from this inequality we have

$$\lim_{\epsilon\to 0}\mathbf{M}(\zeta_{2\sigma}^\epsilon)=0.\tag{4.4}$$

Next we estimate the expectation of the random variable $\zeta^{\epsilon}_{1\sigma}(\omega_\epsilon)$. It is clear that

$$\max_{j\neq i}\frac{1}{|x^j-x^i|^{3(\sigma-1)}}\leqslant L_\epsilon^{3(\sigma-1)}+\sum_{j\neq i}\frac{\chi_{L_\epsilon}(|x^j-x^i|)}{|x^j-x^i|^{3(\sigma-1)}}$$

for any $L_\epsilon>0$. Here $\chi_{L_\epsilon}(t)$ is the indicator of the segment $[0,L_\epsilon^{-1}]$. Therefore, it follows from the properties of the distribution functions (see the conditions of Theorem 2.1) that

$$\begin{aligned}\mathbf{M}(\zeta^{\epsilon}_{1\sigma})&=\int_0^\infty\int_G\cdots\int_0^\infty\int_G\sum_{i=1}^{N_\epsilon}b^{\sigma}_{\epsilon}(a_i)\max_{j\neq i}\frac{1}{|x^j-x^i|^{3(\sigma-1)}}\\&\times f^{\epsilon}_{N_\epsilon}(x^1,\ldots,x^{N_\epsilon};a_1,\ldots,a_{N_\epsilon})\mathrm{d}x^1\,\mathrm{d}a_1\cdots\mathrm{d}x^{N_\epsilon}\,\mathrm{d}a_{N_\epsilon}\leqslant C_1L_\epsilon^{3(\sigma-1)}N_\epsilon b^{\sigma}_{\epsilon}(\epsilon^{\alpha})\\&+\sum_{i=1}^{N_\epsilon}\sum_{j\neq i}\int_0^\infty\int_G\cdots\int_0^\infty\int_G\frac{b^{\sigma}_{\epsilon}(a_i)\chi_{L_\epsilon}(|x^j-x^i|)}{|x^j-x^i|^{3(\sigma-1)}}\\&\times f^{\epsilon}_{N_\epsilon}(x^1,\ldots,x^{N_\epsilon};a_1,\ldots,a_{N_\epsilon})\mathrm{d}x^1\,\mathrm{d}a_1\cdots\mathrm{d}x^{N_\epsilon}\,\mathrm{d}a_{N_\epsilon}\leqslant C_1L_\epsilon^{3(\sigma-1)}\epsilon^{-3}b^{\sigma}_{\epsilon}(\epsilon^{\alpha})+N_\epsilon(N_\epsilon\\&-1)\int_G\int_0^\infty\int_G\int_0^\infty\frac{b^{\sigma}_{\epsilon}(a_1)\chi_{L_\epsilon}(|x^2-x^1|)}{|x^2-x^1|^{3(\sigma-1)}}f^{\epsilon}_1(x^1;a_1)f^{\epsilon}_1(x^2;a_2)\mathrm{d}a_1\,\mathrm{d}x^1\,\mathrm{d}a_2\,\mathrm{d}x^2\\&\leqslant C_1L_\epsilon^{3(\sigma-1)}\epsilon^{\sigma\eta-3}+C_2\epsilon^{\sigma\eta-6}\int_0^{L^{-1}}\frac{r^2\,\mathrm{d}r}{r^{3(\sigma-1)}}\leqslant C_1(\sigma)[L_\epsilon^{3(\sigma-1)}\epsilon^{\sigma\eta-3}+L_\epsilon^{3\sigma-6}\epsilon^{\sigma\eta-6}],\end{aligned}\tag{4.5}$$

where $C_1(\sigma)$ is a constant independent of ϵ and $\eta=\eta(\alpha,\beta)$ is defined as follows:

$$\eta(\alpha,\beta)=\begin{cases}\beta+2\alpha & \text{for } 2<\alpha\leqslant 3,\beta\geqslant 3-2\alpha \text{ and } \alpha\geqslant 3,\beta\geqslant-\alpha,\\ \alpha & \text{for } \alpha\geqslant 3,\beta<-\alpha.\end{cases}$$

Notice, that when we calculated the integral with respect to r from 0 to L_ϵ^{-1} we used the condition $\sigma<2$ for the first time.

Now we choose L_ϵ as follows :

$$L_\epsilon=\begin{cases}\epsilon^{-1} & \text{for } 2<\alpha\leqslant 3,\\ \epsilon^{-\alpha/3} & \text{for } 3\leqslant\alpha\leqslant\infty.\end{cases}$$

Since $\eta(\alpha,\beta)\geqslant 3$ for $2<\alpha\leqslant 3$ and $\eta(\alpha,\beta)\geqslant\alpha$ for $3\leqslant\alpha\leqslant\infty$, it follows from (4.5) that

$$\overline{\lim_{\epsilon\to 0}}\,\mathbf{M}(\zeta^{\epsilon}_{1\sigma})\leqslant 2C_1(\sigma).\tag{4.6}$$

The statement of the lemma follows now from (4.2), (4.4), and (4.6). □

We next show that condition (b) also holds in probability.

Let $\varphi(x)$ be an arbitrary function from $C(\bar{G})$. Consider a random variable

$$\zeta^{\epsilon}_{\varphi}(\omega_\epsilon)=\int_G p_{\alpha\beta}(x,\omega_\epsilon)\varphi(x)\mathrm{d}x,$$

where $p_{\alpha\beta}(x,\omega_\epsilon)$ is defined by (3.3)–(3.5).

Lemma 4.4: Suppose that the conditions (1)–(3) of Theorem 2.1 hold, then

$$\lim_{\epsilon\to 0}P_\epsilon\left\{\omega_\epsilon\in\Omega_\epsilon:\left|\zeta^{\epsilon}_{\varphi}(\omega_\epsilon)-\int_G p(x)\varphi(x)\mathrm{d}x\right|<\delta\right\}=1,$$

where $p(x)$ is the function defined by (2.6) and (2.7).

Proof: It follows from the Chebyshev's inquality[23] that

$$P_\epsilon\{\omega_\epsilon \in \Omega_\epsilon : |\zeta_\varphi^\epsilon(\omega_\epsilon) - \mathbf{M}(\zeta_\varphi^\epsilon)| < \delta\} \geqslant 1 - \frac{\mathbf{D}(\zeta_\varphi^\epsilon)}{\delta^2}, \tag{4.7}$$

where $\mathbf{M}(\zeta_\varphi^\epsilon)$ and $\mathbf{D}(\zeta_\varphi^\epsilon)$ are the expectation and the variance of the random variable ζ_φ^ϵ, respectively.

Using (3.3) we can represent ζ_φ^ϵ as follows :

$$\zeta_\varphi^\epsilon(\omega_\epsilon) = \sum_{i=1}^{N_\epsilon} p_i^\epsilon \varphi(x_\epsilon^i),$$

where $x_\epsilon^i = x_\epsilon^i(\omega_\epsilon)$ are the random centers of the balls B_ϵ^i and $p_i^\epsilon = p_{si}^\epsilon(\omega_\epsilon) + p_{vi}^\epsilon(\omega_\epsilon)$ are the random variables which are defined by (3.4) and (3.5). Using this representation, the properties of the distribution functions, and condition (1) we have

$$\begin{aligned}\mathbf{M}(\zeta_\varphi^\epsilon) &= \int_0^\infty \int_G \cdots \int_0^\infty \int_G \sum_{i=1}^{N_\epsilon} p^\epsilon(a_i)\varphi(x^i) f_{N_\epsilon}^\epsilon(x^1,\ldots,x^{N_\epsilon};a_1,\ldots,a_{N_\epsilon})\mathrm{d}x^1\,\mathrm{d}a_1\cdots\mathrm{d}x^{N_\epsilon}\,\mathrm{d}a_{N_\epsilon} \\ &= N_\epsilon \int_G \int_0^\infty p^\epsilon(a)\varphi(x) f_1^\epsilon(x;a)\mathrm{d}x\,\mathrm{d}a = N_\epsilon \int_G \int_0^\infty p^\epsilon(a)\varphi(x)\epsilon^{-\alpha} f(x;\epsilon^{-\alpha}a)\mathrm{d}x\,\mathrm{d}a,\end{aligned}$$

where $p^\epsilon(a) = p_s^\epsilon(a) + p_v^\epsilon(a)$ and $p_s^\epsilon(a)$, $p_v^\epsilon(a)$ are defined by (3.4) and (3.5) with a instead of $a_{i\epsilon}$.

Since $N_\epsilon = \epsilon^{-3}$, from this equality, condition (3) and (3.4) and (3.5), we get

$$\mathbf{M}(\zeta_\varphi^\epsilon) = \int_G \varphi(x) \int_0^\infty p_{\alpha\beta}(a) f(x;a)\mathrm{d}a\,\mathrm{d}x = \int_G p(x)\varphi(x)\mathrm{d}x \equiv p_\varphi, \tag{4.8}$$

where $p_{\alpha\beta}(x)$ is defined by (2.7) and $p(x)$ is defined by (2.6).

Similarly, taking into account (4.8) and condition (2), we estimate the variance

$$\begin{aligned}\mathbf{D}(\zeta_\varphi^\epsilon) = \mathbf{M}[(\zeta_\varphi^\epsilon - \mathbf{M}(\zeta_\varphi^\epsilon))^2] &= \int_0^\infty \int_G \cdots \int_0^\infty \int_G \left(\sum_{i=1}^{N_\epsilon} p^\epsilon(a_i)\varphi(x^i) - p_\varphi \right)^2 \\ &\times f_{N_\epsilon}^\epsilon(x^1,\ldots,x^{N_\epsilon};a_1,\ldots,a_{N_\epsilon})\mathrm{d}x^1\,\mathrm{d}a_1\cdots\mathrm{d}x^{N_\epsilon}\,\mathrm{d}a_{N_\epsilon} = \epsilon^6 \int_0^\infty \int_G \cdots \int_0^\infty \int_G \sum_{i=1}^{N_\epsilon} (\epsilon^{-3}p^\epsilon(a_i)\varphi(x^i) \\ &- p_\varphi)^2 f_{N_\epsilon}^\epsilon(x^1,\ldots,x^{N_\epsilon};a_1,\ldots,a_{N_\epsilon})\mathrm{d}x^1\,\mathrm{d}a_1\cdots\mathrm{d}x^{N_\epsilon}\,\mathrm{d}a_{N_\epsilon} \\ &+ \epsilon^6 \int_0^\infty \int_G \cdots \int_0^\infty \int_G \sum_{\substack{i,j=1 \\ i\neq j}}^{N_\epsilon} (\epsilon^{-3}p^\epsilon(a_i)\varphi(x^i) - p_\varphi)(\epsilon^{-3}p^\epsilon(a_j)\varphi(x^j) - p_\varphi) \\ &\times f_{N_\epsilon}^\epsilon(x^1,\ldots,x^{N_\epsilon};a_1,\ldots,a_{N_\epsilon})\mathrm{d}x^1\,\mathrm{d}a_1\cdots\mathrm{d}x^{N_\epsilon}\,\mathrm{d}a_{N_\epsilon} = N_\epsilon\epsilon^6 \int_0^\infty \int_G (\epsilon^{-3}p^\epsilon(a)\varphi(x) \\ &- p_\varphi)^2 f_1^\epsilon(x;a)\mathrm{d}x\,\mathrm{d}a + N_\epsilon(N_\epsilon - 1)\epsilon^6 \int_0^\infty \int_G \int_0^\infty \int_G (\epsilon^{-3}p^\epsilon(a_1)\varphi(x^1) - p_\varphi)(\epsilon^{-3}p^\epsilon(a_2)\varphi(x^2) \\ &- p_\varphi) f_1^\epsilon(x^1;a_1) f_1^\epsilon(x^2;a_2)\mathrm{d}x^1\,\mathrm{d}a_1\,\mathrm{d}x^2\,\mathrm{d}a_2 = \epsilon^3 \int_0^\infty \int_G (p_{\alpha\beta}(a)\varphi(x) - p_\varphi)^2 f(x;a)\mathrm{d}x\,\mathrm{d}a \\ &+ (1-\epsilon^3) \int_0^\infty \int_G \int_0^\infty \int_G (p_{\alpha\beta}(a_1)\varphi(x^1) - p_\varphi)(p_{\alpha\beta}(a_2)\varphi(x^2) \\ &- p_\varphi) f(x^1;a_1) f(x^2;a_2)\mathrm{d}x^1\,\mathrm{d}a_1\,\mathrm{d}x^2\,\mathrm{d}a_2.\end{aligned}$$

It follows from (4.8) that the second term on the right-hand side of the last equality is equal to zero. Therefore, we get

$$\mathbf{D}(\zeta_{\varphi}^{\epsilon}) \leqslant C\epsilon^{3}. \tag{4.9}$$

The statement of the lemma follows now from (4.7)–(4.9). □

V. END OF THE PROOF OF THEOREM 2.1

Consider the following events in probability space Ω_ϵ:

$$A_{1\epsilon} = \{\omega_\epsilon \in \Omega_\epsilon : a_0\epsilon^\alpha \leqslant a_{i\epsilon}(\omega_\epsilon) \leqslant A_0\epsilon^\alpha; (\alpha > 2), i = 1,\ldots,N_\epsilon\},$$

$$A_{2\epsilon} = \{\omega_\epsilon \in \Omega_\epsilon : R_{i\epsilon} \geqslant a_{i\epsilon}^{\kappa}, (2/\alpha < \kappa < 1), i = 1,\ldots,N_\epsilon\},$$

$$A_{3\epsilon}(N) = \left\{ \omega_\epsilon \in \Omega_\epsilon : \sum_{i=1}^{N_\epsilon} \frac{b_{i\epsilon}^{\sigma}}{R_{i\epsilon}^{3(\sigma-1)}} < N, (3/2 < \sigma < 2) \right\},$$

$$A_{4\epsilon}(j,m) = \left\{ \omega_\epsilon \in \Omega_\epsilon : \left| \int_G p_\epsilon(x,\omega_\epsilon)\varphi_j(x)\mathrm{d}x - \int_G p(x)\varphi_j(x)\mathrm{d}x \right| < \frac{1}{m} \right\},$$

$$A_{5\epsilon}(\nu) = \{\omega_\epsilon \in \Omega_\epsilon : \rho(\omega_\epsilon) > \nu\},$$

where $\varphi_j(x)$ $(j=1,2,\ldots)$ is a sequence of functions which is dense $C(\bar{G})$, $\rho(\omega_\epsilon)$ is a random value defined by (2.3), $\nu > 0$, and $m \in \mathbf{N}$.

It follows from condition (1) of Theorem 2.1 that

$$P_\epsilon\{A_{1\epsilon}\} = 1 \tag{5.1}$$

for any $\epsilon > 0$.

Assume that the conclusion of Theorem 2.1 does not hold. Then there exist $\delta > 0$, $\nu > 0$, and a sequence $\{\epsilon_k \to 0, k = 1,2,\ldots\}$ such that

$$\lim_{\epsilon = \epsilon_k \to 0} P_\epsilon\{A_{5\epsilon}(\nu)\} > \delta. \tag{5.2}$$

On the other hand, it follows from the Corollary 4.2 and Lemma 4.3 and 4.4 that for any j, $m \in \mathbf{N}$ and $N > 0$ there exist $C(\sigma)$ and $\hat{\epsilon} = \hat{\epsilon}(\delta, N, j, m)$ such that

$$P_\epsilon\{A_{2\epsilon}\} \geqslant 1 - \frac{\delta}{4},$$

$$P_\epsilon\{A_{3\epsilon}(N)\} \geqslant 1 - \frac{C(\delta)}{N},$$

$$P_\epsilon\{A_{4\epsilon}(j,m)\} \geqslant 1 - \frac{\delta}{2^{j+m+2}}, \tag{5.3}$$

for any $\epsilon < \hat{\epsilon}$.

Set $N = 4C(\delta)/\delta$ and consider the event

$$A_{\epsilon_k} = A_{1\epsilon_k} \cap A_{2\epsilon_k} \cap A_{3\epsilon_k}(N) \cap \left[\bigcap_{m=1}^{m_k} \bigcap_{j=1}^{j_k} A_{4\epsilon_k}(j,m) \right] \cap A_{5\epsilon_k}(\nu), \tag{5.4}$$

where we choose the numbers m_k and j_k to be such that the inequalities (5.3) hold for $\epsilon=\epsilon_k$ and $m \leqslant m_k$, $j \leqslant j_k$, $N=4C(\delta)/\delta$. Since $\epsilon_k \to 0$ as $k \to \infty$, the numbers m_k and j_k tend to infinity as $k \to \infty$.

Now we show that there is no k for which the event $A_{\epsilon_k} \subset \Omega_{\epsilon_k}$ is not empty. It follows from our choice of N and inequalities (5.3) that

$$P_{\epsilon_k}\left\{ \bar{A}_{2\epsilon_k} \cup \bar{A}_{3\epsilon_k}(N) \cup \left[\bigcup_{m=1}^{m_k} \bigcup_{j=1}^{j_k} \bar{A}_{4\epsilon_k}(j,m) \right] \right\} \leqslant \frac{\delta}{4} + \frac{\delta}{4} + \delta \sum_{j,m=1}^{\infty} \frac{1}{2^{j+m+2}} = \frac{3}{4}\delta.$$

Therefore,

$$P_{\epsilon_k}\left\{ A_{2\epsilon_k} \cap A_{3\epsilon_k}(N) \cap \left[\bigcap_{m=1}^{m_k} \bigcap_{j=1}^{j_k} A_{4\epsilon_k}(j,m) \right] \right\} \geqslant 1 - \frac{3}{4}\delta. \tag{5.5}$$

Here the bar denotes the complementary event.

It follows from (5.4), (5.1), (5.2), and (5.5) that the events A_{ϵ_k} $(k=1,2,\ldots)$ are not empty. For any A_{ϵ_k} we choose a point $\omega(\epsilon_k)=\omega_k$ from this set and consider the corresponding realization of the balls $B^i_{\epsilon_k}(\omega_k)$ $(i=1,\ldots,N_{\epsilon_k})$ in G and the values $\rho(\omega_k)$ constructed by using the minimizers $u_{\epsilon_k}(x,\omega_k) \in M(\omega_k)$ of problem (2.1) and (2.2) in the domain $G_{\epsilon_k}(\omega_k)=G \setminus \cup_i B^i_{\epsilon_k}(\omega_k)$.

It follows from the definition of A_{ϵ_k} that all the conditions of Theorem 3.1 are satisfied as $\epsilon \to 0$ but $\rho(\omega_k)$ does not tend to zero. This contradiction proves Theorem 2.1. (Also see Ref. 24.)

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Ginzburg–Landau description of confinement and quantization effects in mesoscopic superconductors

L. F. Chibotaru and A. Ceulemans
Quantum Chemistry Group, Department of Chemistry, K. U. Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium

M. Morelle, G. Teniers, C. Carballeira,[a] and V. V. Moshchalkov
Nanoscale Superconductivity and Magnetism Group, Department of Physics and Astronomy, K. U. Leuven, Celestijnenlaan 200 D, B-3001 Leuven, Belgium

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An approach to the Ginzburg–Landau problem for superconducting regular polygons is developed making use of an analytical gauge transformation for the vector potential $\mathbf{A}$ which gives $A_n=0$ for the normal component along the boundary line of different symmetric polygons. As a result the corresponding linearized Ginzburg–Landau equation reduces to an eigenvalue problem in the basis set of functions obeying Neumann boundary condition. Such basis sets are found analytically for several symmetric structures. The proposed approach allows for accurate calculations of the order parameter distributions at low calculational cost (small basis sets) for moderate applied magnetic fields. This is illustrated by considering the nucleation of superconductivity in squares, equilateral triangles and rectangles, where vortex patterns containing antivortices are obtained on the T_c–H phase boundary. The calculated phase boundaries are compared with the experimental $T_c(H)$ curves measured for squares, triangles, disks, rectangles, and loops. The stability of the symmetry consistent solutions against small deviations from the phase boundary line deep into the superconducting state is investigated by considering the full Ginzburg–Landau functional. It is shown that below the nucleation temperature symmetry-switching or symmetry-breaking phase transitions can take place. The symmetry-breaking phase transition has the same structure as the pseudo-Jahn-Teller instability of high symmetry nuclear configurations in molecules. The existence of these transitions is predicted to be strongly dependent on the size of the samples. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2013107]

I. INTRODUCTION

"Confinement" and "quantization" are two closely related definitions: if a particle is "confined" then its energy is "quantized," and vice versa. According to the dictionary, to "confine" means to "restrict within limits," to "enclose," and even to "imprison." A typical example, illustrating the relation between confinement and quantization, is the restriction of the motion of a particle by enclosing it within an infinite potential well of size L_A.

Recent impressive progress in nanofabrication has made it possible to realize the whole range of confinement lengths L_A, from 1 μm (photo- and e-beam lithography), via 1 nm to 1 Å (single atom manipulation) and, through that, to control the confinement energy (temperature) from a few mK higher up to far above room temperature.

This progress has stimulated dramatically the experimental and theoretical studies of different

[a]On leave from Laboratorio de Baixas Temperaturas e Superconductividade, Departamento de Física da Materia Condensada, Universidade de Santiago de Compostela, E-15782 Santiago de Compostela, Spain.

nanostructured materials and individual nanostructures. The interest towards such structures arises from the remarkable principle of "quantum design," when quantum mechanics can be efficiently used to tailor the physical properties of nanostructured materials.

Modifying the sample topology in nanostructured materials creates a unique possibility to impose the desired boundary conditions, and through that to change the properties of the sample. A Fermi liquid or a superconducting condensate confined within such materials will be subjected to severe constraints and, as a result, the properties of these materials will be strongly affected by the boundary conditions.[1]

While a normal metallic system should be considered quantum mechanically by solving the Schrödinger equation:

$$\frac{1}{2m}(-\imath\hbar\vec{\nabla}-e\vec{A})^2\Psi+U\Psi=E\Psi, \tag{1}$$

a superconducting system is described by the two coupled Ginzburg–Landau (GL) equations,[2]

$$\frac{1}{2m^\star}(-i\hbar\vec{\nabla}-e^\star\vec{A})^2\Psi_s+\beta|\Psi_s|^2\Psi_s=-\alpha\Psi_s, \tag{2}$$

$$\vec{j}=\vec{\nabla}\times\vec{h}=\frac{e^\star}{2m^\star}[\Psi_s^\star(-\imath\hbar\vec{\nabla}-e^\star\vec{A})\Psi_s+\Psi_s(\imath\hbar\vec{\nabla}-e^\star\vec{A})\Psi_s^\star], \tag{3}$$

with $\vec{A}$ the vector potential which corresponds to the microscopic field $\vec{h}=\mathrm{rot}\,\vec{A}/\mu_0$, U the potential energy, E the total energy, α a temperature dependent parameter changing sign from $\alpha>0$ to $\alpha<0$ as T is decreased through T_c, β a positive temperature independent constant, $m^\star$ the effective mass which can be chosen arbitrarily and is generally taken as twice the free electron mass m.

Note that the first GL equation [Eq. (2)], with the nonlinear term $\beta|\Psi_s|^2\Psi_s$ neglected, is the analogue of the Schrödinger equation [Eq. (1)] with $U=0$, when making a few substitutions, $\Psi_s\leftrightarrow\Psi$, $e^\star\leftrightarrow e$, $-\alpha\leftrightarrow E$, and $m^\star\leftrightarrow m$. The superconducting order parameter Ψ_s corresponds to the wave function Ψ in Eq. (1). The effective charge $e^\star$ in the GL equations is $2e$, i.e., the charge of a Cooper pair, while the temperature dependent GL parameter α,

$$-\alpha=\frac{\hbar^2}{2m^\star\xi^2(T)}, \tag{4}$$

plays the role of E in the Schrödinger equation. Here $\xi(T)$ is the temperature dependent coherence length,

$$\xi(T)=\frac{\xi(0)}{\sqrt{1-\dfrac{T}{T_{c0}}}}. \tag{5}$$

The boundary conditions for interfaces normal metal vacuum and superconductor vacuum are, however, different,[3]

$$\Psi\Psi^\star|_b=0, \tag{6}$$

$$(-\imath\hbar\vec{\nabla}-e^\star\vec{A})\Psi_s|_{\perp,b}=0, \tag{7}$$

i.e., for normal metallic systems *the density* is zero at the boundary (Dirichlet boundary condition), while for superconducting systems, *the current density* has no component perpendicular to the boundary. As a consequence, the supercurrent cannot flow through the boundary. The nucleation of the superconducting condensate is favored at the superconductor/vacuum interfaces, thus leading

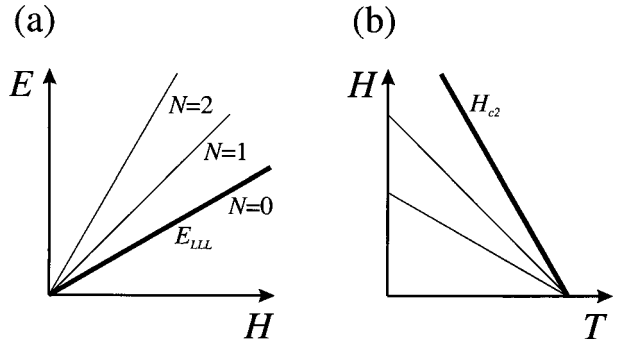

FIG. 1. Landau level scheme in the bulk. From the lowest Landau level $E_{\mathrm{LLL}}(H)=\hbar\omega/2$ [panel (a)] the second critical field $H_{c2}(T)$ [panel (b)] is derived.

to the appearance of superconductivity, at the third critical field $H_{c3}(T)$, in a surface sheet with a thickness $\xi(T)$.

For bulk superconductors the surface-to-volume ratio is negligible and therefore superconductivity in the bulk is not affected by a thin superconducting surface layer. For nanostructured superconductors with antidot arrays, however, the boundary conditions [Eq. (7)] and the surface superconductivity introduced through them become very important if $L_A \leqslant \xi(T)$. The advantage of superconducting materials in this case is that it is not even necessary to go to nm scale (like for normal metals), since for L_A of the order of 0.1–1.0 μm the temperature range where $L_A \leqslant \xi(T)$, spreads over 0.01–0.1 K below T_c due to the divergence of $\xi(T)$ at $T \to T_{c0}$ [Eq. (5)].

In principle, the mesoscopic regime $L_A \leqslant \xi(T)$ [and $L_A \leqslant \lambda(T)$, with λ the magnetic penetration depth] can eventually be reached even in bulk superconducting samples with $L_A \sim 1$ cm^{-1} m, since $\xi(T)$ [and $\lambda(T)$ as well] diverges at $T \to T_{c0}$. However, the temperature window where $L_A \leqslant \xi(T)$ is so narrow, not more than ~ 1 nK below T_{c0}, that one needs ideal sample homogeneity and perfect temperature stability.

In the mesoscopic regime $L_A \leqslant \xi(T)$, which is quite easily realized in nanostructured materials, the surface superconductivity can cover the whole available space occupied by the material, thus spreading superconductivity all over the sample. It is then evident that in this case the surface effects play the role of bulk effects.

Using the similarity between the linearized GL equation [Eq. (2)] and the Schrödinger equation [Eq. (1)], the approach to determine $T_c(H)$ can be formalized as follows: since the parameter $-\alpha$ [Eqs. (2) and (4)] plays the role of energy E [Eq. (1)], then *the highest possible temperature $T_c(H)$ for the nucleation of the superconducting state in presence of the magnetic field H always corresponds to the lowest Landau level $E_{\mathrm{LLL}}(H)$* found by solving the Schrödinger equation [Eq. (1)] with "superconducting" boundary conditions [Eq. (7)].

Figure 1 illustrates the application of this basic rule to the calculation of the upper critical field $H_{c2}(T)$, indeed, if the well-known classical Landau solution for the lowest level in a bulk sample $E_{\mathrm{LLL}}(H)=\hbar\omega/2$, where $\omega=e^{\star}\mu_0 H/m^{\star}$ is the cyclotron frequency, is taken, then, from $-\alpha = E_{\mathrm{LLL}}(H)$, we have

$$\frac{\hbar^2}{2m^{\star}\xi^2(T)} = \left.\frac{\hbar\omega}{2}\right|_{H=H_{c2}} \tag{8}$$

with the help of Eq. (4). We obtain

$$\mu_0 H_{c2}(T) = \frac{\Phi_0}{2\pi\xi^2(T)}, \tag{9}$$

with $\Phi_0 = h/e^{\star} = h/2e$ the superconducting flux quantum.

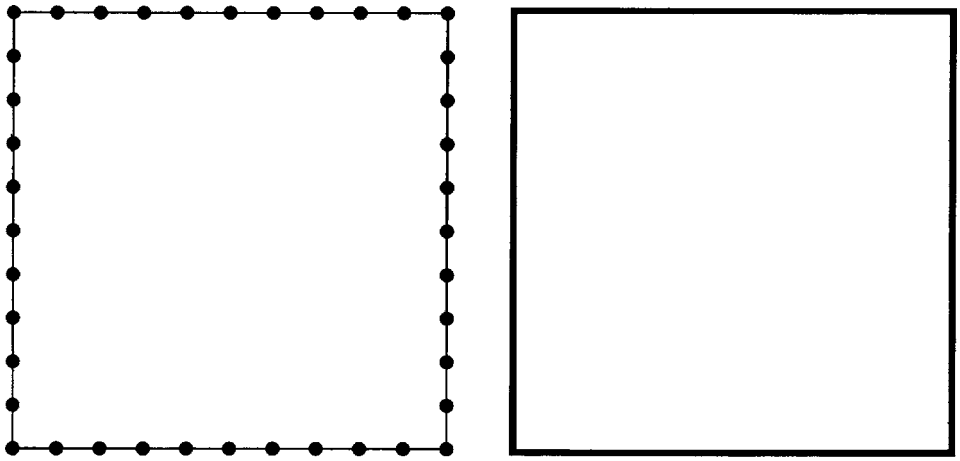

FIG. 2. Domains (bold dots and lines) of the boundary line where the condition in Eq. (7) is satisfied exactly for the case of finite grid (a) and appropriate vector potential gauge (b) methods.

In nanostructured superconductors, where the boundary conditions [Eq. (7)] strongly influence the Landau level scheme, $E_{\mathrm{LLL}}(H)$ must be calculated for each specific confinement geometry. By measuring the shift of the critical temperature $T_c(H)$ in a magnetic field, one can compare the experimental phase boundary $T_c(H)$ with the calculated level $E_{\mathrm{LLL}}(H)$ and thus check the effect of the confinement topology on the superconducting phase boundary for a series of nanostructured superconducting samples. The transition between normal and superconducting states is usually very sharp and therefore the lowest Landau level can be easily traced as a function of applied magnetic field. The midpoint of the resistive transition from the superconducting to the normal state is usually taken as the criterion to determine $T_c(H)$.

This defines the main strategy of our paper to use systematically the GL approach to calculate the condensate density and the energy levels [including $E_{\mathrm{LLL}}(H)$ for superconducting samples of different geometries and topologies and to compare the calculated lowest level $E_{\mathrm{LLL}}(H)$] with the measured $T_c(H)$ phase boundary.

The presence of the vector potential in the boundary condition, Eq. (4), seriously complicates the solution of the Ginzburg–Landau equations for samples of arbitrary geometry. Existing treatments use numerical methods like the method of finite differences. This way proved to be successful for the description of superconductivity in mesoscopic structures[4,5] although it is usually achieved at the expense of high computational costs. The problem, however, simplifies very much if one can find a gauge for the vector potential ($\tilde{\mathbf{A}}$) giving zero normal component on the boundary line

$$\tilde{\mathbf{A}}|_n = 0. \tag{10}$$

In these cases the superconducting boundary condition in Eq. (7) reduces to the Neumann boundary condition,

$$\nabla\Psi|_n = 0, \tag{11}$$

which is much easier to satisfy. Such gauges have been found in the past for infinite slabs,[6] semiplanes with a wedge,[7,8] and disks.[9–12]

The major difference between the above approaches is the extent to which they fulfill the superconducting boundary condition. As Fig. 2 shows, the method of finite differences satisfies Eq. (7) only on a finite set of points along the boundary line, while by using an appropriate gauge for the vector potential (10) we are able *to satisfy the boundary condition everywhere on the*

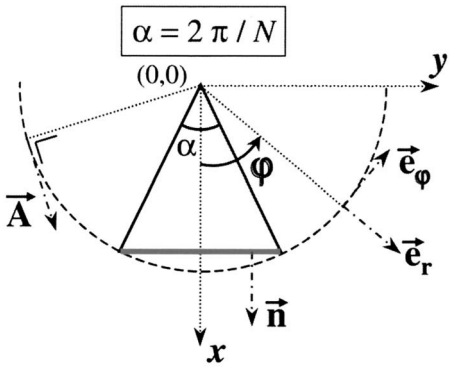

FIG. 3. Piece of a regular polygon containing one edge (thick line). The origin of the coordinate system is chosen in the center of the polygon. $\mathbf{n}$ is the unit vector normal to the edge. $\mathbf{e}_r$ and $\mathbf{e}_\varphi$ are unit vectors of the cylindrical coordinate system. The z axis coincides with the N fold rotational axis of the polygon.

boundary. Since Eq. (7) is nothing but a sort of quantization condition for our problem, we can conclude that finite grid methods always imply an *approximate* solution of Eq. (7), while the methods using the appropriate gauge for the vector potential treat it *exactly*. This is crucial for the proper description of the order parameter in the cases when the boundary becomes important, i.e., for low values of the applied flux.

In this paper we review the development of this second type of approach to the Ginzburg–Landau problem for symmetric superconducting polygons in external magnetic field. In Secs. II and III we present the derivation of vector potential gauge and the basis set for several symmetric structures. The application of this approach to the description of the nucleation of superconductivity in different polygons is given in Sec. IV. Here the evolution of the vortex patterns as a function of applied magnetic field is investigated in detail. We also compare the calculated superconducting/normal phase boundary lines with the experimental ones. The evolution from a disk to thin loops is discussed in Sec. V. In Sec. VI we study the stability of the LGL solutions corresponding to nucleated phases and the conditions for the arising of different phase transitions when the temperature is lowered from the nucleation point. Finally Sec. VII gives some conclusions and the perspective for the future work.

II. VECTOR POTENTIAL GAUGE FOR SYMMETRIC POLYGONS

Consider a regular polygon with N edges. It has a symmetry axis of order N, corresponding to rotations by angles which are multiples of $2\pi/N$. An external homogeneous magnetic field applied along this axis can be described by a vector potential

$$\mathbf{A} = \tfrac{1}{2}\mathbf{H} \times \mathbf{r}, \tag{12}$$

where the radius vector lies in the xy plane (Fig. 3) and $\mathbf{H} \| \mathbf{z}$. Equation (12) defines the cylindrical gauge for $\mathbf{A}$. It is often preferred over many other possible choices[13] due to the high symmetry which allows to preserve the rotational symmetry of the system without field. The direction of $\mathbf{A}$ is tangential to concentric circumferences, $\mathbf{A} \| \mathbf{e}_\varphi$, which are also equipotential lines for the vector potential.

As one can see from Fig. 3, the vector potential in Eq. (12) is not tangential to the boundary line (i.e., the edges) of a polygon. On the edge shown in Fig. 3 it contains a normal component

$$A_n(\varphi) = -C \tan \varphi,$$

$$C = \tfrac{1}{4} H a, \tag{13}$$

where φ is the polar angle and a is the diameter of the circumference inscribed in the regular polygon. Our purpose is to find a new vector potential which would be tangential to the edges. This can be done by the following gauge transformation:[13]

$$\tilde{\mathbf{A}} = \mathbf{A} + \nabla S, \tag{14}$$

where $\mathbf{A}$ is the old and $\tilde{\mathbf{A}}$ is the new vector potential and S is an arbitrary scalar function. This function is found from the condition $\tilde{A}_n = 0$ on the boundary line. This is equivalent to the equation

$$A_n = -\nabla_n S, \tag{15}$$

which must be obeyed on each edge. In order to keep the rotational symmetry of the regular polygon $\tilde{\mathbf{A}}$ and S should be periodic functions of φ with the period α (Fig. 3). Because $\tilde{\mathbf{A}}$ is real, this suggests the following general form for S (in polar coordinates):

$$S(r,\varphi) = \sum_m [R_m^s(r)\sin(Nm\varphi) + R_m^c(r)\cos(Nm\varphi)], \tag{16}$$

where m are non-negative integers. Due to the rotational periodicity of the function S it is enough to satisfy Eq. (15) on one single edge. The form in Eq. (16) is further simplified due to the symmetry requirement that $\tilde{\mathbf{A}}$ is purely tangential on the radial lines defined by $\varphi = \pm\alpha/2$ and $\varphi = 0$ (Fig. 3). The latter requirement means that ∇S is purely tangential on the radial line $\varphi = 0$ which can only be the case if one takes $R_m^c(r) = 0$ in Eq. (16).

Next we simplify the remaining part of the form (16) by confining ourselves to one single term in the summation. Obviously this cannot be the term $m = 0$ because ∇S should be dependent on φ as it is easily seen from Eqs. (13) and (15). Therefore the simplest possible term is $m = 1$ which leads to the ansatz,

$$S_N(r,\varphi) = R_N(r)\sin(N\varphi). \tag{17}$$

Substituting Eqs. (13) and (17) into (15), after eliminating the r variable on the edge line,

$$r = \frac{a}{2\cos\varphi},$$

$$\frac{\partial}{\partial r} = \frac{2}{a}\frac{\cos^2\varphi}{\sin\varphi}\frac{\partial}{\partial\varphi}, \tag{18}$$

one obtains the following equation in φ:

$$\tilde{R}_N' \sin(N\varphi)\cos^2\varphi - \tilde{R}_N \sin(N\varphi)'\sin^2\varphi = \tan^2\varphi, \tag{19}$$

where the prime in the superscript means the first derivative after φ and the following notation was introduced:

$$\tilde{R}_N(\varphi) = \frac{2}{aC} R_N\left(\frac{a}{2\cos\varphi}\right). \tag{20}$$

Bringing Eq. (19) to the form

$$\tilde{R}_N' + \xi(\varphi)\tilde{R}_N = \eta(\varphi), \tag{21}$$

where

$$\xi(\varphi) = -N\cot(N\varphi)\tan^2\varphi,$$

$$\eta(\varphi) = \csc(N\varphi)\tan^2\varphi/\cos^2\varphi, \tag{22}$$

allows us to write down the general solution[14]

$$\tilde{R}_N(\varphi) = \frac{1}{\mu(\varphi)}\left(\int \eta(\varphi)\mu(\varphi)\mathrm{d}\varphi + C_1\right),$$

$$\mu(\varphi) = \exp\left(\int \xi(\varphi)\mathrm{d}\varphi\right). \tag{23}$$

The solution (23) describes the radial function in Eq. (17) only for values of r which are radius vectors of the points on the edge's line. One can extend this solution over the whole range of r by the inverse transformation to (18), $a/2\cos\varphi \to r$. Then using again Eqs. (14), (17), and (20) we can express the polar components of the gauge transformed vector potential $\tilde{\mathbf{A}}$,

$$\tilde{A}_r = \frac{\partial R_N(r)}{\partial r}\sin(N\varphi),$$

$$\tilde{A}_\varphi = \frac{1}{2}Hr + \frac{N}{r}R_N(r)\cos(N\varphi), \tag{24}$$

through the solution (23). The constant C_1 contained in that solution should be chosen in such a way as to provide nondivergent components of the vector potential (24). In contrast to $\mathbf{A}$ in Eq. (12), the vector potential defined by Eqs. (24) does not obey the Coulomb gauge, $\nabla\cdot\mathbf{A}=0$. Hence the term $\nabla\cdot\mathbf{A}$ plays the role of a scalar potential in a Hamiltonian and should be nondivergent either. Fortunately both requirements are met within the area of the polygon under the simple condition $C_1=0$.

Analytical expressions of Eqs. (23) for some regular polygons are given in Ref. 15.

In the case of equilateral triangle the solutions (24) have the form

$$\tilde{A}_r = \tfrac{27}{2}Ha\left(9r'^8 - 7r'^6 + \tfrac{5}{3}r'^4\right)\sin 3\varphi,$$

$$\tilde{A}_\varphi = \tfrac{1}{2}Hr + \tfrac{81}{2}Ha\left(r'^8 - r'^6 + \tfrac{1}{3}r'^4\right)\cos 3\varphi,$$

$$r' = r/\sqrt{3}a, \tag{25}$$

where a is the side length of the triangle. Figure 4 shows how the gauge transformed vector potential looks for the equilateral triangle. We can see that it gradually changes from the cylindrical gauge in the central region to a triangular pattern close to the edges. According to this gauge transformation one should add to Eq. (4) the following divergency term:

$$\nabla\cdot\tilde{\mathbf{A}} = H\frac{9\sqrt{3}}{2}\left(72r'^7 - 40r'^5 + \frac{16}{3}r'^3\right)\sin 3\varphi. \tag{26}$$

In the case of a square the solutions of Eqs. (23) and (24) yield the following gauge transformed vector potential (Fig. 5):

$$\tilde{A}_r = -\frac{1}{4\sqrt{2}}Ha(1+u)^{3/2}[-1+u+(1+2u-u^2)e^{-u}Ei(u)]\sin 4\varphi,$$

$$\tilde{A}_\varphi = \frac{1}{2}Hr + \frac{1}{2\sqrt{2}}Ha(1+u)^{3/2}[1-ue^{-u}Ei(u)]\cos 4\varphi,$$

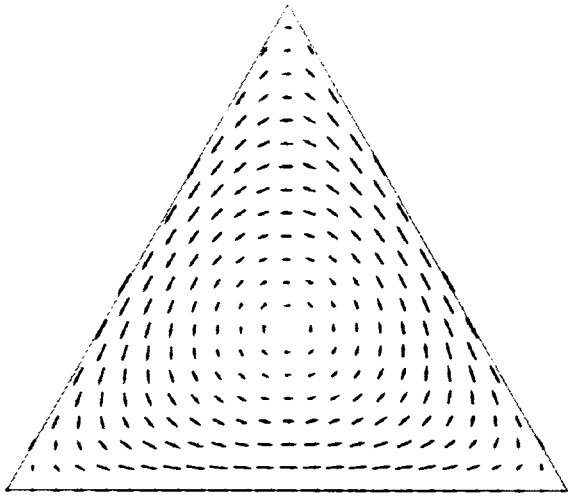

FIG. 4. Vector potential for the equilateral triangle (arbitrary units) after the gauge transformation, described by Eqs. (25).

$$u = 2(r/a)^2 - 1, \tag{27}$$

where $Ei(u)$ is the exponential integral function[16] and a is the side length of the square. In full analogy with the previous case (Fig. 4), this vector potential coincides with the cylindrical gauge in the central region and smoothly changes into a square symmetry pattern when approaching the boundaries. The corresponding divergency term is obtained as follows:

$$\boldsymbol{\nabla} \cdot \tilde{\mathbf{A}} = H\frac{(1+u)^2}{2u}[-1-5u+u^2-u(3-6u+u^2)e^{-u}Ei(u)]\sin 4\varphi. \tag{28}$$

The results for the square are easily extended over arbitrary rectangles, described by the aspect

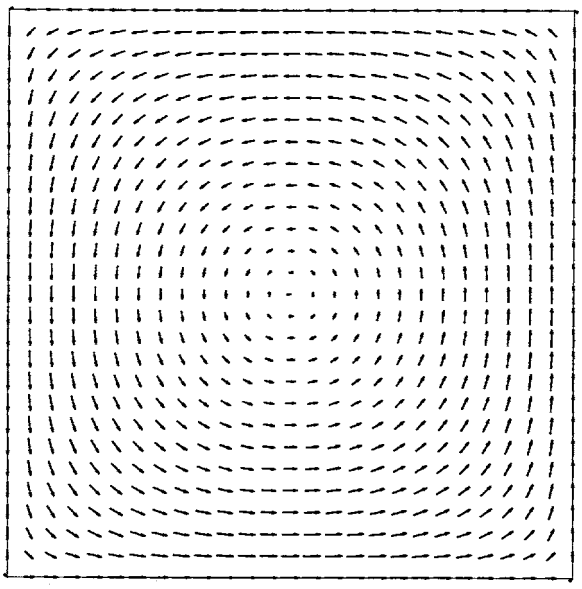

FIG. 5. Vector potential for the square (arbitrary units) after the gauge transformation, described by Eqs. (27).

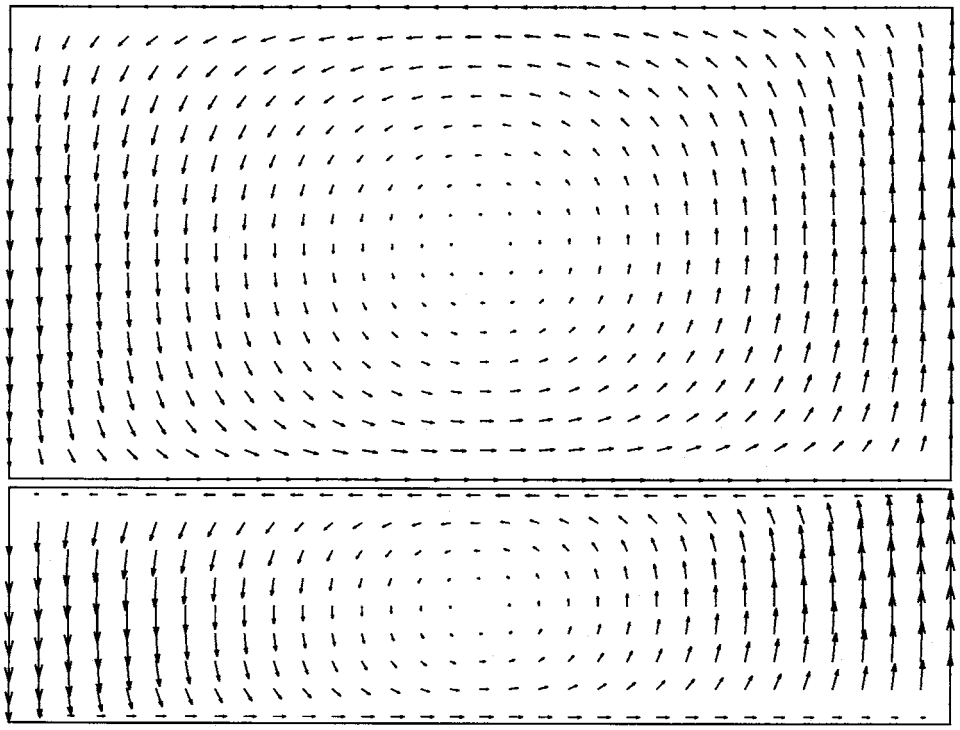

FIG. 6. Vector potential for the rectangle (arbitrary units) with aspect ratio two (top) and four (bottom) after the gauge transformation, described by Eqs. (14), (27), and (29).

ratios $\zeta=a/b$, where a and b are the lengths of the two sides. Directing the Cartesian axes x and y along the sides a and b, respectively, we find the following relation for the scalar function S entering the gauge transformed vector potential (14) for the rectangle:

$$S_{\mathrm{rect}}(x,y) = S_{\mathrm{sq}}\left(\frac{1}{\sqrt{\zeta}}x, \sqrt{\zeta}y\right), \tag{29}$$

where S_{sq} is the scalar function for the square with the side length $a/\sqrt{\zeta}=\sqrt{\zeta}b$. After substitution of Eq. (29) into (14), written in polar coordinates, we can make direct use of Eqs. (27). The resulting gauge transformed vector potential is shown in Fig. 6. The divergency term to be inserted into Eq. (4) is just ΔS_{rect}.

Another extension of the above approach concerns symmetric nonhomogeneous applied magnetic fields. These can be induced, for instance, by setting a cylindrical quantum dot uniformly magnetized along its axis on the top of a superconducting sample.[17,18] This magnetic field together with an independent homogeneous component corresponds to a vector potential of cylindrical symmetry[19]

$$A_{\varphi}(r) = \frac{1}{2}Hr + 4M\sqrt{\frac{R}{r}}\int_0^l \frac{\left[\left(1-\frac{k^2}{2}\right)K(k) - E(k)\right]}{k}\mathrm{d}z,$$

$$k^2 = \frac{4rR}{(r+R)^2+z^2}, \tag{30}$$

where R, l, and M are the radius, the height, and the density of magnetization of the cylindrical dot, respectively; K and E are elliptic integrals of first and second kind, respectively, and H is the

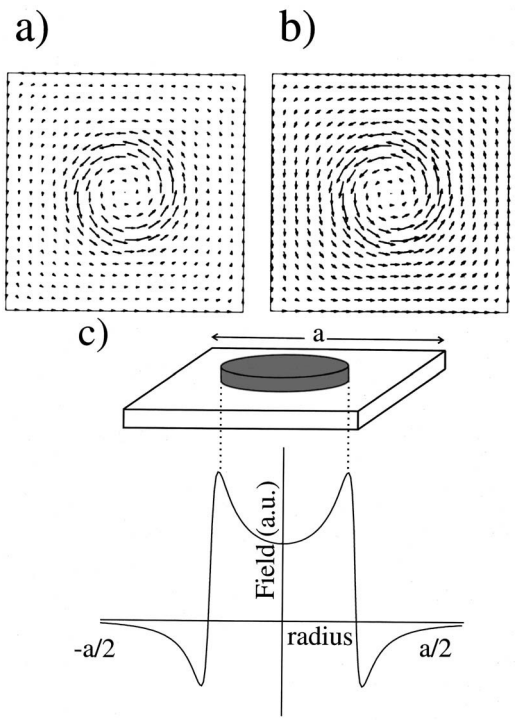

FIG. 7. Vector potential for a square with cylindrical uniformly magnetized quantum dot (a) in an external homogeneous magnetic field producing one flux quantum in the sample, (b) in zero external field. The dot has a radius 0.2 times and a height 0.032 times the sample size a and the magnetization produces one flux quantum in the sample. (c) Schematic drawing of the superconducting square with the magnetic dot (gray) and the corresponding field profile.

intensity of the homogeneous magnetic field as before. Repeating all derivations with the new applied vector potential (30) instead of the cylindrical one (12) we obtain similar results as in Eqs. (22), (23), and (24), where the second equation from (22) should be replaced by

$$\eta(\varphi) = \csc(N\varphi)\frac{\tan^2\varphi}{\cos\varphi}A_\varphi\left(\frac{a}{2\cos\varphi}\right), \tag{31}$$

and A_φ should replace $Hr/2$ in the second equation of (24). However now we can no longer find the primitive in the first equation of (23) in analytical form. This complication can be avoided if we approximate the function $A_\varphi(r)$ by polynomials. This can be done for arbitrary parameters of the dot, which allows to obtain the explicit expressions for the components of the gauge transformed vector potential.[20] Figure 7 shows the gauge transformed vector potential for a square with a cylindrical magnetic dot on top of it. We can see that the behavior of $\tilde{\mathbf{A}}$ as function of r is similar to the previous cases.

III. BASIS SET FOR THE GL PROBLEM OF SYMMETRIC POLYGONS

Having found a gauge for the vector potential ($\tilde{\mathbf{A}}$) satisfying the condition (10) on the boundary line, it follows immediately from Eq. (7) that the order parameter can be expanded into a set of functions, $\{\psi_m\}$,

$$\Psi = \sum_m c_m\psi_m, \tag{32}$$

obeying the Neumann boundary condition,

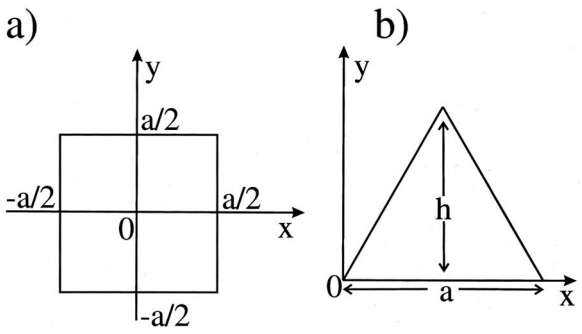

FIG. 8. Coordinate systems used in the derivation of the basis set for a square (a) and an equilateral triangle (b).

$$\nabla \psi_m|_n = 0. \tag{33}$$

For calculational convenience the functions ψ_m are supposed to form an orthonormal set. Furthermore, in order to reduce the dimension of the basis set these functions should be as close as possible to the expected solutions of Eq. (4). Since we are interested in solutions for moderate values of applied magnetic fluxes both requirements are met for sets of low-lying eigenfunctions of the zero-field (i.e., particle in the polygonal box) eigenvalue problem,

$$-\frac{\hbar^2}{2m^*}\Delta\psi_m = \epsilon_m \psi_m, \tag{34}$$

obeying the boundary condition (33).

Consider a regular polygon shaped sample of a constant width in a homogeneous magnetic field applied along the direction perpendicular to the polygonal surface ($\mathbf{H}\|\mathbf{z}$). Then the associated vector potential $\mathbf{A}$ is directed in the xy plane (see Fig. 3). Since $A_z=0$ and the other two components depend on x and y only, the solution of Eq. (34) factorizes as $\Psi(x,y)\Phi(z)$. The z-dependent component of the solution satisfying the boundary condition $d\Phi/dz=0$, $z=\pm d/2$, and corresponding to the lowest value of $-\alpha$ in Eq. (4) has the form $\Phi=$const. This means that the superconductivity nucleates homogeneously across the width of the sample and the solution of the LGL equation reduces to a two-dimensional (2D) problem.

The transformation (14) and (17) keeps the symmetry of the vector potential [and of Eqs. (4)] equal to the rotational symmetry of the sample, described by the point group C_N. Since the LGL equation is a linear eigenvalue problem its solutions, according to Wigner's theorem,[21] are characterized by irreducible representations (irreps) of the corresponding symmetry group. The point group C_N is Abelian and therefore contains N different one-dimensional irreps which transform as

$$\psi_n(\varphi) \sim \exp(in\varphi),$$

$$n = 0,1,\ldots,N-1, \tag{35}$$

under rotations around the z axis by symmetry angles, the smallest of which coincides with the angle α in Fig. 3. The symmetry analysis provides a set of N labels to assign eigenfunctions and splits the matrix eigenvalue equation into diagonal blocks corresponding to different irreps[21] which simplifies the calculations.

A. Square and rectangle

In these geometries the boundary conditions allow the separation of variables in the eigenvalue problem (34) if one chooses the coordinate axes parallel to corresponding edges [Fig. 8(a)].

Along each coordinate the problem reduces to a particle in the box with infinite potential walls.[21] The corresponding solution for the boundary conditions (33) has the form (l is the dimension of the box)

$$\psi_k^1(x) = \sqrt{\frac{2}{l}}\cos kx, \quad k = \frac{2n\pi}{l},$$

$$\psi_k^2(x) = \sqrt{\frac{2}{l}}\sin kx, \quad k = \frac{(2n+1)\pi}{l},$$

$$n = 0,1,2,\ldots . \tag{36}$$

The full solutions in a rectangular box are just the products $\psi_{k_x}(x)\psi_{k_y}(y)$ and correspond to the energy,

$$E_{k_x k_y} = \frac{\hbar^2(k_x^2 + k_y^2)}{2m^*}. \tag{37}$$

These solutions however do not correspond to any definite symmetry. Therefore they should be symmetrized if we want to take advantage of the symmetry of the samples as discussed above.

A *square* in homogeneous magnetic field has the symmetry described by the rotational point group C_4, which contains the irreps A, B, E_+, and E_- with the corresponding numbers $n=0$, 2, 1, and -1 (or 3) in Eq. (35). Using the conventional symmetry projection technique[21] the symmetrized basis set is easily constructed from the solutions in Eq. (37). Thus we obtain the following types of solutions, for the irrep A:

$$\psi_A^1 = \frac{\sqrt{2}}{a}[\cos k_1 x \cos k_2 y + \cos k_2 x \cos k_1 y],$$

$$k_1 > k_2 \geqslant 0, \quad k_i = \frac{2n_i\pi}{a},$$

$$\psi_A^2 = \frac{2}{a}\cos kx \cos ky, \quad k = \frac{2n\pi}{a} \geqslant 0,$$

$$\psi_A^3 = \frac{\sqrt{2}}{a}[\sin k_1 x \sin k_2 y - \sin k_2 x \sin k_1 y],$$

$$k_1 > k_2 > 0, \quad k_i = \frac{(2n_i+1)\pi}{a}, \tag{38}$$

for the irrep B,

$$\psi_B^1 = \frac{\sqrt{2}}{a}[\cos k_1 x \cos k_2 y - \cos k_2 x \cos k_1 y],$$

$$k_1 > k_2 \geqslant 0, \quad k_i = \frac{2n_i\pi}{a},$$

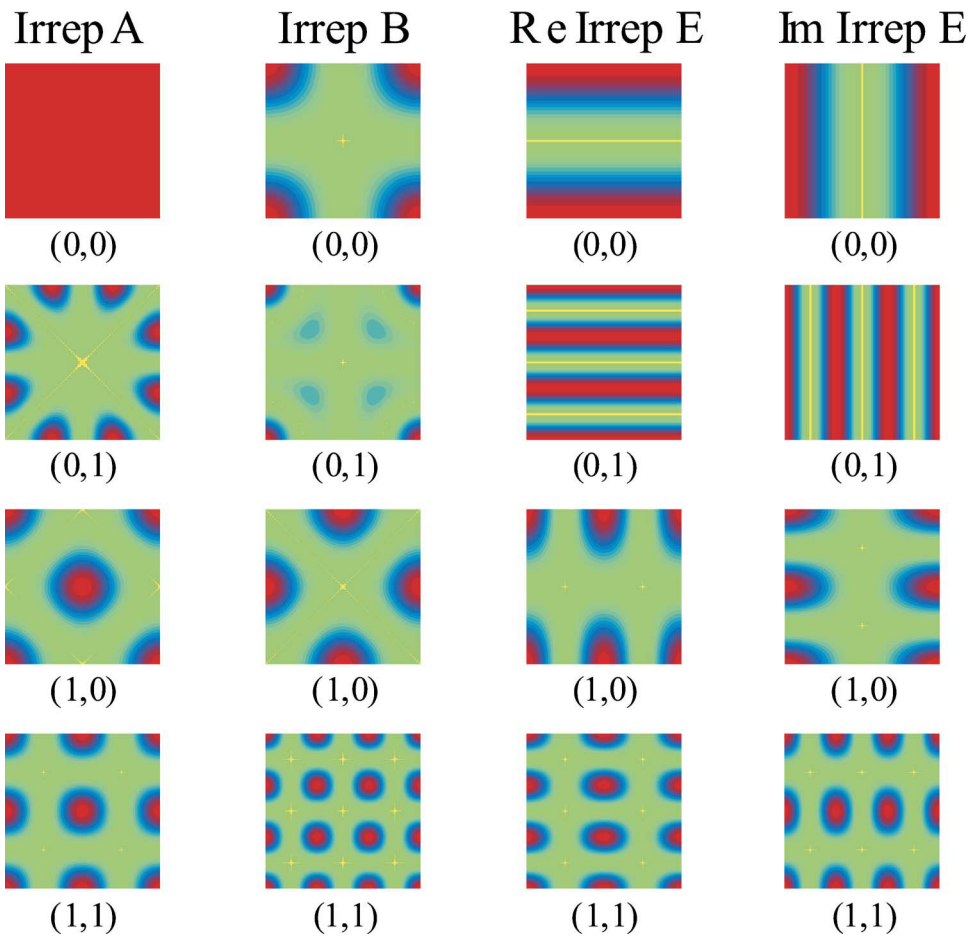

FIG. 9. (Color online) Symmetrized basis functions for a square. The highest density is shown in darker shades and the lowest $|\psi|^2$ values are lighter shades. The numbers in parentheses stand for n_1 and n_2, respectively.

$$\psi_B^2 = \frac{2}{a}\sin kx \sin ky, \quad k = \frac{(2n+1)\pi}{a} > 0,$$

$$\psi_B^3 = \frac{\sqrt{2}}{a}[\sin k_1 x \sin k_2 y + \sin k_2 x \sin k_1 y],$$

$$k_1 > k_2 > 0, \quad k_i = \frac{(2n_i+1)\pi}{a} \tag{39}$$

and for the irrep E,

$$\psi_{E_{+,-}} = \frac{\sqrt{2}}{a}[\cos k_1 x \sin k_2 y \pm i \cos k_1 y \sin k_2 x],$$

$$k_1 = \frac{2n_1\pi}{a} \geqslant 0, \quad k_2 = \frac{(2n_2+1)\pi}{a} \geqslant 0, \tag{40}$$

where n_i are integers. Figure 9 shows graphically some of these symmetrized functions.

In a *rectangle* the symmetry in homogeneous magnetic field is described by the point group

C_2 containing only two irreps, A and B. The reduction of symmetry with respect to the square induces the following reduction of the irreps of C_4: $A,B\rightarrow A$, $E_+,E_-\rightarrow B$. The basis function resulting from this reduction have the following form, for irrep A:

$$\psi_A^1=\frac{2}{\sqrt{ab}}\cos k_1x\cos k_2y,$$

$$k_1=\frac{2n_1\pi}{a},\quad k_2=\frac{2n_2\pi}{b},$$

$$\psi_A^2=\frac{2}{\sqrt{ab}}\sin k_1x\sin k_2y,$$

$$k_1=\frac{(2n_1+1)\pi}{a},\quad k_2=\frac{(2n_2+1)\pi}{b}, \tag{41}$$

and for the irrep B,

$$\psi_B^1=\frac{2}{\sqrt{ab}}\cos k_1x\sin k_2y,$$

$$k_1=\frac{2n_1\pi}{a},\quad k_2=\frac{2(n_2+1)\pi}{b},$$

$$\psi_B^2=\frac{2}{\sqrt{ab}}\sin k_1x\cos k_2y,$$

$$k_1=\frac{(2n_1+1)\pi}{a},\quad k_2=\frac{2n_2\pi}{b} \tag{42}$$

where n_i are integers.

B. Equilateral triangle

This case is more involved since the geometry of the boundary does not allow the separation of variables in the eigenvalue problem (34). Nevertheless it is still possible to express the solutions as a linear combination of a small number ($\leqslant 6$) of plane waves as shown below.

The equilateral triangle in a homogeneous magnetic field has a symmetry corresponding to the rotational point group C_3, which contains the irreps A, E_+, and E_- matching the numbers $n=0$, 1, and -1 (or 2) in Eq. (35), respectively. We make use of this symmetry in the next section when we analyze the solutions of the corresponding LGL equation. The particle in the box problem, however, is characterized by a higher symmetry group C_{3v}, containing in addition three vertical reflection planes, which are absent when the magnetic field is applied. It is convenient to use this higher symmetry group in further derivation. The method used here follows closely the one employed by Li and Blinder for a triangular box with Dirichlet boundary conditions.[22] For an equilateral triangle located with respect to Cartesian axes as shown in Fig. 8(b) we introduce three variables (h is the height of the triangle),

$$u=\frac{2\pi}{h}y,$$

$$v = \frac{2\pi}{h}\left(-\frac{1}{2}y + \frac{\sqrt{3}}{2}x\right),$$

$$w = \frac{2\pi}{h}\left(-\frac{1}{2}y - \frac{\sqrt{3}}{2}x\right) + 2\pi, \tag{43}$$

which are obviously linearly dependent. These variables are transformed into each other under symmetry operations of the C_{3v} group and obey simple relations on the boundaries of the triangle. For instance, on the edge $y=0$ [Fig. 8(b)] we have

$$u = 0, \quad v = 2\pi - w. \tag{44}$$

Equation (34) is satisfied for a harmonic function with arbitrary linear combination of x and y in the argument. It is convenient to take this function in the form $f(pu-qv)$,[22] where u and v are variables introduced in Eq. (43), corresponding to the energy (in units of $\hbar^2/2m^*$),

$$E_{pq} = 4\frac{\pi^2}{h^2}(p^2 + pq + q^2). \tag{45}$$

Starting from the function f, we construct wave functions of definite symmetry by using the method of symmetry projection.[21] The projected functions are linear combinations of functions f of different arguments, all of which obviously correspond to the same energy (45). Due to this symmetrization it is enough to satisfy the boundary condition (33) on a single edge, e.g., $y=0$ [Fig. 8(b)]. Equation (44) shows that on that boundary the wave function depends on a single variable v. The boundary condition is then satisfied by choosing appropriate values of the constants p and q which, at their turn, define the allowed values of the energy (45).

Irrep A_1: The boundary condition at the edge $y=0$ is obtained in the form

$$\left.\frac{\partial \psi_{A_1}}{\partial u}\right|_{u=0} = (2p+q)(f'_u[-qv] + f'_u[qv - 2\pi q]) + (-p+q)(f'_u[-(p+q)v + 2\pi p] + f'_u[(p+q)v - 2\pi q]) - (p+2q)(f'_u[-pv + 2\pi p] + f'_u[pv]) = 0. \tag{46}$$

Since f is a harmonic function with the period 2π, the above equation is only satisfied for integer values of p and q and $f=\cos$. Furthermore, the function ψ_{A_1} is invariant under the following replacements of the two constants: $p,q \to q,p$, $p,q \to -p,-q$ and $p+q,-p \to p,q$. This restricts p and q to positive values. Rewriting this function in x and y variables we obtain (without normalization)

$$\psi^{A_1}_{pq}(x,y) = \cos\frac{\pi}{h}(2p+q)y \cos\frac{\pi}{h}\sqrt{3}qx + \cos\frac{\pi}{h}(-p+q)y \cos\frac{\pi}{h}\sqrt{3}(p+q)x + \cos\frac{\pi}{h}(p+2q)y \cos\frac{\pi}{h}\sqrt{3}px,$$

$$p \geqslant q = 0,1,2,\ldots. \tag{47}$$

Irrep A_2: The boundary conditions for ψ_{A_2} lead to an equation similar to (46) with the only difference that now differences of derivatives f'_u enter in each of the square brackets instead of their sum. This means that the only choice for the harmonic function is $f=\sin$. The constants p and q are again integers and obey the same symmetry relations as in the previous case. Therefore, we obtain for the irrep A_2 the following unnormalized eigenfunctions:

$$\psi_{pq}^{A_2}(x,y) = -\sin\frac{\pi}{h}\sqrt{3}qx\cos\frac{\pi}{h}(2p+q)y + \sin\frac{\pi}{h}\sqrt{3}(p+q)x\cos\frac{\pi}{h}(-p+q)y$$
$$-\sin\frac{\pi}{h}\sqrt{3}px\cos\frac{\pi}{h}(p+2q)y,$$

$$p \geqslant q = 1,2,\ldots . \tag{48}$$

Note that in the presence of homogeneous magnetic field both ψ_{A_1} and ψ_{A_2} reduce to the same irrep A of the group C_3.

Irrep E: Because this irrep is twofold degenerate the corresponding two eigenfunctions are defined up to an arbitrary linear combination. It is convenient to choose these functions as complex conjugate to each other because then they belong automatically to the irreps E_+ and E_- of the group C_3, respectively. This requirement leaves us the only choice for the harmonic function, $\exp[i(pu-qv)]$. After similar derivations as in previous cases we obtain for the unnormalized eigenfunctions $[\psi^{E_-}=(\psi^{E_+})^*]$

$$\psi_{pq}^{E_-}(x,y) = \exp\left\{\frac{\pi i}{h}[(2p+q)y-\sqrt{3}qx]\right\} + \exp\left\{\frac{\pi i}{h}[(p+2q)y-\sqrt{3}px]\right\}$$
$$+\exp\left\{\frac{\pi i}{h}[(-p+q)y+\sqrt{3}(p+q)x]-2\pi qi \pm \frac{2\pi}{3}i\right\}$$
$$+\exp\left\{\frac{\pi i}{h}[-(p+2q)y-\sqrt{3}px]+2\pi pi \mp \frac{2\pi}{3}i\right\}$$
$$+\exp\left\{\frac{\pi i}{h}[(p-q)y+\sqrt{3}(p+q)x]-2\pi pi \pm \frac{2\pi}{3}i\right\}$$
$$+\exp\left\{\frac{\pi i}{h}[-(2p+q)y-\sqrt{3}qx]+2\pi qi \mp \frac{2\pi}{3}i\right\}, \tag{49}$$

where the two signs correspond to the following quantum numbers:

$$q = n + 1/3, \quad p = q, q+1, q+2, \ldots, \quad \text{upper sign},$$

$$q = n + 2/3, \quad p = q, q+1, q+2, \ldots, \quad \text{lower sign},$$

$$n = 0,1,2,\ldots . \tag{50}$$

Note that these eigenfunctions are characterized by fractional quantum numbers p and q.

Figure 10 shows the graphics of some of the solutions (47), (48), and (49) for low values of (p,q). Note that these solutions are very similar for the solutions or the Schrödinger equation for a particle in an equilateral triangle.[22]

The above approach cannot be extended straightforwardly to other geometries. The reason for this is a theorem stating that only in the cases of square and triangular boxes the eigenfunctions can be expanded in a finite set of plane waves.[23] On the other hand, if the boundary line does not deviate strongly from a circumference (as, e.g., in higher polygons), we can again construct a finite basis set by making a radial rescaling of the eigenfunctions for a disk with equal area.[24]

IV. NUCLEATION OF SUPERCONDUCTIVITY IN BASIC POLYGONS

Using the developments of the preceding sections we can solve now the LGL equation (34) with the boundary condition (7) for several symmetric structures. An important feature of vector potential gauge approach is its ability to provide accurate description of the order parameter

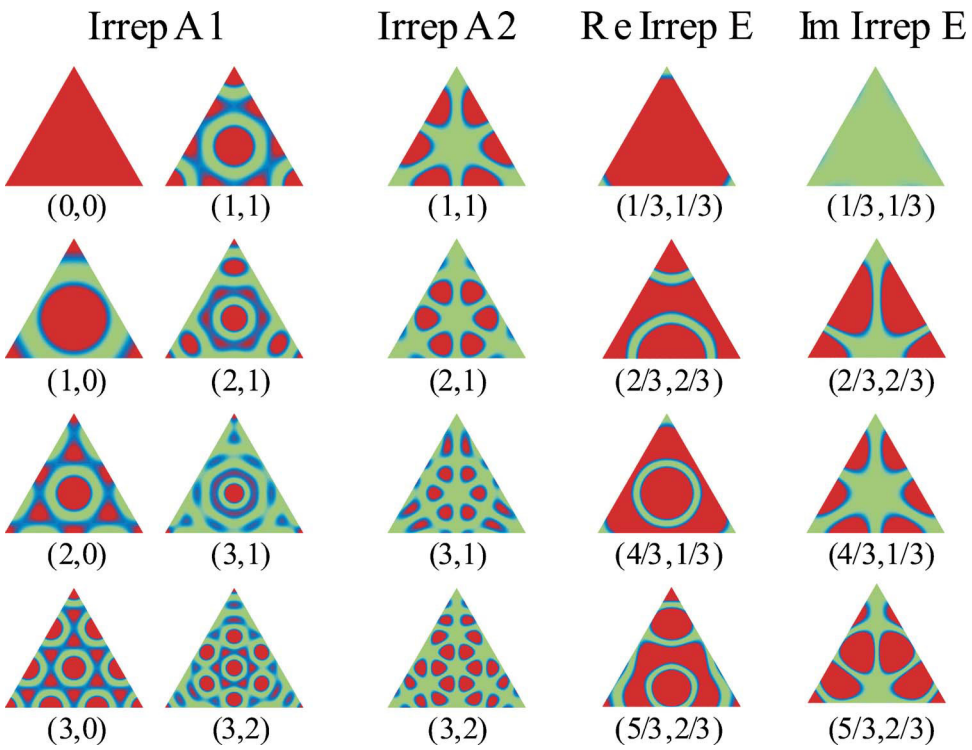

FIG. 10. (Color online) Symmetrized basis functions for an equilateral triangle. The highest density is shown in darker shades and the lowest $|\psi|^2$ values are lighter shades. The numbers in parentheses stand for p and q, respectively.

already for quite limited sizes of the basis sets at moderate applied fields. An accurate calculation of Ψ is often crucial for a correct description of vortex patterns in mesoscopic samples. In this connection we mention that reflections in vertical planes, if they are contained in the symmetry group of the sample, act as time inversion operators, $\sigma_v\Psi=\Psi^*$. Therefore $\Psi^*\Psi$ is invariant under these reflections and the density distribution of the order parameter is described by the full symmetry of the sample.

A. The triangle and square

As shown above it is possible to classify the solutions for a square and a triangle according to the irreducible representations (irreps) of the symmetry groups C_3 and C_4. This classification will include different order parameter patterns, since the solutions are contained in different subclasses characterized by a certain irrep. As can be seen in Figs. 11 and 12 the eigenvalues of the LGL equation belonging to the different irreps will form the complete spectrum of eigenvalues.[25,26] However, *eigenvalues belonging to the same irrep will never cross*. Moreover the lowest eigenvalues form separated bands existing out of an eigenvalue for each irrep, which are crossing in a regular pattern. In this way the H–T phase boundary $T_c(H)$, which is the lowest eigenvalue $E_{\mathrm{LLL}}(H)$, shows an oscillatory cusplike behavior as a function of flux and with every cusp the solution corresponds to a different irrep. The sequence of the $T_c(H)$ oscillations is always A, E_+, B, and E_- in the case of a square, and A, E_+, and E_- in the case of a triangle. The vorticity increases by one when passing a cusp along the H–T phase boundary with increasing field (cf. the Little-Parks experiment) and consequently to the next irrep.

Even as the symmetry of the structure gives rise to a cusplike H–T phase boundary, it still shows a predominantly linear dependence between the magnetic field and the temperature. This is not surprising since a linear H–T phase boundary is the solution for the bulk problem. However, the slope has changed compared to the bulk case, as can be seen in Fig. 13. When comparing the

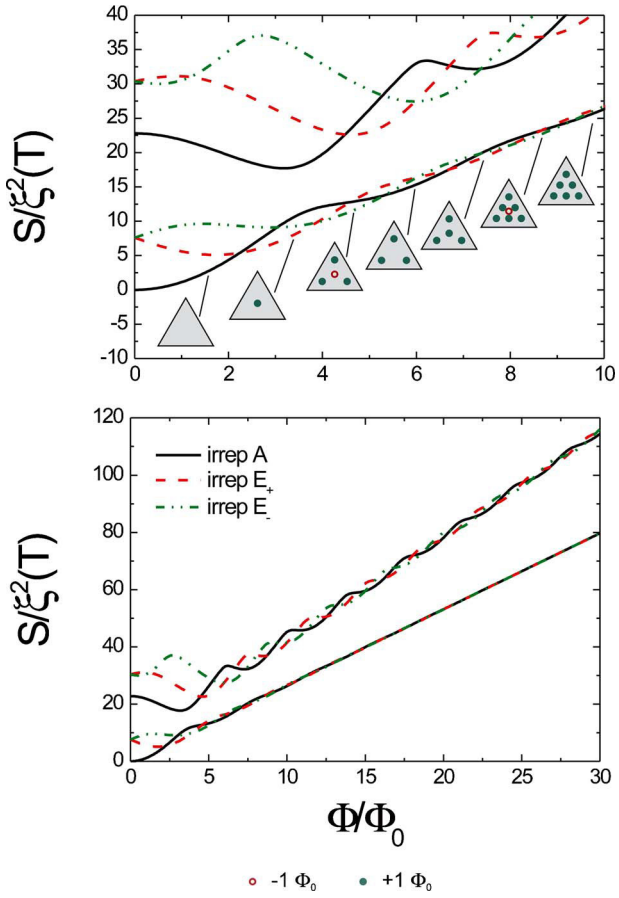

FIG. 11. (Color online) Lower eigenvalues of the LGL equation for the mesoscopic triangle, as a function of the magnetic flux Φ/Φ_0, with superconductor-vacuum boundary conditions. The different lines correspond to the three irreducible representations (irreps) A (full black line), E_+ (dashed red line) and E_- (dashed-dotted-dotted green line). Since the problem has a discrete C_3 symmetry there is a 'repulsion' of the levels, giving a regular pattern of avoided crossing between levels belonging to the same irrep. The flux is defined as $\Phi=\mu_0 HS$, with S the surface of the triangle, $\mu_0 H$ the applied magnetic field and $\Phi_0=h/2e$ the superconducting flux quantum. The lowest sequence of the cusp-like pieces from different irreps forms the lowest eigenvalue $E_{\mathrm{LLL}}(H)$, directly corresponding to the $T_c(H)$ line. For detailed comparison with the experiment see Fig. 19. Along the vertical axis, the critical temperature T_c is linearly decreasing with increasing $S/\xi^2(T)$.

considered shapes with equal surface, it is evident that superconductivity nucleates with decreasing magnetic field H and temperature T, first in the triangle, then the square, the disk[12,28–35] and finally in the bulk material. This can be understood from the results obtained on the nucleation of superconductivity in an infinite wedge[7,8,36–39] where the nucleation field $H_{c3}^{\star}$ increases with reducing angle Γ of the infinite wedge. Consequently we should observe the largest $H_{c3}^{\star}$ for the triangle, since the triangle has the smallest angles in the corners. That is precisely what we observe.

Furthermore, the phase boundary for the square has been calculated by other groups, like Jadallah *et al.*[27] and Schweigert *et al.*[37,40,41] When comparing for instance the positions of the cusps at the phase boundary we see a good agreement between the different calculations at lower fields. However, at higher fields we see a slight deviation between our results and the results of Jadallah *et al.*[27] (see Table I).

Additionally, there is a good agreement between the amplitudes of the oscillations found in our work[26] and Schweigert *et al.*[41] and for certain values of magnetic field and temperature we also find the same vortex patterns. However we also find some large differences in the vortex patterns, specifically vortex-antivortex patterns compared to a giant vortex.

Since the rotational axis in the triangle is of finite order we do not expect the giant vortex state

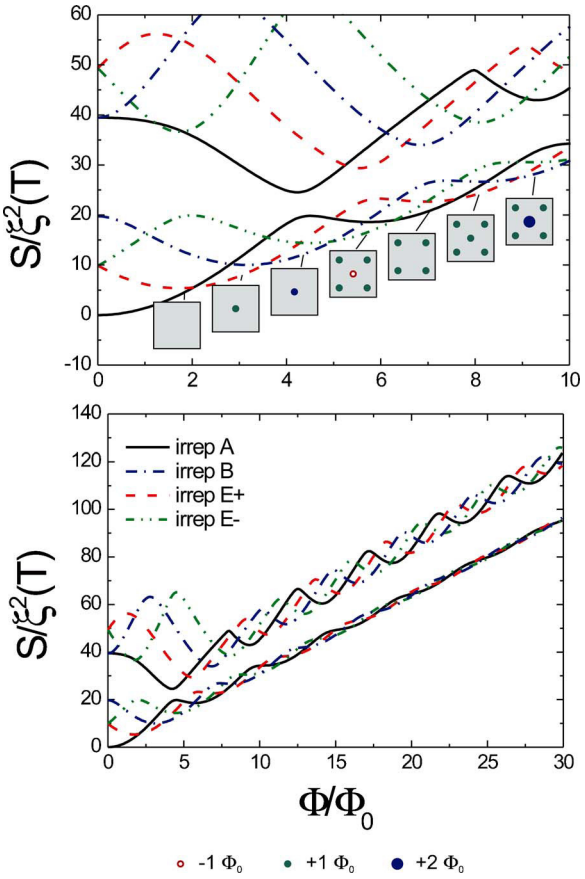

FIG. 12. Lower eigenvalues of the LGL equation for the mesoscopic square, as a function of the magnetic flux Φ/Φ_0, with superconductor-vacuum boundary conditions. The different lines correspond to the four irreducible representations (irreps) A (full black line), B (dashed-dotted line), E_+ (dashed line), and E_- (dashed-dotted-dotted line). Since the problem has a discrete C_4 symmetry there is a 'repulsion' of the levels, giving a regular pattern of avoided crossing between levels belonging to the same irrep. The flux is defined as $\Phi=\mu_0 HS$, with S the surface of the square, $\mu_0 H$ the applied magnetic field and $\Phi_0=h/2e$ the superconducting flux quantum. The lowest sequence of the cusp-like pieces from different irreps forms the lowest eigenvalue $E_{\mathrm{LLL}}(H)$, directly corresponding to the $T_c(H)$ line. For detailed comparison with the experiment see Fig. 20. Along the vertical axis, the critical temperature T_c is linearly decreasing with increasing $S/\xi^2(T)$.

to be always a ground state solution. Actually there are no vortices in the first state ($L=0$), there is one Φ_0 vortex in the cental position in the second state ($L=1$), and there is one $-\Phi_0$ antivortex in the center and three Φ_0 vortices at the diagonal positions in the third state ($L=-1+3=2$). This sequence is periodically repeated when going to higher applied fluxes. For instance, the fourth state ($L=3$) will contain three Φ_0 vortices dispatched along the diagonals of the triangle. Figure 14 shows the distribution of the order parameter in the above states. The total winding number is a sum of the vorticity numbers of the central and diagonal vortices as follows:

$$L = n + 3m,$$

$$n = 0, 1, -1, \tag{51}$$

where $m=0, 1, \ldots$ is the number of vortex triades. The number n in this equation matches the corresponding irrep via Eq. (35).

The seven insets in Fig. 12 show schematically the distribution of vortices in the square, which are clearly different from the giant vortex states.

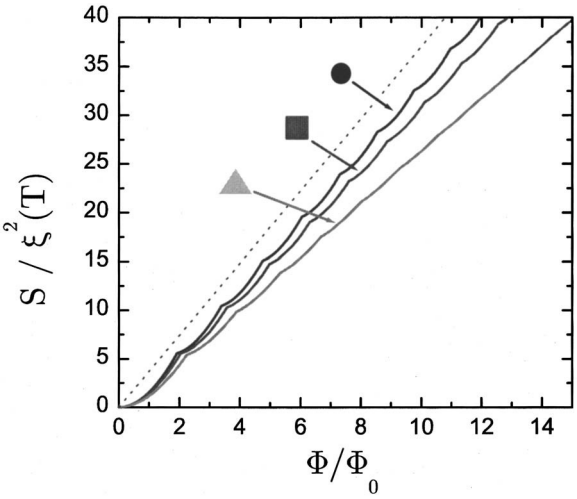

FIG. 13. The calculated *H–T* phase boundary for a disk, square, and triangle. The dotted straight line is the surface critical field for a semi-infinite slab with a straight superconductor/vacuum border $H_{c3}=1.69\,H_{c2}$.

In the case of small L's, vortices can occupy one central and four diagonal positions. In contrast to the diagonal vortices which always enclose a single quantum Φ_0, the central vortex can have different winding numbers in order to conserve the total vorticity of a given state. The contribution of the two kinds of vortices (central+four diagonal) to the total winding number of the states shown in Fig. 12 is given by

$$L = n + 4m,$$

$$n = 0,1,2,-1, \tag{52}$$

where $m=0$, 1. Note that the four numbers in the second equation match the n numbers in the expressions for the basis functions of the corresponding irreps, Eq. (35). This is not surprising since these resemble the eigenfunctions of a 2D rotator with momentum n.

As a result the nature of the central vortex changes, whenever vorticity is changed by one. Thus the central vortex is absent in the first state, it is a Φ_0 vortex in the second state, it is a giant vortex in the third state and it is an *antivortex* (the winding number is negative!) in the fourth state

TABLE I. Calculated cusps positions in $T_c(\Phi)$ for the triangle, the square, and the disk at particular values of the normalized flux Φ/Φ_0. The different calculated values for the square deviate slightly at high winding number L.

$L\rightarrow L+1$ After Ref.	Triangle 25	Square 26	Square 27	Disk 28
$0\rightarrow 1$	2.24	2.04	2.0	1.92
$1\rightarrow 2$	3.88	3.58	3.6	3.39
$2\rightarrow 3$	5.32	4.98	5.0	4.75
$3\rightarrow 4$	6.69	6.32	6.3	6.05
$4\rightarrow 5$	8.01	7.61	7.6	7.31
$5\rightarrow 6$	9.30	8.87	8.9	8.54
$6\rightarrow 7$	10.57	10.12	10.1	9.76
$7\rightarrow 8$	11.82	11.34	11.4	10.96
$8\rightarrow 9$	13.05	12.54	12.7	12.15
$9\rightarrow 10$	14.27	13.74	13.9	13.33

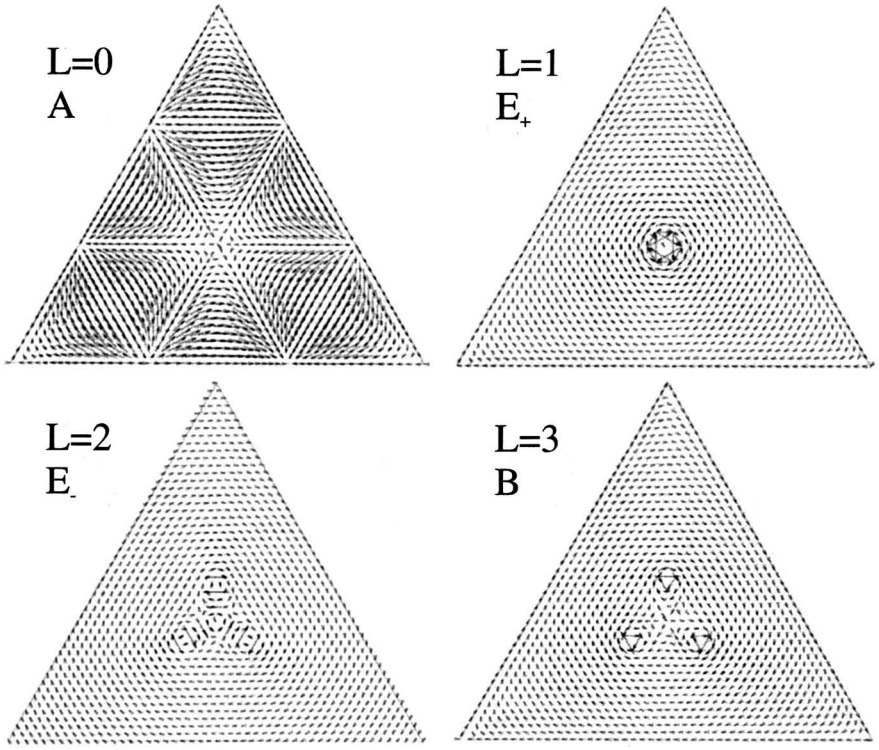

FIG. 14. Gradients of phase of the order parameter at the middle of the lowest four cusps in the $T_c(H)$ phase diagram in Fig. 11. Large arrows rotating clockwise encircle the vortices and those rotating in the anticlockwise direction display the antivortex. The panel for the E_- state, zoomed 16 times, shows the presence of an Φ_0 antivortex in the center.

(see Fig. 12). The sequence of winding numbers of the central vortex $(-1, 0, 1, 2)$ is periodically repeated when going to the right of the phase diagram.

Because the kinetic energy of a vortex is proportional to L^2, the system prefers to split the giant vortex into a sum of smaller vortices[42] if there are no special symmetry restrictions. Another energy based reason is that vortices get attracted to the corners as it was shown for the case of a semi-infinite plane with a wedge.[39] This explains why the four dispatched vortices prefer to stay on the diagonal positions in the ground states. The combination of these two arguments explains why only four numbers mentioned above appear as winding numbers for the central vortex. On the other hand, the formation of antivortices is dictated completely by the discrete symmetry. Indeed, in the state with $L=3$, one cannot distribute three Φ_0 vortices on the square keeping the symmetry. The dilemma is solved by having four diagonal Φ_0 vortices and adding one antivortex in the center.

Figure 15(a) shows the distribution of the order parameter corresponding to the antivortex solution. The central antivortex is separated from vortices on the square diagonals by about 2% of the edge length. The maximal value of the order parameter on the line connecting the antivortex with one vortex does not exceed one-thousandth of its value in the corners of the square. Note that this solution is obtained within the present approach by using a moderate basis set. To reproduce these features by finite grid methods a very large basis set corresponding to at least a 400×400 grid should be involved in the calculations.[43]

At higher values of applied field the additional vortices will continue to occupy the diagonal positions as shown in Fig. 16 for states of symmetry A.

On the whole, the nucleation of superconductivity in squares has similar features with the equilateral triangles. We expect most of these features to be general for higher order regular polygons too since they are based on symmetry grounds. For instance, the avoided crossing

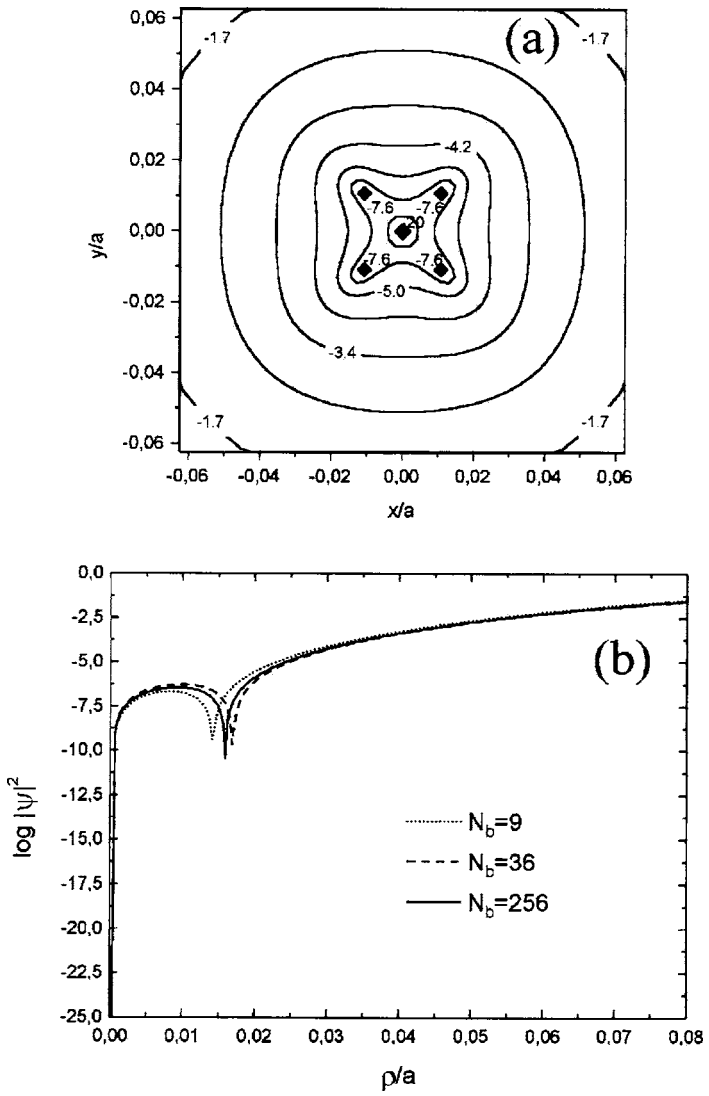

FIG. 15. Order parameter plots corresponding to the ground state of the square in an applied magnetic flux $\Phi=5.5\Phi_0$. The contour plot (a) shows (in logarithmic scale) the vortex pattern in the central region of the square zoomed in eight times after convergence with respect to the basis set size was achieved. The panel (b) displays the cross section in the diagonal direction $\rho=0$ is the center of the square) for different sizes of basis sets used in the calculations.

patterns of levels belonging to the same irrep is a common feature. One can see that it is more pronounced in the triangle (Fig. 11) than in the square (Fig. 12) and will generally diminish with increasing order of the polygon, disappearing completely in the case of disk ($N\rightarrow\infty$). The same for the vortex patterns; they are expected to shrink with increasing N and merge into giant vortex states in the limit of the disk. The asymptotic behavior of the ground state solutions in the limit of high applied field corresponds to the N-fold degenerate ground Landau level, the components of which belong to N different irreps of the corresponding polygon. This becomes infinitely degenerate in the case of disk, containing all different rotational (vorticity) states as components.[11]

B. Experimental phase boundary

To check the theoretical prediction for the lowest Landau level $E_{\mathrm{LLL}}(H)$ for different geometries (triangle, square, disk), superconducting Al samples have been made to measure the $T_c(H)$ line.

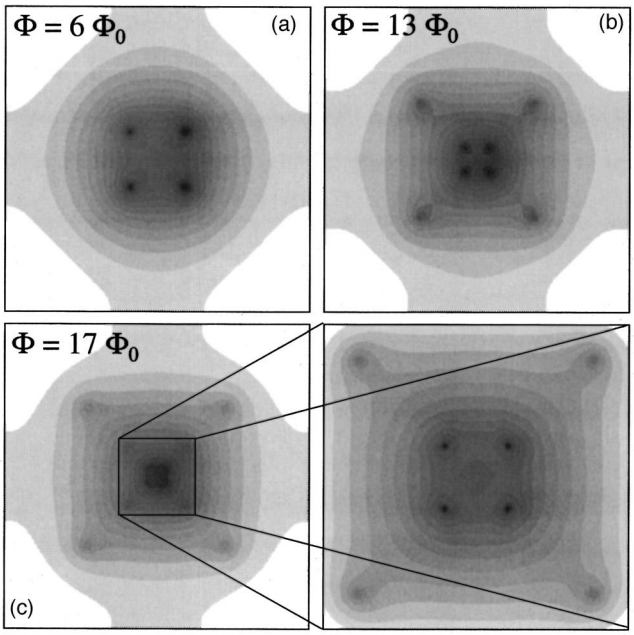

FIG. 16. Three vortex patterns corresponding to the symmetry A of the order parameter and the total vorticity $L=4$ (a), $L=8$ (b), and $L=12$ (c). In all cases the vortices are arranged symmetrically along the diagonals of the square. The panel in the left bottom corner shows the zoomed in central region of the plot c.

1. Sample characteristics

Figure 17 shows AFM and SEM micrographs of the triangle, the square and the disk. Wedge shaped current and voltage leads with an opening angle of $\Gamma=15°$ and with a narrow width of the interface between the structure and the current leads were used in order to minimize their influence on the superconducting properties of the structure.[44,45] The square and the disk were evaporated in the same run. A thickness $\tau=39$ nm was obtained from x-ray and AFM measurements. The radius of the disk, measured with AFM and SEM, was 1 μm. For the square, lateral dimensions of 2×2 μm^2 were obtained. The samples have a coherence length, determined from a coevaporated reference sample, of $\xi(0)=156$ nm and a critical temperature of $T_c=1.32$ and 1.33 K for the square and the disk, respectively. The equilateral triangle has a thickness $\tau=43$ nm, a basis of 2.33 μm. A coherence length of $\xi(0)=130$ nm and critical temperature of $T_c=1.34$ K were found for this sample.

The $T_c(H)$ phase boundary is measured by four-point resistance measurements using a lock-in amplifier. An ac transport current of 0.1 μA is sent through the two current leads (horizontal

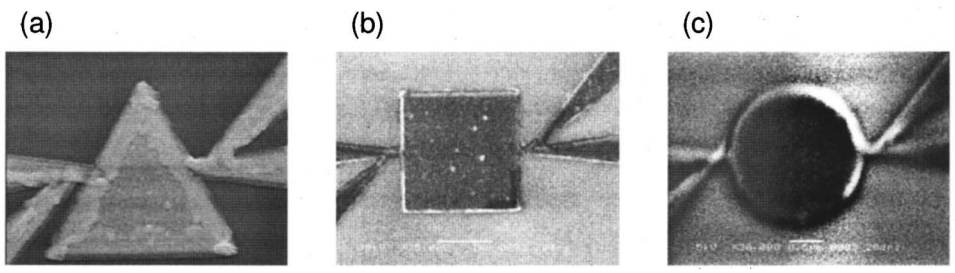

FIG. 17. AFM and SEM micrograph of an Al triangle (a) with basis of 2.33 μm, of a square (b) with a lateral dimension of 2 μm and of a disk (c) with a radius of 1 μm.

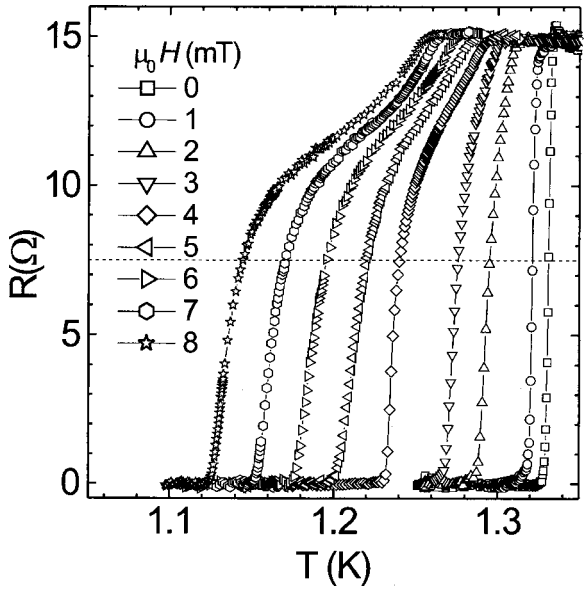

FIG. 18. Resistive transitions $R(T)$ for the triangle in different magnetic fields. From $\mu_0 H=0$ mT (open squares) to 8 mT (open stars). The dashed line shows the resistance criterion used to determine the $T_c(H)$ phase boundary.

contacts in Fig. 28). In order to construct the H–T phase diagram a set of $R(H)$ magnetoresistance curves are measured at various temperatures. The phase line is in a next step extracted from the data using a certain resistance criterion R_c.

2. Triangle

Figure 18 shows the resistive transitions of a mesoscopic triangle with wedge shaped contacts. The $R(T)$ curves are composed of two parts with different slopes. The upper part of this double transition shows a slowly decaying resistance while a steeper drop is seen in the lower part. This effect becomes more pronounced with increasing magnetic field. The appearance of the two distinct parts in the transition curves arises from the different field dependence of the nucleation temperature in the triangle and in the wedge shaped contacts.[45] The upper part of the $R(T)$ curves corresponds to the nucleation in the contacts followed by the nucleation in the triangle for lower temperatures at the lower part. The square and the disk show very similar resistive transitions.

The result of a continuous $T_c(H)$ measurement of a mesoscopic triangle is given in Fig. 19. The $T_c(H)$ phase boundary, measured for the triangle, is shown as open circles in Fig. 19 with the coherence length $\xi(0)=130$ nm determined from a coevaporated reference film and the surface $S=2.36\ \mu\text{m}^2$ found from AFM and SEM investigations. The open squares represent the measured phase boundary with the best fitting parameters, the best value for the coherence length is $\xi(0)=118$ nm and the effective area of the sample $S=2.25\ \mu\text{m}^2$. This leads to a difference of 10% between the measured and the fitted coherence length and a difference of 5% between the measured and the fitted sample areas S. After this small correction an excellent agreement between the experiment and the theory is observed. The amplitude of the oscillations and the position of the cusps are in perfect accordance.

From the AFM and SEM measurements, features that could be attributed to resist at the boundaries of the structures were observed. Since the area written by e-beam lithography was $S=2.25\ \mu\text{m}^2$, we believe that the exact surface of the Al triangle is slightly lower than the measured one ($S=2.36\ \mu\text{m}^2$). Another explanation for the different obtained values of the fitting parameter for the area of the triangle and the measured area could be the error margin on the measured value. A possible reason for the deviation between measured and the fitted coherence length might be the presence of the wedge contacts. The wedge-shaped contacts will probably not change the value of

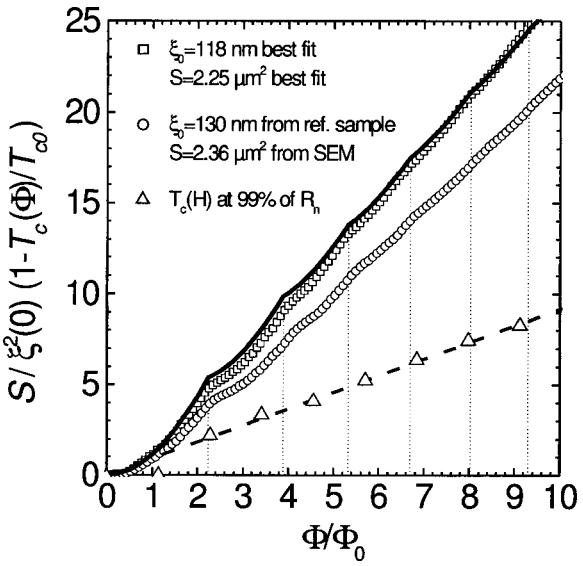

FIG. 19. Experimental $T_c(H)$ phase boundary of an equilateral triangle with wedge-shaped contacts. The open circles represent the data obtained using the measured sample size $S=2.36\ \mu\text{m}^2$ and the coherence length $\xi(0)=130$ nm. The best agreement between the measured and the theoretical phase boundary was found using the parameters $S=2.25\ \mu\text{m}^2$ $\xi(0)=110$ nm, see the open squares in the figure. The full line represents the theoretical curve (Ref. 32). The open triangles are taken from the resistance transition $R(T)$ for a resistance criterion of 99% R_n. The dashed line is the theoretical phase boundary of the wedge-shaped contacts with opening angle $\Gamma=15°$.

the coherence length, but shift the phase boundary of the triangle in the direction of the phase boundary for a wedge with opening angle $\Gamma=15°$. Another possibility for this small discrepancy could be a difference between the coherence length of the coevaporated reference film and the coherence length of the mesoscopic triangle that cannot be measured directly. A potential origin of the discrepancy between the two coherence lengths could be a slight contamination of Al by the resist used in the preparation of the mesoscopic structures, that would decrease the elastic mean free path ℓ_{el} and consequently also ξ. A lower resistance criterion (smaller than the 50% of R_n criterion used) for the determination of the phase boundary, will give a small reduction of the divergence, but cannot remove completely the difference between the two coherence length values. Another reason for this small discrepancy could arise from the not perfectly shaped triangles. Since the opening angle of the corners plays the major role in the determination of the slope of the $T_c(H)$ curve, we could expect that not perfectly sharp corners would decrease the critical field. In our experiment, the measured phase boundaries are shifted to the opposite direction, so that it cannot be attributed to the rounded corners of the triangles.

The open triangles in Fig. 19 show the critical temperature of the triangle for a chosen resistive criterion equal to 99% of the normal state resistance from the $R(T)$ curves. A perfect agreement between the theoretical phase boundary of the contacts and the point on the $R(T)$ curve where the resistance starts to drop is observed. The double resistance transition observed in the measurements (see Fig. 18) is therefore due to two different superconducting/normal transitions. From this observation, it is clear that the resistance criterion for the determination of the phase boundary of the structure must be chosen in the low resistance region of the $R(T)$ transition. If the resistance chosen for this criterion is too high, the nonlocal effect of the contacts on the triangle will be probed.

3. Square

The experimental phase boundary of a square is displayed in Fig. 20 and is compared with the theoretical calculations. While previous measurements[2,46] showed a strongly oscillating $T_c(H)$ dependence superimposed with a pronounced quadratic background, our results are in very good

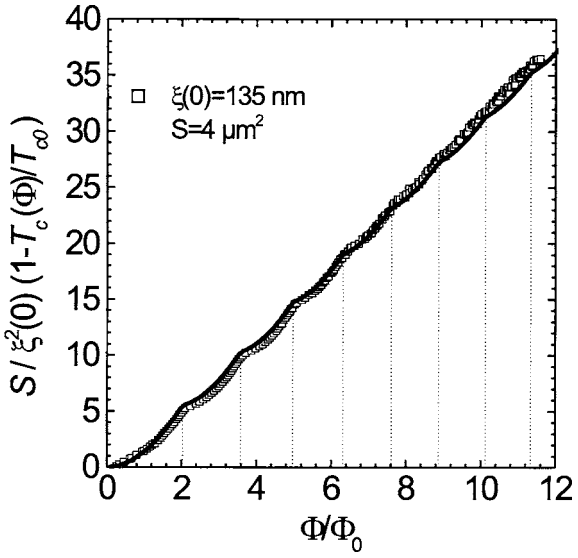

FIG. 20. Experimental $T_c(H)$ phase boundary of a square. The open squares represent the measured value using the measured sample size $S=4\ \mu\text{m}^2$ and the coherence length $\xi(0)=135$ nm. The full line is the theoretical curve $E_{\text{LLL}}(H)$.[26]

agreement with the theoretical predictions. Only a smaller coherence length $\xi(0)=135$ nm was used. The second parameter S used to compare the experimental and the theoretical data was found to be in the error margin of the determined area from SEM and AFM measurements. The main difference between the presented experimental phase boundary and previous reports is the shape and the size of the current and voltage contacts that can be extremely invasive in mesoscopic superconductors.

4. Disk

The $T_c(H)$ phase boundary of the disk is shown in Fig. 21 using a resistance criterion of

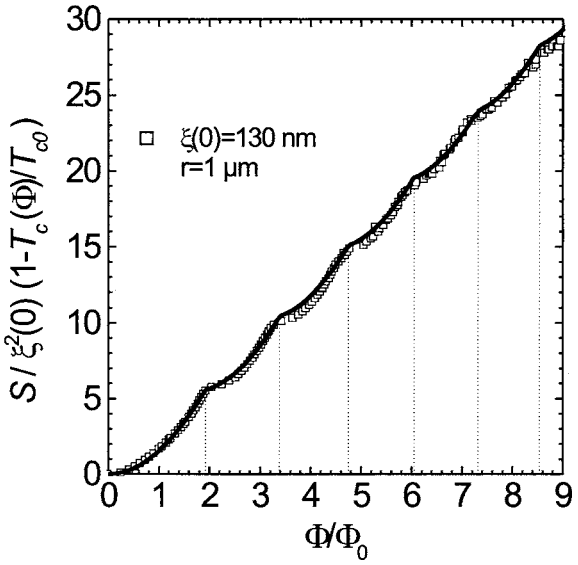

FIG. 21. Experimental $T_c(H)$ phase boundary of a disk determined for a resistance criterion of $2/3\ R_n$. The open squares represent the measured value using the radius $r=1\ \mu$m and the coherence length $\xi(0)=130$ nm. The full line is the theoretical curve $E_{\text{LLL}}(H)$.

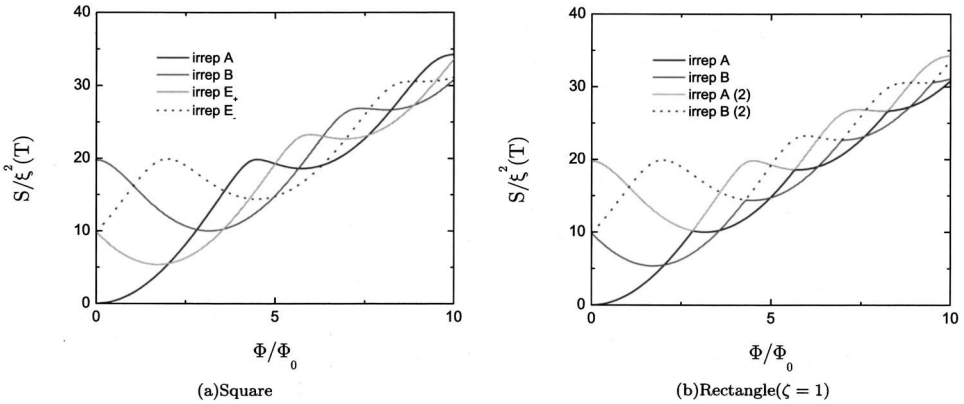

FIG. 22. In the case of the square [panel (a)] the lowest Landau level is constructed by the four lowest eigenvalues, corresponding to different irreps. However, the lowest Landau level $E_{\mathrm{LLL}}(H)$ in the rectangle with aspect ratio one [panel (b)] is obtained from just the lowest two eigenvalues, and the same spectrum of eigenvalues is formed with the two lowest pairs of eigenvalues. Deviations from aspect ratio one for the rectangle will lead to a gap between these two pairs of eigenvalues.

$2/3\,R_n$. Already in 1965, Saint-James calculated the phase boundary of a singly connected cylinder[9] with the gauge chosen as $\vec{A}=(\mu_0 Hr/2)\vec{e}_\phi$. With this particular choice, the superconducting boundary condition is imposed only on the gradient of the order parameter $|\Psi|$ along the radial axis. Since under these conditions $|\Psi|$ has no z-dependence, the phase boundary of a disk or an infinitely long cylinder will be the same. The solution of the linearized GL equation for a disk is a Kummer function of the first kind.[28,29] The nucleation temperature at a fixed magnetic field value can be found by taking the vorticity L that minimizes the eigenvalue giving rise to a cusplike phase boundary as shown by the full line in Fig. 21.

In order to fit the theoretical curve, the measured value of the radius $r=1$ μm and a slightly different coherence length of 130 nm, instead of the value of 154 nm determined from the reference sample, were used. After this small correction a good agreement is found between the theoretical and the experimental phase boundary for the position of the cusps. However, as in the measurements of Buisson *et al.*,[47] where a substantially larger disk was measured, the amplitude of the oscillation in the experimental curve is stronger than for the theoretical predictions. In our experiment, an excellent agreement between the theory and the experiment was found (see Fig. 21) by using a resistance criterion of $2/3\,R_n$. The positions of the cusps as well as the amplitude of the oscillations in the experimental curve match the theoretical phase boundary.

C. From square to rectangle

When crossing over from a square ($\zeta=1$) to a rectangle, we should go from a fourfold to a twofold rotational symmetry. The lowest Landau level in a superconducting square follows a cusplike profile corresponding to successive crossings of the solutions corresponding to four different representations. This is reproduced in the rectangle with aspect ratio one by a pair of crossing irreducible representations (irreps). However to obtain the full spectrum of eigenvalues formed by the four lowest crossing solutions in a square, two pairs of crossing irreps are needed, not only the lowest solutions but also the first excited ones of the A and B symmetry (see Fig. 22).[48] Departure from aspect ratio one leads to a splitting between the lowest and first excited solutions. Small deviations from the square have no noticeable effect on the lowest Landau level. All aspect ratios close to one have a lowest Landau level showing an oscillatory behavior with a predominantly linear background dependence on the field.

At a field of 5 up to 6.3 Φ/Φ_0 we find that the lowest Landau level corresponds to a solution with vorticity three. Although the energy levels and vorticity of all rectangles with an aspect ratio very close to one are the same, the vortex pattern can nevertheless be very different (Fig. 23). In

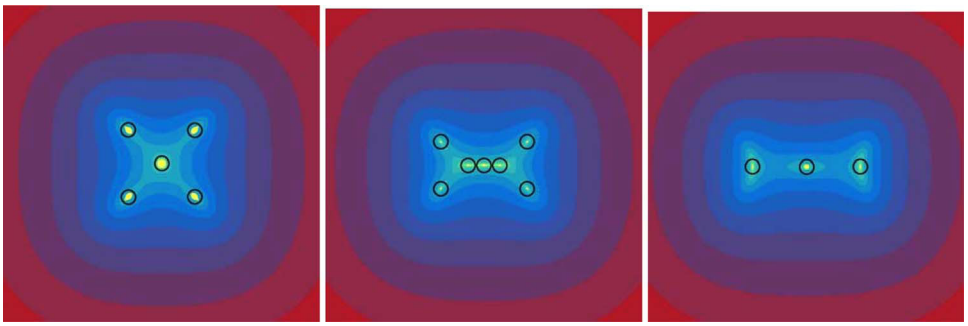

FIG. 23. (Color online) The figures show the density of the order parameter $|\psi|^2$ of the central $(a/10)\times(b/10)$ region in the rectangle in a log scale, where a is the long side and b is the short side. The highest density is shown in darker shades and the lowest $|\psi|^2$ values are in lighter shades, indicating the position of vortices and antivortices. Every shade corresponds to roughly half an order of magnitude. At a field of 5.5 Φ/Φ_0 the rectangles with, respectively, aspect ratio 1, 1.01, and 1.02 have very different vortex patterns. For aspect ratio one we observe the known configuration with one antivortex in the center and four vortices on the diagonals. However, at aspect ratio 1.01 we see four vortices on the diagonals, one in the center and two antivortices next to the central vortex. Finally at aspect ratio 1.02 we find that there are three vortices positioned on the long axis of the rectangle.

a *square* vorticity three is formed by *four vortices on the diagonals and one antivortex in the center*. At an aspect ratio 1.02 vorticity three already corresponds to *three vortices on a row* along the longest axis. However when we consider an aspect ratio 1.01, which lies between these two values, the pattern is more complex. The vortex pattern is now built up from four vortices on the diagonals, one vortex in the center and two antivortices located on the left and right from the central vortex along the long axis. This suggests the following evolution from aspect ratio 1 to aspect ratio 1.02. By varying the aspect ratio from one the antivortex in the center splits into two antivortices plus one vortex in the center. These antivortices move away from the center along the long axis, where each antivortex merges with the pair of vortices, respectively, at the left and right of the antivortex, leaving as a result three vortices on the longest axis. We must point out that the vortex pattern observed at aspect ratio 1.01 with a central vortex and two neighboring antivortices is in itself embedded into a region where the order parameter is already suppressed by orders of magnitude, which implies that we can also consider this structure as one elongated antivortex with a nontrivial $(-1+1-1)$ core structure.

1. Larger aspect ratios

It is surprising to see that the H–T phase boundary [Fig. 24(a)] remains almost the same for the aspect ratio between 1 and 1.333. However, the amplitude of the oscillations within the same irrep is reduced without substantial change in the lowest Landau level. Only when the aspect ratio becomes two or larger, a noticeable shift in the lowest Landau level is seen. Except for the first cusp the lowest Landau level still shows an oscillatory behavior on top of a linear dependence on the field, though with a reduced slope. At an aspect ratio of four we can hardly observe the crossing of the different irreps as they almost completely merge together, only the first cusp remains clearly visible. For fields higher than the first crossing of solutions, the field dependence becomes again linear. The same pattern persists for even higher aspect ratios. However, the field, at which the solutions for the first time cross, increases with the aspect ratio (Fig. 25). This crossing of the two irreps corresponds to the appearance of the first vortex in the rectangle, because the irrep B describes solutions that have a vortex in the center, while the irrep A solutions are without a vortex in the center. As a consequence every crossing of the solutions corresponding to the two irreps, will change the vorticity by one. The H–T phase boundaries for the different aspect ratios not only show the same behavior, they additionally can be scaled on one *universal* curve, apart from the oscillations [Fig. 24(b)]. The scaling is performed by dividing $S/\xi^2(T)$ and Φ/Φ_0 by the aspect ratio ζ,

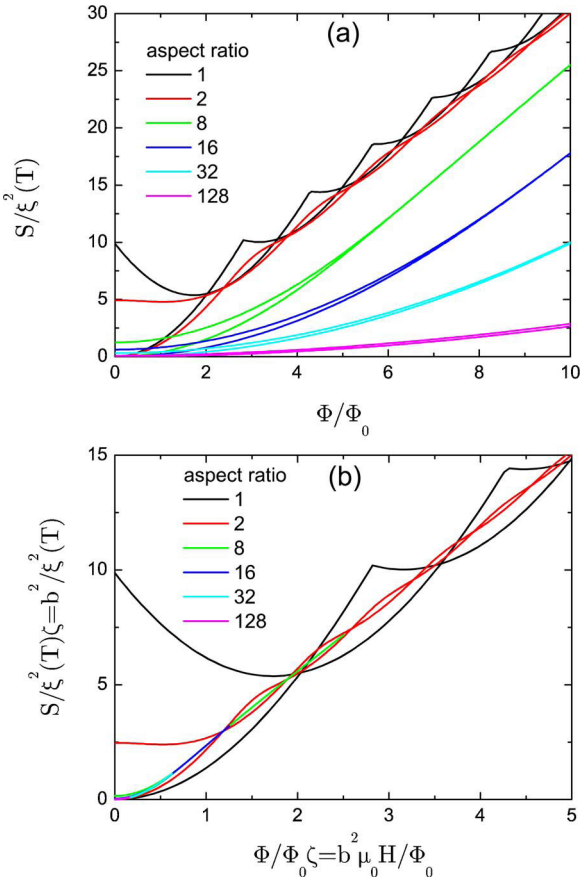

FIG. 24. (Color online) (a) Calculated superconducting H–T phase boundary for rectangles with different aspect ratios. The superconducting phase is located above (lower T) and the normal phase below the H–T phase boundary. For every aspect ratio the lowest two eigenvalues of the LGL equation for the mesoscopic rectangles with superconductor-vacuum boundary conditions as a function of magnetic flux Φ/Φ_0 are shown, with the lowest eigenvalue $E_{\mathrm{LLL}}(H)$ corresponding to the phase boundary. The different shades correspond to different aspect ratios, as indicated in the figure, however with the same surface S. The lowest graph at zero field for the same shade is the solution for irrep A and the highest graph is the solution for irrep B. The flux is defined as $\Phi=\mu_0 HS$ with S the surface of the rectangle, $\mu_0 H$ the applied magnetic field. (b) Different H–T phase boundaries show fundamentally the same behavior in a different field and temperature range, by scaling the different curves with the aspect ratio ζ onto the same universal curve, apart from the oscillations.

$$\frac{ab}{\xi^2(T)\zeta}=\frac{b^2}{\xi^2(T)},\quad \frac{\Phi}{\Phi_0\zeta}=\frac{ab\mu_0 H}{\Phi_0\zeta}=\frac{b^2\mu_0 H}{\Phi_0}. \tag{53}$$

Therefore we can conclude that the length b of the shortest side of the rectangle controls to a large part the behavior of the superconducting mesoscopic rectangle, such as the entry of the first vortex and the slope of the phase boundaries.

Since the curves can be scaled on a universal curve neglecting the cusps, it is also possible to describe the H–T phase boundary with a single function with the same dependence on the aspect ratio as the scaling,

$$\frac{S}{\xi^2(T)}=\frac{3}{\zeta}\left(\frac{\Phi}{\Phi_0}\right)^2\quad\left(\frac{\Phi}{\Phi_0}<0.535\zeta\right), \tag{54}$$

$$\frac{S}{\xi^2(T)}=6\left(\frac{\Phi}{\Phi_0}\right)-3(0.535)^2\zeta\quad\left(\frac{\Phi}{\Phi_0}\geqslant 0.535\zeta\right). \tag{55}$$

However, this fit only works well at aspect ratio $\zeta\geqslant 4$ where the cusps are negligible.

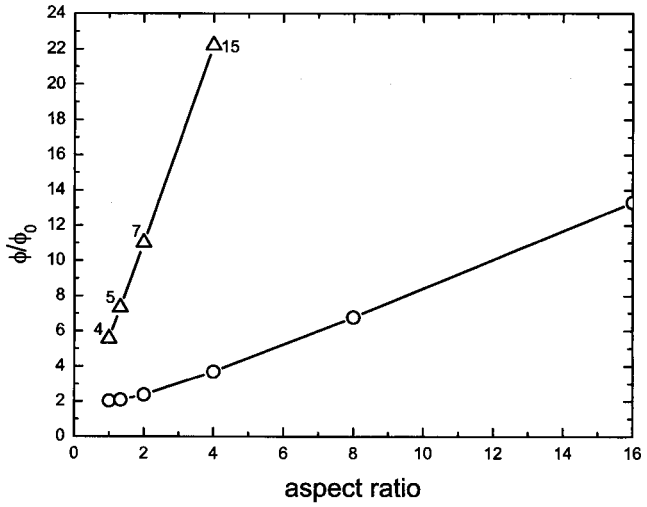

FIG. 25. The circles show the flux at which the first vortex enters the rectangle. The open triangles are the first points on the T_c–H phase boundary where vortices are located on the bisectors for the different aspect ratios. The numbers next to the squares indicate the corresponding number of vortices present in the rectangle at these fields.

In the case of aspect ratio 1.333 the vortices are situated in the central region on the longest axis of the rectangle. However, when the vorticity equals four, the vortices are sitting very close together. As a consequence the vortices move away from the axis and instead are placed on the *bisectors*, which go from the corners to the long axis of the rectangle (see also Fig. 27). The subsequent vortices appear again on the longest axis until the vorticity becomes 12. At this point another four vortices move away from the axis towards the corners along the bisectors. This of course is in contrast to the square where all the vortices are always on the diagonals at the H–T phase boundary in the considered field range.

The preference for positioning the vortices on the bisectors originates from the observed Meissner currents (Fig. 26) which make a hard bend there up to the longest axis (very weak screening), therefore the kinetic energy of the supercurrents is lower when a vortex is present on these bisectors compared to when a vortex is positioned away from the bisectors and from the

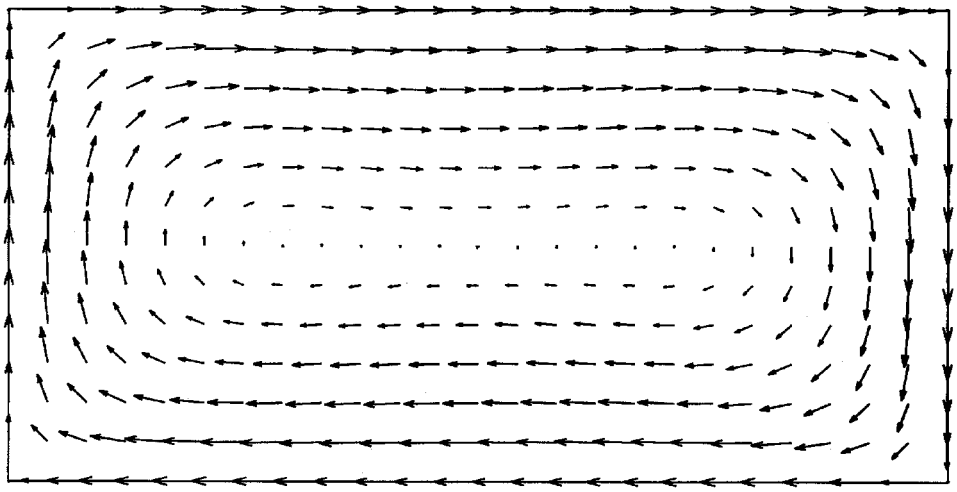

FIG. 26. The graph shows the supercurrents in arbitrary units in a rectangle with aspect ratio two just before the entrance of the first vortex at a magnetic field giving rise to magnetic flux of $\Phi=2.2\Phi_0$.

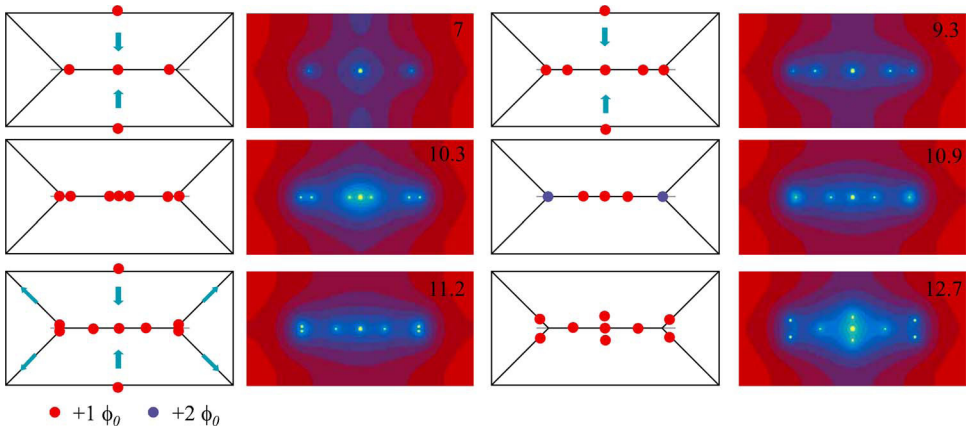

FIG. 27. (Color online) The figures show the evolution of the vortex pattern in the rectangle with aspect ratio two while following a single solution corresponding to irrep B with increasing field. The same shade conventions as in Fig. 23 were used. The numbers indicate the flux in the rectangle in units of the flux quantum Φ_0. The black lines are constructed by dividing the long axis with length a in three regions. Both outer regions have a length of $b/2$. If we would remove the central region, a square would remain with the black lines forming its diagonals.

central region of the longest axis. A similar pattern of Meissner currents leads to a discontinuity along the bisectors in the problem of the entry of flux lines in a rectangle away from the H–T phase boundary observed by magneto-optical techniques.[49–51]

The same scheme repeats itself for aspect ratio two. However we must wait until there are seven vortices in the rectangle before four vortices start to be located on the bisectors. For the aspect ratio four it takes 15 vortices to initiate the vortex redistribution from the axis to the bisectors. So it is clear that with growing aspect ratio the field at which the vortices start to take positions on the bisectors increases. From Fig. 25 we can see that the lowest field at which vortices appear first at the bisectors increases linearly with the aspect ratio for at least the lowest aspect ratios. For aspect ratios beyond four we cannot go high enough in field with a basis set of 1764 basis functions to see vortices on the bisectors. For the largest aspect ratios even the entrance of the first vortex in the rectangle is beyond the field range accessible for a limited number of basis functions in the set.

In summary it has been shown that the vortex pattern in a rectangle is composed of a central row of vortices along the longest axis and the vortices that are situated on the bisectors. These bisectors span the left and right $b/2$ region, where b is the short side of the rectangle. The vortices forming a row parallel to the longest axis only move into these two outer regions when they are ready to reposition themselves onto the bisectors, as shown in Fig. 27. When following the same irrep with increasing field (Fig. 27), we can observe the vortices enter in pairs through the centers of the long edges. When more vortices accumulate on the central line, migration starts to the outer $b/2$ regions. In this region on the longest axis two pairs of vortices will merge at the two points where the bisectors cross and form two giant vortices with vorticity two. These giant vortices split again into separate vortices which move along the bisectors now.

2. Lines

When increasing the aspect ratio to large values, the rectangle eventually resembles a line. The H–T phase boundary for a line with a width smaller than the coherence length $\xi(T)$ in a perpendicular magnetic field is well known for the London limit since it coincides with the problem of a thin (thickness $\ll\xi(T)$) superconducting plane in a parallel magnetic field.[1,52] We have

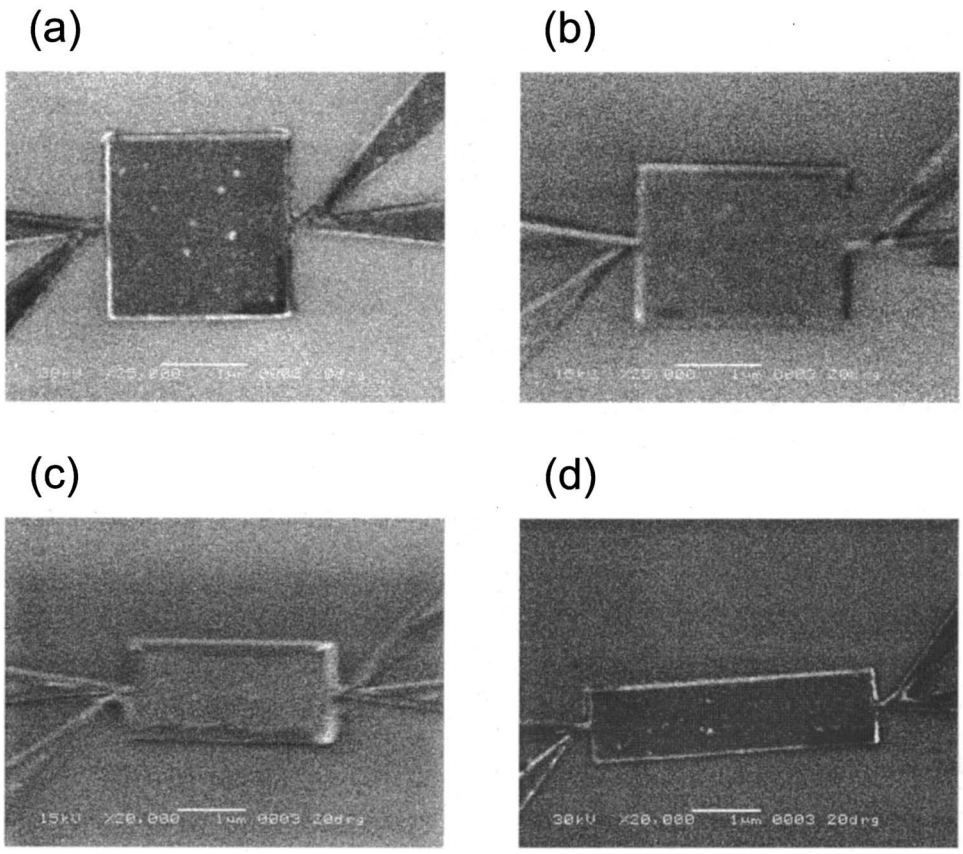

FIG. 28. SEM micrograph (a) of an Al square with lateral dimensions 2×2 μm^2 ($\zeta=1$) and of a rectangle with lateral dimensions of (b) 1.73×2.31 μm^2 ($\zeta=4/3$), (c) 1.41×2.83 μm^2 ($\zeta=2$), and (d) 1×4 μm^2 ($\zeta=4$).

$$\frac{1}{\xi^2(T)}=\frac{\pi^2w^2\mu_0^2H^2}{3\Phi_0^2}. \tag{56}$$

We can get an approximation for the rectangle with large aspect ratio when we substitute the width w^2 with $b^2=ab/\zeta$ where ζ is the aspect ratio, a is the long side, and b is the short side of the rectangle,

$$\frac{ab}{\xi^2(T)}=\frac{\mu_0^2\pi^2}{3\zeta}\left(\frac{\Phi}{\Phi_0}\right)^2. \tag{57}$$

This solution, which is obtained by minimizing the GL free energy in the London limit, is only valid when $|\Psi|$ is approximately spatially constant. Consequently the valid field region will increase with aspect ratio, since the field of the first entrance of a vortex increases with increasing aspect ratio. For instance, we determined that within the shown field region this approximation already coincides perfectly with our calculations for a rectangle with aspect ratio 64.

D. Experimental phase boundary

To investigate experimentally the crossover square-rectangle, four rectangles with different aspect ratio ($\zeta=1$, $4/3$, 2, and 4) were studied. They were all evaporated in the same run. The four structures have the same area of $S=4$ μm^2. A SEM micrograph of the studied samples is shown in Fig. 28. The rectangles with aspect ratio $\zeta=1$, $4/3$, 2, and 4 have dimensions of 2×2 μm^2,

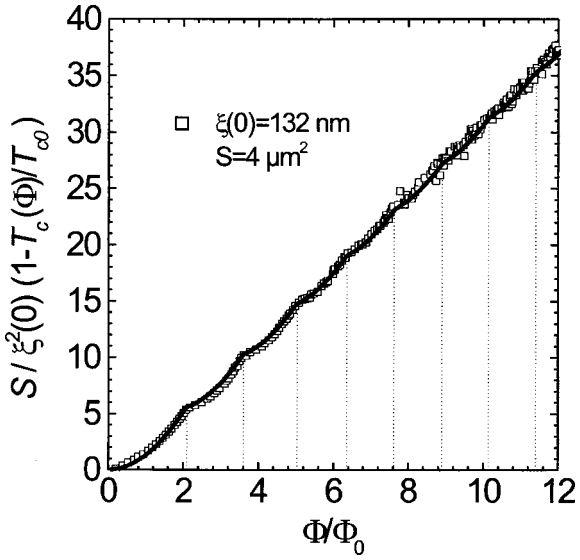

FIG. 29. Experimental $T_c(H)$ phase boundary of a rectangle with $\zeta=4/3$. The open squares represent the measured value using the measured sample size $S=4\ \mu\text{m}^2$ and the coherence length $\xi(0)=132$ nm. The full line is the theoretical curve $E_{\text{LLL}}(H)$.

$1.73\times2.31\ \mu\text{m}^2$, $1.41\times2.83\ \mu\text{m}^2$, and $1\times4\ \mu\text{m}^2$. The thickness τ is 39 nm and the coherence length of the coevaporated reference sample is 156 nm.

The experimental $T_c(H)$ curve of the different rectangles is presented in Figs. 29, 30, and 31. The critical temperature of the rectangles with $\zeta=4/3$ (Fig. 29) and 2 (Fig. 30) shows small oscillations superimposed with a linear dependence of the magnetic field. They have an almost identical phase boundary as the square (see Fig. 20). Only very small changes in the position of the cusps are observed. The magnetic field value where the vorticity changes from L to $L+1$ is slightly delayed when changing the value of ζ from one. No significant change in the slope and the amplitude of the oscillations could be observed.

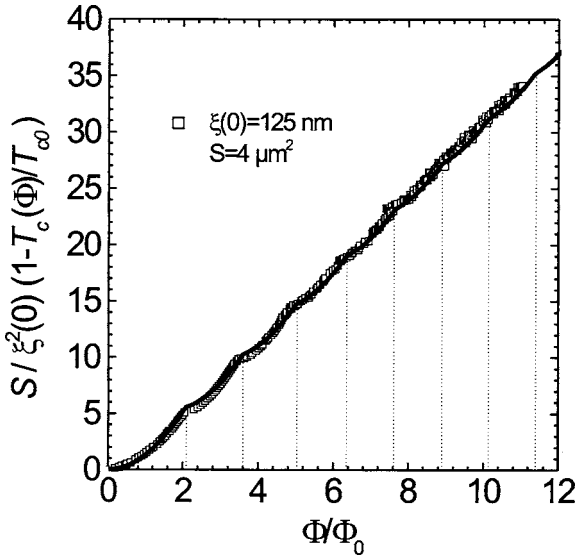

FIG. 30. Experimental $T_c(H)$ phase boundary of a rectangle with $\zeta=2$. The open squares represent the measured value using the measured sample size $S=4\ \mu\text{m}^2$ and the coherence length $\xi(0)=125$ nm. The full line is the theoretical curve $E_{\text{LLL}}(H)$.

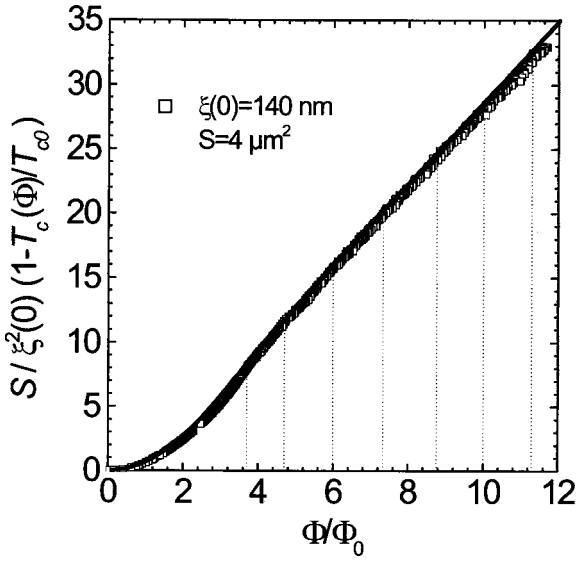

FIG. 31. Experimental $T_c(H)$ phase boundary of a rectangle with $\zeta=4$. The open squares represent the measured value using the measured sample size $S=4$ μm^2 and the coherence length $\xi(0)=140$ nm for a resistance criterion of 40% of R_n. The full line is the theoretical curve $E_{\mathrm{LLL}}(H)$.

A very good agreement between the experimental and the theoretical curves, as well as for the position of the cusp as for the amplitude of the oscillations, is obtained for these two rectangles. Even a large deformation of the square ($\zeta=2$) gives only minor changes in the phase boundary.

For a rectangle with aspect ratio $\zeta=4$, the phase boundary (Fig. 31) is strongly transformed compared to the case of the square. The oscillations are hardly seen and the position of the first vortex entry is delayed to $\Phi/\Phi_0\cong 3.7$ (left dotted line in Fig. 31) instead of the value of $\Phi/\Phi_0 \cong 2$ found for a square. A good agreement between the experimental and the theoretical curves is obtained for a resistance criterion of 40% of R_n.

V. SUPERCONDUCTING RINGS

A. Theoretical formalism

Bruyndoncx *et al.*[53] solved the linear GL equation for a loop of finite width by neglecting the induced magnetic fields. These two assumptions are valid near the phase boundary where $\Psi \rightarrow 0$. Using polar coordinates, with the gauge chosen as $\vec{A}=(\mu_0 Hr/2)\vec{e}_\phi$ so that the vector potential has no radial component, the boundary conditions reduce to the simple case of the Neumann boundary conditions,

$$\left.\frac{\partial|\Psi(r)|}{\partial r}\right|_{r=r_o,r=r_i}=0. \tag{58}$$

The solution for Ψ in cylindrical coordinates takes the following form:[11,28,29,54,55]

$$\Psi(\Phi,\varphi)=e^{-iL\varphi}\left(\frac{\Phi}{\Phi_0}\right)^{L/2}\exp\left(-\frac{\Phi}{2\Phi_0}\right)\times\left(c_1 M\left(-n,L+1,\frac{\Phi}{\Phi_0}\right)+c_2 U\left(-n,L+1,\frac{\Phi}{\Phi_0}\right)\right), \tag{59}$$

where the number n determines the energy eigenvalue and M and U are Kummer functions of the first and second kind, respectively.

The eigenenergies of Eq. (4) are

$$|-\alpha| = \hbar \frac{2e\mu_0 H}{m^\star}\left(n+\frac{1}{2}\right) = \hbar\omega\left(n+\frac{1}{2}\right). \tag{60}$$

It is worth emphasizing that the parameter n depends on L but is not necessarily an integer number. This can be rewritten as

$$\frac{r_o^2}{\xi^2(T_c)} = \frac{r_o^2}{\xi^2(0)}\left(1-\frac{T_c(H)}{T_{c0}}\right) = 4\left(n+\frac{1}{2}\right)\frac{\Phi}{\Phi_0} = \epsilon(H_{c3}^*)\frac{\Phi}{\Phi_0}. \tag{61}$$

The Landau levels in a bulk superconductor are recovered by substituting $n=0,1,2,\ldots$ in Eqs. (60) and (61), meaning that the lowest level $n=0$ corresponds to the upper critical field. It is important to note that the lowest Landau level ($n=0$) for a bulk superconductor is degenerate in the phase winding number L, and therefore the eigenfunction can be expanded as $\Psi=\Sigma c_L \Psi_L$.

Using $\mathrm{d}M(a,c,y)/\mathrm{d}y=(a/c)M(a+1,c+1,y)$ and $\mathrm{d}U(a,c,y)/\mathrm{d}y=-aU(a+1,c+1,y)$ for the derivatives of the first and second type of Kummer functions, respectively,[16] and inserting Eq. (59) into Eq. (58) gives

$$\begin{aligned} c_1\left[\left(L-\frac{\Phi}{\Phi_0}\right)M(-n,L+1,\Phi/\Phi_0) - \frac{2n}{L+1}\frac{\Phi}{\Phi_0}M(-n+1,L+2,\Phi/\Phi_0)\right] \\ + c_2\left[\left(L-\frac{\Phi}{\Phi_0}\right)U(-n,L+1,\Phi/\Phi_0) + 2n\frac{\Phi}{\Phi_0}U(-n+1,L+2,\Phi/\Phi_0)\right]\Bigg|_b = 0, \end{aligned} \tag{62}$$

which must be solved numerically for each integer value of L, resulting in a set of values $n(L,\Phi)$, with $\Phi=\mu_0 H\pi r_o^2$.

For a disk geometry,[9,11,47] we must take $c_2=0$ in Eqs. (59) and (62) in order to avoid the divergency of $U(a,c,y\to 0)=\infty$ at the origin. Following the lowest Landau level at each value Φ, one ends up with a cusplike $T_c(H)$ phase boundary,[9] which is composed of values $n<0$ in Eq. (60), thus leading to $H_{c3}^*(T)>H_{c2}(T)$. A similar calculation was performed for a single circular microhole in a plane film by Bezryadin *et al.*,[54,55] where $c_1=0$ in Eqs. (59) and (62), since $M(a,c,y\to\infty)=\infty$. Here as well, the lowest Landau level consists of solutions with $n<0$. At each cusp in $T_c(\Phi)$, the system makes a transition $L\leftrightarrow L+1$, i.e., a vortex penetrates or is expelled from the sample.

The loops of finite width discussed in this section have two superconducting/vacuum interfaces, one at the outer radius r_o, and one at the inner radius r_i. Consequently, the boundary condition [Eq. (62)] must be fulfilled at both r_o and r_i. As a result, we have a system of two equations and two variables n and c_2 ($c_1=1$ is chosen), which were solved for different values of $x=r_i/r_o$. Note that in this case n is a positive or a negative number, just found from these two equations, it is not necessarily a positive integer number.

B. Sample properties

A SEM micrograph of the different studied samples prepared with *e*-beam lithography is given in Fig. 32. All the structures consist of disks with external radii of $r_o=1$ μm. The radii of the holes, determined from SEM micrograph, were $r_i=0$ μm (a), $r_i=0.1$ μm (b), $r_i=0.3$ μm (c), $r_i=0.5$ μm (d), and $r_i=0.7$ μm (e). All the samples were evaporated in the same run, except for the thinnest loop. A different evaporation will only slightly alter the superconducting properties like the coherence length and the critical temperature. Wedge shaped contacts with opening angle $\Gamma=15°$ are used in order to minimize the influence of the contacts on the superconducting properties of the structures.[44,45] The coherence length determined from a macroscopic coevaporated sample was found to be $\xi(0)=156$ nm for the disk and the three loops with a small opening. The thickness was $\tau=39$ nm. For the sample presented in Fig. 32(e), a coherence length of $\xi(0)=120$ nm was determined in the same way as for the other structures. A thickness of $\tau=54$ nm was found from low angle x-ray diffraction on a coevaporated film and from AFM for the loop with $r_i=0.7$ μm.

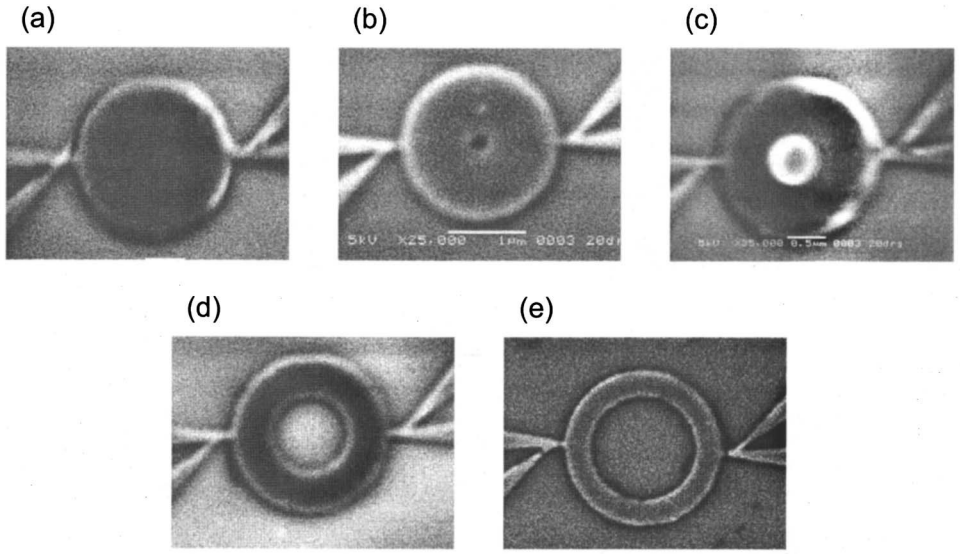

FIG. 32. SEM micrograph of (a) an Al disk with outer radius $r_o=1$ μm and of a loop with outer radius $r_o=1$ μm and inner radius (b) $r_i=0.1$ μm, (c) $r_i=0.3$ μm, (d) $r_i=0.5$ μm, and (e) $r_i=0.7$ μm.

C. Resistance transitions

The superconducting/normal resistance transitions for the disk and the rings with an inner to outer radius ratio $x=r_i/r_o=0.7$ are shown in Fig. 33. The five different samples have a very similar temperature dependence of the resistance at different magnetic field as the samples with wedge shaped contacts with opening angle $\Gamma=15°$ presented above. They are characterized by a slowly decreasing resistance at high temperatures arising from the nucleation of superconductivity in the wedge contacts, followed by a sharp drop of the resistance once superconductivity nucleates in the ring.[56] The samples with $x=0.3$, $x=0.5$, and $x=0.7$ show a different behavior at low magnetic

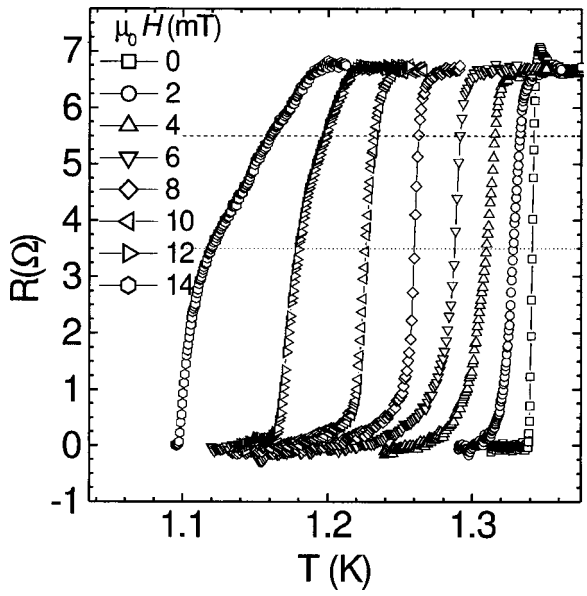

FIG. 33. Resistive transitions $R(T)$ for a loop with inner to outer radius ratio $x=0.7$ in different magnetic fields. The dashed and dotted lines show the resistance criteria used to determine the $T_c(H)$ phase boundary.

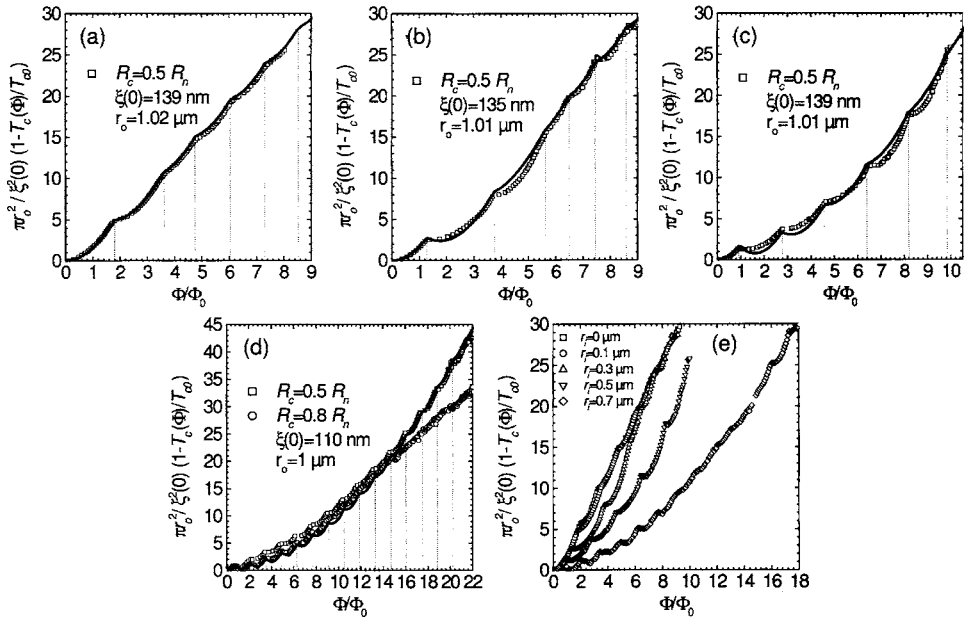

FIG. 34. The $T_c(H)$ phase boundary of a loop with inner to outer radius ratio (a) $x=0.1$, (b) $x=0.3$, (c) $x=0.5$, and (d) $x=0.7$. The open squares [and the open circles in (d)] represent the measured data. The solid lines are the calculated $E_{\mathrm{LLL}}(H)$. The experimental $T_c(H)$ phase boundaries of the different structures are compared in (e).

fields. There, the situation is reversed. A sharp transition is first observed, followed by a broad transition at low resistance. We will show below that the broad transition also corresponds to the nucleation in the wedges. This effect is observed in a broader magnetic field range when the ratio x increases.

D. $T_c(H)$ phase boundaries

The experimental phase boundary of the disk has already been presented in Fig. 21. The data for the ring with $x=0.1$ are shown in Fig. 34(a). The flux Φ on the field axis denotes the flux $\Phi=\mu_0 H\pi r_o^2$ through the ring and the hole. The H–T diagram of the ring with the smallest hole resembles strongly the $T_c(H)$ line of the disk displayed in Fig. 21. The phase boundary has a linear background superimposed with oscillations. A very good agreement between the measured and the calculated curves is found.

Figure 34(b) shows the H–T diagram of the ring with $x=0.3$. Here, the linear dependence is only seen for vorticity $L>4$. At lower magnetic field, a parabolic background suppression of T_c is observed. The crossover from the linear to the parabolic regime occurs at $\pi r_o^2/\xi^2(T)\approx 20$. This corresponds to a value $r_o-r_i\approx 1.8\ \xi(T)$, which is in a good agreement with the thickness $\tau=1.84\ \xi(T)$ for a crossover from a one-dimensional (1D) to a 2D regime for a thin film in a parallel magnetic field.[57,58]

A good agreement with the position of the cusps in the theoretical curve has been found. The amplitude of the oscillations in the experimental curve deviates slightly from the calculated one. At $L=1$, between the first and the second $T_c(H)$ cusps, the experimental oscillation is less pronounced. For higher vorticity, the opposite situation is seen where the amplitude of the experimental oscillations is larger than in the theoretical curve.

The penetration of the first vortex in the ring occurs at a lower magnetic field value than for the ring with the smallest hole [see Fig. 34(a)], while the transitions $L=1\leftrightarrow 2$ to $L=5\leftrightarrow 6$ occur at a higher magnetic field. That the transitions take place at lower magnetic field value for a ring with thinner lines is expected since the transition between L and $L+1$ occurs at $\Phi/\Phi_0=L+1/2$ for an infinitely thin loop or cylinder. At higher magnetic fields, a giant vortex state is formed[53] and the

disk with a small hole in the center behaves like the disk without hole. This, however, cannot fully explain why the change in vorticity is delayed at high magnetic fields by introducing a small hole in a disk.

The measured $T_c(H)$ phase boundary of the ring with ratio $x=0.5$ is shown in Fig. 34(c). In the temperature range accessible with our experimental setup, only a parabolic background dependence of the critical temperature on the magnetic field has been measured. By comparing the experimental results with the calculations, a similar behavior as for the ring with $x=0.3$ is seen. The position of the cusps in the experimental curve matches with the calculated transitions. However, no good agreement is found for the amplitude of the oscillations. For the vorticities $L=1$ and 2, the amplitude is lower in the experimental curve, while for $L>3$, the amplitude is larger. At low L, the transition between states with different vorticities occurs at a lower magnetic field than for the disk, while the transitions $L=3\leftrightarrow 4$, $L=4\leftrightarrow 5$ and $L=5\leftrightarrow 6$ take place at a higher magnetic field, similar to what was observed for the ring with $x=0.3$.

The H–T diagram of the ring with the thinnest line ($x=0.7$) is shown in Fig. 34(d). Two experimental curves are presented, one for $R_c=0.5R_n$ (open squares) and the second for $R_c=0.8R_n$ (open circles). It can be seen that at a higher resistance criterion the parabolic dependence switches to a linear regime at high magnetic field. For the curve calculated with the low resistance criterion, a quasiparabolic background suppression of $T_c(H)$ is observed over the whole measured range. The amplitude of the $T_c(H)$ oscillations is larger than in the samples with smaller x and the transition between states with different vorticities is almost periodic in field. A good agreement between the theoretical curve and the experimental curve with $R_c=0.5R_n$ is seen at high magnetic fields. At lower magnetic fields, a good agreement is found when using a higher resistance criterion.

The phase boundaries of the four different loops are compared with the critical temperature of the disk in Fig. 34(e). All the curves overlap with each other for $L=0$. *It is interesting to note that an opening in the disk does not affect the phase boundary as long as no vortex is trapped inside the superconductor*. Only the magnetic field range over which the state with $L=0$ exists at the phase boundary is lowered by introducing a hole in the disk. The $T_c(H)$ line of the disk with the smallest hole in the middle does not deviate substantially from the phase boundary of the disk without any opening. Only small changes in the position of the cusps is observed at low vorticity. For larger holes, the crossover from 2D to 1D regime is clearly seen. The samples with the thinnest lines do not show the 2D regime in the studied temperature interval and only the parabolic dependence is seen.

In order to reveal the origin of this different behavior at low and high magnetic field, a contour plot of the resistance $R(H,T)$ is presented in Fig. 35. Two different parts are clearly distinguished. Below 10 mT, the low resistance is linear, while the high resistance exhibits a parabolic background superimposed with oscillations. Above 10 mT, the opposite situation occurs, where the low resistance has a parabolic decay with small oscillations while the high resistance decreases monotonously. The parabolic part coincides with the nucleation of superconductivity in the loop shown as a full line. The linear part arises from the nucleation in the wedge contacts.

By fitting the theoretical critical temperature of a wedge with opening angle $\Gamma=15°$ to the linear part of the contour plot (dashed line), a coherence length $\xi(0)=140$ nm is obtained. This differs from the coherence length $\xi(0)=110$ nm that was used to find a good agreement between the experiment and the theoretical curve of a loop. A possible origin of this discrepancy could be a width of the loop that has been evaluated to be smaller than the real size. An estimate of the thickness that would satisfy the coherence length used for the calculation of the wedge contacts can be obtained from the analysis of the nucleation field of a thin wire of a film in a parallel magnetic field. From the calculation of the nucleation field of a thin film in a parallel field,[52] a value for the width of the loop of 0.38 μm is obtained instead of 0.3 μm found from SEM measurements. This difference is too large to be explained only by an error in the characterization of the sample. The opening angle of the contacts can be determined with a high accuracy so that a divergence arising from a wrong determination of Γ could be excluded. It means that either the nucleation of superconductivity is delayed in the wedges due to the presence of the loop or that the

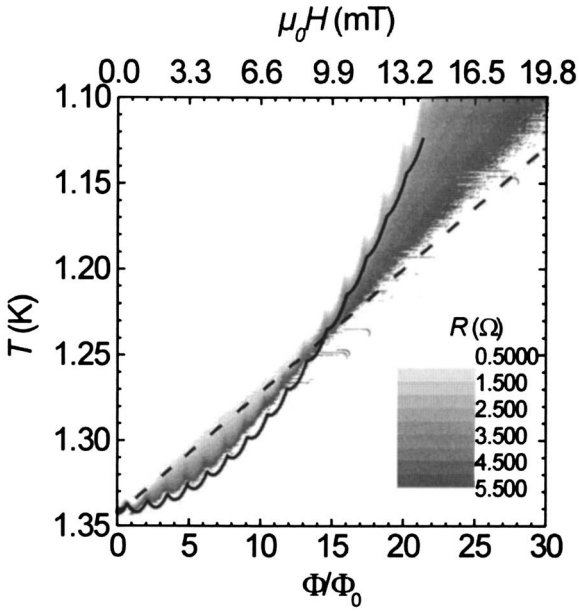

FIG. 35. Contour plot of the resistance $R(H,T)$ of a loop with $x=0.7$. The full line represents the calculated phase boundary of a loop with $r_i=0.7$ μm and $r_o=1$ μm, using a coherence length of 110 nm. The dashed line is the theoretical critical temperature of a wedge with opening angle $\Gamma=15°$ with $\xi=140$ nm.

nucleation in the loop is enhanced by the contacts. It is also possible that the coherence length in the loop is slightly different from that in the wedge. The sample geometry can indeed affect the superconducting parameters λ and ξ in a structure of mesoscopic size similar to the case of a thin film where the effective penetration depth increases as $\lambda'=\lambda^2/\tau$, taking into account the demagnetization effects. The renormalization of λ and ξ should therefore be calculated in a self-consistent way from the sample geometry.

The shape of the resistive curves in Fig. 33 can be easily understood from Fig. 35. It was clearly seen that in low magnetic fields the nucleation first occurs in the ring and is then followed by the nucleation in the contacts. Due to the different field dependence of the $T_c(H)$ of the ring and the contacts, the opposite occurs in higher magnetic fields. Two different shapes are therefore distinguished in the resistive curves depending on the part where superconductivity starts to nucleate. The same happens in the rings with $x=0.3$ and $x=0.5$ since T_c also has a parabolic field dependence for low fields. The normal parts of the sample can however partially become superconducting by the proximity effect with the neighboring superconducting part.

VI. STABILITY OF THE LGL SOLUTIONS AND THE PHASE TRANSITIONS BELOW THE NUCLEATION TEMPERATURE

The lowest level E_{LLL} of the LGL equation, describing the nucleation of superconductivity in applied magnetic field, $T_c(H)$, is always nondegenerate for finite size samples.[59] Therefore the corresponding solution is fully consistent with the symmetry of the sample in applied field as we have seen in the preceding section. This is opposite to the case of bulk type-II superconductors without boundaries, where $E_{\mathrm{LLL}}(H)$ is an infinitely degenerate Landau level while the nucleating order parameter is a combination of its degenerate components,[42] always of broken symmetry (BS) type. Besides the symmetry, the discreteness of the spectrum of the LGL equation in mesoscopic superconductors implies the stability of the shape of the nucleated order parameter in a range of temperatures close to the $T_c(H)$ line. Such stability of a symmetric order parameter has been found for mesoscopic cylinders,[30,34,40,60,61] squares and triangles.[62–66] Remarkably, a similar phenomenon is encountered in molecular physics where it is known as the pseudo-Jahn-Teller effect.[67]

In this section we investigate the mechanisms of phase transitions from a nucleated order parameter of a mesoscopic superconductor to another symmetry or broken symmetry phase when temperature is lowered.[68] We find that in the case of BS phase transitions most often only one single LGL solution of different symmetry effectively admixes to the nucleated phase. In this case the description of the phase transition is equivalent to the description of vibronic instability in a simple (two-level) pseudo-Jahn-Teller problem. Such analogy is specific to mesoscopic superconductors, which have discrete LGL spectrum, and gives a "molecular" view on the mechanism of BS phase transitions in mesoscopic samples. We also investigate the existence of different phases as a function of the samples size and find that the region on the phase diagram corresponding to the nucleated order parameter of S solution increases with reducing the size. The critical sizes, corresponding to the disappearence of BS phase transitions (when the nucleated S phases persist down to $T=0$) are predicted to be in the range of micrometers for conventional superconductors, i.e., within the reach of current experimental techniques. This opens possibilities for the experimental verification of different transitions predicted here on the basis of the similarities with pseudo-Jahn-Teller mechanism.

As before we consider a superconducting polygon of size a (a^2 is the surface of the sample) and thickness d in a perpendicular uniform magnetic field H. For small ($a \sim \xi$, the coherence length) and thin ($d \ll \xi$) samples one can neglect the variation of the order parameter across thickness[30,40] and the distortion of the magnetic field induced by screening and vortex currents. The order parameter Ψ is found from the minimization of the two-dimensional GL functional,

$$\Delta F = \int \left[\alpha |\Psi|^2 + \frac{1}{2}\beta |\Psi|^4 + \frac{1}{2m^*} \left| \left(-i\hbar \nabla - \frac{2e}{c}\mathbf{A} \right) \Psi \right|^2 \right] \mathrm{d}S, \tag{63}$$

with the boundary condition (7). Minimizing (63) without the term $\sim|\Psi|^4$ results in the linear eigenvalue equation (4) with the solutions which we further denote by ϕ_i, ϵ_i. The lowest solution ϕ_1 describes the nucleation phase boundary via the equation $\epsilon_1 = -\alpha$. The eigenvalues ϵ_i, measured in units of $\hbar^2/2m^* a^2 (\epsilon_i')$, depend only on the applied magnetic flux $\Phi = Ha^2$, presented in units of the superconducting flux quantum Φ_0. The eigenstates of (34), normalized to unity within the surface of the sample, are used further as the basis set for the order parameter,

$$\Psi = \sum_{i=1}^{N} c_i \phi_i, \tag{64}$$

where N is the dimension of the basis set. Substitution of (64) into (63) yields ΔF as a function of the expansion coefficients

$$\Delta F = \sum_i \alpha_i |c_i|^2 + \frac{\beta}{2a^2} \sum_{ijkl} A_{ij}^{kl} c_i^* c_j^* c_k c_l,$$

$$\alpha_i \equiv \alpha + \epsilon_i, \tag{65}$$

where the parameters

$$A_{ij}^{kl} = a^2 \int \phi_i^* \phi_j^* \phi_k \phi_l \, \mathrm{d}S \tag{66}$$

depend only on the geometry but not on the size of the sample. A_{ii}^{ii} is precisely the Abrikosov parameter β_A[69] for the state ϕ_i, which is a measure of its "flatness."

The actual parameters defining the relative free energy in Eq. (65) can be found as follows. If we use coefficients $c_i \to a\sqrt{-\alpha_1/\beta} c_i$ and measure the free energy in units of $a^2\alpha_1^2/\beta$ (α_1 corresponds to the lowest LGL eigenvalue ϵ_1) then the right-hand side of Eq. (65) will depend (besides

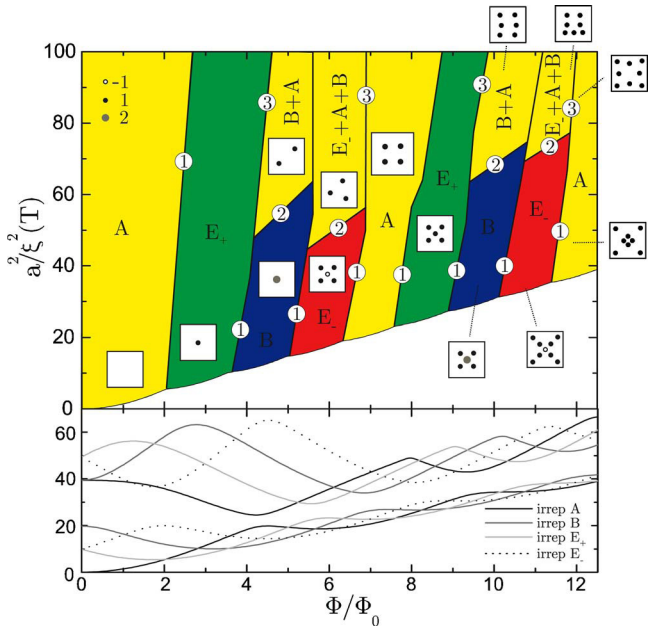

FIG. 36. (Color online) Lower panel, LGL solutions ϵ_i' for a square with superconductor-vacuum boundary condition, characterized by irreps A ($m=0$), B ($m=2$), E_+ ($m=1$), and E_- ($m=-1$). Upper panel, the corresponding phase diagram obtained by Monte Carlo calculations. For each phase, the vortex structure is shown schematically and the involved irreps are indicated. The number at each boundary line denotes the type of transition (Table II). In the color online version: the colors stand for the winding number of the central vortex: 0 (yellow), 1 (green), 2 (blue), and −1 (red).

A_{ij}^{kl}) only on the ratios $\alpha_i/\alpha_1=(a^2/\xi^2+\epsilon_i')/(a^2/\xi^2+\epsilon_1')$. Hence the GL functional for a given sample (measured in units of $a^2\alpha_1^2/\beta$) and the emerging phase diagram are only dependent on $(a/\xi(T))^2$ and Φ/Φ_0.

As we have already seen (Figs. 11 and 12), the spectrum of eigenvalues of the LGL equation is strongly influenced by the symmetry of the problem. If the sample has a rotational symmetry axis C_n, the Landau levels are split in groups of n levels belonging to different irreps, because only these can intersect each other. In addition, the C_n symmetry imposes the selection rules on integrals in Eq. (66), $m_k+m_l-m_i-m_j=0$, similar to the case of cylindrical symmetry.[34,60]

Because the fourth order terms in (65) are overall positive, it is generally expected that only the states ϕ_i with $\alpha_i<0$ will effectively contribute to the order parameter. In the close vicinity to the nucleation phase boundary only α_1 is negative, therefore $\Psi\approx c_1\phi_1$, with $c_1=a\sqrt{-\alpha_1/\beta A_{11}^{11}}$ $\sim\sqrt{(a/\xi)^2-\epsilon_1'}$ and the free energy $\Delta F_1=-(\alpha_1^2/2\beta A_{11}^{11})a^2$. The only allowed admixtures in this phase are from the excited LGL states of the same irrep, $\phi_{1'}$, described by the coefficients $c_{1'}$,

$$\frac{c_{1'}}{c_1}\approx-\frac{A_{11'}^{11}c_1^2}{\alpha_{1'}/\beta+[2A_{11'}^{11'}+|A_{11'}^{11}|\cos(\chi_{1'1'}^{11}-2\chi_{11'}^{11})]c_1^2}, \tag{67}$$

where $\chi_{ij}^{kl}=\arg A_{ij}^{kl}$. In the temperature region where $\alpha_{1'}>0$ the coefficients $c_{1'}$ in (67) show smooth behavior, with continuous derivatives with respect to temperature. The symmetry-preserving phase transitions can therefore occur only when some of $\alpha_{1'}$ become negative. However in symmetric samples the ϕ_i states which are close to ϵ_1 are always of different symmetry (lower panel in Fig. 36) so that many of the corresponding parameters α_i will become negative before $\alpha_{1'}$. We can conclude that the nucleated order parameter will undergo a phase transition *modifying its symmetry* when temperature is lowered.

Even if there are many LGL states with $\alpha_i<0$ at a given temperature, only a few of them actually contribute to the order parameter. This is due to the fact that while the terms $\sim A_{ii}^{ii}$ and $\sim A_{ii}^{jj}$ give net contributions to "repulsion," the other terms, which could become negative, partially

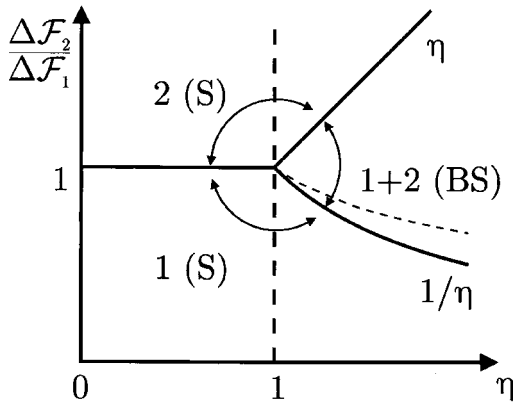

FIG. 37. Diagram of thermodynamically stable phases (solid lines) for the effective two-state model (68) as a function of the parameters from Eqs. (69) and (70). 1, 2 are pure phases and 1+2 is the mixed one.

cancel out when N is increased. One can check indeed that already for $N>3$ there are less available phases of complex c_i coefficients than A_{ij}^{kl} terms to be optimized. The mutual reduction of these terms increases with the number of mixed LGL states which means that at a certain value of N further admixture will become unfavorable. It is expected therefore that only a few different irreps will effectively admix at the transition point.

Next we adopt a general description of the phase transitions from a nucleated order parameter, which is achieved by the following consideration. Given the small number of different irreps among the states ϕ_i which admix at the transition point, we can always divide the corresponding $\{c_i\}$ in two groups so as to bring the functional (65) to the following basic form:

$$\Delta F = \tilde{\alpha}_1 c_1'^2 + \tilde{\alpha}_2 c_2'^2 + \frac{\beta}{2a^2}(A_{11}c_1'^4 + A_{22}c_2'^4 + 2A_{12}c_1'^2 c_2'^2), \tag{68}$$

where c_1' and c_2' are the norms of the coefficients in the first and the second group, respectively, while the parameters $\tilde{\alpha}_1$, $\tilde{\alpha}_2(<0)$ and A_{11}, A_{22}, $A_{12}(>0)$ are functions of associated angular variables to be specified below. The two groups contain different irreps, in numbers n_1 and n_2, correspondingly (ϕ_1 belongs to the first group). Minimization with respect to c_1' and c_2' for fixed values of the five parameters in (68) results in three (meta)stable phases,

$$\Delta F_1 = -\frac{\tilde{\alpha}_1^2}{2\beta A_{11}}a^2, \quad \Delta F_2 = -\frac{\tilde{\alpha}_2^2}{2\beta A_{22}}a^2,$$

$$\frac{\Delta F_{12}}{\Delta F_1} = \frac{(\sqrt{\eta \Delta F_2/\Delta F_1} - 1)^2}{\eta - 1} + 1, \tag{69}$$

where

$$\eta = \frac{A_{11}A_{22}}{A_{12}^2}. \tag{70}$$

The first two are pure phases, with $c_2'=0$ and $c_1'=0$, respectively, while ΔF_{12} is the mixed one $(c_1', c_2' \neq 0)$. Figure 37 shows the diagram of the thermodynamically stable phases. The vertical line $\eta=1$ divides the diagram in two regions. On the left-hand side we have a switch between pure phases (first-order transition). On the right-hand side the two phase boundary lines correspond to the second order transitions. At temperatures close to the lower phase boundary, $T=T_{\mathrm{BS}}-\Delta T$, $\xi=\xi_{\mathrm{BS}}-\Delta\xi$, the BS phase will grow as $c_2' \sim \sqrt{\Delta T}$, $\sqrt{\Delta\xi}$.

Now the free energy expressions (69) are minimized with respect to the remaining variables from $\tilde{\alpha}_i$ and A_{ij} resulting in the lowest energy phase for a given temperature. Since we are looking for phase transitions from the nucleated S-order parameter, the pure phase 1 in Fig. 37 always corresponds to ϕ_1 with possible small admixtures of the same symmetry, Eq. (67). Depending on the symmetries of other LGL states which admix through the transition we can have several types of phase transitions which are investigated below. As in the case of ϕ_1, the contributions from states of other symmetries are mainly represented by one LGL state. Therefore to simplify further analysis we will consider that only one state per irrep contributes.

In the case of a single admixed state (ϕ_2) one should substitute $c_1=c_1'$ and $c_2=c_2'$ in Eq. (68) and $\tilde{\alpha}_i=\alpha_i$, $A_{ii}=A_{ii}^{ii}$ and $A_{12}=2A_{12}^{12}-|A_{11}^{22}|$ into (69) and (70). When the interaction between these states, A_{12}, is larger than $\sqrt{A_{11}^{11}A_{22}^{22}}$, the order parameter corresponds either to ϕ_1 or ϕ_2 (left-hand side of the diagram in Fig. 37). The transition from ϕ_1 to ϕ_2 takes place when

$$\frac{\alpha_2}{\alpha_1} > \sqrt{\frac{A_{22}^{22}}{A_{11}^{11}}}. \tag{71}$$

The left-hand side of this equation increases with lowering the temperature, being always <1. Therefore the transition between symmetric states can only occur if $A_{22}^{22}<A_{11}^{11}$. When the interaction is weaker, $\eta>1$, the transition from ϕ_1 to a BS order parameter (right-hand side of the phase diagram) can arise under the condition

$$\frac{\alpha_2}{\alpha_1} > \frac{A_{12}}{A_{11}^{11}}. \tag{72}$$

When two states of different symmetry mix with ϕ_1, two situations can occur.

(1) If the involved irreps obey the inequalities $m_1+m_3-2m_2\neq 0,\pm n$, $m_1+m_2-2m_3\neq 0,\pm n$, then one has $c_1=c_1'$, $c_2=c_2'\cos\varphi$, $c_3=c_2'\sin\varphi$, and

$$\tilde{\alpha}_1=\alpha_1,$$

$$\tilde{\alpha}_2=\alpha_2\cos^2\varphi+\alpha_3\sin^2\varphi,$$

$$A_{11}=A_{11}^{11},$$

$$A_{22}=A_{22}^{22}\cos^4\varphi+A_{33}^{33}\sin^4\varphi+(A_{23}^{23}-|A_{22}^{33}|/2)\sin^2 2\varphi,$$

$$A_{12}=2A_{12}^{12}\cos^2\varphi+2A_{13}^{13}\sin^2\varphi-|A_{11}^{23}|\sin 2\varphi, \tag{73}$$

Substituting (73) into Eqs. (69) and minimizing with respect to φ we obtain again three thermodynamically stable phases of Fig. 37 for corresponding equilibrium values of φ. The difference is that now the left-hand side of the diagram describes the switch between the symmetric (ϕ_1) and the broken-symmetry ($\phi_2+\phi_3$) phases, while the BS phase on the right-hand side of the diagram corresponds to $\phi_1+\phi_2+\phi_3$.

(2) If the first or the second relation for irreps becomes equality then $c_1=c_1'\cos\varphi$, $c_2=c_2'$, $c_3=c_1'\sin\varphi$, or $c_1=c_1'\cos\varphi$, $c_2=c_1'\sin\varphi$, $c_3=c_2'$, respectively. Therefore for $\eta<1$ we can only have a symmetry-changing transition from ϕ_1 to ϕ_2 (or ϕ_3). However for $\eta>1$, at φ corresponding to thermodynamically stable BS phase $\phi_1+\phi_2+\phi_3$, the lowest boundary line in Fig. 37 separates this phase from the metastable one $\phi_1+\phi_3$ (or $\phi_1+\phi_2$). Therefore the phase transition from ϕ_1 will take place along the line which lies somewhere higher (dashed line in Fig. 37), i.e., it is of the first order. This type of transition is associated with a small jump of c_1, hence it is close to second order.

TABLE II. Possible transitions from a symmetric vortex phase.

Type[a]	η	n_1	n_2	n_f[b]	Order (symmetry)
1	<1	1	1	1	I (S)
2	>1	1	$\geqslant 1$	n_2+1	II (BS)
3	<1	1	>1	n_2	I (BS)
4	>1	>1	$\geqslant 1$	n_2+n_1	I (BS)

[a]Numbers used in Fig. 36.
[b]Number of irreps in the final state.

Considering higher numbers of mixing irreps will not result in qualitatively new phase transitions which are thus of four types (Table II).

The diagram of the lowest transitions from symmetric phases in a thin square was evaluated within the above approach, which compares well with an accurate Monte Carlo calculation[70] shown in the upper panel of Fig. 36. The critical values of ξ calculated by the two approaches differ by only several percents. One finds indeed that only a few states effectively admix to the order parameter. The described region in the phase diagram becomes relatively large with decreasing a. For small enough samples some phase boundary lines pass above $(a/\xi(0))^2$ and the nucleated symmetric phases remain thermodynamically stable down to $T=0$. Thus the transition from the phase with an antivortex in the center ($\Phi/\Phi_0=5.5\leftrightarrow 6.5$) to a BS phase with the same vorticity but without antivortex is suppressed for $a<(7\leftrightarrow 8)\xi(0)$ (≈ 1 μm for Al).

It follows from Fig. 36 that the phase boundary lines separating the areas with different vorticity have positive slopes and correspond to transitions of type 1 (Table II) in the lower part of the diagram.[71] The reason is the increase of Abrikosov parameters β_A in the lowest group of LGL states (Fig. 36) when passing through the corresponding avoided crossings towards increased fields. Indeed, it was shown[24] that the lowest Landau level of each irrep maps into cylindrical states with rotational numbers L to the left and $L+n$ to the right of the avoided crossing, respectively. Therefore for two lowest LGL states the Abrikosov parameter is smaller for the ground state to the left and for the excited one to the right of their intersection, so that the condition (71) can only be obeyed in the latter case.

On the other hand, the obtained transitions to broken-symmetry phases are always of the second order and go mostly via a two-state mixing scenario (in the phases E_-+A+B in Fig. 36 the admixture of B states is relatively small). The direct analogy for this in molecular physics is the pseudo-Jahn-Teller (PJT) instability of symmetric geometry of a molecule with respect to a low symmetry nuclear distortion (q). Usually such an instability results from a strong interaction of the ground electronic state (ϕ_1) with an excited state (ϕ_2), induced by q, which is described by the Hamiltonian,[67]

$$H_{\mathrm{PJT}}=\frac{1}{2}Kq^2+\begin{pmatrix}-\Delta & V_q\\ V_q & \Delta\end{pmatrix}, \tag{74}$$

where 2Δ is the energy gap between the ground and the excited states in the symmetric nuclear configuration, V is the vibronic constant, and K is the force constant. The instability occurs when $V^2/K>\Delta$ and it results in an equilibrium distortion $q^{(0)}$ (Fig. 38) and a broken-symmetry electronic ground state.

The PJT instability can be described by considering a functional depending on electronic variables only.[72] To obtain such a functional, we average H_{PJT} over $\Psi=c_1\phi_1+c_2\phi_2$, find the equilibrium value of q as function of c_1 and c_2 and substitute it back into the average,

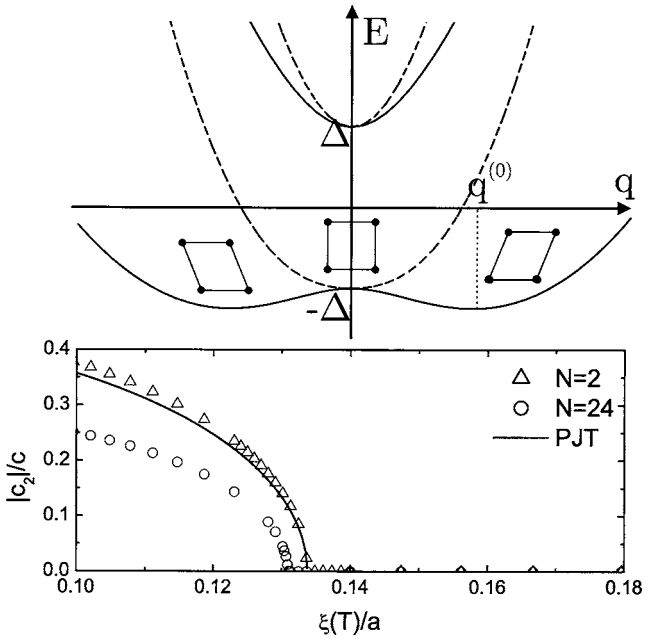

FIG. 38. Upper panel, adiabatic potential for two nondegenerate electronic terms of a square molecule in the case of weak (dashed lines) and strong (solid lines) pseudo-Jahn-Teller effect. Lower panel, temperature dependence of the normalized coefficient of admixture of the excited (A) state close to the $B \rightarrow B+A$ transition at $\Phi=4.5\Phi_0$ (Fig. 36) evaluated by Monte Carlo calculations and the pseudo-Jahn-Teller effect using the correspondence relations (77). The numbers in the inset denote the dimension of the basis set in the Monte Carlo calculations.

$$\langle \Psi | H_{\mathrm{PJT}} | \Psi \rangle^0 = -\frac{2V^2}{K} c_1^2 c_2^2 + \Delta(-c_1^2 + c_2^2). \tag{75}$$

Next we introduce polar coordinates, $c_1=c\cos\varphi$, $c_2=c\sin\varphi$ for the PJT functional (75) and $c_1=A_{11}^{-1/4}c\cos\varphi$, $c_2=A_{22}^{-1/4}c\sin\varphi$ for the functional (68), where φ plays now the role of the order parameter for the BS state. The φ-dependent part of both functionals has now the following common form:

$$\Delta E(\varphi) = -Ac^4 \sin^2 2\varphi - Bc^2 \cos^2\varphi, \tag{76}$$

where $A=V^2/2K$, $B=\Delta$ for the PJT problem and $A=(\beta/4a^2)(1-\eta^{-1/2})$, $B=(\alpha_2 A_{22}^{-1/2}-\alpha_1 A_{11}^{-1/2})/2$ for the case of superconductor. The main difference between them is that $c=1$ in the former and $c\neq 1$ in the second case. Therefore the correspondence between PJT and GL parameters is the following:

$$V^2/K \rightarrow \frac{|\alpha_1|}{2\sqrt{A_{11}}}\left(1-\frac{1}{\sqrt{\eta}}\right),$$

$$2\Delta \rightarrow \frac{\alpha_2}{\sqrt{A_{22}}} - \frac{\alpha_1}{\sqrt{A_{11}}}. \tag{77}$$

Lower panel in Fig. 38 shows how the broken symmetry phase appears for vortex molecules. We can see that the evolution of the order parameter with temperature is reproduced by the pseudo-Jahn-Teller effect. In the case $N=2$, only the ground B and the first excited A LGL states are taken into account. The accurate calculation involving $N=24$ LGL states shifts the transition point obtained in the $N=2$ calculation only by $\approx 2\%$. This shift mainly arises due to the renormalization of the effective parameters in Eq. (68) when more LGL states are taken into account.

As a result of this renormalization the nucleated phase becomes optimized so that the transition takes place at a lower temperature compared to the two-state approximation.

As the analysis shows the specific structural similarity between the pseudo-Jahn-Teller and GL symmetry breaking mechanisms is due to the presence of a quartic dependence on the expansion coefficients. A different mechanism of symmetry breaking was described by Berger for the case of the Schrödinger equation for a cylinder.[73] In this case breaking of axial symmetry was obtained through the induced magnetic field and the quadratic term in the GL potential was not considered.

The symmetric order parameters are found to be remarkably stable below the nucleation temperature, which is a pure mesoscopic effect. Besides, the mesoscopic samples show a rich variety of vortex phases compared to bulk type II superconductors where only the Abrikosov vortex lattice occurs. By using an effective two-state model the nature of the transition to these phases has been revealed and four distinct types of transitions have been found. The symmetry-breaking phase transition has the same structure as the pseudo-Jahn-Teller instability of high symmetry nuclear configurations in molecules. This analogy provides an interesting connection between real and vortex molecules.

The existence of phases can be experimentally verified by using various local probe techniques such as Hall probe microscopy, STM and AFM. The phase diagram is found to be strongly dependent on the samples size. In particular, the region on the phase diagram corresponding to the nucleated (symmetric) order parameter enlarges with reducing the size of the sample. The critical size corresponding to the complete disappearance of the BS phase (the nucleated *S*-phase persists until $T=0$) is predicted to be of the order of micrometers for conventional superconductors, such as Al, Pb. These predictions can be checked experimentally on different mesoscopic superconducting systems.

VII. CONCLUSIONS

An analytical gauge transformation for the vector potential is derived with a vanishing normal component at the boundary line of any regular polygon. With this vector potential gauge, the linearized Ginzburg–Landau problem reduces to an eigenvalue equation in a basis set of functions obeying Neumann boundary conditions, which can be found for different regular polygons. The proposed approach allows for accurate evaluations of the order parameter distributions and proves to be especially efficient at moderate values of applied magnetic fields. For low values of applied magnetic fluxes the order parameter for superconducting square and equilateral triangle contains an antivortex in the center. These solutions are found to be stable with respect to small deviations from the phase boundary line and can be probed by techniques which are sensible to the superfluid density, for example, by using scanning tunnelling microscopy. The calculated lowest energy levels $E_{\mathrm{LLL}}(H)$ show a very good agreement with the measured phase boundaries $T_c(H)$ for a variety of different geometries (triangles, squares, disks, rectangles, loops). By using full GL equations symmetry-breaking transitions deeper in the superconducting state have been studied. A remarkable similarity of these transitions for vortex molecules with pseudo-Jahn-Teller effect for real molecules has been revealed.

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Numerical approximations of the Ginzburg–Landau models for superconductivity

Qiang Du[a)]
Department of Mathematics, Pennsylvania State University, University Park, Pennsylvania 16802

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In this paper, we review various methods for the numerical approximations of the Ginzburg–Landau models of superconductivity. Particular attention is given to the different treatment of gauge invariance in both the finite element, finite difference, and finite volume settings. Representative theoretical results, typical numerical simulations, and computational challenges are presented. Generalizations to other relevant models are also discussed. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The macroscopic model of Ginzburg and Landau[43,91] has been widely used to study both low-temperature and high-temperature superconductors. Due to its highly nonlinear nature, the complex energy landscape and the exotic dynamic responses of its solution to external conditions, its numerical simulations have become valuable tools in order to better understand the properties of the Ginzburg–Landau (GL) models and to provide further theoretical insight into the intriguing superconductivity phenomena.

The development of approximation methods of the Ginzburg–Landau model goes back to the 1950s shortly after the inception of the model.[58] Particularly notable works include the seminal paper by Abrikosov[2] on the vortex state in type-II superconductors based on the linearization of GL equations near the upper critical field. The systematic studies of the GL models from the numerical analysis point of view, to our knowledge, have not been seriously developed until the publication of Ref. 43. In Ref. 43, both rigorous mathematical theory on the well-posedness of the equilibrium GL models and their physical background were presented, along with the systematic development of finite element approximation methods. The work in Ref. 43 was partly motivated by Refs. 3 and 29 of casting the equilibrium models into a variational framework. Extensions to the dynamic models, i.e., the time-dependent Ginzburg–Landau (TDGL) equations were subsequently made.[32,31] Since then, many other works have appeared in the literature, including the development of different types of numerical approximations of Ginzburg–Landau-type models, their rigorous theoretical analysis as well as extensive simulations. By now, almost all aspects of modern numerical analysis have been utilized by people working on the numerical solutions of the GL models, ranging from the design and applications of various discretization methods and fast algorithms, domain decomposition and parallelization techniques, and adaptive computation strategies. In this paper, we briefly review some of the works concerning the numerical approximations of the Ginzburg–Landau models. In terms of spatial discretization methods, we consider, in particular, the finite difference methods, finite element methods and finite volume methods. We also discuss various time-stepping schemes for time dependent models. As there have been a large amount of works on the numerical simulations of the GL models in the last few decades, we make no attempt to provide a comprehensive survey on all existing works on the subject due to limited

[a)]Electronic mail: qdu@math.psu.edu

space. In particular, our review of the vast physics literature is very much limited to those that have also received much attention in the numerical analysis community or have been examined more rigorously in the mathematics literature.

The rest of the paper is organized as follows: in Sec. II, we briefly recall the GL models and their basic features. In Sec. III, various numerical schemes are discussed, and in Sec. IV, some sample simulation results are presented and some concluding remarks are given in Sec. V.

We end the introduction by stating that much of the research works discussed in the paper are aimed at the development and refinement of mezoscale and macroscale models for superconductivity so to enlarge the range of physical problems for which such models are valid; the analysis of these models in order to gain further understanding of their properties and of their solutions, and for the most part of the paper, the development, analysis, and the implementation of algorithms for the numerical simulation of the superconductivity models.

II. GINZBURG–LANDAU MODELS

Let $\Omega \subset R^d$ $(d=2, 3)$ be the region occupied by the superconducting sample. The primary variables used in the GL models are the complex scalar-valued *order parameter* ψ, the real vector-valued *magnetic potential* $\mathbf{A}$, and the real scalar-valued electric potential $\overline{\Phi}$. In a nondimensional form, these variables are related to the physical variables by

$$\text{density of superconducting charge carriers,} \quad |\psi|^2,$$

$$\text{induced magnetic field,} \quad \text{curl } \mathbf{A},$$

$$\text{current,} \quad \mathbf{J} = \mathbf{curl}\ \text{curl } \mathbf{A},$$

$$\text{electric field,} \quad \frac{\partial}{\partial t}\mathbf{A} + \nabla\overline{\Phi}.$$

A. Ginzburg–Landau free energy

Given a constant applied magnetic field H, the conventional Ginzburg–Landau free energy, below the critical transition temperature, is

$$\mathcal{G}(\psi,\mathbf{A}) = \int_\Omega \left(\frac{1}{2}\left| \left(\frac{i}{\kappa}\nabla + \mathbf{A} \right)\psi \right|^2 + \frac{1}{4}(1-|\psi|^2)^2 + \frac{1}{2}|\text{curl } \mathbf{A} - H|^2 \right) \mathrm{d}\Omega,$$

where κ, the Ginzburg–Landau parameter, is a material constant representing the ratio of the penetration depth and the coherence length.

Note that for the general three-dimensional (3D) problems, the interactions between the fields inside the superconducting sample and the external field are important. Various measurement of critical fields are also affected by the geometrical shape of the sample.[72,69,78,85] To apply the Ginzburg–Landau theory in such situations, a coupled system of equations must be solved in both the sample and its exterior. Energetically speaking, in the case where Ω is a bounded domain in 3D, it may be necessary to reformulate the free energy as follows:

$$\mathcal{G}(\psi,\mathbf{A}) = \int_\Omega \left(\frac{1}{2}\left| \left(\frac{i}{\kappa}\nabla + \mathbf{A} \right)\psi \right|^2 + \frac{1}{4}(1-|\psi|^2)^2 \right) \mathrm{d}\Omega + \frac{1}{2}\int_{R^3} |\text{curl } \mathbf{A} - H|^2 \, \mathrm{d}R^3.$$

The minimizers of the GL energy functional satisfy the Euler-Lagrange equations, also called the GL equations, of the form

$$\left(\frac{i}{\kappa}\nabla + \mathbf{A}\right)^2 \psi - \psi + |\psi|^2\psi = 0, \tag{2.1}$$

$$\mathbf{curl}\ \mathrm{curl}\ \mathbf{A} + \frac{i}{2\kappa}(\psi^*\nabla\psi - \psi\nabla\psi^*) + |\psi|^2\mathbf{A} = 0. \tag{2.2}$$

Here, ψ^* is the complex conjugate of ψ. With the present nondimensionalization, $|\psi|=1$ and $|\psi|=0$ correspond to the perfectly superconducting state and the normal state.

This set of nonlinear Ginzburg–Landau equations in the (bounded) interior of Ω is coupled with the linear Maxwell equations in the (unbounded) exterior $\Omega^e = R^3 \backslash \overline{\Omega}$ with far field conditions at infinity and interface conditions on $\Gamma = \partial\Omega$. If we only consider the interior problem (typically valid for a two-dimensional cross section of a long 3D cylinder with the applied magnetic field perpendicular to the cross section), then on Γ, it is customary to use the natural boundary conditions

$$\left(\frac{i}{\kappa}\nabla\psi + \mathbf{A}\psi\right)\cdot\mathbf{n} = 0, \tag{2.3}$$

$$\mathrm{curl}\ \mathbf{A} = H. \tag{2.4}$$

More general boundary conditions have also been studied. For instance, to study the proximity effect, one may use

$$\left(\frac{i}{\kappa}\nabla\psi + \mathbf{A}\psi\right)\cdot\mathbf{n} = -i\gamma\psi.$$

We refer to Refs. 14, 43, and 91 for more discussions.

B. Time-dependent Ginzburg–Landau equations

Let η_1 and η_2 be given relaxation parameters, the conventional time-dependent Ginzburg–Landau (TDGL) model is given by

$$\eta_1\left(\frac{\partial\psi}{\partial t} + i\kappa\overline{\Phi}\psi\right) + \left(\frac{i}{\kappa}\nabla + \mathbf{A}\right)^2\psi - \psi + |\psi|^2\psi = 0, \tag{2.5}$$

$$\eta_2\left(\frac{\partial\mathbf{A}}{\partial t} + \nabla\overline{\Phi}\right) + \mathbf{curl}\ \mathrm{curl}\ \mathbf{A} + \frac{i}{2\kappa}(\psi^*\nabla\psi - \psi\nabla\psi^*) + |\psi|^2\mathbf{A} = 0, \tag{2.6}$$

with boundary conditions

$$\left(\frac{i}{\kappa}\nabla\psi + \mathbf{A}\psi\right)\cdot\mathbf{n} = 0, \tag{2.7}$$

$$\mathrm{curl}\ \mathbf{A} = H, \tag{2.8}$$

$$\eta_2\left(\frac{\partial\mathbf{A}}{\partial t} + \nabla\overline{\Phi}\right)\cdot\mathbf{n} = \mathbf{J}_a\cdot\mathbf{n}, \tag{2.9}$$

where $\mathbf{J}_a$ is an applied current. The initial conditions are

$$\psi(\mathbf{x},0)=\psi_0(\mathbf{x}) \quad \text{and} \quad \mathbf{A}(\mathbf{x},0)=\mathbf{A}_0(\mathbf{x}) \quad \text{in } \Omega.$$

Note that we only focus on the interior problem for now and we assume that η_1 and η_2 are both positive real numbers (dynamics with complex valued η_1 have been studied[30]).

First, it is convenient to introduce an auxiliary variable $\Phi_a(\mathbf{x},t)=(\mathbf{J}_a\cdot\mathbf{x})/\eta_2$ and define $\Phi=\overline{\Phi}-\Phi_a$. The triple $(\psi,\mathbf{A},\Phi)$ is often used as the primary variables for the TDGL equations which are related to the energy functional by

$$\eta_1\left(\frac{\partial\psi}{\partial t}+i\kappa\overline{\Phi}\psi\right)=-\frac{\partial\mathcal{G}}{\partial\psi}(\psi,\mathbf{A}), \tag{2.10}$$

$$\eta_2\left(\frac{\partial\mathbf{A}}{\partial t}+\nabla\Phi\right)=-\frac{\partial\mathcal{G}}{\partial\mathbf{A}}(\psi,\mathbf{A}). \tag{2.11}$$

C. Gauge invariance

Both the GL and the TDGL equations enjoy the *gauge invariance* property, see Refs. 32 and 72 for more detailed discussions.

Numerical minimization of the free energy functional is made difficult due to the gauge invariance. However, a nice remedy has been developed to avoid such pitfalls.[43] Define

$$\mathcal{F}(\psi,\mathbf{A})=\mathcal{G}(\psi,\mathbf{A})+\int_\Omega |\text{div }\mathbf{A}|^2\,d\mathbf{x}. \tag{2.12}$$

By choosing proper gauge transformation, the following can be shown.

Theorem 2.1: *The following minimization problems are equivalent*:

$$\begin{array}{lll} \textbf{Min} & \mathcal{G}(\psi,\mathbf{A}) & \\ s.t. & \psi\in\mathcal{H}^1(\Omega), & \Leftrightarrow \\ & \mathbf{A}\in\mathbf{H}^1(\Omega) & \end{array} \quad \begin{array}{lll} \textbf{Min} & \mathcal{G}(\psi,\mathbf{A}) & \\ s.t. & \psi\in\mathcal{H}^1(\Omega), & \Leftrightarrow \\ & \mathbf{A}\in\mathbf{H}^1_n(\text{div},\Omega) & \end{array} \quad \begin{array}{lll} \textbf{Min} & \mathcal{F}(\psi,\mathbf{A}) & \\ s.t. & \psi\in\mathcal{H}^1(\Omega), & \\ & \mathbf{A}\in\mathbf{H}^1_n(\Omega). & \end{array}$$

where $\mathbf{H}^1_n(\Omega)$ *is a subspace of* $\mathbf{H}^1(\Omega)$ *with vanishing normal component on the boundary while* $\mathbf{H}^1_n(\text{div},\Omega)$ *is a subspace of divergence free vector valued functions in* $\mathbf{H}^1_n(\Omega)$.

With the equivalent formulation, one can simply enforce the Coulomb gauge implicitly by solving for the variational problems with respect to $\mathcal{F}$ in $\mathcal{H}^1(\Omega)\times\mathbf{H}^1_n(\Omega)$. The penalty term $\|\text{div }\mathbf{A}\|^2$ serves as a null Lagrangian which vanishes at the energy minimizer.

The TDGL equations (2.10) and (2.11) may be viewed as the gauge invariant gradient flow of the free energy. By examining the various choices of the gauge, the well posedness of the system was first reported in 1992 at the first world congress of nonlinear analysts.[33,32] Sharper results based on some better energy estimates and the long time solution behavior have later been studied, for instance, in Refs. 72, 90, and 56.

III. NUMERICAL APPROXIMATIONS

Due to the complexity stemming from the full nonlinearity of the GL models, analytical studies have been limited to special cases. Numerical approximations, on the other hand, have provided researchers useful tools to understand the models and to simulate the physical properties of the superconductors. The systematic study of the GL models from the numerical analysis point of view was first made in Ref. 43. Later, many works on the numerical approximations of Ginzburg–Landau type models and their rigorous theoretical analysis have appeared. Here, we briefly discuss the finite difference,[3,21,26,29,35,55,57,59,61] finite element,[4,17,20,18,40,43–45,62,93,95] and finite volume methods[46–48] for spatial discretizations. We also discuss various time-stepping schemes for time-dependent models[31,79,80] and some parallel and adaptive algorithms.

A. Finite element approximations

The basic theory of conforming finite element approximations for the steady state GL equations in a bounded domain has been presented in Ref. 43. Let us choose a pair of conforming finite element spaces $\mathcal{V}_k^h \times \mathbf{V}_k^h \subset \mathcal{H}^1(\Omega) \times \mathbf{H}_n^1(\Omega)$ where h being a mesh parameter, and assume that they satisfy the approximation properties

$$\inf_{g^h \in \mathcal{V}_k^h} \|\psi - g^h\|_1 \leqslant ch^r \|\psi\|_{r+1},$$

$$\inf_{\mathbf{B^h} \in \mathbf{V_k^h}} \|\mathbf{A} - \mathbf{B^h}\|_1 \leqslant \mathbf{ch^r} \|\mathbf{A}\|_{\mathbf{r+1}}$$

for functions ψ and $\mathbf{A}$ of sufficient regularity.

Then, the discrete Galerkin finite element approximation can be formulated as follows:[43]

$$\mathbf{Min}\ \mathcal{F}(\psi^h, \mathbf{A}^h),$$

$$\text{s.t.}\ (\psi^h, \mathbf{A}^h) \in \mathcal{V}_k^h \times \mathbf{V}_k^h.$$

It has been shown that the above problems generate a sequence of convergent approximate solutions as $h \to 0$ under the minimal regularity condition. Moreover, optimal order of error estimates of the following type have been derived for nonsingular solution branches:

$$\|\psi - \psi^h\|_1 + \|\mathbf{A} - \mathbf{A}^h\|_1 \leqslant ch^k \{\|\psi\|_{k+1} + \|\mathbf{A}\|_{k+1}\}.$$

It is worthwhile to note that no inf-sup condition is required for the finite element spaces. The gauge condition is not strictly imposed for finite mesh parameter h, but it is shown to be valid in the limit as $h \to 0$.

The finite element methods have later been generalized to other related models, such as the d-wave GL equations,[93] optimal control of GL models[60] and the Lawrence-Doniach models for layered superconductors.[41,62] In Refs. 44 and 45, various numerical simulations have been conducted based on the finite element approximations.

The application of finite element method to TDGL has been considered in Ref. 31. Besides the basic convergence results for semidiscrete scheme, both first order and second in time discretization schemes have also been presented. Let Δt_n be the step size and $(\psi_n^h, \mathbf{A}_n^h)$ the numerical solution at time t_n. When the applied current is absent, the first order backward Euler scheme can be given a variational form, find $(\psi_{n+1}^h, \mathbf{A}_{n+1}^h)$ such that it solves the problem

$$\mathbf{Min}\ \mathcal{G}_{\Delta t_n}(\psi, \mathbf{A}) = \mathcal{G}(\psi, \mathbf{A}) + \frac{1}{\Delta t_n} \int_\Omega [\eta_1 |\psi - \psi_n^h|^2 + \eta_2 |\mathbf{A} - \mathbf{A}_n^h|^2] \mathrm{d}\Omega.$$

It turns out that a second order in time scheme can also be similarly formulated, first find $(\psi_*^h, \mathbf{A}_*^h)$ that minimizes

$$\mathcal{G}(\psi, \mathbf{A}) + \frac{1}{2\Delta t_n} \int_\Omega [\eta_1 |\psi - \psi_n^h|^2 + \eta_2 |\mathbf{A} - \mathbf{A}_n^h|^2] \mathrm{d}\Omega,$$

then we let $(\psi_{n+1}^h, \mathbf{A}_{n+1}^h) = 2(\psi_*^h, \mathbf{A}_*^h) - (\psi_n^h, \mathbf{A}_n^h)$. We note that the derivation of error estimates of the fully discrete scheme was, however, not rigorously provided there. By using a mixed formulation, Ref. 17 has presented a more complete theory for the approximation of the TDGL along with optimal order error estimates in two space dimension. Later, Ref. 20 considered approximations to a related optimal control problem. Generalizations to the time-dependent Lawrence-Doniach model have been presented in Ref. 62.

B. Finite difference approximations

Same as in the approximations of many other physical problems, the finite difference approximations of the GL models have been the most widely used approach. Though conventional difference schemes have been studied in Refs. 55 and 67, much of the focus has been on the gauge invariant difference approximation. The motivation has come from the fact that the underlying physical model enjoys the gauge invariance property. In Ref. 3, a gauge invariant finite difference scheme was proposed for the steady-state GL equations on a uniform rectangular grid, in the spirit of discrete gauge field theory. Many subsequent works have followed up on such an approach via an introduction of the so-called link and bond variables, and various extensions have also been made.[21,22,55,57,59,61,66,68] For the approximation of the magnetic vector potential, such an approach is naturally related to the idea of staggered grid (marker-and-cell) used in computational electromagnetics and fluid dynamics.

For simplicity, let us consider the two-dimensional setting with a uniform rectangular mesh of grid size h. Following the notation in Ref. 35, the discrete gauge invariant energy functional is given by

$$\mathcal{G}^h(\vec{\psi},\vec{A}) = \frac{1}{2}\sum_{jk}\frac{1}{\kappa^2}|\psi_k \exp(-i\kappa a_{jk}h) - \psi_j|^2 + \sum_j \frac{h^2}{4}(1-|\psi_j|^2)^2 + \frac{1}{2}\sum_{jklm}(a_{jk}+a_{kl}+a_{lm}+a_{mj}-Hh)^2, \tag{3.1}$$

where the first sum is over all neighboring edges, the second over all vertices and the third over all square cells. $\vec{\psi}=\{\psi_j\}$ are the approximations of the order parameter at the cell vertices and $\vec{A}=\{a_{jk}\}$ are the approximations of the signed tangential component of the magnetic vector potential at the midpoint of the cell edges.

The gauge invariant backward Euler scheme is given by[35]

$$\eta_1\frac{\psi_j^n - \psi_j^{n-1}\exp(-i\kappa\overline{\Phi}_j^n\Delta t)}{\Delta t} = -\frac{1}{h^2}\frac{\partial \mathcal{G}^h}{\partial \psi_j^n}(\vec{\psi}^n,\vec{A}^n)$$

and

$$\eta_2\left(\frac{a_{jk}^n - a_{jk}^{n-1}}{\Delta t} + \frac{\Phi_k^n - \Phi_j^n}{h}\right) = -\frac{1}{h^2}\frac{\partial \mathcal{G}^h}{\partial a_{jk}^n}(\vec{\psi}^n,\vec{A}^n)$$

for $n=1,2,\ldots,N=T/\Delta t$. Here, $\{\overline{\Phi}_j^n\}$ are the approximations of the scalar electric potential. Note that the equations at the nodes on the boundary may require slight modifications. A complete and rigorous analysis for such a discretization has been provided in Ref. 35, including the proof of the discrete maximum principle, discrete energy law, and optimal order error estimates.

It remains to be seen if a higher order in time fully discrete gauge invariant scheme can be developed for the TDGL equations.

We note here also that, in practical numerical simulations, explicit or semi-implicit in time difference schemes have been mostly employed. In general, these schemes are only conditionally stable at best.

C. Finite volume approximations

As more and more attention is being paid to the study of the effect of the sample geometry and topology on the superconductivity phenomena, methods based on unstructured grids become more competitive in such cases. Besides the finite element methods we have discussed, finite volume methods have also been developed which have the combined advantage of being able to work with an unstructured grid while preserving the discrete gauge invariance.[48,46,47]

A standard extension to the staggered grid used in the gauge invariant difference approximation is the Voronoi-Delaunay pair. Given a set of distinct points $\{x_j\}_{j=1}^n \subset R^2$, we can define for each point $x_j, j=1,\ldots,n$, the corresponding Voronoi region $V_j, j=1,\ldots,n$, by

$$V_j = \{\mathbf{y} \in R^2 || x_j - y| < |x_k - y| \quad \text{for } 1 \leqslant k \leqslant n \quad \text{and} \quad k \neq j\}.$$

We refer to $\{V_j\}_{j=1}^n$ as the *Voronoi tessellation* corresponding to the generators $\{x_j\}_{j=1}^n$. The dual tessellation to a Voronoi tessellation consisting of triangles is referred to as a *Delaunay triangulation*. Given a discrete vector field $\vec{A}$ tangentially defined at the midpoints of the triangle edges of a Delaunay triangulation, it is easily seen that such vectors are normal to the edges of the Voronoi regions. Thus, discrete calculus can be defined for the curl operator on the Delaunay triangles and for the div operator on the Voronoi cells.

Then, the central idea for finding a suitable discretization of the GL energy functional is to construct a gauge invariant approximation to $|\nabla\psi - i\kappa\mathbf{A}\psi|$. It was noticed in Ref. 48 that one may first project the vector $v = \nabla\psi - i\kappa\mathbf{A}\psi$ into the tangential components along the triangle edges and obtain the following simple identity

$$|\tau_{ijk}||v|^2 = \sum \cot\,\theta_i |v \cdot (x_j - x_k)|^2,$$

where the sum is over all three edges and θ_i is the opposite angle. Notice that if we let θ_{i1} and θ_{i2} be the two opposing angles corresponding to the same edge $x_j x_k$, then

$$\cot\,\theta_{i1} + \cot\,\theta_{i2} = \frac{|\Gamma_{jk}|}{|x_j - x_k|},$$

where Γ_{jk} is the common edge between the two adjacent Voronoi regions V_{i1} and V_{i2}. Now, $|v \cdot (x_j - x_k)|$ can be approximated by $|\psi_k \exp(-i\kappa a_{jk}|x_j - x_k|) - \psi_j|$.

Thus, the Ginzburg–Landau functional is discretized as follows:[48]

$$\mathcal{F}^h(\vec{\psi}^h, \vec{A}^h) = \sum_{j=1}^n \frac{1}{4|V_j|}(1 - |\psi_j|^2)^2 + \sum_{j=1}^n \left\{ \sum_{k \in \chi_j} \frac{|\Gamma_{jk}|}{2\kappa^2 |x_j - x_k|} |\psi_k \exp(-i\kappa a_{jk}|x_j - x_k|) - \psi_j|^2 \right\}$$
$$+ \sum_{\tau_{jkl}} \frac{1}{2\tau_{jkl}}(a_{jk}h_{jk} + a_{kl}h_{kl} + a_{lj}h_{lj} - H\tau_{jkl})^2, \tag{3.2}$$

where for any j, the index set χ_j denotes the indices of all vertices which are adjacent to the vertex $\mathbf{x}_j$. The discrete gauge invariance is understood in the sense that

$$\mathcal{G}^h(\vec{\psi}^h, \vec{A}^h) = \mathcal{G}^h(T^h_\phi(\vec{\psi}^h, \vec{A}^h)),$$

where the transformation T^h is defined by the map

$$\psi_j \to \psi_j e^{i\kappa\phi_j}, \quad a_{jk} \to a_{jk} + \frac{\phi_k - \phi_j}{|x_j - x_k|},$$

corresponding to any scale field $\vec{\phi}^h$.

The gauge invariant difference approximation on a rectangular grid discussed earlier is in fact a special case of the above finite volume scheme. This can be seen by making the equivalence of the rectangular cells with the Voronoi cells and the equivalence of the dual cells with pairs of right Delaunay triangles sharing a common edge opposing the right angles.

Similar to the technique introduced in Ref. 43 and in the finite difference setting, a modified functional can be defined to enforce the gauge choice implicitly. Let us define

$$\mathcal{F}^h(\vec{\psi}^h, \vec{A}^h) = \mathcal{G}^h(\vec{\psi}^h, \vec{A}^h) + \sum_j \frac{1}{|V_j|}\left(\sum_{k \in \chi_j} a_{kj}|\Gamma_{kj}| \right)^2.$$

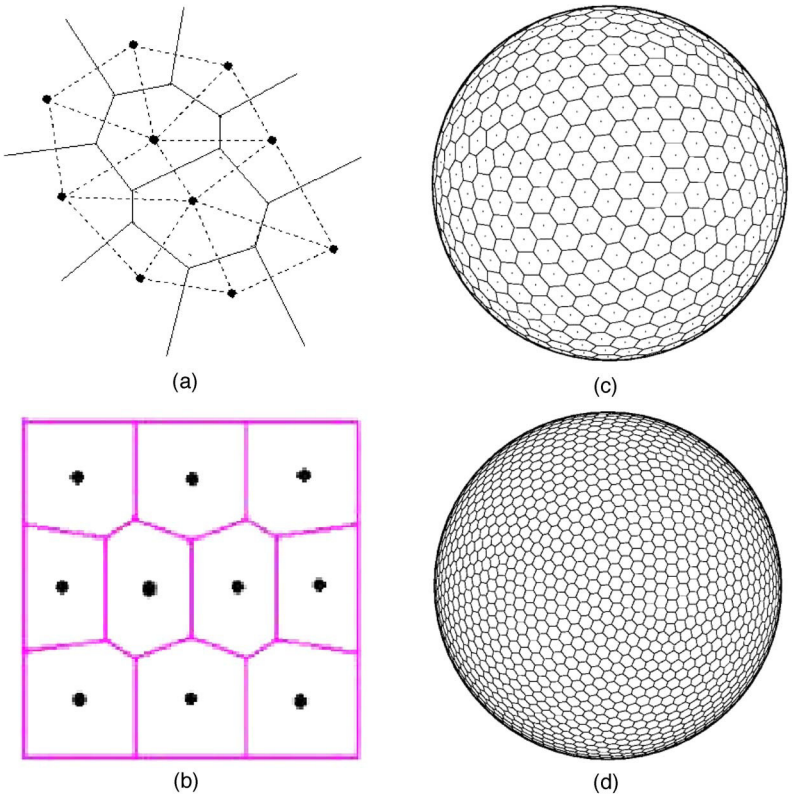

FIG. 1. (Color online) A planar Voronoi-Delaunay pair, a CVT in a square and two SCVTs of different resolution.

Then, it is easy to show that the minimizer of $\mathcal{F}^h$ is also a minimizer of $\mathcal{G}^h$ and it is also divergence free in the discrete sense:

$$\sum_{k\in\chi_j} a_{kj}|\Gamma_{kj}| = 0, \quad \forall\, j.$$

Moreover, it has been shown that the minimizer of $\mathcal{F}^h$ satisfies the discrete maximum principle, $|\psi_j| \leqslant 1$ for all j. This, coupled with suitable energy estimates, leads to the convergence of the discrete approximations as the mesh size goes to zero.[48]

In Refs. 46 and 47, such finite volume scheme was extended to solve a reduced set of TDGL models defined on a thin spherical shell. In addition to the basic convergence properties, a feature of the discussions in Refs. 46 and 47 is the consideration of a special Voronoi-Delaunay pair, namely, the spherical centroidal Voronoi tessellations and the corresponding Delaunay triangulations,[42] see Fig 1. The SCVTs are natural extensions of the centroidal Voronoi tessellations in Euclidean spaces.[39] It has been shown that by using the SCVTs, the discrete approximations exhibit a higher order convergence comparing with the conventional Voronoi-Delaunay pair.

Detailed numerical simulations have also been performed in Refs. 46 and 47 using the SCVT based gauge invariant finite volume scheme. Both static vortex configurations and vortex dynamics under applied current have been studied.

D. Artificial boundary conditions

For a full three-dimensional simulation of the GL model, taking into account the effect of the induced magnetic field of the superconducting sample on the field exterior to the sample, the numerical solution of the Ginzburg–Landau equations in the superconducting sample needs to be solved in conjunction with the solution of the Maxwell equations in the exterior.

To overcome the unboundedness of the exterior domain, approximations must be introduced or alternative formulations must be considered. The crudest but often very effective approximation is simply to ignore the effect in the exterior completely. Such approximations are particularly valid for high-kappa materials (in such cases, some reduced GL models have been proposed and used in numerical simulations of vortex lines.[15,25,40]

As an alternative, a rigorous theory based on artificial boundary conditions has been presented in Ref. 51 to transform the computation domain to a finite ball enclosing the superconducting sample.

The key step is to note that the magnetic energy $\|\mathrm{curl}\,\mathbf{A}\|^2_{L^2(R^3)}$, coupled with the null-Lagrangian term $\|\mathrm{div}\,\mathbf{A}\|^2_{L^2(R^3)}$ used to enforce the Coulomb gauge, is equivalent to $\|\nabla\mathbf{A}\|^2_{L^2(R^3)}$ which can be decomposed as $\|\nabla\mathbf{A}\|^2_{L^2(B_r)}+\|\nabla\mathbf{A}\|^2_{L^2(B_r^e)}$. Here B_r denotes a ball of radius r and $B_r^e = R^3\backslash B_r$ denotes its exterior.

For $\mathbf{A}$'s that are harmonic in B_r^e, we have

$$\|\nabla\mathbf{A}\|^2_{B_r^e} = \int_{S_r} \mathbf{A}\frac{\partial\mathbf{A}}{\partial\mathbf{n}}\mathrm{d}S = \int_{S_r} \mathbf{A}J(\mathbf{A})\mathrm{d}S,$$

where S_r denotes the sphere of radius r, J is the Stekelov-Poincaré operator (or the Dirichlet to Neumann map). Since J can be explicitly expressed with the help of Legendre functions, various orders of approximations can be constructed.

Briefly, let the Legendre polynomial and Legendre function be given by

$$P_n^0(t) = P_n(t) = \frac{1}{2^n n!}\frac{d^n(t^2-1)^n}{\mathrm{d}t^n}, \quad P_n^m(t) = (1-t^2)^{m/2}\frac{d^m}{\mathrm{d}t^m}P_n(t),$$

and let

$$G(\gamma) = -\frac{1}{4\pi R^3} - \sum_{n=1}^{\infty}\frac{(n+1)(2n+1)}{4\pi R^3}P_n(\cos\,\gamma),$$

for γ defined by $\cos\,\gamma = \cos\,\theta\cos\,\theta' + \sin\,\theta\sin\,\theta'\cos(\varphi-\varphi')$ for a pair of points $x=(r,\theta,\varphi)$ and $y=(r,\theta',\varphi')$. Then, with $\mathbf{A}_0$ satisfying $\mathrm{curl}\,\mathbf{A}_0 = H$, we have the following equivalent form of the energy functional[51]

$$\mathcal{F}(\psi,\mathbf{A}) = \int_\Omega \frac{1}{4}(1-|\psi|^2)^2\,\mathrm{d}\Omega + \frac{1}{2}\int_\Omega \left|\left(\frac{i}{\kappa}\nabla + \mathbf{A} + \mathbf{A}_0\right)\psi\right|^2\mathrm{d}\Omega + \frac{1}{2}\int_{B_r}|\nabla\mathbf{A}|^2\,\mathrm{d}x$$
$$+ \int_{S_r}\int_{S_r}\mathbf{A}(x)\cdot G(\gamma)I\cdot\mathbf{A}(y)\mathrm{d}x\,\mathrm{d}y.$$

In a nut-shell, the exterior energy is now effectively transformed into an energy defined on the boundary of the ball.

Various approximations of the boundary energy can be made, for instance, using a finite element discretization in the interior of B_r, the following discrete problem has been considered in Ref. 51:

$$\mathcal{F}(\psi^h,\mathbf{A}^h) = \frac{1}{2}\int_\Omega \left|\left(\frac{i}{\kappa}\nabla + \mathbf{A}^h + \mathbf{A}_0\right)\psi^h\right|^2\mathrm{d}\Omega + \int_\Omega \frac{1}{4}(1-|\psi^h|^2)^2\,\mathrm{d}\Omega + \frac{1}{2}\int_{B_r}|\nabla\mathbf{A}^h|^2\,\mathrm{d}x$$
$$+ \sum_{n=1}^{N}\frac{(n+1)(2n+1)}{4\pi r^3}\int_{S_r}\int_{S_r}\mathbf{A}^h(x)P_n(\cos\,\gamma)\mathbf{A}^h(y)\mathrm{d}x\,\mathrm{d}y.$$

Let $r_1=\mathrm{diam}(\Omega)$, under the approximation assumptions on the finite element spaces made earlier, the following has been proved.

Theorem 3.1: *For a smooth exact solution on a nonsingular solution branch, the approximate solutions satisfy the following error estimates: for h small and* $r>r_1$,

$$\|\psi-\psi^h\|_{1,\Omega}+\|\mathbf{A}-\mathbf{A}^h\|_{1,B_r}\leqslant c_1h^k(\|\psi\|_{k+1,\Omega}+\|\mathbf{A}\|_{k+1,B_r})+c_2(\Omega,r)(r_1/r)^N\|\mathbf{A}\|_{1,B_r},$$

for some constants c_1 *and* $c_2=c_2(\Omega,r)$ *independent of h and N.*

It has been seen in numerical computation that in practice with $N=6$, it is sufficient to choose the computational domain with r no more than twice the diameter of Ω in order to obtain good accuracy of the approximation in the exterior domain.[51]

E. More on time discretization

For TDGL models, while most of the rigorous mathematical analysis have been focused on the fully implicit in time discretizations, explicit marching schemes and semi-implicit marching schemes[94] have also been frequently used in numerical simulations due to their simplicity in implementation.

Theoretically, to make the time-marching more efficient, other useful ideas have also been considered in the literature. For example, a linearized crank-Nicolson scheme has been considered in Ref. 79, similar to the semi-implicit approach. Analytical studies of an alternating marching scheme have also been made in Ref. 80 where for the order parameter and magnetic potential are solved in alternating steps and thus reducing the size of the implicit nonlinear system by half.

To effectively solve the nonlinear and linear systems employed in the implicit schemes, constructions of suitable preconditioners can be very helpful. In this regard, the Sobolev gradient methods studied in Refs. 82 and 83 fit into such a framework. Essentially, the gradient flows in the H^{-1} space considered there are equivalent to employing the inverse of Laplace operator Δ^{-1} as the preconditioner for the standard gradient flow in the L^2 space.

For high values of κ, the Ginzburg–Landau parameter, the original GL models can often be simplified. A particular simplification corresponding to high applied magnetic field has been considered in Refs. 15 and 40. The reduced equations are very much similar to the so-called Gross-Pitaevskii equations used to model the BEC superfluid.[5] In Ref. 9, a class of efficient splitting schemes for computing the ground state solutions of the BEC condensate based on the normalized gradient flow has been studied which may be readily applied to the solution of the reduced GL models.

F. Multilevel, adaptive and parallel algorithms

The numerical simulations of the vortex state in type-II superconductors based on the GL models become computationally challenging when there is a need to resolve a large number of vortices. More efficient implementations of the numerical schemes thus become necessary. There have been a lot of interesting attempts made along this direction. For example, multilevel finite element methods have been analyzed in Ref. 63 for a *d*-wave GL model, following earlier works of Refs. 36 and 93. Posterior error estimates and adaptive finite element methods have been studied in Refs. 18 and 64 with both rigorous analysis and numerical examples.

Parallelization is naturally another important avenue for greater computational efficiency. In Ref. 59, parallelized MPI-based implementation of the explicit finite difference discretization schemes has been presented along with many large scale simulations. Using a natural domain decomposition strategy, a number of parallel algorithms for the simulation of layered superconductors based on the Lawrence Doniach model have been studied in Ref. 41. The implementation has been made first using PVM, with an MPI version developed subsequently. Numerical results indicated significant speed-ups and good scalability. Moreover, interesting numerical simulations of three-dimensional vortex tubes, their dynamics and pinning effect have been made there as well.

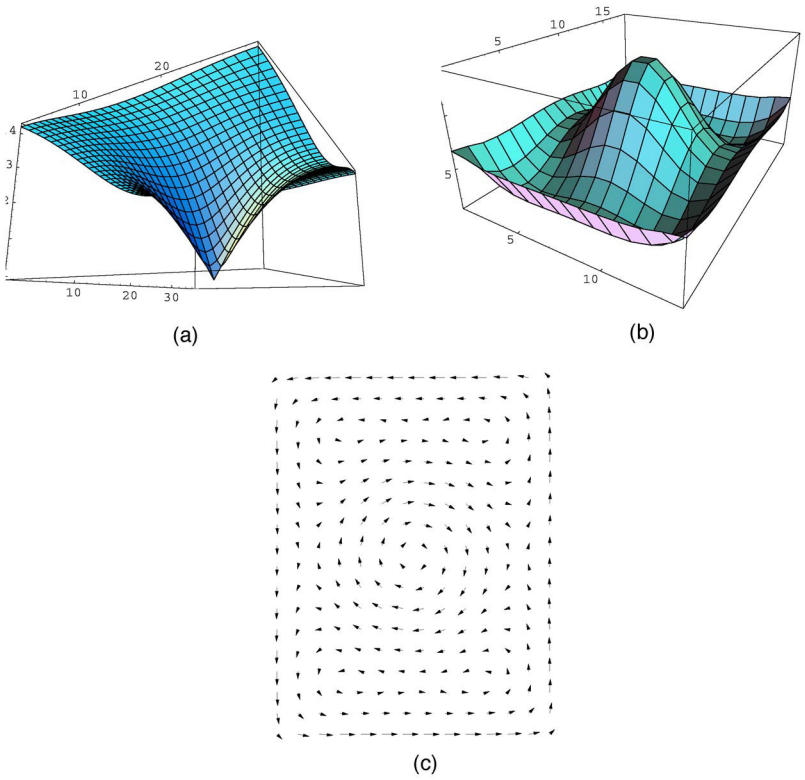

FIG. 2. (Color online) Magnitude of the order parameter, induced field and supercurrent in a 2D rectangular domain.

IV. NUMERICAL SIMULATIONS AND OTHER COMPUTATIONAL ISSUES

We now briefly describe some results of numerical simulations conducted throughout the last decade. These are based on either the finite element codes or the finite volume codes discussed earlier. We refer to Refs. 4, 23–25, 38, 46, and 47 for additional simulations.

A. Vortex solutions

A well-known feature of superconductivity is the phenomena of quantized vortices. For type-II superconductors, the study of Abrikosov on the vortex lattices based on the GL models has become a seminal work that exhibits the great predictive power of the GL theory.

In Fig. 2, we present a few typical plots for the numerical solutions of the steady state GL equations which include a surface plot of the magnitude of the order parameter, a surface plot of the induced magnetic field given by curl **A** and a vector plot of the superconducting current. The solution corresponds to one with a single vortex at the center of a rectangular superconducting sample.[4]

More systematic analysis and simulations of the phase transitions, vortex nucleation, and critical fields can be found in, for instance, Refs. 4, 7, 8, 11, 12, 65, 72, 85, 89, and 88, and the references cited therein.

B. Pinning of vortices in superconducting sample

One of the more intriguing features of superconductivity is the effect of vortex pinning which preserves the superconducting properties in a superconductor despite the penetration of the applied magnetic field.

The GL models have been used to study the pinning effect from many different angles, for instance, pinning due to variable thickness in thin films,[13,27,28,72] spatial inhomogeneities and

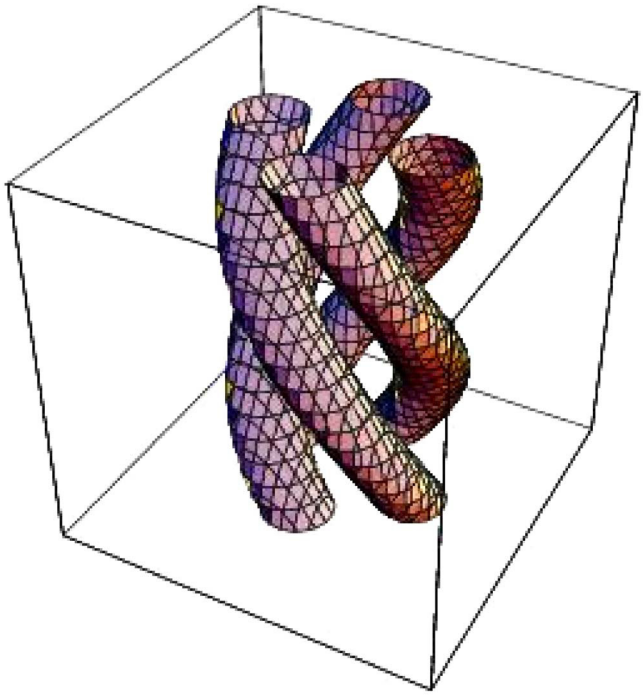

FIG. 3. (Color online) Isosurface plot of vortex tubes pinned in a 3D sample.

normal inclusions and anisotropy.[14,25,49,50] In Fig. 3, three-dimensional vortex tubes pinned by normal inclusions are shown which were computed via the Lawrence-Doniach variant of the GL model in Ref. 41. Due to the collective pinning force, the vortex tubes are no longer strictly aligned in the direction of the applied magnetic field.

C. Vortex state in a thin superconducting spherical shell

The geometry of spherical shell is not only used in superconductivity applications, but also provides an ideal setting for one to examine the vortex state.

With increasing values of the applied magnetic field, some of the energy minimizing superconducting and vortex solutions are given in Fig. 4. We refer to Ref. 46 for more detailed descriptions of the corresponding parameter values.

In Fig. 5, minimum energy values $\mathcal{G}(H)$ corresponding to different external magnetic field strengths H are plotted, along with the magnetization curve given by the derivatives of minimum energy $\mathcal{G}(H)$.

The spatially homogeneous applied magnetic field naturally produces vortices of opposite signs on the two hemispherical shells, thus providing a window for us to see the details of vortex nucleation and vortex annihilation (see Ref. 10 for some analysis in a simpler setting). In Fig. 6, with the applied magnetic field aligned along the poles, the density plots of order parameter show that a pair of vortices of opposite signs first nucleate near the equator, then later split and move into the interior of the hemispheres.[46]

Other simulations on vortex annihilation can be found in Ref. 40 in the planar domain, aided by an applied current.

D. Vortex motion driven by an applied current

An applied current J generally exerts a Lorentz force $F=J\times B$ on each vortex core such that the motion of vortices would induce an electric field, and thus produces electrical resistance. Thus,

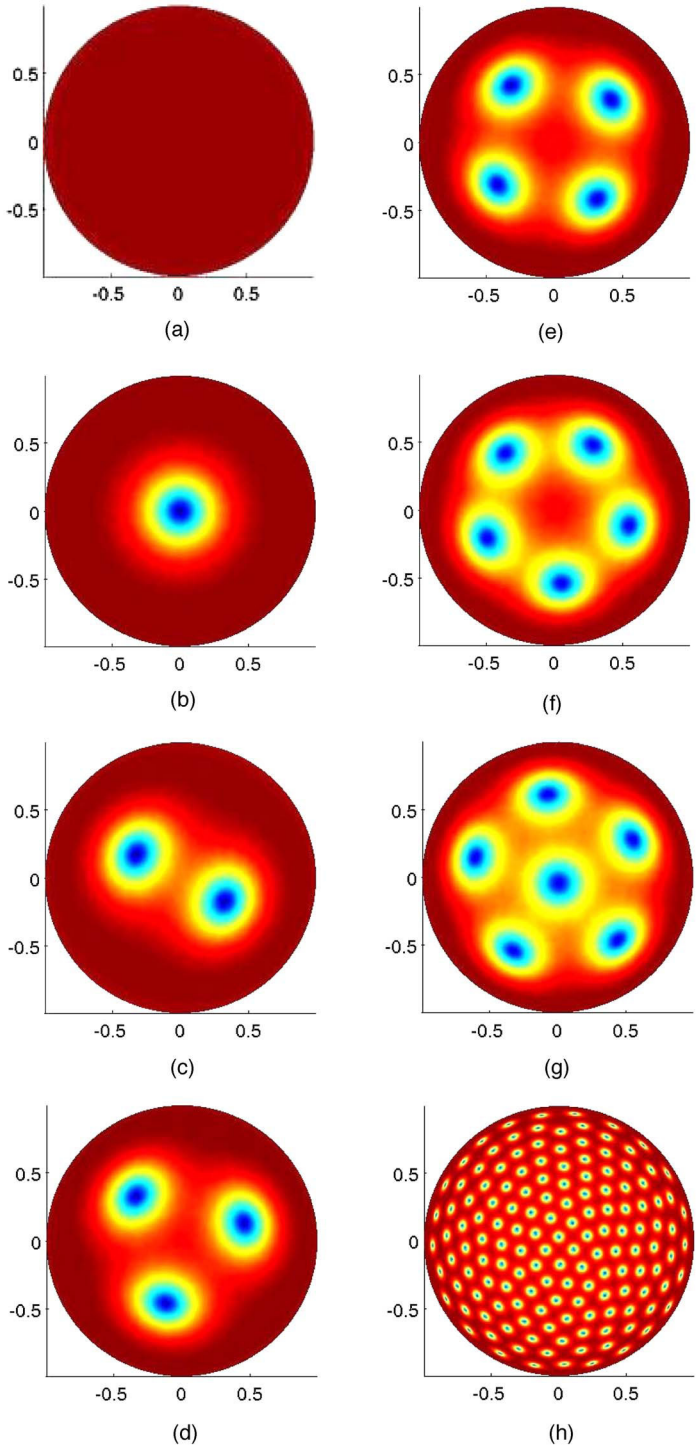

FIG. 4. (Color online) Energy minimizing vortex configurations on the upper hemisphere.

in superconductivity, it is important to understand the interaction of the vortices with the applied current and study the critical values of the applied current which will dislodge the vortices from their equilibrium positions.

In Fig. 7, contour plots of the order parameter are given, corresponding to solution of the

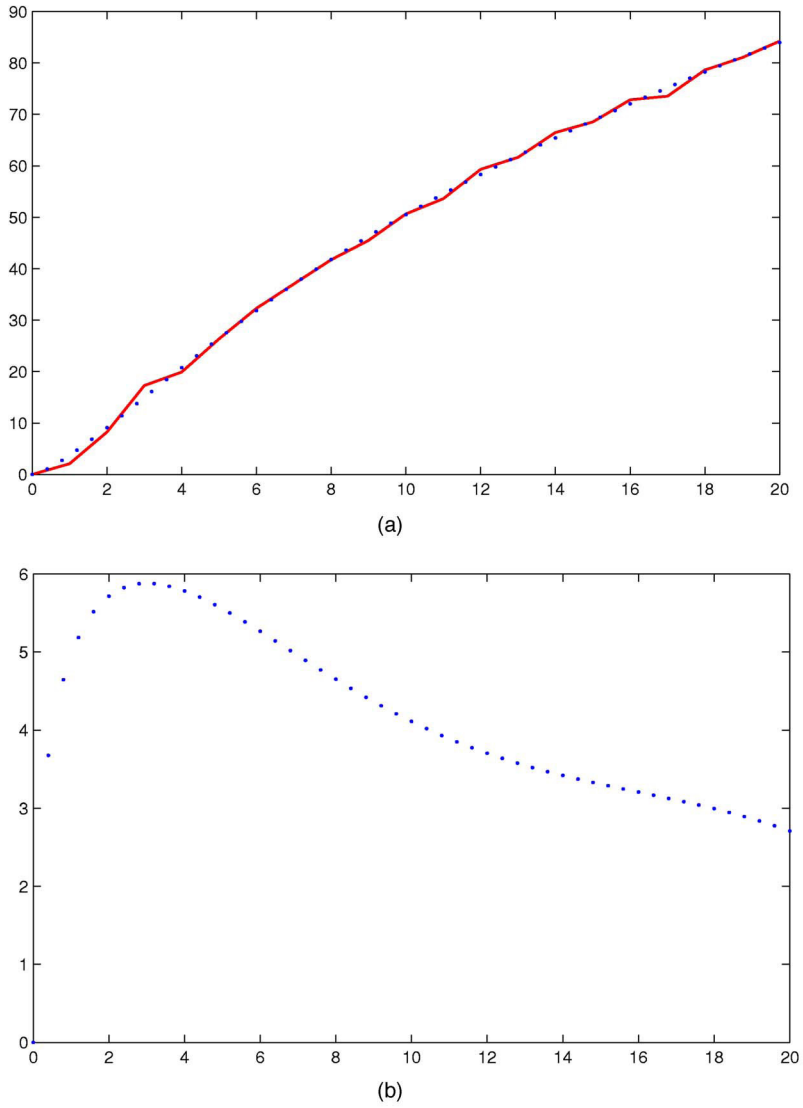

FIG. 5. (Color online) Minimum energy values with its polynomial fitting and the magnetization curve.

TDGL in a two-dimensional square with a constant applied current imposed along the vertical direction. A single vortex starts to move from the left to the right due to the Lorentz force.

E. Effect of thermal fluctuation

The effect of thermal fluctuations play a central role on the pinning of vortices in type-II superconductors. In Refs. 23 and 24, such effects have been examined through stochastic variants of a time-dependent Ginzburg–Landau model valid for high values of the Ginzburg–Landau parameter. Both additive and multiplicative noise variants have been considered. Many numerical computations have been presented that illustrate the effects that noise has on the dynamics of vortex nucleation and vortex motion. In Fig. 8, isosurface plots of vortex tubes are presented corresponding to different values of variance of the additive noise term using for the simulation of Langevin dynamics. The snapshots are taken at the same time instant and the vortex lattice melting effect can be observed in the process.

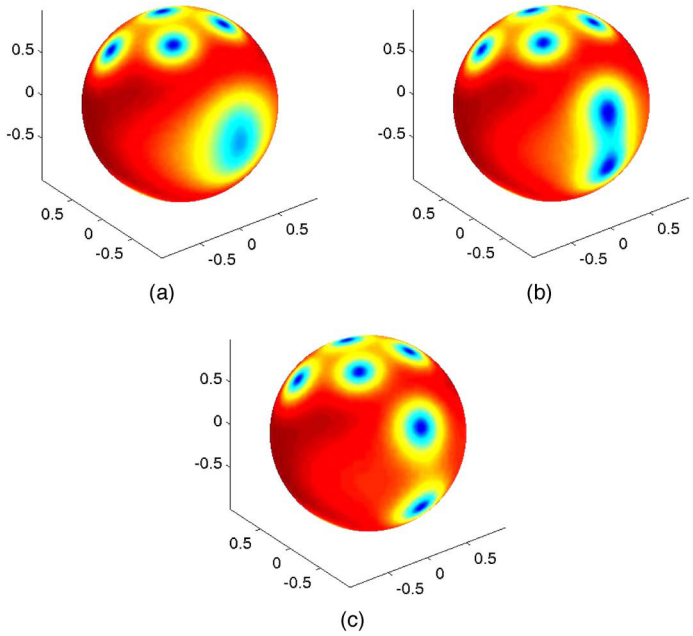

FIG. 6. (Color online) The nucleation and the splitting of vortex pairs near the equator.

F. Variants of Ginzburg–Landau models

The great success of the Ginzburg–Landau models for low T_c superconductivity generated tremendous interests in extending them to other settings including layered materials and high T_c superconductors. For example, in Ref. 36, simulations of a d-wave GL model have been carried out, the vortex solutions there typically display a fourfold symmetry. In certain parameter regimes, the basic stability properties of single and multiple vortices deviated significantly from the single component counterpart, see Fig. 9 for an illustration of a stable double vortex profile.

More analytical and numerical studies of d-wave GL models can be found in Refs. 73, 86, and 93. Numerical studies of other extensions of the GL models have also been performed, for instance, see Ref. 6 for simulations based on the SO(5) model.

Related to the vortex state in superconductors, the 1995 experimental confirmation of Bose-Einstein condensation (BEC) in alkali-metal gases provides another avenue to study the phenomena of quantized vortices. In recent BEC experiments, vortices have been nucleated with the help of laser stirring and rotating magnetic traps. Remarkably, many of the phenomenological properties of quantized vortices have been well captured by mathematical models such as the Gross-Pitaevskii (GP) equations. In the case of rotating magnetic traps, the mathematical form of the GP

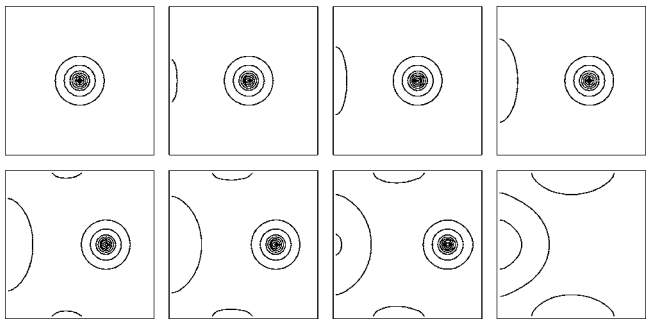

FIG. 7. Motion of vortices in the presence of an applied current.

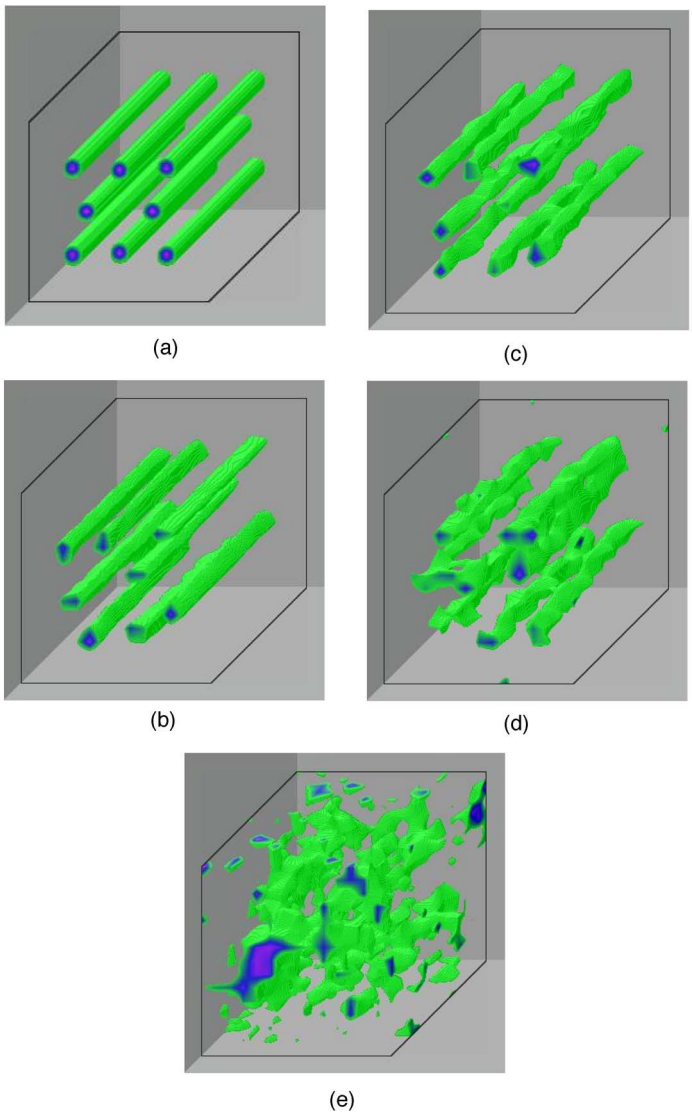

FIG. 8. (Color online) Snapshots of the vortex tubes in a cubic sample with increasing additive noises.

equations have close resemblance with the high-kappa Ginzburg–Landau (GL) model.[40] Utilizing the mathematical theory and the numerical codes developed for the GL,[5] presented a similar mathematical framework for rigorously characterizing the critical velocities for the vortex nucleation in a BEC cloud subject to a rotating magnetic trap. A class of splitting schemes for com-

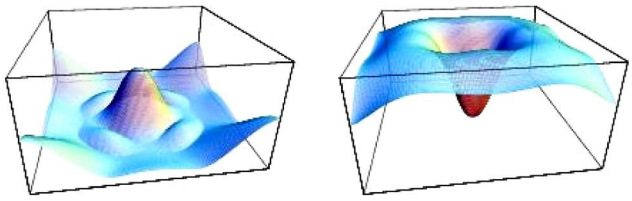

FIG. 9. (Color online) Surface plots of the s and d wave density for a double vortex profile in a GL $s+d$ model.

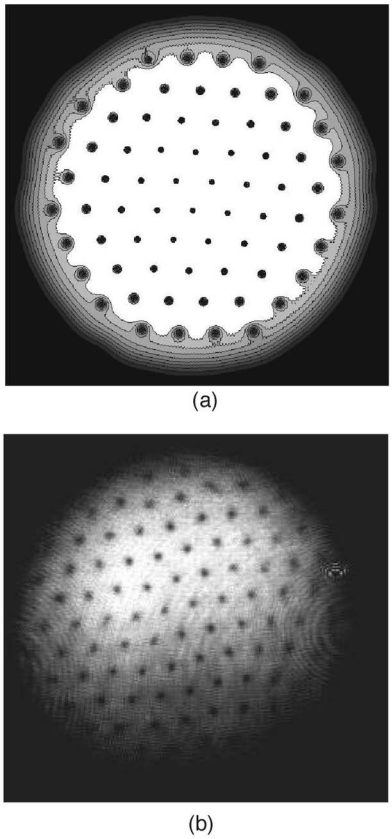

FIG. 10. Vortices in BEC: our numerical simulation (left) vs the MIT experiment (right) (Ref. 1).

puting the ground state solutions of the BEC condensate based on the normalized gradient flow has also been presented.[9] In Fig. 10, we provide a particular comparison of experimental pictures and the result of numerical simulations of the vortex solution with parameters taken from the experimental values based on the code developed in Ref. 5.

G. Computational challenges

The interests of the vortex state not only lie in the study of the vortex structures for a few isolated vortices, but also in the study of the collective effect of a large number of vortices and vortex lattices and their interactions with material structure and defects as well as the impact of sample topology and geometry. Simulations of GL models have been performed recently on structures like buckyballs and for MgB2 thin films. (See Fig. 11.)

In practice, numerical simulations of exceedingly large numbers of vortices based on the GL models remain computationally challenging, partly due to the intriguing properties associated with the vortex quantization effect. More specifically, for a square sample with n vortices in the interior, the phase angle of the complex order parameter will endure a change of $2n\pi$ around the boundary of the sample. If m points are needed to resolve a single period of phase winding, then $mn/4$ points will roughly be needed on each edge of the square. Thus, a uniform mesh will require up to $m^2n^2/16$ grid points. For large n and even moderate values of m, this can become very demanding computationally even for two-dimensional problems, not to mention the more challenging three-dimensional cases.

Naturally, adaptive schemes may save the computational cost significant, but with densely packed vortices, refinement may be required almost everywhere, and their efficiency are thus reduced. In particular, we note that it is not sufficient to only refine near the vortex cores as the

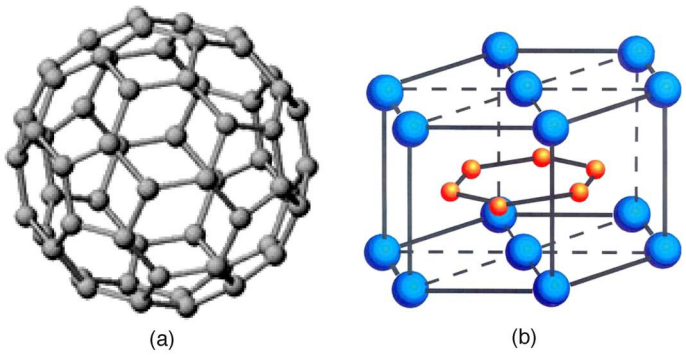

FIG. 11. (Color online) A buckyball and the atomic structure of MgB2.

correct resolution of the highly oscillatory phase change is also very important, see Fig. 12 for an interesting illustration on how the real and imaginary parts of the order parameter behave in comparison with the magnitude for a solution with 22 pairs of vortices in a spherical shell simulation.[47] Resolving the highly oscillatory phase for the Ginzburg–Landau simulation is a challenge that can be compared with resolving the solution of the Hemholtz equation with high frequency. In addition, it is easy to see that the variation in the phase variable starts to become increasingly dramatic when getting closer to the boundary (equator). How to effectively tackle such solution behavior remains to be investigated.

On the other hand, for high-T_c superconductors, codes for mezoscale GL models cannot hope to be of direct use in the design of devices due to the presence of a large number of vortices. Whenever computational or analytical results are used in such an environment, they are based on simple homogenized or macroscopic models.

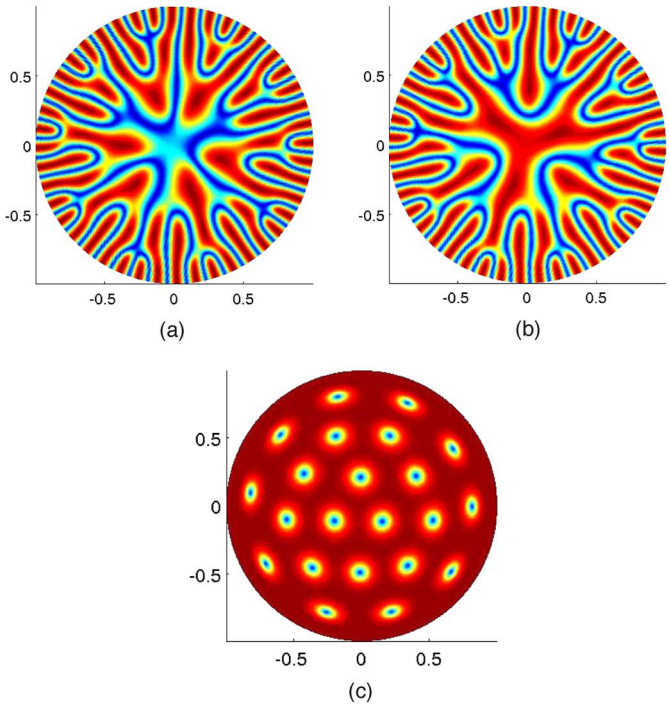

FIG. 12. (Color online) The absolute value of the real (left) and imaginary (center) parts of ψ and the magnitude $|\psi|$.

Recently, mean field models have been derived to describe the vortex state using a vortex density ω. These models are closely related to the GL models as one normally first derives a discrete set of motion laws for individual vortices based on the GL dynamics and a vortex density model is then derived when the number of vortices becomes large.[16,53,71,81,87] Let u denote the averaged magnetic field, a simplest two-dimensional version of such a model is given by

$$u - \lambda^2 \Delta u = \omega \quad \text{in } \Omega \times (0,T),$$

$$\omega_t - \nabla \cdot (\omega \nabla u) = 0 \quad \text{in } \Omega \times (0,T),$$

with suitable initial and boundary conditions. There have been a lot of studies made both from analytical and computational aspects[19,37,38,52,54,74] in recent years. It is perceivable that more efficient simulation schemes on the vortex state can be developed with a multiscale approach that combines GL model or vortex dynamic laws and the mean field models together. (Also see Refs. 34, 70, 75–77, 84, and 92.)

V. CONCLUSION

Superconductivity is one of the grand challenges identified as being crucial to future economic prosperity and scientific leadership. In this paper, various methods for the numerical approximations of the Ginzburg–Landau models of superconductivity are discussed, with an emphasis on the application to the study of vortex dynamics.

From a practical point of view, large-scale numerical simulations of the magnetic vortices complement physical experiments due to the complex three-dimensional, time-dependent, stochastic and multiscale nature of the phenomena. Thus, the development and analysis of efficient and reliable numerical algorithms remain important tasks. These algorithms and codes may ultimately prove to be useful to physicists and engineers in their study of superconducting phenomena and other related problems such as the BEC superfluidity.

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Topologically driven local minimizers of the Oseen-Frank energy

Yun-hui Kim,[a] Jacob Rubinstein,[b] and Peter Sternberg[c]
Department of Mathematics, Indiana University, Bloomington, Indiana 47405

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The analogy between certain liquid crystals and superconductivity has been recognized and explored by a number of scientists. In particular, mathematical techniques first developed within the Ginzburg–Landau theory of superconductivity have proven useful when adapted to the setting of liquid crystals. Here we pursue nontrivial stable liquid crystal configurations, motivated by an approach used by the authors in the setting of Ginzburg–Landau to produce persistent currents in topologically nontrivial domains. Our starting point is the Oseen-Frank energy for a nematic, but we add to the standard model a term that penalizes deviation of the director from a given plane. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The analogy between certain liquid crystals and superconductivity has been recognized and explored by a number of scientists. In particular, mathematical techniques first developed within the Ginzburg–Landau theory of superconductivity have proved useful when adapted to the setting of liquid crystals (see e.g., Ref. 1). Here we pursue nontrivial stable liquid crystal configurations, motivated by the approach in the paper[2] where the authors use the Ginzburg–Landau model to produce persistent currents in topologically nontrivial domains. Our starting point is the Oseen-Frank energy for a nematic.[3,4] We add to the standard model a term that penalizes deviation of the director from a given plane. Therefore, the energy takes the form

$$F_\alpha(\mathbf{n}) = \int_\Omega \{k_1|\mathrm{div}\ \mathbf{n}|^2 + k_2|\mathbf{n}\cdot\mathrm{curl}\ \mathbf{n}|^2 + k_3|\mathbf{n}\times\mathrm{curl}\ \mathbf{n}|^2 + (k_2+k_4)[\mathrm{tr}(\nabla\mathbf{n})^2 - (\mathrm{div}\ \mathbf{n})^2] + \alpha|\mathbf{n}\cdot\mathbf{e}_3|^2\}\mathrm{d}x.$$

Here $\Omega\subset\mathbb{R}^3$ is a bounded, smooth domain occupied by the liquid crystal sample, $\mathbf{n}$ is a Frank director $\mathbf{n}:\Omega\to S^2$, the factors k_i are material constants, and $\mathbf{e}_3$ is the standard unit vector in the z direction in $\mathbb{R}^3$. The constants $\{k_i\}_{i=1}^4$ are generally assumed to satisfy

$$k_1,k_2,k_3>0, \quad k_2>|k_4|, \quad 2k_1\geqslant k_2+k_4. \tag{1}$$

We have included the last term with positive α to describe the interaction with an external electric or magnetic field.[3,5] The fact that α is positive means that the model is only relevant to certain materials.[3,5] We take the field to be uniform in the $\mathbf{e}_3$ direction, and in the case of an electric field we neglect the dipole contribution of the director. In this article we will explore the asymptotic regime $\alpha\gg 1$ so that alignment of the director perpendicular to $\mathbf{e}_3$ is heavily favored, whence we are led to consider the functional

[a]Electronic mail: yunhkim@indiana.edu
[b]Electronic mail: jrubinst@indiana.edu
[c]Electronic mail: sternber@indiana.edu

$$F_\infty(\mathbf{n}) := \int_\Omega [k_1|\text{div } \mathbf{n}|^2 + k_2|\mathbf{n}\cdot\text{curl } \mathbf{n}|^2 + k_3|\mathbf{n}\times\text{curl } \mathbf{n}|^2] + (k_2+k_4)[\text{tr}(\nabla\mathbf{n})^2 - (\text{div } \mathbf{n})^2]\text{d}x.$$

One should view F_∞ as arising formally in the limit $\alpha\to\infty$ where the extreme cost of out-of-plane alignment for the director leads to consideration of this functional over directors $\mathbf{n}$ taking values on the unit circle S^1 in the xy plane rather than on S^2.

Our main result is the assertion that, under certain conditions on Ω, there exist nontrivial local minimizers of the energy F_α for α sufficiently large. We wish to emphasize that these stable critical points locally minimize the energy among all nearby competitors in a suitable topology, without the imposition of Dirichlet boundary conditions as is often the case in the literature. As such, wherever these solutions are smooth, they will satisfy the so-called "natural boundary conditions" for the problem associated with setting the first variation of energy to zero and integrating by parts.

The technique, which we borrow from Ref. 2, involves looking for local minimizers for F_α near local minimizers of F_∞. The fact that one can find nontrivial local minimizers of F_∞ is not obvious given that one is not forcing the director into a non-constant configuration through a Dirichlet condition. It relies crucially on the assumption that the sample Ω occupies a region of nontrivial topology. We now make this hypothesis explicit:
Henceforth we assume that Ω *has the topology of a one-holed torus in* $\mathbb{R}^3$.

We should note that more exotic local minimizers can be found by the same methods if one takes Ω to be a many-holed torus but we will not pursue that here. The effect of this topological assumption is to allow us to introduce a notion of winding number for S^1-valued functions defined on Ω. We will make this notion precise in the next section. We can then minimize F_∞ among S^1-valued competitors of a given winding number m to obtain interesting solutions. Through a perturbative variational calculus, for each m we will then find local minimizers of the full energy F_α for large values of α near these local minimizers of F_∞.

In the final section we include some further observations about the limiting energy F_∞ in the case where $\Omega\subset\mathbb{R}^2$ is an annulus and the director $\mathbf{n}:\Omega\to S^1$.

II. EXISTENCE OF LOCAL MINIMIZERS

We begin by recalling the notion of winding number appropriate to our setting, namely the 1-homotopy type of an S^1-valued map. For smooth functions mapping Ω into S^1, one can simply consider the restriction of such a map to any oriented simple closed loop encircling the hole in Ω and measure the classical winding number. By a standard continuity argument, this number will not depend on the particular loop chosen. However, the natural space of competitors for both F_α and more crucially for F_∞ is not smooth maps but rather maps whose first derivatives are all square integrable, namely the Sobolev spaces $H^1(\Omega;S^2)$ and $H^1(\Omega;S^1)$ respectively, cf. Ref. 6.

Let us then recall the definition of the H^1-norm of a function $\mathbf{n}:\Omega\to\mathbb{R}^k$, $k\geqslant 1$:

$$\|\mathbf{n}\|^2_{H^1(\Omega;\mathbb{R}^m)} = \sum_{j=1}^k \|n^{(j)}\|^2_{L^2(\Omega)} + \sum_{j=1}^k \|\nabla n^{(j)}\|^2_{L^2(\Omega)} = \sum_{j=1}^k \left\{ \int_\Omega |n^{(j)}|^2 dx + \int_\Omega |\nabla n^{(j)}|^2 \text{d}x \right\}$$

where $n^{(j)}$ denotes the j^{th} component of the vector-valued function $\mathbf{n}$.

It is well-known that H^1 functions defined on a set $\Omega\subset\mathbb{R}^3$ need not be continuous so some care must be taken to define the 1-homotopy type of such a Sobolev map. This difficulty was overcome in Ref. 7, where the author studies the harmonic map problem for functions of a given 1-homotopy type. A key tool is the following lemma.

Lemma 1: (Ref. 7) *For each* $K>0$ *there is an* $\epsilon>0$ *such that if* f_1 *and* f_2 *are Lipschitz continuous mappings from* Ω *into* S^1 *satisfying the conditions*

$$\|f_1 - f_2\|_{L^2(\Omega)} < \varepsilon, \quad \|\nabla f_i\|_{L^2(\Omega)} \leqslant K \quad \text{for } i = 1,2, \tag{2}$$

then f_1 *and* f_2 *have the same 1-homotopy type.*

Armed with this information one can for instance appeal to the density of smooth maps taking Ω into S^1 (see, e.g., Ref. 8) to partition the space $H^1(\Omega;S^1)$ according to 1-homotopy type by defining for each integer m the set $H^1_m(\Omega;S^1)\subset H^1(\Omega;S^1)$ as the closure under the H^1-norm of smooth maps of 1-homotopy type m. Equally important from the standpoint of invoking the direct method in the calculus of variations, one has the following consequence of Lemma 1 and the weak compactness of bounded sets in H^1 (cf. Ref. 6): Suppose a sequence $\{\mathbf{n}_j\}\subset H^1_m(\Omega;S^1)$ satisfies the uniform bound

$$\|\mathbf{n}_j\| \leqslant M$$

for some positive constant M. Then there exists a subsequence $\{\mathbf{n}_{jk}\}$ and a function $\mathbf{n} \in H^1_m(\Omega;S^1)$ such that

$$\mathbf{n}_{j_k} \rightharpoonup \mathbf{n} \text{ in } H^1 \text{ as } k\to\infty.$$

In particular, the set $H^1_m(\Omega;S^1)$ is closed under weak H^1 convergence.

With these preliminaries in hand, we now establish the existence of minimizers for the limiting functional F_∞ within each 1-homotopy class. To this end, for each integer m we introduce the notation

$$\mu_m := \inf_{\mathbf{n}\in H^1_m(\Omega;S^1)} F_\infty(\mathbf{n}) \tag{3}$$

and

$$\mathcal{A}_m := \{\mathbf{n} \in H^1_m(\Omega;S^1): F_\infty(\mathbf{n}) = \mu_m\} \tag{4}$$

and establish:

Proposition 1: For every integer m, the set of minimizers $\mathcal{A}_m$ is nonempty.

Proof: Existence will follow from the direct method. Indeed, if $\{\mathbf{n}_j\}$ denotes a minimizing sequence for the problem (3), then the identity

$$|\nabla\mathbf{n}|^2 = \mathrm{tr}(\nabla\mathbf{n})^2 + |\mathrm{curl}\,\mathbf{n}|^2 \tag{5}$$

(cf. Ref. 4, Lemma 3.3) and our assumptions (1) readily imply the bound

$$\bar{k}\int_\Omega |\nabla\mathbf{n}_j|^2 \mathrm{d}x \leqslant 2\mu_m, \tag{6}$$

where $\bar{k} := \min\{k_2, k_3, k_2+k_4\} > 0$. Hence by Lemma 1 and the discussion following it, there exists a subsequence $\{\mathbf{n}_{jk}\}$ and a function $\mathbf{n}\in H^1_m(\Omega;S^1)$ such that

$$\mathbf{n}_{j_k} \rightharpoonup \mathbf{n} \text{ in } H^1, \quad \mathbf{n}_{j_k} \to \mathbf{n} \text{ in } L^2 \text{ as } k\to\infty. \tag{7}$$

Rearranging the terms in F_∞ as

$$F_\infty(\mathbf{n}_{j_k}) = \int_\Omega [(k_1-k_2-k_4)|\mathrm{div}\,\mathbf{n}_{j_k}|^2 + k_2|\mathbf{n}_{j_k}\cdot\mathrm{curl}\,\mathbf{n}_{j_k}|^2 + k_3|\mathbf{n}_{j_k}\times\mathrm{curl}\,\mathbf{n}_{j_k}|^2 + (k_2+k_4)\mathrm{tr}(\nabla\mathbf{n}_{j_k})^2]\mathrm{d}x,$$

we observe that the integrand is a convex function of the partial derivatives of $\mathbf{n}_{jk}$ and so (7) implies that the energy is lower-semi-continuous (cf. Ref. 9):

$$\liminf_{k\to\infty} F_\infty(\mathbf{n}_{j_k}) \geqslant F_\infty(\mathbf{n}).$$

Hence $\mathbf{n}\in\mathcal{A}_m$. □

Remark: We leave open the question as to whether the minimizer of F_∞ in $H^1_m(\Omega;S^1)$ is

unique. Resolving this does not seem to be easy but in any event, it will not be needed for the main result.

Before proceeding to the main result we require a few simple consequences of Lemma 1. For these we introduce notation for the H^1 distance to the set $\mathcal{A}_m$:

$$d(\mathbf{n},\mathcal{A}_m) := \inf_{\tilde{\mathbf{n}}\in\mathcal{A}_m} \|\mathbf{n}-\tilde{\mathbf{n}}\|_{H^1}. \tag{8}$$

First we note some compactness properties of the set $\mathcal{A}_m$:

Lemma 2: Let m be any integer.

(i) *For any sequence $\{\tilde{\mathbf{n}}_j\}\subset\mathcal{A}_m$ there exists a subsequence $\{\tilde{\mathbf{n}}_{jk}\}$ and a function $\tilde{\mathbf{n}}\in\mathcal{A}_m$ such that $\tilde{\mathbf{n}}_{jk}\to\tilde{\mathbf{n}}$ strongly in H^1.*

(ii) *For any $\mathbf{n}\in H^1(\Omega;S^2)$ and any positive constant C, the condition $d(\mathbf{n},\mathcal{A}_m)\leqslant C$ implies that there exists a function $\tilde{\mathbf{n}}\in\mathcal{A}_m$ such that*

$$\|\mathbf{n}-\tilde{\mathbf{n}}\|_{H^1(\Omega;\mathbb{R}^3)} \leqslant C.$$

Proof: To prove (i), we apply the bound (6) to the sequence $\{\tilde{\mathbf{n}}_j\}$ to obtain a weak H^1-limit $\tilde{\mathbf{n}}$ of a subsequence $\{\tilde{\mathbf{n}}_{jk}\}$. As was noted in the proof of Proposition 1, the energy F_∞ is lower-semi-continuous under weak H^1 convergence so with the aid of Lemma 1 we immediately conclude that $\tilde{\mathbf{n}}\in\mathcal{A}_m$. However, using that in fact each term in F_∞ is weakly-lower-semicontinuous we can further assert that

$$\lim_{k\to\infty}\int_\Omega |\tilde{\mathbf{n}}_{j_k}\cdot\operatorname{curl}\tilde{\mathbf{n}}_{j_k}|^2 dx = \int_\Omega |\tilde{\mathbf{n}}\cdot\operatorname{curl}\tilde{\mathbf{n}}|^2 dx,$$

$$\lim_{k\to\infty}\int_\Omega |\tilde{\mathbf{n}}_{j_k}\times\operatorname{curl}\tilde{\mathbf{n}}_{j_k}|^2 dx = \int_\Omega |\tilde{\mathbf{n}}\times\operatorname{curl}\tilde{\mathbf{n}}|^2 dx,$$

and

$$\lim_{k\to\infty}\int_\Omega \operatorname{tr}(\nabla\tilde{\mathbf{n}}_{j_k})^2 dx = \int_\Omega \operatorname{tr}(\nabla\tilde{\mathbf{n}})^2 dx,$$

for otherwise $F_\infty(\tilde{\mathbf{n}})<\mu_m$, a contradiction. Hence, via (5) we see that $\|\nabla\tilde{\mathbf{n}}jk\|_{L^2}\to\|\nabla\tilde{\mathbf{n}}\|_{L^2}$ and the convergence of the subsequence is indeed strong in H^1.

The proof of (ii) follows immediately from the definition (8) and property (i). □

The next lemma says that functions H^1 close to the set $\mathcal{A}_m$ must lie in $H^1_m(\Omega;S^1)$.

Lemma 3: For each m there is a positive number γ_m such that if $\mathbf{n}\in H^1(\Omega;S^1)$ satisfies $d(\mathbf{n},\mathcal{A}_m)<\gamma_m$, then $\mathbf{n}$ belongs to $H^1_m(\Omega;S^1)$.

Proof: First note that if $\tilde{\mathbf{n}}\in\mathcal{A}_m$ then using (6) we have

$$\int_\Omega |\nabla\tilde{\mathbf{n}}|^2 \leqslant \frac{2\mu_m}{\bar{k}}.$$

Now let $K=4\mu_m/\bar{k}+1$ and let $\varepsilon=\varepsilon(K)$ be the value guaranteed by Lemma 1. Set $\gamma_m=\min\{1/\sqrt{2},(1/2)\sqrt{\varepsilon}\}$.

Then suppose

$$d(\mathbf{n},\mathcal{A}_m) < \gamma_m, \tag{9}$$

and pick an element $\tilde{\mathbf{n}}$ in $\mathcal{A}_m$ such that $\|\mathbf{n}-\tilde{\mathbf{n}}\|_{H^1(\Omega;\mathbb{R}^3}<\gamma_m$. It follows that

$$\|\nabla \mathbf{n}\|^2_{L^2(\Omega;S^1)} \leqslant 2(\|\nabla \tilde{\mathbf{n}}\|^2_{L^2(\Omega;S^1)} + \gamma_m^2) < K.$$

Similarly, (9) implies that $\|\mathbf{n}-\tilde{\mathbf{n}}\|_{L^2(\Omega;S^1)} < \varepsilon/4$. Taking smooth sequences $\{f_j\}$ and $\{\tilde{f}_j\}$ in $H^1(\Omega;S^1)$ satisfying $f_j \to \mathbf{n}$ and $\tilde{f}_j \to \tilde{\mathbf{n}}$ in H^1, we see from Lemma 1 that both sequences lie in $H^1_m(\Omega;S^1)$ for j large. Hence $\mathbf{n}$ does as well. □

We can now state our main result:

Theorem 1: For each m there exists a positive number α_m such that for all $\alpha > \alpha_m$, the functional F_α possesses an H^1-local minimizer $\mathbf{n}^m_\alpha$. Further, $d(\{\mathbf{n}^m_\alpha\}, \mathcal{A}_m) \to 0$ as $\alpha \to \infty$.

Remark: By an H^1-local minimizer we mean a function $\mathbf{n}^m_\alpha \in H^1(\Omega;\mathbb{R}^3)$ such that

$$F_\alpha(\mathbf{n}^m_\alpha) \leqslant F_\alpha(\mathbf{n}) \quad \text{whenever} \quad \|\mathbf{n}^m_\alpha - \mathbf{n}\|_{H^1(\Omega;S^2)} < \delta$$

for some $\delta > 0$. Such a function will in particular be a critical point of the functional F_α and so will weakly satisfy the associated Euler-Lagrange equation and natural boundary conditions. The regularity theory for F_α originally developed in[11] for Dirichlet boundary conditions says that minimizers with be smooth off of a set of finite zero-dimensional Hausdorff measure. We have not checked but we suspect that such a theory would apply to this present setting of natural boundary conditions as well. The technical issue would be handling the last (null-Lagragian) term carrying coefficient k_2+k_4 which in this non-Dirichlet setting cannot be equated to a constant.

Remark: In modeling a nematic liquid crystal, the "head" and "tail" of the director are indistinguishable. One way to capture this is to pose the minimization of F_α over unit vectors taking values in $\mathbb{P}^2$, two-dimensional projective space where antipodal points on S^2 are associated. The previous theorem can readily be phrased with $\mathbb{P}^2$ replacing $\mathbb{S}^2$. In fact, if one takes this tack, then local minimizers can be found corresponding to all of the half-integer winding numbers as well. The proof below is unchanged by the substitution of $\mathbb{P}^2$ for S^2 and the consideration of the limiting energy F_∞ for mappings $\mathbf{n}:\Omega \to \mathbb{P}^1$.

Proof: Fix an integer m and consider the variational problem

$$\inf_{\{\mathbf{n} \in H^1(\Omega;S^2):\, d(\mathbf{n},\mathcal{A}_m) \leqslant (1/2)\gamma_m\}} F_\alpha(\mathbf{n}), \tag{10}$$

where γ_m is the value from Lemma 3. Exploiting the convexity of the various terms in F_α as well as the uniform H^1-bound valid for any minimizing sequence $\{\mathbf{n}_j\}$, the direct method succeeds here in a manner similar to that used in solving (3). The only new issue is that one must invoke Lemma 2 and the lower-semi-continuity of the H^1-norm under weak convergence to assure that the weak limit $\mathbf{n}^m_\alpha$ of a subsequence $\{\mathbf{n}_{j_k}\}$ will satisfy the admissibility condition $d(\mathbf{n}^m_\alpha, \mathcal{A}_m) \leqslant \frac{1}{2}\gamma_m$. We would like to argue that the minimizer $\mathbf{n}^m_\alpha$ to the constrained problem (10) is in fact an H^1-local minimizer of F_α. This would follow if one could show that the constraint is not exhausted, that is, if one could demonstrate that $d(\mathbf{n}^m_\alpha, \mathcal{A}_m) < \frac{1}{2}\gamma_m$. We will achieve this for α sufficiently large by in fact arguing that

$$d(\mathbf{n}^m_\alpha, \mathcal{A}_m) \to 0 \text{ as } \alpha \to \infty. \tag{11}$$

We proceed by contradiction and suppose that for some subsequence $\{\alpha_j\} \to \infty$ there exists a positive number η such that

$$d(\mathbf{n}^m_{\alpha_j}, \mathcal{A}_m) \geqslant \eta \text{ for all } j. \tag{12}$$

Note that necessarily, $\eta \leqslant \frac{1}{2}\gamma_m$.

Since all elements of $\mathcal{A}_m$ are uniformly bounded in H^1 by some constant depending on m, the condition $d(\mathbf{n}^m_\alpha, \mathcal{A}_m) \leqslant \frac{1}{2}\gamma_m$ implies an H^1 bound on the sequence $\{\mathbf{n}^m_\alpha\}$ that is independent of α. Hence, after passing to another subsequence (whose notation we suppress), we can conclude that there exists a function $\mathbf{\Phi} \in H^1(\Omega;S^2)$ satisfying

$$\mathbf{n}_{\alpha_j}^m \rightharpoonup \mathbf{\Phi} \quad \text{in} \quad H^1(\Omega;S^2) \quad \text{as} \quad \alpha_j \to \infty. \tag{13}$$

Now observe that for any element $\tilde{\mathbf{n}} \in \mathcal{A}_m$ one has

$$F_{\alpha_j}(\mathbf{n}_{\alpha_j}^m) \leqslant F_{\alpha_j}(\tilde{\mathbf{n}}) = F_\infty(\tilde{\mathbf{n}}) = \mu_m,$$

so that

$$\int_\Omega (\mathbf{n}_{\alpha_j}^m \cdot \mathbf{e}_3)^2 \mathrm{d}x \leqslant \frac{1}{\alpha_j}\mu_m \to 0 \text{ as } \alpha_j \to \infty.$$

Hence, $\int_\Omega(\mathbf{\Phi}\cdot\mathbf{e}_3)^2\mathrm{d}x=0$ and $\mathbf{\Phi} \in H^1(\Omega;S^1)$.

Next we apply Lemma 2 (ii) and note that for each j there exists an element $\tilde{\mathbf{n}}_j \in \mathcal{A}_m$ such that $\|\mathbf{n}_{\alpha_j}^m - \tilde{\mathbf{n}}_j\|_{H^1(\Omega;\mathbb{R}^3)} \leqslant \frac{1}{2}\gamma_m$. Then by Lemma 2 (i), there exists a strong limit $\tilde{\mathbf{n}} \in \mathcal{A}_m$ of a subsequence of $\{\tilde{\mathbf{n}}_j\}$ and the lower-semi-continuity of the H^1-norm under weak convergence implies that $\|\Phi - \tilde{\mathbf{n}}\|_{H^1(\Omega;\mathbb{R}^3)} \leqslant \frac{1}{2}\gamma_m$ as well. Applying Lemma 3, we conclude that $\Phi \in H_m^1(\Omega;S^1)$.

Finally, we once again exploit the convexity of the integrand of F_α and (13) to see that for any element $\tilde{\mathbf{n}} \in \mathcal{A}_m$ one has

$$F_\infty(\mathbf{\Phi}) \leqslant \liminf_{\alpha_j\to\infty} F_\infty(\mathbf{n}_{\alpha_j}^m) \leqslant \limsup_{\alpha_j\to\infty} F_\infty(\mathbf{n}_{\alpha_j}^m) \leqslant \limsup_{\alpha_j\to\infty} F_{\alpha_j}(\mathbf{n}_{\alpha_j}^m) \leqslant \limsup_{\alpha_j\to\infty} F_{\alpha_j}(\tilde{\mathbf{n}}) = F_\infty(\tilde{\mathbf{n}}) = \mu_m. \tag{14}$$

Consequently, $F_\infty(\mathbf{\Phi})=\mu_m$ since $\mathbf{\Phi}$ is admissible in (3) so that $\mathbf{\Phi} \in \mathcal{A}_m$ and all of the inequalities in (14) are in fact equalities. In particular, we have

$$\lim_{\alpha_j\to\infty} F_\infty(\mathbf{n}_{\alpha_j}^m) = F_\infty(\mathbf{\Phi})$$

and the lower-semi-continuity of each term of F_∞ separately under the convergence (13), along with the identity (5) implies that $\mathbf{n}_{\alpha_j}^m \to \mathbf{\Phi}$ strongly in H^1. Hence, $d(\mathbf{\Phi},\mathcal{A}_m) \geqslant \eta$ by (12), which is impossible since $\mathbf{\Phi} \in \mathcal{A}_m$. □

III. REMARKS ON THE TWO-DIMENSIONAL CASE

The entire analysis above is valid also for the case where Ω is an annulus in $\mathbb{R}^2$, or any other smooth planar domain with nontrivial topology. In this section we discuss aspects of the limiting problem of minimizing F_∞ in this 2D setting. When Ω is planar, the limit functional F_∞ takes a rather simple form

$$F_\infty(\mathbf{n}) = \int_\Omega [k_1|\mathrm{div}\ \mathbf{n}|^2 + k_3|\mathrm{curl}\ \mathbf{n}|^2]\mathrm{d}x \tag{15}$$

for $\mathbf{n}:\Omega\to S^1$. In particular, a calculation shows that the null-Lagrangian term involving $(\nabla\mathbf{n})^2 - (\mathrm{div}\ \mathbf{n})^2$ integrates to zero in this setting. We note that F_∞ in the form (15) has also arisen in the literature[10] as a simplification of the Oseen-Frank energy even without an external field under the special geometric assumption that Ω lies in $\mathbb{R}^2$ and the assumption that the director has zero third component.

One immediate conclusion is that in the one-constant case, i.e., when $k_1=k_3$, the phase φ of any critical point is a harmonic function. Moreover, the second variation is positive there and one can show that such a critical point is an isolated local minimizer (up to a constant phase shift). Of course, this is not surprising, since in such a special case the functional F_∞ is proportional to $\int_\Omega|\nabla\mathbf{n}|^2\mathrm{d}x$, which was considered in Refs. 2 and 7. The only novelty in the liquid crystal problem is the existence of extra solutions since $\mathbf{n}$ actually takes values in one-dimensional projective space, $\mathbb{P}^1$ (see the second Remark following Theorem 1). We point out though that unlike the

one-constant case, in the general case $k_1 \neq k_3$, the energy is *not* invariant to a constant shift of the phase.

Returning to the general case $k_1 \neq k_3$, we ask whether particular solutions can be found in the special geometry where Ω is a symmetric annulus (i.e. a domain bounded by concentric circles). Using polar coordinates (r, θ), we claim:

Proposition 2: Assume that Ω *is a symmetric annulus. Then the minimizer of (15) in the class of homotopy type* $m=1$ *is* $\mathbf{n}=(\cos\theta, \sin\theta)$ *if* $k_3 > k_1$, *or* $\mathbf{n}=(-\sin\theta, \cos\theta)$ *if* $k_1 > k_3$.

Proof: Assume that $k_3 > k_1$. Then for every $\mathbf{n}$

$$F_\infty(\mathbf{n}) = \int_\Omega k_1 |\nabla \mathbf{n}|^2 \mathrm{d}x + (k_3 - k_1) \int_\Omega |\mathrm{curl}\, \mathbf{n}|^2 \mathrm{d}x.$$

It is well known that $\mathbf{n}=(\cos\theta, \sin\theta)$ minimizes $\int_\Omega k_1 |\nabla \mathbf{n}|^2 \mathrm{d}x$ in the class of homotopy class 1. It also follows from a simple calculation that curl $(\cos\theta, \sin\theta)=0$. This establishes the proposition for $k_3 > k_1$, and the other case follows similarly. □

The success in finding a simple solution for the case $m=1$, motivates the search for solutions of the form $\mathbf{n}=\mathbf{n}(\theta)$ for other homotopy types as well. Indeed Landau and Lifshitz (Ref. 10, Chap. VI) propose such a solution in the entire plane. They introduce the notation ψ to denote the angle between the director $\mathbf{n}$ with the radius vector to the point $(\cos\theta, \sin\theta)$. Assuming an ansatz $\psi = \psi(\theta)$, they look for a minimizer $\mathbf{n}$ of F_∞ in the restricted family

$$\mathbf{n} = (\cos(\theta + \psi(\theta)), \sin(\theta + \psi(\theta))). \tag{16}$$

Under this restriction, the functional F_∞ can be written as

$$\frac{1}{4}(k_1 + k_3) \int (1 - \gamma \cos 2\psi)(1 + (\psi')^2) \frac{1}{r} \mathrm{d}\theta\, \mathrm{d}r, \tag{17}$$

where $\gamma=(k_3-k_1)/(k_3+k_1)$, and primes mean differentiation with respect to θ. The problem of minimizing the functional $\int_0^{2\pi}(1-\gamma\cos 2\psi)(1+(\psi')^2)\mathrm{d}\theta$ leads to the Euler Lagrange equation

$$(1 - \gamma \cos 2\psi)\psi'' = \gamma \sin 2\psi (1 - (\psi')^2). \tag{18}$$

Since the special case $m=1$ was already previously established, one can assume $m \neq 1$. A short calculation shows that the Euler-Lagrange equation (18) can be integrated in the form

$$\theta = \int_0^\psi q \left(\frac{1 - \gamma \cos 2\phi}{1 - \gamma q^2 \cos 2\phi} \right)^{1/2} \mathrm{d}\varphi, \tag{19}$$

where the integration constant q is determined by the condition

$$(m-1)q \int_0^\pi \left(\frac{1 - \gamma \cos 2\psi}{1 - \gamma q^2 \cos 2\psi} \right)^{1/2} \mathrm{d}\psi = \pi. \tag{20}$$

However, if the solution of Ref. 10 is considered over the infinite plane, as proposed by the authors, the energy density has a nonintegrable singularity at the origin. Landau and Lishitz propose to remedy the problem by introducing a small cutoff radius. Instead of using an artificial cutoff radius, one may ask whether the symmetric solution can be used in an annulus, where the origin is kept well outside the domain. Unfortunately, it turns out that the case $m=1$ is special–it is the only homotopy class in which a minimizer can have the symmetry $\mathbf{n}=\mathbf{n}(\theta)$ when $k_1 \neq k_3$. One can see this by calculating the natural boundary conditions for the functional (15). A short computation gives

$$k_1 \nabla \mathbf{n} \cdot \nu + (k_1 - k_3)(\nabla \times \mathbf{n}) \times \nu = \lambda \mathbf{n}, \tag{21}$$

where ν is the unit normal to the boundary and λ is a proportionality constant. Substituting the ansatz (16), and using the symmetry of the annulus, the condition (21) becomes

$$(k_1 - k_3)(1 + \psi')\sin(\psi)(\sin\theta, -\cos\theta) = \lambda(\cos(\theta + \psi), \sin(\theta + \psi)).$$

Clearly, the only solutions to the previous equation are $\psi = 0$, $\lambda = 0$ and $\psi = \pi/2$, $\lambda = k_3 - k_1$. Both solutions correspond to a degree 1 director field.

Finally, we make some observations regarding the functional F_∞ of (15) for a general two-dimensional domain having the topology of an annulus. For this purpose we express the director $\mathbf{n}$ as $\mathbf{n} = (\cos\varphi, \sin\varphi)$ for some phase function $\varphi(x, y)$. The functional can be written explicitly in terms of φ in the form

$$F_\infty(\phi) = \int L(\phi, \nabla\phi) = \int k_1(\varphi_y \cos\varphi - \varphi_x \sin\varphi)^2 + k_3(\varphi_x \cos\varphi + \varphi_y \sin\varphi)^2$$

Varying the phase φ by a function $\beta(x, y) \in H^1(\Omega)$, one can compute the first and second variations:

$$\delta F_\infty = \int (k_3 - k_1)\beta\left\{(\varphi_y^2 - \varphi_x^2)\frac{\sin 2\varphi}{2} + \varphi_x\varphi_y \cos 2\varphi\right\} + (k_1 \cos\varphi^2 + k_3 \sin\varphi^2)\beta_y\varphi_y$$
$$+ (k_3 - k_1)\beta_y\varphi_x \sin\varphi\cos\varphi + (k_3 - k_1)\beta_x\varphi_y \sin\varphi\cos\varphi + (k_1 \sin\varphi^2 + k_3 \cos\varphi^2)\beta_x\varphi_x,$$

and

$$\delta^2 F_\infty = \int k_1(\beta_x \sin\varphi - \beta_y \cos\varphi)^2 + k_3(\beta_x \cos\varphi + \beta_y \sin\varphi)^2 + 2(k_3 - k_1)$$
$$\times \beta_x\beta(\varphi_y \cos 2\varphi - \varphi_x \sin 2\varphi) + 2(k_3 - k_1)\beta_y\beta(\varphi_x \cos 2\varphi + \varphi_y \sin 2\varphi)$$
$$+ (k_3 - k_1)\beta^2\{(\varphi_y^2 - \varphi_x^2)\cos 2\varphi - 2\varphi_x\varphi_y \sin 2\varphi\}.$$

Consider the special case where the variation β is constant. Since the second variation must be nonnegative at a minimum, we conclude that

$$(k_3 - k_1)\int_\Omega \{(\varphi_y^2 - \varphi_x^2)\cos 2\varphi - 2\varphi_x\varphi_y \sin 2\varphi\} = (k_3 - k_1)\int_\Omega (|\mathrm{div}\,\mathbf{n}|^2 - |\mathrm{curl}\,\mathbf{n}|^2)\mathrm{d}x \geq 0. \tag{22}$$

Fix now a positive k, and set $k_3 = k + \delta$, $k_1 = k - \delta$, for some $|\delta| < k$. For each δ define $E(\delta) = \min F_\infty$ in the homotopy class m (we suppress the m dependency of E).

Proposition 3: The function E is even, i.e. $E = E(|\delta|)$, and moreover, E decreases as a function of $|\delta|$.

Proof: To prove the evenness of E, observe that a shift of $\pi/2$ in the phase φ swaps (up to a sign) the div and curl of a director $\mathbf{n}$. Hence, if $\mathbf{n}_\delta = (\cos\psi_\delta, \sin\psi_\delta)$ is a minimizer achieving $E(\delta)$ and we let $\mathbf{n}_\delta^\perp = (-\sin\psi_\delta, \cos\psi_\delta)$ then we have

$$E(\delta) = F_\infty^\delta(\mathbf{n}_\delta) = F_\infty^{-\delta}(\mathbf{n}_\delta^\perp) \geq E(-\delta)$$

and the reverse inequality follows by similar reasoning.

To see the monotonicity of E, we introduce the notation $\mathbf{n}_i$ for a minimizer of F_∞ when $\delta = \delta_i$ (we fix k and m). Assume without loss of generality that $\delta_1 > 0$. Then, the inequality (22) implies $\int_\Omega (|\mathrm{div}\,\mathbf{n}_1|^2 - |\mathrm{curl}\,\mathbf{n}_1|^2)\mathrm{d}x \geq 0$. Thus, for $\delta_2 > \delta_1$:

$$F_{\infty}^{\delta_2}(\mathbf{n}_1) = E(\delta_1) - (\delta_2 - \delta_1)\int_{\Omega}(|\text{div } \mathbf{n}_1|^2 - |\text{curl } \mathbf{n}_1|^2)\text{d}x.$$

Therefore $E(\delta_2) \leqslant F_{\infty}^{\delta_2}(\mathbf{n}_1) \leqslant E(\delta_1)$. □

Finally, inspecting the first variation for the case of constant variation β, we observe that at a minimizer $\mathbf{n}$ the quantities curl $\mathbf{n}$ and div $\mathbf{n}$ are orthogonal:

$$\int_{\Omega} \text{div } \mathbf{n} \text{ curl } \mathbf{n}\, \text{d}x = 0.$$

We hope to study the minimization of F_{∞} over a given 1-homotopy type further since much remains to be understood. In particular, the limiting cases where either k_1 or k_2 vanish look intriguing and we suspect that for $m \neq 1$, the infimum may not even be attained.

IV. SUMMARY

We proved that liquid crystal samples that occupy a topologically nontrivial domain can exhibit nontrivial local minimizers when they are subjected to a strong external field penalizing deviation from a given plane. These patterns are the liquid crystal analogue of the well-known persistent current phenomenon in superconductivity.

There are several differences between the homotopy solutions derived here and the persistent current solutions in superconductivity. First, the set of homotopy types in the liquid crystal problem is twice as large as the corresponding set in superconductivity, since the director is a headless vector. Another difference is in the way in which the local minimizers are generated. To generate a persistent current, one subjects the superconducting toroidal sample to a large magnetic field. After a supercurrent circulates in the sample, the external field is abruptly shut down trapping the supercurrent. In the liquid crystal setup, a way to generate the local minimizers is to apply boundary conditions that force a director distribution with a given degree, and then to eliminate abruptly these boundary conditions. A third difference is that the limit problem (where the director $\mathbf{n}$ in liquid crystals, or the wave function in superconductivity, are confined to the unit circle S^1) is more general and more difficult in the liquid crystal setup. In fact, we are able to say very little on this limit problem. Finally, we point out that while the phenomenon of persistent currents has been extensively observed experimentally, we are not aware of an experimental demonstration of the patterns we predict here in the liquid crystal problem.

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Global bifurcation structure of a one-dimensional Ginzburg–Landau model

Satoshi Kosugi, Yoshihisa Morita, and Shoji Yotsutani
Department of Applied Mathematics and Informatics, Ryukoku University, Seta, Otsu 520-2194, Japan

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We consider an equation of a simplified Ginzburg–Landau model of superconductivity in a one-dimensional ring. The equation for a complex order parameter ψ has two real parameters μ and λ related to the magnitude of an applied magnetic field and the Ginzburg–Landau parameter, respectively. The purpose of this paper is to reveal a global bifurcation structure for the equation in the parameter space (μ,λ). In particular we show that there exist modulating amplitude solutions which bifurcate from constant amplitude solutions, and how the bifurcation branches of such solutions continue or disappear as μ varies. We also determine the minimizer of the energy functional. © *2005 American Institute of Physics.*
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I. INTRODUCTION

There are many studies on the Ginzburg–Landau equation in phase transition problems of hydrodynamics, chemical reactions, and superconductivity. In the theory of superconductivity the Ginzburg–Landau equation is a model describing a macroscopic superconducting state (Refs. 4 and 11) and it is widely accepted as an established model describing various superconducting phenomena near the critical temperature. In the last two decades the Ginzburg–Landau equation has been extensively studied by mathematicians. We still have many interesting and unsolved mathematical problems in relevance to the superconductivity.

In this paper we are dealing with a simplified model of the superconductivity in a thin uniform superconducting ring. The energy functional in a one-dimensional form of such a model is given by

$$E(\psi;\lambda,h) := \int_0^{2\pi} \frac{1}{2}|D_h\psi|^2 + \frac{\lambda}{4}(1-|\psi|^2)^2 \mathrm{d}x, \quad D_h := \frac{d}{\mathrm{d}x} - ih(x), \tag{1.1}$$

where ψ is a complex-valued order parameter ($|\psi|^2$ expresses the density of superconducting electrons), λ is a positive parameter, and $h(x)$ is a periodic C^1 function. Note that $h(x)$ is the projection of magnetic potential of an applied magnetic field to the tangent direction of a parametrized ring (see Ref. 10 for the derivation of the above model). We consider this functional on the space of 2π-periodic functions in $H^1_{\mathrm{loc}}(\mathbb{R})$. Then the Euler-Lagrange equation of this functional is given by

$$\begin{aligned} &D_h^2\psi + \lambda(1-|\psi|^2)\psi = 0, \quad x \in \mathbb{R}, \\ &\psi(x+2\pi) = \psi(x), \quad x \in \mathbb{R}, \end{aligned} \tag{1.2}$$

which is the Ginzburg–Landau equation of this model. One feature of (1.2) is that (1.2) is transformed into the equation

$$u_{xx} + \lambda(1 - |u|^2)u = 0, \quad x \in \mathbb{R},$$
$$u(x + 2\pi)\exp(2\pi\mu i) = u(x), \quad x \in \mathbb{R}, \tag{1.3}$$

by the change of variable

$$\psi = u \exp\left(i \int_0^x h(s)\mathrm{d}s \right), \tag{1.4}$$

where

$$\mu := \frac{1}{2\pi}\int_0^{2\pi} h(s)\mathrm{d}s. \tag{1.5}$$

It is clear that (1.3) with (1.5) is equivalent to (1.2).

We give a remark on (1.3). For each $\tilde{\mu} \in \mathbb{R}$, let $\tilde{\mu}_0$ be a constant such that $\tilde{\mu}_0 \in [-1/2, 1/2]$ and $\tilde{\mu} - \tilde{\mu}_0 \in \mathbb{Z}$. Since $\exp(2\pi\tilde{\mu}_0 i) = \exp(2\pi\tilde{\mu} i)$, a solution to (1.3) for $\mu = \tilde{\mu}_0$ gives a solution to (1.3) for $\mu = \tilde{\mu}$ and vice versa. Thus it suffices to solve (1.3) for $\mu \in [-1/2, 1/2]$. However we assume $\mu \in \mathbb{R}$ throughout the paper for a simple expression of each solution to (1.2), which is given by (1.4). We also note that if $u(x)$ is a solution of (1.3), the symmetry of the equation allows solutions $u(x)e^{ic}$ and $u(x+c)$ for any constant $c \in \mathbb{R}$. However we will not mention this fact explicitly unless we need to state it clearly.

In Refs. 2 and 12 primary bifurcations from the trivial solution $\psi = 0$ (or $u = 0$) are shown together with secondary bifurcations around higher degenerate bifurcation points. Since their analysis on the secondary bifurcations only works in neighborhoods of the singular points, we are interested in a global structure of the secondary bifurcating solutions. Moreover our goal is to solve (1.3) for every $\mu \in \mathbb{R}$ and $\lambda > 0$ completely and to show how the configuration of the solutions changes as the parameters vary. As for a specific case $\mu \in \mathbb{Z}$, we have already obtained a complete global bifurcation diagram for λ in Ref. 7. We will extend that study to the present case (see also Refs. 5 and 8). However the bifurcation structure exhibits more complex pattern for $2\mu \notin \mathbb{Z}$. In fact the symmetry with respect to the reflection $x \to -x$ is lost if $2\mu \notin \mathbb{Z}$. Nonetheless the approach developed in Ref. 7 fortunately works in the present situation so that a modification of the argument can provide an explicit expression of every solution. With some additional investigation we can observe how the secondary bifurcating solution deforms as μ varies until it disappears through other bifurcation.

To obtain every solution, we first classify all the solutions to (1.3) [or (1.2)] except for the trivial solution $u = 0$ into three types (according to their configuration) as follows:

(I) Solutions with zero.

(IIa) Solutions with constant amplitude.

(IIb) Solutions with modulating but nonvanishing amplitude.

The idea of this classification is quite simple but crucial for our argument. We here made a little modification of the classification found in Ref. 7 for convenience of dealing with the present problem.

Before going to our result, we will explain some known results for these solutions in brief. Every type (I) solution is written in the form

$$u(x) = \exp(ic)\phi(x),$$

where c is a constant of $\mathbb{R}$ and ϕ is a real-valued function (see Sec. II). Moreover a type (I) solution with n zeros exists if and only if $\lambda > n^2/4$ and $\mu - n/2 \in \mathbb{Z}$. In fact, for such a fixed μ, the type (I) solution bifurcates from the trivial solution $u = 0$ at $\lambda = n^2/4$ as λ increases. We denote the type (I) solution with n zeros by $u^{\mathrm{s}}_{\lambda,n}(x)$.

As for type (IIa) solutions of (1.3) it is easy to obtain

$$u^{c}_{\lambda,\mu,m} := \sqrt{1-(m-\mu)^2/\lambda}\,\exp\left(i(m-\mu)x\right), \tag{1.6}$$

for each $m \in \mathbb{Z}$. This solution exists if and only if (μ,λ) satisfies

$$\lambda > \lambda_{\mu,m} := (m-\mu)^2.$$

Then a type (IIa) solution of (1.2) is given by

$$\psi = u^{c}_{\lambda,\mu,m}(x)\exp\left(i\int_0^x h(s)\mathrm{d}s\right),$$

which has the winding number m in the complex plane around the origin.

Next consider type (IIb) solutions. They do not bifurcate from the trivial solution as λ increases. Along the branch of $u^{c}_{\lambda,\mu,m}$, we can find bifurcation points

$$\lambda = \lambda_{\mu,m,n} := 3(m-\mu)^2 - n^2/2 \quad (n \in \mathbb{N}, \lambda_{\mu,m,n} > \lambda_{\mu,m}), \tag{1.7}$$

by investigating the linearized stability of the solution $u^{c}_{\lambda,\mu,m}$. This suggests that a type (IIb) solution bifurcates from the type (IIa) solution at $\lambda=\lambda_{\mu,m,n}$. As a matter of fact there is an intersection point

$$(\mu,\lambda) = ((m_1+m_2)/2, (m_1-m_2)^2/4), \tag{1.8}$$

of two bifurcation curves $\lambda=\lambda_{\mu,m_1}$ and $\lambda=\lambda_{\mu,m_2}$ of type (IIa) solutions. A standard local bifurcation analysis around this critical point does work to reveal that a type (IIb) solution certainly bifurcates in a neighborhood of $u=0$ around the above critical values of (μ,λ) (Ref. 12, see also Refs. 2 and 9 for bifurcations under small perturbation due to nonuniform thickness of the ring).

Besides the local bifurcation structure, as mentioned before, we are interested in a global one of (1.3), consequently (1.2). Moreover we desire to see how the configuration of the secondary bifurcating solution changes as the parameter μ varies.

Now we are going to our results. We notice that a type (IIb) solution is written as $u = w(x)\exp(i\theta(x))$ where $w(x)$ is 2π-periodic and $\theta(x)$ satisfies $\theta(x+2\pi)-\theta(x)=2(m-\mu)\pi$ for an integer m. We let n be the number of local minima of $w(x)$ in the interval $[0,2\pi)$. Since $w(x)$ is not constant, n is a positive integer. We call n the number of modulations for the solution. We denote the solution with such numbers m and n by $u^{o}_{\lambda,\mu,m,n}(x)$ and let

$$D^{-}_{m,n} := \{(\mu,\lambda): \mu < m - n/2, \lambda > \lambda_{\mu,m,n}\}, \tag{1.9}$$

$$D^{+}_{m,n} := \{(\mu,\lambda): \mu > m + n/2, \lambda > \lambda_{\mu,m,n}\}. \tag{1.10}$$

Then we can prove that there exists a solution $u^{o}_{\lambda,\mu,m,n}(x)$ if and only if $(\mu,\lambda) \in D^{-}_{m,n} \cup D^{+}_{m,n}$. This solution is unique up to rotation and translation. Moreover this solution bifurcates from the type (IIa) solution $u^{c}_{\lambda,\mu,m}$ as (μ,λ) pass through the part of $\partial D^{\pm}_{m,n}$

$$\{(\mu,\lambda): \mu < m - n/2, m + n/2 < \mu, \lambda = \lambda_{\mu,m,n}\}$$

(see Proposition 3.1 in Sec. III). We note that $w(x)$ can be expressed by the Jacobi elliptic function.

We are now in a position to propose the main theorem of this paper.

Theorem 1.1: *Let $\lambda>0$. Given 2π-periodic C^1-function h, define μ by (1.5). Then any nontrivial solution to (1.2) is one of the following:*

(I) $\psi^{s}_{\lambda,\mu,n,\omega}(x)e^{ic} = u^{s}_{\lambda,n}(x+\omega)\exp(i\int_0^x h(s)\mathrm{d}s + ic)$ for $n \in \mathbb{N}$ satisfying $n^2/4 < \lambda, \mu - n/2 \in \mathbb{Z}$,

(IIa) $\psi^{c}_{\lambda,\mu,m}(x)e^{ic} = u^{c}_{\lambda,\mu,m}(x)\exp(i\int_0^x h(s)\mathrm{d}s + ic)$ for $m \in \mathbb{Z}$ satisfying $\lambda_{\mu,m} < \lambda$,

(IIb) $\psi^{o}_{\lambda,\mu,m,n,\omega}(x)e^{ic} = u^{o}_{\lambda,\mu,m,n}(x+\omega)\exp(i\int_0^x h(s)\mathrm{d}s + ic)$ for $(m,n) \in \mathbb{Z}\times\mathbb{N}$ satisfying $n^2/4 < \lambda_{\mu,m,n} < \lambda$,

where c and ω are real numbers. Moreover if $h(x)$ is given as

$$h(x) = \mu h_e(x), \quad \frac{1}{2\pi}\int_0^{2\pi} h_e(x)\mathrm{d}x = 1, \tag{1.11}$$

and if $m \in \mathbb{Z}, n \in \mathbb{N}$, *and* $\lambda > n^2/4$ *are fixed, then the set* $\{\psi(\cdot;\mu): \mu^-_{\lambda,m,n} < \mu < \mu^+_{\lambda,m-n,n}\}$ *which is defined as*

$$\psi(x;\mu) := \begin{cases} \psi^o_{\lambda,\mu,m,n,\omega}(x), & \mu^-_{\lambda,m,n} < \mu < m - n/2, \\ i\psi^s_{\lambda,\mu,n,\omega}(x), & \mu = m - n/2, \\ -\psi^o_{\lambda,\mu,m-n,n,\omega}(x), & m - n/2 < /\mu < /\mu^+_{\lambda,m-n,n} \end{cases} \tag{1.12}$$

is a continuous curve in $C(\mathbb{R};\mathbb{C})$, *where*

$$\mu^{\pm}_{\lambda,m,n} := m \pm \sqrt{\lambda/3 + n^2/6}. \tag{1.13}$$

We note that any sectorial region $D^-_{m,n}$ is adjacent to $D^+_{m-n,n}$. The last assertion implies that a solution in one of these adjacent regions is continuously deformed up to a solution in the other region in the way of the statement. Since the two solutions are topologically different, the branch contains a solution with zeros at $\mu = m - n/2$. Then the number of modulations turns to be the number of zeros at this critical value of μ (for the configuration of solutions see figures in Sec. IV).

We next give a remark on the stability of solutions. As seen in Ref. 12, it is known that a type (IIa) solution $\psi^c_{\lambda,\mu,m}$ is stable (or unstable) if $\lambda > \lambda_{\mu,m,1}$ (or $\lambda < \lambda_{\mu,m,1}$). On the other hand, the stability (or instability) region for a type (IIb) solution is not clear. Our result tells the following: as λ increases, a type (IIb) solution $\psi^o_{\lambda,\mu,m,n,\omega}$ bifurcates from the type (IIa) solution $\psi^c_{\lambda,\mu,m}$ that is unstable up to $\lambda = \lambda_{\mu,m,1} > \lambda_{\mu,m,n} (n > 1)$, and no bifurcation takes places from $\psi^o_{\lambda,\mu,m,n,\omega}$. We thereby infer that every type (IIb) solution is unstable globally. To prove it rigorously, we need some stability analysis for $\psi^o_{\lambda,\mu,m,n,\omega}$, which would be a future work.

Nonetheless by explicit computations of the energy (1.1) for the solutions, we obtain the minimizer for given $\lambda > 0$ and $\mu \in \mathbb{R}$ as follows.

Theorem 1.2: *Assume* $\lambda > 0$ *and* $h(x)$ *satisfy (1.11). Given* $m \in \mathbb{Z}$, *let*

$$\mathcal{D}_m := \{(\mu,\lambda): m - 1/2 \leqslant \mu \leqslant m + 1/2,\ (\mu - m)^2 < \lambda\}. \tag{1.14}$$

Then the type (IIa) solution $\psi^c_{\lambda,\mu,m}$ *is a minimizer of (1.1) if* $(\lambda,\mu) \in \mathcal{D}_m$, *while the trivial solution* $\psi = 0$ *is a minimizer if* $(\mu,\lambda) \notin (\cup_{m=1}^{\infty} \mathcal{D}_m)$. *Moreover for* $(\mu,\lambda) \in \mathrm{Int}\, \mathcal{D}_m$, $\psi^c_{\lambda,\mu,m}$ *is a unique minimizer up to the rotation.*

We note that for $\mu = m - 1/2$ (or $m + 1/2$) both $\psi^c_{\lambda,\mu,m}$ and $\psi^c_{\lambda,\mu,m-1}$ (or $\psi^c_{\lambda,\mu,m+1}$) are the minimizer if $\lambda > 1/4$.

In the next section we derive type (I) solutions. Though the result is known (for instance, see Ref. 2), we give a proof for the reader's convenience. In fact the argument of the proof would be helpful when we consider a more difficult case of type (IIb) solutions. In Sec. III we are dealing with type (IIb) solutions and provide a proposition which guarantees the existence of the solution. The proof of the proposition will be postponed until Sec. V, where some lemma is only stated because it is essentially proved in Ref. 7. In Sec. IV we give various figures for existence regions of solutions in (μ,λ) space, bifurcation diagrams and configurations of type (IIb) solutions. In Sec. VI we will prove Theorem 1.2 and give a remark in the final section on the computations arising in Sec. VI.

II. TYPE (I) SOLUTIONS

In this section we treat type (I) solutions to (1.3). We will show that, given $n \in \mathbb{N}$, there exists a solution to (1.3) which has n zero points on $[0, 2\pi)$ if and only if

$$\lambda > n^2/4, \quad \mu = m + n/2 \quad (\forall m \in \mathbb{Z}), \tag{2.1}$$

and each solution is written in the form

$$u = u^s_{\lambda,n}(x+\omega)\exp(ic), \quad u^s_{\lambda,n} := k\sqrt{2/(1+k^2)}\,\mathrm{sn}(nK(k)x/\pi,k),$$

where c and ω are arbitrary constants of $\mathbb{R}$, $k \in (0,1)$ is a unique solution to

$$\sqrt{1+k^2}K(k) = \pi\sqrt{\lambda}/n, \tag{2.2}$$

$\mathrm{sn}(x,k)$ is the Jacobi elliptic function whose inverse is given by

$$\mathrm{sn}^{-1}(u,k) = \int_0^u \frac{1}{\sqrt{1-\tau^2}\sqrt{1-k^2\tau^2}}\mathrm{d}\tau,$$

and $K(k)$ is a complete elliptic integral

$$K(k) := \int_0^1 \frac{1}{\sqrt{1-\tau^2}\sqrt{1-k^2\tau^2}}\mathrm{d}\tau.$$

Recall that $\mathrm{sn}(x,k)$ is extended to $\mathbb{R}$ with period $4K(k)$ and it is not difficult to show $\phi = u^s_{\lambda,n}$ is a solution to the real-valued equation

$$\phi_{xx} + \lambda(1-\phi^2)\phi = 0. \tag{2.3}$$

To achieve the above result, we first show that if a nontrivial solution to (1.3) has a zero point, then 2μ is an integer and the solution is a real-valued function multiplied by a complex constant. The argument below is essentially due to Ref. 3. Consider a nontrivial solution $u(x)$ which vanishes at $x = x_0$. Denote $u(x) = u_1(x) + iu_2(x)$. Then (1.3) allows the expression

$$\begin{aligned} &(u_1)_{xx} + Q(x)u_1 = 0, \qquad x \in \mathbb{R}, \\ &(u_2)_{xx} + Q(x)u_2 = 0, \qquad x \in \mathbb{R}, \end{aligned} \quad Q(x) := \lambda(1 - |u(x)|^2).$$

Since $u_j(x_0) = u_j(x_0 + 2\pi) = 0 (j = 1,2)$, each u_j is an eigenfunction of the operator

$$L := \frac{d^2}{\mathrm{d}x^2} + Q(x), \quad D(L) = \{u \in H^2(x_0, x_0+2\pi) : u(x_0) = u(x_0+2\pi) = 0\}$$

corresponding to zero eigenvalue if $u_j \not\equiv 0$. It thus follows that $c_1u_1 = c_2u_2$ for some constants $c_1, c_2 \in \mathbb{R}[(c1, c2) \neq (0,0)]$ from the Sturm-Liouville theorem, which tells that the dimension of each eigenspace is one. Set $\phi := \sqrt{1 + c_1^2/c_2^2}u_1$ (or $\sqrt{1 + c_2^2/c_1^2}u_2$). Then the solution u is written in

$$u(x) = \phi(x)\exp(ic)$$

for a constant $c \in \mathbb{R}$. Thus the second condition of (1.3) implies

$$\phi(x + 2\pi)\exp(2\pi\mu i) = \phi(x). \tag{2.4}$$

Since $\phi(x)$ is real valued, 2μ must be an integer.

We next verify that any solution ϕ of (2.3) with (2.4) is written in the form $\phi = u^s_{\lambda,n}$ up to translation and (2.1) is a necessary and sufficient condition of existence. As seen below, it follows from an elementary argument of ordinary differential equations.

Let ϕ be a nontrivial solution having zeros to (2.3) with (2.4). Without loss of generality we may assume $\phi(0) = \phi(2\pi) = 0$ and $\phi_x(0) > 0$. Thus there exists a point $x_1 \in (0, 2\pi)$ such that

$$\phi_x(x_1) = 0, \quad \phi_x(x) > 0 \quad \forall\, x \in [0, x_1).$$

Set $\alpha = \phi(x_1)$. Then the equation (2.3) implies

$$\frac{d\phi}{dx} = \sqrt{\lambda(\alpha^2 - \phi^2)(\beta^2 - \phi^2)/2} \quad \forall\, x \in [0, x_1], \tag{2.5}$$

where

$$\alpha^2 + \beta^2 = 2, \quad 0 < \alpha < \beta. \tag{2.6}$$

Changing variable $\xi(x) := \phi(x)/\alpha$, we have

$$x = \frac{\sqrt{2}}{\beta\sqrt{\lambda}} \int_0^{\phi(x)/\alpha} \frac{1}{\sqrt{(1-\xi^2)(1-(\alpha/\beta)^2\xi^2)}} d\xi, \quad \forall\, x \in [0, x_1]$$

and hence

$$x_1 = \sqrt{2}K(k)/\beta\sqrt{\lambda}, \quad k := \alpha/\beta. \tag{2.7}$$

As a consequence ϕ is written in the form

$$\phi(x) = \alpha\, \mathrm{sn}(K(k)x/x_1, k) \tag{2.8}$$

and this equality is satisfied on the whole $\mathbb{R}$. By the condition (2.4) and

$$\mathrm{sn}(x + 2K(k)n, k) = (-1)^n \mathrm{sn}(x, k), \quad x \in \mathbb{R}, \quad n \in \mathbb{N},$$

there exist $n \in \mathbb{N}$ and $m \in \mathbb{Z}$ such that

$$x_1 = \pi/n, \quad \mu = m + n/2. \tag{2.9}$$

On the other hand, with the aid of (2.6) and the definition of k we obtain

$$\alpha = k\sqrt{2/(1+k^2)}, \quad \beta = \sqrt{2/(1+k^2)}. \tag{2.10}$$

Thus (2.8) and (2.7) yield the expression of $u^{\mathrm{s}}_{\lambda,n}$ and

$$x_1 = \sqrt{1+k^2}K(k)/\sqrt{\lambda}, \tag{2.11}$$

respectively. By (2.9) and (2.11), k must satisfy (2.2).

Consequently the equation (2.3) with (2.4) has a nontrivial solution with n zeros in $[0, 2\pi)$ which is uniquely given by $u^{\mathrm{s}}_{\lambda,n}$ (up to translation) with $k \in (0,1)$ satisfying (2.2) and $\mu = m + n/2 (m \in \mathbb{Z})$.

Now let us consider (2.2). Since

$$K(0) = \frac{\pi}{2}, \quad \frac{dK}{dk} > 0, \quad \lim_{k \to 1} K(k) = \infty, \tag{2.12}$$

(2.2) has a unique solution if and only if $n^2 < 4\lambda$. In conclusion we can assert that any type (I) solution ϕ of (2.3) with (2.4) is written in the form $\phi = u^{\mathrm{s}}_{\lambda,n}$ and the solution exists if and only if (2.1) is satisfied.

III. TYPE (IIb) SOLUTIONS: SECONDARY BIFURCATING SOLUTIONS

In this section we consider a solution with modulating amplitude but nonvanishing everywhere. It is not so simple to obtain globally in the parameters λ and μ, since the solution bifurcates from not a trivial solution but a type (IIa) solution. Namely this solution is a secondary bifurcating solution from the zero solution. Fortunately the method developed in the previous paper[7] still works in this present two-parameters case.

Since $|u(x)| > 0$, we can write $u = w(x) \exp(i\theta(x))$ where $w(x) > 0$. Setting it into Eq. (1.3) yields

$$w_{xx} - \theta_x^2 w + \lambda(1 - w^2)w = 0 \quad (x \in \mathbb{R}), \quad (w^2\theta_x)_x = 0 \quad (x \in \mathbb{R}). \tag{3.1}$$

Then the periodic condition in (1.3) is reduced to $w(x+2\pi)=w(x)$ and

$$\theta(x + 2\pi) + 2\pi\mu = \theta(x) + 2m\pi, \tag{3.2}$$

for an integer m. Integrating the equation $(w^2\theta_x)_x=0$, we have that

$$\theta_x = b/w^2 \tag{3.3}$$

for a constant $b \in \mathbb{R}$. Integrating this equality again and using (3.2), we obtain

$$2(m - \mu)\pi = b\int_0^{2\pi} \frac{1}{w(x)^2}\mathrm{d}x.$$

Thus the equation (3.1) is reduced to

$$\begin{gathered} w_{xx} - b^2/w^3 + \lambda(1 - w^2)w = 0, \quad x \in \mathbb{R}, \\ b = 2(m - \mu)\pi \Big/ \int_0^{2\pi} \frac{\mathrm{d}x}{w(x)^2}, \\ w(x + 2\pi) = w(x), \quad x \in \mathbb{R}, \\ w(x) > 0, \quad x \in \mathbb{R}. \end{gathered} \tag{3.4}$$

Then a solution ψ of (1.2) is obtained by solving the above equation and it is written in the form

$$\psi = w(x)\exp\left\{2(m - \mu)\pi i\int_0^x \frac{1}{w(s)^2}\mathrm{d}s \Big/ \int_0^{2\pi} \frac{1}{w(s)^2}\mathrm{d}s + i\int_0^x h(s)\mathrm{d}s\right\}.$$

We note that (3.4) has a constant solution

$$w = \sqrt{1 - (m - \mu)^2/\lambda}$$

if $\lambda > (m-\mu)^2$. This gives a type (IIa) solution. Since w stands for the amplitude of a solution ψ, we exclude this constant solution. To find all the solutions of (3.4), we also give attention to a solution with n modulating amplitude, that is, a $2\pi/n$-periodic solution of (3.4) for $n \in \mathbb{N}$.

Consequently all type (IIb) solutions are obtained by solving the following system of equations for $w(x)$ and b:

$$\begin{gathered} w_{xx} - b^2/w^3 + \lambda(1 - w^2)w = 0, \quad x \in \mathbb{R}, \\ w(x) > 0, \quad x \in \mathbb{R}, \\ T_w = 2\pi/n, \end{gathered} \tag{3.5}$$

and

$$b = 2(m - \mu)\pi \Big/ \int_0^{2\pi} \frac{1}{w(x)^2}\mathrm{d}x, \tag{3.6}$$

for each $m \in \mathbb{Z}, n \in \mathbb{N}, \mu \in \mathbb{R}$, and $\lambda > 0$, where T_w denotes the fundamental period of $w(x)$.

We here introduce some notations which will be used in our argument. Define

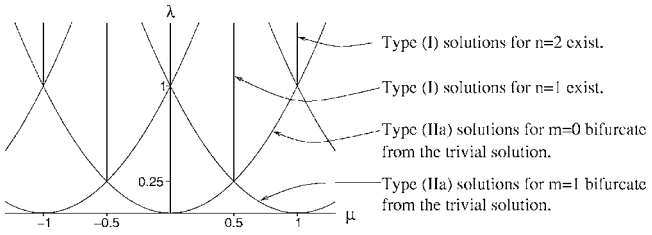

FIG. 1. Bifurcation curves and existence regions of types (I) and (IIa) solutions.

$$\Pi(\nu,k) := \int_0^1 \frac{1}{(1+\nu\tau^2)\sqrt{1-\tau^2}\sqrt{1-k^2\tau^2}}\mathrm{d}\tau, \tag{3.7}$$

$$\alpha(k) := 2/3 - 2n^2K(k)^2(k^2+1)/3\lambda\pi^2, \tag{3.8}$$

$$\beta(k) := 2/3 - 2n^2K(k)^2(1-2k^2)/3\lambda\pi^2, \tag{3.9}$$

$$\gamma(k) := 2/3 - 2n^2K(k)^2(k^2-2)/3\lambda\pi^2. \tag{3.10}$$

The following result establishes not only the existence but also the configuration of every secondary bifurcating solution.

Proposition 3.1: Given $m \in \mathbb{Z}$ *and* $n \in \mathbb{N}$, *let* $D^{\pm}_{m,n}$ *be as in (1.9) and (1.10). For* $(\mu,\lambda) \in D^{+}_{m,n} \cup D^{-}_{m,n}$, *there exists a solution*

$$u^{\mathrm{o}}_{\lambda,\mu,m,n} := w(x)\exp(i\theta(x)),$$

$$w(x) := \sqrt{\frac{2}{3} + \frac{2n^2K(k)^2}{\lambda\pi^2}\left\{k^2\,\mathrm{sn}^2\left(\frac{nK(k)}{\pi}x,k\right) - \frac{k^2+1}{3}\right\}}, \tag{3.11}$$

$$\theta(x) := 2(m-\mu)\pi\left(\int_0^{2\pi}\frac{\mathrm{d}y}{w(y)^2}\right)^{-1}\int_0^x \frac{\mathrm{d}y}{w(y)^2},$$

where $k \in (0,1)$ *is a unique solution of*

$$2(m-\mu)^2K(k)^2 - \lambda\gamma(k)\Pi(\beta(k)/\alpha(k)-1,k)^2\beta(k)/\alpha(k) = 0, \quad \alpha(k) > 0.$$

If $(\mu,\lambda) \notin D^{+}_{m,n} \cup D^{-}_{m,n}$, *there is no solution written as (3.11). Moreover for* $(\mu,\lambda) \in D^{+}_{m,n} \cup D^{-}_{m,n}$, *the solution* $u^{\mathrm{o}}_{\lambda,\mu,m,n}$ *satisfies*

$$u^{\mathrm{o}}_{\lambda,\mu,m,n} - u^{\mathrm{c}}_{\lambda,\mu,m} \to 0 \quad \text{uniformly on } \mathbb{R} \quad \text{as } \lambda \to \lambda_{\mu,m,n}, \tag{3.12}$$

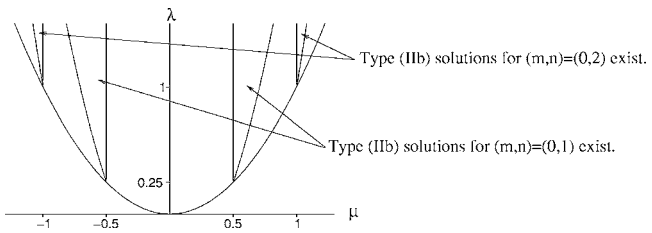

FIG. 2. Existence regions of type (IIb) solutions with $m=0$.

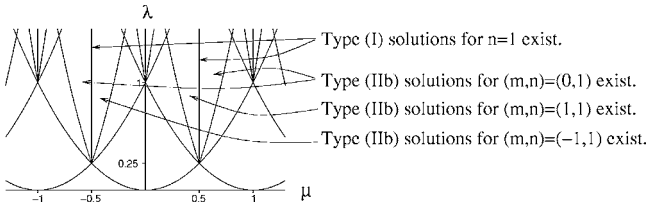

FIG. 3. Existence regions of types (I), (IIa), and (IIb) solutions with $m=-1$, 0, 1.

$$u^{o}_{\lambda,\mu,m,n} - u^{c}_{\lambda,\mu,m} \to 0 \quad \text{uniformly on } \mathbb{R} \text{ as } \mu \to m \pm \sqrt{\lambda/3 + n^2/6}, \tag{3.13}$$

$$u^{o}_{\lambda,\mu,m,n} \pm i u^{s}_{\lambda,n} \to 0 \quad \text{uniformly on } \mathbb{R} \text{ as } \mu \to m \pm n/2. \tag{3.14}$$

Proposition 3.1 implies that the secondary bifurcations take place on

$$\cup_{m\in\mathbb{Z},n\in\mathbb{N}}\{(\mu,\lambda):\mu < m - n/2, m + n/2 < \mu, \lambda = \lambda_{\mu,m,n}\}.$$

Moreover we easily see that any sectorial region $D^{-}_{m,n}$ is adjacent to $D^{+}_{m-n,n}$. Thus we obtain the following corollary.

Corollary 3.1: Let $\lambda > n^2/4$ *and fix it. Define*

$$u(x;\mu) := \begin{cases} u^{o}_{\lambda,\mu,m,n}(x), & \mu^{-}_{\lambda,m,n} < \mu < m - n/2, \\ i u^{s}_{\lambda,n}(x), & \mu = m - n/2, \\ -u^{o}_{\lambda,\mu,m-n,n}(x), & m - n/2 < \mu < \mu^{+}_{\lambda,m-n,n}. \end{cases}$$

Then $\{u(\cdot;\mu):\mu^{-}_{\lambda,m,n} < \mu < \mu^{+}_{\lambda,m-n,n}\}$ *is a continuous curve in* $C(\mathbb{R};\mathbb{C})$.

IV. BIFURCATION DIAGRAMS

In this section we observe bifurcation diagrams for the solutions of Theorem 1.1. These bifurcation diagrams are drawn by using the explicit form of the solutions obtained in Proposition 3.1. We can also exhibit the configuration of type (IIb) solutions for various values of μ.

From Figs. 1–3 we fix the parameter space $(\mu,\lambda) \in \mathbb{R}\times\mathbb{R}^{+}$. Figure 1 shows three bifurcation curves of type (IIa) for $m=-1$, 0, 1 and the straight lines on which type (I) solutions exist.

We see in Fig. 2 existence regions of type (IIb) solutions for $(m,n)=(0,1)$, (0,2) and in Fig. 3 existence regions for $(m,n)=(-2,1),(-2,2),(-1,1),(-1,2)$, (0,1), (0,2), (1,1), (1,2), (2,1), and (2,2).

In Fig. 4 a bifurcation diagram of solutions as λ increases for fixed $\mu=1/4$ is shown. We can observe four branches of type (IIa) solutions and branches of type (IIb) bifurcating from the type

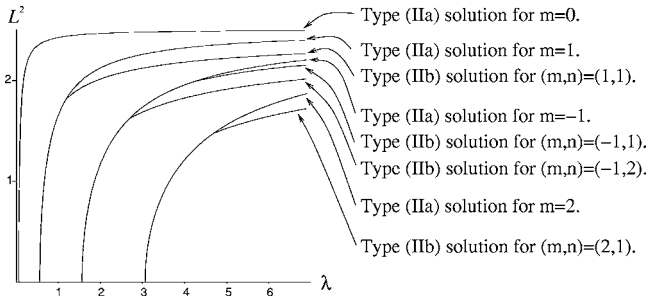

FIG. 4. Bifurcation diagram for λ at $\mu=1/4$. Vertical axis stands for L^2 amplitude.

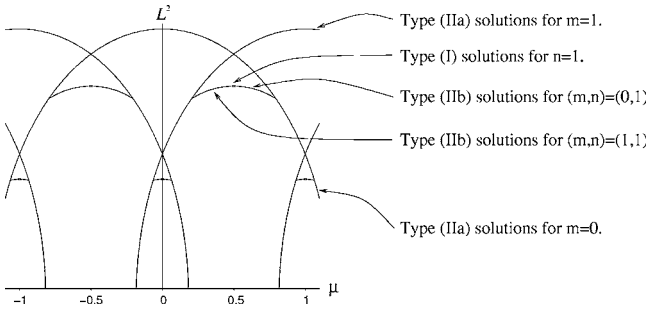

FIG. 5. Bifurcation diagram for μ at $\lambda=1.4$. Vertical axis stands for L^2 amplitude.

(IIa) solutions. On the other hand, Fig. 5 shows a bifurcation diagram as μ varies for fixed $\lambda=1.4$. Three branches of type (IIa) and 10 branches of type (IIb). Small circles separating two branches of type (IIb) indicate type (I) solutions.

Figures 6 and 7 show bifurcation sheets. In Fig. 6 we can observe the bifurcation sheets of types (IIa) and (IIb) solutions on (μ,λ) plane. The vertical axis stands for L^∞ amplitude. In Fig. 7 we also provide bifurcation sheets having cross sections on $\lambda=0.20$, 0.60, 0.85, and 1.40, respectively. The vertical axis stands for L^2 amplitude.

We display the change of configuration in the complex plane of type (IIb) solutions to (1.2) as μ increases. We set $h=$constant (i.e., $\mu=h$) in Figs. 8–10. In Figs. 8 and 9 we fix $\lambda=1.4$ (as in Fig. 5) and plot the solutions on the curves defined by (1.12) for $(m,n)=(0,1)-(-1,1)$ and $(m,n)=(1,2)-(-1,2)$ respectively. We chose six values of μ in the intervals $[-0.795\,822, -0.204\,178]$ and $[-0.064\,5813, 0.064\,5813]$ for Figs. 8 and 9 respectively. Note that the fourth shot (in the left of the second column) of each figure shows type (I) solution. The first shot and the last shot are type (IIa) solutions. We see in Fig. 8 that a solution with $(m,n)=(0,1)$ in the second shot (the winding number 0 and 1 modulation of amplitude) is changed into a solution with

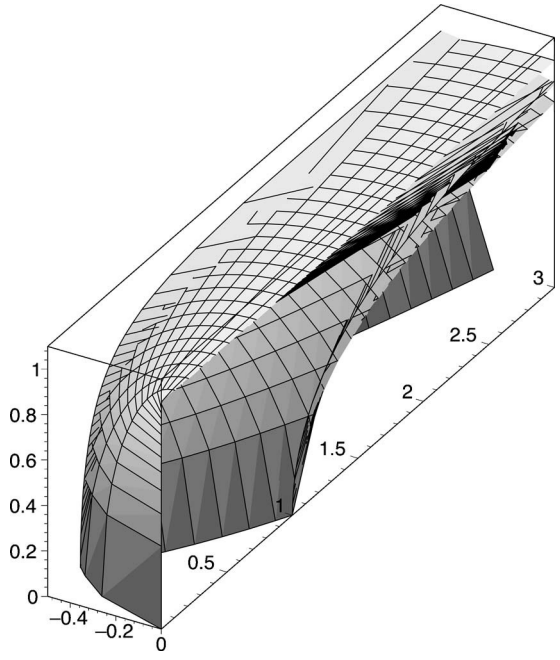

FIG. 6. Bifurcation sheets for (μ,λ). Vertical axis stands for L^∞ amplitude.

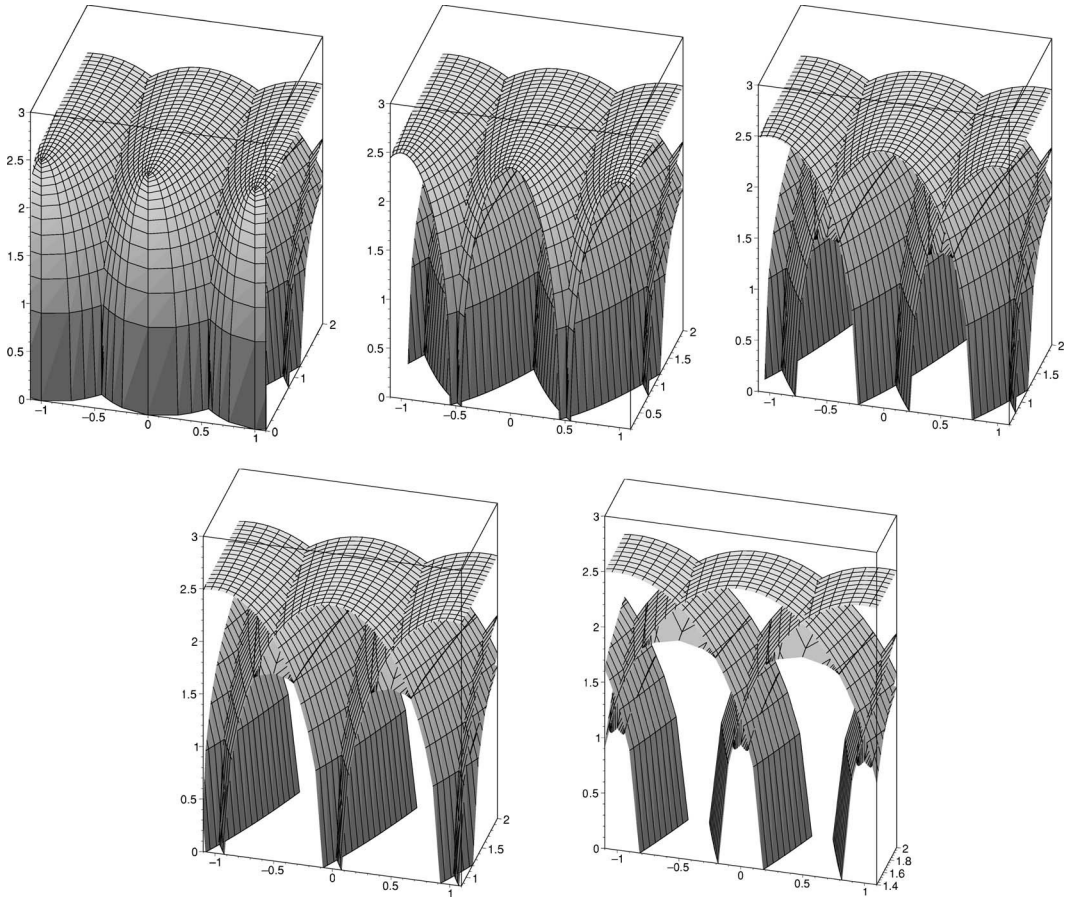

FIG. 7. Bifurcation sheets for (μ,λ). Vertical axis stands for L^2 amplitude.

$(m,n)=(-1,1)$ in the fifth shot. On the other hand, we do not see the change of the winding number of the solutions in Fig. 9, since we are not able to distinguish the sign of the winding number in this figure.

In Fig. 10 for fixed $\lambda=25/2$ we plot the solutions for μ in the interval $[2-5/\sqrt{3},-3+5/\sqrt{3}]$. A solution with $(m,n)=(2,5)$ of the first shot is changed into a solution with $(m,n)=(-3,5)$ in the sixth shot. The fifth shot shows the type (I) solution for $\mu=-1/2$.

V. PROOF OF THEOREM 1.1

We will give the proof of Theorem 1.1. It suffices to prove Proposition 3.1 by (1.4) and Corollary 3.1. Except for the argument related to the continuity of the branch of type (IIa) up to a type (I) solution as $\mu\to m\pm n/2$, the proof is substantially owing to Ref. 7. Therefore we will avoid repeating lengthy arguments in this paper, for example, the proof of Lemma 5.1 below. For the complete proof, the readers can refer to Ref. 7 complementarily.

We first solve (3.5) [without considering (3.6)]. Since w is a nonconstant periodic function in C^2, there exist $x_1,x_2\in\mathbb{R}$ such that $x_1<x_2$ and

$$w_x(x_1)=w_x(x_2)=0,\quad w_x(x)>0\quad(\forall x\in(x_1,x_2)). \tag{5.1}$$

Multiplying $2w_x$ to the equation in (3.5), we have

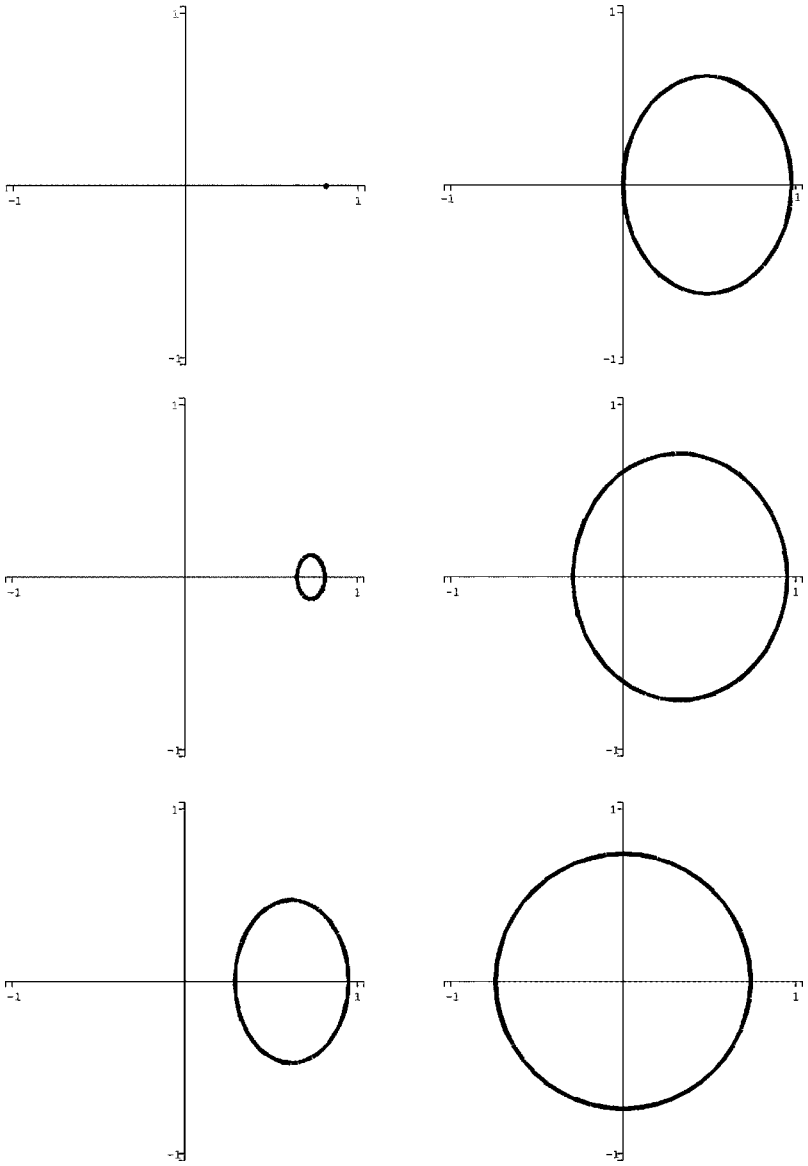

FIG. 8. Type (IIb) $[(m,n)=(0,1),(-1,1)]$ and type (I) solutions in $\mathbb{C}$.

$$\frac{d}{dx}\left((w_x)^2+\frac{b^2}{w^2}+\frac{\lambda}{2}(2w^2-w^4)\right)=0.$$

Thus

$$w_x(x)^2=\frac{\lambda\{w(x)^2-w(x_1)^2\}}{2w(x)^2w(x_1)^2}\left(\{w(x)^2+w(x_1)^2-2\}w(x)^2w(x_1)^2+\frac{2b^2}{\lambda}\right). \tag{5.2}$$

Set $x=x_2$ in (5.2) and

$$\alpha=w(x_1)^2, \quad \beta=w(x_2)^2.$$

Then we obtain $(\beta+\alpha-2)\alpha\beta+2b^2/\lambda=0$, which implies

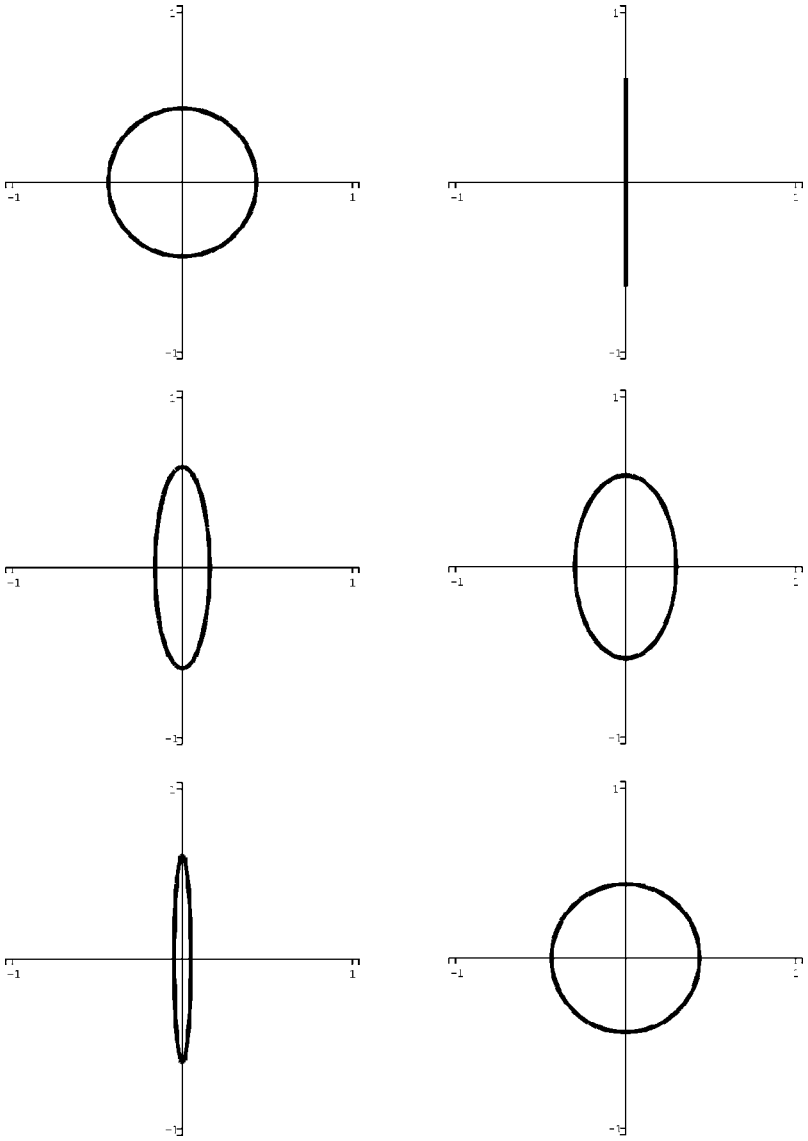

FIG. 9. Type (IIb) $[(m,n)=(1,2),(-1,2)]$ and type (I) solutions in $\mathbb{C}$.

$$2b^2/\lambda = \alpha\beta\gamma, \quad \gamma := 2-\alpha-\beta. \tag{5.3}$$

Introducing the variable

$$v(x) := w(x)^2,$$

and substituting (5.3) into (5.2), we can easily verify

$$(v_x(x))^2 = 2\lambda(v(x)-\alpha)(v(x)-\beta)(v(x)-\gamma), \quad \forall\, x \in \mathbb{R}.$$

Since

$$0 < \alpha < v(x) < \beta, \quad v_x(x) > 0 \quad (\forall x \in (x_1,x_2)),$$

the ordering $\gamma \geqslant \beta$ holds. In the sequel

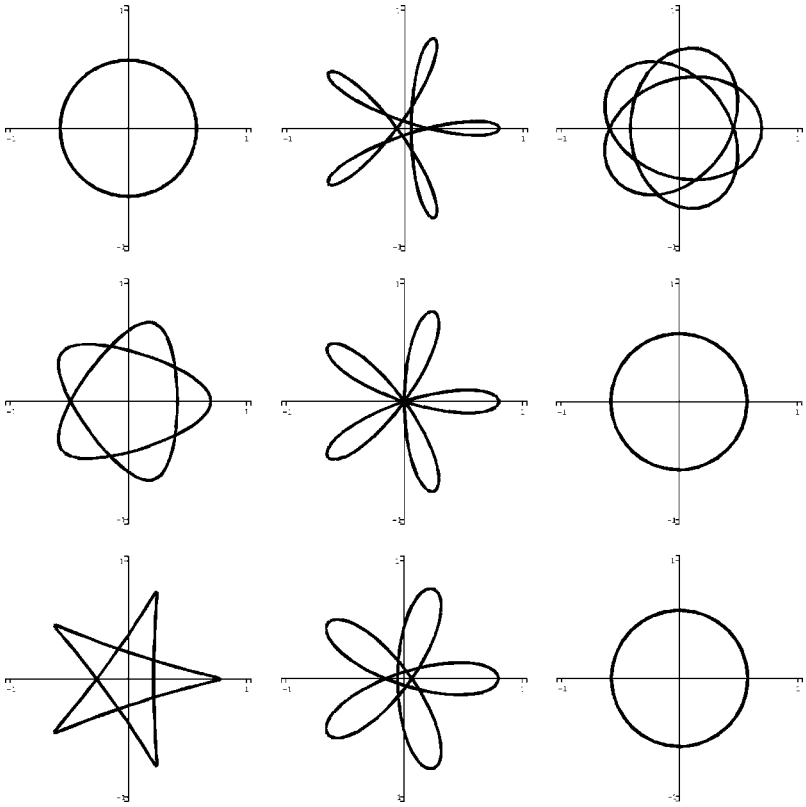

FIG. 10. Type (IIb) $[(m,n)=(2,5),(-3,5)]$ and type (I) solutions in $\mathbb{C}$.

$$v_x(x) = \sqrt{2\lambda(v(x)-\alpha)(v(x)-\beta)(v(x)-\gamma)}, \quad \forall\, x \in [x_1,x_2],$$
$$0 < \alpha < \beta \leqslant \gamma, \quad \alpha+\beta+\gamma = 2. \tag{5.4}$$

Next we solve (5.4). By integration of (5.4),

$$x - x_1 = \frac{1}{\sqrt{2\lambda}} \int_\alpha^{v(x)} \frac{\mathrm{d}y}{\sqrt{(y-\alpha)(y-\beta)(y-\gamma)}}, \quad \forall\, x \in [x_1,x_2]. \tag{5.5}$$

Changing the variable $y=\alpha+(\beta-\alpha)\tau^2$ in (5.5) and setting

$$k := \sqrt{(\beta-\alpha)/(\gamma-\alpha)}, \tag{5.6}$$

we see

$$\frac{\mathrm{d}y}{\sqrt{(y-\alpha)(y-\beta)(y-\gamma)}} = \frac{2\,\mathrm{d}\tau}{\sqrt{(\gamma-\alpha)(1-\tau^2)(1-k^2\tau^2)}}.$$

Applying this to (5.5) yields

$$x - x_1 = \sqrt{\frac{2}{\lambda(\gamma-\alpha)}}\,\mathrm{sn}^{-1}\left(\sqrt{\frac{v(x)-\alpha}{\beta-\alpha}}, k\right), \quad \forall\, x \in [x_1,x_2]. \tag{5.7}$$

Thus on the interval $[x_1,x_2]$ we obtain

$$w(x)=\sqrt{v(x)}=\sqrt{\alpha+(\beta-\alpha)\mathrm{sn}^2\left(\sqrt{\frac{\lambda(\gamma-\alpha)}{2}}(x-x_1),k\right)}. \tag{5.8}$$

Since this $w(x)$ is defined over $\mathbb{R}$ and periodic with period $2K(k)\sqrt{2/\lambda(\gamma-\alpha)}$ [$\mathrm{sn}^2(x,k)$ has a period $2K(k)$], $T_w=2\pi/n$ implies

$$2K(k)\sqrt{2/\lambda(\gamma-\alpha)}=2\pi/n. \tag{5.9}$$

Combining (5.3), (5.6), and (5.9), we obtain the expressions (3.8), (3.9), and (3.10). In the sequel we obtained solutions of (3.5). In fact let $n\in\mathbb{N}$ and $\lambda>0$. Then $(w(x),\lambda,b)$ satisfies (3.5) if and only if there exist $x_1\in\mathbb{R}$ and $k\in(0,1)$ such that $\alpha=\alpha(k)>0$ and

$$w(x+x_1)=\sqrt{\alpha+(\beta-\alpha)\mathrm{sn}^2\left(\frac{nK(k)}{\pi}x,k\right)},$$
$$b^2=\frac{\lambda\alpha\beta\gamma}{2}. \tag{5.10}$$

Now we take the condition (3.6) into account. Since $T_w=2\pi/n$ and a symmetry,

$$\int_0^{2\pi}\frac{dx}{w(x)^2}=\int_0^{2\pi}\frac{dx}{w(x+x_1)^2}=2n\int_0^{\pi/n}\frac{dx}{w(x+x_1)^2}.$$

The similar argument used in the derivation of (5.5) and (5.7) leads us to

$$\int_0^{\pi/n}\frac{dx}{w(x+x_1)^2}=\frac{1}{\sqrt{2\lambda}}\int_\alpha^\beta\frac{dy}{y\sqrt{(y-\alpha)(y-\beta)(y-\gamma)}}=\sqrt{\frac{2}{\lambda}}\frac{\Pi(\beta/\alpha-1,k)}{\alpha\sqrt{\gamma-\alpha}}, \tag{5.11}$$

where Π is the complete elliptic integral defined by (3.7). Since $\alpha>0$ and $\gamma-\alpha=2n^2K(k)^2/\lambda\pi^2$, the equation (3.6) is written as

$$b=(m-\mu)\alpha K(k)/\Pi(\beta/\alpha-1,k).$$

Substituting this into the second equation in (5.10), we can reduce our problem to solving the equation

$$2(m-\mu)^2K(k)^2-\lambda\gamma\Pi(\beta/\alpha-1,k)^2\beta/\alpha=0 \tag{5.12}$$

under the constraint $\alpha>0$. To simplify the notation in the rest of this paper, we denote the left-hand side of Eq. (5.12) by $\rho(k,\lambda,\mu)$ for each $n\in\mathbb{N}$ and $m\in\mathbb{Z}$, that is, we set

$$\rho(k,\lambda,\mu):=2(m-\mu)^2K(k)^2-\lambda\gamma\Pi(\beta/\alpha-1,k)^2\beta/\alpha. \tag{5.13}$$

Summarizing the above argument, we can assert that for each given $n\in\mathbb{N}$, $m\in\mathbb{Z}$, $\mu\in\mathbb{R}$, $\lambda>0$, and $x_1\in\mathbb{R}$, every nonconstant solution of (3.5) with (3.6) is written as

$$w(x+x_1)=\sqrt{\alpha+(\beta-\alpha)\mathrm{sn}^2\left(\frac{nK(k)}{\pi}x,k\right)},\quad b=\mathrm{sgn}(m-\mu)\sqrt{\frac{\lambda\alpha\beta\gamma}{2}}, \tag{5.14}$$

if $(k,\lambda)\in\Sigma$ is a solution of $\rho(k,\lambda,\mu)=0$, where

$$\Sigma:=\{(k,\lambda)\in(0,1)\times\mathbb{R}^+:\alpha(k)>0\}. \tag{5.15}$$

The following proposition guarantees the unique existence of a solution to $\rho=0$.

Proposition 5.1: Let $n\in\mathbb{N}$, $m\in\mathbb{Z}$ and let $D^{\pm}_{m,n}$ be the ones defined in (1.9) and (1.10).

(i) *The equation (5.12) has a solution $(k,\lambda)=(k(\lambda,\mu),\lambda)\in\Sigma$ if*

$$(\mu,\lambda) \in D^-_{m,n} \cup D^+_{m,n}, \tag{5.16}$$

where Σ *is defined by (5.15). Moreover* $k(\lambda,\mu)$ *is unique for each* $(\mu,\lambda) \in D^-_{m,n} \cup D^+_{m,n}$.

(ii) *Let* $(\mu,\lambda) \in D^-_{m,n} \cup D^+_{m,n}$. *Then*

$$k(\lambda,\mu) \to 0 \quad \text{as } \lambda \to 3(\mu-m)^2 - n^2/2, \tag{5.17}$$

$$k(\lambda,\mu) \to 0 \quad \text{as } \mu \to m \pm \sqrt{\lambda/3 + n^2/6}, \tag{5.18}$$

$$\alpha(k(\lambda,\mu)) \to 0 \quad \text{as } \mu \to m \pm n/2. \tag{5.19}$$

(iii) *There is no solution to (5.12) in* Σ *if*

$$(\mu,\lambda) \notin \bigcup_{m\in\mathbb{Z},n\in\mathbb{N}} (D^-_{m,n} \cup D^+_{m,n}).$$

Proof of Proposition 5.1 (i): Let $k=k_\alpha(\lambda) \in (0,1)$ satisfy $\alpha(k)=0$. It is easy to verify that $k=k_\alpha(\lambda)$ is uniquely determined for each $\lambda > n^2/4$ and Σ is written in the form

$$\Sigma = \{(k,\lambda): 0 < k < k_\alpha(\lambda), \lambda > n^2/4\}.$$

We here remark that $\Sigma=\emptyset$ if $\lambda \leqslant n^2/4$. Using the same computation as in the proof of Proposition 3.1 (i) of Ref. 7, we can see

$$\rho(0,\lambda,\mu) = \frac{\pi^2}{6}\left(\frac{6(m-\mu)^2 - n^2}{2} - \lambda\right) \tag{5.20}$$

and

$$\lim_{k\uparrow k_\alpha(\lambda)} \rho(k,\lambda,\mu) = (4(m-\mu)^2 - n^2)\frac{K(k_\alpha(\lambda))^2}{2}. \tag{5.21}$$

Indeed the latter limit is obtained by verifying

$$\sqrt{\beta/\alpha}\Pi(\beta/\alpha - 1, k) \to \pi/2 \quad (k\uparrow k_\alpha(\lambda)). \tag{5.22}$$

Thus the function $\rho(\cdot,\cdot,\mu)$ is extended as a continuous function on $\bar{\Sigma}\backslash\{\lambda=n^2/4\}$. Consequently $\rho(0,\lambda,\mu)\rho(k_\alpha(\lambda),\lambda,\mu) < 0$ is satisfied if and only if

$$\frac{6(m-\mu)^2 - n^2}{2} < \lambda, \quad 0 < 4(m-\mu)^2 - n^2, \tag{5.23}$$

because the inequality $\lambda > n^2/4$ implies

$$\frac{6(m-\mu)^2 - n^2}{2} - \lambda < \frac{3(4(m-\mu)^2 - n^2)}{4}.$$

Therefore it follows from the continuity of $\rho(k,\lambda,\mu)$ that (5.12) has a solution $k=k(\lambda,\mu)$ if (μ,λ) satisfies (5.16) for each $n \in \mathbb{N}$ and $m \in \mathbb{Z}$.

The following lemma implies that a solution $k=k(\lambda,\mu)$ to (5.12) is unique for each (μ,λ) if it exists in $(0,k_\alpha(\lambda))$. By this lemma we can conclude the proof of Proposition 5.1 (i). □

Lemma 5.1: If $k \in (0,k_\alpha(\lambda))$ *satisfies* $\rho(k,\lambda,\mu)=0$, *then*

$$\frac{\partial\rho}{\partial k}(k,\lambda,\mu) > 0.$$

The proof of Lemma 5.1 is performed literally in the same way as in Ref. 7; we omit it (see the proof of Lemma 3.5 in Ref. 7).

Proof of Proposition 5.1 (ii): We first show (5.17). It is clear that, for fixed μ which satisfies $(\mu-m)^2>n^2/4$, both $\rho(0,\lambda,\mu)$ and $\rho(k_\alpha(\lambda),\lambda,\mu)$ are strictly positive if $\lambda\in(n^2/4,\lambda_{\mu,m,n})$. From Lemma 5.1, it follows that

$$\rho(k,\lambda,\mu)>0,\quad \forall\, k\in[0,k_\alpha(\lambda)],\quad \forall\,\lambda\in(n^2/4,\lambda_{\mu,m,n}) \tag{5.24}$$

and hence

$$\rho(k,\lambda_{\mu,m,n},\mu)=\lim_{\lambda\uparrow\lambda_{\mu,m,n}}\rho(k,\lambda,\mu)\geqslant 0,\quad \forall\, k\in[0,k_\alpha(\lambda_{\mu,m,n})].$$

Using, (5.20) and (5.21), and Lemma 5.1 again, we can assert that

$$\begin{gathered}\rho(k,\lambda_{\mu,m,n},\mu)>0,\quad \forall\, k\in(0,k_\alpha(\lambda_{\mu,m,n})],\\ \rho(0,\lambda_{\mu,m,n},\mu)=0.\end{gathered} \tag{5.25}$$

Let $\{\lambda_\sigma\}$ be any sequence satisfying $\lambda_\sigma\downarrow\lambda_{\mu,m,n}$ as $\sigma\to\infty$. Since $k(\lambda,\mu)$ is bounded and ρ is continuous, there exists a subsequence $\{\lambda_{\sigma'}\}\subset\{\lambda_\sigma\}$ such that a limit k_* of $k(\lambda_{\sigma'},\mu)$ as $\sigma'\to\infty$ exists in $[0,k_\alpha(\lambda_{\mu,m,n})]$ and $\rho(k_*,\lambda_{\mu,m,n},\mu)=0$. Thus the limit k_* must be 0 by (5.25). This concludes the proof of (5.17).

As for the proof of (5.18), we can prove it similarly as right above, so omit it.

Now we prove (5.19), that is,

$$\lim_{\mu\to m\pm n/2}k(\lambda,\mu)=k_\alpha(\lambda) \tag{5.26}$$

for $(\mu,\lambda)\in D^+_{m,n}\cup D^-_{m,n}$. Let $\lambda>n^2/4$ be fixed. Both $\rho(0,\lambda,\mu)$ and $\rho(k_\alpha(\lambda),\lambda,\mu)$ are strictly negative if μ satisfies

$$m-n/2<\mu<m+n/2.$$

Lemma 5.1 implies

$$\rho(k,\lambda,\mu)<0,\quad \forall\, k\in[0,k_\alpha(\lambda)],\quad \forall\,\mu\in(m-n/2,m+n/2). \tag{5.27}$$

Thus

$$\rho(k,\lambda,m\pm n/2)\leqslant 0,\quad \forall\, k\in[0,k_\alpha(\lambda)]. \tag{5.28}$$

Combining (5.20), (5.21), and (5.28), and Lemma 5.1, we obtain

$$\begin{gathered}\rho(k,\lambda,m\pm n/2)<0,\quad \forall\, k\in[0,k_\alpha(\lambda)),\\ \rho(k_\alpha(\lambda),\lambda,m\pm n/2)=0.\end{gathered} \tag{5.29}$$

Therefore it follows that $k(\lambda,\mu)\to k_\alpha(\lambda)$ as $\mu\to m\pm n/2$ from the similar argument in the proof of (5.17). □

Proof of Proposition 5.1 (iii): Let $m\in\mathbb{Z}$ and $n\in\mathbb{N}$ be fixed. As mentioned in the proof of (i), $\Sigma=\emptyset$ if $\lambda\leqslant n^2/4$. Thus it suffices to prove $\rho(k,\lambda,\mu)\neq 0$ for $\forall k\in(0,k_\alpha(\lambda))$ if $(\mu,\lambda)\in\{(\mu,\lambda):\lambda>n^2/4\}\setminus(D^+_{m,n}\cup D^-_{m,n})$. By virtue of (5.24) and (5.25), it is clear that $\rho(k,\lambda,\mu)>0$ for $\forall k\in(0,k_\alpha(\lambda))$ if $n^2/4<\lambda\leqslant\lambda_{\mu,m,n}$. On the other hand, it follows from (5.27) and (5.29) that $\rho(k,\lambda,\mu)<0$ for $\forall k\in(0,k_\alpha(\lambda))$ if $m-n/2\leqslant\mu\leqslant m+n/2$ and $\lambda>n^2/4$. Therefore (iii) was proved. □

Using Proposition 5.1, we will complete the proof of Proposition 3.1, thus Theorem 1.1.

Proof of Proposition 3.1: As observed above, we proved that the type (IIa) solution is written in the form (5.14). On the other hand, Proposition 5.1 directly leads to existence and nonexistence conditions of the type (IIb) solutions which are stated in Proposition 3.1. Substituting (3.8) and (3.9) into (5.14) with $x_1=0$, we obtain (3.11). Thus the former part of the proposition was proved.

For the proof of the latter part of Proposition 3.1 it suffices to prove, (3.12), (3.13), and (3.14). In the rest of the proof, $w=w(x)$ denotes (5.14) with $x_1=0$ for simplicity of notation.

We first prove (3.12). It follows from (5.17) that if $(\mu,\lambda)\in D^-_{m,n}\cup D^+_{m,n}$ and $\lambda\to\lambda_{\mu,m,n}$, then $k(\lambda,\mu)\to 0$. Thus

$$\alpha\to 2/3-n^2/6\lambda_{\mu,m,n}=1-(\mu-m)^2/\lambda_{\mu,m,n}\quad\text{as }\lambda\to\lambda_{\mu,m,n},\tag{5.30}$$

$$\beta-\alpha\to 0\quad\text{as }\lambda\to\lambda_{\mu,m,n}.\tag{5.31}$$

For each $\ell\in\mathbb{Z}$, if $x\in[2\pi\ell,2\pi(\ell+1)]$ then

$$\begin{aligned}\theta(x)-(m-\mu)x&=(m-\mu)\left\{2\pi\int_0^x\frac{1}{w(y)^2}\mathrm{d}y\Big/\int_0^{2\pi}\frac{1}{w(y)^2}dy-x\right\}\\&=(m-\mu)\left\{2\pi\int_0^{x-2\pi\ell}\frac{1}{w(y)^2}\mathrm{d}y\Big/\int_0^{2\pi}\frac{1}{w(y)^2}\mathrm{d}y+2\pi\ell-x\right\}.\end{aligned}$$

Since

$$\sqrt{\alpha(k(\lambda,\mu))}\leqslant w(x)\leqslant\sqrt{\beta(k(\lambda,\mu))},$$

a simple calculation yields

$$\frac{\alpha-\beta}{\beta}(x-2\pi\ell)\leqslant 2\pi\int_0^{x-2\pi\ell}\frac{1}{w(y)^2}\mathrm{d}y\Big/\int_0^{2\pi}\frac{1}{w(y)^2}\mathrm{d}y+2\pi\ell-x\leqslant\frac{\beta-\alpha}{\alpha}(x-2\pi\ell)$$

and hence we obtain

$$\sup_{x\in[2\pi\ell,2\pi(\ell+1)]}\left|\theta(x)-(m-\mu)x\right|\leqslant\frac{2\pi|m-\mu|(\beta-\alpha)}{\alpha},\quad\forall\,\ell\in\mathbb{Z}.$$

It is clear that

$$\begin{aligned}|u^{\mathrm{o}}_{\lambda,\mu,m,n}(x)-u^{\mathrm{c}}_{\lambda,\mu,m}(x)|&=\left|w(x)\exp(i\theta(x)-i(m-\mu)x)-\sqrt{1-(m-\mu)^2/\lambda}\right|\leqslant|w(x)||\exp(i\theta(x)\\&\quad-i(m-\mu)x)-1|+\left|w(x)-\sqrt{1-(m-\mu)^2/\lambda}\right|,\end{aligned}$$

and

$$\sup_{x\in\mathbb{R}}\left|w(x)-\sqrt{1-(m-\mu)^2/\lambda}\right|\to 0\quad\text{as }\lambda\to\lambda_{\mu,m,n}$$

in terms of (5.30) and (5.31). It is also clear that

$$\begin{aligned}|\exp(i\theta(x)-i(m-\mu)x)-1|^2&=\{\cos(\theta(x)-(m-\mu)x)-1\}^2+\sin^2(\theta(x)-(m-\mu)x)\\&\leqslant 4\sin^4(\pi|m-\mu|(\beta-\alpha)/\alpha)+\sin^2(2\pi|m-\mu|(\beta-\alpha)/\alpha)\end{aligned}$$

and hence

$$\sup_{x\in\mathbb{R}}\left|\exp(i\theta(x)-i(m-\mu)x)-1\right|\to 0\quad\text{as }\lambda\to\lambda_{\mu,m,n},$$

by (5.31). Therefore (3.12) follows.

Similarly, (3.13) follows from (5.18).

Next we prove (3.14). We only consider $\mu\to m-n/2$ because the other case is easily done with a little modification of the argument. Let $(\mu,\lambda)\in D^-_{m,n}$ and λ be fixed. We first consider the limit of $w=w(x)$ as $\mu\to m-n/2$. Since $\alpha(k_\alpha(\lambda))=0$ holds and (5.19) implies $k(\lambda,\mu)\to k_\alpha(\lambda)$ as $\mu\to m-n/2$, we obtain

$$\beta-\alpha\to 2k_\alpha(\lambda)^2/(k_\alpha(\lambda)^2+1)\quad(\mu\to m-n/2).$$

Hence

$$w(x)\to k_\alpha(\lambda)\sqrt{2/(k_\alpha(\lambda)^2+1)}\left|\mathrm{sn}(nK(k_\alpha(\lambda))x/\pi,k_\alpha(\lambda))\right|, \tag{5.32}$$

uniformly for x as $\mu\to m-n/2$. On the other hand, noticing that $k=k_\alpha(\lambda)$ satisfies (2.2), we can write $u^{\mathrm{s}}_{\lambda,n}$ as

$$u^{\mathrm{s}}_{\lambda,n}(x)=k_\alpha(\lambda)\sqrt{2/(1+k_\alpha(\lambda)^2)}\,\mathrm{sn}(nK(k_\alpha(\lambda))x/\pi,k_\alpha(\lambda)).$$

We thereby obtain the following: For any $\varepsilon>0$, there exists $\delta_1=\delta_1(\varepsilon)>0$ such that

$$\sup_{x\in\mathbb{R}}\left|w(x)-\left|u^{\mathrm{s}}_{\lambda,n}(x)\right|\right|\leqslant\varepsilon \tag{5.33}$$

for $\forall\mu\in(m-n/2-\delta_1,m-n/2)$. We here remark that $u^{\mathrm{s}}_{\lambda,n}(x)$ is defined independently of μ, although it is not a solution to (1.3) if $2\mu\notin\mathbb{Z}$. Since $u^{\mathrm{s}}_{\lambda,n}(x)$ vanishes at $x=2\ell\pi/n(\ell\in\mathbb{Z})$, we can verify that, for any $\varepsilon>0$, there exists $d_1=d_1(\varepsilon)$ such that

$$\max_{\ell\in\mathbb{Z}}\sup_{|x-2\ell\pi/n|\leqslant d_1}\left|u^{\mathrm{s}}_{\lambda,n}(x)\right|\leqslant\varepsilon \tag{5.34}$$

thus

$$\max_{\ell\in\mathbb{Z}}\sup_{|x-2\ell\pi/n|\leqslant d_1}\left|w(x)\right|\leqslant 2\varepsilon, \tag{5.35}$$

for $\forall\mu\in(m-n/2-\delta_1,m-n/2)$.

We next deal with θ. Combining (3.8), (3.10), and (5.11), we have

$$\int_0^{2\pi}\frac{1}{w(x)^2}\mathrm{d}x=\frac{2\pi\Pi(\beta/\alpha-1,k)}{\alpha K(k)}.$$

Arbitrarily given $\ell\in\mathbb{Z}$, if $x\in(2\pi\ell/n,2\pi(\ell+1)/n)$, then

$$\int_0^x\frac{1}{w(s)^2}\mathrm{d}s=\frac{(2\ell+1)\pi\Pi(\beta/\alpha-1,k)}{n\alpha K(k)}+\int_{(2\ell+1)\pi/n}^x\frac{1}{w(s)^2}\mathrm{d}s,$$

while

$$\int_0^{2\pi\ell/n}\frac{1}{w(s)^2}\mathrm{d}s=\frac{2\ell\pi\Pi(\beta/\alpha-1,k)}{n\alpha K(k)},$$

where $(2\ell+1)\pi/n$ is the middle point of the interval $(2\pi\ell/n,2\pi(\ell+1)/n)$. Thus

$$\theta(x)=\begin{cases}\dfrac{(m-\mu)(2\ell+1)\pi}{n}+\dfrac{(m-\mu)\alpha K(k)}{\Pi(\beta/\alpha-1,k)}\displaystyle\int_{(2\ell+1)\pi/n}^x\frac{1}{w(s)^2}\mathrm{d}s\\ \text{if } x\in(2\pi\ell/n,2\pi(\ell+1)/n)\quad(\ell\in\mathbb{Z}),\\ \dfrac{2(m-\mu)\ell\pi}{n}\quad\text{if } x=2\pi\ell/n\quad(\ell\in\mathbb{Z}).\end{cases} \tag{5.36}$$

The limit of θ as $\mu\to m-n/2$ is achieved as follows. Recalling (5.22), we see

$$\alpha/\Pi(\beta/\alpha-1,k)\to 0\quad(\mu\uparrow m-n/2). \tag{5.37}$$

It is also clear that

$$\left| \int_{(2\ell+1)\pi/n}^{x} \frac{1}{w(s)^2} \mathrm{d}s \right| \leqslant \frac{\pi}{n} \frac{1}{w(d_1)^2}, \quad \forall\, x \in [2\pi\ell/n + d_1, 2\pi(\ell+1)/n - d_1],$$

where $d_1 = d_1(\varepsilon)$ is as in (5.34) and (5.35). Thus it follows from (5.32), (5.36), and (5.37), and the above inequality that for any $\varepsilon > 0$ there exists $\delta_2 = \delta_2(\varepsilon, d_1(\varepsilon)) > 0$ such that

$$\sup_{x \in (2\pi\ell/n + d_1, 2\pi(\ell+1)/n - d_1)} |\theta(x) - (2\ell+1)\pi/2| \leqslant \varepsilon, \ \ \forall\, \mu \in (m - n/2 - \delta_2, m - n/2). \tag{5.38}$$

Now we estimate

$$|u^{\mathrm{o}}_{\lambda,\mu,m,n}(x) - i u^{\mathrm{s}}_{\lambda,n}(x)|^2 = w(x)^2 \cos^2\theta(x) + \{w(x)\sin\theta(x) - u^{\mathrm{s}}_{\lambda,n}(x)\}^2. \tag{5.39}$$

For $\varepsilon > 0$, set

$$\delta = \delta(\varepsilon) := \min\{\delta_1(\varepsilon), \delta_2(\varepsilon, d_1(\varepsilon))\}. \tag{5.40}$$

Then it is clear that, if $\mu \in (m - n/2 - \delta, m - n/2)$,

$$\begin{aligned} \sup_{x \in \mathbb{R}} w(x)^2 \cos^2\theta(x) &\leqslant \max_{\ell \in \mathbb{Z}} \sup_{|x - 2\ell\pi/n| \leqslant d_1} w(x)^2 \cos^2\theta(x) + \max_{\ell \in \mathbb{Z}} \sup_{x \in (2\pi\ell/n + d_1, 2\pi(\ell+1)/n - d_1)} w(x)^2 \cos^2\theta(x) \\ &\leqslant 4\varepsilon^2 + \max_{\ell \in \mathbb{Z}} \cos^2((2\ell+1)\pi/2 + \varepsilon) \leqslant 4\varepsilon^2 + \sin^2\varepsilon, \end{aligned} \tag{5.41}$$

where we used $0 < w(x) < 1$. We estimate the second term on the right-hand side of (5.39). Since (5.35) and (5.34), we have an estimate in the neighborhoods of zero points of $u^{\mathrm{s}}_{\lambda,n}$ as

$$\max_{\ell \in \mathbb{Z}} \sup_{|x - 2\ell\pi/n| \leqslant d_1} \{w(x)\sin\theta(x) - u^{\mathrm{s}}_{\lambda,n}(x)\}^2 \leqslant 9\varepsilon^2$$

for $\mu \in (m - n/2 - \delta, m - n/2)$. In the complement to the neighborhoods of the zero points of $u^{\mathrm{s}}_{\lambda,n}$, the second term of the right-hand side of (5.39) is estimated as follows: Let $\mu \in (m - n/2 - \delta, m - n/2)$ and $x \in (2\pi\ell/n + d_1, 2\pi(\ell+1)/n - d_1)$. Then

$$\begin{aligned} |w(x)\sin\theta(x) - u^{\mathrm{s}}_{\lambda,n}(x)| &= |w(x)\sin\theta(x) - |u^{\mathrm{s}}_{\lambda,n}(x)|(-1)^{\ell}| \\ &\leqslant \big|w(x) - |u^{\mathrm{s}}_{\lambda,n}(x)|\big||\sin\theta(x)| + |u^{\mathrm{s}}_{\lambda,n}(x)||\sin\theta(x) - (-1)^{\ell}| \leqslant \varepsilon \\ &\quad + k_{\alpha}(\lambda)\sqrt{2/(1 + k_{\alpha}(\lambda)^2)}\,|\sin\theta(x) - (-1)^{\ell}| \leqslant \varepsilon + \sqrt{2}\,|\sin\theta(x) - (-1)^{\ell}|. \end{aligned}$$

Using (5.38) and

$$\begin{aligned} |\sin\theta(x) - (-1)^{\ell}| &= |(-1)^{\ell}\{\cos(\theta(x) - (2\ell+1)\pi/2) - 1\}| \\ &= 2\sin^2\{(\theta(x) - (2\ell+1)\pi/2)/2\} \leqslant 2\sin^2(\varepsilon/2), \end{aligned}$$

we obtain

$$\sup_{x \in (2\pi\ell/n + d_1, 2\pi(\ell+1)/n - d_1)} |w(x)\sin\theta(x) - u^{\mathrm{s}}_{\lambda,n}(x)| \leqslant \varepsilon + 2\sqrt{2}\sin^2(\varepsilon/2). \tag{5.42}$$

In consequence, combining (5.41) and (5.42), we obtain that there exists $C > 0$ such that for any $\varepsilon > 0$,

$$\sup_{x \in \mathbb{R}} |u^{\mathrm{o}}_{\lambda,\mu,m,n}(x) - i u^{\mathrm{s}}_{\lambda,n}(x)| \leqslant C\varepsilon, \quad \forall\, \mu \in (m - n/2 - \delta, m - n/2).$$

Therefore it completes the proof of (3.14). In conclusion we obtained Proposition 3.1. □

VI. PROOF OF THEOREM 1.2

It is clear that for $\lambda \in (0,1/4]$ the assertion of the theorem is true. Throughout the section we assume $\lambda > 1/4$. Recall the assumption of Theorem 1.2. We denote the energies for the solutions as

$$E^{\mathrm{s}}_{\lambda,n}(\mu) := E(\psi^{\mathrm{s}}_{\lambda,\mu,n};\lambda,\mu h_e),$$

$$E^{\mathrm{c}}_{\lambda,m}(\mu) := E(\psi^{\mathrm{c}}_{\lambda,\mu,m};\lambda,\mu h_e),$$

$$E^{\mathrm{o}}_{\lambda,m,n}(\mu) := E(\psi^{\mathrm{o}}_{\lambda,\mu,m,n};\lambda,\mu h_e).$$

For simplicity of notation we drop ω in the expression of the solutions in the statement of the theorem.

Fix arbitrary $m \in \mathbb{Z}$. We let $(\mu_0,\lambda) \in \operatorname{Int} \mathcal{D}_m$. For the proof of the theorem it suffices to show the following facts:

(i) Given $(\mu,\lambda) \in \mathcal{D}_m$, it holds that

$$\begin{gathered}(\mu - m)(\mathrm{d}E^{\mathrm{c}}_{\lambda,m}(\mu)/\mathrm{d}\mu) > 0,\\ E^{\mathrm{c}}_{\lambda,m}(\mu_0) < E^{\mathrm{c}}_{\lambda,m}(m \pm 1/2) \leqslant E^{\mathrm{c}}_{\lambda,\ell}(m \pm 1/2) \leqslant E^{\mathrm{c}}_{\lambda,\ell}(\mu), \quad \ell \neq m.\end{gathered} \tag{6.1}$$

(ii) Given $\ell \in \mathbb{Z}$ and $(\mu,\lambda) \in D^{-}_{\ell,n} \cup D^{+}_{\ell,n}$, it holds that

$$E^{\mathrm{o}}_{\lambda,\ell,n}(\mu) > E^{\mathrm{s}}_{\lambda,n}(\ell \pm n/2). \tag{6.2}$$

(iii) Given $\ell \in \mathbb{Z}, n, n' \in \mathbb{N}$, and $\lambda > n^2/4$, it holds that

$$E^{\mathrm{s}}_{\lambda,n}(\ell \pm n/2) = \begin{cases} E^{\mathrm{s}}_{\lambda,n}(m \pm 1/2) & \text{if } n \text{ is odd},\\ E^{\mathrm{s}}_{\lambda,n}(m \pm 1) & \text{if } n \text{ is even}, \end{cases} \tag{6.3}$$

$$E^{\mathrm{s}}_{\lambda,n}(\ell \pm n/2) > E^{\mathrm{s}}_{\lambda,n'}(\ell \pm n'/2), \quad (n > n'). \tag{6.4}$$

(iv) Given a pair $(m,n) \in \mathbb{Z} \times \mathbb{N}$, $\psi^{\mathrm{s}}_{\lambda,m\pm n/2,n}$ is unstable.

Indeed from (ii) and (iii) it follows that if $\ell \neq m$ and $(\mu,\lambda) \in \mathcal{D}_m \cap (D^{-}_{\ell,n} \cup D^{+}_{\ell,n})$,

$$E^{\mathrm{o}}_{\lambda,\ell,n}(\mu) > E^{\mathrm{s}}_{\lambda,n}(\ell \pm n/2) \geqslant E^{\mathrm{s}}_{\lambda,1}(m \pm 1/2).$$

Thus any type (IIb) solution cannot be a minimizer at $\mu = m \pm 1/2$. [Note that $\psi^{\mathrm{o}}_{\lambda,\mu,m,n}$ does not exist if $(\mu,\lambda) \in \mathcal{D}_m$.] The assertion of (iv) assures that the minimizer at $\mu = m \pm 1/2$ must be the type (IIa) solution with the least energy. Thus from (i) it follows that

$$E^{\mathrm{o}}_{\lambda,\ell,n}(\mu) > E^{\mathrm{c}}_{\lambda,m}(\mu) \quad (\ell \neq m, (\mu,\lambda) \in \mathcal{D}_m \cap (D^{-}_{\ell,n} \cup D^{+}_{\ell,n})),$$

which implies $\psi^{\mathrm{c}}_{\lambda,\mu,m}$ is the minimizer.

Now we prove (i)–(iv). From

$$E^{\mathrm{c}}_{\lambda,m}(\mu) = \pi(m-\mu)^2\{1 - (m-\mu)^2/2\lambda\}, \quad \lambda > (m-\mu)^2,$$

we can see the conclusion of (i). Since the verification is simple, we omit the proof of (i).

The inequality of (ii) immediately follows from Proposition 5.1 and the next lemma.

Lemma 6.1: Let $k = k(\mu,\lambda)$ be the unique solution of $\rho(k,\lambda,\mu) = 0$ in (5.12). Then $E^{\mathrm{o}}_{\lambda,m,n}(\mu)$ is written as

$$E^{\mathrm{o}}_{\lambda,m,n}(\mu) = I(k(\mu,\lambda)),$$

$$I(k) := -2n^4(1-k^2+k^4)K(k)^4/9\lambda\pi^3 + 4n^2(-2+k^2)K(k)^2/9\pi + 4n^2E(k)K(k)/3\pi + 5\lambda\pi/18, \tag{6.5}$$

where $E(k)$ is an elliptic integral

$$E(k) := \int_0^1 \sqrt{(1-k^2\xi^2)/(1-\xi^2)}\,\mathrm{d}\xi.$$

In the parameter region $D^-_{\ell,n}$ (or $D^+_{\ell,n}$) the inequality

$$\frac{d}{\mathrm{d}\mu}E^{\mathrm{o}}_{\lambda,m,n}(\mu) < 0 \quad (\text{or} > 0) \tag{6.6}$$

holds.

From this lemma and Theorem 1.1 it follows that

$$E^{\mathrm{o}}_{\lambda,\ell,n}(\mu) > \lim_{\mu\to\ell\pm n/2} E^{\mathrm{o}}_{\lambda,\ell,n}(\mu) = E^{\mathrm{s}}_{\lambda,n}(\ell \pm n/2), \quad (\mu,\lambda) \in D^-_{\ell,n} \cup D^+_{\ell,n}.$$

The proof of Lemma 6.1 will be done in the last part of this section.

Next consider (iii). We can verify the following.

Lemma 6.2: Let $k=k^{\mathrm{s}}(n,\lambda)$ be the unique solution to (2.2). Then $E^{\mathrm{s}}_{\lambda,n}(\mu)$ is written as

$$E^{\mathrm{s}}_{\lambda,n}(\mu) = I^{\mathrm{s}}(k^{\mathrm{s}}(n,\lambda)),$$

$$I^{\mathrm{s}}(k) := \lambda\pi(k^2-1)(3k^2+5)/6(k^2+1)^2 + 4\lambda\pi E(k)/3(k^2+1)K(k),$$

and it holds that

$$\frac{\mathrm{d}I^{\mathrm{s}}}{\mathrm{d}k}(k) < 0. \tag{6.7}$$

By this lemma we can prove (iii) as follows: For fixed $n \in \mathbb{N}$, $E^{\mathrm{s}}_{\lambda,n}(\mu)$ is defined if $\lambda > n^2/4$ and $\mu - n/2 \in \mathbb{Z}$. Since (2.2) and $I^{\mathrm{s}}(k)$ are independent of μ, $E^{\mathrm{s}}_{\lambda,n}(\mu) = E^{\mathrm{s}}_{\lambda,n}(\mu\pm 1)$ if $\mu - n/2 \in \mathbb{Z}$. Hence (6.3) follows. On the other hand, (6.4) holds by (6.7), because (2.12) implies $k^{\mathrm{s}}(n,\lambda) > k^{\mathrm{s}}(n',\lambda)$ if $n < n'$.

The proof of Lemma 6.2 will be done in the similar way to that of Lemma 6.1. We leave it to the readers because it is a straightforward computation and simpler than that of Lemma 6.1.

The proof of (iv) can be carried out by applying the arguments in Ref. 1 and Sec. 3.3 of Ref. 6 in the following way: Since the equation has the invariance under the rotation, the linearized operator at $\psi^{\mathrm{s}}_{\lambda,\mu,n}$ has zero eigenvalue with the corresponding eigenfunction $i\psi^{\mathrm{s}}_{\lambda,\mu,n}$. By virtue of the special form of the solution we can show that this eigenvalue problem is reduced to decoupled real-valued scalar equations of the Sturm-Liouville type. One of those scalar eigenvalue problems allows the zero eigenvalue coming from the invariance under the rotation. Since the corresponding eigenfunction has a vanishing point, Sturm-Liouville theorem tells it cannot be that of the least eigenvalue. As a consequence the solution is unstable (see Ref. 1 for the detail of the argument).

Now we present a proof of Lemma 6.1.

Proof of Lemma 6.1: The key computation is to verify (6.5). Once we establish, (6.5) we have

$$\frac{\mathrm{d}E^{\mathrm{o}}_{\lambda,m,n}}{\mathrm{d}\mu}(\mu) = -\frac{\mathrm{d}I}{\mathrm{d}k}\frac{\partial\rho}{\partial\mu} \Big/ \frac{\partial\rho}{\partial k}.$$

By virtue of the formulas

$$\frac{\mathrm{d}K}{\mathrm{d}k}(k)=\frac{E(k)}{(1-k^2)k}-\frac{K(k)}{k},\quad \frac{\mathrm{d}E}{\mathrm{d}k}(k)=\frac{E(k)}{k}-\frac{K(k)}{k},$$

a direct computation leads us to

$$\frac{\mathrm{d}I}{\mathrm{d}k}(k)=\frac{4n^4K(k)^3\{(2-k^2)(1-k^2)K(k)-2(1-k^2+k^4)E(k)\}}{9\lambda\pi^3k(1-k^2)}+\frac{4n^2\{K(k)^2(1-k^2)+2(k^2-2)E(k)K(k)+3E(k)^2\}}{9k\pi(1-k^2)}.$$

By Lemma 5.1 and a simple computation (see Lemma 3.6 and the proof of Lemma 3.5 in Ref. 7) we obtain

$$\frac{\mathrm{d}I}{\mathrm{d}k}(k)<0,\quad \frac{\partial\rho}{\partial\mu}=-4(m-\mu)K(k)^2,\quad \frac{\partial\rho}{\partial k}>0.$$

This implies (6.6).

Now we show (6.5). Let $u^{\mathrm{o}}_{\lambda,\mu,m,n}=w(x)\exp(i\theta(x)), v(x)=w(x)^2$, and let k be the unique solution of (5.12). In the next computation α,β, and γ are the parameters defined in, (3.8), (3.9), and (3.10), respectively. It is obvious from, (3.3), (5.3), and (5.4) that

$$\begin{aligned}E^{\mathrm{o}}_{\lambda,m,n}(\mu)&=\frac{1}{2}\int_0^{2\pi}(w_x)^2+w^2(\theta_x)^2+\frac{\lambda}{2}(1-w^2)^2\,\mathrm{d}x\\&=\frac{1}{2}\int_0^{2\pi}\frac{\lambda(v-\alpha)(v-\beta)(v-\gamma)}{2v}+\frac{\lambda\alpha\beta\gamma}{2v}+\frac{\lambda}{2}(1-v)^2\,\mathrm{d}x\\&=n\lambda\int_0^{\pi/n}(v^2-2v)\mathrm{d}x+\frac{\lambda\pi}{2}(\alpha\beta+\beta\gamma+\gamma\alpha+1).\end{aligned}\tag{6.8}$$

Using (5.4) and the change of variable $v=(\beta-\alpha)\tau^2+\alpha$, we have

$$\begin{aligned}n\lambda\int_0^{\pi/n}(v^2-2v)\mathrm{d}x&=n\sqrt{\frac{\lambda}{2}}\int_\alpha^\beta\frac{v^2-2v}{\sqrt{(v-\alpha)(v-\beta)(v-\gamma)}}\mathrm{d}v\\&=\frac{n\sqrt{2\lambda}}{\sqrt{\gamma-\alpha}}\int_0^1\frac{(\beta-\alpha)^2\tau^4+2(\alpha-1)(\beta-\alpha)\tau^2+(\alpha-2)\alpha}{\sqrt{(1-\tau^2)(1-k^2\tau^2)}}\mathrm{d}\tau.\end{aligned}\tag{6.9}$$

Notice that from

$$\frac{d}{\mathrm{d}\tau}\left(\tau\sqrt{(1-\tau^2)(1-k^2\tau^2)}\right)=\frac{3k^2\tau^4-2(k^2+1)\tau^2+1}{\sqrt{(1-\tau^2)(1-k^2\tau^2)}},$$

it follows

$$\int_0^1\frac{\tau^4}{\sqrt{(1-\tau^2)(1-k^2\tau^2)}}\mathrm{d}\tau=\int_0^1\frac{2(k^2+1)\tau^2-1}{3k^2\sqrt{(1-\tau^2)(1-k^2\tau^2)}}\mathrm{d}\tau.$$

Thus by

$$\int_0^1\frac{\tau^2}{\sqrt{(1-\tau^2)(1-k^2\tau^2)}}\mathrm{d}\tau=\frac{1}{k^2}(K(k)-E(k)),\tag{6.10}$$

we have the formula

$$\int_0^1 \frac{\tau^4}{\sqrt{(1-\tau^2)(1-k^2\tau^2)}}\mathrm{d}\tau = \frac{1}{3k^4}\{(k^2+2)K(k) - 2(k^2+1)E(k)\}. \tag{6.11}$$

Substituting (3.8), (3.9), (3.10), (6.10), and (6.11) into (6.8) and (6.9), we obtain the desired equality (6.5). □

VII. A CONCLUDING REMARK

As pointed out in the Introduction, we do not have the rigorous instability result for the solutions with modulating amplitude. If we could verify it, the proof of Theorem 1.2 would be greatly simplified. However, the computations in Sec. VI help us to see how the energy of the solution can be expressed. In addition to the result in Sec. VI we can prove

$$E^{\mathrm{c}}_{\lambda,m}(\mu) < E^{\mathrm{s}}_{\lambda,n}(\mu) \quad (\mu = m \pm n/2, \lambda > n^2/4),$$

though we need a lengthy computation. By using this inequality, instead of (iv) in Sec. VI, we can also obtain the same conclusion of Theorem 1.2.

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Bifurcation and stability of superconductivity[a)]

Tian Ma
Department of Mathematics, Xian Jiaotong University, Xian, People's Republic of China, and Department of Mathematics, Sichuan University, Chengdu, People's Republic of China

Shouhong Wang[b)]
Department of Mathematics, Indiana University, Bloomington, Indiana 47405

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In this article, we present a bifurcation and stability analysis on time-dependent Ginzburg–Landau model of superconductivity. It is proved in particular that there are two different phase transitions from the normal state to superconducting states or vice versa: one is continuous, and the other is jump. These two transitions are precisely determined by a simple nondimensional parameter, which links the superconducting behavior with the geometry of the material, the applied field and the physical parameters. The rigorous analysis is conducted using a bifurcation theory newly developed by the authors, and provides some interesting physical predictions. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2012128]

I. INTRODUCTION

The main objective of this article is to study the nature of the phase transition from normal to superconducting states, which occurs when the temperature of a sample decreases. The rigorous analysis is conducted using a new bifurcation theory developed recently by the authors.

Superconductivity was first discovered in 1911 by H. Kamerlingh Onnes, who found that Mercury had zero electric resistance when the temperature decreases below some critical value T_c. Since then, one has found that large number of metals and alloys possess the superconducting property. In the superconducting state once a current is set up in a metal ring, it is expected that no change in this current occurs in times more that 10^{10} years (see Ref. 1). In 1933, the other important superconducting property, called the diamagnetism or the Meissner effect, was discovered by W. Meissner and R. Ochsenfield. They found that not only a magnetic field is excluded from entering a superconductor, but also that a field in an originally normal sample is expelled as it is cooled below T_c.

One central problem in the theory of superconductivity is the nature of the phase transition between a normal state, characterized by an order parameter that vanishes identically, and a superconducting state, characterized by the order parameter that is not identically zero. In this article, we address this problem by conducting rigorous bifurcation and stability analysis for the time dependent Ginzburg–Landau (TDGL) model of superconductivity.

The TDGL model of superconductivity involves an order parameter ψ, and the magnetic potential A. The problem is forced by an applied field H_a [see (2.1)–(2.3)]. The associated Ginzburg–Landau free energy is given by (see Ref. 1)

[a)]*Dedicated to Professor Louis Nirenberg on the occasion of his eightieth birthday with great affection and admiration.*
[b)]Electronic mail: showang@indiana.edu

$$f = f_{n0} + a|\psi|^2 + \frac{b}{2}|\psi|^4 + \frac{1}{2m_s}\left|\left(\frac{h}{i}\nabla - \frac{e_s}{c}A\right)\psi\right|^2 + \frac{h^2}{8\pi}, \tag{1.1}$$

where h is the Planck constant, c the speed of light, e_s and m_s the charge and mass of a Cooper pair, and the parameters $a=a(T)$ and $b=b(T)$ are coefficients satisfying the following conditions (see, among others, Ref. 2):

$$a = a(T)\begin{cases} >0 & \text{for } T > T_c \\ <0 & \text{for } T < T_c, \end{cases}$$

$$b = b(T) > 0.$$

Here T the temperature of the sample, and T_c the critical temperature where incipient superconductivity property can be observed.

With proper scaling, a nondimensional parameter α plays a key role in the phase transition (or bifurcation), which is given in terms of dimensional quantities by

$$\alpha = \alpha(T) = -\frac{2a\sqrt{b}m_s D}{e_s^3 h} = \frac{2\sqrt{b}m_s D N_0}{e_s^3 h}\frac{T_c - T}{T_c}, \tag{1.2}$$

where D is the diffusion coefficient, and the last equality was derived using (2.4) based on the Bardeen-Cooper-Schrieffer (BCS) theory.

The main objectives of this article is to establish a nonlinear bifurcation and stability theory for the Ginzburg–Landau equations. It is clear that such a nonlinear bifurcation and stability theory should at least include

(1) a bifurcation theorem when the parameter α crosses some critical numbers for all physically sound boundary conditions and geometry of the domain,
(2) asymptotic stability of bifurcated solutions, and
(3) the vortex structure and its stability and transitions in the physical space.

This bifurcation and stability analysis uses a new bifurcation theory for partial differential equations (PDEs) developed recently by the authors. This bifurcation theory is based on a new notion of bifurcation, called attractor bifurcation, and its corresponding theory introduced in Refs. 3 and 4. With the bifurcation theory, many bifurcation problems in science and engineering are becoming more accessible. In particular, applications are made for variety of PDEs from science and engineering, including, in particular, the Kuramoto-Sivashinshy equation, the Cahn-Hillard equation, the complex Ginzburg–Landau equation, Reaction-diffusion equations in biology and chemistry, the Rayleigh-Bénard convection problem, and the Taylor problem.

We now address different aspects of such a nonlinear bifurcation and stability theory for the TDGL model of superconductivity obtained in this article.

First, we proceed with the reduction of the infinite dimensional dynamical system governed by the TDGL equations to a finite dimensional system defined on the center manifold. One important ingredient of the analysis is the approximation of the center manifold function, which is part of the new bifurcation theory. With this reduction in our disposal, a general bifurcation theorem follows from the general strategy of attractor bifurcations, as required in part (1) mentioned previously. We prove in particular that there are two different phase transitions from the normal state to superconducting states or vice versa: one is continuous shown schematically in Fig. 1, and the other is jump shown in Figs. 2 and 3. These two transitions are precisely determined by a simple parameter R defined by (4.22) for transitions near a complex simple eigenvalue of the linearized problem [respectively, by two parameters R_1 and R_2 defined by (4.44) for transitions near an eigenvalues with higher multiplicity]. The parameter R links the superconducting behavior with the geometry of the material, the applied field and the physical parameters.

Second, as an attractor, the bifurcated attractor has asymptotic stability in the sense that it attracts all solutions with initial data in the phase space outside of the stable manifold of the trivial

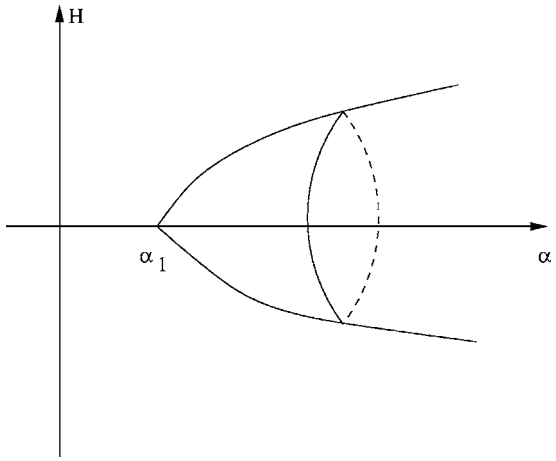

FIG. 1. For each $\alpha \leqslant \alpha_1$, the normal state is stable. For $\alpha > \alpha_1$, the normal state is unstable, the TDGL bifurcates to an S^1 attractor, representing stable superconducting state.

solution. Therefore bifurcation analysis for steady state problems provides in general only partial answers to the problem, and is not enough for solving the stability problem. Hence it appears that the right notion of asymptotic stability after the first bifurcation should be best described by the attractor near, but excluding, the trivial state. It is one of our main motivation for introducing attractor bifurcation.

Consider the TDGL model for the case where the first eigenvalue of the linearized problem is complex simple (i.e., has real multiplicity 2). When $R<0$, we obtain a continuous transition from the normal state to superconducting states. In particular, we prove in Theorem 4.1 that (a) the bifurcated attractor is a circle S^1, consisting of only steady states, (b) the solutions in the bifurcated attractor are in superconducting states, and (c) the bifurcated attractor attracts bounded open sets $U\backslash\Gamma$ in the phase space, where Γ is the stable manifold of the trivial solution. Consequently we prove in particular that under a fluctuation deviating both the normal and superconducting states, the sample will soon be restored to the superconducting states.

When $R>0$, we obtain a jump transition from the normal state to superconducting states or vice versa. In particular, from Theorems 4.2 and 4.3, as shown in Figs. 2 and 3, there are two

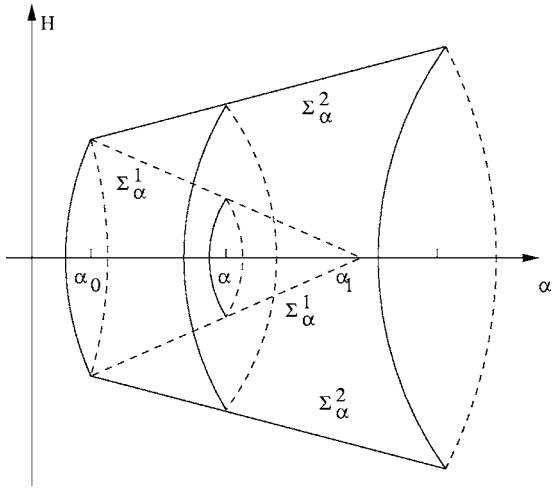

FIG. 2. For each $\alpha \in (\alpha_0, \alpha_1)$, Σ^1_α is a repeller, containing *unstable* superconducting states. For each $\alpha_0 < \alpha$, Σ^2_α is an attractor, containing *stable* superconductivity states.

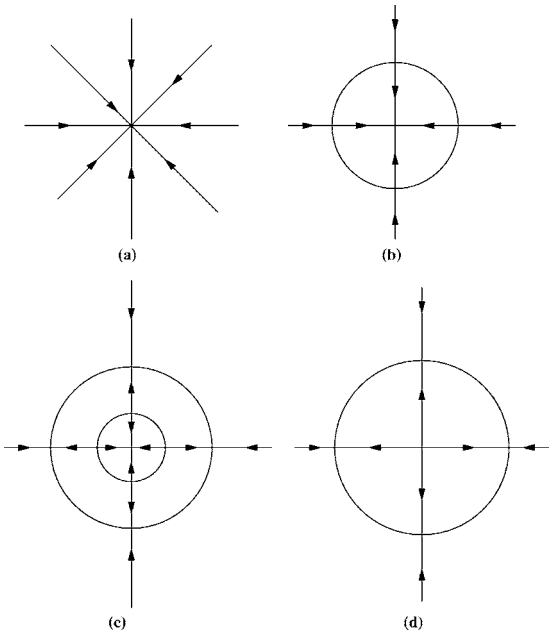

FIG. 3. Phase diagrams on the center manifold for various α: (a) case $\alpha<\alpha_0$, (b) case $\alpha=\alpha_0$, (c) case $\alpha_0<\alpha<\alpha_1$, and (d) case $\alpha_1\leqslant\alpha$

critical temperatures T_c^0 and T_c^1 ($T_c^0>T_c^1$) such that when $T_c^1<T$ (or $\alpha<\alpha_1$), physically observable states consists of the normal state, and the superconducting states in Σ_α^2, and when $T_c^1>T$ (or $\alpha>\alpha_1$), physically observable states are in Σ_α^2. In addition, the transitions at T_c^1 and T_c^0 are jump transitions.

Third, one important aspect of studies in superconductivity is the existence (appearance) and structure of vortices of the supercurrent. The associated mathematical question is to link the solutions of the PDEs (the TDGL model in this article) to the structure of the solutions in the "physical space." In fluid mechanics context, this corresponds to linking the kinematics to dynamics, and an attempt by the authors is summarized in Ref. 5. For the TDGL model, the existence of vortices and the structure of the supercurrent is analyzed using this philosophy.

Fourth, it is noteworthy to mention that although we used the steady state equations to derive the existence of one of the steady state bifurcation branches, the dynamic properties (the basin attraction, stability, introduction of the parameters R, R_1 and R_2, etc) and the branch Σ_α^2 are of a truly dynamical nature.

There have been extensive studies on bifurcation and stability analysis for superconductivity; see among others.[6–10] In particular, we point out recent work by Berger and Rubinstein[11] and Chapman,[12] where similar questions on different phase transitions of the Ginzburg–Landau model were addressed. In Ref. 11, the study is based on evaluating the second variation of the Ginzburg–Landau functional, whereas in Ref. 12, an asymptotic method traced back to Ref. 13 is used.

This article is organized as follows. Section II introduces the TDGL model. In Sec. III, after a brief introduction of the attractor bifurcation theory and center manifold functions, we prove a special case of the attractor bifurcation called S^1 attractor bifurcation. Section IV states and proves the main theorems on stability and bifurcation of the TGDL equations. Conclusions and physical remarks are given in Sec. V.

II. TDGL MODEL

A. The equations

Let $\Omega\subset\mathbb{R}^n$ ($n=2$ or 3) be a bounded open set. We consider the attractor bifurcation of the TDGL equations of superconductivity defined on Ω. The following three unknown functions are

involved in the mathematical formulation: a complex valued function $\psi:\Omega\to\mathbb{C}$ for the order parameter, a vector valued function $A:\Omega\to\mathbb{R}^3$ for the magnetic potential and a scalar function $\phi:\Omega\to\mathbb{R}^1$ for the electric potential. The TDGL model reads

$$\frac{h^2}{2m_sD}\left(\frac{\partial}{\partial t}+\frac{ie_s}{h}\phi\right)\psi+a\psi+b|\psi|^2\psi+\frac{1}{2m_s}\left(hi\nabla+\frac{e_s}{c}A\right)^2\psi=0, \tag{2.1}$$

$$J=-\sigma\left(\frac{1}{c}A_t+\nabla\phi\right)-\frac{e_s^2}{m_sc}|\psi|^2A-\frac{e_shi}{2m_s}(\psi^*\nabla\psi-\psi\nabla\psi^*), \tag{2.2}$$

$$\frac{4\pi}{c}J=\mathrm{curl}^2A-\mathrm{curl}\,H_a, \tag{2.3}$$

where σ the conductivity of the normal phase, J the supercurrent, and ψ^* the complex conjugate of ψ. In the BCS theory, the parameters $a=a(T)$ and $b=b(T)$ are given (see Ref. 2) by

$$\begin{aligned} a(T)&=N(0)\frac{T-T_c}{T_c},\\ b(T)&=0.098\frac{N(0)}{(k_bT_c)^2}. \end{aligned} \tag{2.4}$$

Equations (2.1) and (2.2) are the TDGL equations generalized by P. L. Gor'kov and G. M. Éliashberg,[1,14] and (2.3) is the classical Maxwell equation. The order parameter ψ describes the local density n_s of superconducting electrons: $|\psi|^2=n_s$. In addition, ψ is proportional to the energy gap parameter Δ near T_c, which appears in the BCS theory.

B. Scaling

From both the mathematical and physical points of view, we introduce here two nondimensional forms of the TDGL equations: one of which is used often in the literature, and the other is more suitable for the bifurcation and stability analysis presented in this article.

For convenience, we start with the dimensions of various physical quantities. Let m be the mass, L the typical length scale, t the time, and E the energy. Then we have

$$E:L^2m/t,\quad h:Et,\quad D:L^2/t,\quad e_s^2:EL,$$

$$\sigma:1/t,\quad c:L/t,\quad a:E,\quad b:EL^3,$$

$$\psi:1/L^{3/2},\quad A:(E/L)^{1/2},\quad H:(E/L^3)^{1/2}.$$

Then we introduce some physical parameters:

$$|\psi_0|^2=|a|/b,$$

$$H_c=(4\pi|a|^2/b)^{1/2},$$

$$\lambda=\lambda(T)=(m_sc^2b/4\pi e_s^2|a|)^{1/2},$$

$$\xi=\xi(T)=h/(2m_s|a|)^{1/2},$$

$$\kappa=\lambda/\xi,$$

$$\eta = 4\pi\sigma D/c^2,$$

$$\tau = \lambda^2/D.$$

Physically, $|\psi_0|^2$ stands for the equilibrium density, H_c for the thermodynamic critical field, $\lambda = \lambda(T)$ for the penetration depth, $\xi(T)$ for the coherence length, and τ for the relaxation time. The ratio of the two characteristic lengths $\kappa = \lambda/\xi$ is called the Ginzburg–Landau parameter of the substance. When $0 < \kappa < 1/\sqrt{2}$, the material is of the first type, and when $\kappa > 1/\sqrt{2}$, the material is of the second type.

We now introduce the nondimensional variables (those with a prime):

$$x = \lambda x', \quad t = \tau t', \quad \psi = \psi_0 \psi',$$

$$A = \frac{\sqrt{2}H_c\lambda}{\kappa}A', \quad \phi = \frac{D\sqrt{2}H_c}{\kappa}\phi', \quad H_a = \frac{\sqrt{2}H_c}{\kappa}H_a'.$$

Then we have the following traditional nondimensional TDGL equations (we henceforth drop the primes)

$$\psi_t + i\kappa\phi\psi + \kappa^2(|\psi|^2 - 1)\psi + (i\nabla + A)^2\psi = 0,$$

$$\eta(A_t + \nabla\phi) + \frac{i}{2}(\psi^*\nabla\psi - \psi\nabla\psi^*) + |\psi|^2 A + \operatorname{curl}^2 A - \operatorname{curl} H_a = 0,$$

for the case where $a < 0$, or equivalently $T < T_c$.

As mentioned before, we need to introduce another non-dimensional form for the stability and bifurcation study. To this end, we set

$$l = \frac{\sqrt{b}}{e_s}, \quad \tau_0 = \frac{hl}{e_s^2}, \quad \phi_0 = \frac{e_s^2}{\sqrt{b}},$$

$$A_0 = \left(\frac{e_s h c^2}{D\sqrt{b}}\right)^{1/2}, \quad \alpha = -\frac{2a\sqrt{b}m_s D}{e_s^3 h}, \quad \mu = \frac{hD}{\sqrt{b}e_s},$$

$$\beta = \frac{2m_s D}{h}, \quad \zeta = \frac{4\pi\sigma l e_s^2}{c^2 h}, \quad \gamma = \frac{4\pi e_s^2}{m_s c^2 l},$$

and

$$x = lx', \quad t = \tau_0 t', \quad \psi = l^{-3/2}\psi',$$

$$A = A_0 A', \quad \phi = \phi_0\phi', \quad H_a = l^{-1}A_0 H_a'.$$

Then we have the second type of non-dimensional TDGL equations (we drop the primes also):

$$\begin{aligned} &\psi_t + i\phi\psi = -(i\mu\nabla + A)^2\psi + \alpha\psi - \beta|\psi|^2\psi, \\ &\zeta(A_t + \mu\nabla\phi) = -\operatorname{curl}^2 A + \operatorname{curl} H_a - \gamma|\psi|^2 A - \frac{\gamma\mu i}{2}(\psi^*\nabla\psi - \psi\nabla\psi^*). \end{aligned} \tag{2.5}$$

We shall see in later discussions that the parameter α plays a key role in the phase transition (or bifurcation), which is given in terms of dimensional quantities by

$$\alpha = \alpha(T) = \frac{2\sqrt{b}m_s D N_0}{e_s^3 h}\frac{T_c - T}{T_c}.$$

C. Boundary conditions

A physically sound boundary condition for the order parameter is given by

$$C_1\left(ih\nabla + \frac{e_s}{c}A\right)\psi \cdot n = -C_2 ih\psi \quad \text{on } \partial\Omega, \tag{2.6}$$

which means that no current passes through the boundary, where n is the unit outward normal vector at $\partial\Omega$, and $C_1, C_2 \geqslant 0$ are constants depending on the material to which the contact is made. Physically, they satisfy[1,2]

$$C_2 = 0, \quad C_1 \neq 0 \quad \text{for an insulator on } \partial\Omega,$$

$$C_1 = 0, \quad C_2 \neq 0 \quad \text{for a magnetic material}, \tag{2.7}$$

$$0 < C_2/C_1 < \infty \quad \text{for a normal metal}.$$

We note that Eqs. (2.1)–(2.3) with (2.6) is invariant under the following gauge transformation

$$(\psi, A, \phi) \to \left(\psi e^{i\theta}, A - \frac{hc}{e_s}\nabla\theta, \phi - \frac{h}{e_s}\theta_t\right),$$

where θ is an arbitrary function. If we take θ such that

$$\frac{hc}{e_s}\Delta\theta = \operatorname{div} A \quad \text{in } \Omega,$$

$$\frac{hc}{e_s}\frac{\partial\theta}{\partial n} = A \cdot n \quad \text{on } \partial\Omega,$$

then we obtain an additional equation and a boundary condition; see also Refs. 2 and 15:

$$\operatorname{div} A = 0, \tag{2.8}$$

$$A_n = A \cdot n = 0 \quad \text{on } \partial\Omega. \tag{2.9}$$

Another boundary condition often imposed for A is as follows:

$$\operatorname{curl} A \times n = H_a \times n \quad \text{on } \partial\Omega. \tag{2.10}$$

D. Nondimensional TDGL model

In summary, with the gauge taken such that (2.8) and (2.9) hold true, the nondimensional TDGL equations are

$$\psi_t + i\phi\psi = -(i\mu\nabla + A)^2\psi + \alpha\psi - \beta|\psi|^2\psi,$$

$$\zeta(A_t + \mu\nabla\phi) = -\operatorname{curl}^2 A + \operatorname{curl} H_a - \gamma|\psi|^2 A - \frac{\gamma\mu i}{2}(\psi^*\nabla\psi - \psi\nabla\psi^*), \tag{2.11}$$

$$\operatorname{div} A = 0.$$

The initial conditions are given by

$$\psi(0) = \psi_0, \quad A(0) = A_0. \tag{2.12}$$

The boundary conditions are one of the following:

Neumann boundary condition: For the case where Ω is enclosed by an insulator:

$$\frac{\partial \psi}{\partial n} = 0, \quad A_n = 0, \quad \operatorname{curl} A \times n = H_a \times n \quad \text{on } \partial\Omega. \tag{2.13}$$

Dirichlet boundary condition: For the case where Ω is enclosed by a magnetic material:

$$\psi = 0, \quad A_n = 0, \quad \operatorname{curl} A \times n = H_a \times n \text{ on } \partial\Omega. \tag{2.14}$$

Robin boundary condition: For the case where Ω is enclosed by a normal metal:

$$\frac{\partial \psi}{\partial n} + C\psi = 0, \quad A_n = 0, \quad \operatorname{curl} A \times n = H_a \times n \text{ on } \partial\Omega. \tag{2.15}$$

Remark 2.1: If the material is a loop, or a plate $\Omega = \tilde{\Omega} \times (0,h)$ with the height h being small in comparison to the diameter of $\tilde{\Omega}$, then it is reasonable to consider the boundary condition with periodicity either in x direction or in (x,y) directions.

III. DYNAMIC BIFURCATION THEORY

A. Attractor bifurcation

We recall in this section a general theory on attractor bifurcation developed by the authors.[3,4,16]

Let H and H_1 be two Hilbert spaces, and $H_1 \hookrightarrow H$ be a dense and compact inclusion. We consider the following nonlinear evolution equations:

$$\begin{aligned} \frac{du}{dt} &= L_\lambda u + G(u,\lambda), \\ u(0) &= u_0, \end{aligned} \tag{3.1}$$

where $u:[0,\infty) \to H$ is the unknown function, $\lambda \in \mathbb{R}$ is the system parameter, and $L_\lambda : H_1 \to H$ are parameterized linear completely continuous fields depending continuously on $\lambda \in \mathbb{R}^1$, which satisfy

$$\begin{aligned} &L_\lambda = -A + B_\lambda \quad \text{a sectorial operator}, \\ &A: H_1 \to H \quad \text{a linear homeomorphism}, \\ &B_\lambda: H_1 \to H \quad \text{parameterized linear compact operators}. \end{aligned} \tag{3.2}$$

It is easy to see[17] that L_λ generates an analytic semigroup $\{e^{-tL_\lambda}\}_{t \geqslant 0}$. Then we can define fractional power operators L_λ^α for any $0 \leqslant \alpha \leqslant 1$ with domain $H_\alpha = D(L_\lambda^\alpha)$ such that $H_{\alpha_1} \subset H_{\alpha_2}$ if $\alpha_1 > \alpha_2$, and $H_0 = H$.

Further, we assume that the nonlinear terms $G(\cdot,\lambda): H_\alpha \to H$ for some $0 \leqslant \alpha < 1$ are a family of parameterized C^r bounded operators $(r \geqslant 1)$ depending continuously on the parameter $\lambda \in \mathbb{R}^1$, such that

$$G(u,\lambda) = o(\|u\|_{H_\alpha}), \quad \forall\, \lambda \in \mathbb{R}^1. \tag{3.3}$$

In this paper, we are interested in the sectorial operator $L_\lambda = -A + B_\lambda$ such that there exist an eigenvalue sequence $\{\rho_k\} \subset \mathbb{C}^1$ and an eigenvector sequence $\{e_k, h_k\} \subset H_1$ of A:

$$Az_k = \rho_k z_k, \quad z_k = e_k + ih_k,$$

$$\text{Re } \rho_k \to \infty (k \to \infty), \tag{3.4}$$

$$|\text{Im } \rho_k / (\text{Re } \rho_k)| \leqslant C,$$

for some $C > 0$, and such that $\{e_k, h_k\}$ is a basis of H.

Condition (3.4) implies that A is a sectorial operator. For the operator $B_\lambda : H_1 \to H$, we also assume that there is a constant $0 < \theta < 1$ such that

$$B_\lambda : H_\theta \to H \text{ bounded}, \quad \forall\, \lambda \in \mathbb{R}^1. \tag{3.5}$$

Under conditions (3.4) and (3.5), the operator $L_\lambda = -A + B_\lambda$ is a sectorial operator.

Let $\{S_\lambda(t)\}_{t \geqslant 0}$ be an operator semi-group generated by Eq. (3.1), then the solution of (3.1) can be expressed as

$$u(t) = S_\lambda(t) u_0, \quad t \geqslant 0.$$

Definition 3.1: *A set $\Sigma \subset H$ is called an invariant set of* (3.1) *if $S(t)\Sigma = \Sigma$ for any $t \geqslant 0$. An invariant set $\Sigma \subset H$ of* (3.1) *is said to be an attractor if Σ is compact, and there exists a neighborhood $U \subset H$ of Σ such that for any $\varphi \in U$ we have*

$$\lim_{t \to \infty} \text{dist}_H (u(t, \varphi), \Sigma) = 0.$$

The set U is called a basin of attraction of Σ.

Definition 3.2: (1) *We say that Eq. (3.1) bifurcates from $(u, \lambda) = (0, \lambda_0)$ an invariant set Ω_λ, if there exists a sequence of invariant sets $\{\Omega_{\lambda_n}\}$ of* (3.1) *such that $0 \notin \Omega_{\lambda_n}$, and*

$$\lim_{n \to \infty} \lambda_n = \lambda_0,$$

$$\lim_{n \to \infty} \max_{x \in \Omega_{\lambda_n}} |x| = 0.$$

(2) *If the invariant sets Ω_λ are attractors of* (3.1), *then the bifurcation is called attractor bifurcation.*

A complex number $\beta = \alpha_1 + i\alpha_2 \in \mathbb{C}$ is called an eigenvalue of L_λ if there are $x, y \in H_1$ such that

$$L_\lambda x = \alpha_1 x - \alpha_2 y,$$

$$L_\lambda y = \alpha_2 x + \alpha_1 y.$$

Now let the eigenvalues (counting the multiplicity) of L_λ be given by

$$\beta_1(\lambda), \beta_2(\lambda), \ldots, \quad \beta_k(\lambda) \in \mathbb{C},$$

where $\mathbb{C}$ is the complex space. Suppose that

$$Re\beta_i(\lambda) \begin{cases} < 0 & \text{if } \lambda < \lambda_0, \\ = 0 & \text{if } \lambda = \lambda_0, \\ > 0 & \text{if } \lambda > \lambda_0, \end{cases} \qquad \forall\, 1 \leqslant i \leqslant m, \tag{3.6}$$

$$Re\beta_j(\lambda_0) < 0 \quad \forall\, m+1 \leqslant j. \tag{3.7}$$

Let the eigenspace of L_λ at λ_0 be

$$E_0 = \bigcup_{k\in\mathbb{N}} \bigcup_{1\leqslant i\leqslant m} \{u,v \in H_1 | (L_{\lambda_0} - \beta_i(\lambda_0))^k w = 0, w = u + iv\}.$$

It is known that $\dim E_0 = m$.

Theorem 3.3: (attractor bifurcation).[3,4] *Assume that the conditions* (3.3)–(3.7) *hold true, and* $u=0$ *is a locally asymptotically stable equilibrium point of* (3.1) *at* $\lambda=\lambda_0$. *Then the following assertions hold true.*

(1) (3.1) *bifurcates from* $(u,\lambda)=(0,\lambda_0)$ *to an attractor* $\mathcal{A}_\lambda$ *for* $\lambda>\lambda_0$, *with* $m-1\leqslant \dim \mathcal{A}_\lambda \leqslant m$, *which is connected when* $m>1$;
(2) *The attractor* $\mathcal{A}_\lambda$ *is a limit of a sequence of m-dimensional annulus* M_k *with* $M_{k+1}\subset M_k$; *especially if* $\mathcal{A}_\lambda$ *is a finite simplicial complex, then* $\mathcal{A}_\lambda$ *has the homotopy type of* S^{m-1};
(3) *For any* $u_\lambda \in \mathcal{A}_\lambda$, u_λ *can be expressed as*

$$u_\lambda = v_\lambda + o(\|v_\lambda\|_{H_1}), \quad v_\lambda \in E_0;$$

(4) *There is an open set* $U\subset H$ *with* $0\in U$ *such that the attractor* $\mathcal{A}_\lambda$ *bifurcated from* $(0,\lambda_0)$ *attracts* $U\backslash\Gamma$ *in H, where* Γ *is the stable manifold of* $u=0$ *with co-dimension m.*

B. Center manifold functions

In this section, we introduce a method to derive the first order approximation of the central manifold functions, which was used in Ref. 4. For convenience, we first introduce the center manifold theorem in infinite dimensional spaces.

Let H_1 and H be decomposed into

$$\begin{aligned} H_1 &= E_1^\lambda \oplus E_2^\lambda, \\ H &= \widetilde{E}_1^\lambda \oplus \widetilde{E}_2^\lambda, \end{aligned} \tag{3.8}$$

for λ near $\lambda_0 \in \mathbb{R}^1$, where E_1^λ, E_2^λ are invariant subspaces of L_λ, such that

$$\dim E_1^\lambda < \infty,$$

$$\widetilde{E}_1^\lambda = E_1^\lambda,$$

$$\widetilde{E}_2^\lambda = \text{closure of } E_2^\lambda \text{ in } H.$$

In addition, L_λ can be decomposed into $L_\lambda = \mathcal{L}_1^\lambda \oplus \mathcal{L}_2^\lambda$ such that for any λ near λ_0,

$$\begin{aligned} \mathcal{L}_1^\lambda &= L_{\lambda E_1^\lambda}: E_1^\lambda \to \widetilde{E}_1^\lambda, \\ \mathcal{L}_2^\lambda &= L_{\lambda E_2^\lambda}: E_2^\lambda \to \widetilde{E}_2^\lambda, \end{aligned} \tag{3.9}$$

where the eigenvalues of $\mathcal{L}_2^\lambda$ possess negative real parts, and the eigenvalues of $\mathcal{L}_1^\lambda$ possess nonnegative real parts at $\lambda=\lambda_0$.

Thus, for λ near λ_0, Eq. (3.1) can be written as

$$\frac{dx}{dt} = \mathcal{L}_1^\lambda x + G_1(x,y,\lambda),$$
$$\frac{dy}{dt} = \mathcal{L}_2^\lambda y + G_2(x,y,\lambda), \tag{3.10}$$

where $u=x+y \in H_1$, $x \in E_1^\lambda$, $y \in E_2^\lambda$, $G_i(x,y,\lambda)=P_iG(u,\lambda)$, and $P_i: H \to \tilde{E}_i^\lambda$ are canonical projections. Further, let

$$E_2^\lambda(\alpha) = \text{closure of } E_2^\lambda \text{ in } H_\alpha,$$

with $\alpha<1$ given in (3.3).

The following center manifold theorem is classical.[17]

Theorem 3.4: *Assume* (3.2), (3.3), (3.8), and (3.9). *Then there exists a neighborhood of* λ_0 *given by* $|\lambda-\lambda_0|<\delta$ *for some* $\delta>0$, *a neighborhood* $U_\lambda \subset E_1^\lambda$ *of* $x=0$, *and a* C^1 *function* $\Phi(\cdot,\lambda): U_\lambda \to E_2^\lambda(\theta)$ *depending continuously on* λ, *such that*

(1) $\Phi(0,\lambda)=0$, $\Phi_x'(0,\lambda)=0$,
(2) *the set*

$$M_\lambda = \{(x,y) \in H | x \in U_\lambda, y = \Phi(x,\lambda) \in E_2^\lambda(\theta)\},$$

called the center manifolds, are locally invariant for (3.1), *i.e., for each* $u_0 \in M_\lambda$

$$u_\lambda(t,u_0) \in M_\lambda, \quad \forall\, 0 \leqslant t < t(u_0)$$

for some $t(u_0)>0$, *where* $u_\lambda(t,u_0)$ *is the solution of* (3.1);
(3) *if* $(x_\lambda(t), y_\lambda(t))$ *is a solution of* (3.10), *then there is a* $\beta_\lambda>0$ *and* $k_\lambda>0$ *with* k_λ *depending on* $(x_\lambda(0), y_\lambda(0))$ *such that*

$$\|y_\lambda(t) - \Phi(x_\lambda(t),\lambda)\|_H \leqslant k_\lambda e^{-\beta_\lambda t}.$$

Now we give a formula to calculate the center manifold function. Let the nonlinear operator G be given by

$$G(u,\lambda) = G_k(u,\lambda) + o(|u|^k), \tag{3.11}$$

for $k \geqslant 2$, where $G_k(u,\lambda)$ is a k-multilinear operator:

$$G_k: H_1 \times \cdots \times H_1 \to H,$$

$$G_k(u,\lambda) = G_k(u,\ldots,u,\lambda).$$

The following theorem gives an approximation of the center manifold function; see Ref. 4.

Theorem 3.5: *Under the conditions of Theorem 3.4, the center manifold function* $\Phi(x,\lambda)$ *can be expressed as*

$$\Phi(x,\lambda) = (-\mathcal{L}_2^\lambda)^{-1} P_2 G_k(x,\lambda) + O(|\mathrm{Re}\,\beta(\lambda)| \cdot \|x\|^k) + o(\|x\|^k), \tag{3.12}$$

where $\mathcal{L}_2^\lambda$ *is given by* (3.9), $P_2: H \to \tilde{E}_2$ *the canonical projection*, $x \in E_1^\lambda$, *and* $\beta(\lambda) = (\beta_1(\lambda),\ldots,\beta_m(\lambda))$ *the eigenvalues of* $\mathcal{L}_1^\lambda$.

C. S^1 attractor bifurcation

In this section, we prove that the bifurcated attractor Ω_λ of (3.1) from an eigenvalue with multiplicity two is homeomorphic to a circle S^1.

Let v be a two-dimensional $C^r (r \geqslant 1)$ vector field given by

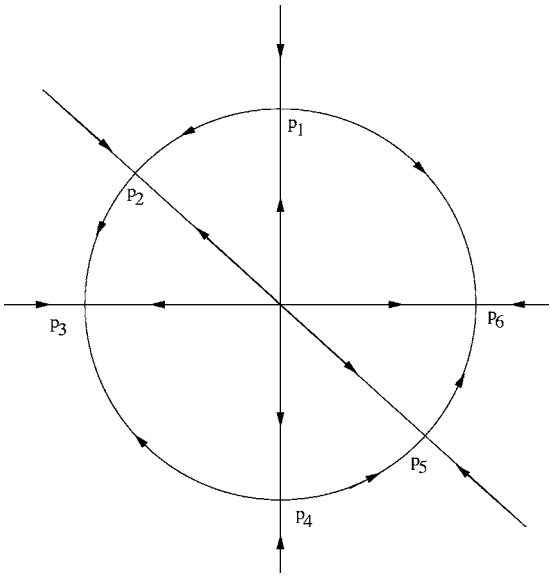

FIG. 4. Ω_λ has $4N+n$ ($N=1$ and $n=2$ shown here) singular points, where p_1,p_4 are saddles, p_3,p_6 are nodes, and p_2,p_5 are singular points with index zero.

$$v_\lambda(x) = \lambda x - G(x,\lambda), \tag{3.13}$$

for $x \in \mathbb{R}^2$. Here

$$G(x,\lambda) = G_k(x,\lambda) + o(|x|^k),$$

where G_k is a k-multilinear field, which satisfies that

$$C_1|x|^{k+1} \leqslant (G_k(x,\lambda),x) \leqslant C_2|x|^{k+1}, \tag{3.14}$$

for some constants $C_2 > C_1 > 0$, $k=2m+1$, and $m \geqslant 1$.

Theorem 3.6: *Under condition* (3.14), *vector field (3.13) bifurcates from* $(x,\lambda)=(0,0)$ *on* $\lambda > 0$ *to an attractor* Ω_λ, *which is homeomorphic to* S^1. *Moreover, one and only one of the following is true*.

(1) Ω_λ *is a periodic orbit*,
(2) Ω_λ *consists of only singular points, or*
(3) Ω_λ *contains at most* $2(k+1)=4(m+1)$ *singular points, and has* $4N+n(N+n \geqslant 1)$ *singular points*, $2N$ *of which are saddle points*, $2N$ *of which are stable node points (possibly degenerate), and* n *of which have index zero, as shown in Fig. 4 for* $N=1$ *and* $n=2$.

Proof: We proceed in the following five steps.

(1) Obviously (3.14) implies that $x=0$ is asymptotically stable for (3.13) at $\lambda=0$. Hence, by Theorem 3.3, the vector field v_λ bifurcates from $(x,\lambda)=(0,0)$ to an attractor Ω_λ on $\lambda>0$, which has the homology type of a circle S^1.

(2) Let Ω_λ have no singular points. Then, Ω_λ must contain at least a periodic orbit. We need to show that Ω_λ contains only one periodic orbit.

Take the polar coordinate system $(x_1,x_2)=(r\cos\theta, r\sin\theta)$. Then the vector field v_λ becomes

$$\frac{dr}{d\theta} = r\frac{\cos\theta v_1 + \sin\theta v_2}{\cos\theta v_2 - \sin\theta v_1}. \tag{3.15}$$

We see that

$$\cos\theta v_1 = \lambda r\cos^2\theta - \cos\theta g_1(r\cos\theta, r\sin\theta, \lambda),$$

$$\sin\theta v_2 = \lambda r\sin^2\theta - \sin\theta g_2(r\cos\theta, r\sin\theta, \lambda),$$

$$\cos\theta v_2 = \lambda r\cos\theta\sin\theta - \cos\theta\, g_2(r\cos\theta, r\sin\theta, \lambda),$$

$$\sin\theta v_1 = \lambda r\sin\theta\cos\theta - \sin\theta\, g_1(r\cos\theta, r\sin\theta, \lambda),$$

where $G(x,\lambda)=(g_1(x,\lambda), g_2(x,\lambda))$. Let

$$g_i(x,\lambda) = g_{ki}(x,\lambda) + o(|x|^k), \quad i = 1,2.$$

By (3.14) and (3.15) is rewritten as

$$\frac{dr}{d\theta} = \frac{\lambda - r^{2m}(\cos\theta\, g_{k1} + \sin\theta\, g_{k2}) + o(r^{2m})}{r^{2m-1}(\sin\theta\, g_{k1} - \cos\theta\, g_{k2} + O(r))}. \tag{3.16}$$

Based on (3.14), we have

$$C_1 \leqslant \cos\theta\, g_{k1}(\cos\theta, \sin\theta, \lambda) + \sin\theta\, g_{k2}(\cos\theta, \sin\theta, \lambda) \leqslant C_2. \tag{3.17}$$

On the other hand, by assumption, Ω_λ contains a periodic orbit for any $\lambda > 0$ sufficiently small. Hence

$$0 < C \leqslant \sin\theta\, g_{k1}(\cos\theta, \sin\theta, \lambda) - \cos\theta\, g_{k2}(\cos\theta, \sin\theta, \lambda) + O(r), \tag{3.18}$$

for any $0 \leqslant \theta \leqslant 2\pi$ and some constant $C > 0$. Condition (3.18) amounts to saying that the orbits of v_λ are circular around $x=0$.

Let $r(\theta, r_0)$ be the solution of (3.16) with initial value $r(0, r_0) = r_0$. Then we have the following Taylor expansion:

$$r^{2m}(\theta, r_0) = r_0^{2m} + R(\theta)\cdot o(|r_0|^{2m}), \quad R(0) = 0. \tag{3.19}$$

It follows from (3.16) and (3.19) that

$$\frac{1}{2m}[r^{2m}(2\pi, r_0) - r^{2m}(0, r_0)] = \int_0^{2\pi} \frac{\lambda - r^{2m}\alpha(\theta) + o(r^{2m})}{\beta(\theta) + O(r)} d\theta = 2\pi(a\lambda - b r_0^{2m}) + o(r_0^{2m}), \tag{3.20}$$

where

$$a = \int_0^{2\pi} \frac{1}{\beta(\theta) + O(r)} d\theta,$$

$$b = \int_0^{2\pi} \frac{\alpha(\theta)}{\beta(\theta) + O(r)} d\theta,$$

$$\alpha(\theta) = \cos\theta\, g_{k1} + \sin\theta\, g_{k2},$$

$$\beta(\theta) = \sin\theta\, g_{k1} - \cos\theta\, g_{k2}.$$

From (3.20) we see that the periodic solutions of v_λ near $x=0$ correspond to positive solutions of

$$2\pi(a\lambda - br_0^{2m}) + o(r_0^{2m}) = 0. \tag{3.21}$$

By (3.17) and (3.18), $a>0$ and $b>0$. Therefore, (3.21) has a unique positive solution near $r=0$:

$$r_0 = \left(\frac{a\lambda}{b}\right)^{1/2m} + o(\lambda^{1/2m}),$$

for any $\lambda>0$ sufficiently small. Thus, Ω_λ has a unique periodic orbit.

(3) We claim that if Ω_λ contains either finite number of singular points or a cycle of singular points, and if it contains finite number of singular points, then there are at most $2(k+1)$ of them near $x=0$.

In fact, if

$$\frac{g_1(x,\lambda)}{g_2(x,\lambda)} = \frac{x_1}{x_2},$$

then Ω_λ has a cycle of singular points. Otherwise, by (3.14), the number of singular points of v_λ is finite. The maximal number of singular points for v_λ is determined by the following equation

$$\lambda x - G_k(x,\lambda) = 0. \tag{3.22}$$

Since G_k is a k-multilinear vector field, the singular points of (3.22) must be on the straight lines $x_2=zx_1$, where z satisfies

$$z = \frac{g_{k2}(x_1,x_2,\lambda)}{g_{k1}(x_1,x_2,\lambda)} = \frac{g_{k2}(1,z,\lambda)}{g_{k1}(1,z,\lambda)}. \tag{3.23}$$

The number of solutions of (3.23) is at most $k+1$. Since $k=$odd, the number of solutions of (3.22) is at most $2(k+1)$.

(4) Let Ω_λ contain a circle S^1 of singular points, then we shall see that $\Omega_\lambda=S^1$.

Under the polar coordinate system, we have

$$v_r(\theta,r) = (v_x,x) = \lambda r^2 - r^{k+1}\alpha(\theta) + o(r^{k+1}),$$

where $\alpha(\theta)$ is defined by (3.20). By (3.17),

$$0 < C_1 \leqslant \alpha(\theta) \leqslant C_2, \quad \forall\, 0 \leqslant \theta \leqslant 2\pi.$$

It is clear that for each $\theta\,(0\leqslant\theta\leqslant 2\pi)$, v_r has a unique zero point $r_\lambda(\theta)>0$ near $r=0$. Hence the set

$$\widetilde{\Omega}_\lambda = \{(\theta, r_\lambda(\theta)) | v_r(\theta, r_\lambda(\theta)) = 0, \quad 0 \leqslant \theta \leqslant 2\pi\}$$

is homeomorphic to a cycle S^1, and all singular points of v near $x=0$ are on $\widetilde{\Omega}_\lambda$. It implies that $\widetilde{\Omega}_\lambda \subset \Omega_\lambda$. Let

$$g_{kl} = \sum_{i+j=k} \alpha_{ij}^l x_1^i x_2^j, \quad l=1,2. \tag{3.24}$$

By Step 3, we know that $x_2 g_{k1} = x_1 g_{k2}$. Then we infer from (3.14) that

$$0 < \alpha_{k0}^1 = \alpha_{k-11}^2. \tag{3.25}$$

For the singular point $(\tilde{x}_1,0) \in \widetilde{\Omega}_\lambda$ of v_λ, we have

$$\begin{aligned} \operatorname{div} v_\lambda(\tilde{x}_1,0) &= 2\lambda - k\alpha_{k0}^1 \tilde{x}_1^{k-1} - \alpha_{k-11}^2 \tilde{x}_1^{k-1} + o(\tilde{x}_1^{k-1}) \\ &= (\text{by } \alpha_{k0}^1 \tilde{x}_1^{k-1} = \lambda \text{ and } (3.25)) = -(k-1)\lambda + o(\lambda) < 0, \end{aligned}$$

for any $\lambda>0$ sufficiently small.

In the same fashion, for any point $\tilde{x} \in \tilde{\Omega}_\lambda$, we take an orthogonal system transformation such that $\tilde{x}$ is on the $\tilde{x}_1$ axis, then we can prove that

$$\operatorname{div} v_\lambda(x) < 0, \quad \forall\, x \in \tilde{\Omega}_\lambda,$$

which implies that $\Omega_\lambda = \tilde{\Omega}_\lambda = S^1$.

(5) Ω_λ contains finite number of singular points. We show that $\Omega_\lambda = S^1$.

By the Brouwer degree theory, it follows from (3.14) that

$$\deg(v_\lambda, \Omega, 0) = 1, \quad |\lambda| \geqslant 0 \text{ sufficiently small},$$

in some neighborhood $\Omega \subset \mathbb{R}^2$ of $x=0$. It is known that

$$\operatorname{ind}(v_\lambda, 0) = 1, \quad |\lambda| \neq 0.$$

Hence we have

$$\sum_{z_i \in \Omega_\lambda} \operatorname{ind}(v_\lambda, z_i) = 0. \tag{3.26}$$

Let $z \in \Omega_\lambda$ be a singular point of v_λ. Without loss of generality, we take the orthogonal coordinate system such that $z=(x_1, 0)$. Then by (3.14) and (3.24), the Jacobian matrix of v_λ at z is given by

$$Dv_\lambda(z) = \begin{pmatrix} -(k-1)\lambda + o(\lambda) & * \\ 0 & (1 - \alpha^2_{k-11}/\alpha^1_{k0})\lambda \end{pmatrix}, \tag{3.27}$$

where $\alpha^1_{k0} > 0$. Obviously, $Dv_\lambda(z)$ has an eigenvalue $\beta = -(k-1)\lambda + o(\lambda) \neq 0$. Hence for any singular point $z \in \Omega_\lambda$ of v_λ, the index of v_λ at z can only be either 1, -1 or 0. It is easy to see that if the index is 1, then z is a stable node point.

Let the index of v_λ at z be -1:

$$\operatorname{index}(v_\lambda, z) = -1. \tag{3.28}$$

When $\alpha^2_{k-11} \neq \alpha^1_{k0}$, z is nondegenerate. Therefore, v_λ has a unique unstable manifold at z. When $\alpha^2_{k-11} = \alpha^1_{k0}$,

$$\operatorname{div} u_\lambda(z) = -(k-1)\lambda + o(\lambda) < 0. \tag{3.29}$$

If the unstable manifold of v_λ at z is not unique, then the local structure of v_λ at z is topologically equivalent to that as shown in Fig. 5.

On the other hand, (3.29) means that there is a neighborhood $\mathcal{O} \subset \mathbb{R}^2$ of $x=0$, such that

$$\operatorname{div} u_\lambda(x) < 0, \quad \forall\, x \in \mathcal{O},$$

which implies that for any open set $\tilde{\mathcal{O}} \subset \mathcal{O}$,

$$|\tilde{\mathcal{O}}| > |\tilde{\mathcal{O}}_t|, \quad 0 < t < t_0, \tag{3.30}$$

where $t_0 > 0$ depends on $\tilde{\mathcal{O}}$, $\tilde{\mathcal{O}}_t = S(t)\tilde{\mathcal{O}}$ and $S(t)$ is the flow semigroup generated by v_λ.

However, it is clear that for any open set $\tilde{\mathcal{O}} \subset \mathcal{O}$ in domain P as shown in Fig. 5, the property (3.30) is not true. Therefore, the unstable manifold of v_λ at z must be unique.

We can prove in the same fashion that if the index of v_λ at z is 0, then the unstable manifold of v_λ at z is also unique.

By the Poincaré-Bendixson theorem, all unstable manifolds of the singular points of v_λ at z with index -1 and 0 are connected to the singular points with index 1 and 0, as shown in Fig. 4.

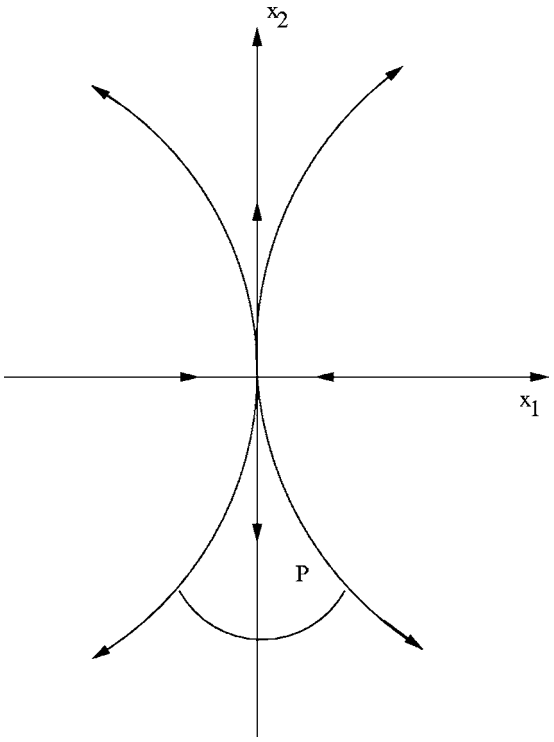

FIG. 5. Schematic illustrating the proof of Theorem 3.6.

Thus by the uniqueness of unstable manifolds for each singular point with either index -1 or index 0, the set of all singular points and unstable manifolds is a circle S^1, and $\Omega_\lambda = S^1$.

The proof is complete. □

IV. ATTRACTOR BIFURCATION FOR TDGL EQUATIONS

A. Mathematical setting

It is known that for a given applied field H_a with $\operatorname{div} H_a = 0$, there exists a field A_a such that

$$\begin{aligned} &\operatorname{curl} A_a = H_a \quad \text{in } \Omega, \\ &\operatorname{div} A_a = 0 \quad \text{in } \Omega, \\ &A_a \cdot n = 0 \quad \text{on } \partial\Omega. \end{aligned} \tag{4.1}$$

Let $A = \mathcal{A} + A_a$. Then (2.11) are rewritten as

$$\psi_t + i\phi\psi = -(i\mu\nabla + A_a)^2\psi + \alpha\psi - 2A_a \cdot \mathcal{A}\psi - 2i\mu\mathcal{A} \cdot \nabla\psi - |\mathcal{A}|^2\psi - \beta|\psi|^2\psi,$$

$$\zeta(\mathcal{A}_t + \mu\nabla\phi) = -\operatorname{curl}^2 \mathcal{A} - \gamma A_a|\psi|^2 - \gamma\mathcal{A}|\psi|^2 - \frac{\gamma\mu i}{2}(\psi^*\nabla\psi - \psi\nabla\psi^*), \tag{4.2}$$

$$\operatorname{div} \mathcal{A} = 0,$$

with the following initial and boundary conditions

$$\psi(0) = \psi_0, \quad A(0) = A_0, \tag{4.3}$$

$$\mathcal{A}_n = 0, \quad \text{curl}\, \mathcal{A} \times n = 0 \quad \text{on } \partial\Omega, \tag{4.4}$$

together with one of the following three boundary conditions for ψ:

Neumann boundary condition:

$$\frac{\partial \psi}{\partial n} = 0 \quad \text{on } \partial\Omega, \tag{4.5}$$

Dirichlet boundary condition:

$$\psi = 0 \quad \text{on } \partial\Omega, \tag{4.6}$$

Robin boundary condition:

$$\frac{\partial \psi}{\partial n} + C\psi = 0 \quad \text{on } \partial\Omega. \tag{4.7}$$

Hereafter we use $H^k(\Omega, \mathbb{C})$ for the Sobolev spaces of complex valued functions defined on Ω, and $H^k(\Omega, \mathbb{R}^3)$ for the Sobolev spaces of vector valued functions. Let

$$H_B^2(\Omega, \mathbb{C}) = \{\psi \in H^2(\Omega, \mathbb{C}) | \psi \text{ satisfy one of (4.5) - (4.7)}\},$$

$$D^2(\Omega, \mathbb{R}^3) = \{\mathcal{A} \in H^2(\Omega, \mathbb{R}^3) | \text{div}\, \mathcal{A} = 0, \quad \mathcal{A} \text{ satisfy (4.4)}\},$$

$$\mathcal{L}^2(\Omega, \mathbb{R}^3) = \{\mathcal{A} \in L^2(\Omega, \mathbb{R}^3) | \text{div}\, \mathcal{A} = 0, \quad \mathcal{A}_n|_{\partial\Omega} = 0\}.$$

We set

$$H = L^2(\Omega, \mathbb{C}) \times \mathcal{L}^2(\Omega, \mathbb{R}^3),$$

$$H_1 = H_B^2(\Omega, \mathbb{C}) \times D^2(\Omega, \mathbb{R}^3).$$

Let

$$P: L^2(\Omega, \mathbb{R}^3) \to \mathcal{L}^2(\Omega, \mathbb{R}^3)$$

be the Leray projection. Then it is known that the function ϕ in (4.2) is determined uniquely up to constants by

$$\zeta\mu \nabla \phi = (I - P)\left[\frac{\gamma\mu}{2} i(\psi \nabla \psi^* - \psi^* \nabla \psi) - \gamma|\psi|^2(\mathcal{A} + A_a)\right], \tag{4.8}$$

where I is the identity on $L^2(\Omega, \mathbb{R}^3)$. Namely, for every $u = (\psi, \mathcal{A}) \in H_1$, there is a unique solution of (4.8) up to constants. Therefore, we define a nonlinear operator $\Phi: H_1 \to L^2(\Omega)$ by

$$\Phi(u) = \phi = \text{the solution of (4.8) with} \int_\Omega \phi \mathrm{d}x = 0. \tag{4.9}$$

B. Eigenvalue problems

In order to describe the dynamic bifurcation of the Ginzburg–Landau equations, it is necessary to consider the eigenvalue problems of the linearized equations.

Let α_1 be the first eigenvalue of the following equation

$$(i\mu\nabla + A_a)^2\psi = \alpha\psi, \quad \forall\, x \in \Omega, \tag{4.10}$$

with one of the boundary conditions (4.5)–(4.7). It is clear that (4.10) can be equivalently expressed as

$$\begin{aligned} -\mu^2\Delta\psi_1 + |A_a|^2\psi_1 - 2\mu A_a\cdot\nabla\psi_2 &= \alpha\psi_1, \\ -\mu^2\Delta\psi_2 + |A_a|^2\psi_2 + 2\mu A_a\cdot\nabla\psi_1 &= \alpha\psi_2, \end{aligned} \tag{4.11}$$

where $\psi = \psi_1 + i\psi_2$.

It is not difficult to check that (4.11) with one of the boundary conditions (4.5)–(4.7) are symmetric. Therefore, there are an infinite real eigenvalue sequence of (4.10):

$$\begin{aligned} &\alpha_1 < \alpha_2 < \cdots, \\ &\lim_{k\to\infty}\alpha_k = \infty, \end{aligned} \tag{4.12}$$

and an eigenvector sequence

$$\{e_n \in H_B^2(\Omega,\mathbb{C}) | n = 1,2,\ldots\}, \tag{4.13}$$

which is an orthogonal basis of $L^2(\Omega,\mathbb{C})$.

The eigenvalues of (4.10) always have even multiplicity, i.e. if ψ is an eigenvector of (4.10), then $e^{i\theta}\psi(\theta\in\mathbb{R}^1)$ are also eigenvectors corresponding to the same eigenvalue. Let the first eigenvalue α_1 have multiplicity $2m(m\geqslant 1)$ with eigenvectors

$$e_{2k-1} = \psi_{k1} + i\psi_{k2}, \quad e_{2k} = -\psi_{k2} + i\psi_{k1}, \quad 1 \leqslant k \leqslant m. \tag{4.14}$$

We know that α_1 enjoys the following properties:

$$\begin{aligned} &\alpha_1 = \alpha_1(A_a) \quad \text{depends continuously on } A_a, \\ &\alpha_1(A_a) > 0 \quad \text{for } A_a \neq 0, \\ &\alpha_1(0) = 0 \quad \text{for the boundary condition (4.5)}, \\ &\alpha_1(0) > 0 \quad \text{for either (4.6) or (4.7)}. \end{aligned} \tag{4.15}$$

Now, we consider another eigenvalue problem, which is also crucial for the attractor bifurcation of (4.2). The problem reads

$$\begin{aligned} &\operatorname{curl}^2 A + \nabla\phi = \rho A, \\ &\operatorname{div} A = 0, \\ &A_n|_{\partial\Omega} = 0, \quad \operatorname{curl} A\times n|_{\partial\Omega} = 0. \end{aligned} \tag{4.16}$$

We remark that the boundary condition in (4.16), i.e., (4.4), is the free boundary condition, which can be expressed as

$$A_n|_{\partial\Omega} = 0, \qquad \left.\frac{\partial A_\tau}{\partial n}\right|_{\partial\Omega} = 0, \tag{4.17}$$

where τ is the tangent vector on $\partial\Omega$.

To see this, for a given point $x_0 \in \partial\Omega$, we take (τ_1, τ_2, n) as an orthogonal coordinate system, where τ_1, τ_2 are unit tangent vectors and n the outward unit vector at $x_0 \in \partial\Omega$. We infer then from the condition $A_n|_{\partial\Omega}=0$ that

$$\operatorname{curl} A(x_0) = -\frac{\partial A_{\tau_2}}{\partial n}\tau_1 + \frac{\partial A_{\tau_1}}{\partial n}\tau_2 + \left(\frac{\partial A_{\tau_2}}{\partial \tau_1} - \frac{\partial A_{\tau_1}}{\partial \tau_2}\right) n \Bigg|_{x=x_0}.$$

Hence we have

$$\operatorname{curl} A(x_0) \times n = \frac{\partial A_{\tau_1}}{\partial n}\tau_1 + \frac{\partial A_{\tau_2}}{\partial n}\tau_2 \Bigg|_{x=x_0},$$

which implies that (4.4) is equivalent to (4.17).

It is known that there are a real eigenvalue sequence

$$0 < \rho_1 < \rho_2 < \cdots,$$
$$\lim_{k\to\infty} \rho_k = \infty, \tag{4.18}$$

and an eigenvector sequence

$$\{a_k \in D^2(\Omega, \mathbb{R}^3) | k = 1,2,\ldots\}, \tag{4.19}$$

which constitutes an orthogonal basis of $\mathcal{L}^2(\Omega, \mathbb{R}^3)$.

C. Main theorems

In superconductivity, the parameter α cannot exceed a maximal value $\alpha(T) \leqslant \alpha(0)$. Hence, we have to impose a basic hypothesis:

$$\alpha_1 < \alpha(0) = \frac{2\sqrt{b} m_s D N_0}{e_s^3 h}, \tag{4.20}$$

where α_1 is the first eigenvalue of (4.10), and N_0 the density of states at the Fermi level.

In this subsection, we consider the case where the first eigenvalue α_1 of (4.10) has multiplicity two. We start with the introduction of a physical parameter, which determines completely the dynamic properties of the bifurcation behavior of the TDGL equations.

Let $e \in H^2(\Omega, \mathbb{C})$ be a first eigenvector of (4.10). Then there is a unique solution for

$$\operatorname{curl}^2 \mathcal{A}_0 + \nabla\phi = |e|^2 A_a + \frac{\mu}{2} i(e^* \nabla e - e \nabla e^*),$$
$$\operatorname{div} \mathcal{A}_0 = 0, \tag{4.21}$$
$$\mathcal{A}_0 \cdot n|_{\partial\Omega} = 0, \quad \operatorname{curl} \mathcal{A}_0 \times n|_{\partial\Omega} = 0.$$

We define a physical parameter R as follows

$$R = -\frac{\beta}{\gamma} + \frac{2\int_\Omega |\operatorname{curl} \mathcal{A}_0|^2 dx}{\int_\Omega |e|^4 dx}. \tag{4.22}$$

It is clear that the parameter R is independent of the choice of the first eigenvectors of (4.10). Since the first eigenvector e of (4.10) and $h_0=\operatorname{curl} A_0$ given by (4.21) depend on the applied magnetic potential A_a and the geometric properties of Ω, the parameter R is essentially a function of A_a,Ω and physical parameters β,γ,μ.

The parameter R defined by (4.22) can be equivalently expressed as follows

$$R=-\frac{\beta}{\gamma}+\frac{2\sum_{k=1}^{\infty}\frac{1}{\rho_k}\left[\int_\Omega(|e|^2A_a+2\mu e_2\nabla e_1)\cdot a_k\right]^2}{\int_\Omega|e|^4\mathrm{d}x}, \tag{4.23}$$

where $e=e_1+ie_2,\rho_k$ are the eigenvalue of (4.16) given by (4.18), and $\{a_k\}$ are the normalized eigenvectors given by (4.19).

The main results in this section are the following theorems. Here, we always assume that the first eigenvalue α_1 of (4.10) with one of the boundary conditions (4.5)–(4.7) is complex simple, and the condition (4.20) holds true.

Theorem 4.1: *If the number R defined by* (4.22) *satisfies $R<0$, then for the problem* (4.2)–(4.4) *with one of* (4.5)–(4.7), *the following assertions hold true.*

(1) *If $\alpha\leqslant\alpha_1$, the steady state $(\psi,\mathcal{A})=0$ is locally asymptotically stable for the problem.*
(2) *The equations bifurcate from $((\psi,\mathcal{A}),\alpha)=(0,\alpha_1)$ to an attractor Σ_α for $\alpha>\alpha_1$, which is homeomorphic to S^1, and consists of steady state solutions of the problem.*
(3) *There is a neighborhood $U\subset H$ of $(\psi,\mathcal{A})=0$ such that the attractor Σ_α attracts $U\backslash\Gamma$ in H, where Γ is the stable manifold of $(\psi,\mathcal{A})=0$ with co-dimension two in H.*
(4) *Each $(\psi,\mathcal{A})\in\Sigma_\alpha$ can be expressed as*

$$\psi=\left|\frac{\alpha-\alpha_1}{R_1}\right|^{1/2}e+o\left(\left|\frac{\alpha-\alpha_1}{R_1}\right|^{1/2}\right),$$

$$\operatorname{curl}^2\mathcal{A}=-\gamma\left|\frac{\alpha-\alpha_1}{R_1}\right|\cdot[|e|^2A_a+\mu\operatorname{Im}(e\nabla e^*)]+o\left(\frac{\alpha-\alpha_1}{R_1}\right), \tag{4.24}$$

$$R_1=\frac{\gamma R\int_\Omega|e|^4\mathrm{d}x}{\int_\Omega|e|^2\mathrm{d}x},$$

where e is the first eigenvector of (4.10).

Theorem 4.2: *If $R>0$, then for the problem* (4.2)–(4.4) *with one of* (4.5)–(4.7), *we have the following assertions:*

(1) *The steady state $(\psi,\mathcal{A})=0$ is locally asymptotically stable at $\alpha<\alpha_1$, and unstable at $\alpha\geqslant\alpha_1$.*
(2) *The equations bifurcate from $((\psi,\mathcal{A}),\alpha)=(0,\alpha_1)$ to an invariant set Σ_α on $\alpha<\alpha_1$, and have no bifurcation on $\alpha>\alpha_1$.*
(3) *$\Sigma_\alpha=S^1$ is a circle consisting of steady states, and has a two-dimensional unstable manifold.*

Theorems 4.1 and 4.2 show that the two cases with $R<0$ and $R>0$ have completely different superconducting transition characteristics; see Sec. V for further discussion.

It is easy to check that if $\alpha=0$, $(\Psi,\mathcal{A})=0$ is globally asymptotically stable for (4.2)–(4.4) with one of (4.5)–(4.7); see Ref. 15. The following theorem is a direct consequence of the existence of global attractor for the TDGL model and Theorem 4.2.

Theorem 4.3: *For the case where* $R>0$, *there exists a saddle-node bifurcation point* $\alpha_0(0<\alpha_0<\alpha_1)$ *for the TDGL equations, such that the following statements hold true, which are described schematically by Figures 2 and 3:*

(1) *At* $\alpha=\alpha_0$, *there is an invariant set* $\Sigma_0=\Sigma_{\alpha_0}$ *with* $0\notin\Sigma_0$.
(2) *For* $\alpha<\alpha_0$, *there is no invariant set near* Σ_0.
(3) *For* $\alpha_0<\alpha<\alpha_1$, *there are two connected branches of invariant sets* Σ_α^1 *and* Σ_α^2, *and* Σ_α^2 *extends to* $\alpha\geqslant\alpha_1$ *and near* α_1 *as well*.
(4) *For each* $\alpha>\alpha_0$,
   (a) Σ_α^2 *is an attractor with* $\mathrm{dist}(\Sigma_\alpha^2,0)>0$ *at* $\alpha=\alpha_1$,
   (b) Σ_α^2 *consists of steady state solutions and orbits connecting them, and*
   (c) Σ_α^2 *contains at least one cycle of steady states*.
(5) *For* $\alpha_0<\alpha<\alpha_1$,
   (a) Σ_α^1 *is a repeller with* $0\notin\Sigma_\alpha^1$,
   (b) Σ_α^1 *consists of steady state solutions and orbits connecting them*,
   (c) Σ_α^1 *contains at least one cycle of steady states, and*
   (d) *when* α *is near* α_1, Σ_α^1 *is exactly the* $\Sigma_\alpha=S^1$ *given in Theorem 4.2, consisting exactly of steady states*.

D. Proof of Theorems 4.1 and 4.2

We proceed in several steps as follows.

(1) We set the mappings $L_\alpha=-K+B_\alpha$ and $G:H_1\to H$ by

$$Ku=\begin{pmatrix}(i\mu\nabla+A_a)^2\psi\\ \zeta^{-1}\mathrm{curl}^2\mathcal{A}\end{pmatrix},$$

$$B_\alpha u=\begin{pmatrix}\alpha\psi\\ 0\end{pmatrix},$$

$$G(u)=\begin{pmatrix}i\psi\Phi(u)+2A_a\cdot\mathcal{A}\psi+2i\mu\mathcal{A}\cdot\nabla\psi+|\mathcal{A}|^2\psi+\beta|\psi|^2\psi\\ P\left[\gamma\zeta^{-1}A_a|\psi|^2+\gamma\zeta^{-1}\mathcal{A}|\psi|^2+\frac{\gamma\mu i}{2\zeta}(\psi^*\nabla\psi-\psi\nabla\psi^*)\right]\end{pmatrix},$$

where $u=(\psi,\mathcal{A})$, $\Phi(u)$ is defined by (4.9), and P the Leray projection. Thus, the problem (4.2)–(4.4) with one of the boundary conditions (4.5)–(4.7) can be rewritten in the following operator form

$$\frac{\mathrm{d}u}{\mathrm{d}t}=L_\alpha u+G(u),\quad u=(\psi,\mathcal{A})\in H_1,$$
$$u(0)=u_0. \tag{4.25}$$

We see that $L_\alpha:H_1\to H$ is a sectorial operator, and the eigenvalues of L_α satisfy that

$$\beta_1(\alpha)=\beta_2(\alpha)=\alpha-\alpha_1\begin{cases}<0 & \text{if } \alpha<\alpha_1\\ =0 & \text{if } \alpha=\alpha_1\\ >0 & \text{if } \alpha>\alpha_1,\end{cases} \tag{4.26}$$

and for $j\geqslant 3$,

$$\beta_j(\alpha_1) = \alpha_1 - \alpha_k \text{ or } -\zeta^{-1}\rho_l,$$
$$\beta_j(\alpha_1) < 0, \tag{4.27}$$

for some $k>1$, $l\geqslant 1$.

It is clear that the operator $\Phi: H_1 \to L^2(\Omega, \mathbb{C})$ defined by (4.9) is C^∞, and by the estimates proved in Ref. 15 for Φ, we have

$$\int_\Omega |\Phi(u)\psi|^2 \mathrm{d}x \leqslant \left[\int_\Omega |\Phi(u)|^3 \mathrm{d}x\right]^{2/3}\left[\int_\Omega |\psi|^6 \mathrm{d}x\right]^{1/3} \leqslant C(\|u\|^2_{H_{1/2}} + \|u\|_{H_{1/2}}\|\psi\|^2_{L^4})^2\|\psi\|^2_{L^6},$$

where $H_{1/2}$ is the closure of H_1 for the H^{-1}-norm. Hence, it is not difficult to check that there is a number $1/2<\sigma<1$ such that $G: H_\sigma \to H$ is C^∞.

(2) It is known that the dynamic bifurcation of (4.25) is determined by its reduced equation to the center manifold.

Let

$$\psi_0 \in E_1 = \{ze | z \in \mathbb{C} \text{ and } e \text{ the first eigenvector of (4.10)}\}.$$

Then the reduced equation of (4.25) is given by

$$\frac{\mathrm{d}\psi_0}{\mathrm{d}t} = \beta_1(\alpha)\psi_0 - P_1 G(\psi_0 + \tilde{\psi}(\psi_0), \tilde{\mathcal{A}}(\psi_0)), \tag{4.28}$$

where $P_1: H \to E_1$ is the canonical projection, and $\tilde{\Phi}(\psi_0) = (\tilde{\psi}(\psi_0), \tilde{\mathcal{A}}(\psi_0)) \in H_1$ the center manifold function.

The k multilinear operators ($k=2,3$) in G are given by

$$G_2(u) = -\begin{pmatrix} 2A_a \cdot \mathcal{A}\psi + 2i\mu\mathcal{A}\cdot\nabla\psi \\ \zeta^{-1}\gamma A_a|\psi|^2 + \dfrac{\gamma\mu}{2\zeta} i(\psi^*\nabla\psi - \psi\nabla\psi^*) \end{pmatrix},$$

$$G_3(u) = -\begin{pmatrix} i\psi\Phi_2(u) + |\mathcal{A}|^2\psi + \beta|\psi|^2\psi \\ \gamma\zeta^{-1}\mathcal{A}|\psi|^2 \end{pmatrix},$$

where $\Phi_2(u)$ is the bilinear operator in $\Phi(u)$.

By the first approximation of the center manifold reduction, the center manifold function $\tilde{\Phi} = (\tilde{\psi}(\psi_0), \tilde{\mathcal{A}}(\psi_0))$ satisfies that

$$\mathrm{curl}^2\,\tilde{\mathcal{A}} + \mu\nabla\phi = -\gamma A_a|\psi_0|^2 - \frac{\gamma\mu}{2} i(\psi_0^*\nabla\psi_0 - \psi_0\nabla\psi_0^*) + o(\|\psi_0\|^2, |\beta_1(\alpha)|\cdot\|\psi_0\|), \tag{4.29}$$

$$\tilde{\psi}(\psi_0) = O(\|\tilde{\mathcal{A}}(\psi_0)\|\cdot\|\psi_0\|) = O(\|\psi_0\|^3). \tag{4.30}$$

Based on (4.28) and (4.30), (4.28)can be expressed as

$$\frac{\mathrm{d}\psi_0}{\mathrm{d}t} = \beta_1(\alpha)\psi_0 - g_3(\psi_0) + o(\|\psi_0\|^3) + O(\|\psi_0\|^3|\beta_1(\alpha)|), \tag{4.31}$$

where

$$g_3(\psi_0) = P_1[\beta|\psi_0|^2\psi_0 + 2A_a\cdot\tilde{\mathcal{A}}_2\psi_0 + 2i\mu\tilde{\mathcal{A}}_2\cdot\nabla\psi_0 + i\Phi_2\psi_0], \tag{4.32}$$

$$\operatorname{curl}^2 \tilde{\mathcal{A}}_2 + \nabla\phi = -\gamma A_a|\psi_0|^2 - \frac{\gamma\mu}{2} i(\psi_0^* \nabla \psi_0 - \psi_0 \nabla \psi_0^*),$$

$$\operatorname{div} \tilde{\mathcal{A}}_2 = 0,$$

$$\tilde{\mathcal{A}}_2 \cdot n|_{\partial\Omega} = 0, \quad \operatorname{curl} \tilde{\mathcal{A}}_2 \times n|_{\partial\Omega} = 0. \tag{4.33}$$

Equations (4.31) and (4.32) are the third-order expression of the reduction of (4.27) to the center manifold.

(3) From (4.32), we obtain

$$\langle g_3(\psi_0), \psi_0\rangle = \operatorname{Re}\int_\Omega g_3(\psi_0)\psi_0^* dx = \int_\Omega [\beta|\psi_0|^4 + 2|\psi_0|^2 A_a \cdot \tilde{\mathcal{A}}_2 + 2\mu\tilde{\mathcal{A}}_2 \cdot (\psi_2^0 \nabla \psi_1^0 - \psi_1^0 \nabla \psi_2^0)]dx$$

$$= \int_\Omega [\beta|\psi_0|^4 + 2|\psi_0|^2 A_a \cdot \tilde{\mathcal{A}}_2 + 4\mu\psi_2^0 \tilde{\mathcal{A}}_2 \cdot \nabla\psi_1^0]dx, \tag{4.34}$$

where $\psi_0 = \psi_1^0 + i\psi_2^0$.

Let $\tilde{\mathcal{A}}_2$ have the Fourier expansion for the basis (4.19) of $\mathcal{L}^2(\Omega, \mathbb{R}^3)$ as follows:

$$\tilde{\mathcal{A}}_2 = \sum_{k=1}^{\infty} y_k a_k.$$

Then, for (4.33) we can derive the solution y_k:

$$y_k = -\frac{\gamma}{\rho_k}\int_\Omega [|\psi_0|^2 A_a \cdot a_k + 2\mu\psi_2^0 a_k \cdot \nabla\psi_1^0]dx. \tag{4.35}$$

Inserting (4.35) into (4.34) we find

$$\langle g_3(\psi_0), \psi_0\rangle = \beta\int_\Omega |\psi_0|^4 dx - 2\gamma\sum_{k=1}^{\infty}\frac{1}{\rho_k}\left[\left(\int_\Omega |\psi_0|^2 A_a \cdot a_k dx\right)^2 + 4\mu\left(\int_\Omega |\psi_0|^2 A_a \cdot a_k dx\right)\right.$$
$$\left.\times\left(\int_\Omega \psi_2^0 a_k \cdot \nabla\psi_1^0 dx\right) + 4\mu^2\left(\int_\Omega \psi_2^0 a_k \cdot \nabla\psi_1^0 dx\right)^2\right]. \tag{4.36}$$

Let $\psi_0 = x_1 e_1 + x_2 e_2$, where $(x_1, x_2) \in \mathbb{R}^2$, and e_1 and e_2 are as in (4.14). Then we have

$$\psi_0 = \psi_1^0 + i\psi_2^0,$$

$$\psi_1^0 = x_1\psi_{11} - x_2\psi_{12},$$

$$\psi_2^0 = x_1\psi_{12} + x_2\psi_{11}.$$

Thus, we see that

$$\int_\Omega |\psi_0|^4 dx = \int_\Omega (|\psi_1^0|^2 + |\psi_2^0|^2)^2 dx = (x_1^2 + x_2^2)\int_\Omega |e_1|^4 dx, \tag{4.37}$$

$$\int_\Omega |\psi_0|^2 A_a \cdot a_k dx = (x_1^2 + x_2^2)\int_\Omega |e_1|^2 A_a \cdot a_k dx, \tag{4.38}$$

$$\int_\Omega \psi_2^0 a_k \cdot \nabla \psi_1^0 \mathrm{d}x = (x_1^2 + x_2^2) \int_\Omega \psi_{12} a_k \cdot \nabla \psi_{11} \mathrm{d}x. \tag{4.39}$$

Here, in (4.39) we use the following equality:

$$\int_\Omega \psi a_k \cdot \nabla \psi \mathrm{d}x = -\frac{1}{2} \int_\Omega \psi^2 \operatorname{div} a_k \, \mathrm{d}x = 0,$$

for any real function ψ.

Putting (4.37)–(4.39) into (4.36) we find

$$\langle g_3(\psi_0), \psi_0 \rangle = -\gamma R (x_1^2 + x_2^2)^2 \int_\Omega |e_1|^4 \mathrm{d}x, \tag{4.40}$$

where R is as in (4.23). It is easy to see that both numbers in (4.22) and (4.23) are the same.

(4) We shall prove that the Ginzburg–Landau equations bifurcate from $((\psi, \mathcal{A}), \alpha) = (0, \alpha_1)$ to at least one steady state solution.

Formally, there are two steady state Ginzburg–Landau systems, i.e. the stationary equations obtained directly from (4.2) which read

$$\begin{aligned} (i\mu + A_a)^2 \psi + i\Phi\psi &= \alpha\psi - 2A_a \cdot A\psi - 2i\mu\mathcal{A} \cdot \nabla\psi - \mathcal{A}^2\psi - \beta|\psi|^2\psi, \\ \operatorname{curl}^2 \mathcal{A} + \zeta\mu \nabla \Phi &= -\gamma(\mathcal{A} + A_a)|\psi|^2 - \frac{\gamma\mu}{2} i(\psi^* \nabla \psi - \psi \nabla \psi^*), \end{aligned} \tag{4.41}$$

and the other one given by

$$\begin{aligned} (i\mu \nabla + A_a)^2 &= \lambda\psi - 2A_a \cdot \mathcal{A}\psi - 2i\mu\mathcal{A} \nabla \psi - \mathcal{A}^2\psi - \beta|\psi|^2\psi, \\ \operatorname{curl}^2 \mathcal{A} &= -\gamma(\mathcal{A} + A_a)|\psi|^2 - \frac{\gamma\mu i}{2}(\psi^* \nabla \psi - \psi \nabla \psi^*). \end{aligned} \tag{4.42}$$

The form (4.42) was derived by Ginzburg and Landau in 1950 as the Euler-Lagrange equations of the free energy. In Ref. 15, it is proved that if $u = (\psi, \mathcal{A}) \in H_1$ and $\Phi \in H^1(\Omega)$ is a solution of (4.41) with (4.4) and (4.5), then we have that $\Phi = 0$. It is easy to prove in the same fashion that this assertion also holds true for the boundary conditions (4.6) and (4.7). Therefore, both steady state equations (4.41) and (4.42) are exactly the same.

The Ginzburg–Landau energy for Eq. (4.42) read

$$\begin{aligned} E = \frac{1}{2} \int_\Omega \left[|(i\mu \nabla + \mathcal{A} + A_a)\psi|^2 + \frac{\beta}{2}|\psi|^4 - \alpha|\psi|^2 + \gamma^{-1}|\operatorname{curl}\mathcal{A}|^2 \right] \\ \times \mathrm{d}x \left(+ \frac{1}{2}\mu^2 c \int_{\partial\Omega} |\psi|^2 \mathrm{d}s \quad \text{for boundary condition (4.7)} \right). \end{aligned}$$

Therefore, by the classical bifurcation theorem for potential operators (see Refs. 18–20), the steady state equations (4.42) with (4.4) and one of the boundary conditions (4.5)–(4.7) must bifurcate to at least one solution from $((\psi, \mathcal{A}), \alpha) = (0, \alpha_1)$.

(5) Proof of Theorem 4.1: When $R < 0$, by (4.31) and (4.40), we can obtain assertion (1), and we infer from Theorem 3.6 that the Ginzburg–Landau equations bifurcate from $((\psi, \mathcal{A}), \alpha) = (0, \alpha_1)$ a cycle Σ_α of attractor for $\alpha > \alpha_1$. By Step 4, the attractor Σ_α contains a singular point. Because of the invariance of the Ginzburg–Landau equations for the gauge transformation

$$\psi \to \psi e^{i\theta}, \quad \theta \in \mathbb{R}^1,$$

the steady state solutions of the Ginzburg–Landau equations appear as a circle S^1. Hence the attractor $\Sigma_\alpha = S^1$ consists of steady state solutions. Assertion (2) is proved.

Assertion (3) follows from Theorem 3.3, and Assertion (4) can be directly derived from Eqs. (4.31) and (4.40). Thus, Theorem 4.1 is proved.

(6) Proof of Theorem 4.2: When $R > 0$, the the time-reversed semigroup $S_\alpha(-t)$ generated by (4.31) has the same dynamic properties as the following equation

$$\frac{d\psi_0}{dt} = (\alpha_1 - \alpha)\psi_0 + g_3(\psi_0) + o(\|\psi_0\|^3, |\alpha - \alpha_1|\|\psi_0\|^2). \tag{4.43}$$

In the same fashion as used in Step 5, from (4.40) we infer that the semi-group $\widetilde{S}_\alpha(t)$ generated by (4.43) bifurcates from $(\psi_0, \alpha) = (0, \alpha_1)$ to an S^1 attractor Σ_α for $\alpha < \alpha_1$, which consists of singular points of (4.43). Hence, for the semi-group $S_\lambda(t)(=\widetilde{S}_\lambda(-t))$ generated by (4.31) with $R > 0$, the Assertions (1)–(3) hold true.

Thus, Theorem 4.2 is proved.

E. Bifurcation from general eigenvalues

Although the bifurcation from general eigenvalues of (4.10) has less physical interest, we consider this problem partially for the mathematical completeness.

Before our discussion, we remark that one can prove[21] that the first eigenvalue λ_1 with complex simplicity is generic. Namely, if we set

$$\mathcal{H}^1 = \{A \in H^1(\Omega, \mathbb{R}^3) | A \cdot n|_{\partial\Omega} = 0, \quad \operatorname{div} A = 0\},$$

then, there is an open and dense set $U \subset \mathcal{H}^1$ such that for any $A_a \in U$, the first eigenvalue $\lambda_1(A_a)$ of (4.10) is complex simple. However, we cannot exclude the existence of a bounded domain $\Omega \subset \mathbb{R}^3$ and a vector $A_a \in \mathcal{H}^1$ such that the first eigenvalue $\lambda_1(\Omega, A_a)$ of (4.10) has higher complex multiplicity.

Let α_k be an eigenvalue of (4.10) with complex multiplicity $m \geqslant 1$, and E_k be the eigenspace of α_k, i.e.

$$E_k = \{\psi \in H_B^2(\Omega, \mathbb{C}) | (i\mu\nabla + A_a)^2 \psi = \alpha_k \psi\}.$$

It is clear that $\dim E_k = 2 \dim_{\mathbb{C}} E_k = 2m$.

Let F be function defined on E_k:

$$F(\psi) = 2\sum_{n=1}^{\infty} \frac{1}{\rho_n}\left[\int_\Omega (|\psi|^2 A_a + 2\mu\psi_2 \nabla \psi_1) a_n dx\right]^2,$$

where $\psi = \psi_1 + i\psi_2 \in E_k$, and ρ_n, a_n are as in (4.18) and (4.19).

Set

$$R_1 = \sup_{\psi \in E_k, \psi \neq 0} \frac{F(\psi)}{\int_\Omega |\psi|^4 dx},$$
$$R_2 = \inf_{\psi \in E_k, \psi \neq 0} \frac{F(\psi)}{\int_\Omega |\psi|^4 dx}. \tag{4.44}$$

Then, we have the following theorem.

Theorem 4.4: *For the problem* (4.2)–(4.4) *with one of* (4.5)–(4.7), *we have the following assertions*.

(1) *If the physical parameter* $\beta/\gamma > R_1$, *then this problem bifurcates from* $((\psi,\mathcal{A}),\alpha)=(0,\alpha_k)$ *to an invariant set* Σ_α *for* $\alpha>\alpha_k$.
(2) *If* $\beta/\gamma < R_2$, *then this problem bifurcates from* $((\psi,\mathcal{A}),\alpha)=(0,\alpha_k)$ *to an invariant set* Σ_α *for* $\alpha<\alpha_k$.
(3) *The invariant set* Σ_α *is a* $(2m-1)$*-dimensional homological sphere, i.e.* $2m-1 \leqslant \dim \Sigma_\alpha \leqslant 2m$, *and* Σ_α *has the same homology as a* $(2m-1)$*-dimensional sphere*.
(4) Σ_α *contains at least a circle of singular points of the equations*.
(5) *When* $m=1$, Σ_α *is a circle* S^1.
(6) *When* $\alpha_k=\alpha_1$ *and* $\beta/\gamma > R_1$, Σ_α *is an attractor, which attracts an open set* $U\backslash\Gamma$, *where* $U\subset H$ *is a neighborhood of* $(\psi,\mathcal{A})=0$, *and* Γ *is the stable manifold of* $(\psi,\mathcal{A})=0$ *with co-dimension* $2m$ *in* H.

Remark 4.5: We conjecture that the bifurcated invariant set Σ_α in Theorem 4.4 is homeomorphic to a $(2m-1)$-dimensional sphere S^{2m-1}, and Σ_α contains at least m circles consisting of singular points.

When $m=1$, these two numbers R_1 and R_2 are the same: $R_1=R_2$, and $R=R_1-\beta/\gamma$ is as in (4.22).

The proof of Theorem 4.4 is the same as that of Theorems 4.1 and 4.2; we omit the details.

V. CONCLUSIONS AND REMARKS

A. General remarks

The permanent current, called supercurrent, is expressed in the Ginzburg–Landau equations by (2.2). In the steady state case, the supercurrent in the second type of nondimensional form is written as

$$J_s = J_s(\psi,\mathcal{A}) = -\gamma(A_a+\mathcal{A})|\psi|^2 - \frac{\gamma\mu}{2} i(\psi^*\nabla\psi - \psi\nabla\psi^*). \tag{5.1}$$

To take the Meissner effect into account in the Ginzburg–Landau equation. Mathematically speaking, in the normal state, the magnetic field H in a sample should be $H=H_a+\mathcal{H}$, $H_a=\operatorname{curl} A_a$ is the applied field and $\mathcal{H}=\operatorname{curl}\mathcal{A}$ the nonequilibrium fluctuation, and in the superconducting state $H=\operatorname{curl}\mathcal{A}$. In the both cases, $\mathcal{A}$ satisfy the Ginzburg–Landau equation (4.2) and boundary condition (4.4). Namely, we can express the magnetic field H in a sample Ω in the following form

$$\begin{gathered} H=\operatorname{curl} A, \quad \forall\, x\in\Omega, \\ A=\begin{cases} A_a+\mathcal{A} & \text{in the normal state,} \\ \mathcal{A} & \text{in the superconducting state,} \end{cases} \end{gathered} \tag{5.2}$$

and the supercurrent J_s in the nondimensional form also is given by

$$J_s = \operatorname{curl}^2 \mathcal{A}. \tag{5.3}$$

Here $\mathcal{A}$ satisfies (4.2) and (4.4).

An equilibrium state $(\tilde{\psi},\tilde{\mathcal{A}})$ of the TDGL equations (4.2) is called in the normal state if $\tilde{\psi}=0$, and $(\tilde{\psi},\tilde{\mathcal{A}})$ is called in the superconducting state if $\tilde{\psi}\neq 0$. A solution $(\psi,\mathcal{A})$ of (4.2) is said in the normal state if $(\psi,\mathcal{A})$ is in a domain of attraction of a normal equilibrium state, otherwise $(\psi,\mathcal{A})$ is said in the superconducting state.

We consider the simplest case where the applied field vanishes $A_a=0$. In this case, the eigenvalue equation (4.10) becomes

$$-\mu\Delta\psi = \alpha\psi. \tag{5.4}$$

The first eigenvalue α_1 of (5.4) with one of the boundary conditions (4.5)–(4.7) is simple, and the eigenvector is real. Therefore, the parameter R defined by (4.22) reads

$$R = -\frac{\beta}{\gamma} < 0.$$

By Theorem 4.1, when the parameter $\alpha(T) \leqslant \alpha_1$ the solutions $(\psi, \mathcal{A})$ of (4.2) is in the normal state, and when $\alpha(T) > \alpha_1$, $(\psi, \mathcal{A})$ with the initial $(\psi_0, \mathcal{A}_0)$ in $U\backslash\Gamma$ is in the superconducting states.

When $A_a = 0$, the steady state solutions $(\tilde{\psi}, \tilde{\mathcal{A}})$ of (4.2) are real, i.e. $\tilde{\psi} = e^{i\theta}\psi$, $I_m\psi = 0$. Hence

$$\tilde{\psi}^* \nabla \tilde{\psi} - \psi \nabla \psi^* = 0,$$

which implies that $\tilde{A} = 0$. Thus, the supercurrent (5.3) (or (5.1)) vanishes

$$J_s = 0.$$

This shows that with zero applied field $H_a = 0$, there is no current in a superconductor.

Implications of (4.20): For the Neumann boundary condition (4.5), i.e. the sample is enclosed by an insulator, the first eigenvalue $\alpha_1 = 0$ for (5.4), which is independent of Ω, the geometry of sample. Therefore, the condition (4.20) always holds true.

However, for the Dirichlet and the Robin boundary conditions (4.6) and (4.7), the situation is different. It is known that the first eigenvalue α_1 of (5.4) depends on Ω. In particular,

$$\alpha_1 = \alpha_1(\Omega) \to \infty \quad \text{if} |\Omega| \to 0$$

The condition (4.20) implies that for the cases where the samples are enclosed by a magnetic material or a normal metal, the volume of a sample must be greater than some critical value $|\Omega| > V_c > 0$. Otherwise no superconducting state occurs at any temperature. This property also holds true for the case where there is an applied magnetic field H_a present. Of course, in this case, the critical volume V_c depends on H_a as well.

B. Transitions in the case with $R < 0$

As mentioned earlier, there are two transitions determined by a simple parameter R defined by (4.22) for transitions near a complex simple eigenvalue of the linearized problem (respectively by two parameters R_1 and R_2 defined by (4.44) for transitions near an eigenvalues with higher multiplicity). The parameter R links the superconducting behavior with the geometry of the material, the applied field and the physical parameters. For simplicity, we address here only the case near a complex simple eigenvalue of the linearized problem, and physical conclusions can be derived in the same fashion.

Let a magnetic field $H_a = \text{curl}\, A_a$ be applied. By the bifurcation theorems, the critical temperature T_c^1 of superconducting transition satisfies then $T_c^1 < T_c$, where T_c is given in (2.4) and T_c^1 satisfies that

$$\alpha(T_c^1) = \alpha_1 > 0, \tag{5.5}$$

where $\alpha_1 = \alpha_1(A_a)$ is the first eigenvalue of (4.10). It is known that

$$\alpha_1(A_a) \to \infty \quad \text{if} \quad |A_a| \to \infty.$$

It implies that the applied magnetic field H_a can not be very strong for superconductivity as required by the condition (4.20).

From Theorems 4.1 and 4.2, we see that the number R defined by (4.22) is an important parameter to distinguish two different types of superconducting transitions. We first examine the case where $R < 0$.

By Theorem 4.1, when $\alpha > \alpha_1$, Eq. (4.2) bifurcate from $((\psi, \mathcal{A}, \alpha) = (0, \alpha_1)$ to a steady state solution $(\psi_\alpha, \mathcal{A}_\alpha)$ which is an attractor attracting an open set $U \backslash \Gamma \subset H$. Physically speaking, this theorem leads to the following properties of superconducting transitions in the case where $R < 0$; see Fig. 1.

Theorem 5.1: *Let $R < 0$ and $m = 1$ as in Theorem 4.1, and T_c^1 be given by* (5.5). *Then the following physical properties hold true*

(1) *When the control temperature decreases (resp. increases) and crosses the critical temperature T_c^1, there will be a phase transition of the sample from the normal to superconducting states (respectively from superconducting to normal state).*
(2) (Stability) *When the control temperature $T \geqslant T_c^1$, under a fluctuation deviating the normal state, the sample will soon be restored to the normal state. In addition, when $T < T_c^1$, under a fluctuation deviating both the normal and superconducting states, the sample will soon be restored to the superconducting states.*
(3) *In general, the supercurrent given by*

$$J_s(\alpha) = -\gamma(A_a + \mathcal{A}_\alpha)|\psi_\alpha|^2 - \frac{\gamma\mu}{2} i(\psi_\alpha^* \nabla \psi_\alpha - \psi_\alpha \nabla \psi_\alpha^*)$$

is nonzero, i.e., $J_s \neq 0$ for $\alpha_1 < \alpha (T < T_c^1)$.
(4) (Continuity) *The order parameter Ψ_α and supercurrent $J_s(\alpha)$ depend continuously on the parameter α (or the control temperature T), namely*

$$\psi_\alpha \to 0, \quad J_s(\alpha) \to 0, \quad \text{if } \alpha \to \alpha_1 + 0 \ (\text{or}, T \to T_c^1 - 0). \tag{5.6}$$

(5) *The superconducting state of the system is dominated by the lowest-energy eigenfunction of* (4.10) *in the sense given by* (4.24).

C. Transitions with $R > 0$

Transitions in this case are precisely described by Theorems 4.2 and 4.3, as shown in Figs. 2 and 3. In particular, we have the following theorem, which recapitulates some phase transition properties obtained in Theorems 4.2 and 4.3 in physical terms.

Theorem 5.2: *Consider a material described by the TDGL with $R > 0$. There are two critical temperatures T_c^0 and T_c^1 $(T_c^0 > T_c^1)$ such that*

$$\alpha(T_c^i) = \alpha_i \quad (i = 0, 1),$$

and the following phase transition properties hold true:

(1) *When the control temperature T decreases and crosses T_c^1, or equivalently α increases and crosses α_1, the stability of the normal state changes from stable to unstable.*
(2) *When $T_c^1 < T$ (or $\alpha < \alpha_1$), physically observable states consists of the normal state, and the superconducting states in Σ_α^2. When $T_c^1 > T$ (or $\alpha > \alpha_1$), physically observable states are in Σ_α^2.*
(3) (Instability) *When the control temperature T is in the interval: $T_c^1 < T < T_c^0$ (or $\alpha_0 < \alpha < \alpha_1$), the superconducting states given Σ_α^1 are unstable, i.e., with a fluctuation deviating a superconducting state in Σ_α^1, transition to either the normal state or a superconducting state in Σ_α^2 will occur.*
(4) (Discontinuity) *At the critical temperature T_c^0 (respectively at T_c^1) of the phase transitions, there is a jump from the superconducting states to the normal state (respectively from the normal state to superconducting states).*
(5) *The other lower-energy eigenfunctions possibly have a stronger influence for the superconducting states.*

It is noteworthy to remark that the phase transitions in the case where $R > 0$ is very different from the transitions for the case where $R < 0$ as described.

Physical significance of R: We note that the parameter β/γ can be characterized by the Ginzburg–Landau parameter κ and the parameter μ:

$$\frac{\beta}{\gamma} = \kappa^2\mu^2, \quad \kappa^2 = \frac{m_s^2c^2}{2\pi e_s^2h^2}b, \quad \mu^2 = \frac{h}{e_s}\frac{D}{\sqrt{b}}. \tag{5.7}$$

In the Ginzburg–Landau energy, the term

$$E_0 = \int_\Omega |e|^4 \mathrm{d}x \tag{5.8}$$

represents the nonlinear part of the energy of the superconducting electrons in the lowest-energy state, and the term

$$E_m = \int_\Omega H_0^2 \mathrm{d}x, \quad h_0 \text{ satisfies (4.21)}, \tag{5.9}$$

is the energy contributed by the magnetic field associated with the supercurrent

$$\operatorname{curl} h_0 = |e|^2 A_a + \frac{\mu}{2} i(e^* \nabla e - e \nabla e^*),$$

which is generated by the applied magnetic potential A_0 and the superconducting electrons in the lowest-energy states.

By (4.2) and (4.22), we obtain from (5.7)–(5.9) that

$$R = -\kappa^2\mu^2 + \frac{2E_m}{E_0}. \tag{5.10}$$

Hence, the type of superconducting phase transitions among the two described above for a given material depends on the "competition" between the two energies E_0 and E_m:

$$R\begin{cases} <0 \quad \text{if and only if } \dfrac{\kappa^2}{2}E_0 > \dfrac{1}{\mu^2}E_m, \\ >0 \quad \text{if and only if } \dfrac{\kappa^2}{2}E_0 < \dfrac{1}{\mu^2}E_m. \end{cases} \tag{5.11}$$

According to the Abrikosov theory, the materials with $\kappa^2<2$ and $\kappa^2>2$ are of types I and II, respectively. From (5.11), we infer that for given geometrical shape of sample and applied magnetic field, a type I material favors more to the jumped phase transition (i.e., the case $(R>0)$), and a type II material favors the continuous phase transition (i.e the case $(R<0)$).

D. Topological structure of supercurrents

In 1957, Abrikosov predicted that in the mixed state of type II superconductors, there is a square array of vortices of supercurrents, and this vortex array was confirmed by experiments later.

In the two-dimensional case, by Theorems 4.1 and 4.2, the bifurcated attractor contains superconducting states $(\psi, \mathcal{A})$ such that the supercurrent $J_s = J_s(\psi, \mathcal{A})$ given by (5.1) is in general not identically zero and

$$\operatorname{div} J_s = 0, \quad J_s \cdot n\big|_{\partial\Omega} = 0. \tag{5.12}$$

Thanks to (5.12), the geometric theory for two-dimensional incompressible flows developed recently by the authors[5] can be applied to study the structure of the supercurrent J_s in the physical space. For this purpose, we first recall briefly some basic results and concepts directly related to the study of the structure of J_s.

Structure of 2D Incompressible flows: First, let $C^r(\Omega,\mathbb{R}^2)$ be the space of all C^r vector fields on Ω, and

$$D^r(\Omega)=\{v\in C^r(\Omega,\mathbb{R}^2)|v\cdot n|_{\partial\Omega}=0,\ \mathrm{div}\ v=0\}.$$

Let $v\in D^r(\Omega)$. A point $p\in\Omega$ is called a singular point of v if $v(p)=0$; a singular point p of v is called nondegenerate if the Jacobian matrix $Dv(p)$ is invertible; v is called regular if all singular points of v are non-degenerate. An interior nondegenerate singular point of v can be either a center or a saddle, and a nondegenerate boundary singularity must be a saddle. Saddles of v must be connected to saddles. An interior saddle $p\in\Omega$ is called self-connected if p is connected only to itself, i.e., p occurs in a graph whose topological form is that of the number 8.

Second, let $v\in D^r(\Omega)$ be regular, and Ω be a connected domain with k holes. Let C be the number of centers of v, S the number of interior saddles, and B the number of boundary saddles. Then[5,22]

$$C-S-\frac{B}{2}=1-k. \tag{5.13}$$

Third, again, let $v\in D^r(\Omega)$, and $p\in M$ be a center. Then there is an open neighborhood C of p, such that for any $x\in C(x\neq p)$, the orbit $\{\Phi(x,t)\}_{t\in\mathbb{R}}$ is closed. The largest such neighborhood C of p is called a circle cell of v. Let $B\subset M$ be an open set, such that for any $x\in B$, the orbit $\{\Phi(x,t)\}_{t\in\mathbb{R}}$ is closed, and each connected component Σ of ∂B is not a single point. Then B is called a circle band of v.

Then it is proved that[5,23] for a regular divergence-free vector field $v\in D^r(\Omega)(r\geqslant 1)$, the topological structure of v consists of finite number of circle cells, circle bands, and saddle connections.

Fourth, two vector fields $u,v\in D^r(\Omega,\mathbb{R}^2)$ are called topologically equivalent if there exists a homeomorphism of $\varphi:\Omega\to\Omega$, which takes the orbits of u to orbits of v and preserves their orientation. A vector field $v\in D^r(\Omega,\mathbb{R}^2)$ is called structurally stable in $D^r(\Omega,\mathbb{R}^2)$ if there exists a neighborhood $U\subset D^r(\Omega,\mathbb{R}^2)$ of v such that for any $u\in U$, u and v are topologically equivalent.

Then it is proved that $v\in D^r(\Omega,\mathbb{R}^2)(r\geqslant 1)$ is structurally stable in $D^r(\Omega,\mathbb{R}^2)$ if and only if a) v is regular, b) all interior saddles of v are self-connected, and c) each boundary saddle point is connected to boundary saddle points on the same connected component of the boundary. Moreover, the set of all structurally stable vector fields is open and dense in $D^r(\Omega,\mathbb{R}^2)$.

Structure of J_s: Now we are in position to study the structure of the supercurrent J_s in the physical space. First observe that in the context of superconductivity, the centers of the supercurrent correspond to vortices. Hence the following is a direct consequence of (5.13), which predicts the existence of vortices.

Theorem 5.3. *Let the domain be simply connected. If the supercurrent J_s for a given superconducting state is regular, then there is at least one vortex for this superconducting state.*

When $R<0$, the superconducting states in the bifurcated attractor is dictated by the first eigenfunction e of (4.10). By Theorem 4.1 and the structural stability theorem mentioned above, the structure of the supercurrent J_s for the superconducting states in the bifurcated attractor is determined by the structure of the following vector field:

$$J_0=-A_a|e|^2-\frac{\mu}{2}i(e^*\nabla e-e\nabla e^*)+\nabla\phi, \tag{5.14}$$

which satisfies that $\mathrm{div}\ J_0=0$ and $J_0\cdot n|_{\partial\Omega}=0$. Then it is easy to obtain the following result.

Theorem 5.4: *Assume that the vector field J_0 given by* (5.14) *is structurally stable in $D^r(\Omega,\mathbb{R}^2)(r\geqslant 1)$. Then there are an $\epsilon>0$ and a time $t_0>0$ such that if $\alpha_1<\alpha<\alpha_1+\epsilon$ and $t>t_0$, then for any initial data $(\psi_0,\mathcal{A}_0)\in U\backslash\Gamma$ where $U\backslash\Gamma\subset H$ is the open set given in Theorem 4.1, the supercurrent*

$$J_s(\psi_\alpha, \mathcal{A}_\alpha) = -\gamma(A_a + \mathcal{A}_\alpha)|\psi_\alpha|^2 - \frac{\gamma\mu}{2} i(\psi^* \nabla_\alpha \psi_\alpha - \psi_\alpha \nabla \psi_\alpha^*),$$

corresponding to the solution $(\psi_\alpha, \mathcal{A}_\alpha)$ *is structurally stable, and is topologically equivalent to* J_0.

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Inequalities for experimental tests of the Kochen-Specker theorem

Koji Nagata
National Institute of Information and Communications Technology, 4-2-1 Nukuikita, Koganei, Tokyo 184-8795, Japan

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We derive inequalities for n-partite states under the assumption that the hidden-variable theoretical joint probability distribution for any pair of commuting observables is equal to the quantum mechanical one. Fine showed that this assumption is connected to the no-hidden-variables theorem of Kochen and Specker (KS theorem). These inequalities give a way to experimentally test the KS theorem. The fidelity to the Bell states which is larger than $1/2$ is sufficient for the experimental confirmation of the KS theorem. Hence, the Werner state is enough to test experimentally the KS theorem. Furthermore, it is possible to test the KS theorem experimentally using uncorrelated states. An n-partite uncorrelated state violates the n-partite inequality derived here by an amount that grows exponentially with n. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2081115]

I. INTRODUCTION

From the incompleteness argument of the EPR paper,[1] hidden-variable interpretation of quantum mechanics (QM) has been an attractive topic of research.[2,3] There are two main approaches to study this conceptual foundation of QM. One is the Bell-EPR theorem.[4] This theorem says that the statistical prediction of QM violates the inequality following from the EPR-locality principle. The EPR-locality principle tells that a result of measurement pertaining to one system is independent of any measurement performed simultaneously at a distance on another system.

The other is the no-hidden-variables theorem of Kochen and Specker (KS theorem).[5] The original KS theorem says the nonexistence of a real-valued function which is multiplicative and linear on commuting operators so that QM cannot be imbedded into the KS type of hidden-variable theory. The proof of the KS theorem relies on intricate geometric argument. Fine connected[6,7] the KS theorem to the assumption, to be called Fine's assumption, that the hidden-variable theoretical joint probability distribution for any commuting pair of observables is equal to a quantum mechanical one. Greenberger, Horne, and Zeilinger discovered[8] the so-called GHZ theorem for four-partite GHZ states and the KS theorem has taken very simple form since then (see also Refs. 9–12).

In 1990, Mermin considered the Bell-EPR theorem of multipartite systems and derived multipartite Bell's inequality.[13] It has shown that the n-partite GHZ state violates the Bell-Mermin inequality by an amount that grows exponentially with n. After this work, several multipartite Bell's inequalities have been derived.[14,15] They also exhibit that QM violates local hidden-variable theory by a similar way.

As for the KS theorem, most researches are related to "all versus nothing" demolition of the KS type of hidden-variable theory.[16] (Of course, Bell's inequalities are available for a test of the KS theorem.) Recently, it has begun to research the KS theorem using inequalities (see Refs. 17). To find such inequalities to test the KS theorem is particularly useful for experimental investigation.[18] Since the KS theorem was purely related to the algebraic structure of quantum operators and was independent of states, it might be possible to find an inequality that is violated by QM when the system is in an uncorrelated state.[19] If so, we ask what an amount of a violation is like.

In this paper, we shall derive two inequalities following from the assumption pointed out[6,7] by Fine as a test for the KS theorem for n spin-1/2 states. A violation of Fine's assumption implies that there exists a pair of commuting observables such that the hidden-variable theoretical joint distribution of them does not agree with QM, or hidden-variables cannot exist in the sense that the KS theorem holds.

One of the inequalities says that the fidelity to the Bell states, which is larger than 1/2, allows a proof of the KS theorem. This says the Werner state[19] which admits local hidden-variable theory is enough to test experimentally the KS theorem. And we reveal possible modification of the Bell-Mermin inequality on combining Mermin's geometric idea[13] and a commutative operator group presented by Nagata *et al.*[20] We show that when n exceeds 2, not only n-partite GHZ states but also n-partite uncorrelated states violate the modified inequality derived here. The amount of a violation grows exponentially with n, which is a factor of $O(2^{n/2})$ at the macroscopic level.

Our result says that QM exhibits an exponentially stronger refutation of the KS type of hidden-variable theory, as the number of parties constituting the state increases linearly. The feature is independent of the requirement that the system be prepared in an entangled state. In other words, we can say that the KS theorem is more serious in high-dimensional settings than in low-dimensional ones. Further, we can see the local hidden-variable theory violates the KS type of hidden-variable theory.

This paper is organized as follows. In Sec. II, we fix several notations and prepare for arguments of this paper. In Sec. III, we review the statistical KS theorem and mention that its inequality version is necessary for an experimental test. In Sec. IV, we present an inequality which follows from Fine's assumption for two-spin-1/2 states and derive a sufficient condition to allow a proof of the KS theorem, which states that the fidelity to the Bell states is larger than 1/2. Since the fidelity to the Bell states is 5/8, the two-spin-1/2 Werner state violates the inequality. In Sec. V, we modify the Bell-Mermin inequality. It follows from Fine's assumption. And we show that not only n-partite GHZ states but also n-partite uncorrelated states violate the inequality by an amount that grows exponentially with n. Section VI summarizes this paper.

II. NOTATION AND PREPARATIONS

Throughout this paper, we assume von Neumann's projective measurements and we confine ourselves to the finite-dimensional and the discrete spectrum case. Let $\mathbf{R}$ denote the reals where $\pm\infty \notin \mathbf{R}$. We assume every eigenvalue in this paper lies in $\mathbf{R}$. Further, we assume that every Hermitian operator is associated with a unique observable because we do not need to distinguish between them in this paper.

We assume the validity of QM and we would like to investigate if the KS type of hidden-variable interpretation of QM is possible. Let $\mathcal{O}$ be the space of Hermitian operators described in a finite-dimensional Hilbert space, and $\mathcal{T}$ be the space of density operators described in the Hilbert space. Namely, $\mathcal{T}=\{\psi \mid \psi \in \mathcal{O} \wedge \psi \geqslant 0 \wedge \mathrm{Tr}[\psi]=1\}$. Now we define the notation θ which represents one result of quantum measurement. Suppose that the measurement of a Hermitian operator A for a system in the state ψ yields a value $\theta(A) \in \mathbf{R}$. We assume that the following two propositions (BSF and QDJ) hold. Here, $\chi_{\Delta}(x), (x \in \mathbf{R})$ represents the characteristic function. Δ is any subset of the reals $\mathbf{R}$.

Proposition: BSF (*the Born statistical formula*),

$$\mathrm{Prob}(\Delta)^{\psi}_{\theta(A)} = \mathrm{Tr}[\psi \chi_{\Delta}(A)]. \tag{2.1}$$

The whole symbol $(\Delta)^{\psi}_{\theta(A)}$ is used to denote the proposition that $\theta(A)$ lies in Δ if the system is in the state ψ. And Prob denotes the probability that the proposition holds.

Proposition: QDJ (*the quantum-mechanical joint probability distribution for commuting observables*),

$$\mathrm{Prob}(\Delta,\Delta')^{\psi}_{\theta(A),\theta(B)} = \mathrm{Tr}[\psi\chi_{\Delta}(A)\chi_{\Delta'}(B)] \tag{2.2}$$

for every commuting pair A,B in $\mathcal{O}$. The notation on the LHS of (2.2) is a generalization of the symbol $(\Delta)^{\psi}_{\theta(A)}$ to express the proposition that $\theta(A)$ and $\theta(B)$ lie in Δ and in Δ', respectively, if the system is in the state ψ.

Let us consider a classical probability space $(\Omega,\Sigma,\mu_{\psi})$, where Ω is a nonempty sample space, Σ is a σ-algebra of subsets of Ω, and μ_{ψ} is a σ-additive normalized measure on Σ such that $\mu_{\psi}(\Omega)=1$. The subscript ψ expresses that the probability measure is determined uniquely when the state ψ is specified.

Let us introduce measurable functions (classical random variables) onto $\Omega(f:\Omega\mapsto\mathbf{R})$, which is written as $f_A(\omega)$ for an operator $A\in\mathcal{O}$. Here $\omega\in\Omega$ is a hidden variable. We introduce appropriate notation. $P(\omega)\simeq Q(\omega)$ means $P(\omega)=Q(\omega)$ holds almost everywhere with respect to μ_{ψ} in Ω. One may assume the probability measure μ_{ψ} is chosen such that the following relation is valid:

$$\mathrm{Tr}[\psi A] = \int_{\omega\in\Omega} \mu_{\psi}(\mathrm{d}\omega) f_A(\omega) \tag{2.3}$$

for every Hermitian operator A in $\mathcal{O}$. Please notice the assumption for the probability measure μ_{ψ} does not disturb the KS theorem. See the lemma (B1) in Appendix B.

Proposition: HV (*the deterministic hidden-variable interpretation of QM*).

Measurable function $f_A(\omega)$ exists for every Hermitian operator A in $\mathcal{O}$.

Proposition: D (*the probability distribution rule*),

$$\mu_{\psi}(f_A^{-1}(\Delta)) = \mathrm{Prob}(\Delta)^{\psi}_{\theta(A)}. \tag{2.4}$$

Proposition: JD (*the joint probability distribution rule*),

$$\mu_{\psi}(f_A^{-1}(\Delta)\cap f_B^{-1}(\Delta')) = \mathrm{Prob}(\Delta,\Delta')^{\psi}_{\theta(A),\theta(B)} \tag{2.5}$$

for every commuting pair A,B in $\mathcal{O}$.

Proposition: FUNC A.E. (*the functional rule holding almost everywhere*),

$$f_{g(A)}(\omega) \simeq g(f_A(\omega)) \tag{2.6}$$

for every function $g:\mathbf{R}\mapsto\mathbf{R}$.

Proposition: PROD A.E. (*the product rule holding almost everywhere*).

If Hermitian operators A and B commute, then

$$f_{AB}(\omega) \simeq f_A(\omega)\cdot f_B(\omega). \tag{2.7}$$

Theorem:[6]

$$\mathrm{HV}\wedge\mathrm{JD}\Rightarrow\mathrm{HV}\wedge\mathrm{D}\wedge\mathrm{FUNC\ A.E.} \tag{2.8}$$

Proof: See (B6) in Appendix B.

Theorem:[6]

$$\mathrm{HV}\wedge\mathrm{FUNC\ A.E.}\Rightarrow\mathrm{HV}\wedge\mathrm{PROD\ A.E.} \tag{2.9}$$

Proof: See (B14) in Appendix B.

III. THE STATISTICAL KOCHEN-SPECKER THEOREM

In this section, we want to review the statistical KS theorem (see also Ref. 17). In what follows, we assume HV and JD hold. This implies that we can use D, FUNC A.E., and PROD A.E.. We follow the statistical version of the KS theorem proposed by Peres[11] and refined by Mermin[12] for two-spin-1/2 states. One then can see that

$$X(\omega) := f_{\sigma_x^1\sigma_x^2}(\omega) f_{\sigma_y^1\sigma_y^2}(\omega) f_{\sigma_z^1\sigma_z^2}(\omega) \simeq f_{\sigma_x^1\sigma_x^2\sigma_y^1\sigma_y^2\sigma_z^1\sigma_z^2}(\omega) = f_{-I}(\omega)$$
$$\Rightarrow \int_{\omega\in\Omega} \mu_\psi(\mathrm{d}\omega) X(\omega) = \mathrm{Tr}[\psi(-I)] = -1, \tag{3.1}$$

where I represents the identity operator for the four-dimensional space. By the way we can factorize two of the terms as $f_{\sigma_x^1\sigma_x^2} \simeq f_{\sigma_x^1} f_{\sigma_x^2}$ and $f_{\sigma_y^1\sigma_y^2} \simeq f_{\sigma_y^1} f_{\sigma_y^2}$. Further, we have $f_{\sigma_x^1\sigma_y^2} \simeq f_{\sigma_x^1} f_{\sigma_y^2}$ and $f_{\sigma_y^1\sigma_x^2} \simeq f_{\sigma_y^1} f_{\sigma_x^2}$. Hence we get $f_{\sigma_x^1\sigma_x^2} f_{\sigma_y^1\sigma_y^2} \simeq f_{\sigma_x^1\sigma_y^2} f_{\sigma_y^1\sigma_x^2}$ and

$$X(\omega) \simeq f_{\sigma_x^1\sigma_y^2}(\omega) f_{\sigma_y^1\sigma_x^2}(\omega) f_{\sigma_z^1\sigma_z^2}(\omega) \simeq f_{\sigma_x^1\sigma_y^2\sigma_y^1\sigma_x^2\sigma_z^1\sigma_z^2}(\omega) = f_I(\omega) \Rightarrow \int_{\omega\in\Omega} \mu_\psi(\mathrm{d}\omega) X(\omega) = \mathrm{Tr}[\psi I] = 1 \tag{3.2}$$

in contradiction to (3.1). Thereby, we see that HV does not hold if we accept JD.

We follow the statistical version of the KS theorem proposed in Refs. 9 and 12 for three-spin-1/2 states. Then, one can see that

$$Y(\omega) := f_{\sigma_x^1\sigma_y^2\sigma_y^3}(\omega) f_{\sigma_y^1\sigma_x^2\sigma_y^3}(\omega) f_{\sigma_y^1\sigma_y^2\sigma_x^3}(\omega) f_{\sigma_x^1\sigma_x^2\sigma_x^3}(\omega) \simeq f_{\sigma_x^1\sigma_y^2\sigma_y^3\sigma_y^1\sigma_x^2\sigma_y^3\sigma_y^1\sigma_y^2\sigma_x^3\sigma_x^1\sigma_x^2\sigma_x^3}(\omega)$$
$$= f_{-I}(\omega) \Rightarrow \int_{\omega\in\Omega} \mu_\psi(\mathrm{d}\omega) Y(\omega) = \mathrm{Tr}[\psi(-I)] = -1, \tag{3.3}$$

where I represents the identity operator for the eight-dimensional space. By the way, we can factorize each of the four terms as

$$f_{\sigma_x^1\sigma_y^2\sigma_y^3}(\omega) \simeq f_{\sigma_x^1}(\omega) f_{\sigma_y^2}(\omega) f_{\sigma_y^3}(\omega) \tag{3.4}$$

and so on to get

$$Y(\omega) \simeq (f_{\sigma_x^1}(\omega))^2 (f_{\sigma_y^1}(\omega))^2 (f_{\sigma_x^2}(\omega))^2 (f_{\sigma_y^2}(\omega))^2 (f_{\sigma_x^3}(\omega))^2 (f_{\sigma_y^3}(\omega))^2 \simeq f_I(\omega) f_I(\omega) f_I(\omega) f_I(\omega) f_I(\omega) f_I(\omega)$$
$$\simeq f_I(\omega) \Rightarrow \int_{\omega\in\Omega} \mu_\psi(\mathrm{d}\omega) Y(\omega) = \mathrm{Tr}[\psi I] = 1 \tag{3.5}$$

in contradiction to (3.3).

These two examples provide the statistical KS theorem, which says demolition of HV or of JD. We have the following result.

Theorem: (*The statistical Kochen-Specker theorem.*)

For every quantum state described in a Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ or $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$, $(\mathrm{Dim}(\mathcal{H}_j) = 2, (j = 1, 2, 3))$,

$$\mathrm{HV} \wedge \mathrm{JD} \Rightarrow \perp. \tag{3.6}$$

That is, these two propositions do not hold at the same time.

These examples are sufficient to show that HV cannot be possible in any state if we accept JD. However, they are not of suitable form to test experimentally the KS theorem. Because, in a real experiment, we cannot claim a sharp value as an expectation with arbitrary precision. Therefore, its inequality version is necessary for an experimental test of the KS theorem.

IV. INEQUALITY FOR TWO-PARTITE STATES

In this section, we shall derive the inequality version statistical KS theorem for two-spin-1/2 states. Then, we show that the two-spin-1/2 Werner state[19] violates the inequality. Since the Werner state satisfies all Bell's inequalities, the inequality derived in this section does not belong

to the category of Bell's inequalities. The inequality is just the inequality concerned with the KS theorem. In the following, we assume that HV and JD hold. Let x,y be real numbers with $x,y \in \{-1,+1\}$, then we have

$$(1+x+y-xy) = \pm 2. \tag{4.1}$$

Theorem:[21] For every state ψ described in a Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$, $(\mathrm{Dim}(\mathcal{H}_j)=2,(j=1,2))$,

$$\mathrm{HV} \wedge \mathrm{JD}(\wedge \sigma_x^1\sigma_y^2\sigma_y^1\sigma_x^2 = \sigma_z^1\sigma_z^2) \Rightarrow 1 + \mathrm{Tr}[\psi\sigma_x^1\sigma_x^2] + \mathrm{Tr}[\psi\sigma_y^1\sigma_y^2] - \mathrm{Tr}[\psi\sigma_z^1\sigma_z^2] \leqslant 2. \tag{4.2}$$

Proof: From PROD A.E., we have

$$(f_{\sigma_k^1\sigma_k^2}(\omega))^2 \simeq f_I(\omega) \simeq +1 \Leftrightarrow f_{\sigma_k^1\sigma_k^2}(\omega) \simeq \pm 1, (k=x,y). \tag{4.3}$$

Hence, the (4.1) says

$$U(\omega) := 1 + f_{\sigma_x^1\sigma_x^2}(\omega) + f_{\sigma_y^1\sigma_y^2}(\omega) - f_{\sigma_x^1\sigma_x^2}(\omega) f_{\sigma_y^1\sigma_y^2}(\omega) \Rightarrow U(\omega) \simeq \pm 2 \tag{4.4}$$

and

$$\int_{\omega\in\Omega} \mu_\psi(\mathrm{d}\omega) U(\omega) \leqslant 2. \tag{4.5}$$

On using $f_{\sigma_x^1\sigma_x^2} f_{\sigma_y^1\sigma_y^2} \simeq f_{\sigma_x^1\sigma_y^2} f_{\sigma_y^1\sigma_x^2} \simeq f_{\sigma_z^1\sigma_z^2}$ we get

$$\int_{\omega\in\Omega} \mu_\psi(\mathrm{d}\omega) f_{\sigma_x^1\sigma_x^2}(\omega) f_{\sigma_y^1\sigma_y^2}(\omega) = \int_{\omega\in\Omega} \mu_\psi(\mathrm{d}\omega) f_{\sigma_x^1\sigma_y^2}(\omega) f_{\sigma_y^1\sigma_x^2}(\omega) = \int_{\omega\in\Omega} \mu_\psi(\mathrm{d}\omega) f_{\sigma_z^1\sigma_z^2}(\omega), \tag{4.6}$$

where we have used the quantum mechanical rule $\sigma_x^1\sigma_y^2\sigma_y^1\sigma_x^2 = \sigma_z^1\sigma_z^2$. Hence we conclude

$$\int_{\omega\in\Omega} \mu_\psi(\mathrm{d}\omega) U(\omega) \leqslant 2 \Leftrightarrow 1 + \mathrm{Tr}[\psi\sigma_x^1\sigma_x^2] + \mathrm{Tr}[\psi\sigma_y^1\sigma_y^2] - \mathrm{Tr}[\psi\sigma_z^1\sigma_z^2] \leqslant 2. \tag{4.7}$$

QED

A violation of the inequality (4.7) implies demolition of HV or of JD in the state ψ. Note the following quantum mechanical relation:

$$1 + \mathrm{Tr}[\psi\sigma_x^1\sigma_x^2] + \mathrm{Tr}[\psi\sigma_y^1\sigma_y^2] - \mathrm{Tr}[\psi\sigma_z^1\sigma_z^2] \leqslant 2 \Leftrightarrow \mathrm{Tr}[\psi|\pi\rangle\langle\pi|] \leqslant 1/2, \tag{4.8}$$

where

$$|\pi\rangle := \frac{|+_1,-_2\rangle + |-_1,+_2\rangle}{\sqrt{2}}. \tag{4.9}$$

Therefore the statistical KS theorem holds if the fidelity to the Bell state $|\pi\rangle$ is larger than $1/2$. Note the fidelity to the Bell states of the two-spin-$1/2$ Werner state[19] is $5/8(>1/2)$. The Werner state W is

$$W = (1/2)|\pi\rangle\langle\pi| + (1/8)I, \tag{4.10}$$

where I is the identity operator on the four-dimensional space. Hence, this quantum state which admits local hidden-variable theory allows a proof of the KS theorem.

V. INEQUALITY FOR MULTIPARTITE STATES

In what follows, we shall modify the Bell-Mermin inequality.[13] We derive an n-partite inequality which is satisfied if both HV and JD hold. We show n-partite uncorrelated states violate

the inequality when $n \geqslant 3$, by an amount that grows exponentially with n. Please note that any uncorrelated states satisfy all Bell's inequalities.[19] Hence, the modified inequality does not belong to the category of Bell's inequalities. In this section, we assume $n \geqslant 2$. Let us denote $\{1,2,\ldots,n\}$ by $\mathbf{N}_n$.

Definition: [*commutative group* (Λ_n) *of Hermitian operators*]

$O_p^n (p \in \{0,1,\ldots,2^n-1\}, n \geqslant 2)$ are Hermitian operators defined by

$$O_p^n := \prod_{j=1}^{n} (\sigma_z^j)^{b_j} (\sigma_x^j)^{b_0} = (\sigma_z^1)^{b_1} (\sigma_z^2)^{b_2} (\sigma_z^3)^{b_3} (\sigma_z^4)^{b_4} \cdots (\sigma_z^{n-1})^{b_{n-1}} (\sigma_z^n)^{b_n} \times (\sigma_x^1)^{b_0} (\sigma_x^2)^{b_0} (\sigma_x^3)^{b_0} \cdots (\sigma_x^{n-1})^{b_0} (\sigma_x^n)^{b_0}, \tag{5.1}$$

where the superscript j of the Pauli operators denotes the party j and the n-bit sequence $b_0 b_1 \cdots b_{n-1}$ is the binary representation of p, and $b_n \in \{0,1\} \wedge b_n \equiv \Sigma_{j=1}^{n-1} b_j (\mathrm{mod}\ 2)$. Thus, the parity of $b_1 b_2 \cdots b_n$ is even. (Here, σ_k^1 means $\sigma_k^1 \otimes_{j=2}^{n} I^j$ and so on. Omitting the identity operator, we abbreviate those as above.)

The operator O_0^n is the identity operator on the 2^n-dimensional space, and the other operators $O_1^n, \ldots, O_{2^n-1}^n$ have two eigenvalues, ± 1. In the following, there are the cases where we abbreviate O_0^n as I.

Example: If $p \in \{0,1,\ldots,2^{n-1}-1\}$, then $b_0 = 0$ and $(\sigma_x^j)^{b_0} = \otimes_{k=1}^{n} I^k = O_0^n$ for all j. That is, the binary representation of p takes, for example, the following form:

$$p_1 := \overbrace{01001\cdots01}^{B_1} (= b_0 b_1 \cdots b_{n-1}), \tag{5.2}$$

where B_1 represents the sum of the number of 1. Then, $b_n \in \{0,1\} \wedge b_n \equiv B_1 (\mathrm{mod}\ 2)$ holds. Suppose $b_n = 1$ holds, then $(\sigma_z^n)^{b_n} = \sigma_z^n$. Then, the corresponding Hermitian operator $O_{p_1}^n$ is as follows:

$$O_{p_1}^n = \sigma_z^1 I^2 I^3 \sigma_z^4 \cdots I^{n-2} \sigma_z^{n-1} \sigma_z^n \times I^1 I^2 I^3 I^4 \cdots I^{n-1} I^n = (\sigma_z^1 I^1) I^2 I^3 (\sigma_z^4 I^4) \cdots I^{n-2} (\sigma_z^{n-1} I^{n-1}) (\sigma_z^n I^n) = \sigma_z^1 I^2 I^3 \sigma_z^4 \cdots I^{n-2} \sigma_z^{n-1} \sigma_z^n, \tag{5.3}$$

where the number of $(\sigma_z I) = \sigma_z$ is even because of the definition of b_n.

Example: If $p \in \{2^{n-1}, 2^{n-1}+1, \ldots, 2^n-1\}$, then $b_0 = 1$ and $(\sigma_x^j)^{b_0} = \sigma_x^j$ for all j. That is, the binary representation of p takes, for example, the following form:

$$p_2 := \overbrace{11001\cdots01}^{B_2}, \tag{5.4}$$

where B_2 represents the sum of the number of 1. Then, $b_n \in \{0,1\} \wedge b_n \equiv B_2 (\mathrm{mod}\ 2)$ holds. Suppose $b_n = 0$ holds, then $(\sigma_z^n)^{b_n} = O_0^n$. Then the corresponding Hermitian operator $O_{p_2}^n$ is as follows:

$$O_{p_2}^n = \sigma_z^1 I^2 I^3 \sigma_z^4 \cdots I^{n-2} \sigma_z^{n-1} I^n \times \sigma_x^1 \sigma_x^2 \sigma_x^3 \cdots \sigma_x^{n-1} \sigma_x^n = (\sigma_z^1 \sigma_x^1) \sigma_x^2 \sigma_x^3 (\sigma_z^4 \sigma_x^4) \cdots \sigma_x^{n-2} (\sigma_z^{n-1} \sigma_x^{n-1}) \sigma_x^n = (i\sigma_y^1) \sigma_x^2 \sigma_x^3 (i\sigma_y^4) \cdots \sigma_x^{n-2} (i\sigma_y^{n-1}) \sigma_x^n, \tag{5.5}$$

where the number of $(\sigma_z \sigma_x) = i\sigma_y$ is even.

Example: The binary representation of 2^{n-1} takes the following form:

$$2^{n-1} = 1\overbrace{0000\cdots00}^{n-1}. \tag{5.6}$$

Then the corresponding Hermitian operator $O_{2^{n-1}}^n$ is as follows:

$$O_{2^{n-1}}^n = I^1 I^2 I^3 I^4 \cdots I^{n-1} I^n \times \sigma_x^1 \sigma_x^2 \sigma_x^3 \cdots \sigma_x^{n-1} \sigma_x^n = \sigma_x^1 \sigma_x^2 \sigma_x^3 \cdots \sigma_x^{n-1} \sigma_x^n. \tag{5.7}$$

Lemma: If $O_p^n, O_q^n \in \Lambda_n$, then

$$O_p^n O_q^n = O_{p\oplus q}^n (\in \Lambda_n), \tag{5.8}$$

where $p \oplus q$ is the bitwise XOR (exclusive OR) of p and q.

Proof: See (A1) in Appendix A.

From the lemma (5.8), the set of 2^n operators $\{O_p^n\}$ forms a commutative group isomorphic to $(Z_2)^n$. We have denoted this commutative group as Λ_n. Let us define another set of operators.

Definition: $R_p^n (p \in \{0,1,\ldots,2^n-1\}, n \geqslant 2)$ are operators defined by

$$R_p^n := \prod_{j=1}^{n} (\sigma_z^j)^{e_j} (\sigma_x^j)^{e_0}, \tag{5.9}$$

where the superscript j of the Pauli operators denotes the party j and the n-bit sequence $e_0 e_1 \cdots e_{n-1}$ is the binary representation of p, and $e_n \in \{0,1\} \wedge e_n \equiv \Sigma_{j=1}^{n-1} e_j + 1 (\mathrm{mod}\ 2)$. Thus, unlike O_p^n, the parity of $e_1 e_2 \cdots e_n$ is odd.

Example: If $p \in \{0,1,\ldots,2^{n-1}-1\}$, then $e_0 = 0$ and $(\sigma_x^j)^{e_0} = \otimes_{k=1}^n I^k = O_0^n$ for all j. That is, the binary representation of p takes, for example, the following form:

$$p_3 := 0\overbrace{1001\cdots01}^{B_3} (= e_0 e_1 \cdots e_{n-1}), \tag{5.10}$$

where B_3 represents the sum of the number of 1. Then, $e_n \in \{0,1\} \wedge e_n \equiv B_3 + 1 (\mathrm{mod}\ 2)$ holds. Suppose $e_n = 1$ holds, then $(\sigma_z^n)^{e_n} = \sigma_z^n$. Then, the corresponding Hermitian operator $R_{p_3}^n$ is as follows:

$$\begin{aligned} R_{p_3}^n &= \sigma_z^1 I^2 I^3 \sigma_z^4 \cdots I^{n-2} \sigma_z^{n-1} \sigma_z^n \times I^1 I^2 I^3 I^4 \cdots I^{n-1} I^n = (\sigma_z^1 I^1) I^2 I^3 (\sigma_z^4 I^4) \cdots I^{n-2} (\sigma_z^{n-1} I^{n-1}) (\sigma_z^n I^n) \\ &= \sigma_z^1 I^2 I^3 \sigma_z^4 \cdots I^{n-2} \sigma_z^{n-1} \sigma_z^n, \end{aligned} \tag{5.11}$$

where the number of $(\sigma_z I) = \sigma_z$ is odd because of the definition of e_n.

Example: If $p \in \{2^{n-1}, 2^{n-1}+1, \ldots, 2^n-1\}$, then $e_0 = 1$ and $(\sigma_x^j)^{e_0} = \sigma_x^j$ for all j. That is, the binary representation of p takes, for example, the following form:

$$p_4 := 1\overbrace{1001\cdots01}^{B_4}, \tag{5.12}$$

where B_4 represents the sum of the number of 1. Then, $e_n \in \{0,1\} \wedge e_n \equiv B_4 + 1 (\mathrm{mod}\ 2)$ holds. Suppose $e_n = 0$ holds, then $(\sigma_z^n)^{e_n} = O_0^n$. Then the corresponding non-Hermitian operator $R_{p_4}^n$ is as follows:

$$\begin{aligned} R_{p_4}^n &= \sigma_z^1 I^2 I^3 \sigma_z^4 \cdots I^{n-2} \sigma_z^{n-2} I^n \times \sigma_x^1 \sigma_x^2 \sigma_x^3 \cdots \sigma_x^{n-1} \sigma_x^n = (\sigma_z^1 \sigma_x^1) \sigma_x^2 \sigma_x^3 (\sigma_z^4 \sigma_x^4) \cdots \sigma_x^{n-2} (\sigma_z^{n-1} \sigma_x^{n-1}) \sigma_x^n \\ &= (i\sigma_y^1) \sigma_x^2 \sigma_x^3 (i\sigma_y^4) \cdots \sigma_x^{n-2} (i\sigma_y^{n-1}) \sigma_x^n, \end{aligned} \tag{5.13}$$

where the number of $(\sigma_z \sigma_x) = i\sigma_y$ is odd. R_p^n / i and $i R_p^n$ are Hermitian operators if $p \in \{2^{n-1}, 2^{n-1}+1, \ldots, 2^n-1\}$.

Lemma:

$$\frac{1}{2}\left(\prod_{j=1}^{n} (I^j + \sigma_z^j) + \prod_{j=1}^{n} (I^j - \sigma_z^j) \right) = \sum_{p=0}^{2^{n-1}-1} O_p^n,$$

$$\frac{1}{2}\left(\prod_{j=1}^{n} (I^j + \sigma_z^j) - \prod_{j=1}^{n} (I^j - \sigma_z^j) \right) = \sum_{p=0}^{2^{n-1}-1} R_p^n,$$

$$\frac{1}{2}\left(\prod_{j=1}^{n}(\sigma_x^j+i\sigma_y^j)+\prod_{j=1}^{n}(\sigma_x^j-i\sigma_y^j)\right)=\sum_{p=2^{n-1}}^{2^n-1}O_p^n,$$

$$\frac{1}{2}\left(\prod_{j=1}^{n}(\sigma_x^j+i\sigma_y^j)-\prod_{j=1}^{n}(\sigma_x^j-i\sigma_y^j)\right)=\sum_{p=2^{n-1}}^{2^n-1}R_p^n. \tag{5.14}$$

Proof: See (A7) and (A14) in Appendix A.

Lemma:

$$\mathrm{HV}\wedge\mathrm{FUNC\ A.E.}\Rightarrow \mathrm{Re}\left(\prod_{j=1}^{n}(f_{\sigma_x^j}(\omega)+if_{\sigma_y^j}(\omega))\right)\simeq\sum_{p=2^{n-1}}^{2^n-1}f_{O_p^n}(\omega),$$

$$\mathrm{Im}\left(\prod_{j=1}^{n}(f_{\sigma_x^j}(\omega)+if_{\sigma_y^j}(\omega))\right)\simeq\sum_{p=2^{n-1}}^{2^n-1}f_{R_p^n/i}(\omega). \tag{5.15}$$

Proof: See (A21) in Appendix A.

Theorem:[21] For every state ψ described in a Hilbert space $\otimes_{j=1}^{n}\mathcal{H}_j$, $(\mathrm{Dim}(\mathcal{H}_j)=2,(j\in\mathbf{N}_n,n\geqslant 2))$,

$$\mathrm{HV}\wedge\mathrm{JD}(\wedge(i\sigma_y^j)(i\sigma_y^j)\sigma_x^j\sigma_x^j=\sigma_z^j\sigma_z^j)\Rightarrow\sum_{p=0}^{2^{n-1}-1}\mathrm{Tr}[\psi O_p^n]\leqslant\begin{cases}2^{n/2} & n=\text{even},\\ 2^{(n-1)/2} & n=\text{odd}.\end{cases} \tag{5.16}$$

Proof: From PROD A.E., we have

$$(f_{\sigma_k^j}(\omega))^2\simeq f_{O_0^n}(\omega)\simeq+1\Leftrightarrow f_{\sigma_k^j}(\omega)\simeq\pm 1,\quad(j\in\mathbf{N}_n,k=x,y). \tag{5.17}$$

Now, we define F^ψ by

$$F^\psi:=\int_{\omega\in\Omega}\mu_\psi(\mathrm{d}\omega)G(\omega), \tag{5.18}$$

where $G(\omega)$ is defined by

$$G(\omega):=\mathrm{Re}\left(\prod_{j=1}^{n}(f_{\sigma_x^j}(\omega)+if_{\sigma_y^j}(\omega))\right)\prod_{j=1}^{n}f_{\sigma_x^j}(\omega). \tag{5.19}$$

From the geometric argument by Mermin in Ref. 13 and (5.17), we have

$$G(\omega)\leqslant\begin{cases}2^{n/2} & n=\text{even}\\ 2^{(n-1)/2} & n=\text{odd}\end{cases}\qquad(\mu_\psi-\text{a.e.}). \tag{5.20}$$

In more detail, almost everywhere with respect to μ_ψ in Ω, the maximum of $G(\omega)$ is equal to the real part of a product of complex numbers each of which has magnitude of $\sqrt{2}$ and a phase of $\pm\pi/4$ or $\pm 3\pi/4$ since absolute value of $\Pi_{j=1}^{n}f_{\sigma_x^j}(\omega)$ is unity almost everywhere with respect to μ_ψ. When n is even the product can lie along the real axis and can attain a maximum value of $2^{n/2}$, when n is odd the product must lie along an axis at 45° to the real axis and its real part can only attain the maximum value $2^{(n-1)/2}$. Therefore, the value $G(\omega)$ is bounded as (5.20) almost everywhere in Ω, and hence F^ψ is bounded as

$$F^{\psi} \leqslant \begin{cases} 2^{n/2} & n = \text{even}, \\ 2^{(n-1)/2} & n = \text{odd}. \end{cases} \tag{5.21}$$

From (5.7), it is easy to see that

$$\prod_{j=1}^{n} f_{\sigma_x^j}(\omega) \simeq f_{O^n_{2^{n-1}}}(\omega). \tag{5.22}$$

Therefore, from (5.19) and the lemma (5.15), we have

$$G(\omega) \simeq \left(\sum_{p=2^{n-1}}^{2^n-1} f_{O^n_p}(\omega) \right) f_{O^n_{2^{n-1}}}(\omega). \tag{5.23}$$

Noting $[O_p^n, O_q^n] = \mathbf{0}, \forall O_p^n, O_q^n \in \Lambda_n$ [see the lemma (5.8)], PROD A.E. tells the following relations:

$$f_{O^n_p}(\omega) f_{O^n_q}(\omega) \simeq f_{O^n_{p\oplus q}}(\omega), \quad (\forall O_p^n, O_q^n \in \Lambda_n). \tag{5.24}$$

It is easy to see that

$$\{O_p^n O^n_{2^{n-1}} | p \in \{2^{n-1}, 2^{n-1}+1, \ldots, 2^n - 1\}\} = \{O_p^n | p \in \{0, 1, \ldots, 2^{n-1} - 1\}\}. \tag{5.25}$$

Here, we have used the quantum mechanical rule $(i\sigma_y^i)(i\sigma_y^j)\sigma_x^i\sigma_x^j = \sigma_z^i\sigma_z^j (i, j \in \mathbf{N}_n, i \neq j)$. [Equation (5.25) is also obvious from the expression (5.1) and (5.7)]. Therefore, we get

$$G(\omega) \simeq \sum_{p=0}^{2^{n-1}-1} f_{O^n_p}(\omega). \tag{5.26}$$

Thus from (5.18) we conclude

$$F^{\psi} = \int_{\omega \in \Omega} \mu_{\psi}(\mathrm{d}\omega) \left(\sum_{p=0}^{2^{n-1}-1} f_{O^n_p}(\omega) \right) = \sum_{p=0}^{2^{n-1}-1} \mathrm{Tr}[\psi O_p^n]. \tag{5.27}$$

QED

Now, it follows from the lemma (5.14) that

$$|+_1;+_2;\cdots;+_n\rangle\langle+_1;+_2;\cdots;+_n| + |-_1;-_2;\cdots;-_n\rangle\langle-_1;-_2;\cdots;-_n| = \frac{1}{2^n}\left(\prod_{j=1}^{n} (I^j + \sigma_z^j) + \prod_{j=1}^{n} (I^j - \sigma_z^j) \right)$$

$$= \frac{1}{2^{n-1}} \left(\sum_{p=0}^{2^{n-1}-1} O_p^n \right), \tag{5.28}$$

where $O_p^n = \Pi_{j=1}^n (\sigma_x^j)^{b_0} (\sigma_z^j)^{b_j}$ and $\sigma_z^j |\pm_j\rangle = \pm |\pm_j\rangle$. Hence we have

$$F^{\psi} = \sum_{p=0}^{2^{n-1}-1} \mathrm{Tr}[\psi O_p^n] = \mathrm{Tr}[\psi H_n], \tag{5.29}$$

where [see (5.28)]

$$H_n := 2^{n-1}(|+_1;+_2;\cdots;+_n\rangle\langle+_1;+_2;\cdots;+_n| + |-_1;-_2;\cdots;-_n\rangle\langle-_1;-_2;\cdots;-_n|). \tag{5.30}$$

Now, let ψ be $|\Psi\rangle\langle\Psi|$ where

$$|\Psi\rangle := \alpha|+_1;+_2;\cdots;+_n\rangle + \beta|-_1;-_2;\cdots;-_n\rangle, (|\alpha|^2 + |\beta|^2 = 1). \tag{5.31}$$

This state $|\Psi\rangle$ is an n-partite uncorrelated state if α or β is zero and $|\Psi\rangle$ is an n-partite GHZ state if $\alpha=\beta=1/\sqrt{2}$.

The quantum theoretical prediction says the expectation value $\mathrm{Tr}[|\Psi\rangle\langle\Psi|H_n]$ should take a value of 2^{n-1} for the state $|\Psi\rangle$ in spite of any value of α and of β, and we get

$$F^{|\Psi\rangle} = 2^{n-1}. \tag{5.32}$$

When n exceeds 2, this value $F^{|\Psi\rangle}$ is larger than the bound (5.21), which exceeds (5.21) by the exponentially larger factor of $2^{(n-2)/2}$ (for n even) or $2^{(n-1)/2}$ (for n odd). This implies demolition of HV or of JD in the state $|\Psi\rangle$. Thus, we have derived the exponentially stronger violation of HV$\wedge$JD, irrespective of quantum entanglement effects.

VI. SUMMARY

In summary, we showed that the fidelity to the Bell states which is larger than $1/2$ is sufficient to allow a proof of the KS theorem. Thus, the Werner state is enough to test experimentally the KS theorem. We also have derived an n-partite inequality following from HV$\wedge$JD. We have shown that an n-partite uncorrelated state violates the inequality by a factor of $O(2^{n/2})$ at the macroscopic level. Hence, it turns out that QM exhibits an exponentially stronger violation of HV$\wedge$JD, as the number of parties constituting the state increases, irrespective of entanglement effects.

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APPENDIX A

Lemma: If $O_p^n, O_q^n \in \Lambda_n$, then

$$O_p^n O_q^n = O_{p\oplus q}^n (\in \Lambda_n), \tag{A1}$$

where $p\oplus q$ is the bitwise XOR (exclusive OR) of p and q.

Proof: Suppose that the binary representations of p and q are $b_0 b_1 \cdots b_{n-1}$ and $c_0 c_1 \cdots c_{n-1}$, respectively. Suppose that $b_n \in \{0,1\} \wedge b_n \equiv \Sigma_{j=1}^{n-1} b_j (\mathrm{mod}\ 2)$ and $c_n \in \{0,1\} \wedge c_n \equiv \Sigma_{j=1}^{n-1} c_j (\mathrm{mod}\ 2)$ hold. This means that

$$c_j \in \{0,1\}\ \forall\, j \wedge \sum_{j=1}^{n} c_j \equiv 0 (\mathrm{mod}\ 2). \tag{A2}$$

This yields ($b_0 \in \{1,0\}$)

$$\left[\prod_{j=1}^{n} (\sigma_x^j)^{b_0}, \prod_{j=1}^{n} (\sigma_z^j)^{c_j}\right] = \mathbf{0}. \tag{A3}$$

Then from (5.1) we have

$$O_p^n = \prod_{j=1}^{n} (\sigma_z^j)^{b_j} (\sigma_x^j)^{b_0}, \quad O_q^n = \prod_{j=1}^{n} (\sigma_z^j)^{c_j} (\sigma_x^j)^{c_0} \Rightarrow O_p^n O_q^n = \prod_{j=1}^{n} (\sigma_z^j)^{b_j} (\sigma_x^j)^{b_0} (\sigma_z^j)^{c_j} (\sigma_x^j)^{c_0}$$
$$= \prod_{j=1}^{n} (\sigma_z^j)^{b_j} (\sigma_z^j)^{c_j} (\sigma_x^j)^{b_0} (\sigma_x^j)^{c_0} = \prod_{j=1}^{n} (\sigma_z^j)^{d_j} (\sigma_x^j)^{d_0} = O_{p\oplus q}^n, \tag{A4}$$

where

$$d_j \in \{0,1\} \wedge d_j \equiv b_j + c_j (\mathrm{mod}\, 2). \tag{A5}$$

Here,

$$d_n \equiv \sum_{j=1}^{n-1} b_j + \sum_{j=1}^{n-1} c_j (\mathrm{mod}\, 2) \equiv \sum_{j=1}^{n-1} (b_j + c_j) (\mathrm{mod}\, 2) \equiv \sum_{j=1}^{n-1} d_j (\mathrm{mod}\, 2). \tag{A6}$$

Hence, d_n can be assumed such that $d_n \in \{0,1\}$ and $d_n \equiv \Sigma_{j=1}^{n-1} d_j (\mathrm{mod}\, 2)$ hold. QED

Lemma:

$$\frac{1}{2}\left(\prod_{j=1}^{n} (I^j + \sigma_z^j) + \prod_{j=1}^{n} (I^j - \sigma_z^j) \right) = \sum_{p=0}^{2^{n-1}-1} O_p^n,$$
$$\frac{1}{2}\left(\prod_{j=1}^{n} (I^j + \sigma_z^j) - \prod_{j=1}^{n} (I^j - \sigma_z^j) \right) = \sum_{p=0}^{2^{n-1}-1} R_p^n. \tag{A7}$$

Proof: If the following relations hold for all $m, (2 \leqslant m \leqslant n)$,

$$\frac{1}{2}\left(\prod_{j=1}^{m} (I^j + \sigma_z^j) + \prod_{j=1}^{m} (I^j - \sigma_z^j) \right) = \sum_{p=0}^{2^{m-1}-1} O_p^m, \tag{A8}$$

$$\frac{1}{2}\left(\prod_{j=1}^{m} (I^j + \sigma_z^j) - \prod_{j=1}^{m} (I^j - \sigma_z^j) \right) = \sum_{p=0}^{2^{m-1}-1} R_p^m, \tag{A9}$$

then the theorem holds. Here, O_p^m means $O_p^m \otimes_{j=m+1}^{n} I^j$ and so on. Omitting the identity operator, we abbreviate those as above. Remember, σ_k^1 means $\sigma_k^1 \otimes_{j=2}^{n} I^j$ and so on.

In the case where $m=2$: The left-hand side (LHS) of (A8) is $(I^1 I^2 + \sigma_z^1 \sigma_z^2) \otimes_{j=3}^{n} I^j$ and right-hand side (RHS) of (A8) is also $(I^1 I^2 + \sigma_z^1 \sigma_z^2) \otimes_{j=3}^{n} I^j$. LHS of (A9) is $(I^1 \sigma_z^2 + \sigma_z^1 I^2) \otimes_{j=3}^{n} I^j$ and RHS of (A9) is also $(I^1 \sigma_z^2 + \sigma_z^1 I^2) \otimes_{j=3}^{n} I^j$. Therefore (A8) and (A9) hold when $m=2$. In the following, if possible, we omit the identity operator.

Suppose that (A8) and (A9) hold for $m=k-1$. Then we have

$$\prod_{j=1}^{k-1} (I^j + \sigma_z^j) = \sum_{p=0}^{2^{k-2}-1} O_p^{k-1} + \sum_{p=0}^{2^{k-2}-1} R_p^{k-1},$$
$$\prod_{j=1}^{k-1} (I^j - \sigma_z^j) = \sum_{p=0}^{2^{k-2}-1} O_p^{k-1} - \sum_{p=0}^{2^{k-2}-1} R_p^{k-1}, \tag{A10}$$

On the other hand, we have

$$
\begin{aligned}
&(I^k+\sigma_z^k)\left(\sum_{p=0}^{2^{k-2}-1}O_p^{k-1}+\sum_{p=0}^{2^{k-2}-1}R_p^{k-1}\right)\\
&=\left(\sum_{p=0}^{2^{k-2}-1}O_p^{k-1}I^k+\sum_{p=0}^{2^{k-2}-1}R_p^{k-1}\sigma_z^k\right)+\left(\sum_{p=0}^{2^{k-2}-1}O_p^{k-1}\sigma_z^k+\sum_{p=0}^{2^{k-2}-1}R_p^{k-1}I^k\right)\\
&=\sum_{p=0}^{2^{k-1}-1}O_p^k+\sum_{p=0}^{2^{k-1}-1}R_p^k
\end{aligned}
\tag{A11}
$$

and

$$
\begin{aligned}
&(I^k-\sigma_z^k)\left(\sum_{p=0}^{2^{k-2}-1}O_p^{k-1}-\sum_{p=0}^{2^{k-2}-1}R_p^{k-1}\right)\\
&=\left(\sum_{p=0}^{2^{k-2}-1}O_p^{k-1}I^k+\sum_{p=0}^{2^{k-2}-1}R_p^{k-1}\sigma_z^k\right)-\left(\sum_{p=0}^{2^{k-2}-1}O_p^{k-1}\sigma_z^k+\sum_{p=0}^{2^{k-2}-1}R_p^{k-1}I^k\right)\\
&=\sum_{p=0}^{2^{k-1}-1}O_p^k-\sum_{p=0}^{2^{k-1}-1}R_p^k.
\end{aligned}
\tag{A12}
$$

Therefore we have

$$
\begin{aligned}
\prod_{j=1}^{k}(I^j+\sigma_z^j)&=\sum_{p=0}^{2^{k-1}-1}O_p^k+\sum_{p=0}^{2^{k-1}-1}R_p^k,\\
\prod_{j=1}^{k}(I^j-\sigma_z^j)&=\sum_{p=0}^{2^{k-1}-1}O_p^k-\sum_{p=0}^{2^{k-1}-1}R_p^k.
\end{aligned}
\tag{A13}
$$

This implies that (A8) and (A9) hold for $m=k$. QED

Lemma:

$$
\begin{aligned}
\frac{1}{2}\left(\prod_{j=1}^{n}(\sigma_x^j+i\sigma_y^j)+\prod_{j=1}^{n}(\sigma_x^j-i\sigma_y^j)\right)&=\sum_{p=2^{n-1}}^{2^n-1}O_p^n,\\
\frac{1}{2}\left(\prod_{j=1}^{n}(\sigma_x^j+i\sigma_y^j)-\prod_{j=1}^{n}(\sigma_x^j-i\sigma_y^j)\right)&=\sum_{p=2^{n-1}}^{2^n-1}R_p^n.
\end{aligned}
\tag{A14}
$$

Proof: If the following relations hold for all $m,(2\leqslant m\leqslant n)$,

$$
\frac{1}{2}\left(\prod_{j=1}^{m}(\sigma_x^j+i\sigma_y^j)+\prod_{j=1}^{m}(\sigma_x^j-i\sigma_y^j)\right)=\sum_{p=2^{m-1}}^{2^m-1}O_p^m,
\tag{A15}
$$

$$
\frac{1}{2}\left(\prod_{j=1}^{m}(\sigma_x^j+i\sigma_y^j)-\prod_{j=1}^{m}(\sigma_x^j-i\sigma_y^j)\right)=\sum_{p=2^{m-1}}^{2^m-1}R_p^m,
\tag{A16}
$$

then the theorem holds. Here, O_p^m means $O_p^m \otimes_{j=m+1}^{n} I^j$ and so on.

In the case where $m=2$: LHS of (A15) is $(\sigma_x^1\sigma_x^2+i\sigma_y^1 i\sigma_y^2)\otimes_{j=3}^{n} I^j$ and RHS of (A15) is also $(\sigma_x^1\sigma_x^2+i\sigma_y^1 i\sigma_y^2)\otimes_{j=3}^{n} I^j$. LHS of (A16) is $(\sigma_x^1 i\sigma_y^2+i\sigma_y^1\sigma_x^2)\otimes_{j=3}^{n} I^j$ and RHS of (A16) is also $(\sigma_x^1 i\sigma_y^2 + i\sigma_y^1\sigma_x^2)\otimes_{j=3}^{n} I^j$. Therefore (A15) and (A16) hold when $m=2$. In the following, if possible, we omit the identity operator.

Suppose that (A15) and (A16) hold for $m=k-1$. Then we have

$$\prod_{j=1}^{k-1}(\sigma_x^j + i\sigma_y^j) = \sum_{p=2^{k-2}}^{2^{k-1}-1} O_p^{k-1} + \sum_{p=2^{k-2}}^{2^{k-1}-1} R_p^{k-1},$$
$$\prod_{j=1}^{k-1}(\sigma_x^j - i\sigma_y^j) = \sum_{p=2^{k-2}}^{2^{k-1}-1} O_p^{k-1} - \sum_{p=2^{k-2}}^{2^{k-1}-1} R_p^{k-1}. \tag{A17}$$

On the other hand, we have

$$\begin{aligned}(\sigma_x^k + i\sigma_y^k)&\left(\sum_{p=2^{k-2}}^{2^{k-1}-1} O_p^{k-1} + \sum_{p=2^{k-2}}^{2^{k-1}-1} R_p^{k-1}\right)\\ &= \left(\sum_{p=2^{k-2}}^{2^{k-1}-1} O_p^{k-1}\sigma_x^k + \sum_{p=2^{k-2}}^{2^{k-1}-1} R_p^{k-1} i\sigma_y^k\right) + \left(\sum_{p=2^{k-2}}^{2^{k-1}-1} O_p^{k-1} i\sigma_y^k + \sum_{p=2^{k-2}}^{2^{k-1}-1} R_p^{k-1}\sigma_x^k\right)\\ &= \sum_{p=2^{k-1}}^{2^k-1} O_p^k + \sum_{p=2^{k-1}}^{2^k-1} R_p^k\end{aligned} \tag{A18}$$

and

$$\begin{aligned}(\sigma_x^k - i\sigma_y^k)&\left(\sum_{p=2^{k-2}}^{2^{k-1}-1} O_p^{k-1} - \sum_{p=2^{k-2}}^{2^{k-1}-1} R_p^{k-1}\right)\\ &= \left(\sum_{p=2^{k-2}}^{2^{k-1}-1} O_p^{k-1}\sigma_x^k + \sum_{p=2^{k-2}}^{2^{k-1}-1} R_p^{k-1} i\sigma_y^k\right) - \left(\sum_{p=2^{k-2}}^{2^{k-1}-1} O_p^{k-1} i\sigma_y^k + \sum_{p=2^{k-2}}^{2^{k-1}-1} R_p^{k-1}\sigma_x^k\right)\\ &= \sum_{p=2^{k-1}}^{2^k-1} O_p^k - \sum_{p=2^{k-1}}^{2^k-1} R_p^k.\end{aligned} \tag{A19}$$

Therefore we have

$$\prod_{j=1}^{k}(\sigma_x^j + i\sigma_y^j) = \sum_{p=2^{k-1}}^{2^k-1} O_p^k + \sum_{p=2^{k-1}}^{2^k-1} R_p^k,$$
$$\prod_{j=1}^{k}(\sigma_x^j - i\sigma_y^j) = \sum_{p=2^{k-1}}^{2^k-1} O_p^k - \sum_{p=2^{k-1}}^{2^k-1} R_p^k. \tag{A20}$$

This implies that (A15) and (A16) hold for $m=k$. QED

Lemma:

$$\mathrm{HV} \wedge \mathrm{FUNC\ A.E.} \Rightarrow \mathrm{Re}\left(\prod_{j=1}^{n}(f_{\sigma_x^j}(\omega)+if_{\sigma_y^j}(\omega))\right) \simeq \sum_{p=2^{n-1}}^{2^n-1} f_{O_p^n}(\omega),$$
$$\mathrm{Im}\left(\prod_{j=1}^{n}(f_{\sigma_x^j}(\omega)+if_{\sigma_y^j}(\omega))\right) \simeq \sum_{p=2^{n-1}}^{2^n-1} f_{R_p^n/i}(\omega). \tag{A21}$$

Proof: If the following relations hold for all $m, (2 \leqslant m \leqslant n)$,

$$\mathrm{Re}\left(\prod_{j=1}^{m}(f_{\sigma_x^j}(\omega)+if_{\sigma_y^j}(\omega))\right) \simeq \sum_{p=2^{m-1}}^{2^m-1} f_{O_p^m}(\omega), \tag{A22}$$

$$\mathrm{Im}\left(\prod_{j=1}^{m}(f_{\sigma_x^j}(\omega)+if_{\sigma_y^j}(\omega))\right) \simeq \sum_{p=2^{m-1}}^{2^m-1} f_{R_p^m/i}(\omega), \tag{A23}$$

then the theorem holds. Here, $f_{O_p^m}$ means $f_{O_p^m \otimes_{j=m+1}^{n} I^j}$ and so on.

In the case where $m=2$: LHS of (A22) is $f_{(\sigma_x^1\sigma_x^2)\otimes_{j=3}^{n} I^j}+f_{(i\sigma_y^1 i\sigma_y^2)\otimes_{j=3}^{n} I^j}$ almost everywhere and RHS of (A22) is $f_{(\sigma_x^1\sigma_x^2)\otimes_{j=3}^{n} I^j}+f_{(i\sigma_y^1 i\sigma_y^2)\otimes_{j=3}^{n} I^j}$. LHS of (A23) is $f_{(\sigma_x^1\sigma_y^2)\otimes_{j=3}^{n} I^j}+f_{(\sigma_y^1\sigma_x^2)\otimes_{j=3}^{n} I^j}$ almost everywhere and RHS of (A23) is $f_{(\sigma_x^1\sigma_y^2)\otimes_{j=3}^{n} I^j}+f_{(\sigma_y^1\sigma_x^2)\otimes_{j=3}^{n} I^j}$. Therefore (A22) and (A23) hold when $m=2$. Here, we have used PROD A.E.. In the following, if possible, we omit the identity operator.

Suppose that (A22) and (A23) hold for $m=k-1$. Then we have

$$\prod_{j=1}^{k-1}(f_{\sigma_x^j}+if_{\sigma_y^j}) \simeq \sum_{p=2^{k-2}}^{2^{k-1}-1} f_{O_p^{k-1}} + \sum_{p=2^{k-2}}^{2^{k-1}-1} if_{R_p^{k-1}/i},$$
$$\prod_{j=1}^{k-1}(f_{\sigma_x^j}-if_{\sigma_y^j}) \simeq \sum_{p=2^{k-2}}^{2^{k-1}-1} f_{O_p^{k-1}} - \sum_{p=2^{k-2}}^{2^{k-1}-1} if_{R_p^{k-1}/i}. \tag{A24}$$

FUNC A.E. says

$$(-1)f_A(\omega) \simeq f_{(-1)A}(\omega). \tag{A25}$$

PROD A.E. says

$$f_{O_p^{k-1}} f_{\sigma_x^k} \simeq f_{O_p^{k-1}\sigma_x^k} \tag{A26}$$

and so on. Hence, we have

$$
\begin{aligned}
&(f_{\sigma_x^k}+if_{\sigma_y^k})\left(\sum_{p=2^{k-2}}^{2^{k-1}-1}f_{O_p^{k-1}}+\sum_{p=2^{k-2}}^{2^{k-1}-1}if_{R_p^{k-1}/i}\right)\\
&\quad=\left(\sum_{p=2^{k-2}}^{2^{k-1}-1}f_{O_p^{k-1}}f_{\sigma_x^k}+\sum_{p=2^{k-2}}^{2^{k-1}-1}if_{R_p^{k-1}/i}if_{\sigma_y^k}\right)+\left(\sum_{p=2^{k-2}}^{2^{k-1}-1}f_{O_p^{k-1}}if_{\sigma_y^k}+\sum_{p=2^{k-2}}^{2^{k-1}-1}if_{R_p^{k-1}/i}f_{\sigma_x^k}\right)\\
&\quad\simeq\left(\sum_{p=2^{k-2}}^{2^{k-1}-1}f_{O_p^{k-1}\sigma_x^k}+\sum_{p=2^{k-2}}^{2^{k-1}-1}f_{R_p^{k-1}i\sigma_y^k}\right)+\left(\sum_{p=2^{k-2}}^{2^{k-1}-1}if_{O_p^{k-1}i\sigma_y^k/i}+\sum_{p=2^{k-2}}^{2^{k-1}-1}if_{R_p^{k-1}\sigma_x^k/i}\right)\\
&\quad=\sum_{p=2^{k-1}}^{2^k-1}f_{O_p^k}+\sum_{p=2^{k-1}}^{2^k-1}if_{R_p^k/i}
\end{aligned}
\tag{A27}
$$

and

$$
\begin{aligned}
&(f_{\sigma_x^k}-if_{\sigma_y^k})\left(\sum_{p=2^{k-2}}^{2^{k-1}-1}f_{O_p^{k-1}}-\sum_{p=2^{k-2}}^{2^{k-1}-1}if_{R_p^{k-1}/i}\right)\\
&\quad=\left(\sum_{p=2^{k-2}}^{2^{k-1}-1}f_{O_p^{k-1}}f_{\sigma_x^k}+\sum_{p=2^{k-2}}^{2^{k-1}-1}if_{R_p^{k-1}/i}if_{\sigma_y^k}\right)-\left(\sum_{p=2^{k-2}}^{2^{k-1}-1}f_{O_p^{k-1}}if_{\sigma_y^k}+\sum_{p=2^{k-2}}^{2^{k-1}-1}if_{R_p^{k-1}/i}f_{\sigma_x^k}\right)\\
&\quad\simeq\left(\sum_{p=2^{k-2}}^{2^{k-1}-1}f_{O_p^{k-1}\sigma_x^k}+\sum_{p=2^{k-2}}^{2^{k-1}-1}f_{R_p^{k-1}i\sigma_y^k}\right)-\left(\sum_{p=2^{k-2}}^{2^{k-1}-1}if_{O_p^{k-1}i\sigma_y^k/i}+\sum_{p=2^{k-2}}^{2^{k-1}-1}if_{R_p^{k-1}\sigma_x^k/i}\right)\\
&\quad=\sum_{p=2^{k-1}}^{2^k-1}f_{O_p^k}-\sum_{p=2^{k-1}}^{2^k-1}if_{R_p^k/i}.
\end{aligned}
\tag{A28}
$$

Therefore we have

$$
\begin{aligned}
\prod_{j=1}^{k}(f_{\sigma_x^j}+if_{\sigma_y^j})&\simeq\sum_{p=2^{k-1}}^{2^k-1}f_{O_p^k}+\sum_{p=2^{k-1}}^{2^k-1}if_{R_p^k/i},\\
\prod_{j=1}^{k}(f_{\sigma_x^j}-if_{\sigma_y^j})&\simeq\sum_{p=2^{k-1}}^{2^k-1}f_{O_p^k}-\sum_{p=2^{k-1}}^{2^k-1}if_{R_p^k/i}.
\end{aligned}
\tag{A29}
$$

This implies that (A22) and (A23) hold for $m=k$. QED

APPENDIX B

Lemma: Let S_A stand for the spectrum of the Hermitian operator A. If

$$
\mathrm{Tr}[\psi A]=\sum_{y\in S_A}\mathrm{Prob}(\{y\})^{\psi}_{\theta(A)}y,
$$

$$
E_{\psi}(A):=\int_{\omega\in\Omega}\mu_{\psi}(\mathrm{d}\omega)f_A(\omega),
$$

then

$$\mathrm{HV} \wedge \mathrm{D} \Rightarrow \mathrm{Tr}[\psi A] = E_{\psi}(A). \tag{B1}$$

Proof: Note

$$\omega \in f_A^{-1}(\{y\}) \Leftrightarrow f_A(\omega) \in \{y\} \Leftrightarrow y = f_A(\omega),$$

$$\int_{\omega \in f_A^{-1}(\{y\})} \frac{\mu_{\psi}(\mathrm{d}\omega)}{\mu_{\psi}(f_A^{-1}(\{y\}))} = 1,$$

$$y \neq y' \Rightarrow f_A^{-1}(\{y\}) \cap f_A^{-1}(\{y'\}) = \phi. \tag{B2}$$

Hence we have

$$\begin{aligned}
\mathrm{Tr}[\psi A] &= \sum_{y \in S_A} \mathrm{Prob}(\{y\})^{\psi}_{\theta(A)} y = \sum_{y \in \mathbf{R}} \mathrm{Prob}(\{y\})^{\psi}_{\theta(A)} y = \sum_{y \in \mathbf{R}} \mu_{\psi}(f_A^{-1}(\{y\}))y \\
&= \sum_{y \in \mathbf{R}} \mu_{\psi}(f_A^{-1}(\{y\}))y \int_{\omega \in f_A^{-1}(\{y\})} \frac{\mu_{\psi}(\mathrm{d}\omega)}{\mu_{\psi}(f_A^{-1}(\{y\}))} \\
&= \sum_{y \in \mathbf{R}} \int_{\omega \in f_A^{-1}(\{y\})} \mu_{\psi}(f_A^{-1}(\{y\})) \frac{\mu_{\psi}(\mathrm{d}\omega)}{\mu_{\psi}(f_A^{-1}(\{y\}))} f_A(\omega) = \int_{\omega \in \Omega} \mu_{\psi}(\mathrm{d}\omega) f_A(\omega) = E_{\psi}(A).
\end{aligned} \tag{B3}$$

QED

Lemma:

$$\chi_{\Delta}(g(x)) = \chi_{g^{-1}(\Delta)}(x), (x \in \mathbf{R})$$

and

$$\mathrm{Prob}(\Delta)^{\psi}_{\theta(g(A))} = \mathrm{Tr}[\psi \chi_{\Delta}(g(A))] = \mathrm{Tr}[\psi \chi_{g^{-1}(\Delta)}(A)] = \mathrm{Prob}(g^{-1}(\Delta))^{\psi}_{\theta(A)}. \tag{B4}$$

Proof: Obvious.
Lemma:

$$\mathrm{QJD} \Rightarrow \mathrm{BSF},$$

$$\mathrm{HV} \wedge \mathrm{JD} \Rightarrow \mathrm{HV} \wedge \mathrm{D} \tag{B5}$$

Proof: Obvious.
Theorem:[6]

$$\mathrm{HV} \wedge \mathrm{JD} \Rightarrow \mathrm{HV} \wedge \mathrm{D} \wedge \mathrm{FUNC\ A.E.} \tag{B6}$$

Proof: Suppose JD holds. Let y be any real number, and let $S := \{\omega | f_{g(A)}(\omega) = y\}$ and $T := \{\omega | g(f_A(\omega)) = y\}$. We want $\mu_{\psi}(\bar{S} \cap T) = \mu_{\psi}(S \cap \bar{T}) = 0$. This is valid if we have $\mu_{\psi}(S) = \mu_{\psi}(T) = \mu_{\psi}(S \cap T)$ since

$$\begin{aligned}
\mu_{\psi}(S \cap \bar{T}) + \mu_{\psi}(S \cap T) &= \mu_{\psi}(S), \\
\mu_{\psi}(\bar{S} \cap T) + \mu_{\psi}(S \cap T) &= \mu_{\psi}(T).
\end{aligned} \tag{B7}$$

Note

$$\omega \in f_{g(A)}^{-1}(\{y\}) \Leftrightarrow f_{g(A)}(\omega) \in \{y\} \Leftrightarrow y = f_{g(A)}(\omega) \tag{B8}$$

and

$$\omega \in f_A^{-1}(g^{-1}(\{y\})) \Leftrightarrow f_A(\omega) \in g^{-1}(\{y\}) \Leftrightarrow g(f_A(\omega)) \in \{y\} \Leftrightarrow y = g(f_A(\omega)). \tag{B9}$$

The lemma (B5) says that JD yields D. Then, from the lemma (B4), we have

$$\begin{aligned}\mu_\psi(T) &= \mu_\psi(\{\omega | \omega \in f_A^{-1}(g^{-1}(\{y\}))\}) \\ &= \mathrm{Prob}(g^{-1}(\{y\}))_{\theta(A)}^{\psi} = \mathrm{Prob}(\{y\})_{\theta(g(A))}^{\psi} = \mu_\psi(\{\omega | \omega \in f_{g(A)}^{-1}(\{y\})\}) = \mu_\omega(S).\end{aligned} \tag{B10}$$

Using the spectral representation of A, it follows that $\chi_\Delta(A)\chi_{g(\Delta)}(g(A)) = \chi_\Delta(A)$ for any set Δ, where $g(\Delta) = \{g(x) | x \in \Delta\}$. Because, $\chi_\Delta(z) = 1 \Leftrightarrow z \in \Delta \Rightarrow g(z) \in g(\Delta) \Leftrightarrow \chi_{g(\Delta)}(g(z)) = 1$ holds ($z \in \mathbf{R}$). Hence,

$$\mathrm{Prob}(\Delta, g(\Delta))_{\theta(A),\theta(g(A))}^{\psi} = \mathrm{Tr}[\psi\chi_\Delta(A)\chi_{g(\Delta)}(g(A))] = \mathrm{Tr}[\psi\chi_\Delta(A)] = \mathrm{Prob}(\Delta)_{\theta(A)}^{\psi}. \tag{B11}$$

On the other hand, we have $g(g^{-1}(\Delta)) = \Delta$ because $g(g^{-1}(\Delta)) = \{g(x) | x \in g^{-1}(\Delta)\} = \{g(x) | g(x) \in \Delta\} = \Delta$. Therefore, on substituting $g^{-1}(\{y\})$ into Δ, we have

$$\mathrm{Prob}(g^{-1}(\{y\}), \{y\})_{\theta(A),\theta(g(A))}^{\psi} = \mathrm{Prob}(g^{-1}(\{y\}))_{\theta(A)}^{\psi} = \mu_\psi(T). \tag{B12}$$

But, from JD we have

$$\mathrm{Prob}(g^{-1}(\{y\}), \{y\})_{\theta(A),\theta(g(A))}^{\psi} = \mu_\psi(f_A^{-1}(g^{-1}(\{y\})) \cap f_{g(A)}^{-1}(\{y\})) = \mu_\psi(T \cap S). \tag{B13}$$

QED

Theorem:[6]

$$\mathrm{HV} \wedge \mathrm{FUNC\ A.E.} \Rightarrow \mathrm{HV} \wedge \mathrm{PROD\ A.E.} \tag{B14}$$

Proof: Suppose that A and B are two commuting Hermitian operators. This means that there exists a basis $\{P_i\}$ by which we can expand $A = \Sigma_i a_i P_i$, and such that B can also be expanded in the form $B = \Sigma_i b_i P_i$. Now construct a Hermitian operator $O := \Sigma_i o_i P_i$ with real numbers o_i. None of them is equal. Namely, O is assumed to be nondegenerate by construction. Let us define functions j and k by $j(o_i) := a_i$ and $k(o_i) := b_i$, respectively. Then we can see that if A and B commute, there exists a nondegenerate Hermitian operator O such that $A = j(O)$ and $B = k(O)$. Therefore, we can introduce a function h such that $AB = h(O)$ where $h := j \cdot k$. So we have the following:

$$f_{AB}(\omega) = f_{h(O)}(\omega) \simeq h(f_O(\omega)) = j(f_O(\omega)) \cdot k(f_O(\omega)) \simeq f_{j(O)}(\omega) \cdot f_{k(O)}(\omega) = f_A(\omega) \cdot f_B(\omega), \tag{B15}$$

where FUNC A.E. has been used. QED

Lemma:[7] If

$$\mu_\psi(\bar{S} \cap S') = \mu_\psi(\overline{S'} \cap S) = \mu_\psi(\bar{T} \cap T') = \mu_\psi(\overline{T'} \cap T) = 0,$$

then

$$\mu_\psi(S \cap T) = \mu_\psi(S' \cap T'). \tag{B16}$$

Proof: Note

$$\mu_\psi(\bar{S} \cap S' \cap T) + \mu_\psi(S \cap S' \cap T) = \mu_\psi(S' \cap T), \tag{B17}$$

$$\mu_\psi(\overline{S'} \cap S \cap T) + \mu_\psi(S \cap S' \cap T) = \mu_\psi(S \cap T).$$

If the following relation holds

$$\mu_\psi(\bar{S} \cap S') = \mu_\psi(\overline{S'} \cap S) = 0, \tag{B18}$$

then

$$\mu_\psi(\bar{S} \cap S' \cap T) = \mu_\psi(\overline{S'} \cap S \cap T) = 0. \tag{B19}$$

Therefore, from (B17), we have

$$\mu_\psi(S \cap S' \cap T) = \mu_\psi(S' \cap T) = \mu_\psi(S \cap T). \tag{B20}$$

Similar to the argument by changing S to T, S' to T', and T to S', we get

$$\mu_\psi(T \cap T' \cap S') = \mu_\psi(T' \cap S') = \mu_\psi(T \cap S'). \tag{B21}$$

From the relations (B20) and (B21), we conclude

$$\mu_\psi(T \cap S) = \mu_\psi(T' \cap S'). \tag{B22}$$

QED

Lemma:

$$\text{HV} \wedge \text{PROD A.E.} \Rightarrow f_{\chi_\Delta(A)}(\omega) \in \{0,1\}, \quad (\mu_\psi - \text{a.e.}). \tag{B23}$$

Proof: Obvious.

Theorem:[7]

$$\text{HV} \wedge \text{D} \wedge \text{PROD A.E.} \Rightarrow \text{HV} \wedge \text{JD} \tag{B24}$$

Proof: Suppose $[A,B]=\mathbf{0}$ holds. It follows from QJD, BSF, and D that

$$\begin{aligned}\text{Prob}(\Delta,\Delta')^{\psi}_{\theta(A),\theta(B)} &= \text{Tr}[\psi\chi_\Delta(A)\chi_{\Delta'}(B)] = \text{Tr}[\psi\chi_{\{1\}}(\chi_\Delta(A)\chi_{\Delta'}(B))] = \text{Prob}(\{1\})^{\psi}_{\theta(\chi_\Delta(A)\chi_{\Delta'}(B))} \\ &= \mu_\psi(f^{-1}_{\chi_\Delta(A)\chi_{\Delta'}(B)}(\{1\})).\end{aligned} \tag{B25}$$

PROD A.E. and the lemma (B23) say that

$$\begin{aligned}(\text{B25}) &= \mu_\psi(\{\omega|\omega \in f^{-1}_{\chi_\Delta(A)\chi_{\Delta'}(B)}(\{1\})\}) = \mu_\psi(\{\omega|f_{\chi_\Delta(A)\chi_{\Delta'}(B)}(\omega)=1\}) = \mu_\psi(\{\omega|f_{\chi_\Delta(A)}(\omega)\cdot f_{\chi_{\Delta'}(B)}(\omega) \\ &= 1\}) = \mu_\psi(\{\omega|f_{\chi_\Delta(A)}(\omega) = f_{\chi_{\Delta'}(B)}(\omega)=1\}) = \mu_\psi(f^{-1}_{\chi_\Delta(A)}(\{1\}) \cap f^{-1}_{\chi_{\Delta'}(B)}(\{1\})).\end{aligned} \tag{B26}$$

On the other hand, we have

$$\begin{aligned}\mu_\psi(f^{-1}_{\chi_\Delta(A)}(\{1\}) \cap f_A^{-1}(\Delta)) &= \mu_\psi(\{\omega|f_{\chi_\Delta(A)}(\omega) = 1 \wedge f_A(\omega) \in \Delta\}) = \mu_\psi(\{\omega|f_{\chi_\Delta(A)}(\omega)\cdot f_A(\omega) \in \Delta\}) \\ &= \mu_\psi(\{\omega|f_{\chi_\Delta(A)\cdot A}(\omega) \in \Delta\}) = \mu_\psi(f^{-1}_{\chi_\Delta(A)\cdot A}(\Delta)) = \text{Prob}(\Delta)^{\psi}_{\theta(\chi_\Delta(A)\cdot A)} \\ &= \text{Tr}[\psi\chi_\Delta(\chi_\Delta(A)\cdot A)] = \text{Tr}[\psi\chi_\Delta(A)].\end{aligned} \tag{B27}$$

We also obtain

$$\mu_\psi(f^{-1}_{\chi_\Delta(A)}(\{1\})) = \text{Tr}[\psi\chi_{\{1\}}(\chi_\Delta(A))] = \text{Tr}[\psi\chi_\Delta(A)] = \mu_\psi(f_A^{-1}(\Delta)). \tag{B28}$$

Note [see (B7)]

$$\mu_\psi(S \cap T) = \mu_\psi(S) = \mu_\psi(T) \Leftrightarrow \mu_\psi(S \cap \bar{T}) = \mu_\psi(\bar{S} \cap T) = 0. \tag{B29}$$

Therefore, from Eq. (B27) and Eq. (B28), we have

$$\mu_\psi(f^{-1}_{\chi_\Delta(A)}(\{1\}) \cap \overline{f_A^{-1}(\Delta)}) = \mu_\psi(\overline{f^{-1}_{\chi_\Delta(A)}(\{1\})} \cap f_A^{-1}(\Delta)) = 0. \tag{B30}$$

Similarly we can get

$$\mu_\psi(f^{-1}_{\chi_{\Delta'}(B)}(\{1\}) \cap f_B^{-1}(\Delta')) = \mathrm{Tr}[\psi\chi_{\Delta'}(B)], \quad \mu_\psi(f^{-1}_{\chi_{\Delta'}(B)}(\{1\})) = \mu_\psi(f_B^{-1}(\Delta')) = \mathrm{Tr}[\psi\chi_{\Delta'}(B)], \tag{B31}$$

and we have

$$\mu_\psi(f^{-1}_{\chi_{\Delta'}(B)}(\{1\}) \cap \overline{f_B^{-1}(\Delta')}) = \mu_\psi(\overline{f^{-1}_{\chi_{\Delta'}(B)}(\{1\})} \cap f_B^{-1}(\Delta')) = 0. \tag{B32}$$

Hence, from the lemma (B16), we have

$$\mu_\psi(f^{-1}_{\chi_\Delta(A)}(\{1\}) \cap f^{-1}_{\chi_{\Delta'}(B)}(\{1\})) = \mu_\psi(f_A^{-1}(\Delta) \cap f_B^{-1}(\Delta')). \tag{B33}$$

Therefore, from (B26), we conclude

$$\mathrm{Prob}(\Delta,\Delta')^{\psi}_{\theta(A),\theta(B)} = \mu_\psi(f_A^{-1}(\Delta) \cap f_B^{-1}(\Delta')), \tag{B34}$$

which is JD. QED

Theorem:[6]

$$\mathrm{HV} \wedge \mathrm{D} \wedge \mathrm{FUNC\ A.E.} \Rightarrow \mathrm{HV} \wedge \mathrm{JD} \tag{B35}$$

Proof: Suppose $[A,B]=\mathbf{0}$ holds. It follows from BSF, QJD, D, FUNC A.E., and PROD A.E. that

$$\begin{aligned}
\mathrm{Prob}(\Delta,\Delta')^{\psi}_{\theta(A),\theta(B)} &= \mathrm{Tr}[\psi\chi_\Delta(A)\chi_{\Delta'}(B)] = \mathrm{Tr}[\psi\chi_{\{1\}}(\chi_\Delta(A)\chi_{\Delta'}(B))] = \mathrm{Prob}(\{1\})^{\psi}_{\theta(\chi_\Delta(A)\chi_{\Delta'}(B))} \\
&= \mu_\psi(f^{-1}_{\chi_\Delta(A)\chi_{\Delta'}(B)}(\{1\})) = \mu_\psi(\{\omega|\omega \in f^{-1}_{\chi_\Delta(A)\chi_{\Delta'}}(\{1\})\}) = \mu_\psi(\{\omega|f_{\chi_\Delta(A)\chi_{\Delta'}(B)}(\omega) \\
&= 1\}) = \mu_\psi(\{\omega|f_{\chi_\Delta(A)}(\omega) \cdot f_{\chi_{\Delta'}(B)}(\omega) = 1\}) = \mu_\psi(\{\omega|\chi_\Delta(f_A(\omega)) \cdot \chi_{\Delta'}(f_B(\omega)) = 1\}) \\
&= \mu_\psi(\{\omega|\chi_\Delta(f_A(\omega)) = \chi_{\Delta'}(f_B(\omega)) = 1\}) = \mu_\psi(\{\omega|f_A(\omega) \in \Delta \wedge f_B(\omega) \in \Delta'\}) \\
&= \mu_\psi(f_A^{-1}(\Delta) \cap f_B^{-1}(\Delta')).
\end{aligned} \tag{B36}$$

QED

Now we summarize the inclusion relation as follows:

$$\mathrm{HV} \wedge \mathrm{JD} \Leftrightarrow \mathrm{HV} \wedge \mathrm{D} \wedge \mathrm{FUNC\ A.E.} \Leftrightarrow \mathrm{HV} \wedge \mathrm{D} \wedge \mathrm{PROD\ A.E.} \tag{B37}$$

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[21] We know that every proposition is true if the presupposition is false [see Eq. (3.6)]. Therefore, one might think that theorem (4.2) and theorem (5.16) are trivial. However, this is not the matter of our argument. We have used a quantum mechanical rule $\sigma_x^1\sigma_x^2\sigma_y^1\sigma_y^2\sigma_z^1\sigma_z^2=-I$ in the proof of the theorem (3.6). But, we have not used the quantum mechanical rule in the proof of the theorem (4.2). Likewise, a quantum mechanical rule $\sigma_x^i\sigma_y^j\sigma_y^i\sigma_x^j\sigma_z^i\sigma_z^j=I$, $(i,j\in\mathbf{N}_n, i\neq j)$ is needless to prove the theorem (5.16), while we have used the quantum mechanical rule in the proof of the theorem (3.6). Obviously, $\sigma_x^i\sigma_y^j\sigma_y^k\sigma_y^i\sigma_x^j\sigma_y^k\sigma_y^i\sigma_y^j\sigma_x^k\sigma_x^i\sigma_x^j\sigma_x^k=-I$, $(i,j,k\in\mathbf{N}_n, i\neq j\neq k\neq i)$ is needless to prove the theorem (5.16). Of course, Gleason's theorem is needless. Therefore, we can derive these inequalities (4.2) and (5.16) from more precise and weaker presupposition which should not be necessarily false.

Real trajectories in the semiclassical coherent state propagator

Marcel Novaes[a)]
Instituto de Física "Gleb Wataghin," Universidade Estadual de Campinas, 13083-970 Campinas, São Paulo, Brazil

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The semiclassical approximation to the coherent state propagator requires complex classical trajectories in order to satisfy the associated boundary conditions, but finding these trajectories in practice is a difficult task that may compromise the applicability of the approximation. In this work several approximations to the coherent state propagator are derived that make use only of real trajectories, which are easier to handle and have a more direct physical interpretation. It is verified in a particular example that these real trajectories approximations may have excellent accuracy. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2038608]

I. INTRODUCTION

The path integral representation of the coherent state propagator $K(z_1,z_2,T)=\langle z_2|e^{-iHT/\hbar}|z_1\rangle$, where the $|z_i\rangle$ are the usual harmonic oscillator coherent states, appeared in the works of Klauder and collaborators[1,2] and of Weissman.[3] A semiclassical, or stationary phase, approximation leads to classical trajectories satisfying Hamilton equations of motion but subject to special boundary conditions that can only be satisfied in a complex phase space. Aguiar and Baranger also considered this problem[4] and discovered an extra term, which they called $\mathcal{I}$, in the semiclassical approximation that had been overlooked in previous studies and that turns out to be essential for a correct theory[5] (the semiclassical spin propagator has a similar term,[6] known as the Solari-Kochetov correction). Numerical calculations involving complex trajectories in the semiclassical coherent state propagator have been done for a variety of systems: Adachi considered a one-dimensional (1D) and time-dependent problem with chaotic dynamics;[7] Rubin and Klauder,[2] as well as Xavier and Aguiar,[8] have treated 1D bound systems; 1D tunneling was considered in Ref. 9 and also in Ref. 10; Van Voorhis and Heller presented calculations for one and two dimensions[11] and for the N-dimensional Henon-Heiles potential;[12] Ribeiro *et al.* have worked with the two-dimensional chaotic Nelson potential[13] (numerical applications involving the spin coherent states have also appeared[14]). Semiclassical approximations based on complex trajectories for the coordinate wave function, i.e., for the mixed representation $K(x,z,T)=\langle x|e^{-iHT/\hbar}|z\rangle$, were also developed, initially for the one-dimensional case[15–17] and then generalized to many dimensions.[18] The actual calculation of complex trajectories involves two difficulties: first, the effective dimensionality of the phase space is doubled, since both real and imaginary parts of position and momentum must be computed; second, the boundary conditions are defined part at initial time and part at final time, and finding the appropriate classical trajectory becomes a difficult problem known as "root search." Therefore approximations that make use only of real trajectories are certainly desirable.

Since the propagator $K(z_1,z_2,T)$ is a function of time, any complex trajectory that satisfies the boundary conditions at time T must belong to a whole "branch" of trajectories, parametrized by T. In general, for a given system and for fixed values of z_1 and z_2 there are several such branches. In practice, once a solution is found for a particular value of T, one may obtain all elements of the same branch by making small steps forward or backward in time and using appropriate iteractive

[a)]Electronic mail: mnovaes@ifi.unicamp.br

procedures. It may happen that for a certain value of time a relevant complex trajectory has a small (or even null) imaginary part, and in that case its branch was called "nearly real" by Van Voorhis and Heller.[11,12] It is possible that more than one "nearly real" branch contribute to the semiclassical propagator for a given time, and thus one may consider only these branches and still accurately reproduce interference effects.

A similar analysis can be made for the mixed propagator $K(x,z,T)$, but in this case one usually holds T fixed and considers x as a parameter. Varying x thus produces a "family" of trajectories, and again there may exist several such families. However, there is always a value of x for which the involved trajectory is real, and its family was called the "main family" by Aguiar *et al.*[16] Using the main contribution alone is sometimes a very good approximation, but it cannot reproduce interference because only one trajectory enters the calculation at a time. On the other hand, as already noted, finding all the necessary complex trajectories (i.e., performing the "root search") is usually a difficult problem, especially in more than one dimension. Therefore the possibility was considered[16,18] of employing only real trajectories in the semiclassical approximation to $K(x,z,T)$. This was done by approximating the complex trajectories by real ones, that are compatible with the quantum uncertainties and satisfy less restrictive boundary conditions. The final real trajectories approximations are in principle less accurate than the original complex one, but they are much simpler and sometimes have practically the same accuracy.[16,18]

The purpose of the present work is to present semiclassical approximations to $K(z_1,z_2,T)$ that are based only on real classical trajectories, thus making the calculation much more tractable. One method that accomplishes exactly this is the "cellular dynamics," initially developed by Heller[19] (see also Ref. 20) and later generalized and applied to the stadium billiard with great success.[21] This technique has shown to be accurate even for long times,[21,22] and it is actually very close in spirit to the present work, in the sense that the contribution of a complex classical trajectory is expanded to second order in the vicinity of a real one. However, Heller's starting point is the Van-Vleck-Gutzwiller formula for the semiclassical propagator,[23] while we start from the formulation of Baranger *et al.*,[5] and our results are slightly different from those of Heller. We also consider a variety of boundary conditions that the real trajectories may satisfy, something not discussed at length in Ref. 21.

Another approach to the semiclassical coherent state propagator that is based on real trajectories is the so-called initial value representations, such as that of Herman and Kluk.[24] Recent reviews of this method can be found in Ref. 25. Initial value methods are usually easy to apply and reasonably accurate for long times, but they require a numerical integration over all possible initial conditions. Since the present method requires only a few trajectories, at least for short times, it provides a much clearer physical picture.

This article is divided as follows. In the next section we give a brief account of the semiclassical approximation to the coherent state propagator $K(z_1,z_2,T)$ and the complex trajectories. In Sec. III we present the approximations that are based on the real trajectories defined by z_1 or by z_2. Real trajectories that satisfy mixed boundary conditions are investigated in Sec. IV. We present an application to a nonlinear oscillator in Secs. V and VI and we conclude in Sec. VII.

II. THE SEMICLASSICAL COHERENT STATE PROPAGATOR

The coherent states of a harmonic oscillator of mass m and angular frequency ω are defined by

$$|z\rangle = \exp\{za^\dagger - z^* a\}|0\rangle, \tag{2.1}$$

where $|0\rangle$ is the oscillator ground state. The operators $a^\dagger$ and a are, respectively, creation and annihilation operators, related to position Q and momentum P by

$$a = \frac{1}{\sqrt{2}}\left(\frac{Q}{b} + i\frac{P}{c}\right), \quad a^\dagger = \frac{1}{\sqrt{2}}\left(\frac{Q}{b} - i\frac{P}{c}\right). \tag{2.2}$$

The parameters b and c define natural scales of the problem, and are such that $bc=\hbar$ and $c/b=m\omega$. It is easy to see that if we write

$$z = \frac{1}{\sqrt{2}}\left(\frac{q}{b} + i\frac{p}{c}\right) \tag{2.3}$$

then q and p are average values,

$$\langle z|Q|z\rangle = q, \quad \langle z|P|z\rangle = p. \tag{2.4}$$

The parameters b and c are related to quantum uncertainties,

$$\Delta Q = \frac{b}{\sqrt{2}}, \quad \Delta P = \frac{c}{\sqrt{2}}, \tag{2.5}$$

and we see that coherent states are minimum uncertainty states.

These coherent states are never orthogonal,

$$\langle z_2|z_1\rangle = \exp\left\{-\tfrac{1}{2}|z_1|^2 - \tfrac{1}{2}|z_2|^2 + z_1 z_2^*\right\}, \tag{2.6}$$

and in the position representation they are Gaussians,

$$\langle x|z\rangle = \pi^{-1/4} b^{-1/2} \exp\left\{-\frac{(x-q)^2}{2b^2} + \frac{i}{\hbar}p(x-q)\right\}. \tag{2.7}$$

In terms of the usual basis of number states $|n\rangle$, defined such that $a^\dagger a|n\rangle = n|n\rangle$, the coherent states may be written as

$$|z\rangle = e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}}|n\rangle. \tag{2.8}$$

It is easy to see that they are eigenstates of the annihilation operator, $a|z\rangle = z|z\rangle$.

In order to write the semiclassical approximation to the quantum coherent state propagator

$$K(z_1, z_2, T) = \langle z_2|e^{-iHT/\hbar}|z_1\rangle, \tag{2.9}$$

we must consider a complex version of the phase space, i.e., we must make use of a coordinate $q(t)$ and a momentum $p(t)$ that are complex numbers. Following the approach of Ref. 5 we define

$$u(t) = \frac{1}{\sqrt{2}}\left(\frac{q(t)}{b} + i\frac{p(t)}{c}\right), \quad v(t) = \frac{1}{\sqrt{2}}\left(\frac{q(t)}{b} - i\frac{p(t)}{c}\right). \tag{2.10}$$

It is of fundamental importance to realize that $v(t)$ is not the complex conjugate of $u(t)$. In terms of these variables the boundary conditions become

$$u(0) = u' = z_1, \quad v(T) = v'' = z_2^*. \tag{2.11}$$

There is nothing special about the values $u(T) = u''$ and $v(0) = v'$, they are to be determined dynamically. We use hereafter a prime (double prime) to denote initial (final) values, in order to simplify the formulas and stay close to the notation of Ref. 5.

The canonical semiclassical coherent state propagator is

$$K_{\mathrm{sc}}(z_1, z_2, T) = \mathcal{N} \sum_{\mathrm{c.t.}} \sqrt{\frac{i}{\hbar}\frac{\partial^2 S}{\partial u' \, \partial v''}} \exp\left\{\frac{i}{\hbar}(S + \mathcal{I})\right\}, \tag{2.12}$$

where $\mathcal{N} = \exp\left\{-\frac{1}{2}|z_1|^2 - \frac{1}{2}|z_2|^2\right\}$ is a normalization factor, the summation is over all classical trajectories satisfying the boundary conditions, and the complex action is given by

$$S(u',v'',T)=\int_0^T dt\left[\frac{i\hbar}{2}(\dot{u}v-\dot{v}u)-\mathcal{H}\right]-\frac{i\hbar}{2}(u'v'-u''v''). \tag{2.13}$$

This is related to the usual Hamilton action

$$S_H=\int_0^T (p\dot{q}-\mathcal{H})dt \tag{2.14}$$

by

$$S=S_H-\frac{q'p'-q''p''}{2}-\frac{i\hbar}{2}(u'v'-u''v''). \tag{2.15}$$

The Hamiltonian that governs the classical movement according to the usual Hamilton equations

$$\dot{q}=\frac{\partial\mathcal{H}}{\partial p},\quad \dot{p}=-\frac{\partial\mathcal{H}}{\partial q}, \tag{2.16}$$

is the average value of the quantum Hamiltonian in coherent states,

$$\mathcal{H}=\langle z|H|z\rangle, \tag{2.17}$$

which is sometimes called the smoothed Hamiltonian. The quantity $\mathcal{I}$ is related to its second derivative,

$$\mathcal{I}=\frac{1}{2}\int_0^T \frac{\partial^2\mathcal{H}}{\partial u\,\partial v}\mathrm{d}t. \tag{2.18}$$

The prefactor in (2.12) can be written only in terms of the complex tangent matrix. The classical tangent matrix of a certain trajectory is the linear application that relates initial and final displacements about it. We take into account the quantum uncertainties to define it as follows:

$$\begin{pmatrix}\delta q''/b\\ \delta p''/c\end{pmatrix}=\begin{pmatrix}m_{qq} & m_{qp}\\ m_{pq} & m_{pp}\end{pmatrix}\begin{pmatrix}\delta q'/b\\ \delta p'/c\end{pmatrix}. \tag{2.19}$$

The complex tangent matrix, on the other hand, is defined as

$$\begin{pmatrix}\delta u''\\ \delta v''\end{pmatrix}=\begin{pmatrix}M_{uu} & M_{uv}\\ M_{vu} & M_{vv}\end{pmatrix}\begin{pmatrix}\delta u'\\ \delta v'\end{pmatrix}. \tag{2.20}$$

The relation between the matrix elements of these different representations is as follows:

$$2M_{uu}=m_{qq}+m_{pp}+im_{pq}-im_{qp}, \tag{2.21}$$

$$2M_{uv}=m_{qq}-m_{pp}+im_{pq}+im_{qp}, \tag{2.22}$$

$$2M_{vu}=m_{qq}-m_{pp}-im_{pq}-im_{qp}, \tag{2.23}$$

$$2M_{vv}=m_{qq}+m_{pp}-im_{pq}+im_{qp}. \tag{2.24}$$

It is possible to show that the second derivative of the complex action is given by

$$\frac{i}{\hbar}\frac{\partial^2 S}{\partial u'\,\partial v''}=\frac{1}{M_{vv}}, \tag{2.25}$$

and therefore the semiclassical coherent state propagator becomes

$$K_{\mathrm{sc}}(z_1,z_2,T)=\sum_{\mathrm{c.t.}}\frac{\mathcal{N}}{\sqrt{M_{vv}}}\exp\left\{\frac{i}{\hbar}(\mathcal{I}+S)\right\}. \tag{2.26}$$

Upon fixing z_1 and z_2, the squared modulus of this propagator may be interpreted as a time dependent transition probability. On the other hand, if we fix z_1 and T and consider z_2 as a variable then $|K(z_1,z_2,T)|^2$ is a phase space representation, a Husimi function, of the evolved state $e^{-iHT/\hbar}|z_1\rangle$.

If it happens that M_{vv} tends to zero for a certain combination of (z_1,z_2,T), then we see that the semiclassical approximation (2.26) diverges. This is called a phase space caustic[2,7,12,16] and the quadratic approximation used in the derivation of (2.26) is not valid in its vicinity. In order to obtain an uniform approximation that remains valid at caustics it is necessary to employ a conjugate application of the Bargmann representation, as discussed in Ref. 26. We shall not be concerned with caustics in this work.

III. THE "LEAVING" AND THE "ARRIVING" TRAJECTORIES

We have seen that the classical trajectories entering the semiclassical propagator are determined by mixed boundary conditions. The initial position and momentum q' and p' are not the real numbers q_1 and p_1, but rather some complex numbers such that $u'=z_1$. Conversely, the final values q'',p'' are not q_2,p_2 but are such that $v''=z_2^*$. It is in general not an easy task to find such trajectories in practice, even for simple systems. However, it may happen that the complex trajectory is close enough to a real one so that we may still obtain a reasonable result by expanding the propagator to second order in the vicinity of this real trajectory.[16,18] We investigate this problem with some detail in the next sections.

A. Leaving

Let us suppose a certain complex classical trajectory that is to be used in the calculation of the semiclassical propagator, and let us assume it is not very different from the real trajectory that starts at the point (q_1,p_1). We call this the "leaving" trajectory because it leaves the phase space point corresponding to the initial coherent state. After a time T the position and the momentum will be some real numbers (q_f,p_f), generally different from the pair (q_2,p_2). We will expand the complex action up to second order around this trajectory. If q' is the initial complex position and p' is the initial complex momentum, we may write

$$q'=q_1+\Delta q_1,\quad p'=p_1+\Delta p_1, \tag{3.1}$$

where Δq_1 and Δp_1 are assumed to be small (complex) quantities. Moreover, if q'' is the final complex position and p'' is the final complex momentum, we may write in a similar way

$$q''=q_f+\Delta q_f,\quad p''=p_f+\Delta p_f. \tag{3.2}$$

Therefore we have the approximation

$$\begin{aligned}S(u',v'',T)\approx S(z_1,v_r,T)+&\left.\frac{\partial S}{\partial q'}\right|_r\Delta q_1+\left.\frac{\partial S}{\partial p'}\right|_r\Delta p_1+\frac{1}{2}\left.\frac{\partial^2 S}{\partial q'^2}\right|_r\Delta q_1^2+\left.\frac{\partial^2 S}{\partial q'\,\partial p'}\right|_r\Delta q_1\Delta p_1\\&+\frac{1}{2}\left.\frac{\partial^2 S}{\partial p'^2}\right|_r\Delta p_1^2,\end{aligned} \tag{3.3}$$

where the subscript r means that the quantity must be evaluated at the real trajectory (therefore $v_r'=b^{-1}q_1-ic^{-1}p_1$ and $u_r''=b^{-1}q_f+ic^{-1}p_f$). In order to obtain the derivatives of the action, we resort to Eqs. (2.10) and (2.15). Noticing that

$$\left.\frac{\partial S_H}{\partial q'}\right|_r = -p_i + \frac{\partial S_H}{\partial q''}\frac{\partial q''}{\partial q'}, \qquad \left.\frac{\partial S_H}{\partial p'}\right|_r = \frac{\partial S_H}{\partial q''}\frac{\partial q''}{\partial p'}, \tag{3.4}$$

one can obtain the derivatives of the total action, which are given by

$$\left.\frac{\partial S}{\partial q'}\right|_r = -\frac{ic}{\sqrt{2}}[v_r' + (m_{qq} - im_{pq})u_r''], \qquad \left.\frac{\partial S}{\partial p'}\right|_r = \frac{b}{\sqrt{2}}[v_r' - (m_{pp} + im_{qp})u_r'']. \tag{3.5}$$

From the definition of the tangent matrix we have

$$\frac{\partial q''}{\partial q'} = m_{qq}, \quad \frac{\partial q''}{\partial p'} = \frac{b}{c}m_{qp}, \quad \frac{\partial p''}{\partial q'} = \frac{c}{b}m_{pq}, \quad \frac{\partial p''}{\partial p'} = m_{pp}, \tag{3.6}$$

which determines, to first order, the final differences in terms of the initial ones:

$$\Delta q_2 = m_{qq}\Delta q_1 + \frac{b}{c}m_{qp}\Delta p_1, \quad \Delta p_2 = \frac{c}{b}m_{pq}\Delta q_1 + m_{pp}\Delta p_1. \tag{3.7}$$

On the other hand, the boundary conditions

$$\frac{q'}{b} + i\frac{p'}{c} = \frac{q_1}{b} + i\frac{p_1}{c}, \quad \frac{q''}{b} - i\frac{p''}{c} = \frac{q_2}{b} - i\frac{p_2}{c}, \tag{3.8}$$

provide the secondary relations

$$b^{-1}[\Delta q_2 + (q_f - q_2)] = ic^{-1}[\Delta p_2 + (p_f - p_2)], \quad b^{-1}\Delta q_1 = -ic^{-1}\Delta p_1. \tag{3.9}$$

Solving for Δq_1 and Δp_1 in terms of $(q_f - q_2)$ and $(p_f - p_2)$ we have

$$\Delta q_1 = -M_{vv}^{-1}[(q_f - q_2) - ib(p_f - p_2)/c], \quad \Delta p_1 = ic\Delta q_1/b. \tag{3.10}$$

Substituting this in (3.3) one can see that the first-order terms give

$$\left.\frac{\partial S}{\partial q'}\right|_r \Delta q_1 + \left.\frac{\partial S}{\partial p'}\right|_r \Delta p_1 = -\frac{i\hbar}{\sqrt{2}}u_r''\left[\frac{q_f - q_2}{b} - i\frac{p_f - p_2}{c}\right] = -i\hbar u_r''(v_r'' - z_2^*). \tag{3.11}$$

It is easy to take derivatives of Eq. (3.5) in order to calculate the quadratic terms. In so doing we neglect derivatives of the tangent matrix elements, because this would be a higher order correction. Adding up all quadratic terms and making the proper identifications, we see that it can be related to the difference $(v_r'' - z_2^*)$ as

$$\text{quadratic terms} = -\frac{i\hbar}{2}M_{uv}M_{vv}^{-1}(v_r'' - z_2^*)^2. \tag{3.12}$$

Therefore the final result is the following:

$$K_{q_1p_1}(z_1, z_2, T) = \frac{\mathcal{N}}{\sqrt{(M_{vv})_r}}\exp\left\{\frac{i}{\hbar}(\mathcal{I}_r + S_r) + u_r''(v_r'' - z_2^*) + \frac{1}{2}\frac{M_{uv}}{M_{vv}}(v_r'' - z_2^*)^2\right\}. \tag{3.13}$$

The subscript in $K_{q_1p_1}$ denotes that this formula was obtained using the "leaving" trajectory. Notice that the prefactor and the extra term were not expanded but simply evaluated at the real trajectory, which is consistent with the original quadratic derivation of the semiclassical approximation. It is also important to remember that even though the action S_r is evaluated at a real trajectory, it continues to be a complex number.

The expression (3.13) depends quadratically on the difference between the final value of the variable v along the real trajectory and the value that it would have in the complex trajectory. If by

some reason the situation is such that v_r'' and z_2^* coincide, then this formula and the original one (2.12) will give the same result. One may argue that it is possible to obtain the same expression by expanding the action as

$$S \approx S_r + \left.\frac{\partial S}{\partial v''}\right|_r (v_r'' - z_2^*) + \frac{1}{2}\left.\frac{\partial^2 S}{\partial v''^2}\right|_r (v_r'' - z_2^*)^2. \tag{3.14}$$

This is certainly true and actually an easy calculation. We have chosen the long way of using the position/momentum variables because this will be the only possibility in the next section.

B. Arriving

What we call the "arriving" trajectory is the real trajectory that starts in a certain initial point (q_i, p_i) and after a time T arrives at the point (q_2, p_2). We can use this trajectory to approximate the semiclassical propagator in the very same way that we did with the "leaving" trajectory. Similar to the previous arguments, we write

$$q' = q_i + \Delta q_1, \quad p' = p_i + \Delta p_1, \quad q'' = q_2 + \Delta q_2, \quad p'' = p_2 + \Delta p_2. \tag{3.15}$$

Inverting Eq. (2.19) we see that

$$\frac{\partial q'}{\partial q''} = m_{pp}, \quad \frac{\partial q'}{\partial p''} = -\frac{b}{c} m_{qp}, \quad \frac{\partial p'}{\partial q''} = -\frac{c}{b} m_{pq}, \quad \frac{\partial p'}{\partial p''} = m_{qq}. \tag{3.16}$$

Using these relations we can write the initial differences in terms of the final ones, analogous to what we did in (3.7). Using the boundary conditions it is possible to show that

$$\Delta q_2 = -M_{vv}^{-1}[(q_i - q_1) + ib(p_i - p_1)/c], \quad \Delta p_2 = -ic\Delta q_2/b. \tag{3.17}$$

The first derivatives of the action are in this case given by

$$\left.\frac{\partial S}{\partial q''}\right|_r = -\frac{ic}{\sqrt{2}}[u_r'' + (m_{pp} - im_{pq})v_r'], \qquad \left.\frac{\partial S}{\partial p''}\right|_r = -\frac{b}{\sqrt{2}}[u_r'' - (m_{qq} + im_{qp})v_r']. \tag{3.18}$$

We now expand the complex action to second order around this real trajectory. After simplifications, we obtain

$$K_{q_2 p_2}(z_1, z_2, T) = \frac{\mathcal{N}}{\sqrt{(M_{vv})_r}} \exp\left\{\frac{i}{\hbar}(\mathcal{I}_r + S_r) + v_r'(u_r' - z_1) + \frac{1}{2}\frac{M_{vu}}{M_{vv}}(u_r' - z_1)^2\right\}, \tag{3.19}$$

where the meaning of the subscript is evident. This time the expression depends on the difference between the initial value of the variable u in the real trajectory and the value that it would have in the complex one. Its interpretation is quite close to that of (3.13).

IV. OTHER POSSIBLE REAL TRAJECTORIES

In the previous section we saw that we may expand the semiclassical propagator in the vicinity of the real trajectories determined by the initial or by the final labels, (q_1, p_1) and (q_2, p_2), which we called the "leaving" and the "arriving" trajectories, respectively. Although these are probably the most natural real trajectories approximations, we can devise four more possibilities that are also interesting. Of course one may use any real trajectory to build an approximation—in fact, in principle it should be possible to find the "best" choice by a variational approach, but this seems to be a highly nontrivial problem—but the idea here is to obtain explicit formulas for the most natural cases. These are the four trajectories that are determined by pairwise combination of the coherent state labels.

We shall present a detailed calculation for the case when the trajectories determined by the pair (q_1, q_2) are used. All other cases can be treated in a very similar way, and for them we shall be less explicit.

A. From q_1 to q_2

Let us consider a trajectory which satisfies the following boundary conditions: it leaves q_1 at time zero and arrives at q_2 at time T. Its initial and final momenta, p_i and p_f, remain unknown, but are real numbers. Different from the previous section, now there may be more than one trajectory satisfying these requirements. We write

$$q' = q_1 + \Delta q_1, \quad q'' = q_2 + \Delta q_2, \quad p' = p_i + \Delta p_i, \quad p'' = p_f + \Delta p_f. \tag{4.1}$$

The initial and final momenta are regarded as functions of the initial and final positions. Therefore we may write

$$\Delta p_i = \left.\frac{\partial p'}{\partial q'}\right|_r \Delta q_1 + \left.\frac{\partial p'}{\partial q''}\right|_r \Delta q_2, \quad \Delta p_f = \left.\frac{\partial p''}{\partial q'}\right|_r \Delta q_1 + \left.\frac{\partial p''}{\partial q''}\right|_r \Delta q_2, \tag{4.2}$$

where again the subscript r means that the quantity must be evaluated at the real trajectory. On the other hand the boundary conditions $u' = z_1$ and $v'' = z_2^*$ imply that

$$\Delta p_i = \frac{ic}{b}\Delta q_1 - (p_i - p_1), \quad \Delta p_f = -\frac{ic}{b}\Delta q_2 - (p_f - p_2). \tag{4.3}$$

Since we are considering q' and q'' as independent variables, the partial derivatives in (4.2) are given by

$$\frac{\partial p'}{\partial q'} = -\frac{c}{b}\frac{m_{qq}}{m_{qp}}, \quad \frac{\partial p'}{\partial q''} = \frac{c}{b}\frac{1}{m_{qp}}, \quad \frac{\partial p''}{\partial q'} = -\frac{c}{b}\frac{1}{m_{qp}}, \quad \frac{\partial p''}{\partial q''} = \frac{c}{b}\frac{m_{pp}}{m_{qp}}, \tag{4.4}$$

where we have used that $m_{qq}m_{pp} - m_{qp}m_{pq} = 1$. Substituting this in (4.2) and using (4.3) we have

$$\frac{\Delta q_1}{b} = \frac{m_{qp}}{c}\frac{[(p_f - p_2) - M_2(p_i - p_1)]}{1 - M_1 M_2}, \quad \frac{\Delta q_2}{b} = \frac{m_{qp}}{c}\frac{[M_1(p_f - p_2) - (p_i - p_1)]}{1 - M_1 M_2}, \tag{4.5}$$

where we have defined the complex numbers

$$M_1 = m_{qq} + i m_{qp}, \quad M_2 = m_{pp} + i m_{qp}. \tag{4.6}$$

We now expand the complex action around this real trajectory up to second order,

$$S \approx S_r + \left.\frac{\partial S}{\partial q'}\right|_r \Delta q_1 + \left.\frac{\partial S}{\partial q''}\right|_r \Delta q_2 + \frac{1}{2}\left.\frac{\partial^2 S}{\partial q'^2}\right|_r \Delta q_1^2 + \left.\frac{\partial^2 S}{\partial q'\,\partial q''}\right|_r \Delta q_1 \Delta q_2 + \frac{1}{2}\left.\frac{\partial^2 S}{\partial q''^2}\right|_r \Delta q_2^2. \tag{4.7}$$

Noticing that

$$\left.\frac{\partial S_H}{\partial q'}\right|_r = -p_i, \qquad \left.\frac{\partial S_H}{\partial q''}\right|_r = p_f, \tag{4.8}$$

we can obtain the derivatives of the total action,

$$\left.\frac{\partial S}{\partial q'}\right|_r = \frac{c}{\sqrt{2}m_{qp}}[u_r'' - v_r'(m_{qq} + i m_{qp})], \qquad \left.\frac{\partial S}{\partial q''}\right|_r = \frac{c}{\sqrt{2}m_{qp}}[v_r' - u_r''(m_{pp} + i m_{qp})]. \tag{4.9}$$

After simplifications, the linear terms can be written as

$$\text{linear terms} = -\frac{b}{\sqrt{2}}[v'(p_i - p_1) - u''(p_f - p_2)]. \tag{4.10}$$

We now calculate the second derivatives and substitute (4.5) in (4.7). After many simplifications, the final result can be shown to be

$$K_{q_1 q_2}(z_1, z_2, T) = \sum_{\text{c.t}} \frac{\mathcal{N}}{\sqrt{(M_{vv})_r}} \exp\left\{ \frac{i}{\hbar}(\mathcal{I}_r + S_r) + \frac{iz_2}{\sqrt{2}c}(p_f - p_2) - \frac{iz_1^*}{\sqrt{2}c}(p_i - p_1) \right\}$$
$$\times \exp\left\{ -\frac{A_1}{2c^2}(p_i - p_1)^2 - \frac{A_2}{2c^2}(p_f - p_2)^2 - \frac{A_{12}}{2c^2}(p_i - p_1)(p_f - p_2) \right\}, \tag{4.11}$$

where

$$A_1 = 1 - \frac{1}{2}\left(\frac{1 - M_1^* M_2}{1 - M_1 M_2}\right), \quad A_2 = 1 - \frac{1}{2}\left(\frac{1 - M_2^* M_1}{1 - M_1 M_2}\right), \quad A_{12} = \frac{2im_{qp}}{1 - M_1 M_2}. \tag{4.12}$$

This expression is more complicated than the ones we obtained in Sec. III. This is so because the classical trajectories involved are determined by mixed boundary conditions, i.e., their initial and final positions. Its structure is nevertheless still the same: it depends on differences between the values of the variables in the real trajectories and the corresponding coherent state labels. The most important property of this formula is that the initial momentum p_i is not known *a priori*. It must be determined as a function of the given parameters, and in fact there may be more than one possible value for it. Notice that since p_i and also p_f depend nontrivially on z_1, z_2 and T this formula is not a simple Gaussian as it may seem at first. Once again, even though the function S_r is evaluated at a real classical trajectory, it will in general be a complex number.

Notice that the differences $p_i - p_1$ and $p_f - p_2$ are always divided by the momentum uncertainty c. Therefore only classical trajectories whose initial momentum is within a distance c from p_1 may be important for the semiclassical propagator. The same reasoning applies to the final momentum. We see that the real trajectories to be used in this formalism must be compatible with the quantum uncertainty principle.

As a simple illustration of this formula, let us consider a harmonic oscillator of unit mass and angular frequency $\omega = c/b$. An initial condition (q', p') leads, after a time T, to the final values

$$q'' = q' \cos(\omega T) + \frac{p'}{\omega} \sin(\omega T), \quad p'' = -\omega q' \sin(\omega T) + p' \cos(\omega T). \tag{4.13}$$

If we impose that the trajectory must start in q_1 and end in q_2 then it is easy to see that there is only one possibility that satisfies these boundary conditions, for which

$$p_i = \frac{\omega(q_2 - q_1 \cos(\omega T))}{\sin(\omega T)}, \quad p_f = \frac{\omega(q_2 \cos(\omega T) - q_1)}{\sin(\omega T)}. \tag{4.14}$$

In this case we have $m_{qp} = \sin(\omega T)$ and $M_1 = M_2 = e^{i\omega T}$, which leads to $A_1 = A_2 = 1$ and $A_{12} = -e^{-i\omega T}$. The $e^{i\mathcal{I}_r/\hbar}$ term cancels the prefactor. Finally, using that $S_r = e^{-i\omega T}(q_1/b + ip_i/c)(q_2/b - ip_f/c)/2i$ we obtain

$$K_{q_1 q_2}(z_1, z_2, T) = \exp\left\{ -\tfrac{1}{2}(|z_1|^2 + |z_2|^2) + e^{-i\omega T} z_1 z_2^* \right\}, \tag{4.15}$$

which is precisely the exact result. This comes as no surprise since the exact action in this case is of second order to begin with and thus all semiclassical approximations we consider in this work will be exact.

B. From q_1 to p_2

We now consider the real trajectory that starts in $q'=q_1$ with a certain momentum $p'=p_i$ and, after a time T, is in a final point $q''=q_f$ with the momentum $p''=p_2$. We therefore treat q' and p'' as independent variables, in which case we have the following partial derivatives:

$$\frac{\partial p'}{\partial q'}=-\frac{c}{b}\frac{m_{pq}}{m_{pp}},\quad \frac{\partial p'}{\partial p''}=\frac{\partial q''}{\partial q'}=\frac{1}{m_{pp}},\quad \frac{\partial q''}{\partial p''}=\frac{b}{c}\frac{m_{qp}}{m_{pp}}. \tag{4.16}$$

We may calculate the action's first derivatives,

$$\left.\frac{\partial S}{\partial q'}\right|_r=-\frac{ic}{\sqrt{2}m_{pp}}[u_r''+v_r'(m_{pp}-im_{pq})],\qquad \left.\frac{\partial S}{\partial p''}\right|_r=\frac{b}{\sqrt{2}m_{pp}}[v_r'-u_r''(m_{pp}+im_{qp})], \tag{4.17}$$

and after writing

$$q'=q_1+\Delta q_1,\quad q''=q_f+\Delta q_f,\quad p'=p_i+\Delta p_i,\quad p''=p_2+\Delta p_2, \tag{4.18}$$

we may also obtain, using an expansion analogous to (4.2) and the boundary conditions, the relations

$$\frac{\Delta q_1}{b}=-\frac{im_{pp}}{c}\frac{[M_2(p_i-p_1)-ic(q_f-q_2)/b]}{1+M_2M_3^*}, \tag{4.19}$$

$$\frac{\Delta p_2}{c}=-\frac{im_{pp}}{b}\frac{[M_3(q_f-q_2)-ib/c(p_i-p_1)]}{1+M_2M_3^*}, \tag{4.20}$$

where M_2 has already been defined and $M_3=m_{pp}+im_{pq}$.

After calculating the action's second derivatives, the final result is

$$K_{q_1p_2}(z_1,z_2,T)=\sum_{\text{c.t}}\frac{\mathcal{N}}{\sqrt{(M_{vv})_r}}\exp\left\{\frac{i}{\hbar}(\mathcal{I}_r+S_r)-\frac{z_2}{\sqrt{2}b}(q_f-q_2)-\frac{iz_1^*}{\sqrt{2}c}(p_i-p_1)\right\}$$
$$\times\exp\left\{-\frac{B_1}{2c^2}(p_i-p_1)^2-\frac{B_2}{2b^2}(q_f-q_2)^2+\frac{B_{12}}{\hbar}(p_i-p_1)(q_f-q_2)\right\}, \tag{4.21}$$

where the coefficients are given by

$$B_1=1-\frac{1}{2}\left(\frac{1-M_2M_3}{1+M_2M_3^*}\right),\quad B_2=1-\frac{1}{2}\left(\frac{1-M_2^*M_3^*}{1+M_2M_3^*}\right),\quad B_{12}=\frac{im_{pp}}{1+M_2M_3^*}. \tag{4.22}$$

We see that the semiclassical propagator obtained is quite similar in structure to the one presented in Sec. IV A. Only this time we have position and momentum in a more equal footing. As p_i-p_1 is always divided by c and q_f-q_2 is always divided by b, we see that again the quantum uncertainties play a fundamental role in selecting the relevant classical trajectories.

C. From p_1 to q_2

It is also possible to fix the initial momentum as p_1 and then search for an initial position q_i such that the final position is q_2. In that case the final momentum will be some p_f. Proceeding in complete analogy with the previous cases, we take p' and q'' to be independent variables and calculate derivatives of q', p'' and S with respect to them. After obtaining the values of Δp_1 and Δq_2 in terms of (q_i-q_1) and (p_f-p_2) and expanding the action to second order, the final result will be

$$K_{p_1q_2}(z_1,z_2,T)=\sum_{\text{c.t}}\frac{\mathcal{N}}{\sqrt{(M_{vv})_r}}\exp\left\{\frac{i}{\hbar}(\mathcal{I}_r+S_r)+\frac{iz_2}{\sqrt{2}c}(p_f-p_2)-\frac{z_1^*}{\sqrt{2}b}(q_i-q_1)\right\}$$
$$\times\exp\left\{-\frac{C_1}{2b^2}(q_i-q_1)^2-\frac{C_2}{2c^2}(p_f-p_2)^2-\frac{C_{12}}{\hbar}(q_i-q_1)(p_f-p_2)\right\},\quad(4.23)$$

where the coefficients are given by

$$C_1=1-\frac{1}{2}\left(\frac{1-M_1^*M_4^*}{1+M_1M_4^*}\right),\quad C_2=1-\frac{1}{2}\left(\frac{1-M_1M_4}{1+M_1M_4^*}\right),\quad C_{12}=\frac{im_{qq}}{1+M_1M_4^*},\qquad(4.24)$$

with $M_4=m_{qq}+im_{pq}$.

D. From p_1 to p_2

Finally, we consider the trajectory determined by the pair (p_1,p_2). This has initial and final positions q_i and q_f, respectively. The procedure to obtain the semiclassical approximation is certainly clear by now, so it will not be repeated in any detail. The final result in this case will be

$$K_{p_1p_2}(z_1,z_2,T)=\sum_{\text{c.t}}\frac{\mathcal{N}}{\sqrt{(M_{vv})_r}}\exp\left\{\frac{i}{\hbar}(\mathcal{I}_r+S_r)-\frac{z_1^*}{\sqrt{2}b}(q_i-q_1)-\frac{z_2}{\sqrt{2}b}(q_f-q_2)\right\}$$
$$\times\exp\left\{-\frac{D_1}{2b^2}(q_i-q_1)^2-\frac{D_2}{2b^2}(q_f-q_2)^2-\frac{D_{12}}{b^2}(q_i-q_1)(q_f-q_2)\right\},\quad(4.25)$$

where the coefficients are given by

$$D_1=1-\frac{1}{2}\left(\frac{1-M_3M_4^*}{1-M_3^*M_4^*}\right),\quad D_2=1-\frac{1}{2}\left(\frac{1-M_3^*M_4}{1-M_3^*M_4^*}\right),\quad D_{12}=\frac{im_{pq}}{1-M_3^*M_4^*}.\qquad(4.26)$$

E. Summary of Sec. IV

In this section we have obtained four different semiclassical approximations to the quantum coherent state propagator that are based only on real trajectories. The trajectories considered share the property that they are not determined by initial or final values, but satisfy mixed boundary conditions. Therefore finding them in practice is not trivial, but is certainly easier than finding the original complex ones. All the semiclassical propagators obtained are in principle able to reproduce quantum effects such as interference, since there may be more than one classical trajectory involved. They will be affected by caustics just like the original formula (2.26), but the location of such caustics will change because $(M_{vv})_r$ is different for each one of them.

Which one of the several formulas obtained here and in Sec. III is more accurate will depend on the particular problem at hand. We have considered only initial and final coherent states with the same value of the parameter b, but a generalization of the semiclassical propagator was presented[27] for more general b's, and the calculations presented here may be adapted to that case with no essential difficulty. Let us suppose for a moment that the initial coherent state $|z_1\rangle$ has a position uncertainty b_1 while $|z_2\rangle$ has a position uncertainty b_2. If these numbers are small that means the states are very narrow in the position representation, while having a large uncertainty in momentum. In that case we conjecture that an approximation in the spirit of $K_{q_1q_2}$ would be the most effective one. If b_1 is small but b_2 is large, than $K_{q_1p_2}$ would be a better candidate, and so on. Of course for the free particle and the harmonic oscillator they are all exact, regardless of the values of b_1 and b_2.

In Sec. V, we present an application of the formalism just presented to a nonlinear system. The purpose is not to attempt an exhaustive investigation of the several possibilities, but rather to

illustrate the method in a simple case. We have chosen a system for which many analytical results are possible so that the main properties of the theory do not disappear under numerical calculations.

V. APPLICATION TO A NONLINEAR OSCILLATOR: SHORT TIME

We consider the nonlinear Hamiltonian

$$H = \hbar\omega(a^\dagger a)^2 = \frac{1}{\hbar\omega}\frac{(p^2+\omega^2q^2-\hbar\omega)^2}{4}, \tag{5.1}$$

which is diagonal in the usual number basis,

$$H|n\rangle = E_n|n\rangle = \hbar\omega n^2|n\rangle. \tag{5.2}$$

The quantum propagator in this case is quite simple:

$$K(z_1,z_2,T) = \langle z_2|e^{-iHT/\hbar}|z_1\rangle = \mathcal{N}\sum_{n=0}^{\infty}\frac{(z_1z_2^*)^n}{n!}e^{-in^2\omega T}. \tag{5.3}$$

We shall be interested, for simplicity, only in the diagonal case

$$K(z_1,z_1,T) = e^{-|z_1|^2}\sum_{n=0}^{\infty}\frac{|z_1|^{2n}}{n!}e^{-in^2\omega T}, \tag{5.4}$$

whose squared modulus is the return probability,

$$P(z_1,T) = |K(z_1,z_1,T)|^2. \tag{5.5}$$

This function is periodic with period $T_r=2\pi/\omega$. In the semiclassical limit the term that is responsible for the largest contribution to the sum in (5.4) is $n_0\approx|z_1|^2$. If we linearize the exponent in the vicinity of this term we have

$$P(z_1,T) \approx e^{-2|z_1|^2}\left|\sum_{n\approx n_0}\frac{|z_1|^{2n}}{n!}e^{2in_0n\omega T}\right|^2. \tag{5.6}$$

Notice that expression (5.6) has a distinct time scale,

$$T_c = \frac{\pi}{n_0\omega}. \tag{5.7}$$

The quantities T_r and T_c are usually called revival time and classical time.[28]

For short times, we can approximate $|K(z_1,T)|^2\approx 1-(\langle H^2\rangle-\langle H\rangle^2)T^2/\hbar^2$, where $\langle\cdot\rangle$ denotes an average value in the state $|z_1\rangle$. For the system in question, this gives

$$P(z_1,T) \approx 1-(4|z_1|^6+6|z_1|^4+|z_1|^2)\omega^2T^2. \tag{5.8}$$

Let us write $z_1=(q+ip)/\sqrt{2}$ and take for simplicity the value $q=0$. Since the movement in phase space has circular symmetry, this choice is of no fundamental importance. The short-time expansion (5.8) becomes simply

$$P(z_1,T) \approx 1-\tfrac{1}{2}(p^6+3p^4+p^2)T^2. \tag{5.9}$$

Let us now turn to the semiclassical approximation. From now on we set $\hbar=\omega=1$, which implies $b=c=1$. The smoothed Hamiltonian associated with (5.1) is

$$\mathcal{H} = \frac{(p^2+q^2)(p^2+q^2+2)}{4} = uv(uv+1), \tag{5.10}$$

and the corresponding Hamilton equations are

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial p} = \sigma p, \quad \dot{p} = -\frac{\partial \mathcal{H}}{\partial q} = -\sigma q, \tag{5.11}$$

where we have defined $\sigma = p^2+q^2+1$. If we note that $\{\sigma, \mathcal{H}\}=0$, and thus that σ is a constant of the motion, then it is clear that

$$q'' = q'\cos(\sigma t) + p'\sin(\sigma t), \quad p'' = p'\cos(\sigma t) - q'\sin(\sigma t). \tag{5.12}$$

We see that the classical trajectories have a period of motion that is energy-dependent and given by $2\pi/\sigma$. If we remember that $n_0+1/2=(q^2+p^2)/2$ we see that in the semiclassical limit this time scale becomes precisely T_c.

The tangent matrix that is associated with the classical trajectory that starts in (q',p') can be obtained by simply differentiating the equations of motion. We must remember that the angular frequency σ is not uniform. The result is

$$\begin{pmatrix} m_{qq} & m_{qp} \\ m_{pq} & m_{pp} \end{pmatrix} = \begin{pmatrix} \cos(\sigma t) & \sin(\sigma t) \\ -\sin(\sigma t) & \cos(\sigma t) \end{pmatrix} \begin{pmatrix} 1+2q'p't & 2p'^2 t \\ -2q'^2 t & 1-2q'p't \end{pmatrix}. \tag{5.13}$$

The action of such a trajectory is easily seen to be

$$S = \frac{(\sigma-1)^2 T}{4} - i\frac{(\sigma-1)}{2}, \tag{5.14}$$

while the extra term is

$$\mathcal{I} = (\sigma - 1/2)T. \tag{5.15}$$

The result of this semiclassical approximation based on complex trajectories will be given in Sec. VI.

A. The "leaving" and the "arriving" trajectories

The first possibility we consider is to approximate the return probability by using only the real trajectory that leaves the position $q=0$ with momentum p. The tangent matrix for that trajectory is

$$\begin{pmatrix} m_{qq} & m_{qp} \\ m_{pq} & m_{pp} \end{pmatrix} = \begin{pmatrix} \cos(\sigma t) & \sin(\sigma t) \\ -\sin(\sigma t) & \cos(\sigma t) \end{pmatrix} \begin{pmatrix} 1 & 2p^2 T \\ 0 & 1 \end{pmatrix}, \tag{5.16}$$

which gives the values

$$M_{uv} = -ip^2 T e^{-i\sigma T}, \quad M_{vv} = (1+ip^2 T)e^{i\sigma T}. \tag{5.17}$$

The angular frequency is $\sigma = p^2+1$ and the final points in phase space are $q_f = p\sin(\sigma T)$ and $p_f = p\cos(\sigma T)$. This corresponds to

$$u_r'' = (v_r'')^* = \frac{ip}{\sqrt{2}} e^{-i\sigma T}. \tag{5.18}$$

Inserting all this information, together with (5.14) and (5.15), into the formula (3.13) we have

$$K_{q_1p_1}(z_1,T)=\frac{1}{\sqrt{1+ip^2T}}\exp\left\{\frac{iT}{4}(p^4+2p^2)-ip^2e^{-i\sigma T/2}\sin(\sigma T/2)\right\}$$
$$\times\exp\left\{\frac{ip^4T}{(1+ip^2T)}e^{-i\sigma T}\sin^2(\sigma T/2)\right\}. \tag{5.19}$$

The first thing we note is that for $p=0$ we obtain the exact result $K=1$. Moreover, in the short time regime we can expand (5.19) and obtain

$$|K_{q_1p_1}(z_1,T)|^2\approx 1-\frac{1}{2}(p^6+3p^4+p^2)T^2 \quad \text{(short times)}, \tag{5.20}$$

which again reproduces the exact calculation. For later times we should not expect exact agreement.

Let us now turn to the "arriving" trajectory, the one that starts in q_i,p_i and arrives at the position $q=0$ with momentum p after a time T. The tangent matrix is less trivial than in the previous case, but in the end we get

$$M_{vu}=-ip^2Te^{-i\sigma T}, \quad M_{vv}=(1+ip^2T)e^{i\sigma T}. \tag{5.21}$$

Since q^2+p^2 is a conserved quantity, we have $\sigma=q_i^2+p_i^2+1=p^2+1$. After the whole calculation is done, we find out that $K_{q_2p_2}=K_{q_1p_1}$. This indicates that perhaps these two approximations will always have the same content of information, something that is not completely unexpected because of the dual role of $|z_1\rangle$ and $|z_2\rangle$ in the quantum propagator.

B. The $q_1\to q_2$ possibility

In that case the trajectories that enter the approximation have initial momentum given by

$$p_i\sin[(p_i^2+1)T]=0. \tag{5.22}$$

Of course one solution to this equation is

$$p_i(=p_f)=0, \tag{5.23}$$

in which case the particle simply stays still and $\sigma=1$. It is easy to see that for this trajectory the tangent matrix is very simple,

$$\begin{pmatrix} m_{qq} & m_{qp} \\ m_{pq} & m_{pp} \end{pmatrix}=\begin{pmatrix} \cos(T) & \sin(T) \\ -\sin(T) & \cos(T) \end{pmatrix}, \tag{5.24}$$

and therefore $M_1=M_2=M_{vv}=e^{iT}$. The contribution of this trajectory to the propagator is

$$K_0=\exp\{-ip^2\sin(T/2)e^{-iT/2}\}, \tag{5.25}$$

where we have used $S_r+\mathcal{I}_r=T/2$. Notice that for $p=0$ we again have the exact result $K_0=1$. We also note that the function $|K_0|^2$ has a period of 2π, which of course corresponds to the quantum revival time.

We now turn to the other solutions of Eq. (5.22). They are of the form

$$p_i^2(n)=\frac{2n\pi}{T}-1, \tag{5.26}$$

where n is an integer, which leads to $\sigma_n=2n\pi/T$. In this case we have less trivial trajectories, for which the tangent matrix is given by

$$\begin{pmatrix} m_{qq} & m_{qp} \\ m_{pq} & m_{pp} \end{pmatrix} = \begin{pmatrix} 1 & 2p_i^2 T \\ 0 & 1 \end{pmatrix}, \tag{5.27}$$

and we see that the prefactor is $M_{vv}=(1+ip_i^2T)$, while $M_1=M_2=-4p_i^4T^2$. The action and the extra term are given by $S_r=(p_i^4T-2ip_i^2)/4$ and $\mathcal{I}_r=(p_i^2+1/2)T$. The coefficients in (4.11) are

$$A_1 = A_2 = 1 + \frac{ip_i^2 T}{2(1+ip_i^2 T)}, \quad A_{12} = -\frac{1}{1+ip_i^2 T}. \tag{5.28}$$

After many simplifications, we obtain

$$K_{q_1 q_2} = \sum_{n=0}^{\infty} K_n, \tag{5.29}$$

where the contribution of the trajectory with label n (different from zero) is given by

$$K_n = \frac{1}{\sqrt{1+ip_i^2 T}} \exp\left\{ -\frac{ip_i^2 T}{1+ip_i^2 T}(p_i - p)^2 + \frac{iT}{4}(p_i^4 + 4p_i^2 + 2) \right\}. \tag{5.30}$$

Note that for short times $p_i(n)$ is very large, so K_n becomes negligible and K_0 gives the only contribution. However, it predicts the initial decay $|K_0|^2 \approx 1-2p^2T^2$, which is very slow compared to the exact calculation (5.9). The two results agree only for very small values of the momentum p.

Concerning the contributions K_n, we see that for a given instant of time the value of n that will contribute the most is that for which $p_i(n)$ is as close as possible to p, because of the Gaussian decay in (5.30). If we impose $p_i^2(n) \approx p^2$ we have $T \approx 2n\pi/(p^2+1)$, which means that the return probability has a maximum at the classical period, in agreement with the exact result.

C. The $q_1 \to p_2$ possibility

If we impose that the classical trajectory starts in $q=0$ with momentum p_i and ends at q_f with momentum p, we have

$$q_f = p_i \sin(\sigma T), \quad p = p_i \cos(\sigma T), \quad \sigma = p_i^2 + 1. \tag{5.31}$$

These transcendental equations have no explicit solution. If we confine ourselves to the short time regime, then we can write $p_i \approx p$ and $q_f \approx p(p^2+1)T$. The tangent matrix is given by

$$\begin{pmatrix} m_{qq} & m_{qp} \\ m_{pq} & m_{pp} \end{pmatrix} = \begin{pmatrix} \cos(\sigma t) & \sin(\sigma t) \\ -\sin(\sigma t) & \cos(\sigma t) \end{pmatrix} \begin{pmatrix} 1 & 2p_i^2 T \\ 0 & 1 \end{pmatrix}, \tag{5.32}$$

and we obtain $M_2=e^{i\sigma T}(1+2ip_i^2T)$ and $M_3=e^{-i\sigma T}-2p_i^2T$. Substituting this in (4.21), we obtain

$$|K_{q_1 p_2}|^2 \approx 1 - \left(p^6 + \frac{5}{2}p^4 + p^2 \right) T^2 \quad \text{(short times)}, \tag{5.33}$$

which decays faster than the exact result but is a better approximation than the one obtained using the $q_1 \to q_2$ trajectory. We see that the different approximations may lead to very different results.

D. The $p_1 \to q_2$ possibility

The equations of motion in this case are

$$0 = q_i \cos(\sigma T) + p \sin(\sigma T), \quad p_f = -q_i \sin(\sigma T) + p \cos(\sigma T), \quad \sigma = q_i^2 + p^2 + 1, \tag{5.34}$$

while the tangent matrix is

$$\begin{pmatrix} m_{qq} & m_{qp} \\ m_{pq} & m_{pp} \end{pmatrix} = \begin{pmatrix} \cos(\sigma t) & \sin(\sigma t) \\ -\sin(\sigma t) & \cos(\sigma t) \end{pmatrix} \begin{pmatrix} 1+2q_i pT & 2p^2 T \\ -2q_i^2 T & 1-2q_i pT \end{pmatrix}. \tag{5.35}$$

The situation here regarding solubility of the equations is even worse than in the previous case. Once again we restrict the analysis to the short time regime. Then it is possible to write the first equation as $q_i \approx -p\sigma T/2$ and find

$$q_i \approx -\frac{1}{2pT}(1-\sqrt{1-4p^2T^2(p^2+1)}), \tag{5.36}$$

which we substitute in the first equation to find p_f. Carrying out the whole calculation will give in the end

$$|K_{p_1 q_2}|^2 \approx 1-\frac{1}{2}(p^6+3p^4+p^2)T^2 \quad \text{(short times)}, \tag{5.37}$$

which agress with the exact result.

E. The $p_1 \to p_2$ possibility

Finally, in the last possibility we have

$$q_f = q_i \cos(\sigma T) + p \sin(\sigma T), \quad p = -q_i \sin(\sigma T) + p \cos(\sigma T), \quad \sigma = q_i^2 + p^2 + 1. \tag{5.38}$$

In the short time limit we have again

$$q_i \approx -\frac{1}{2pT}(1-\sqrt{1-4p^2T^2(p^2+1)}), \tag{5.39}$$

and the final result is

$$|K_{p_1 p_2}|^2 \approx 1-\frac{p^4}{2}T^2 \quad \text{(short times)}. \tag{5.40}$$

This is kind of intermediate between the result we found in Sec. V B and that of Secs. V C and V D.

VI. APPLICATION TO A NONLINEAR OSCILLATOR: NUMERICAL RESULTS

Before we consider the semiclassical approximations based on real trajectories for longer times, let us see how well the original one (2.26) compares to the exact result. This has been considered in detail in Ref. 29, so we just present the result. Given the initial condition $u'=z_1$, for each time T we must find a value for v' such that $v''=z_2^*=z_1^*$. This problem usually has more than one solution, and we must add their contributions coherently. In Fig. 1 we see the return probability as a function of time (in units of T_c) for the case $p=10$, which we have chosen to ensure that we are in the semiclassical limit. The corresponding classical period is $T_c \approx 0.062$. The exact and the semiclassical results are indistinguishable in this scale.

In Sec. V we saw how the different approximations based on real trajectories performed in the short time regime. The exact result was reproduced only by the "leaving" and the "arriving" formulas and by $K_{p_1 q_2}$. We now turn to the less simple case of arbitrary T, when the classical trajectories and the associated propagators must be computed numerically.

Let us start with the propagator $K_{q_1 p_1}$, which is based on a real periodic orbit. Its initial decay is exact, and we can see how well it does for later times in Fig. 2. It is able to reproduce the height of the peaks with great accuracy, but not their widths. Since there is never more than one contribution for each time, it never displays any interference effects.

This is not the case for $K_{q_1 q_2}$. We see from (5.29) and (5.30) that it consists in the sum of many contributions. We focus on the values $n=1, 2, 3$. Their individual contributions are depicted in Fig.

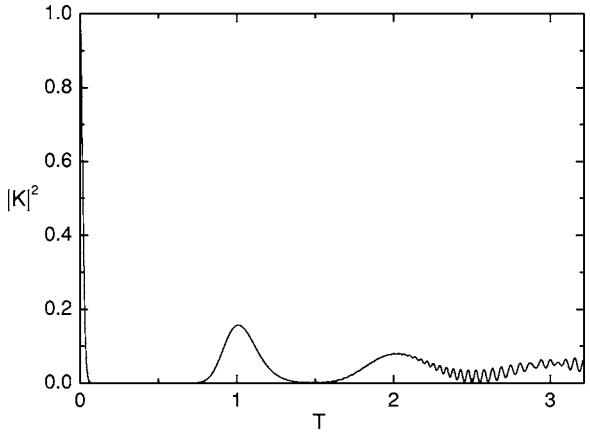

FIG. 1. Squared modulus of the exact propagator for $q=0$ and $p=10$. The semiclassical approximation based on complex trajectories is indistinguishable from it in this scale. Time is in units of the classical period.

3. Notice that the second and third peaks overlap. When we calculate the total propagator, this gives rise to interference. The final result is indistinguishable from the exact one (for $T>T_c/2$, because we have ignored K_0 which gives a bad initial decay).

So far the propagators could be obtained analytically. Since the calculation of $K_{q_1p_2}$ depends on the solution of the transcendental equation (5.31), we must resort to numerical routines. Let us try to find solutions to the second equation in (5.31) in the vicinity of the first period, $T\approx T_c$. In Fig. 4(a) we see that there are two solutions (solid lines) for $T<T_c$ and no solution at all for $T>T_c$. This is because the cosine function with a real argument is always less than unity, and thus p_i must always be greater than p. The complex solutions do not have this obstruction, as we can also see in Fig. 4(a) (dashed line), where we plot the real part of the complex momentum that satisfies the boundary conditions (2.11). Therefore the semiclassical approximation based on the complex trajectory can reproduce the whole peak, while $K_{q_1p_2}$ is discontinuous.

In Fig. 4(b) we see the squared modulus of the exact propagator and the values of $|K_{q_1p_2}|^2$ obtained using the two available real trajectories. Note that one should not add these results. They are independent and we may choose any of them, because both real trajectories are good approximations to the actual complex one (the real trajectories do not come from a saddle point approxi-

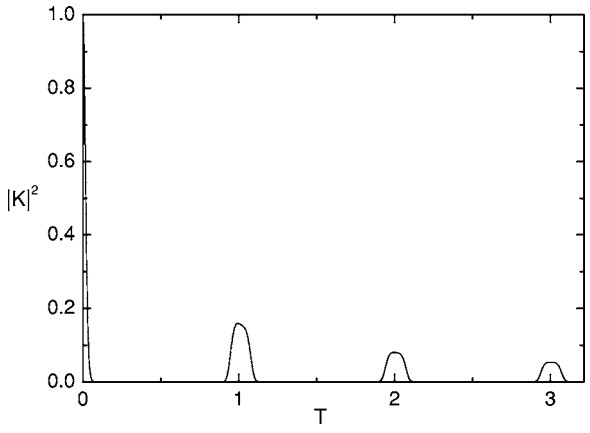

FIG. 2. The function $|K_{q_1p_1}|^2$ as a function of time. It reproduces well the height of the peaks, but not their widths, and shows no interference.

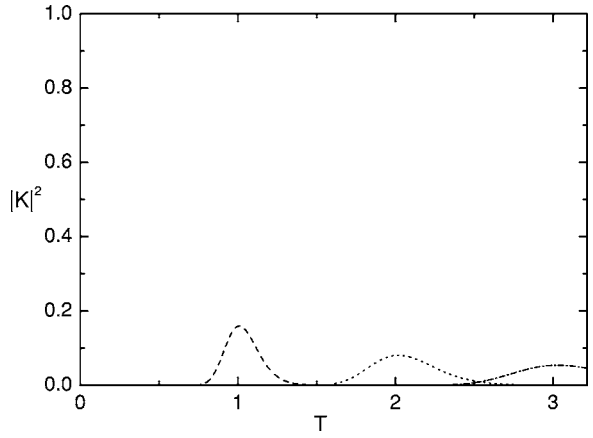

FIG. 3. The individual contributions $|K_n|^2$ for the approximation $K_{q_1q_2}$. We show the cases $n=1$, 2, and 3. When they are added there is interference, and the exact result of Fig. 1 is reproduced with extraordinary accuracy for $T>T_c/2$ (we have not included K_0 in the calculation).

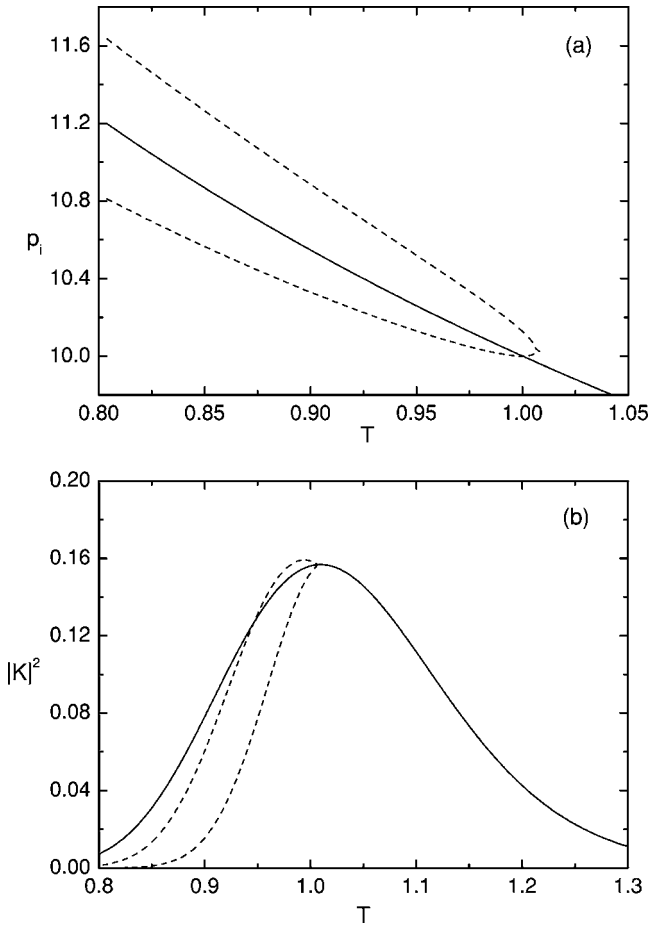

FIG. 4. Top panel: real solutions to the equation $p=p_i\cos((p_i^2+1)T)$ in the vicinity of the classical period (dashed lines). We also show the real part of the momentum for the complex trajectory (solid line). Bottom panel: approximation $|K_{q_1p_2}|^2$ (dashed lines) compared to the exact result (solid line). Since there are no real trajectories for $T>T_c$, the propagator becomes truncated. For $T<T_c$ there are two possibilities.

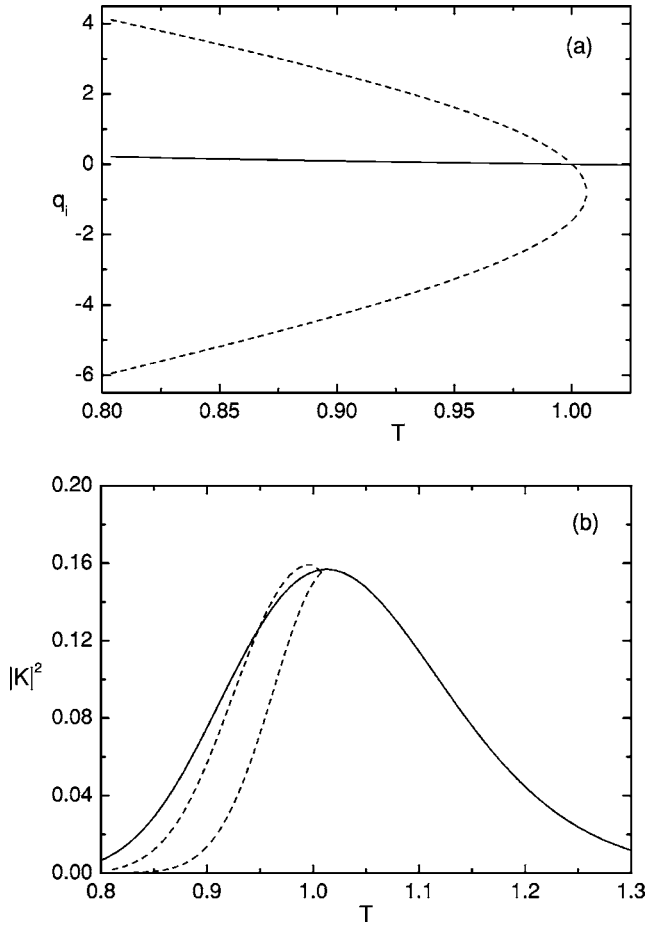

FIG. 5. Top panel: real solutions to the equation $0=q_i\cos(\sigma T)+p\cos(\sigma T)$, where $\sigma=q_i^2+p^2+1$, in the vicinity of the classical period (dashed lines). We also show the real part of the position for the complex trajectory (solid line). Bottom panel: approximation $|K_{p_1q_2}|^2$ (dashed lines) compared to the exact result (solid line). The situation is analogous to Fig. 4.

mation). As observed in Refs. 16 and 18, the mixed propagator $\langle \mathbf{x}|e^{-iHT/\hbar}|\mathbf{z}\rangle$ can also be discontinuous when calculated using real trajectories. But in that case there are caustics involved, while here we have an algebraic obstruction.

The discussion of the approximation $K_{p_1q_2}$ is quite similar to the above. The solutions to the first equation in (5.34) are shown in Fig. 5(a), where we also show the real part of the complex position that satisfies the boundary conditions (2.11). Again there is no solution for $T>T_c$ and the semiclassical propagator is discontinuous, as we appreciate in Fig. 5(b). The results are practically the same as in Fig. 4(b).

Finally, the propagator $K_{p_1p_2}$. This time we solve numerically the conditions (5.38) and find that there is a single real trajectory for $T<T_c$ and no one for $T>T_c$. The final result is in Fig. 6.

VII. CONCLUSIONS

Several approximations to the semiclassical coherent state propagator $\langle z_2|e^{-iHT/\hbar}|z_1\rangle$ were presented that are based solely on real classical trajectories. Two of these approximations do not involve mixed boundary conditions and thus are not hindered by the associated "root search" problem. The remaining four possibilities are based on trajectories that are determined by initial and final data, but since they are real for all times they are simpler to determine than the original complex ones.

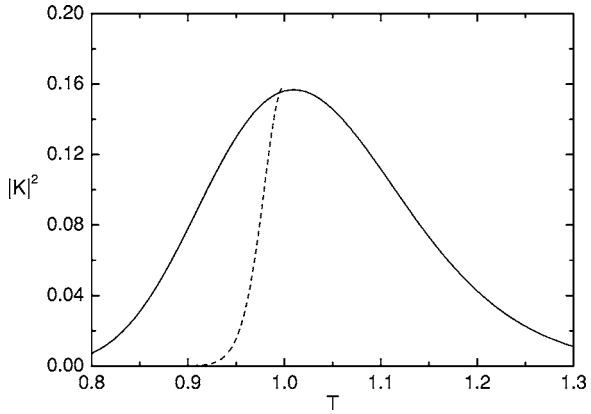

FIG. 6. Approximation $|K_{p_1p_2}|^2$ (dashed line) compared to the exact result (solid line). This time only one real trajectory exists for $T<T_c$, but again the propagator is truncated.

As a testing ground we have used the nonlinear system $H=(a^\dagger a)^2$. Only one of the approximations, namely $K_{q_1q_2}$, reproduced the exact result to the fine details. This is certainly due to the particular initial coherent state that was chosen, one corresponding to $q=0$ and $p=10$. Had we chosen for example $q=10$ and $p=0$ and then $K_{p_1p_2}$ would give excellent results. We could also consider a nondiagonal propagator, and in that case we would expect $K_{q_1p_2}$, for example, to improve its performance.

Straightforward extensions of this work include the already mentioned case of different position uncertainties (squeezed states) and also higher dimensional systems. It is also possible to fix the time T and the initial state $|z_1\rangle$ and to regard $|K(z_1,z_2,T)|^2$ as a Husimi function defined in the z_2 plane. This is technically more difficult than what we have presented here, because it involves finding classical trajectories—usually more than one—parametrized by points in the plane.

Similar results can be obtained for the semiclassical $SU(2)$, or spin, coherent state propagator, even though the introduction of position and momentum variables in that case is not as natural. The associated phase space is also two-dimensional, but since it has curvature the calculations may be a little more involved. The same may be said about the semiclassical $SU(1,1)$ coherent state propagator. Since these groups have wide applications, it would be interesting to also have the corresponding approximations based on real trajectories.

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Teleportation schemes in infinite dimensional Hilbert spaces

Karl-Heinz Fichtner[a)]
Institut für Angewandte Mathematik, Friedrich-Schiller-Unversität Jena, 07740 Jena, Germany

Wolfgang Freudenberg[b)]
Institut für Mathematik, PF 101344, Brandenburgische Technische Universität Cottbus, 03013 Cottbus, Germany

Masanori Ohya[c)]
Department of Information Science, Tokyo University of Science, Noda City, Chiba 278-8510, Japan

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The success of quantum mechanics is due to the discovery that nature is described in infinite dimension Hilbert spaces, so that it is desirable to demonstrate the quantum teleportation process in a certain infinite dimensional Hilbert space. We describe the teleportation process in an infinite dimensional Hilbert space by giving simple examples. © *2005 American Institute of Physics.*
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I. INTRODUCTION

In quantum communication theory, we code information by quantum states and send it through a quantum device that is properly designed. If one can send any quantum state from an input system to an output system as it is, that is, if one can find such a method sending an input state without changing it, then it will be an ultimate way for information transmission. It is in quantum teleportation that we can discuss such an ultimate communication system.

The problem of quantum teleportation is whether there exists a physical device and a key (or a set of keys) by which a quantum state attached to a sender (Alice) is completely transmitted and a receiver (Bob) can reconstruct the state sent. Bennett *et al.*[1] showed that such teleportation is possible through a device (channel) made from proper (EPR) entangled states of Bell basis. The basic idea behind their discussion is to divide the information encoded in the state into two parts, classical and quantum, and send them through different channels, a classical channel and an EPR channel. The classical channel is nothing but a simple correspondence between sender and receiver, and the EPR channel is constructed by using a certain entangled state. However the EPR channel is not so stable due to quick decoherence. Fichtner and Ohya[2,3] studied the quantum teleportation by means of general beam splitting processes in Bose Fock space so that it contains the EPR channel as a special case, and they constructed a stable teleportation process with coherent entangled states.

However, all these discussions have been based on finite dimensionality of the Hilbert spaces, attached to Alice and Bob. As is well known, success of quantum mechanics is due to the discovery that nature is described in infinite dimension Hilbert spaces, so that it is desirable to demonstrate the quantum teleportation process in a certain infinite dimensional Hilbert space. This paper is a trial to describe the teleportation process in an infinite dimensional Hilbert space by

[a)]Electronic mail: fichtner@mathematik.uni-jena.de
[b)]Electronic mail: freudenberg@math.tu-cottbus.de
[c)]Electronic mail: ohya@is.noda.tus.ac.jp

giving simple examples. In Sec. II, we fix the notations based on Fock space discussion of the series of papers.[2–4] In Sec. III, the channel expression of the teleportation is reviewed and the entanglement between Alice and Bob is constructed by an isometry operator, on which an operator expression of the teleportation channel is given, and some extreme cases of the teleportation are considered. To be closer to usual teleportation schemes and to get simple and explicit results we consider in Sec. IV the case of product states. In Sec. V, the existence of unitary keys is discussed.

II. BASIC NOTIONS AND NOTATIONS

We consider three complex Hilbert spaces $\mathcal{H}_1$, $\mathcal{H}_2$, and $\mathcal{H}_3$. To Alice there are attached the Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. Alice wants to teleportate a state ρ on $\mathcal{H}_1$ to Bob to whom there is attached the Hilbert space $\mathcal{H}_3$. Usually it is assumed that all three Hilbert spaces are finite-dimensional ones. This is also necessary for obtaining perfect teleportation. In the present article we will consider the case of Hilbert spaces being separable but not necessarily finite dimensional. We assume that all three spaces are either infinite-dimensional separable Hilbert spaces or finite-dimensional ones with same finite dimension. The paper continues and generalizes results obtained in Refs. 2–4.

Let us be given orthonormal bases,

$$(\xi_k^1)_{k\in G}, \quad (\xi_k^2)_{k\in G}, \quad (\xi_k^3)_{k\in G}, \tag{1}$$

in $\mathcal{H}_1$, $\mathcal{H}_2$, and $\mathcal{H}_3$ where the at most countable index set G is an abelian (additive) group with operation $\oplus$. An important case is that G is the set of integers $\mathbb{Z}$ where the group operation $\oplus$ will be usual addition. Since we need the structure of a group it is more convenient for our purposes to choose only orthonormal bases consisting of two-sided infinite sequences. To include usual teleportation models (with finite index space G) we consider also the case $G=\{1,\ldots,N\}$ with N belonging to the set $\mathbb{N}$ of natural numbers. In this case the operation $\oplus: G\times G\to G$ is defined by $k\oplus l := (k+l) \bmod N$. The operation inverse to $\oplus$ we denote by $\ominus$. In the latter case $k\ominus l=k-l$ if $k>l$ and $k\ominus l=k-l+N$ if $k\leqslant l$.

The algebra of all bounded linear operators on a Hilbert space $\mathcal{H}$ we will denote by $\mathcal{B}(\mathcal{H})$. Throughout this article we will assume that all states on a Hilbert space $\mathcal{H}$ are normal states (on $\mathcal{B}(\mathcal{H})$). The set of all normal states we denote by $\mathcal{S}(\mathcal{H})$.

Let $V\in\mathcal{B}(\mathcal{H}_2)$ be an arbitrary unitary operator. Consequently, the sequence $(\eta_n)_{n\in G}$ with $\eta_n := V\xi_n^2, n\in G$ is a second orthonormal basis in $\mathcal{H}_2$. Thus there exists a sequence $(b_{kl})_{k,l\in G}$ such that

$$\eta_k = \sum_{l\in G} b_{kl}\xi_l^2 \quad (k\in G). \tag{2}$$

Obviously, the sequence $(b_{kl})_{k,l\in G}$ has to fulfill

$$\sum_{l\in G} \overline{b_{kl}} b_{ml} = \delta_{k,m} \quad (k,m\in G), \tag{3}$$

where $\delta_{k,m}$ denotes the Kronecker symbol. Observe that for all $m,k\in G$ it holds $\langle \eta_m, \xi_k^2\rangle = \overline{b_{mk}}$. Consequently, we obtain

$$\xi_k^2 = \sum_{m\in G} \overline{b_{mk}}\eta_m \quad (k\in G). \tag{4}$$

Since V^* is again unitary and $\xi_n^2 = V^*\eta_n$ we also have

$$\sum_{l\in G} \overline{b_{lk}} b_{lm} = \delta_{k,m} \quad (k,m\in G). \tag{5}$$

Remark: To simplify notations only if there appear ambiguities we will separate multiple indices by "commas," i.e., usually we write b_{kl} instead of $b_{k,l}$.

Further, we consider a sequence $(U_m)_{m\in G}$ of unitary operators on $\mathcal{H}_2$ acting as shift operators on the elements of the (original) basis:

$$U_m\xi_k^2 = \xi_{k\oplus m}^2 \quad (m,k \in G). \tag{6}$$

The Hilbert space $\mathcal{H}_2$ is connected by simple isometries S_1 to $\mathcal{H}_1$ and S_3 to $\mathcal{H}_3$:

$$S_1{:}\mathcal{H}_2 \to \mathcal{H}_1 \otimes \mathcal{H}_2, \quad S_1(\xi_k^2) = \xi_k^1 \otimes \xi_k^2 \quad (k \in G), \tag{7}$$

$$S_3{:}\mathcal{H}_2 \to \mathcal{H}_2 \otimes \mathcal{H}_3, \quad S_3(\xi_k^2) = \xi_k^2 \otimes \xi_k^3 \quad (k \in G). \tag{8}$$

Finally, we construct a new basis in $\mathcal{H}_1 \otimes \mathcal{H}_2$ by setting

$$\xi_{km} = (\mathbb{1} \otimes U_m)S_1\eta_k = (\mathbb{1} \otimes U_m)S_1V\xi_k^2 \quad (k,m \in G), \tag{9}$$

where $\mathbb{1}$ denotes the identical operator (from the context it always will be clear on which space $\mathbb{1}$ operates). Observe that for $k,m \in G$

$$\xi_{km} = (\mathbb{1} \otimes U_m)\sum_{l\in G} b_{kl}(\xi_l^1 \otimes \xi_l^2) = \sum_{l\in G} b_{kl}(\xi_l^1 \otimes \xi_{l\oplus m}^2). \tag{10}$$

Proposition 1: The sequence $(\xi_{km})_{k,m\in G}$ is an orthonormal basis in $\mathcal{H}_1 \otimes \mathcal{H}_2$.

Proof: For $n,m,r,s \in G$ we get using (10) and (3)

$$\begin{aligned}\langle \xi_{nm}, \xi_{rs}\rangle &= \sum_{k,l\in G} \overline{b_{nk}} b_{rl}\langle \xi_k^1 \otimes \xi_{k\oplus m}^2, \xi_l^1 \otimes \xi_{l\oplus s}^2\rangle = \sum_{k,l\in G} \overline{b_{nk}} b_{rl}\langle \xi_k^1, \xi_l^1\rangle\langle \xi_{k\oplus m}^2, \xi_{l\oplus s}^2\rangle \\ &= \sum_{k\in G} \overline{b_{nk}} b_{rk}\langle \xi_{k\oplus m}^2, \xi_{k\oplus s}^2\rangle = \delta_{n,r}\cdot\delta_{m,s}.\end{aligned}$$

Thus $(\xi_{km})_{k,m\in G}$ is an orthonormal system in $\mathcal{H}_1 \otimes \mathcal{H}_2$.

To prove completeness we check whether the Parseval equality

$$\|\Phi\|^2 = \sum_{n,m\in G} |\langle \Phi, \xi_{nm}\rangle|^2$$

holds for all $\Phi \in \mathcal{H}_1 \otimes \mathcal{H}_2$. Let

$$\Phi = \sum_{r,s\in G} \alpha_{rs}\xi_r^1 \otimes \xi_s^2. \tag{11}$$

Then

$$\langle \Phi, \xi_{nm}\rangle = \sum_{r,s,k\in G} \overline{\alpha_{rs}} b_{nk}\langle \xi_r^1 \otimes \xi_s^2, \xi_k^1 \otimes \xi_{k\oplus m}^2\rangle = \sum_{r,s\in G} \overline{\alpha_{rs}} b_{nr}\langle \xi_s^2, \xi_{r\oplus m}^2\rangle = \sum_{r\in G} \overline{\alpha_{r,r\oplus m}} b_{nr}.$$

Using (5) this implies

$$\begin{aligned}\sum_{n,m\in G} |\langle \Phi, \xi_{nm}\rangle|^2 &= \sum_{n,m,r,s\in G} \overline{\alpha_{s,s\oplus m}}\alpha_{r,r\oplus m}\overline{b_{nr}} b_{ns} = \sum_{m,r,s\in G} \overline{\alpha_{s,s\oplus m}}\alpha_{r,r\oplus m}\sum_{n\in G} \overline{b_{nr}} b_{ns} \\ &= \sum_{m,r,s\in G} \overline{\alpha_{s,s\oplus m}}\alpha_{r,r\oplus m}\delta_{r,s} = \sum_{m,r\in G} |\alpha_{r,r\oplus m}|^2 = \sum_{m,r\in G} |\alpha_{r,m}|^2 = \|\Phi\|^2.\end{aligned}$$

This ends the proof. □

We denote by $F_{nm} \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ the projection onto ξ_{nm}, i.e.,

$$F_{nm} := |\xi_{nm}\rangle\langle \xi_{nm}| = \langle \xi_{nm}, \cdot\rangle\xi_{nm} \quad (n,m \in G). \tag{12}$$

Remark: We will use as well the "scalar product" notation as also the "bra and ket" symbols.

However, using the symbol $|\Phi\rangle$ let us make the convention that the symbol has to denote the normalization of the vector Φ, i.e.,

$$|\Phi\rangle := \frac{\Phi}{\|\Phi\|}. \tag{13}$$

Observe that for $\Phi \in \mathcal{H}_1 \otimes \mathcal{H}_2$ given by (11) and for all $n,m \in G$ one obtains

$$\begin{aligned} F_{nm}\Phi &= \langle \xi_{nm}, \Phi\rangle \xi_{nm} = \sum_{k\in G} \overline{b_{nk}} \langle \xi_k^1 \otimes \xi_{k\oplus m}^2, \Phi\rangle \xi_{nm} = \sum_{k,r,s\in G} \overline{b_{nk}} \alpha_{rs} \langle \xi_k^1 \otimes \xi_{k\oplus m}^2, \xi_r^1 \otimes \xi_s^2\rangle \xi_{nm} \\ &= \left(\sum_{k\in G} \overline{b_{nk}} \alpha_{k,k\oplus m} \right) \xi_{nm}. \end{aligned} \tag{14}$$

Especially,

$$F_{nm}(\xi_r^1 \otimes \xi_s^2) = \delta_{s,r\oplus m} \cdot \overline{b_{nr}} \xi_{nm}. \tag{15}$$

In the subsequent sections we investigate concrete teleportation channels. For this we need an explicit expression for $(F_{nm} \otimes \mathbb{1})(\mathbb{1} \otimes S_3)$ which maps $\mathcal{H}_1 \otimes \mathcal{H}_2$ into $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$.

Proposition 2: Let $\Phi \in \mathcal{H}_1 \otimes \mathcal{H}_2$ be given by (11). For all $n,m \in G$ it holds

$$(F_{nm} \otimes \mathbb{1})(\mathbb{1} \otimes S_3)\Phi = \xi_{nm} \otimes \sum_{r\in G} \overline{b_{nr}} \alpha_{r,r\oplus m} \xi_{r\oplus m}^3. \tag{16}$$

Proof: Using definition (8) of the imbedding operator S_3 and (15) we obtain for all $n,m \in G$

$$\begin{aligned} (F_{nm} \otimes \mathbb{1})(\mathbb{1} \otimes S_3)\Phi &= \sum_{r,s\in G} \alpha_{rs} (F_{nm} \otimes \mathbb{1})(\mathbb{1} \otimes S_3) \xi_r^1 \otimes \xi_s^2 = \sum_{r,s\in G} \alpha_{rs} (F_{nm} \otimes \mathbb{1}) \xi_r^1 \otimes \xi_s^2 \otimes \xi_s^3 \\ &= \sum_{r,s\in G} \alpha_{rs} \overline{b_{nr}} \xi_{nm} \otimes \xi_s^3 \cdot \delta_{s,r\oplus m} = \sum_{r\in G} \alpha_{r,r\oplus m} \overline{b_{nr}} \xi_{nm} \otimes \xi_{r\oplus m}^3. \end{aligned}$$

This proves (16). □

Corollary 3: Let $\Phi \in \mathcal{H}_1 \otimes \mathcal{H}_2$ be given by (11) and assume $\|\Phi\| = 1$. For all $n,m \in G$ it holds

$$(F_{nm} \otimes \mathbb{1})(\mathbb{1} \otimes S_3)|\Phi\rangle\langle\Phi|(\mathbb{1} \otimes S_3^*)(F_{nm} \otimes \mathbb{1}) = F_{nm} \otimes \langle \Psi_{nm}, \cdot \rangle \Psi_{nm} \tag{17}$$

with

$$\Psi_{nm} = \sum_{r\in G} \overline{b_{nr}} \alpha_{r,r\oplus m} \xi_{r\oplus m}^3. \tag{18}$$

Proof: Immediately from Proposition 2 we obtain

$$\begin{aligned} (F_{nm} \otimes \mathbb{1})(\mathbb{1} \otimes S_3)|\Phi\rangle\langle\Phi|(\mathbb{1} \otimes S_3^*)(F_{nm} \otimes \mathbb{1}) &= \left\langle \sum_{r\in G} \alpha_{r,r\oplus m} \overline{b_{nr}} \xi_{nm} \otimes \xi_{r\oplus m}^3, \cdot \right\rangle \sum_{s\in G} \alpha_{s,s\oplus m} \overline{b_{ns}} \xi_{nm} \\ &\otimes \xi_{s\oplus m}^3 = |\xi_{nm}\rangle\langle\xi_{nm}| \\ &\otimes \left\langle \sum_{r\in G} \alpha_{r,r\oplus m} \overline{b_{nr}} \xi_{r\oplus m}^3, \cdot \right\rangle \sum_{s\in G} \alpha_{s,s\oplus m} \overline{b_{ns}} \xi_{s\oplus m}^3. \end{aligned}$$

This proves (17). □

Corollary 3 allows us to get explicit formulas for

$$(F_{nm} \otimes \mathbb{1})(\mathbb{1} \otimes S_3)\varkappa(\mathbb{1} \otimes S_3^*)(F_{nm} \otimes \mathbb{1}),$$

where $\varkappa$ is a normal state on $\mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$.

Let $\varkappa$ be given in the form

$$\varkappa = \sum_{u,v \in G} \lambda_{uv} |\Phi_{uv}\rangle\langle\Phi_{uv}| \tag{19}$$

with $(\Phi_{uv})_{u,v \in G}$ being an orthonormal sequence in $\mathcal{H}_1 \otimes \mathcal{H}_2$,

$$\Phi_{uv} = \sum_{r,s \in G} \alpha_{uvrs} \xi^1_r \otimes \xi^2_s \tag{20}$$

and $(\lambda_{uv})_{u,v \in G}$ fulfilling

$$\sum_{u,v \in G} \lambda_{uv} = 1, \quad \lambda_{uv} \geqslant 0. \tag{21}$$

Of course, we have for all $u, \tilde{u}, v, \tilde{v} \in G$

$$\sum_{r,s \in G} \overline{\alpha_{uvrs}} \alpha_{\tilde{u}\tilde{v}rs} = \delta_{u,\tilde{u}} \cdot \delta_{v,\tilde{v}}. \tag{22}$$

As an immediate consequence of Corollary 3 we obtain the following result.

Proposition 4: Let $\varkappa$ be given by (19). For all $n, m \in G$ it holds

$$\begin{aligned}(F_{nm} \otimes \mathbb{1})(\mathbb{1} \otimes S_3)\varkappa(\mathbb{1} \otimes S_3^*)(F_{nm} \otimes \mathbb{1}) &= F_{nm} \otimes \sum_{u,v \in G} \lambda_{uv} \langle \Psi_{uvnm}, \cdot \rangle \Psi_{uvnm} \\ &= F_{nm} \otimes \sum_{u,v \in G} \lambda_{uv} \|\Psi_{uvnm}\|^2 \cdot |\Psi_{uvnm}\rangle\langle\Psi_{uvnm}| \end{aligned} \tag{23}$$

with

$$\Psi_{uvnm} = \sum_{r \in G} \overline{b_{nr}} \alpha_{uvr,r\oplus m} \xi^3_{r\oplus m}. \tag{24}$$

Remark: Observe that the vectors Ψ_{uvnm} usually are not normalized. Further, in general the sequence $(\Psi_{uvnm})_{u,v \in G}$ is not an orthogonal one.

III. THE TELEPORTATION CHANNEL

A. The measurement

Now we apply the model which was used in several papers[2,3,5] for the description of a teleportation scheme. The measurement will be done with the operator

$$F = \sum_{n,m \in G} z_{nm} F_{nm}, \tag{25}$$

where $(z_{nm})_{n,m \in G}$ is a sequence of real numbers and $(F_{nm})_{n,m \in G}$ is the family of orthogonal projections on $\mathcal{H}_1 \otimes \mathcal{H}_2$ introduced in Sec. II (cf. (12) and (10)). In the above-mentioned articles one considers the case of a given state ρ on $\mathcal{H}_1$ (that has to be teleportated to Bob) and an entangled state σ on $\mathcal{H}_2 \otimes \mathcal{H}_3$. Thus the whole system is prepared in the state $\rho \otimes \sigma$. Alice makes a measurement (restricted to $\mathcal{H}_1 \otimes \mathcal{H}_2$) with the operator F given by (25), i.e., the operator $F \otimes \mathbb{1}$ is applied to the system being in the state $\rho \otimes \sigma$. As the result of the measurement Alice obtains a value z_{nm} for some $n, m \in G$. Consequently, after the measurement the whole system will be in the state θ_{nm} on $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$ given by

$$\theta_{nm} := \frac{(F_{nm} \otimes \mathbb{1})\rho \otimes \sigma(F_{nm} \otimes \mathbb{1})}{\mathrm{tr}((F_{nm} \otimes \mathbb{1})\rho \otimes \sigma(F_{nm} \otimes \mathbb{1}))}, \tag{26}$$

where tr denotes the full trace with respect to $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$. Bob who is informed about the result of the measurement controls the state $\tilde{\Lambda}_{nm}(\rho)$ on $\mathcal{H}_3$ being the partial trace of θ_{nm} with respect to $\mathcal{H}_1 \otimes \mathcal{H}_2$:

$$\tilde{\Lambda}_{nm}(\rho) := \mathrm{tr}_{12}(\theta_{nm}) = \frac{\mathrm{tr}_{12}((F_{nm}\otimes \mathbb{1})\rho\otimes\sigma(F_{nm}\otimes\mathbb{1}))}{\mathrm{tr}((F_{nm}\otimes\mathbb{1})\rho\otimes\sigma(F_{nm}\otimes\mathbb{1}))}, \tag{27}$$

where tr_{12} denotes the partial trace on $\mathcal{H}_1\otimes\mathcal{H}_2$. Of course we have to assume that the denominator in (26), respectively, in (27) is nonzero. Otherwise, the left-hand side has to be set equal to zero. The mapping $\tilde{\Lambda}_{nm}:\mathcal{S}(\mathcal{H}_1)\to\mathcal{S}(\mathcal{H}_3)$ is called a *teleportation channel*.

The teleportation works perfectly if Bob is able to reconstruct the initial state ρ from $\tilde{\Lambda}_{nm}(\rho)$. We will return to this question in the subsequent sections. Teleportation channels $\tilde{\Lambda}_{nm}$ of the above-mentioned type might be useful also for modeling other transformations of states. For instance in Ref. 4 we proposed an extremely simplified model of certain recognition processes based on a teleportation channel. In this model the spaces $\mathcal{H}_1$, $\mathcal{H}_2$, and $\mathcal{H}_3$ represent the processing part (brain), the memory before and after recognition.

B. The entanglement

Instead of the state $\rho\otimes\sigma$ on $\mathcal{H}_1\otimes\mathcal{H}_2\otimes\mathcal{H}_3$ we will consider now states of the form

$$(\mathbb{1}\otimes S_3)\varkappa(\mathbb{1}\otimes S_3^*) \tag{28}$$

with $\varkappa$ being a state on $\mathcal{H}_1\otimes\mathcal{H}_2$ and S_3 isometry (8) coupling $\mathcal{H}_1$ to $\mathcal{H}_3$. The simple entanglement between $\mathcal{H}_2$ and $\mathcal{H}_3$ is achieved just by applying S_3. Especially, if $\varkappa$ has the form $\varkappa=\rho^1\otimes\rho^2$ with ρ^j being a state on $\mathcal{H}_j$, $j=1,2$ then using the above cited notations from Refs. 2 and 3 we get $\rho=\rho^1$ and $\sigma=S_3\rho^2S_3^*$. This case of $\varkappa$ being a product state we will discuss in Sec. IV.

We will consider now the channel $\Lambda_{nm}:\mathcal{S}(\mathcal{H}_1\otimes\mathcal{H}_2)\to\mathcal{S}(\mathcal{H}_3)$ given by

$$\Lambda_{nm}(\varkappa) = \frac{\mathrm{tr}_{1,2}((F_{nm}\otimes\mathbb{1})(\mathbb{1}\otimes S_3)\varkappa(\mathbb{1}\otimes S_3^*)(F_{nm}\otimes\mathbb{1}))}{\mathrm{tr}((F_{nm}\otimes\mathbb{1})(\mathbb{1}\otimes S_3)\varkappa(\mathbb{1}\otimes S_3^*)(F_{nm}\otimes\mathbb{1}))}, \tag{29}$$

where as in (27) tr_{12} denotes the partial trace with respect to $\mathcal{H}_1\otimes\mathcal{H}_2$ and tr the full trace on $\mathcal{H}_1\otimes\mathcal{H}_2\otimes\mathcal{H}_3$. Again we have to assume that the denominator in (29) is greater than zero. Otherwise we set $\Lambda_{nm}(\varkappa)=0$. Observe that for product states $\varkappa=\rho\otimes\sigma$ one has the relation $\tilde{\Lambda}_{nm}(\rho)=\Lambda_{nm}(\rho\otimes\sigma)$.

Remark: Since $\mathrm{tr}_{1,2}((F_{nm}\otimes\mathbb{1})(\mathbb{1}\otimes S_3)\varkappa(\mathbb{1}\otimes S_3^*)(F_{nm}\otimes\mathbb{1}))$ is a positive linear functional on $\mathcal{H}_3$ the denominator in (29) can be equal to zero only if this functional is zero. In other words, in this case no information about the measured value z_{nm} can be transmitted to Bob (in a brain model this would mean that no information about the input signal will be stored in the memory). The following result is an immediate consequence of Proposition 4.

Theorem 5: *Let $\varkappa$ be a state on $\mathcal{H}_1\otimes\mathcal{H}_2$ given by (19)–(21). Then for all $n,m\in G$*

$$\Lambda_{nm}(\varkappa) = \frac{\sum_{u,v\in G}\lambda_{uv}\langle\Psi_{uvnm},\cdot\rangle\Psi_{uvnm}}{\mathrm{tr}_3\left(\sum_{u,v\in G}\lambda_{uv}\langle\Psi_{uvnm},\cdot\rangle\Psi_{uvnm}\right)} \tag{30}$$

where $\Psi_{uvnm}\in\mathcal{H}_3$ is given by (24), and $\Lambda_{nm}(\varkappa)$ has to be set equal to zero if the denominator in (30) is equal to zero (tr_3 denotes the trace in $\mathcal{H}_3$).

Sometimes it is more convenient (cf. the second remark in this article) to write (30) in the form

$$\Lambda_{nm}(\varkappa) = \frac{\sum_{u,v\in G}\lambda_{uv}\|\Psi_{uvnm}\|^2|\Psi_{uvnm}\rangle\langle\Psi_{uvnm}|}{\mathrm{tr}\left(\sum_{u,v\in G}\lambda_{uv}\|\Psi_{uvnm}\|^2|\Psi_{uvnm}\rangle\langle\Psi_{uvnm}|\right)}. \tag{31}$$

Of course, mixed states are not necessarily transformed into mixed ones—possibly there is only one pair u,v such that $\|\Psi_{uvnm}\|>0$. However, immediately from (30) we may conclude the following proposition.

Proposition 6: If $\varkappa$ is a pure state on $\mathcal{H}_1 \otimes \mathcal{H}_2$ then $\Lambda_{nm}(\varkappa)$ is a pure state on $\mathcal{H}_3$ or equal to zero.

C. Examples

Example 1: Let $\varkappa = |\Phi\rangle\langle\Phi|$ be a pure state on $\mathcal{H}_1 \otimes \mathcal{H}_2$, $\|\Phi\| = 1$, $\Phi = \Sigma_{r,s \in G} \alpha_{rs} \xi_r^1 \otimes \xi_s^2$. Then we obtain

$$\Lambda_{nm}(\varkappa) = \frac{1}{\|\Psi_{nm}\|^2} \langle \Psi_{nm}, \cdot \rangle \Psi_{nm} = |\Psi_{nm}\rangle\langle\Psi_{nm}|$$

with

$$\Psi_{nm} = \sum_{r \in G} \overline{b_{nr}} \alpha_{r,r \oplus m} \xi_{r \oplus m}^3,$$

provided $\|\Psi_{nm}\| > 0$. Especially, for $\varkappa = |\Phi\rangle\langle\Phi|$ with $\Phi = \xi_r^1 \otimes \xi_s^2$ we get

$$\Lambda_{nm}(\varkappa) = |\xi_{r \oplus m}^3\rangle\langle\xi_{r \oplus m}^3|$$

provided $b_{n,s \ominus m} \neq 0$.

Let us discuss this result. Measuring the value z_{nm} means that there was made the projection onto $\xi_{nm} = \Sigma_{r \in G} b_{nr} (\xi_r^1 \otimes \xi_{r \oplus m}^2)$. Observe that $\Sigma_{r \in G} |b_{nr}|^2 |\alpha_{r,r \oplus m}|^2 = \|\Psi_{nm}\|^2 > 0$ if and only if there exists at least one $r \in G$ such that $b_{nr} \neq 0$ and $\alpha_{r,r \oplus m} \neq 0$. Obviously, there exists $r \in G$ such that $b_{nr} \neq 0$. The number $\alpha_{r,r \oplus m}$ is the coefficient of the basis element $\xi_r^1 \otimes \xi_{r \oplus m}^2$ in the expansion of $\varkappa = |\Phi\rangle\langle\Phi|$. So only if $\varkappa$ is receptive for the signal $\xi_r^1 \otimes \xi_{r \oplus m}^2$ for at least one admissible r there will be an output transmitted to Bob.

Example 2: We consider the case $G = \mathbb{Z}$ and fix an $N \in \mathbb{N}$. Let the state $\varkappa$ be a finite mixture of basis elements with equal weights:

$$\varkappa = \sum_{u,v=-N}^{N} \frac{1}{(2N+1)^2} |\xi_u^1 \otimes \xi_v^2\rangle\langle\xi_u^1 \otimes \xi_v^2|. \tag{32}$$

Since in this case $\alpha_{uvrs} = \delta_{u,r} \cdot \delta_{v,s}$ we get from (24)

$$\Psi_{uvnm} = \begin{cases} \delta_{v,u+m} \cdot \overline{b_{nu}} \xi_{u+m}^3, & u,v \in \{-N, \ldots, N\} \\ 0 & \text{elsewhere}. \end{cases}$$

Especially,

$$\|\Psi_{uvnm}\|^2 = \begin{cases} |b_{nu}|^2, & u,v \in \{-N, \ldots, N\}, v - u = m \\ 0 & \text{elsewhere}. \end{cases}$$

The conditions $u, v \in \{-N, \ldots, N\}$ and $v - u = m$ imply $m \leqslant 2N$. So we finally get for $n \in G$ and $m \leqslant 2N$

$$\Lambda_{nm}(\varkappa) = \frac{1}{C} \sum_{u=-N}^{N-m} |b_{nu}|^2 |\xi_{u+m}^3\rangle\langle\xi_{u+m}^3|$$

provided

$$C = \sum_{u=-N}^{N-m} |b_{nu}|^2 > 0.$$

For $m > 2N$ the numerator in (30) is equal to zero. That means that measuring the value z_{nm} with $m > 2N$ it is not possible to send any information to Bob.

In further investigations one should consider more refined measurements than simple projections onto one-dimensional subspaces which are obtained just by a change of the basis and a shifting procedure. The next examples elucidates that the whole procedure becomes trivial if we even do not change the basis.

Example 3: Let us consider the (extreme) case that the second basis in $\mathcal{H}_2$ is the old one, i.e., $\eta_n=\xi_n^2$ for all $n\in G$. This implies $b_{nk}=\delta_{n,k}$, and the projection operator F_{nm} is the projection onto $\xi_{nm}=\xi_n^1\otimes\xi_{n\oplus m}^2$. Let $\varkappa$ be an arbitrary normal state on $\mathcal{H}_1\otimes\mathcal{H}_2$ given in the forms (19)–(21). If $\Sigma_{u,v}\lambda_{uv}|\alpha_{uvn,n\oplus m}|^2=0$ there will be no output, i.e., $\Lambda_{nm}(\varkappa)=0$. If $\Sigma_{u,v}\lambda_{uv}|\alpha_{uvn,n\oplus m}|^2>0$ we obtain $\Lambda_{nm}(\varkappa)=|\xi_{n\oplus m}^3\rangle\langle\xi_{n\oplus m}^3|$. Only if the vector $\xi_n^1\otimes\xi_{n\oplus m}^3$ appears in at least one nonzero component Φ_{uv} of the state $\varkappa$ some information will be transmitted and the final state $\Lambda_{nm}(\varkappa)$ will be the pure state $|\xi_{n\oplus m}^3\rangle\langle\xi_{n\oplus m}^3|$.

IV. TRANSFORMATION OF PRODUCT STATES

To be closer to usual teleportation schemes and to get simple and explicit results we want to consider in the sequel the case that the state $\varkappa$ on $\mathcal{H}_1\otimes\mathcal{H}_2$ is a product state:

$$\varkappa=\rho^1\otimes\rho^2 \tag{33}$$

where $\rho^1\in\mathcal{S}(\mathcal{H}_1)$ and $\rho^2\in\mathcal{S}(\mathcal{H}_2)$. Assume $(\Phi_u^1)_{u\in G}$, $(\Phi_u^2)_{u\in G}$ are orthonormal sequences in $\mathcal{H}_1$, respectively, $\mathcal{H}_2$ such that

$$\rho^j=\sum_{u\in G}\lambda_u^j|\Phi_u^j\rangle\langle\Phi_u^j| \quad (j=1,2) \tag{34}$$

with

$$\sum_{u\in G}\lambda_u^j=1, \quad \lambda_v^j\geqslant 0 \quad (j=1,2,v\in G) \tag{35}$$

and Φ_u^j having the representation

$$\Phi_u^j=\sum_{r\in G}\alpha_{ur}^j\xi_r^j \quad (j=1,2,u\in G). \tag{36}$$

Using the notations from (19)–(21) we thus get in that case

$$\lambda_{uv}=\lambda_u^1\cdot\lambda_v^2, \quad \alpha_{uvrs}=\alpha_{ur}^1\cdot\alpha_{vs}^2 \quad (u,v,r,s\in G).$$

Obviously, we have

$$\sum_{r\in G}\bar{\alpha}_{ur}^j\alpha_{vr}^j=\delta_{u,v} \quad (j=1,2,u,v\in G).$$

From (24) we conclude

$$\Psi_{uvnm}=\sum_{r\in G}\overline{b_{nr}}\alpha_{ur}^1\cdot\alpha_{v,r\oplus m}^2\xi_{r\oplus m}^3 \quad (u,v,n,m\in G) \tag{37}$$

and Theorem 5 can be written in the following form.

Theorem 7: *Let $\varkappa=\rho^1\otimes\rho^2$ be a state on $\mathcal{H}_1\otimes\mathcal{H}_2$ given by* (34)–(36). *Then for all $n,m\in G$*

$$\Lambda_{nm}(\rho^1\otimes\rho^2)=\frac{\sum_{u,v\in G}\lambda_u^1\cdot\lambda_v^2\langle\Psi_{uvnm},\cdot\rangle\Psi_{uvnm}}{\mathrm{tr}_3\left(\sum_{u,v\in G}\lambda_u^1\cdot\lambda_v^2\langle\Psi_{uvnm},\cdot\rangle\Psi_{uvnm}\right)} \tag{38}$$

where $\Psi_{uvnm}\in\mathcal{H}_3$ is given by (37) *and where we have to assume that the denominator in* (30) *is greater than zero* (tr_3 *again denotes the trace in* $\mathcal{H}_3$).

We want to express the channel Λ_{nm} acting from $\mathcal{S}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ to $\mathcal{S}(\mathcal{H}_3)$ by a consecutive application of single channels having an intuitive meaning.

First for each $h \in \mathcal{H}_2$ we introduce an operator $A_h : \mathcal{H}_3 \to \mathcal{H}_3$ by

$$A_h f = \sum_{r \in G} \langle \xi_r^2, h \rangle \langle \xi_r^3, f \rangle \xi_r^3 \quad (f \in \mathcal{H}_3). \tag{39}$$

Especially, for all $r \in G$ we have

$$A_h \xi_r^3 = \langle \xi_r^2, h \rangle \xi_r^3 \tag{40}$$

and

$$A_{\xi_r^2} = |\xi_r^3\rangle\langle\xi_r^3|. \tag{41}$$

Obviously,

$$\|A_h f\|^2 = \sum_{r \in G} |\langle \xi_r^2, h \rangle \langle \xi_r^3, f \rangle|^2 \leqslant \|h\|^2 \|f\|^2,$$

so, for each $h \in \mathcal{H}_2$ it holds $A_h \in \mathcal{B}(\mathcal{H}_3)$.

For each $h \in \mathcal{H}_2$ the adjoint of A_h is given by

$$A_h^* f = \sum_{r \in G} \overline{\langle \xi_r^2, h \rangle} \langle \xi_r^3, f \rangle \xi_r^3 \quad (f \in \mathcal{H}_3). \tag{42}$$

On $\mathcal{H}_3$ we define for all $m \in G$ (in the same way as on $\mathcal{H}_2$—cf. (6)) the shift operator $V_m : \mathcal{H}_3 \to \mathcal{H}_3$ characterized by

$$V_m \xi_r^3 = \xi_{r \oplus m}^3 \quad (r \in G) \tag{43}$$

being a unitary operator on $\mathcal{H}_3$.

Finally, let $J_1 : \mathcal{H}_1 \to \mathcal{H}_3$ and $J_2 : \mathcal{H}_2 \to \mathcal{H}_3$ be the isomorphisms exchanging the corresponding basis elements, i.e.,

$$J_1 \xi_r^1 = \xi_r^3, \quad J_2 \xi_r^2 = \xi_r^3 \quad (r \in G). \tag{44}$$

Lemma 8: For all $u, v, n, m \in G$ it holds

$$\Psi_{uvnm} = A_{\Phi_v^2}(V_m A_{\overline{\eta}_n}(J_1 \Phi_u^1)), \tag{45}$$

where $\Psi_{uvnm} \in \mathcal{H}_3$ is given by (37), *the vectors Φ_v^j by* (36) *and $\overline{\eta}_n$ by*

$$\overline{\eta_n} = \sum_{l \in G} \overline{b_{nl}} \xi_l^2 \tag{46}$$

(*cf. definition* (2) *of* η_n).

Proof: From

$$J_1 \Phi_u^1 = \sum_{r \in G} \alpha_{ur}^1 \xi_r^3$$

we conclude

$$V_m A_{\bar{\eta}_n}(J_1\Phi_u^1) = V_m\left(\sum_{r\in G}\alpha_{ur}^1\langle\xi_r^2,\bar{\eta}_n\rangle\xi_r^3\right) = V_m\left(\sum_{r\in G}\alpha_{ur}^1\overline{b_{nr}}\xi_r^3\right) = \sum_{r\in G}\alpha_{ur}^1\overline{b_{nr}}\xi_{r\oplus m}^3$$

$$A_{\Phi_v^2}V_m A_{\bar{\eta}_n}(J_1\Phi_u^1) = \sum_{r\in G}\alpha_{ur}^1\overline{b_{nr}}A_{\Phi_v^2}\xi_{r\oplus m}^3 = \sum_{r\in G}\alpha_{ur}^1\overline{b_{nr}}\alpha_{v,r\oplus m}^2\xi_{r\oplus m}^3$$

what proves because of (37) Lemma 8. □

Observe that for all $h\in\mathcal{H}_2$, $f\in\mathcal{H}_3$ and $r\in G$

$$\langle\xi_r^2,h\rangle\langle\xi_r^3,f\rangle = \langle\xi_r^2,J_2^*f\rangle\langle\xi_r^3,J_2h\rangle.$$

From definition (39) of the operator A_h we thus immediately conclude

Lemma 9: For all $h\in\mathcal{H}_2$, $f\in\mathcal{H}_3$

$$A_h f = A_{J_2^*f}(J_2h). \tag{47}$$

The following property of the operators A_h will be basic for our description of the channel Λ_{nm}.

Lemma 10: Let τ be a positive trace-class operator on $\mathcal{H}_2$ (possibly also the operator being identically zero) and let us be given two different representations of τ

$$\tau = \sum_{k\in G}\gamma_k^1|h_k^1\rangle\langle h_k^1| = \sum_{k\in G}\gamma_k^2|h_k^2\rangle\langle h_k^2| \tag{48}$$

with $\gamma_k^j\geqslant 0$ and $(h_k^j)_{k\in G}$, $j=1,2$ being orthonormal bases in $\mathcal{H}_2$. Then for each positive trace-class operator α on $\mathcal{H}_3$ we have

$$\sum_{k\in G}\gamma_k^1 A_{h_k^1}\alpha A_{h_k^1}^* = \sum_{k\in G}\gamma_k^2 A_{h_k^2}\alpha A_{h_k^2}^*. \tag{49}$$

Proof: It is sufficient to consider the case

$$\alpha = |f\rangle\langle f| \quad (f\in\mathcal{H}_3, \|f\|=1).$$

Using Lemma 9 we get for all $g\in\mathcal{H}_3$ and $j=1,2$

$$\sum_{k\in G}\gamma_k^j A_{h_k^j}|f\rangle\langle f|A_{h_k^j}^* g = \sum_{k\in G}\gamma_k^j A_{h_k^j}f\langle A_{h_k^j}f,g\rangle = \sum_{k\in G}\gamma_k^j A_{J_2^*f}J_2h_k^j\langle A_{J_2^*f}h_k^j,g\rangle = \sum_{k\in G}\gamma_k^j A_{J_2^*f}J_2|h_k^j\rangle\langle h_k^j|J_2^*A_{J_2^*f}^* g$$
$$= A_{J_2^*f}J_2\sum_{k\in G}\gamma_k^j|h_k^j\rangle\langle h_k^j|J_2^*A_{J_2^*f}^* g = A_{J_2^*f}J_2\tau J_2^*A_{J_2^*f}^* g.$$

Consequently, left- and right-hand sides of (49) coincide—the expression in (49) does not depend on the special representation of τ in some basis in $\mathcal{H}_2$.

□

Let us remark that τ may be a finite rank operator since we did not exclude $\gamma_k^j=0$.

Denote by $\mathcal{T}_j$ the set of all positive trace-class operators on $\mathcal{H}_j$, $j=1,2,3$. For each $\tau\in\mathcal{T}_2$ we define a mapping $K_\tau:\mathcal{T}_3\to\mathcal{T}_3$ by the ansatz

$$K_\tau(\alpha) = \sum_{k\in G}\gamma_k A_{h_k}\alpha A_{h_k}^* \quad (\alpha\in\mathcal{T}_3), \tag{50}$$

where

$$\tau = \sum_{k\in G}\gamma_k|h_k\rangle\langle h_k| \quad (j=1,2) \tag{51}$$

with $\gamma_k\geqslant 0$ and $(h_k)_{k\in G}$ being an orthonormal basis in $\mathcal{H}_2$. Lemma 10 guarantees that the mapping K_τ is well defined, i.e., the definition (50) does not depend on the special representation of τ in some basis of $\mathcal{H}_2$.

In the sequel let us make the convention to denote the normalization of a positive trace-class operator $\varkappa$ by $\hat{\varkappa}$, i.e.,

$$\hat{\varkappa} = \frac{\varkappa}{\mathrm{tr}\varkappa} \tag{52}$$

provided $\mathrm{tr}\,\varkappa > 0$.

Now, we are able to express the channel $\Lambda_{nm}(\varkappa)$ as a consecutive application of single channels. This explicit construction will be done only for product states $\varkappa = \rho^1 \otimes \rho^2$. Besides the channel K_τ defined by (50) we still need two other channels—one lifting the state from $\mathcal{H}_1$ to $\mathcal{H}_3$ by the isomorphism J_1 given by (44) and one shifting the states on $\mathcal{H}_3$ with the shift operator V_m defined by (43). We define $K: \mathcal{T}_1 \to \mathcal{T}_3$ by

$$K(\alpha) = J_1 \alpha J_1^* \quad (\alpha \in \mathcal{T}_1) \tag{53}$$

and for $m \in G$ the mapping $K_m: \mathcal{T}_3 \to \mathcal{T}_3$ by

$$K_m(\alpha) = V_m \alpha V_m^* \quad (\alpha \in \mathcal{T}_3). \tag{54}$$

Theorem 11: *For all* $\rho^1 \in \mathcal{S}(\mathcal{H}_1)$, $\rho^2 \in \mathcal{S}(\mathcal{H}_2)$ *and* $n, m \in G$ *it holds*

$$\Lambda_{nm}(\rho^1 \otimes \rho^2) = \hat{K}_{\rho^2} \circ K_m \circ K_{|\overline{\eta_n}\rangle\langle\overline{\eta_n}|} \circ K(\rho^1) \tag{55}$$

provided $\mathrm{tr}\, K_{\rho^2} \circ K_m \circ K_{|\overline{\eta_n}\rangle\langle\overline{\eta_n}|} \circ K(\rho^1) > 0$. *Hereby,* $\overline{\eta_n}$ *is given by* (46).

Proof: Let $\rho^1 \otimes \rho^2$ be given by (34)–(36).

Using (38) in Theorem 7 and the representation (45) of Ψ_{uvnm} we obtain for all $u, v, n, m \in G$

$$\begin{aligned}
\sum_{u,v \in G} \lambda_u^1 \cdot \lambda_v^2 \langle \Psi_{uvnm}, \cdot \rangle \Psi_{uvnm} &= \sum_{u,v \in G} \lambda_u^1 \cdot \lambda_v^2 A_{\Phi_v^2} V_m A_{\overline{\eta}_n} J_1 |\Phi_u^1\rangle\langle\Phi_u^1| J_1^* A_{\overline{\eta}_n}^* V_m^* A_{\Phi_v^2}^* \\
&= \sum_{v \in G} \lambda_v^2 A_{\Phi_v^2} V_m A_{\overline{\eta}_n} J_1(\rho^1) J_1^* A_{\overline{\eta}_n}^* V_m^* A_{\Phi_v^2}^* \\
&= \sum_{v \in G} \lambda_v^2 A_{\Phi_v^2} V_m A_{\overline{\eta}_n} K(\rho^1) A_{\overline{\eta}_n}^* V_m^* A_{\Phi_v^2}^* \\
&= \sum_{v \in G} \lambda_v^2 A_{\Phi_v^2} V_m (K_{|\overline{\eta_n}\rangle\langle\overline{\eta_n}|} \circ K(\rho^1)) V_m^* A_{\Phi_v^2}^* \\
&= \sum_{v \in G} \lambda_v^2 A_{\Phi_v^2} (K_m \circ K_{|\overline{\eta_n}\rangle\langle\overline{\eta_n}|} \circ K(\rho^1)) A_{\Phi_v^2}^* \\
&= K_{\rho^2} \circ K_m \circ K_{|\overline{\eta_n}\rangle\langle\overline{\eta_n}|} \circ K(\rho^1).
\end{aligned}$$

Since $\Lambda_{nm}(\rho^1 \otimes \rho^2)$ is just the normalization of the previous expression using the notation (52) we finally obtain (55). □

The aim of teleportation models is to find methods of transmission of states on $\mathcal{H}_1$ to states on $\mathcal{H}_3$ in such a way that Bob is able to reconstruct perfectly or in a nearly perfect way the emitted state—having only knowledge about the result of a certain measurement. In Sec. III we already gave some examples illustrating the model. For the states considered in these examples it will be impossible to reconstruct all original states. However, one is not interested only in perfect teleportations but also in the deformation of the state, the degree of destruction of the input signal, etc. In Ref. 4 we considered the special case of all spaces being equal and finite dimensional. For examples in this case we refer to this article. Further, one can ask for subsets of $\mathcal{S}(\mathcal{H}_1)$ for which perfect teleportation can be achieved. We continue to illustrate the channels and operations previously introduced by simple examples connected with product states. The aim of the examples below is just to illustrate the mechanism of the procedure.

In what follows, summands for which $\|\Psi_{uvnm}\|=0$ just have to be cancelled. If it is equal to zero no information about the input signal (the measurement of the value z_{nm}) will pass to Bob. Such cases of non-perfect teleportation were considered in Ref. 3.

Example 4: Let us consider the extreme case that $\rho^1=|\xi_k^1\rangle\langle\xi_k^1|$ *for some* $k\in G$. *Then* $K(\rho^1)=|\xi_k^3\rangle\langle\xi_k^3|$, *which implies*

$$K_{|\overline{\eta_n}\rangle\langle\overline{\eta_n}|}\circ K(\rho^1)=|b_{nk}|^2|\xi_k^3\rangle\langle\xi_k^3|.$$

Consequently,

$$K_m\circ K_{|\overline{\eta_n}\rangle\langle\overline{\eta_n}|}\circ K(\rho^1)=|b_{nk}|^2|\xi_{k\oplus m}^3\rangle\langle\xi_{k\oplus m}^3|.$$

From (40) *we know that for each* $h\in\mathcal{H}_2$ *it holds*

$$A_h|\xi_{k\oplus m}^3\rangle\langle\xi_{k\oplus m}^3|A_h^*=|\langle\xi_{k\oplus m}^2,h\rangle|^2|\xi_{k\oplus m}^3\rangle\langle\xi_{k\oplus m}^3|.$$

For arbitrary state ρ^2 *on* $\mathcal{H}_2$ *this leads to*

$$K_{\rho^2}\circ K_m\circ K_{|\overline{\eta_n}\rangle\langle\overline{\eta_n}|}\circ K(\rho^1)=|b_{nk}|^2\mathrm{tr}_2(\rho^2|\xi_{k\oplus m}^2\rangle\langle\xi_{k\oplus m}^2|)\cdot|\xi_{k\oplus m}^3\rangle\langle\xi_{k\oplus m}^3|.$$

Finally, if $|b_{nk}|^2\mathrm{tr}_2(\rho^2|\xi_{k\oplus m}^2\rangle\langle\xi_{k\oplus m}^2|)>0$ *we obtain*

$$\Lambda_{nm}(\rho^1\otimes\rho^2)=|\xi_{k\oplus m}^3\rangle\langle\xi_{k\oplus m}^3|.$$

□

We try to give again a possible interpretation of the result. Measuring z_{nm} we made a projection onto $\xi_{nm}=\Sigma_{r\in G}b_{nr}(\xi_r^1\otimes\xi_{r\oplus m}^2)$. At least one of the coefficients $b_{nr}, r\in G$ has to be different from zero. The state Alice wants to teleportate consists only of the elementary signal ξ_k^1 since $\rho^1=|\xi_k^1\rangle\langle\xi_k^1|$. This implies that only the signal $\xi_k^1\otimes\xi_{k\oplus m}^2$ is able to pass. So it is necessary that $b_{nk}\neq 0$. The information about the index n is not contained in the elementary signal $\xi_k^1\otimes\xi_{k\oplus m}^2$ and will not be contained in the output sent to Bob. However, $b_{nk}\neq 0$ is necessary to get an output at all. Further, for the state ρ^2 given by (34)–(36) one easily checks

$$\mathrm{tr}_2(\rho^2|\xi_{k\oplus m}^2\rangle\langle\xi_{k\oplus m}^2|)=\sum_{u\in G}\lambda_u^2|\alpha_{u,k\oplus m}^2|^2.$$

Consequently, to obtain the output $|\xi_{k\oplus m}^3\rangle\langle\xi_{k\oplus m}^3|$ at least for one Φ_u^2 with $\lambda_u^2>0$ it must hold $\alpha_{u,k\oplus m}^2\neq 0$. If Bob would know that only states of the form $\rho^1=|\xi_k^1\rangle\langle\xi_k^1|$ for some $k\in G$ are sent by Alice he obviously has unitary keys to reconstruct the original state. This of course requires that all $b_{nk}\neq 0$ and that the state ρ^2 is such that for all $k\in G$ there exists at least one $u\in G$ such that $\lambda_u^2>0$ and $\alpha_{uk}^2\neq 0$.

Example 5: Now we consider the other extreme case that ρ^2 *is just an elementary signal, i.e., there exists an* $k\in G$ *such that* $\rho^2=|\xi_k^2\rangle\langle\xi_k^2|$. *Analogous calculation as in Example 4 shows that*

$$\Lambda_{nm}(\rho^1\otimes\rho^2)=|\xi_k^3\rangle\langle\xi_k^3|,$$

where we have to assume that $\mathrm{tr}_1(\rho^1|\xi_{k\ominus m}^1\rangle\langle\xi_{k\ominus m}^1|)>0$. *We already observed in the example above that* ρ^2 *should contain as much information as possible. In the case* $\rho^2=|\xi_k^2\rangle\langle\xi_k^2|$ *Bob obtains no information at all abut the state* ρ^1. *Independently of the result* z_{nm} *of the measurement performed by Alice either* $\Lambda_{nm}(\rho^1\otimes\rho^2)=0$ *or equal to* $|\xi_k^3\rangle\langle\xi_k^3|$. *So we have the most extreme case of loss of information*.

V. EXISTENCE OF UNITARY KEYS

We will consider again the case of product states $\varkappa=\rho^1\otimes\rho^2$ on $\mathcal{H}_1\otimes\mathcal{H}_2$ where $\rho^1\in\mathcal{S}(\mathcal{H}_1)$ and $\rho^2\in\mathcal{S}(\mathcal{H}_2)$. That means that the entangled state σ considered in Refs. 2 and 3 has the form $\sigma=S_3\rho^2S_3^*$. For fixed state ρ^2 on $\mathcal{H}_2$ we consider the channel $\tilde{\Lambda}_{nm}:\mathcal{S}(\mathcal{H}_1)\to\mathcal{S}(\mathcal{H}_3)$ given by

$$\tilde{\Lambda}_{nm} := \Lambda_{nm}(\cdot \otimes \rho^2),$$

i.e., (cf. (27) and (29))

$$\tilde{\Lambda}_{nm}(\rho^1) = \frac{\mathrm{tr}_{1,2}((F_{nm} \otimes \mathbb{1})(\mathbb{1} \otimes S_3)\rho^1 \otimes \lambda(\mathbb{1} \otimes S_3^*)(F_{nm} \otimes \mathbb{1}))}{\mathrm{tr}((F_{nm} \otimes \mathbb{1})(\mathbb{1} \otimes S_3)\rho^1 \otimes \lambda(\mathbb{1} \otimes S_3^*)(F_{nm} \otimes \mathbb{1}))}. \tag{56}$$

Let $\mathcal{G} \subseteq \mathcal{S}(\mathcal{H}_1)$ be a fixed set of states on $\mathcal{H}_1$.

Definition 12: We say that the teleportation scheme is perfect if for each $n,m \in G$ there exists a unitary operator $V_{nm}: \mathcal{H}_1 \to \mathcal{H}_3$ such that

$$\tilde{\Lambda}_{nm}(\rho^1) = V_{nm}\rho^1 V_{nm}^* \quad (\rho^1 \in \mathcal{G}) \tag{57}$$

and

$$\sum_{n,m \in G} \mathrm{tr}((F_{nm} \otimes \mathbb{1})(\mathbb{1} \otimes S_3)\rho^1 \otimes \rho^2(\mathbb{1} \otimes S_3^*)(F_{nm} \otimes \mathbb{1})) = 1 \quad (\rho^1 \in \mathcal{G}). \tag{58}$$

The unitary operators V_{nm} are called unitary keys.

Usually, perfect teleportation means that the above-mentioned conditions hold for all $\rho^1 \in \mathcal{S}(\mathcal{H}_1)$ (cf. Refs. 2, 3, and 5). The restriction of the set of states that have to be teleportated enlarges the possibilities for perfect or "nearly" perfect models. Condition (57) means that Bob can reconstruct the original state ρ^1 from the knowledge of the result z_{nm} of the measurement and of the received state $\tilde{\Lambda}_{nm}(\rho^1)$ where it is assumed that Bob possesses for each $n,m \in G$ the appropriate key V_{nm}. This follows obviously form $\rho^1 = V_{nm}^* \tilde{\Lambda}_{nm}(\rho^1) V_{nm}$. Finally, (58) means that with probability one Bob will find the proper key, i.e., with certainty there will be a result z_{nm} of measurement for which he has unitary keys.

Let us have a closer look to formula (55). The channel K_m is built with the help of the unitary V_m. The same is true for K since $J_1 J_1^* = J_1^* J_1 = \mathbb{1}$. The channel $K_{|\overline{\eta_n}\rangle\langle\overline{\eta_n}|}$ destroys any hope for unitary keys. An easy calculation shows that for each $f \in \mathcal{H}_3$ it holds

$$A_{\overline{\eta_n}}^* A_{\overline{\eta_n}} f = A_{\overline{\eta_n}} A_{\overline{\eta_n}}^* f = \sum_{r \in G} |b_{nr}|^2 \langle \xi_r^3, f \rangle \xi_r^3. \tag{59}$$

We see that only if G is finite and all $|b_{nk}|$ are equal A will be unitary (up to a constant that vanishes after normalization). This is in accordance with (and another proof of) the fact that perfect teleportation requires finite dimensional spaces and maximal entanglement.

VI. CONCLUDING REMARKS

The aim of this article is to touch the problem of teleportation schemes in infinite-dimensional spaces. The previous results still have to be supplemented by calculations of fidelity and other characteristics. Just to achieve simple explicit expressions we illustrated the model on the most simple sequence of elementary signals (ξ_k^j). To obtain more interesting models one has to refine the above-mentioned models:

(1) consider more complex measurements than simple one-dimensional projections F_{nm},
(2) if the Hilbert space is a symmetric Fock space take *truncated* coherent vectors (exponential vectors with "removed" vacuum part) as basis and beam splittings for the entanglement,
(3) replace the isomorphisms J_1, J_2 and the trivial isometries S_1, S_3 by more complex ones.[6–11]

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Continuity bounds on the quantum relative entropy

Koenraad M. R. Audenaert[a] and Jens Eisert[b]
Blackett Laboratory, Imperial College London, Prince Consort Rd, London SW7 2BW, United Kingdom and Institute for Mathematical Sciences, Imperial College London, Exhibition Rd, London SW7 2BW, United Kingdom

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The quantum relative entropy is frequently used as a distance, or distinguishability measure between two quantum states. In this article we study the relation between this measure and a number of other measures used for that purpose, including the trace norm distance. More specifically, we derive lower and upper bounds on the relative entropy in terms of various distance measures for the difference of the states based on unitarily invariant norms. The upper bounds can be considered as statements of continuity of the relative entropy distance in the sense of Fannes. We employ methods from optimisation theory to obtain bounds that are as sharp as possible. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2044667]

I. INTRODUCTION

The relative entropy of states of quantum systems is a measure of how well one quantum state can be operationally distinguished from another. Defined as

$$S(\rho\|\sigma) = \mathrm{Tr}[\rho(\log\rho - \log\sigma)]$$

for states ρ and σ, it quantifies the extent to which one hypothesis ρ differs from an alternative hypothesis σ in the sense of quantum hypothesis testing.[1–5] Dating back to work by Umegaki,[6] the relative entropy is a quantum generalization of the Kullback–Leibler relative entropy for probability distributions in mathematical statistics.[7] The quantum relative entropy plays an important role in quantum statistical mechanics[5] and in quantum information theory, where it appears as a central notion in the study of capacities of quantum channels[8–11] and in entanglement theory.[11–13]

In *finite-dimensional Hilbert spaces*, the relative entropy functional is manifestly continuous.[5] For states on infinite-dimensional Hilbert spaces the relative entropy functional is not trace norm continuous any more, but-as the von-Neumann entropy—lower semi-continuous. That is, for sequences of states $\{\sigma_n\}_n$ and $\{\rho_n\}_n$ converging in trace norm to states σ and ρ, i.e., $\lim_{n\to\infty}\|\sigma_n - \sigma\|_1 = 0$ and $\lim_{n\to\infty}\|\rho_n - \rho\|_1 = 0$, we merely have $S(\rho\|\sigma) \leqslant \liminf_{n\to\infty} S(\rho_n\|\rho_n)$. However, for systems for which the Gibbs state exists, these discontinuities can be tamed[5] when considering compact subsets of state space with finite mean energy. In a similar manner, entropic measures of entanglement can become trace norm continuous on subsets with bounded energy.[14] For considerations of the continuity of the relative entropy in classical contexts, see Ref. 15. In particular, if $\{\sigma_n\}_n$ is a sequence of states of fixed finite dimension satisfying

$$\lim_{n\to\infty}\|\sigma_n - \sigma\|_1 = \lim_{n\to\infty}\mathrm{Tr}|\sigma_n - \sigma| = 0 \tag{1}$$

for a given state σ, then

[a]Electronic address: k.audenaert@imperial.ac.uk
[b]Electronic address: jense@imperial.ac.uk

$$\lim_{n\to\infty} S(\sigma_n\|\sigma) = 0.$$

In practical contexts, however, more precise estimates can be necessary, in particular in an asymptotic setting. Consider a state ρ on a Hilbert space $\mathcal{H}$, and a sequence $\{\sigma_n\}_n$, where σ_n is a state on $\mathcal{H}^{\otimes n}$, the n-fold tensor product of $\mathcal{H}$. The sequence is said to asymptotically approximate ρ if σ_n tends to $\rho^{\otimes n}$ for $n\to\infty$. More precisely, one typically requires that

$$\lim_{n\to\infty} \|\sigma_n - \rho^{\otimes n}\|_1 = 0. \tag{2}$$

Now, as an alternative to the trace norm distance, one can consider the use of the Bures distance. The Bures distance D is defined as

$$D(\rho_1,\rho_2) = 2(1 - F(\rho_1,\rho_2))^{1/2},$$

in terms of the Uhlmann fidelity

$$F(\rho_1,\rho_2) = \mathrm{Tr}(\rho_1^{1/2}\rho_2\rho_1^{1/2})^{1/2}.$$

Because of the inequalities[16]

$$1 - F(\rho_1,\rho_2) \leqslant \mathrm{Tr}|\rho_1 - \rho_2| \leqslant (1 - F^2(\rho_1,\rho_2))^{1/2}, \tag{3}$$

the trace norm distance tends to zero if and only if the Bures distance tends to zero, which shows that, for the purpose of state discrimination, both distances are essentially equivalent and one can use whichever is most convenient.

A natural question that now immediately arises is whether the same statement is true for the relative entropy. To find an answer to that one would need inequalities like (3) connecting the quantum relative entropy, used as a distance measure, to the trace norm distance, or similar distance measures.

In this article, we do just that: we find upper bounds on the relative entropy functional in terms of various norm differences of the two states. As such, the presented bounds are very much in the same spirit as Fannes' inequality, sharpening the notion of continuity for the von Neumann entropy.[17] It has already to be noted here that one of the main stumbling blocks in this undertaking is the well-known fact that the relative entropy is not a very good distance measure, as it gives infinite distance between nonidentical pure states. However, we will present a satisfactory solution, based on using the minimal eigenvalue of the state that is the second argument of the relative entropy. Apart from the topic of upper bounds, we also study lower bounds on the relative entropy, giving a complete picture of the relation between norm based distances and relative entropy.

We start in Sec. II with presenting a short motivation of how this article came about. Section III contains the relevant notations, definitions, and basic results that will be used in the rest of the paper. In Sec. IV we discuss some properties of unitarily invariant (UI) norms that will allow us to consider all UI norms in one go. The first upper bounds on the relative entropy $S(\rho\|\sigma)$ are presented in Sec. V, one bound being quadratic in the trace norm distance of ρ and σ and the other logarithmic in the minimal eigenvalue of σ. Both bounds separately capture an essential behavior of the relative entropy, and it is argued that finding a single bound that captures both behaviors at once is not a trivial undertaking. Nevertheless, we will succeed in doing this in Sec. VII by constructing upper bounds that are as sharp as possible for given trace norm distance *and* minimal eigenvalue of σ. In Sec. VI we use similar techniques to derive lower bounds that are as sharp as possible. Finally, in Sec. IX, we come back to the issue of state discrimination mentioned at the beginning.

II. BACKGROUND

In Ref. 18 (Example 6.2.31, p. 279) we find the following upper bound on the relative entropy, valid for all ρ and for nonsingular σ:

$$S(\rho\|\sigma) \leqslant \frac{\|\rho-\sigma\|_\infty}{\lambda_{\min}(\sigma)}. \tag{4}$$

This bound is linear in the operator norm distance between ρ and σ and has a $1/x$ dependence on $\lambda_{\min}(\sigma)$. For several purposes, such a bound is not necessarily sharp enough. The impetus for the present article was given by the observation that sharper upper bounds on the relative entropy should be possible than (4). Specifically, there should exist bounds that are

1. *quadratic* in $\rho-\sigma$, and/or
2. depend on $\lambda_{\min}(\sigma)$ in a *logarithmic* way.

A simple argument shows that a logarithmic dependence on $\lambda_{\min}(\sigma)$ can be achieved instead of an $1/x$ dependence. Note that $0 \geqslant \log \sigma \geqslant \mathbb{1}\cdot\log \lambda_{\min}(\sigma)$. Thus,

$$S(\rho\|\sigma) = \mathrm{Tr}[\rho(\log\rho - \log\sigma)] \leqslant -S(\rho) - \log\lambda_{\min}(\sigma) \leqslant -\log\lambda_{\min}(\sigma). \tag{5}$$

Concerning the quadratic dependence on $\rho-\sigma$, we can put $\rho=\sigma+\varepsilon\Delta$, with $\mathrm{Tr}[\Delta]=0$, and calculate the derivative

$$\lim_{\varepsilon\to 0} S(\sigma+\varepsilon\Delta\|\sigma)/\varepsilon$$

and find that this turns out to be zero for any nonsingular σ. Indeed, the gradient of the relative entropy $S(\rho\|\sigma)$ with respect to ρ is, $\mathbb{1}+\log\rho-\log\sigma$ (see Lemma 1). Hence, for $\rho=\sigma$ and $\mathrm{Tr}[\Delta]=0$,

$$\lim_{\varepsilon\to 0} S(\sigma+\varepsilon\Delta\|\sigma)/\varepsilon = \mathrm{Tr}[\Delta(\mathbb{1}+\log\sigma-\log\sigma)] = 0.$$

This seems to imply that for small ε, $S(\sigma+\varepsilon\Delta\|\sigma)$ must at least be quadratic in ε, and, therefore, upper bounds might exist that indeed are quadratic in ε. Further, Ref. 4 contains the following quadratic lower bound (Theorem 1.15)

$$S(\rho\|\sigma) \geqslant \tfrac{1}{2}\|\rho-\sigma\|_1^2. \tag{6}$$

The rest of the article will be devoted to finding firm evidence for these intuitions, by exploring the relation between relative entropy and norm based distances, culminating in a number of bounds that are the sharpest possible.

III. NOTATION

In this article, we will use the following notations. We will use the standard vector and matrix bases: e^i is the vector with the ith element equal to 1, and all other elements being equal to 0. $e^{i,j}$ is the matrix with i,j element equal to 1 and all other elements 0. For any diagonal matrix A, we write A_i as a shorthand for $A_{i,i}$, and $\mathrm{Diag}(a_1,a_2,\ldots)$ is the diagonal matrix with a_i as diagonal elements. We reserve two symbols for the following special matrices:

$$E := \mathrm{Diag}(1,0,\ldots,0) = e^{1,1}, \tag{7}$$

and

$$F := \mathrm{Diag}(1,-1,0,\ldots,0) = e^{1,1} - e^{2,2}. \tag{8}$$

The positive semidefinite order is denoted using the $\geqslant$ sign: $A \geqslant B$ iff $A-B \geqslant 0$ (positive semidefinite).

The (quantum) relative entropy is denoted as $S(\rho\|\sigma)=\mathrm{Tr}[\rho(\log\rho-\log\sigma)]$. All logarithms in this article are natural logarithms. When ρ and σ are both diagonal (i.e., when we encounter the commutative, classical case) we use the shorthand

$$S((r_1,r_2,\ldots)\|(s_1,s_2,\ldots)) := S(\mathrm{Diag}(r_1,r_2,\ldots)\|\mathrm{Diag}(s_1,s_2,\ldots)).$$

Lemma 1: The gradient of the relative entropy $S(\rho\|\sigma)$ with respect to its first argument ρ, being nonsingular, is given by $\mathbb{1}+\log\rho-\log\sigma$.

Proof: The calculation of this derivative is straightforward. Since the classical entropy function $x\mapsto h(x):=-x\log x$ is continuously differentiable on (0,1), and therefore,

$$\left.\frac{\partial}{\partial\varepsilon}\right|_{\varepsilon=0} S(\rho+\varepsilon\Delta)=\mathrm{Tr}[\Delta h'(\rho)],$$

we can write

$$\lim_{\varepsilon\to 0} S(\rho+\varepsilon\Delta\|\sigma)/\varepsilon=\mathrm{Tr}[\Delta(\mathbb{1}+\log\rho-\log\sigma)].$$

□

Finally, we recall a number of series expansions related to the logarithm, which are valid for $-1<y<1$,

$$\log(1-y)=-\sum_{k=1}^{\infty}\frac{y^k}{k},$$

$$\log(1+y)+\log(1-y)=-\sum_{k=1}^{\infty}\frac{y^{2k}}{k},$$

$$\log(1+y)-\log(1-y)=2\sum_{k=0}^{\infty}\frac{y^{2k+1}}{2k+1}.$$

These expansions will be made extensive use of.

IV. UNITARILY INVARIANT NORMS

In this section we collect the main definitions and known results about unitarily invariant norms along with a number of refinements that will prove to be very useful for the rest of the article.

A *unitarily invariant norm* (UI norm), denoted with $|||.|||$, is a norm on square matrices that satisfies the property

$$|||UAV|||=|||A|||\tag{9}$$

for all A and for unitary U, V ([1], Sec. IV B). Perhaps the most important property of UI norms is that they only depend on the singular values of the matrix A. If A is positive semidefinite, then $|||A|||$ depends only on the eigenvalues of A.

A very important class of UI norms are the *Ky Fan norms* $\|.\|_{(k)}$, which are defined as follows: for any given square $n\times n$ matrix A, with singular values $s_j^{\downarrow}(A)$ (sorted in nonincreasing order) and $1\leqslant k\leqslant n$, the k-Ky Fan norm is the sum of the k largest singular values of A:

$$\|A\|_{(k)}=\sum_{j=1}^{k} s_j^{\downarrow}(A).$$

Two special Ky Fan norms are the *operator norm* and the *trace norm*,

$$\|A\|_{\infty}=\|A\|_{(1)},\quad \|A\|_{\mathbf{Tr}}=\|A\|_1=\|A\|_{(n)}.\tag{10}$$

The importance of the Ky Fan norms derives from their leading role in Ky Fan's *Dominance Theorem* (Ref. 19, Theorem IV.2.2):

Theorem 1 (Ky Fan Dominance): *Let A and B be any two $n\times n$ matrices. If B majorizes A*

in all the Ky Fan norms,

$$\|A\|_{(k)} \leqslant \|B\|_{(k)},$$

for all $k=1,2,\ldots$, *then it does so in all other UI norms as well*,

$$|||A||| \leqslant |||B|||.$$

From Ky Fan's Dominance Theorem follows the following well-known norm dominance statement.

Lemma 2: For any matrix A, and any unitarily invariant norm $|||.|||$,

$$\|A\|_\infty \leqslant \frac{|||A|||}{|||E|||} \leqslant \|A\|_1.$$

Proof: We need to show that, for every A,

$$|||(\|A\|_\infty)E||| \leqslant |||A||| \leqslant |||(\|A\|_1)E|||,$$

holds for every unitarily invariant norm. By Ky Fan's dominance theorem, we only need to show this for the Ky Fan norms. All the Ky Fan norms of E are 1, and

$$\|A\|_\infty = \|A\|_{(1)} \leqslant \|A\|_{(k)} \leqslant \|A\|_{(d)} = \|A\|_1$$

follows from the definition of the Ky Fan norms. □

The main mathematical object featuring in this article is not the state, but rather the difference Δ of two states, $\Delta := \rho - \sigma$, and for that object a stronger dominance result obtains. We first show that the largest norm difference between two states occurs for orthogonal pure states. Indeed, by convexity of norms, $|||\rho-\sigma|||$ is maximal in pure ρ and σ. A simple calculation then reveals that, for any unitarily invariant norm,

$$||| \, |\psi\rangle\langle\psi| - |\phi\rangle\langle\phi| \, ||| = (1 - |\langle\psi|\phi\rangle|^2)^{1/2} |||F|||.$$

This achieves its maximal value $|||F|||$ for ψ orthogonal to ϕ, showing that it makes sense to normalise a norm distance $|||\rho-\sigma|||$ by division by $|||F|||$. We will call this a *rescaled* norm. We now have the following dominance result for rescaled norms of differences of states:

Lemma 3: For any Hermitian A, with $\mathrm{Tr}[A]=0$,

$$\frac{\|A\|_\infty}{\|F\|_\infty} \leqslant \frac{|||A|||}{|||F|||} \leqslant \frac{\|A\|_1}{\|F\|_1}.$$

Note that equality can be obtained for any value of $|||A|||$, by setting $A=cF$.

Proof: We need to show, for all traceless Hermitian A, that

$$|||(\|A\|_\infty)F||| \leqslant |||A||| \leqslant |||(\|A\|_1/2)F||| \tag{11}$$

holds for every unitarily invariant norm. Again by Ky Fan's dominance theorem, we only need to do this for the Ky Fan norms $\|.\|_{(k)}$. Since

$$\|F\|_{(k)} = \begin{cases} 1, & k=1 \\ 2, & k>1, \end{cases}$$

and

$$\|X\|_\infty = \|X\|_{(1)} \leqslant \|X\|_{(k)} \leqslant \|X\|_{(d)} = \|X\|_1,$$

the inequalities (11) follow trivially for $k>1$. The case $k=1$ is covered by Lemma 4. □

Lemma 4: For any Hermitian A, with $\mathrm{Tr}[A]=0$,

$$\|A\|_1 \geqslant 2\|A\|_\infty.$$

Proof: Let the Jordan decomposition of A be

$$A = A_+ - A_-, \tag{12}$$

with $A_+, A_- \geqslant 0$. Since $\mathrm{Tr}[A]=0$, clearly $\mathrm{Tr}[A_+]=\mathrm{Tr}[A_-]$ holds. Thus, $\|A\|_1=\mathrm{Tr}|A|=\mathrm{Tr}[A_+]+\mathrm{Tr}[A_-]=2\mathrm{Tr}[A_+]$. Also,

$$\|A\|_\infty = \max(\|A_+\|_\infty, \|A_-\|_\infty). \tag{13}$$

Hence, $\|A\|_\infty \leqslant \max(\|A_+\|_1, \|A_-\|_1)=\mathrm{Tr}[A_+]=\|A\|_1/2$. □

In this article, we will also be dealing with $\Delta=\rho-\sigma$ under the constraint $\sigma \geqslant \beta\mathbb{1}$. Obviously we have

$$\beta \leqslant 1/d.$$

We now show that under this constraint, any rescaled norm of Δ is upper bounded by $1-\beta$.

Lemma 5: For any state ρ, and states σ such that $\sigma \geqslant \beta\mathbb{1}$,

$$T := |||\rho - \sigma|||/|||F||| \leqslant 1 - \beta. \tag{14}$$

Proof: We proceed by maximizing T under the constraint $\sigma \geqslant \beta\mathbb{1}$. Convexity of norms yields that T is maximal when ρ and σ are extremal,[20] hence in ρ being a pure state $|\phi\rangle\langle\phi|$ and σ being of the form

$$\sigma = \beta\mathbb{1} + (1 - \beta d)|\psi\rangle\langle\psi|. \tag{15}$$

Fixing $\phi=e^1$, we need to maximize

$$|||e^{1,1} - \beta\mathbb{1} - (1 - \beta d)|\psi\rangle\langle\psi|||$$

over all ψ. Put $\psi=(\cos\alpha, \sin\alpha, 0, \ldots, 0)^T$, then the eigenvalues of the matrix are

$$\lambda_\pm = ((d-2)\beta \pm ((\beta d)^2 + 4(1-\beta d)\sin^2\alpha)^{1/2})/2$$

and $-\beta$ (with multiplicity $d-2$). One finds that, for $d>2$, $\lambda_+, |\lambda_-| \geqslant \beta$, for any value of α, and both λ_+ and $|\lambda_-|$ are maximal for $\alpha=\pi/2$, as would be expected. The maximal Ky Fan norms of this matrix are therefore

$$\|\,.\,\|_{(1)} = \lambda_+ = 1 - \beta,$$

$$\|\,.\,\|_{(k)} = \lambda_+ + |\lambda_-| + (k-2)\beta = (2 - \beta d) + (k-2)\beta,$$

for $k>1$. Hence, for every Ky Fan norm, the maximum norm value is obtained for orthogonal ϕ and ψ. By the Ky Fan dominance theorem, this must then hold for any UI norm. In case of the trace norm, as well as of the operator norm, the rescaled value of the maximum is $1-\beta$. By Lemma 3, this must then be the maximal value for any rescaled norm. □

Remark: For the Schatten q-norm, $|||F|||=2^{1/q}$. The largest value of $|||F|||$ is 2, obtained for the trace norm, and the smallest value is 1, for the operator norm.

V. SOME SIMPLE UPPER BOUNDS

In this section we present our first attempts at finding upper bounds that capture the essential features of relative entropy. In Sec. III A we present a bound that is indeed quadratic in the trace norm distance, the existence of which was already hinted at in Sec. II. Likewise, in Sec. III B, we find a bound that is logarithmic in the minimal eigenvalue of σ, again in accordance with previous intuition. Combining the two bounds into one that has both of these features turns out to be not so

easy. In fact, in Sec. III C a number of arguments are given that initially hinted at the impossibility of realising sich a combined bound. Nevertheless, we will succeed in finding a combined bound later on in the article, by using techniques from optimisation theory.[20]

A. A quadratic upper bound

Lemma 6: For any positive definite matrix A and Hermitian Δ such that $A+\Delta$ is positive definite,

$$\log(A+\Delta)-\log(A) \leqslant \int_0^\infty \mathrm{d}x (A+x)^{-1}\Delta(A+x)^{-1}.$$

Proof: Since the logarithm is strictly matrix concave,[21] for all $t\in[0,1]$:

$$\log((1-t)A+tB) \geqslant (1-t)\log(A)+t\log(B).$$

Setting $B=A+\Delta$ and rearranging terms then gives

$$\frac{\log(A+t\Delta)-\log(A)}{t} \geqslant \log(A+\Delta)-\log(A),$$

for all $t\in[0,1]$. A fortiori, this holds in the limit for t going to zero, and then the left-hand side is just the Fréchet derivative of log at A in the direction Δ. □

This Lemma allows us to give a simple upper bound on $S(\sigma+\Delta\|\sigma)$. Note that if $A\geqslant B$ then $\mathrm{Tr}[CA]\geqslant\mathrm{Tr}[CB]$ for any $C\geqslant 0$. Therefore, we arrive at

$$S(\rho\|\sigma)=\mathrm{Tr}[(\sigma+\Delta)(\log(\sigma+\Delta)-\log(\sigma))] \leqslant \int_0^\infty \mathrm{d}x\,\mathrm{Tr}[(\sigma+\Delta)(\sigma+x)^{-1}\Delta(\sigma+x)^{-1}]$$

$$=\int_0^\infty \mathrm{d}x\,\mathrm{Tr}[(\sigma+x)^{-1}\sigma(\sigma+x)^{-1}\Delta]+\int_0^\infty \mathrm{d}x\,\mathrm{Tr}[\Delta(\sigma+x)^{-1}\Delta(\sigma+x)^{-1}].$$

The first integral evaluates to $\mathrm{Tr}[\Delta]$, because

$$\int_0^\infty \mathrm{d}x \frac{s}{(s+x)^2}=1$$

for any $s>0$, and therefore gives the value 0. The second integral can be evaluated most easily in a basis in which σ is diagonal. Denoting by s_i the eigenvalues of σ, we get

$$\int_0^\infty \mathrm{d}x\,\mathrm{Tr}[\Delta(\sigma+x)^{-1}\Delta(\sigma+x)^{-1}]=\sum_{i,j}\Delta_{i,j}\Delta_{j,i}\int_0^\infty \mathrm{d}x (s_i+x)^{-1}(s_j+x)^{-1}$$

$$=\sum_{i\neq j}\Delta_{i,j}\Delta_{j,i}\frac{\log s_i-\log s_j}{s_i-s_j}+\sum_i(\Delta_{i,i})^2\frac{1}{s_i}. \tag{16}$$

The coefficients of $\Delta_{i,j}\Delta_{j,i}$ are easily seen to be always positive, and furthermore, bounded from above by $1/\lambda_{\min}(\sigma)$. Hence we get the upper bound

$$\int_0^\infty \mathrm{d}x\,\mathrm{Tr}[\Delta(\sigma+x)^{-1}\Delta(\sigma+x)^{-1}] \leqslant \frac{\mathrm{Tr}[\Delta^2]}{\lambda_{\min}(\sigma)},$$

yielding an upper bound on the relative entropy which is, indeed, quadratic in Δ:

Theorem 2: *For states ρ and σ with $\Delta=\rho-\sigma$, $T=\|\Delta\|_2$ and $\beta=\lambda_{\min}(\sigma)$,*

$$S(\rho\|\sigma) \leqslant \frac{T^2}{\beta}. \tag{17}$$

B. An upper bound that is logarithmic in the minimum eigenvalue of σ

We have already found a sharper bound than (4) concerning its dependence on $\lambda_{\min}(\sigma)$. However, the bound (5) is not sharp at all concerning its dependence on $\rho-\sigma$. A slight modification can greatly improve this. First note

$$|\mathrm{Tr}[\Delta \log \sigma]| \leqslant \|\Delta\|_1 \cdot \|\log \sigma\|_\infty = \mathrm{Tr}|\Delta| \cdot |\log \lambda_{\min}(\sigma)|.$$

This inequality can be sharpened, since $\mathrm{Tr}[\Delta]=0$ and σ is a state. Let $\Delta=\Delta_+-\Delta_-$ be the Jordan decomposition of Δ, then

$$|\mathrm{Tr}[\Delta \log \sigma]| \leqslant \|\Delta_+\|_1 \cdot |\log \lambda_{\min}(\sigma)|, \tag{18}$$

and hence

$$|\mathrm{Tr}[\Delta \log \sigma]| \leqslant \mathrm{Tr}|\Delta|/2 \cdot |\log \lambda_{\min}(\sigma)|.$$

Further, we have Fannes' continuity of the von Neumann entropy,[15]

$$|S(\sigma+\Delta) - S(\sigma)| \leqslant T \log d + \min\left(-T \log T, \frac{1}{e}\right),$$

where d is the dimension of the underlying Hilbert space and $T := \mathrm{Tr}|\Delta|$. Combining all this with

$$S(\sigma+\Delta\|\sigma) = -(S(\sigma+\Delta) - S(\sigma)) - \mathrm{Tr}[\Delta \log \sigma]$$

gives rise to the subsequent upper bound, logarithmic in the smallest eigenvalue of σ.

Theorem 3: *For all states ρ and σ on a d-dimensional Hilbert space, with $T=\|\rho-\sigma\|_1$ and $\beta=\lambda_{\min}(\sigma)$,*

$$S(\rho\|\sigma) \leqslant T \log d + \min\left(-T \log T, \frac{1}{e}\right) - \frac{T \log \beta}{2}. \tag{19}$$

C. A combination of two bounds?

The following question comes to mind almost automatically: can we combine the two bounds (17) and (19) into a single bound that is both quadratic in Δ and logarithmic in $\lambda_{\min}(\sigma)$? This would certainly be a very desirable feature for a good upper bound. For instance, could it be true that

$$S(\rho\|\sigma) \leqslant C \cdot \mathrm{Tr}[(\rho-\sigma)^2] \cdot |\log \lambda_{\min}(\sigma)|,$$

for some constant $C>0$? Unfortunately, the answer to this first attempt is negative. In fact, the proposed inequality is violated no matter how large the value of C.

Proposition 1: For any $r>0$ there exist states σ and ρ such that

$$S(\rho\|\sigma) > r \cdot \mathrm{Tr}[(\rho-\sigma)^2] \cdot |\log \lambda_{\min}(\sigma)|. \tag{20}$$

Proof: It suffices to consider the case that σ, ρ are states acting on the Hilbert space $\mathbb{C}^2$, and that σ and ρ commute. Hence, the statement must only be shown for two probability distributions

$$P = (p, 1-p), \quad Q = (q, 1-q).$$

Without loss of generality we can require q to be in $[0, 1/2]$. Then, one has to show that for any $r>0$ there exist p, q such that the C^∞ function f, defined as

$$f(p,q,r) = r((p-q)^2 + (2-p-q)^2)|\log(q)| - (p\log(p/q) + (1-p)\log[(1-p)/(1-q)]),$$

assumes a negative value. Now, for any $r>1$, fix a $q \in (0,1/2)$ such that $-4r(q\log q)<1$. Clearly,

$$f(q,q,r) = 0, \qquad \frac{\partial}{\partial p}\bigg|_{p=q} f(p,q,r) = 0.$$

Then

$$\frac{\partial^2}{\partial p^2}\bigg|_{p=q} f(p,q,r) = -\frac{1}{1-q} - \frac{1}{q} - 4r\log(q) < -\frac{1}{q} - 4r\log(q) < 0.$$

This means that there exists an $\varepsilon>0$ such that $f(p,q,r)<0$ for $p \in [q, q+\varepsilon]$, which in turn proves the validity of (20). □

The underlying reason for this failure is that the two bounds (19) and (17) are incompatible, in the sense that there are two different regimes where either one or the other dominates. To see when the logarithmic dependence dominates, let us again take the basis where σ is diagonal, with s_i being the main diagonal elements. When keeping $\Delta=\rho-\sigma$ fixed and $s_1=\lambda_{\min}(\sigma)$ tends to zero, then

$$\lim_{s_1\to 0} S(\sigma+\Delta\|\sigma)/|\log s_1| = \Delta_{1,1} < \infty.$$

Hence, in the regime where $\lambda_{\min}(\sigma)$ tends to zero and $\rho-\sigma$ is fixed, the bound (19) is the appropriate one.

The other regime is the one where σ is fixed and $\rho-\sigma$ tends to zero. This can be intuitively seen by considering the case where the states ρ and σ commute (the classical case). Let p_i and q_i be the diagonal elements of ρ and σ, respectively, in a diagonalizing basis, and $r_i=p_i-q_i$. Then

$$S(\rho\|\sigma) = \sum_i (q_i + r_i)\log(1 + r_i/q_i).$$

We can develop $S(\rho\|\sigma)$ as a Taylor series in the r_i, giving

$$S(\rho\|\sigma) = \sum_i \frac{r_i^2}{2q_i} + O(r_i^3).$$

Hence, in the regime where $\rho-\sigma$ tends to zero and σ is otherwise fixed, the relative entropy exhibits the behaviour of bound (17).

In terms of the matrix derivatives, this notion can be made more precise as follows. Denote the bound (19) as

$$g(\rho\|\sigma) = \frac{\mathrm{Tr}[(\rho-\sigma)^2]}{\lambda_{\min}(\sigma)}$$

for states ρ,σ, then clearly

$$\lim_{\varepsilon\to 0} g(\sigma+\varepsilon\Delta\|\sigma)/\varepsilon = 0.$$

On using the integral representation of the second Fréchet derivative of the matrix logarithm,[4]

$$\frac{\partial^2}{\partial\varepsilon^2}\bigg|_{\varepsilon=0} \log(\sigma+\varepsilon\Delta) = -2\int_0^\infty \mathrm{d}x(\sigma+x)^{-1}\Delta(\sigma+x)^{-1}\Delta(\sigma+x)^{-1},$$

one obtains

$$\left.\frac{\partial^2}{\partial\varepsilon^2}\right|_{\varepsilon=0} S(\sigma+\varepsilon\Delta\|\sigma) = -2\,\mathrm{Tr}\left[\sigma\int_0^\infty \mathrm{d}x(\sigma+x)^{-1}\Delta(\sigma+x)^{-1}\Delta(\sigma+x)^{-1}\right] + 2\,\mathrm{Tr}\left[\Delta\int_0^\infty \mathrm{d}x(\sigma+x)^{-1}\Delta(\sigma+x)^{-1}\right].$$

The right-hand side is bounded from above by

$$\left.\frac{\partial^2}{\partial\varepsilon^2}\right|_{\varepsilon=0} S(\sigma+\varepsilon\Delta\|\sigma) \leqslant \int_0^\infty \mathrm{d}x\,\mathrm{Tr}[\Delta(\sigma+x)^{-1}\Delta(\sigma+x)^{-1}],$$

see Refs. 4 and 22. This bound can be written as in Eq. (16). Therefore, one can conclude that

$$\left.\frac{\partial^2}{\partial\varepsilon^2}\right|_{\varepsilon=0} S(\sigma+\varepsilon\Delta\|\sigma) = \left.\frac{\partial^2}{\partial\varepsilon^2}\right|_{\varepsilon=0} g(\sigma+\varepsilon\Delta\|\sigma)$$

holds for all Δ satisfying $\mathrm{Tr}[\Delta]=0$ if and only if $\sigma=\mathbb{1}/d$, where d is the dimension of the underlying Hilbert space. These considerations seem to spell doom for any attempt at "unifying" the two kinds of upper bounds. However, below we will see how a certain change of perspective will allow us to get out of the dilemma.

VI. A SHARP LOWER BOUND IN TERMS OF NORM DISTANCE

We define $S_{\min}(T)$ with respect to a norm to be the smallest relative entropy between two states that have a distance of exactly T in that norm, that is

$$S_{\min}(T) = \min_{\rho,\sigma}\{S(\rho\|\sigma):|||\rho-\sigma||| = T\}. \tag{21}$$

When one agrees to assign $S(\rho\|\sigma)=+\infty$ for nonpositive ρ, the definition of $S_{\min}$ can be rephrased as

$$S_{\min}(T) = \min_{\Delta,\sigma}\{S(\sigma+\Delta\|\sigma):|||\Delta||| = T,\mathrm{Tr}[\Delta]=0\}. \tag{22}$$

Intuitively one would guess that $S_{\min}$ is monotonously increasing with T. The following lemma shows that this is true, but some care is required in proving it.

Lemma 7: For $T_1\leqslant T_2$, $S_{\min}(T_1)\leqslant S_{\min}(T_2)$.

Proof: Keep σ fixed and define

$$f_\sigma(T) = \min_{\Delta}\{S(\sigma+\Delta\|\sigma):|||\Delta||| = T,\mathrm{Tr}[\Delta]=0\},$$

so that $S_{\min}(T)=\min_\sigma f_\sigma(T)$. Considering $S(\sigma+\Delta\|\sigma)$ as a function of Δ, it is convex and minimal in the origin $\Delta=0$. Further, for the norm balls

$$\mathcal{B}(T) := \{\Delta:|||\Delta||| \leqslant T,\mathrm{Tr}[\Delta]=0\} \tag{23}$$

we have

$$\{0\} = \mathcal{B}(0) \subseteq \mathcal{B}(T_1) \subseteq \mathcal{B}(T_2). \tag{24}$$

This is sufficient to prove that $0=f_\sigma(0)\leqslant f_\sigma(T_1)\leqslant f_\sigma(T_2)$. Now, since this holds for any σ, it also holds when minimising over σ, and that is just the statement of the lemma. □

As a direct consequence, a third equivalent definition of $S_{\min}(T)$ is

$$S_{\min}(T) = \min_{\Delta,\sigma}\{S(\sigma+\Delta\|\sigma):|||\Delta||| \geqslant T,\mathrm{Tr}[\Delta]=0\}. \tag{25}$$

We now show that one can restrict oneself to the commutative case.

Lemma 8: The minimum in Eq. (22) is obtained for σ and Δ commuting.

Proof: Fix Δ and consider a basis in which Δ is diagonal. Let $\rho \mapsto \mathrm{Diag}(\rho)$ be the completely positive trace-preserving map which, in that basis, sets all off-diagonal elements of ρ equal to zero. Thus $\mathrm{Diag}(\Delta)=\Delta$. By monotonicity of the relative entropy,

$$S(\sigma+\Delta\|\sigma) \geqslant S(\mathrm{Diag}(\sigma)+\Delta\|\mathrm{Diag}(\sigma)).$$

Minimizing over all states σ then gives

$$\min_{\sigma} S(\sigma+\Delta\|\sigma) \geqslant \min_{\sigma} S(\mathrm{Diag}(\sigma)+\Delta\|\mathrm{Diag}(\sigma)) = \min_{\sigma}\{S(\sigma+\Delta\|\sigma):[\sigma,\Delta]=0\}.$$

On the other hand, the states σ that commute with Δ are included in the domain of minimization of the left-hand side, hence equality holds. □

For later reference we define the auxiliary function

$$s(x) := \min_{0<r<1-x} S((r+x,1-r-x)\|(r,1-r)), \tag{26}$$

for $0 \leqslant x < 1$. An equivalent expression for this function is given by

$$s(x) := \min_{x<r<1} S((r-x,1-r+x)\|(r,1-r)). \tag{27}$$

The first three nonzero terms in its series expansion around $x=0$ are given by

$$s(x) = 2x^2 + \frac{4}{9}x^4 + \frac{32}{135}x^6 + O(x^8) \tag{28}$$

(obtained using a computer algebra package). Further calculations reveal that some of the higher-order coefficients are negative, the first one being the coefficient of x^{62}. One can easily prove[23] that the lowest order expansion $2x^2$ is actually a lower bound. It is, therefore, the sharpest quadratic lower bound. For values of x up to $1/2$, the error incurred by considering only the lowest order term in (28) is at most 6.5%. For larger values of x, the error increases rapidly. In fact, when x tends to its maximal value of 1, $s(x)$ tends to infinity, as can easily be seen from the minimisation expression (r tends to 0); accordingly, the series expansion diverges. For values of $x > 4/5$, $s(x)$ is well approximated by its upper bound

$$s(x) \leqslant \lim_{r\to 1-x} S((r+x,1-r-x)\|(r,1-r)) = -\log(1-x).$$

This is illustrated in Fig. 1.

Let us now come back to Eq. (22), with σ and Δ diagonal, and $|||.|||$ any unitarily invariant norm. Let σ and Δ have diagonal elements σ_k and Δ_k, respectively. Fixing Δ, we minimize first over σ. This is a convex problem and any local minimum is automatically a global minimum.[20] The corresponding Lagrangian is

$$\mathcal{L} = \sum_k \sigma_k(1+\Delta_k/\sigma_k)\log(1+\Delta_k/\sigma_k) - \nu\left(\sum_k \sigma_k - 1\right). \tag{29}$$

The derivative of the Lagrangian with respect to σ_k is

$$\frac{\partial \mathcal{L}}{\partial \sigma_k} = \log(1+\Delta_k/\sigma_k) - \Delta_k/\sigma_k - \nu. \tag{30}$$

This must vanish in a critical point, giving the expression

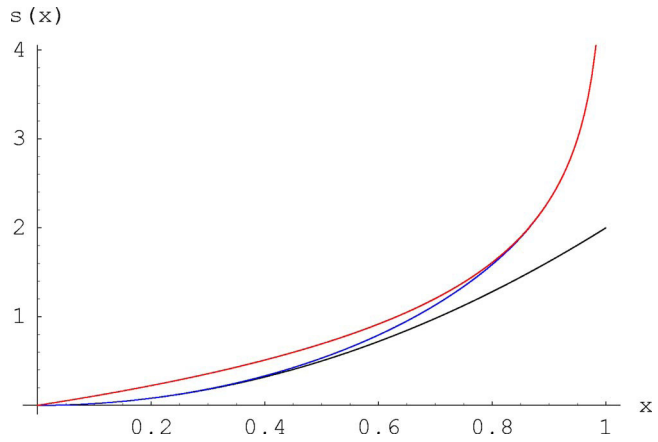

FIG. 1. (Color online) Function s defined in Eq. (26) (middle curve), the lower bound $2x^2$ (lower curve), and the upper bound $-\log(1-x)$ (upper curve).

$$\log(1+\Delta_k/\sigma_k) = \Delta_k/\sigma_k + \nu. \tag{31}$$

Now note that the equation $\log(1+x)-x=b$, for $b<0$ has only two real solutions, one positive and one negative, and none for $b>0$. Therefore, for any $k\Delta_k/\sigma_k$ can assume only one of these two possible values. Let K be an integer between 1 and $d-1$. Without loss of generality we can set

$$\Delta_k/\sigma_k = \begin{cases} c_p, & 1 \leqslant k \leqslant K \\ -c_m, & K < k \leqslant d, \end{cases} \tag{32}$$

where c_p and c_m are positive numbers, to be determined along with K. The requirement $\Sigma_k\Delta_k = 0$ imposes

$$c_p \sum_{k=1}^{K} \sigma_k - c_m \sum_{k=K+1}^{d} \sigma_k = 0,$$

which upon defining

$$r := \sum_{k=1}^{K} \sigma_k, \tag{33}$$

turns into

$$c_p r = c_m(1-r) =: c. \tag{34}$$

Substituting Eqs. (32) and (33), the function to be minimized becomes

$$r(1+c_p)\log(1+c_p) + (1-r)(1-c_m)\log(1-c_m),$$

which, given Eq. (34), can be rewritten as

$$S((r+c, 1-r-c)\|(r, 1-r)).$$

The one remaining constraint $|||\Delta||| = T$ likewise becomes

$$|||(c_p\sigma_1, \ldots, c_p\sigma_K, -c_m\sigma_{K+1}, \ldots, -c_m\sigma_d)||| = T.$$

Defining

$$\tau' := (\sigma_1, \ldots, \sigma_K)/r,$$

$$\tau'' := (\sigma_{K+1}, \ldots, \sigma_d)/(1-r),$$

this turns into

$$T = |||(c_p r\tau'; -c_m(1-r)\tau'')||| = c|||(\tau';\tau'')|||,$$

where we have exploited the homogeneity of a norm. Note that by their definition, τ' and τ'' are vectors consisting of positive numbers adding up to 1.

The minimization itself thus turns into

$$S_{\min}(T) = \min_{r,\tau',\tau''} S((r+c,1-r-c)\|(r,1-r)),$$

where $c := T/|||(\tau';\tau'')|||$. Quite obviously, the minimum over c is obtained for the smallest possible c, hence

$$S_{\min}(T) = \min_{r} S((r+T/\gamma,1-r-T/\gamma)\|(r,1-r)) = s(T/\gamma),$$

with

$$\gamma = \max_{\tau',\tau''} |||(\tau';\tau'')|||.$$

By convexity of a norm, this maximum is obtained in an extreme point, so

$$\gamma = |||F|||.$$

Incidentally, by Lemma 5, this value is also the maximum

$$\max_{\rho,\sigma} |||\rho-\sigma|||,$$

over all possible states ρ and σ, i.e., γ is the largest possible value of T for the given norm. We have thus proven

Theorem 4: *For any unitarily invariant norm* $|||.|||$, *we have the sharp lower bound*

$$S(\rho\|\sigma) \geqslant s(|||\rho-\sigma|||/|||F|||). \tag{35}$$

A few remarks are in order at this point:

(1) Within the setting of finite-dimensional systems, this theorem generalizes a result of Refs. 4 and 24 for the trace norm to all unitarily invariant norms. This article also uses the technique of getting lower bounds by projecting on an abelian subalgebra and then exploiting the case of a two-dimensional support as the worst case scenario.

(2) If we take the results of Refs. 4 and 24 for granted and combine it with Lemma 3, we immediately get

$$S(\rho\|\sigma) \geqslant s(\|\rho-\sigma\|_1/\|F\|_1) \geqslant s(|||\rho-\sigma|||/|||F|||).$$

(3) The divergence of s at $x=1$ is easily understood. The largest norm difference between two states occurs for orthogonal pure states, in which case their relative entropy is infinite.

VII. SHARP UPPER BOUNDS IN TERMS OF NORM DISTANCE

Let now $S_{\max}(T,\beta)$ be the largest relative entropy between ρ and σ that have a normalized distance of exactly T and $\lambda_{\min}(\sigma)=\beta$, so let

$$S_{\max}(T,\beta) := \max_{\rho,\sigma}\left\{ S\left(\rho||\sigma\right): \frac{|||\rho-\sigma|||}{|||F|||} = T, \lambda_{\min}(\sigma) = \beta \right\}. \tag{36}$$

The need for the extra parameter β arises because for $\beta=0$, $S_{\max}$ is infinite, as can be seen by taking different pure states for ρ and σ. We can rephrase this definition as

$$S_{\max}(T,\beta) = \max_{\Delta,\sigma}\left\{ S(\sigma+\Delta\|\sigma): \frac{|||\Delta|||}{|||F|||} = T, \mathrm{Tr}[\Delta]=0, \sigma+\Delta \geqslant 0, \lambda_{\min}(\sigma)=\beta \right\}. \tag{37}$$

Because Δ commutes with the identity matrix, there is a unique common least upper bound on $\beta\mathbb{1}$ and $-\Delta$, which we will denote by $\max(\beta\mathbb{1},-\Delta)$. In the eigenbasis of Δ, this is a diagonal matrix with diagonal elements $\max(\beta,-\Delta_i)$. The constraints $\sigma\geqslant\beta$ and $\sigma+\Delta\geqslant 0$ can therefore be combined into the single constraint

$$\sigma \geqslant \max(\beta\mathbb{1},-\Delta). \tag{38}$$

The extremal σ obeying this constraint are

$$\sigma = \max(\beta\mathbb{1},-\Delta) + \eta|\psi\rangle\langle\psi|, \tag{39}$$

where ψ is any state vector, and

$$\eta := 1 - \mathrm{Tr}[\max(\beta\mathbb{1},-\Delta)]. \tag{40}$$

Therefore, the constrained maximisation over σ can be replaced by an unconstrained maximisation over all pure states of the function

$$S(\Delta + \max(\beta\mathbb{1},-\Delta) + \eta|\psi\rangle\langle\psi| \,\|\max(\beta\mathbb{1},-\Delta) + \eta|\psi\rangle\langle\psi|). \tag{41}$$

Of course, all of this puts constraints on Δ as well. Indeed, in order that states σ obeying (38) exist, $\max(\beta\mathbb{1},-\Delta)$ must obey the condition

$$\mathrm{Tr}[\max(\beta\mathbb{1},-\Delta)] \leqslant 1. \tag{42}$$

We now have to distinguish between two cases: the case $d=2$, and the case $d>2$.

A. The case $d=2$

For the $d=2$ case, the maximization over Δ is trivial. In its eigenbasis, Δ is a multiple of $\mathrm{Diag}(1,-1)=F$. Hence, fixing the eigenbasis of Δ (which we can do because of unitary invariance of the relative entropy), and fixing

$$|||\Delta|||/|||F||| = T, \tag{43}$$

actually leaves just one possibility for Δ, namely $\Delta=TF$. The term $\max(\beta\mathbb{1},-\Delta)$ leads to two cases: $T\leqslant\beta$ and $T>\beta$.

The condition $T\leqslant\beta$ implies, by Lemma 3, that $\|\Delta\|_\infty\leqslant\beta$ and, hence,

$$\max(\beta\mathbb{1},-\Delta) = \mathrm{Diag}(\beta,\beta),$$

$$\eta = 1-2\beta.$$

The remaining maximization of (41) is therefore given by

$$\max_{\psi} S(\mathrm{Diag}(\beta+T,\beta-T)+(1-2\beta)|\psi\rangle\langle\psi|\,\|\mathrm{Diag}(\beta,\beta)+(1-2\beta)|\psi\rangle\langle\psi|). \tag{44}$$

Positivity of η requires $\beta\leqslant 1/2$. By unitary invariance of the relative entropy, and invariance of diagonal states under diagonal unitaries (phase factors), we can restrict ourselves to vectors ψ of the form $\psi=(\cos\alpha,\sin\alpha)^T$.

Lemma 9: For a state vector $\psi=(\cos\alpha,\sin\alpha)^T$, *the function to be maximized in (44) is convex in* $\cos(2\alpha)$.

Proof: Let D_1 be the determinant of the first argument. It is linear in $t:=\cos(2\alpha)$:

$$D_1=\beta^2-T^2+(1-2\beta)(\beta-Tt).$$

After some basic algebra involving eigensystem decompositions of the states, the function to be maximized in (44) is found to be given by

$$f(x):=((1-x)\log(1-x)+(1+x)\log(1+x))/2+(-1+2\beta-2Tt)(\log(1-\beta)-\log\beta)/2$$
$$-(\log(4-4\beta)+\log\beta)/2,$$

where $x=(1-4D_1)^{1/2}$. We will now show that this function is convex in t. Since the second and third terms are linear in t, we only need to show convexity for the first term. The series expansion of the first term is

$$((1-x)\log(1-x)+(1+x)\log(1+x))/2=\sum_{k=1}^{\infty}\frac{x^{2k}}{2k(2k-1)}.$$

Every term in the expansion is a positive power of x^2 with positive coefficient and is therefore convex in x^2, which itself is linear in t.The sum is therefore also convex in t. □

By the previous lemma, the maximum of the maximization over ψ is obtained for extremal values of t, that is: either $\psi=(1,0)^T$ or $\psi=(0,1)^T$. Evaluation of the maximum is now straightforward and it can be checked that the choice $\psi=(1,0)^T$ always yields the largest value of the relative entropy.

We will now more specifically look at the case where $T>\beta$. In this case, we get

$$\max(\beta\mathbb{1},-\Delta)=\mathrm{Diag}(\beta,T),$$

$$\eta=1-\beta-T,$$

and the remaining maximization of (41) is given by

$$\max_{\psi} S(\mathrm{Diag}(\beta+T,0)+(1-\beta-T)|\psi\rangle\langle\psi|\,\|\mathrm{Diag}(\beta,T)+(1-\beta-T)|\psi\rangle\langle\psi|). \tag{45}$$

Positivity of η requires $\beta\leqslant 1/2$ and $T\leqslant 1-\beta$. Again, we can restrict ourselves to states $\psi=(\cos\alpha,\sin\alpha)^T$. We also have the equivalent of Lemma 9, which needs more work in this case.

Lemma 10: For a state vector $\psi=(\cos\alpha,\sin\alpha)^T$, *the function to be maximised in (45) is convex in* $\cos(2\alpha)$.

Proof: Let D_1 and D_2 be the determinant of the first and second argument, respectively. Both are linear in $t:=\cos(2\alpha)$:

$$D_1=(1-\beta-T)(\beta+T)(1-t)/2,$$

$$D_2=((\beta+T-\beta^2-T^2)+(1-\beta-T)(T-\beta)t)/2.$$

In the (D_1,D_2) plane, this describes a line segment with gradient

$$K := -\frac{T-\beta}{T+\beta},$$

which lies in the interval $[-1,0]$.

Again, after some basic algebra, the function to be maximized in (45) is identified to be $f((1-4D_1)^{1/2},(1-4D_2)^{1/2})$, where

$$f(x,y) := ((1-x)\log(1-x)+(1+x)\log(1+x))/2 + ((x^2+y^2-2y-4T^2)\log(1-y) - (x^2+y^2+2y-4T^2)\log(1+y))/4y.$$

We will now show that $f((1-4D_1)^{1/2},(1-4D_2)^{1/2})$ is convex in t. First, note that

$$f(x,y) = f_0(x,y) + T^2 f_1(y).$$

The term $f_1(y)$ is itself convex in t: its series expansion is

$$f_1(y) = (\log(1+y)-\log(1-y))/y = 2\sum_{k=0}^{\infty}\frac{y^{2k}}{2k+1},$$

which by the positivity of all its coefficients is convex in y^2, and y^2 is linear in t.

The other term, $f_0(x,y)$ is given by a sum of three terms

$$f_0(x,y) = \frac{1}{2}((1-x)\log(1-x)+(1+x)\log(1+x)) + \frac{1}{4}((y-2)\log(1-y)-(y+2)\log(1+y)) - \frac{x^2}{4}(\log(1+y)-\log(1-y))/y.$$

Replacing each of the three terms by its series expansion yields

$$f_0(x,y) = \sum_{k=1}^{\infty}\frac{x^{2k}}{2k(2k-1)} + \sum_{k=1}^{\infty}(k-1)\frac{y^{2k}}{2k(2k-1)} - \frac{x^2}{2}\sum_{k=0}^{\infty}\frac{y^{2k}}{2k+1}.$$

To show that this function is convex in t, we will evaluate it along the curve

$$x^2 = u+p,$$

$$y^2 = v+Kp,$$

with gradient K between 0 and -1, and u and v lying in the interval $[0,1]$, and check positivity of its second derivative with respect to p at $p=0$:

$$\left.\frac{\partial^2}{\partial p^2}\right|_{p=0} f_0(x,y) = \sum_{k=2}^{\infty}\frac{k-1}{2k-1}u^{k-2} + (k-1)\left(K\frac{(k-1)K-2}{2k-1} - K^2\frac{k}{2k+1}u\right)v^{k-2}.$$

The coefficient of u^{k-2} is clearly positive, hence the derivative is positive if the coefficient of v^{k-2} is positive for all allowed values of u and K. The worst case occurs for $u=1$, yielding a coefficient

$$K\frac{(k-1)K-2}{2k-1} - K^2\frac{k}{2k+1} = \frac{-K(2+4k+K)}{(2k-1)(2k+1)}.$$

For values of K between 0 and -1, this is indeed positive. □

By the previous lemma, the maximum of the maximization over ψ is obtained for extremal values of t, that is: either $\psi=(1,0)^T$ or $\psi=(0,1)^T$. Evaluation of the maximum is again straightforward, and calculations show that sometimes $\psi=(1,0)^T$ yields the larger value, and sometimes $\psi=(0,1)^T$. In this way we have obtained the upper bounds.

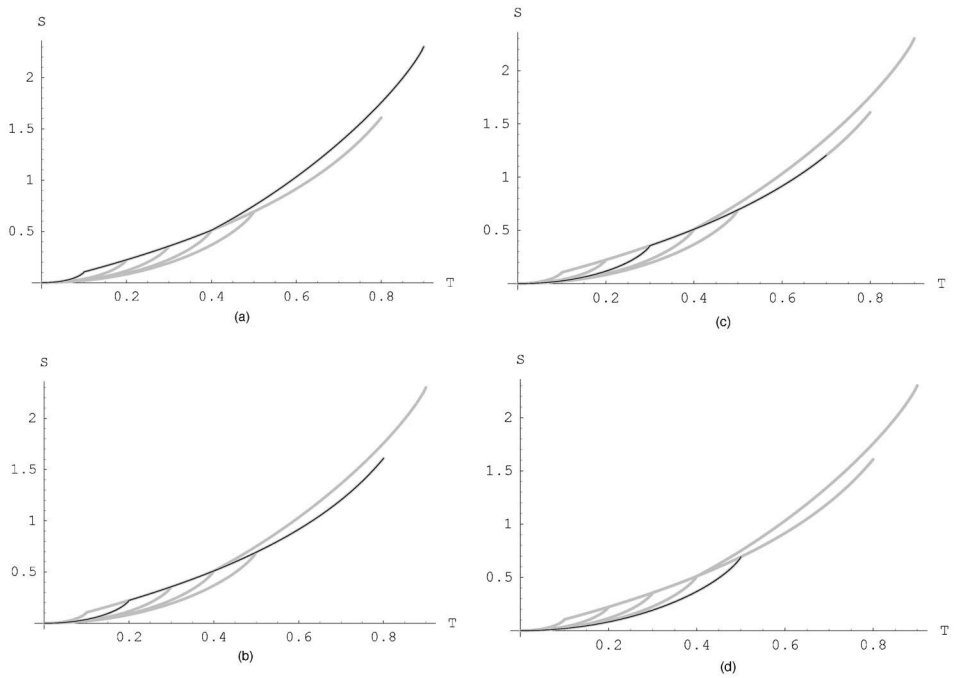

FIG. 2. Upper bounds of Theorem 5 on $S=S(\rho\|\sigma)$ vs. the rescaled norm distance $T=|||\rho-\sigma|||/|||F|||$, for $d=2$, and for values of smallest eigenvalue of σ (a) $\beta=0.1$, (b) 0.2, (c) 0.3, and (d) 0.5. The two regimes $T\leqslant\beta$ and $\beta\leqslant T\leqslant 1-\beta$ can be clearly identified. For ease of comparison, each curve is shown superimposed on the curves for $\beta=0.1$, 0.2, 0.3, 0.4, and 0.5 shaded line.

Theorem 5: *Let* $\Delta=\rho-\sigma$, $T=|||\Delta|||/|||F|||$ *and* $\beta=\lambda_{\min}(\sigma)$. *For* $d=2$, *and* $T\leqslant\beta$,

$$S(\rho\|\sigma)\leqslant(T+1-\beta)\log\frac{T+1-\beta}{1-\beta}+(\beta-T)\log(1-T/\beta). \tag{46}$$

For $d=2$, *and* $T>\beta$,

$$S(\rho\|\sigma)\leqslant\max(-\log(1-T)\ ,$$

$$(\beta+T)\log(1+T/\beta)+\ (1-\beta-T)\log(1-T/(1-\beta))). \tag{47}$$

It is interesting to study the behavior of the bound in the case of large β. More specifically, an approximation for bound (46), valid for $T\ll\beta$, is

$$S(\rho\|\sigma)\leqslant\sum_{k=2}^{\infty}\frac{T^k}{k(k-1)}\left(\frac{1}{\beta^k}-\frac{(-1)^k}{(1-\beta)^k}\right)\approx\frac{T^2}{2\beta(1-\beta)}, \tag{48}$$

Figure 2 illustrates the combined upper bounds of Theorem 5 ($d=2$) for various values of β.

B. The case $d>2$

In case d is larger than 2, it is not clear how to proceed in the most general setting, for general UI norms, as the maximization over Δ must explicitly be performed. In the following, we will restrict ourselves to using the trace norm, which is in some sense the most important one anyway. That is, the requirements on Δ are

$$\|\Delta\|_1=2T, \tag{49}$$

$$\mathrm{Tr}[\Delta] = 0, \tag{50}$$

$$\mathrm{Tr}[\max(\beta\mathbb{1}, -\Delta)] \leqslant 1. \tag{51}$$

The following very simple lemma will prove to be a powerful tool.

Lemma 11: For all A, B, and C, *positive semidefinite operators*,

$$S(A + C\|B + C) \leqslant S(A\|B).$$

Proof: First note that for any $a > 0$,

$$S(aA\|aB) = \mathrm{Tr}[aA(\log(aA) - \log(aB))] = aS(A\|B).$$

This, together with joint convexity of the relative entropy in its arguments (which need not be normalized to trace 1), leads to

$$S(A + C\|B + C) = 2S\left(\frac{A + C}{2}\middle\|\frac{B + C}{2}\right) \leqslant S(A\|B) + S(C\|C) = S(A\|B).$$

□

The Lemma immediately yields an upper bound on (41): letting

$$\sigma := \max(\beta\mathbb{1}, -\Delta) + \eta|\psi\rangle\langle\psi|,$$

such that we obtain

$$S(\Delta + \sigma\|\sigma) \leqslant S(\Delta + \max(\beta\mathbb{1}, -\Delta)\|\max(\beta\mathbb{1}, -\Delta)) = S((\Delta + \beta\mathbb{1})_+\|\beta\mathbb{1} + (\Delta + \beta\mathbb{1})_-). \tag{52}$$

To continue, we consider two cases.

Case 1: When $T \leqslant \beta$, requirement (51) is automatically satisfied, and $\max(\beta\mathbb{1}, -\Delta) = \beta\mathbb{1}$. Let Δ_+ and Δ_- be the positive and negative part of Δ, respectively. That is, $\Delta = \Delta_+ - \Delta_-$, with Δ_+ and Δ_- nonnegative and orthogonal. Because we are using the trace norm we can rewrite the conditions on Δ as

$$\|\Delta\|_1 = \mathrm{Tr}[\Delta_+] + \mathrm{Tr}[\Delta_-] = 2T,$$

$$\mathrm{Tr}[\Delta] = \mathrm{Tr}[\Delta_+] - \mathrm{Tr}[\Delta_-] = 0,$$

hence

$$\mathrm{Tr}[\Delta_+] = \mathrm{Tr}[\Delta_-] = T.$$

By Lemma 11, (41) is upper bounded by $S(\Delta + \beta\mathbb{1}\|\beta\mathbb{1})$. By convexity, its maximum over Δ_+, $\Delta_- \geqslant 0$, with $\mathrm{Tr}[\Delta_+] = \mathrm{Tr}[\Delta_-] = T$, is obtained in Δ_+ and Δ_- of rank 1, giving as upper bound

$$S(\Delta + \sigma\|\sigma) \leqslant (\beta + T)\log\frac{\beta + T}{\beta} + (\beta - T)\log\frac{\beta - T}{\beta}.$$

The upper bound can be achieved in dimensions $d \geqslant 3$ for all values of $T \leqslant \beta$ by setting $\Delta = TF$ and $\psi = e^3$.

Case 2: In the other case, when $T > \beta$, we have to deal with condition (51). To do that we split Δ into three nonnegative parts,

$$\Delta = \Delta_+ - \Delta_0 - \Delta_-, \tag{53}$$

with Δ_+, Δ_0 and Δ_-, operating on orthogonal subspaces V_+, V_0 and V_-, respectively, with

$$\Delta_+ \geqslant 0,$$

$$0 \geqslant -\Delta_0 \geqslant -\beta\mathbb{1}_0,$$

$$-\beta\mathbb{1}_- \geqslant -\Delta_-.$$

We denote the projectors on these subspaces by $\mathbb{1}_+$, $\mathbb{1}_0$, and $\mathbb{1}_-$. Then

$$(\Delta+\beta)_+ = \Delta_+ - \Delta_0 + \beta\mathbb{1}_{+0},$$

where $\mathbb{1}_{+0} := \mathbb{1}_+ + \mathbb{1}_0$. The conditions on Δ, $\mathrm{Tr}[\Delta]=0$ and $\mathrm{Tr}[|\Delta|]=2T$ translate to

$$\mathrm{Tr}[\Delta_+] = \mathrm{Tr}[\Delta_0] + \mathrm{Tr}[\Delta_-] = T.$$

Due to the orthogonality of positive and negative part, (52) can be simplified to $S((\Delta+\beta\mathbb{1})_+ \| \beta\mathbb{1}_{+0})$. After subtracting $\beta\mathbb{1}_0 - \Delta_0$ from both arguments, we get

$$S(\Delta_+ + \beta\mathbb{1}_+ \| \beta\mathbb{1}_+ + \Delta_0),$$

which is an upper bound on (52), by Lemma 11. Ignoring condition (51) on Δ, we get

$$S_{\max} \leqslant \max_{\substack{\Delta_+ \geqslant 0 \\ \mathrm{Tr}[\Delta_+]=T}} S(\Delta_+ + \beta\mathbb{1}_+ \| \beta\mathbb{1}_+).$$

By convexity, the maximum is obtained for Δ_+ rank 1, giving the upper bound

$$S_{\max} \leqslant (T+\beta)\log((T+\beta)/\beta).$$

To see that this bound is sharp for (almost) any value of T, consider the two states

$$\rho = \mathrm{Diag}(T+\beta, 0, 0^{\times J}, \beta^{\times K}, \beta+\eta),$$

$$\sigma = \mathrm{Diag}(\beta, T-J\beta, \beta^{\times J}, \beta^{\times K}, \beta+\eta),$$

$$\eta := 1 - T - (d-1-J)\beta.$$

Here, J is an integer between 0 and $d-3$ and $k=d-3-J$. Conditions on J are $J\beta \leqslant T$ (so that $\sigma \geqslant 0$) and $T \leqslant 1-(d-1-J)\beta$ (so that $\eta \geqslant 0$). This choice of states can thus be obtained for $\beta \leqslant T \leqslant 1-2\beta$. It can be seen that $\|\rho-\sigma\|_1 = 2T$ and

$$S(\rho\|\sigma) = (T+\beta)\log((T+\beta)/\beta). \tag{54}$$

The result of the foregoing can be subsumed into the following theorem.

Theorem 6: *Let* $\Delta=\rho-\sigma$, $T=\|\Delta\|_1/2$ *and* $\beta=\lambda_{\min}(\sigma)$. *If* $T \leqslant \beta$ *then*

$$S(\rho\|\sigma) \leqslant (\beta+T)\log\frac{\beta+T}{\beta} + (\beta-T)\log\frac{\beta-T}{\beta}, \tag{55}$$

and this upper bound is sharp when $d>2$. *If* $\beta \leqslant T \leqslant 1-\beta$ *then*

$$S(\rho\|\sigma) \leqslant (\beta+T)\log\frac{\beta+T}{\beta}. \tag{56}$$

When $d>2$, *this bound is sharp for (at least)* $\beta \leqslant T \leqslant 1-2\beta$.

Figure 3 illustrates these bounds and shows their superiority to the previously obtained bound (19).

Again, it is interesting to look at the bound for large β. An approximation for bound (55), valid for $T \ll \beta$, is given by

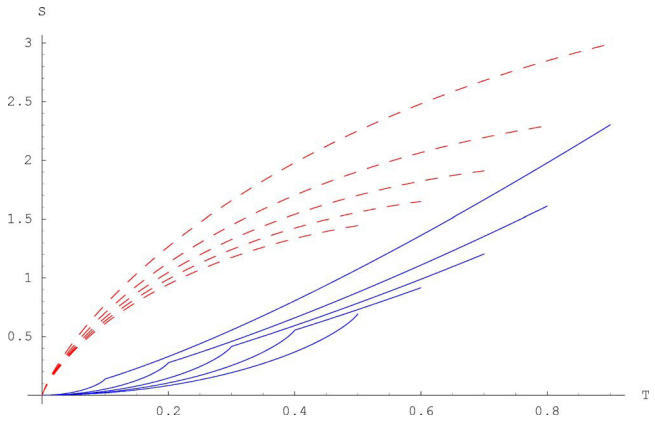

FIG. 3. (Color online) Comparison between upper bounds (19), (55), and (56) on $S=S(\rho\|\sigma)$ vs. the trace norm distance $T=\|\rho-\sigma\|_1/2$, for various values of β, the smallest eigenvalue of σ. The upper set of dashed curves depict bound (19) (with $d=3$) for $\beta=0.1$ (lower curve), 0.2, 0.3, 0.4, and 0.5 (upper curve). The lower set of full line curves depict bounds (55) and (56) for $\beta=0.1$ (upper curve), 0.2, 0.3, 0.4, and 0.5 (lower curve). The two regimes $T\leqslant\beta$ and $\beta\leqslant T\leqslant 1-\beta$ can be clearly seen.

$$S(\rho\|\sigma)\leqslant\sum_{k=1}^{\infty}\frac{T^{2k}}{k(2k-1)\beta^{2k-1}}\approx\frac{T^2}{\beta}. \tag{57}$$

VIII. APPLICATION TO STATE APPROXIMATION

In the following paragraph we will give an application of our bounds to state approximation. Consider a state ρ on a Hilbert space $\mathcal{H}$, and a sequence $\{\sigma_n\}_n$ where σ_n is a state on $\mathcal{H}^{\otimes n}$. As before, the sequence is said to asymptotically approximate ρ if for n tending to infinity, $\|\sigma_n-\rho^{\otimes n}\|_1=\mathrm{Tr}|\sigma_n-\rho^{\otimes n}|$ tends to zero. Let us define T_n as

$$T_n:=\mathrm{Tr}|\rho^{\otimes n}-\sigma_n|/2.$$

Because of the lower bound (6), we get

$$S_n:=S(\rho^{\otimes n}\|\sigma_n)\geqslant 2T_n^2,$$

and this bound is sharp. Hence, T_n goes to zero if S_n does.

On the other hand, T_n going to zero does not necessarily imply S_n going to zero. Indeed, S_n can be infinite for any finite value of n when $\rho^{\otimes n}$ is not restricted to the range of σ_n. In particular, the relative entropy distance between two pure states is infinite unless the states are identical. At first sight, this seems to render the relative entropy useless as a distance measure. Nevertheless, sense can be made of it by imposing an additional requirement that the range of σ_n must contain the range of $\rho^{\otimes n}$. Let us then restrict σ_n to the range of $\rho^{\otimes n}$, as the relative entropy only depends on that part of σ_n. Letting d be the rank of ρ, the dimension of the range of $\rho^{\otimes n}$ is d^n. Let β_n be the smallest nonzero eigenvalue of σ_n on that range; β_n is at most $1/d^n$.

The behavior of the relative entropy then very much depends on the relation between β_n and T_n. Since β_n decreases at least exponentially, we only need to consider the case $T_n\geqslant\beta_n$, and use the bound (56)

$$S_n\leqslant(\beta_n+T_n)\log\left(1+\frac{T_n}{\beta_n}\right).$$

In the worst-case behavior of T_n (T_n/β_n tending to infinity) the bound can be approximated by

$$S_n \leqslant T_n \log \frac{T_n}{\beta_n} = T_n(\log T_n - \log \beta_n) \approx T_n |\log \beta_n|.$$

To guarantee convergence of S_n we therefore need T_n to converge to 0 at least as fast as $1/|\log \beta_n|$, which in the best case goes as $1/n$. Note that bound (19) yields the same requirement, but as this bound is not a sharp one it could have been too strong a requirement. This gives us the subsequent theorem.

Theorem 7: *Consider a state ρ on a finite-dimensional Hilbert space $\mathcal{H}$ and a sequence $\{\sigma_n\}_n$ of states σ_n on $\mathcal{H}^{\otimes n}$. The sequence $\{\sigma_n\}_n$ asymptotically approximates ρ in the trace norm, if*

$$\lim_{n\to\infty} S(\rho^{\otimes n} \| \sigma_n) = 0. \tag{58}$$

Conversely, if the range of σ_n includes the range of $\rho^{\otimes n}$ and $\|\rho^{\otimes n} - \sigma_n\|_1$ *converges to zero faster than $1/|\log \beta_n|$, where β_n is the minimal eigenvalue of σ_n restricted to the range of $\rho^{\otimes n}$, then* $\lim_{n\to\infty} S(\rho^{\otimes n} \| \sigma_n) = 0$.

IX. SUMMARY

In this article, we have discussed several lower and upper bounds on the relative entropy functional, thereby sharpening the notion of continuity of the relative entropy for states which are close to each other in the trace norm sense.

The main results are the sharp lower bound from Theorem 4, and the sharp upper bounds of Theorems 5 ($d=2$) and 6 ($d>2$). Theorems 4 and 5 give the relation between relative entropy and norm distances based on any unitarily invariant norm, while Theorem 6 holds only for the trace norm distance. These results have been obtained employing methods from optimization theory.

ACKNOWLEDGMENTS

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The frequency spectrum of the Casimir effect

Andrew S. I. D. Lang[a)]
Computer Science and Mathematics Department, Oral Roberts University, Tulsa, Oklahoma 74171

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The frequency spectrum of the Casimir effect between parallel plates is studied. Calculations are performed for both the massless scalar field and the electromagnetic field cases, first using a spectral weight function, and then via the Fourier transform of the renormalized expectation of the Casimir energy-momentum operator. The Casimir force is calculated using the spectrum for two plates which are perfectly transparent in a frequency band. The result of this calculation suggests a way to detect the frequency spectrum of the Casimir effect. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2046529]

I. INTRODUCTION

The Casimir effect[1] is a force between two physical objects, classically a pair of perfectly conducting parallel plates, resulting from quantum vacuum fluctuations of the electromagnetic field between them. In recent years, this relatively small effect has been detected in the laboratory.[2] It has also been extensively studied, see Bordag *et al.*[3] for a comprehensive review, and Milton[4] for a more recent one.

Between two perfectly conducting parallel plates, the Casimir effect can be calculated by subtracting the infinite regularized vacuum zero-point energy per unit area of the electromagnetic field

$$E_v(l) = \hbar c \lim_{\Omega\to\infty} \frac{3l}{\pi^2}\Omega^4, \tag{1}$$

from the again infinite regularized zero-point energy per unit area for the electromagnetic field between the two plates

$$E_p(l) = \hbar c \lim_{\Omega\to\infty} \left(\frac{3l}{\pi^2}\Omega^4 - \frac{1}{720}\frac{\pi^2}{l^3} + O\left(\frac{1}{\Omega}\right)\right), \tag{2}$$

to obtain a renormalized energy between the two plates of

$$E(l) = \hbar c \lim_{\Omega\to\infty} \left(-\frac{1}{720}\frac{\pi^2}{l^3} + O\left(\frac{1}{\Omega}\right)\right) = -\frac{\pi^2\hbar c}{720 l^3}. \tag{3}$$

Even though the zero-point energies given by (1) and (2) are infinite, for which as yet there is no complete understanding, most physics only involves differences in energies. So by renormalizing, taking the limit only after we have performed the subtraction, we obtain a finite negative energy between the plates. It is this renormalized energy that results in an attractive Casimir force between the two plates of

[a)]Electronic mail: alang@oru.edu

$$F(l) = -\frac{\partial E}{\partial l} = -\frac{\pi^2 \hbar c}{240 l^4}. \tag{4}$$

See Ref. 5 for further details. The method used previously for calculating the vacuum energy, though rather elegant, does not show the immense cancelation between the frequency modes which renders the renormalized energy finite. To make this cancelation more explicit, a spectral function $\sigma(\omega)$ can be introduced.

Work begun by Ford[6] for the scalar fields case, followed by Hacyan *et al.*[7] for the electromagnetic field case, shows that such a spectral function can be defined in at least two ways. Ford[6] introduces a spectral weight function which samples the frequency spectrum, and Hacyan *et al.*[7] take the Fourier transform of the renormalized expectation of the Casimir energy-momentum operator. The spectral weight function method is used to assign a frequency spectrum for the energy density between the two plates, whose integral over all frequencies gives the net energy per unit area (3), whereas the Fourier transform method defines a spectrum for the Casimir force, whose integral over all frequencies gives the net force per unit area (4).

This article reviews and extends previous work in this area and proposes an experimental test for the validity of assigning frequency spectra by using frequency band-gap materials.

II. ASSIGNING A FREQUENCY SPECTRUM USING A SPECTRAL WEIGHT FUNCTION

Following Ford,[6] we may use the Plana summation formula

$$\sum_{n=1}^{\infty} f(n) + \frac{1}{2} f(0) = \int_0^{\infty} f(x)\mathrm{d}x + \mathrm{i}\int_0^{\infty} \frac{f(\mathrm{i}t) - f(-\mathrm{i}t)}{\exp(2\pi t) - 1}\mathrm{d}t, \tag{5}$$

instead of the standard regularization and renormalization technique outlined previously, to rewrite the zero-point energy between the plates as an integral

$$E_p(l) = {\sum_{n=0}^{\infty}}' \hbar\omega_n = \int_0^{\infty} \hbar\omega(n)\mathrm{d}n + \mathrm{i}\hbar\int_0^{\infty} \frac{\omega(\mathrm{i}t) - \omega(-\mathrm{i}t)}{\exp(2\pi t) - 1}\mathrm{d}t, \tag{6}$$

where the prime indicates a factor of $\frac{1}{2}$ should be introduced when $n=0$, and the particular form of the frequency modes ω_n depends on the type of field between the plates and the number of spatial dimensions. Subtracting from (6) the zero-point energy of the vacuum

$$E_v(l) = \int_0^{\infty} \hbar\omega(n)\mathrm{d}n, \tag{7}$$

we obtain the *convergent* integral for the renormalized energy

$$E(l) = \mathrm{i}\hbar\int_0^{\infty} \frac{\omega(\mathrm{i}t) - \omega(-\mathrm{i}t)}{\exp(2\pi t) - 1}\mathrm{d}t. \tag{8}$$

To measure the contribution that each mode, ω_0 say, gives to the total energy, we introduce a spectral weight function

$$W_m(\omega) = \left(\frac{2m}{\omega_0}\right)^{2m+1} \frac{\omega^{2m}}{(2m)!} e^{-m\omega/\omega_0}, \tag{9}$$

which has the following properties:

$$\int_0^{\infty} W(\omega)\mathrm{d}\omega = 1, \tag{10}$$

$$\int_0^\infty W(\omega)\mathrm{d}\omega_0 = 1, \tag{11}$$

$$\lim_{m\to\infty} W(\omega) = \delta(\omega - \omega_0). \tag{12}$$

For $m \gg 1$, the spectral weight function (9) is sharply peaked about ω_0, so by substituting it into the equation for the energy density (8), we reproduce Ford's expression for the contribution that ω_0 gives to the total vacuum energy between the plates[6]

$$\sigma(\omega_0) = \mathrm{i}\hbar \int_0^\infty \frac{\omega(\mathrm{i}t)W(\mathrm{i}t) - \omega(-\mathrm{i}t)W(-\mathrm{i}t)}{\exp(2\pi t) - 1}\mathrm{d}t. \tag{13}$$

By integrating this expression over all frequencies we recover the energy density, i.e.,

$$E(l) = \int_0^\infty \sigma(\omega)\mathrm{d}\omega. \tag{14}$$

Thus $\sigma(\omega)$ is a **spectrum for the Casimir energy**.

A. Energy spectrum for the massless scalar field

The massless scalar field in two dimensions with periodic boundary conditions $\mathbb{S}^1 \times \mathbb{R}$ gives rise to normal modes[6]

$$\omega_n = \frac{2n\pi c}{l}, \quad n = 0, \pm 1, \pm 2, \ldots . \tag{15}$$

These modes give a rise to a formally divergent vacuum energy

$$E_p(l) = \sum_{n=0}^{\infty}{}' \frac{2n\pi\hbar c}{l^2} \tag{16}$$

which has a renormalized value

$$E(l) = -\frac{\pi\hbar c}{6l^2}. \tag{17}$$

Substituting the normal modes (15) into (13) and integrating gives

$$\sigma(\omega_0) = (-1)^{m+1}\frac{(2m+1)\hbar c}{\pi^{2m+1}l^2}\left(\frac{m}{\omega_0}\right)^{2m+1}\left[\zeta\left(2m+2, 1 - \frac{\mathrm{i}m}{\pi\omega_0}\right) + \zeta\left(2m+2, 1 + \frac{\mathrm{i}m}{\pi\omega_0}\right)\right], \tag{18}$$

where $\zeta(s,a)$ is the Hurwitz zeta function defined by

$$\zeta(s,a) = \sum_{k=0}^{\infty} \frac{1}{(k+a)^s}. \tag{19}$$

Plotting the energy spectrum for the massless scalar field in $\mathbb{S}^1 \times \mathbb{R}$ we see that it is an oscillatory function of decaying amplitude with maxima at integer values of ω_0, see Fig. 1. It is easy to verify that for all m, the integral over all frequencies is, as required, the energy density, i.e.,

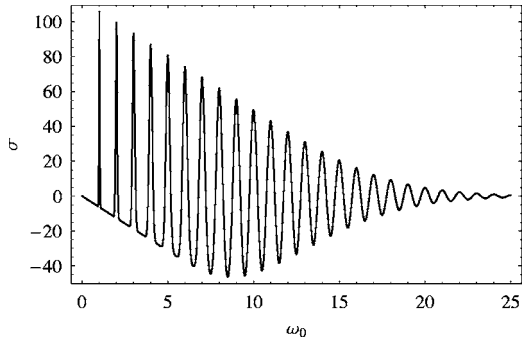

FIG. 1. Energy spectrum $\sigma(\omega_0)$ for the massless scalar field in $\mathbb{S}^1\times\mathbb{R}$ plotted using $m=1000$, $\hbar=c=l=1$.

$$E(l)=\int_0^\infty \sigma(\omega)\mathrm{d}\omega=-\frac{\pi\hbar c}{6l^2}. \tag{20}$$

Thus $\sigma(\omega)$, given by (18), is the energy spectrum for the massless scalar field in $\mathbb{S}^1\times\mathbb{R}$. Comparing the energy spectrum (18) with Ford's[6] equations [(2.13)–(2.15)], it can be shown that (18) is equivalent to Ford's expression for $\sigma(\omega)$.

The energy spectrum for the four-dimensional massless scalar field can be calculated similarly. The massless scalar field in four-dimensions with periodic boundary conditions $\mathbb{S}^1\times\mathbb{R}^3$ gives rise to normal modes[6]

$$\omega_n=c\sqrt{k^2+\left(\frac{2n\pi}{l}\right)^2},\quad n=0,\pm 1,\pm 2,\ldots\ . \tag{21}$$

These modes give a rise to a formally divergent vacuum energy

$$E_p(l)=\frac{\hbar c}{2\pi l}\int_0^\infty {\sum_{n=0}^{\infty}}' k\sqrt{k^2+\left(\frac{2n\pi}{l}\right)^2}\,\mathrm{d}k. \tag{22}$$

Using the change of variables $x^2=k^2+4n^2\pi^2/l^2$ and regularizing, by introducing the convergence factor $e^{-\alpha x}$ yields

$$E_p(l)=\lim_{\alpha\to 0}\frac{\hbar c}{2\pi l}{\sum_{n=0}^{\infty}}'\int_{2n\pi/l}^\infty x^2e^{-\alpha x}\mathrm{d}k.$$

$$=\lim_{\alpha\to 0}\frac{\hbar c}{2\pi l}{\sum_{n=0}^{\infty}}'\left(\frac{2}{\alpha^3}+\frac{4n\pi}{\alpha^2 l}+\frac{4n^2\pi^2}{\alpha l^2}\right)e^{-2n\pi\alpha/l}. \tag{23}$$

As mentioned in Sec. I, we can renormalize this expression by subtracting the zero-point energy of the vacuum to obtain the energy between the plates. Instead we proceed here to derive an expression for the energy spectrum. Substituting

$$\omega(n)=\frac{c}{2\pi l}\left(\frac{2}{\alpha^3}+\frac{4n\pi}{\alpha^2 l}+\frac{4n^2\pi^2}{\alpha l^2}\right)e^{-2n\pi\alpha/l} \tag{24}$$

into (13), where $W_m(\omega)$ is as before, we obtain (after some algebra)

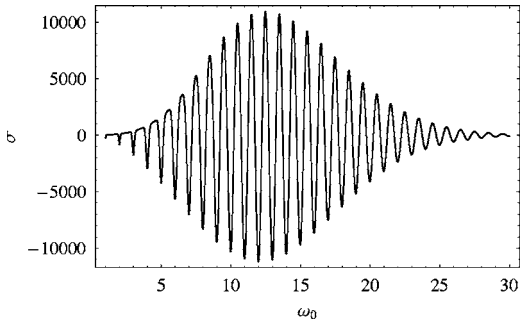

FIG. 2. Energy spectrum $\sigma(\omega_0)$ for the massless scalar field in $\mathbb{S}^1\times\mathbb{R}^3$ plotted using $m=1000$, $\hbar=c=l=1$.

$$\sigma(\omega_0)=\frac{i\hbar c}{\pi\omega_0 l^3\alpha^3}\frac{(-1)^m(2m)^{2m+1}}{(2m)!}\int_0^\infty dt\left(\frac{t}{\omega_0}\right)^{2m}(\coth(\pi t)-1)$$
$$\times\left[(l^2-2\alpha^2\pi^2t^2)\sin\left[2t\left(\frac{\alpha\pi}{l}+\frac{m}{\omega_0}\right)\right]-2\alpha l\pi t\cos\left[2t\left(\frac{\alpha\pi}{l}+\frac{m}{\omega_0}\right)\right]\right]. \tag{25}$$

Integrating and taking the limit as $\alpha\to 0$ gives

$$\sigma(\omega_0)=(-1)^{m+1}\frac{(2m+1)(2m+2)(2m+3)\hbar c}{6\pi^{2m+2}l^4}\left(\frac{m}{\omega_0}\right)^{2m+1}$$
$$\times\left[\zeta\left(2m+4,1-\frac{im}{\pi\omega_0}\right)+\zeta\left(2m+4,1+\frac{im}{\pi\omega_0}\right)\right]. \tag{26}$$

Plotting the energy spectrum for the massless scalar field in $\mathbb{S}^1\times\mathbb{R}^3$ we see a slightly different shaped oscillatory function than before, the amplitude initially increasing before it decays to zero. Again, the maxima are at integer values of ω_0, see Fig. 2. It is again easy to verify that for all m, the integral over all frequencies is, as required, the energy density, i.e.,

$$E(l)=\int_0^\infty\sigma(\omega)d\omega=-\frac{\pi^2\hbar c}{90l^4}. \tag{27}$$

Thus $\sigma(\omega)$, given by (26), is the energy spectrum for the massless scalar field in $\mathbb{S}^1\times\mathbb{R}^3$. Comparing the energy spectrum (26) with Ford's[6] equation (3.18) it can be shown that (26) is equivalent to Ford's expression for $\sigma(\omega)$ but is given here in a more compact form.

B. Energy spectrum for the electromagnetic field

For two perfectly conducting parallel plates, the frequency modes for the electromagnetic field are given by[5]

$$\omega_n=c\sqrt{k_x^2+k_y^2+\left(\frac{n^2\pi^2}{l^2}\right)^2},\quad n=0,\pm1,\pm2,\ldots\ . \tag{28}$$

These modes give rise to a formally divergent vacuum energy

$$E_p(l)=\frac{\hbar c}{4\pi^2}{\sum_{n=0}^{\infty}}'\int_0^\infty\int_0^\infty\sqrt{k_x^2+k_y^2+(n^2\pi^2/l^2)^2}dk_xdk_y=\frac{\hbar c}{4\pi^2}{\sum_{n=0}^{\infty}}'\int_0^\infty 2\pi k\sqrt{k^2+(n^2\pi^2/l^2)^2}dk_x. \tag{29}$$

Using the change of variables $x^2=k^2+n^2\pi^2/l^2$ and regularizing, by introducing the convergence factor $e^{-\alpha x}$, yields

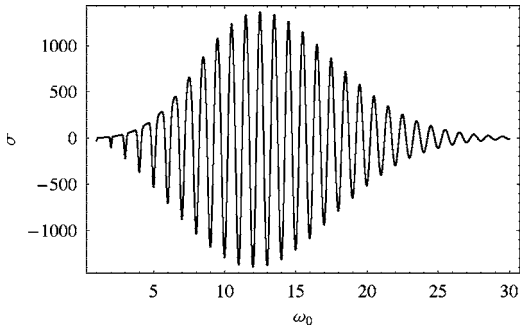

FIG. 3. Energy spectrum $\sigma(\omega_0)$ for the electromagnetic field in between parallel plates plotted using $m=1000$, $\hbar=c=l=1$.

$$E_p(l) = \lim_{\alpha\to 0} \frac{\hbar c}{2\pi} {\sum_{n=0}^{\infty}}' \int_{n\pi/l}^{\infty} x^2 e^{-\alpha x} \mathrm{d}x = \lim_{\alpha\to 0} \frac{\hbar c}{2\pi} {\sum_{n=0}^{\infty}}' \left(\frac{1}{\pi\alpha^3} + \frac{n}{l\alpha^2} + \frac{n^2\pi}{2l^2\alpha} \right) e^{-n\pi\alpha/l}. \tag{30}$$

We can renormalize this expression by subtracting the zero-point energy of the vacuum to obtain the energy between the plates (3). Instead we proceed here to derive an expression for the energy spectrum. Substituting

$$\omega(n) = \frac{c}{2\pi} \left(\frac{1}{\pi\alpha^3} + \frac{n}{l\alpha^2} + \frac{n^2\pi}{2l^2\alpha} \right) e^{-n\pi\alpha/l} \tag{31}$$

into (13), where $W_m(\omega)$ is as before, we obtain (after some algebra)

$$\sigma(\omega_0) = \frac{\mathrm{i}\hbar c}{2\pi\omega_0 l^2\alpha^3} \frac{(-1)^m m}{(2m)!} \int_0^{\infty} \left(\frac{2mt}{\omega_0} \right)^{2m} (\coth(\pi t) - 1) \times \left[\exp\left[\mathrm{i}t \left(\frac{2m}{\omega_0} + \frac{\pi\alpha}{l} \right) \right] ((\mathrm{i}+1)l + \pi t\alpha)((\mathrm{i}-1)l + \pi t\alpha) - c.c. \right] \mathrm{d}t. \tag{32}$$

Integrating and taking the limit as $\alpha\to 0$ gives

$$\sigma(\omega_0) = (-1)^m \frac{(2m+1)(2m+2)(2m+3)\hbar c}{48\pi^{2m+2} l^3} \left(\frac{m}{\omega_0} \right)^{2m+1} \times \left[\zeta\left(2m+4, 1 - \frac{\mathrm{i}m}{\pi\omega_0} \right) + \zeta\left(2m+4, 1 + \frac{\mathrm{i}m}{\pi\omega_0} \right) \right]. \tag{33}$$

Plotting the energy spectrum for the electromagnetic field, see Fig. 3, we see that it is, up to scaling, identical to the plot of energy spectrum for the massless scalar field in $\mathbb{S}^1\times\mathbb{R}^3$, see Fig. 2. This is not surprising as the equations for σ are nearly identical, see Eq. (26). As before, the amplitude initially increases before it decays to zero and the maxima are at integer values of ω_0. Integrating over all frequencies for any m gives, as required, the energy density, i.e.,

$$E(l) = \int_0^{\infty} \sigma(\omega)\mathrm{d}\omega = -\frac{\pi^2\hbar c}{720 l^3}. \tag{34}$$

Thus $\sigma(\omega)$, given by (33), is the energy spectrum for the electromagnetic field between two perfectly conducting parallel plates in vacuum.

III. ASSIGNING A FREQUENCY SPECTRUM USING FOURIER TRANSFORMS

An alternative definition of a frequency spectrum for the Casimir effect has been proposed by Hacyan *et al.*[7] They define the spectrum as the Fourier transform of the renormalized expectation value of the energy-momentum stress operator for a quantized field, i.e.,

$$\varsigma(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty} \langle T^{zz}(\tau)\rangle_{\mathrm{R}} e^{-\mathrm{i}\omega\tau}\mathrm{d}\tau, \tag{35}$$

where z is the direction normal to the plates. Integrating this expression over all frequencies we recover, not the energy density, but the Casimir force itself. That is

$$F(l) = \int_0^{\infty} \varsigma(\omega)\mathrm{d}\omega. \tag{36}$$

Thus $\varsigma(\omega)$ given by (35) is a **spectrum for the Casimir force**.

The renormalized stress tensor for the electromagnetic field between two perfectly conducting parallel plates in vacuum in given by[7]

$$\langle T^{zz}(\tau)\rangle_{\mathrm{R}} = \frac{2\hbar c}{\pi^2}\sum_{n=1}^{\infty} \frac{\tau^2 + 3(2ln)^2}{(\tau^2 - (2ln)^2)^3}. \tag{37}$$

Substituting this expression into (35) gives the spectrum

$$\varsigma(\omega) = \frac{\hbar c}{\pi^2 l^3}\sum_{n=1}^{\infty}\left(\frac{l\omega}{2n^2}\cos(2ln\omega) + \frac{2l^2\omega^2n^2 - 1}{4n^3}\sin(2ln\omega)\right). \tag{38}$$

By introducing a convergence term $e^{-\alpha\omega}$, and integrating over all frequencies, we recover the Casimir force as follows:

$$\begin{aligned} F(l) &= \lim_{\alpha\to 0}\frac{\hbar c}{\pi^2 l^3}\sum_{n=1}^{\infty}\int_0^{\infty}\left(\frac{l\omega}{2n^2}\cos(2ln\omega) + \frac{2l^2\omega^2n^2 - 1}{4n^3}\sin(2ln\omega)\right)e^{-\alpha\omega}\mathrm{d}\omega \\ &= \lim_{\alpha\to 0}\frac{\hbar c}{\pi^2}\sum_{n=1}^{\infty}\frac{-24l^2n^2 + 2\alpha^2}{(4l^2n^2 + \alpha^2)^3} = \lim_{\alpha\to 0}\frac{\hbar c}{\pi^2}\left(\frac{\pi^3\coth(\pi\alpha/2l)\mathrm{csch}^2(\pi\alpha/2l)}{8l^3\alpha} - \frac{1}{\alpha^4}\right) \\ &= \lim_{\alpha\to 0}\hbar c\left(\frac{-\pi^2}{240l^4} + \frac{\pi^2\alpha^2}{3024l^6} + O(\alpha)^3\right) = -\frac{\pi^2\hbar c}{240l^4}. \end{aligned} \tag{39}$$

Thus $\varsigma(\omega)$, given by (38), is the force spectrum for the electromagnetic field between two perfectly conducting parallel plates in vacuum. Ford[8] has shown that this force spectrum may also be derived directly from Lifshitz theory.[9]

The force spectrum (38) may be expressed in the following form, useful for evaluating and plotting

$$\begin{aligned} \varsigma(\omega) = \frac{\hbar c}{\pi^2}\Bigg\{ &\frac{\mathrm{i}\omega^2}{4l}[\ln(1 - e^{2\mathrm{i}l\omega}) - \ln(1 - e^{-2\mathrm{i}l\omega})] + \frac{\omega}{4l^2}[\mathrm{Li}_2(e^{2\mathrm{i}l\omega}) - \mathrm{Li}_2(e^{-2\mathrm{i}l\omega})] + \frac{\mathrm{i}}{8l^3}[\mathrm{Li}_3(e^{2\mathrm{i}l\omega}) \\ &- \mathrm{Li}_3(e^{-2\mathrm{i}l\omega})]\Bigg\}, \end{aligned} \tag{40}$$

where $\mathrm{Li}_2(z)$ and $\mathrm{Li}_3(z)$ are the dilogarithm and trilogarithm functions, respectively, defined in general by

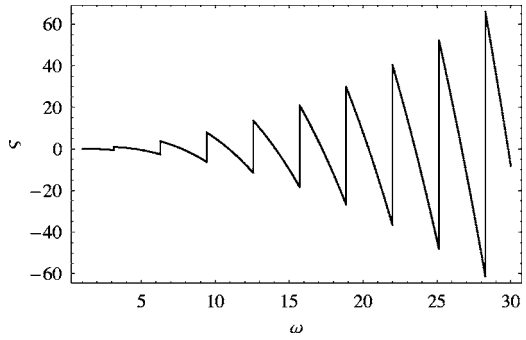

FIG. 4. Force spectrum $\varsigma(\omega)$ for the electromagnetic field plotted using $\hbar=c=l=1$.

$$\mathrm{Li}_n(z)=\sum_{k=1}^{\infty}\frac{z^k}{k^n}. \tag{41}$$

Plotting the force spectrum for fixed l, see Fig. 4, we see that it has a different form than the energy spectra. First, the location of the extrema depends explicitly on l, the separation between the plates. Specifically, the extrema occur for $\omega=n\pi/l$; $n=1,2,\ldots$ instead of integer values of ω as we saw for the energy spectra. Second, the amplitude of the force spectrum does not decay to zero as $\omega\to 0$, as it does for the energy spectra, but instead it increases without bound. Since integrating the force spectrum over all ω gives the Casimir force, we clearly see here the almost total cancelation that must occur between all the modes to render the Casimir force finite. These two properties suggest that for certain physical materials (and by varying l), the frequency mode cancelation may be disturbed to produce designer Casimir forces of almost any magnitude, both attractive and repulsive.

IV. CASIMIR FORCE BETWEEN IDEAL FREQUENCY BAND AND FREQUENCY BAND-GAP MATERIALS

In this section, the term **frequency band** material is used to mean a physical material that is perfectly reflecting in a narrow frequency interval and perfectly transparent outside of that interval. Similarly, the term **frequency band-gap** material is used to mean a physical material that is perfectly reflecting for all frequencies except for a narrow frequency interval, for which it is perfectly transparent. Such ideal materials, of course, do not exist. In fact, a spatially homogeneous dielectric material is restricted by the Kramers–Kronig relations from having the type of discontinuous response I assume[10] and the results of Lifshitz[9] restrict the Casimir force between two homogeneous dielectric half-spaces to be always attractive and no greater than the Casimir

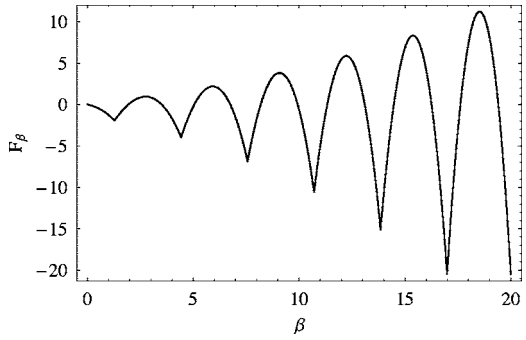

FIG. 5. Casimir force for a frequency band material with fixed ω_0 and varying band width β plotted using $\hbar=c=l=1$ and $\omega_0=5$.

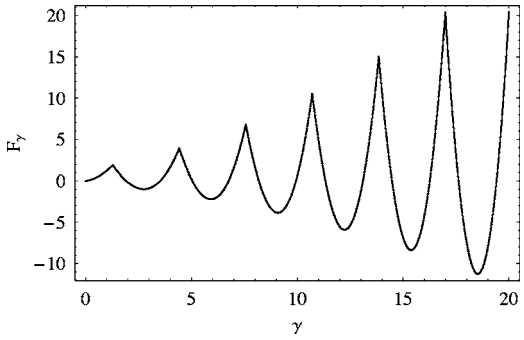

FIG. 6. Casimir force for a frequency band-gap material with fixed ω_0 and varying band-gap width γ plotted using $\hbar=c=l=1$ and $\omega_0=5$.

force between two perfectly reflecting parallel plates. It is possible however to do better with inhomogeneous materials such as photonic crystals which are regular arrays of materials with different refractive indices.[11] Photonic crystals have been made which are essentially perfectly reflecting over a finite frequency band, and partially reflecting (having rather complicated transmission spectra) outside this band.[12–14]

In the preceeding section, we explicitly saw the cancelation, alluded to in Sec. I, between the frequency modes which gives a finite Casimir force. It was Ford and Sopova[8,15,16] who first speculated that "one might be able to upset this cancelation in some way," and alter the magnitude and even direction of the Casimir force. For frequency band material plates, which are perfectly reflecting in the interval $(\omega_0, \omega_0+\beta)$ say, the Casimir force is given by[8]

$$F_\beta(l,\omega_0) = \int_{\omega_0}^{\omega_0+\beta} \varsigma(\omega)\mathrm{d}\omega. \tag{42}$$

Similarly, for frequency band-gap material plates, which are perfectly reflecting everywhere except in the interval $(\omega_0, \omega_0+\gamma)$ say, the Casimir force is given by

$$F_\gamma(l,\omega_0) = F(l) - F_\beta(l,\omega_0). \tag{43}$$

Substituting the force spectrum (40) into (42), we obtain

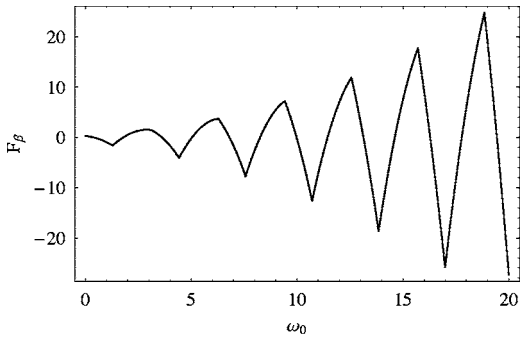

FIG. 7. Casimir force for a frequency band material with fixed β and varying band width ω_0 plotted using $\hbar=c=l=1$ and $\beta=5$.

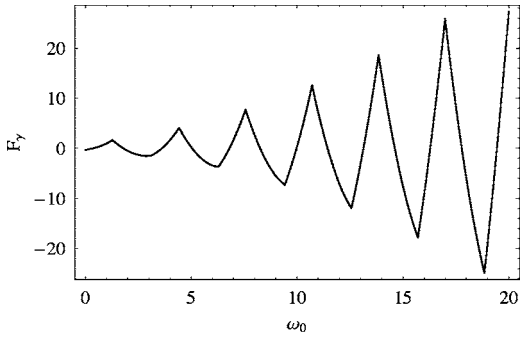

FIG. 8. Casimir force for a frequency band-gap material with fixed γ and varying band-gap width ω_0 plotted using $\hbar = c = l = 1$ and $\gamma = 5$.

$$F_\beta(l,\omega_0) = -\frac{\hbar c}{16\pi^2 l^4}\{2l^2(\omega_0+\beta)^2[\mathrm{Li}_2(e^{2il(\omega_0+\beta)}) + \mathrm{Li}_2(e^{-2il(\omega_0+\beta)})] - 2l^2\omega_0^2[\mathrm{Li}_2(e^{2il\omega_0}) + \mathrm{Li}_2(e^{-2il\omega_0})] + 4il\beta[\mathrm{Li}_3(e^{2il(\omega_0+\beta)}) + \mathrm{Li}_3(e^{-2il(\omega_0+\beta)})] - 4il\omega[\mathrm{Li}_3(e^{2il\omega_0}) + \mathrm{Li}_3(e^{-2il\omega_0})] - 3[\mathrm{Li}_4(e^{2il(\omega_0+\beta)}) + \mathrm{Li}_4(e^{-2il(\omega_0+\beta)})] + 3[\mathrm{Li}_4(e^{2il\omega_0}) + \mathrm{Li}_4(e^{-2il\omega_0})]\}. \quad (44)$$

Plotting the Casimir band force and the Casimir band-gap force for constant ω_0 and l, we see that the force oscillates with the amplitude increasing as the frequency band (or band gap) increases, see Figs. 5 and 6. Also we have an infinite number of equilibria points where the force between the plates equals zero. Since l is constant here, the two plots are reflections of each other about the line $F = F(l)/2$.

Plotting the Casimir band force and the Casimir band-gap force for constant β, γ and l, we see that the force again oscillates with the amplitude increasing as the frequency ω_0 increases, see Figs. 7 and 8. We again have an infinite number of equilibria points where the force between the plates equals zero, and since l is constant, the graphs are reflections of each other about the line $F = F(l)/2$. One thing to note here is that as $\beta \to 0^+$, the graph of $F_\beta(l,\omega_0)$ tends to the graph of $\varsigma(\omega)$. Thus one way to test the theoretical frequency spectra is to use a narrow frequency band material to sample the contribution that each frequency mode contributes to the total force. This can also be done using a narrow frequency band-gap materials via Eq. (43). Ideally one would like to have a material in which you could control where the frequency band (or band-gap) began and its width. Plotting the Casimir band force and the Casimir band-gap force for constant β, γ, and ω_0 and for varying l, we see that the force again oscillates but this time the amplitude decreases as the separation l increases, see Figs. 9 and 10. This is clearly what we would expect from physical principles. We have an infinite number of equilibria points where the force between the plates equals zero. These equilibria points alternate between being unstable $F' > 0$ and stable $F' < 0$ for

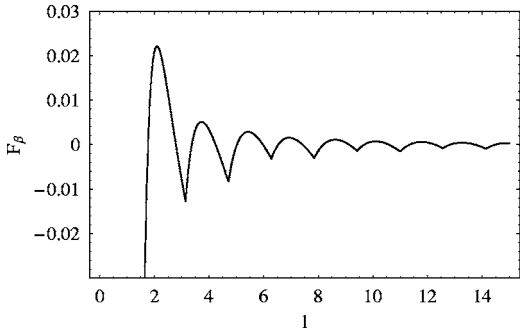

FIG. 9. Casimir force for a frequency band material with fixed β and ω_0 with varying l plotted using $\hbar = c = \beta = \omega_0 = 1$.

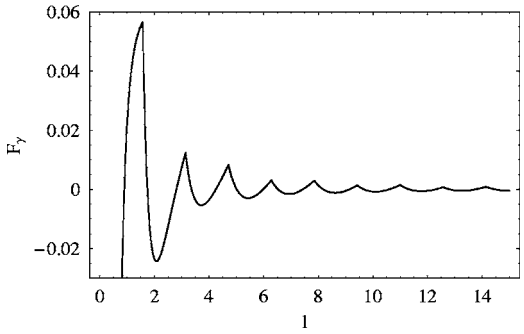

FIG. 10. Casimir force for a frequency band-gap material with fixed γ and ω_0 with varying l plotted using $\hbar=c=\gamma=\omega_0=1$.

both the band and band-gap cases. Unlike the previous two sets of plots, the Casimir force $F(l)$ is not constant, this is why the two plots are not merely reflections of each other about the line $F=F(l)/2$. We have here another possible experimental test for the force spectrum. By taking a frequency band (or band-gap) material and measuring the Casimir force at varying distances, we should be able to detect the oscillation in the force that comes from the spectrum. If at all possible, care should be taken to produce a material where the width of the band (or band gap) corresponds to an ω_0, for which the magnitude of the force is a maximum. This occurs when

$$\gamma = \frac{n\pi}{l} - \omega_0. \tag{45}$$

Plotting the Casimir band-gap force in two dimensions for constant γ, see Fig. 11, with lighter gray levels corresponding to repulsive forces and darker levels corresponding to attractive forces, and with the zero force equilibria indicated with the black curves. We see that oscillations die out as l increases for all ω_0, even though the amplitude increases as ω_0 increases. Plotting the Casimir band-gap force in two dimensions for constant l, see Fig. 12, again with lighter gray levels corresponding to repulsive forces and darker gray levels corresponding to attractive forces, and with the zero force equilibria indicated with the black curves. We see the amplitude of the force oscillations increases as both ω_0 and γ increase.

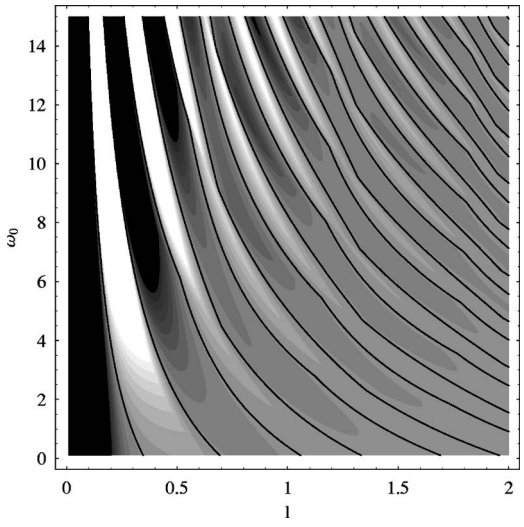

FIG. 11. Casimir force for a frequency band-gap material with fixed γ plotted using $\hbar=c=1$ and $\gamma=5$.

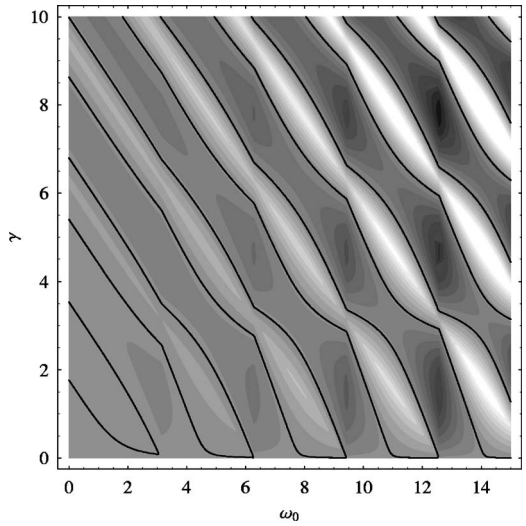

FIG. 12. Casimir force for a frequency band-gap material with fixed l plotted using $\hbar=c=l=1$.

V. DISCUSSION AND CONCLUSION

In the previous sections, we have reviewed the two main ways of assigning a frequency spectrum for the Casimir effect. First by using a spectral weight function to assign an energy spectrum and second by using the Fourier transform of the energy density to assign a force spectrum. Calculations were performed for both the massless scalar field and the electromagnetic field. New exact forms for the various spectra were presented in all cases.

There is some doubt to the validity of assigning a spectrum to the Casimir effect, as a theoretical understanding of how exactly the individual modes contribute to the total force will not be complete until the individual infinite zero-point energies are themselves better understood. Possible experiments were proposed to test the validity of the models. Such experimental tests may be done using either frequency band or frequency band-gap materials. Some limitations to this are the physical restrictions of any plasma frequency of the material and also the smoothness of the interface, where we would like to keep the variations in l small compared to $1/\omega_0$.[6] Also, as already mentioned, there may be restrictions imposed by causality and passivity considerations.[10] Another possible way to detect such a frequency spectrum is via a Casimir-Polder spectrum, whereby an experiment to detect the force between a dielectric wall and small metal sphere is conducted.[15,16]

For possible future work, the Casimir force between photonic band gap materials with a more realistic band gap structure needs to be calculated. Also, other geometries need to be considered, especially the cases of a sphere and a cylinder. Assigning a spectrum to these geometries now seems accessible via a generalized Plana summation formula.[17]

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Minimum orbit dimension for local unitary action on *n*-qubit pure states

David W. Lyons[a)]
Mathematical Sciences, Lebanon Valley College, Annville, Pennsylvania 17003

Scott N. Walck[b)]
Department of Physics, Lebanon Valley College, Annville, Pennsylvania 17003

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The group of local unitary transformations partitions the space of n-qubit quantum states into orbits, each of which is a differentiable manifold of some dimension. We prove that all orbits of the n-qubit quantum state space have dimension greater than or equal to $3n/2$ for n even and greater than or equal to $(3n+1)/2$ for n odd. This lower bound on orbit dimension is sharp, since n-qubit states composed of products of singlets achieve these lowest orbit dimensions. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2048327]

I. INTRODUCTION

Quantum entanglement theory can be regarded as the branch of nonrelativistic quantum mechanics that seeks to understand the states and dynamics of composite quantum systems with a fixed number of subsystems. Composite quantum systems can exhibit correlations among subsystems in ways that classically describable composite systems cannot. A (pure) state of a composite quantum system is called entangled if it cannot be described by specifying (pure) states for each of the subsystems.

Quantum entanglement plays a particularly important role in quantum information, where the subsystems are quantum bits or qubits (a spin-1/2 particle is a physical realization of a qubit). An n-qubit system is the quantum analog of an n-bit computer or communications channel. Because quantum computing algorithms and quantum communications protocols utilize entanglement as an essential resource, potential applications of quantum information theory provide motivation for a more complete description of entanglement (see Refs. 1 and 2 for surveys of a broad range of topics in this area).

A fundamental problem in the theory of quantum entanglement is to describe the types of entanglement that are achievable for a composite quantum system. We regard two states of a composite quantum system as having the same type of entanglement if unitary operations on the subsystems, called local unitary or LU transformations, can transform one quantum state into the other. Local unitary transformations form a Lie group which acts on the manifold of quantum states, partitioning it into orbits. Each orbit is a differentiable manifold that represents a type of quantum entanglement. The *orbit space*—the set of orbits made into a topological space by the quotient topology—is the collection of entanglement types.

A theory of quantum entanglement based on local unitary transformations seeks to describe the orbit spaces and the orbits themselves for composite quantum systems. Much of the progress toward understanding the orbit spaces of quantum systems comes from invariant theory—the study of functions which are constant along orbits.[3–12] One hopes to use these invariants, which are usually polynomial functions of state vector coefficients, to distinguish and classify orbits. Rains[3] and Grassl *et al.*[4] laid the groundwork for a systematic approach using this philosophy. The

[a)]Electronic mail: lyons@lvc.edu
[b)]Electronic mail: walck@lvc.edu

success in choosing particular, finite sets of invariants to label points in the orbit space has so far been limited to small numbers of qubits. Makhlin[6] gave a set of 18 polynomial invariants that separate orbits for two-qubit mixed states. Sudbery[5] gave a set of six polynomial invariants that separate orbits for 3-qubit pure states. Acín *et al.*[13,14] gave a convenient set of nonpolynomial invariants and a classification of 3-qubit pure states based on it.

In this paper we pursue a strategy inspired by Linden and Popescu,[15,16] who approached entanglement properties of quantum states working on the Lie algebra level to study the orbits themselves. We develop a general technique for calculating the orbit dimension of a state and use this to prove a lower bound on orbit dimension. We have also used our methods to provide a proof[17] of the authors' claim in Refs. 15 and 16 that almost all states have orbit dimension $3n$ [we take the manifold of pure n-qubit states to be the projective space $\mathbb{P}((\mathbb{C}^2)^{\otimes n})$ and the group of local unitary transformations to be $G=\mathrm{SU}(2)^n$].

Most of the progress in understanding orbits and orbit dimensions has been for systems of only two or three qubits. Carteret and Sudbery[18] described the nongeneric orbits (including orbit dimensions) for pure 3-qubit states. Życzkowski *et al.*[19,20] analyze orbits for bipartite states. Few general results are known about those orbits which are the most interesting from the quantum information point of view, namely the nongeneric or exceptional orbits of n-qubit states (basic examples are the singlet state of two qubits and the GHZ state of three qubits). The main result in the present paper is at least a small step towards the larger goal of orbit classification for general n.

A. Physical significance of the result

In this paper, we identify the minimum orbit dimension of n-qubit quantum states. States that have the minimum orbit dimension are, in some sense, the "rarest" quantum states. Until now, it has been known that singlet states have minimum orbit dimension for two qubits, and one could conjecture that some n-qubit generalization of the singlet state would have minimum orbit dimension for n qubits, but it was not clear how the singlet should be generalized to maintain the minimum orbit dimension as n increases. For example, one generalization of the singlet is the so-called n-cat state, $1/\sqrt{2}|00\cdots00\rangle+1/\sqrt{2}|11\cdots11\rangle$, of which the GHZ state is an example for three qubits. But the n-cat generalization of the singlet does not maintain the minimum orbit dimension for higher qubit numbers. As we show in this paper, it is the product of singlet states (for even qubit numbers) or the product of singlets and one unentangled qubit (for odd qubit numbers) that is the generalization of singlets that achieves minimum orbit dimension. This suggests a special role for the 2-qubit singlet state in the theory of n-qubit quantum entanglement.

B. Proof strategy and outline

To establish the minimum orbit dimension, we show that the orbit dimension of a given state is (one less than) the rank of a real matrix M associated to that state. The matrix M arises naturally via consideration of the action of the local unitary group on an infinitesimal level, that is, the action of the Lie algebra of the local unitary group. The column vectors of M can be identified with complex vectors. We then establish lower bounds on the rank of M by showing that a sufficient number of real dot products of columns of M can be arranged, possibly after local unitary operations, to vanish. Instead of working directly with real dot products, it is convenient to calculate complex inner products; the vanishing of the real part of a complex inner product guarantees that the real dot product is zero [see (15) below].

In Sec. III we introduce the matrix M. To establish the necessary cancellations among terms of complex inner products of columns of M requires careful bookkeeping and a technical lemma; we present this machinery in Sec. IV. Next we establish orthogonality among columns of M in Sec. V and Sec. VI. We then use these results to prove minimum orbit dimension in Sec. VII.

II. CONVENTIONS AND NOTATION

A. Hilbert space, state space and the local unitary group

Let $H=(\mathbb{C}^2)^{\otimes n}$ denote the Hilbert space of pure states of a system of n qubits and let $\mathbb{P}(H)$ denote the projectivization of H which is the state space of the system. We take the local unitary group to be $G=\mathrm{SU}(2)^n$. These definitions constitute a minor departure, made for the sake of clarity and compactness of exposition, from the widespread practice of taking state space to be the set of normalized state vectors and resolving phase ambiguity by including an extra U(1) factor in the local unitary group.

B. Multi-index notation for Hilbert space basis vectors

Let $|0\rangle,|1\rangle$ denote the standard basis for $\mathbb{C}^2$ and write $|i_1 i_2 \cdots i_n\rangle$ for $|i_1\rangle\otimes|i_2\rangle\otimes\cdots\otimes|i_n\rangle$ in $(\mathbb{C}^2)^{\otimes n}$. For a multi-index $I=(i_1 i_2 \cdots i_n)$ with $i_k=0,\ 1$ for $1\leqslant k\leqslant n$, we will write $|I\rangle$ to denote $|i_1 i_2 \cdots i_n\rangle$. Let i_k^c denote the bit complement

$$i_k^c=\begin{cases}0 & \text{if } i_k=1,\\ 1 & \text{if } i_k=0,\end{cases}$$

and let I_k denote the multi-index

$$I_k := (i_1 i_2 \cdots i_{k-1} i_k^c i_{k+1} \cdots i_n)$$

obtained from I by taking the complement of the kth bit for $1\leqslant k\leqslant n$. Similarly, let I_{kl} denote the multi-index

$$I_{kl} := (i_1 i_2 \cdots i_{k-1} i_k^c i_{k+1} \cdots i_{l-1} i_l^c i_{l+1} \cdots i_n)$$

obtained from I by taking the complement of the kth and lth bits for $1\leqslant k<l\leqslant n$.

C. Standard identification of $\mathbb{C}^N$ with $\mathbb{R}^{2N}$

We identify the complex vectors in $\mathbb{C}^N$ with real vectors in $\mathbb{R}^{2N}$ via

$$\mathbb{C}^N \leftrightarrow \mathbb{R}^{2N},$$

$$(z_1,z_2,\ldots,z_N) \leftrightarrow (a_1,b_1,a_2,b_2,\ldots,a_N,b_N), \tag{1}$$

where $z_j=a_j+ib_j$ for $1\leqslant j\leqslant N$.

III. LIE ALGEBRA ACTION

The Lie algebra su(2) of SU(2) is the set of traceless skew Hermitian matrices,

$$\mathrm{su}(2)=\left\{\begin{bmatrix} it & u \\ -\bar{u} & -it\end{bmatrix} : t\in\mathbb{R}, u\in\mathbb{C}\right\}$$

and the Lie algebra $LG=(\mathrm{su}(2))^n$ of the local unitary group $G=(\mathrm{SU}(2))^n$ is the set of n-tuples of matrices of this form.

A local unitary operator $g=(g_1,g_2,\ldots,g_n)$ in G acts on a product state vector $|v\rangle=|v_1\rangle\otimes|v_2\rangle\otimes\cdot\otimes|v_n\rangle$ in Hilbert space $H=(\mathbb{C}^2)^{\otimes n}$ by

$$g\cdot|v\rangle = g_1|v_1\rangle\otimes g_2|v_2\rangle\otimes\cdots\otimes g_n|v_n\rangle. \tag{2}$$

The induced action on $|v\rangle$ by $X=(X_1,X_2,\ldots,X_n)$ in LG is given by

$$X \cdot |v\rangle = \sum_{i=1}^{n} |v_1\rangle \otimes \cdots \otimes |v_{i-1}\rangle \otimes X_i |v_i\rangle \otimes |v_{i+1}\rangle \otimes \cdots \otimes |v_n\rangle. \tag{3}$$

This action extends linearly to all of Hilbert space as follows. Let $|\psi\rangle = \Sigma_I c_I |I\rangle$ be an element in Hilbert space H, and let $X = (X_1, X_2, \ldots, X_n)$ be an element of LG with

$$X_k = \begin{bmatrix} it_k & u_k \\ -\overline{u_k} & -it_k \end{bmatrix} \quad \text{for } 1 \leqslant k \leqslant n.$$

A straightforward calculation shows that the action of X on $|\psi\rangle$ is given by

$$X \cdot |\psi\rangle = \sum_I \left(\sum_{k=1}^{n} (-1)^{i_k} [c_I i t_k + c_{I_k} \mathrm{conj}^{i_k}(u_k)] \right) |I\rangle, \tag{4}$$

where $\mathrm{conj}^1(z) = \overline{z}$ and $\mathrm{conj}^0(z) = z$. Let a_I, b_I denote the real and imaginary parts of the coefficient c_I in the expression for $|\psi\rangle$, and let r_k, s_k denote the real and imaginary parts of the entry u_k in X_k. The real and imaginary parts of the Ith coefficient on the right-hand side of Eq. (4) are the following:

$$\mathrm{Re}\langle I|X|\psi\rangle = \sum_{k=1}^{n} [(-1)^{i_k}(-b_I t_k) + (-1)^{i_k} a_{I_k} r_k - b_{I_k} s_k], \tag{5}$$

$$\mathrm{Im}\langle I|X|\psi\rangle = \sum_{k=1}^{n} [(-1)^{i_k}(a_I t_k) + (-1)^{i_k} b_{I_k} r_k + a_{I_k} s_k]. \tag{6}$$

Given a state x in $\mathbb{P}(H)$, the isotropy Lie subalgebra LI_x of the isotropy subgroup I_x is determined by the following condition.

Proposition 3.1: Isotropy Lie algebra condition: Let $x \in \mathbb{P}(H)$ be a state and let $|\psi\rangle$ be a Hilbert space representative for x. The element $X \in LG$ is in the Lie algebra LI_x of the isotropy subgroup I_x of x if and only if

$$X \cdot |\psi\rangle = i\theta |\psi\rangle$$

for some real θ.

Together with (5) and (6), Proposition 3.1 implies the following.

Corollary 3.2: Let X, x and $|\psi\rangle$ be as above. Suppose that X is in LI_x. Then for each multi-index I, we have the following pair of equations:

$$\sum_{k=1}^{n} [(-1)^{i_k}(-b_I t_k) + (-1)^{i_k} a_{I_k} r_k - b_{I_k} s_k] = -b_I \theta, \tag{7}$$

$$\sum_{k=1}^{n} [(-1)^{i_k}(a_I t_k) + (-1)^{i_k} b_{I_k} r_k + a_{I_k} s_k] = a_I \theta, \tag{8}$$

for some real number θ.

By adding $b_I\theta$, respectively $a_I\theta$, to both sides of Eq. (7), respectively (8), the corollary shows that calculating the Lie algebra LI_x is a matter of solving a homogeneous real linear system of 2^{n+1} equations (two for each of the 2^n multi-indices) in the $3n+1$ unknowns t_k, r_k, s_k, θ. Let

$$M(t_1, r_1, s_1, t_2, r_2, s_2, \ldots, t_n, r_n, s_n, \theta) = 0 \tag{9}$$

denote the linear system of 2^{n+1} equations given by (7) and (8), so that the $2^{n+1} \times (3n+1)$ matrix for M has all entries of the form $\pm a_I, \pm b_I$.

Here is the fundamental observation which reduces the problem of orbit dimension to finding the rank of M.

Proposition 3.3: Orbit dimension as rank of M: Let x be a state, let $|\psi\rangle$ be a Hilbert space representative for x, and let M be the associated matrix constructed from the coordinates of $|\psi\rangle$ as described above. Then we have

$$\operatorname{rank} M = \dim \mathcal{O}_x + 1.$$

Proof: We can think of M as the matrix of a linear map $M: LG \times \mathbb{R} \to \mathbb{R}^{2^{n+1}}$ via the identification

$$\mathbb{R}^{3n} \leftrightarrow LG,$$

$$(t_1, r_1, s_1, t_2, r_2, s_2, \ldots, t_n, r_n, s_n) \leftrightarrow (X_1, X_2, \ldots, X_n),$$

where

$$X_k = \begin{bmatrix} it_k & r_k + is_k \\ -r_k + is_k & -it_k \end{bmatrix}.$$

Consider a solution (X, θ) of $M(X, \theta) = 0$. Proposition 3.1 says that $|\psi\rangle$ is an eigenvector for X with eigenvalue $i\theta$, so θ is determined by X. Since $X \in LI_x$ if and only if $M(X, \theta) = 0$ for some θ, it follows that $\dim LI_x = \dim \ker M$. From this we have

$$\dim LI_x = \dim \ker M = \text{number of columns of } M - \operatorname{rank} M = 3n + 1 - \operatorname{rank} M.$$

Thus we have $\dim \mathcal{O}_x = \dim G - \dim LI_x = 3n - (3n + 1 - \operatorname{rank} M) = \operatorname{rank} M - 1$. □

Next we introduce three operators on H whose purpose is to simplify calculations (specifically, inner products of column vectors) to establish the rank of M,

$$\text{Let } A = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \text{and } C = \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix}$$

denote the standard basis for su(2), so that the element

$$X = \begin{bmatrix} it & r + is \\ -r + is & -it \end{bmatrix}$$

is written $X = tA + rB + sC$ with respect to this basis.

[This basis is standard in the sense that A, B, C correspond to the truly standard basis vectors $\mathbf{i} = (0,1,0,0)$, $\mathbf{j} = (0,0,1,0)$, $\mathbf{k} = (0,0,0,1)$ of the pure quaternions, under the natural identification $\begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix} \leftrightarrow a + b\mathbf{j}$. In terms of the Pauli spin matrices, we have $A = i\sigma_z$, $B = i\sigma_y$, and $C = i\sigma_x$ where $\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$, and $\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$.]

Define elements A_k, B_k, C_k of LG for $1 \leqslant k \leqslant n$ to have A, B, C, respectively, in the kth coordinate and zero elsewhere.

$$A_k = \left(0, \ldots, 0, \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, 0, \ldots, 0\right),$$

$$B_k = \left(0, \ldots, 0, \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, 0, \ldots, 0\right),$$

$$C_k = \left(0,\ldots,0,\begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix},0,\ldots,0\right).$$

Applying (4), we have the following:

$$A_k|\psi\rangle = \sum_I i(-1)^{i_k} c_I |I\rangle, \tag{10}$$

$$B_k|\psi\rangle = \sum_I (-1)^{i_k} c_{I_k} |I\rangle, \tag{11}$$

$$C_k|\psi\rangle = \sum_I i c_{I_k} |I\rangle. \tag{12}$$

Simple checking shows that the complex vectors on the right-hand sides of the above three equations identify with columns of M via the standard identification (1). The rightmost column of M identifies with $-i|\psi\rangle$. Thus we may view M as the $(3n+1)$-tuple of complex vectors,

$$M = (A_1|\psi\rangle, B_1|\psi\rangle, C_1|\psi\rangle, \ldots, A_n|\psi\rangle, B_n|\psi\rangle, C_n|\psi\rangle, -i|\psi\rangle). \tag{13}$$

It is convenient to gather the columns of M into 3-tuples. We define the *triple* T_k to be the set of vectors

$$T_k = \{A_k|\psi\rangle, B_k|\psi\rangle, C_k|\psi\rangle\} \tag{14}$$

for $1 \leqslant k \leqslant n$. We view the vectors both as real and also as complex via (1).

IV. TECHNICAL LEMMAS

In this section we present combinatorial machinery that will be used to establish orthogonality among columns of the matrix M described in the preceding section.

Lemma 4.1: Let $L=(i_{jk})$ be an $\ell \times m$ matrix with entries in $\mathbb{Z}_2=\{0,1\}$, and let $E=((-1)^{i_{jk}})$. We view L as the matrix of a $\mathbb{Z}_2$-linear map $\mathbb{Z}_2^m \to \mathbb{Z}_2^\ell$ and we view E as the matrix of an $\mathbb{R}$-linear map. Suppose that E has a nontrivial kernel. Then either L has a nontrivial kernel or there is some $v \in \mathbb{Z}_2^m$ such that $Lv=(1,1,\ldots,1)$.

Proof: Assume the hypotheses of the lemma. Let N be the $\ell \times m$ matrix whose entries are all ones. As matrices over $\mathbb{R}$, observe that $E=N-2L$.

Since E has integer coefficients, there is a nonzero kernel vector v with integer coordinates. Dividing by a power of 2, if necessary, we may rescale v so that the integer coordinates are not all even. We have $0=Ev=(N-2L)v$, so $Lv=(N/2)v=(s/2)c$, where c is the column vector of all ones and s is the sum of the entries in v. Since Lv is a vector with integer entries, $Lv=(s/2)c$ implies s is even. Now we can read the equation $Lv=(s/2)c \bmod 2$. If $s/2=0 \bmod 2$, then $v \bmod 2$ is a nonzero kernel vector for L since not all coordinates of v are even. If $s/2=1 \bmod 2$, then $c=(1,1,\ldots,1)$ is in the image of L. □

Corollary 4.2: Let $\xi_1,\xi_2,\ldots,\xi_m$ be real numbers, not necessarily distinct, and not all of which are zero. Let D_m be the $2^m \times 2^m$ diagonal matrix whose r,r entry is

$$\sum_{i=1}^m (-1)^{r_i}\xi_i,$$

where $r=(r_m r_{m-1}\cdots r_2 r_1)$ is the binary expansion of the integer r in the range $0 \leqslant r \leqslant 2^m-1$. Suppose that D_m has at least one zero eigenvalue. Let $r^1,r^2,\ldots,r^\ell$ be the row numbers of the zero eigenvalues of D_m. Then there is a nonempty set $\mathcal{K}=\{k_1,k_2,\ldots,k_{m'}\}$ with $1 \leqslant k_1 < k_2 < \cdots < k_{m'} \leqslant m$ and m' even so that

$$\sum_{k\in\mathcal{K}} r_k^1 = \sum_{k\in\mathcal{K}} r_k^2 = \cdots = \sum_{k\in\mathcal{K}} r_k^\ell,$$

where the sums are taken mod 2.

Proof: Let $L=(r_j^i)$ and let $E=((-1)^{r_j^i})$. Since E kills the nonzero vector $(\xi_1,\xi_2,\ldots,\xi_m)$, Lemma 4.1 applies. If L is not injective, let $v=(v_1,v_2,\ldots,v_m)$ be a nonzero kernel vector and let $k_1,k_2,\ldots,k_{m'}$ be the indices i in the range from 1 to m inclusive for which $v_i=1$. Then the mod 2 equation $Lv=0$ yields

$$0 = \sum_{k\in\mathcal{K}} r_k^1 = \sum_{k\in\mathcal{K}} r_k^2 = \cdots = \sum_{k\in\mathcal{K}} r_k^\ell.$$

If there is a $v=(v_1,v_2,\ldots,v_m)$ such that $Lv=(1,1,\ldots,1)$, then setting $k_1,k_2,\ldots,k_{m'}$ to be the indices i for which $v_i=1$, then we have

$$1 = \sum_{k\in\mathcal{K}} r_k^1 = \sum_{k\in\mathcal{K}} r_k^2 = \cdots = \sum_{k\in\mathcal{K}} r_k^\ell.$$

To see that m' must be even, note that if

$$0 = \sum_{i=1}^{m} (-1)^{r_i}\xi_i$$

then we also have

$$0 = -\sum_{i=1}^{m} (-1)^{r_i}\xi_i = \sum_{i=1}^{m} (-1)^{r_i^c}\xi_i.$$

So if $r^1=r$ is a row number for a zero entry in D_m, so is $r^2=r^c$, where r^c is the binary string obtained from r by complementing each bit. Since these two rows have opposite parity in each bit, m' cannot be odd. This completes the proof. □

Definition 4.3: For the set $\mathcal{K}=\{k_1,k_2,\ldots,k_{m'}\}$ arising from zero entries in D_m in row numbers $r^1,r^2,\ldots,r^J$ as in 4.2 above, we define the *parity of* $\mathcal{K}$ to be the common value in $\mathbb{Z}_2$ of the sums

$$\sum_{k\in\mathcal{K}} r_k^1 = \sum_{k\in\mathcal{K}} r_k^2 = \cdots = \sum_{k\in\mathcal{K}} r_k^\ell.$$

Now we are ready to establish lower bounds on the rank of M by showing that inner products of certain pairs of columns can be arranged (via local unitary equivalence operations) to vanish.

V. ORTHOGONALITY RESULTS

Throughout this section, let $|\psi\rangle=\Sigma_I c_I|I\rangle\in H$ be a Hilbert space vector, and let M be the associated matrix as defined in Sec. III.

We make repeated use of the following elementary observation about the relationship between complex and real inner products. Let u,v be vectors in $\mathbb{C}^N$ and let u',v' be the corresponding vectors in $\mathbb{R}^{2N}$ given by the standard identification (1). The complex inner product $\langle u|v\rangle$ and the real dot product $u'\cdot v'$ are related by

$$\mathrm{Re}(\langle u|v\rangle = u'\cdot v'. \tag{15}$$

We shall consider complex inner products given in Table I among the column vectors of M given in (13). For the sake of compactness we have omitted a factor of $-i$ in the inner products (A), (E), and (I). With or without the factor $-i$, their vanishing guarantees the orthogonality of the rightmost column vector $-i|\psi\rangle$ of M to $A_k|\psi\rangle, B_k|\psi\rangle$, and $C_k|\psi\rangle$.

Our first proposition is that each triple spans three real dimensions.

Proposition 5.1: Triples span three dimensions: Let $T_k=\{A_k|\psi\rangle, B_k|\psi\rangle, C_k|\psi\rangle\}$ *be a triple of*

TABLE I. Inner products of pairs of columns of M.

$\langle\psi\|A_k\|\psi\rangle=\Sigma_I i(-1)^{i_k}\|c_I\|^2$	(A)
$\langle\psi\|A_j^\dagger A_k\|\psi\rangle=\Sigma_I(-1)^{i_j+i_k}\|c_I\|^2$	(B)
$\langle\psi\|B_j^\dagger A_k\|\psi\rangle=\Sigma_I i(-1)^{i_j+i_k}\overline{c_{I_j}}c_I$	(C)
$\langle\psi\|C_j^\dagger A_k\|\psi\rangle=\Sigma_I(-1)^{i_k}\overline{c_{I_j}}c_I$	(D)
$\langle\psi\|B_k\|\psi\rangle=\Sigma_I(-1)^{i_k}\overline{c_I}c_{I_k}$	(E)
$\langle\psi\|A_j^\dagger B_k\|\psi\rangle=\Sigma_I-i(-1)^{i_j+i_k}\overline{c_I}c_{I_k}$	(F)
$\langle\psi\|B_j^\dagger B_k\|\psi\rangle=\Sigma_I(-1)^{i_j+i_k}\overline{c_{I_j}}c_{I_k}$	(G)
$\langle\psi\|C_j^\dagger B_k\|\psi\rangle=\Sigma_I-i(-1)^{i_j}\overline{c_{I_j}}c_{I_k}$	(H)
$\langle\psi\|C_k\|\psi\rangle=\Sigma_I i\overline{c_I}c_{I_k}$	(I)
$\langle\psi\|A_j^\dagger C_k\|\psi\rangle=\Sigma_I(-1)^{i_j}\overline{c_I}c_{I_k}$	(J)
$\langle\psi\|B_j^\dagger C_k\|\psi\rangle=\Sigma_I i(-1)^{i_j}\overline{c_{I_j}}c_{I_k}$	(K)
$\langle\psi\|C_j^\dagger C_k\|\psi\rangle=\Sigma_I\overline{c_{I_j}}c_{I_k}$	(L)

columns of M. The three vectors in the triple are orthogonal when viewed as real vectors.

Proof: To prove the proposition, we show that inner products (F), (J), and (K) in Table I are pure imaginary for the case $j=k$. First, for (F), the Ith summand is

$$-i(-1)^{i_k+i_k}\overline{c_I}c_{I_k}=-i\overline{c_I}c_{I_k}$$

and the I_kth summand is

$$-i(-1)^{i_k+1+i_k+1}\overline{c_{I_k}}c_I=-i\overline{c_{I_k}}c_I.$$

The sum of the Ith and the I_kth summands is therefore $-2i\,\mathrm{Re}(\overline{c_I}c_{I_k})$. By pairing the summands in this way, we see that $\langle\psi|A_k^\dagger B_k|\psi\rangle$ is pure imaginary. Thus it follows from (15) that $A_k|\psi\rangle, B_k|\psi\rangle$ are orthogonal as real vectors.

Next we consider (J) with $j=k$. The Ith summand is $(-1)^{i_k}\overline{c_I}c_{I_k}$, while the I_kth summand is $(-1)^{i_k+1}\overline{c_{I_k}}c_I$. Thus the sum of the Ith and I_kth summands is $(-1)^{i_k}2i\,\mathrm{Im}(\overline{c_I}c_{I_k})$, which is pure imaginary, so $A_k|\psi\rangle, C_k|\psi\rangle$ are orthogonal as real vectors.

Finally we check (K) for $j=k$. In this case the Ith summand is $i(-1)^{i_k}|c_{I_k}|^2$ so the inner product is pure imaginary. Therefore $B_k|\psi\rangle, C_k|\psi\rangle$ are orthogonal as real vectors. This establishes the proposition. □

Next we show that a nontrivial linear dependence among the columns $A_k|\psi\rangle$ as real vectors guarantees that certain columns among the $B_k|\psi\rangle, C_k|\psi\rangle$ are orthogonal to spans of certain sets of triples.

Proposition 5.2: Main orthogonality proposition: Suppose that

$$\sum_{k=1}^{m}\xi_k A_{j_k}|\psi\rangle=0$$

for some $1\leqslant j_1<j_2<\cdots<j_m\leqslant n$, ξ_j *real and not all zero. Then there is a nonempty subset* $K\subseteq\{j_1,j_2,\ldots,j_m\}$ *containing an even number of elements such that* $B_k|\psi\rangle$ *and* $C_k|\psi\rangle$ *are orthogonal to* $-i|\psi\rangle$ *and to* $A_j|\psi\rangle, B_j|\psi\rangle, C_j|\psi\rangle$ *for all* $k\in K$, $j\notin K$.

Proof: Let D_m be the matrix constructed from $\xi_1,\ldots,\xi_m$ as described in the technical lemmas section. Let c_I be a nonzero state vector coefficient. By (10), the Ith coordinate of $\Sigma_{k=1}^m\xi_k A_{j_k}|\psi\rangle$ is $ic_I\Sigma_k(-1)^{i_{j_k}}\xi_k$, so the hypothesis $\Sigma_{k=1}^m\xi_k A_{j_k}|\psi\rangle=0$ guarantees that D_m has at least one zero eigenvalue, namely $\Sigma_k(-1)^{i_{j_k}}\xi_k$ where I is any multi-index for which $c_I\neq 0$. Therefore $\xi_1,\xi_2,\ldots,\xi_m$ and D_m meet the hypothesis of corollary 4.2.

Let $\mathcal{K}=\{k_1,k_2,\ldots,k_{m'}\}$ be the subset of $\{1,2,\ldots,m\}$ whose existence is guaranteed by 4.2 with corresponding parity b as defined in 4.3, and let $K=\{j_{k_1},j_{k_2},\ldots,j_{k_{m'}}\}$. The set of multi-indices of state basis vectors $|I\rangle$ is partitioned by K into two equal-sized equivalence classes by the following equivalence relation.

$$(i_1,i_2,\ldots,i_n)\sim(i'_1,i'_2,\ldots,i'_n)\Leftrightarrow\sum_{k\in K}i_k=\sum_{k\in K}i'_k \bmod 2 \tag{16}$$

In words, $I\sim I'$ if the parity of the sum of bits in columns in K is the same for I and I'. Let $\mathcal{P}$ be the set of multi-indices of parity class b and let $\mathcal{P}'$ be the opposite parity class.

We claim that all complex inner products of the form (E)–(L) in Table I vanish for $k\in K$ and $j\notin K$. From this it follows from (15) that the corresponding real dot products also vanish. Observe that for any I for which $c_I\neq 0$ we have $\Sigma_k(-1)^{i_{j_k}}\xi_k=0$, so I is in parity class $\mathcal{P}$. So if I,J are multi-indices in opposite parity classes, at least one of c_I,c_J must be zero. If $k\in K$ and $j\notin K$ then multi-indices I,I_k are in opposite parity classes, and also I_j,I_k are in opposite parity classes. Since every summand in each of the inner products (E)–(L) has a factor either of the form $\overline{c_I}c_{I_k}$ or of the form $\overline{c_{I_j}}c_{I_k}$ with $k\in K$ and $j\notin K$, all of the inner products vanish.

This completes the proof. □

Proposition 5.3: Suppose that for some $1\leq l<l'\leq n$ *we have* $A_l|\psi\rangle=A_{l'}|\psi\rangle$ *and* $C_l|\psi\rangle=C_{l'}|\psi\rangle$. *Then* $A_k|\psi\rangle,B_k|\psi\rangle$, *and* $C_k|\psi\rangle$ *are each orthogonal to* $-i|\psi\rangle$ *and to* $A_j|\psi\rangle,B_j|\psi\rangle,C_j|\psi\rangle$ *for all* $k\in\{l,l'\}$, $j\notin\{l,l'\}$.

Proof: We claim that all of the complex [and hence also real, by (15)] inner products (A)–(L) vanish for $k\in\{l,l'\}$ and $j\notin\{l,l'\}$. We begin by applying Proposition 5.2 to the hypothesis $A_l|\psi\rangle=A_{l'}|\psi\rangle$. In the notation of 5.2 we have $m=2$ and therefore also $m'=2$ since m' is an even number in the range $0<m'\leq m$, so $K=\{l,l'\}$. Thus we have from 5.2 that $B_k|\psi\rangle$ and $C_k|\psi\rangle$ are orthogonal to $-i|\psi\rangle$ and to $A_j|\psi\rangle,B_j|\psi\rangle,C_j|\psi\rangle$ for all $k\in\{l,l'\}$, $j\notin\{l,l'\}$.

It remains to be shown that $A_l|\psi\rangle,A_{l'}|\psi\rangle$ are also orthogonal to $-i|\psi\rangle$ and to $A_j|\psi\rangle,B_j|\psi\rangle,C_j|\psi\rangle$ for all $j\notin\{l,l'\}$.

The hypothesis $C_l|\psi\rangle=C_{l'}|\psi\rangle$ implies that $c_{I_l}=c_{I_{l'}}$, or equivalently, that $c_I=c_{I_{ll'}}$ for all I. This implies that summands of the inner products (A)–(D) cancel in pairs for $k\in\{l,l'\}$, $j\notin\{l,l'\}$, as follows. The Ith summand of (A) is $i(-1)^{i_k}|c_I|^2$ and the $I_{ll'}$th summand is $i(-1)^{i_k+1}|c_I|^2$. The Ith summand of (B) is $(-1)^{i_j+i_k}|c_I|^2$ and the $I_{ll'}$th summand is $(-1)^{i_j+i_k+1}|c_I|^2$. The Ith summand of (C) is $i(-1)^{i_j+i_k}\overline{c_{I_j}}c_I$ and the $I_{ll'}$th summand is $i(-1)^{i_j+i_k+1}\overline{c_{I_j}}c_I$. The Ith summand of (D) is $(-1)^{i_k}\overline{c_{I_j}}c_I$ and the $I_{ll'}$th summand is $(-1)^{i_k+1}\overline{c_{I_j}}c_I$.

This completes the proof. □

VI. LOCAL UNITARY ADJUSTMENT

In this section we adapt the orthogonality results of the preceding section to hypotheses involving more general linear dependencies.

Let us write $\langle T_{i_1},T_{i_2},\ldots,T_{i_r}\rangle$ to denote the subspace of the (real) column space of M spanned by the vectors in the triples $T_{i_1},\ldots,T_{i_r}$ viewed as real vectors.

Proposition 6.1: Main orthogonality proposition generalized: Suppose that

$$\dim\langle T_{j_1},T_{j_2},\ldots,T_{j_m}\rangle<3m$$

for some $1\leq j_1<j_2<\cdots<j_m\leq n$. *Then there is a nonempty subset* $K\subseteq\{j_1,j_2,\ldots,j_m\}$ *containing an even number of elements such that there are two orthogonal vectors* $|\zeta_k\rangle,|\eta_k\rangle$ *in* $\langle T_k\rangle$, *both of which are orthogonal to* $-i|\psi\rangle,A_j|\psi\rangle,B_j|\psi\rangle$ *and to* $C_j|\psi\rangle$ *for all* $k\in K$, $j\notin K$.

Proof: Let us write the linear dependency as a relation

$$\sum_{i=1}^{m} \xi_i |\phi_i\rangle = 0,$$

where ξ_i is real, $|\phi_i\rangle$ lies in $\langle T_{j_i}\rangle$, $\langle \phi_i|\phi_i\rangle = \langle \psi|\psi\rangle$ for $1 \leqslant i \leqslant m$, and not all the ξ_i are zero. Write each $|\phi_i\rangle$ as a linear combination

$$|\phi_i\rangle = \alpha_i A_{j_i}|\psi\rangle + \beta_i B_{j_i}|\psi\rangle + \gamma_i C_{j_i}|\psi\rangle$$

with α_i, β_i, and γ_i real. Let $R_i \in \mathrm{SO}(\mathrm{su}(2))$ be such that

$$R_i(A) = \alpha_i A + \beta_i B + \gamma_i C.$$

Since the adjoint representation $\mathrm{Ad}: \mathrm{SU}(2) \to \mathrm{SO}(\mathrm{su}(2))$ is surjective, we can choose $U_{j_i} \in \mathrm{SU}(2)$ such that $\mathrm{Ad}(U_{j_i}^{\dagger}) = R_i$, that is, $U_{j_i}^{\dagger} X U_{j_i} = R_i X$ for all $X \in \mathrm{su}(2)$. For $j \notin \{j_1, j_2, \ldots, j_m\}$, set U_j equal to the identity. Finally, let $U \in G = \mathrm{SU}(2)^n$ be $U = \prod_{i=1}^{n} U_i$.

Now observe that

$$\sum_{i=1}^{m} \xi_i (U^{\dagger} A_{j_i} U)|\psi\rangle = \sum_{i=1}^{m} \xi_i |\phi_i\rangle = 0.$$

Applying U to both sides, we get

$$\sum_{i=1}^{m} \xi_i A_{j_i} (U|\psi\rangle) = 0.$$

Let M' be the matrix for the state vector $U|\psi\rangle$. Applying the main orthogonality proposition 5.2 to M', we get that $B_k(U|\psi\rangle), C_k(U|\psi\rangle)$ are orthogonal to $U|\psi\rangle$ and to $A_j U|\psi\rangle, B_j U|\psi\rangle, C_j U|\psi\rangle$ for $k \in K$, $j \notin K$. Now set

$$|\zeta_k\rangle = U^{\dagger} B_k U|\psi\rangle,$$

$$|\eta_k\rangle = U^{\dagger} C_k U|\psi\rangle$$

for $k \in K$. Since U is unitary, we have that $|\zeta_k\rangle, |\eta_k\rangle$ are orthogonal to $U^{\dagger}U|\psi\rangle = |\psi\rangle$ and to $U^{\dagger}A_j U|\psi\rangle, U^{\dagger}B_j U|\psi\rangle, U^{\dagger}C_j U|\psi\rangle$ for $k \in K$, $j \notin K$. Since the three vectors $U^{\dagger}A_j U|\psi\rangle, U^{\dagger}B_j U|\psi\rangle, U^{\dagger}C_j U|\psi\rangle$ have the same span as $A_j|\psi\rangle, B_j|\psi\rangle, C_j|\psi\rangle$ for all j, the proposition is established. □

Proposition 6.2: Generalization of 5.3: Suppose that $\dim\langle T_l, T_{l'}\rangle \leqslant 4$ *for some* $1 \leqslant l < l' \leqslant n$. *Then* $A_k|\psi\rangle, B_k|\psi\rangle$, *and* $C_k|\psi\rangle$ *are each orthogonal to* $-i|\psi\rangle$ *and to* $A_j|\psi\rangle, B_j|\psi\rangle, C_j|\psi\rangle$ *for all* $k \in \{l, l'\}$, $j \notin \{l, l'\}$.

Proof: The proof is very similar to the proof of 6.1.

Since $\dim\langle T_l, T_{l'}\rangle \leqslant 4$, the dimension of the intersection $\langle T_l\rangle \cap \langle T_{l'}\rangle$ is at least two. Choose orthogonal vectors $|\phi\rangle, |\phi'\rangle$ in $\langle T_l\rangle \cap \langle T_{l'}\rangle$ with $\langle \phi|\phi\rangle = \langle \phi'|\phi'\rangle = \langle \psi|\psi\rangle$. Write linear combinations,

$$|\phi\rangle = \alpha_k A_k|\psi\rangle + \beta_k B_k|\psi\rangle + \gamma_k C_k|\psi\rangle,$$

$$|\phi'\rangle = \alpha'_k A_k|\psi\rangle + \beta'_k B_k|\psi\rangle + \gamma'_k C_k|\psi\rangle,$$

and let $R_k \in \mathrm{SO}(\mathrm{su}(2))$ be such that

$$R_k(A) = \alpha_k A + \beta_k B + \gamma_k C,$$

$$R_k(C) = \alpha'_k A + \beta'_k B + \gamma'_k C,$$

for $k \in \{l, l'\}$.

Since the adjoint representation $\mathrm{Ad}:\mathrm{SU}(2)\to\mathrm{SO}(\mathrm{su}(2))$ is surjective, we can choose $U_k \in \mathrm{SU}(2)$ such that $\mathrm{Ad}(U_k^\dagger)=R_k$, that is, $U_k^\dagger X U_k = R_k X$ for all $X\in\mathrm{su}(2)$. For $j\notin\{l,l'\}$, set U_j equal to the identity. Finally, let $U\in G=\mathrm{SU}(2)^n$ be $U=\prod_{i=1}^n U_i$.

Now observe that

$$U^\dagger A_l U|\psi\rangle = |\phi\rangle = U^\dagger A_{l'} U|\psi\rangle,$$

$$U^\dagger C_l U|\psi\rangle = |\phi'\rangle = U^\dagger C_{l'} U|\psi\rangle.$$

Applying U to both sides, we get

$$A_l U|\psi\rangle = A_{l'} U|\psi\rangle,$$

$$C_l U|\psi\rangle = C_{l'} U|\psi\rangle.$$

Let M' be the matrix for the state vector $U|\psi\rangle$. Applying 5.3 M', we get that $A_k(U|\psi\rangle), B_k(U|\psi\rangle), C_k(U|\psi\rangle)$ are orthogonal to $U|\psi\rangle$ and to $A_jU|\psi\rangle, B_jU|\psi\rangle, C_jU|\psi\rangle$ for $k\in\{l,l'\}$, $j\notin\{l,l'\}$. Since U is unitary, we have that $U^\dagger A_k U|\psi\rangle, U^\dagger B_k U|\psi\rangle, U^\dagger C_k U|\psi\rangle$ are orthogonal to $U^\dagger U|\psi\rangle=|\psi\rangle$ and to $U^\dagger A_j U|\psi\rangle, U^\dagger B_j U|\psi\rangle, U^\dagger C_j U|\psi\rangle$ for $k\in\{l,l'\}$, $j\notin\{l,l'\}$. Since the three vectors $U^\dagger A_j U|\psi\rangle, U^\dagger B_j U|\psi\rangle, U^\dagger C_j U|\psi\rangle$ have the same span as $A_j|\psi\rangle, B_j|\psi\rangle, C_j|\psi\rangle$ for all j, the proposition is established. □

VII. MINIMUM ORBIT THEOREM

Theorem 7.1: *Minimum orbit dimension: For the local unitary group action on state space for n qubits, the smallest orbit dimension is*

$$\min\{\dim \mathcal{O}_x : x\in\mathbb{P}(H)\} = \begin{cases} \frac{3n}{2}, & n \text{ even}, \\ \frac{3n+1}{2}, & n \text{ odd}. \end{cases}$$

We begin the proof by exhibiting a state for which the claimed minimum dimension is realized.

Let $|s\rangle=|01\rangle-|10\rangle$ be a Hilbert space representative of the singlet state, let $X=\begin{bmatrix} it & u \\ -\bar{u} & -it \end{bmatrix}$ be an element of su(2). We have

$$(X,X)\cdot|s\rangle = 0$$

so (X,X) is in the isotropy Lie algebra of the state represented by $|s\rangle$.

From this it follows that $(X_1,X_1,X_2,X_2,\ldots,X_k,X_k)$ stabilizes the $2k$-qubit state x represented by

$$\underbrace{|s\rangle\otimes|s\rangle\otimes\cdots\otimes|s\rangle}_{k \text{ copies}}$$

for all $X_1,X_2,\ldots,X_k$ in su(2). Therefore LI_x has dimension at least $3k=3n/2$ for $n=2k$, and therefore $\dim \mathcal{O}_x \leqslant 3n-3n/2=3n/2$ for n even.

Observe that $\left(X_1,X_1,X_2,X_2,\ldots,X_k,X_k,\begin{bmatrix} it & 0 \\ 0 & -it \end{bmatrix}\right)$ stabilizes the $(2k+1)$-qubit state x represented by $|s\rangle\otimes|s\rangle\otimes\cdots\otimes|s\rangle\otimes|0\rangle$ (by a phase factor), so the dimension of LI_x is at least $3k+1=(3n-1)/2$ for $n=2k+1$, and therefore $\dim \mathcal{O}_x \leqslant 3n-(3n-1)/2=(3n+1)/2$ for n odd.

These calculations establish that

$$\min\{\dim \mathcal{O}_x : x \in \mathbb{P}(H)\} \leqslant \begin{cases} \frac{3n}{2}, & n \text{ even}, \\ \frac{3n+1}{2}, & n \text{ odd}. \end{cases} \tag{17}$$

Next we show that this bound on orbit dimension is sharp by establishing a lower bound for the rank of M. From 3.3 the desired lower bound for the minimum orbit dimension follows immediately from 7.2 below.

Proposition 7.2: Minimum rank of M: Let x be a state for a system of n qubits, let $|\psi\rangle$ be a Hilbert space representative for x, and let M be the real matrix associated to $|\psi\rangle$ as defined in Sec. III. *We have*

$$\operatorname{rank} M \geqslant \begin{cases} \frac{3n}{2} + 1, & n \textit{ even}, \\ \frac{3n+1}{2} + 1, & n \textit{ odd}. \end{cases}$$

Proof: Let $\mathcal{C} = \{A_1|\psi\rangle, B_1|\psi\rangle, C_1|\psi\rangle, \ldots, A_n|\psi\rangle, B_n|\psi\rangle, C_n|\psi\rangle, -i|\psi\rangle\}$ denote the set of columns of M. For a subset $\mathcal{S} \subseteq \mathcal{C}$, let $\langle \mathcal{S} \rangle$ denote the real span of the column vectors contained in $\mathcal{S}$. Let $\mathcal{S}_0$ be a subset of $\mathcal{C}$ which is the union of some number p of triples, and is maximal with respect to the property that $\langle \mathcal{S}_0 \rangle$ contains a subspace W for which

(i)

$$\dim W \geqslant \begin{cases} \frac{3p}{2}, & p \text{ even}, \\ \frac{3p+1}{2}, & p \text{ odd}, \end{cases}$$

(ii)

$$W \perp \langle \mathcal{C} \setminus \mathcal{S}_0 \rangle.$$

We separate the argument into cases. We show that in every case, either 7.2 holds or we can derive a contradiction by constructing a superset $\mathcal{S}_1$ of $\mathcal{S}_0$ which is the union of some number $p' > p$ of triples and which contains a subspace W' satisfying properties (i) and (ii) with p' in place of p. The construction of $\mathcal{S}_1$ violates the maximality of $\mathcal{S}_0$ and therefore rules out the case in question.

Case 1: Suppose that $p = n$, so that $\mathcal{C} \setminus \mathcal{S}_0 = \{-i|\psi\rangle\}$. Then property (ii) guarantees that $\operatorname{rank} M \geqslant \dim W + 1$, so property (i) guarantees that 7.2 holds.

Case 2: Suppose that $p < n$ and that the remaining triples $T_{j_1}, T_{j_2}, \ldots, T_{j_{n-p}}$ in $\mathcal{C} \setminus \mathcal{S}_0$ have the maximum possible span, that is,

$$\dim\langle T_{j_1}, T_{j_2}, \ldots, T_{j_{n-p}} \rangle = 3(n-p).$$

Properties (i) and (ii) imply that

$$\operatorname{rank} M \geqslant \dim W + \dim\langle \mathcal{C} \setminus \mathcal{S}_0 \rangle \geqslant \frac{3p}{2} + 3(n-p) = \frac{6n-3p}{2}$$

$$\geqslant \frac{6n-(3n-3)}{2} \quad (\text{since } p \leqslant n-1) = \frac{3n+3}{2} = \frac{3n+1}{2} + 1$$

and so 7.2 holds. Note that if $p = n-1$, the hypothesis of full span is met by 5.1. Therefore in the remaining cases we need only consider $p \leqslant n-2$.

Case 3: Suppose $p \leqslant n-2$ and that there is a pair of triples $T_l, T_{l'}$ in $\mathcal{C} \setminus \mathcal{S}_0$ with $1 \leqslant l < l' \leqslant n$ such that $\dim\langle T_l, T_{l'} \rangle \leqslant 4$. Let $\mathcal{S}_1 = \mathcal{S}_0 \cup T_l \cup T_{l'}$, let $p' = p+2$, and let $W' = W \oplus \langle T_l \cup T_{l'} \rangle$, where "$\oplus$" denotes the orthogonal direct sum. That the sum is orthogonal is guaranteed by property (ii) for W. Proposition 6.2 implies that property (ii) also holds for the pair $(\mathcal{S}_1, W')$ and that $\dim W' \geqslant \dim W + 3$. It follows that if p is even, so is p' and we have

$$\dim W' \geqslant \frac{3p}{2} + 3 = \frac{3p+6}{2} = \frac{3(p+2)}{2} = \frac{3p'}{2}$$

and similarly if p and p' are odd we have

$$\dim W' \geqslant \frac{3p+1}{2} + 3 = \frac{3p'+1}{2}$$

so $(\mathcal{S}_1, W')$ satisfies property (i). Thus $\mathcal{S}_1$ violates the maximality of $\mathcal{S}_0$, so we conclude that the hypothesis of case 3 is impossible.

Case 4: Suppose $p \leqslant n-2$ and that there is a pair of triples $T_l, T_{l'}$ in $\mathcal{C}\backslash\mathcal{S}_0$ with $1 \leqslant l < l' \leqslant n$ such that $\dim\langle T_l, T_{l'}\rangle = 5$. Applying 6.1 we have four vectors

$$|\zeta_l\rangle, |\eta_l\rangle \in \langle T_l\rangle, \quad |\zeta_{l'}\rangle, |\eta_{l'}\rangle \in \langle T_{l'}\rangle$$

which must span at least three dimensions, so once again $\mathcal{S}_1 = \mathcal{S}_0 \cup T_l \cup T_{l'}$ with the subspace

$$W' = W \oplus \langle |\zeta_l\rangle, |\eta_l\rangle, |\zeta_{l'}\rangle, |\eta_{l'}\rangle\rangle$$

violates the maximality of $\mathcal{S}_0$. We conclude that the hypothesis of case 4 is impossible.

Case 5: The only remaining possibility is that $p \leqslant n-3$. Let $\mathcal{T} = \{T_{j_1}, T_{j_2}, \ldots, T_{j_m}\}$ be a set of triples in $\mathcal{C}\backslash\mathcal{S}_0$ with $m \geqslant 3$ minimal with respect to the property

$$\dim\langle T_{j_1}, T_{j_2}, \ldots, T_{j_m}\rangle < 3m.$$

Applying 6.1 we have two vectors

$$|\zeta_k\rangle, |\eta_k\rangle \in \langle T_k\rangle$$

for each of the $m' \geqslant 2$ elements $k \in K$. Let

$$\mathcal{S}_1 = \mathcal{S}_0 \cup \left(\bigcup_{k\in K} T_k\right),$$

let $p' = p + m'$, and let

$$W' = W \oplus \langle \{|\zeta_k\rangle, |\eta_k\rangle\}_{k\in K}\rangle.$$

Note that property (ii) holds for $(\mathcal{S}_1, W')$. If $m' < m$, then the $2m'$ vectors in $\{|\zeta_k\rangle, |\eta_k\rangle\}_{k\in K}$ are independent by the minimality of $\mathcal{T}$, so we have

$$\dim W' \geqslant \dim W + 2m' \geqslant \frac{3p}{2} + 2m' = \frac{3p' + m'}{2} \geqslant \frac{3p'+1}{2}$$

so property (i) holds for $(\mathcal{S}_1, W')$, but this contradicts the maximality of $\mathcal{S}_0$. Finally, if $m' = m$, then $m \geqslant 4$ (since m' is even) and at least $2(m-1)$ of the vectors in $\{|\zeta_k\rangle, |\eta_k\rangle\}_{k\in K}$ must be independent, again by the minimality of $\mathcal{T}$. If p is even, then $p' = p + m$ is also even and we have

$$\dim W' \geqslant \dim W + 2(m-1) \geqslant \frac{3p}{2} + 2(m-1) = \frac{3p' + m - 4}{2} \geqslant \frac{3p'}{2}.$$

If p is odd, then $p' = p + m$ is odd and we have

$$\dim W' \geqslant \dim W + 2(m-1) \geqslant \frac{3p+1}{2} + 2(m-1) = \frac{3p' + m - 3}{2} \geqslant \frac{3p'+1}{2}.$$

Thus $\mathcal{S}_1$ with the subspace W' violates the maximality of $\mathcal{S}_0$. We conclude that the hypothesis of case 5 is impossible.

Having exhausted all possible cases, this completes the proof of 7.2, and hence of Theorem 7.1. □

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Ground state of the massless Nelson model in a non-Fock representation

Itaru Sasaki[a)]
Department of Mathematics, Hokkaido University, Sapporo 060-0810, Japan

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We consider a model of a particle coupled to a massless scalar field (the massless Nelson model) in a non-Fock representation. We prove the existence of a ground state of the system, applying the method of Griesemer, Lieb, and Loss. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2050507]

I. INTRODUCTION

The Nelson model is a quantum mechanical model which describes an interaction between some quantum mechanical particles and a Bose field.[8] In this article, we present a criterion for a Nelson model to have a ground state.

We consider one particle under the influence of an external potential V and coupled to a scalar Bose field. The Hilbert space of the system is given by

$$\mathcal{F} := L^2(\mathbb{R}^3) \otimes \mathcal{F}_{\mathrm{b}}(L^2(\mathbb{R}^3)), \tag{1}$$

where $\mathcal{F}_{\mathrm{b}}(L^2(\mathbb{R}^3))$ is the Boson Fock space over $L^2(\mathbb{R}^3)$. The standard Nelson Hamiltonian is of the form

$$H_m^V := (-\Delta + V) \otimes \mathbb{1} + \mathbb{1} \otimes H_f(m) + \lambda \phi^{\oplus}(v), \quad \text{on } \mathcal{F},$$

where $\mathbb{1}$ denotes identity, Δ is the generalized Laplacian on $L^2(\mathbb{R}^3)$, $\lambda \in \mathbb{R}$ is a coupling constant, and $H_f(m)$ and $\phi^{\oplus}(v)$ are defined by

$$H_f(m) := \int_{\mathbb{R}^3} \omega_m(k) a(k)^* a(k) \mathrm{d}k,$$

$$\phi^{\oplus}(v) := \frac{1}{\sqrt{2}} \int_{\mathbb{R}^3} (v(x,k) \otimes a(k)^* + v(x,k)^* \otimes a(k)) \mathrm{d}k,$$

with

$$\omega_m(k) := \sqrt{k^2 + m^2}, \quad v(x,k) := \frac{1}{\sqrt{(2\pi)^3}} \frac{\hat{\rho}(k)}{|k|^{1/2}} e^{-ikx},$$

where $|k|^{-1/2}\hat{\rho} \in \mathrm{Dom}(\omega_m^{-1/2})$ and $a(k)^*, a(k)$ are the distribution kernels of the creation and annihilation operators on $\mathcal{F}_{\mathrm{b}}(L^2(\mathbb{R}^3))$ ($\mathrm{Dom}(A)$ means the domain of operator A). The problem on the ground state of H_m^V can be classified as follows:

(i) the massive case: $m > 0$

[a)]Electronic mail: i-sasaki@math.sci.hokudai.ac.jp

$$\text{(ii) the massless case: } m=0 \begin{cases} |k|^{-1/2}\hat{\rho} \in \mathrm{Dom}(\omega_0^{-1}) \text{: infrared regular} \\ |k|^{-1/2}\hat{\rho} \notin \mathrm{Dom}(\omega_0^{-1}) \text{: infrared singular.} \end{cases}$$

In almost all cases, to prove existence of a ground state for the massive case is easy. The first result on the ground state problem, to our knowledge, is due to Spohn.[12] In Ref. 12 he proved existence of a ground state in the case where the infrared regular (I.R.) condition holds and $(-\Delta+V+i)^{-1}$ is compact. If $(-\Delta+V+i)^{-1}$ is not compact, this theorem shows that a ground state exists if the I.R. condition holds and the coupling constant λ is small enough. After the work of Spohn,[12] C. Gérard proved existence of a ground state of an extended model of the Nelson model in the case where an abstract particle Hamiltonian K (which corresponds to $-\Delta+V$ in the previous context) has compact resolvent and an I.R. like condition holds.[3] On the other hand, Lörinczi *et al.*[7] showed that H_0^V has *no* ground state if the infrared singular (I.S.) condition holds in spite of the condition $V(x) > C|x|^{\alpha}(C, \alpha > 0)$ (also refer to Ref. 2 about the absence of ground states). Recently, Hirokawa *et al.*[5] proved existence of a ground state for the renormalized Nelson model.

In the case where the I.S. condition holds, H_0^V may not have a ground state,[7] but Arai[1] showed that a massless Nelson model in *a non-Fock representation* has a ground state.

We work with the non-Fock representation introduced in Ref. 1. In this representation the massless Nelson model we consider is of the form:

$$\tilde{H}^V := (-\Delta + V) \otimes \mathbb{1} + \mathbb{1} \otimes H_f(0) + \lambda \phi^{\oplus}(G) - \lambda^2 \mathcal{V}(\hat{x}) \otimes \mathbb{1} + \lambda^2 \mathcal{W} \mathbb{1},$$

where $\mathcal{V}(\hat{x})$ is the multiplication operator by $\mathcal{V}(x) := \mathrm{Re}\langle |k|^{-1/2} v(0), |k|^{-1/2} v(x) \rangle$, $\mathcal{W} := \| |k|^{-1/2} v(0) \|^2$ is a constant, and $G(x,k) := v(x,k) - v(0,k)$. If $m=0$ and the I.R. condition holds, $\tilde{H}^V$ is unitarily equivalent to H_0^V (Proposition 2.1). But if the I.S. condition holds, $\tilde{H}^V$ may not be unitarily equivalent to H_0^V. If the I.S. condition holds, to consider $\tilde{H}^V$ means to choose a non-Fock representation of the canonical commutation relations of a, a^* (see Ref. 1). Note that, in the massless case $m=0$, the Hamiltonian we consider is $\tilde{H}^V$, not H_0^V.

For the non-Fock Hamiltonian $\tilde{H}^V$, we present a criterion for $\tilde{H}^V$ to have a ground state. The criterion is essentially the same condition as in Ref. 4, and we prove existence of a ground state without assuming the I.R. condition. Our strategy is the same as that of Ref. 4. We, however, improved the proof of the photon derivative bound. In the proof of photon derivative bound in Ref. 4, it is difficult to prove that the integer-valued k-dependent sequence $h_l(k)$ is measurable. In our new proof of the photon derivative bound, such uncertain sequence does not appear.

This article is organized as follows. In Sec. II we describe rigorous definitions of our system and state main results. In Sec. III, we prove the main theorem. In the Appendix, we establish a formula which expresses a second quantization operator by the annihilation operators.

II. NOTATION AND MAIN RESULTS

We consider a model of one particle interacting with a scalar Bose field, and in an external potential $V: \mathbb{R}^3_x \to \mathbb{R}$ satisfying $V \in L^1_{\mathrm{loc}}(\mathbb{R}^3_x)$. The Hilbert space for the model is given by $\mathcal{F} := L^2(\mathbb{R}^3_x) \otimes \mathcal{F}_{\mathrm{b}}(L^2(\mathbb{R}^3_k))$, where $\mathcal{F}_{\mathrm{b}}(L^2(\mathbb{R}^3_k))$ is the Boson Fock space over $L^2(\mathbb{R}^3_k)$ (see Ref. 9). For $m \geqslant 0$ we define a function $\omega_m: \mathbb{R}^3_k \to \mathbb{R}$ by $\omega_m(k) := \sqrt{k^2+m^2}$. The multiplication operator by ω_m is denoted by the same symbol. The free Hamiltonian of the scalar Bose field is the second quantization of ω_m (Ref. 9):

$$H_f(m) := \mathrm{d}\Gamma_{\mathrm{b}}(\omega_m). \tag{2}$$

We set $V_{\pm}(x) := \max\{0, \pm V(x)\}$. Throughout this article, we assume that the potential V has the following properties:

[N.1] There exist constants $a < 1$ and $b \in \mathbb{R}$ such that

$$\|V_-^{1/2}\psi\|^2 \leqslant a\|(-\Delta)\psi\|^2 + b\|\psi\|^2, \quad \psi \in C_0^\infty(\mathbb{R}_x^3).$$

The particle Hamiltonian H_p is a self-adjoint operator defined by

$$H_\mathrm{p} := -\Delta \dot{+} V, \quad \text{on } L^2(\mathbb{R}_x^3),$$

where $\dot{+}$ means the form sum. For $f \in L^2(\mathbb{R}_k^3)$ we denote by $a(f)^*$, $a(f)$, the creation and annihilation operators respectively, by $\Phi_\mathrm{S}(f) := \overline{[a(f)+a(f)^*]}/\sqrt{2}$ the Segal field operators ("$-$" means closure). It is well known that $\Phi_\mathrm{S}(f)$ is a self-adjoint operator on $\mathcal{F}_\mathrm{b}(L^2(\mathbb{R}_k^3))$ (see Ref. 10). For $x \in \mathbb{R}_x^3$ and $\hat{\rho} \in L^2(\mathbb{R}_k^3) \cap \mathrm{Dom}(|k|^{-1/2})$ we define $v(x) \in L^2(\mathbb{R}_k^3)$ by

$$v(x)(k) := v(x,k) := \frac{1}{(2\pi)^{3/2}} \frac{\hat{\rho}(k)}{|k|^{1/2}} e^{-ikx}, \quad k \in \mathbb{R}_k^3.$$

The Hilbert space $\mathcal{F}$ can be identified with the fibre direct integral of $\mathcal{F}_\mathrm{b}(L^2(\mathbb{R}_k^3))$ (see Ref. 11):

$$\mathcal{F} = \int_{\mathbb{R}_x^3}^{\oplus} \mathcal{F}_\mathrm{b}(L^2(\mathbb{R}_k^3))\mathrm{d}x.$$

In this identification the operator

$$\phi^\oplus(v) := \int_{\mathbb{R}_x^3}^{\oplus} \Phi_\mathrm{S}(v(x))\mathrm{d}x$$

gives a self-adjoint operator on $\mathcal{F}$.[11]

The Hamiltonian of the standard Nelson model is defined by

$$H_m^V := H_\mathrm{p} \otimes \mathbb{1} + \mathbb{1} \otimes H_f(m) + \lambda\phi^\oplus(v).$$

Here $\lambda \in \mathbb{R}$ is a coupling constant. We set

$$H_0 := H_\mathrm{p} \otimes \mathbb{1} + \mathbb{1} \otimes H_f(m),$$

the free Hamiltonian of the Nelson model. By [N.1], H_p is bounded below. Therefore H_0 is self-adjoint on $D(H_0) = D(H_\mathrm{p} \otimes \mathbb{1}) \cap D(\mathbb{1} \otimes H_f(m))$ and bounded below.

The following fact is well known:

Proposition 2.1: Assume $|k|^{-1/2}\hat{\rho} \in \mathrm{Dom}(\omega_m^{1/2})$ *and (N.1). Then* H_m^V *is self-adjoint on* $\mathrm{Dom}(H_0)$ *and bounded below. Moreover* H_m^V *is essentially self-adjoint on each core for* H_0.

Under the assumption of Proposition 2.1, we set

$$E^V(m) := \inf \sigma(H_m^V),$$

the ground state energy of H_m^V. Where $\sigma(H_m^V)$ means the spectrum of H_m^V. If $E^V(m)$ is an eigenvalue of H_m^V, we say that H_m^V has a ground state and a eigenvector $\Phi_m \in \ker(H_m^V - E^V(m)) \backslash \{0\}$ is called a ground state of H_m^V.

Let $\theta \in C_0^\infty(\mathbb{R}_x^3)$, $\tilde{\theta} \in C^\infty(\mathbb{R}_x^3)$ be functions which satisfy the following properties (i), (ii):

$$\text{(i) } 0 \leqslant \theta(x), \tilde{\theta}(x) \leqslant 1, \quad \theta(x)^2 + \tilde{\theta}(x)^2 = 1, \ (x \in \mathbb{R}_x^3).$$

$$\text{(ii) } \theta(x) = \begin{cases} 1, & |x| \leqslant 1 \\ 0, & |x| \geqslant 2. \end{cases}$$

For $R > 0$ we define particle cutoff functions $\theta_R, \tilde{\theta}_R$ as follows:

$$\theta_R(x) := \theta(x/R), \quad \widetilde{\theta}_R(x) := \widetilde{\theta}(x/R).$$

We abbreviate $\theta_R \otimes \mathbb{1}, \widetilde{\theta}_R \otimes \mathbb{1}$ to $\theta_R, \widetilde{\theta}_R$, respectively if there is no danger of confusion. For a self-adjoint operator T, we denote by $Q(T)$ the form domain of T, and for $\Psi, \Phi \in Q(T)$, we write simply $\langle \Psi, T\Phi \rangle = \int_{\mathbb{R}} \mu \mathrm{d}\langle \Psi, E_T(\mu)\Phi \rangle$, where E_T means the spectral measure of T.

We define a quantity which physically means the minimal energy in the states where the particle is separated more than R away from the origin:

Definition 2.2:

$$E_\infty(R,m) := \inf_{\substack{\Psi \in Q(H_m^V) \\ \|\widetilde{\theta}_R \Psi\| \neq 0}} \frac{\langle \widetilde{\theta}_R \Psi, H_m^V \widetilde{\theta}_R \Psi \rangle}{\langle \Psi, \widetilde{\theta}_R^2 \Psi \rangle}.$$

Remark: For all $R > 0$, it is easy to see that $E^V(m) - E_\infty(R,m) \leqslant 0$.

The following condition is based on Ref. 4.

Hypothesis I (binding condition for $m > 0$):

$$E^V(m) < \limsup_{R \to \infty} E_\infty(R,m).$$

Theorem 2.3: *(Existence of ground state ($m > 0$)). Let $m > 0$. Assume [N.1] and Hypothesis I. Then H_m^V has a ground state.*

Proof: This is done in the same method as in the proof of (Ref. 4, Theorem 4.1). Therefore we omit the proof. ■

In the case $m = 0$, we need more assumptions:

[N.2] $\hat{\rho}/|k| \in L^2(\mathbb{R}_k^3)$.

Under conditions [N.1] and [N.2], the Hamiltonian of the massless Nelson model we consider is:

$$\widetilde{H}^V := H_{\mathrm{p}} \otimes \mathbb{1} + \mathbb{1} \otimes H_f(0) + \lambda \phi^{\oplus}(G) - \lambda^2 \mathcal{V}(\hat{x}) \otimes \mathbb{1} + \lambda^2 \mathcal{W} \mathbb{1},$$

where $\mathcal{W} := \|\omega_0^{-1/2} v(0)\|^2$ is a constant and $\mathcal{V}(\hat{x})$ is the multiplication operator by the function $\mathcal{V}(x) := \mathrm{Re}\langle \omega_0^{-1/2} v(0), \omega_0^{-1/2} v(x) \rangle$.

By [N.2], $\mathcal{V}(x)$ is uniformly continuous and $\lim_{|x| \to 0} \mathcal{V}(x) = 0$. The relation between $\widetilde{H}^V$ and H_0^V is given by the following proposition.

Proposition 2.4: Suppose that the infrared regular condition $\hat{\rho}/|k|^{3/2} \in L^2(\mathbb{R}_k^3)$ holds. Then $\widetilde{H}^V$ is unitarily equivalent to H_0^V.

Proof: By the assumption, the operator $T := \exp[-i\lambda \mathbb{1} \otimes \Phi_{\mathrm{S}}(i|k|^{-1} v(0))]$ is a unitary operator on $\mathcal{F}$ and H_m^V is unitarily equivalent to $\widetilde{H}^V = T H_m^V T^*$. ■

If the infrared singular condition $\hat{\rho}/|k|^{3/2} \notin L^2(\mathbb{R}_k^3)$ holds, this Hamiltonian $\widetilde{H}^V$ gives a Nelson Hamiltonian in a non-Fock representation (see Ref. 1).

For the existence of ground states of $\widetilde{H}^V$, we impose some conditions on $\hat{\rho}$:

[N.3] There exists an open set $S \subset \mathbb{R}^3$, such that $\mathrm{supp}\, \hat{\rho} = \overline{S}$. Moreover, for all $n \in \mathbb{N}$

$$S_n := \{k \in S \,|\, |k| < n\}$$

has the cone-property (see Ref. 6).

[N.4] There exists a function $\eta \in H^1(\mathbb{R}_k^3)$, such that $\hat{\rho} = \chi_S \eta$, where χ_S is the characteristic function of S.

[N.5] $\hat{\rho}$ is continuously differentiable in $S \backslash \{0\}$.

[N.6] $|k|^{-3/2} \hat{\rho}, |k|^{-1/2} |\nabla \hat{\rho}| \in L^p(S)$ for all $p, 1 < p < 2$.

Under the condition [N.1] and [N.2], it is easy to see that $E^V(0) = \inf \sigma(\widetilde{H}^V)$. One of the most important conditions for the existence of ground states of $\widetilde{H}^V$ is

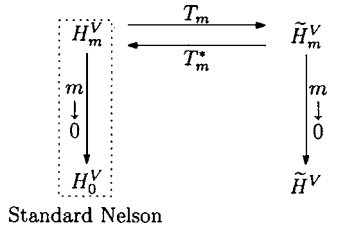

FIG. 1. Author—please provide caption.

Hypothesis II (binding condition for $m=0$):

$$E^V(0) < \limsup_{R\to\infty} E_\infty(R,0). \tag{3}$$

Now we state the main result of this article.

Theorem 2.5. *(Existence of ground state $(m=0)$): Assume [N.1]–[N.6] and Hypothesis II. Then the massless Nelson Hamiltonian $\tilde{H}^V$ has a ground state.*

Remark: In the case $\lim_{|x|\to\infty} V(x)=\infty$, it is easy to see that $\lim_{R\to\infty} E_\infty(R,m)=\infty$. Therefore Hypothesis II holds. On the other hand, if $\lim_{|x|\to\infty} V(x)\to 0$ and the particle Hamiltonian H_{p} has negative energy ground states, then Hypotheses I and II hold (see Ref. 4 Theorem 3.1).

Remark: Let $\Lambda>0$. Then $\hat{\rho}=\chi_\Lambda$ (the characteristic function of the region $|k|<\Lambda$) satisfies the above conditions [N.2]–[N.6]. Note that the function $\hat{\rho}=\chi_\Lambda$ is infrared singular, because $|k|^{-3/2}\hat{\rho}$ is not in $L^2(\mathbb{R}^3)$.

III. PROOF OF THEOREM 2.5

Throughout this section we assume [N.1]–[N.6] and Hypothesis II. In this section, we set $\lambda=1$, because Theorem 2.5 does not depend on λ explicitly (to restore λ, it is enough to replace $\hat{\rho}$ by $\lambda\hat{\rho}$).

For $m>0, T_m := \exp[-i\mathbb{1}\otimes\Phi_{\mathrm{S}}(iv(0/\omega_m))]$ is a unitary operator on $\mathcal{F}$, and we have

$$\tilde{H}_m^V := T_m H_m^V T_m^* = H_{\mathrm{p}}\otimes\mathbb{1} + \mathbb{1}\otimes H_f(m) + \phi^{\oplus}(G) - \mathcal{V}_m(\hat{x})\otimes\mathbb{1} + \mathcal{W}_m\mathbb{1},$$

where $\mathcal{V}_m(\hat{x})$ is the multiplication operator by the function $\mathcal{V}_m(x) := \mathrm{Re}\langle\omega_m^{-1}v(0), v(x)\rangle$ and $\mathcal{W}_m := \|\omega_m^{-1/2}v(0)\|^2$ is a constant. In Fig. 1, we show the relation to the original model.

The ground state energy $E^V(m)$ is monotone increasing in $m\geqslant 0$, and $\lim_{m\to 0} E^V(m)=E^V(0)$ (see Ref. 4, Sec. 5). Therefore, by Hypothesis II, for all sufficiently small $m\geqslant 0$ we have $E^V(m) < \limsup_{R\to\infty} E_\infty(R,0)$. Since $E_\infty(R,m)$ is monotone increasing in $m\geqslant 0$, there exists a constant m such that

$$E^V(m) < \limsup_{R\to\infty} E_\infty(R,m) \quad (0\leqslant m<\mathsf{m}).$$

In what follows, we consider only the case $0<m<\mathsf{m}$. Hence, by Theorem 2.3, H_m^V has a ground state Φ_m. We set $\tilde{\Phi}_m := T_m\Phi_m$ a ground state of $\tilde{H}_m^V$.

Lemma 3.1. (Exponential decay): Let $\beta>0$ be a constant such that

$$\beta^2 < \limsup_{R\to\infty} E_\infty(R,m) - E^V(m) \quad (0<m<\mathsf{m}).$$

Then, for all large $R>0$,

$$\|\exp(\beta|x|)\tilde{\Phi}_m\|^2 \leqslant C\left(1+\frac{1}{E_\infty(R,m)-E^V(m)-\beta^2+o(1/R^0)}\right)\|\tilde{\Phi}_m\|^2,$$

where the constant $C>0$ does not depend on m with $C\leqslant\frac{3}{2}e^{4\beta R}$.

Proof: See Ref. 4. ■

Let $f \in \mathrm{Dom}(\omega_m)$. Since $\mathrm{Dom}(\tilde{H}_m^V) = \mathrm{Dom}(H_\mathrm{p} \otimes \mathbb{1}) \cap \mathrm{Dom}(\mathbb{1} \otimes H_f(m))$, $a(f)\tilde{\Phi}_m \in Q(\tilde{H}_m^V)$. Hence, for all $\Psi \in \mathrm{Dom}(H_m^V)$, we have

$$\langle (\tilde{H}_m^V - E^V(m))\Psi, a(f)\tilde{\Phi}_m \rangle = -\langle \Psi, a(\omega_m f)\tilde{\Phi}_m \rangle - \frac{1}{\sqrt{2}} \langle \Psi, \langle f, G(\hat{x}) \rangle \tilde{\Phi}_m \rangle.$$

Here we use the canonical commutation relations of a, a^*, and $\langle f, G(\hat{x}) \rangle$ is the multiplication operator by the function $\langle f, G(x) \rangle$. Since $\Psi \in \mathrm{Dom}(\tilde{H}_m^V)$ is arbitrary, $a(f)\tilde{\Phi}_m \in \mathrm{Dom}(\tilde{H}_m^V)$, and hence,

$$\langle a(f)\tilde{\Phi}_m, a(\omega_m f)\tilde{\Phi}_m \rangle + \frac{1}{\sqrt{2}} \langle a(f)\tilde{\Phi}_m, \langle f, G(\hat{x}) \rangle \tilde{\Phi}_m \rangle \leqslant 0. \tag{4}$$

Lemma 3.2 (Photon number bound): For all $0 < m < \mathsf{m}$, *we have*

$$\| a(k)\tilde{\Phi}_m \|^2 \leqslant \frac{1}{2(2\pi)^3} \frac{|k|}{\omega_m(k)^2} |\hat{\rho}(k)|^2 \| |x| \tilde{\Phi}_m \|^2, \quad \text{a.e. } k \in \mathbb{R}^3. \tag{5}$$

Proof: Let $q(k)$ be a bounded real-valued measurable function. We choose some complete orthonormal system $\{f_i\}_{i=1}^\infty \subset \mathrm{Dom}(\omega_m)$. By (4), we have

$$\sum_{i=1}^\infty \langle a(\omega_m^{-1/2} q f_i)\tilde{\Phi}_m, a(\omega_m^{1/2} q f_i)\tilde{\Phi}_m \rangle + \frac{1}{\sqrt{2}} \sum_{i=1}^\infty \langle a(\langle \omega_m^{-1/2} q f_i, G(\hat{x}) \rangle \omega_m^{-1/2} q f_i)\tilde{\Phi}_m, \tilde{\Phi}_m \rangle \leqslant 0.$$

By Lemma A.1 in the Appendix, we have

$$\langle \tilde{\Phi}_m, \mathrm{d}\Gamma(q^2)\tilde{\Phi}_m \rangle \leqslant -\frac{1}{\sqrt{2}} \langle a(\omega_m^{-1} q^2 G(\hat{x}))\tilde{\Phi}_m, \tilde{\Phi}_m \rangle \leqslant \frac{1}{\sqrt{2}} \int_{\mathbb{R}^3} \mathrm{d}k \frac{q(k)^2}{\omega_m(k)} |\langle G(\hat{x}, k)^* a(k)\tilde{\Phi}_m, \tilde{\Phi}_m \rangle|.$$

Note that q is arbitrary. Hence, we obtain

$$\| a(k)\tilde{\Phi}_m \|^2 \leqslant \frac{1}{\sqrt{2}} \frac{1}{\omega_m(k)} \| a(k)\tilde{\Phi}_m \| \, \| G(\hat{x}; k)\tilde{\Phi}_m \|, \quad \text{a.e. } k.$$

By the definition of G, we have $|G(x, k)|^2 \leqslant |\hat{\rho}(k)|^2 |k| |x|^2 / (2\pi)^3$. Therefore, (5) holds. ■

We write $\tilde{\Phi}_m = (\tilde{\Phi}_m^{(n)})_{n=0}^\infty$ with $\tilde{\Phi}_m^{(n)} \in L^2(\mathbb{R}_x^3) \otimes (\otimes_s^n L^2(\mathbb{R}_k^3))$, $n \geqslant 0$, where $\otimes_s^n L^2(\mathbb{R}_k^3)$ is the n-fold symmetric tensor product of $L^2(\mathbb{R}_k^3)$.

Lemma 3.3 (Photon derivative bound): Let $0 < m < \mathsf{m}$. *Then, for all* $\tilde{\Phi}_m^{(n)}$ *is in the Sobolev space* $H^1(\mathbb{R}_x^3 \times S^{3n})$, *and* $\mathcal{F}$*-valued function* $a(k)\tilde{\Phi}_m$ *is strongly differentiable in* $k \in S \backslash \{0\}$ *for all directions with*

$$\partial_j a(k)\tilde{\Phi}_m = (\partial_j \tilde{\Phi}_m^{(1)}(k), \sqrt{2}\partial_j \tilde{\Phi}_m^{(2)}(k, \cdot), \ldots, \sqrt{n}\partial_j \tilde{\Phi}_m^{(n)}(k, \cdot), \ldots), \quad j = 1, 2, 3,$$

$$\| \nabla_k a(k)\tilde{\Phi}_m \|^2 \leqslant \frac{1}{(2\pi)^3} \frac{1}{\omega_m(k)^2} \left[3\frac{|\hat{\rho}(k)|^2}{|k|} + |k| |\nabla \hat{\rho}(k)|^2 \right] \| |\hat{x}| \tilde{\Phi}_m \|^2,$$

where ∂_j *and* ∇_k *means the differential operator for j-th component of k and the nabla operator for the coordinate k.*

Proof: For $h \in \mathbb{R}^3$ and a function $f(k)$, we define

$$(\Delta_h f)(k) := f(k+h) - f(k).$$

We consider (4) with f replaced by $\Delta_{-h}\omega_m^{-1/2} q f_i$. Here q and f_i are the same function as in the proof of the above Lemma. By Lemma A.1, we have

$$\sum_{i=1}^{\infty} \langle a(\Delta_{-h}\omega_m^{-1/2} q f_i)\tilde{\Phi}_m, a(\omega_m \Delta_{-h}\omega_m^{-1/2} q f_i)\tilde{\Phi}_m\rangle = \langle \tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta_{-h}\omega_m^{-1} q^2 \Delta_h \omega_m)\tilde{\Phi}_m\rangle. \tag{6}$$

We introduce an operator $(T_h f)(k) := f(k+h)$. It is easy to see that $\Delta_h \omega_m = (\Delta_h \omega_m) T_h + \omega_m \Delta_h$. Therefore, we have

$$(6) = \langle \tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta_{-h} q^2 \Delta_h)\tilde{\Phi}_m\rangle + \langle \tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta_{-h} q^2 \omega_m^{-1}(\Delta_h \omega_m) T_h)\tilde{\Phi}_m\rangle.$$

On the other hand,

$$\sum_{i=1}^{\infty} \langle a(\Delta_{-h}\omega_m^{-1/2} q f_i)\tilde{\Phi}_m, \langle \Delta_{-h}\omega_m^{-1/2} q f_i, G(\hat{x})\rangle \tilde{\Phi}_m\rangle = \langle a(\Delta_{-h}\omega_m^{-1} q^2 \Delta_h G(\hat{x}))\tilde{\Phi}_m, \tilde{\Phi}_m\rangle.$$

Therefore, we obtain

$$\langle \tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta_{-h} q^2 \Delta_h)\tilde{\Phi}_m\rangle \leqslant -\langle \tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta_{-h} q^2 \omega_m^{-1}(\Delta_h \omega_m) T_{-h})\tilde{\Phi}_m\rangle - \frac{1}{\sqrt{2}}\langle a(\Delta_{-h}\omega_m^{-1} q^2 \Delta_h G(\hat{x}))\tilde{\Phi}_m, \tilde{\Phi}_m\rangle. \tag{7}$$

By the Schwarz inequality, we have

$$|\langle a(\Delta_{-h}\omega_m^{-1} q^2 \Delta_h G(\hat{x}))\tilde{\Phi}_m, \tilde{\Phi}_m\rangle| = \langle \Phi, \mathrm{d}\Gamma(\Delta_{-h} q^2 \Delta_h)\Phi\rangle^{1/2} \left[\int_{\mathbb{R}^3} \mathrm{d}k \frac{q(k)^2}{\omega_m(k)^2} \|(\Delta_h G(\hat{x}))(k)\tilde{\Phi}_m\|^2\right]^{1/2}.$$

By using the general inequality $|\langle \Phi, \mathrm{d}\Gamma(S^* T)\Psi\rangle| \leqslant \langle \Phi, \mathrm{d}\Gamma(S^* S)\Phi\rangle^{1/2} \langle \Psi, \mathrm{d}\Gamma(T^* T)\Psi\rangle^{1/2}$, we have

$$\begin{aligned} |\langle \tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta_{-h} q^2 \omega_m^{-1}(\Delta_h \omega_m) T_h)\tilde{\Phi}_m\rangle| &\leqslant \langle \tilde{\Phi}_m, \mathrm{d}\Gamma((\Delta_{-h} q)(\Delta_{-h} q)^*)\tilde{\Phi}_m\rangle^{1/2} \\ &\quad \times \langle \tilde{\Phi}_m, \mathrm{d}\Gamma(T_{-h}(\Delta_h \omega_m) q^2 \omega_m^{-2}(\Delta_h \omega_m) T_h)\tilde{\Phi}_m\rangle^{1/2}. \end{aligned}$$

Hence, we obtain

$$\begin{aligned} \langle \tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta_{-h} q^2 \Delta_h)\tilde{\Phi}_m\rangle &\leqslant \int_{\mathbb{R}^3} \mathrm{d}k \frac{q(k)^2}{\omega_m(k)^2} \|(\Delta_h G(\hat{x}))(k)\tilde{\Phi}_m\|^2 \\ &\quad + 2\langle \tilde{\Phi}_m, \mathrm{d}\Gamma(T_{-h}(\Delta_h \omega_m) q^2 \omega_m^{-2}(\Delta_h \omega_m) T_h)\tilde{\Phi}_m\rangle \\ &= \int_{\mathbb{R}^3} \mathrm{d}k \frac{q(k)^2}{\omega_m(k)^2} \|(\Delta_h G(\hat{x}))(k)\tilde{\Phi}_m\|^2 + 2 \\ &\quad \times \int_{\mathbb{R}^3} \mathrm{d}k \frac{q(k-h)^2}{\omega_m(k-h)^2} |(\Delta_h \omega_m)(k-h)|^2 \|a(k)\tilde{\Phi}_m\|^2. \end{aligned}$$

By (5), this is dominated by

$$\int_{\mathbb{R}^3} \mathrm{d}k \frac{q(k)^2}{\omega_m(k)^2} \|(\Delta_h G(\hat{x}))(k)\tilde{\Phi}_m\|^2 + \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \mathrm{d}k \frac{q(k)^2}{\omega_m(k)^2} |(\Delta_h \omega_m)(k)|^2 \frac{|k+h|\hat{\rho}(k+h)^2}{\omega_m(k+h)^2} \||x|\tilde{\Phi}_m\|^2.$$

Since the function q is arbitrary, we have

$$\|\Delta_h a(k)\tilde{\Phi}_m\|^2 \leqslant \frac{\|(\Delta_h G(\hat{x}))(k)\tilde{\Phi}_m\|^2}{\omega_m(k)^2} + \frac{|k+h|\hat{\rho}(k+h)^2|(\Delta_h\omega_m)(k)|^2}{(2\pi)^3\omega_m(k+h)^2\omega_m(k)^2}\||x|\tilde{\Phi}_m\|^2,$$

for a.e. $k \in \mathbb{R}^3$. By using the definition of $G(x,k)$, we have

$$\sqrt{(2\pi)^3}|\Delta_h G(x,k)| \leqslant \frac{|h||k+h||x|}{|k+h|^{1/2}|k|}|\hat{\rho}(k+h)| + \frac{|h||x|}{|k|^{1/2}}|\hat{\rho}(k+h)| + |k|^{1/2}|x||\hat{\rho}(k+h)-\hat{\rho}(k)|,$$

and it is easy to see that $|(\Delta_h\omega_m)(k)| \leqslant |h|$. Therefore we obtain

$$\|\Delta_h a(k)\tilde{\Phi}_m\|^2 \leqslant \frac{1}{(2\pi)^3}\frac{1}{\omega_m(k)^2}\left[3\frac{|h|^2}{|k|^2}|k+h||\hat{\rho}(k+h)|^2 + 3\frac{|h|^2}{|k|}|\hat{\rho}(k+h)|^2 + 3|k||\hat{\rho}(k+h)-\hat{\rho}(k)|^2 + \frac{|k+h||\hat{\rho}(k+h)|^2|h|^2}{\omega_m(k+h)^2}\right]\||x|\tilde{\Phi}_m\|^2. \tag{8}$$

By this inequality with [N.5], we see that $\mathcal{F}$-valued function $a(k)\tilde{\Phi}_m$ is strongly continuous in $k \in S\backslash\{0\}$. Next, we show that $a(k)\tilde{\Phi}_m$ is strongly differentiable. For this purpose, we introduce the operator $\Delta_{h,\ell}$ by

$$(\Delta_{h,\ell}f)(k) = \frac{f(k+h)-f(k)}{|h|} - \frac{f(k+\ell)-f(k)}{|\ell|}, \quad k,\ell \in \mathbb{R}^3.$$

We define $\Delta^*_{h,\ell} := \Delta_{-h,-\ell}$. Returning to (4) with f replaced by $\Delta^*_{h,\ell}\omega_m^{-1/2}qf_i$ and summing over $i = 1,\ldots,\infty$ we have

$$\langle\tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta^*_{h,\ell}q^2\omega_m^{-1}\Delta_{h,\ell}\omega_m)\tilde{\Phi}_m\rangle + \frac{1}{\sqrt{2}}\langle a(\Delta^*_{h,\ell}\omega_m^{-1}q^2\Delta_{h,\ell}G(\hat{x}))\tilde{\Phi}_m, \tilde{\Phi}_m\rangle \leqslant 0.$$

It is easy to see that $\Delta_{h,\ell}\omega_m = \omega_m\Delta_{h,\ell} + F_h - F_\ell$, where $F_h := (\Delta_h\omega_m)|h|^{-1}T_h$. Hence, we have

$$\langle\tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta^*_{h,\ell}q^2\Delta_{h,\ell})\tilde{\Phi}_m\rangle \leqslant -\frac{1}{\sqrt{2}}\langle a(\Delta^*_{h,\ell}\omega_m^{-1}q^2\Delta_{h,\ell}G(\hat{x}))\tilde{\Phi}_m, \tilde{\Phi}_m\rangle \tag{9}$$

$$+ \langle\tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta^*_{h,\ell}q^2\omega_m^{-1}F_h)\tilde{\Phi}_m\rangle + \langle\tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta^*_{h,\ell}q^2\omega_m^{-1}F_\ell)\tilde{\Phi}_m\rangle. \tag{10}$$

By the Schwarz inequality, we have

$$|\text{r.h.s. of (9)}| \leqslant \langle\tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta^*_{h,\ell}q^2\Delta_{h,\ell})\tilde{\Phi}_m\rangle^{1/2}\left[\int_{\mathbb{R}^3}\mathrm{d}k\frac{q(k)^2}{\omega_m(k)^2}\|(\Delta_{h,\ell}G(\hat{x}))(k)\tilde{\Phi}_m\|^2\right]^{1/2},$$

$$|(10)| \leqslant |\langle\tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta^*_{h,\ell}q^2\omega_m^{-1}[\Delta^*_{h,\ell}\omega_m]T_h)\tilde{\Phi}_m\rangle| \tag{11}$$

$$+ \left|\left\langle\tilde{\Phi}_m, \mathrm{d}\Gamma\left(\Delta^*_{h,\ell}q^2\omega_m^{-1}\left[\frac{\Delta_\ell}{|\ell|}\omega_m\right](T_h - T_\ell)\right)\tilde{\Phi}_m\right\rangle\right|. \tag{12}$$

Moreover,

$$\begin{aligned}\text{r.h.s. of (11)} &\leqslant \langle\tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta^*_{h,\ell}q^2\Delta_{h,\ell})\tilde{\Phi}_m\rangle^{1/2}\langle\tilde{\Phi}_m, \mathrm{d}\Gamma(T_{-h}q^2\omega_m^{-2}[\Delta^*_{h,\ell}\omega_m]^2T_h)\tilde{\Phi}_m\rangle^{1/2} \\ &= \langle\tilde{\Phi}_m, \mathrm{d}\Gamma(\Delta^*_{h,\ell}q^2\Delta_{h,\ell})\tilde{\Phi}_m\rangle^{1/2}\left[\int_{\mathbb{R}^3}\mathrm{d}kq(k)^2\omega_m^{-2}(k)[\Delta^*_{h,\ell}\omega_m]^2(k)\|a(k+h)\tilde{\Phi}_m\|^2\right]^{1/2},\end{aligned}$$

and

$$\text{r.h.s. of (12)} \leqslant \langle\widetilde{\Phi}_m, \mathrm{d}\Gamma(\Delta_{h,\ell}^* q^2 \Delta_{h,\ell})\widetilde{\Phi}_m\rangle^{1/2} \left\langle \widetilde{\Phi}_m, \mathrm{d}\Gamma\left((T_{-h} - T_{-\ell}) \left[\frac{\Delta_\ell}{|\ell|}\omega_m \right]^2 q^2 \omega_m^{-2} (T_h - T_\ell) \right) \right\rangle^{1/2}$$
$$\leqslant \langle\widetilde{\Phi}_m, \mathrm{d}\Gamma(\Delta_{h,\ell}^* q^2 \Delta_{h,\ell})\widetilde{\Phi}_m\rangle^{1/2} \left[\int_{\mathbb{R}^3} \mathrm{d}k q(k)^2 \omega_m(k)^{-2} \| a(k+h)\widetilde{\Phi}_m - a(k+\ell)\widetilde{\Phi}_m \|^2 \right]^{1/2}.$$

This inequality yields

$$\begin{aligned}\langle\widetilde{\Phi}_m, \mathrm{d}\Gamma(\Delta_{h,\ell}^* q^2 \Delta_{h,\ell})\widetilde{\Phi}_m\rangle \leqslant{}& \frac{3}{2}\int_{\mathbb{R}^3} \mathrm{d}k \frac{q(k)^2}{\omega_m(k)^2} \| (\Delta_{h,\ell} G(\hat{x}))(k)\widetilde{\Phi}_m \|^2 \\ &+ 3\int_{\mathbb{R}^3} \mathrm{d}k \frac{q(k)^2}{\omega_m(k)^2} |\Delta_{h,\ell}^* \omega_m|^2(k) \| a(k+h)\widetilde{\Phi}_m \|^2 \\ &+ 3\int_{\mathbb{R}^3} \mathrm{d}k \frac{q(k)^2}{\omega_m(k)^2} \| a(k+h)\widetilde{\Phi}_m - a(k+\ell)\widetilde{\Phi}_m \|^2.\end{aligned}$$

Since the function q is arbitrary, we have

$$\begin{aligned}\| \Delta_{h,\ell} a(k)\widetilde{\Phi}_m \|^2 \leqslant \frac{3}{\omega_m(k)^2} \Bigg[& \frac{1}{2} \| (\Delta_{h,\ell} G(\hat{x}))(k)\widetilde{\Phi}_m \|^2 + |\Delta_{h,\ell}^* \omega_m|^2(k) \| a(k+h)\widetilde{\Phi}_m \|^2 \\ & + \| a(k+h)\widetilde{\Phi}_m - a(k+\ell) \|^2 \Bigg], \quad \text{a.e. } k \in \mathbb{R}^3. \end{aligned} \tag{13}$$

Remembering the condition [N.5] and that $a(k)\widetilde{\Phi}_m$ is continuous, we get,

$$\lim_{h,\ell\to\infty} \| \Delta_{|h|e,|\ell|e} a(k)\widetilde{\Phi}_m \|^2 = 0, \quad \text{a.e. } k \in S\setminus\{0\},$$

for all $e \in \mathbb{R}^3$. Therefore the $\mathcal{F}$-valued function $\Delta_{|h|e} a(k)\widetilde{\Phi}_m/|h|$ is a Cauchy sequence in $|h|$ as $|h| \to 0$. Namely, for all directions, $a(k)\widetilde{\Phi}_m$ is strongly differentiable in $k \in S\setminus\{0\}$. Let $e_j (j = 1,2,3)$ be the unit vectors of the jth direction, and let

$$v_j(k) := \text{s-lim}_{|h|\to 0} \frac{1}{|h|} \Delta_{|h|e_j} a(k)\widetilde{\Phi}_m, \quad \text{a.e. } k \in S.$$

Next, we show that $\widetilde{\Phi}_m^{(n)} \in H^1(\mathbb{R}_x^3 \times S^{3n})$ for all $n \in \mathbb{N}$. Let $\psi \in C_0^\infty(\mathbb{R}_x^3) \times S^{3n}$. Then, we have

$$\begin{aligned}&\int_{\mathbb{R}^{3(n+1)}} (\partial_j \psi)(x,k,K)\widetilde{\Phi}_m^{(n)}(x,k,K)\mathrm{d}x\mathrm{d}k\mathrm{d}K \\ &= \lim_{h\to 0} \frac{1}{|h|} \int_{\mathbb{R}^{3(n+1)}} [\psi(x,k,K) - \psi(x,k,-|h|e_j,K)]\widetilde{\Phi}_m^{(n)}(x,k,K)\mathrm{d}x\mathrm{d}k\mathrm{d}K \\ &= -\lim_{h\to 0} \frac{1}{|h|} \int_{\mathbb{R}^3} \mathrm{d}k \left[\int_{\mathbb{R}^{3(n+1)}} \psi(x,k,K)[\widetilde{\Phi}_m^{(n)}(x,k+|h|e_j,K) - \widetilde{\Phi}_m^{(n)}(x,k,K)]\mathrm{d}x\mathrm{d}K \right],\end{aligned}$$

where $K = (k_1, k_2, \ldots, k_{n-1}) \in \mathbb{R}^{3(n-1)}$. On the other hand,

$$\left| \int_{\mathbb{R}^3} \mathrm{d}k \left[\int_{\mathbb{R}^{3n}} \mathrm{d}x\mathrm{d}K \psi(x,k,K) \left\{ \frac{1}{|h|} [\tilde{\Phi}_m^{(n)}(x,k+|h|e_j,K) + \tilde{\Phi}_m^{(n)}(x,k,K)] - v_j^{(n)}(x,k,K) \right\} \right] \right|$$
$$\leqslant \int_{\mathbb{R}^3} \mathrm{d}k \|\psi(k,\cdot)\|_{L^2(\mathbb{R}^{3n})} \left\| \frac{1}{|h|} (\Delta_{|h|e_j} a(k) \tilde{\Phi}_m)^{(n)} - v_j^{(n)}(k) \right\|$$
$$\leqslant \int_{\mathbb{R}^3} \mathrm{d}k \|\psi(k,\cdot)\|_{L^2(\mathbb{R}^{3n})} \left\| \frac{1}{|h|} \Delta_{|h|e_j} a(k) \tilde{\Phi}_m - v_j(k) \right\|. \tag{14}$$

Returning to (13) with $h \to |h|e_j$, $\ell \to |\ell|e_j$ and $\lim_{|\ell|\to 0}$, we have

$$\left\| \frac{1}{|h|} \Delta_h a(k) \tilde{\Phi}_m - v_j(k) \right\|^2 \leqslant \frac{3}{\omega_m(k)^2} \left[\frac{1}{2} \left\| \left(\frac{1}{h} (\Delta_{he_j} G)(\hat{x},k) - \partial_j G(\hat{x},k) \right) \tilde{\Phi}_m \right\|^2 + \frac{2|h|}{\omega_m(k)} \|a(k+h)\tilde{\Phi}_m\|^2 \right.$$
$$\left. + \|a(k+h)\tilde{\Phi}_m - a(k)\tilde{\Phi}_m\|^2 \right], \quad \text{a.e. } k \in \mathbb{R}^3,$$

where we use the elementary inequality $|(1/h)\Delta_{he_j}\omega_m(k) - \partial_j\omega_m(k)| \leqslant 2|h|/\omega_m(k)$. Since the set $S_\psi := \mathrm{supp}\|\psi(k,\cdot)\|$ is a subset of S, $k+h \in S$ for all h and $k \in S_\psi$ with $|h| < \mathrm{dist}\{S_\psi, S\}$. Using this fact and (8), we obtain

$$\lim_{|h|\to 0} \int_{\mathbb{R}^3} \mathrm{d}k \|\psi(k,\cdot)\|_{L^2(\mathbb{R}^{3n})} \left[|h| \frac{\|a(k+h)\tilde{\Phi}_m\|}{\omega_m(k)^2} + \frac{\|a(k+h)\tilde{\Phi}_m - a(k)\tilde{\Phi}_m\|}{\omega_m(k)} \right] = 0.$$

By condition [N.4] and the dominated convergence theorem, we have

$$\|\chi_{S_\psi}|h|^{-1}\Delta_h\hat{\rho} - \partial_j\hat{\rho}\|^2 \leqslant \||h|^{-1}\Delta_h\eta - \partial_j\eta\|^2_{L^2(\mathbb{R}^3)} \leqslant \int_{\mathbb{R}^3_y} \left| \frac{e^{-i|h|y_j} - 1}{|h|y_j} + i \right|^2 y_j^2 |(\mathsf{F}\eta)(y)|^2 \mathrm{d}y \to 0, (|h| \to 0),$$

where F means Fourier transformation. By this formula and simple but tedious estimates, we can show that

$$\lim_{|h|\to 0} \int_{\mathbb{R}^3} \mathrm{d}k \|\psi(k,\cdot)\|_{L^2(\mathbb{R}^{3n})} \cdot \frac{1}{\omega_m} \left\| \left(\frac{1}{h} (\Delta_{he_j} G)(\hat{x},k) - \partial_j G(\hat{x},k) \right) \tilde{\Phi}_m \right\| = 0.$$

These facts mean that

$$\lim_{h\to 0} (14) = 0.$$

Therefore, $\tilde{\Phi}_m^{(n)} \in H^1(\mathbb{R}^3_x \times S^{3n})$. ■

Pick a sequence $m_1 > m_2 > \cdots$ tending to zero and we set

$$\tilde{\Phi}_j := \tilde{\Phi}_{m_j}, \quad j = 1,2, \ldots .$$

Since $\tilde{\Phi}_j$'s are normalized, a subsequence of $\{\tilde{\Phi}_j\}_j$ has a weak limit $\tilde{\Phi}$ (the subsequence denoted by the same symbol).

Lemma 3.4: $\tilde{\Phi} \in \mathrm{Dom}(\tilde{H}^V)$ *and*,

$$\tilde{H}^V\tilde{\Phi} = E^V(0)\tilde{\Phi}. \tag{15}$$

Proof: First, we show that $\tilde{\Phi} \in Q(\tilde{H}^V) = \mathrm{Dom}(H_f(0)^{1/2}) \cap Q(H_\mathrm{p})$. For all $\Psi \in \mathrm{Dom}(H_f(0)^{1/2})$, we have

$$|\langle\tilde{\Phi},H_f(0)^{1/2}\Psi\rangle| = \lim_{j\to\infty}|\langle H_f(0)^{1/2}\tilde{\Phi}_j,\Psi\rangle| = \limsup_{j\to\infty}\|H_f(0)^{1/2}\tilde{\Phi}_j\|\,\|\Psi\|.$$

Since H_{p} is bounded below, we have

$$\|H_f(0)^{1/2}\tilde{\Phi}_j\|^2 \leqslant \text{const.}\langle\tilde{\Phi}_j,(\tilde{H}^V(m_j)-E^V(m_j)+1)\tilde{\Phi}_j\rangle \leqslant \text{const.},$$

where const. is a constant independent of j. Hence $\tilde{\Phi}\in\mathrm{Dom}(H_f(0)^{1/2})$. Similarly we have $\tilde{\Phi}\in Q(H_{\mathrm{p}})$. Since $E^V(m_j)\to E^V(0)(j\to\infty)$, we have

$$\|(\tilde{H}^V-E^V(0))^{1/2}\tilde{\Phi}_j\|^2 \leqslant \|(\tilde{H}^V(m_j)-E^V(0))^{1/2}\tilde{\Phi}_j\|^2 \leqslant (E^V(m_j)-E^V(0))\|\tilde{\Phi}_j\|^2 \to 0,$$

as $j\to\infty$. Therefore $(\tilde{H}^V-E^V(0))^{1/2}\tilde{\Phi}=0$. This means $\tilde{\Phi}\in\mathrm{Dom}(\tilde{H}^V)$ and $\tilde{H}^V\tilde{\Phi}=E^V(0)\tilde{\Phi}$. ■

By this lemma, if $\tilde{\Phi}\neq 0$ then $\tilde{\Phi}$ is a ground state of $\tilde{H}^V$. This proof is essentially same as (Ref. 4 and 7 Proof of Theorem 2.1), so we omit it (notice that the condition [N.3] and [N.6] were used there).

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APPENDIX: PARSEVAL's EQUALITY FOR THE ANNIHILATION OPERATORS

Let $\mathcal{K}$ be a complex separable Hilbert space, and let $\mathcal{F}_{\mathrm{b}}(\mathcal{K})$ be the Boson Fock space over $\mathcal{K}$. We denote by N_{b} the number operator on $\mathcal{F}_{\mathrm{b}}(\mathcal{K})$. Let S and T be densely defined closed linear operators on $\mathcal{K}$, such that $\mathrm{Dom}(S)\cap\mathrm{Dom}(T)$ is dense.

Lemma A.1 (Parseval's equality for the annihilation operators): Assume that, for vectors $\Psi,\Phi\in\mathrm{Dom}(N_{\mathrm{b}}^{1/2})$, *there exist constants* $\alpha,\beta(\alpha+\beta=1,\alpha,\beta\geqslant 0)$ *such that*,

$$N_{\mathrm{b}}^{\alpha-1}\Phi\in\mathrm{Dom}(\mathrm{d}\Gamma(T^*)),\quad N_{\mathrm{b}}^{\beta-1}\Psi\in\mathrm{Dom}(\mathrm{d}\Gamma(S^*)).$$

Then, for all complete orthonormal basis $\{f_j\}_{j=1}^{\infty}\subset\mathrm{Dom}(S)\cap\mathrm{Dom}(T)$, *the following equality holds:*

$$\sum_{j=1}^{\infty}\langle a(Sf_j)\Psi,a(Tf_j)\Phi\rangle = \sum_{n=1}^{\infty} n\langle S^*\otimes\mathbb{1}_{n-1}\Psi^{(n)},T^*\otimes\mathbb{1}_{n-1}\Phi^{(n)}\rangle_{\otimes^n\mathcal{K}}. \tag{A1}$$

In particular, if $\Phi\in\mathrm{Dom}(\mathrm{d}\Gamma(ST^*))$, *then*

$$\sum_{j=1}^{\infty}\langle a(Sf_j)\Psi,a(Tf_j)\Phi\rangle = \langle\Psi,\mathrm{d}\Gamma(ST^*)\Phi\rangle. \tag{A2}$$

Proof: It is enough to show in the case that $\mathcal{K}$ is L^2-space on a measurable space. For simplicity, we prove (A1) only in the case $\mathcal{K}=L^2(\mathbb{R}^3)$. Using the definition of $a(f)$, we have

$$\begin{aligned}\langle a(Sf_j)\Psi,a(Tf_j)\Phi\rangle &= \int \mathrm{d}k\int \mathrm{d}k'(Sf_j)(k)(Tf_j)^*(k')\langle a(k)\Psi,a(k')\Phi\rangle\\ &= \int \mathrm{d}k\int \mathrm{d}k'\sum_{n=1}^{\infty} n\int \mathrm{d}K(Sf_j)(k)(Tf_j)^*(k')\Psi^{(n)}(k,K)^*\Phi^{(n)}(k',K),\end{aligned}$$

where $K=(k_2,\ldots,k_n)$, $\mathrm{d}K=\mathrm{d}k_2\cdots\mathrm{d}k_n$. In the above equation, the integral and the summation commute, because

$$\int \mathrm{d}k \int \mathrm{d}k' \sum_{n=1}^{\infty} n \int \mathrm{d}K |(Sf_j)(k)(Tf_j)^*(k')\Psi^{(n)}(k,K)^*\Phi^{(n)}(k',K)|$$

$$\leqslant \int \mathrm{d}k\mathrm{d}k' |(Sf_j)(k)(Tf_j)(k')| \left[\sum_{n=1}^{\infty} n \int \mathrm{d}K |\Psi^{(n)}(k,K)|^2\right]^{1/2} \left[\sum_{n=1}^{\infty} n \int \mathrm{d}K |\Phi^{(n)}(k',K)|^2\right]^{1/2}$$

$$= \int \mathrm{d}k\mathrm{d}k' |(Sf_j)(k)| \cdot |(Tf_j)(k')| \cdot \|a(k)\Psi\| \, \|a(k')\Phi\|$$

$$\leqslant \|Sf_j\| \, \|Tf_j\| \left[\int \mathrm{d}k \|a(k)\Psi\|^2\right]^{1/2} \left[\int \mathrm{d}k \|a(k')\Phi\|^2\right]^{1/2}$$

$$= \|Sf_j\| \, \|Tf_j\| \, \|N_{\mathrm{b}}^{1/2}\psi\| \, \|N_{\mathrm{b}}^{1/2}\Phi\| < \infty,$$

and hence one can apply Fubini's theorem. Hence,

$$\sum_{j=1}^{\infty} \langle a(Sf_j)\Psi, a(Tf_j)\Phi\rangle = \sum_{j=1}^{\infty} \sum_{n=0}^{\infty} n \int \mathrm{d}K \langle (T^* \otimes \mathbb{1}\Phi^{(n)})(\cdot,K), f_j(\cdot)\rangle \langle f_j(\cdot), (S^* \otimes \mathbb{1}\Psi^{(n)})(\cdot,K)\rangle.$$

Using Bessel's inequality, we have

$$\left| \sum_{j=1}^{N} \langle (T^* \otimes \mathbb{1}\Phi^{(n)})(\cdot,K), f_j(\cdot)\rangle \langle f_j(\cdot), (S^* \otimes \mathbb{1}\Psi^{(n)})(\cdot,K)\rangle \right| \leqslant \|(T^* \otimes \mathbb{1}\Phi^{(n)})(\cdot,K)\| \, \|(S^* \otimes \mathbb{1}\Psi^{(n)})(\cdot,K)\|$$

$$\leqslant \frac{1}{2n}\{n^{2\alpha}\|(T^* \otimes \mathbb{1}\Phi^{(n)})(\cdot,K)\|^2 + n^{2\beta}\|(S^* \otimes \mathbb{1}\Psi^{(n)})(\cdot,K)\|^2\}, \quad \text{a.e. } K \in \mathbb{R}^{3(n-1)}. \tag{A3}$$

By assumption for Ψ, Φ, we have

$$\sum_{n=1}^{\infty} n \int \mathrm{d}K (\text{r.h.s. of (A3)}) = \frac{1}{2}\sum_{n=1}^{\infty} \|n^{\alpha}T^* \otimes \mathbb{1}\Phi^{(n)}\|^2 + \frac{1}{2}\sum_{n=1}^{\infty} \|n^{\beta}S^* \otimes \mathbb{1}\Psi^{(n)}\|^2 < \infty.$$

Hence, by applying the dominated convergence theorem and the standard parseval equality, we obtain (A1). ■

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Application of pseudo-Hermitian quantum mechanics to a $\mathcal{PT}$-symmetric Hamiltonian with a continuum of scattering states

Ali Mostafazadeh[a)]
Department of Mathematics, Koç University, 34450 Sariyer, Istanbul, Turkey

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We extend the application of the techniques developed within the framework of the pseudo-Hermitian quantum mechanics to study a unitary quantum system described by an imaginary $\mathcal{PT}$-symmetric potential $v(x)$ having a continuous real spectrum. For this potential that has recently been used, in the context of optical potentials, for modeling the propagation of electromagnetic waves traveling in a waveguide half and half filled with gain and absorbing media, we give a perturbative construction of the physical Hilbert space, observables, localized states, and the equivalent Hermitian Hamiltonian. Ignoring terms of order three or higher in the non-Hermiticity parameter ζ, we show that the equivalent Hermitian Hamiltonian has the form $p^2/2m+(\zeta^2/2)\Sigma_{n=0}^{\infty}\{\alpha_n(x),p^{2n}\}$ with $\alpha_n(x)$ vanishing outside an interval that is three times larger than the support of $v(x)$, i.e., in 2/3 of the physical interaction region the potential $v(x)$ vanishes identically. We provide a physical interpretation for this unusual behavior and comment on the classical limit of the system. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2063168]

I. INTRODUCTION

During the past seven years there have appeared over 200 research papers on $\mathcal{PT}$-symmetric quantum systems. This was initially triggered by the surprising observation of Bessis and Zinn-Justin and its subsequent numerical verification by Bender and his co-workers[1] that certain non-Hermitian but $\mathcal{PT}$-symmetric Hamiltonians, such as

$$H=p^2+x^2+i\epsilon x^3 \text{ with } \epsilon\in\mathbb{R}^+, \tag{1}$$

have a purely real spectrum. This observation suggested the possibility to use these Hamiltonians in the description of certain quantum systems. Since the $\mathcal{PT}$-symmetry of a non-Hermitian Hamiltonian H, i.e., the condition $[H,\mathcal{PT}]=0$, did not ensure the reality of its spectrum, a crucial task was to seek the necessary and sufficient conditions for the reality of the spectrum of a given non-Hermitian Hamiltonian H. This was achieved in Ref. 2 where it was shown, under the assumptions of the diagonalizability of H and discreteness of its spectrum, that the reality of the spectrum was equivalent to the existence of a positive-definite inner product $\langle\cdot,\cdot\rangle_+$ that rendered the Hamiltonian self-adjoint, i.e., for any pair (ψ,ϕ) of state vectors $\langle\psi,H\phi\rangle_+=\langle H\psi,\phi\rangle_+$.

Another condition that is equivalent to the reality of the spectrum of H is that it can be mapped to a Hermitian Hamiltonian h via a similarity transformation;[2,3] there is an invertible Hermitian operator ρ such that

$$H=\rho^{-1}h\rho. \tag{2}$$

The positive-definite inner product $\langle\cdot,\cdot\rangle_+$ and the operator ρ entering (2) are determined by a positive-definite operator η_+ according to[2,3]

[a)]Electronic mail: amostafazadeh@ku.edu.tr

$$\langle \cdot, \cdot \rangle_+ := \langle \cdot | \eta_+ \cdot \rangle, \tag{3}$$

$$\rho = \sqrt{\eta_+}, \tag{4}$$

and the Hamiltonian satisfies the η_+-pseudo-Hermiticity condition:[4]

$$H^\dagger = \eta_+ H \eta_+^{-1}. \tag{5}$$

Here $\langle \cdot | \cdot \rangle$ stands for the standard (L^2) inner product that determines the (reference) Hilbert space $\mathcal{H}$ as well as the adjoint $H^\dagger$ of H.[5] (The adjoint $A^\dagger$ of an operator A is the unique operator satisfying, for all $\psi, \phi \in \mathcal{H}$, $\langle \psi | A^\dagger \phi \rangle = \langle A\psi | \phi \rangle$. A is called Hermitian if $A^\dagger = A$.)

It is this, so-called metric operator, η_+ that determines the kinematic structure (the physical Hilbert space and the observables) of the desired quantum system. Note however that η_+ is not unique[6–8] (it is only unique up to symmetries of the Hamiltonian[7]). In Ref. 2 we have not only established the existence of a positive definite metric operator η_+ and the corresponding positive-definite inner product $\langle \cdot, \cdot \rangle_+$ for a diagonalizable Hamiltonian with a discrete real spectrum, but we have also explained the role of antilinear symmetries such as $\mathcal{PT}$ and offered a method for computing the most general η_+. [For a treatment of nondiagonalizable pseudo-Hermitian Hamiltonians see Refs. 9–11. Note that diagonalizability of the Hamiltonian is a necessary condition for applicability of the standard quantum measurement theory.[5] It is also necessary for the unitarity of the time-evolution, for a nondiagonalizable Hamiltonian is never Hermitian (its evolution operator is never unitary[11]) with respect to a positive-definite inner product.[9,10]] An alternative approach that yields a positive-definite inner product for a class of $\mathcal{PT}$-symmetric models is that of Ref. 12. As shown in Refs. 7 and 13, the $\mathcal{CPT}$-inner product proposed in Ref. 12 is identical to the inner product $\langle \cdot, \cdot \rangle_+ = \langle \cdot | \eta_+ \cdot \rangle$ for a particular choice of η_+.

Under the above-mentioned conditions every Hamiltonian having a real spectrum determines a set $\mathcal{U}_{H+}$ of positive-definite metric operators. To formulate a consistent unitary quantum theory having H as its Hamiltonian, one needs to choose an element η_+ of $\mathcal{U}_{H+}$. (Alternatively one may choose sufficiently many operators with real spectrum to construct a so-called irreducible set of observables which subsequently fixes a metric operator η_+.[14]) Each choice fixes a positive-definite inner product $\langle \cdot, \cdot \rangle_+$ and defines the physical Hilbert space $\mathcal{H}_{\text{phys}}$ and the observables. The latter are by definition[15] the operators O that are self-adjoint with respect to $\langle \cdot, \cdot \rangle_+$, alternatively they are η_+-pseudo-Hermitian. These can be constructed from Hermitian operators o acting in $\mathcal{H}$ according to[5]

$$O = \rho^{-1} o \rho. \tag{6}$$

In particular, one can define η_+-pseudo-Hermitian position X and momentum P operators,[5,15] express H as a function of X and P, and determine the underlying classical Hamiltonian for the system by letting $\hbar \to 0$ in the latter expression.[5,16] Alternatively, one may calculate the equivalent Hermitian Hamiltonian h and obtain its classical limit (again by letting $\hbar \to 0$).

Another application of the η_+-pseudo-Hermitian position operator X is in the construction of the physical localized states:

$$|\xi^{(x)}\rangle := \rho^{-1} |x\rangle. \tag{7}$$

These in turn define the physical position wave function, $\Psi(x) := \langle \xi^{(x)}, \psi \rangle_+ = \langle x | \rho | \psi \rangle$, and the invariant probability density,

$$\varrho(x) := \frac{|\Psi(x)|^2}{\int_{-\infty}^{\infty} |\Psi(x)|^2 \mathrm{d}x} = \frac{|\langle x|\rho|\psi\rangle|^2}{\langle \psi, \psi \rangle_+}, \tag{8}$$

for a given state vector $|\psi\rangle$.[5,16]

The above-mentioned prescription for treating $\mathcal{PT}$-symmetric and more generally pseudo-Hermitian Hamiltonians with a real spectrum has been successfully applied in the study of the $\mathcal{PT}$-symmetric square well in Ref. 5 and the cubic anharmonic oscillator (1) in Ref. 16—See also Ref. 17. Both these systems have a discrete nondegenerate energy spectrum, and the results of Refs. 4 and 2 are known to apply to them. The aim of the present paper is to seek whether these results (in particular the construction method for η_+) may be used for treating a system with a continuous spectrum. (The question whether the theory of pseudo-Hermitian operators as outlined in Refs. 4 and 2 is capable of treating a system having scattering states was posed to the author by Zafar Ahmed during the second International Workshop on Pseudo-Hermitian Hamiltonians in Quantum Physics, held in Prague, 14–16 June, 2004.) This question is motivated by the desire to understand field-theoretical analogues of $\mathcal{PT}$-symmetric systems which should admit an S-matrix formulation. Furthermore, there are some basic questions related to the nonlocal nature of the Hermitian Hamiltonian h and the pseudo-Hermitian observables such as X and P especially for $\mathcal{PT}$-symmetric potentials with a compact support (i.e., potentials vanishing outside a compact region).

To achieve this aim we will focus our attention on a simple toy model recently considered as an effective model arising in the treatment of the electromagnetic waves traveling in a planar slab waveguide that is half and half filled with gain and absorbing media.[18] This model has a standard Hamiltonian,

$$H=\frac{p^2}{2m}+v(x), \tag{9}$$

and a $\mathcal{PT}$-symmetric imaginary potential,

$$v(x):=i\zeta\left[\theta\left(x+\frac{L}{2}\right)+\theta\left(x-\frac{L}{2}\right)-2\theta(x)\right]=\begin{cases}0 & \text{for } |x|\geqslant\frac{L}{2} \text{ or } x=0\\ i\zeta & \text{for } x\in\left(-\frac{L}{2},0\right)\\ -i\zeta & \text{for } x\in\left(0,\frac{L}{2}\right),\end{cases} \tag{10}$$

where $L\in(0,\infty)$ is a length scale, $\zeta\in[0,\infty)$ determines the degree of non-Hermiticity of the system, and θ is the step function:

$$\theta(x):=\begin{cases}0 & \text{for } x<0\\ \frac{1}{2} & \text{for } x=0\\ 1 & \text{for } x>0.\end{cases} \tag{11}$$

The Hamiltonian (9) differs from a free particle Hamiltonian only within $(-L/2,L/2)$ where it coincides with the Hamiltonian for the $\mathcal{PT}$-symmetric square well.[5,19]

It is important to note that unlike in Ref. 18 we will consider the potential (10) as defining a fundamental (noneffective) quantum system having a unitary time-evolution (and S-matrix). Therefore our approach will be completely different from that pursued in Ref. 18 and the earlier studies of effective (optical) non-Hermitian Hamiltonians.[20]

Among the main reasons for our consideration of the potential (10) is that its eigenvalue problem can be solved exactly and analytically. However, the computation of the metric operator and consequently that of physical observables, localized states, associated Hermitian Hamiltonian, etc., are extremely involved, and we could only carry them out using first-order perturbation theory.

To the best of the author's knowledge, the only other non-Hermitian Hamiltonian with a continuous (and doubly degenerate) spectrum that is shown to admit a similar treatment is the one

arising in the two-component formulation of the free Klein-Gordon equation.[21,22] Compared to (9), this Hamiltonian defines a technically much simpler system to handle, because it is essentially a tensor product of an ordinary Hermitian Hamiltonian and a 2×2 matrix pseudo-Hermitian Hamiltonian.

II. METRIC OPERATOR

The essential ingredient of our approach is the metric operator η_+. For a diagonalizable Hamiltonian with a discrete spectrum it can be expressed as

$$\eta_+ = \sum_n \sum_{a=1}^{d_a} |\phi_n,a\rangle\langle\phi_n,a|, \tag{12}$$

where n, a, and d_n are a spectral label, a degeneracy label, and the multiplicity (degree of degeneracy) for the eigenvalue E_n of H, respectively, and $\{|\phi_n,a\rangle\}$ is a complete set of eigenvectors of $H^\dagger$ that together with the eigenvectors $|\psi_n,a\rangle$ of H form a biorthonormal system.[4,2]

Now, consider a diagonalizable Hamiltonian with a purely continuous doubly degenerate real spectrum $\{E_k\}$, where $k\in(0,\infty)$. We will extend the application of (12) to this Hamiltonian by changing $\Sigma_n\cdots$ to $\int dk\cdots$. This yields

$$\eta_+ = \int_0^\infty dk(|\phi_k,+\rangle\langle\phi_k,+| + |\phi_k,-\rangle\langle\phi_k,-|), \tag{13}$$

where we have used $\pm$ as the values of the degeneracy label a.[22] The biorthonormal system $\{|\psi_k,a\rangle,|\phi_k,a\rangle\}$ satisfies

$$H|\psi_k,a\rangle = E_k|\psi_k,a\rangle, \quad H^\dagger|\phi_k,a\rangle = E_k|\phi_k,a\rangle, \tag{14}$$

$$\langle\phi_k,a|\psi_\ell,b\rangle = \delta_{ab}\delta(k-\ell), \quad \int_0^\infty (|\psi_k,+\rangle\langle\phi_k,+| + |\psi_k,-\rangle\langle\phi_k,-|)\mathrm{d}k = 1, \tag{15}$$

where δ_{ab} and $\delta(k)$ stand for the Kronecker and Dirac delta functions, respectively, $k\in(0,\infty)$, and $a,b\in\{-,+\}$,

We define the eigenvalue problem for the Hamiltonian (9) using the oscillating (plane wave) boundary conditions at $x=\pm\infty$ similar to the free particle case which corresponds to $\zeta=0$. To simplify the calculation of the eigenvectors we first introduce the following dimensionless quantities:

$$\mathrm{x} := \left(\frac{2}{L}\right)x, \quad \mathrm{p} := \left(\frac{L}{2\hbar}\right)p, \quad Z := \left(\frac{mL^2}{2\hbar^2}\right)\zeta, \quad \mathrm{H} := \left(\frac{mL^2}{2\hbar^2}\right)H = \mathrm{p}^2 + \mathrm{v}(\mathrm{x}), \tag{16}$$

$$\mathrm{v}(\mathrm{x}) := iZ[\theta(\mathrm{x}+1) + \theta(\mathrm{x}-1) - 2\theta(\mathrm{x})] = \begin{cases} 0 & \text{for } |\mathrm{x}|\geqslant 1 \text{ or } \mathrm{x}=0 \\ iZ & \text{for } \mathrm{x}\in(-1,0) \\ -iZ & \text{for } \mathrm{x}\in(0,1). \end{cases} \tag{17}$$

The eigenvalue problem for the scaled Hamiltonian H corresponds to the solution of the differential equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{dx}^2} + \mathrm{v}(\mathrm{x}) - \mathrm{E}_k\right]\psi(\mathrm{x}) = 0, \tag{18}$$

that is subject to the condition that ψ is a differentiable function at the discontinuities $\mathrm{x}=-1,0,1$ of v. Introducing $\psi_1:(-\infty,-1]\to\mathbb{C}$, $\psi_-:[-1,0]\to\mathbb{C}$, $\psi_+:[0,1]\to\mathbb{C}$, and $\psi_2:[1,\infty)\to\mathbb{C}$ according to

$$\psi(\mathrm{x}) =: \begin{cases} \psi_1(\mathrm{x}) & \text{for } \mathrm{x} \in (-\infty,-1] \\ \psi_-(\mathrm{x}) & \text{for } \mathrm{x} \in [-1,0] \\ \psi_+(\mathrm{x}) & \text{for } \mathrm{x} \in [0,1] \\ \psi_2(\mathrm{x}) & \text{for } \mathrm{x} \in [1,\infty), \end{cases} \tag{19}$$

we have

$$\psi_1(-1) = \psi_-(-1), \quad \psi_1'(-1) = \psi_-'(-1), \tag{20}$$

$$\psi_-(0) = \psi_+(0), \quad \psi_-'(0) = \psi_+'(0), \tag{21}$$

$$\psi_+(1) = \psi_2(1), \quad \psi_+'(1) = \psi_2'(1). \tag{22}$$

Now, imposing the plane-wave boundary condition at $\mathrm{x}=\pm\infty$ and demanding that the eigenfunctions ψ be $\mathcal{PT}$-invariant, which implies

$$\psi_-(0) = \psi_+(0)^*, \quad \psi_-'(0) = -\psi_+'(0)^*, \tag{23}$$

we find $E_k=k^2$, i.e., the spectrum is real positive and continuous, and

$$\psi_1(\mathrm{x}) = A_1 e^{ik\mathrm{x}} + B_1 e^{-ik\mathrm{x}}, \quad \psi_2(\mathrm{x}) = A_2 e^{ik\mathrm{x}} + B_2 e^{-ik\mathrm{x}}, \quad \psi_\pm(\mathrm{x}) = A_\pm e^{ik_\pm \mathrm{x}} + B_\pm e^{-ik_\pm \mathrm{x}}, \tag{24}$$

where

$$k_\pm := \sqrt{k^2 \pm iZ}, \tag{25}$$

$$A_1 = A_2^* = \frac{e^{ik}}{\sqrt{2\pi}}[L_-(k)u + K_-(k)v], \quad B_1 = B_2^* = \frac{e^{-ik}}{\sqrt{2\pi}}[L_-(-k)u + K_-(-k)v], \tag{26}$$

$$L_-(k) := \frac{1}{2}\left(\cos k_- - \frac{ik_- \sin k_-}{k}\right), \quad K_-(k) := \frac{1}{2}\sqrt{\frac{k_+}{k_-}}\left(\frac{k_- \cos k_-}{k} - i \sin k_-\right), \tag{27}$$

$$A_\pm = \frac{1}{\sqrt{8\pi}}\left[u + \left(\frac{k_+}{k_-}\right)^{\mp 1/2} v\right], \quad B_\pm = \frac{1}{\sqrt{8\pi}}\left[u - \left(\frac{k_+}{k_-}\right)^{\mp 1/2} v\right], \tag{28}$$

and $u,v \in \mathbb{R}$ are arbitrary constants (possibly depending on k and/or Z and not both vanishing).

The presence of the free parameters u and v is an indication of a double degeneracy of the eigenvalues $E_k=k^2$. We will select u and v in such a way as to ensure that in the limit $Z\to 0$ we recover the plane-wave solutions of the free particle Hamiltonian, i.e., we demand $\lim_{Z\to 0} \psi(x) = e^{\pm ikx}/\sqrt{2\pi}$. This condition is satisfied if we set

$$u = 1, \quad v = \pm 1. \tag{29}$$

In the following we use the superscript $\pm$ to identify the value of a quantity obtained by setting $u=1$ and $v=\pm 1$. In this way we introduce $A_1^\pm$, $B_1^\pm$, $A_2^\pm$, $B_2^\pm$, $A_\pm^\pm$, $B_\pm^\pm$, and $\psi^\pm$. The latter define the basis (generalized[23]) eigenvectors $|\psi_k,\pm\rangle$ by $\langle \mathrm{x}|\psi_k,\pm\rangle := \psi^\pm(\mathrm{x})$.

The next step is to obtain $|\phi_k,\pm\rangle$. In view of the identity $\mathrm{H}^\dagger = \mathrm{H}|_{Z\to -Z}$, we can easily obtain the expression for the eigenfunctions ϕ of $H^\dagger$. Introducing

$$\phi(\mathrm{x}) =: \begin{cases} \phi_1(\mathrm{x}) & \text{for } \mathrm{x} \in (-\infty,-1] \\ \phi_-(\mathrm{x}) & \text{for } \mathrm{x} \in [-1,0] \\ \phi_+(\mathrm{x}) & \text{for } \mathrm{x} \in [0,1] \\ \phi_2(\mathrm{x}) & \text{for } \mathrm{x} \in [1,\infty), \end{cases} \tag{30}$$

we have

$$\phi_1(\mathrm{x}) = C_1 e^{ik\mathrm{x}} + D_1 e^{-ik\mathrm{x}}, \quad \phi_2(\mathrm{x}) = C_2 e^{ik\mathrm{x}} + D_2 e^{-ik\mathrm{x}}, \quad \phi_\pm(\mathrm{x}) = C_\pm e^{ik_\mp \mathrm{x}} + D_\pm e^{-ik_\mp \mathrm{x}}, \tag{31}$$

where

$$C_1 = C_2^* = \frac{e^{ik}}{\sqrt{2\pi}}[L_+(k)r + K_+(k)s], \quad D_1 = D_2^* = \frac{e^{-ik}}{\sqrt{2\pi}}[L_+(-k)r + K_+(-k)s], \tag{32}$$

$$L_+(k) := L_-(-k)^*, \quad K_+(k) := -K_-(-k)^*, \tag{33}$$

$$C_\pm = \frac{1}{\sqrt{8\pi}}\left[r + \left(\frac{k_+}{k_-}\right)^{\pm 1/2} s\right], \quad D_\pm = \frac{1}{\sqrt{8\pi}}\left[r - \left(\frac{k_+}{k_-}\right)^{\pm 1/2} s\right], \tag{34}$$

and $r,s \in \mathbb{R}$ are (possibly k- and/or Z-dependent) parameters that are to be fixed by imposing the biorthonormality condition (15). The latter is equivalent to a set of four (complex) equations [corresponding to the four possible choices for the pair of indices (a,b) in the first equation in (15)] which are to be solved for the two real unknowns r and s. This together with the presence of the delta function in two of these equations make the existence of a solution quite nontrivial.

We checked these equations by expanding all the quantities in powers of the non-Hermiticity parameter Z up to (but not including) terms of order two and found after a long and tedious calculation (partly done using MATHEMATICA) that indeed all four of these equations are satisfied, if we set $r=u=1$ and $s=v=\pm 1$. Again we will refer to this choice using superscript $\pm$. In particular, we have $\phi^\pm = \psi^\pm|_{Z\to -Z}$ and $\langle \mathrm{x}\,|\,\phi_k,\pm\rangle := \phi^\pm(\mathrm{x})$.

Having obtained $|\phi_k,\pm\rangle$ we are in a position to calculate the metric operator (13). We carried out this calculation using first-order perturbation theory in Z. It involved expanding the $\phi_1^\pm(\mathrm{x})$, $\psi_2^\pm(\mathrm{x})$, and $\psi_\pm^\pm(\mathrm{x})$ in powers of Z, substituting the result in

$$\langle \mathrm{x}|\,\eta_+\,|\mathrm{y}\rangle = \int_0^\infty [\phi^+(\mathrm{y})^*\phi^+(\mathrm{x}) + \phi^-(\mathrm{y})^*\phi^-(\mathrm{x})]dk \tag{35}$$

which follows from (13), and using the identities:

$$\int_{-\infty}^{\infty} e^{iak}dk = 2\pi\delta(a), \quad \int_{-\infty}^{\infty} \frac{e^{iak}}{k}dk = i\pi\,\mathrm{sign}(a), \quad \int_{-\infty}^{\infty} \frac{e^{iak}-e^{ibk}}{k^2}dk = \pi(|b|-|a|) \tag{36}$$

[where $a,b \in \mathbb{R}$ and $\mathrm{sign}(a) := \theta(a) - \theta(-a)$] to perform the integral over k for all 16 possibilities for the range of values of the pair of independent variables (x,y) in (35). This is an extremely lengthy calculation whose detail we will not include here. It is absolutely remarkable that the expressions for $\langle \mathrm{x}|\,\eta_+\,|\mathrm{y}\rangle$ that we obtain for these 16 possibilities may be combined to yield a single formula that is valid for all $\mathrm{x},\mathrm{y} \in \mathbb{R}$, namely

$$\langle \mathrm{x}|\,\eta_+\,|\mathrm{y}\rangle = \delta(\mathrm{x}-\mathrm{y}) + \frac{i}{8}(4 + 2|\mathrm{x}+\mathrm{y}| - |\mathrm{x}+\mathrm{y}+2| - |\mathrm{x}+\mathrm{y}-2|)\mathrm{sign}(\mathrm{x}-\mathrm{y})Z + \mathcal{O}(Z^2), \tag{37}$$

where $\mathcal{O}(Z^2)$ stands for terms of order two and higher in powers of Z. Note that $\langle \mathrm{x}|\,\eta_+\,|\mathrm{y}\rangle^* = \langle \mathrm{y}|\,\eta_+\,|\mathrm{x}\rangle$, which is consistent with the Hermiticity of η_+.

III. PHYSICAL OBSERVABLES AND LOCALIZED STATES

The physical observables of the system described by the Hamiltonian (9) are obtained from the Hermitian operators acting in $\mathcal{H}=L^2(\mathbb{R})$ by the similarity transformation (6). This equation involves the positive square root ρ of η_+ which takes the form[16]

$$\rho^{\pm 1} = e^{\mp Q/2}, \tag{38}$$

if we express η in the exponential form

$$\eta_+ = e^{-Q}. \tag{39}$$

In view of (38) and the Backer-Campbell-Hausdorff identity,

$$e^{-A}Be^{A} = B + [B,A] + \frac{1}{2!}[[B,A],A] + \ldots \tag{40}$$

(where A and B are linear operators), physical observables (6) satisfy[16]

$$O = o - \tfrac{1}{2}[o,Q] + \tfrac{1}{8}[[o,Q],Q] + \ldots . \tag{41}$$

If we expand η_+ and Q in powers of Z,

$$\eta_+ = 1 + \sum_{\ell=1}^{\infty} \eta_{+_\ell} Z^\ell, \quad Q = \sum_{\ell=1}^{\infty} Q_\ell Z^\ell, \tag{42}$$

where η_{+_ℓ} and Q_ℓ are Z-independent Hermitian operators, we find using (39) that

$$Q_1 = -\eta_{+_1}, \quad Q_2 = -\eta_{+_2} + \tfrac{1}{2}\eta_{+_1}^2. \tag{43}$$

Combining this relation with (41), we have

$$O = o - \tfrac{1}{2}[o,Q_1]Z + \tfrac{1}{8}(-4[o,Q_2] + [[o,Q_1],Q_1])Z^2 + \mathcal{O}(Z^3). \tag{44}$$

In the following we calculate the η_+-pseudo-Hermitian position (X) and momentum (P) operators,[16] up to (but not including) terms of order Z^2. This is because so far we have only calculated η_{+_1} which in view of (37) satisfies

$$\langle \mathrm{x}|\eta_{+_1}|\mathrm{y}\rangle = \tfrac{i}{8}(4 + 2|\mathrm{x}+\mathrm{y}| - |\mathrm{x}+\mathrm{y}+2| - |\mathrm{x}+\mathrm{y}-2|)\mathrm{sign}(\mathrm{x}-\mathrm{y}), \quad \forall\, \mathrm{x},\mathrm{y} \in \mathbb{R}. \tag{45}$$

Substituting the scaled position (x) and momentum (p) operator for o in (44), using (45), and doing the necessary algebra, we find

$$\langle \mathrm{x}|\mathrm{X}|\mathrm{y}\rangle = \mathrm{x}\,\delta(\mathrm{x}-\mathrm{y}) + \frac{i}{16}(4 + 2|\mathrm{x}+\mathrm{y}| - |\mathrm{x}+\mathrm{y}+2| - |\mathrm{x}+\mathrm{y}-2|)|\mathrm{x}-\mathrm{y}|Z + \mathcal{O}(Z^2), \tag{46}$$

$$\langle \mathrm{x}|\mathrm{P}|\mathrm{y}\rangle = -i\partial_{\mathrm{x}}\delta(\mathrm{x}-\mathrm{y}) + \tfrac{1}{8}[2\,\mathrm{sign}(\mathrm{x}+\mathrm{y}) - \mathrm{sign}(\mathrm{x}+\mathrm{y}+2) - \mathrm{sign}(\mathrm{x}+\mathrm{y}-2)]\mathrm{sign}(\mathrm{x}-\mathrm{x})Z + \mathcal{O}(Z^2), \tag{47}$$

where $\mathrm{X} := 2X/L$ and $\mathrm{P} := LP/(2\hbar)$ are dimensionless η_+-pseudo-Hermitian position and momentum operators, respectively.

As seen from (46), both X and P are manifestly nonlocal and non-Hermitian (but pseudo-Hermitian) operators. If we scale back the relevant quantities in (46) and (47) according to (16), we find

$$\langle x|X|y\rangle = x\,\delta(x-y) + \frac{im}{4\hbar^2}(2L + 2|x+y| - |x+y+L| - |x+y-L|)|x-y|\zeta + \mathcal{O}(\zeta^2), \tag{48}$$

$$\langle x|P|y\rangle = -i\hbar\partial_x\delta(x-y) + \frac{m}{4\hbar}[2\,\mathrm{sign}(x+y) - \mathrm{sign}(x+y+L) - \mathrm{sign}(x+y-L)]\mathrm{sign}(x-y)\zeta + \mathcal{O}(\zeta^2). \tag{49}$$

Note that the contributions of order ζ to P vanish, if both x and y take values outside $[-L/2, L/2]$.

Next, we compute the localized states $\xi^{(x)}$ of the system. The corresponding state vectors are defined by (7). Using this equation as well as (38), (42), (43), (45), and (16) we have the following expression for the x-representation of a localized state $\xi^{(y)}$ centered at $y \in \mathbb{R}$:

$$\langle x|\xi^{(y)}\rangle = \delta(x-y) - \frac{im\zeta}{8\hbar^2}(2L + 2|x+y| - |x+y+L| - |x+y-1|)\mathrm{sign}(x-y) + \mathcal{O}(\zeta^2). \tag{50}$$

Because the linear term in ζ is imaginary, the presence of a weak non-Hermiticity only modifies the usual (Hermitian) localized states by making them complex (nonreal) while keeping their real part intact. Note however that for a fixed y the imaginary part of $\langle x|\xi^{(y)}\rangle$ does not tend to zero as $|x-y| \to \infty$. This observation which seems to be in conflict with the usual notion of localizability has a simple explanation. Because the usual x operator is no longer an observable, it does not describe the position of the particle. This is done by the pseudo-Hermitian position operator X; it is the physical position wave function $\Psi(x) := \langle \xi^{(x)}, \psi\rangle_+$ that defines the probability density of localization in space (8). The physical position wave function for the localized state $\xi^{(y)}$ is given by $\langle \xi^{(x)}, \xi^{(y)}\rangle_+ = \langle x|y\rangle = \delta(x-y)$ which is the expected result.

IV. EQUIVALENT HERMITIAN HAMILTONIAN AND CLASSICAL LIMIT

The calculation of the equivalent Hermitian Hamiltonian h for the Hamiltonian (9) is similar to that of the physical observables. In view of (2), (38), (40), and (42), and the last equation in (16) which we express as

$$\mathrm{H} = \mathrm{p}^2 + i\nu(\mathrm{x})Z \text{ with } \nu(\mathrm{x}) := \theta(\mathrm{x}+1) + \theta(\mathrm{x}-1) - 2\theta(\mathrm{x}), \tag{51}$$

we have

$$\mathrm{h} = \mathrm{p}^2 + h_1 Z + h_2 Z^2 + \mathcal{O}(Z^3), \tag{52}$$

$$\mathrm{h}_1 := i\nu(\mathrm{x}) + \tfrac{1}{2}[\mathrm{p}^2, Q_1], \tag{53}$$

$$\mathrm{h}_2 := \tfrac{1}{8}\{4[\mathrm{p}^2, Q_2] + 4i[\nu(\mathrm{x}), Q_1] + [[\mathrm{p}^2, Q_1], Q_1]\}. \tag{54}$$

where

$$\mathrm{h} := \rho\mathrm{H}\rho^{-1} = mL^2 h/(2\hbar^2) \tag{55}$$

is the dimensionless Hermitian Hamiltonian associated with H.

Next, we substitute (43) and (45) in the identity $\langle \mathrm{x}|[\mathrm{p}^2, Q_1]|\mathrm{v}\rangle = (\partial_\mathrm{y}^2 - \partial_\mathrm{x}^2)\langle \mathrm{x}|Q_1|\mathrm{y}\rangle$, and perform the necessary algebra. We then find $\langle \mathrm{x}|[\mathrm{p}^2, Q_1]|\mathrm{v}\rangle = -2i\nu(\mathrm{x})\delta(\mathrm{x}-\mathrm{y})$. Therefore,

$$[\mathrm{p}^2, Q_1] = -2i\nu(\mathrm{x}), \tag{56}$$

and in view of (53)

$$\mathrm{h}_1 = 0. \tag{57}$$

This was actually to be expected, for both the operators appearing on the right-hand side of (53) are anti-Hermitian, while its left-hand side is Hermitian. The fact that an explicit calculation of the right-hand side of (53) yields the desired result, namely (57), is an important check on the validity

of our calculation of η_{+_1}. It may also be viewed as an indication of the consistency and general applicability of our method, that was initially formulated for systems with a discrete spectrum.[5,16]

According to (57),

$$\mathrm{h} = \mathrm{p}^2 + \mathrm{h}_2 Z^2 + \mathcal{O}(Z^3). \tag{58}$$

Hence, in order to obtain a better understanding of the nature of the system described by the Hamiltonian H, we need to calculate h_2. As we will next show, the knowledge of $\langle \mathrm{x}|\eta_{+_1}|\mathrm{y}\rangle$ turns out to be sufficient for the calculation of h_2. To see this we first employ (56) to express h_2 in the form

$$\mathrm{h}_2 = \tfrac{1}{4}(2[\mathrm{p}^2, Q_2] + i[\nu(\mathrm{x}), Q_1]). \tag{59}$$

Now, we recall that p^2, Q_2, $\nu(\mathrm{x})$, and Q_1 are all Hermitian operators. Therefore $[\mathrm{p}^2, Q_2]$ and $i[\nu(\mathrm{x}), Q_1]$ are, respectively, anti-Hermitian and Hermitian. In view of (59) and the Hermiticity of h_2, this implies that

$$[\mathrm{p}^2, Q_2] = 0. \tag{60}$$

Hence,

$$\mathrm{h}_2 = \frac{i}{4}[\nu(\mathrm{x}), Q_1] = \frac{i}{4}[\eta_{+1}, \nu(\mathrm{x})], \tag{61}$$

where we have also made use of the first equation in (43). We should also mention that the identities (56) and (60) can be directly obtained from the pseudo-Hermiticity condition (5) by substituting (39) in (5) and using (40) and (42).

We can easily use (45) and (61) to yield the expression for the integral kernel of h_2, namely

$$\langle \mathrm{x}|\mathrm{h}_2|\mathrm{y}\rangle = \tfrac{1}{32}(4 + 2|\mathrm{x}+\mathrm{y}| - |\mathrm{x}+\mathrm{y}+2| - |\mathrm{x}+\mathrm{y}-2|)\mathrm{sign}(\mathrm{x}-\mathrm{y})[\nu(\mathrm{x}) - \nu(\mathrm{y})], \quad \forall\, \mathrm{x},\mathrm{y} \in \mathbb{R}. \tag{62}$$

As seen from this equation, $\langle \mathrm{x}|\mathrm{h}_2|\mathrm{y}\rangle = 0$, if $\mathrm{x} \notin [-1,1]$ and $\mathrm{y} \notin [-1,1]$.

We can express h_2 as a function of x and p by performing a Fourier transformation on the y variable appearing in (62), i.e., computing

$$\langle \mathrm{x}|\mathrm{h}_2|\mathrm{p}\rangle := (2\pi)^{-1/2} \int_{-\infty}^{\infty} \langle \mathrm{x}|\mathrm{h}_2|\mathrm{y}\rangle e^{i\mathrm{p}\mathrm{y}} d\mathrm{y}. \tag{63}$$

This yields h_2 as a function of x and p, if we order the factors by placing x's to the left of p's. We can easily do this by expanding $\langle \mathrm{x}|\mathrm{h}_2|\mathrm{p}\rangle$ in powers of p. Denoting the x-dependent coefficients by ω_n, we then have

$$\mathrm{h}_2 = \sum_{n=0}^{\infty} \omega_n(\mathrm{x})\mathrm{p}^n, \tag{64}$$

where we have made the implicit assumption that $\langle \mathrm{x}|\mathrm{h}_2|\mathrm{p}\rangle$ is a real-analytic function of p.

The Fourier transform of $\langle \mathrm{x}|\mathrm{h}_2|\mathrm{y}\rangle$ can be performed explicitly. [One way of doing this is to use the integral representations of the absolute value and sign function, as given in (36), to perform the y-integrations in (63) and use the identities

$$\int_{-\infty}^{\infty} \frac{e^{iau} du}{u(u-k)} = \frac{i\pi}{k}(e^{iak} - 1)\mathrm{sign}(a),$$

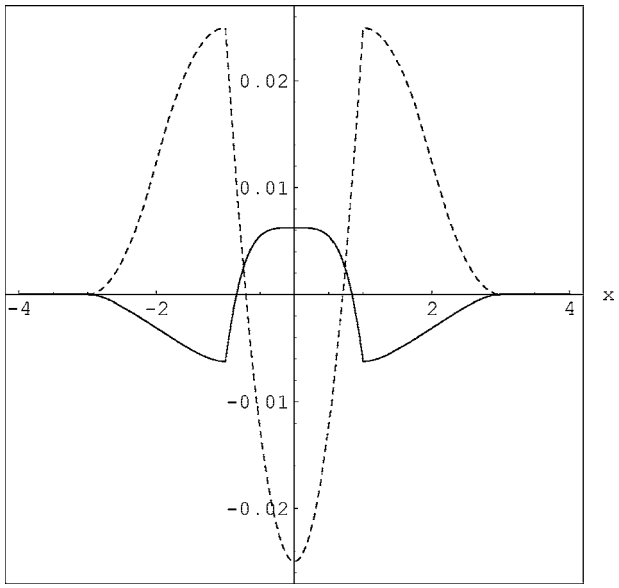

FIG. 1. Graph of the real part of ω_0 (dashed curve) and ω_2 (full curve).

$$\int_{-\infty}^{\infty} \frac{e^{iau}du}{u(u-k)^2} = \frac{i\pi}{k^2}[1+(iak-1)e^{iak}]\text{sign}(a), \quad \forall\, a,k \in \mathbb{R},$$

to evaluate the remaining two integrals. The resulting expression is too lengthy and complicated to be presented here.] We have instead used MATHEMATICA to calculate $\langle x|h_2|p\rangle$ and found the coefficients ω_n for $n \leqslant 5$. It turns out that indeed $\langle x|h_2|p\rangle$ does not have a singularity at $p=0$, and that $\omega_0, \omega_2, \omega_4$ are real and vanish outside $(-3,3)$ while $\omega_1, \omega_3, \omega_5$ are imaginary and proportional to $\theta(x)-1/2$ outside $(-3,3)$. As we will explain momentarily these properties are necessary to ensure the Hermiticity of h.

Figures 1, 2, and 3 show the plots of real part of ω_n for $n=0,2,4$ and the imaginary part of ω_n

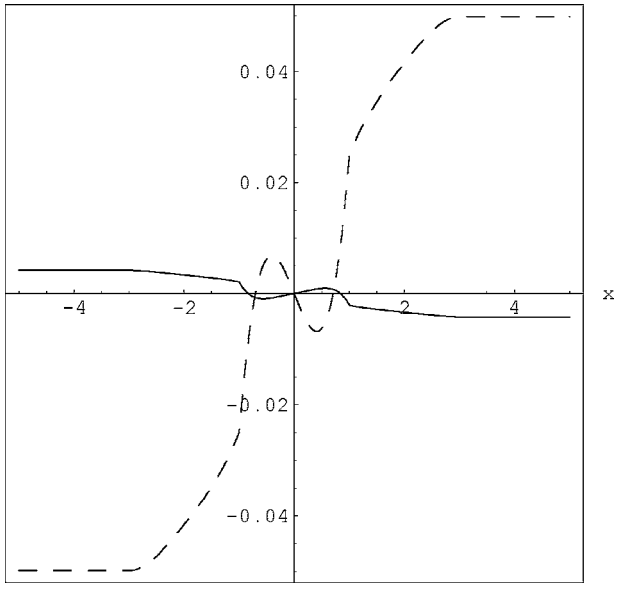

FIG. 2. Graph of the imaginary part of ω_1 (dashed curve) and ω_3 (full curve).

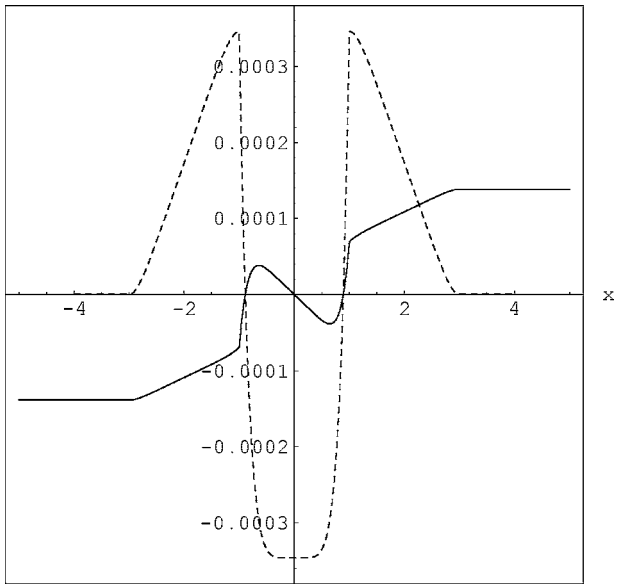

FIG. 3. Graph of the real part of ω_4 (dashed curve) and the imaginary part of ω_5 (full curve).

for $n=1,3,5$. As seen from these figures (the absolute value of) ω_n sharply decreases with n, which suggests that a truncation of (64) yields a good approximation for the action of h_2 on the wave functions with bounded and sufficiently small x-derivatives.

If we use $\langle \mathrm{p}|\mathrm{h}_2|\mathrm{x}\rangle=\langle \mathrm{x}|\mathrm{h}_2|\mathrm{p}\rangle^*$ to determine the form of h_2 and suppose that $\omega_{2n}(\mathrm{x})$ are real and $\omega_{2n+1}(\mathrm{x})$ are imaginary for all $n=0,1,2,3,\ldots$, we find

$$\mathrm{h}_2=\sum_{n=0}^{\infty}\mathrm{p}^n\omega_n(\mathrm{x})^*=\sum_{n=0}^{\infty}[\mathrm{p}^{2n}\omega_{2n}(\mathrm{x})-\mathrm{p}^{2n+1}\omega_{2n+1}(\mathrm{x})].$$

Adding both sides of this relation to those of (64) and diving by two, we obtain

$$\mathrm{h}_2=\frac{1}{2}\sum_{n=0}^{\infty}\{a_n(\mathrm{x}),\mathrm{p}^{2n}\},\quad a_n(\mathrm{x}):=\omega_{2n}(\mathrm{x})+i\omega'_{2n+1}(\mathrm{x}),\tag{65}$$

where $\{\cdot,\cdot\}$ stands for the anticommutator, a prime denotes a derivative, and we have made use of the identity: $[f(\mathrm{x}),\mathrm{p}^m]=\{if'(\mathrm{x}),\mathrm{p}^{m-1}\}$. It is important to note that because $\omega_{2n}(\mathrm{x})$ are real and $\omega_{2n+1}(\mathrm{x})$ are imaginary, $a_n(\mathrm{x})$ are real. Moreover, outside $(-3,3)$, $\omega_{2n}(\mathrm{x})$, $\omega'_{2n+1}(\mathrm{x})$, and consequently a_n vanish. Therefore, we can express h_2 in the manifestly Hermitian form (65) with all the x-dependent coefficient functions vanishing outside $(-3,3)$. Figure 4 shows the plots of a_n for $n=0,1,2$. They are all even functions of x with an amplitude of variations that decreases rapidly as n increases.

Next, we scale back the relevant quantities and use (16), (55), (58), and (65) to obtain

$$h=\frac{p^2}{2m}+\frac{\zeta^2}{2}\sum_{n=0}^{\infty}\{\alpha_n(x),p^{2n}\}+\mathcal{O}(\zeta^3),\quad \alpha_n(x):=2m\left(\frac{L}{2\hbar}\right)^{2(n+1)}a_n\left(\frac{2x}{L}\right).\tag{66}$$

In view of the fact that a_n and α_n are real-valued even functions, h is a manifestly Hermitian $\mathcal{P}$- and $\mathcal{T}$-symmetric Hamiltonian. We can also express it in the form

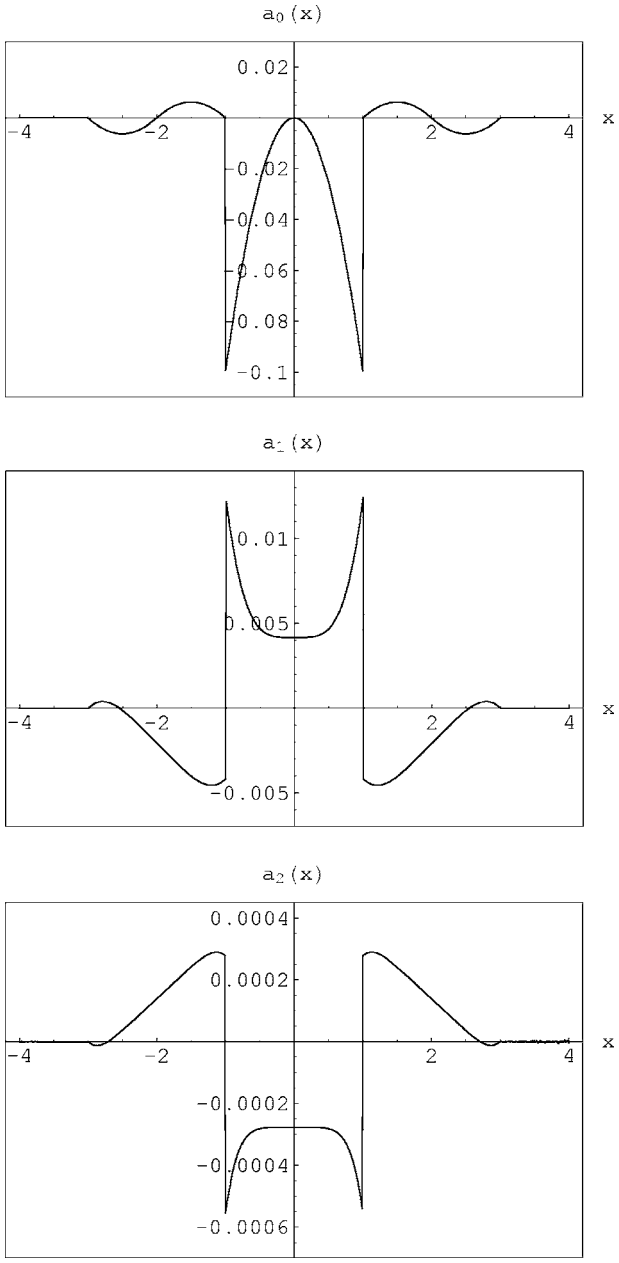

FIG. 4. Graph of a_0, a_1, and a_2.

$$h = \frac{1}{4}\{m_{\text{eff}}^{-1}(x), p^2\} + w(x) + \frac{\zeta^2}{2}\sum_{n=2}^{\infty}\{\alpha_n(x), p^{2n}\} + \mathcal{O}(\zeta^3), \tag{67}$$

where

$$m_{\text{eff}}(x) := \frac{m}{1 + 2m\zeta^2\alpha_1(x)}, \quad w(x) := \zeta^2\alpha_0(x).$$

Therefore, for low energy particles where one may neglect terms involving fourth and higher powers of p, the Hamiltonian h and consequently H describe motion of a particle with an effective position dependent mass $m_{\text{eff}}(x)$ that interacts with the potential $w(x)$. Figure 5 shows a graph of

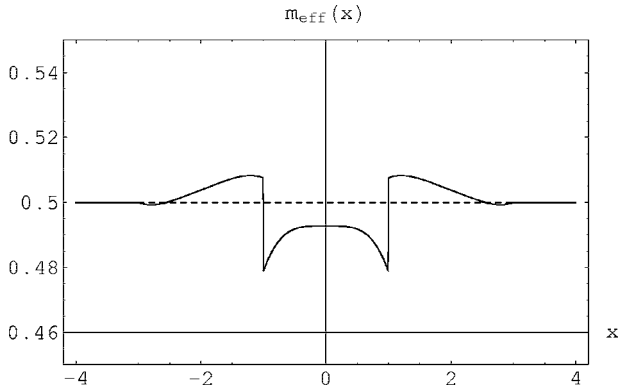

FIG. 5. Graph of the effective mass m_{eff} (full curve) for $m=\frac{1}{2}$, $\hbar=1$, $L=2$, and $\zeta=\frac{1}{3}$. The dashed curve represents $m=\frac{1}{2}$.

$m_{\text{eff}}(x)$ for $m=1/2$, $\hbar=1$, $L=2$, and $\zeta=1/3$. For the same values of these parameters, $w(x)=a_0(x)/9$. See Fig. 4 for a graph of a_0.

If we replace (x,p) of (66) and (67) with their classical counterparts (x_c,p_c), we obtain the "classical" Hamiltonian:

$$\widetilde{H}_c=\frac{p_c^2}{2m}+\frac{\zeta^2}{2}\sum_{n=0}^{\infty}\alpha_n(x_c)p_c^{2n}+\mathcal{O}(\zeta^3)=\frac{p_c^2}{2m_{\text{eff}}(x_c)}+w(x_c)+\frac{\zeta^2}{2}\sum_{n=2}^{\infty}\alpha_n(x_c)p_c^{2n}+\mathcal{O}(\zeta^3), \tag{68}$$

which coincides with the free particle Hamiltonian outside the *physical interaction region*, i.e., $(-3L/2,3L/2)$. The fact that this region is three times larger than the support $(-L/2,L/2)$ of the potential $v(x)$ is quite surprising. Note also that $\widetilde{H}_c$ is an even function of both the position x_c and momentum p_c variables.

Figure 6 shows the phase space trajectories associated with the Hamiltonian $\widetilde{H}_c$ for $L=2$, $\hbar=1$, $m=1/2$, $\zeta=Z=1/3$. For large values of the momentum the trajectories are open curves describing the scattering of a particle due to an interaction that takes place within the physical interaction region, $(-3,3)$. For sufficiently small values of the momentum closed trajectories are

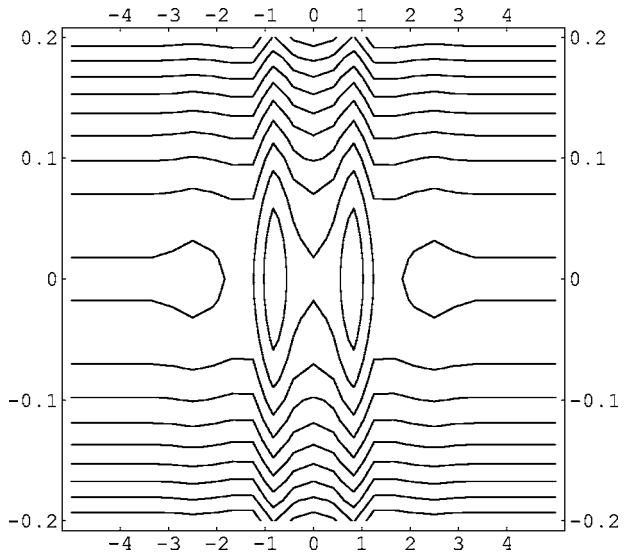

FIG. 6. Phase space trajectories of the Hamiltonian $\widetilde{H}_c(x_c,p_c)$ for $m=\frac{1}{2}$, $\hbar=1$, $L=2$, and $\zeta=\frac{1}{3}$. The horizontal and vertical axes are, respectively, those of x_c and p_c.

generated. These describe a particle that is trapped inside the physical interaction region. This is consistent with the fact that for small p_c, $\widetilde{H}_c$ is dominated by the potential term $w(x_c)$ which in view of its relation to $a_0(x)$ and Fig. 4 can trap the particle.

We wish to emphasize that because we have not yet taken the $\hbar \to 0$ limit of $\widetilde{H}_c$, we cannot identify it with the the true classical Hamiltonian H_c for the quantum Hamiltonian h and consequently H. Given the limitations of our perturbative calculation of $\widetilde{H}_c$, we are unable to determine this limit. (This is in contrast with both the $\mathcal{PT}$-symmetric square well and the $\mathcal{PT}$-symmetric cubic anharmonic oscillator studied in Refs. 5 and 16, respectively. In the former system the presence of an exceptional spectral point imposes the condition that ζ must be of order $\hbar^2$ or higher and consequently the classical system is the same as that of the Hermitian infinite square well.[5] In the latter system, the $\hbar \to 0$ limit of the associated Hermitian Hamiltonian can be easily evaluated and classical Hamiltonian obtained.[16]) Therefore, we cannot view the presence of closed phase space trajectories for $\widetilde{H}_c$ as evidence for the existence of bound states of h and H. This is especially because these trajectories are associated with very low momentum values where the quantum effects are expected to be dominant.

V. CONCLUSION

In this paper we explored for the first time the utility of the methods of pseudo-Hermitian quantum mechanics in dealing with a non-Hermitian $\mathcal{PT}$-symmetric potential $v(x)$ that has a continuous spectrum. We were able to solve the eigenvalue problem for this potential exactly and obtain the explicit form of the metric operator, the pseudo-Hermitian position and momentum operators, the localized states, and the equivalent Hermitian Hamiltonian perturbatively.

Our analysis revealed the surprising fact that the physical interaction region for this model is three times larger than the support of the potential, i.e., there is a region of the configuration space in which $v(x)$ vanishes but the interaction does not seize.

A simple interpretation for this peculiar property is that the argument x of the potential $v(x)$ is not a physical observable and the support $(-L/2, L/2)$ of $v(x)$ being a range of eigenvalues of x does not have a direct physical meaning. This observation underlines the importance of the Hermitian representation of non-Hermitian (inparticular $\mathcal{PT}$-symmetric) Hamiltonians having a real spectrum.

The Hermitian representation involves a nonlocal Hamiltonian that is not suitable for the computation of the energy spectrum or the S-matrix of the theory. Yet it provides invaluable insight in the physical meaning and potential applications of pseudo-Hermitian and $\mathcal{PT}$-symmetric Hamiltonians and is indispensable for the determination of the other observables of the corresponding quantum systems.

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On the semigroup decomposition of the time evolution of quantum mechanical resonances

Y. Strauss[a)]
Einstein Institute of Mathematics, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

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A way of utilizing Lax-Phillips type semigroups for the description of time evolution of resonances for scattering problems involving Hamiltonians with a semibounded spectrum was recently introduced by Strauss. In the proposed framework the evolution is decomposed into a background term and an exponentially decaying resonance term evolving according to a semigroup law given by a Lax-Phillips-type semigroup; this is called the semigroup decomposition. However, the proposed framework assumes that the *S*-matrix in the energy representation is the boundary value on the positive real axis of a bounded analytic function in the upper half-plane. This condition puts strong restrictions on possible applications of this formalism. In this paper it is shown that there is a simple way of weakening the assumptions on the *S*-matrix analyticity while still obtaining the semigroup decomposition of the evolution of a resonance. © *2005 American Institute of Physics.*
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I. INTRODUCTION

There has been a recent effort to adapt the formalism of the scattering theory developed by Lax and Phillips[1] into the framework of quantum mechanics. An initial effort in this direction[2–4] was followed by the introduction of a more general formalism by Strauss, Eisenberg, and Horwitz[5] which was subsequently applied to certain Lee-Friedrichs-type models in relativistic quantum field theory[6,7] and, more recently, to the analysis of the Stark effect.[8] In a parallel work Baumgartel[9] has used a modification of the Lax-Phillips scattering theory in order to deal with quantum mechanical resonances. In particular, he has shown the relevancy of this modified structure for the construction of appropriate Gamow vectors for resonances of certain scattering problems.

It is readily observed that the class of problems which can be analyzed within the framework introduced in Ref. 5 is limited by the very fact that it essentially maintains the original structure of the Lax-Phillips theory. In this formalism the generator of evolution is required to have an unbounded spectrum from below as well as from above, thus a large class of quantum mechanical scattering problems is excluded from its range of applicability. A way of overcoming this difficulty, when dealing with scattering problems for which the generator of evolution has a semibounded absolutely continuous spectrum, was recently proposed in Ref. 10.

The basic setting analyzed in Ref. 10 is a scattering problem involving a "free" unperturbed Hamiltonian $\mathbf{H}_0$ and a perturbed Hamiltonian $\mathbf{H}$ defined on a Hilbert space $\mathcal{H}$ where we assume that the absolutely continuous spectrum of both $\mathbf{H}_0$ and $\mathbf{H}$ satisfies $\text{ess Supp}\,\sigma_{\text{ac}}(\mathbf{H}_0) = \text{ess Supp}\,\sigma_{\text{ac}}(\mathbf{H}) = \mathbb{R}^+$ and that the Møller wave operators $\Omega^{\pm}(\mathbf{H}_0, \mathbf{H})$ exist and are complete. In order to obtain the desired result, described below, it is assumed further that the *S*-matrix in the energy representation, denoted by $\tilde{S}$, is a boundary value on $\mathbb{R}^+$ of an $\mathcal{H}^{\infty}(\Pi)$ function where, denoting by Π the upper half of the complex plane, $\mathcal{H}^{\infty}(\Pi)$ is the class of functions which are bounded analytic in Π.

[a)]Electronic mail: ystrauss@math.huji.ac.il

Suppose that under the assumptions mentioned above $\tilde{S}$, as an analytic function in Π, has a simple zero in the upper half-plane at a point $\bar{\mu}$ with $\mathrm{Im}\,\mu<0$ and $\mathrm{Re}\,\mu>0$. It is then easy to show that there exists an analytic continuation of $\tilde{S}$ across the positive real axis and that this analytic continuation has a simple pole below the real axis at the point $z=\mu$ which is considered to be associated with a scattering resonance (this is usually referred to as a second sheet pole of the S-matrix). Denote by $\mathbf{U}(t)$ the unitary evolution generated by the full scattering Hamiltonian $\mathbf{H}$ and by $\mathcal{H}_{\mathrm{ac}}$ the subspace of $\mathcal{H}$ corresponding to the ac spectrum of $\mathbf{H}$. It is shown in Ref. 10 that the pole of $\tilde{S}$ at $z=\mu$ (or rather the zero at $\bar{\mu}$) induces a decomposition of any matrix element $(g,\mathbf{U}(t)f)_{\mathcal{H}_{\mathrm{ac}}}$, for $t\geqslant 0$ and f and g belonging to a certain dense set in $\mathcal{H}_{\mathrm{ac}}$, into a term evolving according to a semigroup law and a background term. In a sense to be made precise in the next section the semigroup term is of Lax-Phillips type and the eigenvalue of the generator of the semigroup is exactly μ, i.e., the location of the pole of the S-matrix $\tilde{S}$. One may say that the semigroup part of the evolution is driven by the pole of the S-matrix. The identification of the eigenvalue of the generator of the semigroup with the location of the S-matrix pole is made through a mechanism originating from the Sz.-Nagy–Foias theory of contractions on Hilbert space.[11] The decomposition of the matrix element $(g,\mathbf{U}(t)f)_{\mathcal{H}_{\mathrm{ac}}}$ in the form

$$(g,\mathbf{U}(t)f)_{\mathcal{H}_{\mathrm{ac}}}=R^{sg}(g,f;t)+\alpha(g,f)e^{-i\mu t},\quad t\geqslant 0 \tag{1}$$

induced via the Sz.-Nagy–Foias mechanism by a pole of the scattering matrix $\tilde{S}$ at $z=\mu$ will be called the *semigroup decomposition* of the time evolution of a resonance. The second term in Eq. (1) is the semigroup contribution and the first term is the background term.

One important drawback of the framework developed in Ref. 10 is the strong assumption made on the analyticity properties of the S-matrix. While the assumption that $\tilde{S}$ is the boundary value of an $\mathcal{H}^{\infty}(\Pi)$ function allows for the application of the proposed framework in certain situations including, for example, certain Friedrichs-type models or compactly supported perturbations of the Laplacian, it excludes large classes of quantum mechanical scattering problems for which the scattering matrix does not have the necessary analyticity properties. The main focus of the present paper is on an attempt to overcome this obstacle.

The paper is organized as follows: A short summary of the framework for the description of the time evolution of resonances developed in Ref. 10 is given in Sec. II. As mentioned above this framework assumes certain strong analyticity properties for the S-matrix in the upper half-plane. The weakening of these strong assumptions is dealt with in Sec. III. Section IV contains a few comments which are included in order to elucidate some important points in the formalism introduced in the preceding two sections. Final remarks are made in Sec. V.

II. THE SEMIGROUP DECOMPOSITION FOR RESONANCE EVOLUTION

This section provides a short summary of the formalism introduced in Ref. 10. As mentioned in Sec. I, the result, Eq. (1), is obtained under the assumption that $\tilde{S}$, the S-matrix in the energy representation, is the boundary value on $\mathbb{R}^{+}$ of a function in $\mathcal{H}^{\infty}(\Pi)$. In the next section it is shown that it is possible to obtain the same results with a weaker assumption on the analyticity of the S-matrix.

We start the discussion in this section with the definition of a Lax-Phillips-type semigroup. Consider a Hilbert space $\mathcal{H}$ and an evolution group of unitary operators $\{\mathbf{U}(t)\}_{t\in\mathbb{R}}$ on $\mathcal{H}$. The starting point for the Lax-Phillips scattering theory is the assumption that there exist in $\mathcal{H}$ two distinguished subspaces $\mathcal{D}_{-}$ and $\mathcal{D}_{+}$ with the properties

$$\mathcal{D}_{-}\perp\mathcal{D}_{+},$$

$$\mathbf{U}(t)\mathcal{D}_{-}\subset\mathcal{D}_{-},\quad t\leqslant 0,$$

$$\mathbf{U}(t)\mathcal{D}_+ \subset \mathcal{D}_+, \quad t \geqslant 0,$$

$$\cap_t \mathbf{U}(t)\mathcal{D}_\pm = \{0\},$$

$$\overline{\cup_t \mathbf{U}(t)\mathcal{D}_\pm} = \mathcal{H}. \tag{2}$$

The subspaces $\mathcal{D}_-$ and $\mathcal{D}_+$ are called, respectively, the *incoming subspace* and *outgoing subspace* for the evolution $\mathbf{U}(t)$. The main object investigated in the Lax-Phillips theory is the Lax-Phillips semigroup which is defined to be the family $\{\mathbf{Z}(t)\}_{t\geqslant 0}$ of operators on $\mathcal{H}$ given by

$$\mathbf{Z}(t) = \mathbf{P}_+\mathbf{U}(t)\mathbf{P}_-, \quad t \geqslant 0. \tag{3}$$

Here $\mathbf{P}_-$ is the orthogonal projection of $\mathcal{H}$ onto the orthogonal complement of $\mathcal{D}_-$ and $\mathbf{P}_+$ is the orthogonal projection of $\mathcal{H}$ onto the orthogonal complement of $\mathcal{D}_+$. The family $\{\mathbf{Z}(t)\}_{t\geqslant 0}$ forms a strongly continuous contractive semigroup on $\mathcal{K}=\mathcal{H}\ominus(\mathcal{D}_-\oplus\mathcal{D}_+)$ with $s-\lim_{t\to\infty}\mathbf{Z}(t)x=0$ for every $x\in\mathcal{K}$.

Under the assumptions in Eq. (2) Lax and Phillips prove the existence of two *translation representations* for $\mathcal{H}$. In the *incoming translation representation* $\mathcal{H}$ is mapped onto the Hilbert space $L^2_{\mathcal{N}}(\mathbb{R})$ of functions taking their values in a Hilbert space $\mathcal{N}$ (called auxiliary space), $\mathcal{D}_-$ is mapped onto $L^2_{\mathcal{N}}(\mathbb{R}^-)$ and the evolution $\mathbf{U}(t)$ is represented as translation to the right by t units. Analogously, in the *outgoing translation representation* $\mathcal{H}$ is mapped onto $L^2_{\mathcal{N}}(\mathbb{R})$, $\mathcal{D}_+$ is mapped onto $L^2_{\mathcal{N}}(\mathbb{R}^+)$ and the evolution $\mathbf{U}(t)$ is again represented by translation to the right. The mapping S^{LP} of the incoming translation representation onto the outgoing translation representation is the *Lax-Phillips S-matrix*. One usually does not work with the translation representations but rather with their Fourier transforms called, respectively, the *incoming spectral representation and outgoing spectral representation*. According to the Paley-Wiener theorem[12] in the incoming spectral representation $\mathcal{D}_-$ is represented by $\mathcal{H}^+_{\mathcal{N}}(\mathbb{R})$ where $\mathcal{H}^+_{\mathcal{N}}(\mathbb{R})$ is the space of boundary values on $\mathbb{R}$ of functions in $\mathcal{H}^2_{\mathcal{N}}(\Pi)$, the space of (vector valued) Hardy class functions on the upper half-plane. By the same theorem $\mathcal{D}_+$ is represented in the outgoing spectral representation by the function space $\mathcal{H}^-_{\mathcal{N}}(\mathbb{R})$ containing boundary values of functions in $\mathcal{H}^2_{\mathcal{N}}(\bar{\Pi})$ where $\bar{\Pi}$ is the lower half-plane. The Lax-Phillips S-matrix in the spectral representation, i.e., the Fourier transform of the Lax-Phillips S-matrix, will be denoted by $\mathcal{S}^{\mathrm{LP}}$. The operator $\mathcal{S}^{\mathrm{LP}}: L^2_{\mathcal{N}}(\mathbb{R})\mapsto L^2_{\mathcal{N}}(\mathbb{R})$ is realized as a multiplicative, operator valued function $\Theta(\cdot)$, such that $\Theta(\sigma)$ maps $\mathcal{N}$ onto $\mathcal{N}$ for each $\sigma\in R$. The operator valued function $\Theta(\cdot)$ is characterized by its action on $\mathcal{H}^+_{\mathcal{N}}(\mathbb{R})$ as being as *inner function*[13–15] [the notation in this paper does not distinguish between an operator defined on the space $\mathcal{H}^2_{\mathcal{N}}(\Pi)$ and the corresponding operator defined on the space of boundary value functions $\mathcal{H}^+_{\mathcal{N}}(\mathbb{R})$; since the two spaces are isomorphic the same notation is being used for both].

As mentioned above the main object of interest in the Lax-Phillips theory is the Lax-Phillips semigroup. In the outgoing spectral representation an element $\mathbf{Z}(t):\mathcal{K}\mapsto\mathcal{K}$ of the Lax-Phillips semigroup is represented by $\hat{Z}(t)$, $\hat{\mathcal{K}}\mapsto\hat{\mathcal{K}}$ defined by

$$\hat{Z}(t) = T_{u(t)}|\hat{\mathcal{K}}, \quad t \geqslant 0, \tag{4}$$

where

$$\hat{\mathcal{K}} = L^2_{\mathcal{N}}(\mathbb{R}) \ominus (\mathcal{H}^-_{\mathcal{N}}(\mathbb{R}) \oplus \mathcal{S}^{\mathrm{LP}}\mathcal{H}^+_{\mathcal{N}}(\mathbb{R})) = L^2_{\mathcal{N}}(\mathbb{R}) \ominus (\mathcal{H}^-_{\mathcal{N}}(\mathbb{R}) \oplus \Theta(\cdot)\mathcal{H}^+_{\mathcal{N}}(\mathbb{R})) \tag{5}$$

and where $T_{u(t)}:\mathcal{H}^+_{\mathcal{N}}(\mathbb{R})\mapsto\mathcal{H}^+_{\mathcal{N}}(\mathbb{R})$ is a *Toeplitz operator*[13,16,17] with symbol $u(t)$ define by

$$[u(t)f](\sigma) = e^{-i\sigma t}f(\sigma), \quad f\in L^2_{\mathcal{N}}(\mathbb{R}), \quad \sigma\in\mathbb{R}. \tag{6}$$

The structure of the semigroup $\hat{Z}(t)$, representing $\mathbf{Z}(t)$ in the outgoing spectral representation, can be understood in the context of the construction of *functional models* for continuous contractive semigroups on Hilbert space, a part of the Sz.-Nagy–Foias theory of contraction operators on

Hilbert space.[11] We call an operator a *model operator* for a class of operators if every operator in that class is similar to a multiple of a part of it (a part of an operator is defined to be the restriction of the operator to one of its invariant subspaces). By a functional model we mean that the model operator is defined on suitable function spaces. In fact, Eq. (4) provides a functional model for a Lax-Phillips type semigroup. From this point of view the semigroup is a fundamental object, the Lax-Phillips Hilbert space and incoming and outgoing subspaces are obtained in the process of a *unitary dilation* of the semigroup and there always exits a similarity, in fact a unitary, transformation of $\mathbf{Z}(t)$ into its functional model representation in terms of $\hat{Z}(t)$.

We notice that Eq. (5) can be written in the form

$$\hat{\mathcal{K}} = \mathcal{H}^+_{\mathcal{N}}(\mathbb{R}) \ominus \Theta(\cdot)\mathcal{H}^+_{\mathcal{N}}(\mathbb{R}). \tag{7}$$

In fact, Eq. (4) together with Eq. (7) are considered to be the canonical functional model for a Lax-Phillips-type semigroup. Here we consider an *isometric dilation* of the semigroup and we end up with a functional model defined on the Hardy space $\mathcal{H}^+_{\mathcal{N}}(\mathbb{R})$.[10,11] We are interested in this canonical functional model for the Lax-Phillips semigroup and accordingly, for $\Theta(\cdot)$ an inner function, we call a semigroup of the form

$$\hat{Z}(t) = T_{u(t)}|(\mathcal{H}^+_{\mathcal{N}}(\mathbb{R}) \ominus \Theta(\cdot)\mathcal{H}^+_{\mathcal{N}}(\mathbb{R})), \quad t \geqslant 0 \tag{8}$$

a semigroup of *Lax-Phillips type* [in the mathematical literature a functional model for $\mathbf{Z}(t)$ in the form of Eq. (8) follows from the observation that the contractive semigroup $\{\mathbf{Z}^*(t)\}_{t\geqslant 0}$ belongs to the class C_0].

A semigroup of the form given in Eq. (8) is one ingredient entering into the formalism developed in Ref. 10. Another important ingredient is the notion of Hilbert space nesting introduced into the study of quantum mechanical resonances by Grossman.[18] A nesting map of a Hilbert space $\mathcal{H}_1$ into a Hilbert space $\mathcal{H}_0$ is a linear mapping $\theta: \mathcal{H}_1 \to \mathcal{H}_0$ such that

(1) the domain of θ is $\mathcal{H}_1$ and θ is continuous on $\mathcal{H}_1$,
(2) the range $\theta\mathcal{H}_1 \subset \mathcal{H}_0$ is dense in $\mathcal{H}_0$,
(3) θ is injective.

A map with the properties (1)–(3) is also known as a *quasi affine map* (for interesting properties of such maps see, for example, Ref. 11). The adjoint of a nesting map θ, defined by

$$(f, \theta g)_{\mathcal{H}_0} = (\theta^* f, g)_{\mathcal{H}_1},$$

is a nesting of $\mathcal{H}_0$ into $\mathcal{H}_1$. A slightly more extended version of the following theorem was proved in Ref. 10.

Theorem 1 (outgoing\incoming contractive nesting): *Let* $\mathbf{H}_0$ *and* $\mathbf{H}$ *be self-adjoint operators on a Hilbert space* $\mathcal{H}$. *Let* $\{\mathbf{U}(t)\}_{t\in\mathbb{R}}$ *be the unitary evolution group on* $\mathcal{H}$ *generated by* $\mathbf{H}$ [i.e., $\mathbf{U}(t) = \exp(-i\mathbf{H}t)$]. *Denote by* $\mathcal{H}^0_{\mathrm{ac}}$ *and* $\mathcal{H}_{\mathrm{ac}}$, *respectively, the absolutely continuous subspaces of* $\mathbf{H}_0$ *and* $\mathbf{H}$. *Assume that the absolutely continuous spectrum of* $\mathbf{H}_0$ *and* $\mathbf{H}$ *has multiplicity one and that* ess Supp $\sigma_{\mathrm{ac}}(\mathbf{H}_0) =$ ess Supp $\sigma_{\mathrm{ac}}(\mathbf{H}) = \mathbb{R}^+$. *Assume furthermore that the Møller wave operators* $\mathbf{\Omega}^{\pm}(\mathbf{H}_0, \mathbf{H}): \mathcal{H}^0_{\mathrm{ac}} \mapsto \mathcal{H}_{\mathrm{ac}}$ *exist and are complete. Then there are mappings* $\hat{\mathbf{\Omega}}_{\pm}: \mathcal{H}_{\mathrm{ac}} \mapsto \mathcal{H}^+(\mathbb{R})$ *such that*

(i) $(\mathcal{H}_{\mathrm{ac}}, \mathcal{H}^+(\mathbb{R}), \hat{\mathbf{\Omega}}_{\pm})$ *are contractive Hilbert space nestings of* $\mathcal{H}_{\mathrm{ac}}$ *into* $\mathcal{H}^+(\mathbb{R})$,
(ii) *for every* $t \geqslant 0$ *and every* $f \in \mathcal{H}_{\mathrm{ac}}$ *we have*

$$\hat{\mathbf{\Omega}}_{\pm}\mathbf{U}(t)f = T_{u(t)}\hat{\mathbf{\Omega}}_{\pm}f, \tag{9}$$

where $T_{u(t)}$ *is the Toeplitz operator with symbol* $u(t)$. ■

The nesting $(\mathcal{H}_{\mathrm{ac}}, \mathcal{H}^+(\mathbb{R}), \hat{\mathbf{\Omega}}_-)$ is called below the *incoming contractive nesting* of $\mathcal{H}_{\mathrm{ac}}$ and we

denote $f_{\text{in}}=\hat{\mathbf{\Omega}}_{-}f$. Similarly $(\mathcal{H}_{\text{ac}},\mathcal{H}^{+}(\mathbb{R}),\hat{\mathbf{\Omega}}_{+})$ is called the *outgoing contractive nesting* and we denote $f_{\text{out}}=\hat{\mathbf{\Omega}}_{+}f$. The natural definition of the *nested S-matrix* is then $S_{\text{nest}}\equiv\hat{\mathbf{\Omega}}_{+}\hat{\mathbf{\Omega}}_{-}^{-1}$ and we have

$$f_{\text{out}}=\hat{\mathbf{\Omega}}_{+}\hat{\mathbf{\Omega}}_{-}^{-1}f_{\text{in}}=S_{\text{nest}}f_{\text{in}}.$$

Let $U:\mathcal{H}_{\text{ac}}^{0}\mapsto L^{2}(\mathbb{R}^{+})$ be the unitary transformation of $\mathcal{H}_{\text{ac}}^{0}$ into the spectral representation for $\mathbf{H}_{0}$ (the energy representation). If $\mathbf{S}=(\mathbf{\Omega}^{-})^{*}\mathbf{\Omega}^{+}$ is the scattering operator associated with $\mathbf{H}_{0}$ and $\mathbf{H}$ then $\tilde{S}:L^{2}(\mathbb{R}^{+})\mapsto L^{2}(\mathbb{R}^{+})$ defined by

$$\tilde{S}\equiv U\mathbf{S}U^{*}$$

is the energy representation of the S-matrix. Define a map $\theta:\mathcal{H}^{+}(\mathbb{R})\mapsto L^{2}(\mathbb{R}^{+})$ by taking, for each function $f\in\mathcal{H}^{2}(\Pi)$ the restriction on $\mathbb{R}^{+}$ of the boundary value of f on $\mathbb{R}$. Then, by a theorem of Van Winter,[19] θ is a nesting of $\mathcal{H}^{+}(\mathbb{R})$ into $L^{2}(\mathbb{R}^{+})$. The map $\theta^{*}:L^{2}(\mathbb{R}^{+})\mapsto\mathcal{H}^{+}(\mathbb{R})$ is well defined and is a nesting of $L^{2}(\mathbb{R}^{+})$ into $\mathcal{H}^{+}(\mathbb{R})$. It is shown in Ref. 10 that

$$S_{\text{nest}}=\theta^{*}\tilde{\mathbf{S}}(\theta^{*})^{-1} \tag{10}$$

[in fact Eq. (10) is taken in Ref. 10 to be the definition of S_{nest}].

In Sec. III we will need an explicit form for the map θ^{*}. The following Lemma provides the needed expression.[10]

Lemma 1: Define the inclusion map $I:L^{2}(\mathbb{R}^{+})\mapsto L^{2}(\mathbb{R})$ by

$$(If)(\sigma)=\begin{cases}f(\sigma), & \sigma\geqslant 0,\\ 0, & \sigma<0.\end{cases} \tag{11}$$

Let P_{+} be the orthogonal projection of $L^{2}(\mathbb{R})$ onto $\mathcal{H}^{+}(\mathbb{R})$. Then for any $f\in L^{2}(\mathbb{R}^{+})$ we have

$$\theta^{*}f=P_{+}If. \tag{12}$$

■

We are now able to state the semigroup decomposition result following from the $\mathcal{H}^{\infty}(\Pi)$ assumption on the S-matrix mentioned in Sec. I. Assume therefore that $\tilde{S}$, the S-matrix in the energy representation, is the boundary value on $\mathbb{R}^{+}$ of an $\mathcal{H}^{\infty}(\Pi)$ function which will be denoted by $\mathcal{S}$. If $\mathcal{S}$ has only a simple zero in the upper half-plane then, according to the canonical factorization theorems for $\mathcal{H}^{p}$ functions,[14,15] we can write $\mathcal{S}$ in the form

$$\mathcal{S}(z)=\mathcal{B}_{\mu}(z)\mathcal{G}(z), \tag{13}$$

where $\mathcal{B}_{\mu}$ is a simple *Blaschke* factor of the form (for the definition of Blaschke products see, for example, Refs. 14 and 15)

$$\mathcal{B}_{\mu}(z)=\frac{z-\bar{\mu}}{z-\mu} \tag{14}$$

and $\mathcal{G}\in\mathcal{H}^{\infty}(\Pi)$ has no zeros in Π. Under the above assumptions we have the following result on the semigroup decomposition for the $\mathcal{H}^{\infty}$ case.[10]

Proposition 1 ($\mathcal{H}^{\infty}$ case): Assume that the S-matrix $\tilde{S}:L^{2}(\mathbb{R}^{+})\mapsto L^{2}(\mathbb{R}^{+})$ is the boundary value on $\mathbb{R}^{+}$ of some function $\mathcal{S}\in\mathcal{H}^{\infty}(\Pi)$. Suppose, furthermore that $\mathcal{S}$ has a single, simple zero at the point $z=\bar{\mu}$, $\operatorname{Im}\mu<0$ in Π. For any $f\in\mathcal{H}_{\text{ac}}$ let $f_{\text{in}}=\hat{\mathbf{\Omega}}_{-}f$ and $f_{\text{out}}=\hat{\mathbf{\Omega}}_{+}f$. We have

$$f_{\text{out}}=S_{\text{nest}}f_{\text{in}}=\mathcal{B}_{\mu}\theta^{*}\tilde{\mathcal{G}}(\theta^{*})^{-1}f_{\text{in}}-i2\operatorname{Im}\mu[P_{-}\mathcal{G}\bar{f}_{\text{in}}](\mu)x_{\mu}, \tag{15}$$

where P_{-} is the orthogonal projection of $L^{2}(\mathbb{R})$ on $\mathcal{H}^{-}(\mathbb{R})$, $\bar{f}_{\text{in}}\in\mathcal{H}^{-}(\mathbb{R})$ is such that $P_{\mathbb{R}^{-}}(f_{\text{in}}+\bar{f}_{\text{in}})=0$, $\tilde{\mathcal{G}}$ is the boundary value on $\mathbb{R}^{+}$ of a function $\mathcal{G}\in\mathcal{H}^{\infty}(\Pi)$ and $\mathcal{G}$ has no zeros in Π. The vector

$x_\mu \in \mathcal{H}^+(\mathbb{R})$ is given by $x_\mu(\sigma)=(\sigma-\mu)^{-1}$ ($[P_-\mathcal{G}f_{\rm in}^-](\mu)$ is the value of the function $[P_-\mathcal{G}f_{\rm in}^-] \in \mathcal{H}^-(\mathbb{R})$ at $\mu \in \bar{\Pi}$). ■

Define

$$\hat{\mathcal{K}}_\mu \equiv \mathcal{H}^+(\mathbb{R}) \ominus \mathcal{B}_\mu \mathcal{H}^+(\mathbb{R}), \tag{16}$$

then $\hat{\mathcal{K}}_\mu$ is a one-dimensional subspace of $\mathcal{H}^+(\mathbb{R})$ and $x_\mu \in \hat{\mathcal{K}}_\mu$. Since $\mathcal{B}_\mu$ is an inner function for $\mathcal{H}^+(\mathbb{R})$ we can define the Lax-Phillips type semigroup $\{\hat{Z}(t)\}_{t\geqslant 0}$ by

$$\hat{Z}(t) \equiv T_{u(t)}|\hat{\mathcal{K}}_\mu, \quad t \geqslant 0. \tag{17}$$

Then x_μ is an eigenvector of the generator of $\{\hat{Z}(t)\}_{t\geqslant 0}$ and

$$\hat{Z}(t)x_\mu = e^{-i\mu t}x_\mu, \quad t \geqslant 0.$$

Thus, for any $f \in \mathcal{H}_{\rm ac}$ we find that

$$\begin{aligned}\hat{\mathbf{\Omega}}_+\mathbf{U}(t)f = T_{u(t)}f_{\rm out} &= T_{u(t)}\mathcal{B}_\mu\theta^*\tilde{\mathcal{G}}(\theta^*)^{-1}f_{\rm in} - i(2\ \mathrm{Im}\ \mu[P_-\mathcal{G}f_{\rm in}^-](\mu))\hat{Z}(t)x_\mu \\ &= T_{u(t)}\mathcal{B}_\mu\theta^*\tilde{\mathcal{G}}(\theta^*)^{-1}f_{\rm in} - i(2\ \mathrm{Im}\ \mu[P_-\mathcal{G}f_{\rm in}^-](\mu))e^{-i\mu t}x_\mu, \quad t \geqslant 0. \end{aligned} \tag{18}$$

Define

$$\Lambda_{\hat{\mathbf{\Omega}}_+} = \hat{\mathbf{\Omega}}_+^*\hat{\mathbf{\Omega}}_+\mathcal{H}_{\rm ac}. \tag{19}$$

The linear space $\Lambda_{\hat{\mathbf{\Omega}}_+} \subset \mathcal{H}_{\rm ac}$ is dense in $\mathcal{H}_{\rm ac}$. By the injective property of both $\hat{\mathbf{\Omega}}_+$ and $\hat{\mathbf{\Omega}}_+^*$, for any element $g \in \Lambda_{\hat{\mathbf{\Omega}}_+}$ we can find a unique $h_g \in \mathcal{H}_{\rm ac}$ such that $g=\hat{\mathbf{\Omega}}_+^*\hat{\mathbf{\Omega}}_+h_g$. For any $g \in \Lambda_{\hat{\mathbf{\Omega}}_+}$, $f \in \mathcal{H}_{\rm ac}$ and for $t \geqslant 0$ we have

$$\begin{aligned}(g,\mathbf{U}(t)f)_{\mathcal{H}_{\rm ac}} &= (\hat{\mathbf{\Omega}}_+^*\hat{\mathbf{\Omega}}_+h_g,\mathbf{U}(t)f)_{\mathcal{H}_{\rm ac}} = (\hat{\mathbf{\Omega}}_+h_g,\hat{\mathbf{\Omega}}_+\mathbf{U}(t)f)_{\mathcal{H}^+(\mathbb{R})} = (h_{g,\rm out},T_{u(t)}f_{\rm out})_{\mathcal{H}^+(\mathbb{R})} \\ &= (h_{g,\rm out},u(t)\mathcal{B}_\mu\theta^*\tilde{\mathcal{G}}(\theta^*)^{-1}f_{\rm in})_{\mathcal{H}^+(\mathbb{R})} - i(2\ \mathrm{Im}\ \mu[P_-\mathcal{G}f_{\rm in}^-](\mu))e^{-i\mu t}(h_{g,\rm out},x_\mu)_{\mathcal{H}^+(\mathbb{R})}. \end{aligned} \tag{20}$$

Equation (20) is of the form given in Eq. (1) and its rhs provides (for $t \geqslant 0$) the semigroup decomposition of the matrix element $(g,\mathbf{U}(t)f)_{\mathcal{H}_{\rm ac}}$. The zero of the S-matrix at $z=\bar{\mu}$ in Π is related, via the Sz.-Nagy–Foias mechanism described in Ref. 10, to the Lax-Phillips-type semigroup structure leading to the exponential decay of the second term on the rhs of Eq. (20).

As discussed in detail in Ref. 10, Eq. (20) is a direct result of the assumption on the analyticity properties of the S-matrix. In particular, this result is a consequence of the fact that the $\mathcal{H}^\infty$ assumption imply the canonical factorization in Eq. (13). As mentioned in Sec. I above, the assumption that the S-matrix $\tilde{S}$ is a boundary value of a bounded analytic function in the upper half-plane is stronger than what one would consider as desirable. Large classes of models for quantum mechanical scattering phenomena do not possess the assumed analyticity properties and hence cannot be analyzed within the framework developed in Ref. 10. A way of resolving this difficulty is suggested in the next section.

III. MODIFIED ASSUMPTIONS ON *S*-MATRIX ANALYTICITY

In this section it is shown that weaker assumptions on the analyticity of the S-matrix lead to a result very similar to the semigroup decomposition of Eq. (20). Thus, we assume that the S-matrix is analytic in a certain region above the real axis, that it can be analytically continued

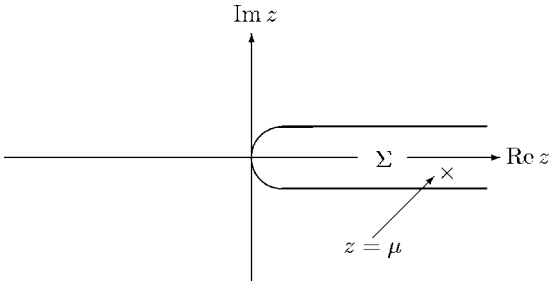

FIG. 1. *S*-matrix analyticity properties. We assume that $\tilde{\mathcal{S}}$ has a meromorphic extension to the region Σ with a simple pole at $z=\mu$.

across $\mathbb{R}^+$ and that the resulting function is meromorphic in an open region Σ containing $\mathbb{R}^+$ with a single, simple pole at $z=\mu$, $\mathrm{Im}\,\mu<0$ inside Σ as depicted in Fig. 1. We have the following theorem.

Theorem 2: *Under the assumptions of Theorem 1, let* **S** *be the scattering operator associated with* $\mathbf{H}_0$ *and* **H** *and let* $\tilde{\mathcal{S}}:L^2(\mathbb{R}^+)\mapsto L^2(\mathbb{R}^+)$ *be the S-matrix in the energy representation (i.e.,* $\tilde{\mathcal{S}} \equiv U\mathbf{S}U^*$ *as above). Assume that* $\tilde{\mathcal{S}}$ *has an extension to a meromorphic function* $\mathcal{S}$ *defined in the region* Σ *with a single, simple, pole at* $z=\mu$, $\mathrm{Im}\,\mu<0$, *and no other pole in* $\bar{\Sigma}$, *the closure of* Σ, *as in Fig. 1.*

For any $f\in\mathcal{H}_{\mathrm{ac}}$ *use the nesting maps* $\hat{\mathbf{\Omega}}_\pm$ *to define* $f_{\mathrm{out}}=\hat{\mathbf{\Omega}}_+f$ *and* $f_{\mathrm{in}}=\hat{\mathbf{\Omega}}_-f$. *Then there exists a unique element* $\psi_\mu\in\mathcal{H}_{\mathrm{ac}}$, *such that*

$$f_{\mathrm{out}} = S_{\mathrm{nest}}f_{\mathrm{in}} = \mathcal{B}_\mu\theta^*\tilde{\mathcal{G}}(\theta^*)^{-1}f_{\mathrm{in}} + i2\,\mathrm{Im}\,\mu(\psi_\mu,f)_{\mathcal{H}_{\mathrm{ac}}}x_\mu, \tag{21}$$

where θ^* *is the map given in Lemma 1,* $x_\mu\in\mathcal{H}^+(\mathbb{R})$ *is given by* $x_\mu(\sigma)=(\sigma-\mu)^{-1}$, $\mathcal{B}_\mu$ *is the Blaschke factor defined in Eq. (14) and the complex valued function* $\tilde{\mathcal{G}}$ *is defined on* $\mathbb{R}^+$ *and is the restriction to* $\mathbb{R}^+$ *of a function* $\mathcal{G}$ *holomorphic in* Σ *and having no zeros on* $\bar{\Sigma}$. ■

Proof: Let $\tilde{\mathcal{S}}$ be the *S*-matrix in the energy representation and assume that it has a meromorphic extension $\mathcal{S}$ in Σ with a simple pole at μ. Then $\mathcal{S}$ has in Σ the representation

$$\mathcal{S}(z) = (z-\mu)^{-1}\mathcal{G}'(z), \tag{22}$$

where $\mathcal{G}'$ is analytic in Σ and has no zero at $z=\mu$. Now, if $\mathcal{S}$ is expressed by Eq. (22) below the real axis then, by the unitarity of $\tilde{\mathcal{S}}$, the restriction of $\mathcal{S}$ to $\mathbb{R}^+$, we find that in the region $\Sigma\cap\Pi$ we can write $\mathcal{S}$ in the form

$$\mathcal{S}(z) = (\bar{\mathcal{S}}(\bar{z}))^{-1} = (z-\bar{\mu})(\overline{\mathcal{G}'}(\bar{z}))^{-1}, \quad \mathrm{Im}\,z>0.$$

Since $\mathcal{G}'$ has no zero at $z=\mu$ then $(\overline{\mathcal{G}'}(\bar{z}))^{-1}$ does not have a pole at $z=\bar{\mu}$ and we conclude that $\mathcal{S}$ has a representation in Σ expressed by

$$\mathcal{S}(z) = \frac{z-\bar{\mu}}{z-\mu}\mathcal{G}(z) = \mathcal{B}_\mu(z)\mathcal{G}(z), \quad z\in\Sigma, \tag{23}$$

where $\mathcal{G}(z)$ has no zero or pole in Σ. We see that $\mathcal{S}$ has in Σ a representation similar to Eq. (13) with the difference being in the fact that this representation is limited to the region Σ.

The *S*-matrix $\tilde{S}$ is given by the restriction of $\mathcal{S}$ in Eq. (23) to $\mathbb{R}^+$, i.e., $\tilde{S}(\lambda)=\mathcal{B}_\mu(\lambda)\tilde{\mathcal{G}}(\lambda)$, $\lambda\in\mathbb{R}^+$. Plugging this form of the *S*-matrix into the expression of the nested *S*-matrix S_{nest} in Eq. (10), we cannot use the methods of Ref. 10 to obtain the desired results since we no longer assume that $\mathcal{S}$ is an $\mathcal{H}^\infty(\Pi)$ function. However, we can avoid the need for this assumption by writing

$$f_{\text{out}} = S_{\text{nest}} f_{\text{in}} = \theta^* \tilde{S}(\theta^*)^{-1} f_{\text{in}} = \theta^* \mathcal{B}_\mu \tilde{\mathcal{G}}(\theta^*)^{-1} f_{\text{in}} = P_+ I \mathcal{B}_\mu \tilde{\mathcal{G}}(\theta^*)^{-1} f_{\text{in}}$$
$$= P_+ \mathcal{B}_\mu (P_+ + P_-) I \tilde{\mathcal{G}}(\theta^*)^{-1} f_{\text{in}} = \mathcal{B}_\mu \theta^* \tilde{\mathcal{G}}(\theta^*)^{-1} f_{\text{in}} + P_+ \mathcal{B}_\mu P_- \bar{\theta}^* \tilde{\mathcal{G}}(\theta^*)^{-1} f_{\text{in}}, \tag{24}$$

where $\bar{\theta}^* = P_- I$. We see that the first term on the rhs of Eq. (24) is identical in form to the first term on the rhs of Eq. (15). In the second term on the rhs of Eq. (24) the operator $P_+ \mathcal{B}_\mu P_- : \mathcal{H}^-(\mathbb{R}) \mapsto \mathcal{H}^+(\mathbb{R})$ is a *Hankel operator* with a one-dimensional range. In fact, for any $g \in \mathcal{H}^+(\mathbb{R})$ and $f \in \mathcal{H}^-(\mathbb{R})$ we have

$$(\mathcal{B}_\mu g, P_+ \mathcal{B}_\mu P_- f)_{\mathcal{H}^+(\mathbb{R})} = (\mathcal{B}_\mu g, \mathcal{B}_\mu f)_{L^2(\mathbb{R})} = 0.$$

Hence Ran $(P_+ \mathcal{B}_\mu P_-) = \hat{\mathcal{K}}_\mu$, where $\hat{\mathcal{K}}_\mu$ is given in Eq. (16). Define the subspace $\hat{\mathcal{K}}_{\bar{\mu}} \subset \mathcal{H}^-(\mathbb{R})$ by

$$\hat{\mathcal{K}}_{\bar{\mu}} \equiv \mathcal{H}^-(\mathbb{R}) \ominus \mathcal{B}_{\bar{\mu}} \mathcal{H}^-(\mathbb{R}).$$

with $\mathcal{B}_{\bar{\mu}}(z) = (z-\mu)/(z-\bar{\mu})$ [$\mathcal{B}_{\bar{\mu}}$ is an inner function for $\mathcal{H}^-(\mathbb{R})$] and denote by $P_{\hat{\mathcal{K}}_{\bar{\mu}}}$ the orthogonal projection on this subspace. Then we also have $P_+ \mathcal{B}_\mu P_- = P_+ \mathcal{B}_\mu P_- P_{\hat{\mathcal{K}}_{\bar{\mu}}}$ since

$$P_+ \mathcal{B}_\mu P_- (\mathcal{B}_{\bar{\mu}} \mathcal{H}^-(\mathbb{R})) = 0.$$

We conclude that

$$P_+ \mathcal{B}_\mu P_- = P_{\hat{\mathcal{K}}_\mu} P_+ \mathcal{B}_\mu P_- P_{\hat{\mathcal{K}}_{\bar{\mu}}}. \tag{25}$$

Using Eq. (25) in Eq. (24) we obtain

$$f_{\text{out}} = \mathcal{B}_\mu \theta^* \tilde{\mathcal{G}}(\theta^*)^{-1} f_{\text{in}} + P_{\hat{\mathcal{K}}_\mu} P_+ \mathcal{B}_\mu P_- P_{\hat{\mathcal{K}}_{\bar{\mu}}} \bar{\theta}^* \tilde{\mathcal{G}}(\theta^*)^{-1} f_{\text{in}}. \tag{26}$$

According to Eq. (16) and Eq. (26) we expect that the second term on the rhs of Eq. (26) is proportional to the vector $x_\mu \in \mathcal{H}^+(\mathbb{R})$. Indeed this is verified by explicit calculation. For the projection operators $P_\pm$ we have the standard expressions

$$[P_\pm f](\sigma') = \frac{1}{2\pi i} \int_{\mathbb{R}} \frac{1}{\sigma' \pm i\epsilon - \sigma} f(\sigma) \mathrm{d}\sigma, \quad f \in L^2(\mathbb{R}).$$

Hence, for $f \in \mathcal{H}^-(\mathbb{R})$ we have

$$[P_+ \mathcal{B}_\mu P_- f](\sigma) = [P_+ \mathcal{B}_\mu f](\sigma) = \frac{1}{2\pi i} \int_{\mathbb{R}} \frac{1}{\sigma + i\epsilon - \sigma'} \frac{\sigma' - \bar{\mu}}{\sigma' - \mu} f(\sigma') = \frac{1}{\sigma - \mu} i 2 \,\mathrm{Im}\, \mu f(\mu). \tag{27}$$

If the S-matrix $\tilde{S}$ has a meromorphic extension $\mathcal{S}$ in Σ with a simple pole at $z = \mu$ then the holomorphic factor of $\mathcal{S}$ in Σ can be found from Eq. (23) and is given by $\mathcal{G} = \mathcal{B}_{\bar{\mu}} \mathcal{S}$. Hence we have

$$[\bar{\theta}^* \mathcal{G}(\theta^*)^{-1} f_{\text{in}}](\mu) = [P_- I \mathcal{B}_{\bar{\mu}} \tilde{\mathcal{S}}(\theta^*)^{-1} f_{\text{in}}](\mu)$$
$$= \frac{1}{2\pi i} \int_{\mathbb{R}^+} \frac{1}{\lambda - \mu} (\mathcal{B}_{\bar{\mu}} \tilde{\mathcal{S}}(\theta^*)^{-1} f_{\text{in}})(\lambda)$$
$$= \frac{1}{2\pi i} \int_{\mathbb{R}^+} \frac{1}{\lambda - \bar{\mu}} (\tilde{\mathcal{S}}(\theta^*)^{-1} f_{\text{in}})(\lambda) = [\theta^* \tilde{\mathcal{S}}(\theta^*)^{-1} f_{\text{in}}](\bar{\mu}) = f_{\text{out}}(\bar{\mu}). \tag{28}$$

Furthermore, it was shown in Ref. 10 that the nesting maps $\hat{\mathbf{\Omega}}_\pm$ are given by $\hat{\mathbf{\Omega}}_\pm = \theta^* U(\mathbf{\Omega}^\mp)^*$ [where, as above, $U : \mathcal{H}_{\text{ac}}^0 \mapsto L^2(\mathbb{R}^+)$ is the mapping onto the $\mathbf{H}_0$ spectral representation] so that, for every $f \in \mathcal{H}_{\text{ac}}$, we have

$$f_{\text{out}}(\bar{\mu}) = \frac{1}{2\pi i}\int_{\mathbb{R}^+} \frac{1}{\lambda - \bar{\mu}}(U(\mathbf{\Omega}^-)^* f)(\lambda) = (\psi_\mu, f)_{\mathcal{H}_{\text{ac}}}, \tag{29}$$

where we define $\psi_\mu = \mathbf{\Omega}^- U^* \tilde{\psi}_\mu$ with $\tilde{\psi}_\mu \in L^2(\mathbb{R}^+)$, $\tilde{\psi}_\mu(\lambda) = (2\pi i)^{-1}(\lambda - \mu)^{-1}$. Combining Eqs. (26)–(29) we obtain the result Eq. (21). ■

In order to see how Theorem 2 is used we go back to Eq. (20). From this equation, together with Eq. (26) and Eq. (21) we find, for any $f \in \mathcal{H}_{\text{ac}}$ and any $g \in \Lambda_{\hat{\mathbf{\Omega}}_+}$,

$$\begin{aligned}(g, \mathbf{U}(t)f)_{\mathcal{H}_{\text{ac}}} &= (h_{g,\text{out}}, T_{u(t)} f_{\text{out}})_{\mathcal{H}^+(\mathbb{R})} = (h_{g,\text{out}}, u(t)\mathcal{B}_\mu \theta^* \tilde{\mathcal{G}}(\theta^*)^{-1} f_{\text{in}})_{\mathcal{H}^+(\mathbb{R})} \\ &\quad + (h_{g,\text{out}}, \hat{Z}(t) P_{\hat{\mathcal{K}}_\mu} P_+ \mathcal{B}_\mu P_- P_{\hat{\mathcal{K}}_{\bar{\mu}}} \overline{\theta}^* \tilde{\mathcal{G}}(\theta^*)^{-1} f_{\text{in}})_{\mathcal{H}^+(\mathbb{R})} \\ &= (h_{g,\text{out}}, u(t)\mathcal{B}_\mu \theta^* \tilde{\mathcal{G}}(\theta^*)^{-1} f_{\text{in}})_{\mathcal{H}^+(\mathbb{R})} + e^{-i\mu t}(h_{g,\text{out}}, x_\mu)_{\mathcal{H}^+(\mathbb{R})}(\psi_\mu, f)_{\mathcal{H}_{\text{ac}}}. \end{aligned} \tag{30}$$

Equation (30) has the general form of Eq. (1) and provides the semigroup decomposition in the case that the S-matrix $\tilde{S}$ has a meromorphic extension to the region Σ in Fig. 1. It can be easily shown that Eq. (30) reduces to Eq. (20) if $\tilde{S}$ is in fact the boundary value on $\mathbb{R}^+$ of a function belonging to $\mathcal{H}^\infty(\Pi)$.

We observe that if in Eq. (30) the state $f \in \mathcal{H}_{\text{ac}}$ is chosen to be orthogonal to ψ_μ then the exponentially decaying term on the rhs of Eq. (30), originating from the Lax-Phillips-type semigroup evolution associated with the pole of the S-matrix, does not appear. This enables us to make a direct correspondence between the state ψ_μ and the resonance contribution to the time evolution. Since, as is seen in Sec. IV below, no state in $\mathcal{H}_{\text{ac}}$ can be mapped into an exact resonance state in the Hardy space $\mathcal{H}^+(\mathbb{R})$ and there always exists some nonzero background contribution, the vector $\psi_\mu \in \mathcal{H}_{\text{ac}}$ will be called an *approximate resonance state*. Using Dirac's notation, let us denote by $\{|E^-\rangle\}_{E\in\mathbb{R}^+}$ the set of outgoing scattering states, i.e., outgoing solutions of the Lipmann-Schwinger equation. It is then easy to see that for $f \in \mathcal{H}_{\text{ac}}$ we have

$$(U(\mathbf{\Omega}^-)^* f)(E) = \langle E^- | f \rangle, \quad E \in \mathbb{R}^+$$

and the definition of the state ψ_μ [see Eq. (29)] implies that it is given by the simple expression

$$|\psi_\mu\rangle = \frac{1}{2\pi i}\int_{\mathbb{R}^+} dE \frac{1}{E - \mu}|E^-\rangle. \tag{31}$$

IV. COMMENTS

This section contains some comments on the framework described in Sec. II and further extended in Sec. III. The discussion below is presented in a slightly more general form than is strictly necessary in order to relate it to the formalism of Secs. II and III. The more general form of the statements made below places the remarks at the end of the present section, on the Bohm-Gadella rigged Hardy space formalism for the resonance problem,[20] into their natural context.

Let $\mathcal{S}$ denote the *Schwartz class* of rapidly decreasing functions in $C^\infty(\mathbb{R})$. Let $\mathcal{S}'$ denote the space of *tempered distributions* on $\mathcal{S}$. We shall need the following definition.[21]

Definition 1 (*the space* $\mathcal{H}^p(\mathbb{C}\backslash\mathbb{R})$)*: For any fixed* $p \in (0,\infty)$ *let* $\mathcal{H}^p(\mathbb{C}\backslash\mathbb{R})$ *denote the space of analytic functions on* $\mathbb{C}\backslash\mathbb{R}$ *for which*

$$\|f\| = \sup_{y\neq 0}\left\{\int_{\mathbb{R}} |f(x+iy)|^p \, dx\right\}^{1/p} < \infty.$$

It can be shown[21] that every function $F \in \mathcal{H}^p(\mathbb{C}\backslash\mathbb{R})$ is associated with a unique tempered distribution $\ell_F \in \mathcal{S}'$ defined by

$$\ell_F(\psi) = \lim_{y\to 0^+} \int \{F(x+iy) - F(x-iy)\}\psi(x)\mathrm{d}x, \quad \psi \in \mathcal{S}. \tag{32}$$

Denote the set of all distributions arising in this way by $H^p(\mathbb{R})$. Then, conversly, for any $p \in (0,\infty)$ and for any distribution $\ell \in H^p(\mathbb{R})$, one can find the unique function $F_\ell \in \mathcal{H}^p(\mathbb{C}\backslash\mathbb{R})$ that defines the distribution ℓ through Eq. (32) via the formula[21]

$$F_\ell(z) = \frac{1}{2\pi i}\ell\left(\frac{1}{\cdot - z}\right). \tag{33}$$

Equation (33) can be thought of as a generalization of the Cauchy integral formula for the recovery of an $\mathcal{H}^p$ function from its boundary value on $\mathbb{R}$.

Even though Eq. (32) and Eq. (33) are valid for any $p \in (0,\infty)$, for $p \in (1,\infty)$ we have the further identification of the space $H^p(\mathbb{R})$ with the space $L^p(\mathbb{R})$ in the sense that any function $f \in L^p(\mathbb{R})$ defines a tempered distribution on $\mathcal{S}$ by

$$\ell_f(\psi) = \int_{\mathbb{R}} f(x)\psi(x)\mathrm{d}x, \quad \psi \in \mathcal{S} \tag{34}$$

and that for any $f \in L^p(\mathbb{R})$ there exists a unique $F_f \in \mathcal{H}^p(\mathbb{C}\backslash\mathbb{R})$ such that $\ell_{F_f} = \ell_f$, i.e., Eqs. (32) and (34) define the same tempered distribution on $\mathcal{S}$.

Finally, we will also need the following result.[21]

Proposition 2: A distribution $\ell \in H^p(\mathbb{R})$ has support which omits an open interval $I \in \mathbb{R}$ if and only if the corresponding function $F_\ell \in \mathcal{H}^p(\mathbb{C}\backslash\mathbb{R})$ given by Eq. (33) has an analytic continuation across the interval I.

Consider now the map $\theta^*: L^2(\mathbb{R}^+) \mapsto \mathcal{H}^+(\mathbb{R})$ and its inverse $(\theta^*)^{-1}: \theta^* L^2(\mathbb{R}^+) \mapsto L^2(\mathbb{R}^+)$. An explicit expression for θ^* is given in Eq. (12). Breaking the action of θ^* into two steps we first have, for any $f \in L^2(\mathbb{R}^+)$,

$$If = P_+ If + P_- If = \theta^* f + \bar{\theta}^* f = f_+ + f_-, \quad f_+ \in \mathcal{H}^+(\mathbb{R}), \quad f_- \in \mathcal{H}^-(\mathbb{R}), \tag{35}$$

where $f_+ = P_+ If$, $f_- = P_- If$. In the second step we take the $\mathcal{H}^+(\mathbb{R})$ piece, i.e.,

$$\theta^* f = P_+ If = f_+.$$

On the other hand, the discussion preceding Proposition 2 implies that if we apply the inclusion map $I: L^2(\mathbb{R}^+) \mapsto L^2(\mathbb{R})$ then, for any element $f \in L^2(\mathbb{R}^+)$, the element $If \in L^2(\mathbb{R})$ is associated with a unique function $F_f \in \mathcal{H}^2(\mathbb{C}\backslash\mathbb{R})$ such that

$$(If)(\sigma) = \lim_{\epsilon\to 0^+} \{F_f(\sigma + i\epsilon) - F_f(\sigma - i\epsilon)\}. \tag{36}$$

In fact, the function $F_f \in \mathcal{H}^2(\mathbb{C}\backslash\mathbb{R})$ is easily found from Eq. (35). We first use the isomorphism of $\mathcal{H}^+(\mathbb{R})$ and $\mathcal{H}^2(\Pi)$ to extend the map θ^* to a mapping $\theta_\pi^*: L^2(\mathbb{R}^+) \mapsto \mathcal{H}^2(\Pi)$. Subsequently we simply define

$$F_f(z) = \begin{cases} f_+(z) = (\theta_\pi^* f)(z), & \mathrm{Im}\, z > 0, \\ -f_-(z) = -(\bar{\theta}_\pi^* f)(z), & \mathrm{Im}\, z < 0. \end{cases} \tag{37}$$

Moreover, Proposition 2 shows that F_f defined in Eq. (37) is in fact analytic on $\mathbb{C}\backslash\mathbb{R}^+$. Denoting the subspace of $\mathcal{H}^2(\mathbb{C}\backslash\mathbb{R})$ of functions analytic on $\mathbb{R}^-$ by $\mathcal{H}^2(\mathbb{C}\backslash\mathbb{R}^+)$ we conclude that there exists a surjective map $A: L^2(\mathbb{R}^+) \mapsto \mathcal{H}^2(\mathbb{C}\backslash\mathbb{R}^+)$ with $Af = F_f$ for $f \in L^2(\mathbb{R}^+)$, $F_f \in \mathcal{H}^2(\mathbb{C}\backslash\mathbb{R}^+)$. Note that

$$(Af)(z) = F_f(z) = (\theta_\pi^* f)(z), \quad \text{Im } z > 0. \tag{38}$$

In addition, we note that Eqs. (36)–(38) provide us with a procedure for the construction of the map $(\theta^*)^{-1}$. Given $f_+ \in \theta^* L^2(\mathbb{R}^+) \subset \mathcal{H}^+(\mathbb{R})$ we use the Cauchy integral formula to obtain the function $f_+ \in \mathcal{H}^2(\Pi)$. We know from Eq. (38) and Eq. (37) that there is a unique function $f \in L^2(\mathbb{R}^+)$ such that $f_+ \in \mathcal{H}^2(\Pi)$ is the restriction to Π of a function $F_f = Af \in \mathcal{H}^2(\mathbb{C}\backslash\mathbb{R}^+)$. Hence we can analytically continue f_+ across $\mathbb{R}^-$ into the lower half-plane and obtain the full function F_f. The reconstruction of the corresponding function $f \in L^2(\mathbb{R}^+)$ is then obtained by using Eq. (36). The process of analytically continuing f_+ across $\mathbb{R}^-$ is done in Ref. 10 essentially by using the Van Winter theorem and explicit integral expressions for the map $(\theta^*)^{-1}$ are obtained.

Next we turn to a discussion of the resonance states. Let

$$R_s \equiv \{x_\mu | x_\mu \in \mathcal{H}^+(\mathbb{R}),\ x_\mu(\sigma) = (\sigma - \mu)^{-1},\ \sigma \in \mathbb{R},\ \text{Im } \mu < 0\}. \tag{39}$$

Obviously, it is not possible to analytically continue any element $x_\mu \in R_s$ across $\mathbb{R}^-$ in order to obtain a function in $\mathcal{H}^2(\mathbb{C}\backslash\mathbb{R}^+)$. By Eq. (38) we obtain the following.

Lemma 2: Define the set $R_s \subset \mathcal{H}^+(\mathbb{R})$ according to Eq. (39). Then $R_s \subset \mathcal{H}^+(\mathbb{R})\backslash\hat{\mathbf{\Omega}}_\pm \mathcal{H}_{\text{ac}}$.

Now, for any given S-matrix $\widetilde{S}$ the eigenvector of the Lax-Phillips-type semigroup in the second term on the rhs of Eq. (30) is proportional to some $x_\mu \in R_s$. Identifying the Hardy space state $x_\mu \in \mathcal{H}^+(\mathbb{R})$ as a pure, exponentially decaying, resonance state, Lemma 2 provides a formal verification for the impossibility of the association of any unique state in the original Hilbert space $\mathcal{H}_{\text{ac}}$ with a pure resonance. For this reason the time evolution (e.g., the survival amplitude) of any state in $\mathcal{H}_{\text{ac}}$ always contains some background contribution and is never purely exponentially decaying.

The final remark in this section is concerned with the Bohm-Gadella rigged Hilbert space formalism for the problem of resonances.[20] The main tool in this formalism is a Gelfand triplet $\Delta_+ \subset \mathcal{H}^+(\mathbb{R}) \subset \Delta_+^*$ constructed by a rigging of the Hardy space $\mathcal{H}^+(\mathbb{R})$. The smaller sector Δ_+ of the Gelfand triple is taken to be $\Delta_+ \equiv \mathcal{H}^+(\mathbb{R}) \cap \mathcal{S}$ where $\mathcal{S}$ again denotes the Schwartz space. The larger sector Δ_+^* contains all the continuous linear functionals on Δ_+. One then uses a pullback procedure in order to obtain a rigged Hilbert space $\Phi \subset L^2(\mathbb{R}^+) \subset \Phi^*$ centered around the Hilbert space $L^2(\mathbb{R}^+)$. The procedure of pull back uses the map θ. We first define $\Phi \equiv \theta\Delta_+$ and then the pull back procedure is used in order to define the set Φ^* of functionals on Φ. Denoting the evaluation of the functional F on a test function f in the rigged Hilbert spaces $\Phi \subset L^2(\mathbb{R}^+) \subset \Phi^*$ or $\Delta_+ \subset \mathcal{H}^+(\mathbb{R}) \subset \Delta_+^*$ by $\langle f, F\rangle_{L^2}$ and $\langle f, F\rangle_{\mathcal{H}^+}$, respectively, the pull back of a functional $F \in \Delta_+^*$ is defined to be

$$\langle f, \widehat{(\theta^{-1})^*} F\rangle_{L^2} \equiv \langle \theta^{-1} f, F\rangle_{\mathcal{H}^+}, \quad f \in \Phi, \quad F \in \Delta_+^*. \tag{40}$$

The map $\widehat{(\theta^{-1})^*}: \Delta_+^* \mapsto \Phi^*$ on the lhs of Eq. (40) is an extension to Δ_+^* of the map $(\theta^{-1})^*$. But on its domain of definition in $\mathcal{H}^+(\mathbb{R})$ we have $(\theta^{-1})^* = (\theta^*)^{-1}$. Hence Eq. (40) can serve just as well to define an extension of the map $(\theta^*)^{-1}$, i.e., we have

$$\langle f, \widehat{(\theta^*)^{-1}} F\rangle_{L^2} \equiv \langle \theta^{-1} f, F\rangle_{\mathcal{H}^+}, \quad f \in \Phi, \quad F \in \Delta_+^*. \tag{41}$$

For any function $F \in \theta^* L^2(\mathbb{R}^+) \subset \mathcal{H}^+(\mathbb{R}) \subset \Delta_+^*$ we have $(f, \widehat{(\theta^*)^{-1}} F\rangle_{L^2} = (f, (\theta^*)^{-1} F)_{L^2(\mathbb{R}^+)}$ and $\widehat{(\theta^*)^{-1}} F$ is then identified with a function in $L^2(\mathbb{R}^+)$ by the procedure for the construction of $(\theta^*)^{-1}$ described above. Here $F \in \theta^* L^2(\mathbb{R}^+)$ is a function in $\mathcal{H}^2(\mathbb{C}\backslash\mathbb{R}^+)$. However, the map $\widehat{(\theta^*)^{-1}}$, defined on Δ_+^*, is certainly well defined for the whole Hardy space $\mathcal{H}^+(\mathbb{R})$ and, in particular, it is well defined in the distributional sense for any resonance state $x_\mu \in R_s \subset \mathcal{H}^+(\mathbb{R})$. Indeed, a resonance in the Bohm-Gadella theory has the form $\widehat{(\theta^*)^{-1}} x_\mu$ for some $x_\mu \in R_s$. Moreover, since the elements of R_s cannot be analytically continued into functions in $\mathcal{H}^2(\mathbb{C}\backslash\mathbb{R}^+)$, they belong to $\Delta_+^* \backslash \theta^* L^2(\mathbb{R}^+)$.

V. CONCLUSIONS

A way of utilizing Lax-Phillips-type semigroups for the description of the time evolution of quantum mechanical resonances was suggested in Ref. 10. The present paper addresses the main difficulty with the framework introduced in Ref. 10 and described in Sec. II above, i.e., the assumption that the S-matrix is the boundary value on $\mathbb{R}^+$ of a function in $\mathcal{H}^\infty(\Pi)$. Such a requirement is not satisfied by large classes of quantum mechanical scattering problems. It is shown in Sec. III above that this condition can be weakened to the assumption that the given S-matrix is analytic in a region Σ as in Fig. 1. In addition, it is shown in Sec. IV that, if we regard a resonance as a quantum object and we look for a Hilbert space state describing it, our expectation that no such state can be found in the Hilbert space $\mathcal{H}$ for the scattering problem is valid. In fact a resonance, identified as an eigenvector of the Lax-Phillips-type semigroup responsible for the exponential decay of the second term on the rhs of the semigroup decomposition in Eq. (30), exists as an element of the Hilbert space $\mathcal{H}^+(\mathbb{R})$, but cannot be associated with any element in $\mathcal{H}_{\mathrm{ac}}$ in the sense that it is outside of the range of the nesting map $\hat{\mathbf{\Omega}}_+$. This implies that the background term, i.e., the first term on the rhs of Eq. (30), exists for any choice of the vectors $g, f \in \mathcal{H}_{\mathrm{ac}}$ and is never zero. However, the formalism developed above does provide a clear identification of a well-defined approximate resonance state $\psi_\mu \in \mathcal{H}_{\mathrm{ac}}$ associated with the resonance contribution to the time evolution (i.e., the semigroup term).

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Geometry of *C*-flat connections, coarse graining and the continuum limit

Jorge Martínez,[a] Claudio Meneses,[b] and José A. Zapata[c]
Instituto de Matemáticas, Universidad Nacional Autónoma de México, A.P. 61-3, Morelia Mich. 58090, México

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A notion of effective gauge fields which does not involve a background metric is introduced. The role of scale is played by cellular decompositions of the base manifold. Once a cellular decomposition is chosen, the corresponding space of effective gauge fields is the space of flat connections with singularities on its codimension two skeleton, $\mathcal{A}_{C\text{-flat}}/\bar{\mathcal{G}}_{M,\star} \subset \bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$. If cellular decomposition C_2 is finer than cellular decomposition C_1, there is a coarse graining map $\pi_{C_2\to C_1}: \mathcal{A}_{C_2\text{-flat}}/\bar{\mathcal{G}}_{M,\star} \to \mathcal{A}_{C_1\text{-flat}}/\bar{\mathcal{G}}_{M,\star}$. We prove that the triple $(\mathcal{A}_{C_2\text{-flat}}/\bar{\mathcal{G}}_{M,\star}, \pi_{C_2\to C_1}, \mathcal{A}_{C_1\text{-flat}}/\bar{\mathcal{G}}_{M,\star})$ is a principal fiber bundle with a preferred global section given by the natural inclusion map $i_{C_1\to C_2}: \mathcal{A}_{C_1\text{-flat}}/\bar{\mathcal{G}}_{M,\star} \to \mathcal{A}_{C_2\text{-flat}}/\bar{\mathcal{G}}_{M,\star}$. Since the spaces $\mathcal{A}_{C\text{-flat}}/\bar{\mathcal{G}}_{M,\star}$ are partially ordered (by inclusion) and this order is directed in the direction of refinement, we can define a continuum limit, $C \to M$. We prove that, in an appropriate sense, $\lim_{C\to M} \mathcal{A}_{C\text{-flat}}/\bar{\mathcal{G}}_{M,\star} = \bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$. We also define a construction of measures in $\bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$ as the continuum limit (not a projective limit) of effective measures. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2037527]

I. MOTIVATION

The Wilsonian renormalization group is fundamental in standard constructions of quantum field theories. The notions of *effective theories at given scales, coarse graining and the ultraviolet/continuum limit* are essential for that scheme.

There are important physical systems for which there is no natural concept of scale which can be used to describe an effective theory as needed by standard renormalization group ideas. Any system that includes gravitational phenomena is in this category of systems because a scale is defined through a metric which in these cases is a dynamical variable. Thus, a definition of effective theories and coarse graining calls for an "extension of the concept of scale."

It is of course possible to introduce a fiducial metric and use its induced notion of scale to define effective theories and coarse graining. In fact this alternative has been developed in recent years.[1]

We will study a proposal of effective theories and coarse graining for gauge theories which emulates structures from lattice gauge theory to situations that are free of a background metric. In standard lattice gauge theory one works with a family of effective theories (labeled by increasingly finer lattices) describing the same system. The key ingredient that fine-tunes all these theories with observation and with each other is a renormalization procedure.

General relativity can be formulated as a gauge theory, but if one wishes to represent the diffeomorphism symmetry it is impossible to use a single embedded lattice to host the theory. A

[a]Electronic mail: yorch@matmor.unam.mx
[b]Electronic mail: claudio@matmor.unam.mx
[c]Electronic mail: zapata@math.unam.mx

solution to this problem is given by the kinematics of loop quantization "which is a lattice gauge theory for a lattice that is infinitely refined" (for a precise statement see Ref. 2). Since there was a single lattice—even if infinitely refined—there was no sequence of effective theories that let one implement Wilson's renormalization group and that in a continuum limit selected a dynamics for the loop quantized theory.

A goal of our research program[2] is to provide a family of effective theories connected to each other by coarse graining maps that average away fluctuations and whose infinite refinement limit takes us to a loop quantized theory. The dynamics of the continuum limit will be defined only after fine-tuning all the effective theories by a renormalization procedure. The proposal is simple and natural in the context of loop quantization. However, there is no claim of uniqueness; we know other families of effective theories with similar structure. Physical applications are still being developed. The most illustrative result at the moment is that when the same ideas are applied to the Ising model one recovers the standard renormalization by blocking. In addition, an extension to irregular lattices of the the blocking and bond-moving procedure of Migdal and Kadanoff is natural in our framework.[3]

A regularization procedure is included in our framework because the configuration spaces of the effective theories lie inside the space of generalized connections, $\mathcal{A}_{\text{"scale"}} \subset \bar{\mathcal{A}}_M$. Thus any observable in the continuum (cylindrical function) is automatically regularized to an observable of the effective theory. This same feature lets us define the continuum limit of the effective theories. For example, the vacuum expectation value of a cylindrical function in the continuum $\langle f \rangle_M$ is defined as the continuum limit of the vacuum expectation value of the same function evaluated in the effective theory defined at a given "scale," "$\langle f \rangle_M = \lim_{\text{"scale"}\to 0} \langle f|_{\mathcal{A}_{\text{"scale"}}} \rangle_{\text{"scale"}}$." Our structure should be compared with others using the restriction of the space of connections to a fixed graph (embedded lattice) $\mathcal{A}_\gamma$ as the home for an effective theory. In that case one would have to provide a separate regularization of observables from $\bar{\mathcal{A}}_M$ to act on each of the spaces $\mathcal{A}_\gamma$ contained in the sequence used to define the continuum limit. Moreover, this family of regularization procedures would have to satisfy compatibility conditions to define a continuum theory.

The specific goal of this paper is to present a geometrical study of a family of configuration spaces of effective theories and of the coarse graining maps that relate them to each other and to the space of generalized connections of loop quantization. The aim is to provide a solid ground for implementing a Wilsonian renormalization in a framework that is independent of a background metric. Eventually, this will serve to define the dynamics (physical measure) of loop quantized theories as the continuum limit of the dynamics of our effective theories.

This paper has the following organization. The next section introduces C-flat connections as effective gauge fields. It also studies the geometry of a C-flat connection and of the space of C-flat connections, as well defines the continuum limit $C \to M$. Section III defines coarse graining maps, studies the resulting geometry, and writes an "exact renormalization prescription" that links different effective measures. Section IV is about the action of diffeomorphisms on the spaces of C-flat connections; it also defines a space of diffeomorphism invariant effective configurations. Finally, the Appendix contains detailed definitions of some preliminary material.

II. A MODEL OF EFFECTIVE GAUGE FIELDS

The access to only finitely many measurement devices implies that only partial knowledge of the system is available. In order to have a presumed state of the system in the continuum for each set of measurements, one complements this partial knowledge with regularity assumptions. A set of measuring devices and complementary regularity assumptions "turn on" some degrees of freedom at a given "measuring scale." This intuitive idea of "measuring scale" is behind all our definitions.

In this paper, the role of scale is played by cellular decompositions of the base manifold. Once a cellular decomposition is chosen, there are regularity assumptions tailored to it. The idea is that inside each cell of the cellular decomposition the connection will be as regular as possible. Ironically these regularity assumptions take us to distributional configurations, configurations that

are not smooth connections but generalized connections. The particular kind of generalized connections (see the Appendix for a definition) that we work with are flat everywhere except for the codimension two cells of the cellular decomposition. The available observables at this "measuring scale" are holonomies along the links of a lattice constructed from the cellular decomposition.

Definition 1 (C-flat connections): A generalized connection is considered to be C-flat, $A \in \mathcal{A}_{C\text{-}flat} \subset \bar{\mathcal{A}}_M$, *if and only if its restriction to each cell of C is flat.*

Notice first that the cells of a cellular decomposition are disjoint, $c_\alpha \cap c_\beta = \emptyset$ if $\alpha \neq \beta$. Thus, there are many nonflat connections which are *C*-flat.

Also notice that in the context of generalized connections the concept of flatness is phrased in terms of the path independence of parallel transport. With this in mind our definition may be clear as it stands, but the following characterization in terms of the holonomy maps induced by *C*-flat connections is most useful in the rest of the paper.

The presence of a cellular decomposition *C* induces a natural equivalence relation among directed paths. Two oriented paths γ_1, γ_2 are defined to be *C-equivalent*, $\gamma_1 \sim_C \gamma_2$, if the two sequences of cells (of any dimension) induced by traversing the curves coincide.

Lemma 1: $\mathcal{A}_{C\text{-}flat}/\bar{\mathcal{G}}_{M,\star}$ *can be characterized as the subset of generalized connections modulo gauge transformations,* $\bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$, *whose elements are those and only those which satisfy*

$$[A](\gamma_1) = [A](\gamma_2)$$

for any two closed oriented paths based at $\star \in M$ *which are C-equivalent,*

$$\gamma_1 \sim_C \gamma_2.$$

The proof of this lemma is a simple application of the reconstruction theorems[4] to our context.

In the rest of this section we will talk about three different subjects in the corresponding sections. In the first section we will describe the geometry of single flat connections; in the second we will elaborate on the space $\mathcal{A}_{C\text{-flat}}$, and in the third we will present configuration spaces that are relevant for the continuum limit in our framework.

A. Geometry of a *C*-flat connection

A good starting point for studying the geometry of *C*-flat connections is the previous lemma; by using it, it is easy to see that the "regularity" assumptions yield generalized connections that may not even be continuous. Consider, for example, a smooth deformation of a given closed curve. According to our lemma, once a *C*-flat connection is chosen, the holonomy of the curve would be independent of the deformation unless its *C*-equivalence class changes. At that point of the deformation process the holonomy may experience a drastic change.

Moreover, since $\bar{\mathcal{G}}_{M,\star}(\mathcal{A}_{C\text{-flat}}) = \mathcal{A}_{C\text{-flat}}$ and $\bar{\mathcal{G}}_{M,\star}$ includes discontinuous gauge transformations, we see that even the gauge equivalence class of an everywhere flat connection has representatives which are not continuous.

However, the distributional nature of our connections modulo gauge is of a very tame type. Essentially they are the familiar spaces of flat connections with "conical" singularities along the codimension two skeleton of *C*. To see that this is the case consider a small loop contained in a single cell of maximum dimension and deform it continuously until it crosses one codimension one cell. The holonomy along the loop before the deformation was the identity and after the deformation it is still the identity because the loop is *C*-equivalent to another loop constructed as $l = c^{-1} \circ c$ (where *c* is an open curve starting in one maximal dimension cell, crossing a codimension one cell, and ending at another maximal dimension cell). Then the codimension one cells cannot host curvature singularities. However, drastic changes in the holonomy during continuous deformations may result from crossing (or hitting) cells of codimension greater or equal to two. (In our framework also the holonomies along curves that pass through singularities are defined. In some contexts these nongeneric curves may be regarded as not important.) This observation is formally stated as a direct corollary of Lemma 1 and the reconstruction theorems.[4]

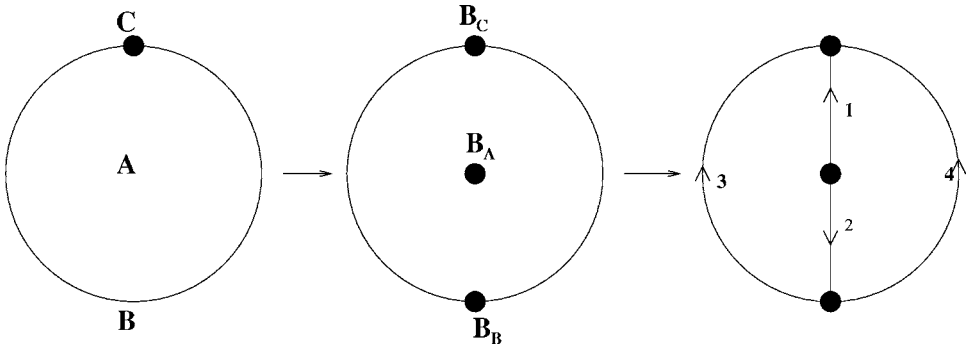

FIG. 1. Construction of $L(C)$.

Corollary 1: For any $[A]\in\mathcal{A}_{C\text{-}flat}/\bar{\mathcal{G}}_{M,\star}$ *there is a unique (up to fiber bundle equivalence) smooth bundle* Φ *over* $M-C^{(n-2)}$ *and a representative* $A\in[A]$ *such that*

$$A|_{M-C^{(n-2)}}\in\mathcal{A}^{\infty}_{M-C^{(n-2)},\Phi}.$$

Moreover, in this domain its curvature is defined and vanishes.

One can expect that the topological charges that characterize the topology and geometry of such singularities will play an important role when investigating the dynamical properties of certain types of fields. Within our framework it would be natural to choose stronger regularity assumptions to make the space of effective configurations at scale C the space of C-flat connections with a restricted type of topological charges at the singularities.

B. Geometry of the space of *C*-flat connections

The space $\mathcal{A}_{C\text{-flat}}$ is infinite dimensional, but we can expect $\mathcal{A}_{C\text{-flat}}/\bar{\mathcal{G}}_{M,\star}$ to be finite dimensional because flat connections modulo gauge do not have any local degrees of freedom. We will show that this is indeed the case by conveniently characterizing gauge equivalence classes of C-flat connections in terms of lattice gauge theory connections.

The starting point is again Lemma 1. Observe that the lattice dual to C contains representatives of the C-equivalence classes of "most" curves, but not all. Hence the space of connections on a lattice dual to C has almost all the holonomy information in $\mathcal{A}_{C\text{-flat}}/\bar{\mathcal{G}}_{M,\star}$, but some is missing. Then we complete the dual lattice to include curves C-equivalent to curves passing through cells of codimension bigger than one; call the resulting lattice $L(C)$. By definition oriented paths in $L(C)$ label C-equivalence classes of oriented paths in M. In the case of simplicial cellular decompositions $L(C)$ is the one skeleton of their barycentric subdivision, $L(C)=\mathrm{Sd}(C)^{(1)}$ (see the Appendix for a definition). In Fig. 1 we present another simple example.

An embedding $\mathrm{Emb}_{L(C)}:L(C)\to M$ can be used to define a fiber bundle with (one-dimensional) base $L(C)$ starting from the fiber bundle (E,φ,M). The total space would be $\varphi^{-1}(\mathrm{Emb}_{L(C)}[L(C)])$, and projection $\varphi|_{\mathrm{Emb}_{L(C)}[L(C)]}$. Apart from pulling back the bundle, $\mathrm{Emb}_{L(C)}$ pulls back connections from $\bar{\mathcal{A}}_M$ to the space of connections on the bundle, $\mathrm{Emb}^{\star}_{L(C)}:\bar{\mathcal{A}}_M\to\mathcal{A}_{L(C)}$.

Clearly not all embeddings are of our interest. To maintain the meaning of directed paths in $L(C)$ as representatives of C-equivalence classes of directed paths in M we restrict ourselves to *representative embeddings*. These are embeddings $\mathrm{Emb}_{L(C)}:L(C)\to M$ such that the inverse image of any oriented path γ in M is a path in $L(C)$ which labels the C-equivalence class of γ.

We denote the group of $\star$-based oriented loops on M by $\mathcal{P}_{M,\star}$; we also denote the induced group of C-equivalent classes of loops by $\mathcal{P}_{C,\star}$ and by $\mathcal{P}_{L(C),b}[\mathrm{Emb}_{L(C)}(b)=\star]$ the analogous object in $L(C)$.

Note that for any representative embedding

$$\mathrm{Emb}_{L(C)}:\mathcal{P}_{L(C),b}\to\mathcal{P}_{C,\star}$$

is an isomorphism independent of the choice of representative embedding [with $\mathrm{Emb}_{L(C)}(b)=\star$]. Thus we also have the natural isomorphism

$$\mathrm{Emb}^{\star}_{L(C)}:\mathrm{Hom}(\mathcal{P}_{C,\star},G)\to\mathrm{Hom}(\mathcal{P}_{L(C),b},G),$$

where $\mathrm{Hom}(\mathcal{P}_{C,\star},G)$ is naturally embedded in $\mathrm{Hom}(\mathcal{P}_{M,\star},G)$.

Using the reconstruction theorems[4] this can be stated in a more familiar language as follows: there is a natural isomorphism

$$\mathrm{Emb}^{\star}_{L(C)}:\mathcal{A}_{C\text{-flat}}/\bar{\mathcal{G}}_{M,\star}\to\mathcal{A}_{L(C)}/\mathcal{G}_{L(C),b}$$

which is independent of the choice of representative embedding $\mathrm{Emb}_{L(C)}:L(C)\to M$ [with $\mathrm{Emb}_{L(C)}(b)=\star$].

It is important to remark that simplicity appears only at the gauge invariant level; for example, since the space $\mathcal{A}_{C\text{-flat}}$ is infinite dimensional it is not isomorphic to a lattice gauge theory configuration space. Working on infinite dimensional quotient spaces is difficult, but we know that the complications must be inessential. This motivates us to study the same spaces in a partially gauge fixed context. It can be thought of as a strengthening of our previous regularity assumptions with extra gauge fixing conditions.

Once a local trivialization is chosen, we can assign group elements to holonomy mappings of open paths. Using this fact, a partially gauge fixed version of the space of C-flat connections is easily characterized as follows: we say that $A\in\mathcal{A}_{C\text{-flat},A_0}$ if and only if the generalized connection $A\in\bar{\mathcal{A}}_M$ is such that the holonomies along any (possibly open) oriented paths are equal, $A(\gamma_1)=A(\gamma_2)\in G$, whenever $\gamma_1\sim_C\gamma_2$. The space $\mathcal{A}_{C\text{-flat},A_0}$ depends on the local trivialization. It is more convenient to say that it depends on an auxiliary flat connection A_0 (the one induced by the local trivialization). Using this notation it is clear that generic gauge transformations do not leave it invariant, but $g(\mathcal{A}_{C\text{-flat},A_0})=\mathcal{A}_{C\text{-flat},g(A_0)}$. The gauge transformations that do leave it invariant form a finite dimensional subgroup of the group of gauge transformations denoted by $\mathcal{G}_{C,A_0,\star}\subset\bar{\mathcal{G}}_{M,\star}$. We can also define this space of residual gauge transformations in terms of the local trivialization as composed by gauge transformations such that $g(p)=g(q)\in G$ whenever p and q are in the same cell.

It is clear that, after the partial gauge fixing $P_{A_0}:\mathcal{A}_{L(C)}\to\mathcal{A}_{L(C),A_0}$, these spaces of connections can be parametrized by the assignment of group elements to C-equivalence classes of paths, or more conveniently to paths in $L(C)$. Then the local trivialization induces isomorphisms $\mathcal{A}_{L(C),A_0}\sim G^{N_1}$ and $\mathcal{G}_{L(C),A_0}\sim G^{N_0-1}$ where N_1 and N_0 are, respectively, the number of edges and vertices in $L(C)$. In this way a local trivialization sets $\mathcal{A}_{C\text{-flat}}/\mathcal{G}_{M,\star}$ in correspondence with G^{N_1}/G^{N_0-1}, where G^{N_0-1} acts by the relevant adjoint action as in the gauge transformations of lattice gauge theory.

We remark that in principle our parametrizations of $\mathcal{A}_{C\text{-flat},A_0}$ and $\mathcal{G}_{C,A_0,\star}$ hold only inside the open set U where A_0 is defined. We can choose an open cover of M in which each open set is a union of cells in C, and proceed as above for each open set. Then we paste all the local parametrizations with the aid of some transition functions. This strategy leads to definitions of partial gauge fixing of $\mathcal{A}_{C\text{-flat}}$ and $\mathcal{G}_{C,\star}$ that hold in all of M. For any choice of transition functions we have a true partial gauge fixing; in the sense that the resulting space contains elements of all the gauge equivalence classes. Thus all the choices of transition functions are equivalent. This radical difference with the theory of smooth bundles is due to working with $\bar{\mathcal{G}}_{M,\star}$. Since this fact makes all the topological considerations almost trivial we will not be concerned about them in the rest of this paper.

Let us summarize the results stated above in the form of a lemma.

Lemma 2: The following spaces are naturally isomorphic:

$$\frac{\mathcal{A}_{C\text{-}flat}}{\bar{\mathcal{G}}_{M,\star}} \sim \frac{\mathcal{A}_{C\text{-}flat,A_0}}{\mathcal{G}_{C,A_0,\star}} \text{ and } \frac{\mathcal{A}_{L(C)}}{\mathcal{G}_{L(C),b}} \sim \frac{\mathcal{A}_{L(C),A_0}}{\mathcal{G}_{L(C),A_0,b}}.$$

Additionally

$$\mathrm{Emb}^{\star}_{L(C)}: \frac{\mathcal{A}_{C\text{-}flat}}{\bar{\mathcal{G}}_{M,\star}} \to \frac{\mathcal{A}_{L(C)}}{\mathcal{G}_{L(C),b}} \text{ and } \mathrm{Emb}^{\star}_{L(C)}: \mathcal{A}_{C\text{-}flat,A_0} \to \mathcal{A}_{L(C),A_0}$$

are natural isomorphisms which are independent of the choice of representative embedding $\mathrm{Emb}_{L(C)}: L(C) \to M$ [*with* $\mathrm{Emb}_{L(C)}(b) = \star$].

Thus,

$$\mathcal{A}_{C\text{-}flat}/\bar{\mathcal{G}}_{M,\star} \sim G^{N_1(L(C))}/G^{N_0(L(C))-1}.$$

Our intuition about the lack of local degrees of freedom in C-flat connections is realized in the form of an identification between the space of C-flat connections modulo gauge transformations and a finite dimensional quotient space.

Within the partially gauge fixed construction both gauge invariance and diffeomorphism invariance are broken by the regularity assumptions. However, note that the original construction does not break gauge invariance, but still breaks diffeomorphism invariance. In a separate presentation we will construct an "extended" space of effective configurations which admits a nontrivial action of the diffeomorphism group, and that after a partial gauge fixation yields our space $\mathcal{A}_{C\text{-flat}}$.[5]

C. Configuration spaces relevant for the continuum limit

A most important element in renormalization is the change to a coarser or finer scale, and a limit in which the scale is the smallest possible (the continuum limit). Thus, in any extended notion of scale used to formulate effective theories there must be a relation that lets us know if a measuring "scale" is finer than another one, and the limit of the smallest "scale" must make sense.

Recall that the set of cellular decompositions of a manifold admits a partial order relation that tells us if a cellular decomposition C_2 is finer than cellular decomposition $C_1 (C_1 \leqslant C_2)$, and that this partial order is directed in the direction of refinement towards "the finest cellular decomposition" $(C \to M)$. [We remark that the directionality of the set of cellular decompositions holds in the piecewise linear and piecewise analytic categories, but not in the smooth category.] This partial order is preserved by our assignment of effective theories to cellular decompositions in the sense of "being contained in" as subsets of $\bar{\mathcal{A}}_M$ or subsets of $\bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$. (Later on we will use the notation $i_C: \mathcal{A}_{C\text{-flat}} \to \bar{\mathcal{A}}_M$ and $i_C: \mathcal{A}_{C_1\text{-flat}}/\bar{\mathcal{G}}_{M,\star} \to \bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$ for the inclusion maps.)

Lemma 3: Our assignment of effective gauge fields to cellular decompositions respects the partial order relation. Namely, $C_1 \leqslant C_2$ *implies*

$$\mathcal{A}_{C_1\text{-}flat} \subseteq \mathcal{A}_{C_2\text{-}flat}, \quad \mathcal{A}_{C_1\text{-}flat,A_0} \subseteq \mathcal{A}_{C_2\text{-}flat,A_0},$$

$$\mathcal{A}_{C_1\text{-}flat}/\bar{\mathcal{G}}_{M,\star} \subseteq \mathcal{A}_{C_2\text{-}flat}/\bar{\mathcal{G}}_{M,\star},$$

and $i_{C_1 \to C_2}$ *will denote all the respective refining maps.*

[The injective map $\mathrm{Emb}^{\star}_{L(C_2)} \circ i_{C_1 \to C_2} \circ (\mathrm{Emb}^{\star}_{L(C_1)} | \mathcal{A}_{C_1\text{-flat},A_0})^{-1}: \mathcal{A}_{L(C_1),A_0} \to \mathcal{A}_{L(C_2),A_0}$, which is not really an inclusion, will also be denoted by $i_{C_1 \to C_2}$. Similarly, at the partially gauge fixed level we will use the same notation for the maps induced by the refining. The ambiguity should be resolved by the context.]

Now let us introduce some configuration spaces that will be the kinematical basis of the continuum limit. First we present the space of connections that are eventually C-flat (given the directed partial order of the cellular decompositions). This space can also be seen as the space of connections that are C-flat according to some cellular decomposition.

Definition 2:

$$\tilde{\mathcal{A}}_M = \cup_C \mathcal{A}_{C\text{-}flat}.$$

There are smaller configuration spaces labeled by a given triangulation Δ of M that are also relevant for the continuum limit. These are constructed iterating the refining operation called barycentric subdivision (see the Appendix).

Definition 3:

$$\tilde{\mathcal{A}}_{M,\Delta} = \cup_n \mathcal{A}_{\mathrm{Sd}^n(\Delta)\text{-}flat}.$$

We will see in the next section that $\tilde{\mathcal{A}}_{M,\Delta}$ can also be constructed as a projective limit, while $\tilde{\mathcal{A}}_M$ cannot.

The interesting property is that while each $\mathcal{A}_{C\text{-flat}}$ captures very little of the information stored in $\bar{\mathcal{A}}_M$, both $\tilde{\mathcal{A}}_M$ and $\tilde{\mathcal{A}}_{M,\Delta}$ can be used to approximate any generalized connection arbitrarily well.

Theorem 1:

$$\lim_{C\to M} \mathcal{A}_{C\text{-}flat} = \lim_{n\to\infty} \mathcal{A}_{\mathrm{Sd}^n(\Delta)\text{-}flat} = \bar{\mathcal{A}}_M$$

in the sense that the subset of generalized connections composed by elements that are eventually in $\mathcal{A}_{C\text{-}flat}$ ($\mathcal{A}_{\mathrm{Sd}^n(\Delta)\text{-}flat}$) *is* $\tilde{\mathcal{A}}_M$ ($\tilde{\mathcal{A}}_{M,\Delta}$) *which is dense in* $\bar{\mathcal{A}}_M$.

Proof: While the restriction of two distinct cylindrical functions $f, g \in \mathrm{Cyl}(\mathcal{A}_M)$ to some $\mathcal{A}_{C\text{-flat}}$ may agree, it is a clear fact that if $f|_{\tilde{\mathcal{A}}_{M,\Delta}} = g|_{\tilde{\mathcal{A}}_{M,\Delta}}$ then $f=g$. In particular, if $f|_{\tilde{\mathcal{A}}_{M,\Delta}}=0$ then f is the zero of the algebra $\mathrm{Cyl}(\mathcal{A}_M)$.

Now suppose that $\tilde{\mathcal{A}}_M$ is not dense in $\bar{\mathcal{A}}_M$. Then there is $A \in \bar{\mathcal{A}}_M$ and a whole neighborhood of it $\mathcal{N}_A$ such that $\mathcal{N}_A \subset \bar{\mathcal{A}}_M - \tilde{\mathcal{A}}_M$. Thus, there is a nonzero continuous function $f \in \mathrm{Cyl}(\mathcal{A}_M)$ such that $f|_{\bar{\mathcal{A}}_M - \mathcal{N}_A}=0$. In particular our assumption implies that there is a $f \in \mathrm{Cyl}(\mathcal{A}_M)$ which $f|_{\tilde{\mathcal{A}}_M}=0$ while it is not the zero of $\mathrm{Cyl}(\mathcal{A}_M)$. The contradiction implies that $\tilde{\mathcal{A}}_M$ is indeed dense in $\bar{\mathcal{A}}_M$.□

Although $\tilde{\mathcal{A}}_M$ and its subset $\tilde{\mathcal{A}}_{M,\Delta}$ are both dense inside $\bar{\mathcal{A}}_M$, in the measure theoretical sense they are both small subsets of $\bar{\mathcal{A}}_M$. The formal statement at the gauge invariant level is the following.

Theorem 2: *As subsets of the space* $\bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$ *equipped with the measure* μ_{AL}, $\tilde{\mathcal{A}}_{M,\Delta}/\bar{\mathcal{G}}_{M,\star}$ *and* $\tilde{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$ *are thin sets.*

Proof: The proof is a simple adaptation of a theorem by Mourao, Thiemann, and Velhinho on the support of the Ashtekar-Lewandowski measure[6] (Theorem I.212).

We will construct a map

$$h^s : \bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star} \to G^{[0,1]}$$

that will let us study "a piece of $\bar{\mathcal{A}}_M$." To make this possible we consider $G^{[0,1]}$ equipped with a different topology and measure theoretical structure than the usual ones. For the moment consider $G^{[0,1]}$ as a set; its structure will be defined below to be compatible with the structure of $\bar{\mathcal{A}}_M$ through the map h^s.

Consider a one parameter family of loops based at $\star \in M$, $s(t) \in \mathcal{P}_\star$, $t \in [0,1]$, such that $s(0)=\mathrm{id}_\star$ and $s(1)$ is a holonomicaly nontrivial loop. Generalized connections assign group elements to loops, $A(s(t)) \in G$. The latter can be seen as a function from $[0, 1]$ to G, or equivalently an element of $G^{[0,1]}$. Thus, a one parameter family of loops $s(t)$ induces a map from $\bar{\mathcal{A}}_M$ to $G^{[0,1]}$. This is our map $h^s : \bar{\mathcal{A}}_M \to G^{[0,1]}$.

Given a choice of finitely many points $t_i \in [0,1]$ consider it as an assignment from $G^{[0,1]}$ to some G^n. Thus continuous functions from $f : G^n \to \mathbb{C}$ induce *cylindrical functions* $f_{\{t_i\}} : G^{[0,1]} \to \mathbb{C}$. Clearly the pull back of these functions by h^s are cylindrical functions of $\bar{\mathcal{A}}_M$. We endow $G^{[0,1]}$

with the weakest topology that makes cylindrical functions continuous and also consider these cylinder functions the basis of its measure theoretical structure. Additionally, the push forward of the Ashtekar-Lewandowski measure is the natural homogeneous measure on $G^{[0,1]}$ endowed with this structure.

Consider the subset $D \subset G^{[0,1]}$ defined by those functions $h:[0,1] \to G$ that are nowhere continuous *according to the usual topologies* of $[0, 1]$ and G.

Thiemann proves that $G^{[0,1]} - D$ is contained in a measure zero set of $G^{[0,1]}$ with respect to the homogeneous measure.[6]

Our result follows from the fact that $h^s(\tilde{\mathcal{A}}_{M,\Delta}/\bar{\mathcal{G}}_{M,\star}) \subset G^{[0,1]} - D$ and $h^s(\tilde{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}) \subset G^{[0,1]} - D$. □

Given that our spaces of effective configurations are nested in the sense of Lemma 3, each $\mathcal{A}_{C\text{-flat}}$ can be used to regularize (approximate) any cylindrical function from the continuum or from a finer cellular decomposition. This regularization is naturally performed by the pull back of the inclusion maps $i_C: \mathcal{A}_{C_1\text{-flat}}/\bar{\mathcal{G}}_{M,\star} \to \bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$ or $i_{C_1 \to C_2}: \mathcal{A}_{C_1\text{-flat}}/\bar{\mathcal{G}}_{M,\star} \to \mathcal{A}_{C_2\text{-flat}}/\bar{\mathcal{G}}_{M,\star}$.

Now we will define measures in $\bar{\mathcal{A}}_M$ as the continuum limit of effective measures.

Definition 4 (continuum limit of effective theories): Consider a collection of measures $\{\mu_C\}$ [*or* $\{\mu_n\}$], *one measure in each of the spaces of effective configurations* $\{\mathcal{A}_{C\text{-}flat}\}$ [*or* $\{\mathcal{A}_{\mathrm{Sd}^n(\Delta)\text{-}flat}\}$].

When the measures converge, the continuum limit measure μ_M, *will be a measure in* $\bar{\mathcal{A}}_M$ *defined by its action on cylindrical functions as follows:*

$$\mu_M(f) \doteq \lim_{C \to M} \mu_C(i_C^\star f)$$

or

$$\mu_M(f) \doteq \lim_{n \to \infty} \mu_n(i_C^\star f)$$

for any cylindrical function $f \in Cyl(\mathcal{A}_M)$.

Clearly the continuum limit of effective measures as $C \to M$ is a much stronger condition than the limit using a sequence of refinements of a given triangulation. The limit $C \to M$ needs that an effective measure be defined for any C and that different refinement sequences of effective measures have the same limit. If our objective is to define measures in the continuum, we should use the limit $n \to \infty$ because it is more economical, but the limit $C \to M$ has the advantage of being manifestly independent of any choice of "discretization" (refining sequence).

The measures in finer and coarser effective theories should be related if they describe the same physical system. In Sec. III C we will show how a finer measure is coarse grained to produce a measure for a coarser effective theory. If in a given refining sequence the measures at coarser scales are constructed by coarse graining finer measures, we say that the measures are projectively compatible. In all these cases the limit $n \to \infty$ of our previous definition exists, but it is trivial in the sense that starting from a high enough n_0 for any $n \geqslant n_0 \mu_n(i_C^\star f)$ is independent of n. The known examples of measures that can be constructed in this way include the Ashtekar-Lewandowski measure (the homogeneous measure) and distributional measures peaked on flat connections.

Our objective is to emulate the lattice gauge theory procedure to find a theory in the continuum, which is much more powerful. There are many examples of collections $\{\mu_n\}$ which are not projectively compatible, but as n increases they become more and more compatible in the sense of the definition given above. It is easy to exhibit examples of nontrivial convergence for sigma models, and one can also construct them for gauge fields.

When the continuum limit exist, the measure μ_M can be coarse grained to define measures in all the spaces $\mathcal{A}_{\mathrm{Sd}^n(\Delta)\text{-flat}}$. Clearly this sequence of measures will be projectively compatible. These measures should be considered as "completely renormalized." In general they differ from the original effective measure used to construct the continuum limit measure, but in the sense of the limit defined above they differ less and less as we approach the continuum limit.

In a restricted version of our framework where we consider only regular cellular decomposi-

tions we can simply declare that the effective measures are the ones used in lattice gauge theory (by a renormalization group procedure). From this point of view there is a whole body of evidence supporting the existence of nontrivial physically interesting measures. A more detailed study of the relation between our framework and standard lattice gauge theory is needed.

The question arises of which measures on $\bar{\mathcal{A}}_M$ can be constructed as a continuum limit. This question and many others are outside of the scope of this paper. A detailed measure theoretical study of this continuum limit is certainly needed.

III. COARSE GRAINING AND FIBER BUNDLE STRUCTURE

Consider a situation in which we have two effective theories, one of which is based on finer knowledge of the system. The coarser and the finer effective theories should be related by a renormalization procedure which adjusts the coupling constants to account for the bulk effect of averaging out the degrees of freedom of the finer theory which are considered as fluctuations over the degrees of freedom relevant for the coarser theory.

In the preceding section we defined spaces of effective connections. The space of connections related to a finer theory contains that of a coarser theory. Physically this will let us treat the degrees of freedom used to describe coarser configurations as background degrees of freedom.

In this section we define a coarse graining procedure based on a choice of fibration which organizes the remaining degrees of freedom of the finer theory as fluctuations over each of the coarser (background) configurations. This fibration and Fubini's theorem tell us how to integrate out the fluctuations; a measure for the coarser theory is induced by coarse graining the measure for the finer theory.

Definition 5 (coarse graining maps): A natural coarse graining in our setting is induced by a choice of representative embedding $\mathrm{Emb}_{L(C)}: L(C) \to M$,

$$\pi_C \doteq (\,\mathrm{Emb}^{\star}_{L(C)}|_{\mathcal{A}_{C\text{-}flat}/\bar{\mathcal{G}}_{M,\star}})^{-1} \circ \mathrm{Emb}^{\star}_{L(C)}: \bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star} \to \mathcal{A}_{C\text{-}flat}/\bar{\mathcal{G}}_{M,\star},$$

where $\mathrm{Emb}^{\star}_{L(C)}: \mathcal{A}_{C\text{-}flat}/\bar{\mathcal{G}}_{M,\star} \to \mathcal{A}_{L(C)}/\mathcal{G}_{L(C),b}$ *is an isomorphism*,

$$\pi_C \doteq (\,\mathrm{Emb}^{\star}_{L(C)}|_{\mathcal{A}_{C\text{-}flat,A_0}})^{-1} \circ P_{A_0} \circ \mathrm{Emb}^{\star}_{L(C)}: \bar{\mathcal{A}}_M \to \mathcal{A}_{C\text{-}flat,A_0},$$

where $P_{A_0}: \mathcal{A}_{L(C)} \to \mathcal{A}_{L(C),A_0}$ *is the partial gauge fixing and* $\mathrm{Emb}^{\star}_{L(C)}: \mathcal{A}_{C\text{-}flat,A_0} \to \mathcal{A}_{L(C),A_0}$ *is an isomorphism. Given* $C_1 \leqslant C_2$,

$$\pi_{C_2 \to C_1} \doteq \pi_{C_1}|_{\mathcal{A}_{C_2\text{-}flat}/\bar{\mathcal{G}}_{M,\star}}: \mathcal{A}_{C_2\text{-}flat}/\bar{\mathcal{G}}_{M,\star} \to \mathcal{A}_{C_1\text{-}flat}/\bar{\mathcal{G}}_{M,\star},$$

$$\pi_{C_2 \to C_1} \doteq \pi_{C_1}|_{\mathcal{A}_{C_2\text{-}flat,A_0}}: \mathcal{A}_{C_2\text{-}flat,A_0} \to \mathcal{A}_{C_1\text{-}flat,A_0}.$$

[When working on the spaces $\mathcal{A}_{L(C_i)}$ the relevant coarse graining map is $\pi_{C_2 \to C_1} = \mathrm{Emb}^{\star}_{1,2}$, where $\mathrm{Emb}_{1,2}: L(C_1) \to L(C_2)$ represents a C_2-equivalence class of representative embeddings $\mathrm{Emb}_{L(C_1)}$. Note that this map is not a projection. The ambiguity in our notation should be resolved by the context.]

In the rest of this section we will treat three different subjects in corresponding sections. In the first section we will give a minimal example of our spaces of effective configurations and coarse graining maps; in addition we use the example to motivate the general result of the following section. In the second section we present a theorem describing the fiber bundle structure induced by our coarse graining maps. In the final section we then study the effect of coarse graining on measures; in particular we treat the issue of renormalization prescriptions, conditions that relate the measures on different effective theories "asking them to describe the same physical system."

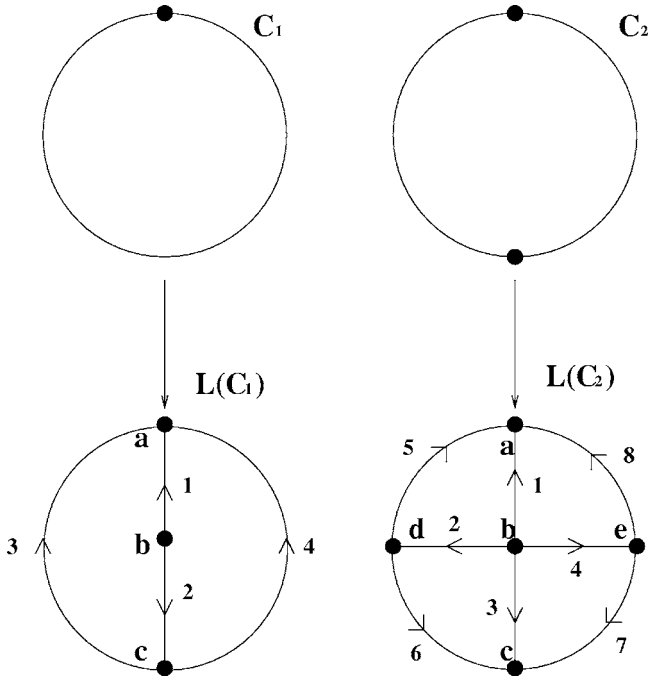

FIG. 2. Two cellular decompositions of the disc, $C_1 \leqslant C_2$.

A. A minimal example

Here we present a minimal example and use it to begin our exploration of the general properties of the coarse graining map. For concreteness we present it at the partially gauge fixed level.

Consider a closed disc (a two-dimensional closed ball) with the cellular decompositions C_1, C_2 described in Fig. 2. These cellular decompositions induce the auxiliary lattices $L(C_1)$, $L(C_2)$ also depicted in the figure. In the parametrizations described in the preceding section we can write

$$A \in \mathcal{A}_{L(C_1),A_0} \quad \text{as } A = (g_1, g_2, g_3, g_4) \in G^4,$$

$$g \in \mathcal{G}_{L(C_1),A_0} \quad \text{as } g = (g_a, g_b, g_c) \in G^3,$$

$$A' \in \mathcal{A}_{L(C_2),A_0} \quad \text{as } A' = (g'_1, g'_2, g'_3, g'_4, g'_5, g'_6, g'_7, g'_8) \in G^8,$$

and

$$g' \in \mathcal{G}_{L(C_2),A_0} \quad \text{as } g' = (g'_a, g'_b, g'_c, g'_d, g'_e) \in G^5.$$

We will also use the subgroup of gauge transformations that are the identity at a vertex, our notation will be

$$g \in \mathcal{G}_{L(C_1),A_0,b} \quad \text{as } g = (g_a, g_c) \in G^2$$

and

$$g' \in \mathcal{G}_{L(C_2),A_0,b} \quad \text{as } g' = (g'_a, g'_c, g'_d, g'_e) \in G^4.$$

The corresponding connections modulo gauge can be written as

$$[A] \in \mathcal{A}_{L(C_1),A_0}/\mathcal{G}_{L(C_1),A_0,b} \quad \text{as } A=(g_{l1},g_{l2}) \in G^2$$

and

$$[A'] \in \mathcal{A}_{L(C_2),A_0}/\mathcal{G}_{L(C_2),A_0,b} \quad \text{as } [A']=(g'_{l'1},g'_{l'2},g'_{l'3},g'_{l'4}) \in G^4,$$

where $l1=2^{-1}\circ 3^{-1}\circ 1$ and $l2=1^{-1}\circ 4\circ 2$ are loops in $L(C_1)$ based at b, and $l'1=2^{-1}\circ 5^{-1}\circ 1$, $l'2=3^{-1}\circ 6\circ 2$, $l'3=4^{-1}\circ 7^{-1}\circ 3$ and $l'4=1^{-1}\circ 8\circ 4$ are loops in $L(C_2)$ based at b.

The maps induced by refining (the inclusion of C-flat connections) on connections $i_{C_1\to C_2}:\mathcal{A}_{L(C_1),A_0}\to\mathcal{A}_{L(C_2),A_0}$ and gauge transformations $i_{C_1\to C_2}:\mathcal{G}_{L(C_1),A_0}\to\mathcal{G}_{L(C_2),A_0}$ are

$$i_{C_1\to C_2}(A)=(g_1,g_2,g_2,g_2,g_3,\mathrm{id},\mathrm{id},g_4),$$

$$i_{C_1\to C_2}(g)=(g_a,g_b,g_c,g_c,g_c).$$

In addition, the three different coarse graining maps depending on the choice of embedding $\mathrm{Emb}_{1,2}:L(C_1)\to L(C_2)$ are

$$\pi_1(A')=(g'_1,g'_2,g'_5,g'_8(g'_7)^{-1}g'_6),$$

$$\pi_1(g')=(g'_a,g'_b,g'_d),$$

$$\pi_2(A')=(g'_1,g'_3,g'_5(g'_6)^{-1},g'_8(g'_7)^{-1}),$$

$$\pi_2(g')=(g'_a,g'_b,g'_c),$$

$$\pi_3(A')=(g'_1,g'_4,g'_5(g'_6)^{-1}g'_7,g'_8),$$

$$\pi_3(g')=(g'_a,g'_b,g'_e).$$

It is easy to verify that the maps $i_{C_1\to C_2}$ and π_i descend to the quotient by gauge transformations since $i_{C_1\to C_2}(g(A))=i_{C_1\to C_2}(g)(i_{C_1\to C_2}(A))$ and $\pi_i(g'(A'))=\pi_i(g')(\pi_i(A'))$.

We will work out the example using the projection π_1. The other projections π_i yield the same structures. Our study will show that in this example $(\mathcal{A}_{L(C_2),A_0},\pi_1,\mathcal{A}_{L(C_1),A_0})$ and $(\mathcal{A}_{L(C_2),A_0}/\mathcal{G}_{L(C_2),A_0,b},\pi_1,\mathcal{A}_{L(C_1),A_0}/\mathcal{G}_{L(C_2),A_0,b})$ are principal fiber bundles with structure group G^4 and G^2, respectively. In addition, they have a preferred global section induced by the refining maps (inclusion of C-flat connections).

On the other hand, $(\mathcal{A}_{L(C_2),A_0}/\mathcal{G}_{L(C_2),A_0},\pi_1,\mathcal{A}_{L(C_1),A_0}/\mathcal{G}_{L(C_2),A_0})$ has the structure of a bundle where neither the total space nor the base are manifolds and where most fibers are homeomorphic to G^2, the only exceptions being the fibers over nongeneric connections modulo gauge, which are not typical. For example, the fiber over the flat connection is the quotient space generated by two copies of the gauge group modulo the adjoint action, $G^2/\mathrm{Ad}\,G$. We will not study this space directly; the most illuminating fact about it is that it is the quotient of the principal fiber bundle, $(\mathcal{A}_{L(C_2),A_0}/\mathcal{G}_{L(C_2),A_0,b},\pi_1,\mathcal{A}_{L(C_1),A_0}/\mathcal{A}_{L(C_2),A_0,b})$ by G, that is a finite-dimensional Lie group.

Now we start with the study of the typical fiber of

$$(\mathcal{A}_{L(C_2),A_0},\pi_1,\mathcal{A}_{L(C_1),A_0}).$$

Given any $A_0=(g_1^\circ,g_2^\circ,g_3^\circ,g_4^\circ)\in\mathcal{A}_{L(C_1),A_0}$ the fiber over it can be parametrized as

$$\pi_1^{-1}(A_0)=\{(g_1^\circ,g_2^\circ,g_3,g_4,g_3^\circ,g_7(g_8)^{-1}g_4^\circ,g_7,g_8)\}.$$

Then all the fibers of $(\mathcal{A}_{L(C_2),A_0},\pi_1,\mathcal{A}_{L(C_1),A_0})$ are homeomorphic to G^4.

A bit of graphical thinking will let us understand this example and generalize the result. At the nongauge invariant level G^4 appears because we have eight unknowns [the number of edges in $L(C_2)$] and four restrictions [the number of edges in $L(C_1)$]. Once we have found one solution to the conditions, we can generate more solutions in two ways, (i) modifying only holonomies along edges in the graph $L(C_2)-\mathrm{Emb}_{1,2}(L(C_1))$, (ii) modifying holonomies along edges of $L(C_2)$ covered by $\mathrm{Emb}_{1,2}(L(C_1))$ without modifying the induced holonomies in the edges of $L(C_1)$.

In our example (i) corresponds to modifying the components of A' assigned to edges 3,4 of $L(C_2)$. Whereas (ii) must be achieved by modifications that involve the components of A' assigned to edges 6,7,8 of $L(C_2)$ without modifying the holonomy along the image by $\mathrm{Emb}_{1,2}$ of edge 4 of $L(C_1)$. Of course, these modifications can be of the form of "gauge transformations" acting on vertices c, e of $L(C_2)$. Moreover, these transformations of the "gauge transformation" style together with type (i) transformations generate all the possible modifications of solutions to the restrictions.

Then, consider the following $G^2\times G^2$ left action on $\mathcal{A}_{L(C_2),A_0}$,

$$\mathcal{F}_{\nu_3,\nu_4;\nu_c,\nu_e}(g_1^\circ,\ldots,g_8^\circ)=(g_1^\circ,g_2^\circ,\nu_c g_3^\circ\nu_3^{-1},\nu_e g_4^\circ\nu_4^{-1},g_5^\circ,\nu_c g_6^\circ,\nu_c g_7^\circ\nu_e^{-1},g_8^\circ\nu_e^{-1}).$$

In our notation type (i) transformations are parametrized by $(\nu_3,\nu_4)\in G^2$ and type (ii) transformations are parametrized by $(\nu_c,\nu_e)\in G^2$.

Our argument in the preceding paragraph implies that the map $\mathcal{F}_\nu$ preserves fibers, $\pi_1(A_0')=\pi_1(\mathcal{F}_\nu(A_0'))$. Furthermore, it gives a bijection between each fiber and G^4. Then $(\mathcal{A}_{L(C_2),A_0},\pi_1,\mathcal{A}_{L(C_2),A_0})$ is a G^4 principal fiber bundle.

Now we would like to describe the typical fiber of

$$(\mathcal{A}_{L(C_2),A_0}/\mathcal{G}_{L(C_2),A_0,b},\pi_1,\mathcal{A}_{L(C_1),A_0}/\mathcal{G}_{L(C_1),A_0,b});$$

the procedure will follow our previous analysis closely. Given any $[A_0]=(g_{l1}^\circ,g_{l2}^\circ)\in\mathcal{A}_{L(C_1),A_0}/\mathcal{G}_{L(C_1),A_0,b}$ the fiber over it can be parametrized as

$$\pi_1^{-1}([A_0])=\{(g_{l1}^\circ,g'_{l'2},g'_{l'3},g_2^\circ g'^{-1}_{l'3}g'^{-1}_{l'2})\}.$$

Then all the fibers of $(\mathcal{A}_{L(C_2),A_0}/\mathcal{G}_{L(C_2),A_0,b},\pi_1,\mathcal{A}_{L(C_1),A_0}/\mathcal{G}_{L(C_1),A_0,b})$ are homeomorphic to G^2.

Consider the following G^2 left action on $\mathcal{A}_{L(C_2),A_0}/\mathcal{G}_{L(C_2),A_0,b}$:

$$\widetilde{\mathcal{F}}_{\nu_1,\nu_2}(g'_{l'1},g'_{l'2},g'_{l'3},g'_{l'4}) \tag{1}$$

$$=(g'_{l'1},\nu_1 g'_{l'2},\nu_2 g'_{l'3}\nu_1^{-1},g'_{l'4}\nu_2^{-1}).$$

Note that it is the action induced by $\mathcal{F}_\nu$ at the gauge invariant level.

Clearly the map $\widetilde{\mathcal{F}}_\nu$ preserves fibers, $\pi_1([A_0'])=\pi_1(\widetilde{\mathcal{F}}_\nu([A_0']))$. Furthermore, it gives a bijection between each fiber and G^2. Then $(\mathcal{A}_{L(C_2),A_0}/\mathcal{G}_{L(C_2),A_0,b},\pi_1,\mathcal{A}_{L(C_1),A_0}/\mathcal{G}_{L(C_1),A_0,b})$ is a G^2 principal fiber bundle.

B. Fiber bundle structure

Theorem 3: *Given a cellular decomposition and a refinement of it, $C_1\leqslant C_2$, the triples $(\mathcal{A}_{C_2\text{-}flat}/\mathcal{G}_{C_2,\star},\pi_{C_2\to C_1},\mathcal{A}_{C_1\text{-}flat}/\mathcal{G}_{C_1,\star})$ and $(\mathcal{A}_{C_2\text{-}flat,A_0},\pi_{C_2\to C_1},\mathcal{A}_{C_1\text{-}flat,A_0})$ are principal fiber bundles with a preferred global section induced by the refining maps (inclusion of C-flat connections).*

Proof: The proof of the general case is entirely analogous to our treatment of the example. Here we present it only at the gauge invariant level.

$\mathcal{A}_{C_2\text{-flat}}/\mathcal{G}_{C_2,\star}$—or equivalently, $\mathcal{A}_{L(C_2)}/\mathcal{G}_{L(C_2),b}$—is parametrized by $G^{N_1(L(C_2))-(N_0(L(C_2))-1)}$.

Once the base space point is fixed in the parametrization of $\mathcal{A}_{C_1\text{-flat}}/\mathcal{G}_{C_1,\star}$ as $G^{N_1(L(C_1))-(N_0(L(C_1))-1)}$, the locus of the fiber over it is found by solving $N_1(L(C_1))-(N_0(L(C_1))-1)$ conditions on the variables $G^{N_1(L(C_2))-(N_0(L(C_2))-1)}$.

When a solution has been found for these equations, one can find all the other solutions through a $G^{[N_1(L(C_2))-(N_0(L(C_2))-1)]-[N_1(L(C_1))-(N_0(L(C_1))-1)]}$ action, $\tilde{\mathcal{F}}_\nu$, of the "gauge transformation type" (1).

Clearly the map $\tilde{\mathcal{F}}_\nu$ preserves fibers and gives a bijection between each fiber and $G^{[N_1(L(C_2))-(N_0(L(C_2))-1)]-[N_1(L(C_1))-(N_0(L(C_1))-1)]}$. □

Since the C-effective theory is isomorphic to a lattice gauge theory, it is clear that configuration observables correspond to holonomies and momentum observables correspond to left invariant vector fields. The set of these observables is an algebra under a Poisson bracket product and is called the holonomy flux algebra, H-F(C).

The pull back of the coarse graining map takes holonomies from H-F(C_1) to H-F(C_2) and the left invariant push forward of the refining map can be used to bring fluxes from H-F(C_1) to H-F(C_2). We call this map $\widehat{\pi^\star_{C_2\to C_1}}$. It turns out that

Corollary 2: If $C_1 \leqslant C_2$,

$$\widehat{\pi^\star_{C_2\to C_1}}\text{:H-}F(C_1) \to \text{H-}F(C_2)$$

is a $\star$*-algebra embedding.*

The proof of this statement, a detailed study of coarse graining within the algebraic approach and phase space effective theories will be treated elsewhere.

C. Coarse graining effective measures

In Sec. III C we defined a construction of measures in $\bar{\mathcal{A}}_M$ as a continuum limit of effective measures on the spaces $\mathcal{A}_{C\text{-flat}}$. If $C_1 \leqslant C_2$, the effective measures μ_{C_1} and μ_{C_2} must be related by coarse graining (at least approximately) because they define effective theories for the same physical system. Assume that we have chosen a projection map $\pi_{C_2\to C_1}$, which amounts to having chosen certain degrees of freedom on $\mathcal{A}_{C_2\text{-flat}}$ as fluctuations over the background configurations $i_{C_1\to C_2}\mathcal{A}_{C_1\text{-flat}}$.

Definition 6 (exact renormalization prescription):

$$(\pi_{C_2\to C_1})_\star \mu_{C_2} = \mu_{C_1}.$$

The definition means that for any cylindrical function f of $\mathcal{A}_{C_1\text{-flat}}$ we have $\int_{\mathcal{A}_{C_1\text{-flat}}} f\, \mathrm{d}\mu_{C_1} = \int_{\mathcal{A}_{C_2\text{-flat}}} \pi^\star_{C_2\to C_1} f\, \mathrm{d}\mu_{C_2}$. Its physical interpretation is that any scale C_1 observable can either be measured by μ_{C_1} on the space $\mathcal{A}_{C_1\text{-flat}}$ or be "observed at scale C_2" as a rather coarse function and measured by μ_{C_2} on the space $\mathcal{A}_{C_2\text{-flat}}$ *producing exactly the same results.*

Given any refining sequence $C1 \leqslant C_2 \leqslant \cdots \leqslant C_n \leqslant \cdots$ there are choices of projections that make the corresponding exact renormalization prescriptions *compatible*. This is because the following lemma holds.

Lemma 4: Given any three cellular decompositions related by refinement $C_1 \leqslant C_2 \leqslant C_3$ *there are choices of embeddings* $\mathrm{Emb}_{i,j}: L(C_i) \to L(C_j)$ *which induce projections* $\pi_{C_j\to C_i} = \mathrm{Emb}^\star_{i,j}: \mathcal{A}_{L(C_j)} \to \mathcal{A}_{L(C_i)}$ *that make the following triangle diagram commute:*

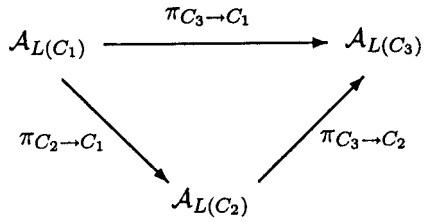

Proof: Fix $\mathrm{Emb}_{1,2}: L(C_1)\to L(C_2)$ and $\mathrm{Emb}_{2,3}: L(C_2)\to L(C_3)$. Clearly $\mathrm{Emb}_{2,3}\circ\mathrm{Emb}_{1,2}: L(C_1)\to L(C_3)$ sends holonomicaly independent paths into holonomicaly independent paths, and it also represents a C_3-equivalence class of embeddings $\mathrm{Emb}_{L(C_1)}: L(C_1)\to M$ as required. □

In particular one can choose compatible exact renormalization prescriptions for the refining sequence $\Delta\leqslant \mathrm{Sd}(\Delta)\leqslant\cdots\leqslant \mathrm{Sd}^n(\Delta)\leqslant\cdots$. In this case a solution of such chain of conditions would yield a sequence of projectively compatible measures $\{\mu_n\}$. Thus, the continuum limit of definition (4) would exist and define a measure μ_M on $\bar{\mathcal{A}}_M$.

It is important to remark that a collection of compatible embeddings that makes the exact renormalization prescriptions compatible can also be used to define the projective limit more commonly used in loop quantization and that the results are compatible in the following sense.

Theorem 4: *Given a family of compatible projections* $\{\pi_{n+1\to n}: \mathcal{A}_{\mathrm{Sd}^{n+1}(\Delta)\text{-}flat}\to\mathcal{A}_{\mathrm{Sd}^{n}(\Delta)\text{-}flat}\}$ *the projective limit of the spaces* $\mathcal{A}_{\mathrm{Sd}^{n}(\Delta)\text{-}flat}$ *is* $\tilde{\mathcal{A}}_{M,\Delta}$.

In addition, the collection of projectively compatible measures $\{\mu_n\}$ *defines a measure* $\tilde{\mu}_M$ *on* $\tilde{\mathcal{A}}_{M,\Delta}$ *which is compatible with our continuum limit measure in the sense that*

$$i_\star\tilde{\mu}_M=\mu_M,$$

where $i:\tilde{\mathcal{A}}_{M,\Delta}\to\bar{\mathcal{A}}_M$ *is the inclusion map.*

The proof of this theorem is a simple corollary of definitions. Of course the continuum limit in these cases is trivial in the sense that starting from a high enough n_0 for any $n\geqslant n_0\mu_n(i_C^\star f)$ is independent of n.

Our continuum limit of measures significantly extends the projective limit and this extension is of interest for physical applications. We say that because there are many examples of collections $\{\mu_n\}$ which are not projectively compatible, but as n increases they become more and more compatible in a way that makes the continuum limit exist. More significantly, the construction of measures by standard lattice gauge theory can be imported to a restricted version of our framework where we consider only regular cellular decompositions. From this point of view there is a whole body of evidence supporting the existence of nontrivial physically interesting measures.

In standard lattice gauge theory the used renormalization prescriptions are much weaker than our exact renormalization prescription: they ask only that some correlation functions chosen by their physical importance be preserved by coarse graining. Also, the allowed measures in LGT are of a very constrained type; only a few coupling constants completely specify their measures. With a smaller space of allowed measures and weaker renormalization prescriptions they are able to generate a flow in the space of coupling constants, which flows in the direction of refinement. We have followed and implemented their ideas in a few examples of our framework.[3]

What about compatible renormalization prescriptions relating the effective theories assigned to all the cellular decompositions? Consider two refining sequences that share a cellular decomposition C. A choice of compatible projections for a refining sequence completely determines the embedding map $\mathrm{Emb}_{L(C)}: L(C)\to M$. Thus, if one chooses independently the two families of compatible projections, it could happen that the induced embedding $\mathrm{Emb}_{L(C)}: L(C)\to M$ may be different for the two sequences. This would mean that the projection from $\bar{\mathcal{A}}_M$ to $\mathcal{A}_{C\text{-flat}}$ would depend on the coarse graining route. If the coarse graining between two effective theories depends on the coarse graining route, there would be one exact renormalization prescription per path and they would not be compatible with each other.

Again we stress that the lattice gauge theory experience tells us that nonexact renormalization

prescriptions are more interesting than exact ones. Then, the more relevant question would be about compatibility of (nonexact) renormalization prescriptions. In this context it is known that coarse graining does depend on the coarse graining route. A familiar example is performing Migdal-Kadanoff blocking in two dimensions first in the x direction and then in the y direction, or reversing the order of the blocking.

IV. ACTION OF "DIFFEOMORPHISMS"

Clearly general fiber bundle maps do not leave the spaces of C-flat connections invariant, but their action is very simple.

Theorem 5: *$\mathcal{A}_{C\text{-}flat} \subset \bar{\mathcal{A}}_M$ is not left invariant by the pull back of fiber bundle automorphisms. Instead*

$$f^\star(\mathcal{A}_{C\text{-}flat}) = \mathcal{A}_{\tilde{f}^{-1}C\text{-}flat},$$

where $\tilde{f}$ is the map induced by f in the base space.

We leave the simple proof of this theorem to the reader.

In this work the relevant fiber bundle maps are the ones that preserve the space of cellular decompositions of the base space that we are considering. Thus, we should focus either on piecewise analytic (also called stratified analytic) or on piecewise linear maps. However, we loosely refer to them as "diffeomorphisms."

For convenience we write $\mathcal{A}_{C\text{-flat}}/\bar{\mathcal{G}}_{M,\star}$ as $(\mathcal{A}/\mathcal{G})_C$.

If the theory under study has diffeomorphism symmetry our construction of spaces of effective configurations breaks that symmetry. However, we can define a space of "diffeomorphism" invariant configurations by injecting $(\mathcal{A}/\mathcal{G})_C$ into $\bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$ and using the notion of "diffeomorphism" equivalence there.

Definition 7: Two connections modulo gauge $[A_1],[A_2] \in (\mathcal{A}/\mathcal{G})_C$ are said to be "diffeomorphism" equivalent,

$$[A_1] \sim_d [A_2],$$

if and only if there is a "diffeomorphism" $\tilde{f}$ of M (that has $\star \in M$ as a fixed point and) such that $\tilde{f}^\star[A_1]=[A_2]$. (We are considering the action $\tilde{f}^\star$ defined by $f^\star: \bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star} \to \bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$ for any bundle map f that induces $\tilde{f}$ on the base space and whose restriction to the fiber over $\star \in M$ is the identity.)

Consider two cellular decompositions C_1 and $C_2=\tilde{f}(C_1)$ [with $\tilde{f}(\star)=\star$]. Clearly the quotient spaces $(\mathcal{A}/\mathcal{G})_{C_1}/\sim_d$ and $(\mathcal{A}/\mathcal{G})_{C_2}/\sim_d$ are identified by $\tilde{f}^\star$. Moreover, the identification would be the same for any other "diffeomorphism" which relates the two cellular decompositions and has $\star \in M$ as a fixed point.

Thus, we define the space of "diffeomorphism" invariant effective configurations at scale $[C]$ as

$$\left(\frac{\mathcal{A}}{\mathcal{G}\times\mathcal{D}}\right)_{[C]} \doteq \frac{\left(\frac{\mathcal{A}}{\mathcal{G}}\right)_C}{\sim_d},$$

for any C in the "diffeomorphism" equivalence class $[C]$ (relative to the subgroup of "diffeomorphisms" that fixes $\star \in M$).

It is important to remark that the equivalence relation $\sim_d$ is not induced by the space of automorphisms of the abstract cellular complex underlying C. Even for a regular cellular decomposition whose automorphism group is large, $\sim_d$ is larger than the equivalence relation induced by automorphisms of C.

There is a construction of effective configurations—$\mathcal{A}_{K\text{-flat}} \subset \bar{\mathcal{A}}_M$ (where K is an abstract cellular complex)—which does not break the "diffeomorphism" symmetry. One can take quotient by the "diffeomorphism" group of $\mathcal{A}_{K\text{-flat}}$ to find a space of "diffeomorphism" invariant configurations finding the same space that we just defined.[5]

From the point of view of the framework mentioned above, the framework presented in this paper is *partially gauge fixed with respect to the "diffeomorphism" group*. The complex nature of the equivalence relation $\sim_d$ in $(\mathcal{A}/\mathcal{G})_C$ as compared to the transparent action of the "diffeomorphism" group in $\bar{\mathcal{A}}_M$ means that this partial gauge fixation would not help if we want to analyze the "diffeomorphism" symmetry. However, many other aspects (including those presented in this paper) are much simpler to study in the gauge fixed framework.

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APPENDIX

For the convenience of the reader we give a minimal recollection of definitions and properties needed in the main body of the paper. The subjects covered are

(1) generalized connections,
(2) cellular decompositions of a manifold and the limit $C \to M$.

Generalized connections

Generalized connections lie at the core of loop quantized theories.

Consider a G-principal fiber bundle (E, φ, M). In the physics literature it is customary to denote the space of smooth G-connections on that fiber bundle simply by $\mathcal{A}_M$. However, topologically different G-bundles over M lead to different spaces of smooth connections.

A *generalized connection* $A \in \bar{\mathcal{A}}_M$ is an assignment (a semigroup morphism) of holonomies to oriented paths in M,

$$A(\gamma): \varphi^{-1}(s(\gamma)) \to \varphi^{-1}(t(\gamma)),$$

where $s(\gamma)$ and $t(\gamma)$ denote the source and target points of γ. A holonomy must be compatible with the right G-action on the fiber bundle, $A(\gamma)[xg] = A(\gamma)[x]g$ for any $g \in G$ and any $x \in \varphi^{-1}(s(\gamma))$. Holonomies can be composed when the corresponding paths can. Asking that the assignment be a morphism means that $A(\gamma_2 \circ \gamma_1) = A(\gamma_2) \circ A(\gamma_1)$. We remark that paths of the form $c^{-1} \circ c$ are regarded as equivalent to the path that stays at the single point $s(c)$; thus $A(c^{-1}) = A(c)^{-1}$.

It is important to emphasize that there are no requirements of smoothness or even continuity for the holonomy assignments with respect to deformations of the path. Analogously the group of gauge transformations acts on holonomy assignments without any continuity restrictions. If one imposes restrictions of this type on the space of connections and the space of gauge transformations, one can recover the space of smooth connections modulo gauge.

At the gauge invariant level the focus changes to group homomorphisms from the group of $\star \in M$-based oriented loops (modulo an equivalence relation that prevents holonomical triviality), $\mathcal{P}_{M,\star}$, to G. The space of such homomorphisms is the space of gauge equivalence classes of generalized connections

$$\bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star} = \mathrm{Hom}(\mathcal{P}_{M,\star}, G).$$

Again no continuity restrictions are imposed. If one imposes this type of conditions one can reconstruct the space of smooth connections modulo gauge. In fact, it is in exactly these terms these the reconstruction theorems are enounced and proven.[4]

Instead of placing continuity restrictions from classical considerations, one defines a different topology for $\bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$. By definition this is the weakest topology for which cylindrical functions, $\mathrm{Cyl}(\bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star})$, are continuous. Cylindrical functions are functions on $\bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$ induced by continuous functions on finitely many copies of G by the choice of a based loop for each copy of G. With respect to this topology, the space $\bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$ is independent of the topology of the total space of the fiber bundle. This finishes with our definition of $\bar{\mathcal{A}}_M/\bar{\mathcal{G}}_{M,\star}$.

Cellular decompositions and the limit $C \to M$

A typical example of a cellular decomposition is a triangulation of the sphere whose cells are four triangles, six edges, and four vertices.

A *cellular decomposition* C of a manifold M is a presentation of it as a union of disjoint cells,

$$M = \cup_{c_\alpha \in C} c_\alpha,$$

$$c_\alpha \cup c_\beta = \emptyset \quad \text{if } \alpha \neq \beta.$$

Each cell c_α is the image of an open convex polyhedron in $\mathbb{R}^{n(\alpha)}$ with $n(\alpha)$ between zero and $\dim M$. Then, we can specify a cell by a pair consisting of an open convex polyhedron in $\mathbb{R}^n$ and a map that takes the polyhedron to M,

$$c_\alpha = (p_\alpha, \phi_\alpha).$$

To be precise we must identify the types of maps we consider. In this work we consider maps $\phi_\alpha: \mathbb{R}^{n(\alpha)} \to M$ which are either piecewise analytic or piecewise linear.

The n-skeleton of a cellular decomposition $C^{(n)}$ is the collection of cells of dimension smaller or equal to n. For example, $C^{(\dim M)}$ is C and $C^{(0)}$ is the set of vertices of C. In our work we use the one-dimensional complex $C^{(1)}$ because it is a lattice.

Notice that the set of cellular decompositions of a manifold admits a partial order relation that tells us if a cellular decomposition C_2 is finer than another one C_1. We write

$$C_1 \leqslant C_2$$

if any cell in the coarser decomposition is a finite union of cells of the finer decomposition.

Triangulations (or simplicial decompositions) are particular examples of cellular decompositions where the polyhedra used are only simplices. In this category of cellular decompositions one can easily define the *barycentric subdivision* operation that produces a finer cellular decomposition, $\Delta \leqslant \mathrm{Sd}(\Delta)$. The triangulation $\mathrm{Sd}(\Delta)$ is easily constructed inductively.

(1) To each simplicial cell $\delta_\alpha \in \Delta$ one assigns a zero-dimensional cell in $\mathrm{Sd}(\Delta)$ called the barycenter of δ_α. (For zero-dimensional cells the barycenter coincides with the original cell.)
(2) For one-dimensional simplicial cells the cone over their boundary with vertex in their barycenter is a simplicial subdivision of δ_α. We call it the barycentric subdivision of δ_α, $\mathrm{Sd}(\delta_\alpha)$.
(3) The barycentric subdivision of the union of cells is by definition the union of the barycentric subdivision of the cells, $\mathrm{Sd}(\delta_\alpha \cup \delta_\beta) = \mathrm{Sd}(\delta_\alpha) \cup \mathrm{Sd}(\delta_\beta)$.
(4) Assume that Sd is defined for cells of dimension $n-1$.
(5) The boundary of an n-dimensional simplicial cell $\partial(\delta_\alpha)$ is the union of $(n-1)$-dimensional simplicial cells. The cone over $\mathrm{Sd}(\partial(\delta_\alpha))$ with vertex in the barycenter of δ_α is defined as $\mathrm{Sd}(\delta_\alpha)$.

The partial order of cellular decompositions is *directed* in the direction of refinement. This means that given any two cellular decompositions C_1, C_2 there is third one such that $C_1 \leqslant C_3$ and $C_2 \leqslant C_3$. With this property in mind, we restrict to piecewise analytic or piecewise linear cellular decompositions; the directionality property would not hold if we allowed any smooth map.

The directionality property is the one that will let us talk about the continuum limit as a limit towards "the finest cellular decomposition." For example, if there is any physically meaningful number calculated in an effective theory associated to a cellular decomposition $N(C)$, we would like it to have a finite limit when we remove the cutoff. Our notation is $N(M)=\lim_{C\to M} N(C)$, where the directionality property of the partial order gives a meaning to the limit "in terms of epsilons and deltas as in ordinary calculus." When one is talking about objects different than numbers one must specify the meaning of $\lim_{C\to M}$; here we simply remark that the directionality of the partial order makes it possible to define a variety of such limits.

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Function group approach to unconstrained Hamiltonian Yang–Mills theory

Antti Salmela[a)]
Theoretical Physics Division, Department of Physical Sciences, University of Helsinki, P.O. Box 64, FIN-00014 Helsinki, Finland

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Starting from the temporal gauge Hamiltonian for classical pure Yang–Mills theory with the gauge group SU(2) a canonical transformation is initiated by parametrizing the Gauss law generators with three new canonical variables. The construction of the remaining variables of the new set proceeds through a number of intermediate variables in several steps, which are suggested by the Poisson bracket relations and the gauge transformation properties of these variables. The unconstrained Hamiltonian is obtained from the original one by expressing it in the new variables and then setting the Gauss law generators to zero. This Hamiltonian turns out to be local and it decomposes into a finite Laurent series in powers of the coupling constant. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2040327]

I. INTRODUCTION

An important and still open problem of quantum chromodynamics is to work out analytical predictions for the low-energy states of the theory. In order to make these predictions we need a proper quantum Yang–Mills theory which is valid in the low-energy regime. However, for many reasons it has turned out to be a difficult task to construct a useful physical Hamiltonian. One of the problems encountered is the implementation of Gauss's law in the Hamiltonian formalism. Up to this date, several methods have been developed to tackle it,[1–13] and this paper aims to provide a method, which is motivated by Lie's theory of function groups and their canonical representations.

Usually one starts with an extended quantum Hamiltonian where the physical subspace consists of states that are annihilated by the Gauss law generators. In this paper, by contrast, the order of quantization and constraining is reversed and Gauss's law is incorporated into the Hamiltonian formalism already at the classical level with the help of a suitable canonical transformation. Whenever one performs canonical transformations in a classical Hamiltonian gauge theory, one must choose the new variables in a way that makes their fundamental Poisson bracket relations compatible with the gauge algebra satisfied by the Gauss law generators. This is often done by the method of Abelianization, where the Gauss law generators are multiplied by suitable matrices that transform them into mutually involutive canonical momenta. In this paper, however, the opposite strategy is followed and the generator algebra is taken as given. The generators are then parametrized with the minimum number of canonical variables in such a way that the gauge algebra is satisfied as a consequence of the fundamental Poisson brackets of the new variables. The remaining variables of the new set are finally constructed by following the logical steps implied by this parametrization. The procedure is carried through for pure SU(2) Yang–Mills theory, but a generalization to other Lie groups is discussed in the end.

The actual construction of the canonical transformation is done in several steps in Sec. II. The procedure is a bit lengthy, but it may be worthwhile to give a presentation where the underlying logic is made clear and where possibilities for modifications and generalizations are also offered.

[a)]Electronic mail: antti.salmela@helsinki.fi

The final transformation is then used in the third section, where the unconstrained Hamiltonian is derived and expanded in a finite series involving both positive and negative powers of the coupling constant. The last section is devoted to conclusions. Throughout the paper Einstein's summation convention will be used with spatial and Lie algebra metrics normalized to positive unity. The generators of the SU(2) algebra are, as usual, taken to be $T_a=\frac{1}{2}\sigma_a$, where the σ_a's stand for the Pauli matrices.

II. CONSTRUCTION OF THE CANONICAL TRANSFORMATION

A. Parametrization of the Gauss law generators

We start with the temporal gauge ($A_0^a=0$) Hamiltonian

$$H=\int\left(\frac{1}{2}\Pi_{ka}\Pi^{ka}+\frac{1}{4}F_{kl}^{a}F_{a}^{kl}\right)\mathrm{d}^3\mathbf{x}, \tag{1}$$

where the field tensor F_{kl}^a is defined by

$$F_{kl}^{a}=\partial_l A_k^a-\partial_k A_l^a+g\varepsilon_{bc}{}^{a}A_k^b A_l^c.$$

The variables $A_k^a(\mathbf{x})$ and $\Pi_{ka}(\mathbf{x})$ are canonically conjugate, i.e., they satisfy the fundamental Poisson bracket relations

$$\{A_k^a(\mathbf{x}),\Pi_{lb}(\mathbf{y})\}=\delta_{kl}\delta^a{}_b\delta(\mathbf{x}-\mathbf{y}).$$

From these relations it follows that the Gauss law generators

$$G_a=\partial^k\Pi_{ka}-g\varepsilon_b{}^c{}_a A^{kb}\Pi_{kc} \tag{2}$$

obey the SU(2) algebra

$$\{G_a(\mathbf{x}),G_b(\mathbf{y})\}=-g\varepsilon_{ab}{}^{c}G_c(\mathbf{y})\delta(\mathbf{x}-\mathbf{y}). \tag{3}$$

They also generate time-independent gauge transformations of the canonical variables as follows:

$$\begin{aligned}\{G_a(\mathbf{x}),A_k^b(\mathbf{y})\}&=-\delta_a{}^b\partial_k^{(x)}\delta(\mathbf{x}-\mathbf{y})-g\varepsilon_{ca}{}^{b}A_k^c(\mathbf{y})\delta(\mathbf{x}-\mathbf{y}),\\ \{G_a(\mathbf{x}),\Pi_{kb}(\mathbf{y})\}&=-g\varepsilon^{c}{}_{ab}\Pi_{kc}(\mathbf{y})\delta(\mathbf{x}-\mathbf{y}).\end{aligned} \tag{4}$$

The canonical equations of motion

$$\dot{A}_k^a(\mathbf{x})=\frac{\delta H}{\delta\Pi_a^k(\mathbf{x})},\quad \dot{\Pi}_{ka}(\mathbf{x})=-\frac{\delta H}{\delta A^{ka}(\mathbf{x})} \tag{5}$$

reproduce the dynamical Yang–Mills equations

$$\ddot{A}_k^a(\mathbf{x})-\left[\delta^a{}_c\partial^l-g\varepsilon_{bc}{}^{a}A^{lb}(\mathbf{x})\right]F_{kl}^{c}(\mathbf{x})=0,$$

but not Gauss's law

$$G_a(\mathbf{x})=0.$$

However, the Gauss law generators are constants of motion, i.e.,

$$\dot{G}_a(\mathbf{x})=0$$

in the dynamics described by the equations (5). This property ensures that the implementation of Gauss's law can be done consistently with the Hamiltonian equations of motion. Unfortunately we cannot just use (2) to eliminate redundant coordinates in the limit $G_a\to 0$, because we do not know

which coordinates to eliminate or how to deal with the canonical conjugates of these redundant variables.

The first stage in the function group approach consists of replacing the Gauss law generators with such canonical variables that will vanish in the limit when Gauss's law is put into force. At this point we recall that in Lie's work a function group is defined as a set of variables equipped with Poisson brackets that close on the set.[14] According to Lie, every function group can be transformed into a form where every variable either has a canonically conjugate counterpart in the set or its Poisson brackets with the remaining variables vanish. Applying this idea to the function group formed by the G_a's, we parametrize it with three canonical variables p_1, p_2, and q_2 as follows:

$$\begin{aligned} G_1 &= \sqrt{p_1^2 - p_2^2}\cos(gq_2), \\ G_2 &= -\sqrt{p_1^2 - p_2^2}\sin(gq_2), \\ G_3 &= p_2. \end{aligned} \tag{6}$$

It is easy to check that the SU(2) algebra relations (3) are satisfied if the Poisson brackets of the new variables are canonical, i.e., if

$$\{q_2(\mathbf{x}), p_2(\mathbf{y})\} = \delta(\mathbf{x} - \mathbf{y})$$

and all the other brackets vanish. Conversely, we can invert this transformation and check that the variables

$$\begin{aligned} p_1 &= \sqrt{G_1^2 + G_2^2 + G_3^2}, \\ p_2 &= G_3, \\ q_2 &= -\frac{2}{g}\arctan\left(\frac{\sqrt{G_1^2 + G_2^2} - G_1}{G_2}\right) \end{aligned} \tag{7}$$

satisfy the fundamental Poisson bracket relations by virtue of the algebra (3).

The parametrization (6) is by no means the only possibility of defining a canonical representation, but it is one of the simplest with respect to the properties of the SU(2) algebra. Namely, Eq. (3) allows us to identify the G_a's with the basis vectors of the SU(2) algebra and the Poisson bracket with the commutator. We can now make use of the fact that for all semisimple Lie groups the Casimir operators together with the basis of the Cartan subalgebra span an Abelian subspace of the enveloping algebra. With higher-dimensional Lie groups this Abelian subspace can be augmented by Casimir operators of some lower-dimensional subalgebras. Since all canonical momenta must have vanishing Poisson brackets with each other, we see that the maximal set of momenta can be obtained from the maximal Abelian subspace of the enveloping algebra. This is the idea behind the transformation (7), where we now recognize p_1^2 as the Casimir operator of SU(2) and p_2 as the usual basis vector for the Cartan subalgebra. Once this choice has been made, the form of q_2 follows from the consistency of the canonical Poisson brackets with the algebra (3). However, the fundamental Poisson bracket relations do not determine the canonical conjugate of p_1 uniquely and we can thus leave the specific form of q_1 open at this stage. The next step is to extend the transformation (7) to the remaining variables.

B. Gauge-invariant variables

Let ξ_i stand for any new canonical variable not equal to those already fixed. By the requirement that the Poisson brackets between ξ_i and the members of the set $\{q_1, p_1, q_2, p_2\}$ vanish and with the help of the parametrization (6) we see that

$$\{G_a(\mathbf{x}),\xi_i(\mathbf{y})\}=0, \quad a=1,2,3, \tag{8a}$$

$$\frac{\delta\xi_i(\mathbf{y})}{\delta p_1(\mathbf{x})}=0. \tag{8b}$$

In particular, Eq. (8a) means that all the remaining variables must be invariant under topologically trivial gauge transformations. Since we have already defined three non-gauge-invariant variables (q_1,q_2,p_2), they completely fix the gauge angles (modulo constant gauge transformations) in the new set of variables. The gauge-invariant fields must therefore be constructed by transforming the old variables into a gauge where q_1, q_2, and p_2 are absent. Note that the term "gauge" does not imply neglecting any dynamical degrees of freedom at this stage, it only describes the way that the gauge-invariant variables of the new set are formed. In other words, the new variables consist of both gauge-dependent and gauge-invariant degrees of freedom. Although it may sound a little paradoxical, the gauge-invariant variables also satisfy a gauge condition due to the fact that, by construction, the gauge-dependent degrees of freedom have been transformed away. (This procedure is discussed in a more general context in Ref. 4.)

Let us begin with the elimination of q_2 and p_2. When these variables tend to zero, Eq. (6) shows that the components G_a tend to $\delta_{a1}p_1$. The intermediate variables $\hat{A}_k^a$ and $\hat{\Pi}_{ka}$ are then determined by the requirement that this property holds exactly, i.e.,

$$\begin{aligned}\hat{A}_k^a &= (O_1)^a{}_b A_k^b - \frac{1}{2g}\varepsilon_{bc}{}^a\left(O_1\partial_k O_1^T\right)^{cb},\\ \hat{\Pi}_{ka} &= (O_1)_a{}^b \Pi_{kb},\end{aligned} \tag{9}$$

where the orthogonal matrix O_1 satisfies the relation

$$\hat{G}_a=(O_1)_a{}^b G_b=\delta_{a1}p_1. \tag{10}$$

This is clearly fulfilled if we take

$$O_1=\begin{pmatrix} \sqrt{1-\left(\frac{p_2}{p_1}\right)^2}\cos(gq_2) & -\sqrt{1-\left(\frac{p_2}{p_1}\right)^2}\sin(gq_2) & \frac{p_2}{p_1} \\ \frac{p_2}{p_1}\cos(gq_2) & -\frac{p_2}{p_1}\sin(gq_2) & -\sqrt{1-\left(\frac{p_2}{p_1}\right)^2} \\ \sin(gq_2) & \cos(gq_2) & 0 \end{pmatrix} \tag{11a}$$

$$=\begin{pmatrix} \frac{G_1}{\sqrt{G_1^2+G_2^2+G_3^2}} & \frac{G_2}{\sqrt{G_1^2+G_2^2+G_3^2}} & \frac{G_3}{\sqrt{G_1^2+G_2^2+G_3^2}} \\ \frac{G_1G_3}{\sqrt{G_1^2+G_2^2}\sqrt{G_1^2+G_2^2+G_3^2}} & \frac{G_2G_3}{\sqrt{G_1^2+G_2^2}\sqrt{G_1^2+G_2^2+G_3^2}} & -\frac{\sqrt{G_1^2+G_2^2}}{\sqrt{G_1^2+G_2^2+G_3^2}} \\ -\frac{G_2}{\sqrt{G_1^2+G_2^2}} & \frac{G_1}{\sqrt{G_1^2+G_2^2}} & 0 \end{pmatrix}. \tag{11b}$$

It is interesting to note that the condition (10) falls in the category of Abelian gauges,[15] where the gauge is partially fixed by diagonalizing some homogeneously transforming object. In our case this object is the Gauss law generator $G=G^aT_a$, which is transformed into the direction of T_1. The residual U(1) gauge transformations are generated by T_1, and Eq. (10) then suggests that q_1 and p_1 are associated with this gauge freedom. More precisely, using the inverse formula (7) together with the properties (4) we can calculate the brackets

$$\{p_1(\mathbf{x}),\widehat{A}^a_k(\mathbf{y})\} = -\,\delta^a{}_1\partial^{(x)}_k\delta(\mathbf{x}-\mathbf{y}) - g\varepsilon_{b1}{}^a\widehat{A}^b_k(\mathbf{y})\,\delta(\mathbf{x}-\mathbf{y}),$$
$$\{p_1(\mathbf{x}),\widehat{\Pi}_{ka}(\mathbf{y})\} = -\,g\varepsilon^b{}_{1a}\widehat{\Pi}_{kb}(\mathbf{y})\,\delta(\mathbf{x}-\mathbf{y}), \tag{12}$$

which prove that p_1 indeed generates U(1) rotations in the direction of T_1. On the other hand,

$$\{p_1(\mathbf{x}),\widehat{A}^a_k(\mathbf{y})\} = -\,\frac{\delta\widehat{A}^a_k(\mathbf{y})}{\delta q_1(\mathbf{x})}, \quad \{p_1(\mathbf{x}),\widehat{\Pi}_{ka}(\mathbf{y})\} = -\,\frac{\delta\widehat{\Pi}_{ka}(\mathbf{y})}{\delta q_1(\mathbf{x})},$$

and combining these equations with the brackets (12) we get the following functional differential equations for the fields $\widehat{A}^a_k$ and $\widehat{\Pi}_{ka}$:

$$\frac{\delta\widehat{A}^a_k(\mathbf{y})}{\delta q_1(\mathbf{x})} = \delta^a{}_1\partial^{(x)}_k\delta(\mathbf{x}-\mathbf{y}) + g\varepsilon_{b1}{}^a\widehat{A}^b_k(\mathbf{y})\,\delta(\mathbf{x}-\mathbf{y}),$$

$$\frac{\delta\widehat{\Pi}_{ka}(\mathbf{y})}{\delta q_1(\mathbf{x})} = g\varepsilon^b{}_{1a}\widehat{\Pi}_{kb}(\mathbf{y})\,\delta(\mathbf{x}-\mathbf{y}).$$

Given that these equations hold, it is then easy to see that new fields $\mathcal{A}^a_k$ and π_{ka} defined by

$$\mathcal{A}^a_k = (O_2)^a{}_b\widehat{A}^b_k - \frac{1}{2g}\varepsilon_{bc}{}^a\left(O_2\partial_k O_2^T\right)^{cb},$$
$$\pi_{ka} = (O_2)_a{}^b\widehat{\Pi}_{kb}, \tag{13}$$

$$O_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(gq_1) & -\sin(gq_1) \\ 0 & \sin(gq_1) & \cos(gq_1) \end{pmatrix} \tag{14}$$

are independent of q_1, i.e.,

$$\frac{\delta\mathcal{A}^a_k(\mathbf{y})}{\delta q_1(\mathbf{x})} = 0, \quad \frac{\delta\pi_{ka}(\mathbf{y})}{\delta q_1(\mathbf{x})} = 0. \tag{15}$$

Combining the transformations (9) and (13) we can express the new variables in terms of the original fields A^a_k, Π_{ka} and the variables $\{q_1,p_1,q_2,p_2\}$. Employing formulas (4) and (6) together with the identity

$$\{G_a(\mathbf{x}),q_1(\mathbf{y})\} = -\,\frac{\delta G_a(\mathbf{x})}{\delta p_1(\mathbf{y})}$$

it is then a straightforward albeit rather lengthy exercise to check that the new variables are really gauge invariant,

$$\{G_a(\mathbf{x}),\mathcal{A}^b_k(\mathbf{y})\} = 0, \quad \{G_a(\mathbf{x}),\pi_{kb}(\mathbf{y})\} = 0.$$

The requirement (8a) is thus satisfied, but this is not yet sufficient to make $\mathcal{A}^a_k$ and π_{ka} independent of p_1. Moreover, the new fields are redundant in number, because they satisfy the relation

$$\mathcal{G}_a = \partial^k\pi_{ka} - g\varepsilon_b{}^c{}_a\mathcal{A}^{kb}\pi_{kc} = \delta_{a1}p_1, \tag{16}$$

which is actually more like a functional identity rather than a constraint, because it follows immediately from the transformations (9) and (13). Finally, $\mathcal{A}^a_k$ and π_{ka} are not canonical variables

due to the fact that the gauge transformation matrices (11) and (14) depend on the original fields. Employing the fundamental Poisson brackets of the original variables and the gauge transformation properties (4) it is relatively straightforward to work out the brackets of $\mathcal{A}_k^a$ and π_{ka}, but the calculations are lengthy. In fact, it becomes almost inevitable to use computer software capable of symbolic manipulations to perform these extensive calculations. Eventually we obtain the following result:

$$\begin{aligned}\{\mathcal{A}_k^a(\mathbf{x}),\pi_{lb}(\mathbf{y})\} &= \frac{1}{p_1(\mathbf{y})}\left[\delta^a{}_b\pi_{l1}(\mathbf{y})-\delta_{b1}\pi_l^a(\mathbf{y})\right]\partial_k^{(x)}\delta(\mathbf{x}-\mathbf{y})\\ &\quad+\left[\frac{g}{2p_1(\mathbf{y})}\left(\delta^a{}_1\varepsilon_{bc}{}^d+\delta_{b1}\varepsilon^a{}_c{}^d+\delta^d{}_1\varepsilon^a{}_{bc}+\delta_{c1}\varepsilon^a{}_b{}^d\right)\mathcal{A}_k^c(\mathbf{y})\pi_{ld}(\mathbf{y})+\delta_{kl}\delta^a{}_b\right]\delta(\mathbf{x}-\mathbf{y})\\ &\quad+\left[\delta^a{}_1\partial_k^{(x)}-g\varepsilon_{c1}{}^a\mathcal{A}_k^c(\mathbf{x})\right]\frac{\delta\pi_{lb}(\mathbf{y})}{\delta p_1(\mathbf{x})}+g\varepsilon^c{}_{1b}\pi_{lc}(\mathbf{y})\frac{\delta\mathcal{A}_k^a(\mathbf{x})}{\delta p_1(\mathbf{y})},\end{aligned}\tag{17a}$$

$$\begin{aligned}\{\mathcal{A}_k^a(\mathbf{x}),\mathcal{A}_l^b(\mathbf{y})\} &= \frac{1}{g}\varepsilon_1{}^{ab}\partial_l^{(y)}\left[\frac{1}{p_1(\mathbf{y})}\partial_k^{(x)}\delta(\mathbf{x}-\mathbf{y})\right]+\frac{1}{p_1(\mathbf{y})}\left[\delta^{ab}\mathcal{A}_{l1}(\mathbf{y})-\delta^b{}_1\mathcal{A}_l^a(\mathbf{y})\right]\partial_k^{(x)}\delta(\mathbf{x}-\mathbf{y})\\ &\quad-\partial_l^{(y)}\left[\frac{1}{p_1(\mathbf{y})}\left(\delta^{ab}\mathcal{A}_{k1}(\mathbf{y})-\delta^a{}_1\mathcal{A}_k^b(\mathbf{y})\right)\delta(\mathbf{x}-\mathbf{y})\right]\\ &\quad+\frac{g}{2p_1(\mathbf{y})}\left(\delta^a{}_1\varepsilon^b{}_{cd}+\delta^b{}_1\varepsilon^a{}_{cd}+\delta_{d1}\varepsilon^{ab}{}_c+\delta_{c1}\varepsilon^{ab}{}_d\right)\mathcal{A}_k^c(\mathbf{y})\mathcal{A}_l^d(\mathbf{y})\delta(\mathbf{x}-\mathbf{y})\\ &\quad+\left[\delta^a{}_1\partial_k^{(x)}-g\varepsilon_{c1}{}^a\mathcal{A}_k^c(\mathbf{x})\right]\frac{\delta\mathcal{A}_l^b(\mathbf{y})}{\delta p_1(\mathbf{x})}-\left[\delta^b{}_1\partial_l^{(y)}-g\varepsilon_{c1}{}^b\mathcal{A}_l^c(\mathbf{y})\right]\frac{\delta\mathcal{A}_k^a(\mathbf{x})}{\delta p_1(\mathbf{y})},\end{aligned}\tag{17b}$$

$$\begin{aligned}\{\pi_{ka}(\mathbf{x}),\pi_{lb}(\mathbf{y})\} &= \frac{g}{2p_1(\mathbf{y})}\left(\delta_{a1}\varepsilon_b{}^{cd}+\delta_{b1}\varepsilon_a{}^{cd}+\delta^d{}_1\varepsilon_{ab}{}^c+\delta^c{}_1\varepsilon_{ab}{}^d\right)\pi_{kc}(\mathbf{y})\pi_{ld}(\mathbf{y})\delta(\mathbf{x}-\mathbf{y})\\ &\quad-g\varepsilon^c{}_{1a}\pi_{kc}(\mathbf{x})\frac{\delta\pi_{lb}(\mathbf{y})}{\delta p_1(\mathbf{x})}+g\varepsilon^c{}_{1b}\pi_{lc}(\mathbf{y})\frac{\delta\pi_{ka}(\mathbf{x})}{\delta p_1(\mathbf{y})}.\end{aligned}\tag{17c}$$

As there are redundant coordinates in this set of variables, we should verify that these brackets are compatible with (16). Indeed, starting from the brackets (17) it is possible to derive the result

$$\{\mathcal{G}_a(\mathbf{x}),\mathcal{A}_k^b(\mathbf{y})\}=0,\quad \{\mathcal{G}_a(\mathbf{x}),\pi_{kb}(\mathbf{y})\}=0,$$

which is consistent with (15) and (16). Our next task is to parametrize $\mathcal{A}_k^a$ and π_{ka} with new canonical variables in such a way that the relations (16) and (17) are satisfied.

C. Canonical variables

The elimination of the residual U(1) gauge degree of freedom with the transformation (13) was rather symbolic by nature, because the form of q_1 was not specified. The advantage of doing so is the fact that the Poisson brackets (17) now hold for all possible U(1) gauges and we can thus experiment with different gauge choices. Once a choice is made, its consistency with the brackets (17) then yields equations that determine the p_1 dependence of $\mathcal{A}_k^a$ and π_{ka}. The ingredients for choosing the gauge can be read off from the transformation formula (13). It is seen that the available objects fall in three categories, where the pairs $(\hat{A}_k^2,\hat{A}_k^3)$ and $(\hat{\Pi}_{k2},\hat{\Pi}_{k3})$ form SO(2) doublets, the components $\hat{\Pi}_{k1}$ are invariant and $\hat{A}_k^1$ transforms as a photon. Although every gauge is possible from the physical point of view, yet in practice some gauges are not manifestly compatible with the brackets (17). For example, in the Coulomb gauge we should choose q_1 in such a way that the equation $\partial^k\mathcal{A}_k^1=0$ would hold as a functional identity, as indicated by (15).

Therefore the Poisson brackets $\{\partial^k \mathcal{A}_k^1(\mathbf{x}), \partial^l \mathcal{A}_l^1(\mathbf{y})\}$ should also vanish identically, but according to the relations (17b) this is not the case. Probably this contradiction stems from the canonical structure of the variables already fixed, and the problem could possibly be circumvented by adjusting q_1 and the definitions (7) suitably.

In the following calculations the unitary gauge

$$\pi_{12}(\mathbf{x}) = 0$$

will be employed. Its consistency with the resulting identity $\{\pi_{12}(\mathbf{x}), \pi_{12}(\mathbf{y})\}=0$ is obvious and it corresponds to defining q_1 by

$$q_1 = \frac{2}{g} \arctan\left(\frac{\sqrt{\widehat{\Pi}_{12}^2 + \widehat{\Pi}_{13}^2} - \widehat{\Pi}_{13}}{\widehat{\Pi}_{12}} \right). \tag{18}$$

Using formulas (4), (7), and (11b) it is a straightforward but lengthy calculation to verify that the fundamental Poisson bracket relations between q_1 and the variables $\{p_1, q_2, p_2\}$ indeed hold. Now the functional identities

$$\{\mathcal{A}_k^a(\mathbf{x}), \pi_{12}(\mathbf{y})\} = 0, \quad \{\pi_{ka}(\mathbf{x}), \pi_{12}(\mathbf{y})\} = 0$$

combined with the brackets (17) give the following equations:

$$\frac{\delta \mathcal{A}_k^a(\mathbf{x})}{\delta p_1(\mathbf{y})} = -\frac{1}{g p_1(\mathbf{y})} \frac{\pi_{11}(\mathbf{y})}{\pi_{13}(\mathbf{y})} \delta^a{}_2 \partial_k^{(x)} \delta(\mathbf{x}-\mathbf{y}) + \frac{1}{\pi_{13}(\mathbf{y})} \left(\frac{\pi_{11}(\mathbf{y})}{p_1(\mathbf{y})} \varepsilon_{b2}{}^a \mathcal{A}_k^b(\mathbf{y}) - \frac{1}{g} \delta_{k1} \delta^a{}_2 \right) \delta(\mathbf{x}-\mathbf{y}),$$

$$\frac{\delta \pi_{ka}(\mathbf{x})}{\delta p_1(\mathbf{y})} = \frac{1}{p_1(\mathbf{y})} \frac{\pi_{11}(\mathbf{y})}{\pi_{13}(\mathbf{y})} \varepsilon^b{}_{2a} \pi_{kb}(\mathbf{y}) \delta(\mathbf{x}-\mathbf{y}).$$

At first sight these equations look a bit frightening, but they turn out to be solvable with a reasonable effort. The solution can be written as a gauge transformation in the direction of T_2,

$$\mathcal{A}_k^a = (O_3)^a{}_b \left(\mathcal{Q}_k^b - \frac{1}{g} \delta_{k1} \delta^b{}_2 \frac{p_1}{\mathcal{P}_{11}} \cos\phi \right) - \frac{1}{2g} \varepsilon_{bc}{}^a \left(O_3 \partial_k O_3^T \right)^{cb},$$
$$\pi_{ka} = (O_3)_a{}^b \mathcal{P}_{kb}, \tag{19}$$

with

$$O_3 = \begin{pmatrix} \sin\phi & 0 & -\cos\phi \\ 0 & -1 & 0 \\ -\cos\phi & 0 & -\sin\phi \end{pmatrix},$$
$$\sin\phi = \frac{\beta}{p_1}, \tag{20}$$

where $\mathcal{Q}_k^a$, $\mathcal{P}_{ka}$, and β are constants of integration, i.e.,

$$\frac{\delta \mathcal{Q}_k^a(\mathbf{x})}{\delta p_1(\mathbf{y})} = 0, \quad \frac{\delta \mathcal{P}_{ka}(\mathbf{x})}{\delta p_1(\mathbf{y})} = 0, \quad \frac{\delta \beta(\mathbf{x})}{\delta p_1(\mathbf{y})} = 0,$$

and

$$\mathcal{P}_{12}(\mathbf{x}) = \mathcal{P}_{13}(\mathbf{x}) = 0. \tag{21}$$

These constant fields fulfill both of the requirements (8), and therefore they should be adopted as new variables. The transformation formula is the inverse of (19), that is,

$$\begin{gathered}\mathcal{Q}_k^a = (O_3)^a{}_b\left(\mathcal{A}_k^b + \frac{1}{g}\delta_{k1}\delta^b{}_2 p_1 \frac{\pi_{13}}{\pi_{11}^2 + \pi_{13}^2}\right) - \frac{1}{2g}\varepsilon_{bc}{}^a\left(O_3\partial_k O_3^T\right)^{cb}, \\ \mathcal{P}_{ka} = (O_3)_a{}^b\pi_{kb},\end{gathered} \tag{22}$$

where we now write the gauge angle as

$$\sin\phi = \frac{\pi_{11}}{\sqrt{\pi_{11}^2 + \pi_{13}^2}}, \quad \cos\phi = -\frac{\pi_{13}}{\sqrt{\pi_{11}^2 + \pi_{13}^2}}. \tag{23}$$

Note that the matrix O_3 is both orthogonal and symmetric.

In order to proceed towards our final canonical transformation we must now find out whether the newest set of variables can be made canonical in accordance with the relation (16). Using (19) it is easy to see that the corresponding relation in the new variables reads

$$\partial^k\mathcal{P}_{ka} - g\varepsilon_b{}^c{}_a\mathcal{Q}^{kb}\mathcal{P}_{kc} = \delta_{a1}\beta. \tag{24}$$

The Poisson brackets are evaluated by inserting expressions (22) into the relations (17). Again this is a formidable calculation which requires extensive use of computer software. Here is the result,

$$\begin{gathered}\{\mathcal{Q}_k^a(\mathbf{x}), \mathcal{P}_{lb}(\mathbf{y})\} = \delta_{kl}\delta^a{}_b\delta(\mathbf{x}-\mathbf{y}), \quad k \neq 1, \\ \{\mathcal{Q}_1^a(\mathbf{x}), \mathcal{P}_{11}(\mathbf{y})\} = \delta^a{}_1\delta(\mathbf{x}-\mathbf{y}), \\ \{\mathcal{Q}_1^a(\mathbf{x}), \mathcal{P}_{lb}(\mathbf{y})\} = -\frac{1}{\mathcal{P}_{11}(\mathbf{y})}\left[\delta^a{}_b\mathcal{P}_{l1}(\mathbf{y}) - \delta_{b1}\mathcal{P}_l^a(\mathbf{y})\right]\delta(\mathbf{x}-\mathbf{y}), \quad l \neq 1, \\ \{\mathcal{Q}_k^a(\mathbf{x}), \mathcal{Q}_l^b(\mathbf{y})\} = 0, \quad k \neq 1, \quad l \neq 1, \\ \{\mathcal{Q}_k^a(\mathbf{x}), \mathcal{Q}_1^b(\mathbf{y})\} = -\frac{1}{g}\varepsilon_1{}^{ab}\frac{1}{\mathcal{P}_{11}(\mathbf{y})}\partial_k^{(x)}\delta(\mathbf{x}-\mathbf{y}) + \frac{1}{\mathcal{P}_{11}(\mathbf{y})}\left[\delta^{ab}\mathcal{Q}_{k1}(\mathbf{y}) - \delta^a{}_1\mathcal{Q}_k^b(\mathbf{y})\right]\delta(\mathbf{x}-\mathbf{y}), \quad k \neq 1,\end{gathered} \tag{25}$$

$$\begin{gathered}\{\mathcal{Q}_1^a(\mathbf{x}), \mathcal{Q}_1^b(\mathbf{y})\} = -\frac{1}{\mathcal{P}_{11}(\mathbf{y})}\left[\delta^a{}_1\mathcal{Q}_1^b(\mathbf{y}) - \delta^b{}_1\mathcal{Q}_1^a(\mathbf{y}) + \frac{1}{g}\varepsilon_1{}^{ab}\frac{\beta(\mathbf{y}) - \partial_1^{(y)}\mathcal{P}_{11}(\mathbf{y})}{\mathcal{P}_{11}(\mathbf{y})}\right]\delta(\mathbf{x}-\mathbf{y}), \\ \{\mathcal{P}_{ka}(\mathbf{x}), \mathcal{P}_{lb}(\mathbf{y})\} = 0, \\ \{\beta(\mathbf{x}), \mathcal{Q}_k^a(\mathbf{y})\} = -\delta^a{}_1\partial_k^{(x)}\delta(\mathbf{x}-\mathbf{y}) - g\varepsilon_{b1}{}^a\mathcal{Q}_k^b(\mathbf{y})\,\delta(\mathbf{x}-\mathbf{y}), \\ \{\beta(\mathbf{x}), \mathcal{P}_{ka}(\mathbf{y})\} = -g(1-\delta_{k1})\varepsilon^b{}_{1a}\mathcal{P}_{kb}(\mathbf{y})\,\delta(\mathbf{x}-\mathbf{y}).\end{gathered}$$

Remember that $\mathcal{P}_{12}=\mathcal{P}_{13}=0$ in these relations. It is now easy to construct the desired canonical fields. The brackets (25) suggest that we choose the pairs

$$(\mathcal{Q}_1^1, \mathcal{P}_{11}), \quad (\mathcal{Q}_k^a, \mathcal{P}_{ka}), \quad k \neq 1 \tag{26}$$

as canonically conjugate variables. If we then solve the remaining variables from Eq. (24),

$$\beta = \partial_1 \mathcal{P}_{11} + \sum_{k=2}^{3} \left(\partial_k \mathcal{P}_{k1} - g\varepsilon_b{}^c{}_1 \mathcal{Q}_k^b \mathcal{P}_{kc} \right), \tag{27a}$$

$$\mathcal{Q}_1^2 = -\frac{1}{g\mathcal{P}_{11}} \sum_{k=2}^{3} \left(\partial_k \mathcal{P}_{k3} - g\varepsilon_b{}^c{}_3 \mathcal{Q}_k^b \mathcal{P}_{kc} \right), \tag{27b}$$

$$\mathcal{Q}_1^3 = \frac{1}{g\mathcal{P}_{11}} \sum_{k=2}^{3} \left(\partial_k \mathcal{P}_{k2} - g\varepsilon_b{}^c{}_2 \mathcal{Q}_k^b \mathcal{P}_{kc} \right), \tag{27c}$$

it turns out that all the Poisson brackets in the set (25) involving these variables follow from the fundamental brackets of the pairs (26). Unfortunately the variables (26), although gauge-invariant and canonical, are still not useful for implementing the Gauss law. The reason is Eq. (20), which shows that β tends to zero in the limit when p_1 vanishes. Looking at expression (27a), we see that it would be difficult to implement the requirement $\beta \to 0$ using the variables (26). A suitable canonical transformation is needed.

D. Canonical U(1) transformation

Passing to the variables (26), we have replaced the original SU(2) fields with a set of gauge-invariant canonical fields. However, the Poisson brackets (25) show that these variables have an inner U(1) symmetry, which is generated by β. Note that this symmetry has nothing to do with the original SU(2) symmetry since all the variables (26) and the generator β, defined by Eq. (27a), are gauge invariant with respect to the generators G_a. Even so, we can apply the procedures of Secs. II A–II C also to this U(1) symmetry and choose β as a new canonical momentum variable, i.e.,

$$p_3 = \partial_1 \mathcal{P}_{11} + \sum_{k=2}^{3} \left(\partial_k \mathcal{P}_{k1} - g\varepsilon_b{}^c{}_1 \mathcal{Q}_k^b \mathcal{P}_{kc} \right). \tag{28}$$

The canonical conjugate of p_3 then determines the gauge angle associated with transformations generated by p_3, but again we leave the specific form of q_3 open at this stage. Since both q_3 and p_3 must have vanishing Poisson brackets with the remaining variables of the final canonical set, we conclude that the remaining variables must be functionally independent of q_3 and p_3. The elimination of q_3 can be done, as before, with a gauge transformation in the T_1 direction,

$$\begin{aligned} \widehat{\mathcal{Q}}_k^a &= (O_4)^a{}_b \mathcal{Q}_k^b - \frac{1}{2g} \varepsilon_{bc}{}^a \left(O_4 \partial_k O_4^T \right)^{cb}, \\ \widehat{P}_{ka} &= (O_4)_a{}^b \mathcal{P}_{kb}, \end{aligned} \tag{29}$$

where

$$O_4 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(gq_3) & -\sin(gq_3) \\ 0 & \sin(gq_3) & \cos(gq_3) \end{pmatrix}.$$

The Poisson brackets of the new variables follow from the algebra (25), the result being

$$\{\widehat{Q}_k^a(\mathbf{x}),\widehat{P}_{lb}(\mathbf{y})\}=\delta_{kl}\delta^a{}_b\delta(\mathbf{x}-\mathbf{y})+\left[\delta^a{}_1\partial_k^{(x)}-g\varepsilon_{c1}{}^a\widehat{Q}_k^c(\mathbf{x})\right]\frac{\delta\widehat{P}_{lb}(\mathbf{y})}{\delta p_3(\mathbf{x})}+g\varepsilon^c{}_{1b}\widehat{P}_{lc}(\mathbf{y})\frac{\delta\widehat{Q}_k^a(\mathbf{x})}{\delta p_3(\mathbf{y})},$$

$$\{\widehat{Q}_k^a(\mathbf{x}),\widehat{Q}_l^b(\mathbf{y})\}=\left[\delta^a{}_1\partial_k^{(x)}-g\varepsilon_{c1}{}^a\widehat{Q}_k^c(\mathbf{x})\right]\frac{\delta\widehat{Q}_l^b(\mathbf{y})}{\delta p_3(\mathbf{x})}-\left[\delta^b{}_1\partial_l^{(y)}-g\varepsilon_{c1}{}^b\widehat{Q}_l^c(\mathbf{y})\right]\frac{\delta\widehat{Q}_k^a(\mathbf{x})}{\delta p_3(\mathbf{y})},\tag{30}$$

$$\{\widehat{P}_{ka}(\mathbf{x}),\widehat{P}_{lb}(\mathbf{y})\}=-g\varepsilon^c{}_{1a}\widehat{P}_{kc}(\mathbf{x})\frac{\delta\widehat{P}_{lb}(\mathbf{y})}{\delta p_3(\mathbf{x})}+g\varepsilon^c{}_{1b}\widehat{P}_{lc}(\mathbf{y})\frac{\delta\widehat{P}_{ka}(\mathbf{x})}{\delta p_3(\mathbf{y})}.$$

For the sake of clarity only those brackets have been written down that hold for the actual variables

$$(\widehat{Q}_1^1,\widehat{P}_{11}),\quad(\widehat{Q}_k^a,\widehat{P}_{ka}),\quad k\neq 1.$$

In order to define variables independent of p_3 we must now specify the U(1) gauge by fixing q_3. In the following we choose

$$q_3=\frac{2}{g}\arctan\left(\frac{\sqrt{\mathcal{P}_{22}^2+\mathcal{P}_{23}^2}-\mathcal{P}_{23}}{\mathcal{P}_{22}}\right),\tag{31}$$

which corresponds to the identity

$$\widehat{P}_{22}(\mathbf{x})=0.\tag{32}$$

Making use of the brackets (25) it is possible to verify that q_3 and p_3 indeed satisfy

$$\{q_3(\mathbf{x}),p_3(\mathbf{y})\}=\delta(\mathbf{x}-\mathbf{y}),$$

while their brackets with the variables $\{q_1,p_1,q_2,p_2\}$ vanish due to the fact that both $\mathcal{Q}_k^a$ and $\mathcal{P}_{ka}$ meet the requirements (8). As before, the functional identities

$$\{\widehat{Q}_k^a(\mathbf{x}),\widehat{P}_{22}(\mathbf{y})\}=0,\quad\{\widehat{P}_{ka}(\mathbf{x}),\widehat{P}_{22}(\mathbf{y})\}=0$$

lead to the equations

$$\frac{\delta\widehat{Q}_k^a(\mathbf{x})}{\delta p_3(\mathbf{y})}=-\frac{1}{g\widehat{P}_{23}(\mathbf{y})}\delta_{k2}\delta^a{}_2\delta(\mathbf{x}-\mathbf{y}),$$

$$\frac{\delta\widehat{P}_{ka}(\mathbf{x})}{\delta p_3(\mathbf{y})}=0,$$

whose solutions read

$$\widehat{Q}_k^a=Q_k^a-\frac{1}{g}\delta_{k2}\delta^a{}_2\frac{p_3}{P_{23}},$$
$$\widehat{P}_{ka}=P_{ka},\tag{33}$$

where Q_k^a and P_{ka} are constants of integration, i.e.,

$$\frac{\delta Q_k^a(\mathbf{x})}{\delta p_3(\mathbf{y})} = 0, \quad \frac{\delta P_{ka}(\mathbf{x})}{\delta p_3(\mathbf{y})} = 0.$$

Now we choose these constants as new variables. Equation (28) then leads to the relation

$$\partial_1 P_{11} + \sum_{k=2}^{3} \left(\partial_k P_{k1} - g\varepsilon_b{}^c{}_1 Q_k^b P_{kc} \right) = 0, \tag{34}$$

which holds as a functional identity, implying that the new variables contain one redundant coordinate. The Poisson brackets of Q_k^a and P_{ka} are easily evaluated with the help of the relations (30). The result reads

$$\{Q_k^a(\mathbf{x}), P_{lb}(\mathbf{y})\} = \delta_{kl}\delta^a{}_b \delta(\mathbf{x}-\mathbf{y}) - \delta_{k2}\delta^a{}_2 \varepsilon^c{}_{1b} \frac{1}{P_{23}(\mathbf{y})} P_{lc}(\mathbf{y})\, \delta(\mathbf{x}-\mathbf{y}),$$

$$\{Q_k^a(\mathbf{x}), Q_l^b(\mathbf{y})\} = 0, \quad (k,a) \neq (2,2), \quad (l,b) \neq (2,2),$$

$$\{Q_k^a(\mathbf{x}), Q_2^2(\mathbf{y})\} = -\frac{1}{gP_{23}(\mathbf{y})} \left[\delta^a{}_1 \partial_k^{(x)} - g\varepsilon_{c1}{}^a Q_k^c(\mathbf{x}) \right] \delta(\mathbf{x}-\mathbf{y}), \quad (k,a) \neq (2,2), \tag{35}$$

$$\{Q_2^2(\mathbf{x}), Q_2^2(\mathbf{y})\} = 0,$$

$$\{P_{ka}(\mathbf{x}), P_{lb}(\mathbf{y})\} = 0,$$

showing that the pairs

$$(Q_1^1, P_{11}), \quad (Q_2^a, P_{2a}), \quad a = 1,3, \quad (Q_3^a, P_{3a}), \quad a = 1,2,3$$

are the most natural choice for final canonical variables. Solving (34) for the redundant coordinate,

$$Q_2^2 = \frac{1}{gP_{23}} \left(\partial^k P_{k1} - g\varepsilon_b{}^c{}_1 Q_3^b P_{3c} \right), \tag{36}$$

it is easy to see that all of the Poisson bracket relations (35) hold true. Our search for suitable canonical variables is now over.

E. Results

Starting from the original canonical fields (A_k^a, Π_{ka}) and passing through four sets of intermediate variables we have found the final canonical pairs

$$\begin{gathered} (q_i, p_i), \quad i = 1,2,3, \\ (Q_1^1, P_{11}), \\ (Q_2^a, P_{2a}), \quad a = 1,3, \\ (Q_3^a, P_{3a}), \quad a = 1,2,3. \end{gathered} \tag{37}$$

Equation (7) relates p_1, q_2, and p_2 to the original variables, and a formula for q_1 is obtained by combining Eqs. (18), (9), and (11b). The momentum p_3 is most easily calculated by combining Eqs. (20), (23), (13), and (9), while it takes successive applications of Eqs. (31), (22), (13), and (9) to work out a formula for q_3. The remaining variables of the set (37) are then obtained by performing the transformations (33), (29), (22), (13), and (9) one after the other. Again the

manipulations are so lengthy that computer assistance is required. Introducing the notation

$$\|X\| := \sqrt{X_a X^a}$$

for the Lie algebra norm, the results can be written as follows:

$$q_1 = \frac{2}{g}\arctan\left(\frac{\sqrt{\widehat{\Pi}_{12}^2+\widehat{\Pi}_{13}^2}-\widehat{\Pi}_{13}}{\widehat{\Pi}_{12}}\right), \tag{38a}$$

$$\widehat{\Pi}_{12} = \frac{1}{\|G\|}\left[\frac{G_3}{\sqrt{G_1^2+G_2^2}}\left(G_1\Pi_{11}+G_2\Pi_{12}\right)-\sqrt{G_1^2+G_2^2}\Pi_{13}\right],$$

$$\widehat{\Pi}_{13} = \frac{1}{\sqrt{G_1^2+G_2^2}}\left(-G_2\Pi_{11}+G_1\Pi_{12}\right),$$

$$q_2 = -\frac{2}{g}\arctan\left(\frac{\sqrt{G_1^2+G_2^2}-G_1}{G_2}\right), \tag{38b}$$

$$q_3 = \frac{2}{g}\arctan\left(\frac{\sqrt{\mathcal{P}_{22}^2+\mathcal{P}_{23}^2}-\mathcal{P}_{23}}{\mathcal{P}_{22}}\right), \tag{38c}$$

$$\mathcal{P}_{22} = \frac{1}{\|\mathcal{N}\|}\varepsilon^{abc}G_a\Pi_{1b}\Pi_{2c},$$

$$\mathcal{P}_{23} = \frac{1}{\|\mathcal{N}\|}\frac{1}{\|\Pi_1\|}\left(\delta^{ad}\delta^{bc}-\delta^{ab}\delta^{cd}\right)G_a\Pi_{1b}\Pi_{1c}\Pi_{2d},$$

$$\mathcal{N}_a = \varepsilon_a{}^{bc}G_b\Pi_{1c},$$

$$p_1 = \|G\|, \tag{38d}$$

$$p_2 = G_3, \tag{38e}$$

$$p_3 = \frac{G^a\Pi_{1a}}{\|\Pi_1\|}, \tag{38f}$$

$$Q_k^a = \Omega^a{}_b A_k^b - \frac{1}{2g}\varepsilon_{bc}{}^a\left(\Omega\partial_k\Omega^T\right)^{cb}, \tag{38g}$$

$$P_{ka} = \Omega_a{}^b\Pi_{kb}, \tag{38h}$$

where

$$\Omega_a{}^b = \left(O_4O_3O_2O_1\right)_a{}^b$$

$$= \delta_{a1}\frac{1}{\|\Pi_1\|}\Pi_1^b + \delta_{a2}\frac{1}{\|N\|}\varepsilon^{bcd}\Pi_{2c}\Pi_{1d} + \delta_{a3}\frac{1}{\|\Pi_1\|}\frac{1}{\|N\|}\left(\delta^{be}\delta^{cd} - \delta^{bc}\delta^{de}\right)\Pi_{1c}\Pi_{1d}\Pi_{2e}, \tag{39}$$

$$N_a = \varepsilon_a{}^{bc}\Pi_{1b}\Pi_{2c}.$$

This transformation is singular when $||\Pi_1||$ or $||N||$ vanishes, corresponding to points where the gauge angles (23) and (38c) become ambiguous. These singularities are Gribov ambiguities[16] peculiar to unitary gauges, and it is well known that such ambiguities appear in almost every gauge.[17]

When inverting the transformation (38), it should be noted that formula (38g) holds for variables of the set (37) only. The general expression reads

$$Q_k^a + \frac{1}{g}\delta_{k1}(O_4)^a{}_2\frac{p_1}{P_{11}}\sqrt{1-\left(\frac{p_3}{p_1}\right)^2} - \frac{1}{g}\delta_{k2}\delta^a{}_2\frac{p_3}{P_{23}}$$

$$= \Omega^a{}_b A_k^b - \frac{1}{2g}\varepsilon_{bc}{}^a\left(\Omega\partial_k\Omega^T\right)^{cb}.$$

This equation determines the original gauge potential A_k^a as a function of the variables (37), provided that we use Eqs. (27), (36), (29), and (33) to define those components Q_k^a that are not regarded as free variables. In the same way we can invert the momentum transformation equation (38h), taking into account the definitions (21) and (32). The result is

$$A_k^a = \left(\Omega^T\right)^a{}_b\left(Q_k^b + \frac{1}{g}\delta_{k1}(O_4)^b{}_2\frac{p_1}{P_{11}}\sqrt{1-\left(\frac{p_3}{p_1}\right)^2} - \frac{1}{g}\delta_{k2}\delta^b{}_2\frac{p_3}{P_{23}}\right) - \frac{1}{2g}\varepsilon_{bc}{}^a\left(\Omega^T\partial_k\Omega\right)^{cb}, \tag{40a}$$

$$\Pi_{ka} = \left(\Omega^T\right)_a{}^b P_{kb}, \tag{40b}$$

where

$$Q_1^2 = -\frac{1}{gP_{11}}\sum_{k=2}^{3}\left(\partial_k P_{k3} - g\varepsilon_b{}^c{}_3 Q_k^b P_{kc}\right) + \frac{1}{g}p_3\frac{P_{21}}{P_{11}P_{23}},$$

$$Q_1^3 = \frac{1}{gP_{11}}\left(\partial_3 P_{32} - \sum_{k=2}^{3} g\varepsilon_b{}^c{}_2 Q_k^b P_{kc}\right),$$

$$Q_2^2 = \frac{1}{gP_{23}}\left(\partial^k P_{k1} - g\varepsilon_b{}^c{}_1 Q_3^b P_{3c}\right), \tag{41}$$

$$P_{12} = P_{13} = P_{22} = 0,$$

and Ω^T is expressed in the variables (q_i, p_i), i.e.,

$$\Omega^T = \begin{pmatrix} \sqrt{1-\left(\frac{p_2}{p_1}\right)^2}\cos(gq_2) & \frac{p_2}{p_1}\cos(gq_2) & \sin(gq_2) \\ -\sqrt{1-\left(\frac{p_2}{p_1}\right)^2}\sin(gq_2) & -\frac{p_2}{p_1}\sin(gq_2) & \cos(gq_2) \\ \frac{p_2}{p_1} & -\sqrt{1-\left(\frac{p_2}{p_1}\right)^2} & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(gq_1) & \sin(gq_1) \\ 0 & -\sin(gq_1) & \cos(gq_1) \end{pmatrix}$$
$$\times \begin{pmatrix} \frac{p_3}{p_1} & 0 & \sqrt{1-\left(\frac{p_3}{p_1}\right)^2} \\ 0 & -1 & 0 \\ \sqrt{1-\left(\frac{p_3}{p_1}\right)^2} & 0 & -\frac{p_3}{p_1} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(gq_3) & \sin(gq_3) \\ 0 & -\sin(gq_3) & \cos(gq_3) \end{pmatrix}.$$

The transformation equations can also be obtained from a generating functional of the form

$$F\left[p_1, q_2, p_3, \{Q_k^{a'}\}, \{\Pi_{ka}\}\right] = \int \mathcal{F}(\mathbf{x}) \mathrm{d}^3\mathbf{x}, \tag{42}$$

where

$$\mathcal{F} = \frac{2}{g}\eta p_1 \arctan\left(\frac{\sqrt{1-\left(\frac{p_3}{p_1}\right)^2}\|\Pi_1\| - \left[\Pi_{11}\sin(gq_2) + \Pi_{12}\cos(gq_2)\right]}{\sqrt{\Pi_{13}^2 - \left(\frac{p_3}{p_1}\right)^2\|\Pi_1\|^2 + \left[\Pi_{11}\cos(gq_2) - \Pi_{12}\sin(gq_2)\right]^2}} \right)$$
$$+ \frac{2}{g}p_3 \arctan\left(\left[\|\Pi_1\|\left[N_1\sin(gq_2) + N_2\cos(gq_2)\right]\sqrt{1-(p_3/p_1)^2} \right.\right.$$
$$\left. + \eta\|N\|\left[\Pi_{13}^2 - \left(\frac{p_3}{p_1}\right)^2\|\Pi_1\|^2 + \left[\Pi_{11}\cos(gq_2) - \Pi_{12}\sin(gq_2)\right]^2 \right]^{1/2} \right]$$
$$\times \left[\left(\sqrt{1-(p_3/p_1)^2}K_1 - \frac{p_3}{p_1}\|N\|\Pi_{11} \right)\sin(gq_2) \right.$$
$$\left. + \left(\sqrt{1-(p_3/p_1)^2}K_2 - \frac{p_3}{p_1}\|N\|\Pi_{12} \right)\cos(gq_2) \right] \Bigg/ \left[-(K_1^2 + K_2^2) + \left(\frac{p_3}{p_1}\right)^2\|\Pi_1\|^2 N_3^2 \right.$$
$$\left. + \left[K_1\cos(gq_2) - K_2\sin(gq_2)\right]^2 + \left(\frac{p_3}{p_1}\right)^2\|\Pi_1\|^2\left[N_1\cos(gq_2) - N_2\sin(gq_2)\right]^2 \right] \Bigg)$$
$$- Q^{ka'}\Omega_{a'}{}^{b}\Pi_{kb} + \frac{1}{2g}\varepsilon_{bc}{}^{a}\left(\Omega^T\partial_3\Omega\right)^{cb}\Pi_{3a} - \frac{1}{2g}\Pi_{11}N_1\partial_2\left(\frac{1}{\Pi_{12}^2 + \Pi_{13}^2}\right)$$
$$+ \frac{1}{g}\frac{\Pi_{21}(\Pi_{13}\partial_2\Pi_{12} - \Pi_{12}\partial_2\Pi_{13}) + \Pi_{11}(\Pi_{13}\partial_1\Pi_{12} - \Pi_{12}\partial_1\Pi_{13})}{\Pi_{12}^2 + \Pi_{13}^2}$$
$$- \frac{1}{g}\left[\partial_1\|\Pi_1\| + \partial_2\left(\|\Pi_1\|\frac{\Pi_{12}\Pi_{22} + \Pi_{13}\Pi_{23}}{\Pi_{12}^2 + \Pi_{13}^2} \right) \right]\arctan\left(\frac{K_1}{\|\Pi_1\|N_1} \right)$$

$$+\frac{1}{2g}\left[\partial_2\left(\frac{\Pi_{11}N_1}{\Pi_{12}^2+\Pi_{13}^2}\right)\right]\ln\left(\frac{\|N\|^2}{M^8}\right)$$

and

$$K_a=\varepsilon_a{}^{bc}\Pi_{1b}N_c=\left(\delta_a{}^c\delta^{bd}-\delta_a{}^d\delta^{bc}\right)\Pi_{1b}\Pi_{1c}\Pi_{2d}.$$

The components N_a are those defined in (39) and M denotes a constant with the dimension of energy. There is also a real phase η which can take the values ± 1. Expression (39) is used for the matrix Ω, and the primed index a' stands as a reminder of the fact that only independent components $Q_k^{a'}$, i.e., those included in the list (37) should be summed over. Now the transformation equations read

$$q_1(\mathbf{x})=\frac{\delta F}{\delta p_1(\mathbf{x})}, \tag{43a}$$

$$p_2(\mathbf{x})=-\frac{\delta F}{\delta q_2(\mathbf{x})}, \tag{43b}$$

$$q_3(\mathbf{x})=\frac{\delta F}{\delta p_3(\mathbf{x})}, \tag{43c}$$

$$P_{ka'}(\mathbf{x})=-\frac{\delta F}{\delta Q^{ka'}(\mathbf{x})}, \tag{43d}$$

$$A_k^a(\mathbf{x})=-\frac{\delta F}{\delta \Pi_a^k(\mathbf{x})}. \tag{43e}$$

Equations (43a)–(43c) reproduce Eqs. (38a), (38e), and (38c) in a form where the components G_a are expressed in the variables $\{p_1,q_2,p_3,\Pi_{1a}\}$ by inverting Eqs. (38d), (38b), and (38f), i.e.,

$$\begin{aligned}G_1=&\left(\frac{p_3}{p_1}\|\Pi_1\|\left[\Pi_{11}\cos(gq_2)-\Pi_{12}\sin(gq_2)\right]\right.\\&\left.-\eta\Pi_{13}\sqrt{\Pi_{13}^2-\left(\frac{p_3}{p_1}\right)^2\|\Pi_1\|^2+\left[\Pi_{11}\cos(gq_2)-\Pi_{12}\sin(gq_2)\right]^2}\right)\\&\times\frac{p_1\cos(gq_2)}{\Pi_{13}^2+\left[\Pi_{11}\cos(gq_2)-\Pi_{12}\sin(gq_2)\right]^2},\end{aligned}$$

$$\begin{aligned}G_2=&-\left(\frac{p_3}{p_1}\|\Pi_1\|\left[\Pi_{11}\cos(gq_2)-\Pi_{12}\sin(gq_2)\right]\right.\\&\left.-\eta\Pi_{13}\sqrt{\Pi_{13}^2-\left(\frac{p_3}{p_1}\right)^2\|\Pi_1\|^2+\left[\Pi_{11}\cos(gq_2)-\Pi_{12}\sin(gq_2)\right]^2}\right)\\&\times\frac{p_1\sin(gq_2)}{\Pi_{13}^2+\left[\Pi_{11}\cos(gq_2)-\Pi_{12}\sin(gq_2)\right]^2},\end{aligned} \tag{44}$$

$$\begin{aligned}G_3=&\left(\frac{p_3}{p_1}\|\Pi_1\|\Pi_{13}+\eta\left[\Pi_{11}\cos(gq_2)-\Pi_{12}\sin(gq_2)\right]\right.\\&\left.\times\sqrt{\Pi_{13}^2-\left(\frac{p_3}{p_1}\right)^2\|\Pi_1\|^2+\left[\Pi_{11}\cos(gq_2)-\Pi_{12}\sin(gq_2)\right]^2}\right)\\&\times\frac{p_1}{\Pi_{13}^2+\left[\Pi_{11}\cos(gq_2)-\Pi_{12}\sin(gq_2)\right]^2},\end{aligned}$$

where the sign η must be chosen so that

$$\left(\frac{p_3}{p_1}\|\Pi_1\|\left[\Pi_{11}\cos(gq_2)-\Pi_{12}\sin(gq_2)\right]\right.$$

$$\left.-\eta\Pi_{13}\sqrt{\Pi_{13}^2-\left(\frac{p_3}{p_1}\right)^2\|\Pi_1\|^2+\left[\Pi_{11}\cos(gq_2)-\Pi_{12}\sin(gq_2)\right]^2}\right)\geqslant 0.$$

Equations (43d) and (38h) are equivalent, and with the help of Eqs. (38c), (38h), and (44) it is also possible to see the equivalence of Eqs. (43e) and (40a). Although the generating functional looks rather complicated, its mere existence is sufficient to confirm that the transformation (38) is canonical. We have now all the necessary tools at hand for constructing the physical Hamiltonian.

III. PHYSICAL VARIABLES

The greatest advantage in passing to the new variables (37) is the fact that their behavior in the limit $G_a\to 0$ is relatively simple to analyze. Of course, if we were to be exact, we would have to specify this limit precisely by starting from Eq. (2) and then defining suitable norms and function spaces for the fields A_k^a and Π_{ka}. Instead of doing so let us adopt a physicist's point of view and assume that it does not matter much which particular function spaces we use if our fields are sufficiently smooth and vanish rapidly enough at infinity. Looking at Eqs. (38d)–(38f) we see then that Gauss's law is implemented in the new variables by setting

$$p_1=p_2=p_3=0. \tag{45}$$

That these constraints are preserved in time in the dynamics described by the Hamiltonian (1) is evident because p_1 and p_2 are constants of motion and $\dot{p}_3$ is proportional to the Gauss law generators. Equations (38a)–(38c) reveal similarly that the angles q_1, q_2, and q_3 become ambiguous when $G_a\to 0$ and therefore we must discard these variables as nonphysical. The physical variables are then the pairs $(Q_k^{a'},P_{ka'})$, as their defining equations (38g) and (38h) are independent of G_a. Since the generating functional (42) does not contain explicit time dependence, the dynamics of $Q_k^{a'}$ and $P_{ka'}$ is governed by the Hamiltonian (1) under the constraint (45), i.e.,

$$H_{\text{phys}}=H_{|p_1=p_2=p_3=0}.$$

A formula for the Hamiltonian (1) in the variables (37) is most easily obtained with the help of Eq. (40). Since the Hamiltonian is invariant under gauge transformations of this form, we immediately get the result

$$H=\int\left(\frac{1}{2}P_{ka}P^{ka}+\frac{1}{4}\widetilde{\Phi}_{kl}^a\widetilde{\Phi}_a^{kl}\right)d^3\mathbf{x},$$

where

$$\widetilde{\Phi}_{kl}^a=\partial_l\widetilde{Q}_k^a-\partial_k\widetilde{Q}_l^a+g\varepsilon_{bc}{}^a\widetilde{Q}_k^b\widetilde{Q}_l^c,$$

$$\widetilde{Q}_k^a=Q_k^a+\frac{1}{g}\delta_{k1}(O_4)^a{}_2\frac{p_1}{P_{11}}\sqrt{1-\left(\frac{p_3}{p_1}\right)^2}-\frac{1}{g}\delta_{k2}\delta^a{}_2\frac{p_3}{P_{23}},$$

and the definitions (41) are implied. Imposing the constraint (45), it is then easy to see that

$$H_{\text{phys}} = \int \left(\frac{1}{2} P_{ka} P^{ka} + \frac{1}{4} \Phi^a_{kl} \Phi^{kl}_a \right) d^3\mathbf{x}, \tag{46}$$

where

$$\Phi^a_{kl} = \partial_l Q^a_k - \partial_k Q^a_l + g \varepsilon_{bc}{}^a Q^b_k Q^c_l$$

and

$$\begin{aligned} Q^2_1 &= -\frac{1}{g P_{11}} \sum_{k=2}^{3} \left(\partial_k P_{k3} - g \varepsilon_b{}^c{}_3 Q^b_k P_{kc} \right), \\ Q^3_1 &= \frac{1}{g P_{11}} \left(\partial_3 P_{32} - \sum_{k=2}^{3} g \varepsilon_b{}^c{}_2 Q^b_k P_{kc} \right), \\ Q^2_2 &= \frac{1}{g P_{23}} \left(\partial^k P_{k1} - g \varepsilon_b{}^c{}_1 Q^b_3 P_{3c} \right), \end{aligned} \tag{47}$$

$$P_{12} = P_{13} = P_{22} = 0.$$

Equations (38h) and (39) also show that

$$P_{11} \geqslant 0, \quad P_{23} \geqslant 0.$$

It may be a little surprising that the Hamiltonian (46) is local, because one would expect the Gauss law to produce nonlocal terms. However, the locality of H_{phys} becomes easy to understand if we look at the definitions (47). Our gauge choices have annihilated three momentum components, and when we solve Gauss's law for the coordinates conjugate to these momenta, the result is local. One should also note that the Hamiltonian density is singular at points where P_{11} or P_{23} vanishes. These are exactly the same points where the gauge transformation matrix (39) becomes ambiguous.

Now we would like to examine what the Hamiltonian (46) looks like at small and large values of the coupling constant g. For that purpose we note that every component Q^a_k consists of terms proportional to g^{-1} and terms independent of g. Therefore the field tensor components Φ^a_{kl} range from g^{-1} to g^1 and as a result, the Hamiltonian density takes the form

$$\mathcal{H}_{\text{phys}} = \frac{1}{2g^2} \mathcal{H}^{(0)} + \frac{1}{g} \mathcal{H}^{(1)} + \mathcal{H}^{(2)} + g \mathcal{H}^{(3)} + \frac{g^2}{2} \mathcal{H}^{(4)}. \tag{48}$$

At small values of g the dominant term is $\mathcal{H}^{(0)}$, and it is rather straightforward to work out that

$$\begin{aligned}\mathcal{H}^{(0)} = &\left[-\partial_2\left(\frac{1}{P_{11}}\sum_{k=2}^{3}\partial_k P_{k3}+\frac{P_{21}}{P_{11}P_{23}}\sum_{k=1}^{3}\partial_k P_{k1}\right)-\partial_1\left(\frac{1}{P_{23}}\sum_{k=1}^{3}\partial_k P_{k1}\right)\right]^2\\ &+\left[-\partial_3\left(\frac{1}{P_{11}}\sum_{k=2}^{3}\partial_k P_{k3}+\frac{P_{21}}{P_{11}P_{23}}\sum_{k=1}^{3}\partial_k P_{k1}\right)\right]^2+\left[\partial_2\left(\frac{\partial_3 P_{32}}{P_{11}}\right)\right]^2+\left[\partial_3\left(\frac{\partial_3 P_{32}}{P_{11}}\right)\right]^2\\ &+\left[-\frac{\partial_3 P_{32}}{P_{11}P_{23}}\sum_{k=1}^{3}\partial_k P_{k1}\right]^2+\left[\partial_3\left(\frac{1}{P_{23}}\sum_{k=1}^{3}\partial_k P_{k1}\right)\right]^2. \qquad (49)\end{aligned}$$

This expression looks a bit complicated, but it is noteworthy that $\mathcal{H}^{(0)}$ does not depend on the coordinates Q_k^a. At large values of g we similarly find the dominant term to be

$$\begin{aligned}\mathcal{H}^{(4)} = &\{[\left(P_{33}Q_3^1-P_{31}Q_3^3\right)\left(P_{33}Q_3^2-P_{32}Q_3^3\right)+P_{23}Q_3^2\left(P_{33}Q_2^1-P_{31}Q_2^3\right)+P_{23}P_{32}\left(Q_2^3Q_3^1-Q_2^1Q_3^3\right)]^2\\ &+P_{23}^2[-P_{11}Q_1^1Q_2^3+Q_2^1\left(P_{23}Q_2^1-P_{21}Q_2^3+P_{33}Q_3^1-P_{31}Q_3^3\right)]^2+[P_{23}Q_2^1\left(-P_{32}Q_3^1+P_{31}Q_3^2\right)\\ &-\left(P_{11}Q_1^1+P_{21}Q_2^1\right)\left(P_{33}Q_3^2-P_{32}Q_3^3\right)]^2+[-P_{23}Q_3^2\left(P_{23}Q_2^1-P_{21}Q_2^3+P_{33}Q_3^1\right)+Q_3^3\left(P_{23}P_{32}Q_3^1\\ &+P_{21}P_{33}Q_3^2\right)-P_{21}P_{32}\left(Q_3^3\right)^2]^2+P_{23}^2[Q_3^1\left(P_{23}Q_2^1-P_{21}Q_2^3+P_{33}Q_3^1\right)-Q_3^3\left(P_{11}Q_1^1+P_{31}Q_3^1\right)]^2\\ &+[-P_{23}P_{32}\left(Q_3^1\right)^2+P_{23}Q_3^2\left(P_{11}Q_1^1+P_{31}Q_3^1\right)+P_{21}Q_3^1\left(-P_{33}Q_3^2+P_{32}Q_3^3\right)]^2+P_{11}^2[-P_{23}Q_2^3Q_3^2\\ &-Q_3^3\left(P_{33}Q_3^2-P_{32}Q_3^3\right)]^2+\left(P_{11}P_{23}\right)^2\left(Q_2^3Q_3^1-Q_2^1Q_3^3\right)^2+P_{11}^2[P_{23}Q_2^1Q_3^2+Q_3^1\left(P_{33}Q_3^2\right.\\ &\left.-P_{32}Q_3^3\right)]^2\}/\left(P_{11}P_{23}\right)^2. \qquad (50)\end{aligned}$$

This is also a rather complicated expression, being fourth order in the coordinates Q_k^a and fractional in the momenta P_{ka}. Finally we should note that the form of the decomposition (48) is actually a matter of choice, since it is always possible to scale the variables by

$$(Q_k^a, P_{ka}) \to (g^{\alpha_{ka}}Q_k^a, g^{-\alpha_{ka}}P_{ka}),$$

where the α_{ka}'s are arbitrary constants. However, scalings like this would alter the g dependence of the field tensor Φ_{kl}^a and the covariant derivative. As a result, the interpretation of g would also change. In the present form g is defined so that the limit $g \to 0$ corresponds to an Abelian theory. The singular behavior of $\mathcal{H}_{\text{phys}}$ in this limit then stems from an obvious qualitative difference between Abelian and non-Abelian theories in the function group method. Namely, the algebra (3) shows that for a non-Abelian theory ($g \neq 0$) the Gauss law generators must be parametrized with variables that contain one canonically conjugate pair, whereas in the Abelian case ($g=0$) this parametrization cannot contain canonical pairs at all. Also the solution of Gauss's law given in (47) is genuinely non-Abelian and impossible to extend to the Abelian case.

When quantizing the Hamiltonian (46), we could try to quantize one of the limiting cases (49) or (50) first and then develop a perturbation expansion in appropriate powers of g. At least the weak coupling Hamiltonian (49), despite its complicated appearance, looks easy to quantize as its eigenstates would consist of common eigenstates of the momentum operators. The strong coupling Hamiltonian (50) is considerably more difficult to quantize in the canonical approach because we would have to solve problems connected with the ordering of operators and with the regularization of higher order functional derivatives defined at the same point in space. Moreover, it is not clear whether large values of the bare coupling constant are physically relevant. As a general feature of quantization one should also take into account that two classical systems connected by a canonical transformation do not necessarily yield unitarily equivalent quantum systems. For example, in quantum mechanics it is often difficult to find a unitary transformation corresponding to action-angle variables in classical mechanics.[18] The fact that the transformation (38) is nonlinear might thus have an effect on the quantization of the Hamiltonian (46). Finding a suitable quantization procedure remains a problem to study.

IV. CONCLUSIONS

The unconstrained Hamiltonian (46) lies at the end of a long journey which started from the temporal gauge Hamiltonian (1) and passed through the transformation (38), making it finally possible to implement Gauss's law in the new variables (37). The canonical pairs (q_i, p_i) turned out to be nonphysical, which led to the conclusion that the physical degrees of freedom are described by the gauge-invariant fields $(Q_k^{a'}, P_{ka'})$. Equation (47) then defined those components that are not free variables. The actual construction of the variables (37) relied on the parametrization (6) and the complementary choices (18), (28), and (31). One could also easily experiment with different choices and derive alternative Hamiltonians corresponding to them by applying the general principles stated in Sec. II. In particular, the Poisson bracket relations (17) allow for a large variety of possible U(1) gauges, given only that the initial choice (7) is made.

An extension of this construction to more general Lie groups is relatively straightforward to outline. One should begin by deriving a parametrization of the Gauss law generators similar to (6). Identifying the G_a's with elements of the corresponding Lie algebra, one should select the maximum number of new canonical momenta from the maximal Abelian subspace of the enveloping algebra. The remaining variables needed for the parametrization should then be chosen so that the Lie algebra relations

$$\{G_a(\mathbf{x}), G_b(\mathbf{y})\} = -gf_{ab}{}^c G_c(\mathbf{y})\delta(\mathbf{x}-\mathbf{y})$$

would hold as a consequence of the canonical Poisson brackets. After identifying which variables are gauge-dependent one should define gauge-invariant variables by transforming the gauge-dependent degrees of freedom away. The details of the construction would then depend on the Poisson brackets of the gauge-invariant variables and the way of defining those gauge degrees of freedom that are not fixed by the parametrization of the Gauss law generators. No doubt that the calculations would be much more complicated than in the SU(2) case. In addition to generalizing the Lie group, one could also extend the method by adding matter fields, in particular fermions, into the theory. However, it seems that the question of quantization deserves the most attention in the future because it is crucial for the physical applicability of the Hamiltonian (46).

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A note on BRST quantization of SU(2) Yang-Mills mechanics

A. Fuster[a] and J. W. van Holten[b]
NIKHEF, Amsterdam, the Netherlands

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The quantization of SU(2) Yang-Mills theory reduced to 0+1 space-time dimensions is performed in the BRST framework. We show that in the unitary gauge $A_0=0$ the BRST procedure has difficulties which can be solved by introduction of additional singlet ghost variables. In the Lorenz gauge $\dot{A}_0=0$ one has additional unphysical degrees of freedom, but the BRST quantization is free of the problems of the unitary gauge. © *2005 American Institute of Physics.*
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I. SU(2) YANG-MILLS MECHANICS

We consider SU(2) Yang-Mills mechanics obtained by the reduction of SU(2) Yang-Mills field theory in $(D+1)$-dimensional space-time to a finite-dimensional quantum system, by taking the dynamical variables to depend on the time coordinate t only. The Lagrangian of such a theory is

$$L_{\mathrm{YMQM}} = \tfrac{1}{2}(F^a_{0i})^2 - \tfrac{1}{4}(F^a_{ij})^2, \tag{1}$$

where $i,j=(1,\ldots,D)$, and

$$F^a_{0i} = \dot{A}^a_i - g\epsilon^{abc}A^b_0A^c_i, \quad F^a_{ij} = -g\epsilon^{abc}A^b_iA^c_j. \tag{2}$$

Such a system has been widely studied in the context of nonperturbative aspects of (super) Yang-Mills theories,[1,2] and as a first step in the regularized dynamics of membrane theory.[3–5]

The Lagrangian is invariant under time-dependent gauge transformations with parameters $\Lambda^a(t)$, taking the infinitesimal form

$$\delta A^a_0 = \dot{\Lambda}^a - g\epsilon^{abc}A^b_0\Lambda^c, \quad \delta A^a_i = -g\epsilon^{abc}A^b_i\Lambda^c. \tag{3}$$

This invariance allows us to impose a gauge condition leaving the physical dynamics unchanged. The simplest choice is

$$A^a_0 = 0. \tag{4}$$

With this condition the effective Lagrangian for the remaining D-dimensional vector potentials $\mathbf{A}_a$ becomes [we do not distinguish between upper and lower adjoint indices $(a,b,c,\ldots)$ for SU(2)]

$$L_{\mathrm{eff}} = \tfrac{1}{2}\dot{\mathbf{A}}^2_a - V[\mathbf{A}], \tag{5}$$

with the potential

[a]Electronic mail: fuster@nikhef.nl
[b]Electronic mail: v.holten@nikhef.nl

$$V[\mathbf{A}] = \frac{g^2}{4}(\mathbf{A}_a^2\mathbf{A}_b^2 - (\mathbf{A}_a \cdot \mathbf{A}_b)^2). \tag{6}$$

In addition, we must impose a set of (first-class) constraints corresponding to the previous equations of motion for A_0^a,

$$G^a \equiv g\ \epsilon^{abc}A_i^b F_{0i}^c \simeq g\ \epsilon_{abc}\mathbf{A}_b \cdot \dot{\mathbf{A}}_c = 0. \tag{7}$$

Thus, the physical trajectories in configuration space in the gauge (4) are the solutions of the Euler-Lagrange equations derived from (5) subject to the additional constraints (7).

In addition to the pure Yang-Mills theory described by the action (1), one can also construct various supersymmetric extensions, based on the reduction of supersymmetric Yang-Mills field theory in $D=1$, 3, 5, 9. The spectra of these theories differ in certain aspects,[1,6,3,4,7–9] but for the problem addressed in this paper those differences are not relevant.

To keep track of the constraints, especially in the context of the Yang-Mills quantum theory, we follow the BRST procedure. (For reviews, see Refs. 10 and 11.) Thus we introduce anticommuting ghost degrees of freedom (b^a, c^a) as well as commuting auxiliary scalars N^a in such a way, that the total gauge-fixed action becomes invariant under a set of special ghost-dependent gauge transformations, the rigid BRST invariance. The anticommuting BRST differentials δ_Ω are defined before gauge fixing as follows:

$$\begin{gathered}\delta_\Omega A_0^a = (D_0 c)^a = \dot{c}^a - g\epsilon^{abc}A_0^b c^c, \quad \delta_\Omega A_i^a = (D_i c)^a = -g\epsilon^{abc}A_i^b c^c, \\ \delta_\Omega c^a = \frac{g}{2}\epsilon^{abc}c^b c^c, \\ \delta_\Omega b^a = iN^a, \quad \delta_\Omega N^a = 0.\end{gathered} \tag{8}$$

The gauge invariance of the classical action (1) implies its invariance under the BRST transformations by construction. The BRST differential has the standard property that $\delta_\Omega^2 = 0$. The implementation of the BRST construction for the gauge $A_0 = 0$ is, to impose this gauge condition using the Nakanishi-Lautrup fields N^a as Lagrange multipliers, and complete the effective Lagrangian so as to make it fully BRST invariant. For the case at hand this results in the effective Lagrangian,

$$L_{\text{eff}} = L_{\text{YMQM}} + N^a A_0^a + ib^a(\dot{c}^a - g\epsilon^{abc}A_0^b c^c). \tag{9}$$

We can use the gauge condition implied by the Nakanishi-Lautrup fields to eliminate A_0^a and N^a simultaneously; in a path-integral formulation, this implies integrating out a δ-functional $\delta(A_0)$. The result is

$$L_{\text{eff}} = \tfrac{1}{2}\dot{\mathbf{A}}_a^2 - \tfrac{1}{4}(F_{ij}^a)^2 + ib_a\dot{c}_a. \tag{10}$$

Note that for $D=3$ we can construct a magnetic field by $1/2\ \epsilon_{ijk}F_{jk}^a = B_i^a$, but this does not hold for general D. The effective Lagrangian (10) is invariant under the reduced form of the BRST variations (8) obtained by taking $A_0^a = 0$, and using the equation of motion for N^a,

$$\delta b^a = iN^a \simeq ig\epsilon^{abc}(A_i^b F_{0i}^c - ic^b b^c). \tag{11}$$

The BRST invariance of the effective Lagrangian implies an anticommuting conserved charge by Noether's theorem. The BRST charge takes the form

$$\Omega = c^a G^a - \frac{ig}{2}\epsilon^{abc}c^a c^b b^c. \tag{12}$$

The first-class constraints of the classical theory are summarized effectively by the statement that $\Omega = 0$; more precisely, in the phase-space formulation, all brackets of physical quantities with Ω

must vanish, physical quantities must be BRST invariant; this is discussed in more detail in the next section.

II. QUANTUM THEORY

In the quantum theory the dynamical variables A_i^a and their conjugate momenta $P_i^a = \dot{A}_i^a$, as well as the Faddeev-Popov ghosts are operators satisfying (anti-)commutation relations

$$[A_i^a, P_j^b] = i\ \delta^{ab}\delta_{ij}, \quad [c^a, b^b]_+ = \delta^{ab}. \tag{13}$$

The Hamiltonian is given by

$$H_{\text{eff}} = \tfrac{1}{2}\mathbf{P}_a^2 + \tfrac{1}{4}F_{ij}^{a\,2}, \tag{14}$$

as for pure Yang-Mills theory, in fact. The Hamiltonian determines the time evolution of any quantity X constructed from the Yang-Mills or ghost operators by the Schrödinger equation

$$\dot{X} = i[H, X]. \tag{15}$$

Gauge transformations on $(\mathbf{A}_a, \mathbf{P}_a)$ are generated by the SU(2) charges

$$G_a = g\ \epsilon_{abc}\mathbf{A}_b \cdot \mathbf{P}_c, \tag{16}$$

such that

$$\delta_a X = i[G_a, X], \quad \delta_a G_b = i[G_a, G_b] = -\,g\ \epsilon_{abc}G_c, \tag{17}$$

while more generally the BRST transformations are given by

$$\delta_\Omega X = i[\Omega, X]_\pm, \tag{18}$$

where the sign depends on the fermionic parity of the quantity X, + (anticommutator) for fermionic X and − (commutator) for bosonic X. In particular, the commutation relation (17) for the gauge charges together with the ghost anticommutator (13) implies the nilpotency of the BRST charge,

$$\Omega^2 = 0. \tag{19}$$

To complete the theory we must define an inner product on the extended state space, such that zero-norm states decouple and physical states have positive norm. For this to happen, it is necessary that the BRST operator is self-adjoint with respect to this inner product. In the coordinate representation, with states being represented by wave functions $\Psi[\mathbf{A}, c]$, such an inner product is defined by the integral[12]

$$(\Phi, \Psi) = i \int \mathrm{d}c^1 \mathrm{d}c^2 \mathrm{d}c^3 \int \prod_{i,a} \mathrm{d}A_i^a \Phi^\dagger[\mathbf{A}, c]\Psi[\mathbf{A}, c]. \tag{20}$$

It is easily seen that with this definition the ghost operators (b, c) are self-adjoint themselves. It follows directly that, indeed,

$$(\Omega\Phi, \Psi) = (\Phi, \Omega\Psi). \tag{21}$$

III. PHYSICAL STATES

The physical states of Yang-Mills quantum mechanics are constructed by solving for the eigenstates and eigenvalues of the Hamiltonian (14) subject to the constraint of BRST invariance.

One useful way to construct states is by the Fock-space approach,[7] in which one starts with an oscillator basis for the dynamical degrees of freedom defined by

$$\mathbf{a}_a = \frac{1}{\sqrt{2}}(\mathbf{A}_a + i\mathbf{P}_a), \quad \mathbf{a}_a^\dagger = \frac{1}{\sqrt{2}}(\mathbf{A}_a - i\mathbf{P}_a). \tag{22}$$

These creation and annihilation operators satisfy the standard commutation relations

$$[\mathbf{a}_a, \mathbf{a}_b^\dagger] = \delta_{ab} 1_D, \tag{23}$$

where 1_D is the D-dimensional unit matrix. As implied by Eq. (13) the ghost operators already behave like fermionic ladder operators. One is free to consider either c^a or b^a as creation operator; we choose c^a. Fock states are now constructed as polynomials in $\mathbf{a}_a^\dagger$ and c^a acting on an empty state Ψ_0 defined by

$$\mathbf{a}_a \Psi_0 = b^a \Psi_0 = 0. \tag{24}$$

Such a construction differs from the standard (bosonic or fermionic) creation and annihilation operators in that c^a and b^a are self-adjoint with respect to the inner product (20) rather than adjoint to each other. A similar treatment of ghost ladder operators can be found in Ref. 13.

The Hamiltonian can be represented as a matrix in a basis of Fock states. Subsequent diagonalization would give the spectrum of the theory. [Note one can only construct a basis of finite dimension and therefore any results would be approximate (see Ref. 7).]

In the context of the coordinate representation this construction is realized by taking

$$\mathbf{a}_a = \frac{1}{\sqrt{2}}\left(\mathbf{A}_a + \frac{\partial}{\partial \mathbf{A}_a}\right), \quad b^a = \frac{\partial}{\partial c^a}, \tag{25}$$

and

$$\Psi_0 = N e^{-\frac{1}{2}\mathbf{A}_a \cdot \mathbf{A}_a}, \tag{26}$$

with N a normalization factor. In this representation the gauge generators are of the form

$$G_a = -ig\ \epsilon_{abc} \mathbf{a}_b^\dagger \cdot \mathbf{a}_c. \tag{27}$$

We analyze next the restrictions imposed by the BRST symmetry on states in order to be physical. In the BRST formalism physical states are identified with the cohomology classes of the nilpotent BRST charge Ω,

$$\mathcal{H}^{\text{phys}} \simeq \frac{\text{Ker}\,\Omega}{\text{Im}\,\Omega}. \tag{28}$$

This implies that physical states Ψ are BRST invariant,

$$\Omega\Psi = 0, \quad (\Psi, \Psi) = 1, \tag{29}$$

and state vectors differing by a BRST-exact state are identified,

$$\Psi \sim \Psi' = \Psi + \Omega\Lambda. \tag{30}$$

Therefore matrix elements of physical operators between physical states must be invariant under the BRST transformations (30):

$$(\Phi, X\Psi) = (\Phi, X\Psi'), \quad \text{if } [\Omega, X]_\pm = 0. \tag{31}$$

These properties are guaranteed if BRST-exact states of the form $\Omega\Lambda$ decouple from the physical state space and have zero norm,

$$(\Psi,\Omega\Lambda)=(\Omega\Psi,\Lambda)=0,\quad (\Omega\Lambda,\Omega\Lambda)=(\Lambda,\Omega^2\Lambda)=0. \tag{32}$$

Observe that it is crucial for these results that the BRST charge is self-adjoint with respect to the physical inner product.

To do any practical calculation one needs an explicit expression for the physical state vectors; this can be achieved by selecting one element from each equivalence class, using the nilpotent co-BRST operator

$$^*\Omega = G^a b^a - \frac{ig}{2}\epsilon^{abc}c^a b^b b^c,\quad {}^*\Omega^2 = 0. \tag{33}$$

Indeed, the co-BRST condition

$$^*\Omega\Psi = 0, \tag{34}$$

acts as a gauge fixing condition for the BRST transformations (30), reducing the state space as required.[12] States satisfying both $\Omega\Psi = {}^*\Omega\Psi = 0$ are called BRST harmonic. Physical states are defined as BRST harmonic states of finite norm. We build first Fock states which are BRST harmonic.

Define the (total) ghost number as the operator

$$N_g = c^a b^a. \tag{35}$$

Splitting the Fock space in four sectors corresponding to the eigenvalues n_g of N_g, 0,…,3, we construct states in each ghost sector as follows:

$$\Psi^{(0)}[M] = M[\mathbf{a}^\dagger]\Psi_0,$$

$$\Psi^{(1)}_a[M] = c_a M[\mathbf{a}^\dagger]\Psi_0,$$

$$\tilde{\Psi}^{(2)}_a[M] = \tfrac{1}{2}\epsilon_{abc}c^a c^b M[\mathbf{a}^\dagger]\Psi_0,$$

$$\tilde{\Psi}^{(3)}[M] = \frac{1}{3!}\epsilon_{abc}c^a c^b c^c M[\mathbf{a}^\dagger]\Psi_0.$$

Here $M[\mathbf{a}^\dagger]$ is some gauge-invariant polynomial in the operators $\mathbf{a}^\dagger$,

$$M[\mathbf{a}^\dagger] = \sum_n \mu_{a_1\cdots a_n}\mathbf{a}^\dagger_{a_1}\cdots\mathbf{a}^\dagger_{a_n}, \tag{36}$$

and the coefficients $\mu_{a_1\cdots a_n}$ are invariant SU(2) tensors.

The complete set of solutions consists of two distinct classes, the states at ghost number $n_g=0$, $\Psi^{(0)}_M$, and those at ghost number $n_g=3$, $\tilde{\Psi}^{(3)}[M]$. We discuss next the possibility for these states to have finite norm (see also Refs. 14 and 15). The spectrum of the Hamiltonian in such a basis would be guaranteed to be physical.

IV. INNER PRODUCT AND GHOST VACUUM

The existence of two classes of BRST-harmonic states at different ghost number is of crucial importance for the construction of a nontrivial physical inner product.[11,14] Indeed, if we would only have the states at $n_g=0$ it is quite obvious from the definition (20) that the vacuum state Ψ_0 would have zero norm,

$$(\Psi_0,\Psi_0)=0, \tag{37}$$

while the BRST-invariant 3-ghost operator has a nonzero vacuum expectation value,

$$\frac{i}{3!}\epsilon^{abc}\langle c^a c^b c^c\rangle = \frac{i}{3!}(\Psi_0, \epsilon^{abc} c^a c^b c^c \Psi_0) = 1. \tag{38}$$

The problem clearly is in the definition of the ghost vacuum, in combination with the fact that the ghosts are self-conjugate. Therefore the ghost creation operators c^a do not act as annihilation operators on the conjugate (bra) vectors; if they would, the BRST charge would not be self-adjoint. In particular, it is not an option to replace the space of bra states by the BRST-dual states

$$\tilde{\Psi}^\dagger[M] = \frac{i}{3!}\Psi^\dagger[M]\epsilon^{abc} c^a c^b c^c, \tag{39}$$

as proposed in Refs. 14 and 16, which is equivalent to the replacement of the inner product (20) by

$$(\Phi, \Psi) \to \langle \Phi, \Psi\rangle = \frac{i}{3!}\epsilon^{abc}(\Phi, c^a c^b c^c \Psi). \tag{40}$$

In fact, it is clear that the ghost variables have vanishing matrix elements between any of the states (physical or unphysical):

$$\langle \Phi, c^a \Psi\rangle = 0, \quad \forall\, \Psi, \Phi, \tag{41}$$

i.e., the ghosts would effectively vanish as operators, and the same is true for the BRST charge Ω.

Part of the solution of this problem, also along the lines suggested in Ref. 16, is to use the existence of the second set of solutions of the BRST and co-BRST constraints with $n_g = 3$ to change the definition of the ghost vacuum. If we define a new vacuum state,

$$\Psi_+ = \frac{1}{\sqrt{2}}\left(1 + \frac{i}{3!}\epsilon^{abc} c^a c^b c^c\right)\Psi_0, \tag{42}$$

with corresponding physical excited states $\Psi_+[M] = M[\mathbf{a}^\dagger]\Psi_+$, the ghost operators remain self-adjoint and the vacuum is normalizable,

$$(\Psi_+, \Psi_+) = 1. \tag{43}$$

A drawback is, that the vacuum Ψ_+ has no well-defined ghost number, and not even a well-defined Grassmann parity, being a sum of an even and odd ghost number state. Moreover, the vacuum expectation value of the ghosts (38) is changed, but still nonvanishing; actually we now have

$$\frac{i}{3!}\epsilon^{abc}\langle c^a c^b c^c\rangle_+ = \frac{i}{3!}(\Psi_+, \epsilon^{abc} c^a c^b c^c \Psi_+) = \frac{1}{2}, \tag{44}$$

and similarly

$$\frac{i}{3!}\epsilon^{abc}\langle b^a b^b b^c\rangle_+ = \frac{1}{2}. \tag{45}$$

Although these expectation values are BRST invariant, they carry a nonzero ghost number, a manifestation of the noninvariance of both the vacuum and the inner product itself under ghost rescaling.

Both problems can be solved by introducing a fourth ghost θ, with conjugate antighost ζ,

$$[\theta, \zeta]_+ = 1. \tag{46}$$

The new ghost θ is taken to be a BRST singlet and has ghost number $n_g(\theta) = -3$; thus it has the same quantum numbers as the invariant antighost operator, while ζ has the quantum numbers of the corresponding ghost operator,

$$\theta \sim \frac{i}{3!}\epsilon^{abc}b^a b^b b^c, \quad \zeta \sim \frac{i}{3!}\epsilon^{abc}c^a c^b c^c. \tag{47}$$

We then define the physical vacuum state

$$\Phi_0 = \frac{1}{\sqrt{2}}\left(1 + \frac{1}{3!}\theta\ \epsilon^{abc}c^a c^b c^c\right)\Psi_0, \tag{48}$$

and the physical excited states

$$\Phi[M] = M[\mathbf{a}^\dagger]\Phi_0. \tag{49}$$

These physical states have a well-defined ghost number $n_g(\Phi_M)=0$ and Grassmann parity (even). This is especially important in the supersymmetric extensions of the theory, as the action of the gaugino operators would otherwise cause problems with sign changes for odd ghost number terms.

Simultaneously we also redefine the inner product (20) in the coordinate representation the full state space to

$$(\Phi,\Psi) = \int \mathrm{d}\theta \int \mathrm{d}c^1\mathrm{d}c^2\mathrm{d}c^3 \int \prod_{i,a} \mathrm{d}A_i^a \Phi^\dagger[\mathbf{A},c]\Psi[\mathbf{A},c]. \tag{50}$$

With respect to this inner product, all ghosts, including the new singlet ghost, are self-adjoint, and so is the BRST charge Ω. Observe that the ghost integration measure now has vanishing ghost number as well. Finally, the 3-ghost operator vacuum expectation value vanishes trivially,

$$\frac{i}{3!}\epsilon^{abc}\langle c^a c^b c^c\rangle_\theta = \frac{i}{3!}(\Phi_0, \epsilon^{abc}c^a c^b c^c \Phi_0) = 0. \tag{51}$$

Of course, there arise new vacuum expectation values

$$\frac{1}{3!}\langle \theta\ \epsilon^{abc}c^a c^b c^c\rangle_\theta = \frac{1}{3!}\langle \zeta\ \epsilon^{abc}b^a b^b b^c\rangle_\theta = \frac{1}{2}, \tag{52}$$

but these expectation values are both BRST invariant and have vanishing ghost number.

In passing, let us point out a further result of some interest, it is possible to define new antighost operators β^a and η by

$$\beta^a = b^a + \tfrac{1}{2}\epsilon^{abc}\theta c^b c^c, \quad \eta = \zeta - \frac{1}{3!}\epsilon^{abc}c^a c^b c^c. \tag{53}$$

These redefinitions preserve the ghost number. Moreover, one easily establishes the anticommutation relations

$$[c^a,\beta^b]_+ = \delta^{ab}, \quad [\theta,\eta]_+ = 1, \quad [\eta,\beta^a]_+ = [\theta,c^a]_+ = 0, \tag{54}$$

with all other anticommutators vanishing as well. In addition

$$\beta^a\Phi_0 = \eta\ \Phi_0 = 0, \tag{55}$$

suggesting that Φ_0 is the actual Fock vacuum for the new antighosts (η,β^a). Unfortunately, it is to be noted that these antighosts are no longer self-adjoint with respect to the inner product (50),

$$\beta_a^\dagger = b^a - \tfrac{1}{2}\epsilon^{abc}\theta c^b c^c, \quad \eta^\dagger = \zeta + \frac{1}{3!}\epsilon^{abc}c^a c^b c^c. \tag{56}$$

Hence these operators do not annihilate the conjugate vacuum, for a general state vector Ψ,

$$(\Phi_0, \beta^a \Psi) = (\beta_a^\dagger \Phi_0, \Psi) \neq 0. \tag{57}$$

Moreover, the conjugate ghosts have nontrivial anticommutation relations with the original antighosts, e.g.,

$$[\beta_a^\dagger, \eta]_+ = -\epsilon^{abc} c^b c^c, \quad [\beta_a^\dagger, \beta^b]_+ = -\epsilon^{abc} \theta c^c. \tag{58}$$

Therefore the ghost variables (β^a, η) are not of much use in the construction of states. Nevertheless, they do provide a good way to characterize the ghost dependence of the physical states by the conditions (55).

V. LORENZ GAUGE

We will now show, that the problems with the definition of physical states and inner products sketched in Sec. IV do not exist in the Lorenz gauge quantization. The starting point for our analysis is again the classical theory defined in Eqs. (1)–(3), and the representation of the nilpotent BRST algebra defined in Eq. (8). In the $(0+1)$-dimensional reduction of the Yang-Mills theory, the Lorenz gauge takes the form

$$\dot{A}_0 = 0. \tag{59}$$

A convenient BRST-invariant extension of the classical Lagrangian for this gauge is

$$L_{\text{Lorenz}} = L_{\text{YMQM}} + N^a \dot{A}_0^a - \tfrac{1}{2} N_a^2 - i\dot{b}^a (D_0 c)^a \simeq \tfrac{1}{2}(D_0 \mathbf{A}^a)^2 + \tfrac{1}{2}(\dot{A}_0^a)^2 - \tfrac{1}{4}(F_{ij}^a)^2 - i\dot{b}^a (D_0 c)^a, \tag{60}$$

where the last line results from elimination of the auxiliary fields N^a. The corresponding Hamiltonian is

$$H_{\text{Lorenz}} = \frac{1}{2}(\mathbf{P}^a + g\epsilon^{abc} A_0^b \mathbf{A}^c)^2 + \frac{1}{2}(P_0^a)^2 + \frac{1}{4}(F_{ij}^a)^2 - \frac{g^2}{2}(\epsilon^{abc} A_0^b \mathbf{A}^c)^2 + i(u^a - ig\epsilon^{abc} A_0^b c^c) v^a, \tag{61}$$

where the canonical momenta are defined by

$$\mathbf{P}_a = (D_0 \mathbf{A})^a, \quad P_0^a = \dot{A}_0^a,$$

$$u^a = -(D_0 c)^a, \quad v^a = \dot{b}^a. \tag{62}$$

The conserved BRST charge takes the form

$$\Omega = G^a c^a - \frac{ig}{2}\epsilon^{abc} c^a c^b v^c + P_0^a u^a, \tag{63}$$

with the gauge charges G^a as in Eq. (16). As neither of the expressions (61) and (63) suffer from ordering ambiguities, they can be interpreted directly as quantum operators, with the fundamental commutation relations given by

$$[\mathbf{A}_a, \mathbf{P}_b] = i\delta_{ab} 1_D, \quad [A_0^a, P_0^b] = i\delta^{ab},$$
$$[c^a, v^b]_+ = \delta^{ab}, \quad [b^a, u^b]_+ = \delta^{ab}. \tag{64}$$

The quantum equations of motion and the BRST transformations then again take the form (15) and (18). In the coordinate representation, the BRST-invariant inner product of two wave functions in the full ghost-extended Hilbert space now takes the form

$$(\Phi,\Psi)=i\int\prod_a \mathrm{d}b^a\mathrm{d}c^a\int\prod_a \mathrm{d}A_0^a\int\prod_{i,a}\mathrm{d}A_i^a\Phi^\dagger[\mathbf{A},A_0,c,b]\Psi[\mathbf{A},A_0,c,b]. \tag{65}$$

To fix the BRST gauge, we introduce the co-BRST operator

$${}^*\Omega=G^a v^a+\frac{ig}{2}\epsilon^{abc}c^a v^b v^c+P_0^a b^a. \tag{66}$$

Requiring states to be simultaneously BRST and co-BRST invariant leads to the conditions

$$G^a\Psi=0,\quad \Sigma^a\Psi=0,\quad P_0^a\Psi=0, \tag{67}$$

where

$$\Sigma^a=ig\epsilon^{abc}c^b v^c, \tag{68}$$

is the generator of the rigid SU(2) transformations, which is still an invariance of the theory, on the conjugate ghosts variables (c^a,v^a). In contrast to the unitary gauge $A_0^a=0$, in the Lorenz gauge the BRST conditions do not fix the physical states complelety. We can still impose a further constraint fixing the dependence of physical states on the antighost variables (b^a,u^a), by requiring states to be rigid SU(2) singlets with respect to all variables,

$$\tilde{\Sigma}^a\Psi=0,\quad \tilde{\Sigma}^a=ig\epsilon^{abc}b^b u^c. \tag{69}$$

Indeed, it is easily checked that $\tilde{\Sigma}^a$ is a BRST and co-BRST invariant operator; therefore the constraint can be imposed consistently on all physical states.

The full set of solutions of conditions (67) and (69) are wave functions which are SU(2) singlets (i.e., gauge invariant), which do not depend on A_0^a, and whose ghost dependence is a constraint to the form

$$\Psi_{\mathrm{phys}}[\mathbf{A},c,b]=\Psi_1[\mathbf{A}]+\frac{i}{3!}\epsilon^{abc}c^a c^b c^c\Psi_2[\mathbf{A}]+\frac{i}{3!}\epsilon^{abc}b^a b^b b^c\Psi_3[\mathbf{A}]+\frac{i}{(3!)^2}(\epsilon^{abc}c^a c^b c^c)\times(\epsilon^{def}b^d b^e b^f)\Psi_4[\mathbf{A}]. \tag{70}$$

With the standard assignment of the ghost number +1 for c^a and −1 for b^a, requiring the states to have vanishing ghost number and definite Grassmann parity imposes the further constraint

$$\Psi_2[\mathbf{A}]=\Psi_3[\mathbf{A}]=0. \tag{71}$$

Finally, requiring the inner product (65) to be positive definite in the subspace of physical states, we must fix the space of physical states to be represented by factorized wave functions,

$$\Psi_{\mathrm{phys}}=\frac{1}{\sqrt{2}}\left[1+\frac{i}{(3!)^2}(\epsilon^{abc}c^a c^b c^c)(\epsilon^{def}b^d b^e b^f)\right]\Psi_M=\frac{1}{\sqrt{2}}\left(1-i\prod_a(c^a b^a)\right)\Psi_M, \tag{72}$$

where Ψ_M can be taken as a physical Fock state of the form (36). Observe that the operator $(i/3!)\epsilon^{abc}b^a b^b b^c$ plays the same role here as the extra ghost θ in our construction of the states in the unitary gauge. Obviously, as in the unitary gauge, we can define a ghost operator with nonzero vacuum expectation value

$$\frac{i}{(3!)^2}\left\langle\prod_a(c^a b^a)\right\rangle=\frac{1}{2}, \tag{73}$$

but like (52) it is BRST invariant and has vanishing ghost number. Finally, defining the vacuum state of the physical subspace as

$$\Phi_0 = \frac{1}{\sqrt{2}}\left(1 - i\prod_a (c^a b^a)\right)\Psi_0, \tag{74}$$

where Ψ_0 is the Fock vacuum of the Yang-Mills system, one can again define ghost operators anihilating Φ_0 by taking

$$\gamma^a = c^a + \frac{i}{2\cdot 3!}\epsilon^{abc}v^b v^c \epsilon^{def}u^d u^d u^f, \quad \beta^a = b^a - \frac{i}{2\cdot 3!}\epsilon^{abc}u^b u^c \epsilon^{def}v^d v^d v^f. \tag{75}$$

As might be expected from our previous analysis, these operators are not self-adjoint and do not define a good basis for a complete Fock-space construction in the ghost sector. Nevertheless, the conditions

$$\gamma^a \Phi_0 = \beta^a \Phi_0 = 0 \tag{76}$$

provide a convenient way to characterize the physical ghost vacuum.

Finally we should remark, that in the physical subspace the integration over A_0^a is of course divergent in the absence of damping, as the physical wave functions are A_0 independent. This divergence can be absorbed in a wave-function renormalization factor

$$N = \frac{1}{\sqrt{\int \Pi_a \mathrm{d}A_0^a}}. \tag{77}$$

Knowing this, we can remove the A_0^a from the physical inner product and effectively set $N=1$; we observe, that N is BRST invariant, and the procedure does not jeopardize the BRST invariance of the integration measure.

VI. DISCUSSION

In this paper we have shown, that although the physical content of the $(0+1)$-dimensional Yang-Mills theory is clearest in the unitary gauge $A_0^a=0$, the BRST quantization works in a more straightforward way in the Lorenz gauge $\dot{A}_0^a=0$. An important part of the discussion and analysis was based on the construction of a BRST-invariant inner product with respect to which the BRST charge Ω is self-adjoint.

To get a little more algebraic and geometric insight into the constructions, consider again the unitary gauge, in which a general state is represented by a wave function

$$\Psi[c] = \psi + c^a \psi_a + \frac{i}{2!}c^a c^b \psi_{ab} + \frac{i}{3!}c^a c^b c^c \psi_{abc}. \tag{78}$$

Defining the dual wave function

$$\tilde{\Psi}[c] = \tilde{\psi} + c^a \tilde{\psi}_a + \frac{i}{2!}c^a c^b \tilde{\psi}_{ab} + \frac{i}{3!}c^a c^b c^c \tilde{\psi}_{abc} \tag{79}$$

with components

$$\tilde{\psi} = \frac{1}{3!}\epsilon_{abc}\psi_{abc}, \quad \tilde{\psi}_a = \frac{1}{2!}\epsilon_{abc}\psi_{bc},$$
$$\tilde{\psi}_{ab} = \epsilon_{abc}\psi_c, \quad \tilde{\psi}_{abc} = \epsilon_{abc}\psi, \tag{80}$$

we recognize that the physical states (42) are characterized as the self-dual states $\tilde{\Psi}=\Psi$, such that the inner product (20) becomes

$$i\int \mathrm{d}c^1\mathrm{d}c^2\mathrm{d}c^3\Psi^\dagger\Psi = \frac{1}{3!}\epsilon_{abc}(\psi^\dagger_{abc}\psi + \psi^\dagger\psi_{abc} + 3\psi^\dagger_a\psi_{bc} + 3\psi^\dagger_{ab}\psi_c) = 2\psi^\dagger\psi + 2\psi^\dagger_a\psi_a. \tag{81}$$

In particular, with $\tilde{\psi}=\psi=\sqrt{2}\psi_M$ and $\psi_a=\tilde{\psi}_a=0$, this reduces to

$$i\int \mathrm{d}c^1\mathrm{d}c^2\mathrm{d}c^3\Psi^\dagger[M]\Psi[M] = \psi^\dagger_M\psi_M. \tag{82}$$

Hence this inner product is positive definite for physical states. Of course, one can also consider the anti-self-dual states $\tilde{\Psi}=-\Psi$, which than have a negative definite norm. This should not surprise us, as the existence of a self-adjoint nilpotent BRST operator $\Omega^2=0$ is possible only in a space with indefinite norm. The important point is, that the space of physical states should have positive norm, and that is realized in the subspace of self-dual states.

Generalization of this discussion to the Lorenz gauge is simple. Each component in the wave-function expansion (78) now is a function of the additional ghost variables b_a, and we can again distinguish between components which are self-dual or anti-self-dual with respect to the expansion in b_a. In this formulation the physical states are then identified with the wave functions for which the components of zero ghost number are completely self-dual, i.e., self-dual both with respect to the c-ghost duality and with respect to the b-ghost duality.

We have discussed in particular the case of SU(2) Yang-Mills theory. The generalization to SU(N) is straightforward; with $r=N^2-1$ generators, and the same number of ghost and antighost variables, the self-dual physical states in the unitary gauge are of the form

$$\Psi[c] = \frac{1}{\sqrt{2}}\left(1 + \frac{i^{[r/2]}}{r!}\epsilon^{a_1\cdots a_r}c^{a_1}\cdots c^{a_r}\right)\psi_M. \tag{83}$$

For odd r (even N), both ghost number and Grassmann parity of the wave functions are ill defined; for even r (odd N), it is only the ghost number which is violated. In both cases, introduction of a singlet ghost θ with ghost number $n_g(\theta)=-r$ solves the problems. On the other hand, in the Lorenz gauge this is taken care of automatically by the antighost variables, as the operator

$$\frac{i^{[r/2]}}{r!}\epsilon^{a_1\cdots a_r}b^{a_1}\cdots b^{a_r} \tag{84}$$

has the same quantum numbers and plays the same role.

Finally we note, that as we have constructed precisely one BRST-invariant wave function for each physical state, in the supersymmetric extension the computation of the Witten index[17,9] is not affected by including the ghost degrees of freedom in the appropriate way (also see Refs. 18–20).

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$AdS_{d+1} \rightarrow AdS_d$

T. E. Clark[a)]
Department of Physics, Purdue University, West Lafayette, Indiana 47907-1396

S. T. Love[b)]
Department of Physics, Purdue University, West Lafayette, Indiana 47907-1396
and Fermi National Accelerator Laboratory, P.O. Box 500, Batavia, Illinois 60510

Muneto Nitta[c)]
Department of Physics, Tokyo Institute of Technology, Tokyo 152-8551, Japan

T. ter Veldhuis[d)]
Department of Physics and Astronomy, Macalester College, Saint Paul, MN 55105-1899

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Coset methods are used to construct the action describing the dynamics of the (massive) Nambu-Goldstone scalar degree of freedom associated with the spontaneous breaking of the isometry group of AdS_{d+1} space to that of an AdS_d subspace. The resulting action is an $SO(2,d)$ invariant AdS generalization of the Nambu-Goto action. The vector field theory equivalent action is also determined. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2048307]

I. INTRODUCTION

The AdS/CFT correspondence originally proposed by Maldecena[1] has sparked an enormous amount of theoretical investigation and speculation.[2] The nature of this connection has been recently considered[3,4] for the case of an AdS_d defect (brane) embedded in an underlying AdS_{d+1} space so that the $SO(2,d)$ isometry group of the AdS_{d+1} metric is spontaneously broken to the $SO(2,d-1)$ isometry group of the AdS_d space. It turns out that this case also provides a surprising example of a localized $D=4$ gravity in which the metric differs drastically from the Minkowski metric only far from the brane.[3] Moreover, when a CFT is coupled to AdS gravity, it has been shown that the AdS graviton obtains a mass by means of the AdS Higgs mechanism with the graviton absorbing a massive AdS vector[5] Nambu-Goldstone field.[3,6,7]

As a consequence of the embedding of the AdS_d brane in AdS_{d+1} space, it follows that $(d+1)$ of the pseudotranslations and Lorentz transformations of the AdS_{d+1} space are spontaneously broken. As is typical of spontaneous space-time symmetry breaking,[8] however, not all of the broken symmetries give rise to independent Nambu-Goldstone degrees of freedom. In fact, there is only a single Nambu-Goldstone boson, denoted $\phi(x)$, associated with a broken pseudotranslation generator which is independent. Here x^μ, $\mu=0,1,\ldots,d-1$, are coordinates parametrizing the AdS_d space. In this paper, we construct the action governing the dynamics of this Nambu-Goldstone boson. This mode has a natural interpretation as describing the coordinate oscillations of the brane into the target space covolume. As such we obtain the AdS space generalization of the Nambu-Goto action.

AdS_{d+1} space can be simply described as the $SO(2,d)$ invariant hyperboloidal hypersurface

[a)]Electronic mail: clark@physics.purdue.edu
[b)]Electronic mail: love@physics.purdue.edu
[c)]Electronic mail: nitta@th.phys.titech.ac.jp
[d)]Electronic mail: terveldhuis@macalester.edu

$$\frac{1}{m^2} = X_0^2 - X_1^2 - X_2^2 - \cdots - X_d^2 + X_{d+1}^2 = X^{\mathcal{M}} \hat{\eta}_{\mathcal{M}\mathcal{N}} X^{\mathcal{N}}, \tag{1.1}$$

embedded in a $(d+2)$-dimensional pseudo-Euclidean space defined with invariant interval

$$\mathrm{d}s^2 = \mathrm{d}X^{\mathcal{M}} \hat{\eta}_{\mathcal{M}\mathcal{N}} \mathrm{d}X^{\mathcal{N}} \tag{1.2}$$

characterized by the metric tensor $\hat{\eta}_{\mathcal{M}\mathcal{N}}$ of signature $(+1,-1,-1,\ldots,-1,+1)$, where $\mathcal{M},\mathcal{N} = 0,1,\ldots,d,d+1$. Here $X^{\mathcal{M}}$ are the pseudo-Euclidean space homogeneous coordinates and m is a constant inverse length scale characterizing the AdS_{d+1} space.

AdS_{d+1} space containing an AdS_d brane, which is a d-dimensional world volume with an AdS metric embedded as a $X^d=0$ hypersurface, can be described by the coordinates $X^{\mathcal{M}} = (X^\mu, X^d, X^{d+1})$ with

$$X^\mu = a(x^2) x^\mu \cosh(mr), \quad \mu = 0,1,\ldots,d-1,$$

$$X^d = \frac{1}{m}\sinh(mr), \tag{1.3}$$

$$X^{d+1} = \frac{1}{m} b(x^2)\cosh(mr).$$

Here x^μ are the intrinsic coordinates of the AdS_d world volume and $-\infty < r < \infty$ is the covolume coordinate. To satisfy Eq. (1.1) of the AdS_{d+1} hyperbola, $a(x^2)$ and $b(x^2)$ are related as

$$1 = m^2 x^2 a^2(x^2) + b^2(x^2). \tag{1.4}$$

Hence the $\mathrm{SO}(2,d)$ invariant interval, Eq. (1.2), becomes

$$\mathrm{d}s^2 = e^{2A(r)} \mathrm{d}\overline{s^2} - \mathrm{d}r^2, \tag{1.5}$$

where the warp factor is $A(r) = \ln\cosh(mr)$ and $\mathrm{d}\overline{s^2} = \mathrm{d}x^\mu \overline{g}_{\mu\nu}(x) \mathrm{d}x^\nu$ is the AdS_d invariant interval with $\overline{g}_{\mu\nu}$ the AdS_d metric tensor.

The AdS_d subspace has the isotropic coordinates x^μ of an $\mathrm{SO}(2,d-1)$ invariant hyperboloid, $1/m^2 = X_0^2 - X_1^2 - \cdots - X_{d-1}^2 + X_{d+1}^2$, embedded at $r=0=X^d$. This subsurface maintains the coordinate relation Eq. (1.4). This in turn leads to a form for the AdS_d metric tensor given by

$$\begin{aligned}\overline{g}_{\mu\nu}(x) &= a^2(x^2) P_{T\mu\nu}(x) + \left[\left(a(x^2) + 2x^2 \frac{\mathrm{d}a(x^2)}{\mathrm{d}x^2} \right)^2 + 4\frac{x^2}{m^2} \left(\frac{\mathrm{d}b(x^2)}{\mathrm{d}x^2} \right)^2 \right] P_{L\mu\nu}(x) \\ &= a^2(x^2) P_{T\mu\nu}(x) + \frac{\left(a(x^2) + 2x^2 \frac{\mathrm{d}a(x^2)}{\mathrm{d}x^2} \right)^2}{\left(1 - m^2 x^2 a^2(x^2)\right)} P_{L\mu\nu}.\end{aligned} \tag{1.6}$$

Here the transverse and longitudinal projectors for x^μ are defined as

$$P_{T\mu\nu}(x) = \eta_{\mu\nu} - \frac{x_\mu x_\nu}{x^2},$$

$$P_{L\mu\nu}(x) = \frac{x_\mu x_\nu}{x^2}, \tag{1.7}$$

and $\eta_{\mu\nu}$ is the metric tensor for d-dimensional Minkowski space having signature $(+1,-1,\ldots,-1)$. Throughout this paper, indices are raised, lowered, and contracted using $\eta_{\mu\nu}$ so that,

for instance $x^2 \equiv x^\mu \eta_{\mu\nu} x^\nu$. Any use of a curved metric will be noted explicitly. Further discussion of AdS coordinates and some specfic choices for $a(x^2)$ and $b(x^2)$ are found in Appendix A.

Since the embedding of the AdS_d brane breaks the AdS_{d+1} space-time symmetries to those of AdS_d, the associated Nambu-Goldstone bosons act as coordinates of the coset manifold corresponding to the $SO(2,d) \to SO(2,d-1)$ breakdown. In this paper, we show, using coset methods,[9–11] that the $SO(2,d)$ invariant action governing the dynamics of the Nambu-Goldstone boson degree of freedom takes the form

$$\Gamma = -\sigma \int d^d x \det \overline{e}(x) \cosh^d(m\phi(x)) \sqrt{1 - \frac{\mathcal{D}_\ell \phi(x)\, \eta^{\ell n} \mathcal{D}_n \phi(x)}{\cosh^2(m\phi(x))}}. \tag{1.8}$$

Here $\mathcal{D}_n = \overline{e}_n^{-1\mu}(x)\partial_\mu$ is the $SO(2,d-1)$ covariant derivative with $n = 0,1,\ldots,d-1$. The AdS_d vielbein, $\overline{e}_\mu^{\ n}$, corresponding to the metric tensor $\overline{g}_{\mu\nu} = \overline{e}_\mu^{\ \ell} \eta_{\ell n} \overline{e}_\nu^{\ n}$ is given by

$$\begin{aligned} \overline{e}_\mu^{\ n}(x) &= a(x^2) P_{T\mu}^{\ \ n}(x) + \sqrt{\left[\left(a(x^2) + 2x^2 \frac{da(x^2)}{dx^2}\right)^2 + 4\frac{x^2}{m^2}\left(\frac{db(x^2)}{dx^2}\right)^2\right]} P_{L\mu}^{\ \ n}(x) \\ &= a^2(x^2) P_{T\mu}^{\ \ n}(x) + \frac{a(x^2) + 2x^2 \frac{da(x^2)}{dx^2}}{\sqrt{1 - m^2 x^2 a^2(x^2)}} P_{L\mu}^{\ \ n}. \end{aligned} \tag{1.9}$$

The overall positive constant σ (brane tension) carries mass dimension d. Note that the overall sign of the action is fixed so that the ϕ kinetic energy term is positive. Equation (1.8) is the AdS generalization of the Nambu-Goto action for an AdS_d brane embedded in AdS_{d+1} space. We see that the Nambu-Goldtone mode is massive and has nonderivative self-interactions.

The outline of the paper is as follows. The coset method construction is presented in Sec. II along with the explicit form of the nonlinear realizations of the $SO(2,d)$ transformations of the Nambu-Goldstone fields. The action building blocks secured from the Maurer-Cartan one-form also appear in this section. Section III includes the transformation properties of the Maurer-Cartan one form along with the construction of the $SO(2,d)$ invariant AdS_d action. In addition, this section contains the general AdS_d coordinate transformations. The form of the AdS_d action is shown to remain invariant under these coordinate transformations. Finally in Sec. III, the vector field theory equivalent of this action is also secured. In this construction, it is the longitudnal component of the vector field which plays the role of the massive Nambu-Goldstone degree of freedom. In the Poincaré limit, $m \to 0$, the usual equivalence of this action to a tensor gauge theory[12] action is obtained.[13] There are two appendixes. Appendix A contains a discussion of the various AdS coordinate systems used in the paper, while the AdS isometry charge algebra is reviewed in Appendix B.

II. THE COSET CONSTRUCTION

The isometry group of the AdS_{d+1} hyperboloid [cf. Eq. (1.1)] is $SO(2,d)$ while that of the AdS_d subspace is $SO(2,d-1)$. The action governing the dynamics of the Nambu-Goldstone modes associated with the symmetry breakdown $SO(2,d) \to SO(2,d-1)$ can be constructed by means of the coset method. This technique begins by introducing the coset element $\Omega \in SO(2,d)/SO(1,d-1)$ where $SO(1,d-1)$ corresponds to the Lorentz (stability) group of transformations in AdS_d. The $AdS_d = SO(2,d-1)/SO(1,d-1)$ coordinates, y^μ, act as parameters for pseudotranslations in the world volume and are part of the coset so that

$$\Omega(y) = e^{iy^\mu P_\mu} e^{i\phi(y) Z} e^{iv^\mu(y) K_\mu}. \tag{2.1}$$

Here the symmetry generators P_μ, Z, and K_μ, as well as the Lorentz transformations generators $M_{\mu\nu}$, are defined in Appendix B. The coset so defined corresponds to a particular choice of coordinates, specifically denoted as y^μ, for the AdS_d world volume. The fields are also defined as functions of y^μ. Other coordinate choices, generically denoted by x^μ, can and will be used. In

order to transform to these coordinates, the y^μ will be defined as a function of the x^μ coordinates, $y^\mu = y^\mu(x)$. Likewise in this case, the fields will also be relabeled as functions of x^μ. That is, $\phi(y) = \phi(y(x)) \to \phi(x)$ and $v^m(y) = v^m(y(x)) \to v^m(x)$. Hence the coset element has the same operator structure as in Eq. (2.1) but now the fields and y are functions of x so that $\Omega(y) = \Omega(y(x)) \to \Omega(x) = e^{iy^\mu(x)P_\mu} e^{i\phi(x)Z} e^{iv^\mu(x)K_\mu}$. For the present, we use the y^μ coordinates and the fields are considered functions of y^μ. The Nambu-Goldstone field $\phi(y)$ along with $v^\mu(y)$ act as the remaining coordinates needed to parametrize the coset manifold $\mathrm{SO}(2,d)/\mathrm{SO}(2,d-1)$.

Left multiplication of the coset elements Ω by an $\mathrm{SO}(2,d)$ group element

$$g = e^{i\epsilon^\mu P_\mu} e^{izZ} e^{ib^\mu K_\mu} e^{(i/2)\lambda^{\mu\nu} M_{\mu\nu}}, \tag{2.2}$$

which is specified by the (space-time independent) infinitesimal parameters $\epsilon^\mu, z, b^\mu, \lambda^{\mu\nu}$, results in transformations of the space-time coordinates and the Nambu-Goldstone fields according to the general form[9]

$$g\Omega = \Omega' h. \tag{2.3}$$

The transformed coset element, Ω', is a function of the transformed world volume coordinates and the total variations of the fields,

$$\Omega' = e^{iy'^\mu P_\mu} e^{i\phi'(y')Z} e^{iv'^\mu(y')K_\mu}, \tag{2.4}$$

while h is a field dependent element of the stability group $\mathrm{SO}(1,d-1)$,

$$h = e^{(i/2)\theta^{\mu\nu}(y) M_{\mu\nu}}. \tag{2.5}$$

Exploiting the algebra of the $\mathrm{SO}(2,d)$ charges displayed in Appendix B, along with extensive use of the Baker-Campbell-Hausdorf formulas, the AdS transformations are obtained as

$$\begin{aligned} y'^\mu = {} & \left[1 - z\sqrt{m^2}\tanh\sqrt{m^2\phi^2}\frac{\sin\sqrt{m^2y^2}}{\sqrt{m^2y^2}} \right] y^\mu - \lambda^{\mu\nu} y_\nu + [P_L^{\mu\nu}(y) + \sqrt{m^2y^2}\cot\sqrt{m^2y^2} P_T^{\mu\nu}(y)]\epsilon_\nu \\ & + \frac{\tanh\sqrt{m^2\phi^2}}{\sqrt{m^2}} \left[\cos\sqrt{m^2y^2} P_L^{\mu\nu}(y) + \frac{\sqrt{m^2y^2}}{\sin\sqrt{m^2y^2}} P_T^{\mu\nu}(y) \right] b_\nu, \end{aligned}$$

$$\phi'(y') = \phi(y) + z\cos\sqrt{m^2y^2} + b_\mu y^\mu \frac{\sin\sqrt{m^2y^2}}{\sqrt{m^2y^2}},$$

$$\begin{aligned} v'^\mu(y') = {} & v^\mu(y) - \lambda^{\mu\nu} v_\nu - \frac{m^2}{2}\frac{\tan\sqrt{m^2y^2/4}}{\sqrt{m^2y^2/4}}(\epsilon^\mu y^\nu - \epsilon^\nu y^\mu) v_\nu \\ & - z\frac{m^2}{\cosh\sqrt{m^2\phi^2}}\frac{\sin\sqrt{m^2y^2}}{\sqrt{m^2y^2}}[P_L^{\mu\nu}(v) + \sqrt{v^2}\coth\sqrt{v^2} P_T^{\mu\nu}(v)] y_\nu \\ & + \sqrt{m^2/4}\frac{\tan\sqrt{m^2y^2/4}}{\sqrt{m^2y^2/4}}\tanh\sqrt{m^2\phi^2}(b^\mu y^\nu - b^\nu y^\mu) v_\nu \\ & + \frac{1}{\cosh\sqrt{m^2\phi^2}}[P_L^{\mu\nu}(v) + \sqrt{v^2}\coth\sqrt{v^2} P_T^{\mu\nu}(v)][\cos\sqrt{m^2y^2} P_{L\nu\rho}(y) + P_{T\nu\rho}(y)] b^\rho, \end{aligned}$$

$$\theta^{\mu\nu}(y)=\lambda^{\mu\nu}+\frac{m^2}{2}\frac{\tan\sqrt{m^2y^2/4}}{\sqrt{m^2y^2/4}}(\epsilon^\mu y^\nu-\epsilon^\nu y^\mu)-z\frac{m^2}{\cosh\sqrt{m^2\phi^2}}\frac{\sin\sqrt{m^2y^2}}{\sqrt{m^2y^2}}(v^\mu y^\nu-v^\nu y^\mu)\frac{\tanh\sqrt{v^2/2}}{\sqrt{v^2}}$$
$$-\sqrt{m^2/4}\frac{\tan\sqrt{m^2y^2/4}}{\sqrt{m^2y^2/4}}\tanh\sqrt{m^2\phi^2}(b^\mu y^\nu-b^\nu y^\mu)-\frac{1}{\cosh\sqrt{m^2\phi^2}}\frac{\tanh\sqrt{v^2/2}}{\sqrt{v^2}}$$
$$\times[\cos\sqrt{m^2y^2}P_L^{\mu\rho}(y)b_\rho v^\nu+P_T^{\mu\rho}(y)b_\rho v^\nu-(\mu\leftrightarrow\nu)]. \tag{2.6}$$

The nonlinearly realized $SO(2,d)$ transformations induce a field dependent general coordinate transformation of the world volume space-time coordinates. Using the y^μ coordinate transformation given above, the AdS_{d+1} general coordinate transformation for the world volume space-time coordinate differentials is given by

$$dy'^\mu=dy^\nu\overline{G}_\nu{}^\mu, \tag{2.7}$$

with $\overline{G}_\nu{}^\mu=\partial y'^\mu/\partial y^\nu$. The $SO(2,d)$ invariant interval can be formed using the metric tensor $g_{\mu\nu}(y)$ so that $ds^2=dy^\mu g_{\mu\nu}(y)dy^\nu=ds'^2=dy'^\mu g'_{\mu\nu}(y')dy'^\nu$ where the metric tensor transforms as

$$g'_{\mu\nu}(y')=\overline{G}^{-1\rho}_\mu g_{\rho\sigma}(y)\overline{G}^{-1\sigma}_\nu. \tag{2.8}$$

The form of the vielbein (and hence the metric tensor) as well as the $SO(2,d)$ covariant derivatives of the Nambu-Goldstone boson fields and the spin connection can be extracted from the Maurer-Cartan one-form, $\Omega^{-1}d\Omega$, which can be expanded in terms of the generators as

$$\Omega^{-1}d\Omega=i\left[\omega^m P_m+\omega_Z Z+\omega_K^m K_m+\tfrac{1}{2}\omega_M^{mn}M_{mn}\right]. \tag{2.9}$$

Italic indices $m,n=0,1,\ldots,d-1$, are used to distinguish tangent space (italic indices) transformation properties from world volume (greek indices) transformation properties. Recall all contracted indices (italic or greek) are summed using the d-dimensional Minkowski metric tensor. Applying the Feynman formula for the variation of an exponential operator in conjunction with the Baker-Campell-Hausdorff formulas, the individual world volume one-forms appearing in the above decomposition of the Maurer-Cartan one-form are secured as

$$\omega^m=-\frac{\sinh\sqrt{v^2}}{\sqrt{v^2}}v^m d\phi+\cosh\sqrt{m^2\phi^2}[P_T^{mn}(v)+\cosh\sqrt{v^2}P_L^{mn}(v)]\overline{\omega}_n,$$

$$\omega_Z=\cosh\sqrt{v^2}\left[d\phi-\cosh\sqrt{m^2\phi^2}\overline{\omega}_m v^m\frac{\tanh\sqrt{v^2}}{\sqrt{v^2}}\right],$$

$$\omega_K^m=dv^m-\left(\frac{\sinh\sqrt{v^2}}{\sqrt{v^2}}-1\right)\frac{[v^m v_n dv^n-v^2dv^m]}{v^2}-\overline{\omega}_M^{mn}v_n\frac{\sinh\sqrt{v^2}}{\sqrt{v^2}}$$
$$+\sqrt{m^2}\sinh\sqrt{m^2\phi^2}[P_L^{mn}(v)+\cosh\sqrt{v^2}P_T^{mn}(v)]\overline{\omega}_n,$$

$$\omega_M^{mn}=\overline{\omega}_M^{mn}+[\cosh\sqrt{v^2}-1]\frac{v^m dv^n-v^n dv^m}{v^2}-(\cosh\sqrt{v^2}-1)[P_{Lr}^m(v)\overline{\omega}_M^{nr}-P_{Lr}^n(v)\overline{\omega}_M^{mr}]$$
$$+\sqrt{m^2}\sinh\sqrt{m^2\phi^2}\frac{\sinh\sqrt{v^2}}{\sqrt{v^2}}\overline{\omega}_r[v^m P_T^{rn}(v)-v^n P_T^{rm}(v)]. \tag{2.10}$$

In these expressions, the AdS_d covariant coordinate differential, $\overline{\omega}^m$, and spin connection, $\overline{\omega}_M^{mn}$, are obtained from the AdS_d coordinate one-form $(e^{-iy^m P_m})d(e^{iy^n P_n})=i\left[\overline{\omega}^m P_m+\frac{1}{2}\overline{\omega}_M^{mn}M_{mn}\right]$ as

$$\overline{\omega}^m = \frac{\sin\sqrt{m^2y^2}}{\sqrt{m^2y^2}} P_T^{mn}(y)\mathrm{d}y_n + P_L^{mn}(y)\mathrm{d}y_n,$$
$$\overline{\omega}_M^{mn} = [\cos\sqrt{m^2y^2} - 1]\frac{(y^m\mathrm{d}y^n - y^n\mathrm{d}y^m)}{y^2}. \tag{2.11}$$

The differential $\overline{\omega}^m$ is related to the y^μ world volume coordinate differential via the vielbein $\overline{e}_\mu{}^m(y)$ as

$$\overline{\omega}^m = \mathrm{d}y^\mu \overline{e}_\mu{}^m(y). \tag{2.12}$$

Using Eq. (2.11) along with $d=\mathrm{d}y^\mu\partial_\mu^y$, this vielbein is obtained as

$$\overline{e}_\mu{}^m(y) = \frac{\sin\sqrt{m^2y^2}}{\sqrt{m^2y^2}} P_{T\mu}{}^m(y) + P_{L\mu}{}^m(y). \tag{2.13}$$

Thus it is seen that the y coordinates correspond to the choice of embedding coordinates [cf. Eq. (1.3)]

$$a(y^2) = \frac{\sin\sqrt{m^2y^2}}{\sqrt{m^2y^2}},$$
$$b(y^2) = \cos(\sqrt{m^2y^2}). \tag{2.14}$$

The two sets of bases for coordinate differentials, $\mathrm{d}y^\mu$ and the AdS_{d+1} covariant one-form ω^m, are related to each other through the vielbein $e_\mu{}^m(y)$,

$$\omega^m(y) = \mathrm{d}y^\mu e_\mu{}^m(y). \tag{2.15}$$

Again using that $d=\mathrm{d}y^\mu\partial_\mu^y$, it follows from the first equality in Eq. (2.10) that the vielbein $e_\mu{}^m$ can be factorized as

$$e_\mu{}^m(y) = \overline{e}_\mu{}^n(y) N_n{}^m(y), \tag{2.16}$$

where the Nambu-Goto vielbein, $N_n{}^m(y)$, is

$$N_n{}^m(y) = -v^m\frac{\sinh\sqrt{v^2}}{\sqrt{v^2}}\mathcal{D}_n\phi + \cosh\sqrt{m^2\phi^2}[P_{Tn}^m(v) + \cosh\sqrt{v^2}P_{Ln}^m(v)], \tag{2.17}$$

and the AdS_d covariant derivative is defined as $\mathcal{D}_n=\overline{e}_n^{-1\mu}(y)\partial_\mu^y$.

III. THE INVARIANT ACTION

To construct an $\mathrm{SO}(2,d)$ invariant action, we begin by using [cf. Eqs. (2.3) and (2.5)]

$$\Omega'(y') = g\Omega(y)e^{-(i/2)\theta^{mn}(y)M_{mn}} \tag{3.1}$$

and isolating the coefficient of P_m in the decomposition of $(\Omega^{-1}\mathrm{d}\Omega)'(y')$ giving

$$\omega'^m(y')P_m = \omega^m(y)e^{(i/2)\theta^{lr}(y)M_{lr}}P_m e^{-(i/2)\theta^{st}(y)M_{st}}. \tag{3.2}$$

Next, from the $\mathrm{SO}(2,d)$ algebra (see Appendix B) it follows that

$$e^{(i/2)\theta^{lr}M_{lr}}P_m e^{-(i/2)\theta^{st}M_{st}} = \Lambda_m{}^n(\theta)P_n, \tag{3.3}$$

where $\Lambda_m{}^n(\theta)$ is an AdS_d (local) Lorentz transformation with parameter $\theta^{rs}(y)$ so that $\det\Lambda=1$.

Thus

$$\omega'^{m}(y') = dy'^{\nu} e'^{m}_{\nu}(y') = \omega^{n}(y)\Lambda_{n}{}^{m} = dy^{\rho} e_{\rho}{}^{n}(y)\Lambda_{n}{}^{m}, \tag{3.4}$$

where $dy'^{\mu} = dy^{\rho}\overline{G}_{\rho}{}^{\mu}$, Eq. (2.7). Consequently the vielbeins are related as

$$e_{\rho}{}^{n}(y)\Lambda_{n}{}^{m} = \overline{G}_{\rho}{}^{\nu} e'^{m}_{\nu}(y'). \tag{3.5}$$

Taking the determinant (using $\det \Lambda = 1$) then yields $\det e' = (\det \overline{G})^{-1} \det e$. Since the Jacobian of the $y^{\mu} \to y'^{\mu}$ transformation is simply

$$d^{d}y' = d^{d}y \det \overline{G}, \tag{3.6}$$

it follows that $d^{d}y' \det e'(y') = d^{d}y \det e(y)$. Thus an $SO(2,d)$ invariant action is constructed as

$$\Gamma = -\sigma \int d^{d}y \det e(y), \tag{3.7}$$

with the vacuum energy denoted by σ. Note that the action is simply the negative of the brane tension integrated over the invariant AdS volume.

An additional general coordinate transformation can be made taking the y^{μ} coordinates to the x^{μ} coordinates, $y^{\mu} = y^{\mu}(x)$, so that the $SO(2,d)$ invariant interval will assume the form $ds^2 = dx^{\mu} g_{\mu\nu}(x) dx^{\nu}$ with the metric tensor given by

$$g_{\mu\nu}(x) = \frac{\partial y^{\rho}(x)}{\partial x^{\mu}} g_{\rho\sigma}(y(x)) \frac{\partial y^{\sigma}(x)}{\partial x^{\nu}} = a_{\mu}{}^{\rho}(x) g_{\rho\sigma}(y(x)) a_{\nu}{}^{\sigma}(x). \tag{3.8}$$

The transformation matrix associated with this change of variables is defined to be $a_{\mu}{}^{\rho}(x) = \partial y^{\rho}(x)/\partial x^{\mu}$. Consequently the $SO(2,d)$ transformations similarly induce a field dependent general coordinate transformation of these new world volume coordinates

$$x'^{\mu} = x^{\mu} + a^{-1\mu}_{\nu}(x)\, \delta y^{\nu}(x), \tag{3.9}$$

where the corresponding $SO(2,d)$ variation of y^{μ} is given in Eq. (2.6), $\delta y^{\mu} = y'^{\mu} - y^{\mu}$. From Eq. (3.9), the new coordinate differentials transform as

$$dx'^{\mu} = dx^{\nu} G_{\nu}{}^{\mu}, \tag{3.10}$$

with $G_{\nu}{}^{\mu} = \partial x'^{\mu}/\partial x^{\nu}$. Relating the coordinate differentials through the transformation matrix, $dy^{\mu} = dx^{\nu}(\partial y^{\mu}/\partial x^{\nu}) = dx^{\nu} a_{\nu}{}^{\mu}$ and likewise for the $SO(2,d)$ transformed coordinates, $dy'^{\mu} = dx'^{\nu}(\partial y'^{\mu}/\partial x'^{\nu}) = dx'^{\nu} a'^{\mu}_{\nu}$, the variation of the transformation matrix is obtained,

$$a'^{\mu}_{\nu} = \frac{\partial y'^{\mu}}{\partial x'^{\nu}} = \frac{\partial y'^{\mu}}{\partial y^{\sigma}} \frac{\partial y^{\sigma}}{\partial x^{\rho}} \frac{\partial x^{\rho}}{\partial x'^{\nu}} = G^{-1\rho}_{\nu} a_{\rho}{}^{\sigma} \overline{G}_{\sigma}{}^{\mu}. \tag{3.11}$$

Hence the invariance of the interval in terms of the new x^{μ} coordinates is secured since $g'_{\mu\nu}(x') = G^{-1\rho}_{\mu} g_{\rho\sigma}(x) G^{-1\sigma}_{\nu}$.

The covariant coordinate differential one-forms are related to the new coordinate differentials dx^{μ} through the vielbein $e_{\mu}{}^{m}(x)$ as

$$\omega^{m}(x) = dx^{\mu} e_{\mu}{}^{m}(x). \tag{3.12}$$

Thus the y^{μ} and the x^{μ} coordinate vielbein are related by the transformation matrix

$$e_{\mu}{}^{m}(x) = a_{\mu}{}^{\nu} e_{\nu}{}^{m}(y). \tag{3.13}$$

In a similar fashion, the $\overline{\omega}^{m}$ one-form can also be expanded in terms of dx^{μ} as $\overline{\omega}^{m} = dx^{\mu}\, \overline{e}_{\mu}{}^{m}(x) = dy^{\mu}\, \overline{e}_{\mu}{}^{m}(y)$ thus giving

$$\overline{e}_{\mu}{}^{m}(x) = a_{\mu}{}^{\nu}\overline{e}_{\nu}{}^{m}(y). \tag{3.14}$$

The AdS_d covariant derivative has the same form in either coordinate system,

$$\mathcal{D}_m = \overline{e}{}^{-1\mu}_{m}(y)\partial^{y}_{\mu} = \overline{e}{}^{-1\mu}_{m}(y)a^{-1\nu}_{\mu}\partial^{x}_{\nu} = \overline{e}{}^{-1\mu}_{m}(x)\partial^{x}_{\mu} \tag{3.15}$$

as does the Nambu-Goto vielbein $N_n{}^m$. Thus Eq. (2.17), after making the replacements $\phi(y) = \phi(y(x)) \to \phi(x)$ and $v^m(y) = v^m(y(x)) \to v^m(x)$, reads

$$N_n{}^m(x) = -v^m\frac{\sinh(\sqrt{v^2})}{\sqrt{v^2}}\mathcal{D}_n\phi + \cosh\sqrt{m^2\phi^2}\left[P^m_{Tn}(v) + \cosh(\sqrt{v^2})P^m_{Ln}(v)\right]. \tag{3.16}$$

It follows that the x coordinate vielbein also has the factorized form

$$e_{\mu}{}^{m}(x) = a_{\mu}{}^{\nu}e_{\nu}{}^{m}(y) = a_{\mu}{}^{\nu}\overline{e}_{\nu}{}^{n}(y)N_n{}^m(y) = \overline{e}_{\mu}{}^{n}(x)N_n{}^m(x). \tag{3.17}$$

Using Eq. (3.13), the $\mathrm{SO}(2,d)$ invariant action in the x coordinate system then becomes

$$\begin{aligned}\Gamma &= -\sigma\int \mathrm{d}^d y \det e(y) = -\sigma\int \mathrm{d}^d x \det a \det a^{-1}\det e(x)\\ &= -\sigma\int \mathrm{d}^d x \det e(x) = -\sigma\int \mathrm{d}^d x \det \overline{e}(x)\det N(x).\end{aligned} \tag{3.18}$$

Finally, the determinant of the Nambu-Goto vielbein is evaluated as

$$\det N = \cosh^d(m\phi)\cosh(\sqrt{v^2})\left[1 - \left(v^n\frac{\tanh(\sqrt{v^2})}{\sqrt{v^2}}\right)\left(\frac{\mathcal{D}_n\phi}{\cosh(m\phi)}\right)\right], \tag{3.19}$$

so that the action (3.18) reads

$$\Gamma = -\sigma\int \mathrm{d}^d x \det \overline{e}(x)\cosh^d(m\phi)\cosh(\sqrt{v^2})\left[1 - \left(v^n\frac{\tanh(\sqrt{v^2})}{\sqrt{v^2}}\right)\left(\frac{\mathcal{D}_n\phi}{\cosh(m\phi)}\right)\right]. \tag{3.20}$$

Note that the v^n field is not an independent dynamical degree of freedom since it enters the action with no derivative. Hence it can be expressed in terms of the Nambu-Goldstone boson ϕ through its field equation as

$$v_n\frac{\tanh\sqrt{v^2}}{\sqrt{v^2}} = \frac{\mathcal{D}_n\phi}{\cosh\sqrt{m^2\phi^2}}. \tag{3.21}$$

This relation is identical to that obtained by setting to zero the $\mathrm{SO}(2,d)$ invariant second equality in Eq. (2.10) from the expansion of the Maurer-Cartan one-form, $\omega_Z = 0$. This is referred to as the "inverse Higgs mechanism."[8] Exploiting this relation, the final form of the Nambu-Goto action for an AdS_d brane embedded in AdS_{d+1} target space is secured,

$$\Gamma = -\sigma\int \mathrm{d}^d x \det e = -\sigma\int \mathrm{d}^d x \det \overline{e}\cosh^d(m\phi)\sqrt{1 - \frac{\mathcal{D}_\ell\phi\eta^{\ell n}\mathcal{D}_n\phi}{\cosh^2(m\phi)}}. \tag{3.22}$$

This is the AdS space generalization of the Nambu-Goto action for the Nambu-Goldstone mode. Expanding the action through terms bilinear in ϕ gives

$$\Gamma = -\sigma \int d^d x \det \overline{e} \left\{ 1 + \frac{1}{2}(d\ m^2)\phi^2 - \frac{1}{2}\partial_\mu \phi \overline{g}^{\mu\nu}\partial_\nu \phi + \cdots \right\}. \tag{3.23}$$

It is seen that the Nambu-Goldstone boson carries the $(E,s)=(d,0)$ representation[5] of $SO(2,d-1)$. That is, it has mass squared equal to $d\ m^2$ and hence energy d in units of m while being spin zero.

Note that the form of the action, Eq. (3.22), also follows from the invariant interval of the AdS_{d+1} space, Eq. (1.5), provided one identifies the covolume coordinate r with the Nambu-Goldstone field $\phi(x), r\to\phi(x)$. Using this identification, the interval can be written as $ds^2 = dx^\mu g_{\mu\nu}(x) dx^\nu$, with

$$g_{\mu\nu}(x) = \overline{g}_{\mu\nu}(x)\cosh^2(m\phi) - \partial_\mu\phi\partial_\nu\phi. \tag{3.24}$$

The $SO(2,d)$ invariant AdS_d brane action, Γ, can then be constructed from $g_{\mu\nu}$ as

$$\Gamma = -\sigma \int d^d x \sqrt{-(-1)^d \det g_{\mu\nu}}. \tag{3.25}$$

Introducing the AdS_d vielbein, $\overline{e}_\mu{}^m(x)$, via $\overline{g}_{\mu\nu} = \overline{e}_\mu{}^m \eta_{mn} \overline{e}_\nu{}^n$, as in Eq. (1.9), and likewise the AdS_{d+1} vielbein, $e_\mu{}^m(x)$ as $g_{\mu\nu} = e_\mu{}^m \eta_{mn} e_\nu{}^n$, it then follows that $e_\mu{}^m$ has the factorized form

$$e_\mu{}^n(x) = \overline{e}_\mu{}^\ell(x) N_\ell{}^n(x), \tag{3.26}$$

where the Nambu-Goto vielbein, $N_n{}^m$ is given by

$$N_\ell{}^n(x) = \delta_\ell{}^n \cosh(m\phi(x)) + \left[\sqrt{(\cosh^2(m\phi(x)) - \mathcal{D}_r\phi(x)\,\eta^{rs}\mathcal{D}_s\phi(x))} - \cosh(m\phi(x))\right] \frac{\mathcal{D}_\ell\phi(x)\mathcal{D}^n\phi(x)}{(\mathcal{D}\phi)^2(x)}. \tag{3.27}$$

The action can then be expressed in terms of the vielbein as

$$\begin{aligned}\Gamma &= -\sigma \int d^d x \det e(x) = -\sigma \int d^d x \det \overline{e}(x) \det N(x) \\ &= -\sigma \int d^d x \det \overline{e}(x) \cosh^d(m\phi(x)) \sqrt{1 - \frac{\mathcal{D}_\ell\phi(x)\,\eta^{\ell n}\mathcal{D}_n\phi(x)}{\cosh^2(m\phi(x))}},\end{aligned} \tag{3.28}$$

which is precisely Eq. (3.22).

Next reconsider the action with both Nambu-Goldstone fields ϕ and v^m present and independent as given in Eq. (3.20),

$$\Gamma = -\sigma \int d^d x \det \overline{e} \left[\cosh^d(\sqrt{m^2\phi^2}) \cosh(\sqrt{v^2}) - \cosh^{d-1}\sqrt{(m^2\phi^2)} \frac{\sinh(\sqrt{v^2})}{\sqrt{v^2}} v^m \mathcal{D}_m\phi \right]. \tag{3.29}$$

Defining the (ϕ independent) vector density field F^μ as

$$F^\mu \equiv \det \overline{e} \frac{\sinh(\sqrt{v^2})}{\sqrt{v^2}} v^n \overline{e}_n^{-1\mu}, \tag{3.30}$$

the v^n dependent terms can be expressed as F^μ and

$$\det \overline{e} \cosh(\sqrt{v^2}) = \sqrt{(\det \overline{e})^2 + F^\mu \overline{g}_{\mu\nu} F^\nu} = \sqrt{-(-1)^d \det \overline{g}_{\mu\nu} + F^\mu \overline{g}_{\mu\nu} F^\nu} = \sqrt{-(-1)^d \det(\overline{g}_{\mu\nu} + F_\mu F_\nu)}, \tag{3.31}$$

where the covariant vector field is

$$F_\mu = \frac{1}{\det \overline{e}} \overline{g}_{\mu\nu} F^\nu. \tag{3.32}$$

The action can then be written as

$$\Gamma = -\sigma \int \mathrm{d}^d x [\sqrt{-(-1)^d \det(\overline{g}_{\mu\nu} + F_\mu F_\nu)} \cosh^d(m\phi) - F^\mu \partial_\mu \phi \cosh^{d-1}(m\phi)]. \tag{3.33}$$

Expressing the second term on the right-hand side as

$$\partial_\mu \phi \cosh^{d-1}(m\phi) = \partial_\mu f(\phi) \tag{3.34}$$

so that $\mathrm{d}f/\mathrm{d}\phi = \cosh^{d-1}(m\phi)$, the action, after integrating the second term by parts, can be written as

$$\Gamma = -\sigma \int d^d x [\sqrt{-(-1)^d \det(\overline{g}_{\mu\nu} + F_\mu F_\nu)} \cosh^d(m\phi) + f(\phi) \partial_\mu F^\mu]. \tag{3.35}$$

Note that in the Poincaré limit, $m \to 0$, the action reduces to $\Gamma \to -\sigma \int \mathrm{d}^d x [\sqrt{1+F^2} + \phi \partial_\mu F^\mu]$. In that case, the ϕ field equation, $\delta\Gamma/\delta\phi = 0 = \partial_\mu F^\mu$, is just the Bianchi identity for F^μ. That is, the dual of F^μ is closed. Hence F^μ can be (locally) expressed as $F^\mu = \epsilon^{\mu\nu(\rho)} \partial_\nu B_{(\rho)}$, where the $(d-2)$-form $B_{(\rho)}$ is a tensor gauge potential. Eliminating the ϕ term from the action by integration by parts, the tensor gauge theory action dual to the bosonic Poincaré brane Nambu-Goto action is obtained.[13] The situation for $m \neq 0$ is quite different.

Now the ϕ field equation

$$\frac{\delta\Gamma}{\delta\phi} = 0 = -\sigma \frac{\mathrm{d}f(\phi)}{\mathrm{d}\phi} [\partial_\mu F^\mu + \mathrm{d}\ m \sinh(m\phi) \det \overline{e} \cosh(\sqrt{v^2})] \tag{3.36}$$

can be used to eliminate it from the action. Introducing a Lagrange multiplier field L to enforce this equality, the action becomes

$$\Gamma = -\sigma \int \mathrm{d}^d x [\sqrt{-(-1)^d \det(\overline{g}_{\mu\nu} + F_\mu F_\nu)} (T(\phi) + L\ \mathrm{d}\ m \sinh(m\phi)) + L \partial_\mu F^\mu], \tag{3.37}$$

where

$$T(\phi) = \cosh^d(m\phi) - \mathrm{d}\ m\ f(\phi) \sinh(m\phi). \tag{3.38}$$

After employing Eq. (3.36) to eliminate the ϕ and L fields, the action takes the form

$$\Gamma = -\sigma \int \mathrm{d}^d x \sqrt{(-1)^{d-1} \det(\overline{g}_{\mu\nu} + F_\mu F_\nu)} T(F). \tag{3.39}$$

Here $T(\phi) = T(\phi(F)) \to T(F)$ where the implicit dependence of ϕ on F^μ is given by

$$\sinh m\phi = -\frac{\partial_\mu F^\mu}{\mathrm{d}\ m \sqrt{-(-1)^d \det(\overline{g}_{\mu\nu} + F_\mu F_\nu)}}, \tag{3.40}$$

which follows from the equation of motion (3.36).

Expanding T through terms bilinear in the field gives

$$T(F) = 1 - \frac{1}{2} \mathrm{d}\ m^2 \phi^2 + \mathcal{O}(\phi^3) = 1 - \left(\frac{1}{\mathrm{d}\ m^2 \det^2 \overline{e}} \right) (\partial_\mu F^\mu)^2 + \cdots. \tag{3.41}$$

Substituting this into Eq. (3.39) and expanding the square root, the bilinear in the field F^μ form of the action becomes

$$\Gamma = -\sigma \int d^d x \det \overline{e} \left\{ 1 + \left(\frac{1}{m^2 d \det^2 \overline{e}} \right) \left[\frac{1}{2}(m^2 d) F^\mu \overline{g}_{\mu\nu} F^\nu - \frac{1}{2} \partial_\mu F^\mu \partial_\nu F^\nu + \cdots \right] \right\}. \quad (3.42)$$

The ellipses refer to the F^μ field self-interactions.

The F_μ field equation then gives

$$\det \overline{e}\, \overline{g}^{\mu\nu} \partial_\nu \left(\frac{1}{\det \overline{e}} \partial_\lambda F^\lambda \right) - \mathrm{d}\, m^2 F^\mu = J^\mu, \quad (3.43)$$

where J_μ contains the F field self-interactions contained in the ellipses. Taking the divergence of Eq. (3.43), it follows that the longitudnal projection $F_L \equiv (1/\det \overline{e}) \partial_\mu F^\mu$ satisfies the equation

$$\left[\overline{g}^{\mu\nu} \partial_\mu \partial_\nu - \mathrm{d}\, m^2 + \frac{1}{\det \overline{e}} \partial_\mu (\det \overline{e}\, \overline{g}^{\mu\nu}) \partial_\nu \right] F_L = \frac{1}{\det \overline{e}} \partial_\mu J^\mu. \quad (3.44)$$

The differential operator on the left-hand side acting on F_L is identical to the differential operator acting on ϕ which appears in the ϕ field equation resulting from the AdS Nambu-Goto action. Thus the longitudinal mode F_L describes a propagating scalar degree of freedom with mass $\mathrm{d}\, m^2$ and Eq. (3.39) is the vector field action equivalent to the Nambu-Goto action in AdS space. On the other hand, using the field equation (3.43), the transverse component of F is constrained to satisfy

$$\mathrm{d}\, m^2 \epsilon^{\mu_1 \mu_2 \cdots \mu_d} \partial_{\mu_1} \left[\frac{1}{\det \overline{e}} \overline{g}_{\mu_2 \nu} F^\nu \right] = -\epsilon^{\mu_1 \mu_2 \cdots \mu_d} \partial_{\mu_1} \left[\frac{1}{\det \overline{e}} \overline{g}_{\mu_2 \nu} J^\nu \right]. \quad (3.45)$$

Indeed this equivalence can be run in reverse. Starting with Eq. (3.39), the Lagrange multiplier field L can be reintroduced to give Eq. (3.37) [recall that $T(\phi) = \cosh^d(m\phi) - \mathrm{d}\, m\, g(\phi) \sinh(m\phi)$]. The fields ϕ, F^μ, and L are all independent. Hence the ϕ field equation, $\delta\Gamma/\delta\phi = 0$ implies that $L = g(\phi)$. Substituting this into the action along with the definition of F^μ in terms of v^n, Eq. (3.30), and integrating by parts, the Nambu-Goto action equation (3.29) is once again obtained.

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APPENDIX A: AdS COORDINATES

An AdS_d brane embedded as a $r=0$ hypersurface in an AdS_{d+1} target space has intrinsic coordinates x^μ with the pseudo-Euclidean $(d+2)$-dimensional homogeneous coordinates given as in Eq. (1.3),

$$X^\mu = a(x^2) x^\mu \cosh(mr),$$

$$X^d = \frac{1}{m} \sinh(mr), \quad (A1)$$

$$X^{d+1} = \frac{1}{m} b(x^2) \cosh(mr).$$

The AdS_{d+1} target space and the embedded AdS_d brane hyperbolic equations require the coordinate relation $1 = m^2 x^2 a^2 + b^2$. This leads to a form of the AdS_d metric tensor, Eq. (1.6),

$$\overline{g}_{\mu\nu}(x) = a^2(x^2)P_{T\mu\nu}(x) + \left[\left(a(x^2) + 2x^2\frac{da(x^2)}{dx^2}\right)^2 + 4\frac{x^2}{m^2}\left(\frac{db(x^2)}{dx^2}\right)^2\right]P_{L\mu\nu}(x)$$
$$= a^2(x^2)P_{T\mu\nu}(x) + \frac{\left(a(x^2) + 2x^2\frac{da(x^2)}{dx^2}\right)^2}{1 - m^2x^2a^2(x^2)}P_{L\mu\nu} \tag{A2}$$

and the AdS_d vielbein, Eq. (1.9),

$$\overline{e}_\mu{}^m(x) = a(x^2)P_{T\mu}{}^m(x) + \sqrt{\left[\left(a(x^2) + 2x^2\frac{da(x^2)}{dx^2}\right)^2 + 4\frac{x^2}{m^2}\left(\frac{db(x^2)}{dx^2}\right)^2\right]}P_{L\mu}{}^m(x)$$
$$= a(x^2)P_{T\mu}{}^m(x) + \frac{\left(a(x^2) + 2x^2\frac{da(x^2)}{dx^2}\right)}{\sqrt{1 - m^2x^2a^2(x^2)}}P_{L\mu}{}^m(x). \tag{A3}$$

Only the case where a and b are functions of x^2 are considered.

The coset construction setup naturally led to a specific choice of intrinsic coordinates denoted by y^μ for which the functions a and b were given by Eq. (2.14),

$$a(y^2) = \frac{\sin(\sqrt{m^2y^2})}{\sqrt{m^2y^2}},$$
$$b(y^2) = \cos\sqrt{m^2y^2}. \tag{A4}$$

Hence the embedding relations for these homogeneous coordinates are

$$X^\mu = y^\mu\frac{\sin(\sqrt{m^2y^2})}{\sqrt{m^2y^2}}\cosh(mr),$$
$$X^d = \frac{1}{m}\sinh(mr), \tag{A5}$$
$$X^{d+1} = \frac{1}{m}\cos(\sqrt{m^2y^2})\cosh(mr).$$

The metric on the AdS_d brane was then given by the vielbein, Eq. (2.13),

$$\overline{e}_\mu{}^n(y) = \frac{\sin(\sqrt{m^2y^2})}{\sqrt{m^2y^2}}P_{T\mu}{}^n(y) + P_{L\mu}{}^n(y). \tag{A6}$$

A different choice of intrinsic coordinates x^μ that leaves the AdS_d vielbein $\overline{e}_\mu{}^n$ diagonal is given by

$$a(x^2) = \frac{4}{4 + m^2x^2},$$
$$b(x^2) = \left(\frac{4 - m^2x^2}{4 + m^2x^2}\right), \tag{A7}$$

hence the embedding relations for the homogeneous coordinates become

$$X^\mu = a(x^2)x^\mu \cosh(mr),$$

$$X^d = \frac{1}{m}\sinh(mr), \tag{A8}$$

$$X^{d+1} = a(x^2)\frac{1}{m}\left(\frac{4-m^2x^2}{4}\right)\cosh(mr).$$

The metric on the AdS_d brane is then given by the vielbein,

$$\overline{e_\mu}^n(x) = a(x^2)\delta_\mu{}^n = \left(\frac{4}{4+m^2x^2}\right)\delta_\mu{}^m. \tag{A9}$$

Note that in the Poincaré limit, $m \to 0$, this reduces to the Minkowski metric and vielbein.

The transformation between the x and y coordinates is found by substituting the transformation $y^\mu = x^\mu f(x^2)$ into the expression for $\overline{\omega}^m$ in Eq. (2.11) and requiring a diagonal vielbein. In the process, the function $a(x^2)$ is also determined. The resulting differential equation for f,

$$2x^2 f'(x^2) = -f(x^2)\left(1 - \frac{\sin\sqrt{m^2x^2f(x^2)}}{\sqrt{m^2x^2f(x^2)}}\right), \tag{A10}$$

has the solution

$$f(x^2) = \frac{2\tan^{-1}\sqrt{m^2x^2/4}}{\sqrt{m^2x^2}}. \tag{A11}$$

Hence the coordinate transformation is given by

$$y^\mu = x^\mu \frac{\tan^{-1}\sqrt{m^2x^2/4}}{\sqrt{m^2x^2/4}}, \tag{A12}$$

while the inverse relation is

$$x^\mu = y^\mu \frac{\tan\sqrt{m^2y^2/4}}{\sqrt{m^2y^2/4}}. \tag{A13}$$

In the Poincaré limit, the x and y coordinates are identical, $y^\mu = x^\mu$. In AdS space the transformation matrix between these coordinates is

$$a_\mu{}^\nu(x) = \partial^x_\mu y^\nu(x) = \frac{\tan^{-1}\sqrt{m^2x^2/4}}{\sqrt{m^2x^2/4}}P_{T\mu}{}^\nu(x) + a(x^2)P_{L\mu}{}^\nu(x). \tag{A14}$$

This choice of coordinates has the advantage of simplifying the variations of the fields as well as the transformations of the coordinates themselves. Transforming Eq. (2.6) from y to x coordinates yields

$$x'^\mu = x^\mu + \frac{1}{4}(4-m^2x^2)\epsilon^\mu + \frac{m^2}{2}(\epsilon_\nu x^\nu)x^\mu - \lambda^{\mu\nu}x_\nu - zx^\mu\sqrt{m^2}\tanh\sqrt{m^2\phi^2}$$
$$+ \frac{1}{4}\frac{\tanh\sqrt{m^2\phi^2}}{\sqrt{m^2}}[(4-m^2x^2)P_L^{\mu\nu}(x) + (4+m^2x^2)P_T^{\mu\nu}(x)]b_\nu,$$

$$\phi'(x') = \phi(x) + z\left[\frac{4-m^2x^2}{4+m^2x^2}\right] + a(x^2)x^\mu b_\mu,$$

$$v'^{\mu}(x') = v^{\mu}(x) - \lambda^{\mu\nu}v_{\nu} - \frac{m^2}{2}(\epsilon^{\mu}x^{\nu} - \epsilon^{\nu}x^{\mu})v_{\nu} - za(x^2)\frac{m^2}{\cosh\sqrt{m^2\phi^2}}[P_L^{\mu\nu}(v) + \sqrt{v^2}\coth\sqrt{v^2}P_T^{\mu\nu}(v)]x_{\nu}$$
$$+ \frac{\sqrt{m^2}}{2}\tanh\sqrt{m^2\phi^2}(b^{\mu}x^{\nu} - b^{\nu}x^{\mu})v_{\nu} + \frac{1}{\cosh\sqrt{m^2\phi^2}}[P_L^{\mu\nu}(v) + \sqrt{v^2}\coth\sqrt{v^2}P_T^{\mu\nu}(v)]$$
$$\times\left[P_{T\nu\rho}(x) + \left(\frac{4-m^2x^2}{4+m^2x^2}\right)P_{L\nu\rho}(x)\right]b^{\rho},$$

$$\theta^{\mu\nu} = \lambda^{\mu\nu} + \frac{m^2}{2}(\epsilon^{\mu}x^{\nu} - \epsilon^{\nu}x^{\mu}) - za(x^2)\frac{m^2}{\cosh\sqrt{m^2\phi^2}}\frac{\tanh\sqrt{v^2/2}}{\sqrt{v^2}}(v^{\mu}x^{\nu} - v^{\nu}x^{\mu})$$
$$- \frac{\sqrt{m^2}}{2}\tanh\sqrt{m^2\phi^2}(b^{\mu}x^{\nu} - b^{\nu}x^{\mu}) - \frac{1}{\cosh\sqrt{m^2\phi^2}}\frac{\tanh\sqrt{v^2/2}}{\sqrt{v^2}}$$
$$\times\left[P_T^{\mu\rho}(x)b_{\rho}v^{\nu} + \left(\frac{4-m^2x^2}{4+m^2x^2}\right)P_L^{\mu\rho}(x)b_{\rho}v^{\nu} + -(\mu\leftrightarrow\nu)\right]. \tag{A15}$$

APPENDIX B: AdS SYMMETRY CHARGE ALGEBRA

AdS_{d+1} space can be viewed as a hyperboloid embedded in a $(d+2)$-dimensional pseudo-Euclidean space. The equation of such a hypersurface is given in Eq. (1.1),

$$\frac{1}{m^2} = X_0^2 - X_1^2 - X_2^2 - \cdots - X_d^2 + X_{d+1}^2 = X^{\mathcal{M}}\hat{\eta}_{\mathcal{M}\mathcal{N}}X^{\mathcal{N}}. \tag{B1}$$

Here the pseudo-Euclidean metric tensor $\hat{\eta}_{\mu\nu}$ has signature $(+1,-1,-1,\cdots,-1,+1)$ and $\mathcal{M},\mathcal{N} = 0,1,\cdots,d,d+1$. It follows that the isometry group of this AdS_{d+1} space is $\mathrm{SO}(2,d)$. Denoting the symmetry generators as $M^{\mathcal{M}\mathcal{N}}$, they obey the algebra

$$[M^{\mathcal{M}\mathcal{N}},M^{\mathcal{R}\mathcal{S}}] = -i(\hat{\eta}^{\mathcal{M}\mathcal{R}}M^{\mathcal{N}\mathcal{S}} - \hat{\eta}^{\mathcal{M}\mathcal{S}}M^{\mathcal{N}\mathcal{R}} + \hat{\eta}^{\mathcal{N}\mathcal{S}}M^{\mathcal{M}\mathcal{R}} - \hat{\eta}^{\mathcal{N}\mathcal{R}}M^{\mathcal{M}\mathcal{S}}). \tag{B2}$$

The $\mathrm{SO}(1,d)$ subgroup of Lorentz transformations in AdS_{d+1} space is generated by the charges M^{MN}, where $M,N=0,1,\ldots,d$. The remaining $\mathrm{SO}(2,d)$ generators are the pseudotranslations in AdS_{d+1} space and are given by the Lorentz group vectors $P^M = mM^{d+1,M}$. In terms of P^M and M^{MN}, the $\mathrm{SO}(2,d)$ algebra (B2) reads

$$[M^{MN},M^{RS}] = -i(\eta^{MR}M^{NS} - \eta^{MS}M^{NR} + \eta^{NS}M^{MR} - \eta^{NR}M^{MS}),$$

$$[M^{MN},P^L] = i(P^M\eta^{NL} - P^N\eta^{ML}), \tag{B3}$$

$$[P^M,P^N] = -im^2M^{MN},$$

where the $(d+1)$-dimensional Minkowski metric $\eta_{MN}=(+1,-1,-1,\ldots,-1)$.

An AdS_d brane embedded in the AdS_{d+1} space as a $X^d=0$ hypersurface is described by the hyperboloidal hypersurface

$$\frac{1}{m^2} = X_0^2 - X_1^2 - \cdots - X_{d-1}^2 + X_{d+1}^2. \tag{B4}$$

The brane spontaneously breaks the isometry group of the AdS_{d+1} space from $\mathrm{SO}(2,d)$ to $\mathrm{SO}(2,d-1)$, which is the isometry group of the AdS_d space. The $\mathrm{SO}(2,d)$ generators can be expressed in terms of the unbroken $\mathrm{SO}(1,d-1)$ Lorentz subgroup representation content of the $\mathrm{SO}(2,d-1)$ symmetry group of the brane. The unbroken $\mathrm{SO}(2,d-1)$ symmetry group is generated

by the subgroup Lorentz transformation generators $M^{\mu\nu}$, where $\mu,\nu=0,1,2,\ldots,d-1$ and the pseudotranslations in AdS_d space with charges P^μ. The remaining charges are the generating elements of the $SO(2,d)/SO(2,d-1)$ coset. They are the broken $SO(2,d)$ symmetry transformation charges. $Z=P_d$ generates the broken $SO(2,d)$ pseudotranslations in the X_d direction, while $K^\mu=M^{d\mu}$ generates the broken AdS_{d+1} Lorentz transformations. Thus the $SO(2,d)$ algebra, Eqs. (B2) and (B3), can be written in terms of the $P^\mu, M^{\mu\nu}, Z$, and K^μ charges as

$$
\begin{aligned}
[M^{\mu\nu},M^{\rho\sigma}] &= -i(\eta^{\mu\rho}M^{\nu\sigma}-\eta^{\mu\sigma}M^{\nu\rho}+\eta^{\nu\sigma}M^{\mu\rho}-\eta^{\nu\rho}M^{\mu\sigma}),\\
[M^{\mu\nu},P^\lambda] &= i(P^\mu\eta^{\nu\lambda}-P^\nu\eta^{\mu\lambda}),\\
[M^{\mu\nu},K^\lambda] &= i(K^\mu\eta^{\nu\lambda}-K^\nu\eta^{\mu\lambda}),\\
[M^{\mu\nu},Z] &= 0,\\
[P^\mu,P^\nu] &= -im^2M^{\mu\nu},\\
[K^\mu,K^\nu] &= iM^{\mu\nu},\\
[P^\mu,K^\nu] &= i\eta^{\mu\nu}Z,\\
[P^\mu,Z] &= -im^2K^\mu,\\
[Z,K^\mu] &= iP^\mu.
\end{aligned}
\tag{B5}
$$

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Rigorous dynamics and radiation theory for a Pauli-Fierz model in the ultraviolet limit

Massimo Bertini[a)]
Dipartimento di Matematica, Università di Milano, I-20133 Milano, Italy

Diego Noja[b)]
Dipartimento di Matematica e Applicazioni, Università di Milano-Bicocca, I-20126, Milano, Italy

Andrea Posilicano[c)]
Dipartimento di Scienze Fisiche e Matematiche, Università dell'Insubria, I-22100 Como, Italy

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The present paper is devoted to the detailed study of quantization and evolution of the point limit of the Pauli-Fierz model for a charged oscillator interacting with the electromagnetic field in dipole approximation. In particular, a well defined dynamics is constructed for the classical model, which is subsequently quantized according to the Segal scheme. To this end, the classical model in the point limit, already obtained by Noja and Posilicano [Ann. I.H.P. Phys. Theor. **71**, 425 (1999)], is reformulated as a second order abstract wave equation, and a consistent quantum evolution is given. This allows a study of the behavior of the survival and transition amplitudes for the process of decay of the excited states of the charged particle, and the emission of photons in the decay process. In particular, for the survival amplitude the exact time behavior is found. This is completely determined by the resonances of the systems plus a tail term prevailing in the asymptotic, long time regime. Moreover, the survival amplitude exhibits in a fairly clear way the Lamb shift correction to the unperturbed frequencies of the oscillator. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2009607]

I. INTRODUCTION

In recent years a considerable effort was tributed by the mathematical physics community to the problem of a rigorous formulation of the dynamics of the main models in nonrelativistic quantum field theory. In particular, a comprehensive study of the Pauli-Fierz model, the model which describes the low energy interaction of nonrelativistic matter and electromagnetic radiation, was undertaken by various authors, both in its full form, or making resort to different approximations, such as rotating wave approximation, dipole approximation, or others. Correspondingly, a wealth of results concerning various aspects of the model have been obtained, concerning self-adjointness of the Hamiltonian, existence, multiplicity or also nonexistence of the ground state and related infrared behavior, and detailed study of the spectral properties of the model and of its resonances. In the present paper we give a comprehensive analysis of some of the previous problems in the special case of a point charged oscillator interacting with the electromagnetic field in dipole approximation. While this model is unrealistically simple compared to the case, to give an example, of the hydrogen atom interacting with the full (not dipole) radiation field, (about which a lot is known thanks to the work of Lieb *et al.*[10,14] and Frölich *et al.*,[3,4] the original

[a)]Electronic mail: bertini@mat.unimi.it
[b)]Electronic mail: noja@matapp.unimib.it
[c)]Electronic mail: posilicano@uninsubria.it

contribution of the present work resides in the fact that we are able to cope with the point limit of the model. The removal of the ultraviolet cutoff in the interaction between matter and radiation is in its generality, a difficult and unsolved problem, and in particular one not faced off in the quoted rigorous literature. In some previous papers of the last two authors (Refs. 16 and 17 and references therein) the renormalized dynamics of the classical Pauli-Fierz model in dipole approximation (Ref. 18) and for fairly general external potentials, was rigorously constructed and analyzed. In particular, it was shown that the evolution of the Pauli-Fierz model in the point limit is given by an abstract wave equation generated by a family of operators related to the so-called point interactions (see Ref. 1 and references therein). Given the classical model in the ultraviolet limit, a second step would be to construct the quantized model. The harmonic potential has the unique feature of giving rise to linear equations of motion, so that the classical equations for the system take the form of an abstract linear wave equation. This allows a plain quantization *à la* Segal of the model, which seems otherwise quite problematic (in contrast with the case of the regularized Pauli-Fierz model, where canonical quantization works; a detailed study of the canonically quantized regularized dipole Pauli-Fierz model with an external harmonic potential was given by Arai in Ref. 2). So we confine ourself to this case, about which we give in the next section a self-contained treatment independent and different in spirit from Ref. 17, to clarify some of the themes discussed above. We outline briefly our main results. The classical evolution of the system is given by the abstract wave equation

$$(\partial_{tt}^2 + L_{\mathrm{e}})\xi = 0$$

for the couple $\xi=(A,p)$ where A is the vector potential of the electromagnetic field in Coulomb gauge and p is the particle momentum variable (see Sec. II for the explanation of this choice). Here L_{e} is a self-adjoint operator in $L^2_*(\mathbb{R}^3)\oplus\mathbb{R}^3$ ($*$ stands for "divergenceless") such that its resolvent can be explicitly calculated (see Lemma 2.2 and Theorem 2.3).

The operator L_{e} has a single negative eigenvalue and the rest of its spectrum is purely absolutely continuous and coincides with $[0,+\infty)$. Thus, to quantize the abstract wave equation above according to the Segal method, one must take L_{e}^+, i.e., L_{e} projected onto the spectral subspace corresponding to $\sigma_{\mathrm{ac}}(L_{\mathrm{e}})$. The (first) quantized dynamics of the system is defined through the Schrödinger-type equation $i\dot{\psi}=(L_{\mathrm{e}}^+)^{1/2}\psi$, defined on the complex Hilbert space $L^2_*(\mathbb{R}^3;\mathbb{C}^3)\oplus\mathbb{C}^3$ and the Hamiltonian of the quantized system of particle and field is given by the second quantization $\mathrm{d}\Gamma((L_{\mathrm{e}}^+)^{1/2})$, on the Fock space over $L^2_*(\mathbb{R}^3;\mathbb{C}^3)\oplus\mathbb{C}^3$.

A preliminary but essential step in the description of the properties of the system is to write the first quantized evolution in terms of the resolvent of the original classical operator L_{e}^+. By Stone formula, spectral theorem and after some work, one gets (see Lemma 2.5) a representation (perhaps new or at least not known to us) for the transition amplitudes $\langle\psi_1, e^{-it(L_{\mathrm{e}}^+)^{1/2}}\psi_2\rangle$ between one particle states in terms of the resolvent of L_{e}. Correspondingly, one has an expression for the survival and transition amplitudes for the second quantized model on the Fock space, just using functoriality of Γ. Our main concern here is in the calculation of two relevant characteristics of the evolution. The first is the survival amplitude $\mathcal{S}(t)$ of the unperturbed first excited bound state of the oscillator. The second is the amplitude transition $\mathcal{A}(t)$ between states with the photon field in the vacuum state and the oscillator in the first excited state, and states with one photon and the oscillator in the ground state. The survival and transition amplitudes relative to more general states factorize in a sum of product of these two simpler types. The survival amplitude $\mathcal{S}(t)$ has a particularly neat form (see Theorem 3.3),

$$\mathcal{S}(t) = c_1 e^{-\lambda_{\mathrm{e}}|t|} + c_2 e^{-\gamma_{\mathrm{e}}|t|}e^{-i\omega_{\mathrm{e}}t} + c_3 e^{-\lambda_{\mathrm{e}}|t|}\mathrm{Ei}(\lambda_{\mathrm{e}}|t|).$$

In this formula, the complex numbers

$$z_k := (-1)^k\omega_{\mathrm{e}} - i\gamma_{\mathrm{e}}, \quad k=1,2$$

coincide with the complex poles of the analytically continued resolvent of L_{e}^+; $-\lambda_{\mathrm{e}}^2$ is the unique negative eigenvalue of L_{e}, and by Ei we mean the exponential integral function. The complex

numbers c_1, c_2, and c_3 depend on the physical parameters. So, in the time evolution of the survival amplitude for the bound states of the oscillator it is possible to distinguish three different time behaviors. The first term, depends on a resonance on the imaginary axis originated from the projection onto the positive spectral subspace; it is a pure exponentially decaying term (for positive times) and the characteristic time of the decay, for realistic values of mass and charge of the electron, has an order of 10^{-23} s, an exceedingly small time. The second term is an exponentially damped oscillation described in terms of the complex resonance poles. In particular, the imaginary part of the resonance γ_{e} gives as usual a measure of the lifetime of the excited unperturbed states, or, equivalently, the breadth of the spectral lines of the spontaneous decay of the excited states (according to the Breit-Wigner law, see Ref. 7); while the real part gives the position of the maximum in the emission of the spectral line. In terms of given physical parameters of the systems, the behavior of these quantities is the following:

$$\omega_{\mathsf{e}} = \omega_0 + \frac{28\omega_0^3}{3m^2c^6}\mathsf{e}^4 + O(\mathsf{e}^5), \quad \gamma_{\mathsf{e}} = \frac{2\omega_0^2}{3mc^3}\mathsf{e}^2 + O(\mathsf{e}^5)$$

Here the symbols m, c, and e denote the (renormalized) phenomenological mass, the velocity of light and the electric charge, respectively. The noteworthy fact is the Lamb shift in the expression of ω_{e}. The maximum in the emission does not appear in correspondence of the unperturbed frequency of the oscillator, but at a displaced frequency. The last term, taking into account the asymptotic behavior of the exponential integral, is of the order $1/t$ for $t \gg 1$. The appearance of a slowly decaying tail implies a departure from the purely exponential decay given by the Breit-Wigner law, and is well known both in theoretical models and experimental studies. See Lemma 2.5 and the following remarks for an interpretation of its origin.

The transition amplitudes $\mathcal{A}(t)$ have a form very similar to the one for $\mathcal{S}(t)$ (see Theorem 3.5), and to them apply the same remarks and comments concerning their time behavior.

II. AN EXACTLY SOLUBLE MODEL IN CLASSICAL AND QUANTUM ELECTRODYNAMICS

A. Classical theory

The classical Pauli-Fierz model for a particle with charge e, charge density $\mathsf{e}\rho_r$ and bare mass m_r interacting with the electromagnetic field in dipole approximation and subjected to a restoring harmonic force, is described by the Hamiltonian

$$H = 2\pi c^2\langle E,E\rangle + \frac{1}{8\pi}\langle A,\Delta A\rangle + \frac{1}{2m_r}\left|p - \frac{\mathsf{e}}{c}\langle \rho_r,A\rangle\right|^2 + \frac{1}{2}\alpha|q|^2,$$

where $E = \dot{A}/(4\pi c^2)$ is the canonical variable conjugated to A and p is the canonical momentum conjugated to the particle position q. The model is written in the Coulomb gauge, so the fields are divergenceless. A suitable phase space for this dynamical system is $H^1_*(\mathbb{R}^3) \oplus L^2_*(\mathbb{R}^3) \oplus \mathbb{R}^3 \oplus \mathbb{R}^3$ where $H^1_*(\mathbb{R}^3)$ denotes the space of divergenceless locally square integrable vector fields with square integrable first derivatives. A point electron should have a Dirac measure as charge distribution, and the regular form factor ρ_r is introduced to give meaning to the equations of motion. So r must be interpreted as a measure of the particle radius. In the point limit, as $r \downarrow 0$, the charge distribution ρ_r weakly converges to δ_0, and the Hamilton equations corresponding to the Pauli-Fierz Hamiltonian lose their original meaning. A well-defined dynamical system is recovered only at the expense of renormalizing the bare mass m_r. This procedure is analyzed in detail in Ref. 16 and we content ourself to say here that the correct prescription is given by the well-known relation between the bare, electromagnetic (m_{em}) and renormalized (m) masses,

$$m = m_r + m_{\mathrm{em}} = m_r + \frac{8\pi}{3}\frac{\mathsf{e}^2}{c^2}\langle(-\Delta)^{-1}\rho_r, \rho_r\rangle.$$

Keeping m fixed to the physical value, this is the only choice for the bare mass which allows to obtain a nontrivial limit for the Pauli-Fierz model. From now on, with the symbol m_r we mean precisely the function $m_r(\mathsf{e}, m)$ given by the above relation.

The rigorous deduction of the limit dynamics is carried out in Ref. 17 for a general external potential; specializing the result to the case of the harmonic potential one obtains the equations

$$\dot{A} = 4\pi c^2 E,$$

$$\dot{E} = -\frac{1}{4\pi} H_m^p A,$$

$$\dot{q} = Q_A,$$

$$\dot{p} = -\alpha q.$$

The p-dependent operator H_m^p is an affine deformation of a linear self-adjoint operator in the class of point interactions (see Ref. 1 and references therein for the use of point interactions in quantum mechanics), H_m^p is linear if and only if $p=0$ and H_m^0 is the vector-valued version of one of such linear operators; Q_A is a certain linear functional which in some sense extract the singular part of the vector potential.

While obtaining a well-defined dynamics in the point limit it is an interesting and not obvious result, it remains unclear how to quantize such a system. So, according to the point of view we adopt in this paper, and in view of the Segal quantization of the system, we would like to work with (abstract) second order wave equations of the form

$$\ddot{\xi}(t) = -L\xi(t),$$

with a suitable self-adjoint operator L. This is not the case of the previous system of equation, due to the presence of a tight relation between the dynamical variables contained in the definition of the operator H_m^p. Going back to the regularized system, the second order equations corresponding to the Hamiltonian given above are not better from this point of view; they are

$$\frac{1}{c^2}\ddot{A} = \Delta A + \frac{4\pi\mathsf{e}}{c} M\dot{q}\rho,$$

$$m_r\ddot{q} = -\frac{\mathsf{e}}{c}\langle\rho_r, \dot{A}\rangle - \alpha q,$$

and the presence of $\dot{q}$ and $\dot{A}$ on the right-hand side make them not of the desired form. So we prefer to give a construction of the limit dynamics independent of the one given in Ref. 17. In fact, making resort to the Hamiltonian regularized equations above, it is simple to overcome this problem. Deriving with respect to time the equation which gives $\dot{p}$ and using the other equations, one obtains that the couple $\xi=(A, p)$ satisfies the abstract second-order wave equation

$$\ddot{\xi} = -L_{\mathsf{e}}^r \xi,$$

where the operator L_{e}^r is given by

$$L_{\mathrm{e}}^r(A,p)=\left(-c^2\Delta A-\frac{4\pi \mathrm{e}c}{m_r}M\left(p-\frac{\mathrm{e}}{c}\langle\rho_r,A\rangle\right)\rho_r,\frac{\alpha}{m_r}\left(p-\frac{\mathrm{e}}{c}\langle\rho_r,A\rangle\right)\right).$$

The analogous result is obtained by means of the canonical transformation which exchanges the particle position and momentum (see also Ref. 22),

$$q=-P,\quad p=Q.$$

The change of dynamical variable from q to p in the second order (or Lagrangian) formalism is not particularly relevant to the analysis of the problems we are interested in, and the interpretation of the results we get. For example, the time behavior of the classical position q, which is important in the calculation of the survival amplitude of the bound states of the oscillator, is quite simply related to the time behavior of the variable p, up to a constant, the derivative of the momentum gives the position, and this relation is preserved in the limit dynamics.

Another important point to note, is that the operator L_{e}^r is a finite rank perturbation of the noninteracting operator $L_0=(-c^2\Delta,0)$. This simple structure suggests the possibility that the operator L_{e}^r has a limit for $r\downarrow 0$, and being an unbounded operator such a limit, if existing, should be sought in the resolvent sense. The calculation of the resolvent of the operator L_{e}^r is lenghty but elementary. We omit the proof and give the result in the following.

Lemma 2.1: For every $z\in\mathbb{C}_{\pm}$, the resolvent of L_{e}^r is given by

$$(L_{\mathrm{e}}^r-z^2)^{-1}(A,p)=(\mathcal{G}_z^{\pm}*A,0)-\Lambda^r(z)R_{\mathrm{e}}^r(z)(A,p),$$

where

$$\Lambda^r(z)=\frac{-1}{m_r k_1^r k_2^r},\quad \mathcal{G}_z^{\pm}(x)=\frac{1}{c^2}\frac{e^{\pm iz|x|/c}}{4\pi|x|},\quad \pm\operatorname{Im} z>0,$$

$$R_{\mathrm{e}}^r(z)(A,p)=(R_{\mathrm{e}}^{1r}(z)(A,p),R_{\mathrm{e}}^{2r}(z)(A,p)),$$

$$R_{\mathrm{e}}^{1r}(z)(A,p)=\frac{4\pi\mathrm{e}}{c}M\left(\left(z^2c\mathrm{e}\langle(-c^2\Delta-z^2)^{-1}A,\rho_r\rangle+c^2\frac{m_rk_1^r}{\alpha}(z^2+k_2^r)p\right)(-c^2\Delta-z^2)^{-1}\rho_r\right),$$

$$R_{\mathrm{e}}^{2r}(z)(A,p)=\alpha\frac{\mathrm{e}}{c}\langle(-c^2\Delta-z^2)^{-1}A,\rho_r\rangle+m_rk_1^rp,$$

$$k_1^r=1+\tfrac{8}{3}\pi\mathrm{e}^2\langle(-c^2\Delta-z^2)^{-1}\rho_r,\rho_r\rangle,$$

$$k_2^r=\frac{\alpha}{m_r}-z^2-\frac{8}{3}\frac{\alpha\pi\mathrm{e}^2}{m_r^2k_1^r}\langle(-c^2\Delta-z^2)^{-1}\rho_r,\rho_r\rangle.$$

The next step is the point limit $r\downarrow 0$. The result is analogous to the corresponding result given in Ref. 16 for the case of a free particle, and the proof is modelled on one of the well known ways of defining point interactions (see Ref. 1). We give only an outline of the proof.

Lemma 2.2: Let $\rho_r\to\delta_0$ weakly as $r\downarrow 0$. For every fixed $z\in\mathbb{C}_{\pm}$, $(L_{\mathrm{e}}^r-z^2)^{-1}$ converges as $r\downarrow 0$ in the norm resolvent sense to the operator

$$(\mathcal{G}_z^{\pm}*A,0)-\Lambda_{\pm}(z)R_{\mathrm{e}}^{\pm}(z)(A,p),$$

where, setting $\omega_0^2:=\alpha/m$,

$$R_{\mathrm{e}}^{\pm}(z)(A,p)=\left(\frac{4\pi\mathrm{e}}{c}M(z^2c\mathrm{e}\langle\mathcal{G}_{z^*}^{\mp},A\rangle+c^2p)\mathcal{G}_z^{\pm},m\omega_0^2\frac{\mathrm{e}}{c}\langle\mathcal{G}_{z^*}^{\mp},A\rangle+\left(m\pm i\frac{2\mathrm{e}^2}{3c^3}z\right)p\right),$$

$$\Lambda_{\pm}(z) = \frac{1}{\pm i\dfrac{2\mathsf{e}^2}{3c^3}z^3 - m(\omega_0^2 - z^2)}.$$

Such an operator is the resolvent of a self-adjoint operator L_{e} *on* $L^2_*(\mathbb{R}^3)\oplus\mathbb{R}^3$ *when on the component* $\mathbb{R}^3$ *one considers the scalar product* $\langle p_1,p_2\rangle := \kappa_0 p_1\cdot p_2$, *with* $\kappa_0 := 4\pi c^2/m\omega_0^2$.

Proof: The proof of the convergence of the regularized resolvent is a direct consequence of the following limiting relations:

$$\lim_{r\downarrow 0}(-c^2\Delta - z^2)^{-1}\rho_r = \mathcal{G}_z^{\pm},$$

$$\lim_{r\downarrow 0} k_1^r = 0, \quad \lim_{r\downarrow 0} k_1^r m_r = m \pm i\frac{2\mathsf{e}^2}{3c^3}z,$$

$$\lim_{r\downarrow 0} k_2^r = -\frac{\pm i\dfrac{2\mathsf{e}^2}{3c^3}z^3 - m(\omega_0^2 - z^2)}{m \pm i\dfrac{2\mathsf{e}^2}{3c^3}z}.$$

Checking that the limit operator is the resolvent of a self-adjoint operator is routine. See Ref. 16 for a similar verification. □

By the resolvent just constructed it is straightforward to derive the actions of L_{e} itself and of its spectral properties.

Theorem 2.3: *The action and domain of the self-adjoint operator*

$$L_{\mathsf{e}}: D(L_{\mathsf{e}}) \subseteq L^2_*(\mathbb{R}^3)\oplus\mathbb{R}^3 \to L^2_*(\mathbb{R}^3)\oplus\mathbb{R}^3$$

are given by

$$L_{\mathsf{e}}(A,p) = \left(-c^2\Delta A_0, \omega_0^2\left(p - \frac{\mathsf{e}}{c}A_0(0)\right)\right),$$

$$D(L_{\mathsf{e}}) = \left\{(A,p)\in L^2_*(\mathbb{R}^3)\oplus\mathbb{R}^3 : A = A_0 + \frac{4\pi\mathsf{e}}{c}Mv\mathcal{G}, \sqrt{-\Delta}A_0, \Delta A_0 \in L^2_*(\mathbb{R}^3), v\in\mathbb{R}^3, mv = p - \frac{\mathsf{e}}{c}A_0(0)\right\},$$

where

$$\mathcal{G}(x) = \frac{1}{4\pi|x|}.$$

Moreover,

$$\sigma_p(L_{\mathsf{e}}) = \{-\lambda_{\mathsf{e}}^2\}, \quad \sigma_{\mathrm{ess}}(L_{\mathsf{e}}) = \sigma_{\mathrm{ac}}(L_{\mathsf{e}}) = [0,+\infty), \quad \sigma_{\mathrm{sc}}(L_{\mathsf{e}}) = \varnothing,$$

where

$$\lambda_{\mathsf{e}} = \frac{3mc^3}{2\mathsf{e}^2} + O(\mathsf{e}^2)$$

is the unique real (and positive) solution of the third order equation

$$\frac{2e^2}{3c^3}\lambda^3 - m(\omega_0^2 + \lambda^2) = 0.$$

We emphasize that, due to the fact that the operator L_e has been constructed as a norm resolvent limit of the operator L_e^r, the flow generated by the limit operator coincides with the limit of the regularized flow, in the relevant norms of the phase space and uniformly in time. This allows to consider L_e as the generator of the limit dynamics. As a second remark, note that the algebraic equation $\Lambda_\pm(z)^{-1}=0$ is nothing but the characteristic equation of the Abraham-Lorentz (AL) equation (see, e.g., Ref. 15) in the particular case of an harmonic external force, i.e.,

$$-\tau_0 \dddot{q} + \ddot{q} + \omega_0 q = 0, \quad \tau_0 = \frac{2e^2}{3mc^3},$$

the equation which classically describes the behavior of the particle position in the nonrelativistic regime (the classical relativistic equation was obtained by Dirac in Ref. 9). In particular, the negative eigenvalue of L_e corresponds to the so-called runaway solution of the AL equation. In the traditional approaches, this solution is discarded due to its unphysical character. From the present point of view, we give up the (important) interpretative problem related to the presence of these instabilities, and take the attitude according to which the suppression of runaway behavior corresponds to reduction of the dynamics on the stable subspace, or equivalently, restriction to the absolutely continuous component of the spectrum. This should correspond, in ordinary scattering theory for Schrödinger operators, to the elimination of bound states. The procedure to obtain this reduction can be explicitly performed as follows. Let us consider, from now on, L_e as acting on the complex Hilbert space $L^2_*(\mathbb{R}^3;\mathbb{C}^3)\oplus\mathbb{C}^3$. It is self-adjoint when on the component $\mathbb{C}^3$ one considers the scalar product $\langle\zeta_1,\zeta_2\rangle := \kappa_0 \zeta_1^* \cdot \zeta_2$.

Given ζ_1,ζ_2,ζ_3, an orthonormal base in $\mathbb{C}^3$, and defining

$$\mathcal{G}_{\lambda_e}(x) := \frac{1}{c^2}\frac{e^{-\lambda_e|x|/c}}{4\pi|x|}, \quad \kappa := \left(\frac{2\pi e^2\lambda_0^3}{m^2\omega_0^4 c} + \kappa_0\right)^{1/2}, \quad \kappa_1 := \frac{e}{c}\lambda_e^2\kappa_0,$$

let

$$\psi_i^0 = \frac{1}{\kappa}(-\kappa_1 M\zeta_i \mathcal{G}_{\lambda_e}, \zeta_i), \quad i=1,2,3$$

be the normalized eigenvectors corresponding to the eigenvalue $-\lambda_e^2$. Then the projection P_e onto the absolutely continuous subspace of the operator L_e is given by

$$P_e\psi \equiv \psi^+ = \psi - \sum_{i=1,2,3}\langle\psi,\psi_i^0\rangle\psi_i^0.$$

In particular

$$P_e(0,\zeta) = \frac{\kappa_2}{\kappa^2}\left(\frac{12\pi c^4}{e}M\zeta\mathcal{G}_{\lambda_e},\lambda_e\zeta\right), \quad \kappa_2 := \frac{4\pi e^2\lambda_e^2}{m^2\omega_0^4 c}.$$

We define the positive self-adjoint operator L_e^+ by $L_e^+ := P_e L_e$, and from now on we consider this reduced operator as the generator of the physical limit dynamics.

B. Quantum theory

The operator L_e^+ generates the classical evolution, whereas, according to the results summarized in the appendix, the corresponding quantum evolution is given in terms of its square root $(L_e^+)^{1/2}$. More explicitly, denoting by $\mathcal{F}(L^2_*(\mathbb{R}^3;\mathbb{C}^3)\oplus\mathbb{C}^3)$ the bosonic Fock space over $L^2_*(\mathbb{R}^3;\mathbb{C}^3)\oplus\mathbb{C}^3$, i.e.,

$$\mathcal{F}(L^2_*(\mathbb{R}^3;\mathbb{C}^3)\oplus\mathbb{C}^3) := \bigoplus_{n\geqslant 0} S_n (L^2_*(\mathbb{R}^3;\mathbb{C}^3)\oplus\mathbb{C}^3)^{\otimes n},$$

where S_n denotes the symmetrization operator on the nth sector, the quantum Hamiltonian on $\mathcal{F}(L^2_*(\mathbb{R}^3;\mathbb{C}^3)\oplus\mathbb{C}^3)$ corresponding to the second quantization of the classical wave equation

$$(\partial^2_{tt} + L^+_{\mathsf{e}})(A,p) = 0$$

is given by

$$\mathsf{H}_{\mathsf{e}} := \hbar\, \mathrm{d}\Gamma((L^+_{\mathsf{e}})^{1/2}).$$

Note that the noninteracting Hamiltonian

$$\mathsf{H}_0 := \hbar\, \mathrm{d}\Gamma(L_0^{1/2}) \equiv \hbar\, \mathrm{d}\Gamma(\sqrt{-\Delta}\oplus\omega_0)$$

is unitarily equivalent to

$$\hbar\, \mathrm{d}\Gamma(\sqrt{-\Delta})\otimes 1 + 1\otimes \hbar\, \mathrm{d}\Gamma(\omega_0),$$

defined on the Hilbert space

$$\mathcal{F}(L^2_*(\mathbb{R}^3;\mathbb{C}^3))\otimes\mathcal{F}(\mathbb{C}^3) := \bigoplus_{n\geqslant 0} S_n L^2_*(\mathbb{R}^3;\mathbb{C}^3)^{\otimes n} \otimes \bigoplus_{n\geqslant 0} S_n(\mathbb{C}^3)^{\otimes n}.$$

The unitary operator

$$\mathsf{U}:\mathcal{F}(L^2_*(\mathbb{R}^3;\mathbb{C}^3)\oplus\mathbb{C}^3) \to \mathcal{F}(L^2_*(\mathbb{R}^3;\mathbb{C}^3))\otimes\mathcal{F}(\mathbb{C}^3) \tag{1}$$

giving the stated equivalence is defined by

$$\mathsf{U}\Omega := \Omega\otimes\Omega, \quad \mathsf{U}\mathsf{C}(\psi)\mathsf{U}^{-1} = \mathsf{C}(\varphi)\otimes 1 + 1\otimes \mathsf{C}(\zeta),$$

where Ω denotes the vacuum, $\psi=(\varphi,\zeta)$ and C is the usual creation operator. Moreover $\hbar\, \mathrm{d}\Gamma(\omega_0)$ is unitarily equivalent to the usual harmonic oscillator Hamiltonian on $L^2(\mathbb{R}^3;\mathbb{C})$ given by the self-adjoint operator

$$-\frac{\hbar^2}{2m}\Delta + \frac{m\omega_0^2}{2}q^2.$$

Concerning the interacting Hamiltonian H_{e}, the present one is its first *explicit* construction in the ultraviolet limit and the problem arises if other representations more directly confrontable with usual canonical formulation could be given. We emphasize the fact that in our description, already at the classical level, the point limit produces an intimate interlacing between field singularities and particle variables, through the definition of the domain of the operator L_{e} itself, and this fact introduces essential difficulties in tracing the relation with the canonical formalism based on the usual regularized Pauli-Fierz Hamiltonian, where this constraint disappears. Nevertheless, in the quoted Arai paper (Ref. 2), a reconstruction theorem based on the limit of the Wightman functions of the regularized model is outlined. It could be interesting to analyze the relations between two approaches.

Since the resolvent of L_{e} is quite explicit, making use of the Birman-Kato invariance principle to deal with the group generated by the square root, and of the Birman-Kuroda completeness theorem (see Ref. 6) which is applicable because $(L_{\mathsf{e}}+z)^{-1}-(L_0+z)^{-1}$ is a finite rank operator, one immediately obtains the following.

Theorem 2.4: *Let P_0 and P_{e} be the orthogonal projections onto the absolutely continuous subspaces of L_0 and L_{e}, respectively. Then the Möller wave operators exist, they are complete and,*

$$\Omega_{\pm}(\mathsf{H}_{\mathsf{e}},\mathsf{H}_0) := \text{s-}\lim_{t\to\pm\infty} e^{-it\mathsf{H}_{\mathsf{e}}/\hbar} e^{-it\mathsf{H}_0/\hbar}\Gamma(P_0) = \Gamma(\Omega_{\pm}(L_{\mathsf{e}},L_0)),$$

$$\Omega_{\pm}(\mathsf{H}_0,\mathsf{H}_e) := \text{s-}\lim_{t\to\pm\infty} e^{-it\mathsf{H}_0/\hbar}e^{-it\mathsf{H}_e/\hbar}\Gamma(P_e) = \Gamma(\Omega_{\pm}(L_0,L_e)).$$

A final result of this paragraph is a formula for the evaluation of transition amplitudes of the Schrödinger-type propagator $e^{-it(L_e^+)^{1/2}}$, that is the scalar product of the type $\langle\psi_1, e^{-it(L_e^+)^{1/2}}\psi_2\rangle$, in terms of boundary values of the resolvent of the classical operator L_e. In the formula the special form of the operator L_e plays no rule, and it holds true for a positive generator A whatsoever. By linearity it will be sufficient to suppose that ψ_1 and ψ_2 are real valued. Since (see the Appendix for the definition of $W_{L_e^+}$)

$$((iW_{L_e^+} - z)^{-1})(\psi,0) = (z(L_e^+ - z^2)^{-1}\psi, -i\psi - iz^2(L_e^+ - z^2)^{-1}\psi),$$

by Lemma A.2 and Lemma A.3 one obtains

$$\begin{aligned}\langle\psi_1, e^{-it(L_e^+)^{1/2}}\psi_2\rangle = &\lim_{a\uparrow\infty}\lim_{\epsilon\downarrow 0}\frac{1}{2\pi i}\int_{-a}^{a} d\lambda\, e^{-it\lambda}(\langle\psi_1,((\lambda+i\epsilon)(L_e-(\lambda+i\epsilon)^2)^{-1}\\ &-(\lambda-i\epsilon)(L_e-(\lambda-i\epsilon)^2)^{-1})\psi_2^+\rangle)\\ &+\lim_{a\uparrow\infty}\lim_{\epsilon\downarrow 0}\frac{1}{2\pi i}\int_{-a}^{a} d\lambda\, e^{-it\lambda}(\langle\psi_1,((\lambda+i\epsilon)^2(L_e-(\lambda+i\epsilon)^2)^{-1}\\ &-(\lambda-i\epsilon)^2(L_e-(\lambda-i\epsilon)^2)^{-1})(L_e^+)^{-1/2}\psi_2^+\rangle).\end{aligned}$$

Moreover, using first resolvent identity and

$$(L_e^+)^{-1/2} = \frac{1}{\pi}\int_{\mathbb{R}} ds(L_e^+ + s^2)^{-1}$$

it turns that

$$\langle\psi_1,(L_e-z^2)^{-1}(L_e^+)^{-1/2}\psi_2^+\rangle = \frac{1}{\pi}\int_{\mathbb{R}}\frac{ds}{s^2+z^2}\langle\psi_1,(L_e-z^2)^{-1}\psi_2^+\rangle - \frac{1}{\pi}\int_{\mathbb{R}}\frac{ds}{s^2+z^2}\langle\psi_1,(L_e+s^2)^{-1}\psi_2^+\rangle.$$

Thus for any couple ψ_1,ψ_2 for which the limits

$$\langle\psi_1,(L_e-\lambda_{\pm}^2)^{-1}\psi_2^+\rangle := \lim_{\epsilon\downarrow 0}\langle\psi_1,(L_e-(\lambda\pm i\epsilon)^2)^{-1}\psi_2^+\rangle$$

exist, one obtains the following.

Lemma 2.5:

$$\begin{aligned}\langle\psi_1, e^{-it(L_e^+)^{1/2}}\psi_2\rangle = &\lim_{a\uparrow\infty}\frac{1}{2\pi i}\int_{-a}^{a} d\lambda\, e^{-it\lambda}\lambda(\langle\psi_1,((L_e-\lambda_+^2)^{-1}-(L_e-\lambda_-^2)^{-1})\psi_2^+\rangle)\\ &+\frac{1}{\pi}\int_{\mathbb{R}}\frac{ds}{2\pi i}\int_{\mathbb{R}} d\lambda\,\frac{e^{-it\lambda}\lambda^2}{s^2+\lambda^2}\langle\psi_1,((L_e-\lambda_+^2)^{-1}-(L_e-\lambda_-^2)^{-1})\psi_2^+\rangle.\end{aligned}$$

Note that the second contribution in the previous formula comes from the nonlocal relation between the real phase space classical variables and the complexified ones, described in Lemma A.3. Performing however the s integral one obtains, under the same condition of the previous result, the following alternative representation:

$$\langle \psi_1, e^{-it(L_e^+)^{1/2}}\psi_2\rangle = \lim_{a\uparrow\infty}\frac{1}{2\pi i}\int_0^a d\lambda\, e^{-it\lambda}\lambda(\langle\psi_1,((L_e-\lambda_+^2)^{-1}-(L_e-\lambda_-^2)^{-1})\psi_2^+\rangle).$$

This last representation has a more direct meaning, in that it is an integral extended over the spectrum of the operator $(L_e^+)^{1/2}$. Moreover, it presents the evolution generated by $(L_e^+)^{1/2}$ as a Fourier transform of a function (for every fixed couple of states ψ_1 and ψ_2) supported on a half-line. As a consequence of the Paley-Wiener theorem, the evolution of the amplitude transition cannot have a leading large time contribution of exponential type, but a slower one should appear (see Refs. 11 and 12 for an early application of this remark to the time decay of amplitude transition). The exact time behavior cannot be precised without the knowledge of further details about the generator. To this end it more practical to use the formula given in Lemma 2.5, as we see in the following section.

III. RADIATION THEORY

A. Generalities

In this section we want to give some details of the quantum dynamics of the model we are studying. In particular, we want to estimate, under the dynamics generated by H_e, the survival amplitudes of the bound states of H_0 and the probability amplitudes of the transitions between two of such states with emission of photons. We begin with some preliminaries on the general structure of the amplitude transitions in our model.

In the space $\mathcal{F}(L^2_*(\mathbb{R}^3;\mathbb{C}^3))\otimes\mathcal{F}(\mathbb{C}^3)$ a bound state (n level) for the Hamiltonian operator H_0 is represented by a vector of the kind

$$\Omega\otimes S_n(\zeta_1\otimes\cdots\otimes\zeta_n).$$

According to (1) this state is represented in $\mathcal{F}(L^2_*(\mathbb{R}^3;\mathbb{C}^3)\oplus\mathbb{C}^3)$ by the vector

$$S_n((0,\zeta_1)\otimes\cdots\otimes(0,\zeta_n)).$$

By (1) again, a more general state with m photons, of the kind

$$S_m(\varphi_1\otimes\cdots\otimes\varphi_m)\otimes S_n(\zeta_1\otimes\cdots\otimes\zeta_n),$$

is represented in $\mathcal{F}(L^2_*(\mathbb{R}^3;\mathbb{C}^3)\oplus\mathbb{C}^3)$ by the vector

$$S_{m+n}((\varphi_1,0)\otimes\cdots\otimes(\varphi_m,0)\otimes(0,\zeta_1)\otimes\cdots\otimes(0,\zeta_n)).$$

Note that, being $\mathsf{H}_e=\hbar\,d\Gamma((L_e^+)^{1/2})$, any sector in $\mathcal{F}(L^2_*(\mathbb{R}^3;\mathbb{C}^3)\oplus\mathbb{C}^3)$ is preserved under $e^{-it\mathsf{H}_e}$. Thus only the transitions from a n level to a m level with the emission of $n-m$ photons are allowed.

On the other hand, as we shall see, asymptotically the particle part of the wave function of the state relaxes to the ground state, and this yelds to the asymptotic conservation of the photon number in the scattering process. This property was devised by Arai in Ref. 2 for the regularized Pauli-Fierz model with quadratic potential, as a consequence of the factorization properties of the scattering matrix, and we find it again in the point model.

Since

$$\begin{aligned}e^{-it\mathsf{H}_e/\hbar}S_n(\psi_1\otimes\cdots\otimes\psi_n)&=\Gamma(e^{-it(L_e^+)^{1/2}})S_n(\psi_1\otimes\cdots\otimes\psi_n)\\&=\frac{1}{n!}\sum_\sigma e^{-it(L_e^+)^{1/2}}\psi_{\sigma_1}\otimes\cdots\otimes e^{-it(L_e^+)^{1/2}}\psi_{\sigma_n},\end{aligned}$$

the survival amplitude of the bound state $\Omega\otimes S_n(\zeta_1\otimes\cdots\otimes\zeta_n)$ is given by

$$\frac{1}{n!}\sum_{\sigma}\prod_{j=1}^{n}\langle(0,\zeta_{\sigma_j}),e^{-it(L_{\mathrm{e}}^{+})^{1/2}}(0,\zeta_j)\rangle,$$

whereas the the probability amplitude of the transition

$$\Omega\otimes S_n(\zeta_1\otimes\cdots\otimes\zeta_n)\leftrightarrow S_m(\varphi_1\otimes\cdots\otimes\varphi_m)\otimes S_{n-m}(\xi_{m+1}\otimes\cdots\otimes\xi_{n-m})$$

is given by

$$\frac{1}{n!}\sum_{\sigma}\prod_{\sigma_j\leqslant m}\langle(\varphi_{\sigma_j},0),e^{-it(L_{\mathrm{e}}^{+})^{1/2}}(0,\zeta_j)\rangle\prod_{\sigma_k>m}\langle(0,\xi_{\sigma_k}),e^{-it(L_{\mathrm{e}}^{+})^{1/2}}(0,\zeta_k)\rangle.$$

B. Survival amplitudes

After these general remarks, we evaluate the survival amplitudes for the bound states of the unperturbed dynamics along the perturbed evolution. To simplify the exposition we break the analysis in a number of lemmata.

Lemma 3.1: For any $\zeta_1,\zeta_2\in\mathbb{C}^3$ *one has*

$$\langle(0,\zeta_1),e^{-it(L_{\mathrm{e}}^{+})^{1/2}}(0,\zeta_2)\rangle=\mathcal{S}(t)\bar{\zeta}_1\cdot\zeta_2,$$

where

$$\mathcal{S}(t)=-\frac{2\kappa_0\kappa_2}{\kappa^2}I(t)$$

and, with $\pm t>0$,

$$I(t)=\mp e^{\mp\lambda_{\mathrm{e}}t}i\lambda_{\mathrm{e}}\frac{p(-i\lambda_{\mathrm{e}})}{q(-i\lambda_{\mathrm{e}})}\pm e^{\mp\gamma_{\mathrm{e}}t}\frac{e^{-i\omega_{\mathrm{e}}t}2z_{\pm}}{z_{\pm}+i\lambda_{\mathrm{e}}}\frac{p(z_{\pm})}{q'(z_{\pm})}+J_1(t)+J_2(t),$$

$$J_1(t)=\frac{1}{\pi}\int_{\mathbb{R}}\mathrm{d}s\frac{e^{\mp|s|t}|s|}{2(|s|+\lambda_{\mathrm{e}})}\frac{p(i|s|)}{q(i|s|)},$$

$$J_2(t)=\frac{1}{\pi}\int_{\mathbb{R}}\mathrm{d}s\left(\frac{e^{\mp|s|t}|s|}{2(|s|-\lambda_{\mathrm{e}})}\frac{p(-i|s|)}{q(-i|s|)}-\frac{e^{\mp\lambda_{\mathrm{e}}t}\lambda_{\mathrm{e}}^2}{s^2-\lambda_{\mathrm{e}}^2}\frac{p(-i\lambda_{\mathrm{e}})}{q(-i\lambda_{\mathrm{e}})}\right),$$

$$p(z)=\frac{\mathrm{e}^2\lambda_{\mathrm{e}}}{3c^3}z+i\frac{m}{\lambda_{\mathrm{e}}}\left(\omega_0^2+\frac{\lambda_{\mathrm{e}}^2}{2}\right),$$

$$q(z)=\frac{2\mathrm{e}^2}{3c^3}z^2+i\frac{m\omega_0^2}{\lambda_{\mathrm{e}}^2}(z+i\lambda_{\mathrm{e}}),$$

where

$$z_{\pm}:=\pm\omega_{\mathrm{e}}-i\gamma_{\mathrm{e}},$$

$$\omega_{\mathrm{e}}=\omega_0+\frac{28\omega_0^3}{3m^2c^6}\mathrm{e}^4+O(\mathrm{e}^5),\quad \gamma_{\mathrm{e}}=\frac{2\omega_0^2}{3mc^3}\mathrm{e}^2+O(\mathrm{e}^5)$$

are the two roots of $q(z)$.

Proof: Let $z\in\mathbb{C}_{\pm}$. Taking in account the algebraic equation satisfied by λ_{e} and the identity

$$\langle \mathcal{G}_{z^*}^{\mp}, \mathcal{G}_{\lambda_e} \rangle = \frac{1}{4\pi c^3} \frac{1}{\lambda_e \mp iz}$$

we have, for the projected resolvent,

$$\begin{aligned}\langle (0,\zeta_1), (L_e - z^2)^{-1}(0,\zeta_2)^+ \rangle &= -\kappa_0 \frac{\kappa_2}{\kappa^2} \Lambda_\pm(z) \left(m\omega_0^2 8\pi c^3 \langle \mathcal{G}_{z^*}^{\mp}, \mathcal{G}_{\lambda_e} \rangle + \left(m \pm i \frac{2e^2}{3c^3} z \right) \lambda_e \right) \zeta_1^* \cdot \zeta_2 \\ &= \frac{-2\kappa_0\kappa_2}{\kappa^2(\pm iz - \lambda_e)} \frac{\left(\pm i \frac{e^2 \lambda_e}{3c^3} z - \frac{m}{\lambda_e} \left(\omega_0^2 + \frac{\lambda_e^2}{2} \right) \right) (\pm iz + \lambda_e)}{\left(\frac{2e^2}{3c^3} z^2 + \frac{m\omega_0^2}{\lambda_e^2} (\pm iz - \lambda_e) \right) (\pm iz + \lambda_e)} \zeta_1^* \cdot \zeta_2 .\end{aligned}$$

Thus using the representation formula given in Lemma 2.5, we get

$$\langle (0,\zeta_1), e^{-it(L_e^+)^{1/2}} (0,\zeta_2) \rangle = -\frac{2\kappa_0\kappa_2}{\kappa^2} \left(I_1(t) + \frac{1}{\pi} \int_{\mathbb{R}} ds\, I_2(t,s) \right) \zeta_1^* \cdot \zeta_2,$$

where

$$I_1(t) := \frac{1}{2\pi i} \lim_{a \uparrow \infty} \int_{-a}^{a} d\lambda\, e^{-it\lambda} \lambda (f(\lambda) - f(-\lambda)),$$

$$I_2(t,s) := \frac{1}{2\pi i} \int_{\mathbb{R}} d\lambda\, e^{-it\lambda} \lambda^2 \frac{f(\lambda) - f(-\lambda)}{s^2 + \lambda^2},$$

$$f(\lambda) := \frac{1}{\lambda + i\lambda_e} \frac{\frac{e^2 \lambda_e}{3c^3} \lambda + i \frac{m}{\lambda_e} \left(\omega_0^2 + \frac{\lambda_e^2}{2} \right)}{\frac{2e^2}{3c^3} \lambda^2 + i \frac{m\omega_0^2}{\lambda_e^2} (\lambda + i\lambda_e)} \equiv \frac{1}{\lambda + i\lambda_e} \frac{p(\lambda)}{q(\lambda)}.$$

Then, by residue theorem and Jordan's lemma, when $\pm t > 0$, one obtains

$$I_1(t) = \mp e^{\mp \lambda_e t} i\lambda_e \frac{p(-i\lambda_e)}{q(-i\lambda_e)} \pm e^{\mp \gamma_e t} \sum_{k=1,2} \frac{e^{\mp (-1)^k i \omega_e t} z_k}{z_k + i\lambda_e} \frac{p(z_k)}{q'(z_k)},$$

where $z_k := (-1)^k \omega_e - \gamma_e$, and

$$\begin{aligned}I_2(t,s) = &-\frac{e^{\mp \lambda_e t} \lambda_e^2}{s^2 - \lambda_e^2} \frac{p(-i\lambda_e)}{q(-i\lambda_e)} + e^{\mp t\gamma_e} \sum_{k=1,2} \frac{z_k}{s^2 + z_k^2} \frac{e^{\mp (-1)^k i\omega_e t} z_k}{z_k + i\lambda_e} \frac{p(z_k)}{q'(z_k)} \\ &+ e^{\mp |s| t} \frac{|s|}{2} \left(\frac{1}{|s| \mp \lambda_e} \frac{p(\mp i|s|)}{q(\mp i|s|)} + \frac{1}{|s| \pm \lambda_e} \frac{p(\pm i|s|)}{q(\pm i|s|)} \right).\end{aligned}$$

Since

$$\frac{1}{\pi} \int_{\mathbb{R}} ds \frac{z_k}{s^2 + z_k^2} = (-1)^k,$$

one has

$$I_1(t)+\frac{1}{\pi}\int_{\mathbb{R}}\mathrm{d}s\, I_2(t,s)= \mp e^{\mp\lambda_e t}i\lambda_e\frac{p(-i\lambda_e)}{q(-i\lambda_e)}\pm e^{\mp\gamma_e t}\frac{e^{-i\omega_e t}2z_k}{z_k+i\lambda_e}\frac{p(z_k)}{q'(z_k)}+\frac{1}{\pi}\int_{\mathbb{R}}\mathrm{d}s\left(\frac{e^{\mp|s|t}|s|}{2(|s|-\lambda_e)}\frac{p(-i|s|)}{q(-i|s|)}\right.$$
$$\left.-\frac{e^{\mp\lambda_e t}\lambda_e^2}{s^2-\lambda_e^2}\frac{p(-i\lambda_e)}{q(-i\lambda_e)}\right)+\frac{1}{\pi}\int_{\mathbb{R}}\mathrm{d}s\frac{e^{\mp|s|t}|s|}{2(|s|+\lambda_e)}\frac{p(i|s|)}{q(i|s|)},$$

where $k=2$ if $t>0$ and $k=1$ if $t<0$. □

We distinguish three contributions in the previous formula for $I(t)$. The one on the first line is due to the resonances of the system. In particular, we have a purely exponential term with lifetime λ_e, coming from the projection on the stable subspace of the system, which dies out very quickly; and terms exponentially damped, due to the complex resonances. These last resonances are typical of the Breit-Wigner distribution, and they are the only terms which survive to the usual single pole approximation for the resolvent. They give both the breadth of emission lines in the spectrum (or equivalently the lifetime of the process) and the Lamb shift, as recalled in the introduction. The other contributions to the survival amplitude need more direct analysis. To simplify the exposition we confine to the case of $t>0$, the case $t<0$ being completely analogous. The term $J_1(t)$ is nothing more than the Laplace transform (which we denote by the symbol $\mathcal{L}$), a rational function. It is a tedious but standard calculation to verify that such a Laplace transform is in fact the sum of a pure exponential and a damped oscillation with the same characteristic exponents as the ones coming from the first group of terms. So, the term $J_1(t)$ corresponds to a further resonance contribution.

Concerning $J_2(t)$ the following result holds true.

Lemma 3.2: There exist complex constants c_1, c_2, c_3 such that, for $t>0$,

$$J_2(t)=\frac{1}{\pi}\mathcal{L}\left(\frac{c_1 s+c_2}{(s-\gamma_e)^2+\omega_e^2}\right)+\frac{c_3}{\pi}PV\int_0^\infty\frac{e^{-st}}{s-\lambda_e}\mathrm{d}s.$$

Proof: Introducing a parameter ϵ to isolate the singularity in λ_e, one can write

$$J_2(t)=\frac{2}{\pi}\int_0^{+\infty}\mathrm{d}s\left(\frac{e^{-|s|t}|s|}{2(|s|-\lambda_e)}\frac{p(-i|s|)}{q(-i|s|)}-\frac{e^{-\lambda_e t}\lambda_e^2}{s^2-\lambda_e^2}\frac{p(-i\lambda_e)}{q(-i\lambda_e)}\right)$$
$$=\lim_{\epsilon\downarrow 0}\left(\frac{2}{\pi}\left(\int_0^{\lambda_e-\epsilon}\mathrm{d}s\frac{e^{-|s|t}|s|}{2(|s|-\lambda_e)}\frac{p(-i|s|)}{q(-i|s|)}+\int_{\lambda_e+\epsilon}^{+\infty}\mathrm{d}s\frac{e^{-|s|t}|s|}{2(|s|-\lambda_e)}\frac{p(-i|s|)}{q(-i|s|)}\right)\right.$$
$$\left.-\frac{2}{\pi}\left(\int_0^{\lambda_e-\epsilon}\mathrm{d}s\frac{e^{-\lambda_e t}\lambda_e^2}{s^2-\lambda_e^2}\frac{p(-i\lambda_e)}{q(-i\lambda_e)}+\int_{\lambda_e+\epsilon}^{+\infty}\frac{e^{-\lambda_e t}\lambda_e^2}{s^2-\lambda_e^2}\frac{p(-i\lambda_e)}{q(-i\lambda_e)}\mathrm{d}s\right)\right),$$

and the integrals in the second braces is vanishing for every ϵ. So, one remains with

$$J_2(t)=\frac{2}{\pi}PV\int_0^\infty\frac{e^{-st}s}{2(s-\lambda_e)}\frac{p(-is)}{q(-is)}.$$

Finally, the rational function in the above integral can be decomposed in a singular (not integrable) part and an integrable one, obtaining

$$J_2(t)=\frac{1}{\pi}\mathcal{L}\left(\frac{c_1 s+c_2}{(s-\gamma_e)^2+\omega_e^2)}\right)+\frac{c_3}{\pi}PV\int_0^\infty\frac{e^{-st}}{s-\lambda_e}\mathrm{d}s,$$

where c_1, c_2, and c_3 are constants depending on the parameters. □

The first integral has the time behavior of the other already studied contributions, and the last one is related to the exponential integral function

$$\frac{c_3}{\pi} PV \int_0^\infty \frac{e^{-st}}{s-\lambda_e} ds = -\frac{c_3}{\pi} e^{-\lambda_e t} \mathrm{Ei}(\lambda_e t).$$

From the well-known asymptotic behavior for large arguments of the exponential integral function, one can deduce that the leading contribution for large times to the survival amplitude is of the order $1/t$ when $t \gg 1$. In summary, collecting the previous calculations, we end with the following result.

Theorem 3.3: *There exist complex constants c_1, c_2, c_3 depending on the physical parameters e, m, c, ω_0 such that the survival amplitude is given by*

$$\mathcal{S}(t) = c_1 e^{-\lambda_e |t|} + c_2 e^{-\gamma_e |t|} e^{-i\omega_e t} + c_3 e^{-\lambda_e |t|} \mathrm{Ei}(\lambda_e |t|).$$

C. Transition amplitudes

Now we turn to the evaluation of the transition amplitudes. As we see in the previous theorem, the unperturbed excited states of the oscillator decay. The transition to a lower energy state takes place with the emission of electromagnetic radiation, photons in the Fock space. To give a quantitative estimate of the probability of emission of photons one must decide which functions describe the one particle states of the electromagnetic field one is interested in. We choose to calculate the transition amplitudes in the case of a regularized plane wave of (approximatively) given momentum.

Classically, a natural choice for the functions φ representing the photons of energy $\hbar\nu$ should be the divergence-free plane waves of the kind

$$\varphi(x) := k \wedge \zeta e^{-i\nu k \cdot x/c}, \quad |k| = 1.$$

Of course such functions are not square integrable and so we consider the divergence-free regularization defined by

$$\varphi^\epsilon(x) := \left(k - \frac{i\epsilon}{\nu} \frac{x}{|x|} \right) \wedge \zeta e^{-i\alpha k \cdot x/c - \epsilon |x|/c}, \quad \nu > 0, \quad \epsilon > 0, \quad |k| = 1.$$

We choose this one as the one-particle wave functions describing photons. Eventually, we are interested in removing the cutoff ϵ from the amplitude transitions.

We anticipate the definitions of some quantities appearing in the statement and proof of the following result. To evaluate the resolvent between states relevant to the transitions, one needs the scalar product $\langle \varphi^\epsilon, \mathcal{G}_z^\pm \rangle$. Assuming that k is along the z axis and ζ is along the y axis, by elementary calculations one obtains

$$\chi^\epsilon(\pm z) := \langle \varphi^\epsilon, \mathcal{G}_z^\pm \rangle \equiv k \wedge \zeta^* \frac{1}{\alpha} \left(\frac{\alpha^2 - \epsilon(\epsilon \mp iz)}{\alpha^2 + (\epsilon \mp iz)^2} - \frac{i\epsilon}{2\alpha^2} \ln \frac{\alpha + i\epsilon \pm z}{\alpha - i\epsilon \mp z} \right) \equiv (k \wedge \zeta^*)(\chi_r^\epsilon(\pm z) + \chi_l^\epsilon(\pm z)).$$

We have written the function $\chi^\epsilon(\pm z)$ just defined, as the sum $\chi_r^\epsilon(\pm z) + \chi_l^\epsilon(\pm z)$ with two summands, a rational one and a logarithmic one. The first, $\chi_r^\epsilon(\pm z)$ has poles at the points $\pm\alpha \pm i\epsilon$, and at the same points the logaritmic part $\chi_l^\epsilon(\pm z)$ has branching points. Due to this fact, some cautions are needed in the use of the residue theorem to evaluate transition amplitudes. Note, moreover, that these branching points of χ are to be thought of as artificial byproducts of the regularization of the plane wave, and that the poles of the function χ_r correspond to the frequencies of the plane wave. These poles depend on the particular wave function representing the photon, at variance with the poles of the function $1/q(z)$, which are determined by the physical parameters of the system. We indicate with $\mathcal{C}$ the logarithmic cut in the complex plane, and we distinguish the components of the cut with real part of a fixed sign $(\pm)$, with $\mathcal{C}^\pm$. With these premises, we state the following.

Lemma 3.4: For any $\zeta_1, \zeta_2 \in \mathbb{C}^3$ one has

$$\langle (\varphi_1^\epsilon, 0), e^{-it(L_e^+)^{1/2}} (0, \zeta_2) \rangle = \mathcal{A}^\epsilon(t) k \cdot (\zeta_1^* \wedge \zeta_2),$$

where

$$\mathcal{A}^{\epsilon}(t) = -\frac{4\pi e}{c}\frac{\kappa_2}{\kappa^2} I^{\epsilon}(t)$$

and, with $\pm t > 0$,

$$\begin{aligned} I^{\epsilon}(t) = {} & \mp e^{\mp \lambda_e t}\lambda_e^2 \frac{\chi(-i\lambda_e)}{q(-i\lambda_e)} \pm e^{\mp \gamma_e t}\frac{e^{-i\omega_e t} 2z_{\pm}}{z_{\pm}+i\lambda_e}\frac{2z_{\pm}+i\lambda_e}{q'(z_{\pm})}\chi(z_{\pm}) \\ & \pm e^{\mp \epsilon t}\frac{e^{\mp i\nu t}2(\pm\nu - i\epsilon)}{\pm\nu + i(\lambda_e - \epsilon)}\frac{2\nu + i(\lambda_e - 2\epsilon)}{q(\pm\nu - i\epsilon)}\frac{\mp\nu - i\epsilon}{2\nu} \\ & + \frac{i}{\pi}\int_{\mathbb{R}} ds \left(\frac{e^{\mp\lambda_e t}\lambda_e^3}{s^2-\lambda_e^2}\frac{\chi(-i\lambda_e)}{q(-i\lambda_e)} + \frac{e^{\mp|s|t}|s|(-2|s|+\lambda_e)}{2(|s|-\lambda_e)}\frac{\chi(-i|s|)}{q(-i|s|)}, \right) \\ & + \frac{i}{\pi}\int_{\mathbb{R}} ds \frac{e^{\mp|s|t}|s|(2|s|+\lambda_e)}{2(|s|+\lambda_e)}\frac{\chi(i|s|)}{q(i|s|)} + \frac{\epsilon}{\nu^3}\int_{\mathcal{C}} dz\, e^{-itz}\frac{2z+i\lambda_e}{z+i\lambda_e}\frac{1}{q(z)} \\ & + \pi\frac{\epsilon}{\nu^3}\left(\int_{\mathcal{C}^+} dz\, e^{-itz}\frac{2z+i\lambda_e}{z+i\lambda_e}\frac{z}{q(z)} - \int_{\mathcal{C}^-} dz\, e^{-itz}\frac{2z+i\lambda_e}{z+i\lambda_e}\frac{z}{q(z)} \right), \end{aligned}$$

Proof: One has, proceeding as in the proof of Lemma 3.1,

$$\langle (\varphi_1^{\epsilon},0), (L_e - z^2)^{-1}(0,\zeta_2)^{+}\rangle = \frac{4\pi c e \kappa_2}{\kappa^2(\mp iz+\lambda_e)}\frac{(\pm 2iz-\lambda_e)(\pm iz+\lambda_e)}{\left(\frac{2e^2}{3c^3}z^2 - \frac{m\omega_0^2}{\lambda_e^2}(\mp iz+\lambda_e)\right)(\pm iz+\lambda_e)}\chi^{\epsilon}(\pm z)(k\wedge\zeta_1^*)\cdot\zeta_2.$$

Therefore,

$$\langle (\varphi_1^{\epsilon},0), e^{-it(L_e^+)^{1/2}}(0,\zeta_2)\rangle = -\frac{4\pi e}{c}\frac{\kappa_2}{\kappa^2}\left(I_1(t) + \frac{1}{\pi}\int_{\mathbb{R}} ds\, I_2(t,s)\right)(k\wedge\zeta_1^*)\cdot\zeta_2,$$

where (we omit the dependence on ϵ)

$$I_1(t) := \frac{1}{2\pi i}\lim_{a\uparrow\infty}\int_{-a}^{a} d\lambda\, e^{-it\lambda}\lambda(g(\lambda)-g(-\lambda)),$$

$$I_2(t,s) := \frac{1}{2\pi i}\int_{\mathbb{R}} d\lambda\, e^{-it\lambda}\lambda^2\frac{g(\lambda)-g(-\lambda)}{s^2+\lambda^2},$$

$$g(\lambda) := \frac{2\lambda+i\lambda_e}{\lambda+i\lambda_e}\frac{\chi(\lambda)}{q(\lambda)}.$$

Now, let us choose a path in the complex lower half-plane which has the real axis as the upper side, avoids the cuts of the function χ_l (say, the straight half lines parametrized as $z=\pm\nu+u-i\epsilon$, $\pm u>0$), and close itself at ∞ along a great circle, as in the previous lemma. There will be contributions due to the residues of the function $1/q(z)$, the residues of the function $\chi_r(z)$, and to the discontinuity of the logarithmic part of $\chi_l(z)$ along the cut. In the end, one obtains, when $\pm t > 0$,

$$I_1(t) = \mp e^{\mp\lambda_e t}\lambda_e^2\frac{\chi(-i\lambda_e)}{q(-i\lambda_e)} \pm e^{\mp\gamma_e t}\sum_{k=1,2}\frac{e^{\mp(-1)^k i\omega_e t}z_k}{z_k+i\lambda_e}\frac{2z_k+i\lambda_e}{q'(z_k)}\chi(z_k) \pm e^{\mp\epsilon t}\sum_{k=1,2}\frac{e^{\mp i\nu t}w_k}{w_k+i\lambda_e}\frac{2w_k+i\lambda_e}{q(w_k)}r_k + \int_{\mathcal{C}}\frac{2z+i\lambda_e}{z+i\lambda_e}\frac{e^{-itz}}{q(z)},$$

where $z_\pm$ are the poles of q, $w_k := (-1)^k\nu - i\epsilon$ are the two poles of $\chi_r(z)$ and r_k the residues of χ_r, and finally $\mathcal{C}$ is the path along the cut of the logarithmic term.

Moreover, we have

$$I_2(t,s) = i\frac{e^{\mp\lambda_e t}\lambda_e^3}{s^2-\lambda_e^2}\frac{\chi(-i\lambda_e)}{q(-i\lambda_e)} + e^{\mp\gamma_e t}\sum_{k=1,2}\frac{z_k}{s^2+z_k^2}\frac{e^{\mp(-1)^k i\omega_e t}z_k}{z_k+i\lambda_e}\frac{2z_k+i\lambda_e}{q'(z_k)}\chi(z_k) + e^{\mp\epsilon t}\sum_{k=1,2}\frac{w_k}{s^2+w_k^2}\frac{e^{\mp i\nu t}w_k}{w_k+i\lambda_e}\frac{2w_k+i\lambda_e}{q(w_k)}r_k + ie^{\mp|s|t}\frac{|s|}{2}\left(\frac{\mp 2|s|+\lambda_e}{|s|\mp\lambda_e}\frac{\chi(\mp i|s|)}{q(\mp i|s|)} + \frac{\pm 2|s|+\lambda_e}{|s|\pm\lambda_e}\frac{\chi(\pm i|s|)}{q(\pm i|s|)}\right) + \int_{\mathcal{C}}e^{-itz}\frac{2z+i\lambda_e}{z+i\lambda_e}\frac{z^2}{q(z)}\frac{1}{s^2+z^2}.$$

Therefore one obtains

$$\begin{aligned} I_1(t) + \frac{1}{\pi}\int_{\mathbb{R}} ds\, I_2(t,s) = {} & \mp e^{\mp\lambda_e t}\lambda_e^2\frac{\chi(-i\lambda_e)}{q(-i\lambda_e)} \pm e^{\mp\gamma_e t}\frac{e^{-i\omega_e t}2z_k}{z_k+i\lambda_e}\frac{2z_k+i\lambda_e}{q'(z_k)}\chi(z_k) \\ & \pm e^{\mp\epsilon t}\frac{e^{\mp i\nu t}2w_k}{w_k+i\lambda_e}\frac{2w_k+i\lambda_e}{q(w_k)}r_k \\ & + \frac{i}{\pi}\int_{\mathbb{R}} ds\left(\frac{e^{\mp\lambda_e t}\lambda_e^3}{s^2-\lambda_e^2}\frac{\chi(-i\lambda_e)}{q(-i\lambda_e)} + \frac{e^{\mp|s|t}|s|(-2|s|+\lambda_e)}{2(|s|-\lambda_e)}\frac{\chi(-i|s|)}{q(-i|s|)}\right) \\ & + \frac{i}{\pi}\int_{\mathbb{R}} ds\frac{e^{\mp|s|t}|s|(2|s|+\lambda_e)}{2(|s|+\lambda_e)}\frac{\chi(i|s|)}{q(i|s|)} + \frac{\epsilon}{\nu^3}\int_{\mathcal{C}} dz\, e^{-itz}\frac{2z+i\lambda_e}{z+i\lambda_e}\frac{1}{q(z)} \\ & + \pi\frac{\epsilon}{\nu^3}\left(\int_{\mathcal{C}^+} dz\, e^{-itz}\frac{2z+i\lambda_e}{z+i\lambda_e}\frac{z}{q(z)} - \int_{\mathcal{C}^-} dz\, e^{-itz}\frac{2z+i\lambda_e}{z+i\lambda_e}\frac{z}{q(z)}\right), \end{aligned}$$

where $k=2$ if $t>0$ and $k=1$ if $t<0$ and $\mathcal{C}^\pm$ are the components of $\mathcal{C}$ with $\pm\mathrm{Sign}(\mathrm{Re}(z))>0$, respectively.

□

Now we can give the time behavior of the various terms, as in the previous theorem. A first group of terms is composed by the resonant contributions. One can distinguish natural resonances, depending on the structural parameters only (the physical constants e,m,c), and the resonance due to the incident photon. For $\epsilon\downarrow 0$ this last contribution reduces to a strictly oscillating term, as expected. A second group of terms is given by the s integrals. We give their behavior for vanishing ϵ only. The calculation is similar to the one already given for the survival amplitude, and one has in the end Laplace transforms of rational functions with poles at the resonances, producing other exponentials of the type already seen, and an exponential integral function. So the leading behavior of the type t^{-1} survives to the $\epsilon\downarrow 0$ limit.

The last group of terms are the contour complex integrals. These could be analyzed asymptotically as Fourier integrals of rational functions, but they vanish as $\epsilon\downarrow 0$. Summarizing we can state the following.

Theorem 3.5: *There exist complex constants C_1,C_2,C_3 depending on the physical parameters m, e, c, ω_0, ν, and a function $R(t)$ such that*

$$\lim_{\epsilon \downarrow 0} \mathcal{A}^{\epsilon}(t) = C_1 e^{-\lambda_{\mathrm{e}}|t|} + C_2 e^{-\gamma_{\mathrm{e}}|t|} e^{-i\omega_{\mathrm{e}} t} + C_3 e^{-i\nu t} + R(t)$$

with

$$R(t) = O(1/t), \quad |t| \gg 1.$$

APPENDIX: QUANTIZATION OF ABSTRACT WAVE EQUATIONS

In this appendix we give a brief and self-contained introduction to the quantization of second order abstract wave equations, along the lines traced by Segal in the 1950s and 1960s and with an emphasis on the aspects of direct concern with our work. We refer for details and different approaches to Refs. 23 and 13 as regards abstract wave equations and to Refs. 21 and 5 as regards quantization.

Let $B: D(B) \subseteq \mathcal{H} \to \mathcal{H}$ be an injective self-adjoint operator on the real Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle)$. We denote by $\mathcal{H}^1$, the Hilbert space given by the domain of B with the scalar product $\langle \cdot, \cdot \rangle_1$ leading to the graph norm, i.e.,

$$\langle \phi_1, \phi_2 \rangle_1 := \langle B\phi_1, B\phi_2 \rangle + \langle \phi_1, \phi_2 \rangle.$$

We then define the Hilbert space $\bar{\mathcal{H}}^1$ by completing the pre-Hilbert space $D(B)$ endowed with the scalar product

$$[\phi_1, \phi_2]_1 := \langle B\phi_1, B\phi_2 \rangle.$$

We extend the self-adjoint operator B to $\bar{\mathcal{H}}^1$ by considering $\bar{B}: \bar{\mathcal{H}}^1 \to \mathcal{H}$, the closed bounded extension of the densely defined linear operator

$$B: \mathcal{H}^1 \subseteq \bar{\mathcal{H}}^1 \to \mathcal{H}.$$

Since B is self-adjoint one has $\mathrm{Ran}(B)^{\perp} = \mathrm{Ker}(B)$, so that, being B injective, $\mathrm{Ran}(B)$ is dense in $\mathcal{H}$. Therefore we can define $\bar{B}^{-1}: \mathcal{H} \to \bar{\mathcal{H}}^1$ as the closed bounded extension of the densely defined linear operator

$$B^{-1}: \mathrm{Ran}(B) \subseteq \mathcal{H} \to \mathcal{H}^1.$$

One can then verify that $\bar{B}$ is boundedly invertible with inverse given by $\bar{B}^{-1}$.

Given $\bar{B}$ we can now introduce the space $\bar{\mathcal{H}}^2$ defined by

$$\bar{H}^2 := \{\phi \in \bar{\mathcal{H}}_1 : \bar{B}\phi \in \mathcal{H}_1\}.$$

On the Hilbert space $\bar{\mathcal{H}}^1 \oplus \mathcal{H}$ with scalar product

$$\langle\langle (\phi_1, \dot{\phi}_1), (\phi_2, \dot{\phi}_2) \rangle\rangle := \langle \bar{B}\phi_1, \bar{B}\phi_2 \rangle + \langle \dot{\phi}_1, \dot{\phi}_2 \rangle$$

we define the linear operator

$$W_B: \bar{\mathcal{H}}_2 \oplus \mathcal{H}^1 \subseteq \bar{\mathcal{H}}^2 \oplus \mathcal{H} \to \bar{\mathcal{H}}^1 \oplus \mathcal{H}, \quad W_B(\phi, \dot{\phi}) := (\dot{\phi}, -B\bar{B}\phi).$$

Theorem A.1: *The linear operator W_B is skew-adjoint.*

Being W_B skew-adjoint, by the Stone theorem it generates the strongly continuous one-parameter group of isometric operators e^{tW_B}. By defining $(\phi(t), \dot{\phi}(t)) := e^{tW_B}(\phi, \dot{\phi})$, one has that, in the case $\phi \in \bar{\mathcal{H}}^2$, $\dot{\phi} \in \mathcal{H}^1$, $\phi(t)$ is the unique strong solution of the Cauchy problem

$$\ddot{\phi}(t) = -B\bar{B}\phi(t),$$

$$\phi(0) = \phi, \quad \dot{\phi}(0) = \dot{\phi}.$$

Given an arbitrary real Hilbert space $(\mathcal{K}, \langle\cdot,\cdot\rangle_{\mathcal{K}})$ we will denote by $(\mathcal{K}_c, \langle\cdot,\cdot\rangle_c)$ its standard complexification, i.e., $\mathcal{K}_c = \mathcal{K}\oplus\mathcal{K}$, the multiplication by the complex unity being defined by $i\psi := J\psi$, $J(\varphi_1,\varphi_2) := (-\varphi_2,\varphi_1)$, and

$$\langle\psi_1,\psi_2\rangle_c := \langle\psi_1,\psi_2\rangle_{\mathsf{K}\oplus\mathsf{K}} - i\langle\psi_1, J\psi_2\rangle_{\mathsf{K}\oplus\mathsf{K}}.$$

Given any linear operator $A: D(A)\subseteq\mathcal{K}\to\mathcal{K}$ on $\mathcal{K}$, we define $A_c: D(A_c)\subset\mathcal{K}_c\to\mathcal{K}_c$ by $D(A_c) := D(A)\times D(A)$, $A_c(\varphi_1,\varphi_2) := (A\varphi_1, A\varphi_2)$. Conversely, given any linear operator $L: D(L)\subset\mathcal{K}_c \to\mathcal{K}_c$, $L(\varphi_1,\varphi_2)\equiv(L_1(\varphi_1,\varphi_2), L_2(\varphi_1,\varphi_2))$, we define $L_r: D(L_r)\subseteq\mathcal{K}\to\mathcal{K}$ by $D(L_r) := \{\phi \in \mathsf{K}: (\phi,0)\in D(L)\}$, $L_r := L_1(\varphi,0)$.

By the above definitions B_c is self-adjoint and $(W_B)_c = W_{B_c}$, where

$$W_{B_c}: \bar{\mathcal{H}}^2_c \oplus \mathcal{H}^1_c \subseteq \bar{\mathcal{H}}^2_c \oplus \mathcal{H}_c \to \bar{\mathcal{H}}^1_c \oplus \mathcal{H}_c, \quad W_{B_c}(\psi,\dot{\psi}) := (\dot{\psi}, -B_c\bar{B}_c\psi).$$

By the Stone formula one has the following.

Lemma A.2:

$$e^{tW_B} = \lim_{a\uparrow\infty}\lim_{\epsilon\downarrow 0}\frac{1}{2\pi i}\int_{-a}^{a} \mathrm{d}\lambda\, e^{-it\lambda}((iW_{B_c} - (\lambda + i\epsilon))^{-1} - (iW_{B_c} - (\lambda - i\epsilon))^{-1})_r.$$

The following lemma translates the wave flow in a Schrödinger-type one.

Lemma A.3: The map

$$C_B: \bar{\mathcal{H}}^1 \oplus \mathcal{H} \to \mathcal{H}_c, \quad C_B(\phi,\dot{\phi}) := (\bar{B}\phi, \dot{\phi})$$

is unitary once one makes $\bar{\mathcal{H}}^1\oplus\mathcal{H}$ a complex Hilbert space by introducing the complex structure $J_B(\phi,\dot{\phi}) := (-\bar{B}^{-1}\dot{\phi}, \bar{B}\phi)$ and by defining $i(\phi,\dot{\phi}) := J_B(\phi,\dot{\phi})$ and the scalar product

$$\langle\langle(\phi_1,\dot{\phi}_1),(\phi_2,\dot{\phi}_2)\rangle\rangle_B := \langle\langle(\phi_1,\dot{\phi}_1),(\phi_2,\dot{\phi}_2)\rangle\rangle - i\langle\langle(\phi_1,\dot{\phi}_1), J_B(\phi_2,\dot{\phi}_2)\rangle\rangle.$$

Moreover

$$e^{tW_B} = C_B^* e^{-itB_c} C_B.$$

Once we have transformed the abstract wave equation $\ddot{\phi}(t) = -B\bar{B}\phi(t)$, defined on the real Hilbert space $\bar{\mathcal{H}}^1\oplus\mathcal{H}$, into the Schrödinger equation $i\dot{\psi} = B_c\psi$, defined on the complex Hilbert space $\mathcal{H}_c$, we can then (second) quantize it in the standard way. Let us define K to be the bosonic Fock space over $\mathcal{H}_c$ (see Ref. 19, Sec. II.4, for the definition). For any $\psi\in\mathcal{H}$ we define the self-adjoint operator on K given by the Segal field $\mathsf{S}(\psi) := (1/\sqrt{2})(\mathsf{C}(\psi) + \mathsf{C}^*(\psi))$, were C and C^* denote the usual creation and destruction operators (see Ref. 20, Sec. X.7, for the definition). Given the Segal field S we can then define the Weyl system $\mathsf{W}(\psi) := e^{i\mathsf{S}}\psi$, so that

$$\mathsf{W}(\psi_1+\psi_2) = e^{(i/2)\langle\psi_1,\psi_2\rangle_c}\mathsf{W}(\psi_1)\mathsf{W}(\psi_2).$$

The unitary strongly continuous one-parameter group of evolution on K defined by $\mathsf{U}(t) := \Gamma(e^{-itB_c})$ satisfies the relations

$$\mathsf{W}(e^{-itB_c}\psi) = \mathsf{U}(t)\mathsf{W}(\psi)\mathsf{U}(t)^*$$

and we denote by $\mathrm{d}\Gamma(B_c)$ the self-adjoint operator on K which generates $\mathsf{U}(t)$ (we refer to Ref. 20, Sec. II.4, and Ref. 8 for the definitions of Γ and $\mathrm{d}\Gamma$). The quantum Hamiltonian corresponding to the (second) quantization of the abstract wave equation $\ddot{\phi}(t) = -B\bar{B}\phi(t)$ is defined by $\mathsf{H} := \hbar\,\mathrm{d}\Gamma(B_c)$. Suppose now that we start with a self-adjoint operator A on the real Hilbert space $\mathcal{K}$. Denoting by A^+ the positive part of A and by $\mathcal{K}^+$ the projection of $\mathcal{K}$ onto the positive spectral subspace. Then

we can apply the previous construction to $B:=(A^+)^{1/2}$, considered as an injective self-adjoint operator on $\mathcal{H}:=\mathcal{K}^+$. However, since

$$\langle \psi_1, e^{-it(A^+)_c^{1/2}} \psi_2 \rangle = \langle \psi_1^+, e^{-it(A^+)_c^{1/2}} \psi_2^+ \rangle,$$

where ψ^+ denotes the projection of ϕ on $\mathcal{K}^+$, we will work with $\mathrm{d}\Gamma((A^+)_c^{1/2})$ on the bosonic Fock space over $\mathcal{K}$.

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Solutions of the massive SU(*N*) Yang–Mills equations by harmonic maps

H. J. Wospakrik
Department of Mathematical Sciences, University of Durham, Durham DH1 3LE, United Kingdom and Department of Physics, Institute of Technology Bandung, Jalan Ganesha 10, Bandung 40132, Indonesia

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We consider classical static solutions of the pure massive SU(N) Yang–Mills field equations in (3+1)-dimensional space–time. By applying harmonic map ansatz, constructed from the harmonic maps $S^2 \to CP^{N-1}$, we construct some bounded spherically symmetric solutions having finite energies for $N=2$, 3, and 4 cases.
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I. INTRODUCTION

It is well known that the pure massless (3+1)-dimensional SU(N) Yang–Mills theories do not admit static classical finite-energy solutions.[1,2] This fact is related to the conformal invariance of the action which implies that the corresponding stress-energy tensor is traceless. As mass terms in the action break this conformal invariance, this raises the expectation that finite-energy solutions might exist in the pure massive SU(N) Yang–Mills theories. This expectation is our main concern in this paper.

The pure massive case is of course pathological, as its action is nongauge invariant. In order to get rid of this nongauge invariance, in Sec. II we consider a Stückelberg-type gauge invariant formalism,[3] where SU(N) chiral currents $\tilde{U}^{-1}\partial_\mu \tilde{U}$ with $\tilde{U} \in \mathrm{SU}(N)$ are added to render the massive terms gauge invariant. The pure massive case now corresponds to choosing the special gauge $\tilde{U}=I$. We then observe that if, within this special gauge, we choose the massive gauge potential to be of *almost* pure gauge form, we recover the SU(N) Skyrme models action,[4] which adds strong support to our previous expectation.

Armed with this observation, in Sec. III we turn to consider a static magnetic type case where we show that the corresponding energy satisfies a Hobart–Derrick-type stability condition[5,6] for the existence of finite energy solutions. By performing a Bogomolnyi-type analysis to the energy, we found that the energy has a lower bound that is proportional to a metric independent integral we call B-integral, which is analogous to the topological charge of the SU(N) Skyrme models.[4]

To construct these solutions, in Sec. IV we consider the spherically symmetric case where we apply harmonic map ansatz for the gauge potentials that were introduced by Ioannidou and Sutcliffe in their study of non-Bogomolnyi BPS monopoles.[7] The ansatz is constructed by using $(N-1)$ rank-1 projectors of the harmonic maps $S^2 \to CP^{N-1}$ as formulated in Ref. 8. Here, the two-dimensional (2D) harmonic map construction, which is a generalization of geodesic concept in differential geometry,[9] is used to describe the angular dependence of the field configurations. This has the advantage of reducing the complicated matrix field equations into simpler sets of nonlinear ordinary differential equations (ODEs) for the profile functions $g_l(r)$, $l=0,1,\ldots,(N-1)$, i.e., the radial dependence part of the fields.

In Sec. V, we study spherically symmetric solutions of the equations (numerically) for lower N cases (2, 3, and 4), where we found that by letting the profile functions $g_l(r)$ vanish at $r \to \infty$ and appropriately choosing the boundary conditions to be imposed at the origin $r=0$, some bounded solutions with finite energies can be constructed.

II. MASSIVE SU(*N*) YANG–MILLS THEORIES AND SKYRME MODELS

Let $\tilde{U}(x)$ be an SU(N) group valued function of space–time coordinates. Then a Stückelberg-type formalism of massive SU(N) Yang–Mills theories is given by the action[3]

$$S = \int \mathrm{d}^4x \, \mathrm{Tr}\Big[-\tfrac{1}{2}F^{\mu\nu}F_{\mu\nu} + M^2(A^\mu - \tilde{L}^\mu)(A_\mu - \tilde{L}_\mu)\Big], \tag{1}$$

where Tr is for trace and where

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + i[A_\mu, A_\nu], \tag{2}$$

$$\tilde{L}_\mu = -i\tilde{U}^{-1}\partial_\mu \tilde{U}, \tag{3}$$

with M as a mass parameter and where we have chosen arbitrarily the gauge coupling $e=1$. The gauge potential A_μ and the left chiral current $\tilde{L}_\mu$ have values in the Lie algebra Su(N) and here we have chosen them to be Hermitian, i.e., $A_\mu^\dagger = A_\mu$ and $\tilde{L}_\mu^\dagger = \tilde{L}_\mu$, respectively.

We note that the action (1) is *invariant* under the gauge transformations,

$$A'_\mu = \Omega^{-1}A_\mu\Omega - i\Omega^{-1}\partial_\mu\Omega, \tag{4}$$

$$\tilde{U}' = \tilde{U}\Omega, \tag{5}$$

where $\Omega \in \mathrm{SU}(N)$. On the other hand, as under the scale transformation $x^\mu \to \lambda x^\mu$, the gauge potential and the chiral current scale as $\lambda A_\mu(\lambda x)$ and $\lambda\tilde{L}_\mu(\lambda x)$, respectively, we see that the mass term breaks the scale invariancy of the action (1).

The corresponding Euler–Lagrange equations are

$$D_\mu F^{\mu\nu} - M^2(A^\nu - \tilde{L}^\nu) = 0, \tag{6}$$

$$\partial_\mu A^\mu - D_\mu \tilde{L}^\mu = 0, \tag{7}$$

where for any $G \in \mathrm{Su}(N)$,

$$D_\mu G \equiv \partial_\mu G + i[A_\mu, G]. \tag{8}$$

Taking $\Omega = \tilde{U}^{-1}$ in (4) and (5), $\tilde{U}$ becomes the unit element I and the action (1) reduces to

$$S = \int \mathrm{d}^4x \, \mathrm{Tr}\Big[-\tfrac{1}{2}F^{\mu\nu}F_{\mu\nu} + M^2A^\mu A_\mu\Big], \tag{9}$$

i.e., it is the *pure massive* SU(N) Yang–Mills action. The field equations (6) and (7) then reduce to

$$D_\mu F^{\mu\nu} - M^2A^\nu = 0, \tag{10}$$

$$\partial_\mu A^\mu = 0, \tag{11}$$

respectively.

Equation (11) means that the gauge potential A_μ satisfies the *Lorentz condition*. Thus, we may interpret the action (9) as a gauge fixed version of the gauge invariant action (1). As the field equations (10) and (11) imply 3 degrees of freedom (polarization states) for each vector field A_μ^a where a is the Lie algebra index, we call the gauge $\tilde{U}=I$ the *physical* or *unitary gauge*. In the following, by massive SU(N) Yang–Mills theories we mean the pure case (9).

Now, let us make the following observation by choosing the gauge potential A_μ in the action

(9) to be of *almost* pure-gauge form, i.e.,

$$A_\mu = iqU^{-1}\partial_\mu U, \tag{12}$$

where U takes value in the group SU(N), and q is a space–time independent free parameter. In terms of U, the gauge field strength $F_{\mu\nu}$, according to (2), becomes

$$F_{\mu\nu} = -iq(1+q)[L_\mu, L_\nu], \tag{13}$$

where

$$L_\mu = U^{-1}\partial_\mu U. \tag{14}$$

Thus we see that, if we choose $q=-1$ then $F_{\mu\nu}=0$ and so the corresponding gauge potential A_μ is a pure gauge.

Setting (12) and (13) into the action (9) yields a new action

$$S = \int \mathrm{d}^4x \, \mathrm{Tr}\left(\tfrac{1}{2}q^2(1+q)^2[L^\mu, L^\nu][L_\mu, L_\nu] - q^2M^2L^\mu L_\mu\right), \tag{15}$$

which coincides with the SU(N) Skyrme models action,[4] with the parameters identification,

$$F = 4qM, \quad a = \frac{1}{4q(1+q)}, \tag{16}$$

where F is the pion decay constant, and a the Skyrme models dimensionless constant.

As the SU(N) Skyrme models have finite (or solitonic) solutions called skyrmions, this coincidence gives us a strong basis to expect that massive SU(N) Yang–Mills theories might admit finite energy solutions as well. To check this further, in the following sections, III–V, we choose to study the static magnetic type case.

III. STATIC MAGNETIC TYPE ENERGY AND *B*-INTEGRAL

As we are interested in the static magnetic type case, we exclude the electric type fields by imposing

$$A_0 = 0, \quad \partial_0 A_a = 0, \tag{17}$$

from which it follows that

$$F_{0a} = 0, \tag{18}$$

where $a=1, 2, 3$. Then, from the action (9), the static magnetic type energy of the massive SU(N) Yang–Mills fields is

$$E = \int \mathrm{d}^3x \, \mathrm{Tr}\left[\tfrac{1}{2}F_{ab}^2 + M^2A_a^2\right]. \tag{19}$$

In Ref. 10, Sheng had shown that the static magnetic type massive SU(N) Yang–Mills fields in $(n+1)-D$ space–time with $n\neq 3$ do not allow for the existence of finite-energy static solutions. Thus, the $n=3$ case that we are considering here evades Sheng nonexistence theorems which was left as an open problem in Ref. 10.

To examine this $n=3$ case explicitly, let us study the scale stability of the energy integral (19) under the scale transformation, $\vec{x}\to\lambda\vec{x}$. As the gauge potentials A_μ scale as

$$A_\mu(\vec{x}) \to \lambda A_\mu(\lambda\vec{x}), \tag{20}$$

from which

$$F_{\mu\nu}(\vec{x}) \to \lambda^2 F_{\mu\nu}(\lambda\vec{x}), \tag{21}$$

the energy integral (19) scales as

$$E \to E[\lambda] = \int \frac{\mathrm{d}^3(\lambda x)}{\lambda^3} \mathrm{Tr}\left[\tfrac{1}{2}\lambda^4 F_{ab}(\lambda\vec{x})^2 + M^2\lambda^2 A_a(\lambda\vec{x})^2\right]$$

$$= \lambda E_F + \frac{1}{\lambda} E_M, \tag{22}$$

where E_F and E_M are the F-term and the massive term, respectively. Thus we see that the pure massive SU(N) Yang–Mills static energy (19) scales in the same fashion as the static energy of the SU(N) Skyrme models.[4] As

$$\left.\frac{\mathrm{d}E[\lambda]}{\mathrm{d}\lambda}\right|_{\lambda=1} = E_F - E_M, \tag{23}$$

$$\left.\frac{\mathrm{d}^2E[\lambda]}{\mathrm{d}\lambda^2}\right|_{\lambda=1} = 2E_M, \tag{24}$$

the extremum condition guarantees that $E_M = E_F$. Thus we see that the Hobart–Derrick-type stability condition[5,6] could be satisfied, and so we conclude that static massive SU(N) Yang–Mills field theories admit the existence of finite-energy solutions as we expected.

Next, we note that the energy integral (19) can be expressed in the form of a perfect square term plus "something" as follows:

$$E = \int \mathrm{d}^3x\, \mathrm{Tr}\left[\left(\tfrac{1}{2}\epsilon_{abc}F_{ab} - MA_c\right)^2 + M\epsilon_{abc}F_{ab}A_c\right]. \tag{25}$$

The second term in (25) has structure which is independent of the metric tensor, which raises the expectation that it is a topological quantity. As it is proportional to the baryon number B of the SU(N) Skyrme models if A_μ is of almost pure gauge form, so for convenience we keep the same letter B for it, and define

$$B = \frac{1}{16\pi}\int \mathrm{d}^3x\, \mathrm{Tr}[\epsilon_{abc}F_{ab}A_c]. \tag{26}$$

For later reference, we call it by the name *B-integral*. From (25) it is obvious that, for finite B,

$$E \geqslant 16\pi MB, \tag{27}$$

and so the lower bound of the energy would be saturated if

$$\epsilon_{abc}F_{ab} - 2MA_c = 0, \tag{28}$$

which is analogous to Bogomolnyi's bound in Yang–Mills–Higgs monopole theories.[7] Note that (28) is consistent with the Lorentz condition (11) in this static magnetic type case.

In terms of the spherical polar coordinates (r, θ, ϕ), the energy (19) becomes

$$E = \int \mathrm{d}r(\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi)\mathrm{Tr}\left[F_{r\theta}^2 + \frac{1}{\sin^2\theta}F_{r\phi}^2 + \frac{1}{r^2\sin^2\theta}F_{\theta\phi}^2 + M^2r^2A_r^2 + M^2A_\theta^2 + \frac{M^2}{\sin^2\theta}A_\phi^2\right]. \tag{29}$$

As we are going to apply the harmonic maps $S^2 \to CP^{N-1}$ to this problem, in the following we choose to use the stereographic (holomorphic) coordinates $(\xi, \bar{\xi})$ for S^2 where ξ is related to the θ, φ, via $\xi = \tan(\theta/2)e^{i\varphi}$. The angular derivatives ∂_θ and ∂_ϕ then read

$$\partial_\theta = \frac{(1+|\xi|^2)}{2|\xi|}(\xi\partial_\xi + \bar{\xi}\partial_{\bar{\xi}}), \tag{30}$$

$$\partial_\phi = i(\xi\partial_\xi - \bar{\xi}\partial_{\bar{\xi}}), \tag{31}$$

respectively, where $|\xi| = \sqrt{|\xi|^2}$, whereas for the volume element,

$$\mathrm{d}^3x = r^2\,\mathrm{d}r[\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi] = r^2\,\mathrm{d}r\left[\frac{2i\,\mathrm{d}\bar{\xi}\,\mathrm{d}\xi}{(1+|\xi|^2)^2}\right]. \tag{32}$$

The transformation relations between the angular components of the gauge potential and field strength in the spherical polar and holomorphic coordinates are

$$A_\theta = \frac{(1+|\xi|^2)}{2|\xi|}(\xi A_\xi + \bar{\xi}A_{\bar{\xi}}), \tag{33}$$

$$A_\phi = i(\xi A_\xi - \bar{\xi}A_{\bar{\xi}}), \tag{34}$$

$$F_{r\theta} = \frac{(1+|\xi|^2)}{2|\xi|}(\xi F_{r\xi} + \bar{\xi}F_{r\bar{\xi}}), \tag{35}$$

$$F_{r\phi} = i(\xi F_{r\xi} - \bar{\xi}F_{r\bar{\xi}}), \tag{36}$$

$$F_{\theta\phi} = i|\xi|(1+|\xi|^2)F_{\bar{\xi}\xi}. \tag{37}$$

In terms of the complex quantities on the right-hand side of (33)–(37), the energy (29) in the spherical holomorphic coordinates $(r,\xi,\bar{\xi})$ is

$$E = 2i\int \mathrm{d}r\,\mathrm{d}\xi\,\mathrm{d}\bar{\xi}\,\mathrm{Tr}\left[F_{r\bar{\xi}}F_{r\xi} - \frac{(1+|\xi|^2)^2}{4r^2}F_{\bar{\xi}\xi}F_{\bar{\xi}\xi} + \frac{M^2r^2}{(1+|\xi|^2)^2}A_rA_r + M^2A_{\bar{\xi}}A_\xi\right], \tag{38}$$

and the field equations (10) become

$$D_{\bar{\xi}}F_{\xi r} + D_\xi F_{\bar{\xi}r} - \frac{2Mr^2}{(1+|\xi|^2)^2}A_r = 0, \tag{39}$$

$$D_rF_{r\bar{\xi}} - D_{\bar{\xi}}\left[\frac{(1+|\xi|^2)^2}{2r^2}F_{\bar{\xi}\xi}\right] - M^2A_{\bar{\xi}} = 0, \tag{40}$$

while the Lorentz condition (11) becomes

$$\partial_r(r^2A_r) + \frac{(1+|\xi|^2)^2}{2}[\partial_\xi A_{\bar{\xi}} + \partial_{\bar{\xi}}A_\xi] = 0. \tag{41}$$

IV. SU(*N*) HARMONIC MAP ANSATZ

In this section, we solve the massive SU(N) Yang–Mills field equations (39) and (40) together with the constraint (41), numerically, by using harmonic maps $S^2 \to CP^{N-1}$. Our harmonic map ansatz for the gauge potentials, following Ioannidou and Sutcliffe,[7] are given by

$$A_r = 0, \quad A_{\bar{\xi}} = i\sum_{k=0}^{N-2} g_k[P_k, \partial_{\bar{\xi}} P_k], \tag{42}$$

where $P_k = P_k(\xi, \bar{\xi})$ are rank-1 projector fields of the $CP^{N-1}\sigma$ model,[8] and where g_k, the profile functions, are dependent on the radial coordinate r only.

Following the construction in Ref. 8, the projectors P_k are given by

$$P_k = M_k |M_k|^{-2} M_k^\dagger \quad (k = 0, 1, \ldots, N-1), \tag{43}$$

where M_k are a set of N mutually orthogonal N-component vector fields that are constructed by the Gram–Schmidt procedure from the holomorphic vector fields, M_0, $\partial_\xi M_0, \ldots, \partial_\xi^{(N-1)} M_0$.

Note that, in (43) and the rest of our discussion, summation convention on repeated indices are no longer held. Notice also that the upper sum in (42) is $(N-2)$ as the projectors P_k satisfy the completeness relation, $P_0 + P_1 + \cdots + P_{N-1} = I_N$ where I_N is the $(N \times N)$ unit matrix.

As M_0 is holomorphic, i.e., $\partial_{\bar{\xi}} M_0 = 0$, the following properties of the constructed matrices M_k in (43) hold:[8]

$$\partial_{\bar{\xi}} M_k = -M_{k-1} |M_{k-1}|^{-2} |M_k|^2, \tag{44}$$

$$\partial_\xi (M_k |M_k|^{-2}) = M_{k+1} |M_k|^{-2}. \tag{45}$$

Now, from the construction (43) we see that $A_{\bar{\xi}} = (A_\xi)^\dagger$ and that, as the projectors P_k satisfy the $CP^{N-1}\sigma$ model equation,[8] $[P_k, \partial_{\bar{\xi}\bar{\xi}} P_k] = 0$, it follows from the ansatz (42) that the gauge potentials A_ξ and $A_{\bar{\xi}}$ satisfy the identity

$$\partial_\xi A_{\bar{\xi}} + \partial_{\bar{\xi}} A_\xi = 0, \tag{46}$$

and so (41) is solved by this ansatz automatically.

Furthermore, we find that with the ansatz (42), Eq. (39) is also satisfied identically. Thus, the only nontrivial equation left is (40). To derive the explicit equations for the profile functions g_k from (40), we need to extract out the angular dependence in a consistent way. To carry out this manipulation directly is a formidable task due to the complexities in evaluating the derivatives of the projectors. In order to get rid of it, we reduce the dependencies on the holomorphic coordinates $(\xi, \bar{\xi})$ by multiplying (40) from the right by the mutually orthogonal vector fields $M_l[l = 0, \ldots, (N-1)]$, i.e.,

$$\left(D_r F_{r\bar{\xi}} - D_{\bar{\xi}} \left[\frac{(1 + |\xi|^2)^2}{2r^2} F_{\bar{\xi}\bar{\xi}} \right] - M^2 A_{\bar{\xi}} \right) M_l = 0, \tag{47}$$

and then use the following properties of the projector operators $P_k = M_k |M_k|^{-2} M_k^\dagger$ and its derivatives applied to M_l:

$$P_k M_l = \delta_{kl} M_l, \tag{48}$$

$$(\partial_\xi P_k) M_l = (\delta_{kl} - \delta_{k,l+1}) M_{l+1}, \tag{49}$$

$$(\partial_{\bar{\xi}} P_k) M_l = \kappa_{l-1} (\delta_{k,l-1} - \delta_{kl}) M_{l-1}, \tag{50}$$

where

$$\kappa_l = |M_l|^{-2} |M_{l+1}|^2. \tag{51}$$

In deriving the above results we have taken M_0 to be holomorphic and we have used the derivative properties of M_l as given by Eqs. (44) and (45). Note that, by definition, $\kappa_{-1} = 0$. For example, in deriving (50) we first write

$$(\partial_{\bar{\xi}} P_k) M_l = \partial_{\bar{\xi}}(P_k M_l) - P_k \partial_{\bar{\xi}} M_l. \tag{52}$$

Then, using (44) and (48), i.e., $\partial_{\bar{\xi}} M_l = -\kappa_{l-1} M_{l-1}$, gives (50).

Hence, the action of the gauge potential, as given by the ansatz (42), on the vectors M_l are

$$A_{\xi} M_l = -iG_l M_{l+1}, \tag{53}$$

$$A_{\bar{\xi}} M_l = iG_{l-1}\kappa_{l-1} M_{l-1}, \tag{54}$$

where

$$G_l = (g_l + g_{l+1}), \tag{55}$$

from which we derive that

$$F_{r\xi} M_l = -i\dot{G}_l M_{l+1}, \tag{56}$$

$$F_{r\bar{\xi}} M_l = i\dot{G}_{l-1}\kappa_{l-1} M_{l-1}, \tag{57}$$

$$F_{\bar{\xi}\xi} M_l = i(\tilde{Q}_l \kappa_l - \tilde{Q}_{l-1}\kappa_{l-1}) M_l, \tag{58}$$

where

$$\tilde{Q}_l = G_l(2 - G_l). \tag{59}$$

Note that, by definition, $g_l = 0$ if $l \notin [0, 1, \ldots, (N-2)]$.

Let us now return to Eq. (47). We observe that, in order to have a compatible set of equations for the profile functions g_l, we must choose the vectors M_l in such a way that each factor $(1+|\xi|^2)^2\kappa_l$ is equal to a constant, i.e.,

$$\kappa_l = \frac{\mathcal{K}_l}{(1+|\xi|^2)^2}, \tag{60}$$

where $\mathcal{K}_l$ are some constants depending on the index l. In fact, we found that the condition (60) is satisfied if we choose the initial vector M_0 to be given by the *Veronese map*,[11]

$$M_0 = [1, \sqrt{C_1^{N-1}}\xi, \ldots, \sqrt{C_k^{N-1}}\xi^k, \ldots, \xi^{N-1}]^T, \tag{61}$$

where C_k^{N-1} are binomial coefficients.

With this choice then from the construction of the vectors M_l we obtain[4]

$$\mathcal{K}_l = (l+1)(N-l-1) = \mathcal{N}_l. \tag{62}$$

Using (53)–(57) and (60) for κ_l then for the first two terms of Eq. (40), we obtain

$$\left(D_r F_{r\bar{\xi}} - D_{\bar{\xi}}\left[\frac{(1+|\xi|^2)^2}{2r^2} F_{\bar{\xi}\xi}\right]\right) M_l$$
$$= i\left(\ddot{G}_{l-1} + \frac{1}{2r^2}[\mathcal{N}_l \tilde{Q}_l - 2\mathcal{N}_{l-1}\tilde{Q}_{l-1} + \mathcal{N}_{l-2}\tilde{Q}_{l-2}](1 - G_{l-1})\right)\kappa_{l-1} M_{l-1}. \tag{63}$$

Substituting (54) and (63) in Eq. (40), and noticing that M_l are independent vector fields, we find that the profile functions g_l satisfy the following second order nonlinear ordinary differential equations:

$$\ddot{G}_l + \frac{1}{2r^2}[\mathcal{N}_{l+1}\widetilde{Q}_{l+1} - 2\mathcal{N}_l\widetilde{Q}_l + \mathcal{N}_{l-1}\widetilde{Q}_{l-1}](1-G_l) - M^2 G_l = 0. \tag{64}$$

Thus we see that the harmonic map ansatz (42) with the initial vector M_0 given by the Veronese map (61) is an exact spherically symmetric solution of the massive Yang–Mills field equations (39)–(41).

Next, we want to express the static magnetic type energy (19) in terms of the profile functions g_l. To simplify the evaluation of the traces in (19), we choose to use the formula

$$\mathrm{Tr}[R] = \sum_{k=0}^{N-1} \frac{1}{|M_k|^2} M_k^{\dagger}[R]M_k, \tag{65}$$

where R is a $(N\times N)$ nonsingular complex matrix which is diagonal in each basis vector $M_k (k=0,1,\ldots,N-1)$. Note that the upper sum in (65) is $(N-1)$, instead of $(N-2)$, because here we must sum over the whole *complete set* of basis vectors M_k in C^N.

Using (53)–(57) and (60) we obtain

$$\mathrm{Tr}(F_{r\bar{\xi}}F_{r\xi}) = \frac{1}{(1+|\xi|^2)^2}\sum_{k=0}^{N-2} \mathcal{N}_l \dot{G}_l^2, \tag{66}$$

$$\mathrm{Tr}(F_{\xi\bar{\xi}}F_{\bar{\xi}\xi}) = -\frac{1}{(1+|\xi|^2)^4}\sum_{k=0}^{N-1} (\mathcal{N}_l\widetilde{Q}_l - \mathcal{N}_{l-1}\widetilde{Q}_{l-1})^2, \tag{67}$$

$$\mathrm{Tr}(A_{\bar{\xi}}A_{\xi}) = \frac{1}{(1+|\xi|^2)^2}\sum_{k=0}^{N-2} \mathcal{N}_l G_l^2, \tag{68}$$

where, by definition, $G_{N-1}=0$ and $\mathcal{N}_{-1}=0$.

With the above results for the traces, the static energy (38), written in a symmetrical form, becomes

$$E = 4\pi\int_0^{\infty} \mathrm{d}r \sum_{l=0}^{N-1}\left[\mathcal{N}_l\dot{G}_l^2 + \frac{1}{4r^2}(\mathcal{N}_l\widetilde{Q}_l - \mathcal{N}_{l-1}\widetilde{Q}_{l-1})^2 + M^2\mathcal{N}_l G_l^2\right]. \tag{69}$$

We note that equations for the critical points of the energy (69) coincide with the equations for the profile functions g_l in (64) as we expected. From this expression we see that the energy is finite provided the profile functions G_l, for all $l=0,1\ldots,(N-2)$, are bounded and that they approach zero at infinity as re^{-Mr} and at the origin the boundary conditions, $G_l=0$ or 2, are imposed.

The B-integral in this coordinate system is

$$B = -\frac{2i}{16\pi}\int \mathrm{d}r\,\mathrm{d}\xi\,\mathrm{d}\bar{\xi}\,\mathrm{Tr}[F_{r\bar{\xi}}A_{\bar{\xi}} + F_{\bar{\xi}r}A_{\xi}], \tag{70}$$

and so using the formula (65) to express the traces, we obtain

$$B = -\frac{1}{2}\sum_{l=0}^{N-2}\mathcal{N}_l\int_0^{\infty}\mathrm{d}r(\dot{G}_l G_l) = -\frac{1}{4}\sum_{l=0}^{N-2}\mathcal{N}_l[G_l^2(r)]_{r=0}^{\infty}, \tag{71}$$

where $\mathcal{N}_l$ is given by (62). Thus, by taking the boundary conditions $G_l(\infty)=0$, we see that the B-integral is determined solely by the boundary conditions at the origin.

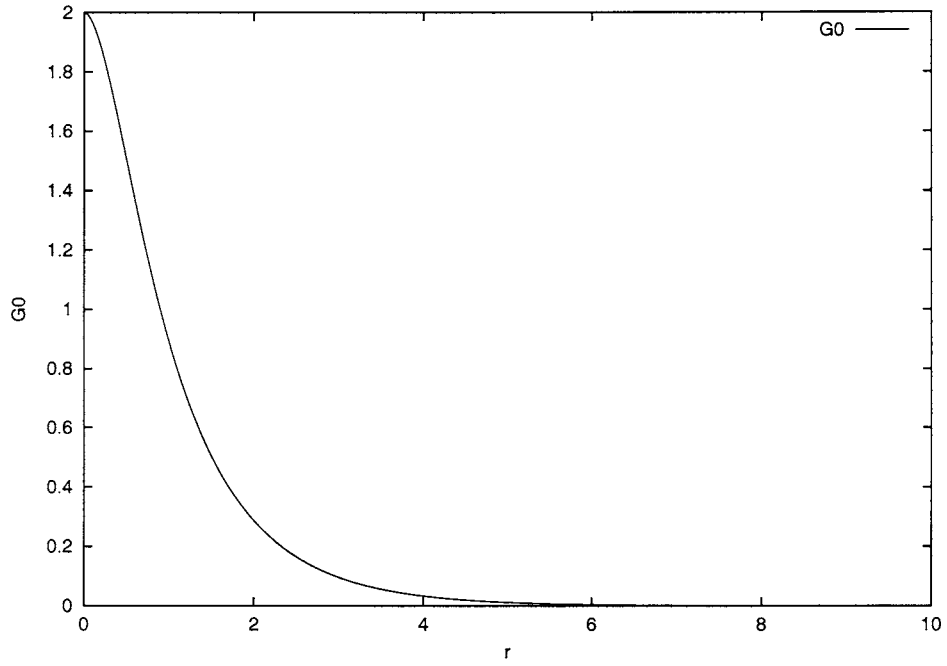

FIG. 1. Profile function of the massive SU(2) YM field for $M=1$.

V. SPHERICALLY SYMMETRIC SOLUTIONS

In this section, we have a look at the numerical solutions of the profile equations (64) for some different values of the mass M by imposing the boundary conditions, $G_l(\infty)=0$ and $G_l(0)=0$ or 2, as required for having finite-energy solutions. In fact, we only consider the cases $N=2$, 3, and 4.

A. SU(2)

Here we have only one profile function G_0, with $\mathcal{N}_0=1$, so the profile equations (64) reduce to a single equation,

$$\ddot{G}_0 - \frac{1}{r^2}\tilde{Q}_0(1-G_0) - M^2 G_0 = 0. \tag{72}$$

Solving (72) for some different values of the mass M with the boundary condition $G_0(0)=2$ at the origin, we have found that each solution G_0 is bounded. In Fig. 1 we show the solution for $M=1$.

We have also computed the corresponding energy from (69), i.e.,

$$E = 4\pi \int_0^\infty \mathrm{d}r \left[\dot{G}_0^2 + \frac{1}{2r^2}\tilde{Q}_0^2 + M^2 G_0^2 \right], \tag{73}$$

and the results for four different mass parameters, i.e., $M=1$, 5, 10, and 50, are summarized in Table I.

TABLE I. Energies of the massive SU(2) YM fields.

$G_0(0)$	B	$E_{M=1}/4\pi$	$E_{M=5}/4\pi$	$E_{M=10}/4\pi$	$E_{M=50}/4\pi$
2	1	4.946 29e+00	2.473 20e+01	4.946 70e+01	2.477 55e+02

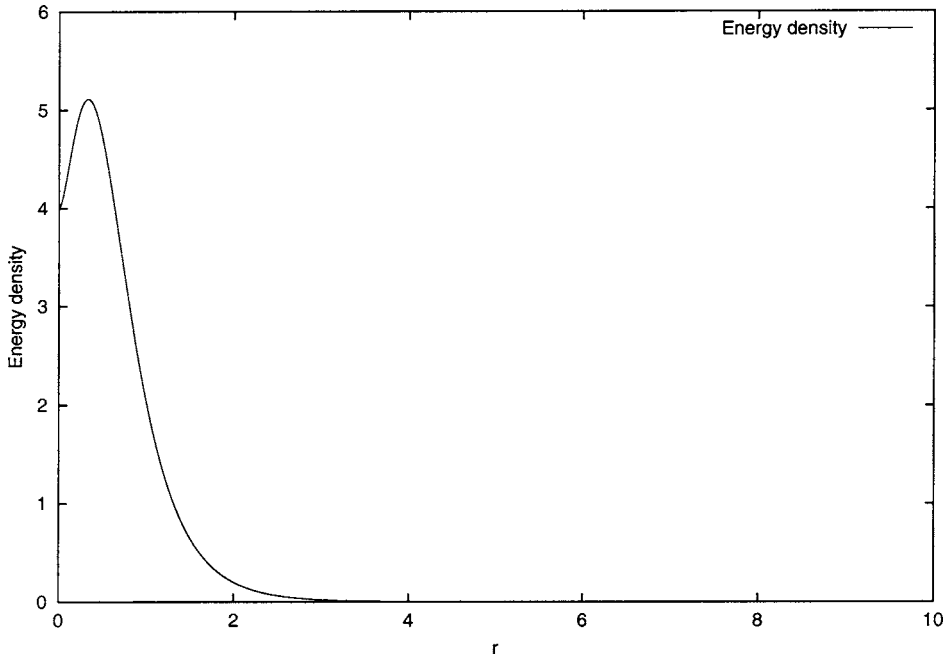

FIG. 2. Energy density of the massive SU(2) YM field for $M=1$.

In Fig. 2 we show the radial energy density for $M=1$ and we see that it looks like a trough ball.

These solutions has B-integral equal to 1 and so, according to (27), the lower bound of the energy is $E/(4\pi)=4M$. We see that each energy is about 25% higher than the corresponding lower bound value.

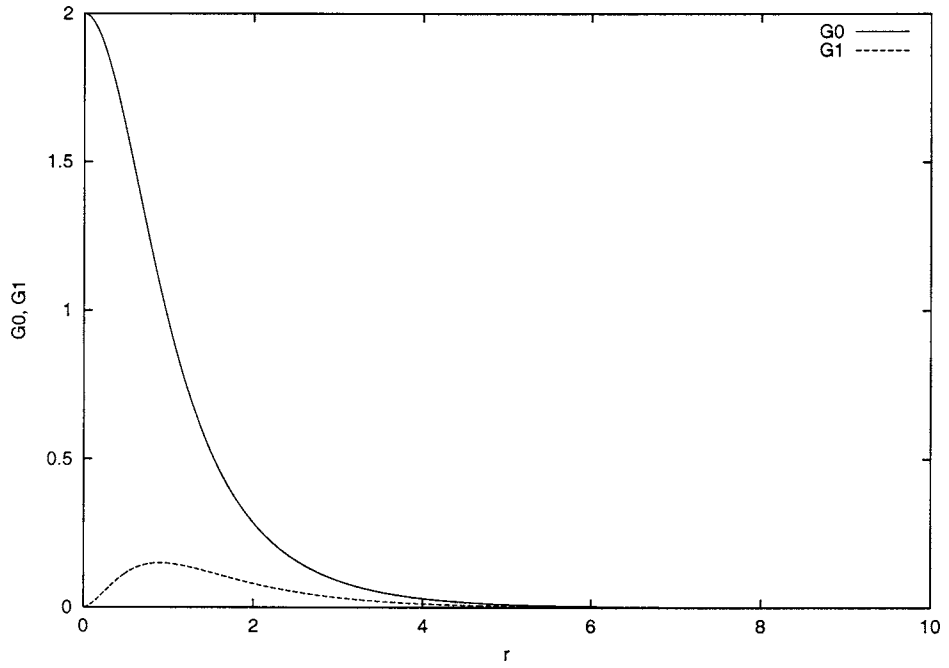

FIG. 3. Profile functions of the massive SU(3) YM fields for $M=1$, $G_0(0)=2$, and $G_1(0)=0$.

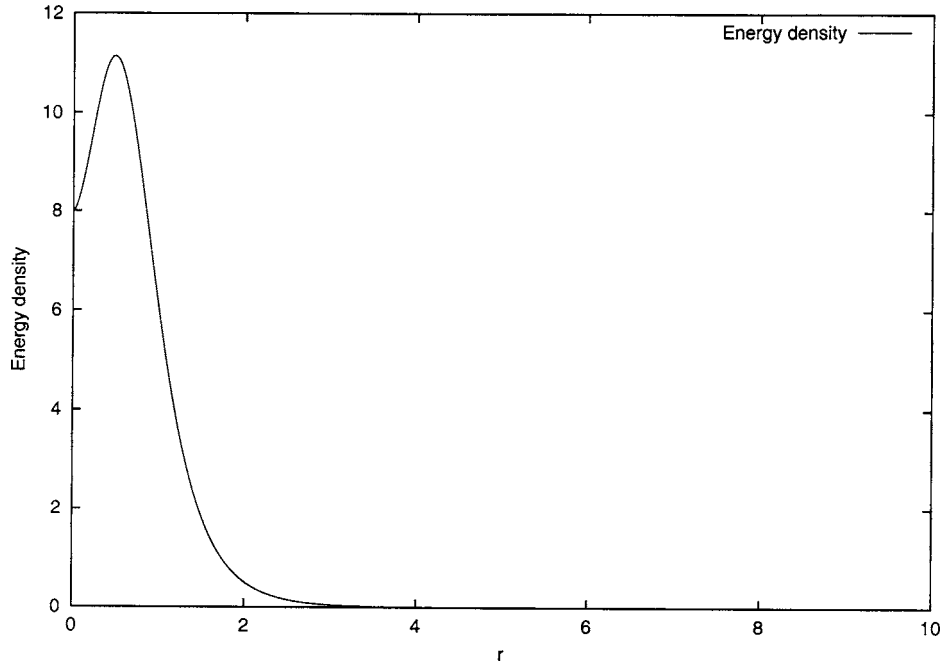

FIG. 4. Energy density of the massive SU(3) YM fields for $M=1$, $G_0(0)=2$, and $G_1(0)=0$.

For the boundary condition $G_0(0)=0$, we have found that Eq. (72) has trivial solution $G_0(r)=0$.

B. SU(3)

For $N=3$, we have two profile functions G_0 and G_1 which satisfy

$$\ddot{G}_0 - \frac{1}{r^2}[2\tilde{Q}_0 - \tilde{Q}_1](1-G_0) - M^2 G_0 = 0, \tag{74}$$

$$\ddot{G}_1 - \frac{1}{r^2}[-\tilde{Q}_0 + 2\tilde{Q}_1](1-G_1) - M^2 G_1 = 0, \tag{75}$$

as $\mathcal{N}_0=\mathcal{N}_1=2$.

We have solved these equations for each of the following two different choices of boundary conditions imposing at the origin $(G_0(0), G_1(0))=(2,0)$ and (2, 2), and we have also found that the corresponding solutions are bounded. In Fig. 3, we show the graphs of these solutions for $M=1$, and the corresponding radial energy distribution is presented in Fig. 4. In Table II we have summarized the result of energies computed from (69), i.e.,

TABLE II. Energies of the massive SU(3) YM fields.

$G_0(0)$	$G_1(0)$	B	$E_{M=1}/4\pi$	$E_{M=5}/4\pi$	$E_{M=10}/4\pi$	$E_{M=50}/4\pi$
2	0	2	1.190 80*e*+01	5.954 09*e*+01	1.190 87*e*+02	5.962 17*e*+02
2	2	4	2.164 98*e*+01	1.082 51*e*+02	2.165 16*e*+02	1.084 40*e*+03

TABLE III. Energies of the massive SU(4) YM fields (reduced case).

$G(0)$	$G_1(0)$	B	$E_{M=1}/4\pi$	$E_{M=5}/4\pi$	$E_{M=10}/4\pi$	$E_{M=50}/4\pi$
0	2	4	2.690 92e+01	1.345 50e+02	2.691 20e+02	1.348 17e+03
2	0	6	3.665 47e+01	1.832 76e+02	3.665 67e+02	1.834 96e+03

$$E = 4\pi(2)\int_0^\infty \mathrm{d}r\left(\dot{G}_0^2 + \dot{G}_1^2 + \frac{1}{r^2}[\tilde{Q}_0^2 - \tilde{Q}_0\tilde{Q}_1 + \tilde{Q}_1^2] + M^2G_0^2 + M^2G_1^2\right), \tag{76}$$

for different values of mass M.

We notice that Eqs. (74) and (75) are symmetric with respect to the interchange $G_0 \leftrightarrow G_1$. This allows us to set $G_0 = G_1$ which reduces the system to a single SU(2) profile equation (72). This configuration has $B=4$ [taking $G_0(0)=2$] and having energy 4 times the energy of a SU(2) configuration.

C. SU(4)

Here we have three profile functions G_0, G_1, and G_2, with $\mathcal{N}_0=\mathcal{N}_2=3$ and $\mathcal{N}_1=4$, so the profile equations (64) reduce to

$$\ddot{G}_0 - \frac{1}{r^2}[3\tilde{Q}_0 - 2\tilde{Q}_1](1-G_0) - M^2G_0 = 0, \tag{77}$$

$$\ddot{G}_1 - \frac{1}{2r^2}[-3\tilde{Q}_0 + 8\tilde{Q}_1 - 3\tilde{Q}_2](1-G_1) - M^2G_1 = 0, \tag{78}$$

$$\ddot{G}_2 - \frac{1}{r^2}[-2\tilde{Q}_1 + 3\tilde{Q}_2](1-G_2) - M^2G_2 = 0, \tag{79}$$

The corresponding energy (69) is

$$E = 4\pi\int_0^\infty \mathrm{d}r\left(3\dot{G}_0^2 + 4\dot{G}_1^2 + 3\dot{G}_2^2 + \frac{1}{2r^2}[9\tilde{Q}_0^2 - 12\tilde{Q}_0\tilde{Q}_1 + 16\tilde{Q}_1^2 - 12\tilde{Q}_1\tilde{Q}_2 + 9\tilde{Q}_2^2]\right.$$
$$\left. + 3M^2G_0^2 + 4M^2G_1^2 + 3M^2G_2^2\right). \tag{80}$$

We observe that the system (77)–(79) has symmetry $G_0 \leftrightarrow G_2$, which allows us to set $G_0 = G_2 = G$ by keeping G_1 arbitrary. The energies for this configuration are summarized in Table III.

In addition, letting $G_0=G_1=G_2=G$, the above system of equations reduces to the SU(2) profile equation (72). This configuration has $B=10$ [taking $G(0)=2$] and has energy 10 times the energy of one SU(2) configuration.

TABLE IV. Energies of the massive SU(4) YM fields.

$G_0(0)$	$G_1(0)$	$G_2(0)$	B	$E_{M=1}/4\pi$	$E_{M=5}/4\pi$	$E_{M=10}/4\pi$	$E_{M=50}/4\pi$
0	0	2	3	1.917 95e+01	9.589 85e+01	1.918 04e+02	9.601 04e+02
0	2	0	4	2.777 12e+01	1.388 60e+02	2.777 48e+02	1.393 03e+03
2	0	2	6	3.665 40e+01	1.832 73e+02	3.665 68e+02	1.835 97e+03
0	2	2	7	4.136 43e+01	2.068 26e+02	4.136 80e+02	2.072 68e+03

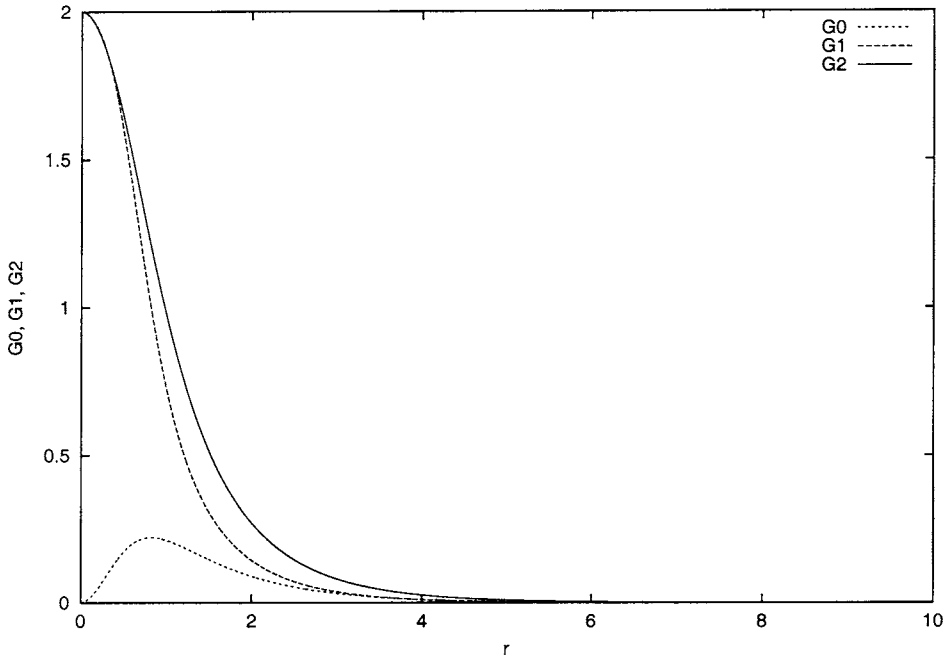

FIG. 5. Profile functions of the massive SU(4) YM fields for $M=1$, $G_0(0)=0$, $G_1(0)=2$, and $G_2(0)=2$.

In Table IV, we have summarized the values of energies for general configurations $G_0 \neq G_1 \neq G_2$ for four different combinations of boundary conditions at the origin. In Fig. 5, we show the graphs of the solutions for $M=1$, $G_0(0)=0$, $G_1(0)=2$, and $G_2(0)=2$. The corresponding radial energy distribution is presented in Fig. 6.

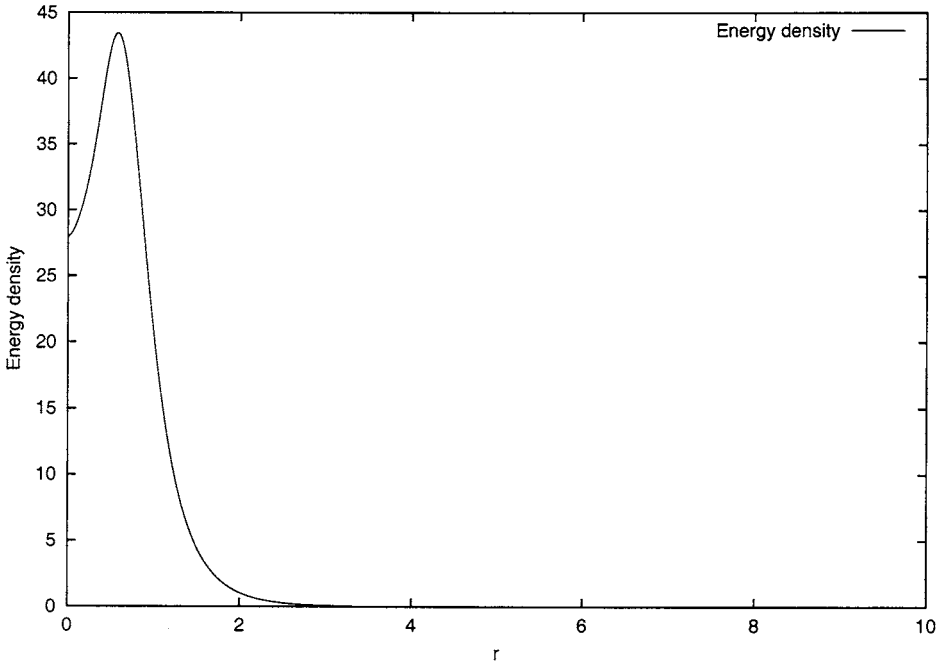

FIG. 6. Energy density of the massive SU(4) YM fields for $M=1$, $G_0(0)=0$, $G_1(0)=2$, and $G_2(0)=2$.

VI. CONCLUSIONS

In this paper we considered the pure massive SU(N) Yang–Mills theories where we first showed that for the case when the gauge potential is chosen to be of almost pure gauge form, the theories reduce to the SU(N) Skyrme models. When we studied the static magnetic type case we found that the energy is bounded from below by a topological chargelike quantity that we called by the name B-integral.

To solve the corresponding static equations, we used Ioannidou–Sutcliffe harmonic map ansatz that they introduced in their study of non-Bogomolnyi BPS monopoles.[7] This ansatz enabled us to construct some bounded solutions having finite energies for $N=2$, 3, and 4 cases. These solutions are very special in the sense that they depend very much on the chosen boundary conditions to be imposed on the profile functions g_k, i.e., $g_k=-2$, 0 or 2 at the origin and zero at infinity. We also showed that each solution is classified by the B-integral which is an integer number.

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Ground state energy of the polaron in the relativistic quantum electrodynamics

Itaru Sasaki[a)]
Department of Mathematics, Hokkaido University, Sapporo 060-0810, Japan

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We consider the polaron model in the relativistic quantum electrodynamics. We prove that the ground state energy of the model is finite for all values of the fine-structure constant and the ultraviolet cutoff Λ. Moreover we give an upper bound and a lower bound of the ground state energy. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2084749]

I. INTRODUCTION AND MAIN RESULTS

We consider the relativistic quantum electrodynamics (QED) for a fixed total momentum—the polaron model of the relativistic QED. The Hamiltonian, which describes a Dirac particle minimally coupled to the quantized radiation field, commutes with the total momentum operator, and has a direct integral decomposition with respect to the total momentum operator.[1,2] Each fiber in this direct integral decomposition is just the Hamiltonian of the polaron we consider. The Hilbert space of the polaron model is defined by

$$\mathcal{F} := \mathbb{C}^4 \otimes \mathcal{F}_{\mathrm{b}}(L^2(\mathbb{R}^3 \times \{1,2\})), \tag{1}$$

where

$$\mathcal{F}_{\mathrm{b}}(L^2(\mathbb{R}^3 \times \{1,2\})) := \bigotimes_{n=0}^{\infty} \left[\bigotimes_{s}^{n} (L^2(\mathbb{R}^3 \times \{1,2\})) \right] \tag{2}$$

is the photon Fock space ($\otimes_s^n$ denotes n-fold symmetric tensor product). For a closable operator T on $L^2(\mathbb{R}^3 \times \{1,2\})$ we denote by $\mathrm{d}\Gamma_{\mathrm{b}}(T)$, the second quantization operator of T (see Ref. 3). Let $a(f)$, $f \in L^2(\mathbb{R}^3 \times \{1,2\})$ be the annihilation operator on the photon Fock space. For a function $g_j \in L^2(\mathbb{R}^3 \times \{1,2\})$, $j=1,2,3$, we set

$$A_j := a(g_j) + a(g_j)^*, \quad j = 1,2,3. \tag{3}$$

Let $\{\alpha_1, \alpha_2, \alpha_3, \beta\}$ be the 4×4-Dirac matrices, i.e., $\{\alpha_i, \alpha_j\} = 2\delta_{i,j}$, $\{\alpha_i, \beta\} = 0$, $\beta^2 = 1$, $i,j = 1,2,3$. Here $\{A,B\} := AB + BA$. For three objects a_1, a_2, a_3 we set $\mathbf{a} = (a_1, a_2, a_3)$, and write $\mathbf{a} \cdot \mathbf{b} := \Sigma_{j=1}^3 a_j b_j$, provided that $a_j b_j$ and $\Sigma_{j=1}^3 a_j b_j$ are defined.

The Hamiltonian of the polaron model we consider is

$$H(\mathbf{p}) := \boldsymbol{\alpha} \cdot \mathbf{p} + M\beta + \mathrm{d}\Gamma_{\mathrm{b}}(\omega) - \boldsymbol{\alpha} \cdot \mathrm{d}\Gamma_{\mathrm{b}}(\mathbf{k}) - q\boldsymbol{\alpha} \cdot \mathbf{A}, \tag{4}$$

where $\mathbf{p} \in \mathbb{R}^3$ is the fixed total momentum, $M \geqslant 0$ is the mass of the Dirac particle, $q \in \mathbb{R}$ is a constant proportional to the fine-structure constant, and $\omega = |\mathbf{k}|$ is the one-photon Hamiltonian ($\mathbf{k} \in \mathbb{R}^3$). Note that we omit the symbol $\otimes$ between the Hilbert space for the Dirac matrices $\mathbb{C}^4$ and the photon Fock space $\mathcal{F}_{\mathrm{b}}(L^2(\mathbb{R}^3 \times \{1,2\}))$. The most important example of $\{g_j\}_{j=1}^3$ is of the form

[a)]Electronic mail: i-sasaki@math.sci.hokudai.ac.jp

$$f_j(\mathbf{k},r) := \frac{\chi_\Lambda(\mathbf{k})}{|\mathbf{k}|^{1/2}} e_j^{(r)}(\mathbf{k}), \tag{5}$$

where the measurable functions $\mathbf{e}^{(1)}(\mathbf{k}), \mathbf{e}^{(2)}(\mathbf{k})$ are the polarization vectors:

$$\mathbf{k}\cdot\mathbf{e}^{(r)}(\mathbf{k}) = 0, \quad \mathbf{e}^{(r)}(\mathbf{k})\cdot\mathbf{e}^{(s)}(\mathbf{k}) = \delta_{r,s}, \quad \text{a.e.}\mathbf{k} \in \mathbb{R}^3, \quad r,s = 1,2, \tag{6}$$

and $\chi_\Lambda(\mathbf{k})$ is the characteristic function of the ball $\{\mathbf{k}\in\mathbb{R}^3 | |\mathbf{k}| < \Lambda\}$, $\Lambda > 0$.

We define

$$E_0(\mathbf{p}) := \inf_{\substack{\Psi\in \mathrm{Dom}(H(\mathbf{p})) \\ \|\Psi\|=1}} \langle \Psi, H(\mathbf{p})\Psi\rangle \tag{7}$$

the ground state energy of $H(\mathbf{p})$, where "Dom" means operator domain. We assume the following.

Hypothesis I: $g_j \in \mathrm{Dom}(\omega^{-1/2}) \cap \mathrm{Dom}(\omega)$, $\langle g_j, g_\ell\rangle \in \mathbb{R}$, $j,\ell = 1,2,3$.

It should be noted that it is highly nontrivial whether or not $E_0(\mathbf{p})$ is finite, because $H(\mathbf{p})$ contains the term $-\boldsymbol{\alpha}\cdot \mathrm{d}\Gamma_b(\mathbf{k})$. This is the main problem discussed in the present paper.

We prove that the ground state energy $E_0(\mathbf{p})$ is finite under suitable conditions:

Theorem 1.1: *Assume Hypothesis I, and*

$$G(\mathbf{g}) := \sup_{\mathbf{k}\in\mathbb{R}^3\setminus\{0\}} \frac{1}{|\mathbf{k}|} \sum_{r=1,2} \int_{\mathbb{R}^3} \frac{|\mathbf{k}\cdot\mathbf{g}(\mathbf{k}',r)|^2}{|\mathbf{k}||\mathbf{k}'| - \mathbf{k}\cdot\mathbf{k}'} \mathrm{d}\mathbf{k}' < \infty. \tag{8}$$

Then, the ground state energy $E_0(\mathbf{p})$ is finite:

$$E_0(\mathbf{p}) > -\infty. \tag{9}$$

In particular, if $g_j = f_j$, $j=1,2,3$, the ground state energy $E_0(\mathbf{p})$ is finite.

For a vector $u \in \mathbb{C}^4$, we set $a_j := \langle u, \alpha_j u\rangle_{\mathbb{C}^4}$, and

$$\mathcal{E}(\Lambda_1, u) := \mathbf{p}\cdot\mathbf{a} + M\langle u, \beta u\rangle + 4\pi\Lambda q^2 \frac{1-|\mathbf{a}|^2}{|\mathbf{a}|} \log\left(\frac{1+|\mathbf{a}|}{1-|\mathbf{a}|}\right) - 4\pi\Lambda q^2.$$

In the physical case (i.e., the function g_j's are given by (5)), the lower bound of $E_0(\mathbf{p}) + \sqrt{|\mathbf{p}|^2 + M^2}$ are proportional to Λ.

Theorem 1.2: *Let $g_j = f_j$, $j=1,2,3$. Then*

$$C_1\Lambda - \sqrt{|\mathbf{p}|^2 + M^2} \leqslant E_0(\mathbf{p}), \tag{10}$$

$$E_0(\mathbf{p}) \leqslant C_2(\Lambda), \tag{11}$$

where

$$C_1 := \inf_{\epsilon,\epsilon'>0} \left\{ \epsilon|q| + 16\pi q^2 + \left(\epsilon' + \frac{1}{\epsilon'}\right) 4\pi q^2, \sqrt{\frac{4\pi|q|}{3\epsilon} + \left(1 + \frac{1}{\epsilon'}\right) 4\pi q^2} \right\}, \tag{12}$$

$$C_2(\Lambda) := \inf_{\substack{u\in\mathbb{C}^4 \\ \|u\|_{\mathbb{C}^4}=1}} \mathcal{E}(\Lambda, u). \tag{13}$$

II. PROOF OF THEOREM 1.1 AND 1.2

Lemma 2.1: Let A be a positive self-adjoint operator on a Hilbert space $\mathcal{H}$. Let B be a symmetric operator with $\mathrm{Dom}(A) \subset \mathrm{Dom}(B)$ *and*

$$\|B\Psi\| \leqslant \|A\Psi\|, \quad \Psi \in \mathrm{Dom}(A). \tag{14}$$

Then, for all $\Psi \in D(A)$, $\langle \Psi, (A+B)\Psi \rangle \geqslant 0$.

Proof: By the Kato–Rellich theorem,[4] for all $\epsilon \in (-1,1)$, $A+\epsilon B$ is self-adjoint and $A+\epsilon B \geqslant 0$. Therefore $\langle \Psi, (A+B)\Psi \rangle \geqslant 0$ for all $\Psi \in \mathrm{Dom}(A)$. ■

By this lemma, it suffices to show that there exists a constant $E \geqslant 0$ such that

$$\|(\mathrm{d}\Gamma_b(\omega)+E)\Psi\|^2 \geqslant \|\boldsymbol{\alpha}\cdot(\mathrm{d}\Gamma_b(\mathbf{k})+q\mathbf{A})\Psi\|^2, \quad \Psi \in \mathrm{Dom}(\mathrm{d}\Gamma_b(\omega)). \tag{15}$$

We use the following representation for $\boldsymbol{\alpha}$ matrices:

$$\alpha_j = \begin{bmatrix} \sigma_j & 0 \\ 0 & -\sigma_j \end{bmatrix}, \quad j=1,2,3,$$

with $(\sigma_1,\sigma_2,\sigma_3)$ being the Pauli matrices. Using the anticommutation relation of α_1, α_2, and α_3, we have

$$\|\boldsymbol{\alpha}\cdot(\mathrm{d}\Gamma_b(\mathbf{k})+q\mathbf{A})\Psi\|^2 = \sum_{j=1}^{3}\|(\mathrm{d}\Gamma_b(k_j)+qA_j)\Psi\|^2 - q\langle \Psi, \mathbf{S}\cdot[a(i\mathbf{k}\times\mathbf{g})+a(i\mathbf{k}\times\mathbf{g})^*]\Psi\rangle, \tag{16}$$

where $S_j=\sigma_j\oplus\sigma_j$, $j=1,2,3$. The Hilbert space $\mathbb{C}^4\otimes[\otimes_s^n L^2(\mathbb{R}^3\times\{1,2\})]$ is naturally embedded in $L^2(\mathbb{R}^3\times\{1,2\};\mathbb{C}^4\otimes[\otimes_s^{(n-1)}L^2(\mathbb{R}^3\times\{1,2\})])$. For a vector $\Psi\in\mathbb{C}^4\otimes[\otimes_s^n L^2(\mathbb{R}^3\times\{1,2\})]$, we denote its value at point $(\mathbf{k},r)\in\mathbb{R}^3\times\{1,2\}$ by $\Psi(\mathbf{k},r,\cdot)$.

For $\Psi=(\Psi^{(n)})_{n=0}^{\infty}\in\mathrm{Dom}(\mathrm{d}\Gamma_b(\omega))$, we define

$$a^{(r)}(\mathbf{k})\Psi := (\Psi^{(1)}(\mathbf{k},r), \sqrt{2}\Psi^{(2)}(\mathbf{k},r,\cdot), \ldots, \sqrt{n}\Psi^{(n)}(\mathbf{k},r,\cdot), \ldots) \in \mathcal{F}, \quad \mathbf{k}\in\mathbb{R}^3, \quad r=1,2, \tag{17}$$

a Fock space valued function. This operator $a^{(r)}(\mathbf{k})$ is the distributional kernel of the annihilation operator.

Lemma 2.2: For all $\Psi\in\mathrm{Dom}(\mathrm{d}\Gamma_b(\omega))$ *and* $\epsilon>0$, *the following inequality holds:*

$$|q\langle \Psi, \mathbf{S}\cdot[a(i\mathbf{k}\times\mathbf{g})+a(i\mathbf{k}\times\mathbf{g})^*]\Psi\rangle| \leqslant |q|\epsilon\langle\Psi,\mathrm{d}\Gamma_b(\omega)\Psi\rangle + \frac{|q|}{\epsilon}\langle\mathbf{g},\omega\mathbf{g}\rangle\|\Psi\|^2, \tag{18}$$

where $\langle\mathbf{g},\omega\mathbf{g}\rangle := \Sigma_{j=1}^3\langle g_j,\omega g_j\rangle$.

Proof:

$$\begin{aligned}
\text{left-hand side of (18)} &= 2|q|\left|\mathrm{Re}\sum\!\!\!\!\!\!\int_{\mathbb{R}^3}\langle\Psi, -i\mathbf{S}\cdot(\mathbf{k}\times\mathbf{g}(\mathbf{k},r))a^{(r)}(\mathbf{k})\Psi\rangle\mathrm{d}\mathbf{k}\right| \\
&\leqslant 2|q|\sum\!\!\!\!\!\!\int_{\mathbb{R}^3}\|\mathbf{S}\cdot(\mathbf{k}\times\mathbf{g}(\mathbf{k},r))\Psi\|\,\|a^{(r)}(\mathbf{k})\Psi\|\mathrm{d}\mathbf{k} \\
&= 2|q|\sum\!\!\!\!\!\!\int_{\mathbb{R}^3}|\mathbf{k}|^{1/2}|\mathbf{g}(\mathbf{k},r)|\cdot\|\,|\mathbf{k}|^{1/2}a^{(r)}(\mathbf{k})\Psi\|\cdot\|\Psi\|\mathrm{d}\mathbf{k} \leqslant 2|q| \\
&\quad\times\langle\mathbf{g},\omega\mathbf{g}\rangle^{1/2}\left[\sum\!\!\!\!\!\!\int_{\mathbb{R}^3}\|\,|\mathbf{k}|^{1/2}a^{(r)}(\mathbf{k})\Psi\|^2\right]^{1/2}\|\Psi\| \\
&\leqslant |q|\epsilon\langle\Psi,\mathrm{d}\Gamma_b(\omega)\Psi\rangle + \frac{|q|}{\epsilon}\langle\mathbf{g},\omega\mathbf{g}\rangle\|\Psi\|^2,
\end{aligned}$$

where $\sum\!\!\!\!\!\!\int := \Sigma_{r=1,2}\int$. ■

Lemma 2.3: For all $\Psi\in\mathrm{Dom}(\mathrm{d}\Gamma_b(\omega))$ *and* $\epsilon>0$, *the following inequality holds*:

$$\langle \Psi, \mathbf{A}^2 \Psi \rangle \leqslant \left(2 + \epsilon + \frac{1}{\epsilon}\right) \langle \omega^{-1/2}\mathbf{g}, \omega^{-1/2}\mathbf{g} \rangle \langle \Psi, \mathrm{d}\Gamma_{\mathrm{b}}(\omega)\Psi \rangle + \left(1 + \frac{1}{\epsilon}\right) \langle \mathbf{g}, \mathbf{g} \rangle \|\Psi\|^2. \tag{19}$$

Proof:

$$\begin{aligned}
\langle \Psi, \mathbf{A}^2 \Psi \rangle &\leqslant \sum_{j=1}^{3} \left[(1+\epsilon) \|a(g_j)\Psi\|^2 + \left(1 + \frac{1}{\epsilon}\right) \|a(g_j)^* \Psi\|^2 \right] \\
&\leqslant \sum_{j=1}^{3} \left[(1+\epsilon) \| \, |\mathbf{k}|^{-1/2} g_j \|^2 \cdot \|\mathrm{d}\Gamma_{\mathrm{b}}(\omega)^{1/2}\Psi\|^2 + \left(1 + \frac{1}{\epsilon}\right) \| |\mathbf{k}|^{-1/2} g_j \|^2 \cdot \|\mathrm{d}\Gamma_{\mathrm{b}}(\omega)^{1/2}\Psi\|^2 \right. \\
&\quad \left. + \left(1 + \frac{1}{\epsilon}\right) \|g_j\|^2 \cdot \|\Psi\|^2 \right].
\end{aligned}$$

■

The following Lemma is the most important fact in the proof of Theorem 1.1.

Lemma 2.4: For all $\Psi \in \mathrm{Dom}(\mathrm{d}\Gamma_{\mathrm{b}}(\omega))$, *the following inequality holds*:

$$\begin{aligned}
&\|\mathrm{d}\Gamma_{\mathrm{b}}(\omega)\Psi\|^2 - \sum_{j=1}^{3} \|\mathrm{d}\Gamma_{\mathrm{b}}(k_j)\Psi\|^2 - q\langle \mathrm{d}\Gamma_{\mathrm{b}}(\mathbf{k})\Psi, \mathbf{A}\Psi \rangle - q\langle \mathbf{A}\Psi, \mathrm{d}\Gamma_{\mathrm{b}}(\mathbf{k})\Psi \rangle \\
&\quad \geqslant -4q^2 G(\mathbf{g}) \langle \Psi, \mathrm{d}\Gamma_{\mathrm{b}}(\omega)\Psi \rangle - q\langle \Psi, (a(\mathbf{k}\cdot\mathbf{g})^* + a(\mathbf{k}\cdot\mathbf{g}))\Psi \rangle.
\end{aligned} \tag{20}$$

Proof: We define

$$F := \frac{\mathbf{k}\cdot\mathbf{g}(\mathbf{k}', \mu)}{|\mathbf{k}|\cdot|\mathbf{k}| - \mathbf{k}\cdot\mathbf{k}'}. \tag{21}$$

For all $\Psi \in \mathrm{Dom}(\mathrm{d}\Gamma_{\mathrm{b}}(\omega))$, we have

$$\begin{aligned}
\text{left-hand side of (20)} = \int_{\mathbb{R}^3} \mathrm{d}\mathbf{k} \int'_{\mathbb{R}^3} \mathrm{d}\mathbf{k}' (|\mathbf{k}|\cdot|\mathbf{k}'| - \mathbf{k}\cdot\mathbf{k}') \|(b - 2qF)a\Psi\|^2 - q\langle \Psi, [a(\mathbf{k}\cdot\mathbf{g}) \\
+ a(\mathbf{k}\cdot\mathbf{g})^*]\Psi \rangle - 4q^2 \int_{\mathbb{R}^3} \mathrm{d}\mathbf{k} \left[\int'_{\mathbb{R}^3} \mathrm{d}\mathbf{k}' (|\mathbf{k}|\cdot|\mathbf{k}'| - \mathbf{k}\cdot\mathbf{k}')^{-1} |\mathbf{k}\cdot\mathbf{g}(\mathbf{k}', \mu)|^2 \right] \\
\times \|a\Psi\|^2,
\end{aligned}$$

where $a := a^{(r)}(\mathbf{k})$, $b := a^{(\mu)}(\mathbf{k}')$, and $\int' := \Sigma_{\mu=1,2} \int$. Since $|\mathbf{k}|\cdot|\mathbf{k}'| - \mathbf{k}\cdot\mathbf{k}' \geqslant 0$, inequality (20) holds. ■

Proof of Theorem 1.1: Using Lemmas 2.2–2.4, we get

$$\begin{aligned}
(\mathrm{d}\Gamma_{\mathrm{b}}(\omega) + E)^2 - \sum_{j=1}^{3} (\mathrm{d}\Gamma_{\mathrm{b}}(k_j) + qA_j)^2 - q\mathbf{S}\cdot[a(i\mathbf{k}\times\mathbf{g}) + a(i\mathbf{k}\times\mathbf{g})^*] &\geqslant 2E\mathrm{d}\Gamma_{\mathrm{b}}(\omega) + E^2 \\
- 4q^2 G(\mathbf{g})\mathrm{d}\Gamma_{\mathrm{b}}(\omega) - q[a(\mathbf{k}\cdot\mathbf{g})^* + a(\mathbf{k}\cdot\mathbf{g})] - |q|\mathrm{d}\Gamma(\omega) - |q|\langle \mathbf{g}, \omega\mathbf{g} \rangle - 4\langle \omega^{-1/2}\mathbf{g}, \omega^{-1/2}\mathbf{g} \rangle \mathrm{d}\Gamma_{\mathrm{b}}(\omega) \\
- 2\langle \mathbf{g}, \mathbf{g} \rangle,
\end{aligned}$$

in the sense of quadratic form on $\mathrm{Dom}(\mathrm{d}\Gamma_{\mathrm{b}}(\omega))$. Since $a(\mathbf{k}\cdot\mathbf{g}) + a(\mathbf{k}\cdot\mathbf{g})^*$ is $\mathrm{d}\Gamma_{\mathrm{b}}(\omega)^{1/2}$ bounded, for a large $E > 0$ we have

$$(\mathrm{d}\Gamma_{\mathrm{b}}(\omega) + E)^2 - \sum_{j=1}^{3} (\mathrm{d}\Gamma_{\mathrm{b}}(k_j) + qA_j)^2 - q\mathbf{S}\cdot[a(i\mathbf{k}\times\mathbf{g}) + a(i\mathbf{k}\times\mathbf{g})] \geqslant 0.$$

By Lemma 2.1, for a large $E \geqslant 0$, we obtain

$$\mathrm{d}\Gamma_{\mathrm{b}}(\omega)-\boldsymbol{\alpha}\cdot\mathrm{d}\Gamma_{\mathrm{b}}(\mathbf{k})-q\boldsymbol{\alpha}\cdot\mathbf{A}\geqslant -E, \tag{22}$$

in the sense of quadratic form on $\mathrm{Dom}(\mathrm{d}\Gamma_{\mathrm{b}}(\omega))$. This inequality implies that $E_0(\mathbf{p})$ is finite.

Next we show that $G(\mathbf{f})<\infty$ if $g_j=f_j(j=1,2,3)$. By the definitions of $\mathbf{e}^{(r)}(\mathbf{k})$, the vectors $\mathbf{k}/|\mathbf{k}|$, $\mathbf{e}^{(1)}(\mathbf{k})$, $\mathbf{e}^{(2)}(\mathbf{k})$ are the orthonormal basis of $\mathbb{C}^3$. Therefore

$$G(\mathbf{f})=\sup_{\mathbf{k}\in\mathbb{R}^3\setminus\{0\}}\frac{1}{|\mathbf{k}|}\int_{\mathbb{R}^3}\frac{\chi_\Lambda(\mathbf{k}')\mathrm{d}\mathbf{k}'}{|\mathbf{k}||\mathbf{k}'|-\mathbf{k}\cdot\mathbf{k}'}\cdot\frac{1}{|\mathbf{k}'|}\left[|\mathbf{k}|^2-\frac{(\mathbf{k}\cdot\mathbf{k}')^2}{|\mathbf{k}'|^2}\right]=\int_{\mathbb{R}^3}\frac{\chi_\Lambda(\mathbf{k}')}{|\mathbf{k}'|^2}\mathrm{d}\mathbf{k}'=4\pi\Lambda.$$

■

Proof of Theorem 1.2: First we show (10). We set $g_j=f_j(j=1,2,3)$. It is easy to see that

$$H(\mathbf{p})\geqslant-\sqrt{|\mathbf{p}|^2+M^2}+\mathrm{d}\Gamma_{\mathrm{b}}(\omega)-\boldsymbol{\alpha}\cdot\mathrm{d}\Gamma_{\mathrm{b}}(\mathbf{k})-q\boldsymbol{\alpha}\cdot\mathbf{A}. \tag{23}$$

By the definition of $\mathbf{e}^{(r)}(\mathbf{k})$, we have $\mathbf{k}\cdot\mathbf{f}(\mathbf{k},r)=0(\mathbf{k}\in\mathbb{R}^3,r=1,2)$. Therefore, using Lemmas 2.2–2.4, we have

$$\begin{aligned}&(\mathrm{d}\Gamma_{\mathrm{b}}(\omega)+C_1\Lambda)^2-(\mathrm{d}\Gamma_{\mathrm{b}}(\mathbf{k})+q\mathbf{A})^2-q\mathbf{S}\cdot[a(i\mathbf{k}\times\mathbf{f})+a(i\mathbf{k}\times\mathbf{f})^*]\\&\quad\geqslant\left(2C_1\Lambda-2|q|\epsilon\Lambda-4q^2G(\mathbf{f})-\left(2+\epsilon'+\frac{1}{\epsilon'}\right)\langle\omega^{-1/2}\mathbf{f},\omega^{-1/2}\mathbf{f}\rangle\right)\mathrm{d}\Gamma_{\mathrm{b}}(\omega)\\&\qquad+C_1^2\Lambda^2-\frac{|q|}{2\epsilon\Lambda}\langle\mathbf{f},\omega\mathbf{f}\rangle-\left(1+\frac{1}{\epsilon'}\right)q^2\langle\mathbf{f},\mathbf{f}\rangle,\quad\epsilon,\epsilon'>0.\end{aligned} \tag{24}$$

It is easy to see that $\langle\omega^{-1/2}\mathbf{f},\omega^{-1/2}\mathbf{f}\rangle=8\pi\Lambda$, $\langle\mathbf{f},\omega\mathbf{f}\rangle=8\pi\Lambda^3/3$, $\langle\mathbf{f},\mathbf{f}\rangle=4\pi\Lambda^2$. Hence, by the definition of C_1, the left-hand side of (24) is positive for suitable $\epsilon,\epsilon'>0$. Thus, using Lemma 2.1 (and (16)), we have

$$H(\mathbf{p})\geqslant-\sqrt{|\mathbf{p}|^2+M^2}-C_1\Lambda. \tag{25}$$

For normalized vectors $u\in\mathbb{C}^4$, $\psi\in\mathrm{Dom}(\mathrm{d}\Gamma_{\mathrm{b}}(\omega))$ we define

$$a_j:=\langle u,\alpha_j u\rangle,\quad h(\mathbf{a}):=\mathrm{d}\Gamma_{\mathrm{b}}(\omega-\mathbf{a}\cdot\mathbf{k})-q\mathbf{a}\cdot\mathbf{A},$$

$$\Psi:=u\otimes\psi\in\mathcal{F}.$$

Note that $\omega-\mathbf{a}\cdot\mathbf{k}\geqslant0$ and $\omega-\mathbf{a}\cdot\mathbf{k}$ is injective as a multiplication operator. We have

$$\langle\Psi,H(\mathbf{p})\Psi\rangle=\mathbf{a}\cdot\mathbf{p}+M\langle u,\beta u\rangle+\langle\psi,h(\mathbf{a})\psi\rangle. \tag{26}$$

Since $h(\mathbf{a})$ is a van Hove type Hamiltonian, we have

$$\begin{aligned}\inf\sigma(h(\mathbf{a}))&=-q^2\|(|\mathbf{k}|-\mathbf{a}\cdot\mathbf{k})^{-1/2}\mathbf{a}\cdot\mathbf{f}\|^2=-4\pi\Lambda q^2+q^2(1-|\mathbf{a}|^2)\int_{\mathbb{R}^3}\mathrm{d}\mathbf{k}\frac{\chi_\Lambda(\mathbf{k})}{|\mathbf{k}|^2-(\mathbf{a}\cdot\mathbf{k})^2}\\&=-4\pi\Lambda q^2+2\pi\Lambda q^2(1-|\mathbf{a}|^2)\frac{1}{|\mathbf{a}|}\log\left(\frac{1-|\mathbf{a}|}{1+|\mathbf{a}|}\right),\end{aligned}$$

where σ means the spectrum (e.g., Ref. 3). Thus we have

$$E_0(\mathbf{p})\leqslant\inf_{u\in\mathbb{C}^4;\|u\|=1}\inf_{\psi\in\mathrm{Dom}(\mathrm{d}\Gamma_{\mathrm{b}}(\omega))}\langle\Psi,H(\mathbf{p})\Psi\rangle=\inf_{u\in\mathbb{C}^4;\|u\|=1}\mathcal{E}(u).$$

■

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Induced matter: Curved *N*-manifolds encapsulated in Riemann-flat *N*+1 dimensional space

Harry I. Ringermacher
General Electric Global Research Center, Schenectady, New York 12309

Lawrence R. Mead[a)]
Department of Physics and Astronomy, University of Southern Mississippi, Hattiesburg, Mississippi 39406

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Liko and Wesson have recently introduced a new five-dimensional induced matter solution of the Einstein equations, a negative curvature Robertson-Walker space embedded in a Riemann-flat five-dimensional manifold. We show that this solution is a special case of a more general theorem prescribing the structure of certain $N+1$ dimensional Riemann-flat spaces which are all solutions of the Einstein equations. These solutions encapsulate N-dimensional curved manifolds. Such spaces are said to "induce matter" in the submanifolds by virtue of their geometric structure alone. We prove that the N-manifold can be any maximally symmetric space. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2042968]

The concept of "induced matter," was originally introduced by Wesson.[1,2] While investigating five-dimensional (5D) Kaluza-Klein theory, he recognized that a curved 4-space could be embedded in a Ricci-flat ($R_{AB}=0$; $A,B,\ldots\in\{0,1,2,3,4\}$) 5-space. This is a reflection of the Campbell-Magaard theorem[3] which, applied to 5D, states that it is always possible to embed a curved four-dimensional (4D) manifold in a 5D Ricci-flat space. Seahra and Wesson[4] provide an overview and rigorous proof of the Campbell-Magaard theorem with applications to higher dimensions. Wesson takes "induced matter" to mean that the left-hand geometric side extra terms of the flat 5D Ricci-tensor provide the source terms in the 4D curved Ricci-tensor of the embedded space. A "weak" version of this concept utilizing an embedding of the Friedmann-Roberston-Walker (FRW) 4-space in a Minkowski 5-space has been used to visualize the big bang sectionally.[5] Here, the 5-space is Riemann-flat ($R_{ABCD}=0$) since it is Minkowski. There is no physics in the 4D subspace, except with reference to the original FRW coordinates. This simply provides a Euclidean embedding diagram.

More recently, Liko and Wesson have introduced a new 5D, Riemann-flat solution[6] which they found could "encapsulate" a 4D curved FRW space. We use the term "encapsulate" as distinct from embed since in this 5-space, the coordinates are not Minkowski. The 4D subspace is itself curved in the same 5D coordinates. It is true that a flattening transformation can be found to a 5D Minkowski space. However, this would simply produce another embedding diagram. The physics seems to lie in the encapsulating 5D metric. We shall use the term "induced matter" to include a Riemann-flat 5D manifold encapsulating a curved 4D subspace. The Liko-Wesson induced matter solution goes on to describe an apparently inflationary universe as a negative curvature FRW space embedded in a special 5D universe. The RW space undergoes accelerated expansion subject to a repulsive "dark energy" ($P=-\rho$). We will show in this paper that the Liko-Wesson solution is a special case of a more general class of maximally symmetric submanifolds embedded in Riemann-

[a)]Author to whom correspondence should be addressed. Electronic mail: lawrence.mead@usm.edu

flat space. A detailed discussion of maximally symmetric submanifolds based on Poincarè metrics and their consequences can be found in Ref. 7. For convenience, we repeat some critical definitions and calculations.

Consider the Riemann manifold defined by

$$\mathrm{d}S^2 = \tilde{g}_{ij}\,\mathrm{d}x^i\,\mathrm{d}x^j. \tag{1}$$

This space is said to be maximally symmetric if and only if it has constant sectional curvature $\kappa=\kappa(i,j)$, for any $1\leqslant i\neq j\leqslant N$. In the plane spanned by the basis vectors $(\hat{e}_i,\hat{e}_j)$ the sectional curvature is defined by

$$\kappa(i,j) = \tilde{g}^{ii}R^j_{iji} \quad (i,j \text{ not summed}). \tag{2}$$

For a maximally symmetric space $R^j_{iji}=\kappa\tilde{g}_{ii}$, $j\neq i$. For such a space,

$$R_{ii} = -\kappa(N-1)\tilde{g}_{ii}. \tag{3}$$

Theorem: Let $\tilde{g}_{ij}$ represent a maximally symmetric space of sectional curvature κ. *The metric*

$$\mathrm{d}S^2 = \mathrm{d}\tau^2 - D\tau^2\tilde{g}_{ij}\,\mathrm{d}x^i\,\mathrm{d}x^j, \quad i,j\ldots,\in\{1,2,\ldots,N\}, \tag{4}$$

is Riemann-flat whenever $D=-\kappa$.

Proof: Consider the metric

$$\mathrm{d}S^2 = \mathrm{d}\tau^2 - f(\tau)^2\tilde{g}_{ij}\,\mathrm{d}x^i\,\mathrm{d}x^j, \tag{5}$$

where $\tilde{g}_{ij}$ denotes a maximally symmetric space. We compute the independent components of the curvature tensor (the overtilde denotes differentiation in τ):

$$R^i_{0j0} = -\frac{f''}{f}\delta^i_j,$$

$$R^0_{i0j} = -ff''\tilde{g}_{ij},$$

$$R^k_{ikj} = \tilde{R}_{ij} - (N-1)f'^2\tilde{g}_{ij} = -\kappa(N-1)\tilde{g}_{ij} - (N-1)f'^2\tilde{g}_{ij} = -(N-1)(f'^2+\kappa)\tilde{g}_{ij}, \tag{6}$$

where we have made use of the result (3). It is evident from (6) that the space will be Riemann-flat if and only if $f''=0$ and $f'^2+\kappa=0$. Let $f(\tau)=\sqrt{D}\tau$. Then $f''=0$ and $f'^2-D=0$. It follows that $D=-\kappa$ and the proof is complete.

Liko and Wesson[6] introduce the line element (with overall sign of $\mathrm{d}S^2$ reversed from ours),

$$\mathrm{d}S^2 = \mathrm{d}\tau^2 - \frac{\tau^2}{L^2}\left[\mathrm{d}t^2 - L^2\sinh^2\left(\frac{t}{L}\right)\mathrm{d}\sigma_3^2\right], \tag{7}$$

where

$$\mathrm{d}\sigma_3^2 = \left(1+\frac{kr^2}{4}\right)^{-2}(\mathrm{d}r^2 + r^2\,\mathrm{d}\theta^2 + r^2\sin^2\theta\,\mathrm{d}\phi^2), \tag{8}$$

is the Robertson-Walker 3-space with $k=-1$.

Define coordinates $x^A=\{\tau,r,\theta,\phi,t\}$, $A\in\{0,1,2,3,4\}$.

We can then identify in (4),

$$\tilde{g}_{ii} = \{-f, -fr^2, -fr^2 \sin^2\theta, 1\}, \quad f = L^2 \sinh^2(t/L)\left(1 + \frac{kr^2}{4}\right)^{-2}, \tag{9}$$

and $D = 1/L^2$. Equation (7) is thus of the form (4) and will satisfy the theorem provided that the sectional curvature of the 4-space is $\kappa = -1/L^2$. Direct evaluation of the sectional curvature for two typical cases (by symmetry, the remaining cases are identical) results in

$$\kappa(1,2) = \tilde{g}^{11} R^2_{121} = -\frac{1}{L^2},$$

$$\kappa(4,2) = \tilde{g}^{44} R^2_{424} = -\frac{1}{L^2}$$

which show that the conditions (6) are met. That is, the 4-space has constant sectional curvature which then results in a Riemann-flat 5-space. We have thus shown that the new metric solution, (7), introduced by Liko and Wesson is a special case of our more general theorem (4) which allows the N-space to be any maximally symmetric manifold.

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Tetrads in geometrodynamics

Alcides Garat[a)]
Instituto de Física, Facultad de Ciencias, Iguá 4225, esq. Mataojo, Montevideo, Uruguay

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A new tetrad is introduced within the framework of geometrodynamics for non-null electromagnetic fields. This tetrad diagonalizes the electromagnetic stress-energy tensor and allows for maximum simplification of the expression of the electromagnetic field. The Einstein-Maxwell equations will also be simplified. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2049167]

I. INTRODUCTION

The theory of geometrodynamics[1] tried to account for the classical problem of the charged particle. It is a point of view where there is nothing except curved spacetime. Electromagnetism is only a manifestation of the curvature. The electric charge was described as the flux of lines of force that emerges from the mouth of a small wormhole in a multiply connected space. An observer with poor resolving power would see the emerging flux as coming from an elementary electric charge.[1] Therefore, it was concluded that if elementary charge can be associated with a geometrical property of the multiply connected spacetime, there should not be a source term in Maxwell's equations. Geometrodynamics is not in agreement with the idea that particles and fields live in a geometrical background as imported entities. However, it presented difficulties, since it was not possible to find a variational principle for this theory. If $F_{\mu\nu}$ is the electromagnetic field and $f_{\mu\nu}=(G^{1/2}/c^2)F_{\mu\nu}$ is the geometrized electromagnetic field, then the Einstein-Maxwell equations can be written,

$$f^{\mu\nu}{}_{;\nu}=0, \tag{1}$$

$$*f^{\mu\nu}{}_{;\nu}=0, \tag{2}$$

$$R_{\mu\nu}=f_{\mu\lambda}f_{\nu}{}^{\lambda}+*f_{\mu\lambda}*f_{\nu}{}^{\lambda}, \tag{3}$$

where $*f_{\mu\nu}=\frac{1}{2}\epsilon_{\mu\nu\sigma\tau}f^{\sigma\tau}$ is the dual tensor of $f_{\mu\nu}$ (Appendix A). The symbol ";" stands for covariant derivative with respect to the metric tensor $g_{\mu\nu}$. The quadratic right-hand side in Eq. (3) is solved in terms of the left-hand side. Then the "square root of the left-hand side" written in terms of the metric tensor is replaced in Eqs. (1) and (2) and two sets of equations have to be satisfied by the metric tensor. On the one hand, the Bianchi identities. They are identically satisfied by the metric tensor, so they were not a problem. On the other hand, a set of integrability conditions that could not be derived from a variational principle. In this work, it is not our goal to solve the problem of the variational principle in geometrodynamics. It is our purpose to introduce a new tetrad, specifically adapted to the geometry of electromagnetic fields in geometrodynamics. This new tetrad could simplify the understanding of the geometry associated with non-null electromagnetic fields. A tetrad is a set of four linearly independent vectors $V^{\alpha}_{(j)}$ that could be defined at every point in a spacetime.[2,3] The index j is the tetrad index and runs from one to four, naming the vectors. It is

[a)]Electronic mail: garat@fisica.edu.uy

possible then, to write at every point in a spacetime, the components of a tensor in terms of the tetrad vectors,

$$Z^{\alpha\beta\ldots}{}_{\mu\nu\ldots} = Z^{rs\ldots}{}_{pq\ldots} V^{\alpha}_{(r)} V^{\beta}_{(s)} V^{(p)}_{\mu} V^{(q)}_{\nu} \ldots , \tag{4}$$

where the quantities $Z^{rs\ldots}{}_{pq\ldots}$ are the tetrad components of the tensor. Our purpose is to find a tetrad in geometrodynamics that diagonalizes the stress-energy tensor and simplifies the expression of the electromagnetic field. We need to understand first the concept of duality rotations. A duality rotation of the electromagnetic field is defined as[1]

$$e^{*\alpha} f_{\mu\nu} = f_{\mu\nu} \cos\alpha + {*f}_{\mu\nu} \sin\alpha, \tag{5}$$

where α is a scalar called the complexion. At every point in spacetime there is a duality rotation by an angle $-\alpha$ that transforms a non-null electromagnetic field into an extremal field,

$$\xi_{\mu\nu} = e^{-*\alpha} f_{\mu\nu}. \tag{6}$$

Extremal fields are essentially electric fields and they satisfy,

$$\xi_{\mu\nu} * \xi^{\mu\nu} = 0. \tag{7}$$

The tetrad that diagonalizes the stress-energy tensor will be written in terms of the extremal field $\xi_{\mu\nu}$, and two other vector fields X^{α} and Y^{α}. It will be proved that these two extra vector fields are available freedom that we have in the construction of a general tetrad for non-null electromagnetic fields. The fact that in geometrodynamics Maxwell's equations (1) and (2) have zero source terms, introduces the existence of two potential vector fields, A^{α} and ${*A}^{\alpha}$, natural candidates for a particular and explicit choice or example of X^{α} and Y^{α}. In this particular example, an unexpected question will arise at this point. If our tetrad involves in its construction the potential vectors A^{α} and ${*A}^{\alpha}$, how is the tetrad going to be affected by electromagnetic gauge transformations? The geometry of electromagnetic fields defines at every point in spacetime two planes related to the symmetries of the stress-energy tensor.[4] Gauge transformations $A^{\alpha} \rightarrow A^{\alpha} + \Lambda^{\cdot\alpha}$, with Λ a scalar function, that leave invariant the electromagnetic field, will generate proper and improper Lorentz transformations on one of the planes. Gauge transformations ${*A}^{\alpha} \rightarrow {*A}^{\alpha} + {*\Lambda}^{\cdot\alpha}$, with ${*\Lambda}$ a scalar function, that leave invariant the dual of the electromagnetic field will generate spatial rotations on the other plane. The possibility of introducing null tetrads in geometrodynamics will also be explored. Finally, the general tetrad will be studied for non-null electromagnetic fields where X^{α} and Y^{α} are considered as generic fields, and the Einstein-Maxwell equations in this general tetrad will be discussed. The explicit example introduced and all its properties will be useful in understanding the general case. The remainder of this paper will be organized as follows. The tetrad that diagonalizes the stress-energy tensor will be introduced in Sec. II. The available freedom that we have in building this tetrad will be analyzed in Sec. III. The geometrical implications of gauge transformations will be discussed in Sec. IV. An isomorphism between the local gauge group and local Lorentz transformations on blades one and two will be included in Sec. V. The normalized tetrad will be studied in Sec. VI. In this last section a new null tetrad will also be introduced. The general case and the Einstein-Maxwell equations written in terms of the general tetrad will be discussed in Sec. VII. Throughout the paper we use the conventions of Ref. 1. In particular we use a metric with sign conventions $-+++$. The only difference in notation with Ref. 1 will be that we will call our geometrized electromagnetic potential A^{α}, where $f_{\mu\nu} = A_{\nu;\mu} - A_{\mu;\nu}$ is the geometrized electromagnetic field $f_{\mu\nu} = (G^{1/2}/c^2) F_{\mu\nu}$.

II. DIAGONALIZATION OF THE STRESS-ENERGY TENSOR

The stress-energy tensor according to Eq. (14a) in Ref. 1, can be written as

$$T_{\mu\nu} = f_{\mu\lambda} f_{\nu}^{\ \lambda} + {}^{*}f_{\mu\lambda}\, {}^{*}f_{\nu}^{\ \lambda}, \tag{8}$$

where ${}^{*}f_{\mu\nu} = \frac{1}{2}\epsilon_{\mu\nu\sigma\tau} f^{\sigma\tau}$ is the dual tensor of $f_{\mu\nu}$. The tensor $\epsilon_{\mu\nu\sigma\tau}$ is studied in Appendix A. The duality rotation given by Eq. (59) in Ref. 1,

$$f_{\mu\nu} = \xi_{\mu\nu} \cos\alpha + {}^{*}\xi_{\mu\nu} \sin\alpha, \tag{9}$$

allows us to express the stress-energy tensor in terms of the extremal field,

$$T_{\mu\nu} = \xi_{\mu\lambda} \xi_{\nu}^{\ \lambda} + {}^{*}\xi_{\mu\lambda}\, {}^{*}\xi_{\nu}^{\ \lambda}. \tag{10}$$

The extremal field $\xi_{\mu\nu}$ and the scalar complexion α are defined through Eqs. (22)–(25) in Ref. 1. It is our purpose to find a tetrad in which the stress-energy tensor is diagonal. This tetrad would simplify the analysis of the geometrical properties of the electromagnetic field. There are four tetrad vectors that at every point in spacetime diagonalize the stress-energy tensor in geometrodynamics,

$$V_{(1)}^{\alpha} = \xi^{\alpha\lambda} \xi_{\rho\lambda} X^{\rho}, \tag{11}$$

$$V_{(2)}^{\alpha} = \sqrt{-Q/2}\, \xi^{\alpha\lambda} X_{\lambda}, \tag{12}$$

$$V_{(3)}^{\alpha} = \sqrt{-Q/2}\, {}^{*}\xi^{\alpha\lambda} Y_{\lambda}, \tag{13}$$

$$V_{(4)}^{\alpha} = {}^{*}\xi^{\alpha\lambda}\, {}^{*}\xi_{\rho\lambda} Y^{\rho}, \tag{14}$$

where $Q = \xi_{\mu\nu}\xi^{\mu\nu} = -\sqrt{T_{\mu\nu}T^{\mu\nu}}$ according to Eq. (39) in Ref. 1. Q is assumed not to be zero, because we are dealing with non-null electromagnetic fields. We are free to choose the vector fields X^{α} and Y^{α}, as long as the four vector fields (11)–(14) are not trivial. Two identities in the extremal field are going to be used extensively in this work, in particular, to prove that tetrads (11)–(14) diagonalizes the stress-energy tensor. The first identity is given by Eq. (64) in Ref. 1,

$$\xi_{\alpha\mu}\, {}^{*}\xi^{\mu\nu} = 0. \tag{15}$$

In order to find the second identity we need Eq. (15) in Ref. 1,

$$f_{\mu\alpha} f^{\nu\alpha} - {}^{*}f_{\mu\alpha}\, {}^{*}f^{\nu\alpha} = \tfrac{1}{2}\delta_{\mu}^{\ \nu} f_{\alpha\beta} f^{\alpha\beta}. \tag{16}$$

When we replace (9) in (16) and make use of (15), the second identity is found,

$$\xi_{\mu\alpha}\xi^{\nu\alpha} - {}^{*}\xi_{\mu\alpha}\, {}^{*}\xi^{\nu\alpha} = \tfrac{1}{2}\delta_{\mu}^{\ \nu} Q. \tag{17}$$

When we make iterative use of (15) and (17) we find,

$$V_{(1)}^{\alpha} T_{\alpha}^{\ \beta} = \frac{Q}{2} V_{(1)}^{\beta}, \tag{18}$$

$$V_{(2)}^{\alpha} T_{\alpha}^{\ \beta} = \frac{Q}{2} V_{(2)}^{\beta}, \tag{19}$$

$$V_{(3)}^{\alpha} T_{\alpha}^{\ \beta} = -\frac{Q}{2} V_{(3)}^{\beta}, \tag{20}$$

$$V_{(4)}^{\alpha} T_{\alpha}^{\ \beta} = -\frac{Q}{2} V_{(4)}^{\beta}. \tag{21}$$

In Ref. 1 the stress-energy tensor was diagonalized through the use of a Minkowskian frame in which the equation for this tensor was given in (34) and (38). In this work, we give the explicit expression for the tetrad in which the stress-energy tensor is diagonal. The freedom we have to choose the vector fields X^α and Y^α represents available freedom that we have to choose the tetrad. If we make use of Eqs. (15) and (17), it is straightforward to prove that (11)–(14) is a set of orthogonal vectors.

III. ELECTROMAGNETIC POTENTIALS IN GEOMETRODYNAMICS

Our goal is to simplify as much as we can the expression of the electromagnetic field through the use of an orthonormal tetrad, so its geometrical properties can be understood in an easier way. As was mentioned earlier we would like to show this simplification through an explicit example by making a convenient and particular choice of the vector fields X^α and Y^α. In geometrodynamics, the Maxwell equations,

$$f^{\mu\nu}{}_{;\nu}=0,$$

$$*f^{\mu\nu}{}_{;\nu}=0, \tag{22}$$

are telling us that two potential vector fields exist,

$$f_{\mu\nu}=A_{\nu;\mu}-A_{\mu;\nu},$$

$$*f_{\mu\nu}=*A_{\nu;\mu}-*A_{\mu;\nu}. \tag{23}$$

For instance, in the Reissner-Nordstrom geometry the only nonzero electromagnetic tensor component is $f_{tr}=A_{r;t}-A_{t;r}$ and its dual $*f_{\theta\phi}=*A_{\phi;\theta}-*A_{\theta;\phi}$. The vector fields A^α and $*A^\alpha$ represent a possible choice in geometrodynamics for the vectors X^α and Y^α. It is not meant that the two vector fields have independence from each other, it is just a convenient choice for a particular example. This choice allows us to write the new tetrad as

$$V^\alpha_{(1)}=\xi^{\alpha\lambda}\xi_{\rho\lambda}A^\rho, \tag{24}$$

$$V^\alpha_{(2)}=\sqrt{-Q/2}\,\xi^{\alpha\lambda}A_\lambda, \tag{25}$$

$$V^\alpha_{(3)}=\sqrt{-Q/2}\,*\xi^{\alpha\lambda}*A_\lambda, \tag{26}$$

$$V^\alpha_{(4)}=*\xi^{\alpha\lambda}*\xi_{\rho\lambda}*A^\rho. \tag{27}$$

A further justification for the choice $X^\alpha=A^\alpha$ and $Y^\alpha=*A^\alpha$ could be illustrated through the Reissner-Nordstrom geometry. In this particular geometry, $f_{tr}=\xi_{tr}$ and $*f_{\theta\phi}=*\xi_{\theta\phi}$, therefore, $A_\theta=0$ and $A_\phi=0$. Then, for the last two tetrad vectors (26) and (27), the choice $Y^\alpha=*A^\alpha$ becomes meaningful under the light of this particular extreme case, when basically there is no magnetic field. However, we have to be careful about the choice we made for X^α and Y^α. The normalization of the tetrad vectors (24)–(27) requires one to know the values of the invariant quantities,

$$V^\alpha_{(1)}V_{(1)\alpha}=(Q/2)A_\mu\xi^{\mu\sigma}\xi_{\nu\sigma}A^\nu, \tag{28}$$

$$V^\alpha_{(2)}V_{(2)\alpha}=(-Q/2)A_\mu\xi^{\mu\sigma}\xi_{\nu\sigma}A^\nu, \tag{29}$$

$$V^\alpha_{(3)}V_{(3)\alpha}=(-Q/2)*A_\mu*\xi^{\mu\sigma}*\xi_{\nu\sigma}*A^\nu \tag{30}$$

$$V^{\alpha}_{(4)}V_{(4)\alpha} = (-Q/2) * A_{\mu} * \xi^{\mu\sigma} * \xi_{\nu\sigma} * A^{\nu}. \tag{31}$$

Then, it is convenient to calculate the invariants (28)–(31) in the Minkowski reference frame given by Eqs. (38) and (39) in Ref. 1,

$$V^{\alpha}_{(1)}V_{(1)\alpha} = (\xi_{01})^4(A^0A_0 + A^1A_1), \tag{32}$$

$$V^{\alpha}_{(2)}V_{(2)\alpha} = -(\xi_{01})^4(A^0A_0 + A^1A_1), \tag{33}$$

$$V^{\alpha}_{(3)}V_{(3)\alpha} = (\xi_{01})^4(*A^2 * A_2 + *A^3 * A_3), \tag{34}$$

$$V^{\alpha}_{(4)}V_{(4)\alpha} = (\xi_{01})^4(*A^2 * A_2 + *A^3 * A_3). \tag{35}$$

Several cases arise. Since $\xi_{01} \neq 0$ because the electromagnetic field is non-null ($Q \neq 0$), the two vector components A_0 and A_1 cannot be simultaneously zero. If in a region of spacetime or in the whole spacetime $A^0A_0 + A^1A_1 > 0$, it would be necessary to switch the first two tetrad vectors, $V^{\alpha}_{(1)} = \sqrt{-Q/2}\xi^{\alpha\lambda}A_{\lambda}$ and $V^{\alpha}_{(2)} = \xi^{\alpha\lambda}\xi_{\rho\lambda}A^{\rho}$. If $A^0A_0 + A^1A_1 = 0$, then we have $V^{\alpha}_{(1)}T_{\alpha}{}^{\beta}V_{(1)\beta} = 0$ and $V^{\alpha}_{(2)}T_{\alpha}{}^{\beta}V_{(2)\beta} = 0$. We are not dealing with this kind of situation in this work. Another choice of X^{α} would be necessary at the points where $A^0A_0 + A^1A_1 = 0$. It is clear that if $A^0A_0 + A^1A_1 < 0$, the following equations hold:

$$-V^{\alpha}_{(1)}V_{(1)\alpha} = V^{\alpha}_{(2)}V_{(2)\alpha} > 0, \tag{36}$$

$$V^{\alpha}_{(3)}V_{(3)\alpha} = V^{\alpha}_{(4)}V_{(4)\alpha} > 0. \tag{37}$$

The treatment of the problem of building tetrad vectors in geometrodynamics, studying their gauge transformation properties and building null tetrads would be analogous for the two cases when $A^0A_0 + A^1A_1 > 0$ or $A^0A_0 + A^1A_1 < 0$. The treatment of just one of the these two possible cases would automatically provide the framework and the ideas to solve the other one. That is why we choose to analyze in detail $A^0A_0 + A^1A_1 < 0$.

IV. GAUGE GEOMETRY

Once we make the choice $X^{\alpha} = A^{\alpha}$ and $Y^{\alpha} = *A^{\alpha}$ the question about the geometrical implications of electromagnetic gauge transformations arises. When we make the transformation,

$$A_{\alpha} \rightarrow A_{\alpha} + \Lambda_{,\alpha}, \tag{38}$$

$f_{\mu\nu}$ remains invariant, and the transformation,

$$*A_{\alpha} \rightarrow *A_{\alpha} + *\Lambda_{,\alpha}, \tag{39}$$

leaves $*f_{\mu\nu}$ invariant, as long as the functions Λ and $*\Lambda$ are scalars. It is valid to ask how the tetrad vectors (24) and (25) are going to transform under (38), (26), and (27) under (39). Schouten defined what he called a two-bladed structure in a spacetime.[4] These blades are the planes determined by the pairs $(V^{\alpha}_{(1)}, V^{\alpha}_{(2)})$ and $(V^{\alpha}_{(3)}, V^{\alpha}_{(4)})$. For simplicity we will study first what we call gauge transformations associated with blade one, the blade generated by the pair $(V^{\alpha}_{(1)}, V^{\alpha}_{(2)})$. Later we will study similar transformations on blade two, the blade generated by $(V^{\alpha}_{(3)}, V^{\alpha}_{(4)})$.

A. Gauge transformations on blade one

In order to simplify the notation we are going to write $\Lambda_{,\alpha} = \Lambda_{\alpha}$. First we study the change in (24) and (25) under (38),

$$\tilde{V}^{\alpha}_{(1)} = V^{\alpha}_{(1)} + \xi^{\alpha\lambda}\xi_{\rho\lambda}\Lambda^{\rho}, \tag{40}$$

$$\tilde{V}^{\alpha}_{(2)} = V^{\alpha}_{(2)} + \sqrt{-Q/2}\xi^{\alpha\lambda}\Lambda_{\lambda}, \tag{41}$$

The second term on the right-hand side of (40) has the orthogonality properties,

$$\xi^{\alpha\lambda}\xi_{\rho\lambda}\Lambda^{\rho}V_{(3)\alpha} = \xi^{\alpha\lambda}\xi_{\rho\lambda}\Lambda^{\rho}V_{(4)\alpha} = 0. \tag{42}$$

The second term on the right-hand side of (41) has similar orthogonality properties,

$$\sqrt{-Q/2}\xi^{\alpha\lambda}\Lambda_{\lambda}V_{(3)\alpha} = \sqrt{-Q/2}\xi^{\alpha\lambda}\Lambda_{\lambda}V_{(4)\alpha} = 0. \tag{43}$$

Since the four vectors (24)–(27) are independent and orthogonal, Eqs. (42) and (43) imply that the second terms on the right-hand sides of (40) and (41) must be a linear combination of the vectors (24) and (25). We proceed then to write Eqs. (40) and (41) as

$$\tilde{V}^{\alpha}_{(1)} = V^{\alpha}_{(1)} + CV^{\alpha}_{(1)} + DV^{\alpha}_{(2)}, \tag{44}$$

$$\tilde{V}^{\alpha}_{(2)} = V^{\alpha}_{(2)} + EV^{\alpha}_{(1)} + FV^{\alpha}_{(2)}. \tag{45}$$

From Eqs. (40) and (44) we know that

$$\xi^{\alpha\lambda}\xi_{\rho\lambda}\Lambda^{\rho} = CV^{\alpha}_{(1)} + DV^{\alpha}_{(2)}, \tag{46}$$

and from Eqs. (41) and (45) we have

$$\sqrt{-Q/2}\xi^{\alpha\lambda}\Lambda_{\lambda} = EV^{\alpha}_{(1)} + FV^{\alpha}_{(2)}. \tag{47}$$

Making use of identities (15)–(17) it can be proved that

$$\xi_{\alpha\sigma}V^{\alpha}_{(1)} = \sqrt{-Q/2}V_{(2)\sigma}, \tag{48}$$

$$\xi_{\alpha\sigma}V^{\alpha}_{(2)} = \sqrt{-Q/2}V_{(1)\sigma}. \tag{49}$$

If we contract Eq. (46) with $\xi_{\alpha\sigma}$ and make use of identities (15)–(17) and Eqs. (48) and (49) we get

$$\sqrt{-Q/2}\xi_{\sigma\lambda}\Lambda^{\lambda} = CV_{(2)\sigma} + DV_{(1)\sigma}. \tag{50}$$

This last equation means that

$$\tilde{V}^{\alpha}_{(2)} = V^{\alpha}_{(2)} + CV^{\alpha}_{(2)} + DV^{\alpha}_{(1)}. \tag{51}$$

Then, from (45) and (51) we have the following relations between coefficients:

$$E = D, \tag{52}$$

$$F = C. \tag{53}$$

Contracting Eq. (50) with $V^{\sigma}_{(1)}$ and $V^{\sigma}_{(2)}$ it can be found that

$$C = (-Q/2)V_{(1)\sigma}\Lambda^{\sigma}/(V_{(2)\beta}V^{\beta}_{(2)}), \tag{54}$$

$$D = (-Q/2)V_{(2)\sigma}\Lambda^{\sigma}/(V_{(1)\beta}V^{\beta}_{(1)}). \tag{55}$$

We would like to calculate the norm of the transformed vectors $\tilde{V}^{\alpha}_{(1)}$ and $\tilde{V}^{\alpha}_{(2)}$,

$$\tilde{V}^{\alpha}_{(1)}\tilde{V}_{(1)\alpha}=[(1+C)^2-D^2]V^{\alpha}_{(1)}V_{(1)\alpha}, \tag{56}$$

$$\tilde{V}^{\alpha}_{(2)}\tilde{V}_{(2)\alpha}=[(1+C)^2-D^2]V^{\alpha}_{(2)}V_{(2)\alpha}, \tag{57}$$

where the relation $V^{\alpha}_{(1)}V_{(1)\alpha}=-V^{\alpha}_{(2)}V_{(2)\alpha}$ has been used. In order for these transformations to keep the timelike or spacelike character of $V^{\alpha}_{(1)}$ and $V^{\alpha}_{(2)}$ the condition $[(1+C)^2-D^2]>0$ must be satisfied. If this condition is fulfilled, then we can normalize the transformed vectors $\tilde{V}^{\alpha}_{(1)}$ and $\tilde{V}^{\alpha}_{(2)}$ as follows:

$$\frac{\tilde{V}^{\alpha}_{(1)}}{\sqrt{-\tilde{V}^{\beta}_{(1)}\tilde{V}_{(1)\beta}}}=\frac{(1+C)}{\sqrt{(1+C)^2-D^2}}\frac{V^{\alpha}_{(1)}}{\sqrt{-V^{\beta}_{(1)}V_{(1)\beta}}}+\frac{D}{\sqrt{(1+C)^2-D^2}}\frac{V^{\alpha}_{(2)}}{\sqrt{V^{\beta}_{(2)}V_{(2)\beta}}}, \tag{58}$$

$$\frac{\tilde{V}^{\alpha}_{(2)}}{\sqrt{\tilde{V}^{\beta}_{(2)}\tilde{V}_{(2)\beta}}}=\frac{D}{\sqrt{(1+C)^2-D^2}}\frac{V^{\alpha}_{(1)}}{\sqrt{-V^{\beta}_{(1)}V_{(1)\beta}}}+\frac{(1+C)}{\sqrt{(1+C)^2-D^2}}\frac{V^{\alpha}_{(2)}}{\sqrt{V^{\beta}_{(2)}V_{(2)\beta}}}. \tag{59}$$

The condition $[(1+C)^2-D^2]>0$ allows for two possible situations, $1+C>0$ or $1+C<0$. For the particular case when $1+C>0$, the transformations (58) and (59) are telling us that an electromagnetic gauge transformation on the vector field A^{α}, that leaves invariant the electromagnetic field $f_{\mu\nu}$, generates a boost transformation on the normalized tetrad vector fields

$$\left(\frac{V^{\alpha}_{(1)}}{\sqrt{-V^{\beta}_{(1)}V_{(1)\beta}}},\frac{V^{\alpha}_{(2)}}{\sqrt{V^{\beta}_{(2)}V_{(2)\beta}}}\right).$$

For the case $1+C<0$, Eqs. (58) and (59) can be rewritten,

$$\frac{\tilde{V}^{\alpha}_{(1)}}{\sqrt{-\tilde{V}^{\beta}_{(1)}\tilde{V}_{(1)\beta}}}=\frac{[-(1+C)]}{\sqrt{(1+C)^2-D^2}}\frac{(-V^{\alpha}_{(1)})}{\sqrt{-V^{\beta}_{(1)}V_{(1)\beta}}}+\frac{[-D]}{\sqrt{(1+C)^2-D^2}}\frac{(-V^{\alpha}_{(2)})}{\sqrt{V^{\beta}_{(2)}V_{(2)\beta}}}, \tag{60}$$

$$\frac{\tilde{V}^{\alpha}_{(2)}}{\sqrt{\tilde{V}^{\beta}_{(2)}\tilde{V}_{(2)\beta}}}=\frac{[-D]}{\sqrt{(1+C)^2-D^2}}\frac{(-V^{\alpha}_{(1)})}{\sqrt{-V^{\beta}_{(1)}V_{(1)\beta}}}+\frac{[-(1+C)]}{\sqrt{(1+C)^2-D^2}}\frac{(-V^{\alpha}_{(2)})}{\sqrt{V^{\beta}_{(2)}V_{(2)\beta}}}. \tag{61}$$

Equations (60) and (61) represent the composition of two transformations—an inversion of the normalized tetrad vector fields

$$\left(\frac{V^{\alpha}_{(1)}}{\sqrt{-V^{\beta}_{(1)}V_{(1)\beta}}},\frac{V^{\alpha}_{(2)}}{\sqrt{V^{\beta}_{(2)}V_{(2)\beta}}}\right),$$

and a boost. If the case is that $[(1+C)^2-D^2]<0$, the vectors $V^{\alpha}_{(1)}$ and $V^{\alpha}_{(2)}$ are going to change their timelike or spacelike character,

$$\tilde{V}^{\alpha}_{(1)}\tilde{V}_{(1)\alpha}=[-(1+C)^2+D^2](-V^{\alpha}_{(1)}V_{(1)\alpha}), \tag{62}$$

$$(-\tilde{V}^{\alpha}_{(2)}\tilde{V}_{(2)\alpha})=[-(1+C)^2+D^2]V^{\alpha}_{(2)}V_{(2)\alpha}. \tag{63}$$

These are improper transformations on blade one. The normalized tetrad vectors $V^{\alpha}_{(1)}$ and $V^{\alpha}_{(2)}$ transform as

$$\frac{\tilde{V}^{\alpha}_{(1)}}{\sqrt{\tilde{V}^{\beta}_{(1)}\tilde{V}_{(1)\beta}}}=\frac{(1+C)}{\sqrt{-(1+C)^2+D^2}}\frac{V^{\alpha}_{(1)}}{\sqrt{-V^{\beta}_{(1)}V_{(1)\beta}}}+\frac{D}{\sqrt{-(1+C)^2+D^2}}\frac{V^{\alpha}_{(2)}}{\sqrt{V^{\beta}_{(2)}V_{(2)\beta}}}, \tag{64}$$

$$\frac{\tilde{V}^{\alpha}_{(2)}}{\sqrt{-\tilde{V}^{\beta}_{(2)}\tilde{V}_{(2)\beta}}}=\frac{D}{\sqrt{-(1+C)^2+D^2}}\frac{V^{\alpha}_{(1)}}{\sqrt{-V^{\beta}_{(1)}V_{(1)\beta}}}+\frac{(1+C)}{\sqrt{-(1+C)^2+D^2}}\frac{V^{\alpha}_{(2)}}{\sqrt{V^{\beta}_{(2)}V_{(2)\beta}}}. \tag{65}$$

For $D>0$ and $1+C>0$ these transformations (64) and (65) represent improper space inversions on blade one. If $D>0$ and $1+C<0$, Eqs. (64) and (65) are improper time reversal transformations on blade one.[5] If the case is that $D<0$, we can proceed to analyze in analogy to (60) and (61). Then, the normalized tetrad vectors transform as

$$\frac{\tilde{V}^{\alpha}_{(1)}}{\sqrt{\tilde{V}^{\beta}_{(1)}\tilde{V}_{(1)\beta}}}=\frac{[-(1+C)]}{\sqrt{-(1+C)^2+D^2}}\frac{(-V^{\alpha}_{(1)})}{\sqrt{-V^{\beta}_{(1)}V_{(1)\beta}}}+\frac{[-D]}{\sqrt{-(1+C)^2+D^2}}\frac{(-V^{\alpha}_{(2)})}{\sqrt{V^{\beta}_{(2)}V_{(2)\beta}}}, \tag{66}$$

$$\frac{\tilde{V}^{\alpha}_{(2)}}{\sqrt{-\tilde{V}^{\beta}_{(2)}\tilde{V}_{(2)\beta}}}=\frac{[-D]}{\sqrt{-(1+C)^2+D^2}}\frac{(-V^{\alpha}_{(1)})}{\sqrt{-V^{\beta}_{(1)}V_{(1)\beta}}}+\frac{[-(1+C)]}{\sqrt{-(1+C)^2+D^2}}\frac{(-V^{\alpha}_{(2)})}{\sqrt{V^{\beta}_{(2)}V_{(2)\beta}}}. \tag{67}$$

For $D<0$ and $1+C<0$ these transformations (66) and (67) represent the composition of inversions, and improper space inversions on blade one. If $D<0$ and $1+C>0$, Eqs. (66) and (67) are inversions composed with improper time reversal transformations on blade one.[5] For $D=1+C$ we can see using Eqs. (44) and (51) that

$$\tilde{V}^{\alpha}_{(1)}=(1+C)V^{\alpha}_{(1)}+(1+C)V^{\alpha}_{(2)}, \tag{68}$$

$$\tilde{V}^{\alpha}_{(2)}=(1+C)V^{\alpha}_{(2)}+(1+C)V^{\alpha}_{(1)}. \tag{69}$$

Equations (68) and (69) show that any vector on blade one transforms as

$$AV^{\alpha}_{(1)}+BV^{\alpha}_{(2)}\rightarrow A\tilde{V}^{\alpha}_{(1)}+B\tilde{V}^{\alpha}_{(2)}=(1+C)(A+B)(V^{\alpha}_{(1)}+V^{\alpha}_{(2)}). \tag{70}$$

This is clearly a noninjective transformation. At the same time we know that there is an inverse transformation,

$$\tilde{\tilde{V}}^{\alpha}_{(1)}=\tilde{V}^{\alpha}_{(1)}-\xi^{\alpha\lambda}\xi_{\rho\lambda}\Lambda^{\rho}=V^{\alpha}_{(1)}, \tag{71}$$

$$\tilde{\tilde{V}}^{\alpha}_{(2)}=\tilde{V}^{\alpha}_{(2)}-\sqrt{-Q/2}\xi^{\alpha\lambda}\Lambda_{\lambda}=V^{\alpha}_{(2)}. \tag{72}$$

Then, the conclusion must be that there could not exist a scalar function that satisfies the initial assumption $D=1+C$. Analogous for $D=-(1+C)$.

B. Gauge transformations on blade two

The change in notation $*\Lambda_{,\alpha}=*\Lambda_{\alpha}$ is going to be adopted. In this section we are interested in the study of the change in (26) and (27) under (39),

$$\tilde{V}^{\alpha}_{(3)}=V^{\alpha}_{(3)}+\sqrt{-Q/2}*\xi^{\alpha\lambda}\Lambda_{\lambda}, \tag{73}$$

$$\tilde{V}^{\alpha}_{(4)} = V^{\alpha}_{(4)} + {}^{*}\xi^{\alpha\lambda} {}^{*}\xi_{\rho\lambda} {}^{*}\Lambda^{\rho}. \tag{74}$$

The second term on the right-hand side of (73) has the orthogonality properties,

$$\sqrt{-Q/2}\, {}^{*}\xi^{\alpha\lambda} {}^{*}\Lambda_{\lambda} V_{(1)\alpha} = \sqrt{-Q/2}\, {}^{*}\xi^{\alpha\lambda} {}^{*}\Lambda_{\lambda} V_{(2)\alpha} = 0. \tag{75}$$

The second term on the right-hand side of (74) has similar orthogonality properties,

$${}^{*}\xi^{\alpha\lambda} {}^{*}\xi_{\rho\lambda} {}^{*}\Lambda^{\rho} V_{(1)\alpha} = {}^{*}\xi^{\alpha\lambda} {}^{*}\xi_{\rho\lambda} {}^{*}\Lambda^{\rho} V_{(2)\alpha} = 0. \tag{76}$$

Since the four vectors (24)–(27) are independent and orthogonal, Eqs. (75) and (76) imply that the second terms on the right-hand sides of (73) and (74) must be a linear combination of the vectors (26) and (27). We proceed then to write equations (73) and (74) as

$$\tilde{V}^{\alpha}_{(3)} = V^{\alpha}_{(3)} + KV^{\alpha}_{(3)} + LV^{\alpha}_{(4)}, \tag{77}$$

$$\tilde{V}^{\alpha}_{(4)} = V^{\alpha}_{(4)} + MV^{\alpha}_{(3)} + NV^{\alpha}_{(4)}. \tag{78}$$

From Eqs. (73) and (77) we know that

$$\sqrt{-Q/2}\, {}^{*}\xi^{\alpha\lambda} {}^{*}\Lambda_{\lambda} = KV^{\alpha}_{(3)} + LV^{\alpha}_{(4)}, \tag{79}$$

and from Eqs. (74) and (78) we have

$${}^{*}\xi^{\alpha\lambda} {}^{*}\xi_{\rho\lambda} {}^{*}\Lambda^{\rho} = MV^{\alpha}_{(3)} + NV^{\alpha}_{(4)}. \tag{80}$$

Making use of identities (15)–(17) it can be proved that

$${}^{*}\xi_{\alpha\sigma} V^{\alpha}_{(3)} = \sqrt{-Q/2} V_{(4)\sigma}, \tag{81}$$

$${}^{*}\xi_{\alpha\sigma} V^{\alpha}_{(4)} = -\sqrt{-Q/2} V_{(3)\sigma}. \tag{82}$$

If we contract Eq. (80) with ${}^{*}\xi_{\alpha\sigma}$ and make use of identities (15)–(17) and Eqs. (81) and (82) we get

$$-\sqrt{-Q/2}\, {}^{*}\xi_{\sigma\lambda} {}^{*}\Lambda^{\lambda} = MV_{(4)\sigma} - NV_{(3)\sigma}. \tag{83}$$

This last equation means that

$$\tilde{V}^{\alpha}_{(3)} = V^{\alpha}_{(3)} + NV^{\alpha}_{(3)} - MV^{\alpha}_{(4)}. \tag{84}$$

Then, from (77) and (84) we have the following relations between coefficients:

$$K = N, \tag{85}$$

$$L = -M. \tag{86}$$

Contracting Eq. (83) with $V^{\sigma}_{(3)}$ and $V^{\sigma}_{(4)}$ it can be found that

$$M = (-Q/2) V_{(3)\sigma} {}^{*}\Lambda^{\sigma} / (V_{(4)\beta} V^{\beta}_{(4)}), \tag{87}$$

$$N = (-Q/2) V_{(4)\sigma} {}^{*}\Lambda^{\sigma} / (V_{(3)\beta} V^{\beta}_{(3)}). \tag{88}$$

We would like to calculate the norm of the transformed vectors $\tilde{V}^{\alpha}_{(3)}$ and $\tilde{V}^{\alpha}_{(4)}$,

$$\tilde{V}^{\alpha}_{(3)}\tilde{V}_{(3)\alpha}=[(1+N)^2+M^2]V^{\alpha}_{(3)}V_{(3)\alpha}, \tag{89}$$

$$\tilde{V}^{\alpha}_{(4)}\tilde{V}_{(4)\alpha}=[(1+N)^2+M^2]V^{\alpha}_{(4)}V_{(4)\alpha}, \tag{90}$$

where the relation $V^{\alpha}_{(3)}V_{(3)\alpha}=V^{\alpha}_{(4)}V_{(4)\alpha}$ has been used. Now, we see that the gauge transformations of the invariants given by (89) and (90) cannot change the spacelike character of vectors $V^{\alpha}_{(3)}$ and $V^{\alpha}_{(4)}$, unless $1+N=M=0$. Apart from that exception, the factor $[(1+N)^2+M^2]$ is always positive, so we would have no problems normalizing the transformed vectors $\tilde{V}^{\alpha}_{(3)}$ and $\tilde{V}^{\alpha}_{(4)}$,

$$\frac{\tilde{V}^{\alpha}_{(3)}}{\sqrt{\tilde{V}^{\beta}_{(3)}\tilde{V}_{(3)\beta}}}=\frac{(1+N)}{\sqrt{(1+N)^2+M^2}}\frac{V^{\alpha}_{(3)}}{\sqrt{V^{\beta}_{(3)}V_{(3)\beta}}}-\frac{M}{\sqrt{(1+N)^2+M^2}}\frac{V^{\alpha}_{(4)}}{\sqrt{V^{\beta}_{(4)}V_{(4)\beta}}}, \tag{91}$$

$$\frac{\tilde{V}^{\alpha}_{(4)}}{\sqrt{\tilde{V}^{\beta}_{(4)}\tilde{V}_{(4)\beta}}}=\frac{M}{\sqrt{(1+N)^2+M^2}}\frac{V^{\alpha}_{(3)}}{\sqrt{V^{\beta}_{(3)}V_{(3)\beta}}}+\frac{(1+N)}{\sqrt{(1+N)^2+M^2}}\frac{V^{\alpha}_{(4)}}{\sqrt{V^{\beta}_{(4)}V_{(4)\beta}}}. \tag{92}$$

As long as $[(1+N)^2+M^2]>0$ the transformations (91) and (92) are telling us that an electromagnetic gauge transformation on the vector field $*A^{\alpha}$ that leaves invariant the dual electromagnetic field $*f_{\mu\nu}$, generates a rotation on the normalized tetrad vector fields

$$\left(\frac{V^{\alpha}_{(3)}}{\sqrt{V^{\beta}_{(3)}V_{(3)\beta}}},\frac{V^{\alpha}_{(4)}}{\sqrt{V^{\beta}_{(4)}V_{(4)\beta}}}\right).$$

V. GROUP ISOMORPHISM

In Secs. IV A and IV B the gauge transformation properties of the tetrad vectors were analyzed. But we can take advantage of the expressions we found for both the transformations on blade one and blade two to prove an important result involving the mappings between the local gauge group and the local Lorentz transformations on both blades. We are going to name LB1 the group of Lorentz transformations on blade one. Analogously we name the group of rotations on blade two, LB2. Making use of expressions (58) and (59), (60) and (61), (64) and (65), (66) and (67), and (91) and (92) we can prove the transformation properties of the local gauge group. We proceed first to study the transformation properties of the elements of the local gauge group on blade one.

A. Isomorphism on blade one

We can readily verify that the identity is given by $\Lambda=0$ or any other constant. Since all the gauge transformations only involve gradients of scalar functions, then the results we are going to find are going to be true, except for additional constants that have no physical or geometrical meaning. If the scalar function Λ generates a Lorentz transformation, then $(-\Lambda)$ generates the inverse Lorentz transformation. It is necessary at this point to understand several details about inverse transformations. Following the notation of the proceeding sections we can introduce on blade one, for instance, the inverse of the direct transformation as

$$\tilde{\tilde{V}}^{\alpha}_{(1)}=\tilde{V}^{\alpha}_{(1)}-\xi^{\alpha\lambda}\xi_{\rho\lambda}\Lambda^{\rho}=V^{\alpha}_{(1)}, \tag{93}$$

$$\tilde{\tilde{V}}^{\alpha}_{(2)}=V^{\alpha}_{(2)}-\sqrt{-Q/2}\xi^{\alpha\lambda}\Lambda_{\lambda}=V^{\alpha}_{(2)}, \tag{94}$$

$$\tilde{C} = (-Q/2)\tilde{V}_{(1)\sigma}(-\Lambda^{\sigma})/(\tilde{V}_{(2)\beta}\tilde{V}^{\beta}_{(2)}), \tag{95}$$

$$\tilde{D} = (-Q/2)\tilde{V}_{(2)\sigma}(-\Lambda^{\sigma})/(\tilde{V}_{(1)\beta}V^{\beta}_{(1)}). \tag{96}$$

We can see that in expressions (95) and (96) the change in sign of the scalar function Λ is not the only change. Therefore, we can also notice that for transformations (58) and (59),

$$\frac{(1+C)}{\sqrt{(1+C)^2 - D^2}} = \frac{(1+\tilde{C})}{\sqrt{(1+\tilde{C})^2 - \tilde{D}^2}}, \tag{97}$$

$$\frac{D}{\sqrt{(1+C)^2 - D^2}} = -\frac{\tilde{D}}{\sqrt{(1+\tilde{C})^2 - \tilde{D}^2}}, \tag{98}$$

while for transformations (64) and (65),

$$\frac{(1+C)}{\sqrt{-(1+C)^2 + D^2}} = -\frac{(1+\tilde{C})}{\sqrt{-(1+\tilde{C})^2 + \tilde{D}^2}}, \tag{99}$$

$$\frac{D}{\sqrt{-(1+C)^2 + D^2}} = \frac{\tilde{D}}{\sqrt{-(1+\tilde{C})^2 + \tilde{D}^2}}. \tag{100}$$

In order to get a better geometrical insight into the results that follow, we are introducing the angle ϕ. For proper transformations on blade one,

$$\cosh\phi = \frac{|1+C|}{\sqrt{(1+C)^2 - D^2}}, \tag{101}$$

while for improper transformations,

$$\cosh\phi = \frac{|D|}{\sqrt{-(1+C)^2 + D^2}}. \tag{102}$$

For instance, if the scalar function Λ_1 generates a boost ϕ_1, and the scalar function Λ_2 generates a boost ϕ_2, then it is straightforward to see that the subsequent transformation, first by Λ_1 and then by Λ_2 generates a boost $\phi_1 + \phi_2$. In general, if the scalar function Λ_1 generates a Lorentz transformation on blade one, and the scalar function Λ_2 generates another Lorentz transformation on blade one, then it is straightforward to see that the subsequent transformation, first by Λ_1 and then by Λ_2, generates the composition of the two Lorentz transformations.

Therefore, we proved that the transformations (58) and (59), (60) and (61), (64) and (65), and (66) and (67), represent a mapping between the local gauge group and the group LB1. Both groups are Abelian and have the same dimension. If in addition we manage to prove that this mapping is injective, and the image is not a subgroup of LB1, then the mapping would be an isomorphism. To this end, using equations (54) and (55), (87) and (88) we can write

$$(-Q/2)\Lambda^{\alpha} = -CV^{\alpha}_{(1)} - DV^{\alpha}_{(2)} + MV^{\alpha}_{(3)} + NV^{\alpha}_{(4)}, \tag{103}$$

such that

$$D = (1+C)\tanh\phi \quad \text{for proper transformations}, \tag{104}$$

$$D = (1+C)/\tanh\phi \quad \text{for improper transformations}. \tag{105}$$

It is simple to check that Eq. (104) is valid for $1+C>0$ or $1+C<0$, and Eq. (105) is also valid for $D>0$ or $D<0$. Once we are given a ϕ, the functions C, M, and N should be found through the use of the integrability conditions $\Lambda_{\alpha;\beta}=\Lambda_{\beta;\alpha}$. We know that if $\phi_1\neq\phi_2$, then $\tanh\phi_1\neq\tanh\phi_2$ and $\tanh\phi_1\neq 1/\tanh\phi_2$. Then, accordingly, the corresponding scalar functions Λ_1 and Λ_2 are not going to be the same. Conversely, we can ask if it is possible to map two different scalar functions Λ_1 and Λ_2 into the same Lorentz transformation. If this is possible, then we can first generate a Lorentz transformation by Λ_1 and then another one by $-\Lambda_2$. The result should be the identity, because $-\Lambda_2$ generates the inverse Lorentz transformation of Λ_1. Therefore $\Lambda_1-\Lambda_2$ must be a constant. Summarizing, the injectivity remains proved. The last point to make clear is related to the image of this mapping. The question to answer is if the image of this mapping is a subgroup of LB1. Let us suppose that there is a certain local gauge transformation Λ, such that $1+C>0$, with $-1<C<0$. Then, there is always the transformation $n\Lambda$ with n a natural number, $C_n=nC$. $1+C_n=1+nC=1-n|C|$. For n sufficiently large $1+C_n$ is going to become negative. If $C>0$, there is the transformation $-n\Lambda$ with n a natural number, $C_n=-nC$. $1+C_n=1-nC=1-n|C|$. Once more for n sufficiently large $1+C_n$ is going to become negative. Following similar ideas, but now if $1+C>D>0$ we can prove for instance, that if $-1<C<0$, for n sufficiently large, $D_n>0>1+C_n$, and analogous for $C>0$. Then, the mapping image obviously cannot be a subgroup of LB1. Therefore the mapping is surjective.

Theorem 1: *The mapping between the local gauge group of transformations is isomorphic to the group LB1 defined above*.

B. Isomorphism on blade two

The proof for the mapping between the local gauge group and the rotations on blade two is analogous to the previous one. For rotations all the considerations about inverse transformations and composition of transformations apply in a similar fashion as for the ones on blade one. The precisions we have to make on blade two regard fundamentally the injectivity. We can introduce the angle φ as

$$\cos\varphi=\frac{(1+N)}{\sqrt{(1+N)^2+M^2}}. \tag{106}$$

Then, we can use again Eq. (103), along with

$$M=(1+N)\tan\varphi. \tag{107}$$

Once we are given a φ, the functions C, D, and N should be found through the use of the integrability conditions $\Lambda_{\alpha;\beta}=\Lambda_{\beta;\alpha}$. For rotations, we know that $\tan(\varphi)=\tan(\varphi-\pi)$, but simultaneously we have that $\mathrm{sg}(M_\varphi)=-\mathrm{sg}(M_{(\varphi-\pi)})$ and $\mathrm{sg}(1+N_\varphi)=-\mathrm{sg}(1+N_{(\varphi-\pi)})$. The last sign equalities arise from the fact that under a change $\varphi\rightarrow\varphi-\pi$, the sine and cosine change their signs. All these results put together mean that given a pair of different angles φ_1 and φ_2, the corresponding scalar functions Λ_1 and Λ_2 are not going to be the same. Conversely, we can ask if it is possible to transform two different scalar functions Λ_1 and Λ_2 into the same φ. If this is possible, then we can proceed exactly as for the blade one case, we can first generate a rotation transformation by Λ_1 and then another one by $-\Lambda_2$. The result should be the identity, because $-\Lambda_2$ generates a rotation transformation by $-\varphi$. Therefore $\Lambda_1-\Lambda_2$ must be a constant, and the injectivity remains proved.

Theorem 2: *The mapping between the local gauge group of transformations is isomorphic to the group LB2 defined above*.

VI. TETRADS

A. Orthonormal tetrad

It was found in Sec. III that for an electromagnetic vector potential A^α, with $A^0A_0+A^1A_1<0$ in the Minkowski reference frame given by Eqs. (38) and (39) in Ref. 1, it was possible to normalize the tetrad vectors fields (24)–(27). Then, at the points in spacetime where the set of four vectors (24)–(27) is not trivial, we can proceed to normalize,

$$U^\alpha = \xi^{\alpha\lambda}\xi_{\rho\lambda}A^\rho/(\sqrt{-Q/2}\sqrt{A_\mu\xi^{\mu\sigma}\xi_{\nu\sigma}A^\nu}), \tag{108}$$

$$V^\alpha = \xi^{\alpha\lambda}A_\lambda/(\sqrt{A_\mu\xi^{\mu\sigma}\xi_{\nu\sigma}A^\nu}), \tag{109}$$

$$Z^\alpha = *\,\xi^{\alpha\lambda} * A_\lambda/(\sqrt{*A_\mu * \xi^{\mu\sigma} * \xi_{\nu\sigma} * A^\nu}), \tag{110}$$

$$W^\alpha = *\,\xi^{\alpha\lambda} * \xi_{\rho\lambda} * A^\rho/(\sqrt{-Q/2}\sqrt{*A_\mu * \xi^{\mu\sigma} * \xi_{\nu\sigma} * A^\nu}). \tag{111}$$

The notation we are using to name the four tetrad vectors (108)–(111) is the same notation used in Ref. 2, even though the geometrical meaning is different. The four vectors (108)–(111) have the following algebraic properties:

$$-U^\sigma U_\alpha = V^\alpha V_\alpha = Z^\alpha Z_\alpha = W^\alpha W_\alpha = 1. \tag{112}$$

Any other scalar product is zero. It is possible to find expressions for the metric tensor and the stress-energy tensor in the new tetrad (108)–(111). The new expression for the metric tensor is

$$g_{\alpha\beta} = -U_\alpha U_\beta + V_\alpha V_\beta + Z_\alpha Z_\beta + W_\alpha W_\beta. \tag{113}$$

The stress-energy tensor can be written,

$$T_{\alpha\beta} = (Q/2)[-U_\alpha U_\beta + V_\alpha V_\beta - Z_\alpha Z_\beta - W_\alpha W_\beta]. \tag{114}$$

In order to find the expression for the electromagnetic field in terms of the tetrad (108)–(111), it is necessary to find some previous results. Using Eqs. (15) and (17) it is possible to prove that

$$U^\alpha\xi_{\alpha\beta} = \sqrt{-Q/2}V_\beta, \tag{115}$$

$$V^\alpha\xi_{\alpha\beta} = \sqrt{-Q/2}U_\beta, \tag{116}$$

$$Z^\alpha * \xi_{\alpha\beta} = \sqrt{-Q/2}W_\beta, \tag{117}$$

$$W^\alpha * \xi_{\alpha\beta} = -\sqrt{-Q/2}Z_\beta. \tag{118}$$

Equations (112) and (115)–(118) allow us to find the expressions for the extremal field in terms of the new tetrad,

$$U^\alpha\xi_{\alpha\beta}V^\beta = \sqrt{-Q/2}, \tag{119}$$

$$Z^\alpha * \xi_{\alpha\beta}W^\beta = \sqrt{-Q/2}. \tag{120}$$

The extremal field tensor and its dual can then be written,

$$\xi_{\alpha\beta} = -2\sqrt{-Q/2}U_{[\alpha}V_{\beta]}, \tag{121}$$

$$*\xi_{\alpha\beta} = 2\sqrt{-Q/2}Z_{[\alpha}W_{\beta]}. \tag{122}$$

Equations (121) and (122) are providing the necessary information to express the electromagnetic field in terms of the new tetrad,

$$f_{\alpha\beta} = -2\sqrt{-Q/2}\cos\alpha U_{[\alpha}V_{\beta]} + 2\sqrt{-Q/2}\sin\alpha Z_{[\alpha}W_{\beta]}. \tag{123}$$

B. Null tetrad

We are ready now to introduce a new null tetrad. It will be defined as

$$K_\alpha = \frac{1}{\sqrt{2}}(U_\alpha + V_\alpha), \tag{124}$$

$$L_\alpha = \frac{1}{\sqrt{2}}(U_\alpha - V_\alpha), \tag{125}$$

$$T_\alpha = \frac{1}{\sqrt{2}}(Z_\alpha + \imath W_\alpha), \tag{126}$$

$$\bar{T}_\alpha = \frac{1}{\sqrt{2}}(Z_\alpha - \imath W_\alpha), \tag{127}$$

where $\imath$ is the imaginary complex unit, $\imath^2=-1$. The notation we are using to name the null tetrad vectors (124)–(127) is the same as in Ref. 2. Again it should be noticed that even though the null tetrad notation is the same as in Ref. 2, the geometrical meaning is not the same. This new null tetrad (124)–(127) satisfies the following algebraic relations;

$$K^\alpha K_\alpha = K^\alpha T_\alpha = L^\alpha L_\alpha = L^\alpha T_\alpha = T^\alpha T_\alpha = 0, \tag{128}$$

and

$$K^\alpha L_\alpha = -1, \tag{129}$$

$$T^\alpha \bar{T}_\alpha = 1. \tag{130}$$

It can also be proved in the Minkowskian reference frame given by Eqs. (38) and (39) in Ref. 1, and through the use of the results found in Appendices A and B that the identity,

$$\epsilon_{\alpha\beta\mu\nu}K^\alpha L^\beta T^\alpha \bar{T}^\nu = -\imath, \tag{131}$$

is satisfied. Then, the metric tensor can be written in terms of the new null tetrad,

$$g_{\alpha\beta} = T_\alpha \bar{T}_\beta + \bar{T}_\alpha T_\beta - K_\alpha L_\beta - K_\beta L_\alpha. \tag{132}$$

Using (124)–(127) it is straightforward to prove that (132) is equivalent to (113). In terms of the new null tetrad the stress-energy tensor can be expressed,

$$T_{\alpha\beta} = (-Q/2)[K_\alpha L_\beta + K_\beta L_\alpha + T_\alpha \bar{T}_\beta + T_\beta \bar{T}_\alpha]. \tag{133}$$

It is not difficult to prove that (133) and (114) are equivalent. We would like to find the expression for the electromagnetic field in terms of the new null tetrad. It is necessary to find first the components of the external tensor and its dual in terms of the new null tetrad. Making use of (119) and (120) we find,

$$K^\alpha \xi_{\alpha\beta} L^\beta = -\sqrt{-Q/2}, \tag{134}$$

$$T^{\alpha} * \xi_{\alpha\beta}\bar{T}^{\beta} = -\iota\sqrt{-Q/2}. \tag{135}$$

Now, we have the expressions for the extremal field tensor and its dual in terms of the new null tetrad,

$$\xi_{\alpha\beta} = 2\sqrt{-Q/2}K_{[\alpha}L_{\beta]}, \tag{136}$$

$$*\xi_{\alpha\beta} = 2\iota\sqrt{-Q/2}T_{[\alpha}\bar{T}_{\beta]}. \tag{137}$$

Equations (136) and (137) allow us to find the electromagnetic field expressed in terms of the new null tetrad,

$$f_{\alpha\beta} = 2\sqrt{-Q/2}\cos\alpha K_{[\alpha}L_{\beta]} + 2\iota\sqrt{-Q/2}\sin\alpha T_{[\alpha}\bar{T}_{\beta]}. \tag{138}$$

C. Bivectors

It is possible to express any antisymmetric second-rank tensor, as a linear combination of the following bivectors:

$$U_{\alpha\beta} = \bar{T}_{\alpha}L_{\beta} - \bar{T}_{\beta}L_{\alpha}, \tag{139}$$

$$V_{\alpha\beta} = K_{\alpha}T_{\beta} - K_{\beta}T_{a}, \tag{140}$$

$$W_{\alpha\beta} = T_{\alpha}\bar{T}_{\beta} - T_{\beta}\bar{T}_{\alpha} - K_{\alpha}L_{\beta} + K_{\beta}L_{\alpha}. \tag{141}$$

These bivectors are combinations of the null tetrad vectors (124)–(127), and making use of (131) it can be proved that they are also self-dual,

$$\tilde{U}_{\alpha\beta} = \tfrac{1}{2}\epsilon_{\alpha\beta\mu\nu}U^{\mu\nu} = -\iota U_{\alpha\beta}, \tag{142}$$

$$\bar{V}_{\alpha\beta} = -\iota V_{\alpha\beta}, \tag{143}$$

$$\tilde{W}_{\alpha\beta} = -\iota W_{\alpha\beta}. \tag{144}$$

One more time, the notation for (139)–(141) is analogous to the one in Ref. 2 but the geometrical meaning is different. The self-dual bivectors (139)–(141) have the following associated scalar products:

$$W_{\alpha\beta}V^{\alpha\beta} = W_{\alpha\beta}U^{\alpha\beta} = V_{\alpha\beta}V^{\alpha\beta} = U_{\alpha\beta}U^{\alpha\beta} = 0, \tag{145}$$

$$W_{\alpha\beta}W^{\alpha\beta} = -4, \tag{146}$$

$$U_{\alpha\beta}V^{\alpha\beta} = 2. \tag{147}$$

It was our purpose since the beginning of this work to find the simplest possible expression for the electromagnetic field through the use of null tetrads in geometrodynamics. Now, we would like to see what is the expression in the new bivectors (139)–(141) for the self-dual electromagnetic bivector,

$$\Phi_{\alpha\beta} = f_{\alpha\beta} + \iota * f_{\alpha\beta}. \tag{148}$$

Making use of expressions (136), (137), and (141) it is possible to write

$$\Phi_{\alpha\beta} = -\sqrt{-Q/2}e^{(-\iota\alpha)}W_{\alpha\beta}. \tag{149}$$

The standard way of expressing the bivector (148) is through an expansion in the three standard bivectors given by Eq. (18.9) in Ref. 2, which in turn are built in terms of the familiar NP tetrads.[3] The new null tetrad (124)–(127) has the advantage that in the particular problem of geometrodynamics the expression of the bivector (148) given by (149) is the simplest possible one, since we can write it only in terms of one of the three independent new bivectors, expression (141). The two scalar functions associated with the electromagnetic field are included in the complex factor $-\sqrt{-Q/2}e^{(-\iota\alpha)}$. This example shows the simplifying power of the new tetrad built specifically for the problem of geometrodynamics.

VII. GENERAL TETRAD

In Sec. III a particular example of an explicit choice of the vector fields X_α and Y_α was introduced ($X_\alpha = A_\alpha$ and $Y_\alpha = *A_\alpha$) within the framework of geometrodynamics. Through this example several properties of these new tetrads were discussed. The transformation properties induced by usual gauge transformations $A^\alpha \to A^\alpha + \Lambda'^\alpha$ and $*A^\alpha \to *A^\alpha + *\Lambda'^\alpha$ were analyzed in Sec. IV. Let us assume that it is possible to normalize the general tetrad (11)–(14). For generic fields X_α and Y_α, we can proceed to study the transformation properties of the normalized version of (11) and (12) under the transformation $X_\alpha \to X_\alpha + V_\alpha$, where V_α is any well-behaved vector field in spacetime. The necessary steps to study these tetrad transformations are a replica of the ones taken in Sec. IV A. The conclusions are analogous. In a similar way, the normalized version of (13) and (14) can be transformed under $Y_\alpha \to Y_\alpha + W_\alpha$, where W_α is any well-behaved vector field. Again, the steps and conclusions involved in the study of these tetrad transformations are a replica of the ones taken in Sec. IV B. Once we introduced these new tetrad transformations for the general case, we can easily prove that $X_\alpha \to X_\alpha + V_\alpha$ and $Y_\alpha \to Y_\alpha + W_\alpha$ leave invariant two tensors, $g_{\alpha\beta}$ and $f_{\alpha\beta}$. The fact that these tetrad transformations leave invariant the metric tensor means that they are symmetries of the geometry. They also leave invariant the electromagnetic tensor, which means that they represent symmetries of the electromagnetic geometry. But the important issue is that they do not alter the tensors that carry the physical information. The new tetrads (11)–(14) when normalized can be used to simplify the Einstein-Maxwell equations in the Newman-Penrose tetrad formalism. It is worth noticing the substantial simplification that the new tetrads would introduce in the Einstein-Maxwell equations. As an example, the vacuum Maxwell equations using the notation given in Ref. 7 are given by

$$D\phi_1 = 2\rho\phi_1, \tag{150}$$

$$\delta\phi_1 = -2\tau\phi_1, \tag{151}$$

$$\bar{\delta}\phi_1 = -2\pi\phi_1, \tag{152}$$

$$\Delta\phi_1 = -2\mu\phi_1. \tag{153}$$

It is important to notice that the tetrads will be independent variables. For a non-null solution to the set of Einstein-Maxwell equations we can find the scalars α and Q from $\phi_1 = -\sqrt{-Q/2}e^{(-\iota\alpha)}$. Expression (136) will provide the relation between the extremal field and the new tetrads. The electromagnetic field will be available through expression (138) and the metric tensor will be given by (132) once a tetrad is known for a particular solution. The overall effect of the new tetrads is to reallocate or reorganize algebraic information in the Einstein-Maxwell equations making it easier to find new possible solutions.

VIII. CONCLUSIONS

A new tetrad that diagonalizes the electromagnetic stress-energy tensor for non-null electromagnetic fields was introduced. However, this tetrad has an inherent freedom in the choice of two vector fields. Geometrodynamics is an arena in which an explicit example or choice can be given for these two vector fields, because Maxwell's equations are providing two vector potentials. The simplicity of the expression for the electromagnetic field in this new tetrad and the associated null tetrad becomes evident. It was also proved that the local gauge group is related to the group LB1, and also to the group LB2 through an isomorphism. In the last section the tetrad is also considered without making any specific choice for these two vector fields. It is found that there are transformations that leave invariant the metric and electromagnetic tensors simultaneously. It was also proved that when written in terms of the new tetrad, the Einstein-Maxwell equations are substantially simplified.

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APPENDIX A

The Levi-Civita pseudotensor can be transformed into a tensor through the use of factors $\sqrt{-g}$, where g is the determinant of the metric tensor. We use the notation $e_{\alpha\beta\mu\nu}=[\alpha\beta\mu\nu]$ for the covariant components of the Levi-Civita pseudotensor in the Minkowskian frame given in Ref. 1,

$$e_{\alpha\beta\mu\nu}=\begin{cases}1 \text{ if } \alpha\beta\mu\nu \text{ is an even permutation of } 0123\\ -1 \text{ if } \alpha\beta\mu\nu \text{ is an odd permutation of } 0123\\ 0 \text{ if } \alpha\beta\mu\nu \text{ are not all different.}\end{cases}$$

It can be noticed that the signs in $e^{\alpha\beta\mu\nu}$ are going to be opposite to the standard notation.[5] The reason for this is that we want to keep the compatibility with Ref. 1 where the definition $e_{0123}=[0123]=1$ was adopted. With these definitions we see that in a spacetime with a metric $g_{\alpha\beta}$,

$$e^{\alpha\beta\mu\nu}=\frac{e^{\alpha\beta\mu\nu}}{\sqrt{-g}}=-\frac{[\alpha\beta\mu\nu]}{\sqrt{-g}} \tag{A1}$$

are the components of a contravariant tensor.[5–7] The covariant components of (A1) are

$$\epsilon_{\alpha\beta\mu\nu}=e_{\alpha\beta\mu\nu}\sqrt{-g}=[\alpha\beta\mu\nu]\sqrt{-g}, \tag{A2}$$

where

$$g_{\alpha\sigma}g_{\beta\rho}g_{\mu\kappa}g_{\nu\lambda}e^{\sigma\rho\kappa\lambda}=-ge_{\alpha\beta\mu\nu} \tag{A3}$$

is satisfied.

APPENDIX B

The tetrad vectors $(U^\alpha,V^\alpha,Z^\alpha,W^\alpha)$ have the following expressions in the Minkowski reference frame given by Eqs. (38) and (39) in Ref. 1,

$$U^0=-A^0/\sqrt{-(A^0A_0+A^1A_1)}, \tag{B1}$$

$$U^1=-A^1/\sqrt{-(A^0A_0+A^1A_1)}, \tag{B2}$$

$$V^0=-\xi_{01}A^1/(|\xi_{01}|\sqrt{-(A^0A_0+A^1A_1)}), \tag{B3}$$

$$V^1 = -\xi_{01}A^0/(|\xi_{01}|\sqrt{-(A^0A_0 + A^1A_1)}), \tag{B4}$$

$$Z^2 = -\xi_{01} * A^3/(|\xi_{01}|\sqrt{*A^2 * A_2 + *A^3 * A_3}), \tag{B5}$$

$$Z^3 = \xi_{01} * A^2/(|\xi_{01}|\sqrt{*A^2 * A_2 + *A^3 * A_3}), \tag{B6}$$

$$W^2 = *A^2/\sqrt{*A^2 * A_2 + *A^3 * A_3}, \tag{B7}$$

$$W^3 = *A^3/\sqrt{*A^2 * A_2 + *A^3 * A_3}, \tag{B8}$$

where $|\xi_{01}| = \sqrt{(\xi_{01})^2}$.

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Analytic structure of radiation boundary kernels for blackhole perturbations

Stephen R. Lau[a)]
Center for Gravitational Wave Astronomy, University of Texas at Brownsville, Brownsville, Texas 78520

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Exact outer boundary conditions for gravitational perturbations of the Schwarzschild metric feature integral convolution between a time-domain boundary kernel and each radiative mode of the perturbation. For both axial (Regge–Wheeler) and polar (Zerilli) perturbations, we study the Laplace transform of such kernels as an analytic function of (dimensionless) Laplace frequency. We present numerical evidence indicating that each such frequency-domain boundary kernel admits a "sum-of-poles" representation. Our work has been inspired by Alpert, Greengard, and Hagstrom's analysis of nonreflecting boundary conditions for the ordinary scalar wave equation. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2073287]

I. INTRODUCTION

Now 50 years old, the perturbation theory of Schwarzschild blackholes remains a timely subject with fundamental applications. The covariant d'Alembertian (or wave equation) associated with the Schwarzschild line-element describes scalar "perturbations." Classical Schwarzschild blackholes are spherically symmetric and static in time, and these symmetries allow for combined multipole and Fourier (or Laplace) decompositions. As a result, perturbations may be described via a denumerable collection of ODE rather than the d'Alembertian PDE. Similar ODE describe electromagnetic "perturbations"[1] and gravitational perturbations (small genuine fluctuations in the background geometry),[2,3] although their derivation is more complicated since the multipole decomposition involves either vector or tensor spherical harmonics. Remarkably, via the technique of "despinning" based on the eth operator,[4] such ODEs can be related to scalar wave equations.

Wheeler considered the case of electromagnetic perturbations in 1955,[1] showing for a given multipole that each of the two electromagnetic polarization states are described by a copy of a single ODE. Regge and Wheeler then derived a similar ODE describing odd-parity (or axial) gravitational perturbations in 1957,[2] and Zerilli introduced an ODE describing even-parity (or polar) gravitational perturbations in 1970.[3] In the 1970s Chandrasekhar and Detweiler demonstrated that the Zerilli equation can be derived from the Regge–Wheeler equation, although the derivation involves differential operations (see Ref. 5, and references therein). In their treatment[6] of *intertwining operators*, Anderson and Price clarified the relationship between solutions to the Regge–Wheeler and Zerilli ODEs. Application of a first-order differential operator transforms smooth solutions of one equation into solutions of the other.

Schwarzschild perturbation theory has played a central role in several modern areas of classical and quantum gravity. Although the following is by no means an exhaustive list, we mention four salient applications: the "close-limit" approximation for blackhole collisions, a time-domain approach to the radiation reaction problem, the asymptotic form of high frequency quasinormal modes, and quantum uncertainty in blackhole horizons. Price and Pullin, assuming that the colliding blackholes are initially cloaked in a common horizon, have used first-order perturbation

[a)]Present address: Department of Mathematics and Statistics, MSC03 2150, 1 University of New Mexico, Albuquerque, New Mexico 87131-0001; electronic mail: srlau@math.unm.edu

theory and the Zerilli equation to compute the energy radiated away by gravitational waves.[7] They initially applied their close-limit approximation to time-symmetric initial data. More general data were subsequently considered,[8] and the accuracy of the approximation studied via second-order perturbation theory.[9,10] Lousto has studied the binary radiation reaction problem in the extreme mass ratio limit via time-domain calculations.[11] His approach relies on numerical simulation of Schwarzschild perturbations, and he has developed a fourth-order convergent algorithm for such simulations.[12] Interest in the quasinormal mode spectrum of classical Schwarzschild blackholes has been renewed by possible connections with the Barbero-Immirzi parameter in loop quantum gravity.[13–15] While these issues are beyond us, we note that they have focused attention on the asymptotic form of high frequency quasinormal modes[16,17] (a purely classical issue). Most recently, York and Schmekel have considered a truncated superspace of blackhole fluctuations, using path integral quantization to derive a Schrödinger equation and estimate the quantum uncertainty in the horizon.[18] York and Schmekel's analysis constitutes an improved derivation of results already found by York via semiclassical arguments.[19]

This paper addresses the mathematical issue of *exact* radiation outer boundary conditions (ROBC) for Schwarzschild blackhole perturbations. Our work is based on an approach[20] developed by Alpert, Greengard, and Hagstrom (AGH) for nonreflecting boundary conditions and time-domain wave propagation on flat spacetime. Beyond being of theoretical interest, such boundary conditions are relevant for numerical simulations. Indeed, long-time simulations require some form of domain reduction, that is specification of appropriate boundary conditions at the "edge" of the computational domain. Exact outer boundary conditions for gravitational perturbations of Schwarzschild blackholes feature integral convolution between a time-domain boundary kernel and each angular mode of the perturbation. For both axial (Regge–Wheeler) and polar (Zerilli) perturbations, we study the Laplace transform of the such kernels as an analytic function of (dimensionless) Laplace frequency σ. We present numerical evidence indicating that each such gravitational boundary kernel admits a "sum-of-poles" representation. These representations are similar to those considered by AGH for wave propagation on flat $3+1$ and $2+1$ spacetimes. We hope to interest analysts in our conjectured sum-of-poles representation and the theorems we believe are lurking behind it.

We have considered such boundary conditions in detail before[21,22] (hereafter referred to as Papers I and II). However, this paper goes beyond these references in the following ways. First, we consider the Zerilli equation, not considered at all in Papers I and II. Second, we focus here on the analytic structure of gravitational kernels (both Regge–Wheeler and Zerilli cases), whereas Paper I almost exclusively considered kernels for scalar wave propagation. Although the theory and methods in Papers I and II were also spelled out for the gravitational (spin 2) Regge–Wheeler equation, we consider these results in more detail here. We also discuss the asymptotic agreement between Schwarzschild ROBC and flatspace nonreflecting boundary conditions, remarking on some fine points unmentioned in our earlier work. Part of this paper roughly parallels Sec. III from Paper I, which documented several numerical tests of the sum-of-poles representation for scalar (spin 0) kernels. Here we run through those same tests for the gravitational kernels, and also carry out another test based on the Argument principle. A longer paper on numerical implementation of these ideas, complete with extensive numerical tables, is forthcoming,[23] and in part this paper is meant to lay more groundwork for that longer work.

II. PRELIMINARIES

A. Wave equations for gravitational perturbations

In terms of dimensionless time τ and radius $\rho > 1$, the standard Schwarzschild line-element reads

$$\mathrm{d}s^2 = -F\mathrm{d}\tau^2 + F^{-1}\mathrm{d}\rho^2 + \rho^2(\mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\phi^2), \tag{1}$$

where $F(\rho) = 1 - \rho^{-1}$. With M the mass parameter of the solution, standard physical coordinates are then $t = 2M\tau$ and $r = 2M\rho$. We also consider a dimensionless Laplace frequency σ related to the

physical frequency s via $\sigma=2Ms$. As is well known (see, for example, Ref. 24), radiative perturbations of the Schwarzschild metric are ultimately described by wave equations for angular modes $\rho^{-1}\Psi_{\ell m}(\tau,\rho)$. From now on, we drop the "azimuthal" index m and write $\Psi_\ell(\tau,\rho)$, since all equations depend only on the "orbital" index ℓ. In terms of the Regge–Wheeler tortoise coordinate $\rho_*=\rho+\log(\rho-1)$, the perturbation Ψ_ℓ obeys the wave equation

$$\frac{\partial^2\Psi_\ell}{\partial\tau^2}-\frac{\partial^2\Psi_\ell}{\partial\rho_*^2}+V(\rho)\Psi_\ell=0. \tag{2}$$

For axial perturbations $V(\rho)$ is the Regge–Wheeler potential

$$V^{RW}(\rho)=\left(1-\frac{1}{\rho}\right)\left[\frac{\ell(\ell+1)}{\rho^2}+\frac{1-j^2}{\rho^3}\right], \tag{3}$$

where $j=2$. Scalar and electromagnetic perturbations correspond to $j=0$ and 1, respectively.

Equation (2) also describes polar perturbations, although in this case $V(\rho)$ is the Zerilli potential

$$V^{Z}(\rho)=\left(1-\frac{1}{\rho}\right)\left[\frac{8n^2(n+1)\rho^3+12n^2\rho^2+18n\rho+9}{\rho^3(2n\rho+3)^2}\right], \tag{4}$$

where $n=\frac{1}{2}(\ell-1)(\ell+2)$. Throughout this paper we consider the same objects for the Regge–Wheeler and Zerilli cases, and we shall make use of the following convention. An object without a superscript letter, say $V(\rho)$, will refer to the generic object, and could correspond to either of the two cases (actually four cases, since the Regge–Wheeler scenario is three cases in itself). Superscript letters will denote the specific cases. For example, we have $V^{RW}(\rho)$ and $V^{Z}(\rho)$ as above. We will also sometimes use a superscript F to denote corresponding flatspace objects, for example

$$V^{F}(\rho)=\frac{\ell(\ell+1)}{\rho^2} \tag{5}$$

as the flatspace potential.

Formal Laplace transformation of the Regge–Wheeler wave equation (2) yields a second-order ODE

$$L^{RW}\hat{\Psi}_\ell=0,\quad L^{RW}=\frac{\mathrm{d}^2}{\mathrm{d}\rho_*^2}-V^{RW}(\rho)-\sigma^2, \tag{6}$$

where σ is Laplace frequency. This equation is—apart from a transformation on the dependent variable—a special case of the *confluent Heun equation*.[25,26] Therefore, implementation of ROBC for the Regge–Wheeler equation involves confluent Heun functions, whereas the flatspace implementation of AGH[20] involves Bessel functions (closely related to *confluent* hypergeometric functions).

Likewise, we may consider formal Laplace transformation of the Zerilli wave equation (2),

$$L^{Z}\hat{\Psi}_\ell=0,\quad L^{Z}=\frac{\mathrm{d}^2}{\mathrm{d}\rho_*^2}-V^{Z}(\rho)-\sigma^2. \tag{7}$$

Solutions of (6) with $j=2$ are related to solutions of (7) and *vice versa* by the intertwining relations[6]

$$D_+L^{RW}=L^{Z}D_+,\quad D_-L^{Z}=L^{\mathrm{RW}}D_-, \tag{8}$$

with

$$D_{\pm} = \frac{\mathrm{d}}{\mathrm{d}\rho_*} \pm \left[\frac{2}{3} n(n+1) + \frac{3(\rho-1)}{\rho^2(3+2n\rho)} \right]. \tag{9}$$

We have mentioned that Papers I and II examined the exact ROBC for the Regge–Wheeler equation, although mostly focusing on the $j=0$ case. A natural question then is whether or not these boundary conditions can be easily carried over to the Zerilli case via use of intertwining relations. It would seem the answer is "no," and we have been unable to make direct use of our previous work on ROBC via the intertwining relations. Although we believe the issue may merit further study, in this paper we develop and describe Zerilli ROBC from scratch.

B. Radiation outer boundary conditions

Let us assume initial data of compact support, and that the radial location ρ_B of the outer boundary B lies beyond the support of the data. Then the exact nonlocal ROBC is the following differential-integral identity:[21]

$$\left(\frac{\partial \Psi_\ell}{\partial \tau} + \frac{\partial \Psi_\ell}{\partial \rho_*} \right) \Bigg|_{\rho=\rho_B} = \frac{F(\rho_B)}{\rho_B} \int_0^\tau \omega_\ell(\tau-\tau';\rho_B) \Psi_\ell(\tau',\rho_B) \mathrm{d}\tau'. \tag{10}$$

The ROBC equates an outgoing characteristic derivative of the field with an integral convolution of the field history. Although the conditions (10) are equally valid for the Regge–Wheeler and Zerilli cases, we must consider two separate kernels: $\omega_\ell^{RW}(\tau;\rho_B)$ and $\omega_\ell^{Z}(\tau;\rho_B)$. As a function of complex Laplace frequency σ, Paper I has considered the Laplace transform $\hat{\omega}_\ell^{RW}(\sigma;\rho_B)$ of the integral kernel $\omega_\ell^{RW}(\tau;\rho_B)$, in particular arguing that it admits a "sum-of-poles" representation quite similar to the representation of frequency-domain kernels for flatspace wave propagation in $2+1$ dimensions. Such representations involve both a finite pole sum as well as a continuous sector.[20] The analysis in Paper I mostly concentrated on the $\hat{\omega}_\ell^{RW}(\sigma;\rho_B)$ relevant for scalar wave propagation (that is for $j=0$), and did not consider the Zerilli equation at all. In the following we consider the analytic structure of both $\hat{\omega}_\ell^{RW}(\sigma;\rho_B)$ for $j=2$ and $\hat{\omega}_\ell^{Z}(\sigma;\rho_B)$ in some detail.

Paper I has developed numerical methods for evaluating $\hat{\omega}_\ell(\sigma;\rho_B)$ along the axis of imaginary Laplace frequency, precisely the contour over which the inverse Laplace transform is taken to obtain the time-domain kernel. We further touch upon these methods in the following, but mention here that they rely on stable numerical integration over various paths in both the complex ρ and complex $z=\sigma\rho$ planes. All of our work in this paper is based upon these methods, and we have used them to plot in Fig. 1 the $j=2$ Regge–Wheeler profiles Re $\hat{\omega}_2^{RW}(\mathrm{i}y;15)$ and Im $\hat{\omega}_2^{RW}(\mathrm{i}y;15)$ for real y. Although different, the corresponding Zerilli profiles would be indistinguishable to the eye, were they also plotted in Fig. 1.

C. Kernel compression

With the ability to generate such numerical profiles for exact frequency-domain kernels, we have employed the technique of kernel compression in order to construct highly accurate numerical kernels which allow for efficient evaluation of the convolution appearing in (10). Introduced by AGH[20] and described further in both Ref. 27 and Paper II, compression is vital both for high-ℓ kernels as well as low-ℓ kernels which are dominated by costly continuous sectors (such sectors are further described in the following). The technique produces a rational function,

$$\hat{\xi}_\ell(\sigma;\rho_B) = \sum_{k=1}^{d} \frac{\gamma_{\ell,k}(\rho_B)}{\sigma - \beta_{\ell,k}(\rho_B)}, \tag{11}$$

which approximates $\hat{\omega}_\ell(\sigma;\rho_B)$ and is in fact a sum of d simple poles. The pole locations $\beta_{\ell,k}(\rho_B)$ and strengths $\gamma_{\ell,k}(\rho_B)$—output from the compression algorithm—lie in the left-half plane. The approximation is rigged to satisfy

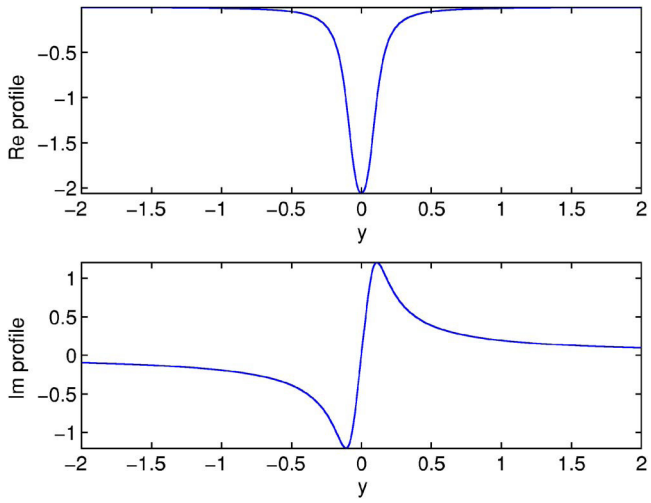

FIG. 1. (Color online) Re $\hat{\omega}_2^{RW}(\mathrm{iy};15)$ and Im $\hat{\omega}_2^{RW}(\mathrm{iy};15)$ profiles for the $j=2$ frequency domain kernel $\hat{\omega}_2^{RW}(\mathrm{iy};15)$. As indicated, $\ell=2$ and $\rho_B=15$.

$$\sup_{y\in R}\frac{|\hat{\xi}_\ell(\mathrm{iy};\rho_B)-\hat{\omega}_\ell(\mathrm{iy};\rho_B)|}{|\hat{\omega}_\ell(\mathrm{iy};\rho_B)|}<\varepsilon, \tag{12}$$

where ε is a chosen numerical tolerance. Theoretically, this bound on the relative supremum error in the frequency domain ensures a long-time bound on the relative convolution error associated with (10), as discussed in Ref. 20 and Paper II. This convolution error arises when using the approximate time-domain kernel

$$\xi_\ell(\tau;\rho_B)=\sum_{k=1}^{d}\gamma_{\ell,k}(\rho_B)\exp[\beta_{\ell,k}(\rho_B)\tau] \tag{13}$$

in place of the true kernel $\omega_\ell(\tau;\rho_B)$. Since $\xi_\ell(\tau;\rho_B)$ is a sum of exponentials, due to recursive identities an approximation of the convolution (10) based on $\xi_\ell(\tau;\rho_B)$ is not memory intensive. We list representative compressed kernels for Regge–Wheeler and Zerilli kernels in Tables I and II. The two kernels are strikingly similar, although they differ by a relative supremum error of about 3.03×10^{-2}, well below their stated $\varepsilon=10^{-10}$ tolerances. Extensive numerical tables of compressed kernels are being prepared and will appear in Ref. 23.

D. Quasinormal ringing and decay tail

Providing little detail, we now carry out a simple experiment meant only to indicate that the described ROBC work well for long-time simulations. More careful experiments were considered in Paper II (for Regge–Wheeler cases only) and will be considered in Ref. 23. In terms of retarded time $\mu=\tau-\rho_*$ and the pulse function

$$g(\mu)=\begin{cases}[\mu(\mu+4)]^4/256 & \text{for } -4\leqslant\mu\leqslant0\\ 0 & \text{otherwise,}\end{cases} \tag{14}$$

we construct the $\ell=2$ wave packet

$$\Psi_2(0,\rho)=g(-\rho_*) \tag{15}$$

as initial data for the Zerilli equation. The initial packet is then of unit height and compactly supported on $0\leqslant\rho_*\leqslant4$. To complete the data, we assume that

TABLE I. Compressed $j=2$ Regge–Wheeler kernel for $\ell=2$, $\rho_B=15$, $\varepsilon=10^{-10}$. There are $d=10$ poles and strengths, and complex conjugation of the ninth entries gives the tenth entries. Zeros correspond to outputs from the compression algorithm which are less than 10^{-30} in absolute value.

k	Re $\beta^{RW}_{2,k}(15)$	Im $\beta^{RW}_{2,k}(15)$
1	−3.756 161 769 22E−01	0
2	−2.522 858 979 20E−01	0
3	−1.714 587 811 91E−01	0
4	−1.165 624 902 43E−01	0
5	−7.643 319 902 76E−02	0
6	−4.680 910 579 81E−02	0
7	−2.637 301 379 27E−02	0
8	−1.256 529 945 67E−02	0
9	−9.477 951 789 47E−02	5.993 120 249 47E−02
k	Re $\gamma^{RW}_{2,k}(15)$	Im $\gamma^{RW}_{2,k}(15)$
1	−9.428 154 407 64E−06	0
2	−3.660 463 100 52E−04	0
3	−3.740 273 835 89E−03	0
4	−8.727 342 659 27E−03	0
5	−1.471 891 363 42E−03	0
6	−5.013 569 886 68E−05	0
7	−9.734 236 210 68E−07	0
8	−7.288 070 250 58E−09	0
9	−8.948 361 729 91E−02	6.206 435 489 37E−02

TABLE II. Compressed Zerilli kernel for $\ell=2$, $\rho_B=15$, $\varepsilon=10^{-10}$. There are $d=10$ poles and strengths, and complex conjugation of the ninth entries gives the tenth entries. Zeros correspond to outputs from the compression algorithm which are less than 10^{-30} in absolute value.

k	Re $\beta^{Z}_{2,k}(15)$	Im $\beta^{Z}_{2,k}(15)$
1	−3.708 271 031 77E−01	0
2	−2.489 162 785 32E−01	0
3	−1.690 979 832 83E−01	0
4	−1.148 943 408 03E−01	0
5	−7.531 695 951 30E−02	0
6	−4.612 526 333 39E−02	0
7	−2.598 806 812 76E−02	0
8	−1.238 195 997 59E−02	0
9	−9.340 658 398 50E−02	5.898 027 899 71E−02
k	Re $\gamma^{Z}_{2,k}(15)$	Im $\gamma^{Z}_{2,k}(15)$
1	−8.949 811 305 35E−06	0
2	−3.479 035 876 70E−04	0
3	−3.560 015 286 14E−03	0
4	−8.350 117 682 48E−03	0
5	−1.413 065 450 24E−03	0
6	−4.817 773 441 34E−05	0
7	−9.356 938 500 95E−07	0
8	−7.006 520 225 51E−09	0
9	−8.701 548 441 97E−02	6.018 039 999 46E−02

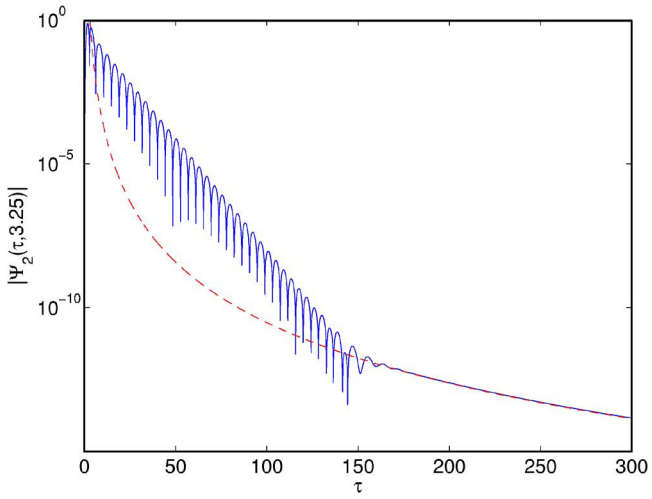

FIG. 2. (Color online) Quasinormal ringing and decay tail.

$$\left[\frac{\partial\Psi_2}{\partial\tau}+\frac{\partial\Psi_2}{\partial\rho_*}\right]\Bigg|_{\tau=0}=0, \tag{16}$$

so that the pulse starts as essentially outgoing. We place the inner boundary at $\rho_*=-175$, and adopt (10) as the boundary condition at $\rho=\rho_B=15$, with an approximation of the exact ROBC based on the compressed kernel listed in Table II.

We evolve the data until $\tau=300$, using the MacCormack predictor-corrector algorithm. (A scheme in consistent conservation form[28] when applied to a hyperbolic conservation law.) Throughout the evolution, we record the value $\Psi_2(\tau,3.25)$ of the field, that is to say, we record the history of the field in time at the fixed location $\rho=3.25$ (actually at the grid point nearest this location). Notice that the total run time is not long enough for the history $\Psi_2(\tau,3.25)$ to be influenced by reflection off of the inner boundary. The absolute value of the history is depicted as a linear-log plot in Fig. 2. It exhibits *quasinormal ringing*[24] until about $\tau=150$, and afterward a *Price tail* with the field decaying as $t^{-(2\ell+3)}=t^{-7}$.[24] This late-time behavior stems from backscatter of the outgoing packet off of the long-range potential $V^Z(\rho)$. The dashed curve $3000t^{-7}$ has been eyeballed to fit the late-time decay tail.

III. SUM-OF-POLES REPRESENTATION

A. Flatspace frequency-domain nonreflecting kernel and outgoing solution

AGH have considered nonreflecting boundary conditions (NRBC) for both 3+1 and 2+1 flatspace wave propagation, thoroughly treating both theoretical description and numerical approximation of NRBC for both scenarios.[20] For later comparison with the two gravitational scenarios, let us briefly recall the principal theoretical aspects of their work for the 3+1 scenario. To facilitate the comparison, we will use the same letters ρ, τ, and σ used for our dimensionless Schwarzschild coordinates, although for the flatspace case r, t, and s would be more standard notations. Their boundary condition for a flatspace order-ℓ multipole $\rho^{-1}\Psi_\ell$ is

$$\left(\frac{\partial\Psi_\ell}{\partial\tau}+\frac{\partial\Psi_\ell}{\partial\rho}\right)\Bigg|_{\rho=\rho_B}=\frac{1}{\rho_B}\int_0^\tau \omega_\ell^F(\tau-\tau';\rho_B)\Psi_\ell(\tau',\rho_B)\mathrm{d}\tau', \tag{17}$$

comparable with (10). The exact TDRK $\omega_\ell^F(\tau;\rho_B)$ appearing in (17) is now also a time-domain nonreflecting kernel (TDNK), and it is the inverse Laplace transform of an exact frequency-domain nonreflecting kernel (FDNK) admitting the following representation:[20]

$$\hat{\omega}_\ell^F(\sigma;\rho_B) = \sum_{k=1}^{\ell} \frac{b_{\ell,k}/\rho_B}{\sigma - b_{\ell,k}/\rho_B}, \tag{18}$$

where the $b_{\ell,k}$ are the zeros of the classical MacDonald function $K_{\ell+1/2}(z)$, a modified cylindrical Bessel function. Here the Bessel order is a half-integer, since we are considering the radial wave equation stemming from ordinary wave propagation on $3+1$ flat spacetime, and these functions have the form[29]

$$\begin{aligned}
K_{1/2}(z) &= \sqrt{\frac{\pi}{2z}} e^{-z}, \\
K_{3/2}(z) &= \sqrt{\frac{\pi}{2z}} e^{-z}\left(1 + \frac{1}{z}\right), \\
K_{5/2}(z) &= \sqrt{\frac{\pi}{2z}} e^{-z}\left(1 + \frac{3}{z} + \frac{3}{z^2}\right), \\
K_{7/2}(z) &= \sqrt{\frac{\pi}{2z}} e^{-z}\left(1 + \frac{6}{z} + \frac{15}{z^2} + \frac{15}{z^3}\right), \\
&\vdots \\
K_{\ell+1/2}(z) &= \sqrt{\frac{\pi z}{2}} (-1)^\ell z^\ell \left(\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^\ell \frac{e^{-z}}{z}.
\end{aligned} \tag{19}$$

The function $K_{\ell+1/2}(z)$ has ℓ simple zeros $\{b_{\ell,k}: k=1,\ldots,\ell\}$. When scaled by order, these zeros $(\ell+1/2)^{-1} b_{\ell,k}$ are known to accumulate on a fixed transcendental curve $\mathcal{C}$ in the left-half plane[20,30] (the numerical methods developed in Paper I take advantage of this fact). Although this accumulation is asymptotic with large order $\ell+1/2 \to \infty$, Fig. 3 shows that the agreement holds even for the lowest ℓ, at least to the eye. The curve $\mathcal{C}$ shown in Fig. 3 has parametric form[30,27]

$$z(\lambda) = -\sqrt{\lambda^2 - \lambda \tanh\lambda} \pm \mathrm{i}\sqrt{\lambda \coth\lambda - \lambda^2}, \tag{20}$$

for λ in the domain $[0,\lambda_0]$ with $\lambda_0 \simeq 1.1997$ such that $\tanh\lambda_0 = 1/\lambda_0$. In terms of the "normalized-at-infinity" outgoing solution [in the introduction of Paper II, the correspondence between $W_\ell(z)$ and $K_{\ell+1/2}(z)$ is off by a factor of $\pi/2$]

$$W_\ell(z) = \sqrt{\frac{2z}{\pi}} \exp(z) K_{\ell+1/2}(z), \tag{21}$$

we have

$$\hat{\omega}_\ell^F(\sigma;\rho_B) = \sigma\rho_B \frac{W_\ell'(\sigma\rho_B)}{W_\ell(\sigma\rho_B)} \tag{22}$$

as another expression for the flatspace frequency-domain kernel.[20] In passing, we remark that although the exact FDNK (18) is already a rational function, the technique of kernel compression still proves useful for high-ℓ FDNK, since for a given tolerance ε compression of (18) yields a numerical kernel with far fewer poles.[20]

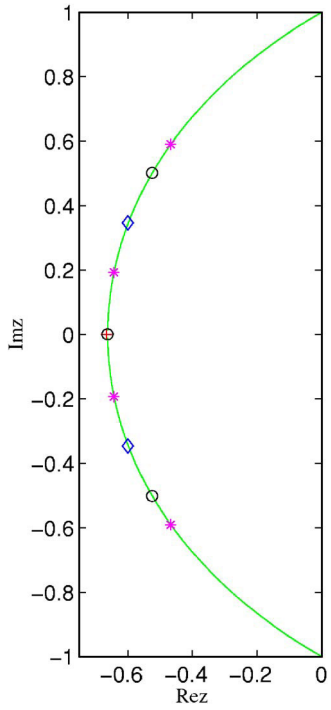

FIG. 3. (Color online) Scaled zeros of MacDonald functions. Here we plot scaled zeros $(\ell+1/2)^{-1}b_{\ell,k}$ for $\ell=1,2,3,4$. The cross is the scaled zero of $K_{1/2}(z)$, the diamonds are the scaled zeros of $K_{3/2}(z)$, the circles are the scaled zeros of $K_{5/2}(z)$, and the stars are the scaled zeros of $K_{7/2}(z)$.

B. Gravitational FDRK and outgoing solution

Let us first consider the relationship between a gravitational FDRK $\hat{\omega}_\ell(\sigma;\rho_B)$ described earlier and solutions to the formal Laplace transform

$$\frac{\mathrm{d}^2\hat{\Psi}_\ell}{\mathrm{d}\rho_*^2} - V(\rho)\hat{\Psi}_\ell = \sigma^2\hat{\Psi}_\ell \tag{23}$$

of the generic equation (2). Here we mostly just collect relevant formulas. These formulas are derived in the first section of Paper I, and the derivation presented there goes through for Regge–Wheeler case ($j=0,1,2$ considered there) as well as the Zerilli case (not considered there). Whence the formulas we consider now are valid for all cases.

We "peel off" the exponential behavior of the field by setting $\hat{\Psi}_\ell=\exp(-\sigma\rho_*)\hat{\Phi}_\ell$, whereupon finding

$$\frac{\mathrm{d}^2\hat{\Phi}_\ell}{\mathrm{d}\rho^2} + \left(-2\sigma - \frac{1}{\rho} + \frac{1-2\sigma}{\rho-1}\right)\frac{\mathrm{d}\hat{\Phi}_\ell}{\mathrm{d}\rho} - \frac{\rho^2 V(\rho)}{(\rho-1)^2}\hat{\Phi}_\ell = 0 \tag{24}$$

as the ODE satisfied by $\hat{\Phi}_\ell$. When numerically integrating (24) in various contexts, we have found it useful to work instead with $z=\sigma\rho$, re-expressing the equation as follows:

$$\frac{\mathrm{d}^2\hat{\Phi}_\ell}{\mathrm{dz}^2} + \left(-2 - \frac{1}{z} + \frac{1-2\sigma}{z-\sigma}\right)\frac{\mathrm{d}\hat{\Phi}_\ell}{\mathrm{dz}} - \frac{z^2 V(z/\sigma)}{\sigma^2(z-\sigma)^2}\hat{\Phi}_\ell = 0. \tag{25}$$

Let $W_\ell(z;\sigma)$ denote the outgoing solution to (25). This solution obeys[30]

$$W_\ell(z;\sigma) \sim \sum_{k=0}^{\infty} d_k(\sigma) z^{-k} \tag{26}$$

as $z \to \infty$, and we describe it as "normalized at infinity." Appendix B considers the recursion relations defining the $d_k^{RW}(\sigma)$ and $d_k^{Z}(\sigma)$. As described in Paper I, the flatspace solution $W_\ell(z)$ in (21) is formally $W_\ell(z) = W_\ell^{RW}(z;0)$ in terms of the Regge–Wheeler case $W_\ell^{RW}(z;\sigma)$.

In our notation $W_\ell(\sigma\rho;\sigma)$ is the outgoing solution to (24), and Paper I expresses the FDRK in terms of it as

$$\hat{\omega}_\ell(\sigma;\rho_B) = \sigma\rho_B \frac{W_\ell'(\sigma\rho_B;\sigma)}{W_\ell(\sigma\rho_B;\sigma)}, \tag{27}$$

where the prime denotes differentiation in the first slot of $W_\ell(z;\sigma)$. Since we have peeled off the exponential factor $\exp(-\sigma\rho_*)$ earlier and now work with an outgoing solution $W_\ell(\sigma\rho,\sigma)$ which is normalized at infinity, the FDRK (27) is more apt to have a well-defined inverse Laplace transform.

Paper I has described a collection of numerical methods which allow us to (i) evaluate $W_\ell(\sigma\rho_B;\sigma)$ for σ in the left-half plane and (ii) evaluate $\hat{\omega}_\ell(\mathrm{i}y;\rho_B)$ for real y. We remark that Leaver has analytically represented a solution, say the outgoing one $W_\ell^{RW}(\sigma\rho_B;\sigma)\exp(-\sigma\rho_*)$, to the frequency-domain Regge–Wheeler equation as an infinite series in Coulomb wave functions, where the expansion coefficients obey a three-term recursion relation. In fact, such series expansions hold more generally for the generalized spheroidal wave equation (essentially the confluent Heun equation).[31] The methods described in Paper I are not based on the appropriate Leaver series, rather they rely on direct integration of (25). As such they can and have now been carried over to the Zerilli case. We note that the Zerilli equation is not directly related to the confluent Heun equation; whence it is not immediately evident how to evaluate $W_\ell^{Z}(\sigma\rho_B;\sigma)$ via a Leaver series.

Roughly, our method for evaluating $W_\ell(\sigma\rho_B;\sigma)$ is as follows. For a fixed frequency σ, initial data at a large radius are obtained for (25) using the asymptotic expansion (26). Then (25) is integrated over a suitable path in the complex $z=\sigma\rho$ plane to a terminal point $z_B=\sigma\rho_B$. To convey the basic idea behind our numerical evaluation of the FDRK $\hat{\omega}_\ell(\mathrm{i}y;\rho_B)$ itself, we introduce

$$w_\ell(z;\sigma) = z\frac{W_\ell'(z;\sigma)}{W_\ell(z;\sigma)}. \tag{28}$$

Then the FDRK is $\hat{\omega}_\ell(\sigma;\rho_B) = w_\ell(\sigma\rho_B;\sigma)$, and we have from (25) that $w_\ell(z;\sigma)$ obeys the first-order nonlinear equation

$$\frac{\mathrm{d}w_\ell}{\mathrm{d}z} + \frac{w_\ell^2}{z} + \left(-2 - \frac{2}{z} + \frac{1-2\sigma}{z-\sigma}\right) w_\ell - \frac{z^3 V(z/\sigma)}{\sigma^2 (z-\sigma)^2} = 0. \tag{29}$$

We calculate values $\hat{\omega}_\ell(\mathrm{i}y;\rho_B) = w_\ell(\mathrm{i}y\rho_B;\mathrm{i}y)$ via direct numerical integration of (29). To achieve stability and high accuracy, the methods associated with both (i) and (ii) evaluations require integration over nontrivial paths in the z plane. Moreover, for technical reasons the integration employed for kernel evaluation (ii) is sometimes carried out in the complex ρ plane rather than complex z plane. Finally, we remark that to produce the origin value $\hat{\omega}_\ell(0;\rho_B)$ of the kernel, we do not integrate (29). Rather, we make use of an exact series expression, one given for the Regge–Wheeler cases in Paper I and for the Zerilli case in Appendix A.

C. Gravitational sum-of-poles representation

For the case of $j=0$ scalar perturbations Paper I has documented compelling numerical evidence indicating that the FDRK (27) admits an explicit "sum-of-poles" representation,

$$\hat{\omega}_\ell(\sigma;\rho_B)=\sum_{k=1}^{N_\ell}\frac{\alpha_{\ell,k}(\rho_B)}{\sigma-\sigma_{\ell,k}(\rho_B)}-\frac{1}{\pi}\int_0^\infty\frac{f_\ell(\chi;\rho_B)}{\sigma+\chi}\mathrm{d}\chi, \tag{30}$$

in terms of complex frequency σ. When we discussed compressed kernels before, we introduced approximate pole locations $\beta_{\ell,k}(\rho_B)$ and strengths $\gamma_{\ell,k}(\rho_B)$. We now consider N_ℓ (an integer) *physical pole locations* $\sigma_{\ell,k}(\rho_B)$ and *physical pole strengths* $\alpha_{\ell,k}(\rho_B)$, all of which lie in the left-half plane. Also appearing in (30) is a *cut profile* $f_\ell(\chi;\rho_B)$, and like the pole locations and strengths it depends on the value of ρ_B. [It may or may not be the case that an approximate location $\beta_{\ell,k}(\rho_B)$, for example, approximates a physical one $\sigma_{\ell,k}(\rho_B)$. It is the compressed kernel $\hat{\xi}_\ell(\mathrm{i}y;\rho_B)$ in whole which approximates the physical FDRK $\hat{\omega}_\ell(\mathrm{i}y;\rho_B)$ uniformly in $y\in\mathbb{R}$.] In principle the integer N_ℓ also depends on ρ_B, but turns out to be constant over sizable regions of the relevant parameter space (more comments on this point to follow). The kth pole strength and cut profile are given, respectively, by

$$\alpha_{\ell,k}(\rho_B)=-\rho_B\sigma'_{\ell,k}(\rho_B),\quad f_\ell(\chi;\rho_B)=\mathrm{Im}\;\hat{\omega}_\ell(\chi e^{i\pi};\rho_B), \tag{31}$$

with $\chi\geqslant 0$ and the prime here standing for $\partial/\partial\rho_B$ differentiation.

We will argue that the representation (30) is also valid for both $j=2$ Regge–Wheeler and Zerilli gravitational cases, and this conjecture is the main result of our paper. Note that (30) is not really a "sum of poles." Indeed, recall that in the sense of complex analysis a pole is an *isolated* singularity. Strictly speaking then, the cut integral in (30) does not correspond to a "continuous distribution of poles" (an oxymoron). Nevertheless, we shall continue to describe the representation (30) as a "sum of poles."

We stress that (30) is a representation for a *boundary* integral kernel. Its inverse Laplace transform, the TDRK $\omega_\ell(\tau;\rho_B)$, lives on the history of the spatial boundary B. Indeed, (10) makes no reference to the details of the initial data and is certainly not a spatial convolution over initial data. Moreover, the pole locations $\sigma_{\ell,k}(\rho_B)$ are not quasinormal modes. An infinite number of quasinormal modes belong to each ℓ value, and these characteristic frequencies do not depend on any particular choice of outer boundary radius ρ_B. Quasinormal modes are associated with a boundary value problem specifying that $\hat{\Psi}_\ell$ is downgoing at the horizon and outgoing at infinity. The locations $\sigma_{\ell,k}(\rho_B)$ are finite in number, and they do depend on ρ_B. They can be associated with a boundary value problem specifying that $\hat{\Psi}_\ell$ is outgoing at infinity and vanishes at ρ_B. [As such, the locations $\sigma_{\ell,k}(\rho_B)$ are analogous to the "flatspace quasinormal modes" considered in Ref. 32, a misleading terminology for our paper.] Likewise, the cut integral appearing in (30) is not the branch-cut contribution to the usual Green's function studied in the quasinormal mode problem.[33]

IV. NUMERICAL STUDY

In this section we both provide further qualitative description of the key representation (30) and justify it numerically. To argue that the representation (30) is valid for both $j=2$ Regge–Wheeler and Zerilli gravitational cases, we offer nearly the same evidence as that offered in Paper I for the case of scalar perturbations. However, here we also consider one extra numerical experiment based on the Argument principle. Our main numerical justification is to compare values $\hat{\omega}_\ell(\mathrm{i}y;\rho_B)$ of the kernel obtained via two independent approaches. These are the following:

(1) Direct integration of (29) as alluded to earlier [a process which makes no use whatsoever of the conjecture representation (30)].
(2) Approximation of the sum-of-poles representation itself (by this we do *not* mean kernel compression).

In the second approach, we "build" the kernel as

$$\hat{\omega}_\ell(\mathrm{i}y;\rho_B) \simeq \sum_{k=1}^{N_\ell} \frac{\alpha_{\ell,k}(\rho_B)+\delta\alpha_{\ell,k}(\rho_B)}{\mathrm{i}y-\sigma_{\ell,k}(\rho_B)-\delta\sigma_{\ell,k}(\rho_B)} - \frac{1}{\pi}\int_{\chi_{\min}}^{\chi_{\max}} \frac{f_\ell(\chi;\rho_B)+\delta f_\ell(\chi;\rho_B)}{\mathrm{i}y+\chi}\mathrm{d}\chi, \tag{32}$$

where the δ terms represent numerical errors and the integral over the chosen window $[\chi_{\min},\chi_{\max}]$ must be handled via numerical quadrature. We have used Simpson's rule, respectively, with 2048, 2048, 1024, 2048, 1024, 2048, 1024, 2048, 512 subintervals for $\ell=2,3,4,5,6,7,8,9,10$ (odd ℓ requires more subintervals). We stress that this latter approach to evaluation, quite unlike the first approach, requires that we numerically compute all pole locations and strengths and well as the cut profile. To locate poles, zeros in σ of $W_\ell(\sigma\rho_B;\sigma)$, we have used the secant algorithm. The $\partial/\partial\rho_B$ derivatives of the $\sigma_{\ell,k}(\rho_B)$ needed to compute the strengths $\alpha_{\ell,k}(\rho_B)$ are obtained by first building a high-order interpolating polynomial $T_{\ell,k}(1/\rho_B)$ for each $\sigma_{\ell,k}(\rho_B)$ based on Chebyshev nodes in $1/\rho_B$. Derivatives are then found via differentiation of the Chebyshev polynomial. This procedure is described in more detail in Paper I where it was used for the $j=0$ Regge–Wheeler case.

We remark that this direct approximation (32) to the sum-of-poles representation (30) is certainly not a compressed kernel. Indeed, as mentioned, this brute-force approximation of (30) typically requires thousands of poles (stemming from the numerical quadrature of the cut integral) to achieve the same error tolerance achieved by a compressed kernel comprised of ten or so poles.

Besides making the comparison outlined in the last paragraph, we also wish to provide further qualitative description of the sum-of-poles representation (30). We describe both the poles and the cut profile in more detail, and also compare the representation to the strikingly similar representation (18) of the FDNK $\hat{\omega}_\ell^F(\sigma;\rho_B)$ for a flatspace order-ℓ multipole. We have found that both gravitational kernels, $\hat{\omega}_\ell^{RW}(\sigma;\rho_B)$ and $\hat{\omega}_\ell^Z(\sigma;\rho_B)$, indeed agree with $\hat{\omega}_\ell^F(\sigma;\rho_B)$ in the $\rho_B\to\infty$ limit, although here we will focus on the Zerilli case. One certainly expects such agreement, since the Schwarzschild solution is asymptotically flat. However, the nature of this asymptotic agreement is rather interesting, and we point out some subtleties not mentioned in Paper I.

A. Pole locations and strengths

For the most part, here we give what amounts to a qualitative description. Using our method for evaluating the outgoing solution $W_\ell(\sigma\rho_B;\sigma)$, we may plot the modulus $|W_\ell(\sigma\rho_B;\sigma)|$ in order to suggest rough values for zeros (that is, roots) of the function. Provided such a zero is simple, it will correspond to a pole appearing in the representation (30). Over the parameter space $\rho_B\geqslant 15$ and $\ell=2,3,\ldots,10$, and for both Zerilli and $j=2$ Regge–Wheeler cases, we have found that the number N_ℓ of zeros $\sigma_{\ell,k}(\rho_B)$ is as follows: $N_2=2$, $N_3=4=N_4$, $N_5=6=N_6$, $N_7=8=N_8$, $N_9=10=N_{10}$. For a fixed choice of ℓ and ρ_B, these zeros form a crescent pattern in the left-half σ plane.

For example, Fig. 4 depicts the modulus $|W_3^Z(\sigma 15;\sigma)|$ in the indicated region of the left-half σ plane. Four zeros appear to be evident in the figure, and in order to further explore whether or not they are indeed zeros, we appeal to the Argument principle. We focus on the two upper locations shown closer up in Fig. 5. Let $h(\sigma)=W_3^Z(\sigma 15;\sigma)$ represent our numerically computed function. [Due to small errors in the asymptotic expansion (26) used to generate initial data for an evaluation based on integrating (25), $h(\sigma)$ will actually represent the product of $W_3^Z(\sigma 15;\sigma)$ and an analytic function of σ which slowly varies over the region of interest. However, Paper I showed that the choice of integration path in the $z=\sigma\rho$ plane results in exponential suppression of the second solution to (25), and absolute differences in the zero *locations* of $h(\sigma)$ and those of $W_3^Z(\sigma 15;\sigma)$ are of size 10^{-13} in modulus.] We numerically compute

$$\frac{1}{2\pi\mathrm{i}}\oint_{\text{square}} \frac{h'(\sigma)}{h(\sigma)}\mathrm{d}\sigma \simeq 1.999\,732 - \mathrm{i}4.185\,506\times 10^{-5} \tag{33}$$

over the square (running in the counterclockwise sense) shown in Fig. 5. On each side of the square we have introduced 1024 subintervals, and used the trapezoid rule. Since we are unable to numerically evaluate $h'(\sigma)$ directly, we approximate this derivative using difference quotients (this requires two extra function evaluations beyond the corners). Using a sequence of discretizations, we have confirmed that the integral convergences to 2 at a second-order rate, suggesting that the

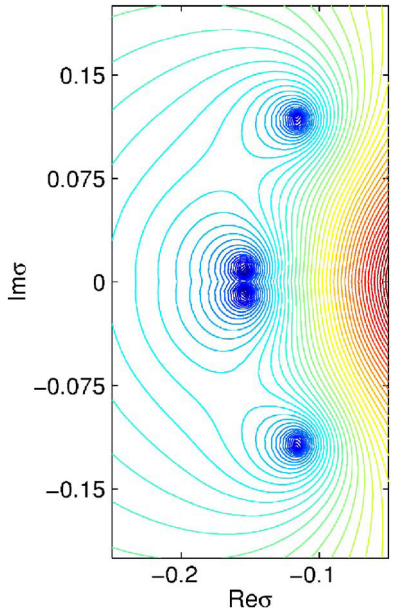

FIG. 4. (Color online) Zeros $\{\sigma^Z_{3,k}(15):1\leqslant k\leqslant 4\}$ in frequency of $W^Z_3(\sigma 15;\sigma)$. The contour lines are of $\log_{10}|W^Z_3(\sigma 15;\sigma)|$, with the logarithm distributing contour lines more evenly.

square indeed encloses two simple zeros. As a second example, consider the modulus $|W^Z_8(\sigma 25;\sigma)|$ plotted in Fig. 6 over the indicated region (four other zeros, conjugate to those shown, are located in the third quadrant). For the analogous line integral over the square shown (and using 2048 cells on each side for the trapezoidal integration), we find a value of $3.999\,975-\mathrm{i}5.169\,761\times 10^{-5}$, suggesting four simple zeros.

As with the scalar case, we find for the Zerilli and $j=2$ Regge–Wheeler cases that the zeros $\sigma_{\ell,k}(\rho_B)$ in frequency of $W_\ell(\sigma\rho_B;\sigma)$ behave asymptotically as

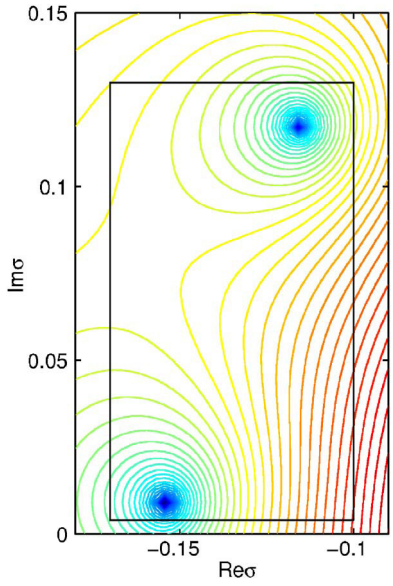

FIG. 5. (Color online) Zeros in frequency of $W^Z_3(\sigma 15;\sigma)$. The plot here is a blow-up of the one shown in Fig. 4.

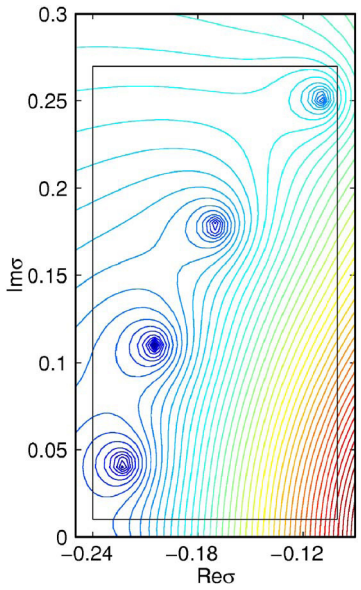

FIG. 6. (Color online) Zeros in frequency of $W_8^Z(\sigma 25;\sigma)$. The contour lines are of $\log_{10}|W_8^Z(\sigma 25;\sigma)|$, with the logarithm distributing contour lines more evenly.

$$\sigma_{\ell,k}(\rho_B) \sim b_{\ell,k}/\rho_B \tag{34}$$

in the $\rho_B \to \infty$ limit. However, let us offer several important observations in order to sharpen the precise nature of this asymptotic agreement. First, in the opposite limit as $\rho_B \to 1^+$, we do not believe N_ℓ remains constant. Indeed, we expect the phenomenon of "zero pair creation" in this limit, as described in Paper I for the scalar $j=0$ Regge–Wheeler FDRK. Although we believe that the sum-of-poles representation remains valid for ρ_B close (but not equal) to unity, description of the FDRK and implementation of ROBC both become more difficult in this limit. For these reasons, we have required $\rho_B \geqslant 15$. Second, for odd ℓ there is an "extra" zero. That is to say, for odd ℓ the number $N_\ell = \ell + 1$ of zeros $\sigma_{\ell,k}(\rho_B)$ is greater by one than the number ℓ of MacDonald zeros (provided ρ_B is large enough, otherwise N_ℓ could be a larger integer still). We will argue that this curious feature is not at odds with the asymptotic result (34). Let us focus on the Zerilli case, with the understanding that similar statements apply to the $j=2$ Regge–Wheeler case.

For even $\ell = 2,4,6,8,10$ and $\rho_B \geqslant 15$, the number of zeros $\sigma_{\ell,k}^Z(\rho_B)$ is $N_\ell = \ell$, the same as the number of $b_{\ell,k}/\rho_B$. As an illustration, Fig. 7 depicts the six zeros $\sigma_{6,k}^Z(\rho_B)$ of $W_6^Z(\sigma\rho_B;\sigma)$ as diamonds for $\rho_B = 15,16,\ldots,30$. We also plot the corresponding MacDonald–Bessel zeros $b_{6,k}/\rho_B$ as crosses. The collection $\sigma_{6,k}^Z(15)$ of zeros is the outermost crescent of diamonds, while the collection $\sigma_{6,k}^Z(30)$ is the innermost (and similarly for the crescents of Bessel crosses). The plot is clearly not at odds with the asymptotic formula (34) above.

As mentioned, for odd $\ell = 1,3,5,7,9$ and $\rho_B \geqslant 15$, the number of zeros $\sigma_{\ell,k}^Z(\rho_B)$ is $N_\ell = \ell + 1$, that is one more than the corresponding number of MacDonald–Bessel zeros. For odd ℓ there is a single MacDonald–Bessel zero which lies on the negative real axis. As with the $j=0$ Regge–Wheeler case, we find for odd ℓ that two zeros of $W_\ell^Z(\sigma\rho_B;\sigma)$ correspond to this single real MacDonald–Bessel zero. Moreover, as ρ_B gets large each of these two zeros is asymptotic to the single MacDonald–Bessel zero. This phenomenon is evident in Fig. 8, and corresponding plots for other odd ℓ are similar. The existence of an "extra" zero is at first sight troubling in light of the expected asymptotic agreement between $\hat{\omega}_\ell^Z(\mathrm{i}y;\rho_B)$ and $\hat{\omega}_\ell^F(\mathrm{i}y;\rho_B)$. However, we argue in the following that the pole and cut contributions to the gravitational FDRK in tandem do yield the correct asymptotic agreement.

So far we have only considered locations $\sigma_{\ell,k}^Z(\rho_B)$ associated with Zerilli kernels. To the eye, both Figs. 7 and 8 would be the same had we instead plotted the corresponding locations $\sigma_{\ell,k}^{RW}(\rho_B)$

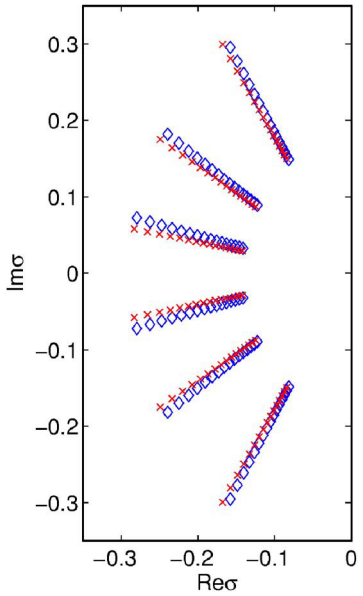

FIG. 7. (Color online) Zeros $\{\sigma^{Z}_{6,k}(\rho_B): 1 \leqslant k \leqslant 6\}$ in frequency of $W^{Z}_{6}(\sigma\rho_B;\sigma)$. Diamonds represent the zeros $\sigma_{6,k}(\rho_B)$, while the crosses represent the $b_{6,k}/\rho_B$. All zeros for $\rho_B=15,16,\ldots,30$ are shown. The outermost crescent of locations corresponds to $\rho_B=15$ and the innermost to $\rho_B=30$.

associated with $j=2$ Regge–Wheeler kernels. For the examples we have considered, $|\sigma^{Z}_{\ell,k}(\rho_B) - \sigma^{RW}_{\ell,k}(\rho_B)|$ is typically on the order of 10^{-5} to 10^{-3}. However, from Paper I results we know that this difference is seven to ten orders of magnitude larger than our knowledge of these locations. As an example, we list the two conjugate locations $\sigma_{2,k}(15)$ for $j=0$ Regge–Wheeler, $j=2$ Regge–Wheeler, and Zerilli cases. Respectively, these are

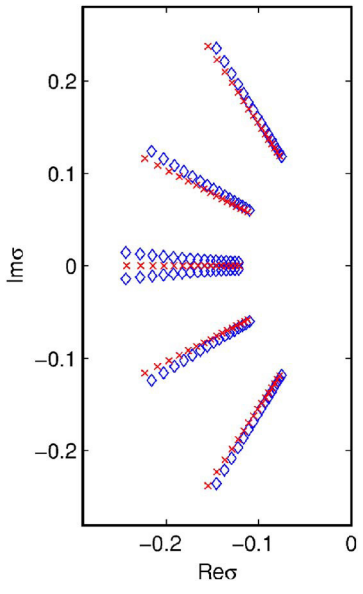

FIG. 8. (Color online) Zeros $\{\sigma^{Z}_{5,k}(\rho_B): 1 \leqslant k \leqslant 6\}$ in frequency of $W^{Z}_{5}(\sigma\rho_B;\sigma)$. Diamonds represent the zeros $\sigma^{Z}_{5,k}(\rho_B)$, while the crosses represent $b_{5,k}/\rho_B$. All zeros for $\rho_B=15,16,\ldots,30$ are shown. The outermost crescent of locations corresponds to $\rho_B=15$ and the innermost to $\rho_B=30$. For each ρ_B two diamonds correspond to the single cross lying on the negative real axis.

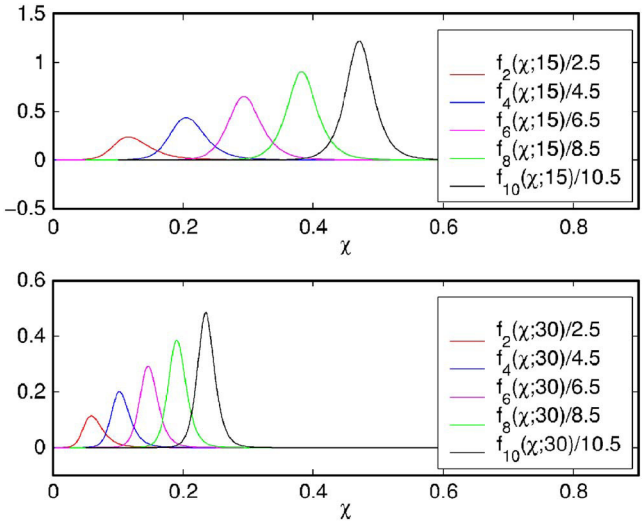

FIG. 9. (Color online) Scaled even cut profiles for Zerilli kernels. In each plot the leftmost profile is $f_2^Z(\chi;\rho_B)/2.5$ and the rightmost $f_{10}^Z(\chi;\rho_B)/10.5$.

$$-0.096\,885\,391\,711\,329 \pm i0.061\,245\,961\,499\,841.$$

$$-0.094\,779\,501\,145\,744 \pm i0.059\,927\,941\,363\,806,$$

$$-0.093\,406\,539\,086\,840 \pm i0.058\,977\,077\,340\,679.$$

These locations are all quite similar, and they may be compared to the roots $b_{2,k}/15$: $-(3/2 \pm i\sqrt{3}/2)/15 = -0.1 \pm i0.057\,735\,026\,918\,96$. In this short list the last location, say, clearly corresponds in some sense to the ninth pole location in the compressed kernel in Table II, but note that the absolute difference between the value here and the table value is more than the stated $\varepsilon = 10^{-10}$ tolerance for the compressed kernel. See the information in square brackets just after Eq. (30).

B. Cut profile

Using the type (i) numerical method from Paper I described earlier [which also returns derivative information for $W'_\ell(\sigma\rho_B;\sigma)$], we have generated Zerilli cut profiles $f_\ell^Z(\chi;\rho_B)$ for various ℓ and ρ_B. Figure 9 depicts profiles for even ℓ. To the eye the cut profiles shown match $j=2$ Regge–Wheeler profiles $f_\ell^{RW}(\chi;\rho_B)$ corresponding to the same parameter choices. However, the Zerilli and Regge–Wheeler even profiles are indeed different, as is shown by an example plot in Fig. 11. Near the peak of this plotted difference, the accuracy to which we know the Zerilli and Regge–Wheeler profiles is some ten orders of magnitude greater than the difference. Notice that these even cut profiles *weaken* as ρ_B gets larger, and we believe that the cut contribution to an even-ℓ gravitational FDRK "dies out" as ρ_B gets large. Based on our earlier claim that for an even-ℓ gravitational FDRK we have the same number $N_\ell = \ell$ of zeros $\sigma_{\ell,k}(\rho_B)$ as Bessel zeros $b_{\ell,k}/\rho_B$, and that these zeros lock on to the latter as ρ_B gets large, we conjecture that the even-ℓ kernels $\hat{\omega}_\ell^Z(iy;\rho_B)$ and $\hat{\omega}_\ell^{RW}(iy;\rho_B)$ both approach $\hat{\omega}_\ell^F(iy;\rho_B)$ uniformly in y as $\rho_B \to \infty$.

We plot odd-ℓ Zerilli cut profiles in Fig. 10. Like before with the even-ℓ profiles, to the eye these could be either Zerilli or $j=2$ Regge–Wheeler profiles. However, as is evident in the bottom plot shown in Fig. 11, these cases are different. Notice that for odd ℓ the cut profiles *strengthen* as ρ_B increases. We believe that such a strengthening profile in tandem with the two zeros closest to the real axis as a whole combine to asymptotically agree with the single MacDonald–Bessel zero $b_{\ell,0}/\rho_B$ located on the negative real axis. [For notational simplicity we have now labeled this zero

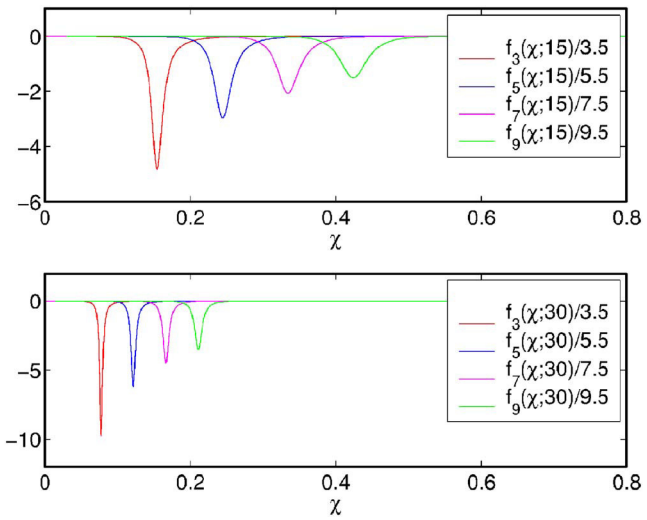

FIG. 10. (Color online) Scaled odd cut profiles for Zerilli kernels. In each plot the leftmost profile is $f_3^Z(\chi;\rho_B)/3.5$ and the rightmost $f_9^Z(\chi;\rho_B)/9.5$.

by $k=0$. Before it would have corresponded to $k=\frac{1}{2}(\ell+1)$ for odd ℓ, if $k=1,\ldots,\ell$ for the zeros $b_{\ell,k}$ of $K_{\ell+1/2}(z)$.] In other words, for odd ℓ the cut profile in effect cancels one of the zeros $\sigma_{\ell,k}^Z(\rho_B)$, so that again we have agreement between the gravitational FDRK $\hat{\omega}_\ell^Z(\mathrm{i}y;\rho_B)$ and flatspace FDNK $\hat{\omega}_\ell^F(\mathrm{i}y;\rho_B)$ uniformly in y as $\rho_B\to\infty$. While we cannot precisely describe how this cancellation of the extra zero occurs, we believe that it stems from the following two conjectures, claimed to hold as $\rho_B\to\infty$. First, the cut profile becomes sharply concentrated for χ near $-b_{\ell,0}/\rho_B$. Second,

$$-\frac{1}{\pi}\int_0^\infty f_\ell^Z(\chi;\rho_B)\mathrm{d}\chi\sim -b_{\ell,0}/\rho_B. \tag{35}$$

Preliminary numerical investigations indicate that both claims are in fact valid, but the issue deserves further study (preferably theoretical). All statements made in this paragraph also pertain to $\hat{\omega}_\ell^{RW}(\mathrm{i}y;\rho_B)$.

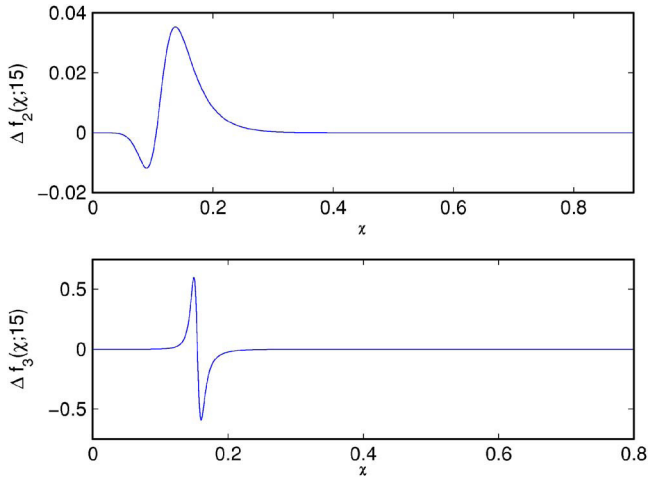

FIG. 11. (Color online) Difference between Regge–Wheeler and Zerilli cut profiles. Here we plot example differences with the notation $\Delta f_\ell(\chi;15)=f_\ell^{RW}(\chi;15)-f_\ell^Z(\chi;15)$.

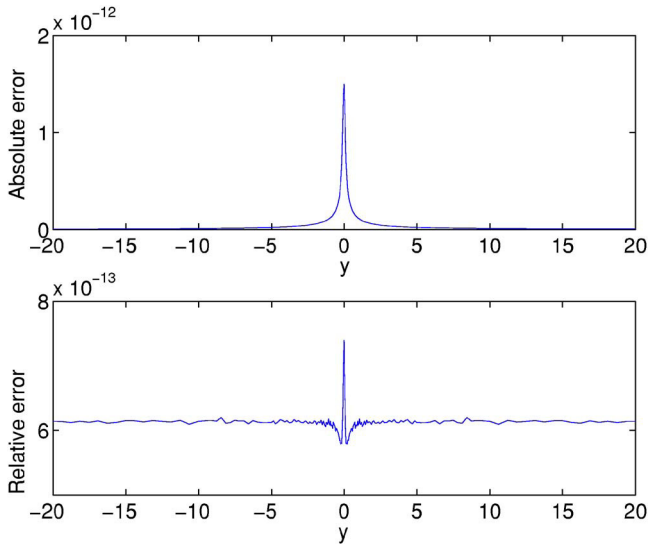

FIG. 12. (Color online) Relative and absolute numerical errors. Here we plot numerical errors corresponding to $|\Delta\hat{\omega}_2^Z(\mathrm{i}y;15)|$ and $|\Delta\hat{\omega}_2^Z(\mathrm{i}y;15)|/|\hat{\omega}_2^Z(\mathrm{i}y;15)|$ for the Zerilli case with $\ell=2$ and $\rho_B=15$.

C. Numerical validation of the sum-of-pole representation

Up to this point we have mainly given a qualitative description of what we believe are the main features of the sum-of-poles representation (30). In order to quantitatively test our representation (30), we compare the two numerical approaches for evaluating either $\hat{\omega}_\ell^Z(\mathrm{i}y;\rho_B)$ or $\hat{\omega}_\ell^{RW}(\mathrm{i}y;\rho_B)$ outlined at the beginning of this section. Figure 12 depicts such a comparison for the Zerilli case with $\ell=2$ and $\rho_B=15$. To make the plots in the figure, we have used a y grid with 5 adaptive levels, each with 32 grid points. The adaptive grid provides more resolution near the origin where we expect the largest errors. We have then generated two separate numerical arrays of values $\hat{\omega}_2^Z(\mathrm{i}y;15)$ on the y grid, the first obtained by integrating the ODE (29) and the second via the direct construction (32). Both arrays of numerical values are obtained in double precision arithmetic. Over the y grid, the plots depict the absolute error $|\Delta\hat{\omega}_2^Z(\mathrm{i}y;15)|$ and relative error $|\Delta\hat{\omega}_2^Z(\mathrm{i}y;15)|/|\hat{\omega}_2^Z(\mathrm{i}y;15)|$, and they indicate striking agreement between the two methods. We note that the maximum value of the absolute error in the top plot is 1.49×10^{-12}, and the maximum value of the relative error in the bottom plot is 7.35×10^{-13}. We can now perform the same experiment over a range of ρ_B values, say $\rho_B=15,16,\ldots,30$. For each choice of ρ_B we compute maximum values of absolute and relative error over the y grid. It turns out that the same values above corresponding to $\rho_B=15$ are the largest errors encountered.

We now perform the same experiment for each $\ell\leqslant10$ and for both $j=2$ Regge–Wheeler and Zerilli cases. That is to say, for each ℓ we compute the maximum absolute error $|\Delta\hat{\omega}_\ell(\mathrm{i}y;\rho_B)|$ and maximum relative error $|\Delta\hat{\omega}_\ell(\mathrm{i}y;\rho_B)|/|\hat{\omega}_\ell(\mathrm{i}y;\rho_B)|$ uniformly over the described y grid and all $\rho_B=15,16,\ldots,30$. For the Zerilli case we list these errors in the Table III. Errors for the $j=2$ Regge–Wheeler case are comparable.

V. CONCLUSION

For both flatspace 3+1 and flatspace 2+1 wave propagation and nonreflecting boundary conditions, AGH proved several theorems related to both the exact sum-of-poles representation for a FDNK (also a FDRK, but we have used FDNK for the special flatspace case) and its numerical approximation.[20] In particular, they proved that a FDNK admits a rational approximation as a compressed kernel, and for a given large Bessel order ν (for the 3+1 case $\nu=\ell+1/2$) and choice of ε tolerance they estimated the required number d of poles appearing in the compressed kernel. In addition to some techniques stemming from the fast multipole method, their proofs rely heavily

TABLE III. Zerilli errors.

ℓ	Max relative error	Max absolute error
2	7.35×10^{-13}	1.49×10^{-12}
3	3.63×10^{-12}	9.50×10^{-12}
4	8.63×10^{-13}	2.47×10^{-12}
5	1.27×10^{-12}	4.68×10^{-12}
6	6.17×10^{-13}	2.15×10^{-12}
7	6.93×10^{-13}	4.69×10^{-12}
8	3.03×10^{-13}	1.51×10^{-12}
9	5.10×10^{-13}	3.51×10^{-12}
10	9.71×10^{-14}	8.92×10^{-13}

on the well-understood theory of Bessel functions. In particular, AGH made extensive use of integral representations, order recursion relations, and detailed understanding of the scaling behavior for both the poles and (for the 2+1 case) the cut profile. [The 2+1 case, associated with integer-order Bessel functions, is analytically richer than the 3+1 case, as for the 2+1 case there is a continuous sector associated with the sum-of-poles representation for the FDNK. This sector is at least qualitatively similar to the one in (30).]

While the numerical evidence amassed here is extremely convincing, it does not constitute a mathematical proof that a gravitational FDRK admits the representation (30), and we hope that our numerical investigation spurs the interest of analysts capable of theoretically investigating our conjectured representation. Were (30) established theoretically, we believe approximation theorems—similar to those proved by AGH but pertaining to our gravitational ROBC—would follow. One might prove that a gravitational FDRK also admits a rational approximation as a compressed kernel, and determine the asymptotic growth of the number d of approximating poles as $\ell\to\infty, \varepsilon\to0^+$. Since numerically constructed compressed kernels have performed spectacularly in implementations of ROBC (see Paper II), we have good reason to believe that approximation theorems must hold. Such theorems are bound to involve the details of the underlying special functions. Unfortunately, relative to Bessel functions, significantly less is known about the special functions considered here, confluent Heun functions for the Regge–Wheeler cases and seemingly more exotic functions for the Zerilli case. Indeed, we are unaware of useful integral representations, and while appropriate Leaver series are certainly of formal interest, they would not seem a good platform for carrying out the requisite asymptotic analysis. While our own knowledge of modern analysis would seem not up to such theoretical investigation, we believe our results offer fertile new ground for more capable analysts.

ACKNOWLEDGMENTS

I thank C. R. Evans, C. O. Lousto, and R. H. Price for clarifying remarks about blackhole perturbation theory, and gratefully acknowledge support from NSF Grant No. PHY0514282.

APPENDIX A: ORIGIN VALUE OF THE FDRK

For the $j=0,1,2$ Regge–Wheeler cases Paper I has expressed the origin value $\hat{\omega}_\ell^{RW}(0;\rho_B)$ of the FDRK in terms of an infinite series in ρ_B^{-1}, where the expansion coefficients obey a two-term recursion relation (see Sec. 3.2.3 of that reference). All expansion coefficients are positive, and the value $\hat{\omega}_\ell^{RW}(0;\rho_B)$ can be accurately approximated in terms of two partial sums. This series was used numerically to evaluate the kernel at the origin $\sigma=0$, a frequency value for which direct integration of (29) proved problematic.

To express $\hat{\omega}_\ell^{Z}(0;\rho_B)$ for the Zerilli case of polar perturbations, we have used a similar series expression, although now the series coefficients obey a four-term rather than two-term recursion relation. We have obtained this series via the following recipe. First, we set $\sigma=0$ in (24) and use (4), thereby reaching

$$\frac{d^2\hat{\Phi}_\ell}{d\rho^2}+\left(-\frac{1}{\rho}+\frac{1}{\rho-1}\right)\frac{d\hat{\Phi}_\ell}{d\rho}-\left[\frac{8n^2(n+1)\rho^3+12n^2+18n\rho+9}{\rho^2(\rho-1)(2n\rho+3)^2}\right]\hat{\Phi}_\ell=0. \tag{A1}$$

Next, plugging the expansion

$$\hat{\Phi}_\ell=\sum_{k=0}^{\infty}a_k\rho^{-(\ell+k)} \tag{A2}$$

into (A1), assuming $a_0=1$, and balancing terms, we find the recursion relation

$$\beta_k a_{k+3}+\gamma_k a_{k+2}+\delta_k a_{k+1}+\epsilon_k a_k=0, \tag{A3}$$

where

$$\begin{aligned}\beta_k&=4n^2[(\ell+k+3)(\ell+k+4)-2(n+1)],\\ \gamma_k&=4n(\ell+k+2)[(3-n)(\ell+k+3)-n]-12n^2,\\ \delta_k&=(\ell+k+1)[(9-12n)(\ell+k+2)-12n]-18n,\\ \epsilon_k&=-9(\ell+k+1)^2.\end{aligned} \tag{A4}$$

Again $n=\frac{1}{2}(\ell-1)(\ell+2)$, and in the start-up, $\delta_{-2}=0=\epsilon_{-2}$, and $\epsilon_{-1}=0$. The origin value of the FDRK is

$$\hat{\omega}_\ell^Z(0;\rho_B)=-\sum_{k=0}^{\infty}(\ell+k)a_k\rho_B^{-(\ell+k)}\Bigg/\sum_{k=0}^{\infty}a_k\rho_B^{-(\ell+k)}. \tag{A5}$$

Despite the four-term recursion relation used to generate the series and its ρ derivative, in using (A5) we have encountered no numerical instabilities.

APPENDIX B: ASYMPTOTIC EXPANSION FOR OUTGOING SOLUTION

To generate initial data for our numerical methods based on path integration in the complex z plane (or sometimes the complex ρ plane), we use the asymptotic expansion (26) about the irregular singular point at infinity. Paper I describes this expansion for all the Regge–Wheeler cases, showing that the $d_k^{RW}(\sigma)$ obey a three-term recursion relation. For the Zerilli case, we write the expansion coefficients as $d_k^Z(\sigma)=g_k(\sigma)\sigma^k$, then finding that the $g_k(\sigma)$ obey the five-term recursion relation

$$A_k g_{k+4}+B_k g_{k+3}+C_k g_{k+2}+D_k g_{k+1}+E_k g_k=0, \tag{B1}$$

where

$$\begin{aligned}A_k&=8\sigma n^2(k+4),\\ B_k&=4n(k+3)[6\sigma+n(k+4)]-8n^2(n+1),\\ C_k&=(k+2)[18\sigma-4n^2+(12n-4n^2)(k+3)]-12n^2,\\ D_k&=(k+1)[(9-12n)(k+2)-12n]-18n,\end{aligned} \tag{B2}$$

$$E_k = -9(k+1)^2.$$

Here again $n=\frac{1}{2}(\ell-1)(\ell+2)$, and in the start-up $C_{-3}=D_{-3}=E_{-3}=0$, $D_{-2}=E_{-2}=0$, and $E_{-1}=0$. Typically, we have used fewer than ten terms in the expansion (26) to generate initial data for numerical integration, and have encountered no problems in using this expansion (despite potentially tricky issues associated with high-order recursions). We have used dimensionless coordinates and Laplace rather than Fourier transform. Adjusting for these choices, (B1) and (B2) agree with an expansion given by Chandrasekhar and Detweiler in Ref. 34.

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Fields of accelerated sources: Born in de Sitter

Jiří Bičák[a] and Pavel Krtouš[b]
Institute of Theoretical Physics, Charles University, V Holešovičkách 2, 180 00 Prague 8, Czech Republic and Max-Planck Institute for Gravitational Physics, Albert Einstein Institute, 14476 Golm, Germany

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This paper deals thoroughly with the scalar and electromagnetic fields of uniformly accelerated charges in de Sitter space–time. It gives details and makes various extensions of our Physical Review Letter from 2002. The basic properties of the classical Born solutions representing two uniformly accelerated charges in flat space–time are first summarized. The worldlines of uniformly accelerated particles in de Sitter universe are defined and described in a number of coordinate frames, some of them being of cosmological significance, the others are tied naturally to the particles. The scalar and electromagnetic fields due to the accelerated charges are constructed by using conformal relations between Minkowski and de Sitter space. The properties of the generalized "cosmological" Born solutions are analyzed and elucidated in various coordinate systems. In particular, a limiting procedure is demonstrated which brings the cosmological Born fields in de Sitter space back to the classical Born solutions in Minkowski space. In an extensive Appendix, which can be used independently of the main text, nine families of coordinate systems in de Sitter space–time are described analytically and illustrated graphically in a number of conformal diagrams. © *2005 American Institute of Physics.*
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I. INTRODUCTION

In 1969, on the 60th anniversary of Max Born's[1] first analysis of the field of a uniformly accelerated charge, Ginzburg, Nobelist in 2003, reanalyzed[2–4] this—what he called—"perpetual problem of classical physics," with the conclusion that the problem "is already clear enough not to be regarded as perpetual." Ginzburg confirmed the presence of radiation and emphasized that the vanishing of the radiation reaction force during the uniformly accelerated motion of the charge "is in no way paradoxical, in spite of the presence of radiation," since "a nonzero total energy flux through a surface surrounding a charge at a zero radiation force is exactly equal to the decrease of the field energy in the volume enclosed by this surface." Despite Ginzburg's view, however, the problem does not seem to lose its "perpetuity." A number of distinguished physicists who dealt with it before Ginzburg like Sommerfeld, Schott, von Laue, Pauli and others have, after Ginzburg, been followed by such authors as, for example, Bondi,[5] Boulware,[6] Peierls,[7] Thirring[8] and others.[9–12]

The fields and radiation patterns from uniformly accelerated general multipole particles were also studied.[13] The December 2000 issue of Annals of Physics contains three papers by Eriksen and Grøn[14–16] with numerous references on "electrodynamics of hyperbolically accelerated charges." (Yet, except for Refs. 1 and 6, the explicit citations above are not contained in Refs. 14–16.)

Space–times describing "uniformly accelerated particles or black holes" play fundamental role in general relativity. They are the only explicit solutions of Einstein's field equations known which

[a]Electronic mail: bicak@mbox.troja.mff.cuni.cz
[b]Electronic mail: pavel.krtous@mff.cuni.cz

are radiative and represent the fields of finite sources. Born fields in electrodynamics are produced by two charges moving along an "axis of symmetry" in opposite directions with uniform accelerations of the same magnitude. They have two symmetries: they are axially symmetric and symmetric with respect to the boosts along the axis of symmetry. Their general-relativistic counterparts, the boost-rotation symmetric space–times, are unique because of a theorem which roughly states that in axially symmetric, locally asymptotically flat space–times the only additional symmetry that does not exclude radiation is the boost symmetry. The boost-rotation symmetric space–times have been used in gravitational radiation theory, quantum gravity, and as test beds in numerical relativity; their general structure is described in Ref. 17, their applications and new references are given in the reviews.[18–20] One of the best known examples, the so-called C-metric, describing uniformly accelerated black holes, is the only boost-rotation symmetric solution known also for a nonvanishing cosmological constant Λ. Asymptotically this "generalized" C-metric approaches de Sitter space–time if $\Lambda>0$. It is well known from the classical work of Penrose[21] on the asymptotic properties of fields and space–times that, in contrast to asymptotically Minkowskian space–times with null (lightlike) conformal infinities $\mathcal{I}^{\pm}$, asymptotically de Sitter vacuum space–times have two disjoint conformal infinities, past and future, which are both *spacelike*. When $\Lambda<0$, as in anti-de Sitter space, the conformal infinity is timelike, and it is not disjoint. (In the analytically extended C-metrics, there is an infinite number of such infinities which can be reached by going "through" black holes like with a Reissner-Nordtröm black hole, but this is not pertinent to the present work.)

The importance of de Sitter space–time in the history of modern cosmology seems to grow steadily. The "flat" de Sitter universe became the standard cosmological model in steady state theory, more recently, as the "first approximation" of inflationary models, and today, with indications that $\Lambda>0$ in our Universe, it is an asymptote of all indefinitely expanding Friedmann-Robertson-Walker models with $\Lambda>0$. In fact much more general cosmological models with $\Lambda>0$ approach de Sitter model asymptotically in time. This manifestation of the validity of the "cosmic no-hair conjecture,"[22,23] will also be noticed in the properties of the fields analyzed in this work.

Motivated by the role of the Born solution in classical electrodynamics, by the importance of the boost-rotation symmetric space–times in general relativity, and by the relevance of de Sitter space in contemporary cosmology, we have recently generalized the Born solution for scalar and electromagnetic fields to the case of two charges uniformly accelerated in de Sitter universe.[24] In the present paper we give calculations and detailed proofs of the results and statements briefly sketched in our paper.[25] In addition, we investigate the character of the field in a number of various coordinate systems which are relevant either in a general-relativistic context or from a cosmological perspective.

The appropriate coordinates and corresponding tetrad fields were important in finding our recent results on a general asymptotic behavior of fields in the neighborhood of future infinity $\mathcal{I}^{+}$ in asymptotically de Sitter space–times.[26] In obtaining these results we were inspired by the inspection of the electromagnetic fields from uniformly accelerated charges in de Sitter universe.

It was known from the work of Penrose since late 1960s that the radiation field is "less invariantly" defined when $\mathcal{I}^{+}$ is spacelike—that it depends on the direction in which $\mathcal{I}^{+}$ is approached. However, no explicit models were available. The investigation of the test fields of accelerated charges in de Sitter universe has served as a useful example; it was then generalized also to the study of asymptotic and radiative properties of the C-metric with $\Lambda>0$ (Ref. 27), as well as to the case of the C-metric with $\Lambda<0$ when infinity is timelike.[28] (For other recent works on the "cosmological" C-metric, see, e.g., Refs. 29 and 30.) These studies led to a more general conclusion[26] that the directional pattern of gravitational and electromagnetic radiation near de Sitter-like conformal infinity has a universal character, determined by the algebraic (Petrov) type of a solution of the Maxwell/Einstein equations considered. In particular, the radiation field vanishes along directions opposite to principal null directions. Very recently analogous conclusions have been obtained for space–times with anti-de Sitter asymptotics.[31]

Since past and future infinities are spacelike in de Sitter space–time, there exist particle and

event horizons. Under the presence of the horizons, purely retarded fields (appropriately defined) become singular or even cannot be constructed at the "creation light cones," i.e., at future light cones of the "points" at $\mathcal{I}^-$ at which the sources "enter" the universe. In Ref. 24 we analyzed this phenomenon in detail and constructed smooth (outside the sources) fields involving both retarded and advanced effects. As demonstrated in Ref. 24, to be "born in de Sitter" is quite a different matter than to be "born in Minkowski." This reveals the double meaning of the second—perhaps somewhat enigmatic—part of the title of this paper.

Its plan is as follows. In order to gain an understanding of the generalized Born solution in de Sitter space it is advantageous to be familiar with some details of the classical Born solution in Minkowski space. Hence, its properties most relevant for our purpose are summarized in Sec. II. Here we also discuss why in Minkowski space problems with purely retarded fields of uniformly accelerated particles do not arise.

There exists vast literature on de Sitter space in which various types of coordinates are employed. We shall construct fields in de Sitter space by using its conformal relations to Minkowski space. For our aim coordinate systems on conformally compactified spaces and their properties will be particularly useful. These, together with several "cosmological" and "static" coordinate systems, will be described and graphically illustrated in conformal diagrams in Sec. III. What is meant by "uniformly accelerated particles in de Sitter space" is defined and the properties of the corresponding worldlines are studied in Sec. IV. For technical reasons it is more advantageous to consider particles which asymptotically start and end at the poles of coordinates covering de Sitter space, i.e., particles "born at the poles" (Sec. IV A). In order to find a direct relation between the standard form of the Born solution produced by two charges at each time located symmetrically with respect to the origin of Minkowski space and the generalized Born solution in de Sitter space, it is necessary to construct also worldlines of uniformly accelerated particles which are "born at the equator" (Sec. IV B).

With the worldlines of accelerated particles available, it is advantageous to consider coordinates in de Sitter space which are centered on these worldlines. These "accelerated coordinates" and "Robinson-Trautman coordinates" are obtained, in a constructive manner, in Sec. V.

Section VI is devoted to the fields from particles "born at the poles." Here we also study in detail their properties in various coordinate systems introduced before. The fields of particles "born at the equator" are found in Sec. VII by a simple rotation. Starting from these fields we demonstrate by means of which limiting procedure the standard Born field in Minkowski space can be regained. Finally, we conclude by few remarks in Sec. VIII.

The paper contains a rather extensive Appendix in which nine families of coordinate systems employed in the main text are described in detail, illustrated graphically, their relations are given, and corresponding metric forms as well as orthonormal tetrads are presented. We believe the Appendix can be used as a general-purpose catalogue in other studies of physics in de Sitter space–time.

II. BORN IN MINKOWSKI

It was Einstein in 1908, inspired by a letter from Planck, who first defined a uniformly accelerated motion in special relativity.[32,33] A particle is in uniformly accelerated motion if its acceleration has a fixed constant value in instantaneous rest frames of the particle. This can be stated in a covariant form (see, e.g., Ref. 34) as

$$P^{\alpha}_{\mu}\dot{a}^{\mu} = \dot{a}^{\alpha} - (a^{\mu}a_{\mu})u^{\alpha} = 0, \tag{2.1}$$

u^{α} being four-velocity, $\dot{} \equiv u^{\mu}\nabla_{\mu}$ covariant derivative with respect to proper time, $a^{\alpha}=\dot{u}^{\alpha}$ four-acceleration, and $P^{\alpha}_{\mu}=\delta^{\alpha}_{\mu}+u^{\alpha}u_{\mu}$ is the projection tensor into the hypersurface orthogonal to u^{α}. Equation (2.1) implies $\dot{a}^{\mu}a_{\mu}=0$ so that the condition of uniform acceleration guarantees that the magnitude of the four-acceleration is constant,

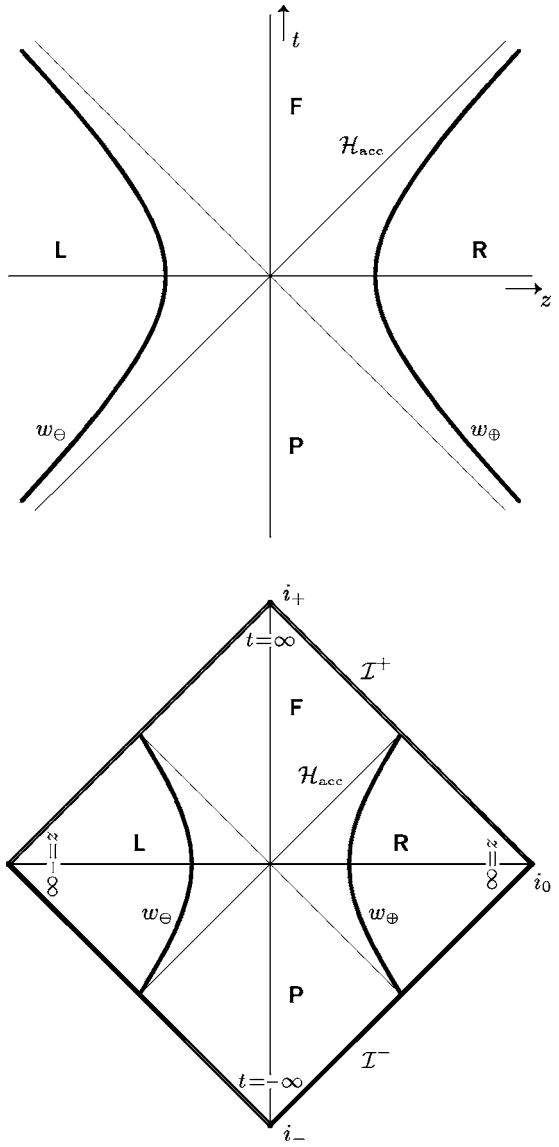

FIG. 1. A pair of uniformly accelerated charges in Minkowski space–time (with the conformal diagram below). The boost Killing vector is timelike in regions **L** and **R**; it is spacelike in **F** and **P**. The charges are causally disconnected by null hypersurfaces ("the roof") $-t^2+z^2=0$. These hypersurfaces represent the acceleration horizon for uniformly accelerated observers with respect to which the charges are at rest.

$$a_{\mathrm{M}} = \sqrt{\mathrm{a}^\mu \mathrm{a}_\mu} = \text{constant}, \tag{2.2}$$

although $\dot{\mathrm{a}}^\mu \neq 0$. Integrating Eq. (2.1) in Minkowski space–time, one finds that the worldline of a uniformly accelerated particle is a hyperbola.[35,36] One can then choose an inertial frame, in which the initial three-velocity and three-acceleration are parallel; in such frames the motion is spatially one-dimensional. It can be produced by placing a test charged particle into a homogeneous electric field with initial velocity aligned with the field. The motion along the z axis is illustrated in Fig. 1. There, in fact, *two* particles uniformly accelerated in opposite directions are shown, the one moving along the positive ($\varepsilon=+1$ for particle $w_\oplus$ in the figure) and the second one along the negative z axis ($\varepsilon=-1$ for particle $w_\ominus$); their worldlines parametrized by proper time λ_{M} are

$$z = \varepsilon b_{\mathrm{o}} \cosh\frac{\lambda_{\mathrm{M}}}{b_{\mathrm{o}}}, \quad t = b_{\mathrm{o}} \sinh\frac{\lambda_{\mathrm{M}}}{b_{\mathrm{o}}}, \quad x = y = 0, \tag{2.3}$$

or

$$z = \varepsilon\sqrt{t^2 + b_{\mathrm{o}}^2}. \tag{2.4}$$

Here we have chosen the particles to be at rest at $z=\varepsilon b_{\mathrm{o}}$ at $t=0$. Then their three-acceleration at initial moment $t=0$ is $a_{\mathrm{M}}=|\mathrm{d}^2z/\mathrm{d}t^2|=1/b_{\mathrm{o}}$. As $t\to\infty$, the three-velocity $v_{\mathrm{M}}=|\mathrm{d}z/\mathrm{d}t|=t/\sqrt{t^2+b_{\mathrm{o}}^2}$ approaches the velocity of light. This is the well-known hyperbolic motion.

The worldlines of the particles coincide with the orbits of the boost Killing vector in the t–z plane,

$$\xi_{\mathrm{boost}} = z\frac{\partial}{\partial t} + t\frac{\partial}{\partial z}. \tag{2.5}$$

These orbits, given by $-t^2+z^2=$constant, $x,y=$constant, are timelike at $-t^2+z^2>0$, but they are spacelike at $-t^2+z^2<0$. The fields (scalar, electromagnetic, higher-spin) produced by charged particles in the hyperbolic motion will have boost-rotational symmetry. They are thus static in the region $-t^2+z^2>0$—"below the roof" as introduced in Ref. 17, however, we can expect them to be radiative in the region $-t^2+z^2<0$—"above the roof."

Consider a massless scalar field Φ with the scalar charge source S satisfying, in a general four-dimensional space–time, the wave equation

$$\left[\Box - \tfrac{1}{6}R\right]\Phi = S, \tag{2.6}$$

in which $\Box \equiv g^{\mu\nu}\nabla_\mu\nabla_\nu$ is the curved-space d'Alambertian, and R is the scalar curvature (of course, in Minkowski space $R=0$). We are interested in a field due to two monopole particles with the same constant scalar charge of magnitude s moving along hyperbolae (2.3). The source at a space–time point x is thus given by

$$S = S_{\oplus} + S_{\ominus}, \quad S_{\varepsilon} = s\int \delta(x - w_{\varepsilon}(\lambda_{\mathrm{M}}))\mathrm{d}\lambda_{\mathrm{M}}, \tag{2.7}$$

where $w_{\varepsilon}(\lambda_{\mathrm{M}})$ denotes the worldlines of the particles. The resulting fields may be written as

$$\Phi = \Phi_{\oplus} + \Phi_{\ominus}, \tag{2.8}$$

where Φ_{ε} is produced by S_{ε}. The retarded and advanced fields of these sources are constructed and analyzed in detail in Ref. 17. It can be demonstrated that the retarded and advanced fields due to the particle $w_{\oplus}$ or $w_{\ominus}$ are all given by exactly *identical* expression

$$\Phi_{\mathrm{BM}} = \frac{s}{4\pi}\frac{1}{\mathcal{R}}, \tag{2.9}$$

which, however, occurs in different regions of space–time. Namely,

$$\Phi_{\mathrm{ret/adv}\ \varepsilon} = \frac{s}{4\pi}\frac{1}{\mathcal{R}}\theta\,(\varepsilon z \pm t), \tag{2.10}$$

θ being the step function and upper/lower sign is valid for retarded/advanced case. The quantity $\mathcal{R}$ in the denominator is given by

$$\mathcal{R} = \frac{1}{2b_o}((b_o^2 + t^2 - r^2)^2 + 4b_o^2 r^2 \sin^2 \vartheta)^{1/2}. \tag{2.11}$$

It has the meaning of a retarded or advanced distance—it is a spatial distance of the "observation" (field) point from the position of the source at retarded or advanced time. Here, as usual, $x=r\sin\vartheta\cos\varphi$, $y=r\sin\vartheta\sin\varphi$, $z=r\cos\vartheta$. The fields (2.9), as well as (2.10), are, at first glance, axially (rotationally) symmetric. They are also unchanged under the boost along the z axis.

The field Φ_{BM} can, in fact, be viewed as the field due to both accelerated particles, i.e., as the field corresponding to the source (2.7). Inspecting regions at which the retarded and advanced fields (2.10) are nonvanishing we discover that Φ_{BM} admits the interpretation as arising from 1-parametric combination of retarded and advanced effects from both particles,

$$\Phi_{\mathrm{BM}} = \xi\,\Phi_{\mathrm{ret}\oplus} + (1-\xi)\,\Phi_{\mathrm{adv}\oplus} + (1-\xi)\,\Phi_{\mathrm{ret}\ominus} + \xi\,\Phi_{\mathrm{adv}\ominus}, \tag{2.12}$$

where $\xi\in\mathbb{R}$ is an arbitrary constant parameter. In particular, choosing $\xi=\frac{1}{2}$, the field Φ_{BM} arises from $\frac{1}{2}(\Phi_{\mathrm{ret}}+\Phi_{\mathrm{adv}})$ from both particles. With $\xi=1$, the field can be interpreted as being caused by purely retarded effects from particle $w_\oplus$ in region $z+t>0$, and by purely advanced effects from particle $w_\ominus$ in region $z+t<0$.

The case of electrodynamics is very similar. The solution corresponding to the scalar field (2.9) was found by Born in 1909.[1] It is customarily given in cylindrical coordinates (see, e.g., Refs. 34, 37, and 14), however, in order to compare it with its generalization to de Sitter universe, it is more convenient to write it down in spherical coordinates,

$$\begin{aligned}\mathrm{F}_{\mathrm{BM}} = -\frac{e}{4\pi}\frac{1}{2b_o}\frac{1}{\mathcal{R}^3}(&-(b_o^2+t^2-r^2)\cos\vartheta\,\mathrm{d}t\wedge\mathrm{d}r + (b_o^2+t^2+r^2)r\sin\vartheta\,\mathrm{d}t\wedge\mathrm{d}\vartheta.\\ &-2tr^2\sin\vartheta\,\mathrm{d}r\wedge\mathrm{d}\vartheta\end{aligned} \tag{2.13}$$

The field can be obtained from the Liénard-Wiechert retarded and advanced potentials of two charged particles moving along hyperbolae (2.3), however, in contrast to the scalar case when charges are exactly the same, the electric charges have opposite signs. Similarly to the scalar case, the field is smooth everywhere, except for the places where the particles occur. F_{BM} can be interpreted in the precisely same way as the scalar field (2.9), i.e., as the 1-parametric combination of retarded and advanced effects from both charges, analogously to Eq. (2.12). However, in the electromagnetic case an exact form of retarded and advanced fields from a single particle is a more subtle issue. Considering that the field in the region $z+t>0$ may be interpreted as the retarded effect emitted from the charge which moves along $z>0$, it is natural to try to exclude advanced effects of the other particle by requiring the field to vanish in the region $z+t<0$ (cf. Fig. 1). The field is then not smooth at the null hypersurface $z=-t$. In the scalar case such a field does represent the pure retarded field of the single particle, cf. Eq. (2.10). However, in the electromagnetic case the field $\mathrm{F}_{\mathrm{BM}}\theta(z+t)$ corresponds to sources consisting not only of the particle but also of a "charged wall" moving along hypersurface $z+t=0$ with velocity of light.[38,5] Nevertheless, it is possible to obtain[6,39,40] a pure retarded field of the only single particle by modifying the field with a delta function valued term localized on $z+t=0$.

In de Sitter space such a modification is not feasible because the advanced fields cannot be excluded. The underlying cause is the null character of the past conformal infinity in Minkowski space–time, whereas in de Sitter space–time both future and past conformal infinities are spacelike. As a consequence, the Gauss constraint restricts the data at the spacelike past infinity, and it can be shown that a purely retarded field of a pointlike charge cannot satisfy this constraint.[24] The absence of purely retarded fields is also related to a different character of the past horizon of a particle. Since the worldline of a particle "enters" the universe through the past spacelike infinity, there exists the past particle horizon, called also the creation light cone. In de Sitter space a purely retarded electromagnetic field of a pointlike charge cannot be constructed on the whole cone. In Minkowski space–time the creation light cone of a particle moving asymptotically in the past

freely, coincides with the whole past null infinity, and thus it does not belong to the physical space–time. Eternally accelerated particles can "enter" the Minkowski space–time at a point of the past null infinity—as, for example, uniformly accelerated particles do. Like in de Sitter case, in conformal space–time the past horizon of such particles forms the null cone but, in contrast to de Sitter space, it has one generator in common with the null infinity. In physical space–time this horizon thus corresponds to a null hyperplane—for the particle $w_{\oplus}$ it is just the hyperplane $z+t=0$ (cf. Fig. 1)—and so its spatial sections are not compact. Thanks to this noncompactness the "bad" behavior of the retarded field on the horizon can be "pushed out of sight" to the infinity. We analyzed this issue in detail in Ref. 24.

III. MANY FACES OF DE SITTER

The fields due to various types of uniformly accelerated sources in de Sitter space–time found in Ref. 24, as well as those described briefly in Ref. 25, were constructed by employing the conformal relation between Minkowski and de Sitter space–times. When analyzing the worldlines of the sources in de Sitter space–time and their relation to the corresponding worldlines in Minkowski space–time we need to introduce appropriate coordinate systems. Suitable coordinates will later be used to exhibit various properties of the fields. An extensive literature exists on various types of coordinates in de Sitter space (e.g., Refs. 41 and 42); we will survey some of them in this section. In particular, we relate them to the corresponding coordinates on conformally related Minkowski spaces since this does not appear to be given elsewhere. In the next section, after identifying the worldlines of uniformly accelerated particles in de Sitter space, we shall construct coordinate systems tied to such particles, such as Rindler-type "accelerated" coordinates, or Robinson-Trautman-type coordinates in which the null cones emanating from the particles have especially simple forms. These coordinate systems will turn out to be very useful in analyzing the fields. Here, in the main text, however, only a brief description of relevant coordinates will be given. More details, including both formulas and illustrations, are relegated to the Appendix.

As it is well known from textbooks on general relativity (for a recent pedagogical exposition, see Ref. 43), de Sitter space–time, which is the solution of Einstein vacuum equations with a cosmological term $\Lambda>0$, is best visualized as the four-dimensional hyperboloid imbedded in flat five-dimensional Minkowski space. It is the homogeneous space of constant curvature equal to 4Λ. Hereafter, we use the quantity

$$\ell_\Lambda = \sqrt{\frac{3}{\Lambda}} \tag{3.1}$$

(with the dimension of length) to parametrize the radius of the curvature.

The entire de Sitter space–time can be covered by a single coordinate system—which we call standard coordinates—$\tau\in\mathbb{R}$, $\chi\in(0,\pi)$, $\vartheta\in(0,\pi)$, $\varphi\in(-\pi,\pi)$ in which the metric reads

$$g_{\mathrm{dS}} = -\,\mathrm{d}\tau^2 + \ell_\Lambda^2 \cosh^2\frac{\tau}{\ell_\Lambda}(\mathrm{d}\chi^2 + \sin^2\chi\,\mathrm{d}\omega^2), \tag{3.2}$$

$$\mathrm{d}\omega^2 = \mathrm{d}\vartheta^2 + \sin^2\vartheta\,\mathrm{d}\varphi^2. \tag{3.3}$$

Clearly, we can imagine the space–time as the time evolution of a 3-sphere which shrinks from infinite extension at $\tau\to-\infty$ to a radius ℓ_Λ, and then expands again in a time-symmetric way. Hence, we also call τ,χ the spherical cosmological coordinates. The coordinate lines are shown in the conformal diagram, Fig. 2.

In cosmology the most popular "flat" de Sitter universe is obtained by considering only a half of de Sitter hyperboloid foliated by flat three-dimensional spacelike hypersurfaces labeled by timelike coordinate $\check{\tau}\in\mathbb{R}$, cf. Fig. 3. Together with appropriate radial coordinate $\check{r}\in\mathbb{R}^+$, the coordinates, which we call flat cosmological coordinates, are given in terms of τ,χ by

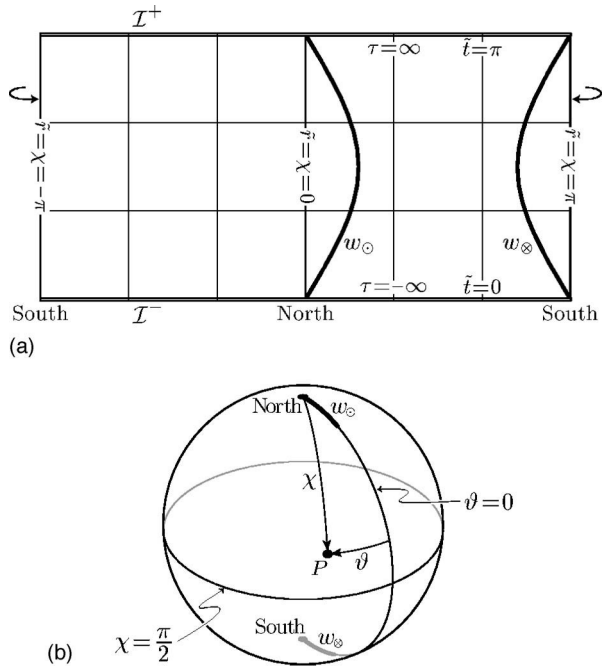

FIG. 2. The spherical cosmological coordinates and a pair of uniformly accelerated particles $w_\odot$ and $w_\otimes$ in de Sitter universe: the conformal diagram (above) and projection on the spacelike cut τ=constant in the standard cosmological spherical coordinates (angle φ suppressed). The whole de Sitter space–time could be represented by just the "right half" of the conformal diagram. For convenience, we admit negative values of radial coordinates and identify $\tilde{r}=\chi=-\pi$ and $\tilde{r}=\chi=\pi$ [see the text below Eq. (3.12) and the Appendix].

$$\check{\tau}=\ell_\Lambda \log\left(\sinh\frac{\tau}{\ell_\Lambda}+\cosh\frac{\tau}{\ell_\Lambda}\cos\chi\right), \quad \check{r}=\ell_\Lambda\frac{\sin\chi}{\cos\chi+\tanh(\tau/\ell_\Lambda)}, \tag{3.4}$$

implying the well-known "inflationary" metric

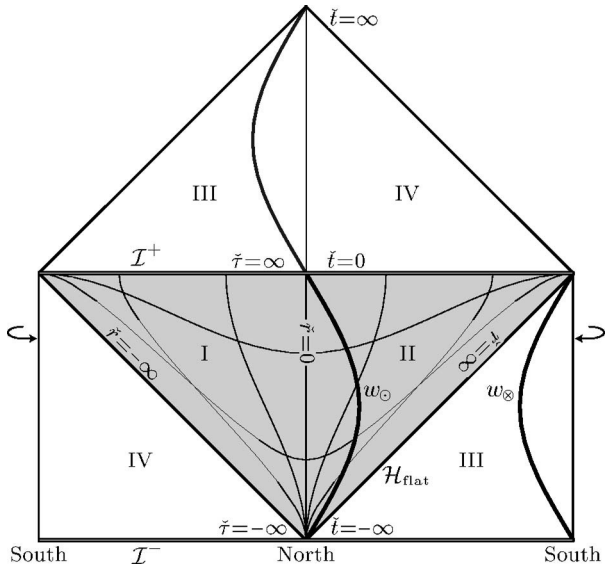

FIG. 3. The flat cosmological coordinates and particles $w_\odot, w_\otimes$ in de Sitter space and in conformally related Minkowski space. The flat cosmological coordinates cover shaded region. Its boundary, $\check{r}=\pm\infty$, represents the horizon for observers at rest in these coordinates.

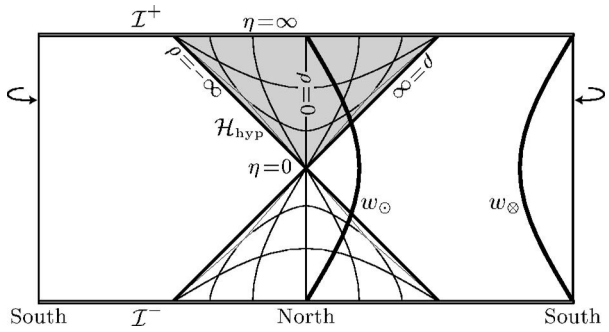

FIG. 4. The hyperbolic cosmological coordinates. They cover only the shaded region and, therefore, only a part of the worldline $w_\odot$. The horizon $\mathcal{H}_{\rm hyp}$ arises for the observers who are at rest in the hyperbolic cosmological coordinates.

$$g_{\rm dS} = -\,\mathrm{d}\check{\tau}^2 + \exp\frac{2\check{\tau}}{\ell_\Lambda}(\mathrm{d}\check{r}^2 + \check{r}^2\,\mathrm{d}\omega^2). \tag{3.5}$$

These coordinates cover only "one-half" of de Sitter space as indicated by shading in Fig. 3.

de Sitter introduced his model in what we call hyperbolic cosmological coordinates $\eta\in\mathbb{R}$, $\rho\in\mathbb{R}^+$ (see Fig. 4) related to τ,χ by

$$\cosh\frac{\eta}{\ell_\Lambda} = \cosh\frac{\tau}{\ell_\Lambda}\cos\chi, \quad \tanh\frac{\rho}{\ell_\Lambda} = \coth\frac{\tau}{\ell_\Lambda}\sin\chi. \tag{3.6}$$

The metric

$$g_{\rm dS} = -\,\mathrm{d}\eta^2 + \sinh^2\frac{\eta}{\ell_\Lambda}\left(\mathrm{d}\rho^2 + \ell_\Lambda^2\sinh^2\frac{\rho}{\ell_\Lambda}\mathrm{d}\omega^2\right) \tag{3.7}$$

shows that the time slices η=constant have the geometry of constant negative curvature, i.e., as the standard time slices in an open FRW universe.

The last commonly used coordinates in de Sitter space–time are static coordinates $T\in\mathbb{R}$, $R\in(0,\ell\Lambda)$,

$$T = \frac{\ell_\Lambda}{2}\log\left|\frac{\cos\chi+\tanh(\tau/\ell_\Lambda)}{\cos\chi-\tanh(\tau/\ell_\Lambda)}\right|, \quad R = \ell_\Lambda\cosh\frac{\tau}{\ell_\Lambda}\sin\chi, \tag{3.8}$$

covering also only a part of the universe. The metric in these coordinates reads

$$g_{\rm dS} = -\left(1-\frac{R^2}{\ell_\Lambda^2}\right)\mathrm{d}T^2 + \left(1-\frac{R^2}{\ell_\Lambda^2}\right)^{-1}\mathrm{d}R^2 + R^2\,\mathrm{d}\omega^2, \tag{3.9}$$

revealing that $\partial/\partial T$ is a timelike Killing vector in the region $0<R<\ell_\Lambda$.

Among the coordinates introduced until now only the standard coordinates $\tau,\chi,\vartheta,\varphi$ cover the whole de Sitter space–time globally. One can easily extend flat cosmological coordinates to cover (though not smoothly) the whole de Sitter hyperboloid, which will be useful in discussion of the conformally related Minkowski space–time, cf. Eq. (3.13). We shall also use extensions of the static coordinates into the whole space–time, using definitions (3.8), but allowing $R\in\mathbb{R}^+$. In regions where $R>\ell_\Lambda$ coordinates T and R interchange their character, $\partial/\partial T$ becomes a spacelike Killing vector (analogously to $\partial/\partial t$ inside a Schwarzschild black hole). However, the static coordinates T,R are not globally smooth and uniquely valued. Namely, $T\to\infty$ at the cosmological horizons $R=\ell_\Lambda$. The static coordinates, extended to the whole de Sitter space, are illustrated in Fig. 5. Here we also indicate the regions in which $\partial/\partial T$ is spacelike by bold **F** ("future") and **P** ("past"), whereas the regions in which it is timelike are denoted by **N** (containing the "north pole" $\chi=0$) and **S** (containing the "south pole" $\chi=\pi$). Hereafter, this notation will be used repeatedly.

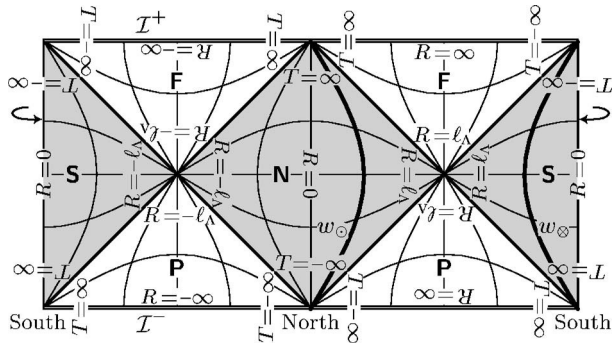

FIG. 5. The static coordinates and the worldlines of particles $w_\odot$ and $w_\otimes$. These coordinates can be defined in the whole space–time, however several coordinate patches, in diagram indicated by shaded and nonshaded regions, have to be used (cf. sections 5 and 6 of the Appendix). These regions are separated by the cosmological horizons at $R=\ell_\Lambda$, where $T=\pm\infty$. The vector $\partial/\partial T$ is a Killing vector of de Sitter space–time. It is timelike in the domains **N** and **S** (shaded regions) and spacelike in the domains **F** and **P**. The histories of both particles $w_\odot$ and $w_\otimes$ belong to the domains **N** and **S**.

The conformal structure of Minkowski and de Sitter space–times, their conformal relation, and their conformal relation to various regions of the Einstein static universe have been discussed extensively in literature (see, e.g., Refs. 44–47). The complete compactified picture of these space–times, in particular the three-dimensional diagram of the compactified Minkowski and de Sitter spaces $M^{\#}$ as parts of the Einstein universe represented by *a solid* cylinder can be found in Ref. 24. We refer the reader especially to Sec. III of Ref. 24 where we explain and illustrate the compactification in detail. In the present paper we shall confine ourselves to the two-dimensional Penrose diagrams.

The basic standard rescaled coordinates covering globally de Sitter space–time including the conformal infinity are simply related to the standard coordinates as follows:

$$\tan\frac{\tilde{t}}{2}=\exp\frac{\tau}{\ell_\Lambda},\quad \tilde{r}=\chi, \tag{3.10}$$

$\tilde{t}\in(0,\pi),\tilde{r}\in(0,\pi)$. The metric (3.2) becomes

$$g_{\mathrm{dS}}=\ell_\Lambda^2\sin^{-2}\tilde{t}\,(-\mathrm{d}\tilde{t}^2+\mathrm{d}\,\tilde{r}^2+\sin^2\tilde{r}\,\mathrm{d}\omega^2), \tag{3.11}$$

demonstrating explicitly the conformal relations of de Sitter space–time to the Einstein universe,

$$g_{\mathrm{E}}=\Omega_{\mathrm{dS}}^2\,g_{\mathrm{dS}},\quad \Omega_{\mathrm{dS}}=\sin\tilde{t}. \tag{3.12}$$

Therefore, we also call coordinates $\tilde{t},\tilde{r}$ the conformally Einstein coordinates. The conformal diagram of de Sitter space–time is illustrated in Fig. 2. The past and future infinities, $\tilde{t}=0$ and $\tilde{t}=\pi$ are spacelike, the worldlines of the north and south poles (given by the choice of the origin of the coordinates) are described by $\tilde{r}=\chi=0$ and $\tilde{r}=\chi=\pi$.

The whole de Sitter space–time could be represented by just the "right half" of Fig. 2. Indeed, it is customary to draw this half only and to consider any point in the figure as a 2-sphere, except for the poles $\tilde{r}=0,\pi$. As we shall see, the formulas relating coordinates on the conformally related de Sitter and Minkowski space–times have simpler forms if we admit negative values of the radial coordinate $\tilde{r}\in(-\pi,0)$ covering the left half of the diagram. We shall thus consider the two-dimensional diagrams as in Fig. 2 to represent the cuts of de Sitter space–time along the axis going through the origins (through north and south poles—analogously to the cuts along the z axis in E^3). The axis, i.e., the main circle of the spatial spherical section of de Sitter space–time, is typically chosen as $\vartheta=0,\pi$. Thus, in the diagram the point with $\tilde{r}=-\tilde{r}_{\mathrm{o}}<0$, $\vartheta=\vartheta_{\mathrm{o}}$, $\varphi=\varphi_{\mathrm{o}}$ is identical to that with $\tilde{r}=\tilde{r}_{\mathrm{o}}$, $\vartheta=\pi-\vartheta_{\mathrm{o}}$, and $\varphi=\varphi_{\mathrm{o}}+\pi$. We use the same convention also for other radial coordinates appearing later, as explicitly stated in the Appendix (cf. also Appendix in

Ref. 24). We admit negative radial coordinates only when describing various relations between the coordinate systems. In the expressions for the fields in the following sections only positive radial coordinates are considered.

As mentioned above, in Ref. 24 we constructed fields on de Sitter space–time by conformally transforming the fields from Minkowski space–time. Now "different Minkowski spaces" can be used in the conformal relation to de Sitter space, depending on which region of a Minkowski space is mapped onto which region of de Sitter space. Consider, for example, Minkowski space with metric g_{M} given in spherical coordinates $\check{t},\check{r},\vartheta,\varphi$. Identify it with de Sitter space by relations

$$\check{t}=\frac{\ell_\Lambda \sin\tilde{t}}{\cos\tilde{t}-\cos\tilde{r}}, \quad \check{r}=\frac{\ell_\Lambda \sin\tilde{r}}{\cos\tilde{r}-\cos\tilde{t}}, \tag{3.13}$$

the inverse relation (A11) is given in the Appendix. In the coordinates $\check{t}$, $\check{r}$, ϑ, φ the de Sitter metric (3.11) becomes

$$g_{\mathrm{dS}}=\frac{\ell_\Lambda^2}{\check{t}^2}\,(-\,\mathrm{d}\check{t}^2+\mathrm{d}\check{r}^2+\check{r}^2\,\mathrm{d}\omega^2), \tag{3.14}$$

so that

$$g_{\mathrm{dS}}=\Omega_{\check{\mathrm{M}}}^2 g_{\check{\mathrm{M}}}, \quad \Omega_{\check{\mathrm{M}}}=\frac{\ell_\Lambda}{\check{t}}. \tag{3.15}$$

The coordinates $\check{t}$, $\check{r}$, ϑ, φ can, of course, be used in both de Sitter and Minkowski spaces. Figure 3 illustrates the coordinate lines. It also shows how four regions I, II, III, and IV of Minkowski space are mapped onto four regions of de Sitter space by relations (3.13). We call $\check{t}$, $\check{r}$ rescaled flat cosmological coordinates since their radial coordinate $\check{r}$ coincides with that of the flat cosmological coordinates (3.4) and the time coordinate is simply related to $\check{\tau}$ as

$$\check{t}=-\,\ell_\Lambda \exp(-\,\check{\tau}/\ell_\Lambda). \tag{3.16}$$

The caron or the check (still better "háček") "$\vee$" formed by cosmological horizon at $\check{t}=\pm\infty$ in de Sitter space (cf. Fig. 3) inspired our notation of these coordinates. It is possible to introduce analogously the coordinates $\hat{t}$, $\hat{r}$ given in the Appendix, Eqs. (A39) and (A40), that cover nicely the past conformal infinity but are not smooth at the cosmological horizon $\hat{t}=\pm\infty$; in this case they form the hat "$\wedge$" in the conformal diagram (see Fig. 16 in the Appendix).

From relations (3.13) it is explicitly seen why, when writing down mappings between de Sitter and Minkowski spaces and drawing the corresponding two-dimensional conformal diagrams, it is advantageous to admit negative radial coordinates. If we would restrict all radial coordinates to be non-negative, we would have to consider the second relation in Eq. (3.13) with different signs for regions III and II in de Sitter space: in III $\check{r}=\ell_\Lambda \sin\tilde{r}/(\cos\tilde{r}-\cos\tilde{t})$, but in III we would have $\check{r}=-\ell_\Lambda \sin\tilde{r}/(\cos\tilde{r}-\cos\tilde{t})$.

Another mapping of Minkowski on de Sitter space will be used to advantage in the explicit manifestation that the generalized Born solution in de Sitter space goes over to the classical solution (2.13). Instead of the mapping (3.13), consider the relations

$$t=-\,\frac{\ell_\Lambda \cos\tilde{t}}{\cos\tilde{r}+\sin\tilde{t}}, \quad r=\frac{\ell_\Lambda \sin\tilde{r}}{\cos\tilde{r}+\sin\tilde{t}} \tag{3.17}$$

[see Eq. (A17) for the inverse mapping], which turn the metric (3.11) into

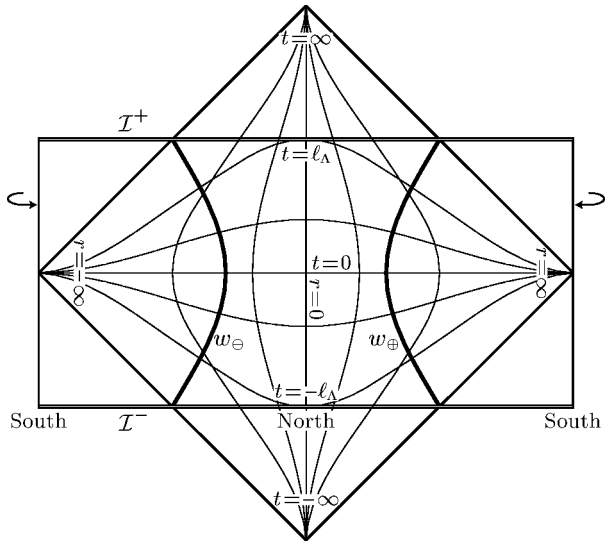

FIG. 6. The conformally Minkowski coordinates. They cover the whole conformally related Minkowski space but only a part of corresponding de Sitter space. This Minkowski space is related to that in Fig. 3 by a shift "downwards" by $\pi/2$ in the direction of the conformally Einstein coordinate $\tilde{\tau}$.

$$g_{\mathrm{dS}} = \left(\frac{2\ell_\Lambda^2}{\ell_\Lambda^2 - t^2 + r^2}\right)^2 (-\,\mathrm{d}t^2 + \mathrm{d}r^2 + r^2\,\mathrm{d}\omega^2). \tag{3.18}$$

We again obtain the de Sitter metric in the form explicitly conformal to the Minkowski metric with, however, a different conformal factor from that in Eq. (3.15),

$$g_{\mathrm{dS}} = \Omega_{\mathrm{M}}^2 g_{\mathrm{M}}, \quad \Omega_{\mathrm{M}} = \frac{2\ell_\Lambda^2}{\ell_\Lambda^2 - t^2 + r^2}. \tag{3.19}$$

[For the use of the de Sitter metric in "atypical" form (3.18) in the work on the domain wall space–times, see Ref. 48). The relation of Minkowski space to de Sitter space based on the mapping (3.17) is illustrated in Fig. 6. Clearly, the Minkowski space in this figure is shifted "downwards" by $\pi/2$ in $\tilde{\tau}$ coordinate, as compared with Minkowski space in Fig. 3. Indeed, replacing $\tilde{\tau}$ by $\tilde{\tau}+\pi/2$ in Eq. (3.13), we get $\check{t}=t$, $\check{r}=r$ with t, r given by Eq. (3.17). Since coordinates t, r, ϑ, φ are not connected directly with any cosmological model and correspond to Minkowski space "centered" on de Sitter space (Fig. 6), we just call them conformally Minkowski coordinates.

In Ref. 24 still another Minkowski space is related to de Sitter space—one which is shifted "downward" in $\tilde{\tau}$ coordinate by another $\pi/2$. As mentioned below Eq. (3.16), the cosmological horizon forms hat "$\wedge$" in this case and the corresponding coordinates are accordingly denoted as $\hat{t}$, $\hat{r}$. They are given explicitly in section 3 of the Appendix and Fig. 16.

The three sets of coordinates $\check{t}$, $\check{r}$, t, r, and $\hat{t}$, $\hat{r}$ (with the same ϑ, φ) relating naturally "three" Minkowski spaces to de Sitter space are suitable for different purposes. The third set describes conveniently the past infinity of de Sitter space—that is why it was used extensively in Ref. 24 where we were interested in how the sources enter (are "born in") de Sitter universe. The second set will be needed in Sec. VII for exhibiting the flat-space limit of the generalized Born solution. The first set describes nicely the future infinity and will be employed when analyzing radiative properties of the fields.

With all the coordinates discussed above, corresponding double null coordinates can be associated; some of them will also be used in the following. Their more detailed description and illustration is presented in section 10 of the Appendix.

Before concluding this section let us notice that the observers which are at rest in cosmological coordinate systems τ, χ, $\check{\tau}$, $\check{r}$, and η, ρ move along the geodesics with proper time τ, $\check{\tau}$, and η respectively. These geodesics are also the orbits of the conformal Killing vectors. Indeed, the symmetries of Minkowski space–time and of the Einstein universe become conformal symmetries in conformally related de Sitter space–time. In particular, we shall employ the fact that since $\partial/\partial\check{t}$ and $\partial/\partial t$ are timelike Killing vectors in Minkowski space–time and $\partial/\partial\tilde{t}$ is a timelike Killing vector in the Einstein universe, the vectors

$$\frac{\partial}{\partial\tilde{t}}, \quad \frac{\partial}{\partial\check{t}}, \quad \text{and} \quad \frac{\partial}{\partial t} \tag{3.20}$$

are timelike conformal Killing vectors in de Sitter space–time. As mentioned below Eq. (3.9), $\partial/\partial T$ is a Killing vector which is timelike for $|R|<\ell_\Lambda$.

IV. UNIFORMLY ACCELERATED PARTICLES IN DE SITTER

A. Particles born at the poles

In Sec. II we defined uniformly accelerated motion in Minkowski space–time. However, the formulas given there, being in covariant forms, remain valid in de Sitter space–time. As explained in Ref. 24 in detail, a simple way of obtaining a worldline of a uniformly accelerated particle in de Sitter space–time is to consider a suitable particle moving with a *uniform velocity* in Minkowski space–time and use the conformal relation between the spaces.

Consider a particle moving with a constant velocity of magnitude

$$v_{\check{M}} = \tanh\alpha_o = \text{constant}, \tag{4.1}$$

such that for $\alpha_o>0$ it moves in a negative direction along the $\check{z}$ axis of the inertial frame in Minkowski space $\check{M}$ with coordinates $\check{t}$, $\check{r}$, ϑ, φ and passes through $\check{r}=0$ at $\check{t}=0$,

$$\check{t} = \lambda_{\check{M}}\cosh\alpha_o, \quad \check{r} = -\lambda_{\check{M}}\sinh\alpha_o, \quad \vartheta = 0. \tag{4.2}$$

Substituting into transformation (A11), we find

$$\tilde{t} = \arctan\left(-2\ell_\Lambda\frac{\lambda_{\check{M}}\cosh\alpha_o}{\lambda_{\check{M}}^2-\ell_\Lambda^2}\right), \quad \tilde{r} = \arctan\left(-2\ell_\Lambda\frac{\lambda_{\check{M}}\sinh\alpha_o}{\lambda_{\check{M}}^2+\ell_\Lambda^2}\right), \tag{4.3}$$

or expressing Minkowski proper time $\lambda_{\check{M}}$ in terms of the proper time of de Sitter space–time,

$$\lambda_{\check{M}} = \mp\,\ell_\Lambda\exp(\mp(\cosh\alpha_o)\lambda_{dS}/\ell_\Lambda), \tag{4.4}$$

we obtain

$$\tilde{t} = \operatorname{arccot}\left(-\frac{\sinh((\cosh\alpha_o)\lambda_{dS}/\ell_\Lambda)}{\cosh\alpha_o}\right), \quad \tilde{r} = \operatorname{arccot}\left(\pm\frac{\cosh((\cosh\alpha_o)\lambda_{dS}/\ell_\Lambda)}{\sinh\alpha_o}\right), \quad \vartheta = 0. \tag{4.5}$$

Here $\lambda_{dS}\in\mathbb{R}$, arccot takes values such that $\tilde{t}\in(0,\pi)$ and $\tilde{r}\in(0,\pi)$ for $\alpha_o>0$, or $\tilde{r}\in(-\pi,0)$ for $\alpha_o<0$. Upper sign is valid for the particle starting and ending with $\tilde{r}=0$ (particle $w_\odot$ in Fig. 7), lower sign for the particle starting and ending at $\tilde{r}=\pi$ (particle $w_\otimes$ in Fig. 7).

One can make sure by direct calculations of the four-acceleration (for its simplest form in the static coordinates, see below) that these worldlines describe the uniformly accelerated motion as defined in Sec. II, the magnitude of the acceleration being

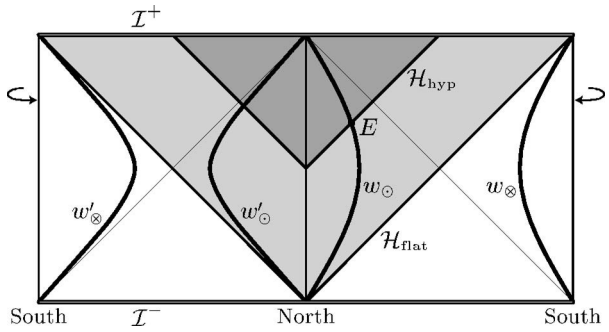

FIG. 7. The worldlines of uniformly accelerated charges. The particles $w_\odot$ and $w'_\odot$ start and end at the "north pole," $w_\otimes, w'_\otimes$ start and end at the south pole. Particles $w'_\odot, w'_\otimes$ have a higher magnitude of acceleration $a_{\rm dS}$ than particles $w_\odot, w_\otimes$. They are characterized by a negative parameter $\alpha_{\rm o}$, whereas particles $w_\odot, w_\otimes$ have a positive $\alpha_{\rm o}$.

$$a_{\rm dS} = \sqrt{\mathrm{a}^\mu \mathrm{a}_\mu} = |\ell_\Lambda^{-1} \sinh \alpha_{\rm o}|. \tag{4.6}$$

Since de Sitter universe represents the asymptotic state of all three types of indefinitely expanding FRW models with $\Lambda > 0$, it is of interest to find out the form of these worldlines in the three types of cosmological frames—spherical, flat, and hyperbolic—introduced in Sec. II.

In terms of cosmological spherical coordinates the worldlines are given by

$$\tau = \ell_\Lambda \,\mathrm{arcsinh}\left(\frac{\sinh((\cosh \alpha_{\rm o})\lambda_{\rm dS}/\ell_\Lambda)}{\cosh \alpha_{\rm o}}\right), \quad \chi = \mathrm{arccot}\left(\pm\frac{\cosh((\cosh \alpha_{\rm o})\lambda_{\rm dS}/\ell_\Lambda)}{\sinh \alpha_{\rm o}}\right), \quad \vartheta = 0. \tag{4.7}$$

In flat cosmological coordinates, which cover only half of de Sitter space, we obtain just particle $w_\odot$ described by the worldline

$$\check{\tau} = \lambda_{\rm dS} \cosh \alpha_{\rm o} - \ell_\Lambda \log \cosh \alpha_{\rm o}, \quad \check{r} = \ell_\Lambda \sinh \alpha_{\rm o} \exp(-(\cosh \alpha_{\rm o})\lambda_{\rm dS}/\ell_\Lambda). \tag{4.8}$$

Finally, in hyperbolic cosmological coordinates, which are also not global, we obtain again one particle's worldline only given in terms of its proper time as

$$\eta = \ell_\Lambda \,\mathrm{arccosh}\,\frac{\cosh((\cosh \alpha_{\rm o})\lambda_{\rm dS}/\ell_\Lambda)}{\cosh \alpha_{\rm o}}, \quad \rho = \ell_\Lambda \,\mathrm{arccoth}\frac{\sinh((\cosh \alpha_{\rm o})\lambda_{\rm dS}/\ell_\Lambda)}{\sinh \alpha_{\rm o}}. \tag{4.9}$$

These formulas have no meaning for $|\lambda_{\rm dS}/\ell_\Lambda \cosh \alpha_{\rm o}| < |\alpha_{\rm o}|$ where the inverse hyperbolic functions are not defined. This corresponds to the fact that for such $\lambda_{\rm dS}$ the particle occurs in the region where the hyperbolic cosmological coordinates are not defined (cf. Fig. 4). Excluding the proper time we find the worldlines to be given by remarkably simple formulas in the three systems of the cosmological coordinates,

(a) spherical,

$$\sin \chi = \pm \tanh \alpha_{\rm o} / \cosh \frac{\tau}{\ell_\Lambda}; \tag{4.10}$$

(b) flat,

$$\frac{\check{r}}{\ell_\Lambda} = \tanh \alpha_{\rm o} / \exp \frac{\check{\tau}}{\ell_\Lambda}; \tag{4.11}$$

(c) hyperbolic,

$$\sinh\frac{\rho}{\ell_\Lambda}=\tanh\alpha_o\big/\sinh\frac{\eta}{\ell_\Lambda}. \tag{4.12}$$

It is of interest to see what are the physical radial velocities which will be observed by three types of the fundamental cosmological observers, i.e., those with fixed χ, $\check{r}$, and ρ, respectively, whose proper times are τ, $\check{\tau}$, and η, respectively. Such velocities can be defined by the covariant expression

$$v_{\text{obs}}=\mathrm{u}_\alpha\,\mathrm{e}_1^\alpha\frac{\mathrm{d}\lambda_{\text{dS}}}{\mathrm{d}\lambda_{\text{obs}}}, \tag{4.13}$$

where u^α is the particle's four-velocity, λ_{dS} its proper time, e_1^α is the unit spacelike vector in the direction of the radial coordinate $x^1=\chi$, $\check{r}$, and ρ, respectively, i.e., in directions $\partial/\partial\chi$, $\partial/\partial\check{r}$, and $\partial/\partial\rho$, and λ_{obs} is the proper time of an observer, i.e., τ, $\check{\tau}$, or η, respectively. Since all three cosmological metrics are diagonal the expression (4.13) takes on the form

$$v_{\text{obs}}=\sqrt{g_{\text{dS}11}}\frac{dx^1}{d\lambda_{\text{obs}}}. \tag{4.14}$$

The results are of interest,

$$v_{\text{obs}(\chi)}=\mp\frac{\operatorname{sign}\tau\sinh\alpha_o}{\sqrt{\sinh^2\alpha_o+\coth^2(\tau/\ell_\Lambda)}}, \tag{4.15}$$

$$v_{\text{obs}(\check{r})}=-\tanh\alpha_o, \tag{4.16}$$

$$v_{\text{obs}(\rho)}=-\frac{\sinh\alpha_o}{\sqrt{\sinh^2\alpha_o+\tanh^2(\eta/\ell_\Lambda)}}. \tag{4.17}$$

Consider first the picture in spherical cosmological coordinates, Eqs. (4.7) and (4.10). Only in this frame both particles are present. They start asymptotically at antipodes of the spatial section of de Sitter space at $\mathcal{I}^-(\tau\to-\infty)$ and move one towards the other until $\tau=0$, the moment of maximal contraction of de Sitter space ("the neck" of de Sitter hyperboloid), when they stop, $v_{\text{obs}(\chi)}=0$. Then they move, in a time-symmetric manner, apart from each other until they reach future infinity asymptotically at the antipodes from which they started. In contrast to the flat space case, the particles do not approach the velocity of light in this global spherical cosmological coordinate system, the asymptotical magnitude of their velocity being equal to $|\tanh\alpha_o|$ [cf. Eq. (4.15)]. Hence, curiously enough, the particles approach the antipodes asymptotically with a finite nonvanishing velocity (for an intuitive insight into this effect, see below).

Although the particles $w_\odot$ and $w_\otimes$ do not approach infinities with velocity of light, they *are* causally disconnected as the analogous pair of particles in Minkowski space (cf. Fig. 1 and Fig. 7). No retarded or advanced effects from the particle $w_\odot$ can reach the particle $w_\otimes$ and vice versa.

Next, consider flat and hyperbolic observers. As seen from Eq. (4.16), with respect to the flat cosmological coordinates the particle $w_\odot$ moves with the same velocity $|\tanh\alpha_o|$ all the time. And the same velocity is asymptotically, at $\eta\to\infty$, reached by this particle in the hyperbolic cosmological coordinates. The magnitude of the asymptotic values of the velocity at $\mathcal{I}^+$ is, in fact, equal to the velocity (4.1) of the particle in Minkowski space from which we constructed uniformly accelerated worldlines by a conformal transformation. The identity of all these velocities is understandable, the magnitude of the velocity with respect to an observer can be determined by projecting the particle's four-velocity on the observer's four-velocity, i.e., by the angle between these directions. In de Sitter space all three types of cosmological observers reach $\mathcal{I}^+$ with the same four-velocity; moreover, this four-velocity is at $\mathcal{I}^+$ identical to the four-velocity of observers

at rest in conformally related Minkowski space. But a conformal transformation preserves the angles and thus, the velocities with respect to the three types of cosmological observers in de Sitter space and the velocity in the conformally related Minkowski space must all be equal—given by the "Lorentzian" angle α_o.

It is worth noticing yet what is the *initial* velocity of the particle $w_\odot$ in hyperbolic cosmological coordinates. Regarding Fig. 4 we have $\eta\to-\infty$, $\rho\to 0$ at the "starting point" of the particle at $\mathcal{I}^-$. From Eq. (4.17) we get $v_{\mathrm{obs}(\rho)}\to-\tanh\alpha_o$ which in the magnitude is the same as in spherical cosmological coordinates but has opposite sign since the particle moves in the direction of increasing negative ρ. More interesting is how the particle enters the upper region of the hyperbolic coordinates. Figure 4 suggests that its velocity must approach the velocity of light since at this boundary the fundamental observers of the hyperbolic cosmological frame themselves approach the velocity of light. Indeed, at this boundary $\eta=0,\rho=\infty$, and the expression (4.17) implies $v_{\mathrm{obs}(\rho)}\to-1$.

By far the simplest description of the particles is obtained in the static coordinates T,R. Using, for example, the relation $R=\ell_\Lambda\sin\tilde{r}/\sin\tilde{t}$ [cf. Eqs. (A64) and (A77)], and substituting from Eq. (4.5), we find that the worldlines of both particles $w_\odot$ and $w_\otimes$ are given by remarkably lucid forms

$$T=\lambda_{\mathrm{dS}}\cosh\alpha_o=\frac{\lambda_{\mathrm{dS}}}{\sqrt{1-R_o^2/\ell_\Lambda^2}},\quad R=\ell_\Lambda\tanh\alpha_o\equiv R_o. \tag{4.18}$$

These expressions imply that the four-acceleration $\mathrm{a}^\alpha=\mathrm{u}^\mu\nabla_\mu\mathrm{u}^\alpha$ is simply

$$\mathrm{a}=-\frac{R_o}{\ell_\Lambda^2}\frac{\partial}{\partial R}=-\frac{1}{\ell_\Lambda}\tanh\alpha_o\frac{\partial}{\partial R}=a_o\mathrm{e}_R, \tag{4.19}$$

where e_R is a unit spatial vector in the direction $\partial/\partial R$ of the static radial coordinate R, and we introduced constant

$$a_o=-\ell_\Lambda^{-1}\sinh\alpha_o=-\frac{R_o/\ell_\Lambda^2}{\sqrt{1-R_o^2/\ell_\Lambda^2}} \tag{4.20}$$

which represents the "oriented" value of the acceleration of the particles.

We thus find the uniformly accelerated particles in de Sitter space–time to be at rest in the static coordinates at fixed values $R=R_o$ of the radial coordinate. Two charges moving along the orbits of the boost Killing vector (2.5) in Minkowski space are at rest in the Rindler coordinate system and have a constant distance from the space–time origin, as measured along the slices orthogonal to the Killing vector. Similarly, we see that the worldlines $w_\odot$ and $w_\otimes$ are the orbits of the static Killing vector $\partial/\partial T$ of de Sitter space. The particle $w_\odot$ (respectively, $w_\otimes$) has, as measured at fixed T, a constant proper distance from the origin $\tilde{t}=\pi/2$ $(\tau=0)$, $\tilde{r}=\chi=0$ (respectively, $\tilde{r}=\chi=\pi$). As with Rindler coordinates in Minkowski space, the static coordinates cover only a "half" of de Sitter space. In the other half the Killing vector becomes spacelike. Owing to "cosmic repulsion" caused by the presence of Λ, fundamental cosmological observes moving along geodesics χ,ϑ,φ constant are "repelled" one from the others. Their initial implosion starting at $\tau\to-\infty$ is stopped at $\tau=0$ and changes into expansion. Clearly, a particle with constant $R=R_o$—hence a constant proper distance from the particle at $R=0=\chi$—must be accelerated towards that "central" particle.

In Eq. (4.20) we have denoted the radial tetrad component of the acceleration in the static coordinates by a_o; notice that, in contrast to the magnitude of the acceleration $a_{\mathrm{dS}}=|a_o|$ [cf. Eq. (4.6)], a_o can be negative as, in fact, it is the case with both particles $w_\odot$ and $w_\otimes$, assuming that the static radial coordinate of the particles is positive, $R=R_o>0$. Geometrically, the four-vectors of the acceleration of the particles point in opposite directions—towards $\chi=0$, the other towards $\chi=\pi$. Since, however, one needs two sets of the static coordinates to cover both particles, and the radial coordinate R increases from both $\chi=0$ and $\chi=\pi$ worldlines (cf. Fig. 5), the accelerations of both particles point in the direction of decreasing R's and is thus negative. All the particles we are

considering perform one-dimensional motion only, hence we use for the description of their worldlines the same convention as for the two-dimensional diagrams with time and radial coordinates—we allow the radial coordinate to take negative values. Thus, for example, consider a particle with worldline $w'_\odot$ which is a "reflection" of the worldline $w_\odot$ with respect to $\tilde{r}=\chi=0$ (see Fig. 7). The particle $w'_\odot$ moves in the region of negative $\tilde{r}$, respectively R, it has an acceleration positive, $a_o=-\ell_\Lambda^{-1}\sinh\alpha_o>0$ (i.e., $\alpha_o<0$), and its four-acceleration vector is pointing in the direction of increasing R. With our convention, the particle $w'_\odot$ is just that which moves from $\chi=0$ along the $\vartheta=\pi$ direction. This convention will be particularly useful when we shall construct worldlines of uniformly accelerated particles which start and end at the equator. Those which move in the region $\chi>\pi/2$ will have negative a_o, those moving with $\chi<\pi/2$ will have positive a_o—see Sec. IV B.

An intuitive geometrical understanding of the worldlines of uniformly accelerated particles in de Sitter space–time can be gained by considering de Sitter space as a four-dimensional hyperboloid $-Z_0^2+Z_1^2+Z_2^2+Z_3^2+Z_4^2=\ell_\Lambda^2$ in five-dimensional Minkowski space. The spherical cosmological coordinates $\tau,\chi,\vartheta,\varphi$ are then identical to the hyperspherical coordinates on this hyperboloid. The worldlines of the north and south poles, $\chi=0,\pi$, can be obtained by cutting the hyperboloid by a timelike 2-plane $\mathcal{T}_2$, given by $Z_2=Z_3=Z_4=0$. The worldlines of our uniformly accelerated particles $w_\odot$ and $w_\otimes$ then arise when the hyperboloid is cut by a timelike 2-plane $\mathcal{T}_2^*$ parallel to $\mathcal{T}_2$ at a distance $R_o=\ell_\Lambda\tanh(\alpha_o/\ell_\Lambda)$ from the origin.[43] $\mathcal{T}_2^*$ is thus given by $Z_2=R_o$, $Z_3=Z_4=0$. From the definition of the hyperspherical coordinates it follows $\vartheta=0,\pi$ and $Z_2=\ell_\Lambda\cosh(\tau/\ell_\Lambda)\sin\chi\cos\vartheta=R_o$, i.e., $\sin\chi=\pm\tanh\alpha_o/\cosh(\tau/\ell_\Lambda)$, which is just Eq. (4.10) describing $w_\odot$ and $w_\otimes$.

From this construction, the curious result mentioned above—that $w_\odot$ and $w_\otimes$ approach antipodes $\chi=0$ and $\chi=\pi$ asymptotically with a fixed speed $|\tanh\alpha_o|$ in spherical cosmological coordinates—is not so surprising: thanks to the expansion of de Sitter space–time fundamental cosmological observers with arbitrarily small $\chi=\text{constant}>0$ will, in the limit $\tau\to\infty$, eventually cross the plane $\mathcal{T}_2^*$, and thus the particle $w_\odot$; however at any finite but arbitrarily large τ there will be observers with $\chi=\text{constant}$ which are still moving towards the particle $w_\odot$. The same, of course, is true with the symmetrically located particle $w_\otimes$ and corresponding observers close to $\chi=\pi$.

B. Particles born at the equator

In the classical Born solutions both charges are, at all times, located symmetrically with respect to the origin of the Minkowski coordinates (see Fig. 1). In order to demonstrate explicitly that a limiting procedure exists in which our generalized Born's solution goes over to its classical counterpart, we shall now construct the pair of uniformly accelerated particles which are, at all times, symmetrically located with respect to the origin of the standard spherical coordinates in de Sitter space, i.e., with respect to the "north pole" at $\chi=0$. Asymptotically at $\tau\to-\infty$ these two particles both start ("are born") with the same speed at the equator, $\chi=\pi/2$, at the antipodal points $\vartheta=0$ and $\vartheta=\pi$. As the universe contracts, they both move symmetrically along the axis $\vartheta=0,\pi$, reach some limiting value χ_o at the moment of time symmetry, and accelerate back towards the equator, reaching the initial positions asymptotically at $\tau\to+\infty$. These two particles are illustrated in Fig. 8, with their worldlines denoted by $w_\oplus$ and $w_\ominus$. In Fig. 9, a snapshot at $\tau=\text{constant}$ is depicted. Comparing Fig. 8 with Fig. 7, it is evident that the particles $w_\oplus$ and $w_\ominus$ are located with respect to the point $\chi=\pi/2$, $\vartheta=0$ in exactly the same manner as the particles $w_\odot$ and $w_\otimes$ are located with respect to the pole $\chi=0$ (or, rather, as the particles $w'_\odot$, $w'_\otimes$, since we chose $w_\oplus$, $w_\ominus$ to have positive a_o in Fig. 8).

Owing to the global homogeneity of de Sitter space and the spherical geometry of its slices $\tau=\text{constant}$, the worldlines of the particles $w_\oplus$ and $w_\ominus$ can be constructed by a suitable rotation of the worldlines of the particles $w_\odot$ and $w_\otimes$. In Sec. VII the same rotation will be applied to obtain

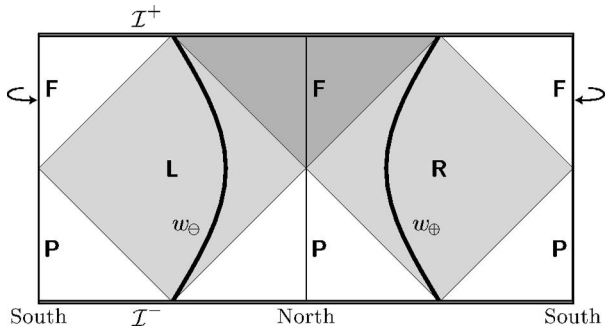

FIG. 8. The worldlines of uniformly accelerated charges located symmetrically with respect to the origin (north pole) of the standard spherical coordinates in de Sitter space. The particles "start" and "end" at the equator. They are causally disconnected as a corresponding pair in Minkowski space (cf. Fig. 1). The "oriented" value a_o of the acceleration of these particles is positive [cf. the "rotated" version of Eq. (4.20)].

the fields of these particles "born at the equator." We rotate the coordinates χ, ϑ, φ into coordinates $\bar{\chi}$, $\bar{\vartheta}$, $\bar{\varphi}$ which, as a pole, have the point $\chi=\pi/2$, $\vartheta=0$ (see Fig. 9). The relations between these coordinates follow from the spherical geometry:

$$\cos\bar{\chi}=\sin\chi\cos\vartheta,\quad \tan\bar{\vartheta}=-\tan\chi\sin\vartheta,\quad \bar{\varphi}=\varphi. \tag{4.21}$$

The new worldlines, $w_\oplus$ and $w_\ominus$, will then be given by Eqs. (4.7) in which χ, ϑ, φ are replaced by rotated coordinates $\bar{\chi}$, $\bar{\vartheta}$, $\bar{\varphi}$. Substituting for these by using relations (4.21), we find the worldlines $w_\oplus$, $w_\ominus$ in the original coordinates to be described by the expressions

$$\tau=\ell_\Lambda\,\mathrm{arcsinh}\left(\frac{\sinh((\cosh\alpha_o)\lambda_{dS}/\ell_\Lambda)}{\cosh\alpha_o}\right),\quad \chi=\pm\arctan\left(-\frac{\cosh((\cosh\alpha_o)\lambda_{dS}/\ell_\Lambda)}{\sinh\alpha_o}\right),\quad \vartheta=0, \tag{4.22}$$

with the values of arctan from $(0,\pi)$ and upper (lower) sign corresponding to the particle starting at the positive (negative) value of χ, i.e., to the particle $w_\oplus$ (or $w_\ominus$, respectively).

Excluding the proper time λ_{dS}, we arrive at simple result [cf. Eq. (4.10)]

$$\cos\chi=-\frac{\tanh\alpha_o}{\cosh(\pi/\ell_\Lambda)}. \tag{4.23}$$

As $\tau\to\pm\infty$, then indeed $|\chi|\to\pi/2$; at $\tau=0$, $|\chi|=\arccos(-\tanh\alpha_o)=\arccos(-R_o/\ell_\Lambda)$, in agreement with the "deviation" of the "original" particles $w_\odot$, $w_\otimes$ from $\chi=0$ at $\tau=0$. In the spherical rescaled coordinates, Eqs. (4.22) read

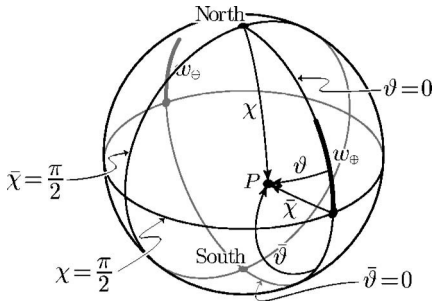

FIG. 9. The rotated spherical coordinates $\bar{\chi},\bar{\vartheta}$ on 3-sphere (the cut φ=constant). The relation between the coordinates is given in Eq. (4.21).

$$\tilde{t} = \operatorname{arccot}\left(- \frac{\sinh((\cosh \alpha_o)\lambda_{dS}/\ell_\Lambda)}{\cosh \alpha_o} \right),$$

$$\tilde{r} = \pm \operatorname{arccot}\left(- \frac{\cosh((\cosh \alpha_o)\lambda_{dS}/\ell_\Lambda)}{\sinh \alpha_o} \right), \tag{4.24}$$

$$\vartheta = 0,$$

again with the values of arctan and arccot from $(0, \pi)$. Equation (4.23) becomes

$$\cos \tilde{r} = - \tanh \alpha_o \sin \tilde{t}. \tag{4.25}$$

Although the flat (rescaled) cosmological coordinates cover only parts of the worldlines $w_\oplus$, $w_\ominus$ (see Figs. 8 and 3), we transcribe the equations above also into these frames in which the particles "emerge" at $\check{\tau}$, $\check{t} \to -\infty$ at the cosmological horizon at $\check{r} = \pm\infty$. We find

$$\frac{\check{\tau}}{\ell_\Lambda} = - \log\left(\frac{- \cosh \alpha_o}{- \sinh((\cosh \alpha_o)\lambda_{dS}/\ell_\Lambda) + \sinh \alpha_o} \right),$$

$$\frac{\check{t}}{\ell_\Lambda} = \frac{\cosh \alpha_o}{- \sinh((\cosh \alpha_o)\lambda_{dS}/\ell_\Lambda) + \sinh \alpha_o}, \tag{4.26}$$

$$\frac{\check{r}}{\ell_\Lambda} = \mp \frac{\cosh((\cosh \alpha_o)\lambda_{dS}/\ell_\Lambda)}{- \sinh((\cosh \alpha_o)\lambda_{dS}/\ell_\Lambda) + \sinh \alpha_o},$$

so that Eq. (4.25) translates into the relations

$$\begin{aligned} \check{r} &= \pm \sqrt{\ell_\Lambda^2 + \check{t}^2 - 2\ell_\Lambda \check{t} \tanh \alpha_o}, \\ \check{r} &= \pm \ell_\Lambda \sqrt{1 + 2 \tanh \alpha_o \exp(- \check{\pi}/\ell_\Lambda) + \exp(- 2\check{\pi}/\ell_\Lambda)}. \end{aligned} \tag{4.27}$$

As $\check{\tau} \to +\infty$, we have $\check{r} \to \pm \ell_\Lambda$, as it corresponds to $\chi \to \pm \pi/2$; at $\check{\tau} \to -\infty$, we get $\check{r} \to \pm\infty$—here the particles enter flat cosmological frame at the horizon (cf. Fig. 8).

The worldlines $w_\oplus$, $w_\ominus$ are situated outside the regions covered by our choice of the hyperbolic cosmological coordinates. Similarly, we get only finite parts of $w_\oplus$, $w_\ominus$ in our static coordinates. Of course, we could rotate the static coordinates to cover both particles but then we arrive at exactly the same picture as with the particles $w_\odot$, $w_\otimes$ considered above.

Our primary reason to discuss the pair $w_\oplus$, $w_\ominus$ is to demonstrate explicitly how our fields go over into the classical Born solution in the limit of vanishing Λ. For this purpose, it will be important to have available also the description of the worldlines $w_\oplus$, $w_\ominus$ in the Minkowski coordinates introduced in Eqs. (3.17). As it is obvious from Fig. 6, these coordinates cover both worldlines $w_\oplus$ and $w_\ominus$ completely. Using the relations inverse to Eqs. (3.17) given in the Appendix, Eq. (A17), we find Eqs. (4.24) to imply

$$t = b_o \sinh \frac{\lambda_M}{b_o}, \quad r = \pm b_o \cosh \frac{\lambda_M}{b_o}, \quad \vartheta = 0, \tag{4.28}$$

where

$$\frac{b_o}{\ell_\Lambda} = \exp \alpha_o = \sqrt{1 + a_o^2 \ell_\Lambda^{-2}} - a_o \ell_\Lambda = \sqrt{\frac{\ell_\Lambda + R_o}{\ell_\Lambda - R_o}}, \tag{4.29}$$

and λ_M is the proper time measured in Minkowski space M related to de Sitter space by conformal mapping (3.18) and (3.19),

$$\lambda_M = \exp \alpha_o \cosh \alpha_o \, \lambda_{dS}. \tag{4.30}$$

Consequently,

$$r = \pm \sqrt{t^2 + b_o^2}, \quad \vartheta = 0, \tag{4.31}$$

which is the simplest form of the hyperbolic motion with the uniform acceleration $1/b_o$ as measured in Minkowski space [cf. Eqs. (2.3)].

V. FRAMES CENTERED ON ACCELERATED PARTICLES

For the investigation of the radiative properties and other physical aspects of the fields, the use of (physically equivalent) particles $w_\odot, w_\otimes$, i.e., those "born at the poles" of spherical coordinates is technically more advantageous. We shall now return back and construct frames with the origins located directly on these particles. In such frames, various properties of the fields will become more transparent than in the coordinates introduced so far.

As we have seen in the preceding section, the uniformly accelerated particles $w_\odot$ and $w_\otimes$ are at rest in static coordinates T, R at given $R = R_o = -a_o \ell_\Lambda^2 / \sqrt{1 + a_o^2 \ell_\Lambda^2}$, where $|a_o|$ is the magnitude of the acceleration. In order to investigate the properties of the fields, in particular, in order to see what is the structure of the field along the null cones with vertices at the particle's position, i.e., what is the field "emitted" by the particle at a given time, it is useful to construct coordinate frames centered on the accelerated particles. Such systems of coordinates are used to describe accelerating black holes in general relativity (like C-metrics, known also for $\Lambda \neq 0$, cf. Refs. 27 and 28), so that their properties on de Sitter background may indicate what is their meaning in more general cases—in situations when they are centered on gravitating objects rather than on test particles.

We shall now describe three coordinate systems of this type: the accelerated coordinates, the C-metric-like coordinates, and the Robinson-Trautman coordinates, all centered on the worldlines $w_\odot$ and $w_\otimes$. Instead of writing down just the transformation formulas, we wish to indicate some steps how these coordinates can be obtained naturally. We list only the main transformation relations here, many other formulas and forms of the metrics can be found in the Appendix. Let us also note that in this section we assume $R_o, \alpha_o > 0$, i.e., $a_o < 0$, and we use only static radial coordinate with positive values, i.e., $R > 0$.

A. Accelerated coordinates

We begin with the construction of accelerated coordinates $T', R', \vartheta', \varphi$. This type of coordinates was recently introduced[49] by another method in the context of the C-metric with $\Lambda > 0$. In the preceding section we obtained the worldlines $w_\odot, w_\otimes$ of uniformly accelerated particles in de Sitter space by starting from a particle moving with a uniform velocity $v_{\breve{M}} = \tanh \alpha_o$ in a negative direction of the $\breve{z}$ axis in the inertial frame $\breve{t}, \breve{r}, \vartheta, \varphi$ in Minkowski space $\breve{M}$ which passes through $\breve{r} = 0$ at $\breve{t} = 0$ [see Eqs. (4.1) and (4.2)]; and we used then the conformal relation between Minkowski and de Sitter spaces to find $w_\odot, w_\otimes$. Therefore, let us first construct a frame centered on the uniformly moving particle in $\breve{M}$. Using spherical coordinates again, this boosted frame denoted by primes is related to the original one simply by

$$\begin{aligned} \breve{t}' &= \breve{t} \cosh \alpha_o + \breve{r} \cos \vartheta \sinh \alpha_o, \\ \breve{r}' \cos \vartheta' &= \breve{t} \sinh \alpha_o + \breve{r} \cos \vartheta \cosh \alpha_o, \end{aligned} \tag{5.1}$$

$$\check{r}' \sin \vartheta' = r \sin \vartheta,$$

the φ-coordinate does not change and will be suppressed in the following. From here

$$\begin{aligned} -\check{t}'^2 + \check{r}'^2 &= -\check{t}^2 + \check{r}^2, \\ \tan \vartheta' &= \frac{\sin \vartheta}{(\check{t}/\check{r})\sinh \alpha_o + \cos \vartheta \cosh \alpha_o}. \end{aligned} \tag{5.2}$$

The original frame $\check{t}, \check{r}, \vartheta$ in Minkowski space $\check{M}$ is related to the static coordinates T, R, ϑ in de Sitter space by [cf. Eqs. (A67) and (A80)]

$$T = -\frac{\ell_\Lambda}{2} \log \left| \frac{\check{t}^2 - \check{r}^2}{\ell_\Lambda^2} \right|, \quad R = -\ell_\Lambda \frac{\check{r}}{\check{t}}, \quad \vartheta = \vartheta. \tag{5.3}$$

The metrics of the two spaces are related by $g_{\mathrm{dS}} = (\ell_\Lambda^2/\check{t}^2) g_{\check{M}}$, g_{dS} being given by Eq. (3.9)—cf. Eq. (3.14). Now, let us introduce coordinates T', R', ϑ' given in terms of $\check{t}', \check{r}', \vartheta'$ by exactly the same formulas as coordinates T, R, ϑ are given in terms of $\check{t}, \check{r}, \vartheta$ in Eq. (5.3). In this way we obtain $g_{\mathrm{dS}'} = (\ell_\Lambda^2/\check{t}'^2) g_{\check{M}}$. Combining the last relation with $g_{\mathrm{dS}} = (\ell_\Lambda^2/\check{t}^2) g_{\check{M}}$, we find the metric of the original de Sitter space in the new coordinates T', R', ϑ' in the form

$$g_{\mathrm{dS}} = \frac{\check{t}'^2}{\check{t}^2} g_{\mathrm{dS}'}, \tag{5.4}$$

$g_{\mathrm{dS}'}$ is given by the "primed" version of Eq. (3.9). Expressing then the factor $(\check{t}'/\check{t})^2$ by using Eqs. (5.1) and (5.2), and "primed" relations (5.3), we arrive at the de Sitter metric in the accelerated coordinates in the form

$$g_{\mathrm{dS}} = \frac{1 - R_o^2/\ell_\Lambda^2}{[1 + (R' R_o/\ell_\Lambda^2)\cos \vartheta']^2} \left(-\left(1 - \frac{R'^2}{\ell_\Lambda^2}\right) \mathrm{d}T'^2 + \left(1 - \frac{R'^2}{\ell_\Lambda^2}\right)^{-1} \mathrm{d}R'^2 + R'^2 (\mathrm{d}\vartheta'^2 + \sin^2 \vartheta' \, \mathrm{d}\varphi^2) \right). \tag{5.5}$$

Here the accelerated coordinates $T', R', \vartheta', \varphi$ are given in terms of static coordinates by the relation obtained by the procedure described above as follows:

$$\begin{aligned} R' &= \ell_\Lambda \sqrt{1 - \frac{(1 - R^2/\ell_\Lambda^2)(1 - R_o^2/\ell_\Lambda^2)}{[1 - (R R_o/\ell_\Lambda^2)\cos \vartheta]^2}}, \\ T' &= T, \quad \tan \vartheta' = \frac{\sqrt{1 - R_o^2/\ell_\Lambda^2} R \sin \vartheta}{R \cos \vartheta - R_o}. \end{aligned} \tag{5.6}$$

Notice that the time coordinate of static and accelerated frames coincide. Technically, this is easy to see from the first relation in Eqs. (5.2) and (5.3). Intuitively, this is evident since the uniformly accelerated particles are at rest in the static coordinates, as well as in the accelerated coordinates, the only difference being that they are located at the origin of the accelerated frame. Setting $R_o = 0$ in Eq. (5.6), we get $R' = R$, $\vartheta' = \vartheta$, as expected. The static coordinates are centered on the poles $\chi = 0, \pi$, hence, on the *un*accelerated worldlines. The name accelerated coordinates *is* thus inspired by the fact that their origin is accelerated, and the value of this acceleration enters the form of the metric (5.5) explicitly through the quantity R_o.

The two-dimensional conformal diagram of de Sitter space with coordinate lines $T' = \text{constant}$, $R' = \text{constant}$ of the accelerated frame is given in Fig. 10. For details, see the figure caption. Here let us just notice that the cosmological horizons are still described by $R'^2 = \ell_\Lambda^2$.

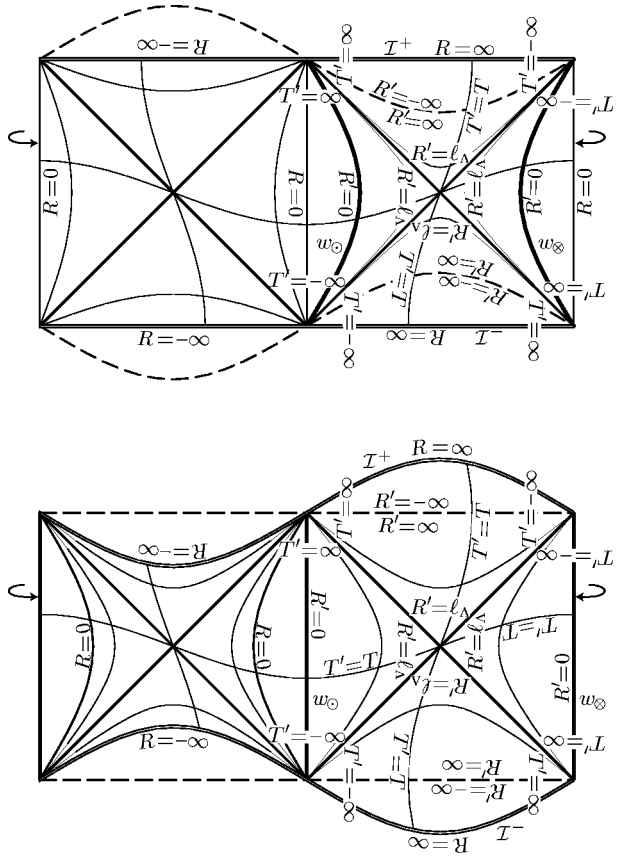

FIG. 10. The two-dimensional conformal diagrams of de Sitter space based on the static, nonaccelerated coordinates (upper diagram), and on the accelerated coordinates (lower diagram). Starting from static coordinates T,R,ϑ,φ, one can draw the conformal diagram of the axis $\vartheta=0,\pi$ in which the conformal past and future infinities, $\mathcal{I}^\pm(R=\pm\infty)$, are horizontal (double) lines. In addition to static coordinates T,R, also accelerated coordinates T',R' are indicated in both diagrams. These have a coordinate singularity for $R'=\infty$ (drawn as a dashed line). The origins of the accelerated coordinates, $R'=0$ (thick lines), are worldlines of uniformly accelerated particles. In the conformal diagram of the axis $\vartheta'=0,\pi$ based on accelerated coordinates, the origins $R'=0$ and the coordinate singularity $R'=\infty$ of the accelerated frame are straight lines; the true infinities $\mathcal{I}^\pm$ have a "bulge" upwards or "downwards," depending on the angle ϑ'. The hypersurface $R'=\infty$ corresponds to the boosted hyperplane $\check{t}'=0$, whereas the conformal infinity corresponds to $\check{t}=0$ (the relation of both hyperplanes can be well understood in the diagram of the conformally related Minkowski space $\check{M}$). The diagrams in which the conformal infinities $\mathcal{I}^\pm$ are not straight naturally arise in the studies of the C-metric with $\Lambda>0$ [de Sitter space being a special case of this class of the metrics (Ref. 27)]. In general, outside the axis $\vartheta=\vartheta'=0,\pi$, the transformations between the static and accelerated coordinates mix radial and angular coordinates R, ϑ and R',ϑ', as is seen also in the following Fig. 11. The sections $\vartheta'=$constant (for some general ϑ') are also shown in Fig. 21 in the Appendix.

Infinite values of R' can, however, be encountered "before" the conformal infinities $\mathcal{I}^\pm$ are reached. This depends on the angle ϑ'. Indeed, $R'=\infty$ corresponds to $\check{t}'=0$, whereas $\mathcal{I}^\pm$ is given by $\check{t}=0$, i.e.,

$$R'=-\frac{\ell_\Lambda^2}{R_\mathrm{o}}\frac{1}{\cos\vartheta'}, \tag{5.7}$$

[cf. metric (5.5)]. Relation of these two surfaces is best viewed in Minkowski space $\check{M}$. We see that for $\vartheta,\vartheta'<\pi/2$, the conformal infinity $\mathcal{I}^+$ ($\mathcal{I}^-$) lies "above" ("below") the surface $R'=\pm\infty$. Thus the infinity $R'=\pm\infty$ is just a coordinate singularity, which can be removed using, for example, the C-metric-like coordinate v introduced below.

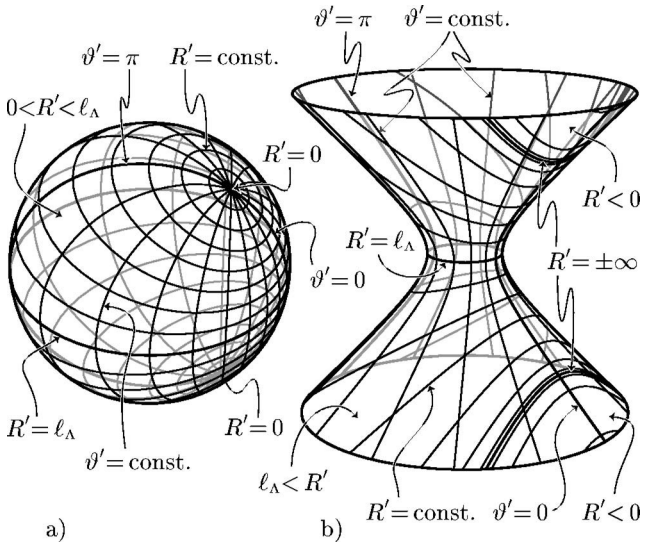

FIG. 11. The accelerated coordinates R', ϑ' on the sections $T'=$constant of de Sitter space (coordinate φ suppressed). In the region where $\partial/\partial T'$ is timelike ($0<R'<\ell_\Lambda$), the cut $T'=$constant is a spacelike sphere [diagram (a)]. In the region where $\partial/\partial T'$ is spacelike ($\ell_\Lambda<R'$ and $R'<0$), it is a timelike hyperboloid [diagram (b)]. The diagrams are not in the same scale—the radius of the sphere and of the neck of the hyperboloid should be the same. The axis $\vartheta'=0,\pi$ corresponds to the lines $T'=$constant of Fig. 10. The coordinate singularity $R'=\pm\infty$ is also indicated. For more details see the text.

Figure 11(a) shows the cut $T=T'=$constant located in the region of de Sitter space where the Killing vector $\partial/\partial T=\partial/\partial T'$ is timelike ($R,R'<\ell_\Lambda$); φ-direction is suppressed. The cut is a spacelike sphere S^3 with homogeneous spherical metric. The coordinate lines $R'=$constant and $\vartheta'=$constant are plotted, with two origins $R'=0$ indicated, here the accelerated particles occur. The coordinate R' grows from $R'=0$ at the origins to the equator where $R'=\ell_\Lambda$. In Fig. 11(b) the cut $T=T'=$constant located in the regions where $\partial/\partial T=\partial/\partial T'$ is spacelike ($R,R'>\ell_\Lambda$) is illustrated, again with φ-direction suppressed. Here the cut is timelike with the geometry of three-dimensional de Sitter space. The coordinate lines $R'=$constant and $\vartheta'=$constant are also shown.

As we have just seen, the points with $R'=\infty$ can be "nice" points in de Sitter manifold. It may thus be convenient to introduce the inverse of R' as a new coordinate. Also, we consider $-\cos\vartheta'$ as a coordinate, and make the time coordinate dimensionless. We thus arrive at the C-metric-like coordinates $\tau, \upsilon, \xi, \varphi$,

$$\tau=\frac{T'}{\ell_\Lambda},\quad \upsilon=\frac{\ell_\Lambda}{R'},\quad \xi=-\cos\vartheta'. \tag{5.8}$$

The metric (5.5) becomes

$$g_{\mathrm{dS}}=\mathfrak{r}^2\left(-(\upsilon^2-1)\mathrm{d}\tau^2+\frac{1}{\upsilon^2-1}\mathrm{d}\upsilon^2+\frac{1}{1-\xi^2}\mathrm{d}\xi^2+(1-\xi^2)\mathrm{d}\varphi^2\right), \tag{5.9}$$

with the conformal factor $\mathfrak{r}$ given by

$$\mathfrak{r}=\frac{\ell_\Lambda}{\upsilon\cosh\alpha_{\mathrm{o}}-\xi\sinh\alpha_{\mathrm{o}}}. \tag{5.10}$$

This is de Sitter space–time in the "C-metric form:" setting the mass and charge parameters, m and e, equal to zero in the the C-metric with a positive cosmological constant [written in the form (2.8) of Ref. 27], and choosing the acceleration parameter equal to $A=\ell_\Lambda^{-1}|\sinh\alpha_{\mathrm{o}}|=|a_{\mathrm{o}}|$, we obtain the metric (5.9).

B. Robinson-Trautman coordinates

In order to arrive naturally to the Robinson-Trautman form of the metric, notice that the coefficients in the metric (5.9) become singular at $v \to \pm 1$, similarly as they do on the horizon of the Schwarzschild space–time in the standard Schwarzschild coordinates. Analogously to that case, we choose a "tortoise-type" coordinate $v_\star$ by

$$v_\star = \frac{1}{2} \log \left| \frac{1-v}{1+v} \right| . \tag{5.11}$$

Similarly to the Schwarzschild case again, we introduce a suitable *null* coordinate $\mathfrak{u}$ in terms of the radial and time coordinates τ and $v_\star$ as follows:

$$\mathfrak{u} = (\ell_\Lambda \tanh \alpha_\mathrm{o})(\tau + v_\star). \tag{5.12}$$

Together with the conformal factor $\mathfrak{r}$ defined in Eq. (5.10), we arrive at the de Sitter metric in coordinates $\mathfrak{u}, \mathfrak{r}, \xi, \varphi$ [cf. Eq. (A109)] which is very near to being in the Robinson-Trautman form. However, there is a nonvanishing mixed metric coefficient at $\mathrm{d}\mathfrak{u} \vee \mathrm{d}\xi$ which is absent in the Robinson-Trautman metric. Such a term can be made to vanish by introducing a new angular coordinate ψ by

$$\psi = \operatorname{arctanh} \xi + \frac{\mathfrak{u}}{\ell_\Lambda} \sinh \alpha_\mathrm{o}. \tag{5.13}$$

The de Sitter metric then becomes

$$g_{\mathrm{dS}} = -H\, \mathrm{d}\mathfrak{u}^2 - \mathrm{d}\mathfrak{u} \vee \mathrm{d}\mathfrak{r} + \frac{\mathfrak{r}^2}{P^2}(\mathrm{d}\psi^2 + \mathrm{d}\varphi^2), \tag{5.14}$$

where

$$\begin{gathered} H = -\frac{\mathfrak{r}^2}{\ell_\Lambda^2} + 2\frac{\mathfrak{r}}{\ell_\Lambda} \sinh \alpha_\mathrm{o} \tanh\left(\psi - \frac{\mathfrak{u}}{\ell_\Lambda} \sinh \alpha_\mathrm{o} \right) + 1, \\ P = \cosh\left(\psi - \frac{\mathfrak{u}}{\ell_\Lambda} \sinh \alpha_\mathrm{o} \right). \end{gathered} \tag{5.15}$$

This is precisely the form of the Robinson-Trautman metric—see, e.g., Ref. 50. Tracking back the transformations leading to the metric (5.14), the connection between the Robinson-Trautman coordinates and the static coordinates T, R, ϑ, φ turns out to be not as complicated as our procedure might have indicated, in particular, for the radial coordinate. We find a nice formula for $\mathfrak{r}$,

$$\mathfrak{r} = \frac{\ell_\Lambda}{\sqrt{1 - \dfrac{R_\mathrm{o}^2}{\ell_\Lambda^2}}} \left(\left(1 - \frac{R R_\mathrm{o}}{\ell_\Lambda^2} \cos \vartheta \right)^2 - \left(1 - \frac{R^2}{\ell_\Lambda^2} \right) \left(1 - \frac{R_\mathrm{o}^2}{\ell_\Lambda^2} \right) \right)^{1/2}, \tag{5.16}$$

whereas the other two coordinates are simply expressed only in terms of accelerated coordinates $T' = T, R', \vartheta', \varphi$,

$$\mathfrak{u} = \sqrt{1 - \frac{R_\mathrm{o}^2}{\ell_\Lambda^2}} \left(T' + \frac{\ell_\Lambda}{2} \log \left| \frac{R' - \ell_\Lambda}{R' + \ell_\Lambda} \right| \right), \quad \psi = \frac{R_\mathrm{o}}{\ell_\Lambda} \left(\frac{T'}{\ell_\Lambda} + \frac{1}{2} \log \left| \frac{R' - \ell_\Lambda}{R' + \ell_\Lambda} \right| \right) + \log \left| \tan \frac{\vartheta'}{2} \right| . \tag{5.17}$$

Coordinates R', ϑ' can then be obtained in terms of the original static coordinates by using Eqs. (5.6).

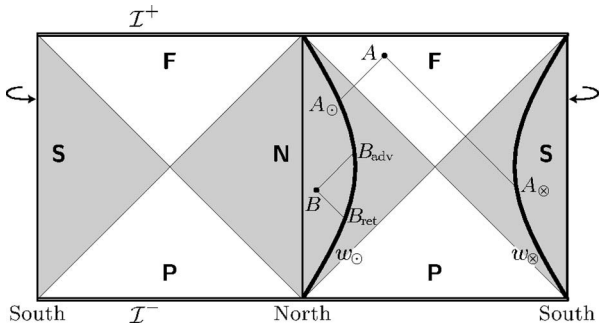

FIG. 12. The field at an event A can be interpreted as $1/2$ of the sum of the retarded fields produced by particle $w_\odot$ at $A_\odot$ and particle $w_\otimes$ at $A_\otimes$. The field at B can be interpreted as $1/2$ of the sum of the retarded and advanced effects from particle $w_\odot$. The affine parameter distances $BB_{\rm ret}$ and $BB_{\rm adv}$ are equal, the same being true for the distances $AA_\odot$ and $AA_\otimes$.

The Robinson-Trautman coordinates with metric (5.14) are centered on the accelerated particles. As with static or accelerated frames, we need two sets of such coordinates to cover both $w_\odot$ and $w_\otimes$. The relations to the static coordinates become, of course, much simpler if the particles are not accelerated, $R_{\rm o}=0$, and when both the Robinson-Trautman and static coordinates are centered on the pole $\chi=0$,

$$\mathfrak{r}=R, \quad \psi=\log\tan\frac{\vartheta}{2}, \quad \mathfrak{u}=T+\frac{\ell_\Lambda}{2}\log\left|\frac{R-\ell_\Lambda}{R+\ell_\Lambda}\right|. \tag{5.18}$$

However, even "accelerated" Robinson-Trautman coordinates possess some very convenient features. The radial coordinate $\mathfrak{r}$ is an affine parameter along null rays $\mathfrak{u},\psi,\varphi=$constants, normalized at the particle's worldline by the condition

$$\frac{\partial^\mu}{\partial\mathfrak{r}}g_{{\rm dS}\mu\nu}\mathfrak{u}^\nu=-1, \tag{5.19}$$

where $\mathfrak{u}$ is the particle's four-velocity. These null rays form a diverging but nonshearing and nonrotating congruence of geodesics. The null vector $\partial/\partial\mathfrak{r}$, tangent to the rays, is parallelly propagated along them. Its divergence is given by $\nabla_\mu(\partial^\mu/\partial\mathfrak{r})=2/\mathfrak{r}$ so that $\mathfrak{r}$ is both the affine parameter and the luminosity distance (see, e.g., Ref. 51). With Robinson-Trautman coordinates, one can also associate a null tetrad [explicitly written down in the Appendix, Eq. (A114)] which is parallelly transported along the null rays from the particle ($\mathfrak{r}=0$) up to infinity ($\mathfrak{r}=\infty$).

Owing to the boost symmetry of both the worldlines and de Sitter space, an interesting feature arises, which is analogous to the situation in Minkowski space. Consider a point B in region **N** (Fig. 12). There are two generators of the null cone with the origin at B which cross the worldline $w_\odot$ at two points, $B_{\rm ret}$ and $B_{\rm adv}$. Then the affine parameter distance $BB_{\rm ret}$ is the same as $BB_{\rm adv}$. (In order to go towards the past from $B_{\rm adv}$ to B, the "advanced" Robinson-Trautman coordinates built on the past null cones with origins on $w_\odot$ can easily be introduced.) This is evident because B lies on one orbit of the boost Killing vector $\partial/\partial T$ and a boost can be applied which leaves the worldline $w_\odot$ invariant but moves B into event B' on the slice of time symmetry, $\tau=0$ (also $T=T'=0$), where the particle is at rest. Then $B_{\rm adv}$ and $B_{\rm ret}$ move to the new points $B'_{\rm adv},B'_{\rm ret}$, which are located symmetrically with respect to $\tau=0$. The equality of the affine parameter distances then follows from the symmetry immediately. Similarly, for an event A in region **F** one can show that the affine parameter distance $AA_\odot$ is equal to the distance $AA_\otimes$ (see Fig. 12). The point A lies on a boost orbit (which now has a spatial character) along which it can be brought, by an appropriate boost, to the point located symmetrically between the worldlines $w_\odot$ and $w_\otimes$ (lying so on the equator, $\chi=\pi/2$). The same consideration can, of course, be applied to an event in the "past" region **P**—showing that the affine distances along future-oriented null rays from an event to the particles are equal.

Although the symmetries just described are common to the worldlines of uniformly accelerated particles in Minkowski and de Sitter space–times, an important difference exists. In Minkowski space, the affine parameter distance along the null ray from an event on particle's worldline, such as $A_\odot$, to an "observation" point A is equal to the proper distance between $A_\perp$ and $A_\odot$ where $A_\perp$ is the orthogonal projection of A onto the spacelike slice $T=T(A_\odot)$. This is not the case in de Sitter space if, as it appears natural, under an orthogonal projection we understand the projection of the observation point A onto the spacelike slice $T=$constant containing $A_\odot$ performed along a timelike geodesic orthogonal to such a slice. Nevertheless, the proper distance s between $A_\odot$ and $A_\perp$ is still related to the affine parameter distance $\mathfrak{r}$ by a simple expression

$$\frac{\mathfrak{r}}{\ell_\Lambda} = \tan \frac{s}{\ell_\Lambda}. \tag{5.20}$$

This relation can be derived as follows. Consider, without loss of generality, $A_\odot$ located at the turning point of the particle $w_\odot$ at $T=0$. The condition that the events A and $A_\odot$ are connected by a null ray implies that the distance s between $A_\odot$ and $A_\perp$ is the same as the time interval between $A_\perp$ and A as measured by the metric (3.12) of the conformally related static Einstein universe. Since A occurs at some time $\tilde{t}$ whereas $A_\odot$ and $A_\perp$ at $\tilde{t}=\pi/2$ (i.e., at static time $T=0$), this time interval is equal to $\ell_\Lambda(\tilde{t}-\pi/2)$, cf. Eq. (3.11). The static radial coordinate R of A thus reads [cf. Eqs. (A64) and (A77)]

$$R = \frac{\sin \tilde{r}}{\sin \tilde{t}} = \frac{\sin \tilde{r}}{\cos(s/\ell_\Lambda)}. \tag{5.21}$$

The slice $T=0$ has a geometry of the 3-sphere of radius ℓ_Λ. Using the standard law of cosines in spherical trigonometry for the sides of the triangle spanned by $A_\odot, A_\perp$, and the north pole, we can eliminate $\tilde{r}$. Finally, employing Eq. (5.16), we obtain the result (5.20). Clearly, near the particle $w_\odot$ we have $s \ll \ell_\Lambda$, and Eq. (5.20) then gives $\mathfrak{r} \approx s$, as in Minkowski space.

In the following section we shall explore the character of the fields of the particles $w_\odot$ and $w_\otimes$. We shall see that the affine parameter distance $\mathfrak{r}$ will play most important role, simplifying their description enormously. Namely, as we will see in Sec. VI B, Eq. (6.28), the affine parameter $\mathfrak{r}$ is identical to the factor $\mathcal{Q}$ which will be introduced in the following and will appear in all expressions for the fields.

VI. FIELDS OF UNIFORMLY ACCELERATED SOURCES AND THEIR MANY FACES

In this section we wish to construct the scalar and electromagnetic fields of uniformly accelerated (scalar and electric) charges in de Sitter universe. A general procedure, suitable in case of any—not necessarily uniform—acceleration would be to seek for appropriate Green's functions. Alternatively, in particular for sources moving along uniformly accelerated worldlines, we can make use of the conformal relations between Minkowski and de Sitter spaces, and of the properties of scalar and electromagnetic fields under conformal mappings. This method is advantageous not only for finding the fields in de Sitter space–time, but also for understanding their relationships to the known fields of corresponding sources in special relativity. The only delicate issue is the fact that there are no conformal mappings between Minkowski and de Sitter space which are globally smooth. We discussed, in Sec. III, how various regions of one space can be mapped onto the regions of the other space. In Ref. 24 we carefully treated the fields at the hypersurfaces where the conformal transformation fails to be regular. In order to obtain well-behaved fields, one must continue analytically across such a hypersurface the field obtained in one region into the whole de Sitter space. In Sec. II in Ref. 24, we also analyzed in detail the behavior of the scalar field wave equation with sources and of Maxwell's equations with sources under (general) conformal transformations.

In Ref. 24 we primarily concentrated on the absence of purely retarded fields at the past infinity $\mathcal{I}^-$ of de Sitter space–time—in fact, in any space–time in which $\mathcal{I}^-$ is spacelike. In order

to analyze this problem we also considered, in addition to monopole charges, more complicated sources like rigid and geodesic dipoles; and we constructed some retarded solutions to show their patological features. However, we confined ourselves to the sources the worldlines of which start and end at the poles; we did not employ coordinates best suited for exhibiting the properties of the fields at future infinity $\mathcal{I}^+$, and the frames corresponding to cosmological models like flat ($k=0$) or hyperbolic ($k=-1$) cosmological coordinates; and we did not give the physical components of the fields. In the following we shall find the fields and discuss their properties in various physically important coordinate systems, in particular those significant at $\mathcal{I}^+$ or in a cosmological context. In the next section, we also obtain the fields due to the uniformly accelerated scalar and electric charges starting at $\mathcal{I}^-$ at $\chi=\pi/2$ ("born at the equator"). This, among others, will be important when we wish to regain the classical Born fields in the limit $\Lambda\to 0$.

We start by using the analysis of the conformal behavior of the fields and sources given in Sec. II in Ref. 24, and we also take over from Ref. 24 the resulting forms of the fields due to the sources starting and ending at the poles of de Sitter space, as described in standard coordinates.

A. Fields in coordinates centered on the poles

Consider two uniformly accelerated point sources starting at $\mathcal{I}^-$ (i.e., at $\tau\to-\infty$, $\tilde{t}\to 0$) at the poles $\chi=\tilde{r}=0$ and $\chi=\tilde{r}=\pi$ (Fig. 7). Their worldlines $w_\odot, w_\otimes$ are given by Eqs. (4.7) [or (4.24)] in these standard (rescaled) coordinates, by Eqs. (4.8) and (4.9) in the flat and hyperbolic cosmological coordinates, and by Eqs. (4.18) in the static coordinates. Their simplest description is, of course, given by $R'=0$ and $\mathfrak{r}=0$ in the accelerated and Robinson-Trautman coordinates since these frames are centered exactly on their worldlines. In Sec. IV we discussed physical velocities and other properties of these particles.

Now, as noticed at the beginning of Sec. IV, these two worldlines can be obtained by conformally mapping the worldline of one uniformly moving particle in Minkowski space into de Sitter space. The fields of uniformly moving sources in Minkowski space are just boosted Coulomb fields. Under a conformal rescaling of the metric, $g_{\alpha\beta}\to\hat{g}_{\alpha\beta}=\Omega^2 g_{\alpha\beta}$, the fields behave as follows: $\Phi\to\hat{\Phi}=\Omega^{-1}\Phi$, $\mathrm{F}_{\alpha\beta}\to\hat{\mathrm{F}}_{\alpha\beta}=\mathrm{F}_{\alpha\beta}$ (see Ref. 24, Sec. II, where the behavior of the source terms is also analyzed). Hence, the fields due to two uniformly accelerated sources in de Sitter space–time can be obtained by conformally transforming the boosted Coulomb fields in Minkowski space–time. Employing the conformal mapping (3.13)–(3.15), we arrive at the following results.[52] The scalar field is given by the expression

$$\Phi=\frac{s}{4\pi}\frac{1}{\mathcal{Q}}, \tag{6.1}$$

where

$$\mathcal{Q}=\ell_\Lambda\left[\left(\sqrt{1+a_\mathrm{o}^2\ell_\Lambda^2}+a_\mathrm{o}\ell_\Lambda\cosh\frac{\tau}{\ell_\Lambda}\sin\chi\cos\vartheta\right)^2-\left(1-\cosh^2\frac{\tau}{\ell_\Lambda}\sin^2\chi\right)\right]^{1/2}, \tag{6.2}$$

or, written in the standard rescaled coordinates,

$$\mathcal{Q}=\ell_\Lambda\left[\left(\sqrt{1+a_\mathrm{o}^2\ell_\Lambda^2}+a_\mathrm{o}\ell_\Lambda\frac{\sin\tilde{r}}{\sin\tilde{t}}\cos\vartheta\right)^2-1+\frac{\sin^2\tilde{r}}{\sin^2\tilde{t}}\right]^{1/2}. \tag{6.3}$$

This field is produced by two identical charges of magnitude s moving along worldlines $w_\odot$ and $w_\otimes$. It is smooth everywhere outside the charges and it can be written as a symmetric combination of retarded and advanced effects from both charges [cf. Eq. (6.6) in Ref. 24].

Similarly to the scalar-field case, by using conformal technique the electromagnetic field produced by two uniformly accelerated charges moving along $w_\odot$ and $w_\otimes$ can be obtained in the form

$$\mathrm{F}=\frac{e}{4\pi}\frac{\ell_\Lambda^2}{\mathcal{Q}^3}\cosh\frac{\tau}{\ell_\Lambda}\Bigg[a_\mathrm{o}\ell_\Lambda\sin\chi\cos\chi\sin\vartheta\,\mathrm{d}\tau\wedge\mathrm{d}\vartheta$$
$$-\left(\sqrt{1+a_\mathrm{o}^2\ell_\Lambda^2}\cosh\frac{\tau}{\ell_\Lambda}\sin\chi+a_\mathrm{o}\ell_\Lambda\cos\vartheta\right)\mathrm{d}\tau\wedge\mathrm{d}\chi$$
$$+a_\mathrm{o}\ell_\Lambda^2\sinh\frac{\tau}{\ell_\Lambda}\cosh\frac{\tau}{\ell_\Lambda}\sin^2\chi\sin\vartheta\,\mathrm{d}\chi\wedge\mathrm{d}\vartheta \tag{6.4}$$

where $\mathcal{Q}$ is again given by Eq. (6.2). As in the scalar-field case, the field is smooth, nonvanishing in the whole de Sitter space–time and involving thus both retarded and advanced effects (cf. Sec. VII A in Ref. 24). However, an important difference between the scalar and electromagnetic case exists: the magnitude of the scalar charges is the same, whereas the electromagnetic charges producing the fields (6.4) have opposite signs. This is analogous to the situation in Minkowski space–time described in Sec. II [see the discussion below Eq. (2.13)]. At the root of this fact appears to be CPT theorem—cf. Ref. 53 for the analogous gravitational case where the masses of the particles uniformly accelerated in the opposite direction are the same. In de Sitter space–time, as in any space–time with compact spacelike sections, a simpler argument exists: the total charge in a compact space must vanish as a consequence of the Gauss theorem.[24]

To gain a better physical insight into the electromagnetic fields, we shall introduce the orthonormal tetrad $\{\mathrm{e}_\mu\}$ and the dual tetrad $\{\mathrm{e}^\mu\}$ tied to each coordinate frame used, and we shall decompose the electromagnetic field F into the electric and magnetic parts. Such a decomposition, of course, depends on the choice of the tetrad. For example, in the standard spherical coordinates τ, χ, ϑ, φ the electromagnetic field (2-form) F can be written as

$$\mathrm{F}=\mathrm{E}^\chi\mathrm{e}^\chi\wedge\mathrm{e}^\tau+\mathrm{E}^\vartheta\mathrm{e}^\vartheta\wedge\mathrm{e}^\tau+\mathrm{E}^\varphi\mathrm{e}^\varphi\wedge\mathrm{e}^\tau+\mathrm{B}^\chi\mathrm{e}^\vartheta\wedge\mathrm{e}^\varphi+\mathrm{B}^\vartheta\mathrm{e}^\varphi\wedge\mathrm{e}^\chi+\mathrm{B}^\varphi\mathrm{e}^\chi\wedge\mathrm{e}^\vartheta, \tag{6.5}$$

and the electric and magnetic field spatial vectors are given in terms of their frame components as follows:

$$\mathrm{E}=\mathrm{E}^\chi\mathrm{e}_\chi+\mathrm{E}^\vartheta\mathrm{e}_\vartheta+\mathrm{E}^\varphi\mathrm{e}_\varphi,$$
$$\mathrm{B}=\mathrm{B}^\chi\mathrm{e}_\chi+\mathrm{B}^\vartheta\mathrm{e}_\vartheta+\mathrm{B}^\varphi\mathrm{e}_\varphi. \tag{6.6}$$

In the present case of the standard spherical coordinates, using the explicit forms of the tetrad given in Appendix [Eqs. (A10)], we find

$$\mathrm{E}_\mathrm{sph}=\frac{e}{4\pi}\frac{\ell_\Lambda}{\mathcal{Q}^3}\left[-a_\mathrm{o}\ell_\Lambda\cos\chi\sin\vartheta\,\mathrm{e}_\vartheta+\left(\sqrt{1+a_\mathrm{o}^2\ell_\Lambda^2}\cosh\frac{\tau}{\ell_\Lambda}\sin\chi+a_\mathrm{o}\ell_\Lambda\cos\vartheta\right)\mathrm{e}_\chi\right],$$
$$\mathrm{B}_\mathrm{sph}=\frac{e}{4\pi}\frac{a_\mathrm{o}\ell_\Lambda^2}{\mathcal{Q}^3}\sinh\frac{\tau}{\ell_\Lambda}\sin\chi\sin\vartheta\,\mathrm{e}_\varphi. \tag{6.7}$$

In Appendix the orthonormal tetrads tied to the coordinate systems considered in this paper are all listed explicitly. The only exception is the Robinson-Trautman coordinate system with one coordinate null and thus with a nondiagonal metric; in this case the null tetrad is given in which the Newman-Penrose-type components are more telling.

The tetrad components of the electric intensity and the magnetic induction vectors are physically meaningful objects, they can be measured by observers who move with the four-velocities given by the timelike vector of the tetrad (as, e.g., e_τ for spherical cosmological observers), and are equipped with an orthonormal triad of the spacelike vectors (e.g., e_χ, e_ϑ, e_φ).

We first list the resulting electromagnetic field tensor and its electric and magnetic parts in the coordinate systems centered on the poles $\chi=0,\pi$. The scalar field is always given by expression

(6.1), the explicit form of the scalar factor $\mathcal{Q}$ changes according to the coordinates used. Since this factor enters all the electromagnetic quantities as well, we always give $\mathcal{Q}$ first and then write the electromagnetic field quantities.

In the flat cosmological coordinates [see Eqs. (3.4) and (3.5)] we find

$$\mathcal{Q}=\ell_\Lambda\left[\left(\cosh\alpha_o-\sinh\alpha_o\frac{\check r}{\ell_\Lambda}\exp\frac{\check\tau}{\ell_\Lambda}\cos\vartheta\right)^2-\left(1-\frac{\check r^2}{\ell_\Lambda^2}\exp\left(2\frac{\check\tau}{\ell_\Lambda}\right)\right)\right]^{1/2}, \tag{6.8}$$

$$\begin{aligned}F=&-\frac{e}{4\pi}\frac{1}{\mathcal{Q}^3}\exp\frac{\check\tau}{\ell_\Lambda}\left[\ell_\Lambda\check r\sinh\alpha_o\sin\vartheta\,d\check\tau\wedge d\vartheta+\left(\check r\cosh\alpha_o\exp\frac{\check\tau}{\ell_\Lambda}-\ell_\Lambda\sinh\alpha_o\cos\vartheta\right)d\check\tau\wedge d\check r\right.\\&\left.+\check r^2\sinh\alpha_o\exp\left(2\frac{\check\tau}{\ell_\Lambda}\right)\sin\vartheta\,d\check r\wedge d\vartheta\right],\end{aligned} \tag{6.9}$$

$$\begin{aligned}E_{flat}=&\frac{e}{4\pi}\frac{\ell_\Lambda}{\mathcal{Q}^3}\left[\sinh\alpha_o\sin\vartheta\,e_{\vartheta}-\left(\cosh\alpha_o\frac{\check r}{\ell_\Lambda}\exp\frac{\check\tau}{\ell_\Lambda}-\sinh\alpha_o\cos\vartheta\right)e_{\check r}\right],\\B_{flat}=&-\frac{e}{4\pi}\frac{\ell_\Lambda\sinh\alpha_o}{\mathcal{Q}^3}\frac{\check r}{\ell_\Lambda}\exp\frac{\check\tau}{\ell_\Lambda}\sin\vartheta\,e_\varphi.\end{aligned} \tag{6.10}$$

In the hyperbolic cosmological coordinates [see Eqs. (3.6) and (3.7)], the results are slightly lengthier,

$$\mathcal{Q}=\ell_\Lambda\left[\left(\cosh\alpha_o-\sinh\alpha_o\sinh\frac{\eta}{\ell_\Lambda}\sinh\frac{\rho}{\ell_\Lambda}\cos\vartheta\right)^2-\left(1-\sinh^2\frac{\eta}{\ell_\Lambda}\sinh^2\frac{\rho}{\ell_\Lambda}\right)\right]^{1/2}, \tag{6.11}$$

$$\begin{aligned}F=&-\frac{e}{4\pi}\frac{\ell_\Lambda}{\mathcal{Q}^3}\left[\sinh\frac{\eta}{\ell_\Lambda}\left(\cosh\alpha_o\sinh\frac{\eta}{\ell_\Lambda}\sinh\frac{\rho}{\ell_\Lambda}-\sinh\alpha_o\cos\vartheta\right)d\eta\wedge d\rho\right.\\&+\sinh\alpha_o\sinh\frac{\eta}{\ell_\Lambda}\sinh\frac{\rho}{\ell_\Lambda}\cosh\frac{\rho}{\ell_\Lambda}\sin\vartheta\,\ell_\Lambda d\eta\wedge d\vartheta\\&\left.+\sinh\alpha_o\sinh^2\frac{\eta}{\ell_\Lambda}\cosh\frac{\eta}{\ell_\Lambda}\sinh^2\frac{\rho}{\ell_\Lambda}\sin\vartheta\,\ell_\Lambda\,d\rho\wedge d\vartheta\right]\end{aligned} \tag{6.12}$$

$$\begin{aligned}E_{hyp}=&\frac{e}{4\pi}\frac{\ell_\Lambda}{\mathcal{Q}^3}\left[\sinh\alpha_o\cosh\frac{\rho}{\ell_\Lambda}\sin\vartheta\,e_{\vartheta}+\left(\cosh\alpha_o\sinh\frac{\eta}{\ell_\Lambda}\sinh\frac{\rho}{\ell_\Lambda}-\sinh\alpha_o\cos\vartheta\right)e_\rho\right],\\B_{hyp}=&-\frac{e}{4\pi}\frac{\ell_\Lambda}{\mathcal{Q}^3}\sinh\alpha_o\cosh\frac{\eta}{\ell_\Lambda}\sinh\frac{\rho}{\ell_\Lambda}\sin\vartheta\,e_\varphi.\end{aligned} \tag{6.13}$$

Much simpler expressions for the fields arise in the static coordinates [see Eqs. (3.8) and (3.9)]. We obtain

$$\mathcal{Q}^2=\frac{(\ell_\Lambda^2-RR_o\cos\vartheta)^2}{(\ell_\Lambda^2-R_o^2)}-(\ell_\Lambda^2-R^2), \tag{6.14}$$

$$\mathrm{F} = -\frac{e}{4\pi}\frac{\ell_\Lambda}{\sqrt{\ell_\Lambda^2 - R_\mathrm{o}^2}}\frac{1}{\mathcal{Q}^3}\left[(R - R_\mathrm{o}\cos\vartheta)\,\mathrm{d}T\wedge\mathrm{d}R + \left(1 - \frac{R^2}{\ell_\Lambda^2}\right)RR_\mathrm{o}\sin\vartheta\,\mathrm{d}T\wedge\mathrm{d}\vartheta\right], \quad (6.15)$$

$$\mathrm{E}_{\mathrm{stat}} = \frac{e}{4\pi}\frac{1}{\mathcal{Q}^3}\left[\frac{\ell_\Lambda(R - R_\mathrm{o}\cos\vartheta)}{\sqrt{\ell_\Lambda^2 - R_\mathrm{o}^2}}\mathrm{e}_R + R_\mathrm{o}\sin\vartheta\,\mathrm{e}_\vartheta\right], \quad \mathrm{B}_{\mathrm{stat}} = 0. \quad (6.16)$$

Since for practical calculations and for an understanding of the conformal relations between Minkowski and de Sitter spaces the rescaled coordinates are very useful, we also give the fields in these coordinates. The rescaled coordinates are tied with the same orthonormal tetrad as nonrescaled ones, and they define the same splitting into electric and magnetic parts (E and B are the same spatial vectors); the functional dependence on the coordinates, however, is different. In the standard rescaled (conformally Einstein) coordinates [see Eqs. (3.10)–(3.12)], which cover the whole de Sitter space–time including its conformal infinities globally, we get Eq. (6.3) for $\mathcal{Q}$ and

$$\mathrm{F} = -\frac{e}{4\pi}\frac{1}{\mathcal{Q}^3}\frac{\ell_\Lambda^3}{\sin^3\tilde{t}}\Big[a_\mathrm{o}\ell_\Lambda\cos\tilde{t}\sin^2\tilde{r}\sin\vartheta\,\mathrm{d}\tilde{r}\wedge\mathrm{d}\vartheta + \Big(\sqrt{1 + a_\mathrm{o}^2\ell_\Lambda^2}\sin\tilde{r} + a_\mathrm{o}\ell_\Lambda\sin\tilde{t}\cos\vartheta\Big)\mathrm{d}\tilde{t}\wedge\mathrm{d}\tilde{r}$$
$$- a_\mathrm{o}\ell_\Lambda\sin\tilde{t}\cos\tilde{r}\sin\tilde{r}\sin\vartheta\,\mathrm{d}\tilde{t}\wedge\mathrm{d}\vartheta\Big], \quad (6.17)$$

$$\mathrm{E}_{\mathrm{sph}} = \frac{e}{4\pi}\frac{\ell_\Lambda}{\mathcal{Q}^3}\left[-a_\mathrm{o}\ell_\Lambda\cos\tilde{r}\sin\vartheta\,\mathrm{e}_\vartheta + \left(\sqrt{1 + a_\mathrm{o}^2\ell_\Lambda^2}\,\frac{\sin\tilde{r}}{\sin\tilde{t}} + a_\mathrm{o}\ell_\Lambda\cos\vartheta\right)\mathrm{e}_\chi\right],$$
$$\mathrm{B}_{\mathrm{sph}} = -\frac{e}{4\pi}\frac{a_\mathrm{o}\ell_\Lambda^2}{\mathcal{Q}^3}\cot\tilde{t}\sin\tilde{r}\sin\vartheta\,\mathrm{e}_\varphi, \quad (6.18)$$

whereas in the flat rescaled cosmological coordinates (3.13)–(3.15), which cover globally the conformally related Minkowski space (see also Fig. 3), we arrive at

$$\mathcal{Q} = \ell_\Lambda\left[\left(\cosh\alpha_\mathrm{o} + \sinh\alpha_\mathrm{o}\frac{\check{r}}{\check{t}}\cos\vartheta\right)^2 - \left(1 - \frac{\check{r}^2}{\check{t}^2}\right)\right]^{1/2}, \quad (6.19)$$

$$\mathrm{F} = \frac{e}{4\pi}\frac{1}{\mathcal{Q}^3}\frac{\ell_\Lambda^3}{\check{t}^3}\Big[\sinh\alpha_\mathrm{o}\,\check{r}^2\sin\vartheta\,\mathrm{d}\check{r}\wedge\mathrm{d}\vartheta + (\cosh\alpha_\mathrm{o}\,\check{r} + \sinh\alpha_\mathrm{o}\,\check{t}\cos\vartheta)\mathrm{d}\check{t}\wedge\mathrm{d}\check{r}$$
$$- \sinh\alpha_\mathrm{o}\,\check{t}\check{r}\sin\vartheta\,\mathrm{d}\check{t}\wedge\mathrm{d}\vartheta\Big], \quad (6.20)$$

$$\mathrm{E}_{\mathrm{flat}} = \frac{e}{4\pi}\frac{\ell_\Lambda}{\mathcal{Q}^3}\left[\sinh\alpha_\mathrm{o}\sin\vartheta\,\mathrm{e}_\vartheta - \left(\cosh\alpha_\mathrm{o}\frac{\check{r}}{\check{t}} + \sinh\alpha_\mathrm{o}\cos\vartheta\right)\mathrm{e}_{\check{r}}\right],$$
$$\mathrm{B}_{\mathrm{flat}} = \frac{e}{4\pi}\frac{\ell_\Lambda\sinh\alpha_\mathrm{o}}{\mathcal{Q}^3}\frac{\check{r}}{\check{t}}\sin\vartheta\,\mathrm{e}_\varphi. \quad (6.21)$$

In various contexts the electromagnetic field four-potential form A, implying the field F=dA, may be needed. In the standard rescaled (conformally Einstein) coordinates the potential reads

$$\mathrm{A} = -\frac{e}{4\pi}\frac{1}{\mathcal{Q}}\frac{\ell_\Lambda}{\sin\tilde{t}}\frac{\sqrt{1+a_\mathrm{o}^2\ell_\Lambda^2}\sin\tilde{t}+a_\mathrm{o}\ell_\Lambda\sin\tilde{r}\cos\vartheta}{\sin^2\tilde{t}-\sin^2\tilde{r}}(\sin\tilde{t}\cos\tilde{r}\,\mathrm{d}\tilde{t}-\cos\tilde{t}\sin\tilde{r}\,\mathrm{d}\tilde{r}). \tag{6.22}$$

From this expression the frame components can easily be obtained and the four-potential form can be transformed directly to any coordinate system of interest. The four-potential acquires a particularly simple form in static coordinates,

$$A = -\frac{e}{4\pi}\frac{1}{\mathcal{Q}}\frac{\ell_\Lambda^2 - RR_\mathrm{o}\cos\vartheta}{\ell_\Lambda\sqrt{\ell_\Lambda^2 - R_\mathrm{o}^2}}\mathrm{d}T. \tag{6.23}$$

Inspecting now the expressions (6.4)–(6.21), we first notice few basic features of the fields. As a consequence of the axisymmetry, the azimuthal φ component of the electric field vanishes. On the other hand, only the azimuthal φ component of the magnetic field is nonzero. At the axis of symmetry, $\vartheta=0,\pi$, the latitudinal ϑ component of the electric field and magnetic field vanish as $\sim\sin\vartheta$. The electric field points along the axis.

In the classical Born solution in Minkowski space, both charges are, at any time, located symmetrically with respect to the equatorial plane $\vartheta=\pi/2$. Consequently, the radial part of the electric field vanishes for $\vartheta=\pi/2$ [cf. Eq. (2.13)]. In de Sitter space–time the charges outgoing from the poles are, at all times, symmetrically located with respect to the sphere $\chi=\pi/2$ (illustrated as the circle in Fig. 2). We thus expect the ϑ component of the electric field to vanish for $\chi=\pi/2$. This, indeed, follows from Eq. (6.7). This symmetry can be seen only in the standard spherical coordinates since the sphere $\chi=\pi/2$ is not covered by the hyperbolic cosmological coordinates and in the flat cosmological coordinates only one particle occurs.

Another typical feature of the Born solution in Minkowski space is its time symmetry. As a consequence, the magnetic field vanishes at $t=0$ [cf. Eq. (2.13)]. In the past, it was this fact which led some investigators, Pauli[54] among them, to the conclusion that there is "no formation of a wave zone nor any corresponding radiation" since $\mathrm{B}=0$ at $t=0$. However, it is not at a spacelike hypersurface $t=$constant but at $\mathcal{I}^+$, which is reached by taking $u=t-r$ constant, $t,r\to\infty$, where the Born field has typical radiative features, i.e., $|\mathrm{E}|=|\mathrm{B}|\sim r^{-1}$ (see Refs. 37, 53, and 25). In our generalized Born solution, the time symmetry of the fields is clearly demonstrated in the global standard coordinates, under inversion $\tau\to-\tau$ the electric field in Eq. (6.7) is invariant, whereas the magnetic field changes the sign; $\mathrm{B}_\varphi=0$ at $\tau=0$. The field also exhibits radiative character when we approach $\mathcal{I}^+$ in an appropriate way, as it is briefly indicated in Ref. 25. A detailed analysis of the radiative properties of the generalized Born field will be given elsewhere.

The fields take the simplest form in the static coordinates, Eq. (6.15). In these coordinates the particles are at rest, and they both have a constant distance from the poles; their world lines are the orbits of the "static" Killing vector $\partial/\partial T$ of de Sitter space. The electric field is time independent, the magnetic field vanishes. This is fully analogous to the Born field in Minkowski space–time, it is static, and purely electric in the Rindler coordinates, the time coordinate of which is aligned along the orbit of the boost Killing vectors (see, e.g., Ref. 6). However, as we discussed in Sec. III, the static coordinates cover only a "half" of de Sitter space. In the other half, the Killing vector $\partial/\partial T$ becomes spacelike. It is in this nonstatic domain (regions **F** and **P** in Fig. 12) where we expect, in analogy with the results in Minkowski space–time, to find fields which have radiative properties. $\partial/\partial T$ is the Killing vector also in the nonstatic regions, however, it is spacelike here, as it is typical for a boost Killing vector in Minkowski space. The fields of uniformly accelerated charges in de Sitter space–time are invariant under the boosts along $\partial/\partial T$ everywhere. They are thus boost-rotation symmetric as the Born fields in Minkowski space–time.

In the cosmological coordinates, respectively, in their rescaled versions, the fields are, of course, time dependent. Here we expect the effects of the expansion/contraction of de Sitter universe to be manifested. Indeed, considering in any of the cosmological frames the spatial coordinates fixed, and examining the fields along the timelike geodesics, we discover that the fields exponentially decay at large times, i.e., as $\mathcal{I}^+$ is approached. More specifically, with the

spherical coordinates χ, ϑ, φ fixed, the factor $\mathcal{Q}$ behaves as $\exp(\tau/\ell_\Lambda)$ at large times τ, and hence, we obtain $\mathrm{E}_{\mathrm{sph}} \approx c_1 \exp(-2\tau/\ell_\Lambda)\mathrm{e}_\chi + c_2 \exp(-3\tau/\ell_\Lambda)\mathrm{e}_\vartheta$, $\mathrm{B}_{\mathrm{sph}} \approx b_1 \exp(-2\tau/\ell_\Lambda)\mathrm{e}_\varphi, c_1, c_2, b_1$ being constants. The electric field thus becomes radial at large τ. Similarly, in flat cosmological coordinates we find $\mathrm{E}_{\mathrm{flat}} \approx c_1 \exp(-2\check{\tau}/\ell_\Lambda)\mathrm{e}_{\check{r}}$, $\mathrm{B}_{\mathrm{flat}} \approx b_1 \exp(-2\check{\tau}/\ell_\Lambda)\mathrm{e}_\varphi$. In the hyperbolic cosmological coordinates the proper time η appears instead of $\check{\tau}$. The rapid decay of the fields along timelike worldlines at large times is caused by the exponential expansion (at large times) of the spatial slices τ=constant (respectively, $\check{\tau}, \eta$=constant). Although our fields are just test fields, their exponential decay is another manifestation of the "cosmic no-hair phenomenon:" geodesic observers in space–times with $\Lambda > 0$ see at large times these space–times to approach the de Sitter universe exponentially fast—the universe becomes "bald" (see, e.g., Refs. 22 and 23). Clearly, as one approaches past infinity $\mathcal{I}^-$ ($\tau \to -\infty$), the fields also decay exponentially.

It is interesting to notice the character of the field as it would be seen by the observers at rest with respect to the hyperbolic cosmological coordinates in the limit at which the particles "enter" the region covered by these observers across the horizon $\tilde{t} = \tilde{r}$ (cf. Fig. 4), given in the hyperbolic coordinates by $\eta \to 0$, $\rho \to \infty$. As discussed in Sec. IV, the observed velocity (4.17) of the charges at this boundary is (in the limit) equal to the velocity of light. Employing the transformation formulas (A86), it is easy to see that at this boundary $|\sinh(\eta/\ell_\Lambda)\sinh(\rho/\ell_\Lambda)| \to 1$. Hence, the factor $\mathcal{Q}$ is finite here (as it is evident from its scalar character and its finiteness in the global standard coordinates). Also, the radial part of the electric field remains finite. However, E^ϑ diverges as $\exp(\rho/\ell_\Lambda)$ here, indicating that the field has a character of an impulse, in fact, rather of an impulsive wave—indeed, Eq. (6.10) implies $|\mathrm{E}^\vartheta| = |\mathrm{B}^\varphi|$. The situation appears to be analogous to the field of a static charge viewed from an inertial frame boosted to the velocity of light in Minkowski space–time (see, e.g., Ref. 55).

B. Fields in coordinates centered on the particles

As expected, a remarkable simplification occurs when the fields are evaluated in the coordinates at the origin of which the charges are situated at all times. Since the accelerated coordinates T', R', ϑ' and the C-metric-like coordinates are simply related by Eqs. (5.8), the discussion of the field properties is the same in both these frames. Namely, notice that both coordinate systems are tied with the same orthonormal tetrad, and they thus define the same splitting of the field into the electric and magnetic parts. In these coordinates, we find the factor $\mathcal{Q}$ to read

$$\mathcal{Q} = \cosh\alpha_{\mathrm{o}} \frac{1}{R'} + \sinh\alpha_{\mathrm{o}} \frac{1}{\ell_\Lambda} \cos\vartheta' = \frac{1}{\ell_\Lambda}(v\cosh\alpha_{\mathrm{o}} - \xi\sinh\alpha_{\mathrm{o}}). \tag{6.24}$$

The scalar field is again given by $\Phi = (s/4\pi)\mathcal{Q}^{-1}$, and the electromagnetic field also acquires now an extremely simple form,

$$\mathrm{F} = \frac{e}{4\pi}\frac{1}{R'^2}\mathrm{d}R' \wedge \mathrm{d}T' = \frac{e}{4\pi}\mathrm{d}\tau \wedge \mathrm{d}v, \tag{6.25}$$

$$\mathrm{E}_{\mathrm{acc}} = \frac{e}{4\pi}\frac{1}{\mathcal{Q}^2}e_{R'}, \quad \mathrm{B}_{\mathrm{acc}} = 0. \tag{6.26}$$

The magnetic field vanishes in the frame tied to the accelerated and C-metric coordinates, the electric field has precisely the Coulomb form, with the factor $\mathcal{Q}$ playing the role of a distance.

As signalized above already, the factor $\mathcal{Q}$ turns out to be the Robinson-Trautman radial coordinate [see Eq. (6.28) below], i.e., the affine parameter distance along null geodesics. The geometrical role of $\mathcal{Q}$ was elucidated in Sec. V B. Considering a fixed point in de Sitter universe and a light cone emanating from this point, three typical situations can arise as illustrated in Fig. 12. For a point B from the regions **N** or **S**, there are two null geodesics, one past-pointing, the other future-pointing, each of which crosses the worldline of the same particle, say $w_\odot$ (in case of B from **N**), at points B_{ret} and B_{adv} (see Fig. 12). Since $\mathcal{Q}$ is equal to the (specific) affine parameter

distance which is the same from B_{ret} as from B_{adv} (see Sec. V B), we can interpret the field (6.26) as arising from purely retarded, respectively, advanced effects from B_{ret}, respectively B_{adv}; or, equivalently, as a combination of retarded and advanced effects from these points. In the second situation, when the fixed point, say A, is located "above the roof" (in the region **F**), there are two past-oriented null geodesics emanating from it which cross now both particles $w_{\odot}$ and $w_{\otimes}$ at points $A_{\odot}$ and $A_{\otimes}$ (see Fig. 12). The field can be interpreted as arising from retarded effects only, either as a combination from both particles $w_{\odot}$ and $w_{\otimes}$, or as the retarded field from just one of them. Finally, for a point from the region **P** the field can analogously be interpreted in terms of advanced effects.

As we discussed in Sec. V A and illustrate in detail in Appendix, the accelerated coordinates (similarly as the static coordinates to which they go over for a vanishing acceleration) are static, i.e., the vector $\partial/\partial T'$ tangent to the orbits of the Killing vector is timelike, only in the regions **N** and **S** (cf. Figs. 10 and 12). Observers following the orbits of the Killing vector are thus confined to the regions **N** and **S**, and they cannot detect the fields in the region **F** (respectively, **P**). Nevertheless, notice that although the time coordinate T' diverges at the horizon $R=\ell_{\Lambda}$, the radial coordinate R' is perfectly finite there, $R'=\ell_{\Lambda}$ [cf. Eq. (5.6) with $R=\ell_{\Lambda}$], and the field (6.25) is meaningful in the region **F** (or **P**) as well. Since here the roles of the coordinates R' and T' are interchanged, R' becoming a time coordinate, the field becomes time dependent. As mentioned above, we do not expect to find radiative properties in the regions **N** and **S**. Indeed, in accelerated coordinates the field (6.26) is static Coulomb field, with $\mathcal{Q}$ playing the role of a distance. However, the radiative properties of the whole field in the wave zone in the region **F** are not evident from the time-dependent, purely electric field in the accelerated coordinates with R' as a time coordinate.

It is worthwhile to recall that with finite sources in Minkowski space–time the field at any event is of a general algebraic type; only asymptotically, at large distances, its features approach those of a null field ($\mathrm{E}^2-\mathrm{B}^2=0$, $\mathrm{E}\cdot\mathrm{B}=0$), if there is a radiation (see, e.g., Refs. 56 and 45). In case of a non-null field, one can always introduce a frame in which the electric and magnetic fields are collinear, or, in the language of the Newman-Penrose formalism, to choose such a null tetrad k, l, m, $\bar{\mathrm{m}}$, corresponding to the orthonormal tetrad, that the only nonvanishing null-tetrad component is $\Phi_1=1/(2\sqrt{2})\ (\mathrm{E}-i\mathrm{B})\cdot(\mathrm{k}-\mathrm{l})$ [see Eqs. (A114) for the explicit expressions of the null tetrad and Eqs. (A4) for the null-tetrad components of the electromagnetic field]. Such a situation arises precisely for the null tetrad associated with the accelerated coordinates: the null-tetrad components are simply

$$\Phi_1^{\mathrm{acc}}=-\frac{1}{2}\frac{e}{4\pi}\frac{1}{\mathcal{Q}^2},\quad \Phi_0^{\mathrm{acc}}=\Phi_2^{\mathrm{acc}}=0. \tag{6.27}$$

The vanishing of the other two null-tetrad components, Φ_0^{acc} and Φ_2^{acc}, has a deeper algebraic explanation: the null tetrad tied to the accelerated coordinates is special in the sense that it contains both principal null directions of the electromagnetic field. Inspecting the form of the null tetrad constructed from the orthonormal tetrad (A95), we observe that both these principal null directions are tangent to the "radial" surfaces ϑ', $\varphi=$constant in the accelerated coordinates.

The radiative properties are well exhibited in the Robinson-Trautman coordinates. As we discussed in Sec. V B, these coordinates are tied to the future null cones centered on the worldline of a particle. We consider the null cones with vertices on the particle $w_{\odot}$. Let us recall that the radial coordinate $\mathfrak{r}$ is the affine parameter along the generators of the null cones, each of which is given by $\mathfrak{u}$, ψ, φ fixed. Now, as mentioned above, it turns out that the factor $\mathcal{Q}$ is precisely equal to this affine parameter $\mathfrak{r}$,

$$\mathcal{Q}=\mathfrak{r}. \tag{6.28}$$

The scalar field is then simply given by

$$\Phi = \frac{s}{4\pi}\frac{1}{\mathfrak{r}}. \tag{6.29}$$

A remarkably nice form also acquires the electromagnetic field,

$$F = \frac{e}{4\pi}\left(\frac{1}{\mathfrak{r}^2}\mathrm{d}\mathfrak{u}\wedge\mathrm{d}\mathfrak{r} + a_{\mathrm{o}}\sin^2\vartheta'\mathrm{d}\mathfrak{u}\wedge\mathrm{d}\vartheta'\right) = \frac{e}{4\pi}\left(\frac{1}{\mathfrak{r}^2}\mathrm{d}\mathfrak{u}\wedge\mathrm{d}\mathfrak{r} + a_{\mathrm{o}}\sin^2\vartheta'\mathrm{d}\mathfrak{u}\wedge\mathrm{d}\psi\right). \tag{6.30}$$

The Newman-Penrose scalars are defined in terms of the null tetrad (A114), which is parallelly propagated from the source to the "observation point" along the rays $\mathfrak{u}$, ψ, φ=constant. They look as follows:

$$\Phi_0^{\mathrm{RT}} = 0, \quad \Phi_1^{\mathrm{RT}} = -\frac{1}{2}\frac{e}{4\pi}\frac{1}{\mathfrak{r}^2}, \quad \Phi_2^{\mathrm{RT}} = \frac{1}{\sqrt{2}}\frac{e}{4\pi}\frac{1}{\mathfrak{r}}a_{\mathrm{o}}\sin\vartheta'. \tag{6.31}$$

Now the radiative character of the field is transparent: the first term entering the peeling behavior, the scalar Φ_2, decays indeed as $\mathfrak{r}^{-1}$, and it is nonvanishing for a nonzero acceleration a_{o}. In the expressions (6.30) and (6.31), the de Sitter background is completely "hidden." The same form of the fields are obtained in case of uniformly accelerated charges in Minkowski space if the coordinates built on the null cones emanating from the particles are employed. A difference between both cases reveals itself only in the explicit dependence of the affine parameter $\mathfrak{r}$ on the coordinates of space–time points.

VII. BORN IN DE SITTER

Finally, we turn to the fields from the particles symmetrically located with respect to the origin $\chi=0$ (the "north pole") of the standard spherical coordinates. The particles are thus "born" asymptotically at the equator, $\chi=\pi/2$, at $\tau\to-\infty$, and return back at $\tau\to\infty$ with the opposite speeds (Fig. 8). Their fields, of course, are intrinsically the same as those considered in the preceding section but only now they represent the direct generalization of the classical Born solutions due to uniformly accelerated charges symmetrically located with respect to the origin of Minkowski space.

We shall find the generalized Born fields easily by using the transformation (4.21) which we applied to obtain the worldlines of the particles born at the equator from those born at the poles. The scalar field due to two equal scalar charges s moving along the worldlines $w_{\oplus}$ and $w_{\ominus}$ reads

$$\Phi = \frac{s}{4\pi}\Omega_{\mathrm{M}}^{-1}\frac{1}{\mathcal{R}}, \tag{7.1}$$

where the factor $\mathcal{R}$ is determined by

$$\mathcal{R} = \frac{\ell_\Lambda}{1+\cosh\dfrac{\tau}{\ell_\Lambda}\cos\chi}\left[\cosh^2\frac{\tau}{\ell_\Lambda}\sin^2\chi\sin^2\vartheta + \left(\sqrt{1+a_{\mathrm{o}}^2\ell_\Lambda^2}\cosh\frac{\tau}{\ell_\Lambda}\cos\chi - a_{\mathrm{o}}\ell_\Lambda\right)^2\right]^{1/2}, \tag{7.2}$$

and the conformal factor Ω_{M} is given by [cf. Eq. (3.19)]

$$\Omega_{\mathrm{M}} = 1+\cosh\frac{\tau}{\ell_\Lambda}\cos\chi. \tag{7.3}$$

This factor is left in the explicit form here, in contrast to the preceding section, since it explicitly exhibits conformal relation of the scalar field under conformal mappings (3.19) between de Sitter space and Minkowski space M. This relation will be used in the following to perform the limit from the Born field in de Sitter to the Born field in Minkowski space–time.

The electromagnetic field produced by charge e moving along the worldline $w_{\oplus}$ and by symmetrically located charge $-e$ moving along $w_{\ominus}$ has the following form:

$$\mathrm{F}_{\mathrm{BdS}} = \frac{e}{4\pi}\frac{\ell_\Lambda^2}{\mathcal{R}^3}\frac{\cosh\dfrac{\tau}{\ell_\Lambda}\sin\vartheta}{\left(1+\cosh\dfrac{\tau}{\ell_\Lambda}\cos\chi\right)^3}\Bigg[a_{\mathrm{o}}\ell_\Lambda^2\sinh\frac{\tau}{\ell_\Lambda}\cosh\frac{\tau}{\ell_\Lambda}\sin^2\chi\,\mathrm{d}\chi\wedge\mathrm{d}\vartheta$$

$$+\left(\sqrt{1+a_{\mathrm{o}}^2\ell_\Lambda^2}\cosh\frac{\tau}{\ell_\Lambda}\cos\chi - a_{\mathrm{o}}\ell_\Lambda\right)\cot\vartheta\,\mathrm{d}\tau\wedge\mathrm{d}\chi \tag{7.4}$$

$$-\left(\sqrt{1+a_{\mathrm{o}}^2\ell_\Lambda^2}\cosh\frac{\tau}{\ell_\Lambda} - a_{\mathrm{o}}\ell_\Lambda\cos\chi\right)\sin\chi\,\mathrm{d}\tau\wedge\mathrm{d}\vartheta\Bigg].$$

with factor $\mathcal{R}$ given by (7.2). In the tetrad tied to the standard spherical coordinates the electric and magnetic fields become

$$\mathrm{E}^{\mathrm{BdS}}_{\mathrm{sph}} = -\frac{e}{4\pi}\frac{\ell_\Lambda}{\mathcal{R}^3}\frac{1}{\left(1+\cosh\dfrac{\tau}{\ell_\Lambda}\cos\chi\right)^3}\Bigg[\left(\sqrt{1+a_{\mathrm{o}}^2\ell_\Lambda^2}\cosh\frac{\tau}{\ell_\Lambda}\cos\chi - a_{\mathrm{o}}\ell_\Lambda\right)\cot\vartheta\,\mathrm{e}_\chi$$

$$-\left(\sqrt{1+a_{\mathrm{o}}^2\ell_\Lambda^2}\cosh\frac{\tau}{\ell_\Lambda} - a_{\mathrm{o}}\ell_\Lambda\cos\chi\right)\sin\chi\,\mathrm{e}_\vartheta\Bigg], \tag{7.5}$$

$$\mathrm{B}^{\mathrm{BdS}}_{\mathrm{sph}} = \frac{e}{4\pi}\frac{a_{\mathrm{o}}\ell_\Lambda^2}{\mathcal{R}^3}\frac{\sinh\dfrac{\tau}{\ell_\Lambda}\sin\chi\sin\vartheta}{\left(1+\cosh\dfrac{\tau}{\ell_\Lambda}\cos\chi\right)^3}\,\mathrm{e}_\varphi.$$

In the standard rescaled (conformally Einstein) coordinates the expressions (7.4) and (7.5) slightly simplify

$$\frac{\mathcal{R}}{\ell_\Lambda} = \frac{\left[\left(a_{\mathrm{o}}\ell_\Lambda\sin\tilde{t} - \sqrt{1+a_{\mathrm{o}}^2\ell_\Lambda^2}\cos\tilde{r}\right)^2 + \sin^2\tilde{r}\sin^2\vartheta\right]^{1/2}}{\sin\tilde{t}+\cos\tilde{r}}, \tag{7.6}$$

$$\Omega_{\mathrm{M}} = \frac{\cos\tilde{r}+\sin\tilde{t}}{\sin\tilde{t}}, \tag{7.7}$$

$$\mathrm{F}_{\mathrm{BdS}} = -\frac{e}{4\pi}\frac{\ell_\Lambda^3}{\mathcal{R}^3}\frac{\sin\vartheta}{(\sin\tilde{t}+\cos\tilde{r})^3}\Big[a_{\mathrm{o}}\ell_\Lambda\sin^2\tilde{r}\cos\tilde{t}\,\mathrm{d}\tilde{r}\wedge\mathrm{d}\vartheta$$

$$-\left(\sqrt{1+a_{\mathrm{o}}^2\ell_\Lambda^2}\cos\tilde{r} - a_{\mathrm{o}}\ell_\Lambda\sin\tilde{t}\right)\cot\vartheta\,\mathrm{d}\tilde{t}\wedge\mathrm{d}\tilde{r} \tag{7.8}$$

$$+\left(\sqrt{1+a_{\mathrm{o}}^2\ell_\Lambda^2} - a_{\mathrm{o}}\ell_\Lambda\cos\tilde{r}\sin\tilde{t}\right)\sin\tilde{r}\,\mathrm{d}\tilde{t}\wedge\mathrm{d}\vartheta$$

$$\mathrm{E}^{\mathrm{BdS}}_{\mathrm{CE}} = \frac{e}{4\pi}\frac{\ell_\Lambda \sin^2\tilde{t}}{\mathcal{R}^3(\sin\tilde{t}+\cos\tilde{r})^3}\Big[-\Big(\sqrt{1+a_\mathrm{o}^2\ell_\Lambda^2}\cos\tilde{r}-a_\mathrm{o}\ell_\Lambda\sin\tilde{t}\Big)\cos\vartheta\,\mathrm{e}_{\tilde{r}} + \Big(\sqrt{1+a_\mathrm{o}^2\ell_\Lambda^2}-a_\mathrm{o}\ell_\Lambda\sin\tilde{t}\cos\tilde{r}\Big)\sin\vartheta\,\mathrm{e}_\vartheta\Big], \tag{7.9}$$

$$\mathrm{B}^{\mathrm{BdS}}_{\mathrm{CE}} = -\frac{e}{4\pi}\frac{a_\mathrm{o}\ell_\Lambda^2\sin^2\tilde{t}}{\mathcal{R}^3(\sin\tilde{t}+\cos\tilde{r})^3}\cos\tilde{t}\sin\tilde{r}\sin\vartheta\,\mathrm{e}_\varphi.$$

The character of these fields was discussed in the preceding section for the particles $w_\odot$ and $w_\otimes$. One must only rotate all the structures by $\pi/2$ in the χ direction; hence, for example, the sphere of symmetry changes from $\chi=\pi/2$ to $\vartheta=\pi/2$.

There is some interest in having the fields available also in the hyperbolic cosmological coordinates. They cover only those regions of the fields in which we assume the radiative properties will be manifested. The sources producing the fields are not covered by these coordinates (cf. Fig. 8). The fields in the hyperbolic cosmological coordinates look as follows:

$$\mathcal{R} = \frac{1}{2b_\mathrm{o}}\left[\left(b_\mathrm{o}^2+\ell_\Lambda^2\tanh^2\frac{\eta}{2\ell_\Lambda}\right)^2+4b_\mathrm{o}^2\tanh^2\frac{\eta}{2\ell_\Lambda}\sinh^2\frac{\rho}{\ell_\Lambda}\sin^2\vartheta\right]^{1/2}, \tag{7.10}$$

$$\Omega_\mathrm{M} = 1+\cosh\frac{\eta}{\ell_\Lambda} = 2\cosh^2\frac{\eta}{2\ell_\Lambda}, \tag{7.11}$$

$$\mathrm{F}_{\mathrm{BdS}} = \frac{e}{4\pi}\frac{\ell_\Lambda^3}{\mathcal{R}^3}\frac{1}{2b_\mathrm{o}\Omega_\mathrm{M}^2} \times\left[\left(\frac{b_\mathrm{o}^2}{\ell_\Lambda^2}+\tanh^2\frac{\eta}{2\ell_\Lambda}\right)\sinh\frac{\eta}{\ell_\Lambda}\left(\frac{1}{\ell_\Lambda}\cos\vartheta\,\mathrm{d}\eta\wedge\mathrm{d}\rho-\sinh\frac{\rho}{\ell_\Lambda}\cosh\frac{\rho}{\ell_\Lambda}\sin\vartheta\,\mathrm{d}\eta\wedge\mathrm{d}\vartheta\right) -\left(\frac{b_\mathrm{o}^2}{\ell_\Lambda^2}-\tanh^2\frac{\eta}{2\ell_\Lambda}\right)\sinh^2\frac{\eta}{\ell_\Lambda}\sinh^2\frac{\rho}{\ell_\Lambda}\sin\vartheta\,\mathrm{d}\rho\wedge\mathrm{d}\vartheta\right], \tag{7.12}$$

$$\mathrm{E}^{\mathrm{BdS}}_{\mathrm{hyp}} = \frac{e}{4\pi}\frac{\ell_\Lambda^2}{\mathcal{R}^3}\frac{1}{2b_\mathrm{o}\Omega_\mathrm{M}^2}\left(\frac{b_\mathrm{o}^2}{\ell_\Lambda^2}+\tanh^2\frac{\eta}{2\ell_\Lambda}\right)\left(-\cos\vartheta\,\mathrm{e}_\rho+\cosh\frac{\rho}{\ell_\Lambda}\sin\vartheta\,\mathrm{e}_\vartheta\right), \tag{7.13}$$

$$\mathrm{B}^{\mathrm{BdS}}_{\mathrm{hyp}} = -\frac{e}{4\pi}\frac{\ell_\Lambda^2}{\mathcal{R}^3}\frac{\sinh\dfrac{\rho}{\ell_\Lambda}}{2b_\mathrm{o}\Omega_\mathrm{M}^2}\left(\frac{b_\mathrm{o}^2}{\ell_\Lambda^2}-\tanh^2\frac{\eta}{2\ell_\Lambda}\right)\sin\vartheta\,\mathrm{e}_\varphi.$$

Finally, we wish to describe the limiting procedure which leads from the generalized Born solutions directly to their counterparts in Minkowski space–time. For this purpose it is natural to employ the conformally Minkowski coordinates t,r,ϑ,φ introduced in Eq. (3.17), with the inverse transformation given in Appendix, Eq. (A17). Transforming the fields of the particles $w_\oplus$, $w_\ominus$ from the conformally Einstein coordinates to the conformally Minkowski coordinates, we arrive at the following intriguing forms. The scalar field is given by Eq. (7.1) where now the factors $\mathcal{R}$ and Ω_M are determined by

$$\mathcal{R} = \frac{1}{2b_\mathrm{o}}\sqrt{(b_\mathrm{o}^2+t^2-r^2)^2+4b_\mathrm{o}^2r^2\sin^2\vartheta}, \tag{7.14}$$

$$\Omega_{\mathrm{M}} = \frac{2\ell_\Lambda^2}{\ell_\Lambda^2 - t^2 + r^2}. \tag{7.15}$$

Notice that factor $\mathcal{R}$ coincides with the expression (2.11) in Minkowski space. The electromagnetic field reads

$$\begin{aligned} \mathrm{F}_{\mathrm{BdS}} = &- \frac{e}{4\pi}\frac{1}{2b_{\mathrm{o}}}\frac{1}{\mathcal{R}^3}[-2tr^2 \sin\vartheta\, \mathrm{d}r\wedge \mathrm{d}\vartheta - (b_{\mathrm{o}}^2 + t^2 - r^2)\cos\vartheta\, \mathrm{d}t\wedge \mathrm{d}r \\ &+ r(b_{\mathrm{o}}^2 + t^2 + r^2)\sin\vartheta\, \mathrm{d}t\wedge \mathrm{d}\vartheta], \end{aligned} \tag{7.16}$$

and the electric and magnetic parts of the field turn out to be

$$\begin{aligned} \mathrm{E}_{\mathrm{CM}}^{\mathrm{BdS}} &= \frac{e}{4\pi}\frac{1}{\mathcal{R}^3}\frac{1}{2b_{\mathrm{o}}\Omega_{\mathrm{M}}^2}[(b_{\mathrm{o}}^2 + t^2 - r^2)\cos\vartheta\, \mathrm{e}_r - (b_{\mathrm{o}}^2 + t^2 + r^2)\sin\vartheta\, \mathrm{e}_\vartheta], \\ \mathrm{B}_{\mathrm{CM}}^{\mathrm{BdS}} &= \frac{e}{4\pi}\frac{1}{\mathcal{R}^3}\frac{1}{b_{\mathrm{o}}\Omega_{\mathrm{M}}^2} tr\sin\vartheta\, \mathrm{e}_\varphi. \end{aligned} \tag{7.17}$$

To connect these fields with their counterparts in flat space, note first that they are conformally related by the conformal transformation (3.19). Under the conformal mapping, the field Φ_{BdS} must be multiplied by factor Ω_{M}, which gives $\Phi_{\mathrm{M}} = (s/4\pi)\mathcal{R}^{-1}$, and $\mathrm{F}_{\mathrm{BdS}}$ in (7.16) remains unchanged. The transformed fields then coincide with the classical Born fields (2.9), (2.11), and (2.13).

In order to see the limit for $\Lambda \to 0$, we parametrize the sequence of de Sitter spaces by Λ, and identify them in terms of coordinates t, r, ϑ, φ. As $\Lambda = 3/\ell_\Lambda^2 \to 0$, Eq. (3.19) implies $(\Omega_{\mathrm{M}})_\Lambda \to 2$, $(g_{\mathrm{dS}})_\Lambda \to 4g_{\mathrm{M}}$. After the trivial rescaling of t, r by factor 2, the standard Minkowski metric is obtained. The limit of the scalar and electromagnetic fields (7.1) and (7.16), in which b_{o} is kept constant [with $a_{\mathrm{o}} = (1 - b_{\mathrm{o}}^2\ell_\Lambda^{-2})/(2b_{\mathrm{o}})$—cf. Eq. (4.29)], leads precisely to the scalar and electromagnetic Born fields (2.9) and (2.13) in flat space. Because of the rescaling of the coordinates by factor 2, we get the physical acceleration equal to $1/b_{\mathrm{o}} = 2a_{\mathrm{o}}$, and the scalar field rescaled by $1/2$. The explicit limiting procedure carrying the generalized Born fields in de Sitter universe back into the classical Born solution in Minkowski space has thus been demonstrated.

VIII. CONCLUDING REMARKS

Since 1998 the observations of high-redshift supernovae indicate, with an increasing evidence, that we live in an accelerating universe with a positive cosmological constant (for most recent observations see, e.g., Ref. 57). Vacuum energy seems to dominate in the universe and it is thus of interest to understand fundamental physics in the vacuum dominated de Sitter space–time.

In the present work, we constructed the fields of uniformly accelerated charges in this universe. They go over to the classical Born fields in Minkowski space in the limit of a vanishing cosmological constant. Aside from some similarities found, the generalized fields provide the models showing how a positive cosmological constant implies essential differences from physics in flat space–time. For example, advanced effects occur inevitably due to the spacelike character of the past infinity $\mathcal{I}^-$ and its consequence—the existence of the past particles' horizons, respectively, of the "creation light cones" of the particles' worldlines.

Since de Sitter space–time, according to our present understanding, appears to be not only an appropriate basic model for studying future cosmological epochs, but it is commonly used also for exploring the inflationary era, various physical processes have been investigated in de Sitter space from the perspective of the early universe, among them, the effects of quantum field theory. Also in quantum contexts, however, problems arise from combining the causal structure of the full de Sitter space–time with the constraint equations (see Ref. 58 for a recent review). These problems are associated with the "insufficiency of purely retarded fields" in space–times with a spacelike $\mathcal{I}^-$. We analyzed this issue in detail for the classical electromagnetic and scalar fields with sources in Ref. 24.

Another intriguing implication of the rapid expansion of de Sitter universe due to a positive cosmological constant is manifested in the exponential decay of the fields at large times. We noticed this "cosmic no-hair phenomenon" explicitly on the late-time behavior of the fields due to accelerated charges.

In the present paper we wished to give all details on the construction of the fields and on coordinate frames useful in understanding their various aspects, including their relation to their counterparts in flat space–time. We did not here analyze the radiative characteristics of the fields. In the Introduction we indicated that radiative properties depend on the way in which a given point of infinity is approached. This is briefly described at the end of our paper.[25]

In de Sitter space–time it is not *a priori* clear, as it is in special relativity, how to define global physical quantities like energy or energy flux. Such issues connected with the question of radiation from "Born in de Sitter" will be considered in a future presentation.

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APPENDIX A: THE PALETTE OF COORDINATE SYSTEMS IN DE SITTER SPACE–TIME

Nine families of coordinate systems are here introduced, described analytically and illustrated graphically. The corresponding forms of de Sitter metric, orthonormal tetrads and interrelations between the systems are given. All these systems are suitable for exhibiting various features of de Sitter space; two families are directly associated with uniformly accelerated particles. Although the majority (though not all) of these coordinate systems undoubtedly appeared in literature in some form already, they are scattered and, as far as we know, not summarized as comprehensively as in the following. In the main text we refer frequently to this Appendix, but the Appendix can be read independently. We hope it can serve as a catalogue useful for analyzing various aspects of physics in de Sitter universe.

By a family of coordinate systems we mean the systems with the same coordinate lines; e.g., $\{x^\mu\}$ and $\{y^\mu\}$ where $x^1=x^1(y^1)$, $x^2=x^2(y^2)$, etc. Seven of our families have the same spherical angular coordinates ϑ,φ, accelerated and Robinson-Trautman coordinates mix three coordinates, only azimuthal coordinate φ remains unchanged.

The homogeneous normalized metric on two-spheres (the metric "in angular direction") is denoted by

$$\mathrm{d}\omega^2 = \mathrm{d}\vartheta^2 + \sin^2\vartheta\,\mathrm{d}\varphi^2. \tag{A1}$$

The radial coordinates label directions pointing out from the pole and acquire only positive values. However, transformations among coordinates take simpler forms if we allow radial coordinates to take on negative values as well. This causes no problems if, denoting by t and r the prototypes of time and radial coordinates, we adopt the convention that the following two values of coordinates describe the same point:

$$\{t,r,\vartheta,\varphi\} \leftrightarrow \{t,-r,\pi-\vartheta,\varphi+\pi\}. \tag{A2}$$

Hence, intuitively we may consider a point with $-r<0$ and ϑ,φ fixed to lie on diametrically opposite side of the pole $r=0$ with respect to the point $r>0,\vartheta,\varphi$.

The orthonormal tetrad $\mathrm{e}_t,\mathrm{e}_r,\mathrm{e}_\vartheta,\mathrm{e}_\varphi$ associated with a coordinate system is tangent to the coordinate lines and oriented (with few exceptions) in the directions of growing coordinates. It is chosen in such a way that the external product $\mathrm{e}^t\wedge\mathrm{e}^r\wedge\mathrm{e}^\vartheta\wedge\mathrm{e}^\varphi$ of 1-forms of the dual tetrad has

always the same orientation. Since all forms of the metric contain the term (A1) the only component $(e_\varphi)^\varphi$ of the tetrad vector e_φ in coordinate frame $\{\partial/\partial x^\mu\}$ is related to the ϑ-component of e_ϑ as

$$(e_\varphi)^\varphi = \frac{1}{\sin\vartheta}(e_\vartheta)^\vartheta, \tag{A3}$$

and we thus omit e_φ henceforth.

In the standard Newman-Penrose null complex tetrad $k, l, m, \bar{m}$ with only nonvanishing inner products $k\cdot l=-1$, $m\cdot\bar{m}=1$, the electromagnetic field F is represented by three complex components:

$$\Phi_0 = F_{\alpha\beta}\, k^\alpha m^\beta, \quad \Phi_2 = F_{\alpha\beta}\, \bar{m}^\alpha l^\beta, \quad \Phi_1 = \tfrac{1}{2}\, F_{\alpha\beta}\,(k^\alpha l^\beta - m^\alpha \bar{m}^\beta). \tag{A4}$$

The null tetrad can be specified directly [as it will be done in the case of Robinson-Trautman coordinates in Eq. (A114)], or it can be associated with any orthonormal tetrad, say t, q, r, s, by relations

$$k = \frac{1}{\sqrt{2}}(t+q), \quad l = \frac{1}{\sqrt{2}}(t-q), \quad m = \frac{1}{\sqrt{2}}(r - i\,s), \quad \bar{m} = \frac{1}{\sqrt{2}}(r + i\,s). \tag{A5}$$

Here, t and q are timelike and spacelike unit vectors, respectively, typically in a direction of "time" and "radial" coordinate, and r, s are spacelike unit vectors in angular directions, $r=e_\vartheta$, $s=e_\varphi$.

For each coordinate family we give the diagram illustrating section ϑ, φ=constant with the radial coordinate taking on both positive and negative values. The diagrams thus represent the history of the entire main circle of the spatial spherical section of de Sitter universe. The left and right edges of the diagrams represent the south pole and should be considered as identified; the central vertical line describes the history of the north pole. Recalling the meaning of the negative radial coordinate we could eliminate the left half of each of the diagrams by transforming it into the right one by replacements $\{\vartheta,\varphi\}\to\{\pi-\vartheta,\varphi+\pi\}$. However, it is instructive to keep both halves for better understanding of the spatial topology of the sections. All diagrams are compactified—they are adapted to the standard rescaled coordinates $\tilde{t}$, $\tilde{r}$ (see below). The past and future conformal infinites are drawn as double lines. The ranges of time and radial coordinates are shown, the orientation of coordinate labels indicates the directions of the growth of corresponding coordinates.

We will also introduce several sign factors. The values of these factors in different domains of space–time are indicated in Fig. 13.

1. The spherical cosmological family:

The first family consists of the standard or spherical cosmological coordinates τ, χ, ϑ, φ, and of the standard rescaled or conformally Einstein coordinates $\tilde{t}$, $\tilde{r}$, ϑ, φ (where $\tilde{r}\equiv\chi$). These coordinates cover de Sitter space–time globally. They are associated with cosmological observers with homogeneous spatial sections of positive spatial curvature. The coordinates are adjusted to the spherical symmetry of the spatial sections, χ, ϑ, and φ are standard angular coordinates. The coordinate τ is a proper time along the worldlines of the cosmological observers given by χ, ϑ, φ=constant. The vector $\partial/\partial\tau$ is a conformal Killing vector which is everywhere timelike. The rescaled coordinates $\tilde{t}$, $\tilde{r}$, ϑ, φ can also be viewed as the standard coordinates of the conformally related Einstein universe; they cover smoothly both conformal infinities $\mathcal{I}^\pm$ of de Sitter space–time. (See Fig. 14.)

Metric and relation between coordinates

$$g = -\,d\tau^2 + \ell_\Lambda^2 \cosh^2(\tau/\ell_\Lambda)(d\chi^2 + \sin^2\chi\, d\omega^2), \tag{A6}$$

$$g = \ell_\Lambda^2 \sin^{-2}\tilde{t}\,(-\,d\tilde{t}^2 + d\tilde{r}^2 + \sin^2\tilde{r}\, d\omega^2), \tag{A7}$$

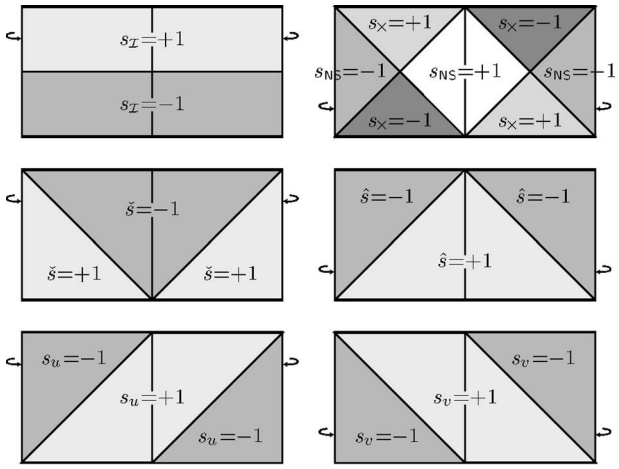

FIG. 13. The values of the factors $s_{\mathcal{I}}$, s_{NS}, $s_\times$, $\check{s}$, $\hat{s}$, s_u, and s_v in various regions of de Sitter space. The factors are defined in Eqs. (A21), (A36), (A61), (A73), (A74), and (A128), respectively. The factor $s_\times$ is used only in the expressions for static coordinates in the region where the Killing vector is spacelike. Therefore, we indicated the values of $s_\times$ only in those regions, although Eq. (A74) defines $s_\times$ everywhere. The factors $s_\times$, s_u, and s_v are defined only for any given section ϑ=constant, but not as unique functions on the whole space–time (they are not symmetric with respect to the pole). This is related to our convention using negative radial coordinates, cf. the text below Eq. (A1).

$$\tan\frac{\tilde{t}}{2}=\exp\frac{\tau}{\ell_\Lambda},\quad \cot\tilde{t}=-\sinh\frac{\tau}{\ell_\Lambda},\quad \sin\tilde{t}=\cosh^{-1}\frac{\tau}{\ell_\Lambda},\quad \cos\tilde{t}=-\tanh\frac{\tau}{\ell_\Lambda}, \tag{A8a}$$

$$\tilde{r}=\chi. \tag{A8b}$$

The ranges of coordinates are

$$\tau\in\mathbb{R},\quad \chi\in(-\pi,\pi),\quad \tilde{t}\in(0,\pi),\quad \tilde{r}\in(-\pi,\pi), \tag{A9}$$

with negative values of radial coordinates χ, $\tilde{r}$ interpreted in accordance with Eq. (A2).

Orthonormal tetrad,

$$\mathrm{e}_\tau=\frac{\partial}{\partial\tau}=\frac{1}{\ell_\Lambda}\sin\tilde{t}\,\frac{\partial}{\partial\tilde{t}},$$

$$\mathrm{e}_\chi=\frac{1}{\ell_\Lambda}\cosh^{-1}\frac{\tau}{\ell_\Lambda}\frac{\partial}{\partial_\chi}=\frac{1}{\ell_\Lambda}\sin\tilde{t}\,\frac{\partial}{\partial\tilde{r}}, \tag{A10}$$

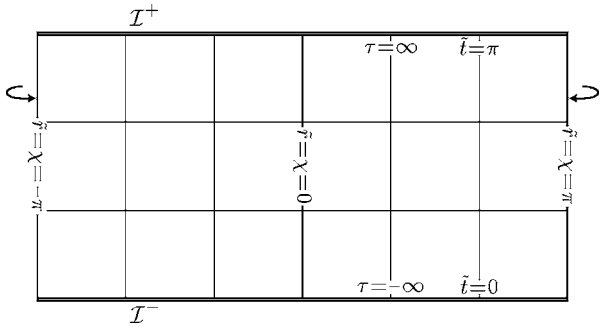

FIG. 14. The spherical cosmological family of coordinates.

$$\mathrm{e}_\vartheta = \frac{1}{\ell_\Lambda}\frac{1}{\cosh(\pi/\ell_\Lambda)\sin\chi}\frac{\partial}{\partial\vartheta} = \frac{1}{\ell_\Lambda}\frac{\sin\tilde{t}}{\sin\tilde{r}}\frac{\partial}{\partial\vartheta}\,.$$

Relation to flat cosmological family,

$$\tan\tilde{t} = \frac{2\ell_\Lambda\hat{t}}{\ell_\Lambda^2 - \hat{t}^2 + \hat{r}^2} = \frac{2\ell_\Lambda\check{t}}{\ell_\Lambda^2 - \check{t}^2 + \check{r}^2}\,, \quad \tan\tilde{r} = \frac{2\ell_\Lambda\hat{r}}{\ell_\Lambda^2 + \hat{t}^2 - \hat{r}^2} = \frac{2\ell_\Lambda\check{r}}{\ell_\Lambda^2 + \check{t}^2 - \check{r}^2}\,. \tag{A11}$$

Relation to hyperbolic cosmological coordinates,

$$\cot\tilde{t} = -\sinh\frac{\eta}{\ell_\Lambda}\cosh\frac{\rho}{\ell_\Lambda}\,, \quad \tan\tilde{r} = \tanh\frac{\eta}{\ell_\Lambda}\sinh\frac{\rho}{\ell_\Lambda}\,. \tag{A12}$$

Relation to static family in timelike domains **N**, **S**,

$$\tan\tilde{t} = -s_{\mathbf{NS}}\frac{\ell_\Lambda}{\sqrt{\ell_\Lambda^2 - R^2}}\sinh^{-1}\frac{T}{\ell_\Lambda}, \quad \tan\tilde{r} = s_{\mathbf{NS}}\frac{R}{\sqrt{\ell_\Lambda^2 - R^2}}\cosh^{-1}\frac{T}{\ell_\Lambda}, \tag{A13}$$

$$\tan\tilde{t} = -s_{\mathbf{NS}}\frac{\cosh\dfrac{\bar{r}}{\ell_\Lambda}}{\sinh\dfrac{\bar{t}}{\ell_\Lambda}}\,, \quad \tan\tilde{r} = s_{\mathbf{NS}}\frac{\sinh\dfrac{\bar{r}}{\ell_\Lambda}}{\cosh\dfrac{\bar{t}}{\ell_\Lambda}}\,, \tag{A14}$$

where $s_{\mathbf{NS}} = +1(-1)$ in domain **N** (**S**), cf. Eq. (A61).

Relation to static family in spacelike domains **F**, **P**,

$$\tan\tilde{t} = \frac{-s_{\mathcal{I}}\ell_\Lambda}{\sqrt{R^2 - \ell_\Lambda^2}}\cosh^{-1}\frac{T}{\ell_\Lambda}, \quad \tan\tilde{r} = \frac{s_{\mathcal{I}}R}{\sqrt{R^2 - \ell_\Lambda^2}}\sinh^{-1}\frac{T}{\ell_\Lambda}, \tag{A15}$$

$$\tan\tilde{t} = s_\times\frac{\sinh\dfrac{\bar{r}}{\ell_\Lambda}}{\cosh\dfrac{\bar{t}}{\ell_\Lambda}}\,, \quad \tan\tilde{r} = s_\times\frac{\cosh\dfrac{\bar{r}}{\ell_\Lambda}}{\sinh\dfrac{\bar{t}}{\ell_\Lambda}}\,, \tag{A16}$$

where $s_{\mathcal{I}} = -\mathrm{sign}\cos\tilde{t}$ and $s_\times = -s_{\mathcal{I}}\,\mathrm{sign}\,\tilde{r}$, cf. Eqs. (A73) and (A74).

Relation to conformally Minkowski coordinates,

$$\cot\tilde{t} = \frac{2\ell_\Lambda t}{t^2 - r^2 - \ell_\Lambda^2}\,, \quad \tan\tilde{r} = \frac{2\ell_\Lambda r}{t^2 - r^2 + \ell_\Lambda^2}\,. \tag{A17}$$

2. The flat cosmological family, type "$\vee$":

The first flat cosmological coordinate family (Fig. 15) consists of the flat cosmological coordinates $\check{\tau}$, $\check{r}$, ϑ, φ and of the rescaled flat cosmological coordinates $\check{t}$, $\check{r}$, ϑ, φ. Hypersurfaces $\check{\tau}$ =constant are homogeneous flat spaces and coordinate lines $\check{r}$, ϑ, φ=constant are worldlines of cosmological observers orthogonal to these hypersurfaces. They are geodesic with proper time $\check{\tau}$, the vector $\partial/\partial\check{\tau}$ is a conformal Killing vector. The coordinates cover de Sitter space–time smoothly, except for the past cosmological horizon, $\tilde{r}=\tilde{t}$, of the north pole where $\check{r}$, $\check{t}\to\pm\infty$. The coordinates thus split into two coordinate patches—"above" and "below" the horizon. The domain above the horizon has a cosmological interpretation of an exponentially expanding flat three-space. The rescaled coordinates can be viewed as inertial coordinates in the conformally related Minkowski space $\check{M}$, cf. Fig. 3; the domain above the horizon corresponds to the "lower half," $\check{t}<0$, of $\check{M}$, the domain below corresponds to the "upper half," $\check{t}>0$.

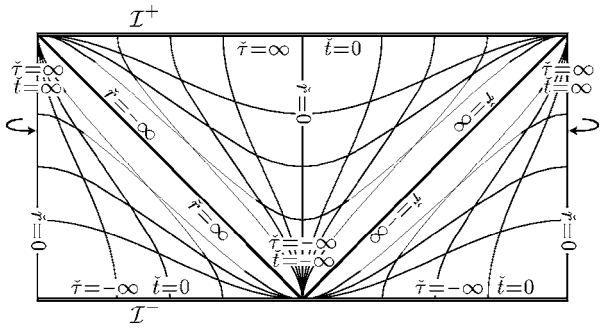

FIG. 15. The flat cosmological family, type "∨."

Metric and relation between coordinates,

$$g=\frac{\ell_\Lambda^2}{\check{t}^2}(-\,\mathrm{d}\check{t}^2+\mathrm{d}\check{r}^2+\check{r}^2\,\mathrm{d}\omega^2), \tag{A18}$$

$$g=-\,\mathrm{d}\check{\tau}^2+\exp(-\check{s}2\check{\tau}/\ell_\Lambda)(\mathrm{d}\check{r}^2+\check{r}^2\,\mathrm{d}\omega^2). \tag{A19}$$

$$\check{t}=\check{s}\,\ell_\Lambda\exp\left(\check{s}\frac{\check{\tau}}{\ell_\Lambda}\right), \tag{A20}$$

$$\check{s}=\operatorname{sign}\check{t}. \tag{A21}$$

The ranges of coordinates are

$$\begin{aligned}&\check{\tau}\in\mathbb{R},\quad \check{t}\in\mathbb{R}^-,\quad \check{r}\in\mathbb{R}\ \text{above the horizon},\\ &\check{\tau}\in\mathbb{R},\quad \check{t}\in\mathbb{R}^+,\quad \check{r}\in\mathbb{R}\ \text{below the horizon},\end{aligned} \tag{A22}$$

with negative values of radial coordinate $\check{r}$ interpreted as described in Eq. (A2).

Orthonormal tetrad,

$$\begin{aligned}&\mathrm{e}_{\check{t}}=\frac{\partial}{\partial\check{\tau}}=\frac{\check{s}\check{t}}{\ell_\Lambda}\frac{\partial}{\partial\check{t}},\quad \mathrm{e}_{\check{r}}=\exp\frac{\check{s}\check{\tau}}{\ell_\Lambda}\frac{\partial}{\partial\check{r}}=\frac{\check{s}\check{t}}{\ell_\Lambda}\frac{\partial}{\partial\check{r}},\\ &\mathrm{e}_{\vartheta}=-\frac{\check{s}}{\check{r}}\exp\frac{\check{s}\check{\tau}}{\ell_\Lambda}\frac{\partial}{\partial\vartheta}=-\frac{1}{\ell_\Lambda}\frac{\check{t}}{\check{r}}\frac{\partial}{\partial\vartheta}.\end{aligned} \tag{A23}$$

Relation to spherical cosmological family,

$$\check{t}=\frac{-\,\ell_\Lambda\cosh^{-1}(\tau/\ell_\Lambda)}{\cos\chi+\tanh(\tau/\ell_\Lambda)},\quad \check{r}=\frac{\ell_\Lambda\cosh^{-1}(\tau/\ell_\Lambda)}{\cos\chi+\tanh(\tau/\ell_\Lambda)}, \tag{A24}$$

$$\check{t}=\frac{\ell_\Lambda\sin\tilde{t}}{\cos\tilde{t}-\cos\tilde{r}},\quad \check{r}=\frac{\ell_\Lambda\sin\tilde{r}}{\cos\tilde{r}-\cos\tilde{t}}. \tag{A25}$$

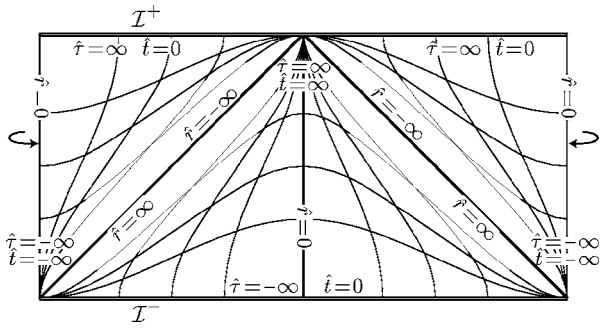

FIG. 16. The flat cosmological family, type "∧."

Relation to flat cosmological family, type "∧",

$$\check t=-\frac{\hat t\ell_\Lambda^2}{\hat t^2-\hat r^2}\,,\quad \check r=\frac{\hat r\ell_\Lambda^2}{\hat t^2-\hat r^2}\,, \tag{A26}$$

$$\begin{gathered}\check t\hat r+\hat t\check r=0\,,\quad \hat t\check t+\hat r\check r=-\ell_\Lambda^2\,,\\ (-\hat t^2+\hat r^2)(-\check t^2+\check r^2)=\ell_\Lambda^4\,,\quad (\hat t+\hat r)(\check t+\check r)=(\hat t-\hat r)(\check t-\check r)=-\ell_\Lambda^2\,.\end{gathered} \tag{A27}$$

Relation to static family in timelike domains $\mathbf{N},\mathbf{S}$,

$$\frac{\check t}{\ell_\Lambda}=-s_{\mathbf{NS}}\frac{\ell_\Lambda}{\sqrt{\ell_\Lambda^2-R^2}}\exp\!\left(-\frac{T}{\ell_\Lambda}\right),\quad \frac{\check r}{\ell_\Lambda}=s_{\mathbf{NS}}\frac{R}{\sqrt{\ell_\Lambda^2-R^2}}\exp\!\left(-\frac{T}{\ell_\Lambda}\right), \tag{A28}$$

$$\check t=-s_{\mathbf{NS}}\ell_\Lambda\exp\!\left(-\frac{\overline t}{\ell_\Lambda}\right)\cosh\frac{\overline r}{\ell_\Lambda}\,,\quad \check r=s_{\mathbf{NS}}\ell_\Lambda\exp\!\left(-\frac{\overline t}{\ell_\Lambda}\right)\sinh\frac{\overline r}{\ell_\Lambda}\,, \tag{A29}$$

where $s_{\mathbf{NS}}=+1(-1)$ in domain $\mathbf{N}(\mathbf{S})$, cf. Eq. (A61).

Relation to static family in spacelike domains $\mathbf{F},\mathbf{P}$,

$$\frac{\check t}{\ell_\Lambda}=s_\times\frac{\ell_\Lambda}{\sqrt{R^2-\ell_\Lambda^2}}\exp\!\left(-\frac{T}{\ell_\Lambda}\right),\quad \frac{\check r}{\ell_\Lambda}=-s_\times\frac{R}{\sqrt{R^2-\ell_\Lambda^2}}\exp\!\left(-\frac{T}{\ell_\Lambda}\right), \tag{A30}$$

$$\check t=s_\times\ell_\Lambda\exp\!\left(-\frac{\overline t}{\ell_\Lambda}\right)\sinh\frac{\overline r}{\ell_\Lambda}\,,\quad \check r=-s_\times\ell_\Lambda\exp\!\left(-\frac{\overline t}{\ell_\Lambda}\right)\cosh\frac{\overline r}{\ell_\Lambda}\,, \tag{A31}$$

where $s_\times=\operatorname{sign}\widetilde r\,\operatorname{sign}\cos\widetilde t$, cf. Eqs. (A73) and (A74).

Relation to conformally Minkowski coordinates,

$$\frac{\check t}{\ell_\Lambda}=-\frac{\ell_\Lambda^2-t^2+r^2}{(\ell_\Lambda+t)^2-r^2}\,,\quad \frac{\check r}{\ell_\Lambda}=\frac{2\ell_\Lambda r}{(\ell_\Lambda+t)^2-r^2}\,. \tag{A32}$$

3. The flat cosmological family, type "∧":

The second flat cosmological coordinate family (Fig. 16) consists of the flat cosmological coordinates $\hat\tau,\hat r,\vartheta,\varphi$ and of the rescaled flat cosmological coordinates $\hat t,\hat r,\vartheta,\varphi$. They can be built analogously to the flat coordinates introduced above, with north and south poles interchanged only. They thus have similar properties. Hypersurfaces $\hat t=$constant are homogeneous flat three-spaces, coordinate lines $\hat r,\vartheta,\varphi=$constant are geodesics with proper time $\hat\tau$, and $\partial/\partial\hat\tau$ is a conformal Killing vector. The coordinates cover de Sitter space–time everywhere except the future

cosmological horizon, $\tilde{r}=\pi-\tilde{t}$, of the north pole (i.e., the past horizon of the south pole), and the rescaled coordinates can be viewed as inertial coordinates in the conformally related Minkowski space $\hat{M}$.

Metric and relation between coordinates,

$$g=\frac{\ell_\Lambda^2}{\hat{t}^2}(-\,\mathrm{d}\hat{t}^2+\mathrm{d}\hat{r}^2+\hat{r}^2\,\mathrm{d}\omega^2), \tag{A33}$$

$$g=-\,\mathrm{d}\hat{\tau}^2+\exp(-\hat{s}2\hat{\tau}/\ell_\Lambda)(\mathrm{d}\hat{r}^2+\hat{r}^2\,\mathrm{d}\omega^2), \tag{A34}$$

$$\hat{t}=\hat{s}\ell_\Lambda\exp\left(\hat{s}\frac{\hat{\tau}}{\ell_\Lambda}\right), \tag{A35}$$

where

$$\hat{s}=\operatorname{sign}\hat{t}. \tag{A36}$$

The ranges of coordinates are

$$\begin{gathered}\hat{\tau}\in\mathbb{R},\quad \hat{t}\in\mathbb{R}^-,\quad \hat{r}\in\mathbb{R}\ \text{above the horizon},\\ \hat{\tau}\in\mathbb{R},\quad \hat{t}\in\mathbb{R}^+,\quad \hat{r}\in\mathbb{R}\ \text{below the horizon},\end{gathered} \tag{A37}$$

with negative values of radial coordinate $\hat{r}$ interpreted as described in Eq. (A2).

Orthonormal tetrad,

$$\begin{gathered}\mathrm{e}_{\hat{t}}=\frac{\partial}{\partial\hat{\tau}}=\frac{\hat{s}\hat{t}}{\ell_\Lambda}\frac{\partial}{\partial\hat{t}},\quad \mathrm{e}_{\hat{r}}=\exp\frac{\hat{s}\hat{\tau}}{\ell_\Lambda}\frac{\partial}{\partial\hat{r}}=\frac{\hat{s}\hat{t}}{\ell_\Lambda}\frac{\partial}{\partial\hat{r}},\\ \mathrm{e}_{\vartheta}=\frac{\hat{s}}{\hat{r}}\exp\frac{\hat{s}\hat{\tau}}{\ell_\Lambda}\frac{\partial}{\partial\vartheta}=\frac{1}{\ell_\Lambda}\frac{\hat{t}}{\hat{r}}\frac{\partial}{\partial\vartheta}.\end{gathered} \tag{A38}$$

Relation to spherical cosmological family,

$$\hat{t}=\frac{\ell_\Lambda\cosh^{-1}(\tau/\ell_\Lambda)}{\cos\chi-\tanh(\tau/\ell_\Lambda)},\quad \hat{r}=\frac{\ell_\Lambda\cosh^{-1}(\tau/\ell_\Lambda)}{\cos\chi-\tanh(\tau/\ell_\Lambda)}, \tag{A39}$$

$$\hat{t}=\frac{\ell_\Lambda\sin\tilde{t}}{\cos\tilde{t}+\cos\tilde{r}},\quad \hat{r}=\frac{\ell_\Lambda\sin\tilde{r}}{\cos\tilde{r}+\cos\tilde{t}}. \tag{A40}$$

Relation to flat cosmological family, type "$\wedge$",

$$\hat{t}=-\frac{\check{t}\ell_\Lambda^2}{\check{t}^2-\check{r}^2},\quad \hat{r}=\frac{\check{r}\ell_\Lambda^2}{\check{t}^2-\check{r}^2}, \tag{A41}$$

$$\begin{gathered}\check{t}\hat{r}+\hat{t}\check{r}=0,\quad \hat{t}\check{t}+\hat{r}\check{r}=-\,\ell_\Lambda^2,\\ (-\,\hat{t}^2+\hat{r}^2)(-\,\check{t}^2+\check{r}^2)=\ell_\Lambda^4,\quad (\hat{t}+\hat{r})(\check{t}+\check{r})=(\hat{t}-\hat{r})(\check{t}-\check{r})=-\,\ell_\Lambda^2.\end{gathered} \tag{A42}$$

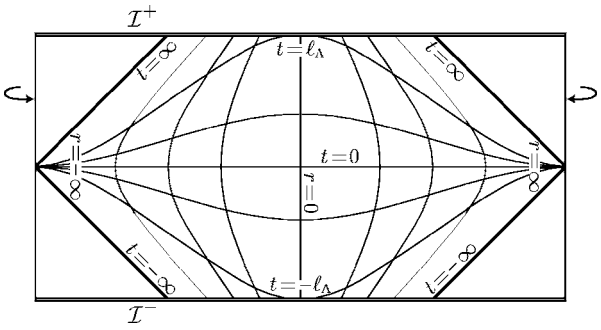

FIG. 17. The conformally Minkowski family of coordinates.

Relation to static family in timelike domains **N**, **S**,

$$\frac{\hat{t}}{\ell_\Lambda} = s_{\mathbf{NS}} \frac{\ell_\Lambda}{\sqrt{\ell_\Lambda^2 - R^2}} \exp \frac{T}{\ell_\Lambda}, \quad \frac{\hat{r}}{\ell_\Lambda} = s_{\mathbf{NS}} \frac{R}{\sqrt{\ell_\Lambda^2 - R^2}} \exp \frac{T}{\ell_\Lambda}, \tag{A43}$$

$$\hat{t} = s_{\mathbf{NS}} \ell_\Lambda \exp \frac{\overline{t}}{\ell_\Lambda} \cosh \frac{\overline{r}}{\ell_\Lambda}, \quad \hat{r} = s_{\mathbf{NS}} \ell_\Lambda \exp \frac{\overline{t}}{\ell_\Lambda} \sinh \frac{\overline{r}}{\ell_\Lambda}, \tag{A44}$$

where $s_{\mathbf{NS}} = +1(-1)$ in domain **N** (**S**), cf. Eq. (A61).

Relation to static family in spacelike domains **F**, **P**,

$$\frac{\hat{t}}{\ell_\Lambda} = s_\times \frac{\ell_\Lambda}{\sqrt{R^2 - \ell_\Lambda^2}} \exp \frac{T}{\ell_\Lambda}, \quad \frac{\hat{r}}{\ell_\Lambda} = s_\times \frac{R}{\sqrt{R^2 - \ell_\Lambda^2}} \exp \frac{T}{\ell_\Lambda}, \tag{A45}$$

$$\hat{t} = s_\times \ell_\Lambda \exp \frac{\overline{t}}{\ell_\Lambda} \sinh \frac{\overline{r}}{\ell_\Lambda}, \quad \hat{r} = s_\times \ell_\Lambda \exp \frac{\overline{t}}{\ell_\Lambda} \cosh \frac{\overline{r}}{\ell_\Lambda}, \tag{A46}$$

where $s_\times = \operatorname{sign} \tilde{r} \operatorname{sign} \cos \tilde{t}$, cf. Eqs. (A73) and (A74).

Relation to conformally Minkowski coordinates,

$$\frac{\hat{t}}{\ell_\Lambda} = \frac{\ell_\Lambda^2 - t^2 + r^2}{(\ell_\Lambda - t)^2 - r^2}, \quad \frac{\hat{r}}{\ell_\Lambda} = \frac{2\ell_\Lambda r}{(\ell_\Lambda - t)^2 - r^2}. \tag{A47}$$

4. The conformally Minkowski family:

The conformally Minkowski coordinates t, r, ϑ, φ can be understood as spherical coordinates in the conformally related Minkowski space M. The coordinates do not cover de Sitter space–time globally—they cover only a region around north pole, see Fig. 17. The boundary of this region is given by the conformal infinity of the Minkowski space–time. These coordinates are useful for studying the limit $\Lambda \to 0$.

The metric,

$$g = \left(\frac{2\ell_\Lambda^2}{\ell_\Lambda^2 - t^2 + r^2} \right)^2 (-\mathrm{d}t^2 + \mathrm{d}r^2 + r^2 \, \mathrm{d}\omega^2), \tag{A48}$$

the ranges of coordinates

$$t \in \mathbb{R}, \quad r \in \mathbb{R}, \quad \text{such that } t^2 - r^2 < \ell_\Lambda^2, \tag{A49}$$

with negative values of radial coordinate r interpreted as described in Eq. (A2).

Orthonormal tetrad,

$$\mathrm{e}_t = \frac{\ell_\Lambda^2 - t^2 + r^2}{2\ell_\Lambda^2}\frac{\partial}{\partial t}, \quad \mathrm{e}_r = \frac{\ell_\Lambda^2 - t^2 + r^2}{2\ell_\Lambda^2}\frac{\partial}{\partial r}, \quad \mathrm{e}_\vartheta = \frac{\ell_\Lambda^2 - t^2 + r^2}{2\ell_\Lambda^2}\frac{1}{r}\frac{\partial}{\partial t}. \tag{A50}$$

Relation to spherical cosmological family,

$$t = -\frac{\ell_\Lambda \cos\tilde{t}}{\cos\tilde{r} + \sin\tilde{t}}, \quad r = \frac{\ell_\Lambda \sin\tilde{r}}{\cos\tilde{r} + \sin\tilde{t}}. \tag{A51}$$

Relation to flat cosmological family,

$$\begin{aligned} \frac{t}{\ell_\Lambda} &= -\frac{\ell_\Lambda^2 - \hat{t}^2 + \hat{r}^2}{(\ell_\Lambda + \hat{t})^2 - \hat{r}^2} = \frac{\ell_\Lambda^2 - \check{t}^2 + \check{r}^2}{(\ell_\Lambda - \check{t})^2 - \check{r}^2}, \\ \frac{r}{\ell_\Lambda} &= \frac{2\ell_\Lambda \hat{r}}{(\ell_\Lambda + \hat{t})^2 - \hat{r}^2} = \frac{2\ell_\Lambda \check{r}}{(\ell_\Lambda - \check{t})^2 - \check{r}^2}. \end{aligned} \tag{A52}$$

Relation to hyperbolic cosmological coordinates,

$$\frac{t}{\ell_\Lambda} = \tanh\frac{\eta}{2\ell_\Lambda}\cosh\frac{\beta}{\ell_\Lambda}, \quad \frac{r}{\ell_\Lambda} = \tanh\frac{\eta}{2\ell_\Lambda}\sinh\frac{\beta}{\ell_\Lambda}. \tag{A53}$$

Relation to static family in timelike domains **N**, **S**,

$$\frac{t}{\ell_\Lambda} = \frac{\sinh\dfrac{\bar{t}}{\ell_\Lambda}}{\cosh\dfrac{\bar{t}}{\ell_\Lambda} + s_{\mathbf{NS}}\cosh\dfrac{\bar{r}}{\ell_\Lambda}}, \quad \frac{r}{\ell_\Lambda} = \frac{\sinh\dfrac{\bar{r}}{\ell_\Lambda}}{\cosh\dfrac{\bar{r}}{\ell_\Lambda} + s_{\mathbf{NS}}\cosh\dfrac{\bar{t}}{\ell_\Lambda}}, \tag{A54}$$

$$\frac{t}{\ell_\Lambda} = \frac{\sqrt{\ell_\Lambda^2 - R^2}\sinh\dfrac{T}{\ell_\Lambda}}{s_{\mathbf{NS}}\ell_\Lambda + \sqrt{\ell_\Lambda^2 - R^2}\cosh\dfrac{T}{\ell_\Lambda}}, \quad \frac{r}{\ell_\Lambda} = \frac{R}{\ell_\Lambda + s_{\mathbf{NS}}\sqrt{\ell_\Lambda^2 - R^2}\cosh\dfrac{T}{\ell_\Lambda}}, \tag{A55}$$

where $s_{\mathbf{NS}} = +1(-1)$ in domain **N** (**S**), cf. Eq. (A61).

Relation to static family in spacelike domains **F**, **P**,

$$\frac{t}{\ell_\Lambda} = \frac{\cosh\dfrac{\bar{t}}{\ell_\Lambda}}{\sinh\dfrac{\bar{t}}{\ell_\Lambda} - s_\times\sinh\dfrac{\bar{r}}{\ell_\Lambda}}, \quad \frac{r}{\ell_\Lambda} = \frac{\cosh\dfrac{\bar{r}}{\ell_\Lambda}}{\sinh\dfrac{\bar{r}}{\ell_\Lambda} - s_\times\cosh\dfrac{\bar{t}}{\ell_\Lambda}}, \tag{A56}$$

$$\frac{t}{\ell_\Lambda} = \frac{\sqrt{R^2 - \ell_\Lambda^2}\cosh\dfrac{T}{\ell_\Lambda}}{-s_\times\ell_\Lambda + \sqrt{R^2 - \ell_\Lambda^2}\sinh\dfrac{T}{\ell_\Lambda}}, \quad \frac{r}{\ell_\Lambda} = \frac{R}{\ell_\Lambda - s_\times\sqrt{R^2 - \ell_\Lambda^2}\sinh\dfrac{T}{\ell_\Lambda}}, \tag{A57}$$

with $s_\times = \mathrm{sign}\,\tilde{r}\,\mathrm{sign}\cos\tilde{t}$, cf. Eqs. (A73) and (A74).

***5. The static family in timelike domains* N *and* S:** This family consists of the static coordinates T, R, ϑ, φ and the "tortoise" static coordinates $\bar{t}$, $\bar{r}$, ϑ, φ. The metric does not depend on time coordinate $T = \bar{t}$—the coordinates are associated with a Killing vector. Since the Killing vector

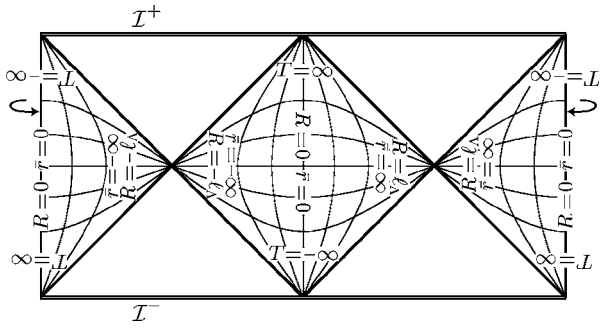

FIG. 18. The static family of coordinates, timelike domains.

changes its character, the coordinates do not cover the space–time smoothly. We first describe the static coordinates in domains **N** and **S**, where the Killing vector is timelike. In domain **N** the orbits of the Killing vector (corresponding to the worldlines of static observers) start and end at the north pole, in domain **S**—at the south pole. They are orthogonal to slices $T=$constant, each of which consists of two hemispheres (one in domain **N**, the other in **S**) with homogeneous spherical 3-metric. The distances between static observers (measured within these slices) do not change. Since the static observers must overcome first the cosmological contraction and then the expansion, they move with a (uniform) acceleration. (See Fig. 18.)

Metric and relation between coordinates,

$$g=\cosh^{-2}\frac{\bar{r}}{\ell_\Lambda}\left(-\mathrm{d}\bar{t}^{\,2}+\mathrm{d}\bar{r}^2+\ell_\Lambda^2\sinh^2\frac{\bar{r}}{\ell_\Lambda}\mathrm{d}\omega^2\right), \tag{A58}$$

$$g=-\left(1-\frac{R^2}{\ell_\Lambda^2}\right)\mathrm{d}T^2+\left(1-\frac{R^2}{\ell_\Lambda^2}\right)^{-1}\mathrm{d}R^2+R^2\,\mathrm{d}\omega^2, \tag{A59}$$

$$T=\bar{t}, \tag{A60a}$$

$$\exp\frac{\bar{r}}{\ell_\Lambda}=\sqrt{\frac{\ell_\Lambda+R}{\ell_\Lambda-R}}\,,\quad \sinh\frac{\bar{r}}{\ell_\Lambda}=\frac{R}{\sqrt{\ell_\Lambda^2-R^2}}\,,$$
$$\tanh\frac{\bar{r}}{\ell_\Lambda}=\frac{R}{\ell_\Lambda},\quad \cosh\frac{\bar{r}}{\ell_\Lambda}=\frac{\ell_\Lambda}{\sqrt{\ell_\Lambda^2-R^2}}, \tag{A60b}$$

$$s_{\mathbf{NS}}=\begin{cases}+1 & \text{in domain } \mathbf{N},\\ -1 & \text{in domain } \mathbf{S}.\end{cases} \tag{A61}$$

The ranges of coordinates are

$$T\in\mathbb{R},\quad R\in(-\ell_\Lambda,\ell_\Lambda),\quad \bar{t}\in\mathbb{R},\quad \bar{r}\in\mathbb{R}, \tag{A62}$$

with negative values of coordinates R and $\bar{r}$ interpreted as described in Eq. (A2).

Orthonormal tetrad,

$$\mathrm{e}_T=\left(1-\frac{R^2}{\ell_\Lambda^2}\right)^{-1/2}\frac{\partial}{\partial T}=\cosh\frac{\bar{r}}{\ell_\Lambda}\frac{\partial}{\partial\bar{t}},\quad \mathrm{e}_R=\left(1-\frac{R^2}{\ell_\Lambda^2}\right)^{1/2}\frac{\partial}{\partial R}=\cosh^{-1}\frac{\bar{r}}{\ell_\Lambda}\frac{\partial}{\partial\bar{r}}\,, \tag{A63}$$

$$\mathrm{e}_\vartheta = \frac{1}{R}\frac{\partial}{\partial\vartheta} = \frac{1}{\ell_\Lambda}\coth\frac{\bar r}{\ell_\Lambda}\frac{\partial}{\partial\vartheta}\,.$$

Relation to spherical cosmological family,

$$T = \frac{\ell_\Lambda}{2}\log\frac{\cos\tilde r-\cos\tilde t}{\cos\tilde r+\cos\tilde t}, \quad R = \ell_\Lambda\frac{\sin\tilde r}{\sin\tilde t}\,, \tag{A64}$$

$$\bar t = \frac{\ell_\Lambda}{2}\log\left(\tan\frac{\tilde t+\tilde r}{2}\tan\frac{\tilde t-\tilde r}{2}\right), \quad \bar r = \frac{\ell_\Lambda}{2}\log\left(\tan\frac{\tilde t+\tilde r}{2}\cot\frac{\tilde t-\tilde r}{2}\right),$$

$$\exp\frac{\bar t}{\ell_\Lambda} = \sqrt{\frac{\cos\tilde r-\cos\tilde t}{\cos\tilde r+\cos\tilde t}}, \quad \sinh\frac{\bar t}{\ell_\Lambda} = \frac{-s_{\mathbf{NS}}\cos\tilde t}{\sqrt{\cos^2\tilde r-\cos^2\tilde t}}\,,$$

$$\tanh\frac{\bar t}{\ell_\Lambda} = -\frac{\cos\tilde t}{\cos\tilde r}, \quad \cosh\frac{\bar t}{\ell_\Lambda} = \frac{s_{\mathbf{NS}}\cos\tilde r}{\sqrt{\cos^2\tilde r-\cos^2\tilde t}}\,, \tag{A65}$$

$$\exp\frac{\bar r}{\ell_\Lambda} = \sqrt{\frac{\sin\tilde t+\sin\tilde r}{\sin\tilde t-\sin\tilde r}}, \quad \sinh\frac{\bar r}{\ell_\Lambda} = \frac{\sin\tilde r}{\sqrt{\sin^2\tilde t-\sin^2\tilde r}}\,,$$

$$\tanh\frac{\bar r}{\ell_\Lambda} = \frac{\sin\tilde r}{\sin\tilde t}, \quad \cosh\frac{\bar r}{\ell_\Lambda} = \frac{\sin\tilde t}{\sqrt{\sin^2\tilde t-\sin^2\tilde r}}.$$

Relation to flat cosmological family,

$$\bar t = \frac{\ell_\Lambda}{2}\log\frac{\hat t^2-\hat r^2}{\ell_\Lambda^2} = -\frac{\ell_\Lambda}{2}\log\frac{\check t^2-\check r^2}{\ell_\Lambda^2}, \quad \bar r = \frac{\ell_\Lambda}{2}\log\frac{\hat t+\hat r}{\hat t-\hat r} = \frac{\ell_\Lambda}{2}\log\frac{\check t-\check r}{\check t+\check r}\,, \tag{A66}$$

$$\frac{T}{\ell_\Lambda} = \frac{1}{2}\log\frac{\hat t^2-\hat r^2}{\ell_\Lambda^2} = -\frac{1}{2}\log\frac{\check t^2-\check r^2}{\ell_\Lambda^2}, \quad \frac{R}{\ell_\Lambda} = \frac{\hat r}{\hat t} = -\frac{\check r}{\check t}\,. \tag{A67}$$

Relation to conformally Minkowski coordinates,

$$\tanh\frac{T}{\ell_\Lambda} = \frac{2\ell_\Lambda t}{\ell_\Lambda^2+t^2-r^2}\,, \quad \frac{R}{\ell_\Lambda} = \frac{2\ell_\Lambda r}{\ell_\Lambda^2+r^2-t^2}\,, \tag{A68}$$

$$\bar t = \frac{\ell_\Lambda}{2}\log\frac{(\ell_\Lambda+t)^2-r^2}{(\ell_\Lambda-t)^2-r^2}\,, \quad \bar r = \frac{\ell_\Lambda}{2}\log\frac{(\ell_\Lambda+r)^2-t^2}{(\ell_\Lambda-r)^2-t^2}\,. \tag{A69}$$

***6. The static family in spacelike domains* F *and* P**:

Here we describe the static coordinates T, R, ϑ, φ and the "tortoise" static coordinates $\bar t, \bar r, \vartheta, \varphi$ from the preceding section in domains **F** and **S** where the Killing vector is spacelike. These "nonstatic" domains extend up to infinity, namely, domain **F** up to $\mathcal{I}^+$, domain **P** up to $\mathcal{I}^-$. The orbits of the Killing vector start at the south pole and end at the north pole in **F**, and they point in opposite direction in **P**. The motion along them could thus be characterized as a "translation" from one pole to the other. The Lorentzian hypersurfaces $T=$constant are homogeneous spaces with positive curvature, i.e., three-dimensional de Sitter space–times. (See Fig. 19.)

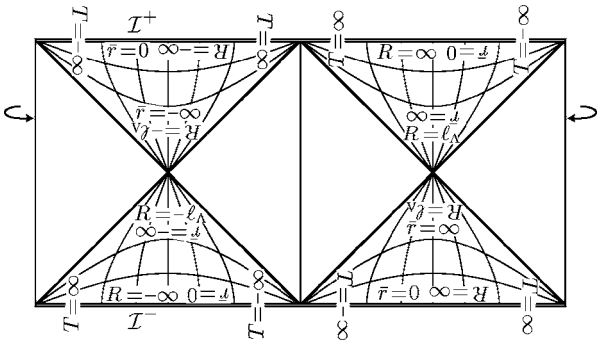

FIG. 19. The static family of coordinates, spacelike domains.

Metric and relation between coordinates,

$$g = \sinh^{-2}\frac{\bar{r}}{\ell_\Lambda}\left(-\mathrm{d}\bar{r}^2 + \mathrm{d}\bar{t}^2 + \ell_\Lambda^2 \cosh^2\frac{\bar{r}}{\ell_\Lambda}\mathrm{d}\omega^2\right), \tag{A70}$$

$$g = -\left(1 - \frac{R^2}{\ell_\Lambda^2}\right)\mathrm{d}T^2 + \left(1 - \frac{R^2}{\ell_\Lambda^2}\right)^{-1}\mathrm{d}R^2 + R^2\,\mathrm{d}\omega^2, \tag{A71}$$

$$T = \bar{t}, \tag{A72a}$$

$$\exp\frac{\bar{r}}{\ell_\Lambda} = \sqrt{\frac{R+\ell_\Lambda}{R-\ell_\Lambda}}, \quad \left|\sinh\frac{\bar{r}}{\ell_\Lambda}\right| = \frac{\ell_\Lambda}{\sqrt{R^2-\ell_\Lambda^2}}, \qquad \tanh\frac{\bar{r}}{\ell_\Lambda} = \frac{\ell_\Lambda}{R}, \quad \cosh\frac{\bar{r}}{\ell_\Lambda} = \frac{|R|}{\sqrt{R^2-\ell_\Lambda^2}}. \tag{A72b}$$

The signature factors $s_\mathcal{I}$ and $s_\times$ are defined as

$$s_\mathcal{I} = \begin{cases} +1 & \text{in domain } \mathbf{F}, \\ -1 & \text{in domain } \mathbf{P}, \end{cases} \tag{A73}$$

$$s_\times = -\,s_\mathcal{I}\,\mathrm{sign}\,\tilde{r}. \tag{A74}$$

The coordinates ranges are

$$T \in \mathbb{R}, \quad |R| \in (\ell_\Lambda, \infty), \quad \bar{t} \in \mathbb{R}, \quad \bar{r} \in \mathbb{R}, \tag{A75}$$

with negative values of coordinates R and $\bar{r}$ interpreted as described in Eq. (A2).

Orthonormal tetrad,

$$\mathrm{e}_T = \left(\frac{R^2}{\ell_\Lambda^2} - 1\right)^{-1/2}\frac{\partial}{\partial T} = \left|\sinh\frac{\bar{r}}{\ell_\Lambda}\right|\frac{\partial}{\partial \bar{t}}, \qquad \mathrm{e}_R = \left(\frac{R^2}{\ell_\Lambda^2} - 1\right)^{1/2}\frac{\partial}{\partial R} = -\left|\sinh^{-1}\frac{\bar{r}}{\ell_\Lambda}\right|\frac{\partial}{\partial \bar{r}}, \quad \mathrm{e}_\vartheta = \frac{1}{R}\frac{\partial}{\partial \vartheta} = \frac{1}{\ell_\Lambda}\left|\tanh\frac{\bar{r}}{\ell_\Lambda}\right|\frac{\partial}{\partial \vartheta}. \tag{A76}$$

Relation to spherical cosmological family,

$$T=\frac{\ell_\Lambda}{2}\log\frac{\cos\tilde{t}-\cos\tilde{r}}{\cos\tilde{t}+\cos\tilde{r}}\,,\quad R=\ell_\Lambda\frac{\sin\tilde{r}}{\sin\tilde{t}}\,,\tag{A77}$$

$$\bar{t}=\frac{\ell_\Lambda}{2}\log\left(-\tan\frac{\tilde{t}+\tilde{r}}{2}\tan\frac{\tilde{t}-\tilde{r}}{2}\right),\quad \bar{r}=\frac{\ell_\Lambda}{2}\log\left(-\tan\frac{\tilde{t}+\tilde{r}}{2}\cot\frac{\tilde{t}-\tilde{r}}{2}\right),$$

$$\exp\frac{\bar{t}}{\ell_\Lambda}=\sqrt{\frac{\cos\tilde{t}-\cos\tilde{r}}{\cos\tilde{t}+\cos\tilde{r}}}\,,\quad \sinh\frac{\bar{t}}{\ell_\Lambda}=\frac{s_{\mathcal{I}}\cos\tilde{r}}{\sqrt{\cos^2\tilde{t}-\cos^2\tilde{r}}}\,,$$

$$\tanh\frac{\bar{t}}{\ell_\Lambda}=-\frac{\cos\tilde{r}}{\cos\tilde{t}}\,,\quad \cosh\frac{\bar{t}}{\ell_\Lambda}=\frac{-s_{\mathcal{I}}\cos\tilde{t}}{\sqrt{\cos^2\tilde{t}-\cos^2\tilde{r}}}\,,\tag{A78}$$

$$\exp\frac{\bar{r}}{\ell_\Lambda}=\sqrt{\frac{\sin\tilde{r}+\sin\tilde{t}}{\sin\tilde{r}-\sin\tilde{t}}}\,,\quad \left|\sinh\frac{\bar{r}}{\ell_\Lambda}\right|=\frac{\sin\tilde{t}}{\sqrt{\sin^2\tilde{r}-\sin^2\tilde{t}}}\,,$$

$$\tanh\frac{\bar{r}}{\ell_\Lambda}=\frac{\sin\tilde{t}}{\sin\tilde{r}}\,,\quad \cosh\frac{\bar{r}}{\ell_\Lambda}=\frac{|\sin\tilde{r}|}{\sqrt{\sin^2\tilde{r}-\sin^2\tilde{t}}}\,.$$

Relation to flat cosmological family,

$$\bar{t}=\frac{\ell_\Lambda}{2}\log\frac{-\hat{t}^2+\hat{r}^2}{\ell_\Lambda^2}=-\frac{\ell_\Lambda}{2}\log\frac{-\check{t}^2+\check{r}^2}{\ell_\Lambda^2}\,,\quad \bar{r}=\frac{\ell_\Lambda}{2}\log\frac{\hat{r}+\hat{t}}{\hat{r}-\hat{t}}=\frac{\ell_\Lambda}{2}\log\frac{\check{r}-\check{t}}{\check{r}+\check{t}}\,,\tag{A79}$$

$$\frac{T}{\ell_\Lambda}=\frac{1}{2}\log\frac{-\hat{t}^2+\hat{r}^2}{\ell_\Lambda^2}=-\frac{1}{2}\log\frac{-\check{t}^2+\check{r}^2}{\ell_\Lambda^2}\,,\quad \frac{R}{\ell_\Lambda}=\frac{\hat{r}}{\hat{t}}=-\frac{\check{r}}{\check{t}}\,.\tag{A80}$$

Relation to conformally Minkowski coordinates,

$$\coth\frac{T}{\ell_\Lambda}=\frac{2\ell_\Lambda t}{\ell_\Lambda^2+t^2-r^2}\,,\quad \frac{R}{\ell_\Lambda}=\frac{2\ell_\Lambda r}{\ell_\Lambda^2+r^2-t^2}\,,\tag{A81}$$

$$\bar{t}=\frac{\ell_\Lambda}{2}\log\left(-\frac{(\ell_\Lambda+t)^2-r^2}{(\ell_\Lambda-t)^2-r^2}\right),\quad \bar{r}=\frac{\ell_\Lambda}{2}\log\left(-\frac{(\ell_\Lambda+r)^2-t^2}{(\ell_\Lambda-r)^2-t^2}\right).\tag{A82}$$

7. The hyperbolic cosmological family:

The third type of cosmological coordinates are the hyperbolic cosmological coordinates η, ρ, ϑ, φ. The hypersurfaces η=constant are homogeneous spaces with negative curvature, coordinate lines ρ,ϑ,φ=constant correspond to the worldlines of cosmological observers orthogonal to these slices, and the vector $\partial/\partial\eta$ is a timelike conformal Killing vector. The coordinates cover space–time only partially—they can be introduced in two disconnected domains near the north pole, namely, in the past of the event $\tilde{t}=\pi/2$, $\tilde{r}=0$ (where $\eta<0$), and in the future of this event (where $\eta>0$). (see. Fig. 20.)

The metric,

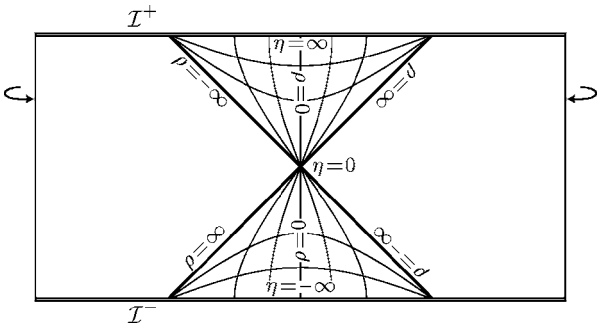

FIG. 20. The hyperbolic cosmological family of coordinates.

$$g=-\,\mathrm{d}\eta^2+\sinh^2\frac{\eta}{\ell_\Lambda}\left(\mathrm{d}\rho^2+\ell_\Lambda^2\sinh^2\frac{\rho}{\ell_\Lambda}\mathrm{d}\omega^2\right). \tag{A83}$$

The ranges of coordinates and the signature factor $s_\mathcal{I}$ are

$$\begin{aligned}&\eta\in\mathbb{R}^+,\quad \rho\in\mathbb{R},\quad s_\mathcal{I}=+1\quad \text{in the future patch},\\ &\eta\in\mathbb{R}^-,\quad \rho\in\mathbb{R},\quad s_\mathcal{I}=-1\quad \text{in the past patch},\end{aligned} \tag{A84}$$

with negative values of radial coordinate ρ interpreted as described in Eq. (A2).

Orthonormal tetrad,

$$\mathrm{e}_\eta=\frac{\partial}{\partial\eta},\quad \mathrm{e}_\rho=\sinh^{-1}\frac{\eta}{\ell_\Lambda}\frac{\partial}{\partial\rho},\quad \mathrm{e}_\vartheta=\sinh^{-1}\frac{\eta}{\ell_\Lambda}\sinh^{-1}\frac{\rho}{\ell_\Lambda}\frac{\partial}{\partial\rho}. \tag{A85}$$

Relation to spherical cosmological family,

$$\tanh\frac{\eta}{2\ell_\Lambda}=s_\mathcal{I}\sqrt{\frac{\cos\tilde{r}-\sin\tilde{t}}{\cos\tilde{r}+\sin\tilde{t}}},\quad \tanh\frac{\rho}{\ell_\Lambda}=-\frac{\sin\tilde{r}}{\cos\tilde{t}}. \tag{A86}$$

Relation to conformally Minkowski coordinates,

$$\tanh\frac{\eta}{2\ell_\Lambda}=s_\mathcal{I}\frac{\sqrt{t^2-r^2}}{\ell_\Lambda},\quad \tanh\frac{\rho}{\ell_\Lambda}=\frac{r}{t}. \tag{A87}$$

8. The accelerated coordinate family:

This family consists of the accelerated coordinates T',R',ϑ',φ, and the C-metric-like coordinates $\tau,\upsilon,\xi,\varphi$ (τ being different from τ of the standard coordinates). Contrary to the previous cases the accelerated coordinates are centered on uniformly accelerated origins, $R'=0$ corresponds to two worldlines with acceleration $|a_\mathrm{o}|$. The transformation relations to the systems introduced above mix these three coordinates in general.

The accelerated coordinates are closely related to the static system. Their time coordinates coincide, $T'=T$, and coordinate lines R',ϑ',φ=constant are the same as those with R,ϑ,φ=constant. Both coordinate systems are identical for $a_\mathrm{o}=0$. Sections T,T',φ=constant with $R,R'<\ell_\Lambda$ have geometry of 2-sphere with parallels and meridians given by the coordinate lines of the static coordinates R,ϑ. The lines of coordinates R',ϑ' are the deformed version of static ones, their poles are shifted along meridian $\vartheta=0$ towards each other, cf. Fig. 11.

Two conformal diagrams of sections ϑ',φ=constant ($\vartheta'<\pi/2$ on the right, $\vartheta'>\pi/2$ on the left), adapted to the accelerated coordinates, are depicted in Fig. 21. The shape of the diagram varies with different values of ϑ'; indeed, the position of infinity is given by $R'=-\ell_\Lambda^2/R_\mathrm{o}\cos^{-1}\vartheta'$. See also Fig. 10 for sections $\vartheta'=0,\pi$.

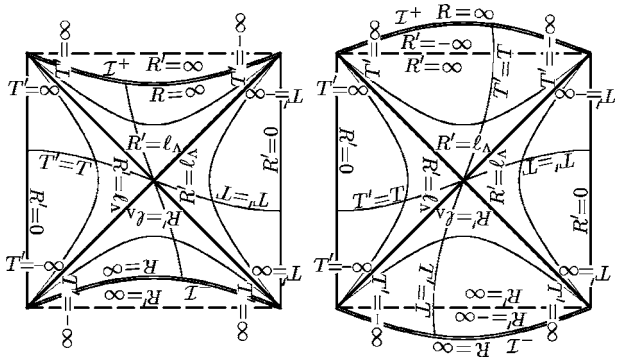

FIG. 21. The accelerated family of coordinates.

The C-metric-like coordinates rescale only the values of the accelerated coordinates and regularize the coordinate singularity $R'=\pm\infty$. de Sitter metric in these coordinates is a zero-mass limit of the C-metric (the metric describing accelerated black holes; see, e.g., Refs. 28 and 29, cf. also Ref. 59).

Finally, we use four parameters a_o,α_o,R_o,b_o to parametrize the acceleration. They are related as follows:

$$\begin{aligned}
\sinh\alpha_o &= \frac{R_o}{\sqrt{\ell_\Lambda^2-R_o^2}} = \frac{b_o^2-\ell_\Lambda^2}{2\ell_\Lambda b_o} = -a_o\ell_\Lambda,\\
\cosh\alpha_o &= \frac{\ell_\Lambda}{\sqrt{\ell_\Lambda^2-R_o^2}} = \frac{b_o^2+\ell_\Lambda^2}{2\ell_\Lambda b_o} = \sqrt{1+a_o^2\ell_\Lambda^2},\\
\tanh\alpha_o &= \frac{R_o}{\ell_\Lambda} = \frac{b_o^2-\ell_\Lambda^2}{b_o^2+\ell_\Lambda^2} = -\frac{a_o\ell_\Lambda}{\sqrt{1+a_o^2\ell_\Lambda^2}},\\
\exp\alpha_o &= \sqrt{\frac{\ell_\Lambda+R_o}{\ell_\Lambda-R_o}} = \frac{b_o}{\ell_\Lambda} = \sqrt{1+a_o^2\ell_\Lambda^2}-a_o\ell_\Lambda.
\end{aligned} \tag{A88}$$

Metric and relation between coordinates,

$$g=\Omega^2\left[-\left(1-\frac{R'^2}{\ell_\Lambda^2}\right)\mathrm{d}T'^2+\left(1-\frac{R'^2}{\ell_\Lambda^2}\right)^{-1}\mathrm{d}R'^2+R'^2\,\mathrm{d}\omega^{2\prime}\right], \tag{A89}$$

$$g=\mathfrak{r}^2\left[-(v^2-1)\mathrm{d}\tau^2+\frac{1}{v^2-1}\mathrm{d}v^2+\frac{1}{1-\xi^2}\mathrm{d}\xi^2+(1-\xi^2)\mathrm{d}\varphi^2\right], \tag{A90}$$

where

$$\mathrm{d}\omega^{2\prime}=(\mathrm{d}\vartheta'^2+\sin^2\vartheta'\,\mathrm{d}\varphi^2), \tag{A91}$$

$$\Omega=\frac{\sqrt{1-R_o^2/\ell_\Lambda^2}}{1+(R'R_o/\ell_\Lambda^2)\cos\vartheta'}=\frac{\mathfrak{r}}{R'}=\frac{\mathfrak{r}v}{\ell_\Lambda}, \tag{A92}$$

$$\mathfrak{r}=\frac{\ell_\Lambda}{v\cosh\alpha_o-\xi\sinh\alpha_o}=\Omega R'=\Omega\frac{\ell_\Lambda}{v}, \tag{A93}$$

$$\tau = \frac{T'}{\ell_\Lambda}, \quad \upsilon = \frac{\ell_\Lambda}{R'}, \quad \xi = -\cos\vartheta', \tag{A94}$$

Orthonormal tetrad:

$$\mathrm{e}_{T'} = |\Omega|^{-1}\left(1 - \frac{R'^2}{\ell_\Lambda^2}\right)^{-1/2}\frac{\partial}{\partial T'} = \frac{1}{\mathfrak{r}\sqrt{\upsilon^2 - 1}}\frac{\partial}{\partial T'},$$

$$\mathrm{e}_{R'} = |\Omega|^{-1}\left(1 - \frac{R'^2}{\ell_\Lambda^2}\right)^{1/2}\frac{\partial}{\partial R'} = \frac{1}{\mathfrak{r}}\sqrt{\upsilon^2 - 1}\frac{\partial}{\partial R'}, \tag{A95}$$

$$\mathrm{e}_{\vartheta'} = \frac{1}{\Omega R'}\frac{\partial}{\partial\vartheta'} = \frac{1}{\mathfrak{r}}\frac{\partial}{\partial\vartheta'}.$$

Relation to static coordinates,

$$T = T',$$

$$R\cos\vartheta = \frac{R'\cos\vartheta' + R_\mathrm{o}}{1 + (R'R_\mathrm{o}/\ell_\Lambda^2)\cos\vartheta'}, \quad R\sin\vartheta = \frac{R'\sin\vartheta'\sqrt{1 - \dfrac{R_\mathrm{o}^2}{\ell_\Lambda^2}}}{1 + (R'R_\mathrm{o}/\ell_\Lambda^2)\cos\vartheta'},$$

$$\frac{R^2}{\ell_\Lambda^2} = 1 - \frac{(1 - R'^2/\ell_\Lambda^2)(1 - R_\mathrm{o}^2/\ell_\Lambda^2)}{(1 + (R'R_\mathrm{o}/\ell_\Lambda^2)\cos\vartheta')^2}, \quad \tan\vartheta = \frac{R'\sin\vartheta'\sqrt{1 - \dfrac{R_\mathrm{o}^2}{\ell_\Lambda^2}}}{R'\cos\vartheta' + R_\mathrm{o}}. \tag{A96}$$

The inverse relations have the same form with T, R, ϑ and T', R', ϑ' interchanged only and α_o replaced by $-\alpha_\mathrm{o}$,

$$\Omega = \frac{\sqrt{1 - R_\mathrm{o}^2/\ell_\Lambda^2}}{1 + (R'R_\mathrm{o}/\ell_\Lambda^2)\cos\vartheta'} = \frac{1 - (RR_\mathrm{o}/\ell_\Lambda^2)\cos\vartheta}{\sqrt{1 - R_\mathrm{o}^2/\ell_\Lambda^2}}, \tag{A97}$$

$$\left(1 + \frac{R'R_\mathrm{o}}{\ell_\Lambda^2}\cos\vartheta'\right)\left(1 - \frac{RR_\mathrm{o}}{\ell_\Lambda^2}\cos\vartheta\right) = 1 - \frac{R_\mathrm{o}^2}{\ell_\Lambda^2}, \tag{A98}$$

$$\frac{1 - R'^2/\ell_\Lambda^2}{1 + (R'R_\mathrm{o}/\ell_\Lambda^2)\cos\vartheta'} = \frac{1 - R^2/\ell_\Lambda^2}{1 - (RR_\mathrm{o}/\ell_\Lambda^2)\cos\vartheta}. \tag{A99}$$

Relation to Robinson-Trautman coordinates,

$$T' = \mathfrak{u}\cosh\alpha_\mathrm{o} - \frac{\ell_\Lambda}{2}\log\left|\frac{\ell_\Lambda - \mathfrak{r}(\sinh\alpha_\mathrm{o}\cos\vartheta' + \cosh\alpha_\mathrm{o})}{\ell_\Lambda - \mathfrak{r}(\sinh\alpha_\mathrm{o}\cos\vartheta' - \cosh\alpha_\mathrm{o})}\right|,$$

$$R' = \frac{\mathfrak{r}\cosh\alpha_\mathrm{o}}{1 - (\mathfrak{r}/\ell_\Lambda)\sinh\alpha_\mathrm{o}\cos\vartheta'}, \quad \left|\tan\frac{\vartheta'}{2}\right| = \exp\left(\psi - \frac{\mathfrak{u}}{\ell_\Lambda}\sinh\alpha_\mathrm{o}\right), \tag{A100}$$

$$\tau = \frac{\mathfrak{u}}{\ell_\Lambda}\cosh\alpha_\mathrm{o} - \frac{1}{2}\log\left|\frac{\ell_\Lambda - \mathfrak{r}(\sinh\alpha_\mathrm{o}\cos\vartheta' + \cosh\alpha_\mathrm{o})}{\ell_\Lambda - \mathfrak{r}(\sinh\alpha_\mathrm{o}\cos\vartheta' - \cosh\alpha_\mathrm{o})}\right|, \tag{A101}$$

$$v=\frac{\ell_\Lambda}{\mathfrak{r}\cosh\alpha_o}-\tanh\alpha_o\cos\vartheta',\quad \xi=\tanh\left(\psi-\frac{\mathfrak{u}}{\ell_\Lambda}\sinh\alpha_o\right),$$

where $\cos\vartheta'=-\xi$ is given in terms of the Robinson-Trautman coordinates by the last equation.

Relation to flat cosmological family: If we introduce the spherical coordinates $\check{t}'$, $\check{r}'$, ϑ', φ boosted with respect to the flat cosmological coordinates $\check{t}$, $\check{r}$, ϑ, φ by a boost α_o (in the sense of Minkowski space $\check{M}$), we find that the accelerated coordinates T', R' are related to $\hat{t}'$, $\hat{r}'$ in exactly the same way as the static coordinates T, R are related to the coordinates $\check{t}$, $\check{r}$. The boost $\check{t}'=\check{t}\cosh\alpha_o+\check{z}\sinh\alpha_o$, $\check{x}'=\check{x}$, $\check{y}'=\check{y}$, $\check{z}'=\check{t}\sinh\alpha_o+\check{z}\cosh\alpha_o$, rewritten in the spherical coordinates $\check{r}'\cos\vartheta'=\check{z}'$, $\check{r}'\sin\vartheta'=\sqrt{\check{x}'^2+\check{y}'^2}$, reads

$$\begin{aligned}\check{t}'&=\check{t}\cosh\alpha_o+\check{r}\cos\vartheta\sinh\alpha_o,\\ \check{r}'\cos\vartheta'&=\check{t}\sinh\alpha_o+\check{r}\cos\vartheta\cosh\alpha_o,\\ \check{r}'\sin\vartheta'&=\check{r}\sin\vartheta,\end{aligned}\tag{A102}$$

and relations analogous to Eqs. (A67) and (A80) are

$$T'=-\frac{\ell_\Lambda}{2}\log\left|\frac{\check{t}'^2-\check{r}'^2}{\ell_\Lambda^2}\right|,\quad R'=-\ell_\Lambda\frac{\check{r}'}{\check{t}'}\,.\tag{A103}$$

Similarly, the formulas relating the accelerated coordinates to the coordinates $\hat{t}$, $\hat{r}$, ϑ are

$$\begin{aligned}\hat{t}'&=\hat{t}\cosh\alpha_o-\hat{r}\cos\vartheta\sinh\alpha_o,\\ \hat{r}'\cos\vartheta'&=-\hat{t}\sinh\alpha_o+\hat{r}\cos\vartheta\cosh\alpha_o,\\ \hat{r}'\sin\vartheta'&=\hat{r}\sin\vartheta,\end{aligned}\tag{A104}$$

$$T'=\frac{\ell_\Lambda}{2}\log\left|\frac{\hat{t}'^2-\hat{r}'^2}{\ell_\Lambda^2}\right|,\quad R'=\ell_\Lambda\frac{\hat{r}'}{\hat{t}'}\,.\tag{A105}$$

The conformal factor takes the form

$$\Omega=\frac{\check{t}'}{\check{t}}=\frac{\hat{t}'}{\hat{t}}=\cosh\alpha_o-\frac{R}{\ell_\Lambda}\sinh\alpha_o\cos\vartheta.\tag{A106}$$

9. The Robinson-Trautman coordinates:

In the Robinson-Trautman coordinates $\mathfrak{u},\mathfrak{r},\psi,\varphi$ (or in their complex version $\mathfrak{u},\mathfrak{r},\zeta,\bar{\zeta}$), de Sitter metric takes the standard Robinson-Trautman form (see Fig. 22).[50] The coordinate $\mathfrak{u}$ is null, the "radial" coordinate $\mathfrak{r}$ is an affine parameter along coordinate lines $\mathfrak{u},\psi,\varphi=$constant. These lines are null geodesics generating light cones with vertices at the origin $\mathfrak{r}=0$. The coordinates ψ,φ (or $\zeta,\bar{\zeta}$) are angular coordinates, however, they are not functions of the accelerated angular coordinates ϑ',φ only [cf. Eq. (A112)]. Because ϑ',φ have a clearer geometrical meaning, we list some formulas also in the mixed coordinate system $\mathfrak{u},\mathfrak{r},\vartheta',\varphi$.

The origin $\mathfrak{r}=0$ of the Robinson-Trautman coordinates is centered on the worldline of the uniformly accelerated observer moving with the acceleration $|a_o|=|\ell_\Lambda^{-1}\sinh\alpha_o|$. The coordinates are thus closely related to the accelerated coordinates.

The coordinates $\mathfrak{u},\mathfrak{r},\psi,\varphi$ do not cover the whole space–time smoothly. They can be introduced smoothly in the future of the north pole, or in the past of the south pole. At the boundary of these two domains, $\mathfrak{u}\to\pm\infty$.

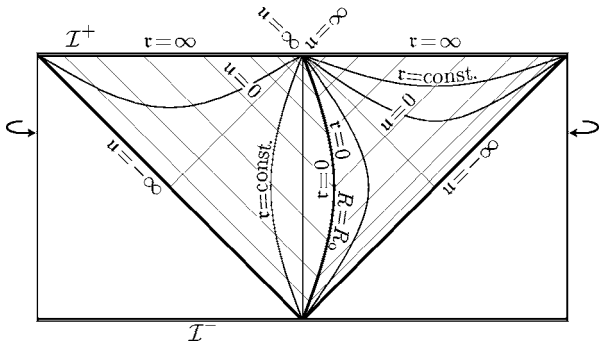

FIG. 22. The Robinson-Trautman coordinates.

Metric and relation between coordinates,

$$g = -H\,\mathrm{d}\mathfrak{u}^2 - \mathrm{d}\mathfrak{u}\vee\mathrm{d}\mathfrak{r} + \frac{\mathfrak{r}^2}{P^2}(\mathrm{d}\psi^2+\mathrm{d}\varphi^2), \tag{A107}$$

$$g = -H\,\mathrm{d}\mathfrak{u}^2 - \mathrm{d}\mathfrak{u}\vee\mathrm{d}\mathfrak{r} + \frac{\mathfrak{r}^2}{P^2}\mathrm{d}\zeta\vee\mathrm{d}\bar{\zeta}, \tag{A108}$$

$$g = -\cosh^2\alpha_0\frac{\mathfrak{r}^2}{\ell_\Lambda^2}(v^2-1)\mathrm{d}\mathfrak{u}^2 - \mathrm{d}\mathfrak{u}\vee\mathrm{d}\mathfrak{r} + \cosh\alpha_0\frac{\mathfrak{r}^2}{\ell_\Lambda}\sin\vartheta'\,\mathrm{d}\mathfrak{u}\vee\mathrm{d}\vartheta' + \mathfrak{r}^2(\mathrm{d}\vartheta'^2+\sin^2\vartheta'\,\mathrm{d}\varphi^2), \tag{A109}$$

$$H = -\frac{\mathfrak{r}^2}{\ell_\Lambda^2} + 2\frac{\mathfrak{r}}{\ell_\Lambda}\sinh\alpha_0\tanh\left(\psi - \frac{\mathfrak{u}}{\ell_\Lambda}\sinh\alpha_0\right) + 1 = -\frac{\mathfrak{r}^2}{\ell_\Lambda^2} - 2\frac{\mathfrak{r}}{\ell_\Lambda}\sinh\alpha_0\cos\vartheta' + 1, \tag{A110}$$

$$P = \cosh\left(\psi - \frac{\mathfrak{u}}{\ell_\Lambda}\sinh\alpha_0\right) = \frac{1}{\sin\vartheta'}, \tag{A111}$$

$$\begin{aligned}\psi &= \frac{\mathfrak{u}}{\ell_\Lambda}\sinh\alpha_0 + \log\left|\tan\frac{\vartheta'}{2}\right|,\\ \left|\tan\frac{\vartheta'}{2}\right| &= \exp\left(\psi - \frac{\mathfrak{u}}{\ell_\Lambda}\sinh\alpha_0\right),\end{aligned} \tag{A112}$$

$$\begin{aligned}\zeta &= \frac{1}{\sqrt{2}}(\psi - i\varphi), \quad \psi = \frac{1}{\sqrt{2}}(\zeta+\bar{\zeta}),\\ \bar{\zeta} &= \frac{1}{\sqrt{2}}(\psi + i\varphi), \quad \varphi = \frac{i}{\sqrt{2}}(\zeta-\bar{\zeta}).\end{aligned} \tag{A113}$$

Null tetrad: Since the Robinson-Trautman coordinates are closely related to the congruence of null geodesics, it is convenient to introduce the null tetrad which is parallelly transported along these geodesics $\mathfrak{u}, \psi, \varphi$=constant,

$$\mathrm{k}_{\mathrm{RT}}=\frac{1}{\sqrt{2}}\frac{\partial}{\partial\mathfrak{r}},\quad \mathrm{l}_{\mathrm{RT}}=-\frac{1}{\sqrt{2}}H\frac{\partial}{\partial\mathfrak{r}}+\sqrt{2}\frac{\partial}{\partial\mathfrak{u}},$$

$$\mathrm{m}_{\mathrm{RT}}=\frac{1}{\sqrt{2}}\frac{P}{\mathfrak{r}}\left(\frac{\partial}{\partial\psi}-i\frac{\partial}{\partial\varphi}\right),\quad \bar{\mathrm{m}}_{\mathrm{RT}}=\frac{1}{\sqrt{2}}\frac{P}{\mathfrak{r}}\left(\frac{\partial}{\partial\psi}+i\frac{\partial}{\partial\varphi}\right). \tag{A114}$$

Relation to accelerated coordinate family,

$$\mathfrak{r}=\frac{R'\sqrt{1-R_{\mathrm{o}}^2/\ell_\Lambda^2}}{1+(R'R_{\mathrm{o}}/\ell_\Lambda^2)\cos\vartheta'},$$

$$\mathfrak{u}=\sqrt{1-\frac{R_{\mathrm{o}}^2}{\ell_\Lambda^2}}\left(T'+\frac{\ell_\Lambda}{2}\log\left|\frac{R'-\ell_\Lambda}{R'+\ell_\Lambda}\right|\right), \tag{A115}$$

$$\psi=\frac{R_{\mathrm{o}}}{\ell_\Lambda}\left(\frac{T'}{\ell_\Lambda}+\frac{1}{2}\log\left|\frac{R'-\ell_\Lambda}{R'+\ell_\Lambda}\right|\right)+\log\left|\tan\frac{\vartheta'}{2}\right|,$$

$$\mathfrak{r}=\frac{\ell_\Lambda}{v\cosh\alpha_{\mathrm{o}}-\xi\sinh\alpha_{\mathrm{o}}},$$

$$\mathfrak{u}=\frac{\ell_\Lambda}{\cosh\alpha_{\mathrm{o}}}\left(\tau+\frac{1}{2}\log\left|\frac{1-v}{1+v}\right|\right), \tag{A116}$$

$$\psi=\tanh\alpha_{\mathrm{o}}\left(\tau+\frac{1}{2}\log\left|\frac{1-v}{1+v}\right|\right)+\frac{1}{2}\log\left|\frac{1+\xi}{1-\xi}\right|.$$

Relation to static family,

$$\mathfrak{r}=\frac{\ell_\Lambda}{\sqrt{1-R_{\mathrm{o}}^2/\ell_\Lambda^2}}\left[\left(1-\frac{RR_{\mathrm{o}}}{\ell_\Lambda^2}\cos\vartheta\right)^2-\left(1-\frac{R^2}{\ell_\Lambda^2}\right)\left(1-\frac{R_{\mathrm{o}}^2}{\ell_\Lambda^2}\right)\right]^{1/2}, \tag{A117}$$

$$\mathfrak{r}\sin\vartheta'=R\sin\vartheta,\quad \mathfrak{r}\cos\vartheta'=\frac{R\cos\vartheta-R_{\mathrm{o}}}{\sqrt{1-R_{\mathrm{o}}^2/\ell_\Lambda^2}}, \tag{A118}$$

$$R\sin\vartheta=\mathfrak{r}\sin\vartheta',\quad R\cos\vartheta=\mathfrak{r}\cos\vartheta'\sqrt{1-R_{\mathrm{o}}^2/\ell_\Lambda^2}+R_{\mathrm{o}}. \tag{A119}$$

10. The null family:

Finally, we return back to the coordinate systems which employ standard coordinates ϑ, φ. Time and radial coordinates can be transformed into two null coordinates. Such null coordinates can be associated with most coordinate families introduced above. Coordinates $\tilde{u}$, $\tilde{v}$ are related to the standard coordinates; $\check{u}$, $\check{v}$ and $\hat{u}$, $\hat{v}$ to the flat cosmological coordinates; u, v to the conformally Minkowski; and $\bar{u}$, $\bar{v}$ to the static coordinates. Coordinate vectors $\{\partial/\partial\tilde{u},\partial/\partial\tilde{v}\}$, $\{\partial/\partial\check{u},\partial/\partial\check{v}\}$, etc., are the pairs of independent null vectors in the radial 2-slices ϑ, φ=constant. We do not allow the radial coordinate to be negative in the definitions of null coordinates because this would interchange the meaning of u and v. The null coordinates are thus drawn in the right half of Fig. 23 only.

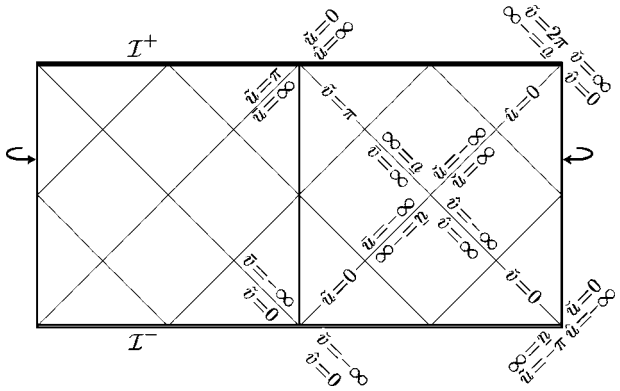

FIG. 23. The null family of coordinates

Metric and relation to other coordinates,

$$g = \frac{\ell_\Lambda^2}{1-\cos(\tilde{u}+\tilde{v})}(-\,\mathrm{d}\tilde{u}\vee\mathrm{d}\tilde{v} + (1-\cos(\tilde{u}-\tilde{v}))\mathrm{d}\omega^2), \tag{A120}$$

$$g = \frac{\ell_\Lambda^2}{(\hat{u}+\hat{v})^2}(-\,2\,\mathrm{d}\hat{u}\vee\mathrm{d}\hat{v} + (\hat{u}-\hat{v})^2\,\mathrm{d}\omega^2), \tag{A121}$$

$$g = \frac{\ell_\Lambda^2}{(\check{u}+\check{v})^2}(-\,2\,\mathrm{d}\check{u}\vee\mathrm{d}\check{v} + (\check{u}-\check{v})^2\,\mathrm{d}\omega^2), \tag{A122}$$

$$g = \left(\frac{\ell_\Lambda^2}{\ell_\Lambda^2 - uv}\right)^2(-\,2\,\mathrm{d}u\vee\mathrm{d}v + (u-v)^2\,\mathrm{d}\omega^2), \tag{A123}$$

$$g = \left(\exp\frac{\bar{u}}{\ell_\Lambda} + \exp\frac{\bar{v}}{\ell_\Lambda}\right)^{-2}\left(-\,2\exp\frac{\bar{u}+\bar{v}}{\ell_\Lambda}\mathrm{d}\bar{u}\vee\mathrm{d}\bar{v} + \ell_\Lambda^2\left(\exp\frac{\bar{u}}{\ell_\Lambda} - \exp\frac{\bar{v}}{\ell_\Lambda}\right)^2\mathrm{d}\omega^2\right). \tag{A124}$$

The relation of time and radial coordinates $\overset{*}{t}$, $\overset{*}{r}$ to the corresponding null coordinates $\overset{*}{u}$, $\overset{*}{v}$ is given by the usual formulas,

$$\begin{aligned} \overset{*}{t} &= \tfrac{1}{2}(\overset{*}{v}+\overset{*}{u}), \quad \overset{*}{u} = \overset{*}{t} - \overset{*}{r}, \\ \overset{*}{r} &= \tfrac{1}{2}(\overset{*}{v}-\overset{*}{u}), \quad \overset{*}{v} = \overset{*}{t} + \overset{*}{r}. \end{aligned} \tag{A125}$$

Here $\{\overset{*}{t},\overset{*}{r}\}$ stands for $\{\tilde{t},\tilde{r}\}$, $\{\check{t},\check{r}\}$, $\{\hat{t},\hat{r}\}$, $\{t,r\}$, and $\{\bar{t},\bar{r}\}$, respectively; similarly with $\{\overset{*}{u},\overset{*}{v}\}$.

Relation between null coordinates: The coordinates $\hat{u}$, $\hat{v}$, u, v, and $\check{u}$, $\check{v}$ can be viewed as null coordinates in the conformally related Minkowski spaces $\hat{M}$, M, and $\check{M}$; these are shifted with respect to each other by $\pi/2$ in the direction of the conformally Einstein time coordinate $\tilde{t}$, or associated null coordinates,

$$\frac{\hat{u}}{\ell_\Lambda} = \tan\frac{\tilde{u}}{2}, \quad \frac{\hat{v}}{\ell_\Lambda} = \tan\frac{\tilde{v}}{2},$$

$$\frac{u}{\ell_\Lambda}=\tan\left(\frac{\tilde{u}}{2}-\frac{\pi}{4}\right),\quad \frac{v}{\ell_\Lambda}=\tan\left(\frac{\tilde{v}}{2}-\frac{\pi}{4}\right), \tag{A126}$$

$$\frac{\check{u}}{\ell_\Lambda}=\tan\left(\frac{\bar{u}}{2}-\frac{\pi}{2}\right),\quad \frac{\check{v}}{\ell_\Lambda}=\tan\left(\frac{\bar{v}}{2}-\frac{\pi}{2}\right).$$

The remaining coordinates $\bar{u}$, $\bar{v}$ are related to the conformally Einstein null coordinates $\tilde{u}$, $\tilde{v}$ by the "compactification transformation,"

$$\tan\frac{\tilde{u}}{2}=s_u\exp\frac{\bar{u}}{\ell_\Lambda},\quad \tan\frac{\tilde{v}}{2}=s_v\exp\frac{\bar{v}}{\ell_\Lambda}. \tag{A127}$$

Here the sign factors s_u and s_v are given by

$$s_u=\operatorname{sign}\tan\frac{\tilde{u}}{2},\quad s_v=\operatorname{sign}\tan\frac{\tilde{v}}{2}. \tag{A128}$$

Relations (A126) and (A127) between null coordinates can also be rewritten as follows:

$$\tan\frac{\tilde{u}}{2}=s_u\exp\frac{\bar{u}}{\ell_\Lambda}=\frac{\hat{u}}{\ell_\Lambda}=-\frac{\ell_\Lambda}{\check{u}}=\frac{\ell_\Lambda+u}{\ell_\Lambda-u},$$

$$\tan\tilde{u}=-s_u\sinh^{-1}\frac{\bar{u}}{\ell_\Lambda}=\frac{2\hat{u}\ell_\Lambda}{\ell_\Lambda^2-\hat{u}^2}=\frac{2\check{u}\ell_\Lambda}{\ell_\Lambda^2-\check{u}^2}=\frac{u^2-\ell_\Lambda^2}{2u\ell_\Lambda},$$

$$\sin\tilde{u}=s_u\cosh^{-1}\frac{\bar{u}}{\ell_\Lambda}=\frac{2\hat{u}\ell_\Lambda}{\ell_\Lambda^2+\hat{u}^2}=\frac{-2\check{u}\ell_\Lambda}{\ell_\Lambda^2+\check{u}^2}=\frac{\ell_\Lambda^2-u^2}{\ell_\Lambda^2+u^2}, \tag{A129}$$

$$\cos\tilde{u}=-\tanh\frac{\bar{u}}{\ell_\Lambda}=\frac{\ell_\Lambda^2-\hat{u}^2}{\ell_\Lambda^2+\hat{u}^2}=\frac{\hat{u}^2-\ell_\Lambda^2}{\hat{u}^2+\ell_\Lambda^2}=\frac{-2u\ell_\Lambda}{\ell_\Lambda^2+u^2},$$

$$\frac{\hat{u}}{\ell_\Lambda}=\tan\frac{\tilde{u}}{2}=s_u\exp\frac{\bar{u}}{\ell_\Lambda}=-\frac{\ell_\Lambda}{\check{u}}=\frac{\ell_\Lambda+u}{\ell_\Lambda-u}, \tag{A130}$$

$$-\frac{\check{u}}{\ell_\Lambda}=\cot\frac{\tilde{u}}{2}=s_u\exp\left(-\frac{\bar{u}}{\ell_\Lambda}\right)=\frac{\ell_\Lambda}{\hat{u}}=\frac{\ell_\Lambda-u}{\ell_\Lambda+u}, \tag{A131}$$

$$\frac{u}{\ell_\Lambda}=-\frac{1-\sin\tilde{u}}{\cos\tilde{u}}=-\frac{\cos\tilde{u}}{1+\sin\tilde{u}}=\left(\tanh\frac{\bar{u}}{2\ell_\Lambda}\right)^{s_u}=\frac{\hat{u}-\ell_\Lambda}{\hat{u}+\ell_\Lambda}=\frac{\ell_\Lambda+\check{u}}{\ell_\Lambda-\check{u}}, \tag{A132}$$

$$\frac{\bar{u}}{\ell_\Lambda}=\log\left|\tan\frac{\tilde{u}}{2}\right|=\log\left|\frac{\hat{u}}{\ell_\Lambda}\right|=\log\left|\frac{\ell_\Lambda}{\check{u}}\right|=\log\left|\frac{\ell_\Lambda+u}{\ell_\Lambda-u}\right|=2\operatorname{arctanh}\left(\frac{u}{\ell_\Lambda}\right)^{s_u}, \tag{A133}$$

$$\hat{u}\check{u}=-\ell_\Lambda^2,\quad \frac{\hat{u}}{\ell_\Lambda}+\frac{\ell_\Lambda}{\check{u}}=0. \tag{A134}$$

The same relations hold for coordinates v, $\tilde{v}$, $\hat{v}$, $\check{v}$ and $\bar{v}$.

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$\mathfrak{sl}_2$ Gaudin model with jordanian twist

N. Cirilo António[a)]
Departamento de Matemática, Instituto Superior Técnico, UTL, Lisbon, Portugal

N. Manojlović[b)]
Departamento de Matemática, FCT, Universidade do Algarve, Campus de Gambelas, 8005-139 Faro, Portugal

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$\mathfrak{sl}_2$ Gaudin model with jordanian twist is studied. This system can be obtained as the semiclassical limit of the *XXX* spin chain deformed by the jordanian twist. The appropriate creation operators that yield the Bethe states of the Gaudin model and consequently its spectrum are defined. Their commutation relations with the generators of the corresponding loop algebra as well as with the generating function of integrals of motion are given. The inner products and norms of Bethe states and the relation to the solutions of the Knizhnik-Zamolodchikov equations are discussed. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2036932]

I. INTRODUCTION

The quantum inverse scattering method (QISM) was largely created by Faddeev and his school at St. Petersburg as a quantum counterpart of the classical inverse scattering method.[1–4] Classifying quantum solvable systems with respect to the underlying dynamical symmetry algebras, one could say that the Gaudin models[5,6] can be seen as the simplest ones being based on loop algebras. Their Hamiltonians are related to classical r-matrices,

$$H^{(a)} = \sum_{b \neq a}^{N} r_{ab}(z_a - z_b). \tag{1.1}$$

The condition of their commutativity $[H^{(a)}, H^{(b)}]=0$ is nothing else but the classical Yang-Baxter equation

$$[r_{ab}(z_a - z_b), r_{ac}(z_a - z_c) + r_{bc}(z_b - z_c)] + [r_{ac}(z_a - z_c), r_{bc}(z_b - z_c)] = 0, \tag{1.2}$$

where r is antisymmetric and belongs to the tensor product $\mathfrak{g} \otimes \mathfrak{g}$ of a Lie algebra $\mathfrak{g}$, or its representations and the indices fix the corresponding factors in the N-fold tensor product of this algebra. The Gaudin models based on the classical r-matrices of simple Lie algebras attracted a lot of attention.[7–11] Their spectrum and corresponding eigenfunctions were obtained using different methods such as coordinate and algebraic Bethe ansatz, separated variables, etc. The correlation functions of the $\mathfrak{sl}_2$ Gaudin system were calculated by means of the Gauss factorization.[8] A connection between the Bethe vectors of the Gaudin models for simple Lie algebras to the solutions of the Knizhnik-Zamolodchikov equation was established in Refs. 9–11. An explanation of this connection based on Wakimoto modules at critical level of the underlying affine algebra was given in Ref. 10.

The algebraic Bethe Ansatz for the Gaudin model based on the $\mathfrak{sl}_2$ invariant classical r-matrix deformed by the constant jordanian r-matrix was postulated in Ref. 12. Following the ideas used

[a)]Electronic mail: nantonio@math.ist.utl.pt
[b)]Electronic mail: nmanoj@ualg.pt

in the case of the $\mathfrak{osp}(1|2)$ trigonometric Gaudin model,[13] Kulish noticed that the similarity transformation by $\exp(\alpha X^+)\otimes\exp(\alpha X^+)$ on the $\mathfrak{sl}_2$ trigonometrical classical r-matrix,

$$r_{\mathrm{trig}}(\lambda)=\frac{e^{-\lambda}}{\sinh(\lambda)}r^{(+)}+\frac{e^{\lambda}}{\sinh(\lambda)}r^{(-)}=\frac{e^{-\lambda}}{\sinh(\lambda)}\left(\frac{1}{2}h\otimes h+2X^+\otimes X^-\right)+\frac{e^{\lambda}}{\sinh(\lambda)}\left(\frac{1}{2}h\otimes h+2X^-\otimes X^+\right),$$

setting $\lambda\to\epsilon\lambda$, $\alpha\to\xi/2\epsilon$ and after the scaling limit

$$\lim_{\epsilon\to 0}\epsilon r_{\mathrm{trig}}(\epsilon\lambda)=\frac{1}{\lambda}(h\otimes h+2(X^+\otimes X^-+X^-\otimes X^+))+\xi(h\otimes X^+-X^+\otimes h),$$

yields the $\mathfrak{sl}_2$-invariant classical r-matrix deformed by the jordanian r-matrix. Moreover the highest weight vector of the corresponding Gaudin model is preserved. Based on these arguments Kulish postulated the Bethe vectors, the spectrum, and the Bethe equations of the system.

Alternatively, the jordanian twist[14–16]

$$\mathcal{F}^J=e^{h\otimes\sigma}=\exp\left(h\otimes\tfrac{1}{2}\ln(1+2\theta X^+)\right) \tag{1.3}$$

can be applied to the $\mathfrak{sl}_2$-invariant spin system based on the Yang quantum R-matrix,

$$R(\lambda;\eta)=I+\frac{\eta}{\lambda}\mathcal{P}, \tag{1.4}$$

where $\mathcal{P}$ is the permutation matrix in the tensor product $\mathbb{C}^2\otimes\mathbb{C}^2$, to obtain the twisted $\mathfrak{sl}_2$ spin system.[14,17] The semiclassical limit $\eta\to 0$ of this system yields the same Gaudin model discussed by Kulish.[12] The twisted XXX spin chain related to the quantum R-matrix,

$$R(\lambda;\eta;\theta)=R^J(\theta)+\frac{\eta}{\lambda}\mathcal{P}, \tag{1.5}$$

where $R^J(\theta)=\mathcal{F}^J_{21}(\mathcal{F}^J_{12})^{-1}$ is the $\mathfrak{sl}_2$ jordanian quantum R-matrix studied in Refs. 18–20, whose homogeneous case was analyzed in Ref. 14, will be discussed elsewhere,[17] here will only be presented the aspects relevant to the study of the corresponding Gaudin model.

The $\mathfrak{L}$-operator of the quantum spin system on a one-dimensional lattice with N sites coincides with R-matrix acting on a tensor product $V_0\otimes V_a$ of auxiliary space $V_0=\mathbb{C}^2$ and the space of states at site $a=1,2,\ldots,N$,

$$\mathfrak{L}_{0a}(\lambda-z_a)=\begin{pmatrix}e^{-\sigma_a} & \theta h_a e^{\sigma_a}\\ 0 & e^{\sigma_a}\end{pmatrix}+\frac{\eta}{\lambda-z_a}\begin{pmatrix}\frac{h_a}{2} & X_a^-\\ X_a^+ & -\frac{h_a}{2}\end{pmatrix}, \tag{1.6}$$

where z_a is a parameter of inhomogeneity (site dependence). Corresponding monodromy matrix $\mathfrak{T}$ is an ordered product of the $\mathfrak{L}$ operators,

$$\mathfrak{T}(\lambda;\{z_a\}_1^N)=\mathfrak{L}_{0N}(\lambda-z_N)\cdots\mathfrak{L}_{01}(\lambda-z_1)=\prod_{a=1}^{\overleftarrow{N}}\mathfrak{L}_{0a}(\lambda-z_a)=\begin{pmatrix}A(\lambda) & B(\lambda)\\ C(\lambda) & D(\lambda)\end{pmatrix}. \tag{1.7}$$

The commutation relations of the $\mathfrak{T}$-matrix entries follow form the FRT relation

$$R_{12}(\lambda-\mu;\eta;\theta)\mathfrak{T}_1(\lambda)\mathfrak{T}_2(\mu)=\mathfrak{T}_2(\mu)\mathfrak{T}_1(\lambda)R_{12}(\lambda-\mu;\eta;\theta). \tag{1.8}$$

Multiplying (1.8) by R_{12}^{-1} and taking the trace over $\mathbb{C}^2\otimes\mathbb{C}^2$, one gets commutativity of the transfer matrix

$$\mathfrak{t}(\lambda)=\operatorname{tr}\mathfrak{T}(\lambda)=A(\lambda)+D(\lambda) \tag{1.9}$$

for different values of the spectral parameter $\mathfrak{t}(\lambda)\mathfrak{t}(\mu)=\mathfrak{t}(\mu)\mathfrak{t}(\lambda)$.

It is of interest to choose different spins l_a at different sites of the lattice, hence the following space of states:

$$\mathcal{H}=\bigotimes_{a=1}^{N}V_a^{(l_a)},$$

with the highest spin vector $\Omega_+=\otimes_{a=1}^{N}\omega_a$. It is straightforward to show that

$$C(\lambda)\Omega_+=0, \tag{1.10}$$

and

$$A(\lambda)\Omega_+=a(\lambda)\Omega_+=\prod_{a=1}^{N}\left(\frac{\lambda-z_a+\ell_a\eta/2}{\lambda-z_a}\right)\Omega_+, \tag{1.11}$$

$$D(\lambda)\Omega_+=d(\lambda)\Omega_+=\prod_{a=1}^{N}\left(\frac{\lambda-z_a-\ell_a\eta/2}{\lambda-z_a}\right)\Omega_+. \tag{1.12}$$

As the first step in the application of the algebraic Bethe Ansatz to the twisted *XXX* spin chain one can confirm that the highest spin vector Ω_+ is an eigenvector of the transfer matrix (1.9),

$$\mathfrak{t}(\lambda)\Omega_+=\Lambda_0(\lambda)\Omega_+, \tag{1.13}$$

with $\Lambda_0(\lambda)=a(\lambda)+d(\lambda)$. The next step is to show that $\Psi_1(\mu)=B(\mu)\Omega_+$ is also an eigenvector of the transfer matrix

$$\begin{aligned}\mathfrak{t}(\lambda)\Psi_1(\mu)=\mathfrak{t}(\lambda)B(\mu)\Omega_+=\Lambda_1(\lambda,\mu)\Psi_1(\mu)+\frac{\eta}{\lambda-\mu}(a(\mu)-d(\mu))\Psi_1(\lambda)\\ -\theta(a(\mu)-d(\mu))(a(\lambda)-d(\lambda))\Omega_+,\end{aligned} \tag{1.14}$$

where the eigenvalue $\Lambda_1(\lambda,\mu)$ and the Bethe equations are given by

$$\Lambda_1(\lambda,\mu)=\Lambda_0(\lambda)-\frac{\eta}{\lambda-\mu}(a(\lambda)-d(\lambda)), \tag{1.15}$$

$$a(\mu)-d(\mu)=0. \tag{1.16}$$

The following steps of the algebraic Bethe Ansatz are analogous having the same eigenvalues and Bethe equations as in the invariant case,[14] the details will be presented elsewhere.[17]

The corresponding Gaudin model can be obtained from the spin system via the semiclassical limit[7,21] by setting $\theta=-(\eta/2)\xi$ and using the expansion in powers of η of the monodromy matrix

$$\mathfrak{T}(\lambda)=\mathrm{I}+\frac{\eta}{2}L(\lambda)+\mathcal{O}(\eta^2), \tag{1.17}$$

where

$$L(\lambda)=\begin{pmatrix} h(\lambda) & 2X^{-}(\lambda) \\ 2X^{+}(\lambda) & -h(\lambda) \end{pmatrix} \tag{1.18}$$

and

$$h(\lambda)=\sum_{a=1}^{N}\left(\frac{h_a}{\lambda-z_a}+\xi X_a^{+}\right),\quad X^{-}(\lambda)=\sum_{a=1}^{N}\left(\frac{X_a^{-}}{\lambda-z_a}-\frac{\xi}{2}h_a\right),\quad X^{+}(\lambda)=\sum_{a=1}^{N}\frac{X_a^{+}}{\lambda-z_a}. \tag{1.19}$$

Substituting the expansion of the monodromy matrix (1.17) and

$$R(\lambda;\eta;\theta)\big|_{\theta=-(\eta/2)\xi}=\mathrm{I}+\frac{\eta}{2}r_{\xi}(\lambda)+\mathcal{O}(\eta^2), \tag{1.20}$$

with

$$r_{\xi}(\lambda)=\begin{pmatrix} \frac{1}{\lambda} & \xi & -\xi & 0 \\ 0 & -\frac{1}{\lambda} & \frac{2}{\lambda} & \xi \\ 0 & \frac{2}{\lambda} & -\frac{1}{\lambda} & -\xi \\ 0 & 0 & 0 & \frac{1}{\lambda} \end{pmatrix}, \tag{1.21}$$

into the FRT relations (1.8), the first nontrivial term, the coeficient of η^2, is the so-called Sklyanin bracket[7]

$$[L_1(\lambda),L_2(\mu)]=-[r_{\xi}(\lambda-\mu),L_1(\lambda)+L_2(\mu)]. \tag{1.22}$$

Moreover the central element $\Delta(\lambda)$,[2] of the algebra (1.8), admits the expansion in η such that the second order term of $\mathfrak{t}(\lambda)-\Delta(\lambda)$ is the generating function of the integrals of motion of the corresponding Gaudin model,[7]

$$t(\lambda)=\tfrac{1}{2}\mathrm{Tr}\,L^2(\lambda). \tag{1.23}$$

The first step in the application of the algebraic Bethe Ansatz, to the Gaudin models, is to define appropriate creation operators that yield the Bethe states and consequently the spectrum of the generating function $t(\lambda)$. The creation operators used in the $\mathfrak{sl}_2$-invariant Gaudin model coincide with one of the L-matrix entry.[5,7] However, in the present case these operators are not homogeneous polynomials of the generator $X^{-}(\lambda)$ and can be defined by the recursive relation as proposed by Kulish.[12] It is convenient to define $B_M^{(k)}(\mu_1,\ldots,\mu_M)$, a more general set of operators, in order to simplify the calculation of the commutators between the creation operators and the generating function of the integrals of motion $t(\lambda)$. These operators are symmetric functions of their arguments and they satisfy certain recursive relations. Their commutation relations with the generators of the loop algebra are straightforward to calculate and they are essential in the main step of the algebraic Bethe Ansatz. The creation operators of the $\mathfrak{sl}_2$ Gaudin model with jordanian twist are the particular case $B_M(\mu_1,\ldots,\mu_M)=B_M^{(0)}(\mu_1,\ldots,\mu_M)$. Thus the commutation relations between the creation operators and $t(\lambda)$ are easily calculated. Therefore the corresponding Bethe vectors can be defined by the action of the creation operators on the highest spin vector Ω_+ and thus the spectrum of the system is determined. In this way the algebraic Bethe Ansatz is fully implemented confirming the result of Kulish[12] that the spectrum of the system coincides with the one of the $\mathfrak{sl}_2$-invariant model and consequently the twisted Gaudin Hamiltonians have the same spectrum as in the $\mathfrak{sl}_2$-invariant case, although the Bethe vectors of the two systems are different. However the Bethe vectors, in this case, are not eigenstates of the global Cartan generator h_{gl}.

Besides the problem of determining the spectrum of the system, via algebraic Bethe Ansatz, some properties of the creation operators are fundamental in calculating the inner products and the norms of the Bethe states. In particular, it turns out that the relation between the creation operators of the system and the ones in the untwisted case is essential in determining the inner products of the Bethe vectors. In addition, it is necessary to consider the dual creation operators $B_M^*(\mu_1,\ldots,\mu_M)$ obtained by using the dual Gaudin model based on the following classical r-matrix:

$$r^*(\lambda)=\frac{1}{\lambda}(h\otimes h+2(X^+\otimes X^-+X^-\otimes X^+))+\xi(h\otimes X^--X^-\otimes h). \tag{1.24}$$

As opposed to the $\mathfrak{sl}_2$-invariant case, the Bethe vectors $\Psi_M(\mu_1,\ldots,\mu_M)$ are not orthogonal for different M's. It should also be mentioned that, due to the jordanian twist, the dual generating function of integrals of motion $t^*(\lambda)$ is not equal to $t(\lambda)$, the generating function of integrals of motion of the original model, contrary to the $\mathfrak{sl}_2$-invariant case, thus these operators are not Hermitian.

A connection between the Bethe vectors, when the Bethe equations are not imposed on their parameters, of the twisted Gaudin model to the solutions of the corresponding Knizhnik-Zamolodchikov equation, similarly to the $\mathfrak{sl}_2$-invariant model, is based on some analytical properties of the creation operators $B_M(\mu_1,\ldots,\mu_M)$.

The paper is organized as follows. In Sec. II we discuss the Gaudin model based on the $\mathfrak{sl}_2$ invariant r-matrix with jordanian twist emphasizing the creation operators B_M. Using the previously established properties of the creation operators B_M, in Sec. III the spectrum and the Bethe vectors of the system are given. The dual creation operators are used to obtain the expressions for inner products and norms of Bethe states. In conclusion a relation between the Bethe vectors and the solutions to the Knizhnik-Zamolodchikov equation are discussed. In the appendix the proofs of the lemmas are given.

II. $_2$ TWISTED GAUDIN MODEL

The $\mathfrak{sl}_2$-invariant classical r-matrix with jordanian twist[22,18,19] is the following element of $\mathfrak{sl}_2\otimes\mathfrak{sl}_2$:

$$r_\xi(\lambda)=\frac{c_2^\otimes}{\lambda}+\xi r^J=\frac{1}{\lambda}(h\otimes h+2(X^+\otimes X^-+X^-\otimes X^+))+\xi(h\otimes X^+-X^+\otimes h). \tag{2.1}$$

The matrix form of $r_\xi(\lambda)$ in the fundamental representation of $\mathfrak{sl}_2$ follows from (2.1) by replacing the appropriate matrices for the generators of $\mathfrak{sl}_2$ given explicitly by

$$r_\xi(\lambda)=\begin{pmatrix}\frac{1}{\lambda} & \xi & -\xi & 0\\ 0 & -\frac{1}{\lambda} & \frac{2}{\lambda} & \xi\\ 0 & \frac{2}{\lambda} & -\frac{1}{\lambda} & -\xi\\ 0 & 0 & 0 & \frac{1}{\lambda}\end{pmatrix}, \tag{2.2}$$

here $\lambda\in\mathbb{C}$ is the spectral and $\xi\in\mathbb{C}$ is the twisting parameter. Definition of the Gaudin model requires not only the classical r-matrix but also the L operator

$$L(\lambda)=\begin{pmatrix} h(\lambda) & 2X^{-}(\lambda) \\ 2X^{+}(\lambda) & -h(\lambda) \end{pmatrix}, \tag{2.3}$$

whose entries $(h(\lambda),X^{\pm}(\lambda))$ are generators of the loop algebra $\mathcal{L}_{\xi}(\mathfrak{sl}_2)$ defined by the Sklyanin linear bracket

$$[L_1(\lambda),L_2(\mu)]=-[r_{12}(\lambda-\mu),L_1(\lambda)+L_2(\mu)]. \tag{2.4}$$

The corresponding commutation relations between the generators are explicitly given by

$$\begin{aligned}
&[h(\lambda),h(\mu)]=2\xi(X^{+}(\lambda)-X^{+}(\mu)),\\
&[X^{-}(\lambda),X^{-}(\mu)]=-\xi(X^{-}(\lambda)-X^{-}(\mu)),\\
&[X^{+}(\lambda),X^{-}(\mu)]=-\frac{h(\lambda)-h(\mu)}{\lambda-\mu}+\xi X^{+}(\lambda),\\
&[X^{+}(\lambda),X^{+}(\mu)]=0,\\
&[h(\lambda),X^{-}(\mu)]=2\frac{X^{-}(\lambda)-X^{-}(\mu)}{\lambda-\mu}+\xi h(\mu),\\
&[h(\lambda),X^{+}(\mu)]=-2\frac{X^{+}(\lambda)-X^{+}(\mu)}{\lambda-\mu}.
\end{aligned} \tag{2.5}$$

The usual $\mathfrak{sl}_2$ loop algebra is recovered be setting $\xi=0$.

In order to define a dynamical system besides the algebra of observables $\mathcal{L}_{\xi}(\mathfrak{sl}_2)$ a Hamiltonian should be specified. Due to the Sklyanin linear bracket (2.4) the elements

$$t(\lambda)=\tfrac{1}{2}\mathrm{Tr}\,L^2(\lambda)=h^2(\lambda)+2(X^{+}(\lambda)X^{-}(\lambda)+X^{-}(\lambda)X^{+}(\lambda))=h^2(\lambda)-2h'(\lambda)+2(2X^{-}(\lambda)+\xi)X^{+}(\lambda) \tag{2.6}$$

generate an Abelian subalgebra

$$t(\lambda)t(\mu)=t(\mu)t(\lambda). \tag{2.7}$$

One way to show (2.7) is to notice that the commutation relation between $t(\lambda)$ and $L(\mu)$ can be written in the form

$$[t(\lambda),L(\mu)]=[M(\lambda,\mu),L(\mu)], \tag{2.8}$$

using (2.4)–(2.6) it is straightforward to calculate $M(\lambda,\mu)$,

$$\begin{aligned}
M(\lambda,\mu)&=-\mathrm{Tr}_1(r_{12}(\lambda-\mu)L_1(\lambda))-\frac{1}{2}\mathrm{Tr}_1(r_{12}^2(\lambda-\mu))\\
&=\begin{pmatrix} -2\dfrac{h(\lambda)}{\lambda-\mu}+2\xi X^{+}(\lambda) & -4\dfrac{X^{-}(\lambda)}{\lambda-\mu}-2\xi h(\lambda) \\ -4\dfrac{X^{+}(\lambda)}{\lambda-\mu} & 2\dfrac{h(\lambda)}{\lambda-\mu}-2\xi X^{+}(\lambda) \end{pmatrix}-\frac{3}{(\lambda-\mu)^2}I_2.
\end{aligned} \tag{2.9}$$

Thus the commutators between the generating function $t(\lambda)$ and the generators of the loop algebra follow from (2.8) and (2.9):

$$[t(\lambda),X^+(\mu)]=4\frac{X^+(\mu)h(\lambda)-X^+(\lambda)h(\mu)}{\lambda-\mu}-4\xi X^+(\lambda)X^+(\mu), \tag{2.10}$$

$$[t(\lambda),h(\mu)]=8\frac{X^-(\mu)X^+(\lambda)-X^-(\lambda)X^+(\mu)}{\lambda-\mu}-4\xi h(\lambda)X^+(\mu), \tag{2.11}$$

$$[t(\lambda),X^-(\mu)]=4\frac{X^-(\lambda)h(\mu)-X^-(\mu)h(\lambda)}{\lambda-\mu}+2\xi h(\lambda)h(\mu)+4\xi X^-(\mu)X^+(\lambda)+2\xi^2X^+(\mu). \tag{2.12}$$

Preserving some generality, the representation space $\mathcal{H}$ of the Sklyanin algebra (2.4) and (2.5) can be a highest spin $\rho(\lambda)$ representation with the highest spin vector Ω_+,

$$X^+(\lambda)\Omega_+=0,\quad h(\lambda)\Omega_+=\rho(\lambda)\Omega_+. \tag{2.13}$$

The spectrum and the eigenstates of $t(\lambda)$ can be studied in this general setting. However to have a physical interpretation a local realization

$$\mathcal{H}=V_1\otimes\cdots\otimes V_N \tag{2.14}$$

as tensor product of $\mathfrak{sl}_2$-modules is needed. Then the L operator is given by

$$L(\lambda)=\sum_{a=1}^{N}\left(\frac{1}{\lambda-z_a}\begin{pmatrix}h_a & 2X_a^-\\ 2X_a^+ & -h_a\end{pmatrix}+\xi\begin{pmatrix}X_a^+ & -h_a\\ 0 & -X_a^+\end{pmatrix}\right), \tag{2.15}$$

where $Y_a=(h_a,X_a^\pm)\in\mathrm{End}(V_a)$ are $\mathfrak{sl}_2$ generators in representation V_a, associated with each site a. For convenience, the generators $Y(\lambda)=(h(\lambda),X^\pm(\lambda))$ are written down explicitly,

$$h(\lambda)=\sum_{a=1}^{N}\left(\frac{h_a}{\lambda-z_a}+\xi X_a^+\right),\quad X^-(\lambda)=\sum_{a=1}^{N}\left(\frac{X_a^-}{\lambda-z_a}-\frac{\xi}{2}h_a\right),\quad X^+(\lambda)=\sum_{a=1}^{N}\frac{X_a^+}{\lambda-z_a}. \tag{2.16}$$

In this realization it is useful to consider the expressions of the generators of the global $\mathfrak{sl}_2$ Lie algebra in terms of the local ones,

$$Y_{\mathrm{gl}}=\sum_{a=1}^{N}Y_a, \tag{2.17}$$

where $Y=(h,X^\pm)$. Also, the following notation is useful:

$$Y(\lambda)_0=\left.Y(\lambda)\right|_{\xi=0}, \tag{2.18}$$

then $h(\lambda)=h(\lambda)_0+\xi X_{\mathrm{gl}}^+$.

A representation of the model with the above Gaudin realization is obtained by considering at each site a an irreducible representation $V_a^{(\ell_a)}$ of $\mathfrak{sl}_2$ with highest weight ℓ_a corresponding to a singular vector $\omega_a\in V_a^{(\ell_a)}$ such that $X_a^+\omega_a=0$ and $h_a\omega_a=\ell_a\omega_a$. Thus the space of states is

$$\mathcal{H}=V_1^{(\ell_1)}\otimes\cdots\otimes V_N^{(\ell_N)}, \tag{2.19}$$

with the highest spin vector (2.13),

$$\Omega_+=\omega_1\otimes\cdots\otimes\omega_N \tag{2.20}$$

and the corresponding highest spin

$$\rho(\lambda)=\sum_{a=1}^{N}\frac{\ell_a}{\lambda-z_a}. \tag{2.21}$$

The Gaudin Hamiltonians,

$$H^{(a)}=\sum_{b\neq a}^{N} r_{ab}(z_a-z_b)=\sum_{b\neq a}^{N}\left(\frac{c_2^{\otimes}(a,b)}{z_a-z_b}+\xi(h_aX_b^{+}-X_a^{+}h_b)\right), \tag{2.22}$$

where $c_2^{\otimes}(a,b)=h_a\otimes h_b+2(X_a^{+}\otimes X_b^{-}+X_a^{-}\otimes X_b^{+})$, can be obtained as the residues of the generating function $t(\lambda)$ at the points $\lambda=z_a$, $a=1,\ldots,N$ using the expansion

$$t(\lambda)=\sum_{a=1}^{N}\left(\frac{c_2(a)}{(\lambda-z_a)^2}+\frac{2H^{(a)}}{\lambda-z_a}\right)+\xi^2\sum_{a,b=1}^{N}X_a^{+}X_b^{+}, \tag{2.23}$$

here $c_2(a)=h_a^2+2h_a+4X_a^{-}X_a^{+}$ is the $\mathfrak{sl}_2$ Casimir at site a. As opposed to the $\mathfrak{sl}_2$-invariant case, the generating function (2.23) commutes only with the generator X_{gl}^{+}.

The first step in the algebraic Bethe Ansatz is to define appropriate creation operators that yield the Bethe states and consequently the spectrum of the generating function $t(\lambda)$. The creation operators used in the $\mathfrak{sl}_2$-invariant Gaudin model coincide with one of the L-matrix entries.[5,7] However, in the present case these operators are not homogeneous polynomials of the generator $X^{-}(\lambda)$. It is convenient to define a more general set of operators in order to simplify the presentation.

Definition 2.1: Given two integers M and $k\geqslant 0$ consider the operators

$$\begin{aligned}B_M^{(k)}(\mu_1,\ldots,\mu_M)&=(X^{-}(\mu_1)+k\xi)(X^{-}(\mu_2)+(k+1)\xi)\cdots(X^{-}(\mu_M)+(M+k-1)\xi)\\&=\prod_{n=k}^{M+k-1}{}^{\rightarrow}(X^{-}(\mu_{n-k+1})+n\xi),\end{aligned} \tag{2.24}$$

with $B_0^{(k)}=1$ and $B_M^{(k)}=0$ for $M<0$.

The following lemma describes some properties of the $B_M^{(k)}(\mu_1,\ldots,\mu_M)$ operators which will be used later on.

Lemma 2.1: Some useful properties of $B_M^{(k)}(\mu_1,\ldots,\mu_M)$ operators are the following:

(i) *The operators $B_M^{(k)}(\mu_1,\ldots,\mu_M)$ are symmetric functions of their arguments.*

(ii) $B_M^{(k)}(\mu_1,\ldots,\mu_M)=B_{M-1}^{(k)}(\mu_1,\ldots,\mu_{M-1})(B_1^{(0)}(\mu_M)+(M+k-1)\xi)$.

(iii) $B_M^{(k)}(\boldsymbol{\mu})=B_M^{(k-1)}(\boldsymbol{\mu})+\xi\sum_{i=1}^{M}B_{M-1}^{(k)}(\boldsymbol{\mu}^{(i)})$, *here $\boldsymbol{\mu}$ is a set of $M=|\boldsymbol{\mu}|$ complex scalars with a particular ordering $\boldsymbol{\mu}=\{\mu_1,\ldots,\mu_M\}$ assumed for convenience and the notation*

$$\boldsymbol{\mu}^{(i_1,\ldots,i_k)}=\boldsymbol{\mu}\setminus\{\mu_{i_1},\ldots,\mu_{i_k}\}$$

for any distinct $i_1,\ldots,i_k\in\{1,\ldots,M\}$.

(iv) $B_M^{(k)}(\boldsymbol{\mu})=B_1^{(k)}(\mu_1)B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(1)})$.

Implementation of the algebraic Bethe Ansatz requires the commutation relations between the generators of the loop algebra $\mathcal{L}_{\xi}(\mathfrak{sl}_2)$ and the $B_M^{(k)}(\mu_1,\ldots,\mu_M)$ operators. To this end we first introduce the notation for the Bethe operators

$$\hat{\beta}_M(\lambda;\boldsymbol{\mu})=h(\lambda)+\sum_{\mu\in\boldsymbol{\mu}}\frac{2}{\mu-\lambda}, \tag{2.25}$$

where $\boldsymbol{\mu}=\{\mu_1,\ldots,\mu_{M-1}\}$ and $\lambda\in\mathbb{C}\setminus\boldsymbol{\mu}$. In the particular case $M=1$, $\hat{\beta}_1(\lambda;\varnothing)=h(\lambda)$ and will be denoted by $\hat{\beta}_1(\lambda)$. The required commutators are given in the following lemma.

Lemma 2.2: The commutation relation between the generators $h(\lambda)$, $X^{\pm}(\lambda)$, *and the* $B_M^{(k)}(\mu_1,\ldots,\mu_M)$ *operators are given by*

$$h(\lambda)B_M^{(k)}(\boldsymbol{\mu}) = B_M^{(k)}(\boldsymbol{\mu})h(\lambda) + 2\sum_{i=1}^{M}\frac{B_M^{(k)}(\lambda\cup\boldsymbol{\mu}^{(i)}) - B_M^{(k)}(\boldsymbol{\mu})}{\lambda-\mu_i} + \xi\sum_{i=1}^{M} B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(i)})\hat{\beta}_M(\mu_i;\boldsymbol{\mu}^{(i)}), \tag{2.26}$$

$$X^{+}(\lambda)B_M^{(k)}(\boldsymbol{\mu}) = B_M^{(k)}(\boldsymbol{\mu})X^{+}(\lambda) - \sum_{i=1}^{M} B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(i)})\frac{\hat{\beta}_M(\lambda;\boldsymbol{\mu}^{(i)}) - \hat{\beta}_M(\mu_i;\boldsymbol{\mu}^{(i)})}{\lambda-\mu_i} - 2\sum_{\substack{i,j=1\\ i<j}}^{M}\frac{B_{M-1}^{(k+1)}(\{\lambda\}\cup\boldsymbol{\mu}^{(i,j)})}{(\lambda-\mu_i)(\lambda-\mu_j)}$$
$$+ \xi\sum_{i=1}^{M} B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(i)})X^{+}(\lambda), \tag{2.27}$$

$$X^{-}(\lambda)B_M^{(k)}(\boldsymbol{\mu}) = B_M^{(k)}(\boldsymbol{\mu})(X^{-}(\lambda)+M\xi) - \xi\sum_{i=1}^{M} B_M^{(k)}(\lambda\cup\boldsymbol{\mu}^{(i)}) = B_{M+1}^{(k)}(\lambda\cup\boldsymbol{\mu}) - \xi\sum_{i=1}^{M} B_M^{(k)}(\lambda\cup\boldsymbol{\mu}^{(i)}). \tag{2.28}$$

The B operators that define the Bethe states of the system were proposed by Kulish.[12] These operators are the particular case $k=0$ of (2.24) and will be denoted by $B_M(\mu_1,\ldots,\mu_M)=B_M^{(0)}(\mu_1,\ldots,\mu_M)$. A recursive relation of the B operators follows from (ii) of Lemma 2.1,

$$B_M(\boldsymbol{\mu}) = B_{M-1}(\boldsymbol{\mu}^{(M)})(X^{-}(\mu_M)+(M-1)\xi). \tag{2.29}$$

It may be useful to write down explicitly the first few B operators,

$$B_0 = 1, \quad B_1(\mu) = X^{-}(\mu), \quad B_2(\mu_1,\mu_2) = X^{-}(\mu_1)X^{-}(\mu_2) + \xi X^{-}(\mu_1),$$

$$B_3(\mu_1,\mu_2,\mu_3) = X^{-}(\mu_1)X^{-}(\mu_2)X^{-}(\mu_3) + 2\xi X^{-}(\mu_1)X^{-}(\mu_2) + \xi X^{-}(\mu_1)X^{-}(\mu_3) + 2\xi^2 X^{-}(\mu_1).$$

As a particular case of Lemma 2.2 the commutation relation between loop algebra generators $h(\lambda)$, $X^{\pm}(\lambda)$ and the B operators are given by setting $k=0$ in (2.26)–(2.28),

$$h(\lambda)B_M(\boldsymbol{\mu}) = B_M(\boldsymbol{\mu})h(\lambda) + \sum_{i=1}^{M}\left(2\frac{B_M(\lambda\cup\boldsymbol{\mu}^{(i)}) - B_M(\boldsymbol{\mu})}{\lambda-\mu_i} + \xi B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})\hat{\beta}_M(\mu_i;\boldsymbol{\mu}^{(i)})\right), \tag{2.30}$$

$$X^{+}(\lambda)B_M(\boldsymbol{\mu}) = B_M(\boldsymbol{\mu})X^{+}(\lambda) - \sum_{i=1}^{M} B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})\left(\frac{\hat{\beta}_M(\lambda;\boldsymbol{\mu}^{(i)}) - \hat{\beta}_M(\mu_i;\boldsymbol{\mu}^{(i)})}{\lambda-\mu_i} - \xi X^{+}(\lambda)\right)$$
$$- 2\sum_{\substack{i,j=1\\ i<j}}^{M}\frac{B_{M-1}^{(1)}(\{\lambda\}\cup\boldsymbol{\mu}^{(i,j)})}{(\lambda-\mu_i)(\lambda-\mu_j)}, \tag{2.31}$$

$$X^{-}(\lambda)B_M(\boldsymbol{\mu}) = B_M(\boldsymbol{\mu})(X^{-}(\lambda)+M\xi) - \xi\sum_{i=1}^{M} B_M(\lambda\cup\boldsymbol{\mu}^{(i)}). \tag{2.32}$$

The crucial step in the algebraic Bethe Ansatz is to determine the commutation relations between the creation operators, in this case the B operators, and the generating function $t(\lambda)$. The main lemma, based on the results established previously in this section, will given a complete expression for the required commutator.

Lemma 2.3: The generating function $t(\lambda)$ has the following commutation relation with the B operators:

$$
\begin{aligned}
t(\lambda)B_M(\boldsymbol{\mu}) = B_M(\boldsymbol{\mu})&\left(t(\lambda) - \sum_{i=1}^{M}\frac{4h(\lambda)}{\lambda-\mu_i} + \sum_{i<j}^{M}\frac{8}{(\lambda-\mu_i)(\lambda-\mu_j)}\right) + 4\sum_{i=1}^{M}\frac{B_M(\lambda\cup\boldsymbol{\mu}^{(i)})}{\lambda-\mu_i}\hat{\beta}_M(\mu_i;\boldsymbol{\mu}^{(i)})\\
&+ 2\xi\sum_{i=1}^{M}B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})h(\lambda)\hat{\beta}_M(\mu_i;\boldsymbol{\mu}^{(i)}) + 4\xi\sum_{\substack{i,j=1\\ i\neq j}}^{M}\frac{B_{M-1}^{(1)}(\lambda\cup\boldsymbol{\mu}^{(i,j)}) - B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})}{\lambda-\mu_j}\hat{\beta}_M(\mu_i;\boldsymbol{\mu}^{(i)})\\
&+ \xi^2\sum_{\substack{i,j=1\\ i\neq j}}^{M}B_{M-2}^{(2)}(\boldsymbol{\mu}^{(i,j)})\hat{\beta}_{M-1}(\mu_j;\boldsymbol{\mu}^{(i,j)})\hat{\beta}_M(\mu_i;\boldsymbol{\mu}^{(i)}) + 4M\xi B_M(\boldsymbol{\mu})X^{+}(\lambda)\\
&+ 2\xi^2\sum_{i=1}^{M}B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})X^{+}(\mu_i).
\end{aligned}
\tag{2.33}
$$

Proof: The case $M=1$ can be obtained directly from the M matrix (2.9) and is given by (2.12). For $M>1$ the commutator between the operator $t(\lambda)$ and the corresponding B operator is to be calculated directly using expression (2.6),

$$
\begin{aligned}
[t(\lambda),B_M(\boldsymbol{\mu})] = [h(\lambda),[h(\lambda),B_M(\boldsymbol{\mu})]] &+ 2[h(\lambda),B_M(\boldsymbol{\mu})]h(\lambda) - 2\frac{d}{d\lambda}[h(\lambda),B_M(\boldsymbol{\mu})]\\
&+ 2(2X^{-}(\lambda)+\xi)[X^{+}(\lambda),B_M(\boldsymbol{\mu})] + 4[X^{-}(\lambda),B_M(\boldsymbol{\mu})]X^{+}(\lambda).
\end{aligned}
$$

The terms in the preceding expression only involve the commutators between the generators of the loop algebra and the B operators. Each term in the above equation will be calculated separately. Using the commutators (2.26) and (2.30)–(2.32) the first term is given by

$$
\begin{aligned}
[h(\lambda),[h(\lambda),B_M(\boldsymbol{\mu})]] = B_M(\boldsymbol{\mu})&\sum_{i<j}^{M}\frac{8}{(\lambda-\mu_i)(\lambda-\mu_j)}\\
&- 4\sum_{i=1}^{M}\left(\frac{B_M(\{\lambda\}\cup\boldsymbol{\mu}^{(i)}) - B_M(\boldsymbol{\mu})}{(\lambda-\mu_i)^2} - \frac{\frac{d}{d\lambda}B_M(\{\lambda\}\cup\boldsymbol{\mu}^{(i)})}{\lambda-\mu_i}\right)\\
&+ 8\sum_{i<j}^{M}\frac{X^{-}(\lambda)B_{M-1}^{(1)}(\{\lambda\}\cup\boldsymbol{\mu}^{(i,j)})}{(\lambda-\mu_i)(\lambda-\mu_j)} - 4\sum_{i=1}^{M}\frac{B_M(\{\lambda\}\cup\boldsymbol{\mu}^{(i)})}{\lambda-\mu_i}\sum_{j\neq i}^{M}\frac{2}{\lambda-\mu_j}\\
&+ 4\xi\sum_{i<j}^{M}\frac{B_{M-1}^{(1)}(\{\lambda\}\cup\boldsymbol{\mu}^{(i,j)})}{(\lambda-\mu_i)(\lambda-\mu_j)} + 2\xi\sum_{i=1}^{M}B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})\frac{\hat{\beta}_M(\lambda;\boldsymbol{\mu}^{(i)}) - \hat{\beta}_M(\mu_i\boldsymbol{\mu}^{(i)})}{\lambda-\mu_i}\\
&+ \xi\sum_{i\neq j}^{M}\left(4\frac{B_{M-1}^{(1)}(\lambda\cup\boldsymbol{\mu}^{(i,j)}) - B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})}{\lambda-\mu_j} + \xi B_{M-2}^{(2)}(\boldsymbol{\mu}^{(i,j)})\hat{\beta}_{M-1}(\mu_j;\boldsymbol{\mu}^{(i,j)})\right)\\
&\times\hat{\beta}_M(\mu_i;\boldsymbol{\mu}^{(i)}) + 2\xi^2\sum_{i=1}^{M}B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})(X^{+}(\lambda)-X^{+}(\mu_i)).
\end{aligned}
$$

The commutator between the generator $h(\lambda)$ and $B_M(\boldsymbol{\mu})$ is also used to determine the next two terms

$$2[h(\lambda),B_M(\boldsymbol{\mu})]h(\lambda)=B_M(\boldsymbol{\mu})\sum_{i=1}^{M}\frac{-4h(\lambda)}{\lambda-\mu_i}+4\sum_{i=1}^{M}\frac{B_M(\{\lambda\}\cup\boldsymbol{\mu}^{(i)})}{\lambda-\mu_i}h(\lambda)+2\xi\sum_{i=1}^{M}B_{M-1}^{(1)}$$
$$\times(\boldsymbol{\mu}^{(i)})h(\lambda)\hat{\beta}_M(\mu_i;\boldsymbol{\mu}^{(i)})-4\xi^2\sum_{i=1}^{M}B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})(X^+(\lambda)-X^+(\mu_i)),$$

and after differentiating (2.30),

$$-2\frac{d}{d\lambda}[h(\lambda),B_M(\boldsymbol{\mu})]=4\sum_{i=1}^{M}\frac{B_M(\{\lambda\}\cup\boldsymbol{\mu}^{(i)})-B_M(\boldsymbol{\mu})}{(\lambda-\mu_i)^2}-\frac{\frac{d}{d\lambda}B_M(\{\lambda\}\cup\boldsymbol{\mu}^{(i)})}{\lambda-\mu_i}.$$

The next term follows directly from (2.31),

$$2(2X^-(\lambda)+\xi)[X^+(\lambda),B_M(\boldsymbol{\mu})]=-4\sum_{i=1}^{M}B_M(\{\lambda\}\cup\boldsymbol{\mu}^{(i)})\frac{\hat{\beta}_M(\lambda;\boldsymbol{\mu}^{(i)})-\hat{\beta}_M(\mu_i;\boldsymbol{\mu}^{(i)})}{\lambda-\mu_i}$$
$$-8\sum_{i<j}^{M}\frac{X^-(\lambda)B_{M-1}^{(1)}(\{\lambda\}\cup\boldsymbol{\mu}^{(i,j)})}{(\lambda-\mu_i)(\lambda-\mu_j)}-2\xi\sum_{i=1}^{M}B_{M-1}^{(1)}$$
$$\times(\boldsymbol{\mu}^{(i)})\frac{\hat{\beta}_M(\lambda;\boldsymbol{\mu}^{(i)})-\hat{\beta}_M(\mu_i;\boldsymbol{\mu}^{(i)})}{\lambda-\mu_i}-4\xi\sum_{i<j}^{M}\frac{B_{M-1}^{(1)}(\{\lambda\}\cup\boldsymbol{\mu}^{(i,j)})}{(\lambda-\mu_i)(\lambda-\mu_j)}$$
$$+4\xi\sum_{i=1}^{M}B_M(\{\lambda\}\cup\boldsymbol{\mu}^{(i)})X^+(\lambda)+2\xi^2\sum_{i=1}^{M}B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})X^+(\lambda).$$

The last term is obtained from (2.32),

$$4[X^-(\lambda),B_M(\boldsymbol{\mu})]X^+(\lambda)=4M\xi B_M(\boldsymbol{\mu})X^+(\lambda)-4\xi\sum_{i=1}^{M}B_M(\{\lambda\}\cup\boldsymbol{\mu}^{(i)})X^+(\lambda).$$

When all terms in $[t(\lambda),B_M(\boldsymbol{\mu})]$ are put together it is straightforward to obtain the formula (2.33) □

Besides the problem of determining the spectrum of the system, via algebraic Bethe Ansatz, some properties of the B operators are fundamental in calculating the inner products and the norms of the Bethe states. To this end the relation between the B operators and the untwisted ones is established using the Gaudin realization (2.16),

$$B_M(\boldsymbol{\mu})=\sum_{k=0}^{M-1}\xi^k\sum_{j_1<\cdots<j_{M-k}}^{M}B_{M-k}(\mu_{j_1},\ldots,\mu_{j_{M-k}})_0\hat{p}_k^{(M-k)}+\xi^M\hat{p}_M,\tag{2.34}$$

where

$$B_{M-k}(\mu_{j_1},\ldots,\mu_{j_{M-k}})_0=B_{M-k}(\mu_{j_1},\ldots,\mu_{j_{M-k}})|_{\xi=0}$$

and also

$$\hat{p}_i^{(j)}=\left(-\frac{h_{\mathrm{gl}}}{2}+j\right)\cdots\left(-\frac{h_{\mathrm{gl}}}{2}+i+j-1\right)\quad\text{with }\hat{p}_i=\hat{p}_i^{(0)}\tag{2.35}$$

are operators defined for any integers i and j.

Moreover, some analytical properties of the B operators are important when solving the corresponding Knizhnik-Zamolodchikov equation.

Lemma 2.4: The B operators satisfy the following identity:

$$\frac{\partial}{\partial z_a} B_M(\boldsymbol{\mu}) = -\sum_{i=1}^{M} \frac{\partial}{\partial \mu_i} (X_a^-(\mu_i) B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})), \tag{2.36}$$

where $X_a^-(\mu_i) = [X_a^-/(\mu_i - z_a)] - (\xi/2)h_a$ *for site* $a = 1, \ldots, N$.

Using the relevant properties of the B operators established in this section, the fundamental description of the $\mathfrak{sl}_2$ Gaudin model with jordanian twist can be obtained.

III. SPECTRUM AND BETHE VECTORS OF THE TWISTED $_2$ GAUDIN MODEL

In this section the spectrum and the Bethe vectors of the twisted $\mathfrak{sl}_2$ Gaudin model as well as their inner products and norms will be determined by applying the algebraic Bethe Ansatz. The first step is to define the Bethe vectors $\Psi_M(\boldsymbol{\mu}) = B_M(\boldsymbol{\mu})\Omega_+$ by the action of the B operators on the highest spin vector Ω_+. Then the key observation is that highest spin vector Ω_+ is an eigenvector of the generating function of integrals of motion $t(\lambda)$. Finally the spectrum of the system is obtained as a consequence of the commutation relations between $t(\lambda)$ and $B_M(\boldsymbol{\mu})$ Lemma 2.3 (2.33). The unwanted terms coming from the commutator are annihilated by the Bethe equations on the parameters $\boldsymbol{\mu} = \{\mu_1, \ldots, \mu_M\}$ as well as by the condition $X^+(\lambda)\Omega_+ = 0$. Hence the algebraic Bethe Ansatz can be resumed in the following theorem.

Theorem 3.1: *The highest weight vector* Ω_+ *is an eigenvector of* $t(\lambda)$,

$$t(\lambda)\Omega_+ = \Lambda_0(\lambda)\Omega_+ \tag{3.1}$$

with the corresponding eigenvalue,

$$\Lambda_0(\lambda) = \rho^2(\lambda) - 2\rho'(\lambda) = \sum_{a=1}^{N} \frac{2}{\lambda - z_a} \left(\sum_{b \neq a}^{N} \frac{\ell_a \ell_b}{z_a - z_b} \right) + \sum_{a=1}^{N} \frac{\ell_a(\ell_a + 2)}{(\lambda - z_a)^2}. \tag{3.2}$$

Furthermore, the action of the B operators on the highest spin vector Ω_+ *yields the Bethe vectors*,

$$\Psi_M(\boldsymbol{\mu}) = B_M(\boldsymbol{\mu})\Omega_+, \tag{3.3}$$

such that

$$t(\lambda)\Psi_M(\boldsymbol{\mu}) = \Lambda_M(\lambda; \boldsymbol{\mu})\Psi_M(\boldsymbol{\mu}), \tag{3.4}$$

with the eigenvalues

$$\Lambda_M(\lambda; \boldsymbol{\mu}) = \rho_M^2(\lambda; \boldsymbol{\mu}) - 2\frac{\partial \rho_M}{\partial \lambda}(\lambda; \boldsymbol{\mu}) \quad \textit{and} \quad \rho_M(\lambda; \boldsymbol{\mu}) = \rho(\lambda) - \sum_{i=1}^{M} \frac{2}{\lambda - \mu_i}, \tag{3.5}$$

provided that the Bethe equations are imposed on the parameters $\boldsymbol{\mu} = \{\mu_1, \ldots, \mu_M\}$,

$$\sum_{a=1}^{N} \frac{\ell_a}{\mu_i - z_a} - \sum_{j \neq i}^{M} \frac{2}{\mu_i - \mu_j} = 0, \quad i = 1, \ldots, M. \tag{3.6}$$

Proof: A consequence of (2.6), (2.13), (2.20), and (2.21) is

$$t(\lambda)\Omega_+ = (h^2(\lambda) - 2h'(\lambda))\Omega_+ = (\rho^2(\lambda) - 2\rho'(\lambda))\Omega_+ = \Lambda_0(\lambda)\Omega_+.$$

The action of $t(\lambda)$ on the Bethe vectors $\Psi_M(\boldsymbol{\mu})$ (3.3) is evident from Lemma 2.3,

$$
\begin{aligned}
t(\lambda)\Psi_M(\boldsymbol{\mu}) &= t(\lambda)B_M(\boldsymbol{\mu})\Omega_+ = \Lambda_0(\lambda)\Psi_M(\boldsymbol{\mu}) + [t(\lambda), B_M(\boldsymbol{\mu})]\Omega_+ \\
&= \left(\Lambda_0(\lambda) - \sum_{i=1}^{M}\frac{4\rho(\lambda)}{\lambda-\mu_i} + \sum_{i<j}^{M}\frac{8}{(\lambda-\mu_i)(\lambda-\mu_j)}\right)\Psi_M(\boldsymbol{\mu}) \\
&\quad + 4\sum_{i=1}^{M}\frac{\Psi_M(\lambda\cup\boldsymbol{\mu}^{(i)})}{\lambda-\mu_i}\rho_M(\mu_i;\boldsymbol{\mu}^{(i)}) + 2\xi\sum_{i=1}^{M}\left(\rho(\lambda)\Psi^{(1)}_{M-1}(\boldsymbol{\mu}^{(i)})\right. \\
&\quad \left. + 2\sum_{i\neq j}^{M}\frac{\Psi^{(1)}_{M-1}(\lambda\cup\boldsymbol{\mu}^{(i,j)}) - \Psi^{(1)}_{M-1}(\boldsymbol{\mu}^{(i)})}{\lambda-\mu_j}\right)\rho_M(\mu_i;\boldsymbol{\mu}^{(i)}) \\
&\quad + \xi^2\sum_{i=1}^{M}\left(\sum_{j\neq i}^{M}\rho_{M-1}(\mu_j;\boldsymbol{\mu}^{(i,j)})\Psi^{(2)}_{M-2}(\boldsymbol{\mu}^{(i,j)})\right)\rho_M(\mu_i;\boldsymbol{\mu}^{(i)}),
\end{aligned}
\tag{3.7}
$$

where $\Psi^{(k)}_M(\boldsymbol{\mu}) = B^{(k)}_M(\boldsymbol{\mu})\Omega_+$ and $X^+(\lambda)\Omega_+ = 0$. When the Bethe equations are imposed on the parameters $\boldsymbol{\mu} = \{\mu_1, \ldots, \mu_M\}$,

$$
\rho_M(\mu_i;\boldsymbol{\mu}^{(i)}) = \sum_{a=1}^{N}\frac{\ell_a}{\mu_i - z_a} - \sum_{j\neq i}^{M}\frac{2}{\mu_i-\mu_j} = 0, \quad i = 1, \ldots, M, \tag{3.8}
$$

the unwanted terms in (3.7) vanish and hence $t(\lambda)\Psi_M(\boldsymbol{\mu}) = \Lambda_M(\boldsymbol{\Lambda};\boldsymbol{\mu})\Psi_M(\boldsymbol{\mu})$ with

$$
\Lambda_M(\lambda;\boldsymbol{\mu}) = \Lambda_0(\lambda) - \sum_{i=1}^{M}\frac{4\rho(\lambda)}{\lambda-\mu_i} + \sum_{i<j}^{M}\frac{8}{(\lambda-\mu_i)(\lambda-\mu_j)} = \rho^2_M(\lambda;\boldsymbol{\mu}) - 2\frac{\partial\rho_M}{\partial\lambda}(\lambda;\boldsymbol{\mu}). \tag{3.9}
$$

□

Due to the pole expansion (2.23) of $t(\lambda)$ the previous theorem yields the spectrum of the Gaudin Hamiltonians.

Corollary 3.1: The Bethe vectors $\Psi_M(\boldsymbol{\mu})$ are eigenvectors of the Gaudin Hamiltonians (2.22),

$$
H^{(a)}\Psi_M(\boldsymbol{\mu}) = E^{(a)}_M\Psi_M(\boldsymbol{\mu}) \tag{3.10}
$$

with the eigenvalues

$$
E^{(a)}_M = \sum_{b\neq a}^{N}\frac{\ell_a\ell_b}{z_a - z_b} - \sum_{i=1}^{M}\frac{2\ell_a}{z_a-\mu_i}. \tag{3.11}
$$

Remark 3.1: The fact that the spectrum of the $\mathfrak{sl}_2$-invariant Gaudin model remains is not affected by the jordanian twist can also be deduced from the following expression:

$$
t(\lambda) = t(\lambda)_0 + 2\xi(h(\lambda)_0X^+_{\mathrm{gl}} + 2\hat{p}^{(1)}_1X^+(\lambda)) + \xi^2(X^+_{\mathrm{gl}})^2. \tag{3.12}
$$

Remark 3.2: From the Gaudin realization (2.16) follows that $\xi X^+_{\mathrm{gl}} = \lim_{\lambda\to\infty} h(\lambda)$ and together with (2.30) is straightforward to obtain the action of the global generator X^+_{gl} on the Bethe vectors

$$
X^+_{\mathrm{gl}}\Psi_M(\boldsymbol{\mu}) = \sum_{i=1}^{M}\beta_M(\mu_i;\boldsymbol{\mu}^{(i)})\Psi^{(1)}_{M-1}(\boldsymbol{\mu}^{(i)}). \tag{3.13}
$$

Thus the Bethe vectors are annihilated by the global generator X^+_{gl},

$$
X^+_{\mathrm{gl}}\Psi_M(\boldsymbol{\mu}) = 0 \tag{3.14}
$$

once the Bethe equations (3.5) are imposed.

Remark 3.3: Analogously from (2.16) follows that $-(\xi/2)h_{\mathrm{gl}} = \lim_{\lambda\to\infty} X^-(\lambda)$ and with (2.32) and (ii) of Lemma 2.1 shows that Bethe vectors are not eigenstates of the global generator h_{gl},

$$h_{\mathrm{gl}}\Psi_M(\boldsymbol{\mu}) = -2p_1^{(M)}\Psi_M(\boldsymbol{\mu}) + 2\xi p_1^{(M-1)}\sum_{i=1}^{M}\Psi_{M-1}(\boldsymbol{\mu}^{(i)}), \tag{3.15}$$

where $p=-\frac{1}{2}\sum_{a=1}^{N}\ell_a$ *and* $p_l^{(k)}=(p+k)_l=(p+k)\cdots(p+l+k-1)$ *is the Pochhammer symbol.*

As it was shown already, the jordanian twist of the $\mathfrak{sl}_2$-invariant Gaudin model preserves its spectrum but the Bethe vectors are different, thus their inner products and norms are changed also. In order to determine the inner products and norms of the Bethe vectors it is of interest to consider the dual B operators, obtained by using the dual

$$(X^-)^*(\lambda) = \sum_{a=1}^{N}\left(\frac{X_a^+}{\lambda - z_a} - \frac{\xi}{2}h_a\right), \tag{3.16}$$

explicitly given by

$$B_M^*(\lambda_1, \ldots, \lambda_M) = \prod_{\substack{k=1\\ \leftarrow}}^{M}((X^-)^*(\lambda_k) + (k-1)\xi). \tag{3.17}$$

As opposed to the $\mathfrak{sl}_2$-invariant case here evidently the dual B operators do not annihilate the highest spin vector Ω_+,

$$B_M^*(\boldsymbol{\mu})\Omega_+ = \xi^M p_M \Omega_+. \tag{3.18}$$

Moreover the Bethe vectors are not orthogonal and their norms depend on the twist parameter.

Lemma 3.1: Consider integers $M_1, M_2 \geqslant 0$, $M=\min\{M_1, M_2\}$ *and complex numbers* $\boldsymbol{\lambda}=\{\lambda_1, \ldots, \lambda_{M_1}\}$ *and* $\boldsymbol{\mu}=\{\mu_1, \ldots, \mu_{M_2}\}$ *such that* $\boldsymbol{\lambda}\cap\boldsymbol{\mu}=\emptyset$. *Then the inner products between Bethe vectors is given by*

$$\begin{aligned}\langle\Psi_{M_1}(\boldsymbol{\lambda})|\Psi_{M_2}(\boldsymbol{\mu})\rangle &= p_{M_1}p_{M_2}\xi^{M_1+M_2} + \sum_{k=1}^{M} p_{M_1-k}^{(k)}p_{M_2-k}^{(k)}\xi^{M_1+M_2-2k}\\ &\times \sum_{i_1<\cdots<i_k}^{M_1}\ \sum_{j_1<\cdots<j_k}^{M_2}\langle\Psi_k(\lambda_{i_1}, \ldots, \lambda_{i_k})|\Psi_k(\mu_{j_1}, \ldots, \mu_{j_k})\rangle_0,\end{aligned} \tag{3.19}$$

where $\langle\cdot|\cdot\rangle_0=\langle\cdot|\cdot\rangle|_{\xi=0}$ *denotes the corresponding inner product of the* $\mathfrak{sl}_2$*-invariant Gaudin model.*[8]

Proof: The Bethe vectors are obtained from the action of the B operators (2.34) on Ω_+,

$$\Psi_M(\boldsymbol{\mu}) = B_M(\boldsymbol{\mu})\Omega_+ = p_M\xi^M\Omega_+ + \sum_{k=0}^{M-1}p_k^{(M-k)}\xi^k\sum_{j_1<\cdots<j_{M-k}}^{M}\Psi_{M-k}(\mu_{j_1}, \ldots, \mu_{j_{M-k}})_0,$$

where $\Psi_M(\boldsymbol{\mu})_0=B_M(\boldsymbol{\mu})|_{\xi=0}\Omega_+$ are the corresponding Bethe vectors of the $\mathfrak{sl}_2$-invariant Gaudin model. Then the inner product of the Bethe vectors of the twisted model are

$$\begin{aligned}\langle\Psi_{M_1}(\boldsymbol{\lambda})|\Psi_{M_2}(\boldsymbol{\mu})\rangle &= p_{M_1}p_{M_2}\xi^{M_1+M_2} + \sum_{k=0}^{M_1-1}\sum_{l=0}^{M_2-1}p_k^{(M_1-k)}p_l^{(M_2-l)}\xi^{k+l}\\ &\times\sum_{i_1<\cdots<i_{M_1-k}}^{M_1}\ \sum_{j_1<\cdots<j_{M_2-l}}^{M_2}\langle\Psi_{M_1-k}(\lambda_{i_1}, \ldots, \lambda_{i_{M_1-k}})|\Psi_{M_2-l}(\mu_{j_1}, \ldots, \mu_{j_{M_2-l}})\rangle_0\\ &= p_{M_1}p_{M_2}\xi^{M_1+M_2} + \sum_{n=1}^{M-1}p_{M_1-n}^{(n)}p_{M_1-n}^{(n)}\xi^{M_1+M_2-2n}\end{aligned}$$

$$\times \sum_{i_1<\cdots<i_n}^{M_1} \sum_{j_1<\cdots<j_n}^{M_2} \langle \Psi_n(\lambda_{i_1}, \ldots, \lambda_{i_n}) | \Psi_n(\mu_{j_1}, \ldots, \mu_{j_n}) \rangle_0.$$

□

The norms of the Bethe vector follow from the previous lemma.

Corollary 3.2: The norms of Bethe vectors $\Psi_M(\boldsymbol{\mu})$ are given by

$$\|\Psi_M(\boldsymbol{\mu})\|^2 = \sum_{k=0}^{M} (p_{M-k}^{(k)})^2 \xi^{2(M-k)} \sum_{\substack{i_1<\cdots<i_k \\ j_1<\cdots<j_k}}^{M} \langle \Psi_k(\mu_{i_1}, \ldots, \mu_{i_k}) | \Psi_k(\mu_{j_1}, \ldots, \mu_{j_k}) \rangle_0. \tag{3.20}$$

IV. CONCLUSION

The Gaudin model based on the $\mathfrak{sl}_2$ classical r-matrix with jordanian twist is studied. This system can be obtained as the semiclassical limit of the *XXX* spin chain deformed by the jordanian twist. Alternatively, applying a certain similarity transformation on the XXZ Gaudin model and using the scaling limit, Kulish[12] was able to postulate the spectrum and the Bethe states of the system.

The result of Kulish[12] that the spectrum of the system coincides with the one of the $\mathfrak{sl}_2$-invariant model is demonstrated by full implementation of the algebraic Bethe Ansatz. In order to construct the Bethe vectors it is necessary to consider the creation operators which are not homogeneous polynomials of one of the generators of the corresponding loop algebra. However, it was convenient to consider a more general set of operators $B_M^{(k)}(\mu_1, \ldots, \mu_M)$, in order to simplify the calculation of the commutators between the creation operators and the generating function of the integrals of motion $t(\lambda)$. These operators are symmetric functions of their arguments and they satisfy certain recursive relations. Their commutation relations with the generators of the loop algebra are given and they are essential in the main step of the algebraic Bethe Ansatz. The creation operators are the particular case $B_M(\mu_1, \ldots, \mu_M) = B_M^{(0)}(\mu_1, \ldots, \mu_M)$. Thus the commutation relations between the creation operators and $t(\lambda)$ are easily calculated. The corresponding Bethe vectors are defined by the action of the creation operators on the highest spin vector Ω_+ and the spectrum of the system is determined. However, the Bethe vectors in this case, are not eigenstates of the global Cartan generator h_{gl}.

Some properties of the creation operators are fundamental in calculating the inner products and the norms of the Bethe states. It is necessary to consider the dual creation operators $B_M^*(\mu_1, \ldots, \mu_M)$ obtained by using the dual Gaudin model. The Bethe vectors $\Psi_M(\mu_1, \ldots, \mu_M)$ are not orthogonal for different M's. Moreover, contrary to the $\mathfrak{sl}_2$-invariant case, the generating function of integrals of motion is not Hermitian.

The well known relation[9,10] between the off-shell Bethe vectors of the Gaudin models related to simple Lie algebras and the solutions of Knizhnik-Zamolodchikov equation[23]

$$\kappa \frac{\partial}{\partial z_a} \psi(z_1, \ldots, z_N) = H^{(a)} \psi(z_1, \ldots, z_N), \tag{4.1}$$

where $H^{(a)}$ are the Gaudin Hamiltonians (1.1), also holds for the KZ equation related to the $\mathfrak{sl}_2$ classical r-matrix with the jordanian twist. This relation is obtained by considering a Bethe vector $\Psi(\vec{\mu}|\vec{z})$, where the corresponding Bethe equations are not imposed, and the integral representation of solutions to the Knizhnik-Zamolodchikov equation,

$$\psi(z_1, \ldots, z_N) = \oint \cdots \oint \phi(\vec{\mu}|\vec{z}) \Psi(\vec{\mu}|\vec{z}) \mathrm{d}\vec{\mu}, \tag{4.2}$$

where $\phi(\vec{\mu}|\vec{z})$ is a scalar function

$$\phi(\vec{\mu}|\vec{z}) = \prod_{i<j}^{M} (\mu_i - \mu_j)^{4/\kappa} \prod_{a<b}^{N} (z_a - z_b)^{\ell_a \ell_b/\kappa} \prod_{a=1}^{N} \prod_{k=1}^{M} (z_a - \mu_k)^{-2\ell_a/\kappa}. \tag{4.3}$$

The partial derivatives of the scalar factor (4.3) are simply written

$$\kappa \partial_{z_a}(\phi) = E_M^{(a)} \phi \quad \text{and} \quad \kappa \partial_{\mu_i}(\phi) = -2\rho_M(\mu_i; \boldsymbol{\mu}^{(i)})\phi. \tag{4.4}$$

It is a simple matter to check that ψ given by (4.2) satisfies (4.1). Due to the Leibniz rule $\partial_{z_a}(\phi\Psi) = \partial_{z_a}(\phi)\Psi + \phi\partial_{z_a}(\Psi)$ and the residue of (3.7) at $\lambda = z_a$,

$$H^{(a)}\Psi(\boldsymbol{\mu}) = E_M^{(a)}\Psi(\boldsymbol{\mu}) - 2\sum_{i=1}^{M} \Psi_M^{(i,a)}(\boldsymbol{\mu})\rho_M(\mu_i; \boldsymbol{\mu}^{(i)}), \tag{4.5}$$

where $\Psi_M^{(i,a)}(\boldsymbol{\mu}) = X_a^-(\mu_i) B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})\Omega_+$ and $X_a^-(\mu_i) = [X_a^-/(\mu_i - z_a)] - (\xi/2)h_a$, we have

$$\kappa\partial_{z_a}(\phi\Psi) = H^{(a)}(\phi\Psi) + 2\phi\sum_{i=1}^{M} \Psi_M^{(i,a)}(\boldsymbol{\mu})\rho_M(\mu_i; \boldsymbol{\mu}^{(i)}) + \kappa\phi\partial_{z_a}(\Psi) = H^{(a)}(\phi\Psi) - \kappa\sum_{i=1}^{M} \partial_{\mu_i}(\phi\Psi_M^{(i,a)}). \tag{4.6}$$

To obtain the final formula we have used the Lemma 2.4 and formulas (4.4). Moreover, a closed contour integration of $\phi\Psi$ with respect to $\mu_1, \ldots, \mu_M$ will cancel the contribution from the sum and therefore $\psi(z_1, \ldots, z_N)$ given by (4.2) will satisfy Knizhnik-Zamolodchikov equation.

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APPENDIX: PROOFS OF LEMMAS

Proof of Lemma 2.1: The recurrence relations in (ii) and (iv) are evident from Definition 2.1.

(i) Given a fixed integer k, induction on M is used. Consider $M=2$ in definition (2.24),

$$B_2^{(k)}(\mu_1, \mu_2) = X^-(\mu_1)X^-(\mu_2) + (k+1)\xi X^-(\mu_1) + k\xi X^-(\mu_2) + k(k+1)\xi^2, \tag{A1}$$

then using (2.5) it is straightforward to check that $B_2^{(k)}(\mu_1, \mu_2) = B_2^{(k)}(\mu_2, \mu_1)$.

Assume $B_N^{(k)}(\mu_1, \ldots, \mu_N)$ is symmetric for $M-1 \geqslant N$. For $1 \leqslant i < j < M$ it is clear from (ii) that

$$B_M^{(k)}(\mu_1, \ldots, \mu_i, \ldots, \mu_j, \ldots, \mu_M) = B_M^{(k)}(\mu_1, \ldots, \mu_j, \ldots, \mu_i, \ldots, \mu_M).$$

The symmetry of $B_M^{(k)}(\mu_1, \ldots, \mu_M)$ with respect to μ_{M-1} and μ_M must be shown. To this end the recurrence relation in (ii) is to be iterated twice and the appropriate terms combined

$$\begin{aligned} B_M^{(k)}(\mu_1, \ldots, \mu_M) &= B_{M-2}^{(k)}(\mu_1, \ldots, \mu_{M-2})(X^-(\mu_{M-1}) + (M+k-2)\xi)(X^-(\mu_M) + (M+k-1)\xi) = B_{M-1}^{(k)} \\ &\quad \times(\mu_1, \ldots, \mu_{M-2}, \mu_M)(X^-(\mu_{M-1}) + (M+k-2)\xi) \\ &\quad + B_{M-2}^{(k)}(\mu_1, \ldots, \mu_{M-2})([X^-(\mu_{M-1}), X^-(\mu_M)] + \xi(X^-(\mu_{M-1}) + (M+k-2)\xi)) \\ &= B_{M-1}^{(k)}(\mu_1, \ldots, \mu_{M-2}, \mu_M)(X^-(\mu_{M-1}) + (M+k-2)\xi) + \xi B_{M-1}^{(k)}(\mu_1, \ldots, \mu_{M-2}, \mu_M) \\ &= B_M^{(k)}(\mu_1, \ldots, \mu_{M-2}, \mu_M, \mu_{M-1}). \end{aligned}$$

(iii) Applying the induction on M, for a fixed integer k. Set $M=2$, it is a direct consequence of (A1) that

$$B_2^{(k)}(\mu_1,\mu_2) = B_2^{(k-1)}(\mu_1,\mu_2) + \xi(B_1^{(k)}(\mu_1) + B_1^{(k)}(\mu_2)).$$

Assume (iii) is true for $M-1$ then

$$\begin{aligned} B_M^{(k)}(\boldsymbol{\mu}) &= \left(B_{M-1}^{(k-1)}(\boldsymbol{\mu}^{(M)}) + \xi \sum_{i=1}^{M-1} B_{M-2}^{(k)}(\boldsymbol{\mu}^{(i,M)}) \right)(X^-(\mu_M) + (M+k-1)\xi) \\ &= B_M^{(k-1)}(\boldsymbol{\mu}) + \xi B_{M-1}^{(k-1)}(\boldsymbol{\mu}^{(M)}) + \xi \sum_{i=1}^{M-1} (B_{M-1}^{(k)}(\boldsymbol{\mu}^{(i)}) + \xi B_{M-2}^{(k)}(\boldsymbol{\mu}^{(i,M)})) \\ &= B_M^{(k-1)}(\boldsymbol{\mu}) + \xi \sum_{i=1}^{M-1} B_{M-1}^{(k)}(\boldsymbol{\mu}^{(i)}) + \xi B_{M-1}^{(k)}(\boldsymbol{\mu}^{(M)}) = B_M^{(k-1)}(\boldsymbol{\mu}) + \xi \sum_{i=1}^{M} B_{M-1}^{(k)}(\boldsymbol{\mu}^{(i)}). \end{aligned}$$

□

Proof of Lemma 2.2: From Definition 2.1 $B_1^{(k)}(\mu) = X^-(\mu) + k\xi$, and commutators (2.5) it is clear that $M=1$ in (2.26) and (2.28) is given by

$$[h(\lambda), B_1^{(k)}(\mu)] = [h(\lambda), X^-(\mu)] = 2\frac{B_1^{(k)}(\lambda) - B_1^{(k)}(\mu)}{\lambda - \mu} + \xi\hat{\beta}_1(\mu),$$

$$[X^+(\lambda), B_1^{(k)}(\mu)] = [X^+(\lambda), X^-(\mu)] = -\frac{\hat{\beta}_1(\lambda) - \hat{\beta}_1(\mu)}{\lambda - \mu} + \xi X^+(\lambda),$$

$$[X^-(\lambda), B_1^{(k)}(\mu)] = [X^-(\lambda), X^-(\mu)] = \xi B_1^{(k)}(\mu) - \xi B_1^{(k)}(\lambda).$$

The induction method is used to demonstrate Lemma 2.2. Assume that (2.26)–(2.28) hold for $B_N^{(k)}(\boldsymbol{\mu}), M-1 \geqslant N \geqslant 1$ then, to show that these formulas are valid for M, the recurrence relation (ii) in Lemma 2.1 is used,

$$\begin{aligned} [h(\lambda), B_M^{(k)}(\boldsymbol{\mu})] &= [h(\lambda), B_{M-1}^{(k)}(\boldsymbol{\mu}^{(M)})](B_1(\mu_M) + (M+k-1)\xi) + B_{M-1}^{(k)}(\boldsymbol{\mu}^{(M)})[h(\lambda), X^-(\mu_M)] \\ &= \sum_{i=1}^{M-1} \left(2\frac{B_M^{(k)}(\{\lambda\} \cup \boldsymbol{\mu}^{(i)}) - B_M^{(k)}(\boldsymbol{\mu})}{\lambda - \mu_i} + \xi B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(i)})\hat{\beta}_{M-1}(\mu_i; \boldsymbol{\mu}^{(i,M)}) \right) \\ &\quad + \xi \sum_{i=1}^{M-1} B_{M-2}^{(k+1)}(\boldsymbol{\mu}^{(i,M)})[h(\mu_i), X^-(\mu_M)] + B_{M-1}^{(k)}(\boldsymbol{\mu}^{(M)}) \left(2\frac{B_1(\lambda) - B_1(\mu_M)}{\lambda - \mu_M} + \xi h(\mu_M) \right) \\ &= 2\sum_{i=1}^{M} \frac{B_M^{(k)}(\{\lambda\} \cup \boldsymbol{\mu}^{(i)}) - B_M^{(k)}(\boldsymbol{\mu})}{\lambda - \mu_i} + \xi \sum_{i=1}^{M-1} B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(i)}) \left(\hat{\beta}_{M-1}(\mu_i; \boldsymbol{\mu}^{(i,M)}) + \frac{2}{\mu_M - \mu_i} \right) \\ &\quad + \xi B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(M)}) \sum_{i=1}^{M-1} \frac{2}{\mu_i - \mu_M} + \xi \left(B_{M-1}^{(k)}(\boldsymbol{\mu}^{(M)}) + \xi \sum_{i=1}^{M-1} B_{M-2}^{(k+1)}(\boldsymbol{\mu}^{(i,M)}) \right) h(\mu_M) \\ &= \sum_{i=1}^{M} \left(2\frac{B_M^{(k)}(\lambda \cup \boldsymbol{\mu}^{(i)}) - B_M^{(k)}(\boldsymbol{\mu})}{\lambda - \mu_i} + \xi B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(i)})\hat{\beta}_M(\mu_i; \boldsymbol{\mu}^{(i)}) \right), \end{aligned}$$

here we used, where appropriate, the induction hypothesis, the commutators $[h(\lambda), X^-(\mu)]$, and properties (ii) and (iv) in Lemma 2.1. Thus (2.26) is proved,

$$
\begin{aligned}
[X^+(\lambda),B_M^{(k)}(\boldsymbol{\mu})] &= [X^+(\lambda),B_{M-1}^{(k)}(\boldsymbol{\mu}^{(M)})](B_1(\mu_M)+(M+k-1)\xi)+B_{M-1}^{(k)}(\boldsymbol{\mu}^{(M)})[X^+(\lambda),X^-(\mu_M)]\\
&= -\sum_{i=1}^{M-1} B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(i)})\frac{\hat{\beta}_{M-1}(\lambda;\boldsymbol{\mu}^{(i,M)})-\hat{\beta}_{M-1}(\mu_i;\boldsymbol{\mu}^{(i,M)})}{\lambda-\mu_i}-2\sum_{i<j}^{M-1}\frac{B_{M-1}^{(k+1)}(\{\lambda\}\cup\boldsymbol{\mu}^{(i,j)})}{(\lambda-\mu_i)(\lambda-\mu_j)}\\
&\quad+\xi\sum_{i=1}^{M-1} B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(i)})X^+(\lambda)+\left(B_{M-1}^{(k)}(\boldsymbol{\mu}^{(M)})+\xi\sum_{i=1}^{M-1}B_{M-2}^{(k+1)}(\boldsymbol{\mu}^{(i,M)})\right)\\
&\quad\times\left(-\frac{h(\lambda)-h(\mu_M)}{\lambda-\mu_M}+\xi X^+(\lambda)\right)-\sum_{i=1}^{M-1}B_{M-2}^{(k+1)}\\
&\quad\times(\boldsymbol{\mu}^{(i,M)})\frac{[h(\lambda),X^-(\mu_M)]-[h(\mu_i),X^-(\mu_M)]}{\lambda-\mu_i}\\
&= -\sum_{i=1}^{M-1} B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(i)})\frac{\hat{\beta}_{M}(\lambda;\boldsymbol{\mu}^{(i)})-\hat{\beta}_{M}(\mu_i;\boldsymbol{\mu}^{(i)})}{\lambda-\mu_i}-2\sum_{i<j}^{M-1}\frac{B_{M-1}^{(k+1)}(\{\lambda\}\cup\boldsymbol{\mu}^{(i,j)})}{(\lambda-\mu_i)(\lambda-\mu_j)}\\
&\quad+\xi\sum_{i=1}^{M} B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(i)})X^+(\lambda)-B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(M)})\frac{\hat{\beta}_{M}(\lambda;\boldsymbol{\mu}^{(M)})-\hat{\beta}_{M}(\mu_M;\boldsymbol{\mu}^{(M)})}{\lambda-\mu_M}\\
&\quad-2\sum_{i=1}^{M-1}\frac{B_{M-1}^{(k+1)}(\{\lambda\}\cup\boldsymbol{\mu}^{(i,M)})}{(\lambda-\mu_i)(\lambda-\mu_M)}\\
&= -\sum_{i=1}^{M} B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(i)})\frac{\hat{\beta}_{M}(\lambda;\boldsymbol{\mu}^{(i)})-\hat{\beta}_{M}(\mu_i;\boldsymbol{\mu}^{(i)})}{\lambda-\mu_i}-2\sum_{i<j}^{M}\frac{B_{M-1}^{(k+1)}(\{\lambda\}\cup\boldsymbol{\mu}^{(i,j)})}{(\lambda-\mu_i)(\lambda-\mu_j)}\\
&\quad+\xi\sum_{i=1}^{M} B_{M-1}^{(k+1)}(\boldsymbol{\mu}^{(i)})X^+(\lambda),
\end{aligned}
$$

here we used, where appropriate, the commutators $[h(\lambda),X^-(\mu)]$ and $[X^+(\lambda),X^-(\mu)]$. Thus (2.27) is proved,

$$
\begin{aligned}
[X^-(\lambda),B_M^{(k)}(\boldsymbol{\mu})] &= [X^-(\lambda),B_{M-1}^{(k)}(\boldsymbol{\mu}^{(M)})](B_1(\mu_M)+(M+k-1)\xi)+B_{M-1}^{(k)}(\boldsymbol{\mu}^{(M)})[X^-(\lambda),B_1(\mu_M)]\\
&= \left((M-1)\xi B_{M-1}^{(k)}(\boldsymbol{\mu}^{(M)})-\xi\sum_{i=1}^{M-1}B_{M-1}^{(k)}(\{\lambda\}\cup\boldsymbol{\mu}^{(i,M)})\right)(B_1(\mu_M)+(M+k-1)\xi)\\
&\quad+\xi B_{M-1}^{(k)}(\boldsymbol{\mu}^{(M)})(B_1(\mu_M)-B_1(\lambda))=M\xi B_M^{(k)}(\boldsymbol{\mu})-\xi\sum_{i=1}^{M}B_M^{(k)}(\{\lambda\}\cup\boldsymbol{\mu}^{(i)}),
\end{aligned}
$$

here we used, where appropriate, the commutators $[X^-(\lambda),X^-(\mu)]$. □

Proof of Lemma 2.4: In the case for $M=1$ the proof is straightforward,

$$
\frac{\partial}{\partial z_a}B_1(\mu)=\frac{X_a^-}{(\mu-z_a)^2}=-\frac{\partial}{\partial\mu}\left(\frac{X_a^-}{\mu_i-z_a}-\frac{\xi}{2}h_a\right)=-\frac{\partial}{\partial\mu}X_a^-(\mu_i).
$$

Assume (2.36) is true for any set $\boldsymbol{\mu}$ with $|\boldsymbol{\mu}|<M$ complex numbers. Use formula (2.29) and the induction hypothesis together with (1) of Lemma 2.1 we can write

$$\frac{\partial}{\partial z_a}B_M(\boldsymbol{\mu}) = \frac{\partial}{\partial z_a}(B_{M-1}(\boldsymbol{\mu}^{(M)})(B_1(\mu_M) + (M-1)\xi))$$

$$= -\sum_{i=1}^{M-1}\frac{\partial}{\partial \mu_i}(X_a^-(\mu_i)B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})) - \frac{\partial}{\partial \mu_M}B_{M-1}(\boldsymbol{\mu}^{(M)})X_a^-(\mu_M)$$

$$= -\sum_{i=1}^{M-1}\frac{\partial}{\partial \mu_i}(X_a^-(\mu_i)B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})) - \frac{\partial}{\partial \mu_M}\left(X_a^-(\mu_M)B_{M-1}(\boldsymbol{\mu}^{(M)}) + \frac{[B_{M-1}(\boldsymbol{\mu}^{(M)}), X_a^-]}{\mu_M - z_a}\right)$$

$$= -\sum_{i=1}^{M}\frac{\partial}{\partial \mu_i}(X_a^-(\mu_i)B_{M-1}^{(1)}(\boldsymbol{\mu}^{(i)})).$$

□

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Breakdown of Lindstedt expansion for chaotic maps

Guido Gentile[a)]
Dipartimento di Matematica, Università di Roma Tre, Roma 00146, Italy

Titus S. van Erp[b)]
Laboratoire de Physique/Centre Européen de Calcul Atomique et Moléculaire, Ecole Normale Supérieure de Lyon, 69364 Lyon Cedex 07, France

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In a previous paper of one of us [Europhys. Lett. **59**, 330–336 (2002)] the validity of Greene's method for determining the critical constant of the standard map (SM) was questioned on the basis of some numerical findings. Here we come back to that analysis and we provide an interpretation of the numerical results, by showing that the conclusions of that paper were wrong as they relied on a plausible but untrue assumption. Hence no contradiction exists with respect to Greene's method. We show that the previous results, based on the expansion in Lindstedt series, do correspond to the critical constant but for a different map: the semi-standard map (SSM). For such a map no Greene's method analog is at disposal, so that methods based on Lindstedt series are essentially the only possible ones. Moreover, we study the expansion for two simplified models obtained from the SM and SSM by suppressing the small divisors. We call them the simplified SM and simplified SSM, respectively; the first case turns out to be related to Kepler's equation after a proper transformation of variables. In both cases we give an analytical solution for the radius of convergence, that represents the singularity in the complex plane closest to the origin. Also here, the radius of convergence of the simplified SM turns out to be lower than that of the simplified SSM. However, despite the absence of small divisors these two radii are lower than those of the true maps (i.e., of the maps with small divisors) when the winding number equals the golden mean. Finally, we study the analyticity domain and, in particular, the critical constant for the two maps without small divisors. The analyticity domain turns out to be a perfect circle for the simplified SSM (as for the SSM itself), while it is stretched along the real axis for the simplified SM, yielding a critical constant which is larger than its radius of convergence. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The Taylor-Chirikov map[12,23] or standard map (SM) is one of the best known nonlinear models showing the onset of chaos in Hamiltonian systems. It describes with some level of approximation many physical systems. Among these there are numerous applications to plasma physics, the field in which it was originally introduced. The SM is also exactly related to the time evolution of the "kicked rotor" and the equilibrium condition for a chain of masses superpositioned on a periodic potential. The latter model is known as the Frenkel-Kontorova (FK) model. This model is of equal importance for solid state physics as the SM is for plasma physics. It has, e.g., been applied to Josephson junctions arrays, charge density waves and surface friction.[19] More importantly, due to their simplicity and, yet, the complex behavior they show, these minimalistic

[a)]Electronic mail: gentile@mat.uniroma3.it
[b)]Electronic mail: tsvanerp@cecam.fr

models have had an enormous impact for the understanding in complex phenomena such as nonlinearity, chaos, quasi-periodicity, and commensurate-incommensurate transitions. Although now part of any textbook in nonlinear physics and studied extensively over many years, the SM and FK still bear many unsolved problems. The most intriguing one of these is the sudden transition from smooth to chaotic orbits in the SM when the coupling parameter K is increased above a critical value K_c. In the FK model this transition is connected to change from a sliding to a pinned state and bears the name of Aubry transition (or analyticity breaking transition).

The theoretical framework that characterizes this transition originates from the Kolmogorov-Arnol'd-Moser (KAM) theorem,[2] that deals with the problem of small divisors that can occur in any perturbation expansion for quasi-integrable systems. In fact, the KAM theorem can be used to prove the non-chaotic behavior of the SM for very small coupling K and sufficiently irrational winding number ω. Other arguments can then be applied to prove that a chaotic regime exists for values of K large enough giving an upper bound to K_c. For ω equal to the golden mean there exists an analytical bound by Mather, $K_c<4/3$,[34] and the computer assisted proof of MacKay and Percival $K_c<63/64\approx 0.9844$.[33] Moreover, another computer assisted analysis of Jungreis excluded the value $K=0.9718$ for possible occurrence of invariant circles (smooth orbits).[27]

There exist several methods to calculate K_c precisely, among which Greene's method[23] has shown to be one of the most effective giving the estimate $K_c=0.971\,635$. This method is based on the assumption that the dissolution of invariant curves can be associated with the sudden change from stability to instability of nearby closed orbits. The renormalization technique of MacKay (cf. Ref. 32, Sec. 4.4.1) is a further refinement of this method and has established the same value (cf. p. 199 of the quoted reference) with higher digit precision with respect to the original Greene's result. Yet, Greene's hypothesis has only been partly proven. A result by Falcolini and de la Llave[16] and, independently, by MacKay[31] yields that the critical constants for symplectic maps can never be higher than the ones obtained by Greene's method. Recently, the result has been extended to nontwist maps by Delshams and de la Llave.[14] Hence, $K_c\leqslant 0.971\,635$ for the SM with the golden mean as winding number. We mention that MacKay also showed that Greene's method does not apply to every map.[31] However, in the case of the SM, the situations for which no rigorous result can be given are considered unlikely; cf. the discussion in Refs. 16 and 31.

Another way to calculate (or, at least, to estimate) K_c is through the Lindstedt series expansion. Any smooth invariant curve in the SM can be described, for complex K small enough, say $|K|<\rho$, where ρ will depend on the winding number of the curve, by an analytic function which conjugates the dynamics to the unperturbed one. Of course ρ provides a lower bound for K_c, which is essentially the maximum real value of K for which there is an analytic invariant curve with the fixed winding number (more precise definitions will be given below). By writing down the Taylor expansion and equating the Taylor orders in the functional equation satisfied by this conjugation function, the Fourier-Taylor coefficients can, in principle, be derived from the ones of lower order. In Ref. 42 an evaluation of this expansion, always in the case of the golden mean, to high orders led the authors to infer a convergence to a value $K_c\sim 0.979\,78$, which is higher than Greene's result. [Note that the fact that ρ and K_c are different cannot be invoked to explain the discrepancy because of the direction of the inequality between the two quantities. One could also wonder what information about K_c can be inferred from ρ other than a lower bound. In general none, but one has strong numerical evidence that $\rho=K_c$ for the golden mean.] In this paper, we revisit that analysis and show that an apparent plausible assumption made in Ref. 42 is falsified beyond Taylor order $n>200$. As a result, the Lindstedt expansion does not contradict Greene's result. The value $K_c\sim 0.979\,78$, however, does correspond to the critical value for a different map, the semi-standard map (SSM); cf. also Ref. 24. We come back to this in Sec. III; though, we note straight away that this method is fundamental for the SSM, where no analog of Greene's method exists (see also the comments at the end of Sec. II).

Aubry[3] proposed another method, which is probably not very effective for high precision evaluation in a computer algorithm, but still interesting. It is based on an eigenvalue calculation of the dynamical matrix for the FK chain close to the critical point. Although this, in principle, requires the diagonalization of an infinite matrix, one can use the fact that the eigenvector of the

lowest mode tends to localize.[43] The instability of the FK chain can then be determined in successive approximants by calculating the determinants of finite matrices of increasing size.

Another effective method is the frequency analysis method proposed by Laskar, which has been applied to the standard map in Ref. 30, giving for the golden mean a critical value $K_c = 0.9718$, which is close to Greene's value. In Ref. 11 it has been used to study numerically the dependence of the critical constant on the winding number.

Finally we mention the use of Padé approximants to study numerically the entire analyticity domain. [The (L,M)-Padé approximant for a function $f(x)$ is given by the ratio of two polynomials, $f(x) \approx P_L(x)/Q_M(x)$, with $P_L = p_0 + p_1 x + \cdots + p_L x^L$ and $Q_M = 1 + q_1 x + \cdots + q_M x^M$. Hence, the simple Taylor expansion of order n can be considered as a special case of Padé approximant with $L=n$ and $M=0$.] This is a powerful numerical tool even if it is less precise than other methods for detecting the critical constant K_c and not completely under control from a rigorous point of view. It has, for instance, been employed in Ref. 4 and, very recently, in Ref. 5, where the existence of a natural boundary for the analyticity domain of the SM has been checked numerically. Always with the aim of studying the analyticity domain Falcolini and de la Llave[17] developed a variant of Greene's method working for complex values of the parameter K that gives an alternative to the Padé approximants approach. An implementation of Padé approximants is given in Sec. IV, though for a case in which the analytical solution is known.

Eventually, these approaches are assumed to converge to the same value. However, the proof of this is highly non trivial. The ultimate goal, of course, would be to gain an analytical expression for K_c. This is still far beyond our capabilities. Inspired by the desire to investigate further the influence of the small divisors in the Lindstedt series expansion, we introduce two simplified models by setting rigorously all the divisors equal to 1 both for the SSM and the SM. In the latter case, this is a very well-known model, Kepler's equation,[50] which turns out to have a very similar transition and can be solved analytically. The radii of convergence are found to be lower than those determined with the methods described above for the SM and SSM, respectively, in the case of golden mean winding numbers.

This paper is organized as follows. In Sec. II we recall the definition of the SM and SSM. In Sec. III we come back to the analysis of Ref. 42 showing that, contrary to what was asserted in that paper, the Lindstedt expansion does not violate Greene's method, and we make the comparison between the SM and SSM. In our opinion the analysis in Sec. III gives some insight onto the mechanism of break up of the invariant curves, and leaves some open problems: this will be discussed to more extent in Sec. V. In Sec. IV we present a model in which we suppress the small divisors and give an analytical expression both for the radius of convergence and the critical constant. Moreover, the analysis in Sec. IV has some consequence on the cases with small divisors in relation with the appearance of a natural boundary in the analyticity domain; this is further discussed in Sec. V. Finally we end up with the conclusions in Sec. V.

II. THE (SEMI-) STANDARD MAP

The SM and SSM can be written as

$$\begin{pmatrix} x_{i+1} \\ x_i \end{pmatrix} = \mathrm{T}\begin{pmatrix} x_i \\ x_{i-1} \end{pmatrix} = \begin{pmatrix} 2x_i + V'(x_i) - x_{i-1} \\ x_i \end{pmatrix}, \tag{1}$$

with $\{x_i\}$ defined mod 1, and

$$V'(x) = \begin{cases} \dfrac{K}{2\pi}\sin(2\pi x) & \text{for the SM,} \\ \dfrac{K}{4\pi i}\exp(i2\pi x) & \text{for the SSM.} \end{cases} \tag{2}$$

The resulting sequence $\{x_i \bmod 1\}$, for $i=2,\ldots\infty$, originating from a starting point (x_1,x_0) corresponds to a discrete trajectory on an invariant curve, when the latter exists. Such a trajectory for

the SM can be related to the equilibrium positions of an infinite FK chain where particles with harmonic nearest neighbor coupling are placed on a periodic potential $V(x)=K(2\pi)^{-2}(1-\cos(2\pi x))$. The SSM has not a similar counterpart, but is much simpler in its mathematics, and this is basically the reason why it was considered by Greene and Percival.[24] By definition, in terms of the lift of the map, the winding number or rotation number of an orbit is given by

$$\omega \equiv \langle x_{i+1} - x_i \rangle \equiv \lim_{n\to\infty} \sum_{i=0}^{n} \frac{x_{i+1} - x_i}{n} = \lim_{n\to\infty} \frac{x_n - x_0}{n}, \tag{3}$$

when the limit exists. For low coupling K and ω incommensurate to the periodicity of V', there exists a continuous function $g(x;K,\omega)$ such that the positions $\{x_i \bmod 1\}$ can be expressed as $x_i = g(i\omega+\varphi;K,\omega)$, where φ is an arbitrary phase. This function is often called the conjugating function or, in context with the FK model, the modulation or hull function. Its shape depends on the winding number ω and on the coupling parameter K.

The conjugating function satisfies the functional equation

$$2g(x;K,\omega) - g(x+\omega;K,\omega) - g(x-\omega;K,\omega) = -V'(x+g(x;K,\omega)). \tag{4}$$

For K large enough the function $g(x;K,\omega)$ becomes discontinuous. For the SM this implies that the orbits become chaotic and for the FK that the chain of particles gets pinned together with the appearance of a phonon gap.

There are several quantities of interest which one can introduce in order to study the transition from regular to chaotic dynamics. As the function $g(x;K,\omega)$ is analytic for K close to the origin one can consider its series expansion in powers of K,

$$g(x;K,\omega) = \sum_{n=1}^{\infty} K^n g^{(n)}(x;\omega), \tag{5}$$

and define the radius of convergence $\rho(\omega)$ as

$$\rho(\omega) = \inf_{x\in[0,1]} \left(\limsup_{n\to\infty} \left| g^{(n)}(x;\omega) \right|^{1/n} \right)^{-1}. \tag{6}$$

Note that the infimum appears in the definition of the radius of convergence because, as a result of the incommensurate winding number ω, each invariant curve is filled densely by any trajectory lying on it. Hence, existence of the invariant curve itself requires the latter to be defined for all $x \in [0,1]$.

The critical constant is defined as the (positive) real value $K_c(\omega)$ such that for $K > K_c(\omega)$ the conjugating function is not analytic any more. [The reason why one usually does not consider the negative critical constant, that is the negative value $K_c'(\omega)$ such that for $K < K_c'(\omega)$ there is no longer an analytic invariant curve, is that $K_c'(\omega) = -K_c(\omega)$ for the SM.] It is believed that the analyticity domain of the conjugating function has a natural boundary,[4,5,24] this means that $g(x;K,\omega)$ has a set of singularities in terms of K that form a closed curve around the origin in the complex plane. Hence, the radius of convergence $\rho(\omega)$ corresponds to the singularity closest to the origin, while the critical constant $K_c(\omega)$ corresponds to the intersection of this curve with the (positive) real axis. By definition one has $K_c(\omega) \geqslant \rho(\omega)$, so that by estimating the radius of convergence one finds a lower bound for the critical constant. Furthermore, it is generally accepted that $K_c(\tau) = \rho(\tau)$ for the golden mean [the golden mean is sometimes in other literature defined as the inverse of this value, $(\sqrt{5}+1)/2 = \tau^{-1} \approx 1.618\,034$ $\tau = (\sqrt{5}-1)/2 \approx 0.618\,034$], whereas there is strong numerical evidence that $K_c(\omega)$ can be much larger than $\rho(\omega)$ for winding numbers which have very large partial quotients in their continued fraction expansion.[9,11] [For an introduction of the continued fraction theory and a discussion of the basic properties we refer to the classical textbook by Hardy and Wright.[26] In the continued fraction expansion of a number $\omega = [a_0, a_1, a_2, \ldots] = a_0 + 1/(a_1 + 1/(a_2 + 1/(\cdots)))$, the numbers a_j are called the partial quotients,

while the rational numbers $q_j/p_j=[a_0,a_1,a_2,\ldots,a_j]$ are called the best approximants for ω.] It is also commonly believed (on the basis of numerical simulations and heuristic arguments) that $K_c(\omega)$ has the highest value for the golden mean $\omega=\tau$.

So far, the most accurate method to calculate K_c is based on Greene's method (also known as residue criterion). In this method the infinite trajectory $\{x_i \bmod 1\}$ with irrational winding number ω is approached by successive approximants which are periodic trajectories with rational winding numbers $\omega_j=p_j/q_j$ tending to ω, and $x_{i+q_j} \bmod 1=x_i$. Hence, p_j and q_j are at each level j two integer values whose ratio gives a better estimate of ω for each increment in j and $\omega=\lim_{j\to\infty}\omega_j$. These numbers can, for instance, be obtained using the best approximants in the continued fraction expansion of ω. For $\omega=\tau$ this results in the ratios of subsequent Fibonacci numbers ($\tau\approx F_{j-1}/F_j$ with $F_0=F_1=1$ and $F_j=F_{j-1}+F_{j-2}$ for $j>1$). Conclusively, Greene's method tells how to construct the periodic orbits and to measure their stability by means of a suitable quantity, called the residue, which does not tend to zero any more for $K>K_c$.

Besides being only partly proven, Greene's method has also some other limitations. For instance, this method does not work for other interesting models, as the SSM and Siegel's problem,[39] where the construction of periodic orbits fails. One can also easily check the nonexistence of smooth periodic orbit by a first orders perturbation theory. The best general alternative is the Lindstedt series expansion. This method is more generally applicable (it also works for the SSM and for any Hamiltonian systems close to an integrable one), but, in view of a numerical implementation, is less accurate than Greene's method for the SM and, in general, is more suitable for studying the radius of convergence rather than the critical constant.

III. THE LINDSTEDT SERIES EXPANSION

A. Standard map

A way to study the transition is by means of the Lindstedt series, which in this case means the expansion of the function $g(x;K,\omega)$ both in Fourier and in Taylor series. Such expansions were originally introduced by Lindstedt and Newcomb to study problems in celestial mechanics.[37] By defining the Fourier transform as

$$g(x;K,\omega)=\sum_{k=-\infty}^{+\infty}\hat{g}_k(K,\omega)e^{2\pi ikx} \quad \text{with inverse,}$$
$$\hat{g}_k(K,\omega)=\int_0^1 \mathrm{d}x\, g(x;K,\omega)e^{-2\pi ikx}, \tag{7}$$

and expanding

$$\hat{g}_k(K,\omega)=K\hat{g}_k^{(1)}(\omega)+K^2\hat{g}_k^{(2)}(\omega)+K^3\hat{g}_k^{(3)}(\omega)+\cdots, \tag{8}$$

we end up with Fourier-Taylor coefficients $\hat{g}_k^{(n)}(\omega)$, where n is the Taylor index and k is the Fourier index. Of course, $\hat{g}_k^{(n)}(\omega)$ depends on ω, but henceforth we withdraw such a dependence in order not to overwhelm the notation, whenever no ambiguity can arise.

Now, using Eq. (4) we can relate the Fourier-Taylor coefficients of order n by the ones with lower Taylor index by[42]

$$D_k^2\hat{g}_k^{(n)}=\frac{i}{4\pi}\{\delta_{1,k}-\delta_{-1,k}\}\delta_{1,n}+\frac{i}{4\pi}\sum_{m=1}^{\infty}\frac{(i2\pi)^m}{m!}\sum_{n_1+n_2+\cdots+n_m=n-1}\left\{\sum_{k_1+k_2+\ldots+k_m=k-1}\hat{g}_{k_1}^{(n_1)}\hat{g}_{k_2}^{(n_2)}\cdots\hat{g}_{k_m}^{(n_m)}-(-1)^m\sum_{k_1+k_2+\cdots+k_m=k+1}\hat{g}_{k_1}^{(n_1)}\hat{g}_{k_2}^{(n_2)}\cdots\hat{g}_{k_m}^{(n_m)}\right\}, \tag{9}$$

with

$$D_k^2 \equiv \frac{1}{\hat{g}_k(K,\omega)} \int_0^1 \mathrm{d}x (2g(x;K,\omega) - g(x+\omega;K,\omega) - g(x-\omega;K,\omega)) e^{-2\pi i k x}$$
$$= 2(1-\cos(2\pi k\omega)) = (2\sin(\pi k\omega))^2, \tag{10}$$

and where $\Sigma_{n_1+n_2+\cdots+n_m=n\pm1}$ implies a summation of all possible integers $n_1, n_2, \ldots, n_m$ with the constraint that $\sum_{i=1}^{m} n_i = n \pm 1$. There are ways to reduce the number of summations in Eq. (9). One possible way was proposed in Ref. 42 to construct an extended matrix $P(n,k,m)$ defined as

$$P(n,k,m) = \frac{(2\pi i)^m}{m!} \sum_{n_1+n_2+\cdots+n_m=n} \sum_{k_1+k_2+\cdots+k_m=k} \hat{g}_{k_1}^{(n_1)} \hat{g}_{k_2}^{(n_2)} \cdots \hat{g}_{k_m}^{(n_m)}. \tag{11}$$

One can show that $P(n,k,m)=0$ if $|k|>n$ or $m>n$. This gives rise to the following recursive relations:[42]

$$P(1,\pm 1,1) = \frac{\mp 1}{2D_1^2},$$

$$P(n,k,1) = -\frac{1}{2} D_k^{-2} \sum_{m=1}^{n-1} [P(n-1,k-1,m) - (-1)^m P(n-1,k+1,m)],$$

$$P(n,k,m) = \frac{1}{m} \sum_{n'=1}^{n-m+1} \sum_{k'=\max\{-n',k-n+n'\}}^{\min\{n',k+n-n'\}} P(n',k',1) P(n-n',k-k',m-1), \quad 1 < m \leqslant n, \tag{12}$$

from which we can distract the Fourier-Taylor coefficients by

$$\hat{g}_k^{(n)} = \frac{P(n,k,1)}{2\pi i}. \tag{13}$$

The entries of P are all real and obey the symmetry relation $P(n,k,m)=(-1)^m P(n,-k,m)$. Moreover, besides being zero for $|k|>n$ and $m>n, P(n,k,m)$ has zero values whenever $k+n$ is odd. Hence, $k=n,n-2,\ldots,-n$ are the only non-zero entries of P.

The relations of Eqs. (12) are very efficient to evaluate $\hat{g}_k^{(n)}$, and they were used in Ref. 42 to reach a Taylor order of approximately $n=200$. To go beyond this limit, sufficient computer power and time is needed as both the computation time and the number of non-zero matrix entries increase with $\sim n^3$. Hence, memory can become a severe problem as the number of entries that must be stored can easily go beyond the maximum allowed allocation limit of the computing system. Also the precision must be high enough in order to minimize numerical errors, but this problem is easily solved without requiring a precision as high as in the case of winding numbers close to rational numbers, as in Ref. 5, where the small divisors could become really small and up to 480 digits were needed. In this work, we reached the level $n=700$ (see Fig. 1) and we believe that going beyond this order is not very profitable for obtaining a more accurate evaluation of K_c. We come back to these results after addressing the small divisor problem that arises from Eq. (12).

From Eq. (10) and the second line in Eq. (12) one sees that even for irrational values of ω, the terms D_k^{-2} can become arbitrarily high for some k. This effect is a typical example of the small divisor problem (or small denominator problem), that can strongly prevent the convergence of any perturbation series. In fact, in general it requires a stronger condition than irrationality, such as a Diophantine condition.[2] [The usual Diophantine condition requires $|\omega q - p| > 1/C_0 |q|^\gamma$ for all $(p,q) \in \mathbb{Z}^2$ with $q \neq 0$ and for suitable positive constants C_0 and γ. But one can require also the Bryuno condition, which is a condition stronger than irrationality but weaker than the usual Diophantine condition; cf. for instance Refs. 8 and 21 in the case of the SM.] Among all the irrational numbers, the golden mean τ suffers the least from the small divisor problem and has

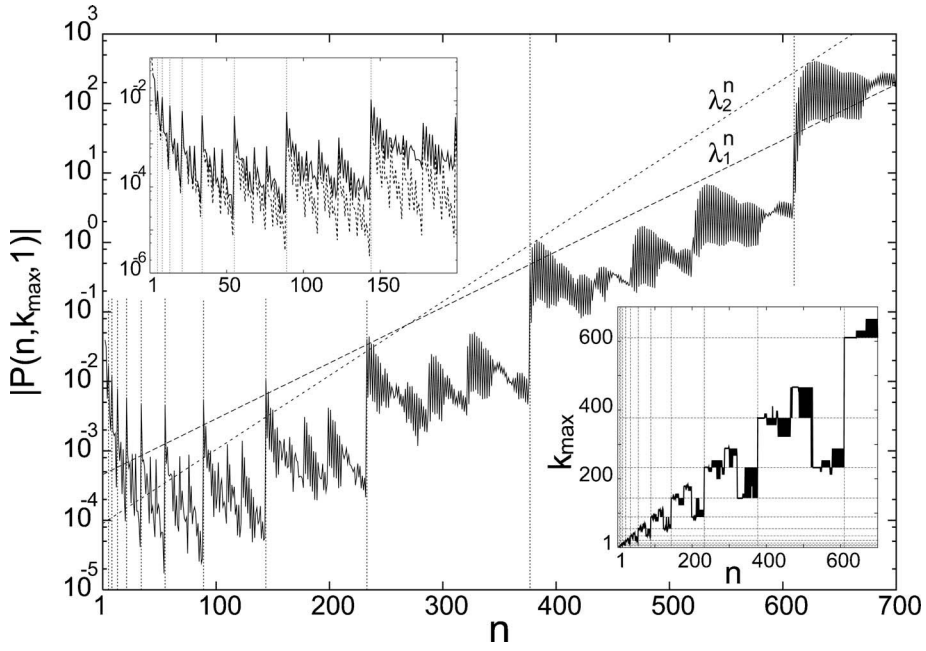

FIG. 1. $|P(n,k_{\max},1)|$ as a function of n. This is defined as the maximum value of $|P(n,k,1)|$ of all k; hence, $k_{\max}=k_{\max}(n)$ is defined as the k value where $|P(n,k,1)|$ has this maximum. The inset in the lower corner shows $k_{\max}$ as a function of n. The inset in the left upper corner is an enlargement of the first 200 terms together with $|P(n,n,1)|$ (dashed line). From these figures, one can clearly detect sudden boosts in the function $|P(n,k_{\max},1)|$ where $k_{\max}=n$ at the Fibonacci values (dashed vertical lines). However, whereas for $n<200$ the character is sharply peaked at these values, its behavior changes for higher orders. Still $k_{\max}=n$ for n a Fibonacci number, but the intersecting line described by $\alpha_1\lambda_1^n$ does no longer dominate the complete evolution of all the $|P(n,k,1)|$ terms. $\lambda_1=1.0186$ is determined by the line through $(n,k)=(F_{13},F_{13})=(377,377)$ and $(n,k)=(F_{14},F_{14})=(610,610)$. $\lambda_2=1.0248$ is set by the line through $(n,k)=(383,377)$ and $(n,k)=(622,610)$ where $|P(n,k_{\max}(n),1)|^{1/n}$ shows local maxima in n. The inversed values, $\lambda_1^{-1}\approx 0.9817$ and $\lambda_2^{-1}\approx 0.9758$ are assumed to converge for higher n to K_c for the SSM and SM, respectively.

therefore the highest convergence radius $K_c(\tau)$. The golden mean is "relatively difficult" to approximate by rational numbers as those arising, for instance, from the continued fraction expansion (one can say that it is the "most irrational number"). [A more formal statement is that τ allows the smallest values of C_0 and γ in the Diophantine condition. Hence, it is the number that is the most distant from all rational numbers.] As addressed above, the best approximants for the golden mean are given by the ratios F_j/F_{j+1}, where $\{F_j\}$ is the sequence of the Fibonacci numbers. Therefore, the small divisors will be largest for $k=F_j$. From the exact relation $F_{j-1}-F_j\tau=(-\tau)^{j+1}$, one can show that for $j\to\infty$,

$$D_{F_j}^{-2}\approx\frac{1}{4\pi^2}\left(\frac{1}{\tau^2}\right)^{j+1}\sim(2.618)^{j+1}. \tag{14}$$

However, we would like to stress that the small divisor problem is not the only mechanism causing the breakdown of the perturbative approach. This becomes evident in Sec. IV where we introduce the model that arises when we rigorously set $D_k^{-2}=1$ for all k in the series of Eq. (12). Clearly, this simplified expansion cannot be affected by the small divisors. However, it still has a radius of convergence and a critical constant, as shown by the analytical solution. As the radius of convergence ρ of this simplified model is found to be lower than $\rho(\tau)=K_c(\tau)$ for the SM, it proves that the golden mean winding number is remarkably resistant to the problem of small divisors. The full analysis of this model is given in Sec. IV.

Coming back to the results of Fig. 1, we see that indeed the evolution of $P(n,k,1)$ makes sudden jumps at the Fibonacci numbers as expected from Eq. (14). Besides, deceptively the values

$n=k=F_j$ seem to determine the whole power law behavior of $\hat{g}_k^{(n)}$, which is true until Taylor order $n\sim 200$. This assumption made in Ref. 42 allows for a further simplification of Eq. (12) by defining the reduced matrix $Q(n,m)\equiv P(n,n,m)$ obeying the relations

$$Q(1,1)=\frac{-1}{2D_1^2},$$

$$Q(n,1)=-\frac{1}{2}D_n^{-2}\sum_{m=1}^{n-1}Q(n-1,m), \tag{15}$$

$$Q(n,m)=\frac{1}{m}\sum_{n'=1}^{n-m+1}Q(n',1)Q(n-n',m-1),\quad 1<m\leqslant n.$$

This set of equations make high order ($\sim n=F_{20}=10\,946$) evaluations accessible for computer calculations. At this order the value of the radius of convergence seems to stabilize near $\rho=0.979\,78$, but this is still higher than the one obtained by Greene's method. As a consequence, validity of Greene's method was questioned in Ref. 42.

The more elaborated calculations in this work show that the assumption made in Ref. 42 was actually wrong as shown by the high order behavior in Fig. 1. Still, we find that $k=n$ gives the maximum for $|P(n,k,1)|$ whenever n is a Fibonacci number. However, the character of the evolution changes from being peaked to more smooth oscillations. Clearly, the line connecting the points $(F_j,|P(F_j,F_j,1)|)$ does no longer dominate the increment of the entries of P for $n>200$. As $|P(n,k_{\max}(n),1)|^{1/n}$ shows local maxima for $(n,k_{\max})=(383,377)$ and $(n,k_{\max})=(622,610)$ just after F_{13} and F_{14}, we fitted the line $\alpha_2\lambda_2^n$ through the corresponding points. From this fit, $\lambda_2=1.0248$, the estimate for $K_c\approx\lambda_2^{-1}=0.9758$ is obtained. Although still higher than Greene's value, it is already considerably lower than $\rho=0.979\,78$ obtained from Eqs. (15) for $n=F_{20}=10\,946$. Note that the latter approach of Ref. 42 for this lower approximant $n=F_{14}=610$, as obtained from the line λ_1^n (see Fig. 1), would result in $\rho\approx 1/\lambda_1=0.9817$, still approximately 0.002 higher than the nearly converged value of $\rho=0.979\,78$. Hence, a decay of 0.004 from 0.9758 at $n=622$ to 0.9716 at $n\to\infty$ is not unlikely. As a consequence, contrary to the results of the restricted series (15), there is no evidence at all that the full Lindstedt series (12) violates Greene's hypothesis. This also shows that a further simplification of Eqs. (12) is not easily obtained and that an accurate evaluation of K_c based on the Lindstedt perturbation is severely demanding.

B. Semi-standard map

When evaluating Eq. (1) for the SSM (2), the factors $\delta_{-1,k}$ and $-(-1)^m\Sigma\cdots$ are not present in Eq. (9). It is then straightforward to show that the only non zero entries of $P(n,k,m)$ in (11) are those with $n=k$. Hence, the assumption made in Ref. 42 that gave rise to Eqs. (15) does not correspond to the critical constant of the SM, but still gives the correct value for SSM. A result by Davie[13] shows that, for maps including the ones we are considering, the radius of convergence (6) is equal to

$$\rho(\omega)=\left(\limsup_{n\to\infty}\max_{|k|\leqslant n}\left|\hat{g}_k^{(n)}(\omega)\right|^{1/n}\right)^{-1}. \tag{16}$$

Therefore, the radius of convergence for the SM cannot be larger than the radius of convergence of the SSM, but of course it implies only a lower bound on the critical constant. Numerically by using Padé approximants in Ref. 5 it has been found that for certain values of the winding number ω, the radius of convergence of the SM is strictly smaller than the radius for the SSM. For the golden mean it is hard to improve upon simple power series using Padé, but for other numbers closer to resonant values it is possible and the phenomenon becomes much more evident.

The fact that the radius of convergence for these numbers is lower for the SM than for the SSM implies, by (16), that dominant contributions arise from terms with Taylor orders n for which $|\hat{g}_{k_{\max}}^{(n)}| > |\hat{g}_n^{(n)}|$, where $k_{\max}=k_{\max}(n)$ is defined as the value of k maximizing $|P(n,k,1)|$ at fixed n. This is exactly what emerges from the numerics as noted above and shown in Fig. 1 for $n > 200$. Clearly, this is not the case for the SSM where one can limit to $k=n$. Hence, in Ref. 42 $K_c(\tau)=\rho(\tau)$ was actually determined for the SSM to be 0.979 78 at Taylor order $n=F_{20}=10\,946$. In the calculations of this work, we went to order $n=F_{24}=75\,025$, that gave the value 0.979 37. As the root criterion saturates very slowly, the numerical results provide essentially only an (accurate) upper bound for the radius of convergence.

To summarize, we found that, also for the golden mean, the radius of convergence for the SM is strictly less than the radius of convergence for the SSM. Therefore, as a general comment we can remark that for the SM the presence of all harmonics in the Fourier expansion of the Taylor coefficients, that is $g^{(n)}(x;\omega)=\Sigma_{k\in\mathbb{Z}}\hat{g}_k^{(n)}(\omega)e^{2\pi ix}$, has a double effect. On the one hand, the radius of convergence becomes smaller with respect to that of the SSM. On the other hand, the critical constant $K_c(\omega)$ can be larger than its radius of convergence $\rho(\omega)$. For the golden mean the two values are equal as emerges numerically,[17] but for other values they can be appreciably different. One can imagine that the first phenomenon is due to the presence of contributions $\hat{g}_k^{(n)}(\omega)$ larger (in modulus) than $\hat{g}_n^{(n)}(\omega)$, while the second one is a consequence of deep cancellations between the harmonics of given perturbative order. These two effects are, in general, much more dominant for winding numbers ω close to rational values (see for instance Refs. 5, 6, and 8–10).

IV. SETTING SMALL DIVISORS TO UNITY

A. Introduction of the simplified maps

An interesting study appears if we set rigorously all possible small divisors equal to unity, $D_k=1$ for all k in Eqs. (12) and (15). Although the inspiration of this model was simply the study of the perturbation expansion when the small divisors have no effect, we can retrace from this series back to a functional relation as the one in Eq. (4) for a function $h(x;K)$,

$$h(x;K)+\frac{K}{4\pi i}\exp\left(i2\pi(x+h(x;K))\right)=0 \quad \text{for the SSM and,}$$
$$h(x;K)+\frac{K}{4\pi}\sin(2\pi(x+h(x;K)))=0 \quad \text{for the SM,} \tag{17}$$

where ω has vanished. Hence, the divergence of the simplified series corresponds to values K where the functional equations (17) have no analytical solution any more. A logical next step would be to relate Eqs. (17) to the iteration of a map similar to Eq. (1). As the relation (17) no longer contains the arguments $x\pm\omega$ this is not so evident. However, one can relate the function $h(x;K)$ to the hull function of a FK-type system. It can be shown that this corresponds to a one-dimensional Einstein solid that is interacting with an external incommensurate potential. (The Einstein model is a well-known approximation in solid physics where the vibrations of a lattice of N atoms is treated as a set of $3N$ independent harmonic oscillators in one dimension.[29]) Due to the lack of neighbor interaction, which makes each particle independent, it is highly unusual to describe for such a system the equilibrium coordinates by a collective hull function. Still, there are no restrictions not to do so and one can even give such a function a physical meaning. As known from the FK model, the continuous shape of the hull function is directly associated with the existence of a sliding mode where the FK chain can slide over the periodic potential without cost of energy.[19,43] In this case, the complete phonon spectrum is given by the sum of oscillations of the individual particles that are not zero in general. The sliding mode appears when we add an extra degree of freedom to the system as shown in Fig. 2.

Here, all particles have no interaction with their neighbors, but are connected to an upper rod. When the rod has an infinite mass compared to the particle masses, the system is basically an

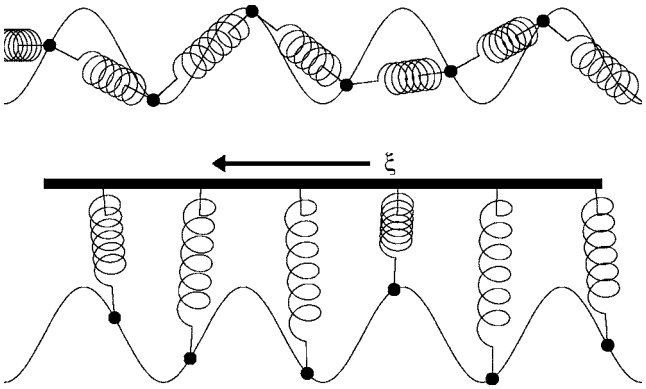

FIG. 2. Illustration of the FK model (top) and the system that obeys Eq. (17) (bottom). The latter corresponds also to the FKT model without neighbor interaction. All particles are connected to the upper rod whose position is given by ξ. A sliding mode exists when ξ can be varied without cost of energy.

Einstein solid. However, if we assume that the position of the rod may vary according to a coordinate ξ an extra phonon mode exist that is zero for $K<K_c$ in this system. Hence, the breakdown of the Lindstedt expansion (12) with $D_k=1$ for all k can be also related to a real physical sliding-pinning transition. The model as illustrated in Fig. 2 is also equal to a special case of the Frenkel-Kontorova-Tomlinson (FKT) model where each particle is connected to a rod by a spring with spring constant c_r and additionally to its neighbors with a coupling c_n. [The simple Tomlinson model[41] is not the system in Fig. 2 as this usually consists of only one single oscillator (particle). This ancient model is now often applied to simulate the "stick-slip" motion of an atomic force microscope (AFM) tip over a sample surface.] The FKT model has been proposed to study more realistically the frictional behavior between atomic surfaces.[25,45,46] The model that is described by Eq. (17) simply corresponds to the FKT system with $c_r=1$ and $c_n=0$. The nice thing is that the perturbation series of Eqs. (17) can be solved exactly. To show this, we will start with the more simple SSM case.

B. Radii of convergence for simplified maps

1. Simplified SSM

It can be convenient to use the following normalization:

$$R(n,m) = n\,!\,(-2)^n Q(n,m), \tag{18}$$

with matrix entries that are integer and positive and with $R(n,n)=1$. From Eqs. (12) and (18) with $D_n^{-2}=1$ we derive

$$\begin{aligned} R(n,1) &= n\sum_{m=1}^{n-1} R(n-1,m), \\ R(n,m) &= \frac{1}{m}\sum_{n'=1}^{n-m+1}\binom{n}{n'}R(n',1)R(n-n',m-1), \quad 1<m\leqslant n. \end{aligned} \tag{19}$$

Note that the recursive relations in Eq. (19) for $m>1$ coincide with those satisfied by the Stirling numbers of the first and second kind, $S_n^{(m)}$ and $\mathfrak{S}_n^{(m)}$, respectively. [The Stirling numbers of the first kind $S_n^{(m)}$ are defined by the requirement that $(-1)^{n-m}S_m^{(n)}$ is the number of permutations of n symbols which have exactly m cycles. The Stirling number of the second kind $\mathfrak{S}_n^{(m)}$ is equal to the way of partioning a set of n elements into m non-empty subsets. See Ref. 1, p. 824, Secs. 24.1.3 and 24.1.4, with $r=m-1$.] Of course what is different is the relation for $m=1$.

From relations (19) with $R(1,1)=1$ the following exact equality can be proven:

$$R(n,m) = n^{n-m}\binom{n-1}{m-1}. \tag{20}$$

The proof of this equation is given in the appendixes in two ways. In Appendix A we derive this proof using the argument of induction. In Appendix B we give a proof based on the tree formalism that was first introduced in Refs. 15 and 36, then extended and formalized in Ref. 20. The first proof is quite elementary, but a little elongated. The second is short, but less self-contained as it requires some knowledge of the previous publications about the tree formalism (but of course it becomes very simple for any reader acquainted with such a technique). Furthermore, the latter is most practical for the more complicated proof for the simplified SM in Eq. (17). Now, from Eqs. (18) and (20) we deduce that

$$Q(n,1) = (-1)^n \frac{n^{n-1}}{2^n n!}, \tag{21}$$

which shows a power law behavior $\sim a\lambda^n$ for large n giving the radius of convergence as $\rho = 1/\lambda$. Hence,

$$\ln|Q(n,1)| \sim (n-1)\ln(n) - n\ln(2) - \ln(n!). \tag{22}$$

Then by using (this is a refinement of the well-known Stirling's formula $\ln n! \approx n\ln n - n$)[47]

$$\ln(n!) \approx \left(n+\tfrac{1}{2}\right)\ln n - n + \tfrac{1}{2}\ln(2\pi), \tag{23}$$

we get

$$\ln|Q(n,1)| = n(1-\ln(2)) - \tfrac{3}{2}\ln(n) - \tfrac{1}{2}\ln(2\pi) \Rightarrow |Q(n,1)| \sim \frac{1}{\sqrt{2\pi n^3}}\left(\frac{1}{2}e\right)^n, \tag{24}$$

yielding a radius of convergence $\rho = 2/e \approx 0.735\,759$. This value is less than the SSM value or SM value. This can be a bit contraintuitive, as one could have expected that the possible occurrence of small divisors would give a lower ρ. Apparently, this does not happen for the golden mean. This can be understood by the following reasoning. Although the small divisor factors D_k^{-2} can become arbitrarily large for some k giving a boost to the series (12) and (15), at most values of k they will be considerable smaller than 1 resulting in an opposite effect. Hence, for the golden mean as winding number the latter effect seems to be more dominant yielding an even higher value for ρ than the case where all D_k^{-2} terms are equal to 1. We can say that, in fact, for the golden mean the small divisors "are not so bad," whereas they become really small for winding numbers much closer to rational values (that is with very large partial quotients in their continued fraction expansion).

2. Simplified SM

The simplified SM considered in Eq. (17) is well known in celestial mechanics[50] after applying the following variable transformation. Write $K/2 = -\mathfrak{e}$ and $2\pi x = \mathfrak{M}$ where $\mathfrak{e}$ is the eccentricity and $\mathfrak{M}$ is the mean anomaly. Then the eccentric anomaly $E = 2\pi(x + h(x;K))$ is related to $\mathfrak{M}$ through Kepler's equation $\mathfrak{M} = E - \mathfrak{e}\sin E$, which is exactly the second equation in Eq. (17).

The recursive relations (12) with $D_k^{-2} = 1$ have also an exact solution that we write here,

$$P(n,k,1)=\begin{cases}\dfrac{(-1)^{n+(n-k)/2}}{2^n}\dfrac{k^{n-1}}{((n-k)/2)!\,((n+k)/2)!}, & \text{for } |k|\leqslant n \text{ and } k+n \text{ is even}\\ 0 & \text{otherwise,}\end{cases} \tag{25}$$

which can be obtained by the Lagrange inversion theorem.[48,50] We present a derivation of this relation based on the tree formalism in Appendix B.

Then, by using Eq. (16) we see that we must compute the maximum over k of $|P(n,k,1)|$. It is immediate to realize that the maximum is reached for some $k>n/2$; by assuming that the maximum is reached for some k which is not too close to n (an assumption that we shall verify *a posteriori*), we can approximate the factorial appearing in Eq. (25) with Stirling's formula (23). This gives rise to

$$\begin{aligned}|P(n,k,1)| &\sim \frac{1}{2^n}\frac{k^{n-1}e^n}{\left(\frac{1}{2}(n-k)\right)^{\frac{1}{2}(n-k)}\left(\frac{1}{2}(n+k)\right)^{\frac{1}{2}(n+k)}}\frac{1}{\left(\frac{1}{4}(n^2-k^2)\right)^{\frac{1}{2}}}\\ &\sim \frac{2e^n}{n^2}\frac{1}{\sigma(1-\sigma^2)^{\frac{1}{2}}}\left(\frac{\sigma}{(1-\sigma)^{\frac{1}{2}(1-\sigma)}(1+\sigma)^{\frac{1}{2}(1+\sigma)}}\right)^n,\end{aligned} \tag{26}$$

where we have defined $\sigma=k/n\in[-1,1]$. Hence, we must compute the maximum of the function

$$E(\sigma)=\sigma\exp\left(-\frac{1-\sigma}{2}\ln(1-\sigma)-\frac{1+\sigma}{2}\ln(1+\sigma)\right). \tag{27}$$

By taking the derivative $\partial E(\sigma)/\partial\sigma=0$, we find that the maximum is reached at a value $\sigma_{\max}$ that satisfies the following relation:

$$2+\sigma_{\max}\ln(1-\sigma_{\max})-\sigma_{\max}\ln(1+\sigma_{\max})=0, \tag{28}$$

yielding $\sigma_{\max}\approx 0.833\,557$. Hence, $k_{\max}=\sigma_{\max}n\approx 0.833\,557n$. Using Eq. (28), $E(\sigma_{\max})$ simplifies to $E(\sigma_{\max})=(1/e)[\sigma_{\max}/(\sqrt{1-\sigma_{\max}^2})]$. Inserting this relation into Eq. (26) gives

$$|P(n,k_{\max},1)|\sim\frac{2}{n^2\sigma_{\max}^2}\lambda^{n+1}, \tag{29}$$

with $\lambda=[\sigma_{\max}/(\sqrt{1-\sigma_{\max}^2})]$. This yields a radius of convergence $\rho=\lambda^{-1}\approx 0.662\,743$, which is known as the Laplace limit.[18] This value is again smaller than the radius of convergence of the true SM [recall that for the golden mean the radius of convergence $\rho(\tau)$ equals $K_c(\tau)$]. Moreover, similar to the true maps, this SM-analog transition value ρ is lower than the one of the SSM.

C. The critical constant and the analyticity domain

The argument above gives only information about the location of the singularities closest to the origin. The solution of the functional equations (17) could still exist for real values of K larger than the radius ρ. This would correspond to the situation where $h(x;K)$ is still analytic for $K>\rho$ real, but at which the power series (5) and (8) are no longer defined. In particular, there could be no singularity at all on the real axis so that an analytical form of $h(x;K)$ could still exist for $K\to\infty$. To analyze the extent of the analyticity domain and the critical constants, we need to "evaluate" the summations of Eqs. (5) and (8). This means that we need to find the functional form $h(x;K)$ that corresponds to the power series, but, contrary to the summation itself, can still be perfectly defined for $|K|>\rho$.

In the following analysis, we will show that the analyticity domains for the simplified maps are, like those for the true maps, also constrained by a closed boundary. More precisely, we find that for fixed x there are only a few singularities, but the union over all $x\in[0,1]$ of such singularities reconstruct a closed curve surrounding the origin. Hence, outside this natural bound-

ary there is no function $h(x;K)$ that can be obtained by an analytic continuation of the power series around $K=0$. Although very unlikely, this does not completely exclude the existence of a very different function, say $\tilde{h}(x;K)$, that is defined outside this domain and obeys Eq. (17) and may even persist for $K\to\infty$. Recurrence phenomena, such as appearance and disappearance of an invariant curve with given winding number when varying the parameter K, are known to occur for certain maps,[49] but, for instance, this is not the case of the SM.

1. Simplified SSM

As for this model one has $\hat{h}_k(K)=\hat{h}_k^{(k)}K^k$, we can directly write down the summation of Eq. (5) for the function $h(x;K)$,

$$h(x;K)=\sum_{k=1}^{\infty}\hat{h}_k^{(k)}K^k e^{2\pi ikx}. \tag{30}$$

Inserting the expression (21) gives

$$h(x;K)=\frac{1}{2\pi i}\sum_{k=1}^{\infty}(-1)^k\frac{k^{k-1}}{2^k k!}K^k e^{2\pi ikx}=\frac{1}{2\pi i}\sum_{k=1}^{\infty}|Q(k,1)|K^k e^{\pi ik(2x+1)}. \tag{31}$$

To find the full analyticity domain of $h(x;K)$, one basically must fix a certain value for x, say $x=x'$, and search for the singularities in K of the function $h(x';K)$ by, e.g., using the Padé approximants method. Then, one must repeat, in principle, this procedure for all possible values of x and collect the set of all singularities to construct the full analyticity domain. Finally, the radius of convergence ρ is then the complex singularity closest to the origin, while K_c is the smallest (positive) real singularity, if any.

Vice versa, we could also fix the argument ϕ of the complex value K, such that $K=|K|e^{i\phi}$. The summation (31) will then be maximized for $x=-\left[(\phi/2\pi)+\frac{1}{2}\right]$, where each term in the sum turns into a positive value. For these values of K and x, by using the inclusion argument and the root criterion on the delimiting series, one can show that the radius of convergence is given by $2/e$. Hence, for each x there is one singularity at $K=-(2/e)e^{-i2\pi x}$, and the complete set over all x forms a closed curve that is a circle around the origin.

Note that this is very different from the true maps with the small divisors. Although not proven, numerical studies (for instance Ref. 5 and references quoted therein) suggest that for the true SM and SSM the function $g(x;K,\omega)$ has for each value of x, independently of its value, an infinite set of singularities forming the same (for each x) natural boundary. Numerical analysis[5] shows that the natural boundary of the true SSM, at fixed x, is a circle just as in this simplified model when the union on all x is taken. [It is easy to prove that the analyticity domain in K, that is by taking the union over all values of $x\in[0,1]$, is a circle for the true SSM, as first pointed out in Ref. 35. However, to our knowledge, there is no analytical proof that it is a circle for a fixed value of x.] This property appears to be true irrespective to the choice of ω as long as it fulfills a Diophantine condition,[2] or even a Bryuno condition. For the SM with golden mean as winding number this curve resembles close to a circle, but not very smooth and slightly elongated (about 1%) along the imaginary axis.[17]

2. Simplified SM

Taking the power series (8) for $\hat{h}_k(K)$ for the simplified SM using Eq. (25) we have

$$\hat{h}_k(K)=\sum_{n=1}^{\infty}\frac{1}{2\pi i}P(n,k,1)K^n=\frac{1}{2\pi i}\sum_{n=|k|,|k|+2,\ldots}^{\infty}K^n\frac{(-1)^{n+(n-k)/2}}{2^n}\frac{k^{n-1}}{((n-k)/2)!\,((n+k)/2)!}. \tag{32}$$

Changing variables to $j=(n-|k|)/2$ gives

$$\hat{h}_k(K) = \frac{(-1)^k}{2\pi i k} \sum_{j=0}^{\infty} \frac{(-1)^j}{2^{2j+|k|} j\,!\,(j+|k|)!} (|k|K)^{2j+|k|} = \frac{(-1)^k}{2\pi i k} J_{|k|}(K|k|), \tag{33}$$

with $J_v(z)$ the Bessel function of the first kind[22,44] defined (for integers v) as

$$J_v(z) \equiv \sum_{j=0}^{\infty} \frac{(-1)^j}{2^{2j+v} j\,!\,(j+v)!} z^{2j+v}. \tag{34}$$

As these Bessel functions $J_v(z)$ have no singularities in z, neither has $\hat{h}_k(K)$ in K. Therefore, the Fourier coefficients do not give direct information about K_c. On the other hand, one can conclude from Eqs. (33) and (34) that $|\hat{h}_k(K)|$ is maximized for pure imaginary K, so that the singularity closest to the origin is lying on the imaginary axis, on a distance ρ from the origin. Here, the individual terms in Eq. (34) can not cancel as $(-1)^j$ is then neutralized by $z^{2j} \sim K^{2j} = (-1)^j |K|^{2j}$.

We can now try to evaluate the Fourier series (7) for $h(x;K)$,

$$h(x;K) = \sum_{k=-\infty}^{+\infty} \frac{(-1)^k}{2\pi i k} J_{|k|}(|k|K) \exp(2\pi i k x) = \sum_{k=1}^{\infty} \frac{(-1)^k}{\pi k} J_k(kK) \sin(2\pi k x). \tag{35}$$

Further simplification is achieved by taking the derivative with respect to x and searching the singularities in

$$h'(x;K) = \sum_{k=1}^{\infty} 2(-1)^k J_k(kK) \cos(2\pi k x) \tag{36}$$

instead of $h(x;K)$; this is allowed as the two problems are equivalent.

From the series (36) we can guess for which values of x the singularities will be K_c and ρ respectively. As $J_k(kK)$ is positive for real values $0 < K < 1$ (see p. 534 in Ref. 44), we need to compensate the $(-1)^k$ term by $\cos(2\pi k x)$. This is achieved for $x = \frac{1}{2}$ that reduces Eq. (36) to

$$h'(1/2;K) = 2\sum_{k=1}^{\infty} J_k(kK), \tag{37}$$

which has the exact solution [see formula (1) on p. 615 in Ref. 44]

$$2\sum_{k=1}^{\infty} J_k(kK) = \frac{K}{1-K}. \tag{38}$$

Hence, $h'(1/2;K)$ has a singularity at $K=1$, yielding the critical constant $K_c = 1$, a well known result in celestial mechanics.[50]

The complete analyticity domain can be found in Ref. 50, p. 219. In Fig. 3 we represent what can be obtained by using Padé approximants for some values of x. What emerges is that the function $h(x;K)$ has for each value of x a pair of complex singularities closest to the origin symmetric with respect to the real axis. For x going from 0 to 1/2 such singularities move continuously from -1 to 1 along two (symmetric) curves which pass through the points $\pm i\rho$ at $x = 1/4$ (see Fig. 3). Hence the entire set of singularities closest to the origin lies on a curve which is smooth except at $K = \pm 1$, where it has a discontinuity in its first derivative (cf. again Ref. 50, p. 219).

An important feature is, however, that, as already noted in a similar context by Simon,[40] a natural boundary in K for fixed x seems to appear only in the presence of small divisors. In fact, the latter give rise to the occurrence of sudden peaks yielding a pattern similar to lacunary series,[28] for which natural boundaries can be proved to arise. Hence, these peaks seem to be responsible for the formation of the natural boundary as suggested by Prange (cf. again Ref. 40).

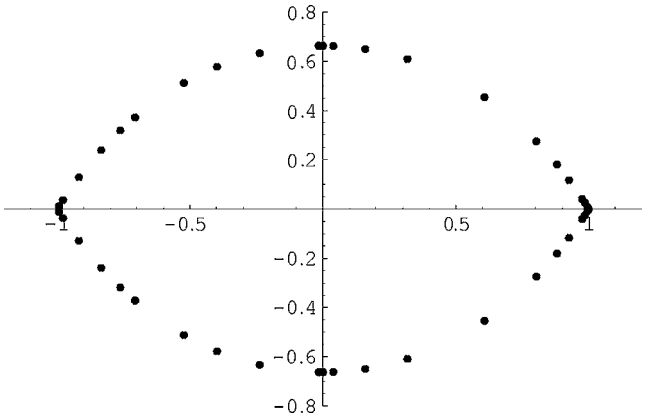

FIG. 3. Singularities in K of the function $h(x;K)$ for the SM without small divisors for x varying in [0,1]. The radius of convergence ρ corresponds to the value $x=1/4$, while the critical constant $K_c=1$ corresponds to $x=1/2$. The curve is symmetric with respect to both the real and the imaginary axes.

V. CONCLUSIONS

We showed by a numerical evaluation of the Lindstedt series up to order $n=700$ that a previously assumed violation of Greene's criterion[42] was ungrounded. The assumption that allowed the restricted series (15) was falsified for orders $n>200$. The resulting critical constant did not correspond to the SM, but is still the true one for the SSM. From our numerics, we conclude that, for the golden mean, the SSM critical constant is strictly higher than the SM. This seems to be generally true for all winding numbers, but it is specifically difficult to prove for the golden mean where both constants are very close. Still, the numerics up to order $n=700$ do not give a complete convergence. An evaluation that would compare to the accuracy of Greene's method would rely on a prohibitive computational effort.

Note that our analysis leaves some open problems. As we have seen, the small divisors introduce some sudden jumps in the coefficients $\hat{g}_k^{(n)}(\omega)$ whenever k is a Fibonacci number, or more generally (for $\omega\neq\tau$) the denominator of a best approximant for the winding number ω, and one has $|k|\leqslant n$ for the SM, hence one could think, as done in Ref. 42, that the most dominant terms in the Taylor expansion of $g(x;K,\omega)$ are those with n the denominator of a best approximant and $k=n$. In principle this conjecture could seem very plausible, but in fact, as the analysis above shows, it is wrong, even if it appears as numerically supported up to rather high Taylor orders n (up to $n\sim 200$). If one bears in mind Davie's result (16), the only possibility left is that there are Taylor orders n such that $|P(n,k,1)|$ is maximized for $k=k_{\max}(n)<n$. It would be interesting to study the dependence of $k_{\max}(n)$ on n. An interesting problem would be also to understand which are the values of n at which the peaks of $|P(n,k_{\max},1)|$ appear. They are very likely related to the best approximants, but the exact nature of such a relationship deserves further investigation. An already remarked consequence of our analysis is that also for the golden mean the SM has a radius of convergence lower than that of the SSM. Even if such a property has been numerically checked for other winding numbers,[10] it is not *a priori* obvious that it must hold for the golden mean. [To make an analogy, also the equality $\rho(\omega)=K_c(\omega)$ is certainly false for most of ω, but still it holds for $\omega=\tau$.] Our result suggests that the radius of convergence for the SM is always less than that of the SSM for all winding numbers, but we leave such a property as a conjecture.

In addition to the analysis performed in Sec. III, we have proposed a simplified model that appears when the small divisors in the SM and SSM are suppressed. We show that this model maintains many features of the SM and SSM. It has an analytical solution in both cases, and it corresponds to Kepler's equation in case of the SM. Also here, the analog of the SM has a lower value of ρ than that of the SSM. Moreover, surprisingly, the radii of convergence are lower than the true models for golden mean winding numbers. This proves that the golden mean winding number is remarkably resistant to the small divisor effect and falsifies a common misconception

that the small divisor problem is the dominant and only mechanism for the analyticity breaking transition. The fact, that the simplified model still has a transition with a value even lower than the true maps for the golden mean, shows that this is not the case.

Finally, we studied the full analyticity domain for the two models (the case of the SM was well known in literature, as it correspond to the celebrated Kepler's equation). Also here, there are striking differences between the simplified and the true maps. Similar to the true maps, the set of singularities form a natural boundary. However, whereas the SM and SSM all the singularities in K for the function $g(x;K,\omega)$ are present for any value of x (that is there is a natural boundary at fixed x), the situation is quite different for the simplified maps. The simplified SSM has only one singularity in the complex K plane for the function $h(x;\boldsymbol{K})$ at each value of x. The simplified SM has for each value of x two singularities symmetric with respect to the real axis, except for the singularities on the real axis for $x=0$ and $x=1/2$ which are single. The closed natural boundary is retained after gathering all singularities for all x.

This natural boundary is a perfect circle in case of the simplified SSM (such as it is for the true SSM), while it is a more stretched curve for the simplified SM with a discontinuity in the first derivative on the real axis at $K=\pm 1$. This shows that the radius of convergence of the simplified SSM equals its critical constant, as it was found for the true SSM. In contrast, the simplified SM has a critical constant of $K_c=1$ that is higher than its radius of convergence. In that respect, the simplified SM resembles more the true SM with winding numbers close to rational values. Also this is a bit of a surprise, as one would expect the contrary, but it is consistent with the trend mentioned above. It is almost as if the model, in which all small divisors were eliminated, still suffers more from this effect than the true SM with the golden mean, somehow the small divisors for the golden mean introduce sort of a rotational symmetry for the analyticity domain.

Therefore, we believe that the study of these kinds of simplified analytical models are a worthy prerequisite for the understanding of the SM, SSM, and FK models and, in particular, the influence of the small divisors. For instance, our results about the simplified SSM give further support that the existence of a natural boundary at a single fixed x is created by the presence of small divisors, in agreement with the general remarks at the end of Sec. IV. In particular, this shows that the circular shape of the analyticity domain of the SSM is not simply due to the fact that the corresponding conjugating function depends on K and x through the variable $\eta=K e^{2\pi i x}$ (see Appendix B). On the contrary, there is some deeper reason for this to occur as the above argument cannot explain the existence of the natural boundary, neither its circular shape, for a single fixed value of x.

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APPENDIX A: INDUCTION PROOF

Proof of Eq. (20): Assuming that relation (20) is true up to some Taylor order $n-1$, then the first relation of Eq. (19) for n yields

$$R(n,1)=n\sum_{m=1}^{n-1}\frac{(n-1)^{n-1-m}}{(m-1)!}\frac{(n-2)!}{(n-1-m)!}$$
$$=n\sum_{m=0}^{n-2}\frac{(n-1)^{m}}{(n-2-m)!}\frac{(n-2)!}{m!}=n\sum_{m=0}^{n-2}(n-1)^{m}\binom{n-2}{m}=n((n-1)+1)^{n-2}=n^{n-1}. \tag{A1}$$

The second relation of Eq. (19) is slightly more difficult. One can write

$$
\begin{aligned}
R(n,m) &= \frac{1}{m}\sum_{n'=1}^{n-m+1}\binom{n}{n'}\binom{n-n'-1}{m-2}n'^{(n'-1)}(n-n')^{(n-n'-m+1)} \\
&= \frac{1}{m}\sum_{n'=1}^{n-m+1}\frac{n!}{n'!\,(n-n')!}\frac{(n-n'-1)!}{(m-2)!\,(n-n'-m+1)!}n'^{(n'-1)}(n-n')^{(n-n'-m+1)} \\
&= \frac{1}{m}\sum_{n'=1}^{n-m+1}\frac{n!}{n'!\,(m-2)!\,(n-n'-m+1)!}n'^{(n'-1)}(n-n')^{(n-n'-m)} \\
&= \frac{1}{m}\sum_{n'=1}^{n-m+1}\frac{n!}{(m-2)!\,(n-m+1)!}\binom{n-m+1}{n'}n'^{(n'-1)}(n-n')^{(n-n'-m)} \\
&= \frac{m-1}{m}\sum_{n'=1}^{n-m+1}\binom{n}{m-1}\binom{n-m+1}{n'}n'^{(n'-1)}(n-n')^{(n-n'-m)} \\
&= \frac{m-1}{m}\binom{n}{m-1}\sum_{n'=0}^{n-m}\binom{n-m+1}{n'+1}(n'+1)^{n'}(n-n'-1)^{(n-n'-1-m)} \\
&= \frac{(m-1)(n-m+1)}{m}\binom{n}{m-1}\sum_{n'=0}^{n-m}\binom{n-m}{n'}(n'+1)^{n'-1}(n-n'-1)^{(n-n'-1-m)}. \qquad \text{(A2)}
\end{aligned}
$$

Using Abel's identity[38]

$$
(x+y)(x+y-a\tilde{n})^{\tilde{n}-1} = \sum_{k=0}^{\tilde{n}}\binom{\tilde{n}}{k}xy(x-ak)^{k-1}[y-a(\tilde{n}-k)]^{\tilde{n}-k-1}, \qquad \text{(A3)}
$$

with $k=n'$, $\tilde{n}=n-m$, $a=-1$, $x=1$, $y=m-1$ yields

$$
mn^{n-m-1} = \sum_{n'=0}^{n-m}\binom{n-m}{n'}(m-1)(1+n')^{n'-1}(n-n'-1)^{n-m-n'-1}, \qquad \text{(A4)}
$$

hence

$$
\begin{aligned}
R(n,m) &= \frac{(m-1)(n-m+1)}{m}\binom{n}{m-1}\sum_{n'=0}^{n-m}\binom{n-m}{n'}(n'+1)^{n'-1}(n-n'-1)^{(n-n'-1-m)} \\
&= (n-m+1)\binom{n}{m-1}n^{n-m-1} = \frac{n-m+1}{n}\frac{n!}{(m-1)!\,(n-m+1)!}n^{n-m} \\
&= \frac{(n-1)!}{(m-1)!\,(n-m)!}n^{n-m} = \binom{n-1}{m-1}n^{n-m}, \qquad \text{(A5)}
\end{aligned}
$$

which concludes the proof as the case $n=1$ is trivial.

APPENDIX B: TREE FORMALISM

Proof of Eq. (20) for $m=1$: First of all, by defining $\alpha=2\pi x$ and $u(\alpha)=2\pi g(x;K,\omega)$ (of course, besides α,u also depends on K and ω) one can write the functional relation that the function $u(\alpha)$ must satisfy as $u(\alpha)+(K/2i)\exp(i\alpha+iu(\alpha))=0$ for the SSM and $u(\alpha)+K\sin(\alpha+u(\alpha))=0$ for the SM. Note that in the case of the SSM the function u, which in principle depends on two parameters K and α (for a given ω), is in fact a function of the only parameter $\eta\equiv Ke^{i\alpha}$.

In terms of the function $u(\alpha)$ the functional equation (4) becomes, for the SM,

$$2u(\alpha) - u(\alpha + 2\pi\omega) - u(\alpha - 2\pi\omega) = -K \sin(\alpha + u(\alpha)), \tag{B1}$$

in which we recognize Eq. (1.4) of Ref. 6, with $\varepsilon = K$. For the SSM we have the same equation with the sine function replaced with $(2i)^{-1} \exp(i\alpha + iu(\alpha))$. Then we can envisage the same tree expansion as in Ref. 6; see formula (2.2), where, to make a relation with the notations we are using now, k and ν are what we are denoting with n and k, respectively. (In fact we need only p. 162 of the quoted reference, where the tree formalism is introduced.) Moreover $\gamma(\nu_{\ell_v}) = -D_{\nu_{\ell_v}}$, hence it is -1 in our case, and one has $\nu_v = 1$ for the SSM and $\nu_u \in \{\pm 1\}$ for the SM. At the end we find

$$\hat{h}_k^{(n)} = \frac{1}{2\pi i} \frac{(-1)^n}{2^n} \sum_{\vartheta \in \mathcal{T}_{n,k}} \mathrm{Val}(\vartheta), \quad \mathrm{Val}(\vartheta) = \prod_{u \in \vartheta} \frac{1}{m_u!} \nu_u^{m_u + 1}, \tag{B2}$$

where the trees ϑ, the branching numbers m_u and the set of trees $\mathcal{T}_{n,k}$ of order n (that is with n nodes) and with momentum k flowing through the root line (that is such that $\Sigma_{u \in \vartheta} \nu_u = k$) are defined as in Ref. 6. Extensions of notations to more general maps are easily obtained; see for instance Ref. 7.

In the case of the SSM, Eq. (B2) reduces to

$$\hat{h}_n^{(n)} = \frac{1}{2\pi i} \frac{(-1)^n}{2^n} \sum_{\vartheta \in \mathcal{T}_{n,n}} \mathrm{Val}(\vartheta), \quad \mathrm{Val}(\vartheta) = \prod_{u \in \vartheta} \frac{1}{m_u!}, \tag{B3}$$

as $\nu_u \equiv 1$, and the sum over trees of order n can be written as a sum over all possible configurations of branching numbers $\{m_u\}_{u \in \vartheta}$ with the constraint $\Sigma_{u \in \vartheta} m_u = n - 1$, indeed they are the only labels of the trees, and their values uniquely determine the elements of $\mathcal{T}_{n,n}$. Therefore we can rewrite $\hat{h}_n^{(n)}$ as

$$\hat{h}_n^{(n)} = \frac{1}{2\pi i} \frac{(-1)^n}{2^n} \sum_{m_1 + \cdots + m_n = n-1} \frac{1}{m_1 ! \cdots m_n!} = \frac{1}{2\pi i} \frac{(-1)^n}{2^n} \frac{n^{n-1}}{n!}, \tag{B4}$$

where we have used the multinomial theorem

$$\sum_{m_1 + \cdots + m_n = p} \frac{n!}{m_1 ! \ldots m_n!} x_1^{m_1} \cdots x_n^{m_n} = (x_1 + \cdots + x_n)^p, \tag{B5}$$

which extends the binomial theorem to $n > 2$; see Ref. 1, Sec 24.1.3.

Proof of Eq. (25): In the case of the SM, without small divisors, we can still use formula (B2), but now one can have $\nu_u = \pm 1$.

As $k = \Sigma_{u \in \vartheta} \nu_u$ we see that, first, k can assume only the values $-n, -n+2, -n+4, \ldots, n-4, n-2, n$ [so that, in particular, $(n \pm k)/2$ is even], and, second, in order to have a contribution to $\hat{h}_k^{(n)}$ we must set $(n-k)/2$ mode labels ν_u equal to -1 and the remaining $(n+k)/2$ mode labels equal to 1. Moreover for any tree $\vartheta \in \mathcal{T}_{n,k}$ we can write

$$\prod_{u \in \vartheta} \nu_u^{m_u + 1} = \left(\prod_{u \in \vartheta} \nu_u \right) \left(\prod_{u \in \vartheta} \nu_u^{m_u} \right) = (-1)^{(n-k)/2} \prod_{u \in \vartheta} \nu_u^{m_u}, \tag{B6}$$

which inserted into Eq. (B2) gives, by using again the multinomial theorem,

$$\begin{aligned} \hat{h}_k^{(n)} &= \frac{1}{2\pi i} \frac{(-1)^{n+(n-k)/2}}{2^n} \binom{n}{(n-k)/2} \sum_{m_1 + \cdots + m_n = n-1} \frac{\nu_1^{m_1} \cdots \nu_n^{m_n}}{m_1 ! \cdots m_n!} \\ &= \frac{1}{2\pi i} \frac{(-1)^{n+(n-k)/2}}{2^n} \frac{k^{n-1}}{((n-k)/2) ! \, ((n+k)/2)!}, \end{aligned} \tag{B7}$$

which yields Eq. (25).

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Jacobi structures in $\mathbb{R}^3$

F. Haas[a)]
UNISINOS, Ciências Exatas e Tecnológicas, Av. Unisinos, 950, 93022-000, São Leopoldo, RS, Brazil

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The most general Jacobi brackets in $\mathbb{R}^3$ are constructed after solving the equations imposed by the Jacobi identity. Two classes of Jacobi brackets were identified, according to the rank of the Jacobi structures. The associated Hamiltonian vector fields are also constructed. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Jacobi brackets have all properties of Poisson brackets, except from the fact that they are not necessarily derivations. A manifold endowed with a Jacobi bracket is called a Jacobi manifold. In this context, Jacobi manifolds are natural generalizations of Poisson, contact and locally conformal symplectic manifolds. Jacobi manifolds were introduced by Lichnerowicz[1] and, in a local Lie algebra setting, by Kirillov.[2] The general properties of Jacobi manifolds are discussed, for instance, in Refs. 3 and 4. Some recent advances on the study of Jacobi manifolds can be found in Refs. 5–16.

The present work is devoted to the explicit construction of Jacobi structures. Although contact and locally conformal symplectic manifolds are general concrete examples of Jacobi manifolds, there is a lack of knowledge of other possible classes of Jacobi brackets even for low dimensional manifolds. An exception in this regard is given by linear Jacobi structures on vector bundles.[17] This is to be compared with the Poisson manifolds case, where, in recent years, there has been much work for the explicit construction of Poisson structures, generalizing the well-known case of Lie-Poisson structures.[18–22] In particular, there have been intensive efforts in the derivation of new classes of three-dimensional Poisson structures, with application to three-dimensional dynamical systems.[23–31] More recently, Ay *et al.*[32] have found the general solution of the determining equation for Poisson structures in $\mathbb{R}^3$. The purpose of the present work is to extend this result, obtaining the general form of Jacobi structures in $\mathbb{R}^3$. Our approach is not applicable to generic three-dimensional manifolds.

The paper is organized as follows. In Sec. II, we briefly review the basic definitions about Jacobi manifolds. In Sec. III, we consider the specific case of Jacobi structures in $\mathbb{R}^3$. The determining equations for Jacobi brackets in $\mathbb{R}^3$ are obtained and solved. In Sec. IV, the associated Hamiltonian vector fields are discussed. Section V is reserved to our conclusions.

II. JACOBI MANIFOLDS

Here we review the essential results about Jacobi manifolds. More detailed accounts on the subject can be found in Refs. 1–4. By definition, a Jacobi structure on a manifold M is a 2-vector $\mathbf{\Lambda}$ and a vector field $\mathbf{E}$ on M such that

$$[\mathbf{\Lambda},\mathbf{\Lambda}] = 2\mathbf{E} \wedge \mathbf{\Lambda}, \quad [\mathbf{E},\mathbf{\Lambda}] = 0, \tag{1}$$

where $[,]$ is the Schouten-Nijenhuis bracket.[33] Let $C^\infty(M,\mathbb{R})$ be the algebra of C^∞ real-valued functions on M. If $(M,\mathbf{\Lambda},\mathbf{E})$ is a Jacobi structure, then the space $C^\infty(M,\mathbb{R})$ endowed with a

[a)]Electronic mail: ferhaas@unisinos.br

mapping $\{,\}: C^\infty(M,\mathbb{R})\times C^\infty(M,\mathbb{R})\to C^\infty(M,\mathbb{R})$ becomes a local Lie algebra in the sense of Kirillov.[2] This so-called Jacobi bracket $\{,\}$ is defined by

$$\{f,g\} = \mathbf{\Lambda}(\mathrm{d}f,\mathrm{d}g) + f\mathbf{E}(g) - g\mathbf{E}(f), \tag{2}$$

for all $f,g\in C^\infty(M,\mathbb{R})$. The Jacobi bracket is $\mathbb{R}$ bilinear, skew-symmetric, and satisfies the Jacobi identity. In other words,

$$\{c_1 f + c_2 g, h\} = c_1\{f,h\} + c_2\{g,h\},$$

$$\{f,g\} = -\{g,f\},$$

$$\{\{f,g\},h\} + \{\{g,h\},f\} + \{\{h,f\},g\} = 0, \tag{3}$$

for all $f,g,h\in C^\infty(M,\mathbb{R})$ and $c_1,c_2\in\mathbb{R}$. The local Lie algebra character of $C^\infty(M,\mathbb{R})$ is assured by

$$\text{support}\{f,g\}\subseteq \text{support } f\cap \text{support } g, \tag{4}$$

for all $f,g\in C^\infty(M,\mathbb{R})$.

In addition, the Jacobi bracket is a first-order differential operator in each of its arguments using ordinary multiplication of functions,

$$\{fg,h\} = f\{g,h\} + \{f,h\}g - fg\{1,h\}, \tag{5}$$

for all $f,g,h\in C^\infty(M,\mathbb{R})$. As apparent from (5), the Jacobi bracket is not a derivation unless the constant unit function has a vanishing Jacobi bracket with all functions in $C^\infty(M,\mathbb{R})$. It happens if and only if the vector field $\mathbf{E}$ vanish, $\mathbf{E}\equiv 0$. If $\mathbf{E}\equiv\mathbf{0}$, then $(M,\mathbf{\Lambda})$ is a Poisson manifold. In this sense, Jacobi manifolds are generalizations of Poisson manifolds. Examples of manifolds with Jacobi but not Poisson structures are contact and locally conformal symplectic manifolds.

As shown by Lichnerowicz,[1] any Jacobi structure $(M,\mathbf{\Lambda},\mathbf{E})$ can be associated to a higher-dimensional Poisson structure $(\mathbf{\Pi},M\times\mathbb{R})$, defined by

$$\mathbf{\Pi}(\mathbf{x},t) = \exp(-t)\left(\mathbf{\Lambda}(\mathbf{x}) + \frac{\partial}{\partial t}\wedge\mathbf{E}\right), \tag{6}$$

where (x,t) are local coordinates in $(\mathbf{\Pi},M\times\mathbb{R})$. While Eq. (6) provides a simple recipe to obtain a Poisson structure from a Jacobi structure in a lower-dimensional manifold, it is not trivial to construct a Jacobi structure in the manifold M itself. Hence the importance of deriving concrete examples of Jacobi structures in manifolds like $\mathbb{R}^3$, for instance.

In a local coordinate chart x^i, for $i=1,\ldots,n$ with $n=\dim M$, we have the following expressions for the tensor field $\mathbf{\Lambda}$, the vector field $\mathbf{E}$, and the Jacobi bracket of two functions f and g,

$$\mathbf{\Lambda} = \tfrac{1}{2}\Lambda^{ij}\partial_i\wedge\partial_j, \quad \mathbf{E} = E^i\partial_i,$$

$$\{f,g\} = \Lambda^{ij}\partial_i f\partial_j g + fE^i\partial_i g - gE^i\partial_i f. \tag{7}$$

The summation convention was used, as well as the notation $\partial_i = \partial/\partial x^i$. In addition, the Schouten-Nijenhuis bracket conditions (1) traduces into

$$\Lambda^{im}\partial_m\Lambda^{jk} + \Lambda^{jm}\partial_m\Lambda^{ki} + \Lambda^{km}\partial_m\Lambda^{ij} + \Lambda^{ij}E^k + \Lambda^{jk}E^i + \Lambda^{ki}E^j = 0, \tag{8}$$

$$E^k\partial_k\Lambda^{ij} - \Lambda^{ik}\partial_k E^j + \Lambda^{jk}\partial_k E^i = 0. \tag{9}$$

As can be verified, Eqs. (8) and (9) are completely equivalent to the Jacobi identity for the Jacobi bracket (2). In this context, we call (8) and (9) the Jacobi equations. The general solution for the Jacobi equations yields the general form of the Jacobi structures in $\mathbb{R}^n$. Ay *et al.* have solved the

Jacobi equations for $n=3$ and $\mathbf{E}=\mathbf{0}$, that is, the Poisson case in $\mathbb{R}^3$. In the next section we allow for nonvanishing vector fields $\mathbf{E}$, looking for the general class of Jacobi structures in $\mathbb{R}^3$.

III. JACOBI STRUCTURES IN $\mathbb{R}^3$

Consider the $\mathbb{R}^3$ case, introducing a vector field $\mathbf{A}=A^i\partial_i$ according to

$$\Lambda^{ij}=\varepsilon_{ijk}A^k, \tag{10}$$

using the Levi-Civita symbol ε_{ijk}. In other words, $\mathbf{A}=(\Lambda^{23},\Lambda^{31},\Lambda^{12})$. In terms of this vector field $\mathbf{A}$, the Jacobi equations (8) and (9) are rewritten as

$$\mathbf{A}\cdot(\nabla\times\mathbf{A}-\mathbf{E})=0, \tag{11}$$

$$\mathbf{E}\times(\nabla\times\mathbf{A})+\mathbf{A}\nabla\cdot\mathbf{E}=\nabla(\mathbf{A}\cdot\mathbf{E}), \tag{12}$$

using standard symbols of vector calculus in $\mathbb{R}^3$.

Using (11) and (12) we can proceed to construct Jacobi structures using the well-known language of vector calculus in $\mathbb{R}^3$. Before we do that, it is interesting to interpret geometrically equation (11). Consider $(M,\mathbf{\Lambda},\mathbf{E})$ a given Jacobi structure and let $\mathbf{\Lambda}^\sharp:T^*M\to TM$ be the vector bundle map associated with $\mathbf{\Lambda}$. In other words, for all $\mathbf{p}\in M,\zeta,\eta\in T_p^*M$,

$$\mathbf{\Lambda}(\zeta,\eta)=\langle\eta,\mathbf{\Lambda}^\sharp(\zeta)\rangle, \tag{13}$$

where $\langle,\rangle$ denotes the natural pairing. In terms of the vector field $\mathbf{A}$, the last equation shows that the image of the vector bundle map $\Lambda^\sharp$ is the plane orthogonal to $\mathbf{A}$. Taking into account (11), written as $\mathbf{A}\cdot\mathbf{E}=\mathbf{A}\cdot\nabla\times\mathbf{A}$, we conclude that the condition $\mathbf{A}\cdot\nabla\times\mathbf{A}\neq0$ would imply that the vector $\mathbf{E}$ does not belong to the image of $\mathbf{\Lambda}^\sharp$, or, in other words, that the rank of the Jacobi structure is everywhere 3. On the other hand, the condition $\mathbf{A}\cdot\nabla\times\mathbf{A}\equiv0$ would imply that the vector $\mathbf{E}$ takes its values in the image of $\mathbf{\Lambda}^\sharp$. Together with $\mathbf{A}\neq0$, that means that the rank of the Jacobi structure would be everywhere 2.

Now consider the calculation of Jacobi structures. For $\mathbf{A}\equiv0$, Eqs. (11) and (12) are identically satisfied for arbitrary $\mathbf{E}$, but this will not produce very interesting Jacobi structures. Disregarding the too trivial case $\mathbf{A}\equiv0$, we conclude that Eq. (11) is equivalent to

$$\mathbf{E}=\nabla\times\mathbf{A}-\mathbf{g}\times\mathbf{A}, \tag{14}$$

for some vector field $\mathbf{g}$ in $\mathbb{R}^3$, to be determined. The Poisson case $\mathbf{E}=\mathbf{0}$ is obtained for

$$\nabla\times\mathbf{A}=\mathbf{g}\times\mathbf{A}. \tag{15}$$

As shown by Ay and co-workers in a different notation,[32] the general solution for (15) is given by

$$\mathbf{A}=\mu\nabla\psi, \tag{16}$$

for $\mu,\psi\in C^\infty(\mathbb{R}^3,\mathbb{R})$. The solution (16) has shown to be valid[32] also in the neighborhood of some classes of irregular points, where $\mathbf{A}=\mathbf{0}$. The corresponding vector field $\mathbf{g}$ is given by

$$\mathbf{g}=\frac{\nabla\mu}{\mu}. \tag{17}$$

Returning to the not necessarily Poisson case and substituting the form (14) into (12), we get the following condition:

$$\nabla(\mathbf{A}\cdot\nabla\times\mathbf{A})=\mathbf{g}(\mathbf{A}\cdot\nabla\times\mathbf{A})-\mathbf{A}(\mathbf{A}\cdot\nabla\times\mathbf{g}). \tag{18}$$

In the remaining part of the section we examine the general solution for (18), thus determining the possible classes of Jacobi structures in $\mathbb{R}^3$. We consider two cases, according to the rank of the Jacobi structure.

A. Rank 3 Jacobi structures

Suppose

$$\mathbf{A}\cdot\nabla\times\mathbf{A}\neq 0. \tag{19}$$

In this situation, $(\mathbb{R}^3,\mathbf{\Lambda})$ is certainly not a Poisson structure, with 2-vector $\mathbf{\Lambda}$ specified by (10). However, we can construct Jacobi structures defining a vector field $\mathbf{h}$ such that

$$\mathbf{g}=\nabla\phi+\mathbf{h}, \tag{20}$$

for

$$\phi=\ln(\mathbf{A}\cdot\nabla\times\mathbf{A}). \tag{21}$$

Of course the function ϕ is not well defined unless $\mathbf{A}\cdot\nabla\times\mathbf{A}$ is not identically vanishing. Inserting (20) into (18), the result is

$$\mathbf{h}(\mathbf{A}\cdot\nabla\times\mathbf{A})-\mathbf{A}(\mathbf{A}\cdot\nabla\times\mathbf{h})=0. \tag{22}$$

The cross product of (22) with $\mathbf{A}$ gives

$$\mathbf{A}\times\mathbf{h}=\mathbf{0}\rightarrow\mathbf{h}=\alpha\mathbf{A}, \tag{23}$$

for an arbitrary real-valued function α on $\mathbb{R}^3$. We can take $\alpha\equiv 0$ without loss of generality, since, according to (14) and (20), this function will add nothing to the vector field $\mathbf{E}$. Hence, in the rank 3 case the determining equation (18) is solved for any vector field $\mathbf{A}$ satisfying $\mathbf{A}\cdot\nabla\times\mathbf{A}\neq 0$, taking $\mathbf{g}=\nabla\phi$ with ϕ given by (21). The corresponding vector field $\mathbf{E}$ follows from (14). After using some vector identities, the result is

$$\mathbf{E}=e^{\phi}\nabla\times(e^{-\phi}\mathbf{A}). \tag{24}$$

Using (2) and (10) and the above solution $\mathbf{E}$, we get the Jacobi bracket between any functions $f,g\in C^{\infty}(\mathbb{R}^3,\mathbb{R})$,

$$\{f,g\}=\mathbf{A}\cdot\nabla f\times\nabla g+e^{\phi}(f\nabla g-g\nabla f)\cdot\nabla\times(e^{-\phi}\mathbf{A}). \tag{25}$$

It takes a simpler form for $\phi=$constant, in which case

$$\{f,g\}=\mathbf{A}\cdot\nabla f\times\nabla g+(f\nabla g-g\nabla f)\cdot\nabla\times\mathbf{A}. \tag{26}$$

In conclusion, the Jacobi bracket (25) has three free ingredients, namely the three components of the vector field $\mathbf{A}$, as long as $\mathbf{A}\cdot\nabla\times\mathbf{A}$ is not identically null. For simplicity, we do not consider the behavior of the solution in the neighborhood of points into domains $\Omega\subset\mathbb{R}^3$ where $\mathbf{A}\cdot\nabla\times\mathbf{A}=0$.

On $\mathbb{R}^3$, rank 3 Jacobi structures are in one-to-one correspondence with contact 1-forms. Specifically, giving a contact 1-form θ on $\mathbb{R}^3$ such that $\theta\wedge\mathrm{d}\theta\neq 0$, there is a Jacobi structure $(\mathbb{R}^3,\mathbf{\Lambda},\mathbf{E})$ satisfying $\mathbf{\Lambda}\wedge\mathbf{E}\neq 0$ and $i_{\theta}(\mathbf{\Lambda})=0$, $i_{\mathbf{E}}(\theta)=1$. In the case of the rank 3 Jacobi structures of this section, using Cartesian coordinates we can show that

$$\mathbf{\Lambda}\wedge\mathbf{E}=\mathbf{A}\cdot\mathbf{E}\frac{\partial}{\partial x}\wedge\frac{\partial}{\partial y}\wedge\frac{\partial}{\partial z}=\mathbf{A}\cdot\nabla\times\mathbf{A}\frac{\partial}{\partial x}\wedge\frac{\partial}{\partial y}\wedge\frac{\partial}{\partial z}\neq 0. \tag{27}$$

Since $\mathbf{\Lambda}\wedge\mathbf{E}$ is nowhere zero, there is a contact 1-form θ associated to this Jacobi structure. It can be shown that

$$\theta=e^{-\phi}A^i\,\mathrm{d}x^i \tag{28}$$

satisfies

$$i_{\theta}(\mathbf{\Lambda})=-e^{-\phi}(\mathbf{A}\times\mathbf{A})\cdot\nabla=0, \tag{29}$$

$$i_{\mathbf{E}}(\theta) = e^{-\phi}\mathbf{A}\cdot(\nabla\times\mathbf{A}-\nabla\phi\times\mathbf{A}) = e^{-\phi}\mathbf{A}\cdot\nabla\times\mathbf{A} = 1, \tag{30}$$

the last equality following from the definition of ϕ. Moreover,

$$\theta\wedge \mathrm{d}\theta = e^{-\phi}\,\mathrm{d}x\wedge\mathrm{d}y\wedge\mathrm{d}z, \tag{31}$$

which never vanishes. Therefore, the 1-form θ given by (28) qualifies as the contact 1-form associated to rank 3 Jacobi structures in $\mathbb{R}^3$. As a corollary, we conclude that

$$\mathrm{d}\theta = e^{-\phi}(\partial_i A^j - A^j\partial_i\phi)\mathrm{d}x^i\wedge\mathrm{d}x^j \tag{32}$$

is a symplectic structure on the vector bundle $\ker\theta\to\mathbb{R}^3$ defined as the set of vector fields orthogonal to $\mathbf{A}$ at every point.

Another way to interpret the above construction is in terms of the characteristic distribution[2,3] of the Jacobi structure $(\mathbb{R}^3,\mathbf{\Lambda},\mathbf{E})$, defined as the subbundle D of $T(\mathbb{R}^3)$ spanned by the set of all Hamiltonian vector fields. In other words, $D_{\mathbf{p}}=\mathrm{Span}\{\mathbf{\Lambda}^{\sharp}(\zeta)(\mathbf{p}),\mathbf{E}(\mathbf{p}),\forall\,\zeta\in T^*(\mathbb{R}^3)\}$ is the fiber at a point $\mathbf{p}\in\mathbb{R}^3$. The characteristic distribution of a Jacobi structure is completely integrable, defining a foliation whose leaves are contact manifolds or locally conformal symplectic manifolds. The leaves of the foliation can be represented as the level sets of a function $f(x,y,z)$. In terms of the vector fields $\mathbf{A}$ and $\mathbf{E}$, the determining equations of the foliation are given by

$$\mathbf{A}\times\nabla f = 0, \tag{33}$$

$$\mathbf{E}\cdot\nabla f = 0. \tag{34}$$

For the rank 3 Jacobi structures of this section, inserting (24) into (34) and considering equation (33) gives

$$\nabla\times\mathbf{A}\cdot\nabla f = 0, \tag{35}$$

which is redundant since $\nabla\times\mathbf{A}\cdot\nabla f=\nabla\cdot(\mathbf{A}\times\nabla f)=0$ in virtue of (33). Hence, for rank 3 Jacobi structures in $\mathbb{R}^3$ the vector field $\mathbf{A}$ is always normal to the leaves of the foliation, as stated in (33).

B. Rank 2 Jacobi structures

For

$$\mathbf{A}\cdot\nabla\times\mathbf{A}\equiv 0, \tag{36}$$

the determining equation (18) simplifies to

$$\mathbf{A}\cdot\nabla\times\mathbf{g} = 0, \tag{37}$$

excluding the trivial case $\mathbf{A}=\mathbf{E}=\mathbf{0}$. As shown by Ay and co-workers,[32] the general solution for (36) is given in terms of two scalar functions μ and ψ, as in Eq. (16). Using (16), the Eq. (37) traduces into

$$\nabla\psi\cdot\nabla\times\mathbf{g} = \nabla\cdot(\mathbf{g}\times\nabla\psi) = 0, \tag{38}$$

showing that the vector field $\mathbf{g}\times\nabla\psi$ is solenoidal. Hence, there are real smooth functions ξ_1 and ξ_2 on $\mathbb{R}^3$ such that

$$\mathbf{g}\times\nabla\psi = \nabla\xi_1\times\nabla\xi_2 \tag{39}$$

in a neighborhood U of every regular point of $\mathbf{g}\times\nabla\psi$. We exclude the trivial case $\nabla\psi=0$.

Inversion of (39) gives

$$\mathbf{g} = \frac{\nabla\psi \times (\nabla\xi_1 \times \nabla\xi_2)}{|\nabla\psi|^2} + \alpha \nabla\, \psi, \tag{40}$$

where α is an arbitrary real-valued smooth function on $\mathbb{R}^3$ and

$$\nabla\psi \cdot \nabla\xi_1 \times \nabla\xi_2 = 0 \tag{41}$$

for consistency with (39). Equation (41) implies a functional dependence between ψ, ξ_1, and ξ_2,

$$\psi = \psi(\xi_1, \xi_2). \tag{42}$$

Since we have solved the determining equation (18), we can construct the vector field $\mathbf{E}$, using Eqs. (14), (16), and (40). This procedure gives

$$\mathbf{E} = \nabla\mu \times \nabla\psi - \mu \nabla\, \xi_1 \times \nabla\xi_2. \tag{43}$$

The corresponding Jacobi bracket reads

$$\{f,g\} = \mu \nabla\, \psi \cdot \nabla f \times \nabla g + (f \nabla\, g - g \nabla\, f) \cdot (\nabla\mu \times \nabla\psi - \mu \nabla\, \xi_1 \times \nabla\xi_2). \tag{44}$$

Notice that the real function α in (40) does not appear in the final form of the Jacobi bracket. Therefore, the Jacobi structure described by (44) has only four ingredients, namely μ, ξ_1, ξ_2, and $\psi(\xi_1, \xi_2)$.

The presence of the function μ in the Jacobi bracket can be eliminated by a conformal transformation. Indeed,[15] if $(M, \mathbf{\Lambda}, \mathbf{E})$ is a Jacobi structure in a manifold M, then $(M, \widetilde{\mathbf{\Lambda}}, \widetilde{\mathbf{E}})$ is also a Jacobi structure in M, where $\widetilde{\mathbf{\Lambda}}$ and $\widetilde{\mathbf{E}}$ are obtained from the conformal change

$$\widetilde{\mathbf{\Lambda}} = \lambda \mathbf{\Lambda}, \quad \widetilde{\mathbf{E}} = \lambda \mathbf{E} + \mathbf{\Lambda}^{\sharp}(\mathrm{d}\lambda), \tag{45}$$

for any $\lambda \in C^{\infty}(\mathbb{R}^3, \mathbb{R})$. Applying such a conformal transformation to everywhere rank 2 Jacobi structures in $\mathbb{R}^3$ using $\lambda = 1/\mu$ gives

$$\widetilde{\Lambda}^{ij} = \varepsilon_{ijk}\partial_k\psi, \quad \widetilde{E} = -\nabla\xi_1 \times \nabla\xi_2, \tag{46}$$

with no presence of the arbitrary function μ. However, this does not mean that μ is to be taken as irrelevant in applications for dynamical systems, for instance.

A Jacobi structure everywhere of rank 2 on $\mathbb{R}^3$ determines a foliation of $\mathbb{R}^3$ whose leaves are locally conformal symplectic surfaces.[2,3] Perhaps the simplest way to describe such a foliation is in terms of the characteristic distribution of the Jacobi structure, as follows from (33) and (34). Representing, as before, the leaves of the foliation as the level sets of a function $f(x,y,z)$ and using (16) and (43) in (34), we get

$$\mathbf{E} \cdot \nabla f = -\mu \nabla\, \xi_1 \times \nabla\xi_2 \cdot \nabla f \equiv 0, \tag{47}$$

showing that $f = f(\xi_1, \xi_2)$. When we insert this result into (33) with $\mathbf{A}$ given by (16), we conclude that

$$\frac{\partial\psi}{\partial\xi_1}\frac{\partial f}{\partial\xi_2} - \frac{\partial\psi}{\partial\xi_2}\frac{\partial f}{\partial\xi_1} = 0, \tag{48}$$

showing that f and ψ are functionally dependent. In conclusion, for rank 2 Jacobi structures in $\mathbb{R}^3$ there exists a locally conformal symplectic foliation whose leaves can be represented by the level sets of the function $\psi(x,y,z)$ entering the Jacobi bracket.

The degenerate character of rank 2 Jacobi structures in $\mathbb{R}^3$ allows to search for Casimir functions associated to the Jacobi bracket. These Casimir functions can be defined in analogy with the Casimir functions of degenerate Poisson manifolds. In other words, we define Casimir func-

tions as the nonconstant functions having a vanishing Jacobi bracket with any other function on $\mathbb{R}^3$. Let a Casimir function be denoted by $C=C(x,y,z)$. In terms of the vector fields **A** and **E**, we have

$$\{f,C\}=(\nabla C\times\mathbf{A}-C\mathbf{E})\cdot\nabla f+f\mathbf{E}(C)\equiv 0 \tag{49}$$

for an arbitrary smooth function $f\in C^{\infty}(\mathbb{R}^3,\mathbb{R})$. Since f is arbitrary, Eq. (49) is decomposed in two parts,

$$\nabla C\times\mathbf{A}=C\mathbf{E}, \tag{50}$$

$$\mathbf{E}(C)=0. \tag{51}$$

Observe that the Casimirs are preserved by the flow of the vector field **E**. In addition, notice that, for $C\neq 0$, Eq. (51) follows from (50) taking the scalar product with ∇C. Therefore, (50) is sufficient for the construction of the Casimirs.

For $C\neq 0$, scalar product of (50) with **A** implies

$$\mathbf{A}\cdot\mathbf{E}=0, \tag{52}$$

incidentally the condition for rank 2 Jacobi structures in $\mathbb{R}^3$. Therefore, nontrivial Casimirs can exist only in the case of rank 2 Jacobi structures, as expected. As will be explicitly shown in what follows, the condition (50) is not only necessary but also sufficient for the existence of nontrivial Casimirs.

Equation (50), written in terms of **A** as given in (16) and **E** as given in (43), reads, after some simple algebra considering $\mu\neq 0$,

$$\nabla\Gamma\times\nabla\psi=-\nabla\xi_1\times\nabla\xi_2, \tag{53}$$

where

$$\Gamma=\ln\left(\frac{C}{\mu}\right). \tag{54}$$

After solving (53) for Γ, the Casimirs follows trivially from (54).

Scalar product of (53) with $\nabla\Gamma$ gives

$$\nabla\Gamma\cdot\nabla\xi_1\times\nabla\xi_2=0, \tag{55}$$

showing that

$$\Gamma=\Gamma(\xi_1,\xi_2). \tag{56}$$

Inserting this information on the functional dependence of Γ in (50), we get

$$\left(\frac{\partial\Gamma}{\partial\xi_1}\frac{\partial\psi}{\partial\xi_2}-\frac{\partial\Gamma}{\partial\xi_2}\frac{\partial\psi}{\partial\xi_1}+1\right)\nabla\xi_1\times\nabla\xi_2=0. \tag{57}$$

Since this equation holds for arbitrary ξ_1, ξ_2, we conclude that

$$\frac{\partial\Gamma}{\partial\xi_1}\frac{\partial\psi}{\partial\xi_2}-\frac{\partial\Gamma}{\partial\xi_2}\frac{\partial\psi}{\partial\xi_1}=-1. \tag{58}$$

Equation (58) can be solved by the method of characteristics. The characteristic equations can be written as

$$\frac{\mathrm{d}\xi_1}{\partial\psi/\partial\xi_2} = -\frac{\mathrm{d}\xi_2}{\partial\psi/\partial\xi_1} = -\,\mathrm{d}\Gamma. \tag{59}$$

One of the characteristics is readily identified as $\psi(\xi_1,\xi_2)$. Without loss of generality, suppose $\partial\psi/\partial\xi_1 \neq 0$ in some neighborhood. Then, the inverse function theorem allows to consider $\xi_1 = \xi_1(\xi_2;\psi)$, written locally as a function of ξ_2 and ψ. This allows writing the general solution for (58) according to

$$\Gamma = \int_{\xi_1=\xi_1(\xi_2;\psi)} \frac{\mathrm{d}\xi_2}{\partial\psi/\partial\xi_1} + \bar{\Gamma}(\psi), \tag{60}$$

where $\bar{\Gamma}$ is an arbitrary function of the indicated argument.

Equation (60), together with (54), provides a recipe to compute the Casimirs of a given rank 2 Jacobi structure in $\mathbb{R}^3$. Perhaps it would be interesting to provide a concrete example of the procedure. Consider a rank 2 Jacobi structure in $\mathbb{R}^3$ defined by

$$\xi_1 = x, \quad \xi_2 = y, \quad \psi = x^2 + y^2, \quad \mu = 1. \tag{61}$$

With (60) and then (54), we obtain the Casimirs in the form

$$C = \bar{C}(r^2)e^{\theta/2}, \tag{62}$$

using cylindrical coordinates and defining

$$\bar{C}(\psi) = e^{\bar{\Gamma}(\psi)}. \tag{63}$$

In addition, we observe that in this case the leaves of the foliation of $\mathbb{R}^3$ in locally conformal symplectic surfaces are given by the cylinders defined by $\psi = x^2 + y^2 = \text{constant}$.

In the next section, we discuss the Hamiltonian vector fields associated to the two types of Jacobi structures derived.

IV. HAMILTONIAN VECTOR FIELDS ASSOCIATED TO JACOBI STRUCTURES IN $\mathbb{R}^3$

For a function $H \in C^\infty(M,\mathbb{R})$, the Hamiltonian vector field $\mathbf{v}_H$ associated with H is defined by[1]

$$\mathbf{v}_H = \mathbf{\Lambda}^\sharp(\mathrm{d}H) + H\mathbf{E}. \tag{64}$$

In this context, the function H is said to be the Hamiltonian for the vector field $\mathbf{v}_H$. In particular,

$$\mathbf{v}_1 = \mathbf{E}, \tag{65}$$

that is, the unit function $H=1$ is a Hamiltonian associated to any vector field $\mathbf{E}$. In this sense, any dynamical system in a manifold M can be viewed as a Hamiltonian system with Jacobi structure given by Hamiltonian function $H=1$, vector field $\mathbf{E}$ being the dynamical vector field itself and tensor field $\mathbf{\Lambda} \equiv 0$. In addition,

$$\mathbf{v}_{\{f,g\}} = [\mathbf{v}_f, \mathbf{v}_g], \tag{66}$$

for any $f,g \in C^\infty(M,\mathbb{R})$, so that the mapping which associates a function with the corresponding Hamiltonian vector field is a Lie algebra homomorphism. Finally, notice that the Hamiltonian is not always a constant of motion, even if time independent. In fact, for a time-independent Hamiltonian function,

$$\frac{\mathrm{d}H}{\mathrm{d}t} = H\mathbf{E}(H). \tag{67}$$

Hence, H is a constant of motion if and only if it is preserved by the flow associated to the vector field $\mathbf{E}$.

In a local coordinate chart x^i, for $i=1,\ldots,n$ with $n=\dim M$, the Hamiltonian vector field at (64) and the corresponding Hamilton equations in M are then

$$\dot{x}^i = v_H^i = \Lambda^{ij}\partial_j H + HE^i, \tag{68}$$

where $\mathbf{v}_H = v_H^i \partial_i$. For $\mathbb{R}^3$ and in terms of the vector field $\mathbf{A}$, the result is

$$\dot{\mathbf{r}} = \nabla H \times \mathbf{A} + H\mathbf{E}, \tag{69}$$

where $\mathbf{r}=(x,y,z)$. The expression (69) can be used to compute the Hamiltonian vector fields associated to the Jacobi structures of Sec. III. The two classes of Jacobi structures are treated separately.

A. Hamiltonian vector fields associated to rank 3 Jacobi structures

The class of Jacobi structures described in Sec. III A yields the following Hamilton equations, taking $\mathbf{E}$ as in (24):

$$\dot{\mathbf{r}} = \nabla \times (H\mathbf{A}) + H\mathbf{A} \times \nabla\phi, \tag{70}$$

with Hamiltonian H and ϕ as in (21).

At first sight, it appears that a simple rescaling $\mathbf{A} \to \bar{\mathbf{A}} = H\mathbf{A}$ would be sufficient to incorporate H into the new vector field $\bar{\mathbf{A}}$, eliminating one irrelevant function. However, the dependence of ϕ on $\mathbf{A}$ prevents this possibility. Indeed, consider $\bar{\mathbf{A}}$ and $\bar{\phi}$ given by

$$\bar{\mathbf{A}} = H\mathbf{A}, \quad \bar{\phi} = \ln(\bar{\mathbf{A}} \cdot \nabla \times \bar{\mathbf{A}}). \tag{71}$$

With these definitions, (70) reads

$$\dot{\mathbf{r}} = \nabla \times \bar{\mathbf{A}} + \bar{\mathbf{A}} \times \nabla\bar{\phi} + 2\frac{\nabla H}{H} \times \bar{\mathbf{A}}. \tag{72}$$

The last term in (72) is H dependent. Therefore, we are left with a dynamical system (70) determined by four functions, namely the three components of $\mathbf{A}$ and the Hamiltonian function H.

Among the whole class (70), an interesting subclass is provided by the choices

$$\nabla \times \mathbf{A} = \lambda\mathbf{A}, \quad H = 1, \tag{73}$$

where $\lambda \in C^\infty(\mathbb{R}^3, \mathbb{R})$ is an arbitrary smooth function. With the choice (73), we get

$$\dot{\mathbf{r}} = \lambda\mathbf{A} + \mathbf{A} \times \nabla\phi, \tag{74}$$

so that the Hamiltonian vector field is immediately decomposed into a parallel and a perpendicular part to the vector field $\mathbf{A}$.

As seen in (73), $\mathbf{A}$ is in the class of the force free vector fields.[34] For instance, a force free field is given by the Arnold-Beltrami-Childress (ABC) vector field,

$$\mathbf{A} = (a\sin z + c\cos y, b\sin x + a\cos z, c\sin y + b\cos x), \tag{75}$$

for a,b,c real nonnegative parameters. In this case, $\lambda=1$. The ABC flow is known to be generically nonintegrable. For instance, for $a=b=c$ there is even an analytic proof of nonintegrability.[35] Inserting (75) into (74), we would obtain a perturbed ABC flow endowed with a Jacobi bracket structure. It would be interesting to investigate the integrability properties of such a system.

To conclude, notice that the dynamical vector field v_H associated to (70) is not necessarily solenoidal, because

$$\nabla \cdot \mathbf{v}_H = \nabla\phi \cdot \nabla \times (H\mathbf{A}), \tag{76}$$

an expression which may be nonvanishing.

B. Hamiltonian vector fields associated to rank 2 Jacobi structures

The class of Jacobi structures described in Sec. III B yields the following Hamilton equations:

$$\dot{\mathbf{r}} = \nabla(\mu H) \times \nabla\psi - \mu H \nabla\, \xi_1 \times \nabla\xi_2. \tag{77}$$

Without any loss of generality, for this class of dynamical systems we can set $H=1$, thanks to the rescaling $\mu \to \mu H$. Hence, we adopt the choice $H=1$ in the following. The dynamical system (77) contains four free functions, namely μ, ξ_1, ξ_2, and $\psi(\xi_1, \xi_2)$.

Notice that ψ is a constant of motion if time independent, because

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} = -\,\mu\, \nabla\, \psi \cdot \nabla\xi_1 \times \nabla\xi_2 = 0. \tag{78}$$

Therefore, to obtain a Hamiltonian description of a dynamical system in $\mathbb{R}^3$ using a Jacobi structure of the extended Poisson type, one must know a first integral. This is a most restrictive condition, in comparison with the case of the preceding section.

Using (50) and (51) and taking $H=1$, one can show that the Casimirs of the rank 2 Jacobi structures in $\mathbb{R}^3$ are preserved by the flow of the associated Hamiltonian vector field,

$$\mathbf{v}_H(C) = 0, \tag{79}$$

where C is any Casimir function. Since one can readily derive all Casimirs from the recipe described by Eqs. (54) and (60), we conclude that a constant of motion ψ plus a rank 2 Jacobi structure amounts to complete integrability, with the corresponding time-independent constants of motion being ψ and C.

To conclude, we observe that the Hamiltonian vector field $\mathbf{v}_H$ associated to (77) (with $H=1$) is not necessarily solenoidal,

$$\nabla \cdot \mathbf{v}_H = -\,\nabla\mu \cdot \nabla\xi_1 \times \nabla\xi_2, \tag{80}$$

which may be nonvanishing.

V. CONCLUSION

The two admissible classes of Jacobi structures in $\mathbb{R}^3$ were constructed. For simplicity, neighborhood of points into domains $\Omega \subset \mathbb{R}^3$ where the vector field $\mathbf{A}$ vanish were not considered. In this sense the results of the work are not completely general.

One of the reasons why Poisson structures are so ubiquitous rests in their applications for dynamical systems.[18–32] Certainly Jacobi structures have not been already applied at the same level in connection with dynamical systems. The results of Sec. IV shows the possible classes of Hamiltonian vector fields endowed with Jacobi structures in $\mathbb{R}^3$. This is a first step towards a more detailed examination of the possibilities opened by Jacobi structures for dynamical systems. For instance, one can ask about the existence of some kind of energy Casimir method for Hamiltonian systems on Jacobi manifolds. In addition, notice that the inverse problem of the construction of a nontrivial Jacobi bracket associated to a given dynamical system was not considered here. This seems to be a difficult task. For instance, due to the dependence of the ϕ function on $\mathbf{A}$, the equation (70) is a nonlinear equation for $\mathbf{A}$ for a given dynamical vector field. However, the class of Hamiltonian equations in Sec. IV A is possibly more interesting for applications, since one does not need to obtain a first integral for it. In contrast, the Hamiltonian description in Sec. IV B must be constructed in terms of a function ψ which was shown to be a first integral for the dynamical system, if $\partial\psi/\partial t = 0$. Therefore, it is more difficult to derive Jacobi structures of the type in Sec. IV B, considering nonintegrable dynamical systems in $\mathbb{R}^3$.

Recently, there has been interest on Leibniz manifolds,[36] that is, manifolds endowed with brackets satisfying the derivation property but not necessarily the Jacobi identity. These Leibniz manifolds provide another possible alternative to generalize Poisson manifolds. It would be interesting to extend the results of the present work to Leibniz structures in $\mathbb{R}^3$.

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Wigner-Moyal description of free variable mass Klein-Gordon fields

J. P. Santos and L. O. Silva[a)]
GoLP/Centro de Física dos Plasmas, Instituto Superior Técnico, 1049-001 Lisboa, Portugal

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A system of coupled kinetic transport equations for the Wigner distributions of a free variable mass Klein-Gordon field is derived. This set of equations is formally equivalent to the full wave equation for electromagnetic waves in nonlinear dispersive media, thus allowing for the description of broadband radiation-matter interactions and the associated instabilities. The standard results for the classical wave action are recovered in the short wavelength limit of the generalized Wigner-Moyal formalism for the wave equation. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The Wigner-Moyal formalism provides an alternative formulation for nonrelativistic Quantum Mechanics, where the wave function is replaced by a quasiparticle distribution function, the Wigner distribution, in phase space, which evolves in time according to a transport equation for the Wigner-Moyal distribution.[1] One of the main advantages of the Wigner-Moyal formalism is the possibility to describe quantum fields with nontrivial statistical properties.[2]

Since the evolution of electromagnetic waves can be described, in the paraxial approximation, by a Schrödinger-like equation it is not surprising that the Wigner-Moyal formalism has been used to describe waves propagating in an inhomogeneous, dispersive, anisotropic and slowly varying in time medium.[3] However, the propagation of electromagnetic waves is, in general, a two mode problem as clearly stated by the second-order time derivative in the wave equation for electromagnetic waves in any medium.[4] Previous works[5] have only dealt with the single mode problem, formally equivalent to propagating a nonlinear Schrödinger-like field, but this approach clearly breaks down when backscattering of the field is an important ingredient for the full dynamics of the system, as it usually occurs in laser/radiation-matter interactions at high intensities.

In this paper, we build an alternative description for the propagation of electromagnetic waves in dispersive and nonlinear media, capable of capturing both forward and backscattering dynamics of the electromagnetic waves, by generalizing the work developed by Javanainen *et al.*[6] to a variable mass problem. In the short wavelength approximation the results regarding the classical wave action (e.g., Ref. 7) are recovered.

We first construct a 2×2 Wigner matrix[6] on the basis of the Hamiltonian form of the Klein-Gordon equation of a charged scalar particle field, introduced by Feshbach and Villars.[8] The diagonal elements describe forward and backward photon densities and off-diagonal elements correspond to cross-densities in phase space. In the corresponding quantum problem, the mass is assumed to be fixed;[6] here a further generalization is performed in order to study the variable mass problem, since the response of the medium (in our case, a cold plasma) exhibits spatial and temporal dependencies. The motivation of this approach is to develop the relativistic phase-space description of the dynamics of Klein-Gordon particles analogously to the Hamiltonian description used earlier by Bialynichi-Birula, Górnicki, and Rafelski for the Dirac particles.[9] The advantage of

[a)]Electronic mail: luis.silva@ist.utl.pt

this method, compared with the manifestly covariant descriptions of Ref. 10, is that a single time parameter is used to describe the dynamics; as a result, the phase space is a genuine dynamical system with its fully prescribed dynamics, and its conservation laws.

In order for the discussion to be self-contained, a brief outline of the Feshbach and Villars Hamiltonian formulation for the Klein-Gordon equation is given in Sec. II, along with the definition of the 2×2 Wigner matrix. In Sec. III, we present the derivation of the generalized Boltzmann-Vlasov equation of motion for the Wigner matrix, and the set of coupled equations for the four real phase-space densities, which are related to the diagonal and cross-densities of the Klein-Gordon particles and their antiparticles, are derived. A physical interpretation of the phase-space densities is provided. In Sec. IV the short wavelength approximation of the Boltzmann-Vlasov equation of motion for the Wigner matrix is performed, and the well-known results of the classical wave action (e.g., Ref. 7 and references therein) are recovered. Finally, in Sec. V, we state our conclusions.

II. THE FESHBACK-VILLARS FORMALISM FOR ELECTROMAGNETIC WAVES AND THE WIGNER MATRIX

The propagation of an electromagnetic wave in a dispersive medium is described by the Klein-Gordon equation:[4]

$$\varepsilon^2\partial_t^2\Phi - \varepsilon^2 c^2\vec{\nabla}_{\mathbf{r}}^2\Phi + \omega_p^2(\mathbf{r},t)\Phi = 0. \tag{1}$$

Here, Φ stands for one of the spatial components of the vector potential, in the Coulomb gauge, and c is the speed of light in vacuum. The CGS system of units is assumed throughout the paper, except where explicitly noted. We observe that ω_p plays the role of the mass of the Klein-Gordon field. For a cold plasma $\omega_p(\mathbf{r},t)$ is the electron plasma frequency, a function of time and space, given by $\omega_p(\mathbf{r},t)=(4\pi e^2 n_e/m_e\gamma)^{1/2}$ where e is the electron charge, m_e is the electron mass, $n_e(\Phi(\mathbf{r},t),\mathbf{r},t)$ is the electron density in the plasma, and $\gamma(\Phi(\mathbf{r},t),\mathbf{r},t)$ is the relativistic Lorentz factor of the plasma electrons. The electron plasma frequency can be an arbitrary function of both time and space, and it may be a source of nonlinearity.[11] Equivalently, Eq. (1) is also the starting point for nonlinear optics,[12] which traditionally uses the index of refraction instead of ω_p to describe the properties of the media.

A distinguishing feature of this problem is the presence of a positive dimensionless parameter ε. This parameter can be taken inversely proportional to the scale size of the spatial inhomogeneities, being small, but finite, for a slowing varying medium. We stress that our discussion is valid for $\varepsilon=1$, which corresponds to the usual wave equation. The inclusion of this small parameter will allow us to easily perform the analysis in the short-wavelength limit in Sec. IV.

To find the Hamiltonian form of Eq. (1), we follow the Feshbach-Villars[8] description, defining

$$\phi,\chi = \frac{1}{2}\left(\Phi \pm \frac{i\varepsilon}{\omega_{p0}}\partial_t\Phi\right), \tag{2}$$

where ω_{p0}^2 is the background electron plasma frequency, independent of time and space, such that $\omega_p^2(\mathbf{r},t)=\omega_{p0}^2+\tilde{\omega}_p^2(\mathbf{r},t)$. Equation (1) can then be written as

$$i\varepsilon\partial_t\phi = -\frac{\varepsilon^2 c^2}{2\omega_{p0}}\vec{\nabla}_{\mathbf{r}}^2(\phi+\chi) + \frac{\tilde{\omega}_p^2}{2\omega_{p0}}(\phi+\chi) + \omega_{p0}\phi, \tag{3a}$$

$$i\varepsilon\partial_t\chi = \frac{\varepsilon^2 c^2}{2\omega_{p0}}\vec{\nabla}_{\mathbf{r}}^2(\phi+\chi) - \frac{\tilde{\omega}_p^2}{2\omega_{p0}}(\phi+\chi) - \omega_{p0}\chi. \tag{3b}$$

There are several ways of separating Eq. (1) in two coupled equations, respecting definitions (2). Equation (3) denotes the correct expansion for the scalar potential, $\tilde{\omega}_p^2$, and guarantees, unlike the prescription proposed in Ref. 6, that the short wavelength limit leads to the standard classical wave action conservation, as shown in Sec. IV.

If we now introduce Ψ, the two-component vector potential, as

$$\Psi = \begin{bmatrix} \phi \\ \chi \end{bmatrix}, \tag{4}$$

Eq. (3) can be rewritten as

$$i\varepsilon\partial_t\Psi = \frac{(\tau_3 + i\tau_2)}{2\omega_{p0}}(-\varepsilon^2 c^2\vec{\nabla}_{\mathbf{r}}^2 + \tilde{\omega}_p^2)\Psi + \omega_{p0}\tau_3\Psi = \mathcal{H}_m\Psi, \tag{5}$$

where $\mathcal{H}_m$ is the Hamiltonian matrix. In Eq. (5), and henceforth, the notation

$$\tau_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \tau_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

$$\tau_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \tau_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{6}$$

is used to represent the Pauli matrices.

Equation (5) is a Schrödinger-like equation. Thus, the usual Wigner formalism can be applied to a 2×2 igner matrix, instead of using the Wigner formalism on a scalar function. Defining the 2×2 Wigner matrix using the Feshbach-Villars representation:[6]

$$W(\mathbf{k},\mathbf{r},t) \equiv \left(\frac{1}{2\pi\varepsilon}\right)^3 \int_{\mathbb{R}^3} d\mathbf{y} e^{i(\mathbf{k}\cdot\mathbf{y})/\varepsilon}\Psi(\mathbf{r}_-,t)\overline{\Psi}(\mathbf{r}_+,t), \tag{7}$$

where $\overline{\Psi} = \Psi^\dagger\tau_3$ denotes the Feshbach-Villars adjoint of the vector potential Ψ, $\mathbf{r}_\pm = \mathbf{r} \pm \mathbf{y}/2$, and $\mathbb{R}^3$ the usual three-dimensional Cartesian space. By construction, W is an Hermitian matrix in the Feshbach-Villars sense, namely $\overline{W} \equiv \tau_3 W^\dagger \tau_3 = W$, and its explicit form can be expressed in terms of the field components ϕ and χ, yielding

$$W = \begin{bmatrix} W_{\phi\phi} & -W_{\phi\chi}^* \\ W_{\phi\chi} & -W_{\chi\chi} \end{bmatrix}, \tag{8}$$

where

$$W_{\phi\phi} = \left(\frac{1}{2\pi\varepsilon}\right)^3 \int_{\mathbb{R}^3} d\mathbf{y} e^{i(\mathbf{k}\cdot\mathbf{y})/\varepsilon}\phi^*(\mathbf{r}_+,t)\phi(\mathbf{r}_-,t), \tag{9a}$$

$$W_{\phi\chi} = \left(\frac{1}{2\pi\varepsilon}\right)^3 \int_{\mathbb{R}^3} d\mathbf{y} e^{i(\mathbf{k}\cdot\mathbf{y})/\varepsilon}\phi^*(\mathbf{r}_+,t)\chi(\mathbf{r}_-,t), \tag{9b}$$

$$W_{\chi\chi} = \left(\frac{1}{2\pi\varepsilon}\right)^3 \int_{\mathbb{R}^3} d\mathbf{y} e^{i(\mathbf{k}\cdot\mathbf{y})/\varepsilon}\chi^*(\mathbf{r}_+,t)\chi(\mathbf{r}_-,t). \tag{9c}$$

It is useful to calculate the equation governing the time evolution of $\overline{\Psi}$. Taking the conjugate transpose of Eq. (5), and multiplying on the right by τ_3, we obtain

$$i\varepsilon\partial_t\overline{\Psi} = -\overline{\Psi}\frac{(\tau_3 + i\tau_2)}{2\omega_{p0}}(-\varepsilon^2 c^2\overleftarrow{\nabla}_{\mathbf{r}}^2 + \tilde{\omega}_p^2) - \overline{\Psi}\tau_3\omega_{p0} = -\overline{\Psi}\mathcal{H}_m, \tag{10}$$

where we used $\tau_i^\dagger = \tau_i, i \in \{0,1,2,3\}$ and $\{\tau_i, \tau_j\} = 2\tau_0\delta_{ij}$, $i,j \in \{1,2,3\}$. Equation (10) demonstrates that the Hamiltonian matrix is not Hermitian. As a consequence the transport equation for the Wigner matrix will have to include both commutators and anticommutators.

III. GENERALIZED BOLTZMANN-VLASOV EQUATION OF MOTION

The equation of motion for the Wigner matrix (7), can be derived from the Schrödinger-type equations (5) and (10) for, respectively, $\Psi(\mathbf{r}_-,t)$ and $\overline{\Psi}(\mathbf{r}_+,t)$, following a standard procedure.[13]

From Eqs. (5), (7), and (10) we obtain

$$\partial_t W(\mathbf{k},\mathbf{r},t) = \mathcal{R}_1 + \mathcal{R}_2 - \frac{i}{\varepsilon}\omega_{p0}[\tau_3, W], \tag{11}$$

where

$$\partial_t W(\mathbf{k},\mathbf{r},t) = \left(\frac{1}{2\pi\varepsilon}\right)^3 \int_{\mathbb{R}^3} \mathrm{d}\mathbf{y} e^{i(\mathbf{k}\cdot\mathbf{y})/\varepsilon}[\partial_t \Psi(\mathbf{r}_-,t)\overline{\Psi}(\mathbf{r}_+,t) + \Psi(\mathbf{r}_-,t)\partial_t\overline{\Psi}(\mathbf{r}_+,t)], \tag{12a}$$

$$\mathcal{R}_1 = \frac{i\varepsilon c^2}{\omega_{p0}}\left(\frac{1}{2\pi\varepsilon}\right)^3 \int_{\mathbb{R}^3} \mathrm{d}\mathbf{y} e^{i(\mathbf{k}\cdot\mathbf{y})/\varepsilon}\left\{(\tau_3 + i\tau_2)\left[\frac{\vec{\nabla}_{\mathbf{r}}^2}{2}\Psi(\mathbf{r}_-,t)\right]\overline{\Psi}(\mathbf{r}_+,t) - \Psi(\mathbf{r}_-,t)\left[\frac{\vec{\nabla}_{\mathbf{r}}^2}{2}\overline{\Psi}(\mathbf{r}_+,t)\right](\tau_3 + i\tau_2)\right\}, \tag{12b}$$

$$\mathcal{R}_2 = \frac{i}{2\varepsilon\omega_{p0}}\left(\frac{1}{2\pi\varepsilon}\right)^3 \int_{\mathbb{R}^3} \mathrm{d}\mathbf{y} e^{i(\mathbf{k}\cdot\mathbf{y})/\varepsilon}[\Psi(\mathbf{r}_-,t)\overline{\Psi}(\mathbf{r}_+,t)(\tau_3 + i\tau_2)\widetilde{\omega}_{p_+}^2 - (\tau_3 + i\tau_2)\widetilde{\omega}_{p_-}^2\Psi(\mathbf{r}_-,t)\overline{\Psi}(\mathbf{r}_+,t)], \tag{12c}$$

where $\widetilde{\omega}_{p_\pm}^2 = \widetilde{\omega}_p^2(\mathbf{r}_\pm,t)$. Note that $[A,B]$ represents the usual commutator between operator A and B, and that we also used the following identities:

$$\vec{\nabla}_{\mathbf{r}_\pm} g(\mathbf{r}_\pm,t) = \vec{\nabla}_{\mathbf{r}} g(\mathbf{r}_\pm,t) = \pm 2\vec{\nabla}_{\mathbf{y}} g(\mathbf{r}_\pm,t), \tag{13}$$

where $g(\mathbf{r},t)$ stands for a first-order differentiable function of $\mathbf{r}$, and an arbitrary function of t.

The first term on the right-hand side of Eq. (11), $\mathcal{R}_1$, is the kinetic contribution for the equation of motion, and it is always present, independently of the potential $\widetilde{\omega}_p^2(\mathbf{r},t)$, whereas the second term, $\mathcal{R}_2$, accounts for the potential contribution. After some lengthy calculations $\mathcal{R}_1$ can also be written as

$$\mathcal{R}_1 = -\frac{c^2\mathbf{k}\cdot\vec{\nabla}_{\mathbf{r}}}{2\omega_{p0}}\{\tau_3 + i\tau_2, W\} - \frac{i}{\varepsilon}[\mathcal{H}_0(\mathbf{k})(\tau_3 + i\tau_2), W] + \mathcal{Q}, \tag{14}$$

where

$$\mathcal{H}_0(\mathbf{k}) = \frac{c^2}{\omega_{p0}}\mathbf{k}^2, \tag{15a}$$

$$\mathcal{Q} = -2\frac{i\varepsilon c^2}{\omega_{p0}}\left(\frac{1}{2\pi\varepsilon}\right)^3 \int_{\mathbb{R}^3} \mathrm{d}\mathbf{y} e^{i(\mathbf{k}\cdot\mathbf{y})/\varepsilon}[(\tau_3 + i\tau_2)\vec{\nabla}_{\mathbf{y}}\Psi(\mathbf{r}_-,t)\cdot\vec{\nabla}_{\mathbf{y}}\overline{\Psi}(\mathbf{r}_+,t) - \vec{\nabla}_{\mathbf{y}}\Psi(\mathbf{r}_-,t)\cdot\vec{\nabla}_{\mathbf{y}}\overline{\Psi}(\mathbf{r}_+,t)(\tau_3 + i\tau_2)] \tag{15b}$$

and $\{A,B\}$ represents the usual anticommutator. Consequently, the equation of motion already denotes the effects of the non-Hermiticity of the Hamiltonian $\mathcal{H}_m$, as previously noted.

The form of Eq. (15b) suggests that a second-order derivative in space, and a commutator must be involved; in fact, $\mathcal{Q}$ can be rewritten as

$$\mathcal{Q} = \frac{i\varepsilon c^2}{\omega_{p0}}\left[(\tau_3 + i\tau_2)\frac{\vec{\nabla}_{\mathbf{r}}^2}{8}, W\right] + \frac{i}{\varepsilon}\left[\frac{1}{2}\mathcal{H}_0(\hat{\mathbf{k}})(\tau_3 + i\tau_2), W\right] \tag{16}$$

leading to

$$\mathcal{R}_1 = -\frac{c^2\mathbf{k}\cdot\vec{\nabla}_{\mathbf{r}}}{2\omega_{p0}}\{\tau_3 + i\tau_2, W\} - \frac{i}{\varepsilon}\left[\frac{1}{2}\mathcal{H}_0(\hat{\mathbf{k}})(\tau_3 + i\tau_2), W\right] \tag{17}$$

with the generalized wave number $\hat{\mathbf{k}}^2 = \mathbf{k}^2 - \varepsilon^2\vec{\nabla}_{\mathbf{r}}^2/4$

To calculate $\mathcal{R}_2$, we observe first that the inverse Fourier transform of the Wigner matrix (7) yields the vector potential matrix $\Psi(\mathbf{r}_+, t)\overline{\Psi}(\mathbf{r}_-, t)$, viz.:

$$\Psi(\mathbf{r}_+, t)\overline{\Psi}(\mathbf{r}_-, t) = \int_{\mathbb{R}^3} \mathrm{d}\mathbf{k}' e^{-i(\mathbf{k}'\cdot\mathbf{y})/\varepsilon} W(\mathbf{k}', \mathbf{r}, t). \tag{18}$$

Combining Eq. (18) and Eq. (12c) leads to

$$\mathcal{R}_2 = \frac{i}{2\varepsilon\omega_{p0}}\left(\frac{1}{2\pi\varepsilon}\right)^3 \int_{\mathbb{R}^3}\mathrm{d}\mathbf{k}' \int_{\mathbb{R}^3}\mathrm{d}\mathbf{y} e^{i[(\mathbf{k}-\mathbf{k}')\cdot\mathbf{y}]/\varepsilon}[W(\mathbf{k}', \mathbf{r}, t)(\tau_3 + i\tau_2)\tilde{\omega}_{p_+}^2 - (\tau_3 + i\tau_2)W(\mathbf{k}', \mathbf{r}, t)\tilde{\omega}_{p_-}^2]. \tag{19}$$

Since $\tilde{\omega}_{p_\pm}^2 = e^{\pm i\mathbf{y}/2i\cdot\vec{\nabla}_{\mathbf{r}}}\tilde{\omega}_p^2(\mathbf{r}, t)$, and in the case of a sufficient regular function g:[13]

$$\int_{-\infty}^{+\infty} e^{iyk'} g(iy)F(k')\mathrm{d}k' = \int_{-\infty}^{+\infty} e^{iyk'} g\left(-\frac{\partial}{\partial k'}\right)F(k')\mathrm{d}k'. \tag{20}$$

Thus, $\mathcal{R}_2$ can be expressed as

$$\mathcal{R}_2 = \frac{i\tilde{\omega}_p^2(\mathbf{r}, t)}{2\varepsilon\omega_{p0}}\cos\left(\frac{\varepsilon}{2}\overleftarrow{\nabla}_{\mathbf{r}}\cdot\vec{\nabla}_{\mathbf{k}}\right)[W, (\tau_3 + i\tau_2)] + \frac{\tilde{\omega}_p^2(\mathbf{r}, t)}{2\varepsilon\omega_{p0}}\sin\left(\frac{\varepsilon}{2}\overleftarrow{\nabla}_{\mathbf{r}}\cdot\vec{\nabla}_{\mathbf{k}}\right)\{W, (\tau_3 + i\tau_2)\}. \tag{21}$$

Combining Eqs. (17) and (21) in Eq. (11), the generalized Boltzmann-Vlasov equation of motion for the Wigner matrix is

$$\partial_t W(\mathbf{k}, \mathbf{r}, t) + (\hat{D} - \hat{S})\tfrac{1}{2}\{\tau_3 + i\tau_2, W(\mathbf{k}, \mathbf{r}, t)\} + \frac{i}{\varepsilon}[\mathcal{H}_0(\hat{\mathbf{k}}) + \hat{C}]\frac{1}{2}[(\tau_3 + i\tau_2), W(\mathbf{k}, \mathbf{r}, t)] + \frac{i\omega_{p0}}{\varepsilon}[\tau_3, W(\mathbf{k}, \mathbf{r}, t)] = 0, \tag{22}$$

where

$$\hat{D} = \frac{c^2}{\omega_{p0}}\mathbf{k}\cdot\vec{\nabla}_{\mathbf{r}}, \quad \hat{S} = \frac{\tilde{\omega}_p^2(\mathbf{r}, t)}{\varepsilon\omega_{p0}}\sin\left(\frac{\varepsilon}{2}\overleftarrow{\nabla}_{\mathbf{r}}\cdot\vec{\nabla}_{\mathbf{k}}\right), \quad \hat{C} = \frac{\tilde{\omega}_p^2(\mathbf{r}, t)}{\omega_{p0}}\cos\left(\frac{\varepsilon}{2}\overleftarrow{\nabla}_{\mathbf{r}}\cdot\vec{\nabla}_{\mathbf{k}}\right). \tag{23}$$

In the argument of the trigonometric functions, the operator $\overleftarrow{\nabla}_{\mathbf{r}}$ acts on the electron plasma frequency, and the operator $\vec{\nabla}_{\mathbf{k}}$ acts on the components of the Wigner matrix $W(\mathbf{k}, \mathbf{r}, t)$. The matrix operator $\mathcal{H}_0(\hat{\mathbf{k}})$ reduces, in the short wavelength approximation, to the free particle Hamiltonian $\mathcal{H}_0(\mathbf{k})$. Both $\hat{C}$ and $\hat{S}$ can be expanded in a power series, containing only even powers of ε and, therefore, $\hat{S}$ and $\hat{C}$ in Eqs. (23) have regular limits when $\varepsilon \to 0$.

The operators (23) can also be cast in an integral form, which is more useful for numerical implementations:

$$\hat{C},\hat{S}f(\mathbf{k},\mathbf{r},t) = \int_{\mathbb{R}^3} d\mathbf{k}' \mathcal{K}^{\pm}(\mathbf{k}-\mathbf{k}',\mathbf{r},t) f(\mathbf{k}',\mathbf{r},t), \tag{24}$$

where

$$\mathcal{K}^{\pm}(\mathbf{k},\mathbf{r},t) = \frac{i}{2\varepsilon\omega_{p0}}\left(\frac{1}{2\pi\varepsilon}\right)^3 \int_{\mathbb{R}^3} d\mathbf{y} e^{i(\mathbf{k}\cdot\mathbf{y})/\varepsilon}(\tilde{\omega}_{p_+}^2 - \tilde{\omega}_{p_-}^2). \tag{25}$$

Equation (22) describes the equation of motion for the Wigner matrix, and therefore it describes the transport of W in phase space. Even though it is formally equivalent to the wave equation (1), it is more useful to represent our field in terms of real Wigner distributions. Since the Pauli matrices form a basis for the 2×2 complex matrix space, W admits the expansion

$$W = \tfrac{1}{2}(\tau_0 W_0 + i\tau_1 W_1 - i\tau_2 W_2 + \tau_3 W_3), \tag{26}$$

where all the $W_i, i \in \{0,1,2,3\}$ are real distributions. Since W is not Hermitian, an expansion in the form $W=\Sigma_{i=0}^{3} W_i \tau_i$, where all the $W_i, i \in \{0,1,2,3\}$, are real functions, is not possible. Nevertheless, W is Hermitian in the Feshbach-Villars sense and the natural expansion with real coefficients is given by Eq. (26). It is easily seen that $W_0 = W_{\phi\phi} - W_{\chi\chi}$, $W_1 = 2\,\mathrm{Im}(W_{\phi\chi})$, $W_2 = 2\,\mathrm{Re}(W_{\phi\chi})$, and $W_3 = W_{\phi\phi} + W_{\chi\chi}$. The physical meaning of $W_2(\mathbf{k},\mathbf{r},t) + W_3(\mathbf{k},\mathbf{r},t)$ is of interest, because it is related to the Wigner function of the vector potential Φ. In fact, with

$$W_{\Phi\Phi}(\mathbf{k},\mathbf{r},t) = \left(\frac{1}{2\pi\varepsilon}\right)^3 \int_{\mathbb{R}^3} d\mathbf{y} e^{i(\mathbf{k}\cdot\mathbf{y})/\varepsilon} \Phi^*(\mathbf{r}_+,t)\Phi(\mathbf{r}_-,t), \tag{27}$$

where $\Phi^*(\mathbf{r},t)$ stands for the complex conjugate of $\Phi(\mathbf{r},t)$, then

$$W_{\Phi\Phi} = W_2(\mathbf{k},\mathbf{r},t) + W_3(\mathbf{k},\mathbf{r},t) = W_{\phi\phi} + W_{\chi\chi} + 2\,\mathrm{Re}(W_{\phi\chi}). \tag{28}$$

The vector potential is completely characterized by the distribution function $W_{\Phi\Phi}$, which can be calculated for different electromagnetic field configurations. Furthermore, there is a one-to-one correspondence between the distribution $W_{\Phi\Phi}$, and the vector potential Φ, apart from a constant phase shift ϕ_0. Defining the inverse Fourier transform of $W_{\Phi\Phi}$, as

$$\mathcal{F}_{\mathbf{k},\mathbf{y}}^{-1}(\mathbf{y},\mathbf{r},t) = \int_{\mathbb{R}^3} d\mathbf{k} e^{-i(\mathbf{k}\cdot\mathbf{y})/\varepsilon}[W_2(\mathbf{k},\mathbf{r},t) + W_3(\mathbf{k},\mathbf{r},t)], \tag{29}$$

$\Phi(\mathbf{r},t)$ is determined by

$$\Phi(\mathbf{r},t) = \frac{\mathcal{F}_{\mathbf{k},\mathbf{r}}^{-1}\left(\mathbf{r},\frac{\mathbf{r}}{2},t\right)}{\sqrt{\mathcal{F}_{\mathbf{k},\mathbf{r}}^{-1}(0,0,t)}} e^{i\phi_0}. \tag{30}$$

In Eq. (30) ϕ_0 is determined from the initial conditions, and the inverse Fourier transform of the Wigner function is assumed to be different from 0 at $t=0$.

The imaginary part of the cross-density $W_{\phi\chi}, W_1$, is the classical equivalent of the quantum "Zitterbewegung,"[6] and it represents the interference between forward and backward photons. For Wigner matrices of a free forward plane wave or a free backward plane wave, of momentum $\mathbf{k}_0, W_1$ is zero.

As a simple illustration, let us consider a vector potential described by the superposition of two plane waves $\Phi(\mathbf{r},t) = \Phi_0 \exp[i(\mathbf{k}_0\cdot\mathbf{r} - \omega_0 t)] + \Phi_1 \exp[i(\mathbf{k}_1\cdot\mathbf{r} - \omega_1 t)]$, propagating in an uniform medium with $\tilde{\omega}_p^2(\mathbf{r},t) = 0$. For this field:

$$\phi(\mathbf{r},t)=\frac{\Phi_0}{2}\left(\frac{\omega_{p0}+\omega_0}{\omega_{p0}}\right)e^{i(\mathbf{k}_0\cdot\mathbf{r}-\omega_0 t)}+\frac{\Phi_1}{2}\left(\frac{\omega_{p0}+\omega_1}{\omega_{p0}}\right)e^{i(\mathbf{k}_1\cdot\mathbf{r}-\omega_1 t)}, \tag{31a}$$

$$\chi(\mathbf{r},t)=\frac{\Phi_0}{2}\left(\frac{\omega_{p0}-\omega_0}{\omega_{p0}}\right)e^{i(\mathbf{k}_0\cdot\mathbf{r}-\omega_0 t)}+\frac{\Phi_1}{2}\left(\frac{\omega_{p0}-\omega_1}{\omega_{p0}}\right)e^{i(\mathbf{k}_1\cdot\mathbf{r}-\omega_1 t)}. \tag{31b}$$

The corresponding components of the Wigner matrix are

$$W_{\phi\phi}(\mathbf{k},\mathbf{r},t)=\frac{(\omega_0+\omega_{p0})^2}{4\omega_{p0}^2}\Phi_0^2\delta(\mathbf{k}-\mathbf{k}_0)+\frac{(\omega_1+\omega_{p0})^2}{4\omega_{p0}^2}\Phi_1^2\delta(\mathbf{k}-\mathbf{k}_1)+\frac{(\omega_{p0}+\omega_0)(\omega_{p0}+\omega_1)}{2\omega_{p0}^2}\Phi_0\Phi_1\cos(\eta)\delta\left(\mathbf{k}-\frac{\mathbf{k}_0+\mathbf{k}_1}{2}\right), \tag{32a}$$

$$W_{\phi\chi}(\mathbf{k},\mathbf{r},t)=-\frac{\mathbf{k}_0^2c^2}{4\omega_{p0}^2}\Phi_0^2\delta(\mathbf{k}-\mathbf{k}_0)-\frac{\mathbf{k}_1^2c^2}{4\omega_{p0}^2}\Phi_1^2\delta(\mathbf{k}-\mathbf{k}_1)+\frac{\Phi_0\Phi_1}{2}\times\left\{\left[1-\frac{\omega_0\omega_1}{\omega_{p0}^2}\right]\cos(\eta)+i\frac{\omega_0-\omega_1}{\omega_{p0}}\sin(\eta)\right\}\delta\left(\mathbf{k}-\frac{\mathbf{k}_0+\mathbf{k}_1}{2}\right), \tag{32b}$$

$$W_{\chi\chi}(\mathbf{k},\mathbf{r},t)=\frac{(\omega_0-\omega_{p0})^2}{4\omega_{p0}^2}\Phi_0^2\delta(\mathbf{k}-\mathbf{k}_0)+\frac{(\omega_1-\omega_{p0})^2}{4\omega_{p0}^2}\Phi_1^2\delta(\mathbf{k}-\mathbf{k}_1)+\frac{(\omega_{p0}-\omega_0)(\omega_{p0}-\omega_1)}{2\omega_{p0}^2}\Phi_0\Phi_1\cos(\eta)\delta\left(\mathbf{k}-\frac{\mathbf{k}_0+\mathbf{k}_1}{2}\right), \tag{32c}$$

where $\eta=\Delta_{\mathbf{k}}\cdot\mathbf{r}-\Delta_\omega t$, $\Delta_{\mathbf{k}}=\mathbf{k}_1-\mathbf{k}_0$, $\Delta_\omega=\omega_1-\omega_0$, $\delta(\mathbf{k})$ represents the Dirac delta distribution and $\omega_{0,1}=\sqrt{\mathbf{k}_{0,1}^2c^2+\omega_{p0}^2}$. The presence of two photon beams associated with the two plane waves is easily seen. Furthermore there is a "third wave" which results from the interference between the two plane waves. In this case, W_1 is different from zero, since it accounts for the interference between forward and backward photons. W_0 is associated with the effective photon density, i.e., it is positive when the forward photon density is bigger than the backward photon density.

Using the decomposition $W=\mathrm{Re}(W)+i\,\mathrm{Im}(W)$ in Eq. (22), one can derive a set of two coupled real equations:

$$\partial_t 2\,\mathrm{Re}(W)+(\hat{D}-\hat{S})\frac{1}{2}\{\tau_3+i\tau_2,2\,\mathrm{Re}(W)\}-\frac{1}{\varepsilon}[\mathcal{H}_0(\hat{\mathbf{k}})+\hat{C}]\frac{1}{2}[(\tau_3+i\tau_2),\tau_1]W_1-\frac{\omega_{p0}}{\varepsilon}[\tau_3,\tau_1]W_1=0, \tag{33a}$$

$$\partial_t(\tau_1W_1)+\frac{1}{\varepsilon}[\mathcal{H}_0(\hat{\mathbf{k}})+\hat{C}]\frac{1}{2}[(\tau_3+i\tau_2),2\,\mathrm{Re}(W)]+\frac{\omega_{p0}}{\varepsilon}[\tau_3,2\,\mathrm{Re}(W)]=0, \tag{33b}$$

where we have used $\{\tau_i,\tau_j\}=2\tau_0\delta_{ij}$, $i,j\in\{1,2,3\}$ and $2\,\mathrm{Im}(W)=\tau_1W_1$. From expansion (26) it is easily seen that $2\,\mathrm{Re}(W)=\tau_0W_0-i\tau_2W_2+\tau_3W_3$ and, therefore, the four real phase-space densities obey the set of transport equations:

$$\partial_t W_0+(\hat{D}-\hat{S})(W_2+W_3)=0, \tag{34a}$$

$$\partial_t W_1-\frac{1}{\varepsilon}[\mathcal{H}_0(\hat{\mathbf{k}})+\hat{C}](W_2+W_3)-\frac{2}{\varepsilon}\omega_{p0}W_2=0, \tag{34b}$$

$$\partial_t W_2 - (\hat{D} - \hat{S}) W_0 + \frac{1}{\varepsilon}[\mathcal{H}_0(\hat{\mathbf{k}}) + \hat{C}] W_1 + \frac{2}{\varepsilon}\omega_{p0} W_1 = 0, \tag{34c}$$

$$\partial_t W_3 + (\hat{D} - \hat{S}) W_0 - \frac{1}{\varepsilon}[\mathcal{H}_0(\hat{\mathbf{k}}) + \hat{C}] W_1 = 0. \tag{34d}$$

The set of equations (34) is the main result of this paper. With the appropriate definitions for W_i, the set of equations (34) is formally equivalent to Eq. (1), and therefore opens the way to an appropriate description of the propagation of electromagnetic waves with arbitrary spectral content in nonlinear dispersive media.[14]

IV. THE SHORT WAVELENGTH LIMIT

We now examine the short wavelength limit of the Boltzmann-Vlasov equation of motion (22) by examining the limit $\varepsilon \to 0$. In order to consider the short wavelength limit of (22) we first observe that

$$\lim_{\varepsilon\to 0} \hat{S} = \frac{\vec{\nabla}_{\mathbf{r}} \tilde{\omega}_p^2(\mathbf{r},t)}{2\omega_{p0}} \cdot \vec{\nabla}_{\mathbf{k}}, \quad \lim_{\varepsilon\to 0} \hat{C} = \frac{\tilde{\omega}_p^2(\mathbf{r},t)}{\omega_{p0}}, \quad \lim_{\varepsilon\to 0} \hat{\mathbf{k}} = \mathbf{k}. \tag{35}$$

Let the superscript (0) represent any function in the short wavelength limit. In the limit $\varepsilon \to 0$, the set of equations (33) converges to a meaningful limit only if $W_1 \to 0$ faster than $\varepsilon \to 0$; hence $W^{(0)}$ must be real, i.e., $W_1^{(0)} = 0$. The same conclusions can also be obtained using the coarse-graining technique introduced by Shin and Rafelski.[15] Using the results in (35) and the previous considerations, Eq. (33) can be written, in the $\epsilon \to 0$ limit, as

$$\partial_t W^{(0)} + \left[\frac{c^2}{\omega_{p0}} \mathbf{k} \cdot \vec{\nabla}_{\mathbf{r}} - \frac{1}{2} \frac{\vec{\nabla}_{\mathbf{r}} \tilde{\omega}_p^2(\mathbf{r},t)}{\omega_{p0}} \cdot \vec{\nabla}_{\mathbf{k}} \right] \frac{1}{2} \{ (\tau_3 + i\tau_2), W^{(0)} \} = 0, \tag{36a}$$

$$\left[(c^2\mathbf{k}^2 + \tilde{\omega}_p^2(\mathbf{r},t)) \frac{(\tau_3 + i\tau_2)}{2\omega_{p0}} + \omega_{p0}\tau_3, W^{(0)} \right] = 0. \tag{36b}$$

Our first goal now is to find a matrix operator that transforms Eq. (36b) into a necessary condition for $W' = U^{-1} W^{(0)} U$ to be diagonal. This will significantly reduce the amount of calculations needed to identify the form of the classical wave action, since the system will be reduced to two degrees of freedom. The matrix operator that performs this task is

$$U(\zeta) = e^{-\tau_1 \zeta}, \tag{37}$$

where

$$\zeta = \frac{1}{2} \log \left[\frac{\omega(\mathbf{k},\mathbf{r},t)}{\omega_{p0}} \right],$$

and with $\omega(\mathbf{k},\mathbf{r},t) = \sqrt{\mathbf{k}^2 c^2 + \omega_{p0}^2 + \tilde{\omega}_p^2(\mathbf{r},t)}$. On performing the similarity transformation induced by U in Eq. (36b), we obtain

$$\omega(\mathbf{k},\mathbf{r},t)[\tau_3, W'] = 0, \tag{38}$$

where

$$U^{-1}(\tau_3 + i\tau_2) U = \frac{\omega_{p0}}{\omega(\mathbf{k},\mathbf{r},t)} (\tau_3 + i\tau_2). \tag{39}$$

From Eq. (38) we can see that W' must be a linear combination of τ_0 and τ_3, since all the other Pauli matrices do not commute with τ_3. One can choose this linear combination to be parametrized by two real functions f and g, such that

$$W' = \frac{f-g}{2}\tau_0 + \frac{f+g}{2}\tau_3. \tag{40}$$

Performing the transformation (37) in Eq. (36a), with W' given by Eq. (40), the diagonal part leads to

$$\partial_t f(\mathbf{k},\mathbf{r},t) + \frac{c^2\mathbf{k}}{\omega(\mathbf{k},\mathbf{r},t)}\cdot\vec{\nabla}_{\mathbf{r}} f(\mathbf{k},\mathbf{r},t) - \frac{1}{2}\frac{\vec{\nabla}_{\mathbf{r}}\tilde{\omega}_p^2(\mathbf{r},t)}{\omega_{p0}}\cdot\vec{\nabla}_{\mathbf{k}} f(\mathbf{k},\mathbf{r},t) = 0, \tag{41a}$$

$$\partial_t g(\mathbf{k},\mathbf{r},t) - \frac{c^2\mathbf{k}}{\omega(\mathbf{k},\mathbf{r},t)}\cdot\vec{\nabla}_{\mathbf{r}} g(\mathbf{k},\mathbf{r},t) + \frac{1}{2}\frac{\vec{\nabla}_{\mathbf{r}}\tilde{\omega}_p^2(\mathbf{r},t)}{\omega_{p0}}\cdot\vec{\nabla}_{\mathbf{k}} g(\mathbf{k},\mathbf{r},t) = 0. \tag{41b}$$

Equations (41a) and (41b) clearly resemble the classical wave action conservation for forward and backward radiation, respectively.[7] However to confirm this fact, the relation between f, g, and $W^{(0)}_{\Phi\Phi}$ needs to be established. On one hand, we know that $\mathrm{Re}(W)$ is $1/2(\tau_0 W_0 - i\tau_2 W_2 + \tau_3 W_3)$. On the other hand, in the short wavelength limit, $\mathrm{Re}(W)$ is $W^{(0)}$. Thus, we conclude that

$$W^{(0)} = \tfrac{1}{2}(\tau_0 W_0^{(0)} - i\tau_2 W_2^{(0)} + \tau_3 W_3^{(0)}). \tag{42}$$

Performing the transformation induced by U in Eq. (42) we obtain

$$2W' = (f-g)\tau_0 + (f+g)\tau_3 = U^{-1}(\tau_0 W_0^{(0)} - i\tau_2 W_2^{(0)} + \tau_3 W_3^{(0)})U, \tag{43}$$

which after some manipulation can be reduced to the set of algebraic equations:

$$f - g = W_0^{(0)}, \tag{44a}$$

$$f + g = \frac{R^2+1}{2R}W_3^{(0)} + \frac{R^2-1}{2R}W_2^{(0)}, \tag{44b}$$

$$0 = \frac{R^2+1}{2R}W_2^{(0)} + \frac{R^2-1}{2R}W_3^{(0)}, \tag{44c}$$

where we have defined $R = \omega(\mathbf{k},\mathbf{r},t)/\omega_{p0}$. From Eq. (44), one infers

$$f + g = \frac{\omega(\mathbf{k},\mathbf{r},t)}{\omega_{p0}}W^{(0)}_{\Phi\Phi} = \frac{c^2}{2\omega_{p0}}J(\mathbf{k},\mathbf{r},t), \tag{45}$$

where $J(\mathbf{k},\mathbf{r},t)$ represents the classical wave action, as defined in Ref. 7. Thus, in the short wavelength limit, Eqs. (41a) and (41b) state that the classical wave action, $J(\mathbf{k},\mathbf{r},t)$, is conserved along the geometrical optics ray, independent of the adiabaticity condition.[16]

To conclude the discussion of the short wavelength limit, we observe that when $\varepsilon \to 0$ in Eq. (3) χ is negligible, since reflected waves are exponentially small.[17] Dropping the small component χ in Eq. (3) and eliminating the ω_{p0} term by setting $\phi(\mathbf{r},t) = \tilde{\phi}(\mathbf{r},t)\exp(-i\omega_{p0}t/\varepsilon)$, yields the paraxial wave equation:[18]

$$2i\omega_{p0}\varepsilon\partial_t\tilde{\phi} = -\varepsilon^2 c^2\vec{\nabla}_{\mathbf{r}}^2\tilde{\phi} + \tilde{\omega}_p^2\tilde{\phi}. \tag{46}$$

This equation is formally equivalent to the Schrödinger equation, and the Wigner-Moyal formalism can be followed in a straightforward way. This is the approach followed by Besieris and

Tappert.[2,3] As expected, this path also leads to classical wave action conservation in the same limit we have explored here, but fails to capture the dynamics of the backscattered component of the radiation field.

V. CONCLUSIONS

In order to establish a description of the propagation of electromagnetic waves in nonlinear dispersive media, including the two modes described by the wave equation, we have employed the Feshbach-Villars description of the Klein-Gordon field with a variable mass term, and the corresponding 2×2 Wigner matrix. The equations of motion for the Wigner matrix lead to a set of four coupled equations for four real phase-space densities, whose physical meanings are clearly identified. The general Boltzmann-Vlasov equations of motion account for the backscattered waves, and for the interference between forward and backward radiation. These equations replace the standard Wigner-Moyal description of classical fields,[3] generalizing it to the two mode problem with variable mass terms, and are formally equivalent to the full wave equation.

The short wavelength limit of the Boltzmann-Vlasov equations of motion was considered, and it was shown they reduce to uncoupled equations for the forward and backward radiation phase-space densities. In this limit, the standard results regarding wave action conservation,[7] are recovered.

The formalism introduced here provides a complete description for the electromagnetic field in nonlinear dispersive media, and opens the way to the description of broadband radiation driven parametric instabilities in nonlinear media. Applications of this formalism will be presented elsewhere.

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Rigid body mechanics in Galilean spacetimes

Ajit Bhand[a] and Andrew D. Lewis
Department of Mathematics and Statistics, Queen's University, Kingston, Ontario K7L3N6, Canada

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An observer-independent formulation of rigid body dynamics is provided in the general setting of a Galilean spacetime. The equations governing the motion of a rigid body undergoing a rigid motion in a Galilean spacetime are derived on the basis of the principle of conservation of spatial momentum. The formulation of rigid body dynamics is then studied in the presence of an observer. It is seen that an observer defines a connection such that there exist rigid motions that are horizontal with respect to this connection that give the same physical motion of the rigid body, and for which the general equations of motion are exactly the usual Euler equations for a rigid body undergoing rigid motion. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The main aim of this paper is to understand the dynamics of a rigid body in the general framework of a Galilean spacetime. We study how the physical motion of a rigid body is related to "rigid motions"—the set of mappings belonging to the group of Galilean transformations from a Galilean spacetime to itself, called the Galilean group. We present a new formulation of rigid body dynamics that is independent of an observer. Note that the momentum associated with a particle undergoing motion in a Galilean spacetime is thought of as observer-dependent quantity in the literature (see, for example, Ref. 1). In this paper we take the view that momentum is an intrinsic property of a rigid body in motion, and that it is possible to define it without using any external structure. An observer merely affects the way the momentum is *measured*.

The problem of deriving equations of motion for a rigid body in a Newtonian setting has a rich history. Galileo (1564–1642) carried out the first systematic study of rigid bodies in motion. Newton (1643–1727) built on the foundations laid by Galileo, and came up with equations of motion for a particle in an inertial frame. Later on, Euler (1703–1783) derived the equations of motion for a rigid body fixed at a point in $\mathbb{R}^3$. A modern treatment of this subject, from a general point of view of mechanics on Lie groups, can be found in Refs. 2 and 3. The role of the Galilean structure of the Newtonian spacetime has been understood in the case of the dynamics of a particle.[1,3] A Galilean covariant formulation of the classical mechanics of a single particle has been studied in Ref. 4, and, of course, the dynamics of a rigid body in a fixed Galilean frame has been investigated quite thoroughly.[3,5] However, to our knowledge, the role played by the Galilean structure has not been explained for *rigid body* mechanics. Unlike a particle or a rigid body fixed at a point in $\mathbb{R}^3$, in the general setting of a Galilean spacetime, there does not exist an exact correspondence between rigid motions and physical motions of a rigid body. We address this issue in detail and derive the "Galilean-Euler equations" for a rigid body.

We also show that an observer in a Galilean spacetime, apart from providing a reference frame for observing Newton's laws, also provides an isomorphism from the "abstract" Galilean group to the "standard" or "canonical" Galilean group which consists of rotations, spatial translations, uniform velocity boosts, and time translations. Furthermore, an observer defines a connection such

[a]Electronic mail: ajit@mast.queensu.ca

that, for any given rigid motion, there exists a rigid motion that is horizontal with respect to this connection that gives the same physical motion of the body as the given rigid motion, and for which the generalized equations of motion reduce to the usual Euler equations for a rigid body.

It should be noted that notions of Galilean spacetimes more general than ours have also been studied in the literature. For example, the full machinery of affine differential geometry has been used in Ref. 6 (see also Ref. 7) while a notion of "inertial relations" has been used in Refs. 8–10 to characterize more general Galilean spacetimes.

It is also worth noting that Souriau's approach[11] is different from ours. In particular, he considers a symplectic formulation and his definition of momentum is based on the "Lagrange two-form." Souriau also works with the canonical Galilean group, so obscuring the role of the observer.

This paper is organized as follows. In Sec. II, we present the mathematical preliminaries relevant to our investigation. Several important concepts like affine spaces and subspaces, observers, Galilean spacetimes, and the Galilean group are introduced and their various properties are described. The notion of a rigid body, along with its attendant features, is introduced in Sec. III. In particular, the inertia tensor of a rigid body is defined and its properties are thoroughly explained. In Sec. IV, the structure of the canonical, as well as the abstract, Galilean group is investigated in detail. It is shown that an observer induces an isomorphism between the Galilean group and the canonical group. Next, "canonical velocities" are defined. These are curves in the Lie algebra of the Galilean group. With this background, we first look at rigid motions in Sec. V. Various quantities associated with a rigid motion, such as the body and spatial linear and angular velocities, are defined. Throughout this section, the treatment is observer-independent. The discussion then focuses on angular and spatial momenta, and finally the generalized equations of motion (called the Galilean-Euler equations) for a rigid body are derived. In Sec. VI, the formulation presented in Sec. V is studied in the *presence* of an observer. It is shown that, in such a case, we recover the familiar quantities associated with the classical treatment of rigid body mechanics. The Galilean-Euler equations are also studied in the presence of an observer, and the connection induced by the observer (called the Galilean connection) is defined. It is shown that, for each constant velocity boost, we recover the classical Euler equations for a rigid body.

II. GALILEAN SPACETIME

In this section, we present the mathematical background and introduce the notation to be used in the following sections. In Sec. II A, we define affine spaces and subspaces; the principle objects of interest in this paper. In Sec. II B, we introduce the notion of a Galilean spacetime and describe the affine spaces naturally associated with it. We also introduce the set of Galilean velocities. Next, we define observers in a Galilean spacetime and discuss their properties. Finally, in Sec. II E, we define the Galilean group of a Galilean spacetime and introduce the fundamental maps associated with a Galilean mapping.

A. Affine spaces

In this section, we define affine spaces and subspaces, and record some of their properties. We refer to Ref. 12 for more details.

Definition 2.1: Let V be an $\mathbb{R}$-vector space. An *affine space* modeled on V is a pair $(\mathcal{A}, \phi)$ where $\mathcal{A}$ is a set and $\phi: V \times \mathcal{A} \to \mathcal{A}$ is a map with the following properties:

(i) for every $x, y \in \mathcal{A}$, there exists $v \in V$ such that $y = \phi(v, x)$;
(ii) $\phi(v, x) = x$ for every $x \in \mathcal{A}$ implies that $v = 0$;
(iii) $\phi(0, x) = x$, for each $x \in \mathcal{A}$;
(iv) $\phi(u + v, x) = \phi(u, \phi(v, x))$.

We shall now cease to use the map ϕ and instead use the more suggestive notation $\phi(v, x) = v + x$. By definition, if $x, y \in \mathcal{A}$, there exists a unique $v \in V$ such that $y = v + x$. In this case we shall

denote $v=y-x$. By a slight abuse of notation, we shall denote an affine space $(\mathcal{A},\phi)$ simply by $\mathcal{A}$. If $\mathcal{A}$ is an affine space modeled on V and we fix a point $x\in\mathcal{A}$, then $\mathcal{A}$ is isomorphic to the vector space V. We denote this vector space by $\mathcal{A}_x$.

Definition 2.2: Let $\mathcal{A}$ and $\mathcal{B}$ be affine spaces. A map $f:\mathcal{A}\to\mathcal{B}$ is an *affine map* if, for each $x\in\mathcal{A}$, the map f is an $\mathbb{R}$-linear map between the vector spaces $\mathcal{A}_x$ and $\mathcal{B}_{f(x)}$.

A subset $\mathcal{B}$ of an affine space modeled on V is an *affine subspace* if there is a subspace U of V with the property that $y-x\in U$ for every $x,y\in\mathcal{B}$. In this case, $\mathcal{B}$ is itself an affine space modeled on U. It can be shown that if $\mathcal{B}$ is an affine subspace of $\mathcal{A}$, then there exists a subspace U of V such that, for any fixed $x\in\mathcal{B}$, we have $\mathcal{B}=\{u+x\,|\,u\in U\}$.

B. Time and distance

We begin by giving the basic definition of a Galilean spacetime and by providing meaning to the intuitive notions of time and distance.

Definition 2.3: A *Galilean spacetime* is a quadruple $\mathcal{G}=(\mathcal{E},V,g,\tau)$ where

(i) V is a four-dimensional $\mathbb{R}$-vector space,
(ii) $\tau:V\to\mathbb{R}$ is a surjective linear map called the *time map*,
(iii) g is an inner product on $\ker(\tau)$, and
(iv) $\mathcal{E}$ is an affine space modeled on V.

Points in $\mathcal{E}$ are called *events*—thus $\mathcal{E}$ is a model for the spatiotemporal world of Newtonian mechanics. With the time map, we may measure the time between two events $x_1,x_2\in\mathcal{E}$ as $\tau(x_2-x_1)$. Events $x_1,x_2\in\mathcal{E}$ are called *simultaneous* if $\tau(x_2-x_1)=0$; that is, if $x_2-x_1\in\ker(\tau)$.

We may define the *distance* between simultaneous events $x_1,x_2\in\mathcal{E}$ to be equal to $\sqrt{g(x_2-x_1,x_2-x_1)}$. Note that this method for defining distance does not allow us to measure distances between events that are *not* simultaneous. In particular, it does not make sense to talk about two nonsimultaneous events as occurring in the same place.

Simultaneity is an equivalence relation on $\mathcal{E}$ and the quotient we denote by $I_{\mathcal{G}}=\mathcal{E}/\sim$, with $\sim$ denoting the relation of simultaneity. $I_{\mathcal{G}}$ is simply the collection of equivalence classes of simultaneous events. We call it the *set of instants*. We denote by $\pi_{\mathcal{G}}:\mathcal{E}\to I_{\mathcal{G}}$ the canonical projection.

For $s\in I_{\mathcal{G}}$, we denote by $\mathcal{E}(s)$ the collection of events $x\in\mathcal{E}$ with the property that $\pi_{\mathcal{G}}(x)=s$. Thus events in $\mathcal{E}(s)$ are simultaneous. We next denote by $V_{\mathcal{G}}$ the vectors $v\in V$ for which $\tau(v)=1$. We call vectors in $V_{\mathcal{G}}$ *Galilean velocities*. The following result is easy to prove.

Proposition 2.4: The following statements hold:

(i) *for each $s\in I_{\mathcal{G}}$, $\mathcal{E}(s)$ is a three-dimensional affine space modeled on* $\ker(\tau)$*;*
(ii) *$I_{\mathcal{G}}$ is a one-dimensional affine space modeled on* $\mathbb{R}$*;*
(iii) *$V_{\mathcal{G}}$ is an affine space modeled on* $\ker(\tau)$.

C. Observers

An observer is to be thought of intuitively as someone who is present at each instant. Such an observer should be moving at a "uniform velocity." Note that, in a Galilean spacetime, the notion of "stationarity" makes no sense. We now provide our definition of an observer.

Definition 2.5: An *observer* in a Galilean spacetime $\mathcal{G}=(\mathcal{E},V,g,\tau)$ is a one-dimensional affine subspace $\mathcal{O}$ of $\mathcal{E}$ with the property that $\pi_{\mathcal{G}}|\mathcal{O}$ is surjective.

The definition thus requires that $\mathcal{O}$ not be comprised entirely of simultaneous events. As a consequence of the definition, we have the following result.

Proposition 2.6: If $\mathcal{O}$ is an observer in a Galilean spacetime $\mathcal{G}=(\mathcal{E},V,g,\tau)$, then, for each $s_0\in I_{\mathcal{G}}$, there exists a unique point $x_0\in\mathcal{O}\cap\mathcal{E}(s_0)$.

Proof: Given $s_0\in I_{\mathcal{G}}$, there exists $x_0\in\mathcal{O}$ such that $\pi_{\mathcal{G}}(x_0)=s_0$. Since $\mathcal{O}$ is a one-dimensional affine space with the property that $\pi_{\mathcal{G}}|\mathcal{O}$ is surjective, there exists a one-dimensional subspace $W\subset V$ such that

$$\mathcal{O} = (w + x_0 | w \in W),$$

where W is not contained in $\ker(\tau)$. By construction, $x_0 \in \mathcal{E}(s_0) \cap \mathcal{O}$. This means that, for each $s_0 \in I_{\mathcal{G}}$, the intersection $\mathcal{E}(s_0) \cap \mathcal{O}$ is nonempty. Next, let $y_0 \in \mathcal{E}(s_0) \cap \mathcal{O}$. Now, $y_0 \in \mathcal{E}(s_0)$ implies that $y_0 - x_0 \in \ker(\tau)$. On the other hand, $y_0 \in \mathcal{O}$ implies that $y_0 - x_0 \in W$. This means that $y_0 = x_0$ which proves the uniqueness of x_0. □

This means that an observer does exactly what it should: it resides in exactly one place at each instant. By requiring that $\mathcal{O}$ be an affine subspace, we ensure that it has a "uniform velocity" and so is an appropriate reference for observing Newton's laws. We shall denote by $\mathcal{O}_s$ the unique point in the intersection $\mathcal{O} \cap \mathcal{E}(s)$.

Since an observer $\mathcal{O}$ is a one-dimensional affine subspace, there is a unique one-dimensional subspace U of V upon which $\mathcal{O}$ is modeled. Therefore, there exists a unique vector $v_{\mathcal{O}} \in U \cap V_{\mathcal{G}}$ with the property that $\tau(v_{\mathcal{O}}) = 1$. Conversely, given $v \in V_{\mathcal{G}}$ and $x \in \mathcal{E}$, there exists a unique observer $\mathcal{O}$ such that $x \in \mathcal{O}$ and $v = v_{\mathcal{O}}$. We call $v_{\mathcal{O}}$ the *Galilean velocity* of the observer $\mathcal{O}$. It provides a reference velocity with which we can measure other velocities. Indeed, given an observer $\mathcal{O}$, we may define an associated map $P_{\mathcal{O}} : V \to \ker(\tau)$ by $P_{\mathcal{O}}(v) = v - (\tau(v))v_{\mathcal{O}}$. In particular, if $v \in V_{\mathcal{G}}$, we note that $v = v_{\mathcal{O}} + P_{\mathcal{O}}(v)$. Thus $P_{\mathcal{O}}$ can be thought of as giving the velocity of v relative to the observer's Galilean velocity $v_{\mathcal{O}}$. Note that such velocities always live in the three-dimensional vector space $\ker(\tau)$ that is to be thought of as the space of velocities that are familiar in mechanics. Such velocities are, however, only defined relative to an observer.

D. World lines

Intuitively, a world line is to be thought of as being the spatiotemporal history of something moving in the spacetime. We make the following definition.

Definition 2.7: Let $\mathcal{G} = (\mathcal{E}, V, g, \tau)$ be a Galilean spacetime. A *world line* in $\mathcal{G}$ is a section of $\pi_{\mathcal{G}} : \mathcal{E} \to I_{\mathcal{G}}$.

A world line $c : I_{\mathcal{G}} \to \mathcal{E}$ is *differentiable* at $s_0 \in I_{\mathcal{G}}$ if the limit

$$c'(s_0) := \lim_{t \to 0} \frac{c(t + s_0) - c(s_0)}{t}$$

exists. Since c is a section of $\pi_{\mathcal{G}}$, we have $\tau(c(t+s_0) - c(s_0)) = t$ and so $c'(s_0) \in V_{\mathcal{G}}$, provided it exists. Similarly, for a differentiable world line, if the limit

$$\lim_{t \to 0} \frac{c'(t + s_0) - c'(s_0)}{t}$$

exists, we denote it by $c''(s_0)$, the acceleration of the world line at the instant s_0. Since

$$\tau(c''(s_0)) = \lim_{t \to 0} \frac{\tau(c'(t + s_0) - c'(s_0))}{t} = \lim_{t \to 0} \frac{1 - 1}{t} = 0,$$

we have $c''(s_0) \in \ker(\tau)$.

E. Galilean mappings

If $\mathcal{G}_i = (\mathcal{E}_i, V_i, g_i, \tau_i)$, $i = 1, 2$, are two Galilean space-times, a *Galilean mapping* from $\mathcal{G}_1$ to $\mathcal{G}_2$ is a map $\psi : \mathcal{E}_1 \to \mathcal{E}_2$ with the following properties:

(i) ψ is an affine map;
(ii) $\tau_2(\psi(x_1) - \psi(x_2)) = \tau_1(x_1 - x_2)$ for $x_1, x_2 \in \mathcal{E}_1$;
(iii) $g_2(\psi(x_1) - \psi(x_2), \psi(x_1) - \psi(x_2)) = g_1(x_1 - x_2, x_1 - x_2)$ for simultaneous events $x_1, x_2 \in \mathcal{E}_1$.

The set of Galilean mappings from a Galilean spacetime $\mathcal{G}$ to itself is a Lie group (under composition of Galilean mappings), and we call it the *Galilean group* of the Galilean spacetime $\mathcal{G}$. We

shall denote this group by $\mathrm{Gal}(\mathcal{G})$ and its Lie algebra by $\mathfrak{gal}(\mathcal{G})$. If $\psi \in \mathrm{Gal}(\mathcal{G})$, then there are induced natural mappings of V, $I_{\mathcal{G}}$, and $\mathbb{R}$ as follows.

Lemma 2.8: Let $\mathcal{G}=(\mathcal{E},V,g,\tau)$ be a Galilean spacetime with $\psi \in \mathrm{Gal}(\mathcal{G})$. The following mappings are well defined:

(i) *the mapping $\psi_V: V \to V$ defined by $\psi_V(v)=\psi(v+x_0)-\psi(x_0)$, where $x_0 \in \mathcal{E}$;*
(ii) *the mapping $\psi_{I_{\mathcal{G}}}: I_{\mathcal{G}} \to I_{\mathcal{G}}$ defined by $\psi_{I_{\mathcal{G}}}(s)=\pi_{\mathcal{G}}(\psi(x))$, where $x \in \mathcal{E}(s)$;*
(iii) *the mapping $\psi_\tau: \mathbb{R} \to \mathbb{R}$ defined by $\psi_\tau(t)=t+\psi_{I_{\mathcal{G}}}(s)-s$, for $s \in I_{\mathcal{G}}$. Furthermore,*
(iv) *$\psi_V(v)=\psi(x_1)-\psi(x_2)$, where $x_1-x_2=v$, and*
(v) *there exists $t_\psi \in \mathbb{R}$ such that $\psi_{I_{\mathcal{G}}}(s)=s+t_\psi$ and $\psi_\tau(t)=t+t_\psi$.*

Proof: (i) Let $x_0, \bar{x}_0 \in \mathcal{E}$. We have

$$\psi(v+x_0)-\psi(x_0)=\psi((v+(x_0-\tilde{x}_0))+\tilde{x}_0)-\psi((x_0-\tilde{x}_0)+\tilde{x}_0)=\psi((x_0-\tilde{x}_0)+\tilde{x}_0)+\psi(v+\tilde{x}_0)-\psi(\tilde{x}_0)$$
$$-\psi((x_0-\tilde{x}_0)+\tilde{x}_0)=\psi(v+\tilde{x}_0)-\psi(\tilde{x}_0),$$

where we have used the property

$$\psi((v_1+v_2)+x)=(\psi(v_1+x)+\psi(v_2+x))-\psi(x),$$

since ψ is an affine map. This property is readily verified using the definition of an affine map. We will now show that $\ker(\tau)$ is an invariant subspace for ψ_V. We let $x, \tilde{x} \in \mathcal{E}$ have the property that $x-\tilde{x}=u \in \ker(\tau)$. Then

$$\tau(\psi_V(u))=\tau(\psi(x)-\psi(\tilde{x}))=\tau(u)=0,$$

where we have used property (ii) of Galilean mappings.

(ii) Let $x, \tilde{x} \in \mathcal{E}(s)$. There exists $u \in \ker(\tau)$ such that $\tilde{x}=u+x$. Now we compute

$$\pi_{\mathcal{G}}(\psi(\tilde{x}))-\pi_{\mathcal{G}}(\psi(x))=\tau(\psi(\tilde{x})-\psi(x))=\tau(\psi_V(\tilde{x}-x))=\tau(\psi_V(u))=0,$$

using the fact that $\ker(\tau)$ is an invariant subspace for ψ_V.

(iii) We must show that the definition is independent of the choice of $s \in I_{\mathcal{G}}$. For $\tilde{s} \in I_{\mathcal{G}}$, we compute

$$t+\psi_{I_{\mathcal{G}}}(\tilde{s})-\tilde{s}=t+\psi_{I_{\mathcal{G}}}(s+(\tilde{s}-s))-s+(s-\tilde{s})=t+\psi_{I_{\mathcal{G}}}(s+(\tilde{s}-s))-\psi_{I_{\mathcal{G}}}(s)+\psi_{I_{\mathcal{G}}}(s)-s+(s-\tilde{s})$$
$$=t+\psi_{I_{\mathcal{G}}}(s)-s.$$

(iv) We have

$$\psi(x_1)-\psi(x_2)=\psi((x_1-x_2)+x_2)-\psi(x_2)=\psi_V(x_1-x_2),$$

as desired.

(v) Let $x_0 \in \mathcal{E}$ and let $t_\psi=\tau(\psi(x_0)-x_0)$. For $s \in I_{\mathcal{G}}$, let $x \in \mathcal{E}(s)$. We then have

$$\psi_{I_{\mathcal{G}}}(s)-s=\psi_{I_{\mathcal{G}}}(s)-\pi_{\mathcal{G}}(x)=\pi_{\mathcal{G}}(\psi(x))-\pi_{\mathcal{G}}(x)=\tau(\psi(x)-\psi(x_0))+\tau(\psi(x_0)-x_0)+\tau(x_0-x)$$
$$=\tau(\psi(x_0)-x_0)=t_\psi,$$

where we have used the property (ii) of Galilean mappings. This shows that the definition of t_ψ is independent of x_0, and that $\psi_{I_{\mathcal{G}}}(s)=t_\psi+s$, as desired. From (iii) it also follows that $\psi_\tau(t)=t_\psi+t$. □

Remarks 2.9: (1) In the proof of the lemma we showed that, given $\psi \in \mathrm{Gal}(\mathcal{G})$, ψ_V leaves $\ker(\tau)$ invariant. We shall see in the next section that $\psi_V|_{\ker(\tau)}$ has a mechanical interpretation.

(2) Using the definition of a Galilean mapping, it is easy to see that $V_{\mathcal{G}}$ is also invariant under ψ_V.

Given a Galilean spacetime $\mathcal{G}$, we let $O(\ker(\tau))$ denote the g-orthogonal linear mappings of $\ker(\tau)$. The Lie algebra of $O(\ker(\tau))$ we denote by $\mathfrak{o}(\ker(\tau))$, recalling that it is the collection of g-skew symmetric linear mappings of $\ker(\tau)$. We identify $\ker(\tau)$ with $\mathfrak{o}(\ker(\tau))$ by the "hat" map (see Ref. 5) given by $\omega \mapsto \hat{\omega}$. This is a generalization of the map from $\mathbb{R}^3$ to $\mathfrak{o}(3)$ defined by

$$\begin{bmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{bmatrix} \mapsto \begin{bmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{bmatrix},$$

and may be explicitly defined by choosing an orthonormal basis for $\ker(\tau)$ and then applying this transformation to the components in this basis. Since the vector product in $\mathbb{R}^3$ commutes with orthogonal transformations, this definition is independent of the choice of orthonormal basis. In like manner, one can define $u_1 \times u_2$ for any $u_1, u_2 \in \ker(\tau)$ as the generalization of the $\mathbb{R}^3$ vector product.

III. RIGID BODIES

In order to talk about momenta, we need the notion of a rigid body. In this section we provide our definition for a rigid body and provide some implications of this definition. We begin by proving, in our Galilean setting, some of the basic properties of the inertia tensor of a rigid body.

A. Definitions

Let $\mathcal{G}=(\mathcal{E}, V, g, \tau)$ be a Galilean spacetime. A *rigid body* is a pair $(\mathcal{B}, \mu)$, where $\mathcal{B} \subset \mathcal{E}(s_0)$ is a compact subset of simultaneous events, and μ is a mass-distribution on $\mathcal{E}(s_0)$ with support equal to $\mathcal{B}$. Our definition thus allows such degenerate rigid bodies as point masses, and bodies whose mass distribution is contained in a line in $\mathcal{E}(s_0)$. We denote

$$\mu(\mathcal{B}) = \int_{\mathcal{B}} \mathrm{d}\mu$$

as the *mass* of the body.

The *center of mass* of the body $(\mathcal{B}, \mu)$ is the point

$$x_c = \frac{1}{\mu(\mathcal{B})} \int_{\mathcal{B}} (x - x_0) \mathrm{d}\mu + x_0.$$

Note that the integrand is in $\ker(\tau)$ and so too will be the integral. The following lemma gives some of the basic properties of this definition. If $\mathcal{S} \subset \mathcal{A}$ is a subset of an affine space $\mathcal{A}$, we let $\mathrm{conv}(\mathcal{S})$ denote the convex hull of $\mathcal{S}$ and $\mathrm{aff}(\mathcal{S})$ denote the affine hull of $\mathcal{S}$. If X is a topological space with subsets $T \subset S \subset X$, $\mathrm{int}_S(T)$ denotes the interior of T relative to the induced topology on S.

Lemma 3.1: Let $(\mathcal{B}, \mu)$ be a rigid body in a Galilean spacetime with $\mathcal{B} \subset \mathcal{E}(s_0)$. The following statements hold:

(i) *the expression*

$$x_c = \frac{1}{\mu(\mathcal{B})} \int_{\mathcal{B}} (x - x_0) \mathrm{d}\mu + x_0$$

is independent of the choice of $x_0 \in \mathcal{E}(s_0)$;

(ii) *x_c is the unique point in $\mathcal{E}(s_0)$ with the property that $\int_{\mathcal{B}} (x - x_c) \mathrm{d}\mu = 0$;*

(iii) *$x_c \in \mathrm{int}_{\mathrm{aff}(\mathcal{B})}(\mathrm{conv}(\mathcal{B}))$.*

Proof: (i) To check that the definition of x_c is independent of $x_0 \in \mathcal{E}(s_0)$, we let $\tilde{x}_0 \in \mathcal{E}(s_0)$ and compute

$$\frac{1}{\mu(\mathcal{B})}\int_{\mathcal{B}}(x-\tilde{x}_0)\mathrm{d}\mu+\tilde{x}_0=\frac{1}{\mu(\mathcal{B})}\int_{\mathcal{B}}(x-x_0)\mathrm{d}\mu+\frac{1}{\mu(\mathcal{B})}\int_{\mathcal{B}}(x_0-\tilde{x}_0)\mathrm{d}\mu$$
$$+(\tilde{x}_0-x_0)+x_0=\frac{1}{\mu(\mathcal{B})}\int_{\mathcal{B}}(x-x_0)\mathrm{d}\mu+x_0.$$

(ii) By definition of x_c and by part (i), we have

$$x_c=\frac{1}{\mu(\mathcal{B})}\int_{\mathcal{B}}(x-x_c)\mathrm{d}\mu+x_c,$$

from which it follows that

$$\int_{\mathcal{B}}(x-x_c)\mathrm{d}\mu=\mu(\mathcal{B})(x_c-x_c)=0.$$

Now suppose that $\tilde{x}_c\in\mathcal{E}(s_0)$ is an arbitrary point with the property that

$$\int_{\mathcal{B}}(x-\tilde{x}_c)\mathrm{d}\mu=0.$$

Then, by (i),

$$x_c=\frac{1}{\mu(\mathcal{B})}\int_{\mathcal{B}}(x-\tilde{x}_c)\mathrm{d}\mu+\tilde{x}_c,$$

from which we conclude that $\tilde{x}_c=x_c$.

(iii) If x_c is on the relative boundary of $\mathrm{conv}(\mathcal{B})$ or not in $\mathcal{B}$ at all, then there exists a hyperplane P in $\mathcal{E}(s_0)$ passing through x_c such that there are points in $\mathcal{B}$ which lie on one side of P, but there are no points in $\mathcal{B}$ on the opposite side. In other words, there exists $\lambda\in\ker(\tau)^\star$ such that the set

$$\{x\in\mathcal{B}|\lambda(x-x_c)>0\}$$

is nonempty, but the set

$$\{x\in\mathcal{B}|\lambda(x-x_c)<0\}$$

is empty. But this would imply that

$$\int_{\mathcal{B}}\lambda(x-x_c)\mathrm{d}\mu>0,$$

contradicting (ii). □

B. The inertia tensor

The properties of a rigid body are characterized by three things: (1) its mass, (2) its center of mass, and (3) its inertia tensor. We now define the latter. The *inertia tensor* about $x_0\in\mathcal{E}(s_0)$ of a rigid body $(\mathcal{B},\mu)$ is defined to be the linear map $\mathbb{I}_{x_0}:\ker(\tau)\to\ker(\tau)$ given by

$$\mathbb{I}_{x_0}(u)=\int_{\mathcal{B}}(x-x_0)\times(u\times(x-x_0))\mathrm{d}\mu.$$

We denote the inertia tensor about the center of mass of $(\mathcal{B},\mu)$ by $\mathbb{I}_c$. Next, we record some basic properties of the inertia tensor.

Proposition 3.2: The inertia tensor $\mathbb{I}_{x_0}$ of a rigid body $(\mathcal{B},\mu)$ is symmetric with respect to the inner product g.

Proof: Using the vector identity $g(u,v\times w)=g(w,u\times v)$, we compute

$$g(\mathbb{I}_{x_0}(u_1),u_2)=\int_{\mathcal{B}} g((x-x_0)\times(u_1\times(x-x_0)),u_2)\mathrm{d}\mu=\int_{\mathcal{B}} g(u_1\times(x-x_0)\ ,(u_2\times(x-x_0))\mathrm{d}\mu$$

$$=\int_{\mathcal{B}} g(u_1,(x-x_0)\times(u_2\times(x-x_0)))\mathrm{d}\mu=g(u_1,\mathbb{I}_{x_0}(u_2)),$$

which is what we wished to show. □

C. Eigenvalues of the inertia tensor

Since $\mathbb{I}_{x_0}$ is symmetric, its eigenvalues are real. Furthermore, they are non-negative. The following result demonstrates this, as well as other eigenvalue related assertions.

Proposition 3.3: Let $(\mathcal{B},\mu)$ be a rigid body with $\mathcal{B}\subset\mathcal{E}(s_0)$ and let $x_0\in\mathcal{E}(s_0)$. Let $\mathbb{I}_{x_0}$ denote the inertia tensor of $(\mathcal{B},\mu)$ about x_0. The following statements hold:

(i) *the eigenvalues of the inertia tensor $\mathbb{I}_{x_0}$ of the rigid body are real and non-negative;*
(ii) *if $\mathbb{I}_{x_0}$ has a zero eigenvalue, then the other two eigenvalues are equal;*
(iii) *if $\mathbb{I}_{x_0}$ has two zero eigenvalues, then $\mathbb{I}_{x_0}=0$.*

Proof: (i) Since $\mathbb{I}_{x_0}$ is symmetric, its eigenvalues will be non-negative if and only if the quadratic form $u\mapsto g(\mathbb{I}_{x_0}(u),u)$ is positive-semidefinite. For $u\in\ker(\tau)$, we compute

$$g(\mathbb{I}_{x_0}(u),u)=\int_{\mathcal{B}} g(u,(x-x_0)\times(u\times(x-x_0)))\mathrm{d}\mu=\int_{\mathcal{B}} g(u\times(x-x_0),u\times(x-x_0))\mathrm{d}\mu.$$

Since the integrand is non-negative, so too will be the integral.

(ii) Let I_1 be the zero eigenvalue with v_1 a unit eigenvector. We claim that the support of the mass distribution μ must be contained in the line

$$\ell_{v_1}=\{sv_1+x_0|s\in\mathbb{R}\}.$$

To see that this must be so, suppose that the support of μ is not contained in ℓ_{v_1}. Then there exists a Borel set $S\subset\mathcal{E}(s_0)\backslash\ell_{v_1}$ such that $\mu(S)>0$. This would imply that

$$g(\mathbb{I}_{x_0}(v_1),v_1)=\int_{\mathcal{B}} g(v_1\times(x-x_0),v_1\times(x-x_0))\mathrm{d}\mu\geqslant\int_{S} g(v_1\times(x-x_0),v_1\times(x-x_0))\mathrm{d}\mu.$$

Since $S\cap\ell_{v_1}=\varnothing$, it follows that, for all points $x\in S$, the vector $x-x_0$ is not collinear with v_1. Therefore

$$g(v_1\times(x-x_0),v_1\times(x-x_0))>0$$

for all $x\in S$, and this would imply that $g(\mathbb{I}_{x_0}(v_1),v_1)>0$. But this contradicts v_1 being an eigenvector with zero eigenvalue, and so the support of $\mathcal{B}$ must be contained in the line ℓ_{v_1}.

To see that this implies that the remaining two eigenvectors are equal, we shall show that any vector that is g-orthogonal to v_1 is an eigenvector for $\mathbb{I}_{x_0}$. First write

$$x-x_0=f^1(x)v_1+f^2(x)v_2+f^3(x)v_3$$

for functions $f^i:\mathcal{E}(s_0)\to\mathbb{R}$, $i=1,2,3$. Since the support of μ is contained in the line ℓ_{v_1}, we have

$$\int_{\mathcal{B}} (x-x_0)\times(u\times(x-x_0))\mathrm{d}\mu = v_1\times(u\times v_1)\int_{\mathcal{B}} (f^1(x))^2\mathrm{d}\mu$$

for all $u\in\ker(\tau)$. Now recall the property of the cross product that $v_1\times(u\times v_1)=u$, provided that u is orthogonal to v_1 and that v_1 has unit length. Therefore, we see that for any u that is orthogonal to v_1, we have

$$\mathbb{I}_{x_0}(u) = \left(\int_{\mathcal{B}} (f^1(x))^2\mathrm{d}\mu\right)u,$$

meaning that all such vectors u are eigenvectors with the same eigenvalue, which is what we wished to show.

(iii) It follows from the above arguments that, if two eigenvalues I_1 and I_2 are zero, then the support of μ must lie in the intersection of the lines ℓ_{v_1} and ℓ_{v_2} (here v_i is an eigenvector for I_i, $i=1,2$), and this intersection is a single point that must therefore be x_0. From this and the definition of $\mathbb{I}_{x_0}$, it follows that $\mathbb{I}_{x_0}=0$. □

Note that, in proving the result, we have proved the following corollary.

Corollary 3.4: Let $(\mathcal{B},\mu)$ *be a rigid body with inertia tensor* $\mathbb{I}_{x_0}$. *The following statements are true:*

(i) $\mathbb{I}_{x_0}$ *has a zero eigenvalue if and only if* $\mathcal{B}$ *is contained in a line through* x_0;
(ii) *if* $\mathbb{I}_{x_0}$ *has two zero eigenvalues, then* $\mathcal{B}=\{x_0\}$, *i.e.,* $\mathcal{B}$ *is a particle located at* x_0;
(iii) *if there is no line through* x_0 *that contains the support of* μ, *then the inertia tensor is an isomorphism.*

In coming to an understanding of the "appearance" of a rigid body, it is most convenient to refer to its inertia tensor $\mathbb{I}_c$ about its center of mass. Let $\{I_1,I_2,I_3\}$ be the eigenvalues of $\mathbb{I}_c$ that we call the *principal inertias* of $(\mathcal{B},\mu)$. If $\{v_1,v_2,v_3\}$ are orthonormal eigenvectors associated with these eigenvalues, we call these the *principal axes* of $(\mathcal{B},\mu)$. Related to these is the *inertial ellipsoid* which is the ellipsoid in $\ker(\tau)$ given by

$$E(\mathcal{B}) = \{x^1v_1+x^2v_2+x^3v_3\in\ker(\tau)\,|\,I_1(x^1)^2+I_2(x^2)^2+I_3(x^3)^2=1\},$$

provided that none of the eigenvalues of $\mathbb{I}_{x_0}$ are zero. If one of the eigenvalues *does* vanish, then by Proposition 3.3, the other two eigenvalues are equal. If we suppose that $I_1=0$ and that $I_2=I_3=I$, then in the case of a single zero eigenvalue, the inertial ellipsoid is

$$E(\mathcal{B}) = \left\{x^1v_1+x^2v_2+x^3v_3\in\ker(\tau)\,|\,x^2=x^3=0, x^1\in\left\{-\frac{1}{\sqrt{I}},\frac{1}{\sqrt{I}}\right\}\right\}.$$

In the most degenerate case, when all eigenvalues are zero, we define $E(\mathcal{B})=\{0\}$. These latter two inertial ellipsoids correspond to cases (i) and (ii) in Corollary 3.4.

To relate these properties of the eigenvalues of $\mathbb{I}_c$ with the inertial ellipsoid $E(\mathcal{B})$, it is helpful to introduce the notion of an axis of symmetry for a rigid body. We let $\mathbb{I}_c$ be the inertia tensor about the center of mass, and denote by $\{I_1,I_2,I_3\}$ its eigenvalues and $\{v_1,v_2,v_3\}$ its orthogonal eigenvectors. A vector $v\in\ker(\tau)\backslash\{0\}$ is an *axis of symmetry* for $(\mathcal{B},\mu)$ if, for every $R\in O(\ker(\tau))$ which fixes v, we have $R(E(\mathcal{B}))=E(\mathcal{B})$. The following result gives the relationship between axes of symmetry and the eigenvalues of $\mathbb{I}_c$.

Proposition 3.5: Let $(\mathcal{B},\mu)$ *be a rigid body with inertia tensor* $\mathbb{I}_c$ *about its center of mass. Let* $\{I_1,I_2,I_3\}$ *be the eigenvalues of* $\mathbb{I}_c$ *with orthonormal eigenvectors* $\{v_1,v_2,v_3\}$. *If* $I_1=I_2$, *then* v_3 *is an axis of symmetry for* $(\mathcal{B},\mu)$.

Conversely, if $v\in\ker(\tau)$ *is an axis of symmetry, then* v *is an eigenvector of* $\mathbb{I}_c$. *If* I *is the eigenvalue for which* v *is an eigenvector, then the other two eigenvalues of* $\mathbb{I}_c$ *are equal.*

Proof: Write $I_1=I_2=I$. We then see that any vector $v\in\mathrm{span}_{\mathbb{R}}\{v_1,v_2\}$ will have the property

that $\mathbb{I}_c(v)=Iv$. Now, let $R\in O(\ker(\tau))$ fix the vector v_3. Because R is orthogonal, if we have $v\in \mathrm{span}_{\mathbb{R}}\{v_1,v_2\}$, then $R(v)\in \mathrm{span}_{\mathbb{R}}\{v_1,v_2\}$. Also, if $v=a^1v_1+a^2v_2$, then,

$$R(v)=(\cos\theta a^1+\sin\theta a^2)v_1+(-\sin\theta a^1+\cos\theta a^2)v_2 \tag{1}$$

for some $\theta\in\mathbb{R}$, since R is simply a rotation in the plane spanned by v_1,v_2. Now let $u\in E(\mathcal{B})$. We then write $u=x^1v_1+x^2v_2+x^3v_3$ and note that

$$I(x^1)^2+I(x^2)^2+I_3(x_3)^2=1.$$

It is now a straightforward calculation to verify that $R(u)\in E(\mathcal{B})$ using (1) and the fact that R fixes v_3. This shows that $R(E(\mathcal{B}))=E(\mathcal{B})$, and so v_3 is an axis of symmetry for $(\mathcal{B},\mu)$.

For the second part of the proposition, let v be an axis of symmetry for $(\mathcal{B},\mu)$. Denote the set of orthogonal mappings that fix v by $O(v)$. That is, let

$$O(v)=\{R\in O(\ker(\tau))\,|\,R(v)=v\}.$$

Now $R\in O(v)$ has the property that $R(E(\mathcal{B}))=E(\mathcal{B})$, and thus maps principal axes of $(\mathcal{B},\mu)$ to principal axes. Since $\{v_1,v_2,v_3\}$ form an orthonormal basis for $\ker(\tau)$, it is clear that, for every $R\in O(v)$, the set $\{R(v_1),R(v_2),R(v_3)\}$ is also an orthonormal basis. It can be seen that every vector orthogonal to v is a principal axis and thus, without loss of generality, we can take $v/\|v\|=v_3$. It is now clear that $\mathbb{I}_c$ acts on $v^\perp$ by scalars, and thus v is an eigenvector of $\mathbb{I}_c$. The result now follows. □

IV. THE STRUCTURE OF THE GALILEAN GROUP

As defined previously, the Galilean group of a Galilean spacetime $\mathcal{G}=(\mathcal{E},V,g,\tau)$ is the set of affine maps from $\mathcal{E}$ to itself that preserve simultaneity of events and the distance between simultaneous events. In this section, we shall examine the Galilean group and describe its properties. In Sec. IV A we study the canonical Galilean group and show that it consists of rotations, translations, velocity boosts, and temporal origin shifts. We also look at its subgroups and describe the various fundamental objects associated with it. In Sec. IV B, we study the abstract Galilean group $\mathrm{Gal}(\mathcal{G})$. We show that, in the presence of an observer, the Galilean group is isomorphic to the canonical Galilean group. Finally, in Sec. VI A, we introduce canonical velocities and describe their images under the isomorphism of the Lie algebras induced by the Lie group isomorphism constructed previously.

A. The canonical Galilean group

In this section, we study the Galilean group of a canonical Galilean spacetime, which is a generalization of the "standard" Galilean spacetime $\mathbb{R}^3\times\mathbb{R}$. To be precise, given a Galilean spacetime $\mathcal{G}=(\mathcal{E},V,g,\tau)$, the *canonical* spacetime of $\mathcal{G}$ is the Galilean spacetime $\mathcal{G}_{\mathrm{can}}:=(\mathcal{E}_{\mathrm{can}}:=\ker(\tau)\oplus\mathbb{R},V=\ker(\tau)\oplus\mathbb{R},g,\tau)$. We now investigate the structure of the canonical Galilean group $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$. The next proposition shows that $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$ decomposes into rotations, spatial translations, Galilean velocity boosts, and temporal translations.

Proposition 4.1: The Galilean group $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$ *of the canonical spacetime* $\mathcal{G}_{\mathrm{can}}$ *is isomorphic to* $(O(\ker(\tau))\ltimes\ker(\tau))\ltimes(\ker(\tau)\times\mathbb{R})$, *where* $\ltimes$ *denotes semidirect product of groups. The group operation on* $O(\ker(\tau))\ltimes\ker(\tau))\ltimes(\ker(\tau)\times\mathbb{R})$ *is given by*

$$(R_1,r_1,u_1,t_1)\cdot(R_2,r_2,u_2,t_2)=(R_1\circ R_2,r_1+R_1(r_2)+t_2u_1,u_1+R_1(u_2),t_1+t_2),$$

where $(R_i,r_i,u_i,t_i)\in O(\ker(\tau))\ltimes\ker(\tau))\ltimes(\ker(\tau)\times\mathbb{R}$, $i=1,2$.

Proof: We first find the form of a Galilean transformation $\phi:\mathcal{E}_{\mathrm{can}}\to\mathcal{E}_{\mathrm{can}}$. Recall that, since ϕ is an affine map, it has the form $\phi(x,t)=A(x,t)+(r,\sigma)$ where $A:\ker(\tau)\oplus\mathbb{R}\to\ker(\tau)\oplus\mathbb{R}$ is $\mathbb{R}$-linear and where $(r,\sigma)\in\ker(\tau)\oplus\mathbb{R}$. Given vector spaces U and V, we denote the set of linear maps from U to V by $L(U,V)$. Let us write $A(x,t)=(A_{11}x+A_{12}t,A_{21}x+A_{22}t)$ where $A_{11}\in L(\ker(\tau),\ker(\tau))$, $A_{12}\in L(\mathbb{R},\ker(\tau))$, $A_{21}\in L(\ker(\tau),\mathbb{R})$, and $A_{22}\in L(\mathbb{R},\mathbb{R})$. By property (iii) of

Galilean mappings, A_{11} is a g-orthogonal transformation of $\ker(\tau)$. Property (ii) of Galilean mappings implies that

$$A_{22}(t_2-t_1)+A_{21}(x_2-x_1)=t_2-t_1, \quad t_1,t_2\in\mathbb{R}, x_1x_2\in\ker(\tau).$$

Thus, taking $x_1=x_2$, we see that $A_{22}=1$. This in turn implies that $A_{21}=0$. Gathering this information shows that a Galilean transformation has the form

$$\phi:\begin{bmatrix}x\\t\end{bmatrix}\mapsto\begin{bmatrix}R & u\\0 & 1\end{bmatrix}\begin{bmatrix}x\\t\end{bmatrix}+\begin{bmatrix}r\\\sigma\end{bmatrix},$$

where $R\in O(\ker(\tau))$, $\sigma\in\mathbb{R}$, and $r,u\in\ker(\tau)$. This proves the first part of the proposition. Now, it is easy to see that, if ϕ_i, $i=1,2$, are Galilean transformations given by

$$\phi_i:\begin{bmatrix}x\\t\end{bmatrix}\mapsto\begin{bmatrix}R_i & u_i\\0 & 1\end{bmatrix}\begin{bmatrix}x\\t\end{bmatrix}+\begin{bmatrix}r_i\\\sigma_i\end{bmatrix}, \quad i=1,2,$$

then

$$\phi_1\circ\phi_2:\begin{bmatrix}x\\t\end{bmatrix}\mapsto\begin{bmatrix}R_1\circ R_2 & u_1+R_1(u_2)\\0 & 1\end{bmatrix}\begin{bmatrix}x\\t\end{bmatrix}+\begin{bmatrix}r_1+R_1(r_2)+\sigma_2u_1\\\sigma_1+\sigma_2\end{bmatrix}.$$

which gives us the desired group operation. □

Remarks 4.2: (1) It is clear from this proposition that $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$ is a ten-dimensional group. This is not altogether obvious from the definition.

(2) The meaning of the appearance of two semi-direct products in the decomposition of $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$ should be understood correctly. They arise because $\ker(\tau)\times\mathbb{R}$ is a normal subgroup of $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$ and the quotient group itself is a semi-direct product of $O(\ker(\tau))$ and $\ker(\tau)$.

(3) A canonical Galilean transformation may now be written as a composition of one of three basic classes of transformations.

(i) *A spatiotemporal shift of origin:*

$$\begin{bmatrix}x\\t\end{bmatrix}\mapsto\begin{bmatrix}x\\t\end{bmatrix}+\begin{bmatrix}r\\\sigma\end{bmatrix},$$

for $r\in\ker(\tau)$, $\sigma\in\mathbb{R}$.

(ii) *A "rotation" of reference frame:*

$$\begin{bmatrix}x\\t\end{bmatrix}\mapsto\begin{bmatrix}R & 0\\0 & 1\end{bmatrix}\begin{bmatrix}x\\t\end{bmatrix},$$

for $R\in O(\ker(\tau))$.

(iii) *A (Galilean) velocity boost:*

$$\begin{bmatrix}x\\t\end{bmatrix}\mapsto\begin{bmatrix}\mathrm{id}_{\ker(\tau)} & u\\0 & 1\end{bmatrix}\begin{bmatrix}x\\t\end{bmatrix},$$

for $u\in\ker(\tau)$.

The names we have given these fundamental transformations are suggestive. A shift of the spatiotemporal origin should be thought of as moving the origin to a new position, and resetting the clock, but maintaining the same orientation in space. A rotation of reference frame means the origin stays in the same place, and uses the same clock but rotates the "point of view." The final basic transformation, a velocity boost, means that the origin maintains its orientation and uses the same clock, but now moves with a certain velocity with respect to the previous origin.

B. The structure of the abstract Galilean group

In the usual presentation of Galilean invariant mechanics (e.g., Ref. 11), one considers a spacetime $\mathbb{R}^3 \times \mathbb{R}$ and Galilean invariance is imposed by asking that the system admit the Galilean group as a symmetry group. In this case, the Galilean group naturally breaks down into rotations, translations, Galilean boosts (constant velocity shifts), and temporal origin shifts. In our abstract setting, the Galilean group $\mathrm{Gal}(\mathcal{G})$ does not admit such a decomposition. Note that this is similar to what one sees in an affine Euclidean space where a decomposition of an isometry into rotation and translation is not possible until one chooses an origin about which to measure rotations. However, the presence of an observer in a Galilean spacetime defines, for each instant, an isomorphism from the abstract Galilean group $\mathrm{Gal}(\mathcal{G})$ into the canonical group $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$.

Proposition 4.3: Let $\mathcal{G}=(\mathcal{E}, V, g, \tau)$ be a Galilean spacetime with $\mathcal{O}$ an observer. The following statements hold.

(i) *The mapping from V to $\ker(\tau) \oplus \mathbb{R}$ defined by $v \mapsto (P_{\mathcal{O}}(v), \tau(v))$ is an isomorphism.*

(ii) *For each $s_0 \in I_{\mathcal{G}}$, the observer at s_0, $\mathcal{O}_{s_0}$, induces a natural isomorphism $\iota_{\mathcal{O}_{s_0}}$ from $\mathrm{Gal}(\mathcal{G})$ to the group $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$. Explicitly, if $\psi \in \mathrm{Gal}(\mathcal{G})$ with t_ψ as defined in Lemma 2.8, and if $R_\psi \in O(\ker(\tau))$ and $r_{\psi,\mathcal{O}} \in \ker(\tau)$ satisfy*

$$\psi(x) = (R_\psi(x - \mathcal{O}_{s_0}) + r_{\psi,\mathcal{O}}) + \mathcal{O}_{t_\psi + s_0}, \quad x \in \mathcal{E}(s_0),$$

then

$$\iota_{\mathcal{O}_s}(\psi) = (R_\psi, r_{\psi,\mathcal{O}}, u_{\psi,\mathcal{O}}, t_\psi),$$

where $u_{\psi,\mathcal{O}} = P_{\mathcal{O}}(\psi_V(v_{\mathcal{O}}))$.

Proof: (i) It suffices to show that the mapping $v \mapsto (P_{\mathcal{O}}(v), \tau(v))$ is injective. If $\tau(v)=0$, then $v \in \ker(\tau)$. Now, if we also have

$$P_{\mathcal{O}}(v) = v - (\tau(v))v_{\mathcal{O}} = 0,$$

we must have $v=0$, thus the mapping is injective as desired.

(ii) We first assign to each $(R, r, u, t) \in \mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$ a Galilean mapping ψ, and show that the construction implies that $(R, r, u, t) = (R_\psi, r_{\psi,\mathcal{O}}, u_{\psi,\mathcal{O}}, t_\psi)$, thus showing that $\iota_{\mathcal{O}_{s_0}}$ is invertible. Now, given $(R, r, u, t) \in \mathrm{Gal}_{\mathrm{can}}(\mathcal{G})$, we define a map $\psi: \mathcal{E} \to \mathcal{E}$ by

$$\psi(x) = tv_{\mathcal{O}} + (R(x - \mathcal{O}_{\pi_{\mathcal{G}}(x)}) + (\pi_{\mathcal{G}}(x) - s_0)u + r) + \mathcal{O}_{\pi_{\mathcal{G}}(x)}. \tag{2}$$

We now show that this mapping is Galilean. First we show that it is affine. For $v \in V$, we compute

$$\begin{aligned}
\psi(v + \mathcal{O}_{s_0}) - \psi(\mathcal{O}_{s_0}) &= tv_{\mathcal{O}} + (R(v + \mathcal{O}_{s_0} - \mathcal{O}_{\tau(v)+s_0}) + ((\tau(v) + s_0) - s_0)u + r) \\
&\quad + \mathcal{O}_{\tau(v)+s} - (tv_{\mathcal{O}} + r + \mathcal{O}_{s_0}) \\
&= R(v + \mathcal{O}_{s_0} - (\tau(v)v_{\mathcal{O}} + \mathcal{O}_{s_0})) + \tau(v)(u + v_{\mathcal{O}}) \\
&= R(v - \tau(v)v_{\mathcal{O}}) + \tau(v)(u + v_{\mathcal{O}}) \\
&= R(P_{\mathcal{O}}(v)) + \tau(v)(u + v_{\mathcal{O}}).
\end{aligned} \tag{3}$$

Thus the map $v \mapsto \psi(v + \mathcal{O}_{s_0}) - \psi(\mathcal{O}_{s_0})$ is linear, so ψ is affine. Similarly, we calculate

$$\tau(\psi(x_1) - \psi(x_2)) = \tau(tv_{\mathcal{O}} + \mathcal{O}_{\pi_{\mathcal{G}}(x_1)}) - \tau(tv_{\mathcal{O}} + \mathcal{O}_{\pi_{\mathcal{G}}(x_2)}) = t + \pi_{\mathcal{G}}(x_1) - (t + \pi_{\mathcal{G}}(x_2)) = \tau(x_1 - x_2).$$

So property (ii) of Galilean mappings is satisfied. Next, for $s_0 \in I_{\mathcal{G}}$, consider $y_1, y_2 \in \mathcal{E}(s_0)$. We compute

$$\psi(y_1) - \psi(y_2) = tv_{\mathcal{O}} + R(y_1 + \mathcal{O}_{s_0}) + (s_0 - s_0)u + r + \mathcal{O}_{s_0} - (tv_{\mathcal{O}} + R(y_2 - \mathcal{O}_{s_0}) + (s_0 - s_0)u + r + \mathcal{O}_{s_0})$$
$$= R(y_1 - y_2).$$

Thus ψ satisfies property (iii) of Galilean mappings. Next we show that $(R,r,u,t) = (R_\psi, r_{\psi,\mathcal{O}}, u_{\psi,\mathcal{O}}, t_\psi)$. By restricting ψ to $\mathcal{E}(s_0)$ we get

$$(\psi|\mathcal{E}(s_0))(x) = tv_{\mathcal{O}} + (R(x - \mathcal{O}_{s_0}) + r) + \mathcal{O}_{s_0} = (R(x - \mathcal{O}_{s_0}) + r) + \mathcal{O}_{t+s_0}.$$

However, the definition of R_ψ and $r_{\psi,\mathcal{O}}$ gives

$$R(x - \mathcal{O}_{s_0}) + r = R_\psi(x - \mathcal{O}_{s_0}) + r_{\psi,\mathcal{O}},$$

for each $x \in \mathcal{E}(s_0)$. Taking $x = \mathcal{O}_{s_0}$ gives $r = r_{\psi,\mathcal{O}}$, from which it follows that $R = R_\psi$. Also, for $x \in \mathcal{E}(s_0)$, we have

$$\psi_{I_{\mathcal{G}}}(s_0) = \pi_{\mathcal{G}}(\psi(x)) = t + s_0.$$

From Lemma 2.8, it follows that $t = t_\psi$. From (3) we also have

$$P_{\mathcal{O}}(\psi_V(v_{\mathcal{O}})) = R(P_{\mathcal{O}}(v_{\mathcal{O}})) + \tau(v_{\mathcal{O}})u = u,$$

using the fact that $P_{\mathcal{O}}(v_{\mathcal{O}}) = 0$. This shows that $u = u_{\psi,\mathcal{O}}$. We have now shown that, for every $(R,r,u,t) \in \mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$, there is a Galilean mapping ψ such that $\iota_{\mathcal{O}_{s_0}}(\psi) = (R,r,u,t)$. Thus we have shown that $\iota_{\mathcal{O}_{s_0}}$ is surjective. Next we show that it is injective. For this, let $\tilde{\psi} \in \mathrm{Gal}(\mathcal{G})$ be such that, for $x \in \mathcal{E}$,

$$\tilde{\psi}(x) = tv_{\mathcal{O}} + (R(x - \mathcal{O}_{s_0}) + (\pi_{\mathcal{G}}(x) - s_0)u + r) + \mathcal{O}_{\pi_{\mathcal{G}}(x)}.$$

that is, suppose that

$$\iota_{\mathcal{O}_{s_0}}(\tilde{\psi}) = (R,r,u,t) = \iota_{\mathcal{O}_{s_0}}(\psi).$$

We shall show that $\tilde{\psi} = \psi$. Since $\tilde{\psi}(\mathcal{O}_{s_0}) = \psi(\mathcal{O}_{s_0})$, using (3) this will follow if we can show that $\tilde{\psi}_V = \psi_V$. As in (i), we note that $V \simeq \ker(\tau) \oplus \mathbb{R}$ and the preimage of (u,t) under this isomorphism is $u + tv_{\mathcal{O}}$. We also write

$$\psi_V(u + tv_{\mathcal{O}}) = A_{11}(u) + A_{12}(t) + (A_{21}(u) + A_{22}(t))v_{\mathcal{O}},$$

for linear mappings $A_{11}: \ker(\tau) \to \ker(\tau)$, $A_{12}: \mathbb{R} \to \ker(\tau)$, $A_{21}: \ker(\tau) \to \mathbb{R}$, and $A_{22}: \mathbb{R} \to \mathbb{R}$. The property (ii) of Galilean mappings implies that ψ_V has $\ker(\tau)$ as an invariant subspace. Thus $A_{21} = 0$. We next calculate

$$\tau(\psi_V(tv_{\mathcal{O}})) = \tau(\psi(tv_{\mathcal{O}} + \mathcal{O}_{s_0})) - \tau(\psi(\mathcal{O}_{s_0})) = \tau(tv_{\mathcal{O}} + \mathcal{O}_{s_0}) - \tau(\mathcal{O}_{s_0}) = t.$$

This gives $A_{22}(t) = t$. With $t = 0$, property (iii) of Galilean mappings implies that $A_{11} \in O(\ker(\tau))$. Thus we have

$$\psi_V(u + tv_{\mathcal{O}}) = \tilde{R}(u) + t(\tilde{u} + v_{\mathcal{O}}), \tag{4}$$

for some $\tilde{R} \in O(\ker(\tau))$ and $\tilde{u} \in \ker(\tau)$. Since $\psi|\mathcal{E}(s) = \tilde{\psi}|\mathcal{E}(s)$ we have

$$\psi_V(u) = \tilde{\psi}(u + \mathcal{O}_{s_0}) - \tilde{\psi}(\mathcal{O}_{s_0}) = R_\psi(u),$$

giving $\tilde{R} = R$. From (3) we also have

$$P_{\mathcal{O}}(\psi_V(v_{\mathcal{O}}) = \tilde{u},$$

from which we get $u=\tilde{u}$. This shows that $\psi_V=\tilde{\psi}_V$, thus showing that, if $\psi_1,\psi_2\in\mathrm{Gal}(\mathcal{G})$ satisfy $\iota_{\mathcal{O}_{s_0}}(\psi_1)=\iota_{\mathcal{O}_{s_0}}(\psi_2)$, then $\psi_1=\psi_2$. Therefore, $\iota_{\mathcal{O}_{s_0}}$ is injective.

Finally we show that $\iota_{\mathcal{O}_{s_0}}$ is a homomorphism. We let $\psi_1,\psi_2\in\mathrm{Gal}(\mathcal{G})$ and denote $\iota_{\mathcal{O}_{s_0}}(\psi_i)=(R_i,r_i,u_i,t_i)$, $i=1,2$. We also let $\iota_{\mathcal{O}_{s_0}}(\psi_1\circ\psi_2)=(R_{12},r_{12},u_{12},t_{12})$. First, we compute

$$\begin{aligned}(\psi_1\circ\psi_2)_V(v) &= (\psi_1\circ\psi_2)(v+\mathcal{O}_{s_0})-(\psi_1\circ\psi_2)(\mathcal{O}_{s_0}) = \psi_1(\psi_2(v+\mathcal{O}_{s_0}))-\psi_1(\psi_2(\mathcal{O}_{s_0}))\\ &= \psi_1(tv_{\mathcal{O}}+R_2(v+\mathcal{O}_{s_0}-\mathcal{O}_{\tau(v)+s_0})+\tau(v)u_2+r_2+\mathcal{O}_{\tau(v)+s_0})-\psi_1(tv_{\mathcal{O}}+r+\mathcal{O}_{s_0})\\ &= \psi_1((tv_{\mathcal{O}}+r)+R_2(P_{\mathcal{O}}(v))+\tau(v)(u_2+v_{\mathcal{O}})+\mathcal{O}_{s_0})-\psi_1(tv_{\mathcal{O}}+r_2+\mathcal{O}_{s_0})\\ &= \psi_{1,V}(R_2(P_{\mathcal{O}}(v))+\tau(v)(u_2+v_{\mathcal{O}}))=\psi_{1,V}(\psi_{2,V}(v)).\end{aligned}$$

From this we deduce that

$$R_{12}(u)+t(u_{12}+v_{\mathcal{O}})=R_1\circ R_2(u)+t(u_1+R_1(u_2)+v_{\mathcal{O}}),$$

for each $(u,t)\in\ker(\tau)\oplus\mathbb{R}$. Thus we have

$$R_{12}=R_1\circ R_2,\quad u_{12}=u_1+R_1(u_2).$$

Next we have

$$\psi_1\circ\psi_2(\mathcal{O}_{s_0})=r_{12}+\mathcal{O}_{t_{12}+s_0}. \tag{5}$$

Also,

$$\psi_2(\mathcal{O}_{s_0})=r_2+\mathcal{O}_{t_2+s_0}.$$

Therefore

$$\begin{aligned}\psi_1\circ\psi_2(\mathcal{O}_{s_0}) &= \psi_1(r_2+\mathcal{O}_{t_2+s_0})=R_1(r_2+\mathcal{O}_{t_2+s_0}-\mathcal{O}_{t_2+s_0})+t_2u_1+r_1+\mathcal{O}_{s_0+t_2+t_1}\\ &= R_1r_2+t_2u_1+r_1+\mathcal{O}_{s_0+t_1+t_2}.\end{aligned}$$

Comparing this to (5) we get

$$r_{12}=R_1r_2+t_2u_1+r_1,\quad t_{12}=t_1+t_2.$$

Thus we have shown that the group action defined on $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$ agrees with that on $\mathrm{Gal}(\mathcal{G})$ under the bijection $\iota_{\mathcal{O}_{s_0}}$. □

We end this section by listing some of the subgroups of $\mathrm{Gal}(\mathcal{G})$ that we shall have occasion to use in the sequel. The following result is easy to prove.

Proposition 4.4: The following statements hold:

(i) *the following are subgroups of* $\mathrm{Gal}(\mathcal{G})$*:*

- *(a)* $\mathrm{Gal}_0(\mathcal{G}):=\{\psi\in\mathrm{Gal}(\mathcal{G}):\psi_{I_{\mathcal{G}}}=\mathrm{id}_{I_{\mathcal{G}}}\}$;
- *(b)* $N:=\{\psi\in\mathrm{Gal}(\mathcal{G}):\ \psi_V|_{\ker(\tau)}=\mathrm{id}_{\ker(\tau)}\}$;
- *(c)* $N_0:=N\cap\mathrm{Gal}_0(\mathcal{G})$.

(ii) *the set* $\mathrm{Lin}(\mathcal{G}):=\{\psi_V\,|\,\psi\in\mathrm{Gal}(\mathcal{G})\}$ *is a Lie group.*

V. OBSERVER-INDEPENDENT FORMULATION OF RIGID BODY MECHANICS

In this section we formulate rigid mechanics in an observer independent manner. All of the classical concepts in Eulerian rigid body mechanics—motions, body and spatial velocities, body and spatial momenta, and the equations of motion—are given definitions independent of an observer.

A. Rigid motions

A *rigid motion* in a Galilean spacetime $\mathcal{G}=(\mathcal{E},V,g,\tau)$ is a smooth mapping $\Psi:\mathbb{R}\to\mathrm{Gal}(\mathcal{G})$ with the property that $(\Psi(t))_{I_\mathcal{G}}(s)=s+t$, for each $t\in\mathbb{R}$ (see Sec. II E). In other words, if we denote $\Psi_t:=\Psi(t)$, then a rigid motion Ψ has the property that $\Psi_t(x)\in\mathcal{E}(t+\pi_\mathcal{G}(x))$ for each $x\in\mathcal{E}(s)$. Thus a rigid motion maps points in $\mathcal{E}(s)$ to $\mathcal{E}(s)$ at $t=0$, and for $t\neq 0$, the points get shifted by the affine action of $\mathbb{R}$ on $I_\mathcal{G}$. Let us give some of the basic properties of rigid motions. The following result is immediate.

Lemma 5.1: Given a rigid motion Ψ, for each $x\in\mathcal{E}$ the map $I_\mathcal{G}\ni s\mapsto\Psi_{s-\pi_\mathcal{G}(x)}(x)\in\mathcal{E}$ is a world line.

The next result shows how we can extract the "rotational component" of a rigid motion for each $t\in\mathbb{R}$.

Proposition 5.2: Let Ψ be a rigid motion in a Galilean specetime $\mathcal{G}=(\mathcal{E},V,g,\tau)$. Then, for each $t\in\mathbb{R}$, we have $\Psi_{t,V}|_{\ker(\tau)}\in O(\ker(\tau))$.

Proof: From Lemma 2.8, it is clear that $\Psi_{t,V}$ maps $\ker(\tau)$ to itself. Next for simultaneous events x_1 and x_2, we compute

$$\begin{aligned} g(\Psi_{t,V}|_{\ker(\tau)}(x_1-x_2),\Psi_{t,V}|_{\ker(\tau)}(x_1-x_2)) &= g(\Psi_{t,V}(x_1-x_2),\Psi_{t,V}(x_1-x_2)) \\ &= g(\Psi_t(x_1)-\Psi_t(x_2),\Psi(x_1)-\Psi_t(x_2)) \\ &= g(x_1-x_2,x_1-x_2), \end{aligned}$$

where we have used the properties of the rigid motion and Lemma 2.8. This shows that $\Psi_{t,V}|_{\ker(\tau)}\in O(\ker(\tau))$ as desired. □

This proposition shows that, given a rigid motion Ψ in a Galilean spacetime, we can associate to this rigid motion a unique map from $\mathbb{R}\to O(\ker(\tau))$. We denote this map by R_Ψ.

B. Spatial and body velocities

In this section we define the concepts of spatial and body velocities corresponding to a rigid motion Ψ. Intuitively, the configuration of a rigid body is given by its "orientation" and "position" (with respect to an initial orientation and position). To make this precise, let us denote $Q:=O(\ker(\tau))\times\mathcal{E}$. If we choose a reference configuration, say $q_0=(R_0,x_0)\in Q$, it is easy to see that a Galilean mapping $\phi\in\mathrm{Gal}(\mathcal{G})$ maps q_0 to another point in Q as follows:

$$\mathrm{Gal}(\mathcal{G})\times Q\to Q,$$

$$(\phi,(R_0,x_0))\mapsto(R_\phi R_0,\phi(x_0)),\quad \phi\in\mathrm{Gal}(\mathcal{G}).$$

This defines an action of $\mathrm{Gal}(\mathcal{G})$ on Q which we represent by Φ. In other words, we have $\Phi(\phi,(R_0,x_0))=(R_\phi R_0,\phi(x_0))$. For each $q\in Q$ and $g\in\mathrm{Gal}(\mathcal{G})$, we define the maps $\Phi_q:\mathrm{Gal}(\mathcal{G})\to Q$ and $\Phi_g:Q\to Q$ by $\Phi_q(g):=\Phi(g,q)=:\Phi_q(g)$. The action Φ also defines an action of $\mathrm{Gal}(\mathcal{G})$ on $O(\ker(\tau))$ and $\mathcal{E}$, respectively. The latter action is denoted by $\Psi^\mathcal{E}$. Given $\zeta\in\mathfrak{gal}(\mathcal{G})$, denote the infinitesimal generator corresponding to ζ at $(R_0,x_0)\in Q$ by $\zeta_Q(R_0,x_0)$. It is easy to see that $\zeta_Q(R_0,x_0)$ can be written as

$$\zeta_Q(R_0,x_0) = (\zeta_{O(\ker(\tau))}(R_0), \zeta_{\mathcal{E}}(x_0)),$$

where $\zeta_{O(\ker(\tau))}(R_0)$ is the infinitesimal generator at $R_0 \in O(\ker(\tau))$ corresponding to ζ of the action of $\mathrm{Gal}(\mathcal{G})$ on $O(\ker(\tau))$, and $\zeta_{\mathcal{E}}(x_0)$ is the infinitesimal generator at $x_0 \in \mathcal{E}$ corresponding to ζ of the action of $\mathrm{Gal}(\mathcal{G})$ on $\mathcal{E}$.

Now, given a rigid motion Ψ, define curves $\xi_\Psi(t)$ and $\eta_\Psi(t) \in \mathfrak{gal}(\mathcal{G})$ as follows:

$$\eta_\Psi(t) = \Psi_t^{-1}\dot{\Psi}_t, \quad \xi_\Psi(t) = \dot{\Psi}_t\Psi_t^{-1}.$$

Notice that $\xi_\Psi(t) = \mathrm{Ad}_{\Psi_t}\eta_\Psi(t)$. These curves $\xi_\Psi(t)$ and $\eta_\Psi(t)$ are called "spatial velocity" and "body velocity," respectively, in the literature (see, for example, Ref. 5) and the interpretation for defining them in this way is somewhat unintuitive. In the sequel, given a rigid motion Ψ, we think of velocities at a point $q_0 = (R_0, x_0) \in Q$ as tangent vectors defined by the infinitesimal generators corresponding to the curves $\eta_\Psi(t)$ and $\xi_\Psi(t)$, respectively, at q_0. The idea is that a rigid motion generates a curve in Q (starting at q_0) given by $\Psi_t(q_0) := (R_\Psi(t)R_0, \Psi_t(x_0))$, and the tangent vector to this curve at a point corresponds to the velocity at that point. We now give our definitions for spatial and body velocities, respectively. First, given a rigid motion Ψ, we define maps $\Omega, \omega : \mathbb{R} \to \mathfrak{o}(\ker(\tau))$ by $\hat{\Omega}_\Psi(t) := R_\Psi^{-1}(t)\dot{R}_\Psi(t)$ and $\hat{\omega}_\Psi(t) := \dot{R}_\Psi(t)R_\Psi^{-1}(t)$, respectively. We also represent by $\tau_{\mathrm{ang}} : TQ \to T(O(\ker(\tau)))$ and $\tau_{\mathrm{lin}} : TQ \to T\mathcal{E}$ the respective projections. Denote by $\Theta_{\mathrm{ang}} : T(O(\ker(\tau))) \to O(\ker(\tau)) \times \mathfrak{o}(\ker(\tau))$ the right-trivialization of $T(O(\ker(\tau)))$. Thus $\Theta_{\mathrm{ang}}(v_g) = (g, T_gR_{g^{-1}}v_g)$ for $v_g \in T_g(O(\ker(\tau)))$ and $g \in O(\ker(\tau))$. Similarly, denote by $\Theta_{\mathrm{lin}} : T\mathcal{E} \to \mathcal{E} \times V$ the natural trivialization of $T\mathcal{E}$. Let us denote by pr_2 the projection onto the second components of $O(\ker(\tau)) \times \mathfrak{o}(\ker(\tau))$ and $\mathcal{E} \times V$, respectively. With an abuse of notation, we represent the maps $\mathrm{pr}_2 \circ \Theta_{\mathrm{ang}}$ and $\mathrm{pr}_2 \circ \Theta_{\mathrm{lin}}$ by Θ_{ang} and Θ_{lin}, respectively.

Definition 5.3: Let Ψ be a rigid motion in a Galilean spacetime $\mathcal{G}$.

(i) The *body velocity* is the map $V_\Psi^b : Q \times \mathbb{R} \to TQ$ given by

$$V_\Psi^b(R,x,t) = (\eta_\Psi(t))_Q(R,x).$$

The maps $V_{\Psi,\mathrm{ang}}^b := \Theta_{\mathrm{ang}} \circ \tau_{\mathrm{ang}} \circ V_\Psi^b$ and $V_{\Psi,\mathrm{lin}}^b := \Theta_{\mathrm{lin}} \circ \tau_{\mathrm{lin}} \circ V_\Psi^b$ are called *body angular velocity* and *body linear velocity*, respectively.

(ii) The *spatial velocity* is the map $V_\Psi^s : Q \times \mathbb{R} \to TQ$ defined by

$$V_\Psi^s(R,x,t) = (\xi_\Psi(t))_Q(R,x).$$

The maps $V_{\Psi,\mathrm{ang}}^s := \Theta_{\mathrm{ang}} \circ \tau_{\mathrm{ang}} \circ V_\Psi^s$ and $V_{\Psi,\mathrm{lin}}^s := \Theta_{\mathrm{lin}} \circ \tau_{\mathrm{lin}} \circ V_\Psi^s$ are called *spatial angular velocity* and *spatial linear velocity*, respectively.

Let us make a few comments about these definitions.

Remarks 5.4: (1) We identify the TQ-valued velocities with the corresponding $Q \times (\mathfrak{o}(\ker(\tau)) \times V)$-valued trivialization. Let us provide some intuition for these definitions. Notice that, for $q \in Q$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}(\Psi_t(q)) = T_q\Phi_{\Psi_t}(\xi_\Psi(t)^{-1}\dot{\xi}_\Psi(t))_Q(q) = T_q\Phi_{\Psi_t}(V_\Psi^b(q,t)).$$

Therefore, $V_\Psi^b(q,t) = T_q\Phi_{\Psi_t^{-1}}((\mathrm{d}/\mathrm{d}t)(\Psi_t(q)))$. The body velocity can therefore be thought of as the velocity of the curve $\Psi_t(q)$ at $t \in \mathbb{R}$ as seen in the "frame" fixed at q.

(2) The definition of spatial velocity is less intuitive. It will become clearer once we prove Proposition 5.6.

(3) It is not clear at this stage how our definitions are consistent with the existing ones. We shall see, in Sec. VI B, that in the presence of an observer, the body and spatial velocities correspond to "canonical" velocities.

The definitions lead to the following relationship between body and spatial velocities, which we shall have occasion to use.

Lemma 5.5: $V^s_\Psi(R_\Psi(t)R,\Psi_t(x),t)=T_{(R,x)}\Phi_{\Psi_t}V^b_\Psi(R,x,t)$.

Proof: Given an action $\Phi:G\times Q\to Q$ of a Lie group G on a manifold Q, we have, for $\zeta\in\mathfrak{g}$ and $g\in G$, $(\mathrm{Ad}_g\zeta)_Q(g\cdot q)=T_q\Phi_g\zeta_Q(q)$. The result follows directly from this equality. □

Next, we write down the expressions for linear and angular velocities.

Proposition 5.6: Let Ψ be a motion in a Galilean spacetime $\mathcal{G}$. Then

(i) $V^b_{\Psi,\mathrm{ang}}(R,x,t)=\hat{\Omega}_\Psi(t)$,
(ii) $V^b_{\Psi,\mathrm{lin}}(R,x,t)=\Psi^{-1}_{t,V}(\mathrm{d}/\mathrm{d}t\Psi_t(x))$,
(iii) $V^s_{\Psi,\mathrm{ang}}(R,x,t)=\hat{\omega}_\Psi(t)$, *and*
(iv) $V^s_{\Psi,\mathrm{lin}}(R,x,t)=-\Psi_{t,V}(\mathrm{d}/\mathrm{d}t\Psi_t^{-1}(x))$.

Proof: (i) The projection $\tau_{\mathrm{ang}}(V^b_{\Psi,\mathrm{ang}}(R,x,t))$ is actually the infinitesimal generator corresponding to $(\Psi_{t,V}|^{-1}_{\ker(\tau)}\dot{\Psi}_{t,V}|_{\ker(\tau)})=\hat{\Omega}_\Psi(t)$. We compute

$$V^b_{\Psi,\mathrm{ang}}(R,x,t)=\left.\frac{\mathrm{d}}{\mathrm{d}s}\exp(s\hat{\Omega}_\Psi(t))R\right|_{s=0}=\hat{\Omega}_\Psi(t)R.$$

Thus $V^b_{\Psi,\mathrm{ang}}(R,x,t)=\hat{\Omega}_\Psi(t)$.

(ii) The body linear velocity $V^b_{\Psi,\mathrm{lin}}(R,x,t)$ is the infinitesimal generator corresponding to $\eta_\Psi(t)$ at $x\in\mathcal{E}$ of the action of $\mathrm{Gal}(\mathcal{G})$ on $\mathcal{E}$. We compute

$$\begin{aligned}V^b_{\Psi,\mathrm{lin}}(R,x,t)&=T_e\Phi^{\mathcal{E}}_x(T_{\Psi_t}L_{\Psi_t^{-1}}\dot{\Psi}_t)=T_{\Psi_t}(\Phi_{\Psi_t^{-1}}\Phi^{\mathcal{E}}_x)(\dot{\Psi}_t)\\&=\left.\frac{\mathrm{d}}{\mathrm{d}s}\Phi_{\Psi_t^{-1}}\Phi^{\mathcal{E}}_x\circ(\Psi_{t+s})\right|_{s=0}=\left.\frac{\mathrm{d}}{\mathrm{d}s}\Phi_{\Psi_t^{-1}}(\Psi_{t+s}(x))\right|_{s=0}\\&=T_{\Psi_t(x)}\Phi_{\Psi_t^{-1}}\frac{\mathrm{d}}{\mathrm{d}t}(\Psi_t(x))=\Psi^{-1}_{t,V}\frac{\mathrm{d}}{\mathrm{d}t}(\Psi_t(x)).\end{aligned}$$

This is what we wanted to prove.

(iii) This is identical to the proof of part (i).

(iv) The spatial linear velocity $V^s_{\Psi,\mathrm{lin}}(R,x,t)$ is the infinitesimal generator corresponding to $\xi_\Psi(t)$ at $x\in\mathcal{E}$ of the action of $\mathrm{Gal}(\mathcal{G})$ on $\mathcal{E}$. Notice that, by differentiating $\Psi_t\Psi_t^{-1}=\mathrm{id}_{\mathcal{E}}$, we get

$$T_{\Psi_t}R_{\Psi_t^{-1}}\dot{\Psi}_t=-T_{\Psi_t^{-1}}L_{\Psi_t}\dot{\Psi}_t^{-1}.$$

We compute

$$\begin{aligned}V^s_{\Psi,\mathrm{lin}}(R,x,t)&=T_e\Phi^{\mathcal{E}}_x(T_{\Psi_t}R_{\Psi_t^{-1}}\dot{\Psi}_t)=-T_e\Phi^{\mathcal{E}}_x(T_{\Psi_t}L_{\Psi_t}\dot{\Psi}_t^{-1})\\&=-\left.\frac{\mathrm{d}}{\mathrm{d}s}\Phi_{\Psi_t}\Phi^{\mathcal{E}}_x(\Psi^{-1}_{t+s})\right|_{s=0}=-\left.\frac{\mathrm{d}}{\mathrm{d}s}\Phi_{\Psi_t}(\Psi^{-1}_{t+s}(x))\right|_{s=0}\\&=-T_{\Psi_t^{-1}(x)}\Phi_{\Psi_t}\frac{\mathrm{d}}{\mathrm{d}t}(\Psi_t^{-1}(x))=-\Psi_{t,V}\frac{\mathrm{d}}{\mathrm{d}t}(\Psi_t^{-1}(x)),\end{aligned}$$

as desired. □

Thus, the spatial velocity at $(q_0,t)\in Q\times\mathbb{R}$ is obtained by taking the tangent vector to the curve $\Psi_t^{-1}(q_0)$, and then "pushing" this vector by the map $(-T_{\Psi_t^{-1}(x)}\Phi_{\Psi_t})$. In other words, $V^s_\Psi(q_0,t)$ can be thought of as the velocity of a point in Q traveling through q_0 at time t. This is exactly the interpretation of spatial velocity given in Ref. 5

C. Spatial and body momenta

In this section we define the spatial and body momenta for a rigid body. We identify $\mathfrak{o}(\ker(\tau))$ with $\ker(\tau)$ by the inverse of the map defined earlier and denote the angular velocities thought of as taking values in $\ker(\tau)$ by $V^b_{\Psi,\mathrm{ang}}$ and $V^s_{\Psi,\mathrm{ang}}$. Given a rigid body $(\mathcal{B},\mu)$, a rigid motion Ψ, and a curve $u:\mathbb{R}\to\ker(\tau)$, we define the *instantaneous inertia tensor* $\mathbb{I}_c(t):\ker(\tau)\to\ker(\tau)$ by

$$\mathbb{I}_c(t)(u(t)) = \int_{\mathcal{B}(t)} (\Psi_t(x)-\Psi_t(x_c)) \times (u(t)\times(\Psi_t(x)-\Psi_t(x_c)))\,\mathrm{d}\mu(t),$$

where $\mathcal{B}(t)=\Psi_t(\mathcal{B})$ and $u(t)\in\ker(\tau)$. Notice that, since the integrand is in $\ker(\tau)$, so too will be the integral. The following result shows what the spatial angular momentum looks like in terms of the inertia tensor of the body about its center of mass.

Lemma 5.7: $\mathbb{I}_c(t)(\omega_\Psi(t))=R_\Psi(t)\mathbb{I}_c(R_\Psi^{-1}(t)\omega_\Psi(t))$.

Proof: We represent by $\mathcal{B}(t)$ the rigid body after it has undergone the transformation Ψ_t and the corresponding mass distribution by $\mathrm{d}\mu(t)$. We compute

$$\begin{aligned}
\mathbb{I}_c(t)(\omega_\Psi(t)) &= \int_{\mathcal{B}(t)} (\Psi_t(x)-\Psi_t(x_c)) \times (\omega_\Psi(t)\times(\Psi_t(x)-\Psi_t(x_c)))\mathrm{d}\mu(t)\\
&= \int_{\mathcal{B}(t)} (\Psi_{t,V}(x-x_c)) \times (\omega_\Psi(t)\times(\Psi_{t,V}(x-x_c)))\mathrm{d}\mu(t)\\
&= \int_{\mathcal{B}(t)} (R_\Psi(t)(x-x_c)) \times (\omega_\Psi(t)\times(R_\Psi(t)(x-x_c)))\mathrm{d}\mu(t)\\
&= R_\Psi(t)\int_{\mathcal{B}} (x-x_c)\times(R_\Psi^{-1}(t)\omega_\Psi(t)\times(x-x_c))\mathrm{d}\mu = R_\Psi(t)\mathbb{I}_c(R_\Psi^{-1}(t)\omega_\Psi(t)),
\end{aligned}$$

where we have used the fact that $x-x_c\in\ker(\tau)$, and therefore $\Psi_{t,V}(x-x_c)=R_\Psi(t)(x-x_c)$. □

We can now define spatial and body momenta.

Definition 5.8: Let $(\mathcal{B},\mu)$ be a rigid body in a Galilean spacetime $\mathcal{G}$ and let Ψ be a rigid motion.

(i) *The spatial momentum is a map* $p_{\Psi,\mathcal{B}}:\mathbb{R}\to\ker(\tau)\times V$ *given by*

$$p_{\Psi,\mathcal{B}}(t) = (\mathbb{I}_c(t)V^s_{\Psi,\mathrm{ang}},\mu(\mathcal{B})V^s_{\Psi,\mathrm{lin}})(R_\Psi(t),\Psi_t(x_c),t).$$

(ii) *The body momentum is the map* $P_{\Psi,\mathcal{B}}:\mathbb{R}\to\ker(\tau)\times V$ *given by*

$$P_{\Psi,\mathcal{B}}(t) = (\mathbb{I}_c(t)V^b_{\Psi,\mathrm{ang}},\mu(\mathcal{B})V^b_{\Psi,\mathrm{lin}})(\mathrm{id}_{\ker(\tau)},x_c,t).$$

The following result can be readily proved using Lemma 5.5.

Proposition 5.9: Let $(\mathcal{B},\mu)$ *be a rigid body in a Galilean spacetime* $\mathcal{G}$ *and let* Ψ *be a rigid motion. Then*

(i) $p_{\Psi,\mathcal{B}}(t)=(\mathbb{I}_c(t)\omega_\Psi(t),\mu(\mathcal{B})\mathrm{d}/\mathrm{d}t\Psi_t(x_c))$,
(ii) $P_{\Psi,\mathcal{B}}(t)=(R_\Psi(t)^{-1}\mathbb{I}_c(t)\omega_\Psi(t),\mu(\mathcal{B})\Psi_{t,V}^{-1}\mathrm{d}/\mathrm{d}t\Psi_t(x_c))$.

Given a rigid body $(\mathcal{B},\mu)$, define an equivalence class of Galilean mappings as follows. Two mappings ϕ and $\psi\in\mathrm{Gal}(\mathcal{G})$ are called $\mathcal{B}$-*equivalent* if $\phi(\mathcal{B})=\psi(\mathcal{B})$. It is easy to see that this is an equivalence relation. In such a case, we denote the equivalence class containing ϕ by $[\phi]_\mathcal{B}$. In other words, any two mappings in the equivalence class $[\phi]_\mathcal{B}$ map the rigid body $\mathcal{B}$ to the same set of points in $\mathcal{E}$. The following result is readily verified.

Proposition 5.10: $\phi\in[\psi]_\mathcal{B}$ *if and only if* $\phi(x_c)=\psi(x_c)$ *and* $R_\phi=R_\psi$.

Proof: If $\phi\in[\psi]_\mathcal{B}$ then, for each $x\in\mathcal{B}$, we have $\phi(x)=\psi(x)$. Since $\mathcal{B}$ is a subset of $\mathcal{E}(s_0)$

(which is an affine space modeled on $\ker(\tau)$), we can write $x \in \mathcal{B}$ as $x = x_c + w$ for some $w \in \ker(\tau)$. We thus have

$$\phi(x_c + w) = \psi(x_c + w),$$

which implies that

$$\phi(x_c + w) - \phi(x_c) = \psi(x_c + w) - \psi(x_c).$$

We thus have $\phi_V(w) = \psi_V(w)$ and thus $R_\phi w = R_\psi w$. Conversely, assume that ψ is such that $R_\psi = R_\phi$ and $\psi(x_c) = \phi(x_c)$. By reversing the argument above, it is easy to show that $\phi(x) = \psi(x)$ for all $x \in \mathcal{B}$. □

Given a rigid body $(\mathcal{B}, \mu)$ and a rigid motion Ψ, a rigid motion $\tilde{\Psi}$ is *$\mathcal{B}$-equivalent* to Ψ if $\tilde{\Psi}_t \in [\Psi_t]_{\mathcal{B}}$ for each $t \in \mathbb{R}$. The following result is immediate.

Lemma 5.11: Let $(\mathcal{B}, \mu)$ be a rigid body in a Galilean spacetime and let Ψ be a motion. If a rigid motion $\tilde{\Psi}$ is $\mathcal{B}$-equivalent to Ψ, then $p_{\tilde{\Psi},\mathcal{B}} = p_{\Psi,\mathcal{B}}$.

D. Galilean–Euler equations

In this section we derive the equations of motion for a rigid body in our general framework. As remarked in Sec. I, the problem of finding the equations of motion for rigid bodies has a rich history. The key observation of Newton and Euler is that the free motion of a rigid body is completely determined by imposing conservation of spatial linear and angular momenta. The observation that this approach generalizes to other physical settings such as hydrodynamics was first made by Arnol'd[13] (see also Ref. 2). Using his method, the Euler equations for an incompressible fluid can be written as geodesic equations on a certain infinite-dimensional Lie group. We note that the Galilean group $\mathrm{Gal}(\mathcal{G})$ of a Galilean spacetime $\mathcal{G}$ does not have a natural invariant metric, and thus we cannot use Arnol'd's method in this setup. Intuitively speaking, $\mathrm{Gal}(\mathcal{G})$ is "too big" to uniquely determine the physical motion of the body. We shall have more to say on this matter in Sec. VI E. We use the principle of conservation of spatial momentum to derive differential equations in terms of "spatial" as well as "body" quantities that describe the physical motion of the body. We also show that, if a rigid motion Ψ satisfies these equations for the body $(\mathcal{B}, \mu)$, then every rigid motion $\mathcal{B}$-equivalent to Ψ also satisfies the equations. From the definitions given in the previous section, it can be seen that $p_{\Psi,\mathcal{B}}(t) = (\ell_{\Psi,\mathcal{B}}(t), m_{\Psi,\mathcal{B}}(t)) = (R_\Psi(t) L_{\Psi,\mathcal{B}}(t), \Psi_{t,V} M_{\Psi,\mathcal{B}}(t))$.

Proposition 5.12 (Galilean-Euler equations): Let $(\mathcal{B}, \mu)$ be a rigid body in a Galilean spacetime and let Ψ be a rigid motion. The following statements are equivalent:

(i) *the spatial momentum $p_{\Psi,\mathcal{B}}$ is conserved;*

(ii) *the motion of the body satisfies the spatial Galilean–Euler equations*

$$\mathbb{I}_c(\dot{\omega}_\Psi(t)) = \mathbb{I}_c(\omega_\Psi(t)) \times \omega_\Psi(t)$$

$$\ddot{x}_c(t) = 0,$$

where $\ddot{x}_c(t) = (\mathrm{d}^2/\mathrm{d}t^2)(\Psi_t(x_c))$;

(iii) *the motion of the body satisfies the body Galilean–Euler equations*

$$\dot{L}_{\Psi,\mathcal{B}}(t) = L_{\Psi,\mathcal{B}}(t) \times \Omega_\Psi(t),$$

$$\dot{M}_{\Psi,\mathcal{B}}(t) = -(\eta_V(t))_V(M_{\Psi,\mathcal{B}}(t)),$$

where $(\eta_V(t))_V(M_{\Psi,\mathcal{B}}(t))$ is the infinitesimal generator corresponding to $\eta_V(t) = \Psi_{t,V}^{-1} \dot{\Psi}_{t,V}$ of

the action of $\mathrm{Lin}(\mathcal{G})$ *on* V.

Furthermore,

(iv) *if* $\tilde{\Psi}$ *is a rigid motion* $\mathcal{B}$*-equivalent to* Ψ*, then* Ψ *can be replaced with* $\tilde{\Psi}$ *in the above statements.*

Proof: Conservation of spatial momentum implies that $\dot{p}_{\Psi,\mathcal{B}}(t)=0$. The equation $\ddot{x}_c(t)=0$ immediately follows. To derive the first equation, we note that

$$\mathbb{I}_c(t)\omega_\Psi(t) = R_\Psi(t)\mathbb{I}_c(R_\Psi^{-1}\omega_\Psi(t)).$$

Therefore,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}R_\Psi(t)\mathbb{I}_c(R_\Psi^{-1}\omega_\Psi(t)) &= \dot{R}_\Psi(t)\mathbb{I}_c(R_\Psi^{-1}\omega_\Psi(t) + R_\Psi(t)\mathbb{I}_c(R_\Psi^{-1}\dot{\omega}_\Psi(t))\\ &= \hat{\omega}_\Psi(t)R_\Psi(t)\mathbb{I}_c(R_\Psi^{-1}\omega_\Psi(t)) + R_\Psi(t)\mathbb{I}_c(R_\Psi^{-1}\dot{\omega}_\Psi(t))\\ &= \hat{\omega}_\Psi(t)\mathbb{I}_c(\omega_\Psi(t)) + \mathbb{I}_c(t)\dot{\omega}_\Psi(t) = 0,\end{aligned}$$

by conservation of spatial momentum. Therefore

$$\mathbb{I}_c(\dot{\omega}_\Psi(t)) = -\hat{\omega}_\Psi(t)\mathbb{I}_c(\omega_\Psi(t)) = \mathbb{I}_c(\omega_\Psi)\times\omega_\Psi(t)).$$

Next, we write spatial momentum in terms of the body momentum. That is,

$$p_{\Psi,\mathcal{B}}(t) = (R_\Psi(t)L_{\Psi,\mathcal{B}}, \Psi_{t,V}M_{\Psi,\mathcal{B}}(t)).$$

Conservation of spatial momentum implies that

$$\frac{\mathrm{d}}{\mathrm{d}t}(R_\Psi(t)L_{\Psi,\mathcal{B}}(t)) = 0 \text{ and } \frac{\mathrm{d}}{\mathrm{d}t}(\Psi_{t,V}M_{\Psi,\mathcal{B}}(t)) = 0.$$

The first equation gives

$$0 = (\dot{R}_\Psi(t)L_{\Psi,\mathcal{B}}(t) + (R_\Psi(t)\dot{L}_{\Psi,\mathcal{B}}(t) = R_\Psi(t)\tilde{\Omega}_\Psi(t)L_{\Psi,\mathcal{B}}(t) + R_\Psi(t)\dot{L}_{\Psi,\mathcal{B}}(t).$$

We therefore get

$$\dot{L}_{\Psi,\mathcal{B}}(t) = -\hat{\Omega}_\Psi(t)L_{\Psi,\mathcal{B}}(t) = L_{\Psi,\mathcal{B}}(t)\times\Omega_\Psi(t).$$

Next, consider the second equation. Written appropriately in terms of the action Φ^V of $\mathrm{Lin}(\mathcal{G})$ on V, the equation becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi^V_{\Psi_{t,V}}(M_{\Psi,\mathcal{B}}(t)) = 0.$$

We compute

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi^V_{\Psi_{t,V}}(M_{\Psi,\mathcal{B}}(t)) = T_{M_{\Psi,\mathcal{B}(t)}}\Phi^V_{\Psi_{t,V}}\dot{M}_{\Psi,\mathcal{B}}(t) + T_{M_{\Psi,\mathcal{B}}}\Phi^V_{\Psi_{t,V}}(\eta_V(t))_V\ (M)) = 0,$$

which gives us the requisite equation. The final part of the proposition follows directly from Lemma 5.11. □

Remarks 5.13: (1) Proposition 5.12 shows that if a motion Ψ satisfies the Galilean–Euler equations for a rigid body so does every motion $\mathcal{B}$-equivalent to Ψ. In other words, the Galilean–Euler equations hold for an equivalence class of motions specified by the rigid body.

(2) The Galilean–Euler equations are very general because they have been derived in the setting of an abstract Galilean spacetime without requiring an observer. However, the generality of the treatment makes certain things less obvious. In particular, it is not clear how the classical Euler equations fit into this setup and, if they do, whether or not there is a geometrical explanation for it. We shall see, in the next section, that the presence of an observer allows us to answer these questions.

VI. DYNAMICS OF RIGID BODIES IN THE PRESENCE OF AN OBSERVER

In Sec. V we formulated rigid body dynamics in an observer-independent way. In this section, we shall explore the effect of introducing an observer in this formulation. In Sec. VI A we introduce canonical velocities associated with a rigid motion in the presence of an observer. In Sec. VI B we show that in the presence of an observer, the body and spatial velocities defined in Sec. V project to the corresponding canonical velocities. In the next section, we show that the momenta also project to the well-known quantities in the presence of the observer. Finally, in Sec. VI D, we illustrate how an observer enables us to recover the classical Euler equations for a rigid body.

A. Canonical velocities

Consider a rigid motion Ψ in a Galilean spacetime $\mathcal{G}=(\mathcal{E},V,g,\tau)$. In Sec. V B, we introduced the curves $\eta_\Psi(t)$ and $\xi_\Psi(t)\in\mathfrak{gal}(\mathcal{G})$ corresponding to Ψ. The following result provides a decomposition of these curves in the presence of an observer.

Proposition 6.1: Let $\mathcal{G}=(\mathcal{E},V,g,\tau)$ be a Galilean spacetime with $\mathcal{O}$ an observer and Ψ a rigid motion. For $s_0\in I_\mathcal{G}$, let

$$\iota_{\mathcal{O}_{s_0}}(\Psi_t)=(R_\Psi(t),r_{\Psi,\mathcal{O}}(t),u_{\Psi,\mathcal{O}}(t),t).$$

Then, the following statements hold:

(i) *the image of $\eta_\Psi(t)\in\mathfrak{gal}(\mathcal{G})$ under the isomorphism of the Lie algebras induced by $\iota_{\mathcal{O}_{s_0}}$ is*

$$(\hat{\Omega}_\Psi(t),V_{\Psi,\mathcal{O}}(t)-R_\Psi^{-1}(t)u_{\Psi,\mathcal{O}}(t),R_\Psi^{-1}(t)\dot{u}_{\Psi,\mathcal{O}}(t),1)\in\mathfrak{gal}(\mathcal{G}_{\mathrm{can}});$$

(ii) *the image of $\xi_\Psi(t)\in\mathfrak{gal}(\mathcal{G})$ under the isomorphism of Lie algebra induced by $\iota_{\mathcal{O}_{s_0}}$ is*

$$(\hat{\omega}_\Psi(t),v_{\Psi,\mathcal{O}}(t)-t(\dot{u}_{\Psi,\mathcal{O}}(t)+u_{\Psi,\mathcal{O}}(t)\times\omega_\Psi(t)),\dot{u}_{\Psi,\mathcal{O}}(t)+u_{\Psi,\mathcal{O}}(t)\times\omega_\Psi(t),1)\in\mathfrak{gal}(\mathcal{G}_{\mathrm{can}}),$$

where $V_{\Psi,\mathcal{O}}(t)=R_\Psi^{-1}(t)\dot{r}_{\Psi,\mathcal{O}}(t)$, and $v_{\Psi,\mathcal{O}}(t)=\dot{r}_{\Psi,\mathcal{O}}(t)+r_{\Psi,\mathcal{O}}(t)\times\omega_\Psi(t)$.

Proof: We start by faithfully representing $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$ in a vector space. We let $W=\ker(\tau)\oplus\mathbb{R}\oplus\mathbb{R}$ and, for $g=(R,r,u,t)\in\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$, define an isomorphism ρ_g of W by

$$(\mu,\sigma,\xi)\mapsto(R(\mu)+\sigma u+\xi r,\sigma+\xi t,\xi).$$

One readily verifies that the map $\rho:\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})\to GL(W)$ defined by $\rho(g)=\rho_g$ is a homomorphism. To see that the representation is faithful, suppose that

$$(\mu,\sigma,\xi)\mapsto(R(\mu)+\sigma u+\xi r,\sigma+\xi t,\xi)=(\mu,\sigma,\xi)$$

for all $(\mu,\sigma,\xi)\in W$. Then we must have $\sigma+\xi t=0$, for all $\sigma,\xi\in\mathbb{R}$, implying that $t=0$. Similarly, $R(\mu)+\sigma u+\xi r=\mu$ for all $(\mu,\sigma,\xi)\in W$ implies that $r=0$, $u=0$, and $R=\mathrm{id}_{\ker(\tau)}$. Thus the representation is faithful. In block matrix form, the representation of (R,r,u,t) on W is

$$\begin{bmatrix} R & u & r \\ 0 & 1 & t \\ 0 & 0 & 1 \end{bmatrix} \in GL(W).$$

We then compute

$$\begin{bmatrix} R & u & r \\ 0 & 1 & t \\ 0 & 0 & 1 \end{bmatrix}^{-1} = \begin{bmatrix} R^{-1} & -R^{-1}u & R^{-1}(tu-r) \\ 0 & 1 & -t \\ 0 & 0 & 1 \end{bmatrix}.$$

With this expression, both parts follow from direct computation. □

We call the first two components in (i) respectively, the *canonical body angular velocity*, and the *canonical body linear velocity*, and denote them by $\Omega^{\text{can}}_{\Psi}$ and $V^{\text{can}}_{\Psi,\mathcal{O}}$, respectively. Similarly, we call the first two components in (ii) respectively, the *canonical spatial angular velocity* and the *canonical spatial linear velocity*, and represent them by $\omega^{\text{can}}_{\Psi}$ and $v^{\text{can}}_{\Psi,\mathcal{O}}$, respectively.

B. Linear and angular velocities

Recall that, given a rigid motion Ψ in a Galilean spacetime, the body linear velocity is the map $V^{b}_{\Psi,\text{lin}}: Q\times\mathbb{R}\to V$ given by

$$V^{b}_{\Psi,\text{lin}}(R,x,t) = \Psi^{-1}_{t,V}\left(\frac{\mathrm{d}}{\mathrm{d}t}(\Psi_t(x\ ))\right),$$

and the spatial linear velocity is the map $V^{s}_{\Psi,\text{lin}}: Q\times\mathbb{R}\to V_{\mathcal{G}}$ given by

$$V^{s}_{\Psi,\text{lin}}(R,x,t) = -\Psi_{t,V}\left(\frac{\mathrm{d}}{\mathrm{d}t}(\Psi^{-1}_{t}(x))\right).$$

Let us see what these velocities look like in the presence of an observer. We look at body linear velocity first.

Proposition 6.2: Let Ψ be a rigid motion in a Galilean spacetime $\mathcal{G}=(\mathcal{E},V,g,\tau)$ and let $\mathcal{O}$ be an observer. Then $P_{\mathcal{O}}(V^{b}_{\Psi,\text{lin}}(R,x,t))=V^{\text{can}}_{\Psi,\mathcal{O}}(t)$.

Proof: We know that, for each instant $s_0\in I_{\mathcal{G}}$, there exists an isomorphism $\iota_{\mathcal{O}_{s_0}}$ such that, for a motion Ψ, we have

$$\iota_{\mathcal{O}_{s_0}}(\Psi_t) = (R_{\Psi}(t), r_{\Psi,\mathcal{O}}(t), u_{\Psi,\mathcal{O}}(t), t).$$

Also,

$$\Psi_t(x) = R_{\Psi}(t)(x-\mathcal{O}_{\pi_{\mathcal{G}}(x)}) + (\pi_{\mathcal{G}}(x)-s_0)u_{\Psi,\mathcal{O}}(t) + r_{\Psi,\mathcal{O}}(t) + \mathcal{O}_{\pi_{\mathcal{G}}(x)+t}.$$

Now, for $x\in\mathcal{O}$, we have

$$\Psi_t(x) = r_{\Psi,\mathcal{O}}(t) + \mathcal{O}_{\pi_{\mathcal{G}}(x)+t},$$

so we have

$$\frac{\mathrm{d}}{\mathrm{d}t}(\Psi_t(x)) = \dot{r}_{\Psi,\mathcal{O}}(t) + v_{\mathcal{O}}.$$

Next,

$$\Psi_{t,V}^{-1}\left(\frac{\mathrm{d}}{\mathrm{d}t}\,\Psi_t(x)\right) = \Psi_{t,V}^{-1}(\dot{r}_{\Psi,\mathcal{O}}(t) + v_{\mathcal{O}}) = \Psi_t^{-1}(\dot{r}_{\Psi,\mathcal{O}}(t) + v_{\mathcal{O}} + \mathcal{O}_{s_0}) - \Psi_t^{-1}(\mathcal{O}_{s_0})$$
$$= R_\Psi^{-1}(t)(\dot{r}_{\Psi,\mathcal{O}}(t) + v_{\mathcal{O}} + \mathcal{O}_{s_0} - \mathcal{O}_{1+s_0}) - R_\Psi^{-1}(t)u_{\Psi,\mathcal{O}}(t)$$
$$+ R_\Psi^{-1}(t)(tu_{\Psi,\mathcal{O}}(t) - r_{\Psi,\mathcal{O}}(t)) + (1-t)v_{\mathcal{O}} + \mathcal{O}_{s_0} - R_\Psi^{-1}(t)(tu_{\Psi,\mathcal{O}}(t)$$
$$- r_{\Psi,\mathcal{O}}(t)) + tv_{\mathcal{O}} - \mathcal{O}_{s_0}$$
$$= R_\Psi^{-1}(t)\dot{r}_{\Psi,\mathcal{O}}(t) - R_\Psi^{-1}(t)u_{\Psi,\mathcal{O}}(t) + v_{\mathcal{O}}.$$

From this, the result follows. □

Let us look at the spatial linear velocity now.

Proposition 6.3: Let Ψ be a motion in a Galilean spacetime $\mathcal{G}=(\mathcal{E},V,g,\tau)$ and let $\mathcal{O}$ be an observer. Then $P_{\mathcal{O}}(V^s_{\Psi,\mathrm{lin}}(R,x,t))=v^{\mathrm{can}}_{\Psi,\mathcal{O}}(t)$.

Proof: For $x\in\mathcal{O}$, we compute,

$$\Psi_t^{-1}(x) = R_\Psi^{-1}(t)(tu_{\Psi,\mathcal{O}}(t) - r_{\Psi,\mathcal{O}}(t)) - tv_{\mathcal{O}} + \mathcal{O}_{s_0}.$$

Therefore,

$$\frac{\mathrm{d}}{\mathrm{d}t}(\Psi_t^{-1}(x)) = R_\Psi^{-1}(t)(u_{\Psi,\mathcal{O}}(t) + t\dot{u}_{\Psi,\mathcal{O}}(t) - \dot{r}_{\Psi,\mathcal{O}}(t)) + (-R_\Psi^{-1}(t)\dot{R}_\Psi(t)R_\Psi^{-1}(t))(tu_{\Psi,\mathcal{O}}(t) - r_{\Psi,\mathcal{O}}(t))) - v_{\mathcal{O}}$$
$$= R_\Psi^{-1}(t)(u_{\Psi,\mathcal{O}}(t) + t\dot{u}_{\Psi,\mathcal{O}}(t) - \dot{r}_{\Psi,\mathcal{O}}(t)) - R_\Psi^{-1}(t)\hat{\omega}_\Psi(t)(tu_{\Psi,\mathcal{O}}(t) - r_{\Psi,\mathcal{O}}(t)) - v_{\mathcal{O}}$$
$$= R_\Psi^{-1}(t)u_{\Psi,\mathcal{O}}(t) + R_\Psi^{-1}(t)[t(\dot{u}_{\Psi,\mathcal{O}}(t) + u_\Psi(t)\times\omega_\Psi(t))]$$
$$- R_\Psi^{-1}(t)(\dot{r}_{\Psi,\mathcal{O}}(t) + r_{\Psi,\mathcal{O}}(t)\times\omega_\Psi(t)) - v_{\mathcal{O}}$$
$$= R_\Psi^{-1}(t)u_\Psi(t) - R_\Psi^{-1}(t)(v_{\Psi,\mathcal{O}}(t) - t(\dot{u}_{\Psi,\mathcal{O}}(t) + u_{\Psi,\mathcal{O}}(t)\times\omega_\Psi(t))) - v_{\mathcal{O}}.$$

Let us call the last expression $\dot{\Psi}_t^{-1}(x)$. Now, we compute

$$-\Psi_{t,V}\left(\frac{\mathrm{d}}{\mathrm{d}t}(\Psi_t^{-1}(x))\right) = \Psi_t(-\dot{\Psi}_t^{-1}(x) + \mathcal{O}_{s_0}) - \Psi_t(\mathcal{O}_{s_0})$$
$$= R_\Psi(t)(-\dot{\Psi}_t^{-1}(x) + \mathcal{O}_{s_0} - \mathcal{O}_{1+s_0}) + u_{\Psi,\mathcal{O}}(t) + r_{\Psi,\mathcal{O}}(t) + tv_{\mathcal{O}} + \mathcal{O}_{1+s_0}$$
$$- r_{\Psi,\mathcal{O}}(t) - tv_{\mathcal{O}} - \mathcal{O}_{s_0}$$
$$= R_\Psi(t)(-\dot{\Psi}_t^{-1}(x) - v_{\mathcal{O}}) + u_{\Psi,\mathcal{O}}(t) + v_{\mathcal{O}}$$
$$= R_\Psi(t)(R_\Psi^{-1}(t)(v_{\Psi,\mathcal{O}}(t) - t(\dot{u}_{\Psi,\mathcal{O}}(t) + u_{\Psi,\mathcal{O}}(t)\times\omega_\Psi(t))) - u_{\Psi,\mathcal{O}}(t) + u_{\Psi,\mathcal{O}}(t)$$
$$+ v_{\mathcal{O}} = v_{\Psi,\mathcal{O}}(t) - t(\dot{u}_{\Psi,\mathcal{O}}(t) + u_{\Psi,\mathcal{O}}(t)\times\omega_\Psi(t)) + v_{\mathcal{O}}.$$

From this the result follows. □

We notice that, in the presence of an observer, the spatial linear and body linear velocities project onto the canonical spatial linear and canonical body linear velocities, respectively.

C. Spatial and body momenta

We let $\mathcal{G}=(\mathcal{E},V,g,\tau)$ be a Galilean spacetime with Ψ a rigid motion, $\mathcal{O}$ an observer, and $(\mathcal{B},\mu)$ a rigid body with $\mathcal{B}\in\mathcal{E}(s_0)$. We next see how our definitions of spatial and body momenta look when we have an observer $\mathcal{O}$. In such a case, we have the following result.

Proposition 6.4: Let $\mathcal{G}=(\mathcal{E},V,g,\tau)$ be a Galilean spacetime with Ψ a rigid motion, $\mathcal{O}$ an observer, and $(\mathcal{B},\mu)$ a rigid body with $\mathcal{B}\in\mathcal{E}(s_0)$, and let $m_{\Psi,\mathcal{B}}$, $\ell_{\Psi,\mathcal{B}}$, $M_{\Psi,\mathcal{B}}$, and $L_{\Psi,\mathcal{B}}$ be as defined in Sec. V C. For $s_0\in I_{\mathcal{G}}$, let

$$\iota_{\mathcal{O}_{s_0}}(\Psi_t) = (R_\Psi(t), r_{\Psi,\mathcal{O}}(t), u_{\Psi,\mathcal{O}}(t), t).$$

Then the following statements hold:

(i) $P_{\mathcal{O}}(m_{\Psi,\mathcal{B}}(t)) = \mu(\mathcal{B})\dot{r}_{\Psi,\mathcal{O}}(t)$;
(ii) $P_{\mathcal{O}}(\ell_{\Psi,\mathcal{B}}(t)) = R_\Psi(t)\mathbb{I}_c(R_\Psi^{-1}(t)\omega_\Psi(t))$;
(iii) $P_{\mathcal{O}}(M_{\Psi,\mathcal{B}}(t)) = \mu(\mathcal{B})V^{\text{can}}_{\Psi,\mathcal{O}}(t)$;
(iv) $P_{\mathcal{O}}(L_{\Psi,\mathcal{B}}(t)) = \mathbb{I}_c(R_\Psi^{-1}(t)\omega_\Psi(t))$.

Proof: (i) We compute

$$P_{\mathcal{O}}(m_{\Psi,\mathcal{B}}(t)) = \mu(\mathcal{B})P_{\mathcal{O}}\left(\frac{\mathrm{d}}{\mathrm{d}t}(\Psi_t(x_c))\right) = \mu(\mathcal{B})P_{\mathcal{O}}(\dot{r}_{\Psi,\mathcal{O}}(t) + v_{\mathcal{O}}) = \mu(\mathcal{B})\dot{r}_{\Psi,\mathcal{O}}(t),$$

where we have used the computations carried out in Proposition 6.2.

Parts (ii) and (iv) are easily seen to be true since both $\ell_{\Psi,\mathcal{B}}$ and $L_{\Psi,\mathcal{B}}$ take their values in $\ker(\tau)$ and the projection $P_{\mathcal{O}}$ is the identity map on $\ker(\tau)$.

To obtain (iii), we compute

$$\begin{aligned} P_{\mathcal{O}}(M_{\Psi,\mathcal{B}}(t)) &= \mu(\mathcal{B})P_{\mathcal{O}}(\Psi_{t,V}^{-1}\left(\frac{\mathrm{d}}{\mathrm{d}t}(\Psi_t(x_c))\right) = \mu(\mathcal{B})P_{\mathcal{O}}(\Psi_{t,V}^{-1}(\dot{r}_{\Psi,\mathcal{O}}(t) + v_{\mathcal{O}})) \\ &= \mu(\mathcal{B})P_{\mathcal{O}}(R_\Psi^{-1}(t)\dot{r}_{\Psi,\mathcal{O}}(t) - R_\Psi^{-1}(t)u_{\Psi,\mathcal{O}}(t) + v_{\mathcal{O}}) = \mu(\mathcal{B})V^{\text{can}}_{\Psi,\mathcal{O}}(t), \end{aligned}$$

as desired. □

It is worth pointing out that the classical definition of spatial angular momentum requires an observer, and is different from ours. Given an observer $\mathcal{O}$ and a rigid motion Ψ, the *classical spatial angular momentum* $\ell^{\text{cl}}_{\Psi,\mathcal{B}}$ for a rigid body $(\mathcal{B},\mu)$ about its center of mass x_c is defined as

$$\ell^{\text{cl}}_{\Psi,\mathcal{B}}(t) = \int_{\mathcal{B}} P_{\mathcal{O}}(\Psi_t(x) - x_c) \times P_{\mathcal{O}}\left(\frac{\mathrm{d}}{\mathrm{d}t}(\Psi_t(x) - x_c)\right)\mathrm{d}\mu.$$

One can motivate this definition of spatial angular momentum by recalling how it might be defined for a particle of mass m (see, for example, Ref. 3). If a particle is moving in $\mathbb{R}^3$ following a curve $t \mapsto x(t)$, then we would define the spatial angular momentum at time t to be $mx(t) \times \dot{x}(t)$. This is exactly the intuition behind the definition of $\ell^{\text{cl}}_{\Psi,\mathcal{O}}$. Our definition of body angular momentum agrees with the classical one, and therefore we do not need to consider it separately. We shall see in the next section that the equations of motion derived on the basis of the conservation of classical spatial angular momentum are equivalent to the general spatial Euler equations. We have the following result.

Proposition 6.5: Let $(\mathcal{B},\mu)$ *be a rigid body in a Galilean spacetime* $\mathcal{G}$ *undergoing a rigid motion* Ψ, *and let* $\mathcal{O}$ *be an observer with the property that* $x_c \in \mathcal{O}$. *Then* $\ell^{\text{cl}}_{\Psi,\mathcal{B}}(t) = R_\Psi(t)\mathbb{I}_c(R_\Psi(t)^{-1}\omega_\Psi(t)) + \mu(\mathcal{B})r_{\Psi,\mathcal{O}}(t) \times \dot{r}_{\Psi,\mathcal{O}}(t)$.

Proof: We let $s_0 = \pi_{\mathcal{G}}(x_c)$, and use the isomorphism $\iota_{\mathcal{O}_{s_0}}$ between $\mathrm{Gal}(\mathcal{G})$ and $\mathrm{Gal}(\mathcal{G}_{\text{can}})$ to get

$$\Psi_t(x) = R_\Psi(t)(x - \mathcal{O}_{\pi_{\mathcal{G}}(x)}) + r_{\Psi,\mathcal{O}}(t) + tv_{\mathcal{O}} + \mathcal{O}_{\pi_{\mathcal{G}}(x)}, \quad x \in \mathcal{B},$$

which implies that $\Psi_t(x) - x_c = R_\Psi(t)(x - x_c) + r_{\Psi,\mathcal{O}}(t)$. The result is readily verified by using part (ii) of Lemma 3.1 in the computation of the integral. □

D. Euler equations of a rigid body

In this section we look at the Galilean–Euler equations, as derived in Sec. V D in the presence of an observer. Since we consider the abstract Galilean group in our analysis, derivatives of velocity boosts also appear in the equations. We first write down the general Galilean–Euler equations in the presence of an observer.

Proposition 6.6: Let $(\mathcal{B},\mu)$ *be a rigid body,* Ψ *a rigid motion, and let* $\mathcal{O}$ *be an observer. For* $s_0 \in I_{\mathcal{G}}$, *let*

$$\iota_{\mathcal{O}_{s_0}}(\Psi_t) = (R_\Psi(t), r_{\Psi,\mathcal{O}}(t), u_{\Psi,\mathcal{O}}(t), t)$$

for each $t \in \mathbb{R}$. *The following statements hold:*

(i) the spatial Galilean–Euler equations for Ψ *are equivalent to*

$$\mathbb{I}_c(\dot{\omega}_\Psi(t)) = \mathbb{I}_c(\omega_\Psi(t)) \times \omega_\Psi(t)$$

$$\ddot{r}_{\Psi,\mathcal{O}}(t) = -\ddot{R}_\Psi(t)(x_c - \mathcal{O}_{\pi_{\mathcal{G}}(x_c)}) - (\pi_{\mathcal{G}}(x_c) - s_0)\ddot{u}_{\Psi,\mathcal{O}}(t);$$

(ii) the body Galilean–Euler equations for Ψ *are equivalent to*

$$\dot{L}_{\Psi,\mathcal{B}}(t) = L_{\Psi,\mathcal{B}}(t) \times \Omega_\Psi(t),$$

$$\dot{M}_{\Psi,\mathcal{B}}(t) = P_{\mathcal{O}}(M_{\Psi,\mathcal{B}}(t)) \times \Omega_\Psi(t) - R_\Psi^{-1}(t)\dot{u}_{\Psi,\mathcal{O}}(t).$$

Proof: (i) The first spatial Galilean–Euler equation evolves on $\ker(\tau)$ and thus remains the same under the projection $P_{\mathcal{O}}$. For the second equation, we compute

$$\begin{aligned} 0 = \ddot{x}_c(t) &= \frac{\mathrm{d}}{\mathrm{d}t}(\dot{R}_\Psi(t)(x_c - \mathcal{O}_{\pi_{\mathcal{G}}}(x_c)) + (\pi_{\mathcal{G}}(x_c) - s_0)\dot{u}_{\Psi,\mathcal{O}}(t) + \dot{r}_{\Psi,\mathcal{O}}(t) + v_{\mathcal{O}}) \\ &= \ddot{R}_\Psi(t)(x_c - \mathcal{O}_{\pi_{\mathcal{G}}}(x_c)) + \ddot{r}_{\Psi,\mathcal{O}}(t) + (\pi_{\mathcal{G}}(x_c) - s_0)\ddot{u}_{\Psi,\mathcal{O}}(t), \end{aligned}$$

from which we get the required equation.

(ii) Similarly, the first body Galilean–Euler equation remains unchanged under the projection onto $\ker(\tau)$. To get the second equation we use the definition of $M_{\Psi,\mathcal{O}}$ and the relation $\Psi_V(v) = R_\Psi P_{\mathcal{O}}(v) + \tau(v)(u_{\Psi,\mathcal{O}} + v_{\mathcal{O}})$, and compute

$$\begin{aligned} 0 = \frac{\mathrm{d}}{\mathrm{d}t} m_{\Psi,\mathcal{B}}(t) &= \frac{\mathrm{d}}{\mathrm{d}t}\Psi_{t,V}(M_{\Psi,\mathcal{O}}(t)) = \frac{\mathrm{d}}{\mathrm{d}t}(R_\Psi(t)P_{\mathcal{O}}(M_{\Psi,\mathcal{O}}(t))) + \tau(M_{\Psi,\mathcal{O}}(t))(u_{\Psi,\mathcal{O}}(t) + v_{\mathcal{O}})) \\ &= \dot{R}_\Psi(t)P_{\mathcal{O}}(M_{\Psi,\mathcal{O}}(t)) + R_\Psi(t)\frac{\mathrm{d}}{\mathrm{d}t}(P_{\mathcal{O}}(M_{\Psi,\mathcal{O}}(t))) + \dot{u}_{\Psi,\mathcal{O}}(t) \\ &= R_\Psi(t)\hat{\Omega}P_{\mathcal{O}}(M_{\Psi,\mathcal{O}}(t)) + R_\Psi(t)(\dot{M}_{\Psi,\mathcal{O}}(t))) + \dot{u}_{\Psi,\mathcal{O}}(t), \end{aligned}$$

since $M_{\Psi,\mathcal{O}}(t) \in V_{\mathcal{G}}$ and thus $\dot{M}_{\Psi,\mathcal{O}}(t) = (d/\mathrm{d}t)P_{\mathcal{O}}(M_{\Psi,\mathcal{O}}(t))$. The result now follows. □

Let us now show that we get the same equations of motion if we use the classical spatial angular momentum $\ell^{\mathrm{cl}}_{\Psi,\mathcal{B}}$ instead of $\ell_{\Psi,\mathcal{B}}$. Let us write $p^{\mathrm{cl}}_{\Psi,\mathcal{B}} = (\ell^{\mathrm{cl}}_{\Psi,\mathcal{B}}, m_{\Psi,\mathcal{B}})$ to denote the classical spatial momentum. We also call the equations of motion derived on the basis of the conservation of classical spatial momentum the *classical spatial Euler equations*. We have the following result.

Proposition 6.7: Let $(\mathcal{B},\mu)$ *be a rigid body undergoing a rigid motion* Ψ *in a Galilean spacetime* $\mathcal{G}$. *Let* $\mathcal{O}$ *be an observer with the property that* $x_c \in \mathcal{O}$. *The following statements are equivalent*:

(i) the classical spatial momentum $p^{\mathrm{cl}}_{\Psi,\mathcal{B}}$ *is conserved;*
(ii) the motion of the body satisfies the classical spatial Euler equations

$$\mathbb{I}_c(\dot{\omega}_\Psi(t)) = \mathbb{I}_c(\omega_\Psi(t)) \times \omega_\Psi(t),$$

$$\ddot{r}_{\Psi,\mathcal{O}}(t) = 0.$$

Proof: As before, we let $s_0=\pi_{\mathcal{G}}(x_c)$ and consider the isomorphism $\iota_{\mathcal{O}_{s_0}}$, using which, it is easy to see that the conservation of spatial linear momentum $m_{\Psi,\mathcal{B}}$ implies that $\ddot{r}_{\Psi,\mathcal{O}}(t)=0$. It is a simple computation to show that this also implies that

$$\frac{\mathrm{d}}{\mathrm{d}t}(\ell^{\mathrm{cl}}_{\Psi,\mathcal{B}}(t)) = \frac{\mathrm{d}}{\mathrm{d}t}(R_\Psi(t)\mathbb{I}_c(R_\Psi(t)^{-1}\omega_\Psi(t))) = \frac{\mathrm{d}}{\mathrm{d}t}(l_{\Psi,\mathcal{B}}(t)).$$

The result now follows. □

E. The Galilean connection

In Proposition 6.6, we wrote down the general form of the Galilean–Euler equations in the presence of an observer. Since we have considered the abstract Galilean group in our analysis, we have imposed no restrictions on the velocity boost (the "$u_{\Psi,\mathcal{O}}$" component) corresponding to a rigid motion. This is the reason why the derivatives of these velocity boosts appear in the equations given in Proposition 6.6. Recall that the classical Euler equations for a rigid body do not include these derivative terms because the velocity boosts are assumed to be "uniform." In this section, we explain how, in our general setting, an observer allows us to recover the classical equations of motion for a rigid body by defining a special geometric structure (namely a principal connection) on $\mathrm{Gal}(\mathcal{G})$. We refer to Ref. 14 for the definitions and properties of principal connections.

Let $Q=O(\ker(\tau))\times\mathcal{E}$ and $(\mathcal{B},\mu)$ be a rigid body. For the center of mass $x_c\in\mathcal{E}$ of the rigid body, consider the map

$$\pi_c:\mathrm{Gal}(\mathcal{G})\to Q$$

$$\psi\mapsto(R_\psi,\psi(x_c)).$$

An observer $\mathcal{O}$ defines a map $\pi_{c,\mathcal{O}}:\mathrm{Gal}(\mathcal{G})\to O(\ker(\tau))\times\ker(\tau)\times\mathbb{R}$ given by

$$\psi\mapsto(R_\psi,P_{\mathcal{O}}(\psi(x_c)-x_c),\tau(\psi(x_c)-x_c)).$$

We also know that, for $s_0\in I_{\mathcal{G}}$, there is an isomorphism $\iota_{\mathcal{O}_{s_0}}$ from $\mathrm{Gal}(\mathcal{G})$ to $O(\ker(\tau))\times\ker(\tau)\times\ker(\tau)\times\mathbb{R}$ given by

$$\psi\mapsto(R_\psi,r_{\psi,\mathcal{O}},u_{\psi,\mathcal{O}},t_\psi).$$

For $x_c\in\mathcal{O}$, we can write

$$\psi(x_c)=R_\psi(x_c-x_c)+(\pi_{\mathcal{G}}-s_0)u_{\psi,\mathcal{O}}+r_{\psi,\mathcal{O}}+t_\psi v_{\mathcal{O}}+x_c,$$

and thus we have

$$P_{\mathcal{O}}(\psi(x_c)-x_c)=(\pi_{\mathcal{G}}(x_c)-s_0)u_{\psi,\mathcal{O}}+r_{\psi,\mathcal{O}}.$$

Also, $\tau(\psi(x_c)-x_c)=t_\psi$, so the map $\pi_{c,\mathcal{O}}$ induces a map

$$\pi^{\mathrm{can}}_{c,\mathcal{O}}:\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})\to O(\ker(\tau))\times\ker(\tau)\times\mathbb{R}=\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})/\ker(\tau)$$

$$(R_\psi,r_{\psi,\mathcal{O}},u_{\psi,\mathcal{O}},t_\psi)\mapsto(R_\psi(\pi_{\mathcal{G}}-s_0)u_{\psi,\mathcal{O}}+r_{\psi,\mathcal{O}},t_\psi),$$

where the quotient $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})/\ker(\tau)$ corresponds to the following action of $\ker(\tau)$ on $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$:

$$\ker(\tau)\times\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})\to\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$$

$$(\mu,(R,r,u,s)) \mapsto (R, r-(\pi_{\mathcal{G}}(x_c)-s_0)\mu, u+\mu, s).$$

Thus, $\ker(\tau)$ acts on $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$ by appropriately changing the $r_{\psi,\mathcal{O}}$ and $u_{\psi,\mathcal{O}}$ components of a given $\psi \in \mathrm{Gal}(\mathcal{G})$ such that the resulting mapping gives the same physical motion of the body as ψ, that is, it lies in $[\psi]_{\mathcal{B}}$. We also write $\pi := \pi^{\mathrm{can}}_{c,\mathcal{O}} \circ \iota_{\mathcal{O}_{s_0}} : \mathrm{Gal}(\mathcal{G}) \to \mathrm{Gal}(\mathcal{G}_{\mathrm{can}})/\ker(\tau)$. It is clear that, given $\psi \in \mathrm{Gal}(\mathcal{G})$, a Galilean mapping $\phi \in [\psi]_{\mathcal{B}}$ if and only if $\pi(\phi)=\pi(\psi)$. We have the following result.

Proposition 6.8: Let $(\mathcal{B},\mu)$ be a rigid body in a Galilean spacetime and $\mathcal{O}$ be an observer. For fixed $s_0 \in I_{\mathcal{G}}$, the map $\omega_{\mathrm{can}} : T\mathrm{Gal}(\mathcal{G}_{\mathrm{can}}) \to \ker(\tau)$ given by

$$\omega_{\mathrm{can}}(X_R,X_r,X_u,X_t) = X_u, \quad (X_R,X_r,X_u,X_t) \in T_{(R,r,u,t)}\mathrm{Gal}(\mathcal{G}_{\mathrm{can}}),$$

is a principal connection one-form in the bundle

$$\pi^{\mathrm{can}}_{c,\mathcal{O}} : \mathrm{Gal}(\mathcal{G}_{\mathrm{can}}) \to \mathrm{Gal}(\mathcal{G}_{\mathrm{can}})/\ker(\tau).$$

Proof: Given $X=(X_R,X_r,X_u,X_t) \in T_{(R,r,u,t)}\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$, it is easy to see that

$$T\pi^{\mathrm{can}}_{c,\mathcal{O}}(X_R,X_R,X_u,X_t) = (X_R, X_r + (\pi_{\mathcal{G}}(x_c)-s_0)X_u, X_t).$$

The observer $\mathcal{O}$ allows us to decompose X into its *vertical* and *horizontal* components as follows. We write

$$X = \mathrm{hor}(X) + \mathrm{ver}(X), \tag{6}$$

where

$$\mathrm{hor}(X) = (X_R, X_r + (\pi_{\mathcal{G}}(x_c)-s_0)X_u, 0, X_t),$$

$$\mathrm{ver}(X) = (0, -(\pi_{\mathcal{G}}(x_c)-s_0)X_u, X_u, 0).$$

It can be seen that $T\pi^{\mathrm{can}}_{c,\mathcal{O}}(\mathrm{ver}(X))=0$, and $\omega_{\mathrm{can}}(\mathrm{hor}(X))=0$. Thus (6) defines an Ehresmann connection in $\pi^{\mathrm{can}}_{c,\mathcal{O}} : \mathrm{Gal}(\mathcal{G}_{\mathrm{can}}) \to O(\ker(\tau)) \times \ker(\tau) \times \mathbb{R}$. Next, the infinitesimal generator $\zeta_{\mathrm{Gal}(\mathcal{G})}$ corresponding to $\zeta \in \ker(\tau)$ for the action of $\ker(\tau)$ on $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$ is given by

$$\zeta_{\mathrm{Gal}(\mathcal{G})}(R,r,u,s) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} (R, r-(\pi_{\mathcal{G}}(x_c)-s_0)\exp(\zeta t), u+\exp(\zeta t), s) = (0, -(\pi_{\mathcal{G}}(x_c)-s_0)\zeta, \zeta, 0),$$

and thus, by definition,

$$\omega_{\mathrm{can}}(\zeta_{\mathrm{Gal}(\mathcal{G})}(R,r,u,s)) = \zeta.$$

Next, given $h \in \ker(\tau)$ and $X=(X_R,X_r,X_u,X_t) \in T_{(R,r,u,t)}\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$, it is easy to see that $\omega_{\mathrm{can}}(T_{(R,r,u,t)}\Phi_h X) = \mathrm{ad}_h \cdot \omega_{\mathrm{can}}(X)$, where $\Phi_h : \mathrm{Gal}(\mathcal{G}_{\mathrm{can}}) \to \mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$ is the action of $\ker(\tau)$ on $\mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$ and $\mathrm{ad}_h : \mathfrak{gal}(\mathcal{G}_{\mathrm{can}}) \to \mathfrak{gal}(\mathcal{G}_{\mathrm{can}})$ is defined by $\mathrm{ad}_h(\beta) = T_e L_h R_{h^{-1}}(\beta)$, $\beta \in \mathfrak{gal}(\mathcal{G}_{\mathrm{can}})$. So ω_{can} is indeed a connection one-form. □

Now, it is easy to see that $\ker(\tau)$ also acts on $\mathrm{Gal}(\mathcal{G})$ as follows:

$$\ker(\tau) \times \mathrm{Gal}(\mathcal{G}) \to \mathrm{Gal}(\mathcal{G})$$

$$(\mu, \psi) \mapsto \psi_\mu \circ \psi,$$

where ψ_μ is such that $\iota_{\mathcal{O}_{s_0}}(\psi_\mu) = (\mathrm{id}_{O(\ker(\tau))}, -(\pi_{\mathcal{G}}(x_c)-s_0)\mu, \mu, 0) \in \mathrm{Gal}(\mathcal{G}_{\mathrm{can}})$. In other words, $\ker(\tau)$ acts on $\mathrm{Gal}(\mathcal{G})$ as a subgroup of N_0 that fixes x_c. It can be seen that, for any $x \in \mathcal{E}$, we have $\psi_\mu(x) = x + (\pi_{\mathcal{G}}(x) - \pi_{\mathcal{G}}(x_c))\mu$. As a direct consequence of Proposition 6.8, we have the following corollary.

Corollary 6.9: The $\ker(\tau)$-valued one-form on $\mathrm{Gal}(\mathcal{G})$ defined by $\omega_{\mathcal{O}} = (\iota_{\mathcal{O}_{s_0}})^* \omega_{\mathrm{can}}$ is a connec-

tion one-form in the bundle $\mathrm{Gal}(\mathcal{G}) \to \mathrm{Gal}(\mathcal{G})/\ker(\tau)$. *We call* $\omega_{\mathcal{O}}$ *the* Galilean connection induced by $\mathcal{O}$.

Thus, the Galilean connection $\omega_{\mathcal{O}}$ induced by $\mathcal{O}$ is the pull-back of ω_{can} to $\mathrm{Gal}(\mathcal{G})$ by $\iota_{\mathcal{O}_{s_0}}$. It allows us to recover the classical Euler equations for a rigid body. It may be recalled that these equations do not contain derivatives of velocity boosts (that is, the "$\dot{u}_{\Psi,\mathcal{O}}$" terms) corresponding to the given rigid motion. The next proposition shows that, given a rigid motion, the Galilean connection allows us to choose a rigid motion that gives the same physical motion of the rigid body as the given rigid motion, and such that the corresponding Galilean–Euler equations do not contain the "$\dot{u}_{\Psi,\mathcal{O}}$" terms. This is made precise in the following proposition.

Proposition 6.10: Let $(\mathcal{B},\mu)$ *be a rigid body in a Galilean spacetime*, $\mathcal{O}$ *be an observer such that* $x_c \in \mathcal{O}$, *and* $s_0 \in I_{\mathcal{G}}$. *Then, for every rigid motion* Ψ, *there exists a rigid motion* Φ *with the following properties:*

(i) Φ *is* $\mathcal{B}$*-equivalent to* Ψ*;*
(ii) Φ_t *is horizontal with respect to* $\omega_{\mathcal{O}}$*;*
(iii) The Galilean-Euler equations for Φ *are equivalent to*

$$\mathbb{I}_c(t)(\dot{\omega}_\Phi(t)) = \mathbb{I}_c(t)(\omega_\Phi(t)) \times \omega_\Phi(t),$$

$$\ddot{r}_{\Phi,\mathcal{O}}(t) = 0,$$

$$\dot{L}_{\Phi,\mathcal{B}}(t) = L_{\Phi,\mathcal{B}}(t) \times \Omega_\Phi(t),$$

$$\dot{M}_{\Phi,\mathcal{B}}(t) = P_{\mathcal{O}}(M_{\Phi,\mathcal{B}}(t)) \times \Omega_\Phi(t).$$

Moreover, given $C_0 \in \ker(\tau)$, *the rigid motion* Φ *can be uniquely chosen such that* $u_{\Psi,\mathcal{O}}(t) = C_0$ *for every* $t \in \mathbb{R}$. *In particular, if* $x(t) = \pi(\Psi_t) = (R_\Psi(t), a_{\Psi,\mathcal{O}}(t), t)$, *then,* Φ_t *is the horizontal lift of* $x(t)$ *passing through* $\iota^{-1}_{\mathcal{O}_{s_0}}(R_\Psi(t_0), a_{\Psi,\mathcal{O}}(t_0) - (\pi_{\mathcal{G}}(x_c) - s_0)C_0, C_0, t_0)$ *for some (and therefore every)* $t_0 \in \mathbb{R}$.

Proof: For $x(t) = \pi(\Psi_t) = (R_\Psi(t), a_{\Psi,\mathcal{O}}(t), t) \in O(\ker(\tau)) \times \ker(\tau) \times \mathbb{R}$, we have, for each $t \in \mathbb{R}$,

$$(\pi^{\mathrm{can}}_{c,\mathcal{O}})^{-1}(R_\Psi(t), a_{\Psi,\mathcal{O}}(t), t) = \{(R_\Psi(t), a_{\Psi,\mathcal{O}}(t) - (\pi_{\mathcal{G}}(x_c) - s_0)\tilde{u}(t), \tilde{u}(t), t) \in \mathrm{Gal}(\mathcal{G}_{\mathrm{can}}) \,|\, \tilde{u}(t) \in \ker(\tau)\}.$$

Thus, all rigid motions Φ for which $\iota_{\mathcal{O}_{s_0}}(\Phi_t) \in (\pi^{\mathrm{can}}_{c,\mathcal{O}})^{-1}(R_\Psi(t), a_{\Psi,\mathcal{O}}(t), t)$ for each $t \in \mathbb{R}$, have the property that $\pi(\Psi_t) = \pi(\Phi_t), t \in \mathbb{R}$, and map the rigid body $(\mathcal{B},\mu)$ to the same set of points. Therefore, every such Φ is $\mathcal{B}$-equivalent to Ψ. Now, given $C_0 \in \ker(\tau)$, define a motion Φ by

$$\Phi_t = \iota^{-1}_{\mathcal{O}_{s_0}}(R_\Psi(t), a_{\Psi,\mathcal{O}}(t) - (\pi_{\mathcal{G}}(x_c) - s_0)C_0, C_0, t).$$

Clearly, Φ_t is horizontal and $\Phi_t \in (\pi^{\mathrm{can}}_{c,\mathcal{O}})^{-1}(R_\Psi(t), a_{\Psi,\mathcal{O}}(t), t)$, for each $t \in \mathbb{R}$. It can be directly verified that the curve Φ_t passes through the point $\iota^{-1}_{\mathcal{O}_{s_0}}(R_\Psi(t_0), a_{\Psi,\mathcal{O}}(t_0) - (\pi_{\mathcal{G}}(x_c) - s_0)C_0, C_0, t_0)$ at $t = t_0$, for each $t_0 \in \mathbb{R}$, and thus corresponds to the unique rigid motion Φ with the property that $u_{\Phi,\mathcal{O}}(t) = C_0$, for all $t \in \mathbb{R}$. From Proposition 6.6 we can see that, for $x_c \in \mathcal{O}$, the Galilean–Euler equations for the rigid motion Φ are equivalent to

$$\mathbb{I}_c(t)(\dot{\omega}_\Phi(t)) = \mathbb{I}_c(t)(\omega_\Phi(t)) \times \omega_\Phi(t),$$

$$\ddot{r}_{\Phi,\mathcal{O}}(t) = 0,$$

$$\dot{L}_{\Phi,\mathcal{B}}(t) = L_{\Phi,\mathcal{B}}(t) \times \Omega_\Phi(t),$$

$$\dot{M}_{\Phi,\mathcal{B}}(t) = P_{\mathcal{O}}(M_{\Phi,\mathcal{B}}(t)) \times \Omega_{\Phi}(t).$$

The result now follows. □

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Asymptotic corrections to the eigenvalue density of the GUE and LUE

T. M. Garoni[a)]
Institute for Mathematics and its Applications, University of Minnesota, 400 Lind Hall, 207 Church Street S.E., Minneapolis, Minnesota 55455-0436

P. J. Forrester[b)]
Department of Mathematics and Statistics, University of Melbourne, Parkville, Victoria 3010, Australia

N. E. Frankel[c)]
School of Physics, University of Melbourne, Parkville, Victoria 3010, Australia

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We obtain correction terms to the large N asymptotic expansions of the eigenvalue density for the Gaussian unitary and Laguerre unitary ensembles of random $N \times N$ matrices, both in the bulk of the spectrum and near the spectral edge. This is achieved by using the well known orthogonal polynomial expression for the kernel to construct a double contour integral representation for the density, to which we apply the saddle point method. The main correction to the bulk density is oscillatory in N and depends on the distribution function of the limiting density, while the corrections to the Airy kernel at the soft edge are again expressed in terms of the Airy function and its first derivative. We demonstrate numerically that these expansions are very accurate. A matching is exhibited between the asymptotic expansion of the bulk density, expanded about the edge, and the asymptotic expansion of the edge density, expanded into the bulk. © *2005 American Institute of Physics.*
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I. INTRODUCTION

We consider in this article two classical ensembles of random matrices, the Gaussian unitary ensemble (GUE), and the Laguerre unitary ensemble (LUE). These ensembles can be characterized by their joint eigenvalue probability density functions

$$P_N(x_1,\ldots,x_N) \propto \prod_{l=1}^{N} \omega_N(x_l) \prod_{1\leqslant j<k\leqslant N} (x_k - x_j)^2, \quad x_l \in \Omega, \tag{1}$$

with

$$\omega_N(x) = \begin{cases} \exp(-2Nx^2), & \text{GUE} \\ x^{\alpha}\exp(-4Nx), & \text{LUE}, \end{cases} \tag{2}$$

and

[a)]Electronic mail: garoni@ima.umn.edu; URL: http://www.ima.umn.edu/~garoni
[b)]Electronic mail: P.Forrester@ms.unimelb.edu.au; URL: http://www.ms.unimelb.edu.au/~matpjf/matpjf.html
[c)]Electronic mail: n.frankel@physics.unimelb.edu.au

$$\Omega = \begin{cases} \mathbb{R}, & \text{GUE} \\ (0,\infty), & \text{LUE.} \end{cases} \tag{3}$$

The GUE consists of $N \times N$ Hermitian matrices with independent normally distributed entries on and above the diagonal. It is the cornerstone of random matrix theory.[1–3] The LUE has fundamental applications in mathematical statistics and quantum field theory since it includes Wishart matrices and the Chiral GUE as special cases (the latter after a straightforward change of variables); see, e.g., Ref. 1.

We are interested in the large N behavior of the marginal eigenvalue probability density $\rho_N(x)$, which we hereafter refer to simply as "the density," and which is defined by

$$\rho_N(x) := \int_{\Omega^{N-1}} P_N(x,x_2,\ldots,x_N)\mathrm{d}x_2 \cdots \mathrm{d}x_N. \tag{4}$$

The function $N\,\rho_N(x)$ can be interpreted as the number density of eigenvalues near the point x. We also remark that for the GUE, $N\,\rho_N(x)$ is equal to the number density of a harmonically trapped system of either non-interacting fermions or impenetrable bosons.[4] There is a similar interpretation for the LUE in terms of a Calogero-Sutherland type model.[5] For recent advances in asymptotic questions related to these interpretations, complementary to the present study, see Refs. 6–8.

As background to the present study we note that aspects of the large N form of $\rho_N(x)$ first arose in studies of field theories related to Hermitian matrix models.[9] There, for the GUE the large N asymptotic expansion of the moments

$$m_N(p) := \int_\Omega x^p \rho_N(x)\mathrm{d}x \quad (p = 1,2,\ldots)$$

was sort. By a graphical expansion of the matrix integral, involving cataloging the corresponding maps according to their genus, it was predicted that for certain coefficients $a_{2j}(p)$,

$$m_N^{\mathrm{GUE}}(p) = \sum_{j=0}^{p/2} \frac{a_{2j}(p)}{N^{2j}} \quad (p = 2,4,\ldots), \tag{5}$$

(the odd moments of course vanish). Analogous considerations in the case of the LUE[10] show that

$$m_N^{\mathrm{LUE}}(p) = \sum_{j=0}^{\lfloor (p+1)/2 \rfloor - 1} \frac{\tilde{a}_{2j}(p,\alpha)}{N^{2j}} \quad (p = 1,2,\ldots), \tag{6}$$

for certain coefficients $\tilde{a}_{2j}(p,\alpha)$. Observe in particular that both (5) and (6) contain only even inverse powers of N.

The graphical methods allow $a_0(p)$ in (5) and $\tilde{a}_0(p,\alpha)$ in (6) to be computed in terms of binomial coefficients for all $p = 0,1,\ldots$. This knowledge in turn can be used (see, e.g., Ref. 1) to prove that in the limit $N \to \infty$ with x fixed

$$\rho(x) := \lim_{N\to\infty} \rho_N(x) = \begin{cases} \frac{2}{\pi}\sqrt{1-x^2}, & x \in [-1,1], \quad \text{GUE} \\ \frac{2}{\pi}\sqrt{\frac{1}{x}-1}, & x \in (0,1], \quad \text{LUE}, \\ 0 \quad \text{otherwise}. \end{cases} \tag{7}$$

The first functional form in (7) is referred to as the Wigner semicircle law, whereas the second is sometimes named after Marčenko-Pastur. See, e.g., Refs. 1–3.

The expansions (5) and (6) provide a motivation to undertake a study of the asymptotic form of (4). In the case of the GUE such a result has been given by Kalish and Braak.[11] It states that for $|x| < 1$ and fixed

$$\rho_N(x) = \rho(x) - \frac{2\cos[2\ N\ \pi\ P(x)]}{\pi^3 \rho^2(x)} \frac{1}{N} + O\left(\frac{1}{N^2}\right), \tag{8}$$

where

$$P(x) = 1 + \frac{x}{2}\rho(x) - \frac{1}{\pi}\,\mathrm{Arccos}(x).$$

Thus, one sees that unlike the situation with the moments (5), the leading correction term is $O(1/N)$. Of course, this term is oscillatory so one might anticipate that after integration it contributes at a higher order. However inspection of (8) reveals that the situation is more complex: the oscillatory term is not integrable at the endpoints of the support, $|x|=1$. Indeed, it is well known that with the boundary of the eigenvalue support taken as the origin, a scaling regime distinct from that of the bulk becomes relevant. Explicitly, with $\mathrm{Ai}(x)$ denoting the Airy function, it has been proved that[12]

$$\lim_{N\to\infty} \frac{N^{1/3}}{2} \rho_N^{\mathrm{GUE}}\left(1 + \frac{\xi}{2N^{2/3}}\right) = \lim_{N\to\infty} \frac{(2N)^{1/3}}{2} \rho_N^{\mathrm{LUE}}\left(1 + \frac{\xi}{(2N)^{2/3}}\right) = [\mathrm{Ai}'(\xi)]^2 - \xi[\mathrm{Ai}(\xi)]^2, \tag{9}$$

where ξ is fixed. In view of the breakdown of (8) in the vicinity of the spectrum edge, (referred to as the *soft edge*, since although it defines the edge of the support of $\rho(x)$, for any finite N there is a nonzero probability of finding eigenvalues lying beyond it), we are thus led to also investigate the large N asymptotic expansion extending the limit law (9).

At a technical level, the main achievement of this paper is the derivation of the first correction terms to the limit laws (7) and (9). We do this by utilizing the well known orthogonal polynomial expression for $\rho_N(x)$ to obtain a double integral representation which is amenable to the saddle point method. In the bulk, i.e., in the interior of the support of $\rho(x)$, we show that the asymptotic series progresses in powers of $1/N$, and we obtain the explicit form of the $1/N$ correction. We find for the LUE that the coefficient of the $1/N$ term consists of a component which is oscillatory in N as well a component which is nonoscillatory in N, whereas for the GUE it consists of only an oscillatory component, as shown in (8). For the soft edge we will see that the asymptotic series progresses in powers of $N^{-1/3}$, and we obtain explicit expressions for the coefficients of the $N^{-1/3}$ and $N^{-2/3}$ terms, which again involve Airy functions.

Due to the similarity in the structure of $\rho_N(x)$ for the GUE and LUE, it is convenient to consider both cases simultaneously to avoid unnecessary repetition, and so at each step of our presentation we discuss the GUE and LUE in parallel. In Section II we discuss the double contour integral expression for $\rho_N(x)$ to which we shall apply the saddle point method. Section III contains our discussion of the asymptotics of $\rho_N(x)$ in the bulk whereas Sec. IV discusses the soft edge. In Sec. V we discuss the extent to which our expansions in the bulk match up with those for the soft edge.

Problems relating to the present study, but which remain to be investigated, are discussed in Sec. VI.

II. CONTOUR INTEGRAL EXPRESSION FOR $\rho_N(x)$

For the unitary ensembles there is a well known and very neat expression for $\rho_N(x)$ in terms of orthogonal polynomials, valid for any N and $x \in \Omega$. If we let $\{\pi_j(x)\}_{j=0}^{\infty}$ denote the monic polynomials orthogonal with respect to $\omega_N(x)$ on Ω, then

$$\rho_N(x) = \frac{\omega_N(x)}{N\|\pi_{N-1}\|^2}[\pi'_N(x)\pi_{N-1}(x) - \pi'_{N-1}(x)\pi_N(x)]. \tag{10}$$

The norm in the denominator of (10) is just the L^2 norm associated with $\omega_N(x)$ and Ω. For a derivation of (10) the reader is referred to Refs. 1–3. We remark at this point that there is no

universally agreed scale by which the GUE and LUE are defined. To match our choice of scale and notation in (2) to that employed in Ref. 1 for instance, we observe that

$$\rho_N(x) = \begin{cases} \sqrt{2}N^{-1/2}P_N(\sqrt{2N}x, \sqrt{2N}x), & \text{GUE} \\ 4\ P_N(4Nx,4Nx), & \text{LUE}, \end{cases}$$

where $P_N(x,y)$ (not to be confused with our definition (1) mentioned previously) is the kernel defined in Chap. 4 of Ref. 1 (the kernel is often also denoted $K_N(x,y)$ in the literature).

To investigate the large N behavior of $\rho_N(x)$ it is obviously advantageous to start with the expression (10) rather than with the $(N-1)$-fold integral (4). The $\pi_{N+j-1}(x)$ can be expressed in terms of the standard Hermite and Laguerre polynomials found in Szegö's classic book[13] as follows

$$\pi_{N+j-1}(x) = \begin{cases} 2^{-3(N+j-1)/2}N^{-(N+j-1)/2}H_{N+j-1}(\sqrt{2N}x), & \text{GUE} \\ (-1)^{N+j-1}(N+j-1)!\,(4N)^{-N-j+1}L_{N+j-1}^{(\alpha)}(4Nx), & \text{LUE}. \end{cases} \tag{11}$$

The required asymptotic expansions of the scaled Hermite and Laguerre polynomials appearing in (11) are known to any order both in the bulk and near the soft edge,[14,15] and such asymptotic expansions of scaled orthogonal polynomials are now generically said to be of *Plancherel-Rotach* type (Plancherel and Rotach were the first to compute such asymptotics for the Hermite polynomials). It is reasonable to assume that the most straightforward procedure to obtain the desired asymptotic corrections for $\rho_N(x)$ in each region of interest is to simply insert the corresponding asymptotic expansion for $\pi_{N+j-1}(x)$ into (10). While this is certainly legitimate in principle, and does indeed recover the leading term fairly easily, to derive the correction terms it turns out that such a procedure is rather tedious, and provides little if any insight into the resulting expressions. The source of the complication is that the asymptotic expansions for $\pi_{N+j-1}(x)$ contain a large amount of superfluous information which is canceled when the expansions are substituted into (10). To avoid this, we shall pursue a related, but more direct route.

The Plancherel-Rotach asymptotics for the Hermite and Laguerre polynomials were originally derived by first expressing the polynomials in terms of contour integrals, and then applying the saddle point method. By suitably massaging the standard results in Szegö's book[13] one finds that

$$\pi_{N+j-1}(x) = \begin{cases} c_j(N)\oint \frac{\mathrm{d}z}{2\pi i} e^{2N\,z\,x}\frac{e^{-Nz^2/2}}{z^{N+j}}, & \text{GUE} \\ (-1)^{N+j-1}c_j(N)\oint \frac{\mathrm{d}z}{2\pi i}\frac{e^{-2N\,z\,x}}{z^{N+1}}\left(1+\frac{z}{2}\right)^{N+\alpha}\left(\frac{1}{z}+\frac{1}{2}\right)^{j-1}, & \text{LUE}, \end{cases} \tag{12}$$

$$c_j(N) := \frac{(N+j-1)!}{(2N)^{N+j-1}}. \tag{13}$$

In both cases the contour of integration is a closed positively oriented contour which encircles the origin; in the Laguerre case we further demand that it not contain the point $z=-2$.

Instead of applying the saddle point method to (12) and then substituting the expansions into (10), we shall first insert the contour integrals (12) into (10) to obtain a double integral expression for $\rho_N(x)$, and then perform the saddle point method on this double integral. To highlight the similarity between the GUE and LUE it is convenient in the GUE case to substitute the contour integral for $\pi_{N+j-1}(-x)$ into (10) rather than that for $\pi_{N+j-1}(x)$; since $H_j(-x)=(-1)^jH_j(x)$ this ruse is perfectly harmless. This results in

$$\rho_N(x) = 2\frac{c_0(N)c_1(N)}{\|\pi_{N-1}\|^2}\omega_N(x)J_N(x), \tag{14}$$

where

$$J_N(x) := \oint \frac{dz_1}{2\pi i} \oint \frac{dz_2}{2\pi i} e^{NS(z_1,x)+NS(z_2,x)} G(z_1,z_2) \tag{15}$$

and

$$S(z,x) := \begin{cases} -2z\,x - \log(z) - z^2/2, & \text{GUE} \\ -2z\,x - \log(z) + \log(1+z/2), & \text{LUE}, \end{cases} \tag{16}$$

$$G(z_1,z_2) := u(z_1)u(z_2)\left(1 - \frac{z_1}{z_2}\right), \tag{17}$$

$$u(z) := \begin{cases} 1, & \text{GUE} \\ (1+z/2)^{\alpha-1}, & \text{LUE}. \end{cases} \tag{18}$$

The remainder of this paper will involve a careful asymptotic analysis of the double integral (15).

Before proceeding we note that it is straightforward to show, using standard results in the orthogonal polynomial literature,[13] that

$$\|\pi_{N-1}\|^{-2} = \begin{cases} \dfrac{2^{2N-3/2}}{\sqrt{\pi}} \dfrac{N^{N+1/2}}{N!}, & \text{GUE} \\ \dfrac{(4N)^{2N+\alpha-1}}{\Gamma(N)\Gamma(N+\alpha)}, & \text{LUE}, \end{cases} \tag{19}$$

and hence the asymptotics of the prefactors in (14) is

$$2\frac{c_0(N)c_1(N)}{\|\pi_{N-1}\|^2} = \begin{cases} \sqrt{\dfrac{2}{\pi}} N^{\frac{3}{2}-N}\Gamma(N), & \text{GUE} \\ \dfrac{4^{N+\alpha}N^{\alpha}\Gamma(1+N)}{\Gamma(N+\alpha)}, & \text{LUE}, \end{cases} \tag{20}$$

$$= \begin{cases} 2Ne^{-N}\left[1 + \dfrac{1}{12\,N} + O\left(\dfrac{1}{N^2}\right)\right], & \text{GUE} \\ 4^{N+\alpha}N\left[1 - \dfrac{(\alpha-1)\alpha}{2\,N} + O\left(\dfrac{1}{N^2}\right)\right], & \text{LUE}. \end{cases} \tag{21}$$

Saddle points: Before applying the saddle point method to (15) we need to identify and classify the saddle points of (16). The functions $S(z,x)$ in general have two saddle points at $z = z_\pm$ where

$$z_\pm := \begin{cases} -x \pm i\,\nu(x), & \text{GUE} \\ -1 \pm i\,\nu(x), & \text{LUE}, \end{cases} \tag{22}$$

and

$$\nu(x) := \begin{cases} \sqrt{1-x^2}, & \text{GUE} \\ \sqrt{\frac{1}{x}-1}, & \text{LUE}. \end{cases} \tag{23}$$

We note that for both the GUE and LUE we have

$$\nu(x) = \frac{\pi}{2}\rho(x) \quad \text{for} \quad |x| \leqslant 1, \tag{24}$$

with $\rho(x)$ as defined in (7). (Recall that, as defined in (3), when considering the LUE we always demand that $x>0$, so that (22) is indeed well defined).

Since for $|x| \leqslant 1$ we have

$$\frac{S''(z_\pm,x)}{2} = \begin{cases} \nu(x)e^{\pm i(\pi - \mathrm{Arcsin}(x))}, & \text{GUE} \\ 2x^2\nu(x)e^{\pm i\pi/2}, & \text{LUE}, \end{cases} \tag{25}$$

the saddle points $z=z_\pm$ are both simple when $|x|<1$, i.e., $S''(z_\pm,x)\neq 0$. However, when $x=1$ the two simple saddle points given in (22) coalesce to $z_\pm=-1$ and $S''(z_\pm,1)$ vanishes, so we obtain one double saddle point in this case. Thus we already see why the regions $|x|<1$ and $x\sim 1$ have qualitatively distinct asymptotic behavior. Simple saddle points generically produce Gaussian integrals whereas double saddle points generically produce Airy functions (see e.g., Ref. 16).

III. BULK ASYMPTOTICS FOR THE GUE AND LUE

In the bulk of the spectrum, i.e., for $|x|<1$, we hold x fixed and investigate the asymptotics of (15) as N becomes large. From (22) we see that there are two distinct simple saddle points of $S(z,x)$, which form a complex conjugate pair in this case. Let us define $S_\pm := S(z_\pm,x)$. Then since

$$\mathrm{Re}(S_+) = \mathrm{Re}(S_-), \tag{26}$$

both saddle points contribute to the same order and we deform our contour through both of them. Denoting by $\Omega_\pm$ a contour passing through $z_\pm$ along a path of steepest descent, the standard arguments of the saddle point method (see for e.g., Ref. 16) yield

$$J_N(x) = \left(\int_{\Omega_+}\frac{dz_1}{2\pi i} + \int_{\Omega_-}\frac{dz_1}{2\pi i}\right)\left(\int_{\Omega_+}\frac{dz_2}{2\pi i} + \int_{\Omega_-}\frac{dz_2}{2\pi i}\right) e^{N\,S(z_1,x)+N\,S(z_2,x)}G(z_1,z_2) + O(e^{2N\,\mathrm{Re}(S_+)-N\,\epsilon}), \tag{27}$$

$$= -\sum_{\sigma\in\{-,+\}^2}\int_{\Omega_{\sigma_1}}\frac{dz_1}{2\pi}\int_{\Omega_{\sigma_2}}\frac{dz_2}{2\pi} e^{N\,S(z_1,x)+N\,S(z_2,x)}G(z_1,z_2) + O(e^{2N\,\mathrm{Re}(S_+)-N\,\epsilon}), \tag{28}$$

for suitably small $\epsilon>0$.

We now need to parameterize the contours $\Omega_\pm$. From (25) we see that if we set

$$\theta = \begin{cases} \mathrm{Arcsin}(x)/2, & \text{GUE} \\ \pi/4, & \text{LUE}, \end{cases} \tag{29}$$

then a suitable parameterization of $\Omega_\pm$ is

$$z = z_\pm + e^{\pm i\theta}t, \quad t\in[-\eta,\eta], \tag{30}$$

for sufficiently small $\eta>0$. In (29) the function $\mathrm{Arcsin}:[-1,1]\to[-\pi/2,\pi/2]$ denotes the principle branch of arcsine. With the parameterization (30) the contour Ω_+ is traversed in the negative direction, so we need to compensate for this with an explicit minus sign.

By choosing η sufficiently small $S(z,x)$ is analytic on $\Omega_\pm$ and so using the parameterization (30) we see that

$$S(z,x) = S_\pm - a\,t^2 - a\,t^2\varphi_\pm(t), \quad z\in\Omega_\pm, \tag{31}$$

where

$$a := \begin{cases} \nu(x), & \text{GUE} \\ 2x^2\nu(x), & \text{LUE}, \end{cases} \tag{32}$$

and

$$\varphi_{\pm}(t) := \sum_{k=3}^{\infty} \frac{S^{(k)}(z_{\pm},x)}{S^{(2)}(z_{\pm},x)} \frac{2}{k!} e^{\pm i(k-2)\theta} t^{k-2}. \tag{33}$$

We note that $\varphi_{-}(t)=\varphi_{+}^{*}(t)$, where * denotes complex conjugation.

It is a straightforward exercise to show that $S_{-}=S_{+}^{*}$, and that

$$\mathrm{Re}(S_{+}) = \begin{cases} \frac{1}{2} + x^2, & \text{GUE} \\ 2x - \log(2), & \text{LUE}, \end{cases} \tag{34}$$

$$\mathrm{Im}(S_{+}) = -\pi\, P(x), \tag{35}$$

where

$$P(x) := \int_{x_0}^{x} \rho(t)\mathrm{d}t, \tag{36}$$

$$= \begin{cases} 1 + \frac{x}{2}\rho(x) - \frac{1}{\pi}\mathrm{Arccos}(x), & \text{GUE} \\ 1 + x\ \rho(x) - \frac{2}{\pi}\mathrm{Arccos}(\sqrt{x}), & \text{LUE}. \end{cases} \tag{37}$$

Here x_0 is the left edge of the support of $\rho(x)$ given in (7), i.e., $x_0=-1$, 0, for the GUE and LUE respectively. We note that $P(x)$ is the probability distribution function corresponding to $\rho(x)$. The limiting distribution function $P(x)$ will play a significant role in the bulk asymptotic expansion of $\rho_N(x)$.

With the results (31) and (35) for $S(z,x)$, and the definitions

$$G_{\sigma}(t) := G(z_1,z_2)\big|_{\substack{z_1\to z_{\sigma_1}+e^{i\sigma_1\theta}t_1 \\ z_2\to z_{\sigma_2}+e^{i\sigma_2\theta}t_2}}, \tag{38}$$

$$\mathbb{E}_i^{(B)} := \int_{-\eta}^{\eta} \frac{e^{-aNt_i^2}}{2\pi}\mathrm{d}t_i, \tag{39}$$

where $\mathbb{E}_i^{(B)}$ is an integral operator acting to the right, we can make the change of variables (30) in (28) to obtain

$$J_N(x) = e^{2N\,\mathrm{Re}(S_{+})}\mathbb{E}_1^{(B)}\mathbb{E}_2^{(B)} \sum_{\sigma\in\{-1,+1\}^2} -\sigma_1\sigma_2 e^{i(\sigma_1+\sigma_2)(\theta-N\ \pi\ P(x))} e^{-aNt_1^2\varphi_{\sigma_1}(t_1)-aNt_2^2\varphi_{\sigma_2}(t_2)} G_{\sigma}(t) + O(e^{2N\,\mathrm{Re}(S_{+})-\epsilon\ N}). \tag{40}$$

A small amount of massaging shows that the $(-1,+1)$ term in (40) is the complex conjugate of the $(+1,-1)$ term, and likewise the $(-1,-1)$ term is conjugate to the $(+1,+1)$ term. Suppose now that we define the function $F_{\sigma}(\lambda,t)$ by

$$F_{\sigma}(\lambda,t) := e^{\lambda_1\varphi_{\sigma_1}(t_1)} e^{\lambda_2\varphi_{\sigma_2}(t_2)} G_{\sigma}(t), \tag{41}$$

then

$$J_N(x) = 2\ e^{2N\ \mathrm{Re}(S_+)} \mathrm{Re}\ \mathbb{E}_1^{(B)} \mathbb{E}_2^{(B)} \{F_{+,-}(\lambda,t)|_{\lambda_i=-aNt_i^2} - e^{2i(\theta - N\ \pi\ P(x))} F_{+,+}(\lambda,t)|_{\lambda_i=-aNt_i^2}\} + O(e^{2N\ \mathrm{Re}(S_+)-\epsilon N}). \tag{42}$$

We shall discuss the purpose of the parameters λ_i shortly. Note that the two terms in (42) are qualitatively distinct—the second term is oscillatory in N whereas the first is not.

It is convenient to pause for a moment and multiply (42) by the the explicit forms for the prefactors required in (14) using (21) and (34) to obtain the corresponding expression for $\rho_N(x)$ Since

$$\frac{2c_0(N)c_1(N)}{\|\pi_{N-1}\|^2} \omega_N(x) e^{2N\ \mathrm{Re}(S_+)} = h_0 N \left[1 + \frac{h_1}{N} + O\left(\frac{1}{N^2}\right) \right] \tag{43}$$

with

$$h_0 = \begin{cases} 2, & \text{GUE} \\ 4^\alpha x^\alpha, & \text{LUE}, \end{cases} \tag{44}$$

$$h_1 = \begin{cases} \frac{1}{12}, & \text{GUE} \\ -\frac{\alpha(\alpha-1)}{2}, & \text{LUE}, \end{cases} \tag{45}$$

we have

$$\rho_N(x) = h_0 \left[1 + \frac{h_1}{N} + O\left(\frac{1}{N^2}\right) \right] \times 2\ \mathrm{Re}\ N\ \mathbb{E}_1^{(B)} \mathbb{E}_2^{(B)} \{F_{+,-}(\lambda,t)|_{\lambda_i=-aNt_i^2} - e^{2i(\theta - N\ \pi\ P(x))} F_{+,+}(\lambda,t)|_{\lambda_i=-aNt_i^2}\} + O(e^{-\epsilon N}). \tag{46}$$

The introduction of the auxiliary variables λ_1, λ_2 in (41) is a common ruse applied in the saddle point method (see e.g., Ref. 16) which we now discuss. Suppose that we construct the Maclaurin expansion in t_1, t_2 of $F_\sigma(\lambda, t)$ with λ considered as a fixed parameter

$$F_\sigma(\lambda,t) = \sum_{j=0}^{p} \sum_{k=0}^{j} \frac{t_1^k t_2^{j-k}}{k!\,(j-k)!} \left[\frac{\partial^k}{\partial s_1^k} \frac{\partial^{j-k}}{\partial s_2^{j-k}} F_\sigma(\lambda, s_1, s_2) \right] \Bigg|_{s_1,s_2=0} + O(t_1^{p_1} t_2^{p_2})|_{p_1+p_2=p+1}. \tag{47}$$

If we now set $\lambda_i = -aNt_i^2$ in (47) and perform the integrations required in (46) then we find that each term corresponding to a given value of j in (47) has the same resulting N dependence. This then gives a systematic way of obtaining the corrections out to any given order in N. To see why this occurs, first note that we need only consider the terms in (47) for which both j and k are even since any odd monomials are annihilated by (39), and then further note that with $\lambda_i = -aNt_i^2$ we have

$$N\ \mathbb{E}_1^{(B)} \mathbb{E}_2^{(B)} t_1^{2m_1} t_2^{2m_2} \lambda_1^{l_1} \lambda_2^{l_2} = (-1)^{l_1+l_2} \frac{\Gamma(m_1 + l_1 + 1/2)\Gamma(m_2 + l_2 + 1/2)}{4\ \pi^2 a^{m_1+m_2+1}} N^{-(m_1+m_2)} + O(e^{-a\eta^2 N}), \tag{48}$$

for any $l_1, l_2 \in \mathbb{N}$. Hence, despite the fact that various powers of λ_1 and λ_2 arise when $F_\sigma(\lambda, t)$ is differentiated, for a given value of j all terms end up with the same N dependence after setting $\lambda_i = -aNt_i^2$ and performing the integrations.

Hence, substituting (47) into (46) one can construct the asymptotic series for $\rho_N(x)$ out to any desired order. We shall explicitly construct this series out to order $1/N$ but the generalization to

higher orders is obvious. However, as we shall see the resulting asymptotic expansions obtained by keeping only the $1/N$ correction are already extremely good, and it appears that numerically optimal truncation occurs at this order.

Let us denote by $c_m^{(\sigma)}(x)$ the coefficient of $1/N^m$ in the $1/N$ expansion generated by acting with $N\,\mathbb{E}_1^{(B)}\mathbb{E}_2^{(B)}$ on (47), with λ_i set to $-aNt_i^2$. Then since the only terms which contribute are those for which j and k are even we have

$$\frac{c_m^{(\sigma)}(x)}{N^m} = \sum_{k=0}^{m} \frac{1}{(2k)!\,(2[m-k])!} N\,\mathbb{E}_1^{(B)}\mathbb{E}_2^{(B)} t_1^{2k} t_2^{2(m-k)} \left[\frac{\partial^{2k}}{\partial {s_1}^{2k}} \frac{\partial^{2(m-k)}}{\partial {s_2}^{2(m-k)}} F_\sigma(\lambda, s)\Big|_{s_i=0} \right] \Bigg|_{\lambda_i=-aNt_i^2}. \tag{49}$$

We can re-express $\rho_N(x)$ from (46) in terms of the $c_m^{(\sigma)}(x)$ as follows:

$$\begin{aligned}\rho_N(x) = {} & 2\,h_0 \mathrm{Re}\{c_0^{(1,-1)}(x)\} - 2\,h_0 \mathrm{Re}\{e^{2i(\theta - N\,\pi\,P(x))} c_0^{(1,1)}(x)\} - 2\,h_0 \mathrm{Re}\{e^{2i(\theta - N\,\pi\,P(x))}[c_1^{(1,1)}(x) \\ & + h_1 c_0^{(1,1)}(x)]\}\frac{1}{N} + 2h_0 \mathrm{Re}\{c_1^{(1,-1)}(x) + h_1 c_0^{(1,-1)}(x)\}\frac{1}{N} + O\left(\frac{1}{N^2}\right).\end{aligned} \tag{50}$$

It is not hard to show that the term $2\,h_0\mathrm{Re}\{c_0^{(1,-1)}(x)\}$ is equal to the limiting density $\rho(x)$ from (7) when $|x|<1$, as required, and also that $c_0^{(1,1)}(x)$ vanishes identically (this is actually obvious from (17) and (38)). The explicit construction of the remaining $c_m^{(\sigma)}(x)$ required in (50) is straightforward and we finally obtain the following.

Proposition 1: *Let* $\rho_N(x)$ *be as defined in* (4), *and let x be fixed, with* $|x|<1$ *for the GUE and* $x \in (0,1)$ *for the LUE. Then as* $N \to \infty$ *we have the following:*

For the GUE

$$\rho_N(x) = \rho(x) - \frac{2\cos[2\,N\,\pi\,P(x)]}{\pi^3 \rho^2(x)}\frac{1}{N} + O\left(\frac{1}{N^2}\right), \tag{51}$$

whereas for the LUE

$$\begin{aligned}\rho_N(x) &= \rho(x) - \left(\frac{\cos(2\,N\,\pi\,P(x) - \alpha\,\pi[1 + x\,\rho(x) - P(x)])}{\pi^3 x^2 \rho^2(x)} - \frac{\alpha}{\pi^2 x\,\rho(x)}\right)\frac{1}{N} + O\left(\frac{1}{N^2}\right), \\ &= \rho(x) - \left(\frac{\cos(2\,N\,\pi\,P(x) - 2\,\alpha\,\mathrm{Arccos}(\sqrt{x}))}{\pi^3 x^2 \rho^2(x)} - \frac{\alpha}{\pi^2 x\,\rho(x)}\right)\frac{1}{N} + O\left(\frac{1}{N^2}\right),\end{aligned} \tag{52}$$

where $\rho(x)$ *is given in* (7) *and* $P(x)$ *is the corresponding probability distribution function, given explicitly in* (37).

As remarked in Sec. I, the result (51) was obtained previously in[11] again by steepest descent, but starting from an integral representation derived by super-symmetric arguments rather than orthogonal polynomials.

It is interesting to note that it is the distribution function $P(x)$ of the limiting density $\rho(x)$ which controls the large N oscillations in the $1/N$ correction to $\rho_N(x)$. Note also that while the non-oscillatory correction vanishes at order $1/N$ for the GUE leaving only an oscillatory correction at this order, the LUE has both an oscillatory and a non-oscillatory component to its $1/N$ correction.

To demonstrate to the reader just how accurate the expansions given by Proposition 1 are we provide in Figs. 1 and 2 a numerical comparison of the asymptotic expansions with the exact results computed using the expression (10) in terms of orthogonal polynomials.

IV. SOFT EDGE ASYMPTOTICS FOR THE GUE AND LUE

The appropriate scaling to elucidate the behavior of $\rho_N(x)$ near the soft edge is to set $x = 1 + \xi/N^{2/3}$ for fixed ξ, as appears in (9). Substituting such a scaling into (16) we find

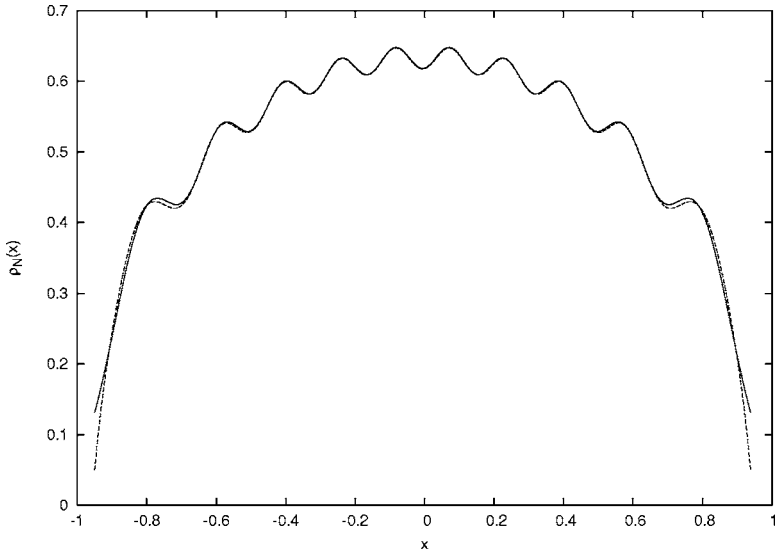

FIG. 1. Comparison of the asymptotic expansion (51), shown as the dashed line, and the exact result (10), shown as the solid line, for the eigenvalue density of the GUE with $N=10$.

$$N\,S\left(z,1+\frac{b^{1/3}}{2}\frac{\xi}{N^{2/3}}\right)=-\xi b^{1/3}N^{1/3}z+N\,S(z), \tag{53}$$

where we have introduced the shorthand $S(z):=S(z,1)$. Here $b>0$ is a free parameter that we can fix later as convenient. Defining

$$\tilde{J}_N(\xi):=J_N\left(1+\frac{b^{1/3}}{2}\frac{\xi}{N^{2/3}}\right), \tag{54}$$

we see that (53) leads to

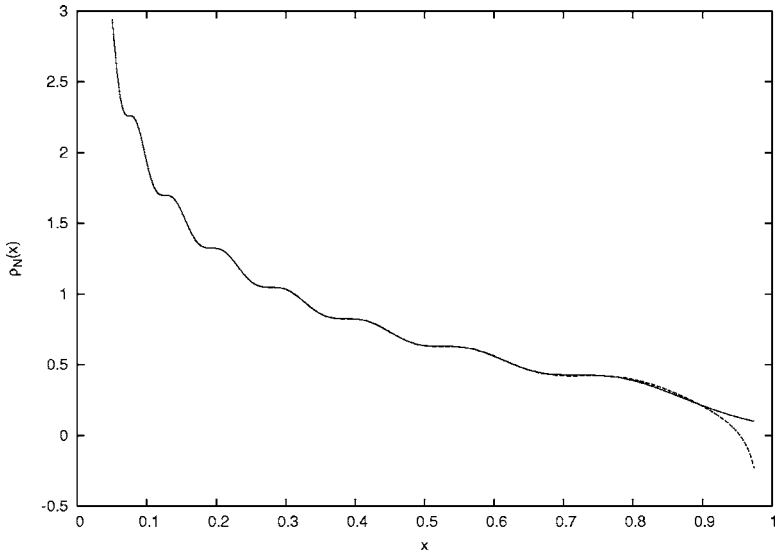

FIG. 2. Comparison of the asymptotic expansion (52), shown as the dashed line, and the exact result (10), shown as the solid line, for the eigenvalue density of the LUE with $\alpha=1/2$ and $N=10$.

$$\widetilde{J}_N(\xi) = \oint \frac{\mathrm{d}z_1}{2\pi i} \exp(N\,S(z_1) - b^{1/3}N^{1/3}z_1\xi) \oint \frac{\mathrm{d}z_2}{2\pi i} \exp(N\,S(z_2) - b^{1/3}N^{1/3}z_2\xi)G(z_1,z_2). \tag{55}$$

The reader might be concerned by the slightly unorthodox term in the exponent proportional to $N^{1/3}$, however it is subdominant to the $N\,S(z)$ term and its presence does not affect any of the usual arguments of the saddle point method; the asymptotic behavior of (55) is determined by $S(z)$. From (22), (23), and (25) we see for both the GUE and LUE that $S(z)$ has one double saddle point, located at $z=-1$. We can deform the contour of integration to a new contour which passes through $z=-1$ along paths of steepest descent. Note that although in (12) the integrals must be positively oriented, since we have two integrals in (55) we are free to orient the integrals in the negative direction since the consequent minus signs cancel. Let us denote by $\mathcal{C}$ the contour consisting of the union of two rays of unit length, the first starting at $z=e^{-i\pi/3}-1$ and ending at $z=-1$ and the second starting at $z=-1$ and ending at $z=e^{i\pi/3}-1$. If we then denote by $\mathcal{A}$ any suitable arc such that $\mathcal{C}\cup\mathcal{A}$ is a simple closed curve enclosing the origin we can write

$$\begin{aligned}\widetilde{J}_N(\xi) = &\left(\int_{\mathcal{C}} + \int_{\mathcal{A}}\right)\frac{\mathrm{d}z_1}{2\pi i} \exp(N\,S(z_1) - b^{1/3}N^{1/3}z_1\xi) \\ &\times \left(\int_{\mathcal{C}} + \int_{\mathcal{A}}\right)\frac{\mathrm{d}z_2}{2\pi i}\exp(N\,S(z_2) - b^{1/3}N^{1/3}z_2\xi)G(z_1,z_2),\end{aligned} \tag{56}$$

$$\begin{aligned}= &\int_{\mathcal{C}} \frac{\mathrm{d}z_1}{2\pi i} \exp(N\,S(z_1) - b^{1/3}N^{1/3}z_1\xi) \int_{\mathcal{C}} \frac{\mathrm{d}z_2}{2\pi i} \exp(N\,S(z_2) - b^{1/3}N^{1/3}z_2\xi)G(z_1,z_2) \\ &+ o(e^{2N\,S(-1)}N^{-p}).\end{aligned} \tag{57}$$

The error bound in (57) holds for all $p\in\mathbb{N}$, and so in what follows we consider p as arbitrarily large. The equality between (56) and (57) can be obtained by noting that we can choose $\mathcal{A}$ to consist of two rays lying along the path of steepest descent away from the endpoints of $\mathcal{C}$, which extend as far as we like into the right half plane, together with an arc to close the contour which we can choose to be as far into the right half plane as desired. With such a choice for $\mathcal{A}$ one can obtain the required bounds by a straightforward generalization of the usual argument used in the saddle point method. For a careful discussion of the saddle point method, suitable for this purpose, see, e.g., Sec. 2.5 of Ref. 16. We note that Ref. 16 refers to the saddle point method as *Perron's method*.

Now let us change variables in (57) according to $t=z+1$, so that the vertex of our contour is now at the origin. We shall denote the image of $\mathcal{C}$ under this change of variables by $\mathcal{B}$. Further, since $S(z)$ is analytic on $\mathcal{C}$ we have

$$S(t-1) = S(-1) + b\frac{t^3}{3} + b\frac{t^3}{3}\varphi(t), \tag{58}$$

where

$$\varphi(t) := \sum_{k=4}^{\infty} \frac{S^{(k)}(-1)}{S^{(3)}(-1)}\frac{3!}{k!}t^{k-3}, \tag{59}$$

and we have now chosen

$$b = \frac{S^{(3)}(-1)}{2}, \tag{60}$$

$$= \begin{cases} 1, & \text{GUE} \\ 2, & \text{LUE.} \end{cases} \tag{61}$$

We also note that by setting $x=1$ in (34) and (35) we have

$$S(-1) = \begin{cases} \frac{3}{2} - i\pi, & \text{GUE} \\ 2 - \log(2) - i\pi, & \text{LUE.} \end{cases} \tag{62}$$

Finally, defining

$$F(\lambda,t) := G(t_1 - 1, t_2 - 1) e^{\lambda_1 \varphi(t_1) + \lambda_2 \varphi(t_2)}, \tag{63}$$

and the integral operator

$$\mathbb{E}_i^{(S)} := \int_{\mathcal{B}} \exp\left(bN \frac{t_i^3}{3} - \xi b^{1/3} N^{1/3} t_i \right) \frac{dt_i}{2\pi i} \tag{64}$$

we have

$$\tilde{J}_N(\xi) = e^{2N \,\mathrm{Re}[S(-1)] + 2b^{1/3}N^{1/3}\xi} [\mathbb{E}_1^{(S)} \mathbb{E}_2^{(S)} F(\lambda,t)|_{\lambda_i = bNt_i^3/3} + o(N^{-p})]. \tag{65}$$

If we now multiply (65) by the prefactors required in (14) using (21) we obtain

$$\frac{(bN)^{1/3}}{2} \rho_N\left(1 + \frac{b^{1/3}}{2} \frac{\xi}{N^{2/3}}\right) = \left[g_0(\xi) + \frac{g_1(\xi)}{N^{1/3}} + \frac{g_2(\xi)}{N^{2/3}} + O\left(\frac{1}{N}\right) \right] \times [N^{4/3} \mathbb{E}_1^{(S)} \mathbb{E}_2^{(S)} F(\lambda,t)|_{\lambda_i = bNt_i^3/3} + o(N^{-p})], \tag{66}$$

where $g_m(\xi)$ is the coefficient of $N^{-m/3}$ in the large N fixed ξ expansion of

$$\begin{cases} e^{-\xi^2/2N^{1/3}}, & \text{GUE} \\ 2^{2\alpha - 2/3} \left(1 + \dfrac{\xi}{(2N)^{2/3}}\right)^{\alpha}, & \text{LUE.} \end{cases} \tag{67}$$

In (66) we have presented only terms $O(1/N)$ in the first factor since this will be sufficient for our purposes in what follows. Higher order terms are easily retained if desired.

Our work is now essentially done. One expands $F(\lambda,t)$ around $t=0$ for fixed λ as in (47) and then sets $\lambda_i = bNt_i^3/3$, analogous to the bulk case. Again, after integration, each value of j in the Maclaurin expansion (47) contributes to the same order in N. To see this explicitly we can use the following lemma.

Lemma 1. Let $\mathcal{B}$ be the contour consisting of the union of a ray starting at $e^{-i\pi/3}$ and ending at the origin, and a ray starting at the origin and ending at $e^{i\pi/3}$. For any $b>0$ and $0<\beta<1/3$ we have for large N that

$$\int_{\mathcal{B}} z^m \exp\left(bN \frac{z^3}{3} - \xi b^{1/3} N^{1/3} z \right) \frac{dz}{2\pi i} = (-1)^m b^{-(m+1)/3} N^{-(m+1)/3} [\mathrm{Ai}^{(m)}(\xi) + O(e^{-\beta bN})],$$

where $\mathrm{Ai}^{(m)}(\xi)$ *is the* m^{th} *derivative of the Airy function* $\mathrm{Ai}(\xi)$.

Proof: This follows from the standard entire contour integral expression for $\mathrm{Ai}(\xi)$ (see e.g., Ref. 17) by simply changing variables $z \mapsto b^{-1/3} N^{-1/3} z$, and noting that the rays defining the contour $\mathcal{B}$ can be extended to infinity at the cost of introducing exponentially subdominant corrections.

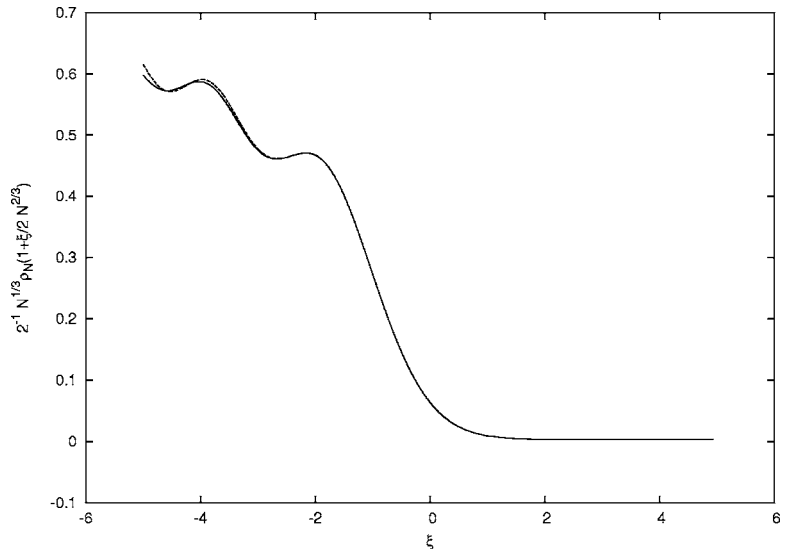

FIG. 3. Comparison of the asymptotic expansion (72), shown as the dashed line, and the exact result (10), shown as the solid line, for the eigenvalue density near the soft edge at $x=1$, for the GUE with $N=10$.

An immediate consequence of Lemma 1 is that with $\lambda_i = bNt_i^3/3$ we have

$$N^{4/3}\mathbb{E}_1^{(S)}\mathbb{E}_2^{(S)}t_1^{k_1}t_2^{k_2}\lambda_1^{l_1}\lambda_2^{l_2} = \frac{(-1)^{l_1+l_2+k_1+k_2}}{3^{l_1+l_2}b^{(k_1+k_2+2)/3}}\mathrm{Ai}^{(k_1+3l_1)}(\xi)\mathrm{Ai}^{(k_2+3l_2)}(\xi)\left(\frac{1}{N^{1/3}}\right)^{k_1+k_2-2} + O(e^{-\beta bN}). \tag{68}$$

Hence, if we construct the Maclaurin expansion of $F(\lambda,t)$ with λ fixed as in (47), and set $\lambda_i = bNt_i^3/3$ and integrate using (68), we obtain an expansion for

$$N^{4/3}\mathbb{E}_1^{(S)}\mathbb{E}_2^{(S)}F(\lambda,t)|_{\lambda_i=bNt_i^3/3} \tag{69}$$

in powers of $N^{-1/3}$. Denoting the coefficient of $N^{-m/3}$ in this expansion by $c_m(\xi)$ we have explicitly that

$$\frac{c_m(\xi)}{N^{m/3}} = \sum_{k=0}^{m+2}\frac{1}{k\,!\,(m+2-k)!}N^{4/3}\mathbb{E}_1^{(S)}\mathbb{E}_2^{(S)}t_1^k t_2^{m+2-k}\left[\frac{\partial^k}{\partial s_1^k}\frac{\partial^{m+2-k}}{\partial s_2^{m+2-k}}F(\lambda,s_1,s_2)\bigg|_{s_1,s_2=0}\right]\Bigg|_{\lambda_i=bNt_i^3/3}. \tag{70}$$

The reader might be concerned that according to (68) the $k_1+k_2=1$ and $k_1+k_2=0$ terms grow with N; however it is not hard to show from (70) that the coefficients $c_{-2}(\xi)$ and $c_{-1}(\xi)$ vanish identically.

We can now express (66) in terms of the coefficients $c_m(\xi)$ as

$$\frac{(bN)^{1/3}}{2}\rho_N\left(1+\frac{b^{1/3}}{2}\frac{\xi}{N^{2/3}}\right) = g_0(\xi)c_0(\xi) + [g_1(\xi)c_0(\xi)+g_0(\xi)c_1(\xi)]\frac{1}{N^{1/3}} + [g_2(\xi)c_0(\xi)+g_1(\xi)c_1(\xi)+g_0(\xi)c_2(\xi)]\frac{1}{N^{2/3}} + O\left(\frac{1}{N}\right). \tag{71}$$

We have explicitly displayed terms $o(1/N)$ here, but it is straightforward to retain as many terms as desired. The expansion constructed from terms $o(1/N)$ however is extremely accurate, as we demonstrate in Figs. 3 and 4, and it appears to be the numerically optimal order at which to truncate the expansions.

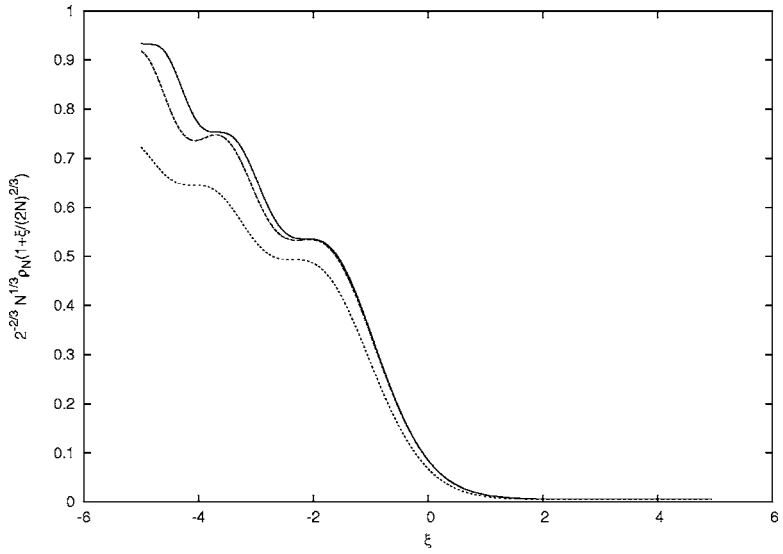

FIG. 4. Comparison of the asymptotic expansion (73), shown as the dashed line, and the exact result (10), shown as the solid line, for the eigenvalue density near the soft edge at $x=1$, for the LUE with $\alpha=1/2$ and $N=20$. Also shown is the limit as $N\to\infty$ given by the Airy kernel (9), shown as the dotted line lying below the other two curves.

The explicit forms for the coefficients $c_m(\xi)$ can be constructed from (70) and substituted into (71). We can also further simplify the Airy derivatives appearing in (68) using the Airy differential equation $\mathrm{Ai}''(\xi)=\xi\,\mathrm{Ai}(\xi)$ so that only $\mathrm{Ai}(\xi)$ and its first derivative appear. We finally obtain the following.

Proposition 2: Let $\rho_N(x)$ be as defined in (4). *Then with ξ fixed, as $N\to\infty$ we have the following:*

For the GUE

$$\frac{N^{1/3}}{2}\rho_N\left(1+\frac{\xi}{2N^{2/3}}\right)=[\mathrm{Ai}'(\xi)]^2-\xi[\mathrm{Ai}(\xi)]^2 - \frac{1}{20}(3\xi^2[\mathrm{Ai}(\xi)]^2-2\xi[\mathrm{Ai}'(\xi)]^2-3\,\mathrm{Ai}(\xi)\mathrm{Ai}'(\xi))\frac{1}{N^{2/3}} + O\left(\frac{1}{N}\right), \tag{72}$$

whereas for the LUE

$$\frac{(2N)^{1/3}}{2}\rho_N\left(1+\frac{\xi}{(2N)^{2/3}}\right)=[\mathrm{Ai}'(\xi)]^2-\xi[\mathrm{Ai}(\xi)]^2+\frac{\alpha}{2^{1/3}}[\mathrm{Ai}(\xi)]^2\frac{1}{N^{1/3}} + \frac{2^{1/3}}{10}(3\xi^2[\mathrm{Ai}(\xi)]^2-2\xi[\mathrm{Ai}'(\xi)]^2+(2-5\alpha^2)\mathrm{Ai}(\xi)\mathrm{Ai}'(\xi))\frac{1}{N^{2/3}} + O\left(\frac{1}{N}\right). \tag{73}$$

Figures 3 and 4 provide a numerical comparison of the asymptotic expansions given in Proposition 2 with the exact results computed using the expression (10) in terms of orthogonal polynomials.

Note that it appears that the GUE converges much faster than the LUE, since while the two curves in (3) are almost indistinguishable at $N=10$ for the GUE, the asymptotic expansion for the

LUE begins to diverge from the exact result in (4) already by $\xi \sim 2$, and both curves are rather different from the limiting Airy kernel expression (9). We investigated the affects of retaining more terms in the expansion for the LUE case; keeping terms $O(1/N)$ did not noticeably change the plots, while keeping terms higher than $1/N$ caused significant divergence of the asymptotic expansion from the exact result. The explanation for this is most likely that, as made precise in the next section, the edge expansions match onto the bulk expansions, and these in turn become more divergent near the edge at each order in $1/N$.

V. MATCHING OF THE BULK AND EDGE EXPANSIONS

In Figs. 1–4 plots of the bulk and edge asymptotic expansions have separately been compared against the exact density for I finite N. Although the scale of the independent variable is different, we can see from Figs. 3 and 4 that the edge asymptotic expansions are accurate approximations to the exact density at least up to the neighborhood of the first local maximum (relative to the edge $\xi=0$), and thus the edge asymptotic expansions should be used instead of the bulk asymptotic expansions in this region.

At a quantitative level, it is possible to exhibit a matching between the various asymptotic expansions. Suppose in (51) we set $x=1+\xi/2N^{2/3}$, and in (52) we set $x=1+\xi/(2N)^{2/3}$, and take $\xi<0$ and fixed. Expanding the right hand sides as an asymptotic series in N gives

$$N^{1/3}\rho_N^{\mathrm{GUE}}(1+\xi/2N^{2/3}) \dot{\sim} \left(\frac{2\sqrt{|\xi|}}{\pi} - \frac{\cos(4|\xi|^{3/2}/3)}{2\pi|\xi|}\right) - \left(\frac{|\xi|^{3/2}}{4\pi} + \frac{\cos(4|\xi|^{3/2}/3)}{8\pi} + \frac{|\xi|^{3/2}\sin(4|\xi|^{3/2}/3)}{20\pi}\right)\frac{1}{N^{2/3}} + O\left(\frac{1}{N^{4/3}}\right), \tag{74}$$

$$(2N)^{1/3}\rho_N^{\mathrm{LUE}}(1+\xi/(2N)^{2/3}) \dot{\sim} \left(\frac{2\sqrt{|\xi|}}{\pi} - \frac{\cos(4|\xi|^{3/2}/3)}{2\pi|\xi|}\right) + \frac{\alpha(1+\sin(4|\xi|^{3/2}/3))}{\pi\sqrt{|\xi|}}\frac{1}{(2N)^{1/3}} + O\left(\frac{1}{N^{2/3}}\right), \tag{75}$$

where the symbol $\dot{\sim}$ denotes that the asymptotic series have been expanded as specified. An important feature is that this procedure mixes the terms which are at different orders in N in (51) and (52).

Let us now compute the $\xi \to -\infty$ asymptotic expansions of the right hand sides of the first two terms in each of (72) and (73), multiplied by 2. Using the fact that for $x \to \infty$ (see e.g., Ref. 17)

$$\mathrm{Ai}(-x) = \frac{1}{\sqrt{\pi}x^{1/4}}\cos\left(\frac{\pi}{4} - \frac{2}{3}x^{3/2}\right) - \frac{5}{48\sqrt{\pi}x^{7/4}}\cos\left(\frac{\pi}{4} + \frac{2}{3}x^{3/2}\right) + O\left(\frac{1}{x^{13/4}}\right),$$

we obtain expansions which reproduce the N-independent terms in (74) and (75), giving furthermore, terms of higher order in $1/|\xi|$. In (75) the term proportional to $1/(2N)^{1/3}$ is reproduced, and this too is accompanied by terms of higher order in $1/|\xi|$. In (74) the term $-|\xi|^{3/2}/4\pi N^{2/3}$ is reproduced, as is the term proportional to $|\xi|^{3/2}\sin(4|\xi|^{3/2}/3)/N^{2/3}$, whereas the term proportional to $\cos(4|\xi|^{3/2}/3)/N^{2/3}$ is out by a rational factor. The explanation for the missing higher order terms in $1/|\xi|$, and incorrect rational factors is most likely due to the fact that terms of all orders in $1/N$ in (51) and (52) contribute to each distinct order in the expansions (74) and (75). Specifically, from the results exhibited above, it would seem that expanding the complete large N asymptotic series for $\rho_N^{\mathrm{GUE}}(x)$ and $\rho_N^{\mathrm{LUE}}(x)$ as in (74) and (75) would give precisely the large $\xi \to -\infty$ expansion of (72) and (73), extended to all orders in N.

VI. DISCUSSION AND QUESTIONS FOR FUTURE STUDIES

From the viewpoint of obtaining accurate numerical approximations to the density, it appears to be optimal to retain only the order $1/N$ corrections in the bulk. However, as remarked at the end

of the previous section, knowledge of higher order terms would allow us to exhibit higher order matching relating the bulk and edge expansions. Higher order non-oscillatory corrections in the bulk are also of interest because they relate to earlier work.[18,19] In particular, in Ref. 18 [Eqs. (2.6), (3.15), (3.24), (3.25)], the nonoscillatory order $1/N^2$ correction to $\rho_N(x)$ for the GUE is calculated by way of the corresponding resolvent to equal

$$\frac{1}{16\pi(1-x^2)^{5/2}}\frac{1}{N^2}.$$

On the other hand, using the method of Sec. III to extend (51) gives the order $1/N^2$ correction as

$$\left(\frac{1}{16\pi(1-x^2)^{5/2}}+\frac{x(15+2x^2)\sin[2N\pi P(x)]}{48\pi(1-x^2)^{5/2}}\right)\frac{1}{N^2},$$

exhibiting precise agreement with the earlier study.

A result of Ref. 18 as it relates to the GUE, and of Ref. 19 as it relates to the LUE in the case $\alpha=0$, is that all corrections to the bulk density which are proportional to odd powers of $1/N$ contain only oscillatory terms. Indeed, the expansions of Proposition 1 are consistent with this result, although its truth in general does not appear to be an easy corollary of the working of Sec. III.

For the LUE, in addition to the bulk and soft edge regimes, there is a distinct regime in the neighborhood of $x=0$ referred to as the hard edge.[12] The bulk expansion (52) diverges for $x\to 0$, and we are faced with the same matching issue as that between the bulk and soft edge expansions. To leading order this matching can be seen by comparing the $x\to\infty$ behavior of the hard edge density known from Ref. 12, with the $x\to 0$ form of the Marčenko-Pastur law in (7). At higher order, correction terms to the hard edge density must be computed. This we hope to address in a future study.

The studies of Refs. 18 and 19 tell us the bulk asymptotic expansion of the smoothed form of not just the density, but the two-point Green function as well. From this the bulk asymptotic expansion of the smoothed two-point correlation can be read off. On the other hand, this latter quantity, and in fact the general k-point correlations, are determined by a single quantity known as the Christoffel-Darboux kernel, generalizing (10). It would thus be of interest to apply the methods of the present study to compute the asymptotic expansion of this kernel for the GUE and LUE, both in the bulk and at the soft edge.

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A field theoretic derivation of the Max Born hypothesis

Abdulmuhsen H. Ali[a)]

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It is shown in this article that the statistical character of the nonrelativistic, one particle quantum probabilities can be inferred from the function which results from the Wigner transformation on the field operator $\hat{\psi}^{\dagger}(\vec{x})$ which, in turn, must be expressed in the occupation number representation. The function which results from the Wigner transformation is shown to be the state function of a single particle which is defined in the conventional quantum mechanics. The integral of the norm squared of that function is proven to be unity which is the step that proves the Max Born hypothesis. The compatibility of the expression for the field amplitude, obtained here, with the measurability of the Bosonic and the Fermionic fields is explained. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2044668]

I. INTRODUCTION

The relation between quantum expectation values and statistical averages is a subject that has been studied very extensively. Early attempts to explore that relation includes the Bohr and the von Neumann reasonings, both of which rule out the possibility of interpreting quantum expectation values in terms of averaging over uniquely determined processes because, as was discussed by Groenewold,[1] these processes may not be well defined either on physical or mathematical grounds. On the other hand, Wigner functions[2] proved to be the main objects through which phase-space *c*-number density functions may be defined.[3] These functions have been studied very extensively, for example, Curtright and Zachos,[3,4] Bohun *et al.*,[5] and Lesche.[6] A Wigner function is the Wigner transform of the quantum density operator,[7,8] and it can be used to calculate averages of a phase space function which will give the statistical average of that particular phase space function and not the quantum expectation value. In spite of the fact that the Wigner function leaves the interpretation of the expectation value as an axiom of quantum mechanics it remains to be the superior function which bridges quantum density operators to statistical averages.

Another way to relate quantum operators to statistical averages is to identify expectation values with statistical averages through an equation which directly relates the quantum probability density to the statistical probability. The purpose of this article is to show that using quantum field theory one can connect the single particle, nonrelativistic, quantum probability density to the statistical probability which is a step that will give the Max Born hypothesis a mathematical proof. This connection is important because it presents a nonaxiomatic approach to the statistical interpretation of the state function's norm square.[9] Consequently, one will be able to study, as will be shown in a future work, the conditions under which the norm square of a one particle state function may fail to represent the probability density. To relate the quantum probability to the statistical probability one needs to apply the Wigner transformation to the field operator $\hat{\psi}^{\dagger}(\vec{x})$, an operator which is introduced in the second quantization and which represents the creation of a particle at the position $\vec{x}$. The matrix element of $\hat{\psi}^{\dagger}(\vec{x})$ should be given in the coordinate representation of N particles. The function $\Psi_{w}^{*}(x,p,\vec{x})$, which denotes the Wigner transform of $\hat{\psi}^{\dagger}(\vec{x})$, will have an N-coordinate dependence, an N-momentum dependence, and an $\vec{x}$ dependence. To eliminate the N coordinates and momenta dependencies an integration over the coordinates fol-

a)Electronic mail: aliamh@hotmail.com

lowed by an ensemble averaging is performed. The resulting function $\bar{\psi}_w^*(\vec{x})$ is proven to obey the Schrödinger equation, and thus is proven to be the state function defined in quantum mechanics. Further, the integral over the spatial coordinates of the norm square of the function $\bar{\psi}_w^*(\vec{x})$ is shown to be unity.

It is worth mentioning that the equation derived here for the field amplitude have a direct proportionality to the average occupation number per state. A consequence of that direct proportionality is the fact that Bosons will have a much stronger field amplitude than Fermions. Fermions are allowed to have an occupation number of either 1 or 0 per state. Bosons, on the other hand, can have up to the total number of particles in the system occupying a single state. With the direct proportionality between the particle field amplitude and the average occupation number per state, for a certain projection, the above-mentioned statistics will lead to a much stronger field amplitude for Bosons than for Fermions. This is consistent with the classical measurability of a field; if a field is to be measurable then the field amplitude must be strong enough to be detected on a classical scale[10] which means that particles having Bose–Einstein statistics have a physically measurable field, for example, the classical electromagnetic fields, and particles obeying the Fermi–Dirac statistics have a field amplitude which, in comparison to the Bosons, is too weak.

II. THE TRANSFORMATION FOR FERMIONS

For any operator $\hat{A}$ the Wigner transformation is defined by[5,7]

$$A_w(x,p) = \int_{R^{3N}} d^{3N}z e^{i(p\cdot z)/\hbar} \left\langle x - \frac{z}{2} \middle| \hat{A} \middle| x + \frac{z}{2} \right\rangle \tag{1}$$

where $x,z,p \in R^{3N}$, R is the real axis, N is the total number of particles, $(p\cdot z)=\Sigma_{\ell=1}^{3N} p_\ell z_\ell$, $\hbar$ is Plank's constant, $d^{3N}z=\Pi_{\ell=1}^{N} d\vec{z}_\ell$, $\vec{z}_\ell \in R^3$, and $A_w(x,p)$ is the classical function corresponding to the quantum operator $\hat{A}$, which may have a position dependence. The interest here is in the spatial integral of the Wigner transformation of the field operator $\hat{\psi}^\dagger(\vec{x})=\Sigma_{j=1}^{\infty}\hat{b}_j^\dagger \phi_j^*(\vec{x})$.[10] The Wigner transform of $\hat{\psi}^\dagger(\vec{x})$ is denoted by $\Psi_w^*(x,p,\vec{x})$, the sum in the expansion of $\hat{\psi}^\dagger(\vec{x})$ runs over single particle states, the $\phi_j(\vec{x})$ is a single particle state function which corresponds to the $N+1st$ particle, and $\vec{x}$ is the position vector of that particle. In particular, the function of interest is

$$\psi_w^*(p,\vec{x}) = \int d^{3N}x \Psi_w^*(x,p,\vec{x}) = \int d^{3N}x d^{3N}z e^{i(p\cdot z)/\hbar} \left\langle x - \frac{z}{2} \middle| \hat{\psi}^\dagger(\vec{x}) \middle| x + \frac{z}{2} \right\rangle, \tag{2}$$

where $d^{3N}x=\Pi_{\ell=1}^{N} d\vec{x}_\ell$. The general plan is to insert the unit operator[11]

$$1^{S,A} = \frac{1}{N!}\sum_{\{n_k\}} |n_1,n_2,\ldots\rangle^{S,A\ S,A}\langle n_1,n_2,\ldots|$$

in the matrix element in the integrand, multiply terms, and then integrate. The superscripts indicate, respectively, the symmetric (Bosonic) and the antisymmetric (Fermionic) state vectors.[7] The matrix element in the integrand will be

$$\begin{aligned}\left\langle x - \frac{z}{2} \middle| \psi^\dagger(\vec{x}) \middle| x + \frac{z}{2} \right\rangle &= {}^{S,A}\left\langle x - \frac{z}{2} \middle| 1^{S,A}\left(\sum_j \hat{b}_j^\dagger \phi_j^*(\vec{x})\right)1^{S,A} \middle| x + \frac{z}{2} \right\rangle^{S,A} = {}^{S,A}\left\langle x - \frac{z}{2} \right| \\ &\times \left(\frac{1}{N!}\sum_{\{n_k\}} |n_1,n_2,\ldots\rangle^{S,A\ S,A}\langle n_1,n_2,\ldots|\right)\sum_j \hat{b}_j^\dagger \phi_j^*(\vec{x}) \\ &\times \left(\frac{1}{N!}\sum_{\{n_k'\}} |n_1',n_2',\ldots\rangle^{S,A\ S,A}\langle n_1',n_2',\ldots|\right)\left| x + \frac{z}{2} \right\rangle^{S,A}\end{aligned}$$

$$= \sum_{\{n_k\}} \sum_{\{n_k'\}} \left(\frac{1}{N!}\right)^2 {}^{S,A}\left\langle x - \frac{z}{2} \,|n_1, n_2, \ldots \right\rangle^{S,A} {}^{S,A}\langle n_1, n_2, \ldots |\left(\sum_j \hat{b}_j^\dagger \phi_j^*(\vec{x})\right)$$
$$\times |n_1', n_2', \ldots\rangle^{S,A S,A}\left\langle n_1', n_2', \ldots \left| x + \frac{z}{2}\right\rangle^{S,A}. \tag{3}$$

The last term in Eq. (3) is the N-particle state function and it will be written as[12]

$${}^{S,A}\left\langle n_1', n_2', \ldots \left| x + \frac{z}{2}\right\rangle^{S,A} = {}^{S,A}\left\langle n_1', n_2', \ldots \left| \vec{x}_1 + \frac{\vec{z}_1}{2}, \ldots, \vec{x}_N + \frac{\vec{z}_N}{2}\right\rangle^{S,A}\right.\right.$$
$$= \Phi^*_{[n_1' n_2' \cdots]}\left(\vec{x}_1 + \frac{\vec{z}_1}{2}, \ldots, \vec{x}_N + \frac{\vec{z}_N}{2}\right)^{S,A}. \tag{4}$$

According to quantum mechanics[12] the square of the amplitude of the Φ function in Eq. (4) will give the simultaneous probability of finding a particle at $\vec{x}_1$, a particle at $\vec{x}_2, \ldots$, and a particle at $\vec{x}_N$ with the knowledge that the "first" state is occupied by n_1 particles, the second state by n_2 particles, the third state by n_3 particles, and so forth. With Eq. (4) the matrix elements of the field operator $\hat{\psi}^\dagger(\vec{x})$ is

$$\left\langle x - \frac{z}{2}\right| \hat{\psi}^\dagger(\vec{x}) \left| x + \frac{z}{2}\right\rangle = \sum_j \sum_{\{n_k'\}} \sum_{\{n_k\}} \left(\frac{1}{N!}\right)^2 \Phi_{[n_1 n_2 \ldots]}\left(\vec{x}_1 - \frac{\vec{z}_1}{2}, \ldots, \vec{x}_N - \frac{\vec{z}_N}{2}\right)^{S,A}$$
$$\times {}^{S,A}\langle n_1, n_2, \ldots |\hat{b}_j^\dagger| n_1', n_2', \ldots\rangle^{S,A} \Phi^*_{[n_1' n_2' \cdots]}\left(\vec{x}_1 + \frac{\vec{z}_1}{2}, \ldots, \vec{x}_N + \frac{\vec{z}_N}{2}\right)^{S,A} \phi_j^*(\vec{x}). \tag{5}$$

The value of the matrix ${}^{S,A}\langle n_1, n_2, \ldots |\hat{b}_j^\dagger| n_1', n_2', \ldots\rangle^{S,A}$ will depend on the type of particles being considered. For Bosons and Fermions it is respectively given by[10]

$${}^{S}\langle n_1, n_2, \ldots, n_j, \ldots |\hat{b}_j^\dagger| n_1', n_2', \ldots, n_j', \ldots\rangle^{S} = \sqrt{n_j' + 1}\, \delta_{n_1, n_1'} \cdots \delta_{n_j, n_j'+1} \cdots, \tag{6}$$

$${}^{A}\langle n_1, n_2, \ldots, n_j, \ldots |\hat{b}_j^\dagger| n_1', n_2', \ldots, n_j', \ldots\rangle^{A} = (-1)^{R_j}\sqrt{1 - n_j'}\, \delta_{n_1, n_1'} \cdots \delta_{n_j, 1 - n_j'} \cdots. \tag{7}$$

The prefactor $(-1)^{R_j}$ with $R_j = \sum_{\nu=1}^{n_{j-1}} n_\nu$ is ± 1 depending on the number of occupied states between n_1 and n_{j-1}.[10] When doing the calculations for Fermions the matrix element of the field operator $\hat{\psi}^\dagger(\vec{x})$ will be

$$\left\langle x - \frac{z}{2}\right| \hat{\psi}^\dagger(\vec{x}) \left| x + \frac{z}{2}\right\rangle = \sum_j \sum_{\{n_k'\}} \sum_{\{n_k\}} \left(\frac{1}{N!}\right)^2 \Phi_{[n_1 n_2 \cdots]}\left(\vec{x}_1 - \frac{\vec{z}_1}{2}, \ldots, \vec{x}_N - \frac{\vec{z}_N}{2}\right)^{A}$$
$$\times (-1)^{R_j}\sqrt{1 - n_j'}\, \delta_{n_1, n_1'} \cdots \delta_{n_j, 1 - n_j'} \cdots \Phi^*_{[n_1' n_2' \cdots]}\left(\vec{x}_1 + \frac{\vec{z}_1}{2}, \ldots, \vec{x}_N + \frac{\vec{z}_N}{2}\right)^{A}$$
$$\times \phi_j^*(\vec{x}) = \sum_j \sum_{\{n_k\}} \left(\frac{1}{N!}\right)^2 \Phi_{[n_1 n_2 \cdots]}\left(\vec{x}_1 - \frac{\vec{z}_1}{2}, \ldots, \vec{x}_N - \frac{\vec{z}_N}{2}\right)^{A}$$
$$\times (-1)^{R_j}\sqrt{n_j}\, \Phi^*_{[n_1 n_2 \cdots]}\left(\vec{x}_1 + \frac{\vec{z}_1}{2}, \ldots, \vec{x}_N + \frac{\vec{z}_N}{2}\right)^{A} \phi_j^*(\vec{x})$$
$$= \sum_j \left(\frac{1}{N!}\right)^2 \left[\sum_{k_1, k_2, \ldots, k_N} \Phi_{k_1, \ldots, k_N}\left(\vec{x}_1 - \frac{\vec{z}_1}{2}, \ldots, \vec{x}_N - \frac{\vec{z}_N}{2}\right)^{A}\right.$$

$$\times \Phi^{*}_{k_1,\ldots,k_N}\left(\vec{x}_1+\frac{\vec{z}_1}{2},\ldots,\vec{x}_N+\frac{\vec{z}_N}{2}\right)^{A}\Bigg](-1)^{(j-1)}\sqrt{n_j}\phi^{*}_{j}(\vec{x}), \tag{8}$$

where the state function has been rewritten as

$$\Phi_{[n_1 n_2\cdots]}\left(\vec{x}_1-\frac{\vec{z}_1}{2},\ldots,\vec{x}_N-\frac{\vec{z}_N}{2}\right)^{S,A}\equiv\Phi_{k_1,\ldots,k_N}\left(\vec{x}_1-\frac{\vec{z}_1}{2},\ldots,\vec{x}_N-\frac{\vec{z}_N}{2}\right)^{S,A} \tag{9}$$

which makes the statement that this is an N-particle state function with particles in the levels $k_1,\ldots,k_N$. The symmetric and the antisymmetric N-particle state function are, respectively, given by[13]

$$\Phi_{k_1,\ldots,k_N}\left(\vec{x}_1-\frac{\vec{z}_1}{2},\ldots,\vec{x}_N-\frac{\vec{z}_N}{2}\right)^{S}=\frac{1}{\sqrt{N!n_1!n_2!\cdots}}\sum_{p\in S_N}\phi_{k_{p(1)}}\left(\vec{x}_1-\frac{\vec{z}_1}{2}\right)\cdots\phi_{k_{p(N)}}\left(\vec{x}_N-\frac{\vec{z}_N}{2}\right), \tag{10}$$

$$\Phi_{k_1,\ldots,k_N}\left(\vec{x}_1-\frac{\vec{z}_1}{2},\ldots,\vec{x}_N-\frac{\vec{z}_N}{2}\right)^{A}=\frac{1}{\sqrt{N!}}\sum_{p\in S_N}\mathrm{sgn}(p)\phi_{k_{p(1)}}\left(\vec{x}_1-\frac{\vec{z}_1}{2}\right)\cdots\phi_{k_{p(N)}}\left(\vec{x}_N-\frac{\vec{z}_N}{2}\right), \tag{11}$$

where $\mathrm{sgn}(p)=+1$ for even permutations, $\mathrm{sgn}(p)=-1$ for odd permutations, and where S_N is the set of all permutations of the N particles. The permutation of N elements is denoted by[13]

$$p(1,2,\ldots,N)=(p(1),p(2),\ldots,p(N)).$$

The $\phi(\vec{x})_k$'s in Eqs. (10) and (11) are single particle solutions to the Schrödinger equation and form a complete basis in Hilbert space.[13]

The expanded form of the antisymmetric state functions should now be inserted in Eq. (8):

$$\begin{aligned}\left\langle x-\frac{z}{2}\middle|\hat{\psi}^{\dagger}(\vec{x})\middle|x+\frac{z}{2}\right\rangle=\sum_j\left(\frac{1}{N!}\right)\Bigg[&\sum_{k_1,\ldots,k_N}\left(\frac{1}{N!}\right)^2\\&\times\sum_{p'\in S_N}\mathrm{sgn}(p')\sum_{p\in S_N}\mathrm{sgn}(p)\phi_{k_{p(1)}}\left(\vec{x}_1-\frac{\vec{z}_1}{2}\right)\cdots\phi_{k_{p(N)}}\left(\vec{x}_N-\frac{\vec{z}_N}{2}\right)\\&\times\phi^{*}_{k_{p'(1)}}\left(\vec{x}_1+\frac{\vec{z}_1}{2}\right)\cdots\phi^{*}_{k_{p'(N)}}\left(\vec{x}_N+\frac{\vec{z}_N}{2}\right)(-1)^{(j-1)}\sqrt{n_j}\Bigg]\phi^{*}_{j}(\vec{x}).\end{aligned} \tag{12}$$

Now one must substitute (12) into (2) but Eq. (12) is complicated and the calculations at this point will be done for $N=3$ and $j=3$ so that by induction one may obtain the general N particles result. The results below will hold only under the imposition of the ansatz

$$\phi_{k_j}\left(\vec{x}_j-\frac{\vec{z}_j}{2}\right)=\phi_{k_j}(\vec{x}_j)\phi_{k_j}\left(-\frac{\vec{z}_j}{2}\right)$$

and

$$\phi^{*}_{k_j}\left(\vec{x}_j+\frac{\vec{z}_j}{2}\right)=\phi^{*}_{k_j}(\vec{x}_j)\phi^{*}_{k_j}\left(\frac{\vec{z}_j}{2}\right).$$

Thus, according to Eq. (12) for three particles and three quantum states the Wigner transform of the field operator $\hat{\psi}^{\dagger}(\vec{x})$ will be

$$\Psi_w^*(x,p,\vec{x}) = \left(\frac{1}{3!}\right)^3 \int d^3z_1 d^3z_2 d^3z_3 e^{i(p\cdot z)/\hbar} \sum_{j=1}^{3} \sum_{k_1,k_2,k_3} (-1)^{(j-1)} \sqrt{n_j} \phi_j^*(\vec{x}) \Bigg[\sum_{p\in S_3} \prod_{\nu=1}^{3} \phi_{k_{p(\nu)}}(\vec{x}_\nu)$$
$$\times \phi_{k_{p(\nu)}}^*(\vec{x}_\nu) \phi_{k_{p(\nu)}}\left(-\frac{\vec{z}_\nu}{2}\right) \phi_{k_{p(\nu)}}^*\left(\frac{\vec{z}_\nu}{2}\right) - \sum_{p\in S_2} \sum_{m,\ell,j,r=1}^{3}{}' \phi_{k_j}(r) \phi_{k_j}^*(r) \phi_{k_{p(r)}}(\ell) \phi_{k_{p(\ell)}}^*(\ell) \phi_{k_{p(\ell)}}(m)$$
$$\times \phi_{k_{p(r)}}^*(m) - \frac{1}{2} \sum_{p\in S_2} \sum_{j,r=1}^{3}{}' \phi_{k_r}(r) \phi_{k_r}^*(r) \phi_{k_{p(j)}}(\ell) \phi_{k_{p(\ell)}}^*(\ell) \phi_{k_{p(\ell)}}(j) \phi_{k_{p(j)}}^*(j)$$
$$+ \sum_{p'\in S_2} \sum_{p\in S_2} \phi_{k_{p'(1)}}(1) \phi_{k_{p'(2)}}^*(1) \phi_{k_{p'(2)}}(p(2)) \phi_{k_3}^*(p(2)) \phi_{k_3}(p(3)) \phi_{k_{p'(1)}}^*(p(3))$$
$$+ \sum_{p'\in S_2} \sum_{p\in S_2} \phi_{k_{p'(1)}}(1) \phi_{k_{p'(3)}}^*(1) \phi_{k_2}(p(2)) \phi_{k_{p'(1)}}^*(p(2)) \phi_{k_{p'(3)}}(p(3)) \phi_{k_2}^*(p(3))$$
$$+ \sum_{p'\in S_2} \sum_{p\in S_2} \phi_{k_{p'(2)}}(1) \phi_{k_{p'(3)}}^*(1) \phi_{k_{p'(1)}}(p(2)) \phi_{k_{p'(2)}}^*(p(2)) \phi_{k_{p'(3)}}(p(3)) \phi_{k_{p'(1)}}^*(p(3)) \Bigg], \tag{13}$$

where the prime on the summation indicates a restricted sum which means that in taking the sum one should consider terms in which a subscript k_j occurs only twice, and in the last three terms the permutations are $p(m)=j, p(j)=m$. Specifically, in the last term the permutations are $p(m)=j, p(j)=m$ per $\vec{x}_\ell$, $\ell=1,2,3$. The total number of terms in Eq. (13) are 36. The first term in Eq. (13) accounts for 6 of the 36 terms, the second term in equation (13) gives 12 terms out of the 36 terms, the third term in Eq. (13) will give 6 terms out of the 36 terms, and the last three will give 12 terms out of the 36 terms. Also, in Eq. (13) the coordinate dependence of the state functions have been suppressed such that $\phi_{k_\ell}(j) \equiv \phi_{k_\ell}(\vec{x}_j - \vec{z}_j/2)$, and $\phi_{k_\ell}^*(j) \equiv \phi_{k_\ell}^*(\vec{x}_j + \vec{z}_j/2)$. Applying the above-mentioned Ansatz and the orthonormal property of the complete set $\{\phi_j(\vec{x})\}$ will make the last five terms in Eq. (13) vanish when the integrations over the $\vec{x}_j$'s are performed. Given this fact and Eqs. (2) and (13) one can write

$$\psi_w^*(p,\vec{x}) = \int d^{3N}x \Psi_w^*(x,p,\vec{x}) = \left(\frac{1}{3!}\right)^3 \int_{R^9} d^9x \int_{R^9} d^9z e^{i(p\cdot z)/\hbar} \sum_{j=1}^{3} \sum_{k_1,k_2,k_3} (-1)^{(j-1)} \sqrt{n_j} \phi_j^*(\vec{x})$$
$$\times \sum_{p\in S_3} \prod_{\nu=1}^{3} \phi_{k_{p(\nu)}}(\vec{x}_\nu) \phi_{k_{p(\nu)}}^*(\vec{x}_\nu) \phi_{k_{p(\nu)}}\left(-\frac{\vec{z}_\nu}{2}\right) \phi_{k_{p(\nu)}}^*\left(\frac{\vec{z}_\nu}{2}\right). \tag{14}$$

The orthonormal property of the complete set $\{\phi_{k_j}(\vec{x})\}$ will make all the integrals with respect to the $\vec{x}_j$'s be equal to unity

$$\psi_w^*(p,\vec{x}) = \left(\frac{1}{3!}\right)^3 \int_{R^9} d^9z e^{i(p\cdot z)/\hbar} \sum_{j=1}^{3} \sum_{k_1,k_2,k_3} (-1)^{(j-1)} \sqrt{n_j} \phi_j^*(\vec{x}) \sum_{p\in S_3} \prod_{\nu=1}^{3} \phi_{k_{p(\nu)}}\left(-\frac{\vec{z}_\nu}{2}\right) \phi_{k_{p(\nu)}}^*\left(\frac{\vec{z}_\nu}{2}\right). \tag{15}$$

In Eq. (15) employ the closure relation $\Sigma_{k_\ell} \phi_{k_\ell}(\vec{z}_m/2) \phi_{k_\ell}^*(-\vec{z}_m/2) = \delta(\vec{z}_m)$, $\forall j=1,2,3 \ni j \neq \ell$, and $m=1,2,3$. Now integrate over the z coordinate and the function $\psi_w^*(p,\vec{x})$ will reduce to

$$\psi_w^*(p,\vec{x}) = \left(\frac{1}{3!}\right)^3 (2) \sum_{j=1}^{3} \Bigg[\sum_{k_j} (-1)^{(j-1)} \sqrt{n_j} \sum_{\ell=1}^{3} \int d^3z_\ell e^{i(p\cdot\vec{z}_\ell)/\hbar} \phi_{k_j}\left(-\frac{\vec{z}_\ell}{2}\right) \phi_{k_j}^*\left(\frac{\vec{z}_\ell}{2}\right) \Bigg] \phi_j^*(\vec{x}). \tag{16}$$

The dependence on p is eliminated by taking the average $\bar{\psi}_w^*(\vec{x})=\Sigma_{\{n_k\}}\psi_w^*(p,\vec{x})P\{n_k\}$, where

$$P\{n_k\}=\frac{g\{n_k\}e^{-\beta\Sigma_{k=1}^{\infty}n_k(\epsilon_k-\mu)}}{\sum_{\{n_k\}}g\{n_k\}e^{-\beta\Sigma_{k=1}^{\infty}n_k(\epsilon_k-\mu)}}$$

is the probability of finding the set of occupation numbers $\{n_1,n_2,\ldots\}=\{n_k\}_{k=1}^{\infty}$ in the grand canonical ensemble,[7] $g\{n_k\}$ is the statistical weight of the set $\{n_k\}_{k=1}^{\infty}$, ϵ_k is the energy of the single particle state k, μ is the chemical potential, $\beta=1/k_BT$, k_B is the Boltzmann constant, and T is the absolute temperature. The statistical weight $g\{n_k\}$ equals to unity for both Fermions and Bosons. The Fermionic function $\bar{\psi}_w^*(\vec{x})$ will be obtained by virtue of the function $P\{n_k\}$

$$\bar{\psi}_w^*(\vec{x})=\sum_{\{n_k\}}\psi_w^*(p,\vec{x})P\{n_k\}=\left(\frac{1}{3!}\right)^3(2)\sum_{j=1}^{3}\left[\sum_{k_j}(-1)^{(j-1)}\left(\frac{\prod_{r=1}^{3}\sum_{n_r}e^{-\beta n_r(\epsilon_r-\mu)}\sqrt{n_j}}{\prod_{r=1}^{3}\sum_{n_r}e^{-\beta n_r(\epsilon_r-\mu)}}\right)\right.$$
$$\left.\times\sum_{\ell=1}^{3}\int d^3z_\ell e^{i(p\cdot\vec{z}_\ell)/\hbar}\phi_{k_j}\left(-\frac{\vec{z}_\ell}{2}\right)\phi_{k_j}^*\left(\frac{\vec{z}_\ell}{2}\right)\right]\phi_j^*(\vec{x}).$$

The fraction in the parentheses will simplify to the average of $\sqrt{n_j}$ denoted as $\langle\sqrt{n_j}\rangle$

$$\left(\frac{\prod_{r=1}^{3}\sum_{n_r}e^{-\beta n_r(\epsilon_r-\mu)}\sqrt{n_j}}{\prod_{r=1}^{3}\sum_{n_j}e^{-\beta n_r(\epsilon_r-\mu)}}\right)=\frac{\sum_{n_j}\sqrt{n_j}e^{-\beta n_j(\epsilon_j-\mu)}\prod_{\substack{r=1\\r\neq j}}^{3-1}\sum_{n_r}e^{-\beta n_r(\epsilon_r-\mu)}}{\sum_{n_j}e^{-\beta n_j(\epsilon_j-\mu)}\prod_{\substack{r=1\\r\neq j}}^{3-1}\sum_{n_r}e^{-\beta n_r(\epsilon_r-\mu)}}=\frac{\sum_{n_j}\sqrt{n_j}e^{-\beta n_j(\epsilon_j-\mu)}}{\sum_{n_j}e^{-\beta n_j(\epsilon_j-\mu)}}$$
$$=\sum_{n_j}\sqrt{n_j}p_j(n_j)=\langle\sqrt{n_j}\rangle,$$

where

$$p_j(n_j)=\frac{e^{-\beta n_j(\epsilon_j-\mu)}}{\sum_{n_j}e^{-\beta n_j(\epsilon_j-\mu)}}$$

is the probability of finding n_j particles in the subsystem j which has the energy ϵ_j.[7] This last result will simplify the function $\bar{\psi}^*(\vec{x})$ significantly

$$\bar{\psi}_w^*(\vec{x})=\left(\frac{1}{3!}\right)^3(2)\sum_{j=1}^{3}\left[\sum_{k_j}\sum_{\ell=1}^{3}\int d^3z_\ell e^{i(p\cdot\vec{z}_\ell)/\hbar}\phi_{k_j}\left(-\frac{\vec{z}_\ell}{2}\right)\phi_{k_j}^*\left(\frac{\vec{z}_\ell}{2}\right)\right](-1)^{(j-1)}\langle\sqrt{n_j}\rangle\phi_j^*(\vec{x})$$
$$=\left(\frac{1}{3!}\right)^3(2)\sum_{j=1}^{3}\left[\sum_{\ell=1}^{3}\int d^3z_\ell e^{i(p\cdot\vec{z}_\ell)/\hbar}\sum_{k_j}\phi_{k_j}\left(-\frac{\vec{z}_\ell}{2}\right)\phi_{k_j}^*\left(\frac{\vec{z}_\ell}{2}\right)\right](-1)^{(j-1)}\langle\sqrt{n_j}\rangle\phi_j^*(\vec{x})$$

a further simplification is reached by using the closure relation

$$\bar{\psi}_w^*(\vec{x})=\left(\frac{1}{3!}\right)^3(2)\sum_{j=1}^{3}\left[\sum_{\ell=1}^{3}\int d^3z_\ell e^{i(p\cdot\vec{z}_\ell)/\hbar}\delta(\vec{z}_\ell)\right](-1)^{(j-1)}\langle\sqrt{n_j}\rangle\phi_j^*(\vec{x})=\left(\frac{1}{3!}\right)^3(2)\sum_{j=1}^{3}[3](-1)^{(j-1)}$$
$$\times\langle\sqrt{n_j}\rangle\phi_j^*(\vec{x})=\left(\frac{1}{3!}\right)^3(3!)\sum_{j=1}^{3}(-1)^{(j-1)}\langle\sqrt{n_j}\rangle\phi_j^*(\vec{x})$$

or

$$\bar{\psi}_w^*(\vec{x}) = \left(\frac{1}{3!}\right)\left(\frac{1}{(3-1)!\sqrt{3}}\right)\sum_{j=1}^{3}(-1)^{(j-1)}\frac{\langle\sqrt{n_j}\rangle}{\sqrt{3}}\phi_j^*(\vec{x}). \tag{17}$$

By induction the general equation for the average number of particles,[7] $N=\Sigma_j\langle n_j\rangle$, and a denumerable set of states is

$$\psi_w^*(\vec{x}) \equiv \bar{\psi}_w^*(\vec{x})(N!)((N-1)!\sqrt{N}) = \sum_{j=1}^{\infty}(-1)^{(j-1)}\frac{\langle\sqrt{n_j}\rangle}{\sqrt{N}}\phi_j^*(\vec{x}). \tag{18}$$

The following approximation[10] is valid only in the limit of a very large average number of particles N:

$$\ln(N^{1/2}N!(N-1)!) = (1/2)\ln N + \ln N! + \ln(N-1)! \approx (1/2)\ln N + N\ln N - N + (N-1)\ln(N-1)$$
$$-(N-1) = 2N\ln N - (1/2)\ln N - 2N \approx 2N\ln N, \tag{19}$$

where $N \gg 1$ leads to $N \pm 1 \approx N$. Raising both sides in Eq. (19) to the exponent will give the approximate equality, $N^{1/2}N!(N-1)! \approx (N)^{2N}$. Under the large N approximation and the assumption of negligible occupation number fluctuations[7] Eq. (18) is

$$\psi_w^*(\vec{x}) \equiv \bar{\psi}_w^*(\vec{x})(N)^{2N} = \sum_j (-1)^{(j-1)}\left(\frac{\langle n_j\rangle}{N}\right)^{1/2}\phi_j^*(\vec{x}), \tag{20}$$

where the negligible fluctuations of the occupation number leads to $\langle\sqrt{n_j}\rangle \approx \sqrt{\langle n_j\rangle}$. The function $\psi_w^*(\vec{x})$ changes sign according to the way the factor $(-1)^{(j-1)}$ contributes to the sum. With the complex conjugate of Eq. (20)

$$\psi_w(\vec{x}) = \sum_j (-1)^{(j-1)}\left(\frac{\langle n_j\rangle}{N}\right)^{1/2}\phi_j(\vec{x}) \tag{21}$$

and the integration of the product between Eqs. (20) and (21), an insight may be given into the physical meaning of the function $\psi_w(\vec{x})$

$$\int d^3x\psi_w^*(\vec{x})\psi_w(\vec{x}) = \int d^3x\sum_j\sum_k (-1)^{(j+k-2)}\left(\frac{\langle n_j\rangle}{N}\right)^{1/2}\left(\frac{\langle n_k\rangle}{N}\right)^{1/2}\phi_j^*(\vec{x})\phi_k(\vec{x}). \tag{22}$$

By the orthonormal property of the complete set of the basis states, $\int d^3x\phi_j^*(\vec{x})\phi_k(\vec{x}) = \delta_{jk}$, the above-mentioned equation simplifies to

$$\int d^3x\psi_w^*(\vec{x})\psi_w(\vec{x}) = \sum_j\left(\frac{\langle n_j\rangle}{N}\right)^{1/2}\left(\frac{\langle n_j\rangle}{N}\right)^{1/2} = \sum_j\left(\frac{\langle n_j\rangle}{N}\right) = 1, \tag{23}$$

where $(-1)^{j+k-2}=1$ when $j=k$, and $N=\Sigma_j\langle n_j\rangle$. This result makes it clear that, in relation to the statistical average, the product $\psi_w^*(\vec{x})\psi_w(\vec{x})$ may be identified with the probability density known in quantum mechanics. Given that, one can find a general explicit expression for the expansion coefficients of the series expansion of $\psi_w(\vec{x})$,

$$\psi_w(\vec{x}) = \sum_j b_j\phi_j(\vec{x}) = \sum_j (-1)^{j-1}\left(\frac{\langle n_j\rangle}{N}\right)^{1/2}\phi_j(\vec{x}), \tag{24}$$

this equality will, by linear independence, lead to $b_j=(-1)^{j-1}(\langle n_j\rangle/N)^{1/2}$.

III. THE TRANSFORMATION FOR BOSONS

The transformation for Bosons is not too different from the Fermions. In fact the steps are all similar except that in the calculations one needs to exclude the phase factor $(-1)^{(j-1)}$, and include the fact that more than one Boson may occupy the same quantum state. The matrix element for the field operator $\hat{\psi}^{\dagger}(\vec{x})$ in the case of Bosons is

$$\left\langle x-\frac{z}{2}\left|\hat{\psi}^{\dagger}(\vec{x})\right|x+\frac{z}{2}\right\rangle=\sum_{j}\left(\frac{1}{N!}\right)^{2}\left[\sum_{k_1,\ldots,k_N}\Phi_{k_1,\ldots,k_N}\left(\vec{x}_1-\frac{\vec{z}_1}{2},\ldots,\vec{x}_N-\frac{\vec{z}_N}{2}\right)^{S}\right.$$
$$\left.\times\,\Phi^{*}_{k_1,\ldots,k_N}\left(\vec{x}_1+\frac{\vec{z}_1}{2},\ldots,\vec{x}_N+\frac{\vec{z}_N}{2}\right)^{S}\right]\sqrt{n_j}\phi^{*}_{j}(\vec{x}). \tag{25}$$

The numbers $n_1,n_2,\ldots$ are not simply either 1 or 0, because of the Bosons statistics they are allowed to vary from 0 to N. Equation (12) should be written for Bosons

$$\left\langle x-\frac{z}{2}\left|\hat{\psi}^{\dagger}(\vec{x})\right|x+\frac{z}{2}\right\rangle=\sum_{j}\left(\frac{1}{N!n_1!n_2!\cdots}\right)\left[\sum_{k_1,\ldots,k_N}\left(\frac{1}{N!}\right)^{2}\sum_{p'\in S_N}\sum_{p\in S_N}\phi_{k_{p(1)}}\left(\vec{x}_1-\frac{\vec{z}_1}{2}\right)\cdots\phi_{k_{p(N)}}\right.$$
$$\left.\times\left(\vec{x}_N-\frac{\vec{z}_N}{2}\right)\phi^{*}_{k_{p'(1)}}\left(\vec{x}_1+\frac{\vec{z}_1}{2}\right)\cdots\phi^{*}_{k_{p'(N)}}\left(\vec{x}_N+\frac{\vec{z}_N}{2}\right)\sqrt{n_j}\right]\phi^{*}_{j}(\vec{x}). \tag{26}$$

Next apply the same ansatz as with Fermions and integrate with respect to x. All the terms with product of the form $\phi_{k_\ell}(j)\phi^{*}_{k_m}(j)$, $\ni \ell\neq m$, will vanish. Now one can write Eq. (15) for N Bosons

$$\psi^{*}_{w}(p,\vec{x})=\left(\frac{1}{N!}\right)^{2}\frac{1}{N!n_1!n_2!\cdots}\int_{R^{3N}}d^{3N}z e^{i(p\cdot z)/\hbar}\sum_{j=1}^{\infty}\sum_{k_1,\ldots,k_N}\sqrt{n_j}\phi^{*}_{j}(\vec{x})\sum_{p\in S_N}\prod_{\nu=1}^{N}\phi_{k_{p(\nu)}}\left(-\frac{\vec{z}_\nu}{2}\right)\phi^{*}_{k_{p(\nu)}}\left(\frac{\vec{z}_\nu}{2}\right), \tag{27}$$

which when integrated over the z coordinate will give

$$\psi^{*}_{w}(p,\vec{x})=\left(\frac{1}{N!}\right)^{2}\frac{1}{N!n_1!n_2!\cdots}(N-1)!\sum_{j=1}^{\infty}\left[\sum_{k_j}\sqrt{n_j}\sum_{\ell=1}^{N}\int d^{3}z_\ell e^{i(p\cdot\vec{z}_\ell)/\hbar}\phi_{k_j}\left(-\frac{\vec{z}_\ell}{2}\right)\phi^{*}_{k_j}\left(\frac{\vec{z}_\ell}{2}\right)\right]\phi^{*}_{j}(\vec{x}). \tag{28}$$

The Bosonic $\psi^{*}_{w}(p,\vec{x})$ will make it possible to calculate the function $\bar{\psi}^{*}_{w}(\vec{x})$ for Bosons

$$\bar{\psi}^{*}_{w}(\vec{x})=\sum_{\{n_k\}}\psi^{*}_{w}(p,\vec{x})P\{n_k\}=\left(\frac{1}{N!}\right)^{2}\frac{1}{N!n_1!n_2!\cdots}(N-1)!\sum_{j=1}^{\infty}\left[\sum_{\ell=1}^{N}\int d^{3}z_\ell e^{i(p\cdot\vec{z}_\ell)/\hbar}\right.$$
$$\left.\times\sum_{k_j}\phi_{k_j}\left(-\frac{\vec{z}_\ell}{2}\right)\phi^{*}_{k_j}\left(\frac{\vec{z}_\ell}{2}\right)\right]\langle\sqrt{n_j}\rangle\phi^{*}_{j}(\vec{x}) \tag{29}$$

and using the closure relation

$$\bar{\psi}_w^*(\vec{x}) = \left(\frac{1}{N!}\right)^2 \frac{1}{N!n_1!n_2!\cdots}(N-1)!\sum_{j=1}^{\infty}\left[\sum_{\ell=1}^{N}\int d^3z_\ell e^{i(p\cdot\vec{z}_\ell)/\hbar}\delta(\vec{z}_\ell)\right]\langle\sqrt{n_j}\rangle\phi_j^*(\vec{x})$$
$$= \left(\frac{1}{N!}\right)^2 \frac{1}{N!n_1!n_2!\cdots}(N-1)!\sum_{j=1}^{\infty}(N)\langle\sqrt{n_j}\rangle\phi_j^*(\vec{x}) = \left(\frac{1}{N!}\right)\frac{1}{N!n_1!n_2!\cdots}\sum_{j=1}^{\infty}\langle\sqrt{n_j}\rangle\phi_j^*(\vec{x})$$
$$= \left(\frac{1}{N!}\right)\frac{1}{(N-1)!\sqrt{N}n_1!n_2!\cdots}\sum_{j=1}^{\infty}\frac{\langle\sqrt{n_j}\rangle}{\sqrt{N}}\phi_j^*(\vec{x}). \tag{30}$$

The Bosonic $\psi_w^*(\vec{x})$ is

$$\psi_w^*(\vec{x}) \equiv \bar{\psi}_w^*(\vec{x})(N!)(N-1)!\sqrt{N}(n_1!n_2!\cdots) = \sum_{j=1}^{\infty}\frac{\langle\sqrt{n_j}\rangle}{\sqrt{N}}\phi_j^*(\vec{x}). \tag{31}$$

As in the Fermionic case $\psi_w^*(\vec{x})$ will be written for the $N\gg 1$ and the approximation in Eq. (19) will be applied

$$\ln(N^{1/2}N!(N-1)!(n_1!n_2!\cdots)) = (1/2)\ln N + \ln N! + \ln(N-1)! + \sum_{j=1}^{\infty}\ln n_j! \approx (1/2)\ln N + N\ln N$$
$$- N + (N-1)\ln(N-1) - (N-1) + \sum_{j=1}^{\infty}(n_j\ln n_j - n_j) \approx 2N\ln N$$
$$+ \sum_{j=1}^{\infty} n_j\ln n_j = \sum_{j=1}^{\infty}(2N\ln N + n_j\ln n_j) \approx \sum_{j=1}^{\infty}2N\ln N = (N)2N\ln N$$
$$= 2N^2\ln N,$$

where $n_j \ll N, \forall j$. Therefore, for $N\gg 1$ one have

$$\psi_w^*(\vec{x}) \equiv \bar{\psi}_w^*(\vec{x})(N)^{2N^2} = \sum_j\left(\frac{\langle n_j\rangle}{N}\right)^{1/2}\phi_j^*(\vec{x}), \tag{32}$$

where the negligible fluctuation approximation has been applied. The rest of the argument following Eq. (32) will be similar to the fermionic case. Thus, for Bosons, the product $\psi_w^*(\vec{x})\psi_w(\vec{x})$ may be identified with the probability density as well.

IV. THE INCLUSION OF TIME

The time dimension may be added simply by solving the Heisenberg equation[12] for the operator $\hat{b}_j$

$$i\hbar\dot{\hat{b}}_j(t) = [\hat{b}_j(t), \hat{H}(t)] \tag{33}$$

and this will allow the definition of the time-dependent expansion coefficient

$$b_j(t) = (-1)^{(j-1)}\left(\frac{\langle n_j\rangle}{N}\right)^{1/2}e^{-i\epsilon_j t/\hbar}, \tag{34}$$

where ϵ_j is the energy of the j^{th} eigenstate. The transformed function in Eq. (24) may now be written as a field with a position, and a time dependence

$$\psi_w^*(\vec{x},t)=\sum_j(-1)^{(j-1)}\left(\frac{\langle n_j\rangle}{N}\right)^{1/2}e^{+i\epsilon_j t/\hbar}\phi_j^*(\vec{x}) \tag{35}$$

which, in turn, will allow the Wigner transformation with the time dimension

$$\begin{aligned}\psi_w^*(\vec{x},t)&=N\bar{\psi}_w^*(\vec{x},t)=N\sum_{\{n_k\}}\psi_w^*(p,\vec{x},t)P\{n_k\}=N\sum_{\{n_k\}}\int d^{3N}x\Psi_w^*(x,p,\vec{x},t)P\{n_k\}\\&=N\sum_{\{n_k\}}\int_{R^{3N}}d^{3N}xd^{3N}ze^{i(p\cdot z)/\hbar}\left\langle x-\frac{z}{2}\middle|\hat{\psi}^\dagger(\vec{x},t)\middle|x+\frac{z}{2}\right\rangle P\{n_k\}.\end{aligned} \tag{36}$$

V. IN RELATION TO THE SCHRÖDINGER EQUATION

Unless one can show a relation between $\psi_w^*(\vec{x},t)$ and a function which is defined in quantum mechanics, the function $\psi_w^*(\vec{x},t)$ remains to be only the function resulting from the Wigner transform of the operator $\hat{\psi}^\dagger(\vec{x},t)$. To this end one applies the energy operators $\hat{E}=i\hbar\partial/\partial t$, and $\hat{H}=-(\hbar^2/2m)\nabla^2+V(\vec{x})$ separately to the complex conjugate of the function $\psi_w^*(\vec{x},t)$

$$i\hbar\frac{\partial}{\partial t}\psi_w(\vec{x},t)=N\sum_{\{n_k\}}\int_{R^{3N}}d^{3N}xd^{3N}ze^{-i(p\cdot z)/\hbar}\left\langle x+\frac{z}{2}\middle|i\hbar\frac{\partial}{\partial t}\hat{\psi}(\vec{x},t)\middle|x-\frac{z}{2}\right\rangle P\{n_k\}, \tag{37}$$

$$\hat{H}\psi_w(\vec{x},t)=N\sum_{\{n_k\}}\int_{R^{3N}}d^{3N}xd^{3N}ze^{-i(p\cdot z)/\hbar}\left\langle x+\frac{z}{2}\middle|\hat{H}\hat{\psi}(\vec{x},t)\middle|x-\frac{z}{2}\right\rangle P\{n_k\}, \tag{38}$$

which by subtraction leads to

$$\begin{aligned}\hat{H}\psi_w(\vec{x},t)-i\hbar\frac{\partial}{\partial t}\psi_w(\vec{x},t)=N\sum_{\{n_k\}}\int_{R^{3N}}d^{3N}xd^{3N}ze^{-i(p\cdot z)/\hbar}&\left\langle x+\frac{z}{2}\middle|\hat{H}\hat{\psi}(\vec{x},t)\right.\\&\left.-i\hbar\frac{\partial}{\partial t}\hat{\psi}(\vec{x},t)\middle|x-\frac{z}{2}\right\rangle P\{n_k\}.\end{aligned} \tag{39}$$

However, the field equation[12]

$$-\frac{\hbar^2}{2m}\nabla^2\hat{\psi}(\vec{x},t)+V(\vec{x})\hat{\psi}(\vec{x},t)=i\hbar\frac{\partial}{\partial t}\hat{\psi}(\vec{x},t) \tag{40}$$

holds for both Fermions and Bosons, which along with Eq. (39) will give

$$-\frac{\hbar^2}{2m}\nabla^2\psi_w(\vec{x},t)+V(\vec{x})\psi_w(\vec{x},t)=i\hbar\frac{\partial}{\partial t}\psi_w(\vec{x},t). \tag{41}$$

Equation (41) leads to the fact that the function $\psi_w(\vec{x},t)$ is the solution to the Schrödinger equation, thereby proving that the functions $\psi_w^*(\vec{x})$ appearing in Eqs. (20) and (32) are the quantum mechanical wave functions from which the probability density may be calculated by taking the square of the norm for each function. With the understanding that the Fermionic wave function is $(N)^{2N}$ times the Fermionic $\bar{\psi}_w^*(\vec{x})$ and that the Bosonic wave function is $(N)^{2N^2}$ times the Bosonic $\bar{\psi}_w^*(\vec{x})$, the quantum mechanical wave function $\psi_w(\vec{x},t)\equiv\psi(\vec{x},t)$ can now be written for the both types of particles

$$\psi(\vec{x},t) = \sum_j \kappa_j \left(\frac{\langle n_j\rangle}{N}\right)^{1/2} e^{-i\epsilon_j t/\hbar}\phi_j(\vec{x}), \tag{42}$$

where

$$\kappa_j = \begin{cases} (-1)^{(j-1)} & \text{for Fermions} \\ 1 & \text{for Bosons.} \end{cases}$$

According to Eq. (42) projections of the Bosonic field amplitude can be much stronger than the same projections of the Fermionic field amplitude. This is due to the fact that both fields are directly proportional to the average occupation number. If $x \equiv \beta(\epsilon_k - \mu)$ then $x \to 0$ leads to $\langle n_j\rangle \to \infty$ for Bosons and $\langle n_j\rangle \to 1$ for Fermions (Ref. 7, p. 306). Also, for Bosons the κ_j factor is positive for all the terms in Eq. (42), but for Fermions it changes sign which means that some terms will be subtracted from the total sum. Thus, one can conclude that a certain projection of the Bosonic field amplitude can be much stronger than a similar projection of the Fermionic field amplitude for that limit. This is consistent with physical observations.[10]

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APPENDIX: PRODUCT RESULTS OF ANTISYMMETRIZED (SYMMETRIZED) STATE FUNCTIONS

For a two state system $\{k_1,k_2\}$ the product of the anti-symmetrized sums in Eq. (12) is

$$\begin{aligned}
I_2 &= \sum_{k_1,k_2}\sum_{p',p} \mathrm{sgn}(p')\mathrm{sgn}(p)\phi_{k_{p_1}}\left(\vec{x}_1 - \frac{\vec{z}_1}{2}\right)\phi_{k_{p_2}}\left(\vec{x}_2 - \frac{\vec{z}_2}{2}\right)\phi^*_{k_{p_1}}\left(\vec{x}_1 + \frac{\vec{z}_1}{2}\right)\phi^*_{k_{p_2}}\left(\vec{x}_2 + \frac{\vec{z}_2}{2}\right) \\
&= \sum_{k_1}\phi_{k_1}\left(\vec{x}_1 - \frac{\vec{z}_1}{2}\right)\phi^*_{k_1}\left(\vec{x}_1 + \frac{\vec{z}_1}{2}\right)\sum_{k_2}\phi_{k_2}\left(\vec{x}_2 - \frac{\vec{z}_2}{2}\right)\phi^*_{k_2}\left(\vec{x}_2 + \frac{\vec{z}_2}{2}\right) - \sum_{k_1}\phi_{k_1}\left(\vec{x}_1 - \frac{\vec{z}_1}{2}\right)\phi^*_{k_1}\left(\vec{x}_2 + \frac{\vec{z}_2}{2}\right) \\
&\quad \times \sum_{k_2}\phi_{k_2}\left(\vec{x}_2 - \frac{\vec{z}_2}{2}\right)\phi^*_{k_2}\left(\vec{x}_1 + \frac{\vec{z}_1}{2}\right) - \sum_{k_1}\phi_{k_1}\left(\vec{x}_2 - \frac{\vec{z}_2}{2}\right)\phi^*_{k_1}\left(\vec{x}_1 + \frac{\vec{z}_1}{2}\right)\sum_{k_2}\phi_{k_2}\left(\vec{x}_1 - \frac{\vec{z}_1}{2}\right)\phi^*_{k_2}\left(\vec{x}_2 + \frac{\vec{z}_2}{2}\right) \\
&\quad + \sum_{k_1}\phi_{k_1}\left(\vec{x}_2 - \frac{\vec{z}_2}{2}\right)\phi^*_{k_1}\left(\vec{x}_2 + \frac{\vec{z}_2}{2}\right)\sum_{k_2}\phi_{k_2}\left(\vec{x}_1 - \frac{\vec{z}_1}{2}\right)\phi^*_{k_2}\left(\vec{x}_1 + \frac{\vec{z}_1}{2}\right) = \delta(\vec{z}_1)\delta(\vec{z}_2) - \sum_{k_1,k_2}\phi_{k_1}\left(\vec{x}_1 - \frac{\vec{z}_1}{2}\right) \\
&\quad \times \phi^*_{k_1}\left(\vec{x}_2 + \frac{\vec{z}_2}{2}\right)\phi_{k_2}\left(\vec{x}_2 - \frac{\vec{z}_2}{2}\right)\phi^*_{k_2}\left(\vec{x}_1 + \frac{\vec{z}_1}{2}\right) - \sum_{k_1,k_2}\phi_{k_1}\left(\vec{x}_2 - \frac{\vec{z}_2}{2}\right)\phi^*_{k_1}\left(\vec{x}_1 + \frac{\vec{z}_1}{2}\right) \\
&\quad \times \phi_{k_2}\left(\vec{x}_1 - \frac{\vec{z}_1}{2}\right)\phi^*_{k_2}\left(\vec{x}_2 + \frac{\vec{z}_2}{2}\right) + \delta(\vec{z}_2)\delta(\vec{z}_1) = 2!\,\delta(\vec{z}_1)\delta(\vec{z}_2) + \text{other terms} = 2!\prod_{\ell=1}^{2}\delta(\vec{z}_\ell) \\
&\quad + \text{other terms}.
\end{aligned} \tag{A1}$$

For a three state system the product of the anti-symmetrized sums in (12) is

$$\begin{aligned}
I_3 &= \phi_{k_1}(1)\phi_{k_2}(2)\phi_{k_3}(3)\phi^*_{k_1}(1)\phi^*_{k_2}(2)\phi^*_{k_3}(3) - \phi_{k_1}(1)\phi_{k_2}(2)\phi_{k_3}(3)\phi^*_{k_2}(1)\phi^*_{k_1}(2)\phi^*_{k_3}(3) \\
&\quad + \phi_{k_1}(1)\phi_{k_2}(2)\phi_{k_3}(3)\phi^*_{k_2}(1)\phi^*_{k_3}(2)\phi^*_{k_1}(3) - \phi_{k_1}(1)\phi_{k_2}(2)\phi_{k_3}(3)\phi^*_{k_3}(1)\phi^*_{k_2}(2)\phi^*_{k_1}(3) \\
&\quad + \phi_{k_1}(1)\phi_{k_2}(2)\phi_{k_3}(3)\phi^*_{k_3}(1)\phi^*_{k_1}(2)\phi^*_{k_2}(3) - \phi_{k_1}(1)\phi_{k_2}(2)\phi_{k_3}(3)\phi^*_{k_1}(1)\phi^*_{k_3}(2)\phi^*_{k_2}(3) \\
&\quad - \phi_{k_2}(1)\phi_{k_1}(2)\phi_{k_3}(3)\phi^*_{k_1}(1)\phi^*_{k_2}(2)\phi^*_{k_3}(3) + \phi_{k_2}(1)\phi_{k_1}(2)\phi_{k_3}(3)\phi^*_{k_2}(1)\phi^*_{k_1}(2)\phi^*_{k_3}(3)
\end{aligned}$$

$$
\begin{aligned}
&- \phi_{k_2}(1)\phi_{k_1}(2)\phi_{k_3}(3)\phi^*_{k_2}(1)\phi^*_{k_3}(2)\phi^*_{k_1}(3) + \phi_{k_2}(1)\phi_{k_1}(2)\phi_{k_3}(3)\phi^*_{k_3}(1)\phi^*_{k_2}(2)\phi^*_{k_1}(3)\\
&- \phi_{k_2}(1)\phi_{k_1}(2)\phi_{k_3}(3)\phi^*_{k_3}(1)\phi^*_{k_1}(2)\phi^*_{k_2}(3) + \phi_{k_2}(1)\phi_{k_1}(2)\phi_{k_3}(3)\phi^*_{k_1}(1)\phi^*_{k_3}(2)\phi^*_{k_2}(3)\\
&+ \phi_{k_2}(1)\phi_{k_3}(2)\phi_{k_1}(3)\phi^*_{k_1}(1)\phi^*_{k_2}(2)\phi^*_{k_3}(3) - \phi_{k_2}(1)\phi_{k_3}(2)\phi_{k_1}(3)\phi^*_{k_2}(1)\phi^*_{k_1}(2)\phi^*_{k_3}(3)\\
&+ \phi_{k_2}(1)\phi_{k_3}(2)\phi_{k_1}(3)\phi^*_{k_2}(1)\phi^*_{k_3}(2)\phi^*_{k_1}(3) - \phi_{k_2}(1)\phi_{k_3}(2)\phi_{k_1}(3)\phi^*_{k_3}(1)\phi^*_{k_2}(2)\phi^*_{k_1}(3)\\
&+ \phi_{k_2}(1)\phi_{k_3}(2)\phi_{k_1}(3)\phi^*_{k_3}(1)\phi^*_{k_1}(2)\phi^*_{k_2}(3) - \phi_{k_2}(1)\phi_{k_3}(2)\phi_{k_1}(3)\phi^*_{k_1}(1)\phi^*_{k_3}(2)\phi^*_{k_2}(3)\\
&- \phi_{k_3}(1)\phi_{k_2}(2)\phi_{k_1}(3)\phi^*_{k_1}(1)\phi^*_{k_2}(2)\phi^*_{k_3}(3) + \phi_{k_3}(1)\phi_{k_2}(2)\phi_{k_1}(3)\phi^*_{k_2}(1)\phi^*_{k_1}(2)\phi^*_{k_3}(3)\\
&- \phi_{k_3}(1)\phi_{k_2}(2)\phi_{k_1}(3)\phi^*_{k_2}(1)\phi^*_{k_3}(2)\phi^*_{k_1}(3) + \phi_{k_3}(1)\phi_{k_2}(2)\phi_{k_1}(3)\phi^*_{k_3}(1)\phi^*_{k_2}(2)\phi^*_{k_1}(3)\\
&- \phi_{k_3}(1)\phi_{k_2}(2)\phi_{k_1}(3)\phi^*_{k_1}(1)\phi^*_{k_3}(2)\phi^*_{k_2}(3) + \phi_{k_3}(1)\phi_{k_2}(2)\phi_{k_1}(3)\phi^*_{k_1}(1)\phi^*_{k_2}(2)\phi^*_{k_3}(3)\\
&+ \phi_{k_3}(1)\phi_{k_1}(2)\phi_{k_2}(3)\phi^*_{k_1}(1)\phi^*_{k_2}(2)\phi^*_{k_3}(3) - \phi_{k_3}(1)\phi_{k_1}(2)\phi_{k_2}(3)\phi^*_{k_2}(1)\phi^*_{k_1}(2)\phi^*_{k_3}(3)\\
&+ \phi_{k_3}(1)\phi_{k_1}(2)\phi_{k_2}(3)\phi^*_{k_2}(1)\phi^*_{k_3}(2)\phi^*_{k_1}(3) - \phi_{k_3}(1)\phi_{k_1}(2)\phi_{k_2}(3)\phi^*_{k_3}(1)\phi^*_{k_2}(2)\phi^*_{k_1}(3)\\
&+ \phi_{k_3}(1)\phi_{k_1}(2)\phi_{k_2}(3)\phi^*_{k_3}(1)\phi^*_{k_1}(2)\phi^*_{k_2}(3) - \phi_{k_3}(1)\phi_{k_1}(2)\phi_{k_2}(3)\phi^*_{k_1}(1)\phi^*_{k_2}(2)\phi^*_{k_3}(3)\\
&- \phi_{k_1}(1)\phi_{k_3}(2)\phi_{k_2}(3)\phi^*_{k_1}(1)\phi^*_{k_2}(2)\phi^*_{k_3}(3) + \phi_{k_1}(1)\phi_{k_3}(2)\phi_{k_2}(3)\phi^*_{k_2}(1)\phi^*_{k_1}(2)\phi^*_{k_3}(3)\\
&- \phi_{k_1}(1)\phi_{k_3}(2)\phi_{k_2}(3)\phi^*_{k_2}(1)\phi^*_{k_3}(2)\phi^*_{k_1}(3) + \phi_{k_1}(1)\phi_{k_3}(2)\phi_{k_2}(3)\phi^*_{k_3}(1)\phi^*_{k_2}(2)\phi^*_{k_1}(3)\\
&- \phi_{k_1}(1)\phi_{k_3}(2)\phi_{k_2}(3)\phi^*_{k_3}(1)\phi^*_{k_1}(2)\phi^*_{k_2}(3) + \phi_{k_1}(1)\phi_{k_3}(2)\phi_{k_2}(3)\phi^*_{k_1}(1)\phi^*_{k_3}(2)\phi^*_{k_2}(3)\\
&= 6\delta(\vec{z}_1)\delta(\vec{z}_2)\delta(\vec{z}_3) + \text{other terms} = 3!\prod_{\ell=1}^{3}\delta(\vec{z}_\ell) + \text{other terms}. \qquad \text{(A2)}
\end{aligned}
$$

For a symmetrized I_2 and I_3 the $\mathrm{sgn}(p')$ and $\mathrm{sgn}(p)$ need not be included.

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An H-theorem for the general relativistic Ornstein-Uhlenbeck process

M. Rigotti[a] and F. Debbasch[b]
LERMA (ERGA), UMR 8112, UPMC, Site Le Raphaël, 3 rue Galilée 94200 Ivry sur Seine, France

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We construct conditional entropy four-currents for the general relativistic Ornstein-Uhlenbeck process and we prove that the four-divergences of these currents are always non-negative. This *H*-theorem is then discussed in detail. In particular, the theorem is valid in any Lorentzian space-time, even those presenting well-known chronological violations. © *2005 American Institute of Physics.*
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NOTATIONS

In this article, c denotes the speed of light, and the signature of the space-time metric is $(+,-,-,-)$. Indices running from 0 to 3 are indicated by Greek letters. Latin letter indices run instead from 1 to 3. We also introduce the abbreviation $\partial_p^\mu = \partial/\partial p_\mu$ for the partial derivative with respect to an arbitrary component of the momentum p. This notation underlines the fact that this operator transforms as a contravariant vector. Similarly we will often write $\partial_\mu = \partial/\partial x^\mu$, but the latter operator naturally does *not* transform as a tensor. Finally, det g stands for the determinant of the coordinate basis components of the metric tensor g.

I. INTRODUCTION

In Galilean physics, the most common way to quantify the irreversibility of a phenomenon is to introduce an entropy, i.e., a functional of the time-dependent thermodynamical state of the system which never decreases with time. In usual Galilean continuous media theories, the total entropy $\mathcal{S}$ can be written as the integral of an entropy density s over the volume occupied by the system.[24] One also introduces an entropy current $\mathbf{j}_s$ and, since entropy is by definition not generally conserved, the relation $\partial_t s + \nabla \cdot \mathbf{j}_s \geqslant 0$ holds for every evolution of the system.

Traditional relativistic hydrodynamics and kinetic theory deal with the problem in a completely similar manner. An entropy four-current S is associated to the local thermodynamical state of the system;[5,21,14] the total entropy $\mathcal{S}(t_0)$ of the system at time-coordinate $t=t_0$ can be obtained by integrating S over the three-dimensional space-like submanifold $t=t_0$ and the entropy fluxes are obtained by integrating S over two-dimensional submanifolds of space-time. Since entropy is not generally conserved, the simple relation $\nabla \cdot S = \nabla_\mu S^\mu \geqslant 0$ holds for any evolution of the system.

Actually, given a system and its dynamics, any four-vector field S of non-negative divergence which depends on the local thermodynamical state of the system can be considered as an entropy current. In particular, nothing precludes the possibility of associating more than one entropy current to a single local state of a system.

Let us illustrate this remark by considering two special cases of great physical and mathematical interest. Historically speaking, the first statistical theory of out-of-equilibrium systems is Boltzmann's model of dilute Galilean gases.[4,24,13] The local state of the system is encoded in the so-called one particle distribution function f, which obeys the traditional Boltzmann equation. A

[a]On leave from ETH-Hönggerberg, CH-8093 Zürich, Switzerland.
[b]Author to whom correspondence should be addressed; electronic mail: fabrice.debbasch@wanadoo.fr

direct consequence of this equation is that a certain functional of the distribution function never decreases with time. Boltzmann denoted this functional by H and the result is therefore known as Boltzmann's H-theorem. To this day, H is the only-known functional of f that never decreases in time. This H-theorem has later on been extended to the relativistic generalization of Boltzmann's model of dilute gases.[14] Thus, the relativistic Boltzmann gas also admits an entropy (and an entropy current) and it seems that this entropy is unique.

The situation is drastically different for stochastic processes. Indeed, a theorem due to Voigt[26,22] states that, under very general conditions, a stochastic process admits an infinity of entropies: Let X be the variable whose time-evolution is governed by the stochastic process and let $\mathrm{d}X$ be a measure in X-space $\mathcal{X}$ (typically, $\mathrm{d}X$ is the Lebesgue measure if $\mathcal{X}\subset\mathbb{R}^n$). Now let f and g be any two probability distribution functions solutions of the transport equation associated to the stochastic process. Then, the quantity

$$\mathcal{S}_{f|g}(t) = -\int_{\mathcal{X}} f(t,X)\ln\left(\frac{f(t,X)}{g(t,X)}\right)dX \tag{1}$$

is a never decreasing function of time and is called the conditional entropy of f with respect to g. Thus, to any given $f(t,\cdot)$ representing the state of the system at time t, one can associate as many entropies as there are different solutions g of the transport equation so, typically, an infinity. Naturally, if the function g_0 defined by $g_0(t,X)=1$ for all t and X is a solution of the transport equation, the conditional entropy $\mathcal{S}_{f|g_0}$ of any distribution f with respect to g_0 coincides with the Boltzmann entropy of f.

The notion of conditional entropy corresponds to what is sometimes called the Kullback information and we refer the reader to Refs. 19, 18, and 3 for extensive discussions of this concept.

The application of Voigt's theorem to Galilean stochastic processes is of course straightforward and rather well known, but its application to relativistic stochastic processes demands discussion. To be definite, we will now particularize our treatment to the ROUP, which is the first relativistic process to have been introduced in the literature.[7,8,2,1,6]

Given a reference frame (chart) $\mathcal{R}$, the ROUP transcribes as a set of stochastic equations governing the evolution of the position and momentum of a diffusing particle as functions of the time coordinate t in $\mathcal{R}$. This set of equations is a stochastic process in the usual sense of the word, and Voigt's theorem ensures this process admits an infinity of conditional entropies. But, by construction, these entropies *a priori* depend on the reference frame $\mathcal{R}$ and the general theorem does not furnish any information about their tensorial status.

This question has been partly answered for the special relativistic Ornstein-Uhlenbeck process.[1] In flat space-time, the ROUP admits as invariant measure in p-space a Jüttner distribution J;[16] this distribution simply describes a special relativistic equilibrium at the temperature of the fluid surrounding the diffusing particle. It has been shown in Ref. 1 that this Jütnner distribution can be used to construct a four-vector field of non-negative four-divergence which can be interpreted as the conditional entropy current of f with respect to J.

The aim of the present article is to prove the existence of conditional entropy currents for the ROUP in curved space-time. The matter is organized as follows. Section II reviews some basic results pertaining to the ROUP in curved space-time with particular emphasis on the Kolmogorov equation associated to the process. It is also recalled here that, in a generic space-time, this equation does *not* admit any equilibrium stationary solution.[6] In particular, a general relativistic Jütnner distribution is not, generically, a solution of the Kolmogorov equation and, therefore, cannot be used to construct an entropy current in curved space-time. We therefore consider two arbitrary solutions f and g of the Kolmogorov equation and introduce in Sec. III A a candidate for the conditional entropy current of f with respect to g. We then prove in Sec. III B that the four-divergence of this current is always non-negative. This is our main result and it constitutes an H-theorem for the ROUP in curved space-time. Note that the flat space-time version of this H-theorem is itself a new result because our previous work[1] only proved the existence of a single

entropy current for the ROUP in flat space-time, i.e., the conditional entropy current of an arbitrary distribution f with respect to the Jüttner equilibrium distribution J. Finally, the new H-theorem and some of its possible extensions are discussed at length in Sec. IV. The Appendix recalls and, if necessary, proves some simple but important purely geometrical relations useful in deriving the H-theorem.

II. BASICS ON THE ROUP IN CURVED SPACE-TIME

A. Kolmogorov equation

The general relativistic Ornstein-Uhlenbeck process can be viewed as a toy model for the diffusion of a point particle of nonvanishing mass m interacting with both a fluid and a gravitational field. This process is best presented by its Kolmogorov equation in manifestly covariant form.[6] The extended phase-space is the eight-dimensional bundle cotangent to the space-time manifold with local coordinates, say (x^μ, p_ν), $(\mu,\nu)\in\{0,1,2,3\}^2$. At each point in space-time, the four-dimensional (4D) momentum space $\mathcal{P}$ is equipped with the 4D volume measure:

$$\mathcal{D}^4p = \theta(p_0)\,\delta(p^2 - m^2c^2)\frac{1}{\sqrt{-\det g}}d^4p, \tag{2}$$

with $d^4p = dp_0\wedge dp_1\wedge dp_2\wedge dp_3$. This measure behaves as a scalar with respect to arbitrary coordinate changes. Note that integrals over $\mathcal{P}$ defined by using (multiples of) $\mathcal{D}^4p$ as a measure are *de facto* restricted to the (generally position-dependent) mass-shell.

Let f be the probability distribution function in the extended phase-space of a particle diffusing in a surrounding fluid with normalized four-velocity U. As shown in Ref. 6, f obeys a manifestly covariant Kolmogorov equation which can be written in the following compact form:

$$\partial_\mu(p^\mu f) = -\partial_p^\mu\left\{\widetilde{\Gamma}_\mu f + \mathcal{K}_\mu(f)\right\}. \tag{3}$$

The coefficients $\widetilde{\Gamma}_\mu$, which do not constitute a tensor, are defined by

$$\widetilde{\Gamma}_\mu = \Gamma^\lambda_{\mu\nu}g^{\kappa\nu}p_\kappa p_\lambda \tag{4}$$

and

$$\mathcal{K}_\mu(f) = I_\mu f - \partial_p^\nu(J_{\mu\nu}f) \tag{5}$$

with

$$I_\mu = -DK^\alpha{}_\mu{}^\beta{}_\nu\partial_p^\nu\left(\frac{p_\alpha p_\beta}{p\cdot U}\right) + mcF_\mu, \tag{6}$$

$$J_{\mu\nu} = -DK^\alpha{}_\mu{}^\beta{}_\nu\frac{p_\alpha p_\beta}{p\cdot U}. \tag{7}$$

The tensor K is independent of p. It depends on U and on the metric g, but only through the projector Δ on the orthogonal to U, which reads:

$$\Delta^{\mu\nu} = g^{\mu\nu} - U^\mu U^\nu. \tag{8}$$

The explicit expression of K in terms of U and Δ is

$$K^{\alpha\mu\beta\nu} = U^\alpha U^\beta\Delta^{\mu\nu} + U^\mu U^\nu\Delta^{\alpha\beta} - U^\alpha U^\nu\Delta^{\mu\beta} - U^\mu U^\beta\Delta^{\alpha\nu}. \tag{9}$$

Finally, F represents the deterministic part of the force exerted by the fluid on the diffusing particle; its expression as a function of p and U reads

$$F_\mu = -\lambda_{\mu\nu} p^\nu \frac{p^2}{m^2c^2} + \lambda_{\alpha\beta} \frac{p^\alpha p^\beta}{m^2c^2} p_\mu, \tag{10}$$

with

$$\lambda_{\mu\nu} = \frac{\alpha (mc)^2}{(p \cdot U)^2} \Delta_{\mu\nu}, \tag{11}$$

$\alpha > 0$ being the friction coefficient (see Ref. 7). Note that F is by construction orthogonal to p.

It has been shown in Ref. 6 that (3) does not generically admit stationary solutions. In particular, a general relativistic Jüttner distribution cannot be used to construct in curved space-time a preferred conditional entropy current for the ROUP.

III. *H*-THEOREM FOR THE ROUP IN CURVED SPACE-TIME

A. Definition of the conditional entropy currents

Given any two probability distribution functions f and g defined over the extended phase-space, a natural definition for the conditional entropy current of f with respect to g is

$$S_{f|g}(x) = -\int_{\mathcal{P}} p f(x,p) \ln\left(\frac{f(x,p)}{g(x,p)}\right) \mathcal{D}^4 p. \tag{12}$$

This definition is clearly the simplest generalization of Eq. (37) in Ref. 1 to both an arbitrary reference distribution g and a possibly curved space-time background.

We will now prove that for all f and g solutions of the Kolmogorov equation (3), the four-divergence of $S_{f|g}$ is non-negative.

B. Proof of the *H*-theorem

The proof of the H-theorem for the general relativistic Ornstein-Uhlenbeck process will be carried out in two steps.

1. Computation of the four-divergence of the entropy current

Theorem 1: *For any f and g solutions of Kolmogorov equation*

$$\nabla \cdot S_{f|g}(x) = \int_{\mathcal{P}} J_{\mu\nu}(x,p) D^\mu[f/g] D^\nu[f/g] \mathcal{D}^4 p, \tag{13}$$

where J is defined by (7) *and the functional D is given by*

$$D^\mu[f/g] = \partial_p^\mu \ln(f/g). \tag{14}$$

Proof: The main idea behind the proof is to use Kolmogorov equation (3) to convert all the spatial derivatives into derivatives with respect to momentum components. To do this we will deal with various integrals over $\mathcal{P}$ by integrating most of them by parts. This procedure generally leads to the appearance of so-called "border terms." Some of them trivially vanish if we suppose, as is customary in statistical physics, that phase-space distribution functions tend to zero sufficiently rapidly at infinity (in 4D p-space). One is then left with border terms that are to be evaluated on the hyperplane $p \cdot U = 0$. These also vanish for the following reason. Let us choose, at each point in space-time, an orthornormal basis (tetrad) (e_a), $a = 0,1,2,3$ in the tangent space. Introducing the components p_a and U^a of p and U in this base, the normalization condition $U^2 = 1$ reads:

$$U^0 = \sqrt{1 + \sum_{i=1}^{3} (U^i)^2} \tag{15}$$

so that

$$U^0 > \sqrt{\sum_{i=1}^{3} (U^i)^2}. \tag{16}$$

The condition $p \cdot U = 0$ becomes $p_0 U^0 + \Sigma_{i=1}^3 p_i U^i = 0$; since $U^0 > 0$, this translates into

$$p_0 = - \frac{\sum_{i=1}^3 p_i U^i}{U^0}. \tag{17}$$

It follows easily from (16) and (17) that $(p_0)^2 < \Sigma_{i=1}^3 (p_i)^2$ on the hyperplane $p \cdot U = 0$. The Dirac δ distribution which enforces the on mass-shell restriction $p^2 = m^2 c^2$ therefore vanishes on the hyperplane $p \cdot U = 0$, ensuring that the corresponding border terms disappear.

Let us now proceed with the proof of Theorem 1. Direct derivation of Eq. (12) leads to

$$\begin{aligned}
\nabla_\kappa S^\kappa_{f|g} &= -\partial_\kappa \int_{\mathcal{P}} p^\kappa f \ln\left(\frac{f}{g}\right) \mathcal{D}^4 p - \Gamma^\alpha_{\alpha\kappa} \int_{\mathcal{P}} p^\kappa f \ln\left(\frac{f}{g}\right) \mathcal{D}^4 p \\
&= \underbrace{- \int_{\mathcal{P}} \partial_\kappa (p^\kappa f) \ln\left(\frac{f}{g}\right) \mathcal{D}^4 p}_{=\mathcal{A}_1} \underbrace{- \int_{\mathcal{P}} p^\kappa \left[(\partial_\kappa f) - \frac{f}{g} (\partial_\kappa g) \right] \mathcal{D}^4 p}_{=\mathcal{A}_2} \\
&\underbrace{- \int_{\mathcal{P}} p^\kappa f \ln\left(\frac{f}{g}\right) \partial_\kappa (\mathcal{D}^4 p)}_{=\mathcal{A}_3} \underbrace{- \Gamma^\alpha_{\alpha\kappa} \int_{\mathcal{P}} p^\kappa f \ln\left(\frac{f}{g}\right) \mathcal{D}^4 p}_{=\mathcal{A}_4}.
\end{aligned} \tag{18}$$

Using Kolmogorov equation (3), integrating by parts, and inserting the definition of $\mathcal{K}_\mu(f)$ Eq. (5) we obtain for $\mathcal{A}_1$:

$$\begin{aligned}
\mathcal{A}_1 &= \int_{\mathcal{P}} \partial_p^\mu \left\{ \widetilde{\Gamma}_\mu f + \mathcal{K}_\mu(f) \right\} \ln\left(\frac{f}{g}\right) \mathcal{D}^4 p = - \int_{\mathcal{P}} \left\{ \widetilde{\Gamma}_\mu f + \left[I_\mu f - \partial_p^\nu (J_{\mu\nu} f) \right] \right\} \partial_p^\mu \ln\left(\frac{f}{g}\right) \mathcal{D}^4 p \\
&\quad - \int_{\mathcal{P}} \left\{ \widetilde{\Gamma}_\mu f + \mathcal{K}_\mu(f) \right\} \ln\left(\frac{f}{g}\right) \partial_p^\mu (\mathcal{D}^4 p).
\end{aligned} \tag{19}$$

Let us now consider the term $\mathcal{A}_2$:

$$\begin{aligned}
\mathcal{A}_2 &= - \int_{\mathcal{P}} p^\kappa \left[(\partial_\kappa f) - \frac{f}{g} (\partial_\kappa g) \right] \mathcal{D}^4 p \\
&= \underbrace{- \int_{\mathcal{P}} \partial_\kappa (p^\kappa f) \mathcal{D}^4 p}_{=\mathcal{B}_1} + \underbrace{\int_{\mathcal{P}} \partial_\kappa (p^\kappa g) \frac{f}{g} \mathcal{D}^4 p}_{=\mathcal{B}_2}.
\end{aligned} \tag{20}$$

Using again Kolmogorov equation (3) and integrating by parts, we obtain for the term $\mathcal{B}_1$:

$$\mathcal{B}_1 = \int_{\mathcal{P}} \partial_p^\mu \left\{ \widetilde{\Gamma}_\mu f + \mathcal{K}_\mu(f) \right\} \mathcal{D}^4 p = - \int_{\mathcal{P}} \left\{ \widetilde{\Gamma}_\mu f + \mathcal{K}_\mu(f) \right\} \partial_p^\mu (\mathcal{D}^4 p), \tag{21}$$

and for the term $\mathcal{B}_2$:

$$\mathcal{B}_2 = -\int_{\mathcal{P}} \partial_p^\mu \left\{ \widetilde{\Gamma}_\mu g + \mathcal{K}_\mu(g) \right\} \frac{f}{g} \mathcal{D}^4 p = \int_{\mathcal{P}} \left\{ \widetilde{\Gamma}_\mu f + \mathcal{K}_\mu(g) \frac{f}{g} \right\} \partial_p^\mu \ln\left(\frac{f}{g}\right) \mathcal{D}^4 p + \int_{\mathcal{P}} \left\{ \widetilde{\Gamma}_\mu f + \mathcal{K}_\mu(g) \frac{f}{g} \right\} \partial_p^\mu (\mathcal{D}^4 p). \tag{22}$$

Summing (21) and (22) and inserting the definition of $\mathcal{K}_\mu(g)$ Eq. (5) we obtain:

$$\mathcal{A}_2 = \int_{\mathcal{P}} \left\{ \widetilde{\Gamma}_\mu f + \left[I_\mu f - \partial_p^\nu (J_{\mu\nu} g) \frac{f}{g} \right] \right\} \partial_p^\mu \ln\left(\frac{f}{g}\right) \mathcal{D}^4 p + \int_{\mathcal{P}} \left\{ \mathcal{K}_\mu(g) \frac{f}{g} - \mathcal{K}_\mu(f) \right\} \partial_p^\mu (\mathcal{D}^4 p). \tag{23}$$

Putting (19) and (23) together we get:

$$\mathcal{A}_1 + \mathcal{A}_2 = \int_{\mathcal{P}} \left\{ \partial_p^\nu (J_{\mu\nu} f) - \partial_p^\nu (J_{\mu\nu} g) \frac{f}{g} \right\} \partial_p^\mu \ln\left(\frac{f}{g}\right) \mathcal{D}^4 p - \int_{\mathcal{P}} \widetilde{\Gamma}_\mu f \ln\left(\frac{f}{g}\right) \partial_p^\mu (\mathcal{D}^4 p) + \int_{\mathcal{P}} \left\{ \mathcal{K}_\mu(g) \frac{f}{g} - \mathcal{K}_\mu(f) \left[1 + \ln\left(\frac{f}{g}\right) \right] \right\} \partial_p^\mu (\mathcal{D}^4 p). \tag{24}$$

The third integral on the right-hand side of (24) contains two contributions and they both involve the contraction of the operator $\mathcal{K}$ with $\partial_p^\mu(\mathcal{D}^4 p)$. By Eq. (A9), this contraction is proportional to the contraction of $\mathcal{K}$ with p. By definitions (5)–(7), the action of this latter contraction on an arbitrary function h reads:

$$p^\mu \mathcal{K}_\mu(h) = p^\mu \{ I_\mu h - \partial_p^\nu (J_{\mu\nu} h) \} = D K^\alpha{}_\mu{}^\beta{}_\nu p^\mu \frac{p_\alpha p_\beta}{p \cdot U} (\partial_p^\nu h) + mc p^\mu F_\mu h. \tag{25}$$

The tensor $K^{\alpha\mu\beta\nu}$ is antisymmetric upon exchange of the indices μ and α, entailing that $K^{\alpha\mu\beta\nu} p_\alpha p_\mu p_\beta = 0$; moreover, the deterministic four-force F is orthogonal to the momentum p, i.e., $p^\mu F_\mu = 0$. Equation (25) therefore simply reduces to

$$p^\mu \mathcal{K}_\mu(h) = 0. \tag{26}$$

The last integral in (24) therefore disappears, and we can write:

$$\mathcal{A}_1 + \mathcal{A}_2 = \int_{\mathcal{P}} f \underbrace{\left\{ \frac{1}{f} \partial_p^\nu (J_{\mu\nu} f) - \frac{1}{g} \partial_p^\nu (J_{\mu\nu} g) \right\}}_{= J_{\mu\nu} D^\mu [f/g]} D^\mu [f/g] \, \mathcal{D}^4 p - \Gamma^\nu_{\mu\kappa} \int_{\mathcal{P}} p^\kappa p_\nu f \ln\left(\frac{f}{g}\right) \partial_p^\mu (\mathcal{D}^4 p), \tag{27}$$

where we used definition (14) of $D^\mu[\cdot]$ and definition (4) of $\widetilde{\Gamma}_\mu$.

Let us now address the $\mathcal{A}_3$ contribution to Eq. (18). Inserting the expression (A10) for $\partial_\kappa(\mathcal{D}^4 p)$, we have

$$\mathcal{A}_3 = -\int_{\mathcal{P}} p^\kappa f \ln\left(\frac{f}{g}\right) \partial_\kappa (\mathcal{D}^4 p) = \Gamma^\nu_{\kappa\mu} \int_{\mathcal{P}} p^\kappa p_\nu f \ln\left(\frac{f}{g}\right) \partial_p^\mu (\mathcal{D}^4 p) + \Gamma^\alpha_{\alpha\kappa} \int_{\mathcal{P}} p^\kappa f \ln\left(\frac{f}{g}\right) \mathcal{D}^4 p. \tag{28}$$

Inserting Eqs. (28) and (27) in (18), we obtain the wanted simple expression:

$$\nabla_\mu S^\mu_{f|g} = \int_{\mathcal{P}} J_{\mu\nu} D^\mu[f/g] D^\nu[f/g] \mathcal{D}^4 p. \tag{29}$$

□

2. The four-divergence of the entropy current is non-negative

We now state a second theorem, which, together with the previous one, will prove the *H*-theorem.

Theorem 2: *For any two arbitrary distributions f and g, the integrand in* Eq. (13) *of Theorem* 1 *is non-negative, that is*:

$$J_{\mu\nu} D^\mu[f/g] D^\nu[f/g] \geqslant 0. \tag{30}$$

Proof: Let us fix an arbitrary point x in space-time and choose as local reference frame ($\mathcal{R}$) at x the proper rest frame at x of the fluid surrounding the diffusing particle. By definition, in this reference frame, the components of the four-velocity $U(x)$ of the fluid at x are simply $U^\mu = (1/\sqrt{g_{00}})(1,0,0,0)$. Inserting these components into the definition (7) for J, we get

$$J^{00} = -\frac{D}{\sqrt{g_{00}} p_0} g^{ij} p_i p_j, \tag{31}$$

$$J^{0i} = -D\left(\frac{1}{g_{00}}(p_0)^2 g^{0i} - \frac{1}{g_{00}} p_0 g^{i\alpha} p_\alpha\right)\frac{\sqrt{g_{00}}}{p_0} = \frac{D}{\sqrt{g_{00}} p_0} g^{ij} p_0 p_j, \tag{32}$$

$$J^{ij} = -D\left(\frac{1}{g_{00}}(p_0)^2 g^{ij}\right)\frac{\sqrt{g_{00}}}{p_0} = -\frac{D}{\sqrt{g_{00}} p_0} g^{ij} (p_0)^2. \tag{33}$$

We thus find:

$$\begin{aligned} J^{\mu\nu} D_\mu D_\nu &= J^{00} D_0 D_0 + 2 J^{0i} D_0 D_i + J^{ij} D_i D_j \\ &= -\frac{D}{\sqrt{g_{00}} p_0}\left[g^{ij} p_i p_j (D_0)^2 - 2 g^{ij} p_0 p_j D_0 D_i + g^{ij} (p_0)^2 D_i D_j\right] \\ &= -\frac{D}{\sqrt{g_{00}} p_0} \underbrace{\left[p_i D_0 - (p_0)^2 D_i\right]}_{=v_i} g^{ij} \underbrace{\left[p_j D_0 - (p_0)^2 D_j\right]}_{=v_j} \\ &= -\frac{D}{\sqrt{g_{00}} p_0} g^{ij} v_i v_j. \end{aligned} \tag{34}$$

By Lemma 1 presented in the Appendix, the right-hand side of this equation is non-negative, which proves Theorem 2. □

IV. DISCUSSION

This article has been focused on the general relativistic Ornstein-Uhlenbeck process introduced in Ref. 6; we have constructed a conditional entropy four-current associated to any two arbitrary distributions solutions of Kolmogorov equation for the ROUP, and we have proven that the four-divergence of this current is always non-negative; this constitutes an *H*-theorem for the ROUP in curved space-time. It is a twofold generalization of the theorem introduced in Ref. 1. First, the *H*-theorem proved in Ref. 1 concerns flat space-time only. Second, Ref. 1 does not deal with a conditional entropy four-current associated to *two* arbitrary distributions, but only with the conditional entropy four-current of *one* arbitrary distribution with respect to the equilibrium dis-

tribution (invariant measure) of the ROUP in flat space-time. Let us note in this context that the ROUP does not generally admit an equilibrium distribution in curved space-time.[6]

We would like now to comment on this new *H*-theorem. Let us first remark that the theorem is valid in any Lorentzian space-time and for any time-like field U representing the velocity of the fluid in which the particles diffuse. In particular, the theorem is even valid in space-times with closed time-like curves, as the Gödel universe or the extended Kerr black hole,[12] and even if U is tangent to one of these closed time-like curves. The irreversibility measured by the local increase of the conditional entropy currents is entirely due to the Markovian character[25,11,23] of the ROUP and the remarkably general validity of the *H*-theorem proves that this irreversibility is in some sense stronger than all possible general relativistic chronological violations.

It should nevertheless be remarked that, as the Boltzmann-Gibbs entropy current associated to the relativistic Boltzmann equation, the conditional entropy four-currents introduced in Sec. III A are not necessarily time-like. And, even when they are time-like, their time-orientation in an orientable space-time generally depends on the point at which they are evaluated. Let us elaborate on this by first recalling the definition of the Boltzmann-Gibbs entropy current $S_{\mathrm{BG}}[f]$ associated to a distribution f (see Ref. 14):

$$S_{\mathrm{BG}}[f](x) = -\int_{\mathcal{P}} pf \ln f \mathcal{D}^4 p. \tag{35}$$

The normalization of f reads:

$$1 = \int_{\mathcal{T}_\Sigma} f d^3x \mathcal{D}^4 p, \tag{36}$$

where Σ is an arbitrary space-like hypersurface of the space-time $\mathcal{M}$ and where $\mathcal{T}_\Sigma \subset T^*(\mathcal{M})$ is defined by

$$\mathcal{T}_\Sigma = \{(x,p) \in T^*(\mathcal{M}), x \in \Sigma\}. \tag{37}$$

As a probability distribution, f is certainly non-negative; but f may take values both superior and inferior to unity. Therefore, nothing can be said on the sign of the function $f \ln f$ against which the time-like vector p is integrated in (35). This entails that $S_{\mathrm{BG}}[f](x)$ may be either time-like or space-like. Also note that the sign of the zeroth component of $S_{\mathrm{BG}}[f](x)$ cannot be ascertained either; thus, even when time-like, the Boltzmann-Gibbs entropy current may be past as well as future oriented (in a time-orientable space-time).

Similarly, the sign of the function $f(x,p)\ln(f(x,p)/g(x,p))$ appearing in definition (12) of the conditional entropy current $S_{f|g}(x)$ generally depends on p (and x) and $S_{f|g}(x)$ may therefore not be time-like. For the same reason, the sign of the zeroth component of $S_{f|g}(x)$ also generally depends on the point in space-time so that the conditional entropy currents, even when time-like, may not have a definite time-orientation (in a time-orientable space-time).

The Galilean limit deserves a particular discussion. The very notions of time-like and space-like vector-fields do not exist in this limit and only the time-orientation of the conditional entropy currents should be addressed. In the Galilean limit, the zeroth component of $S_{f|g}(x)$ reads

$$s_{f|g}(t,\mathbf{x}) = -\int_{\mathbb{R}^3} f(t,\mathbf{x},\mathbf{p}) \ln\left(\frac{f(t,\mathbf{x},\mathbf{p})}{g(t,\mathbf{x},\mathbf{p})}\right) d^3p; \tag{38}$$

note that this expression coincides with the conditional entropy density of the usual, non relativistic Ornstein-Uhlenbeck process.[22] A reasoning similar to the one presented in the preceding paragraph shows that this density may take positive as well as negative values. The time-orientation of the conditional entropy currents is therefore generally position-dependent, even in the Galilean regime.

However, in the Galilean limit, it surely makes sense to integrate $s_{f|g}(t,\mathbf{x})$ over the whole three-dimensional (3D) space to obtain the total (time-dependent) conditional entropy $\mathcal{S}(t)$ of f with respect to g and this quantity can be proven to be non-positive. The proof[22,3] is based on the so-called Gibbs-Klein inequality[25]

$$F \ln F \geqslant F - 1, \tag{39}$$

valid for any positive real number F and applied to $F(t,\mathbf{x},\mathbf{p})=f(t,\mathbf{x},\mathbf{p})/g(t,\mathbf{x},\mathbf{p})$ (with the hypothesis that g does not vanish anywhere in $\mathbb{R}^3$). One has indeed:

$$\int_{\mathcal{V}} s_{f|g}(t,\mathbf{x})d^3x = -\int_{\mathcal{V}\times\mathbb{R}^3} f(t,\mathbf{x},\mathbf{p})\ln\left(\frac{f(t,\mathbf{x},\mathbf{p})}{g(t,\mathbf{x},\mathbf{p})}\right)d^3x\,d^3p \leqslant \int_{\mathcal{V}\times\mathbb{R}^3}\big(f(t,\mathbf{x},\mathbf{p})-g(t,\mathbf{x},\mathbf{p})\big)d^3x\,d^3p \leqslant 0. \tag{40}$$

This calculation can be extended formally to the special and general relativistic situations, but, since conditional entropy four-currents are then not necessarily time-like, their integrals on space-like 3D submanifolds may take positive or negative values. It is therefore far from clear that the concept of *total* conditional entropy makes sense in the relativistic regime. In particular, the relativistic H-theorem proved in this article should be primarily considered as a purely local result.

Thus, the conceptual status of the entropy currents introduced in Sec. III A is in a certain sense similar to the status of the general relativistic black hole entropies.[28,29,17,15] Indeed, we have shown in this article that stochastic processes theory proves the existence of conditional entropy currents in curved space-time and permits their computation, exactly as quantum field theory and string theory both prove the existence of black-holes entropies and furnish the tools necessary for their computations. But the standard statistical interpretation of conditional entropy currents via their fluxes through 3D space-like submanifolds is certainly not straightforward in curved space-time, as the usual interpretation of entropy and temperature via Gibbs canonical ensembles does not seem to extend smoothly to black hole thermodynamics.[29]

It is our opinion that progress in interpreting the notion of entropy in curved space-time can best be achieved by studying specific examples in particular circumstances where most results can be obtained by explicit or semi-explicit calculations. The ROUP is obviously an interesting tool for such computations and diffusion in space-times exhibiting naked or unnaked singularities should certainly be studied in detail.

Finally, it would naturally be most interesting to determine if H-theorems can also be proved for the two "new" relativistic stochastic processes recently proposed as alternative models of relativistic diffusion in Refs. 10 and 9.

APPENDIX

General relations

A basic assumption of general relativity is that the connection ∇ used in space-time is the Levi-Civita connection of the space-time metric g.[27] Given a coordinate basis, this translates into the following relation between the metric components $g_{\mu\nu}$ and the connection coefficients $\Gamma^{\alpha}_{\mu\nu}$:

$$\partial_\kappa g_{\mu\nu} = \Gamma^{\alpha}_{\kappa\mu} g_{\alpha\nu} + \Gamma^{\alpha}_{\kappa\nu} g_{\mu\alpha}. \tag{A1}$$

Another equivalent form of (A1) is

$$\partial_\kappa g^{\mu\nu} = -\Gamma^{\mu}_{\kappa\alpha} g^{\alpha\nu} - \Gamma^{\nu}_{\kappa\alpha} g^{\mu\alpha}. \tag{A2}$$

A direct consequence of (A2) is that, for any vector p:

$$(\partial_\kappa g^{\mu\nu}) p_\mu p_\nu = -\Gamma^{\mu}_{\kappa\alpha} p^\alpha p_\mu - \Gamma^{\nu}_{\kappa\alpha} p^\alpha p_\nu = -2\Gamma^{\nu}_{\kappa\mu} p_\nu p^\mu. \tag{A3}$$

Another useful relation reads:[20]

$$\partial_\kappa \det g = (\det g) g^{\mu\nu} \partial_\kappa g_{\mu\nu}. \tag{A4}$$

Using (A1), this translates into

$$\partial_\kappa \det g = (\det g) g^{\mu\nu} 2\Gamma^\alpha_{\kappa\mu} g_{\alpha\nu} = 2(\det g)\Gamma^\alpha_{\kappa\alpha}. \tag{A5}$$

A useful lemma

Lemma 1: *Let* (∂_μ) *be a* (*local*) *coordinate basis of a Lorentzian space-time* (*with time-like* ∂_0). *Then*, *at any point x of space-time*, *the set of the six spatial components* $g^{ij}(x)$ *of the inverse metric tensor define a non-positive quadratic form. More precisely*,

$$g^{ij}(x) v_i v_j \leqslant 0 \quad \text{for all } (v_1, v_2, v_3) \in \mathbb{R}^3.^1 \tag{A6}$$

Proof: Let x be a point in space-time and suppose there exists a set of three real numbers (v_1, v_2, v_3) such that $g^{ij}(x) v_i v_j > 0$. Define V, cotangent to the space-time manifold at x, by its components $V_0 = 0$, $V_1 = v_1$, $V_2 = v_2$, $V_3 = v_3$. The vector V is both time-like and orthogonal to ∂_0. The space cotangent to the space-time manifold at x therefore admits a time-like subspace of dimension at least two, which is impossible for a Lorentzian space-time. This proves the lemma.□

Derivatives of the volume measure in momentum-space

Let us now evaluate the partial derivatives of the volume measure $\mathcal{D}^4 p$ with respect to both space-time coordinates and momentum components. The measure $\mathcal{D}^4 p$ is defined by an expression which involves the product of a Heaviside function and a Dirac distribution. Direct derivation of this expression would lead to a product of Dirac distributions, which is not a well-defined mathematical object. To avoid this (at least formal) problem, we introduce a class of regular functions h_ϵ, which uniformly converge towards δ as ϵ tends to zero and write:

$$\partial^\mu_p \{\theta(p_0)\delta(p^2 - m^2c^2)\} = \lim_{\epsilon \to 0} \partial^\mu_p \{\theta(p_0) h_\epsilon (g^{\alpha\beta} p_\alpha p_\beta - m^2 c^2)\}$$

$$= \lim_{\epsilon \to 0} \{\delta(p_0)\delta^\mu_0 h_\epsilon (g^{\alpha\beta} p_\alpha p_\beta - m^2 c^2) + \theta(p_0)\partial^\mu_p [h_\epsilon (g^{\alpha\beta} p_\alpha p_\beta - m^2 c^2)]\}$$

$$= \lim_{\epsilon \to 0} \{\delta(p_0)\delta^\mu_0 h_\epsilon (g^{ij} p_i p_j - m^2 c^2) + \theta(p_0) 2 g^{\mu\nu} p_\nu h'_\epsilon (g^{\alpha\beta} p_\alpha p_\beta - m^2 c^2)\}. \tag{A7}$$

By Lemma 1 (Eq. (A6)), $g^{ij} p_i p_j \leqslant 0$. The argument of h_ϵ in the last line of (A7) is therefore always strictly negative. The term involving h_ϵ thus disappears for $\epsilon \to 0$ and we are left with the result:

$$\partial^\mu_p \{\theta(p_0)\delta(p^2 - m^2c^2)\} = 2p^\mu \theta(p_0)\delta'(p^2 - m^2c^2). \tag{A8}$$

This equation leads directly to the following expression for the partial derivatives of $\mathcal{D}^4 p$ with respect to momentum components:

$$\partial^\mu_p (\mathcal{D}^4 p) = \partial^\mu_p \left\{ \theta(p_0)\delta(p^2 - m^2c^2) \frac{1}{\sqrt{-\det g}} \right\} d^4 p = 2p^\mu \theta(p_0)\delta'(p^2 - m^2c^2) \frac{1}{\sqrt{-\det g}} d^4 p. \tag{A9}$$

[1] See for example Sec. 84 of Ref. 20.

Let us now focus on the derivatives of $\mathcal{D}^4p$ with respect to space-time coordinates. Using Eqs. (A3), (A5), and (A9), we obtain

$$\partial_\kappa(\mathcal{D}^4p) = \partial_\kappa\left\{\theta(p_0)\delta(g^{\mu\nu}p_\mu p_\nu - m^2c^2)\frac{1}{\sqrt{-\det g}}\right\}d^4p = \theta(p_0)(\partial_\kappa g^{\mu\nu})p_\mu p_\nu \delta'(p^2 - m^2c^2)\frac{1}{\sqrt{-\det g}}d^4p$$
$$+ \theta(p_0)\delta(p^2 - m^2c^2)\partial_\kappa\left(\frac{1}{\sqrt{-\det g}}\right)d^4p = -2\Gamma^\nu_{\kappa\mu}p_\nu p^\mu \theta(p_0)\delta'(p^2 - m^2c^2)\frac{1}{\sqrt{-\det g}}d^4p$$
$$- \theta(p_0)\delta(p^2 - m^2c^2)\frac{1}{\sqrt{-\det g}}\frac{\partial_\kappa \det g}{2\det g}d^4p = -\Gamma^\nu_{\kappa\mu}p_\nu\partial^\mu_p(\mathcal{D}^4p) - \Gamma^\alpha_{\kappa\alpha}\mathcal{D}^4p. \quad \text{(A10)}$$

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An application of the inverse scattering transform to the modified intermediate long wave equation

George Scoufis[a)]
School of Quantitative Methods and Mathematical Sciences, University of Western Sydney, Sydney, NSW 1797, Australia

Christopher M. Cosgrove
School of Mathematics and Statistics, University of Sydney, Sydney, NSW 2006, Australia

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The modified intermediate long wave (MILW) equation is a (1+1)-dimensional nonlinear singular integro-differential equation that possesses soliton solutions. In an appropriate limit the MILW equation reduces to the well-known modified Korteweg-de Vries equation. In this paper we solve the initial value problem for the MILW equation through a suitable implementation of the inverse scattering transform and use of the Miura-type transformation that maps solutions of the MILW equation into solutions of a complexified version of the standard intermediate long wave (ILW) equation. The initial value used for the MILW equation is assumed to be real valued, sufficiently smooth, and decaying to zero as the absolute value of the spatial variable approaches large values. An interesting feature of the procedure we develop is that soliton solutions for the ILW and MILW equations can be derived by appropriate specializations of a master set of equations. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1996830]

I. INTRODUCTION AND PRELIMINARY

In a remarkable and seminal paper[1] that appeared in 1967, Gardner, Greene, Kruskal, and Miura (GGKM) derived an exact reduction to a linear problem for the initial value problem associated with the nonlinear evolution equation,

$$u_t + 6uu_x + u_{xxx} = 0, \tag{1.1}$$

where u $(=u(x,t))$ is a real-valued function of x and t over the domain $-\infty < x < \infty$ and $t \geqslant 0$, and u_x denotes $\partial u/\partial x$, etc. Equation (1.1) is known as the "KdV equation," and derives its name from work by Korteweg and de Vries[2] that models weakly nonlinear long waves propagating on the surface of a rectangular canal. However, it was Boussinesq[3] who first derived Eq. (1.1) as a model in a hydrodynamical context.

GGKM[1] solved Eq. (1.1) by leveraging results derived by Gel'fand and Levitan[4] for the solution of the inverse problem associated with the one-dimensional time-independent Schrödinger equation,

$$\psi_{xx} = -(u + \kappa)\psi, \tag{1.2}$$

where $\psi = \psi(x,t)$, κ is the spectral parameter, and u is the potential. Their ingenious method identified the potential in Eq. (1.2) with the desired solution of Eq. (1.1), and eventually arrived at a closed system of linear integral equations from which one can construct the physical variable $u(x,t)$.

The modified Korteweg-de Vries (MKdV) equation,

[a)]Permanent address: National Australia Bank, Level 27, 255 George Street, Sydney, NSW 2000, Australia.

$$\nu_t + 6\nu^2\nu_x + \nu_{xxx} = 0, \tag{1.3}$$

where $\nu = \nu(x,t)$, was pivotal[5,6] in the development of the procedure used by GGKM to solve the initial value problem for Eq. (1.1). Equation (1.3) has important physical applications,[7] but we will focus our attention on a certain transformation that connects Eq. (1.3) to Eq. (1.1). Miura[8] has derived the explicit nonlinear transformation,

$$u = \nu^2 + i\nu_x, \tag{1.4}$$

which maps a *real-valued* solution of Eq. (1.3) into a *complex-valued* solution of Eq. (1.1). (The phrase "complex-valued" will be used throughout this paper to designate a complex-valued function of the two real variables x and t.) The appearance of the imaginary unit i in Eq. (1.4), which can obviously be removed by a complex scaling $\nu \to i\nu$, can be attributed to our selection of positive coefficients throughout Eq. (1.3). Ablowitz *et al.*[9] have shown that Eq. (1.4) maps sparsely onto the set of KdV solutions. Equation (1.4) is the x part of a pair of equations forming a Bäcklund transformation (BT),[10] and it was this particular BT that led GGKM[5] to consider the inverse problem for Eq. (1.2).

The method used by GGKM to solve the initial value problem for the KdV equation has flourished into a systematic mathematical technique known as the "inverse scattering transform" (IST).[11] Initial value problems for numerous nonlinear wave equations have been solved analytically by suitable implementations of the IST.[12–17]

The versatility of the IST is exemplified in its application to nonlinear singular integro-differential equations. The prototype equation of this type that is solvable by an application of the IST is the intermediate long wave (ILW) equation,[18–20]

$$U_t + \frac{1}{\delta}U_x + 2UU_x + \mathbf{T}(U_{xx}) = 0, \tag{1.5}$$

where $U = U(x,t)$ [or, more precisely, $U(x,t;\delta)$], δ is a *positive* parameter, and the operator $\mathbf{T}$ is defined by the Cauchy principal-value integral,

$$(\mathbf{T}f)(x) := \frac{1}{2\delta}(P)\int_{-\infty}^{\infty} \coth\left(\frac{\pi}{2\delta}(\xi - x)\right) f(\xi)\mathrm{d}\xi. \tag{1.6}$$

For convenience, we will use the notation $\mathbf{T}(f(x))$ interchangeably with $(\mathbf{T}f)(x)$. Equation (1.5) models one-dimensional propagation of weakly nonlinear long internal gravity waves in a density-stratified fluid of *finite* total depth.[21,22]

Throughout this paper we assume that any argument of $\mathbf{T}$ satisfies all the conditions necessary to guarantee the validity of our computations. In particular, a necessary condition for the existence of $(\mathbf{T}f)(x)$ is the convergence of the improper Riemann integral $\int_{-\infty}^{\infty} f(x)\mathrm{d}x$. For later purposes, we require that the convergence be absolute. We also assume that $U(x,t)$ and its first few derivatives with respect to x vanish in the limit $x \to \pm\infty$. In Appendix A of this paper the reader will find a useful summary of some relevant mathematical properties of the operator $\mathbf{T}$. An essential property that we use frequently is the fact that $\mathbf{T}$ commutes with differentiation so that, for example, $\mathbf{T}(U_{xx}) = \partial^2\mathbf{T}(U)/\partial x^2$. Appendix B contains a selection of useful $\mathbf{T}$ transforms.

Despite the obvious differences in the mathematical structure of the KdV and ILW equations, these two equations are connected by virtue of the physical systems they describe. Several researchers[18,22,23] have observed that Eq. (1.5) contracts in the shallow-water limit ($\delta \to 0^+$) to the KdV equation (1.1). To carry out the reduction, let

$$U = \tfrac{1}{4}\delta u + O(\delta^2), \quad x = 2x', \quad t = 24\delta^{-1}t'. \tag{1.7}$$

Then, with the help of Eqs. (A3) and (A5) from Appendix A to compute the shallow-water expansion of $\mathbf{T}(U_{xx})$, the left-hand side of Eq. (1.5) becomes

$$\frac{\delta^2}{96}(u_{t'}+6uu_{x'}+u_{x'x'x'})+O(\delta^3).$$

In the deep-water limit ($\delta\to\infty$), Eq. (1.5) becomes the Benjamin-Ono (BO) equation,[24]

$$q_t+2qq_x+\mathbf{H}(q_{xx})=0, \tag{1.8}$$

where $q=q(x,t)$ and $\mathbf{H}$ (the Hilbert transform) is defined by the integral operator,

$$(\mathbf{H}f)(x):=\frac{1}{\pi}(P)\int_{-\infty}^{\infty}\frac{f(\xi)}{\xi-x}\mathrm{d}\xi. \tag{1.9}$$

Transition from Eq. (1.5) to Eq. (1.8) is a direct consequence of the limit given by Eq. (A2) and the mild restriction that $U(x,t)=q(x,t)+O(1/\delta)$ as $\delta\to\infty$. Equation (1.8) was first derived by Benjamin[24] to model the propagation of unidirectional internal waves with finite amplitude in stable heterogeneous fluid systems of *infinite* total depth. Fokas and Ablowitz[25] have solved the initial value problem for Eq. (1.8) by using an implementation of the IST that is conceptually similar to the IST for nonlinear evolution equations that involve three independent variables (two spatial variables and one temporal variable).

A natural extrapolation from Eqs. (1.5) and (1.8) is to construct *modified* versions (in the sense of the MKdV equation) of the ILW and BO equations. The nomenclature that we will use to refer to the two modified-type nonlinear singular integro-differential equations is *modified intermediate long wave* (MILW) equation for the modified version of the ILW equation, and *modified Benjamin-Ono* (MBO) for the modified version of the BO equation. Desirable attributes of the MILW and MBO equations are that (i) MILW$\to$MKdV in the shallow-water limit $\delta\to 0^+$, (ii) MILW$\to$MBO in the deep-water limit $\delta\to\infty$, and (iii) a Miura transformation maps MILW to ILW such that its deep-water limit maps MBO to BO and its shallow-water limit is the classical Miura transformation mapping MKdV to KdV.

The two candidates to represent the MILW and MBO equations are the following nonlinear singular integro-differential equations:[26–29]

$$\text{MILW},\quad V_t+\beta V_x(e^V-1)+\frac{1}{\delta}V_x+V_x\mathbf{T}(V_x)+\mathbf{T}(V_{xx})=0, \tag{1.10}$$

$$\text{MBO},\quad Q_t+\alpha Q_x(e^Q-1)+Q_x\mathbf{H}(Q_x)+\mathbf{H}(Q_{xx})=0, \tag{1.11}$$

where $V=V(x,t)$, $Q=Q(x,t)$, $\mathbf{T}$ is defined by Eq. (1.6), $\mathbf{H}$ is defined by Eq. (1.9), and α and β are real parameters. Both the MILW and MBO equations are integrable soliton equations. The MILW equation in particular possesses an infinite number of conservation laws,[27] a linear scattering problem,[27] a BT,[27,28] and multisoliton solutions.[28]

Despite the important extension that the MILW equation provides to the mathematical theory for the KdV-MKdV pairing and the possible physical applications of the MILW equation (whose dispersion law is the same as the ILW equation), the initial value problem for the MILW equation has not been solved.[30] The corresponding initial value problem for the MBO equation was recently solved by Scoufis and Cosgrove.[31] The main purpose of this paper is to use the IST to derive the solution of the initial value problem for the MILW equation Eq. (1.10). The initial value $V(x,0)$ for the MILW equation is real-valued, sufficiently smooth, decays to zero as $|x|\to\infty$, and is such that $\int_{-\infty}^{\infty}V(x,0)\mathrm{d}x$ converges absolutely, but is otherwise arbitrary.

We now close this section with an outline of how the remainder of this paper is arranged. Section II is devoted to the derivation of the MILW equation and its Miura transformation to the complex-valued ILW equation. In Sec. III we present the linear scattering problem for the MILW equation. Suitable Jost functions are defined in this section, and we also derive equations that characterize the scattering data forming the continuous spectrum. Section IV examines the bound states and extends the previous results to identify the scattering data forming the discrete spec-

trum. The temporal evolution of the scattering data is presented in Sec. V. Section VI carries out the solution of the inverse problem that emerges from our efforts in Sec. III to identify the analytical properties of the scattering data. Soliton solutions for the complex-valued ILW and real-valued MILW equations are derived in Sec. VII by recourse to the results contained in the preceding sections.

II. MATHEMATICAL ORIGIN OF THE MILW EQUATION

Our primary objective in this section is to elucidate the mathematical origin of the MILW equation. The standard ILW equation provides the catalyst for our work in this section. The dependent variable transformation,

$$W(x,t) := \int_{-\infty}^{x} U(\xi,t)\mathrm{d}\xi,$$

accompanied by the boundary conditions $U(x,t)\to 0$ (uniformly in t) as $|x|\to\infty$, facilitates the conversion of Eq. (1.5) into the equation,

$$W_t + \frac{1}{\delta}W_x + (W_x)^2 + \mathbf{T}(W_{xx}) = 0. \tag{2.1}$$

Let W and W' denote two local complex-valued solutions of Eq. (2.1) that are connected by the auto-Bäcklund transformation,[23]

$$(W' + W)_x = \alpha + i\mathbf{T}(W'_x - W_x) + \beta e^{i(W'-W)}, \tag{2.2}$$

$$(W' - W)_t = -(\alpha + \delta^{-1})(W' - W)_x + i(W' + W)_{xx} - i(W' - W)_x\mathbf{T}(W'_x - W_x), \tag{2.3}$$

where α and β denote two arbitrary real nonzero constants. The proof that elimination of W' produces (the x derivative of) Eq. (2.1), and vice versa, makes use of properties of the $\mathbf{T}$ operator given in Appendix A, especially Eq. (A7).

Next, define the single dependent variable V through the equation,

$$V := i(W' - W). \tag{2.4}$$

Eliminating the $(W'+W)$ terms between Eqs. (2.2) and (2.3), and then using Eq. (2.4), we obtain the nonlinear evolution equation,

$$V_t + \left(\alpha + \frac{1}{\delta}\right)V_x + \beta V_x e^V + V_x\mathbf{T}(V_x) + \mathbf{T}(V_{xx}) = 0, \tag{2.5}$$

where $V=V(x,t)$. This is gauge equivalent to the MILW equation. The parameter α is not essential because it can be varied by a gauge transformation $x\to x+kt$. To get the standard form of the MILW equation, we invoke the boundary conditions $U(x,t)\to 0$ and $V(x,t)\to 0$ as $x\to\pm\infty$ and apply the limit expressed by Eq. (A4) to Eq. (2.2). These conditions force the constraint $\alpha=-\beta$. Thus the standard form of the MILW equation is

$$V_t + \frac{1}{\delta}V_x + \beta V_x(e^V - 1) + V_x\mathbf{T}(V_x) + \mathbf{T}(V_{xx}) = 0. \tag{2.6}$$

In the region $0<\delta\ll 1$, Eq. (2.6) contracts to Eq. (1.3), the latter being the self-focusing form of the MKdV equation. The transition from Eq. (2.6) to Eq. (1.3) requires

$$V = \delta\nu + O(\delta^2), \quad \beta = \delta^{-1} + O(\delta), \quad x = 2x', \quad t = 24\delta^{-1}t'. \tag{2.7}$$

Then, with the assistance of Eq. (A3), the left-hand side of Eq. (2.6) reduces to

$$\frac{\delta^2}{24}(\nu_{t'} + 6\nu^2\nu_{x'} + \nu_{x'x'x'}) + O(\delta^3).$$

Alternative forms of the MILW equation appear in the literature. Nakamura,[28] for example, used the auto–BT of the ILW equation to derive a version of the MILW equation in the form,

$$V_t + (u_0 - \mu + \delta^{-1})V_x + \beta V_x e^V + V_x \mathbf{T}(V_x) + \mathbf{T}(V_{xx}) = 0. \tag{2.8}$$

This is Eq. (2.5) with the parameter α renamed. Satsuma *et al.*[27] derived the equation,

$$\tfrac{1}{3}\delta V_t + \delta^{-1} V_x e^V + V_x \mathbf{T}(V_x) + \mathbf{T}(V_{xx}) = 0, \tag{2.9}$$

as their representative of the MILW equation. Gibbons and Kupershmidt[26] derived the equation,

$$V_t = \delta^{-2} V_x (e^{2i\delta V} - 1 - 2i\delta V) + 2iV_x \hat{\mathbf{T}}(V_x) + \delta^{-1}\hat{\mathbf{T}}(V_{xx}), \tag{2.10}$$

where $\hat{\mathbf{T}}$ is the operator defined by Eq. (A9), and we replaced their pure imaginary δ with $i\delta$ and adjusted a factor of 2 in the second to last term. All these equations are equivalent to the MILW equation Eq. (2.6) under gauge transformations of the form, $x' = \pm x + kt$, $t' = lt$, $V' = pV + q$. On the other hand, Degasperis and co-workers[32,33] derived a qualitatively different nonlinear singular integro-differential equation whose shallow-water limit is the MKdV equation, and so we can conclude that the MILW equation is not the only possible candidate for an intermediate version of the MKdV equation. We have selected Eq. (2.6) as our representative of the MILW equation because it is endowed with a transparent deep-water limit as well as a shallow-water limit that leads directly to the MKdV equation after a simple scaling.

Equation (2.2) contains an explicit relationship between solutions of the ILW and MILW equations. Setting $W' = W - iV$, $W_x = U$, and $\alpha = -\beta$, we get

$$U = \tfrac{1}{2}\{\mathbf{T}(V_x) + \beta(e^V - 1) + iV_x\}. \tag{2.11}$$

Equation (2.11) is the Miura-type transformation that maps *real-valued* solutions V of Eq. (2.6) into *complex-valued* solutions U of Eq. (1.5). If we substitute this U into the left-hand side of the ILW equation (1.5), we will obtain an expression that vanishes on account of Eq. (A7). Substituting Eqs. (1.7) and (2.7) into Eq. (2.11), and then using Eq. (A3) to obtain the shallow-water limit of the $\mathbf{T}$ operator, we will arrive at the classical Miura transformation Eq. (1.4).

In the context of this paper, Eq. (2.11) is essential to the scheme we develop to solve the initial value problem for the MILW equation; we now outline this scheme and provide necessary details in Secs. III–VII. Let $V(x,0)$ denote the known or given initial value of $V(x,t)$ in the MILW equation. We will assume that $V(x,0)$ is a sufficiently smooth real-valued function of x and that $V(x,0)$ and its first few derivatives tend to zero as $x \to \pm\infty$ and $\int_{-\infty}^{\infty} V(x,0)\mathrm{d}x$ converges absolutely. Equation (2.11) maps $V(x,0)$ into the complex-valued function $U(x,0)$, where

$$U(x,0) := \tfrac{1}{2}\{\mathbf{T}(V_x(x,0)) + \beta(e^{V(x,0)} - 1) + iV_x(x,0)\}. \tag{2.12}$$

This function $U(x,0)$, which will be the initial value of $U(x,t)$ in the complex-valued ILW equation, can be considered known because $V(x,0)$ has been specified. As a consequence of Eq. (A4) and the boundary conditions on $V(x,0)$, we have $U(x,0) \to 0$ as $|x| \to \infty$ and $\int_{-\infty}^{\infty} U(x,0)\mathrm{d}x$ is absolutely convergent. Equating imaginary parts on each side of Eq. (2.11), we obtain the important equation,

$$V_x(x,t) = 2\,\mathrm{Im}\{U(x,t)\}, \tag{2.13}$$

for $t \geqslant 0$.

We can solve the initial value problem for $U(x,t)$ by appropriately extending the IST for the real-valued ILW equation derived by Kodama, Ablowitz, and Satsuma (KAS)[19] to take account of the initial value given by Eq. (2.12). As soon as $U(x,t)$ is known, we then proceed to determine

$V_x(x,t)$ from Eq. (2.13), and thence $V(x,t)$ itself by a quadrature with respect to x. An arbitrary function of integration that remains in the formula for $V(x,t)$ will be determined by the boundary conditions on $V(x,t)$. The last stage of our solution scheme for Eq. (2.6) uses the equation,

$$\mathrm{Re}\{U(x,t)\} = \tfrac{1}{2}\{\mathbf{T}(V_x) + \beta(e^V - 1)\}, \tag{2.14}$$

to connect all parameters that originate from the IST (for the complex-valued ILW equation) to the fundamental parameter β in Eq. (2.6). Equation (2.14) is formed when we equate real parts on each side of Eq. (2.11).

The simplest conserved quantity for the ILW equation is

$$L := \frac{1}{2\delta}\int_{-\infty}^{\infty} U(x,t)\mathrm{d}x. \tag{2.15}$$

It is independent of time t on account of Eq. (1.5) and its boundary condition. But when $U(x,t)$ is the complex-valued function on the left-hand side of Eq. (2.11), the constant L is real on account of the boundary condition on $V(x,t)$.

Multisoliton solutions of Eq. (2.8) have been derived by Nakamura[28] by the use of Hirota's method.[34,35] These, of course, translate across to our version of the MILW equation (2.6). Suitable modifications of results contained in Refs. 28 and 36 lead to the one-soliton solution,

$$V(x,t) = \log\left(\frac{\cosh[\kappa(x-\varphi t - x_0)] + \cos(\kappa\delta - \gamma)}{\cosh[\kappa(x-\varphi t - x_0)] + \cos(\kappa\delta + \gamma)}\right), \tag{2.16}$$

where κ, x_0, and γ are arbitrary real parameters with $0 < \kappa < \pi/\delta$ and

$$\varphi = \delta^{-1} - \kappa\cot(\kappa\delta). \tag{2.17}$$

The parameter β in the MILW equation is

$$\beta = \frac{\kappa\sin(\kappa\delta + \gamma)}{\sin\kappa\delta\sin\gamma}. \tag{2.18}$$

In Sec. VII, we will derive this result from the IST and substitute it directly into the MILW equation with the aid of the **T** transform formulas in Appendix B. We will also construct the two-soliton and two-breather solutions from the IST.

The shallow-water limit of the one-soliton solution can be obtained from Eq. (2.7). With $\kappa = O(1)$ as $\delta \to 0^+$, we get $\varphi = \kappa^2\delta/3 + O(\delta^3)$. The limiting form of β given by Eq. (2.7) requires that $\gamma = \pm\pi/2 + O(\delta)$. Then with $\kappa = \kappa'/2$ and $x_0 = 2x_0'$, the shallow-water limit of Eq. (2.16) becomes

$$\nu(x',t') = \pm\frac{\kappa'}{\cosh\kappa'(x' - \kappa'^2 t' - x_0')}, \tag{2.19}$$

which is the one-soliton solution of the MKdV equation Eq. (1.3).

To get the deep-water limit $\delta \to \infty$ of Eq. (2.16), let $\kappa = \pi/\delta - \pi/(\lambda\delta^2)$ and $\gamma = \pi y_0/\delta$. The limiting solution is

$$Q(x,t) = \log\left(\frac{\lambda^2(x - \lambda t - x_0)^2 + (1 + \lambda y_0)^2}{\lambda^2(x - \lambda t - x_0)^2 + (1 - \lambda y_0)^2}\right), \tag{2.20}$$

which is the one-soliton solution of the MBO equation Eq. (1.11) with $\alpha = y_0^{-1} - \lambda$.

We would like to close this section by noting that the technique whereby one solves a nonlinear evolution equation by first solving an auxiliary complexified equation, and then using this solution to invert an appropriate Miura-type transformation is not new. The method was first employed by Wadati[37] to solve the Gardner equation.[8] A more traditional approach would be to solve the direct and inverse problems for a suitable set of linear scattering equations for the MILW

equation itself. The only such set that we are aware of are those given by Satsuma *et al.*[27] However, they can be seen by inspection to be gauge equivalent to the scattering equations that we study in the following sections, and so they are really scattering equations for the complexified ILW equation rather than the MILW equation.

III. JOST FUNCTIONS AND THE DIRECT PROBLEM

The initial value problem for the real-valued ILW equation has been solved by the IST developed by KAS.[18,19] A feature of this particular IST is that the solution of the associated inverse problem does not immediately produce a formula for $U(x,t)$, but the auxiliary function,

$$U^{+}(x,t) := \tfrac{1}{2}(\mathbf{I} - i\mathbf{T})U(x,t), \tag{3.1}$$

where $\mathbf{I}$ denotes the identity operator. In fact, both their left and right scattering problems lead to $U^{+}(x,t)$. But because KAS were working in the domain of real variables, they could recover $U(x,t)$ just by taking real parts. With a star (*) denoting complex conjugation, the result can be written,

$$U(x,t) = U^{+}(x,t) + \{U^{+}(x,t)\}^{*}.$$

As we mentioned in Sec. II, our $U(x,t)$ is an intrinsically complex-valued function because it evolves from Eq. (2.12). Therefore, we cannot retrieve the physical variable by such a simple device as taking real parts. Instead, we must construct separate formulas for $U^{+}(x,t)$ and $U^{-}(x,t)$, where

$$U^{\pm}(x,t) := \tfrac{1}{2}(\pm\mathbf{I} - i\mathbf{T})U(x,t), \tag{3.2}$$

before we can build $U(x,t)$ according to

$$U(x,t) = U^{+}(x,t) - U^{-}(x,t). \tag{3.3}$$

Separate equations that each express $U^{+}(x,t)$ and $U^{-}(x,t)$ in terms of appropriate scattering data can be derived through the suitable inclusion of an *indicator* in the linear scattering problem for the real-valued ILW equation. We will use the symbol ϵ, whose permissible values are

$$\epsilon = \pm 1,$$

to denote the necessary indicator. Except for this indicator we will attempt to keep the notation reasonably close to the original papers of KAS (Refs. 18 and 19) and Santini *et al.*[38]

The correct inclusion of ϵ into the linear scattering problem associated with the ILW equation results in the overdetermined system,

$$\psi_{x}^{+\epsilon} = \epsilon i(U-\mu)\psi^{+\epsilon} - \epsilon i\nu\,\psi^{-\epsilon}, \tag{3.4}$$

$$\psi_{t}^{\pm\epsilon} = \epsilon i\psi_{xx}^{\pm\epsilon} - 2\left(\mu + \frac{1}{2\delta}\right)\psi_{x}^{\pm\epsilon} + \{\pm U_{x} - \epsilon i\mathbf{T}(U_{x}) + \Omega\}\psi^{\pm\epsilon}, \tag{3.5}$$

where $\psi=\psi(x,t)$, U is the complex-valued function defined by Eq. (2.11), and μ, ν, and Ω are constants to be made more precise later. Equation (1.5) is produced from the compatibility condition, $\psi_{xt}^{+\epsilon}=\psi_{tx}^{+\epsilon}$.

The functions $\psi^{\pm\epsilon}$ denote continuous boundary values on the real axis of functions that are analytic in the horizontal strips between $\mathrm{Im}(z)=0$ and $\mathrm{Im}(z)=\pm 2\epsilon\delta$ in the complex z plane, where $z=x+iy$ defines the complex extension of x. The functions $\psi^{\pm\epsilon}(x)$ (with the argument t temporarily suppressed in this section and Secs. IV and VI) are connected by the periodicity condition,[18]

$$\psi^{-\epsilon}(x) = \psi^{+\epsilon}(x + 2\epsilon i\delta), \tag{3.6}$$

which prompts the definition,

$$\psi^{\epsilon}(x) := \psi^{\pm\epsilon}(x \pm \epsilon i\delta), \tag{3.7}$$

for an appropriate function $\psi^{\epsilon}(x)$. The reader is warned of a possible source of confusion in this notation. The symbol $\psi^{+\epsilon}$, for example, has two separate and independent indicators attached, the first indicator being inherited from the notation of KAS.[19] Alternative symbols that we could use are $\psi^{+,\epsilon}$ or $\psi^{+}(\ ;\epsilon)$. If we were to change the sign of ϵ, $\psi^{+\epsilon}$ would become $\psi^{+,-\epsilon}$, not $\psi^{-\epsilon}$.

We now begin our analysis of the direct problem for Eq. (3.4). Let λ denote the necessary spectral parameter, which will start off as a real nonzero parameter but will be extended into the complex domain at a later stage. It appears through the boundary conditions,

$$\psi^{\epsilon}(x;\lambda) \sim \exp\left(\pm\tfrac{1}{2}\epsilon i\lambda x\right) \quad \text{as } x \to \pm\infty, \tag{3.8}$$

where Eq. (3.7) contains the relation connecting $\psi^{\epsilon}(x)$ and the eigenfunctions $\psi^{\pm\epsilon}(x)$. The boundary conditions given by Eq. (3.8) induce the following parametrizations for the quantities μ and ν in Eq. (3.4):

$$\mu = \mu(\lambda) = -\tfrac{1}{2}\lambda \coth(\delta\lambda), \tag{3.9}$$

$$\nu = \nu(\lambda) = \tfrac{1}{2}\lambda \operatorname{cosech}(\delta\lambda). \tag{3.10}$$

Let $m^{+\epsilon}(x;\lambda)$ and $\bar{m}^{+\epsilon}(x;\lambda)$ denote the left-hand Jost functions for Eq. (3.4), and let $n^{+\epsilon}(x;\lambda)$ and $\bar{n}^{+\epsilon}(x;\lambda)$ denote the right-hand Jost functions. The Jost functions satisfy Eq. (3.4), are $(+\epsilon)$ functions in x, and possess the large x asymptotics,

$$m^{+\epsilon}(x;\lambda) \sim \exp\left\{-\tfrac{1}{2}\epsilon i\lambda(x-\epsilon i\delta)\right\}, \quad \bar{m}^{+\epsilon}(x;\lambda) \sim \exp\left\{\tfrac{1}{2}\epsilon i\lambda(x-\epsilon i\delta)\right\}, \tag{3.11}$$

as $x \to -\infty$, and

$$n^{+\epsilon}(x;\lambda) \sim \exp\left\{\tfrac{1}{2}\epsilon i\lambda(x-\epsilon i\delta)\right\}, \quad \bar{n}^{+\epsilon}(x;\lambda) \sim \exp\left\{-\tfrac{1}{2}\epsilon i\lambda(x-\epsilon i\delta)\right\}, \tag{3.12}$$

as $x \to +\infty$. The same asymptotics apply in the strips of analyticity adjacent to the real x axis. The following remarks will clarify several issues about these Jost functions:

(i) The bars on m and n do not denote complex conjugation. Thus m^{+} and $\bar{m}^{+}$, for example, denote distinct functions. Complex conjugation will be denoted by a star (*).

(ii) The Jost functions $m^{+\epsilon}$ and $m^{-\epsilon}$ have two separate indicators attached, as outlined in the text after Eq. (3.7). They are related to each other by the vertical periodicity property Eq. (3.6).

(iii) The phrase "$(+\epsilon)$ function in x" (respectively, $-\epsilon$) refers to a function of the real variable x that can be analytically continued into the horizontal strip between $\mathrm{Im}(z)=0$ and $\mathrm{Im}(z)=2\epsilon\delta$ (respectively, $-2\epsilon\delta$) in the complex z plane, where $z=x+iy$, with the function being continuous onto both edges of the strip.

Our analysis of the direct problem for Eq. (3.4) will proceed efficiently if we work with the modified eigenfunctions $\Psi^{\pm\epsilon}(x;\lambda)$, where

$$\Psi^{\pm\epsilon}(x;\lambda) := \psi^{\pm\epsilon}(x;\lambda)\exp\left\{\tfrac{1}{2}\epsilon i\lambda(x \mp \epsilon i\delta)\right\}. \tag{3.13}$$

An important property of the modified eigenfunctions is the vertical periodicity condition,

$$\Psi^{-\epsilon}(x;\lambda) = \Psi^{+\epsilon}(x+2\epsilon i\delta;\lambda), \tag{3.14}$$

which has the same shape as Eq. (3.6). Appropriate use of Eq. (3.13) to express Eqs. (3.4) and (3.5) in terms of $\Psi^{\pm\epsilon}(x;\lambda)$ leads to the system,

$$\epsilon i\Psi_x^{+\epsilon} + \left(\zeta_+(\lambda) + \frac{1}{2\delta}\right)(\Psi^{+\epsilon} - \Psi^{-\epsilon}) = -U\Psi^{+\epsilon}, \tag{3.15}$$

$$\Psi_t^{\pm\epsilon} = \epsilon i\Psi_{xx}^{\pm\epsilon} + 2\zeta_+(\lambda)\Psi_x^{\pm\epsilon} + \{\pm U_x - \epsilon i\mathbf{T}(U_x) + \Gamma\}\Psi^{\pm\epsilon}, \tag{3.16}$$

where $\Gamma := \Omega + \epsilon i\lambda\{\frac{1}{4}\lambda - \zeta_+(\lambda)\}$ and $\zeta_+(\lambda)$ is defined by

$$\zeta_+(\lambda) := \frac{1}{2}\lambda(1 + \coth\,\delta\lambda) - \frac{1}{2\delta} = \frac{\lambda e^{\delta\lambda}}{2\sinh\,\delta\lambda} - \frac{1}{2\delta}. \tag{3.17}$$

Later, we will also need the notation $\zeta_-(\lambda)$, both cases being contained in the definition,

$$\zeta_\epsilon(\lambda) := \frac{1}{2}\lambda(1 + \epsilon\coth\,\delta\lambda) - \frac{\epsilon}{2\delta} = \frac{\epsilon\lambda e^{\epsilon\delta\lambda}}{2\sinh\,\delta\lambda} - \frac{\epsilon}{2\delta}. \tag{3.18}$$

It will be convenient to have the following elementary identities on hand:

$$\zeta_\epsilon(\lambda) + \zeta_{-\epsilon}(\lambda) = \lambda,$$

$$\zeta_\epsilon(-\lambda) = -\zeta_{-\epsilon}(\lambda),$$

$$\left(\zeta_\epsilon(\lambda) + \frac{\epsilon}{2\delta}\right)e^{-2\epsilon\delta\lambda} = \frac{\epsilon}{2\delta} - \zeta_{-\epsilon}(\lambda),$$

$$\dot{\zeta}_\epsilon(\lambda) = \delta e^{\epsilon\delta\lambda}\,\mathrm{cosech}(\delta\lambda)\zeta_{-\epsilon}(\lambda).$$

As a consequence of the transition to modified eigenfunctions, our spectral parameter λ can be replaced by $\zeta_+ := \zeta_+(\lambda)$. In the real domain, this will be straightforward because $\zeta_+(\lambda)$ is a strictly increasing function of λ with range $(-1/(2\delta), +\infty)$. But because $\zeta_+(\lambda)$ has a somewhat complicated inverse in the complex domain, which is discussed below, we will need to keep using both λ and ζ_+ according to convenience.

The asymptotics of the modified Jost functions are

$$M^{+\epsilon}(x;\lambda) \sim 1, \quad \bar{M}^{+\epsilon}(x;\lambda) \sim \exp\{\epsilon i\lambda(x - \epsilon i\delta)\}, \tag{3.19}$$

as $x \to -\infty$ and

$$N^{+\epsilon}(x;\lambda) \sim \exp\{\epsilon i\lambda(x - \epsilon i\delta)\}, \quad \bar{N}^{+\epsilon}(x;\lambda) \sim 1, \tag{3.20}$$

as $x \to +\infty$, where

$$M^{+\epsilon}(x;\lambda) := m^{+\epsilon}(x;\lambda)\exp\left\{\tfrac{1}{2}\epsilon i\lambda(x - \epsilon i\delta)\right\},$$

and similarly for the other three Jost functions. Each of the modified (uppercase) Jost functions is a $(+\epsilon)$ function in x and satisfies the system of Eqs. (3.15) and (3.16). Thereafter, the $(-\epsilon)$ version of each modified Jost function can be constructed using Eq. (3.14).

The analytic properties of the (modified) Jost functions as functions of λ or ζ_+ are essential to our analysis of the direct problem for Eq. (3.15). Unless stated otherwise, in the remainder of this section, any reference to analyticity will be with respect to either λ or ζ_+ in domains to be specified later. The integral equation,

$$\Psi^{+\epsilon}(x;\lambda) = \Psi_0^{+\epsilon}(x;\lambda) + \int_{-\infty}^{\infty} G^\epsilon(x,\eta;\lambda)U(\eta)\Psi^{+\epsilon}(\eta;\lambda)\mathrm{d}\eta, \tag{3.21}$$

is the key to the analytic character of the Jost functions. The function $\Psi_0^{+\epsilon}(x;\lambda)$ denotes a homogeneous solution of Eq. (3.15), namely, a solution of Eq. (3.15) when $U \equiv 0$, and the Green's function $G^\epsilon(x,\eta;\lambda)$ is a $(+\epsilon)$ function in x that satisfies the periodicity condition (3.14) and the differential equation,

$$\epsilon i G_x^{\epsilon} + \left(\zeta_+(\lambda) + \frac{1}{2\delta}\right)(G^{\epsilon} - G^{-\varepsilon}) = -\delta(x-\eta), \tag{3.22}$$

where $G^{\epsilon}=G^{\epsilon}(x,\eta;\lambda)$, $G^{-\epsilon}=G^{\epsilon}(x+2\epsilon i\delta,\eta;\lambda)$, and $\delta(\ )$ denotes the Dirac delta function.

A Fourier integral representation of the Green's function $G^{\epsilon}(x,\eta;\lambda)$ is

$$G^{\epsilon}(x,\eta;\lambda) = \frac{1}{2\pi}\int_C \hat{g}(r;\lambda)e^{i(x-\eta)r}\,\mathrm{d}r, \tag{3.23}$$

where C denotes a suitable infinite horizontal line in the complex r plane and

$$\hat{g}(r;\lambda) := \frac{1+\epsilon\coth\delta r}{2(\epsilon\zeta_{\epsilon}(r)-\zeta_+(\lambda))}. \tag{3.24}$$

The function $\hat{g}(r;\lambda)$ has a straightforward pole structure in the complex r plane when the parameter λ is real. The symmetries,

$$\{\hat{g}(r;\lambda)\}^* = \hat{g}(r^*;\lambda), \quad \hat{g}(-r;\lambda,-\epsilon) = \hat{g}(r;\lambda,\epsilon),$$

allow us to focus on those poles of $\hat{g}(r;\lambda)$ for which $\mathrm{Im}(r)\geqslant 0$. Let $r=r_n(\lambda;\epsilon)$, where $\mathrm{Im}(r_n)>0$ and $n=1,2,3,\ldots$, be a solution of the equation,

$$\epsilon\zeta_{\epsilon}(r) - \zeta_+(\lambda) = 0. \tag{3.25}$$

Equation (3.25) has a countable infinity of solutions because of the multivalued inverse of $\zeta_{\epsilon}(r)$. A straightforward application of the argument principle to the denominator of Eq. (3.24) localizes the simple pole r_n to the horizontal strip,

$$\frac{\pi n}{\delta} < \mathrm{Im}(r_n) < \frac{\pi(2n+1)}{2\delta}, \tag{3.26}$$

for all $n\geqslant 1$. For large n, the asymptotic location of the nth pole is

$$r_n = \frac{(4n+1)i\pi}{4\delta} - \frac{\epsilon}{2\delta}\left\{\log\left(\frac{\pi n}{\delta}\right) - \log\left(\zeta_+(\lambda)+\frac{1}{2\delta}\right)\right\} + O\left(\frac{\log n}{n}\right).$$

In the strip $-\pi/\delta\leqslant \mathrm{Im}(r)\leqslant \pi/\delta$, there are exactly two poles of $\hat{g}(r;\lambda)$, counting multiplicity. These are both real and are located at

$$r_0 = \epsilon\lambda, \quad r_{-1} = 0,$$

in the notation of KAS.[19] If $\lambda=0$, these two poles coincide to form a double pole. There are also a countable infinity of complex values of λ, namely, the roots of $\zeta_-(\lambda)=0$, such that $\hat{g}(r;\lambda)$ has a double pole in r.

This is an appropriate time to discuss the conformal mapping $\lambda\to\zeta_+(\lambda)$ between the complex variables λ and ζ_+. This conformal mapping maps the complex λ plane to a multisheeted covering of the complex ζ_+ plane. The principal ζ_+ sheet is the one where the real interval $-1/(2\delta)<\zeta_+<+\infty$ is the image of the real λ axis. The point $\zeta_+=-1/(2\delta)$ is a logarithmic branch point of the inverse function $\lambda^{-1}(\zeta_+)$. Hence, the principal sheet has a branch cut along the real interval $-\infty<\zeta_+\leqslant -1/(2\delta)$. The inverse function also has quadratic branch points at the complex zeros of $\mathrm{d}\zeta_+/\mathrm{d}\lambda=\delta e^{\delta\lambda}\zeta_-(\lambda)/\sinh(\delta\lambda)$. On the principal sheet, these occur at $\zeta_+=\zeta_0^{\pm}$, where

$$\zeta_0^{\epsilon} := \delta^{-1}(1.044\,421\,5078 + \epsilon i 3.730\,744\,6428),$$

to 10 decimal places. The corresponding points in the complex λ plane are exactly the same because $\zeta_+(\zeta_0^{\epsilon})=\zeta_0^{\epsilon}-\zeta_-(\zeta_0^{\epsilon})=\zeta_0^{\epsilon}$. Let the branch cuts in the complex ζ_+ plane run horizontally to the right from $\zeta_0^{\pm}$ to $+\infty+\zeta_0^{\pm}$. The inverse image of the principal sheet is a region in the complex λ

plane that is symmetrically placed about the real axis. (This is the region denoted A in Fig. 1 of Ref. 19.) Its upper boundary consists of three curved pieces joined end to end. The first piece runs from $\lambda=-\infty+i\pi/(2\delta)$ to the pole at $i\pi/\delta$ and is the inverse image of the upper edge of the branch cut running from $\zeta_+=-1/(2\delta)$ to $-\infty$. The second piece runs from $\lambda=i\pi/\delta$ to ζ_0^+ and is the inverse image of the upper edge of the branch cut running from $\zeta_+=+\infty+\zeta_0^+$ to ζ_0^+. The third piece runs from $\lambda=\zeta_0^+$ to $+\infty+\zeta_0^+$ and is the inverse image of the lower edge of the same branch cut running in the opposite sense. Denote the region of the complex λ plane between the real axis and the upper boundary D^+ and the corresponding region in the lower half-plane D^-, and let the curved boundaries be included to the right-hand side of the points $\pm i\pi/\delta$.

A function of λ or ζ_+ whose domain covers the region D^ϵ will be denoted a $(+\epsilon)$ function in either λ or ζ_+ if it is analytic throughout the $(+\epsilon)$ half of the complex ζ_+ plane, which is the half-plane $\mathrm{Im}(\epsilon\zeta_+)>0$, and continuous onto the real interval $-1/(2\delta)<\zeta_+<+\infty$. The important point is that such a function cannot have a quadratic branch point at $\zeta_+=\zeta_0^\epsilon$. Generic entire or meromorphic functions of λ will fail this analyticity test, examples being λ itself, $e^{\pm i\lambda x}$, $\sinh(\delta\lambda)$, and $\zeta_-(\lambda)$. A necessary, but far from sufficient, condition for $f(\lambda)$ to be a $(+\epsilon)$ function in λ is $f'(\zeta_0^\epsilon)=0$.

If $\eta\neq x$, the integral in Eq. (3.23) can be evaluated by summing residues in an appropriate half of the complex r plane (according to Jordan's lemma applied to a semicircular contour of large radius passing between consecutive poles of the integrand). The correct half-plane is the upper half-plane when $\eta<x$ and the lower half-plane when $\eta>x$. The integral diverges logarithmically when $\eta=x$, but this will become an integrable singularity when the Green's function later appears inside an integral with respect to η. It is worth noting that the r_n (which depend on λ and ϵ) are above D^+ and the r_n^* are below D^- whenever λ resides anywhere in $D^\pm$ or the real axis.

An important issue in relation to Eq. (3.23) concerns the choice of the contour C. Poles on the real axis at $r_{-1}=0$ and $r_0=\epsilon\lambda$ (or a double pole when $\lambda=0$) dictate two distinct choices for C, and so we will obtain two distinct Green's functions. Use the notation $C_\pm$ for the horizontal line running from $-\infty\pm i0^+$ to $+\infty\pm i0^+$. The choice $C=C_+$ in Eq. (3.23) leads to the Green's function,

$$G_{-\epsilon}^\epsilon(x,\eta;\lambda)=\frac{\epsilon i}{2\delta}\theta(\eta-x)\left\{\frac{1}{\zeta_+(\lambda)}-\frac{e^{\epsilon i(x-\eta)\lambda}}{\zeta_-(\lambda)}-\epsilon\sum_{n=1}^{\infty}\frac{e^{i(x-\eta)r_n^*}}{r_n^*-\epsilon\zeta_+(\lambda)}\right\}+\frac{i}{2\delta}\theta(x-\eta)\sum_{n=1}^{\infty}\frac{e^{i(x-\eta)r_n}}{r_n-\epsilon\zeta_+(\lambda)},\tag{3.27}$$

$\eta\neq x$, where, for $x\neq 0$, $\theta(x)$ is the Heaviside step function,

$$\theta(x)=\begin{cases}1, & x>0,\\ 0, & x<0.\end{cases}$$

The alternative contour $C=C_-$ gives the Green's function,

$$G_\epsilon^\epsilon(x,\eta;\lambda)=G_{-\epsilon}^\epsilon(x,\eta;\lambda)+\frac{\epsilon i}{2\delta}\left(\frac{e^{\epsilon i(x-\eta)\lambda}}{\zeta_-(\lambda)}-\frac{1}{\zeta_+(\lambda)}\right).\tag{3.28}$$

In the remainder of this paper, superscripts attached to the Green's and Jost functions will continue to indicate analytic character with respect to x as above, whereas subscripts attached to these functions will designate analytic character with respect to λ or ζ_+, in cases when x and λ can be extended into the complex domain. The subscript ϵ denotes a $(+\epsilon)$ function in λ or ζ_+ as discussed above, and such functions must be free of the quadratic branch point at $\zeta_+=\zeta_0^\epsilon$ when written as functions of ζ_+. The analytic character of the Green's functions with respect to ζ_+ can be seen from the integral formulas,

$$G_\epsilon^\epsilon(x,\eta;\lambda)=\frac{1}{4\pi}\int_{C_{-\epsilon}}\frac{1+\coth\,\delta r}{\zeta_+(r)-\zeta_+(\lambda)}e^{\epsilon i(x-\eta)r}\,\mathrm{d}r,\tag{3.29}$$

$$G^{\epsilon}_{-\epsilon}(x,\eta;\lambda)=\frac{1}{4\pi}\int_{C_\epsilon}\frac{1+\coth\,\delta r}{\zeta_+(r)-\zeta_+(\lambda)}e^{\epsilon i(x-\eta)r}\,\mathrm{d}r, \tag{3.30}$$

which can be obtained from Eq. (3.23) by the substitution $r\to\epsilon r$. In the case of real λ, the replacement $\lambda\to-\lambda$ followed by the substitution $r\to r-\lambda$ in the integrals gives the useful reflection formulas,

$$G^{\epsilon}_{\epsilon}(x,\eta;-\lambda)=e^{-\epsilon i\lambda(x-\eta)}G^{\epsilon}_{\epsilon}(x,\eta;\lambda), \tag{3.31}$$

$$G^{\epsilon}_{-\epsilon}(x,\eta;-\lambda)=e^{-\epsilon i\lambda(x-\eta)}G^{\epsilon}_{-\epsilon}(x,\eta;\lambda). \tag{3.32}$$

The boundary conditions given by Eqs. (3.19) and (3.20) provide a means by which we can assign $G^{\epsilon}_{\pm\epsilon}(x,\eta;\lambda)$ to the kernel of Eq. (3.21). Preservation of Eqs. (3.19) and (3.20) leads to the following inhomogeneous Fredholm integral equations of the second kind,

$$\begin{pmatrix}M^{+\epsilon}(x;\lambda)\\ \bar{M}^{+\epsilon}(x;\lambda)\end{pmatrix}=\begin{pmatrix}1\\ \exp(\epsilon i\lambda(x-\epsilon i\delta))\end{pmatrix}+\int_{-\infty}^{\infty}G^{\epsilon}_{\epsilon}(x,\eta;\lambda)U(\eta)\begin{pmatrix}M^{+\epsilon}(\eta;\lambda)\\ \bar{M}^{+\epsilon}(\eta;\lambda)\end{pmatrix}\mathrm{d}\eta, \tag{3.33}$$

$$\begin{pmatrix}N^{+\epsilon}(x;\lambda)\\ \bar{N}^{+\epsilon}(x;\lambda)\end{pmatrix}=\begin{pmatrix}\exp(\epsilon i\lambda(x-\epsilon i\delta))\\ 1\end{pmatrix}+\int_{-\infty}^{\infty}G^{\epsilon}_{-\epsilon}(x,\eta;\lambda)U(\eta)\begin{pmatrix}N^{+\epsilon}(\eta;\lambda)\\ \bar{N}^{+\epsilon}(\eta;\lambda)\end{pmatrix}\mathrm{d}\eta. \tag{3.34}$$

Fredholm's second theorem,[39] when applied to Eqs. (3.33) and (3.34), allows us to conclude that $M^{+\epsilon}(x;\lambda)$, as a function of ζ_+, can be analytically continued to the half-plane $\mathrm{Im}(\epsilon\zeta_+)>0$ and $\bar{N}^{+\epsilon}(x;\lambda)$ can be continued to the half-plane $\mathrm{Im}(\epsilon\zeta_+)<0$. Hence, our conventions allow us to expand the notation as follows:

$$M^{+\epsilon}(x;\lambda)=M^{+\epsilon}_{\epsilon}(x;\lambda),\quad \bar{N}^{+\epsilon}(x;\lambda)=\bar{N}^{+\epsilon}_{-\epsilon}(x;\lambda).$$

The corresponding analytic character of the other two Jost functions is discussed in the next paragraph.

The reflection formulas Eqs. (3.31) and (3.32) for the Green's functions have immediate consequences for the Jost functions. The functions,

$$M^{+\epsilon}_{\epsilon}(x;-\lambda),\quad e^{-\epsilon i\lambda(x-\epsilon i\delta)}\bar{M}^{+\epsilon}(x;\lambda),$$

satisfy the same Fredholm equation. We take as a working hypothesis that the solutions of these Fredholm equations are unique, or, equivalently, that the corresponding homogeneous equations have no nontrivial solutions. Hence we obtain the connection formula,

$$M^{+\epsilon}_{\epsilon}(x;-\lambda)=\bar{M}^{+\epsilon}(x;\lambda)e^{-\epsilon i\lambda(x-\epsilon i\delta)}. \tag{3.35}$$

An identical argument produces the connection formula,

$$\bar{N}^{+\epsilon}_{-\epsilon}(x;-\lambda)=N^{+\epsilon}(x;\lambda)e^{-\epsilon i\lambda(x-\epsilon i\delta)}. \tag{3.36}$$

These play a vital role in Sec. VI. We derived them for real λ but they obviously analytically continue off the real axis. For example, $N^{+\epsilon}(x;\lambda)$ analytically continues into the $(+\epsilon)$ half of the complex ζ_+ plane but fails the analyticity test at $\zeta_+=\zeta_0^{\epsilon}$, having a quadratic branch point there. A similar comment applies to $\bar{M}^{+\epsilon}(x;\lambda)$ in the opposite half-plane.

Linear independence of $N^{+\epsilon}$ and $\bar{N}^{+\epsilon}_{-\epsilon}$ for real $\lambda\neq0$ leads to the identity,

$$M^{+\epsilon}_{\epsilon}(x;\lambda)=A(\lambda)\bar{N}^{+\epsilon}_{-\epsilon}(x;\lambda)+B(\lambda)N^{+\epsilon}(x;\lambda), \tag{3.37}$$

where $A(\lambda)$ and $B(\lambda)$ are defined through the functionals,

$$A(\lambda) = 1 - \frac{\epsilon i}{2\delta\zeta_+(\lambda)} \int_{-\infty}^{\infty} U(\eta) M_\epsilon^{+\epsilon}(\eta;\lambda) \mathrm{d}\eta, \tag{3.38}$$

$$B(\lambda) = \frac{\epsilon i}{2\delta\zeta_-(\lambda)} \int_{-\infty}^{\infty} U(\eta) M_\epsilon^{+\epsilon}(\eta;\lambda) e^{-\epsilon i\lambda(\eta-\epsilon i\delta)} \mathrm{d}\eta. \tag{3.39}$$

Equation (3.37) provides asymptotics for $M_\epsilon^{+\epsilon}(x;\lambda)$ as $x \to +\infty$, which supplements the limit $M_\epsilon^{+\epsilon}(x;\lambda) \to 1$ as $x \to -\infty$ given by Eq. (3.19).

To prove Eqs. (3.37)–(3.39), substitute Eq. (3.28) into Eq. (3.33), and then integrate term by term to obtain the equation

$$M_\epsilon^{+\epsilon}(x;\lambda) = 1 + \int_{-\infty}^{\infty} \tilde{M}(\eta;\lambda) \left\{ G_{-\epsilon}^{\epsilon}(x,\eta;\lambda) - \frac{\epsilon}{2\delta\zeta_+(\lambda)} + \frac{\epsilon i e^{\epsilon i\lambda(x-\eta)}}{2\delta\zeta_-(\lambda)} \right\} \mathrm{d}\eta, \tag{3.40}$$

where $\tilde{M}(\eta;\lambda) := U(\eta) M_\epsilon^{+\epsilon}(\eta;\lambda)$. Using Eq. (3.34) to replace $\bar{N}_{-\epsilon}^{+\epsilon}(x;\lambda)$ and $N^{+\epsilon}(x;\lambda)$ in Eq. (3.37), we obtain

$$M_\epsilon^{+\epsilon}(x;\lambda) = A(\lambda) + B(\lambda) e^{\epsilon i\lambda(x-\epsilon i\delta)} + \int_{-\infty}^{\infty} G_{-\epsilon}^{\epsilon}(x,\eta;\lambda) \tilde{M}(\eta;\lambda) \mathrm{d}\eta. \tag{3.41}$$

Equating (3.40) and (3.41) and then matching the coefficients of $\exp(\epsilon i\lambda x)$ on each side of the resultant identity, we arrive at Eqs. (3.38) and (3.39).

The functions $A(\lambda)$ and $B(\lambda)$, which depend on ϵ, are members of the continuous spectrum, and therefore we must ascertain their analytic character. From Eq. (3.38), we deduce that $A(\lambda)$ is a $(+\epsilon)$ function in λ, except for a possible simple pole at $\lambda=0$, but we will omit the subscript implied by this property except when we need to call attention to it. Analytic continuation of $B(\lambda)$ may be possible, but $B(\lambda)$ only plays a role in the inverse scattering when λ is real and for certain isolated nonreal values of λ for which the integral in Eq. (3.39) converges. The latter have relevance to the bound states below. In general, the integral in Eq. (3.39) diverges when λ is nonreal. If $A(\lambda)$ has a simple pole at $\lambda=0$, then the combinations $A(\lambda)+B(\lambda)$, $B(\lambda)/A(\lambda)$, and $A(\lambda)A(-\lambda)-B(\lambda)B(-\lambda)$ are nonsingular at $\lambda=0$ whenever $\int_{-\infty}^{\infty} xU(x)\mathrm{d}x$ converges absolutely.

In a similar fashion, linear independence of $M_\epsilon^{+\epsilon}$ and $\bar{M}^{+\epsilon}$ when λ is real and nonzero gives

$$\bar{N}_{-\epsilon}^{+\epsilon}(x;\lambda) = G(\lambda) M_\epsilon^{+\epsilon}(x;\lambda) + H(\lambda) \bar{M}^{+\epsilon}(x;\lambda), \tag{3.42}$$

where

$$G(\lambda) = 1 + \frac{\epsilon i}{2\delta\zeta_+(\lambda)} \int_{-\infty}^{\infty} U(\eta) \bar{N}_{-\epsilon}^{+\epsilon}(\eta;\lambda) \mathrm{d}\eta. \tag{3.43}$$

$$H(\lambda) = -\frac{\epsilon i}{2\delta\zeta_-(\lambda)} \int_{-\infty}^{\infty} U(\eta) \bar{N}_{-\epsilon}^{+\epsilon}(\eta;\lambda) e^{-\epsilon i\lambda(\eta-\epsilon i\delta)} \mathrm{d}\eta. \tag{3.44}$$

Equation (3.42) provides asymptotics for $\bar{N}_{-\epsilon}^{+\epsilon}(x;\lambda)$ as $x \to -\infty$. We now have enough information to construct the leading-term asymptotics as $\mathrm{Re}\, x \to \pm\infty$ of all four Jost functions in their strips of analyticity in x. The function $G(\lambda)$ is a $(-\epsilon)$ function in λ except for a possible simple pole at $\lambda=0$, whereas $H(\lambda)$ will only be needed for real λ and a finite number of isolated nonreal values. In the inverse scattering transform, the ratios,

$$R(\lambda) := \frac{B(\lambda)}{A(\lambda)}, \quad S(\lambda) := \frac{H(\lambda)}{G(\lambda)}, \tag{3.45}$$

play an important role and are known as reflection coefficients.

The four functions $A(\lambda)$, $B(\lambda)$, $G(\lambda)$, and $H(\lambda)$ of the real variable λ satisfy several identities. First, identities for argument $-\lambda$ can be deduced from the connection formulas (3.35) and (3.36). The results are

$$A(-\lambda) = -\frac{B(\lambda)G(\lambda)}{H(\lambda)}, \quad B(-\lambda) = \frac{1 - A(\lambda)G(\lambda)}{H(\lambda)}, \tag{3.46}$$

$$G(-\lambda) = -\frac{A(\lambda)H(\lambda)}{B(\lambda)}, \quad H(-\lambda) = \frac{1 - A(\lambda)G(\lambda)}{B(\lambda)}. \tag{3.47}$$

Additional identities involving the indicator $-\epsilon$ can be deduced from the differential equations (3.4) or (3.15). Let us work with lowercase Jost functions $m^{+\epsilon}$ and $\bar{n}^{+\epsilon}$, which satisfy Eq. (3.4). The relation to the corresponding uppercase functions is given by Eq. (3.14). Asymptotics for large positive and negative x can be deduced from Eqs. (3.11)–(3.13), (3.19), (3.20), (3.37), and (3.42).

Suppose $\psi_1^{+\epsilon}(x;\lambda_1)$ is one of these Jost functions and $\psi_2^{+,-\epsilon}(x;\lambda_2)$ is one with the sign of the indicator ϵ changed. Then Eqs. (3.4) and (3.6) imply

$$\psi_{1x}^{+\epsilon}(x;\lambda_1) = \epsilon i\{U(x) - \mu(\lambda_1)\}\psi_1^{+\epsilon}(x;\lambda_1) - \epsilon i\,\nu(\lambda_1)\psi_1^{+\epsilon}(x + 2\epsilon i\,\delta;\lambda_1), \tag{3.48}$$

$$\psi_{2x}^{+,-\epsilon}(x;\lambda_2) = -\epsilon i\{U(x) - \mu(\lambda_2)\}\psi_2^{+,-\epsilon}(x;\lambda_2) + \epsilon i\,\nu(\lambda_2)\psi_2^{+,-\epsilon}(x - 2\epsilon i\,\delta;\lambda_2). \tag{3.49}$$

Thence,

$$\begin{aligned}\epsilon i\frac{\partial}{\partial x}\{\psi_1^{+\epsilon}(x;\lambda_1)\psi_2^{+,-\epsilon}(x;\lambda_2)\} = {}& \{\mu(\lambda_1) - \mu(\lambda_2)\}\psi_1^{+\epsilon}(x;\lambda_1)\psi_2^{+,-\epsilon}(x;\lambda_2)\\ &+ \nu(\lambda_1)\psi_1^{+\epsilon}(x + 2\epsilon i\,\delta;\lambda_1)\psi_2^{+,-\epsilon}(x;\lambda_2)\\ &- \nu(\lambda_2)\psi_1^{+\epsilon}(x;\lambda_1)\psi_2^{+,-\epsilon}(x - 2\epsilon i\,\delta;\lambda_2).\end{aligned}$$

Integrate both sides with respect to x from $-R_1$ to R_2 where R_1 and R_2 are large positive numbers. The second to last and last terms on the right-hand side are, respectively, a $(-\epsilon)$ function in x and a $(+\epsilon)$ function in x, and so we can replace the definite integrals with contour integrals following three sides of a rectangle in their respective strips of analyticity as follows:

$$\int_{-R_1}^{R_2} = \int_{-R_1}^{-R_1-\epsilon i\,\delta} + \int_{-R_1-\epsilon i\,\delta}^{R_2-\epsilon i\,\delta} + \int_{R_2-\epsilon i\,\delta}^{R_2}, \quad \int_{-R_1}^{R_2} = \int_{-R_1}^{-R_1+\epsilon i\,\delta} + \int_{-R_1+\epsilon i\,\delta}^{R_2+\epsilon i\,\delta} + \int_{R_2+\epsilon i\,\delta}^{R_2}.$$

Thereafter, the results simplify with the help of Eq. (3.7). We obtain the result,

$$\begin{aligned}\epsilon i\left[\psi_1^{+\epsilon}(x;\lambda_1)\psi_2^{+,-\epsilon}(x;\lambda_2)\right]_{-R_1}^{R_2} = {}& \{\mu(\lambda_1) - \mu(\lambda_2)\}\int_{-R_1}^{R_2}\psi_1^{+\epsilon}(x;\lambda_1)\psi_2^{+,-\epsilon}(x;\lambda_2)\mathrm{d}x\\ &+ \{\nu(\lambda_1) - \nu(\lambda_2)\}\int_{-R_1}^{R_2}\psi_1^{\epsilon}(x;\lambda_1)\psi_2^{(-\epsilon)}(x;\lambda_2)\mathrm{d}x\\ &- \left\{\nu(\lambda_2)\int_{-R_1-\epsilon i\,\delta}^{-R_1} + \nu(\lambda_1)\int_{-R_1}^{-R_1+\epsilon i\,\delta} - \nu(\lambda_2)\int_{R_2-\epsilon i\,\delta}^{R_2} - \nu(\lambda_1)\int_{R_2}^{R_2+\epsilon i\,\delta}\right\}\\ &\psi_1^{\epsilon}(z;\lambda_1)\psi_2^{(-\epsilon)}(z;\lambda_2)\mathrm{d}z.\end{aligned} \tag{3.50}$$

Note that in all terms containing $\nu(\lambda_1)$ and $\nu(\lambda_2)$, the ψ functions appearing are of the type on the

left-hand side of Eq. (3.7). Because $\mu(\lambda)$ and $\nu(\lambda)$ are *even* functions of λ, a substantial simplification occurs in the two cases $\lambda_2 = \pm\lambda_1$. Then the last identity reduces to

$$\left[\psi_1^{+\epsilon}(x;\lambda)\psi_2^{+,-\epsilon}(x;\pm\lambda)\right]_{-R_1}^{R_2} = \epsilon i\nu(\lambda)\left\{\int_{-R_1-\epsilon i\delta}^{-R_1+\epsilon i\delta} - \int_{R_2-\epsilon i\delta}^{R_2+\epsilon i\delta}\right\}\psi_1^{\epsilon}(z;\lambda)\psi_2^{(-\epsilon)}(z;\pm\lambda)\mathrm{d}z, \tag{3.51}$$

which can be evaluated using asymptotic results alone.

With $+\lambda$ as the second argument of $\psi_2^{+,-\epsilon}$ and using the appropriate asymptotic formulas for $m^{+\epsilon}$ and $\bar{n}^{+\epsilon}$, we get the following four identities:

$$\zeta_+(\lambda)\{A(\lambda)A^{-\epsilon}(\lambda) - 1\} = e^{2\delta\lambda}\zeta_-(\lambda)B(\lambda)B^{-\epsilon}(\lambda), \tag{3.52}$$

$$\zeta_+(\lambda)\{G(\lambda)G^{-\epsilon}(\lambda) - 1\} = e^{2\delta\lambda}\zeta_-(\lambda)H(\lambda)H^{-\epsilon}(\lambda), \tag{3.53}$$

$$G^{-\epsilon}(\lambda) = A(\lambda), \tag{3.54}$$

$$A^{-\epsilon}(\lambda) = G(\lambda). \tag{3.55}$$

Here, $A^{-\epsilon}(\lambda)$ is the result of replacing ϵ with $-\epsilon$ throughout the right-hand side of Eq. (3.38), and similarly for the other functions with indicator $-\epsilon$ attached. Both sides of Eq. (3.54) are $(+\epsilon)$ functions in λ and both sides of Eq. (3.55) are $(-\epsilon)$ functions in λ. These analytic continuations are relevant to the bound states below.

With $-\lambda$ as the second argument of $\psi_2^{+,-\epsilon}$, we get

$$\zeta_+(\lambda)A(\lambda)B^{-\epsilon}(-\lambda) = e^{2\delta\lambda}\zeta_-(\lambda)B(\lambda)A^{-\epsilon}(-\lambda), \tag{3.56}$$

$$\zeta_+(\lambda)G(\lambda)H^{-\epsilon}(-\lambda) = e^{2\delta\lambda}\zeta_-(\lambda)H(\lambda)G^{-\epsilon}(-\lambda), \tag{3.57}$$

$$\zeta_+(\lambda)H^{-\epsilon}(-\lambda) = -e^{2\delta\lambda}\zeta_-(\lambda)B(\lambda), \tag{3.58}$$

$$\zeta_+(\lambda)B^{-\epsilon}(-\lambda) = -e^{2\delta\lambda}\zeta_-(\lambda)H(\lambda). \tag{3.59}$$

These identities allow 12 functions of the real variable λ to be written in terms of four others. They include the identities (3.46) and (3.47) above. In particular, we find

$$\{A(\lambda)A(-\lambda) - B(\lambda)B(-\lambda)\}\{A^{-\epsilon}(\lambda)A^{-\epsilon}(-\lambda) - B^{-\epsilon}(\lambda)B^{-\epsilon}(-\lambda)\} = 1,$$

which implies that $A(\lambda)A(-\lambda) - B(\lambda)B(-\lambda)$ cannot have any zeros on the real line (including $\lambda = 0$, which requires separate treatment). A further consequence is that $B(\lambda)$ and $H(\lambda)$ have the same real zeros, if any. Pure soliton solutions are characterized by $B(\lambda)$ vanishing identically on the real line. In that case, the above identities imply that $H(\lambda)$, $B^{-\epsilon}(\lambda)$, and $H^{-\epsilon}(\lambda)$ also vanish identically, which is of importance in the construction of MILW solitons.

Corresponding identities can be constructed in which the functions with indicator $-\epsilon$ are replaced by complex conjugates. These are less elegant because they contain the imaginary part of $U(x)$ inside definite integrals. The most interesting is the identity corresponding to Eq. (3.54) in which all functions appearing analytically extend to the $(+\epsilon)$ half of the complex ζ_+ plane. This identity is

$$2\delta\zeta_+(\lambda)\{(G(\lambda^*))^* - A(\lambda)\} = -\epsilon\int_{-\infty}^{\infty} V_x M_\epsilon^{+\epsilon}(x;\lambda)(\bar{N}_{-\epsilon}^{+\epsilon}(x;\lambda^*))^* \, dx, \tag{3.60}$$

where the factor V_x comes from Eq. (2.11). In the case of pure multisoliton solutions, we can calculate $A(\lambda)$ and $G(\lambda)$ explicitly (see Sec. VII), in which case we will see by inspection that the left-hand side of Eq. (3.60) vanishes.

IV. THE DISCRETE SPECTRUM

Our calculations have up to this point dealt exclusively with the continuous spectrum for Eq. (3.4). Discrete (complex) eigenvalues for Eq. (3.4) are also possible, leading to a finite number of bound states. While Eqs. (3.37) and (3.42) are not valid off the real λ axis, they survive as leading-term asymptotics in appropriate half-planes.

For the bound states, it is more natural to work with lowercase Jost functions. For $\mathrm{Im}(\epsilon\lambda) > 0$, $m^{+\epsilon}(x;\lambda)$ is locally analytic and has the asymptotic behavior,

$$m^{+\epsilon}(x;\lambda) \sim e^{-\epsilon i\lambda(x-\epsilon i\delta)/2} \quad \text{as } x \to -\infty, \tag{4.1}$$

$$m^{+\epsilon}(x;\lambda) \sim A(\lambda)e^{-\epsilon i\lambda(x-\epsilon i\delta)/2} \quad \text{as } x \to +\infty. \tag{4.2}$$

Thus, in general, $m^{+\epsilon}$ decays as $x \to -\infty$ and grows exponentially as $x \to +\infty$. The exceptional values of λ are the zeros of $A(\lambda)$, if any. Suppose there are q zeros of $A(\lambda)$ in the region D^ϵ of the complex λ plane, namely,

$$\lambda_1, \lambda_2, \ldots, \lambda_q,$$

and let $\zeta_{+j} := \zeta_+(\lambda_j)$. The λ_j are the discrete eigenvalues of Eq. (3.4) in the region D^ϵ and the ζ_{+j} are the corresponding discrete eigenvalues of Eq. (3.15) in the $(+\epsilon)$ half of the complex ζ_+ plane. The asymptotics of $m^{+\epsilon}(x;\lambda)$ as $x \to +\infty$ can be deduced from Eq. (3.28). By using the same argument that led to Eq. (3.37), we get the exact formula,

$$m^{+\epsilon}(x;\lambda_j) = B(\lambda_j)n^{+\epsilon}(x;\lambda_j), \tag{4.3}$$

where $B(\lambda_j)$ is defined by Eq. (3.39) with λ replaced by λ_j and $N^{+\epsilon}(x;\lambda_j)$ [the uppercase Jost function corresponding to $n^{+\epsilon}(x;\lambda_j)$] satisfies the Fredholm equation (3.22) for $N^{+\epsilon}(x;\lambda)$ with λ_j replacing λ. Note that $B(\lambda_j)$ is not, in general, the value that $B(\lambda)$ would take if it could be analytically continued off the real axis to λ_j. For example, $B(\lambda)$ can vanish identically for real λ, but the $B(\lambda_j)$ can never vanish. The asymptotics for $m^{+\epsilon}(x;\lambda_j)$ can now be written,

$$m^{+\epsilon}(x;\lambda_j) \sim \begin{cases} e^{-\epsilon i\lambda_j(x-\epsilon i\delta)/2} & \text{as } x \to -\infty, \\ B(\lambda_j)e^{\epsilon i\lambda_j(x-\epsilon i\delta)/2} & \text{as } x \to +\infty. \end{cases} \tag{4.4}$$

Bound states corresponding to discrete eigenvalues in the region $D^{-\epsilon}$ are constructed similarly. Let $\lambda_j^{-\epsilon}$ denote the result of changing the sign of the indicator ϵ in λ_j. According to Eq. (3.55), which is applicable to $D^{-\epsilon}$, the $\lambda_j^{-\epsilon}$ are the zeros of $G(\lambda)$ in $D^{-\epsilon}$. Then the functions $\bar{n}^{+\epsilon}(x;\lambda_j^{-\epsilon})$, $j=1,2,\ldots,q$, are bound states with

$$\bar{n}^{+\epsilon}(x;\lambda_j^{-\epsilon}) = H(\lambda_j^{-\epsilon})\bar{m}^{+\epsilon}(x;\lambda_j^{-\epsilon}), \tag{4.5}$$

where $H(\lambda_j^{-\epsilon})$ is defined by the integral Eq. (3.44) with $\lambda_j^{-\epsilon}$ replacing λ.

We need to know the precise relationship between the λ_j and the $\lambda_j^{-\epsilon}$. The integral formula Eq. (3.51) is valid for any real or complex value of λ for which the eigenfunctions $\psi_1^{+\epsilon}$ and $\psi_2^{+,-\epsilon}$ are defined. Let us apply it to the case $\psi_1^{+\epsilon} = m^{+\epsilon}(x;\lambda_j)$ and $\psi_2^{+,-\epsilon} = m^{+,-\epsilon}(x;-\lambda_j)$. Suppose that $-\lambda_j$ is not a discrete eigenvalue in $D^{-\epsilon}$ for the case of indicator $-\epsilon$. In that case, we must use the asymptotic formula Eq. (4.2) with the sign of ϵ changed. Equation (3.51) can be simplified to

$$\zeta_+(-\lambda_j)B(\lambda_j)A^{-\epsilon}(-\lambda_j)=0.$$

Now $B(\lambda_j)$ can never vanish and ζ_+ can only vanish at the origin of its own complex plane, which is on the real axis. It follows that the hypothesis that $-\lambda_j$ was not a discrete eigenvalue in $D^{-\epsilon}$ has led to a contradiction, namely, that it is indeed a discrete eigenvalue. For this case, the alternative asymptotics given by Eq. (4.4) with the sign of ϵ changed guarantee that Eq. (3.51) is identically satisfied. The same conclusion would result if we applied Eq. (3.51) to the case $\psi_1^{+\epsilon}=\bar{n}^{+\epsilon}(x;-\lambda_j)$ and $\psi_2^{+,-\epsilon}$ as before. Hence, we have proved that

$$A^{-\epsilon}(-\lambda_j)=0=G(-\lambda_j),\quad A(-\lambda_j^{-\epsilon})=0, \tag{4.6}$$

for $j=1,2,\ldots,q$. Equation (4.6) shows that the $\lambda_j^{-\epsilon}$ are the negatives of the λ_j in some order, and we are free to label these eigenvalues so that

$$\lambda_j^{-\epsilon}=-\lambda_j \tag{4.7}$$

and

$$\lambda_j =: \epsilon i\kappa_j,\quad \mathrm{Re}(\kappa_j)>0, \tag{4.8}$$

$j=1,2,\ldots,q$, with the κ_j being independent of ϵ. This result allows us to write Eq. (4.5) in terms of quantities with the same indicator, namely,

$$\bar{n}^{+\epsilon}(x;-\lambda_j)=H(-\lambda_j)\bar{m}^{+\epsilon}(x;-\lambda_j). \tag{4.9}$$

In view of Eq. (4.8), we can obtain more identities. First, by suitably combining Eqs. (3.28), (3.31), and (3.32), we can get a reflection formula for the Green's functions that extends off the real λ axis. Then it will be found that the connection formula Eq. (3.35) holds for $\lambda=-\lambda_j$ and Eq. (3.36) holds for $\lambda=\lambda_j$. This means that $N^{+\epsilon}(x;\lambda_j)$ is precisely the result that would be obtained by analytic continuation of $N^{+\epsilon}(x;\lambda)$ from the real λ axis to the point $\lambda=\lambda_j$ in D^{ϵ}, which is not obvious from the definition of $N^{+\epsilon}(x;\lambda_j)$, and similarly for $\bar{M}^{+\epsilon}(x;-\lambda_j)$. As already remarked, similar statements are false for $B(\lambda_j)$ and $H(-\lambda_j)$. The large x asymptotics of the connection formulas now give

$$H(-\lambda_j)=\frac{1}{B(\lambda_j)}. \tag{4.10}$$

This can also be proved by substituting $\lambda=-\lambda_j$ into Eq. (3.44) and rearranging.

The relationship between λ_j and λ_j^* is less easy to determine in the case of the complex-valued ILW equation. Calculations similar to the proof of Eq. (4.6) give

$$2\delta e^{\delta\lambda_j}\zeta_-(\lambda_j)B(\lambda_j)(A(-\lambda_j^*))^*=-\epsilon\int_{-\infty}^{\infty}V_x m^{+\epsilon}(x;\lambda_j)(m^{+\epsilon}(x;-\lambda_j^*))^*\,\mathrm{d}x, \tag{4.11}$$

which can also be deduced from Eq. (3.60) by setting $\lambda=-\lambda_j^*$. In the case of the real-valued ILW equation, the right-hand sides of Eqs. (3.60) and (4.11) are zero because V_x is proportional to the imaginary part of $U(x)$. Hence $A(-\lambda_j^*)=0$, which implies that the λ_j are either pure-imaginary or are distributed symmetrically about the imaginary axis of the complex λ plane. Equivalently, the κ_j are either real or are distributed in complex conjugate pairs. The real κ_j which do not have the same real part as any other κ_j give rise to solitons (solitary waves) that travel from left to right with a steady amplitude. When two or more of the κ_j have the same real part, the corresponding solitary waves travel together as a packet known as a *breather* because the combined wave pulsates. KAS (Ref. 19) concluded that all the λ_j were pure imaginary from a different integral identity. In view of the existence of breathers, their conclusion cannot be upheld.

The discrete eigenvalues are also either pure imaginary or are distributed in symmetric pairs across the imaginary axis of the complex λ plane in the case of the particular *complex-valued* ILW equation derived from the real-valued MILW equation via the Miura transformation Eq. (2.11).

Our argument is indirect because we have not found a direct way to prove that the integral on the right-hand side of Eq. (4.11) vanishes identically. In Sec. VII, we prove that the eigenvalues are so distributed for pure soliton solutions. But that implies that they are so distributed for all solutions because the solitary waves or breathers become widely separated from each other and from the background generated by the nonsoliton part at late times. If the eigenvalues were not distributed as stated, the function $V(x,t)$ constructed from Eq. (2.13) would fail the consistency condition Eq. (2.14). We could also employ the same indirect argument to prove that the discrete eigenvalues are *simple* zeros of $A(\lambda)$ and $G(\lambda)$ for the class of complex-valued ILW equations relevant to the MILW equation, but we shall omit that proof.

One final set of identities involves λ derivatives of $A(\lambda)$ at $\lambda=\lambda_j$ and of $G(\lambda)$ at $\lambda=-\lambda_j$. Define the *normalizing coefficients*,

$$C_j := -\epsilon i \frac{\dot{\zeta}_+(\lambda_j)B(\lambda_j)}{\dot{A}(\lambda_j)}, \tag{4.12}$$

$$F_j := \epsilon i \frac{\dot{\zeta}_+(-\lambda_j)H(-\lambda_j)}{\dot{G}(-\lambda_j)}, \tag{4.13}$$

where the dot denotes differentiation with respect to λ. Start again with Eqs. (3.48) and (3.49), but take a derivative of the first equation with respect to λ_1. The steps which led to Eq. (3.51) give the integral identity,

$$\begin{aligned}\left[\psi_{1\lambda}^{+\epsilon}(x;\lambda)\psi_2^{+,-\epsilon}(x;\pm\lambda)\right]_{-R_1}^{R_2} &= \epsilon i\nu(\lambda)\left\{\int_{-R_1-\epsilon i\delta}^{-R_1+\epsilon i\delta} - \int_{R_2-\epsilon i\delta}^{R_2+\epsilon i\delta}\right\}\psi_{1\lambda}^{\epsilon}(z;\lambda)\psi_2^{(-\epsilon)}(z;\pm\lambda)\mathrm{d}z \\ &\quad + \epsilon i\dot{\nu}(\lambda)\left\{\int_{-R_1}^{-R_1+\epsilon i\delta} - \int_{R_2}^{R_2+\epsilon i\delta}\right\}\psi_1^{\epsilon}(z;\lambda)\psi_2^{(-\epsilon)}(z;\pm\lambda)\mathrm{d}z \\ &\quad - \epsilon i\dot{\mu}(\lambda)\int_{-R_1}^{R_2}\psi_1^{+\epsilon}(x;\lambda)\psi_2^{+,-\epsilon}(x;\pm\lambda)\mathrm{d}x \\ &\quad - \epsilon i\dot{\nu}(\lambda)\int_{-R_1}^{R_2}\psi_1^{\epsilon}(x;\lambda)\psi_2^{(-\epsilon)}(x;\pm\lambda)\mathrm{d}x.\end{aligned} \tag{4.14}$$

This identity is applicable to the case $\lambda=\pm\lambda_j$ provided the eigenfunctions appearing are defined for such λ. With $\psi_1^{+\epsilon}=m^{+\epsilon}(x;\lambda_j)$ and $\psi_2^{+,-\epsilon}=m^{+,-\epsilon}(x;-\lambda_j)$, Eq. (4.14) yields

$$\begin{aligned}C_j = -\frac{1}{2\dot{A}(\lambda_j)\dot{A}^{-\epsilon}(-\lambda_j)}\Bigg\{&\frac{\dot{\mu}(\lambda_j)}{\sinh\,\delta\lambda_j}\int_{-\infty}^{\infty}m^{+\epsilon}(x;\lambda_j)m^{+,-\epsilon}(x;-\lambda_j)\mathrm{d}x \\ &+\frac{\dot{\nu}(\lambda_j)}{\sinh\,\delta\lambda_j}\int_{-\infty}^{\infty}m^{\epsilon}(x;\lambda_j)m^{(-\epsilon)}(x;-\lambda_j)\mathrm{d}x\Bigg\}.\end{aligned} \tag{4.15}$$

Similarly,

$$\begin{aligned}F_j = -\frac{1}{2\dot{G}(-\lambda_j)\dot{G}^{-\epsilon}(\lambda_j)}\Bigg\{&\frac{\dot{\mu}(\lambda_j)}{\sinh\,\delta\lambda_j}\int_{-\infty}^{\infty}\bar{n}^{+\epsilon}(x;-\lambda_j)\bar{n}^{+,-\epsilon}(x;\lambda_j)\mathrm{d}x \\ &+\frac{\dot{\nu}(\lambda_j)}{\sinh\,\delta\lambda_j}\int_{-\infty}^{\infty}\bar{n}^{\epsilon}(x;-\lambda_j)\bar{n}^{(-\epsilon)}(x;\lambda_j)\mathrm{d}x\Bigg\}.\end{aligned} \tag{4.16}$$

From these two formulas, we can read off the important identities,

$$C_j^{-\epsilon} = C_j, \quad F_j^{-\epsilon} = F_j. \tag{4.17}$$

In other words, C_j and F_j, like κ_j, are independent of the indicator ϵ. Now we can swap ϵ with $-\epsilon$ in either Eq. (4.12) or Eq. (4.13) and get the simple relationship,

$$\frac{F_j}{C_j} = H(-\lambda_j)H^{-\epsilon}(\lambda_j) = \frac{1}{B(\lambda_j)B^{-\epsilon}(-\lambda_j)}, \tag{4.18}$$

where we used Eq. (4.10). When a particular λ_j is purely imaginary, the coefficients $\dot{\mu}(\lambda_j)/\sinh \delta\lambda_j$ and $\dot{\nu}(\lambda_j)/\sinh \delta\lambda_j$ are real and negative. If, in addition, the function $U(x)$ is real, then C_j and F_j are themselves real and positive, as shown by KAS.[19] But for $U(x)$ derived from Eq. (2.11), the C_j and F_j are, in general, complex numbers. MILW solitons have a direct relationship to the imaginary parts of the C_j and F_j.

This completes our analysis of the direct problem for the complex-valued ILW equation. The *scattering data* consists of the functions,

$$A(\lambda), \quad B(\lambda), \quad G(\lambda), \quad H(\lambda), \tag{4.19}$$

of the real variable λ which comprise the continuous spectrum, with $A(\lambda)$ and $G(\lambda)$ having analytic extensions to half-planes of the complex variable ζ_+ as shown above, and the complex constants,

$$\lambda_j = \epsilon i\kappa_j, \quad B(\lambda_j), \quad H(-\lambda_j), \quad C_j, \quad F_j, \tag{4.20}$$

which form the discrete spectrum. We have derived several identities involving these quantities and the corresponding quantities obtained by changing the sign of the indicator ϵ.

V. TEMPORAL EVOLUTION OF THE SCATTERING DATA

The scattering data derived in the preceding section will evolve in a simple way with respect to time t. This is the standard way that the IST is used to solve an initial value problem. One calculates the scattering data for the initial value $V(x,0)$ at $t=0$ and then evolves the scattering data forward in time according to simple expressions. Finally, when the inverse problem is formulated and solved, one inputs the scattering data at time t and outputs the required potential $V(x,t)$. The solution of the inverse problem for the complex-valued ILW equation and real-valued MILW equation will be given in the next section.

Introduce the argument t into the notation for the scattering data,

$$A(\lambda;t), \quad B(\lambda;t), \quad G(\lambda;t), \quad H(\lambda;t),$$

$$\lambda_j(t), \quad B(\lambda_j;t), \quad H(-\lambda_j;t), \quad C_j(t), \quad F_j(t),$$

$j=1,2,\ldots,q$. Now the four Jost functions, $M_\epsilon^{+\epsilon}(x,t;\lambda)$, $\bar{M}^{+\epsilon}(x,t;\lambda)$, $N^{+\epsilon}(x,t;\lambda)$, and $\bar{N}_{-\epsilon}^{+\epsilon}(x,t;\lambda)$, satisfy Eq. (3.16) for $\Psi^{+\epsilon}(x,t)$. The boundary conditions given by Eqs. (3.19) and (3.20) force the parameter Γ in this equation to be

$$\Gamma = \begin{cases} 0 & \text{when } \Psi^{+\epsilon} = M_\epsilon^{+\epsilon} \text{ or } \bar{N}_{-\epsilon}^{+\epsilon}, \\ -\theta(\lambda) & \text{when } \Psi^{+\epsilon} = \bar{M}^{+\epsilon} \text{ or } N^{+\epsilon}, \end{cases}$$

where

$$\theta(\lambda) := \epsilon i\lambda(\lambda \coth(\delta\lambda) - \delta^{-1}). \tag{5.1}$$

With all terms appearing in Eqs. (3.37) and (3.42) depending on t, differentiation and application of Eq. (3.16) produces the simple differential identities,

$$A_t(\lambda;t)\bar{N}^{+\epsilon}_{-\epsilon}(x,t;\lambda)+\{B_t(\lambda;t)+\Gamma B(\lambda;t)\}N^{+\epsilon}(x,t;\lambda)=0,$$

$$G_t(\lambda;t)M^{+\epsilon}_{\epsilon}(x,t;\lambda)+\{H_t(\lambda;t)+\Gamma H(\lambda;t)\}\bar{M}^{+\epsilon}(x,t;\lambda)=0,$$

where the second value of Γ is applicable. Thus,

$$A(\lambda;t)=A(\lambda;0), \tag{5.2}$$

$$B(\lambda;t)=B(\lambda;0)e^{\theta(\lambda)t}, \tag{5.3}$$

$$G(\lambda;t)=G(\lambda;0), \tag{5.4}$$

$$H(\lambda;t)=H(\lambda,0)e^{\theta(\lambda)t}. \tag{5.5}$$

Because $A(\lambda;t)$ and $G(\lambda;t)$ are time independent, so also are their zeros. Hence, for $j=1,2,\ldots,q$,

$$\lambda_j(t)=\lambda_j(0), \tag{5.6}$$

$$B(\lambda_j;t)=B(\lambda_j;0)e^{\theta(\lambda_j)t}, \tag{5.7}$$

$$H(-\lambda_j;t)=H(-\lambda_j;0)e^{-\theta(\lambda_j)t}, \tag{5.8}$$

$$C_j(t)=C_j(0)e^{\theta(\lambda_j)t}, \tag{5.9}$$

$$F_j(t)=F_j(0)e^{-\theta(\lambda_j)t}. \tag{5.10}$$

Note that $\theta(\lambda_j)$ is independent of the indicator ϵ.

The scattering data at $t=0$ will be regarded as known because they have been constructed out of the initial value $U(x,0)$ of the complex-valued ILW equation, which in turn has been constructed out of the initial value $V(x,0)$ of the MILW equation according to Eq. (2.12). Thus the scattering data are now known for all t.

VI. THE INVERSE PROBLEM AND ITS SOLUTION

In this section, we will formulate and solve the inverse problem for the complex-valued ILW equation. The natural setting is the complex plane of the scattering variable ζ_+ obtained by the conformal mapping $\zeta_+=\zeta_+(\lambda)$, and we intend to use the notation $A(\zeta_+)$ interchangeably with $A(\lambda)$, and similarly with all the other functions of λ or of the λ_j. The scattering data are now understood to be the scattering data at time t,

$$A(\zeta_+),\quad B(\zeta_+;t),\quad G(\zeta_+),\quad H(\zeta_+;t),$$

$$\zeta_{+j}:=\zeta_+(\lambda_j),\quad \zeta_{-j}:=\zeta_-(\lambda_j)=-\zeta_+(-\lambda_j),$$

$$B(\zeta_{+j};t),\quad H(-\zeta_{-j};t),\quad C_j(t),\quad F_j(t),$$

derived in the preceding section. Our aim is to produce an expression for the auxiliary variable,

$$U^{\epsilon}(x,t) := \tfrac{1}{2}\{\epsilon U(x,t) - i(\mathbf{T}U)(x,t)\}, \tag{6.1}$$

in terms of the scattering data, and thence the solution $U(x,t)$ of the complex-valued ILW equation and the solution $V(x,t)$ of the real-valued MILW equation. For convenience, we again suppress the t dependence in the arguments of our functions.

The solution of our inverse problem relies on the interpretation of Eqs. (3.37) and (3.42) as Riemann-Hilbert problems[40] in the complex ζ_+ plane. With the indicator ϵ temporarily attached to A, B, G, and H and the subscript identifying the half-plane of analyticity attached to A and G, these Riemann-Hilbert problems read

$$M_{\epsilon}^{+\epsilon}(x;\zeta_+) = A_{\epsilon}^{\epsilon}(\zeta_+)\bar{N}_{-\epsilon}^{+\epsilon}(x;\zeta_+) + B^{\epsilon}(\zeta_+)N^{+\epsilon}(x;\zeta_+), \tag{6.2}$$

$$\bar{N}_{-\epsilon}^{+\epsilon}(x;\zeta_+) = G_{-\epsilon}^{\epsilon}(\zeta_+)M_{\epsilon}^{+\epsilon}(x;\zeta_+) + H^{\epsilon}(\zeta_+)\bar{M}^{+\epsilon}(x;\zeta_+), \tag{6.3}$$

for real $\zeta_+ > -1/(2\delta)$.

In Sec. III, we took care to identify those functions, denoted $(+\epsilon)$ functions and having the subscript ϵ, that are analytic in ζ_+ throughout the half-plane $\mathrm{Im}(\epsilon\zeta_+) > 0$, and similarly for $(-\epsilon)$ functions. In particular, we proved that

(i) $M_{\epsilon}^{+\epsilon}(x;\zeta_+)$ and $A(\zeta_+)$ are $(+\epsilon)$ functions in ζ_+,

(ii) $\bar{N}_{-\epsilon}^{+\epsilon}(x;\zeta_+)$ and $G(\zeta_+)$ are $(-\epsilon)$ functions in ζ_+,

(iii) $N^{+\epsilon}$ and $\bar{M}^{+\epsilon}$ also have analytic extensions into the half-planes $\mathrm{Im}(\epsilon\zeta_+) > 0$ and $\mathrm{Im}(\epsilon\zeta_+) < 0$, respectively, but they do not extend to the complete half-planes, having quadratic branch points at ζ_0^{ϵ} and $\zeta_0^{-\epsilon}$, respectively.

(iv) $A(\zeta_+)$ has simple zeros at ζ_{+j} and $G(\zeta_+)$ has corresponding simple zeros at $-\zeta_{-j}$, $j = 1,2,\ldots,q$.

(v) $B(\zeta_+)$ is defined for real $\zeta_+ > -1/(2\delta)$ and for the ζ_{+j}; $H(\zeta_+)$ is defined for real $\zeta_+ > -1/(2\delta)$ and for the $-\zeta_{-j}$.

Equation (6.2) can be written,

$$\frac{M_{\epsilon}^{+\epsilon}(x;\zeta_+)}{A(\zeta_+)} = \bar{N}_{-\epsilon}^{+\epsilon}(x;\zeta_+) + R(\zeta_+)N^{+\epsilon}(x;\zeta_+), \tag{6.4}$$

for real $\zeta_+ > -1/(2\delta)$, where

$$R(\zeta_+) := \frac{B(\zeta_+)}{A(\zeta_+)}. \tag{6.5}$$

The ratio $M_{\epsilon}^{+\epsilon}(x;\zeta_+)/A(\zeta_+)$ is meromorphic in the $(+\epsilon)$ half of the complex ζ_+ plane. From Eqs. (3.27), (3.28), (3.33), and (3.38), this ratio tends to $1 + O(1/\zeta_+)$ as $\zeta_+ \to \infty$. Hence, we can write the partial fraction expansion,

$$\frac{M_{\epsilon}^{+\epsilon}(x;\zeta_+)}{A(\zeta_+)} = 1 + \sum_{j=1}^{q} \frac{D_j^{\epsilon}(x)}{\zeta_+ - \zeta_{+j}} + \phi_{\epsilon}^{\epsilon}(x;\zeta_+), \tag{6.6}$$

where $\phi_{\epsilon}^{\epsilon}(x;\zeta_+)$ is a $(+\epsilon)$ function in x and ζ_+ such that $\phi_{\epsilon}^{\epsilon}(x;\zeta_+) \to 0$ as $\zeta_+ \to \infty$, and

$$D_j^{\epsilon}(x) = \lim_{\zeta_+ \to \zeta_{+j}} (\zeta_+ - \zeta_{+j}) \frac{M_{\epsilon}^{+\epsilon}(x;\zeta_+)}{A(\zeta_+)}. \tag{6.7}$$

Examining the leading terms in Eq. (6.2) in the neighborhood of the ζ_{+j}, we arrive at the identification,

$$D_j^{\epsilon}(x) = \epsilon i C_j N^{+\epsilon}(x;\zeta_{+j}), \tag{6.8}$$

where C_j is defined by Eq. (4.12). With the dot denoting differentiation with respect to ζ_+, the expressions for C_j and F_j simplify to

$$C_j = -\epsilon i \frac{B(\zeta_{+j})}{\dot{A}(\zeta_{+j})}, \quad F_j = \epsilon i \frac{H(-\zeta_{-j})}{\dot{G}(-\zeta_{-j})}.$$

Substituting Eq. (6.6) into Eq. (6.2), we find

$$\bar{N}_{-\epsilon}^{+\epsilon}(x;\zeta_+) + R(\zeta_+)N^{+\epsilon}(x;\zeta_+) = 1 + \epsilon i \sum_{j=1}^{q} C_j \frac{N^{+\epsilon}(x;\zeta_{+j})}{\zeta_+ - \zeta_{+j}} + \phi_{\epsilon}^{\epsilon}(x;\zeta_+). \tag{6.9}$$

The function $R(\zeta_+)N^{+\epsilon}(x;\zeta_+)$ is only defined for real $\zeta_+ > -1/(2\delta)$, but we can employ the Plemelj formulas,[40]

$$\hat{R}_{\pm\epsilon}(x;\zeta_+) := \frac{1}{2\pi i}\int_{-1/(2\delta)}^{\infty} \frac{R(\tilde{\zeta})N^{+\epsilon}(x;\tilde{\zeta})}{\tilde{\zeta} - (\zeta_+ \pm \epsilon i 0^+)} \mathrm{d}\tilde{\zeta}, \tag{6.10}$$

to create the decomposition,

$$R(\zeta_+)N^{+\epsilon}(x;\zeta_+) = \epsilon\{\hat{R}_{\epsilon}(x;\zeta_+) - \hat{R}_{-\epsilon}(x;\zeta_+)\}. \tag{6.11}$$

Thus, up to sign, $\hat{R}_{\pm\epsilon}(x;\zeta_+)$ is the $(\pm\epsilon)$ part of $R(\zeta_+)N^{+\epsilon}(x;\zeta_+)$. Substituting Eqs. (6.10) and (6.11) into Eq. (6.9) and equating the $(-\epsilon)$ parts in a manner that respects the asymptotic condition $\bar{N}_{-\epsilon}^{+\epsilon}(x;\zeta_+) \to 1$ as $\zeta_+ \to \infty$ gives

$$\bar{N}_{-\epsilon}^{+\epsilon}(x;\zeta_+) = 1 + \epsilon i \sum_{j=1}^{q} C_j \frac{N^{+\epsilon}(x;\zeta_{+j})}{\zeta_+ - \zeta_{+j}} + \frac{\epsilon}{2\pi i}\int_{-1/(2\delta)}^{\infty} \frac{R(\tilde{\zeta})N^{+\epsilon}(x;\tilde{\zeta})}{\tilde{\zeta} - (\zeta_+ - \epsilon i 0^+)} \mathrm{d}\tilde{\zeta}. \tag{6.12}$$

Equation (6.12) solves the Riemann-Hilbert problem given by Eq. (6.2). It expresses $\bar{N}_{-\epsilon}^{+\epsilon}$ in terms of $N^{+\epsilon}$ and the scattering data. Both sides analytically extend to the half-plane $\mathrm{Im}(\epsilon\zeta_+) < 0$.

With the aid of the connection formula Eq. (3.36), we can eliminate $\bar{N}_{-\epsilon}^{+\epsilon}$ from Eq. (6.12) and get a system of coupled Fredholm equations for $N^{+\epsilon}(x;\zeta_+)$ and $N^{+\epsilon}(x;\zeta_{+j})$, $j = 1, 2, \ldots, q$. The connection formula gives

$$e^{\epsilon i\lambda(x-\epsilon i\delta)} N^{+\epsilon}(x;\zeta_+(-\lambda)) = \Lambda(x;-\zeta_+(\lambda)) + \frac{\epsilon}{2\pi i}\int_{-1/(2\delta)}^{\infty} \frac{R(\tilde{\zeta})N^{+\epsilon}(x;\tilde{\zeta})}{\tilde{\zeta} - \zeta_+(\lambda) + \epsilon i 0^+} \mathrm{d}\tilde{\zeta}, \tag{6.13}$$

where the auxiliary function Λ is defined by

$$\Lambda(x;\zeta) := 1 - \epsilon i \sum_{k=1}^{q} C_k \frac{N^{+\epsilon}(x;\zeta_{+k})}{\zeta + \zeta_{+k}}. \tag{6.14}$$

The involution $\lambda \to -\lambda$ together with the identity $\zeta_+(-\lambda) = -\zeta_-(\lambda)$ transforms Eq. (6.13) into the Fredholm equation,

$$N^{+\epsilon}(x;\zeta_+) = \left\{ \Lambda(x;\zeta_-) + \frac{\epsilon}{2\pi i}\int_{-1/(2\delta)}^{\infty} \frac{R(\tilde{\zeta})N^{+\epsilon}(x;\tilde{\zeta})}{\tilde{\zeta} + \zeta_- + \epsilon i 0^+} \mathrm{d}\tilde{\zeta} \right\} e^{\epsilon i\lambda(x-\epsilon i\delta)}. \tag{6.15}$$

In this equation ζ_- is understood to be the function of the real variable ζ_+ formed by composition of the increasing functions $\zeta_-=\zeta_-(\lambda)$ and $\lambda=\zeta_+^{-1}(\zeta_+)$. Passage to the limit $\lambda\to-\lambda_j$ throughout Eq. (6.13) yields the set of Fredholm equations,

$$N^{+\epsilon}(x;\zeta_{+j})=\left\{\Lambda(x;\zeta_{-j})+\frac{\epsilon}{2\pi i}\int_{-1/(2\delta)}^{\infty}\frac{R(\tilde{\zeta})N^{+\epsilon}(x;\tilde{\zeta})}{\tilde{\zeta}+\zeta_{-j}}\mathrm{d}\tilde{\zeta}\right\}e^{\epsilon i\lambda_j(x-\epsilon i\delta)},\tag{6.16}$$

$j=1,2,\ldots,q$, where $\zeta_{-j}:=\zeta_-(\lambda_j)$. Equations (6.15) and (6.16) form a closed system of $q+1$ Fredholm equations for the $q+1$ unknown functions $N^{+\epsilon}(x;\zeta_+)$ and $N^{+\epsilon}(x;\zeta_{+j})$. The kernels are built out of the scattering data $\zeta_{\pm j}$, C_j, and $R(\zeta_+)$. The other three Jost functions can be calculated in terms of $N^{+\epsilon}(x;\zeta_+)$ by Eqs. (6.12), (6.2), and (6.3).

Large ζ_+ asymptotics for $\bar{N}_{-\epsilon}^{+\epsilon}(x;\zeta_+)$ can be obtained from Eq. (6.12) by standard methods, the expansion to first order being

$$\bar{N}_{-\epsilon}^{+\epsilon}(x;\zeta_+)=1+\frac{1}{\zeta_+}\left\{\epsilon i\sum_{j=1}^{q}C_jN^{+\epsilon}(x;\zeta_{+j})-\frac{\epsilon}{2\pi i}\int_{-1/(2\delta)}^{\infty}R(\tilde{\zeta})N^{+\epsilon}(x;\tilde{\zeta})\mathrm{d}\tilde{\zeta}\right\}+O(1/\zeta_+^2),\tag{6.17}$$

as $\zeta_+\to\infty$. Equation (3.34) can furnish us with a different expression for the large ζ_+ asymptotics of $\bar{N}_{-\epsilon}^{+\epsilon}(x;\zeta_+)$. First, from the formula Eq. (3.30) for the Green's function, we get

$$G_{-\epsilon}^{\epsilon}(x,\eta;\zeta_+)=\frac{\epsilon i}{4\delta\zeta_+}\left\{1+\coth\left(\frac{\pi}{2\delta}(\eta-x-\epsilon i0^+)\right)\right\}+O(1/\zeta_+^2),\tag{6.18}$$

as $\zeta_+\to\infty$. Substituting Eq. (6.18) into Eq. (3.34) gives

$$\bar{N}_{-\epsilon}^{+\epsilon}(x;\zeta_+)=1-\frac{\epsilon}{\zeta_+}\left\{U^{\epsilon}(x)-\frac{1}{2}iL\right\}+O(1/\zeta_+^2),\tag{6.19}$$

where

$$U^{\epsilon}(x)=-\frac{i}{4\delta}\int_{-\infty}^{\infty}\coth\left(\frac{\pi}{2\delta}(\eta-x-\epsilon i0^+)\right)U(\eta)\mathrm{d}\eta=\frac{1}{2}\epsilon U(x)-\frac{1}{2}i\mathbf{T}(U(x))\tag{6.20}$$

and L is the real conserved quantity,

$$L:=\frac{1}{2\delta}\int_{-\infty}^{\infty}U(\xi)\mathrm{d}\xi.$$

Matching the $1/\zeta_+$ terms in the asymptotic expansions Eqs. (6.17) and (6.19), we obtain

$$U^{\epsilon}(x)=\frac{1}{2}iL-i\sum_{j=1}^{q}C_jN^{+\epsilon}(x;\zeta_{+j})+\frac{1}{2\pi i}\int_{-1/(2\delta)}^{\infty}R(\tilde{\zeta})N^{+\epsilon}(x;\tilde{\zeta})\mathrm{d}\tilde{\zeta}.\tag{6.21}$$

A corresponding set of Fredholm equations for the Jost function $\bar{M}^{+\epsilon}(x;\zeta_+)$ can be derived from the Riemann-Hilbert problem Eq. (6.3). These provide alternative expressions for the four Jost functions that are better adapted to asymptotics as $x\to-\infty$. The solution of this Riemann-Hilbert problem is

$$M_{\epsilon}^{+\epsilon}(x;\zeta_+)=1-\epsilon i\sum_{j=1}^{q}F_j\frac{\bar{M}^{+\epsilon}(x;-\zeta_{-j})}{\zeta_++\zeta_{-j}}-\frac{\epsilon}{2\pi i}\int_{-1/(2\delta)}^{\infty}\frac{S(\tilde{\zeta})\bar{M}^{+\epsilon}(x;\tilde{\zeta})}{\tilde{\zeta}-(\zeta_++\epsilon i0^+)}\mathrm{d}\tilde{\zeta}.\tag{6.22}$$

The Fredholm equations analogous to Eqs. (6.15) and (6.16) are

$$\bar{M}^{+\epsilon}(x;\zeta_+) = \left\{ \Lambda_2(x;\zeta_-) - \frac{\epsilon}{2\pi i}\int_{-1/(2\delta)}^{\infty} \frac{S(\tilde{\zeta})\bar{M}^{+\epsilon}(x;\tilde{\zeta})}{\tilde{\zeta}+\zeta_- - \epsilon i 0^+}\mathrm{d}\tilde{\zeta} \right\} e^{\epsilon i\lambda(x-\epsilon i\delta)}, \tag{6.23}$$

$$\bar{M}^{+\epsilon}(x;-\zeta_{-j}) = \left\{ \Lambda_2(x;-\zeta_{+j}) - \frac{\epsilon}{2\pi i}\int_{-1/(2\delta)}^{\infty} \frac{S(\tilde{\zeta})\bar{M}^{+\epsilon}(x;\tilde{\zeta})}{\tilde{\zeta}-\zeta_{+j}}\mathrm{d}\tilde{\zeta} \right\} e^{-\epsilon i\lambda_j(x-\epsilon i\delta)}, \tag{6.24}$$

where

$$S(\zeta_+) := \frac{H(\zeta_+)}{G(\zeta_+)},$$

$$\Lambda_2(x,\zeta) := 1 + \epsilon i\sum_{k=1}^{q} \frac{F_k\bar{M}^{+\epsilon}(x;-\zeta_{-k})}{\zeta-\zeta_{-k}}.$$

Finally, large ζ_+ asymptotics for $M_\epsilon^{+\epsilon}$ give

$$U^{\epsilon}(x) = -\frac{1}{2}iL + i\sum_{j=1}^{q} F_j\bar{M}^{+\epsilon}(x;-\zeta_{-j}) - \frac{1}{2\pi i}\int_{-1/(2\delta)}^{\infty} S(\tilde{\zeta})\bar{M}^{+\epsilon}(x;\tilde{\zeta})\mathrm{d}\tilde{\zeta}. \tag{6.25}$$

We have arrived at two equivalent expressions for $U^{\epsilon}(x,t)$. To get $U^{-\epsilon}(x,t)$, we need to solve the direct and inverse problems with the opposite indicator. This does not necessarily mean starting afresh from the beginning because formulas for the scattering data with the opposite indicator were given in Secs. III and IV. In particular, the κ_j, $C_j(t)$, and $F_j(t)$ are independent of ϵ. When $U^{\epsilon}(x,t)$ and $U^{-\epsilon}(x,t)$ have both been constructed, we can read off

$$U(x,t) = \epsilon\{U^{\epsilon}(x,t) - U^{-\epsilon}(x,t)\}, \tag{6.26}$$

$$(\mathbf{T}U)(x,t) = i\{U^{\epsilon}(x,t) + U^{-\epsilon}(x,t)\}. \tag{6.27}$$

To calculate $V(x,t)$, the solution of the MILW equation from the given initial value $V(x,0)$, first calculate

$$W(x,t) = \int_{-\infty}^{x} U(\xi,t)\mathrm{d}\xi. \tag{6.28}$$

Then

$$V(x,t) = 2\,\mathrm{Im}\{W(x,t)\}. \tag{6.29}$$

Because the operator $\mathbf{T}$ commutes with differentiation, Eq. (2.11) gives us a choice of two formulas for $\mathbf{T}(V_x)$,

$$\mathbf{T}(V_x) = 2\,\mathrm{Im}\{\mathbf{T}U\} = 2\,\mathrm{Re}\{U\} - \beta(e^V - 1), \tag{6.30}$$

which, of course, must be consistent with each other. [Consistency is guaranteed when one is solving an initial value problem, starting with a given $V(x,0)$, but becomes an issue when the starting point is somewhere else, as in the case of the multisoliton solutions in the next section.] One more quadrature will then give $\mathbf{T}V$.

The shallow-water limit of the full IST for the ILW and MILW equations is reasonably straightforward. The functions $U(x,t)$ and $V(x,t)$ require the simple scaling given by Eqs. (1.7) and (2.7), but the Jost functions and the scattering data do not require scaling, as shown by

Satsuma *et al.*[23] On the other hand, the deep-water limit of the IST is more subtle since the ISTs for the ILW and BO equations have features that do not correspond in an obvious way. We refer the reader to Santini *et al.*[38] for the handling of this limit.

VII. SOLITON SOLUTIONS FOR THE ILW AND MILW EQUATIONS

Pure soliton solutions for the real-valued and complex-valued ILW equations occur when the reflection coefficient $R(\lambda;t)$, also written $R(\zeta_+;t)$, vanishes. According to Eqs. (5.3) and (5.5) and identities in Sec. III, whenever the initial value $B(\lambda;0)$ vanishes for real λ, all of the functions,

$$B(\lambda;t), \quad H(\lambda;t), \quad B^{-\epsilon}(\lambda;t), \quad H^{-\epsilon}(\lambda;t),$$

$$R(\lambda;t), \quad S(\lambda;t), \quad R^{-\epsilon}(\lambda;t), \quad S^{-\epsilon}(\lambda;t),$$

vanish together for all real λ and $t \geqslant 0$.

So the integral terms in Eqs. (6.12), (6.15), (6.16), and (6.21)–(6.25) disappear, and the inverse problem reduces to a system of q linear algebraic equations for the case of the q-soliton solution. This will allow us to calculate the physical variables $U(x,t)$, $V(x,t)$, their **T** transforms, and all the Jost functions and other auxiliary functions explicitly in terms of determinants. General formulas for the ILW multisoliton solution have been given by KAS (Ref. 19) and general formulas for the MILW multisoliton solution have been given by Nakamura,[28] the latter demonstrating the power of Hirota's bilinear method.[34,35] However, for the questions that we want to examine regarding MILW solitons, it will be more instructive to look at large x asymptotics of the q-soliton solution and explicit expressions for just the one- and two-soliton solutions of the ILW and MILW equations.

With the help of the time-evolution results in Sec. V, we can write the system of equations for $N^{+\epsilon}(x,t;\lambda_j)$, $j=1,2,\ldots,q$, in the form,

$$N^{+\epsilon}(x,t;\lambda_j) = \left\{ 1 - \epsilon i \sum_{k=1}^{q} \frac{\kappa_k N^{+\epsilon}(x,t;\lambda_k)}{\zeta_{+k} + \zeta_{-j}} e^{\theta_k t - \nu_k} \right\} e^{-\kappa_j (x - \epsilon i \delta)}, \tag{7.1}$$

where

$$\lambda_j = \epsilon i \kappa_j = \zeta_{+j} + \zeta_{-j}, \tag{7.2}$$

$$\theta_j := \theta(\lambda_j) = \kappa_j (\delta^{-1} - \kappa_j \cot \delta \kappa_j), \tag{7.3}$$

$$\nu_j := \log\{\kappa_j / C_j(0)\}. \tag{7.4}$$

The θ_j are real and positive when the corresponding κ_j are real, and similarly for complex conjugate pairs. It will be convenient to define the following auxiliary functions:

$$E_j(x,t) := \exp\{\kappa_j x - \theta_j t + \nu_j\}, \tag{7.5}$$

$$E_j^{\epsilon}(x,t) := \exp\{\kappa_j (x - \epsilon i \delta) - \theta_j t + \nu_j\}. \tag{7.6}$$

Having obtained $N^{+\epsilon}(x,t;\lambda_j)$, the values of $U(x,t)$ and $V(x,t)$ can be deduced from

$$U^{\epsilon}(x,t) = \frac{1}{2} iL - i \sum_{k=1}^{q} \kappa_k N^{+\epsilon}(x,t;\lambda_k) e^{\theta_k t - \nu_k}, \tag{7.7}$$

where L is the real constant defined by Eq. (2.15), by following the steps at the end of the preceding section. An equivalent formula is given by Eq. (6.25) without the integral term. However, because we have disconnected the analysis from the initial value, we no longer know the parameter β in advance, but must calculate it in terms of the other parameters appearing in the

soliton solutions, and also determine any other constraints on the parameters needed to guarantee that $V(x,t)$ is actually a solution of the MILW equation. We also need to determine the relation between the discrete eigenvalues and their complex conjugates.

The asymptotics of $N^{+\epsilon}(x,t;\lambda_j)$ for large positive x are easy to calculate from Eq. (7.1). For large negative x, we get simple determinants that can be evaluated explicitly. The results are

$$N^{+\epsilon}(x,t;\lambda_j) \sim e^{-\kappa_j(x-\epsilon i\delta)}, \tag{7.8}$$

as $x \to +\infty$, and

$$N^{+\epsilon}(x,t;\lambda_j) \sim \frac{1}{B(\lambda_j;t)}\left\{1 - \epsilon i\sum_{k=1}^{q}\frac{\kappa_k e^{-2\nu_k}E_k^{\epsilon}(x,t)}{(\zeta_{+j}+\zeta_{-k})B(\lambda_k;0)B^{-\epsilon}(-\lambda_k;0)}\right\}, \tag{7.9}$$

as $x \to -\infty$, where

$$B(\lambda_j;t) = e^{\theta_j t-\nu_j}\prod_{k\neq j}\frac{\zeta_{+j}-\zeta_{+k}}{\zeta_{+j}+\zeta_{-k}}. \tag{7.10}$$

$$B^{-\epsilon}(-\lambda_j;t) = e^{\theta_j t-\nu_j}\prod_{k\neq j}\frac{\zeta_{-j}-\zeta_{-k}}{\zeta_{-j}+\zeta_{+k}}. \tag{7.11}$$

This $B(\lambda_j;t)$, also written $B(\zeta_{+j};t)$, is identifiable with the $B(\lambda_j)$ appearing on the right-hand side of Eq. (4.3). (In these truncated asymptotic expansions, the next terms involving squares and products of the decaying exponential functions appearing are not necessarily smaller than all of those exponential functions, but they are disjoint from the terms that we have kept.)

From Eq. (6.12), we get the asymptotic expansion,

$$\bar{N}_{-\epsilon}^{+\epsilon}(x,t;\lambda) \sim \frac{1}{A(\lambda)}\left\{1 - \epsilon i\sum_{k=1}^{q}\frac{\kappa_k e^{-2\nu_k}E_k^{\epsilon}(x,t)}{(\zeta_{+}(\lambda)+\zeta_{-k})B(\lambda_k;0)B^{-\epsilon}(-\lambda_k;0)}\right\}, \tag{7.12}$$

as $x \to -\infty$, where

$$A(\lambda) = \prod_{k=1}^{q}\frac{\zeta_{+}(\lambda)-\zeta_{+k}}{\zeta_{+}(\lambda)+\zeta_{-k}}. \tag{7.13}$$

This $A(\lambda)$ is identifiable with the $A(\lambda)$ appearing in Eq. (3.37).

Further calculations along these lines will confirm all the identities among the scattering data given in Secs. III and IV restricted to the case of pure solitons. In particular,

$$G(\lambda) = \frac{1}{A(\lambda)}, \quad H(-\lambda_j;t) = \frac{1}{B(\lambda_j;t)}. \tag{7.14}$$

If we start again with the alternative system Eqs. (6.22)–(6.24), we would arrive at the same asymptotics for the Jost functions with the coefficients $F_j(t)$ given by

$$F_j(t) = \frac{\kappa_j e^{-\theta_j t-\nu_j}}{B(\lambda_j;0)B^{-\epsilon}(-\lambda_j;0)}, \tag{7.15}$$

in agreement with Eq. (4.18). This result permits a simplification of Eqs. (7.9) and (7.12).

The corresponding asymptotics for $U^{\epsilon}(x,t)$ can be calculated from Eq. (7.7) or the corresponding formula deduced from Eq. (6.25). Equation (7.7) yields

$$U^{\epsilon}(x,t) \sim \frac{1}{2}iL - i\sum_{j=1}^{q} \kappa_j E_j^{\epsilon}(x,t)^{-1}, \tag{7.16}$$

as $x \to +\infty$. Similarly, Eq. (6.25) gives

$$U^{\epsilon}(x,t) \sim -\frac{1}{2}iL + i\sum_{j=1}^{q} F_j(t) e^{\kappa_j(x-\epsilon i\delta)}, \tag{7.17}$$

as $x \to -\infty$. Equation (7.7) also gives the same asymptotics as $x \to -\infty$ except that the constant term appears to differ. Equating the constant terms gives the useful identity,

$$\kappa_1 + \kappa_2 + \cdots + \kappa_q = L. \tag{7.18}$$

Thus U^{ϵ} tends to opposite limits at opposite ends of the real axis, in agreement with Eq. (A4) and the boundary condition on U.

The asymptotics for U, $\mathbf{T}U$, W, V, and $\mathbf{T}V$ as $x \to \pm\infty$ can now be calculated from Eqs. (7.16)–(7.18) and (6.26)–(6.30). Our purpose here is to find the constraints, if any, on the real and imaginary parts of the κ_j and ν_j so that we get a consistent q-soliton solution of the MILW equation. For the case $x \to +\infty$, we get

$$U(x,t) \sim \sum_{j=1}^{q} 2\kappa_j \sin \delta\kappa_j E_j(x,t)^{-1}, \tag{7.19}$$

$$\mathbf{T}U(x,t) \sim -L + \sum_{j=1}^{q} 2\kappa_j \cos \delta\kappa_j E_j(x,t)^{-1}, \tag{7.20}$$

$$W(x,t) \sim 2\delta L - \sum_{j=1}^{q} 2 \sin \delta\kappa_j E_j(x,t)^{-1}. \tag{7.21}$$

Before taking the imaginary part of W, let

$$\kappa_j = \mu_j + i\rho_j, \quad \nu_j = \sigma_j + i\tau_j, \tag{7.22}$$

$\mu_j > 0$. Then

$$\theta_j = \frac{\mu_j}{\delta} - \frac{(\mu_j^2 - \rho_j^2)\sin 2\delta\mu_j + 2\mu_j\rho_j \sinh 2\delta\rho_j}{\cosh 2\delta\rho_j - \cos 2\delta\mu_j} + i\left\{\frac{\rho_j}{\delta} + \frac{(\mu_j^2 - \rho_j^2)\sinh 2\delta\rho_j - 2\mu_j\rho_j \sin 2\delta\mu_j}{\cosh 2\delta\rho_j - \cos 2\delta\mu_j}\right\} =: \theta_{jR} + i\theta_{jI}.$$

Then Eq. (6.29) and the first part of Eq. (6.30) give

$$V(x,t) \sim 4\sum_{j=1}^{q} e^{-\mu_j x + \theta_{jR} t - \sigma_j}\{\cosh \delta\rho_j \sin \delta\mu_j \sin(\rho_j x - \theta_{jI} t + \tau_j) - \sinh \delta\rho_j \cos \delta\mu_j \cos(\rho_j x - \theta_{jI} t + \tau_j)\}, \tag{7.23}$$

$$\mathbf{T}V(x,t) \sim 4\sum_{j=1}^{q} e^{-\mu_j x+\theta_{jR}t-\sigma_j}\{\cosh\,\delta\rho_j \cos\,\delta\mu_j \sin(\rho_j x-\theta_{jI}t+\tau_j) - \sinh\,\delta\rho_j \sin\,\delta\mu_j \cos(\rho_j x-\theta_{jI}t+\tau_j)\} + \text{const}, \tag{7.24}$$

as $x \to +\infty$.

An important issue that we did not settle in Sec. IV concerns how the discrete eigenvalues are distributed in the complex plane when the initial value $U(x,0)$ is complex according to Eq. (2.12). We shall now prove that the κ_j are either real or are distributed in complex conjugate pairs, just like the case of the real-valued ILW equation. We will deduce this from the asymptotics of the pure q-soliton solution of the MILW equation. However, the result must hold for all solutions of the complex-valued ILW equation deduced from the real-valued MILW equation because at late times the solitary waves or packets of solitary waves traveling together at the same velocity separate from each other and from the nonsoliton background. If the κ_j were not distributed as stated, the function $V(x,t)$ constructed from Eq. (6.29) would fail the consistency condition given by the second part of Eq. (6.30).

Let us now examine this consistency condition for large $|x|$. At the order at which we are working, e^V-1 has the same asymptotics as V itself. Thus Eqs. (6.30), (7.19), (7.23), and (7.24) give the constraint,

$$\begin{aligned}
&\beta\sum_{j=1}^{q} e^{-\mu_j x+\theta_{jR}t-\sigma_j}\{\cosh\,\delta\rho_j \sin\,\delta\mu_j \sin(\rho_j x-\theta_{jI}t+\tau_j) - \sinh\,\delta\rho_j \cos\,\delta\mu_j \cos(\rho_j x-\theta_{jI}t+\tau_j)\} \\
&= \sum_{j=1}^{q} e^{-\mu_j x+\theta_{jR}t-\sigma_j+\delta\rho_j}\{(\mu_j \cos\,\delta\mu_j + \rho_j \sin\,\delta\mu_j)\sin(\rho_j x-\theta_{jI}t+\tau_j) \\
&\quad + (\mu_j \sin\,\delta\mu_j - \rho_j \cos\,\delta\mu_j)\cos(\rho_j x-\theta_{jI}t+\tau_j)\}.
\end{aligned}$$

Because β is a constant, this equation gives as many distinct equations for β as there are linearly independent functions of x and t appearing.

Suppose that a particular κ_j is not real and that its complex conjugate is not found among the other κ_j. Then the functions of x and t appearing in the jth term are linearly independent of the functions of x and t in the other terms and we can immediately separate out two distinct equations for β,

$$\beta \cosh\,\delta\rho_j \sin\,\delta\mu_j = e^{\delta\rho_j}(\mu_j \cos\,\delta\mu_j + \rho_j \sin\,\delta\mu_j),$$

$$\beta \sinh\,\delta\rho_j \cos\,\delta\mu_j = e^{\delta\rho_j}(\rho_j \cos\,\delta\mu_j - \mu_j \sin\,\delta\mu_j).$$

The same method works for the asymptotics as $x \to -\infty$. The equations analogous to the last two are found to be

$$\beta \cosh\,\delta\rho_j \sin\,\delta\mu_j = e^{-\delta\rho_j}(\mu_j \cos\,\delta\mu_j - \rho_j \sin\,\delta\mu_j),$$

$$\beta \sinh\,\delta\rho_j \cos\,\delta\mu_j = e^{-\delta\rho_j}(\rho_j \cos\,\delta\mu_j + \mu_j \sin\,\delta\mu_j).$$

These four equations admit only the trivial solution $\mu_j=0=\rho_j$, which is out of range. Consequently, we must drop the hypothesis that one of the κ_j is not real while its complex conjugate is not found among the other κ_j. This completes the proof that the κ_j are either real or are distributed in complex conjugate pairs. Since $\lambda_j=\epsilon i\kappa_j$, the eigenvalues λ_j, which live in the region D^ϵ, are therefore either pure imaginary or are distributed symmetrically about the imaginary axis of the complex λ plane. Because the curved boundaries of the regions $D^\pm$ are not symmetric about the imaginary axis, we get the slightly improved inequalities,

$$0 < \mathrm{Re}(\kappa_j) < \pi/\delta, \quad 0 < \mathrm{Im}(\epsilon\lambda_j) < \pi/\delta. \tag{7.25}$$

We now know that $A(-\lambda_j^*)=0=G(\lambda_j^*)$. Hence, we have proved indirectly that the integral on the right-hand side of Eq. (4.11) vanishes identically. Similarly, for the pure soliton solutions at least, Eqs. (7.13) and (7.14) show that $A(\lambda)$ and $G(\lambda^*)$ are complex conjugates of each other when $\mathrm{Re}(\epsilon\lambda)\geqslant 0$ and so the integral on the right-hand side of Eq. (3.60) must vanish in these circumstances.

In the case where all or some of the κ_j are real, the asymptotics of the MILW q-soliton solution give the set of constraints,

$$\beta = \kappa_j(\cot\,\delta\kappa_j + \cot\,\tau_j), \tag{7.26}$$

for each j for which κ_j is real. These express the corresponding τ_j in terms of β and κ_j, there being no loss of generality in restricting τ_j to the interval $(-\pi,\pi)$, with $\tau_j\neq 0$, which allows two values of τ_j for given β and κ_j.

Consider the case where $\kappa_1=\mu_1+i\rho_1$ and $\kappa_2=\mu_1-i\rho_1$, with corresponding ν-parameters, ν_1 and ν_2, which are independent complex numbers (not necessarily complex conjugates). The two corresponding equations for β can be arranged into the form

$$\beta = \kappa_1\{\cot\,\delta\kappa_1 + \cot(i(\nu_2)^* - i\nu_1)\},$$

$$\beta = \kappa_2\{\cot\,\delta\kappa_2 + \cot(i(\nu_1)^* - i\nu_2)\},$$

which have the same shape as Eq. (7.26). Soliton pairs formed in this fashion are known as *breathers*. Physically, they are pulsating solitary waves. Mathematically, the exponential functions appearing will be multiplied by trigonometric functions. More complicated breathers occur when three of more of the κ_j have the same real part.

We have a choice of two ways to construct breathers, both giving the same class of solutions but with different parametrizations. One is to continue with two or more of the κ_j being complex conjugate pairs and use Eq. (2.13) to calculate the real-valued function $V(x,t)$. But a more efficient way is to deduce the breather solutions from the q-soliton solution of the MILW equation having *all real* κ_j by complexifying all the parameters (κ_j, σ_j, and τ_j) *after* applying Eq. (2.13) and taking real slices. Thus, for example, when κ_1 and κ_2 are complex conjugates, take the corresponding parameters σ_1 and σ_2 to be complex conjugates, and similarly for τ_1 and τ_2. Then the complex τ_j obtained in this way will also be constrained by Eq. (7.26).

Let us conclude this section with complete calculations of the one- and two-soliton solutions of the MILW equation and the corresponding Jost functions. For the case $q=1$, Eq. (7.1) gives

$$N^{+\epsilon}(x;\lambda_1) = \frac{e^{-\theta_1 t+\nu_1}}{1+E_1^\epsilon(x,t)}, \tag{7.27}$$

where θ_1 and $E_1^\epsilon(x,t)$ are defined by Eqs. (7.3) and (7.6), respectively. Then Eq. (7.7) gives

$$U^\epsilon(x,t) = \frac{1}{2}i\kappa_1\frac{E_1^\epsilon(x,t)-1}{E_1^\epsilon(x,t)+1}. \tag{7.28}$$

From this we can read off

$$U(x,t) = \frac{\kappa_1\,\sin\,\delta\kappa_1}{\cosh(\kappa_1 x-\theta_1 t+\nu_1)+\cos\,\delta\kappa_1}, \tag{7.29}$$

$$(\mathbf{T}U)(x,t) = -\frac{\kappa_1 \sinh(\kappa_1 x - \theta_1 t + \nu_1)}{\cosh(\kappa_1 x - \theta_1 t + \nu_1) + \cos\,\delta\kappa_1}. \tag{7.30}$$

This is the one-soliton solution of the complex-valued ILW equation. In Appendix B, we give a direct proof that $\mathbf{T}U$ is the $\mathbf{T}$ transform of U according to the definition Eq. (1.6). An easy calculation shows that $U(x,t)$ satisfies the ILW equation.

The four Jost functions for the one-soliton solution are

$$M_\epsilon^{+\epsilon}(x,t;\lambda) = 1 - \frac{\epsilon i\kappa_1 E_1^\epsilon(x,t)}{[\zeta_+(\lambda) + \zeta_{-1}][E_1^\epsilon(x,t)+1]}, \tag{7.31}$$

$$\bar{M}^{+\epsilon}(x,t;\lambda) = e^{\epsilon i\lambda(x-\epsilon i\delta)}\left\{1 + \frac{\epsilon i\kappa_1 E_1^\epsilon(x,t)}{[\zeta_-(\lambda) - \zeta_{-1}][E_1^\epsilon(x,t)+1]}\right\}, \tag{7.32}$$

$$N^{+\epsilon}(x,t;\lambda) = e^{\epsilon i\lambda(x-\epsilon i\delta)}\left\{1 - \frac{\epsilon i\kappa_1}{[\zeta_-(\lambda) + \zeta_{+1}][E_1^\epsilon(x,t)+1]}\right\}, \tag{7.33}$$

$$\bar{N}_{-\epsilon}^{+\epsilon}(x,t;\lambda) = 1 + \frac{\epsilon i\kappa_1}{[\zeta_+(\lambda) - \zeta_{+1}][E_1^\epsilon(x,t)+1]}. \tag{7.34}$$

These can be shown directly to satisfy Eqs. (3.15) and (3.16). The formulas also give the values of $M_\epsilon^{+\epsilon}$ and $N^{+\epsilon}$ at $\lambda=\lambda_1$ and of $\bar{M}^{+\epsilon}$ and $\bar{N}_{-\epsilon}^{+\epsilon}$ at $\lambda=-\lambda_1$. We already know from the general q-soliton results above that

$$A(\lambda) = \frac{\zeta_+(\lambda) - \zeta_{+1}}{\zeta_+(\lambda) + \zeta_{-1}}, \quad G(\lambda) = \frac{1}{A(\lambda)},$$

$$B(\lambda;t) = H(\lambda;t) = 0, \quad B(\lambda_1;t) = e^{\theta_1 t - \nu_1}, \quad H(-\lambda_1;t) = e^{-\theta_1 t + \nu_1},$$

but we can also confirm these results by evaluating the original integrals (3.38), (3.39), (3.43), and (3.44), the integrals for $B(\lambda;t)$ and $H(\lambda;t)$ requiring the rectangular contour with corners at $\eta = \pm R$ and $\pm R + 2\pi i/\kappa_1$.

To get the corresponding one-soliton solution of the MILW equation, follow the steps at the end of Sec. VI. Integrating U gives

$$W(x,t) = 2\tan^{-1}\left(\frac{E_1(x,t)\sin\,\delta\kappa_1}{1 + E_1(x,t)\cos\,\delta\kappa_1}\right), \tag{7.35}$$

where $E_1(x,t)$ is defined by Eq. (7.5). The only parameter that is allowed to be complex is ν_1. Let $\nu_1 = \sigma_1 + i\tau_1$. Then

$$V(x,t) = \log\left(\frac{\cosh(\kappa_1 x - \theta_1 t + \sigma_1) + \cos(\delta\kappa_1 - \tau_1)}{\cosh(\kappa_1 x - \theta_1 t + \sigma_1) + \cos(\delta\kappa_1 + \tau_1)}\right), \tag{7.36}$$

$$(\mathbf{T}V)(x,t) = -2\tan^{-1}\left(\frac{\sin\,\tau_1 \sinh(\kappa_1 x - \theta_1 t + \sigma_1)}{\cos\,\tau_1 \cosh(\kappa_1 x - \theta_1 t + \sigma_1) + \cos\,\delta\kappa_1}\right). \tag{7.37}$$

Appendix B also contains a direct proof that $\mathbf{T}V$ is the $\mathbf{T}$ transform of V. This $V(x,t)$ satisfies the MILW equation with

$$\beta = \kappa_1(\cot\,\delta\kappa_1 + \cot\,\tau_1). \tag{7.38}$$

It is now an easy matter to evaluate the integrals on the right-hand sides of Eqs. (3.60) and (4.11) for the case of the one-soliton solution of the MILW equation. The result in both cases is zero because the integrands are odd functions of $\kappa_1 x - \theta_1 t + \sigma_1$.

For the two-soliton solution, we begin the calculation with

$$N^{+\epsilon}(x,t;\lambda_1) = \frac{N_1}{D_1}, \quad N^{+\epsilon}(x,t;\lambda_2) = \frac{N_2}{D_1}, \tag{7.39}$$

where

$$N_1 = f_3 e^{-\theta_1 t + \nu_1}\{f_4 E_2^{\epsilon}(x,t) + f_2\}, \tag{7.40}$$

$$N_2 = f_4 e^{-\theta_2 t + \nu_2}\{f_3 E_1^{\epsilon}(x,t) - f_2\}, \tag{7.41}$$

$$D_1 = f_3 f_4\{E_1^{\epsilon}(x,t)E_2^{\epsilon}(x,t) + E_1^{\epsilon}(x,t) + E_2^{\epsilon}(x,t)\} + f_1 f_2, \tag{7.42}$$

and the auxiliary constants f_1, f_2, f_3, and f_4 are defined by

$$f_1 := \zeta_{+1} - \zeta_{+2}, \quad f_2 := \zeta_{-1} - \zeta_{-2},$$

$$f_3 := \zeta_{+1} + \zeta_{-2}, \quad f_4 := \zeta_{-1} + \zeta_{+2}.$$

The four Jost functions can be calculated from Eqs. (6.12), (6.15), (6.22), and (6.23). Equation (6.22) gives

$$M_{\epsilon}^{+\epsilon}(x,t;\lambda) = \frac{N_3}{[\zeta_+(\lambda) + \zeta_{-1}][\zeta_+(\lambda) + \zeta_{-2}]D_1}, \tag{7.43}$$

where

$$\begin{aligned} N_3 = f_3 f_4\{&[\zeta_+(\lambda) - \zeta_{+1}][\zeta_+(\lambda) - \zeta_{+2}]E_1^{\epsilon}(x,t)E_2^{\epsilon}(x,t) \\ &+ [\zeta_+(\lambda) - \zeta_{+1}][\zeta_+(\lambda) + \zeta_{-2}]E_1^{\epsilon}(x,t) \\ &+ [\zeta_+(\lambda) + \zeta_{-1}][\zeta_+(\lambda) - \zeta_{+2}]E_2^{\epsilon}(x,t)\} + f_1 f_2[\zeta_+(\lambda) + \zeta_{-1}][\zeta_+(\lambda) + \zeta_{-2}]. \end{aligned} \tag{7.44}$$

Then $\bar{N}_{-\epsilon}^{+\epsilon} = M_{\epsilon}^{+\epsilon}/A(\lambda)$, and the other two Jost functions can be deduced from the connection formulas.

According to Eqs. (6.21) and (6.25),

$$U^{\epsilon}(x,t) = \frac{iN_4}{2D_1}, \tag{7.45}$$

where

$$N_4 = f_3 f_4\{(\kappa_1 + \kappa_2)E_1^{\epsilon}(x,t)E_2^{\epsilon}(x,t) + (\kappa_1 - \kappa_2)[E_1^{\epsilon}(x,t) - E_2^{\epsilon}(x,t)]\} - f_1 f_2(\kappa_1 + \kappa_2). \tag{7.46}$$

Then the two-soliton solution of the complex-valued ILW equation is given by

$$U(x,t) = \frac{N_5}{D_5}, \quad (\mathbf{T}U)(x,t) = \frac{N_6}{D_5}, \tag{7.47}$$

where

$$N_5 = 2f_3f_4\{f_3f_4[\kappa_2 \sin \delta\kappa_2 E_1(x,t) + \kappa_1 \sin \delta\kappa_1 E_2(x,t) + (\kappa_1 - \kappa_2)\sin \delta(\kappa_1 - \kappa_2)]E_1(x,t)E_2(x,t) + f_1f_2[(\kappa_1 + \kappa_2)\sin \delta(\kappa_1 + \kappa_2)E_1(x,t)E_2(x,t) + \kappa_1 \sin \delta\kappa_1 E_1(x,t) + \kappa_2 \sin \delta\kappa_2 E_2(x,t)]\}, \tag{7.48}$$

$$N_6 = -f_3^2f_4^2\{(\kappa_1 + \kappa_2)E_1^2(x,t)E_2^2(x,t) + 2[\kappa_1 \cos \delta\kappa_2 E_1(x,t) + \kappa_2 \cos \delta\kappa_1 E_2(x,t)]E_1(x,t)E_2(x,t) + (\kappa_1 - \kappa_2)[E_1^2(x,t) - E_2^2(x,t)]\} + 2f_1f_2f_3f_4\{\kappa_2 \cos \delta\kappa_1 E_1(x,t) + \kappa_1 \cos \delta\kappa_2 E_2(x,t)\} + f_1^2f_2^2(\kappa_1 + \kappa_2), \tag{7.49}$$

$$D_5 = f_3^2f_4^2\{E_1^2(x,t)E_2^2(x,t) + 2[\cos \delta\kappa_2 E_1(x,t) + \cos \delta\kappa_1 E_2(x,t)]E_1(x,t)E_2(x,t) + E_1^2(x,t) + 2 \cos \delta(\kappa_1 - \kappa_2)E_1(x,t)E_2(x,t) + E_2^2(x,t)\} + 2f_1f_2f_3f_4 \times\{\cos \delta(\kappa_1 + \kappa_2)E_1(x,t)E_2(x,t) + \cos \delta\kappa_1 E_1(x,t) + \cos \delta\kappa_2 E_2(x,t)\} + f_1^2f_2^2. \tag{7.50}$$

To construct the two-soliton solution of the MILW equation, first integrate U to get the potential,

$$W(x,t) = 2 \tan^{-1}\left(\frac{N_7}{D_7}\right), \tag{7.51}$$

where

$$N_7 = f_3f_4\{\sin \delta(\kappa_1 + \kappa_2)E_1(x,t)E_2(x,t) + \sin \delta\kappa_1 E_1(x,t) + \sin \delta\kappa_2 E_2(x,t)\}, \tag{7.52}$$

$$D_7 = f_3f_4\{\cos \delta(\kappa_1 + \kappa_2)E_1(x,t)E_2(x,t) + \cos \delta\kappa_1 E_1(x,t) + \cos \delta\kappa_2 E_2(x,t)\} + f_1f_2. \tag{7.53}$$

There are two ways to arrange the complex parameters to arrive at a real MILW solution using Eq. (6.29), namely, the usual two-soliton consisting of two solitary waves and the two-breather. For the case of two solitary waves, let κ_1 and κ_2 be real with $0 < \kappa_1 < \kappa_2 < \pi/\delta$ and, for $j = 1, 2$, let $\nu_j = \sigma_j + i\tau_j$ and define the auxiliary functions,

$$\widetilde{E}_j(x,t) := \exp(\kappa_j x - \theta_j t + \sigma_j). \tag{7.54}$$

Equations (6.29) and (6.30) give

$$V(x,t) = \log\left(\frac{N_8}{D_8}\right), \quad (\mathbf{T}V)(x,t) = -2 \tan^{-1}\left(\frac{N_9}{D_9}\right), \tag{7.55}$$

where

$$N_8 = f_3^2f_4^2\{\widetilde{E}_1^2(x,t)\widetilde{E}_2^2(x,t) + 2[\cos(\delta\kappa_2 - \tau_2)\widetilde{E}_1(x,t) + \cos(\delta\kappa_1 - \tau_1)\widetilde{E}_2(x,t)]\widetilde{E}_1(x,t)\widetilde{E}_2(x,t) + \widetilde{E}_1^2(x,t) + \widetilde{E}_2^2(x,t) + 2 \cos(\delta\kappa_1 - \delta\kappa_2 - \tau_1 + \tau_2)\widetilde{E}_1(x,t)\widetilde{E}_2(x,t)\} + 2f_1f_2f_3f_4\{\cos(\delta\kappa_1 + \delta\kappa_2 - \tau_1 - \tau_2)\widetilde{E}_1(x,t)\widetilde{E}_2(x,t) + \cos(\delta\kappa_1 - \tau_1)\widetilde{E}_1(x,t) + \cos(\delta\kappa_2 - \tau_2)\widetilde{E}_2(x,t)\} + f_1^2f_2^2, \tag{7.56}$$

$$D_8 = f_3^2f_4^2\{\widetilde{E}_1^2(x,t)\widetilde{E}_2^2(x,t) + 2[\cos(\delta\kappa_2 + \tau_2)\widetilde{E}_1(x,t) + \cos(\delta\kappa_1 + \tau_1)\widetilde{E}_2(x,t)]\widetilde{E}_1(x,t)\widetilde{E}_2(x,t) + \widetilde{E}_1^2(x,t) + \widetilde{E}_2^2(x,t) + 2 \cos(\delta\kappa_1 - \delta\kappa_2 + \tau_1 - \tau_2)\widetilde{E}_1(x,t)\widetilde{E}_2(x,t)\} + 2f_1f_2f_3f_4\{\cos(\delta\kappa_1 + \delta\kappa_2 + \tau_1 + \tau_2)\widetilde{E}_1(x,t)\widetilde{E}_2(x,t) + \cos(\delta\kappa_1 + \tau_1)\widetilde{E}_1(x,t)$$

$$+\cos(\delta\kappa_2+\tau_2)\tilde{E}_2(x,t)\}+f_1^2f_2^2, \tag{7.57}$$

$$N_9=f_3^2f_4^2\{\sin(\tau_1+\tau_2)\tilde{E}_1^2(x,t)\tilde{E}_2^2(x,t)+2[\cos\,\delta\kappa_2\sin\,\tau_1\tilde{E}_1(x,t)+\cos\,\delta\kappa_1\sin\,\tau_2\tilde{E}_2(x,t)]\tilde{E}_1(x,t)\tilde{E}_2(x,t)$$
$$+\sin(\tau_1-\tau_2)[\tilde{E}_1^2(x,t)-\tilde{E}_2^2(x,t)]\}-2f_1f_2f_3f_4\{\cos\,\delta\kappa_1\sin\,\tau_2\tilde{E}_1(x,t)+\cos\,\delta\kappa_2\sin\,\tau_1\tilde{E}_2(x,t)\}$$
$$-f_1^2f_2^2\sin(\tau_1+\tau_2), \tag{7.58}$$

$$D_9=f_3^2f_4^2\{\cos(\tau_1+\tau_2)\tilde{E}_1^2(x,t)\tilde{E}_2^2(x,t)+2[\cos\,\delta\kappa_2\cos\,\tau_1\tilde{E}_1(x,t)$$
$$+\cos\,\delta\kappa_1\cos\,\tau_2\tilde{E}_2(x,t)]\tilde{E}_1(x,t)\tilde{E}_2(x,t)+\cos(\tau_1-\tau_2)[\tilde{E}_1^2(x,t)+\tilde{E}_2^2(x,t)]$$
$$+2\cos\,\delta(\kappa_1-\kappa_2)\tilde{E}_1(x,t)\tilde{E}_2(x,t)\}+2f_1f_2f_3f_4$$
$$\times\{\cos\,\delta(\kappa_1+\kappa_2)\tilde{E}_1(x,t)\tilde{E}_2(x,t)+\cos\,\delta\kappa_1\cos\,\tau_2\tilde{E}_1(x,t)+\cos\,\delta\kappa_2\cos\,\tau_1\tilde{E}_2(x,t)\}$$
$$+f_1^2f_2^2\cos(\tau_1+\tau_2). \tag{7.59}$$

This $V(x,t)$ satisfies the MILW equation with

$$\beta=\kappa_1(\cot\,\delta\kappa_1+\cot\,\tau_1)=\kappa_2(\cot\,\delta\kappa_2+\cot\,\tau_2). \tag{7.60}$$

This two-soliton solution describes two solitary waves traveling from left to right at different speeds, with the taller and thinner wave catching up to the shorter and thicker wave and overtaking it. After the interaction, both waves end up identical in shape to the original waves except for a phase shift, in accordance with the classic profile.

As already mentioned, the best way to construct the two-breather is to complexify the six real parameters in the two-soliton solution just constructed and take the real slice with $\kappa_2=(\kappa_1)^*$, $\sigma_2=(\sigma_1)^*$, and $\tau_2=(\tau_1)^*$. The functions N_8 and D_8 in Eq. (7.55) are real and positive definite for both the two-soliton and two-breather solutions.

To obtain the shallow-water limit of the multisoliton solutions, apply the scalings given by Eq. (2.7) and let all parameters be $O(1)$ as $\delta\to 0^+$ except

$$\tau_j=\pm\tfrac{1}{2}\pi+\delta\tilde{\tau}_j+O(\delta^2).$$

To take the deep-water limit $\delta\to\infty$, let

$$\kappa_j=\frac{\pi}{\delta}-\frac{\pi}{\delta^2\tilde{\lambda}_j},\quad \sigma_j=\frac{\pi\tilde{\sigma}_j}{\delta},\quad \tau_j=\frac{\pi\tilde{\tau}_j}{\delta}.$$

Then the constraints given by Eq. (7.26) reduce to $\tilde{\tau}_j=1/(\beta+\tilde{\lambda}_j)$.

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APPENDIX A: PROPERTIES OF THE OPERATOR T

The singular integral operator **T**, defined by

$$(\mathbf{T}f)(x):=\frac{1}{2\delta}(P)\int_{-\infty}^{\infty}\coth\left(\frac{\pi}{2\delta}(\xi-x)\right)f(\xi)\mathrm{d}\xi=\mathbf{T}(f(x)), \tag{A1}$$

where (P) indicates that the integral is in the Cauchy principal-value sense, appears in the ILW and MILW equations. In this appendix we collate several useful mathematical properties of this

operator. Most of these results are easily proved directly from the definition (some require contour integration), and so we omit these proofs. However, we supply a proof of Eq. (A3) below because of its importance for the shallow-water limit.

The deep-water limit to the BO and MBO equations involves the Hilbert transform operator **H** defined by

$$(\mathbf{H}f)(x) := \frac{1}{\pi}(P)\int_{-\infty}^{\infty}\frac{f(\xi)}{\xi - x}\mathrm{d}\xi = \mathbf{H}(f(x)).$$

Without any additional hypotheses on $f(x)$ apart from the absolute convergence of $\int_{-\infty}^{\infty} f(x)\mathrm{d}x$, we get

$$(\mathbf{T}f)(x) = (\mathbf{H}f)(x) + O(1/\delta), \tag{A2}$$

as $\delta \to \infty$, uniformly for all real x. The O bound can be improved to $O(1/\delta^2)$ uniformly for x on finite intervals if $\int_{-\infty}^{\infty} xf(x)\mathrm{d}x$ converges absolutely.

The corresponding shallow-water limit is given by

$$(\mathbf{T}f)(x) = -\frac{1}{\delta}\int_{-\infty}^{x} f(\xi)\mathrm{d}\xi + L_f + \frac{\delta}{3}f'(x) + \frac{\delta^3}{45}f'''(x) + O(\delta^5), \tag{A3}$$

as $\delta \to 0^+$, where

$$L_f := \frac{1}{2\delta}\int_{-\infty}^{\infty} f(\xi)\mathrm{d}\xi.$$

This is a truncated version of a more general result derived below.

The operator **T** also possesses the following additional properties:[26,27,35,41]

$$\lim_{x\to\pm\infty}(\mathbf{T}f)(x) = \mp L_f, \tag{A4}$$

$$\frac{d}{\mathrm{d}x}\{(\mathbf{T}f)(x)\} = (\mathbf{T}f')(x) = \mathbf{T}(f'(x)), \tag{A5}$$

$$\int_{-\infty}^{\infty} f(x)(\mathbf{T}g)(x)\mathrm{d}x = -\int_{-\infty}^{\infty} g(x)(\mathbf{T}f)(x)\mathrm{d}x, \tag{A6}$$

$$\mathbf{T}(f\mathbf{T}g + g\mathbf{T}f)(x) = (\mathbf{T}f)(x)(\mathbf{T}g)(x) - f(x)g(x) - L_fL_g, \tag{A7}$$

$$\mathbf{T}\left(\log\frac{h(x+i\delta)}{h(x-i\delta)}\right) = -i\log\{h(x+i\delta)h(x-i\delta)\}. \tag{A8}$$

In all cases, it is understood that $f(x)$ and $g(x)$ are sufficiently smooth and decay at a sufficient rate to guarantee existence of the relevant derivatives and integrals and allow interchange of limit operations. In Eq. (A8), $h(z)$ denotes a function of a complex variable z that is analytic in the open strip $-\delta < \mathrm{Im}\, z < \delta$, is continuous and nonzero on the closure of that strip, and tends to 1 uniformly as $\mathrm{Re}\, z \to \pm\infty$ in the closed strip.

A proof of Eq. (A3) is given by Satsuma *et al.*[23] It calls upon a result of Gibbons and Kupershmidt.[26] We believe that the reader would be interested in seeing a proof that proceeds directly from the definition of the **T** operator.

To assist in the derivation, we prefer to use the auxiliary operator,[21]

$$(\hat{\mathbf{T}}f)(x) := \frac{1}{2\delta}(P)\int_{-\infty}^{\infty}\left\{\coth\left(\frac{\pi}{2\delta}(\xi-x)\right)-\operatorname{sgn}(\xi-x)\right\}f(\xi)\mathrm{d}\xi, \tag{A9}$$

which converges more rapidly than the integral for $(\mathbf{T}f)(x)$ (although, of course, it is not suited to contour integration). The two operators $\mathbf{T}$ and $\hat{\mathbf{T}}$ are related by the identity,

$$(\mathbf{T}f)(x) = (\hat{\mathbf{T}}f)(x) + \frac{1}{2\delta}\int_{x}^{\infty} f(\xi)\mathrm{d}\xi - \frac{1}{2\delta}\int_{-\infty}^{x} f(\xi)\mathrm{d}\xi. \tag{A10}$$

First, observe that the change of variable $y=(\xi-x)/\delta$ maps Eq. (A9) into

$$(\hat{\mathbf{T}}f)(x) = \frac{1}{2}(P)\int_{-\infty}^{\infty}\left\{\coth\left(\frac{\pi y}{2}\right)-\operatorname{sgn}(y)\right\}f(x+\delta y)\mathrm{d}y. \tag{A11}$$

Focus now on the shallow-water region, $0<\delta\ll 1$. Assume that $f(x)$ possesses at least three derivatives. The Taylor series (with remainder) for the function $f(x+\delta y)$ in ascending powers of δ or y is

$$f(x+\delta y) = \sum_{m=0}^{2N}\frac{\delta^m y^m}{m!}f^{(m)}(x) + \frac{\delta^{2N+1}y^{2N+1}}{(2N+1)!}f^{(2N+1)}(x+\delta\theta y), \tag{A12}$$

where $0<\theta=\theta(x,y,\delta,N)<1$. Substituting Eq. (A12) into Eq. (A11) and interchanging the order of summation and integration, we obtain

$$(\hat{\mathbf{T}}f)(x) = \frac{1}{2}\sum_{m=0}^{2N}\frac{\delta^m}{m!}f^{(m)}(x)(P)\int_{-\infty}^{\infty}\left\{\coth\left(\frac{\pi y}{2}\right)-\operatorname{sgn}(y)\right\}y^m\,\mathrm{d}y + R_N, \tag{A13}$$

where the remainder term R_N will be given a suitable bound below.

The integral in Eq. (A13) is a principal-value integral only for $m=0$ and, in this case, it vanishes because the integrand is odd. For all other m, the integrals are just convergent improper Riemann integrals. Again, when m is even, they all vanish because the integrands are odd. Hence, the series Eq. (A13) simplifies to

$$(\hat{\mathbf{T}}f)(x) = \sum_{k=1}^{N}\frac{\delta^{2k-1}}{(2k-1)!}f^{(2k-1)}(x)I_k + R_N, \tag{A14}$$

where

$$I_k := \int_0^{\infty}\left\{\coth\left(\frac{\pi y}{2}\right)-1\right\}y^{2k-1}\,\mathrm{d}y. \tag{A15}$$

The integrals I_k can be evaluated in terms of zeta-function values or Bernoulli numbers as follows:

$$I_k = \frac{2}{\pi^{2k}}\int_0^{\infty}\frac{z^{2k-1}}{e^z-1}\mathrm{d}z = \frac{2}{\pi^{2k}}(2k-1)!\zeta(2k) = \frac{2^{2k-1}}{k}|B_{2k}|. \tag{A16}$$

(To distinguish between various conventions for the Bernoulli numbers, we state here that $B_0=1$, $B_1=-1/2$, $B_2=1/6$, $B_3=0$, and $B_4=-1/30$.)

The remainder term can be written,

$$R_N = \frac{\delta^{2N+1}}{2(2N+1)!}\int_0^\infty \left\{\coth\left(\frac{\pi y}{2}\right) - 1\right\} y^{2N+1}\{f^{(2N+1)}(x+\delta\theta y) + f^{(2N+1)}(x-\delta\theta_1 y)\}\mathrm{d}y, \tag{A17}$$

where $\theta_1 := \theta(x,-y,\delta,N)$. A straightforward bound can be obtained if we just assume that the derivatives of $f(x)$ are bounded, that is,

$$|f^{(k)}(x)| \leqslant M_k, \quad -\infty < x < \infty, \tag{A18}$$

at least in the case $k=2N+1$. (Of course, this might not be sharp enough for some applications.) Then the triangle inequality for integrals gives

$$|R_N| \leqslant \frac{M_{2N+1} I_{N+1} \delta^{2N+1}}{(2N+1)!} = \frac{2^{2N+2}\delta^{2N+1}}{(2N+2)!}|B_{2N+2}|M_{2N+1}. \tag{A19}$$

Substituting Eq. (A16) into Eq. (A14), we obtain

$$(\hat{\mathbf{T}}f)(x) = \sum_{k=1}^{N} \frac{2^{2k}\delta^{2k-1}}{(2k)!}|B_{2k}|f^{(2k-1)}(x) + R_N, \tag{A20}$$

which is the (truncated) shallow-water expansion of the operator $\hat{\mathbf{T}}$ in terms of known quantities. According to Eq. (A10), the corresponding expansion for $\mathbf{T}$ is

$$(\mathbf{T}f)(x) = \frac{1}{2\delta}\int_x^\infty f(\xi)\mathrm{d}\xi - \frac{1}{2\delta}\int_{-\infty}^x f(\xi)\mathrm{d}\xi + \sum_{k=1}^{N} \frac{2^{2k}\delta^{2k-1}}{(2k)!}|B_{2k}|f^{(2k-1)}(x) + R_N. \tag{A21}$$

If $f(x)$ were real-analytic or differentiable to all orders, we would obtain an infinite series in ascending powers of δ. Depending on the remainder, it could be either convergent or valid as an asymptotic series for small positive δ. If $f(x)$ is differentiable five times, with a bounded fifth derivative, we get the truncated formula Eq. (A3).

APPENDIX B: SELECTED T TRANSFORMS

In this appendix, we give direct evaluations of $(\mathbf{T}f)(x)$ for a useful class of functions that includes the one-soliton solutions of the ILW and MILW equations (with the time dependence and phase shift suppressed as these can be trivially reinstated later). These results are used in Sec. VII to confirm that the one-soliton solutions do indeed satisfy their respective equations and also to evaluate the parameter β in the one-soliton solution of the MILW equation.

Begin with the two-parameter family of functions,

$$f(x) = \frac{1}{\cosh \kappa x + \cos\theta_0}, \tag{B1}$$

where κ and θ_0 are real with $\kappa > 0$ and $-\pi < \theta_0 < \pi$. In general, the $\mathbf{T}$ transform of $f(x)$ does not have a simple explicit formula, but there are simple formulas in cases where one parameter is arbitrary and the other is suitably restricted. For example, in the case where θ_0 is arbitrary and κ is a rational multiple of π/δ, the integral defining $(\mathbf{T}f)(x)$ can be evaluated by summing residues inside a suitable indented rectangular contour. However, the rectangular contour cannot work in the case relevant to the one-soliton solution of the ILW equation, where κ is arbitrary and $\theta_0 = \kappa\delta$. Several of the more elementary integrals appearing below without proof can be reduced to linear combinations of the following integrals:

$$\int_{-\infty}^{\infty} \frac{\sinh \alpha\mu}{\sinh \beta\mu} \mathrm{d}\mu = \frac{\pi}{\beta} \tan\left(\frac{\pi\alpha}{2\beta}\right), \tag{B2}$$

β real, α complex, $-\beta < \mathrm{Re}\ \alpha < \beta$,

$$\int_{-R}^{R} \frac{\sinh \alpha\mu}{\sinh \beta\mu} \mathrm{d}\mu = \frac{\pi}{\beta} \tan\left(\frac{\pi\alpha}{2\beta}\right) + \frac{2}{\alpha - \beta} e^{(\alpha-\beta)R} + O(e^{-(3\beta - \mathrm{Re}\ \alpha)R}), \tag{B3}$$

as $R \to \infty$, $\beta \leqslant \mathrm{Re}\ \alpha < 3\beta$, $\alpha \neq \beta$, and

$$\int_{-\infty}^{\infty} \frac{\cosh \kappa\alpha x}{\cosh \kappa x + \cos\ \theta_0} \mathrm{d}x = \frac{2\pi \sin\ \alpha\theta_0}{\kappa \sin\ \theta_0 \sin\ \pi\alpha}, \tag{B4}$$

$-1 < \mathrm{Re}\ \alpha < 1$.

Take a Fourier transform of $f(x)$ and rearrange to give the formula,

$$\frac{1}{\cosh \kappa x + \cos\ \theta_0} = \frac{1}{\sin\ \theta_0} \int_{-\infty}^{\infty} \frac{\sinh\ \theta_0\mu}{\sinh\ \pi\mu} e^{i\kappa\mu x}\, \mathrm{d}\mu. \tag{B5}$$

Apply the $\hat{\mathbf{T}}$ operator and interchange the order of integration. A straightforward application of a rectangular contour with corners at $\xi = \pm R$ and $\pm R + 2i\delta$ and indents at $\xi = x$ and $x + 2i\delta$ gives

$$\hat{\mathbf{T}}(e^{i\kappa\mu x}) = i\left(\coth\ \kappa\delta\mu - \frac{1}{\kappa\delta\mu}\right) e^{i\kappa\mu x}.$$

Thence

$$\hat{\mathbf{T}}\left(\frac{1}{\cosh \kappa x + \cos\ \theta_0}\right) = -\frac{1}{\sin\ \theta_0} \int_{-\infty}^{\infty} \frac{\sinh\ \theta_0\mu \sin\ \kappa\mu x}{\sinh\ \pi\mu} \left(\coth\ \kappa\delta\mu - \frac{1}{\kappa\delta\mu}\right) \mathrm{d}\mu. \tag{B6}$$

Parameter differentiation and a rectangular contour give the result,

$$\int_{-\infty}^{\infty} \frac{\sinh\ \theta_0\mu \sin\ \kappa\mu x}{\mu \sinh\ \pi\mu} \mathrm{d}\mu = 2 \tan^{-1}\left(\tan \frac{1}{2}\theta_0 \tanh \frac{1}{2}\kappa x\right). \tag{B7}$$

Thence Eq. (A10) gives our main formula,

$$\mathbf{T}\left(\frac{1}{\cosh \kappa x + \cos\ \theta_0}\right) = -\frac{1}{\sin\ \theta_0} \int_{-\infty}^{\infty} \frac{\sinh\ \theta_0\mu \sin\ \kappa\mu x}{\sinh\ \pi\mu} \coth\ \kappa\delta\mu\, \mathrm{d}\mu, \tag{B8}$$

valid for $\kappa \neq 0$ and $-\pi < \theta_0 < \pi$. Validity extends to $\kappa = 0$ if the $\mathbf{T}$ operator is understood to be a principal value integral in two senses, the second being $(P)\int_{-\infty}^{\infty} = \lim_{R\to\infty} (P)\int_{-R}^{R}$.

It is immediately clear from Eq. (B8) that the case $\theta_0 = \kappa\delta$ can be reduced to two applications of Eq. (B2). The result is

$$\mathbf{T}\left(\frac{1}{\cosh \kappa x + \cos\ \kappa\delta}\right) = -\frac{1}{\sin\ \kappa\delta} \frac{\sinh\ \kappa x}{\cosh\ \kappa x + \cos\ \kappa\delta}, \tag{B9}$$

valid for $-\pi/\delta < \kappa < \pi/\delta$. This integral (with an appropriate shift in x) confirms Eq. (7.30) for the one-soliton solution of the ILW equation.

The integral on the right-hand side of Eq. (B8) also simplifies when θ_0 is a nonzero integer multiple of $\kappa\delta$ or differs from such a value by π. Examples are

$$\mathbf{T}\left(\frac{1}{\cosh \kappa x - \cos \kappa\delta}\right) = \frac{1}{\sin \kappa\delta}\left(\frac{\sinh \kappa x}{\cosh \kappa x - \cos \kappa\delta} - \frac{\pi}{\kappa\delta}\tanh \frac{\pi x}{2\delta}\right), \tag{B10}$$

valid for $0<\kappa<2\pi/\delta$,

$$\mathbf{T}\left(\frac{1}{\cosh \kappa x + \cos 2\kappa\delta}\right) = -\frac{1}{\sin 2\kappa\delta}\left(\frac{\sinh \kappa x}{\cosh \kappa x + \cos 2\kappa\delta} + \tanh \frac{\kappa x}{2}\right), \tag{B11}$$

valid for $-\pi/(2\delta)<\kappa<\pi/(2\delta)$, and

$$\mathbf{T}\left(\frac{1}{\cosh \kappa x - \cos 2\kappa\delta}\right) = \frac{1}{\sin 2\kappa\delta}\left(\frac{\sinh \kappa x}{\cosh \kappa x - \cos 2\kappa\delta} + \coth \frac{\kappa x}{2} - \frac{\pi}{\kappa\delta}\coth \frac{\pi x}{2\delta}\right), \tag{B12}$$

valid for $0<\kappa<\pi/\delta$.

The small κ limits of Eqs. (B10) and (B12) give

$$\mathbf{T}\left(\frac{1}{x^2+\delta^2}\right) = \frac{x}{\delta(x^2+\delta^2)} - \frac{\pi}{2\delta^2}\tanh \frac{\pi x}{2\delta}, \tag{B13}$$

$$\mathbf{T}\left(\frac{1}{x^2+4\delta^2}\right) = \frac{1}{2\delta x} + \frac{x}{2\delta(x^2+4\delta^2)} - \frac{\pi}{4\delta^2}\coth \frac{\pi x}{2\delta}, \tag{B14}$$

which can be proved directly by summing residues in the upper-half ξ plane. More generally,

$$\mathbf{T}\left(\frac{1}{x^2+n^2\delta^2}\right) = \frac{x}{n\delta}\sum_{k=1}^{n}\left(\frac{1}{x^2+(2k-n)^2\delta^2}\right) - \frac{\pi}{2n\delta^2}\coth\left(\frac{\pi x}{2\delta} + \frac{n\pi i}{2}\right). \tag{B15}$$

The aforementioned elementary case where κ is a rational multiple of π/δ is best handled by applying the rectangular contour to the right-hand side of Eq. (B8). The simplest examples are

$$\mathbf{T}\left(\frac{1}{\cosh(\pi x/\delta) + \cos \theta_0}\right) = -\frac{\delta\theta_0 \sinh(\pi x/\delta) + \pi x \sin \theta_0}{\delta\pi \sin \theta_0\{\cosh(\pi x/\delta) + \cos \theta_0\}}, \tag{B16}$$

$$\mathbf{T}\left(\frac{1}{\cosh(\pi x/(2\delta)) + \cos \theta_0}\right) = -\frac{2\delta\theta_0 \sinh(\pi x/\delta) - \pi x \sin 2\theta_0}{\delta\pi \sin \theta_0\{\cosh(\pi x/\delta) - \cos 2\theta_0\}}. \tag{B17}$$

More generally,

$$\begin{aligned}\mathbf{T}\left(\frac{1}{\cosh(m\pi x/(n\delta)) + \cos \theta_0}\right) = &-\frac{1}{m\pi \sin \theta_0\{\cosh(m\pi x/\delta) - (-1)^n \cos n\theta_0\}} \\ &\times \left\{ n\theta_0 \sinh \frac{m\pi x}{\delta} - (-1)^n \frac{m\pi x}{\delta} \sin n\theta_0 \right. \\ &+ 2m\pi \sum_{k=1}^{n-1} (-1)^k \cot \frac{km\pi}{n} \sin k\theta_0 \sinh \frac{(n-k)m\pi x}{n\delta} \\ &\left. + 2n\pi \sum_{h=1}^{m-1} \operatorname{cosec} \frac{hn\pi}{m} \sin \frac{hn\theta_0}{m} \sinh \frac{(m-h)\pi x}{\delta} \right\}.\end{aligned} \tag{B18}$$

Additional consequences of Eq. (B8) can be deduced by parameter differentiation or integration. Multiply both sides by $\sin \theta_0$ and integrate with respect to θ_0. We get

$$\mathbf{T}\left(\log\frac{\cosh\kappa x+\cos\theta_2}{\cosh\kappa x+\cos\theta_1}\right)=\int_{-\infty}^{\infty}\frac{(\cosh\theta_2\mu-\cosh\theta_1\mu)\sin\kappa\mu x}{\mu\sinh\pi\mu}\coth\kappa\delta\mu\,\mathrm{d}\mu, \tag{B19}$$

valid for $-\pi<\theta_j<\pi$, $j=1,2$. A cancellation occurs when $\theta_2+\theta_1=2\kappa\delta$. The result is

$$\begin{aligned}\mathbf{T}\left(\log\frac{\cosh\kappa x+\cos(\kappa\delta+\gamma)}{\cosh\kappa x+\cos(\kappa\delta-\gamma)}\right)&=2\int_{-\infty}^{\infty}\frac{\sinh\gamma\mu\cosh\kappa\delta\mu\sin\kappa\mu x}{\mu\sinh\pi\mu}\mathrm{d}\mu\\&=2\tan^{-1}\left(\frac{\sin\gamma\sinh\kappa x}{\cos\gamma\cosh\kappa x+\cos\kappa\delta}\right).\end{aligned} \tag{B20}$$

Apart from a shift in x, this is the **T** transform of the one-soliton solution of the MILW equation, confirming Eq. (7.37).

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Basic twist quantization of the exceptional Lie algebra g_2

Andrzej Borowiec, Jerzy Lukierski, Vladimir Lyakhovsky,[a)]
Marek Mozrzymas, and Valeriy N. Tolstoy[b)]
Institute for Theoretical Physics, University of Wroclaw, pl. M. Borna 9, 50-204 Wroclaw, Poland

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We present the formulas for twist quantization of g_2, corresponding to the solution of a classical YB equation with support in the eight-dimensional Borel subalgebra of g_2. The considered chain of twists consists of the four factors describing the four steps of quantization: Jordanian twist, the two twist factors extending Jordanian twist and the deformed Jordanian or in a second variant additional Abelian twist. The first two steps describe as well the $sl(3)$ quantization. The coproducts are calculated for each step in explicit form, and for that purpose we present new formulas for the calculation of similarity transformations on the tensor product. We introduce new basic generators in universal enveloping algebra $U(g_2)$ that provide nonlinearities in the algebraic sector maximally simplifying the deformed coproducts. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2041849]

I. INTRODUCTION

In this paper we shall consider the basic nonstandard quantum deformations of complex exceptional Lie algebra g_2. There are four complex semisimple Lie algebras of rank 2, given by $A_2 \simeq sl(3)$, $D_2 \simeq o(4) = o(3) \oplus o(3)$, $B_2 \simeq C_2 \simeq o(5) \simeq sp(4)$ and g_2, with 8, 6, 10, and 14 generators, respectively. The eight-dimensional carrier of classical r matrices that describe our deformations is equal to the Borel subalgebra $\mathfrak{b}_+(g_2)$ of g_2.

There are two natural embeddings related with the group G_2.

(i) $G_2 \subset O(7)$. The fundamental matrix representation of G_2 is seven dimensional. The 7×7 orthogonal matrices $(L_{ab}) \in O(7)$ $(a,b=1,2,\ldots,7)$ belong to the group G_2 if the following cubic constraint is satisfied:[1,2]

$$f_{a_1a_2a_3} = f_{b_1b_2b_3} L_{a_1b_1} L_{a_2b_2} L_{a_3b_3}, \tag{1.1}$$

where the totally antisymmetric cubic tensor f_{abc} describes the multiplication table for imaginary octonions t_a,

$$t_a t_b = f_{abc} t_c, \tag{1.2}$$

and the values of f_{abc} are determined by the following choice (we list only nonvanishing values):

$$f_{127} = f_{157} = f_{163} = f_{264} = f_{245} = f_{374} = f_{576} = 1. \tag{1.3}$$

Therefore there are only seven independent equations (1.1) reducing 21 parameters of $O(7)$ to 14 parameters of the group G_2.

We see that the fundamental seven-dimensional representation $\{7\}$ of Lie algebra g_2 inherits basic properties of the fundamental $o(7)$ representation: reality and its dimensionality. The generators (E^l_k, A_k, B^l) $(k,l=1,2,3)$ of g_2 satisfy the following relations (Refs. 1–5):

[a)]On leave of absence from Sankt-Petersburg University, Ulianovskaya 1, Petrodvoretz, 198904 Sankt Petersburg, Russia
[b)]On leave of absence from Institute of Nuclear Physics, Moscow State University, 119 992 Moscow, Russia

$$[E_k{}^l, E_m{}^n] = \delta_m{}^l E_k{}^n - \delta_k{}^n E_m{}^l, \tag{1.4a}$$

$$[E_k{}^l, A_m] = \delta_m{}^l A_k - \frac{1}{3}\delta_k{}^l A_m, \tag{1.4b}$$

$$[E_k{}^l, B^n] = -\delta_k{}^n B^l + \frac{1}{3}\delta_k{}^l B^n, \tag{1.4c}$$

$$[A_m, B^n] = E_m{}^n, \tag{1.4d}$$

$$[A_m, A_n] = -\frac{4}{3}\epsilon_{mnl} B^l, \tag{1.4e}$$

$$[B^m, B^n] = \epsilon^{mnl} A_l, \tag{1.4f}$$

where

$$E_k{}^k = 0, \tag{1.4g}$$

and we employ the $su(3)$ tensorial basis.

(ii) $sl(3) \subset g_2$ or $su(3) \subset g_2$ (real form). The generators $E_k{}^l$ forming the subalgebra (1.4a) describe $sl(3)$ (if g_2 is a complex Lie algebra) or $su(3)$ (if we introduce in g_2 the suitable real structure). The Lie algebra generators of g_2 belong to a 14-dimensional adjoint representation $\{\underline{14}\}$ that decomposes under $sl(3)$ [or $su(3)$] as follows:

$$\{\underline{14}\} = \{\underline{8}\} + \{\underline{3}\} + \{\overline{\underline{3}}\}. \tag{1.5}$$

In the realization [(1.4a), (1.4b), (1.4c), (1.4d), (1.4e), and (1.4f)] of the Lie algebra g_2, the generators A_m (B^m) transform as fundamental triplet (antitriplet) representations of $sl(3)$ or $su(3)$. These properties can also be seen from the root diagram of g_2 (see Sec. II).

The relations (1.4a), (1.4b), (1.4c), (1.4d), (1.4e), (1.4f), and (1.4g) show that the coset space $S^6 = G_2/SU(3)$ is a nonsymmetric Riemannian space, with torsion described by the nonvanishing rhs of relations (1.4e) and (1.4f). One of our aims in this paper is to provide an algebraic ground for new quantum deformation of the sphere S^6 with torsion.

The embedding of a three-dimensional fundamental representation of $su(3)$ described by Gell-Mann fundamental matrices λ_k ($k=1,\ldots,8$) into a seven-dimensional fundamental representation of g_2 looks as follows:

$$\Lambda_k = \frac{1}{\sqrt{2}}\begin{pmatrix} \lambda_k & 0 & 0 \\ 0 & -\lambda_k^* & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{1.6}$$

where we use the standard normalization

$$\mathrm{Tr}\,\lambda_k\lambda_l = \mathrm{Tr}\,\Lambda_k\Lambda_l = 2\delta_{kl}. \tag{1.7}$$

We identify two Cartan generators of g_2 with the $su(3)$ generators Λ_3 and Λ_8.

Our plan for this paper is the following:

In Sec. II we shall consider the Lie algebra g_2 in the Cartan-Weyl basis (see, e.g., Ref. 6), which is directly linked with the generators (E_k^l, A_k, B^l) satisfying the algebra (1.4a), (1.4b), (1.4c), (1.4d), (1.4e), (1.4f), and (1.4g). We present the important class of triangular r matrices for g_2, satisfying the classical Yang–Baxter equation (CYBE). It appears that the two-parameter families of such r matrices have as its carrier algebra the whole eight-dimensional Borel subalgebra

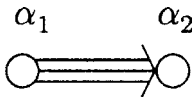

FIG. 1. Dynkin diagram of the Lie algebra g_2.

$\mathfrak{b}_+(g_2) \subset g_2$. We show that the parameters of the considered classical r matrices can achieve fixed nonzero values by means of inner automorphism maps inside g_2 algebra. In Sec. III we shall recall the general formulas that describe the twist quantization method,[7–12] and we shall introduce the general twisting function, describing the twist quantization procedure for g_2 with the eight-dimensional carrier space for its r matrix. In Sec. IV we obtain first the explicit formulas describing the twist quantization of g_2 generated by the $sl(3)$ classical r matrix. It appears that these quantization formulas for g_2 describe the extension of known relations describing the twist quantization of $sl(3)$.[12] In particular, following general techniques presented in Ref. 13, we shall introduce a suitable nonlinear basis in the deformed Hopf algebras. In Sec. V we consider the most general g_2 quantizations containing two additional twists, depending on the g_2 generators from the coset $G_2/sl(3)$. In Sec. VI we present a general discussion and some conclusions. We remark that in Secs. IV and V we shall use new algebraic formulas for calculating twisted coproducts presented in Sec. III D and shall introduce a new basis of $U(g_2)$, which will simplify the twisted coproduct formulas.

The motivation for our work is mainly to present a new mathematical result—an interesting class of quantum deformations for an important Lie algebra. On the other side, it should be stressed that g_2 algebra recently has attracted attention of physicists in the domain of elementary particle physics and fundamental interactions theory. In particular, we recall the following.

(i) In 11-dimensional M theory, there were proposed the internal manifolds with g_2 holonomy as a base for the grand unification describing an extension of the standard model in particle physics (see, e.g., Refs. 14–17). The algebra g_2 implies seven-dimensional internal symmetry space as the privileged one, in obvious connection with the relation $11=4+7$.

(ii) In the reduction of supersymmetric theories from $D=11$ to $D=4$, the g_2 internal symmetry implies a phenomenologically interesting case of $D=4$ models with $N=1$ supersymmetry.[5] In particular, there were also considered standard and supersymmetric extensions of $D=4$ chromodynamics to G_2 gauge theories[5] with an interesting exceptional quark confinement mechanism.

(iii) There are four Hurwitz algebras (real numbers R, complex numbers C, quaternions H, and octonions O); G_2 acts on seven imaginary octonionic units and describes the automorphism group of the octonion algebra. All applications of exceptional and octonions groups to the description of symmetries in elementary particle physics (see, e.g., Ref. 18) is therefore strongly linked with the appearance of G_2 symmetry.

In this paper we consider only the quantum deformations of universal enveloping algebra $U(g_2)$; it is an interesting problem to supplement the considerations with deformations of dual Hopf algebra describing matrix quantum G_2 group and, further, describe, e.g., the quantum deformations of $S^6=G_2/SL(3)$. In such a way one can obtain an example of the six-dimensional counterpart of a two-dimensional Podleś sphere,[19] provided by the deformed coset $SU(2)/U(1)$.

II. CARTAN–WEYL BASIS OF g_2 AND JORDANIAN TYPE CLASSICAL r MATRICES

A. Cartan–Weyl basis of g_2

In order to describe a Cartan–Weyl basis of g_2, let us introduce the Dynkin diagram for its simple roots $\Pi=\{\alpha_1,\alpha_2\}$ (see Fig. 1):

The corresponding standard $A=(a_{ij})$ $(i,j=1,2)$ and symmetric $A^{\mathrm{sym}}=(a_{ij}^{\mathrm{sym}})_{i,j}$ Cartan matrices are given by

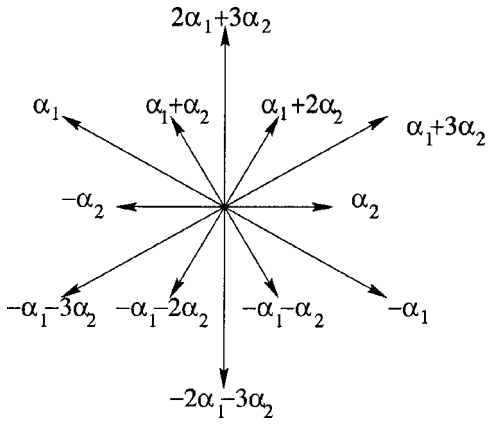

FIG. 2. The root diagram for g_2.

$$A=\begin{pmatrix}2 & -1\\ -3 & 2\end{pmatrix},\quad A^{\mathrm{sym}}=\begin{pmatrix}6 & -3\\ -3 & 2\end{pmatrix}. \tag{2.1}$$

The Lie algebra g_2 is generated by the six Chevalley elements e_{α_i}, $e_{-\alpha_i}$, h_{α_i} $(i=1,2)$ with the defining relations (see, e.g., Ref. 6)

$$[h_{\alpha_i},h_{\alpha_j}]=0,$$

$$[h_{\alpha_i},e_{\pm\alpha_j}]=\pm a_{ij}^{\mathrm{sym}}e_{\pm\alpha_j},$$

$$[e_{\alpha_i},e_{-\alpha_j}]=\delta_{ij}h_{\alpha_i},$$

$$[e_{\pm\alpha_1},[e_{\pm\alpha_1},e_{\pm\alpha_2}]]=0,$$

$$[[[[e_{\pm\alpha_1},e_{\pm\alpha_2}],e_{\pm\alpha_2}],e_{\pm\alpha_2}],e_{\pm\alpha_2}]=0. \tag{2.2}$$

The positive $\Sigma_+(g_2)$ and total $\Sigma(g_2)=\Sigma_+(g_2)\cup(-\Sigma_+(g_2))$ root systems of g_2 are presented in terms of an orthonormalized basis $\{\epsilon_1,\epsilon_2\}$ of a two-dimensional Euclidian space as follows:

$$\Sigma_+(g_2)=\left\{\sqrt{3}\epsilon_1,\epsilon_2,\frac{\sqrt{3}}{2}\epsilon_1\pm\frac{1}{2}\epsilon_2,\frac{\sqrt{3}}{2}\epsilon_1\pm\frac{3}{2}\epsilon_2\right\}, \tag{2.3}$$

$$\Sigma(g_2)=\left\{\pm\sqrt{3}\epsilon_1,\pm\epsilon_2,\pm\frac{\sqrt{3}}{2}\epsilon_1\pm\frac{1}{2}\epsilon_2,\pm\frac{\sqrt{3}}{2}\epsilon_1\pm\frac{3}{2}\epsilon_2\right\}, \tag{2.4}$$

where the simple roots are given by $\alpha_1=(\sqrt{3}/2)\epsilon_1-\frac{3}{2}\epsilon_2$ and $\alpha_2=\epsilon_2$. It is convenient to present the total root system by the root diagram presented in Fig. 2.

For a construction of the composite root vectors e_γ $(\gamma\neq\pm\alpha_1,\pm\alpha_2)$, we fix the following normal ordering of the positive root system $\Sigma_+(g_2)$ (see Ref. 6):

$$\alpha_1,\alpha_1+\alpha_2,2\alpha_1+3\alpha_2,\alpha_1+2\alpha_2,\alpha_1+3\alpha_2,\alpha_2, \tag{2.5}$$

which corresponds to "clockwise" ordering for positive roots in Fig. 2 if we start from the root α_1 to the root α_2. For convenience we introduce the short notations,

$$e_{k,l} := e_{k\alpha_1+l\alpha_2}, \quad h_{k,l} := kh_{\alpha_1} + lh_{\alpha_2}, \tag{2.6}$$

for $k,l=0,\pm 1,\ldots$. According to the ordering (2.5), we set the composite roots generators with suitably chosen numerical coefficients as follows:

$$e_{1,1} = [e_{1,0}, e_{0,1}], \quad e_{-1,-1} = -[e_{-1,0}, e_{0,-1}],$$

$$e_{1,2} = [e_{1,1}, e_{0,1}], \quad e_{-1,-2} = -\frac{3}{4}[e_{0,-1}, e_{-1,-1}],$$

$$e_{1,3} = [e_{1,2}, e_{0,1}], \quad e_{-1,-3} = -\frac{3}{4}[e_{0,-1}, e_{-1,-2}],$$

$$e_{2,3} = [e_{1,3}, e_{1,0}], \quad e_{-2,-3} = -\frac{3}{4}[e_{-1,0}, e_{-1,-3}]. \tag{2.7}$$

The complete set of relations for the Cartan–Weyl basis of g_2 can be read off from the formulas (1.4a), (1.4b), (1.4c), (1.4d), (1.4e), and (1.4f) after the identification

$$h_{1,0} \equiv h_1 = E_2{}^2 - E_3{}^3, \quad h_{0,1} \equiv h_2 = \frac{1}{6}(E_1{}^1 - 2E_2{}^2 + E_3{}^3), \tag{2.8a}$$

and

$$e_{1,0} = E_2{}^3, \quad e_{-1,0} = E_3{}^2,$$

$$e_{0,1} = B^2, \quad e_{0,-1} = A_2,$$

$$e_{1,1} = -B^3, \quad e_{-1,-1} = -A_3,$$

$$e_{1,2} = A_1, \quad e_{-1,-2} = B^1,$$

$$e_{1,3} = E_1{}^2, \quad e_{-1,-3} = E_2{}^1,$$

$$e_{2,3} = E_1{}^3, \quad e_{-2,-3} = E_3{}^1. \tag{2.8b}$$

B. Jordanian-type classical *r* matrices for g_2

First, we introduce some definitions concerning classical r matrices. Let $\mathfrak{g}$ be any simple Lie algebra; then $\mathfrak{g}=\mathfrak{n}_- \oplus \mathfrak{h} \oplus \mathfrak{n}_+$, where $\mathfrak{n}_\pm$ are maximal nilpotent subalgebras and $\mathfrak{h}$ is a Cartan subalgebra. The subalgebra $\mathfrak{n}_+$ ($\mathfrak{n}_-$) is generated by the positive (negative) root vectors e_β ($e_{-\beta}$) for all $\beta \in \Sigma_+(\mathfrak{g})$. The symbol $\mathfrak{b}_+$ will denote the Borel subalgebra of $\mathfrak{g}$, $\mathfrak{b}_+ := \mathfrak{h} \oplus \mathfrak{n}_+$. Let the elements $h_\theta \in \mathfrak{h}$ and $e_\theta \in \mathfrak{n}_+$ satisfy the relation

$$[h_\theta, e_\theta] = e_\theta. \tag{2.9}$$

A two-tensor $r_J(\xi_\theta) \in \mathfrak{b}_+ \otimes \mathfrak{b}_+$ of the form

$$r_\theta(\xi_\theta) = \xi_\theta h_\theta \wedge e_\theta := \xi_\theta(h_\theta \otimes e_\theta - e_\theta \otimes h_\theta) \tag{2.10}$$

satisfies CYBE and it is called the Jordanian classical r matrix. The symbol $\xi_\theta \in \mathbb{C}$ is a deformation parameter. Moreover, let elements $e_{\gamma \pm i}$, indexed by the symbols i and $-i$, $i \in I=\{1,2,\ldots,N\}$, satisfy the relations

$$[h_\theta, e_{\gamma_i}] = (1 - t_{\gamma_i}) e_{\gamma_i}, \quad [h_\theta, e_{\gamma_{-i}}] = t_{\gamma_i} e_{\gamma_{-i}}, \tag{2.11a}$$

$$[e_{\gamma_i}, e_{-\gamma_j}] = \delta_{ij} e_{\gamma_0}, \quad [e_{\gamma \pm i}, e_{\gamma \pm j}] = 0, \tag{2.11b}$$

$$[e_{\gamma \pm i}, e_{\gamma_0}] = 0. \tag{2.11c}$$

It is not difficult to check (see also Ref. 8) that the element

$$r_{\theta;N}(\xi_\theta) = \xi_\theta \left(h_\theta \wedge e_\theta + \sum_{i=1}^{N} e_{\gamma_i} \wedge e_{\gamma - i} \right) \tag{2.12}$$

satisfies CYBE, and it will be called the extended Jordanian r matrix of N order. Let N be of maximal order, i.e., there do not exist other elements $e_{\gamma \pm j} \in \mathfrak{n}_+$, $j > N$ that satisfy the relations (2.11c); then the element (2.12) will be called the extended Jordanian r matrix of maximal order.[20] It is evident that the extended Jordanian r matrix of maximal order is defined by the elements $h_\theta \in \mathfrak{h}$, $e_\theta \in \mathfrak{n}_+$ and the Borel subalgebra $\mathfrak{b}_+$. Here we shall consider a special ("canonical") case when e_θ and $e_{\gamma \pm i}$ $(i = 1, 2, \ldots, N)$ are weight elements with respect to the Cartan subalgebra $\mathfrak{h}$,

$$[h, e_\theta] = (h, \theta) e_\theta, \quad [h, e_{\gamma \pm i}] = (h, \gamma_{\pm i}) e_{\gamma \pm i} \tag{2.13}$$

for any $h \in \mathfrak{h}$ and for all $i = 1, 2, \ldots, N$. Analyzing the structure of the positive root systems of the complex simple Lie algebras, we see that if $e_{\gamma \pm j} \in \mathfrak{n}_+$, the maximal order N of the extended Jordanian r matrix is associated with the maximal root, i.e., the root θ is maximal.

Let us pass now to the Lie algebra $\mathfrak{g} = g_2$. The maximal root generator e_θ is $e_{2,3} = e_{2\alpha_1 + 3\alpha_2}$ and the extended Jordanian matrix of maximal order is provided by formula (2.12) with $N = 2$. It takes the form

$$r_{2,3;2}(\xi) = \xi (h_{2,3} \wedge e_{2,3} + e_{1,1} \wedge e_{1,2} + e_{1,3} \wedge e_{1,0}). \tag{2.14}$$

In order to obtain the generalizations of the r matrix (2.14), one can use the theorem by Belavin and Drinfeld, which states that the sum of two r matrices r_1, r_2 is again a classical r matrix[21] if r_2 has a carrier $L \in g_2$ ($r_2 \in L \otimes L$) that cocommutes with r_1 (i.e., it is a kernel of the bialgebra cobracket).

The maximal subalgebra in g_2, which is a kernel of the Lie bialgebra cobracket determined by the r matrix (2.14) has the following linear basis:

$$L = (h_{0,1}, e_{0,1}, e_{0,-1}, e_{2,3}), \tag{2.15}$$

i.e., $[r_{2,3;2}(\xi), l \otimes 1 + 1 \otimes l] = 0 (l \in L)$. From the generators of the subalgebra L, one can construct the following five classical r matrices: (a) $h_{0,1} \wedge e_{0,1}$, (b) $h_{0,1} \wedge e_{2,3}$, (c) $e_{0,1} \wedge e_{2,3}$, (d) $h_{0,1} \wedge e_{0,-1}$, (e) $e_{0,-1} \wedge e_{2,3}$.

The r matrices that we shall consider below are obtained as the linear combination of (2.14) and the r matrices (a) and (b). One can show that the results of the addition of the r matrix (2.14) and the r matrices (c)–(e) can be obtained from the previous two cases by suitable automorphisms of the algebra g_2.

It follows that we can consider two r matrices as basic ones, or, more explicitly,

$$r_1 = \alpha h_{0,1} \wedge e_{0,1} + \xi (h_{2,3} \wedge e_{2,3} + e_{1,1} \wedge e_{1,2} + e_{1,3} \wedge e_{1,0}), \tag{2.16a}$$

$$r_2 = \beta h_{0,1} \wedge e_{2,3} + \xi (h_{2,3} \wedge e_{2,3} + e_{1,1} \wedge e_{1,2} + e_{1,3} \wedge e_{1,0}), \tag{2.16b}$$

where ξ, α, β are arbitrary.

One can raise the question of whether the classical r matrices (2.16a) and (2.16b) can be extended to carrier space containing also the generators belonging to $\mathfrak{b}_-$. Unfortunately, such an extension, which cannot be eliminated by the inner automorphism of g_2, is not possible for a

purely algebraic reason. One can show that there does not exist an even dimensional subalgebra of g_2, with dimension ten (two extra generators from $\mathfrak{b}_-$), which extends the full Borel subalgebra $\mathfrak{b}_+$. In fact, the consideration of classical r matrices with the carrier in both Borel subalgebras of g_2 that, however, are not simultaneously the classical r matrices for a $sl(3)$ subalgebra is an interesting problem to study, going beyond the scope of the present paper.

Below we shall consider the quantization of g_2 in the four steps, corresponding to the quantization of the following sequence of r matrices.

(i) Jordanian twist quantization,

$$r_J = \xi h_{2,3} \wedge e_{2,3}. \tag{2.17}$$

(ii) Two extended Jordanian twist quantizations,

$$r_{EJ} = \xi(h_{2,3} \wedge e_{2,3} + e_{1,1} \wedge e_{1,2}), \tag{2.18a}$$

$$r_{E'EJ} = \xi(h_{2,3} \wedge e_{2,3} + e_{1,1} \wedge e_{1,2} + e_{1,3} \wedge e_{1,0}). \tag{2.18b}$$

The r matrix r_{EJ} describes the extended Jordanian twist quantization of the $sl(3)$ subalgebra.

(iii) Full twist quantization with additional twist factors describing the deformed Jordanian twist [classical r matrix (2.16a)] and the Abelian twist [classical r matrix (2.16b)].

It should be observed that the parameters α, β, and ξ occurring in the classical r matrices (2.16a) and (2.16b) can be rescaled by inner automorphisms of g_2 algebra as well as by the overall scaling of the r matrices. In particular, performing the two-parameter rescaling by Cartan generators (we use the notation $(ad^{\otimes}a)A \otimes B \equiv [a,A] \otimes B + A \otimes [a,B]$):

$$\exp[ad^{\otimes}(c_1 h_{1,0} + c_2 h_{0,1})] r_1 = e^{(1/2)c_1} r_1,$$

$$\exp[ad^{\otimes}(c_1 h_{1,0} + c_2 h_{0,1})] r_2 = e^{(-(1/2)c_1 + (1/3)c_2)} \beta h_{0,1} \wedge e_{0,1} + e^{(1/2)c_1} r_{E'EJ}, \tag{2.19}$$

we see that while the parameter α remains unchanged, the parameters β and ξ can be rescaled, e.g., to unity. In order to modify the parameter α we can employ the overall scaling of the r matrix. We see therefore, that similarly like in the case of Jordanian deformation of $sl(2)$ or κ deformation of Poincaré algebra, the deformations with different values of the parameters α, β, and ξ are mathematically equivalent (provided $\alpha \neq 0$, $\beta \neq 0$, $\xi \neq 0$) but distinguishable if applied to physical models.

III. TWIST QUANTIZATION METHOD AND THE GENERAL TWIST FUNCTIONS FOR g_2

A. Quantum deformations by twisting coproducts of universal enveloping algebras

Consider the universal enveloping algebra $U(\mathfrak{g})$ of a Lie algebra $\mathfrak{g}$ as a Hopf algebra with the comultiplication $\Delta^{(0)}$ generated by the primitive coproduct in $\mathfrak{g}$. The parametric invertible solution $\mathcal{F}(\xi) = \Sigma f_i^{(1)} \otimes f_i^{(2)} \in U(\mathfrak{g}) \otimes U(\mathfrak{g})$ of the twist equations,[8]

$$\mathcal{F}_{12}(\Delta^{(0)} \otimes 1)(\mathcal{F}) = \mathcal{F}_{23}(1 \otimes \Delta^{(0)})(\mathcal{F}), \tag{3.1}$$

$$(\varepsilon \otimes \mathrm{id})(\mathcal{F}) = (\mathrm{id} \otimes \varepsilon)(\mathcal{F}) = 1 \otimes 1, \tag{3.2}$$

defines the deformed (twisted) Hopf algebra $U_{\mathcal{F}}(\mathfrak{g})$ with the unchanged multiplication, unit and counit [as in $U(\mathfrak{g})$], the twisted comultiplication and antipode defined by the relations

$$\Delta_{\mathcal{F}}(u) = \mathcal{F}\Delta^{(0)}(u)\mathcal{F}^{-1}, \quad u \in U(\mathfrak{g}), \tag{3.3a}$$

$$S_{\mathcal{F}}(u) = vS^{(0)}(u)v^{-1}, \quad v = \sum f_i^{(1)} S^{(0)}(f_i^{(2)}). \tag{3.3b}$$

The twisted algebra $U_{\mathcal{F}}(\mathfrak{g})$ is triangular, with the universal $\mathcal{R}$ matrix,

$$\mathcal{R}_{\mathcal{F}} = \mathcal{F}_{21}\mathcal{F}^{-1}, \tag{3.4}$$

which belongs to some extension of $U(\mathfrak{g}) \otimes U(\mathfrak{g})$. When $\mathcal{F}$ is a smooth function of ξ and $\lim_{\xi\to 0} \mathcal{F} = 1 \otimes 1$ then in the neighborhood of the origin the $\mathcal{R}$-matrix can be presented as

$$\mathcal{R}_{\mathcal{F}} = 1 \otimes 1 + \xi r_{\mathcal{F}} + o(\xi), \tag{3.5}$$

where $r_{\mathcal{F}}$ is the skew-symmetric classical r matrix corresponding to the twist $\mathcal{F}$. Let us write explicitly the r matrix as follows:

$$r_{\mathcal{F}} = a^{ij} I_i \wedge I_j. \tag{3.6}$$

Then we obtain

$$\mathcal{F} = 1 \otimes 1 + \xi \tilde{a}^{ij} I_i \otimes I_j + \mathcal{O}(\xi), \tag{3.7}$$

where $a^{ij} = \frac{1}{2}(\tilde{a}^{ij} - \tilde{a}^{ji})$.

By a nonlinear change of basis in $U(\mathfrak{g})$, one can modify the twisted coproducts and locate part of the deformation in the algebraic sector.

B. Twist deformations for $U(g_2)$ Hopf algebra

Our aim is to construct explicitly such a sequence of the twist deformations $U_{\mathcal{F}}(g_2)$ of the algebra $U(g_2)$ that will lead to the largest possible carrier subalgebra for the corresponding classical r matrices. The final element of the corresponding twists will be the full chain of extended twists whose carrier coincides with the Borel subalgebra of g_2. The peculiarity of the chain twist deformation is that the deformed algebra can be twisted step by step by the consecutive twisting factors with their specific properties. One of the important aims will also be the construction of proper nonlinear basis in $U(g_2)$. Indeed, on each step we shall construct the nonlinear basis in which the costructure of the Hopf algebra $U_{\mathcal{F}}(g_2)$ becomes more transparent.

In Sec. II we have presented the sequence of classical r matrices for $U(g_2)$ [see (2.17), (2.18a), (2.18b), (2.16a), and (2.16b)]. The quantization of these classical r-matrices is performed as follows.

(a) First, we introduce the standard Jordanian twist quantizing the classical r matrix (2.17), corresponding to the long root $2\alpha_1 + 3\alpha_2$ in g_2. We have the following twisting element:[22]

$$\mathcal{F}_J = e^{h_{2,3} \otimes \sigma_{2,3}} = e^{H \otimes \sigma}, \tag{3.8}$$

where

$$H = h_{2,3} = 2h_{1,0} + 3h_{0,1}, \quad \sigma = \ln(1 + e_{2,3}). \tag{3.9}$$

(b) There are four types of the extension twisting factors that can be applied to $U_J(g_2)$:[12]

$$\mathcal{F}_{E_+} = e^{e_{1,1} \otimes e_{1,2} e^{-(1/2)\sigma}}$$

$$\mathcal{F}_{E_-} = e^{-e_{1,2} \otimes e_{1,1} e^{-(1/2)\sigma}}$$

$$\tilde{\mathcal{F}}_{E_+} = e^{e_{1,3} \otimes e_{1,0} e^{-(1/2)\sigma}}$$

$$\widetilde{\mathcal{F}}_{E_-} = e^{-e_{1,0}\otimes e_{1,3}e^{-(1/2)\sigma}}. \tag{3.10}$$

They can be composed to provide the following four types of the two-element extensions of (3.8):

$$\mathcal{F}_{E_{++}} = e^{e_{1,3}\otimes e_{1,0}e^{-(1/2)\sigma}}e^{e_{1,1}\otimes e_{1,2}e^{-(1/2)\sigma}},$$

$$\mathcal{F}_{E_{+-}} = e^{e_{1,3}\otimes e_{1,0}e^{-(1/2)\sigma}}e^{-e_{1,2}\otimes e_{1,1}e^{-(1/2)\sigma}},$$

$$\mathcal{F}_{E_{-+}} = e^{-e_{1,0}\otimes e_{1,3}e^{-(1/2)\sigma}}e^{e_{1,1}\otimes e_{1,2}e^{-(1/2)\sigma}},$$

$$\mathcal{F}_{E_{--}} = e^{-e_{1,0}\otimes e_{1,3}e^{-(1/2)\sigma}}e^{-e_{1,2}\otimes e_{1,1}e^{-(1/2)\sigma}}. \tag{3.11}$$

One can note that exponential factors in the twists (3.11) commute with each other, and do not describe themselves as the solutions of twist equations (3.1) and (3.2) with primitive coproduct $\Delta^{(0)}$. The four twists (3.11) lead to the equivalent Hopf algebras, however, their coalgebra relations differ considerably. The most elegant result is obtained when the extension is chosen as follows:

$$\mathcal{F}_E := \mathcal{F}_{E_{-+}} = \mathcal{F}_{E_-}\mathcal{F}_{E_+} = e^{-e_{1,2}\otimes e_{1,1}e^{-(1/2)\sigma}}e^{e_{1,3}\otimes e_{1,0}e^{-(1/2)\sigma}}, \tag{3.12}$$

with the extended twist

$$\mathcal{F}_{EJ} := e^{-e_{1,2}\otimes e_{1,1}e^{(-1/2)\sigma}}e^{e_{1,3}\otimes e_{1,0}e^{(-1/2)\sigma}}e^{H\otimes\sigma}. \tag{3.13}$$

It should be added that the products of twists $\mathcal{F}_{E_\pm}\mathcal{F}_J$ describe the twist quantization of $sl(3)$ subalgebra.

(c) The additional Abelian twist factor ($h \equiv 3h_{0,1}$),

$$\mathcal{F}_A = e^{h\otimes\sigma}, \tag{3.14}$$

that produces a kind of a "rotation" in the root space of g_2, can enlarge the extended twist (3.13):

$$\mathcal{F}_{AEJ} := e^{h\otimes\sigma}e^{-e_{1,2}\otimes e_{1,1}e^{(-1/2)\sigma}}e^{e_{1,3}\otimes e_{1,0}e^{(-1/2)\sigma}}e^{H\otimes\sigma}. \tag{3.15}$$

In such a way we obtain the quantization of the classical r matrix (2.16b).

(d) We can construct the chain of twists (see, e.g., Refs. 9 and 10) for g_2 by additionally deforming the twisted $U_{EJ}(g_2)$ by the second link of the chain, which is the Jordanian factor:

$$\mathcal{F}_{J'} = e^{h\otimes\sigma}, \tag{3.16}$$

with

$$\omega = \ln\left(1 + e_{0,1} + \frac{1}{2}(e_{1,2})^2\right). \tag{3.17}$$

This gives the quantization with the largest carrier

$$\mathcal{F}_{J'EJ} := e^{h\otimes\omega}e^{-e_{1,2}\otimes e_{1,1}e^{(-1/2)\sigma}}e^{e_{1,3}\otimes e_{1,0}e^{(-1/2)\sigma}}e^{H\otimes\sigma}. \tag{3.18}$$

The twist function (3.18) describes the quantization of the classical r matrix (2.16a). The twist (3.15) can also form the chain with $\mathcal{F}_{J''}=e^{h\otimes\omega''}$ (see Sec. V C). But the Abelian twist factors $\mathcal{F}_A$ and this new Jordanian factor are related by the formula $\mathcal{F}_{J''}\mathcal{F}_A=\mathcal{F}_{J'}$. This means that for any "rotated" extended twist $\mathcal{F}_{AEJ}$ we get the unique chain (3.18).

In Secs. IV and V we shall present the deformed Hopf algebras $U_{\mathcal{F}}(g_2)$ with more details, discuss their properties, and introduce the suitable bases of $U(g_2)$. In such a way we obtain the twist quantizations for g_2 with the largest carrier, which can be described by the chain of twists.

The following paragraph Sec. III C will be devoted to the description of the mathematical framework, which permits us to choose the basis in $U(g_2)$ with simplified coproduct formulas. Subsequently, in Sec. III D we shall derive some new mathematical formulas simplifying the calculation of coproducts in Secs. IV and V.

C. Dual bases and simplification of coalgebra structure

Let $(\mathfrak{g},\mathfrak{g}^{\#})$ be a coboundary Lie bialgebra. The dual Lie algebra $\mathfrak{g}^{\#}$ is determined by the r matrix and can be written explicitly in the form of Lie coalgebra with the cocommutators $\delta(a)=[a\otimes 1+1\otimes a,r]$, $(a\in\mathfrak{g})$. Let $\mathfrak{G}^{\#}$ denote the dual group for $(\mathfrak{g},\mathfrak{g}^{\#})$—the universal covering Lie group with the Lie algebra $\mathfrak{g}^{\#}$. According to the quantum duality principle,[13] the Hopf algebra $U_{\mathcal{F}}(\mathfrak{g})$ naturally treated as quantum algebra with respect to $U(\mathfrak{g})$ can be also considered as a quantum group with respect to Fun $(\mathfrak{G}^{\#})$: $U_{\mathcal{F}}(\mathfrak{g})\approx \mathrm{Fun}_{\xi}(\mathfrak{G}^{\#})$. The coproducts in $U_{\mathcal{F}}(\mathfrak{g})$ describe the deformed group multiplication law of the dual group $\mathfrak{G}^{\#}$. These multiplications are deformed due to the fact that generators in $\mathrm{Fun}_{\xi}(\mathfrak{G}^{\#})$ are subject to the relations of $U(\mathfrak{g})$. The undeformed coproducts for Fun $(\mathfrak{G}^{\#})$ can be obtained by constructing the second classical limit $\mathrm{Fun}_{\xi}(\mathfrak{G}^{\#})\to \mathrm{Fun}(\mathfrak{G}^{\#})$ for the Hopf algebra $U_{\mathcal{F}}(\mathfrak{g})$.[26] Among other important consequences, the quantum duality prescribes the existence of two preferred bases for the Hopf algebra $U_{\mathcal{F}}(\mathfrak{g})$:[25] the natural set of generators for $\mathfrak{g}$ (usually they form the Cartan–Weil basis in $\mathfrak{g}$) and the basis natural for $\mathfrak{G}^{\#}$. The latter may be the exponential basis, generated by the Cartan–Weil basis in $\mathfrak{g}^{\#}$. Evidently, the costructure of $U_{\mathcal{F}}(\mathfrak{g})$ becomes transparent only in terms of the group $\mathfrak{G}^{\#}$ that is in the dual group basis or (keeping in mind the exponential map) in a $\mathfrak{g}^{\#}$ basis. For algebras of $\mathrm{rank}(\mathfrak{g})=1$ one can use the $\mathfrak{g}$ coordinates for the multiplications as well as for the comultiplications. Starting with $\mathrm{rank}(\mathfrak{g})=2$ [see, for example, $U_{\mathcal{F}}(sl(3))$] in Ref. 12 some of the coproducts written in a classical $\mathfrak{g}$ basis (natural $\mathfrak{g}$ coordinates) are complicated, and it is difficult to study their properties. To pass from $\mathfrak{g}$ to $\mathfrak{g}^{\#}$ basis, it is necessary to compare the generators in $U_{\mathcal{F}}(\mathfrak{g})$ induced by the undeformed $U(\mathfrak{g})$ with those corresponding to Fun $(\mathfrak{G}^{\#})$ or to its canonical dual $[\mathrm{Fun}(\mathfrak{G}^{\#})]^{*}\approx U(\mathfrak{g}^{\#})$. The general description of the corresponding algorithm and, in particular, the transformation of the Lie-algebra bases (i.e., the change of coordinates $\mathfrak{g}\leftrightarrow\mathfrak{g}^{\#}$), was presented in Ref. 13. In Sec. IV for the obtained quantum algebras $U_{\mathcal{F}}(\mathfrak{g})$, we shall use both $\mathfrak{g}$ and $\mathfrak{g}^{\#}$ bases and demonstrate their role in the description of algebraic and coalgebraic properties of twist deformations.

D. New algebraic formulas for the similarity transformation of tensor products

Calculations of deformed coproducts rely on the successive application of the following version of the Baker-Campbell-Hausdorff (BCH) formula (the adjoint action in terms of the exponential map):

$$e^{X}Ae^{-X}=\exp(\mathrm{ad}_X)A\equiv\sum_{k=0}^{\infty}\frac{1}{k!}\mathrm{ad}_X^k A=\sum_{k=0}^{\infty}\frac{1}{k!}[X,[\ldots[X,A]\ldots]]. \tag{3.19}$$

More exactly, since one works in the tensor product of two algebras $U\otimes U$, the BCH formula we need is as follows:

$$\begin{aligned} e^{X\otimes Y}(A\otimes B)e^{-X\otimes Y}&=\exp(\mathrm{ad}_{X\otimes Y})(A\otimes B)\\ &=\exp(\mathrm{ad}_X\otimes Y)(A\otimes 1)\exp(X\otimes \mathrm{ad}_Y)(1\otimes B)\\ &=\sum_{k=0}^{\infty}\frac{1}{k!}\mathrm{ad}_X^k A\otimes Y^k\sum_{m=0}^{\infty}\frac{1}{m!}X^m\otimes \mathrm{ad}_Y^m B. \end{aligned} \tag{3.20}$$

The above expression is a product of two infinite series. Fortunately, in most applications impor-

tant for our study here, both series truncate and become finite due to the fact that one acts in the enveloping algebra $U=U_g$ of some finite-dimensional simple Lie algebra g and adjoint actions of non-Cartan elements are nilpotent. The other case that can be handled well occurs when one of the elements, say X, belongs to Cartan subalgebra. Then $\mathrm{ad}_X A \equiv [X,A]=aA$ and $\mathrm{ad}_X^k A=a^k A$, with $a \in \mathbb{C}$. In this case the first factor shrinks into the following simple expression:

$$\sum_{k=0}^{\infty} \frac{1}{k!} \mathrm{ad}_X^k A \otimes Y^k = A \otimes e^{aY}. \tag{3.21}$$

We see that the complexity of calculations heavily depends on the degree of nilpotency. We should also notice that in applications, one of the factors, say $Y=f(E)$, might have a functional form in terms of some generator E, e.g., corresponding to the maximal root vector. We are particularly interested when $f(E)=\ln(1+E)$ or $f(E)=e^E$.

When the degree of nilpotency is lower than two, i.e. $\mathrm{ad}_E^2 B \equiv [E,[E,B]]=0$, one can use the following obvious expression $[f(E),B]=[E,B]f'(E)$ (where f' denotes the derivative of f). This leads to

$$\sum_{m=0}^{\infty} \frac{1}{m!} X^m \otimes \mathrm{ad}_{f(E)}^m B = 1 \otimes B + X \otimes [E,B] f'(E). \tag{3.22}$$

Dealing with these simple techniques permits us to calculate almost all deformed coproducts except the one described by the last twist factor $\mathcal{F}_C$ [see Eq. (5.22)]. In order to complete calculations one needs more general and more sophisticated methods. For this purpose we have found two combinatorial expressions, which turned out to be very useful.

If X and Y are two commuting elements and, in addition, $[X,B]=0$, then

$$Y^X B Y^{-X} \equiv e^{X \ln Y} B e^{-X \ln Y} = \sum_{k=0}^{\infty} X^{\underline{k}} \frac{\mathrm{ad}_Y^k B}{k!} Y^{-k}, \tag{3.23}$$

where the sequence

$$x^{\underline{k}} \equiv \frac{\Gamma(x+1)}{\Gamma(x-k+1)} = x(x-1)\ldots(x-k+1) = \sum_{m=1}^{k} s(k,m) x^m \tag{3.24}$$

stands for the so-called lower (or falling) factorial polynomials and $s(n,k)$ are the Stirling numbers of the first kind.

Notice that if $[Y,B]=0$ and $[Y,X]=0$, one gets

$$Y^X B Y^{-X} \equiv e^{X \ln Y} B e^{-X \ln Y} = \sum_{k=0}^{\infty} \frac{1}{k!} (\ln Y)^k \mathrm{ad}_X^k B. \tag{3.25}$$

Another useful combinatorial formula is

$$e^{Ye^E} B e^{-Ye^E} = \sum_{k=0} \frac{\mathrm{ad}_E^k B}{k!} q_k(Ye^E) = \sum_{m=0} \left(\sum_{k=m} \frac{\mathrm{ad}_E^k B}{k!} S(k,m) \right) Y^m e^{mE}, \tag{3.26}$$

whenever E and B commute with Y. Here the sequence

$$q_k(x) = \sum_{m=0}^{k} S(k,m) x^m \tag{3.27}$$

is given by the so-called Bell polynomials and $S(n,k)$ are Stirling numbers of the second kind. It should be also remarked that both families of polynomials, $x^{\underline{k}}$ and $q_k(x)$, belong to the wide class

of so-called convolution polynomials known also as polynomial sequences of binomial type since, e.g.,

$$q_k(x+y)=\sum_{m=0}^{k}\binom{k}{m}q_m(x)x_{k-m}(y). \tag{3.28}$$

Such polynomials are extensively discussed in combinatorial analysis and umbral calculus (see Refs. 23 and 24). Here we have found operator analogs of some fundamental formulas involving polynomial sequences of binomial type. All of the above formulas can be checked by direct calculation in any order of the power expansion, the nonperturbative proof will be presented elsewhere.

Both formulas (3.23) and (3.26) can be adjusted to the particular situation for nonstandard (Jordanian) and extended twists. For example, adapting to the case of Jordanian twist $\mathcal{F}_J=e^{H\otimes\omega}$ with H being a Cartan element: $[H,A]=aA,\omega=\ln(1+E)$, one gets

$$\mathcal{F}_J A\otimes B\mathcal{F}_J^{-1}=\sum_{k=0}^{\infty}H^k\otimes\frac{\mathrm{ad}_E^k B}{k!}e^{-k\omega}(A\otimes e^{a\omega})=\sum_{k=0}^{\infty}H^kA\otimes\frac{\mathrm{ad}_E^k B}{k!}e^{(a-k)\omega}. \tag{3.29}$$

Similarly, the counterpart of (3.29) for extended twist (double exponential) $\mathcal{F}_E=e^{X\otimes Ye^{f(E)}}$ takes the form

$$\begin{aligned}\mathcal{F}_E(A\otimes B)\mathcal{F}_E^{-1}&=\sum_{m=0}^{\infty}\frac{1}{m!}X^m\otimes\mathrm{ad}_{f(E)}^m Bq_m(Ye^{f(E)})\sum_{k=0}^{\infty}\frac{1}{k!}\mathrm{ad}_X^k A\otimes Y^ke^{kf(E)}\\&=\sum_{k,m\geqslant 0}\frac{1}{m!k!}X^m\,\mathrm{ad}_X^k A\otimes\mathrm{ad}_{f(E)}^m B\sum_{i=0}^{m}S(m,i)Y^{k+i}e^{(k+i)f(E)},\end{aligned} \tag{3.30}$$

provided that $[Y,B]=[Y,E]=0$.

In Secs. IV and V, these last formulas shall be particularly useful.

IV. TWIST QUANTIZATIONS OF g_2 GENERATED BY THE $sl(3)$ TWISTS

We start by considering the two twist factors $\mathcal{F}$ corresponding to the classical r matrix (2.18a) with the carrier subalgebras inside the Borel subalgebra of $sl(3)\subset g_2$. This choice will permit us to construct the first two steps of the twist deformation corresponding to the r matrices (2.16a) and (2.16b). Performing such twisting, one can compare deformed Hopf algebras $U_{\mathcal{F}}(g_2)$ with the known deformation $U_{\mathcal{F}}(sl(3))$.[8,12]

A. The first Jordanian twist

The Jordanian twist $\mathcal{F}_J$ can be based on any two-dimensional Borel subalgebra $\mathfrak{b}_+(sl(2))\subset g_2$. In our case this subalgebra is generated by $\{H\equiv h_{2,3},e_{2,3}\}$. The Jordanian r matrix is given by (2.17), and the corresponding twisting element is $\mathcal{F}_J=e^{H\otimes\sigma}$ [see Eq. (3.8)].

The costructure of the deformed algebra $U_J(g_2)$ is obtained by applying the similarity map (3.3a) to the primitive coproducts in $U(g_2)$. In the carrier subalgebra $\mathfrak{b}_+(sl(2))$, we obtain

$$\Delta_J(e_{2,3})=e_{2,3}\otimes e^{\sigma}+1\otimes e_{2,3},\quad\text{or}\quad\Delta_J(\sigma)=\sigma\otimes 1+1\otimes\sigma, \tag{4.1}$$

$$\Delta_J(H)=H\otimes e^{-\sigma}+1\otimes H. \tag{4.2}$$

The generators of the long root sequences $\pm(\alpha_1+k\alpha_2)$ $(k=0,1,2,3)$ have the coproducts

$$\Delta_J(e_{1,k})=e_{1,k}\otimes e^{1/2\sigma}+1\otimes e_{1,k}, \tag{4.3}$$

$$\Delta_J(e_{-1,-k}) = e_{-1,-k} \otimes e^{-1/2\sigma} + 1 \otimes e_{-1,-k} + (-1)^k H \otimes e_{1,(3-k)} e^{-\sigma}, \tag{4.4}$$

describing one- and two-dimensional subrepresentations of the Borel subalgebra $\mathfrak{b}_+(sl(2))$. The generators with the roots "orthogonal" to $2\alpha_1+3\alpha_2$ remain primitive:

$$\Delta_J(h) = h \otimes 1 + 1 \otimes h, \tag{4.5}$$

$$\Delta_J(e_{0,\pm 1}) = e_{0,\pm 1} \otimes 1 + 1 \otimes e_{0,\pm 1}. \tag{4.6}$$

and describe two-dimensional subrepresentations of $\mathfrak{b}_+(sl(2))$. One can check that in $\mathfrak{g}^{\#} \backslash \mathfrak{b}_+(sl(2))$, the generator H induces a shift $\mathrm{ad}_H : e_{1,(3-k)} \to e_{-1,-k}$, and this is exactly what indicates the last terms of the above coproducts $\Delta_J(e_{-1,-k})$.

The coproduct for the lowest root generator $e_{-2,-3}$,

$$\Delta_J(e_{-2,-3}) = e_{-2,-3} \otimes e^{-\sigma} + 1 \otimes e_{-2,-3} + (H - H^2) \otimes (e^{-\sigma} - e^{-2\sigma}) + 2H \otimes H e^{-\sigma}, \tag{4.7}$$

also refers to a one-dimensional subrepresentation. This can be seen when we pass to the $\mathfrak{g}^{\#}$ basis. The following generator should be redefined here:

$$\widetilde{e_{-2,-3}} := e_{-2,-3} - H^2. \tag{4.8}$$

The coproduct $\Delta_J(\widetilde{e_{-2,-3}})$ is quasiprimitive and similar to $\Delta_J(H)$:

$$\Delta_J(\widetilde{e_{-2,-3}}) = \widetilde{e_{-2,-3}} \otimes e^{-\sigma} + 1 \otimes \widetilde{e_{-2,-3}}. \tag{4.9}$$

For the case of twisted $U_J(sl(2))$ the nonlinear transformation (4.8) was first indicated in Ref. 22.

B. The first extended Jordanian twist

The peculiarity of the chain twist deformation is that the deformed algebra can be twisted further by other twisting factors. The quantization goes step by step and on each level you get the deformed symmetry with its specific properties.

For the carrier $\mathfrak{g}^c \subset sl(3) \subset g_2$, the extension factor should be

$$\mathcal{F}_{E_+} = e^{e_{1,3} \otimes e_{1,0} e^{-(1/2)\sigma}}. \tag{4.10}$$

We remind the reader that $sl(3)$ subalgebra is generated by the following eight elements: $\{H, h, e_{\pm 2,\pm 3}, e_{\pm 1,0}, e_{\pm 1,\pm 3}\}$.

The twist (4.10) is a solution of the twist equations (3.1) and (3.2) for $U_J(g_2)$ and the adjoint operator $\exp(\mathrm{ad}(e_{1,3} \otimes e_{1,0} e^{-(1/2)\sigma}))$ applied to the coproducts in $U_J(g_2)$ will perform the deformation $\mathcal{F}_{E_+} : U_J(g_2) \to U_{E_+J}(g_2)$. The same result can be obtained directly by applying the twist $\mathcal{F}_{E_+J} = (\mathcal{F}_{E_+} \mathcal{F}_J) : U(g_2) \to U_{E_+J}(g_2)$.

In the costructure of $U_{E_+J}(g_2)$, we see the group multiplication of the solvable four-dimensional Lie group (see Ref. 12) with the Lie algebra equivalent to the carrier subalgebra $\mathfrak{g}^c_{E_+J}$ of the twist $\mathcal{F}_{E_+J}$:

$$\Delta_{E_+J}(e_{2,3}) = e_{2,3} \otimes e^{\sigma} + 1 \otimes e_{2,3},$$

$$\Delta_{E_+J}(H) = H \otimes e^{-\sigma} + 1 \otimes H - e_{1,3} \otimes e_{1,0} e^{-(3/2)\sigma},$$

$$\Delta_{E_+J}(e_{1,0}) = e_{1,0} \otimes e^{(1/2)\sigma} + e^{\sigma} \otimes e_{1,0},$$

$$\Delta_{E_+J}(e_{1,3}) = e_{1,3} \otimes e^{-(1/2)\sigma} + 1 \otimes e_{1,3}. \tag{4.11}$$

The other generators of the subalgebra $sl(3)$ form the four-dimensional representation of $\mathcal{L}$:

$$\Delta_{E_+J}(h) = h \otimes 1 + 1 \otimes h,$$

$$\Delta_{E_+J}(e_{-1,-3}) = e_{-1,-3} \otimes e^{-(1/2)\sigma} + 1 \otimes e_{-1,-3} + h \otimes e_{1,0}e^{-\sigma},$$

$$\begin{aligned}\Delta_{E_+J}(e_{-1,0}) = {} & + e_{-1,0} \otimes e^{-(1/2)\sigma} + 1 \otimes e_{-1,0} + H \otimes e_{1,3}e^{-\sigma} - e_{1,3} \otimes e_{1,0}e_{1,3}e^{-(3/2)\sigma} \\ & + e_{1,3} \otimes (H-h)e^{-(1/2)\sigma} - (e_{1,3})^2 \otimes e_{1,0}e^{-2\sigma} - He_{1,3} \otimes (e^{\sigma}-1)e^{-(3/2)\sigma},\end{aligned}$$

$$\begin{aligned}\Delta_{E_+J}(\widetilde{e_{-2,-3}}) = {} & + \widetilde{e_{-2,-3}} \otimes e^{-\sigma} + 1 \otimes \widetilde{e_{-2,-3}} - e_{-1,0} \otimes e_{1,0}e^{-(3/2)\sigma} \\ & + He_{1,3} \otimes e_{1,0}e^{-(3/2)\sigma} + e_{1,3} \otimes e_{-1,-3}e^{-(1/2)\sigma}.\end{aligned} \tag{4.12}$$

Finally on the remaining six-dimensional space we also observed the adjoint action of the carrier subalgebra $\mathfrak{g}^c_{E_+J}$ $(k=1,2)$,

$$\Delta_{E_+J}(e_{1,k}) = e_{1,k} \otimes e^{(1/2)\sigma} + 1 \otimes e_{1,k},$$

$$\Delta_{E_+J}(e_{0,\pm 1}) = e_{0,\pm 1} \otimes 1 + 1 \otimes e_{0,\pm 1} + e_{1,(5+1)/2} \otimes e_{1,(1\pm 1)/2}e^{-(1/2)\sigma},$$

$$\begin{aligned}\Delta_{E_+J}(e_{-1,-k}) = {} & e_{-1,-k} \otimes e^{-(1/2)\sigma} + 1 \otimes e_{-1,-k} + (-1)^k H \otimes e_{1,(3-k)}e^{-\sigma} - e_{(2-k),(5-2k)} \otimes e_{(k-1),(k-2)}e^{-\sigma} \\ & - e_{1,3} \otimes e_{1,0}e_{1,(3-k)}e^{-(3/2)\sigma}.\end{aligned} \tag{4.13}$$

First of all, notice that $sl(3)$ generates the well-known twisted algebra $U_{EJ}(sl(3))$ (8) which here is a Hopf subalgebra $U_{EJ}(sl(3)) \subset U_{E_+J}(g_2)$. Thus, we obtain the intermediate $U_{\mathcal{F}}(sl(3))$ twist quantization inside $U_{\mathcal{F}}(f_2)$.

The nonprimitive terms in $\Delta_{E_+J}(e_{0,\pm 1})$ are in agreement with the structure of $\mathfrak{g}^{\#}$. They describe the action of the dual carrier group $G^{\#}_c$ in the two-dimensional indecomposable representations. The third term in $\Delta_{E_+J}(H)$ [see Eq. (4.11)] is just due to the Heisenberg subgroup in G^*_c.

The essential nonlinearities in the costructure are present in the last terms in $\Delta_{E_+J}(e_{-1,-k})$ as well as in $\Delta_{E_+J}(\widetilde{e_{-2,-3}})$ and $\Delta_{E_+J}(e_{-1,0})$. It should be noticed that the generator $\widetilde{e_{-2,-3}} = e_{-2,-3} - H^2$ is not modified. This is a common property of all the generators with roots opposite the Jordanian carrier.

Let us return to the nontrivial terms in the costructure Δ_{E_+J}. Comparing $\Delta_{E_+J}(e_{-1,0})$, $\Delta_{E_+J}(e_{-1,-k})$ and $\Delta_{E_+J}(e_{0,\pm 1})$ with the canonical multiplication in $U(\mathfrak{g}^{\#})$, we find the following $\mathfrak{g}^{\#}$ basis:

$$\widetilde{e_{-1,0}} = e_{-1,0} - He_{1,3},$$

$$\widetilde{e_{0,-1}} = e_{0,-1} - e_{1,0}e_{1,2}e^{-\sigma},$$

$$\widetilde{e_{0,1}} = e_{0,1} - e_{1,3}e_{1,1},$$

$$\widetilde{e_{-1,-2}} = e_{-1,-2} - He_{1,1}. \tag{4.14}$$

In these terms the action of G^c on the six-dimensional space becomes transparent:

$$\Delta_{E_+J}(\widetilde{e_{0,1}}) = \widetilde{e_{0,1}} \otimes 1 + 1 \otimes \widetilde{e_{0,1}} - e_{1,1} \otimes e_{1,3}e^{(1/2)\sigma},$$

$$\Delta_{E_+J}(\widetilde{e_{0,-1}}) = \widetilde{e_{0,-1}} \otimes 1 + 1 \otimes \widetilde{e_{0,-1}} - e_{1,0}e^{-\sigma} \otimes e_{1,2}e^{-(1/2)\sigma},$$

$$\Delta_{E_+J}(e_{-1,-1}) = e_{-1,-1} \otimes e^{-(1/2)\sigma} + 1 \otimes e_{-1,-1} - H \otimes e_{1,2}e^{-\sigma} - e_{1,3} \otimes \widetilde{e_{0,-1}}e^{-(1/2)\sigma},$$

$$\Delta_{E_+J}(\widetilde{e_{-1,-2}}) = \widetilde{e_{-1,-2}} \otimes e^{-(1/2)\sigma} + 1 \otimes \widetilde{e_{-1,-2}} - e_{1,1} \otimes He^{(1/2)\sigma} - \widetilde{e_{0,1}} \otimes e_{1,0}e^{-\sigma},$$

$$\Delta_{E_+J}(\widetilde{e_{-1,0}}) = \widetilde{e_{-1,0}} \otimes e^{-(1/2)\sigma} + 1 \otimes \widetilde{e_{-1,0}} - e_{1,3} \otimes he^{-(1/2)\sigma},$$

$$\Delta_{E_+J}(\widetilde{e_{-2,-3}}) = \widetilde{e_{-2,-3}} \otimes e^{-\sigma} + 1 \otimes \widetilde{e_{-2,-3}} - \widetilde{e_{-1,0}} \otimes e_{1,0}e^{-(3/2)\sigma} + e_{1,3} \otimes e_{-1,-3}e^{-(1/2)\sigma}. \quad (4.15)$$

V. TWIST DEFORMATIONS SPECIFIC TO g_2

A. The full extended twist

The Jordanian twist $\mathcal{F}_J$ (4.1) can be enlarged by the second extension factor $\mathcal{F}_{E_-}$. Such an extension is the special property of the g_2 root system. It does not exist for any other rank 2 simple Lie algebra. The following element is the solution of the twist equations for the Hopf algebra $U_{E_+J}(g_2)$:

$$\mathcal{F}_{E_-} = e^{-e_{1,2}\otimes e_{1,1}e^{-(1/2)\sigma}}. \quad (5.1)$$

Together with the previously studied twist $\mathcal{F}_{E_+J}$ we obtain the full extended twist,

$$\mathcal{F}_{EJ} = e^{-e_{1,2}\otimes e_{1,1}e^{-(1/2)\sigma}}e^{e_{1,3}\otimes e_{1,0}e^{-(1/2)\sigma}}e^{H\otimes\sigma}. \quad (5.2)$$

The carrier subalgebra $\mathfrak{g}^c_{EJ} \approx \mathfrak{g}^{c\#}_{EJ}$ is six-dimensional, it contains two Heisenberg subalgebras with common central element $e_{2,3}$ and the Cartan generator H. Applying the twist (5.2) to $U(g_2)$ or the second extension (5.1) to the Hopf algebra $U_{E_+J}(g_2)$ (constructed in the previous section) we obtain the new deformed costructure $\Delta_{E_{-+}J}$. The coproducts $\Delta_{EJ} := \Delta_{E_{-+}J}$ for the generators of $\mathfrak{g}^c_{EJ}$ describe the group multiplication in $G^{c\#}_{EJ}$, which is defined by the following relations:

$$\Delta_{EJ}(e_{2,3}) = e_{2,3} \otimes e^{\sigma} + 1 \otimes e_{2,3},$$

$$\Delta_{EJ}(H) = H \otimes e^{-\sigma} + 1 \otimes H - e_{1,3} \otimes e_{1,0}e^{-(3/2)\sigma} + e_{1,2} \otimes e_{1,1}e^{-(3/2)\sigma}. \quad (5.3)$$

$$\Delta_{EJ}(e_{1,l}) = e_{1,l} \otimes e^{(1/2)\sigma} + e^{\sigma} \otimes e_{1,l}, \quad l = 0,1.$$

$$\Delta_{EJ}(e_{1,2+l}) = e_{1,2+l} \otimes e^{-(1/2)\sigma} + 1 \otimes e_{1,2+l}, \quad (5.4)$$

These six coproducts are typical for the extended Jordanian twists:[8] each extension adds a summand in $\Delta_{E_{-+}J}(H)$, the constituent roots generators remain quasiprimitive, and the generator σ deformed by the extension factors.

On the plane "orthogonal" to the initial root $\lambda_0 = 2\alpha + 3\beta$, we find only one primitive generator,

$$\Delta_{EJ}(h) = h \otimes 1 + 1 \otimes h. \quad (5.5)$$

Other two coproducts are deformed:

$$\Delta_{E_{-+}J}(e_{0,1}) = e_{0,1} \otimes 1 + 1 \otimes e_{0,1} - e_{1,2} \otimes e_{1,2}e^{-(1/2)\sigma} + \frac{1}{2}(e_{1,2})^2 \otimes (1 - e^{-\sigma}),$$

$$\Delta_{E_{-+}J}(e_{0,-1}) = e_{0,-1}\otimes 1 + 1\otimes e_{0,-1} - \frac{4}{3}e_{1,1}\otimes e_{1,1}e^{-(1/2)\sigma} - \frac{2}{3}(e^{\sigma}-1)\otimes (e_{1,1})^2 e^{-\sigma}. \tag{5.6}$$

The generators in the negative sector have quite complicated coproducts in $U_{EJ}(g_2)$. For example,

$$\begin{aligned}\Delta_{EJ}(\widetilde{e_{-2,-3}}) = {} & \widetilde{e_{-2,-3}}\otimes e^{-\sigma} + 1\otimes \widetilde{e_{-2,-3}} - (e_{-1,0} - He_{1,3})\otimes e_{1,0}e^{-(3/2)\sigma} + e_{1,3}\otimes e_{-1,-3}e^{-(1/2)\sigma} \\ & - \left(e_{-1,-1} - \frac{1}{4}e_{1,2} + He_{1,2}\right)\otimes e_{1,1}e^{-(3/2)\sigma} - \left(\frac{2}{3}e_{0,1} + \frac{1}{4}(e_{1,2})^2\right)\otimes (e_{1,1})^2 e^{-2\sigma} \\ & + e_{1,2}\otimes \left(e_{-1,-2} - \frac{1}{4}e_{1,1}e^{-\sigma}\right)e^{-(1/2)\sigma} + \frac{1}{2}(e_{1,2})^2\otimes \left(\frac{1}{2}(e_{1,1})^2 e^{-\sigma} + e_{0,-1}\right)e^{-\sigma} \\ & + \frac{2}{9}e_{1,3}\otimes (e_{1,1})^3 e^{-(5/2)\sigma} - \frac{1}{6}(e_{1,2})^3\otimes e_{1,0}e^{-(3/2)\sigma}. \end{aligned}\tag{5.7}$$

Notice that in this expression we use the generators $\widetilde{e_{-2,-3}}$, i.e., we suppose that $\widetilde{e_{-2,-3}}$ will be appropriate for the deformed costructure, not only in $U_{E_{+}J}(g_2)$ but also in $U_{EJ}(g_2)$.

The coproducts for the elements $\{h, e_{0,\pm 1}, e_{-1,-k}, e_{-2,-3}; k=0,\ldots,3\}$ describe the action of the carrier group $G^{c\#}_{EJ}$ in the eight-dimensional subrepresentation.

To make this adjoint action transparent, we perform the coordinate transformation $\mathfrak{g}\Rightarrow\mathfrak{g}^{\#}$ (see Sec. III C). According to the algorithm presented in Ref. 12, the new basic elements are introduced:

$$\widetilde{\widetilde{e_{0,1}}} = e_{0,1} + \frac{1}{2}(e_{1,2})^2,$$

$$\widetilde{\widetilde{e_{0,-1}}} = e_{0,-1} + \frac{2}{3}(e_{1,1})^2 e^{-\sigma},$$

$$\widetilde{\widetilde{e_{-1,-3}}} = e_{-1,-3} + \frac{2}{9}(e_{1,1})^3 e^{-2\sigma},$$

$$\widetilde{\widetilde{e_{-1,-2}}} = e_{-1,-2},$$

$$\widetilde{\widetilde{e_{-1,-1}}} = e_{-1,-1} + He_{1,2},$$

$$\widetilde{\widetilde{e_{-1,0}}} = e_{-1,0} - He_{1,3} + \frac{1}{6}(e_{1,2})^3,$$

$$\widetilde{\widetilde{e_{-2,-3}}} = \widetilde{e_{-2,-3}}. \tag{5.8}$$

We see that the element $e_{-1,-2}$ belongs to the $\mathfrak{g}^{\#}$ basis for the group $G^{\#}_{EJ}$ while the generator $\widetilde{e_{-2,-3}}$ remains unchanged, however, we recall that on the previous step of quantization [in $U_{E_{+}J}(g_2)$] it was nontrivially deformed. The coproducts of generators (5.8) are the following:

$$\Delta_{EJ}(\widetilde{\widetilde{e_{0,1}}}) = \widetilde{\widetilde{e_{0,1}}}\otimes 1 + 1\otimes \widetilde{\widetilde{e_{0,1}}},$$

$$\Delta_{EJ}(\widetilde{\widetilde{e_{0,-1}}}) = \widetilde{\widetilde{e_{0,-1}}}\otimes 1 + 1\otimes \widetilde{\widetilde{e_{0,-1}}},$$

$$\Delta_{EJ}(h) = h \otimes 1 + 1 \otimes h$$

$$\Delta_{EJ}(\widetilde{\widetilde{e_{-1,-3}}}) = (\widetilde{\widetilde{e_{-1,-3}}}) \otimes e^{-(1/2)\sigma} + 1 \otimes (\widetilde{\widetilde{e_{-1,-3}}}) + 3h_{0,1} \otimes e_{1,0}e^{-\sigma} + \widetilde{\widetilde{e_{0,-1}}} \otimes e_{1,1}e^{-\sigma},$$

$$\Delta_{EJ}(e_{-1,-2}) = e_{-1,-2} \otimes e^{-(1/2)\sigma} + 1 \otimes e_{-1,-2} - h_{0,1} \otimes e_{1,1}e^{-\sigma} - \widetilde{\widetilde{e_{0,1}}} \otimes e_{1,0}e^{-\sigma} + e_{1,2} \otimes \widetilde{\widetilde{e_{0,-1}}}e^{-(1/2)\sigma},$$

$$\Delta_{EJ}(\widetilde{\widetilde{e_{-1,-1}}}) = \widetilde{\widetilde{e_{-1,-1}}} \otimes e^{-(1/2)\sigma} + 1 \otimes \widetilde{\widetilde{e_{-1,-1}}} + e_{1,2} \otimes h_{0,1}e^{-(1/2)\sigma} - e_{1,3} \otimes (\widetilde{\widetilde{e_{0,-1}}})e^{-(1/2)\sigma} + \frac{4}{3}(\widetilde{\widetilde{e_{0,1}}}) \otimes e_{1,1}e^{-\sigma},$$

$$\Delta_{EJ}(\widetilde{\widetilde{e_{-1,0}}}) = \widetilde{\widetilde{e_{-1,0}}} \otimes e^{-(1/2)\sigma} + 1 \otimes \widetilde{\widetilde{e_{-1,0}}} - e_{1,3} \otimes 3h_{0,1}e^{-(1/2)\sigma} + e_{1,2} \otimes \widetilde{\widetilde{e_{0,1}}}e^{-(1/2)\sigma},$$

$$\Delta_{EJ}(\widetilde{\widetilde{e_{-2,-3}}}) = \widetilde{\widetilde{e_{-2,-3}}} \otimes e^{-\sigma} + 1 \otimes \widetilde{\widetilde{e_{-2,-3}}} - \widetilde{\widetilde{e_{-1,0}}} \otimes e_{1,0}e^{-(3/2)\sigma} + e_{1,3} \otimes \widetilde{\widetilde{e_{-1,-3}}}e^{-(1/2)\sigma} - \widetilde{\widetilde{e_{-1,-1}}} \otimes e_{1,1}e^{-(3/2)\sigma} - \frac{2}{3}\widetilde{\widetilde{e_{0,1}}} \otimes (e_{1,1})^2e^{-2\sigma} + e_{1,2} \otimes e_{-1,-2}e^{-(1/2)\sigma} + \frac{1}{2}(e_{1,2})^2 \otimes \widetilde{\widetilde{e_{0,-1}}}e^{-\sigma}. \tag{5.9}$$

These coproducts correspond to the adjoint action of the algebra $G_{EJ}^{c\#}$ on the eight-dimensional space $G_2 \backslash \mathfrak{g}_{EJ}^c$. One can notice two subrepresentations on the subspaces spanned by $\{\widetilde{\widetilde{e_{0,\pm 1}}}, h\}$ and $\{\widetilde{\widetilde{e_{-1,-k}}}, \widetilde{\widetilde{e_{-2,-3}}}\}$. On the subspace with the generators $\{\widetilde{\widetilde{e_{0,\pm 1}}}, h\}$, we have the trivial factor representation. This property means that on the plane orthogonal to the initial root we have the $sl(2)$ subalgebra with primitive generators $\{\widetilde{\widetilde{e_{0,\pm 1}}}, h\}$. Such an effect was first described in Ref. 9.

In the deformation $U(g_2) \to U_{EJ}(g_2)$ the costructure (5.3) and (5.4) on the carrier subalgebra is the extended Jordanian twist with two extension factors [as can be seen, for example, in $U_{EJ}(sl(4))$]. The specific properties of g_2 become important in the negative sector [relations (5.9)], where the pecularities of the root system induce additional terms. For example, the coproducts $\Delta_{EJ}(\widetilde{\widetilde{e_{-1,-1}}})$ and $\Delta_{EJ}(\widetilde{\widetilde{e_{-1,-2}}})$ contain the last two terms depending on the generators $\widetilde{\widetilde{e_{0,1}}}$ and $\widetilde{\widetilde{e_{0,-1}}}$.

Comparing the generators $\tilde{\tilde{e}}_{k,l}$ in (5.8) with $\tilde{e}_{k,l}$ [see (4.9) and (4.15)] one can see that most of them have different expressions in terms of the initial $\mathfrak{g}$ basis. The reason is that the twisting (5.2) not only deforms the group $G_{E_+J}^{\#}$ but also changes its realization in terms of the initial g_2 generators.

B. The full chain of twists for G_2: Adding the second Jordanian twist

The existence of the subalgebra $U(sl(2)) \subset U_{EJ}(g_2)$ with primitive generators $\{\widetilde{\widetilde{e_{0,\pm 1}}}, h\}$ shows that the Hopf algebra $U_{EJ}(g_2)$ can be additionally deformed by the second Jordanian twist. In other words, the twist equations (3.1) and (3.2) with $\Delta^{(0)}$ replaced by Δ_{EJ} have the solution $\mathcal{F}_{J'} = e^{h \otimes \omega}$, where ω is given by (3.17), i.e., one can perform the transformation $\mathcal{F}_{J'}: U_{EJ}(g_2) \to U_{J'EJ}(g_2) := U_C(g_2)$. The same result can be achieved by the chain of twists (3.18):

$$\mathcal{F}_C = \mathcal{F}_{J'EJ} = e^{h \otimes \omega}e^{-e_{1,2} \otimes e_{1,1}e^{-(1/2)\sigma}}e^{e_{1,3} \otimes e_{1,0}e^{-(1/2)\sigma}}e^{H \otimes \sigma}, \tag{5.10}$$

applied to the initial $U(g_2)$.

The carrier subalgebra $\mathfrak{g}_C^c$ is the Borel subalgebra $\mathfrak{b}^+(g_2)$. Applying the twist (5.10) to $U(g_2)$, we obtain the deformed costructure $\Delta_{J'EJ} := \Delta_C$ corresponding to the maximal carrier subalgebra in g_2. In the Hopf algebra $U_C(g_2)$ we have two σ-like generators,

$$\Delta_C(\sigma) = \sigma \otimes 1 + 1 \otimes \sigma,$$

$$\Delta_C(\omega) = \omega \otimes 1 + 1 \otimes \omega, \tag{5.11}$$

and the ordinary form of the coproduct for the Cartan generator of $\mathfrak{b}\ sl(2)$ twisted by $\mathcal{F}_{J'} = e^{h\otimes\omega}$:

$$\Delta_C(h) = h \otimes e^{-\omega} + 1 \otimes h.$$

In the coproducts for the elements corresponding to the positive long sequence $\alpha_1 + k\alpha_2$ ($k = 0,1,2,3$), one can trace the adjoint action of the algebra $\mathfrak{g}_C^{\#}$:

$$\Delta_C(e_{1,3}) = e_{1,3} \otimes e^{-(1/2)\sigma+(3/2)\omega} + 1 \otimes e_{1,3},$$

$$\Delta_C(e_{1,2}) = e_{1,2} \otimes e^{-(1/2)\sigma+(1/2)\omega} + 1 \otimes e_{1,2} - h \otimes e_{1,3}e^{-\omega},$$

$$\Delta_C(e_{1,1}) = e_{1,1} \otimes e^{(1/2)\sigma-(1/2)\omega} + e^{\sigma} \otimes e_{1,1} - he^{\sigma} \otimes \left(e_{1,2}e^{-\omega} + \frac{1}{2}e_{1,3}e^{-2\omega}\right) + \frac{1}{2}h^2e^{\sigma} \otimes e_{1,3}e^{-2\omega}, \tag{5.12}$$

$$\Delta_C(e_{1,0}) = e_{1,0} \otimes e^{(1/2)\sigma(3/2)\omega} + e^{\sigma} \otimes e_{1,0} - he^{\sigma} \otimes \left(e_{1,1}e^{-\omega} + \frac{1}{12}e_{1,3}e^{-3\omega} + \frac{1}{2}e_{1,2}e^{-2\omega}\right)$$
$$+ \frac{1}{2}h^2e^{\sigma} \otimes (e_{1,2}e^{-2\omega} + e_{1,3}e^{-3\omega}) - \frac{1}{6}h^3e^{\sigma} \otimes e_{1,3}e^{-3\omega}. \tag{5.13}$$

The terms corresponding to the powers of ad (X_h) of the short root operator dual to h (such as $-\frac{1}{6}h^3e^{\sigma}\otimes e_{1,3}e^{-3w}$ in the last row) are accompanied by the additional summands that will disappear when we pass (via the second classical limit) to the group costructure for $G_C^{\#}$. This is especially evident when $\Delta_C(H)$ is considered:

$$\Delta_C(H) = e^{\mathrm{ad}\ h\otimes\omega}\begin{pmatrix} H \otimes e^{-\sigma} + 1 \otimes H \\ -e_{1,3} \otimes e_{1,0}e^{-(3/2)\sigma} + e_{1,2} \otimes e_{1,1}e^{-(3/2)\sigma} \end{pmatrix}$$
$$= H \otimes e^{-\sigma} + 1 \otimes H + h \otimes \left(-\frac{1}{2}(e_{1,2})^2e^{-\omega} - \frac{1}{2}e_{1,2}e_{1,3}e^{-2\omega} - \frac{1}{3}(e_{1,3})^2e^{-3\omega}\right)$$
$$+ \frac{1}{2}h^2 \otimes (e_{1,3}e_{1,2}e^{-2\omega} + (e_{1,3})^2e^{-3\omega}) + \frac{1}{6}h^3 \otimes (-(e_{1,3})^2e^{-3\omega}) - e_{1,3} \otimes e_{1,0}e^{-(3/2)(\sigma-\omega)}$$
$$- he_{1,3} \otimes \left(-e_{1,1}e^{-(5/2)\sigma+(3/2)\omega} - \frac{1}{12}e_{1,3}e^{-(9/2)\sigma+(3/2)\omega} - \frac{1}{2}e_{1,2}e^{-(7/2)\sigma+(3/2)\omega}\right)$$
$$- \frac{1}{2}h^2e_{1,3} \otimes (e_{1,2}e^{-(7/2)\sigma+(3/2)\omega} + e_{1,3}e^{-(9/2)\sigma+(3/2)\omega})$$
$$+ \frac{1}{6}h^3e_{1,3} \otimes e_{1,3}e^{-(9/2)+\sigma(3/2)\omega} + e_{1,2} \otimes e_{1,1}e^{-(3/2)\sigma+(1/2)\omega} - he_{1,2} \otimes e_{1,2}e^{-(3/2)\sigma-(1/2)\omega}$$
$$- \frac{1}{2}he_{1,2} \otimes e_{1,3}e^{-(3/2)\sigma-(3/2)\omega} + \frac{1}{2}h^2e_{1,2} \otimes e_{1,3}e^{-(3/2)\sigma-(3/2)\omega}. \tag{5.14}$$

One can show that in the second classical limit the large number of terms in (5.14) will disappear.

Let us turn now to the determination of the $\mathfrak{g}_C^{\#}$ basis in $U_C(g_2)$.

In the negative root sector $\mathfrak{n}_-$, the element $e_{0,-1}$ must be evidently changed:

$$\widehat{e_{0,-1}} = \widetilde{\widetilde{e_{0,-1}}} - \frac{1}{3}h^2. \tag{5.15}$$

This is due to the fact that on the subspace generated by $\widetilde{\widetilde{e_{0,1}}}$, $\widetilde{\widetilde{e_{0,-1}}}$, and h the twist deformation performed by $\mathcal{F}_{J'}$ is an ordinary Jordanian deformation for the algebra $sl(2)$. The coproduct for $\widehat{e_{0,-1}}$ is quasiprimitive:

$$\Delta_C(\widehat{e_{0,-1}}) = \widehat{e_{0,-1}} \otimes e^{-\omega} + 1 \otimes \widehat{e_{0,-1}}. \tag{5.16}$$

The other coproducts for negative sector generators are quite complicated, despite the fact that they are obtained in the improved (dual group $G^{\#}_{EJ}$) basis $\{\tilde{\tilde{x}}\}$. The factor $\mathcal{F}_{J'}$ changes the dual group,

$$\mathcal{F}_{J'}: G^{\#}_{EJ} \to G^{\#}_{C}, \tag{5.17}$$

and the corresponding Lie algebra generators must be redefined. Using the technique demonstrated in Sec. III D we get the set of new generators:

$$\widehat{e_{0,1}} = \widetilde{\widetilde{e_{0,1}}} = e_{0,1} + \frac{1}{2}(e_{1,2})^2 = e^{\omega} - 1; \tag{5.18a}$$

$$\widehat{e_{0,-1}} = \widetilde{\widetilde{e_{0,-1}}} - \frac{1}{3}h^2 = e_{0,-1} + \frac{2}{3}(e_{1,1})^2 e^{-\sigma} - \frac{1}{3}h^2; \tag{5.18b}$$

$$\widehat{e_{-1,0}} = \widetilde{\widetilde{e_{-1,0}}} + e_{1,2} + he_{1,3} = e_{-1,0} + (h - H)e_{1,3} + \frac{1}{6}(e_{1,2})^3 + e_{1,2}; \tag{5.18c}$$

$$\widehat{e_{-1,-1}} = \widetilde{\widetilde{e_{-1,-1}}} - \frac{4}{3}e_{1,1}e^{-\sigma+\omega} - \frac{1}{3}he_{1,2} + \frac{1}{3}h^2e_{1,3} = e_{-1,-1} + \left(H - \frac{1}{3}h\right)e_{1,2} - \frac{4}{3}e_{1,1}e^{-\sigma+\omega} + \frac{1}{3}h^2e_{1,3}; \tag{5.18d}$$

$$\widehat{e_{-1,-2}} = \widetilde{\widetilde{e_{-1,-2}}} + e_{1,0}e^{-\sigma+\omega} - \frac{1}{3}h^2e_{1,2} = e_{-1,-2} + e_{1,0}e^{-\sigma+\omega} - \frac{1}{3}h^2e_{1,2}; \tag{5.18e}$$

$$\widehat{e_{-1,-3}} = \widetilde{\widetilde{e_{-1,-3}}} = e_{-1,-3} + \frac{2}{9}(e_{1,1})^3 e^{-2\sigma}; \tag{5.18f}$$

$$\widehat{e_{-2,-3}} = \widetilde{\widetilde{e_{-2,-3}}} + \frac{2}{3}(e_{1,1})^2 e^{-2\sigma+\omega} - \frac{1}{6}h^2(e_{1,2})^2 - \frac{2}{3}h = e_{-2,-3} - H^2 + \frac{2}{3}(e_{1,1})^2 e^{-2\sigma+\omega} - \frac{1}{6}h^2(e_{1,2})^2 - \frac{2}{3}h. \tag{5.18g}$$

In the new basis we find fewer nonzero costructure constants. One of the new generators corresponds to the boundary of $\mathfrak{n}_-$ and thus is quasiprimitive,

$$\Delta_C(\widehat{e_{-1,0}}) = \widehat{e_{-1,0}} \otimes e^{-(1/2)\sigma+(3/2)\omega} + 1 \otimes \widehat{e_{-1,0}} \tag{5.19}$$

[notice that the other boundary element is $\widehat{e_{0,-1}}$ with the coproduct (5.16)].

The number of independent terms in the coproducts corresponds to the number of different decompositions of the vector $\beta \in \Sigma_{\mathfrak{n}_-}$ in terms of the $\mathfrak{g}^{c\#}_C$ roots. This explains why in the sequence $e_{-\alpha_1-k\alpha_2}$ $(k=0,1,2,3)$ the number of terms rapidly increases with k:

$$\Delta_C(\widehat{e_{-1,-1}}) = \widehat{e_{-1,-1}} \otimes e^{-(1/2)\sigma+(1/2)\omega} + 1 \otimes \widehat{e_{-1,-1}} + h \otimes (\widehat{e_{-1,0}} + e_{1,3})e^{-\omega} - e_{1,3} \otimes \widehat{e_{0,-1}}e^{-(1/2)\sigma+(3/2)\omega}; \tag{5.20a}$$

$$\begin{aligned}\Delta_C(\widehat{e_{-1,-2}}) = {} & \widehat{e_{-1,-2}} \otimes e^{-(1/2)\sigma-(1/2)\omega} + 1 \otimes \widehat{e_{-1,-2}} + h \otimes \widehat{e_{-1,-1}}e^{-\omega} + \frac{1}{2}h^2 \otimes \widehat{e_{-1,0}}e^{-2\omega} + e_{1,2} \\ & \otimes \widehat{e_{0,-1}}e^{-(1/2)\sigma+(1/2)\omega} - \frac{1}{2}h \otimes \widehat{e_{-1,0}}e^{-2\omega} - \frac{1}{3}h \otimes e_{1,2}e^{-\omega} - \frac{2}{3}(h-h^2) \otimes e_{1,3}e^{-2\omega};\end{aligned} \tag{5.20b}$$

$$\begin{aligned}\Delta_C(\widehat{e_{-1,-3}}) = {} & \widehat{e_{-1,-3}} \otimes e^{-(1/2)\sigma-(3/2)\omega} + 1 \otimes \widehat{e_{-1,-3}} \\ & + h \otimes \begin{pmatrix} \widehat{e_{-1,-2}}e^{-\omega} + \frac{1}{3}\widehat{e_{-1,0}}e^{-3\omega} - \widehat{e_{0,-1}}e_{1,2}e^{-\omega} - \frac{4}{3}e_{1,1}e^{-\sigma-\omega} \\ - \frac{1}{2}\widehat{e_{-1,-1}}e^{-2\omega} - \frac{1}{2}e_{1,2}e^{-2\omega} - \frac{1}{2}\widehat{e_{0,-1}}e_{1,3}e^{-2\omega} + \end{pmatrix} \\ & + h^2 \otimes \begin{pmatrix} \frac{1}{2}\widehat{e_{-1,-1}}e^{-2\omega} + \frac{1}{2}\widehat{e_{0,-1}}e_{1,3}e^{-2\omega} + \\ + \frac{1}{6}e_{1,2}e^{-2\omega} - \frac{1}{3}e_{1,3}e^{-3\omega} - \frac{1}{2}\widehat{e_{-1,0}}e^{-3\omega} \end{pmatrix} + h^3 \otimes \left(\frac{1}{6}\widehat{e_{-1,0}}e^{-3\omega} + \frac{1}{3}e_{1,3}e^{-3\omega}\right) \\ & + h\widehat{e_{0,-1}} \otimes \left(-e_{1,2}e^{-2\omega} - \frac{1}{2}e_{1,3}e^{-3\omega}\right) + \widehat{e_{0,-1}} \otimes e_{1,1}e^{-\sigma-\omega} + \frac{1}{2}h^2\widehat{e_{0,-1}} \otimes e_{1,3}e^{-3\omega}.\end{aligned} \tag{5.20c}$$

In the twisted algebra $U_C(g_2)$ the group multiplication of $G_C^{\#}$ is nontrivially deformed. In particular, the remaining coproduct $\Delta_C(\widehat{e_{-2,-3}})$ is the largest one: it has 23 terms that correspond to the adjoint action of the dual carrier group $G_C^{c\#}$ on the space of its six-dimensional subrepresentation, and the other 28 terms do appear only due to the noncommutativity of the coordinates:

$$\begin{aligned}\Delta_C(\widehat{e_{-2,-3}}) = {} & \widehat{e_{-2,-3}} \otimes e^{-\sigma} + 1 \otimes \widehat{e_{-2,-3}} - \widehat{e_{-1,0}} \otimes e_{1,0}e^{-(3/2)\sigma+(3/2)\omega} - \widehat{e_{-1,-1}} \otimes e_{1,1}e^{-(3/2)\sigma+(1/2)\omega} \\ & + e_{1,2} \otimes \widehat{e_{-1,-2}}e^{-(1/2)\sigma+(1/2)\omega} + e_{1,3} \otimes \widehat{\widehat{e_{-1,-3}}}e^{-(1/2)\sigma+(3/2)\omega} + \frac{1}{2}(e_{1,2})^2 \otimes \widehat{e_{0,-1}}e^{-\sigma+\omega} \\ & + h \otimes \widehat{e_{-1,-1}}e_{1,2}e^{-\omega} - \frac{1}{2}h^2 \otimes \widehat{e_{-1,-1}}e_{1,3}e^{-2\omega} + he_{1,2} \otimes \widehat{e_{-1,-1}}e^{-(1/2)\sigma-(1/2)\omega} + h\widehat{e_{-1,-1}} \\ & \otimes e_{1,2}e^{-(1/2)\sigma-(1/2)\omega} + \frac{1}{2}h^2e_{1,3} \otimes \widehat{e_{-1,-1}}e^{-(1/2)\sigma-(1/2)\omega} - \frac{1}{2}h^2\widehat{e_{-1,-1}} \otimes e_{1,3}e^{-(1/2)\sigma-(3/2)\omega} \\ & + \frac{1}{2}h^2 \otimes \widehat{e_{-1,0}}e_{1,2}e^{-2\omega} + \frac{1}{2}h^2e_{1,3} \otimes \widehat{e_{0,-1}}e_{1,3}e^{-(1/2)\sigma-(1/2)\omega} - \frac{1}{3}h^3 \otimes \widehat{e_{-1,0}}e_{1,3}e^{-3\omega} \\ & + h\widehat{e_{-1,0}} \otimes e_{1,1}e^{-(3/2)\sigma+(1/2)\omega} - \frac{1}{2}h^2\widehat{e_{-1,0}} \otimes e_{1,2}e^{-(1/2)\sigma+(1/2)\omega} + \frac{1}{2}h^2e_{1,2} \\ & \otimes \widehat{e_{-1,0}}e^{-(1/2)\sigma-(3/2)\omega} + \frac{1}{6}h^3e_{1,3} \otimes \widehat{e_{-1,0}}e^{-(1/2)\sigma-(3/2)\omega} + \frac{1}{6}h^3\widehat{e_{-1,0}} \otimes e_{1,3}e^{-(1/2)\sigma-(3/2)\omega} \\ & + he_{1,3} \otimes \widehat{e_{-1,-2}}e^{-(1/2)\sigma+(1/2)\omega} - he_{1,3} \otimes \widehat{e_{0,-1}}e_{1,2}e^{-(1/2)\sigma+(1/2)\omega}\end{aligned}$$

$$
\begin{aligned}
&- h \otimes \left(\begin{array}{c} \frac{4}{3} e_{1,1} e_{1,3} e^{-\sigma-\omega} + \frac{3}{2} e_{1,2} e_{1,3} e^{-2\omega} + \frac{1}{3} (e_{1,2})^2 e^{-\omega} \\ + \frac{4}{3} (e_{1,3})^2 e^{-3\omega} + \frac{1}{2} \widehat{e_{-1,0}} e_{1,2} e^{-2\omega} \\ + \frac{2}{3} \widehat{e_{-1,0}} e_{1,3} e^{-3\omega} - \frac{1}{2} \widehat{e_{-1,-1}} e_{1,3} e^{-2\omega} \end{array} \right) \\
&- h e_{1,2} \otimes \left(\frac{2}{3} e_{1,2} e^{-(1/2)\sigma-(1/2)\omega} + \frac{5}{12} e_{1,3} e^{-(1/2)\sigma-(3/2)\omega} \right) \\
&- h e_{1,3} \otimes \left(\begin{array}{c} \frac{4}{3} e_{1,1} e^{-(3/2)\sigma+(1/2)\omega} + \frac{1}{2} e_{1,2} e^{-(1/2)\sigma-(1/2)\omega} \\ - \frac{1}{3} \widehat{e_{-1,0}} e^{-(1/2)\sigma-(3/2)\omega} + \frac{1}{2} \widehat{e_{0,-1}} e_{1,3} e^{-(1/2)\sigma-(1/2)\omega} \\ + \frac{1}{2} \widehat{e_{-1,-1}} e^{-(1/2)\sigma-(1/2)\omega} \end{array} \right) \\
&+ h^2 \otimes \left(\frac{1}{2} e_{1,2} e_{1,3} e^{-2\omega} + 2 (e_{1,3})^2 e^{-3\omega} + \widehat{e_{-1,0}} e_{1,3} e^{-3\omega} \right) \\
&+ h^2 e_{1,2} \otimes \left(\frac{1}{2} e_{1,3} e^{-(1/2)\sigma-(3/2)\omega} + \frac{1}{2} \widehat{e_{-1,0}} e^{-(1/2)\sigma-(3/2)\omega} \right) \\
&+ h^2 e_{1,3} \otimes \left(\frac{1}{6} e_{1,2} e^{-(1/2)\sigma-(1/2)\omega} - \frac{1}{3} e_{1,3} e^{-(1/2)\sigma-(3/2)\omega} - \frac{1}{2} \widehat{e_{-1,0}} e^{-(1/2)\sigma-(3/2)\omega} \right) \\
&- \frac{1}{2} h^3 \otimes (e_{1,3})^2 e^{-3\omega} + \frac{1}{3} h^3 e_{1,3} \otimes e_{1,3} e^{-(1/2)\sigma-(3/2)\omega} \\
&+ h \widehat{e_{-1,0}} \otimes \left(\frac{1}{3} e_{1,3} e^{-(1/2)\sigma-(3/2)\omega} + \frac{1}{2} e_{1,2} e^{-(1/2)\sigma-(1/2)\omega} \right) \\
&+ \frac{1}{2} h \widehat{e_{-1,-1}} \otimes e_{1,3} e^{-(1/2)\sigma-(3/2)\omega} - \frac{1}{2} h^2 \widehat{e_{-1,0}} \otimes e_{1,3} e^{-(1/2)\sigma-(3/2)\omega}. \qquad (5.21)
\end{aligned}
$$

Comparing these results with those for other simple Lie algebras (deformed by the full chains of twists) we see that contrary, e.g., to the $sl(n)$ case in the twisted algebra $U_C(G_2)$, the dual generator $\widehat{e_{-2,-3}}$ differs considerably from the "Jordanian" $\widehat{\widehat{e_{-2,-3}}} = e_{-2,-3} - H^2$ and as well most of the coproducts in the negative sector are strongly deformed. In this situation the appropriate basis for the presentation of the costructure plays a very essential role. In the initial $\mathfrak{g}$ basis, the decomposition of the coproduct $\Delta_C(e_{-2,-3})$ contains more than 400 terms. Using the $\mathfrak{g}^{\#}_{EJ}$ basis $\{\tilde{\tilde{x}}\}$, we can reduce this number to 109 and, finally, in the $\mathfrak{g}^{\#}_{C}$ basis, we get the expression (5.21) with 51 terms. The effective technique is needed to perform the corresponding calculations and this is where the modified BCH formulas (3.29) and (3.30) presented in Sec. III D are very useful. The expressions (5.20a), (5.20b), (5.20c), and (5.21) were obtained with their help.

The full chain of twists (5.10) can be parametrized as follows:

$$
\mathcal{F}_C = \mathcal{F}_{J'} \mathcal{F}_E \mathcal{F}_J = e^{h \otimes \omega(\xi,\psi)} e^{-\xi e_{1,2} \otimes e_{1,1} e^{-(1/2)\sigma(\xi)}} e^{\xi e_{1,3} \otimes e_{1,0} e^{-(1/2)\sigma(\xi)}} e^{H \otimes \sigma(\xi)}, \qquad (5.22)
$$

with

$$
\sigma(\xi) = \ln(1 + \xi e_{2,3}),
$$

$$\omega(\xi,\psi)=\ln\left(1+\psi e_{0,1}+\frac{1}{2}\xi\psi(e_{1,2})^2\right). \tag{5.23}$$

Thus, the full chain leads to the two-parameter set of Hopf algebras $U_C(G_2;\xi,\psi)$. In particular, this parametrization provides the possibility to study the second classical limit for $U_C(G_2)$. The latter is obtained by scaling the generators $x\to(1/\varepsilon)x$ and by going to the limit $\varepsilon,\xi,\psi\to 0$, with finite values of $\xi/\varepsilon=\zeta$, $\psi/\varepsilon=\eta$. In such a limit we get the composition law of the dual group $G_C^{\#}$:

$$\begin{aligned}\Delta_C^{\#}(H)&=H\otimes e^{-\sigma(\zeta)}+1\otimes H-\zeta e_{1,3}\otimes e_{1,0}e^{-(3/2)(\sigma(\zeta)-\omega(\zeta,\eta))}+\zeta e_{1,2}\otimes e_{1,1}e^{-(3/2)\sigma(\zeta)+(1/2)\omega(\zeta,\eta)}\\&\quad-\frac{1}{2}\zeta\eta h\otimes(e_{1,2})^2e^{-\omega(\zeta,\eta)}-\zeta\eta he_{1,2}\otimes e_{1,2}e^{-(3/2)\sigma(\zeta)-(1/2)\omega(\zeta,\eta)}\\&\quad+\zeta\eta he_{1,3}\otimes e_{1,1}e^{-(5/2)\sigma(\zeta)+(3/2)\omega(\zeta,\eta)}+\frac{1}{2}\zeta\eta^2h^2e_{1,2}\otimes e_{1,3}e^{-(3/2)\sigma(\zeta)-(3/2)\omega(\zeta,\eta)}\\&\quad+\frac{1}{2}\zeta\eta^2h^2\otimes e_{1,3}e_{1,2}e^{-2\omega(\zeta,\eta)}-\frac{1}{2}\zeta\eta^2h^2e_{1,3}\otimes e_{1,2}e^{-(7/2)\sigma(\zeta)+(3/2)\omega(\zeta,\eta)}\\&\quad-\frac{1}{6}\zeta\eta^3h^3\otimes(e_{1,3})^2e^{-3\omega(\zeta,\eta)}+\frac{1}{6}\zeta\eta^3h^3e_{1,3}\otimes e_{1,3}e^{-(9/2)\sigma(\zeta)(3/2)\omega(\zeta,\eta)},\end{aligned} \tag{5.24a}$$

$$\Delta_C^{\#}(h)=h\otimes e^{-\omega(\zeta,\eta)}+1\otimes h, \tag{5.24b}$$

$$\begin{aligned}\Delta_C^{\#}(e_{1,0})&=e_{1,0}\otimes e^{-(1/2)\sigma(\zeta)-(3/2)\omega(\zeta,\eta)}+e^{\sigma(\zeta)}\otimes e_{1,0}-\eta he^{\sigma(\zeta)}\otimes e_{1,1}e^{-\omega(\zeta,\eta)}\\&\quad+\frac{1}{2}\eta^2h^2e^{\sigma(\zeta)}\otimes e_{1,2}e^{\sigma(\zeta)-2\omega(\zeta,\eta)}-\frac{1}{6}\eta^3h^3e^{\sigma(\zeta)}\otimes e_{1,3}e^{\sigma(\zeta)-3\omega(\zeta,\eta)},\end{aligned} \tag{5.24c}$$

$$\begin{aligned}\Delta_C^{\#}(e_{1,1})&=e_{1,1}\otimes e^{(1/2)\sigma(\zeta)-(1/2)\omega(\zeta,\eta)}+e^{\sigma(\zeta)}\otimes e_{1,1}-\eta he^{\sigma(\zeta)}\otimes e_{1,2}e^{\sigma(\zeta)-\omega(\zeta,\eta)}\\&\quad+\frac{1}{2}\eta^2h^2e^{\sigma(\zeta)}\otimes e_{1,3}e^{\sigma(\zeta)-2\omega(\zeta,\eta)},\end{aligned} \tag{5.24d}$$

$$\Delta_C^{\#}(e_{1,2})=e_{1,2}\otimes e^{-(1/2)\sigma(\zeta)+(1/2)\omega(\zeta,\eta)}+1\otimes e_{1,2}-\eta h\otimes e_{1,3}e^{-\omega(\zeta,\eta)}, \tag{5.24e}$$

$$\Delta_C^{\#}(e_{1,3})=e_{1,3}\otimes e^{-(1/2)\sigma(\zeta)+(3/2)\omega(\zeta,\eta)}+1\otimes e_{1,3}, \tag{5.24f}$$

$$\Delta_C^{\#}(e_{2,3})=e_{2,3}\otimes e^{\sigma(\zeta)}+1\otimes e_{2,3}, \tag{5.24g}$$

$$\Delta_C^{\#}(\omega(\zeta,\eta))=\omega(\zeta,\eta)\otimes 1+1\otimes\omega(\zeta,\eta), \tag{5.24h}$$

$$\Delta_C^{\#}(\widehat{e_{0,-1}})=\widehat{e_{0,-1}}\otimes e^{-\omega(\zeta,\eta)}+1\otimes\widehat{e_{0,-1}}, \tag{5.24i}$$

$$\Delta_C^{\#}(\widehat{e_{-1,0}})=\widehat{e_{-1,0}}\otimes e^{-(1/2)\sigma(\zeta)+(3/2)\omega(\zeta,\eta)}+1\otimes\widehat{e_{-1,0}}, \tag{5.24j}$$

$$\begin{aligned}\Delta_C^{\#}(\widehat{e_{-1,-1}})&=\widehat{e_{-1,-1}}\otimes e^{-(1/2)\sigma(\zeta)+(1/2)\omega(\zeta,\eta)}+1\otimes\widehat{e_{-1,-1}}\\&\quad+\eta h\otimes\widehat{e_{-1,0}}e^{-\omega(\zeta,\eta)}-\zeta e_{1,3}\otimes\widehat{e_{0,-1}}e^{-(1/2)\sigma(\zeta)+(3/2)\omega(\zeta,\eta)},\end{aligned} \tag{5.24k}$$

$$\Delta_C^{\#}(\widehat{e_{-1,-2}}) = \widehat{e_{-1,-2}} \otimes e^{-(1/2)\sigma(\zeta)-(1/2)\omega(\zeta,\eta)} + 1 \otimes \widehat{e_{-1,-2}} + \eta h \otimes \widehat{e_{-1,-1}} e^{-\omega(\zeta,\eta)} + \frac{1}{2}\eta^2 h^2 \otimes \widehat{e_{-1,0}} e^{-2\omega(\zeta,\eta)}$$
$$+ \zeta e_{1,2} \otimes \widehat{e_{0,-1}} e^{-(1/2)\sigma(\zeta)+(1/2)\omega(\zeta,\eta)}, \tag{5.24l}$$

$$\Delta_C^{\#}(\widehat{e_{-1,-3}}) = \widehat{e_{-1,-3}} \otimes e^{-(1/2)\sigma(\zeta)-(3/2)\omega(\zeta,\eta)} + 1 \otimes \widehat{e_{-1,-3}} + h \otimes (\eta \widehat{e_{-1,-2}} e^{-\omega(\zeta,\eta)} - \zeta\eta \widehat{e_{0,-1}} e_{1,2} e^{-\omega(\zeta,\eta)})$$
$$+ h^2 \otimes \left(\frac{1}{2}\eta^2 \widehat{e_{-1,-1}} e^{-2\omega(\zeta,\eta)} + \frac{1}{2}\zeta\eta^2 \widehat{e_{0,-1}} e_{1,3} e^{-2\omega(\zeta,\eta)} \right) + \frac{1}{6}\eta^3 h^3 \otimes \widehat{e_{-1,0}} e^{-3\omega(\zeta,\eta)}$$
$$- \zeta\eta h \widehat{e_{0,-1}} \otimes e_{1,2} e^{-2\omega(\zeta,\eta)} + \zeta \widehat{e_{0,-1}} \otimes e_{1,1} e^{-\sigma(\zeta)-\omega(\zeta,\eta)} + \frac{1}{2}\zeta\eta^2 h^2 \widehat{e_{0,-1}} \otimes e_{1,3} e^{-3\omega(\zeta,\eta)}, \tag{5.24m}$$

$$\Delta_C^{\#}(\widehat{e_{-2,-3}}) = \widehat{e_{-2,-3}} \otimes e^{-\sigma(\zeta)} + 1 \otimes \widehat{e_{-2,-3}} - \zeta \widehat{e_{-1,0}} \otimes e_{1,0} e^{-(3/2)\sigma(\zeta)+(3/2)\omega(\zeta,\eta)}$$
$$+ \zeta e_{1,3} \otimes \widehat{e_{-1,-3}} e^{-(1/2)\sigma(\zeta)+(3/2)\omega(\zeta,\eta)} - \zeta \widehat{e_{-1,-1}} \otimes e_{1,1} e^{-(3/2)\sigma(\zeta)+(1/2)\omega(\zeta,\eta)}$$
$$+ \zeta e_{1,2} \otimes \widehat{e_{-1,-2}} e^{-(1/2)\sigma(\zeta)+(1/2)\omega(\zeta,\eta)} + h \otimes \zeta\eta \widehat{e_{-1,-1}} e_{1,2} e^{-\omega(\zeta,\eta)} - \frac{1}{2}h^2$$
$$\otimes \zeta\eta^2 \widehat{e_{-1,-1}} e_{1,3} e^{-2\omega(\zeta,\eta)} + \zeta\eta h e_{1,2} \otimes \hat{e}_{-1,-1} e^{-(1/2)\sigma(\zeta)-(1/2)\omega(\zeta,\eta)} + \zeta\eta h \widehat{e_{-1,-1}}$$
$$\otimes e_{1,2} e^{-(1/2)\sigma(\zeta)-(1/2)\omega(\zeta,\eta)} + \frac{1}{2}\zeta\eta^2 h^2 e_{1,3} \otimes \widehat{e_{-1,-1}} e^{-(1/2)\sigma(\zeta)-(1/2)\omega(\zeta,\eta)} - \frac{1}{2}\zeta\eta^2 h^2 \widehat{e_{-1,-1}}$$
$$\otimes e_{1,3} e^{-(1/2)\sigma(\zeta)-(3/2)\omega(\zeta,\eta)} + \frac{1}{2}h^2 \otimes \zeta\eta^2 \widehat{e_{-1,0}} e_{1,2} e^{-2\omega(\zeta,\eta)} + \frac{1}{2}\zeta^2\eta^2 h^2 e_{1,3}$$
$$\otimes \widehat{e_{0,-1}} e_{1,3} e^{-(1/2)\sigma(\zeta)-(1/2)\omega(\zeta,\eta)}$$
$$- \frac{1}{3}h^3 \otimes \zeta\eta^3 \widehat{e_{-1,0}} e_{1,3} e^{-3\omega(\zeta,\eta)} + h \widehat{e_{-1,0}} \otimes \zeta\eta e_{1,1} e^{-(3/2)\sigma(\zeta)+(1/2)\omega(\zeta,\eta)}$$
$$- \frac{1}{2}\zeta\eta^2 h^2 \widehat{e_{-1,0}} \otimes e_{1,2} e^{-(1/2)\sigma(\zeta)+(1/2)\omega(\zeta,\eta)} + \frac{1}{2}\zeta\eta^2 h^2 e_{1,2} \otimes \widehat{e_{-1,0}} e^{-(1/2)\sigma(\zeta)-(3/2)\omega(\zeta,\eta)}$$
$$+ \frac{1}{6}\zeta\eta^3 h^3 e_{1,3} \otimes \widehat{e_{-1,0}} e^{-(1/2)\sigma(\zeta)-(3/2)\omega(\zeta,\eta)} + \frac{1}{6}\zeta\eta^3 h^3 \widehat{e_{-1,0}} \otimes e_{1,3} e^{-(1/2)\sigma(\zeta)-(3/2)\omega(\zeta,\eta)}$$
$$+ \zeta\eta h e_{1,3} \otimes \widehat{e_{-1,-2}} e^{-(1/2)\sigma(\zeta)+(1/2)\omega(\zeta,\eta)} - \zeta^2\eta h e_{1,3} \otimes \widehat{e_{0,-1}} e_{1,2} e^{-(1/2)\sigma(\zeta)+(1/2)\omega(\zeta,\eta)}$$
$$+ \frac{1}{2}\zeta^2 (e_{1,2})^2 \otimes \widehat{e_{0,-1}} e^{-\sigma(\zeta)+\omega(\zeta,\eta)}. \tag{5.24n}$$

We have finished the construction of the universal enveloping algebra $U_C(g_2)$ twisted by the full chain of extended twists. The sequence of factors (5.10) cannot be essentially enlarged due to the absence of the Lie-Frobenius subalgebras in g_2 that nontrivially contain $\mathfrak{b}_+(g_2)$ (see the discussion in Sec. II). It is certainly possible to perform the additional Abelian twist $\mathcal{F}_{A'} = e^{\sigma\otimes\omega}$, but in such a case the carrier $\mathfrak{g}_C^{\#}$ is not changed. It appears that adding the twist $\mathcal{F}_{A'}$ leads to the different realization of the same $\mathfrak{g}_C^{\#}$ in terms of the generators of $U_C(g_2)$.

When such a change of the realization of the carrier happens in the intermediate steps of the quantization this can lead to interesting results. We shall study this possibility in the next section.

C. General form of extended twist for g_2: Additional Abelian twist

Let us construct the quantization for the r matrix (2.16b). As it was indicated in Sec. III, this can be performed by the twisting element

$$\mathcal{F}_{AE}(\rho) = e^{\rho h\otimes\sigma} e^{-e_{1,2}\otimes e_{1,1} e^{-(1/2)\sigma}} e^{e_{1,3}\otimes e_{1,0} e^{-(1/2)\sigma}} e^{H\otimes\sigma}. \tag{5.25}$$

Here the parameter ρ is written explicitly because of its specific role. Notice that for any fixed ρ the element $\mathcal{F}_{AE}$ depends on the deformation parameter ξ [due to the ξ-dependence of σ (see Eq. (5.22)]. Studying the parametrized set $\{\mathcal{F}_{AE}(\xi,\rho)\}$ we are dealing with the family of twists indexed by the parameter ρ. We shall demonstrate that, contrary to the case of the deformation parameter ξ where we get equivalent deformed algebras $U_{\mathcal{F}_{AE(\xi,\rho)}} \sim U_{\mathcal{F}_{AE(\xi',\rho)}}$, there are nonzero values of ρ for which the twisted algebras are inequivalent, $U_{\mathcal{F}_{AE(\xi,\rho)}} \not\sim U_{\mathcal{F}_{AE(\xi,\rho')}}$.

In order to construct the twisted Hopf algebra $U_{\mathcal{F}_{AE(\rho)}}(g_2)$, we use the coproducts Δ_{EJ} (5.18)–(5.21) of the full extended twisting (5.3) obtained in Sec. V A and apply the transformation $e^{\rho \mathrm{ad} h\otimes\sigma}$ corresponding to the Abelian twist factor $\mathcal{F}_A = e^{\rho h\otimes\sigma}$. Each nontrivial twisting factor induces the transformation of the dual group and the new dual coordinates are to be constructed. Omitting the intermediate steps we present the results in terms of the new dual $\mathfrak{g}^{\#}_{AE}$ basis:

$$\overline{H} = H + \rho h,$$

$$\overline{e_{-2,-3}} = \widetilde{\widetilde{e_{-2,-3}}} + \rho^2 h^2,$$

$$\overline{e_{-1,0}} = \widetilde{\widetilde{e_{-1,0}}} - \rho h e_{1,3},$$

$$\overline{e_{-1,-1}} = \widetilde{\widetilde{e_{-1,-1}}} + \rho h e_{1,2} \tag{5.26}$$

(the other $\mathfrak{g}^{\#}_{E}$ coordinates $\tilde{\tilde{x}}$ remain unchanged).

According to the properties of the twist $\mathcal{F}_A$ the costructure on its carrier is conserved:

$$\Delta_{AE}(h) = h\otimes 1 + 1\otimes h,$$

$$\Delta_{AE}(e_{2,3}) = e_{2,3}\otimes e^{\sigma} + 1\otimes e_{2,3}. \tag{5.27}$$

The changes in $\Delta_{AE}(\overline{H})$ and in the long sequence $\Delta_{AE}(e_{1,l})$ $(l=0,1,2,3)$ are correlated with the root structure of the extensions:

$$\begin{aligned}\Delta_{AE}(\overline{H}) &= (\overline{H})\otimes e^{-\sigma} + 1\otimes(\overline{H}) - e_{1,3}\otimes e_{1,0} e^{(\rho(\alpha+3\beta)(h)-3/2)\sigma} + e_{1,2}\otimes e_{1,1} e^{(\rho(\alpha+2\beta)(h)-3/2)\sigma} \\ &= (\overline{H})\otimes e^{-\sigma} + 1\otimes(\overline{H}) - e_{1,3}\otimes e_{1,0} e^{(3/2)(\rho-1)\sigma} + e_{1,2}\otimes e_{1,1} e^{(1/2)(\rho-3)\sigma}.\end{aligned}$$

$$\Delta_{AE}(e_{1,k}) = e_{1,0}\otimes e^{(1/2+\rho(\alpha+k\beta)(h))\sigma} + e^{\sigma}\otimes e_{1,0}, \quad k=0,1,$$

$$\Delta_{AE}(e_{1,m}) = e_{1,0}\otimes e^{(-1/2+\rho(\alpha+m\beta)(h))\sigma} + 1\otimes e_{1,0}, \quad m=2,3. \tag{5.28}$$

On the plane orthogonal to the highest root, we find the quasiprimitive costructure:

$$\Delta_{AE}(\widetilde{\widetilde{e_{0,1}}}) = \widetilde{\widetilde{e_{0,1}}}\otimes e^{\rho\sigma} + 1\otimes\widetilde{\widetilde{e_{0,1}}},$$

$$\Delta_{AE}(\widetilde{\widetilde{e_{0,-1}}}) = \widetilde{\widetilde{e_{0,-1}}}\otimes e^{-\rho\sigma} + 1\otimes\widetilde{\widetilde{e_{0,-1}}}. \tag{5.29}$$

In the coproducts for the other basic elements (belonging to $\mathfrak{n}_-$) the additional terms proportional to ρ do appear,

$$\Delta_{AE}(\widetilde{\widetilde{e_{-1,-3}}}) = \widetilde{\widetilde{e_{-1,-3}}} \otimes e^{-(1/2)(1+3\rho)\sigma} + 1 \otimes \widetilde{\widetilde{e_{-1,-3}}} + (1-\rho)h \otimes e_{1,0}e^{-\sigma} + \widetilde{\widetilde{e_{0,-1}}} \otimes e_{1,1}e^{-(1+\rho)\sigma}, \tag{5.30a}$$

$$\Delta_{AE}(e_{-1,-2}) = e_{-1,-2} \otimes e^{-(1/2)(1+\rho)\sigma} + 1 \otimes e_{-1,-2} + \left(\rho - \frac{1}{3}\right)h \otimes e_{1,1}e^{-\sigma} - \widetilde{\widetilde{e_{0,1}}} \otimes e_{1,0}e^{(\rho-1)\sigma} + e_{1,2} \otimes \widetilde{\widetilde{e_{0,-1}}}e^{-(1/2)\sigma(1-\rho)}, \tag{5.30b}$$

$$\Delta_{AE}(\overline{e_{-1,-1}}) = \overline{e_{-1,-1}} \otimes e^{(1/2)(\rho-1)\sigma} + 1 \otimes \overline{e_{-1,-1}} + \left(\frac{1}{3} + \rho\right)e_{1,2} \otimes he^{(1/2)(\rho-1)\sigma} - e_{1,3} \otimes \widetilde{\widetilde{e_{0,-1}}}e^{(1/2)(3\rho-1)\sigma} + \frac{4}{3}\widetilde{\widetilde{e_{0,1}}} \otimes e_{1,1}e^{(\rho-1)\sigma}, \tag{5.30c}$$

$$\Delta_{AE}(\overline{e_{-1,0}}) = \overline{e_{-1,0}} \otimes e^{(1/2)(3\rho-1)\sigma} + 1 \otimes \overline{e_{-1,0}} + e_{1,2} \otimes \widetilde{\widetilde{e_{0,1}}}e^{-(1/2)\sigma(1-\rho)} - (\rho+1)e_{1,3} \otimes he^{(1/2)(3\rho-1)\sigma}, \tag{5.30d}$$

$$\Delta_{AE}(\overline{e_{-2,-3}}) = \overline{e_{-2,-3}} \otimes e^{-\sigma} + 1 \otimes \overline{e_{-2,-3}} + 2\rho h \otimes \overline{H} - \overline{e_{-1,0}} \otimes e_{1,0}e^{(3/2)(\rho-1)\sigma} - \overline{e_{-1,-1}} \otimes e_{1,1}e^{(1/2)(\rho-3)\sigma} + e_{1,2} \otimes e_{-1,-2}e^{(1/2)(\rho-1)\sigma} + e_{1,3} \otimes \widetilde{\widetilde{e_{-1,-3}}}e^{(1/2)(3\rho-1)\sigma} - \frac{2}{3}\widetilde{\widetilde{e_{0,1}}} \otimes (e_{1,1})^2e^{(\rho-2)\sigma} + \frac{1}{2}(e_{1,2})^2 \otimes \widetilde{\widetilde{e_{0,-1}}}e^{(\rho-1)\sigma} + 2\rho he_{1,2} \otimes e_{1,1}e^{(1/2)(\rho-3)\sigma}. \tag{5.30e}$$

In the last expression the additional terms signify that the root vector $\overline{H^*}$ is no longer orthogonal to h^* and the adjoint operator $\mathrm{ad}(\overline{H^*})$ transforms h^* into $\overline{e_{-2,-3}}$.

In comparison with $\Delta_E(\tilde{x})$, the changes of the form of the coproducts Δ_{AE} are small but essential. We immediately see five singular points $\rho = 0, \pm 1, \pm\frac{1}{3}$. In each of them one of the coproducts loses some terms and becomes closer to a quasiprimitive. For example, in the cases $\Delta_{AE_+}(\widetilde{\widetilde{e_{-1,-3}}})$ and $\Delta_{AE_+}(\overline{e_{-1,0}})$ if we use only the $sl(3)$ extension $\mathcal{F}_+ = e^{e_{1,3}\otimes e_{1,0}e^{(-1/2)\sigma}}$ then for $\rho = \pm 1$ these coproducts become quasiprimitive, and we obtain the possibility to perform additional twistings with the carrier algebra nontrivially intersecting with $\mathfrak{n}_-$. In the costructure Δ_{AE} the corresponding enlargement of the carrier cannot be achieved, nevertheless, the singular points are also important. In particular, we see that the standard case Δ_{EJ} corresponds to the singular point $\rho = 0$ while in the general situation the coproduct $\Delta_{AE(\rho)}(\overline{e_{-2,-3}})$ has additional components, and we arrive at different dual algebra $\mathfrak{g}^{\#}_{AE} \neq \mathfrak{g}^{\#}_{E}$. Notice that in all the singular points the corresponding r matrices differ only by the value of the numerical parameter ρ but the results of the quantizations are different and refer to Lie–Poisson structures.

We have already seen that the coproducts $\Delta_{AE}(\widetilde{\widetilde{e_{0,\pm 1}}})$ are now quasiprimitive. Consequently, there still exists the possibility to perform further twisting with the Jordanian factor similar to $\mathcal{F}_{J'}$,

$$\mathcal{F}_{J''} = e^{h\otimes\omega'}, \tag{5.31}$$

with $\omega' = \ln(\widetilde{\widetilde{e_{0,1}}}e^{-\rho\sigma} + e^{-\rho\sigma})$. The twisting element,

$$\mathcal{F}_{J''AE} = e^{h\otimes\omega'} e^{\rho h\otimes\sigma} e^{-e_{1,2}\otimes e_{1,1}e^{-(1/2)\sigma}} e^{e_{1,3}\otimes e_{1,0}e^{-(1/2)\sigma}} e^{H\otimes\sigma}, \tag{5.32}$$

is the solution of the twist equation. Here, contrary to the situation with the full chain of extended twists, we do not obtain a parametrized family of chain deformations. It can be easily checked that [see also Eq. (5.10)]

$$\mathcal{F}_{J''AE} = \mathcal{F}_C = e^{h\otimes\omega} e^{-e_{1,2}\otimes e_{1,1}e^{-(1/2)\sigma}} e^{e_{1,3}\otimes e_{1,0}e^{-(1/2)\sigma}} e^{H\otimes\sigma}. \tag{5.33}$$

The dependence on ρ cancels and we are again with the full chain studied above in Sec. V B. Thus, we have obtained the following result: there is the ρ family of quantum algebras $U_{AE(\rho)}(g_2)$, but the full chain quantization $U_C(g_2)$ is unique.

To complete the analysis of the set of twist deformations for $U(g_2)$, let us consider the generators that can become quasiprimitive (in general, nonsimultaneously) after the action of the full chain of twists $\mathcal{F}_C$. The number q_C^- of such generators is equal to the rank of $\mathfrak{g}$. In our case we have $q_C^-(g_2)=2$, and the corresponding generators are $\widehat{e_{0,-1}}$ and $\widehat{e_{-1,0}}$. Both are quasiprimitive simultaneously but cannot enlarge the space of $\mathfrak{g}_c^C$ up to a (quasi-) Frobenius subalgebra in $U(g_2)$. In the Borel subalgebra $U_C(\mathfrak{b}_+(g_2))$ the number q_C^+ of quasiprimitive generators is equal to the number of simultaneously primitive. For the full chains we have $q_C^+=r$ and in our case (as we have seen above) these primitive generators are σ and ω. This certainly provides the possibility to perform the additional Abelian twist but the corresponding deformation will be equivalent to the redefinition of the Cartan elements in the Jordanian twisting factors.

VI. DISCUSSION AND OUTLOOK

We have described the set $\{U_J, U_{E_+J}, U_{EJ}, U_{J'EJ}, U_{A(\rho)EJ}\}$ of quantized Lie–Poisson structures that were constructed on the space $U(g_2)$ by chains of twist deformations. The dual group coordinates ($\mathfrak{g}^{\#}$ basis) obtained through the second classical limit procedure provide us with the possibility of writing down the explicit form of these Lie–Poisson structures. We have presented in this paper the algebraic and coalgebraic formulas determined by the exceptional Lie algebra g_2, in particular, we get the additional [in comparison with the situation in $U(sl(3))$ and $U(so(5))$] Hopf algebra U_{EJ}; the carrier space for the second Jordanian twist $\mathcal{F}_{J'}$ is deformed [the analogous result was found for $U_{E_+J}(so(5))$ (Refs. 11 and 12)]; the Hopf algebras $\{U_{E_+J}, U_{J'EJ}, U_{AEJ}\}$ in comparison with the analogous quantizations of $U(sl(3))$ and $U(so(5))$ have a more complicated constructure determined by the root system of g_2.

We have also found the peripheric twisted algebras in the set of Hopf algebras $\{U_{A(\rho)EJ}\}$. The number s_C of inequivalent algebras in this set depends on the number l_C^n of extended Jordanian factors in the chain $\mathcal{F}_C$. We conjecture the following relation;

$$s_C = \sum_{i=1}^{l_C^n} (\dim(\mathfrak{g}_c^{(i)}) - 1), \tag{6.1}$$

where $\mathfrak{g}_c^{(i)}$ is the carrier subalgebra of the link $\mathcal{F}^{(i)} \subset \mathcal{F}_C$. This gives three inequivalent subsets for $U_{A(\rho)EJ}(sl(3))$ as well as $U_{A(\rho)EJ}(so(5))$ and five for $U_{A(\rho)EJ}(g_2)$. One of the algebras, $U_{A(0)EJ}(g_2)$, corresponds to the canonical extended twist and four others are the analogs of the peripheric extended deformations[12] in $U_{EJ}(sl(N))$. At the same time we do not have peripheric chains in $U_{\mathcal{F}}(g_2)$. As we have already stressed above, the full chain deformation $U_{\mathcal{F}}(g_2)$ is invariant under the rotation generated by an additional Abelian twist.

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On the continuous spectral component of the Floquet operator for a periodically kicked quantum system

James McCaw[a] and B. H. J. McKellar[b]
School of Physics, Research Centre for High Energy Physics,
The University of Melbourne, Victoria, 3010, Australia

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By a straightforward generalization, we extend the work of Combescure [J. Stat. Phys. **59**, 679 (1990)] from rank-1 to rank-*N* perturbations. The requirement for the Floquet operator to be pure point is established and compared to that in Combescure. The result matches that in McCaw and McKeller [J. Math. Phys. **46**, 032108 (2005)]. The method here is an alternative to that work. We show that if the condition for the Floquet operator to be pure point is relaxed, then in the case of the δ-kicked Harmonic oscillator, a singularly continuous component of the Floquet operator spectrum exists. We also provide an in-depth discussion of the conjecture presented in the work of Combescure of the case where the unperturbed Hamiltonian is more general. We link the physics conjecture directly to a number-theoretic conjecture of Vinogradov [*The Method of Trigonometrical Sums in the Theory of Numbers* (Interscience, London, 1954)] and show that a solution of Vinogradov's conjecture solves the physics conjecture. The result is extended to the rank-*N* case. The relationship between our work and the work of Bourget [J. Math. Anal. Appl. **276**, 28 (2002); **301**, 65 (2005)], on the physics conjecture is discussed. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2035027]

I. INTRODUCTION

The spectral analysis of the Floquet operator (the unitary time-evolution operator over a single kick period) is of great interest for periodically perturbed Hamiltonian systems. There are general arguments[1–5] which indicate that an understanding or classification of the spectrum of the time-evolution operator can provide information on the dynamics of the system. In particular, the existence of a singularly continuous spectrum of the Floquet operator allows for a slow diffusive energy growth over time, typical of a chaotic system. Thus, this work has significance in the broad field of quantum chaos. For a more detailed discussion of the links among spectral analysis, dynamics, and chaos, see the introductory sections of Ref. 1 and references therein.

The work in Ref. 1 established a nonperturbative stability result on the spectral nature of the Floquet operator for simple systems with a rank-*N* perturbation periodic in time. The conditions under which the Floquet spectrum remains pure point were established. Here, we will first show the same result, but in a very different manner, before proceeding to determine when a continuous spectrum may arise. This result sheds further light on the array of possible dynamics that periodically perturbed systems may experience.

We consider Hamiltonians of the form

[a]Electronic mail: j.mccaw@physics.unimelb.edu.au
[b]Electronic mail: b.mckellar@physics.unimelb.edu.au

$$H(t) = H_0 + \left(\sum_{k=1}^{N} \lambda_k |\psi_k\rangle\langle\psi_k| \right) \sum_{n=0}^{\infty} \delta(t - nT), \tag{1}$$

where $\lambda_k \in \mathbb{R}$ and each vector $|\psi_k\rangle$ is a linear combination of the H_0 basis states, $|\phi_n\rangle$,

$$|\psi_k\rangle = \sum_{n=0}^{\infty} (a_k)_n |\phi_n\rangle.$$

The states $|\psi_k\rangle$ are orthogonal

$$\langle\psi_k|\psi_l\rangle = \delta_{kl}.$$

The Floquet operator is

$$V \equiv U(T) = e^{-iH_0 T/\hbar} e^{-i(\Sigma_k \lambda_k |\psi_k\rangle\langle\psi_k|)/\hbar}.$$

(Our Floquet operator differs from that in Combescure[6] and Bourget.[7,8] An erronous T was introduced in Ref. 6 and it has been carried through in the literature. Note that the theorems proved therein are not invalidated in any way by this error.) The basic result, as established in Ref. 1 is that if every $|\psi_k\rangle$ is in $l_1(H_0)$, the spectrum will remain pure point for almost every perturbation strength.

If this condition is dropped for any one of the $|\psi_k\rangle$, then we no longer have $V_{\lambda_1,\ldots,\lambda_N}$ pure point. In fact, on the subspace $\mathcal{H}_k$ defined by that space for which $|\psi_k\rangle$ is a cyclic vector for operator U, the spectrum is purely continuous. At this point, we note that Milek and Seba[5] have incorrectly concluded from Combescure's work that the existence of a ψ such that ψ is in the continuous subspace of $\mathcal{H}$ implies that the whole of $\mathcal{H}$ is continuous for the operator V. This statement would require the assumption that ψ is a cyclic vector for U, which is simply impossible for $|\psi\rangle\langle\psi|$ as an arbitrary projection.

For Milek and Seba's work to be properly justified, we show that a sufficient condition is that Vinogradov's number-theoretic conjecture, stated over 50 years ago, is true. (The reference is to the 1954 English translation of Vinogradov's original work, published in 1947. The work in Vinogradov's 1947 monograph incorporates results from a series of papers and a first monograph from 1937. It is unknown to us when the conjecture referred to was first presented, but it was at least 50 years ago.) This observation is linked to the conjecture put forward by Combescure[6] and partially addressed by Bourget.[7] After the completion of this work, we became aware of a recent paper by Bourget[8] which successfully resolves the issues with Milek and Seba's work by building on the earlier work in Ref. 7. Bourget's new work in no way invalidates the arguments presented here—the two approaches are complimentary.

In Sec. II we extend Combescure's rank-1 theorem on the pure point spectral nature of V to the rank-N case. In Sec. III we then show the existence of a continuous spectrum for the case where H_0 is the harmonic oscillator and the perturbation is rank-N. In Sec. IV we investigate Combescure's conjecture, the answer provided by Bourget and the link to number theory and Vinogradov's conjecture. Finally, in Sec. V, we extend Milek and Seba's work to the rank-N case, correcting a number of subtle errors. We emphasize that their work has only recently been fully justified (by Bourget in Ref. 8). We provide a complimentary justification, linked to the number-theoretic investigations and Vinogradov's conjecture just mentioned.

II. RANK-*N* GENERALIZATION OF COMBESCURE'S FIRST THEOREM

We consider the measures

$$m_{k,\lambda_k} = \langle\psi_k| E_{\lambda_k}(S) |\psi_k\rangle.$$

Each $|\psi_k\rangle$ admits a cyclic subspace of $\mathcal{H}$, $\mathcal{H}_k$. As argued in the later part of the proof of Theorem 4.3 in Ref. 1, on the space $\mathcal{H} \ominus (\oplus_{k=1}^{N} \mathcal{H}_k)$, the perturbation

$$\sum_{k=1}^{N} \lambda_k |\psi_k\rangle\langle\psi_k|$$

is null and thus $V=U$ is trivially pure point. Henceforth, we may safely restrict our proof to the subspace $\oplus_{k=1}^{N}\mathcal{H}_k$ for which the vectors $|\psi_k\rangle$ form a cyclic set.

Directly following Combescure, the measure for a point $x \in [0, 2\pi)$ for the operator V acting on the state $|\psi_k\rangle$ is given by

$$m_{k,\lambda_k}(\{x\}) = \frac{-4(1+\mu_k)}{\mu_k^2} B_k(x), \tag{2}$$

where

$$\mu_k = e^{i\lambda_k/\hbar} - 1$$

and

$$B_k(x) = \left[\int_0^{2\pi} dm_{k,\lambda_k=0}(\theta)(\sin^2[(x-\theta)/2])^{-1} \right]^{-1}.$$

This result is the essence of Lemma 1 in Ref. 6. When H_0 is pure point, it is a trivial calculation to show that

$$B_k^{-1}(x) = \sum_{n=0}^{\infty} \frac{|(a_k)_n|^2}{\sin^2[(x-\theta_n)/2]}. \tag{3}$$

Corollary 2 in Ref. 6 is replaced with the following.

Theorem II.1: *Assume H_0 is pure point, with $\{\phi_n\}_{n\in\mathbb{N}}$ and $\{\alpha_n\}_{n\in\mathbb{N}}$ as eigenstates and eigenvalues. Let each*

$$\psi_k = \sum_{n=0}^{\infty} (a_k)_n \phi_n$$

be cyclic for H_0 (hence, cyclic for U and V) on $\mathcal{H}_k$ and $\langle\psi_k|\psi_l\rangle = \delta_{kl}$. Then e^{ix} belongs to the point spectrum of $V_{\lambda_1,\ldots,\lambda_N}$ if and only if

$$\prod_{k=1}^{N} B_k^{-1}(x) < \infty,$$

where

$$\theta_n = 2\pi\{\alpha_n/2\pi\hbar\},$$

$\{z\}$ *being the fractional part of z.*

Proof II.1: The proof follows that in Ref. 6. By the cyclicity of each $|\psi_k\rangle$ on $\mathcal{H}_k$ and the argument in Theorem 4.3 of Ref. 1, e^{ix} is an eigenvalue of $V_{\lambda_1,\ldots,\lambda_N}$ if and only if every $m_{k,\lambda_k}(\{\theta\}) \neq 0$ at $\theta=x$. As already mentioned, using

$$\mathrm{d}m_{k,\lambda_k=0} = \sum_{n=0}^{\infty} |(a_k)_n|^2 \delta(\theta-\theta_n)\mathrm{d}\theta$$

we obtain, for each k,

$$B_k^{-1}(x) = \sum_{n=0}^{\infty} \frac{|(a_k)_n|^2}{\sin^2[(x-\theta_n)/2]}.$$

We now consider the eigenvalue e^{ix}. If it were to be that for some k, $m_{k,\lambda_k}(\{x\})=0$, then we would have found a vector, namely $|\psi_k\rangle$, such that $V|\psi_k\rangle$ was continuous. We have in fact found that the whole subspace $\mathcal{H}_k$ is continuous. Thus, for V to be pure point, we require every $m_{k,\lambda_k}(\{\theta\}) \neq 0$. Thus, we are lead to consider the requirement

$$\prod_{k=1}^{N} B_k^{-1}(x) < \infty.$$

□

As in Ref. 6, the relationship

$$\sum_{n=0}^{\infty} |(a_k)_n|^2 \operatorname{cotg}\left(\frac{x-\theta_n}{2}\right) = \operatorname{cotg}\frac{\lambda_k}{2\hbar} \tag{4}$$

also holds for each k. To show (4), we consider each k separately. The proof is the same as for the rank-1 case. See Ref. 6. Points to consider are that each projection operator in the rank-N projection is normalized and hence for every k we have

$$\sum_{n=0}^{N} |(a_k)_n|^2 = 1.$$

□

In order to complete the generalization of Combescure's first theorem, we require, just as in Ref. 6, two additional Lemmas.

Lemma II.2: If $\Sigma_{n=0}^{\infty}|(a_k)_n| < \infty$, *then* $B_k^{-1}(x) < \infty$ *for almost every* $x \in \mathbb{R}$.

For each $k \in 1, \ldots, N$, the proof is identical to that in Ref. 6.

Lemma II.3: The following two statements are equivalent.

(a) *For almost every* $(\lambda_1, \ldots, \lambda_N)$, $V_{\lambda_1,\ldots,\lambda_N}$ *has only a point spectrum.*
(b) *For every* $k \in \{1, \ldots, N\}$ *and for almost every* x, $B_k(x) \neq 0$.

The proof is again virtually identical to Combescure's proof. For each k, the continuous part of the spectrum is supported outside the set $E_k=\{x \in [0,2\pi) : B_k(x) \neq 0\}$ and, for $\lambda_k \neq 0$, the point part of $\mathrm{d}m_{k,\lambda_k}$ is supported by the set E_k. Thus, for $V_{\lambda_1,\ldots,\lambda_N}$ to be pure point for almost every $\lambda_1, \ldots, \lambda_N$ and for every k, we require

$$m_{k,\lambda_k}([0,2\pi) \setminus E_k) = 0.$$

This in turn implies that for every k

$$\int_0^{2\pi} \mathrm{d}\lambda_k' h(\lambda_k') m_{k,\lambda_k}([0,2\pi) \setminus E_k) = 0,$$

where $\lambda_k' = \lambda_k/\hbar$ and

$$h(\lambda) = 2\Re \frac{1}{1 - ce^{i\lambda}}$$

for some $|c| < 1$.

Lemma 5 in Ref. 6 trivially applies for each k. Thus, we have generalized Combescure's work to obtain the result that the Floquet operator for the rank-N perturbed Hamiltonian has a pure point spectrum. The result matches that in Ref. 1.

III. RANK-*N* GENERALIZATION OF COMBESCURE'S SECOND THEOREM

Having shown that the Floquet operator remains pure point for perturbations constructed from the vectors $|\psi_k\rangle \in l_1(H_0)$, Combescure relaxes this condition to allow for the emergence of a continuous spectral component of the Floquet operator. This result is easily generalized to the rank-N case. The key point is that the technique in Ref. 6 applies independently for each k. We do not discuss the details of the rank-1 proof here at all, delaying an analysis to Sec. IV where we will have the opportunity to generalize the result still further. Here, we simply provide the argument for why each k may be treated independently. Before proceeding, some subtleties of what Combescure actually shows are highlighted. They are seemingly overlooked by some in the literature (e.g., Ref. 5).

The cyclicity requirement was essential in the proof that the Floquet operator spectrum was pure point. Here, we can happily ignore the cyclicity conditions, as our only goal is to establish the existence of a state in the continuous subspace $\mathcal{H}_{\text{cont}}$. We need not try and ensure the result obtained by considering $\langle\psi|E(S)|\psi\rangle$ is applicable to all other vectors in $\mathcal{H}$—the very idea is ill-formed as the perturbation is null on a subset of $\mathcal{H}$ and thus there is always part of $\mathcal{H}$ where V has a discrete spectrum. Milek and Seba seem to have missed this point, restating Theorem 1 in Ref. 6 in a way that implies that all ψ are in $\mathcal{H}_{\text{cont}}$.

If

$$\langle\psi_k|E(\{x\})|\psi_k\rangle = 0$$

then $\mathcal{H}_{\text{ac}}$ contains at least the state $|\psi_k\rangle$. The point to be mindful of is that this does not allow one to conclude that the Hilbert space for the operator V has $\mathcal{H}_{pp}=\emptyset$, as implied by Milek and Seba.[5] To draw that conclusion would require an argument to show that a cyclic vector does in fact exist for V. This does not seem possible in the general context we have here.

Combescure's proof (Lemma 6 in Ref. 6) that $\sigma_{\text{cont}}(V)\neq\emptyset$ is based on showing that $B^{-1}(x)\rightarrow\infty$ [Eq. (3)]. As the spectral measure of a single point x is proportional to $B(x)$ [Eq. (2)], if $B^{-1}(x)\rightarrow\infty$, then the contribution of the single point is zero. That is, e^{ix} is in the continuous spectrum of the Floquet operator. Combescure argues (see Sec. IV for details) that

$$B^{-1}(x) \geqslant \#S(x),$$

where $\#S(x)$ is the number of element of a particular set S. She then shows (the bulk of the proof) that $\#S(x)\rightarrow\infty$ and thus $B^{-1}(x)\rightarrow\infty$. We generalize the result in a straightforward manner.

Theorem III.1: *Assume* $\alpha_n=n\hbar\omega$ *with* ω *irrational. If* $|\psi_k\rangle \notin l_1(H_0)$ *for at least one* $k \in 1,\ldots,N$, *then* $\sigma_{\text{cont}}(V)\neq\emptyset$.

Proof III.1: Following the same argument as for the rank-1 case, we take

$$|(a_k)_n| = n^{-\gamma}2\pi$$

for the state $|\psi_k\rangle$, in such a way that the condition $\langle\psi_k|\psi_l\rangle=\delta_{kl}$ is preserved.

With this construction, the proof that the number of elements in $S(x)$ is infinite[6] applies to each subsequence $S_k(x)$. The number of elements, $\#S_k(x)$, in each subsequence for which $|psi_k\rangle \notin l_1(H_0)$, is infinite. The Floquet operator for the rank-N perturbed harmonic oscillator obtains a continuous spectral component. □

Discussion. It must be noted that the proof of Lemma 6 in Ref. 6 is only valid for the eigenvalue spectrum,

$$\alpha_n = n\hbar\omega,$$

of the harmonic oscillator. Combescure does however conjecture that the argument will be valid for more general eigenvalue spectra, including the rotor

$$\alpha_n \propto n^2.$$

For Milek and Seba's numerical work (using the rotor) to be based on valid mathematical arguments, a proof of this conjecture is required. It was only very recently that a proof was developed,[8] some 15 years after the numerical results of Milek and Seba were published. As already mentioned, the work presented here, aiming to justify Milek and Seba's numerical work, was developed independently and is complimentary to Bourget's approach.

In Sec. IV we show that if a conjecture from number theory on the estimation of exponential sums is true, then Milek and Seba's work can be justified. The rank-N generalization is straightforward. Considering the number theory conjecture has stood for some 50 years, it seems we may have to wait quite some time for a proof. (Of course, now that Bourget has provided a direct proof for the rotor, the numerical simulations are on safe ground.)

For more general eigenvalue spectra (loosely $\alpha_n \propto n^j$) the situation is similar. For $j \geqslant 3$ Bourget[7] made significant progress. He has now covered the $j=2$ case.[8] A continuous component of the Floquet operator exists for certain constructions of $|\psi\rangle$. The conditions, for all $j \geqslant 2$, are complicated and more restrictive than the $|\psi\rangle \notin l_1(H_0)$ condition for the harmonic oscillator. The result is easily extended to the rank-N case due to the independence of each k as already discussed. Here, by utilizing a number-theoretic conjecture, we will provide improvements to the work of Bourget (both the $j \geqslant 3$ and $j=2$ cases). See Sec. IV.

Returning to the harmonic oscillator case, by applying Theorem III.1 we may conclude that for each $|\psi_k\rangle \notin l_1(H_0)$, $\mathcal{H}_k$ is purely continuous. Thus, by dropping the l_1 condition for all $|\psi_k\rangle$, we have shown that V is purely continuous on the subspace of $\mathcal{H}$ where the perturbation is nonzero. On the subspace of $\mathcal{H}$ where the perturbation is zero, $V=U$ trivially and thus that portion of the Hilbert space remains pure point.

IV. DISCUSSION OF COMBESCURE'S CONJECTURE

Combescure[6] makes a remark (Remark c.) that she believes Theorem III.1 (Lemma 6, Ref. 6) is generalizable to include systems other than the harmonic oscillator. Explicitly, she conjectures that Hamiltonians, H_0, with eigenvalues, α_n, of the form

$$\alpha_n = \hbar \sum_{j=0}^{p} \beta_j n^j \tag{5}$$

with $\beta_j T/2\pi$ Diophantine for some $j: 1 \leqslant j \leqslant p$ will have the vector ψ in the continuous spectral subspace of V_λ.

At an intuitive level, one would expect this to be true. The precise nature of the eigenvalue spectra (proportional to n or a polynomial in n) should not make a significant difference. Milek[9] argues that Combescure's work can be used in the n^2 case based on evidence from some numerical work that shows that the sequences obtained are "almost random"—however, the argument is not entirely convincing to us. The cited numerical work of Casati *et al.*[10] discusses the existence of correlations in the energy levels, rather than the lack of correlations. While the deviations from a Poisson distribution look small to the naked eye, Casati *et al.*[10] find deviations from the expected Poisson distribution of up to 17 standard deviations. The energy levels are correlated—it is arguable that they are not characterizable as "almost random" as Milek asserts.

In late 2002, Bourget[7] produced a proof of a slightly modified conjecture for all but the $p=2$ case in (5). The techniques used by Bourget are similar to those followed in this work. We will analyze Bourget's work, and highlight the key breakthrough made. We also provide a modified argument to obtain the proof which is, we believe, significantly easier to follow. Importantly, it also covers the $p=2$ case, unresolved by Bourget (until very recently) due to technical difficulties. However, it comes at the expense of relying upon a conjecture. Our result plays a complementary role in understanding, or perhaps appreciating, Bourget's proof. The reliance on the conjecture removes the need for much of the technical wizardry in Bourget's proof, and also strengthens the work. Our analysis also indicates, or highlights, that Combescure's conjecture is solved by a

number-theoretic conjecture that has stood for over 50 years. What seems a perfectly reasonable conjecture on physical grounds is shown to be directly related to an abstract mathematical conjecture.

In what follows, we rely heavily upon the lemmas and theorems in Chapter 2 of Ref. 11. We also use some results on Weyl sums from Ref. 12. Of key importance is an understanding of the proof of Lemma 6 in Ref. 6 on the emergence of a continuous spectrum for the kicked harmonic oscillator. This will be discussed at the appropriate time in this section.

A. Number theory

To discuss the conjecture, we require two concepts from number theory—the classification of irrational numbers and the *discrepancy* of a sequence. We first introduce the concepts and define the relevant ideas. We then proceed to analyze the conjecture and the proof provided by Bourget. As the discussion progresses, the new work that we have done will be presented.

For any number β, we define

(1) $[\beta]$, the integer part of β,
(2) $\{\beta\}$, the fractional part of β, and
(3) $\langle\beta\rangle = \min(\{\beta\}, 1-\{\beta\})$.

$\langle\beta\rangle$ is simply the "distance to the nearest integer." Definition IV.1 is taken directly from Kuipers and Niederreiter (Definition 3.4, p. 121, Ref. 11).

Definition IV.1: η Let be a positive real number or infinity. The irrational β of type η if η is the supremum of all τ for which

$$\lim_{n\to\infty} q^{\tau}\langle q\beta\rangle = 0, \tag{6}$$

where q runs through the positive integers.

The idea behind this definition can be seen by considering *rational* $\beta = p/q'$ for some p and q'. Run through the positive integers q. At $q=q'$, $\langle q\beta\rangle = 0$, so there is no supremum η for τ in (6). In effect, $\eta\to\infty$. For irrational β, $\langle q\beta\rangle$ is never equal to zero but will approach zero. If the approach is very slow, then a small τ is enough to prevent (6) from approaching zero. $\langle q\beta\rangle$ approaching zero slowly is, in a sense, indicative of β being badly approximated by rational numbers. Even for very large q', p/q' remains a poor approximation to β. Thus, the smaller η, the stronger the irrationality of β. This is reasonable in the sense that rational β's act like numbers with $\eta\to\infty$. As stated in Ref. 11, all numbers β have type $\eta \geqslant 1$.

We now define the discrepancy of a sequence—a measure of the nonuniformity of the sequence. We consider a sequence of numbers x_n in $[0, 1)$

$$\omega = (x_n)_{n\in\mathbb{N}} \text{ with } x_n \in [0,1).$$

(Equivalently, consider any sequence x_n and consider the discrepancy of the sequence modulo 1.) For $0 \leqslant a < b \leqslant 1$ and positive integer N, $A([a,b),N)$ counts the number of terms of the sequence (up to x_N) contained in the interval $[a,b)$,

$$A([a,b),N) = \#\{n \leqslant N : x_n \in [a,b)\}.$$

Definition IV.2: The discrepancy D_N of the sequence ω is

$$D_N(\omega) = \sup_{0\leqslant a<b\leqslant 1} \left| \frac{A([a,b),N)}{N} - (b-a) \right|. \tag{7}$$

If the sequence ω is uniformly distributed in $[0, 1)$ then $D_N \to 0$ as $N\to\infty$. In this case, every interval $[a,b]$ in $[0, 1)$ gets its "fair share" of terms from the sequence ω.

Estimating the discrepancy of a sequence will turn out to be vital in the analysis of Combescure's work. The sequence of interest is basically the eigenvalue sequence for H_0, but we will discuss this in greater detail later.

The starting point for the estimations that we require is Eq. (2.42), Chap. 2, Ref. 11. This is a famous result obtained by Erdös and Turán. It states that

$$D_N \leqslant C\left(\frac{1}{m}+\sum_{h=1}^{m}\frac{1}{h}\left|\frac{1}{N}\sum_{n=1}^{N}e^{2\pi i h x_n}\right|\right) \tag{8}$$

for any real numbers $x_1 \ldots x_N$ and any positive integer m. The sum

$$S=\sum_{n=1}^{N}e^{2\pi i h x_n}$$

is an example of a class of exponential sums known as *Weyl sums*, reflecting the pioneering work of Weyl on providing estimations for them. Vinogradov[12] improved on some of the estimations of Weyl. Weyl and Vinogradov's results concern the modulus of the sum, $|S|$, and characterize it as

$$|S| \leqslant \gamma N,$$

where N is the number of terms in the sum and γ tends to zero as $N \to \infty$. The subtle behavior of γ is linked to the rational/irrational nature of the terms in the sequence.

We will use some basic results from the introductory chapter of Ref. 12. In general, we write

$$S=\sum_{n=1}^{N}\exp(2\pi i F(n))$$

for some function $F(n)$. The application here is when

$$F(n)=\beta n^j.$$

For β rational (*not* the case we will be interested in) Hau proved that $|S|$ was of order

$$N^{1-(1/j)+\epsilon}$$

(p. 3, Ref. 12) and that this estimate could not be much improved. Here, we are interested in the case where β is irrational. Estimations are much more difficult, and form the major aspect of the work by Vinogradov. The estimations depend upon making a rational approximation to β and are complicated functions of N and j. Very loosely, he obtains results like

$$|S|=O(N^{1-\rho'}),$$

where

$$\rho'=\frac{1}{3(j-1)^2\log 12j(j-1)}. \tag{9}$$

Vinogradov states

> It is a plausible conjecture that the estimate in (9) holds with ρ' replaced be $1/j-\epsilon\ldots$. A proof or disproof of this conjecture would be very desirable.

As the conjecture plays a central role in what follows, we state it formally.

Conjecture IV.3: Consider the sum

$$S=\sum_{n=1}^{N}\exp 2\pi i n^j\beta_j.$$

For all N greater than some critical value, we have

$$|S| \leqslant cN^{1-(1/j)+\epsilon}$$

for all $\epsilon > 0$ *and some constant* $c \in \mathbb{R}$.

We do not attempt to prove Conjecture IV.3. Given the lengths gone to by Vinogradov to obtain the results presented above, it seems rather unlikely that a proof or disproof will be found any time soon. (Incremental improvements on the estimations presented by Vinogradov in Ref. 12 have been made over time. While Bourget[7,8] makes use of these improved results, the conjecture itself remains unproven which is the only result of any consequence in this discussion.)

B. Upper and lower bounds on discrepancy

Armed with the estimations on Weyl sums, we now proceed to derive both upper and lower bounds on the discrepancy for sequences of the type

$$\omega_j = (n^j \beta)$$

for β of any type $\eta \geqslant 1$. It must be remembered that the upper bound obtained is contingent upon Conjecture IV.3. The lower bound obtained is not dependent upon any unproved conjectures. The result obtained highlights the "best possible" nature of the conjectured upper bound.

First, (Lemma 3.2, p. 122, Ref. 11) is generalized to arbitrary j.

Lemma IV.4: The discrepancy $D_N(\omega_j)$ *of* $\omega_j = (n^j \beta)$ *satisfies*

$$D_N(\omega_j) \leqslant C\left(\frac{1}{m} + N^{1-(1/j)+\epsilon} c' \sum_{h=1}^{m} \frac{1}{h\langle h\beta \rangle}\right)$$

for any positive integer m and $\epsilon > 0$, *where C and c′ are absolute constants.*

Proof (IV.4): Consider (8). It is applicable to the first N terms of the sequence ω_j. We have

$$D_N(\omega_j) \leqslant C\left(\frac{1}{m} + \frac{1}{N}\sum_{h=1}^{m} \frac{1}{h}\left|\sum_{n=1}^{N} e^{2\pi i h n^j \beta}\right|\right) \tag{10}$$

for any positive integer m. Consider the sum over n,

$$\left|\sum_{n=1}^{N} e^{2\pi i h n^j \beta}\right|.$$

Conjecture IV.3 allows this sum to be bounded by

$$cN^{1-(1/j)+\epsilon}.$$

We are free to write

$$c = \frac{c'}{|\sin \pi h\beta|}$$

as $\sin \pi h\beta$ is just some positive real number. Substituting this result into (10), we obtain

$$D_N(\omega_j) \leqslant C\left(\frac{1}{m} + N^{-(1/j)+\epsilon} c' \sum_{h=1}^{m} \frac{1}{h} \frac{1}{|\sin \pi h\beta|}\right).$$

Now following the argument at the end of (Lemma 3.2, Ref. 11) the desired result is obtained.

□

We now give the generalization of (Theorem 3.2, Ref. 11). It provides the "best" upper bound one could hope for when estimating the discrepancy of the sequence $\omega_j=(n^j\beta)$. Again, remember that the proof relies on Conjecture IV.3.

Theorem IV.5: *Assume Conjecture IV.3 is true. Let β be of finite type η. Let j be a positive integer $j\geqslant 1$. Then, for every $\epsilon>0$, the discrepancy $D_N(\omega_j)$ of $\omega_j=(n^j\beta)$ satisfies*

$$D_N(\omega_j) = O(N^{-1/(\eta j)+\epsilon}).$$

Proof (IV.5): Let $\epsilon>0$ be fixed. By (Lemma 3.1 and Lemma 3.3, p. 121-3, Ref. 11),

$$\sum_{h=1}^{m} \frac{1}{h\langle h\beta\rangle} = O(m^{\eta-1+\epsilon'})$$

for a fixed $\epsilon'>0$. Combining this with Lemma IV.4, gives

$$D_N(\omega_j) \leqslant C\left(\frac{1}{m} + N^{-(1/j)+\epsilon''} m^{\eta-1+\epsilon'}\right)$$

for all $m\geqslant 1$. Now choose $m=[N^{1/(\eta j)}]$. We obtain

$$D_N(\omega_j) \leqslant C(N^{-1/(\eta j)} + N^{-(1/j)+\epsilon''+(1/j)-1/(\eta j)+\epsilon'/(\eta j)}) = O(N^{-1/(\eta j)+\epsilon}),$$

where $\epsilon=\epsilon''+\epsilon'/(\eta j)$. □

Theorem IV.5 is, in a sense, optimal. For functions f,g, define $f=\Omega(g)$ if $f/g \nrightarrow 0$.

Theorem IV.6: *Let β be of finite type η. Let j be a positive integer $j\geqslant 1$. Then, for every $\epsilon>0$, the discrepancy $D_N(\omega_j)$ of $\omega_j=(n^j\beta)$ satisfies*

$$D_N(\omega_j) = \Omega(N^{-1/(\eta j)-\epsilon}).$$

Proof (IV.6): Let $\epsilon>0$ be fixed. For any given $\epsilon'>0$, there exists $0<\delta<\eta$ with $1/(\eta-\delta) = (1/\eta)+\epsilon'$. By (Definition 3.4, p. 121, Ref. 11), we have $\lim_{q\to\infty} q^{\eta-(\delta/2)}\langle q\beta-j\rangle=0$ and thus

$$\langle q\beta_j\rangle < q^{-\eta+(\delta/2)}$$

for an infinite number of positive integers q. There are infinitely many positive integers q and p such that

$$|\beta - p/q| < q^{-1-\eta+(\delta/2)}.$$

That is, by choosing q large enough, we can always find a p such that $|q\beta-p|=\langle q\beta\rangle$. As q increases p/q is a better approximation to the irrational β. For θ some irrational with $|\theta|<1$, we have

$$\beta = p/q + \theta q^{-1-\eta+(\delta/2)}.$$

Pick a q such that the above relations are valid. Set

$$N = [q^{j(\eta-\delta)}].$$

Then for $1\leqslant n^j \leqslant N^{1/j}$,

$$n^j\beta = n^j(p/q) + \theta_n,$$

with

$$|\theta_n| = |n^j\theta q^{-1-\eta+(\delta/2)}| < n^j q^{-1-\eta+(\delta/2)} \leqslant q^{[j(\eta-\delta)]^{1/j}-1-\eta+(\delta/2)} = q^{-1-(\delta/2)}.$$

Thus, none of the fractional parts $\{\beta\},\{2^j\beta\},\ldots,\{[N^{1/j}]\beta\}$ lie in the interval $J=[q^{-1-(\delta/2)}, q^{-1}-q^{-1-(\delta/2)})$, so

$$D_N(\omega_j) \geqslant \left| \frac{A(J,N)}{N} - \lambda(J) \right| = \lambda(J)$$

where $\lambda(J)$, is simply the "size" of the set J. For large enough q we have $\lambda(J) \geqslant 1/2q$. But from the definition of N it is clear that

$$N \leqslant q^{j(\eta-\delta)} \leqslant N+1 \leqslant 2N,$$

so

$$q^{-1} \geqslant cN^{-[j(\eta-\delta)]^{-1}}.$$

Combining these inequalities, we obtain

$$D_N(\omega_j) \geqslant c' N^{-[j(\eta-\delta)]^{-1}} = c' N^{-(1/j)(1/(\eta-\delta))} = c' N^{-(1/j)((1/\eta)+\epsilon')} = c' N^{-1/(\eta j)-\epsilon},$$

where $\epsilon = \epsilon'/j$. That is, we have shown, for all $\epsilon > 0$, that

$$D_N(\omega_j) = \Omega(N^{-1/(\eta j)-\epsilon}).$$

□

C. Combescure's conjecture, Bourget's work, and new results

Before discussing the conjecture, we must clearly understand Combescure's proof for the harmonic oscillator case. As stated in Sec. III, the aim is to show that

$$B^{-1}(x) = \sum_{n=0}^{\infty} |a_n|^2 \left(\frac{2}{\sin(x-\theta_n)} \right)^2 \to \infty.$$

We define the set $S(x)$,

$$S(x) = \{n : |x-\theta_n| \leqslant |a_n| = n^{-\gamma} 2\pi\}. \tag{11}$$

Each n is an element of $S(x)$ if x is "close to θ_n." Note that $\theta_n = 2\pi\{\alpha_n/2\pi\hbar\}$, where $\{.\}$ is the fractional part, not "set" and α_n are the eigenvalues of the base Hamiltonian H_0.

Given that $\sin x \leqslant x$ for all $x \geqslant 0$, a lower bound for $B^{-1}(x)$ is obtained,

$$B^{-1}(x) \geqslant \sum_{n=0}^{\infty} |a_n|^2 \left(\frac{2}{x-\theta_n} \right)^2 \geqslant \sum_{n \in S(x)} \frac{4|a_n|^2}{(x-\theta_n)^2} \geqslant 4 \,\#\, S(x). \tag{12}$$

Each $n \in S(x)$ gives a contribution to the sum of greater than one as $|a_n|/|x-\theta_n| \geqslant 1$. By only considering $\#S(x)$, we simply count a "1" each time.

The results on discrepancy of sequences are now used, with the sequence $\omega_{\mathrm{HO}} = (\theta_n/2\pi)$. Note that each element of the sequence ω_{HO} is in $[0, 1)$.

Consider the interval, defined for every $x \in (0, 2\pi)$ and centered around $x/2\pi$,

$$J_N(x) = \left[\frac{x}{2\pi} - N^{-\gamma}, \frac{x}{2\pi} + N^{-\gamma} \right]. \tag{13}$$

For large enough $N, J_N(x) \subset [0,1)$. The size of the interval is $2N^{-\gamma}$. Using this particular subset and noting that the definition of discrepancy (7) involves taking the supremum over all subsets of $[0, 1)$, Combescure obtains

$$|N^{-1} A(J_N(x), N) - 2N^{-\gamma}| \leqslant D_N(\omega_{\mathrm{HO}}).$$

Multiplying through by N gives

$$|A(J_N(x),N) - 2N^{1-\gamma}| \leqslant ND_N(\omega_{\mathrm{HO}}). \tag{14}$$

As $|\psi\rangle \notin l_1(H_0)$

$$\sum |a_n| \to \infty$$

and thus

$$1/2 < \gamma \leqslant 1$$

from simple convergence arguments. Therefore, $N^{1-\gamma}$ grows at a rate less than $N^{1/2}$. [Interestingly, it can in fact not grow at all ($\gamma=1$) which is a subtle point seemingly missed by Combescure and others. The rank-1 projection operator from the vector $|\psi\rangle$ constructed with $\gamma=1$ is not shown to lead to the emergence of a continuous spectrum. Therefore, the statement that $|\psi\rangle \notin l_1(H_0)$ implies $|\psi\rangle \in \mathcal{H}_{\mathrm{cont}}$ is not in fact proved to be true. There are vectors not in $l_1(H_0)$ that may not be in the continuous spectrum. In practice (numerical, experimental work) this should not cause any trouble. It is clearly easy to avoid $\gamma=1$.] At this stage, Combescure utilizes the theorems discussed above on the discrepancy of sequences. For the eigenvalue sequence, $\alpha_n=n\hbar\omega$, of the harmonic oscillator the $j=1$ case of Theorem IV.5 applies which is exactly (Theorem 3.2, Ref. 11). (Do not confuse ω, the harmonic oscillator frequency, with ω_{HO}, the label for the sequence in $[0, 1)$, the discrepancy of which is being bounded.) Combescure obtains the result

$$D_N(\omega_{\mathrm{HO}}) = O(N^{-1(/\eta)+\epsilon}).$$

(This is not based on a conjecture as for $j=1$ a direct proof is possible, bypassing Conjecture IV.3. See. Ref. 11.) For the sequence $\omega_{\mathrm{HO}}, \beta=\omega/2\pi$. If β is an irrational of constant type ($\eta=1$), the strongest type of irrational, then

$$ND_N(\omega_{\mathrm{HO}}) = O(N^{\epsilon}).$$

As the right-hand side of (14) can be made to grow arbitrarily slowly, we conclude that the left-hand side must grow slowly too. Thus, to cancel out the growth of $2N^{1-\gamma}$, $A(J_N(x),N)$ must grow at a rate arbitrarily close to that of $2N^{1-\gamma}$. We see that

$$A(J_N(x),N) \to \infty$$

as $N\to\infty$. It is now a simple observation[6] that this implies that $\#S(x)\to\infty$ and thus $B^{-1}(x)\to\infty$. Thus, e^{ix} is in the continuous spectral subspace of the Floquet operator V.

The importance of the eigenvalue sequence is seen in that if we cannot limit the right-hand side of (14), then we cannot place a lower limit on $A(J_N(x),N)$ and thus we cannot conclude that $B^{-1}(x)\to\infty$. Two barriers to limiting the right-hand side of this equation exist—j and η. If, still in the harmonic oscillator case, we wished for $\beta=\omega/2\pi$ to only be of a weaker type, say $\eta=2$, we would no longer be able to conclude that $B^{-1}\to\infty$. The right-hand side would grow like $N^{(1/2)+\epsilon}$, which is always faster than $2N^{1-\gamma}$ for $1/2<\gamma\leqslant 1$ which grows at a rate of $N^{(1/2)-\epsilon}$. Thus, no suitable lower limit for $A(J_N(x),N)$ can be found. Similarly, if the eigenvalue sequence is generalized (Combescure's conjecture) then we run into trouble. For $j=2$, the lowest possible growth rate for the right-hand side we can obtain, taking Conjecture IV.3 as true, applying Theorem 5 and noting Theorem IV.6 which says we cannot do any better, is, once again, $N^{(1/2)+\epsilon}$. For larger j, the situation only gets worse.

Given these seemingly significant problems, the natural question to ask is: "How does one get around this problem?" The answer is provided in the work of Bourget.[7] Bourget proves a weaker theorem than Combescure's conjecture. Where the same requirement on $|\psi\rangle$ is kept in Ref. 6, that it be in $l_1(H_0)$, Bourget has a j dependent requirement. Essentially, for increasing j the a_n terms used to construct $|\psi\rangle$ must decrease more slowly with n. See Bourget's work for the exact requirement, which depends on the best estimates available for Weyl sums discussed earlier and thus is a nontrivial function of j.

The key insight in obtaining the proof is to modify the set $S(x)$ [Eq. (11)] and the corresponding interval $J_N(x)$ [Eq. (13)] that we consider. Importantly, they become j dependent. Bourget reduces the shrinking rate of the set $J_N(x)$ as a function of N just enough so as to allow the weaker limits on the discrepancy to be good enough to force the right-hand side of the equivalent to (14) to be less than the left-hand side, while keeping strong enough control on terms in the new set $S(x)$ to still argue that $B^{-1}\to\infty$.

Using the best available estimations on Weyl sums and plugging these into the upper bound formulas for discrepancy (as discussed earlier when introducing the work by Vinogradov), Bourget manages to provide a rigorous proof of the existence of a continuous spectral component of the Floquet operator (the essence of Combescure's conjecture) for $j\geqslant 3$[7] and $j=2$.[8] The proof is, unfortunately, unavoidably clouded by the "messy" estimates available for Weyl sums and thus, the essence of the proof is difficult to see. Here, we will revisit the proof, but (utilizing Conjecture IV.3) apply Theorem IV.5 which says (using 2ϵ, rather than ϵ for technical reasons), for all $\epsilon>0$,

$$D_N(\omega)=O(N^{-1/(\eta j)+2\epsilon}).$$

With this very clean estimate, it is far easier to see how Bourget's work provides a proof that a continuous spectral component of the Floquet operator exists. It covers all $j\geqslant 2$. We highlight the fact that a solution to Vinogradov's conjecture provides an elegant solution to Combescure's physics conjecture. The j-dependence of the a_n's used to construct $|\psi\rangle$ is straightforward.

Theorem IV.7: *Assume Conjecture IV.3 is true and thus Theorem IV.5 follows. Assume β is irrational and of type η. Then for all positive integers, j, the Floquet operator, V, has $\sigma_{\mathrm{cont}}(V)\neq\emptyset$ if $1/2<\gamma<1/2+1/(2\eta j)$.*

Proof (IV.7): The proof relies upon the techniques utilized by Bourget. In essence, we simply increase the size of the interval [Eq. (13)] from $2N^{-\gamma}$ to $2N^{2((1/2)-\gamma)}(\log N)^{-1/2}$. The important change is the first factor. The $\log N$ term is essential for technical reasons, but has a negligibly small effect on the shrinkage rate of the interval for large N. As $\log N/N^{4\delta}\to 0$ as $N\to\infty$ for all $\delta>0$, for N large enough we have

$$2N^{2((1/2)-\gamma)}(\log N)^{-1/2}>2N^{2((1/2)-\gamma-\delta)}.$$

Using this underestimate for the size of the interval, we easily obtain the equivalent of (14),

$$|A(J_N(x),N)-2N^{2(1-\gamma-\delta)}|\leqslant ND_N(\omega_j),$$

for the sequence $\omega_j=(n^j\beta)$. Now, using Theorem IV.5, it is evident that to ensure $A(J_N(x),N)\to\infty$, we must have

$$2(1-\gamma-\delta)>1-1/(\eta j)+2\epsilon,$$

or

$$\gamma<1/2+1/(2\eta j)-\epsilon-\delta.$$

The condition

$$1/2<\gamma<1/2+1/(2\eta j), \tag{15}$$

where the "$<$" sign has absorbed the arbitrarily small numbers ϵ and δ, must be satisfied to force $A(J_N(x),N)\to\infty$.

Finally, we must show that $B^{-1}(x)\to\infty$ when this larger interval is used. Corresponding to the new interval $J_N(x)$, we introduce the new set $S(x)$,

$$S(x)=\{n:|x-\theta_n|\leqslant 2\pi N^{2((1/2)-\gamma)}\log N^{-1/2}\}.$$

The estimate (12) is the same, except with the new set $S(x)$, which no longer has all terms greater than unity. Thus, it is not enough to simply count the number of terms in $S(x)$. A more subtle

estimate is required. Replacing the numerator, $|a_n|$, with something smaller, $N^{-\gamma}$, and the denominator, $(x-\theta_n)$, with something larger, $2\pi N^{2((1/2)-\gamma)} \log N^{-1/2}$, we obtain

$$B^{-1}(x) \geqslant \frac{1}{\pi^2} \sum_{n \in S(x)} \frac{\log N}{N^{2(1-\gamma)}},$$

which is essentially the estimate Bourget obtains. The estimate contained therein (Lemma 3.5 in Ref. 7) then shows that $B^{-1}(x) \to \infty$ and the argument is complete. □

Examining (15) we note that for $j=1$ (for $\eta=1$) we recover the simple result of Combescure. For all $j \geqslant 2$, we have a stronger (j-dependent) condition on $|\psi\rangle$ than simply $|\psi\rangle \notin l_1(H_0)$. This complication is the main weakening of Combescure's conjecture that Bourget and we have been forced to make. Note that the restriction on γ takes into account the end point subtleties referred to in the preceding discussions.

We have replaced the requirement that $|\psi\rangle \notin l_1(H_0)$ (i.e., $1/2 < \gamma \leqslant 1$) with the j dependent requirement $1/2 < \gamma < 1/2 + 1/(2j)$. In Bourget's work, the requirement is stronger—directly related to the replacement of the known limits on Weyl sums (in terms of ρ in the earlier sections) with the "best possible" estimate from our Conjecture IV.3 of $(1/j) - \epsilon$.

D. Summary

Reliance on Conjecture IV.3 and the result of Theorem IV.5 derived from it has allowed us to discuss Bourget's proof without the complications of the messy estimations on Weyl sums. Bourget's proof is also n-dependent (m in his work) while ours is n-independent. This simplified discussion highlights the key aspects of Bourget's proof, both for $j \geqslant 3$[7] and $j=2$.[8] It has also shown that the emergence of a continuous spectral component of the Floquet operator is solved by Vinogradov's conjecture. A proof of Vinogradov's conjecture is no longer just of mathematical interest. It has a direct mathematical physics consequence.

Finally, note that the rank-N equivalent of this work follows in the same way as presented for the harmonic oscillator case in Sec. III, providing a complete rank-N generalization of the work of Combescure.[6]

V. GENERALIZING THE RESULTS OF MILEK AND SEBA

Having established that the continuous subspace of $\mathcal{H}$, $\mathcal{H}_{\text{cont}}$ is not empty, we wish to characterize it—by identifying the singular and absolutely continuous components. Here, we extend the result of Milek and Seba to rank-N perturbations.

Theorem V.1: *Assume $H(t)$ is given by* (1) *and that* (2) *applies. Assume that $B_k^{-1}(x) \to \infty$ and thus $\mathcal{H}_{\text{cont}} \neq \emptyset$. Then $\mathcal{H}_{ac} = \emptyset$ and thus $\mathcal{H}_{sc}$ is not-empty. The Floquet operator, V, has a nonempty singular continuous spectrum.*

Proof (V.1): As shown in the proof of Theorem II.4a, (Ref. 1) and easily calculated, the Floquet operator can be written in the form

$$V = U + \sum_{k=1}^{N} R_k,$$

where

$$R_k = (e^{i\lambda_k/\hbar} - 1)|\psi_k\rangle\langle\psi_k|U. \tag{16}$$

We can now use either (Theorem 5, Ref. 13) or (Theorem 1, Ref. 14). The theorem from the paper of Birman and Krein is more direct, so we use it here. It states that if we have two unitary operators, U and V, that differ by a trace class operator, then the wave operators

$$\Omega_{\pm} = \mathrm{s} - \lim_{\nu \to \pm\infty} V^{\nu} U^{-\nu} P_{\mathrm{ac}}(U)$$

exist and their range is the absolutely continuous subspace of V,

$$R(\Omega_{\pm}) = \mathcal{H}_{\mathrm{ac}}(V). \tag{17}$$

We must show that the difference $V-U$ is finite. With the notation in Ref. 1, where the perturbation W is given by $A^{*}A$ and

$$A = |\psi\rangle\langle\psi|,$$

with

$$|\psi\rangle = \sum_{n} a_n \phi_n,$$

we obtain

$$\mathrm{Tr}\, A^{*}A = \mathrm{Tr}\, A = \sum_{l} \langle \phi_l | A | \phi_l \rangle = \sum_{l,m,n} \langle \phi_l | a_n | \phi_n \rangle \langle \phi_m | a_m^{*} | \phi_l \rangle = \sum_{l,m,n} a_n a_m^{*} \delta_{ln} \delta_{ml} = \sum_{l} |a_l|^2 = 1$$

as $|\psi\rangle \in l_2(H_0)$ and is normalized. The perturbation to the Hamiltonian is trace class. The difference in unitary operators, U and V, is also trace class. By the triangle inequality for norms,

$$\|R_k\|_{\mathrm{Tr}} \leqslant \|(e^{i\lambda_k/\hbar} - 1)\| \, \| \, |\psi_k\rangle\langle\psi_k| \|_{\mathrm{Tr}} \|U\|_{\mathrm{Tr}}.$$

As $\|U\|_{\mathrm{Tr}} = 1$,

$$\mathrm{Tr}\left(\sum_{k=1}^{N} R_k \right) \leqslant \sum_{k} \|(e^{i\lambda_k/\hbar} - 1 \, \| \sum_{l,m,n} \langle \phi_l | (a_k)_n | \phi_n \rangle \langle \phi_m | (a_k)_m^{*} | \phi_l \rangle = \sum_{k} |e^{i\lambda_k \hbar} - 1| = \sum_{k} \sqrt{2(1 - \cos \lambda_k/\hbar)}.$$

Armed with a trace-class perturbation, we conclude that the wave operators exist. The existence of the operators $\Omega_{\pm}$ means that they are defined for all vectors in the Hilbert Space $\mathcal{H}$. Note [Eq. (17)] that the subspace $\mathcal{H}_{\mathrm{ac}}(V)$ is equal to the range of these operators. However, $P_{\mathrm{ac}}(U)$ gives zero when acting on any state in $\mathcal{H}$ because U is pure point. Thus, $\mathcal{H}_{\mathrm{ac}}(V)$ is empty. As $\mathcal{H}_{\mathrm{cont}}$ is not empty, $\mathcal{H}_{\mathrm{sc}}$ must be nonempty, and we have proved that a singular continuous subspace of the Floquet operator V exists. □

The key assumption in Theorem V.1 is that $B_k^{-1}(x) \to \infty$. This is certainly true for $j=1$ if $|\psi_k\rangle \neq l_1(H_0)$. For $j \geqslant 2$, Bourget[7,8] showed that one can construct vectors $|\psi_k\rangle$ for which $B_k^{-1}(x) \to \infty$. The results were discussed in detail in Sec. IV. We have shown, in Conjecture IV.7, that if Conjecture IV.3 is true then this result may be improved—the requirements on the states $|\psi_k\rangle$ are less restrictive. The result was also extended to rank-N perturbations.

Discussion. Milek and Seba make a number of incorrect statements in obtaining this result for the rank-1 case. First, they state that the operator $R=[\exp(i\lambda/\hbar)-1]|\psi\rangle\langle\psi|U$ is rank-1 which it is not—the presence of the unitary operator U stops R from being rank-1. [As we are dealing with the rank-1 case, the subscript k may be dropped from (16).] This is not, however, important. The applicability of the theorems in Refs. 13 and 14 does not rely upon the rank of the operator R, but upon it being of trace-class. Second, they claim that the existence of the wave operators implies that

$$\sigma_{\mathrm{ac}}(V) \subset \sigma_{\mathrm{ac}}(U). \tag{18}$$

This is, again, not true. Given that $\sigma_{\mathrm{ac}}(U)$ is empty, it is indeed possible to conclude that $\sigma_{\mathrm{ac}}(V)$ is empty, as discussed earlier, but the relation (18) does not follow. Consider the situation where $\sigma_{\mathrm{cont}}(U)$ is not empty. Then there is a set of vectors in $\mathcal{H}$ which are continuous for U. These vectors form the domain for the operator V^{ν} in the wave operators. The action with V^{ν} does not however keep us in the subspace $\mathcal{H}_{\mathrm{cont}}(U)$ as the space we get to (the range for V^{ν}) is only

invariant for $\mathcal{H}_{\mathrm{cont}}(V)$, not $\mathcal{H}_{\mathrm{cont}}(U)$. Thus, we may obtain a vector, necessarily in $\mathcal{H}_{\mathrm{cont}}(V)$ due to invariance, but possibly in $\mathcal{H}_{\mathrm{s}}(U)$, and thus, we cannot conclude that $\sigma_{\mathrm{ac}}(V) \subset \sigma_{\mathrm{ac}}(U)$. These two points discussed do not make the final results of Milek and Seba wrong, but "only" the proofs.

Of greatest concern is the use of Lemma 6 in Ref. 6 without justification. Milek and Seba have assumed that Combescure's conjecture is true. It has taken 15 years, and a significant amount of work by Bourget, for that to be shown to be the case. We have shown that the conjecture is directly linked to a long-standing number-theoretic conjecture. The work has also been extended to cover rank-N perturbations.

VI. SUMMARY

We have generalized the work of both Combescure[6] and Milek and Seba[5] from rank-1 to rank-N. We have also discussed in detail Combescure's conjecture, our work on estimations of discrepancy and the demonstration by Bourget[7] that a continuous spectral component of the Floquet operator does exist for certain constructions of $|\psi\rangle$. This covers the essential aim of Combescure's conjecture on the existence of a continuous spectral component. A clear view of the essence of Bourget's proof has been provided by taking a reasonable number-theoretic conjecture to be true. With this clear view, the work of Bourget becomes more accessible. A resolution to Vinogradov's conjecture would have direct implications in mathematical physics.

An in-depth critical analysis of the work of Milek and Seba was also undertaken; we highlighted a number of misconceptions in the work. A proof of Vinogradov's conjecture, allowing our work to provide an elegant solution to Combescure's conjecture, remains desirable.

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On the exceptional $N=6$ superconformal algebra

Elena Poletaeva[a)]
Department of Mathematics, University of California, Riverside, California 92521

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We realize the exceptional $N=6$ superconformal algebra, spanned by 32 fields, inside the Lie superalgebra of pseudodifferential symbols on the supercircle $S^{1|3}$. Correspondingly, we obtain two nonisomorphic one-parameter families of irreducible representations of this superconformal algebra in a superspace spanned by 8 fields. © *2005 American Institute of Physics*. [DOI: 10.1063/1.2035029]

I. INTRODUCTION

A *superconformal algebra* is a simple complex Lie superalgebra $\mathfrak{g}$ spanned by the coefficients of a finite family of pairwise local fields $a(z)=\sum_{n\in\mathbb{Z}}a_{(n)}z^{-n-1}$; one of the members of this family is the Virasoro field $L(z)$.[1–4] Superconformal algebras play an important rôle in the string theory and conformal field theory.

The Lie superalgebra $K(N)$ of contact vector fields with Laurent polynomials as coefficients (with N odd variables) is a superconformal algebra which is characterized by its action on a contact 1-form.[1,2,5,6] These Lie superalgebras are also known to physicists as the $SO(N)$ superconformal algebras.[7] Note that $K(N)$ is spanned by 2^N fields. It is simple if $N\neq 4$, if $N=4$, then the derived Lie superalgebra $K'(4)$ is simple. The nontrivial central extensions of $K(1)$, $K(2)$, and $K'(4)$ are well known: they are isomorphic to the Neveu-Schwarz superalgebra, and the so-called "$N=2$," and "big $N=4$" superconformal algebra, respectively.[7]

The superalgebra $K(6)$ contains a simple subsuperalgebra spanned by 32 fields. This new exceptional superconformal algebra was constructed in Ref. 1 (and denoted by CK_6) and in Ref. 8 (and denoted by $\mathfrak{kas}$); see also Refs. 5 and 9–13. It was proven in Refs. 1 and 5 that CK_6 has no nontrivial central extensions. It was also pointed out that CK_6 appears to be the only new superconformal algebra, which completes their list; see Refs. 2–6.

Martinez and Zelmanov[14,15] obtained CK_6 using their construction of superalgebras $CK(R,d)$, where R is an associative commutative superalgebra with an even derivation d.

In this work we realize CK_6 inside the Poisson superalgebra $P(6)$ of pseudodifferential symbols on the supercircle $S^{1|3}$ and inside its deformation $P_h(6)$.

It is known that a Lie algebra of contact vector fields can be realized as a subalgebra of Poisson algebra.[16] In particular, the Lie algebra $Vect(S^1)$ of complex polynomial vector fields on the circle has a natural embedding into the Poisson algebra $P(0)$ of formal Laurent series on the cylinder $T^*S^1\backslash S^1$. One can consider a family of Lie algebras P_h, $h\in\,]0,1]$, having the same vector space, which contracts to $P(0)$.[17–20] Analogously, $K(2N)$ is embedded into the Poisson superalgebra $P(2N)$ of pseudodifferential symbols on the supercircle $S^{1|N}$, and there is a family of Lie superalgebras $P_h(2N)$, which contracts to $P(2N)$; see Ref. 21.

A natural question is whether there exists an embedding

$$K(2N)\subset P_h(2N). \tag{1.1}$$

Recall that the answer is "yes" if $N=2$, more precisely, there exists an embedding

a)*Electronic mail*: elena@math.ucr.edu

$$\hat{K}'(4) \subset P_h(4), \tag{1.2}$$

where $K'(4)=[K(4),K(4)]$ is a simple ideal of $K(4)$ of codimension one, and $\hat{K}'(4)$ is one of three independent central extensions of $K'(4)$. Associated with the embedding (1.2), there is a one-parameter family of irreducible representations of this central extension $\hat{K}'(4)$ realized on 4 fields.[21]

Note that embedding (1.1) does not hold if $N>2$.[22] However, it is remarkable that it is possible to embed CK_6, which is "one half" of $K(6)$, into $P_h(6)$. We construct two such embeddings, and obtain the corresponding one-parameter families of irreducible representations of CK_6 realized on 8 fields. In particular, we obtain representations of CK_6 in 8 fields, which preserve an odd nondegenerate supersymmetric or superskew-symmetric bilinear form. We also show how the superalgebra CK_6 is generated inside $P_h(6)$.

II. CONTACT SUPERCONFORMAL ALGEBRA *K*(2*N*)

Let $\Lambda(2N)$ be the Grassmann algebra in $2N$ variables $\xi_1,\dots,\xi_N$, $\eta_1,\dots,\eta_N$, and let $\Lambda(1,2N)=\mathbb{C}[t,t^{-1}]\otimes\Lambda(2N)$ be the associative superalgebra with natural multiplication and with the following parity of generators: $p(t)=\overline{0}$, $p(\xi_i)=p(\eta_i)=\overline{1}$ for $i=1,\dots,N$. Let $W(2N)$ be the Lie superalgebra of all derivations of $\Lambda(1,2N)$. Let ∂_t, ∂_{ξ_i}, and ∂_{η_i} stand for $\partial/\partial t,\partial/\partial\xi_i$, and $\partial/\partial\eta_i$, respectively. By definition,

$$K(2N)=\{D\in W(2N)\mid D\Omega=f\Omega \quad \text{for some } f\in\Lambda(1,2N)\}, \tag{2.1}$$

where $\Omega=\mathrm{d}t+\Sigma_{i=1}^{N}(\xi_i\,\mathrm{d}\eta_i+\eta_i\,\mathrm{d}\xi_i)$ is a differential 1-form, which is called a *contact form*; see Refs. 1, 2, 5, 6, 8, and 11–13, and 23. Let the Euler operator be defined by

$$E=\sum_{i=1}^{N}(\xi_i\partial_{\xi_i}+\eta_i\partial_{\eta_i}). \tag{2.2}$$

Set also:

$$\Delta=2-E, \quad H_f=(-1)^{p(f)+1}\sum_{i=1}^{N}(\partial_{\xi_i}f\partial_{\eta_i}+\partial_{\eta_i}f\partial_{\xi_i}), \tag{2.3}$$

for any $f\in\Lambda(1,2N)$.

There is a one-to-one correspondence between the differential operators $D\in K(2N)$ and the functions $f\in\Lambda(1,2N)$. The correspondence $f\leftrightarrow D_f$ is given by

$$D_f=\Delta(f)\frac{\partial}{\partial t}+\frac{\partial f}{\partial t}E-H_f. \tag{2.4}$$

The contact bracket on $\Lambda(1,2N)$ is

$$\{f,g\}_K=\Delta(f)\partial_t g-\partial_t f\Delta(g)-\{f,g\}_{P.b}, \tag{2.5}$$

where

$$\{f,g\}_{P.b}=(-1)^{p(f)+1}\sum_{i=1}^{N}(\partial_{\xi_i}f\partial_{\eta_i}g+\partial_{\eta_i}f\partial_{\xi_i}g) \tag{2.6}$$

is the Poisson bracket. Thus $[D_f,D_g]=D_{\{f,g\}_K}$.

Let $\Theta=\xi_1\xi_2\xi_3\eta_1\eta_2\eta_3$.

Proposition 2.1: (See Refs. 1,5, and 8.) The superalgebra $K(6)$ contains an exceptional $N=6$ superconformal algebra CK_6. It is spanned by the following 32 fields:

$$L_n = t^{n+1} - (\partial_t)^3 t^{n+1}\Theta,$$

$$G_n^i = t^{n+1}\xi_i + (\partial_t)^2 t^{n+1}\partial_{\eta_i}\Theta, \quad \widetilde{G}_n^i = t^n\eta_i + (\partial_t)^2 t^n \partial_{\xi_i}\Theta, \quad i=1,2,3,$$

$$T_n^{ij} = t^n\xi_i\eta_j - (\partial_t)t^n\partial_{\eta_i}\partial_{\xi_j}\Theta, \quad i\neq j, \quad T_n^i = t^n\xi_i\eta_i - (\partial_t)t^n\partial_{\eta_i}\partial_{\xi_i}\Theta, \quad i=1,2,3,$$

$$S_n^i = t^n\xi_i(\xi_j\eta_j + \xi_k\eta_k), \quad \widetilde{S}_n^i = t^{n-1}\eta_i(\xi_j\eta_j - \xi_k\eta_k), \quad i=1,2,3, \tag{2.7}$$

$$I_n^i = t^{n-1}\xi_i\eta_j\eta_k, \quad i=1,2,3, \quad I_n = t^{n+1}\xi_1\xi_2\xi_3,$$

$$J_n^{ij} = t^{n+1}\xi_i\xi_j - (\partial_t)t^{n+1}\partial_{\eta_i}\partial_{\eta_j}\Theta, \quad \widetilde{J}_n^{ij} = t^{n-1}\eta_i\eta_j - (\partial_t)t^{n-1}\partial_{\xi_i}\partial_{\xi_j}\Theta, \quad i<j,$$

where $n\in\mathbb{Z}$; (i,j,k) is the cycle $(1,2,3)$ in the formulas for $S_n^i, \widetilde{S}_n^i$ and I_n^i.

III. POISSON SUPERALGEBRA $P(2N)$ OF PSEUDODIFFERENTIAL SYMBOLS ON $S^{1|N}$

The *Poisson algebra* $P(0)$ *of pseudodifferential symbols on the circle* is formed by the formal series $A(t,\tau)=\sum_{-\infty}^{n} a_i(t)\tau^i$, where $a_i(t)\in\mathbb{C}[t,t^{-1}]$, and the even variable τ corresponds to ∂_t. The Poisson bracket is defined as follows:

$$\{A(t,\tau),B(t,\tau)\} = \partial_\tau A(t,\tau)\partial_t B(t,\tau) - \partial_t A(t,\tau)\partial_\tau B(t,\tau). \tag{3.1}$$

The Poisson algebra $P(0)$ has a deformation P_h, where $h\in\,]0,1]$. The associative multiplication in the vector space P is determined as follows:

$$A(t,\tau)\circ_h B(t,\tau) = \sum_{n\geqslant 0}\frac{h^n}{n!}\partial_\tau^n A(t,\tau)\partial_t^n B(t,\tau). \tag{3.2}$$

The Lie algebra structure on P_h is given by $[A,B]_h = A\circ_h B - B\circ_h A$, so that the family P_h contracts to $P(0)$. The Lie algebra P_h is called the *Lie algebra of pseudodifferential symbols on the circle*.[17–20]

The *Poisson superalgebra* $P(2N)$ *of pseudodifferential symbols on the supercircle* $S^{1|N}$ has the underlying vector space $P\otimes\Lambda(2N)$. The Poisson bracket is defined as follows:

$$\{A,B\} = \partial_\tau A\partial_t B - \partial_t A\partial_\tau B + \{A,B\}_{P.b}. \tag{3.3}$$

Let $\Lambda_h(2N)$ be an associative superalgebra with generators $\xi_1,\ldots,\xi_N,\ \eta_1,\ldots,\eta_N$ and relations:

$$\xi_i\xi_j = -\xi_j\xi_i, \eta_i\eta_j = -\eta_j\eta_i, \eta_i\xi_j = h\delta_{i,j} - \xi_j\eta_i. \tag{3.4}$$

Let $P_h(2N)=P_h\otimes\Lambda_h(2N)$ be a superalgebra with the product of $A=A_1\otimes X$ and $B=B_1\otimes Y$, where $A_1,B_1\in P_h$, and $X,Y\in\Lambda_h(2N)$, given by

$$AB = \frac{1}{h}(A_1\circ_h B_1)\otimes(XY). \tag{3.5}$$

The Lie bracket in $P_h(2N)$ is $[A,B]_h = AB - (-1)^{p(A)p(B)}BA$, and $\lim_{h\to 0}[A,B]_h = \{A,B\}$. There exist natural embeddings: $W(N)\subset P(2N)$ and $W(N)\subset P_h(2N)$, where $W(N)$ is the Lie superalgebra of all derivations of $\mathbb{C}[t,t^{-1}]\otimes\Lambda(\xi_1,\ldots,\xi_N)$ (∂_{ξ_i} is identified with η_i), so that the commutation relations in $P(2N)$ and in $P_h(2N)$, when restricted to $W(N)$, coincide with the commutation relations in $W(N)$. The Lie superalgebra $P_h(2N)$ is called the *Lie superalgebra of pseudodifferential symbols on* $S^{1|N}$ (see Ref. 21).

IV. REALIZATION OF CK_6 INSIDE THE POISSON SUPERALGEBRA

Theorem 4.1: The superalgebra CK_6 is spanned by the following 32 fields inside $P(6)$:

$$L_{n,0}=t^{n+1}\tau,$$

$$G^i_{n,0}=t^{n+1}\tau\xi_i,\quad \widetilde{G}^i_{n,0}=t^n\eta_i-nt^{n-1}\tau^{-1}\xi_j\eta_i\eta_j,\quad i=1,2,3,$$

$$T^{ij}_{n,0}=t^n\xi_i\eta_j-nt^{n-1}\tau^{-1}\xi_k\xi_i\eta_k\eta_j,\quad i\neq j\neq k,$$

$$\begin{aligned}T^i_{n,0}&=-t^n(\xi_j\eta_j+\xi_k\eta_k)+nt^{n-1}\tau^{-1}\xi_j\xi_k\eta_j\eta_k,\quad i=1,2,3,\\ S^i_{n,0}&=-t^n\xi_i(\xi_j\eta_j+\xi_k\eta_k)+nt^{n-1}\tau^{-1}\xi_i\xi_j\xi_k\eta_j\eta_k,\quad i=1,2,3,\end{aligned}\tag{4.1}$$

$$\widetilde{S}^i_{n,0}=t^{n-1}\tau^{-1}(\xi_j\eta_j-\xi_k\eta_k)\eta_i,\quad i=1,2,3,$$

$$I^i_{n,0}=t^{n-1}\tau^{-1}\xi_i\eta_j\eta_k,\quad i=1,2,3,\quad I_{n,0}=t^{n+1}\tau\xi_1\xi_2\xi_3,$$

$$J^{ij}_{n,0}=t^{n+1}\tau\xi_i\xi_j,\quad \widetilde{J}^{ij}_{n,0}=t^{n-1}\tau^{-1}\eta_i\eta_j,\quad i<j,$$

where $n\in\mathbb{Z}$; (i,j,k) is the cycle $(1,2,3)$ in the formulas for $\widetilde{G}^i_{n,0}$, $T^i_{n,0}$, $S^i_{n,0}$, $\widetilde{S}^i_{n,0}$, and $I^i_{n,0}$.

Proof: Note that there exists an embedding

$$K(2N)\subset P(2N),\quad N\geqslant 0,\tag{4.2}$$

(see Ref. 21). Consider a $\mathbb{Z}$ grading of the associative superalgebra

$$P(2N)=\oplus_{i\in\mathbb{Z}}P_{(i)}(2N)\tag{4.3}$$

defined by $\deg_{Lie}f=\deg f-1$, where deg is defined as follows:

$$\begin{aligned}&\deg t=\deg\xi_i=0\quad \text{for } i=1,\ldots,N,\\ &\deg\tau=\deg\eta_i=1\quad \text{for } i=1,\ldots,N.\end{aligned}\tag{4.4}$$

With respect to the Poisson bracket,

$$\{P_{(i)}(2N),P_{(j)}(2N)\}\subset P_{(i+j)}(2N).\tag{4.5}$$

Thus $P_{(0)}(2N)$ is a subsuperalgebra of $P(2N)$, and we will show that $P_{(0)}(2N)\cong K(2N)$. Equivalently, $P_{(0)}(2N)$ is singled out as the set of all (Hamiltonian) functions $A(t,\tau,\xi_i,\eta_i)\in P(2N)$ such that the corresponding vector fields supercommute with the semi-Euler operator:

$$\left[H_A,\tau\partial_\tau+\sum_{i=1}^N\eta_i\partial_{\eta_i}\right]=0,\tag{4.6}$$

where

$$A(t,\tau,\xi_i,\eta_i)\to H_A=\partial_\tau A\partial_t-\partial_t A\partial_\tau-(-1)^{p(A)}\sum_{i=1}^N(\partial_{\xi_i}A\partial_{\eta_i}+\partial_{\eta_i}A\partial_{\xi_i}).\tag{4.7}$$

To describe an isomorphism of $K(2N)$ with $P_{(0)}(2N)$, we change the variable t in $\Lambda(1|2N)$: $t\overset{\chi}{\to}2t-\Sigma_{i=1}^N\xi_i\eta_i$. Then we have the following contact bracket on $\Lambda(1|2N)$:

$$\{f,g\}_{\widetilde{K}} = \widetilde{\Delta}(f)\partial_t g - \partial_t f\widetilde{\Delta}(g) - \{f,g\}_{P.b}, \tag{4.8}$$

where $\widetilde{\Delta}=1-\widetilde{E}$ and $\widetilde{E}=\Sigma_{i=1}^{N}\eta_i\partial_{\eta_i}$. Note that the corresponding contact form is $\widetilde{\Omega}=\mathrm{d}t+\Sigma_{i=1}^{N}\xi_i\mathrm{d}\eta_i$. Define a map $\varphi:\Lambda(1|2N)\to P_{(0)}(2N)$ as follows:

$$f\overset{\varphi}{\to}A_f=(-1)^s\tau^{1-s}f, \tag{4.9}$$

where s is a scalar given by $\widetilde{E}(f)=sf$. Then

$$\{A_f,A_g\}=A_{\{f,g\}_{\widetilde{K}}}. \tag{4.10}$$

Applying the isomorphism $\psi=\varphi\circ\chi$ to the fields (2.7), we obtain the following fields:

$$\begin{gathered}
\psi(L_n)=2^{n+1}L_{n,0}-2^{n-1}(n+1)(T^1_{n,0}+T^2_{n,0}+T^3_{n,0}),\\
\psi(G^i_n)=2^{n+1}G^i_{n,0}-2^n(n+1)S^i_{n,0},\quad \psi(\widetilde{G}^i_n)=-2^n\widetilde{G}^i_{n,0}+2^{n-1}n\widetilde{S}^i_{n,0},\\
\psi(T^{ij}_n)=-2^nT^{ij}_{n,0},\quad \psi(T^i_n)=2^{n-1}(-T^i_{n,0}+T^j_{n,0}+T^k_{n,0}),\\
\psi(S^i_n)=2^nS^i_{n,0},\quad \psi(\widetilde{S}^i_n)=2^{n-1}\widetilde{S}^i_{n,0},\\
\psi(I^i_n)=2^{n-1}I^i_{n,0},\quad \psi(I_n)=2^{n+1}I_{n,0},\\
\psi(J^{ij}_n)=2^{n+1}J^{ij}_{n,0},\quad \psi(\widetilde{J}^{ij}_n)=2^{n-1}\widetilde{J}^{ij}_{n,0},
\end{gathered} \tag{4.11}$$

where (i,j,k) is the cycle $(1,2,3)$ in the formulas for $\psi(T^i_n)$. □

V. REALIZATION OF CK_6 INSIDE THE LIE SUPERALGEBRA OF PSEUDODIFFERENTIAL SYMBOLS

Given the embedding (4.2) it is natural to ask whether there exists an embedding

$$K(2N)\subset P_h(2N). \tag{5.1}$$

Recall that $K'(4)=[K(4),K(4)]$ is a simple ideal in $K(4)$ of codimension one defined from the exact sequence

$$0\to K'(4)\to K(4)\to \mathbb{C}D_{t^{-1}\xi_1\xi_2\eta_1\eta_2}\to 0. \tag{5.2}$$

Recall also (see Ref. 21) that the superalgebra $K'(4)\subset P(4)$ is spanned by the 16 fields: By the 12 fields:

$$f(\xi_1,\xi_2,t)\tau,\quad f(\xi_1,\xi_2,t)\eta_i\quad (i=1,2), \tag{5.3}$$

which form a subsuperalgebra isomorphic to $W(2)$, and 4 more fields F^i_n, where $0\leqslant i\leqslant 3$ and $n\in\mathbb{Z}$:

$$\begin{gathered}
F^0_n=t^{n-1}\tau^{-1}\eta_1\eta_2,\\
F^i_n=t^{n-1}\tau^{-1}\xi_i\eta_1\eta_2,\quad i=1,2,\\
F^3_n=t^{n-1}\tau^{-1}\xi_1\xi_2\eta_1\eta_2,\quad n\neq 0.
\end{gathered} \tag{5.4}$$

Proposition 5.1: (See Ref. 21.) The superalgebra $\hat{K}'(4)\subset P_h(4)$ is spanned by the 12 fields given in (5.3) and 4 more fields $F^i_{n,h}$:

$$F^0_{n,h}=\tau^{-1}\circ_h t^{n-1}\eta_1\eta_2,$$

$$F^i_{n,h}=\tau^{-1}\circ_h t^{n-1}\eta_1\eta_2\xi_i,\quad i=1,2, \tag{5.5}$$

$$F^3_{n,h}=\tau^{-1}\circ_h t^{n-1}\eta_1\eta_2\xi_1\xi_2+\frac{h}{n}t^n,\quad n\neq 0,$$

and the central element $h\in P_h(4)$, so that $\lim_{h\to 0}\hat{K}'(4)=K'(4)\subset P(4)$.

Note that we cannot obtain the embedding (5.1) if $N>2$.[22] However, the following theorem holds.

Theorem 5.2: There exists an embedding $i_h: CK_6\to P_h(6)$ for each $h\in\,]0,1]$ such that $\lim_{h\to 0} i_h(CK_6)=CK_6\subset P(6)$.

Proof: $i_h(CK_6)$ is spanned by the following fields inside $P_h(6)$:

$$L_{n,h}=t^{n+1}\tau,$$

$$G^i_{n,h}=t^{n+1}\tau\xi_i,\quad \widetilde{G}^i_{n,h}=t^n\eta_i-n\tau^{-1}\circ_h t^{n-1}\eta_i\eta_j\xi_j,\quad i=1,2,3,$$

$$T^{ij}_{n,h}=t^n\xi_i\eta_j-n\tau^{-1}\circ_h t^{n-1}\eta_k\eta_j\xi_k\xi_i,\quad i\neq j\neq k,$$

$$\begin{aligned} T^i_{n,h}&=-t^n(\xi_j\eta_j+\xi_k\eta_k)+n\tau^{-1}\circ_h t^{n-1}\eta_j\eta_k\xi_j\xi_k+ht^n,\quad i=1,2,3,\\ S^i_{n,h}&=-t^n\xi_i(\xi_j\eta_j+\xi_k\eta_k)+n\tau^{-1}\circ_h t^{n-1}\eta_j\eta_k\xi_i\xi_j\xi_k+ht^n\xi_i,\quad i=1,2,3, \end{aligned} \tag{5.6}$$

$$\widetilde{S}^i_{n,h}=\tau^{-1}\circ_h t^{n-1}(\eta_j\eta_i\xi_j-\eta_k\eta_i\xi_k),\quad i=1,2,3,$$

$$I^i_{n,h}=\tau^{-1}\circ_h t^{n-1}\eta_j\eta_k\xi_i,\quad i=1,2,3,\quad I_{n,h}=t^{n+1}\tau\xi_1\xi_2\xi_3,$$

$$J^{ij}_{n,h}=t^{n+1}\tau\xi_i\xi_j,\quad \widetilde{J}^{ij}_{n,h}=\tau^{-1}\circ_h t^{n-1}\eta_i\eta_j,\quad i<j,$$

where $n\in\mathbb{Z}$; (i,j,k) is the cycle $(1,2,3)$ in the formulas for $\widetilde{G}^i_{n,h}$, $T^i_{n,h}$, $S^i_{n,h}$, $\widetilde{S}^i_{n,h}$, and $I^i_{n,h}$. Let $h\in[0,1]$. Set $J^{ij}_{n,h}=-J^{ji}_{n,h}$ and $\widetilde{J}^{ij}_{n,h}=-\widetilde{J}^{ji}_{n,h}$ for $i>j$. Given $h\in[0,1]$, set

$$L_n:=L_{n,h},\quad \ldots,\quad \widetilde{J}^{ij}_n:=\widetilde{J}^{ij}_{n,h}. \tag{5.7}$$

Recall that if $h=0$, then (5.7) gives elements (4.1). The nonvanishing commutation relations between the elements (5.7) are as follows: let $i\neq j\neq k$, then

$$[L_n,L_m]=(m-n)L_{n+m},$$

$$[L_n,G^i_m]=(m-n)G^i_{n+m},\quad [L_n,\widetilde{G}^i_m]=m\widetilde{G}^i_{n+m},$$

$$[L_n,T^{ij}_m]=mT^{ij}_{n+m},\quad [L_n,T^i_m]=mT^i_{n+m},$$

$$[L_n,S^i_m]=mS^i_{n+m},\quad [L_n,\widetilde{S}^i_m]=(m+n)\widetilde{S}^i_{n+m},$$

$$[L_n,I^i_m]=(m+n)I^i_{n+m},\quad [L_n,I_m]=(m-n)I_{n+m},$$

$$[L_n,J^{ij}_m]=(m-n)J^{ij}_{n+m},\quad [L_n,\tilde{J}^{ij}_m]=(m+n)\tilde{J}^{ij}_{n+m},$$

$$[G^i_n,G^j_m]=(m-n)J^{ij}_{n+m},\quad [G^i_n,\tilde{G}^j_m]=mT^{ij}_{n+m},$$

$$[G^i_n,T^{ji}_m]=-G^j_{n+m}+mS^j_{n+m},\quad [G^i_n,T^i_m]=mS^i_{n+m},$$

$$[G^i_n,T^j_m]=G^i_{n+m},\quad [G^i_n,S^j_m]=J^{ij}_{n+m},$$

$$[G^i_n,\tilde{S}^j_m]=T^{ij}_{n+m},\quad [\tilde{G}^i_n,\tilde{G}^j_m]=(m-n)\tilde{J}^{ij}_{n+m},$$

$$[\tilde{G}^i_n,S^i_m]=T^i_{n+m},\quad [\tilde{G}^i_n,S^j_m]=T^{ji}_{n+m},$$

$$[\tilde{G}^i_n,\tilde{S}^j_m]=-\tilde{J}^{ij}_{n+m},\quad [\tilde{G}^i_n,J^{ij}_m]=G^j_{n+m},$$

$$[T^{ij}_n,T^{ji}_m]=T^i_{n+m}-T^j_{n+m},\quad [T^{ij}_n,T^{jk}_m]=T^{ik}_{n+m},$$

$$[T^{ij}_n,T^{ki}_m]=-T^{kj}_{n+m},\quad [T^{ij}_n,T^i_m]=-T^{ij}_{n+m},$$

$$[T^{ij}_n,T^j_m]=T^{ij}_{n+m},\quad [T^{ij}_n,S^j_m]=S^i_{n+m},$$

$$[T^{ij}_n,\tilde{S}^i_m]=\tilde{S}^j_{n+m},\quad [T^{ij}_n,\tilde{S}^k_m]=-2I^i_{n+m},$$

$$[T^{ij}_n,I^j_m]=-\tilde{S}^k_{n+m},\quad [T^{ij}_n,J^{jk}_m]=J^{ik}_{n+m},$$

$$[T^{ij}_n,\tilde{J}^{ik}_m]=-\tilde{J}^{jk}_{n+m},\quad [T^j_n,S^i_m]=-S^i_{n+m},$$

$$[T^j_n,\tilde{S}^i_m]=\tilde{S}^i_{n+m},\quad [T^i_n,I^i_m]=2I^i_{n+m},$$

$$[T^i_n,I_m]=-2I_{n+m},\quad [T^i_n,J^{ij}_m]=[T^j_n,J^{ij}_m]=-J^{ij}_{n+m},$$

$$[T^k_n,J^{ij}_m]=-2J^{ij}_{n+m},\quad [T^i_n,\tilde{J}^{ij}_m]=[T^j_n,\tilde{J}^{ij}_m]=\tilde{J}^{ij}_{n+m},$$

$$[T^k_n,\tilde{J}^{ij}_m]=2\tilde{J}^{ij}_{n+m},\quad [J^{ij}_n,\tilde{J}^{ij}_m]=T^k_{n+m},$$

$$[J^{ij}_n,\tilde{J}^{ik}_m]=-T^{jk}_{n+m},\quad [J^{ij}_n,\tilde{J}^{jk}_m]=T^{ik}_{n+m}. \tag{5.8}$$

Let (i,j,k) be the cycle $(1,2,3)$, then

$$[G^i_n,\tilde{G}^i_m]=L_{n+m}-mT^k_{n+m},\quad [G^i_n,\tilde{S}^i_m]=T^j_{n+m}-T^k_{n+m},$$

$$[G^i_n,I^j_m]=T^{jk}_{n+m},\quad [G^i_n,I^k_m]=-T^{kj}_{n+m},$$

$$[G_n^i, J_m^{jk}] = (m-n)I_{n+m}, \quad [G_n^i, \widetilde{J}_m^{jk}] = (m+n)I_{n+m}^i,$$

$$[G_n^i, \widetilde{J}_m^{ij}] = \widetilde{G}_{n+m}^j - (n+m)\widetilde{S}_{n+m}^j, \quad [G_n^i, \widetilde{J}_m^{ik}] = \widetilde{G}_{n+m}^k,$$

$$[\widetilde{G}_n^i, T_m^{ij}] = \widetilde{G}_{n+m}^j - n\widetilde{S}_{n+m}^j, \quad [\widetilde{G}_n^i, T_m^{ik}] = \widetilde{G}_{n+m}^k - (n+m)\widetilde{S}_{n+m}^k,$$

$$[\widetilde{G}_n^i, T_m^{jk}] = (m+n)I_{n+m}^j, \quad [\widetilde{G}_n^i, T_m^{kj}] = (n-m)I_{n+m}^k,$$

$$[\widetilde{G}_n^i, T_m^j] = -\widetilde{G}_{n+m}^i + m\widetilde{S}_{n+m}^i, \quad [\widetilde{G}_n^i, T_m^k] = -\widetilde{G}_{n+m}^i,$$

$$[\widetilde{G}_n^i, I_m^i] = \widetilde{J}_{n+m}^{jk}, \quad [\widetilde{G}_n^i, I_m] = J_{n+m}^{jk},$$

$$[S_n^i, J_m^{jk}] = -2I_{n+m}, \quad [S_n^i, \widetilde{J}_m^{ij}] = -\widetilde{S}_{n+m}^j,$$

$$[S_n^i, \widetilde{J}_m^{ik}] = \widetilde{S}_{n+m}^k, \quad [S_n^i, \widetilde{J}_m^{jk}] = 2I_{n+m}^i,$$

$$[\widetilde{S}_n^i, J_m^{ij}] = S_{n+m}^j, \quad [\widetilde{S}_n^i, J_m^{ik}] = -S_{n+m}^k,$$

$$[I_n^i, J_m^{jk}] = -S_{n+m}^i, \quad [I_n, \widetilde{J}_m^{ij}] = S_{n+m}^k. \tag{5.9}$$

□

VI. REPRESENTATION OF CK_6 ASSOCIATED WITH ITS EMBEDDING INTO $P_{h=1}(6)$

Recall that the embedding (1.2) for $h=1$ allows us to define a one-parameter family of spinor-like representations of $K'(4)$ in the superspace spanned by 2 even and 2 odd fields, where the central element $1 \in P_1(4)$ acts by the identity operator.[21]

Theorem 6.1: There exists a one-parameter family of irreducible representations of CK_6, depending on parameter $\mu \in \mathbb{C}$, in a superspace spanned by 4 even fields and 4 odd fields.

Proof: Let $V^\mu = t^\mu \mathbb{C}[t,t^{-1}] \otimes \Lambda(3)$, where $\Lambda(3) = \Lambda(\xi_1, \xi_2, \xi_3)$ is the Grassmann algebra, and $\mu \in \mathbb{C}\backslash\mathbb{Z}$. Let $\{v_m^i, \hat{v}_m^i\}$, where $m \in \mathbb{Z}$ and $1 \leqslant i \leqslant 4$, be the following basis in V^μ:

$$v_m^i = \frac{t^{m+\mu}}{m+\mu}\xi_i, \quad \hat{v}_m^i = t^{m+\mu}\xi_j\xi_k, \quad 1 \leqslant i \leqslant 3, \quad v_m^4 = \frac{t^{m+\mu}}{m+\mu}, \quad \hat{v}_m^4 = -t^{m+\mu}\xi_1\xi_2\xi_3, \tag{6.1}$$

where (i,j,k) is the cycle $(1,2,3)$ in the formulas for $\hat{v}_m^i$. We define a representation of CK_6 in V^μ according to the formulas (5.6), where $h=1$. Namely, ξ_i is the operator of multiplication in $\Lambda(3)$, η_i is identified with ∂_{ξ_i}, and τ^{-1} is identified with the antiderivative:

$$\tau^{-1}g(t) = \int g(t)\mathrm{d}t, \quad g \in t^\mu \mathbb{C}[t,t^{-1}]. \tag{6.2}$$

Notice that

$$(\tau^{-1} \circ_{h=1} f)(g) = \tau^{-1}(fg) \tag{6.3}$$

for any $f \in \mathbb{C}[t,t^{-1}]$ and $g \in t^\mu \mathbb{C}[t,t^{-1}]$. Observe that

$$\tau^{-1}\circ_{h=1} f = \sum_{n=0}^{\infty} (-1)^n (\tau^n f)\tau^{-n-1}. \tag{6.4}$$

Thus the formula (6.3) is simply the formula of integration by parts:

$$f\int g\,\mathrm{d}t - f'\int\int g\,\mathrm{d}t^2 + f''\int\int\int g\,\mathrm{d}t^3 - \cdots = \int fg\,\mathrm{d}t. \tag{6.5}$$

The superalgebra CK_6 acts on $V^\mu = Span(v_m^i, \hat{v}_m^i \mid 1 \leqslant i \leqslant 4, m \in \mathbb{Z})$ as follows (see (5.7) for notations):

$$\begin{gathered}
L_n(v_m^i) = (m+n+\mu)v_{m+n}^i, \quad L_n(\hat{v}_m^i) = (m+\mu)\hat{v}_{m+n}^i,\\
G_n^i(v_m^4) = (m+n+\mu)v_{m+n}^i, \quad G_n^i(\hat{v}_m^i) = -(m+\mu)\hat{v}_{m+n}^4,\\
G_n^i(v_m^j) = \hat{v}_{m+n}^k, \quad G_n^i(v_m^k) = -\hat{v}_{m+n}^j,\\
\widetilde{G}_n^i(v_m^i) = v_{m+n}^4, \quad \widetilde{G}_n^i(\hat{v}_m^4) = -\hat{v}_{m+n}^i,\\
\widetilde{G}_n^i(\hat{v}_m^j) = -(m+\mu)v_{m+n}^k, \quad \widetilde{G}_n^i(\hat{v}_m^k) = (m+n+\mu)v_{m+n}^j,\\
T_n^{ij}(v_m^j) = v_{m+n}^i, \quad T_n^{ij}(\hat{v}_m^i) = -\hat{v}_{m+n}^j,\\
T_n^i(v_m^i) = v_{m+n}^i, \quad T_n^i(v_m^4) = v_{m+n}^4,\\
T_n^i(\hat{v}_m^i) = -\hat{v}_{m+n}^i, \quad T_n^i(\hat{v}_m^4) = -\hat{v}_{m+n}^4,\\
S_n^i(v_m^4) = v_{m+n}^i, \quad S_n^i(\hat{v}_m^i) = \hat{v}_{m+n}^4,\\
\widetilde{S}_n^i(\hat{v}_m^j) = v_{m+n}^k, \quad \widetilde{S}_n^i(\hat{v}_m^k) = v_{m+n}^j,\\
I_n^i(\hat{v}_m^i) = -v_{m+n}^i, \quad I_n(v_m^4) = -\hat{v}_{m+n}^4,\\
J_n^{ij}(v_m^4) = \hat{v}_{m+n}^k, \quad J_n^{ij}(v_m^k) = -\hat{v}_{m+n}^4,\\
\widetilde{J}_n^{ij}(\hat{v}_m^k) = -v_{m+n}^4, \quad \widetilde{J}_n^{ij}(\hat{v}_m^4) = v_{m+n}^k,
\end{gathered} \tag{6.6}$$

where (i,j,k) is the cycle $(1,2,3)$ in the formulas for $\widetilde{G}_n^i$, $\widetilde{S}_n^i$, J_n^{ij}, and $\widetilde{J}_n^{ij}$. □

Remark 6.2: We have posed the condition $\mu \in \mathbb{C}\backslash\mathbb{Z}$ in the definition of V^μ. However, formulas (6.6) actually define a representation of CK_6 in a superspace spanned by v_m^i, $\hat{v}_m^i$ for an arbitrary $\mu \in \mathbb{C}$. (See also Sec. VIII.)

VII. SECOND FAMILY OF REPRESENTATIONS OF CK_6

Note that the embedding of infinite-dimensional Lie superalgebras

$$CK_6 \subset K(6), \tag{7.1}$$

considered in this work, is naturally related to the embedding of finite-dimensional Lie superalgebras

$$\hat{\mathcal{P}}(4) \subset P(0|6). \tag{7.2}$$

Recall that $P(0|6)$ is the Poisson superalgebra with 6 odd generators: $\xi_1, \xi_2, \xi_3, \eta_1, \eta_2, \eta_3$, and the Poisson bracket is given by (2.6). The simple Lie superalgebra $\mathcal{P}(n)$ is defined as follows. Let $\widetilde{\mathcal{P}}(n)$ be the Lie superalgebra, which preserves the odd nondegenerate supersymmetric bilinear form antidiag $(1_n, 1_n)$ on the $(n|n)$-dimensional superspace. Thus

$$\widetilde{\mathcal{P}}(n) = \left\{ \begin{pmatrix} A & B \\ C & -A^t \end{pmatrix} \middle| A \in \mathfrak{gl}(n), \quad B^t = B, \quad C^t = -C \right\}. \tag{7.3}$$

$\mathcal{P}(n)$ is a subsuperalgebra of $\widetilde{\mathcal{P}}(n)$ such that $A \in \mathfrak{sl}(n)$.[24] A. Sergeev has proved that $\mathcal{P}(n)$ has a nontrivial central extension if and only if $N=4$; see Refs. 5, 8, 12, and 13. Note that $\dim \hat{\mathcal{P}}(4) = (16|16)$. It was pointed out in Refs. 5, 8, 9, 12, and 13 that $\hat{\mathcal{P}}(4)$ has a family spin_λ of $(4|4)$-dimensional irreducible representations. In fact, there exist two non-isomorphic families: they correspond to two families of embeddings of $\hat{\mathcal{P}}(4)$ into $P(0|6)$.

For every $\lambda \neq 0$ we can realize $\hat{\mathcal{P}}(4)$ inside $P(0|6)$ as follows:

$$\hat{\mathcal{P}}(4) = Span(L, G^i, \widetilde{G}^i, T^{ij}, T^i, S^i, \widetilde{S}^i, I^i, I, J^{ij}, \widetilde{J}^{ij}), \tag{7.4}$$

where

$$L = \lambda, \quad G^i = \lambda \eta_i, \quad \widetilde{G}^i = \xi_i,$$

$$T^{ij} = \eta_i \xi_j, \quad i \neq j, \quad T^i = -\eta_j \xi_j - \eta_k \xi_k,$$

$$S^i = -\eta_i(\eta_j \xi_j + \eta_k \xi_k), \quad \widetilde{S}^i = \frac{1}{\lambda}(\eta_j \xi_j - \eta_k \xi_k)\xi_i, \tag{7.5}$$

$$I^i = \frac{1}{\lambda}\eta_i \xi_j \xi_k, \quad I = \lambda \eta_1 \eta_2 \eta_3,$$

$$J^{ij} = \lambda \eta_i \eta_j, \quad \widetilde{J}^{ij} = \frac{1}{\lambda}\xi_i \xi_j, \quad i < j,$$

so that L is its central element; (i,j,k) is the cycle $(1,2,3)$ in the formulas for T^i, S^i, J^i, and I^i. Correspondingly, there is an embedding $j_h : \hat{\mathcal{P}}(4) \to P_h(0|6)$ given by

$$L_h = \lambda, \quad G_h^i = \lambda \eta_i, \quad \widetilde{G}_h^i = \xi_i,$$

$$T_h^{ij} = \eta_i \xi_j, \quad T_h^i = -\eta_j \xi_j - \eta_k \xi_k + h,$$

$$S_h^i = -\eta_i(\eta_j \xi_j + \eta_k \xi_k) + h\eta_i, \quad \widetilde{S}_h^i = \frac{1}{\lambda}(\xi_j \xi_i \eta_j - \xi_k \xi_i \eta_k),$$

$$I_h^i = \frac{1}{\lambda}\xi_j \xi_k \eta_i, \quad I_h = \lambda \eta_1 \eta_2 \eta_3,$$

$$J_h^{ij} = \lambda \eta_i \eta_j, \quad \tilde{J}_h^{ij} = \frac{1}{\lambda} \xi_i \xi_j, \tag{7.6}$$

and $\lim_{h\to 0} j_h(\hat{\mathcal{P}}(4)) = \hat{\mathcal{P}}(4) \subset P(0|6)$. The nonvanishing commutation relations between the elements (7.5) and between the elements (7.6) are as in (5.8) and (5.9), where the indices $m=n=0$.

Associated to this embedding (for $h=1$) there is a family spin_λ^1 of representations of $\hat{\mathcal{P}}(4)$ in the superspace $\Lambda(\xi_1, \xi_2, \xi_3)$. We choose the basis

$$v^i = \xi_i, \quad \hat{v}^i = \frac{1}{\lambda} \xi_j \xi_k, \quad 1 \leqslant i \leqslant 3, \quad v^4 = 1, \quad \hat{v}^4 = -\frac{1}{\lambda} \xi_1 \xi_2 \xi_3, \tag{7.7}$$

where (i,j,k) is the cycle $(1,2,3)$ in the formulas for $\hat{v}^i$. Explicitly,

$$\text{spin}_\lambda^1 : \begin{pmatrix} A & B \\ C & -A^t \end{pmatrix} + \mathbb{C}L \to \begin{pmatrix} A & B - \lambda \tilde{C} \\ C & -A^t \end{pmatrix} + \mathbb{C}\lambda \cdot 1_{4|4}, \tag{7.8}$$

where $1_{4|4}$ is the identity matrix, and if $C_{ij} = E_{ij} - E_{ji}$, then $\tilde{C}_{ij} = C_{kl}$, so that the permutation $(1,2,3,4) \mapsto (i,j,k,l)$ is even; cf. Refs. 5,8,9,12, and 13. Formula (7.8) also gives the standard representation spin_0^1.

The second family of embeddings of $\hat{\mathcal{P}}(4)$ into $P(0|6)$ and into $P_h(0|6)$ is given by (7.4)–(7.6), where ξ_i is interchanged with η_i for all i in all the formulas. There is a family spin_λ^2 of representations of $\hat{\mathcal{P}}(4)$ associated to this embedding (for $h=1$) in the superspace $\Lambda(\xi_1, \xi_2, \xi_3)$, so that $\Pi(\text{spin}_\lambda^2) \cong \text{spin}_\lambda^1$, as $\hat{\mathcal{P}}(4)$ modules, for all λ.

(Π denotes the change of parity). Theorem 6.1 has the following corollary.

Corollary 7.1: Under the restriction of the representation of CK_6 in V^μ to $\hat{\mathcal{P}}(4)$, V^μ decomposes into a direct sum of irreducible $(4|4)$-dimensional submodules of the family spin_λ^2.

Proof: Naturally, there are embeddings:

$$\hat{\mathcal{P}}(4) \subset CK_6, \quad P(0|6) \subset K(6). \tag{7.9}$$

The first embedding is given as follows:

$$\hat{\mathcal{P}}(4) = \{x \in CK_6 \mid [L_0, x] = 0\}. \tag{7.10}$$

Hence $\hat{\mathcal{P}}(4)$ is spanned by the elements (5.7), where $n=0$, and L_0 is its central element. The nontrivial 2-cocycle on $\mathcal{P}(4)$ is $(G_0^i, \tilde{G}_0^j) = \delta_{i,j} L_0$. It follows from (6.6) that V^μ is a direct sum of $(4|4)$-dimensional $\hat{\mathcal{P}}(4)$ submodules:

$$V^\mu = \oplus_{m \in \mathbb{Z}} V_m^\mu, \quad V_m^\mu = Span(v_m^i, \hat{v}_m^i \mid 1 \leqslant i \leqslant 4), \tag{7.11}$$

where $V_m^\mu \cong \text{spin}_{m+\mu}^2$. □

It is possible to define another embedding of CK_6 into $P(6)$ (respectively, into $P_h(6)$) by interchanging ξ_i with η_i in all the formulas (4.1) (respectively, in (5.6)), and then obtain a one-parameter family of representations of CK_6 in V^μ by repeating the previous construction. Thus the following theorem holds.

Theorem 7.2: Consider the following basis in V^μ:

$$v_m^i = t^{m+\mu} \xi_i, \quad \hat{v}_m^i = \frac{t^{m+\mu}}{m+\mu} \xi_j \xi_k, \quad 1 \leqslant i \leqslant 3, \quad v_m^4 = t^{m+\mu}, \quad \hat{v}_m^4 = -\frac{t^{m+\mu}}{m+\mu} \xi_1 \xi_2 \xi_3, \tag{7.12}$$

where (i,j,k) is the cycle $(1,2,3)$ in the formulas for $\hat{v}_m^i$. Then the action of CK_6 on V^μ is defined as follows

$$L_n(v_m^i) = (m+\mu) v_{m+n}^i, \quad L_n(\hat{v}_m^i) = (m+n+\mu) \hat{v}_{m+n}^i,$$

$$G_n^i(v_m^i) = (m+\mu)v_{m+n}^4, \quad G_n^i(\hat{v}_m^4) = -(m+n+\mu)\hat{v}_{m+n}^i,$$

$$G_n^i(\hat{v}_m^k) = v_{m+n}^j, \quad G_n^i(\hat{v}_m^j) = -v_{m+n}^k,$$

$$\widetilde{G}_n^i(v_m^4) = v_{m+n}^i, \quad \widetilde{G}_n^i(\hat{v}_m^i) = -\hat{v}_{m+n}^4,$$

$$\widetilde{G}_n^i(v_m^k) = -(m+n+\mu)\hat{v}_{m+n}^j, \quad \widetilde{G}_n^i(v_m^j) = (m+\mu)\hat{v}_{m+n}^k,$$

$$T_n^{ij}(v_m^i) = -v_{m+n}^j, \quad T_n^{ij}(\hat{v}_m^j) = \hat{v}_{m+n}^i,$$

$$T_n^i(v_m^i) = -v_{m+n}^i, \quad T_n^i(v_m^4) = -v_{m+n}^4, \tag{7.13}$$

$$T_n^i(\hat{v}_m^i) = \hat{v}_{m+n}^i, \quad T_n^i(\hat{v}_m^4) = \hat{v}_{m+n}^4,$$

$$S_n^i(v_m^i) = -v_{m+n}^4, \quad S_n^i(\hat{v}_m^4) = -\hat{v}_{m+n}^i,$$

$$\widetilde{S}_n^i(v_m^k) = -\hat{v}_{m+n}^j, \quad \widetilde{S}_n^i(v_m^j) = -\hat{v}_{m+n}^k,$$

$$I_n^i(v_m^i) = \hat{v}_{m+n}^i, \quad I_n(\hat{v}_m^4) = v_{m+n}^4,$$

$$J_n^{ij}(\hat{v}_m^k) = -v_{m+n}^4, \quad J_n^{ij}(\hat{v}_m^4) = v_{m+n}^k,$$

$$\widetilde{J}_n^{ij}(v_m^4) = \hat{v}_{m+n}^k, \quad \widetilde{J}_n^{ij}(v_m^k) = -\hat{v}_{m+n}^4,$$

where (i,j,k) is the cycle $(1,2,3)$ in the formulas for $\widetilde{G}_n^i$, $\widetilde{S}_n^i$, J_n^{ij}, and $\widetilde{J}_n^{ij}$. Thus V^μ is a direct sum of $(4|4)$-dimensional $\hat{\mathcal{P}}(4)$ submodules, see (7.11), where $V_m^\mu \cong \mathrm{spin}_{m+\mu}^1$.

VIII. FINAL REMARKS

Theorem 8.1: $CK_6 \subset P_h(6)$ is generated by $t^n\tau\Lambda(\xi_1,\xi_2,\xi_3)$ and $\tau^{-1}\circ_h t^n\eta_i\eta_j$, where $n\in\mathbb{Z}$.

Proof: It follows from (5.7)–(5.9) that $L_{n,h}$, $G_{n,h}^i$, $J_{n,h}^{ij}$, $I_{n,h}$, and $\widetilde{J}_{n,h}^{ij}$ generate CK_6. □

We fix $h=1$. Let $\mu\in(0,1)$. In each V^μ we defined a basis by (6.1). We will denote it now by $\{v_{\underline{m}}^i(\mu),\hat{v}_m^i(\mu)\}$. Let $\underline{V}=Span(v_m^i,\hat{v}_m^i \mid 1\leqslant i\leqslant 4, m\in\mathbb{Z})$, be a superspace such that $p(\hat{v}_m^i)=p(v_m^4)=\overline{0}$, $p(v_m^i)=p(\hat{v}_m^4)=\overline{1}$. Let $v\in V$ and let $v(\mu)\in V^\mu$ be the vector with the same coordinates as v with respect to the basis (6.1). Consider the odd nondegenerate superskew-symmetric bilinear form on each V^μ given by

$$(v_m^i(\mu),\hat{v}_l^i(\mu)) = -(\hat{v}_l^i(\mu),v_m^i(\mu)) = -(v_m^4(\mu),\hat{v}_l^4(\mu)) = (\hat{v}_l^4(\mu),v_m^4(\mu)) = \delta_{m+l,0}, \tag{8.1}$$

where $1\leqslant i\leqslant 3$. The odd nondegenerate superskew-symmetric bilinear form on V is given by

$$(v_m^i,\hat{v}_l^i) = -(\hat{v}_l^i,v_m^i) = -(v_m^4,\hat{v}_l^4) = (\hat{v}_l^4,v_m^4) = \delta_{m+l,0}. \tag{8.2}$$

Theorem 8.2: Let $X\in CK_6$. Then

$$\lim_{\mu\to 0}[(Xv(\mu),w(\mu)) + (-1)^{p(X)p(v(\mu))}(v(\mu),Xw(\mu))] = 0 \quad \text{for all } v,w\in V. \tag{8.3}$$

There is a representation of CK_6 in V given by (6.6), where $\mu=0$, and this action preserves the form (8.2).

Remark 8.3: There is a representation of CK_6 in V given by (7.13), where $\mu=0$, and this action preserves the odd nondegenerate supersymmetric bilinear form on V:

$$(v_m^i,\hat{v}_l^i)=(\hat{v}_l^i,v_m^i)=\delta_{m+l,0},\quad 1\leqslant i\leqslant 4. \tag{8.4}$$

Remark 8.4: Each of the representations of CK_6 in V given by (6.6) and (7.13), where $\mu=0$, decomposes into a direct sum of irreducible $\hat{\mathcal{P}}(4)$ modules:

$$V=\oplus_{m\in\mathbb{Z}}V_m,\quad V_m=Span(v_m^i,\hat{v}_m^i \mid 1\leqslant i\leqslant 4), \tag{8.5}$$

where $V_m\cong \mathrm{spin}_m^2$ for the representation (6.6), and $V_m\cong \mathrm{spin}_m^1$ for the representation (7.13).

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Quantum trigonometric Calogero-Sutherland model, irreducible characters and Clebsch-Gordan series for the exceptional algebra E_7

J. Fernández Núñez and W. García Fuertes
Departamento de Física, Facultad de Ciencias, Universidad de Oviedo, E-33007 Oviedo, Spain

A. M. Perelomov[a)]
Departamento de Física Teórica, Universidad de Zaragoza, E-50009 Zaragoza, Spain

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We reexpress the quantum Calogero-Sutherland model for the Lie algebra E_7 and the particular value of the coupling constant $\kappa=1$ by using the fundamental irreducible characters of the algebra as dynamical variables. For that, we need to develop a systematic procedure to obtain all the Clebsch-Gordan series required to perform the change of variables. We describe how the resulting quantum Hamiltonian operator can be used to compute more characters and Clebsch-Gordan series for this exceptional algebra. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Integrable systems are important because they can be considered as 0th order perturbative approximations to nonintegrable systems. By integrability we mean here integrability in the sense of Liouville, that is, the existence of a complete set of mutually commuting integrals of motion. During the three last decades of the past century, a plethora of highly nontrivial (classical and quantum) mechanical integrable systems were discovered, see Refs. 1 and 2 for comprehensive reviews. Among these, the Calogero-Sutherland models form a distinguished class. The first analysis of a system of this kind was performed by Calogero[3] who studied, from the quantum standpoint, the dynamics on the infinite line of a set of particles interacting pairwise by rational plus quadratic potentials, and found that the problem was exactly solvable. Soon afterwards, Sutherland[4] arrived to similar results for the quantum problem on the circle, this time with trigonometric interaction; and later Moser[5] proved, in terms of Lax pairs, that the classical counterparts of these models also enjoyed integrability.

The identification of the general scope of these discoveries came with the work of Olshanetsky and Perelomov,[6–8] who realized that it is possible to associate models of this kind to all the root systems of the simple Lie algebras, and that all these models are integrable, both in the classical and the quantum framework,[9,10] for interactions of the type rational (or inverse-square), q^{-2}; rational+quadratic, $q^{-2}+\omega^2 q^2$; trigonometric, $\sin^{-2} q$; hyperbolic, $\sinh^{-2} q$. For the most general case, given by the Weierstrass elliptic function $\mathcal{P}(q)$, see Refs. 2 and 10. Nowadays, there is a widespread interest in this kind of integrable systems, and many mathematical and physical applications for them have been found, see for instance Ref. 11. In Physics, we mention, among others, the remarkable connection established[12,13] between the different Calogero-Sutherland models and the properties of the equations describing the physics of disordered wires (the DMPK equation); the results are in good agreement with the experimental observations.

[a)]On leave of absence from the Institute for Theoretical and Experimental Physics, 117259, Moscow, Russia. Electronic mail: perelomo@mpim-bonn.mpg.de

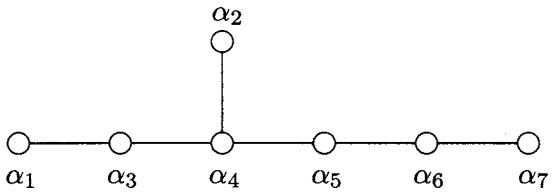

FIG. 1. The Dynkin diagram for the Lie algebra E_7.

The study of the form and properties of the Schrödinger eigenfunctions for the quantum version of these models constitutes by itself an interesting line of research. In fact, these eigenfunctions have very rich mathematical properties. In particular, for the trigonometric case, if we tune the coupling constants to some special values, the wave functions correspond to the characters of the simple Lie algebras, while if we select a different tuning, we can make them to coincide with zonal spherical functions. Thus, the Calogero-Sutherland theories provide us with a new tool for computing these quantities. In this spirit, we will describe in the present paper how to use the trigonometric Calogero-Sutherland model to obtain both particular characters and Clebsch-Gordan series for the exceptional Lie algebra E_7. The main point of our approach is to express the Hamiltonian in a suitable set of independent variables, indeed the fundamental characters of E_7. The use of such types of variables has been quite useful to solve the Schrödinger equation for the models associated to some algebras.[6,14–21]

The organization of the paper is as follows. Section II is a reminder of the properties of E_7 relevant for the contents of the paper. Section III describes the main properties of the Calogero-Sutherland models associated to root systems and explains how to find the Hamiltonian in the variables mentioned above. Section IV gives some account of the computation of the Clebsch-Gordan series of E_7 needed to pass to the new variables. In Sec. V we present the Hamiltonian in these variables and describe its use for computing new characters and to reduce tensor products of representations. Some conclusions are given in Sec. VI, and finally, the appendixes show some explicit results for characters and Clebsch-Gordan series of E_7.

II. SUMMARY OF RESULTS ON THE LIE ALGEBRA E_7

In this section, we review some standard facts about the root and weight systems of the Lie algebra E_7, with the aim of fixing the notation and help the reader to follow the rest of the paper. More extensive and sound treatments of these topics can be found in many excellent textbooks, see for instance Refs. 22 and 23.

The complex Lie algebra E_7 has dimension 133 and rank 7, as the name suggests. From the geometrical point of view, it admits (with some subtleties, see Ref. 24) an interpretation which extends the standard-one for the classical algebras: in the same way that these correspond to the isometries of projective spaces over the first three normed division algebras—$\mathrm{SO}(n+1) \simeq \mathrm{Isom}(\mathbf{R}P^n)$, $\mathrm{SU}(n+1) \simeq \mathrm{Isom}(\mathbf{C}P^n)$, $\mathrm{Sp}(n+1) \simeq \mathrm{Isom}(\mathbf{H}P^n)$—$F_4$, E_6, E_7, and E_8 are the Lie algebras of the projective planes over extensions of the octonions, giving rise to the so-called "magic square," $F_4 \simeq \mathrm{Isom}(\mathbf{O}P^2)$, $E_6 \simeq \mathrm{Isom}[(\mathbf{C}\otimes\mathbf{O})P^2]$, $E_7 \simeq \mathrm{Isom}[(\mathbf{H}\otimes\mathbf{O})P^2]$, $E_8 \simeq \mathrm{Isom}[(\mathbf{O}\otimes\mathbf{O})P^2]$.

The Dynkin diagram of E_7, see Fig. 1, encodes the Euclidean relations $A_{ij}=(\alpha_i,\alpha_j)$ among the simple roots, which are

$$(\alpha_i,\alpha_i)=2, \quad i=1,\ldots,7,$$

$$(\alpha_i,\alpha_{i+2})=-1, \quad i=1,2,$$

$$(\alpha_i,\alpha_{i+1})=-1, \quad i=3,\ldots,6,$$

$$(\alpha_i, \alpha_j) = 0, \quad \text{in all other cases.} \tag{1}$$

Therefore, the Cartan matrix $A=(A_{ij})$ and its inverse $A^{-1}=(A_{ij}^{-1})$ read

$$A = \begin{pmatrix} 2 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 2 \end{pmatrix}, \quad A^{-1} = \frac{1}{2}\begin{pmatrix} 4 & 4 & 6 & 8 & 6 & 4 & 2 \\ 4 & 7 & 8 & 12 & 9 & 6 & 3 \\ 6 & 8 & 12 & 16 & 12 & 8 & 4 \\ 8 & 12 & 16 & 24 & 18 & 12 & 6 \\ 6 & 9 & 12 & 18 & 15 & 10 & 5 \\ 4 & 6 & 8 & 12 & 10 & 8 & 4 \\ 2 & 3 & 4 & 6 & 5 & 4 & 3 \end{pmatrix}. \tag{2}$$

Throughout this paper we will use a realization of this root system in terms of a system of vectors $\{v_i\}_{i=1,\ldots,8}$ of $\mathbf{R}^8$ [endowed with the standard Euclidean product $(,)$] satisfying the relations $(v_i, v_j) = -\frac{1}{8} + \delta_{ij}$.[22] With reference to this system, E_7 is the root system in the hyperplane $V \subset \mathbf{R}^8$ of equation $\sum_i v_i = 0$ given by $\mathcal{R} = \{v_i - v_j, v_i + v_j + v_k + v_l \,|\, i \neq j \neq k \neq l\}$, the positive ones being those in the subset $\mathcal{R}^+ = \{v_i - v_j, v_8 - v_i, v_i + v_j + v_k + v_8 \,|\, i < j < k < 8\}$. There are 63 positive roots, which can be classified by heights as indicated in Table I. The seven simple roots are

$$\alpha_1 = v_1 - v_2, \quad \alpha_2 = v_4 + v_5 + v_6 + v_7,$$

$$\alpha_3 = v_2 - v_3, \quad \alpha_4 = v_3 - v_4,$$

$$\alpha_5 = v_4 - v_5, \quad \alpha_6 = v_5 - v_6,$$

$$\alpha_7 = v_6 - v_7, \tag{3}$$

which clearly satisfy the relations (1).

The hyperplane V can be viewed as $\mathbf{R}^7$, and the basis made with the vectors $v_1, \ldots, v_7$ is related to the canonical basis $\{e_k\}_{k=1,\ldots,7}$ by $v_k = e_k - \frac{1}{7}[1 + (1/\sqrt{8})]\sum_{j=1}^{7} e_j$; thus, the simple roots α_i are given by

$$\alpha_1 = e_1 - e_2,$$

$$\alpha_2 = \frac{1}{7}\left(3 - \frac{2}{\sqrt{2}}\right)\sum_{j=4}^{7} e_j - \frac{4}{7}\left(1 + \frac{1}{\sqrt{8}}\right)\sum_{j=1}^{3} e_j,$$

$$\alpha_k = e_{k-1} - e_k, \quad k = 3, \ldots, 7. \tag{4}$$

The fundamental weights $\lambda_i = \sum_{j=1}^{7} A_{ji}^{-1} \alpha_j$ are

$$\lambda_1 = v_1 - v_8,$$

$$\lambda_2 = -2v_8,$$

$$\lambda_3 = v_1 + v_2 - 2v_8,$$

$$\lambda_4 = v_1 + v_2 + v_3 + 3v - 3v_8,$$

$$\lambda_5 = v_1 + v_2 + v_3 + v_4 - 2v_8,$$

TABLE I. Heights of positive roots of E_7.

ht	Positive roots
1	$\alpha_1,\ \alpha_2,\ \alpha_3,\ \alpha_4,\ \alpha_5,\ \alpha_6,\ \alpha_7$
2	$\alpha_1+\alpha_3,\ \alpha_3+\alpha_4,\ \alpha_4+\alpha_5,\ \alpha_5+\alpha_6,\ \alpha_2+\alpha_4,\ \alpha_6+\alpha_7$
3	$\alpha_1+\alpha_3+\alpha_4,\ \alpha_3+\alpha_4+\alpha_5,\ \alpha_4+\alpha_5+\alpha_6,\ \alpha_2+\alpha_3+\alpha_4,\ \alpha_2+\alpha_4+\alpha_5,\ \alpha_5+\alpha_6+\alpha_7$
4	$\alpha_1+\alpha_3+\alpha_4+\alpha_5,\ \alpha_3+\alpha_4+\alpha_5+\alpha_6,\ \alpha_1+\alpha_2+\alpha_3+\alpha_4,\ \alpha_2+\alpha_3+\alpha_4+\alpha_5,$ $\alpha_2+\alpha_4+\alpha_5+\alpha_6,\ \alpha_4+\alpha_5+\alpha_6+\alpha_7$
5	$\alpha_1+\alpha_3+\alpha_4+\alpha_5+\alpha_6,\ \alpha_1+\alpha_2+\alpha_3+\alpha_4+\alpha_5,\ \alpha_2+\alpha_3+2\alpha_4+\alpha_5,$ $\alpha_2+\alpha_3+\alpha_4+\alpha_5+\alpha_6,\ \alpha_2+\alpha_4+\alpha_5+\alpha_6+\alpha_7,\ \alpha_3+\alpha_4+\alpha_5+\alpha_6+\alpha_7$
6	$\alpha_1+\alpha_2+\alpha_3+2\alpha_4+\alpha_5,\ \alpha_1+\alpha_2+\alpha_3+\alpha_4+\alpha_5+\alpha_6,\ \alpha_2+\alpha_3+2\alpha_4+\alpha_5+\alpha_6,$ $\alpha_1+\alpha_3+\alpha_4+\alpha_5+\alpha_6+\alpha_7,\ \alpha_2+\alpha_3+\alpha_4+\alpha_5+\alpha_6+\alpha_7$
7	$\alpha_1+\alpha_2+2\alpha_3+2\alpha_4+\alpha_5,\ \alpha_2+\alpha_3+2\alpha_4+2\alpha_5+\alpha_6,\ \alpha_1+\alpha_2+\alpha_3+2\alpha_4+\alpha_5+\alpha_6,$ $\alpha_1+\alpha_2+\alpha_3+\alpha_4+\alpha_5+\alpha_6+\alpha_7,\ \alpha_2+\alpha_3+2\alpha_4+\alpha_5+\alpha_6+\alpha_7$
8	$\alpha_1+\alpha_2+2\alpha_3+2\alpha_4+\alpha_5+\alpha_6,\ \alpha_1+\alpha_2+\alpha_3+2\alpha_4+2\alpha_5+\alpha_6,$ $\alpha_1+\alpha_2+\alpha_3+2\alpha_4+\alpha_5+\alpha_6+\alpha_7,\ \alpha_2+\alpha_3+2\alpha_4+2\alpha_5+\alpha_6+\alpha_7$
9	$\alpha_1+\alpha_2+2\alpha_3+2\alpha_4+2\alpha_5+\alpha_6,\ \alpha_1+\alpha_2+\alpha_3+2\alpha_4+2\alpha_5+\alpha_6+\alpha_7,$ $\alpha_1+\alpha_2+2\alpha_3+2\alpha_4+\alpha_5+\alpha_6+\alpha_7,\ \alpha_2+\alpha_3+2\alpha_4+2\alpha_5+2\alpha_6+\alpha_7$
10	$\alpha_1+\alpha_2+\alpha_3+2\alpha_4+2\alpha_5+2\alpha_6+\alpha_7,\ \alpha_1+\alpha_2+2\alpha_3+2\alpha_4+2\alpha_5+\alpha_6+\alpha_7,$ $\alpha_1+\alpha_2+2\alpha_3+3\alpha_4+2\alpha_5+\alpha_6$
11	$\alpha_1+2\alpha_2+2\alpha_3+3\alpha_4+2\alpha_5+\alpha_6,\ \alpha_1+\alpha_2+2\alpha_3+2\alpha_4+2\alpha_5+2\alpha_6+\alpha_7,$ $\alpha_1+\alpha_2+2\alpha_3+3\alpha_4+2\alpha_5+\alpha_6+\alpha_7$
12	$\alpha_1+\alpha_2+2\alpha_3+3\alpha_4+2\alpha_5+2\alpha_6+\alpha_7,\ \alpha_1+2\alpha_2+2\alpha_3+3\alpha_4+2\alpha_5+\alpha_6+\alpha_7$
13	$\alpha_1+\alpha_2+2\alpha_3+3\alpha_4+3\alpha_5+2\alpha_6+\alpha_7,\ \alpha_1+2\alpha_2+2\alpha_3+3\alpha_4+2\alpha_5+2\alpha_6+\alpha_7$
14	$\alpha_1+2\alpha_2+2\alpha_3+3\alpha_4+3\alpha_5+2\alpha_6+\alpha_7$
15	$\alpha_1+2\alpha_2+2\alpha_3+4\alpha_4+3\alpha_5+2\alpha_6+\alpha_7$
16	$\alpha_1+2\alpha_2+3\alpha_3+4\alpha_4+3\alpha_5+2\alpha_6+\alpha_7$
17	$2\alpha_1+2\alpha_2+3\alpha_3+4\alpha_4+3\alpha_5+2\alpha_6+\alpha_7$

$$\lambda_6 = v_1 + v_2 + v_3 + v_4 + v_5 - v_8,$$

$$\lambda_7 = v_1 + v_2 + v_3 + v_4 + v_5 + v_6,$$

as it follows from (2) and (3). As E_7 is simply laced, the geometry of the weight system is summarized by the relations $(\lambda_i,\lambda_j)=A_{ij}^{-1}$. The Weyl vector is

$$\rho = \frac{1}{2}\sum_{\alpha\in\mathcal{R}^+}\alpha = \sum_{i=1}^{7}\lambda_i = \frac{1}{2}(34\alpha_1 + 49\alpha_2 + 66\alpha_3 + 96\alpha_4 + 75\alpha_5 + 52\alpha_6 + 27\alpha_7),$$

and has length $|\rho|=\sqrt{798}/2$. The Weyl formula for dimensions applied to the irreducible representation associated to the integral dominant weight $\mu=\Sigma_{i=1}^{7}m_i\lambda_i$ gives

$$\dim R_\mu = \prod_{\alpha\in\mathcal{R}^+} \frac{(\alpha,\mu+\rho)}{(\alpha,\rho)} = \frac{P}{2^6\cdot 3^6\cdot 4^6\cdot 5^6\cdot 6^5\cdot 7^5\cdot 8^4\cdot 9^4\cdot 10^3\cdot 11^3\cdot 12^2\cdot 13^2\cdot 14\cdot 15\cdot 16\cdot 17},$$

where P is a product extended to the set of positive roots in which the root $\alpha=\Sigma_{i=1}^7 a_i\alpha_i$ contributes with a factor $\mathrm{ht}(\alpha)+\Sigma_{i=1}^7 a_i m_i$, where $\mathrm{ht}(\alpha)$ is the height of α. In particular, for the basic representations R_{λ_k}, one finds

$$\dim R_{\lambda_1} = 133, \quad \dim R_{\lambda_2} = 912,$$

$$\dim R_{\lambda_3} = 8645, \quad \dim R_{\lambda_4} = 365\,750,$$

$$\dim R_{\lambda_5} = 27\,664, \quad \dim R_{\lambda_6} = 1539,$$

$$\dim R_{\lambda_7} = 56.$$

All the irreducible representations are self-adjoint; R_{λ_1} is the adjoint representation and R_{λ_7}, the fundamental one.

III. THE TRIGONOMETRIC CALOGERO-SUTHERLAND MODEL ASSOCIATED TO A ROOT SYSTEM

First of all, we review briefly the general theory of the quantum trigonometric Calogero-Sutherland model related to a root system $\mathcal{R}$ associated to a simple Lie algebra L of rank r, and later study explicity the E_7 case. For Calogero-Sutherland systems other than trigonometric see Ref. 10; see also Ref. 25.

The trigonometric Calogero-Sutherland model related to the root system $\mathcal{R}$ of rank r is the quantum system in a Euclidean space $\mathbf{R}^r$ defined by the standard Hamiltonian operator

$$H = \frac{1}{2}\sum_{j=1}^{r} p_j^2 + \sum_{\alpha\in\mathcal{R}^+} \kappa_\alpha(\kappa_\alpha-1)\sin^{-2}(\alpha,q), \tag{5}$$

where $q=(q_j)$ is a Cartesian coordinate system and $p_j=-i\partial_{q_j}$; $\mathcal{R}^+$ is the set of the positive roots of L, and the coupling constants κ_α are such that $\kappa_\alpha=\kappa_\beta$ if $|\alpha|=|\beta|$. We will restrict ourselves to the case of simply laced root systems (as the E series is), for which the Calogero-Sutherland model depends only on one coupling constant κ.

Although the Hamiltonian (5) is defined in all $\mathbf{R}^r$, the configuration space is confined by the singularities (infinite walls) $(\alpha,q)=0$. If the q coordinates are assumed to take values in the $[0,\pi]$ interval, H can be interpreted as describing the dynamics of a system of r unit mass particles moving on the circle with interaction $V(q)=\kappa(\kappa-1)\Sigma_\alpha \sin^{-2}(\alpha,q)$, but notice that there is not translational invariance. The wave functions must be π periodic.

The main problem is to find the stationary states, i.e., to solve the Schrödinger eigenvalue problem $H\Psi=E\Psi$. The following important facts about this family of quantum mechanical systems were well established in Refs. 6 and 10.

(a) They are integrable, and moreover they are exactly solvable. The configuration space is confined to the Weyl alcove $\Lambda_W=\{q\in\mathbf{R}^r \,|\, 0<(\alpha,q)<\pi\}$.

(b) The ground state energy and (non-normalized) wave function are

$$E_0(\kappa) = 2\rho^2\kappa^2,$$

$$\Psi_0^\kappa(q) = \prod_{\alpha\in\mathcal{R}^+} \sin^\kappa(\alpha,q),$$

while the excited states are indexed by the highest weights $\mu=\Sigma m_i\lambda_i \in P^+$ (P^+ is the cone of dominant weights) of the irreducible representations of L, that is, by the r-tuple of non-negative integers $\mathbf{m}=(m_1,\ldots,m_r)$ (the quantum numbers), and the wave functions satisfy

$$\begin{aligned} H\Psi_{\mathbf{m}}^\kappa &= E_{\mathbf{m}}(\kappa)\Psi_{\mathbf{m}}^\kappa, \\ E_{\mathbf{m}}(\kappa) &= 2(\mu+\kappa\rho,\mu+\kappa\rho). \end{aligned} \tag{6}$$

(c) It is natural to look for the solutions $\Psi_{\mathbf{m}}^\kappa$ in the form

$$\Psi_{\mathbf{m}}^\kappa(q) = \Psi_0^\kappa(q)\Phi_{\mathbf{m}}^\kappa(q), \tag{7}$$

and consequently we are led to the eigenvalue problem

$$\Delta^\kappa\Phi_{\mathbf{m}}^\kappa = \varepsilon_{\mathbf{m}}(\kappa)\Phi_{\mathbf{m}}^\kappa, \tag{8}$$

where Δ^κ is the linear differential operator

$$\Delta^\kappa = -\frac{1}{2}\sum_{j=1}^r \partial_{q_j}^2 - \kappa\sum_{\alpha\in\mathcal{R}^+}\cot(\alpha,q)(\alpha,\nabla_q), \tag{9}$$

and the eigenvalues $\varepsilon_{\mathbf{m}}(\kappa)$ are the energies over the ground level, i.e.,

$$\varepsilon_{\mathbf{m}}(\kappa) = E_{\mathbf{m}}(\kappa) - E_0(\kappa) = 2(\mu,\mu+2\kappa\rho). \tag{10}$$

Taking into account that $(\lambda_j,\lambda_k)=A_{jk}^{-1}$, it is possible to give a more explicit expression for the eigenvalues $\varepsilon_{\mathbf{m}}(\kappa)$,

$$\varepsilon_{\mathbf{m}}(\kappa) = 2\sum_{j,k=1}^r A_{jk}^{-1}m_jm_k + 4\kappa\sum_{j,k=1}^r A_{jk}^{-1}m_j. \tag{11}$$

We will write $\varepsilon_j(\kappa)$ for the fundamental weight λ_j, i.e., for the quantum numbers $(0,\ldots,1^{(j)},\ldots,0)$.

(d) In the case $\kappa=0$ the wave functions (8) are (proportional to) the monomial symmetric functions

$$M_\lambda(q) = \sum_{w\in W} e^{2i(w\cdot\lambda,q)}, \quad \lambda\in P^+, \tag{12}$$

W being the Weyl group of L. And the wave functions in the case $\kappa=1$ are (proportional to) the characters of the irreducible representations

$$\boldsymbol{\chi}_\lambda(q) = \frac{\sum_{w\in W}(\det w)e^{2i(w\cdot(\lambda+\rho),q)}}{\sum_{w\in W}(\det w)e^{2i(w\cdot\rho,q)}}, \quad \lambda\in P^+. \tag{13}$$

Both M_λ and $\boldsymbol{\chi}_\lambda$ are sums over the orbit of λ under W, and consequently, W invariant; as wave functions, they represent superpositions of plane waves whose momenta are consistent with the required π periodicity.

(d) Due to the Weyl symmetry of the Hamiltonian, the wave functions $\Phi^{\kappa}_{\mathbf{m}}(q)$ are W invariant, and the best way to solve the eigenvalue problem (8) is to use the set of independent W-invariant variables $z_k=\boldsymbol{\chi}_{\lambda_k}(q)$, in terms of which the wave functions $\Phi^{\kappa}_{\mathbf{m}}$ are polynomials.

Unfortunately, the expression of these characters z_k in terms of the q variables is complicated and makes the direct change of variables $z=z(q)$ very cumbersome. We are thus forced to follow a much more convenient, indirect route, which has proven to be useful for other root systems.[20,21]

To this goal, the starting point is to write the operator Δ^{κ} in the z variables,

$$\Delta^{\kappa}=\sum_{j,k} a_{jk}(z)\partial_{z_j}\partial_{z_k}+\sum_j [b^0_j(z)+\kappa b^1_j(z)]\partial_{z_j}, \tag{14}$$

with $a_{jk}=a_{kj}$. Now, if we take into account the fact that, as pointed above, $b^0_j(z)+b^1_j(z)=\Delta^1 z_j=\varepsilon_j(1)z_j$, the full expression for the coefficients $b_j(q)=b^0_j(z)+b^1_j(z)$ appearing in Δ^1 is completely determined by the Cartan matrix of the algebra; explicitly,

$$b_j(z)=2\left(A^{-1}_{jj}+2\sum_k A^{-1}_{kj}\right)z_j, \quad j=1,\ldots,r. \tag{15}$$

On the other hand, in order to find the coefficients a_{jk} we will rely on the quadratic Clebsh-Gordan series

$$R_{\lambda_j}\otimes R_{\lambda_k}=\sum_{\mu\in Q_{jk}} N_{\mu;jk}R_{\mu}, \tag{16}$$

where $Q_{jk}\subset P^+$ is the set of dominant weights in the irreducible representation of highest weight $\lambda_j+\lambda_k$, and $N_{\lambda;jk}$ is the multiplicity of the irreducible representation R_{λ} in that series; in particular, $N_{\lambda_j+\lambda_k;jk}=1$. In these expressions we will write $\mathbf{m}$ or $(m_1,\ldots,m_r)$ instead of $\mu=\Sigma_i m_i\lambda_i$. The Clebsh-Gordan series (16) yield the formulas

$$z_j z_k=\sum_{\mathbf{m}\in Q_{jk}} N_{\mathbf{m};jk}\boldsymbol{\chi}_{\mathbf{m}}(z) \tag{17}$$

for the products of fundamental characters $z_j z_k$, and consequently we obtain the coefficients a_{jk} by applying the operator Δ^1 to the two members of (17),

$$2a_{jk}(z)=\sum_{\mathbf{m}\in Q_{jk}} N_{\mathbf{m};jk}\varepsilon_{\mathbf{m}}(1)\boldsymbol{\chi}_{\mathbf{m}}(z)-b_j(z)z_k-b_k(z)z_j, \quad j,k=1,\ldots,r. \tag{18}$$

Therefore, to accomplish the task of fixing the form of the coefficents a_{jk} we need the list of all the quadratic Clebsh-Gordan series, the explicit expressions of the characters entering in them, and the coefficients b_j. Although there are some results for E_7 already available in the literature,[22,26] most of the required Clebsch-Gordan series and characters remain, to our knowledge, to be calculated.

The remaining step to achieve the complete expression of Δ^{κ} is to look for the coefficients $b^0_j(z)$. These can be found if we know enough monomial symmetric functions M_{λ} in terms of the z variables. Suppose that the relations $M_k=M_k(z)$ are known, where $M_k=M_{\lambda_k}$, $k=1,\ldots,r$; then, from the eigenvalue equation $\Delta^0 M_k=\varepsilon_k(0)M_k$ we obtain the following linear system for the b^0's:

$$\sum_{i,j} a_{ij}(z)\frac{\partial^2 M_k}{\partial z_i\partial z_j}+\sum_j b^0_j(z)\frac{\partial M_k}{\partial z_j}=2\lambda_k^2 M_k(z). \tag{19}$$

This system has a unique solution (b^0_j) because each of the sets of characters and monomial symmetric functions constitutes a basis of W-invariant functions.

Recently[27] we have found how to find the functions $M_k(z)$ in the E_6 case. In the present paper we will study only the case $\kappa=1$ and consequently we do not need to calculate the b^0 coefficients now.

IV. THE QUADRATIC CLEBSH-GORDAN SERIES FOR E_7

We have developed a systematic strategy, entirely based on a few elementary facts, to obtain all quantities needed for application of the formula (18). This strategy, which is essentially the same as that used in the previous paper[21] for the case of E_6, was described there in full detail, so we will confine ourselves here to mention some very general but important points. First of all, the series should be computed starting from those involving the most external dots of the Dynkin diagram, and going gradually towards the center of it. This is the order that allows the most efficient use of the orthogonality relations. Second, the orthogonality relations should be used not only to fix the multiplicity of some of the weights of lower height, but also to determine linear equations among the multiplicities of several weights of intermediate height. While for E_6 this is not of great importance, for the more complicated case of E_7 an extensive use of such linear constraints is required. These constraints, along with the bounds on multiplicities established in Ref. 28, make it posible to write a system of diophantine equations with unique solution for these multiplicities. Finally, once all the series are found, the inversion of them to obtain the second-order characters appearing in (18) requires the computation of many other characters of third, fourth, and fifth order. The best way to perform these computations is as follows. Starting from the outer region of the Dynkin diagram, we build in each step the part of the Δ^1 operator which only requires the characters that we already know. Then, we can use one of the procedures described in Sec. V below to compute the characters needed to obtain the next coefficient through (18), and so on. This is possible because (18) gives each coefficient $a_{ij}(z)$ in terms of characters associated to weights whose height is lower or equal than $\lambda_i+\lambda_j$.

By means of these techniques, one finally arrives at the following list of Clebsch-Gordan series:

$$R_{\lambda_1}\otimes R_{\lambda_1}=R_{2\lambda_1}\oplus R_{\lambda_6}\oplus R_{\lambda_3}\oplus R_{\lambda_1}\oplus 1,$$

$$R_{\lambda_1}\otimes R_{\lambda_2}=R_{\lambda_1+\lambda_2}\oplus R_{\lambda_7}\oplus R_{\lambda_2}\oplus R_{\lambda_1+\lambda_7}\oplus R_{\lambda_5},$$

$$R_{\lambda_1}\otimes R_{\lambda_3}=R_{\lambda_1+\lambda_3}\oplus R_{\lambda_4}\oplus R_{\lambda_1}\oplus R_{\lambda_6}\oplus R_{\lambda_3}\oplus R_{2\lambda_1}\oplus R_{\lambda_1+\lambda_6}\oplus R_{\lambda_2+\lambda_7},$$

$$R_{\lambda_1}\otimes R_{\lambda_4}=R_{\lambda_1+\lambda_4}\oplus R_{\lambda_2+\lambda_5}\oplus R_{\lambda_3+\lambda_6}\oplus R_{\lambda_1+\lambda_2+\lambda_7}\oplus R_{\lambda_5+\lambda_7}\oplus R_{2\lambda_2}\oplus R_{\lambda_1+\lambda_3}\oplus R_{\lambda_4}\oplus R_{\lambda_1+\lambda_6}\oplus R_{\lambda_2+\lambda_7}\oplus R_{\lambda_3},$$

$$R_{\lambda_1}\otimes R_{\lambda_5}=R_{\lambda_1+\lambda_5}\oplus R_{\lambda_2+\lambda_6}\oplus R_{\lambda_2}\oplus R_{\lambda_5}\oplus R_{\lambda_1+\lambda_2}\oplus R_{\lambda_1+\lambda_7}\oplus R_{\lambda_3+\lambda_7}\oplus R_{\lambda_6+\lambda_7},$$

$$R_{\lambda_1}\otimes R_{\lambda_6}=R_{\lambda_1+\lambda_6}\oplus R_{\lambda_2+\lambda_7}\oplus R_{\lambda_3}\oplus R_{\lambda_6}\oplus R_{2\lambda_7}\oplus R_{\lambda_1},$$

$$R_{\lambda_1}\otimes R_{\lambda_7}=R_{\lambda_1+\lambda_7}\oplus R_{\lambda_2}\oplus R_{\lambda_7},$$

$$R_{\lambda_2}\otimes R_{\lambda_2}=R_{2\lambda_2}\oplus R_{\lambda_1}\oplus R_{2\lambda_7}\oplus R_{\lambda_6}\oplus R_{2\lambda_1}\oplus R_{\lambda_3}\oplus R_{\lambda_2+\lambda_7}\oplus R_{\lambda_1+\lambda_6}\oplus R_{\lambda_4}\oplus 1,$$

$$R_{\lambda_2}\otimes R_{\lambda_3}=R_{\lambda_2+\lambda_3}\oplus R_{\lambda_1+\lambda_5}\oplus R_{\lambda_2}\oplus R_{\lambda_5}\oplus R_{\lambda_7}\oplus R_{\lambda_2+\lambda_6}\oplus R_{\lambda_3+\lambda_7}\oplus R_{\lambda_6+\lambda_7}\oplus 2R_{\lambda_1+\lambda_7}\oplus 2R_{\lambda_1+\lambda_2}\oplus R_{2\lambda_1+\lambda_7},$$

$$R_{\lambda_2}\otimes R_{\lambda_4}=R_{\lambda_2+\lambda_4}\oplus R_{\lambda_3+\lambda_5}\oplus R_{\lambda_1+\lambda_2+\lambda_6}\oplus R_{2\lambda_2+\lambda_7}\oplus R_{\lambda_1+\lambda_3+\lambda_7}\oplus R_{\lambda_5+\lambda_6}\oplus R_{\lambda_4+\lambda_7}\oplus R_{\lambda_1+\lambda_6+\lambda_7}$$
$$\oplus R_{2\lambda_1+\lambda_2}\oplus 2R_{\lambda_2+\lambda_3}\oplus R_{\lambda_2+2\lambda_7}\oplus 2R_{\lambda_1+\lambda_5}\oplus R_{2\lambda_1+\lambda_7}\oplus 2R_{\lambda_2+\lambda_6}\oplus 2R_{\lambda_3+\lambda_7}\oplus 2R_{\lambda_1+\lambda_2}$$
$$\oplus R_{\lambda_6+\lambda_7}\oplus R_{\lambda_5}\oplus R_{\lambda_1+\lambda_7}\oplus R_{\lambda_2},$$

$$R_{\lambda_2}\otimes R_{\lambda_5}=R_{\lambda_2+\lambda_5}\oplus R_{\lambda_3+\lambda_6}\oplus R_{2\lambda_6}\oplus R_{\lambda_1+\lambda_2+\lambda_7}\oplus R_{2\lambda_2}\oplus R_{\lambda_1+\lambda_3}\oplus R_{\lambda_5+\lambda_7}\oplus R_{\lambda_4}\oplus R_{\lambda_1+2\lambda_7}$$
$$\oplus 2R_{\lambda_1+\lambda_6}\oplus 2R_{\lambda_2+\lambda_7}\oplus R_{2\lambda_7}\oplus R_{2\lambda_1}\oplus R_{\lambda_3}\oplus R_{\lambda_6}\oplus R_{\lambda_1},$$

$$R_{\lambda_2}\otimes R_{\lambda_6}=R_{\lambda_7}\oplus R_{\lambda_2}\oplus 2R_{\lambda_1+\lambda_7}\oplus R_{\lambda_5}\oplus R_{\lambda_6+\lambda_7}\oplus R_{\lambda_1+\lambda_2}\oplus R_{\lambda_3+\lambda_7}\oplus R_{\lambda_2+\lambda_6},$$

$$R_{\lambda_2}\otimes R_{\lambda_7}=R_{\lambda_2+\lambda_7}\oplus R_{\lambda_1}\oplus R_{\lambda_3}\oplus R_{\lambda_6},$$

$$R_{\lambda_3}\otimes R_{\lambda_3}=R_{2\lambda_3}\oplus R_{\lambda_1+\lambda_4}\oplus R_{\lambda_2+\lambda_5}\oplus R_{2\lambda_1+\lambda_6}\oplus R_{\lambda_3+\lambda_6}\oplus 2R_{\lambda_1+\lambda_2+\lambda_7}\oplus R_{2\lambda_6}\oplus R_{\lambda_5+\lambda_7}\oplus R_{3\lambda_1}$$
$$\oplus R_{2\lambda_2}\oplus 2R_{\lambda_1+\lambda_3}\oplus R_{\lambda_1+2\lambda_7}\oplus 2R_{\lambda_4}\oplus 3R_{\lambda_1+\lambda_6}\oplus 2R_{2\lambda_1}\oplus 2R_{\lambda_2+\lambda_7}\oplus R_{2\lambda_7}\oplus 2R_{\lambda_3}$$
$$\oplus 2R_{\lambda_6}\oplus R_{\lambda_1}\oplus 1,$$

$$R_{\lambda_3}\otimes R_{\lambda_4}=R_{\lambda_3+\lambda_4}\oplus R_{\lambda_1+\lambda_2+\lambda_5}\oplus R_{2\lambda_2+\lambda_6}\oplus R_{\lambda_1+\lambda_3+\lambda_6}\oplus R_{2\lambda_5}\oplus R_{\lambda_4+\lambda_6}\oplus R_{2\lambda_1+\lambda_2+\lambda_7}\oplus R_{\lambda_1+2\lambda_6}$$
$$\oplus 2R_{\lambda_2+\lambda_3+\lambda_7}\oplus 2R_{\lambda_1+\lambda_5+\lambda_7}\oplus R_{2\lambda_1+\lambda_3}\oplus R_{2\lambda_1+2\lambda_7}\oplus 2R_{\lambda_1+2\lambda_2}\oplus R_{2\lambda_3}\oplus 3R_{\lambda_1+\lambda_4}$$
$$\oplus 2R_{\lambda_2+\lambda_6+\lambda_7}\oplus 2R_{2\lambda_1+\lambda_6}\oplus 3R_{\lambda_2+\lambda_5}\oplus R_{\lambda_3+2\lambda_7}\oplus 4R_{\lambda_3+\lambda_6}\oplus R_{\lambda_6+2\lambda_7}\oplus 5R_{\lambda_1+\lambda_2+\lambda_7}\oplus R_{2\lambda_6}$$
$$\oplus 2R_{2\lambda_2}\oplus 3R_{\lambda_5+\lambda_7}\oplus R_{3\lambda_1}\oplus 3R_{\lambda_1+\lambda_3}\oplus 2R_{\lambda_1+2\lambda_7}\oplus 3R_{\lambda_4}\oplus 4R_{\lambda_1+\lambda_6}\oplus R_{2\lambda_1}\oplus 3R_{\lambda_2+\lambda_7}$$
$$\oplus R_{2\lambda_7}\oplus 2R_{\lambda_3}\oplus R_{\lambda_6}\oplus R_{\lambda_1},$$

$$R_{\lambda_3}\otimes R_{\lambda_5}=R_{\lambda_3+\lambda_5}\oplus R_{\lambda_1+\lambda_2+\lambda_6}\oplus R_{2\lambda_2+\lambda_7}\oplus R_{\lambda_1+\lambda_3+\lambda_7}\oplus R_{\lambda_5+\lambda_6}\oplus R_{\lambda_4+\lambda_7}\oplus 2R_{\lambda_1+\lambda_6+\lambda_7}\oplus R_{2\lambda_1+\lambda_2}$$
$$\oplus R_{\lambda_2+2\lambda_7}\oplus 2R_{\lambda_2+\lambda_3}\oplus 2R_{\lambda_1+\lambda_5}\oplus R_{3\lambda_7}\oplus 2R_{2\lambda_1+\lambda_7}\oplus 3R_{\lambda_2+\lambda_6}\oplus 3R_{\lambda_3+\lambda_7}\oplus 3R_{\lambda_1+\lambda_2}$$
$$\oplus 2R_{\lambda_6+\lambda_7}\oplus 2R_{\lambda_5}\oplus 3R_{\lambda_1+\lambda_7}\oplus R_{\lambda_2}\oplus R_{\lambda_7},$$

$$R_{\lambda_3}\otimes R_{\lambda_6}=R_{\lambda_3+\lambda_6}\oplus R_{\lambda_1+\lambda_2+\lambda_7}\oplus R_{2\lambda_2}\oplus R_{\lambda_1+\lambda_3}\oplus R_{\lambda_5+\lambda_7}\oplus R_{\lambda_4}\oplus R_{\lambda_1+2\lambda_7}\oplus 2R_{\lambda_1+\lambda_6}\oplus 2R_{\lambda_2+\lambda_7}$$
$$\oplus R_{2\lambda_1}\oplus R_{2\lambda_7}\oplus 2R_{\lambda_3}\oplus R_{\lambda_6}\oplus R_{\lambda_1},$$

$$R_{\lambda_3}\otimes R_{\lambda_7}=R_{\lambda_3+\lambda_7}\oplus R_{\lambda_1+\lambda_7}\oplus R_{\lambda_1+\lambda_2}\oplus R_{\lambda_2}\oplus R_{\lambda_5},$$

$$R_{\lambda_4}\otimes R_{\lambda_4}=R_{2\lambda_4}\oplus R_{\lambda_2+\lambda_3+\lambda_5}\oplus R_{2\lambda_3+\lambda_6}\oplus R_{\lambda_1+2\lambda_5}\oplus R_{\lambda_1+2\lambda_2+\lambda_6}\oplus R_{3\lambda_2+\lambda_7}\oplus R_{\lambda_1+\lambda_4+\lambda_6}$$
$$\oplus 2R_{\lambda_1+\lambda_2+\lambda_3+\lambda_7}\oplus 2R_{\lambda_2+\lambda_5+\lambda_6}\oplus 2R_{\lambda_2+\lambda_4+\lambda_7}\oplus R_{2\lambda_1+2\lambda_6}\oplus R_{2\lambda_1+2\lambda_2}\oplus R_{\lambda_3+2\lambda_6}$$
$$\oplus R_{2\lambda_1+\lambda_5+\lambda_7}\oplus 3R_{\lambda_3+\lambda_5+\lambda_7}\oplus R_{\lambda_1+2\lambda_3}\oplus 2R_{2\lambda_1+\lambda_4}\oplus 4R_{\lambda_1+\lambda_2+\lambda_6+\lambda_7}\oplus R_{3\lambda_6}\oplus 3R_{2\lambda_2+\lambda_3}$$
$$\oplus R_{3\lambda_1+2\lambda_7}\oplus 2R_{\lambda_5+\lambda_6+\lambda_7}\oplus 2R_{2\lambda_2+2\lambda_7}\oplus 2R_{\lambda_1+\lambda_3+2\lambda_7}\oplus 3R_{\lambda_3+\lambda_4}\oplus 6R_{\lambda_1+\lambda_2+\lambda_5}\oplus 4R_{2\lambda_2+\lambda_6}$$
$$\oplus 2R_{\lambda_4+2\lambda_7}\oplus 3R_{\lambda_1+\lambda_6+2\lambda_7}\oplus R_{3\lambda_1+\lambda_6}\oplus 2R_{2\lambda_5}\oplus 6R_{\lambda_1+\lambda_3+\lambda_6}\oplus 6R_{2\lambda_1+\lambda_2+\lambda_7}\oplus 7R_{\lambda_4+\lambda_6}$$
$$\oplus R_{4\lambda_1}\oplus R_{\lambda_2+3\lambda_7}\oplus 4R_{\lambda_1+2\lambda_6}\oplus 9R_{\lambda_2+\lambda_3+\lambda_7}\oplus 9R_{\lambda_1+\lambda_5+\lambda_7}\oplus 3R_{2\lambda_1+\lambda_3}\oplus 6R_{\lambda_1+2\lambda_2}$$

$$\oplus 4R_{2\lambda_1+2\lambda_7} \oplus 4R_{2\lambda_3} \oplus 8R_{\lambda_2+\lambda_6+\lambda_7} \oplus 6R_{\lambda_3+2\lambda_7} \oplus 8R_{\lambda_1+\lambda_4} \oplus 8R_{\lambda_2+\lambda_5} \oplus 8R_{2\lambda_1+\lambda_6} \oplus R_{4\lambda_7}$$
$$\oplus 3R_{\lambda_6+2\lambda_7} \oplus 2R_{3\lambda_1} \oplus 9R_{\lambda_3+\lambda_6} \oplus 4R_{2\lambda_6} \oplus 12R_{\lambda_1+\lambda_2+\lambda_7} \oplus 6R_{\lambda_1+\lambda_3} \oplus 3R_{2\lambda_2} \oplus 7R_{\lambda_5+\lambda_7}$$
$$\oplus 7R_{\lambda_4} \oplus 6R_{\lambda_1+2\lambda_7} \oplus 7R_{\lambda_1+\lambda_6} \oplus 5R_{\lambda_2+\lambda_7} \oplus 2R_{2\lambda_7} \oplus 3R_{2\lambda_1} \oplus 3R_{\lambda_3} \oplus 3R_{\lambda_6} \oplus R_{\lambda_1} \oplus 1,$$

$$R_{\lambda_4} \otimes R_{\lambda_5} = R_{\lambda_4+\lambda_5} \oplus R_{\lambda_2+\lambda_3+\lambda_6} \oplus R_{\lambda_1+\lambda_5+\lambda_6} \oplus R_{2\lambda_3+\lambda_7} \oplus R_{\lambda_1+2\lambda_2+\lambda_7} \oplus R_{\lambda_1+\lambda_4+\lambda_7} \oplus R_{\lambda_2+2\lambda_6}$$
$$\oplus 2R_{\lambda_2+\lambda_5+\lambda_7} \oplus 2R_{\lambda_1+\lambda_2+\lambda_3} \oplus R_{2\lambda_1+\lambda_6+\lambda_7} \oplus R_{3\lambda_2} \oplus 2R_{\lambda_3+\lambda_6+\lambda_7} \oplus 2R_{\lambda_2+\lambda_4} \oplus R_{2\lambda_1+\lambda_5}$$
$$\oplus 3R_{\lambda_3+\lambda_5} \oplus 2R_{\lambda_1+\lambda_2+2\lambda_7} \oplus 5R_{\lambda_1+\lambda_2+\lambda_6} \oplus R_{2\lambda_6+\lambda_7} \oplus R_{\lambda_5+2\lambda_7} \oplus R_{3\lambda_1+\lambda_7} \oplus 4R_{\lambda_1+\lambda_3+\lambda_7}$$
$$\oplus 3R_{\lambda_5+\lambda_6} \oplus 3R_{2\lambda_2+\lambda_7} \oplus 5R_{\lambda_4+\lambda_7} \oplus 3R_{2\lambda_1+\lambda_2} \oplus 5R_{\lambda_2+\lambda_3} \oplus R_{\lambda_1+3\lambda_7} \oplus 5R_{\lambda_1+\lambda_6+\lambda_7}$$
$$\oplus 5R_{\lambda_1+\lambda_5} \oplus 3R_{\lambda_2+2\lambda_7} \oplus 5R_{\lambda_2+\lambda_6} \oplus 4R_{2\lambda_1+\lambda_7} \oplus 5R_{\lambda_3+\lambda_7} \oplus 4R_{\lambda_1+\lambda_2} \oplus R_{3\lambda_7} \oplus 3R_{\lambda_6+\lambda_7}$$
$$\oplus 3R_{\lambda_5} \oplus 3R_{\lambda_1+\lambda_7} \oplus R_{\lambda_2} \oplus R_{\lambda_7},$$

$$R_{\lambda_4} \otimes R_{\lambda_6} = R_{\lambda_4+\lambda_6} \oplus R_{\lambda_2+\lambda_3+\lambda_7} \oplus R_{2\lambda_3} \oplus R_{\lambda_1+\lambda_5+\lambda_7} \oplus R_{\lambda_2+\lambda_6+\lambda_7} \oplus R_{\lambda_1+2\lambda_2} \oplus R_{\lambda_1+\lambda_4} \oplus R_{\lambda_3+2\lambda_7}$$
$$\oplus 2R_{\lambda_2+\lambda_5} \oplus R_{2\lambda_1+\lambda_6} \oplus 2R_{\lambda_3+\lambda_6} \oplus 3R_{\lambda_1+\lambda_2+\lambda_7} \oplus R_{2\lambda_6} \oplus 2R_{\lambda_5+\lambda_7} \oplus R_{2\lambda_2} \oplus R_{\lambda_1+2\lambda_7}$$
$$\oplus 2R_{\lambda_1+\lambda_3} \oplus 3R_{\lambda_4} \oplus 2R_{\lambda_1+\lambda_6} \oplus 2R_{\lambda_2+\lambda_7} \oplus R_{2\lambda_1} \oplus R_{\lambda_3} \oplus R_{\lambda_6},$$

$$R_{\lambda_4} \otimes R_{\lambda_7} = R_{\lambda_4+\lambda_7} \oplus R_{\lambda_2+\lambda_3} \oplus R_{\lambda_1+\lambda_5} \oplus R_{\lambda_2+\lambda_6} \oplus R_{\lambda_3+\lambda_7} \oplus R_{\lambda_1+\lambda_2} \oplus R_{\lambda_5},$$

$$R_{\lambda_5} \otimes R_{\lambda_5} = R_{2\lambda_5} \oplus R_{\lambda_4+\lambda_6} \oplus R_{\lambda_2+\lambda_3+\lambda_7} \oplus R_{\lambda_1+2\lambda_6} \oplus R_{2\lambda_3} \oplus R_{\lambda_1+\lambda_5+\lambda_7} \oplus 2R_{\lambda_2+\lambda_6+\lambda_7} \oplus R_{\lambda_1+2\lambda_2}$$
$$\oplus R_{2\lambda_1+2\lambda_7} \oplus R_{\lambda_1+\lambda_4} \oplus R_{\lambda_3+2\lambda_7} \oplus 2R_{\lambda_2+\lambda_5} \oplus R_{2\lambda_1+\lambda_6} \oplus 3R_{\lambda_3+\lambda_6} \oplus 4R_{\lambda_1+\lambda_2+\lambda_7} \oplus R_{\lambda_6+2\lambda_7}$$
$$\oplus R_{3\lambda_1} \oplus 2R_{2\lambda_6} \oplus 3R_{\lambda_5+\lambda_7} \oplus 2R_{2\lambda_2} \oplus 3R_{\lambda_1+2\lambda_7} \oplus 2R_{\lambda_1+\lambda_3} \oplus 3R_{\lambda_4} \oplus 4R_{\lambda_1+\lambda_6} \oplus 3R_{\lambda_2+\lambda_7}$$
$$\oplus 2R_{2\lambda_7} \oplus 2R_{2\lambda_1} \oplus 2R_{\lambda_3} \oplus 2R_{\lambda_6} \oplus R_{\lambda_1} \oplus 1,$$

$$R_{\lambda_5} \otimes R_{\lambda_6} = R_{\lambda_5+\lambda_6} \oplus R_{\lambda_4+\lambda_7} \oplus R_{\lambda_1+\lambda_6+\lambda_7} \oplus R_{\lambda_2+\lambda_3} \oplus R_{\lambda_2+2\lambda_7} \oplus R_{\lambda_1+\lambda_5} \oplus 2R_{\lambda_2+\lambda_6} \oplus R_{2\lambda_1+\lambda_7}$$
$$\oplus 2R_{\lambda_3+\lambda_7} \oplus 2R_{\lambda_1+\lambda_2} \oplus 2R_{\lambda_6+\lambda_7} \oplus 2R_{\lambda_5} \oplus 2R_{\lambda_1+\lambda_7} \oplus R_{\lambda_2} \oplus R_{\lambda_7}$$

$$R_{\lambda_5} \otimes R_{\lambda_7} = R_{\lambda_5+\lambda_7} \oplus R_{\lambda_4} \oplus R_{\lambda_6} \oplus R_{\lambda_3} \oplus R_{\lambda_1+\lambda_6} \oplus R_{\lambda_2+\lambda_7},$$

$$R_{\lambda_6} \otimes R_{\lambda_6} = R_{2\lambda_6} \oplus R_{\lambda_5+\lambda_7} \oplus R_{\lambda_1} \oplus R_{\lambda_3} \oplus R_{\lambda_4} \oplus 2R_{\lambda_6} \oplus R_{2\lambda_1} \oplus R_{2\lambda_7} \oplus R_{\lambda_1+\lambda_6} \oplus 2R_{\lambda_2+\lambda_7} \oplus R_{\lambda_1+2\lambda_7}$$
$$\oplus 1,$$

$$R_{\lambda_6} \otimes R_{\lambda_7} = R_{\lambda_6+\lambda_7} \oplus R_{\lambda_5} \oplus R_{\lambda_1+\lambda_7} \oplus R_{\lambda_2} \oplus R_{\lambda_7},$$

$$R_{\lambda_7} \otimes R_{\lambda_7} = R_{2\lambda_7} \oplus R_{\lambda_1} \oplus R_{\lambda_6} \oplus 1.$$

We present also a list of second order characters,

$$\chi_{2000000} = z_1^2 - z_3 - z_6 - z_1 - 1,$$

$$\chi_{1100000} = z_1 z_2 - z_5 - z_1 z_7,$$

$$\chi_{1010000} = z_1z_3 - z_4 - z_1z_6 - z_1^2 + z_7^2 + z_3,$$

$$\chi_{1001000} = z_1z_4 - z_2z_5 + z_6^2 - z_5z_7 + z_1z_6 - z_2z_7 - z_7^2 + z_6 + z_1,$$

$$\chi_{1000100} = z_1z_5 - z_2z_6 + z_1z_7 - z_2,$$

$$\chi_{1000010} = z_1z_6 - z_2z_7 - z_7^2 + z_6 + z_1 + 1,$$

$$\chi_{1000001} = z_1z_7 - z_2 - z_7,$$

$$\chi_{0200000} = z_2^2 - z_4 - z_1z_6 - z_1^2 + z_3 + z_6 + z_1,$$

$$\chi_{0110000} = z_2z_3 - z_1z_5 - z_1^2z_7 + z_3z_7 + z_6z_7 + z_1z_7,$$

$$\chi_{0101000} = z_2z_4 - z_3z_5 + z_1z_6z_7 - z_2z_7^2 - z_1z_5 + z_2z_6 - z_6z_7 + z_5 + z_2,$$

$$\chi_{0100100} = z_2z_5 - z_3z_6 - z_6^2 + z_5z_7 + z_1z_7^2 - z_1z_6 - z_6 - z_1,$$

$$\chi_{0100010} = z_2z_6 - z_3z_7 - z_6z_7 + z_5 + z_2,$$

$$\chi_{0100001} = z_2z_7 - z_3 - z_6 - z_1,$$

$$\chi_{0020000} = z_3^2 - z_1z_4 - z_1^2z_6 + z_3z_6 + z_5z_7 - z_1^3 + 2z_1z_3 + z_1z_7^2 - z_4 + z_3 + z_1,$$

$$\chi_{0011000} = z_3z_4 - z_1z_2z_5 + z_4z_6 + z_1z_6^2 + z_1^2z_6 - z_3z_6 - z_6z_7^2 - z_1z_2z_7 + z_2^2 + z_5z_7 - z_4 - z_1z_6 + z_7^2 + z_3 - 1,$$

$$\chi_{0010100} = z_3z_5 - z_1z_2z_6 + z_4z_7 + z_1z_6z_7 + z_2z_7^2 - z_7^3 + z_1^2z_7 - z_2z_6 - z_3z_7 - z_1z_2 + z_6z_7 - z_5 - z_1z_7 - z_2 + z_7,$$

$$\chi_{0010010} = z_3z_6 - z_1z_2z_7 + z_4 + z_1z_6 + z_2z_7 + z_1^2 - z_3 - z_1,$$

$$\chi_{0010001} = z_3z_7 - z_1z_2 + z_7,$$

$$\chi_{0002000} = z_4^2 - z_2z_3z_5 + z_1z_4z_6 + z_3z_6^2 + z_1^2z_5z_7 - 2z_3z_5z_7 - 2z_4z_7^2 - z_1z_6z_7^2 - z_5^2 + 2z_4z_6 + z_1z_6^2 - z_1z_5z_7 + z_2z_5 + z_7^4 - 2z_6z_7^2 + z_6^2 + 2z_4 + z_1z_6 - 2z_7^2 + 2z_6 + 1,$$

$$\chi_{0001100} = z_4z_5 - z_2z_3z_6 + z_1z_4z_7 + z_1^2z_6z_7 - z_3z_5 - z_5z_6 - z_1z_7^3 - z_4z_7 - z_1z_5 + z_7^3 - z_6z_7 + z_1z_7 - z_7,$$

$$\chi_{0001010} = z_4z_6 - z_2z_3z_7 + z_1^2z_7^2 + z_1z_4 - z_3z_7^2 + z_3z_6 - z_5z_7 - 2z_1z_7^2 + z_4 + z_1z_6 - z_7^2 + z_6 + z_1 + 1,$$

$$\chi_{0001001} = z_4z_7 - z_2z_3 + z_1^2z_7 - z_3z_7 - z_5 - z_1z_7 - z_7,$$

$$\chi_{0000200} = z_5^2 - z_4z_6 - z_1z_6^2 + z_1z_5z_7 + z_3z_7^2 - z_3z_6 + z_6z_7^2 - z_6^2 - z_4 - z_1z_6 + z_7^2 - z_3 - 2z_6 - 1,$$

$$\chi_{0000110} = z_5z_6 - z_4z_7 - z_1z_6z_7 + z_1z_5 + z_7^3 + z_3z_7 - z_6z_7 + z_5 - z_7,$$

$$\chi_{0000101} = z_5z_7 - z_4 - z_1z_6 + z_7^2 - z_6 - 1,$$

$$\chi_{0000020} = z_6^2 - z_5z_7 - z_1z_7^2 + z_1z_6 + z_3 + z_6 + z_1,$$

$$\chi_{0000011} = z_6z_7 - z_5 - z_1z_7,$$

$$\chi_{0000002} = z_7^2 - z_6 - z_1 - 1.$$

V. THE CALOGERO-SUTHERLAND HAMILTONIAN Δ^1 IN E_7: SOME APPLICATIONS

The coefficients $b_j(z)$ in the expression of Δ^1 are easily obtained from (15) and (2),

$$b_1(z) = 72z_1, \quad b_2(z) = 105z_2, \quad b_3(z) = 144z_1, \quad b_4(z) = 216z_4,$$

$$b_5(z) = 165z_5, \quad b_6(z) = 112z_5, \quad b_7(z) = 57z_7.$$

After having computed in Sec. IV the necessary series and characters, we can now follow the lines indicated in Sec. III to obtain the Hamiltonian operator in the limit $\kappa=1$. The result for the coefficients $a_{jk}(z)$ in (14) for $\kappa=1$ is

$$a_{11}(z) = 4(-19 - 10z_1 + z_1^2 - z_3 - 5z_6),$$

$$a_{12}(z) = 2(-7z_2 + 2z_1z_2 - 5z_5 - 19z_7 - 13z_1z_7),$$

$$a_{13}(z) = 2(10 - 14z_1 - 19z_1^2 + 13z_3 + 3z_1z_3 - 3z_4 - 4z_6 - 9z_1z_6 - 6z_2z_7 + 9z_7^2),$$

$$\begin{aligned} a_{14}(z) = 2(&-10 - 2z_1 + 18z_1^2 - 7z_2^2 - 24z_3 - 6z_1z_3 + 14z_4 + 4z_1z_4 - 4z_2z_5 + 8z_6 + 12z_1z_6 - 4z_3z_6 + 4z_6^2 \\ &- 14z_2z_7 - 5z_1z_2z_7 - 9z_5z_7 - 9z_7^2 + 9z_1z_7^2), \end{aligned}$$

$$a_{15}(z) = 2(-12z_2 - 6z_1z_2 + 8z_5 + 3z_1z_5 - 5z_2z_6 + 19z_7 + 5z_1z_7 - 5z_3z_7 - 13z_6z_7),$$

$$a_{16}(z) = 4(9 - 3z_1 - 3z_3 + 2z_6 + z_1z_6 - 3z_2z_7 - 9z_7^2),$$

$$a_{17}(z) = 2(-7z_2 - 19z_7 + z_1z_7),$$

$$a_{22}(z) = -40 + 24z_1 - 36z_1^2 + 7z_2^2 + 24z_3 - 4z_4 + 44z_6 - 16z_1z_6 - 12z_2z_7 - 36z_7^2,$$

$$a_{23}(z) = 2(9z_2 - 14z_1z_2 + 4z_2z_3 + 16z_5 - 4z_1z_5 - 5z_2z_6 + 4z_1z_7 - 12z_1^2z_7 + 7z_3z_7 - z_6z_7),$$

$$\begin{aligned} a_{24}(z) = 2(&-7z_2 - 4z_1z_2 - 6z_1^2z_2 - z_2z_3 + 6z_2z_4 + 20z_5 - 6z_1z_5 - 3z_3z_5 + 14z_2z_6 - 4z_1z_2z_6 - 5z_5z_6 \\ &- 10z_1z_7 + 22z_1^2z_7 - 6z_2^2z_7 - 12z_3z_7 - 5z_1z_3z_7 + 12z_4z_7 - \ 10z_6z_7 + 13z_1z_6z_7 - 9z_2z_7^2), \end{aligned}$$

$$\begin{aligned} a_{25}(z) = 40 &- 24z_1 + 12z_1^2 - 14z_2^2 + 12z_3 - 12z_1z_3 + 28z_4 + 9z_2z_5 + 16z_6 - 12z_1z_6 - 8z_3z_6 - 24z_6^2 \\ &+ 12z_2z_7 - 10z_1z_2z_7 + 14z_5z_7 - 2z_7^2 - 2z_1z_7^2, \end{aligned}$$

$$a_{26}(z) = 2(17z_2 - 6z_1z_2 + 8z_5 + 3z_2z_6 - 24z_1z_7 - 5z_3z_7 - 13z_6z_7),$$

$$a_{27}(z) = -48z_1 - 12z_3 - 28z_6 + 3z_2z_7,$$

$$\begin{aligned} a_{33}(z) = 4(&-20 + 16z_1 - 5z_1^2 - 9z_1^3 + 8z_3 + 12z_1z_3 + 3z_3^2 - 7z_4 - z_1z_4 - 2z_2z_5 - 9z_6 + - 3z_1z_6 - 4z_1^2z_6 \\ &+ 2z_3z_6 - 3z_6^2 + 6z_2z_7 - 6z_1z_2z_7 + 8z_5z_7 + z_7^2 + 7z_1z_7^2), \end{aligned}$$

$$\begin{aligned} a_{34}(z) = 2(&-20 - 12z_1 - 6z_1^2 + 6z_1^3 + 9z_2^2 - 7z_1z_2^2 + 20z_3 + 6z_1z_3 - 6z_1^2z_3 + 6z_3^2 - 26z_4 + 6z_1z_4 + 8z_3z_4 \\ &+ 2z_2z_5 - 3z_1z_2z_5 - 5z_5^2 - 2z_6 - 32z_1z_6 + 20z_1^2z_6 - 5z_2^2z_6 - 24z_3z_6 - 4z_1z_3z_6 + 10z_4z_6 + 4z_6^2 \\ &+ 4z_1z_6^2 - 3z_2z_7 - 2z_1z_2z_7 - 5z_1^2z_2z_7 - z_2z_3z_7 + 15z_5z_7 + 4z_2z_6z_7 + 20z_7^2 - 5z_1z_7^2 + 5z_1^2z_7^2 \\ &+ 9z_3z_7^2 - 9z_6z_7^2), \end{aligned}$$

$$\begin{aligned} a_{35}(z) = 2(&-z_2 + z_1z_2 - 6z_1^2z_2 - z_2z_3 - 22z_5 + 15z_1z_5 + 6z_3z_5 - 15z_2z_6 - 4z_1z_2z_6 - 5z_5z_6 + 18z_7 - 5z_1z_7 \\ &+ 11z_1^2z_7 - 6z_2^2z_7 - 6z_3z_7 - 5z_1z_3z_7 + 12z_4z_7 + 45z_6z_7 - 8z_1z_6z_7 + 12z_2z_7^2 - 18z_7^3), \end{aligned}$$

$$\begin{aligned} a_{36}(z) = 2(&20 + 6z_1^2 - 7z_2^2 - 18z_3 - 6z_1z_3 + 14z_4 + 20z_6 + 6z_1z_6 + 4z_3z_6 + 6z_2z_7 - 5z_1z_2z_7 - 5z_5z_7 - z_7^2 \\ &- 13z_1z_7^2), \end{aligned}$$

$$a_{37}(z) = 2(-7z_2 - 6z_1z_2 - 5z_5 + 19z_7 - 13z_1z_7 + 2z_3z_7),$$

$$\begin{aligned} a_{44}(z) = 4(&-10 - 16z_1 + 8z_1^2 - 6z_1^4 - 4z_2^2 - 16z_3 + 24z_1^2z_3 - 4z_2^2z_3 - 12z_3^2 + 8z_4 - 16z_1z_4 - 4z_1^2z_4 \\ &+ 8z_3z_4 + 6z_4^2 + 11z_2z_5 + 2z_1z_2z_5 - z_2z_3z_5 - 12z_5^2 - 2z_1z_5^2 + 4z_6 - 4z_1z_6 - 14z_1^2z_6 + 4z_1^3z_6 \\ &+ 3z_2^2z_6 - 2z_1z_2^2z_6 - 4z_3z_6 - 8z_1z_3z_6 - 2z_3^2z_6 + 6z_4z_6 + 4z_1z_4z_6 - 3z_2z_5z_6 - 2z_6^2 + 4z_1z_6^2 + 4z_3z_6^2 \\ &- 2z_6^3 + z_2z_7 + z_1z_2z_7 + 9z_1^2z_2z_7 - 3z_2^3z_7 - 8z_2z_3z_7 - 3z_1z_2z_3z_7 + 9z_2z_4z_7 - 21z_5z_7 + 6z_1z_5z_7 \\ &+ 4z_1^2z_5z_7 - 9z_3z_5z_7 - 6z_2z_6z_7 + 7z_1z_2z_6z_7 + 9z_5z_6z_7 - 9z_7^2 + 17z_1z_7^2 - 3z_1^2z_7^2 - 2z_1^3z_7^2 + 9z_1z_3z_7^2 \\ &- 9z_4z_7^2 + 9z_6z_7^2 - 9z_1z_6z_7^2), \end{aligned}$$

$$\begin{aligned} a_{45}(z) = 2(&9z_2 - 7z_1z_2 + 13z_1^2z_2 - 7z_2^3 - 12z_2z_3 - 7z_1z_2z_3 + 21z_2z_4 - 28z_5 - 7z_1z_5 + 7z_1^2z_5 - 13z_3z_5 \\ &+ 9z_4z_5 - 3z_2z_6 + 7z_1z_2z_6 - 3z_2z_3z_6 - 19z_5z_6 - 4z_1z_5z_6 - 5z_2z_6^2 + 21z_1z_7 - 24z_1^2z_7 + 6z_1^3z_7 \\ &+ 7z_2^2z_7 - 5z_1z_2^2z_7 + 14z_3z_7 - z_1z_3z_7 - 5z_3^2z_7 - 19z_4z_7 + 10z_1z_4z_7 - z_2z_5z_7 + 10z_1z_6z_7 + 4z_1^2z_6z_7 \\ &+ 5z_6^2z_7 - 2z_2z_7^2 + 4z_1z_2z_7^2 + 9z_5z_7^2 - 9z_1z_7^3), \end{aligned}$$

$$\begin{aligned} a_{46}(z) = 2(&20 + 12z_1 - 18z_1^2 + 12z_1^3 + 7z_2^2 - 6z_1z_2^2 + 12z_3 - 24z_1z_3 - 6z_3^2 + 2z_4 + 12z_1z_4 - z_2z_5 + 2z_6 \\ &+ 8z_1z_6 + 2z_1^2z_6 + 8z_3z_6 + 6z_4z_6 - 4z_6^2 - 6z_2z_7 - z_1z_2z_7 - 4z_2z_3z_7 - 10z_5z_7 - 4z_1z_5z_7 - 5z_2z_6z_7 \\ &- 20z_7^2 + 2z_1z_7^2 + 4z_1^2z_7^2 - 9z_3z_7^2 + 9z_6z_7^2), \end{aligned}$$

$$\begin{aligned} a_{47}(z) = 2(&-5z_2 - 6z_1z_2 - 5z_2z_3 - 19z_5 - 4z_1z_5 - 5z_2z_6 - 19z_7 + 11z_1z_7 + 5z_1^2z_7 - 10z_3z_7 + 3z_4z_7 \\ &+ 9z_6z_7), \end{aligned}$$

$$a_{55}(z) = -60 + 48z_1 - 12z_1^2 - 12z_1z_2^2 - 24z_3 + 24z_1z_3 - 12z_3^2 - 48z_4 + 24z_1z_4 + 12z_2z_5 + 15z_5^2 - 52z_6 + 24z_1^2z_6 - 48z_3z_6 - 4z_4z_6 - 48z_6^2 - 16z_1z_6^2 + 40z_2z_7 + 8z_1z_2z_7 - 8z_2z_3z_7 + 20z_5z_7 + 8z_1z_5z_7 - 24z_2z_6z_7 - 16z_7^2 + 4z_1z_7^2 - 12z_1^2z_7^2 + 32z_3z_7^2 + 28z_6z_7^2,$$

$$a_{56}(z) = 2(7z_2 - z_1z_2 - 5z_2z_3 + 8z_5 + 5z_1z_5 - 7z_2z_6 + 5z_5z_6 - 28z_7 + 19z_1z_7 - 6z_1^2z_7 + 11z_3z_7 - 3z_4z_7 - 17z_6z_7 - 9z_1z_6z_7 - 6z_2z_7^2 + 9z_7^3),$$

$$a_{57}(z) = -20 + 12z_1 - 12z_3 - 8z_4 - 48z_6 - 20z_1z_6 - 12z_2z_7 + 5z_5z_7 + 20z_7^2,$$

$$a_{66}(z) = 4(-14 + 12z_1 - 6z_1^2 + 12z_3 - 2z_4 + 2z_6 + 2z_6^2 - 7z_2z_7 - z_5z_7 - 5z_7^2 - 5z_1z_7^2),$$

$$a_{67}(z) = 2(-7z_2 - 3z_5 - 19z_7 - 11z_1z_7 + 2z_6z_7),$$

$$a_{77}(z) = -60 - 24z_1 - 4z_6 + 3z_7^2.$$

With the explicit expression of Δ^1 at our disposal, we can now try to use the Schrödinger equation as an efficient mean to compute particular characters of E_7. Given that all these characters are polynomials in the z variables, the Schrödinger equation can be solved by applying a systematic procedure, which is suitable to be implemented in a computer program able to carry out symbolic calculations. We propose two alternative methods to find the Schrödinger eigenfunctions.

(1) Given a weight $\nu=\sum_{i=1}^7 n_i\lambda_i \in P^+$, let us denote $z^{\mathbf{n}}$ (or z^ν) the monomial $z^{\mathbf{n}}=\prod_{i=1}^7 z_i^{n_i}$; thus $z_i=z^{\lambda_i}$. The operator Δ^1 acting on $z^{\mathbf{n}}$ gives

$$\Delta^1 z^{\mathbf{n}} = \sum_{\beta\in\Lambda} S_{\beta,\mathbf{n}} z^{\mathbf{n}-\beta} = \varepsilon_{\mathbf{m}}(1) z^{\mathbf{m}} + \sum_{0\neq\beta\in\Lambda} S_{\beta,\mathbf{n}} z^{\mathbf{n}-\beta}, \tag{20}$$

where Λ only includes integral linear combinations of the simple roots with non-negative coefficients and, of course, in the exponent of (20) we express β in the basis of fundamental weights. The eigenfunctions $\boldsymbol{\chi}_{\mathbf{m}}$ can be written as

$$\boldsymbol{\chi}_{\mathbf{m}} = \sum_{\lambda\in Q^+_{\mathbf{m}}} C_\lambda z^{\mathbf{m}-\lambda} = z^{\mathbf{m}} + \sum_{0\neq\lambda\in Q^+_{\mathbf{m}}} C_\lambda z^{\mathbf{m}-\lambda},$$

where again the λ in $Q^+_{\mathbf{m}}$ are integral linear combinations of the simple roots with non-negative coefficients such that they do not give rise to negative powers of the z's. By substituting in the Schrödinger equation $\Delta^1\boldsymbol{\chi}_{\mathbf{m}}=\varepsilon_{\mathbf{m}}(1)\boldsymbol{\chi}_{\mathbf{m}}$ we find the iterative formula

$$C_\lambda = \frac{1}{\varepsilon_{\mathbf{m}}(1) - \varepsilon_{\mathbf{m}-\lambda}(1)} \sum_{0\neq\beta\in\Lambda} S_{\beta,\mathbf{m}-(\lambda-\beta)} C_{\lambda-\beta}.$$

To use this formula in practice, one should take into account the heights of the λ's involved, because each coefficient C_λ can depend only on some of the C_ν such that $\mathrm{ht}(\nu)<\mathrm{ht}(\lambda)$.

(2) The Clebsch-Gordan series for the product $\prod_{i=1}^7 z_i^{m_i}$ reads

$$z_1^{m_1}z_2^{m_2}z_3^{m_3}z_4^{m_4}z_5^{m_5}z_6^{m_6}z_7^{m_7} = \boldsymbol{\chi}_{\mathbf{m}} + \sum_{\beta\in Q_{\mathbf{m}}} D_\beta \boldsymbol{\chi}_{\mathbf{m}-\beta}.$$

Here it is not difficult, in each particular case, to elaborate a list with all the elements in $Q_{\mathbf{m}}$ (i.e., the integral dominant weights appearing in the series). Furthermore, the operator $\Delta^1-\varepsilon_{\mathbf{n}}(1)$ annihilates the character $\boldsymbol{\chi}_{\mathbf{n}}$. Taking this into account, we can make use of the simple-looking formula

$$\boldsymbol{\chi}_{\mathbf{m}}=\left\{\prod_{\beta\in Q_{\mathbf{m}}}[\Delta^1-\varepsilon_{\mathbf{m}-\beta}(1)]\right\}z^{\mathbf{m}}$$

to obtain the eigenfunctions.

Through any of these methods, it is possible to compute the characters rather quickly. As an illustration, we offer a list of the third order characters in Appendix A.

Once we have a method for the computation of the characters, we can extend it to produce an algorithm for calculating the Clebsch-Gordan series. Suppose that we want to obtain the series for $\boldsymbol{\chi}_{\mathbf{m}}\cdot\boldsymbol{\chi}_{\mathbf{n}}$. We list the possible dominant weights entering in the series arranged by heights

$$\boldsymbol{\chi}_{\mathbf{m}}\cdot\boldsymbol{\chi}_{\mathbf{n}}=\boldsymbol{\chi}_{\mathbf{m+n}}+N_{\mu_1}\boldsymbol{\chi}_{\mu_1}+N_{\mu_2}\boldsymbol{\chi}_{\mu_2}+\cdots .$$

The multiplicity N_{μ_1} is simply the difference between the coefficients of z^{μ_1} in $\boldsymbol{\chi}_{\mathbf{m}}\cdot\boldsymbol{\chi}_{\mathbf{n}}$ and in $\boldsymbol{\chi}_{\mathbf{m+n}}$. Then, N_{μ_2} is the difference between the coefficient of z^{μ_2} in $\boldsymbol{\chi}_{\mathbf{m}}\cdot\boldsymbol{\chi}_{\mathbf{n}}$ and the sum of the corresponding coefficients in $\boldsymbol{\chi}_{\mathbf{m+n}}$ and $\boldsymbol{\chi}_{\mu_1}$, and so on. As an example, we present in Appendix B a list with a few cubic Clebsch-Gordan series. The complete list can be found in Ref. 29.

The approach we are describing is also useful to find the general structure of the series for products of some specific types. Let us consider, for instance, series of the type $z_7\boldsymbol{\chi}_{n\lambda_7}$ with arbitrary integer $n>0$. The weights of the representation R_{λ_7} are given by the linear combinations $\pm(v_i+v_j)$, $i\neq j$.[22] If we expand these weights in the basis of fundamental weights, we see that there are only four whose coefficients for all λ_i with $i\neq 7$ are non-negative, λ_7, $\lambda_6-\lambda_7$, $\lambda_1-\lambda_7$, and $-\lambda_7$. Hence, the form of the series should be

$$z_7\boldsymbol{\chi}_{0,0,0,0,0,0,n}=\boldsymbol{\chi}_{0,0,0,0,0,0,n+1}+a\boldsymbol{\chi}_{0,0,0,0,0,1,n-1}+b\boldsymbol{\chi}_{1,0,0,0,0,0,n-1}+c\boldsymbol{\chi}_{0,0,0,0,0,0,n-1}, \tag{21}$$

where we must fix a, b, and c. Now, by solving the Schrödinger equation by means of the first of the two methods described above, one finds

$$\boldsymbol{\chi}_{0,0,0,0,0,0,n}=z_7^n+(1-n)z_6z_7^{n-2}-z_1z_7^{n-2}+\cdots ,$$

$$\boldsymbol{\chi}_{0,0,0,0,0,1,n-1}=z_6z_7^{n-1}-z_1z_7^{n-1}+\cdots .$$

If we substitute this in (21), we can solve for a and b, obtaining $a=b=1$. We can now fix c by adjusting dimensions in (21). This gives $c=1$.

We list below the series of the form $z_7\boldsymbol{\chi}_{n\lambda_k}$ obtained through the same procedure,

$$z_7\boldsymbol{\chi}_{n,0,0,0,0,0,0}=\boldsymbol{\chi}_{n,0,0,0,0,0,1}+\boldsymbol{\chi}_{n-1,1,0,0,0,0,0}+\boldsymbol{\chi}_{n-1,0,0,0,0,0,1},$$

$$z_7\boldsymbol{\chi}_{0,n,0,0,0,0,0}=\boldsymbol{\chi}_{0,n,0,0,0,0,1}+\boldsymbol{\chi}_{0,n-1,1,0,0,0,0}+\boldsymbol{\chi}_{0,n-1,0,0,0,1,0}+\boldsymbol{\chi}_{1,n-1,0,0,0,0,0},$$

$$z_7\boldsymbol{\chi}_{0,0,n,0,0,0,0}=\boldsymbol{\chi}_{0,0,n,0,0,0,1}+\boldsymbol{\chi}_{1,1,n-1,0,0,0,0}+\boldsymbol{\chi}_{0,0,n-1,0,1,0,0}+\boldsymbol{\chi}_{1,0,n-1,0,0,0,1}+\boldsymbol{\chi}_{0,1,n-1,0,0,0,0},$$

$$\begin{aligned}z_7\boldsymbol{\chi}_{0,0,0,n,0,0,0}=&\boldsymbol{\chi}_{0,0,0,n,0,0,1}+\boldsymbol{\chi}_{0,1,1,n-1,0,0,0}+\boldsymbol{\chi}_{1,0,0,n-1,1,0,0}+\boldsymbol{\chi}_{0,1,0,n-1,0,1,0}+\boldsymbol{\chi}_{0,0,1,n-1,0,0,1}\\&+\boldsymbol{\chi}_{1,1,0,n-1,0,0,0}+\boldsymbol{\chi}_{0,0,0,n-1,1,0,0},\end{aligned}$$

$$\begin{aligned}z_7\boldsymbol{\chi}_{0,0,0,0,n,0,0}=&\boldsymbol{\chi}_{0,0,0,0,n,0,1}+\boldsymbol{\chi}_{0,0,0,1,n-1,0,0}+\boldsymbol{\chi}_{1,0,0,0,n-1,1,0}+\boldsymbol{\chi}_{0,1,0,0,n-1,0,1}+\boldsymbol{\chi}_{0,0,1,0,n-1,0,0}\\&+\boldsymbol{\chi}_{0,0,0,0,n-1,1,0},\end{aligned}$$

$$z_7\chi_{0,0,0,0,0,n,0} = \chi_{0,0,0,0,0,n,1} + \chi_{0,0,0,0,1,n-1,0} + \chi_{1,0,0,0,0,n-1,1} + \chi_{0,1,0,0,0,n-1,0} + \chi_{0,0,0,0,0,n-1,1}.$$

VI. CONCLUSIONS

In this paper we have shown how the Calogero-Sutherland Hamiltonian for the Lie algebra E_7 can be used to compute both Clebsch-Gordan series and characters of that algebra. The treatment we have presented can be applied to the cases of other simple algebras. It can be also extended to deal with the system of orthogonal polynomials based on E_7 for general values of the parameter κ. The way in which this should be done is the subject of a research now in progress and will be presented elsewhere.

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APPENDIX A: LIST OF THE CHARACTERS OF E_7 OF THIRD ORDER

$$\chi_{3000000} = z_1^3 - 2z_1z_3 + z_4 - z_1z_6 - z_1^2 + z_2z_7 - z_3 - 2z_1,$$

$$\chi_{2100000} = z_1^2z_2 - z_2z_3 - z_1z_5 - z_1^2z_7 + z_6z_7 - z_5 - z_2,$$

$$\chi_{1200000} = z_1z_2^2 - z_1z_4 - z_2z_5 - z_1^2z_6 + z_3z_6 + z_6^2 - z_1z_2z_7 - z_1^3 + 2z_1z_3 - z_4 + 2z_1z_6 + z_1^2 - z_2z_7 + z_3 + z_6 + z_1,$$

$$\chi_{0300000} = z_2^3 - 2z_2z_4 + z_3z_5 - 2z_1z_2z_6 + z_5z_6 + z_1z_3z_7 - z_4z_7 - 2z_1^2z_2 + 2z_2z_3 + z_1z_5 + z_2z_6 + z_3z_7 + z_1z_2 + z_6z_7 + z_1z_7,$$

$$\chi_{2010000} = z_1^2z_3 - z_3^2 - z_1z_4 - z_1^2z_6 + z_2z_5 - z_3z_6 + z_1z_2z_7 - z_1^3 + z_1z_7^2 - z_2z_7 - z_7^2 + z_6 + z_1 + 1,$$

$$\chi_{1110000} = z_1z_2z_3 - z_2z_4 - z_1^2z_5 + z_5z_6 - z_1^3z_7 + z_1z_3z_7 - z_4z_7 + z_1z_6z_7 + z_1z_5 - z_2z_6 + z_1^2z_7 - z_6z_7 + z_5 + z_1z_7,$$

$$\chi_{0210000} = z_2^2z_3 - z_3z_4 - z_1z_2z_5 + z_5^2 - z_4z_6 - z_1^2z_2z_7 + z_2z_3z_7 + z_1z_5z_7 - z_1z_4 + z_2z_5 + z_1z_2z_7 - z_6^2 + z_5z_7 + z_1z_7^2 - z_1z_6 + z_2z_7 - z_3 - z_6 - z_1,$$

$$\chi_{1020000} = z_1z_3^2 - z_1^2z_4 - z_3z_4 + z_1z_2z_5 - z_1^3z_6 + z_1^2z_2z_7 - z_1^4 - z_2z_3z_7 + z_1^2z_3 + z_1z_5z_7 + z_3^2 + z_1^2z_7^2 - z_2z_6z_7 - z_1z_4 + z_3z_6 - z_1z_2z_7 + 2z_1z_3 - z_5z_7 - z_1z_7^2 + z_4 + 2z_1z_6 + 2z_1^2,$$

$$\chi_{0120000} = z_2z_3^2 - z_1z_2z_4 - z_1z_3z_5 + z_4z_5 - z_1^2z_3z_7 + z_1z_5z_6 + z_3^2z_7 - z_2z_6^2 + z_2z_5z_7 + z_3z_6z_7 + z_1^2z_5 - z_3z_5 - z_1z_2z_6 - z_5z_6 + z_1z_3z_7 + z_2^2z_7 + z_2z_7^2 - z_1z_5 - 2z_2z_6 + z_3z_7 - z_1z_2 + z_6z_7 - z_5 - z_2,$$

$$\chi_{0030000} = z_3^3 - 2z_1z_3z_4 + z_4^2 + z_1^2z_2z_5 - z_2z_3z_5 - 2z_1^2z_3z_6 + 2z_3^2z_6 + z_1z_4z_6 - z_2z_5z_6 + z_3z_6^2 + z_1^3z_2z_7 - 2z_1^3z_3 - 2z_1z_2z_3z_7 + z_2z_4z_7 + z_3z_5z_7 - z_1z_2z_6z_7 + 4z_1z_3^2 + z_1^2z_4 - 3z_3z_4 + z_1z_3z_7^2 - z_1z_2z_5 + z_5z_6z_7 - z_5^2 - z_4z_7^2 + 2z_1z_3z_6 - z_1^2z_2z_7 + z_2^2z_6 - z_4z_6 - z_1z_5z_7 - z_1^2z_7^2 + z_1^2z_3 + 2z_3^2 + z_3z_7^2 - z_1z_4 - z_2z_5$$

$$+ 2z_3z_6 + z_6z_7^2 - z_1z_2z_7 + 2z_1z_3 + z_1z_7^2 + z_4 + z_1z_6 + z_1^2 - z_3 - z_6 - z_1,$$

$$\chi_{2001000} = z_1^2z_4 - z_3z_4 - z_1z_2z_5 + z_5^2 + z_2^2z_6 - 2z_4z_6 - z_2z_6z_7 + z_3z_7^2 - z_1z_4 + z_2z_5 - 2z_1z_2z_7 + z_5z_7 + z_2^2 - z_4 + z_1z_6 + z_1^2 + z_2z_7 + z_7^2 - z_3 - z_6 - z_1 - 1,$$

$$\chi_{1101000} = z_1z_2z_4 - z_1z_3z_5 - z_2^2z_5 + z_2z_3z_6 + z_1z_5z_6 - z_1z_4z_7 + z_2z_6^2 - z_2z_5z_7 - z_1z_2z_7^2 - z_6^2z_7 + z_1^2z_5 - z_3z_5 + z_1z_2z_6 + z_1z_7^3 + z_5z_6 - z_4z_7 - 3z_1z_6z_7 + z_7^3 + 2z_1z_5 + 2z_2z_6 - z_6z_7 + z_1z_2 + z_5 - z_1z_7 - z_7,$$

$$\chi_{0201000} = z_2^2z_4 - z_4^2 - z_2z_3z_5 + z_3^2z_6 + z_1z_5^2 - 2z_1z_4z_6 - z_1^2z_6^2 + z_3z_6^2 + z_1^2z_5z_7 - z_3z_5z_7 - z_1^2z_4 + z_1z_2z_6z_7 - z_2^2z_7^2 - z_5z_6z_7 + z_3z_4 - z_1z_2z_5 - z_1z_3z_7^2 + z_5^2 + z_2^2z_6 + z_4z_7^2 - z_1^3z_6 + 2z_1z_3z_6 + z_1^2z_2z_7 + z_1z_6z_7^2 - z_1z_6^2 - z_1z_2^2 + z_1^2z_7^2 + z_1z_4 + z_2z_5 - z_3z_7^2 - z_6z_7^2 - z_1^2z_6 + 2z_3z_6 + z_6^2 + z_5z_7 + z_2^2 - z_1z_7^2 - z_4 - z_1^2 + z_3 + z_6 + z_1,$$

$$\chi_{1011000} = z_1z_3z_4 - z_4^2 - z_1^2z_2z_5 + z_1z_2^2z_6 + z_1z_5^2 - z_1z_4z_6 - z_2z_4z_7 + z_1^2z_5z_7 - 2z_1z_2z_6z_7 - z_1^2z_4 + z_3z_4 - z_5z_6z_7 + z_1z_3z_7^2 + z_1z_2z_5 - 2z_1^2z_2z_7 + z_4z_7^2 + z_5^2 + z_2z_7^3 + z_1z_5z_7 + z_1^2z_7^2 + 2z_1z_2^2 - z_3z_7^2 + z_1z_3 - z_4 - z_1z_6 - z_2z_7 - z_1^2 + z_3,$$

$$\chi_{0111000} = z_2z_3z_4 - z_3^2z_5 - z_1z_2^2z_5 + z_1z_2z_3z_6 + z_2z_5^2 + z_1^2z_5z_6 - z_3z_5z_6 - z_1^2z_4z_7 - z_5z_6^2 + z_1z_2z_5z_7 - z_1^3z_6z_7 + z_1z_3z_6z_7 + 2z_1^3z_5 - 4z_1z_3z_5 - z_2z_3z_7^2 + 2z_4z_5 + z_2z_3z_6 + z_1^2z_7^3 - 2z_1z_5z_6 + z_1z_4z_7 + 2z_2z_5z_7 - z_3z_6z_7 - z_1^2z_5 - z_3z_5 - z_5z_6 - z_1z_7^3 + z_2z_3 + z_1z_6z_7 - 3z_1z_5 - z_1^2z_7 + z_1z_7,$$

$$\chi_{0021000} = z_3^2z_4 - z_1z_4^2 - z_1z_2z_3z_5 + z_2z_4z_5 + z_1^2z_5^2 + z_1^2z_2^2z_6 - z_3z_5^2 - 2z_1^2z_4z_6 - z_2^2z_3z_6 + 3z_3z_4z_6 - z_2^2z_6^2 - z_1^3z_6^2 - z_5^2z_6 - z_1z_2z_4z_7 + 2z_1z_3z_6^2 + z_1^3z_5z_7 + z_2^2z_5z_7 - z_1z_3z_5z_7 - 2z_1^2z_2z_6z_7 - z_1^3z_4 + z_4z_6^2 + z_4z_5z_7 + z_2z_3z_6z_7 + z_1z_6^3 + 2z_1z_3z_4 - z_1z_5z_6z_7 + z_1^2z_3z_7^2 + z_1^2z_2z_5 - z_1^4z_6 - 2z_2z_3z_5 - z_3^2z_7^2 + z_2z_6^2z_7 + z_1z_4z_7^2 + 3z_1^2z_3z_6 + z_1^2z_6z_7^2 - z_1z_5^2 - z_1^3z_2z_7 - z_3^2z_6 + z_1z_4z_6 - 2z_3z_6z_7^2 - z_6^2z_7^2 + z_1^2z_2^2 - z_2z_5z_6 + 2z_1^2z_6^2 + z_2z_4z_7 - z_1^2z_5z_7 - z_3z_6^2 + z_1^3z_7^2 + z_1z_2z_7^3 + z_1^2z_4 + z_1^3z_6 + z_1z_2z_6z_7 + z_5z_6z_7 - 3z_1z_3z_7^2 - 2z_1z_2z_5 - 2z_1z_6z_7^2 - z_5^2 - z_2z_7^3 - 2z_2^2z_6 + z_1z_6^2 + z_2z_3z_7 + z_3^2 - z_1z_4 + 2z_2z_6z_7 - z_1^2z_7^2 - 2z_2z_5 - z_1^3 + z_3z_6 + 2z_1z_3 - z_2^2 + z_1z_6 + z_2z_7 + z_1^2,$$

$$\chi_{1002000} = z_1z_4^2 - z_1z_2z_3z_5 - z_2z_4z_5 + z_3z_5^2 + z_1^2z_4z_6 + z_2^2z_3z_6 - z_3z_4z_6 - z_1z_2z_4z_7 + z_1^3z_5z_7 - z_1z_3z_5z_7 - z_1^2z_2z_6z_7 - z_1z_5z_6z_7 + z_3^2z_7^2 - z_1z_4z_7^2 + z_2z_3z_5 + z_2z_5z_7^2 - z_3^2z_6 + 2z_1z_4z_6 - z_1z_2z_3z_7 + z_1^2z_6^2 + z_1z_2z_7^3 - 2z_1^2z_5z_7 + z_3z_5z_7 - z_1z_2z_6z_7 + z_5z_6z_7 + z_1^2z_4 + z_2^2z_3 - 2z_3z_4 + 2z_1z_2z_5 + z_1^3z_6 - z_5^2 - 2z_1z_3z_6 - z_1z_6z_7^2 + z_1z_6^2 - 2z_1z_5z_7 + z_1z_4 - z_1^2z_7^2 + 2z_3z_7^2 + z_1^2z_6 - 2z_3z_6 - z_1z_2z_7 + z_1z_6 + z_1^2 - 2z_3,$$

$$\chi_{0102000} = z_2z_4^2 - z_2^2z_3z_5 - z_3z_4z_5 + z_2z_3^2z_6 + z_1z_2z_5^2 - z_4z_5z_6 - z_1z_3z_4z_7 - z_1^2z_2z_6^2 + z_4^2z_7 + 2z_2z_3z_6^2 + 2z_1^2z_2z_5z_7 - z_1z_5z_6^2 - 3z_2z_3z_5z_7 - z_1^2z_3z_6z_7 + 2z_1z_4z_6z_7 + z_1^2z_6^2z_7 + z_3^2z_5 - z_1z_4z_5 - 2z_2z_4z_7^2 - z_2z_5^2 - z_3z_5z_7^2 + 2z_2z_4z_6 - 3z_1^2z_5z_6 + 4z_3z_5z_6 + 2z_1^2z_4z_7 + z_5z_6z_7^2 - z_3z_4z_7 + z_1z_3z_7^3 - 2z_4z_7^3$$

$$+ 2z_1^3z_6z_7 + z_5z_6^2 - 2z_1z_6z_7^3 - 2z_5^2z_7 - 4z_1z_3z_6z_7 + 2z_4z_6z_7 - 2z_1^3z_5 - 2z_1z_2z_4 + 2z_1z_6^2z_7 + z_2z_7^4$$
$$+ 5z_1z_3z_5 + z_4z_5 - 2z_1^2z_2z_6 + z_7^5 + 2z_2z_3z_6 - z_1z_5z_7^2 - 2z_2z_6z_7^2 + 2z_1z_5z_6 + z_2z_6^2 - 2z_1^2z_7^3 + z_3z_7^3$$
$$+ 2z_1^2z_6z_7 - 2z_6z_7^3 - z_3z_6z_7 + 2z_2z_4 + 2z_1z_2z_7^2 + 2z_3z_5 - 2z_1z_2z_6 + z_6^2z_7 - z_5z_7^2 - z_1z_3z_7 + 2z_5z_6$$
$$+ 2z_4z_7 + 2z_1z_6z_7 - 2z_2z_7^2 + z_1z_5 + 2z_1^2z_7 - 2z_7^3 + 2z_2z_6 - z_3z_7 + 2z_6z_7 - 2z_1z_2 + z_5 + z_2 + z_7,$$

$$\chi_{0012000} = z_3z_4^2 - z_2z_3^2z_5 - z_1z_2z_4z_5 + z_1z_3z_5^2 + z_2^2z_5^2 - z_4z_5^2 + z_1z_2^2z_3z_6 - z_2^2z_4z_6 + 2z_4^2z_6 - z_2z_3z_5z_6$$
$$- z_1z_2^2z_6^2 - z_1^2z_2z_4z_7 - z_1^2z_3z_6^2 + z_3^2z_6^2 - z_1z_5^2z_6 + 3z_1z_4z_6^2 + 2z_1^2z_3z_5z_7 - 2z_3^2z_5z_7 + z_1z_2^2z_5z_7$$
$$- z_1z_4z_5z_7 - z_1^3z_2z_6z_7 - z_2z_5z_6^2 + z_1^2z_6^3 + z_2z_5^2z_7 + z_3z_6^3 + z_1z_4^2 + z_2z_4z_6z_7 + z_1z_3^2z_7^2$$
$$- z_1^2z_5z_6z_7 - 2z_3z_5z_6z_7 + z_1^2z_4z_7^2 - z_1^2z_5^2 - z_1z_3^2z_6 - z_2z_4z_5 - 3z_3z_4z_7^2 + 3z_1^2z_4z_6 + z_3z_5^2$$
$$+ z_3z_4z_6 + z_1^3z_6z_7^2 + z_1z_2z_6^2z_7 + z_5z_6^2z_7 + z_1z_2z_5z_7^2 + z_2^2z_6z_7^2 - 2z_1z_3z_6z_7^2 - 4z_4z_6z_7^2$$
$$- 2z_1z_2z_5z_6 - z_5^2z_6 - z_1^2z_2z_3z_7 - 3z_1z_6^2z_7^2 + 2z_1^3z_6^2 - z_2^2z_6^2 + z_1^2z_2z_7^3 - 2z_1^3z_5z_7 - z_1^2z_7^4 + 2z_4z_6^2$$
$$+ z_1z_2z_4z_7 + z_1z_6^3 + z_1^3z_4 + z_1z_3z_5z_7 + z_1z_2^2z_3 + 2z_4z_5z_7 - z_2z_3z_6z_7 - z_2z_6z_7^3 - z_2^2z_4$$
$$- 2z_1z_3z_4 - z_1^2z_3z_7^2 + 4z_1z_5z_6z_7 + z_2z_6^2z_7 + 2z_3z_7^4 + z_3^2z_7^2 + 2z_2z_3z_5 + z_1^4z_6 - 2z_1z_5^2$$
$$- 2z_1z_4z_7^2 + 2z_6z_7^4 - z_1^2z_3z_6 - z_3^2z_6 - z_1z_2^2z_6 - 2z_1^2z_6z_7^2 + z_1z_2z_3z_7 - 2z_2z_5z_6 - z_3z_6z_7^2$$
$$- 2z_6^2z_7^2 + z_1^2z_6^2 - z_1z_2z_7^3 - 2z_5z_7^3 + z_2z_4z_7 - z_1^3z_7^2 + z_3z_5z_7 + 2z_1z_2z_6z_7 - z_1^2z_4 + 3z_1z_3z_7^2$$
$$+ z_2^2z_7^2 + z_3z_4 + 3z_5z_6z_7 - z_1z_2z_5 - z_5^2 - 2z_2^2z_6 - 2z_1z_3z_6 + z_1z_7^4 + 2z_4z_6 - z_2z_7^3 - z_1^2z_2z_7$$
$$- z_2z_3z_7 + 2z_1z_5z_7 + z_1z_4 + 2z_1^2z_7^2 + 2z_2z_6z_7 + z_1^2z_6 - 2z_3z_7^2 - z_2z_5 - z_3z_6 + z_1^3 + z_1z_2z_7$$
$$- 2z_6z_7^2 - z_2^2 + 2z_5z_7 - z_1z_7^2 - 2z_1z_3 - z_1z_6 + z_2z_7 - z_1^2,$$

$$\chi_{0003000} = z_4^3 - 2z_2z_3z_4z_5 + z_3^2z_5^2 + z_1z_2^2z_5^2 + z_2^2z_3^2z_6 - z_3^2z_4z_6 - z_1z_2^2z_4z_6 - z_1z_4z_5^2 + 3z_1z_4^2z_6$$
$$- z_1z_2z_3z_5z_6 - z_2z_4z_5z_6 - z_1^2z_2^2z_6^2 - z_1z_3^2z_6^2 - z_1^2z_5^2z_6 - z_1z_2z_3z_4z_7 + z_3z_5^2z_6 + 3z_1^2z_4z_6^2$$
$$+ z_2^2z_3z_6^2 + z_2z_4^2z_7 + z_1^2z_2^2z_5z_7 + z_1z_3^2z_5z_7 - z_2^2z_3z_5z_7 - 2z_3z_4z_5z_7 - z_1z_2z_5z_6^2 - z_1^2z_2z_3z_6z_7$$
$$+ z_1^3z_6^3 + 2z_1z_2z_4z_6z_7 + z_3^3z_7^2 + z_5^3z_7 - 2z_1z_3z_5z_6z_7 + z_1^2z_4^2 - z_1^2z_2z_3z_5 - z_3z_4^2 + 2z_2z_3^2z_5$$
$$- z_1z_2z_4z_5 - z_3^3z_6 - 2z_1^3z_5^2 + 5z_1z_3z_5^2 + z_1^2z_2z_6^2z_7 + 3z_1^3z_4z_6 - 3z_4^2z_7^2 - 4z_4z_5^2 - 4z_1z_3z_4z_6$$
$$+ z_1z_2^2z_6z_7^2 + z_1z_5^2z_7^2 - z_1z_2z_3^2z_7 + z_3^2z_6z_7^2 + 3z_4^2z_6 - 2z_1^2z_2z_5z_6 - 6z_1z_4z_6z_7^2 - 3z_1^2z_6^2z_7^2$$
$$+ 2z_1^4z_6^2 + 3z_2z_3z_5z_6 - z_1z_2^2z_6^2 + z_1^2z_2z_4z_7 - z_1z_5^2z_6 - 3z_1^2z_3z_6^2 + z_2z_5z_6z_7^2 - z_1^4z_5z_7 + z_1z_2z_3z_7^3$$
$$- z_3^2z_6^2 + 4z_1z_4z_6^2 - 2z_2z_4z_7^3 + z_1^2z_3z_5z_7 + 2z_3^2z_5z_7 + 2z_3z_5z_7^3 + z_1^2z_6^3 - 2z_2z_5^2z_7 - 2z_1z_2z_6z_7^3$$
$$+ z_1^3z_2z_6z_7 + z_1^2z_3z_4 - 3z_1z_2z_3z_6z_7 - z_1^3z_3z_7^2 + z_2^2z_3^2 - z_1^3z_2z_5 + 2z_1^2z_5z_6z_7 - z_1z_2^2z_4 - 2z_3^2z_4$$
$$- 2z_1z_4^2 + 4z_1z_2z_3z_5 + 2z_1z_3^2z_7^2 + 3z_2z_4z_6z_7 - z_1^2z_2^2z_6 - 2z_3z_5z_6z_7 - z_1^2z_5^2 - 2z_1^2z_4z_7^2$$
$$+ 2z_1^3z_3z_6 + 3z_1z_2z_6^2z_7 + 2z_3z_4z_7^2 - 4z_1z_3^2z_6 - 3z_1^3z_6z_7^2 + 3z_4z_7^4 - z_2z_4z_5 - z_1z_2z_5z_7^2$$
$$+ 2z_2^2z_3z_6 + 6z_1z_3z_6z_7^2 + 3z_1z_6z_7^4 + z_5^2z_7^2 + 5z_3z_5^2 - 2z_1^2z_4z_6 + z_1^2z_2z_3z_7 - 2z_3z_4z_6 - z_1z_2z_5z_6$$
$$- 5z_4z_6z_7^2 - z_2z_3^2z_7 + z_1^3z_6^2 + z_1^3z_5z_7 - 3z_1z_6^2z_7^2 - 6z_1z_3z_6^2 - z_1^2z_2z_7^3 + z_2z_7^5 + 2z_4z_6^2 + 2z_4z_5z_7$$
$$- z_7^6 + z_1^2z_2z_6z_7 - z_1z_5z_7^3 - 2z_1z_3z_4 - z_2z_3z_6z_7 + 2z_1z_5z_6z_7 + z_1z_2^2z_7^2 + z_1^2z_7^4 - z_1^2z_2z_5 + 3z_4^2$$
$$+ 2z_3^2z_7^2 - 3z_2z_6z_7^3 - z_1^2z_3z_6 + 3z_2z_3z_5 - 2z_3z_7^4 - 2z_1z_2^2z_6 + 2z_6z_7^4 - 3z_3^2z_6 + 3z_1z_5^2$$
$$+ 3z_1z_4z_7^2 + 2z_2z_6^2z_7 + z_1^2z_6z_7^2 + z_2z_5z_7^2 + 4z_3z_6z_7^2 - z_6^2z_7^2 - 2z_1^2z_6^2 - 3z_1z_2z_3z_7 - 2z_3z_6^2$$

$$+ 3z_2z_4z_7 + 3z_1^2z_5z_7 + z_2^2z_3 - z_5z_7^3 - 4z_3z_5z_7 - z_1z_7^4 + 2z_1^2z_4 + 3z_1z_2z_6z_7 + 3z_1^3z_6 - 2z_3z_4$$
$$+ 3z_1z_3z_7^2 - 8z_1z_3z_6 + z_1^2z_2z_7 - 5z_4z_7^2 + 4z_4z_6 - 3z_2z_7^3 - 2z_1z_6^2 + z_1^2z_3 - z_2z_3z_7 - z_1z_2^2$$
$$+ 2z_7^4 + 4z_2z_6z_7 - 2z_1^2z_7^2 - 2z_3^2 + 4z_3z_7^2 - 4z_1z_4 - 2z_1^2z_6 - 2z_6z_7^2 - 4z_3z_6 - 2z_1z_3 + 3z_1z_7^2$$
$$+ 2z_4 - 4z_1z_6 + z_1^2 + 2z_2z_7 - 2z_3 - z_7^2 - 2z_1,$$

$$\chi_{2000100} = z_1^2z_5 - z_3z_5 - z_1z_2z_6 + z_2^2z_7 - z_4z_7 - z_1z_5 + z_3z_7 - 2z_1z_2 + z_1z_7,$$

$$\chi_{1100100} = z_1z_2z_5 - z_2^2z_6 - z_1z_3z_6 - z_5^2 + z_4z_6 + z_1z_6^2 + z_2z_3z_7 - z_1z_5z_7 + z_2z_6z_7 + z_1^2z_6 - z_2z_5 - z_3z_6 - z_6z_7^2$$
$$- z_2^2 - z_1z_7^2 + z_2z_7 + z_7^2,$$

$$\chi_{0200100} = z_2^2z_5 - z_4z_5 - z_2z_3z_6 + z_3^2z_7 - z_2z_6^2 - z_1z_4z_7 + z_2z_5z_7 + z_3z_6z_7 - z_1^2z_5 - z_1^3z_7 + z_1z_3z_7 + z_1^2z_2$$
$$+ z_4z_7 - z_2z_3 + z_1z_6z_7 + z_2z_7^2 + z_1^2z_7 - 2z_2z_6 - z_1z_2 - z_2,$$

$$\chi_{1010100} = z_1z_3z_5 - z_4z_5 - z_1^2z_2z_6 + z_1z_2^2z_7 + z_2z_6^2 + z_1^2z_6z_7 - z_2z_5z_7 - z_3z_6z_7 - z_2z_4 - z_6^2z_7 - z_1^2z_5 + 2z_3z_5$$
$$- z_1z_2z_6 + 2z_5z_6 + z_1z_3z_7 - z_1z_7^3 - 2z_1^2z_2 - z_2^2z_7 + z_1z_6z_7 + z_2z_3 + z_1z_5 + 2z_2z_6 + z_1^2z_7 + z_7^3$$
$$+ z_1z_2 - z_6z_7 + z_5 + z_2 - z_7,$$

$$\chi_{0110100} = z_2z_3z_5 - z_3^2z_6 - z_1z_5^2 - z_1z_2^2z_6 + z_1z_4z_6 + z_2z_5z_6 + z_1z_2z_3z_7 + 2z_1^2z_6^2 - 2z_3z_6^2 - 2z_1^2z_5z_7 + 2z_3z_5z_7$$
$$+ z_1z_2z_6z_7 - z_6^3 + z_5z_6z_7 - z_3z_4 - z_1^3z_7^2 + z_1z_3z_7^2 + 2z_1^3z_6 - 4z_1z_3z_6 - z_1z_6z_7^2 - 2z_1z_6^2 + 2z_1z_5z_7$$
$$+ z_2z_6z_7 + z_1^2z_7^2 - z_1z_4 + z_3z_7^2 - z_1^2z_6 + 2z_6z_7^2 - 3z_3z_6 - 3z_6^2 + z_1z_7^2 - 3z_1z_6 - z_3 - 2z_6 - z_1,$$

$$\chi_{0020100} = z_3^2z_5 - z_1z_4z_5 - z_1z_2z_3z_6 + z_2z_4z_6 + z_1^2z_2^2z_7 + z_1z_2z_6^2 - z_5z_6^2 - z_1^2z_4z_7 - z_2^2z_3z_7 + 2z_3z_4z_7$$
$$- z_1z_2z_5z_7 + z_5^2z_7 - z_2^2z_6z_7 - z_1z_2z_4 - z_1^3z_5 + z_2^2z_5 - z_1^2z_2z_7^2 + 2z_4z_6z_7 + 3z_1z_3z_5 + z_2z_3z_7^2$$
$$- 2z_4z_5 - z_2z_3z_6 - z_1^4z_7 + z_1z_5z_7^2 - z_1z_2^2z_7 - z_1z_5z_6 + 4z_1^2z_3z_7 + z_2z_6^2 - 2z_3^2z_7 + z_2^3 - z_1^3z_2$$
$$+ 2z_1^2z_6z_7 + z_1z_2z_3 - z_2z_4 + 2z_1^3z_7 - 3z_3z_6z_7 + z_3z_5 - z_6^2z_7 + z_1z_2z_7^2 + z_5z_7^2 - z_2^2z_7 - 3z_1z_3z_7$$
$$- z_5z_6 + 2z_2z_3 + z_1z_7^3 - 4z_1z_6z_7 + z_1z_5 + 2z_2z_6 - z_1^2z_7 - z_3z_7 - z_6z_7 + 2z_1z_2 - z_1z_7,$$

$$\chi_{1001100} = z_1z_4z_5 - z_2z_5^2 - z_1z_2z_3z_6 + z_3z_5z_6 + z_1^2z_4z_7 + z_1z_2z_6^2 + z_2^2z_3z_7 - z_3z_4z_7 + z_5z_6^2 - z_1z_2z_5z_7 - z_5^2z_7$$
$$+ z_1^3z_6z_7 - z_1z_3z_6z_7 - z_1^2z_2z_7^2 - z_1z_2z_4 - z_4z_6z_7 + z_4z_5 - 2z_1z_6^2z_7 + z_2z_3z_7^2 - z_2z_3z_6 + 3z_1z_5z_6$$
$$+ z_3^2z_7 - 2z_1z_4z_7 + z_6z_7^3 - 2z_1^2z_6z_7 - z_1z_2z_3 + z_1^2z_5 + 2z_3z_6z_7 + z_2z_4 + z_1z_2z_7^2 - z_3z_5 + z_1z_2z_6$$
$$- z_5z_7^2 + z_5z_6 + z_1^2z_2 + z_4z_7 + z_1z_7^3 - z_1z_6z_7 - z_2z_3 - z_1z_2 - z_7^3 - z_1z_7 + z_7,$$

$$\chi_{0101100} = z_2z_4z_5 - z_3z_5^2 - z_2^2z_3z_6 + z_1z_2z_5z_6 + z_2z_3^2z_7 + z_1z_3z_6^2 - z_4z_6^2 - z_1z_6^3 - z_1z_3z_5z_7 - z_1^2z_3z_7^2 + z_2z_3z_6z_7$$
$$- z_1z_3z_4 + z_4^2 + z_1^2z_2z_5 + z_1z_5z_6z_7 - 2z_2z_3z_5 - z_2z_5z_7^2 - z_1z_5^2 + z_1z_4z_6 - z_1^2z_6^2 + z_6^2z_7^2 + z_1z_2z_3z_7$$
$$+ z_3z_6^2 + z_1z_2z_6z_7 - z_2^2z_3 + z_1^2z_4 + z_1^3z_7^2 - z_5z_6z_7 - z_3z_4 - z_4z_7^2 - z_2^2z_6 - z_1z_6z_7^2 - z_1z_3z_6 - z_1^2z_2z_7$$
$$+ z_4z_6 + z_1z_6^2 + z_2z_3z_7 - 2z_1^2z_7^2 + z_1^2z_6 + z_3z_7^2 - z_3z_6 + 2z_1z_2z_7 - z_1z_3 - z_5z_7 - z_2^2 + z_4 + z_1z_6$$
$$+ z_1^2 - z_3,$$

$$\chi_{0011100} = z_3z_4z_5 - z_1z_2z_5^2 - z_2z_3^2z_6 + z_1z_3z_5z_6 + z_2^2z_5z_6 + z_1z_2^2z_3z_7 - z_2^2z_4z_7 + z_1^2z_2z_6^2 - z_2z_3z_6^2 + z_4^2z_7$$
$$- z_1^2z_2z_5z_7 - z_2z_6^3 - z_1^2z_2z_4 + z_1^2z_3z_5 - z_1z_2^2z_6z_7 + z_1z_4z_6z_7 + z_2z_5z_6z_7 + z_1z_2^2z_5 - z_1^3z_2z_7^2 - z_1^2z_6^2z_7$$
$$+ z_1z_2z_3z_7^2 + z_3z_6^2z_7 - z_3^2z_5 + z_6^3z_7 + z_1^2z_5z_7^2 - z_1z_2z_3z_6 + z_2z_4z_6 - z_3z_5z_7^2 + z_1z_2z_6z_7^2 + z_2^2z_7^3 + z_1^3z_7^3$$
$$+ z_1^2z_5z_6 + z_1z_3^2z_7 - 2z_3z_5z_6 - z_1z_3z_7^3 + z_1^2z_4z_7 - 2z_3z_4z_7 - z_5z_6z_7^2 - z_4z_7^3 - z_1z_6z_7^3 - z_1z_2z_5z_7$$
$$- z_5z_6^2 + z_5^2z_7 + z_1^2z_2z_7^2 - z_1^2z_2z_3 - z_2^2z_6z_7 + z_4z_6z_7 + 2z_1z_6^2z_7 + 2z_1z_2z_4 + 2z_2^2z_5 - z_1z_3z_5 - 2z_4z_5$$
$$- z_2z_3z_7^2 + 2z_1^2z_2z_6 - 2z_2z_3z_6 - z_2z_6z_7^2 - 2z_1^2z_7^3 + z_3z_7^3 - z_1^2z_3z_7 - 3z_1z_5z_6 + z_3^2z_7 - 2z_2z_6^2 + z_1^3z_2$$
$$- z_1z_4z_7 - 2z_1^2z_5 + z_3z_6z_7 + z_2z_4 - z_1^3z_7 + z_3z_5 + z_6^2z_7 + 2z_1z_3z_7 - z_5z_6 - z_2^2z_7 + z_4z_7 + z_1z_7^3$$
$$+ z_1z_6z_7 - z_2z_7^2 - z_1^2z_2 + z_1z_5 + 2z_1^2z_7 - z_3z_7 - z_1z_7 + z_2,$$

$$\chi_{0002100} = z_4^2z_5 - z_2z_3z_5^2 - z_2z_3z_4z_6 + z_3^2z_5z_6 + z_1z_2^2z_5z_6 + z_2^2z_3^2z_7 - z_3^2z_4z_7 - z_1z_2^2z_4z_7 - z_2z_4z_6^2$$
$$+ 2z_1z_4^2z_7 - z_1z_2z_3z_5z_7 - z_1^2z_5z_6^2 + 2z_3z_5z_6^2 - z_1z_3^2z_6z_7 - z_1^2z_2^2z_6z_7 + z_1^2z_5^2z_7 - z_1z_2z_6^3$$
$$- z_1z_2z_3z_4 + z_2z_4^2 - 2z_3z_5^2z_7 + z_2^2z_3z_6z_7 + 3z_1^2z_4z_6z_7 + z_1z_3^2z_5 - z_3z_4z_6z_7 - z_1^2z_2z_3z_7^2$$
$$+ z_1^2z_2^2z_5 + z_2z_3^2z_7^2 + z_5^2z_6z_7 - z_2^2z_3z_5 - z_1^2z_4z_5 + z_1^3z_6^2z_7 - z_1z_3z_6^2z_7 + z_1z_2z_4z_7^2 + z_1^3z_5z_7^2$$
$$- 2z_1z_3z_5z_7^2 + z_4z_6^2z_7 - z_2z_3^2z_6 - z_5^3 + z_1z_2z_4z_6 + z_3^3z_7 - 3z_4z_5z_7^2 - 3z_1^3z_5z_6 + z_1^2z_2z_6z_7^2$$
$$+ 6z_1z_3z_5z_6 + z_1z_6^3z_7 - z_4z_5z_6 + z_2z_3z_6z_7^2 + 2z_1^3z_4z_7 + z_1z_2^2z_7^3 + z_1^2z_3z_7^3 - 2z_1z_5z_6z_7^2 + z_2z_6^2z_7^2$$
$$- 4z_1z_3z_4z_7 - 4z_1z_4z_7^3 - z_2z_3z_6^2 - 3z_1^2z_6z_7^3 - z_1^2z_2z_5z_7 + z_4^2z_7 + z_1z_5z_6^2 + z_2z_3z_5z_7 + 2z_1^4z_6z_7$$
$$- z_1z_5^2z_7 - 6z_1^2z_3z_6z_7 - z_1z_2z_3^2 - z_1z_2^2z_6z_7 + z_1^2z_2z_4 - 2z_1^4z_5 - z_2z_3z_4 - z_6^2z_7^3 - z_2z_6^3$$
$$+ 2z_3^2z_6z_7 + 5z_1z_4z_6z_7 + z_1z_2^2z_5 + 5z_1^2z_3z_5 + 3z_1^2z_6^2z_7 + z_1^3z_2z_6 - z_1z_2z_7^4 - z_1^2z_5z_7^2 - 3z_1z_4z_5$$
$$+ z_6^3z_7 - z_2z_4z_7^2 + 2z_3z_5z_7^2 + 2z_5z_7^4 - 2z_1^3z_7^3 + z_1z_2z_6z_7^2 - 2z_1z_2z_3z_6 - z_1^3z_3z_7 - z_2z_4z_6$$
$$+ 2z_3z_5z_6 + 2z_1z_3^2z_7 + z_2^2z_3z_7 - 2z_1z_2z_6^2 - 2z_1^2z_4z_7 - z_1z_2z_5z_7 + 2z_1z_7^5 + 3z_1z_3z_7^3 - 2z_5z_6z_7^2$$
$$- z_4z_7^3 + 2z_1^2z_2z_3 - 4z_1z_6z_7^3 + z_5^2z_7 - 2z_2z_3^2 - z_1^2z_2z_7^2 - z_1z_2z_4 + 2z_4z_6z_7 + 3z_1z_6^2z_7$$
$$+ 2z_1z_3z_5 + 3z_2z_3z_7^2 + z_4z_5 + 2z_1z_5z_7^2 - 5z_2z_3z_6 + 2z_1z_5z_6 + 2z_2z_6z_7^2 - z_1z_2^2z_7 + 3z_1z_4z_7$$
$$- 3z_2z_6^2 + 2z_1^2z_7^3 - z_3z_7^3 - 2z_1z_2z_3 - z_6z_7^3 + 3z_1^2z_5 + z_3z_6z_7 + 2z_6^2z_7 - 2z_3z_5 + 2z_1z_2z_7^2$$
$$- 2z_1z_2z_6 - 2z_5z_7^2 + 2z_1^3z_7 - 2z_1z_3z_7 + z_4z_7 + z_1^2z_2 - 3z_1z_7^3 + 3z_1z_6z_7 - 4z_2z_3 + z_2z_7^2$$
$$- z_1z_5 - 3z_2z_6 - 2z_1^2z_7 + z_3z_7 - z_1z_2 + z_6z_7 + z_1z_7 - z_2,$$

$$\chi_{1000200} = z_1z_5^2 - z_1z_4z_6 - z_2z_5z_6 - z_1^2z_6^2 + z_2z_4z_7 + z_3z_6^2 + z_1^2z_5z_7 - z_3z_5z_7 + z_1z_2z_6z_7 + z_6^3 - 2z_5z_6z_7$$
$$- z_1z_2z_5 + z_4z_7^2 + z_5^2 - z_2z_7^3 - z_4z_6 - z_2z_3z_7 + z_1z_5z_7 + z_2z_6z_7 + z_3^2 + z_1^2z_7^2 - z_3z_7^2 - 2z_1z_4 - 2z_1^2z_6$$
$$- z_2z_5 - z_6z_7^2 + 2z_3z_6 - z_1^3 + 2z_6^2 + 2z_1z_3 + z_5z_7 + z_1z_7^2 - 2z_4 - z_1z_6 + z_2z_7 + z_3 - 1,$$

$$\chi_{0100200} = z_2z_5^2 - z_2z_4z_6 - z_3z_5z_6 + z_3z_4z_7 - z_5z_6^2 + z_1z_3z_6z_7 + z_5^2z_7 - z_1^2z_2z_7^2 + z_2z_3z_7^2 + z_1z_5z_7^2 - z_1z_3z_5$$
$$+ z_1^2z_2z_6 - z_2z_3z_6 - z_3^2z_7 - 2z_1z_5z_6 + z_1z_4z_7 + z_2z_5z_7 - z_3z_6z_7 + z_1z_2z_3 - 2z_2z_4 + z_1z_2z_7^2 + z_5z_7^2$$
$$- z_3z_5 + z_1z_7^3 - 2z_5z_6 + z_1^3z_7 - 2z_1z_3z_7 - z_4z_7 - 3z_1z_6z_7 + z_2z_7^2 - z_1z_5 - 2z_1^2z_7 - z_2z_6 + z_1z_2$$
$$- z_5 - z_1z_7 - z_2,$$

$$\chi_{0010200} = z_3z_5^2 - z_3z_4z_6 - z_1z_2z_5z_6 + z_2^2z_6^2 + z_1z_2z_4z_7 - z_4z_6^2 - z_2^2z_5z_7 + 2z_4z_5z_7 + z_1^2z_2z_6z_7 - z_2z_3z_6z_7 - z_1^2z_3z_7^2 - z_1z_2^2z_7^2 - z_4^2 - z_1^2z_2z_5 + z_3^2z_7^2 + z_2z_3z_5 + 2z_1z_4z_7^2 - z_2z_6^2z_7 + z_1z_2^2z_6 + z_1^2z_3z_6 - z_3^2z_6 + z_2z_5z_7^2 + z_1z_5^2 - 4z_1z_4z_6 + z_3z_6z_7^2 + z_2z_5z_6 - 2z_1^2z_6^2 - z_2z_4z_7 + 3z_1^2z_5z_7 + z_6^3 + z_2^2z_3 + z_1z_3^2 - 2z_3z_5z_7 + 2z_1^3z_7^2 - 2z_1^2z_4 - z_1z_2z_6z_7 - z_3z_4 + 2z_2^2z_6 - z_1z_3z_7^2 - 3z_1^3z_6 - z_5z_6z_7 + 2z_1z_3z_6 + z_2z_7^3 - z_1^4 - 2z_4z_6 + z_1z_6^2 - z_2z_3z_7 + z_1z_2^2 - 2z_1z_5z_7 - 2z_1^2z_7^2 + z_1^2z_3 + z_3^2 - 3z_2z_6z_7 + z_3z_7^2 - z_1z_4 + z_2z_5 + 2z_3z_6 + 2z_6^2 - z_5z_7 + z_2^2 + 2z_1z_3 + 3z_1z_6 - 2z_2z_7 + z_1^2 + z_6,$$

$$\chi_{0001200} = z_4z_5^2 - z_4^2z_6 - z_2z_3z_5z_6 + z_3^2z_6^2 + z_2z_3z_4z_7 - z_3^2z_5z_7 + z_1z_2^2z_6^2 - 2z_1z_4z_6^2 - z_1z_2^2z_5z_7 + 3z_1z_4z_5z_7 - z_2z_4z_6z_7 - z_1^2z_2^2z_7^2 - z_1z_4^2 - z_1^2z_6^3 + z_3z_6^3 - z_1z_3^2z_7^2 + 2z_1^2z_5z_6z_7 - z_3z_5z_6z_7 + z_1z_3^2z_6 + z_1^2z_4z_7^2 - 2z_1z_2z_6^2z_7 + z_2z_4z_5 + z_2^2z_3z_7^2 + z_3z_4z_7^2 - z_3z_5^2 + z_1^2z_2^2z_6 + z_5z_6^2z_7 + z_1z_2z_5z_7^2 - z_5^2z_7^2 - z_2^2z_3z_6 + z_1^3z_6z_7^2 - z_1z_3z_6z_7^2 - 3z_1^2z_4z_6 + z_1^2z_2z_7^3 + z_1^2z_2z_3z_7 + 2z_1z_2z_5z_6 - z_2z_3^2z_7 + z_4z_6z_7^2 - z_5^2z_6 - 3z_1^3z_6^2 + z_3^3 + 4z_1z_3z_6^2 + 2z_1^3z_5z_7 + z_1z_6^2z_7^2 - 4z_1z_3z_5z_7 - z_4z_6^2 + z_4z_5z_7 - z_1^2z_2z_6z_7 - 2z_1z_5z_7^3 - z_1^3z_4 - z_1^2z_7^4 + z_1z_6^3 + z_1^4z_7^2 - z_1z_5z_6z_7 - z_1^2z_3z_7^2 + z_2z_6z_7^3 + z_1^2z_2z_5 - z_2z_6^2z_7 - z_3^2z_7^2 - z_4^2 - 2z_1^4z_6 + z_1z_4z_7^2 - z_2z_3z_5 + 2z_1^2z_6z_7^2 - z_1z_5^2 + z_1z_2^2z_6 + 2z_1^2z_3z_6 + 2z_3^2z_6 - 2z_3z_6z_7^2 - z_1z_4z_6 - 2z_1z_2z_3z_7 - z_6^2z_7^2 + z_1^2z_6^2 + 3z_3z_6^2 + z_1^2z_2^2 + z_6^3 - 2z_1^3z_3 - 3z_1^2z_5z_7 + 4z_1z_3^2 - 2z_1z_2z_6z_7 - z_2^2z_3 + z_2^2z_7^2 - z_1^3z_7^2 - z_1z_3z_7^2 + z_1^2z_4 - z_3z_4 + z_4z_7^2 + 6z_1z_3z_6 - z_1z_6z_7^2 - z_2^2z_6 - z_4z_6 + z_1^2z_3 - z_2z_3z_7 + 4z_1z_6^2 + 2z_3^2 - z_2z_6z_7 + z_1^2z_7^2 + 2z_1^2z_6 - z_3z_7^2 - z_1^3 - z_2z_5 - z_6z_7^2 + 3z_3z_6 - 2z_1z_2z_7 + 2z_6^2 + 4z_1z_3 - z_1z_7^2 - z_2^2 - z_4 + 3z_1z_6 + z_1^2 + z_3 + z_6 + z_1,$$

$$\chi_{0000300} = z_5^3 - 2z_4z_5z_6 + z_4^2z_7 + z_2z_3z_6^2 - 2z_1z_5z_6^2 - z_2z_3z_5z_7 + z_2z_6^3 + 2z_1z_5^2z_7 + z_1z_4z_6z_7 - 2z_2z_5z_6z_7 - z_1z_2z_3z_7^2 + z_2z_4z_7^2 - z_1z_4z_5 + z_1z_2z_3z_6 + z_1^2z_5z_7^2 + z_3z_5z_7^2 + z_2z_5^2 - z_2z_4z_6 - z_1z_2z_6z_7^2 + z_5z_6z_7^2 - 2z_1^2z_5z_6 + z_1^2z_4z_7 + z_1z_2z_6^2 - 2z_3z_4z_7 + z_1z_2z_5z_7 + z_1z_3z_7^3 + z_1^3z_6z_7 + z_2z_3^2 - z_1z_2z_4 - z_4z_7^3 - 4z_1z_3z_6z_7 - z_1^3z_5 + z_1^2z_2z_7^2 + z_4z_6z_7 - z_1z_6^2z_7 + 2z_1z_3z_5 - 3z_4z_5 - z_2z_3z_7^2 - z_1^2z_2z_6 + 3z_2z_3z_6 + z_1z_5z_7^2 - z_1z_5z_6 - z_2z_6z_7^2 + 3z_2z_6^2 - 3z_1z_4z_7 - z_1^3z_2 + 3z_1z_2z_3 + z_3z_7^3 - 2z_1^2z_6z_7 + z_6z_7^3 - 2z_3z_6z_7 - 2z_6^2z_7 - 2z_2z_4 - z_1z_2z_7^2 - z_1^2z_5 - z_1^3z_7 + 2z_3z_5 + 2z_1z_2z_6 + z_5z_6 + 2z_4z_7 + z_1z_7^3 + 2z_2z_3 - z_1z_6z_7 + 2z_1z_5 + 2z_2z_6 + 2z_1^2z_7 - 2z_3z_7 + 2z_1z_2 - 2z_6z_7 - 2z_1z_7,$$

$$\chi_{2000010} = z_1^2z_6 - z_3z_6 - z_1z_2z_7 + z_2^2 - z_6^2 + z_5z_7 - z_4 - z_1z_6 + z_2z_7 + z_7^2 - 2z_6 - 1,$$

$$\chi_{1100010} = z_1z_2z_6 - z_2^2z_7 - z_1z_3z_7 - z_5z_6 + z_4z_7 + z_2z_3 + z_1^2z_7 + z_2z_6 - z_3z_7 + z_1z_2 - z_6z_7 - 2z_1z_7 + z_2,$$

$$\chi_{0200010} = z_2^2z_6 - z_4z_6 - z_2z_3z_7 + z_3^2 - z_1z_6^2 + z_1z_5z_7 - z_2z_6z_7 + z_1^2z_7^2 - z_1z_4 + z_2z_5 - 2z_1^2z_6 + 2z_3z_6 - z_1z_2z_7 - z_1^3 + z_6^2 + z_2^2 + 2z_1z_3 + z_1z_6 + z_3 + z_6 + z_1,$$

$$\chi_{1010010} = z_1z_3z_6 - z_4z_6 - z_1z_6^2 - z_1^2z_2z_7 + z_1z_5z_7 + z_1^2z_7^2 + z_1z_2^2 + z_2z_6z_7 - z_1^2z_6 - z_2z_5 - z_3z_7^2 + z_3z_6 + z_1z_2z_7 - z_2^2 - z_1z_7^2,$$

$$\chi_{0110010} = z_2z_3z_6 - z_1z_5z_6 - z_3^2z_7 - z_1z_2^2z_7 + z_1z_4z_7 + z_1z_2z_3 + z_2z_5z_7 + z_1^2z_6z_7 - z_3z_6z_7 + z_1z_2z_7^2 - z_1^2z_5 + z_3z_5 + z_1^3z_7 - z_1z_7^3 - 3z_1z_3z_7 + z_4z_7 + z_2z_3 - z_1z_6z_7 + z_2z_7^2 - z_1^2z_7 - z_3z_7,$$

$$\chi_{0020010} = z_3^2z_6 - z_1z_4z_6 - z_1^2z_6^2 - z_1z_2z_3z_7 + z_2z_4z_7 + z_3z_6^2 + z_1^2z_5z_7 + z_1^2z_2^2 - z_3z_5z_7 + z_1z_2z_6z_7 - z_1^2z_4 - z_2^2z_3 + z_1^3z_7^2 + 2z_3z_4 - z_1z_2z_5 - 2z_1z_3z_7^2 + z_4z_7^2 - 2z_1^3z_6 - z_2^2z_6 + 4z_1z_3z_6 - z_2z_7^3 - z_1^4 + z_1z_6^2 + 3z_1^2z_3 - z_1z_5z_7 - z_1z_2^2 + 2z_2z_6z_7 - z_1^2z_7^2 - z_3^2 + 2z_1^2z_6 - z_2z_5 + z_1^3 - z_2^2 - z_4 + z_2z_7,$$

$$\chi_{1001010} = z_1z_4z_6 - z_2z_5z_6 - z_1z_2z_3z_7 + z_3z_5z_7 + z_1^2z_4 + z_1z_2z_6z_7 + z_2^2z_3 + z_1^3z_7^2 + z_6^3 - z_3z_4 - z_5z_6z_7 - z_1z_3z_7^2 - z_1z_2z_5 - 2z_1z_6z_7^2 - z_4z_6 - z_1^2z_2z_7 + z_1z_6^2 + z_2z_3z_7 + z_1z_5z_7 - 2z_1^2z_7^2 - z_2z_6z_7 + z_3z_7^2 - z_1z_4 + z_3z_6 + z_6z_7^2 + z_6^2 + z_1z_2z_7 + z_1z_7^2 + 2z_1z_6 + z_1^2 - z_3 - z_6 - z_1,$$

$$\chi_{0101010} = z_2z_4z_6 - z_3z_5z_6 - z_2^2z_3z_7 + z_1z_2z_5z_7 + z_2z_3^2 + z_1z_3z_6z_7 - z_4z_6z_7 + z_1^2z_2z_7^2 - z_2z_3z_7^2 - z_1z_3z_5 - z_1^2z_7^3 - z_1^2z_2z_6 + 2z_2z_3z_6 - z_2z_6z_7^2 - z_1^2z_3z_7 - z_1z_5z_6 + z_2z_6^2 + z_6z_7^3 - z_2z_5z_7 + z_3z_6z_7 + z_1z_2z_7^2 + z_1z_2z_3 - z_6^2z_7 - z_1^2z_5 + z_2z_4 - z_5z_7^2 + z_3z_5 + 2z_5z_6 + z_1^3z_7 + z_1z_7^3 - z_1z_3z_7 - 2z_1^2z_2 - z_2^2z_7 + z_4z_7 + 2z_2z_3 + 2z_1z_5 - 2z_2z_7^2 + 3z_2z_6 + z_1z_2 - z_7^3 + z_5 - z_1z_7 + 2z_2 + z_7,$$

$$\chi_{0011010} = z_3z_4z_6 - z_1z_2z_5z_6 - z_2z_3^2z_7 + z_2^2z_5z_7 + z_1z_3z_5z_7 + z_4z_6^2 - z_4z_5z_7 + z_1^2z_2z_6z_7 + z_1z_2^2z_3 + z_1z_6^3 - z_2^2z_4 + z_1^2z_3z_7^2 - z_2z_3z_6z_7 - z_1z_5z_6z_7 + z_4^2 - z_1^2z_2z_5 - z_3^2z_7^2 - z_1z_4z_7^2 - z_1z_2^2z_6 - 2z_1^2z_6z_7^2 - z_1^2z_3z_6 + z_3^2z_6 - z_2z_6^2z_7 + z_2z_5z_7^2 + 2z_1z_4z_6 - z_1^3z_2z_7 + 2z_1^2z_6^2 + z_1z_2z_3z_7 + z_1^2z_5z_7 - z_3z_5z_7 + z_2^2z_7^2 + z_1z_7^4 + z_3z_4 - z_1z_2z_5 + z_1^3z_6 + z_1^2z_2z_7 + z_4z_6 - 2z_2z_3z_7 - 2z_2z_6z_7 - 2z_3z_7^2 - z_7^4 + 2z_3z_6 + z_6z_7^2 - z_5z_7 - z_1z_7^2 + z_4 + z_3 + z_7^2,$$

$$\chi_{0002010} = z_4^2z_6 - z_2z_3z_5z_6 - z_2z_3z_4z_7 + z_3^2z_5z_7 + z_2^2z_3^2 + z_1z_4z_6^2 + z_1z_2^2z_5z_7 - z_1z_4z_5z_7 - z_3^2z_4 - z_2z_4z_6z_7 - z_1z_2^2z_4 + 2z_1z_4^2 + z_3z_6^3 - z_1z_2z_3z_5 - z_3z_5z_6z_7 - z_1z_3^2z_6 - z_1z_2z_6^2z_7 - z_1^2z_2^2z_6 + 3z_1^2z_4z_6 + z_2^2z_3z_6 + z_5^2z_7^2 - z_1^2z_2z_3z_7 - z_3z_4z_6 + z_2z_3^2z_7 - z_5^2z_6 + z_1z_2z_4z_7 - z_1z_3z_6z_7^2 + z_1^3z_6^2 - z_4z_6z_7^2 + z_2z_3z_7^3 + 2z_4z_6^2 - z_1^3z_5z_7 + 3z_1z_3z_5z_7 - 4z_4z_5z_7 + z_2z_6z_7^3 + z_1^2z_2z_6z_7 + 2z_1^3z_4 - z_2z_3z_6z_7 + z_1z_2^2z_7^2 + z_1z_6^3 - 4z_1z_3z_4 - z_1^2z_2z_5 + z_1^2z_3z_7^2 - 2z_1z_5z_6z_7 + 2z_1^4z_6 - z_2z_6^2z_7 + 2z_4^2 - 2z_1z_4z_7^2 + 2z_2z_3z_5 - z_2z_5z_7^2 - z_1^2z_6z_7^2 - z_1z_2^2z_6 - z_1z_5^2 - 5z_1^2z_3z_6 - z_3z_6z_7^2 + z_3^2z_6 + 4z_1z_4z_6 - z_1z_2z_3z_7 + z_1^2z_6^2 - z_6^2z_7^2 + 2z_2z_5z_6 + z_3z_6^2 - z_1z_2z_7^3 - z_2z_4z_7 + 2z_5z_7^3 - z_1^2z_5z_7 + z_6^3 - 2z_1^3z_7^2 + 3z_3z_5z_7 + z_2^2z_3 - 2z_1^2z_4 + 3z_1z_3z_7^2 + z_1z_2z_5 - 2z_5z_6z_7 - 3z_4z_7^2 - 2z_1z_3z_6 + 5z_4z_6 - z_1z_6z_7^2 + 2z_1z_6^2 + z_2z_3z_7 + z_2z_7^3 + z_7^4 + z_1z_5z_7 - z_3^2 - z_1z_2^2 + 2z_1z_4 - 2z_2z_6z_7 + 2z_2z_5 + 2z_1^2z_7^2 - z_1^2z_6 + 2z_1^3 + z_1z_2z_7 - 3z_6z_7^2 + 3z_6^2 - z_5z_7 - 4z_1z_3 + 3z_4 + z_1z_6 - z_2z_7 - 2z_1^2 - 2z_7^2 + 3z_6 + 1,$$

$$\chi_{1000110} = z_1z_5z_6 - z_2z_6^2 - z_1z_4z_7 - z_1^2z_6z_7 + z_3z_6z_7 + z_1z_2z_7^2 + z_2z_4 + z_6^2z_7 + z_1^2z_5 - z_5z_7^2 - z_3z_5 - z_5z_6 + z_4z_7 + z_1z_6z_7 - z_2z_3 - z_2z_7^2 - z_2z_6 - z_1z_2 - z_7^3 + 2z_6z_7 + z_1z_7 + z_7,$$

$$\chi_{0100110} = z_2z_5z_6 - z_3z_6^2 - z_2z_4z_7 - z_6^3 + z_3z_4 + z_1z_3z_7^2 + z_5z_6z_7 - z_4z_7^2 + z_1z_6z_7^2 + z_4z_6 - z_1z_6^2 - z_1^2z_2z_7 + z_2z_3z_7 - z_1z_5z_7 - 2z_1^2z_7^2 - z_3^2 + 2z_1z_4 + 2z_1^2z_6 + z_2z_5 + z_3z_7^2 - 2z_3z_6 + 2z_1z_2z_7 + z_6z_7^2 - 2z_6^2 + 2z_1^3 - 4z_1z_3 + 2z_1z_7^2 + z_4 - 3z_1z_6 - z_1^2 - z_3 - z_6 - 2z_1,$$

$$\chi_{0010110} = z_3z_5z_6 - z_1z_2z_6^2 - z_3z_4z_7 + z_2^2z_6z_7 + z_1z_2z_4 + z_1^2z_2z_7^2 + z_1z_6^2z_7 - z_2z_3z_7^2 - z_2^2z_5 + z_4z_5 - z_1z_5z_7^2 - z_1^2z_7^3 - z_1^2z_3z_7 + z_3^2z_7 - z_1z_2^2z_7 + z_1z_4z_7 + z_1^2z_6z_7 - z_6z_7^3 - z_2z_6^2 + z_2z_5z_7 + z_3z_6z_7 - z_1z_2z_7^2 + 2z_6^2z_7 + z_1^2z_5 + z_5z_7^2 + z_1z_7^3 - z_3z_5 - z_1z_2z_6 + z_2^2z_7 + z_1^3z_7 + z_1z_3z_7 - 2z_5z_6 - z_4z_7 - z_2z_3 - z_1z_5 - z_1^2z_7 - 2z_2z_6 + z_3z_7 + z_6z_7 - z_5 - z_2,$$

$$\chi_{0001110} = z_4z_5z_6 - z_4^2z_7 - z_2z_3z_6^2 + z_3^2z_6z_7 + z_2z_3z_4 - z_3^2z_5 + z_1z_2^2z_6z_7 - z_1z_4z_6z_7 - z_1z_2^2z_5 + 2z_1z_4z_5 - z_2z_4z_7^2 + z_3z_6^2z_7 - z_1z_3^2z_7 - z_1^2z_2^2z_7 + z_1^2z_5z_6 - 2z_3z_5z_6 - 2z_1z_2z_6z_7^2 + z_5z_6z_7^2 - z_5z_6^2 + z_2^2z_3z_7 + 2z_3z_4z_7 + z_1^2z_2z_3 + 2z_1z_2z_5z_7 - z_1z_3z_7^3 - z_5^2z_7 - z_2z_3^2 + z_4z_7^3 - z_1^3z_6z_7 + 4z_1z_3z_6z_7 + z_1^2z_2z_7^2 - 2z_4z_6z_7 + 2z_1^3z_5 + z_2z_7^4 - 5z_1z_3z_5 + z_1z_6^2z_7 + 3z_4z_5 + z_2z_3z_7^2 - z_2z_3z_6 - z_1z_5z_7^2 - z_2z_6z_7^2 + z_1^4z_7 + z_1^2z_7^3 - 2z_1z_5z_6 - z_1^2z_3z_7 - z_3^2z_7 + 2z_1z_4z_7 - z_3z_7^3 + z_2z_5z_7 - 2z_1z_2z_3 + z_3z_6z_7 + z_2z_4 - z_1z_2z_7^2 - z_1^2z_5 - 2z_1^3z_7 - 3z_3z_5 + z_1z_2z_6 - z_5z_7^2 + z_2^2z_7 - z_5z_6 - z_4z_7 - 3z_1z_7^3 + 4z_1z_6z_7 + z_1^2z_2 - z_2z_3 - 3z_1z_5 - z_2z_7^2 + z_3z_7 + z_6z_7 - z_1z_2 + 3z_1z_7,$$

$$\chi_{0000210} = z_5^2z_6 - z_4z_6^2 - z_4z_5z_7 + z_2z_3z_6z_7 - z_1z_6^3 + z_4^2 + z_2z_6^2z_7 - z_2z_3z_5 + z_1z_5^2 + z_1z_4z_6 - z_2z_5z_7^2 - z_2z_5z_6 - z_1z_2z_3z_7 + z_2z_4z_7 + z_3z_6z_7^2 - z_1z_2z_7^3 + z_6^2z_7^2 - z_3z_6^2 + z_3z_5z_7 - z_6^3 + z_1^2z_4 + z_1z_2z_6z_7 + z_5z_6z_7 - z_3z_4 + z_1^3z_6 - 2z_1z_3z_6 - z_4z_6 + z_1^2z_2z_7 - 2z_1z_6^2 + 2z_1z_5z_7 + z_1^2z_7^2 + z_1^2z_3 - z_3^2 - 3z_1z_4 + z_2z_6z_7 + z_6z_7^2 - 2z_1^2z_6 - 3z_3z_6 - 3z_6^2 - z_1^3 - 2z_1z_6 + z_1^2 - z_3 - 2z_6 - z_1,$$

$$\chi_{1000020} = z_1z_6^2 - z_1z_5z_7 - z_2z_6z_7 - z_1^2z_7^2 + z_3z_7^2 + z_2z_5 + z_1^2z_6 - z_3z_6 + z_1z_2z_7 + z_1z_7^2 - z_2z_7,$$

$$\chi_{0100020} = z_2z_6^2 - z_2z_5z_7 - z_3z_6z_7 - z_6^2z_7 + z_3z_5 + z_1z_3z_7 + 2z_5z_6 + z_1z_7^3 - z_4z_7 - 2z_1z_6z_7 - z_1^2z_2 + z_2z_3 - z_2z_7^2 + 2z_1z_5 - z_1^2z_7 + 2z_2z_6 + z_3z_7 + z_1z_2 + z_5 + z_1z_7 + z_2,$$

$$\chi_{0010020} = z_3z_6^2 - z_3z_5z_7 - z_1z_2z_6z_7 + z_2^2z_7^2 + z_1z_2z_5 - z_4z_7^2 - z_2^2z_6 + 2z_4z_6 + z_1^2z_2z_7 - z_1^2z_3 + z_1z_6^2 - z_2z_3z_7 - z_1z_2^2 - z_1z_5z_7 - z_1^2z_7^2 + z_3^2 + 2z_1z_4 + 2z_1^2z_6 - z_1z_2z_7 - z_2^2 + z_1^3 + z_4,$$

$$\chi_{0001020} = z_4z_6^2 - z_4z_5z_7 - z_2z_3z_6z_7 + z_3^2z_7^2 + z_2z_3z_5 + z_1z_2^2z_7^2 - z_3^2z_6 - 2z_1z_4z_7^2 - z_1z_2^2z_6 + 3z_1z_4z_6 - z_2z_4z_7 - z_1z_2z_7^3 + z_1^2z_6^2 + z_5z_7^3 - z_1z_3^2 - z_1^2z_5z_7 + z_3z_5z_7 - z_1^2z_2^2 + 2z_1^2z_4 + z_2^2z_3 - 2z_5z_6z_7 - 2z_1^3z_7^2 + 3z_1z_3z_7^2 + 3z_1^3z_6 + z_5^2 - z_4z_7^2 - 4z_1z_3z_6 + 3z_4z_6 + z_1^2z_2z_7 + z_2z_7^3 + 2z_1^2z_7^2 + 2z_1^4 - z_1z_2^2 - 4z_1^2z_3 + 3z_1z_4 - z_2z_6z_7 + z_3z_7^2 + z_7^4 + z_2z_5 - 3z_6z_7^2 - z_1^2z_6 - 2z_3z_6 + z_6^2 - z_1^3 - 2z_1z_3 + z_2^2 - z_1z_7^2 - z_1z_6 - 2z_1^2 - z_2z_7 - z_7^2 + 2z_6 + 2z_1,$$

$$\chi_{0000120} = z_5z_6^2 - z_5^2z_7 - z_4z_6z_7 + z_2z_3z_7^2 + z_4z_5 - z_1z_6^2z_7 - z_2z_3z_6 - z_1z_5z_7^2 + z_2z_6z_7^2 + 3z_1z_5z_6 - z_2z_6^2 - z_2z_5z_7 - z_1z_2z_3 + z_6z_7^3 + z_3z_6z_7 - z_6^2z_7 + z_2z_4 + z_1^2z_5 - z_1z_2z_7^2 - z_5z_7^2 + 2z_5z_6 - z_1z_7^3 + z_4z_7 + z_1^2z_2 - 2z_2z_3 + 2z_1z_6z_7 + z_2z_7^2 + z_1z_5 - 2z_2z_6 + 2z_1^2z_7 - z_3z_7 - z_1z_2 - z_6z_7 - z_1z_7 - z_2,$$

$$\chi_{0000030} = z_6^3 - 2z_5z_6z_7 + z_4z_7^2 + z_5^2 - z_1z_6z_7^2 - z_4z_6 + z_2z_7^3 + z_1z_6^2 + z_1z_5z_7 - 2z_2z_6z_7 + z_1^2z_7^2 - z_3z_7^2 - z_1z_4 + z_2z_5 - z_1^2z_6 + 2z_3z_6 - z_6z_7^2 - z_1z_2z_7 + 2z_6^2 - z_1z_7^2 - z_1^3 + 2z_1z_3 - z_4 + 3z_1z_6 - z_2z_7 + z_1^2 + z_3 + z_6 + z_1,$$

$$\chi_{2000001} = z_1^2z_7 - z_3z_7 - z_1z_2 - z_6z_7 + z_5 - z_1z_7 + z_2,$$

$$\chi_{1100001} = z_1z_2z_7 - z_2^2 - z_1z_3 - z_5z_7 + z_4 - z_1z_7^2 + z_1z_6 + z_1^2 - z_3,$$

$$\chi_{0200001} = z_2^2z_7 - z_4z_7 - z_2z_3 - z_1z_6z_7 + z_1z_5 - z_2z_6 + z_3z_7 - z_1z_2 + z_6z_7 + z_1z_7 - z_2,$$

$$\chi_{1010001} = z_1z_3z_7 - z_4z_7 - z_1^2z_2 - z_1z_6z_7 + z_7^3 + z_1z_5 + z_2z_6 - z_6z_7 + z_1z_2 + z_5 + z_2 - z_7,$$

$$\chi_{0110001} = z_2z_3z_7 - z_1z_5z_7 - z_3^2 - z_1^2z_7^2 - z_1z_2^2 + z_3z_7^2 + z_1z_4 + z_2z_5 + 2z_1^2z_6 + z_6z_7^2 - 2z_3z_6 + z_1z_2z_7 - z_6^2 + 2z_1^3 - 4z_1z_3 + z_4 - 2z_1z_6 - z_1^2 + z_2z_7 - 2z_3 - 2z_6 - 2z_1,$$

$$\chi_{0020001} = z_3^2z_7 - z_1z_4z_7 - z_1z_2z_3 - z_1^2z_6z_7 + z_3z_6z_7 + z_2z_4 + z_1^2z_5 - z_3z_5 + z_5z_7^2 + z_1z_2z_6 - z_5z_6 + z_1z_7^3 + z_1^2z_2 - z_2z_3 - z_1z_6z_7 - z_1z_5 - z_2z_7^2 - z_1^2z_7 + z_2z_6 + z_3z_7 - z_5,$$

$$\chi_{1001001} = z_1z_4z_7 - z_2z_5z_7 - z_1z_2z_3 + z_6^2z_7 + z_3z_5 - z_5z_7^2 + z_1z_2z_6 + z_1^3z_7 - z_1z_3z_7 - z_1z_6z_7 - z_2z_7^2 + z_1z_5 - 2z_1^2z_7 + z_3z_7 + z_1z_2 - z_7^3 + 2z_6z_7 + z_1z_7 + z_7,$$

$$\chi_{0101001} = z_2z_4z_7 - z_3z_5z_7 - z_2^2z_3 + z_1z_2z_5 + z_1z_3z_6 + z_1z_6z_7^2 - z_2z_7^3 - z_4z_6 + z_1^2z_2z_7 - z_1z_6^2 - z_2z_3z_7 - z_1z_5z_7 - z_1^2z_7^2 + z_2z_6z_7 - z_1^2z_6 - z_2z_5 + z_3z_6 + z_1z_2z_7 - z_2^2 + z_1z_7^2,$$

$$\chi_{0011001} = z_3z_4z_7 - z_1z_2z_5z_7 - z_2z_3^2 + z_1z_3z_5 + z_4z_6z_7 + z_1z_6^2z_7 + z_2^2z_5 - z_4z_5 + z_1^2z_2z_6 - z_2z_3z_6 + z_1^2z_3z_7 - z_3^2z_7 - z_1z_5z_6 - z_1z_4z_7 - z_1^2z_6z_7 - z_2z_6^2 - z_6z_7^3 + z_2z_5z_7 - z_3z_6z_7 + z_6^2z_7 - z_1z_2z_7^2 + z_5z_7^2 - z_5z_6 - z_1^3z_7 + z_1z_3z_7 + z_1z_7^3 + z_2^2z_7 + z_1^2z_2 + z_1z_6z_7 - z_2z_3 - z_1z_5 + z_1^2z_7 - 2z_2z_6 + z_6z_7 - z_1z_2 - z_5 - z_1z_7,$$

$$\chi_{0002001} = z_4^2z_7 - z_2z_3z_5z_7 - z_2z_3z_4 + z_1z_4z_6z_7 + z_3^2z_5 + z_1z_2^2z_5 - z_1z_4z_5 + z_3z_6^2z_7 - z_2z_4z_6 + z_1^2z_5z_7^2 - 2z_3z_5z_7^2 - z_1^2z_5z_6 + z_3z_5z_6 - z_1z_2z_6^2 - 2z_4z_7^3 - z_1z_6z_7^3 - z_1z_3z_6z_7 + 3z_4z_6z_7 - 2z_1^3z_5 + 5z_1z_3z_5 - 3z_4z_5 + 2z_1z_6^2z_7 + z_2z_3z_7^2 - z_1z_5z_7^2 - z_2z_3z_6 + z_2z_6z_7^2 - z_2z_6^2 + 2z_1z_4z_7 + 2z_1^2z_6z_7 + z_7^5 - z_3z_6z_7 - 3z_6z_7^3 + 2z_6^2z_7 + z_5z_7^2 - 2z_2z_4 + 3z_3z_5 - 2z_1z_2z_6 - 2z_1z_7^3 - z_5z_6 + 2z_4z_7 + 3z_1z_6z_7 + 2z_2z_7^2 - z_2z_3 + z_1z_5 - 2z_7^3 - 3z_2z_6 + 3z_6z_7 - z_5 + 2z_1z_7 - 2z_2 + z_7,$$

$$\chi_{1000101} = z_1z_5z_7 - z_2z_6z_7 - z_1z_4 - z_1^2z_6 + z_3z_6 + z_6^2 + z_1z_2z_7 - z_5z_7 + z_1z_7^2 - z_2z_7 - z_7^2 - z_1^2 + z_3 + 2z_6 + 1,$$

$$\chi_{0100101} = z_2z_5z_7 - z_3z_6z_7 - z_6^2z_7 - z_2z_4 + z_5z_7^2 + z_1z_3z_7 + z_1z_7^3 - z_4z_7 - z_1z_6z_7 - z_1z_5 - 2z_1^2z_7 + z_3z_7 + z_1z_2 - z_5 + z_7,$$

$$\chi_{0010101} = z_3z_5z_7 - z_1z_2z_6z_7 - z_3z_4 + z_4z_7^2 + z_1z_6z_7^2 + z_2^2z_6 - z_4z_6 + z_2z_7^3 + z_1^2z_2z_7 - z_7^4 - z_2z_3z_7 - z_1z_5z_7 - 2z_2z_6z_7 - z_1z_4 - z_1^2z_6 + z_2z_5 - z_3z_7^2 + z_3z_6 - 2z_1z_2z_7 - z_1^3 + z_2^2 + z_6z_7^2 + z_6^2 - z_5z_7 + 2z_1z_3 + 2z_1z_6 + z_1^2 - 2z_2z_7 + z_7^2 + z_3 + z_6 + z_1,$$

$$\chi_{0001101} = z_4z_5z_7 - z_2z_3z_6z_7 - z_4^2 + z_1z_4z_7^2 + z_3^2z_6 + z_1z_2^2z_6 - 2z_1z_4z_6 + z_1^2z_6z_7^2 - z_2z_4z_7 - z_1^2z_6^2 + z_3z_6^2 - z_3z_5z_7 - 2z_1z_2z_6z_7 - z_1^2z_4 + z_3z_4 + z_1z_2z_5 - z_1z_7^4 - z_1z_3z_7^2 - 2z_1^3z_6 + 4z_1z_3z_6 - z_4z_6 + z_1z_6z_7^2 + z_2z_7^3 + z_2z_3z_7 + z_1z_6^2 - z_1z_5z_7 + z_7^4 - z_2z_6z_7 + 2z_1^2z_7^2 + 2z_1z_4 - z_3z_7^2 - 2z_6z_7^2 + z_1^2z_6 + 2z_3z_6 - z_1z_2z_7 + z_6^2 - 2z_1z_7^2 + 3z_1z_6 - z_1^2 + z_3 - 2z_7^2 + 2z_6 + 2z_1 + 1,$$

$$\chi_{0000201} = z_5^2z_7 - z_4z_6z_7 - z_4z_5 - z_1z_6^2z_7 + z_2z_3z_6 + z_1z_5z_7^2 - z_1z_5z_6 + z_2z_6^2 - z_2z_5z_7 + z_3z_7^3 + z_6z_7^3 - z_3z_6z_7 - z_6^2z_7 - z_1^2z_5 - z_1z_2z_7^2 + z_3z_5 + z_1z_2z_6 + z_5z_6 - z_1z_3z_7 + z_2z_3 - z_1z_6z_7 + z_1z_5 + 2z_2z_6 + z_1^2z_7 - 2z_3z_7 + z_7^3 + z_1z_2 - 3z_6z_7 + z_5 - z_1z_7 + z_2 - 2z_7,$$

$$\chi_{1000011} = z_1z_6z_7 - z_2z_7^2 - z_7^3 - z_1z_5 - z_1^2z_7 + z_3z_7 + z_1z_2 + 2z_6z_7 - z_5 + 2z_1z_7 + z_7,$$

$$\chi_{0100011} = z_2z_6z_7 - z_3z_7^2 - z_2z_5 - z_6z_7^2 + z_1z_3 + z_5z_7 - z_4 + z_1z_7^2 - z_1z_6 - z_1^2 + z_3,$$

$$\chi_{0010011} = z_3z_6z_7 - z_1z_2z_7^2 - z_3z_5 + z_2^2z_7 + z_1z_6z_7 + z_1^2z_2 - z_2z_3 + z_2z_7^2 - z_1z_5 - z_2z_6 - z_3z_7 - z_1z_2 - z_1z_7 - z_2,$$

$$\chi_{0001011} = z_4z_6z_7 - z_2z_3z_7^2 - z_4z_5 + z_3^2z_7 + z_1^2z_7^3 + z_1z_2^2z_7 - z_1z_4z_7 - z_3z_7^3 - z_1^2z_6z_7 + 2z_3z_6z_7 - z_2z_4 - z_1z_2z_7^2 - z_1z_2z_6 - 2z_1^3z_7 - 2z_1z_7^3 + 3z_1z_3z_7 + 3z_1z_6z_7 + z_2z_7^2 - z_2z_6 + 3z_1^2z_7 + z_3z_7 - z_1z_2 + 2z_1z_7 - z_2,$$

$$\chi_{0000111} = z_5z_6z_7 - z_4z_7^2 - z_5^2 - z_1z_6z_7^2 + z_2z_3z_7 + z_2z_6z_7 + z_7^4 + z_3z_7^2 - z_2z_5 - z_6z_7^2 - z_1z_2z_7 + z_5z_7 - z_1z_7^2 - z_1z_3 + z_4 + z_1z_6 + z_2z_7 - z_7^2 + z_1^2 - z_3,$$

$$\chi_{0000021} = z_6^2z_7 - z_5z_7^2 - z_5z_6 + z_4z_7 - z_1z_7^3 + z_1z_6z_7 + z_2z_7^2 - z_2z_6 + z_1^2z_7 - z_1z_2 - z_2,$$

$$\chi_{1000002} = z_1z_7^2 - z_1z_6 - z_2z_7 - z_1^2 - z_7^2 + z_3 + z_6 + z_1 + 1,$$

$$\chi_{0100002} = z_2z_7^2 - z_2z_6 - z_3z_7 - z_6z_7 - z_2,$$

$$\chi_{0010002} = z_3z_7^2 - z_3z_6 - z_1z_2z_7 + z_2^2 - z_4 + z_7^2 - 1,$$

$$\chi_{0001002} = z_4z_7^2 - z_4z_6 - z_2z_3z_7 + z_3^2 + z_1^2z_7^2 - z_3z_7^2 + z_1z_2^2 - 2z_1z_4 - z_1^2z_6 + z_3z_6 - z_1z_2z_7 - z_1z_7^2 - 2z_1^3 + 4z_1z_3 - 2z_4 + z_1z_6 + z_1^2 + 2z_3 + 2z_1,$$

$$\chi_{0000102} = z_5z_7^2 - z_5z_6 - z_4z_7 + z_2z_3 - z_1z_6z_7 - z_1z_5 + z_7^3 + z_2z_6 - z_6z_7 - z_1z_7 + z_2 - z_7,$$

$$\chi_{0000012} = z_6 z_7^2 - z_6^2 - z_5 z_7 + z_4 - z_1 z_7^2 + z_2 z_7 + z_1^2 - z_3 - z_6 - z_1,$$

$$\chi_{0000003} = z_7^3 - 2z_6 z_7 + z_5 - z_1 z_7 + z_2 - z_7.$$

APPENDIX B: SOME CUBIC CLEBSCH-GORDAN SERIES

$$z_1^3 = \chi_{3000000} + 2\chi_{1010000} + \chi_{0001000} + 3\chi_{1000010} + 3\chi_{2000000} + 2\chi_{0100001} + 4\chi_{0010000} + \chi_{0000002} + 3\chi_{0000010} + 5\chi_{1000000} + \chi_{0000000},$$

$$z_2^3 = \chi_{0300000} + 2\chi_{0101000} + \chi_{0010100} + 3\chi_{1100010} + 2\chi_{0000110} + 2\chi_{1010001} + 3\chi_{0200001} + 4\chi_{0001001} + 4\chi_{2100000} + 4\chi_{1000011} + 5\chi_{0100002} + \chi_{0000003} + 6\chi_{0110000} + 8\chi_{1000100} + 6\chi_{2000001} + 9\chi_{0100010} + 12\chi_{0010001} + 12\chi_{1100000} + 8\chi_{0000011} + 11\chi_{0000100} + 12\chi_{1000001} + 10\chi_{0100000} + 4\chi_{0000001},$$

$$z_3^3 = \chi_{0030000} + 2\chi_{1011000} + \chi_{0002000} + \chi_{2100100} + 3\chi_{0110100} + 2\chi_{1200010} + 3\chi_{2010010} + 3\chi_{0020010} + 2\chi_{1000200} + 6\chi_{1001010} + 3\chi_{2000020} + \chi_{0300001} + 4\chi_{0100110} + 6\chi_{0010020} + 2\chi_{3100001} + 4\chi_{3010000} + 10\chi_{1110001} + 9\chi_{2000101} + 8\chi_{0101001} + \chi_{0000030} + 6\chi_{2200000} + 12\chi_{0010101} + 9\chi_{0210000} + 18\chi_{1100011} + 8\chi_{1020000} + 6\chi_{0200002} + 4\chi_{3000002} + 15\chi_{2001000} + 18\chi_{0011000} + 14\chi_{1010002} + 30\chi_{1100100} + 10\chi_{0000111} + 11\chi_{0000200} + 14\chi_{0001002} + 12\chi_{3000010} + 42\chi_{1010010} + 42\chi_{2100001} + 13\chi_{1000012} + 5\chi_{4000000} + 18\chi_{0200010} + 36\chi_{0001010} + 56\chi_{0110001} + 27\chi_{1000020} + 34\chi_{1200000} + 66\chi_{1000101} + 7\chi_{0100003} + 29\chi_{2000002} + 33\chi_{2010000} + 29\chi_{0020000} + 52\chi_{0100011} + \chi_{0000004} + 45\chi_{0010002} + 72\chi_{1001000} + 63\chi_{2000010} + 61\chi_{0100100} + 90\chi_{0010010} + 21\chi_{0000012} + 112\chi_{1100001} + 21\chi_{3000000} + 29\chi_{0000020} + 75\chi_{0000101} + 33\chi_{0200000} + 74\chi_{1010000} + 48\chi_{1000002} + 72\chi_{0001000} + 88\chi_{1000010} + 66\chi_{0100001} + 30\chi_{2000000} + 50\chi_{0010000} + 17\chi_{0000002} + 30\chi_{0000010} + 16\chi_{1000000} + 2\chi_{0000000},$$

$$z_5^3 = \chi_{0000300} + 2\chi_{0001110} + \chi_{0002001} + \chi_{0110020} + 3\chi_{1000120} + 3\chi_{0110101} + 2\chi_{0020011} + 2\chi_{0111000} + 2\chi_{0100030} + 3\chi_{1000201} + 4\chi_{0020100} + 2\chi_{1200011} + 6\chi_{1001011} + 10\chi_{0100111} + 4\chi_{1110002} + \chi_{0300002} + 3\chi_{2000021} + 8\chi_{0101002} + 9\chi_{0010021} + 4\chi_{1200100} + 6\chi_{1001100} + 12\chi_{1110010} + 3\chi_{0300010} + 6\chi_{2000102} + 12\chi_{0010102} + 8\chi_{0100200} + 6\chi_{1020001} + 18\chi_{0101010} + 6\chi_{2200001} + 18\chi_{1100012} + 4\chi_{0000031} + 6\chi_{0200003} + 14\chi_{0000112} + \chi_{3000003} + 9\chi_{2000110} + 27\chi_{0010110} + 14\chi_{2001001} + 30\chi_{1100020} + 18\chi_{0210001} + 30\chi_{0011001} + 24\chi_{0000120} + 60\chi_{1100101} + 10\chi_{1010003} + 8\chi_{3000011} + 8\chi_{1300000} + 30\chi_{0000201} + 9\chi_{2110000} + 18\chi_{0120000} + 43\chi_{1101000} + 42\chi_{0200011} + 14\chi_{0001003} + 62\chi_{1010011} + 11\chi_{3000100} + 42\chi_{2100002} + 13\chi_{1000013} + 42\chi_{0200100} + 7\chi_{0100004} + 80\chi_{0001011} + 56\chi_{1000021} + 58\chi_{1010100} + 65\chi_{0001100} + 78\chi_{0110002} + 72\chi_{2100010} + 134\chi_{0110010} + 96\chi_{1000102} + 3\chi_{4000001} + 57\chi_{2010001} + 138\chi_{1000110} + 84\chi_{0100012} + 30\chi_{2000003} + 105\chi_{1200001} + 101\chi_{0100020} + \chi_{0000005} + 72\chi_{0020001} + 198\chi_{1001001} + 28\chi_{0300000} + 204\chi_{0100101} + 28\chi_{3100000} + 134\chi_{1110000} + 58\chi_{0010003} + 138\chi_{2000011} + 30\chi_{0000013} + 239\chi_{0010011} + 84\chi_{0000021} + 139\chi_{0101000} + 216\chi_{1100002} + 132\chi_{2000100} + 58\chi_{3000001} + 204\chi_{0010100} + 324\chi_{1100010} + 150\chi_{0200001} + 156\chi_{0000102} + 270\chi_{1010001} + 198\chi_{0000110} + 140\chi_{2100000} + 304\chi_{0001001} + 77\chi_{1000003} + 216\chi_{0110000} + 300\chi_{1000011} + 174\chi_{0100002} + 270\chi_{1000100} + 34\chi_{0000003} + 246\chi_{0100010} + 144\chi_{2000001} + 246\chi_{0010001} + 162\chi_{1100000} + 132\chi_{0000011} + 128\chi_{0000100} + 102\chi_{1000001} + 47\chi_{0100000}$$

$$+ 17\chi_{0000001},$$

$$z_6^3 = \chi_{0000030} + 2\chi_{0000111} + \chi_{0001002} + \chi_{0000200} + 3\chi_{1000012} + 3\chi_{0001010} + 2\chi_{0110001} + 2\chi_{0100003}$$
$$+ \chi_{0020000} + 3\chi_{1000020} + 6\chi_{1000101} + 10\chi_{0100011} + 3\chi_{2000002} + \chi_{0000004} + 9\chi_{0010002} + \chi_{1200000}$$
$$+ 3\chi_{1001000} + 8\chi_{0100100} + 6\chi_{2000010} + 12\chi_{0010010} + 9\chi_{0000012} + 18\chi_{1100001} + 11\chi_{0000020}$$
$$+ 6\chi_{0200000} + 21\chi_{0000101} + 18\chi_{1000002} + \chi_{3000000} + 10\chi_{1010000} + 17\chi_{0001000} + 25\chi_{1000010}$$
$$+ 25\chi_{0100001} + 10\chi_{0000002} + 9\chi_{2000000} + 16\chi_{0010000} + 18\chi_{0000010} + 8\chi_{1000000} + 2\chi_{0000000},$$

$$z_7^3 = \chi_{0000003} + 2\chi_{0000011} + \chi_{0000100} + 3\chi_{1000001} + 2\chi_{0100000} + 4\chi_{0000001}.$$

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Resonances of polyatomic molecules in the Born-Oppenheimer approximation

B. Messirdi[a] and A. Senoussaoui[b]
Faculté des Sciences, Département de Mathématiques, Université d'Oran Es-Senia, B.P. 1524 El-Mnaouer, Oran, Algeria

G. Djellouli
Institut des Sciences Exactes, Centre Universitaire de Saida 20000, Algeria

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We study the spectral properties of polyatomic molecules near a scattering level. We prove that in the Born-Oppenheimer approximation this study can be reduced to the one of a family of finite matrices of semiclassical pseudodifferential operators. More precisely, we show that any resonance of the molecule which is close enough to the real axis can be obtained from the discrete spectrum of one of these matrixes. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2037547]

I. INTRODUCTION

Consider a quantum system of $(n+p+1)$ particles, among which $(n+1)$ (the nuclei) are assumed to be heavy (with a mass of order $M \gg 1$), and p other ones (the electrons) are light (with a mass of order 1). Removing the center of mass motion of this system, and choosing properly the coordinates, one can describe it with a Hamiltonian of the type

$$P = -h^2\Delta_x - \Delta_y + V(x,y) \quad \text{on } L^2(\mathbb{R}^{3(n+p)}),$$

where h is a small parameter proportional to $M^{-1/2}$, and V is the sum of all the interactions between the particles. Moreover, we write $x=(x_1,\ldots,x_n) \in \mathbb{R}^{3n}$ for the Jacobi coordinates of $(n+1)$-nuclei in the center of mass frame; $y=(y_1,\ldots,y_p) \in \mathbb{R}^{3p}$ for the postion of p electrons.

Then, one defines the so-called electronic levels to be the discrete eigenvalues $\lambda_1(x) \leqslant \lambda_2(x) \leqslant \cdots$ of the operator

$$Q(x) = -\Delta_y + V(x,y) \quad \text{on } L^2(\mathbb{R}^{3p}_y).$$

Born and Oppenheimer in Ref. 2 realize that the study of P can be approximately reduced, when h is small, to the one of the family of operators,

$$-h^2\Delta_x + \lambda_j(x) \quad \text{on } L^2(\mathbb{R}^{3n}_x), \quad j = 1,2,\ldots .$$

In particular, when, for example, $\lambda_1(x)$ admits a nondegenerate point well at some energy level λ_0, the eigenvalues of P near λ_0 admits a complete asymptotic expansion in half-powers of h.

Such a result was proved both for smooth interactions in Refs. 6, 14, 13, 18, 19, and 3 and for Coulomb potentials (Refs. 12, 7, and 17). As we shall see, the main problem comes from the fact that, when one has singular (e.g., Coulomb) interactions, the eigenvalues and the eigenfunctions of $Q(x)$ are only C^2 with respect to the x variables (Combes-Seiler[4]).

Nevertheless, one can overcome this difficulty by introducing some x-dependent changes in the y variables that will regularize the potential V, the eigenvalues and the eigenfunctions of $Q(x)$.

[a]Electronic mail: bmessirdi@univ-oran.dz
[b]Present address: Université Libre de Bruxelles, Boulevard du Triomphe, Campus Plaine CP 214, B1050 Brussels, Belgium. Electronic mail: asenouss@ulb.ac.be

Since these changes can only be done locally in x, one then must glue them together, at least in a compact region, and to construct a kind of semiclassical pseudodifferential calculus adapted to these changes.

This will be enough to construct the complete expansion of the discrete spectrum of P, as in Klein-Martinez-Seiler-Wong.[12]

However, this technique is not sufficient when one wants to study the continuous spectrum of P (see Messirdi-Senoussaoui[20]), or *a fortiori* its resonances, the reason for this being that the classically allowed region (with respect to x) becomes unbounded.

We assume that any electron can be ionized near the energy level λ_0, and that the eigenvalues of $\lambda_j(x)$ of the operator $Q(x)$ are not degenerate at infinity [see (2.9) and (2.13) below]. This last assumption is essential to obtain a good behavior of the spectral projectors of $Q(x)$ near infinity. This is because our techniques stand strongly on pseudodifferential calculus, which requires a lot of regularity.

One must first make a change of variables whose purpose is to localize in a compact region the x-dependent singularities with respect to y in the interactions. After that the previous ideas can be adapted to any complex distortion of P (the resonances of P are accessible from the analytic distortions introduced by Hunziker[10] and developed by Messirdi[17,19]), and the study of P can be reduced to the one of a matrix of smooth h-pseudodifferential operators on $L^2(\mathbb{R}^{3n}_x)$.

In this paper, we show that one can reduce the problem to a finite matrix of regular h-pseudodifferential operators for polyatomic molecules and a class of potentials which includes the physically interesting case of Coulombic interactions.

More precisely, we construct a change of type

$$y=(y_1,\ldots,y_p)\mapsto y'=(G^0_x(y_1),\ldots,G^0_x(y_p)),$$

where x is outside the collision set of the molecule, $G^0_x(y_j)=y_j/|x|$ when $|y_j|\leqslant|x|$ and $G^0_x(y_j)=N_{y_j}$ (N is fixed large enough) when $|y_j|\geqslant 2N|x|$. In this way the domain in y will not be changed, the singularities become localized in the ball $|y'|\leqslant 1$ and the distorted operator P_μ of P is now regular. Finally, by the Feshbach method we get the reduction result: z is a resonance of P if and only if there exists μ complex small enough, $\mathrm{Im}\,\mu>0$, such that $0\in\sigma_{\mathrm{disc}}a^{\varsigma}_{\mu,-+}(z)$.

$a^{\varsigma}_{\mu,-+}(z)$ is a finite matrix of h-pseudodifferential operators analytic on μ, and depending on a function ς which regularizes P_μ in the elliptic region.

II. ANALYTIC DISTORTION, RESONANCES, *h*-PSEUDODIFFERENTIAL OPERATORS, HYPOTHESIS AND RESULT

A. Analytic distortion

We study the operator

$$P=-h^2\Delta_x-\Delta_y+V(x,y) \tag{2.1}$$

on $L^2(\mathbb{R}^{3n}_x\times\mathbb{R}^{3p}_y)$, when h tends to 0^+, with $V(x,y)=V(x_1,\ldots,x_n,y_1,\ldots,y_p)$ of the form

$$V(x,y)=\sum_{\substack{j,k=1\\ j\neq k}}^{n}\frac{\alpha_{jk}}{|x_j-x_k|}+\sum_{\substack{1\leqslant l\leqslant p\\ 1\leqslant k\leqslant n}}\left(\frac{\alpha^+_{lk}}{|y_l+x_k|}+\frac{\alpha^-_{lk}}{|y_l-x_k|}\right)+\sum_{\substack{l,q=1\\ l\neq q}}^{p}\frac{\beta_{lq}}{|y_l-y_q|}=W(x)+V_1(x,y), \tag{2.2}$$

where α_{jk}, $\alpha^{\pm}_{lk}$, and β_{lq} are real constants, and $\alpha_{jk}>0$, $\forall\, j,k\in\{1,\ldots,n\}$. $W(x)$ and $V_1(x,y)$ denote, respectively, the interaction potentials between the nuclei of the molecule and between the nuclei electrons and electrons electrons. The constants $\alpha^{\pm}_{lk}$ indicate the charges of the nuclei (in particular, if $\alpha^+_{lk}=\alpha^-_{lk}$, the molecule is symmetric).

It is well known that P with domain in $H^2(\mathbb{R}^{3n}_x\times\mathbb{R}^{3p}_y)$ is self-adjoint in $L^2(\mathbb{R}^{3n}_x\times\mathbb{R}^{3p}_y)$, and one can define the resonances of P by analytic distortion introduced by Hunziker in Ref. 10 and

developed afterwards in Refs. 17 and 18. More precisely, let $\omega \in C^\infty(\mathbb{R}^3,\mathbb{R}^3)$ be a C^∞-vector field satisfying $\omega=0$ near the collision set $\mathcal{C}$ of all the nuclei of the molecule:

$$\mathcal{C}=\{x=(x_1,\ldots,x_n)\in\mathbb{R}^{3n};\exists\, i\neq j, x_i=x_j\} \tag{2.3}$$

and ω is the identity far from $\mathcal{C}$, in the following sense:

$$\omega(x_i)=0 \quad \text{if } x=(x_1,\ldots x_i,\ldots,x_n)\in v(\mathcal{C}), \quad i\in\{1,\ldots,n\},$$

$$\omega(x_i)=x_i \quad \text{if } x=(x_1,\ldots x_i,\ldots,x_n)\notin v(\mathcal{C}), \quad |x_i|\to+\infty, \quad i\in\{1,\ldots,n\},$$

where $v(\mathcal{C})$ denote an adequate small neighborhood of $\mathcal{C}$ in the (t,x), the variable t take different positions from 1 to n. For μ real small enough, the analytic distortion U_μ associated to ω is defined on $C_0^\infty(\mathbb{R}^{3n}\times\mathbb{R}^{3p})$ by

$$U_\mu\varphi(x,y)=\varphi(x_1+\mu\omega(x_1),\ldots,x_n+\mu\omega(x_n),y_1+\mu\omega(y_1),\ldots,y_p+\mu\omega(y_p))|J_\mu(x,y)|^{1/2}, \tag{2.4}$$

where $J_\mu(x,y)=\Pi_{j=1}^n\det(1+\mu D\omega(x_j))\Pi_{l=1}^p\det(1+\mu D\omega(y_l))$ is the Jacobian of the transformation

$$F_\mu:(x,y)\to(x_1+\mu\omega(x_1),\ldots,x_n+\mu\omega(x_n),y_1+\mu\omega(y_1),\ldots,y_p+\mu\omega(y_p)). \tag{2.5}$$

The distorted operator $P_\mu=U_\mu P U_\mu^{-1}$ can be extended to small enough complex values of μ as an analytic family of type A in the sense of Kato.[11]

B. Resonances

We say that a complex number ρ is a resonance of the operator P if $\mathrm{Re}\,\rho>\mathrm{Inf}\,\sigma_{\mathrm{ess}}(P)$ and there exists μ small enough, $\mathrm{Im}\,\mu>0$, such that $\rho\in\sigma_{\mathrm{disc}}(P_\mu)$ (see Ref. 15). We denote

$$\Gamma(P)=\bigcup_{\mathrm{Im}\,\mu>0,\ \mu\ \text{small enough}}\sigma_{\mathrm{disc}}(P_\mu)$$

the set of the resonances of P.

In particular, $\Gamma(P)$ (except limit point at a threshold) is a discrete set, and $\Gamma(P)\subset\{z\in\mathbb{C};\ \mathrm{Im}\,z<0\}$, we consider here just the resonances of P which are near the real axis.

C. *h*-pseudodifferential operators (see, e.g., Refs. 21, 22, and 16)

A family of unbounded operators $A_\mu(h)$ on $L^2(\mathbb{R}^{3n}),\mu\in\mathbb{C}$, with fixed domain $H^{k_0}(\mathbb{R}^{3n}),k_0\geqslant 0$, is said to be h-pseudodifferential if there exists a sequence $(a_j(x,\xi))_{j\geqslant 0}$ of C^∞ functions on $T^*\mathbb{R}^{3n}$ satisfying

$$\forall\,\alpha,\beta\in\mathbb{N}^{3n},\exists\, C_{\alpha\beta}>0,\ |\partial_x^\alpha\partial_\xi^\beta a_j(x,\xi)|\leqslant C_{\alpha\beta}(1+|\xi|^2)^{k_0-|\beta|} \tag{2.6}$$

uniformly on $T^*\mathbb{R}^{3n}$, and such that for any N large enough, $A(h)$ can be written

$$A(h)=\sum_{j=0}^{N}h^j\,\mathrm{Op}(a_j)+h^N R_N(h),$$

where $R_N(h)\in\mathcal{L}(L^2(\mathbb{R}^{3n}))$, for h small enough and Op denotes the usual h-quantization of symbols,

$$\mathrm{Op}(a_j)\varphi(x)=(2\pi h)^{-3n}\int_{\mathbb{R}^{6n}}e^{i(x-y)\xi/h}a_j(x,\xi)\varphi(y)\mathrm{d}y\,\mathrm{d}\xi \tag{2.7}$$

for $\varphi\in C_0^\infty(\mathbb{R}^{3n})$. The right-hand side being defined as an oscillatory integral (see, e.g., Ref. 9). $\Sigma_{j=0}^\infty h^j a_j(x,\xi)$ is called the symbol of $A(h),a_0(x,\xi)$ is its principal symbol.

Finally the family $A_\mu(h), \mu$ complex small enough, depends analytically on μ, if for any h small enough it forms an analytic family of type A, when μ varies in a complex neighborhood of zero independent of h.

D. Hypothesis and result

For $x \in \mathbb{R}^{3n} \backslash \mathcal{C}$, we denote

$$Q(x) = -\Delta_y + V(x,y) \tag{2.8}$$

which acts on $L^2(\mathbb{R}^{3p}_y)$ with domain $H^2(\mathbb{R}^{3p})$ and we fix a scattering energy level $\lambda_0 \in \sigma_{\text{ess}}(P) \backslash \{\text{thresholds of } P\}$ such that

$$\forall x \in \mathbb{R}^{3n} \backslash \mathcal{C}, \sigma(Q(x)) \cap]-\infty, \lambda_0] = \sigma_{\text{disc}}(Q(x)) \cap]-\infty, \lambda_0] \tag{2.9}$$

and such that there exists $M \geqslant 0$ satisfying

$$\forall x \in \mathbb{R}^{3n} \backslash \mathcal{C}, \quad \#\sigma_{\text{disc}}(Q(x)) \geqslant M \quad \text{and } \#\sigma(Q(x)) \cap]-\infty, \lambda_0] \leqslant M. \tag{2.10}$$

Denoting $\lambda_1(x) \leqslant \lambda_2(x) \leqslant \cdots \leqslant \lambda_M(x)$ the first M eigenvalues of $Q(x)$, we assume that there exists a gap between them and the rest of the spectrum $\sigma(Q(x))$ of $Q(x)$; then there exists a constant $\delta > 0$, such that for any $\lambda \in \sigma(Q(x)) \backslash \{\lambda_1(x), \ldots, \lambda_M(x)\}$, one has

$$\operatorname*{Inf}_{x \in \mathbb{R}^{3n} \backslash \mathcal{C}} \operatorname*{Inf}_{1 \leqslant j \leqslant M} |\lambda - \lambda_j(x)| \geqslant \delta, \tag{2.11}$$

(2.11) assures that the spectral projector $\pi(x)$ of $Q(x)$ associated to $\{\lambda_1(x), \ldots, \lambda_M(x)\}$ is C^2 regular with respect to x (see Ref. 4).

We also assume the existence of $C > 0$ such that

$$\operatorname*{Sup}_{x \in \mathbb{R}^{3n} \backslash \mathcal{C}} \tilde{\lambda}_M(x) \leqslant C, \tag{2.12}$$

where

$$\tilde{\lambda}_s(x) = \lambda_s(x) - \sum_{\substack{j,k=1 \\ j \neq k}}^{n} \frac{\alpha_{jk}}{|x_j - x_k|}, \quad 1 \leqslant s \leqslant M,$$

and each of the λ_s's are nondegenerate at infinity,

$$\operatorname*{Inf}_{\substack{x \in \mathbb{R}^{3n} \backslash \mathcal{C} \\ |x| \geqslant c}} \operatorname*{Inf}_{j \neq k} |\lambda_j(x) - \lambda_k(x)| \geqslant \frac{1}{C}. \tag{2.13}$$

The condition (2.12) is automatically satisfied if, e.g., $\alpha^{\pm}_{lk} \leqslant 0$, but (2.13) excludes the case of symmetric molecules, for which $\alpha^{+}_{lk} = \alpha^{-}_{lk}$, $l \in \{1, \ldots, p\}$, $k \in \{1, \ldots, n\}$, but where the projectors of $Q(x)$ depend smoothly on x near infinity (see, e.g., Ref. 5 for $p=1$).

Now we fix $N > 0$ large enough so that $\omega(x_i) = 0$, on

$$\left\{ x = (x_1, \ldots, x_i, \ldots, x_n) \in \mathbb{R}^{3n}; d(x, \mathcal{C}) \leqslant \frac{2}{N} \right\}, \quad i \in \{1, \ldots, n\},$$

where d denotes the Euclidian distance in $\mathbb{R}^{3n}$, and we first regularize P_μ near $\mathcal{C}$ by cancelling the potential $V(x,y)$ in this region with a regular function ζ.

We note $V_N = \{x \in \mathbb{R}^{3n}; d(x, C) \leqslant 1/2N\}$, and we remark that $V_N \cap S^{3n-1} \neq \emptyset$ and $(\mathbb{R}^{3n} \backslash V_N) \cap S^{3n-1} \neq \emptyset$, where S^{3n-1} is the unit sphere of $\mathbb{R}^{3n}$. Let the function $\zeta \in C^\infty(\mathbb{R}^{3n}, \mathbb{R})$ such that

$$\zeta = 1 \quad \text{on } [2/N, +\infty[\cdot [1, +\infty[\cdot (V_N \cap S^{3n-1}),$$
$$\zeta = 0 \quad \text{on } \mathbb{R}^{3n} \setminus [3/2N, +\infty[\cdot [1, +\infty[\cdot (V_N \cap S^{3n-1}), \tag{2.14}$$

the conic form appearing in (2.14) results from the expression $x = d(x,\mathcal{C})[|x|/d(x,\mathcal{C})](x/|x|)$ and the definition of the set V_N. Here we denote by

$$AB = \{z = xy; (x,y) \in A \times B\}.$$

Fixing $\alpha_0 > \lambda_0$, we set

$$Q_\mu^\zeta(x) = -U_\mu \Delta_y U_\mu^{-1} + \zeta(x) V_\mu(x,y) + (1-\zeta(x))\alpha_0,$$

$$V_\mu(x,y) = U_\mu V(x,y) U_\mu^{-1} = V(x_1 + \mu\omega(x_1), \ldots, x_n + \mu\omega(x_n), y_1 + \mu\omega(y_1), \ldots, y_p + \mu\omega(y_p)).$$

We also denote

$$P_\mu^\zeta(x) = -h^2 U_\mu \Delta_x U_\mu^{-1} + Q_\mu^\zeta(x)$$

with domain $H^2(\mathbb{R}^{3n} \times \mathbb{R}^{3p})$.

Let us remark that under rather general assumptions, one can show in a similar way as in Ref. 8 that near λ_0, $\sigma(P_\mu)$ and $\sigma(P_\mu^\zeta)$ coincide up to exponentially small error terms (see Ref. 17). This explains why we will study P_μ^ζ instead of P_μ.

Our main result is the following.

Theorem 2.1: *Under assumptions* (2.10) *to* (2.13), *and for any z complex close enough to* λ_0, *there exists a family of* $M \times M$*-matrices* $E_{\mu,-+}^\zeta(z)$, *of h-pseudodifferential operators on* $\mathbb{R}^{3n}$, *depending analytically on* μ *complex small enough, such that*

$$z \in \Gamma(P^\zeta) \Leftrightarrow \exists\, \mu \in \mathbb{C}, \mu \text{ small enough}, \operatorname{Im}\mu > 0, 0 \in \sigma_{\text{disc}}(E_{\mu,-+}^\zeta(z)).$$

The principal symbol of $E_{\mu,-+}^\zeta(z)$ *is of the form*

$$z - [|(1+\mu D\omega)^{-1}\xi|^2 I_M + \mathcal{M}_\mu^\zeta(x)],$$

where I_M *is the identity of* $\mathbb{C}^M$ *and* $\mathcal{M}_\mu^\zeta(x)$ *is a matrix of* C^∞*-functions on* $\mathbb{R}^{3n}$, *with eigenvalues* $\lambda_1(x_1+\mu\omega(x_1), \ldots, x_n+\mu\omega(x_n)), \ldots, \lambda_M(x_1+\mu\omega(x_1), \ldots, x_n+\mu\omega(x_n))$ *on* $\zeta(x)=1$, *and satisfying* $\operatorname{Re}\mathcal{M}_\mu^\zeta(x) \geqslant \lambda_0 + \delta$ *on* $\zeta(x) \neq 1$ *for some positive constant* δ. *Finally* $E_{\mu,-+}^\zeta(z)$ *depends analytically on z near* λ_0 *and is* $O(3)$*-invariant if the function* ζ *is also chosen* $O(3)$*-invariant, where* $O(3)$ *is the orthogonal group of* $\mathbb{R}^3$.

III. THE DISTORTED FESHBACH METHOD

The Feshbach method is a way to construct an effective Hamiltonian of P which is a nice h-pseudodifferential operator on $\mathbb{R}^{3n}$. To do this we will use a so-called Grushin problem associated to the distorted operator P_μ of P and a convenient choice of sections of Ran $\pi(x)$.

For $x \in \mathbb{R}^{3n} \setminus \mathcal{C}$, we denote

$$Q_\mu(x) = U_\mu Q(x + \mu\omega(x)) U_\mu^{-1}, \tag{3.1}$$

here U_μ is considered as acting on $L^2(\mathbb{R}_y^{3p})$, and we can easily see that $Q_\mu(x)$ extends for small enough μ to an analytic family of type A (see Ref. 19), and that the singularities of $V(x,y)$ are not changed if ω is taken as an odd function.

Denoting also

$$\widetilde{Q}_\mu(x) = Q_\mu(x) - \sum_{\substack{j,k=1 \\ j\neq k}}^{n} \frac{\alpha_{jk}}{|x_j + \mu\omega(x_j) - x_k - \mu\omega(x_k)|},$$

$$\widetilde{Q}(x) = \widetilde{Q}_0(x) = Q(x) - \sum_{\substack{j,k=1 \\ j\neq k}}^{n} \frac{\alpha_{jk}}{|x_j - x_k|}. \tag{3.2}$$

We first have the following.

Lemma 3.1: $\exists C_1 > 0$ *such that for all* $x \in \mathbb{R}^{3n}\backslash C$, *one has*

$$\sum_{\substack{j,k=1 \\ j\neq k}}^{n} \frac{\alpha_{jk}}{|x_j - x_k|} \leqslant \lambda_1(x) + C_1.$$

Proof: We must prove that $(\widetilde{Q}(x)+\lambda)^{-1} \in \mathcal{L}(L^2(\mathbb{R}^{3p}))$ for $\lambda \in \mathbb{R}_+$ large enough independently of x.

For $\forall x \in \mathbb{R}^{3n}\backslash\mathcal{C}$, we have

$$(\widetilde{Q}(x) + \lambda)(-\Delta_y + \lambda)^{-1} = 1 + \widetilde{V}(x,y)(-\Delta_y + \lambda)^{-1}, \tag{3.3}$$

where

$$\widetilde{V}(x,y) = V(x,y) - \sum_{\substack{j,k=1 \\ j\neq k}}^{n} \frac{\alpha_{jk}}{|x_j - x_k|}$$

and

$$\widetilde{V}(x,y)(-\Delta_y + \lambda)^{-1} = \sum_{\substack{1\leqslant l\leqslant p \\ 1\leqslant k\leqslant n}} \left(\frac{\alpha^+_{lk}}{|y_l + x_k|} + \frac{\alpha^-_{lk}}{|y_l - x_k|} \right)(-\Delta_y + \lambda)^{-1} + \sum_{\substack{l,q=1 \\ l\neq q}}^{p} \frac{\beta_{lq}}{|y_l - y_q|}(-\Delta_y + \lambda)^{-1}. \tag{3.4}$$

Each term of (3.4) is unitarily equivalent to the operator $(1/|y_1|)(-\Delta_y+\lambda)^{-1}$. But $1/|y_1|$ is Δ_{y_1}-compact on $L^2(\mathbb{R}^3)$ and by taking the Fourier transform of $(1/|y_1|)(-\Delta_y+\lambda)^{-1}$ this operator can be written $(1/|y_1|)(-\Delta_{y_1}+1)^{-1}(-\Delta_{y_1}+1)(-\Delta_y+\lambda)^{-1}$ or $K_{\xi_1}[(\xi_1^2+1)/(\xi^2+\lambda)]$ where the kernel K_{ξ_1} of the operator $(1/|y_1|)(-\Delta_{y_1}+\lambda)^{-1}$ acts in the ξ_1-variable only and is compact on $L^2(\mathbb{R}^3)$, and $[(\xi_1^2+1)/(\xi^2+\lambda)]$ tends to 0 as λ tends to $+\infty$. Consequently $(1/|y_1|)(-\Delta_y+\lambda)^{-1}$ tends to 0 in norm as λ tends to $+\infty$, and this proves in view of (3.4) that $\widetilde{V}(x,y)(-\Delta_y+\lambda)^{-1}$ tend to 0 in norm as λ tends to $+\infty$ uniformly with respect to x.

Therefore by (3.3), $(\widetilde{Q}(x)+\lambda)$ becomes invertible for any $x \in \mathbb{R}^{3n}\backslash\mathcal{C}$ if λ is chosen sufficiently large enough. □

Now, let $\gamma(x)$ be a continuous family of simple loops of $\mathbb{C}$, enclosing $\widetilde{\lambda}_1(x), \ldots, \widetilde{\lambda}_M(x)$ and having the rest of $\sigma(\widetilde{Q}(x))$ in its exterior. By the gap condition (2.11), we may also assume that

$$\operatorname*{Min}_{x\in\mathbb{R}^{3n}\backslash\mathcal{C}} \operatorname{dist}(\gamma(x), \sigma(\widetilde{Q}(x))) \geqslant \frac{\delta}{2} > 0, \tag{3.5}$$

dist is the distance on $\mathbb{C}$. Moreover, using Lemma 3.1 and condition (2.12), $\gamma(x)$ can be taken in a fixed compact set of $\mathbb{C}$.

We deduce also from the proof of Lemma 3.1 and the assumption (3.5) the following result.

Lemma 3.2: For any $k \in \{1,\dots,n\}, l,q \in \{1,\dots,p\}, l \neq q, \alpha \in \mathbb{N}^{3p}, |\alpha| \leqslant 2$, *the operators*

$$\frac{1}{|y_l \pm x_k|}(\widetilde{Q}(x)-z)^{-1}, \quad \frac{1}{|y_l - y_q|}(\widetilde{Q}(x)-z)^{-1}, \quad \partial^{\alpha}(\widetilde{Q}(x)-z)^{-1}$$

are uniformly bounded on $L^2(\mathbb{R}^{3p})$ *as* $x \in \mathbb{R}^{3n}\backslash\mathcal{C}$ *and* $z \in \gamma(x)$.

We now study the continuity of $\widetilde{Q}_{\mu}(x)$ with respect to μ.

Lemma 3.3: If μ *is a small enough complex number, then for any* $x \in \mathbb{R}^{3n}\backslash\mathcal{C}$ *and* $z \in \gamma(x)$, *the operator* $(\widetilde{Q}_{\mu}(x)-z)^{-1}$ *exists and satisfies uniformly*

$$(\widetilde{Q}_{\mu}(x)-z)^{-1} - (\widetilde{Q}(x)-z)^{-1} = \mathcal{O}(|\mu|).$$

Proof: We have

$$\begin{aligned}(\widetilde{Q}_{\mu}(x)-z) &= 1 + \widetilde{Q}_{\mu}(x) - \widetilde{Q}(x)\widetilde{Q}(x) - z^{-1}\widetilde{Q}(x) - z,\\ \widetilde{Q}_{\mu}(x) - \widetilde{Q}(x) &= \sum_{|\beta|\leqslant 2} |\mu| a_{\beta,\mu}(y)\partial_y^{\beta} + \widetilde{V}_{\mu}(x) - \widetilde{V}(x,y),\end{aligned} \tag{3.6}$$

where

$$\widetilde{V}_{\mu}(x,y) = V_{\mu}(x,y) - \sum_{\substack{j,k=1\\ j\neq k}}^{n} \frac{\alpha_{jk}}{|x_j + \mu\omega(x_j) - x_k - \mu\omega(x_k)|}, \quad \widetilde{V}(x,y) = \widetilde{V}_0(x,y),$$

and the $a_{\beta,\mu}$'s are in $C^{\infty}(\mathbb{R}^{3p})$ and uniformly bounded along with all their derivatives as μ tends to 0 in $\mathbb{C}$ (see Ref. 19). Moreover,

$$\begin{aligned}\widetilde{V}_{\mu}(x,y) - \widetilde{V}(x,y) = &\sum_{\substack{1\leqslant l\leqslant p\\ 1\leqslant k\leqslant n}} \alpha_{lk}^{\pm}\left(\frac{1}{|y_l + \mu\omega(y_l) \pm x_k \pm \mu\omega(x_k)|} - \frac{1}{|y_l \pm x_k|}\right)\\ &+ \sum_{\substack{l,q=1\\ l\neq q}}^{p} \beta_{lq}\left(\frac{1}{|y_l + \mu\omega(y_l) - y_q - \mu\omega(y_q)|} - \frac{1}{|y_l - y_q|}\right)\end{aligned}$$

and thus we have from the construction of the vector field ω,

$$|\widetilde{V}_{\mu}(x,y) - \widetilde{V}(x,y)| \leqslant C_2|\mu|\left(\sum_{\substack{1\leqslant l\leqslant p\\ 1\leqslant k\leqslant n}} \frac{1}{|y_l \pm x_k|} + \sum_{\substack{l,q=1\\ l\neq q}}^{p} \frac{1}{|y_l - y_q|}\right),$$

for some constant $C_2 > 0$. Then, the result follows from (3.6) and Lemma 3.2. □

We can now define for μ, a complex small enough for the spectral projector associated to $\widetilde{Q}_{\mu}(x)$ and the loops $\gamma(x)$,

$$\pi_{\mu}(x) = \frac{1}{2\pi i}\oint_{\gamma(x)} (z - \widetilde{Q}_{\mu}(x))^{-1}\,\mathrm{d}z. \tag{3.7}$$

This projector is of rank M and it helps us to construct the Grushin problem associated to P_{μ}^{ξ}.

On the one hand, using the fact that $\pi(x) = \pi_0(x)$ depends continuously on $x \in \mathbb{R}^{3n}\backslash\mathcal{C}$ (see Ref. 4), we can then find an orthonormal family of M continuous sections $\{v_1(x),\dots,v_M(x)\}$ generating Ran $\pi(x)$. On the other hand, we well know that $\lambda_1(x),\dots,\lambda_M(x)$ depend only on $|x|$ and can be

indexed in such a way each of them becomes analytic with respect to $x \in \mathbb{R}^{3n}\backslash\mathcal{C}$. Let $\{v_{1,\mu}(x),\ldots,v_{M,\mu}(x)\}$ denote a family of Ran $\pi_\mu(x)$, depending analytically on μ for μ small enough and normalized in $L^2(\mathbb{R}^{3p})$ by

$$\langle v_{k,\mu}(x), v_{l,\bar{\mu}}(x)\rangle_{L^2(\mathbb{R}^{3p})} = \delta_{k,l}. \tag{3.8}$$

We associate the two following operators:

$$R_\mu^- : \bigoplus_1^M L^2(\mathbb{R}^{3n}) \to L^2(\mathbb{R}^{3(n+p)}),$$

$$u^- = (u_1^-,\ldots,u_M^-) \mapsto R_\mu^- u^- = \sum_{k=1}^M u_k^- v_{k,\mu}(x), \tag{3.9}$$

$$R_\mu^+ = (R_\mu^-)^* : L^2(\mathbb{R}^{3(n+p)}) \to \bigoplus_1^M L^2(\mathbb{R}^{3n}),$$

$$u \mapsto R_\mu^+ u = \bigoplus_1^M \langle u, v_{k,\bar{\mu}}(x)\rangle_{L^2(\mathbb{R}^{3p})}. \tag{3.10}$$

We then consider a Grushin problem that will lead to the Feshbach reduction. For $z \in \mathbb{C}$, define

$$A_\mu^\zeta(z) = \begin{pmatrix} (P_\mu^\zeta - z) & R_\mu^- \\ R_\mu^+ & 0 \end{pmatrix} \tag{3.11}$$

on

$$H^2(\mathbb{R}^{3(n+p)}) \oplus \left(\bigoplus_1^M L^2(\mathbb{R}^{3n})\right)$$

to

$$L^2(\mathbb{R}^{3(n+p)}) \oplus \left(\bigoplus_1^M H^2(\mathbb{R}^{3n})\right).$$

Using Lemma 3.3, and (2.11), one can easily prove that the operator $\hat{\pi}_\mu(x)(P_\mu^\zeta - z)$ is invertible on $\{u \in H^2(\mathbb{R}^{3(n+p)}); \hat{\pi}_\mu(x)u = u\}$, where $\hat{\pi}_\mu(x) = 1 - \pi_\mu(x)$, and its inverse is bounded and denoted by $P_\mu'^{\xi} - z^{-1}$ for $z \in \mathbb{C}$ close enough to λ_0.

It follows that $A_\mu^\zeta(z)$ is invertible for $z \in \mathbb{C}$ close enough to λ_0,

$$(A_\mu^\zeta(z))^{-1} = \begin{pmatrix} a_\mu^\zeta(z) & a_{\mu,+}^\zeta(z) \\ a_{\mu,-}^\zeta(z) & a_{\mu,-+}^\zeta(z) \end{pmatrix} \tag{3.12}$$

with

$$\begin{gathered} a_\mu^\zeta(z) = (P_\mu'^{\zeta} - z)^{-1}\hat{\pi}_\mu(x), \quad a_{\mu,+}^\zeta(z) = R_\mu^- - a_\mu^\zeta(z)P_\mu^\zeta R_\mu^-, \\ a_{\mu,-}^\zeta(z) = R_\mu^+ - R_\mu^+ P_\mu^\zeta a_\mu^\zeta(z), \quad a_{\mu,-+}^\zeta(z) = zI_M - R_\mu^+(P_\mu^\zeta - P_\mu^\zeta a_\mu^\zeta(z)P_\mu^\zeta)R_\mu^-, \end{gathered} \tag{3.13}$$

where I_M is the identity of $\mathbb{C}^M$, and $a_{\mu,-+}^\zeta(z)$ depends only on x defined from $\oplus_{k=1}^M H^2(\mathbb{R}^{3n})$ to $\oplus_{k=1}^M L^2(\mathbb{R}^{3n})$. Consequently we have the following.

Lemma 3.4: *For $z \in \mathbb{C}$ close enough to λ_0, $z \in \Gamma(P^\zeta)$ if and only if there exists $\mu \in \mathbb{C}$, small enough*, Im $\mu > 0$, *such that* $0 \in \sigma_{\text{disc}}(a_{\mu,-+}^\zeta(z))$.

Now, we can prove with a suitable choice of the family $\{v_{1,\mu}(x),\ldots,v_{M,\mu}(x)\}$ that $a^{\xi}_{\mu,-+}(z)$ becomes a family of $M\times M$ matrices of h-pseudodifferential operators on $\mathbb{R}^{3n}$, analytic with respect to μ complex small enough. The main idea consists, before localizing the singularities of the potential, to construct as in Ref. 12 a x-dependent change of the y variables, in such a way the operators $Q_\mu(x)$ become smooth with respect to x.

IV. LOCALIZATION OF THE SINGULARITIES

In this section we use the idea of Martinez-Messirdi (see Ref. 17). By adequate change of variables we localize in a compact set of $\mathbb{R}^{3n}$ the x-dependent singularities with respect to y appearing in the interaction potentials.

Let $\chi\in C_0^\infty(\mathbb{R}_+)$ satisfying $0\leqslant\chi\leqslant 1$, $\chi'\leqslant 0$ and

$$\chi(s)=\begin{cases}1 & \text{if } 0\leqslant s\leqslant 1,\\ 0 & \text{if } s\geqslant 2.\end{cases}$$

We choose $N\geqslant 1$ large enough such that $\omega(x_i)=0$, $\forall i\in\{1,\ldots,n\}$ on $\{d(x,\mathcal{C})\leqslant 2/N\}$. Let us define for $r\geqslant 1/N$ and $t\geqslant 0$, the function

$$\rho(r,t)=\frac{t}{r}\chi\left(\frac{t}{r}\right)+Nt\left(1-\chi\left(\frac{t}{r}\right)\right). \tag{4.1}$$

We clearly see that

(i) $\partial\rho/\partial t>0$ on $[1/N,+\infty[\times\mathbb{R}_+$,
(ii) $\rho(r,t)$ is surjective on $\mathbb{R}_+$,
(iii) $\forall k\geqslant 1$, $\partial^k\rho/\partial t^k$ is uniformly bounded on $[1/N,+\infty[\times\mathbb{R}_+$.

The function $t\to\rho(r,t)$ is a diffeomorphism on $\mathbb{R}_+$, we denote by α_r its inverse.

By construction, we have $\alpha_r(t)=t/N$ if $t\geqslant 2Nr$ and $\alpha_r(r)=rt$ if $t\leqslant 1$.

For $x\in\mathbb{R}^3$, such that $d(x,\mathcal{C})\geqslant 1/N$, we define the function

$$\theta_x:\mathbb{R}^3\ni s\to\alpha_{|x|}(|s|)\frac{s}{|s|}.$$

θ_x has the following properties.

Lemma 4.1: *(see Ref. 17)*

(i) $\forall x\in\mathbb{R}^{3n}$, $d(x,\mathcal{C})\geqslant 1/N$, *the function* θ_x *is a diffeomorphism of* $\mathbb{R}^3$ *depending smoothly on* x, *and satisfying*
(ii) $\forall\alpha\in\mathbb{N}^{3n}\backslash\{0\}$, $\partial_x^\alpha\theta_x$ *is uniformly bounded on* $\{d(x,\mathcal{C})\geqslant 1/N, s\in\mathbb{R}^3\}$.

$$\theta_x(x_i/|x|)=x_i,\quad x=(x_1,\ldots,x_i,\ldots,x_n),\quad \forall\, i\in\{1,\ldots,n\},$$

$$\theta_x(s)=\frac{s}{N}\quad \textit{if } |s|\geqslant 2N|x|,$$

$$\theta_x(s)=|x|s\quad \textit{if } |s|\leqslant 1.$$

Denote $\tilde{\sigma}_x=\theta_x^{-1}$ the inverse diffeomorphism of θ_x on $\mathbb{R}^3$. It satisfies $\tilde{\sigma}_x(s)=Ns$ if $|s|\geqslant 2|x|$ and $\tilde{\sigma}_x(s)=s/|x|$ if $|s|\leqslant|x|$.

Let the function $\mathbb{R}^{3p}\ni y=(y_1,\ldots,y_p)\to\tilde{\sigma}_x(y)=(\tilde{\sigma}_x(y_1),\ldots,\tilde{\sigma}_x(y_p))$, then σ_x is a diffeomorphism on $\mathbb{R}^{3p}$, moreover the transformed potential $\hat{V}_\mu(x,y)$ of $V_\mu(x,y)$ under the change of variables $y'=\sigma_x(y)$ is given by [denoting $I_\mu(s)=s+\mu\omega(s)$]

$$\hat{V}_\mu(x,y)=\sum_{\substack{j,k=1\\ j\neq k}}^{n}\frac{\alpha_{jk}}{|I_\mu(x_j)-I_\mu(x_k)|}+\sum_{\substack{1\leqslant l\leqslant p\\ 1\leqslant k\leqslant n}}\frac{\alpha_{lk}^{\pm}}{\left|I_\mu(\theta_x(y_l'))\pm I_\mu\left(\theta_x\left(\frac{x_k}{|x|}\right)\right)\right|}+\sum_{\substack{l,q=1\\ l\neq q}}^{p}\frac{\beta_{lk}}{|I_\mu(\theta_x(y_l'))\pm I_\mu(\theta_x(y_q'))|}. \tag{4.2}$$

It is then advantageous to study $\hat{V}_\mu(x,y)$ instead of $V_\mu(x,y)$ because their x-dependent singularities are now localized in the compact set $\cup_{l,k}\{y_l'=\pm x_k/|x|\}$.

V. REGULARIZATION OF THE OPERATOR

Since $\{x\in\mathbb{R}^{3n}, d(x,\mathcal{C})\leqslant 1/N\}\subset\mathbb{R}^{3n}\backslash[3/2N,+\infty[\cdot[1,+\infty[\cdot(V_N\cap S^{3n-1})$, then P^ζ is a nice h-pseudodifferential operator in the region $\mathbb{R}^{3n}\backslash[1/2N,+\infty[\cdot[1,+\infty[\cdot(V_N\cap S^{3n-1})$, with operator valued symbol to regularize P^ζ on the region $[1/2N,+\infty[\cdot[1,+\infty[\cdot(V_N\cap S^{3n-1})$, we use a change of variables similar to the one used in Refs. 12 and 20 coupled with the one of Sec. IV.

For any x_0 fixed in $]1/2N,+\infty]\cdot]1,+\infty]\cdot(V_N\cap S^{3n-1})$ [then $d(x_0,\mathcal{C})\geqslant 1/2N, x_0\notin\mathcal{C}$] and for $x\in\mathbb{R}^{3n}\backslash\mathcal{C}$, with $x/|x|$ close enough to $x_0/|x_0|$ [equivalently $x_j/|x|$ close enough to $x_j^0/|x_0|, \forall j\in\{1,\ldots,n\}, x_0=(x_1^0,\ldots,x_n^0)$], we consider the C^∞-function defined on $\mathbb{R}^3$ by

$$F_{x_0}(x,s)=s+\sum_{j=1}^{n}\left(\frac{x_j}{|x|}-\frac{x_j^0}{|x_0|}\right)(f_j(s)-f_j(-s)), \tag{5.1}$$

where $f_j\in C_0^\infty(\mathbb{R}^3,\mathbb{R})$, $f_j(x_k^0/|x_0|)=\delta_{jk}$, and $f_j(-x_k^0/|x_0|)=0, \forall j,k\in\{1,\ldots,n\}$.

It is clear that for $x/|x|$ in some small neighborhood ω_{x_0} of $x_0/|x_0|$, the function $F_{x_0}(x,.)$ is C^∞-diffeomorphism of $\mathbb{R}^3$, satisfying

$$F_{x_0}\left(x,\frac{x_k^0}{|x_0|}\right)=\frac{x_k}{|x|},\quad F_{x_0}\left(x,-\frac{x_k^0}{|x_0|}\right)=-\frac{x_k}{|x|},\quad \forall k\in\{1,\ldots,n\}. \tag{5.2}$$

$\forall\alpha\in\mathbb{N}^{3n}, \exists c_\alpha>0, \forall x\in\mathbb{R}_+^*\omega_{x_0}, \forall s,s'\in\mathbb{R}^3$,

$$\frac{1}{C_0}|s-s'|\leqslant|F_{x_0}(x,s)-F_{x_0}(x,s')|\leqslant C_0|s-s'|,$$

$$|\partial_x^\alpha F_{x_0}(x,s)-\partial_x^\alpha F_{x_0}(x,s')|\leqslant C_\alpha|s-s'|,$$

$$|\partial_x^\alpha F_{x_0}(x,s)|\leqslant C_\alpha(|\alpha|\geqslant 1). \tag{5.3}$$

With the notations of the preceding section, let us denote for $x\in[1/N,+\infty[\cdot[1,+\infty[\cdot\omega_{x_0}$,

$$G_x^0:\mathbb{R}^{3p}\to\mathbb{R}^{3p},$$

$$y=(y_1,\ldots,y_p)\mapsto G_x^0(y)=(\theta_x(F_{x_0}(x,y_1)),\ldots,\theta_x(F_{x_0}(x,y_p))).$$

Using Lemma 4.1 and the properties (5.3), we obtain the following.

Lemma 5.1: $\forall\alpha\in\mathbb{N}^3$, *there exists a constant* $C_\alpha'>0$ *such that* $\forall x\in[1/N,+\infty[\cdot[1,+\infty[\cdot\omega_{x_0}, \forall y,y'\in\mathbb{R}^{3p}$, *one has*

$$\frac{1}{C_0'}|s-s'|\leqslant|G_x^0(y)-G_x^0(y')|\leqslant C_0'(1+|x|)|y-y'|,$$

$$|\partial_x^\alpha G_x^0(y) - \partial_x^\alpha G_x^0(y')| \leqslant C'_\alpha |y - y'| \quad (|\alpha| \geqslant 1), \tag{5.4}$$

$$|\partial_x^\alpha G_x^0(y)| \leqslant C'_\alpha \quad (|\alpha| \geqslant 1).$$

Now using the fact that G_x^0 is a diffeomorphism of $\mathbb{R}^{3p}$, with the abuse of notation $G_x^0(y) = (G_x^0(y_1), \ldots, G_x^0(y_p))$, we consider the change of variables $y' = (G_x^0)^{-1}(y)$ which transforms the operator Q_μ^ζ into

$$Q_{\mu,x_0}^\zeta(x) = t_{\mu,x_0}(x,y',h\Delta_{y'},h) + \sum_{\substack{j,k=1 \\ j\neq k}}^{n} \frac{\alpha_{jk}\zeta(x)}{|I_\mu(x_j) - I_\mu(x_k)|} + \sum_{\substack{1\leqslant l\leqslant p \\ 1\leqslant k\leqslant n}} \frac{\alpha_{lk}^{\pm}\zeta(x)}{\left| I_\mu(G_x^0(y_l')) \pm I_\mu\left(G_x^0\left(\frac{x_0^k}{|x_0|} \right) \right) \right|}$$

$$+ \sum_{\substack{l,q=1 \\ l\neq q}}^{p} \frac{\beta_{lk}\zeta(x)}{|I_\mu(G_x^0(y_l')) \pm I_\mu(G_x^0(y_q'))|} + (1-\zeta(x))\alpha_0 = t_{\mu,x_0}(x,y',hD_{y'},h) + V_{x_0}^\zeta(x,y'), \tag{5.5}$$

where $t_{\mu,x_0}(x,y',hD_{y'},h)$ is an elliptic second order differential operator in y', the coefficients depending smoothly on x and y' and being uniformly bounded in $\{x \in \mathbb{R}^{3n}, d(x,\mathcal{C}) \leqslant 1/N\} \times \mathbb{R}^{3p}$.

By Lemma 5.1, we obtain that $V_{x_0}^\zeta(x,y')$ is smooth with respect to x as a self-adjoint operator from $H^2(\mathbb{R}^{3p})$ to $L^2(\mathbb{R}^{3p})$.

We have consequently proved the following result.

Proposition 5.2: For $\forall x_0 \in V_N \cap S^{3n-1}$, *there exists a neighborhood* ω_{x_0} *of* x_0 *in* $V_N \cap S^{3n-1}$ *and a* C^∞ *application*,

$$G_0 : [1/N, +\infty[\cdot [1, +\infty[\cdot \omega_{x_0} \times \mathbb{R}^{3p} \to \mathbb{R}^{3p},$$

$$(x,y) \mapsto G_0(x,y) = G_x^0(y),$$

such that for any x, G_x^0 *is a diffeomorphism of* $\mathbb{R}^{3p}$. *If we denote*

$$U_0(x)\varphi(y) = \varphi(G_0(x,y))|\det(\partial_y G_0(x,y))|^{1/2}, \tag{5.6}$$

then the family of operators $Q_{\mu,x_0}^\zeta(x) = U_0(x)Q_\mu^\zeta(x)U_0^{-1}(x)$ *is in* $C_b^\infty([1/N, +\infty[\cdot [1, +\infty[\cdot \omega_{x_0}, \mathcal{L}(H^2(\mathbb{R}^{3p}), L^2(\mathbb{R}^{3p}))$. *($C_b^\infty$ denotes the space of C^∞ functions that have their derivatives uniformly bounded for any order.)*

Remark 5.3: *Under* (5.6) *the operator* P_μ^ζ *is transformed into the differential operator*

$$\tilde{P}_\mu^\zeta = \tilde{t}_{\mu,x_0}(x,y',hD_{y'},h) + Q_{\mu,x_0}^\zeta(x),$$

where $\tilde{t}_{\mu,x_0}$ *has the same properties as* t_{μ,x_0} *in* (5.5).

By compactness, we can cover $V_N \cap S^{3n-1}$ with a finite family of open subsets $(w_j)_{j=1}^{j_0}$, such that for any $j \in \{1, \ldots, j_0\}$ there exists a C^∞ application G_j from $[1/N, +\infty[\cdot [1, +\infty[\cdot w_j \times \mathbb{R}^{3p}$ to $\mathbb{R}^{3p}$, and for any $x \in [1/N, +\infty[\cdot [1, +\infty[\cdot w_j, G_j(x,.)$ is a diffeomorphism of $\mathbb{R}^{3p}$.

If we denote $U_j(x)\varphi(y) = \varphi(G_j(x,y))|\det(\partial_y G_j(x,y))|^{1/2}$, then

$$Q_{\mu,j}^\zeta(x) = U_j(x)Q_\mu^\zeta(x)U_j^{-1}(x) \in C_b^\infty\left(\left]\frac{1}{N}, +\infty\right[\cdot \right]1, +\infty[\cdot \omega_j, \mathcal{L}(H^2(\mathbb{R}^{3p}), L^2(\mathbb{R}^{3p})) \right). \tag{5.7}$$

VI. CHARACTERIZATION OF RESONANCES

Using the idea of Ref. 18 and assumptions (2.10)–(2.13), we can construct as in Refs. 12 and 17 a $L^2(\mathbb{R}^{3p}_y)$-orthonormalized family [see (3.8)] $(\omega_{k,\mu}(x,y))_{1\leqslant k\leqslant M}$ of M continuous functions from $\mathbb{R}^{3n}$ to $H^2(\mathbb{R}^{3p})$ depending analytically on μ, such that

(i) $(\omega_{k,\mu})_{1\leqslant k\leqslant M}$ form a basis of Ran $\pi_\mu(x)$ in $[3/2N,+\infty[\cdot[1,+\infty[\cdot(V_N\cap S^{3n-1})\times\mathbb{R}^{3p}$,
(ii) $\omega_{k,\mu}\in C^\infty(\mathbb{R}^{3n}\backslash[1/2N,+\infty[\cdot[1,+\infty[\cdot(V_N\cap S^{3n-1}),H^2(\mathbb{R}^{3p}))$.
(iii) For $|x|$ large enough, $\omega_{k,\mu}(x,.)$ is an eigenfunction of $Q_\mu(x)$ associated to $\lambda_k(x_1+\mu\omega(x_1),\ldots,x_n+\mu\omega(x_n))$, $x=(x_1,\ldots,x_n)$,
(iv) $\forall j\in\{1,\ldots,j_0\}, U_j(x)\omega_{k,\mu}(x,.)\in C_b^\infty(]1/N,+\infty[\cdot[1,+\infty[\cdot w_j,H^2(\mathbb{R}^{3p}))$.

Now, let for any $j\in\{1,\ldots,j_0\}, \psi_j\in C_0^\infty(w_j)$ be such that $\Sigma_{j=1}^{j_0}\psi_j^4=1$ on $V_N\cap S^{3n-1}$, and $\chi_0\in C^\infty(\mathbb{R}^{3n})$ such that $(1-\chi_0^4)^{1/4}\in C^\infty(\mathbb{R}^{3n})$ and

$$\chi_0=\begin{cases}1 & \text{in } \mathbb{R}^{3n}\backslash[1/N,+\infty[\cdot[1,+\infty[\cdot(V_N\cap S^{3n-1}),\\ 0 & \text{in } [3/2N,+\infty[\cdot[1,+\infty[\cdot(V_N\cap S^{3n-1}).\end{cases}$$

For $j\in\{1,\ldots,j_0\}$, we denote $\chi_j(x)=(1-\chi_0^4(x))^{1/4}\psi_j(x/|x|)$. Thanks to the choice of χ_0, we have

$$\sum_{j=0}^{j_0}\chi_j^4=1 \quad \text{in } \mathbb{R}^{3n}$$
$$\text{supp } \chi_j\subset[1/N,+\infty[\cdot[1,+\infty[\cdot w_j,\ \forall\, j\in\{1,\ldots,j_0\}. \tag{6.1}$$

To study the spectrum of P_μ^ζ near λ_0, we consider the Grushin operator

$$A_\mu^\zeta(z)=\begin{pmatrix}(P_\mu^\zeta-z) & R_\mu^-\\ R_\mu^+ & 0\end{pmatrix}, \tag{6.2}$$

where the operators $R_\mu^\pm$ are defined in (3.9) and (3.10), but here with $\omega_{k,\mu}$, $\omega_{k,\bar\mu}$ instead of $v_{k,\mu}$, $v_{k,\bar\mu}$.

$A_\mu^\zeta(z)$ is invertible as in (3.12) and (3.13), we propose now to construct its inverse in the class of h-pseudodifferential operators.

Denoting $U_0=1$ and extending the action of U_j to functions depending on x and y, we set for $j\in\{0,\ldots,j_0\}$,

$$\mathcal{U}_j=\begin{pmatrix}U_j & 0\\ 0 & 1\end{pmatrix} \text{ on } L^2([1/N,+\infty[\cdot[1,+\infty[\cdot w_j\times\mathbb{R}^{3p})\oplus(L^2(\mathbb{R}^{3n})^M,$$
$$A_{\mu,j}^\zeta(z)=\mathcal{U}_j\chi_jA_\mu^\zeta(z)\mathcal{U}_j^{-1}\chi_j, \tag{6.3}$$

which has a meaning thanks to (6.1).

By (5.7) (which extends to the case $j=0$) and the properties of the family $(\omega_{k,\mu})_{1\leqslant k\leqslant M}$, $A_{\mu,j}^\zeta(z)$ is a h-pseudodifferential operator with a $\mathcal{L}(H^2(\mathbb{R}^{3p})\oplus\mathbb{C}^M,L^2(\mathbb{R}^{3p})\oplus\mathbb{C}^M)$ valued symbol (see Refs. 12 and 20). Its principal symbol is given by

$$P_{\mu,j}^\xi(x,\xi;z)=\chi_j^2(x)\begin{pmatrix}t_\mu(\xi)+Q_{\mu,j}^\zeta(x)-z & R_{\mu,j}^-(x)\\ R_{\mu,j}^+(x) & 0\end{pmatrix}=\chi_j^2(x)\tilde P_{\mu,j}(x,\xi;z), \tag{6.4}$$

where $t_\mu(\xi)$ is the principal symbol of $-h^2U_\mu\Delta_xU_\mu^{-1}$, and $R_{\mu,j}^\pm(x)$ are defined as $R_\mu^\pm$ but with $\omega_{k,\mu}(x,.),\omega_{k,\bar\mu}(x,.)$ replaced by $U_j\omega_{k,\mu}(x,.),U_j\omega_{k,\bar\mu}(x,.)$, $1\leqslant k\leqslant M$.

Since $t_\mu(\xi)$ is elliptic and using the gap assumption (2.11), one can see that, for z close enough to λ_0 and for any $(x,\xi)\in T^*(\text{supp }\chi_j), j=0,\ldots,j_0, \tilde P_{\mu,j}(x,\xi;z)$ is invertible with inverse

$$q_{\mu,j}(x,\xi,z)=\begin{pmatrix} a^{\zeta}_{\mu,j}(x,\xi;z) & R^{-}_{\mu,j}(x) \\ R^{+}_{\mu,j}(x) & b_{\mu}(x,\xi;z)\end{pmatrix}. \tag{6.5}$$

Here $a^{\zeta}_{\mu,j}(x,\xi;z)=\hat{\pi}_{\mu,j}(x)[\hat{\pi}_{\mu,j}(x)(t_{\mu}(\xi)+Q^{\zeta}_{\mu,j}(x)-z)\hat{\pi}_{\mu,j}(x)]^{-1}\hat{\pi}_{\mu,j}(x)$, $\hat{\pi}_{\mu,j}(x)=1-\pi_{\mu,j}(x)$, $\pi_{\mu,j}(x)=U_j(x)\pi(x)U_j^{-1}(x)$, and $b_{\mu}(x,\xi;z)$ is the $M\times M$ matrix defined by

$$b_{\mu}(x,\xi;z)=z-(\langle\omega_{k,\mu}(x,y),(t_{\mu}(\xi)+Q^{\zeta}_{\mu}(x))\omega_{l,\bar{\mu}}(x,y)\rangle_{L^2(\mathbb{R}^{3p})}) \tag{6.6}$$

[in particular, $b_{\mu}(x,\xi;z)$ does not depend on j, if $M=1$ and $\mu=0$, then $t_{\mu}(\xi)=\xi^2$ and $b_{\mu}(x,\xi;z)=z-\xi^2-\langle\omega_1(x,y),Q^{\zeta}(x)\omega_1(x,y)\rangle_{L^2(\mathbb{R}^{3p})}$].

We set

$$B_{\mu}(z)=\sum_{j=0}^{j_0}\mathcal{U}_j^{-1}\chi_j^3(x)\mathrm{Op}(q_{\mu,j}(x,\xi,z))\mathcal{U}_j\chi_j(x) \tag{6.7}$$

[where Op is the usual quantification of symbols defined in (2.7)]. Using the composition theorem of h-pseudodifferential operators (see, e.g., Refs. 1, 16, and 22) we have

$$\begin{aligned} A^{\zeta}_{\mu}(z)B_{\mu}(z)&=1+hR_{\mu}(z),\\ R_{\mu}(z)&=\sum_{j=0}^{j_0}\mathcal{U}_j^{-1}\chi_{j,1}R_{\mu,j}(z)\mathcal{U}_j\chi_{j,1},\end{aligned} \tag{6.8}$$

where $\chi_{j,1}\in C_b^{\infty}(]1/N,+\infty[\cdot]1,+\infty[\cdot w_j)$ is supported in $[1/N,+\infty[\cdot[1,+\infty[\cdot w_{j,1}, w_{j,1}\subset\subset w_j$ for $j\geqslant 1$, $\chi_{0,1}$ is chosen as χ_0, and $R_{\mu,j}(z)$ is a h-pseudodifferential operator uniformly bounded (with respect to h) on $L^2(\mathbb{R}^{3(n+p)})\oplus(H^2(\mathbb{R}^{3n}))^M$.

From (6.8), we deduce

$$A^{\zeta}_{\mu}(z)^{-1}=B_{\mu}(z)\sum_{m=0}^{\infty}(-hR_{\mu}(z))^m. \tag{6.9}$$

Applying the calculus of Ref. 12, (6.9) can be written modulo $\mathcal{O}(h^{\infty})$:

$$A^{\zeta}_{\mu}(z)^{-1}=\sum_{j=0}^{j_0}\mathcal{U}_j^{-1}\tilde{\chi}_j\mathcal{E}_{\mu,j}(z)\mathcal{U}_j\tilde{\chi}_j, \tag{6.10}$$

where the $\mathcal{E}_{\mu,j}(z)$'s are h-pseudodifferential operators depending analytically on μ, $\tilde{\chi}_0$ is defined as χ_0 and $\tilde{\chi}_j\in C_b^{\infty}([1/N,+\infty[\cdot[1,+\infty[\cdot w_j)$ is supported in $]1/N,+\infty[\cdot]1,+\infty[\cdot\tilde{w}_j,\tilde{w}_j\subset\subset w_j, j\in\{1,\ldots,j_0\}$.

Denoting $A^{\zeta}_{\mu}(z)^{-1}$ as in (3.12), we obtain in particular from (6.10) that $a^{\zeta}_{\mu,-+}(z)$ is a $M\times M$ matrix of h-pseudodifferential operator on $\mathbb{R}^{3n}_x$. Moreover, in view of (6.6) and (6.10) and also Corollary 1.4 of Ref. 12, its principal symbol is just $b_{\mu}(x,\xi;z)$.

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Second order superintegrable systems in conformally flat spaces. III. Three-dimensional classical structure theory

E. G. Kalnins
Department of Mathematics and Statistics, University of Waikato, Hamilton, New Zealand

J. M. Kress
School of Mathematics, The University of New South Wales, Sydney NSW 2052, Australia

W. Miller, Jr.
School of Mathematics, University of Minnesota, Minneapolis, Minnesota 55455

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This paper is part of a series that lays the groundwork for a structure and classification theory of second-order superintegrable systems, both classical and quantum, in real or complex conformally flat spaces. Here we consider classical superintegrable systems with nondegenerate potentials in three dimensions. We show that there exists a standard structure for such systems, based on the algebra of 3×3 symmetric matrices, and that the quadratic algebra always closes at order 6. We show that the spaces of truly second-, third-, fourth-, and sixth-order constants of the motion are of dimension 6, 4, 21, and 56, respectively, and we construct explicit bases for the fourth- and sixth order constants in terms of products of the second order constants. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2037567]

I. INTRODUCTION AND EXAMPLES

The goal of this series of papers,[1,2] is a structure and classification theory of second-order superintegrable systems, both classical and quantum, in conformally flat spaces. An n-dimensional Riemannian space is conformally flat if and only if it admits a set of local coordinates $x_1,\ldots,x_n$ such that the contravariant metric tensor takes the form $g^{ij}=\delta^{ij}/\lambda(\mathbf{x})$. In other words, the metric is $ds^2=\lambda(\mathbf{x})(\Sigma_{i=1}^n dx_i^2)$. A classical superintegrable system $\mathcal{H}=\Sigma_{ij}g^{ij}p_ip_j+V(\mathbf{x})$ on the phase space of this manifold is one that admits $2n-1$ functionally independent generalized symmetries (or constants of the motion) $\mathcal{S}_k, k=1,\ldots,2n-1$ with $\mathcal{S}_1=\mathcal{H}$. That is, $\{\mathcal{H},\mathcal{S}_k\}=0$ where

$$\{f,g\}=\sum_{j=1}^{n}(\partial_{x_j}f\partial_{p_j}g-\partial_{p_j}f\partial_{x_j}g)$$

is the Poisson bracket for functions $f(\mathbf{x},\mathbf{p}),g(\mathbf{x},\mathbf{p})$ on phase space.[3–10] Note that $2n-1$ is the maximum possible number of functionally independent symmetries and, locally, such symmetries always exist. (In this paper $n=3$ so we have five functionally independent symmetries.) The main interest is in symmetries that are polynomials in the p_k and are globally defined, except for lower dimensional singularities such as poles and branch points. Many tools in the theory of Hamiltonian systems have been brought to bear on superintegrable perintegrable systems, such as R-matrix theory, Lax pairs, exact solvability, quasiexact solvability, and the Jacobi metric.[11–15] However, the most detailed and complete results are obtained from separation of variables methods in those cases where they are applicable. Standard orthogonal separation of variables techniques are associated with second-order symmetries, e.g., Refs. 16–21 and multiseparable Hamiltonian systems provide numerous examples of superintegrability. In these papers we concentrate on second-order

superintegrable systems, that is those in which the symmetries take the form $\mathcal{S}=\Sigma a^{ij}(\mathbf{x})p_ip_j+W(\mathbf{x})$, quadratic in the momenta.

There is an analogous definition for second-order quantum superintegrable systems with Schrödinger operator

$$H=\Delta+V(\mathbf{x}),\quad \Delta=\frac{1}{\sqrt{g}}\sum_{ij}\partial_{x_i}(\sqrt{g}g^{ij})\partial_{x_j},$$

the Laplace-Beltrami operator plus a potential function.[16] Here there are $2n-1$ second-order symmetry operators

$$S_k=\frac{1}{\sqrt{g}}\sum_{ij}\partial_{x_i}(\sqrt{g}a^{ij}_{(k)})\partial_{x_j}+W^{(k)}(\mathbf{x}),\quad k=1,\ldots,2n-1$$

with $S_1=H$ and $[H,S_k]\equiv HS_k-S_kH=0$. Again multiseparable systems yield many examples of superintegrability, though not all multiseparable systems are superintegrable and not all second-order superintegrable systems are multiseparable. There is also a quantization problem in extending the results for classical systems to operator systems. This problem turns out to be not difficult to solve for the nondegenerate systems that we study in this paper.

Superintegrable systems can (1) be solved explicitly, and (2) they can be solved in multiple ways. It is the information gleaned from comparing the distinct solutions and expressing one solution set in terms of another that is a primary reason for their interest.

We give a few simple three-dimensional (3D) examples to illustrate some of the main features of superintegrable systems. (To make clearer the connection with quantum theory and Hilbert space methods we shall, for these examples alone, adopt standard physical normalizations, such as using the factor $-\frac{1}{2}$ in front of the free Hamiltonian.) Consider the Schrödinger eigenvalue equation $H\Psi=E\Psi$ or ($\hbar=m=1, x_1=x, x_2=y, x_3=z$)

$$H\Psi=-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Psi+V(x,y,z)\Psi=E\Psi. \tag{1}$$

The generalized anisotropic oscillator corresponds to the four-parameter potential

$$V(x,y,z)=\frac{\omega^2}{2}(x^2+y^2+4(z+\rho)^2)+\frac{1}{2}\left[\frac{k_1^2-\frac{1}{4}}{x^2}+\frac{k_2^2-\frac{1}{4}}{y^2}\right]. \tag{2}$$

(This potential is "nondegenerate" in the precise sense that we will explain in Sec. III.) The corresponding Schrödinger equation has separable solutions in five coordinate systems, Cartesian coordinates, cylindrical polar coordinates, cylindrical elliptic coordinates, cylindrical parabolic coordinates, and parabolic coordinates. The energy eigenstates for this equation are degenerate and important special function identities arise by expanding one basis of separable eigenfunctions in terms of another. A second order symmetry operator for this equation is a second-order linear differential operator S such that $[H,S]=0$ where $[A,B]=AB-BA$. A basis for these operators is

$$M_1=\partial_x^2-\omega^2x^2+\frac{k_1^2-\frac{1}{4}}{x^2},\quad M_2=\partial_y^2-\omega^2y^2-\frac{k_2^2-\frac{1}{4}}{y^2}, \tag{3}$$

$$P=\partial_z^2-4\omega^2(z+\rho)^2,\quad L=L_{12}^2-\left(k_1^2-\frac{1}{4}\right)\frac{y^2}{x^2}-\left(k_2^2-\frac{1}{4}\right)\frac{x^2}{y^2}-\frac{1}{2}, \tag{4}$$

$$S_1=-\frac{1}{2}(\partial_xL_{13}+L_{13}\partial_x)+\rho\partial_x^2+(z+\rho)\left(\omega^2x^2-\frac{k_1^1-\frac{1}{4}}{x^2}\right),$$

$$S_2 = -\frac{1}{2}(\partial_y L_{23} + L_{23}\partial_y) + \rho\partial_y^2 + (z+\rho)\left(\omega^2 y^2 - \frac{k_2^2 - \frac{1}{4}}{y^2}\right), \tag{5}$$

where $L_{ij} = x_i\partial_{x_j} - x_j\partial_{x_i}$. Remarkably, these symmetries generate a "quadratic algebra" that closes at level six. Indeed, the nonzero commutators of the above basis are

$$[M_1, L] = [L, M_2] = Q, \quad [L, S_1] = [S_2, L] = B, \quad [M_i, S_i] = A_i, \quad [P, S_i] = -A_i.$$

Nonzero commutators of the basis symmetries with Q (fourth-order symmetries) are expressible in terms of the second-order symmetries,

$$[M_i, Q] = [Q, M_2] = 4\{M_1, M_2\} + 16\omega^2 L, \quad [S_1, Q] = [Q, S_2] = 4\{M_1, M_2\},$$

$$[L, Q] = 4\{M_1, L\} - 4\{M_2, L\} + 16(1 - k_1^2)M_1 - 16(1 - k_2^2)M_2.$$

There are similar expressions for commutators with B and the A_i. Also the squares of Q, B, A_i and products such as $\{Q, B\}$ (all sixth-order symmetries) are expressible in terms of second-order symmetries. For example,

$$Q^2 = \tfrac{8}{3}\{L, M_1, M_2\} + 8\omega^2\{L, L\} - 16(1 - k_1^2)M_1^2 - 16(1 - k_2^2)M_2^2 + \tfrac{64}{3}\{M_1, M_2\} - \tfrac{128}{3}\omega^2 L - 128\omega^2(1 - k_1^2)(1 - k_2^2),$$

$$\{Q, B\} = -\tfrac{8}{3}\{M_2, L, S_1\} - \tfrac{8}{3}\{M_1, L, S_2\} + 16(1 - k_1^2)\{M_2, S_2\} + 16(1 - k_2^2)\{M_1, S_1\} - \tfrac{64}{3}\{M_1, S_2\} - \tfrac{64}{3}\{M_2, S_1\}.$$

Here $\{C_1, \ldots, C_j\}$ is the completely symmetrized product of operators $C_1, \ldots, C_j$. (For complete details of all the possible products and commutators, see Ref. 22.) The point is that the algebra generated by products and commutators of the second order symmetries closes at order 6.

Another example in Euclidean space is given by the Schrödinger equation with three-parameter extended Kepler-Coulomb potential,

$$\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right) + \left[2E + \frac{2\alpha}{\sqrt{x^2 + y^2 + z^2}} - \left(\frac{k_1^2 - \frac{1}{4}}{x^2} + \frac{k_2^2 - \frac{1}{4}}{y^2}\right)\right]\Psi = 0.$$

This equation admits separable solutions in the four coordinates systems: spherical, sphero conical, prolate spheroidal, and parabolic coordinates. Again the bound states are degenerate and important special function identities arise by expanding one basis of separable eigenfunctions in terms of another. However, the space of second-order symmetries is only five dimensional and, although there are useful identities among the generators and commutators that enable one to derive spectral properties algebraically, there is no finite quadratic algebra structure. The key difference with our first example is, as we shall show later, that the three-parameter Kepler-Coulomb potential is degenerate and it cannot be extended to a four-parameter potential.

An example on the three-sphere is given by

$$g^{ij} = \delta_{ij} z_i - z_i z_j, \quad 1 \leqslant i, j \leqslant 3.$$

Then $\det(g^{ij}) = g^{-1} = z_1 z_2 z_3 (1 - z)$ where $z = z_1 + z_2 + z_3$ and

$$g_{ij} = \frac{1}{1 - z} + \frac{\delta_{ij}}{z_i}.$$

Thus $ds^2 = \Sigma_{i,j=1}^3 g_{ij}\, dz_i\, dz_j$. To identify this space we introduce Cartesian coordinates x_0, x_1, x_2, x_3 in four-dimensional Euclidean space and restrict these coordinates by the conditions

$$x_0^2 = 1 - z, \quad x_1^2 = z_1, \quad x_2^2 = z_2, \quad x_3^2 = z_3.$$

Note that $x_0^2+x_1^2+x_2^2+x_3^2=1$. Defining a metric ds^2 by $ds^2=\Sigma_{m=0}^3(dx_m)^2$ we find

$$ds^2 = \frac{1}{4}\sum_{i,j=1}^{3}\left(\frac{1}{1-z}+\frac{\delta_{ij}}{z_i}\right)dz_i\,dz_j.$$

Thus the space corresponds to a portion of the three-sphere S^n. The Schrödinger equation is

$$\left(\Delta + \sum_{i=1}^{3}\frac{\gamma_i}{z_i} + \frac{\gamma_4}{1-z}\right)\Psi = E\Psi,$$

where Δ is the Laplace-Beltrami operator. This is a nondegenerate potential. The six second-order operators

$$S_{ij} = 4z_iz_j(\partial_{z_i}-\partial_{z_j})^2 + 4(g_iz_j - g_jz_i)(\partial_{z_i}-\partial_{z_j}) = S_{ji}, \quad 1 \leqslant i < j \leqslant 3,$$

$$S_{0i} = 4z_i(1-z)\partial_{z_i}^2 + 4[g_i(1-z) - g_0z_i]\partial_{z_i} = S_{i0}, \quad 1 \leqslant i \leqslant 3,$$

for $g_i=1+\frac{1}{2}\sqrt{1-16\gamma_i}$ form a basis for the space of second-order symmetries. In particular

$$8H = \sum_{i,j=1}^{n} S_{ij} + 2\sum_{i=1}^{n} S_{0i}.$$

This equation separates in six coordinate systems on the three sphere. Further it can be shown that the quadratic algebra generated by the second-order symmetries closes at order 6.

For our last example we take the space with metric

$$ds^2 = \lambda(A,B,C,D,E,\mathbf{x})(dx^2+dy^2+dz^2),$$

where

$$\lambda = A(x+iy) + B\left(\frac{3}{4}(x+iy)^2 + \frac{z}{4}\right) + C\left((x+iy)^3 + \frac{1}{16}(x-iy) + \frac{3z}{4}(x+iy)\right)$$
$$+ D\left(\frac{5}{16}(x+iy)^4 + \tfrac{z^2}{16} + \tfrac{1}{16}(x^2+y^2) + \tfrac{3z}{8}(x+iy)^2\right) + E,$$

the nondegenerate potential is $V=\lambda(\alpha,\beta,\gamma,\delta,\epsilon,\mathbf{x})/\lambda(A,B,C,D,E,\mathbf{x})$. If $A=B=C=D=0$ this is a superintegrable system on complex Euclidean space. The quadratic algebra always closes, and for general values of A,B,C,D,E the space is not of constant curvature. This is an example of a superintegrable system that is Stäckel equivalent to a system on complex Euclidean space. We will take up the study of such systems in the next paper in this series.

Observed common features of superintegrable systems (and features that we make precise and verify in these papers) are that they are usually multiseparable and that the eigenfunctions of one separable system can be expanded in terms of the eigenfunctions of another. This is the source of nontrivial special function expansion theorems.[23] The symmetry operators are in formal self-adjoint form and suitable for spectral analysis. Also, the quadratic algebra identities allow us to relate eigenbases and eigenvalues of one symmetry operator to those of another. Indeed the representation theory of the abstract quadratic algebra can be used to derive spectral properties of the second-order generators in a manner analogous to the use of Lie algebra representation theory to derive spectral properties of quantum systems that admit Lie symmetry algebras.[23–26] (Note however that for superintegrable systems with nondegenerate potential, there is no first-order Lie symmetry.)

Another common feature of quantum superintegrable systems is that they can be modified by a gauge transformation so that the Schrödinger and symmetry operators are acting on a space of polynomials.[27] This is closely related to the theory of exactly and quasi exactly solvable systems.[13,28] The characterization of ODE quasiexactly solvable systems as embedded in PDE superintegrable systems provides considerable insight into the nature of these phenomena.

The classical analogs of the above examples are obtained by the replacements $\partial_{x_i} \to p_{x_i}$. Commutators go over to Poisson brackets. The operator symmetries become second-order constants of the motion. Symmetrized operators become products of functions. The quadratic algebra relations simplify, the highest order terms agree with the operator case but there are fewer nonzero lower order terms.

Many examples of 3D superintegrable systems are known, although they have not been classified.[29–34] Here, rather than focus on particular spaces and systems, we employ a theoretical method based on integrability conditions to derive structure common to all such systems, with a view to complete classification, at least for nondegenerate potentials. In this paper we consider classical superintegrable systems on a general 3D conformally flat spaces, real or complex, and uncover their common structure. We show that for systems with nondegenerate potentials there exists a standard structure based on the algebra of 3×3 symmetric matrices, and that the quadratic algebra closes at level 6. For two dimensional (2D) nondegenerate superintegrable systems we can show that the three functionally independent constants of the motion are (with one exception) also linearly independent, so at each regular point we can find a unique constant of the motion that matches a quadratic expression in the momenta at that point. However, for 3D systems we have only five functionally independent constants of the motion and the quadratic forms span a six-dimensional space. This is a major problem. However, for nondegenerate potentials we can prove the "5⇒6 Theorem" to show that the space of second-order constants of the motion is in fact six dimensional, there is a symmetry that is functionally dependent on the symmetries that arise from superintegrability, but linearly independent of them. With that result established, the treatment of the 3D case proceeds in analogy with the nondegenerate 2D case treated in Ref. 1. Though the details are quite complicated, we show that the spaces of truly second-, third-, fourth-, and sixth-order constants of the motion are of dimension 6, 4, 21, and 56, respectively. Finally we construct explicit bases for the fourth- and sixth-order constants in terms of products of the second-order constants. These bases are our principal result. They guarantee closure of the quadratic algebra and provide a means for analyzing its structure. This paper is a major advance toward one of our goals, to obtain a demonstrably complete list of 3D superintegrable potentials.

In the next paper in this series we will show that all 3D superintegrable systems with nondegenerate potential are multiseparable. We will study the Stäckel transform, or coupling constant metamorphosis,[35,36] for 3D classical superintegrable systems. This is a conformal transformation of a superintegrable system on one space to a superintegrable system on another space. We will prove that all nondegenerate 3D superintegrable systems are Stäckel transforms of constant curvature systems. We will also extend our results to the quantum analogs of 2D and 3D classical systems.

II. CONFORMALLY FLAT SPACES IN THREE DIMENSIONS

We assume that there is a coordinate system x,y,z and a nonzero function $\lambda(x,y,z) = \exp[G(x,y,z)]$ such that the Hamiltonian is

$$\mathcal{H} = \frac{p_1^2 + p_2^2 + p_3^2}{\lambda} + V(x,y,z). \tag{6}$$

A quadratic constant of the motion (or generalized symmetry)

$$\mathcal{S}=\sum_{k,j=1}^{3} a^{kj}(x,y,z)p_k p_j + W(x,y,z) \equiv \mathcal{L} + W, \quad a^{jk}=a^{kj} \tag{7}$$

must satisfy $\{\mathcal{H},\mathcal{S}\}=0$. The conditions are thus

$$a_i^{ii} = -G_1 a^{1i} - G_2 a^{2i} - G_3 a^{3i},$$

$$2a_i^{ij} + a_j^{ii} = -G_1 a^{1j} - G_2 a^{2j} - G_3 a^{3j}, \quad i \neq j,$$

$$a_k^{ij} + a_j^{ki} + a_i^{jk} = 0, \quad i,j,k \text{ distinct} \tag{8}$$

and

$$W_k = \lambda \sum_{s=1}^{3} a^{sk} V_s, \quad k=1,2,3. \tag{9}$$

(Here a subscript j denotes differentiation with respect to x_j.) The requirement that $\partial_{x_\ell} W_j = \partial_{x_j} W_\ell, \ell \neq j$ leads from (9) to the second-order Bertrand-Darboux partial differential equations for the potential,

$$\sum_{s=1}^{3} [V_{sj}\lambda a^{s\ell} - V_{s\ell}\lambda a^{sj} + V_s((\lambda a^{s\ell})_j - (\lambda a^{sj})_\ell)] = 0. \tag{10}$$

For second-order superintegrabilty in 3D there must be five functionally independent constants of the motion (including the Hamiltonian itself). Thus the Hamilton-Jacobi equation admits four additional constants of the motion

$$\mathcal{S}_h = \sum_{j,k=1}^{3} a_{(h)}^{jk} p_k p_j + W_{(h)} = \mathcal{L}_h + W_{(h)}, \quad h=1,\ldots,4. \tag{11}$$

We assume that the four functions $\mathcal{S}_h$ together with $\mathcal{H}$ are functionally independent in the six-dimensional phase space, i.e., that the differentials $d\mathcal{S}_h, d\mathcal{H}$ are linearly independent. (Here the possible V will always be assumed to form a vector space and we require functional independence for each such V and the associated $W^{(h)}$. This means that we also require that the five quadratic forms $\mathcal{L}_h, \mathcal{H}_0$ are functionally independent.) We say that the functions are weakly functionally independent if $d\mathcal{S}_h, d\mathcal{H}$ are linearly independent for nonzero potentials, but not necessarily for the zero potential.

III. FUNCTIONAL LINEAR INDEPENDENCE

We first shed some light on the relationship between functional independence and functional linear independence for the set $\{\mathcal{H},\mathcal{S}_1,\ldots,\mathcal{S}_4\}$

Theorem 1: *The functionally independent set* $\{\mathcal{H},\mathcal{S}_1,\ldots,\mathcal{S}_4\}$ *is also functionally linearly independent in the sense that if the relation* $\Sigma_{h=0}^{4} c^{(h)}(x)\mathcal{L}_h \equiv 0$ *holds in an open set, then* $c^{(h)}(x) \equiv 0$ *for all* h.

Proof: Suppose that the set is functionally linearly dependent. Then we can express one of the quadratic parts of the constants of the motion $\hat{\mathcal{L}}_0$ as a linear combination of a linearly independent subset $\{\hat{\mathcal{L}}_1,\ldots,\hat{\mathcal{L}}_r, 1 \leqslant r \leqslant 4\}$,

$$\hat{\mathcal{L}}_0 = \sum_{\ell=1}^{r} c^{(\ell)}(x)\hat{\mathcal{L}}_\ell.$$

Taking the Poisson bracket of both sides of this equation with $(p_1^2+p_2^2+p_3^3)/\lambda$ and using the fact that each of the $\hat{\mathcal{S}}_h$ is a constant of the motion, we obtain the identity

$$\sum_{\ell=1}^{r}\sum_{i,j=1}^{3} (\partial_{x_k} c^{(\ell)}) a^{ij}_{(\ell)} p_i p_j p_k = 0. \tag{12}$$

It is straightforward to check that this identity can be satisfied if and only if

$$\sum_{\ell=1}^{r} (\partial_{x_k} c^{(\ell)}) a^{ij}_{(\ell)} = 0, \quad 1 \leqslant i,j,k \leqslant 3.$$

Since the set $\{\hat{\mathcal{L}}_1,\ldots,\hat{\mathcal{L}}_r\}$, is linearly independent, we have $\partial_{x_k} c^{(\ell)} \equiv 0$ for $1 \leqslant k \leqslant 3, 1 \leqslant \ell \leqslant r$. Hence the $c^{(\ell)}$ are constants, which means that

$$\hat{\mathcal{L}}_0 - \sum_{\ell=1}^{r} c^{(\ell)}\hat{\mathcal{L}}_\ell = c,$$

where c is a constant. Thus the set $\{\mathcal{H}_0,\mathcal{L}_1,\ldots,\mathcal{L}_4\}$ is functionally dependent. This is a contradiction. Q.E.D.

Corollary 1: The weakly functionally independent set $\{\mathcal{H}=\mathcal{S}_0,\mathcal{S}_1,\ldots,\mathcal{S}_4\}$ *is also functionally linearly independent in the sense that if the relation* $\Sigma_{h=0}^4 c^{(h)}(x)\mathcal{S}_h \equiv 0$ *holds in an open set, then* $c^{(h)}(x) \equiv 0$ *for all* h.

Proof: Suppose that the set is functionally linearly dependent. Then we can express one of the constants of the motion $\hat{\mathcal{S}}_{0'}$ as a linear combination of a linearly independent subset $\{\hat{\mathcal{S}}_1,\ldots,\hat{\mathcal{L}}_r, 1 \leqslant r \leqslant 4\}$,

$$\hat{\mathcal{S}}_0 = \sum_{\ell=1}^{r} c^{(\ell)}(x)\hat{\mathcal{S}}_\ell.$$

Taking the Poisson bracket of both sides of this equation with $(p_1^2+p_2^2+p_3^3)/\lambda + V$ and using the fact that each of the $\hat{\mathcal{S}}_h$ is a constant of the motion, we obtain the identities

$$\sum_{\ell=1}^{r} (\partial_{x_k} c^{(\ell)}) a^{ij}_{(\ell)} = 0, \sum_{\ell=1}^{r} \partial_{x_k} c^{(\ell)} W_{(\ell)}, \quad 1 \leqslant i,j,k \leqslant 3.$$

Since the set $\{\hat{\mathcal{S}}_1,\ldots,\hat{\mathcal{S}}_r\}$, is functionally linearly independent, we have $\partial_{x_k} c^{(\ell)} \equiv 0$ for $1 \leqslant k \leqslant 3, 1 \leqslant \ell \leqslant r$. Hence the $c^{(\ell)}$ are constants, which means that

$$\hat{\mathcal{S}}_0 - \sum_{\ell=1}^{r} c^{(\ell)}\hat{\mathcal{S}}_\ell = 0.$$

Thus the set $\{\mathcal{S}_0,\ldots,\mathcal{S}_4\}$ is functionally dependent. This is a contradiction. Q.E.D.

We can write the system of Bertrand-Darboux equations in the matrix form $Cv = \tilde{v}^{(1)}V_1 + \tilde{v}^{(2)}V_2 + \tilde{v}^{(3)}V_3$, or

$$\begin{pmatrix} 0 & a^{12} & a^{11}-a^{22} & a^{31} & -a^{32} \\ a^{13} & 0 & -a^{23} & a^{21} & a^{11}-a^{33} \\ a^{32} & -a^{32} & -a^{13} & a^{22}-a^{33} & a^{12} \end{pmatrix} \begin{pmatrix} V_{33}-V_{11} \\ V_{22}-V_{11} \\ V_{12} \\ V_{32} \\ V_{31} \end{pmatrix}$$
$$= \frac{1}{\lambda}\begin{pmatrix} (\lambda a^{12})_1-(\lambda a^{11})_2 \\ (\lambda a^{31})_1-(\lambda a^{11})_3 \\ (\lambda a^{31})_2-(\lambda a^{21})_3 \end{pmatrix} V_1 + \frac{1}{\lambda}\begin{pmatrix} (\lambda a^{22})_1-(\lambda a^{21})_2 \\ (\lambda a^{32})_1-(\lambda a^{12})_3 \\ (\lambda a^{32})_2-(\lambda a^{22})_3 \end{pmatrix} V_2 + \frac{1}{\lambda}\begin{pmatrix} (\lambda a^{32})_1-(\lambda a^{31})_2 \\ (\lambda a^{33})_1-(\lambda a^{13})_3 \\ (\lambda a^{33})_2-(\lambda a^{23})_3 \end{pmatrix} V_3. \quad (13)$$

Corollary 2: Suppose the set $\{\mathcal{H},\mathcal{S}_1,\ldots,\mathcal{S}_4\}$ *is functionally independent. Then for general* x *the* 4×5 *matrix*

$$A = \begin{pmatrix} a^{33}_{(1)}-a^{11}_{(1)}, & a^{22}_{(1)}-a^{11}_{(1)}, & a^{12}_{(1)}, & a^{31}_{(1)}, & a^{32}_{(1)} \\ a^{33}_{(2)}-a^{11}_{(2)}, & a^{22}_{(2)}-a^{11}_{(2)}, & a^{12}_{(2)}, & a^{31}_{(2)}, & a^{32}_{(2)} \\ a^{33}_{(3)}-a^{11}_{(3)}, & a^{22}_{(3)}-a^{11}_{(3)}, & a^{12}_{(3)}, & a^{31}_{(3)}, & a^{32}_{(3)} \\ a^{33}_{(4)}-a^{11}_{(4)}, & a^{22}_{(4)}-a^{11}_{(4)}, & a^{12}_{(4)}, & a^{31}_{(4)}, & a^{32}_{(4)} \end{pmatrix}$$

has rank 4, *where the functions* $a^{ij}_{(h)}(\mathbf{x})$ *are given by* (11).

There are four sets of equations (13), one for each of the functionally independent symmetries (in addition to the Hamiltonian). We can write them as a single matrix equation $Bv=b$ where B is 12×5, b is 12×1 and

$$v = \begin{pmatrix} V_{33}-V_{11} \\ V_{22}-V_{11} \\ V_{12} \\ V_{32} \\ V_{31} \end{pmatrix}.$$

Lemma 1: If the set $\{\mathcal{H},\mathcal{S}_1,\ldots,\mathcal{S}_4\}$ *is functionally independent, the matrix* B *has rank* 5.

Proof: In the neighborhood of a general point (x_0,y_0,z_0) the matrix A of Corollary 2 has rank 4. Thus the possible reduced row equivalence forms (RREF) for A at (x_0,y_0,z_0) are

$$\text{I}\ \begin{pmatrix} 1, & 0, & 0, & 0, & \alpha \\ 0, & 1, & 0, & 0, & \beta \\ 0, & 0, & 1, & 0, & \gamma \\ 0, & 0, & 0, & 1, & \delta \end{pmatrix};\quad \text{II}\ \begin{pmatrix} 1, & 0, & 0, & \alpha, & 0 \\ 0, & 1, & 0, & \beta, & 0 \\ 0, & 0, & 1, & \gamma, & 0 \\ 0, & 0, & 0, & 0, & 1 \end{pmatrix};\quad \text{III}\ \begin{pmatrix} 1, & 0, & \alpha, & 0, & 0 \\ 0, & 1, & \beta, & 0, & 0 \\ 0, & 0, & 0, & 1, & 0 \\ 0, & 0, & 0, & 0, & 1 \end{pmatrix};$$

$$\text{IV}\ \begin{pmatrix} 1, & \alpha, & 0, & 0, & 0 \\ 0, & 0, & 1, & 0, & 0 \\ 0, & 0, & 0, & 1, & 0 \\ 0, & 0, & 0, & 0, & 1 \end{pmatrix};\quad \text{V}\ \begin{pmatrix} 0, & 1, & 0, & 0, & 0 \\ 0, & 0, & 1, & 0, & 0 \\ 0, & 0, & 0, & 1, & 0 \\ 0, & 0, & 0, & 0, & 1 \end{pmatrix}.$$

For each canonical form it is straightforward to check that the associated 12×5 matrix B has rank 5. Q.E.D.

By choosing a rank 5 minor of B we can solve for v and obtain a solution of the form

$$V_{22} = V_{11} + A^{22}V_1 + B^{22}V_2 + C^{22}V_3,$$

$$V_{33} = V_{11} + A^{33}V_1 + B^{33}V_2 + C^{33}V_3,$$

$$V_{12} = A^{12}V_1 + B^{12}V_2 + C^{12}V_3,$$

$$V_{13} = A^{13}V_1 + B^{13}V_2 + C^{13}V_3,$$

$$V_{23} = A^{23}V_1 + B^{23}V_2 + C^{23}V_3. \tag{14}$$

If the augmented matrix (B,b) has rank $r' > r$ then there will be $r'-r$ additional conditions of the form $D^1_{(s)}V_1 + D^2_{(s)}V_2 + D^3_{(s)}V_3 = 0, s = 1, \ldots, r'-r$. Here the $A^{ij}, B^{ij}, C^{ij}, D^i_{(s)}$ are functions of x that can be calculated explicitly. For convenience we take $A^{ij} \equiv A^{ji}, B^{ij} \equiv B^{ji}, C^{ij} \equiv C^{ji}$.

Suppose now that the superintegrable system is such that $r' = r$ so that relations (14) are equivalent to $Bv = b$. Further, suppose the integrability conditions for system (14) are satisfied identically. In this case we say that the potential is nondegenerate. Otherwise the potential is degenerate. If V is nondegenerate then at any point $\mathbf{x}_0$, where the A^{ij}, B^{ij}, C^{ij} are defined and analytic, there is a unique solution $V(\mathbf{x})$ arbitrarily prescribed values of $V_1(\mathbf{x}_0), V_2(\mathbf{x}_0), V_3(\mathbf{x}_0), V_{11}(\mathbf{x}_0)$ [as well as the value of $V(\mathbf{x}_0)$ itself]. The points $\mathbf{x}_0$ are called *regular*. The points of singularity for the A^{ij}, B^{ij}, C^{ij} form a manifold of dimension <3. Degenerate potentials depend on fewer parameters. For example, we could have $r' = r$ but the integrability conditions are not satisfied identically. This occurs for the generalized Kepler-Coulomb potential where the integrability conditions lead to an additional equation of the form $V_{11} = A^{11}V_1 + B^{11}V_2 + C^{11}V_3$ so that V_{11} cannot be prescribed arbitrarily.

From this point on we assume that V is nondegenerate. Substituting the requirement for a nondegenerate potential (14) into the Bertrand-Darboux equations (10) we obtain three equations for the derivatives a^{jk}_i, the first of which is

$$\begin{aligned}(a^{11}_3 - a^{31}_1)V_1 + (a^{12}_3 - a^{32}_1)V_2 + (a^{13}_3 - a^{33}_1)V_3 + a^{12}(A^{23}V_1 + B^{23}V_2 + C^{23}V_3) - (a^{33} - a^{11}) \\ \times (A^{13}V_1 + B^{13}V_2 + C^{13}V_3) - a^{23}(A^{12}V_1 + B^{12}V_2 + C^{12}V_3) + a^{13}(A^{33}V_1 + B^{33}V_2 + C^{33}V_3) \\ = (-G_3a^{11} + G_1a^{13})V_1 + (-G_3a^{12} + G_1a^{23})V_2 + (-G_3a^{13} + G_1a^{33})V_3,\end{aligned} \tag{15}$$

and the other two are obtained in a similar fashion.

Since V is nondegenerate we can compute all of the third partial derivatives of V. In fact, differentiating each of the equations (14) with respect to $x_j, j = 1, 2, 3$ we obtain 15 equations for the 10 distinct partial derivatives V_{ijk}. For example,

$$\begin{aligned}V_{123} = \partial_2 V_{13} &= A^{13}_2 V_1 + B^{13}_2 V_2 + C^{13}_2 V_3 + A^{13}V_{12} + B^{13}V_{22} + C^{13}V_{23} \\ &= \partial_1 V_{23} = A^{23}_1 V_1 + B^{23}_1 V_2 + C^{23}_1 V_3 + A^{23}V_{11} + B^{23}V_{12} + C^{23}V_{13} \\ &= \partial_3 V_{12} = A^{12}_3 V_1 + B^{12}_3 V_2 + C^{12}_3 V_3 + A^{12}V_{13} + B^{12}V_{23} + C^{12}V_{33},\end{aligned}$$

$$\begin{aligned}V_{111} &= (A^{12}_2 - A^{22}_1)V_1 + (B^{12}_2 - B^{22}_1)V_2 + (C^{12}_2 - C^{22}_1)V_3 - A^{22}V_{11} \\ &\quad + B^{12}V_{22} + (A^{12} - B^{22})V_{12} - C^{22}V_{13} + C^{12}V_{23} \\ &= (A^{13}_3 - A^{33}_1)V_1 + (B^{13}_3 - B^{33}_1)V_2 + (C^{13}_3 - C^{33}_1)V_3 - A^{33}V_{11} \\ &\quad + C^{13}V_{33} + (A^{13} - C^{33})V_{13} - B^{33}V_{12} + B^{13}V_{23},\end{aligned}$$

$$\begin{aligned}V_{223} = (A^{31}_1 + A^{22}_3)V_1 + (B^{31}_1 + B^{22}_3)V_2 + (C^{31}_1 + C^{22}_3)V_3 + A^{31}V_{11} + C^{22}V_{33} + B^{13}V_{21} + (C^{31} + A^{22})V_{13} \\ + B^{22}V_{23} = A^{23}_2 V_1 + B^{23}_2 V_2 + C^{23}_2 V_3 + A^{23}V_{12} + C^{23}V_{32} + B^{23}V_{22},\end{aligned}$$

$$V_{332} = (A_1^{12} + A_2^{33})V_1 + (B_1^{12} + B_3^{33})V_2 + (C_1^{12} + C_2^{33})V_3 + A^{12}V_{11} + B^{33}V_{22} + C^{12}V_{31} + (B^{12} + A^{33})V_{12}$$
$$+ C^{33}V_{23} = A_3^{23}V_1 + B_3^{23}V_2 + C_3^{23}V_3 + A^{23}V_{13} + B^{23}V_{23} + C^{23}V_{33}, \tag{16}$$

with analogous expressions for the other third derivatives. Similarly all higher order derivatives of V can be computed from these. The right-hand side of each of these equations can be expressed as an explicit linear combination of V_1, V_2, V_3, V_{11} with analytic functions of x_1, x_2, x_3 as coefficients. Thus if the potential V belongs to the solution space then V can depend on at most four parameters, in addition to a trivial additive constant. We can choose these parameters to be $V_1(x_0, y_0, z_0), V_2(x_0, y_0, z_0), V_3(x_0, y_0, z_0), V_{11}(x_0, y_0, z_0)$ for any fixed regular point (x_0, y_0, z_0). Then all higher derivatives can be computed by successive differentiation of relations (14). Thus our potential is nondegenerate, i.e., it depends non trivially on these four arbitrary parameters, so that *all* higher-order integrability conditions are satisfied.

Then, equating coefficients of V_1, V_2, V_3, V_{11} on each side of the conditions $\partial_1 V_{23} = \partial_2 V_{13} = \partial_3 V_{12}, \partial_3 V_{23} = \partial_2 V_{33}$, etc., we obtain integrability conditions, the simplest of which include

$$A^{23} = B^{13} = C^{12}, \quad B^{12} - A^{22} = C^{13} - A^{33},$$

$$B^{23} = A^{31} + C^{22}, \quad C^{23} = A^{12} + B^{33},$$

$$A_1^{12} + B^{12}A^{12} + A_2^{33} + A^{33}A^{12} + B^{33}A^{22} + C^{33}A^{23} = A_3^{23} + B^{23}A^{23} + C^{23}A^{33},$$

$$A_2^{13} + A^{13}A^{12} + B^{13}A^{22} + C^{13}A^{23} = A_1^{23} + B^{23}A^{12} + C^{23}A^{13} = A_3^{12} + A^{13}A^{12} + B^{12}A^{23} + C^{12}A^{33}. \tag{17}$$

All of these conditions, analytic expressions in x, y, z, must hold identically in a common domain to have a nondegenerate system. Note that if $r' > r$ then there will be conditions relating the parameters $V_1(x_0, y_0, z_0), V_2(x_0, y_0, z_0), V_3(x_0, y_0, z_0), V_{11}(x_0, y_0, z_0)$, so we cannot have a nondegenerate system in that case.

We can further clarify the situation by introducing the dependent variables $W^{(1)} = V_1, W^{(2)} = V_2, W^{(3)} = V_3, W^{(4)} = V_{11}$, the vector

$$\mathbf{w} = \begin{pmatrix} W^{(1)} \\ W^{(2)} \\ W^{(3)} \\ W^{(4)} \end{pmatrix}, \tag{18}$$

and the matrices

$$\mathbf{A}^{(1)} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ A^{12} & B^{12} & C^{12} & 0 \\ A^{13} & B^{13} & C^{13} & 0 \\ A^{14} & B^{14} & C^{14} & B^{12} - A^{22} \end{pmatrix}, \tag{19}$$

$$\mathbf{A}^{(2)} = \begin{pmatrix} A^{12} & B^{12} & C^{12} & 0 \\ A^{22} & B^{22} & C^{22} & 1 \\ A^{23} & B^{23} & C^{23} & 0 \\ A^{24} & B^{24} & C^{24} & A^{12} \end{pmatrix}, \tag{20}$$

$$\mathbf{A}^{(3)} = \begin{pmatrix} A^{13} & B^{13} & C^{13} & 0 \\ A^{23} & B^{23} & C^{23} & 0 \\ A^{33} & B^{33} & C^{33} & 1 \\ A^{34} & B^{34} & C^{34} & A^{13} \end{pmatrix}, \tag{21}$$

where

$$\begin{aligned} A^{14} &= A_2^{12} - A_1^{22} + B^{12}A^{22} + A^{12}A^{12} - B^{22}A^{12} - C^{22}A^{13} + C^{12}A^{23} \\ &= A_3^{13} - A_1^{33} + B^{13}A^{23} + A^{13}A^{13} - B^{33}A^{12} - C^{33}A^{13} + C^{13}A^{33}, \end{aligned}$$

$$\begin{aligned} B^{14} &= B_2^{12} - B_1^{22} + B^{12}B^{22} + A^{12}B^{12} - B^{22}B^{12} - C^{22}B^{13} + C^{12}B^{23} \\ &= B_3^{13} - B_1^{33} + B^{13}B^{23} + A^{13}B^{13} - B^{33}B^{12} - C^{33}B^{13} + C^{13}B^{33}, \end{aligned}$$

$$\begin{aligned} C^{14} &= C_2^{12} - C_1^{22} + B^{12}C^{22} + A^{12}C^{12} - B^{22}C^{12} - C^{22}C^{13} + C^{12}C^{23} \\ &= C_3^{13} - C_1^{33} + B^{13}C^{23} + A^{13}C^{13} - B^{23}C^{12} - C^{33}C^{13} + C^{13}C^{33}, \end{aligned}$$

$$A^{24} = A_1^{12} + B^{12}A^{12} + C^{12}A^{13}, \quad B^{24} = B_1^{12} + B^{12}B^{12} + C^{12}B^{13},$$

$$C^{24} = C_1^{12} + B^{12}C^{12} + C^{12}C^{13},$$

$$A^{34} = A_1^{13} + B^{13}A^{12} + C^{13}A^{13}, \quad B^{34} = B_1^{13} + B^{13}B^{12} + C^{13}B^{13},$$

$$C^{34} = C_1^{13} + B^{13}C^{12} + C^{13}C^{13}. \tag{22}$$

Then the conditions (17) must hold as well as the integrability conditions for the system

$$\partial_{x_j}\mathbf{w} = \mathbf{A}^{(j)}\mathbf{w}, \quad j = 1,2,3. \tag{23}$$

The integrability conditions are

$$A_i^{(j)} - A_j^{(i)} = A^{(i)}A^{(j)} - A^{(j)}A^{(i)} \equiv [A^{(i)}, A^{(j)}]. \tag{24}$$

The integrability conditions (17) and (24) are analytic expressions in x_1, x_2, x_3 and must hold identically. Then the system has a solution V depending on four parameters (plus an arbitrary additive parameter). For convenience in the arguments to follow we set

$$\mathcal{U}^1 = A_2^{(3)} - A_3^{(2)} - [A^{(2)}, A^{(3)}], \quad \mathcal{U}^2 = A_3^{(1)} - A_1^{(3)} - [A^{(3)}, A^{(1)}],$$

$$\mathcal{U}^3 = A_1^{(2)} - A_2^{(1)} - [A^{(1)}, A^{(2)}], \tag{25}$$

so that the identities are

$$\mathcal{U}^1 = \mathcal{U}^2 = \mathcal{U}^3 = 0. \tag{26}$$

We have shown that a weakly functionally independent set of five symmetries (or constants of the motion) is functionally linearly independent. For systems with nondegenerate potentials, the converse holds.

Theorem 2: *Let*

$$\mathcal{S}_h = \sum_{j,k=1}^{3} a_{(h)}^{jk} p_k p_j + W_{(h)}, \quad h = 1, \ldots, 5, \quad \mathcal{H} = \mathcal{S}_1$$

be functionally linearly independent symmetries for a system with nondegenerate potential $V = W_{(1)}$. *Then these symmetries are weakly functionally independent.*

Proof: By assumption, the set $\{\mathcal{S}_h\}$ is functionally linearly independent. Suppose it is also functionally dependent. This means that the set of differentials $\{\mathrm{d}\mathcal{S}_h\}$ is dependent, i.e., that the 5×6 matrix

$$\begin{pmatrix} \sum_i a^{i1}_{(1)}p_i & \sum_i a^{i2}_{(1)}p_i & \sum_i a^{i3}_{(1)}p_i & K_{14}+\sum_i a^{j1}_{(1)}V_j & K_{15}+\sum_i a^{j2}_{(1)}V_j & K_{16}+\sum_i a^{j3}_{(1)}V_j \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum_i a^{i1}_{(5)}p_i & \sum_i a^{i2}_{(5)}p_i & \sum_i a^{i3}_{(5)}p_i & K_{54}+\sum_i a^{j1}_{(5)}V_j & K_{55}+\sum_i a^{j2}_{(5)}V_j & K_{56}+\sum_i a^{j3}_{(5)}V_j \end{pmatrix},$$

where

$$K_{\ell,3+s} = \sum_{ij} a^{ij}_{(\ell),s}p_i p_j,$$

is of rank <5 for all values of p_j, V_j. Thus all 5×5 minors must vanish identically in p_j, V_j. It is an easy consequence of this that all 5×5 minors of the 5×6 matrix

$$\begin{pmatrix} a^{11}_{(1)} & a^{12}_{(1)} & a^{13}_{(1)} & a^{22}_{(1)} & a^{23}_{(1)} & a^{33}_{(1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a^{11}_{(5)} & a^{12}_{(5)} & a^{13}_{(5)} & a^{22}_{(5)} & a^{23}_{(5)} & a^{33}_{(5)} \end{pmatrix}$$

vanish, hence that this matrix have rank <5. Thus $\{\mathcal{L}_h : h=1,\ldots,5\}$ is functionally linearly dependent. Contradiction. Q.E.D.

Since (as we assume) the potential is nondegenerate, at any regular point $\mathbf{x}_0$ the first derivatives V_1, V_2, V_3 can be chosen arbitrarily. Thus the coefficients of V_j on both sides of equation (13) must be equal. From this, we obtain the relations

$$a^{11}_3 - a^{31}_1 = -a^{12}A^{23} + (a^{33}-a^{11})A^{13} + a^{23}A^{12} - a^{13}A^{33} - G_3a^{11} + G_1a^{13},$$

$$a^{12}_3 - a^{32}_1 = -a^{12}B^{23} + (a^{33}-a^{11})B^{13} + a^{23}B^{12} - a^{13}B^{33} - G_3a^{12} + G_1a^{23},$$

$$a^{13}_3 - a^{33}_1 = -a^{12}C^{23} + (a^{33}-a^{11})C^{13} + a^{23}C^{12} - a^{13}C^{33} - G_3a^{13} + G_1a^{33},$$

with six analogous relations from the other two Bertrand-Darboux equations. Using these nine relations and Eqs. (8) we can solve for all of the first partial derivatives a^{jk}_i to obtain

$$a^{11}_1 = -G_1a^{11} - G_2a^{12} - G_3a^{13},$$

$$a^{22}_2 = -G_1a^{12} - G_2a^{22} - G_3a^{23},$$

$$a^{33}_3 = -G_1a^{13} - G_2a^{23} - G_3a^{33},$$

$$3a^{12}_2 = a^{12}A^{22} - (a^{22}-a^{11})A^{12} - a^{23}A^{13} + a^{13}A^{23} + G_2a^{11} - 2G_1a^{12} - G_2a^{22} - G_3a^{23},$$

$$3a^{11}_2 = -2a^{12}A^{22} + 2(a^{22}-a^{11})A^{12} + 2a^{23}A^{13} - 2a^{13}A^{23} - 2G_2a^{11} + G_1a^{12} - G_2a^{22} - G_3a^{23},$$

$$3a^{13}_3 = -a^{12}C^{23} + (a^{33}-a^{11})C^{13} + a^{23}C^{12} - a^{13}C^{33} - G_1a^{11} - G_2a^{12} - 2G_3a^{13} + G_1a^{33},$$

$$3a^{33}_1 = 2a^{12}C^{23} - 2(a^{33}-a^{11})C^{13} - 2a^{23}C^{12} + 2a^{13}C^{33} - G_1a^{11} - G_2a^{12} + G_3a^{13} - 2G_1a^{33},$$

$$3a_2^{23} = a^{23}(B^{33} - B^{22}) - (a^{33} - a^{22})B^{23} - a^{13}B^{12} + a^{12}B^{13} - G_1a^{13} - 2G_2a^{23} - G_3a^{33} + G_3a^{22},$$

$$3a_3^{22} = -2a^{23}(B^{33} - B^{22}) + 2(a^{33} - a^{22})B^{23} + 2a^{13}B^{12} - 2a^{12}B^{13} - G_1a^{13} + G_2a^{23} - G_3a^{33} - 2G_3a^{22},$$

$$3a_1^{13} = -a^{23}A^{12} + (a^{11} - a^{33})A^{13} + a^{13}A^{33} + a^{12}A^{23} - 2G_1a^{13} - G_2a^{23} - G_3a^{33} + G_3a^{11},$$

$$3a_3^{11} = 2a^{23}A^{12} + 2(a^{33} - a^{11})A^{13} - 2a^{13}A^{33} - 2a^{12}A^{23} + G_1a^{13} - G_2a^{23} - G_3a^{33} - 2G_3a^{11},$$

$$3a_2^{33} = -2a^{13}C^{12} + 2(a^{22} - a^{33})C^{23} + 2a^{12}C^{13} - 2a^{23}(C^{22} - C^{33}) - G_1a^{12} - G_2a^{22} + G_3a^{23} - 2G_2a^{33},$$

$$3a_3^{23} = a^{13}C^{12} - (a^{22} - a^{33})C^{23} - a^{12}C^{13} - a^{23}(C^{33} - C^{22}) - G_1a^{12} - G_2a^{22} - 2G_3a^{23} + G_2a^{33},$$

$$3a_2^{12} = -a^{13}B^{23} + (a^{22} - a^{11})B^{12} - a^{12}B^{22} + a^{23}B^{13} - G_1a^{11} - 2G_2a^{12} - G_3a^{13} + G_1a^{22},$$

$$3a_1^{22} = 2a^{13}B^{23} - 2(a^{22} - a^{11})B^{12} + 2a^{12}B^{22} - 2a^{23}B^{13} - G_1a^{11} + G_2a^{12} - G_3a^{13} - 2G_1a^{22},$$

$$\begin{aligned}3a_1^{23} = {} & a^{12}(B^{23} + C^{22}) + a^{11}(B^{13} + C^{12}) - a^{22}C^{12} - a^{33}B^{13} + a^{13}(B^{33} + C^{23}) - a^{23}(C^{13} + B^{12}) \\ & - 2G_1a^{23} + G_2a^{13} + G_3a^{12},\end{aligned}$$

$$\begin{aligned}3a_3^{12} = {} & a^{12}(-2B^{23} + C^{22}) + a^{11}(C^{12} - 2B^{13}) - a^{22}C^{12} + 2a^{33}B^{13} + a^{13}(-2B^{33} + C^{23}) \\ & + a^{23}(-C^{13} + 2B^{12}) - 2G_3a^{12} + G_2a^{13} + G_1a^{23},\end{aligned}$$

$$\begin{aligned}3a_2^{13} = {} & a^{12}(B^{23} - 2C^{22}) + a^{11}(B^{13} - 2C^{12}) + 2a^{22}C^{12} - a^{33}B^{13} + a^{13}(B^{33} - 2C^{23}) + a^{23}(2C^{13} - B^{12}) \\ & - 2G_2a^{13} + G_1a^{23} + G_3a^{12},\end{aligned} \tag{27}$$

plus the linear relations

$$A^{23} = B^{13} = C^{12}, \quad B^{23} - A^{13} - C^{22} = 0,$$

$$B^{12} - A^{22} + A^{33} - C^{13} = 0, \quad B^{33} + A^{12} - C^{23} = 0.$$

Using the linear relations we can express $C^{12}, C^{13}, C^{22}, C^{23}$, and B^{13} in terms of the remaining 10 functions.

Since the above system of first-order partial differential equations is involutive the general solution for the six functions a^{jk} can depend on at most six parameters, the values $a^{jk}(\mathbf{x}_0)$ at a fixed regular point $\mathbf{x}_0$. For the integrability conditions we define the vector-valued function

$$\mathbf{h}(x,y,z) = \begin{pmatrix} a^{11} \\ a^{12} \\ a^{13} \\ a^{22} \\ a^{23} \\ a^{33} \end{pmatrix}$$

and directly compute the 6×6 matrix functions $\mathcal{A}^{(j)}$ to get the first-order system

$$\partial_{x_j}\mathbf{h} = \mathcal{A}^{(j)}\mathbf{h}, \quad j = 1,2,3. \tag{28}$$

The integrability conditions for this system are are

$$\mathcal{A}_i^{(j)}\mathbf{h} - \mathcal{A}_j^{(i)}\mathbf{h} = \mathcal{A}^{(i)}\mathcal{A}^{(j)}\mathbf{h} - \mathcal{A}^{(j)}\mathcal{A}^{(i)}\mathbf{h} \equiv [\mathcal{A}^{(i)}, \mathcal{A}^{(j)}]\mathbf{h}. \tag{29}$$

In terms of the 6×6 matrices

$$\mathcal{S}^{(1)} = \mathcal{A}_2^{(3)} - \mathcal{A}_3^{(2)} - [\mathcal{A}^{(2)}, \mathcal{A}^{(3)}], \quad \mathcal{S}^{(2)} = \mathcal{A}_3^{(1)} - \mathcal{A}_1^{(3)} - [\mathcal{A}^{(3)}, \mathcal{A}^{(1)}],$$

$$\mathcal{S}^{(3)} = \mathcal{A}_1^{(2)} - \mathcal{A}_2^{(1)} - [\mathcal{A}^{(1)}, \mathcal{A}^{(2)}],$$

the integrabilty conditions are

$$\mathcal{S}^{(1)}\mathbf{h} = \mathcal{S}^{(2)}\mathbf{h} = \mathcal{S}^{(3)}\mathbf{h} = 0. \tag{30}$$

IV. THE 5⇒6 THEOREM

Now assume that the system of equations (27) admits a six-parameter family of solutions a^{jk}. (The requirement of superintegrability appears to guarantee only a five-parameter family of solutions.) Thus at any regular point we can prescribe the values of the a^{jk} arbitrarily. This means that (29) and (30) holds identically in $\mathbf{h}$. Thus $\mathcal{S}^{(1)}=\mathcal{S}^{(2)}=\mathcal{S}^{(3)}=0$. Using these expressions, we can perform a tedious but straightforward Maple-assisted computation that yields

(1) An expression for each of the first partial derivatives $\partial_\ell A^{ij}, \partial_\ell B^{ij}, \partial_\ell C^{ij}$, for the 10 independent functions as homogeneous polynomials of order at most two in the $A^{i'j'}, B^{i'j'}, C^{i'j'}$. There are $30=3\times 10$ such expressions in all. An example is

$$B_2^{12} = \tfrac{2}{3}A^{12}B^{12} - \tfrac{1}{6}B^{12}G_2 - \tfrac{5}{6}G_1A^{12} - \tfrac{1}{6}G_1G_2 + \tfrac{1}{3}B^{22}B^{12} + \tfrac{1}{3}B^{22}G_1 + \tfrac{1}{3}A^{23}B^{23} - \tfrac{7}{6}G_3A^{23} + \tfrac{1}{2}G_{12}.$$

(2) Exactly five quadratic identities for the 10 independent functions,

(a)

$$-A^{23}B^{33} - A^{12}A^{23} + A^{13}B^{12} + B^{22}A^{23} + B^{23}A^{33} + \tfrac{1}{2}A^{22}G_3 - \tfrac{1}{2}A^{33}G_3 - \tfrac{1}{2}B^{12}G_3 - \tfrac{1}{2}G_1G_3 - \tfrac{1}{2}A^{13}G_1 + \tfrac{3}{2}G_{13} - \tfrac{1}{2}A^{23}G_2 - A^{22}B^{23} = 0,$$

(b)

$$(A^{33})^2 + B^{12}A^{33} - A^{33}A^{22} - B^{33}A^{12} - C^{33}A^{13} + B^{22}A^{12} - B^{12}A^{22} + A^{13}B^{23} - (A^{12})^2 + \tfrac{3}{2}G_{22} - \tfrac{1}{2}G_y^2 - \tfrac{3}{2}G_{33} + \tfrac{1}{2}A^{13}G_3 + \tfrac{1}{2}B^{33}G_2 - \tfrac{1}{2}A^{22}G_1 + \tfrac{1}{2}A^{33}G_1 - \tfrac{1}{2}B^{23}G_3 - \tfrac{1}{2}B^{22}G_2 + \tfrac{1}{2}C^{33}G_3 + \tfrac{1}{2}(G_3)^2 = 0,$$

(c)

$$-(B^{33})^2 - B^{33}A^{12} + B^{33}B^{22} + B^{12}A^{33} + B^{23}C^{33} - (B^{23})^2 + (B^{12})^2 + \tfrac{1}{2}(G_1)^2 - \tfrac{3}{2}G_{11} + \tfrac{3}{2}G_{33} - \tfrac{1}{2}B^{33}G_2 - \tfrac{1}{2}A^{33}G_1 - \tfrac{1}{2}(G_3)^2 - \tfrac{1}{2}C^{33}G_3 = 0, \tag{31}$$

(d)

$$-B^{12}A^{23} - A^{33}A^{23} + A^{13}B^{33} + A^{12}B^{23} + \tfrac{3}{2}G_{23} - \tfrac{1}{2}A^{23}G_1 - \tfrac{1}{2}A^{12}G_3 - \tfrac{1}{2}B^{23}G_2 - \tfrac{1}{2}G_2G_3 - \tfrac{1}{2}B^{33}Ga_3 = 0,$$

(e)

$$A^{12}B^{12} + C^{33}A^{23} - A^{23}B^{23} + B^{33}A^{22} - B^{33}A^{33} + \tfrac{3}{2}G_{12} - \tfrac{1}{2}G_1G_2 - \tfrac{1}{2}A^{12}G_1 - \tfrac{1}{2}B^{12}G_2 - \tfrac{1}{2}A^{23}G_3 = 0,$$

There are no nontrivial conditions in which some derivative of G is involved as a factor in each term.

Theorem 3 (5 → 6): *Let V be a nondegenerate potential corresponding to a conformally flat space in three dimensions that is superintegrable, i.e., suppose V satisfies the equations (14), where conditions (17) and (24) hold, and there are five functionally independent constants of the motion. Then the space of second-order symmetries for the Hamiltonian $\mathcal{H}=(p_x^2+p_y^2+p_z^2)/\lambda(x,y,z)+V(x,y,z)$ (excluding multiplication by a constant) is of dimension $D=6$.*

Corollary 3: If $\mathcal{H}+V$ is a superintegrable conformally flat system with nondegenerate potential, then the dimension of the space of second-order symmetries

$$\mathcal{S}=\sum_{k,j=1}^{3} a^{kj}(x,y,z)p_kp_j+W(x,y,z)$$

is 6. At any regular point (x_0,y_0,z_0) and given constants $\alpha^{kj}=\alpha^{jk}$ there is exactly one symmetry $\mathcal{S}$ (up to an additive constant) such that $a^{kj}(x_0,y_0,z_0)=\alpha^{kj}$. Given a set of five functionally independent second-order symmetries $\mathcal{L}=\{\mathcal{S}_\ell:\ell=1,\ldots,5\}$ associated with the potential, there is always a sixth second-order symmetry $\mathcal{S}_6$ that is functionally dependent on $\mathcal{L}$, but functionally linearly independent.

Corollary 4: The previous theorem and corollary remain true for five weakly functionally independent second-order symmetries, if the corresponding quadratic forms $\Sigma_{k,j}a_{(\ell)}^{kj}p_kp_j, 1\leqslant\ell\leqslant 5$ are functionally linearly independent.

Proof of theorem: The proof takes many steps, most of which must be carried out with computer algebra software. We give the logic behind the proof and describe the steps in order.

If there is only a five-parameter family of solutions then (30) holds only for the $\boldsymbol{h}$ that lie in a five-dimensional space. By appropriate Euclidean transformation of coordinates, if necessary, we use Gauss-Jordan elimination and show that there is a basis for the space of the form $\tilde{\mathbf{h}}^j, j=1,\ldots,5$ where

$$(\tilde{\mathbf{h}}^1,\tilde{\mathbf{h}}^2,\tilde{\mathbf{h}}^3,\tilde{\mathbf{h}}^4,\tilde{\mathbf{h}}^5)=\begin{pmatrix}1&0&0&0&0\\0&1&0&0&0\\0&0&1&0&0\\0&0&0&1&0\\0&0&0&0&1\\\alpha_1(x,y,z)&\alpha_2(x,y,z)&\alpha_3(x,y,z)&\alpha_4(x,y,z)&\alpha_5(x,y,z)\end{pmatrix}.$$

Here we mean that if $\mathbf{h}$ belongs to the solution space then there are unique differentiable functions $g_j(x,y,z)$ such that $\mathbf{h}=\Sigma_{j=1}^5 g_j\tilde{\mathbf{h}}^j$. It follows that the integrabilty conditions become

$$\mathcal{S}_{kj}^{(\ell)}+\alpha_j\mathcal{S}_{k6}^{(\ell)}=0,\quad \ell=1,\ldots,3,\quad k=1,\ldots,6,\quad j=1,\ldots,5. \tag{32}$$

Further, the conditions (30) must hold. The question that we need to decide is whether the conditions (30) and (32) imply

$$\mathcal{S}^{(1)}=\mathcal{S}^{(2)}=\mathcal{S}^{(3)}=0.$$

Some of the elements of the matrices $\mathcal{S}^{(i)}$ vanish identically. Indeed

$$\mathcal{S}_{16}^{(1)}=\mathcal{S}_{26}^{(1)}=\mathcal{S}_{46}^{(1)}=\mathcal{S}_{14}^{(2)}=\mathcal{S}_{34}^{(2)}=\mathcal{S}_{64}^{(2)}=\mathcal{S}_{41}^{(3)}=\mathcal{S}_{51}^{(3)}=\mathcal{S}_{61}^{(3)}\equiv 0.$$

Also

$$\mathcal{S}_{16}^{(2)}\equiv\mathcal{S}_{15}^{(1)}\equiv-\mathcal{S}_{11}^{(2)},\quad \mathcal{S}_{54}^{(1)}\equiv-\mathcal{S}_{23}^{(1)},$$

$$\mathcal{S}_{25}^{(1)}\equiv-\mathcal{S}_{31}^{(1)},\quad \mathcal{S}_{34}^{(1)}\equiv\mathcal{S}_{26}^{(2)},\quad 3\mathcal{S}_{11}^{(3)}\equiv 2\mathcal{S}_{11}^{(1)},$$

$$\mathcal{S}_{44}^{(2)} \equiv -\tfrac{2}{3}\mathcal{S}_{22}^{(2)}, \quad \mathcal{S}_{46}^{(3)} \equiv -\mathcal{S}_{43}^{(1)}.$$

This implies that the following conditions must hold no matter what are the values of the α_j:

$$\mathcal{S}_{ij}^{(1)} = 0, \quad i = 1,2,4,6, \quad 1 \leqslant j \leqslant 6, \quad \mathcal{S}_{31}^{(1)} = 0, \tag{33}$$

$$\mathcal{S}_{1j}^{(2)} = \mathcal{S}_{4j}^{(3)} = 0, \quad 1 \leqslant j \leqslant 6, \quad \mathcal{S}_{54}^{(1)} = 0, \quad \mathcal{S}_{44}^{(2)} = 0.$$

We will show that the identities (33), plus the identities (26) (that must always hold) suffice to prove that

$$\mathcal{S}^{(1)} = \mathcal{S}^{(2)} = \mathcal{S}^{(3)} = 0,$$

hence that the integrabilty conditions are satisfied identically and there is a six-parameter family of symmetries. In the first step we compute all of the identities (26) and (33) and use a subset of 17 of the identities (33) and 12 of the identities (26) to solve for each of the 30 independent partial derivatives

$$\partial_k A^{12}, \quad \partial_k A^{13}, \quad \partial_k A^{22}, \quad \partial_k A^{23}, \quad \partial_k A^{33}, \quad \partial_k B^{12}, \quad \partial_k B^{22}, \quad \partial_k B^{23}, \quad \partial_k B^{33}, \quad \partial_k C^{33}, \quad k = 1,2,3,$$

save $\partial_z C^{33}$ which does not occur in these expressions. In each case we obtain an expression for the derivative as a polynomial in the 10 variables $A^{12},\ldots,C^{33}$ with coefficients in the linear and zero-order terms that involve derivatives of G. Then we substitute these expressions back into the remaining conditions (26) and (33). This yields a set of four independent second-order polynomial identities, a subset of the identities (31). These identities are sufficient to verify that

$$\mathcal{S}_{36}^{(1)} = \mathcal{S}_{56}^{(1)} = \mathcal{S}_{26}^{(2)} = \mathcal{S}_{36}^{(2)} = \mathcal{S}_{46}^{(2)} = 0.$$

By conditions (32) this immediately implies $\mathcal{S}^{(1)}=0$, and $\mathcal{S}_{jk}^{(2)}=0$ for $j=2$, 3, 4 and $1\leqslant k\leqslant 6$. Substituting our expressions for the derivatives into these identities we obtain the full set of five identities (31), and can solve for $\partial_x C^{33}$. This set is now sufficient to verify that

$$\mathcal{S}_{56}^{(2)} = \mathcal{S}_{66}^{(2)} = \mathcal{S}_{16}^{(3)} = \mathcal{S}_{26}^{(3)} = \mathcal{S}_{36}^{(3)} = \mathcal{S}_{56}^{(3)} = \mathcal{S}_{66}^{(3)} = 0,$$

which implies $\mathcal{S}^{(2)}=\mathcal{S}^{(3)}=0$. Q.E.D.

V. THIRD-ORDER CONSTANTS OF THE MOTION

Now we investigate the space of third-order constants of the motion, assuming a nondegenerate potential. We have

$$\mathcal{K} = \sum_{k,j,i=1}^{3} a^{kji}(x,y,z)p_k p_j p_i + b^{\ell}(x,y,z)p_{\ell}, \tag{34}$$

which must satisfy $\{\mathcal{H},\mathcal{K}\}=0$. Here a^{kji} is symmetric in the indices k,j,i.

The conditions are

$$a_i^{iii} = -\frac{3}{2}\sum_s a^{sii}(\ln\lambda)_s,$$

$$3a_i^{jii} + a_j^{iii} = -3\sum_s a^{sij}(\ln\lambda)_s, \quad i \neq j,$$

$$a_i^{ijj} + a_j^{iij} = -\frac{1}{2}\sum_s a^{sjj}(\ln\lambda)_s - \frac{1}{2}\sum_s a^{sii}(\ln\lambda)_s, \quad i \neq j,$$

$$2a_i^{ijk} + a_j^{kii} + a_k^{jii} = -\sum_s a^{sjk}(\ln \lambda)_s, \quad i,j,k \text{ distinct}, \tag{35}$$

$$b_k^j + b_j^k = 3\lambda \sum_s a^{skj} V_s, \quad j \neq k, \quad j,k = 1,2,3,$$

$$b_j^j = \frac{3}{2}\lambda \sum_s a^{sjj} V_s - \frac{1}{2}\sum_s b^s (\ln \lambda)_s, \quad j = 1,2,3, \tag{36}$$

and

$$\sum_s b^s V_s = 0. \tag{37}$$

The a^{kji} is just a third-order Killing tensor. We will, as usual, require the potential V to be superintegrable and non degenerate. Again, as usual, we require that the highest order terms, the a^{kji} in the constant of the motion, be independent of the four independent parameters in V. However, the b^ℓ must depend on these parameters. We set

$$b^\ell(x,y,z) = \sum_{j=1}^{3} f^{\ell,j}(x,y,z) V_j(x,y,z).$$

[Here we are excluding the purely first-order symmetries. Also, we could add a term $f^{\ell,11}(x,y,z)V_{11}(x,y,z)$ to the preceding expression. However condition (37) implies $f^{\ell,11} \equiv 0$.] Substituting this expression into (37) we see that

$$f^{\ell,j} + f^{j,\ell} = 0, \quad 1 \leqslant \ell, j \leqslant 3.$$

Further

$$b_j^i = \sum_{\ell \neq 1} (f_j^{i,\ell} V_\ell + f^{i,\ell} V_{j\ell}),$$

where the subscript j denotes the partial derivative with respect to x_j. Substituting these results and expressions (14) into the defining equations (36) and equating coefficients of V_1, V_2, V_3, V_{11}, respectively, we obtain the following independent conditions [$G_s \equiv (\ln \lambda)_s$]:

$$\lambda a^{111} = \frac{2}{3}(f^{1,2}A^{12} + f^{1,3}A^{13}) + \frac{1}{3}\sum_{s=1}^{3} f^{s,1} G_s,$$

$$\lambda a^{222} = \frac{2}{3}(-f^{1,2}B^{12} + f^{2,3}B^{23}) + \frac{1}{3}\sum_{s=1}^{3} f^{s,2} G_s,$$

$$\lambda a^{333} = \frac{2}{3}(-f^{1,3}C^{13} - f^{2,3}C^{23}) + \frac{1}{3}\sum_{s=1}^{3} f^{s,3} G_s,$$

$$\lambda a^{112} = \frac{2}{9}(f^{1,2}(A^{22} + B^{12}) + 2f^{1,3}A^{23} + f^{2,3}A^{13}) + \frac{1}{9}\sum_{s=1}^{3} f^{s,2} G_s,$$

$$\lambda a^{113} = \frac{2}{9}(2f^{1,2}A^{23} + f^{1,3}(A^{33} + C^{13}) - f^{2,3}A^{12}) + \frac{1}{9}\sum_{s=1}^{3} f^{s,3}G_s,$$

$$\lambda a^{122} = \frac{2}{9}(f^{1,2}(-A^{12} + B^{22}) + f^{1,3}B^{23} + 2f^{2,3}A^{23}) + \frac{1}{9}\sum_{s=1}^{3} f^{s,1}G_s,$$

$$\lambda a^{223} = \frac{2}{9}(-2f^{1,2}A^{23} - f^{1,3}B^{12} + f^{2,3}(-B^{22} + B^{33} + C^{23})) + \frac{1}{9}\sum_{s=1}^{3} f^{s,3}G_s,$$

$$\lambda a^{133} = \frac{2}{9}(f^{1,2}C^{23} + f^{1,3}(-A^{13} + C^{33}) - 2f^{2,3}A^{23}) + \frac{1}{9}\sum_{s=1}^{3} f^{s,1}G_s,$$

$$\lambda a^{233} = \frac{2}{9}(-f^{1,2}C^{13} - 2f^{1,3}A^{23} + f^{2,3}(-B^{23} - C^{22} + C^{33})) + \frac{1}{9}\sum_{s=1}^{3} f^{s,2}G_s,$$

$$\lambda a^{123} = \frac{2}{9}(f^{1,2}C^{22} + f^{1,3}B^{33} + f^{2,3}(-B^{12} + C^{13})), \tag{38}$$

$$f_1^{1,2} = \frac{1}{3}(f^{1,2}(A^{22} - 2B^{12}) - f^{1,3}A^{23} + f^{2,3}A^{13}) - \frac{1}{3}\sum_{s=1}^{3} f^{s,2}G_s,$$

$$f_2^{1,2} = \frac{1}{3}(f^{1,2}(-2A^{12} - B^{22}) - f^{1,3}B^{23} + f^{2,3}A^{23}) + \frac{1}{3}\sum_{s=1}^{3} f^{s,1}G_s,$$

$$f_1^{1,3} = \frac{1}{3}(-f^{1,2}A^{23} + f^{1,3}(A^{33} - 2C^{13}) - f^{2,3}A^{12}) - \frac{1}{3}\sum_{s=1}^{3} f^{s,3}G_s,$$

$$f_3^{1,3} = \frac{1}{3}(-f^{1,2}C^{23} + f^{1,3}(-2A^{13} - C^{33}) - f^{2,3}A^{23}) + \frac{1}{3}\sum_{s=1}^{3} f^{s,1}G_s,$$

$$f_2^{2,3} = \frac{1}{3}(f^{1,2}A^{23} - f^{1,3}B^{12} + f^{2,3}(-B^{22} + B^{33} - 2C^{23})) - \frac{1}{3}\sum_{s=1}^{3} f^{s,3}G_s,$$

$$f_3^{2,3} = \frac{1}{3}(f^{1,2}C^{13} - f^{1,3}A^{23} + f^{2,3}(-2B^{23} + C^{22} - C^{33})) + \frac{1}{3}\sum_{s=1}^{3} f^{s,2}G_s, \tag{39}$$

and

$$f_1^{2,3} + f_2^{1,3} = \tfrac{1}{3}(-f^{1,2}C^{22} + f^{1,3}(2B^{33} - 3C^{23}) - f^{2,3}(2B^{12} + C^{13})),$$

$$-f_1^{2,3} + f_3^{1,2} = \tfrac{1}{3}(-f^{1,2}(2A^{13} + B^{23}) - f^{1,3}B^{33} + f^{2,3}(B^{12} + 2C^{13})). \tag{40}$$

We have eight equations for the nine derivatives $f_k^{i,j}$, and by differentiating these we have 18 independent conditions for the 18 second derivatives $f_{k\ell}^{i,j}$. Thus the system closes. A solution is determined by 12 parameters $f_k^{i,j}(\mathbf{x}_0), f_{k\ell}^{i,j}(\mathbf{x}_0)$ at a regular point, and these parameters are constrained by at least eight linearly independent conditions. Thus the solution space, which is obviously of dimension $\geqslant 3$ must be of dimension $\leqslant 4$. We must still apply the conditions that the a^{ijk} are third-order Killing tensors.

Theorem 4: *Let $\mathcal{K}$ be a third-order constant of the motion for a conformally flat superintegrable system with nondegenerate potential V,*

$$\mathcal{K} = \sum_{k,j,i=1}^{3} a^{kji}(x,y,z)p_k p_j p_i + \sum_{\ell=1}^{3} b^{\ell}(x,y,z)p_\ell.$$

Then

$$b^{\ell}(x,y,z) = \sum_{j=1}^{3} f^{\ell,j}(x,y,z)V_j(x,y,z)$$

with $f^{\ell,j}+f^{j,\ell}=0, 1\leqslant \ell, j\leqslant 3$. The a^{ijk}, b^{ℓ} are uniquely determined by the four numbers

$$f^{1,2}(x_0,y_0,z_0), \quad f^{1,3}(x_0,y_0,z_0), \quad f^{2,3}(x_0,y_0,z_0), \quad f_3^{1,2}(x_0,y_0,z_0)$$

at any regular point (x_0,y_0,z_0) of V.

Let

$$\mathcal{S}_1 = \sum a_{(1)}^{kj} p_k p_j + W_{(1)}, \quad \mathcal{S}_2 = \sum a_{(2)}^{kj} p_k p_j + W_{(2)}$$

be second-order constants of the motion for a superintegrable system with nondegenerate potential and let $\mathcal{A}_{(i)}(x,y,z)=\{a_{(i)}^{kj}(x,y,z)\}, i=1, 2$ be 3×3 matrix functions. Then the Poisson bracket of these symmetries is given by

$$\{\mathcal{S}_1,\mathcal{S}_2\} = \sum_{k,j,i=1}^{3} a^{kji}(x,y,z)p_k p_j p_i + b^{\ell}(x,y,z)p_\ell,$$

where

$$f^{k,\ell} = 2\lambda \sum_j (a_{(2)}^{kj} a_{(1)}^{j\ell} - a_{(1)}^{kj} a_{(2)}^{j\ell}). \tag{41}$$

Differentiating, we find

$$f_i^{k,\ell} = 2\lambda \sum_j (\partial_i a_{(2)}^{kj} a_{(1)}^{j\ell} + a_{(2)}^{kj}\partial_i a_{(1)}^{j\ell} - \partial_i a_{(1)}^{kj} a_{(2)}^{j\ell} - a_{(1)}^{kj}\partial_i a_{(2)}^{j\ell}) + G_i f^{k,\ell}. \tag{42}$$

Clearly, $\{\mathcal{S}_1,\mathcal{S}_2\}$ is uniquely determined by the skew-symmetric matrix $[\mathcal{A}_{(2)},\mathcal{A}_{(1)}] \equiv \mathcal{A}_{(2)}\mathcal{A}_{(1)}-\mathcal{A}_{(1)}\mathcal{A}_{(2)}$, hence by the constant matrix $[\mathcal{A}_{(2)}(x_0,y_0,z_0),\mathcal{A}_{(1)}(x_0,y_0,z_0)]$ evaluated at a regular point, and by the number $\mathcal{F}(x_0,y_0,z_0)=f_3^{1,2}(x_0,y_0,z_0)$.

For superintegrable nondegenerate potentials there is a standard structure allowing the identification of the space of second-order constants of the motion with the space S_3 of 3×3 symmetric matrices, as well as identification of the space of third-order constants of the motion with a subspace of the space $K_3\times F$ of 3×3 skew-symmetric matrices K_3, crossed with the line $F=\{\mathcal{F}(\mathbf{x}_0)\}$. Indeed, if $\mathbf{x}_0$ is a regular point then there is a linear correspondence between second-order symmetries $\mathcal{S}$ and their associated symmetric matrices $\mathcal{A}_{(\mathbf{x}_0)}$. Let $\{\mathcal{S}_1,\mathcal{S}_2\}'=\{\mathcal{S}_2,\mathcal{S}_1\}$ be the reversed Poisson bracket. Then the map

$$\{\mathcal{S}_1,\mathcal{S}_2\}' \Leftrightarrow [\mathcal{A}_{(1)}(\mathbf{x}_0),\mathcal{A}_{(2)}(\mathbf{x}_0)]$$

is an algebraic homomorphism. Here, $\mathcal{S}_1,\mathcal{S}_2$ are in involution if and only if matrices $\mathcal{A}_{(1)}\times(\mathbf{x}_0),\mathcal{A}_{(2)}(\mathbf{x}_0)$ commute and $\mathcal{F}(\mathbf{x}_0)=0$. If $\{\mathcal{S}_1,\mathcal{S}_2\}\neq 0$ then it is a third-order symmetry and can be uniquely associated with the skew-symmetric matrix $[\mathcal{A}_{(1)}(\mathbf{x}_0),\mathcal{A}_{(2)}(\mathbf{x}_0)]$ and the parameter $\mathcal{F}(\mathbf{x}_0)$. Let $\mathcal{E}^{ij}$ be the 3×3 matrix with a 1 in row i, column j and 0 for every other matrix element. Then the symmetric matrices

$$\mathcal{A}^{(ij)}=\tfrac{1}{2}(\mathcal{E}^{ij}+\mathcal{E}^{ji})=\mathcal{A}^{(ji)},\quad i,j=1,2,3 \tag{43}$$

form a basis for the 6-dimensional space of symmetric matrices. Moreover,

$$[\mathcal{A}^{(ij)},\mathcal{A}^{(k\ell)}]=\tfrac{1}{2}\big(\delta_{jk}\mathcal{B}^{(i\ell)}+\delta_{j\ell}\mathcal{B}^{(ik)}+\delta_{ik}\mathcal{B}^{(j\ell)}+\delta_{i\ell}\mathcal{B}^{(jk)}\big), \tag{44}$$

where

$$\mathcal{B}^{(ij)}=\tfrac{1}{2}(\mathcal{E}^{ij}-\mathcal{E}^{ji})=-\mathcal{B}^{(ji)},\quad i,j=1,2,3.$$

Here $\mathcal{B}^{(ii)}=0$ and $\mathcal{B}^{(12)},\mathcal{B}^{(23)},\mathcal{B}^{(31)}$ form a basis for the space of skew-symmetric matrices. To obtain the commutation relations for the second-order symmetries we need to use relations (42) to compute the parameter $\mathcal{F}(\mathbf{x}_0)$ associated with each commutator $[\mathcal{A}^{(ij)},\mathcal{A}^{(k\ell)}]$. The results are straightforward to compute, using relations (27).

Commutator	$3\mathcal{F}/\lambda$
$[\mathcal{A}^{(12)},\mathcal{A}^{(11)}]=\mathcal{B}^{(21)}$	$-3A^{13}-B^{23}-G_3$
$[\mathcal{A}^{(13)},\mathcal{A}^{(11)}]=\mathcal{B}^{(31)}$	$A^{12}-B^{33}+G_2$
$[\mathcal{A}^{(22)},\mathcal{A}^{(11)}]=0$	$-4A^{23}$
$[\mathcal{A}^{(23)},\mathcal{A}^{(11)}]=0$	$2(A^{22}-A^{33})$
$[\mathcal{A}^{(33)},\mathcal{A}^{(11)}]=0$	$4A^{23}$
$[\mathcal{A}^{(13)},\mathcal{A}^{(12)}]=\frac{1}{2}\mathcal{B}^{(32)}$	$\frac{1}{2}(3B^{12}-A^{22}+3A^{33}-G_1)$
$[\mathcal{A}^{(22)},\mathcal{A}^{(12)}]=\mathcal{B}^{(21)}$	$-3B^{23}-A^{13}-G_3$
$[\mathcal{A}^{(23)},\mathcal{A}^{(12)}]=\frac{1}{2}\mathcal{B}^{(31)}$	$\frac{1}{2}(-3B^{33}-3A^{12}+2B^{22}+G_2)$
$[\mathcal{A}^{(33)},\mathcal{A}^{(12)}]=0$	$2(B^{23}-A^{13})$
$[\mathcal{A}^{(22)},\mathcal{A}^{(13)}]=0$	$-2B^{33}$
$[\mathcal{A}^{(23)},\mathcal{A}^{(13)}]=\frac{1}{2}\mathcal{B}^{(21)}$	$-C^{33}+\frac{1}{2}B^{23}-\frac{1}{2}A^{13}-\frac{1}{2}G_3$
$[\mathcal{A}^{(33)},\mathcal{A}^{(13)}]=\mathcal{B}^{(31)}$	$A^{12}+B^{33}+G_2$
$[\mathcal{A}^{(23)},\mathcal{A}^{(22)}]=\mathcal{B}^{(32)}$	$A^{33}-A^{22}-B^{12}-G_1$
$[\mathcal{A}^{(33)},\mathcal{A}^{(22)}]=0$	$-4A^{23}$
$[\mathcal{A}^{(33)},\mathcal{A}^{(23)}]=\mathcal{B}^{(32)}$	$A^{22}-A^{33}-B^{12}-G_1$

Suppose the dimension of the space of *truly* third-order symmetries generated by commutators of second-order symmetries is 3. This means that whenever the matrices of two second-order symmetries commute at a regular point $\mathbf{x}_0$, so that $f^{1,2}(x_0,y_0,z_0)=f^{1,3}(x_0,y_0,z_0)=f^{2,3}(x_0,y_0,z_0)=0$, then $f_3^{1,2}(x_0,y_0,z_0)=0$. From the table above we see that

$$A^{23}=0,\quad A^{22}=A^{33},\quad B^{23}=A^{13},\quad B^{33}=0.$$

Further, since $[\mathcal{A}^{(12)},\mathcal{A}^{(11)}]-[\mathcal{A}^{(22)},\mathcal{A}^{(12)}]=0$, etc., we have

$$B^{12}=-\tfrac{1}{2}A^{33},\quad B^{22}=2A^{12},\quad C^{33}=2A^{13}.$$

Substituting these results into the integrability conditions for the potential and the symmetries, we find that there exists a function $U(x,y,z)$ such that

$$A^{33}=2(\ln U)_x,\quad A^{12}=-(\ln U)_y,\quad A^{13}=-(\ln U)_z,$$

where

$$U_{xx} = U_{yy} = U_{zz}, \quad U_{xy} = U_{yz} = U_{zx} = 0.$$

Note that U is an instance of the isotropic oscillator potential

$$U = \alpha(x^2 + y^2 + z^2) + \beta x + \gamma y + \delta z.$$

(Further, the defining second-order symmetries for the isotropic oscillator are only weakly functionally independent.) By analogy with the 2D Stäckel transform studied in Ref. 2 (whose 3D form will be studied in our next presentation) it is straightforward to see that the potential of our system is a Stäckel transform by U of the isotropic oscillator potential. By taking the inverse Stäckel transform we can obtain $A^{ij}=B^{ij}=C^{ij}\equiv 0$ for all i,j. Plugging these values into the integrability conditions for the symmetries, we find that $G_1=G_2=G_3=0$ so λ is a constant. Thus the Stäckel transformed system is just the isotropic harmonic oscillator in flat space.

Corollary 5: Let V be a superintegrable nondegenerate potential on a conformally flat space, not a Stäckel transform of the isotropic oscillator. Then the space of truly third-order constants of the motion is four-dimensional and is spanned by Poisson brackets of the second-order constants of the motion.

VI. THE STANDARD BASIS

To gain a deeper understanding of our standard basis structure, it is useful to reformulate the problem of determining the second-order symmetries for a nondegenerate superintegrable potential. We set

$$W(x) = f^1 V_1 + f^2 V_2 + f^3 V_3 + f^{11} V_{11}$$

and substitute this result into $W_i=\lambda\Sigma_{j=1}^3 a^{ij}V_j$. Additionally we must impose the Killing tensor conditions,

$$a_i^{ii} = -G_1 a^{1i} - G_2 a^{2i} - G_3 a^{3i},$$

$$2a_i^{ij} + a_j^{ii} = -G_1 a^{1j} - G_2 a^{2j} - G_3 a^{3j}, \quad i \neq j,$$

$$a_k^{ij} + a_j^{ki} + a_i^{jk} = 0, \quad i,j,k \text{ distinct}.$$

From the expressions for W_i we obtain the equations for the a^{ij},

$$\begin{aligned}
\lambda a^{11} &= f_1^1 + f^2 A^{12} + f^3 A^{13} + f^{11} A^{14},\\
\lambda a^{12} &= f_2^1 + f^1 A^{12} + f^2 A^{22} + f^3 A^{32} + f^{11} A^{24},\\
\lambda a^{13} &= f_3^1 + f^1 A^{13} + f^2 A^{23} + f^3 A^{33} + f^{11} A^{34},\\
\lambda a^{22} &= f_2^2 + f^1 B^{12} + f^2 B^{22} + f^3 B^{32} + f^{11} B^{24},\\
\lambda a^{23} &= f_3^2 + f^1 B^{13} + f^2 B^{23} + f^3 B^{33} + f^{11} B^{34},\\
\lambda a^{33} &= f_3^3 + f^1 C^{13} + f^2 C^{23} + f^3 C^{33} + f^{11} C^{34},
\end{aligned} \tag{45}$$

and the condition on the first derivatives of the f^i,

$$\begin{aligned}
f_2^1 - f_1^2 &= -f^1 A^{12} + f^2 (B^{12} - A^{22}) + f^3 (B^{13} - A^{23}) + f^{11} (B^{14} - A^{24}),\\
f_3^1 - f_1^3 &= -f^1 A^{13} + f^2 (C^{12} - A^{23}) + f^3 (C^{13} - A^{33}) + f^{11} (C^{14} - A^{34}),
\end{aligned} \tag{46}$$

$$f_3^2 - f_2^3 = f^1(C^{12} - B^{13}) + f^2(C^{22} - B^{23}) + f^3(C^{23} - B^{33}) + f^{11}(C^{24} - B^{34}).$$

Note the expressions for f_1^{11} and f_2^{11} in terms of f^1, f^2, f^{11},

$$f_1^{11} = -f^1 - f^{11}(B^{12} - A^{22}), \quad f_2^{11} = -f^2 - f^{11}A^{12}, \quad f_3^{11} = -f^3 - f^{11}A^{13}.$$

Differentiating (46) with respect to each of x_1, x_2, x_3 and substituting (45) into the Killing equations we see that we can express each of the second derivatives of f^1, f^2, f^3 in terms of lower order derivatives of $f^1, f^2 f^3, f^{11}$. Thus the system is in involution at the second derivative level, but not at the first derivative level because we have only three conditions for the nine derivatives f_j^i. We can uniquely determine a symmetry at a regular point by choosing the 10 parameters

$$(f^1, f^2, f^3, f^{11}, f_1^1, f_2^1, f_3^1, f_2^2, f_3^2, f_3^3).$$

The values of f^1, f^2, f^3, f^{11} at the regular point are analogous to the four parameters that we can add to the potentials in the four parameter family. For our standard basis, we fix $(f^1, f^2, f^3, f^{11})_{\mathbf{x}_0} = (0,0,0,0)$. Then from (45) and (46) we have

$$\begin{pmatrix} f_1^1 & f_2^1 & f_3^1 \\ f_1^2 & f_2^2 & f_3^2 \\ f_1^3 & f_2^3 & f_3^3 \end{pmatrix} = \lambda \begin{pmatrix} a^{11} & a^{12} & a^{13} \\ a^{21} & a^{22} & a^{23} \\ a^{31} & a^{32} & a^{33} \end{pmatrix}.$$

Thus we can define a standard set of basis symmetries $\mathcal{S}^{(jk)} = \Sigma a^{ij}(\mathbf{x}) p_i p_j + W^{(ij)}(\mathbf{x})$ corresponding to a regular point $\mathbf{x}_0$ by

$$\frac{1}{\lambda} \begin{pmatrix} f_1^1 & f_2^1 & f_3^1 \\ f_1^2 & f_2^2 & f_3^2 \\ f_1^3 & f_2^3 & f_3^3 \end{pmatrix}_{\mathbf{x}_0} = \begin{pmatrix} a^{11} & a^{12} & a^{13} \\ a^{21} & a^{22} & a^{23} \\ a^{31} & a^{32} & a^{33} \end{pmatrix}_{\mathbf{x}_0} = \mathcal{A}^{(jk)}, \quad W^{(jk)}(\mathbf{x}_0) = 0.$$

The condition on $W^{(jk)}$ is actually four conditions since $W^{(jk)}$ depends on four parameters.

VII. MAXIMUM DIMENSIONS OF THE SPACES OF POLYNOMIAL CONSTANTS

In order to demonstrate the existence and structure of quadratic algebras for 3D superintegrable systems on conformally flat spaces, it is important to compute the dimensions of the spaces of symmetries of these systems that are of orders 4 and 6. These symmetries are necessarily of a special type. The highest order terms in the momenta are independent of the parameters in the potential, while the terms of order 2 less in the momenta are linear in these parameters, those of order 4 less are quadratic, and those of order 6 less are cubic. We will obtain these dimensions exactly, but first we need to establish sharp upper bounds.

A. Quartic constants

We investigate the space of fourth-order constants of the motion

$$\mathcal{F} = \sum_{\ell,k,j,i=1}^{3} a^{\ell kji}(x,y,z) p_\ell p_k p_j p_i + \sum_{m,q=1}^{3} b^{mq}(x,y,z) p_m p_q + W(x,y,z), \tag{47}$$

which must satisfy $\{\mathcal{H}, \mathcal{F}\} = 0$. Here $a^{\ell kji}, b^{mq}$ are symmetric in all indices.

The conditions are

$$a_i^{iiii} = -2 \sum_s \frac{\lambda_s}{\lambda} a^{siii},$$

$$4a_i^{jiii}+a_j^{iiii}=-6\sum_s\frac{\lambda_s}{\lambda}a^{sjii},\quad i\neq j,$$

$$3a_i^{jjii}+2a_j^{iiij}=-\sum_s\frac{\lambda_s}{\lambda}a^{siii}-3\sum_s\frac{\lambda_s}{\lambda}a^{sijj},\quad i\neq j, \tag{48}$$

$$3a_i^{iijk}+a_j^{kiii}+a_k^{jiii}=-6\sum_s\frac{\lambda_s}{\lambda}a^{sijk},\quad i,j,k \text{ distinct},$$

$$2a_i^{ijjk}+2a_j^{jiik}+a_k^{iijj}=-\sum_s\frac{\lambda_s}{\lambda}(a^{skii}+a^{skjj}),\quad i,j,k \text{ distinct},$$

$$b_i^{jk}+b_k^{ij}+b_j^{ki}=6\lambda\sum_s a^{skji}V_s,\quad i,j,k \text{ distinct},$$

$$2b_i^{ij}+b_j^{ii}=6\lambda\sum_s a^{sjii}V_s-\sum_s\frac{\lambda_s}{\lambda}b^{si},\quad i\neq j, \tag{49}$$

$$b_i^{ii}=2\lambda\sum_{s=1}^{3}a^{siii}V_s-\sum_s\frac{\lambda_s}{\lambda}b^{si},$$

and

$$\lambda\sum_s b^{si}V_s=W_i. \tag{50}$$

Clearly, the $a^{\ell kji}$ is a fourth-order Killing tensor. We require the potential V to be superintegrable and nondegenerate. Also we require that the highest order terms, the $a^{\ell kji}$ in the constant of the motion be independent of the four independent parameters in V. However, the b^{mq} must depend linearly and W quadratically on these parameters.

We set

$$b^{jk}=\sum_{\alpha=1}^{4}f^{jk,\alpha}W^{(\alpha)},\quad f^{jk,\alpha}=f^{kj,\alpha},$$

where $W^{(\alpha)}$ is defined by (18). Then conditions (49) take the form

$$\partial_{x_h}f^{jk,\alpha}+\partial_{x_k}f^{hj,\alpha}+\partial_{x_j}f^{kh,\alpha}-\lambda a^{\alpha hjk}=\cdots, \tag{51}$$

where the right-hand side depends only on the $f^{jk,\alpha}, 1\leqslant j,k,h\leqslant 3$ and we set $a^{4hjk}\equiv 0$. From the integrability conditions $\partial_{x_j}(\partial W/\partial x_i)=\partial_{x_i}(\partial W/\partial x_j), i\neq j$ for Eq. (50) we obtain the conditions

$$\partial_{x_j}f^{\beta k,\alpha}+\partial_{x_j}f^{\alpha k,\beta}-\partial_{x_k}f^{\beta j,\alpha}-\partial_{x_k}f^{\alpha j,\beta}=\cdots, \tag{52}$$

where the right-hand side depends only on the $f^{jk,\alpha}, j\neq k, 1\leqslant\alpha,\beta\leqslant 4$ and we set $f^{4j,\alpha}\equiv 0$.

There are 30 independent equations (51) with $\alpha\neq 4$ and we use 15 of these to define the 15 components a^{ihjk} as linear combinations of $\partial_{x_h}f^{jk,\alpha}$ and $f^{jk,\alpha}$. We can then eliminate the a^{ihjk} from the remaining 15 equations to obtain 15 conditions relating $\partial_{x_h}f^{jk,\alpha}$ and $f^{jk,\alpha}$. There are 18 terms of the form $\partial_{x_h}f^{jk,4}$. Equations (52) with $\alpha=\beta=4$ are satisfied identically. There are nine equations (52) with $\beta=4, 1\leqslant\alpha\leqslant 3$ and 10 equations (51) with $\alpha=4$. Thus all terms of the form $\partial_{x_h}f^{jk,4}$ can be expressed as linear combinations of $f^{jk,\alpha}$. There are a total of 54 distinct terms of the form

$\partial_{x_h} f^{jk,m}, 1 \leqslant h,j,k,m \leqslant 3$. We have seen that there are 15 conditions on these terms remaining from (51); there are an additional 18 such conditions from (52) with $\alpha,\beta \neq 4$. Thus there is a shortfall of 21 conditions on the first derivatives $\partial_{x_h} f^{jk,m}$.

There are a total of 108 distinct terms of the form $\partial_{x_h}\partial_{x_\ell} f^{jk,m}$ with $1 \leqslant hj,k,\ell,m \leqslant 3$. Differentiating with respect to x_1, x_2, and x_3 the 15 first-order conditions of (51), from which the a^{ihjk} have been eliminated, we obtain 45 independent conditions on these second derivatives. Differentiating each of our expressions for the a^{ihjk} and substituting into equations (48) we find 63 additional conditions on the second derivatives. This allows us to express each second-order derivative as a linear combination of lower order derivatives, Thus the system is in involution. Also, we can differentiate the 18 equations from (52) with $\alpha,\beta \neq 4$ to obtain 54 additional conditions on the second derivatives (which may or may not be independent of those already found).

We conclude that any fourth-order symmetry is uniquely determined by the values $f^{jk,\alpha}(\mathbf{x}_0)$ and a subset of 21 of the values $\partial_{x_h} f^{jk,m}(\mathbf{x}_0)$ at a regular point $\mathbf{x}_0$. Note that by adding an appropriate linear combination of purely second-order symmetries to the fourth-order symmetry we can achieve $f^{jk,\alpha}(\mathbf{x}_0)=0$ for all j,k,α, so the maximum possible dimension of the space of purely fourth-order symmetries for a nondegenerate potential is 21.

B. Sixth-order constants

We take the general sixth-order symmetry for a nondegenerate potential to be of the form

$$\mathcal{L} = \sum a^{hijklt} p_h p_i p_j p_k p_l p_t + \sum b^{hijk} p_h p_i p_j p_k + \sum c^{ij} p_i p_j + W,$$

where the functions $a^{hijklt}, b^{hijk}, c^{ij}$ are symmetric in all indices. Here a^{hijklt} is independent of the parameters $V_\alpha, \alpha = 1,\ldots,4$, b^{hijk} is a homogeneous quadratic polynomial in the $W^{(\alpha)}$, c^{ij} is homogeneous fourth order, and W is homogeneous sixth order in the $W^{(\alpha)}$. The Poisson bracket of $\mathcal{H}$ and $\mathcal{L}$ is polynomial in the momenta and the parameters $W^{(\alpha)}$ and for it to vanish at a regular point, each coefficient of this polynomial must vanish separately. The conditions are (for $1 \leqslant i,j,k \leqslant k$ and i,j,k pairwise distinct and for $s=1, 2, 3$)

$$a_i^{iiiiii} = -3\sum_s \frac{\lambda_s}{\lambda} a^{siiiii},$$

$$6a_i^{jiiiii} + a_j^{iiiiii} = -15\sum_s \frac{\lambda_s}{\lambda} a^{sjiiii},$$

$$5a_i^{jjiiii} + 2a_j^{jiiiii} = -\sum_s \frac{\lambda_s}{\lambda} a^{siiiii} - 10\sum_s \frac{\lambda_s}{\lambda} a^{sjjiii},$$

$$4a_i^{jjjiii} + 3a_j^{jjiiii} = -3\sum_s \frac{\lambda_s}{\lambda} a^{sjiiii} - 12\sum_s \frac{\lambda_s}{\lambda} a^{sjjjii},$$

$$5a_i^{jkiiii} + a_k^{jiiiii} + a_j^{kiiiii} = -10\sum_s \frac{\lambda_s}{\lambda} a^{sjkiii},$$

$$4a_i^{jjkiii} + 2a_j^{jkiiii} + a_k^{jjiiii} = -6\sum_s \frac{\lambda_s}{\lambda} a^{sjjkii} - \sum_s \frac{\lambda_s}{\lambda} a^{skiiii},$$

$$3a_i^{jjkkii}+2a_j^{jkkiii}+2a_k^{kjjiii}=-90\sum_s\frac{\lambda_s}{\lambda}a^{sijjkk}-30\sum_s\frac{\lambda_s}{\lambda}a^{skkiii}-30\sum_s\frac{\lambda_s}{\lambda}a^{sjjiii}, \tag{53}$$

$$b_i^{iiii}=3\lambda\sum_s a^{siiiii}W^{(s)}-2\sum_s\frac{\lambda_s}{\lambda}b^{siii},$$

$$b_j^{iiii}+4b_i^{jiii}=15\lambda\sum_s a^{sjiiii}W^{(s)}-6\sum_s\frac{\lambda_s}{\lambda}b^{sjii},$$

$$2b_j^{iiij}+3b_i^{jjii}=15\lambda\sum_s a^{sjjiii}W^{(s)}-\sum_s\frac{\lambda_s}{\lambda}(2b^{siii}+6b^{sjji}), \tag{54}$$

$$b_j^{iiik}+b_k^{iiij}+3b_i^{ijjk}=15\lambda\sum_s a^{siiijk}W^{(s)}-6\sum_s\frac{\lambda_s}{\lambda}b^{sijk},$$

$$b_k^{ijjj}+2b_j^{ijjk}+2b_i^{ijjk}=15\lambda\sum_s a^{siijjk}W^{(s)}-2\sum_s\frac{\lambda_s}{\lambda}(b^{siik}+b^{sjjk}),$$

$$c_i^{ii}=2\lambda\sum_s b^{siii}W^{(s)}-\sum_s\frac{\lambda_s}{\lambda}c^{si},$$

$$2c_i^{ij}+c_j^{ii}=6\lambda\sum_s b^{siij}W^{(s)}-\sum_s\frac{\lambda_s}{\lambda}c^{si}, \tag{55}$$

$$c_k^{ij}+c_j^{ik}+c_i^{kj}=6\lambda\sum_s b^{sijk}W^{(s)},$$

$$\sum_s(c_j^{si}-c_i^{sj})W^{(s)}=\frac{1}{\lambda}\sum_s(c^{sj}(\lambda W^{(s)})_i-c^{si}(\lambda W^{(s)})_j). \tag{56}$$

We set

$$c^{ij}=\sum_{\alpha,\beta=1}^{4}c^{ij,\alpha\beta}W^{(\alpha)}W^{(\beta)},\quad c^{ij,\alpha\beta}=c^{ij,\beta\alpha}.$$

There are $6\times10=60$ independent terms $c^{ij,\alpha\beta}$. There are $60\times3=180$ terms $c_k^{ij,\alpha\beta}$ of which 108 are of the form $c_k^{ij,st}$, 54 are of the form $c_k^{ij,4s}$, and 18 are of the form $c_k^{ij,44}$. Equations (56) give 30 conditions relating the derivatives $c_k^{ij,\alpha\beta}$, 18 conditions relating the derivatives $c_k^{ij,4s}$, and 8 conditions relating the derivatives $c_k^{ij,44}$. The 100 independent equations (55) allow us to solve for the 15 terms $b^{ijk\ell,4}$ and the 45 terms $b^{ijk\ell,s}$ where

$$b^{ijk\ell}=\sum_{\alpha=1}^{4}b^{ijk\ell,\alpha}W^{(\alpha)}.$$

Further, they yield 10 conditions relating the derivatives $c_k^{ij,44}$, 15 equations relating the derivatives $c_k^{ij,4s}$, and 15 equations relating the derivatives $c_k^{ij,st}$. It follows that all 18 terms of the form $c_k^{ij,44}$

can be expressed as linear combinations of the $c^{ij,\alpha\beta}$. There are a total of 78 conditions on the remaining 162 terms.

There are 360 terms $c_{k\ell}^{ij,\alpha\beta}$ of which we can ignore the 36 terms $c_{k\ell}^{ij,44}$. The 84 equations (54) allow us to solve for the 28 terms $a^{hijk\ell m}$ and give 21 conditions for $c_{k\ell}^{ij,4s}$ and 35 conditions for $c_{k\ell}^{ij,st}$. Further differentiating our previously obtained 78 conditions on the first derivatives we obtain $78\times 3=234$ conditions, 99 on $c_{k\ell}^{ij,st}$ and 135 independent conditions on $c_{k\ell}^{ij,st}$. It follows that all 108 terms of the form $c_{k\ell}^{ij,4s}$ can be expressed as linear combinations of lower order terms and there is a total of $35+135=160$ independent conditions on the 216 terms $c_{k\ell}^{ij,st}$. Finally, differentiating the previous conditions obtained for the $c_{k\ell}^{ij,st}$ and using the 31 equations (53) we obtain at least 360 independent conditions for the 360 terms $c_{k\ell m}^{ij,st}$. Thus the maximal number of parameters in a solution of the sixth order symmetry equations is $60+84+56=200$, excluding the 35 independent additive terms $W^{(\alpha)}W^{(\beta)}W^{(\gamma)}$.

We know that the dimension of the space of second-order symmetries for a superintegrable system with nondegenerate potential is 6. Now let us suppose (as we will prove) the dimension of the space of quartic symmetries is 21. Then there are exactly $84=21\times 4$ independent sixth-order symmetries that are also quartic symmetries, and $6\times 10=60$ independent sixth-order symmetries that are also quadratic. Thus the maximal possible dimension of the space of truly sixth-order symmetries is $200-84-60=56$. We will show that this bound of 56 is actually achieved.

VIII. BASES FOR THE FOURTH- AND SIXTH-ORDER CONSTANTS OF THE MOTION

It follows from Sec. VII A that, for a superintegrable system with nondegenerate potential, the dimension of the space of truly fourth-order constants of the motion is at most 21. Note from Sec. VI that at any regular point $\mathbf{x}_0$, we can define a standard basis of six second-order constants of the motion $\mathcal{S}^{(ij)}=A^{(ij)}+W^{(ij)}$ where the quadratic form $A^{(ij)}$ has matrix $\mathcal{A}^{(ij)}$ defined by (43) and $W^{(ij)}$ is the potential term with $W^{(ij)}(\mathbf{x}_0)\equiv 0$ identically in the parameters $W^{(\alpha)}$. By taking homogeneous polynomials of order two in the standard basis symmetries we can construct fourth order symmetries.

Question: Is every fourth-order symmetry a polynomial in the second-order symmetries?

Answer: Yes Also the dimension of the space of fourth-order symmetries is exactly 21.

Theorem 5: *The 21 distinct standard monomials* $\mathcal{S}^{(ij)}\mathcal{S}^{(jk)}$, *defined with respect to a regular point* $\mathbf{x}_0$, *form a basis for the space of fourth-order symmetries*.

Proof: We choose the basis symmetries in the form

$$(1)\quad (\mathcal{S}^{(ii)})^2,\ \mathcal{S}^{(ii)}\mathcal{S}^{(ij)},\ \mathcal{S}^{(ii)}\mathcal{S}^{(jj)},\ \mathcal{S}^{(ii)}\mathcal{S}^{(jk)}$$

$$(2)\quad \mathcal{S}^{(ii)}\mathcal{S}^{(jj)}-(\mathcal{S}^{(ij)})^2$$

$$(3)\quad \mathcal{S}^{(ij)}\mathcal{S}^{(ik)}-\mathcal{S}^{(ii)}\mathcal{S}^{(jk)}$$

for $i,j,k=1,\ldots,3$ i,j,k pairwise distinct (three possibilities).

If we evaluate this set at the regular point the first class of symmetries will be $p_i^4, p_i^3p_jp_i^2p_j^2, p_i^2p_jp_k$, respectively, whereas the last two classes of symmetries will vanish. Thus the only possible linear dependencies are those relating the six symmetries

$$F^{(12)}=\mathcal{S}^{(11)}\mathcal{S}^{(22)}-(\mathcal{S}^{(12)})^2,\quad F^{(13)}=\mathcal{S}^{(11)}\mathcal{S}^{(33)}-(\mathcal{S}^{(13)})^2,\quad F^{(23)}=\mathcal{S}^{(22)}\mathcal{S}^{(33)}-(\mathcal{S}^{(23)})^2,$$

$$G^{(23)}=\mathcal{S}^{(12)}\mathcal{S}^{(13)}-\mathcal{S}^{(11)}\mathcal{S}^{(23)},\quad G^{(13)}=\mathcal{S}^{(12)}\mathcal{S}^{(23)}-\mathcal{S}^{(22)}\mathcal{S}^{(13)},\quad G^{(12)}=\mathcal{S}^{(13)}\mathcal{S}^{(23)}-\mathcal{S}^{(33)}\mathcal{S}^{(12)}.$$

The second-order terms in the symmetry $F^{(ij)}$ are

$$\mathcal{F}^{(ij)}=\mathcal{A}^{(ii)}W^{(jj)}+\mathcal{A}^{(jj)}W^{(ii)}-2\mathcal{A}^{(ij)}W^{(ij)}.$$

Now $\mathcal{F}^{(ij)}$ vanishes at the regular point but its derivatives at the point are

$$\mathcal{F}_i^{(ij)} = p_j^2 V_i - p_i p_j V_j, \quad \mathcal{F}_j^{(ij)} = p_i^2 V_j - p_j p_i V_i, \quad \mathcal{F}_k^{(ij)} = 0.$$

Similarly the second-order terms in the symmetry $G^{(jk)}$ are

$$\mathcal{G}^{(jk)} = \mathcal{A}^{(ij)} W^{(ik)} + \mathcal{A}^{(ik)} W^{(ij)} - \mathcal{A}^{(ii)} W^{(jk)} - \mathcal{A}^{(jk)} W^{(ii)}.$$

Again $\mathcal{G}^{(ij)}$ vanishes at the regular point but its derivatives at the point are

$$\mathcal{G}_i^{(jk)} = \tfrac{1}{2} p_i p_j V_k + \tfrac{1}{2} p_i p_k V_j - p_j p_k V_i, \quad \mathcal{G}_j^{(jk)} = \tfrac{1}{2} p_i p_k V_i - \tfrac{1}{2} p_i^2 V_k, \quad \mathcal{G}_k^{(jk)} = \tfrac{1}{2} p_i p_j V_i - \tfrac{1}{2} p_i^2 V_j.$$

Since V_1, V_2, V_3 are arbitrary, it is clear that these six terms are linearly independent. Thus the 21 symmetries form a basis. Q.E.D.

Now we know that for a superintegrable system with nondegenerate potential the space of purely fourth-order constants of the motion is exactly 21. Thus from Sec. VII B the dimension of the space of purely sixth-order constants of the motion is at most 56. Again we shall show that the 56 independent homogeneous third-order polynomials in the symmetries $\mathcal{S}^{(ij)}$ form a basis for this space.

At the sixth-order level we have the symmetries

$$(1) \quad (\mathcal{S}^{(ii)})^3,\ (\mathcal{S}^{(ii)})^2 \mathcal{S}^{(ij)},\ (\mathcal{S}^{(ii)})^2 \mathcal{S}^{(jj)},\ (\mathcal{S}^{(ii)})^2 \mathcal{S}^{(jk)}$$

for $i,j,k=1,\ldots,3$ i,j,k pairwise distinct (18 possibilities),

$$(2) \quad \mathcal{S}^{(ii)} \mathcal{S}^{(ij)} \mathcal{S}^{(jj)},\ \mathcal{S}^{(ii)} \mathcal{S}^{(ij)} \mathcal{S}^{(jk)},\ \mathcal{S}^{(ii)} \mathcal{S}^{(jj)} \mathcal{S}^{(kk)}$$

$$(3) \quad \mathcal{S}^{(\ell m)} (\mathcal{S}^{(ii)} \mathcal{S}^{(jj)} - (\mathcal{S}^{(ij)})^2)$$

$$(4) \quad \mathcal{S}^{(\ell m)} \left(\mathcal{S}^{(ij)} \mathcal{S}^{(ik)} - \mathcal{S}^{(ii)} \mathcal{S}^{(jk)} \right)$$

for $i,j,k=1,\ldots,3$ i,j,k pairwise distinct (18 possibilities).

Theorem 6: *The 56 distinct standard monomials* $\mathcal{S}^{(hi)} \mathcal{S}^{(jk)} \mathcal{S}^{(\ell m)}$, *defined with respect to a regular* $\mathbf{x}_0$, *form a basis for the space of sixth-order symmetries*.

Proof: Rather than using the monomials directly we choose the polynomials in the forms (1)–(4) above. Suppose some linear combination $\mathcal{C}$ of these 56 polynomials has identically vanishing sixth-order terms. This implies immediately that the coefficients of the first 28 polynomials are zero. Thus $\mathcal{C}$ must be a linear combination of the six fourth-order symmetries $F^{(ij)}, G^{(ij)}$ of Theorem 5. Now the first derivatives of the second-order terms in $\mathcal{C}$ all vanish at $\mathbf{x}_0$ so by the proof of Theorem 5 the linear combination of fourth-order basis symmetries must vanish. Thus we must have $\mathcal{C} \equiv 0$. Then evaluating the expressions

$$\partial_{x_h} \mathcal{C}(\mathbf{x}_0) = 0, \quad \partial^2_{x_h x_\ell} \mathcal{C}(\mathbf{x}_0) = 0.$$

and making use of the expressions for $\mathcal{F}^{ij}, \mathcal{G}^{ij}$ in the proof of Theorem 5 it is straightforward to show that the coefficients of all 28 terms in $\mathcal{C}$ must vanish. The 56 terms are linearly independent and all nonzero linear combinations are truly sixth order. Q.E.D.

We conclude that the quadratic algebra closes.

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A recursive parametrization of unitary matrices

C. Jarlskog[a)]
Division of Mathematical Physics LTH, Lund University, Box 118, S-22100 Lund, Sweden

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A simple recursive scheme for parametrization of n-by-n unitary matrices is presented. The n-by-n matrix is expressed as a product containing the $(n-1)$-by-$(n-1)$ matrix and a unitary matrix that contains the additional parameters needed to go from $n-1$ to n. The procedure is repeated to obtain recursion formulas for n-by-n unitary matrices. © *2005 American Institute of Physics.*
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I. THE PARAMETRIZATION

It has been known for a long time that unitary transformations play a central role in physics. An excellent example is Wigner's paper of 1939,[1] which has had a great impact on the development of physics and is still important.

It is also a known fact that a general n-by-n unitary matrix $X^{(n)}$ may be expressed as a product of three unitary matrices,

$$X^{(n)} = \Phi^{(n)}(\vec{\alpha}) V^{(n)} \Phi^{(n)}(\vec{\beta}), \tag{1}$$

where the matrices Φ are diagonal unitary matrices,

$$\Phi^{(n)}(\vec{\alpha}) = \begin{pmatrix} e^{i\alpha_1} & & & & \\ & e^{i\alpha_2} & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & e^{i\alpha_n} \end{pmatrix}. \tag{2}$$

$\Phi(\vec{\beta})$ is defined analogously; the α's and β's being real. The matrix $X^{(n)}$ has n^2 real parameters. In the following, for simplicity, the word parameter stands for real parameter. The quantities $\vec{\alpha}$ and $\vec{\beta}$ take care of $2n-1$ parameters of $X^{(n)}$ because only the sums $\alpha_i+\beta_j$ enter, where i and j run from 1 to n. The remaining $(n-1)^2$ parameters reside in the nontrivial matrix $V^{(n)}$, which is the subject of this study.

We start by putting $V^{(1)}=1$, whereby $X^{(1)}=e^{i(\alpha_1+\beta_1)}$ is the most general one-by-one unitary "matrix." For $n \geqslant 2$, we write the matrix $V^{(n)}$ in the form

$$V^{(n)} = \begin{pmatrix} V^{(n-1)} + (1-c_n)|A^{(n-1)}\rangle\langle B^{(n-1)}| & s_n|A^{(n-1)}\rangle \\ s_n\langle B^{(n-1)}| & c_n \end{pmatrix}. \tag{3}$$

Here we have introduced an angle denoted by θ_n and have used the common notation $s_n=\sin\theta_n$, $c_n=\cos\theta_n$. The complex vectors "$A^{(n-1)}$" and "$B^{(n-1)}$" each have $n-1$ components, i.e.,

a)Electronic mail: cecilia.jarlskog@matfys.lth.se

$$|A^{(n-1)}\rangle = \begin{pmatrix} a_1^{(n-1)} \\ a_2^{(n-1)} \\ \cdot \\ \cdot \\ a_{n-1}^{(n-1)} \end{pmatrix}, \quad |B^{(n-1)}\rangle = \begin{pmatrix} b_1^{(n-1)} \\ b_2^{(n-1)} \\ \cdot \\ \cdot \\ b_{n-1}^{(n-1)} \end{pmatrix}. \tag{4}$$

Furthermore,

$$\langle B^{(n-1)}| = (b_1^{(n-1)\star}, b_2^{(n-1)\star}, \ldots, b_{n-1}^{(n-1)\star}) \tag{5}$$

and

$$(|A^{(n-1)}\rangle\langle B^{(n-1)}|)_{ij} \equiv a_i^{(n-1)} b_j^{(n-1)\star}. \tag{6}$$

$A^{(n-1)}$ and $B^{(n-1)}$ are not arbitrary but are required to satisfy the conditions

$$\langle A^{(n-1)}|A^{(n-1)} = 1, \quad |B^{(n-1)}\rangle = -V^{(n-1)\dagger}|A^{(n-1)}\rangle, \tag{7}$$

whereby

$$\langle B^{(n-1)}|B^{(n-1)} = 1, \quad |A^{(n-1)}\rangle = -V^{(n-1)}|B^{(n-1)}\rangle. \tag{8}$$

We can easily check that if the matrix $V^{(n-1)}$, in Eq. (3), is unitary so is $V^{(n)}$. In order for $V^{(n)}$ to be the most general n-by-n unitary matrix, modulus the phase matrices Φ, it must have the required number of parameters. The vector $A^{(n-1)}$, having $n-1$ complex components, would seem to represent $2(n-1)$ parameters. But it has only $2(n-2)$ because it is normalized and its overall phase can be absorbed into the matrices Φ, i.e., the transformation

$$|A^{(n-1)}\rangle \to e^{i\eta}|A^{(n-1)}\rangle \tag{9}$$

yields

$$|B^{(n-1)}\rangle \to e^{i\eta}|B^{(n-1)}\rangle \tag{10}$$

and

$$V^{(n)} \to \Phi(0,0,\ldots,e^{-i\eta})V^{(n)}\Phi(0,0,\ldots,e^{i\eta}). \tag{11}$$

The parameter counting, therefore, goes as follows. On the left-hand side of Eq. (3) we need to have $(n-1)^2$ parameters. On the right-hand side, we have $(n-2)^2$ from $V^{(n-1)}$ and $2(n-2)$ from the vector $A^{(n-1)}$. Thus, together with the angle θ_n, the number of parameters is $(n-2)^2+2(n-2)+1$ which equals $(n-1)^2$ as required.

We may use the relation (7) between $A^{(n-1)}$ and $B^{(n-1)}$ to rewrite the matrix $V^{(n)}$ in terms of either $A^{(n-1)}$ or $B^{(n-1)}$. In terms of $A^{(n-1)}$, we have

$$V^{(n)} = \begin{pmatrix} 1-(1-c_n))|A^{(n-1)}\rangle\langle A^{(n-1)}| & s_n|A^{(n-1)}\rangle \\ -s_n\langle A^{(n-1)}| & c_n \end{pmatrix} \begin{pmatrix} V^{(n-1)} & 0 \\ 0 & 1 \end{pmatrix} \equiv A_{n,n-1} \begin{pmatrix} V^{(n-1)} & 0 \\ 0 & 1 \end{pmatrix}. \tag{12}$$

While writing the matrix in terms of $B^{(n-1)}$ yields

$$V^{(n)} = \begin{pmatrix} V^{(n-1)} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1-(1-c_n))|B^{(n-1)}\rangle\langle B^{(n-1)}| & -s_n|B^{(n-1)}\rangle \\ s_n\langle B^{(n-1)}| & c_n \end{pmatrix} \equiv \begin{pmatrix} V^{(n-1)} & 0 \\ 0 & 1 \end{pmatrix} B_{n,n-1}. \tag{13}$$

These relations allow for a systematic construction of unitary matrices order by order. By repeating the above noted procedure for the matrix $V^{(n-1)}$ in terms of $A^{(n-2)}$ and $B^{(n-2)}$, and following down the chain we find the recursion formulas that we are looking for,

$$V^{(n)} = A_{n,n-1}A_{n,n-2}\ldots A_{n,2}A_{n,1}, \tag{14}$$

$$V^{(n)} = B_{n,1}B_{n,2}\ldots B_{n,n-2}B_{n,n-1}. \tag{15}$$

The matrices $A_{n,n-1}$ and $B_{n,n-1}$ were previously defined in Eqs. (12) and (13). For $j<n-1$ we have

$$A_{n,j} = \begin{pmatrix} \begin{pmatrix} 1-(1-c_{j+1}))|A^{(j)}\rangle\langle A^{(j)}| & s_{j+1}|A^{(j)}\rangle \\ -s_{j+1}\langle A^{(j)}| & c_{j+1} \end{pmatrix} & 0 \\ 0 & I_{n-j-1} \end{pmatrix}, \tag{16}$$

$$B_{n,j} = \begin{pmatrix} \begin{pmatrix} 1-(1-c_{j+1}))|B^{(j)}\rangle\langle B^{(j)}| & -s_{j+1}|B^{(j)}\rangle \\ s_{j+1}\langle B^{(j)}| & c_{j+1} \end{pmatrix} & 0 \\ 0 & I_{n-j-1} \end{pmatrix}. \tag{17}$$

Here I_{n-j-1} is the unit matrix of order $n-j-1$. The two unitary matrices $A_{n,j}$ and $B_{n,j}$ are related by

$$A_{n,j} = \begin{pmatrix} V^{(j)} & 0 \\ 0 & I_{n-j} \end{pmatrix}, \quad B_{n,j}\begin{pmatrix} V^{(j)\dagger} & 0 \\ 0 & I_{n-j} \end{pmatrix}. \tag{18}$$

II. SIMPLE EXAMPLES

The simplest case is $n=2$ for which we take $|A^{(1)}\rangle=1$ whereby $|B^{(1)}\rangle=-1$. Using $V^{(1)}=1$ we obtain, from Eqs. (12) and (13),

$$V^{(2)} = A_{2,1} = B_{2,1} = \begin{pmatrix} c_2 & s_2 \\ -s_2 & c_2 \end{pmatrix}. \tag{19}$$

This is the familiar rotation matrix $R_2(\theta_2), \theta_2$ being the rotation angle in two dimensions.

The next simplest case is $n=3$ for which we may either use the "mixed form" or the pure forms. For the mixed form we have

$$V^{(3)} = \begin{pmatrix} R_2(\theta) + (1-c_3)|A^{(2)}\rangle\langle B^{(2)}| & s_3|A^{(2)}\rangle \\ s_3\langle B^{(2)}| & c_3 \end{pmatrix}. \tag{20}$$

Here $R_2(\theta)$ is again the rotation matrix in Eq. (19) and we may put

$$|A^{(2)}\rangle = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}, \quad |B^{(2)}\rangle = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}. \tag{21}$$

From Eq. (7) it follows that

$$|A^{(2)}\rangle = -R_2(\theta)|B^{(2)}\rangle, \quad |B^{(2)}\rangle = -R_2(-\theta)|A^{(2)}\rangle. \tag{22}$$

Hence these vectors represent two parameters, for example

$$|A^{(2)}\rangle = \begin{pmatrix} \cos\gamma \\ \sin\gamma e^{i\delta} \end{pmatrix}, \tag{23}$$

where γ and δ are real. The pure forms are also obtained very simply, for example

$$V^{(3)} = \begin{pmatrix} 1-(1-c_3)|A^{(2)}\rangle\langle A^{(2)}| & s_3|A^{(2)}\rangle \\ -s_3\langle A^{(2)}| & c_3 \end{pmatrix}\begin{pmatrix} R_2(\theta_2) & 0 \\ 0 & 1 \end{pmatrix}, \tag{24}$$

where $A^{(2)}$ is as defined in Eq. (23). Evidently, depending on the application one has in mind some choices may be more convenient than others. This is demonstrated in Refs. 2 and 3 which deal

with the so-called quark and lepton mixing matrices. The essential point is that $V^{(3)}$ is described in a rather simple fashion by four parameters as it should be. For the case of $n=4$ we could, for example, take $A^{(3)}$ to be

$$|A^{(3)}\rangle = \begin{pmatrix} \cos\rho \\ \sin\rho\cos\sigma e^{i\delta_1} \\ \sin\rho\sin\sigma e^{i\delta_2} \end{pmatrix}, \tag{25}$$

where ρ, σ, δ_1, and δ_2 are the four parameters needed to define the most general $A^{(3)}$.

In principle, the above recursive procedure may "easily" be extended to much larger n with the help of computers.

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A nonisospectral extension of the Volterra hierarchy to 2+1 dimensions

P. R. Gordoa and A. Pickering
Area de Matemática Aplicada, ESCET, Universidad Rey Juan Carlos, C/Tulipán s/n, 28933 Móstoles, Madrid, Spain

Z. N. Zhu[a)]
Departamento de Matemáticas, Universidad de Salamanca, Plaza de la Merced 1, 37008 Salamanca, Spain

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We give a new nonisospectral generalization of the Volterra lattice equation to 2+1 dimensions. We use this to construct a new nonisospectral lattice hierarchy in 2+1 dimensions, along with its underlying linear problem. Reductions yield a variety of new integrable hierarchies, including generalizations of known discrete Painlevé hierarchies, all along with their corresponding linear problems. This represents an extension of previously developed techniques to the discrete case. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2041347]

I. INTRODUCTION

The representation of a nonlinear system as the compatibility condition of linear equations is an idea that is central to our understanding of the word "integrability." This concept dates to the introduction of the inverse scattering transform (IST) as a tool for solving the initial value problem, under certain conditions on initial data, for completely integrable partial differential equations (PDEs).[1–3] Of course, this idea is not only useful within the context of PDEs in 1+1 dimensions: it has also been succesfully applied to partial differential equations in multidimensions,[4,5] to differential-difference (or lattice) equations,[6] and to ordinary differential equations,[7] as well as to many other integrable nonlinear systems.

Among our aims in the present paper, we extend ideas related to a particular kind of integrable nonlinear system, namely those having a corresponding *nonisospectral* scattering problem. The first example of a nonlinear equation having such a scattering problem is due to Calogero[8] (see also Ref. 9); since then, a great many papers have been published on such systems, both continuous, e.g. Refs. 10–14, and discrete, e.g., Refs. 15 and 16. In a series of recent papers[17–19] (see also Ref. 20), two of the current authors have shown how certain nonisospectral extensions of well-known integrable equations, to 2+1 dimensions, can be understood as embodying information about the entire hierarchy associated to that integrable equation. This involves interpreting the nonisospectral version of the PDE as defining a recursion relation between successive members of the hierarchy. Thus far, this idea has been used within the context of continuous systems. However, its application to lattice systems would require seeking an equation of the form

$$u_t^{(n)} = R^{(n)} u_\tau^{(n)}, \quad u^{(n)} = u(n,t,\tau), \tag{1}$$

where n is a discrete variable and t and τ are continuous variables, and where $R^{(n)}$ is a discrete recursion operator—together with an underlying non-isospectral linear problem. To the best of our knowledge, such equations are unknown. Here we give an example of such an equation, and show how it can be used to extend the approach used in Refs. 17–20 to the discrete case. In this way we

[a)]Permanent address: Department of Mathematics, Shanghai Jiao Tong University, Shanghai 200030, People's Republic of China.

obtain a new hierarchy of 2+1-dimensional nonisospectral lattice equations.

However, in addition to the role played by equations having nonisospectral scattering problems in the construction of integrable hierarchies and their associated linear problems, there are many other reasons why they are of interest, as discussed in Ref. 18. One such is the link between nonisospectral scattering problems for PDEs or lattice equations, and linear problems for ODEs or discrete equations, respectively.[21] This link, in the case of continuous equations, was exploited, and generalized, in Refs. 17–20. Another of our aims in this paper is to extend these results to the discrete case, by considering reductions to hierarchies of discrete equations.

In fact, the consideration of reductions for the 2+1-dimensional lattice hierarchy constructed here appears to yield richer results than for 2+1-dimensional PDE hierarchies, in the sense that not only do we obtain hierarchies of lattice equations and discrete equations (where previously reductions were to hierarchies of PDEs and ODEs), but also hierarchies of differential-delay equations. The consideration of such reductions is a third aim in our paper.

The layout of our paper is as follows. In Sec. II we construct an equation of the form (1), or, in fact, a generalization thereof, along with an underlying nonisospectral linear problem. This 2+1-dimensional lattice equation is based on the Volterra equation, but is distinct from the 2+1-dimensional Volterra equation considered in Ref. 22. We recall that the Volterra equation itself arises in plasma physics and population dynamics. In Sec. III we use our 2+1-dimensional generalization of the Volterra equation to construct a new 2+1-dimensional lattice hierarchy. In Sec. IV we consider reductions to lattice and differential-delay hierarchies, and in Sec. V to hierarchies of discrete equations. A variety of new results are obtained, including novel differential-delay hierarchies and a new generalized discrete first Painlevé (dP_I) hierarchy. We summarize our results in the Conclusions (Sec. VI).

II. A 2+1 NONISOSPECTRAL VOLTERRA LATTICE EQUATION

We begin by considering a generic nonisospectral discrete linear problem of order p, in 2+1 dimensions (with n a discrete variable, and t and τ continuous variables), of the form

$$E\phi^{(n)} = F^{(n)}\phi^{(n)}, \tag{2}$$

$$\phi_t^{(n)} = \omega(\lambda)\phi_\tau^{(n)} + G^{(n)}\phi^{(n)}, \tag{3}$$

where $\phi^{(n)}=\phi(n,t,\tau)$ is a p vector, $F^{(n)}$ and $G^{(n)}$ are $p\times p$ matrices, E is the shift operator, i.e., $Ez^{(n)}=z^{(n+1)}$, and $\lambda(t,\tau)$ satisfies a nonisospectral condition,

$$\lambda_t = \omega(\lambda)\lambda_\tau + \sum_{j=r}^{s} \gamma_j \lambda^j, \quad \gamma_j = \gamma_j(t,\tau), \tag{4}$$

for some integers r, s. In later sections the notation ∂_x will be used to denote a partial derivative with respect to x, and similarly for other independent variables. The compatibility condition of the system (2) and (3) is

$$F_t^{(n)} - \omega(\lambda)F_\tau^{(n)} + F^{(n)}G^{(n)} - G^{(n+1)}F^{(n)} = 0, \tag{5}$$

or equivalently,

$$F_t^{(n)} - \omega(\lambda)F_\tau^{(n)} - (\Delta G^{(n)})F^{(n)} + [F^{(n)}, G^{(n)}] = 0, \tag{6}$$

where $\Delta G^{(n)}=(E-1)G^{(n)}=G^{(n+1)}-G^{(n)}$ is the discrete derivative of $G^{(n)}$.

We now consider the case $p=2$, and make a choice of $F^{(n)}$ corresponding to the Volterra lattice[23–25] (see also Refs. 21, 26, and 27),

$$F^{(n)} = \begin{pmatrix} 1 & u^{(n)} \\ 1/\lambda & 0 \end{pmatrix}. \tag{7}$$

We also assume $\omega(\lambda)=\lambda$, and $G^{(n)}$ to be of the form

$$G^{(n)} = \lambda \begin{pmatrix} a^{(n)} & b^{(n)} \\ c^{(n)} & d^{(n)} \end{pmatrix} + \begin{pmatrix} e^{(n)} & f^{(n)} \\ g^{(n)} & h^{(n)} \end{pmatrix}, \tag{8}$$

where all entries are functions of (n,t,τ). We note that if we assume $a^{(n)}=b^{(n)}=c^{(n)}=d^{(n)}=0$, then we must have $u_\tau^{(n)}=0$, and so are restricted to equations in (n,t) only.

The substitution of (7) and (8) into (5) with $\omega(\lambda)=\lambda$ leads us to a nonisospectral condition (4) with $r=1$ and $s=2$,

$$\lambda_t = \lambda\lambda_\tau + \gamma_1\lambda + \gamma_2\lambda^2, \tag{9}$$

and corresponding form of the matrix $G^{(n)}$,

$$G^{(n)} = \lambda \begin{pmatrix} \tilde{a} & g^{(n+1)}u^{(n)} \\ 0 & \tilde{a} - \gamma_2 - g^{(n)} \end{pmatrix} + \begin{pmatrix} e^{(n)} & 0 \\ g^{(n)} & e^{(n-1)} - \gamma_1 \end{pmatrix}, \tag{10}$$

where γ_1, γ_2, and $\tilde{a}$ are all arbitrary functions of (t,τ). Clearly, without loss of generality, we may set $\tilde{a}=0$. The compatibility condition (5) consists of the three coupled equations,

$$u_t^{(n)} + u^{(n)}(e^{(n-1)} - e^{(n+1)}) - \gamma_1 u^{(n)} = 0, \tag{11}$$

$$e^{(n)} - e^{(n+1)} + u^{(n)}g^{(n)} - u^{(n+1)}g^{(n+2)} = 0, \tag{12}$$

$$-u_\tau^{(n)} + u^{(n)}(g^{(n+1)} - g^{(n)}) - \gamma_2 u^{(n)} = 0. \tag{13}$$

The second of these equations can be used to eliminate $e^{(n)}$ in the first, to give

$$u_t^{(n)} + u^{(n)}[g^{(n+2)}u^{(n+1)} + u^{(n)}(g^{(n+1)} - g^{(n)}) - g^{(n-1)}u^{(n-1)}] - \gamma_1 u^{(n)} = 0. \tag{14}$$

Alternatively, we may simply solve the second equation to obtain

$$e^{(n)} = (E-1)^{-1}(u^{(n)} - u^{(n+1)}E^2)g^{(n)}, \tag{15}$$

or

$$e^{(n)} = \sum_{j=1}^{n-1} (u^{(j)} - u^{(j+1)}E^2)g^{(j)}, \tag{16}$$

where, without loss of generality, we have set the arbitrary summation function of (t,τ) to zero. Here $g^{(n)}$ is given by the third equation of the system (11)–(13),

$$g^{(n+1)} - g^{(n)} = \gamma_2 + \frac{u_\tau^{(n)}}{u^{(n)}}, \tag{17}$$

as

$$g^{(n)} = (E-1)^{-1}\left(\gamma_2 + \frac{u_\tau^{(n)}}{u^{(n)}}\right) = \tilde{g} + (n-1)\gamma_2 + (E-1)^{-1}\left(\frac{u_\tau^{(n)}}{u^{(n)}}\right), \tag{18}$$

or

$$g^{(n)} = \tilde{g} + (n-1)\gamma_2 + \sum_{j=1}^{n-1} \frac{u_\tau^{(j)}}{u^{(j)}}, \tag{19}$$

where $\tilde{g}=g^{(1)}$ is an arbitrary summation function of (t,τ). We thus obtain that $u^{(n)}$ satisfies a differential-difference equation in 2+1 dimensions,

$$u_t^{(n)} = \mathcal{R}^{(\mathrm{n})} u_\tau^{(n)} + \tilde{g} u^{(n)}(u^{(n-1)} - u^{(n+1)}) + \gamma_1 u^{(n)} + \gamma_2 u^{(n)}((n-2)u^{(n-1)} - u^{(n)} - (n+1)u^{(n+1)}), \tag{20}$$

where $\mathcal{R}^{(\mathrm{n})}$ is the recursion operator of the Volterra lattice,

$$\mathcal{R}^{(\mathrm{n})} = u^{(n)}(1+E^{-1})(u^{(n)} - u^{(n+1)}E^2)(E-1)^{-1}(u^{(n)})^{-1}. \tag{21}$$

(The fact that nonisospectral scattering problems can be used in order to obtain recursion operators is an observation due to one of the current authors.[28]) This last equation represents a nonisospectral generalization of the Volterra lattice to 2+1 dimensions, and is new. We now use this result to construct a hierarchy of nonisospectral differential-difference equations in 2+1 dimensions, along with their underlying linear problems. We do this by following the approach used in Refs. 17–20.

III. A 2+1 NONISOSPECTRAL VOLTERRA LATTICE HIERARCHY

First of all, we note that

$$\mathcal{R}^{(\mathrm{n})} u^{(n)} = u^{(n)}((n-2)u^{(n-1)} - u^{(n)} - (n+1)u^{(n+1)}), \tag{22}$$

and summarize the results of Sec. II as follows: the differential-difference equation,

$$u_t^{(n)} = \mathcal{R}^{(\mathrm{n})} u_\tau^{(n)} + \tilde{g} K_1^{(n)} + \gamma_1 u^{(n)} + \gamma_2 \mathcal{R}^{(\mathrm{n})} u^{(n)}, \tag{23}$$

where

$$K_1^{(n)} = u^{(n)}(u^{(n-1)} - u^{(n+1)}), \tag{24}$$

$\mathcal{R}^{(\mathrm{n})}$ is as given by (21), and $\tilde{g}$, γ_1, and γ_2 are all arbitrary functions of (t,τ), has the linear problem

$$E\phi^{(n)} = \begin{pmatrix} 1 & u^{(n)} \\ 1/\lambda & 0 \end{pmatrix} \phi^{(n)}, \tag{25}$$

$$\phi_t^{(n)} = \lambda \phi_\tau^{(n)} + G^{(n)}\phi^{(n)} = \lambda \phi_\tau^{(n)} + \begin{pmatrix} e^{(n)} & \lambda u^{(n)} g^{(n+1)} \\ g^{(n)} & e^{(n-1)} - \lambda g^{(n)} - \gamma_1 - \lambda\gamma_2 \end{pmatrix} \phi^{(n)}, \tag{26}$$

where

$$e^{(n)} = (E-1)^{-1}(u^{(n)} - u^{(n+1)}E^2) g^{(n)}, \tag{27}$$

$$g^{(n)} = \tilde{g} + (n-1)\gamma_2 + (E-1)^{-1}\left(\frac{u_\tau^{(n)}}{u^{(n)}}\right), \tag{28}$$

and λ satisfies the nonisospectral condition

$$\lambda_t = \lambda\lambda_\tau + \gamma_1\lambda + \gamma_2\lambda^2. \tag{29}$$

We now consider iterating on the above results, following the approach used in Refs. 17–20. We first set $t=t_m$, $\tau=t_{m-1}$, $\tilde{g}=\alpha_m$, $\gamma_1=\beta_m$, and $\gamma_2=0$, in order to obtain the equation we use to iterate between successive members of the hierarchy,

$$u_{t_m}^{(n)} = \mathcal{R}^{(n)} u_{t_{m-1}}^{(n)} + \alpha_m K_1^{(n)} + \beta_m u^{(n)}, \quad m > 1, \tag{30}$$

together with the equations we use to iterate between successive evolution equations for the eigenfunction $\phi^{(n)}$, and between associated nonisospectral conditions,

$$\phi_{t_m}^{(n)} = \lambda \phi_{t_{m-1}}^{(n)} + G_m^{(n)} \phi^{(n)}, \quad \lambda_{t_m} = \lambda \lambda_{t_{m-1}} + \beta_m \lambda, \quad m > 1, \tag{31}$$

where we use the subscript m in $G_m^{(n)}$ to denote the matrix $G^{(n)}$ in (26) with $e^{(n)}$ and $g^{(n)}$ defined as in (27) and (28) but with $\tau = t_{m-1}$, and, of course, with $\tilde{g} = \alpha_m$, $\gamma_1 = \beta_m$, and $\gamma_2 = 0$. We then set $t = t_1$, $\tau = y$, $\tilde{g} = \alpha_1$, $\gamma_1 = \beta_1$, and $\gamma_2 = \beta_0$ in order to obtain the base equation of our hierarchy,

$$u_{t_1}^{(n)} = Q_1^{(n)} = \mathcal{R}^{(n)} u_y^{(n)} + \alpha_1 K_1^{(n)} + \beta_0 \mathcal{R}^{(n)} u^{(n)} + \beta_1 u^{(n)}, \tag{32}$$

together with the corresponding evolution equation for the eigenfunction $\phi^{(n)}$, and the associated nonisospectral condition,

$$\phi_{t_1}^{(n)} = \lambda \phi_y^{(n)} + G_1^{(n)} \phi^{(n)}, \quad \lambda_{t_1} = \lambda \lambda_y + \beta_1 \lambda + \beta_0 \lambda^2, \tag{33}$$

where the subscript 1 in $G_1^{(n)}$ is used to denote $G^{(n)}$ in (26) with $e^{(n)}$ and $g^{(n)}$ as in (27) and (28) but with $\tau = y$, and, of course, with $\tilde{g} = \alpha_1$, $\gamma_1 = \beta_1$, and $\gamma_2 = \beta_0$.

We now consider a generic member of our 2+1-dimensional hierarchy,

$$u_{t_m}^{(n)} = Q_m^{(n)}, \tag{34}$$

together with the corresponding evolution equation for the eigenfunction $\phi^{(n)}$, and associated nonisospectral condition,

$$\phi_{t_m}^{(n)} = \Gamma_m \phi_y^{(n)} + H_m^{(n)} \phi^{(n)}, \quad \lambda_{t_m} = \Lambda_m, \tag{35}$$

which for $m = 1$ correspond to (32) and (33). We thus obtain the recursion relations

$$Q_m^{(n)} = \mathcal{R}^{(n)} Q_{m-1}^{(n)} + \alpha_m K_1^{(n)} + \beta_m u^{(n)}, \tag{36}$$

$$\Gamma_m = \lambda \Gamma_{m-1}, \tag{37}$$

$$H_m^{(n)} = \lambda H_{m-1}^{(n)} + G_m^{(n)}, \tag{38}$$

$$\Lambda_m = \lambda \Lambda_{m-1} + \beta_m \lambda. \tag{39}$$

Iteration then yields the 2+1-dimensional hierarchy

$$u_{t_m}^{(n)} = Q_m^{(n)} = (\mathcal{R}^{(n)})^m u_y^{(n)} + \sum_{j=0}^{m-1} \alpha_{m-j} (\mathcal{R}^{(n)})^j K_1^{(n)} + \sum_{j=0}^{m} \beta_{m-j} (\mathcal{R}^{(n)})^j u^{(n)}, \tag{40}$$

together with the corresponding hierarchy of underlying linear problems,

$$E\phi^{(n)} = \begin{pmatrix} 1 & u^{(n)} \\ 1/\lambda & 0 \end{pmatrix} \phi^{(n)}, \tag{41}$$

$$\phi_{t_m}^{(n)} = \Gamma_m \phi_y^{(n)} + H_m^{(n)} \phi^{(n)} = \lambda^m \phi_y^{(n)} + \left(\sum_{j=1}^{m} \lambda^{m-j} G_j^{(n)} \right) \phi^{(n)}, \tag{42}$$

and associated nonisospectral condition

$$\lambda_{t_m} = \lambda^m \lambda_y + \sum_{j=0}^{m} \lambda^{m+1-j} \beta_j. \tag{43}$$

Here all α_k and β_k are functions of (t_m, y), any m, and each $G_j^{(n)}$ is given by

$$G_j^{(n)} = \begin{pmatrix} A_j^{(n)} & B_j^{(n)} \\ C_j^{(n)} & D_j^{(n)} \end{pmatrix}, \tag{44}$$

where for $j > 1$,

$$A_j^{(n)} = (E-1)^{-1}(u^{(n)} - u^{(n+1)}E^2)\left[\alpha_j + (E-1)^{-1}\left(\frac{Q_{j-1}^{(n)}}{u^{(n)}}\right)\right], \tag{45}$$

$$B_j^{(n)} = \lambda u^{(n)}\left[\alpha_j + (E-1)^{-1}\left(\frac{Q_{j-1}^{(n+1)}}{u^{(n+1)}}\right)\right], \tag{46}$$

$$C_j^{(n)} = \left[\alpha_j + (E-1)^{-1}\left(\frac{Q_{j-1}^{(n)}}{u^{(n)}}\right)\right], \tag{47}$$

$$D_j^{(n)} = (E-1)^{-1}(u^{(n-1)} - u^{(n)}E^2)\left[\alpha_j + (E-1)^{-1}\left(\frac{Q_{j-1}^{(n-1)}}{u^{(n-1)}}\right)\right] - \lambda\left[\alpha_j + (E-1)^{-1}\left(\frac{Q_{j-1}^{(n)}}{u^{(n)}}\right)\right] - \beta_j, \tag{48}$$

and

$$A_1^{(n)} = (E-1)^{-1}(u^{(n)} - u^{(n+1)}E^2)\left[\alpha_1 + (n-1)\beta_0 + (E-1)^{-1}\left(\frac{u_y^{(n)}}{u^{(n)}}\right)\right], \tag{49}$$

$$B_1^{(n)} = \lambda u^{(n)}\left[\alpha_1 + n\beta_0 + (E-1)^{-1}\left(\frac{u_y^{(n+1)}}{u^{(n+1)}}\right)\right], \tag{50}$$

$$C_1^{(n)} = \left[\alpha_1 + (n-1)\beta_0 + (E-1)^{-1}\left(\frac{u_y^{(n)}}{u^{(n)}}\right)\right], \tag{51}$$

$$D_1^{(n)} = (E-1)^{-1}(u^{(n-1)} - u^{(n)}E^2)\left[\alpha_1 + (n-2)\beta_0 + (E-1)^{-1}\left(\frac{u_y^{(n-1)}}{u^{(n-1)}}\right)\right] - \lambda\left[\alpha_1 + (n-1)\beta_0 + (E-1)^{-1}\left(\frac{u_y^{(n)}}{u^{(n)}}\right)\right] - \beta_1 - \lambda\beta_0. \tag{52}$$

The first term on the right-hand-side of Eq. (40) corresponds to a nonisospectral extension of the Volterra lattice hierarchy to 2+1 dimensions; the second term consists of a sum of standard (isospectral) Volterra lattice flows. The third term consists of additional 1+1-dimensional nonisospectral terms, which in the general case are both nonautonomous (depend explicitly on n) and nonlocal.

To the best of our knowledge, the 2+1-dimensional hierarchy (40) is new, although 1+1-dimensional nonisospectral modifications of Volterra lattice flows, or indeed such terms

alone, have been considered before, e.g., in Refs. 21, 26, and 27. We now consider reductions of our hierarchy (40), which yield a variety of new hierarchies, including differential-delay hierarchies and generalized discrete Painlevé hierarchies.

IV. LATTICE AND DIFFERENTIAL-DELAY HIERARCHIES

We begin by remarking that, of course, instead of the hierarchy (40), we can always extend our results in order to obtain linear problems and associated nonisospectral conditions for 2+1 lattice equations of the form

$$\sum_{j=0}^{p} a_j(\mathcal{R}^{(n)})^j u_t^{(n)} + \sum_{j=0}^{q} b_j(\mathcal{R}^{(n)})^j u_y^{(n)} + \sum_{j=0}^{r} c_j(\mathcal{R}^{(n)})^j K_1^{(n)} + \sum_{j=0}^{s} d_j(\mathcal{R}^{(n)})^j u^{(n)} = 0, \tag{53}$$

where all a_k, b_k, c_k, and d_k are functions of (y,t). Thus it is also possible to derive more general results than those presented in Secs. IV and V here. However, for our present purposes, it is sufficient to consider reductions of the hierarchy (40). In this section we give the reduced hierarchies and nonisospectral conditions. We also consider explicitly the case $m=1$, for which we give, in addition, the corresponding linear problems.

First of all we rewrite our earlier results for the case $m=1$, in order to simplify the subsequent presentation of reductions in this particular case. For $m=1$, Eq. (40) gives our 2+1-dimensional nonisospectral Volterra lattice in $u^{(n)}=u(n,t_1,y)$, i.e., Eq. (32),

$$u_{t_1}^{(n)} = \mathcal{R}^{(n)} u_y^{(n)} + \alpha_1 K_1^{(n)} + \beta_0 \mathcal{R}^{(n)} u^{(n)} + \beta_1 u^{(n)}, \tag{54}$$

where α_1, β_0, and β_1 are functions of t_1 and y. In order to avoid nonlocal terms, we write this equation using a potential as

$$\begin{aligned} u_{t_1}^{(n)} = {} & u^{(n)}(u^{(n)}w^{(n)} + u^{(n-1)}w^{(n-1)} - u^{(n)}w^{(n+1)} - u^{(n+1)}w^{(n+2)}) + \alpha_1 u^{(n)}(u^{(n-1)} - u^{(n+1)}) \\ & + \beta_0 u^{(n)}((n-2)u^{(n-1)} - u^{(n)} - (n+1)u^{(n+1)}) + \beta_1 u^{(n)}, \end{aligned} \tag{55}$$

where

$$w^{(n+1)} - w^{(n)} = \frac{u_y^{(n)}}{u^{(n)}}. \tag{56}$$

This equation has the linear problem

$$E\phi^{(n)} = \begin{pmatrix} 1 & u^{(n)} \\ 1/\lambda & 0 \end{pmatrix} \phi^{(n)}, \tag{57}$$

$$\phi_{t_1}^{(n)} = \lambda \phi_y^{(n)} + \begin{pmatrix} v^{(n)} & \lambda u^{(n)}(\alpha_1 + n\beta_0 + w^{(n+1)}) \\ \alpha_1 + (n-1)\beta_0 + w^{(n)} & v^{(n-1)} - \beta_1 - \lambda\beta_0 - \lambda(\alpha_1 + (n-1)\beta_0 + w^{(n)}) \end{pmatrix} \phi^{(n)} \tag{58}$$

where

$$v^{(n+1)} - v^{(n)} = (u^{(n)} - u^{(n+1)}E^2)(\alpha_1 + (n-1)\beta_0 + w^{(n)}) \tag{59}$$

and $\lambda=\lambda(t_1,y)$ satisfies the nonisospectral condition

$$\lambda_{t_1} = \lambda\lambda_y + \beta_1\lambda + \beta_0\lambda^2. \tag{60}$$

We now turn to our reductions.

A. Reductions to 1+1 lattice hierarchies

We begin by considering the reduction $\partial_y=0$ of the hierarchy (40), which yields a hierarchy of nonisospectral extensions of Volterra lattice flows,

$$u^{(n)}_{t_m}=\sum_{j=0}^{m-1}\alpha_{m-j}(\mathcal{R}^{(n)})^jK_1^{(n)}+\sum_{j=0}^{m}\beta_{m-j}(\mathcal{R}^{(n)})^ju^{(n)}, \tag{61}$$

where now all α_k and β_k are functions of each t_m only. The nonisospectral condition satisfied by $\lambda=\lambda(t_m)$ is

$$\lambda_{t_m}=\sum_{j=0}^{m}\lambda^{m+1-j}\beta_j. \tag{62}$$

In the case where all $\beta_k=0$, we obtain the (isospectral) Volterra lattice hierarchy,

$$u^{(n)}_{t_m}=\sum_{j=0}^{m-1}\alpha_{m-j}(\mathcal{R}^{(n)})^jK_1^{(n)}. \tag{63}$$

As remarked earlier, all of these equations are known.

Second, we consider the reduction $\partial_{t_m}=\epsilon\partial_y$, ϵ constant, which then gives the nonisospectral 1+1-dimensional lattice hierarchy,

$$(\mathcal{R}^{(n)})^mu_y^{(n)}-\epsilon u_y^{(n)}+\sum_{j=0}^{m-1}\alpha_{m-j}(\mathcal{R}^{(n)})^jK_1^{(n)}+\sum_{j=0}^{m}\beta_{m-j}(\mathcal{R}^{(n)})^ju^{(n)}=0, \tag{64}$$

where now all α_k and β_k are functions of y only, and where $\lambda=\lambda(y)$ satisfies the corresponding nonisospectral condition

$$(\lambda^m-\epsilon)\lambda_y+\sum_{j=0}^{m}\lambda^{m+1-j}\beta_j=0. \tag{65}$$

In the case where all $\beta_k=0$, we obtain from (64) the isospectral flows

$$(\mathcal{R}^{(n)})^mu_y^{(n)}-\epsilon u_y^{(n)}+\sum_{j=0}^{m-1}\alpha_{m-j}(\mathcal{R}^{(n)})^jK_1^{(n)}=0. \tag{66}$$

Clearly in the hierarchies (64) and (66) we can also consider the special case $\epsilon=0$.

1. Examples: m=1

Our first reduction of (55), $\partial_y=0$, gives the equation in $u^{(n)}=u(n,t_1)$,

$$u^{(n)}_{t_1}=\alpha_1u^{(n)}(u^{(n-1)}-u^{(n+1)})+\beta_0u^{(n)}((n-2)u^{(n-1)}-u^{(n)}-(n+1)u^{(n+1)})+\beta_1u^{(n)}, \tag{67}$$

where now α_1, β_0, and β_1 are functions of t_1 only. This equation has the linear problem

$$E\phi^{(n)}=\begin{pmatrix}1 & u^{(n)}\\ 1/\lambda & 0\end{pmatrix}\phi^{(n)}, \tag{68}$$

$$\phi^{(n)}_{t_1}=\begin{pmatrix}v^{(n)} & \lambda u^{(n)}(\alpha_1+n\beta_0)\\ \alpha_1+(n-1)\beta_0 & v^{(n-1)}-\beta_1-\lambda\beta_0-\lambda(\alpha_1+(n-1)\beta_0)\end{pmatrix}\phi^{(n)}, \tag{69}$$

where $v^{(n)}=v(n,t_1)$ satisfies the equation

$$v^{(n+1)} - v^{(n)} = (u^{(n)} - u^{(n+1)}E^2)(\alpha_1 + (n-1)\beta_0), \tag{70}$$

and where $\lambda = \lambda(t_1)$ satisfies the nonisospectral condition

$$\lambda_{t_1} = \beta_1\lambda + \beta_0\lambda^2. \tag{71}$$

In the case $\beta_0 = \beta_1 = 0$, we have an isospectral linear problem.

Our second reduction of (55), $\partial_{t_1} = \epsilon\partial_y$, gives the equation in $u^{(n)} = u(n,y)$,

$$\begin{aligned} &u^{(n)}(u^{(n)}w^{(n)} + u^{(n-1)}w^{(n-1)} - u^{(n)}w^{(n+1)} - u^{(n+1)}w^{(n+2)}) - \epsilon u_y^{(n)} + \alpha_1 u^{(n)}(u^{(n-1)} - u^{(n+1)}) \\ &\quad + \beta_0 u^{(n)}((n-2)u^{(n-1)} - u^{(n)} - (n+1)u^{(n+1)}) + \beta_1 u^{(n)} = 0, \end{aligned} \tag{72}$$

where $w^{(n)} = w(n,y)$ is related to $u^{(n)}$ as in Eq. (56), and α_1, β_0, and β_1 are now functions of y only. This equation has the linear problem

$$E\phi^{(n)} = \begin{pmatrix} 1 & u^{(n)} \\ 1/\lambda & 0 \end{pmatrix}\phi^{(n)}, \tag{73}$$

$$\phi_y^{(n)} = \frac{1}{\epsilon - \lambda}\begin{pmatrix} v^{(n)} & \lambda u^{(n)}(\alpha_1 + n\beta_0 + w^{(n+1)}) \\ \alpha_1 + (n-1)\beta_0 + w^{(n)} & v^{(n-1)} - \beta_1 - \lambda\beta_0 - \lambda(\alpha_1 + (n-1)\beta_0 + w^{(n)}) \end{pmatrix}\phi^{(n)}, \tag{74}$$

where $v^{(n)} = v(n,y)$ satisfies the equation

$$v^{(n+1)} - v^{(n)} = (u^{(n)} - u^{(n+1)}E^2)(\alpha_1 + (n-1)\beta_0 + w^{(n)}) \tag{75}$$

and $\lambda = \lambda(y)$ satisfies the nonisospectral condition

$$\lambda_y = \frac{1}{\epsilon - \lambda}(\beta_1\lambda + \beta_0\lambda^2). \tag{76}$$

In the case $\beta_0 = \beta_1 = 0$, we have an isospectral linear problem.

B. Reductions to 1+1 differential-delay hierarchies

We now give reductions to 1+1 differential-delay hierarchies (in fact, to hierarchies that are purely differential with respect to one of the independent variables, and differential delay with respect to the other). We believe these results to be new.

We begin by considering what may be described—through an abuse of notation—as the reduction $\partial_{t_m} = \kappa\partial_n (\equiv \kappa\partial_x)$, κ constant, so that E now shifts the continuous variable x. We thus obtain from the hierarchy (40) the 1+1 hierarchy,

$$\kappa u_x(x,y) = \tilde{\mathcal{R}}^m u_y(x,y) + \sum_{j=0}^{m-1} \alpha_{m-j}\tilde{\mathcal{R}}^j\tilde{K}_1 + \sum_{j=0}^{m} \beta_{m-j}\tilde{\mathcal{R}}^j u(x,y), \tag{77}$$

where all α_k and β_k are now functions of y only, where $\tilde{\mathcal{R}}$ is defined as

$$\tilde{\mathcal{R}} = u(x,y)(1 + E^{-1})(u(x,y) - u(x+1,y)E^2)(E-1)^{-1}(u(x,y))^{-1}, \tag{78}$$

and $\tilde{K}_1$ as

$$\tilde{K}_1 = u(x,y)(u(x-1,y) - u(x+1,y)), \tag{79}$$

and where $\lambda = \lambda(y)$ satisfies the corresponding nonisospectral condition,

$$\lambda_y + \sum_{j=0}^{m} \lambda^{1-j}\beta_j = 0. \tag{80}$$

Clearly, in the case where all $\beta_k=0$, i.e., for the hierarchy

$$\kappa u_x(x,y) = \tilde{\mathcal{R}}^m u_y(x,y) + \sum_{j=0}^{m-1} \alpha_{m-j}\tilde{\mathcal{R}}^j\tilde{K}_1, \tag{81}$$

we have an isospectral linear problem.

We now consider an alternative reduction of the hierarchy (40), a reduction perhaps best described—again through an abuse of notation—as $\partial_y=\kappa\partial_n(\equiv\kappa\partial_x)$, κ constant, so that E once again now shifts the continuous variable x. We thus obtain the $1+1$ hierarchy

$$u_{t_m}(x,t_m) = \kappa\overline{\mathcal{R}}^m u_x(x,t_m) + \sum_{j=0}^{m-1} \alpha_{m-j}\overline{\mathcal{R}}^j\overline{K}_1 + \sum_{j=0}^{m} \beta_{m-j}\overline{\mathcal{R}}^j u(x,t_m), \tag{82}$$

where all α_k and β_k are now functions of t_m only, where $\overline{\mathcal{R}}$ is defined as

$$\overline{\mathcal{R}} = u(x,t_m)(1+E^{-1})(u(x,t_m) - u(x+1,t_m)E^2)(E-1)^{-1}(u(x,t_m))^{-1} \tag{83}$$

and $\overline{K}_1$ as

$$\overline{K}_1 = u(x,t_m)(u(x-1,t_m) - u(x+1,t_m)), \tag{84}$$

and where $\lambda=\lambda(t_m)$ satisfies the corresponding nonisospectral condition

$$\lambda_{t_m} = \sum_{j=0}^{m} \lambda^{m+1-j}\beta_j. \tag{85}$$

Once again, in the case where all $\beta_k=0$,

$$u_{t_m}(x,t_m) = \kappa\overline{\mathcal{R}}^m u_x(x,t_m) + \sum_{j=0}^{m-1} \alpha_{m-j}\overline{\mathcal{R}}^j\overline{K}_1, \tag{86}$$

we have an isospectral linear problem.

1. Examples: m=1

Our first reduction of (55), $\partial_{t_1}=\kappa\partial_n(\equiv\kappa\partial_x)$, gives the equation in $u(x,y)$,

$$\begin{aligned}\kappa u_x(x,y) = {} & u(x,y)[u(x,y)w(x,y) + u(x-1,y)w(x-1,y) - u(x,y)w(x+1,y) - u(x+1,y)w(x+2,y)] \\ & + \alpha_1 u(x,y)[u(x-1,y) - u(x+1,y)] + \beta_0 u(x,y)[(x-2)u(x-1,y) - u(x,y) \\ & - (x+1)u(x+1,y)] + \beta_1 u(x,y),\end{aligned} \tag{87}$$

where now α_1, β_0, and β_1 are functions of y only and where

$$w(x+1,y) - w(x,y) = \frac{u_y(x,y)}{u(x,y)}. \tag{88}$$

This equation has the linear problem

$$E\phi(x,y) = \begin{pmatrix} 1 & u(x,y) \\ 1/\lambda & 0 \end{pmatrix}\phi(x,y), \tag{89}$$

$$\kappa\phi_x(x,y) = \lambda\phi_y(x,y) + \begin{pmatrix} v(x,y) & \lambda u(x,y)(\alpha_1 + x\beta_0 + w(x+1,y)) \\ \alpha_1 + (x-1)\beta_0 + w(x,y) & v(x-1,y) - \beta_1 - \lambda\beta_0 - \lambda(\alpha_1 + (x-1)\beta_0 + w(x,y)) \end{pmatrix} \times \phi(x,y), \tag{90}$$

where $v(x,y)$ satisfies the equation

$$v(x+1,y) - v(x,y) = (u(x,y) - u(x+1,y)E^2)(\alpha_1 + (x-1)\beta_0 + w(x,y)) \tag{91}$$

and $\lambda = \lambda(y)$ satisfies the nonisospectral condition

$$\lambda_y + \beta_1 + \beta_0\lambda = 0. \tag{92}$$

In the case $\beta_0 = \beta_1 = 0$ we have an isospectral linear problem.

Our second reduction of (55), $\partial_y = \kappa\partial_n (\equiv \kappa\partial_x)$, gives the equation in $u(x,t_1)$,

$$\begin{aligned} u_{t_1}(x,t_1) = {} & u(x,t_1)[u(x,t_1)w(x,t_1) + u(x-1,t_1)w(x-1,t_1) \\ & - u(x,t_1)w(x+1,t_1) - u(x+1,t_1)w(x+2,t_1)] + \alpha_1 u(x,t_1)[u(x-1,t_1) - u(x+1,t_1)] \\ & + \beta_0 u(x,t_1)[(x-2)u(x-1,t_1) - u(x,t_1) - (x+1)u(x+1,t_1)] + \beta_1 u(x,t_1), \end{aligned} \tag{93}$$

where now α_1, β_0, and β_1 are functions of t_1 only and where

$$w(x+1,t_1) - w(x,t_1) = \kappa\frac{u_x(x,t_1)}{u(x,t_1)}. \tag{94}$$

This equation has the linear problem

$$E\phi(x,t_1) = \begin{pmatrix} 1 & u(x,t_1) \\ 1/\lambda & 0 \end{pmatrix}\phi(x,t_1), \tag{95}$$

$$\phi_{t_1}(x,t_1) = \lambda\kappa\phi_x(x,t_1) + \begin{pmatrix} v(x,t_1) & \lambda u(x,t_1)(\alpha_1 + x\beta_0 + w(x+1,t_1)) \\ \alpha_1 + (x-1)\beta_0 + w(x,t_1) & v(x-1,t_1) - \beta_1 - \lambda\beta_0 - \lambda(\alpha_1 + (x-1)\beta_0 + w(x,t_1)) \end{pmatrix} \times \phi(x,t_1), \tag{96}$$

where $v(x,t_1)$ satisfies the equation

$$v(x+1,t_1) - v(x,t_1) = (u(x,t_1) - u(x+1,t_1)E^2)(\alpha_1 + (x-1)\beta_0 + w(x,t_1)) \tag{97}$$

and $\lambda = \lambda(t_1)$ satisfies the nonisospectral condition

$$\lambda_{t_1} = \beta_1\lambda + \beta_0\lambda^2. \tag{98}$$

In the case $\beta_0 = \beta_1 = 0$, we have an isospectral linear problem.

C. Reductions to ordinary differential-delay hierarchies

Setting $\partial_y = 0$ in (77)—or (abusing notation) $\partial_{t_m} = \kappa\partial_n (\equiv \kappa\partial_x)$ in (61)—yields the hierarchy of ordinary differential-delay equations (recall that E shifts x),

$$\kappa u_x(x) = \sum_{j=0}^{m-1} \alpha_{m-j} \widetilde{\mathcal{R}}^j \widetilde{K}_1 + \sum_{j=0}^{m} \beta_{m-j} \widetilde{\mathcal{R}}^j u(x), \tag{99}$$

where $\widetilde{\mathcal{R}}$ and $\widetilde{K}_1$, which are now y independent, are defined as above. We may also consider the special case where all $\beta_k=0$; we note that in this special case, the ordinary differential-delay equation that results for $m=2$ has been given in Ref. 21.

Setting $\partial_{t_m}=\epsilon\kappa\partial_x$ in (82)—or (abusing notation) $\partial_y=\kappa\partial_n(\equiv\kappa\partial_x)$ in (64)—yields the hierarchy of ordinary differential-delay equations (again, E shifts x),

$$\kappa\overline{\mathcal{R}}^m u_x(x) - \epsilon\kappa u_x(x) + \sum_{j=0}^{m-1} \alpha_{m-j} \overline{\mathcal{R}}^j \overline{K}_1 + \sum_{j=0}^{m} \beta_{m-j} \overline{\mathcal{R}}^j u(x) = 0, \tag{100}$$

where $\overline{\mathcal{R}}$ and $\overline{K}_1$, which now depend only on x, are defined as above. In the above hierarchy we may also consider the special cases $\epsilon=0$ or all $\beta_k=0$.

Clearly, both of the above can be included in the single hierarchy

$$\sigma\overline{\mathcal{R}}^m u_x(x) - \rho u_x(x) + \sum_{j=0}^{m-1} \alpha_{m-j} \overline{\mathcal{R}}^j \overline{K}_1 + \sum_{j=0}^{m} \beta_{m-j} \overline{\mathcal{R}}^j u(x) = 0, \tag{101}$$

where σ and ρ are two arbitrary constants. This hierarchy, which again we believe to be new, arises as the compatibility condition

$$\left(\sum_{j=0}^{m} \lambda^{m+1-j}\beta_j\right) F_\lambda(x) - (\lambda^m\sigma-\rho)F_x(x) + F(x)H_m(x) - H_m(x+1)F(x) = 0 \tag{102}$$

of the associated hierarchy of linear systems,

$$E\phi(x) = F(x)\phi(x), \tag{103}$$

$$\left(\sum_{j=0}^{m} \lambda^{m+1-j}\beta_j\right) \phi_\lambda(x) = (\lambda^m\sigma-\rho)\phi_x(x) + H_m(x)\phi(x), \tag{104}$$

where

$$F(x) = \begin{pmatrix} 1 & u(x) \\ 1/\lambda & 0 \end{pmatrix}, \quad H_m(x) = \sum_{j=1}^{m} \lambda^{m-j} G_j(x), \tag{105}$$

and the matrices $G_j(x)$ are obtained from the $G_j^{(n)}$ of Sec. III in the appropriate way. We remark in passing the great interest of "delay Painlevé equations."[21]

1. Example: m=1

In the case $m=1$, Eq. (101) reads as

$$u(x)[u(x)w(x) + u(x-1)w(x-1) - u(x)w(x+1) - u(x+1)w(x+2)] - \rho u_x(x) + \alpha_1 u(x)[u(x-1) - u(x+1)] + \beta_0 u(x)[(x-2)u(x-1) - u(x) - (x+1)u(x+1)] + \beta_1 u(x) = 0, \tag{106}$$

where now α_1, β_0, and β_1 are constants and where

$$w(x+1) - w(x) = \sigma\frac{u_x(x)}{u(x)}. \tag{107}$$

This equation arises as the compatibility condition of the linear system,

$$E\phi(x) = \begin{pmatrix} 1 & u(x) \\ 1/\lambda & 0 \end{pmatrix} \phi(x), \tag{108}$$

$$\begin{aligned}(\beta_0\lambda^2 + \beta_1\lambda)\phi_\lambda(x) &= (\lambda\sigma - \rho)\phi_x(x) \\ &+ \begin{pmatrix} v(x) & \lambda u(x)(\alpha_1 + x\beta_0 + w(x+1)) \\ \alpha_1 + (x-1)\beta_0 + w(x) & v(x-1) - \beta_1 - \lambda\beta_0 - \lambda(\alpha_1 + (x-1)\beta_0 + w(x)) \end{pmatrix} \\ &\times \phi(x),\end{aligned} \tag{109}$$

where $v(x)$ satisfies the equation

$$v(x+1) - v(x) = (u(x) - u(x+1)E^2)(\alpha_1 + (x-1)\beta_0 + w(x)). \tag{110}$$

V. GENERALIZED DISCRETE PAINLEVÉ HIERARCHIES

If in the 1+1 lattice hierarchy (61) we now take the further reduction $\partial_{t_m}=0$, we obtain a hierarchy of discrete equations:

$$\sum_{j=0}^{m-1} \alpha_{m-j}(\mathcal{R}^{(n)})^j K_1^{(n)} + \sum_{j=0}^{m} \beta_{m-j}(\mathcal{R}^{(n)})^j u^{(n)} = 0. \tag{111}$$

Alternatively, we may derive this discrete hierarchy by taking $\partial_y=0$ in (64), or by making appropriate reductions in the hierarchies (77) and (82), or by setting $\rho=\sigma=0$ in (101). This hierarchy arises as the compatibility condition

$$\left(\sum_{j=0}^{m} \lambda^{m+1-j}\beta_j\right) F_\lambda^{(n)} + F^{(n)}H_m^{(n)} - H_m^{(n+1)}F^{(n)} = 0 \tag{112}$$

of the associated hierarchy of linear problems,

$$E\phi^{(n)} = F^{(n)}\phi^{(n)}, \tag{113}$$

$$\left(\sum_{j=0}^{m} \lambda^{m+1-j}\beta_j\right) \phi_\lambda^{(n)} = H_m^{(n)}\phi^{(n)}, \tag{114}$$

where

$$F^{(n)} = \begin{pmatrix} 1 & u^{(n)} \\ 1/\lambda & 0 \end{pmatrix}, \quad H_m^{(n)} = \sum_{j=1}^{m} \lambda^{m-j} G_j^{(n)}, \tag{115}$$

and the matrices $G_j^{(n)}$ are obtained from those of Sec. III in the appropriate way. Here all α_k and β_k are constants.

This hierarchy contains, in the general case, nonlocal terms: although we could consider this hierarchy in its full generality, by introducing auxiliary potential functions, we prefer here to consider the case where $\beta_k=0$, $k=0,1,\ldots,m-2$, i.e.,

$$P_m^{(n)} \equiv \frac{1}{u^{(n)}}\left(\sum_{j=0}^{m-1} \alpha_{m-j}(\mathcal{R}^{(n)})^j K_1^{(n)} + \beta_{m-1}\mathcal{R}^{(n)}u^{(n)} + \beta_m u^{(n)}\right) = 0. \tag{116}$$

For $m=1$, (116) gives the linear equation

$$P_1^{(n)} \equiv \alpha_1(u^{(n-1)} - u^{(n+1)}) + \beta_0((n-2)u^{(n-1)} - u^{(n)} - (n+1)u^{(n+1)}) + \beta_1 = 0, \tag{117}$$

and for $m=2$, the first of our nonlinear equations,

$$P_2^{(n)} \equiv \alpha_1[u^{(n+1)}(u^{(n)}+u^{(n+1)}+u^{(n+2)})-u^{(n-1)}(u^{(n)}+u^{(n-1)}+u^{(n-2)})]+\alpha_2(u^{(n-1)}-u^{(n+1)})$$
$$+\beta_1((n-2)u^{(n-1)}-u^{(n)}-(n+1)u^{(n+1)})+\beta_2=0. \tag{118}$$

This last equation has the linear problem formed by (113), together with

$$(\beta_1\lambda^2+\beta_2\lambda)\phi_\lambda^{(n)}=\begin{pmatrix} -\alpha_1\lambda u^{(n)}+v^{(n)} & \lambda^2\alpha_1u^{(n)}+\lambda u^{(n)}(\alpha_2+n\beta_1 \\ & -\alpha_1(u^{(n+1)}+u^{(n)})) \\ \lambda\alpha_1+\alpha_2+(n-1)\beta_1 & v^{(n-1)}-\beta_2-\lambda\beta_1 \\ -\alpha_1(u^{(n)}+u^{(n-1)}) & -\lambda(\alpha_2+(n-1)\beta_1 \\ & -\alpha_1(u^{(n)}+u^{(n-1)})) \\ & -\alpha_1\lambda u^{(n-1)}-\alpha_1\lambda^2 \end{pmatrix}\phi^{(n)}, \tag{119}$$

where $v^{(n)}$ satisfies the equation

$$v^{(n+1)}-v^{(n)}=(u^{(n)}-u^{(n+1)}E^2)(\alpha_2+(n-1)\beta_1-\alpha_1(u^{(n)}+u^{(n-1)})). \tag{120}$$

As we now show, Eq. (118) is a generalization of a well-known discrete first Painlevé (dP_I) equation. Thus, our hierarchy of discrete equations (116) corresponds to a new generalized dP_I hierarchy. First we note that (118) can be written in the form

$$(E^2-1)\left[\alpha_1u^{(n-1)}(u^{(n)}+u^{(n-1)}+u^{(n-2)})-\alpha_2u^{(n-1)}+\left(\frac{1}{2}\beta_2\right)n\right]$$
$$-\beta_1(E+1)[u^{(n-1)}+(E-1)((n-1)u^{(n-1)})]=0, \tag{121}$$

and so we can sum to obtain

$$\tilde{P}_2^{(n)} \equiv (E-1)\left[\alpha_1u^{(n-1)}(u^{(n)}+u^{(n-1)}+u^{(n-2)})-\alpha_2u^{(n-1)}+\left(\frac{1}{2}\beta_2\right)n\right]$$
$$-\beta_1[u^{(n-1)}+(E-1)((n-1)u^{(n-1)})]-\omega_2(-1)^n=0, \tag{122}$$

where ω_2 (labeled using m) is an arbitrary constant. This third-order discrete equation can be summed once again in order to give, for each of the cases $\beta_1=0$ and $\beta_1\neq0$, a second-order equation.

In the case $\beta_1=0$, we obtain (after a shift on n) the second-order discrete equation

$$\alpha_1u^{(n)}(u^{(n+1)}+u^{(n)}+u^{(n-1)})-\alpha_2u^{(n)}+\left(\frac{1}{2}\beta_2\right)n-\nu_2-\mu_2(-1)^n=0, \tag{123}$$

where $\mu_2=\frac{1}{2}\omega_2$ and ν_2 is a second arbitrary constant (again labeled using m). Equation (123) is the version of dP_I containing a parity-dependent term, which includes both the first and second Painlevé equations among its continuum limits; see Ref. 29, as well as Refs. 21 and 30. In our framework this equation corresponds to the special case $\beta_1=0$ of our more general integrable discrete equation (118) [or (122)]. We note that it is straightforward, using our above results, to give a linear problem for (123) not involving the potential $v^{(n)}$, whose compatibility condition is precisely Eq. (123) rather than the higher-order equivalents (118) or (122) with $\beta_1=0$.

In the case $\beta_1\neq0$, we obtain the second-order discrete equation

$$D_{34} \equiv u^{(n-1)}(\alpha_1u^{(n)}+\alpha_1u^{(n-1)}-\beta_1n+2\delta)(\alpha_1u^{(n-1)}+\alpha_1u^{(n-2)}-\beta_1(n-1)+2\delta)$$
$$-\frac{\beta_2}{\beta_1}\left(\alpha_1u^{(n-1)}-C-\frac{1}{2}\beta_1(n-1)+\delta\right)\left(\alpha_1u^{(n-1)}+C-\frac{1}{2}\beta_1n+\delta\right)$$
$$-\omega_2(\alpha_1u^{(n-1)}(-1)^{n-1}+\delta(-1)^{n-1}+B_n)=0, \tag{124}$$

where C is an arbitrary constant,

$$\delta = \frac{1}{2}\left(-\alpha_2 + \beta_1 + \alpha_1 \frac{\beta_2}{\beta_1}\right), \tag{125}$$

and

$$B_n = \begin{cases} \dfrac{1}{2}\beta_1 n, & n \text{ even}, \\ -\dfrac{1}{2}\beta_1 (n-1), & n \text{ odd}. \end{cases} \tag{126}$$

Here we have made use of the summing factor $(\alpha_1 u^{(n)} + \alpha_1 u^{(n-1)} - \beta_1 n + 2\delta)$:

$$(\alpha_1 u^{(n)} + \alpha_1 u^{(n-1)} - \beta_1 n + 2\delta)\widetilde{P}_2^{(n)} = (E-1)(D_{34}). \tag{127}$$

Equation (124), which we will call the dP_{34} equation, is a generalized version of the known discrete 34th Painlevé equation. We note that when summing we have retained the parity-dependent terms that appear in (122). In the special case $\omega_2 = 0$ this equation yields the discrete 34th Painlevé equation of Ref. 30.

We see from the previous discussion that we have obtained a new generalized dP_I hierarchy (116): the first member of this hierarchy is a generalized dP_I equation since, for the choice $\beta_1 = 0$, it sums to a known dP_I equation. In addition, we have seen that this first member, for the choice $\beta_1 \neq 0$, sums to a new dP_{34} equation.

We also give here the case $m=3$ of (116), which may be written as

$$\begin{aligned}(E^2-1)\Big[&-\alpha_1 u^{(n-1)}(u^{(n)}u^{(n+1)} + u^{(n)2} + 2u^{(n-1)}u^{(n)} + u^{(n-2)}u^{(n-3)} + u^{(n-2)2} + 2u^{(n-1)}u^{(n-2)} + u^{(n-1)2} \\ &+ u^{(n-2)}u^{(n)}) + \alpha_2 u^{(n-1)}(u^{(n)} + u^{(n-1)} + u^{(n-2)}) - \alpha_3 u^{(n-1)} + \left(\frac{1}{2}\beta_3\right)n\Big] - \beta_2(E+1)\big[u^{(n-1)} \\ &+ (E-1)((n-1)u^{(n-1)})\big] = 0. \end{aligned} \tag{128}$$

The linear problem for this equation may also be given explicitly using the results given earlier, but we choose not to do so here. We note that in the special case $\beta_2 = 0$, we can sum this last equation twice to obtain (again after a shift on n) the fourth-order discrete equation

$$\begin{aligned} &-\alpha_1 u^{(n)}(u^{(n+1)}u^{(n+2)} + u^{(n+1)2} + 2u^{(n)}u^{(n+1)} + u^{(n-1)}u^{(n-2)} + u^{(n-1)2} + 2u^{(n)}u^{(n-1)} + u^{(n)2} + u^{(n-1)}u^{(n+1)}) \\ &+ \alpha_2 u^{(n)}(u^{(n+1)} + u^{(n)} + u^{(n-1)}) - \alpha_3 u^{(n)} + \left(\frac{1}{2}\beta_3\right)n - \nu_3 - \mu_3(-1)^n = 0, \end{aligned} \tag{129}$$

where ν_3 and μ_3 are two arbitrary constants. This last is the fourth-order dP_I equation, as given in Ref. 30. We expect, of course, that our hierarchy (116), in the special case $\beta_{m-1} = 0$, is equivalent to the dP_I hierarchy given in Ref. 30. We also expect that our hierarchy (116), in the case $\beta_{m-1} \neq 0$, sums to give a dP_{34} hierarchy that generalizes the results of Ref. 30 in the same way as does our dP_{34} equation (124).

VI. CONCLUSIONS

Here we briefly summarize our results.

- We have extended the method used in Refs. 17–20 which allows the construction of hierarchies of integrable equations along with their underlying linear problems, from the continuous to the discrete case.
- We have given a new 2+1-dimensional generalization of the Volterra hierarchy.

- We have obtained reductions to a variety of new hierarchies of integrable equations, along with their underlying linear problems. These last derive from those given for the 2+1-dimensional case.
- We have obtained a new generalized dP_I hierarchy, and also a generalized dP_{34} hierarchy, each once again along with their underlying linear problems.

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Quantum spheres for $OSp_q(1/2)$

N. Aizawa
Department of Applied Mathematics, Osaka Women's University, Sakai, Osaka 590-0035, Japan

R. Chakrabarti
Department of Theoretical Physics, University of Madras, Guindy Campus, Chennai 600 025, India

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Using the corepresentation of the quantum supergroup $OSp_q(1/2)$ a general method for constructing noncommutative spaces covariant under its coaction is developed. In particular, a one-parameter family of covariant algebras, which may be interpreted as noncommutative superspheres, is constructed. It is observed that embedding of the supersphere in the $OSp_q(1/2)$ algebra is possible. This realization admits to the infinitesimal characterization by Koornwinder. A covariant oscillator realization of the supersphere is also presented. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2042969]

I. INTRODUCTION

Lie supergroups and superalgebras have been used as basic tools in various fields of theoretical physics. Supersymmetry in quantum field theories and string field theory is the most well-known example of application of Lie superalgebras. Other examples are found in exactly solvable lattice models, interacting boson-fermion models in nuclear physics, extended *t-J* models in condensed matter physics, and so on. On the other hand, importance of noncommutative geometry in theoretical physics, especially in string theory and quantum gravity, has come into focus recently.[1] Therefore if these two notions are combined to form a noncommutative geometry of supersymmetric nature, we can expect that the combination will play important roles in various fields in physics. An attempt to introduce a noncommutative superspace was made by Manin[2] in the context of quantum supergroup. Then differential calculus on the noncommutative superspace was developed by two different approaches.[3,4] The present authors extended the notions of noncommutative differential geometry such as connection and curvature to the supersymmetric case and investigated[5] the superspace for super-Jordanian deformed $OSp(1/2)$ group.

A supersphere having bosonic and fermionic coordinates is defined as an algebra whose defining relations are covariant under the coaction of the quantum supergroup $OSp_q(1/2)$. In this paper, we construct a one-parameter family of superspheres by developing a general procedure based on the representation theory of $OSp_q(1/2)$ and its dual $U_q[osp(1/2)]$. By this method, quantum superspaces and superspheres are described in a unified way. Furthermore, the method can be used to find higher dimensional noncommutative superspaces covariant under $OSp_q(1/2)$. Our work is motivated for two reasons, (1) in order to investigate noncommutative geometry, it is important to have explicit examples of noncommutative superspaces. Manin's work is an analogue of flat space, while here we consider an analogue of curved space. (2) There exist some models of integrable quantum field theories with $OSp(m/2n)$ symmetries where superspheres appear.[6] Consideration of quantum group extensions of such models will require quantum superspheres. We start with the simplest and the most important group $OSp_q(1/2)$ to construct quantum superspheres.

Let us briefly recall the studies of noncommutative sphere based on quantum groups, since supersymmetric counterparts of some of them are considered in this paper. Podleś introduced[7] an algebra which is covariant under the adjoint corepresentation of quantum group $SU_q(2)$. The

algebra is interpreted as a noncommutative version of two sphere, and called q-sphere. The q-sphere has one more parameter in addition to its radius and the deformation parameter q. Thus what Podleś constructed is a one-parameter family of noncommutative two spheres. The parameter is specific to q-sphere and does not have a commutative counterpart. Differential calculus on the q-sphere was initiated by Podleś,[8] then classification of differential structures on q-sphere was made in Refs. 9–11. An interesting relation of q-sphere to q-hypergeometric functions is discussed in Ref. 12, where orthogonal bases on q-sphere are explicitly determined in terms of big q-Jacobi polynomials. The q-sphere can be realized by embedding it in $\mathrm{SU}_q(2)$. This embedding admits an elegant description[13] of q-sphere as an algebra which is invariant under left and right actions of a twisted primitive element of the quantum algebra $\mathrm{U}_q[\mathrm{su}(2)]$. Podleś q-sphere has been generalized in two different directions, higher dimensional and Jordanian SU(2). Higher dimensional q-spheres, more precisely, noncommutative analogue of $(2n+1)$-spheres were constructed in a similar way by replacing $\mathrm{SU}_q(2)$ with $\mathrm{SU}_q(n+1)$. Furthermore, an invariant integral on quantum $(2n+1)$-sphere is obtained in Ref. 14. Another family of quantum two-spheres is obtained[15] by using Jordanian deformation of SL(2). One of its distinctions from Podleś q-sphere is that the Jordanian quantum sphere requires different twisted primitive elements for left and right invariances.

Throughout this paper, the quantum superalgebra $\mathrm{U}_q[\mathrm{osp}(1/2)]$ and the quantum supergroup $\mathrm{OSp}_q(1/2)$ are denoted by $\mathcal{U}$ and $\mathcal{A}$, respectively. We assume that q is generic in this paper. The plan of this paper is as follows. In the first two preliminary sections we fix our notations and conventions, and list formulas used in subsequent sections. Section II is a summary of definitions and representation theory of $\mathcal{U}$. For computational purpose, we give all the defining relations of $\mathcal{A}$ explicitly in Sec. III. A relation between representations of $\mathcal{U}$ and corepresentations of $\mathcal{A}$ is given in Sec. IV. A product law of two corepresentations, which is a quantum supergroup analogue of Wigner's product law in the quantum theory of angular momentum, is also derived in Sec. IV. A general prescription to find an algebra covariant under the coaction of $\mathcal{A}$ is given in Sec. V. As a simple application of the method, the most general form of quantum superspaces is derived. The method is applied to construct a one-parameter family of quantum superspheres in Sec. VI. Properties of the quantum supersphere are examined and the similarities to those for q-sphere are pointed out.

II. $\mathrm{U}_q[\mathrm{osp}(1/2)]$ AND ITS REPRESENTATIONS

A. Definition and representations

The universal enveloping algebra $\mathcal{U}=\mathrm{U}_q[\mathrm{osp}(1/2)]$ is generated by the two even $K^{\pm 1}$, and the two odd elements $v_\pm$ satisfying the commutation properties[16]

$$KK^{-1}=K^{-1}K=1, \quad Kv_\pm = q^{\pm 1/2}v_\pm K,$$

$$\{v_+,v_-\} = -\frac{K^2-K^{-2}}{q^4-q^{-4}}. \tag{2.1}$$

The Casimir element is given by

$$C=\left(\frac{q^{1/2}K^2-q^{-1/2}K^{-2}}{q^4-q^{-4}}\right)^2 - \frac{qK^2+q^{-1}K^{-2}}{(q+q^{-1})(q^2+q^{-2})}v_-v_+ - (q^{1/2}+q^{-1/2})^2 v_-^2 v_+^2. \tag{2.2}$$

The coproduct (Δ), the counit (ϵ), and the antipode (S) maps read

$$\Delta(K^{\pm 1}) = K^{\pm 1}\otimes K^{\pm 1}, \quad \Delta(v_\pm) = v_\pm \otimes K^{-1} + K \otimes v_\pm, \tag{2.3}$$

$$\epsilon(K^{\pm 1}) = 1, \quad \epsilon(v_\pm) = 0, \tag{2.4}$$

$$S(K^{\pm 1}) = K^{\mp 1}, \quad S(v_\pm) = -q^{\mp 1/2}v_\pm. \tag{2.5}$$

The finite dimensional irreducible representations of the $\mathcal{U}$ algebra are said to be of the grade-star[17] type. Each irreducible representation is specified by a non-negative integer ℓ and the corresponding $(2\ell+1)$-dimensional graded vector space $V^{(\ell)}$ that admits a nondegenerate Hermitian bilinear form denoted by (,). The subspaces of $V^{(\ell)}$ having different parities are orthogonal with respect to the bilinear form. The graded adjoint operation $(*)$ is defined by

$$(A^* f,g) = (-1)^{\hat{A}\hat{f}}(f,Ag), \quad A \in \mathcal{U}, \quad f,g \in V^{(\ell)}, \tag{2.6}$$

where $\hat{A}$ denotes the parity of A. The $*$-operation is assumed to be an algebra anti-isomorphism and coalgebra isomorphism,

$$(A_1A_2)^* = (-1)^{\hat{A}_1\hat{A}_2}A_2^*A_1^*, \quad (A_1 \otimes A_2)^* = A_1^* \otimes A_2^*. \tag{2.7}$$

The grade-star representation of $\mathcal{U}$ is characterized by

$$K^* = K, \quad v_\pm^* = \pm(-1)^\varepsilon v_\mp, \quad \varepsilon = 0,1, \tag{2.8}$$

where ε refers to the class of the representation.

Let $\{e_m^\ell(\lambda)\,|\,m=\ell,\ell-1,\ldots,-\ell\}$ be a basis of $V^{(\ell)}$, where each basis vector has a definite parity. The index $\lambda=0,1$ specifies the parity of the highest weight vector $e_\ell^\ell(\lambda)$. The parity of $e_m^\ell(\lambda)$ equals $\ell-m+\lambda$, as it is obtained by the application of $v_-^{\ell-m}$ on $e_\ell^\ell(\lambda)$. For the superalgebras the norm of the representation basis need not be chosen positive definite. In this work, however, we assume the positive definiteness of the basis elements,

$$(e_m^\ell(\lambda), e_{m'}^{\ell'}(\lambda)) = \delta_{\ell\ell'}\delta_{mm'}. \tag{2.9}$$

It turns out that this convention relates the parity λ and the class ε as follows:

$$\lambda = \varepsilon + 1 (\mathrm{mod}\ 2). \tag{2.10}$$

With these settings, the irreducible representations of $\mathcal{U}$ are given by

$$Ke_m^\ell(\lambda) = q^{m/2}e_m^\ell(\lambda),$$

$$v_+e_m^\ell(\lambda) = \sqrt{[\ell-m][\ell+m+1]\varrho}\,e_{m+1}^\ell(\lambda),$$

$$v_-e_m^\ell(\lambda) = (-1)^{\ell-m-1}\sqrt{[\ell+m][\ell-m+1]\varrho}\,e_{m-1}^\ell(\lambda), \tag{2.11}$$

where $[n]$ and ϱ are defined by

$$[n] = \frac{q^{-n/2}-(-1)^n q^{n/2}}{q^{-1/2}+q^{1/2}}, \quad \varrho = \frac{q^{-1/2}+q^{1/2}}{q^{-4}-q^4}. \tag{2.12}$$

Our phase convention for $v_\pm$ agrees with that of Ref. 16, but it differs from that of Ref. 17. For later convenience, the representation matrices for $\ell=1,2$ cases are given explicitly. The generators in the $\ell=1$ representation read

$$K = \mathrm{diag}(q^{1/2},1,q^{-1/2}),$$

$$v_+ = \sqrt{[2]\varrho}\begin{pmatrix}0&1&0\\0&0&1\\0&0&0\end{pmatrix}, \quad v_- = \sqrt{[2]\varrho}\begin{pmatrix}0&0&0\\-1&0&0\\0&1&0\end{pmatrix}, \tag{2.13}$$

and for the $\ell=2$ case they are given by

$$K = \mathrm{diag}(q, q^{1/2}, 1, q^{-1/2}, q^{-1}),$$

$$v_+ = \begin{pmatrix} 0 & \sqrt{[4]\varrho} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{[3]!\varrho} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{[3]!\varrho} & 0 \\ 0 & 0 & 0 & 0 & \sqrt{[4]\varrho} \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$v_- = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ -\sqrt{[4]\varrho} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{[3]!\varrho} & 0 & 0 & 0 \\ 0 & 0 & -\sqrt{[3]!\varrho} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{[4]\varrho} & 0 \end{pmatrix}. \tag{2.14}$$

The eigenvalue of the Casimir element depends only on the highest weight,

$$Ce_m^\ell(\lambda) = \left(\frac{q^{\ell+1/2} - q^{-\ell-1/2}}{q^4 - q^{-4}} \right)^2 e_m^\ell(\lambda). \tag{2.15}$$

The quantity $[n]$, known[16,17] as Kulish symbol, plays a role similar to the q-number. For a positive integer n its factorial is defined as $[n]! \equiv [n][n-1]\cdots[1]$.

B. Tensor product representations

Tensor product of the irreducible representations of $\mathcal{U}$ has been discussed in Refs. 16 and 17. The decomposition of tensor product in the irreducible representations is identical to the classical case

$$V^{(\ell_1)} \otimes V^{(\ell_2)} = V^{(\ell_1+\ell_2)} \oplus V^{(\ell_1+\ell_2-1)} \oplus \cdots \oplus V^{(|\ell_1-\ell_2|)}.$$

The explicit formulas of the Clebsch-Gordan coefficients (CGC) are obtained in Ref. 17. We list below the relations which will be used in the later sections.

In spite of our assumption (2.9) of the positivity of the basis states, the norm of the tensor product of the bases is not always positive definite. For instance, the following norm can be negative for some combinations of ℓ_a, $m_a (a=1,2)$, and λ:

$$(e_{m_1}^{\ell_1}(\lambda) \otimes e_{m_2}^{\ell_2}(\lambda), e_{m_1}^{\ell_1}(\lambda) \otimes e_{m_2}^{\ell_2}(\lambda)) = (-1)^{(\ell_1-m_1+\lambda)(\ell_2-m_2+\lambda)} (e_{m_1}^{\ell_1}(\lambda), e_{m_1}^{\ell_1}(\lambda))(e_{m_2}^{\ell_2}(\lambda), e_{m_2}^{\ell_2}(\lambda)). \tag{2.16}$$

The irreducible basis of the tensor product representations is obtained by using the CGC,

$$e_m^\ell(\ell_1, \ell_2, \Lambda) = \sum_{m_1, m_2} C_{m_1 m_2 m}^{\ell_1 \ell_2 \ell} e_{m_1}^{\ell_1}(\lambda) \otimes e_{m_2}^{\ell_2}(\lambda), \tag{2.17}$$

where $m = m_1 + m_2$, and $\Lambda = \ell_1 + \ell_2 + \ell \pmod 2$ is the parity of the highest weight vector $e_\ell^\ell(\ell_1, \ell_2, \Lambda)$. Since our phase convention for representations of $v_\pm$ differs from that of Ref. 17, we cannot use the expression of CGC given therein. The CGC in our convention is explicitly given by

$$C^{\ell_1\ell_2\ell}_{m_1m_2m} = (-1)^{(\ell_1-\ell+m_2)(\ell-m+\lambda)+(\ell_1-\ell+m_2)(\ell_1-\ell+m_2+1)/2} q^{m_2(m+1)/2+(\ell_1-\ell_2)(\ell_1+\ell_2+1)/4-\ell(\ell+1)/4}$$
$$\times \left([2\ell+1] \frac{[\ell_1+\ell_2-\ell]![\ell+m]![\ell-m]![\ell_1-m_1]![\ell_2-m_2]!}{[\ell_1+\ell_2+\ell+1]![\ell_1-\ell_2+\ell]![-\ell_1+\ell_2+\ell]![\ell_1+m_1]![\ell_2+m_2]!} \right)^{1/2}$$
$$\times \sum_k (-1)^{k(k-1)/2+k(\ell_1+\ell_2-m)} q^{k(\ell+m+1)/2} \frac{[\ell_1+\ell-m_2-k]![\ell_2+m_2+k]!}{[k]![\ell-m-k]![\ell_1-\ell+m_2+k]![\ell_2-m_2-k]!}, \tag{2.18}$$

where the index k runs over all non-negative integers maintaining the arguments of $[x]$ non-negative. The derivation of (2.18) is described in Appendix A. All the CGC are, we note, of parity zero. The basis (2.17) is pseudo-orthogonal,

$$(e^{\ell'}_{m'}(\ell_1,\ell_2,\Lambda), e^{\ell}_{m}(\ell_1,\ell_2,\Lambda)) = (-1)^{(\ell-m+\lambda)(\ell_1+\ell_2+\ell+\lambda)} \delta_{\ell'\ell}\delta_{m'm}. \tag{2.19}$$

The CGC satisfies two pseudo-orthogonality relations,

$$\sum_{m_1,m_2} (-1)^{(\ell_1-m_1+\lambda)(\ell_2-m_2+\lambda)} C^{\ell_1\ell_2\ell'}_{m_1m_2m'} C^{\ell_1\ell_2\ell}_{m_1m_2m} = (-1)^{(\ell-m+\lambda)(\ell_1+\ell_2+\ell+\lambda)} \delta_{\ell\ell'}\delta_{mm'}, \tag{2.20}$$

$$\sum_{\ell,m} (-1)^{(\ell-m+\lambda)(\ell_1+\ell_2+\ell+\lambda)} C^{\ell_1\ell_2\ell}_{m_1'm_2'm} C^{\ell_1\ell_2\ell}_{m_1m_2m} = (-1)^{(\ell_1-m_1+\lambda)(\ell_2-m_2+\lambda)} \delta_{m_1'm_1}\delta_{m_2'm_2}. \tag{2.21}$$

Using (2.21), the construction (2.17) is readily inverted,

$$e^{\ell_1}_{m_1}(\lambda) \otimes e^{\ell_2}_{m_2}(\lambda) = (-1)^{(\ell_1-m_1)(\ell_2-m_2)} \sum_{\ell,m} (-1)^{(\ell-m)(\ell_1+\ell_2+\ell)} C^{\ell_1\ell_2\ell}_{m_1m_2m} e^{\ell}_{m}(\ell_1,\ell_2,\Lambda). \tag{2.22}$$

III. QUANTUM SUPERGROUP $OSp_q(1/2)$

The quantum supergroup $\mathcal{A}=OSp_q(1/2)$ is defined as a Hopf dual to the universal enveloping algebra $\mathcal{U}$.[16] In this section, all defining relations of $\mathcal{A}$ will be given explicitly. The universal $\mathcal{R}$-matrix of $\mathcal{U}$ is given in Ref. 16. For the defining $\ell=1$ representation, it reads

$$\mathcal{R}^{(\ell=1)} = \left(\begin{array}{ccc|ccc|ccc}
q & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & 1 & \cdot & \omega & \cdot & \cdot & \cdot & \cdot & \\
\cdot & \cdot & q^{-1} & \cdot & \lambda & \cdot & \rho & \cdot & \cdot \\
\hline
\cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & 1 & \cdot & \lambda & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \omega & \cdot \\
\hline
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & q^{-1} & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & q
\end{array}\right), \tag{3.1}$$

where

$$\omega = q - q^{-1}, \quad \lambda = -q^{-1/2}\omega, \quad \rho = (1+q^{-1})\omega, \tag{3.2}$$

and the dot is used instead of zero for better readability. Let P be a permutation operator, $P(v \otimes w) = (-1)^{\hat{v}\hat{w}} w \otimes v$. Standard *FRT* (Ref. 18) construction is obtained via the matrix R,

$$R = P\mathcal{R}^{(\ell=1)}P = \left(\begin{array}{ccc|ccc|ccc} q & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & q^{-1} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \omega & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & -\lambda & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \rho & \cdot & -\lambda & \cdot & q^{-1} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \omega & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & q \end{array}\right) \tag{3.3}$$

The quantum T-matrix, whose elements generate the algebra $\mathcal{A}$ is given by

$$T = (t_{ij}) = \begin{pmatrix} a & \alpha & b \\ \gamma & e & \beta \\ c & \delta & d \end{pmatrix}, \tag{3.4}$$

where the entries in latin (greek) characters are of even (odd) parity. The parity of the supermatrix T is zero, i.e., $\hat{t}_{ij}=\hat{i}+\hat{j}$. The RTT-relation describes the exchange properties on the entries of T. The q-orthosymplectic condition reads

$$T^{st}CT = DC, \quad TC^{-1}T^{st} = DC^{-1}, \tag{3.5}$$

where

$$C = \begin{pmatrix} 0 & 0 & -q^{-1/2} \\ 0 & 1 & 0 \\ q^{1/2} & 0 & 0 \end{pmatrix}, \quad C^{-1} = \begin{pmatrix} 0 & 0 & q^{-1/2} \\ 0 & 1 & 0 \\ -q^{1/2} & 0 & 0 \end{pmatrix}, \tag{3.6}$$

and the superdeterminant D is given by

$$D = ad - qbc - q^{1/2}\alpha\delta. \tag{3.7}$$

The T^{st} denotes the supertranspose of T. The supertranspose of an arbitrary matrix is given as $A^{st}_{ij}=(-1)^{\hat{i}(\hat{j}+1)}A_{ji}$. The RTT relations require D to be central.

The coproduct and counit of T are given as usual

$$\Delta(T) = T\dot{\otimes}T, \quad \epsilon(T) = \mathrm{diag}(1,1,1). \tag{3.8}$$

The grouplike property of the superdeterminant $\Delta(D)=D\otimes D$ is obtained by taking the coproduct of both sides of the relation (3.5). This allows us to set the constraint

$$D = ad - qbc - q^{1/2}\alpha\delta = 1. \tag{3.9}$$

The antipode of T satisfies $S(T)T=TS(T)=1$, and it explicitly reads

$$S(T) = C^{-1}T^{st}C = \begin{pmatrix} d & q^{-1/2}\beta & -q^{-1}b \\ -q^{1/2}\delta & e & q^{-1/2}\alpha \\ -qc & -q^{1/2}\gamma & a \end{pmatrix}. \tag{3.10}$$

The RTT relations reveal that not all the entries of T are independent. We express the elements e, β, and γ in terms of the rest. Using (2,2) component of the first relation in (3.5),

$$e^2 = 1 - 2q^{-1/2}\alpha\delta + \omega bc, \tag{3.11}$$

we solve for e and its inverse e^{-1},

$$e = 1 - q^{-1/2}\alpha\delta + (q-1)bc,$$

$$e^{-1} = (1 + q^{-1/2}\alpha\delta - (q-1)bc)(1 + q^{-1}(q-1)^2 bc)^{-1}. \tag{3.12}$$

Inclusion of the element e^{-1} allows us to solve for β and γ,

$$\beta = q^{-3/2}b\delta - q^{1/2}d\alpha, \quad \gamma = q^{-1/2}a\delta - q^{3/2}c\alpha, \quad \alpha\delta = \gamma\beta. \tag{3.13}$$

In summary, the algebra $\mathcal{A}$ is generated by a, b, c, d, α, and δ. The generators satisfy the relations

$$ab = q^2 ba, \quad ac = q^2 ca, \quad [a,d] = -\lambda\alpha\delta + \rho bc,$$

$$a\alpha = q\alpha a, \quad a\delta = q\delta a + q\omega c\alpha, \quad [b,c] = 0,$$

$$bd = q^2 db, \quad b\alpha = q^{-1}\alpha b, \quad b\delta = q\delta b,$$

$$cd = q^2 dc, \quad c\alpha = q^{-1}\alpha c, \quad c\delta = q\delta c,$$

$$d\alpha = q^{-1}\alpha d - \omega\delta b, \quad d\delta = q^{-1}\delta d, \quad \alpha\delta = -q\delta\alpha - q\lambda bc,$$

$$\alpha^2 = -q^{-1}[2]ab, \quad \delta^2 = -q^{-1}[2]cd. \tag{3.14}$$

For later convenience, the commutation relations involving e, β, and γ are listed below,

$$[a,e] = \omega\gamma\alpha, \quad a\beta = q\beta a + q\omega b\gamma, \quad a\gamma = q\gamma a,$$

$$[b,e] = 0, \quad b\beta = q\beta b, \quad b\gamma = q^{-1}\gamma b,$$

$$[c,e] = 0, \quad c\beta = q\beta c, \quad c\gamma = q^{-1}\gamma c,$$

$$[d,e] = \omega\delta\beta, \quad d\beta = q^{-1}\beta d, \quad d\gamma = q^{-1}\gamma d - \omega\beta c,$$

$$[e,\alpha] = -\lambda\gamma b, \quad [e,\beta] = \lambda b\delta, \quad [e,\gamma] = \lambda\alpha c,$$

$$[e,\delta] = -\lambda c\beta, \quad \{\alpha,\beta\} = -\omega eb, \quad \{\alpha,\gamma\} = 0,$$

$$\beta\gamma = -q^{-1}\gamma\beta - \lambda bc, \quad \{\beta,\delta\} = 0, \quad \{\gamma,\delta\} = \omega ce,$$

$$\beta^2 = -q^{-1}[2]bd, \quad \gamma^2 = -q^{-1}[2]ac. \tag{3.15}$$

Additional relations may also be proved,

$$e\alpha = q^{1/2}(b\gamma - \beta a), \quad e\beta = q^{1/2}\delta b - q^{-1/2}\alpha d,$$

$$e\gamma = q^{1/2}(\delta a - c\alpha), \quad e\delta = q^{-1/2}\gamma d - q^{1/2}\beta c. \tag{3.16}$$

The duality between $\mathcal{U}$ and $\mathcal{A}$ is given by a nondegenerate pairing $\langle,\rangle$,

$$\langle K,T\rangle = \mathrm{diag}(q^{1/2},1,q^{-1/2}),$$

$$\langle v_+,T\rangle = \sqrt{[2]\varrho}\begin{pmatrix}0&1&0\\0&0&-1\\0&0&0\end{pmatrix},\quad \langle v_-,T\rangle = \sqrt{[2]\varrho}\begin{pmatrix}0&0&0\\1&0&0\\0&1&0\end{pmatrix}. \tag{3.17}$$

The pairing can be extended to tensor product algebras by setting

$$\langle X_1\otimes X_2,a_1\otimes a_2\rangle = (-1)^{\hat{X}_2\hat{a}_1}\langle X_1,a_1\rangle\langle X_2,a_2\rangle. \tag{3.18}$$

IV. COREPRESENTATIONS OF $\mathcal{A}$

A vector space V is called a right $\mathcal{A}$-comodule if there exists a linear mapping $\varphi_R: V\to V\otimes\mathcal{A}$ satisfying

$$(\varphi_R\otimes \mathrm{id})\circ\varphi_R = (\mathrm{id}\otimes\Delta)\circ\varphi_R,\quad (\mathrm{id}\otimes\epsilon)\circ\varphi_R = \mathrm{id}. \tag{4.1}$$

Similarly, the left $\mathcal{A}$-comodule is defined as a vector space V equipped with a linear mapping $\varphi_L: V\to\mathcal{A}\otimes V$ such that

$$(\mathrm{id}\otimes\varphi_L)\circ\varphi_L = (\Delta\otimes\mathrm{id})\circ\varphi_L,\quad (\epsilon\otimes\mathrm{id})\circ\varphi_L = \mathrm{id}. \tag{4.2}$$

The mapping $\varphi_R(\varphi_L)$ is called a corepresentation, or, equivalently, a right (left) coaction of $\mathcal{A}$ on V.

Employing the duality of the algebras $\mathcal{U}$ and $\mathcal{A}$, we may follow the standard[19] construction of the action of $\mathcal{U}$ on a $\mathcal{A}$-comodule V. Namely, starting from the corepresentations of $\mathcal{A}$, we may obtain representations of $\mathcal{U}$. Reversing the argument, we now obtain the hitherto unknown corepresentations of $\mathcal{A}$ from the already known irreducible representations of $\mathcal{U}$.

Let an arbitrary element $X\in\mathcal{U}$ act on the vector space $V^{(\ell)}$ described in Sec. II A. The matrix representation of X on $V^{(\ell)}$ is denoted by $D^\ell(X;\lambda)$,

$$Xe^\ell_m(\lambda) = \sum_{m'} e^\ell_{m'}(\lambda)D^\ell_{m'm}(X;\lambda). \tag{4.3}$$

The parity of the element $T^\ell_{m'm}(\lambda)$ of $\mathcal{A}$, defined via the duality relation

$$D^\ell_{m'm}(X;\lambda) = (-1)^{\hat{X}(\ell-m'+\lambda)}\langle X,T^\ell_{m'm}(\lambda)\rangle, \tag{4.4}$$

may be assigned as

$$\widehat{T^\ell_{m'm}}(\lambda) = m'+m(\mathrm{mod}\,2). \tag{4.5}$$

To prove this, we compare the parity of both sides of (4.3). The resultant equation $\widehat{D^\ell_{m'm}}(X;\lambda) = \hat{X}+m'+m\ (\mathrm{mod}\,2)$ establishes the relation (4.5). Though we know, via (2.11), that all nonvanishing entries of the representation matrices are even, we should keep the parity of $D^\ell(X;\lambda)$ in the present formulation. Next we obtain the coproduct and counit maps for $T^\ell_{m'm}(\lambda)$,

$$\Delta(T^\ell_{m'm}(\lambda)) = \sum_{m''} T^\ell_{m'm''}(\lambda)\otimes T^\ell_{m''m}(\lambda),\quad \epsilon(T^\ell_{m'm}(\lambda)) = \delta_{m'm}. \tag{4.6}$$

The matrix $D^\ell(X;\lambda)$, being a representation of $X\in\mathcal{U}$, obeys the rule

$$D^{\ell}_{m'm}(XY;\lambda) = \sum_{m''} D^{\ell}_{m'm''}(X;\lambda) D^{\ell}_{m''m}(Y;\lambda) \quad \forall\, X,Y \in \mathcal{U}. \tag{4.7}$$

Both sides [left-hand side (lhs) and right-hand side (rhs)] of (4.7) may be rewritten by using (4.4),

$$\text{lhs} = (-1)^{\widehat{XY}(\ell-m'+\lambda)} \langle XY, T^{\ell}_{m'm}(\lambda)\rangle = (-1)^{\widehat{XY}(\ell-m'+\lambda)} \langle X \otimes Y, \Delta(T^{\ell}_{m'm}(\lambda))\rangle,$$

$$\text{rhs} = \sum_{m''} (-1)^{\hat{X}(\ell-m'+\lambda)+\hat{Y}(\ell-m''+\lambda)} \langle X, T^{\ell}_{m'm''}(\lambda)\rangle \langle Y, T^{\ell}_{m''m}(\lambda)\rangle = \sum_{m''} (-1)^{(\hat{X}+\hat{Y})(\ell-m'+\lambda)} \langle X \otimes Y, T^{\ell}_{m'm''}(\lambda) \otimes T^{\ell}_{m''m}(\lambda)\rangle.$$

The property (4.7) now assumes the form

$$\left\langle X \otimes Y, \Delta(T^{\ell}_{m'm}(\lambda)) - \sum_{m''} T^{\ell}_{m'm''}(\lambda) \otimes T^{\ell}_{m''m}(\lambda) \right\rangle = 0. \tag{4.8}$$

Since the relation (4.8) is true for arbitrary X, Y, and the pairing is nondegenerate, we obtain the coproduct map in (4.6). To obtain the counit map, we consider

$$D^{\ell}_{m'm}(1;\lambda) = \langle 1, T^{\ell}_{m'm}(\lambda)\rangle \equiv \epsilon(T^{\ell}_{m'm}(\lambda)), \tag{4.9}$$

and use the fact that the unit element of $\mathcal{U}$ is always represented by the identity matrix $(\delta_{m'm})$. This completes the proof of (4.6).

Defining the map $\varphi_R : V^{(\ell)} \to V^{(\ell)} \otimes \mathcal{A}$ by

$$\varphi_R(e^{\ell}_m(\lambda)) = \sum_{m'} e^{\ell}_{m'}(\lambda) \otimes T^{\ell}_{m'm}(\lambda), \tag{4.10}$$

it is easy to show, via (4.6), that $V^{(\ell)}$ equipped with φ_R is a right $\mathcal{A}$-comodule. Thus the quantum supermatrix $T^{\ell}(\lambda)$ provides the $(2\ell+1)$-dimensional corepresentation of $\mathcal{A}$ on $V^{(\ell)}$. The relation between representations and corepresentations is summarized in the same form as the nonsuper case,[19]

$$X e^{\ell}_m(\lambda) = (\mathrm{id} \otimes X) \circ \varphi_R(e^{\ell}_m(\lambda)), \tag{4.11}$$

where the action of $\mathcal{U}$ on $\mathcal{A}$ is defined by the nondegenerate pairing. It is easy to find $T^{\ell}(\lambda)$ for $\ell = 0, 1$ from (4.4),

$$T^0_{00}(\lambda) = 1 \quad \text{for } \lambda = 0, 1, \tag{4.12}$$

$$T^1(0) = T = \begin{pmatrix} a & \alpha & b \\ \gamma & e & \beta \\ c & \delta & d \end{pmatrix}, \quad T^1(1) = \begin{pmatrix} a & -\alpha & b \\ -\gamma & e & -\beta \\ c & -\delta & d \end{pmatrix}, \tag{4.13}$$

where the indices of rows and columns of $T^1(\lambda)$ run over 1, 0, and −1.

One of the important properties of the corepresentations $T^{\ell}(\lambda)$ is that they satisfy the product law which gives a rule to combine two corepresentations to get the third one,

$$\delta_{\ell'\ell} T^{\ell}_{m'm}(\Lambda) = \sum_{\substack{m_1,m_2 \\ m_1',m_2'}} (-1)^p C^{\ell_1\ell_2\ell'}_{m_1'm_2'm'} C^{\ell_1\ell_2\ell}_{m_1m_2m} T^{\ell_1}_{m_1'm_1}(\lambda) T^{\ell_2}_{m_2'm_2}(\lambda),$$

$$p=(m_1'+m_1)(\ell_2-m_2'+\lambda)+(\ell_1-m_1')(\ell_2-m_2')+(\ell'-m')(\ell_1+\ell_2+\ell'). \tag{4.14}$$

To prove the above product law, we first derive the fusion rule of representation matrices $D^{\ell}(X;\lambda)$ of $\mathcal{U}$, and then apply the duality argument by the proof of (4.6).

Denoting the coproduct of $X\in\mathcal{U}$ as $\Delta(X)=\Sigma_a X_a\otimes X^a$, we use the projection relation (2.17) to obtain

$$Xe_m^{\ell}(\ell_1,\ell_2,\Lambda)=\sum_{m_1,m_2,a}(-1)^{\hat{X}^a(\ell_1-m_1+\lambda)}C^{\ell_1\ell_2\ell}_{m_1m_2m}X_a e^{\ell_1}_{m_1}(\lambda)\otimes X^a e^{\ell_2}_{m_2}(\lambda). \tag{4.15}$$

We employ (4.3) to compute both sides of (4.15),

$$\begin{aligned}\text{rhs}=&\sum_{\substack{m_1,m_2\\ m_1',m_2'}}\sum_a(-1)^{\hat{X}^a(\ell_1-m_1+\lambda)}(-1)^{(\hat{X}_a+m_1'+m_1)(\ell_2-m_2'+\lambda)}\\ &\times C^{\ell_1\ell_2\ell}_{m_1m_2m}(e^{\ell_1}_{m_1'}\otimes e^{\ell_2}_{m_2'})D^{\ell_1}_{m_1'm_1}(X_a;\lambda)D^{\ell_2}_{m_2'm_2}(X^a;\lambda)\\ =&\sum_{\substack{m_1,m_2\\ m_1',m_2'}}\sum_{a,\ell',m'}(-1)^{\hat{X}^a(\ell_1-m_1+\lambda)+\hat{X}_a(\ell_2-m_2'+\lambda)+p}\\ &\times C^{\ell_1\ell_2\ell'}_{m_1'm_2'm'}C^{\ell_1\ell_2\ell}_{m_1m_2m}e^{\ell'}_{m'}(\ell_1,\ell_2,\Lambda')D^{\ell_1}_{m_1'm_1}(X_a;\lambda)D^{\ell_2}_{m_2'm_2}(X^a;\lambda),\end{aligned}$$

where (2.22) is used in the last equality. The lhs of (4.15) follows directly from (4.3):

$$\text{lhs}=\sum_{m'}e^{\ell}_{m'}(\ell_1,\ell_2,\Lambda)D^{\ell}_{m'm}(X;\Lambda),$$

yielding the product law of $D^{\ell}(X,\lambda)$,

$$\begin{aligned}\delta_{\ell'\ell}D^{\ell}_{m'm}(X,\Lambda)=&\sum_{\substack{m_1,m_2\\ m_1',m_2'}}\sum_a(-1)^{\hat{X}^a(\ell_1-m_1+\lambda)+\hat{X}_a(\ell_2-m_2'+\lambda)+p}\\ &\times C^{\ell_1\ell_2\ell'}_{m_1'm_2'm'}C^{\ell_1\ell_2\ell}_{m_1m_2m}D^{\ell_1}_{m_1'm_1}(X_a;\lambda)D^{\ell_2}_{m_2'm_2}(X^a;\lambda).\end{aligned} \tag{4.16}$$

To derive the fusion rule for $T^{\ell}(\lambda)$, we consider the dual pairing,

$$\begin{aligned}\langle X,T^{\ell_1}_{m_1'm_1}(\lambda)T^{\ell_2}_{m_2'm_2}(\lambda)\rangle=\langle\Delta(X),T^{\ell_1}_{m_1'm_1}(\lambda)\otimes T^{\ell_2}_{m_2'm_2}(\lambda)\rangle=&\sum_a(-1)^{\hat{X}^a(m_1'+m_1)}\\ &\times(-1)^{\hat{X}_a(\ell_1-m_1'+\lambda)+\hat{X}^a(\ell_2-m_2'+\lambda)}D^{\ell_1}_{m_1'm_1}(X_a;\lambda)D^{\ell_2}_{m_2'm_2}(X^a;\lambda),\end{aligned}$$

which, in turn, allows us to evaluate the following sum:

$$\begin{aligned}&\sum_{\substack{m_1,m_2\\ m_1',m_2'}}(-1)^pC^{\ell_1\ell_2\ell'}_{m_1'm_2'm'}C^{\ell_1\ell_2\ell}_{m_1m_2m}\langle X,T^{\ell_1}_{m_1'm_1}(\lambda)T^{\ell_2}_{m_2'm_2}(\lambda)\rangle\\ &\quad=(-1)^{\hat{X}(\ell-m'+\Lambda)}\sum_{\substack{m_1,m_2\\ m_1',m_2'}}\sum_a(-1)^{\hat{X}^a(\ell_1-m_1+\lambda)+\hat{X}_a(\ell_2-m_2'+\lambda)+p}\\ &\qquad\times C^{\ell_1\ell_2\ell'}_{m_1'm_2'm'}C^{\ell_1\ell_2\ell}_{m_1m_2m}D^{\ell_1}_{m_1'm_1}(X_a;\lambda)D^{\ell_2}_{m_2'm_2}(X^a;\lambda)=\delta_{\ell'\ell}(-1)^{\hat{X}(\ell-m'+\Lambda)}D^{\ell}_{m'm}(X;\Lambda)\end{aligned}$$

$$= \langle X, \delta_{\ell'\ell} T^{\ell}_{m'm}(\Lambda) \rangle .$$

The second equality is due to (4.16). Invoking the arbitrariness of $X \in \mathcal{U}$, and the nondegeneracy of dual pairing $\langle , \rangle$, we obtain the fusion rule (4.14).

V. $\mathcal{A}$-COVARIANT ALGEBRAS

A. General prescription

In this section, we will give a general prescription to find $\mathcal{A}$-covariant algebras. By $\mathcal{A}$-covariant algebras, we mean algebras whose defining relations are covariant under the right coaction φ_R of $\mathcal{A}$ defined by (4.10). Probably, the simplest way to find such an algebra is to introduce an algebraic structure on the representation space $V^{(\ell)}$. Assuming μ to be a multiplication map in $V^{(\ell)}$, i.e., $\mu(f \otimes g) = fg; f, g \in V^{(\ell)}$, we specifically construct the following composite object:

$$E^L_M(\Lambda) \equiv \mu(e^L_M(\ell, \ell, \Lambda)) = \sum_{m_1, m_2} C^{\ell\ \ell\ L}_{m_1 m_2 M} e^{\ell}_{m_1}(\lambda) e^{\ell}_{m_2}(\lambda), \tag{5.1}$$

where $\Lambda = L (\mathrm{mod}\, 2)$. The right coaction on $E^L_M(\Lambda)$ is shown to be

$$\varphi_R(E^L_M(\Lambda)) = \sum_{M'} E^L_{M'}(\Lambda) \otimes T^L_{M'M}(\Lambda). \tag{5.2}$$

The proof may be done in a straightforward way by inverting the relation (5.1),

$$e^{\ell}_{m_1}(\lambda) e^{\ell}_{m_2}(\lambda) = (-1)^{(\ell - m_1)(\ell - m_2)} \sum_{L,M} (-1)^{(L-M)L} C^{\ell\ \ell\ L}_{m_1 m_2 M} E^L_M(\Lambda), \tag{5.3}$$

and subsequently using the product law (4.14),

$$\begin{aligned}
\varphi_R(E^L_M(\Lambda)) &= \sum_{m_1, m_2} C^{\ell\ \ell\ L}_{m_1 m_2 M} \varphi_R(e^{\ell}_{m_1}(\lambda)) \varphi_R(e^{\ell}_{m_2}(\lambda)) \\
&= \sum_{\substack{m_1, m_2 \\ m_1', m_2'}} (-1)^{(m_1' + m_1)(\ell - m_2' + \lambda)} C^{\ell\ \ell\ L}_{m_1 m_2 M} e^{\ell}_{m_1'}(\lambda) e^{\ell}_{m_2'}(\lambda) \otimes T^{\ell}_{m_1' m_1}(\lambda) T^{\ell}_{m_2' m_2}(\lambda) \\
&\overset{(5.3)}{=} \sum_{\substack{m_1, m_2 \\ m_1', m_2'}} \sum_{L', M'} (-1)^{p'} C^{\ell\ \ell\ L}_{m_1 m_2 M} C^{\ell\ \ell\ L'}_{m_1' m_2' M'} E^{L'}_{M'}(\Lambda) \otimes T^{\ell}_{m_1' m_1}(\lambda) T^{\ell}_{m_2' m_2}(\lambda) \\
&\overset{(4.14)}{=} \sum_{M'} E^L_{M'}(\Lambda) \otimes T^L_{M'M}(\Lambda),
\end{aligned}$$

where $p' = (m_1' + m_1)(\ell - m_2' + \lambda) + (\ell - m_1')(\ell - m_2') + (L' - M')L'$.

Employing (5.2) we now extract a set of relations which are covariant under φ_R. The $L = 0$ relation $\varphi_R(E^0_0(0)) = E^0_0(0)$ signifies that $E^0_0(0)$ is a scalar under the right coaction. It may be equated to a constant parameter r,

$$E^0_0(0) = \sum_{m_1, m_2} C^{\ell\ \ell\ 0}_{m_1 m_2 0} e^{\ell}_{m_1}(\lambda) e^{\ell}_{m_2}(\lambda) = r. \tag{5.4}$$

If $L = \ell$ and $\lambda = \ell \ (\mathrm{mod}\, 2)$, then $E^{\ell}_m(\lambda)$ and $e^{\ell}_m(\lambda)$ have the same parity, and they transform identically under φ_R. Therefore $E^{\ell}_m(\lambda)$ is, in general, proportional to $e^{\ell}_m(\lambda)$. It may be noted that the following relations are covariant:

$$E_m^\ell(\lambda) = \sum_{m_1,m_2} C_{m_1 m_2 m}^{\ell\ \ell\ \ell} e_{m_1}^\ell(\lambda) e_{m_2}^\ell(\lambda) = \xi e_m^\ell(\lambda), \tag{5.5}$$

where the proportionality constant $\xi \to 0$ as $q \to 1$. For the case $\lambda \neq \ell \pmod 2$, $E_m^\ell(\ell)$ has different parity from $e_m^\ell(\lambda)$, even though they transform identically. In this case, the constant ξ in (5.5) is regarded as a Grassmann number that also vanish at $q=1$. For $L \neq 0, \ell$, the element $E_m^\ell(\ell)$ cannot be proportional to $e_m^\ell(\lambda)$ as they transform differently. The relevant covariant relations are, therefore, of the form

$$E_M^L(\Lambda) = \sum_{m_1,m_2} C_{m_1 m_2 M}^{\ell\ \ell\ L} e_{m_1}^\ell(\lambda) e_{m_2}^\ell(\lambda) = 0. \tag{5.6}$$

As will be seen in the subsequent sections, the simultaneous use of all relations from (5.4)–(5.6) gives an inconsistent result, since some of them do not have correct classical limits. In order to obtain a consistent covariant algebra, we must make a choice regarding the relations to be used for defining the algebra. Then the consistency must be verified. As it is clear from the above discussion, the covariant algebras can have at most two more parameters (r, ξ) in addition to the deformation parameter q. It is emphasized that the origin of the parameters is clearly explained in the framework of the representation theory.

We have formulated a method to construct $\mathcal{A}$-covariant algebras with respect to the right coaction. It is possible to repeat the same discussion for the left coaction.

B. Quantum superspace ($\ell=1, \lambda=0$)

Let us investigate the covariant algebra for the $\ell=1$ case, where the relevant tensor product decomposition is given by $1 \otimes 1 = 2 \oplus 1 \oplus 0$. We assume that $\lambda=0$, and denote the basis of $V^{(1)}$ by $z_m = e_m^1(0)$. Thus $z_{\pm 1}$ are parity even and z_0 is parity odd. The CGC for the decomposition is given in Appendix C. For $L=0$, we obtain from (5.4),

$$q^{1/2} z_{-1} z_1 + z_0^2 - q^{-1/2} z_1 z_{-1} = r. \tag{5.7}$$

For $L=1$, we have $\Lambda \neq \lambda$, and, therefore, the parameter ξ is a Grassmann number,

$$-q^{1/2} z_0 z_1 + q^{-1/2} z_1 z_0 = \xi z_1,$$

$$z_{-1} z_1 + (q^{-1/2} + q^{1/2}) z_0^2 - z_1 z_{-1} = \xi z_0,$$

$$q^{1/2} z_{-1} z_0 - q^{-1/2} z_0 z_{-1} = \xi z_{-1}. \tag{5.8}$$

For $L=2$, we obtain, using (5.6), unacceptable relations such as

$$z_1^2 = 0, \quad q^{-1/2} z_0 z_1 + q^{1/2} z_1 z_0 = 0.$$

Thus we take (5.7) and (5.8) as defining relations of our covariant algebra. We need to check the following conditions in order to verify whether or not the algebra is well defined:

(a) The constant r commutes with all generators.
(b) Product of three generators, say $z_1 z_0 z_{-1}$, has two ways of reversing its ordering,

$$\begin{array}{ccccc} & & z_1 z_0 z_{-1} & \to & z_1 z_{-1} z_0 & & \\ & \nearrow & & & & \searrow & \\ z_0 z_1 z_{-1} & & & & & & z_{-1} z_1 z_0. \\ & \searrow & & & & \nearrow & \\ & & z_0 z_{-1} z_1 & \to & z_{-1} z_0 z_1 & & \end{array}$$

These two ways give the same result.

It is straightforward to verify that the condition (a) is satisfied. The condition (b), however, requires setting $\xi=0$.

Therefore, we define our covariant algebra by combining relations (5.7) and (5.8), while maintaining $\xi=0$,

$$z_1 z_0 = q z_0 z_1, \quad z_0 z_{-1} = q z_{-1} z_0,$$

$$z_1 z_{-1} = q^2 z_{-1} z_1 - q(q^{-1/2} + q^{1/2}) r,$$

$$z_0^2 = -q^{-1}[2] z_1 z_{-1} - q^{-1} r. \tag{5.9}$$

This may be interpreted as the most general form of a quantum superspace. The simplest quantum superspace corresponds to the choice of $r=0$.

C. Quantum superspace ($\ell=1, \lambda=1$)

In this section, we study another quantum superspace where the parity is opposite to the previous example. Setting $\theta_m = e^1_m(1)$, we note that $\theta_{\pm 1}$ have odd parity, while θ_0 has even parity. Following (5.4), we obtain

$$q^{1/2}\theta_{-1}\theta_1 - \theta_0^2 - q^{-1/2}\theta_1\theta_{-1} = r. \tag{5.10}$$

The $L=1$ relations may be obtained from (5.5) except that in this case, as $\Lambda=\lambda$ holds, the parameter ξ is not a Grassmann number. However, these relations such as

$$q^{1/2}\theta_0\theta_1 + q^{-1/2}\theta_1\theta_0 = \xi\theta_1$$

are unacceptable as they include, in the $q \to 1$ limit, anticommutators for the product of even and odd elements. On the other hand, $L=2$ relations have proper classical limits,

$$\theta_{\pm 1}^2 = 0,$$

$$q^{-1/2}\theta_0\theta_1 - q^{1/2}\theta_1\theta_0 = 0,$$

$$q^{-1}\theta_{-1}\theta_1 - [2]\theta_0^2 + q\theta_1\theta_{-1} = 0,$$

$$-q^{-1/2}\theta_{-1}\theta_0 + q^{1/2}\theta_0\theta_{-1} = 0. \tag{5.11}$$

An interesting observation for this case is that we have two kinds of quantum superspaces. First we note that the relations (5.11) are enough to define a covariant algebra, since it may be shown that the condition (b) of Sec. V B is satisfied. Thus the relations (5.11) define a quantum superspace. Alternately, combining (5.11) with (5.10) we obtain another set of covariant relations

$$\theta_{\pm 1}^2 = 0, \quad q\theta_1\theta_0 = \theta_0\theta_1, \quad q\theta_0\theta_{-1} = \theta_{-1}\theta_0,$$

$$\theta_1\theta_{-1} + \theta_{-1}\theta_1 = -\frac{[2]}{[3]} r, \quad \theta_0^2 = -(q^{-1/2} + q^{1/2})\theta_1\theta_{-1} - q^{1/2}\frac{[2]}{[3]} r, \tag{5.12}$$

which have correct classical limit for an arbitrary value of r. With these relations, it may be checked that the conditions (a) and (b) of Sec. V B are satisfied. Thus we define the second quantum superspace by (5.12).

The above quantum superspaces are covariant under the coaction,

$$\varphi_R(\theta_m) = \sum_{m'} \theta_{m'} \otimes T^1_{m'm}(1), \tag{5.13}$$

where $T^1(1)$ is given by (4.13). Defining a new basis of the quantum superspace by

$$\theta'_0 = \theta_0, \quad \theta'_{\pm 1} = -\theta_{\pm 1}, \tag{5.14}$$

we observe that the θ'_m are covariant under the same corepresentation matrix as the case of $\lambda = 0$,

$$\theta'_m = \sum_{m'} \theta'_{m'} \otimes T^1_{m'm}(0). \tag{5.15}$$

VI. $\mathcal{A}$-COVARIANT SPHERE

A. Construction

In this section, we investigate an algebra covariant under the coaction of $T^2(\lambda)$, i.e., the adjoint corepresentation of $\mathcal{A}$. This may be interpreted as a supersymmetric extension of a noncommutative sphere. The corepresentation matrices $T^2(\lambda)$ are found from (2.14) and (4.4), or, alternately, by coupling the elements of two $T^1(\lambda)$ matrices via the product law (4.14). We restrict ourselves to the case of $\lambda = 0$,

$$T^2(0) = \begin{pmatrix} a^2 & \kappa_1 a\alpha & \kappa_3 ab & \kappa_1 \alpha b & b^2 \\ \kappa_1 a\gamma & ae + q^{-1}\gamma\alpha & \kappa_2(a\beta + q^{-1}\gamma b) & -\alpha\beta + q^{-1}eb & \kappa_1 b\beta \\ \kappa_3 ac & \kappa_2(a\delta + c\alpha) & ad + q^{-1}[2]\alpha\delta + q^{-2}bc & \kappa_2(\alpha d + \delta b) & \kappa_3 bd \\ \kappa_1 \gamma c & \gamma\delta + q^{-1}ce & \kappa_2(\gamma d + q^{-1}c\beta) & ed + q^{-1}\beta\delta & \kappa_1 \beta d \\ c^2 & \kappa_1 c\delta & \kappa_3 cd & \kappa_1 \delta d & d^2 \end{pmatrix}, \tag{6.1}$$

where

$$\kappa_1 = \sqrt{\frac{[4]}{q[2]}}, \quad \kappa_2 = \sqrt{q^{-1}[3]}, \quad \kappa_3 = \kappa_1\kappa_2. \tag{6.2}$$

The basis of $V^{(2)}$ is denoted by $Y_m = e^2_m(0)$, where $m = 0, \pm 1, \pm 2$. Here $Y_0, Y_{\pm 2}$ are even, and $Y_{\pm 1}$ are odd. Following the prescription in Sec. V A, we seek a covariant algebra under the right coaction of $T^2(0)$. The CGC for $\ell = 2$ are found in Appendix D. The relation for $L = 0$ is obtained via (5.4),

$$q^{-1}Y_2Y_{-2} - q^{-1/2}Y_1Y_{-1} - Y_0^2 + q^{1/2}Y_{-1}Y_1 + qY_{-2}Y_2 = r, \tag{6.3}$$

where r is a constant. Equation (6.3) may be regarded as the radius relation of the quantum supersphere. Explicit constructions for the $L = 2$ case are obtained from (5.5),

$$q^{-3/2}Y_2Y_0 - \left(\frac{[3]!}{[4]}\right)^{1/2} Y_1^2 - q^{3/2}Y_0Y_2 = \xi Y_2,$$

$$q^{-1/2}\left(\frac{[3]!}{[4]}\right)^{1/2} Y_2Y_{-1} + q^{-1/2}\mu_{21}Y_1Y_0 - q^{1/2}\mu_{22}Y_0Y_1 - q^{1/2}\left(\frac{[3]!}{[4]}\right)^{1/2} Y_{-1}Y_2 = \xi Y_1,$$

$$q^{1/2}Y_2Y_{-2} - \mu_{22}Y_1Y_{-1} + \mu_{23}Y_0^2 - \mu_{21}Y_{-1}Y_1 - q^{-1/2}Y_{-2}Y_2 = \xi Y_0,$$

$$q^{-1/2}\left(\frac{[3]!}{[4]}\right)^{1/2} Y_1Y_{-2} + q^{-1/2}\mu_{21}Y_0Y_{-1} - q^{1/2}\mu_{22}Y_{-1}Y_0 - q^{1/2}\left(\frac{[3]!}{[4]}\right)^{1/2} Y_{-2}Y_1 = \xi Y_{-1},$$

$$q^{-3/2}Y_0Y_{-2} - \left(\frac{[3]!}{[4]}\right)^{1/2} Y_{-1}^2 - q^{3/2}Y_{-2}Y_0 = \xi Y_{-2}, \tag{6.4}$$

where ξ is a constant vanishing in the classical limit, and

$$\mu_{21} = \frac{[2]}{[4]}(q^{-2} + q^{3/2}[2]), \quad \mu_{22} = \frac{[2]}{[4]}(q^2 - q^{-3/2}[2]), \quad \mu_{23} = \frac{[2]^2}{[4]}\left(\frac{[8]}{[4]} + 2\frac{[4]}{[2]} + 1\right). \tag{6.5}$$

The construction (5.6) may be applied to the remaining values of L. The relations for the $L=3$ case read

$$q^{-1}Y_2Y_1 - qY_1Y_2 = 0,$$

$$Y_2Y_0 - \mu_{31}Y_1^2 - Y_0Y_2 = 0,$$

$$qY_2Y_{-1} - \mu_{32}Y_1Y_0 + \mu_{33}Y_0Y_1 - q^{-1}Y_{-1}Y_2 = 0,$$

$$-q^2Y_2Y_{-2} + q^{1/2}([3] + q^2)Y_1Y_{-1} + [3]\omega Y_0^2 + q^{-1/2}([3] + q^{-2})Y_{-1}Y_1 + q^{-2}Y_{-2}Y_2 = 0,$$

$$qY_1Y_{-2} - \mu_{32}Y_0Y_{-1} + \mu_{33}Y_{-1}Y_0 - q^{-1}Y_{-2}Y_1 = 0,$$

$$Y_0Y_{-2} - \mu_{31}Y_{-1}^2 - Y_{-2}Y_0 = 0,$$

$$q^{-1}Y_{-1}Y_{-2} - qY_{-2}Y_{-1} = 0, \tag{6.6}$$

where

$$\mu_{31} = -\frac{\sqrt{[4]!}}{[2]^2}\omega, \quad \mu_{32} = \left(\frac{[4]}{[3]!}\right)^{1/2}(q^2 + q^{-1/2}[2]), \quad \mu_{33} = \left(\frac{[4]}{[3]!}\right)^{1/2}(q^{-2} - q^{1/2}[2]). \tag{6.7}$$

We observe that the relations (6.4) together with (6.6) have the correct classical limits. We have obtained a set of 12 relations for five generators. To test whether they consistently define an algebra, we need to check for the conditions (a) and (b) mentioned in Sec. V B. It may be proved by direct computation that the said conditions are, however, not satisfied.

In order to make the algebra well defined, we incorporate the $L=1$ relations listed below,

$$q^{-3/2}Y_2Y_{-1} - q^{-1/2}\left(\frac{[3]!}{[4]}\right)^{1/2} Y_1Y_0 - q^{1/2}\left(\frac{[3]!}{[4]}\right)^{1/2} Y_0Y_1 + q^{3/2}Y_{-1}Y_2 = 0,$$

$$-q^{-1/2}Y_2Y_{-2} + q^{-1}\mu_{11}Y_1Y_{-1} + \varpi\frac{[3]!}{[4]}Y_0^2 - q\mu_{12}Y_{-1}Y_1 - q^{1/2}Y_{-2}Y_2 = 0,$$

$$-q^{-3/2}Y_1Y_{-2} + q^{-1/2}\left(\frac{[3]!}{[4]}\right)^{1/2} Y_0Y_{-1} + q^{1/2}\left(\frac{[3]!}{[4]}\right)^{1/2} Y_{-1}Y_0 - q^{3/2}Y_{-2}Y_1 = 0, \tag{6.8}$$

where

$$\varpi = q^{1/2} + q^{-1/2}, \quad \mu_{11} = q + q^{-1}\frac{[2]}{[4]}, \quad \mu_{12} = q^{-1} + q\frac{[2]}{[4]}. \tag{6.9}$$

The remaining $L=4$ relations cannot be incorporated, because they contain unacceptable equations such as $Y_{\pm 2}^2 = 0$.

As all the relations in (6.4), (6.6), and (6.8) are covariant by construction, their linear combinations are also covariant. Taking linear combination of the 15 relations, 12 "commutation relations" of generators and three constraints are obtained. The commutation relations read

$$Y_2Y_1 = q^2Y_1Y_2, \quad Y_{-1}Y_{-2} = q^2Y_{-2}Y_{-1},$$

$$q^{-2}Y_2Y_0 = q^2Y_0Y_2 + \varpi\frac{[4][3]}{[6]}\xi Y_2,$$

$$q^{-2}Y_0Y_{-2} = q^2Y_{-2}Y_0 + \varpi\frac{[4][3]}{[6]}\xi Y_{-2},$$

$$q^{-3}Y_2Y_{-1} = q^3Y_{-1}Y_2 + \varpi\frac{[3]\sqrt{[4]!}}{[6]}\xi Y_1,$$

$$q^{-3}Y_1Y_{-2} = q^3Y_{-2}Y_1 + \varpi\frac{[3]\sqrt{[4]!}}{[6]}\xi Y_{-1},$$

$$q^{-1}Y_1Y_0 = qY_0Y_1 + \varpi\frac{[3]!}{[6]}\xi Y_1,$$

$$q^{-1}Y_0Y_{-1} = qY_{-1}Y_0 + \varpi\frac{[3]!}{[6]}\xi Y_{-1},$$

$$q^{-1}\mu_{11}Y_2Y_{-2} = q\mu_{12}Y_{-2}Y_2 - F_1Y_0^2 + F_2Y_0,$$

$$q^{-1/2}Y_1Y_{-1} = -q^{1/2}Y_{-1}Y_1 + \omega Y_0^2 + \frac{\varpi}{q+1+q^{-1}}\xi Y_0,$$

$$Y_1^2 = \frac{1}{\mu_{31}}(Y_2Y_0 - Y_0Y_2), \quad Y_{-1}^2 = \frac{1}{\mu_{31}}(Y_0Y_{-2} - Y_{-2}Y_0), \tag{6.10}$$

where

$$F_1 = \varpi(q^2+q+1+q^{-1}+q^{-2})\frac{[2]^2}{[4]},$$

$$F_2 = \varpi(q^2+2q+2q^{-1}+q^{-2})\frac{[3]![2]}{[6][4]}\xi. \tag{6.11}$$

Classical commutation properties immediately follow from (6.10) in the limit $q \to 1$. Three said constraints are given by

$$Y_2Y_{-1} = \frac{q^2}{[3]}\left(\frac{[3]!}{[4]}\right)^{1/2}Y_1Y_0 + q^{1/2}\frac{[2]}{[6]}\left(\frac{[3]!}{[4]}\right)^{1/2}\xi Y_1,$$

$$Y_1Y_{-2} = \frac{q^2}{[3]}\left(\frac{[3]!}{[4]}\right)^{1/2}Y_0Y_{-1} + q^{1/2}\frac{[2]}{[6]}\left(\frac{[3]!}{[4]}\right)^{1/2}\xi Y_{-1},$$

$$Y_0^2 = q^{-1}\frac{[4]}{[2]}Y_2Y_{-2} - q^{-1/2}(q+q^{-1})\mu_{12}Y_1Y_{-1} - q^{-3/2}\frac{[3]!}{[6]}\xi Y_0. \tag{6.12}$$

The classical limit of these constraints are not required in the commutative case. However, *we need the constraints to satisfy the two important requirements* given in Sec. V B. Verification of these conditions is straightforward but requires dull lengthy computation. Since the two conditions are satisfied, we define a one-parameter family of $\mathcal{A}$-covariant quantum superspheres by the radius relation (6.3), the commutation relations (6.10), and the constraints (6.12). We denote this quantum supersphere by $S^0_{q,\xi}$. The superscript 0 indicates the parity $\lambda=0$ and ξ is a free parameter which does not have a classical counterpart. The origin of the parameter and the fact that the quantum superspheres cannot have more parameters clearly follows from the formulation in Sec. V A.

B. Properties of $S^0_{q,\xi}$

In this section, three properties of the quantum supersphere $S^0_{q,\xi}$ are investigated. First, we consider a realization of $S^0_{q,\xi}$ in terms of elements of $\mathcal{A}$. Then it turns out that this realization admits an infinitesimal characterization of $S^0_{q,\xi}$. A representation of $S^0_{q,\xi}$ in terms of a $\mathcal{U}$-covariant oscillator is also given.

Analogous to the example of Podleś q-sphere, embedding of $S^0_{q,\xi}$ in $\mathcal{A}$ may be done by realizing its generators in terms of entries of $T^2(0)$ matrix. Denoting $T^2(0)$ by T, it is straightforward to verify that the embedding is given by

$$\begin{aligned}
Y_2 &= g_1T_{2,2} + g_2T_{0,2} + g_3T_{-2,2},\\
Y_1 &= g_1T_{2,1} + g_2T_{0,1} + g_3T_{-2,1},\\
Y_0 &= g_1T_{2,0} + g_2T_{0,0} + g_3T_{-2,0},\\
Y_{-1} &= g_1T_{2,-1} + g_2T_{0,-1} + g_3T_{-2,-1},\\
Y_{-2} &= g_1T_{2,-2} + g_2T_{0,-2} + g_3T_{-2,-2},
\end{aligned} \tag{6.13}$$

where the coefficients g_1, g_2, and g_3 need to satisfy the constraint

$$g_1g_3 = \frac{[3]!}{[4]}g_2^2. \tag{6.14}$$

In this embedding, the radius r and the parameter ξ are given as functions of g_2,

$$r = ([2]g_2)^2, \quad \xi = \frac{[6]}{[3]}g_2. \tag{6.15}$$

This embedding allows us to treat $S^0_{q,\xi}$ as a subalgebra of $\mathcal{A}$. This fact suggests that $S^0_{q,\xi}$ has an infinitesimal characterization as shown by Koornwinder.[13] To demonstrate this, we extend the left and right actions of $U_q[su(2)]$ on $SU_q(2)$ defined in Ref. 13 to the supersymmetric case. In the following we assume $u,v\in\mathcal{U}; a,b\in\mathcal{A}$, and use Sweedler's notation to denote coproducts, e.g., $\Delta(a)=\Sigma a_{(1)}\otimes a_{(2)}$. With a slight change of notation from Ref. 13, we now define elements $u\odot a$ and $a\odot u$ of $\mathcal{A}$ by

$$u\odot a = (\mathrm{id}\otimes u)(\Delta(a)) = \sum (-1)^{\hat{u}\hat{a}_{(1)}}a_{(1)}\langle u, a_{(2)}\rangle, \tag{6.16}$$

$$a\odot u=(-1)^{\hat{a}\hat{u}}(u\otimes \mathrm{id})(\Delta(a))=\sum (-1)^{\hat{a}\hat{u}}\langle u,a_{(1)}\rangle a_{(2)}. \tag{6.17}$$

The coassociativity of $\mathcal{A}$ then leads to

$$(uv)\odot a=u\odot(v\odot a),\quad a\odot(uv)=(a\odot u)\odot v. \tag{6.18}$$

Moreover, we also have

$$u\odot(ab)=\sum (-1)^{\hat{u}_{(2)}\hat{a}}(u_{(1)}\odot a)(u_{(2)}\odot b),$$

$$(ab)\odot u=\sum (-1)^{\hat{u}_{(1)}\hat{b}}(a\odot u_{(1)})(b\odot u_{(2)}). \tag{6.19}$$

Thus, $u\odot a$ and $a\odot u$ define left and right actions of u on a, respectively. The actions of generators of $\mathcal{U}$ on the T^{ℓ}-matrix of $\mathcal{A}$ are calculated by using (2.11). Explicitly, the left actions are given by

$$K^{\pm 1}\odot T^{\ell}_{m_1m_2}(\lambda)=q^{\pm m_2/2}T^{\ell}_{m_1m_2}(\lambda),$$

$$v_+\odot T^{\ell}_{m_1m_2}(\lambda)=(-1)^{\ell+m_1+\lambda}\sqrt{[\ell-m_2][\ell+m_2+1]\varrho}\,T^{\ell}_{m_1m_2+1}(\lambda),$$

$$v_-\odot T^{\ell}_{m_1m_2}(\lambda)=(-1)^{m_1+m_2+\lambda+1}\sqrt{[\ell+m_2][\ell-m_2+1]\varrho}\,T^{\ell}_{m_1m_2-1}(\lambda), \tag{6.20}$$

while the right actions read

$$T^{\ell}_{m_1m_2}(\lambda)\odot K^{\pm 1}=q^{\pm m_1/2}T^{\ell}_{m_1m_2}(\lambda),$$

$$T^{\ell}_{m_1m_2}(\lambda)\odot v_+=(-1)^{\ell+m_2+\lambda}\sqrt{[\ell-m_1+1][\ell+m_1]\varrho}\,T^{\ell}_{m_1-1m_2}(\lambda),$$

$$T^{\ell}_{m_1m_2}(\lambda)\odot v_-=(-1)^{m_1+m_2+\lambda}\sqrt{[\ell+m_1+1][\ell-m_1]\varrho}\,T^{\ell}_{m_1+1m_2}(\lambda). \tag{6.21}$$

An element $u\in\mathcal{U}$ possessing a coproduct structure $\Delta(u)=g\otimes u+u\otimes g^{-1}$ with $g\in\mathcal{U}$ being a grouplike element, is known as twisted primitive with respect to g. For a twisted primitive element u, it is straightforward to verify that

$$u\odot a=0\quad\text{and}\quad u\odot b=0\Rightarrow u\odot(ab)=0, \tag{6.22}$$

$$a\odot u=0\quad\text{and}\quad b\odot u=0\Rightarrow (ab)\odot u=0. \tag{6.23}$$

Thus a set of elements of $\mathcal{A}$ annihilated by a twisted primitive element u form a subalgebra of $\mathcal{A}$. Indeed, the quantum supersphere $S^0_{q,\xi}$ embedded into $\mathcal{A}$ is a subalgebra of $\mathcal{A}$ that is annihilated by the twisted primitive element $\mathcal{P}_R$,

$$\mathcal{P}_R=-\sqrt{g_3}v_+ +\sqrt{g_1}v_-, \tag{6.24}$$

$$Y_k\odot\mathcal{P}_R=0,\quad k=\pm 2,\pm 1,0. \tag{6.25}$$

The algebra $\mathcal{U}$ has three twisted primitive elements, $K-K^{-1}$, v_+, and v_-. However, $\mathcal{P}_R$ consists of only odd twisted primitive elements. This is a difference from the q-sphere for $\mathrm{SU}_q(2)$. In that example, all the twisted primitive elements contribute to the annihilation operator of the q-sphere.

We now turn to an oscillator realization of $S^0_{q,\xi}$. In Ref. 20, a $\mathcal{U}$-covariant oscillator algebra is introduced. This oscillator algebra is generated by a pair of even creation/annihilation operators ($^-$,), and an odd operator obeying the relations

$$^{-} = q^{-}, \qquad = q^{-1} \quad , \qquad ^{-} - q^{-2-} = 1,$$

$$^{2} = q^{-1}[2]^{-} + \varpi^{-1}. \tag{6.26}$$

These relations are determined by two steps. First, the action of $\mathcal{U}$ on the oscillator is defined via the coproduct of $\mathcal{U}$. Then the commutation properties of the oscillator is fixed by demanding that the triplet $(^{-}, \ , - \ )$ transforms under the $\ell=1$ representation of $\mathcal{U}$. This suggests that the $\mathcal{U}$-covariant oscillator has a close kinship to the quantum space discussed in Sec. V B. Indeed, the $\mathcal{U}$-covariant oscillator is isomorphic to the quantum plane for a special value of r,

$$z_1 = ^{-}, \quad z_0 = \ , \quad z_{-1} = - \ , \quad r = - q\varpi^{-1}. \tag{6.27}$$

Employing the $\mathcal{U}$-covariant oscillator, it is possible to realize $S^0_{q,\xi}$,

$$Y_2 = ^{-2}, \quad Y_1 = q^{-1/2}\left(\frac{[4]}{[2]}\right)^{1/2} - \ ,$$

$$Y_0 = - \frac{\sqrt{[4]!}}{q[2]} - \ - \frac{q^{-1/2}}{\varpi}\left(\frac{[4]}{[3]!}\right)^{1/2},$$

$$Y_{-1} = - q^{-1/2}\left(\frac{[4]}{[2]}\right)^{1/2} \ , \quad Y_{-2} = \ ^{2}. \tag{6.28}$$

In this realization, the radius r and the parameter ξ of $S^0_{q,\xi}$ assume the following values:

$$r = \frac{q^2}{\varpi^2}\frac{[4]}{[3]!}, \quad \xi = \frac{[6]}{[3]!}r^{1/2}. \tag{6.29}$$

An advantage of this realization is that we may represent $S^0_{q,\xi}$ with matrices, since matrix representation of $\mathcal{U}$-covariant oscillator via that of Biedenharn-Macfarlane q-boson algebra exists.[20]

VII. CONCLUDING REMARKS

We have developed the general prescription for constructing $\mathcal{A}$-covariant algebras. By the method, four $\mathcal{A}$-covariant algebras have been obtained, namely, three quantum superspaces and a one-parameter family of quantum superspheres. The special cases of the quantum superspaces correspond to the Manin's quantum superplane and $\mathcal{U}$-covariant oscillator algebra. The quantum superspheres are realized by $\mathcal{A}$ so that it can be regarded as a subalgebra of $\mathcal{A}$. This subalgebra is characterized by the fact that it is annihilated by the right action of a particular combination of the twisted primitive elements of $\mathcal{U}$. These are the similarities to the q-spheres for $SU_q(2)$. It has also been shown that the quantum superspheres have $\mathcal{U}$-covariant oscillator realization that allows us to have matrix representations of the quantum supersphere.

We believe that the results of this paper are useful for making progress in constructing supersymmetric versions of noncommutative geometry. For instance, we may consider differential calculi on the quantum supersphere, then compute its curvature, metric, and so on based on the framework of Ref. 5. In connection with the classification of differential calculi, it is interesting to determine the dual coalgebra of $S^0_{q,\xi}$. The corresponding computation for $SU_q(2)$ q-sphere was made recently and applied to the classification of differential calculi.[11] Furthermore, the general method in Sec. V A is applied to construct higher dimensional quantum superspaces by taking higher values of ℓ.

It is worth pointing out that, because of the similarity of the representation theory of $\mathcal{U}$ to that of $U_q[su(2)]$, the method developed in Sec. V A is valid for $SU_q(2)$. This procedure allows us to treat quantum plane, deformed oscillator and Podleś q-sphere in a unified way. The reason for q-spheres being a one-parameter family becomes clear in this framework. It is also possible to construct hitherto unknown higher dimensional $SU_q(2)$-covariant quantum spaces. We will present these results elsewhere.

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APPENDIX A: CGC OF $\mathcal{U}$

In this appendix, the general expression of CGC in our conventions is derived. Let us write the highest weight vector as

$$e^{\ell}_{\ell}(\ell_1,\ell_2,\Lambda)=\sum_{m_1,m_2} A_{m_1m_2}e^{\ell_1}_{m_1}(\lambda)\otimes e^{\ell_2}_{m_2}(\lambda), \tag{A1}$$

where, for simplicity of notation, the CGC is denoted by $A_{m_1m_2}$. The highest weight condition $\Delta(v_+)e^{\ell}_{\ell}(\ell_1,\ell_2,\Lambda)=0$ gives the recurrence relation for $A_{m_1m_2}$,

$$\sqrt{[\ell_1-m_1][\ell_1+m_1+1]}q^{-m_2/2}A_{m_1m_2}-(-1)^{\ell_1-m_1+\lambda}q^{(m_1+1)/2}\sqrt{[\ell_2+m_2][\ell_2-m_2+1]}A_{m_1+1m_2-1}=0. \tag{A2}$$

It is easy to find the solution of this relation

$$A_{m_1m_2}=(-1)^{\lambda(\ell_1-m_1)+(\ell_1-m_1)(\ell_1-m_1+1)/2}q^{(\ell+1)(\ell_1-m_1)/2}\times\left(\frac{[\ell_1+\ell_2-\ell]![\ell_1+m_1]![\ell_2+m_2]!}{[\ell_2-\ell_1+\ell]![2\ell_1]![\ell_1-m_1]![\ell_2-m_2]!}\right)^{1/2}A_{\ell_1\ell-\ell_1}. \tag{A3}$$

The normalization of the highest weight vector (A1) determines $A_{\ell_1\ell-\ell_1}$ as follows:

$$\begin{aligned}(e^{\ell}_{\ell}(\ell_1,\ell_2,\Lambda),e^{\ell}_{\ell}(\ell_1,\ell_2,\Lambda))&=\sum_{m_1,m_2}(-1)^{(\ell_1-m_1+\lambda)(\ell_2-m_2+\lambda)}A^2_{m_1m_2}\\&=(-1)^{(\ell_1+\lambda)(\ell_2+\ell+\lambda)}\frac{[\ell_1+\ell_2-\ell]!}{[\ell_2-\ell_1+\ell]![2\ell_1]!}A^2_{\ell_1\ell-\ell_1}\\&\quad\times\sum_{m_1}(-1)^{m_1(\ell_1+\ell_2+\ell+1)}q^{(\ell+1)(\ell_1-m_1)}\frac{[\ell_1+m_1]![\ell_2+\ell-m_1]!}{[\ell_1-m_1]![\ell_2-\ell+m]!}.\end{aligned}$$

The summation over m_1 is computed by using the formula (B5). Setting

$$a=\ell_1-m_1,\quad k=\ell_1+\ell_2-\ell,\quad -n=\ell_1-\ell_2+\ell+1,\quad -r=-\ell_1+\ell_2+\ell+1$$

in (B5), while noticing that all these quantities are positive integers, we obtain

$$\sum_{m_1}(-1)^{(\ell_1-m_1)(\ell_1+\ell_2+\ell+1)}q^{(\ell+1)(\ell_1-m_1)}\frac{[\ell_1+m_1]![\ell_2+\ell-m_1]!}{[\ell_1-m_1]![\ell_2-\ell+m]!}$$
$$=q^{(-\ell_1+\ell_2+\ell+1)(\ell_1+\ell_2-1)/2}\frac{[\ell_1+\ell_2+\ell+1]![\ell_1-\ell_2+\ell]![-\ell_1+\ell_2+\ell]!}{[\ell_1+\ell_2-\ell]![2\ell+1]!}.$$

Thus the norm of the highest weight vector reads

$$\|e_\ell^\ell(\ell_1,\ell_2,\Lambda)\|^2=(-1)^{\lambda(\ell_1+\ell_2+\ell+1)}q^{(-\ell_1+\ell_2+\ell+1)(\ell_1+\ell_2-1)/2}A^2_{\ell_1\ell-\ell_1}\frac{[\ell_1+\ell_2+\ell+1]![\ell_1-\ell_2+\ell]!}{[2\ell+1]![2\ell_1]!}.$$

This leads to

$$A_{\ell_1\ell-\ell_1}=q^{-(-\ell_1+\ell_2+\ell+1)(\ell_1+\ell_2-1)/4}\left(\frac{[2\ell+1]![2\ell_1]!}{[\ell_1+\ell_2+\ell+1]![\ell_1-\ell_2+\ell]!}\right)^{1/2}, \tag{A4}$$

where the phase is chosen such that the expression coincides with the result in Ref. 17.

To obtain the other vectors in this irreducible representation we need the following results, which may be verified by induction:

$$v_-^k e_m^\ell(\lambda)=(-1)^{(\ell-m)k+k(k+1)/2}\left(\frac{[\ell+m]![\ell-m+k]!}{[\ell-m]![\ell+m-k]!}\varrho^k\right)^{1/2}e^\ell_{m-k}(\lambda), \tag{A5}$$

$$\Delta(v_-^n)=\sum_{k=0}^n\begin{bmatrix}n\\k\end{bmatrix}(-1)^{k(n-k)}v_-^{n-k}K^k\otimes v_-^kK^{-n+k}. \tag{A6}$$

Using (A5) we obtain

$$e_m^\ell(\ell_1,\ell_2,\Lambda)=(-1)^{(\ell-m)(\ell-m+1)/2}\left(\frac{[\ell+m]!}{[2\ell]![\ell-m]!\varrho^{\ell-m}}\right)^{1/2}\Delta(v_-^{\ell-m})e_\ell^\ell(\ell_1,\ell_2,\Lambda). \tag{A7}$$

The right-hand side is computed by using (A6) and (A1). After some algebra, we derive

$$\Delta(v_-^{\ell-m})e^{\ell_1}_{m_1}(\lambda)\otimes e^{\ell_2}_{m_2}(\lambda)=\sum_k\begin{bmatrix}\ell-m\\k\end{bmatrix}(-1)^{k(\ell_2-m_2+\lambda)+(\ell_1-m_1)(\ell-m)+(\ell-m)(\ell-m+1)/2}q^{km_1/2+(-\ell+m+k)m_2/2}$$
$$\times\left(\frac{[\ell_1+m_1]![\ell_2+m_2]![\ell_1+\ell-m_1-m-k]![\ell_2-m_2+k]!}{[\ell_1-m_1]![\ell_2-m_2]![\ell_1-\ell+m_1+m+k]![\ell_2+m_2-k]!}\varrho^{\ell-m}\right)^{1/2}$$
$$\times e^{\ell_1}_{m_1-\ell+m+k}(\lambda)\otimes e^{\ell_2}_{m_2-k}(\lambda). \tag{A8}$$

Equations (A3) and (A4) allow us to derive

$$e_m^\ell(\ell_1,\ell_2,\Lambda)=\sum_{m_1,m_2}(-1)^{(\ell_1-\ell+m_2)(\ell-m+\lambda)+(\ell_1-\ell+m2)(\ell_1-\ell+m_2+1)/2}q^{m_2(m+1)/2+(\ell_1-\ell_2)(\ell_1+\ell_2+1)/4-\ell(\ell+1)/4}$$
$$\times\left([2\ell+1]\frac{[\ell_1+\ell_2-\ell]![\ell+m]![\ell-m]![\ell_1-m_1]![\ell_2-m_2]!}{[\ell_1+\ell_2+\ell+1]![\ell_1-\ell_2+\ell]![-\ell_1+\ell_2+\ell]![\ell_1+m_1]![\ell_2+m_2]!}\right)^{1/2}$$
$$\times\sum_k(-1)^{k(k-1)/2+k(\ell_1+\ell_2-m)}q^{k(\ell+m+1)/2}$$
$$\times\frac{[\ell_1+\ell-m_2-k]![\ell_2+m_2+k]!}{[k]![\ell-m-k]![\ell_1-\ell+m_2+k]![\ell_2-m_2-k]!}e^{\ell_1}_{m_1}(\lambda)\otimes e^{\ell_2}_{m_2}(\lambda). \tag{A9}$$

APPENDIX B: SUMMATION FORMULA FOR KULISH SYMBOL

A summation formula for Kulish symbol which is used in the preceding section is derived in this appendix. Corresponding binomial coefficient is usually defined for $y \geqslant x \geqslant 0$ as

$$\begin{bmatrix} y \\ x \end{bmatrix} = \frac{[y]!}{[y-x]![x]!} = \frac{[y][y-1]\cdots[y-x+1]}{[x]!}. \tag{B1}$$

We may extend this to $y<0$ by using the property

$$[-n] = (-1)^{n+1}[n], \quad n \geqslant 0, \tag{B2}$$

and define the binomial coefficient for negative y by the rightmost formula of (B1),

$$\begin{bmatrix} y \\ x \end{bmatrix} = \frac{[-(-y)][-(-y+1)]\cdots[-(-y+x-1)]}{[x]!} = (-1)^{xy+x(x+1)/2}\frac{[-y][-y+1]\cdots[-y+x-1]}{[x]!}.$$

Thus for $y<0$ and $x \geqslant 0$, the binomial coefficient is given by

$$\begin{bmatrix} y \\ x \end{bmatrix} = (-1)^{xy+x(x+1)/2}\begin{bmatrix} x-y-1 \\ x \end{bmatrix}. \tag{B3}$$

The following formula, proved by induction, is found in Ref. 17:

$$\begin{bmatrix} n+r \\ k \end{bmatrix} = \sum_a \begin{bmatrix} n \\ k-a \end{bmatrix}\begin{bmatrix} r \\ a \end{bmatrix}(-1)^{(k-a)(r-a)}q^{(r-a)(n+r)/2-r(n-k+r)/2}, \tag{B4}$$

where a runs over any positive integers such that the arguments of $[x]$ in the binomial coefficients are non-negative. We assume $n,r<0$, and apply (B3) to this formula,

$$\text{lhs} = (-1)^{k(n+r)+k(k+1)/2}\begin{bmatrix} k-n-r-1 \\ k \end{bmatrix},$$

$$\text{rhs} = (-1)^{k(n+r)+k(k+1)/2}q^{rk/2}\sum_a (-1)^{an}q^{-a(n+r)/2}\begin{bmatrix} k-a-n-1 \\ k-a \end{bmatrix}\begin{bmatrix} a-r-1 \\ a \end{bmatrix}.$$

From this, the following summation formula of Kulish symbols is obtained:

$$\sum_a (-1)^{an}q^{-a(n+r)/2}\frac{[k-a-n-1]![a-r-1]!}{[k-a]![a]!} = q^{-rk/2}\frac{[k-n-r-1]![-n-1]![-r-1]!}{[k]![-n-r-1]!}. \tag{B5}$$

APPENDIX C: CGC FOR $1\otimes 1 = 2\oplus 1\oplus 0$

Tables I–III contain the values of $C^{1\ 1\ \ell}_{m_1\ m-m_1\ m}$ for a given ℓ. The columns provide the values of m_1, while the rows indicate m. The rightmost column of Table I, titled as "OF," indicates the overall factors that are common to all entries in the row. In Table II and III, the overall factors are common for all entries of the tables.

TABLE I. $\ell=2$.

	1	0	−1	OF
2	1	0	0	1
1	$(-1)^{\lambda}q^{1/2}$	$q^{-1/2}$	0	$\left(\frac{[2]}{[4]}\right)^{1/2}$
0	q	$(-1)^{\lambda}[2]$	q^{-1}	$\frac{[2]}{\sqrt{[4]!}}$
−1	0	$q^{1/2}$	$(-1)^{\lambda}q^{-1/2}$	$\left(\frac{[2]}{[4]}\right)^{1/2}$
−2	0	0	1	1

TABLE II. $\ell=1$, $\mathrm{OF}=([2]/[4])^{1/2}$.

	1	0	−1
1	$q^{-1/2}$	$(-1)^{\lambda+1}q^{1/2}$	0
0	$(-1)^{\lambda+1}$	$q^{1/2}+q^{-1/2}$	$(-1)^{\lambda}$
−1	0	$(-1)^{\lambda+1}q^{-1/2}$	$q^{1/2}$

TABLE III. $\ell=0$, $\mathrm{OF}=1/\sqrt{[3]}$.

	1	0	−1
0	$q^{-1/2}$	$(-1)^{\lambda+1}$	$-q^{1/2}$

APPENDIX D: CGC FOR 2⊗2=4⊕3⊕2⊕1⊕0

Tables IV–VIII contain the values of $C^{2\ 2\ \ell}_{m_1\ m-m_1\ m}$ for a given ℓ. The columns provide the values

TABLE IV. $\ell=4$.

	2	1	0	−1	−2	OF
4	1	0	0	0	0	1
3	$(-1)^{\lambda}q$	q^{-1}	0	0	0	$\left(\frac{[4]}{[8]}\right)^{1/2}$
2	q^2	$(-1)^{\lambda}\left(\frac{[2][4]}{[3]}\right)^{1/2}$	q^{-2}	0	0	$\left(\frac{[3][4]}{[7][8]}\right)^{1/2}$
1	$(-1)^{\lambda}q^3\sqrt{[4]!}$	$q[4][3]$	$(-1)^{\lambda}q^{-1}[4][3]$	$q^{-3}\sqrt{[4]!}$	0	$\left(\frac{[5]!}{[8]!}\right)^{1/2}$
0	q^4	$(-1)^{\lambda}q^2[4]$	$[4][3]$	$(-1)^{\lambda}q^{-2}[4]$	q^{-4}	$\frac{[4]!}{\sqrt{[8]!}}$
−1	0	$q^3\sqrt{[4]!}$	$(-1)^{\lambda}q[4][3]$	$q^{-1}[4][3]$	$(-1)^{\lambda}q^{-3}\sqrt{[4]!}$	$\left(\frac{[5]!}{[8]!}\right)^{1/2}$
−2	0	0	q^2	$(-1)^{\lambda}\left(\frac{[2][4]}{[3]}\right)^{1/2}$	q^{-2}	$\left(\frac{[3][4]}{[7][8]}\right)^{1/2}$
−3	0	0	0	q	$(-1)^{\lambda}q^{-1}$	$\left(\frac{[4]}{[8]}\right)^{1/2}$
−4	0	0	0	0	1	1

TABLE V. $\ell=3$.

	2	1	0	−1	−2	OF
3	q^{-1}	$(-1)^{\lambda+1}q$	0	0	0	$\left(\frac{[4]}{[8]}\right)^{1/2}$
2	$(-1)^{\lambda+1}$	μ_{31}	$(-1)^{\lambda}$	0	0	$\left(\frac{[4]!}{[6][8]}\right)^{1/2}$
1	q	$(-1)^{\lambda+1}\mu_{32}$	μ_{33}	$(-1)^{\lambda+1}q^{-1}$	0	$\left(\frac{[7][3]}{[8]!}\right)^{1/2}[4]!$
0	$(-1)^{\lambda+1}q^2$	$q^{1/2}([3]+q^2)$	$(-1)^{\lambda}[3]\omega$	$q^{-1/2}([3]+q^{-2})$	$(-1)^{\lambda}q^{-2}$	$\left(\frac{[7]}{[8]!}\right)^{1/2}[4]!$
−1	0	$(-1)^{\lambda+1}q$	μ_{32}	$(-1)^{\lambda+1}\mu_{33}$	q^{-1}	$\left(\frac{[7][3]}{[8]!}\right)^{1/2}[4]!$
−2	0	0	$(-1)^{\lambda+1}$	μ_{31}	$(-1)^{\lambda}$	$\left(\frac{[4]!}{[6][8]}\right)^{1/2}$
−3	0	0	0	$(-1)^{\lambda+1}q^{-1}$	q	$\left(\frac{[4]}{[8]}\right)^{1/2}$

$$\mu_{31}=\frac{\sqrt{[4]!}}{[2]^2}\omega\,,\ \mu_{32}=\left(\frac{[4]}{[3]!}\right)^{1/2}(q^2+q^{-1/2}[2])\,,\ \mu_{33}=\left(\frac{[4]}{[3]!}\right)^{1/2}(q^{-2}-q^{1/2}[2])$$

TABLE VI. $\ell=2$.

	2	1	0	−1	−2	OF
2	$q^{-3/2}$	$(-1)^{\lambda+1}\left(\frac{[3]!}{[4]}\right)^{1/2}$	$-q^{3/2}$	0	0	$\left(\frac{[3][4]}{[6][7]}\right)^{1/2}$
1	$(-1)^{\lambda}q^{-1/2}\left(\frac{[3]!}{[4]}\right)^{1/2}$	$q^{-1/2}\mu_{21}$	$(-1)^{\lambda+1}q^{1/2}\mu_{22}$	$-q^{1/2}\left(\frac{[3]!}{[4]}\right)^{1/2}$	0	$\left(\frac{[3][4]}{[6][7]}\right)^{1/2}$
0	$q^{1/2}$	$(-1)^{\lambda+1}\mu_{22}$	μ_{23}	$(-1)^{\lambda+1}\mu_{21}$	$-q^{-1/2}$	$\left(\frac{[3][4]}{[6][7]}\right)^{1/2}$
−1	0	$q^{-1/2}\left(\frac{[3]!}{[4]}\right)^{1/2}$	$(-1)^{\lambda}q^{-1/2}\mu_{21}$	$-q^{1/2}\mu_{22}$	$(-1)^{\lambda+1}q^{1/2}\left(\frac{[3]!}{[4]}\right)^{1/2}$	$\left(\frac{[3][4]}{[6][7]}\right)^{1/2}$
−2	0	0	$q^{-3/2}$	$(-1)^{\lambda+1}\left(\frac{[3]!}{[4]}\right)^{1/2}$	$-q^{3/2}$	$\left(\frac{[3][4]}{[6][7]}\right)^{1/2}$

$$\mu_{21}=\frac{[2]}{[4]}(q^{-2}+q^{3/2}[2]),\ \mu_{22}=\frac{[2]}{[4]}(q^2-q^{-3/2}[2]),\ \mu_{23}=\frac{[2]^2}{[4]}\left(\frac{[8]}{[4]}+2\frac{[4]}{[2]}+1\right).$$

TABLE VII. $\ell=1$.

	2	1	0	−1	−2	OF
1	$q^{-3/2}$	$(-1)^{\lambda+1}q^{-1/2}\left(\frac{[3]!}{[4]}\right)^{1/2}$	$-q^{1/2}\left(\frac{[3]!}{[4]}\right)^{1/2}$	$(-1)^{\lambda}q^{3/2}$	0	$\left(\frac{[3]!}{[5][6]}\right)^{1/2}$
0	$(-1)^{\lambda+1}q^{-1/2}$	$q^{-1}\mu_{11}$	$(-1)^{\lambda+1}\frac{[3]}{[4]}\omega$	$-q\mu_{12}$	$(-1)^{\lambda+1}q^{1/2}$	$\left(\frac{[3][4]}{[5][6]}\right)^{1/2}$
−1	0	$(-1)^{\lambda+1}q^{-3/2}$	$q^{-1/2}\left(\frac{[3]!}{[4]}\right)^{1/2}$	$(-1)^{\lambda}q^{1/2}\left(\frac{[3]!}{[4]}\right)^{1/2}$	$-q^{3/2}$	$\left(\frac{[3]!}{[5][6]}\right)^{1/2}$

$$\mu_{11}=q+q^{-1}\frac{[2]}{[4]},\ \mu_{12}=q^{-1}+q\frac{[2]}{[4]}$$

TABLE VIII. $\ell=0$.

	2	1	0	−1	−2	OF
0	q^{-1}	$(-1)^{\lambda+1}q^{-1/2}$	−1	$(-1)^{\lambda}q^{1/2}$	q	$\frac{1}{\sqrt{[5]}}$

of m_1, while the rows indicate m. The rightmost column, titled as "OF," indicates the overall factors common to all entries in the row.

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An optimal Monte Carlo algorithm for multivariate Feynman–Kac path integrals

Marek Kwas[a)]
Department of Computer Science, Columbia University, New York, New York 10027 and Institute of Applied Mathematics and Mechanics, University of Warsaw, ul. Banacha 2, 02-097 Warszawa, Poland

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We study a Monte Carlo algorithm for approximating multivariate Feynman–Kac path integrals parameterized by initial value and potential d-variate functions. This problem suffers from the curse of dimensionality in the worst case deterministic setting. That is why we study the randomized setting in which the functions are sampled at randomized points and the algorithm uses a finite number of such samples. We achieve optimality of the randomized algorithm due to variance reduction obtained by Smolyak's algorithm for approximating tensor product functions. The optimal convergence depends on the smoothness of initial value and potential functions. When the initial value and potential functions are r times continuously differentiable we obtain the optimal convergence of order $m^{-1/2-r/d}$ for m function samples. Thus, if r/d is negligible we do not gain much over the commonly used classical Monte Carlo algorithm whose convergence is of order $m^{-1/2}$. Hence, the classical Monte Carlo algorithm turns out to be almost optimal if r/d is small. On the other hand, we can significantly improve the classical Monte Carlo convergence if r/d is not negligible. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Due to numerous applications, approximation of path integrals with respect to the Wiener measure attracts attention in many fields, including physics, chemistry, and financial mathematics. In this article we consider a special case of such integrals, namely, the multivariate Feynman–Kac path integral that yields the solution of the initial value problem for the diffusion equation. This problem depends on d-variate initial value and potential functions.

We know that deterministic algorithms for the problem of approximating multivariate Feynman–Kac path integrals with the worst case error assurance are highly inefficient for large d, see Ref. 1. This is caused by the *provable* curse of dimensionality of this problem. More precisely, the convergence of any deterministic algorithm cannot be better than of order $m^{-r/d}$. Here, r measures the smoothness of the initial value and potential functions and m is the number of function samples. Hence, the convergence decreases exponentially with d. A popular remedy to vanquish the curse of dimensionality is through randomization. For this approach the path integral is approximated by a multivariate integral, and then this integral is approximately evaluated by a randomized algorithm, e.g., by the celebrated Monte Carlo algorithm, see e.g., Refs. 2 and 3. This yields the convergence of order $m^{-1/2}$ and the dependence on d disappears. It is important to study whether the convergence $m^{-1/2}$ can be further improved. We prove that this is indeed possible as long as the smoothness r is positive.

[a)]Current affiliation: University of Information Technology and Management in Rzeszów, Sucharskiego 2, 35-225, Rzeszów, Poland; Electronic mail: mkwas@wsiz.edu.pl

This article uses the technique presented in Ref. 4 which was then generalized and modified in Ref. 1. This technique utilizes the smoothness of the initial value and potential functions and yields an algorithm with the optimal convergence roughly of order $m^{-1/2-r/d}$, see also Ref. 5. This is proved by using techniques developed by information-based complexity whose extensive overview is presented in Ref. 6, see also Ref. 7. Thus, the classical Monte Carlo algorithm turns out to be almost optimal when the ratio r/d is negligible. In this case, the algorithm presented here shows very little advantage. However, when r/d is not negligible the convergence of the classical Monte Carlo algorithm is significantly improved.

We plan to implement and test the algorithm presented here and we will report the results in a follow-up article.

II. MULTIVARIATE FEYNMAN-KAC PATH INTEGRATION

The multivariate Feynman–Kac formula yields the solution of the initial value problem for the diffusion equation

$$\frac{\partial z}{\partial t}(\mathbf{u},t) = \tfrac{1}{2}\Delta z(\mathbf{u},t) + V(\mathbf{u})z(\mathbf{u},t) \text{ for } (\mathbf{u},t) \in \mathbb{R}^d \times (0,\infty), \tag{1}$$

$$z(\mathbf{u},0) = v(\mathbf{u}). \tag{2}$$

Here $v, V: \mathbb{R}^d \to \mathbb{R}$ are the initial value and the potential functions, respectively. As usual Δ denotes the Laplacian.

The solution z of (1) and (2) is given by the Feynman–Kac formula

$$z(\mathbf{u},t) = \int_{\mathcal{C}} v(\mathbf{x}(t)+\mathbf{u}) \exp\left(\int_0^t V(\mathbf{x}(s)+\mathbf{u}) \mathrm{d}s \right) w(\mathrm{d}\mathbf{x}). \tag{3}$$

Here, $\mathcal{C}$ is the set of continuous functions $\mathbf{x}: [0,\infty) \to \mathbb{R}^d$ such that $\mathbf{x}(0)=\mathbf{0}$. The path integral (3) is with respect to the d-dimensional Wiener measure w, see Refs. 8 and 9. In Sec. III we formulate precisely the assumptions about the initial value v and the potential V which make the path integral (3) well defined and permit feasible numerical approximation.

III. ASSUMPTIONS ON INITIAL VALUE AND POTENTIAL FUNCTIONS

We assume that the initial value v and the potential V belong to the normed space F satisfying the following assumptions.

(A1) To make the path integral (3) well defined we assume that for every $\mathbf{u} \in \mathbb{R}^d$, the functional $L_{\mathbf{u}}: F \to \mathbb{R}$ defined by $L_{\mathbf{u}} f = f(\mathbf{u})$ is continuous, and for arbitrary $a, t \in \mathbb{R}_+$ we have

$$\int_{\mathcal{C}} \|L_{\mathbf{x}(t)}\|_F \exp\left(a \int_0^t \|L_{\mathbf{x}(s)}\|_F \mathrm{d}s \right) w(\mathrm{d}\mathbf{x}) < \infty. \tag{4}$$

By Fernique's theorem, see e.g., Ref. 10, condition (4) holds if there exists $\alpha \in (0,2)$ such that $\|L_{\mathbf{x}}\|_F = O(\|\mathbf{x}\|^\alpha)$ for $\|\mathbf{x}\|$ approaching infinity, see Ref. 4 for details. Here and elsewhere, $\|\mathbf{x}\| = \sqrt{\sum_{i=1}^d x_i^2}$ is the Euclidean norm in $\mathbb{R}^d$.

(A2) We assume that F is continuously embedded into $L_\infty(\mathbb{R}^d)$. That is, $F \subset L_\infty(\mathbb{R}^d)$ and there exists a positive K such that

$$\|f\|_{L_\infty(\mathbb{R}^d)} \leqslant K \|f\|_F, \quad \forall\, f \in F. \tag{5}$$

This assumption permits us to relate the multivariate Feynman–Kac path integration problem to uniform approximation. By uniform approximation we mean the approximation of functions from F in the norm of $L_\infty(\mathbb{R}^d)$, i.e., given, $\varepsilon > 0$ we want to find a function $\overline{f} \in L_\infty(\mathbb{R}^d)$ such that

$$\|f-\overline{f}\|_{L_\infty(\mathbb{R}^d)} \leqslant \varepsilon \|f\|_F.$$

(A3) We assume that we can compute a uniform approximation $\overline{f}$ of the function f from the class F by a linear algorithm,

$$\overline{f} = \sum_{i=1}^{n_{\mathrm{APP}}} f(\mathbf{u}_i)\zeta_i, \quad \mathbf{u}_i \in \mathbb{R}^d, \quad \zeta_i \in L_\infty(\mathbb{R}^d), \tag{6}$$

that uses n_{APP} function evaluations and

$$n_{\mathrm{APP}} = n_{\mathrm{APP}}(\varepsilon, F) = O(\varepsilon^{-\alpha(F)}) \quad \text{as } \varepsilon \to 0, \tag{7}$$

for some positive $\alpha(F)$. The asymptotic constant in (7) may depend on the dimension d. Usually the exponent $\alpha(F)$ depends on the smoothness and on the number of variables of functions from F, see Sec. VIII. We stress that these assumptions are not essentially restrictive. It is known that optimal algorithms for the uniform approximation problem are of the form (6), see Ref. 11. Moreover the number of function evaluations often depends on ε as in (7), see also Sec. VIII.

(A4) We restrict the norms of the initial value and potential functions. Namely, we assume that $\|v\|_F \leqslant \beta$ and $\|V\|_f \leqslant B$ for given positive β, B. In other words, the pair (v, V) belong to the class

$$B_F = \{(f_1, f_2) \in F \times F : \|f_1\|_F \leqslant B, \|f_2\|_F \leqslant \beta\}. \tag{8}$$

IV. RANDOMIZED ALGORITHMS

We are interested in approximating $z(\mathbf{u}, t)$, i.e., the exact value of the path integral (3) at a certain point $(\mathbf{u}, t) \in (0, \infty) \times \mathbb{R}^d$. We approximate $z(\mathbf{u}, t)$ by a randomized algorithm Φ. This algorithm uses the initial value and the potential sampled at randomized points. The error of the algorithm Φ is measured by the maximum with respect to the class B_F of the root mean square error with respect to the distribution of randomized points,

$$\sup_{(v,V) \in B_F} (\mathbb{E}(z(\mathbf{u}, t) - \Phi(v, V))^2)^{1/2}. \tag{9}$$

V. FEYNMAN–KAC FORMULA AS A SERIES OF MULTIVARIATE INTEGRALS

We briefly recall some results from Ref. 1, where the worst case approximation of the multivariate Feynman–Kac path integrals is analyzed.

Without loss of generality we can assume $\mathbf{u} = \mathbf{0}$ in (3); otherwise we shift the initial value and the potential appropriately. Then we can express the path integral (3) as a series of multivariate weighted integrals

$$z(\mathbf{0}, t) = \sum_{k=0}^{\infty} I_k(h_k), \tag{10}$$

where $h_k(\mathbf{z}_1, \ldots, \mathbf{z}_{k+1}) = v(\mathbf{z}_{k+1}) \prod_{i=1}^{k} V(\mathbf{z}_i)$, and

$$I_k(h_k) = \int_{\mathbb{R}^{(k+1)d}} h_k(\mathbf{z}_1, \ldots, \mathbf{z}_{k+1}) g_{k+1}(\mathbf{z}_1, \ldots, \mathbf{z}_{k+1}) \mathrm{d}\mathbf{z}_1 \ldots \mathrm{d}\mathbf{z}_{k+1}, \tag{11}$$

with

$$g_k(\mathbf{z}_1, \ldots, \mathbf{z}_{k+1}) = \int_{0 \leqslant t_1 \leqslant \cdots \leqslant t_k \leqslant t} f_{k+1}(t_1, \ldots, t_k, t, \mathbf{z}_1, \ldots, \mathbf{z}_{k+1}) \mathrm{d}t_1 \ldots \mathrm{d}t_k \tag{12}$$

and

$$f_k(t_1,\ldots,t_k,t,\mathbf{z}_1,\ldots,\mathbf{z}_{k+1}) = ((2\pi)^{k+1}t_1(t_2-t_1)\cdots(t-t_k))^{-d/2} \times \exp\left(-\frac{1}{2}\left(\frac{\|\mathbf{z}_1\|^2}{t_1}+\frac{\|\mathbf{z}_2-\mathbf{z}_1\|^2}{t_2-t_1}+\cdots+\frac{\|\mathbf{z}_{k+1}-\mathbf{z}_k\|^2}{t-t_k}\right)\right).$$

Note that the integral (11) depends on the input functions v and V only through the product h_k, whereas the weight functions g_{k+1} are independent of v and V, and

$$\|g_k\|_{L_1(\mathbb{R}^{(k+1)d})} = \frac{t^k}{k!} \quad \text{for } k \geqslant 0. \tag{13}$$

VI. APPROXIMATION OF ONE TERM OF THE SERIES

We present algorithms approximating one term (11) of the series (10). To utilize the power of randomization we apply the technique known as variance reduction which is achieved by Smolyak's algorithm. This algorithm uses deterministic uniform approximation of the function h_k and takes advantage of the smoothness of the functions v and V. For the reader's convenience, we include a short overview of Smolyak's algorithm in the next subsection.

A. Smolyak's algorithm

Smolyak's algorithm can be used to approximate wide spectrum of the tensor product problems. We only sketch this algorithm for uniform approximation, for more details see e.g., Ref. 12.

We define F_k as k-fold tensor product of the space F

$$F_k = \overbrace{F \otimes \cdots \otimes F}^{k}.$$

In this section we assume $k>1$. Clearly the domain of functions from F_k is $\mathbb{R}^{kd}$. We want to approximate a function $f_k \in F_k$ uniformly, i.e., we want to find a function $\overline{f_k} \in L_\infty(\mathbb{R}^{kd})$ such that

$$\|f_k - \overline{f_k}\|_{L_\infty(\mathbb{R}^{kd})} \leqslant \varepsilon \|f\|_{F_k}. \tag{14}$$

Smolyak's algorithm is based on the sequence of uniform approximation algorithms A_i, $i=0,1,\ldots,$

$$A_i f = \sum_{j=1}^{n_i} f(\mathbf{u}_j)\zeta_j, \quad \mathbf{u}_j \in \mathbb{R}^d, \quad \zeta_j \in L_\infty(\mathbb{R}^d). \tag{15}$$

These algorithms approximate functions from the space F as assumed in Secs. III A 2 and III A 3.

We impose three conditions on these algorithms.

(C1) $A_0 \equiv 0$ is the zero algorithm.

(C2) The error of the algorithm A_i satisfies

$$\|f - A_i f\|_{L_\infty(\mathbb{R}^d)} \leqslant C2^{-i}, \quad i=0,1,2,\ldots. \tag{16}$$

for some constant $C>0$.

(C3) The number n_i of function evaluations used by the algorithm A_i is bounded by

$$n(A_i) \leqslant D(2^{i\alpha(F)}-1), \quad i=0,1,2,\ldots$$

for some constant $D>0$, with $\alpha(F)$ defined Sec. III A 3. Note that C2 and C3 are consistent with the assumption Sec. III A 3.

We also define

$$\Delta_i = A_i - A_{i-1}, \quad i = 1,2,3, \ldots,$$

and, finally, for multiindices $\mathbf{i}=[i_1,\ldots,i_k] \in \mathbb{N}^k$ and $q \in \mathbb{N}$, we define

$$U_q = \sum_{1 \leqslant \mathbf{i}, |\mathbf{i}| \leqslant q} \overset{k}{\underset{j=1}{\otimes}} \Delta_{i_j}. \tag{17}$$

The sum above is over all multiindices $\mathbf{i}$ whose all coordinates are at least 1 and $|\mathbf{i}| := \Sigma_{i=1}^k i_k \leqslant q$. We can rewrite (17) as

$$U_q = \sum_{1 \leqslant \mathbf{i}, q-k+1 \leqslant |\mathbf{i}| \leqslant q} (-1)^{q-|\mathbf{i}|} \binom{k-1}{q-|\mathbf{i}|} \overset{k}{\underset{j=1}{\otimes}} A_{i_j},$$

see Ref. 12 for a more detailed analysis. Thus by (15) we obtain

$$U_q(f_k) = \sum_{1 \leqslant \mathbf{i}, q-k+1 \leqslant |\mathbf{i}| \leqslant q} (-1)^{q-|\mathbf{i}|} \binom{k-1}{q-|\mathbf{i}|} \sum_{\mathbf{j} \leqslant \mathbf{n_i}} f_k(\mathbf{u}_{j_1}, \ldots, \mathbf{u}_{j_k}) \zeta_{\mathbf{j}}, \tag{18}$$

where the second sum is over all vectors $\mathbf{j}=[j_1,\ldots,j_k]$ whose coordinates are at most the respective coordinates of the vector $\mathbf{n_i}=[n_{i_1},\ldots,n_{i_k}]$ and $\zeta_{\mathbf{j}} = \otimes_{j=1}^k \zeta_{i_j}$.

Assume, as before, $k>1$. The bound on the error of the algorithm U_q with $q>$k follows from Ref. 12 (Lemma 2),

$$\|f_k - U_q(f_k)\|_{L_\infty(\mathbb{R}^d)} \leqslant CH^{k-1} \binom{q}{k-1} 2^{-q} \|f\|_{F_k}, \tag{19}$$

where $H=\max\{2K,3C\}$. Using Stirling's formula we obtain

$$\|f_k - U_q(f_k)\| \leqslant CH^{k-1} \frac{1}{\sqrt{2\pi}} \sqrt{\frac{q}{k(q-k)}} \left(\frac{qe}{k-1}\right)^{k-1} 2^{-q} e^{1/6q}. \tag{20}$$

Let N_q be the number of function evaluations used by U_q with $q>$k. Then, Ref. 12 (Lemma 7) yields

$$N_q \leqslant D^k \left(1 - \frac{1}{2^{\alpha(F)}}\right)^{k-1} 2^{q\alpha(F)} \binom{q-1}{k-1}. \tag{21}$$

Now, given $\varepsilon>0$ and (20), it is easy to choose $q=q(\varepsilon,k)$ as the smallest integer such that

$$CH^{k-1} \frac{1}{\sqrt{2\pi}} \sqrt{\frac{q}{k(q-k)}} \left(\frac{qe}{k-1}\right)^{k-1} 2^{-q} e^{1/6q} \leqslant \varepsilon. \tag{22}$$

After straightforward but tedious calculations we obtain the following bound on $N_{q(\varepsilon,k)}$, i.e., on the number of function evaluations used by $U_{q(\varepsilon,k)}$,

$$N_{q(\varepsilon,k)} \leqslant D_k \left(\log_2 \frac{1}{\varepsilon}\right)_+^{(k-1)(\alpha(F)+1)} \left(\frac{1}{\varepsilon}\right)^{\alpha(F)} \tag{23}$$

with D_k independent on ε and at most exponential in k.

B. Variance reduction

We now use Smolyak's algorithm to reduce the variance of the function $h_k \in F_{k+1}$ defined in (11). The algorithm U_q applied to the function h_k can be written as

$$U_q(h_k) = \sum_{1\leqslant \mathbf{i}, q-k\leqslant |\mathbf{i}|\leqslant q} (-1)^{q-|\mathbf{i}|}\binom{k}{q-|\mathbf{i}|} \sum_{\mathbf{j}\leqslant \mathbf{n}_\mathbf{i}} v(\mathbf{u}_{j_{k+1}}) \prod_{s=1}^{k} V(\mathbf{u}_{j_s})\zeta_\mathbf{j}.$$

In order to get the error bound of the form

$$\|h_k - U_q(h_k)\|_{L_\infty(\mathbb{R}^{(k+1)d})} \leqslant \varepsilon \|v\|_F \|V\|_F^k, \tag{24}$$

we need to take $q=q(\varepsilon,k+1)$ which was defined in the Sec. VI A. The algorithm $U_{q(\varepsilon,k)}$ requires at most

$$N_{q(\varepsilon,k+1)} \leqslant D_{k+1}\left(\log_2 \frac{1}{\varepsilon}\right)_+^{k(\alpha(F)+1)} \left(\frac{1}{\varepsilon}\right)^{\alpha(F)}$$

function evaluations.

The idea underlying variance reduction is as follows. First we compute

$$\overline{h}_{k,\varepsilon} = U_{q(\varepsilon,k+1)}(h_k)$$

using $N_{q(\varepsilon,k+1)}$ function values. Then we compute

$$I_k(\overline{h}_{k,\varepsilon}) = \sum_{1\leqslant \mathbf{i}, q-k\leqslant |\mathbf{i}|\leqslant q} (-1)^{q-|\mathbf{i}|}\binom{k}{q-|\mathbf{i}|} \sum_{\mathbf{j}\leqslant \mathbf{n}_\mathbf{i}} v(\mathbf{u}_{j_{k+1}}) \prod_{s=1}^{k} V(\mathbf{u}_{j_s}) I_k(\zeta_\mathbf{j})$$

with $q=q(\varepsilon,k+1)$. Observe that the functions $\zeta_\mathbf{j}$ do not depend on the input functions v and V so the integrals $I_k(\zeta_\mathbf{j})$ can be precomputed.

We stress that $\overline{h}_{k,\varepsilon}$ and $I_k(\overline{h}_{k,\varepsilon})$ are deterministic. We then use the classical Monte Carlo algorithm to approximate the multivariate integrals $I_k(h_k-\overline{h}_{k,\varepsilon})$. The error depends on the variance of $h_k-\overline{h}_{k,\varepsilon}$ which is bounded by $\|h_k-\overline{h}_{k,\varepsilon}\|_{L_\infty(\mathbb{R}^{(k+1)d})}$. Since this is now small, we obtain variance reduction.

C. Monte Carlo algorithm

We use a randomized algorithm of the form

$$\phi_{\varepsilon,m}(v,V) = I_k(\overline{h}_{k,\varepsilon}) + \mathrm{MC}_m(h_k - \overline{h}_{k,\varepsilon}). \tag{25}$$

Here

$$\mathrm{MC}_m(f) = \frac{1}{m}\sum_{j=1}^{m} f(x_j) \tag{26}$$

denotes the classical Monte Carlo algorithm with m randomized sample points. Randomized sample points $x_j \in \mathbb{R}^{(k+1)d}$ are chosen with respect to the density $g_{k+1}/\|g_{k+1}\|_{L_1(\mathbb{R}^{(k+1)d})}$.

Using the well known error formula for the classical Monte Carlo algorithm and denoting $\overline{f}_{k,\varepsilon}=h_k-\overline{h}_{k,\varepsilon}$, we conclude that the error of the algorithm $\phi_{\varepsilon,m}$ satisfies

$$(\mathbb{E}(I_k(h_k) - \phi_{\varepsilon,m}(v,V))^2)^{1/2} = (\mathbb{E}(I_k(\overline{f}_{k,\varepsilon}) - \mathrm{MC}_m(\overline{f}_{k,\varepsilon}))^2)^{1/2} = \frac{1}{\sqrt{m}}(\mathrm{Var}(\overline{f}_{k,\varepsilon}))^{1/2},$$

with

$$\mathrm{Var}(\overline{f}_{k,\varepsilon}) = I_k(\overline{f}_{k,\varepsilon}^2) - (I_{k+1}(\overline{f}_{k,\varepsilon}))^2.$$

Clearly, from (24) and then from (8) and (12) we get

$$(\mathrm{Var}(\overline{f}_{k,\varepsilon}))^{1/2} \leqslant \frac{t^k}{k!}\|\overline{f}_{k,\varepsilon}\|_{L_\infty(\mathbb{R}^{(k+1)d})} \leqslant \varepsilon\frac{\|v\|_F\|V\|_F^k t^k}{k!} \leqslant \varepsilon\frac{B\beta^k t^k}{k!}.$$

This yields the error estimate

$$(\mathbb{E}(I_k(h_k) - \phi_{\varepsilon,m}(v,V))^2)^{1/2} \leqslant \frac{\varepsilon}{\sqrt{m}}\frac{B\beta^k t^k}{k!} \tag{27}$$

and the total number $n(\phi_{\varepsilon,m})$ of function evaluations is bounded by

$$n(\phi_{\varepsilon,m}) \leqslant N_{q(\varepsilon,k+1)} + m. \tag{28}$$

VII. THE ALGORITHM

Based on the previous section we are ready to present an algorithm Φ_ε which computes an ε approximation of a multivariate Feynman–Kac path integral, i.e., whose error defined by (9) does not exceed ε. We assume that the initial value and the potential belong to the class B_F. We approximate the consecutive terms $I_k(h_k)$ of the series $z(\mathbf{0},t)=\sum_{k=0}^\infty I_k(h_k)$ by the algorithms $\phi_{\varepsilon_k,m}$ with the accuracy ε_k being

$$\varepsilon_k = \varepsilon^{2/(\alpha(F)+2)}\frac{k!}{B\beta^k t^k 2^{k+1}}, \tag{29}$$

and the number of randomized sample points m being

$$m = \lceil \varepsilon^{-2\alpha(F)/(\alpha(F)+2)} \rceil. \tag{30}$$

Since the required error ε_k goes to infinity super exponentially fast we need to approximate only a finite number of the series terms. Thus the final form of the algorithms approximating $z(\mathbf{0},t)$ is

$$\Phi_\varepsilon(v,V) = \sum_{k=0}^{N_\varepsilon} \phi_{\varepsilon_k,m}$$

with the sum limit N_ε determined in the next section.

A. Error analysis

From (27), (29), and (30), it is easy to check that

$$(\mathbb{E}(I_k(h_k) - \phi_{\varepsilon_k,m}(v,V))^2)^{1/2} \leqslant \frac{\varepsilon}{2^{k+1}}. \tag{31}$$

It is also easy to see that we need to approximate only a few terms of the series. Indeed, for k approaching infinity, we have ε_k also tending to infinity. Assume that

$$k!\varepsilon^{1+\alpha(F)/\alpha(F)+2} \geqslant B\beta^k t^k (2K)^{k+1},$$

with K being the embedding constant in (5). This implies

$$\frac{\varepsilon_k}{m} \geqslant K^{k+1},$$

and by (5) and (27) we see that for such k the deterministic zero algorithm provides sufficient accuracy. Thus, we need to use the algorithms $\phi_{\varepsilon_k,m}$ only for $k=O(\ln \varepsilon^{-1})$. Hence, we get $N_\varepsilon = O(\ln \varepsilon^{-1})$.

Summing up the bounds (31) over $k=1,2,\ldots$ we obtain an error estimate of the algorithm Φ_ε

$$(\mathbb{E}(z(\mathbf{0},t)-\Phi_\varepsilon(v,V))^2)^{1/2}\leqslant\varepsilon. \tag{32}$$

This means that the algorithm Φ_ε computes an ε-approximation of the multivariate Feynman–Kac path integral.

B. Number of function evaluations

In this section we derive estimates on the number of function values $n(\Phi_\varepsilon)$ of the algorithm Φ_ε. By the bounds (23) and (28) we get an obvious estimate

$$n(\Phi_\varepsilon)=O\left(1+\sum_{k=0}^{\infty}D_{k+1}(\log_2\varepsilon_k^{-1})_+^{k(\alpha(F)+1)}\left(\frac{B\beta^k t^k 2^{k+1}}{k!}\right)^{\alpha(F)}\right)\varepsilon^{-2\alpha(F)/(\alpha(F)+2)}.$$

We can now use an argument similar to that in the proof of Ref. 4 (Theorem 1) to show that

$$\sum_{k=0}^{\infty}D_{k+1}(\log_2\varepsilon_k^{-1})_+^{k(\alpha(F)+1)}\left(\frac{B\beta^k t^k 2^{k+1}}{k!}\right)^{\alpha(F)}=O(\varepsilon^{-\delta})$$

for all $\delta>0$. Thus we finally get

$$n(\Phi_\varepsilon)=O(\varepsilon^{-2\alpha(F)/(\alpha(F)+2)-\delta})\quad\text{for all }\delta>0. \tag{33}$$

It is easy to see that both parts of each of the algorithms $\phi_{\varepsilon_k,m}$—the variance reduction and the integral approximation—are linear with respect to the functions h_k. This means that their total computational cost (the number of arithmetic operations and comparisons) is proportional to the number of function evaluations. This also holds for the final algorithm Φ_ε, thus the estimate (33) holds also for the total cost of Φ_ε.

C. Optimality of the algorithm Φ_ε

It turns out that the algorithm Φ_ε is optimal modulo δ in (33), as long as the exponent $\alpha(F)$ in (7) is given as the minimal one. The proof of this fact exceeds the scope of this article and requires a more extensive use of information-based complexity. We refer the reader to the follow-up article[5] for more details.

VIII. EXAMPLE

We now consider an example of the class F of initial value and potential functions satisfying the assumptions from Secs. II and III.

Let F be a class of d variate r times continuously differentiable functions whose supports are contained in a cube $[a,b]^d\subset\mathbb{R}^d, a,b\in\mathbb{R}$. Thus F is a subclass of the Sobolev space $W_\infty^{r,d}([a,b]^d)$ with the norm

$$\|f\|_{W_\infty^{r,d}([a,b]^d)}=\sum_{|\boldsymbol{\alpha}|\leqslant r}\|f^{(\boldsymbol{\alpha})}\|_{L_\infty([a,b]^d)},$$

here $\boldsymbol{\alpha}=[\alpha_1,\ldots,\alpha_d]\in\mathbb{N}^d$ and $f^{(\boldsymbol{\alpha})}=\partial^{|\alpha|}/\partial^{\alpha_1}\ldots\partial^{\alpha_d}$.

Clearly, the assumptions Secs. II A 1 and II A 2 are satisfied. We also know an optimal uniform approximation algorithm that satisfies Sec. II A 3 with the exponent $\alpha(F)=d/r$, see Refs. 11, 13, and 14. Based on this algorithm and the results from Secs. VI and VII we can construct the algorithm Φ_ε computing an ε-approximation of the multivariate Feynman–Kac path integral (3) in the sense of (9) with the number of function evaluations being roughly of order $O(\varepsilon^{-2/(1+2r/d)})$. We see that the exponent of ε^{-1} is at most 2 and decreases with the increase of the ratio r/d. Unfortunately, the factor hidden in the big O notation that comes from the use of uniform approximation and Smolyak's algorithm depends exponentially on the dimension d. The limiting value 2 of the exponent $2/(1+2r/d)$ corresponds to the algorithm without variance reduction.

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Reduction of su(*N*) loop tensors to trees

Maciej Trzetrzelewski[a)]
M. Smoluchowski Institute of Physics, Jagiellonian University, Reymonta 4, 30-059 Cracow, Poland

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We present a systematic method to express all su(N) invariant tensors in terms of forests, i.e., products of tree tensors. © *2005 American Institute of Physics.*
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I. INTRODUCTION

It is a well known fact that in a simple Lie algebra of rank r there are exactly r independent Casimir invariants. This causes a direct restriction on algebra of su(N) tensors since naively one could produce an infinite amount of invariants by contracting d, f tensors. The Cayley-Hamilton theorem, which is the reason why higher Casimir invariants are dependent on the first r ones, clearly gives additional d_{ijk} tensor identities. The systematic, computer friendly, approach to obtain these formulas was presented by Sudbery.[1] One may also define matrices $[F_i]_{jk}=f_{ijk}$, $F=a_iF_i$, $a_i \in \mathbf{C}$ and use Cayley-Hamilton equation to obtain analogous identities for f_{ijk}, which was elaborated in detail in Ref. 2. In this paper we will use a geometrical approach to find formulas on su(N) loop tensors in term of su(N) tree tensors. In this way we give a recursive method which allows one to express any su(N) invariant tensor in terms of basic ones, i.e., forests (products of trees). In Sec. III we prove several lemmas and eventually the main result. In Sec. IV we present a few examples to give insights into the method.

We will use the following conventions:

$$\lambda_i\lambda_j = \frac{2}{N}\delta_{ij}\mathbf{1} + d_{ijk}\lambda_k + if_{ijk}\lambda_k, \tag{1}$$

where λ_i's are su(N) generators in fundamental representation and d_{ijk}, f_{ijk} are completely symmetric/antisymmetric structure tensors. Multiplication law (1) together with Jacobi identities for λ_i's give identities that have been known for a long time.[3] We will make special use of

$$f_{i_1i_2k}d_{ki_3i_4} + f_{i_1i_3k}d_{ki_2i_4} + f_{i_1i_4k}d_{ki_2i_3} = 0, \tag{2}$$

and

$$f_{i_1i_2k}f_{ki_3i_4} = \frac{2}{N}(\delta_{i_1i_3}\delta_{i_2i_4} - \delta_{i_1i_4}\delta_{i_2i_3}) + d_{i_1i_3k}d_{ki_2i_4} - d_{i_1i_4k}d_{ki_2i_3}. \tag{3}$$

II. BIRD TRACKS

In order to grasp the variety of all possible invariant tensors it is helpful to introduce the diagrammatic notation for d and f tensors (Fig. 1). Each leg corresponds to one index and summing over any two indices is simply gluing appropriate legs. This notation is very convenient because now any tensor may be represented by a graph.

[a)]Electronic mail: trzetrzelewski@th.if.uj.edu.pl

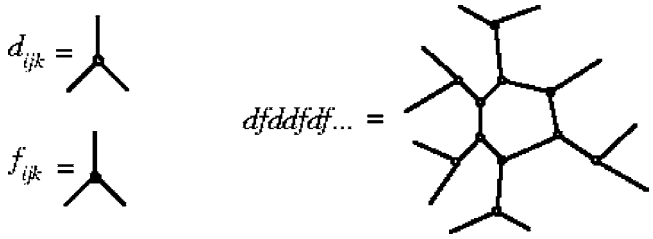

FIG. 1. d_{ijk}, f_{ijk} diagrams and a typical tensor diagram.

Such a diagrammatic approach was already introduced a long time ago by Cvitanovič. The d, f tensors are called bird tracks since they look like tracks of a bird. The reader is referred to Ref. 4 where a vast amount of group properties is rediscovered in such diagrammatic language. Since d_{ijk} is totally symmetric the order of the corresponding legs is irrelevant. For f_{ijk} we have to set, e.g., counterclockwise convention. A special group of diagrams are loop and tree diagrams (Fig. 2).

One may rotate any diagram on the plane without changing the value of the corresponding tensor. Reflections (or rotations in three dimensions) are allowed as well, however in this case one has to take care of the sign since f tensor is antisymmetric. If a diagram consists only of d tensors then reflections will not affect its value. Several definitions are now in order.

The index that corresponds to the d/f tensor is called the d/f index. A loop L_1 is smaller than loop L_2 if the number of f, d tensors in L_2 is smaller than the number of f, d tensors on L_1. Note that, in general, trees can be attached to loops. In that case we will call it a tree loop diagram. Similarly a tree loop L_1 is smaller than tree loop L_2 if the number of f, d tensors within loop in L_2 is smaller than the number of f, d tensors within loop in L_1.

A loop diagram is called n loop if it consists of n tensors. A loop diagram is called d loop if it consists of d tensors only. A loop diagram is called $1f/2f$ loop if it consists of one/two f tensor and d tensors.

III. LOOP REDUCTION

This section consists of several lemmas and eventually a theorem which gives a computational method for expressing loops by trees.

Lemma 1: Any loop is a linear combination of d loops and $1f$ loops.

Proof: Let us rewrite (3) in diagrammatic notation (*). (Instead of writing i_1, i_2, i_3, i_4, etc., we prefer 1, 2, 3, 4 since it causes no misunderstanding and gives a better idea of the structure of indices. Take attention of the order of indices 3 and 4. There is no mistake. The whole diagram is supposed to be read with the counterclockwise convention.) Therefore it is sufficient to consider loops where f tensor is between d tensors (d1)

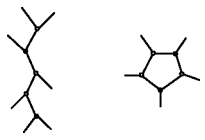

FIG. 2. A tree and a loop diagram.

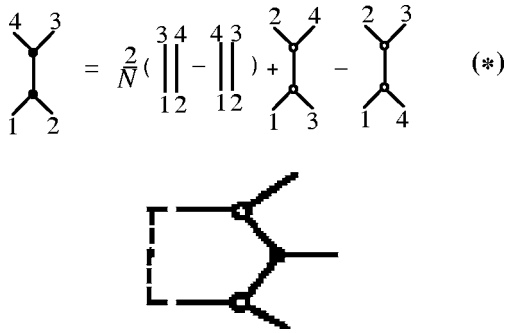

(d1)

However in such case one can use Jacobi identities (2)

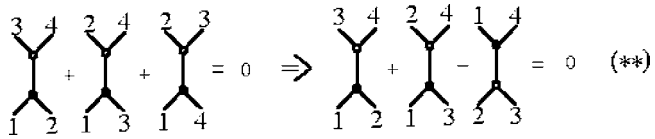

(d2)

therefore attaching (the question mark means that there may be f tensor or d tensor)

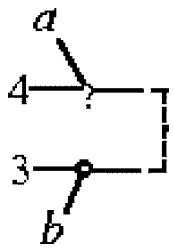

(d3)

we get

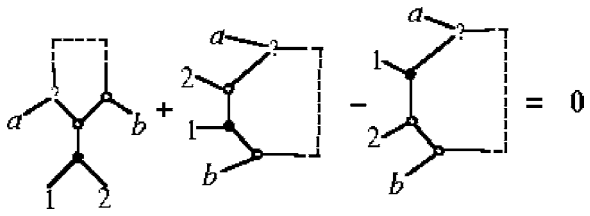

(d4)

The last identity means that we can "move" f tensor along the loop producing a smaller tree loop. Eventually such f tensor will "meet" another f tensor (if there is another one in the loop) and one can use (*) again to get rid of f tensors. This procedure stops on d loops or $1f$ loops. □

Lemma 2: Let A be a d loop or $1f$ loop. Then any permutation of d indices of A does not change the value of A up to trees and smaller tree loops.

Proof: Consider identity (*) and attach the tensor

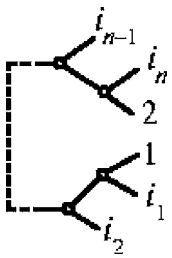

(d5)

where the dashed lines correspond to d tensors only.

The result is

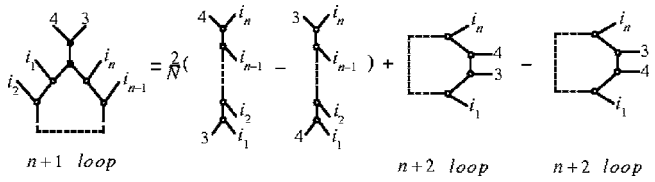

(d6)

Therefore the permutation of indices 3, 4 does not change the d loop up to trees and smaller tree loops. Since indices 3, 4 are not distinguished we can do any permutation of any two indices and the d loop will not change the value up to trees and smaller tree loops. Since any permutation is a proper composition of transpositions the Lemma 2 follows for d loops. The proof for $1f$ loops is analogous. □

Lemma 3: Any $1f$ loop is a linear combination of trees and smaller tree loops.

Proof: Consider the Jacobi identities (**) and attach the tree diagram (consisting of d tensors only)

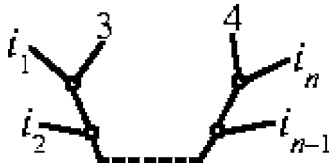

(d7)

The result is

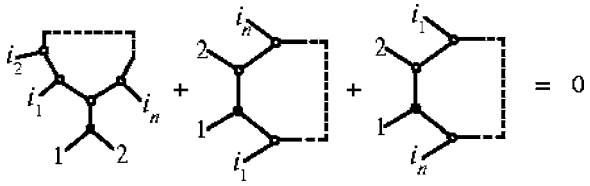

(d8)

From Lemma 2 it follows that

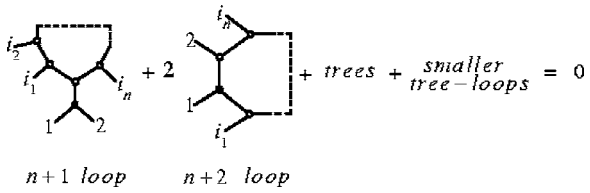

(d9)

Lemma 4: Any d loop is a linear combination of trees and smaller tree loops.

Proof: Consider Jacobi identity (**) and attach the following tree (consisting of one f tensor and $n-1$ d tensors)

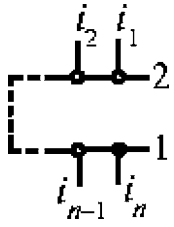

(d10)

The result is

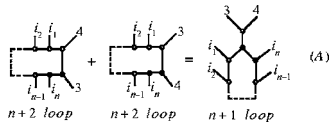

(d11)

Therefore the symmetrization of indices 3, 4 in such $2f$ loop is equal to smaller tree loop. Now for the proof of Lemma 4 consider identity (*) and attach the tree tensor (consisting of d tensors only)

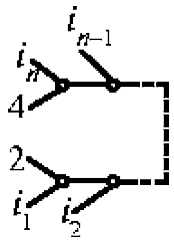

(d12)

The result is

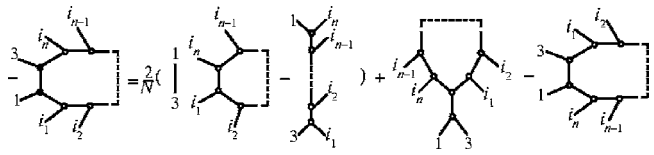

(d13)

Or simply

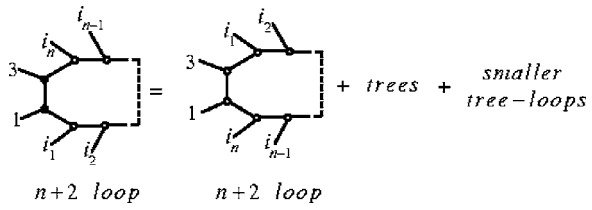

(d14)

According to (A) the symmetrization over indices 1 and i_1 gives

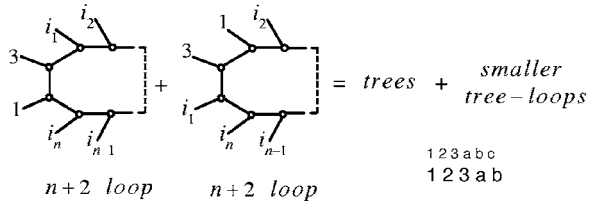

(d15)

Due to Lemma 2, Lemma 4 follows. □

Theorem: Any loop diagram is a linear combination of forests.

Proof: From Lemma 1 it is sufficient to consider d loops and $1f$ loops. From Lemma 3 and Lemma 4 we may recursively reduce $1f$ loop and d loop to arbitrary small loops and ultimately to trees. □

Corollary 1: Any diagram is a linear combination of forests.

Proof: Any loop in the diagram may be replaced by a linear combination of trees. This will in general produce more loops however the number of d, f tensors will be smaller after such replacement. Following the induction with respect to the number of d, f tensors we finely reduce all loops. □

Corollary 2: Any diagram is a linear combination of products of trace tensors $\mathrm{Tr}(\lambda_{i_1}\ldots\lambda_{i_n})$ where λ_i's are su(N) Gell-Mann matrices.

Proof: According to Corollary 1 it is sufficient to consider tree diagrams. With help of (1) we have

$$\mathrm{Tr}(\lambda_{i_1}\ldots\lambda_{i_n}) = \frac{1}{N}\mathrm{Tr}(\lambda_{i_1}\lambda_{i_2})Tr(\lambda_{i_3}\ldots\lambda_{i_n}) + (d_{i_1i_2k} + if_{i_1i_2k})Tr(\lambda_k\lambda_{i_3}\ldots\lambda_{i_n})$$

therefore

$$d_{i_1i_2k}\mathrm{Tr}(\lambda_k\lambda_{i_3}\ldots\lambda_{i_n}) = \frac{1}{2}\mathrm{Tr}(\lambda_{(i_1}\lambda_{i_2)}\lambda_{i_3}\ldots\lambda_{i_n}) - \frac{1}{N}\mathrm{Tr}(\lambda_{i_1}\lambda_{i_2})Tr(\lambda_{i_3}\ldots\lambda_{i_n})$$

and

$$f_{i_1i_2k}Tr(\lambda_k\lambda_{i_3}\ldots\lambda_{i_n}) = \tfrac{1}{2}\mathrm{Tr}(\lambda_{[i_1}\lambda_{i_2]}\lambda_{i_3}\ldots\lambda_{i_n}),$$

hence Corollary 2 follows by induction. □

IV. EXAMPLES

In the following we give su(N) formulas for the lowest d loops, i.e., triangles, squares, and pentagons. The identities for triangles and squares are already in the literature in Refs. 3 and 5, respectively. However to the knowledge of the author these identities are missing for pentagons and higher loops. The results are

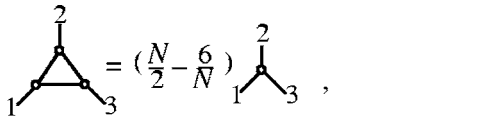

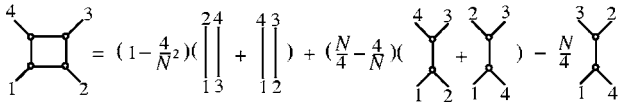

(d16)

and

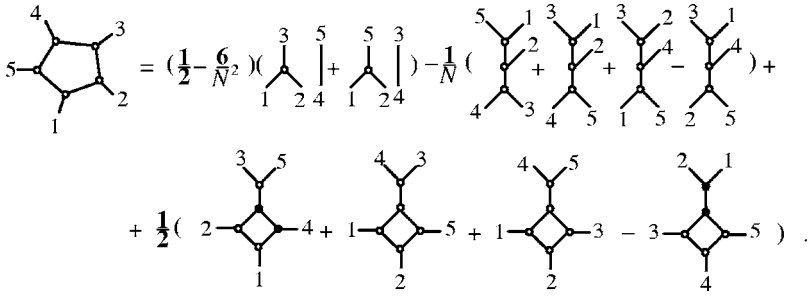

(d17)

The last identity in standard notation is

$$\begin{aligned}\mathrm{Tr}(D_{i_1}D_{i_2}D_{i_3}D_{i_4}D_{i_5}) = \left(\frac{1}{2} - \frac{6}{N}\right)(d_{i_1i_2i_3}\delta_{i_4i_5} + d_{i_1i_2i_5}\delta_{i_4i_3}) + -\frac{1}{N}(d_{i_3i_4k}d_{ki_2l}d_{li_1i_5} + d_{i_4i_5k}d_{ki_2l}d_{li_1i_3}\\ + d_{i_1i_5k}d_{ki_4l}d_{li_2i_3} - d_{i_2i_5k}d_{ki_4l}d_{li_1i_3}) + \frac{1}{2}(\mathrm{Tr}(D_{i_2}D_{i_1}F_{i_4}F_k)d_{ki_5i_3}\\ + \mathrm{Tr}(D_{i_1}D_{i_2}D_{i_5}D_k)d_{ki_3i_4} + \mathrm{Tr}(D_{i_1}D_{i_2}D_{i_3}D_k)d_{ki_5i_4} - \mathrm{Tr}(D_{i_3}D_{i_4}D_{i_5}F_k)f_{ki_1i_2}).\end{aligned}$$

It should be noted that all these identities have been verified in MATHEMATICA with perfect agreement.

V. SUMMARY

The aim of this paper was to give a systematic approach to compute loop tensors. The reason for doing so lies in the analysis of systems based on su(N) group. In fact the author came across this problem while studying supersymmetric Yang-Mills quantum mechanics for arbitrary N and large N limit.[6,7] These issues will be published elsewhere. The method agrees with recent results[2] where the problem was solved via characteristic equation for F matrices. Let us note that it is a laborious task to obtain this equation for arbitrary su(N), therefore a big loop diagram for large N is in general difficult to reduce. In a diagrammatic approach this problem does not exist since we make no use of characteristic equation. Indeed the lemmas presented here are so simple that one could write a computer program for arbitrary loop reduction. What is even more remarkable is that the derivation of our result is based only on Jacobi identities and multiplication law (1). We did not use the relations derived by Sudbery[1] although it is evident that one may contract his formulas with, e.g., d_{ijk} providing a constraint on a d loop.

The diagrammatic method may be applied to arbitrary Lie algebra. However since the multiplication rule (1) is different in other cases than su(N) we expect the conclusions to be different. Indeed in the g_2 case the situation is so different that the simplest triangle d loop is not proportional to d_{ijk} tensor.[8]

Finally let us note that the method[2] gives no information about lower degree traces (e.g., $\mathrm{Tr}(F^4), \mathrm{Tr}(F^6), \mathrm{Tr}(F^8), \mathrm{Tr}(F^{10})$ in su(5) cannot be written as polynomials in lower degree traces). One may however apply different arguments[5] to derive formulas for fourfold traces. Our results also agree with them. Unfortunately these arguments get more complicated while analyzing bigger loops.

ACKNOWLEDGMENTS

The author thanks J. Wosiek and A. Macfarlane for discussions and encouragement. This work was supported by the Polish Committee for Scientific Research under Grant No. PB 1P03B 02427 (2004-2007).

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The antifield Koszul–Tate complex of reducible Noether identities

D. Bashkirov[a)]
Department of Theoretical Physics, Moscow State University, 117234 Moscow, Russia

G. Giachetta[b)]
Department of Mathematics and Informatics, University of Camerino, 62032 Camerino (MC), Italy

L. Mangiarotti[c)]
Department of Mathematics and Informatics, University of Camerino, 62032 Camerino (MC), Italy

G. Sardanashvily[d)]
Department of Theoretical Physics, Moscow State University, 117234 Moscow, Russia

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A generic degenerate Lagrangian system of even and odd fields is examined in algebraic terms of the Grassmann-graded variational bicomplex. Its Euler–Lagrange operator obeys Noether identities which need not be independent, but satisfy first-stage Noether identities, and so on. We show that, if a certain necessary and sufficient condition holds, one can associate to a degenerate Lagrangian system the exact Koszul–Tate complex with the boundary operator whose nilpotency condition restarts all its Noether and higher-stage Noether identities. This complex provides a sufficient analysis of the degeneracy of a Lagrangian system for the purpose of its BV quantization. © *2005 American Institute of Physics.*
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I. INTRODUCTION

As well-known, quantization of a Lagrangian field system essentially depends on the analysis of its degeneracy. One says that a Lagrangian system is degenerate if its Euler–Lagrange operator obeys nontrivial Noether identities. They need not be independent, but satisfy the first-stage Noether identities, which in turn are subject to the second-stage ones, and so on. The hierarchy of reducible Noether identities characterizes the degeneracy of a Lagrangian system in full. Noether's second theorem states the relation between the Noether identities and the gauge symmetries of a Lagrangian system.[1,2] If Noether identities and gauge symmetries are finitely generated, they are parametrized by the modules of antifields and ghosts, respectively. An original Lagrangian is extended to these antifields and ghosts in order to satisfy the so-called master equation. This extended Lagrangian is the starting point of the Batalin–Vilkovisky (BV) quantization of a degenerate Lagrangian field system.[3,4]

Let us note that the notion of a reducible Noether identity has come from that of a reducible constraint. Their Koszul–Tate complex has been invented by analogy with that of constraints[5] under a rather restrictive regularity condition that field equations as well as Noether identities of arbitrary stage can be locally separated into the independent and dependent ones.[6,7] This condition also comes from the case of a constraint locally given by a finite number of functions to which the

[a)]Electronic mail: bashkir@phys.msu.ru
[b)]Electronic mail: giovanni.giachetta@unicam.it
[c)]Electronic mail: luigi.mangiarotti@unicam.it
[d)]Electronic mail: sard@grav.phys.msu.su

inverse mapping theorem can be applied. In contrast with constraints, Noether and higher-stage Noether identities are differential operators. They are locally given by a set of functions and their jet prolongations on an infinite order jet manifold. Since the latter is a Fréchet, but not Banach manifold, the inverse mapping theorem fails to be valid. Here, we follow the general definition of Noether identities of differential operators.[8] This definition reproduces that in Refs. 1 and 2 if Noether identities are finitely generated. Their Koszul–Tate complex is constructed iff a certain homology regularity condition holds.

Our goal is the following. Bearing in mind BV quantization, we address a generic Lagrangian systems of even and odd fields on an arbitrary smooth manifold X ($\dim X=n$). It is algebraically described in terms of a certain bigraded differential algebra (henceforth BGDA) $\mathcal{S}^*_\infty[F;Y]$ which is split into the Grassmann-graded variational bicomplex, generalizing the variational bicomplex on fiber bundles (Sec. II). If a fiber bundle $Y\to X$ of even fields is affine, this algebra has been defined as the product of graded algebras of odd and even fields.[2,9] Here, its definition is generalized to an arbitrary fiber bundle $Y\to X$. In this case, elements of $\mathcal{S}^*_\infty[F;Y]$ are Grassmann-graded differential forms on the infinite order jet manifold $J^\infty Y$ of sections of $Y\to X$, but not on X. Let $L\in\mathcal{S}^{0,n}_\infty[F;Y]$ be a Lagrangian and $\delta L\in\mathcal{S}^{1,n}_\infty[F;Y]$ its Euler–Lagrange operator. We associate to δL the chain complex (13) whose boundaries vanish on-shell, i.e., on $\operatorname{Ker}\delta L$ (Proposition 4). It is a complex of a certain $C^\infty(X)$-module $\mathcal{P}^{0,n}_\infty[\bar{Y}^*;F;Y;\bar{F}^*]$ of Grassmann-graded densities on the infinite order jet manifold $J^\infty Y$. For our purpose, this complex can be replaced with the short zero-exact complex $\mathcal{P}^{0,n}_\infty[\bar{Y}^*;F;Y;\bar{F}^*]_{\leqslant 2}$ (14).

Remark 1: If there is no danger of confusion, elements of homology are identified to its representatives. A chain complex is called r-exact if its homology of $k\leqslant r$ is trivial.

The Noether identities of the Euler–Lagrange operator δL are defined as nontrivial elements of the first homology $H_1(\bar{\delta})$ of the complex (14) (Definition 5). Let this homology be finitely generated by a projective graded $C^\infty(X)$-module of finite rank. In accordance with the Serre–Swan theorem generalized to graded manifolds (Theorem 1), one can introduce the corresponding module of antifields and extend the complex (14) to the one-exact complex $\mathcal{P}^{0,n}_\infty[\bar{E}^*\bar{Y}^*;F;Y;\bar{F}^*\bar{V}^*]_{\leqslant 3}$ (22) with the boundary operator δ_0 (21) whose nilpotency conditions are equivalent to the above-mentioned Noether identities (Proposition 6). First-stage Noether identities are defined as two-cycles of this complex. They are trivial if two-cycles are boundaries, but the converse need not be true. Trivial first-stage Noether identities are boundaries iff a certain homology condition (called the two-homology regularity condition) holds (Proposition 8). In this case, the first-stage Noether identities are identified to nontrivial elements of the second homology of the complex (22). If this homology is finitely generated, the complex (22) is extended to the two-exact complex $\mathcal{P}^{0,n}_\infty[\bar{E}^*_1\bar{E}^*\bar{Y}^*;F;Y;\bar{F}^*\bar{V}^*\bar{V}^*_1]_{\leqslant 4}$ (33) with the boundary operator δ_1 (32) whose nilpotency conditions are equivalent to the Noether and first-stage Noether identities (Proposition 10). If the third homology of this complex is not trivial, the second-stage Noether identities exist, and so on. Iterating the arguments, we come to the following.

We have the $(N+1)$-exact complex $\mathcal{P}^{0,n}_\infty\{N\}_{\leqslant N+3}$ (37) such that (i) the nilpotency conditions of its boundary operator δ_N (35) reproduce Noether and k-stage Noether identities for $k\leqslant N$, (ii) the $(N+1)$-homology regularity condition holds. This condition states that any $\delta_{k<N-1}$-cycle $\phi\in\mathcal{P}^{0,n}_\infty\{k\}_{k+3}$ is a δ_{k+1}-boundary (Definition 11). Then the $(N+1)$-stage Noether identities are defined as $(N+2)$-cycles of this complex. They are trivial if cycles are boundaries, while the converse is true iff the $(N+2)$-homology regularity condition is satisfied. In this case, $(N+1)$-stage Noether identities are identified to nontrivial elements of the $(N+2)$-homology of the complex (37) [item (i) of Theorem 13]. Let this homology be finitely generated. By means of antifields, this complex is extended to the $(N+2)$-exact complex $\mathcal{P}_\infty\{N+1\}_{\leqslant N+4}$ (45) with the boundary operator δ_{N+1} (44) whose nilpotency restarts all the Noether identities up to stage $(N+1)$ [item (ii) of Theorem 13].

This iteration procedure results in the exact Koszul–Tate complex of antifields with the boundary operator whose nilpotency conditions reproduce all Noether and higher Noether identities characterizing the degeneracy of a differential operator δL.

In Sec. V, we address the particular variant of topological BF theory with the Lagrangian (47) for a scalar A and $(n-1)$-form B as an example of a reducible degenerate Lagrangian system[1] where the homology regularity condition is verified (Lemma 14), Noether and k-stage Noether identities are proved to be finitely generated, and its Koszul–Tate complex (62) is constructed.

Remark 2: Throughout the paper, smooth manifolds are assumed to be real, finite-dimensional, Hausdorff, second-countable (consequently, paracompact) and connected. By a Grassmann algebra over a ring $\mathcal{K}$ is meant a $\mathbb{Z}_2$-graded exterior algebra of some $\mathcal{K}$-module. We restrict our consideration to graded manifolds $(Z,\mathfrak{A})$ with structure sheaves $\mathfrak{A}$ of Grassmann algebras of finite rank.[10,11] The symbols $|.|$ and $[.]$ stand for the form degree and Grassmann parity, respectively. We denote by Λ, Σ, Ξ, Ω the symmetric multi-indices, e.g., $\Lambda=(\lambda_1\cdots\lambda_k)$, $\lambda+\Lambda=(\lambda\lambda_1\cdots\lambda_k)$. Summation over a multi-index $\Lambda=(\lambda_1\cdots\lambda_k)$ throughout means separate summation over each index λ_i.

II. GRASSMANN-GRADED LAGRANGIAN SYSTEMS

Let $Y\to X$ be a fiber bundle and J^rY be the jet manifolds of its sections. They form the inverse system

$$X\overset{\pi}{\leftarrow}Y\overset{\pi^1_0}{\leftarrow}J^1Y\leftarrow\cdots J^{r-1}Y\overset{\pi^r_{r-1}}{\leftarrow}J^rY\leftarrow\cdots, \tag{1}$$

where π^r_{r-1} are affine bundles, and $r=0$ conventionally stands for Y. Its projective limit $(J^\infty Y;\pi^\infty_r:J^\infty Y\to J^rY)$ is a paracompact Fréchet manifold. A bundle atlas $\{(U_Y;x^\lambda,y^i)\}$ of $Y\to X$ induces the coordinate atlas

$$\begin{gathered}\{((\pi^\infty_0)^{-1}(U_Y);x^\lambda,y^i_\Lambda)\},\quad y'^i_{\lambda+\Lambda}=\frac{\partial x^\mu}{\partial x'^\lambda}d_\mu y'^i_\Lambda,\quad 0\leqslant|\Lambda|,\\ d_\lambda=\partial_\lambda+\sum_{0\leqslant|\Lambda|}y^i_{\lambda+\Lambda}\partial^\Lambda_i,\quad d_\Lambda=d_{\lambda_1}\circ\cdots\circ d_{\lambda_k},\end{gathered} \tag{2}$$

of $J^\infty Y$, where d_λ are total derivatives. We further assume that the cover $\{\pi(U_Y)\}$ of X is also the cover of atlases of all fiber bundles over X in question. The inverse system (1) yields the direct system

$$\mathcal{O}^*X\overset{\pi^*}{\to}\mathcal{O}^*Y\overset{\pi^{1*}_0}{\to}\mathcal{O}^*_1Y\to\cdots\mathcal{O}^*_{r-1}Y\overset{\pi^{r}_{r-1}{}^*}{\to}\mathcal{O}^*_rY\to\cdots \tag{3}$$

of algebras $\mathcal{O}^*_rY$ of exterior forms on jet manifolds J^rY with respect to the pull-back monomorphisms $\pi^r_{r-1}{}^*$. Its direct limit is the graded differential algebra (henceforth GDA) $\mathcal{O}^*_\infty Y$ of all exterior forms on finite order jet manifolds modulo the pull-back identification.

Let us extend the GDA $\mathcal{O}^*_\infty Y$ to graded forms on graded manifolds whose bodies are jet manifolds J^rY of Y.[2,9] Note that there are different approaches to treat odd fields on a smooth manifold X, but the following variant of the Serre–Swan theorem motivates us to describe them in terms of graded manifolds whose body is X.

Theorem 1: Let Z be a smooth manifold. A Grassmann algebra $\mathcal{A}$ over the ring $C^\infty(Z)$ of smooth real functions on Z is isomorphic to the Grassmann algebra of graded functions on a graded manifold with a body Z iff it is the exterior algebra of some projective $C^\infty(Z)$-module of finite rank.

Proof: The proof follows at once from the Batchelor theorem[10] and the Serre–Swan theorem generalized to an arbitrary smooth manifold.[11,12] The Batchelor theorem states that any graded manifold $(Z,\mathfrak{A})$ with a body Z is isomorphic to the one $(Z,\mathfrak{A}_Q)$ with the structure sheaf $\mathfrak{A}_Q$ of germs of sections of the exterior bundle,

$$\wedge Q^* = \mathbb{R} \underset{Z}{\oplus} Q^* \underset{Z}{\oplus} \overset{2}{\wedge} Q^* \underset{Z}{\oplus} \cdots ,$$

where Q^* is the dual of some vector bundle $Q \to Z$. Let us call $(Z, \mathfrak{A}_Q)$ the simple graded manifold with the structure vector bundle Q. Its ring $\mathcal{A}_Q$ of graded functions (sections of $\mathfrak{A}_Q$) is the $\mathbb{Z}_2$-graded exterior algebra of the $C^\infty(Z)$-module of sections of $Q^* \to Z$. By virtue of the Serre–Swan theorem, a $C^\infty(Z)$-module is isomorphic to the module of sections of a smooth vector bundle over Z iff it is a projective module of finite rank.

In field models, Batchelor's isomorphism is usually fixed from the beginning. Therefore, we further consider simple graded manifolds $(Z, \mathfrak{A}_Q)$. One associates to $(Z, \mathfrak{A}_Q)$ the following BGDA $\mathcal{S}^*[Q;Z]$.[10] Let $\mathfrak{d}\mathfrak{A}_Q$ be the sheaf of graded derivations of $\mathfrak{A}_Q$. Its global sections make up the real Lie superalgebra $\mathfrak{d}\mathcal{A}_Q$ of graded derivations of the $\mathbb{R}$-ring $\mathcal{A}_Q$. Then the Chevalley–Eilenberg complex of $\mathfrak{d}\mathcal{A}_Q$ with coefficients in $\mathcal{A}_Q$ can be constructed.[13] Its subcomplex $\mathcal{S}^*[Q;Z]$ of $\mathcal{A}_Q$-linear morphisms is the Grassmann-graded Chevalley–Eilenberg differential calculus

$$0 \to \mathbb{R} \to \mathcal{A}_Q \overset{d}{\to} \mathcal{S}^1[Q;Z] \overset{d}{\to} \cdots \mathcal{S}^k[Q;Z] \overset{d}{\to} \cdots$$

over a $\mathbb{Z}_2$-graded commutative $\mathbb{R}$-ring $\mathcal{A}_Q$. The graded exterior product $\wedge$ and Chevalley–Eilenberg coboundary operator d (the graded exterior differential) make $\mathcal{S}^*[Q;Z]$ into a BGDA whose elements obey the relations

$$\phi \wedge \phi' = (-1)^{|\phi||\phi'|+[\phi][\phi']} \phi' \wedge \phi, \quad \mathrm{d}(\phi \wedge \phi') = \mathrm{d}\phi \wedge \phi' + (-1)^{|\phi|} \phi \wedge \mathrm{d}\phi' .$$

Given the GDA $\mathcal{O}^*Z$ of exterior forms on Z, there are the monomorphism $\mathcal{O}^*Z \to \mathcal{S}^*[Q;Z]$ and the body epimorphism $\mathcal{S}^*[Q;Z] \to \mathcal{O}^*Z$. The following facts are essential.[9,11] □

Lemma 2: The BGDA $\mathcal{S}^*[Q;Z]$ is a minimal differential calculus over $\mathcal{A}_Q$, i.e., it is generated by elements $\mathrm{d}f$, $f \in \mathcal{A}_Q$.

Lemma 3: Given a ring R, let $\mathcal{K}$, $\mathcal{K}'$ be R-rings and $\mathcal{A}$, $\mathcal{A}'$ the Grassmann algebras over $\mathcal{K}$ and $\mathcal{K}'$, respectively. Then a homomorphism (respectively, a monomorphism) $\rho: \mathcal{A} \to \mathcal{A}'$ yields a homomorphism (respectively, a monomorphism) of the minimal Chevalley–Eilenberg differential calculus over a $\mathbb{Z}_2$-graded R-ring $\mathcal{A}$ to that over $\mathcal{A}'$ given by the map $\mathrm{d}a \mapsto \mathrm{d}(\rho(a))$, $a \in \mathcal{A}$.

One can think of elements of the BGDA $\mathcal{S}^*[Q;Z]$ as being graded exterior forms on Z as follows. Given an open subset $U \subset Z$, let $\mathcal{A}_U$ be the Grassmann algebra of sections of the sheaf $\mathfrak{A}_Q$ over U, and let $\mathcal{S}^*[Q;U]$ be the Chevalley–Eilenberg differential calculus over $\mathcal{A}_U$. Given an open set $U' \subset U$, the restriction morphisms $\mathcal{A}_U \to \mathcal{A}_{U'}$ yield a homomorphism of BGDAs $\mathcal{S}^*[Q;U] \to \mathcal{S}^*[Q;U']$. Thus, we obtain the presheaf $\{U, \mathcal{S}^*[Q;U]\}$ of BGDAs on a manifold Z and the sheaf $\mathfrak{S}^*[Q;Z]$ of BGDAs of germs of this presheaf. Since $\{U, \mathcal{A}_U\}$ is the canonical presheaf of $\mathfrak{A}_Q$, the canonical presheaf of $\mathfrak{S}^*[Q;Z]$ is $\{U, \mathcal{S}^*[Q;U]\}$. In particular, $\mathcal{S}^*[Q;Z]$ is the BGDA of global sections of the sheaf $\mathfrak{S}^*[Q;Z]$, and there is the restriction morphism $\mathcal{S}^*[Q;Z] \to \mathcal{S}^*[Q;U]$ for any open $U \subset Z$. Due to this morphism, elements of $\mathcal{S}^*[Q;Z]$ can be written in the following local form.

Given bundle coordinates (z^A, q^a) on Q and the corresponding fiber basis $\{c^a\}$ for $Q^* \to X$, the tuple (z^A, c^a) is called a local basis for the graded manifold $(Z, \mathfrak{A}_Q)$.[9] With respect to this basis, graded functions read

$$f = \sum_{k=0} \frac{1}{k!} f_{a_1 \cdots a_k} c^{a_1} \cdots c^{a_k}, \quad f \in C^\infty(Z), \tag{4}$$

where we omit the symbol of the exterior product of elements c^a. Due to the canonical vertical splitting $VQ = Q \times Q$, the fiber basis $\{\partial_a\}$ for vertical tangent bundle $VQ \to Q$ of $Q \to Z$ is the dual of $\{c^a\}$. Then graded derivations take the local form $u = u^A \partial_A + u^a \partial_a$, where u^A, u^a are local graded functions. They act on graded functions (4) by the rule

$$u(f_{a\cdots b}c^a\cdots c^b) = u^A\partial_A(f_{a\cdots b})c^a\cdots c^b + u^d f_{a\cdots b}\partial_d \rfloor (c^a\cdots c^b). \tag{5}$$

Relative to the dual local bases $\{\mathrm{d}z^A\}$ for T^*Z and $\{\mathrm{d}c^b\}$ for Q^*, graded one-forms read $\phi = \phi_A\,\mathrm{d}z^A + \phi_a\,\mathrm{d}c^a$. The duality morphism is given by the interior product

$$u \rfloor \phi = u^A\phi_A + (-1)^{[\phi_a]}u^a\phi_a, \quad u \in \mathfrak{d}\mathcal{A}_Q, \quad \phi \in \mathcal{S}^1[Q;Z].$$

The graded exterior differential reads

$$\mathrm{d}\phi = \mathrm{d}z^A \wedge \partial_A\phi + \mathrm{d}c^a \wedge \partial_a\phi,$$

where the derivations ∂_A and ∂_a act on coefficients of graded exterior forms by the formula (5), and they are graded commutative with the graded exterior forms $\mathrm{d}z^A$ and $\mathrm{d}c^a$.

We define jets of odd fields as simple graded manifolds modelled over jet bundles over X.[2,9] This definition differs from the definition of jets of a graded commutative ring[11] and that of jets of a graded fiber bundle,[14] but reproduces the heuristic notion of jets of odd ghosts in Lagrangian BRST theory.[7,15]

Given a vector bundle $F \to X$, let us consider the simple graded manifold $(J^rY, \mathfrak{A}_{F_r})$ whose body is J^rY and the structure bundle is the pull-back

$$F_r = J^rY \underset{X}{\times} J^rF$$

onto J^rY of the jet bundle $J^rF \to X$, which is also a vector bundle. Given the simple graded manifold $(J^{r+1}Y, \mathfrak{A}_{F_{r+1}})$, there is an epimorphism of graded manifolds

$$(J^{r+1}Y, \mathfrak{A}_{F_{r+1}}) \to (J^rY, \mathfrak{A}_{F_r}).$$

It consists of the open surjection π_r^{r+1} and the sheaf monomorphism $\pi_r^{r+1*}\mathfrak{A}_{F_r} \to \mathfrak{A}_{F_{r+1}}$, where $\pi_r^{r+1*}\mathfrak{A}_{F_r}$ is the pull-back onto $J^{r+1}Y$ of the topological fiber bundle $\mathfrak{A}_{F_r} \to J^rY$. This sheaf monomorphism induces the monomorphism of the canonical presheaves $\bar{\mathfrak{A}}_{F_r} \to \bar{\mathfrak{A}}_{F_{r+1}}$, which associates to each open subset $U \subset J^{r+1}Y$ the ring of sections of $\mathfrak{A}_{F_r}$ over $\pi_r^{r+1}(U)$. Accordingly, there is the monomorphism of $\mathbb{Z}_2$-graded rings $\mathcal{A}_{F_r} \to \mathcal{A}_{F_{r+1}}$. By virtue of Lemmas 2and 3, this monomorphism yields the monomorphism of BGDAs,

$$\mathcal{S}^*[F_r;J^rY] \to \mathcal{S}^*[F_{r+1};J^{r+1}Y]. \tag{6}$$

As a consequence, we have the direct system of BGDAs

$$\mathcal{S}^*[Y \underset{X}{\times} F;Y] \to \mathcal{S}^*[F_1;J^1Y] \to \cdots \mathcal{S}^*[F_r;J^rY] \to \cdots, \tag{7}$$

whose direct limit $\mathcal{S}^*_\infty[F;Y]$ is a BGDA of all graded differential forms $\phi \in \mathcal{S}^*[F_r;J^rY]$ on jet manifolds J^rY modulo monomorphisms (6). The monomorphisms $\mathcal{O}^*_rY \to \mathcal{S}^*[F_r;J^rY]$ provide the monomorphism $\mathcal{O}^*_\infty Y \to \mathcal{S}^*_\infty[F;Y]$ of their direct limits. In particular, $\mathcal{S}^*_\infty[F;Y]$ is an $\mathcal{O}^0_\infty Y$-algebra. Accordingly, the body epimorphisms $\mathcal{S}^*[F_r;J^rY] \to \mathcal{O}^*_rY$ yield the epimorphism of $\mathcal{O}^0_\infty Y$-modules $\mathcal{S}^*_\infty[F;Y] \to \mathcal{O}^*_\infty Y$.

If $Y \to X$ is an affine bundle, we recover the BGDA introduced in Refs. 2 and 9 by restricting the ring $\mathcal{O}^0_\infty Y$ to its subring $\mathcal{P}^0_\infty Y$ of polynomial functions, but now elements of $\mathcal{S}^*_\infty[F;Y]$ are graded exterior forms on $J^\infty Y$. Indeed, let $\mathfrak{S}^*[F_r;J^rY]$ be the sheaf of BGDAs on J^rY and $\bar{\mathfrak{S}}^*[F_r;J^rY]$ its canonical presheaf whose elements are the Chevalley–Eilenberg differential calculus over elements of the presheaf $\bar{\mathfrak{A}}_{F_r}$. Then the presheaf monomorphisms $\bar{\mathfrak{A}}_{F_r} \to \bar{\mathfrak{A}}_{F_{r+1}}$ yield the direct system of presheaves

$$\bar{\mathfrak{S}}^*[Y\times F;Y]\to\bar{\mathfrak{S}}^*[F_1;J^1Y]\to\cdots\bar{\mathfrak{S}}^*[F_r;J^rY]\to\cdots, \tag{8}$$

whose direct limit $\bar{\mathfrak{S}}^*_\infty[F;Y]$ is a presheaf of BGDAs on the infinite order jet manifold $J^\infty Y$. Let $\mathfrak{T}^*_\infty[F;Y]$ be the sheaf of BGDAs of germs of the presheaf $\bar{\mathfrak{S}}^*_\infty[F;Y]$. The structure module $\Gamma(\mathfrak{T}^*_\infty[F;Y])$ of sections of $\mathfrak{T}^*_\infty[F;Y]$ is a BGDA such that, given an element $\phi\in\Gamma(\mathfrak{T}^*_\infty[F;Y])$ and a point $z\in J^\infty Y$, there exist an open neighborhood U of z and a graded exterior form $\phi^{(k)}$ on some finite order jet manifold J^kY so that $\phi|_U=\pi^{\infty *}_k\phi^{(k)}|_U$. In particular, there is the monomorphism $\mathcal{S}^*_\infty[F;Y]\to\Gamma(\mathfrak{T}^*_\infty[F;Y])$.

Due to this monomorphism, one can restrict $\mathcal{S}^*_\infty[F;Y]$ to the coordinate chart (2) and say that $\mathcal{S}^*_\infty[F;Y]$ as an $\mathcal{O}^0_\infty Y$-algebra is locally generated by the elements

$$(1,c^a_\Lambda,\mathrm{d}x^\lambda,\theta^a_\Lambda=\mathrm{d}c^a_\Lambda-c^a_{\lambda+\Lambda}\,\mathrm{d}x^\lambda,\theta^i_\Lambda=\mathrm{d}y^i_\Lambda-y^i_{\lambda+\Lambda}\,\mathrm{d}x^\lambda),\quad 0\leqslant|\Lambda|.$$

We agree to call (y^i,c^a) the local basis for $\mathcal{S}^*_\infty[F;Y]$. Let the collective symbol s^A stand for its elements. Accordingly, the notation s^A_Λ and $\theta^A_\Lambda=\mathrm{d}s^A_\Lambda-s^A_{\lambda+\Lambda}\,\mathrm{d}x^\lambda$ is introduced. For the sake of simplicity, we further denote $[A]=[s^A]$.

The BGDA $\mathcal{S}^*_\infty[F;Y]$ is decomposed into $\mathcal{S}^0_\infty[F;Y]$-modules $\mathcal{S}^{k,r}_\infty[F;Y]$ of k-contact and r-horizontal graded forms. Accordingly, the graded exterior differential d on $\mathcal{S}^*_\infty[F;Y]$ falls into the sum $d=d_H+d_V$ of the total and vertical differentials, where

$$d_H(\phi)=\mathrm{d}x^\lambda\wedge d_\lambda(\phi),\quad d_\lambda=\partial_\lambda+\sum_{0\leqslant|\Lambda|}s^A_{\lambda+\Lambda}\partial^\Lambda_A.$$

Given the projector

$$\varrho=\sum_{k>0}\frac{1}{k}\bar{\varrho}\circ h_k\circ h^n,\quad \bar{\varrho}(\phi)=\sum_{0\leqslant|\Lambda|}(-1)^{|\Lambda|}\theta^A\wedge[d_\Lambda(\partial^\Lambda_A\rfloor\phi)],\quad \phi\in\mathcal{S}^{>0,n}_\infty[F;Y],$$

and the graded variational operator $\delta=\varrho\circ d$, the BGDA $\mathcal{S}^*_\infty[F;Y]$ is split into the above-mentioned Grassmann-graded variational bicomplex.[7,8] We restrict our consideration to its short variational subcomplex

$$0\to\mathbb{R}\to\mathcal{S}^0_\infty[F;Y]\overset{d_H}{\to}\mathcal{S}^{0,1}_\infty[F;Y]\cdots\overset{d_H}{\to}\mathcal{S}^{0,n}_\infty[F;Y]\overset{\delta}{\to}\mathbf{E}_1,\quad \mathbf{E}_1=\varrho(\mathcal{S}^{1,n}_\infty[F;Y]).$$

One can think of its even elements

$$\begin{gathered}L=\mathcal{L}\omega\in\mathcal{S}^{0,n}_\infty[F;Y],\quad \omega=\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^n,\\ \delta L=\theta^A\wedge\mathcal{E}_A\omega=\sum_{0\leqslant|\Lambda|}(-1)^{|\Lambda|}\theta^A\wedge d_\Lambda(\partial^\Lambda_A L)\omega\in\mathbf{E}_1\end{gathered} \tag{9}$$

as being a graded Lagrangian and its Euler–Lagrange operator. A pair $(\mathcal{S}^*_\infty[F;Y],L)$ is further called a graded Lagrangian system.

Let $\vartheta\in\mathfrak{d}\mathcal{S}^0_\infty[F;Y]$ be a graded derivation of the $\mathbb{R}$-ring $\mathcal{S}^0_\infty[F;Y]$.[2,9] The interior product $\vartheta\rfloor\phi$ and the Lie derivative $\mathbf{L}_\vartheta\phi$, $\phi\in\mathcal{S}^*_\infty[F;Y]$, are defined by the formulas

$$\vartheta\rfloor\phi=\vartheta^\lambda\phi_\lambda+(-1)^{[\phi_A]}\vartheta^A\phi_A,\quad \phi\in\mathcal{S}^1_\infty[F;Y],$$

$$\vartheta\rfloor(\phi\wedge\sigma)=(\vartheta\rfloor\phi)\wedge\sigma+(-1)^{|\phi|+[\phi][\vartheta]}\phi\wedge(\vartheta\rfloor\sigma),\quad \phi,\sigma\in\mathcal{S}^*_\infty[F;Y],$$

$$\mathbf{L}_\vartheta\phi=\vartheta\rfloor\mathrm{d}\phi+d(\vartheta\rfloor\phi),\quad \mathbf{L}_\vartheta(\phi\wedge\sigma)=\mathbf{L}_\vartheta(\phi)\wedge\sigma+(-1)^{[\vartheta][\phi]}\phi\wedge\mathbf{L}_\vartheta(\sigma).$$

A graded derivation ϑ is said to be contact if the Lie derivative $\mathbf{L}_\vartheta$ preserves the ideal of contact graded forms of the BGDA $\mathcal{S}^*_\infty[F;Y]$. With respect to the local basis $\{s^A\}$ for the BGDA $\mathcal{S}^*_\infty[F;Y]$, any contact graded derivation takes the form

$$\vartheta = \vartheta_H + \vartheta_V = \vartheta^\lambda d_\lambda + \left(\vartheta^A \partial_A + \sum_{0<|\Lambda|} d_\Lambda \vartheta^A \partial_A^\Lambda\right),$$

where the tuple of graded derivations $\{\partial_\lambda, \partial_A^\Lambda\}$ is the dual of the tuple $\{dx^\lambda, ds_\Lambda^A\}$ of generating elements of the $\mathcal{S}^0_\infty[F;Y]$-algebra $\mathcal{S}^*_\infty[F;Y]$, and ϑ^λ, ϑ^A are local graded functions.

We restrict our consideration to vertical contact graded derivations

$$\vartheta = \sum_{0\leqslant|\Lambda|} d_\Lambda \upsilon^A \partial_A^\Lambda. \tag{10}$$

Such a derivation is completely determined by its first summand

$$\upsilon = \upsilon^A(x^\lambda, s_\Lambda^A)\partial_A, \quad 0 \leqslant |\Lambda| \leqslant k, \tag{11}$$

called a generalized graded vector field. It is said to be nilpotent if

$$\mathbf{L}_\vartheta(\mathbf{L}_\vartheta\phi) = \sum_{0\leqslant|\Sigma|,0\leqslant|\Lambda|} (\upsilon_\Sigma^B \partial_B^\Sigma(\upsilon_\Lambda^A)\partial_A^\Lambda + (-1)^{[B][\upsilon^A]}\upsilon_\Sigma^B \upsilon_\Lambda^A \partial_B^\Sigma \partial_A^\Lambda)\phi = 0$$

for any horizontal graded form $\phi \in \mathcal{S}^{0,*}_\infty[F;Y]$. One can show that ϑ (10) is nilpotent only if it is odd and iff all υ^A obey the equality

$$\vartheta(\upsilon^A) = \sum_{0\leqslant|\Sigma|} \upsilon_\Sigma^B \partial_B^\Sigma(\upsilon^A) = 0. \tag{12}$$

For the sake of simplicity, the common symbol further stands for a generalized vector field (11), the contact graded derivation (10) determined by this field and the Lie derivative $\mathbf{L}_\vartheta$. We agree to call all these operators the graded derivation of the BGDA $\mathcal{S}^*_\infty[F;Y]$.

III. NOETHER IDENTITIES IN A GENERAL SETTING

Given a graded Lagrangian system $(\mathcal{S}^*_\infty[F;Y], L)$, let us construct the manifested Koszul–Tate complex of its Noether identities.

The main ingredient in this construction is BGDAs of the following type. Given a vector bundle $E \to X$, let us consider the BGDA $\mathcal{S}^*_\infty[F;E_Y]$, where E_Y denotes the pull-back of E onto Y. There are monomorphisms of $\mathcal{O}^0_\infty Y$-algebras,

$$\mathcal{S}^*_\infty[F;Y] \to \mathcal{S}^*_\infty[F;E_Y], \quad \mathcal{O}^*_\infty E \to \mathcal{S}^*_\infty[F;E_Y],$$

whose images contain the common subalgebra $\mathcal{O}^*_\infty Y$. Let us consider (i) the subring $\mathcal{P}^0_\infty E_Y \subset \mathcal{O}^0_\infty E_Y$ of polynomial functions in fiber coordinates of the vector bundles $J^r E_Y \to J^r Y$, $r \in \mathbb{N}$, (ii) the corresponding subring $\mathcal{P}^0_\infty[F;E_Y] \subset \mathcal{S}^0_\infty[F;E_Y]$ of graded functions with polynomial coefficients belonging to $\mathcal{P}^0_\infty E_Y$, (iii) the subalgebra $\mathcal{P}^*_\infty[F;Y;E]$ of the BGDA $\mathcal{S}^*_\infty[F;E_Y]$ over the subring $\mathcal{P}^0_\infty[F;E_Y]$. Given vector bundles V, V', E, E' over X, we further use the notation

$$\mathcal{P}^*_\infty[V'V;F;Y;EE'] = \mathcal{P}^*_\infty[V' \underset{X}{\times} V \underset{X}{\times} F;Y;E \underset{X}{\times} E'].$$

By a density-dual of a vector bundle $E \to X$ is meant

$$\overline{E}^* = E^* \underset{X}{\otimes} \overset{n}{\wedge} T^*X.$$

For the sake of simplicity, we restrict our consideration to Lagrangian systems where a fiber bundle $Y \to X$ of even fields admits the vertical splitting $VY = Y \times W$, where W is a vector bundle over X. This is the case of almost all field models. In a general setting, one must require that transition functions of fiber bundles over Y under consideration do not vanish on-shell. Let $\overline{Y}^*$ denote the density-dual of W in the above-mentioned vertical splitting.

Proposition 4: One can associate to a graded Lagrangian system $(\mathcal{S}^*_\infty[F;Y],L)$, a chain complex whose boundaries vanish on shell [see the complex (13) below].

Proof: Let us extend the BGDA $\mathcal{S}^*_\infty[F;Y]$ to the BGDA $\mathcal{P}^*_\infty[\overline{Y}^*;F;Y;\overline{F}^*]$ whose local basis is $\{s^A,\overline{s}_A\}$, where $[\overline{s}_A]=([A]+1)\mathrm{mod}\,2$. Following the terminology of Lagrangian BRST theory,[2,5] we call $\overline{s}_A$ the antifields of antifield number 1. The BGDA $\mathcal{P}^0_\infty[\overline{Y}^*;F;Y;\overline{F}^*]$ is provided with the nilpotent graded derivation $\overline{\delta}=\overleftarrow{\partial}{}^A d\mathcal{E}_A$, where $\mathcal{E}_A$ are the graded variational derivatives (9) and the tuple of graded right derivations $\{\overleftarrow{\partial}{}^{\Lambda A}\}$ is the dual of the tuple of contact graded forms $\{\theta_{\Lambda A}\}$. Because of the expression (9) for δL, it is convenient to deal with a graded derivation $\overline{\delta}$ acting on graded functions and forms ϕ on the right by the rule

$$\overline{\delta}(\phi)=\mathrm{d}\phi\rfloor\overline{\delta}+d(\phi\rfloor\overline{\delta}),\quad \overline{\delta}(\phi\wedge\phi')=(-1)^{[\phi']}\overline{\delta}(\phi)\wedge\phi'+\phi\wedge\overline{\delta}(\phi').$$

We call $\overline{\delta}$ the Koszul–Tate differential. Let us consider the module $\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]$ of graded densities. It is split into the chain complex

$$0\leftarrow\mathcal{S}^{0,n}_\infty[F;Y]\overset{\overline{\delta}}{\leftarrow}\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_1\cdots\overset{\overline{\delta}}{\leftarrow}\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_k\cdots \tag{13}$$

graded by the antifield number of its elements. It is readily observed that the boundaries of the complex (13) vanish on-shell.

Note that the homology groups $H_*(\overline{\delta})$ of the complex (13) are $\mathcal{S}^0_\infty[F;Y]$-modules, but these modules fail to be torsion-free. Indeed, given a cycle $\phi\in\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_k$ and an element $f=\overline{\delta}\sigma$ of the ring $\mathcal{S}^0_\infty[F;Y]\subset\mathcal{P}^0_\infty[\overline{Y}^*;F;Y;\overline{F}^*]$, we obtain that $f\phi=\overline{\delta}(\sigma\phi)$ is a boundary. Therefore, one cannot apply the Künneth formula to the homology of this complex, though any term $\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_k$ is isomorphic to the graded commutative k-tensor product of the $\mathcal{S}^0_\infty[F;Y]$-module $\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_1$.

The homology $H_0(\overline{\delta})$ of the complex (13) is not trivial, but this homology and the higher ones $H_{k\geqslant 2}(\overline{\delta})$ are not essential for our consideration. Therefore, we replace the complex (13) with the finite one

$$0\leftarrow\mathrm{Im}\,\overline{\delta}\overset{\overline{\delta}}{\leftarrow}\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_1\overset{\overline{\delta}}{\leftarrow}\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_2 \tag{14}$$

of graded densities of antifield number $k\leqslant 2$. It is exact at $\mathrm{Im}\,\overline{\delta}$, and its first homology coincides with that of the complex (13). Let us consider this homology.

A generic one-chain of the complex (14) takes the form

$$\Phi=\sum_{0\leqslant|\Lambda|}\Phi^{A,\Lambda}\overline{s}_{\Lambda A}\omega,\quad \Phi^{A,\Lambda}\in\mathcal{S}^0_\infty[F;Y], \tag{15}$$

and the cycle condition $\overline{\delta}\Phi=0$ reads

$$\sum_{0\leqslant|\Lambda|}\Phi^{A,\Lambda}d_\Lambda\mathcal{E}_A\omega=0. \tag{16}$$

One can think of this equality as being a reduction condition on the graded variational derivatives $\mathcal{E}_A$. Conversely, any reduction condition of form (16) comes from some cycle (15). The reduction condition (16) is trivial if a cycle is a boundary, i.e., it takes the form

$$\Phi=\sum_{0\leqslant|\Lambda|,|\Sigma|}T^{(A\Lambda)(B\Sigma)}d_\Sigma\mathcal{E}_B\overline{s}_{\Lambda A}\omega,\quad T^{(A\Lambda)(B\Sigma)}=-(-1)^{[A][B]}T^{(B\Sigma)(A\Lambda)}. \tag{17}$$

□

Definition 5: A graded Lagrangian system is called degenerate if there exist nontrivial reduction conditions (16), called Noether identities.

One can say something more if the $\mathcal{S}^0_\infty[F;Y]$-module $H_1(\overline{\delta})$ is finitely generated, i.e., it possesses the following particular structure. There are elements $\Delta \in H_1(\overline{\delta})$ making up a $\mathbb{Z}_2$-graded projective $C^\infty(X)$-module $\mathcal{C}_{(0)}$ of finite rank which, by virtue of the Serre–Swan theorem, is isomorphic to the module of sections of the product $\overline{V}^* \underset{X}{\times} \overline{E}^*$ of the density-duals of some vector bundles $V \to X$ and $E \to X$. Let $\{\Delta_r\}$ be local bases for this $C^\infty(X)$-module. Every element $\Phi \in H_1(\overline{\delta})$ factorizes

$$\Phi = \sum_{0 \leqslant |\Xi|} G^{r,\Xi} d_\Xi \Delta_r \omega, \quad G^{r,\Xi} \in \mathcal{S}^0_\infty[F;Y], \tag{18}$$

$$\Delta_r = \sum_{0 \leqslant |\Lambda|} \Delta_r^{A,\Lambda} \overline{s}_{\Lambda A}, \quad \Delta_r^{A,\Lambda} \in \mathcal{S}^0_\infty[F;Y], \tag{19}$$

via elements of $\mathcal{C}_{(0)}$, i.e., any Noether identity (16) is a corollary of Noether identities

$$\sum_{0 \leqslant |\Lambda|} \Delta_r^{A,\Lambda} d_\Lambda \mathcal{E}_A = 0. \tag{20}$$

Clearly, the factorization (18) is independent of specification of local bases $\{\Delta_r\}$. We say that the Noether identities (20) are complete, and call $\Delta \in \mathcal{C}_{(0)}$ the Noether operators. Note that, being representatives of $H_1(\overline{\delta})$, the graded densities Δ_r (19) are not $\overline{\delta}$-exact.

Proposition 6: If the homology $H_1(\overline{\delta})$ of the complex (14) is finitely generated, this complex can be extended to a one-exact complex with a boundary operator whose nilpotency conditions are just complete Noether identities [see the complex (22) below].

Proof: Let us extend the BGDA $\mathcal{P}^*_\infty[\overline{Y}^*;F;Y;\overline{F}^*]$ to the BGDA $\mathcal{P}^*_\infty[\overline{E}^*\overline{Y}^*;F;Y;\overline{F}^*\overline{V}^*]$ possessing the local basis $\{s^A, \overline{s}_A, \overline{c}_r\}$, where $[\overline{c}_r] = ([\Delta_r]+1) \bmod 2$ and $\mathrm{Ant}[\overline{c}] = 2$. It is provided with the nilpotent graded derivation

$$\delta_0 = \overline{\delta} + \overleftarrow{\partial}^r \Delta_r, \tag{21}$$

called the extended Koszul–Tate differential. Its nilpotency conditions (12) are equivalent to the complete Noether identities (20). Then the module $\mathcal{P}^{0,n}_\infty[\overline{E}^*\overline{Y}^*;F;Y;\overline{F}^*\overline{V}^*]_{\leqslant 3}$ of graded densities of antifield number $\mathrm{Ant}[\phi] \leqslant 3$ is split into the chain complex

$$0 \leftarrow \mathrm{Im}\,\overline{\delta} \xleftarrow{\overline{\delta}} \mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_1 \xleftarrow{\delta_0} \mathcal{P}^{0,n}_\infty[\overline{E}^*\overline{Y}^*;F;Y;\overline{F}^*\overline{V}^*]_2$$

$$\xleftarrow{\delta_0} \mathcal{P}^{0,n}_\infty[\overline{E}^*\overline{Y}^*;F;Y;\overline{F}^*\overline{V}^*]_3. \tag{22}$$

Let $H_*(\delta_0)$ denote its homology. We have $H_0(\delta_0) = H_0(\overline{\delta}) = 0$. Furthermore, any one-cycle Φ up to a boundary takes the form (18) and, therefore, it is a δ_0-boundary,

$$\Phi = \sum_{0 \leqslant |\Sigma|} G^{r,\Xi} d_\Xi \Delta_r \omega = \delta_0 \left(\sum_{0 \leqslant |\Sigma|} G^{r,\Xi} \overline{c}_{\Xi r} \omega \right).$$

Hence, $H_1(\delta_0) = 0$, i.e., the complex (22) is one-exact. □

IV. THE KOSZUL–TATE COMPLEX OF NOETHER IDENTITIES

Turn now to the homology $H_2(\delta_0)$ of the complex (22). A generic two-chain reads

$$\Phi = G + H = \sum_{0\leqslant|\Lambda|} G^{r,\Lambda}\overline{c}_{\Lambda r}\omega + \sum_{0\leqslant|\Lambda|,|\Sigma|} H^{(A,\Lambda)(B,\Sigma)}\overline{s}_{\Lambda A}\overline{s}_{\Sigma B}\omega,$$
$$G^{r,\Lambda}\in\mathcal{S}^0_\infty[F;Y], \quad H^{(A,\Lambda)(B,\Sigma)}\mathcal{V}\in\mathcal{S}^0_\infty[F;Y], \quad \mathcal{V}\in\mathcal{O}^nX. \tag{23}$$

The cycle condition $\delta_0\Phi=0$ takes the form

$$\sum_{0\leqslant|\Lambda|} G^{r,\Lambda}d_\Lambda\Delta_r\omega + \overline{\delta}H = 0. \tag{24}$$

One can think of this equality as being the reduction condition on the Noether operators (19). Conversely, let

$$\Phi = \sum_{0\leqslant|\Lambda|} G^{r,\Lambda}\overline{c}_{\Lambda r}\omega \in \mathcal{P}^{0,n}_\infty[\overline{E}^*\overline{Y}^*;F;Y;\overline{F}^*\overline{V}^*]_2$$

be a graded density such that the reduction condition (24) holds. Obviously, it is a cycle condition of the two-chain (23). The reduction condition (24) is trivial either if a two-cycle Φ (23) is a boundary or its summand G vanishes on-shell.

Definition 7: A degenerate graded Lagrangian system in Proposition 6 is said to be one-stage reducible if there exist nontrivial reduction conditions (24), called the first-stage Noether identities.

Proposition 8: First-stage Noether identities can be identified to nontrivial elements of the homology $H_2(\delta_0)$ iff any $\overline{\delta}$-cycle $\Phi\in\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_2$ is a δ_0-boundary.

Proof: It suffices to show that, if the summand G of a two-cycle Φ (23) is $\overline{\delta}$-exact, then G is a boundary. If $G=\overline{\delta}\Psi$, then

$$\Phi = \delta_0\Psi + (\overline{\delta}-\delta_0)\Psi + H. \tag{25}$$

The cycle condition reads

$$\delta_0\Phi = \overline{\delta}((\overline{\delta}-\delta_0)\Psi + H) = 0.$$

Then $(\overline{\delta}-\delta_0)\Psi+H$ is δ_0-exact since any $\overline{\delta}$-cycle $\phi\in\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_2$, by assumption, is a δ_0-boundary. Consequently, Φ (25) is δ_0-exact. Conversely, let $\Phi\in\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_2$ be an arbitrary $\overline{\delta}$-cycle. The cycle condition reads

$$\overline{\delta}\Phi = 2\Phi^{(A,\Lambda)(B,\Sigma)}\overline{s}_{\Lambda A}\overline{\delta}\overline{s}_{\Sigma B}\omega = 2\Phi^{(A,\Lambda)(B,\Sigma)}\overline{s}_{\Lambda A}d_\Sigma\mathcal{E}_B\omega = 0. \tag{26}$$

It follows that $\Phi^{(A,\Lambda)(B,\Sigma)}\overline{\delta}\overline{s}_{\Sigma B}=0$ for all indices (A,Λ). Omitting a $\overline{\delta}$-boundary term, we obtain

$$\Phi^{(A,\Lambda)(B,\Sigma)}\overline{s}_{\Sigma B} = G^{(A,\Lambda)(r,\Xi)}d_\Xi\Delta_r.$$

Hence, Φ takes the form

$$\Phi = G'^{(A,\Lambda)(r,\Xi)}d_\Xi\Delta_r\overline{s}_{\Lambda A}\omega. \tag{27}$$

We can associate to it the three-chain,

$$\Psi = G'^{(A,\Lambda)(r,\Xi)}\overline{c}_{\Xi r}\overline{s}_{\Lambda A}\omega$$

such that

$$\delta_0\Psi = \Phi + \sigma = \Phi + G''^{(A,\Lambda)(r,\Xi)} d_\Lambda \mathcal{E}_A \overline{c}_{\Xi r}\omega.$$

Owing to the equality $\overline{\delta}\Phi=0$, we have $\delta_0\sigma=0$. Since σ is $\overline{\delta}$-exact, it by assumption is δ_0-exact, i.e., $\sigma=\delta_0\psi$. Then we obtain that $\Phi=\delta_0\Psi-\delta_0\psi$. □

Lemma 9: It is easily justified that a two-cycle $\Phi\in\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_2$ is δ_0-exact iff Φ up to a $\overline{\delta}$-boundary takes the form

$$\Phi = \sum_{0\leqslant|\Lambda|,|\Sigma|} G'^{(r,\Sigma)(r',\Lambda)} d_\Sigma\Delta_r d_\Lambda \Delta_{r'}\omega. \tag{28}$$

If the condition of Proposition 8 (called the two-homology regularity condition) is satisfied, let us assume that the first-stage Noether identities are finitely generated as follows. There are elements $\Delta_{(1)}\in H_2(\delta_0)$ making up a $\mathbb{Z}_2$-graded projective $C^\infty(X)$-module $\mathcal{C}_{(1)}$ of finite rank which is isomorphic to the module of sections of the product $\overline{V}^*_1\underset{X}{\times}\overline{E}^*_1$ of the density-duals of some vector bundles $V_1\to X$ and $E_1\to X$. Let $\{\Delta_{r_1}\}$ be local bases for this $C^\infty(X)$-module. Every element $\Phi\in H_2(\delta_0)$ factorizes

$$\Phi = \sum_{0\leqslant|\Xi|} \Phi^{r_1,\Xi} d_\Xi \Delta_{r_1}\omega, \quad \Phi^{r_1,\Xi}\in\mathcal{S}^0_\infty[F;Y], \tag{29}$$

$$\Delta_{r_1} = G_{r_1} + h_{r_1} = \sum_{0\leqslant|\Lambda|} \Delta^{r,\Lambda}_{r_1}\overline{c}_{\Lambda r} + h_{r_1}, \quad h_{r_1}\omega\in\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*], \tag{30}$$

via elements of $\mathcal{C}_{(1)}$, i.e., any first-stage Noether identity (24) results from the equalities

$$\sum_{0\leqslant|\Lambda|} \Delta^{r,\Lambda}_{r_1} d_\Lambda\Delta_r + \overline{\delta}h_{r_1} = 0, \tag{31}$$

called the complete first-stage Noether identities. Elements of $\mathcal{C}_{(1)}$ are called the first-stage Noether operators. Note that first summands G_{r_1} of operators Δ_{r_1} (30) are not $\overline{\delta}$-exact.

Proposition 10: Given a reducible degenerate Lagrangian system, let the associated one-exact complex (22) obey the two-homology regularity condition and let its homology $H_2(\delta_0)$ (first-stage Noether identities) be finitely generated. Then this complex is extended to the two-exact one with a boundary operator whose nilpotency conditions are equivalent to complete Noether and first-stage Noether identities [see the complex (33) below].

Proof: Let us consider the BGDA $\mathcal{P}^*_\infty[\overline{E}^*_1\overline{E}^*\overline{Y}^*;F;Y;\overline{F}^*\overline{V}^*\overline{V}^*_1]$ with the local basis $\{s^A,\overline{s}_A,\overline{c}_r,\overline{c}_{r_1}\}$, where $[\overline{c}_{r_1}]=([\Delta_{r_1}]+1)\mathrm{mod}\,2$ and $\mathrm{Ant}[\overline{c}_{r_1}]=3$. It can be provided with the first-stage Koszul–Tate differential defined as the nilpotent graded derivation,

$$\delta_1 = \delta_0 + \overleftarrow{\partial}^{r_1}\Delta_{r_1}. \tag{32}$$

Its nilpotency conditions (12) are equivalent to complete Noether identities (20) and complete first-stage Noether identities (31). Then the module $\mathcal{P}^{0,n}_\infty[\overline{E}^*_1\overline{E}^*\overline{Y}^*;F;Y;\overline{F}^*\overline{V}^*\overline{V}^*_1]_{\leqslant 4}$ of graded densities of antifield number $\mathrm{Ant}[\phi]\leqslant 4$ is split into the chain complex

$$0\leftarrow \mathrm{Im}\,\overline{\delta}\overset{\overline{\delta}}{\leftarrow}\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_1\overset{\delta_0}{\leftarrow}\mathcal{P}^{0,n}_\infty[\overline{E}^*\overline{Y}^*;F;Y;\overline{F}^*\overline{V}^*]_2$$

$$\overset{\delta_1}{\leftarrow}\mathcal{P}^{0,n}_\infty[\overline{E}^*_1\overline{E}^*\overline{Y}^*;F;Y;\overline{F}^*\overline{V}^*\overline{V}^*_1]_3\overset{\delta_1}{\leftarrow}\mathcal{P}^{0,n}_\infty[\overline{E}^*_1\overline{E}^*\overline{Y}^*;F;Y;\overline{F}^*\overline{V}^*\overline{V}^*_1]_4. \tag{33}$$

Let $H_*(\delta_1)$ denote its homology. It is readily observed that

$$H_0(\delta_1) = H_0(\overline{\delta}), \quad H_1(\delta_1) = H_1(\delta_0) = 0.$$

By virtue of the expression (29), any two-cycle of the complex (33) is a boundary

$$\Phi = \sum_{0\leqslant|\Xi|} \Phi^{r_1,\Xi} d_\Xi \Delta_{r_1} \omega = \delta_1 \left(\sum_{0\leqslant|\Xi|} \Phi^{r_1,\Xi} \overline{c}_{\Xi r_1} \right) \omega.$$

It follows that $H_2(\delta_1)=0$, i.e., the complex (33) is two-exact.

If the third homology $H_3(\delta_1)$ of the complex (33) is not trivial, there are reduction conditions on the first-stage Noether operators, and so on. Iterating the arguments, we come to the following.

Let $(\mathcal{S}^*_\infty[F;Y],L)$ be a degenerate graded Lagrangian system whose Noether identities are finitely generated. In accordance with Proposition 6, we associate to it the one-exact chain complex (22). Given an integer $N\geqslant 1$, let $V_1,\ldots,V_N,E_1,\ldots,E_N$ be some vector bundles over X and

$$\mathcal{P}^*_\infty\{N\} = \mathcal{P}^*_\infty[\overline{E}^*_N \cdots \overline{E}^*_1 \overline{E}^* \overline{Y}^*; F; Y; \overline{F}^* \overline{V}^* \overline{V}^*_1 \cdots \overline{V}^*_N] \tag{34}$$

a BGDA with local bases $\{s^A, \overline{s}_A, \overline{c}_r, \overline{c}_{r_1}, \ldots, \overline{c}_{r_N}\}$ graded by antifield numbers $\mathrm{Ant}[\overline{c}_{r_k}]=k+2$. Let $k=-1,0$ further stand for $\overline{s}_A$ and $\overline{c}_r$, respectively. We assume the following:

(i) the BGDA $\mathcal{P}^*_\infty\{N\}$ (34) is provided with a nilpotent graded derivation

$$\delta_N = \delta_0 + \sum_{1\leqslant k\leqslant N} \overleftarrow{\partial}^{r_k} \Delta_{r_k}, \tag{35}$$

$$\Delta_{r_k} = G_{r_k} + h_{r_k} = \sum_{0\leqslant|\Lambda|} \Delta^{r_{k-1},\Lambda}_{r_k} \overline{c}_{\Lambda r_{k-1}} + \sum_{0\leqslant\Sigma,0\leqslant\Xi} (h^{(A,\Xi)(r_{k-2},\Sigma)}_{r_k} \overline{s}_{\Xi A} \overline{c}_{\Sigma r_{k-2}} + \cdots), \tag{36}$$

of antifield number -1;

(ii) the module $\mathcal{P}^{0,n}_\infty\{N\}_{\leqslant N+3}$ of graded densities of antifield number $\mathrm{Ant}[\phi]\leqslant N+3$ is split into the $(N+1)$-exact chain complex

$$0 \leftarrow \mathrm{Im}\,\overline{\delta} \overset{\overline{\delta}}{\leftarrow} \mathcal{P}^{0,n}_\infty[\overline{Y}^*; F; Y; \overline{F}^*]_1 \overset{\delta_0}{\leftarrow} \mathcal{P}^{0,n}_\infty\{0\}_2 \overset{\delta_1}{\leftarrow} \mathcal{P}^{0,n}_\infty\{1\}_3 \cdots$$
$$\overset{\delta_{N-1}}{\leftarrow} \mathcal{P}^{0,n}_\infty\{N-1\}_{N+1} \overset{\delta_N}{\leftarrow} \mathcal{P}^{0,n}_\infty\{N\}_{N+2} \overset{\delta_N}{\leftarrow} \mathcal{P}^{0,n}_\infty\{N\}_{N+3}, \tag{37}$$

which satisfies the $(N+1)$-homology regularity condition in accordance with the forthcoming Definition 11. □

Definition 11: One says that the complex (37) obeys the $(N+1)$-homology regularity condition if any $\delta_{k<N-1}$-cycle $\phi\in\mathcal{P}^{0,n}_\infty\{k\}_{k+3}\subset\mathcal{P}^{0,n}_\infty\{k+1\}_{k+3}$ is a δ_{k+1}-boundary.

Remark 3: The $(N+1)$-exactness of the complex (37) implies that any $\delta_{k<N-1}$-cycle $\phi\in\mathcal{P}^{0,n}_\infty\{k\}_{k+3}$, $k<N$, is a δ_{k+2}-boundary, but not necessarily a δ_{k+1} one.

If $N=1$, the complex $\mathcal{P}^{0,n}_\infty\{1\}_{\leqslant 4}$ (37) restarts the complex (33) associated to a first-stage reducible graded Lagrangian system by virtue of Proposition 10. Therefore, we agree to call δ_N (35) the N-stage Koszul–Tate differential. Its nilpotency implies complete Noether identities (20), first-stage Noether identities (31) and the equalities

$$\sum_{0\leqslant|\Lambda|} \Delta^{r_{k-1},\Lambda}_{r_k} d_\Lambda \left(\sum_{0\leqslant|\Sigma|} \Delta^{r_{k-2},\Sigma}_{r_{k-1}} \overline{c}_{\Sigma r_{k-2}} \right) + \overline{\delta} \left(\sum_{0\leqslant\Sigma,0\leqslant\Xi} h^{(A,\Xi)(r_{k-2},\Sigma)}_{r_k} \overline{s}_{\Xi A} \overline{c}_{\Sigma r_{k-2}} \right) = 0, \tag{38}$$

for $k=2,\ldots,N$. One can think of the equalities (38) as being complete k-stage Noether identities because of their properties which we will justify in the case of $k=N+1$. Accordingly, Δ_{r_k} (36) are said to be the k-stage Noether operators.

Let us consider the $(N+2)$-homology of the complex (37). A generic $(N+2)$-chain $\Phi\in\mathcal{P}^{0,n}_\infty\{N\}_{N+2}$ takes the form

$$\Phi = G + H = \sum_{0\leqslant|\Lambda|} G^{r_N,\Lambda}\overline{c}_{\Lambda r_N}\omega + \sum_{0\leqslant\Sigma,0\leqslant\Xi} (H^{(A,\Xi)(r_{N-1},\Sigma)}\overline{s}_{\Xi A}\overline{c}_{\Sigma r_{N-1}} + \cdots)\omega. \tag{39}$$

Let it be a cycle. The cycle condition $\delta_N\Phi=0$ implies the equality

$$\sum_{0\leqslant|\Lambda|} G^{r_N,\Lambda} d_\Lambda\left(\sum_{0\leqslant|\Sigma|} \Delta^{r_{N-1},\Sigma}_{r_N}\overline{c}_{\Sigma r_{N-1}}\right) + \overline{\delta}\left(\sum_{0\leqslant\Sigma,0\leqslant\Xi} H^{(A,\Xi)(r_{N-1},\Sigma)}\overline{s}_{\Xi A}\overline{c}_{\Sigma r_{N-1}}\right) = 0. \tag{40}$$

One can think of this equality as being the reduction condition on the N-stage Noether operators (36). Conversely, let

$$\Phi = \sum_{0\leqslant|\Lambda|} G^{r_N,\Lambda}\overline{c}_{\Lambda r_N}\omega \in \mathcal{P}^{0,n}_\infty\{N\}_{N+2}$$

be a graded density such that the reduction condition (40) holds. Then this reduction condition can be extended to a cycle one as follows. It is brought into the form

$$\delta_N\left(\sum_{0\leqslant|\Lambda|} G^{r_N,\Lambda}\overline{c}_{\Lambda r_N} + \sum_{0\leqslant\Sigma,0\leqslant\Xi} H^{(A,\Xi)(r_{N-1},\Sigma)}\overline{s}_{\Xi A}\overline{c}_{\Sigma r_{N-1}}\right)$$

$$= -\sum_{0\leqslant|\Lambda|} G^{r_N,\Lambda} d_\Lambda h_{r_N} + \sum_{0\leqslant\Sigma,0\leqslant\Xi} H^{(A,\Xi)(r_{N-1},\Sigma)}\overline{s}_{\Xi A} d_\Sigma \Delta_{r_{N-1}}.$$

A glance at the expression (36) shows that the term on the right-hand side of this equality belongs to $\mathcal{P}^{0,n}_\infty\{N-2\}_{N+1}$. It is a δ_{N-2}-cycle and, consequently, a δ_{N-1}-boundary $\delta_{N-1}\Psi$ in accordance with the $(N+1)$-homology regularity condition. Then the reduction condition (40) is a $\overline{c}_{\Sigma r_{N-1}}$-dependent part of the cycle condition

$$\delta_N\left(\sum_{0\leqslant|\Lambda|} G^{r_N,\Lambda}\overline{c}_{\Lambda r_N} + \sum_{0\leqslant\Sigma,0\leqslant\Xi} H^{(A,\Xi)(r_{N-1},\Sigma)}\overline{s}_{\Xi A}\overline{c}_{\Sigma r_{N-1}} - \Psi\right) = 0,$$

but $\delta_N\Psi$ does not make a contribution to this reduction condition.

Being a cycle condition, the reduction condition (40) is trivial either if a cycle Φ (39) is a δ_N-boundary or its summand G is $\overline{\delta}$-exact, i.e., it is a boundary, too, as we have stated above. Then Definition 7 can be generalized as follows.

Definition 12: A degenerate graded Lagrangian system is said to be $(N+1)$-stage reducible if there exist nontrivial reduction conditions (40), called the $(N+1)$-stage Noether identities.

Theorem 13: (i) The $(N+1)$-stage Noether identities can be identified to nontrivial elements of the homology $H_{N+2}(\delta_N)$ of the complex (37) iff this homology obeys the $(N+2)$-homology regularity condition. (ii) If the homology $H_{N+2}(\delta_N)$ is finitely generated as defined below, the complex (37) admits an $(N+2)$-exact extension.

Proof: (i) The $(N+2)$-homology regularity condition implies that any δ_{N-1}-cycle $\Phi\in\mathcal{P}^{0,n}_\infty\{N-1\}_{N+2}\subset\mathcal{P}^{0,n}_\infty\{N\}_{N+2}$ is a δ_N-boundary. Therefore, if Φ (39) is a representative of a nontrivial element of $H_{N+2}(\delta_N)$, its summand G linear in $\overline{c}_{\Lambda r_N}$ does not vanish. Moreover, it is not a $\overline{\delta}$-boundary. Indeed, if $\Phi=\overline{\delta}\Psi$, then

$$\Phi = \delta_N\Psi + (\overline{\delta} - \delta_N)\Psi + H. \tag{41}$$

The cycle condition takes the form

$$\delta_N\Phi = \delta_{N-1}((\overline{\delta} - \delta_N)\Psi + H) = 0.$$

Hence, $(\overline{\delta}-\delta_N)\Psi+H$ is δ_N-exact since any δ_{N-1}-cycle $\phi\in\mathcal{P}^{0,n}_\infty\{N-1\}_{N+2}$ is a δ_N-boundary. Consequently, Φ (41) is a boundary. If the $(N+2)$-homology regularity condition does not hold, trivial reduction conditions (40) also come from nontrivial elements of the homology $H_{N+2}(\delta_N)$. (ii) Let the $(N+1)$-stage Noether identities be finitely generated. Namely, there exist elements $\Delta_{(N+1)}$

$\in H_{N+2}(\delta_N)$ making up a $\mathbb{Z}_2$-graded projective $C^\infty(X)$-module $\mathcal{C}_{(N+1)}$ of finite rank which is isomorphic to the module of sections of the product $\overline{V}^*_{N+1}\underset{X}{\times}\overline{E}^*_{N+1}$ of the density-duals of some vector bundles $V_{N+1}\to X$ and $E_{N+1}\to X$. Let $\{\Delta_{r_{N+1}}\}$ be local bases for this $C^\infty(X)$-module. Then any element $\Phi\in H_{N+2}(\delta_N)$ factorizes

$$\Phi=\sum_{0\leqslant|\Xi|}\Phi^{r_{N+1},\Xi}d_\Xi\Delta_{r_{N+1}}\omega,\quad \Phi^{r_{N+1},\Xi}\in\mathcal{S}^0_\infty[F;Y], \tag{42}$$

$$\Delta_{r_{N+1}}=G_{r_{N+1}}+h_{r_{N+1}}=\sum_{0\leqslant|\Lambda|}\Delta^{r_N,\Lambda}_{r_{N+1}}\overline{c}_{\Lambda r_N}+h_{r_{N+1}}, \tag{43}$$

via elements of $\mathcal{C}_{(N+1)}$. Clearly, this factorization is independent of specification of local bases $\{\Delta_{r_{N+1}}\}$. Let us extend the BGDA $\mathcal{P}^*_\infty\{N\}$ (34) to the BGDA $\mathcal{P}^*_\infty\{N+1\}$ possessing local bases

$$\{s^A,\overline{s}_A,\overline{c}_r,\overline{c}_{r_1},\ldots,\overline{c}_{r_N},\overline{c}_{r_{N+1}}\},\quad \mathrm{Ant}[\overline{c}_{r_{N+1}}]=N+3,\quad [\overline{c}_{r_{N+1}}]=([\Delta_{r_{N+1}}]+1)\mathrm{mod}\,2.$$

It is provided with the nilpotent graded derivation

$$\delta_{N+1}=\delta_N+\overleftarrow{\partial}{}^{r_{N+1}}\Delta_{r_{N+1}} \tag{44}$$

of antifield number -1. With this graded derivation, the module $\mathcal{P}^{0,n}_\infty\{N+1\}_{\leqslant N+4}$ of graded densities of antifield number $\mathrm{Ant}[\phi]\leqslant N+4$ is split into the chain complex,

$$0\leftarrow \mathrm{Im}\,\overline{\delta}\overset{\overline{\delta}}{\leftarrow}\mathcal{P}^{0,n}_\infty[\overline{Y}^*;F;Y;\overline{F}^*]_1\overset{\delta_0}{\leftarrow}\mathcal{P}^{0,n}_\infty\{0\}_2\overset{\delta_1}{\leftarrow}\mathcal{P}^{0,n}_\infty\{1\}_3\cdots$$

$$\overset{\delta_{N-1}}{\leftarrow}\mathcal{P}^{0,n}_\infty\{N-1\}_{N+1}\overset{\delta_N}{\leftarrow}\mathcal{P}^{0,n}_\infty\{N\}_{N+2}\overset{\delta_{N+1}}{\leftarrow}\mathcal{P}^{0,n}_\infty\{N+1\}_{N+3}\overset{\delta_{N+1}}{\leftarrow}\mathcal{P}^{0,n}_\infty\{N+1\}_{N+4}. \tag{45}$$

It is readily observed that this complex is $(N+2)$-exact. In this case, the $(N+1)$-stage Noether identities (40) come from the complete $(N+1)$-stage Noether identities

$$\sum_{0\leqslant|\Lambda|}\Delta^{r_N,\Lambda}_{r_{N+1}}d_\Lambda\Delta_r\omega+\overline{\delta}h_{r_{N+1}}\omega=0,$$

which are reproduced as the nilpotency conditions of the graded derivation (44).

The iteration procedure based on Theorem 13 can be prolonged up to an integer $N_{\max}$ when the $N_{\max}$-stage Noether identities are irreducible, i.e., the homology $H_{N_{\max}+2}(\delta_{N_{\max}})$ is trivial. This iteration procedure may also be infinite. It results in the manifested exact Koszul–Tate complex with the Koszul–Tate boundary operator whose nilpotency conditions reproduce all Noether and higher Noether identities of an original Lagrangian system. □

V. EXAMPLE

Let us consider a fiber bundle

$$Y=\mathbb{R}\underset{X}{\times}\overset{n-1}{\wedge}T^*X, \tag{46}$$

coordinated by $(x^\lambda,A,B_{\mu_1\cdots\mu_{n-1}})$. The corresponding BGDA is $\mathcal{S}^*_\infty[Y]=\mathcal{O}^*_\infty Y$. There is the canonical $(n-1)$-form

$$B = \frac{1}{(n+1)!} B_{\mu_1 \cdots \mu_{n-1}} \, \mathrm{d}x^{\mu_1} \wedge \cdots \wedge \mathrm{d}x^{\mu_{n-1}} \in \mathcal{O}^*_\infty Y$$

on Y (46). A Lagrangian of topological BF theory in question reads

$$L_{\mathrm{BF}} = \frac{1}{n} \mathrm{Ad}_H B. \tag{47}$$

The corresponding Euler–Lagrange operator (9) takes the form

$$\begin{gathered} \delta L = \mathrm{d}A \wedge \mathcal{E}\omega + \mathrm{d}B_{\mu_1 \cdots \mu_{n-1}} \wedge \mathcal{E}^{\mu_1 \cdots \mu_{n-1}} \omega, \\ \mathcal{E} = \epsilon^{\mu\mu_1 \cdots \mu_{n-1}} d_\mu B_{\mu_1 \cdots \mu_{n-1}}, \quad \mathcal{E}^{\mu_1 \cdots \mu_{n-1}} = -\epsilon^{\mu\mu_1 \cdots \mu_{n-1}} d_\mu A, \end{gathered} \tag{48}$$

where ϵ is the Levi–Civita symbol.

Let us extend the BGDA $\mathcal{O}^*_\infty Y$ to the BGDA $\mathcal{P}^*_\infty[\overline{Y}^*; Y]$ where

$$VY = Y \underset{X}{\times} Y, \quad \overline{Y}^* = (\mathbb{R} \underset{X}{\times} \overset{n-1}{\wedge} TX) \underset{X}{\otimes} \overset{n}{\wedge} T^*X.$$

This BGDA possesses the local bases $\{A, B_{\mu_1 \cdots \mu_{n-1}}, \overline{s}, \overline{s}^{\mu_1 \cdots \mu_{n-1}}\}$, where $\overline{s}, \overline{s}^{\mu_1 \cdots \mu_{n-1}}$ are odd of antifield number 1. With the nilpotent Koszul–Tate differential

$$\overline{\delta} = \frac{\overleftarrow{\partial}}{\partial \overline{s}} \mathcal{E} + \frac{\overleftarrow{\partial}}{\partial \overline{s}^{\mu_1 \cdots \mu_{n-1}}} \mathcal{E}^{\mu_1 \cdots \mu_{n-1}},$$

we have the complex (14),

$$0 \leftarrow \mathrm{Im}\, \overline{\delta} \overset{\overline{\delta}}{\leftarrow} \mathcal{P}^{0,n}_\infty[\overline{Y}^*; Y]_1 \overset{\overline{\delta}}{\leftarrow} \mathcal{P}^{0,n}_\infty[\overline{Y}^*; Y]_2.$$

A generic one-chain reads

$$\Phi = \sum_{0 \leqslant |\Lambda|} (\Phi^\Lambda \overline{s}_\Lambda + \Phi^\Lambda_{\mu_1 \cdots \mu_{n-1}} \overline{s}^{\mu_1 \cdots \mu_{n-1}}_\Lambda) \omega,$$

and the cycle condition $\overline{\delta}\Phi = 0$ takes the form

$$\Phi^\Lambda \mathcal{E}_\Lambda + \Phi^\Lambda_{\mu_1 \cdots \mu_{n-1}} \mathcal{E}^{\mu_1 \cdots \mu_{n-1}}_\Lambda = 0. \tag{49}$$

If Φ^Λ and $\Phi^\Lambda_{\mu_1 \cdots \mu_{n-1}}$ are independent of the variational derivatives (48) (i.e., Φ is a nontrivial cycle), the equality (49) is split into the following:

$$\Phi^\Lambda \mathcal{E}_\Lambda = 0, \tag{50}$$

$$\Phi^\Lambda_{\mu_1 \cdots \mu_{n-1}} \mathcal{E}^{\mu_1 \cdots \mu_{n-1}}_\Lambda = 0. \tag{51}$$

The equality (50) holds iff $\Phi^\Lambda = 0$, i.e., there is no Noether identities for $\mathcal{E}$. The equality (51) is satisfied iff

$$\Phi^{\lambda_1 \cdots \lambda_k}_{\mu_1 \cdots \mu_{n-1}} \epsilon^{\mu\mu_1 \cdots \mu_{n-1}} = -\Phi^{\mu\lambda_2 \cdots \lambda_k}_{\mu_1 \cdots \mu_{n-1}} \epsilon^{\lambda_1 \mu_1 \cdots \mu_{n-1}}.$$

It follows that Φ factorizes as

$$\Phi = \sum_{0\leqslant|\Xi|} G^{\Xi}_{\nu_2\cdots\nu_{n-1}} d_{\Xi}\Delta^{\nu_2\cdots\nu_{n-1}}\omega$$

via local graded densities

$$\Delta^{\nu_2\cdots\nu_{n-1}} = \Delta^{\nu_2\cdots\nu_{n-1},\lambda}_{\alpha_1\cdots\alpha_{n-1}}\overline{s}^{\alpha_1\cdots\alpha_{n-1}}_{\lambda} = \delta^{\lambda}_{\alpha_1}\delta^{\nu_2}_{\alpha_2}\cdots\delta^{\nu_{n-1}}_{\alpha_{n-1}}\overline{s}^{\alpha_1\cdots\alpha_{n-1}}_{\lambda} = d_{\nu_1}\overline{s}^{\nu_1\nu_2\cdots\nu_{n-1}}, \tag{52}$$

which provide the complete Noether identities[1]

$$d_{\nu_1}\mathcal{E}^{\nu_1\nu_2\cdots\nu_{n-1}} = 0. \tag{53}$$

The local graded densities (52) form the bases of a projective $C^{\infty}(X)$-module of finite rank which is isomorphic to the module of sections of the vector bundle

$$\overline{V}^* = \wedge^{n-2} TX \underset{X}{\otimes} \wedge^{n} T^*X, \quad V = \wedge^{n-2} T^*X.$$

Therefore, let us extend the BGDA $\mathcal{P}^*_{\infty}[\overline{Y}^*;Y]$ to the BGDA $\mathcal{P}^*_{\infty}\{0\}=\mathcal{P}^*_{\infty}[\overline{Y}^*;Y;V]$ possessing the local bases

$$\{A, B_{\mu_1\cdots\mu_{n-1}}, \overline{s}, \overline{s}^{\mu_1\cdots\mu_{n-1}}, \overline{c}^{\mu_2\cdots\mu_{n-1}}\},$$

where $\overline{c}^{\mu_2\cdots\mu_{n-1}}$ are even of antifield number 2. Let

$$\delta_0 = \overline{\delta} + \frac{\overleftarrow{\partial}}{\partial\overline{c}^{\mu_2\cdots\mu_{n-1}}}\Delta^{\mu_2\cdots\mu_{n-1}}$$

be its nilpotent graded derivation. Its nilpotency is equivalent to the Noether identities (53). Then we have the one-exact complex

$$0 \leftarrow \mathrm{Im}\,\overline{\delta} \overset{\overline{\delta}}{\leftarrow} \mathcal{P}^{0,n}_{\infty}[\overline{Y}^*;Y]_1 \overset{\delta_0}{\leftarrow} \mathcal{P}^{0,n}_{\infty}\{0\}_2 \overset{\delta_0}{\leftarrow} \mathcal{P}^{0,n}_{\infty}\{0\}_3,$$

and so on. Iterating the arguments we come to the following $(N+1)$-exact complex (37) for $N \leqslant n-3$.

Let us consider the vector bundles

$$V_k = \wedge^{n-k-2} T^*X, \quad k = 1, \ldots, N,$$

and the corresponding BGDA

$$\mathcal{P}^*_{\infty}\{N\} = \mathcal{P}^*_{\infty}[\cdots V_3 V_1 \overline{Y}^*; Y; VV_2V_4\cdots],$$

possessing the local bases

$$\{A, B_{\mu_1\cdots\mu_{n-1}}, \overline{s}, \overline{s}^{\mu_1\cdots\mu_{n-1}}, \overline{c}^{\mu_2\cdots\mu_{n-1}}, \ldots, \overline{c}^{\mu_{N+2}\cdots\mu_{n-1}}\},$$

$$[\overline{c}^{\mu_{k+2}\cdots\mu_{n-1}}] = (k+1) \bmod 2, \quad \mathrm{Ant}[\overline{c}^{\mu_{k+2}\cdots\mu_{n-1}}] = k+3.$$

It is provided with the nilpotent graded derivation

$$\delta_N = \delta_0 + \sum_{1\leqslant k\leqslant N} \frac{\overleftarrow{\partial}}{\partial \overline{c}^{\mu_{k+2}\cdots\mu_{n-1}}} \Delta^{\mu_{k+2}\cdots\mu_{n-1}},$$
$$\Delta^{\mu_{k+2}\cdots\mu_{n-1}} = d_{\mu_{k+1}} c^{\mu_{k+1}\mu_{k+2}\cdots\mu_{n-1}}, \tag{54}$$

of antifield number -1. The nilpotency results from the Noether identities (53) and the equalities

$$d_{\mu_{k+2}} \Delta^{\mu_{k+2}\cdots\mu_{n-1}} = 0, \quad k = 0, \ldots, N, \tag{55}$$

which are k-stage Noether identities.[1] Then the above-mentioned $(N+1)$-exact complex is

$$0 \leftarrow \operatorname{Im} \overline{\delta} \overset{\overline{\delta}}{\leftarrow} \mathcal{P}^{0,n}_\infty[\overline{Y}^*; Y]_1 \overset{\delta_0}{\leftarrow} \mathcal{P}^{0,n}_\infty\{0\}_2 \overset{\delta_1}{\leftarrow} \mathcal{P}^{0,n}_\infty\{1\}_3 \cdots$$
$$\overset{\delta_{N-1}}{\leftarrow} \mathcal{P}^{0,n}_\infty\{N-1\}_{N+1} \overset{\delta_N}{\leftarrow} \mathcal{P}^{0,n}_\infty\{N\}_{N+2} \overset{\delta_N}{\leftarrow} \mathcal{P}^{0,n}_\infty\{N\}_{N+3}. \tag{56}$$

It obeys the $(N+2)$-homology regularity condition as follows.

Lemma 14: Any $(N+2)$-cycle $\Phi \in \mathcal{P}^{0,n}_\infty\{N-1\}_{N+2}$ up to a δ_{N-1}-boundary takes the form

$$\Phi = \sum_{k_1+\cdots+k_i+3i=N+2} \sum_{0\leqslant|\Lambda_1|,\ldots,|\Lambda_i|} G^{\Lambda_1\cdots\Lambda_i}_{\mu^1_{k_1+2}\cdots\mu^1_{n-1};\cdots;\mu^i_{k_i+2}\cdots\mu^i_{n-1}}$$
$$d_{\Lambda_1}\Delta^{\mu^1_{k_1+2}\cdots\mu^1_{n-1}} \cdots d_{\Lambda_i}\Delta^{\mu^i_{k_i+2}\cdots\mu^i_{n-1}}\omega, \quad k = -1,0,1,\ldots,N, \tag{57}$$

where $k=-1$ stands for

$$\overline{c}^{\mu_1\cdots\mu_{n-1}} = \overline{s}^{\mu_1\cdots\mu_{n-1}}, \quad \Delta^{\mu_1\cdots\mu_{n-1}} = \mathcal{E}^{\mu_1\cdots\mu_{n-1}}.$$

It follows that Φ is a δ_N-boundary.

Proof: Let us choose some basis element $\overline{c}^{\mu_{k+2}\cdots\mu_{n-1}}$ and denote it simply by $\overline{c}$. Let Φ contain a summand $\phi_1\overline{c}$, linear in $\overline{c}$. Then the cycle condition reads

$$\delta_{N-1}\Phi = \delta_{N-1}(\Phi - \phi_1\overline{c}) + (-1)^{[\overline{c}]}\delta_{N-1}(\phi_1)\overline{c} + \phi\Delta = 0, \quad \Delta = \delta_{N-1}\overline{c}.$$

It follows that Φ contains a summand $\psi\Delta$ such that

$$(-1)^{[\overline{c}]+1}\delta_{N-1}(\psi)\Delta + \phi\Delta = 0.$$

This equality implies the relation

$$\phi_1 = (-1)^{[\overline{c}]+1}\delta_{N-1}(\psi) \tag{58}$$

because the reduction conditions (55) involve total derivatives of Δ, but not Δ. Hence,

$$\Phi = \Phi' + \delta_{N-1}(\psi\overline{c}),$$

where Φ' contains no term linear in $\overline{c}$. Furthermore, let $\overline{c}$ be even and Φ has a summand $\Sigma\phi_r\overline{c}^r$ polynomial in $\overline{c}$. Then the cycle condition leads to the equalities

$$\phi_r\Delta = -\delta_{N-1}\phi_{r-1}, \quad r \geqslant 2.$$

Since ϕ_1 (58) is δ_{N-1}-exact, then $\phi_2=0$ and, consequently, $\phi_{r>2}=0$. Thus, a cycle Φ up to a δ_{N-1}-boundary contains no term polynomial in $\overline{c}$. It reads

$$\Phi = \sum_{k_1+\cdots+k_i+3i=N+2} \sum_{0<|\Lambda_1|,\ldots,|\Lambda_i|} G^{\Lambda_1\cdots\Lambda_i}_{\mu^1_{k_1+2}\cdots\mu^1_{n-1};\cdots;\mu^i_{k_i+2}\cdots\mu^i_{n-1}} \overline{c}^{\mu^1_{k_1+2}\cdots\mu^1_{n-1}}_{\Lambda_1} \cdots \overline{c}^{\mu^i_{k_i+2}\cdots\mu^i_{n-1}}_{\Lambda_i} \omega. \tag{59}$$

However, the terms polynomial in $\overline{c}$ may appear under general covariant transformations

$$\overline{c}'^{\,\nu_{k+2}\cdots\nu_{n-1}} = \det\left(\frac{\partial x^\alpha}{\partial x'^\beta}\right) \frac{\partial x'^{\,\nu_{k+2}}}{\partial x^{\mu_{k+2}}} \cdots \frac{\partial x'^{\,\nu_{n-1}}}{\partial x^{\mu_{n-1}}} \overline{c}^{\mu_{k+2}\cdots\mu_{n-1}}$$

of a chain Φ (59). In particular, Φ contains the summand

$$\sum_{k_1+\cdots+k_i+3i=N+2} F_{\nu^1_{k_1+2}\cdots\nu^1_{n-1};\cdots;\nu^i_{k_i+2}\cdots\nu^i_{n-1}} \overline{c}'^{\,\nu^1_{k_1+2}\cdots\nu^1_{n-1}} \cdots \overline{c}'^{\,\nu^i_{k_i+2}\cdots\nu^i_{n-1}},$$

which must vanish if Φ is a cycle. This takes place only if Φ factorizes through the graded densities $\Delta^{\mu_{k+2}\cdots\mu_{n-1}}$ (54) in accordance with the expression (57).

Following the proof of Lemma 14, one can show that any $(N+2)$-cycle $\Phi \in \mathcal{P}^{0,n}_\infty\{N\}_{N+2}$ up to a boundary takes the form

$$\Phi = \sum_{0\leqslant|\Lambda|} G^\Lambda_{\mu_{N+2}\cdots\mu_{n-1}} \Delta^{\mu_{N+2}\cdots\mu_{n-1}} \omega, \tag{60}$$

i.e., the homology $H_2(\delta_N)$ of the complex (56) is finitely generated by the cycles $\Delta^{\mu_{N+2}\cdots\mu_{n-1}}$. Thus, the complex (56) admits the $(N+2)$-exact extension (45).

The iteration procedure is prolonged until $N=n-3$. Given the BGDA $\mathcal{P}^*\{n-3\}$, the corresponding $(n-2)$-exact complex (56) has the following $(n-1)$-exact extension. Let us consider the BGDA $\mathcal{P}^*\{n-2\}$, where $V_{n-2}=X\times\mathbb{R}$. It possesses the local bases

$$\{A, B_{\mu_1\cdots\mu_{n-1}}, \overline{s}, \overline{s}^{\mu_1\cdots\mu_{n-1}}, \overline{c}^{\mu_2\cdots\mu_{n-1}}, \ldots, \overline{c}^{\mu_{n-1}}, \overline{c}\},$$

where $[\overline{c}]=(n-1) \bmod 2$ and $\mathrm{Ant}[\overline{c}]=n+1$. It is provided with the nilpotent graded derivation

$$\delta_{n-2} = \delta_0 + \sum_{1\leqslant k\leqslant n-3} \frac{\overleftarrow{\partial}}{\partial \overline{c}^{\mu_{k+2}\cdots\mu_{n-1}}} \Delta^{\mu_{k+2}\cdots\mu_{n-1}} + \frac{\overleftarrow{\partial}}{\partial \overline{c}} \Delta, \quad \Delta = d_{\mu_{n-1}} \overline{c}^{\mu_{n-1}}. \tag{61}$$

Then the above-mentioned $(n-1)$-exact complex is

$$\begin{aligned} 0 \leftarrow \mathrm{Im}\,\overline{\delta} \overset{\overline{\delta}}{\leftarrow} \mathcal{P}^{0,n}_\infty[\overline{Y}^*; Y]_1 \overset{\delta_0}{\leftarrow} \mathcal{P}^{0,n}_\infty\{0\}_2 \overset{\delta_1}{\leftarrow} \mathcal{P}^{0,n}_\infty\{1\}_3 \cdots \\ \overset{\delta_{n-3}}{\leftarrow} \mathcal{P}^{0,n}_\infty\{n-3\}_{n-1} \overset{\delta_{n-2}}{\leftarrow} \mathcal{P}^{0,n}_\infty\{n-2\}_n \overset{\delta_{n-2}}{\leftarrow} \mathcal{P}^{0,n}_\infty\{n-2\}_{n+1}. \end{aligned} \tag{62}$$

Following the proof of Lemma 14, one can show that the n-homology regularity condition is satisfied. Therefore, any n-cycle up to a δ_{n-3}-boundary takes the form

$$\Phi = \sum_{0\leqslant|\Lambda|} G^\Lambda \overline{c}_\Lambda.$$

The cycle condition reads

$$\delta_{n-2}\Phi = \sum_{0\leqslant|\Lambda|} G^\Lambda d_\Lambda \Delta = 0.$$

It follows that $G^\Lambda=0$ and, consequently, $\Phi=0$. Thus, the n-homology of the complex (62) is trivial, and this complex is exact. It is a desired Koszul–Tate complex of a Lagrangian system in question. The nilpotency conditions of its boundary operator (61) restarts all the Noether identities of this Lagrangian system. □

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Relativistic harmonic oscillator

Zhi-Feng Li[a)]
Department of Physics, Chongqing University, 400044 Chongqing, China

Jin-Jin Liu
Department of Modern Physics, University of Science and Technology of China, Hefei, China

Wolfgang Lucha[b)]
Institute for High Energy Physics, Austrian Academy of Sciences, Nikolsdorfergasse 18, A-1050 Vienna, Austria

Wen-Gan Ma
Department of Modern Physics, University of Science and Technology of China, Hefei, China

Franz F. Schöberl[c)]
Institute for Theoretical Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria

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We study the semirelativistic Hamiltonian operator composed of the relativistic kinetic energy and a static harmonic-oscillator potential in three spatial dimensions and construct, for bound states with vanishing orbital angular momentum, its eigenfunctions in "compact form," i.e., as power series, with expansion coefficients determined by an explicitly given recurrence relation. The corresponding eigenvalues are fixed by the requirement of normalizability of the solutions. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2054648]

I. INTRODUCTION: RELATIVISTIC HARMONIC-OSCILLATOR PROBLEM

The simplest and perhaps most straightforward generalization of the Schrödinger operators of standard nonrelativistic quantum theory towards the inclusion of relativistic kinematics leads to Hamiltonians H that involve the relativistic kinetic energy, or relativistically covariant form of the free energy, of a particle of mass m and momentum $\mathbf{p}$ given by the square-root operator

$$T(p) \equiv \sqrt{p^2 + m^2}, \quad p \equiv |\mathbf{p}|,$$

and a coordinate-dependent static interaction potential $V(\mathbf{x})$. In the one-body case, they read

$$H = \sqrt{p^2 + m^2} + V(\mathbf{x}). \tag{1}$$

The eigenvalue equation of this Hamiltonian is usually called the "spinless Salpeter equation." It may be regarded as a well-defined approximation to the Bethe-Salpeter formalism[1] for the description of bound states within relativistic quantum field theories, obtained when assuming that all bound-state constituents interact *instantaneously* and propagate like *free* particles.[2] Among others, it yields semirelativistic descriptions of hadrons as bound states of quarks.[3,4]

In general, the above semirelativistic Hamiltonian H is, unfortunately, a *nonlocal* operator, either the relativistic kinetic energy, $T(p)$, *in configuration space* or, in general, the interaction

[a)]Present address: Institute for Theoretical Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria.
[b)]Electronic mail: wolfgang.lucha@oeaw.ac.at
[c)]Electronic mail: franz.schoeberl@univie.ac.at

potential *in momentum space* is a nonlocal operator. Because of the nonlocality it is somewhat difficult to obtain rigorous *analytical* statements about the solutions of its eigenvalue equation. Thus sophisticated methods have been developed to extract information about these solutions; for details and comparisons of the various approaches, consult, for example, Refs. 5–10.

Analytical or, at least, semianalytical (we regard a bound on some eigenvalue of a given self-adjoint operator as *semianalytical* if it can be derived by the—in general, numerical—optimization of an analytically known expression over a single real variable) expressions for both upper and lower bounds on the eigenvalues of some self-adjoint operator may be found by combining the minimum-maximum principle[11–13] and appropriate operator inequalities.[14–18] The outcome of this procedure is sometimes called the "spectral comparison theorem." In Sec. III below, we will use this kind of bounds in order to estimate the accuracy of our findings for the eigenvalues of the operator (1). Accordingly, we recall in the Appendix the proof of the "translation" of some inequality satisfied by two operators into the corresponding relations between their discrete eigenvalues, by briefly sketching all basic assumptions and the line of argument. A very systematic path for obtaining such operator inequalities is provided by rather simple geometrical considerations summarized under the notion "envelope theory."[19–24] These envelope techniques may be generalized to systems composed of arbitrary numbers of relativistically moving interacting particles.[25–27] For particular potentials V, semianalytical lower bounds on the ground-state energy eigenvalue of the semirelativistic Hamiltonian (1), and hence on the entire spectrum of H, can be found by the appropriate generalization of the local-energy theorem[13,28–30] to our case of relativistic kinematics,[23,31] or by applying the optimized (Beckner-Brascamp-Lieb) version of Young's inequality for convolutions to some integral formulation of the spinless Salpeter equation.[32]

Purely numerical solutions of the spinless Salpeter equation may be computed in numerous ways. The semirelativistic Hamiltonian H can be approximated by some effective Hamiltonian which is of nonrelativistic shape but uses parameters that depend on expectation values of the momenta.[33,34] Upper bounds of, in principle, arbitrarily high precision on the eigenvalues of a self-adjoint operator can be found[18,35–39] with the help of the Rayleigh-Ritz (variational) technique as immediate consequence of the minimum-maximum theorem.[11–13] The spinless Salpeter equation may also be converted into an equivalent matrix eigenvalue problem.[40–45]

A particular role for H is played by the spherically symmetric harmonic-oscillator potential

$$V(\mathbf{x}) = ar^2, \quad r \equiv |\mathbf{x}|, \quad a > 0,$$

this potential defines the "relativistic harmonic-oscillator problem," posed by the Hamiltonian

$$H = \sqrt{p^2 + m^2} + ar^2. \tag{2}$$

The eigenvalue equation of H, for eigenstates $|\psi\rangle$, $H|\psi\rangle = E|\psi\rangle$, involves only one parameter, upon factorizing off some overall energy scale $a^{1/3}$ by performing the canonical transformation

$$r \to \frac{r}{a^{1/3}}, \quad p \to a^{1/3} p$$

and rescaling both mass m and eigenvalue E according to $m = a^{1/3}\mu$ and $E = a^{1/3}\varepsilon$, it reads

$$(\sqrt{p^2 + \mu^2} + r^2)|\psi\rangle = \varepsilon|\psi\rangle.$$

In momentum-space representation this eigenvalue equation reduces to a Schrödinger problem,

$$[-\Delta_p + V(p)]\psi(p) = \varepsilon\psi(p), \tag{3}$$

with an interaction potential reminiscent of the square root of the relativistic kinetic energy,

$$V(p) \equiv \sqrt{p^2 + \mu^2}.$$

We would like to take advantage of this facet of the relativistic harmonic-oscillator problem in order to derive for its bound-state eigenfunctions, in this analysis, a compact expression and to move thereby beyond only numerically calculated exact solutions without having to rely on perturbation theory, maybe paving the way for the eventual construction of analytic solutions.

II. ANALYTICAL SOLUTIONS FOR BOUND-STATE EIGENFUNCTIONS

We exploit the fact that, in contrast to the general case, for a harmonic-oscillator potential (as, with due care, for any potential of the form $V \propto r^{2n}$, $n=1, 2, 3, \ldots$) the eigenvalue equation of the Hamiltonian H is an ordinary differential equation, parametrized by μ and its eigenvalue ε.

Focusing on the ground state or purely radial excitations, let us introduce, for eigenstates with vanishing relative orbital angular momentum ℓ, the reduced radial wave function $y(p)$ by

$$y(p) \equiv \sqrt{4\pi} p \psi(p) \quad (\ell = 0),$$

which is, of course, subject to the normalization condition

$$\int_0^\infty dp |y(p)|^2 = 1.$$

In accordance with Eq. (3) the reduced radial wave function satisfies a reduced radial equation,

$$\frac{\mathrm{d}^2 y}{\mathrm{d}p^2}(p) = [V(p) - \varepsilon] y(p). \tag{4}$$

From its definition, this *reduced* radial wave function $y(p)$ must vanish at the origin, $y(0)=0$. Moreover, the analysis of the *normalizable* solutions of the eigenvalue equation (4) reveals that $y(p)$ behaves like p for small p, that is, for $p \ll 1$; hence, its derivative with respect to p at the point $p=0$ is a *nonvanishing* constant, which may be absorbed into the overall normalization,

$$\frac{\mathrm{d}y}{\mathrm{d}p}(0) = 1.$$

We construct all solutions of Eq. (4) in the form of the Taylor-series expansions by using the ansatz

$$y(p) = \sum_{n=0}^{\infty} c_n \frac{p^n}{n!}$$

with the expansion coefficients

$$c_n \equiv \frac{\mathrm{d}^n y}{\mathrm{d}p^n}(0), \quad n = 0,1,2,\ldots .$$

The solution of the eigenvalue equation (4) is then clearly tantamount to the determination of the expansion coefficients c_n. The first three of these expansion coefficients are known trivially,

$$c_0 = y(0) = 0,$$

$$c_1 = \frac{\mathrm{d}y}{\mathrm{d}p}(0) = 1,$$

$$c_2 = \frac{\mathrm{d}^2 y}{\mathrm{d}p^2}(0) = [(V-\varepsilon)y](0) = 0.$$

[For the sake of notational simplicity, we suppress, in accordance with our above remark, in the following that normalization factor of $y(p)$ which guarantees its unity norm and assume $y(p)$ to be normalized such that the value of the first nonvanishing expansion coefficient is one, $c_1=1$.] Upon insertion of the eigenvalue equation (4) followed by the application of Leibniz's theorem, the nontrivial expansion coefficients c_n, $n \geqslant 3$, may be shown to satisfy the recurrence relation

$$\begin{aligned} c_{n+2} &= \frac{\mathrm{d}^{n+2} y}{\mathrm{d}p^{n+2}}(0) = \frac{\mathrm{d}^n}{\mathrm{d}p^n}\left[\frac{\mathrm{d}^2 y}{\mathrm{d}p^2}\right](0) = \frac{\mathrm{d}^n[(V-\varepsilon)y]}{\mathrm{d}p^n}(0) = \sum_{k=0}^{n}\binom{n}{k}\left[\frac{\mathrm{d}^k(V-\varepsilon)}{\mathrm{d}p^k}\frac{\mathrm{d}^{n-k}y}{\mathrm{d}p^{n-k}}\right](0) \\ &= (\mu-\varepsilon)c_n + \sum_{k=1}^{n}\binom{n}{k}\frac{\mathrm{d}^k V}{\mathrm{d}p^k}(0)c_{n-k} = (\mu-\varepsilon)c_n + \sum_{k=1}^{n}\binom{n}{k}\mu^{1-k}d_k c_{n-k}, \quad n = 1,2,3,\ldots . \end{aligned} \tag{5}$$

Here, for the last step, we abbreviated the kth derivative of the potential V by a coefficient d_k,

$$d_k \equiv \mu^{k-1}\frac{\mathrm{d}^k V}{\mathrm{d}p^k}(0) = \frac{\mathrm{d}^k\sqrt{x^2+1}}{\mathrm{d}x^k}(0), \quad x \equiv \frac{p}{\mu}, \quad \mu > 0, \quad k = 0,1,2,\ldots .$$

In the case $\mu=m=0$, the solutions involve Airy's function $\mathrm{Ai}(z)$; cf., e.g., Refs. 18,23,33 and 34. According to the above definition, we have $d_0=1$. Furthermore, by inspection of the function $f(x)=\sqrt{x^2+1}$, it is easy to convince oneself that all odd derivatives of $f(x)$ vanish at $x=0$,

$$d_{2k+1} = 0 \quad \text{for all } k = 0,1,2,\ldots , \tag{6}$$

whereas all even derivatives of $f(x)$ at $x=0$ necessarily satisfy the (simple) recurrence relation

$$d_{2k+2} = (1-4k^2)d_{2k}, \quad k = 0,1,2,\ldots .$$

By induction, the solution of this recurrence relation for the nonvanishing coefficients d_{2k} reads

$$d_{2k} = (-1)^{k-1}(2k-1)\left[\frac{(2k-2)!}{2^{k-1}(k-1)!}\right]^2, \quad k = 1,2,3,\ldots . \tag{7}$$

Taking into account the observation (6), we obtain $c_3=\mu-\varepsilon$ and, for the coefficients c_n, $n \geqslant 4$,

$$c_{n+2} = (\mu-\varepsilon)c_n + \sum_{k=1}^{[n/2]}\binom{n}{2k}\mu^{1-2k}d_{2k}c_{n-2k}, \quad n = 2,3,4,\ldots ,$$

where

$$\left[\frac{n}{2}\right] \equiv \begin{cases} \frac{n}{2} & \text{for } n \text{ even, } n = 2,4,6,\ldots , \\ \frac{n-1}{2} & \text{for } n \text{ odd, } n = 3,5,7,\ldots . \end{cases}$$

Thus the recurrence relation (5) for all expansion coefficients c_n decomposes into one involving only the even coefficients c_{2n}, $n=2, 3, 4, \ldots$, and one involving only the odd coefficients c_{2n+1}, $n=2, 3, 4, \ldots$; recalling $c_0=0$ and $c_2=0$, we conclude that all the *even* coefficients c_n vanish,

$$c_{2n} = 0 \quad \text{for all } n = 0,1,2,\ldots .$$

With the result (7), the recurrence relation for the (nonvanishing) *odd* coefficients finally reads

$$c_{2n+3} = (\mu - \varepsilon)c_{2n+1} + \sum_{k=1}^{n} \binom{2n+1}{2k} \mu^{1-2k} d_{2k} c_{2n-2k+1} = (\mu - \varepsilon)c_{2n+1}$$

$$+ \sum_{k=1}^{n} \binom{2n+1}{2k} c_{2n-2k+1} \mu^{1-2k} (-1)^{k-1} (2k-1) \left[\frac{(2k-2)!}{2^{k-1}(k-1)!} \right]^2, \quad n = 1,2,3,\ldots . \tag{8}$$

In summary, upon constructing the relevant expansion coefficients according to this recurrence relation the analytical expressions for all reduced radial wave functions (of $\ell = 0$ bound states) $y(p)$ of the relativistic harmonic-oscillator problem (2) are given by the power-series expansion

$$y(p) = \sum_{n=0}^{\infty} c_{2n+1} \frac{p^{2n+1}}{(2n+1)!}. \tag{9}$$

The various solutions $y(p)$ of the eigenvalue equation (3) are characterized or discriminated by different sets of expansion coefficients c_n. By construction, apart from the first coefficient c_1, all expansion coefficients for a given solution depend on the corresponding energy eigenvalue ε. Evaluating the recurrence relation (8) for just the first term, the series (9) explicitly starts with

$$y(p) = p \left\{ 1 + (\mu - \varepsilon) \frac{p^2}{3!} + \left[(\mu - \varepsilon)^2 + \frac{3}{\mu} \right] \frac{p^4}{5!} + \cdots \right\}.$$

III. EXPLICIT BOUND-STATE EIGENFUNCTIONS AND ENERGY LEVELS

The central result of our present investigation of the "relativistic harmonic-oscillator problem" defined by the Hamiltonian H of Eq. (2) is an analytical expression for the reduced radial parts $y(p)$ of all eigenfunctions $\psi(p)$ of H for vanishing angular momentum in form of a Taylor series

$$y(p) \equiv \sqrt{4\pi} p \psi(p) = \sum_{n=0}^{\infty} c_{2n+1} \frac{p^{2n+1}}{(2n+1)!},$$

where the corresponding expansion coefficients c_{2n+1}, $n = 0, 1, 2, \ldots$, are either fixed to $c_1 = 1$, $c_3 = \mu - \varepsilon$ or, for c_{2n+1}, $n \geqslant 2$, determined by the recurrence relation (8). For a given solution of this eigenvalue problem these expansion coefficients and thus the resulting reduced radial wave function $y(p)$ depend on the parameter $\mu \equiv m/a^{1/3}$ and the corresponding energy eigenvalue ε. Taking into account the necessary requirement of normalizability of Hilbert-space eigenstates, the inversion of the latter relation may be exploited to determine the energy eigenvalues ε from the knowledge of the dependence of ε on the coefficients c_n, as derived in the preceding section. In order to fulfill its normalization condition, any solution $y(p)$ must vanish in the limit $p \to \infty$,

$$\lim_{p \to \infty} y(p) = 0. \tag{10}$$

Fixing the energy eigenvalue ε of a chosen bound state in this manner and using this particular value of the parameter ε in the expansion (9) then yields the corresponding wave function $y(p)$.

Our principal concern is beyond doubt the semianalytical approach developed in Sec. II and summarized above. Nevertheless, it might be instructive to construct explicitly a few examples of solutions in numerical or graphical form. These results can be compared with the outcome of some straightforward (but merely numerical) integration of the Schrödinger equation (4). This will provide a useful check of the correctness of our solutions and justify the present formalism.

In actual computations, the infinite series (9) must be truncated, for practical purposes, to a reasonably large but definitely finite number N of terms considered in this expansion of $y(p)$,

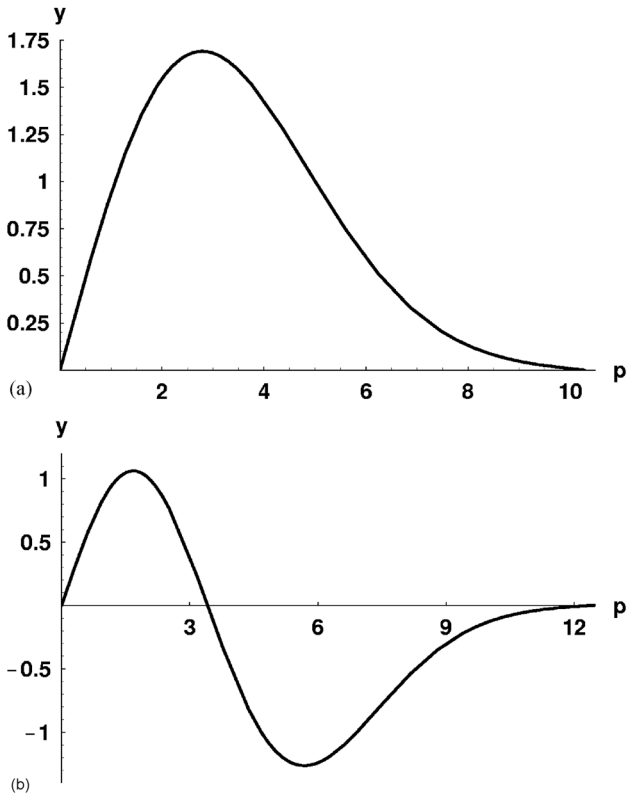

FIG. 1. Radial eigenfunctions in momentum space $y(p) \equiv \sqrt{4\pi} p \psi(p)$ of the ground state (a) and the first radial excitation (b) of the relativistic harmonic-oscillator problem, defined by the Hamiltonian $H=\sqrt{p^2+\mu^2}+r^2$, with $\mu=30$, and for 45 terms in the Taylor expansion of $y(p)$.

$$y(p) \simeq \sum_{n=0}^{N} c_{2n+1} \frac{p^{2n+1}}{(2n+1)!}. \tag{11}$$

In this case, the wave function $y(p)$ will approach zero, as required by the constraint (10), not at infinity but already for a finite value, say $\hat{p}$, of the momentum p— before it starts to diverge. This technique gives the energy eigenvalues ε with a precision determined by one's choice of N, $\varepsilon = \varepsilon(N)$. Likewise, the momentum boundary $\hat{p}$ will also change with N, $\hat{p}=\hat{p}(N)$. For a given value of μ, which quantifies the relative importance of particle mass m and harmonic-oscillator coupling strength a, every wave function resulting from this truncation procedure involves two dimensionless parameters, the relevant energy eigenvalue $\varepsilon(N)$ of the Hamiltonian (2), and the characteristic momentum $\hat{p}(N)$. Their values will be determined simultaneously, in accordance with the above requirement on $y(p)$ [to approach zero at $\hat{p}(N)$] by an appropriate fit procedure. In other words, the value of $\hat{p}(N)$, in particular, cannot be varied freely; it is fixed for chosen N.

Let us illustrate this procedure for both ground state and first radial excitation, i.e., for the two bound states defined by vanishing orbital angular momentum and radial quantum number $n_r=0$, 1, respectively. Figure 1 shows the corresponding reduced radial wave functions $y(p)$ for $\mu=30$ as obtained by inspecting the functional form of $y(p)$ resulting from different choices of ε and $\hat{p}$, if taking into account 45 terms in their Taylor series (9), that is, if choosing $N=44$ in Eq. (11). Table I summarizes the relevant numerical parameter values emerging from such construction.

The exact results can be easily computed with the aid of a (standard) integration technique designed for solving the Schrödinger equation numerically.[46] For our two examples the exact wave functions $y(p)$ prove to be practically indistinguishable, at least by the eye, from the ones extracted from the series (11) with $N=44$. This explains why we refrain from plotting also the former in Fig.

TABLE I. Dimensionless (by scaling) energy eigenvalues $\varepsilon(N)$ and characteristic momenta $\hat{p}(N)$ of the relativistic harmonic-oscillator problem posed by the Hamiltonian $H=\sqrt{p^2+\mu^2}+r^2$ as well as the classical turning points $\bar{p}$ of the corresponding nonrelativistic motion for the ground state and the first radial excitation (identified by their radial quantum number $n_r=0$, 1), with mass vs coupling strength parameter $\mu=30$, and $N=44$ or $N=14$ in our Taylor series (11).

N	n_r	$\varepsilon(N)-\mu$	$\hat{p}(N)$	$\bar{p}$
44	0	0.386 27	10	4.82
	1	0.898 64	12	7.36
14	0	0.388 54	8.5	4.82

1. For the momentum range depicted in Fig. 1, that is, for $0 \leqslant p \leqslant \hat{p}$, the relative differences of the areas under corresponding curves are (of the order) 10^{-8}; more precisely, they are given by 2×10^{-8} for $n_r=0$, the ground state, and 3×10^{-8} for $n_r=1$, the first excited level.

From a straightforward consideration of the "classical turning points" of the corresponding (and well understood) nonrelativistic harmonic-oscillator problem defined by the Hamiltonian

$$H_{\mathrm{NR}} = \mu + \frac{p^2}{2\mu} + r^2,$$

the maximum "classical" momenta, $\bar{p}$, are found, in terms of the radial quantum number n_r, as

$$\bar{p}^2 = (4n_r + 3)\sqrt{2\mu}, \quad n_r = 0,1,2,\ldots .$$

By inspecting Table I we note with satisfaction that for both energy levels under consideration the numerical values of the suitable $\hat{p}$ turn out to be far beyond their classical counterparts $\bar{p}$.

In order to get, at least, some vague idea of the dependence of our findings on the amount of truncation represented by $N<\infty$, we inspect the ground-state wave function $y(p)$ constructed again for $\mu=30$ but by truncating the expansion (9) to the rather modest number of 15 terms, which means to set $N=14$ in Eq. (11). Figure 2 confronts this approximate wave function $y(p)$ with its exact behavior for the ground state. While for small and intermediate momenta there is still perfect agreement with the exact result,[46] we observe a clearly discernible discrepancy between approximate and exact curve for large momenta. Table I tells us that even for $N=14$ our crucial momentum $\hat{p}$ is still comfortably above the corresponding classical turning point, $\bar{p}$. Moreover, comparing

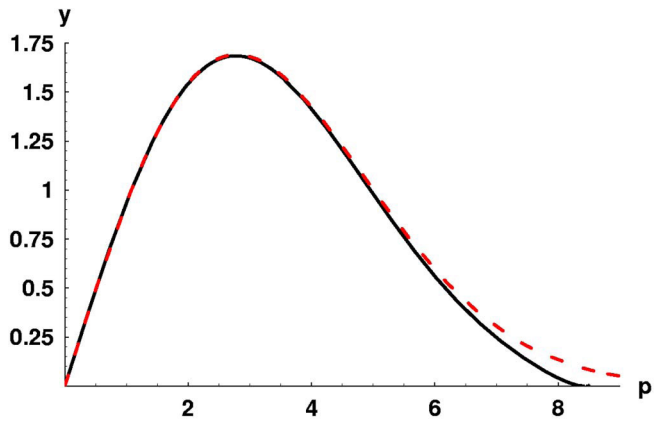

FIG. 2. (Color online) Momentum-space wave function $y(p)$ of Fig. 1(a) resulting from consideration of only 15 terms in its polynomial approximation (11) (full line), in comparison with the corresponding exact ground-state wave function of the relativistic harmonic-oscillator operator (dashed line).

TABLE II. Numerical values of the parameter P_L used by envelope theory for the lower bounds on the energy levels of the relativistic harmonic-oscillator problem in three spatial dimensions, for the lowest-lying $\ell=0$ bound states identified by their radial quantum number $n_r=0, 1, 2, \ldots$.

n_r	P_L
0	1.376 083 5
1	3.181 312 9
2	4.992 554 3
3	6.805 136 9
4	8.618 226 9

the cases $N=14$ and $N=44$, we learn that the value of $\hat{p}$ increases with increasing number N. Of course, the naive expectation would be that $\hat{p}$ behaves like $\hat{p}\to\infty$ for $N\to\infty$, that is, when removing the truncation and restoring the full series expansion for $y(p)$.

The minimum number of terms to be taken into account in the Taylor-series expansions (9) required in order to achieve some given precision of one's results will depend, of course, on both the bound state under study and the desired accuracy. From our above remarks we feel entitled to conclude that a reasonable (and manageable) number $N\simeq 40$ produces satisfactory results.

To our knowledge, at present the best *semianalytical* upper and lower bounds to the energy eigenvalues of the relativistic harmonic-oscillator problem are provided simultaneously by the combination of minimum-maximum principle with operator inequalities[18] and the envelope theory,[19,21] at least for the relativistic harmonic oscillator the envelope bounds[19,21] may be shown[23] to be quantitatively equivalent to the bounds derived in Appendix A of Ref. 18. However, a discussion, in full generality, of all implications of such operator inequalities for the eigenvalues of the operators considered appears clearly off the mainstream of our presentation. Therefore, as already promised in the Introduction, the general relationship is demonstrated in the Appendix. The bounds we need here are derived from this general theorem by specializing to the case of the relativistic harmonic-oscillator problem posed by the Hamiltonian operator (2); all operator inequalities required by this procedure may be generated by, e.g., envelope theory. For a bound state of vanishing relative orbital angular momentum ℓ, that is, for a purely radial excitation, identified by the radial quantum number $n_r=0, 1, 2, \ldots$ (identical to the number of nodes of the corresponding wave function), the bounds on the dimensionless eigenvalue ε read

$$\min_{r>0}\left(\sqrt{\mu^2+\frac{P_L^2}{r^2}}+r^2\right)\leqslant\varepsilon\leqslant\min_{r>0}\left(\sqrt{\mu^2+\frac{P_U^2}{r^2}}+r^2\right),$$

where, in three spatial dimensions, our envelope-theory upper-bound parameter P_U is given by

$$P_U=2n_r+\tfrac{3}{2},\quad n_r=0,1,2,\ldots,$$

while the lower-bound parameter P_L required for our envelope bounds is related to the zeros z_0 of Airy's function Ai(z) (Ref. 47) ($-z_0=2.338\,107, 4.087\,949, 5.520\,560, 6.786\,708, 7.944\,134, \ldots$) by

$$P_{\mathrm{L}}=2\left(\frac{-z_0}{3}\right)^{3/2},\quad \mathrm{Ai}(z_0)=0.$$

Resulting values of P_L for the lowest-lying $\ell=0$ bound states are listed in Table II.[9,19,21–23]

Table III compares, for the lowest four $\ell=0$ energy levels (identified by their radial quantum number $n_r=0, 1, 2, 3$) of our Hamiltonian (2), the approximate eigenvalues, $\varepsilon(N)$, obtained by the present approach by a truncation of the power series (11) to $N=14$ or $N=44$ terms, with the corresponding semianalytical upper (ε_U) and lower (ε_L) bounds mentioned above as well as with the (numerically exact) eigenvalues $\varepsilon_{\mathrm{num}}$, computed by a method developed for the purely numeri-

TABLE III. "Compact-origin" eigenvalues $\varepsilon(N)$, their upper (ε_U) and lower (ε_L) bounds, and their exact values ε_{num} for the lowest $\ell=0$ states of the Hamiltonian $H/a^{1/3}$ in Eq. (2), with $\mu=30$.

Radial excitation n_r	0	1	2	3
$\varepsilon_U-\mu$	0.386 68	0.900 32	1.411 79	1.921 11
$\varepsilon_L-\mu$	0.354 78	0.818 62	1.282 22	1.744 40
$\varepsilon_{\text{num}}-\mu$	0.386 27	0.898 57	1.407 68	1.913 66
$\varepsilon(N=14)-\mu$	0.388 54	0.936 16		
$\varepsilon(N=44)-\mu$	0.386 27	0.898 64	1.410 32	1.943 19

cal solution of (nonrelativistic) Schrödinger equations.[46] For $N=14$, the polynomial in ε resulting from the suitably adapted boundary condition (10) has only two real roots at all. Moreover, both of these approximate values are still above our (semianalytical) upper bounds. In contrast to this rather crude approximation, for $N=44$ the eigenvalues $\varepsilon(N)$ of already the three lowest energy levels fit perfectly to the ranges spanned by the semianalytical bounds. For the ground state, in particular, $\varepsilon(44)$ reproduces the exact result at least to five decimal places.

IV. SUMMARY AND CONCLUSIONS

Our compact result for the reduced $\ell=0$ eigenfunctions of the Hamiltonian (2) is given by the power series (9), with expansion coefficients $c_1=1$, $c_3=\mu-\varepsilon$, and c_{2n+1}, $n\geqslant 2$, determined by the recurrence relation (8). Both the numerical determination of all energy eigenvalues and the explicit construction of the corresponding eigenfunctions of the relativistic harmonic-oscillator problem is then achieved by forcing our solutions to satisfy, in addition, the constraint imposed by the requirement of normalizability of bound-state wave functions. Comparing these explicit solutions with the outcomes of purely numerical integration procedures reveals that at least for the lowest-lying energy levels our semianalytical approach reproduces, already for a truncation of the Taylor series (9) to a moderate number of expansion terms, the exact solutions with high accuracy. Of course, if one is interested only in numerical solutions of the problem under study, their straightforward computation with the help of some integration algorithm should produce the desired result more easily than their extraction from our Taylor series by means of Eq. (10).

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APPENDIX: COMBINATION OF MINIMUM-MAXIMUM PRINCIPLE WITH OPERATOR INEQUALITY: "SPECTRAL COMPARISON THEOREM"

It is a simple exercise to relate discrete eigenvalues of two operators satisfying some inequality.

Consider for some operator A, with domain $\mathcal{D}(A)$, its eigenvalue equation $A|\alpha_k\rangle=a_k|\alpha_k\rangle$, $k=0, 1, 2, \ldots$, for its set of eigenstates $\{|\alpha_k\rangle, k=0,1,2,\ldots\}$, corresponding to its eigenvalues

$$a_k \equiv \frac{\langle\alpha_k|A|\alpha_k\rangle}{\langle\alpha_k|\alpha_k\rangle}, \quad k=0,1,2,\ldots,$$

and likewise for some operator B, with domain $\mathcal{D}(B)$, its eigenvalue equation $B|\beta_k\rangle=b_k|\beta_k\rangle$, $k=0, 1, 2, \ldots$, for its set of eigenstates $\{|\beta_k\rangle, k=0,1,2,\ldots\}$, corresponding to its eigenvalues

$$b_k \equiv \frac{\langle \beta_k | B | \beta_k \rangle}{\langle \beta_k | \beta_k \rangle}, \quad k = 0,1,2,\ldots .$$

Assume that both these operators A and B are self-adjoint, $A^\dagger = A$, $B^\dagger = B$. This implies that all their eigenvalues are real, $a_k^* = a_k$, $b_k^* = b_k$, $k = 0, 1, 2, \ldots$. Let these eigenvalues be ordered according to $a_0 \leqslant a_1 \leqslant a_2 \leqslant \cdots$, $b_0 \leqslant b_1 \leqslant b_2 \leqslant \cdots$. Consider only the discrete eigenvalues a_k of A below the onset of the essential spectrum of the operator A. Assume that the operator A is bounded from below. Assume that the operators A and B are related by an operator inequality of the form $A \leqslant B$, which implies that B too is bounded from below. In order to derive, for any $k = 0, 1, 2, \ldots$, the relationship between a_k and b_k, focus on some arbitrary $(k+1)$-dimensional subspace D_{k+1} of the domain $\mathcal{D}(A)$ of A, $D_{k+1} \subseteq \mathcal{D}(A)$. Employing the appropriate form of the minimum-maximum principle, the operator inequality $A \leqslant B$ translates into an upper bound on the eigenvalue a_k of A which involves all expectation values of B within this subspace D_{k+1},

$$a_k \leqslant \sup_{|\psi\rangle \in D_{k+1}} \frac{\langle \psi | A | \psi \rangle}{\langle \psi | \psi \rangle} \leqslant \sup_{|\psi\rangle \in D_{k+1}} \frac{\langle \psi | B | \psi \rangle}{\langle \psi | \psi \rangle} \quad \text{for all } k = 0,1,2,\ldots . \tag{A1}$$

Now, in order to relate the supremum over the expectation values of B to the eigenvalues b_k of B, consider a particular subspace D_{k+1}, namely, that space that is spanned by the first $k+1$ eigenvectors of the operator B, that is, by precisely those eigenvectors of B that correspond to the first $k+1$ eigenvalues $b_0, b_1, \ldots, b_k$ of B, $D_{k+1} \subseteq \mathcal{D}(B) \subseteq \mathcal{D}(A)$. Then, clearly, every $|\psi\rangle$ in D_{k+1} is a linear combination of the eigenstates $\{|\beta_i\rangle, i = 0, 1, \ldots, k\}$ of B, with coefficients c_i,

$$|\psi\rangle = \sum_{i=0}^{k} c_i |\beta_i\rangle \quad \text{for all } |\psi\rangle \in D_{k+1}.$$

For any subspace D_{k+1}, $k = 0, 1, 2, \ldots$, use of this expansion of $|\psi\rangle$ yields for its norm squared,

$$\langle \psi | \psi \rangle = \sum_{i=0}^{k} |c_i|^2 \langle \beta_i | \beta_i \rangle \quad \text{for all } |\psi\rangle \in D_{k+1}$$

and, with this and $b_i \leqslant b_k$ for all $i = 0, 1, \ldots, k$, an upper bound on all expectation values of B,

$$\langle \psi | B | \psi \rangle = \sum_{i=0}^{k} |c_i|^2 b_i \langle \beta_i | \beta_i \rangle \leqslant b_k \sum_{i=0}^{k} |c_i|^2 \langle \beta_i | \beta_i \rangle = b_k \langle \psi | \psi \rangle \quad \text{for all } |\psi\rangle \in D_{k+1},$$

which means

$$\frac{\langle \psi | B | \psi \rangle}{\langle \psi | \psi \rangle} \leqslant b_k \quad \text{for all } |\psi\rangle \in D_{k+1},$$

$$\frac{\langle \psi | B | \psi \rangle}{\langle \psi | \psi \rangle} = b_k \quad \text{for } |\psi\rangle = |\beta_k\rangle \in D_{k+1}.$$

Therefore the supremum of all expectation values of B over D_{k+1} is just the eigenvalue b_k of B,

$$\sup_{|\psi\rangle \in D_{k+1}} \frac{\langle \psi | B | \psi \rangle}{\langle \psi | \psi \rangle} = b_k \quad \text{for all } k = 0,1,2,\ldots .$$

Thus, inserting this identity in the chain of inequalities (A1) proves that corresponding discrete eigenvalues a_k, b_k of semibounded self-adjoint operators A, B that satisfy $A \leqslant B$ are related by

$$a_k \leqslant b_k \quad \text{for all } k = 0,1,2,\ldots .$$

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Novel solvable extensions of the goldfish many-body model

F. Calogero[a)]
Dipartimento di Fisica, Università di Roma "La Sapienza," Rome, Italy and Istituto Nazionale di Fisica Nucleare, Sezione di Roma, Rome, Italy

S. Iona[b)]
Dipartimento di Fisica, Università di Roma "La Sapienza," Rome, Italy

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A novel *solvable* extension of the goldfish N-body problem is presented. Its Newtonian equations of motion read $\ddot{\zeta}_n=2a\dot{\zeta}_n\zeta_n+2\Sigma_{m=1,m\neq n}^{N}(\dot{\zeta}_n-a\zeta_n^2)(\dot{\zeta}_m-a\zeta_m^2)/(\zeta_n-\zeta_m)$, $n=1,\ldots,N$, where a is an arbitrary (nonvanishing) constant and the rest of the notation is self-evident. The *isochronous* version of this model is characterized by the Newtonian equations of motion $\ddot{z}_n-3i\omega\dot{z}_n-2\omega^2z_n=2a(\dot{z}_n-i\omega z_n)z_n+2\Sigma_{m=1,m\neq n}^{N}(\dot{z}_n-i\omega z_n-az_n^2)(\dot{z}_m-i\omega z_m-az_m^2)/(z_n-z_m)$, $n=1,\ldots,N$, where ω is an arbitrary *positive* constant and the points $z_n(t)$ move now necessarily in the *complex* z-plane. The *generic* solution of this second model is *completely periodic* with a period $T_k=kT$ which is an *integer* multiple k (not larger than $N!$, indeed generally much smaller) of the basic period $T=2\pi/\omega$ and which is independent of the initial data (for sufficiently small, but otherwise arbitrary, changes of such data). These many-body models have an intriguing variety of equilibrium configurations (genuine: with no two particles sitting at the same place), but only for small values of N ($N=2,3,4$ for the first model, $N=2,3,4,5$ for the second). Other versions of these models are also discussed. The study of the behavior of the second, *isochronous* model around its equilibrium configurations yields some amusing *diophantine* results. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2061547]

I. INTRODUCTION

Recently a convenient technique to identify solvable dynamical systems has been introduced and used to identify two solvable extensions of the goldfish many-body model, characterized by the Newtonian equations of motion[3]

$$\ddot{\zeta}_n=2\sum_{m=1,m\neq n}^{N}\frac{\dot{\zeta}_n\dot{\zeta}_m}{\zeta_n-\zeta_m}+a\sum_{m=1}^{N}\frac{\dot{\zeta}_n\dot{\zeta}_m}{\zeta_m}, \tag{1}$$

respectively[4]

$$\ddot{\zeta}_n=2a\dot{\zeta}_n\zeta_n+2\sum_{m=1,m\neq n}^{N}\frac{\dot{\zeta}_n\dot{\zeta}_m}{\zeta_n-\zeta_m}. \tag{2}$$

Here and hereafter, unless otherwise specified, N is an arbitrary positive integer, indices such as n,m run from 1 to N, the dependent variables $\zeta_n\equiv\zeta_n(t)$ are the coordinates of the particles (which are generally supposed to move in the *complex* plane; but *real* solutions also exist if the constant a is *real*), and superimposed dots indicate differentiations with respect to the *real* independent

[a)]Electronic mail: francesco.calogero@roma1.infn.it
[b)]Electronic mail: saiona@tin.it

variable t ("time"). Of course when the constant a vanishes both these N-body problems reduce to the standard goldfish model[1] (and we refer to Ref. 2 for additional information on this model). And *isochronous* variants of these models have also been investigated.[3,4]

In this paper we identify and discuss a third *solvable* extension of the goldfish many-body problem, characterized by the Newtonian equations of motion

$$\ddot{\zeta}_n = 2a\dot{\zeta}_n\zeta_n + 2\sum_{m=1,m\neq n}^{N} \frac{(\dot{\zeta}_n - a\zeta_n^2)(\dot{\zeta}_m - a\zeta_m^2)}{\zeta_n - \zeta_m}, \tag{3}$$

as well as its *isochronous* variant

$$\ddot{z}_n - 3i\omega\dot{z}_n - 2\omega^2 z_n = 2a(\dot{z}_n - i\omega z_n)z_n + 2\sum_{m=1,m\neq n}^{N} \frac{(\dot{z}_n - i\omega z_n - az_n^2)(\dot{z}_m - i\omega z_m - az_m^2)}{z_n - z_m}. \tag{4}$$

In all these models the *arbitrary* constants a and ω could of course be rescaled away, but we prefer to keep them in evidence. Whenever discussing the *isochronous* model (4) we assume the constant ω to be *positive*, $\omega > 0$, and we associate to it the basic *period*

$$T = \frac{2\pi}{\omega}. \tag{5}$$

Of course for $\omega = 0$ the *isochronous* model (4) reduces back to the model (3), but the behavior of the solutions of these two models is *qualitatively* different and it is therefore convenient to treat them separately. Indeed the *generic* motions of the *isochronous* model (4) are *completely periodic* with a period $T_k = kT$ which is an *integer* multiple k of the basic period T and does not depend on the initial data, at least for sufficiently small (but otherwise arbitrary) changes of them (hence having the full dimensionality in phase space). This is in contrast to the phenomenology characteristic of model (3), which features a periodic motion only exceptionally, i.e., only for a special set of initial data (having lower dimensionality in phase space). The more interesting phenomenology obtains when one considers the (nonvanishing!) constant a, and the dependent variables $\zeta_n(t)$, respectively $z_n(t)$, to be *complex*, because motions in the (*complex*) plane allow a much richer gamut of behaviors than motions on the (*real*) line; moreover, as we indicate in the following, it is possible to reinterpret the motions of the points $\zeta_n(t)$ and $z_n(t)$ in the *complex* plane as motions of *real* two-vectors in the (*real*) horizontal plane, allowing thereby a more physical interpretation of these models as genuine many-body problems (with *covariant*, even *rotation-invariant*, Newtonian equations of motion). Of course in the *isochronous* case the dependent variables $z_n(t)$ are *necessarily complex*, because the equations of motion (4) are themselves *complex* (the symbol i appearing in them is of course the imaginary unit, $i \equiv \sqrt{-1}$).

We submit that the phenomenology displayed by these models is sufficiently remarkable to justify calling them "novel," as we did in the title of this paper.

In the following section we report an overview of our main findings, namely the solutions of the two models, first in the *one-body* case and then in the *many-body* case, and their equilibrium configurations (in the *many-body* case). These results are proven in Sec. III, which also contains some other interesting findings. In Sec. IV other versions of these models are introduced and discussed. In Sec. V the behavior is discussed of the *isochronous* model (4), and of its version of Sec. IV, in the neighborhood of their equilibrium configurations, and some amusing *diophantine* relations are thereby obtained.

Finally, we like to add a few words to clarify the character of the model we study in this paper and our justification (admittedly debatable) for referring to it as a "Newtonian many-body problem." We feel entitled to do so because of the possibility to reformulate the *complex* equations of motion (3) and (4), respectively, describing the motions of N points ζ_n and z_n in the *complex* ζ-plane and z-plane, as *real* equations of motions describing the movement of N unit-mass point-particles the positions of which are identified by N *real* two-vectors in the (horizontal) plane. And these *real* equations of motion seem rather naturally interpretable as *Newtonian* equations of

motion, inasmuch as they correspond to the statement that the *acceleration* of each particle is directly given by the *force* that acts on it. Moreover these equations of motion can be formulated in *covariant*, and even in *rotation-invariant*, form (although for simplicity this is explicitly done in the following only in the one-body case, see Sec. II A; the treatment in the many-body case is analogous, as described in detail elsewhere, see for instance Chap. 4 of Ref. 2). And moreover the *forces* featured by this model are just *one-body* and *two-body* forces. On the other hand these forces are *velocity-dependent*, and they do not correspond to any specific physical model; in particular they have no resemblance to the forces characterizing the gravitational N-body problem, which undoubtedly has a much more justified claim than our model to be qualified as "Newtonian"!

II. MAIN RESULTS

In the following we report our main findings. Those for the *one-body* case, treated in Sec. II A, might be considered trivial, but they provide an illuminating introduction to the results for the *many-body* case reported in Sec. II B.

A. The one-body case

For $N=1$ the model (3) reads simply (with $\zeta_1(t) \equiv \zeta(t)$)

$$\ddot{\zeta} = 2a\dot{\zeta}\zeta. \tag{6}$$

This ODE can be reformulated as a problem in the physical (*real*) horizontal plane via the positions

$$\vec{\rho} \equiv (\mathrm{Re}[\zeta], \mathrm{Im}[\zeta], 0), \quad \vec{a} = (\mathrm{Re}[a], -\mathrm{Im}[a], 0); \tag{7}$$

note the minus sign in the second equation. The equation of motion (6) takes then the following *covariant* form:

$$\ddot{\vec{\rho}} = 2[\vec{\rho}(\vec{a} \cdot \dot{\vec{\rho}}) + \dot{\vec{\rho}}(\vec{a} \cdot \vec{\rho}) - \vec{a}(\vec{\rho} \cdot \dot{\vec{\rho}})]. \tag{8a}$$

This Newtonian equation of motion is *covariant*, but not *rotation-invariant*, because the constant vector $\vec{a}$ identifies a preferred direction in the horizontal plane; but this model can be made *rotation-invariant* via the following gimmick: consider the vector $\vec{a}$ in (8a) as an additional *dependent* variable, and then supplement this equation of motion with the additional trivial equation

$$\dot{\vec{a}} = 0. \tag{8b}$$

Note that these two vector equations of motion, (8a) and (8b), are yielded, in the standard manner, by the Hamiltonian

$$H(\vec{\rho}, \vec{a}, \vec{q}; \vec{\pi}, \vec{\alpha}, \vec{\gamma}) = 2(\vec{\pi} \cdot \vec{\rho})(\vec{a} \cdot \vec{\rho}) - (\vec{\pi} \cdot \vec{a})(\vec{\rho} \cdot \vec{\rho}) + (\vec{q} \cdot \vec{\pi}), \tag{9}$$

where $\vec{\rho}$, $\vec{a}$ respectively $\vec{\gamma}$ are the (vector) canonical variables, and $\vec{\pi}$, $\vec{\alpha}$ respectively $\vec{\gamma}$ are the corresponding (vector) canonical momenta: of course the fact that this Hamiltonian does not depend at all on the canonical momenta $\vec{\alpha}$ respectively $\vec{\gamma}$ is consistent with (8b) respectively with the fact that $\vec{q}$ is as well constant. Indeed the first Hamiltonian equation, $\dot{\vec{\rho}} = \partial H / \partial \vec{\pi}$, yielded by the Hamiltonian (9) identifies this vector $\vec{q}$ as the following constant of motion:

$$\vec{q} = \dot{\vec{\rho}} - 2\vec{\rho}(\vec{a} \cdot \vec{\rho}) + \vec{a}(\vec{\rho} \cdot \vec{\rho}), \tag{10}$$

and the time-derivative of this equation yields just the Newtonian equation of motion (8a).

Hereafter we work for convenience with the (*complex*) formulation (6) of the equation of

motion, although we also provide the more physical *real* version of some formulas, as entailed by (7). The solution of the initial-value problem for (6) is

$$\zeta(t) = \frac{\zeta(0) + a^{-1}\Omega \tan(\Omega t)}{1 - a\zeta(0)\Omega^{-1} \tan(\Omega t)}, \tag{11a}$$

$$\Omega^2 = a[\dot{\zeta} - a\zeta^2]. \tag{11b}$$

The right-hand side of (11a) depends clearly on Ω^2 rather than Ω, and this justifies the way we wrote the second of these formulas; and note that, in the definition of Ω^2, it is unnecessary to specify the time at which ζ and $\dot{\zeta}$ are evaluated, since clearly Ω^2 is a constant of motion for the evolution equation (6). The diligent reader will verify that via (7) the solution formula (11a) with (11b) can be written as follows:

$$\vec{\rho}(t) = \frac{\Xi(t)\vec{\rho}(0) + \hat{\Xi}\hat{k} \wedge \vec{\rho}(0) + \Psi(t)\vec{a} + \hat{\Psi}(t)\hat{k} \wedge \vec{a}}{-1 + (\vec{a} \cdot \vec{a})(\vec{\rho}(0) \cdot \vec{\rho}(0))|\Omega^{-1} \tan(\Omega t)|^2 + 2\Xi(t)}, \tag{12a}$$

$$\Omega^2 = (\vec{a} \cdot \vec{q}) + i(\hat{k} \cdot \vec{a} \wedge \vec{q}), \tag{12b}$$

where the constant of motion vector $\vec{q}$ is defined by (10), $\hat{k} \equiv (0,0,1)$ is the unit vector orthogonal to the horizontal plane, the symbol $\wedge$ denotes the standard three-dimensional vector product, and the four *real* functions $\Xi(t)$, $\hat{\Xi}(t)$, $\Psi(t)$, $\hat{\Psi}(t)$ are defined as follows:

$$\Xi(t) = 1 - (\vec{a} \cdot \vec{\rho}(0))\mathrm{Re}\left[\frac{\tan(\Omega t)}{\Omega}\right] + (\hat{k} \cdot \vec{a} \wedge \vec{\rho}(0))\mathrm{Im}\left[\frac{\tan(\Omega t)}{\Omega}\right], \tag{12c}$$

$$\hat{\Xi}(t) = (\vec{a} \cdot \vec{\rho}(0))\mathrm{Im}\left[\frac{\tan(\Omega t)}{\Omega}\right] + (\hat{k} \cdot \vec{a} \wedge \vec{\rho}(0))\mathrm{Re}\left[\frac{\tan(\Omega t)}{\Omega}\right], \tag{12d}$$

$$\Psi(t) = \frac{\Xi(t)\mathrm{Re}[\Omega \tan(\Omega t)] - \hat{\Xi}(t)\mathrm{Im}[\Omega \tan(\Omega t)]}{(\vec{a} \cdot \vec{a})}, \tag{12e}$$

$$\hat{\Psi}(t) = \frac{\Xi(t)\mathrm{Im}[\Omega \tan(\Omega t)] + \hat{\Xi}(t)\mathrm{Re}[\Omega \tan(\Omega t)]}{(\vec{a} \cdot \vec{a})}. \tag{12f}$$

Note that, in writing these formulas, we took good care to distinguish the squared modulus $(\vec{a} \cdot \vec{a}) = |a|^2$ of the (*real*) vector $\vec{a}$, see (7), from the (generally *complex*) number a^2.

Clearly in the *real* case (with a and ζ both *real*) a necessary and sufficient condition to guarantee that this solution, see (11), remains *nonsingular* for all positive time $t > 0$ is validity of the inequality

$$a\dot{\zeta}(0) < 0, \tag{13a}$$

which entails that Ω is *imaginary*. Then

$$\zeta(\pm\infty) = \mp \frac{|\Omega|}{a}. \tag{13b}$$

In the *complex* case the solution (11) is clearly *periodic* with period π/Ω if Ω^2 is *real* and *positive* (in which case we assume Ω to be positive, $\Omega > 0$), provided the imaginary part of $a\zeta(0)$ does *not* vanish, $\mathrm{Im}[a\zeta(0)] \neq 0$ or equivalently $\vec{a} \wedge \vec{\rho}(0) \neq 0$ (to exclude that the solution becomes

singular at some finite time $t=t_s$, $0<t_s<\pi/\Omega$). The condition on the initial data such that indeed Ω^2 be *positive* can be read directly from (11b) or (12b). In the *generic* case when Ω^2 is *not real* the *complex* coordinate $\zeta(t)$ tends—both in the remote past and future—to finite limiting values, see (13b), and the motion is generically *nonsingular*, although there is a lower-dimensional set of initial data yielding singular motions (they are of course those values such that the denominator $1-a\zeta(0)\Omega^{-1}\tan(\Omega t)$ vanishes for some *positive* value of the time t, see (11a)). The diligent reader will formulate the analogous results appropriate to the "physical" formulation in the *real* horizontal plane (see (8a) and (12)).

The *isochronous* version of this model (6) is characterized by the Newtonian equation of motion

$$\ddot{z}-3i\omega\dot{z}-2\omega^2 z=2a(\dot{z}-i\omega z)z. \tag{14}$$

Clearly this equation of motion reduces to the previous one, (6), for $\omega=0$ (entailing $z(t)=\zeta(t)$). As already mentioned, whenever we discuss *isochronous* versions of our models we assume ω to be *positive*, $\omega>0$.

The solution of the initial-value problem for this equation of motion, (14), reads

$$z(t)=\exp(i\omega t)\frac{z(0)+a^{-1}\widetilde{\Omega}\tan(\widetilde{\Omega}\tau)}{1-az(0)\widetilde{\Omega}^{-1}\tan(\widetilde{\Omega}\tau)}, \tag{15a}$$

$$\widetilde{\Omega}^2=a[\dot{z}(0)-i\omega z(0)-az^2(0)]. \tag{15b}$$

Here and always in the following the *complex* time-like variable τ is related to the (*real*, "physical") time variable t by the relation

$$\tau\equiv\tau(t)=\frac{\exp(i\omega t)-1}{i\omega}, \tag{16}$$

which entails that τ is a *periodic* function of t with period T, see (5). And this in turn entails the *isochronous* character of the solution (15a) of (14), which is clearly as well *periodic* with period T, $z(t+T)=z(t)$, for *generic* initial conditions $z(0)$ and $\dot{z}(0)$: the initial data that yield a *singular* solution are indeed *nongeneric*, being characterized by the requirement that the (generally *complex*) denominator $1-az(0)\Omega^{-1}\tan(\widetilde{\Omega}\tau)$, see (15a) with (16), vanishes for some *positive* value of the time $t=\widetilde{t}_s$, with $0<\widetilde{t}_s<T$.

The diligent reader will formulate the analogous results appropriate to the "physical" formulation in the *real* horizontal plane (see (7)).

B. The many-body case

The solution of the initial-value problem for the N-body problem (3) is given by

Proposition 1: the coordinates $\zeta_n(t)$ of the N moving particles are the N eigenvalues of the $N\otimes N$ matrix

$$U(t)=[1-aU(0)t]^{-1}\Bigg\{U(0)+[\chi(t)]^{-1}\Bigg\{[q(t)U(0)+r(t)]P+\Bigg[1-\cos(\Omega t)+\frac{\sin(\Omega t)-\Omega t}{\Omega}aU(0)\Bigg]P[1-aU(0)t]^{-1}U(0)\Bigg\}\Bigg\}, \tag{17a}$$

where

$$\chi(t)=\sum_{n=1}^{N}\left[\left(\frac{\Omega_n^2}{\Omega^2}\right)\frac{\Omega\cos(\Omega t)-\sin(\Omega t)a\zeta_n(0)}{\Omega[1-a\zeta_n(0)t]}\right], \tag{17b}$$

$$q(t) = \sum_{n=1}^{N} \left[\left(\frac{\Omega_n^2}{\Omega^2} \right) \frac{[1 - \cos(\Omega t)][1 + a\zeta_n(0)t] - \Omega t \sin(\Omega t)}{1 - a\zeta_n(0)t} \right], \tag{17c}$$

$$r(t) = \left(\frac{\Omega}{a} \right) \sum_{n=1}^{N} \left[\left(\frac{\Omega_n^2}{\Omega^2} \right) \frac{\Omega \sin(\Omega t) - 2[1 - \cos(\Omega t)]a\zeta_n(0)}{\Omega[1 - a\zeta_n(0)t]} \right], \tag{17d}$$

the diagonal $N \otimes N$ *matrix* $U(0)$ *is given in terms of the initial values of the coordinates* ζ_n *by the simple formula*

$$U(0) = \mathrm{diag}[\zeta_n(0)], \tag{17e}$$

and the dyadic $N \otimes N$ *matrix* P is *defined as follows:*

$$P_{nm} = \frac{\Omega_n \Omega_m}{\Omega^2}. \tag{17f}$$

In these formulas the scalars Ω_n *and* Ω *are defined in terms of the initial data as follows:*

$$\Omega_n = \{a[\dot{\zeta}_n(0) - a\zeta_n^2(0)]\}^{1/2}, \tag{17g}$$

$$\Omega^2 = a \sum_{n=1}^{N} (\dot{\zeta}_n - a\zeta_n^2) = \sum_{n=1}^{N} \Omega_n^2, \tag{17h}$$

so that the dyadic $N \otimes N$ *matrix* P *is actually a* projector, $P^2 = P$.

Several comments on these findings (proven in the following section) are now appropriate. (i) The formula (17h) defines Ω^2 rather than Ω, consistent with the fact that the right-hand side of (17a) is indeed a function of Ω^2 rather than Ω. (ii) In the spirit of the initial value problem the values of $\dot{\zeta}_n$ and ζ_n^2 to be inserted in the right-hand side of expression (17h) of Ω^2 would be evaluated at the initial time $t=0$, as implied by its second version, see (17g); but let us emphasize that this quantity, Ω^2 (see the first version of (17h)), is a constant of motion for our system, as is apparent by summing its equations of motion, (3), over the index n from 1 to N and then noticing that the double sum on the right-hand side vanishes due to the antisymmetry of the summand under exchange of the two dummy indices n and m, while the resulting equation clearly entails that the time-derivative of Ω^2 vanishes. (iii) In writing formula (17a) we assumed that the constant Ω does not vanish; but the formula remains valid, via an obvious limiting procedure, even if Ω does vanish.

Let us emphasize the remarkable time dependence exhibited by the solution formula (17a), that features (see also, (17b)–(17d)) a rational dependence *both* on t and on circular functions of Ωt (with Ω generally *complex*, see (17h)). A terse discussion of this formula is therefore in order.

First let us note that $\chi(0)=1$ (see (17b) with (17g) and (17h)), while $q(0)=r(0)=0$ (see (17c) and (17d)). The consistency of the solution formula (17a) at $t=0$ is thereby apparent.

Second, as $t \to \pm\infty$, there clearly hold (up to corrections of order $1/t$), the asymptotic relations

$$U(t) \approx \left(\frac{\Omega}{a} \right) \frac{b \tan(\Omega t) - 1}{\tan(\Omega t) + b} P \quad \text{if } \mathrm{Im}[\Omega] = 0, \tag{18a}$$

$$U(t) \approx \pm \,\mathrm{sign}[\mathrm{Im}(\Omega)] \frac{i\Omega}{a} P \quad \text{if } \mathrm{Im}[\Omega] \neq 0, \tag{18b}$$

with

$$b = \frac{a}{\Omega}\sum_{n=1}^{N}\left[\zeta_n(0) - \frac{\dot{\zeta}_n(0)}{a\zeta_n(0)}\right]. \tag{18c}$$

We therefore conclude (because the $N\otimes N$ matrix P, being a projector, has a single unit eigenvalue with all the other $N-1$ vanishing) that *generically* (i.e., excluding *nongeneric* solutions that become *singular* due to the occurrence of a particle collision), as $t\to\pm\infty$, *all but one* of the coordinates $\zeta_n(t)$ tend to the origin, while one of them, if $\mathrm{Im}[\Omega]=0$, approaches asymptotically (up to corrections of order $1/t$) the *periodic* trajectory

$$\zeta_{\mathrm{asy}}(t) = \left(\frac{\Omega}{a}\right)\frac{b\tan(\Omega t)-1}{\tan(\Omega t)+b} \tag{19a}$$

(provided $\mathrm{Im}[b]\neq 0$, so that this asymptotic trajectory is *not singular*), and if instead $\mathrm{Im}[\Omega]\neq 0$ it approaches asymptotically (again, up to corrections of order $1/t$) the asymptotic value

$$\bar{\zeta}_{\mathrm{asy}} = \pm\,\mathrm{sign}[\mathrm{Im}(\Omega)]\frac{i\Omega}{a}. \tag{19b}$$

The *isochronous* variant of the model (3) is characterized by the Newtonian equations of motion (4). These equations of motion reduce of course to the previous ones, see (3), for $\omega=0$ (entailing $z_n(t)=\zeta_n(t)$), but, as already indicated earlier, whenever we refer to this *isochronous* model we assume instead that the constant ω is *positive* and we associate with it the basic period T, see (5). Note that in this *isochronous* case the dependent variables $z_n\equiv z_n(t)$ denote N points that move *necessarily* in the *complex* z-plane.

The solution of the initial-value problem for this N-body problem, (4), is given by

Proposition 2: the coordinates $z_n(t)$ of the N moving particles are the N eigenvalues of the $N\otimes N$ matrix

$$\widetilde{U}(t) = \exp(i\omega t)[1-a\widetilde{U}(0)\tau]^{-1}\left\{\widetilde{U}(0) + [\widetilde{\chi}(\tau)]^{-1}\left\{[\widetilde{q}(\tau)\widetilde{U}(0)+\widetilde{r}(\tau)]\widetilde{P} + \left[1-\cos(\widetilde{\Omega}\tau) + \frac{\sin(\widetilde{\Omega}\tau)-\widetilde{\Omega}\tau}{\widetilde{\Omega}}a\widetilde{U}(0)\right]\widetilde{P}[1-a\widetilde{U}(0)\tau]^{-1}\widetilde{U}(0)\right\}\right\} \tag{20a}$$

where $\tau\equiv\tau(t)$ is given by (16),

$$\widetilde{\chi}(\tau) = \sum_{n=1}^{N}\left[\left(\frac{\widetilde{\Omega}_n^2}{\widetilde{\Omega}^2}\right)\frac{\widetilde{\Omega}\cos(\widetilde{\Omega}\tau)-\sin(\widetilde{\Omega}\tau)az_n(0)}{\widetilde{\Omega}[1-az_n(0)\tau]}\right], \tag{20b}$$

$$\widetilde{q}(\tau) = \sum_{n=1}^{N}\left[\left(\frac{\widetilde{\Omega}_n^2}{\widetilde{\Omega}^2}\right)\frac{[1-\cos(\widetilde{\Omega}\tau)][1+az_n(0)\tau]-\widetilde{\Omega}\tau\sin(\widetilde{\Omega}\tau)}{1-az_n(0)\tau}\right], \tag{20c}$$

$$\widetilde{r}(\tau) = \left(\frac{\widetilde{\Omega}}{a}\right)\sum_{n=1}^{N}\left[\left(\frac{\widetilde{\Omega}_n^2}{\widetilde{\Omega}^2}\right)\frac{\widetilde{\Omega}\sin(\widetilde{\Omega}\tau)-2[1-\cos(\widetilde{\Omega}\tau)]az_n(0)}{\widetilde{\Omega}[1-az_n(0)\tau]}\right], \tag{20d}$$

the diagonal *$N\otimes N$ matrix $\widetilde{U}(0)$ is given in terms of the initial values of the coordinates z_n by the simple formula*

$$\widetilde{U}(0) = \mathrm{diag}[z_n(0)], \tag{20e}$$

and the dyadic *$N\otimes N$ matrix $\widetilde{P}$* is *defined as follows:*

$$\widetilde{P}_{nm} = \frac{\widetilde{\Omega}_n \widetilde{\Omega}_m}{\widetilde{\Omega}^2}. \tag{20f}$$

In these formulas the scalars $\widetilde{\Omega}_n$ *and* $\widetilde{\Omega}$ *are defined in terms of the initial data as follows:*

$$\widetilde{\Omega}_n = \{a[\dot{z}_n(0) - i\omega z_n(0) - a z_n^2(0)]\}^{1/2}, \tag{20g}$$

$$\widetilde{\Omega}^2 = a\sum_{n=1}^{N} (\dot{z}_n(0) - i\omega z_n(0) - a z_n^2(0)) = \sum_{n=1}^{N} \widetilde{\Omega}_n^2, \tag{20h}$$

so that the dyadic $N \otimes N$ *matrix* $\widetilde{P}$ *is actually a* projector, $\widetilde{P}^2 = \widetilde{P}$.

The validity of *Proposition 2* is a simple consequence of *Proposition 1*, because the equations of motion (4) of the *isochronous* model are related to those of the previous model (3) by the simple relation (the so-called "trick")

$$z_n(t) = \exp(i\omega t)\zeta_n(\tau) \tag{21}$$

with τ related to t via (16), entailing the following relations among the respective initial data:

$$\zeta_n(0) = z_n(0), \quad \dot{\zeta}_n(0) = \dot{z}_n(0) - i\omega z_n(0). \tag{22}$$

Since clearly the matrix $\widetilde{U}(t)$ is periodic in t with period T,

$$\widetilde{U}(t+T) = \widetilde{U}(t) \tag{23a}$$

(see (20a) with (16) and (5)), the set $\{z_n(t)\}$ of its N eigenvalues is as well *periodic* with the same period; this does not necessarily entail that each of its individual eigenvalues is *periodic* with this period, since during the time evolution (which now necessarily takes place in the *complex* z-plane) an exchange of eigenvalues might occur. But this mechanism can only increase the periodicity of each individual eigenvalue by an integer factor not exceeding $N!$ (indeed, generally much smaller[5]). Hence we conclude that the *generic* solution of the *isochronous* model (4) is (*nonsingular* and) *completely periodic*,

$$z_n(t + \widetilde{T}) = z_n(t), \tag{23b}$$

with a period $\widetilde{T} = kT$, where k is a positive integer not larger (indeed, generally much smaller[5]) than $N!$ (k depends of course on the particular solution under consideration, but its value does not change for sufficiently small changes of the initial data, hence the set of initial data yielding the same period is *open*, with full dimensionality in phase space). The only *nonperiodic* solutions are the *nongeneric* ones that obtain for the *special* set of initial data that cause a "particle collision," namely the coincidence at some time $t_c < T$ of two or more particle positions $z_n(t)$, or equivalently of two or more eigenvalues of the matrix $\widetilde{U}(t_c)$, see (20); the surfaces in phase space on which such special sets of initial data live separate the sets of initial data yielding different periods.

C. Equilibrium configurations in the many-body case

Let us now report our main findings concerning the *equilibrium configurations* of these models, which are of course always defined up to arbitrary permutations of the N equal particles (this obvious *caveat* will not be repeated in the following). But before reporting these findings let us emphasize that here we only consider "genuine" equilibrium configurations, characterized by the requirement that no two particles sit at the same location. Let us also note that, for the first model, (3), clearly any particle sitting initially at the origin with vanishing velocity (i.e., with $\zeta_n(0) = \dot{\zeta}_n(0) = 0$) always remains there without influencing at all the motion of the other particles; and, for the *isochronous* model (4), this is as well true both for a particle sitting at the origin (i.e., with

$z_n(0)=\dot{z}_n(0)=0$) and for a particle sitting at the point $-i\omega/a$ (i.e., with $z_n(0)=-i\omega/a$ and $\dot{z}_n(0)=0$). In the following we also take account of such particles when discussing the equilibrium configurations, but, consistent with the above-mentioned definition of "genuine" equilibrium configurations, we allow at most one particle to sit in such a position.

The first model, (3), has no (genuine) equilibrium configurations for $N\geqslant 5$. For $N=2$ there is only the trivial configuration $\zeta_1=0$, $\zeta_2=\bar{\zeta}$ with $\bar{\zeta}$ an *arbitrary* constant. For $N=3$ at equilibrium its three coordinates ζ_n take three values out of the following four:

$$\tilde{\zeta}_k=\eta\exp\left(\frac{2\pi ki}{3}\right),\quad k=1,2,3 \text{ and } \bar{\zeta}_4=0. \tag{24}$$

For $N=4$ at equilibrium the four coordinates ζ_n take these four values. Here and in the following η is an *arbitrary* (but *nonvanishing*) constant.

To describe the phenomenology of the (genuine) equilibrium configurations of the second, *isochronous* model (4) it is convenient to identify them as follows:

$$z_n(t)=\left(\frac{\omega}{ia}\right)u_n,\quad \dot{z}_n(t)=0,\quad u_n\neq u_m. \tag{25}$$

For $N=2$ there are only two equilibrium configurations: $u_1=0$, $u_2=1$, respectively,

$$u_{1,2}=\frac{3\pm i\sqrt{3}}{2}. \tag{26}$$

For $N=3$, a one-parameter set of equilibrium configurations is

$$u_k(\eta)=1+\eta\exp\left(\frac{2\pi ik}{3}\right),\quad k=1,2,3, \tag{27}$$

with η an *arbitrary* (but *nonvanishing*, $\eta\neq 0$) constant; and there is an additional equilibrium configuration, $u_{1,2}=(3\pm i\sqrt{3})/2$, $u_3=1$. (Note that the configuration with one particle at the origin, say $u_3(\eta)=0$, is included in (27) with $\eta=-1$). For $N=4$ there are *two* one-parameter sets of equilibrium configurations, $u_k=u_k(\eta)$, $k=1,2,3$ (see (27)) and $u_4=0$ and $u_4=1$, respectively (and η again *arbitrary* but *nonvanishing*, $\eta\neq 0$, with, in the first case, the additional restriction $\eta\neq-\exp(-2\pi ik/3)$, $k=1,2,3$, to exclude that any one of the three numbers $u_k(\eta)$ vanish). For $N=5$ there is only a single one-parameter set of equilibrium configurations, $u_k=u_k(\eta)$, $k=1,2,3$, $u_4=0$, $u_5=1$, with $u_k(\eta)$ defined as above, see (27) (and η again *arbitrary* except for the *two* restrictions $\eta\neq 0$ and $\eta\neq-\exp(-2\pi ik/3)$, $k=1,2,3$, to exclude that any one of the three numbers $u_k(\eta)$ vanish or be unity). And for $N>5$ there are no (genuine) equilibrium configurations.

Let us finally note that the equations of motion (4) for the N *complex* dependent variables $z_n(t)$ can be reformulated as *real* and *covariant* Newtonian equations describing the motion of N equal unit-mass point particles moving in the horizontal plane, by introducing as dependent variables the N vectors $\vec{r}_n\equiv\vec{r}_n(t)$ related to the *complex* numbers $z_n(t)$ by the relations $\vec{r}_n(t)\equiv(\mathrm{Re}[z_n(t)],\mathrm{Im}[z_n(t)],0)$, and the constant vector $\vec{a}$ related to the *complex* constant a (see (4)) by the relation $\vec{a}\equiv(\mathrm{Re}[a],-\mathrm{Im}[a],0)$ (note the minus sign in the second component!). All these vectors are formally written as three vectors, but they of course describe motions taking place in the horizontal plane; the three-dimensional notation is convenient to exhibit the covariance of these equations of motion (via the additional introduction of the unit vector $\hat{k}\equiv(0,0,1)$ orthogonal to the horizontal plane). The resulting equations—whose explicit display is left as a trivial if tedious exercise for the diligent reader—are of course *not* invariant under rotations in the plane, since the vector $\vec{a}$ identifies a preferred direction there. They can be made *rotation-invariant* via the following gimmick (see above): consider the vector $\vec{a}$ in these equations as an additional (hence formally time-dependent) variable, and then complement the Newtonian equations of mo-

tion for the N dependent variables $\vec{r}_n(t)$ with the following (also *rotation-invariant*, if quite trivial) equation of motion: $\dot{\vec{a}}=0$.

III. PROOFS, AND SOME OTHER RESULTS

In the following we prove the findings reported in Sec. II, we discuss some of them in more detail than was done there, and we also provide some additional results.

A. Solution of the equations of motion

Let the $N\otimes N$ matrix $U\equiv U(t)$ satisfy the first-order matrix ODE

$$\dot{U}=f(U)+C, \tag{28}$$

where C is a constant $N\otimes N$ matrix and the function $f(u)$ is scalar, namely the matrix $f(U)$ depends on no other matrix besides U, entailing that, for any invertible $N\otimes N$ matrix R,

$$Rf(U)R^{-1}=f(RUR^{-1}). \tag{29}$$

Let us assume now that $U(t)$ is diagonalized by the matrix $R(t)$,

$$U=RZR^{-1}, \quad Z=\mathrm{diag}(\zeta_n), \tag{30}$$

so that the N quantities $\zeta_n\equiv\zeta_n(t)$ are the N eigenvalues of the matrix $U(t)$. Note that, without spoiling the validity of (30), the matrix R could be replaced by the matrix

$$\widetilde{R}=RD, \tag{31}$$

with $D\equiv D(t)$ an *arbitrary diagonal* matrix. Let us also introduce the $N\otimes N$ matrix $\Gamma(t)$ by setting

$$C=R\Gamma R^{-1}, \quad \Gamma=R^{-1}CR. \tag{32}$$

Clearly the relations (30) and (32) entail

$$\dot{U}=R\{\dot{Z}+[M,Z]\}R^{-1}, \quad \dot{C}=R\{\dot{\Gamma}+[M,\Gamma]\}R^{-1}, \tag{33}$$

where we introduced the $N\otimes N$ matrix $M(t)$ by setting

$$M=R^{-1}\dot{R}. \tag{34}$$

Note that the replacement, in this definition of M, of R with $\widetilde{R}$ (see (31)) entails a corresponding replacement of M with

$$\widetilde{M}=\widetilde{R}^{-1}\dot{\widetilde{R}}=D^{-1}MD+D^{-1}\dot{D}. \tag{35}$$

Hence the matrix M is defined up to the addition of the *arbitrary diagonal* matrix $D^{-1}\dot{D}$, which implies that its *diagonal* elements can be assigned *arbitrarily*, provided of course the *off-diagonal* elements are then properly adjusted, see (35).

The original matrix ODE (28) entails, via (33) and (30),

$$\dot{Z}+[M,Z]=\Gamma+f(Z), \tag{36a}$$

and the time-independence of the matrix C entails, via (33) and (32),

$$\dot{\Gamma}+[M,\Gamma]=0. \tag{36b}$$

Let us now write out separately, componentwise, the *diagonal* and *off-diagonal* parts of these two matrix equations (36) (also indicating, for notational convenience, with γ_n and μ_n, respec-

tively, the diagonal elements of the matrices Γ and M, $\gamma_n \equiv \Gamma_{nn}$, $\mu_n \equiv M_{nn}$):

$$\dot{\zeta}_n = \gamma_n + f(\zeta_n), \tag{37a}$$

$$-M_{nm}(\zeta_n - \zeta_m) = \Gamma_{nm}, \quad n \neq m, \tag{37b}$$

$$\dot{\gamma}_n = \sum_{m=1, m\neq n}^{N} (\Gamma_{nm} M_{mn} - \Gamma_{mn} M_{nm}), \tag{37c}$$

$$\dot{\Gamma}_{nm} = -(\mu_n - \mu_m)\Gamma_{nm} + (\gamma_n - \gamma_m) M_{nm} + \sum_{\ell=1, \ell\neq m,n}^{N} (\Gamma_{n\ell} M_{\ell m} - \Gamma_{\ell m} M_{n\ell}), \quad n \neq m. \tag{37d}$$

The first *two* of these four equations can be immediately solved for γ_n and M_{nm}, respectively, whereby the last *two* of these four equations become

$$\ddot{\zeta} = \dot{\zeta}_n f'(\zeta_n) + 2 \sum_{m=1, m\neq n}^{N} \frac{\Gamma_{nm}\Gamma_{mn}}{\zeta_n - \zeta_m}, \tag{38a}$$

$$\dot{\Gamma}_{nm} = -(\mu_n - \mu_m)\Gamma_{nm} - \frac{\{[\dot{\zeta}_n - f(\zeta_n)] - [\dot{\zeta}_m - f(\zeta_m)]\}\Gamma_{nm}}{\zeta_n - \zeta_m} + \sum_{\ell=1, \ell\neq m,n}^{N} \{\Gamma_{n\ell}\Gamma_{\ell m}[(\zeta_n - \zeta_\ell)^{-1} + (\zeta_m - \zeta_\ell)^{-1}]\}, \quad n \neq m. \tag{38b}$$

In (38a) and hereafter the prime appended to a function denotes differentiation with respect to its argument, e.g., $f'(\zeta) \equiv df(\zeta)/d\zeta$.

Let us now set

$$\Gamma_{nm} = \{[\dot{\zeta}_n - g(\zeta_n)][\dot{\zeta}_m - g(\zeta_m)]\}^{1/2} \eta_{nm}, \tag{39}$$

where the quantities $\eta_{nm} \equiv \eta_{nm}(t)$ are new dependent variables (hence this assignment entails no loss of generality), and we reserve the privilege to assign later the function $g(\zeta)$. Insertion of this *ansatz* in (38a) yields

$$\ddot{\zeta}_n = \dot{\zeta}_n f'(\zeta_n) + 2 \sum_{m=1, m\neq n}^{N} \frac{[\dot{\zeta}_n - g(\zeta_n)][\dot{\zeta}_m - g(\zeta_m)]\eta_{nm}\eta_{mn}}{\zeta_n - \zeta_m}, \tag{40a}$$

and its insertion in (38b) yields (via (40a))

$$\frac{\dot{\eta}_{nm}}{\eta_{nm}} + \mu_n - \mu_m - \frac{f(\zeta_n) - g(\zeta_n) - [f(\zeta_m) - g(\zeta_m)]}{\zeta_n - \zeta_m} + \frac{\dot{\zeta}_n[f'(\zeta_n) - g'(\zeta_n)]}{2[\dot{\zeta}_n - g(\zeta_n)]} + \frac{\dot{\zeta}_m[f'(\zeta_m) - g'(\zeta_m)]}{2[\dot{\zeta}_m - g(\zeta_m)]} = \sum_{\ell=1, \ell\neq m,n}^{N} \left\{ [\dot{\zeta}_\ell - g(\zeta_\ell)] \left(\frac{\eta_{n\ell}\eta_{\ell m}}{\eta_{nm}} - 1 \right) [(\zeta_n - \zeta_\ell)^{-1} + (\zeta_m - \zeta_\ell)^{-1}] \right\}, \quad n \neq m. \tag{40b}$$

The system of second-order ODEs (40a) is clearly interpretable as a Newtonian many-body problem, but it contains, in addition to the "particle coordinates" ζ_n, the auxiliary variables η_{nm}, which themselves evolve according to the system of first-order ODEs (40b). Since in this paper we are interested in identifying solvable systems of ODEs interpretable as Newtonian many-body problems *without* additional variables, we now try and see how to get rid of the auxiliary variables

η_{nm}. Clearly a possibility to do so, suggested by the structure of these two systems (40a) and (40b) of ODEs, is to set

$$\eta_{nm}(t) = \frac{\eta_n(t)}{\eta_m(t)}. \tag{41}$$

Via this assignment the auxiliary variables indeed disappear altogether from the first set (40a) of ODEs, which then read

$$\ddot{\zeta}_n = \dot{\zeta}_n f'(\zeta_n) + 2 \sum_{m=1, m\neq n}^{N} \frac{[\dot{\zeta}_n - g(\zeta_n)][\dot{\zeta}_m - g(\zeta_m)]}{\zeta_n - \zeta_m}, \tag{42a}$$

while the second set, (40b), of ODEs becomes

$$\frac{\dot{\eta}_n}{\eta_n} + \mu_n - \left(\frac{\dot{\eta}_m}{\eta_m} + \mu_m\right) = \frac{f(\zeta_n) - g(\zeta_n) - [f(\zeta_m) - g(\zeta_m)]}{\zeta_n - \zeta_m} - \frac{\dot{\zeta}_n[f'(\zeta_n) - g'(\zeta_n)]}{2[\dot{\zeta}_n - g(\zeta_n)]}$$

$$- \frac{\dot{\zeta}_m[f'(\zeta_m) - g'(\zeta_m)]}{2[\dot{\zeta}_m - g(\zeta_m)]}, \quad n \neq m. \tag{42b}$$

There now remains to see whether this second set, (42b), of ODEs can be satisfied.

We note first of all that the left-hand sides of these equations, (25), are antisymmetric under the exchange of the two indices n and m, while the right-hand sides are symmetrical. Hence they must both vanish.

The vanishing of the left-hand side is easily achieved, by setting

$$\mu_n(t) = -\frac{\dot{\eta}_n(t)}{\eta_n(t)}, \tag{43}$$

an assignment which is permitted since we are free to choose at our convenience the diagonal elements $\mu_n(t)$ of the matrix $M(t)$, see the remark made earlier (after (35)).

To achieve the vanishing of the right-hand side of (42b) (which is quite overdetermined, especially because the functions f and g are required to be independent of the "velocities" $\dot{\zeta}$) we can take advantage of our freedom to assign the function $g(\zeta)$. This can be conveniently done in two quite different manners.

A first assignment is

$$g(\zeta) = 0, \tag{44}$$

which has the merit to eliminate altogether from (42b) the presence of the "velocities" $\dot{\zeta}_n$ and $\dot{\zeta}_m$. The requirement that the right-hand sides of (42b) vanish yields then the following (apparently still overdetermined, but see the following) set of ODEs for the function $f(z)$:

$$\frac{f(\zeta_n) - f(\zeta_m)}{\zeta_n - \zeta_m} = \frac{f'(\zeta_n) + f'(\zeta_m)}{2}, \quad n \neq m. \tag{45a}$$

It is easily seen that the general solution of this system of ODEs is

$$f(\zeta) = a\zeta^2 + b\zeta + c, \tag{45b}$$

with a, b, and c three *arbitrary* constants. The corresponding version of the original matrix evolution equation (28) reads

$$\dot{U} = aU^2 + bU + c + C. \tag{46a}$$

Without significant loss of generality this matrix ODE can be replaced by its simpler version

$$\dot{U} = aU^2 + C. \tag{46b}$$

which obtains by setting $b=c=0$ in (46a), but clearly could as well be obtained from (46a) by shifting the two $N\otimes N$ matrices U and C by two appropriate *constant* multiples of the $N\otimes N$ *unit* matrix, resulting merely in a shift of all the eigenvalues $\zeta_n(t)$ of the $N\otimes N$ matrix U by a *common constant*, and in a redefinition of the matrix C which in any case does not feature in the system of ODEs (42a). We conclude that the many-body problem yielded by this choice is characterized by the equations of motion

$$\ddot{\zeta}_n = 2a\dot{\zeta}_n\zeta_n + 2\sum_{m=1,m\neq n}^{N} \frac{\dot{\zeta}_n\dot{\zeta}_m}{\zeta_n - \zeta_m}, \tag{47}$$

yielded by (42a) with (44) and with (45b) which takes now the simpler form

$$f(\zeta) = a\zeta^2. \tag{48}$$

But this many-body model, (47), is *not* new (see (2)): its solvability and properties were demonstrated and investigated in Ref. 4, by a technique analogous to that described earlier except that the starting point in that treatment was the second-order matrix ODE

$$\ddot{U} = a(\dot{U}U + U\dot{U}), \tag{49}$$

rather than the matrix ODE (46b). It is indeed plain that these two matrix ODE, (46b) and (49), are equivalent (at least as long as we restrict our consideration to autonomous equations, namely we consider the scalar a and the matrix C to be time-independent, as we always did hitherto).

A second, and in fact more obvious, assignment of the function $g(\zeta)$ which also achieves the vanishing of the right-hand side of (42b) is

$$g(\zeta) = f(\zeta). \tag{50}$$

Hence, by inserting this assignment in (42a), we conclude that the many-body system

$$\ddot{\zeta}_n = \dot{\zeta}_n f'(\zeta_n) + 2\sum_{m=1,m\neq n}^{N} \frac{[\dot{\zeta}_n - f(\zeta_n)][\dot{\zeta}_m - f(\zeta_m)]}{\zeta_n - \zeta_m} \tag{51}$$

is *solvable*, provided the corresponding $N\otimes N$ matrix evolution ODE (28), with an *arbitrary* constant $N\otimes N$ matrix C, is itself *solvable*: indeed our treatment entails that the time evolution of the N "particle coordinates" $\zeta_n(t)$ coincides then with the time evolution of the N eigenvalues of the $N\otimes N$ matrix $U(t)$ (with an appropriate assignment, in terms of the initial data $\zeta_n(0)$, $\dot{\zeta}_n(0)$, of the initial value $U(0)$ of the matrix $U(t)$ and of the constant matrix C: see the following). Let us also point out that a more general choice of the function $g(\zeta)$, also consistent with the vanishing of the right-hand side of (42b), would add an *arbitrary* constant c to the right-hand side of the formula (50); the alert reader will work out the marginal extension of our results entailed by this possibility.

It is remarkable that, to obtain these Newtonian equations of motion, (51), no restriction has been required so far on the function $f(\zeta)$. However, to the best of our knowledge, the *only* case in which the matrix ODE (28) is *solvable* is for the assignment (45b) of the function $f(\zeta)$, and for the reasons explained earlier no significant loss of generality is then caused by restricting this assignment to the form (48). The corresponding many-body problem is then (3). The corresponding version of the matrix ODE is (46b), and it is easy to verify that the solution to the initial-value problem for this matrix ODE is provided by the following formulas:

$$U(t) = a^{-1}[\cos(Ft) - EF^{-1}\sin(Ft)]^{-1}[F\sin(Ft) + E\cos(Ft)], \tag{52a}$$

$$E = aU(0), \tag{52b}$$

$$F^2 = aC. \tag{52c}$$

Note that the expression on the right-hand side of (52a) depends on the matrix F^2 rather than the matrix F, and this provides a justification for the way we wrote the last of these matrix equations, (52c). We now note that, via (30) and (32), the last two equations can be rewritten as follows:

$$E = aR(0)\mathrm{diag}[\zeta_n(0)][R(0)]^{-1}, \tag{53a}$$

$$F^2 = aR(0)\Gamma(0)[R(0)]^{-1}. \tag{53b}$$

Note that to write the last equation we took advantage of the time-independence of the matrix C in order to evaluate it, conveniently, at $t=0$.

We now note that we are free to assign the initial value $R(0)$ of the diagonalizing matrix $R(t)$, hence we make hereafter the convenient choice $R(0)=1$ (not that these make any substantial difference; we are interested in the eigenvalues of the matrix $U(t)$, see (52a), and the presence of the matrix $R(0)$ in (53) amounts merely to a similarity transformation of the matrix $U(t)$, which does not affect its eigenvalues). Using this choice, as well as (37a) and (39) with (50), (48), and (41), we get

$$E = a\ \mathrm{diag}[\zeta_n(0)], \tag{54}$$

$$(F^2)_{nm} = \delta_{nm}a[\dot{\zeta}_n(0) - a\zeta_n^2(0)] + (1-\delta_{nm})a\{[\dot{\zeta}_n - a\zeta_n^2(0)][\dot{\zeta}_m - a\zeta_n^2(0)]\}^{1/2}\frac{\eta_n(0)}{\eta_m(0)}. \tag{55}$$

We now note that we are as well free to assign the initial values $\eta_n(0)$ of the quantities $\eta_n(t)$, hence we make hereafter the convenient choice $\eta_n(0)=1$ (again, this makes no substantial difference, since clearly the presence of these numbers on the right-hand side of (55) only entails a similarity transformation for the matrix $U(t)$).

We thus see that the matrix F^2 is proportional to the *dyadic* matrix P, see (17f)–(17h):

$$F^2 = \Omega^2 P. \tag{56}$$

We now use the following (rather obvious) property of any *dyadic* matrix W:

$$W_{nm} = v_n v_m \tag{57a}$$

entails

$$\varphi(XW) = \varphi(0) + \frac{\varphi(x)-\varphi(0)}{x}XW \tag{57b}$$

with

$$x = \sum_{n,m=1}^{N} v_n x_{nm} v_m. \tag{57c}$$

Here X is an *arbitrary* $N\otimes N$ matrix whose matrix elements are denoted as x_{nm} and $\varphi(x)$ is any scalar function for which these formulas make good sense. We actually use in the following only the special version of these formulas with $W=P$, see (17f)–(17h), and with a *diagonal* matrix X, namely such that $x_{nm}=x_n\ \delta_{nm}$, in which case the definition (57c) takes the simpler form

$$x = \sum_{n=1}^{N}\left(\frac{\Omega_n^2}{\Omega^2}\right)x_n. \tag{57d}$$

In particular for $X=t^2\mathbf{1}$ and $\varphi(x)=\cos(x^{1/2})$, $\varphi(x)=x^{-1/2}\sin(x^{1/2})$, respectively, $\varphi(x)=x^{1/2}\sin(x^{1/2})$ we get from (56) and (60d), respectively,

$$\cos(Ft) = 1 + [\cos(\Omega t) - 1]P, \tag{58a}$$

$$F^{-1}\sin(Ft) = t + \frac{\sin(\Omega t) - \Omega t}{\Omega}P, \tag{58b}$$

$$F\sin(Ft) = \Omega\sin(\Omega t)P. \tag{59}$$

The insertion in (52a) of these expressions, (58), and of (52b), yields the formula

$$U(t) = \left\{1 + [\cos(\Omega t) - 1]P - aU(0)\left[t + \frac{\sin(\Omega t) - \Omega t}{\Omega}P\right]\right\}^{-1} \cdot \left\{U(0)(1 + [\cos(\Omega t) - 1]P) + \frac{\Omega\sin(\Omega t)}{a}P\right\}, \tag{60a}$$

which can be conveniently rewritten as follows:

$$U(t) = [1 - X^{(1)}(t)P]^{-1}[1 - aU(0)t]^{-1}U(0)[1 - X^{(2)}(t)P], \tag{60b}$$

with the two *diagonal* matrices $X^{(1)}(t)$ and $X^{(2)}(t)$ defined as follows:

$$X^{(1)}(t) = [1 - aU(0)t]^{-1}\left[1 - \cos(\Omega t) + \frac{\sin(\Omega t) - \Omega t}{\Omega}aU(0)\right], \tag{60c}$$

$$X^{(2)}(t) = 1 - \cos(\Omega t) - \Omega\sin(\Omega t)[aU(0)]^{-1}. \tag{60d}$$

Next we use again the formula (57b) with (57d) entailing

$$[1 - X^{(1)}(t)P]^{-1} = 1 + \frac{X^{(1)}(t)P}{1 - x^{(1)}(t)} \tag{61a}$$

with

$$x^{(1)}(t) = \sum_{n=1}^{N}\left(\frac{\Omega_n^2}{\Omega^2}\right)\frac{\Omega[1 - \cos(\Omega t)] + [\sin(\Omega t) - \Omega t]a\zeta_n(0)}{\Omega[1 - a\zeta_n(0)t]}, \tag{61b}$$

and we thereby rewrite (60b) as follows:

$$U(t) = X^{(0)}(t) + \widetilde{X}^{(1)}(t)PX^{(0)}(t) - X^{(0)}(t)X^{(2)}(t)P - \widetilde{X}^{(1)}(t)PX^{(0)}(t)X^{(2)}(t)P, \tag{61c}$$

with the *diagonal* matrices $X^{(0)}(t)$ and $\widetilde{X}^{(1)}(t)$ defined as follows:

$$X^{(0)}(t) = [1 - aU(0)t]^{-1}U(0), \tag{61d}$$

$$\widetilde{X}^{(1)}(t) = \frac{X^{(1)}(t)}{1 - x^{(1)}(t)}. \tag{61e}$$

Finally we note that clearly

$$PX^{(0)}(t)X^{(2)}(t)P = \sum_{n=1}^{N}\left(\frac{\Omega_n^2}{\Omega^2}\right)\frac{[1 - \cos(\Omega t)]a\zeta_n(0) - \Omega\sin(\Omega t)}{a[1 - a\zeta_n(0)t]}P \tag{62}$$

and we thereby get from this formula the solution formula (17). *Proposition 1* is thereby proven.

As for *Proposition 2*, the fact that it is a consequence via (21) with (16) of *Proposition 1* was already explained in the preceding section.

B. Equilibrium configurations

Let us discuss first the (genuine) equilibrium configurations of the system of Newtonian equations of motion (3), namely the solutions (with $\overline{\zeta}_n \neq \overline{\zeta}_m$ if $n \neq m$) of the set of N algebraic equations

$$\sum_{m=1,m\neq n}^{N} \frac{(\overline{\zeta}_m)^2}{\overline{\zeta}_n - \overline{\zeta}_m} = 0. \tag{63}$$

It is obvious that there are no genuine equilibrium configurations for $N=2$, so we can hereafter assume that $N \geqslant 3$. Let us then prove first of all that these equations entail

$$\sum_{n=1}^{N} \overline{\zeta}_n = 0. \tag{64}$$

Indeed by summing (63) over n from 1 to N we get

$$0 = \sum_{m,n=1,m\neq n}^{N} \frac{(\overline{\zeta}_m)^2}{\overline{\zeta}_n - \overline{\zeta}_m} = \sum_{m,n=1,m\neq n}^{N} \frac{(\overline{\zeta}_m)^2 - (\overline{\zeta}_n)^2 + (\overline{\zeta}_n)^2}{\overline{\zeta}_n - \overline{\zeta}_m} = \sum_{m,n=1,m\neq n}^{N} (\overline{\zeta}_m + \overline{\zeta}_n) = 2(N-1)\sum_{n=1}^{N} \overline{\zeta}_n, \tag{65}$$

which proves (64).

Introduce then the polynomial of degree N (assuming that it exists)

$$\psi(\zeta) = \prod_{n=1}^{N} (\zeta - \overline{\zeta}_n). \tag{66a}$$

It is then easy to show (or see Eqs. 2.3.3(12) and 2.3.3(15) of Ref. 2) that

$$\zeta\psi'(\zeta) - N\psi(\zeta) = \psi(\zeta)\sum_{n=1}^{N} (\zeta - \overline{\zeta}_n)^{-1}\overline{\zeta}_n, \tag{66b}$$

$$\zeta^2\psi''(\zeta) - N(N-1)\psi(\zeta) = 2\psi(\zeta)\sum_{n=1}^{N} (\zeta - \overline{\zeta}_n)^{-1} \sum_{m=1,m\neq n}^{N} \frac{(\overline{\zeta}_n)^2}{\overline{\zeta}_n - \overline{\zeta}_m}. \tag{66c}$$

We now replace on the right-hand side of the last formula the quantity $(\overline{\zeta}_n)^2$ with $(\overline{\zeta}_n)^2 - (\overline{\zeta}_m)^2 + (\overline{\zeta}_m)^2$, ignore the last of these three terms thanks to (63), and by taking advantage of (64) and (66b) we find that the polynomial $\psi(\zeta)$ must satisfy the linear ODE

$$\zeta^2\psi''(\zeta) - 2(N-2)\zeta\psi'(\zeta) + N(N-3)\psi(\zeta) = 0. \tag{66d}$$

The *general* solution of this equation is (up to a multiplicative constant)

$$\psi(\zeta) = \zeta^{N-3}(\zeta^3 - \eta^3), \tag{66e}$$

with η an *arbitrary* constant. Clearly this polynomial $\psi(\zeta)$ has the root $\overline{\zeta}=0$ with multiplicity $N-3$, and the three roots $\overline{\zeta}_k = \eta \exp(2\pi ik/3)$. And it is plain that these results entail the findings reported in the preceding section.

Let us then turn our attention to the second, *isochronous* system (4). It is easily seen that

insertion of the definition (25) in the equations of motion (4) yields the following set of N algebraic equations for the N numbers u_n:

$$(u_n - u_n^2)\left\{1 - \sum_{m=1,m\neq n}^{N} \frac{u_m - u_m^2}{u_n - u_m}\right\} = 0. \tag{67a}$$

It is clear from these equations that, if the set $\{u_1, u_2, \ldots, u_N\}$ of N numbers u_n provide a solution to the set of N algebraic equations

$$\sum_{m=1,m\neq n}^{N} \frac{u_m - u_m^2}{u_n - u_m} = 1, \tag{67b}$$

with none of the numbers u_n vanishing ($u_n \neq 0$, $n=1,\ldots,N$), then the set $\{u_1, u_2, \ldots, u_N, 0\}$ of $N+1$ numbers u_n provide a solution to the set of $N+1$ algebraic equations which obtain from (67a) by replacing N with $N+1$ as upper limit of the sum and by letting the index n run from 1 to $N+1$ rather than from 1 to N. Likewise, if the N numbers u_n provide a solution to the set of algebraic equations (67b) with none of these numbers u_n being unity ($u_n \neq 1$, $n=1,\ldots,N$), then the set $\{u_1, u_2, \ldots, u_N, 1\}$ of $N+1$ numbers u_n provide a solution to the set of $N+1$ algebraic equations which obtain from (67a) by replacing N with $N+1$ as upper limit of the sum and by letting the index n run from 1 to $N+1$ rather than from 1 to N. And moreover, if the N numbers u_n provide a solution to the set of algebraic equations (67b) with none of these numbers u_n neither vanishing nor being unity ($u_n \neq 0$ and $u_n \neq 1$, $n=1,\ldots,N$), then the set $\{u_1, u_2, \ldots, u_N, 0, 1\}$ of $N+2$ numbers u_n provide a solution to the set of $N+2$ algebraic equations which obtain from (67a) by replacing N with $N+2$ as upper limit of the sum and by letting the index n run from 1 to $N+1$ rather than from 1 to N. Hence, we can now only focus on the system of algebraic equations (67b), and then extend our conclusions about the equilibrium configurations by taking advantage of these observations.

To find all the solution of (67b) (with $u_n \neq u_m$) we note first of all that this system of N algebraic equations entails

$$S \equiv \sum_{n=1}^{N} u_n = \sum_{n=1}^{N} u_n^2, \tag{68}$$

as can be easily seen by multiplying (67b) by $u_n - u_n^2$, then summing over the index n from 1 to N and noting that thereby the double sum on the left-hand side vanishes due to the antisymmetry of the summand under the exchange of the two dummy indices m and n.

Next we prove that

$$S = \frac{N(N+1)}{2(N-1)}. \tag{69}$$

To obtain this result we sum (67b) from 1 to N over the index n, and use the identities

$$\sum_{m,n=1,m\neq n}^{N} \frac{u_m}{u_n - u_m} = -\frac{1}{2} \sum_{m,n=1,m\neq n}^{N} \frac{u_n - u_m}{u_n - u_m} = -\frac{N(N-1)}{2}, \tag{70a}$$

$$\sum_{m,n=1,m\neq n}^{N} \frac{u_m^2}{u_n - u_m} = -\frac{1}{2} \sum_{m,n=1,m\neq n}^{N} \frac{u_n^2 - u_m^2}{u_n - u_m} = -\sum_{m,n=1,m\neq n}^{N} u_n = -S(N-1). \tag{70b}$$

Next, we multiply by u_n the relation (67b), and again sum from 1 to N over the index n. Now we use the identities

$$\sum_{m,n=1,m\neq n}^{N} \frac{u_n u_m}{u_n - u_m} = 0, \tag{71a}$$

$$\sum_{m,n=1,m\neq n}^{N} \frac{u_n u_m^2}{u_n - u_m} = -\frac{1}{2} \sum_{m,n=1,m\neq n}^{N} \frac{u_n u_m (u_n - u_m)}{u_n - u_m} = -\frac{1}{2} \sum_{m,n=1,m\neq n}^{N} u_n u_m = \frac{S - S^2}{S}. \tag{71b}$$

Note that to obtain the second of these identities we used in the end both formulas (68). In this manner we obtain the relation

$$S(S-3) = 0, \tag{72}$$

which implies that $S=0$ or $S=3$. The first possibility is clearly incompatible with (69). So we conclude that $S=3$, and, via (69), we then conclude that the only values of N for which the set of algebraic equations (67b) can have solutions are $N=2$ and $N=3$. And we can now rewrite the relations (68) in the more explicit form

$$\sum_{n=1}^{N} u_n = \sum_{n=1}^{N} u_n^2 = 3. \tag{73}$$

Using these two formulas as well as (67b) we easily conclude that for $N=2$ the only solution of these equations is (26).

Likewise, for $N=3$, from these equations and one of the equations (67b) one easily gets the solution (27).

Let us also mention that another, perhaps more elegant, route to get all these results is via the same technique used earlier (or see Sec. 2.3.3 of Ref. 2), implying that the solutions u_n of (67b) are the zeros of the polynomial $y(u)$ of degree N (if it exists) that satisfies the ODE

$$uy'' - 2(N-S)y' = u^2 y'' + 2(2-N)uy' + N(N-3)y. \tag{74}$$

In particular, for $S=3$ and for $N=2$ this ODE becomes simply

$$uy'' + 2y' = u^2 y'' - 2y, \tag{75a}$$

and its polynomial solution is (up to a multiplicative constant)

$$y(u) = u^2 - 3u + 3, \tag{75b}$$

and the two zeros of this polynomial are clearly given by (26). Likewise, for $S=3$ and for $N=3$ this ODE, (74), becomes simply

$$uy'' = u^2 y'' - 2uy', \tag{76a}$$

which clearly has (up to a multiplicative constant) the general solution

$$y(u) = (u-1)^3 - \eta^3, \tag{76b}$$

with η an arbitrary constant, implying that its three zeros are indeed given by (27).

IV. OTHER VERSIONS OF THESE SOLVABLE MODELS

In this section we provide other versions of the solvable model (3) and of its *isochronous* variant (4).

The idea is to introduce the time-dependent monic polynomial $\varphi(\zeta,t)$, of degree N in the variable ζ, that has the N zeros $\zeta_n(t)$, and to then consider the time evolution of its N coefficients $b_m(t)$:

$$\varphi(\zeta,t)=\prod_{n=1}^{N}[\zeta-\zeta_n(t)]=\zeta^N+\sum_{m=1}^{N}b_m(t)a^{-m}\zeta^{N-m}. \tag{77}$$

Indeed it is rather easily seen—by using techniques analogous to those used in the preceding section (or see again Sec. 2.3.3 of Ref. 2)—that, if the zeros $\zeta_n(t)$ evolve according to the Newtonian system of ODEs (3), the polynomial $\varphi(\zeta,t)$ evolves according to the second-order PDE

$$\begin{aligned}&\varphi_{tt}+2a\zeta^2\varphi_{\zeta t}+a^2\zeta^4\varphi_{\zeta\zeta}+2[b_1-(N-1)a\zeta]\varphi_t+2a\zeta^2[b_1-(N-2)a\zeta]\varphi_\zeta\\&\quad+[2b_2-2(N-1)ab_1\zeta+N(N-3)a^2\zeta^2]\varphi=0.\end{aligned} \tag{78}$$

Here and throughout subscripted variables denote partial differentiations, e.g., $\varphi_{\zeta t}\equiv\partial^2\varphi(\zeta,t)/\partial\zeta\partial t$.

Clearly this PDE entails that the N coefficients $b_m(t)$ evolve according to the following system of N ODEs:

$$\ddot{b}_m-2m\dot{b}_{m+1}+(m+2)(m-1)b_{m+2}=-2b_1(\dot{b}_m-mb_{m+1})-2b_2b_m, \tag{79a}$$

supplemented by the boundary conditions

$$b_{N+1}=b_{N+2}=0. \tag{79b}$$

Let us recall that, according to the above-announced convention, the index m in (79a) runs from 1 to N (actually (79a) is identically satisfied also for $m=0$, if one sets $b_0=1$, consistently with (77)).

The solvability of this nonlinear system of ODEs is of course implied by the solvability (see *Proposition 1*) of the system (3), since the relation (77) entails that the coefficients b_m can be expressed in terms of the zeros ζ_n,

$$b_1=-a\sum_{n=1}^{N}\zeta_n,\quad b_2=\frac{1}{2}\left(b_1^2-a^2\sum_{n=1}^{N}\zeta_n^2\right),\ \dots\ . \tag{80}$$

Hence, for instance,

$$b_1(t)=-a\ \mathrm{trace}[U(t)],\quad b_N(t)=(-a)^N\det[U(t)], \tag{81}$$

where the $N\otimes N$ matrix $U(t)$ is given by (17)—with the two constant $N\otimes N$ matrices $U(0)$ and C, as well as the scalar Ω, expressed of course via the initial values $b_m(0)$, $\dot{b}_m(0)$ through the explicit formulas that relate the initial values of the N zeros and of their time-derivatives, $\zeta_n(0)$ and $\dot{\zeta}_n(0)$, to these initial values $b_m(0)$, $\dot{b}_m(0)$, see (77) (at $t=0$) and the following formula (at $t=0$) that obtains by differentiating (77) and equates two polynomials in ζ of degree $N-1$:

$$\varphi_t(\zeta,t)=-\varphi(\zeta,t)\sum_{n=1}^{N}[\zeta-\zeta_n(t)]^{-1}\dot{\zeta}_n(t)=\sum_{m=1}^{N}\dot{b}_m(t)a^{-m}\zeta^{N-m}. \tag{82}$$

The fact that the nonlinear system (79) is *solvable* (namely, that its solution can be in principle obtained by merely algebraic operations) is a nontrivial result (up to the observation that all correct mathematical findings are in some sense trivial—after their validity has been proven!). Note that the first ODE of this system, namely that corresponding to $m=1$,

$$\ddot{b}_1-2\dot{b}_2=-2b_1\dot{b}_1, \tag{83a}$$

can be integrated once, yielding

$$b_2 = \tfrac{1}{2}(\dot{b}_1 + b_1^2 + \alpha^2), \tag{83b}$$

with α^2 an arbitrary constant. But, even for $N=2$, the next equation (for $m=2$) of this system,

$$\ddot{b}_2 = -2b_1\dot{b}_2 - 2b_2^2, \tag{84a}$$

which via (83b) becomes the following third-order ODE for the single dependent variable $b_1(t) \equiv \theta(t)$,

$$\dddot{\theta} + 4\ddot{\theta}\theta + 3\dot{\theta}^2 + 6\theta^2\dot{\theta} + \theta^4 + 2\alpha^2(\dot{\theta} + \theta^2) + \alpha^4 = 0, \tag{84b}$$

does not look trivially integrable (even just once, let alone three times!). Indeed the fact that this ODE admits the explicit solution

$$\begin{aligned}\theta(t) = &\left(\left\{\theta(0) + \frac{1}{2}[\theta^2(0) + \dot{\theta}(0) + \alpha^2]t\right\}\cos(\alpha t) + \frac{1}{2}\{\theta^2(0) + \dot{\theta}(0) - \alpha^2 + [\ddot{\theta}(0) + 3\dot{\theta}(0)\theta(0) + \theta^3(0)\right.\\ &\left. + \alpha^2\theta(0)]t\}\frac{\sin(\alpha t)}{\alpha}\right)\cdot\left(\left\{1 - \frac{1}{2\alpha^2}[\ddot{\theta}(0) + 3\dot{\theta}(0)\theta(0) + \theta^3(0) + \alpha^2\theta(0)]t\right\}\cos(\alpha t)\right.\\ &\left. + \frac{1}{2\alpha^2}\{\ddot{\theta}(0) + 3\dot{\theta}(0)\theta(0) + \theta^3(0) + 3\alpha^2\theta(0) + [\theta^2(0) + \dot{\theta}(0) + \alpha^2]\alpha^2 t\}\frac{\sin(\alpha t)}{\alpha}\right)^{-1}\end{aligned} \tag{84c}$$

is remarkable, as the diligent reader who tries and verifies this fact will note (at least if he or she tries to do so without any computer assistance).

An analogous variant of the *isochronous* system (4) leads to the autonomous system of ODEs

$$\begin{aligned}&\ddot{c}_m - i(2m+1)\omega\dot{c}_m - 2m\dot{c}_{m+1} - \omega^2 m(m+1)c_m + 2im(m+1)\omega c_{m+1} + (m+2)(m-1)c_{m+2}\\ &\quad = -2c_1(\dot{c}_m - im\omega c_m - mc_{m+1}) - 2c_2c_m,\end{aligned} \tag{85a}$$

with the boundary conditions

$$c_{N+1} = c_{N+2} = 0, \tag{85b}$$

which might just as well be obtained by inserting the *ansatz*

$$c_m(t) = \exp(im\omega t)b_m(\tau), \quad \tau = \frac{\exp(i\omega t) - 1}{i\omega}, \tag{86}$$

in (79). This of course implies that this system of ODEs, (85a), is just as *solvable* as the system of ODEs for the coefficients $b_m(t)$, see (79) and, e.g., (81); moreover *all* the solutions $c_m(t)$ of this system of N coupled ODEs, (85a), are clearly *periodic* with period T, see (5), $c_m(t+T) = c_m(t)$.

V. BEHAVIOR NEAR THE EQUILIBRIUM CONFIGURATIONS, AND SOME DIOPHANTINE RELATIONS

In the following we discuss the behavior of the *isochronous* system (4), and of its variant (85), in the neighborhood of the respective equilibrium configurations, and we thereby derive some amusing *diophantine* relations.

To get the linearized equations of motion describing the motion of the *isochronous* system (4) in the neighborhood of its equilibrium configuration we set

$$z_n(t) = \left(\frac{\omega}{ia}\right)u_n + \varepsilon w_n(t), \tag{87}$$

where the numbers u_n characterize the equilibrium configurations, see (25), and ε is a small parameter. We thereby obtain the following linearized equations of motion:

$$\ddot{\underline{w}} + i\omega\underline{\Gamma}\,\dot{\underline{\omega}} + \omega^2\underline{\Lambda}\underline{w} = 0, \tag{88}$$

where $\underline{w} \equiv (w_1 \ldots, w_N)$ indicates of course an N-vector and the two $N \otimes N$ matrices $\underline{\Gamma}$ and $\underline{\Lambda}$ are defined as follows:

$$\Gamma_{nm} = \delta_{nm}\left[-3 + 2u_n + 2\sum_{\ell=1,\ell\neq n}^{N}\frac{(u_\ell - u_\ell^2)}{u_n - u_\ell}\right] + (1-\delta_{nm})\frac{2(u_n - u_n^2)}{u_n - u_m}, \tag{89}$$

$$\Lambda_{nm} = 2\delta_{nm}\left[2u_n - 1 + \sum_{\ell=1,\ell\neq n}^{N}\frac{(u_\ell - 2u_\ell u_n + u_n^2)(u_\ell - 1)u_\ell}{(u_n - u_\ell)^2}\right] + (1-\delta_{nm})\frac{2u_n(u_n - 2u_m u_n + u_m^2)(1-u_n)}{(u_n - u_m)^2}. \tag{90}$$

Here and always in the following $\delta_{nm} \equiv \delta_{n,m}$ is the usual Kronecker symbol.

The general solution of the linear system of ODEs (88) reads

$$\underline{w}(t) = \sum_{m=1}^{2N}\alpha_m \exp(i\lambda_m \omega t)\underline{v}^{(m)}, \tag{91}$$

where the $2N$ constants α_n are *arbitrary* and the $2N$ numbers λ_m respectively the $2N$ constant N-vectors $\underline{v}^{(m)}$ are the eigenvalues respectively the eigenvectors of the following eigenvalue problem:

$$[-\lambda_m^2\underline{1} - \lambda_m\underline{\Gamma} + \underline{\Lambda}]\underline{v}^{(m)} = 0, \quad m = 1, \ldots, 2N. \tag{92}$$

Hence the eigenvalues λ_m are the $2N$ roots of the following polynomial equation (of degree $2N$ in λ):

$$D^{(N)}(\lambda) \equiv \det[\lambda^2\underline{1} + \lambda\underline{\Gamma} - \underline{\Lambda}] = 0. \tag{93}$$

But the *exact* solution of the *isochronous* system (4) is *completely periodic* with period T, see (5), hence the same property of isochronicity must be shared by its behavior in the neighborhood of the equilibrium configurations. We therefore conclude that *all* the roots of this algebraic equation must be *integers*. Later we display the corresponding *diophantine equations*.

Analogous results obtain by applying the same approach to the version (85) of our *isochronous* system. To get them we set in (85)

$$c_m(t) = (-i\omega)^m[a_m + \varepsilon\gamma_m(t)], \tag{94}$$

where the N constants a_m satisfy the N algebraic equations

$$-m(m+1)a_m + 2m(m+1)a_{m+1} - (m+2)(m-1)a_{m+2} = 2ma_1(a_m - a_{m+1}) + 2a_2a_m, \tag{95}$$

which obtain (to the zeroth order in ε) by inserting (94) in (85).

Likewise, to the first order in ε, we get the following *linear* system of N equations of motion:

$$\ddot{\gamma}_m - i(2m+1)\omega\dot{\gamma}_m + 2im\omega\dot{\gamma}_{m+1} - 2i\omega a_1\dot{\gamma}_m - m(m+1)\omega^2\gamma_m + 2m(m+1)\omega^2\gamma_{m+1} - 2m\omega^2 a_1\gamma_m - (m^2+m-2)\omega^2\gamma_{m+2} + 2m\omega^2 a_1\gamma_{m+1} - 2\omega^2 a_2\gamma_m - 2m\omega^2 a_m\gamma_1 + 2m\omega^2 a_{m+1}\gamma_1 - 2\omega^2 a_m\gamma_2 = 0, \tag{96a}$$

with the boundary condition

$$\gamma_{N+1}(t) = \gamma_{N+2}(t) = 0. \tag{96b}$$

Equivalently this system of ODEs reads

$$\ddot{\underline{\gamma}} + i\omega \underline{M}\,\dot{\underline{\gamma}} + \omega^2 \underline{L}\,\underline{\gamma} = 0 \tag{97}$$

with the two $N \otimes N$ matrices $\underline{M}$ and $\underline{L}$ defined as follows:

$$M_{nm} = -(2n+1)\delta_{n,m} + 2n\delta_{n+1,m} - 2a_1\delta_{n,m} \tag{98}$$

$$\begin{aligned} N_{nm} = {} & -n(n+1)\delta_{n,m} + 2n(n+1)\delta_{n+1,m} - 2na_1\delta_{n,m} - (n^2+n-2)\delta_{n+2,m} + 2na_1\delta_{n+1,m} - 2a_2\delta_{n,m} \\ & - 2na_n\delta_{1,m} + 2na_{n+1}\delta_{1,m} - 2a_n\delta_{2,m}. \end{aligned} \tag{99}$$

The general solution of this system reads

$$\underline{\gamma}(t) = \sum_{m=1}^{2N} \beta_m \exp(i\lambda_m \omega t)\underline{\mu}^{(m)}, \tag{100}$$

where the $2N$ constants β_n are *arbitrary* and the $2N$ numbers λ_m respectively the $2N$ constant N-vectors $\underline{v}^{(m)}$ are the eigenvalues respectively the eigenvectors of an eigenvalue problem that clearly entails,

$$\widetilde{D}^{(N)}(\lambda) \equiv \det[\lambda^2 \underline{1} + \lambda \underline{M} - \underline{L}] = 0. \tag{101}$$

As indicated by our notation, the eigenvalues λ_m coincide of course with those defined just above; therefore, by the same token this polynomial equation of degree $2N$ in λ must have a *diophantine* character (i.e., integer roots). The corresponding results are exhibited in the following.

Equilibrium configurations and diophantine relations. In the following formulas the symbols $D_j^{(N)}$ and $\widetilde{D}_j^{(N)}$ denote the determinants (93) and (101), respectively with the index j distinguishing (if need be) different equilibrium configuration.

For $N=2$ to the *first* equilibrium configuration

$$u_1 = 0, \quad u_2 = 1; \quad a_1 = -1, \quad a_2 = 0, \tag{102a}$$

there correspond the *diophantine* equations

$$\begin{aligned} D_1^{(2)}(\lambda) \equiv \det\begin{pmatrix} (\lambda-1)(\lambda-2) & 0 \\ 0 & (\lambda+1)(\lambda-2) \end{pmatrix} = \widetilde{D}_1^{(2)}(\lambda) \equiv \det\begin{pmatrix} (\lambda+1)(\lambda-2) & 2(\lambda-2) \\ 0 & (\lambda-1)(\lambda-2) \end{pmatrix} \\ = \lambda^4 - 4\lambda^3 + 3\lambda^2 + 4\lambda - 4 = (\lambda-1)(\lambda+1)(\lambda-2)^2. \end{aligned} \tag{102b}$$

And to the *second* equilibrium configuration,

$$u_{1,2} = \frac{3 \pm i\sqrt{3}}{2}; \quad a_1 = -3, \quad a_2 = 3, \tag{103a}$$

there corresponds the *diophantine* equations

$$\begin{aligned} D_2^{(2)}(\lambda) \equiv \det\begin{pmatrix} \lambda^2 + \lambda(i\sqrt{3}+2) - 2 & -2(\lambda - i\sqrt{3}+1) \\ -2((\lambda + i\sqrt{3}+1)) & \lambda^2 + \lambda(-i\sqrt{3}+2) - 2 \end{pmatrix} = \widetilde{D}_2^{(2)}(\lambda) \\ \equiv \det\begin{pmatrix} (\lambda+5)(\lambda-2) & 2(\lambda-2) \\ 12 & \lambda^2+\lambda+6 \end{pmatrix} = P_4(\lambda). \end{aligned} \tag{103b}$$

Here and in the following

$$P_4(\lambda) \equiv \lambda^4 + 4\lambda^3 - \lambda^2 - 16\lambda - 12 = (\lambda-2)(\lambda+3)(\lambda+2)(\lambda+1). \tag{104}$$

For $N=3$ to the one-parameter set of equilibrium configurations

$$u_k(\eta) = 1 + \eta \exp\left(\frac{2\pi i}{3}k\right), \quad k = 1,2,3,$$
$$a_1 = -3, \quad a_2 = 3, \quad a_3 = -\eta^3 - 1, \tag{105a}$$

there correspond the following *diophantine* equations:

$$D_1^{(3)}(\lambda) \equiv \det[\underline{H}] = \tilde{D}_1^{(3)}(\lambda) \equiv \det\begin{pmatrix} (\lambda+5)(\lambda-2) & 2(\lambda-2) & 0 \\ 4(\eta^3+4) & \lambda^2+\lambda+6 & 4\lambda \\ -6(\eta^3+1) & -2(\eta^3+1) & \lambda(\lambda-1) \end{pmatrix}$$
$$= \lambda^6 + 3\lambda^5 - 5\lambda^4 - 15\lambda^3 + 4\lambda^2 + 12\lambda = \lambda(\lambda-1)P_4(\lambda). \tag{105b}$$

Here and in the following

$$\underline{H}(\lambda,\eta) \equiv \begin{pmatrix} h_1(\lambda,\eta) & h_{12}(\lambda,\eta) & h_{13}(\lambda,\eta) \\ h_{21}(\lambda,\eta) & h_2(\lambda,\eta) & h_{23}(\lambda,\eta) \\ h_{31}(\lambda,\eta) & h_{32}(\lambda,\eta) & h_3(\lambda,\eta) \end{pmatrix}, \tag{106a}$$

$$h_k(\lambda,\eta) \equiv \lambda^2 + \lambda\left[1 + 2\eta\exp\left(\frac{2i\pi k}{3}\right)\right] + \frac{2}{3}\left[\eta\exp\left(\frac{2i\pi k}{3}\right) + 1\right]\left[\eta\exp\left(\frac{2i\pi k}{3}\right) - 2\right], \tag{106b}$$

$$h_{jk}(\lambda,\eta) \equiv -\frac{2}{3}\exp\left(\frac{is_{jk}\pi}{6}\right)\left[\eta\exp\left(\frac{2i\pi j}{3}\right) + 1\right] \cdot \left\{\sqrt{3}\lambda + \exp\left(\frac{is_{jk}\pi}{6}\right)\left[\sqrt{7}\eta\exp\left[i\left(\frac{2\pi k}{3} - s_{jk}\varphi\right)\right] + 1\right]\right\} \tag{106c}$$

where

$$\exp(i\varphi) = \frac{5}{2\sqrt{7}} + \frac{1}{2\sqrt{7}}i\sqrt{3} \tag{106d}$$

and $s_{jk}=+$ if $k=j+1 \bmod(3)$, $s_{jk}=-$ if $k=j+2 \bmod(3)$. Note the independence of the determinants from the value of the *arbitrary* constant η (this remark will not be repeated in the following, when this phenomenon will recur). And to the additional equilibrium configuration,

$$u_{1,2} = \frac{3 \pm i\sqrt{3}}{2}, \quad u_3 = 1; \quad a_1 = -4, \quad a_2 = 6, \quad a_3 = -3, \tag{107a}$$

there correspond the following *diophantine* equations:

$$D_2^{(3)}(\lambda) \equiv \det\begin{pmatrix} \lambda^2+\lambda(i\sqrt{3}+2)-2 & -2(\lambda-i\sqrt{3}+1) & -(i\sqrt{3}+3)(\lambda+1) \\ -2(\lambda+i\sqrt{3}+1) & \lambda^2+\lambda(-i\sqrt{3}+2)-2 & (i\sqrt{3}-3)(\lambda+1) \\ 0 & 0 & (\lambda+4)(\lambda+1) \end{pmatrix}$$
$$= (\lambda+4)(\lambda+1)D_2^{(2)}(\lambda) = \tilde{D}_2^{(3)}(\lambda) \equiv \det\begin{pmatrix} (\lambda+7)(\lambda-2) & 2(\lambda-2) & 0 \\ 36 & \lambda^2+3\lambda+14 & 4(\lambda+1) \\ -18 & -6 & \lambda(\lambda+1) \end{pmatrix}$$
$$= \lambda^6 + 9\lambda^5 + 23\lambda^4 - 5\lambda^3 - 96\lambda^2 - 124\lambda - 48 = (\lambda+1)(\lambda+4)P_4(\lambda). \tag{107b}$$

For $N=4$ to the *first* one-parameter set of equilibrium configurations,

$$u_k(\eta) = 1 + \eta \exp\left(\frac{2\pi i}{3}k\right), \quad k = 1,2,3, \quad u_4 = 0,$$
$$a_1 = -3, \quad a_2 = 3, \quad a_3 = 1 - \eta^3, \quad a_4 = 0, \tag{108a}$$

there correspond the following *diophantine* equations:

$$D_1^{(4)}(\lambda) \equiv \det\begin{pmatrix} \underline{H}(\lambda,\eta) & \vec{\sigma}^T(\lambda,\eta) \\ 0 & (\lambda-1)(\lambda-2) \end{pmatrix} = \tilde{D}_1^{(4)}(\lambda)$$
$$\equiv \det\begin{pmatrix} (\lambda+5)(\lambda-2) & 2\lambda-4 & 0 & 0 \\ 4(\eta^3+4) & \lambda^2+\lambda+6 & 4\lambda & 4 \\ -6(\eta^3+1) & -2(\eta^3+1) & \lambda(\lambda-1) & 6(\lambda-1) \\ 0 & 0 & 0 & (\lambda-1)(\lambda-2) \end{pmatrix}$$
$$= \lambda^8 - 12\lambda^6 + 6\lambda^5 + 39\lambda^4 - 30\lambda^3 - 28\lambda^2 + 24\lambda = \lambda(\lambda-1)^2(\lambda-2)P_4(\lambda); \tag{108b}$$

where the three components of the column three-vector $\vec{\sigma}^T(\lambda,\eta)$ are defined as follows:

$$\sigma_k^T = -2\eta \exp\left(\frac{2\pi i}{3}k\right)(\lambda-1), \quad k = 1,2,3; \tag{108c}$$

and to the second,

$$u_k(\eta) = 1 + \eta \exp\left(\frac{2\pi i}{3}k\right), \quad k = 1,2,3, \quad u_4 = 1,$$
$$a_1 = -4, \quad a_2 = 6, \quad a_3 = -4 - \eta^3, \quad a_4 = 1 + \eta^3, \tag{109a}$$

there correspond the following *diophantine* equations:

$$D_2^{(4)}(\lambda) \equiv \det\begin{pmatrix} \underline{H}(\lambda,\eta) & \vec{\pi}^T(\lambda,\eta) \\ 0 & (\lambda+1)(\lambda+4) \end{pmatrix} = D_2^{(4)}(\lambda)$$
$$\equiv \det\begin{pmatrix} (\lambda+7)(\lambda-2) & 2(\lambda-2) & 0 & 0 \\ 4(\eta^3+10) & 3\lambda+\lambda^2+14 & 4(\lambda+1) & 4 \\ -6(2\eta^3+5) & -2(\eta^3+4) & \lambda(\lambda+1) & 6\lambda \\ 8(\eta^3+1) & 2(\eta^3+1) & 0 & \lambda(\lambda-1) \end{pmatrix}$$
$$= \lambda^8 + 8\lambda^7 + 14\lambda^6 - 28\lambda^5 - 91\lambda^4 - 28\lambda^3 + 76\lambda^2 + 48\lambda$$
$$= \lambda(\lambda+1)(\lambda+4)(\lambda-1)P_4(\lambda), \tag{109b}$$

where the three components of the column three-vector $\vec{\pi}^T(\lambda,\eta)$ are defined as follows:

$$\pi_k^T(\lambda,\eta) = -2\left[\eta \exp\left(\frac{2\pi i}{3}k\right) + 1\right](\lambda+1), \quad k = 1,2,3. \tag{109c}$$

Finally for $N=5$ to the single equilibrium configuration

$$u_k(\eta) = 1 + \eta \exp\left(\frac{2\pi i}{3}k\right), \quad k = 1,2,3, \quad u_4 = 0, \quad u_5 = 1,$$
$$a_1 = -4, \quad a_2 = 6, \quad a_3 = -4 - \eta^3, \quad a_4 = 1 + \eta^3, \quad a_5 = 0, \tag{110a}$$

there correspond the following *diophantine* equations:

$$D^{(5)}(\lambda) \equiv \det\begin{pmatrix} \underline{H}(\lambda,\eta) & \vec{\sigma}^T(\lambda,\eta) & \vec{\pi}^T(\lambda,\eta) \\ 0 & (\lambda-1)(\lambda-2) & 0 \\ 0 & 0 & (\lambda+1)(\lambda+4) \end{pmatrix} = \widetilde{D}^{(5)}(\lambda)$$

$$\equiv \det\begin{pmatrix} (\lambda+7)(\lambda-2) & 2(\lambda-2) & 0 & 0 & 0 \\ 4(\eta^3+10) & \lambda^2+3\lambda+14 & 4(\lambda+1) & 4 & 0 \\ -6(2\eta^3+5) & -2(\eta^3+4) & \lambda(\lambda+1) & 6\lambda & 10 \\ 8(\eta^3+1) & 2(\eta^3+1) & 0 & \lambda(\lambda-1) & 8(\lambda-1) \\ 0 & 0 & 0 & 0 & (\lambda-1)(\lambda-2) \end{pmatrix}$$

$$= \lambda^{10} + 5\lambda^9 - 8\lambda^8 - 54\lambda^7 + 21\lambda^6 + 189\lambda^5 - 22\lambda^4 - 236\lambda^3 + 8\lambda^2 + 96\lambda$$

$$= \lambda(\lambda+1)(\lambda+4)(\lambda-1)^2(\lambda-2)P_4(\lambda). \tag{110b}$$

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On the absence of continuous symmetries for noncommutative 3-spheres

Fedele Lizzi,[a] Allen Stern,[b] and Patrizia Vitale[c]
Dipartement Scienze Fisiche, Università di Napoli Federico II and INFN Sez. di Napoli, Compl. Univ. Monte S. Angelo, Napoli, 80126, Italy

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A large class of noncommutative spherical manifolds was obtained recently from cohomology considerations. A one-parameter family of twisted three-spheres was discovered by Connes and Landi, and later generalized to a three-parameter family by Connes and Dubois-Violette. The spheres of Connes and Landi were shown to be homogeneous spaces for certain compact quantum groups. Here we investigate whether this property can be extended to the noncommutative three-spheres of Connes and Dubois-Violette. Upon restricting to quantum groups which are continuous deformations of Spin(4) and SO(4) with standard coactions, our results suggest that this is not the case. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The recent interest in noncommutative geometry[1] has led to an on-going search for nontrivial examples of noncommutative spaces. Noncommutative generalizations of spheres in various dimensions are known (for a review see Ref. 2), but many of these suffer from a drop in dimensions. Actually, the dimension of a noncommutative space is not uniquely defined. One choice which uses concepts which are natural in noncommutative geometry is the Hochschild dimension. It plays an important role for the three-parameter family of deformations of the sphere S^3 introduced by Connes and Dubois-Violette,[3] which generalizes the one-parameter family discovered previously by Connes and Landi.[4] The Hochschild dimension of the corresponding algebra remains constant (and equal to three) for the deformation. A generalization to higher dimensions is possible for the one-parameter subset, the so-called twisted spheres. This particular subset has another important characteristic. It has been shown[5,6] that the spheres in the one parameter subset carry a coaction of the multiparametric quantum orthogonal groups $\mathrm{SO}_\theta(n+1)$;[7] i.e., they are homogeneous spaces of quantum groups. The aim of this paper is to investigate the possibility of defining a group coaction for the three-parameter 3-spheres as well.

The algebra of the three-parameter spheres S^3_u (Ref. 3) is generated by Hermitian operators $\hat{x}_\mu$, $\mu=0,1,2,3$, subject to

$$\hat{x}_\mu \hat{x}_\mu = \mathbb{1}, \tag{1.1}$$

where $\mathbb{1}$ is the unit operator, and quadratic commutation relations

$$[\hat{x}_\mu, \hat{x}_\nu] = i\hat{E}_{\mu\nu,\rho\sigma}\hat{x}_\rho \hat{x}_\sigma. \tag{1.2}$$

The constant coefficients $\hat{E}_{\mu\nu,\rho\sigma}$ are expressed in terms of four angles ϕ_μ,

[a]Electronic mail: fedele.lizzi@na.infn.it
[b]Also at: Department of Physics, University of Alabama, Tuscaloosa, Alabama 35487, Electronic mail: astern@bama.ua.edu
[c]Electronic mail: patrizia.vitale@na.infn.it

$$\hat{E}_{\mu\nu,\rho\sigma} = \epsilon_{\mu\nu\rho\sigma} \frac{\sin(\phi_\rho - \phi_\sigma)}{\cos(\phi_\mu - \phi_\nu)}, \quad \text{no sum on repeated indices.} \tag{1.3}$$

$\hat{E}_{\mu\nu,\rho\sigma}$ is antisymmetric in the first two indices and symmetric in the last two indices. These commutation relations hold provided no two angles differ by $\pi/2$. Because they depend only on the difference of angles there are three independent deformation parameters, and so one angle, say ϕ_0, can be set to zero. The Connes-Landi case has two of the remaining angles equal with the third zero; e.g., $\phi_1 = \phi_2 = \phi/2$ and $\phi_3 = 0$.[4]

In the search for continuous symmetries, we shall consider linear, as well as spinor, transformations. When all angles are set to zero we require that the symmetries reduce to SO(4) and Spin(4) transformations, respectively. On the other hand, we cannot get Lie group transformations when any of the independent parameters are nonvanishing, since (1.2) would in general not be preserved. If they exist, such symmetries should correspond to quantum group transformations. As the Connes–Dubois–Violette three-spheres are three-parameter deformations of the sphere, their symmetries should correspond to multiparametric deformations of SO(4) and Spin(4). Multiparametric deformations of orthogonal groups[7,8] can be obtained from the standard one-parameter quantum group by applying a twist F, which depends on additional parameters q_{ab}, to the quantum R-matrix. The twist is required to be a specific function in the universal enveloping algebra of the Lie group under consideration. Under these assumptions the quantum deformation becomes at most two-parametric in the case of SO(4). Therefore these kind of q-groups cannot be associated with symmetries for the full three-parameter family of noncommutative spheres. Alternatively, it is possible that there exist symmetries associated with quantum groups which are not deformable to Lie groups. Here, however, our primary focus will be on continuous deformations of Spin(4) and SO(4). We are then justified in looking at the limit of small angles where the search for continuous symmetries is considerably simplified. This is the commutative limit, where the noncommutative sphere goes to S^3, with $\hat{x}_\mu$ going to real commuting coordinates x_μ, $x_\mu x_\mu = 1$, and the noncommutativity gets replaced by a nontrivial Poisson structure on S^3. The commutative limit of the quantum group associated with a continuous symmetry, if it exists, is a Lie-Poisson group,[9] a Lie group with a Poisson bracket on the group manifold which is compatible with the group multiplication.

The search for Lie-Poisson symmetry in the case of the commutative limit of the Connes and Dubois-Violette spheres is carried in Secs. II and III. The Poisson brackets are recovered from (1.2) in the limit of small angles $\phi_\mu \to \epsilon_\mu$

$$\{x_\mu, x_\nu\} = E_{\mu\nu,\rho\sigma} x_\rho x_\sigma, \tag{1.4}$$

where

$$E_{\mu\nu,\rho\sigma} = \epsilon_{\mu\nu\rho\sigma}(\epsilon_\rho - \epsilon_\sigma), \quad \text{no sum on repeated indices.} \tag{1.5}$$

Our approach is to express the Poisson brackets on S^3 in terms of a constant matrix, with the intention of utilizing it as a classical R-matrix for a Lie-Poisson group. In Sec. III we consider Spin(4) transformations. For this one expresses the coordinates in terms of an SU(2) matrix u, with the $\mathrm{Spin}(4) = \mathrm{SU}(2) \times \mathrm{SU}(2)$ transformation given by

$$u \to u' = guh^{-1}, \tag{1.6}$$

where g and h are independent elements of SU(2). The problem is then to find a Poisson structure on Spin(4) which is compatible with the Poisson algebra on S^3. This means that both group multiplication and the action on S^3 are Poisson maps. The former property defines the Lie-Poisson group. Expressing the Poisson brackets on the group in terms of a classical R-matrix, which by definition satisfies the classical Yang-Baxter equations, insures that the Jacobi identity is satisfied. If such a classical R-matrix is found, the group is a Lie-Poisson group, and the space under consideration would be a homogeneous space of the Lie-Poisson group. In Sec. II we find a consistent classical R-matrix only in the Connes-Landi limit, and thus we only get a Poisson map

of Spin(4) in this case. In Sec. III we get the same result for SO(4). We assume the usual linear SO(4) transformations

$$x_\mu \to x'_\mu = M_{\mu\nu} x_\nu, \tag{1.7}$$

$M_{\mu\nu}$ being SO(4) matrix elements. A candidate for the Poisson brackets of $M_{\mu\nu}$ can be written in terms of a constant 16×16 matrix, but the latter only defines a classical R-matrix, i.e., satisfies the classical Yang-Baxter equations, in the Connes-Landi limit.

After ruling out symmetries associated with continuous deformations of Spin(4) and SO(4), there still is the possibility of symmetries at certain finite angles ϕ_μ. This case is more difficult to analyze since it involves going to the full noncommutative theory. In Sec. IV we investigate the full noncommutative theory and search symmetries associated with spinor-type transformations. We express the algebra for the twisted three-sphere in terms of a possible quantum R-matrix. The quantum Yang-Baxter equations should be satisfied for the corresponding quantum group algebra to be coassociative. This cannot be true for arbitrary continuous deformations of the commutative sphere, since in the limit of small angles we recover the system of Sec. II. In Sec. IV we further find no finite values of ϕ_μ, other than those in the Connes-Landi limit, for which the candidate R-matrix satisfies the quantum Yang-Baxter equations.

In Sec. V we Wick rotate the system of Connes and Dubois-Violette, leading to "noncommutative hyperboloids" in Minkowski space, and repeat some of the previous analysis in search of quantum deformations of the Lorentz group which have twisted hyperboloids as homogeneous spaces. As before the search is only successful for a one parameter subset of hyperboloids, namely being the Wick rotation of Connes-Landi spheres.

In Sec. VI we give concluding remarks and discuss the prospects for a more exhaustive study of the full noncommutative theory.

II. POISSON ACTION OF Spin(4)

As u appearing in (1.6) is in the defining representation of SU(2) it can be expressed in terms of the coordinates according to

$$u = x_\mu \tau^\mu, \tag{2.1}$$

where τ^0 is the 2×2 identity matrix $\tau^0 = \mathbb{1}_{2\times 2}$ and τ^i are i times the Pauli matrices, $\tau^i = i\sigma^i$, $i = 1,2,3$. τ^μ satisfy

$$\tfrac{1}{2}\,\mathrm{Tr}(\tau^\mu \tau^\nu) = \eta^{\mu\nu} = \mathrm{diag}(1,-1,-1,-1) \tag{2.2}$$

u has real trace and the traceless part is anti-Hermitian. Hermitian conjugation corresponds to a parity transformation.

We next show that the Poisson brackets (1.4) can be written in the form

$$\{ \underset{1}{u}, \underset{2}{u} \} = \underset{2}{u}\underset{1}{r}\underset{2}{u} - \underset{1}{u}\underset{2}{r}\underset{1}{u}, \tag{2.3}$$

where by u_1 and u_2 is meant $u\otimes \mathbb{1}$ and $\mathbb{1}\otimes u$, respectively, and r is a 4×4 matrix which we need to determine. (For a more general starting ansatz see the end of this section.) From

$$uu^\dagger = u^\dagger u = \mathbb{1}_{2\times 2}, \tag{2.4}$$

r must be Hermitian. From the antisymmetry of the Poisson bracket r should be invariant under exchange of the two tensor product spaces; i.e., $r = r_{12} = r_{21}$. Finally in order to recover the Poisson brackets (1.4) from (2.3) r should satisfy

$$\underset{2}{\tau^\rho}\underset{1}{r}\underset{2}{\tau^\sigma} - \underset{1}{\tau^\rho}\underset{2}{r}\underset{1}{\tau^\sigma} + \underset{2}{\tau^\sigma}\underset{1}{r}\underset{2}{\tau^\rho} - \underset{1}{\tau^\sigma}\underset{2}{r}\underset{1}{\tau^\rho} = 2E_{\mu\nu,\rho\sigma}\underset{1}{\tau^\mu}\underset{2}{\tau^\nu}. \tag{2.5}$$

The solution (up to a term proportional to the identity matrix $\mathbb{1}_{4\times 4} = \tau^0 \times \tau^0$) is

$$r = \kappa_1 \tau^1 \otimes \tau^1 + \kappa_2 \tau^2 \otimes \tau^2 + \kappa_3 \tau^3 \otimes \tau^3, \tag{2.6}$$

where κ_i are given by

$$\begin{aligned} \kappa_1 &= \tfrac{1}{2}(-\epsilon_0 - \epsilon_1 + \epsilon_2 + \epsilon_3), \\ \kappa_2 &= \tfrac{1}{2}(-\epsilon_0 + \epsilon_1 - \epsilon_2 + \epsilon_3), \\ \kappa_3 &= \tfrac{1}{2}(-\epsilon_0 + \epsilon_1 + \epsilon_2 - \epsilon_3). \end{aligned} \tag{2.7}$$

The standard action of Spin(4) on S^3 is (1.6), where g and h are independent elements of SU(2) in the defining representation. The Poisson algebra (2.3) is not preserved under this action. Instead, (2.3) goes to

$$\{ \underset{1}{u'}, \underset{2}{u'} \} = \underset{2\,12}{u'} \underset{12\,1}{r'} \underset{1}{u'} - \underset{1\,21}{u'} \underset{21\,2}{r'} \underset{2}{u'}, \tag{2.8}$$

where

$$\underset{12}{r'} = \underset{1\,2}{g} \underset{2}{h} \underset{2}{r} \underset{2}{h^{-1}} \underset{1}{g^{-1}}. \tag{2.9}$$

On the other hand, if we can consistently assign the following Poisson structure to Spin(4),

$$\{ \underset{1}{g}, \underset{2}{h} \} = -[\, \underset{12}{r}, \underset{1\,2}{gh}\,], \quad \{ \underset{1}{g}, \underset{2}{g} \} = \{ \underset{1}{h}, \underset{2}{h} \} = 0, \tag{2.10}$$

the brackets (2.3) are invariant in the sense that (1.6) is a Poisson map. For these Poisson brackets to be consistent we need that they are antisymmetric and satisfy the Jacobi identity. This means that r should satisfy the classical Yang-Baxter equations,

$$[\, \underset{12}{r}, \underset{13}{r} + \underset{23}{r}\,] + [\, \underset{13}{r}, \underset{23}{r}\,] = I', \tag{2.11}$$

where I' is an adjoint invariant for Spin(4). Note that the classical Yang-Baxter equations did not have to be satisfied for (2.3) to be consistent with the Jacobi identity. It is easily seen that the classical Yang-Baxter and hence the Jacobi identity for (2.10) are satisfied when all κ_i but one vanishes. This corresponds to two angles being equal while the third is zero, i.e., the Connes-Landi case. *Moreover, the Yang-Baxter equations and Jacobi identity are only satisfied in this case,* and thus only then do g and h generate a Lie-Poisson group. In that case we can introduce spinors $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$ and $\bar{\psi} = (\bar{\psi}_1 \bar{\psi}_2)$ with Poisson brackets

$$\{\psi_a, \bar{\psi}_b\} = r_{ad,cb} \psi_c \bar{\psi}_d, \tag{2.12}$$

for which

$$\psi \to \psi' = g\psi, \quad \bar{\psi} \to \bar{\psi}' = \bar{\psi} h^{-1} \tag{2.13}$$

will be a Poisson map. Then the Poisson algebra for $\psi\bar{\psi}$ is identical to that for u in (2.3).

Concerning (2.3), we could start with the most general ansatz which is linear in both u_1 and u_2,

$$\{ \underset{1}{u}, \underset{2}{u} \} = \underset{1\,2}{r^{(1)}} \underset{1\,2}{uu} + \underset{1\,2}{uu} \underset{1\,2}{r^{(2)}} - \underset{2}{u} \underset{1}{r^{(3)}} \underset{1}{u} - \underset{1}{u} \underset{2}{r^{(4)}} \underset{2}{u}, \tag{2.14}$$

where we have introduced four 4×4 matrices $r^{(A)}$, $A = 1,2,3,4$. Now (1.6) is a Poisson map when (2.10) is generalized to

$$\begin{aligned}
\{ \underset{1}{g}, \underset{2}{g} \} &= [r^{(1)}, \underset{1\,2}{gg}], \\
\{ \underset{1}{h}, \underset{2}{h} \} &= [r^{(2)}, \underset{1\,2}{hh}], \\
\{ \underset{1}{g}, \underset{2}{h} \} &= [r^{(3)}, \underset{1\,2}{gh}], \\
\{ \underset{1}{h}, \underset{2}{g} \} &= [r^{(4)}, \underset{1\,2}{hg}].
\end{aligned} \tag{2.15}$$

The matrices $r^{(A)}$, $A=1,2,3,4$, are not fully determined from the Poisson brackets (1.4) of the coordinates. The ambiguity can be fixed once one imposes the requirements that the Poisson brackets for the matrix elements of g and h be antisymmetric and consistent with $\det g = \det h = 1$. However, it can be shown, that then the brackets (2.14) and (2.15) collapse to (2.3) and (2.10), and so the previous conclusions apply.

III. POISSON ACTION OF SO(4)

From the Spin(4) transformations (1.6) we can construct the corresponding SO(4) transformations (1.7), and since the former defines a Poisson map in the Connes-Landi case so does the latter. In that case SO(4) matrix elements $M_{\mu\nu}$ are expressed as quadratic functions of group elements g and h,

$$M_{\mu\nu}(g,h) = \tfrac{1}{2}\mathrm{Tr}(\tau_\mu g \tau^\nu h^{-1}), \tag{3.1}$$

where the indices on τ are raised and lowered with the Minkowski metric (2.2). More generally, if we do not make assumptions like (3.1), it may be possible to find a Poisson map of a group even when no Poisson map is induced by its covering group. However, we find that not to be the case for SO(4) acting on the noncommutative three-sphere, i.e., like Spin(4), SO(4) has a Poisson action only in the Connes-Landi case.

The Poisson brackets (1.4) are not preserved under the action (1.7) of SO(4). Rather they are transformed to

$$\{x'_\mu, x'_\nu\} = E'_{\mu\nu,\rho\sigma} x'_\rho x'_\sigma, \tag{3.2}$$

where

$$E'_{\mu\nu,\rho\sigma} = M_{\mu\alpha} M_{\nu\beta} M_{\rho\gamma} M_{\sigma\delta} E_{\alpha\beta,\gamma\delta}. \tag{3.3}$$

On the other hand, it may be possible to have Poisson brackets on SO(4) which define a Lie-Poisson group and make (1.7) a Poisson map. The Poisson brackets are required to satisfy

$$(\{M_{\mu\gamma}, M_{\nu\delta}\} - E_{\mu\nu,\rho\sigma} M_{\rho\gamma} M_{\sigma\delta} + M_{\nu\sigma} M_{\mu\rho} E_{\rho\sigma,\gamma\delta}) x_\gamma x_\delta = 0, \tag{3.4}$$

in addition to antisymmetry and the Jacobi identity. Equation (3.4) is solved by

$$\{ \underset{1}{M}, \underset{2}{M} \} = [R, \underset{1\,2}{MM}], \tag{3.5}$$

where

$$R_{\mu\nu,\rho\sigma} = E_{\mu\nu,\rho\sigma} + A_{\mu\nu,\rho\sigma}, \tag{3.6}$$

and A is antisymmetric in the last two indices, $A_{\mu\nu,\rho\sigma} = -A_{\mu\nu,\sigma\rho}$. From the requirement that M is orthogonal it follows that R should be a symmetric matrix $R_{\mu\nu,\rho\sigma} = R_{\rho\sigma,\mu\nu}$. This then fixes $A_{\mu\nu,\rho\sigma} = E_{\rho\sigma,\mu\nu}$, and hence R becomes

$$R_{\mu\nu,\rho\sigma} = \epsilon_{\mu\nu\rho\sigma}(\epsilon_\mu - \epsilon_\nu + \epsilon_\rho - \epsilon_\sigma). \tag{3.7}$$

Antisymmetry of the Poisson bracket follows since R is antisymmetric under exchange of the tensor product spaces. The R can be expressed in terms of tensor products of SO(4) generators J_i and $K_i, i=1,2,3$, written in the defining representation,

$$J_1 = \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ -1 & 0 & -1 & 0 \end{pmatrix}, \quad K_1 = \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & -1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ -1 & 0 & 0 & 1 \\ 0 & -1 & -1 & 0 \end{pmatrix},$$

$$J_2 = \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 & -1 \\ -1 & 0 & -1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \end{pmatrix}, \quad K_2 = \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 0 & 0 & -1 \\ 0 & -1 & 1 & 0 \end{pmatrix}, \tag{3.8}$$

$$J_3 = \frac{1}{2}\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \quad K_3 = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

They satisfy

$$[J_i, J_j] = \epsilon_{ijk} J_k,$$

$$[K_i, K_j] = \epsilon_{ijk} K_k, \tag{3.9}$$

$$[J_i, K_j] = 0.$$

Defining $J_\pm = \sqrt{2}(J_1 \pm J_2)$ and $K_\pm = \sqrt{2}(K_1 \pm K_2)$, R can be written

$$R = 2\kappa_1(J_- \otimes K_3 - K_3 \otimes J_-) + 2\kappa_2(K_+ \otimes J_3 - J_3 \otimes K_+) + \kappa_3(K_- \otimes J_+ - J_+ \otimes K_-), \tag{3.10}$$

where κ_i are again given by (2.7). Finally we need to check that (3.5) satisfies the Jacobi identity, or equivalently that R satisfies the classical Yang-Baxter equations,

$$[\underset{12}{R}, \underset{13}{R} + \underset{23}{R}] + [\underset{13}{R}, \underset{23}{R}] = I, \tag{3.11}$$

where I is an adjoint invariant for SO(4). From $[J_i, K_j]=0$, it is easily seen that (3.11) is satisfied when all κ_i but one vanishes. Thus the Jacobi identity is satisfied when two angles are equal and the third is zero. *Just as with Spin(4), the Yang-Baxter equations and Jacobi identity are only satisfied in this case, and* $[M_{\mu\nu}]$ *generate a Lie-Poisson group only in this case*. It can be checked that the results in this case agree with the lowest order commutation relations in Ref. 6.

Above we have argued that we can consistently define a Poisson algebra for SO(4) matrices only in the Connes-Landi case. This algebra is obtainable from the Poisson algebra (2.10) on Spin(4) using (3.1),

$$\{M_{\mu\nu},M_{\rho\sigma}\}(g,h) = \tfrac{1}{4}\underset{12}{\mathrm{Tr}}\ \tau_{\mu}\ \tau_{\rho}\{\ g\ \tau^{\nu}\ h^{-1},g\ \tau^{\sigma}\ h^{-1}\ \}$$
$$= \tfrac{1}{4}\underset{12}{\mathrm{Tr}}\ \tau_{\mu}\ \tau_{\rho}(\ g\ \tau^{\nu}(\ g\ r\ h^{-1} - h^{-1}\ r\ g\ )\tau^{\sigma}\ h^{-1} + g\ \tau^{\sigma}(\ h^{-1}\ r\ g - g\ r\ h^{-1}\ )\tau^{\nu}h^{-1}\ ), \tag{3.12}$$

where Tr_{12} means a trace over both tensor product spaces. We then recover the expression (3.5) with R given by

$$R_{\mu\nu,\rho\sigma} = \tfrac{1}{4}\underset{12}{\mathrm{Tr}}[\tau_{\rho}\otimes\tau^{\nu},\tau^{\mu}\otimes\tau_{\sigma}]r. \tag{3.13}$$

After substituting in the general expression for r given in (2.6) one then gets (3.7).

IV. QUANTUM Spin(4) TRANSFORMATION

Here we generalize to the full noncommutative theory with the goal of searching for symmetries of the noncommutative three-sphere occurring at finite angles ϕ_{μ}. For simplicity we restrict to spinor-type transformations thereby generalizing the discussion of Sec. II.

We begin by replacing the 2×2 matrix u by another 2×2matrix $\hat{u}$, the latter having noncommuting matrix elements. The property of unitarity,

$$\hat{u}\hat{u}^{\dagger} = \hat{u}^{\dagger}\hat{u} = \mathbb{1}_{2\times 2}, \tag{4.1}$$

can be maintained although $\hat{u}$ does not have to have unit determinant. For this (2.1) should be generalized to

$$\hat{u} = \hat{x}_{\mu}e^{i\phi_{\mu}\tau^{\mu}}. \tag{4.2}$$

The sum over $\mu=0,1,2,3$ is assumed. The unitarity condition was shown[3] to be consistent with the commutation relations (1.2). We next show that the commutation relations can be expressed as

$$\underset{1}{\hat{u}}\ \hat{r}\ \underset{2}{\hat{u}} = \underset{2}{\hat{u}}\ \hat{r}\ \underset{1}{\hat{u}} \tag{4.3}$$

for some 4×4 matrix $\hat{r}$. These relations are invariant under interchange of the two tensor product spaces provided $\hat{r}$ is invariant under interchange of the two tensor product spaces; i.e., $\hat{r}=\hat{r}_{12}=\hat{r}_{21}$. In the limit of small angles $\phi_{\mu}\to\epsilon_{\mu}$, $\hat{r}$ should reduce to $\mathbb{1}_{4\times 4}+ir$, with r given in (2.6), for then the commutator of $\hat{u}_1$ with $\hat{u}_2$ goes to i times the Poisson bracket in (2.3),

$$\underset{1}{\hat{u}}\ \underset{2}{\hat{u}} - \underset{2}{\hat{u}}\ \underset{1}{\hat{u}} \to i\ \underset{2}{\hat{u}}\ r\ \underset{1}{\hat{u}} - i\ \underset{1}{\hat{u}}\ r\ \underset{2}{\hat{u}}. \tag{4.4}$$

So the task is to find $\hat{r}$ so that the commutation relations (4.3) agree with (1.2). Substituting (4.2) into (4.3), we get

$$e^{i(\phi_{\rho}+\phi_{\sigma})}(\ \underset{2}{\tau^{\rho}}\ \hat{r}\ \underset{1}{\tau^{\sigma}} - \underset{1}{\tau^{\rho}}\ \hat{r}\ \underset{2}{\tau^{\sigma}}\ )\hat{x}_{\rho}\hat{x}_{\sigma} = 0, \tag{4.5}$$

where the sum over indices is again assumed. We cannot equate coefficients of $\hat{x}_{\rho}\hat{x}_{\sigma}$ to zero because they are not all independent. Rather from (1.2) they are related by

$$\hat{x}_{\rho}\hat{x}_{\sigma} = \tfrac{1}{2}(S_{\rho\sigma,\alpha\beta} + i\hat{E}_{\rho\sigma,\alpha\beta})\hat{x}_{\alpha}\hat{x}_{\beta}, \tag{4.6}$$

where

$$S_{\rho\sigma,\alpha\beta} = \delta_{\alpha\rho}\delta_{\beta\sigma} + \delta_{\alpha\sigma}\delta_{\beta\rho} \tag{4.7}$$

and $\hat{E}_{\rho\sigma,\alpha\beta}$ is given in (1.3). Both $S_{\rho\sigma,\alpha\beta}$ and $\hat{E}_{\rho\sigma,\alpha\beta}$ are symmetric in the last two indices. Equation (4.6) then shows that all quadratic combinations of $\hat{x}_{\mu}$ can be expressed in terms of just the

symmetric ones. If we substitute into (4.5) we can then equate coefficients of all the symmetric combinations of $\hat{x}_\alpha \hat{x}_\beta$ to zero. The result is a generalization of (2.5),

$$\underset{2}{\tau^\rho}\ \underset{}{\hat{r}}\ \underset{1}{\tau^\sigma} - \underset{1}{\tau^\rho}\ \underset{}{\hat{r}}\ \underset{2}{\tau^\sigma} + \underset{2}{\tau^\sigma}\ \underset{}{\hat{r}}\ \underset{1}{\tau^\rho} - \underset{1}{\tau^\sigma}\ \underset{}{\hat{r}}\ \underset{2}{\tau^\rho} = -ie^{i(\phi_\mu+\phi_\nu-\phi_\rho-\phi_\sigma)}\hat{E}_{\mu\nu,\rho\sigma}\left(\underset{2}{\tau^\mu}\ \underset{}{\hat{r}}\ \underset{1}{\tau^\nu} - \underset{1}{\tau^\mu}\ \underset{}{\hat{r}}\ \underset{2}{\tau^\nu}\right). \tag{4.8}$$

Up to an overall constant factor, it is solved by

$$\hat{r} = \frac{1}{2}\begin{pmatrix} e^{2i(\phi_0-\phi_2)}+e^{2i(\phi_0-\phi_1)} & 0 & 0 & e^{2i(\phi_0-\phi_2)}-e^{2i(\phi_0-\phi_1)} \\ 0 & e^{2i(\phi_0-\phi_3)}+1 & e^{2i(\phi_0-\phi_3)}-1 & 0 \\ 0 & e^{2i(\phi_0-\phi_3)}-1 & e^{2i(\phi_0-\phi_3)}+1 & 0 \\ e^{2i(\phi_0-\phi_2)}-e^{2i(\phi_0-\phi_1)} & 0 & 0 & e^{2i(\phi_0-\phi_2)}+e^{2i(\phi_0-\phi_1)} \end{pmatrix}, \tag{4.9}$$

or equivalently,

$$\hat{r} = \mathbb{1}_{4\times 4} + i\hat{\kappa}_\mu \tau^\mu \otimes \tau^\mu, \tag{4.10}$$

with a sum over μ and

$$\begin{aligned} \hat{\kappa}_0 &= \frac{i}{4}(3 - e^{2i(\phi_0-\phi_1)} - e^{2i(\phi_0-\phi_2)} - e^{2i(\phi_0-\phi_3)}), \\ \hat{\kappa}_1 &= -\frac{i}{4}(1 + e^{2i(\phi_0-\phi_1)} - e^{2i(\phi_0-\phi_2)} - e^{2i(\phi_0-\phi_3)}), \\ \hat{\kappa}_2 &= -\frac{i}{4}(1 - e^{2i(\phi_0-\phi_1)} + e^{2i(\phi_0-\phi_2)} - e^{2i(\phi_0-\phi_3)}), \\ \hat{\kappa}_3 &= -\frac{i}{4}(1 - e^{2i(\phi_0-\phi_1)} - e^{2i(\phi_0-\phi_2)} + e^{2i(\phi_0-\phi_3)}). \end{aligned} \tag{4.11}$$

The expressions for $\hat{\kappa}_i, i=1,2,3$, reduce κ_i to (2.7) in the limit of small angles $\phi_\mu \to \epsilon_\mu$, while $\hat{\kappa}_0$ is arbitrary in the limit.

The relations (4.3) are not invariant under Spin(4). Alternatively, we can try to define a deformation of Spin(4), parametrized by two nonsingular 2×2 matrices $\hat{g}$ and $\hat{h}$ with noncommuting matrix elements with an involution. The coaction on $\hat{u}$ is

$$\hat{u} \to \hat{u}' = \hat{g}\hat{u}\hat{h}^{-1}. \tag{4.12}$$

In order to preserve (4.1) we demand that $\hat{g}$ and $\hat{h}$ are unitary. Transformation (4.12) preserves the commutation relations (4.3) provided

$$\underset{1}{\hat{r}}\ \underset{2}{\hat{g}}\ \underset{1}{\hat{h}} = \underset{2}{\hat{h}}\ \underset{1}{\hat{g}}\ \underset{}{\hat{r}}, \quad [\underset{1}{\hat{g}}, \underset{2}{\hat{g}}] = [\underset{1}{\hat{h}}, \underset{2}{\hat{h}}] = 0. \tag{4.13}$$

This is easily shown. Under the coaction, the left-hand side of (4.3) transforms to

$$\begin{aligned} \underset{1}{\hat{u}'}\ \underset{}{\hat{r}}\ \underset{2}{\hat{u}'} &= \underset{1}{\hat{g}}\ \underset{1}{\hat{u}}\ \underset{1}{\hat{h}^{-1}}\ \underset{}{\hat{r}}\ \underset{2}{\hat{g}}\ \underset{2}{\hat{u}}\ \underset{2}{\hat{h}^{-1}} = \underset{1}{\hat{g}}\ \underset{1}{\hat{u}}\ \underset{2}{\hat{g}}\ \underset{}{\hat{r}}\ \underset{1}{\hat{h}^{-1}}\ \underset{2}{\hat{u}}\ \underset{2}{\hat{h}^{-1}} = \underset{2}{\hat{g}}\ \underset{1}{\hat{g}}\ \underset{1}{\hat{u}}\ \underset{}{\hat{r}}\ \underset{2}{\hat{u}}\ \underset{2}{\hat{h}^{-1}}\ \underset{1}{\hat{h}^{-1}} = \underset{2}{\hat{g}}\ \underset{1}{\hat{g}}\ \underset{2}{\hat{u}}\ \underset{}{\hat{r}}\ \underset{1}{\hat{u}}\ \underset{2}{\hat{h}^{-1}}\ \underset{1}{\hat{h}^{-1}} \\ &= \underset{2}{\hat{g}}\ \underset{2}{\hat{u}}\ \underset{1}{\hat{g}}\ \underset{}{\hat{r}}\ \underset{2}{\hat{h}^{-1}}\ \underset{1}{\hat{u}}\ \underset{1}{\hat{h}^{-1}} = \underset{2}{\hat{g}}\ \underset{2}{\hat{u}}\ \underset{2}{\hat{h}^{-1}}\ \underset{}{\hat{r}}\ \underset{1}{\hat{g}}\ \underset{1}{\hat{u}}\ \underset{1}{\hat{h}^{-1}} = \underset{2}{\hat{u}'}\ \underset{}{\hat{r}}\ \underset{1}{\hat{u}'}. \end{aligned} \tag{4.14}$$

In order for the algebra generated by $\hat{g}$ and $\hat{h}$ to be associative it is necessary for $\hat{r}$ to satisfy the quantum Yang-Baxter equations,

$$\underset{12}{\hat{r}}\ \underset{13}{\hat{r}}\ \underset{23}{\hat{r}} = \underset{23}{\hat{r}}\ \underset{13}{\hat{r}}\ \underset{12}{\hat{r}}. \tag{4.15}$$

On the other hand, the quantum Yang-Baxter equations did not have to be satisfied for the algebra generated by $\hat{u}$ to be associative. Finally substitute (4.10) into (4.15). As in the infinitesimal cases, we get an identity only when two angles are equal and the third is zero. Hence the spinor-type transformations (4.12) correspond to symmetries only in the Connes-Landi case. For example, choose $\phi_0=\phi_4=0$ and $\phi_1=\phi_2=\phi/2$. Then $\hat{r}$ simplifies to $\mathrm{diag}(q,1,1,q)$, where $q=e^{-i\phi}$, and the condition (1.1) is equivalent to

$$\det_q \hat{u} \equiv \hat{u}_{11}\hat{u}_{22} - q\hat{u}_{12}\hat{u}_{21} = 1. \tag{4.16}$$

This condition is preserved under (4.12) provided $\det \hat{g}\ \det \hat{h}^{-1}=1$, after using (4.3) along with the commutation relations for matrix elements of $\hat{g}$ with $\hat{h}^{-1}$. It can be checked that both $\det \hat{g}$ and $\det \hat{h}^{-1}$ are Casimirs of the algebra and hence can be set to one. From (4.12) one can obtain the left coaction of the coordinates

$$\hat{x}_\mu \rightarrow \hat{x}'_\mu = \hat{M}_{\mu\nu}\hat{x}_\nu, \tag{4.17}$$

with

$$\hat{M}_{\mu\nu}(\hat{g},\hat{h}) = \tfrac{1}{2}e^{i(\phi_\nu-\phi_\mu)}\,\mathrm{Tr}(\tau_\mu \hat{g}\tau^\nu \hat{h}^{-1}). \tag{4.18}$$

The commutation relations for $\hat{M}_{\mu\nu}$ are then determined from the commutation relations for matrix elements of $\hat{g}$ with $\hat{h}^{-1}$.

V. NONCOMMUTATIVE HYPERBOLOIDS

The sphere of Connes and Dubois-Violette can be Wick rotated to Minkowski space. The result is a three-parameter family of "noncommutative hyperboloids." We can then repeat the previous analysis and search for quantum deformations of the Lorentz group which have noncommutative hyperboloids as homogeneous spaces. For simplicity, we only examine the first order system and write it in spinor notation. The result is that there is a Lie-Poisson action of a Lie-Poisson group acting on a one parameter subgroup of noncommutative hyperboloids, namely the Wick rotated version Connes-Landi spheres.

The Wick rotation of the Poisson structure (1.4) is

$$\{x_\mu, x_\nu\} = E_{\mu\nu,\rho\sigma}x^\rho x^\sigma, \tag{5.1}$$

where $E_{\mu\nu,\rho\sigma}$ are again given in terms of three independent parameters by (1.5) and the indices of x are raised and lowered by the Minkowski metric $\eta_{\mu\nu}=\mathrm{diag}(-1,1,1,1)$. $\eta_{\mu\nu}x^\mu x^\nu$ is a Casimir for the Poisson algebra and so we can restrict to a hyperboloid. In the quantized theory, the time component x_0 will be noncommuting for any nontrivial values of the parameters.

The algebra can be reexpressed in terms of a Hermitian matrix $x=x_\mu\sigma^\mu$, where σ^0 is the 2×2 identity matrix and $\sigma^i, i=1,2,3$, are the Pauli matrices. The Poisson brackets (5.1) can be written as

$$\{\underset{1}{x},\underset{2}{x}\} = i\,\underset{2}{x}\,\underset{1}{r}\,\underset{1}{x} - i\,\underset{1}{x}\,\underset{2}{r}\,\underset{2}{x}, \tag{5.2}$$

using the definition of r in (2.6). The Casimir is now expressed as $\det x$, the latter being invariant under $\mathrm{SL}(2,C)$ transformations

$$x \rightarrow x' = sxs^\dagger, \quad s \in \mathrm{SL}(2,C). \tag{5.3}$$

The Poisson algebra is not preserved under this action, but if we can assign the following Poisson structure to $\mathrm{SL}(2,C)$,

$$\{ \underset{1}{s}, \underset{2}{\bar{s}} \} = -i[\underset{1}{r}, \underset{1}{s} \underset{2}{\bar{s}}], \quad \{ \underset{1}{s}, \underset{2}{s} \} = \{ \underset{1}{s}, \underset{2}{\bar{s}} \} = 0, \tag{5.4}$$

where $\bar{s}=s^{\dagger^{-1}}$, then the brackets (5.2) are invariant in the sense that (5.3) is a Poisson map. Once again for consistency we need to check the Jacobi identity, or equivalently the classical Yang-Baxter equations for r. But as before these conditions are only satisfied when all but one κ_i vanish, and so we only get a consistent deformation of $\mathrm{SL}(2,C)$ in the Connes-Landi limit. For a classification of consistent quantum deformations of $\mathrm{SL}(2,C)$ see Ref. 10.

VI. CONCLUDING REMARKS

Our search for quantum deformations of Spin(4) and SO(4) for which the noncommutative three-spheres of Connes and Dubois-Violette are homogeneous spaces, and which have a smooth commutative limit in the Lie-Poisson sense, has yielded only the known symmetries of twisted Connes-Landi spheres. The question arises as to whether a more involved analysis can yield any other quantum deformations, possibly without a smooth commutative limit. Other possibilities which are currently under investigation would allow for more general Poisson structures on the group at the Poisson level, or commutation relations at the quantum level. In this regard, although the brackets (2.10), if they could have been consistently defined, would have assured that (1.6) is a Poisson map, other possibilities for the Poisson structure on g and h can be explored. For example, one might try dropping the relations $\{g_1,g_2\}=\{h_1,h_2\}=0$. The difficulty is to make this consistent with the requirement that (1.6) be a Poisson map. Moreover, at the quantum level, one can consider generalizing the commutation relations (4.13), possibly dropping $[\hat{g}_1,\hat{g}_2]=[\hat{h}_1,\hat{h}_2]=0$. The task then would be to find the analog of (4.14). Finally, throughout this paper we have insisted upon writing Poisson brackets and commutations relations in terms of an R-matrix. While this is an important case, other possibilities should be investigated for an exhaustive study.

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The Gardner category and nonlocal conservation laws for $N=1$ Super KdV

S. Andrea[a)]
Departamento de Matemáticas, Universidad Simón Bolívar

A. Restuccia[b)]
Departamento de Física, Universidad Simón Bolívar

A. Sotomayor[c)]
Departamento de Ciencias Básicas, Unexpo, Luis Caballero Mejías, Caracas, Venezuela

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The nonlocal conserved quantities of the $N=1$ Super KdV are obtained using a Gardner map. A fermionic substitution semigroup and the resulting Gardner category are defined and several propositions concerning their algebraic structure are obtained. This algebraic framework makes it possible to define general transformations between different nonlinear SUSY differential equations. A SUSY ring extension is then introduced to deal with the nonlocal conserved quantities of SKdV. The algebraic version of the nonlocal conserved quantities is solved in terms of the exponential function applied to the D^{-1} of the local conserved quantities of SKdV. Finally the same formulas are shown to work for rapidly decreasing superfields.
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I. INTRODUCTION

The supersymmetric algebra is the unique extension of the super-Poincaré algebra which is consistent with the S-matrix of quantum field theory. The most remarkable SUSY theory explains how superstrings and other extended SUSY objects can be consistently tied together in what also has been called M-theory.

Free (string) superstring theory is a two-dimensional supersymmetric theory whose local symmetry group is generated by the (Virasoro) Super-Virasoro algebra.

These algebras may be realized as algebras of the (potential) superpotential of (KdV) SKdV[1,2] equations when the second Hamiltonian structure (with the corresponding Poisson structure) is considered.[3]

It is then reasonable to think that the hierarchy of (KdV) SKdV is related to the loop expansion of (string) superstring theory in terms of the genus of Riemann surfaces.[4]

The SKdV hierarchy also arises from supersymmetric quantum mechanics. In fact, it was proven in Refs. 5 and 6 that the entire SKdV hierarchy appears in the asymptotic expansion of the Green's function $g(t,x,\theta,y,\theta')$ of the super heat operator, as $t\to 0^+$ and $g(t,x,\theta,y,\theta')$ is restricted to the diagonal $x=y$, $\theta=\theta'$. The same result holds for the pure "bosonic" (non-SUSY) KdV hierarchy arising from the Green's function of the heat operator with potential, that is, the "Euclidean" Schrödinger operator.[7]

The KdV equation has an infinite number of discrete conserved quantities (CQs). The SUSY extension of these conserved quantities are also CQs for the SKdV equation; but a remarkable

[a)]Electronic mail: sandrea@usb.ve
[b)]Electronic mail: arestu@usb.ve
[c)]Electronic mail: sotomayo@fis.usb.ve

difference between the two equations is that SKdV has a second sequence of CQs, these being nonlocal and intrinsically supersymmetric in nature. They have been interpreted[8] as the Poisson square root of the local CQs, in the sense that

$$\{J,J'\}=H,$$

where J and J' are nonlocal CQs and H is a local CQ of SKdV.

The conservation laws of KdV and SKdV may be obtained from the Lax representations of these equations; for a review see Ref. 8. The nonlocal CQs of SKdV were first obtained by analyzing the infinite set of symmetries of SKdV, e.g., Ref. 9. Later on they were obtained from the Lax operator in Ref. 10.

Another way to obtain these conservation laws is through the supersymmetric extension[1,11] of the Gardner transformation.[12] It may be interpreted as a one-parameter integrable deformation of SKdV. The deformation is

$$\phi=\chi+\varepsilon D^2\chi-\varepsilon^2\chi D\chi,$$

where ε is the deformation parameter.

If the superfield χ satisfies the S-Gardner equation[1] then ϕ satisfies SKdV. Then, using the fact that $H=\int \mathrm{d}x\,\mathrm{d}\theta\chi$ is a conserved quantity of the S-Gardner equation, it was shown[1] that all the local conserved quantities of SKdV arise in the formal expansion of H in powers of ε.

It was left as an open problem, OP1 in the review of Mathieu,[8] to find the nonlocal conserved quantities of SKdV from some integrable ε-deformation.

In the present paper OP1 is solved, by first rephrasing it in a completely algebraic framework. Working first in the free SUSY derivation ring constructed in Ref. 5, a fermionic substitution semigroup is introduced. The resulting Gardner category is an algebraic construction modeled on the possibility of more general Gardner transforms between different nonlinear SUSY differential equations. In the particular case of SKdV the local conserved quantities are constructed from this formalism.

We then introduce SUSY ring extensions in order to deal with the possibility of nonlocal conserved quantities. The algebraic version of the nonlocal CQ problem is solved, using the exponential function applied to the D^{-1} of the local conserved quantities which the ring extensions provide.

Finally the same formulas are shown to work for rapidly decreasing superfields, and the nonlocal CQs so obtained are shown to agree with those found in the literature.

II. THE FERMIONIC SUBSTITUTION SEMIGROUP

Let $\mathcal{A}$ be the free SUSY derivation ring on a single fermionic generator a_1. This ring is generated by its fermionic elements $a_1,a_3,a_5,\ldots$ and bosonic elements $a_2,a_4,a_6,\ldots$ and its superderivation $D:\mathcal{A}\to\mathcal{A}$ is determinated by $Da_n=a_{n+1}$ for $n\geqslant 1$.

The ring extension $\mathcal{A}[\varepsilon]\supset\mathcal{A}$ consists of all formal power series $h=\Sigma_{n=0}^{\infty}\varepsilon^n h_n$ with coefficients $h_n(a_1,a_2,\ldots)\in\mathcal{A}$. Its involution $h\to\bar{h}$ and superderivation $h\to Dh$ are defined componentwise from the same operations in $\mathcal{A}$. The supercommutativity equation $gh=\pm hg$ holds when $\bar{g}=\pm g$ and $\bar{h}=\pm h$, a minus sign when $\bar{g}=-g$ and $\bar{h}=-h$, and a plus sign in the other three cases.

When $f,g\in\mathcal{A}[\varepsilon]$ with $\bar{f}=-f$, the substitution of f in g produces another element $g\circ f\in\mathcal{A}[\varepsilon]$. It is defined by the formulas

$$g=\sum_0^{\infty}\varepsilon^n g_n(a_1,a_2,\ldots),$$

$$g \circ f = \sum_0^\infty \varepsilon^n g_n(f, Df, \dots).$$

The following propositions may be proven.

Proposition 1: When $f, g, h \in \mathcal{A}[\varepsilon]$ *with* $\bar{f} = -f$ *one has*

$$(g+h) \circ f = (g \circ f) + (h \circ f),$$

$$(gh) \circ f = (g \circ f)(h \circ f),$$

which is to say that the operation $g \to g \circ f$ *is a ring homomorphism* $\mathcal{A}[\varepsilon] \to \mathcal{A}[\varepsilon]$, *for any fixed* $\bar{f} = -f$.

Proposition 2: When $f, g \in \mathcal{A}[\varepsilon]$ *with* $\bar{f} = -f$, *one has*

$$D(g \circ f) = (Dg) \circ f.$$

Now let $\mathcal{A}_1[\varepsilon] \subset \mathcal{A}[\varepsilon]$ be the subset of all fermionic elements. The substitution product gives $g \circ f \in \mathcal{A}_1[\varepsilon]$ if $g, f \in \mathcal{A}_1[\varepsilon]$.

Proposition 3: The substitution product is associative:

$$(h \circ g) \circ f = h \circ (g \circ f),$$

when g, h, f *are in* $\mathcal{A}_1[\varepsilon]$.

Thus $\mathcal{A}_1[\varepsilon]$ is made into a semigroup by the substitution construction. Evidently the element $a_1 \in \mathcal{A}_1 \subset \mathcal{A}_1[\varepsilon]$ acts as the identity element of this semigroup.

When an element of $\mathcal{A}_1[\varepsilon]$ has the value a_1 when $\varepsilon = 0$ it is invertible:

Proposition 4: Given $f = a_1 + \varepsilon f_1 + \varepsilon^2 f_2 + \cdots \in \mathcal{A}_1[\varepsilon]$ *there exists* $g = a_1 + \varepsilon g_1 + \varepsilon^2 g_2 + \cdots \in \mathcal{A}_1[\varepsilon]$ *with* $g \circ f = a_1$.

An easy corollary shows that left and right inverses are the same.

Proposition 5: Given $f = a_1 + \Sigma_{k=1}^\infty \varepsilon^k f_k$ *and* $g = a_1 + \Sigma_{k=1}^\infty \varepsilon^k g_k$ *in* $\mathcal{A}_1[\varepsilon]$. *If* $f \circ g = a_1$ *then* $g \circ f = a_1$.

Frechet derivative operator. Associated with the ring $\mathcal{A}$ and its superderivation $D: \mathcal{A} \to \mathcal{A}$ there is a ring $\mathcal{O}_p\mathcal{A}$ whose elements are the finite order differential operators $L = \Sigma_{k=0}^N l_k D^k$ with $l_k \in \mathcal{A}$. Each L acts linearly in $\mathcal{A}$, and the product of two operators is computed from repeated applications of the SUSY product rule $D(gh) = (Dg)h + \bar{g}(Dh)$.

When $\bar{f} = -f \in \mathcal{A}_1[\varepsilon]$, the substitution of f in L is defined by

$$L \circ f = \sum_{k=0}^N (l_k \circ f) D^k.$$

Thus $L \circ f$, a formal power series with operator coefficients, is in the ring $(\mathcal{O}_p\mathcal{A})[\varepsilon]$ whose elements are the sums $\Sigma_{m,n} \varepsilon^m l_{m,n} D^n$ with $l_{m,n} \in \mathcal{A}$ and $l_{m,n} = 0$ for $n \gg 0$, at any given m.

Given $L \in (\mathcal{O}_p\mathcal{A})[\varepsilon]$ and $h \in \mathcal{A}[\varepsilon]$, the element $Lh \in \mathcal{A}[\varepsilon]$ is well-defined because $(\Sigma \varepsilon^m L_m)(\Sigma \varepsilon^n h_n)$ is again a power series with coefficients in $\mathcal{A}$. The effect of f-substitution is as to be expected.

The following proposition may be shown:

Proposition 6: If $L \in (\mathcal{O}_p\mathcal{A})[\varepsilon]$, $h \in \mathcal{A}[\varepsilon]$, and $f \in \mathcal{A}_1[\varepsilon]$, *then*

$$(Lh) \circ f = (L \circ f)(h \circ f).$$

The foregoing constructions come into play when we ask for the first variation of the substitution operation. Given any $f = \Sigma_{m=0}^\infty \varepsilon^m f_m(a_1, a_2, \dots)$ in $\mathcal{A}_1[\varepsilon]$, its Frechet derivative operator is

$$f' = \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} \varepsilon^m \frac{\partial}{\partial a_n} f_m(a_1, a_2, \dots) D^{n-1} \in (\mathcal{O}_p \mathcal{A})[\varepsilon].$$

Then for any $\psi \in \mathcal{A}_1[\varepsilon]$ the substitution by $a_1 + t\psi \in \mathcal{A}_1[\varepsilon]$ gives

$$f \circ (a_1 + t\psi) = f + tf' \psi + \cdots,$$

the full right side of the equation being a power series in t with $\mathcal{A}[\varepsilon]$ coefficients.

A more general formula appears when a_1 is replaced by $\varphi \in \mathcal{A}_1[\varepsilon]$ and

$$f \circ (\varphi + t\psi) = f \circ \varphi + t(f' \circ \varphi)\psi + \cdots,$$

valid when $f, \varphi, \psi \in \mathcal{A}_1[\varepsilon]$.

The chain rule is now immediate.

Proposition 7: When $f, g \in \mathcal{A}_1[\varepsilon]$ one has

$$(f \circ g)' = (f' \circ g) g'.$$

III. THE GARDNER CATEGORY

An element $f = \Sigma_{m=0}^{\infty} \varepsilon^m f_m(a_1, a_2, \dots)$ of $\mathcal{A}_1[\varepsilon]$ may be taken to represent a nonlinear differential equation

$$\frac{\partial}{\partial t} \alpha(x,t) = \sum_{m=0}^{\infty} \varepsilon^m f_m(\alpha(x,t), D_1 \alpha(x,t), \dots),$$

where $\alpha(x,t)$ is a fermionic superfield (see Sec. V) and the superderivation $D_1 = \partial/\partial\theta + \theta(\partial/\partial x)$ is also known as the covariant derivative.

A second element $g \in \mathcal{A}_1[\varepsilon]$ represents a second differential equation, for an unknown superfield $\beta(x,t)$.

Then given a third element $r \in \mathcal{A}_1[\varepsilon]$, one might want the transformation

$$\beta(x,t) = \sum_{m=0}^{\infty} \varepsilon^m r_m(\alpha(x,t), D_1 \alpha(x,t), \dots)$$

to transform solutions of the first equation into solutions of the second. After some computation one sees that this happens if

$$g \circ r = r' f.$$

Accordingly, f and g can be called "objects" in the Gardner category, and r a "morphism" from f to g, written $g \overset{r}{\leftarrow} f$, if the above equality holds in $\mathcal{A}_1[\varepsilon]$.

Obviously the choice $r = a_1 \in \mathcal{A}$, $r' = I \in \mathcal{O}_p \mathcal{A}$ gives the identity automorphism of each object. But the composition of morphisms must be checked.

Proposition 8: Given $f, g, h, r, s \in \mathcal{A}_1[\varepsilon]$.

If $h \overset{s}{\leftarrow} g$ and $g \overset{r}{\leftarrow} f$ then $h \overset{s \circ r}{\leftarrow} f$.

Proof of Proposition 8: From $h \circ s = s' g$ it follows that

$$h \circ s \circ r = s' g \circ r = (s' \circ r)(g \circ r)$$

after applying Proposition 6 to $s' \in \mathcal{O}_p \mathcal{A}[\varepsilon]$ and $g \in \mathcal{A}_1[\varepsilon]$. But $g \circ r = r' f$, giving

$$h \circ (s \circ r) = (s' \circ r) r' f = (s \circ r)' f$$

by the chain rule, Proposition 7. This completes the proof.

The possibility of isomorphism classes in the Gardner category leads one to examine the invertible elements. One has the following result:

Proposition 9: Given $f,g,r,s \in \mathcal{A}_1[\varepsilon]$ *with* $r\circ s=s\circ r=a_1$.

If $g \overset{r}{\leftarrow} f$

then $f \overset{s}{\leftarrow} g$.

The Gardner transform. The SUSY KdV equation is represented by $g=a_7+3a_1a_4+3a_2a_3$, and the Gardner transform by $r=a_1+\varepsilon a_3-\varepsilon^2 a_1a_2$.

A "modified" KdV equation will be represented by some $f \in \mathcal{A}_1[\varepsilon]$. If f can be chosen so that

$$g \circ r = r' f$$

then we will have found an algebraic analog of the Gardner transformation's action on superfield solutions of the two differential equations.

The choice $f=g-3\varepsilon^2\chi$ satisfies $g\circ r=r'f$, which is to say that $g \overset{r}{\leftarrow} f$ in category language.

By Propositions 4 and 5 there exists an inverse Gardner transform

$$s = a_1 - \varepsilon a_3 + \cdots \in \mathcal{A}[\varepsilon]$$

satisfying $r\circ s=s\circ r=a_1$ and hence also, by Proposition 9, $f\circ s=s'g$.

However $f=Dh$ for

$$h = (a_6 + 3a_2^2 - 3a_1a_3) + \varepsilon^2(3a_1a_2a_3 - 2a_2^3).$$

Consequently all the coefficients in the power series $s'g$ are in $D\mathcal{A}\subset\mathcal{A}$.

If $s_n(a_1,a_2,\ldots)$ is the coefficient of ε^n, then this condition implies that $\int \mathrm{d}x\, d\,\theta s_n(\phi,D_1\phi,\ldots)$ remains constant while the superfield ϕ evolves in time with the SUSY KdV equation, and $D_1=\partial/\partial\theta+\theta(\partial/\partial x)$.

IV. RING EXTENSIONS AND NONLOCAL CONSERVATION LAWS

In the general situation $D:\mathcal{B}\to\mathcal{B}$ of an oriented supercommutative ring and a superderivation, an element $u\in\mathcal{B}$ may or may not have the form $u=Dv$ for some $v\in\mathcal{B}$. But for a fermionic $u=-\bar{u}$ one can always pass to the extension $\tilde{D}:\tilde{\mathcal{B}}\to\tilde{\mathcal{B}}$ where $\tilde{\mathcal{B}}$ is the ring of polynomials with $\mathcal{B}$ coefficients in a commuting indeterminate λ, and the new superderivation is $\tilde{D}=D+u(\partial/\partial\lambda)$. (If the extension was unnecessary then $\tilde{D}v=u$ will have more than one solution in $\tilde{B}$.)

The natural first example is given by $u=a_1$, the generator of $\mathcal{A}(a_1,a_2,\ldots)$, the free SUSY derivation ring on a single fermionic generator. The extension just described is $\mathcal{A}(a_0,a_1,a_2,\ldots)$, the free SUSY derivation ring on a bosonic generator a_0, with $Da_n=a_{n+1}$ for $n\geqslant 0$.

The ring of formal power series $\mathcal{A}(a_0,a_1,a_2,\ldots)[\varepsilon]$ has the same universal property seen earlier in the fermionic case. That is, given any $\tilde{D}:\tilde{\mathcal{B}}\to\tilde{\mathcal{B}}$ and some formal power series $b=\Sigma_0^\infty\varepsilon^n b_n$ with all $b_n=\bar{b}_n\in\mathcal{B}$, the substitution operation $g\mapsto g\circ b$ takes $g=\Sigma_0^\infty\varepsilon^n g_n(a_0,a_1,a_2,\ldots)$ to $g\circ b=\Sigma_0^\infty\varepsilon^m g_m(b,\tilde{D}b,\ldots)$.

Then $\Omega(g)=g\circ b$ is a well-defined map of the power series ring extensions

$$\Omega:\mathcal{A}(a_0,a_1,a_2,\ldots)[\varepsilon]\to\tilde{\mathcal{B}}[\varepsilon].$$

In fact Ω is a ring homomorphism which commutes with the respective involutions and satisfies $\Omega D=\tilde{D}\Omega$: The proof is the same as for the Propositions 1 and 2 given earlier.

Ring extensions of the fermionic ring $\mathcal{A}(a_1,a_2,\ldots)$ are now constructed so as to incorporate D^{-1} of all the local conserved quantities of the SUSY KdV equation. From the formulas

$$r = a_1 + \varepsilon a_3 - \varepsilon^2 a_1 a_2$$

for the Gardner transform and

$$s = s_0 + \varepsilon s_1 + \varepsilon^2 s_2 + \cdots$$

for its inverse, which satisfy $r \circ s = s \circ r = a_1$, one can compute for example

$$s_0 = a_1,$$

$$s_1 = -a_3,$$

$$s_2 = a_5 + a_1 a_2,$$

$$s_3 = -a_7 - 2a_1 a_4 - 2a_2 a_3,$$

$$s_4 = a_9 + (3a_1 a_6 + 3a_2 a_5 + 5a_3 a_4) + 2a_1 a_2 a_2.$$

It was shown before that

$$f \circ s = s' g$$

for

$$g = a_7 + 3a_1 a_4 + 3a_2 a_3,$$

$$f = g - 3\varepsilon^2 (a_1 a_2 a_4 + a_2^2 a_3).$$

However $f = Dh$ for $h = (a_6 + 3a_2^2 - 3a_1 a_3) + \varepsilon^2 (3a_1 a_2 a_3 - 2a_2^3)$.

Therefore $D(h \circ s) = s' g$.

As pointed out before, this is a proof that $s_0, s_1, \ldots$ are conserved quantities for the SUSY KdV equation.

For each s_n the ring extension is made which incorporates $\lambda_n = D^{-1} s_n$. Done successively for $s_0, s_1, \ldots$ this gives $\tilde{\mathcal{B}} = \mathcal{A}(\lambda_0, \lambda_1, \ldots)$, the ring of polynomials in the commuting indeterminates $\lambda_0, \lambda_1, \ldots$, with coefficients in $\mathcal{A}(a_1, a_2, \ldots)$. The new superderivation $\tilde{D}: \tilde{\mathcal{B}} \to \tilde{\mathcal{B}}$ is $\tilde{D} = D + \sum_{n=0}^{\infty} s_n (\partial / \partial \lambda_n)$.

Supposing $\mu(\lambda_0, \lambda_1, \ldots)$ to be a polynomial with constant coefficients we ask for the first variation with respect to g. When $\mu = \lambda_n$ this is

$$\dot{\lambda}_n = \left. \frac{\mathrm{d}}{\mathrm{d}t} \right|^{t=0} D^{-1}(s_n \circ (a_1 + tg)) = D^{-1}(s_n' g) = (h \circ s)_n \in \mathcal{A}(a_1, a_2, \ldots),$$

where $(h \circ s)_n$ is the coefficient of ε^n in the power series $h \circ s$.

This shows that $\mu(\lambda_0, \lambda_1, \ldots)$ is a conserved quantity if

$$\sum_{n=0}^{\infty} (h \circ s)_n \frac{\partial \mu}{\partial \lambda_n} \in \tilde{D}(\tilde{\mathcal{B}}).$$

We now work with $\lambda = \sum_0^{\infty} \varepsilon^n \lambda_n \in \tilde{\mathcal{B}}[\varepsilon]$.

Theorem 1: *The coefficients of $e^{\varepsilon \lambda}$ are all nonlocal conserved quantities for the algebraic version of the SUSY KdV equation.*

Proof of Theorem 1: With

$$e^{\varepsilon \lambda} = 1 + \varepsilon \mu_1 + \varepsilon^2 \mu_2 + \cdots,$$

$$\frac{\partial}{\partial \lambda_n} e^{\varepsilon\lambda} = \varepsilon^{n+1} e^{\varepsilon\lambda}$$

one has $(\partial/\partial\lambda_n)\mu_p = \mu_{p-n-1}$ and $\dot{\mu}_p = \Sigma_{n=0}^{p-1} \mu_{p-n-1}\dot{\lambda}_n$.

This is the coefficient of ε^{p-1} in the power series $e^{\varepsilon\lambda}(h \circ s)$.

Evidently $e^{\varepsilon\lambda}(h \circ s) \in \tilde{B}[\varepsilon]$.

The proof of the theorem is complete when we have shown that

$$e^{\varepsilon\lambda}(h \circ s) \in \tilde{D}(\tilde{B}[\varepsilon]).$$

However the substitution operation $\Omega(g) = g \circ \lambda$ gives a ring homomorphism

$$\Omega : \mathcal{A}(a_0, a_1, \ldots)[\varepsilon] \to \tilde{B}[\varepsilon].$$

Obviously $\Omega(e^{\varepsilon a_0}) = e^{\varepsilon\lambda}$, while

$$\Omega(a_1) = a_1 \circ \lambda = D\lambda = s,$$

$$\Omega(a_n) = D^n s \text{ for } n \geqslant 1.$$

This shows that

$$\Omega(h) = h \circ s,$$

giving

$$\Omega(e^{\varepsilon a_0} h(a_1, a_2, \ldots, \varepsilon)) = e^{\varepsilon\lambda}(h \circ s).$$

The search for antiderivatives can therefore be done in the more accessible ring $\mathcal{A}(a_0, a_1, \ldots)[\varepsilon]$. Indeed

$$e^{\varepsilon a_0} h = Dl$$

with $l = e^{\varepsilon a_0}(F_0 + \varepsilon F_1 + \varepsilon^2 F_2)$ and F_0, F_1, F_2 certain fermionic elements of $\mathcal{A}(a_1, a_2, \ldots)$. The desired equation reduces to

$$DF_0 = a_6 + 3a_2 a_2 - 3a_1 a_3,$$

$$DF_1 + a_1 F_0 = 0,$$

$$DF_2 + a_1 F_1 = 3a_1 a_2 a_3 - 2a_2^3,$$

$$a_1 F_2 = 0.$$

These equations are satisfied by

$$F_0 = a_5 + 3a_1 a_2, \quad F_1 = a_1 a_4 - a_2 a_3, \quad F_2 = -2a_1 a_2^2.$$

Because the ring homomorphism satisfies $\Omega D = \tilde{D}\Omega$ we conclude that from

$$\Omega(e^{\varepsilon a_0} h) = e^{\varepsilon\lambda}(h \circ s)$$

we may infer

$$e^{\varepsilon\lambda}(h \circ s) = \tilde{D}(\Omega l).$$

This completes the proof of the theorem.

V. CONSERVATION LAWS FOR SUPERFIELDS

The algebraic constructions done so far will now be applied to the SUSY KdV equation. This equation deals with superfields, which may be described as follows.

Suppose Λ is a finite dimensional Grassmann algebra generated by anticommuting elements $\theta, \eta_1, \eta_2, \ldots$ which satisfy $\theta^2=\eta_1^2=\eta_2^2=\cdots=0$.

Any element of Λ, after reorderings and sign changes, may be written uniquely as

$$\phi = v(\eta_1, \eta_2, \ldots) + \theta u(\eta_1, \eta_2, \ldots).$$

Then the superderivation $\partial/\partial\theta: \Lambda \to \Lambda$ is defined by $\partial\phi/\partial\theta = u$.

A superfield is any infinitely differentiable function $\phi: \mathbb{R} \to \Lambda$, and the ring of all superfields is denoted by $\mathcal{C}^\infty(\mathbb{R}, \Lambda)$. A superfield is called "bosonic" when $\bar{\phi}=\phi$ and fermionic when $\bar{\phi}=-\phi$. To avoid confusion with the algebraic case, the superderivation in this ring is written $D_1 = \partial/\partial\theta + \theta(\partial/\partial x)$.

Thus $\phi(x) = v(x) + \theta u(x)$ and $D_1\phi = u(x) + \theta v'(x)$.

Ring homomorphisms from algebra to analysis are given by substitution of elements of $\mathcal{C}^\infty(\mathbb{R}, \Lambda)$. For example if $\phi=-\bar{\phi}$ in $\mathcal{C}^\infty(\mathbb{R}, \Lambda)$ one has the ring homomorphism

$$\mathcal{A}(a_1, a_2, \ldots) \to \mathcal{C}^\infty(\mathbb{R}, \Lambda)$$

which sends $f(a_1, a_2, \ldots)$ to $f \circ \phi = f(\phi, D_1\phi, \ldots)$. This homomorphism interrelates the two superderivations, in the sense that

$$D_1(f \circ \phi) = (Df) \circ \phi.$$

The associativity equation $(g \circ f) \circ \phi = g \circ (f \circ \phi)$ continues to hold when $f=-\bar{f}$ in $\mathcal{A}(a_1, a_2, \ldots)$ and $\phi=-\bar{\phi}$ in $\mathcal{C}^\infty(\mathbb{R}, \Lambda)$, while $g \in \mathcal{A}(a_1, a_2, \ldots)$ is arbitrary.

For the convergence of integrals one must work in subrings of $\mathcal{C}^\infty(\mathbb{R}, \Lambda)$.

Let $\mathcal{C}^\infty_\downarrow(\mathbb{R}, \Lambda)$ be the superfields that diminish rapidly at $x=\pm\infty$ together with all derivatives. When Φ satisfies $D_1\Phi \in \mathcal{C}^\infty_\downarrow$, Φ and all its derivatives are bounded functions, and in particular $(\partial/\partial\theta)\Phi \in \mathcal{C}^\infty_\downarrow$. Thus $\psi\Phi \in \mathcal{C}^\infty_\downarrow$ when $\psi \in \mathcal{C}^\infty_\downarrow$ and $D_1\Phi \in \mathcal{C}^\infty_\downarrow$.

The nonlocal extension of $\mathcal{C}^\infty_\downarrow$ may be defined to be

$$\mathcal{C}^\infty_{\mathrm{NL}}(\mathbb{R}, \Lambda) = \{\Phi \in \mathcal{C}^\infty(\mathbb{R}, \Lambda) : D_1\Phi \in \mathcal{C}^\infty_\downarrow(\mathbb{R}, \Lambda)\}.$$

Then $\mathcal{C}^\infty_{\mathrm{NL}}$ is again a derivation ring, and it contains $\mathcal{C}^\infty_\downarrow$ as an ideal. The formulas

$$\phi(x) = v(x) + \theta u(x),$$

$$D_1^{-1}\phi(x) = \int_{-\infty}^{x} u(s)\mathrm{d}s + \theta v(x)$$

give an explicit mapping $D_1^{-1}: \mathcal{C}^\infty_\downarrow \to \mathcal{C}^\infty_{\mathrm{NL}}$, with $D_1^{-1}D_1\phi = \phi$ as well as $D_1D_1^{-1}\phi = \phi$ for all $\phi \in \mathcal{C}^\infty_\downarrow$.

When $\Phi(x) = V(x) + \theta U(x) \in \mathcal{C}^\infty_{\mathrm{NL}}$ one can define the integral of $\Phi(x)$ to be

$$\int \Phi = \int_{-\infty}^{\infty} U(x)\mathrm{d}x.$$

Thus, integration is an additive mapping from $\mathcal{C}^\infty_{\mathrm{NL}}(\mathbb{R}, \Lambda)$ to the Grassmann algebra Λ.

And, when $\phi \in \mathcal{C}^\infty_\downarrow \subset \mathcal{C}^\infty_{\mathrm{NL}}$ one has

$$\int D_1\phi = 0.$$

These preparations done we turn to the SUSY KdV equation, which is represented by $g=a_7+3a_1a_4+3a_2a_3$: if ϕ is a time-dependent superfield then

$$\frac{\partial}{\partial t}\phi = \dot{\phi} = g \circ \phi.$$

With $s=\Sigma_0^\infty \varepsilon^n s_n(a_1,a_2,\ldots)$ the inverse Gardner transform, and any $\phi=-\bar{\phi}\in\mathcal{C}_\downarrow^\infty$, we define

$$\Phi = D_1^{-1}(s\circ\phi),$$

a formal power series with $\mathcal{C}_{\mathrm{NL}}^\infty$ coefficients.

Then

$$J(\phi) = \int e^{\varepsilon\Phi}$$

will be shown to be a power series whose coefficients are nonlocal conservation laws for the SUSY KdV equation.

To compute $\dot{\Phi}=\mathrm{d}/\mathrm{d}t|^{t=0}\Phi(\phi+t\dot{\phi})$ we recall first that

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|^{t=0} s\circ(a_1+tg) = D(h\circ s)$$

in the ring of formal power series $\mathcal{A}(a_1,a_2,\ldots)[\varepsilon]$, with $h=\Sigma_0^\infty\varepsilon^n h_n(a_1,a_2,\ldots)$ as computed before.

The substitution homomorphism given by ϕ then gives $(\mathrm{d}/\mathrm{d}t)|^{t=0}s\circ(\phi+t\dot{\phi})=D_1(h\circ s\circ\phi)$. Consequently

$$\dot{\Phi} = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|^{t=0} D_1^{-1}(s\circ(\phi+t\dot{\phi})) = h\circ s\circ\phi.$$

Since $\dot{J}=\varepsilon\int e^{\varepsilon\Phi}\dot{\Phi}$, the proof will be complete when it has been shown that

$$\int e^{\varepsilon\Phi}(h\circ s\circ\phi) = 0.$$

However, it was shown earlier that there exists $F=\Sigma_0^\infty\varepsilon^n F_n(a_1,a_2,\ldots)$ satisfying

$$e^{\varepsilon a_0}h = D(e^{\varepsilon a_0}F)$$

in the ring $\mathcal{A}(a_0,a_1,\ldots)[\varepsilon]$ of formal power series with $\mathcal{A}(a_0,a_1,\ldots)$ coefficients. Under the operation of substitution by Φ this equation becomes

$$e^{\varepsilon\Phi}(h\circ s\circ\phi) = D_1(e^{\varepsilon\Phi}(F\circ s\circ\phi))$$

in the ring $\mathcal{C}_{\mathrm{NL}}^\infty(\mathbb{R},\Lambda)[\varepsilon]$, because $D_1\Phi=s\circ\phi$ and h and F do not involve a_0.

The coefficients of $e^{\varepsilon\Phi}$ are in $\mathcal{C}_{\mathrm{NL}}^\infty$ while the coefficients of $F\circ s\circ\phi$ are in $\mathcal{C}_\downarrow^\infty$.

Therefore their product is in $\mathcal{C}_\downarrow^\infty$, where $\psi\in\mathcal{C}_\downarrow^\infty$ implies $\int D_1\psi=0$.

This completes the proof that $J(\phi)=\int e^{\varepsilon\Phi}$ is a conserved quantity for the SUSY KdV equation.

In closing we may compare $\int e^{\varepsilon\Phi}$ with conserved quantities found in the literature. Starting with $\phi=-\bar{\phi}\in\mathcal{C}_\downarrow^\infty$, the first few coefficients of $\Phi=\Sigma_0^\infty\varepsilon^n\Phi_n=D^{-1}(s\circ\phi)$ can be found from the corresponding coefficients of the inverse Gardner transform $\Sigma_0^\infty\varepsilon^n s_n(a_1,a_2,\ldots)$. After replacing D_1 by the shorter notation $D=\partial/\partial\theta+\theta(\partial/\partial x)$ one finds that

$$\Phi_0 = D^{-1}\phi,$$

$$\Phi_1 = -D\phi,$$

$$\Phi_2 = D^3\phi + D^{-1}(\phi D\phi),$$

$$\Phi_3 = -D^5\phi - 2(D\phi)^2 + 2\phi(D^2\phi).$$

These elements of $\mathcal{C}^{\infty}_{\mathrm{NL}}$ are all bosonic, and the first few coefficients of $e^{\varepsilon\Phi} = 1 + \Sigma_{n=1}^{\infty}\varepsilon^n\Delta_n$ are

$$\Delta_1 = \Phi_0,$$

$$\Delta_2 = \tfrac{1}{2}\Phi_0^2 + \Phi_1,$$

$$\Delta_3 = \tfrac{1}{6}\Phi_0^3 + \Phi_0\Phi_1 + \Phi_2,$$

$$\Delta_4 = \tfrac{1}{24}\Phi_0^4 + \tfrac{1}{2}\Phi_0^2\Phi_1 + \Phi_0\Phi_2 + \tfrac{1}{2}\Phi_1^2 + \Phi_3.$$

Because we are only interested in the integrals of $\Delta_n(\phi)$, terms which fall into $D\mathcal{C}^{\infty}_{\downarrow}$ can be left out because they have identically zero integrals. For example

$$\Phi_0\Phi_1 = -(D^{-1}\phi)(D\phi) = -D((D^{-1}\phi)\phi).$$

After rewriting the Δ_n in terms of $D^{-1}\phi, \phi, \ldots$ and simplifying in the manner just described we arrive at

$$\Delta_1 = D^{-1}\phi,$$

$$\Delta_2 = \tfrac{1}{2}(D^{-1}\phi)^2,$$

$$\Delta_3 = \tfrac{1}{6}(D^{-1}\phi)^3 + D^{-1}(\phi D\phi),$$

$$\Delta_4 = \tfrac{1}{24}(D^{-1}\phi)^4 - \tfrac{1}{2}(D\phi)^2 + (D^{-1}\phi)D^{-1}(\phi D\phi).$$

Replacing ϕ by $-\phi$ in these formulas we obtain constant multiples of the integrands which appear in the nonlocal conserved quantities $J_{\frac{1}{2}}, J_{\frac{3}{2}}, J_{\frac{5}{2}}, J_{\frac{7}{2}}$ presented in Ref. 10.

The sign change comes from the ambiguity $g = \pm a_7 + 3a_1a_4 + 3a_2a_3$ in the definition of the SUSY KdV equation.

The two versions are interchanged by the transformation $T: \mathcal{A}(a_1, a_2, \ldots) \to \mathcal{A}(a_1, a_2, \ldots)$ given by $(Tf)(a_1, a_2, \ldots) = -f(-a_1, -a_2, \ldots)$.

This transformation is not a ring homomorphism but it satisfies $DT = TD$. In terms of the substitution operation, $Tg = -(g \circ (-a_1))$ in general, with $Tf = (-a_1) \circ f \circ (-a_1)$ when $\bar{f} = -f$.

The associativity and the cancellation $(-a_1) \circ (-a_1) = a_1$ then give

$$T(g \circ f) = (Tg) \circ (Tf).$$

Therefore T also exchanges the respective Gardner transforms and conservation laws.

VI. CONCLUSIONS

We introduced the fermionic substitution semigroup and the resulting Gardner category. We obtained several propositions concerning their algebraic structure. This algebraic framework made it possible to define general Gardner transformations between different nonlinear SUSY differen-

tial equations. We then introduced a SUSY ring extension which, in the same algebraic setting, permitted the construction of all the known nonlocal conserved quantities of $N=1$ SKdV. All these nonlocal conserved quantities are then obtained from the Super-Gardner equation using a Gardner map. They may be expressed in terms of the exponential function applied to the D^{-1} of the local conserved quantities of $N=1$ SKdV. As in the case of the local conserved quantities of $N=1$ SKdV, one conserved quantity of the Super-Gardner equation generates all the known nonlocal conserved quantities of $N=1$ SKdV.

An interesting problem to be considered would be to apply the construction we introduced here to obtain the conserved quantities of $N=2$ SKdV.[13]

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On the structure of the supplementary series of unitary, irreducible representations of the proper, orthochronous Lorentz group

J. Kubieniec[a)]
Marian Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, 30-059 Kraków, Poland

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Representations from the supplementary series of unitary, irreducible representations of the proper, orthochronous Lorentz group are classified according to the parameter z, $0<z<1$. The representations with $0<z<1/2$ are qualitatively different from those with $1/2<z<1$. This is shown in the form of the following theorem: the Casimir operator of the little group of a spacelike vector has for $0<z<1/2$ a single bound state, i.e., a single normalizable eigenstate which disappears for $1/2<z<1$. To this end the scalar product for the supplementary series is explicitly calculated in both regions, $0<z<1/2$ and $1/2<z<1$ in a coordinate system provided by common eigenfunctions of the Casimir operator of the little group of a spacelike vector and the commuting generator of a parabolic rotation. The choice of this coordinate system allows to use the well established properties of the Kontorovich-Lebedev pair of integral transforms. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2080455]

I. INTRODUCTION

The supplementary series of unitary, irreducible representations of the proper, orthochronous Lorentz group was discovered simultaneously and independently by Gelfand and Neumark,[1] Bargmann,[2] and Harish-Chandra.[3] It is described in several textbooks, e.g., in the textbook by Gelfand, Graev, and Vilenkin.[4] The structure of the supplementary series was investigated by Mukunda,[5] and Boyer.[6] They calculated the scalar product for the supplementary series in a canonical coordinate system provided by common eigenfunctions of two commuting observables, viz. the Casimir operator of the little group of a spacelike vector and the generator of a rotation. In this way they discovered a bound state of the Casimir operator.

In this paper we shall investigate the structure of the supplementary series in the following way. We shall calculate the scalar product for the supplementary series in a special coordinate system provided by common eigenfunctions of two commuting observables, viz. the Casimir operator of the little group of a spacelike vector and the generator of a parabolic rotation. The reason for the choice of the generator of the parabolic rotation is that common eigenfunctions are then proportional to MacDonald functions of imaginary order. Thus the decomposition of an arbitrary function can be carried out with the aid of the pair of Kontorovich-Lebedev transforms. Moreover, we shall use the theory of the supplementary series described in Ref. 7. This approach makes the Lorentz invariance of all calculations manifest at each step. It also reveals the physical shape of the bound state of the Casimir operator which is completely absent in the papers mentioned above. The mathematics which is necessary to see this was first elaborated by Staruszkiewicz.[8] He discovered a bound state of the first Casimir operator of the proper, orthochronous Lorentz group in his theory of the quantum Coulomb field.

[a)]Electronic mail: jakub@th.if.uj.edu.pl

We use units such that $\hbar=1=c$. We use the metric tensor $g_{\mu\nu}$ such that $xx=g_{\mu\nu}x^\mu x^\nu\equiv(x^0)^2-(x^1)^2-(x^2)^2-(x^3)^2$ is the square of the length of the vector x.

II. THE SUPPLEMENTARY SERIES

We present the supplementary series of unitary, irreducible representations of the proper, orthochronous Lorentz group, following Ref. 7.

The upper light cone (here in the momentum space) is a figure formed by positive frequency null vectors $kk=0$, $k^0>0$. It consists of null directions. A null direction is a set of null vectors parallel to a given null vector. The set of null directions has the Lorentz invariant volume, which Gelfand, Graev, and Vilenkin give on p. 426 of their textbook[4] and Staruszkiewicz[9] applies to calculate several useful integrals,

$$\mathrm{d}^2k=\frac{k^1\,\mathrm{d}k^2\wedge\mathrm{d}k^3+k^2\,\mathrm{d}k^3\wedge\mathrm{d}k^1+k^3\,\mathrm{d}k^1\wedge\mathrm{d}k^2}{k^0}. \tag{1}$$

Here $\wedge$ denotes the outer product. The function $f(k)$ defined on the upper light cone is said to be homogeneous of degree $z-2$, $0<z<1$, if

$$f(\rho k)=\rho^{z-2}f(k)\quad\text{for each }\rho>0. \tag{2}$$

Functions homogeneous of degree $z-2$ form a linear space over the field of complex numbers. Introducing in this space the manifestly Lorentz invariant nonlocal scalar product

$$\langle f|f\rangle_z=\int\frac{\mathrm{d}^2k\,\mathrm{d}^2l}{(kl)^z}\overline{f(k)}f(l) \tag{3}$$

we obtain the Hilbert space appropriate for the supplementary series.

III. THE CASIMIR OPERATOR OF THE LITTLE GROUP OF A SPACELIKE VECTOR AND THE GENERATOR OF A PARABOLIC ROTATION: THEIR COMMON EIGENFUNCTIONS

Let a and b be two fixed orthogonal spacelike vectors, $ab=0$, $aa=-1$, $bb=-1$. Let q be a fixed null vector orthogonal to the vectors a and b, $qq=0$, $aq=0$, $bq=0$.

The set of proper, orthochronous Lorentz transformations which preserve a fixed vector is called the little group of this vector. In what follows we consider the spacelike vector a. The Casimir operator of the little group of this vector written in a manifestly Lorentz invariant form is

$$C=-a_\mu\overset{*}{M}{}^{\mu\nu}a^\rho\overset{*}{M}{}_{\rho\nu}. \tag{4}$$

Here $\overset{*}{M}{}^{\mu\nu}=(1/2)\epsilon^{\mu\nu\rho\sigma}M_{\rho\sigma}$ is the dual pseudotensor associated with generators $M_{\mu\nu}=-M_{\nu\mu}$ of the proper, orthochronous Lorentz group. $\epsilon^{\mu\nu\rho\sigma}$ denotes the Levi-Civita symbol, $\epsilon^{0123}=1$.

There are three kinds of one-parameter subgroups of the proper, orthochronous Lorentz group, elliptic rotations (rotations), which preserve a timelike plane, hyperbolic rotations (Lorentz "boosts"), which preserve a spacelike plane, and parabolic rotations, which preserve a null plane. In what follows we consider the parabolic rotation which preserves the null plane spanned by the spacelike vector a and the null vector q. The generator of this parabolic rotation written in a manifestly Lorentz invariant form is

$$M=a^\mu q^\nu\overset{*}{M}{}_{\mu\nu}=-b^\mu q^\nu M_{\mu\nu}. \tag{5}$$

Let us choose a basis such that $a=(0,0,0,1)$, $b=(0,0,1,0)$, $q=(1,1,0,0)$. Then

$$C=M_{01}^2+M_{02}^2-M_{12}^2, \tag{6}$$

$$M = M_{02} + M_{12}, \tag{7}$$

which shows that C and M commute.

Reflection of the null direction k in the timelike hyperplane orthogonal to the spacelike vector a is the null direction k' such that

$$k' = k + 2(ak)a. \tag{8}$$

It is seen that this reflection changes the sign of the variable ak. Thus its representation in the representation space appropriate for the supplementary series is simply the parity operator P. P is invariant under the little group of a generated by operators $a^\mu M^*_{\mu\nu}$. As a consequence we obtain the following corollary: P commutes with C and M. Hence we can find even and odd common eigenfunctions of C and M, respectively, $f^+_{\tau\lambda}(k)$ and $f^-_{\tau\lambda}(k)$, such that

$$Cf^\pm_{\tau\lambda}(k) = \left(\frac{1}{4} + \tau^2\right) f^\pm_{\tau\lambda}(k),$$

$$Mf^\pm_{\tau\lambda}(k) = \lambda f^\pm_{\tau\lambda}(k),$$

$$Pf^\pm_{\tau\lambda}(k) = \pm f^\pm_{\tau\lambda}(k). \tag{9}$$

The generators of the proper, orthochronous Lorentz group for the spinless case in the momentum space written in a manifestly Lorentz covariant form are

$$M_{\mu\nu} = i\left(k_\mu \frac{\partial}{\partial k^\nu} - k_\nu \frac{\partial}{\partial k^\mu}\right). \tag{10}$$

Since $M_{\mu\nu}(kk) \equiv 0$, the formally four-dimensional differential operator $M_{\mu\nu}$ is in fact an internal differential operator on the light cone $kk=0$. Then the system of partial differential equations (9) can be separated in the stereographic variables ak/qk and bk/qk. One finds thus even and odd common eigenfunctions of C and M to be the following:

$$f^+_{\tau\lambda}(k) = |ak|^{z-2} \left|\lambda \frac{ak}{qk}\right|^{1/2} K_{i\tau}\left(\left|\lambda \frac{ak}{qk}\right|\right) \exp\left(i\lambda \frac{bk}{qk}\right),$$

$$f^-_{\tau\lambda}(k) = \operatorname{sign}(ak)|ak|^{z-2} \left|\lambda \frac{ak}{qk}\right|^{1/2} K_{i\tau}\left(\left|\lambda \frac{ak}{qk}\right|\right) \exp\left(i\lambda \frac{bk}{qk}\right),$$

$$\tau \geqslant 0, \quad -\infty < \lambda < \infty. \tag{11}$$

$K_{i\tau}$ is the MacDonald function of imaginary order $i\tau$ such that

$$K_{i\tau}(|x|) = \int_0^\infty \mathrm{d}t\, e^{-|x|\cosh t} \cos(\tau t) \tag{12}$$

and sign is the signum function.

An arbitrary homogeneous of degree $z-2$ function $f(k)$ defined on the upper light cone can be resolved into even and odd parts, respectively, $f^+(k)$ and $f^-(k)$,

$$f(k) = f^+(k) + f^-(k). \tag{13}$$

Using the pair of Kontorovich-Lebedev transforms[10] we get the decomposition of functions $f^+(k)$, $f^-(k)$,

$$f^{\pm}(k)=\int_0^{\infty}\mathrm{d}\tau\int_{-\infty}^{\infty}\mathrm{d}\lambda\, g^{\pm}(\tau,\lambda)f^{\pm}_{\tau\lambda}(k),$$

$$g^{\pm}(\tau,\lambda)=\frac{1}{2\pi^3}\frac{\tau\sinh(\pi\tau)}{|\lambda|}\int \mathrm{d}^2k|ak|^{2-2z}f^{\pm}(k)\overline{f^{\pm}_{\tau\lambda}(k)}. \tag{14}$$

IV. THE SCALAR PRODUCT FOR THE SUPPLEMENTARY SERIES

It is easy to show that

$$\langle f^{+}_{\tau\lambda}|f^{-}_{\tau'\lambda'}\rangle_z=0. \tag{15}$$

To calculate the scalar product for the supplementary series we need besides the following lemma, which is proved in Appendix A: there exist functions $K^{+}(z;\tau)$, $K^{-}(z;\tau)$ such that

$$\int\frac{\mathrm{d}^2k}{(kl)^z}f^{\pm}_{\tau\lambda}(k)=f^{\pm}_{\tau\lambda}(l)\cdot|al|^{2-2z}\cdot K^{\pm}(z;\tau). \tag{16}$$

The function $K^{+}(z;\tau)$ is calculated in Appendix B. It exists for $1/2<z<1$ and can be expressed by the gamma function Γ,

$$K^{+}(z;\tau)=\pi^2\frac{2^z}{\Gamma^2(z)\sin(\pi z)}\frac{\Gamma\left(\frac{z-1/2+i\tau}{2}\right)\Gamma\left(\frac{z-1/2-i\tau}{2}\right)}{\Gamma\left(\frac{3/2-z+i\tau}{2}\right)\Gamma\left(\frac{3/2-z-i\tau}{2}\right)}. \tag{17}$$

The function $K^{-}(z;\tau)$ is calculated in Appendix C. It exists for $1/2<z<1$ and can be expressed by the gamma function Γ and the generalized hypergeometric function ${}_3F_2$,

$$\begin{aligned}K^{-}(z;\tau)=&\frac{\pi^{3/2}}{2}\frac{2^z}{\Gamma(z)\cos\frac{\pi}{2}\left(z-\frac{1}{2}\right)}\frac{1}{\Gamma\left(\frac{3/2-z+i\tau}{2}\right)\Gamma\left(\frac{3/2-z-i\tau}{2}\right)\cosh\left(\frac{\pi}{2}\tau\right)}\\&\times\left[\frac{1}{1-z}\left(\frac{3/2-z+i\tau}{2}\right)^{-1}{}_3F_2\left(\frac{1}{2},1,\frac{3/2-z+i\tau}{2};2-z,\frac{7/2-z+i\tau}{2};1\right)+\text{c.c.}\right.\\&\left.+2\left(\frac{1/2+z+i\tau}{2}\right)^{-1}{}_3F_2\left(z,1,\frac{1/2+z+i\tau}{2};\frac{3}{2},\frac{5/2+z+i\tau}{2};1\right)+\text{c.c.}\right].\end{aligned} \tag{18}$$

Utilizing Eqs. (14) and (16) we have for $1/2<z<1$,

$$\langle f^{\pm}_{\tau\lambda}|f^{\pm}_{\tau'\lambda'}\rangle_z=2\pi^3\frac{|\lambda|}{\tau\sinh(\pi\tau)}K^{\pm}(z;\tau)\delta(\tau-\tau')\delta(\lambda-\lambda'). \tag{19}$$

Hence the scalar product for the supplementary series valid for $1/2<z<1$ has the form

$$\begin{aligned}\langle f|f\rangle_z=&2\pi^3\int_0^{\infty}\mathrm{d}\tau\int_{-\infty}^{\infty}\mathrm{d}\lambda\frac{|\lambda|}{\tau\sinh(\pi\tau)}K^{+}(z;\tau)|g^{+}(\tau,\lambda)|^2\\&+2\pi^3\int_0^{\infty}\mathrm{d}\tau\int_{-\infty}^{\infty}\mathrm{d}\lambda\frac{|\lambda|}{\tau\sinh(\pi\tau)}K^{-}(z;\tau)|g^{-}(\tau,\lambda)|^2.\end{aligned} \tag{20}$$

To find the equivalent of Eq. (20) valid for $0<z<1/2$ one must notice what follows. For $1/2<z<1$, Eq. (20) can be rewritten as[11]

$$\langle f|f\rangle_z = \int \mathrm{d}^2k\mathrm{d}^2l|ak|^{-z}\overline{f^+(k)}|al|^{-z}f^+(l)\frac{1}{4\pi}\int_0^\infty \mathrm{d}\tau\,\tau\tanh(\pi\tau)P_{-1/2+i\tau}(u)K^+(z;\tau)$$
$$+\int \mathrm{d}^2k\,\mathrm{d}^2l\,\mathrm{sign}(ak)|ak|^{-z}\overline{f^-(k)}\,\mathrm{sign}(al)|al|^{-z}f^-(l)\frac{1}{4\pi}\int_0^\infty \mathrm{d}\tau\,\tau\tanh(\pi\tau)P_{-1/2+i\tau}(u)K^-(z;\tau), \tag{21}$$

where $u=\mathrm{sign}(ak)\mathrm{sign}(al)+kl/(|ak||al|)$. $P_{-1/2+i\tau}$ is the conical function. The original scalar product $\langle f|f\rangle_z$, given by Eq. (3), is an analytic function of z. Thus the correct expression for the scalar product $\langle f|f\rangle_z$ valid for $0<z<1/2$ is the analytic continuation of the functions of z given by the integrals

$$\frac{1}{4\pi}\int_0^\infty \mathrm{d}\tau\,\tau\tanh(\pi\tau)P_{-1/2+i\tau}(u)K^\pm(z;\tau). \tag{22}$$

They can be treated as contour integrals in the complex τ-plane. It is seen then that when z changes from $1/2<z<1$ to $0<z<1/2$, two simple poles of $K^+(z;\tau)$ cross the contour. Residues at these poles must be subtracted, since $\langle f|f\rangle_z$ is a given analytic function of z, the same for all z.

The scalar product for the supplementary series valid for $0<z<1/2$, calculated in accordance with the above mathematical principle, has the form

$$\langle f|f\rangle_z = 2\pi^3\int_0^\infty \mathrm{d}\tau\int_{-\infty}^\infty \mathrm{d}\lambda\frac{|\lambda|}{\tau\sinh(\pi\tau)}K^+(z;\tau)|g^+(\tau,\lambda)|^2$$
$$+2\pi^3\int_0^\infty \mathrm{d}\tau\int_{-\infty}^\infty \mathrm{d}\lambda\frac{|\lambda|}{\tau\sinh(\pi\tau)}K^-(z;\tau)|g^-(\tau,\lambda)|^2$$
$$+16\pi^5\frac{1}{2^z\left(\frac{1}{2}-z\right)^2}\frac{\Gamma(2z)}{\Gamma^2(z)\cos(\pi z)}\int_{-\infty}^\infty \mathrm{d}\lambda|\lambda|\left|g^+\left(i\left(\frac{1}{2}-z\right),\lambda\right)\right|^2. \tag{23}$$

V. SPECTRUM OF THE CASIMIR OPERATOR OF THE LITTLE GROUP OF A SPACELIKE VECTOR

From Eqs. (20) and (23) it follows that the Casimir operator C of the little group of the spacelike vector a, $aa=-1$, given by Eq. (4), has for $0<z<1/2$ a single normalizable eigenstate, i.e., a single bound state which disappears for $1/2<z<1$. One can show that for $0<z<1/2$ the function

$$f_\lambda^+(k) = (qk)^{z-2}\delta\left(\frac{ak}{qk}\right)\exp\left(i\lambda\frac{bk}{qk}\right) \tag{24}$$

is an eigenfunction of C with the eigenvalue $0<z(1-z)<1/4$,

$$Cf_\lambda^+(k) = z(1-z)f_\lambda^+(k). \tag{25}$$

The scalar product of two such functions is[11]

$$\langle f_\lambda^+|f_{\lambda'}^+\rangle_z = 2\pi^2\frac{2^z|\lambda|^{2z-1}}{\Gamma(2z)\cos(\pi z)}\delta(\lambda-\lambda'), \tag{26}$$

which means as usual that wave packets obtained by superposing various values of λ will be normalizable. Thus the momentum wave function of the bound state of C is localized in the circle $ak=0$.

We summarize our results in the form of the following theorem: the spectrum of the Casimir operator C of the little group of the unit spacelike vector a consists of only positive numbers greater than or equal to $1/4$ if $1/2<z<1$ and positive numbers greater than or equal to $1/4$ and additionally the single number $0<z(1-z)<1/4$ if $0<z<1/2$. It reveals that the parameter $z=1/2$ is critical and separates two different classes of representations from the supplementary series.

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APPENDIX A: THE USEFUL LEMMA

Let us notice first that in expressions like $M_{\mu\nu}(k)(kl)$ it is necessary to write the argument k of the differential operator $M_{\mu\nu}$. It indicates the variable with respect to which the differentiation is carried out. Now, applying this convention, we have

$$\int \frac{\mathrm{d}^2k}{(kl)^z} M_{\mu\nu} f(k) = -\int \mathrm{d}^2k\, M_{\mu\nu}(k)(kl)^{-z}\cdot f(k)$$
$$= \int \mathrm{d}^2k\, M_{\mu\nu}(l)(kl)^{-z}\cdot f(k) = M_{\mu\nu}\int \frac{\mathrm{d}^2k}{(kl)^z} f(k) \tag{A1}$$

and

$$\int \frac{\mathrm{d}^2k}{(kl)^z} M_{\mu\nu}M_{\rho\sigma} f(k) = M_{\mu\nu}\int \frac{\mathrm{d}^2k}{(kl)^z} M_{\rho\sigma} f(k) = M_{\mu\nu}M_{\rho\sigma}\int \frac{\mathrm{d}^2k}{(kl)^z} f(k). \tag{A2}$$

As an obvious consequence we obtain

$$\int \frac{\mathrm{d}^2k}{(kl)^z} M f(k) = M\int \frac{\mathrm{d}^2k}{(kl)^z} f(k) \tag{A3}$$

and

$$\int \frac{\mathrm{d}^2k}{(kl)^z} C f(k) = C\int \frac{\mathrm{d}^2k}{(kl)^z} f(k). \tag{A4}$$

The integrals

$$\int \frac{\mathrm{d}^2k}{(kl)^z} f^{\pm}_{\tau\lambda}(k) \tag{A5}$$

are manifestly Lorentz invariant, homogeneous of degree $-z$ in l, and even and odd in a, respectively. On the basis of these facts and Eqs. (A3) and (A4), we infer that there exist functions $K^+(z;\tau,\lambda)$, $K^-(z;\tau,\lambda)$ such that

$$\int \frac{\mathrm{d}^2k}{(kl)^z} f^{\pm}_{\tau\lambda}(k) = f^{\pm}_{\tau\lambda}(l)\cdot |al|^{2-2z}\cdot K^{\pm}(z;\tau,\lambda). \tag{A6}$$

On both sides of Eq. (A6) the eigenvalue λ can be absorbed into the null vector q, which does not change the definition of q. Hence the functions $K^+(z;\tau,\lambda)$, $K^-(z;\tau,\lambda)$ cannot depend on λ and this leads directly to Eq. (16).

APPENDIX B: CALCULATION OF THE FUNCTION $K^+(z;\tau)$

All integrals necessary to calculate the function $K^+(z;\tau)$ are given in Ref. 11.

For the even case in Eq. (16) we substitute $\lambda=1$, multiply both sides by $|bl|^{-\alpha}(ql)^{-\beta}$, $z+\alpha+\beta=2$ and integrate over l. In this way we obtain

$$\int d^2k|ak|^{z-2}\left|\frac{ak}{qk}\right|^{1/2}K_{i\tau}\left(\left|\frac{ak}{qk}\right|\right)\exp\left(i\frac{bk}{qk}\right)\int d^2l(kl)^{-z}|bl|^{-\alpha}(ql)^{-\beta}$$
$$=K^+(z;\tau)\int d^2l|bl|^{-\alpha}(ql)^{-\beta}|al|^{-z}\left|\frac{al}{ql}\right|^{1/2}K_{i\tau}\left(\left|\frac{al}{ql}\right|\right)\exp\left(i\frac{bl}{ql}\right). \tag{B1}$$

The integral

$$\int d^2l(kl)^{-z}|bl|^{-\alpha}(ql)^{-\beta} \tag{B2}$$

is manifestly Lorentz invariant, homogeneous of degree $-z$ in k and $-\beta$ in q, and even in b. On the basis of these facts, we infer that there exists a function $A(z;\alpha)$ such that

$$\int d^2l(kl)^{-z}|bl|^{-\alpha}(ql)^{-\beta}=|bk|^{\beta-z}\cdot(qk)^{-\beta}\cdot A(z;\alpha). \tag{B3}$$

It is easy to show that

$$A(z;\alpha)=2^z\int\frac{d\xi\,d\eta}{|\eta|^\alpha[\xi^2+(\eta-1)^2]^z}, \tag{B4}$$

$\xi=al/ql$ and $\eta=bl/ql$ being the stereographic variables. The integral over ξ can be calculated in a simple way. Then the integral over η boils down to the convolution and can be calculated with the aid of the convolution theorem. It is thus seen that the function $A(z;\alpha)$ exists for $1/2<z<1$, $2-2z<\alpha<1$ and has the form

$$A(z;\alpha)=\frac{2^{z+2}}{\sqrt{\pi}}\frac{\Gamma\left(z-\frac{1}{2}\right)}{\Gamma(z)}\Gamma(2-2z)\cos\frac{\pi}{2}(2-2z)\Gamma(2z+\alpha-2)$$
$$\times\cos\frac{\pi}{2}(2z+\alpha-2)\Gamma(1-\alpha)\cos\frac{\pi}{2}(1-\alpha). \tag{B5}$$

Therefore for $1/2<z<1$, $2-2z<\alpha<1$, Eq. (B1) can be rewritten as

$$A(z;\alpha)\int d^2k|bk|^{2-2z-\alpha}(qk)^{z+\alpha-2}|ak|^{z-2}\left|\frac{ak}{qk}\right|^{1/2}K_{i\tau}\left(\left|\frac{ak}{qk}\right|\right)\exp\left(i\frac{bk}{qk}\right)$$
$$=K^+(z;\tau)\int d^2l|bl|^{-\alpha}(ql)^{z+\alpha-2}|al|^{-z}\left|\frac{al}{ql}\right|^{1/2}K_{i\tau}\left(\left|\frac{al}{ql}\right|\right)\exp\left(i\frac{bl}{ql}\right). \tag{B6}$$

Both integrals in Eq. (B6) exist for $1/2<z<1$, $2-2z<\alpha<1$; the integral on the left-hand side equals

$$2^{z-1/2}\Gamma\left(\frac{z-1/2+i\tau}{2}\right)\Gamma\left(\frac{z-1/2-i\tau}{2}\right)\Gamma(3-2z-\alpha)\cos\frac{\pi}{2}(3-2z-\alpha), \tag{B7}$$

and the integral on the right-hand side equals

$$2^{3/2-z}\Gamma\left(\frac{3/2-z+i\tau}{2}\right)\Gamma\left(\frac{3/2-z-i\tau}{2}\right)\Gamma(1-\alpha)\cos\frac{\pi}{2}(1-\alpha). \tag{B8}$$

This leads directly to Eq. (17).

APPENDIX C: CALCULATION OF THE FUNCTION $K^{-}(z;\tau)$

All integrals necessary to calculate the function $K^{-}(z;\tau)$ are also given in Ref. 11.

For the odd case in Eq. (16) we substitute $\lambda=1$, multiply both sides by $|bl|^{-\alpha}(ql)^{-\beta}\,\mathrm{sign}(al)$, $z+\alpha+\beta=2$ and integrate over l. In this way we obtain

$$\int \mathrm{d}^2k\,\mathrm{sign}(ak)|ak|^{z-2}\left|\frac{ak}{qk}\right|^{1/2}K_{i\tau}\left(\left|\frac{ak}{qk}\right|\right)\exp\left(i\frac{bk}{qk}\right)\int \mathrm{d}^2l(kl)^{-z}|bl|^{-\alpha}(ql)^{-\beta}\,\mathrm{sign}(al)$$

$$=K^{-}(z;\tau)\int \mathrm{d}^2l|bl|^{-\alpha}(ql)^{-\beta}|al|^{-z}\left|\frac{al}{ql}\right|^{1/2}K_{i\tau}\left(\left|\frac{al}{ql}\right|\right)\exp\left(i\frac{bl}{ql}\right). \tag{C1}$$

The integral

$$\int \mathrm{d}^2l(kl)^{-z}|bl|^{-\alpha}(ql)^{-\beta}\,\mathrm{sign}(al) \tag{C2}$$

is manifestly Lorentz invariant, homogeneous of degree $-z$ in k and $-\beta$ in q, even in b, and odd in a. Utilizing these facts we calculate that

$$\int \mathrm{d}^2l(kl)^{-z}|bl|^{-\alpha}(ql)^{-\beta}\,\mathrm{sign}(al)=|bk|^{\beta-z}\cdot(qk)^{-\beta}\cdot\mathrm{sign}(ak)\cdot A(z;\alpha;k), \tag{C3}$$

where

$$A(z;\alpha;k)=2^z\int\frac{\mathrm{d}\xi'\,\mathrm{d}\eta'\,\mathrm{sign}(\xi')}{|\eta'|^{\alpha}\left[\left(\xi'-\left|\frac{ak}{bk}\right|\right)^2+(\eta'-1)^2\right]^z}, \tag{C4}$$

$\xi'=\xi/|bk/qk|$ and $\eta'=\eta/|bk/qk|$ being the scaled stereographic variables. The integral over η' can be calculated in a simple way. It is proportional to the associated Legendre function $P^{1/2-z}_{z+\alpha-3/2}$, which for $\alpha=3/2-z$ has the simplest form, i.e., does not contain the hypergeometric function ${}_2F_1$. Then the integral over ξ' can be calculated. Hence we choose $\alpha=3/2-z$. It is thus seen that the function $A(z;3/2-z;k)\equiv A(z;k)$ exists for $1/2<z<1$ and has the form

$$A(z;k)=2^{2-z}\sqrt{\pi}\frac{\Gamma\left(z-\frac{1}{2}\right)}{\Gamma(z)}\left[\frac{1}{1-z}\zeta^{1-z}(1+\zeta)^{-1/2}\,{}_2F_1\left(\frac{1}{2},1;2-z;\frac{\zeta}{1+\zeta}\right)\right.$$

$$\left.+2\zeta^{1/2}(1+\zeta)^{-z}\,{}_2F_1\left(z,1;\frac{3}{2};\frac{\zeta}{1+\zeta}\right)\right], \tag{C5}$$

where $\zeta=(1/2)(\sqrt{1+|ak/bk|^2}-1)$. Therefore for $1/2<z<1$, $\alpha=3/2-z$, Eq. (C1) can be rewritten as

$$\int \mathrm{d}^2k\,A(z;k)|bk|^{1/2-z}(qk)^{-1/2}|ak|^{z-2}\left|\frac{ak}{qk}\right|^{1/2}K_{i\tau}\left(\left|\frac{ak}{qk}\right|\right)\exp\left(i\frac{bk}{qk}\right)$$

$$=K^{-}(z;\tau)\int \mathrm{d}^2l|bl|^{z-3/2}(ql)^{-1/2}|al|^{-z}\left|\frac{al}{ql}\right|^{1/2}K_{i\tau}\left(\left|\frac{al}{ql}\right|\right)\exp\left(i\frac{bl}{ql}\right). \tag{C6}$$

Both integrals in Eq. (C6) exist for $1/2<z<1$; the integral on the left-hand side equals

$$\frac{\sqrt{2}\pi^{3/2}}{\cosh\left(\frac{\pi}{2}\tau\right)}\frac{\Gamma\left(z-\frac{1}{2}\right)}{\Gamma(z)}\left[\frac{1}{1-z}\left(\frac{3/2-z+i\tau}{2}\right)^{-1}{}_3F_2\left(\frac{1}{2},1,\frac{3/2-z+i\tau}{2};2-z,\frac{7/2-z+i\tau}{2};1\right)+\text{c.c.}\right.$$

$$\left.+2\left(\frac{1/2+z+i\tau}{2}\right)^{-1}{}_3F_2\left(z,1,\frac{1/2+z+i\tau}{2};\frac{3}{2},\frac{5/2+z+i\tau}{2};1\right)+\text{c.c.}\right], \tag{C7}$$

and the integral on the right-hand side equals

$$2^{3/2-z}\Gamma\left(\frac{3/2-z+i\tau}{2}\right)\Gamma\left(\frac{3/2-z-i\tau}{2}\right)\Gamma\left(z-\frac{1}{2}\right)\cos\frac{\pi}{2}\left(z-\frac{1}{2}\right). \tag{C8}$$

This leads directly to Eq. (18).

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Gauge theory on nonassociative spaces

S. Majid[a)]
School of Mathematical Sciences, Queen Mary, University of London, 327 Mile End Rd., London E1 4NS, United Kingdom

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We show how to do gauge theory on the octonions and other nonassociative algebras such as "quasi-$\mathbb{R}^4$" models proposed in string theory. We use the theory of quasialgebras obtained by cochain twist introduced previously. The gauge theory in this case is twisting–equivalent to the usual gauge theory on the underlying classical space. We give a general $U(1)$-Yang–Mills example for any quasialgebra and a full description of the moduli space of flat connections in this theory for the cube $\mathbb{Z}_2^3$ and hence for the octonions. We also obtain further results about the octonions themselves; an explicit Moyal-product description of them as a nonassociative quantization of functions on the cube, and a characterization of their cochain twist as invariant under Fourier transform. © *2005 American Institute of Physics.*
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I. INTRODUCTION

There has been a lot of interest recently in "nonassociative geometry" as a further extension of the ideas of noncommutative geometry, with now the "coordinate algebra" allowed to be nonassociative. The framework which we use of "quasialgebras" was already established and used to describe the octonions as "quasispaces" some years ago.[2] These were, moreover, constructed as a "cochain twist" of a classical associative space. Differential geometry on such quasispaces was introduced in Ref. 1 and in this paper we add "gauge theory."

The need for nonassociative geometry for noncommutative differential forms (even when the coordinate algebra itself remains associative) was shown in Ref. 5, where it was proven that all differential form algebras on the standard q-deformation quantum groups, if they are to be bicovariant and to have classical dimensions, must indeed be nonassociative. Thus the usual assumption in noncommutative geometry, including in Ref. 8, that differential forms should be associative, appears to be too strong. From a physics point of view also, there are suggestions that the world volume algebras on certain string theories are naturally nonassociative[9], and this has been realized quite concretely in some form in the context of reduced matrix models, see Refs. 19, 12, and 20. In the latter is posed the problem of gauge theory on such spaces, with apparently higher order differentials being required. We start by making precise what is fairly clear that the simplified "fuzzy" algebras in Ref. 20 are indeed quasialgebras in our required sense. We then show that in this case there is a natural formulation of gauge theory on them looking much more like the classical case. We describe this theory for any quasialgebra (or algebra in a nonassociative monoidal category) at an algebraic level and give a general construction for examples equivalent to $U(1)$-Yang–Mills in the associative case. The framework allows for non-Abelian gauge theory as well. Also, we do not discuss Lagrangians here but all of the necessary data and methods for these are known in the associative case, see notably Refs. 17 and 18, and apply equivalently to quasialgebras obtained by cochain twists.

As well as covering the strings-motivated example, we explore fully the octonions as finite "quasigeometries" par excellence. We show that the cochain $F(\vec{a},\vec{b})$ in Ref. 2 that modifies the

a)Electronic mail: s.majid@qmul.ac.uk

group algebra of the cube $\mathbb{Z}_2^3$ to the octonion product has the very remarkable feature of being invariant under $\mathbb{Z}_2^3$-Fourier transform. Using this, we also find an explicit more geometrical $\bullet$-product description of the octonion as a nonassociative quantization of the coordinate algebra on the Fourier-dual cube $\mathbb{Z}_2^3$ by means of a (finite difference) bidifferential operator. This is in the spirit of the Moyal-product of functions on $\mathbb{R}^n$, but now nonassociative. The associative quantization (Clifford algebra) case is also covered.

The paper begins in Sec. II with a brief introduction to the theory of quasialgebras obtained by cochain twist,[2,1] as algebras in a (symmetric) monoidal category. Sections II A and II B, respectively, outline the continuous case deforming $\mathbb{R}^n$ and the finite case deforming group algebras. In Sec. III A we recall from Ref. 14 the formulation of gauge theory in such a general monoidal category and the diagrammatic notation for it. Section III B applies this at an algebraic level to describe gauge theory on cochain twist quasialgebras in general. Section III C gives a canonical general example where the "gauge group" can be chosen canonically. Although appearing non-Abelian (and nonassociative) we show that this particular choice gives a theory equivalent to the undeformed $U(1)$-Yang–Mills theory. Note that in noncommutative geometry even the $U(1)$ theory has $F(\alpha)=\mathrm{d}\alpha+\alpha\wedge\alpha$ and we use the phrase Yang–Mills to distinguish this nonlinear theory from the Maxwell case where $F(\alpha)=\mathrm{d}\alpha$.

In Sec. IV we apply the theory of the quasialgebra versions of $\mathbb{R}^n$ of interest in Ref. 19 under heading of a simplified "quasi-$\mathbb{R}^n$." Section IV A introduces the required nonassociative differential calculus and Sec. IV B the promised gauge theory. Finally, in Sec. V we apply the theory of the octonions. Section V A warms up with the new results about the octonions as $\bullet$-product. Section V B has the gauge theory worked out for the octonions. In fact the example of deformed nonassociative gauge theory that we finally arrive at here takes the remarkably workable form

$$F_\bullet(\alpha)=\mathrm{d}\alpha+\sum F(|\alpha|,|\alpha'|)\alpha\bullet\alpha',$$

$$\alpha^\gamma_\bullet=\sum F(|\gamma^{-1}|,|\gamma|)F(|\alpha|,|\gamma|)(\gamma^{-1}\bullet\alpha)\bullet\gamma+\sum F(|\gamma^{-1}|,|\gamma|)\gamma^{-1}\bullet\mathrm{d}\gamma,$$

where the sum is over the different graded Fourier components of each object and to this end α' denotes a second independent copy of α. Such a description also works for the quasi-$\mathbb{R}^4$ if one works in terms of plane waves and their differentials; this is already the case for the octonions where the generators have in our picture the interpretation of deformed plane waves on the cube. In the octonions case $F(\vec{a},\vec{b})$ has values ±1 but is not simply an exponential bilinear of the vector degrees (the three-momentum) as its exponent has cubic terms. It is not known if such quasigeometry of the octonions has a direct physical role, but see for example Ref. 7. We also note the link between the octonions and particle physics;[10] their geometry might play a role in the context of the direct product of spacetime by the finite geometry.

Section V C fills a gap in the literature, namely a complete description of the moduli space of flat $U(1)$-Yang–Mills fields up to gauge transformation on $\mathbb{Z}_2^2$ and $\mathbb{Z}_2^3$, using the same methods as for the symmetric group S_3 in Ref. 18. The above-mentioned equivalence means that the $\mathbb{Z}_2^3$ case also classifies flat connections in the nonassociative theory on the octonions. We note that flat connections on finite groups are also of interest in pure mathematics in connection with Schubert calculus on flag varieties, Ref. 16. Going back to physics, the quantum $U(1)$-Yang–Mills theory on $\mathbb{Z}_2^2$ is fully worked out in Ref. 17 and is renormalizable and computable. The $\mathbb{Z}_2^3$ and octonion cases could in principle be similarly computed. This would be one of several directions for further work.

We also note the related paper[6] where cochain twists are used to describe associative quantizations in which the differential calculus, however, is nonassociative. It turns out that several popular associative quantizations in physics fall into this category; the algebra of coordinates is associative but the nonassociative gauge theory described here still plays a role in view of the differential calculus. Examples in this category include $U(\mathfrak{g})$ as quantization of the Kirillov–Kostant bracket, now expressed as a cochain twist at least to lower order, see Ref. 6.

II. QUASIALGEBRAS BY COCHAIN TWIST

The constructions in the paper come out of quantum group theory (i.e., we use the language of Hopf algebras) but we apply them to classical (not quantum) enveloping algebras and finite group algebras. Thus, let H be a Hopf algebra with coproduct $\Delta: H \to H \otimes H$, counit $\epsilon: H \to \mathbb{C}$ and antipode $S: H \to H$, see Ref. 15. Let $F \in H \otimes H$ be a cochain, i.e., F is invertible and $(\epsilon \otimes \mathrm{id})F = 1 = (\mathrm{id} \otimes \epsilon)F$. Associated to F is its non-Abelian cohomology coboundary

$$\Phi = \partial F = F_{23}((\mathrm{id} \otimes \Delta)F)((\Delta \otimes \mathrm{id})F^{-1})F_{12}^{-1},$$

where $F_{23} = 1 \otimes F \in H^{\otimes 3}$, etc. By construction Φ, called the "associator," is a three-cocycle in the required sense. These data go back to V.G. Drinfeld and it is known that H^F defined by the same algebra as H and with coproduct $\Delta_F = F(\Delta\,)F^{-1}$ and suitable S_F gives a quasi-Hopf algebra.[11]

Now let A be an H-covariant associative algebra. The cochain-twisted quasialgebra A_F is defined as the same vector space as A but with a new product

$$a \bullet b = \cdot(F^{-1} \triangleright (a \otimes b)),$$

where $\triangleright$ denotes the action of each copy of H. The new A_F is nonassociative but obeys

$$(a \bullet b) \bullet c = \bullet(\mathrm{id} \otimes (\bullet))(\Phi \triangleright (a \otimes b \otimes c))$$

for all a, b, c, and is covariant under H^F.

Moreover, when $\Omega(A)$ is an algebra of differential forms on A that is H-covariant, then $\Omega(A_F) = \Omega(A)_F$ defines for us the wedge product algebra of differential forms on A_F, covariant under H^F and again potentially nonassociative.[1] Note that d is not deformed and assumed to commute with the action of H, hence

$$a \bullet \mathrm{d}b = F^{-(1)} \triangleright a \mathrm{d}(F^{-(2)} b), \quad \mathrm{d}a \bullet b = \mathrm{d}(F^{-(1)} \triangleright a) F^{-(2)} \triangleright b, \quad \mathrm{d}a \bullet \mathrm{d}b = (\mathrm{d}F^{-(1)} \triangleright a) \wedge \mathrm{d}(F^{-(2)} \triangleright b)$$

for the deformed wedge product in terms of the undeformed one, where $F^{-1} = F^{-(1)} \otimes F^{-(2)}$ (summation understood) is a notation.

The two examples that will be fully computed in this article are of the general types which we now describe. Note that we work over $\mathbb{C}$ for convenience and because in physical examples there are further unitarity restrictions (otherwise, the general constructions work over any field, though one should avoid certain characteristics in the examples). Also, we use the H-module version of the cochain twist theory as mentioned previously because actions are more familiar to physicists; there is a parallel and in many ways better version of the theory with H coacting on the algebra.

A. Quasi-$\mathbb{R}^n$

Let $H = U(\mathbb{R}^n)$, with Hopf algebra structure

$$\Delta \partial^i = \partial^i \otimes 1 + 1 \otimes \partial^i, \quad \epsilon \partial^i = 0, \quad S\partial^i = -\partial^i.$$

Here $\mathbb{R}^n$ acts on $\mathbb{R}^n$ by translation and hence on its coordinate algebra $A = \mathbb{C}[\mathbb{R}^n]$ by differentiation operators $\partial = \{\partial^i\}$ and we think of the latter quite concretely as generating $U(\mathbb{R}^n)$. Let F be a nowhere vanishing function of two vector coordinates (i.e., a function on $\mathbb{R}^{2n}$) with value 1 when either argument is zero. We consider $F \in H \otimes H$ (or in some completion of this space if F is not a polynomial) as a cochain. Because H is commutative, $H^F = H$ as an algebra and as a coalgebra, but is still regarded with

$$\Phi(\partial_1, \partial_2, \partial_3) = \frac{F(\partial_2, \partial_3) F(\partial_1, \partial_2 + \partial_3)}{F(\partial_1 + \partial_2, \partial_3) F(\partial_1, \partial_2)}$$

as a quasi-Hopf algebra. Here $\partial_1 = \partial \otimes 1 \otimes 1$, $\partial_2 = 1 \otimes \partial \otimes 1$, $\partial_3 = 1 \otimes 1 \otimes \partial$ in $H^{\otimes 3}$ so Φ is a function of these $3n$ variables.

Then A_F has a new product

$$a \bullet b = \cdot F^{-1}(\partial_1, \partial_2) a \otimes b,$$

where $a(x), b(x)$ are acted upon by ∂_1, ∂_2, respectively, and then the result multiplied. Quasiassociativity will take the above-mentioned form, as

$$(a \bullet b) \bullet c = \bullet(\mathrm{id} \otimes (\bullet))\Phi(\partial_1, \partial_2, \partial_3)(a \otimes b \otimes c),$$

where ∂_1 means ∂ acting on a, ∂_2 means ∂ acting on b, ∂_3 means ∂ acting on c, and products are in A_F. Recall that ∂ itself is a vector, namely the momentum vector operator generating translations in $\mathbb{R}^n$.

Of interest in physics seems to be the following special case. Let $\Box = \Sigma \partial^i \otimes \partial^j \eta_{ij} = \partial_1 \cdot \partial_2$ taken with the Euclidean metric say (or any other fixed tensor η on $\mathbb{R}^n$ in place of the dot product). Let f be any nowhere vanishing function in *one* variable and take

$$F(\partial_1, \partial_2) = f(\Box), \quad \Phi(\partial_1, \partial_2, \partial_3) = \frac{f(\Box_{23}) f(\Box_{12} + \Box_{13})}{f(\Box_{13} + \Box_{23}) f(\Box_{12})},$$

where $\Box_{13} = \partial_1 \cdot \partial_3$ is $\Box$ embedded in the first and third tensor positions, etc.

If f is an exponential then $\Phi = 1$ and A_F is associative. For example, if η_{ij} is antisymmetric one has the usual Moyal product for the Heisenberg–Weyl algebra or so-called noncommutative $\mathbb{R}^n$ used for example by Seiberg and Witten for the effective description of the ends of open strings on 2-branes. At the other extreme would be η_{ij} the Euclidean metric in which case the algebra remains commutative and associative. In general if F remains symmetric but f is no longer an exponential then the algebra A_F will be commutative but not associative. This covers the example in Ref. 20 where

$$F(\partial_1, \partial_2) = \left(1 + \frac{\lambda}{m} \Box\right)^{-m}$$

which becomes approximately an exponential $\exp(\lambda \Box)$ as $m \to \infty$. Here λ is the deformation parameter which is taken with value m^{-1} in Ref. 20, but one can also keep these parameters λ, m independent. We have

$$\Phi(\partial_1, \partial_2, \partial_3) = \left(1 + \frac{\frac{\lambda^2}{m^2} \Box_{13}(\Box_{12} - \Box_{23})}{1 + \frac{\lambda}{m}(\Box_{12} + \Box_{13} + \Box_{23}) + \frac{\lambda^2}{m^2} \Box_{23}(\Box_{12} + \Box_{13})}\right)^m.$$

Another interesting family of commutative but nonassociative quasi-$\mathbb{R}^n$ is with

$$F(\partial_1, \partial_2) = e^{-(\lambda/2)\Box^2}, \quad \Phi = e^{-\lambda \Box_{13}(\Box_{12} - \Box_{23})} = e^{-\lambda \eta_{ij} \eta_{kl} (\partial^i \partial^k \otimes \partial^j \otimes \partial^l - \partial^i \otimes \partial^k \otimes \partial^j \partial^l)}$$

when we unpack our compact notation (summation convention understood).

A third variant is with $H = U(\mathbb{R}^n \rtimes \mathbb{R})$ where an extra "dilation" generator D is added. Its relations, coproduct and action on coordinates are

$$[D, \partial^i] = -\partial^i, \quad \Delta D = D \otimes 1 + 1 \otimes D, \quad D \triangleright x_i = x_i$$

(so that D has action p on a monomial of total degree p). In this way $A = \mathbb{C}[\mathbb{R}^n]$ is again covariant under this extended H. One can now have more interesting cochains, for example

$$F = e^{-\lambda \Box - v(D \otimes D)}$$

for a "potential function" v. If $v = 0$ we have $\Phi = 1$ as explained previously. In general, it is tempting to think of the introduction of nonbilinears in the exponent of F as a way to encode interactions as nonassociativity. The passage from the free theory to the interacting theory would then be a matter of a cochain twist by the interaction.[1] This last example is in that spirit.

Clearly a great many models along the above lines are equally possible, as any cochain F is allowed in our framework.

B. Quasi-$\mathbb{Z}_2^n$

Here we take $H=\mathbb{C}(G)$, the functions on a finite group. This has basis of delta functions $\{\delta_a\}$ labeled by $a\in G$ and coproduct $\Delta\delta_a=\Sigma_{bc=a}\delta_b\otimes\delta_c$, counit $\epsilon\delta_a=\delta_{a,e}$ and antipode $S\delta_a=\delta_{a^{-1}}$. Here e is the group identity. We take $A=\mathbb{C}G$ the group algebra of G. This has basis $\{e_a\}$ labeled again by group elements. The product is just the product of G, so $e_ae_b=e_{ab}$. This is covariant under $\mathbb{C}(G)$ with action

$$\delta_a\triangleright e_b=\delta_{a,b}e_b.$$

A cochain on H is a suitable $F\in H\otimes H$, i.e., a nowhere vanishing 2-argument function $F(a,b)$ on the group with value 1 when either argument is the group identity e. Then

$$\Phi(a,b,c)=\frac{F(b,c)F(a,bc)}{F(ab,c)F(a,b)}$$

is the usual group-cohomology coboundary of F and is a group 3-cocycle. Then H^F is the same algebra and coalgebra as H but is viewed as a quasi-Hopf algebra with this Φ. Finally, the canonical example of a quasialgebra here is the twisted group algebra A_F with the new product

$$e_a\bullet e_b=F^{-1}(a,b)e_{ab}.$$

An example is $G=\mathbb{Z}_2^3$ which we write additively as 3-vectors $\vec{a}$ with entires in $\mathbb{Z}_2$. We take

$$\vec{a}^T\begin{pmatrix}1&1&1\\0&1&1\\0&0&1\end{pmatrix}\vec{b}+a_1b_2b_3+b_1a_2b_3+b_1b_2a_3$$

$$F(\vec{a},\vec{b})=(-1)\qquad,\quad \Phi(\vec{a},\vec{b},\vec{c})=(-1)^{\vec{a}\cdot(\vec{b}\times\vec{c})}$$

The new product

$$e_{\vec{a}}\bullet e_{\vec{b}}=F(\vec{a},\vec{b})e_{\vec{a}+\vec{b}}$$

is that of the octonions $\mathbb{O}$ as explained in Ref. 2. If we think of this in the same spirit as the models above, we note that Φ comes from the cubic "interaction term" in the exponent of F. Thus the octonions are a cochain quantization of the finite group $\mathbb{Z}_2^3$ as a quasialgebra. Without the cubic interaction term one has the Clifford algebra in three dimensions. Similarly $n=2$ gives the quaternions or (over $\mathbb{C}$) the algebra of 2×2 matrices.

One can do the same for larger $\mathbb{Z}_2^n$. For the same bilinear form as the previous one, one obtains the Clifford algebra as an associative cochain quantization of $\mathbb{Z}_2^n$, whereas further "interaction" terms give higher Cayley–Dickson and other quasialgebras of interest, see Refs. 2 and 4. Many other examples could be of interest, e.g., for $G=\mathbb{Z}_n$ see Ref. 3.

III. GAUGE THEORY IN MONOIDAL CATEGORIES

With the above-mentioned background the main question we address in this article is that of gauge theory on nonassociative spaces. For the ones in Sec. II A of interest in string theory, a somewhat complex approach has been proposed in Ref. 20 whereas here we propose a simpler one. Briefly, geometry including gauge theory can be done in any monoidal Abelian category $\mathcal{C}$.[13,14] We explain this in Sec. III A and give a concrete algebraic setting in Secs. III B and III C, which are the new results of the section.

Before doing this, let us explain the problem at the simplest level. If we have an associative algebra with a differential calculus obeying the Leibniz rule, one can write down the simplest "$U(1)$-Yang–Mills" theory where a connection is a differential 1-form $\alpha\in\Omega^1$, decreed to transform as

$$\alpha\mapsto \gamma^{-1}\alpha\gamma+\gamma^{-1}\mathrm{d}\gamma \tag{1}$$

for γ any invertible element of the algebra. The fundamental lemma of gauge theory is that then the curvature $F(\alpha)=\mathrm{d}\alpha+\alpha\wedge\alpha$ transforms by conjugation to $\gamma^{-1}F(\alpha)\gamma$. Note that the nonlinear term need not vanish in noncommutative geometry even in this simplest case. The moduli space of flat connections up to gauge transformations is highly nontrivial even for the simplest commutative or noncommutative algebras[18] and carries a lot of "homotopy" information. We will describe it for the functions on the cube $\mathbb{Z}_2^3$ in Sec. V C under a further unitarity restriction (in the *-algebra case one requires $\gamma^*=\gamma^{-1}$, i.e., unitary).

Let us try this now when the algebra is nonassociative. The simplest part of the abovementioned lemma is that $\alpha=\gamma^{-1}\mathrm{d}\gamma$ should have zero curvature. Being careful about brackets, we have

$$\mathrm{d}(\gamma^{-1}\mathrm{d}\gamma)+(\gamma^{-1}\mathrm{d}\gamma)(\gamma^{-1}\mathrm{d}\gamma)=(\mathrm{d}\gamma^{-1})\mathrm{d}\gamma+(\gamma^{-1}\mathrm{d}\gamma)(\gamma^{-1}\mathrm{d}\gamma)=-((\gamma^{-1}\mathrm{d}\gamma)\gamma^{-1})\mathrm{d}\gamma+(\gamma^{-1}\mathrm{d}\gamma)(\gamma^{-1}\mathrm{d}\gamma)$$

which is nonzero precisely when $\gamma^{-1}\mathrm{d}\gamma,\gamma^{-1},\mathrm{d}\gamma$ fail to associate. The computation of $\mathrm{d}\gamma^{-1}$ here is from $\mathrm{d}(\gamma^{-1}\gamma)=0$ and the Leibniz rule, being careful about brackets. This could work for some γ in the algebra but not for all invertible or unitary elements as in the associative case.

A. Diagrammatic gauge theory

A monoidal category $\mathcal{C}$ means a collection of objects with a tensor product between any two objects and an associator natural isomorphism $\Phi_{V,W,Z}:(V\otimes W)\otimes Z\to V\otimes(W\otimes Z)$ for any three objects, obeying the usual properties, notably Mac Lane's pentagon identity. The latter says that the two routes to rebracket

$$((U\otimes V)\otimes W)\otimes Z\to U\otimes(V\otimes(W\otimes Z))$$

are the same. In that case the coherence theorem of Mac Lane says that all other bracketting ambiguities are resolved, i.e., we can and should freely insert associators Φ in order for expressions to make sense and different ways to do that will give the same result. In that case we can adopt a diagrammatic notation in which we omit brackets entirely. We also denote $\otimes$ by omission. We write maps between objects (morphisms) as beads on a string flowing down from one object to the other. We also require direct sums $\oplus$ to be defined and to be compatible in the usual way with $\otimes$. Now, because brackets are omitted, gauge theory *must* work at this level because usual associative gauge theory works when expressed by the same diagrams. In the nonassociative case, however, the translation of the diagrams back into algebra requires the insertion of the nontrivial associator Φ for rebrackettings. We recall here only the "basic level" of gauge theory[13] in this diagrammatic form; there is a more geometrical theory with diagrammatic principal bundles etc.[13]

As an example an associative algebra $\mathcal{A}$ in a monoidal category means an object $\mathcal{A}$ with a product Y such that the two ways to feed the result of Y into another Y give the same. As a result we can depict the iterated product as a node with three lines coming in and one coming out (i.e., collapse the two equivalent tree graphs). We will use such a notation. A coalgebra $\mathcal{B}$ is an object $\mathcal{B}$ with a coproduct $\Delta:\mathcal{B}\to\mathcal{B}\otimes\mathcal{B}$ which we denote by an inverted Y and which "coassociates" similarly. The unit axiom for an algebra says that a 1 branching into a product can be "pruned" off. Similarly a counit $\epsilon:\mathcal{B}\to\underline{1}$ (the latter denoted by omission) is a branch emerging from a coproduct node and can be pruned. More details of "algebra" in such diagrams are in Ref. 15. A coalgebra $\mathcal{B}$ can "coact" on an object $\mathcal{V}$ and we use the inverted Y also to denote the coaction $\mathcal{V}\to\mathcal{V}\otimes\mathcal{B}$.

Similarly, a differential calculus Ω on $\mathcal{A}$ means a graded algebra in the category with $\mathcal{A}$ in degree zero, and d a morphism (hence a node) increasing degree by 1, obeying a graded-Leibniz rule and $\mathrm{d}^2=0$. All of this translates directly into (sums of) diagrams. One usually assumes that Ω

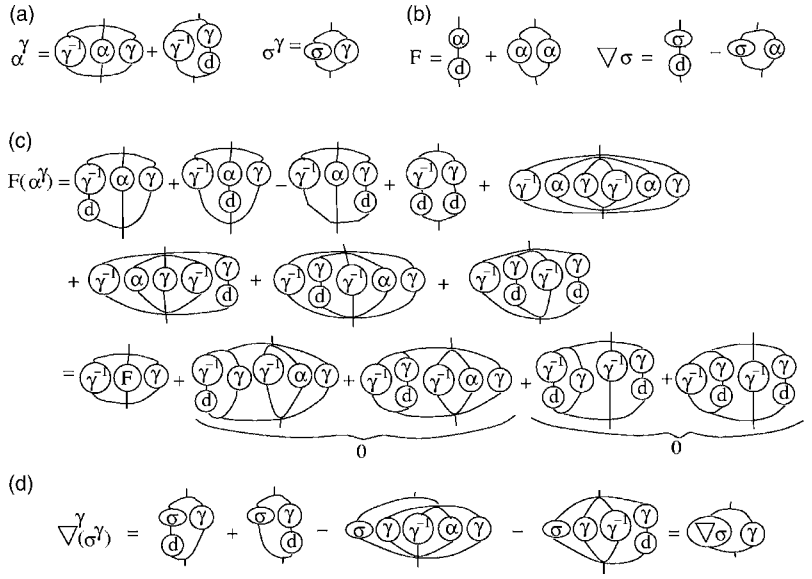

FIG. 1. Local gauge theory in a monoidal category: (a) gauge transform by γ of gauge and matter fields, (b) definition of curvature and covariant derivative, and (c) and (d) proof of covariance of F, ∇.

is generated by $\mathcal{A}$ and the 1-forms Ω^1 but this is not necessary for the basic level of gauge theory that we describe here. We use Y also to denote products in this exterior algebra.

We are now ready to define matter fields as morphisms $\sigma: \mathcal{V} \to \mathcal{A}$. One can consider that σ has "values in $\mathcal{V}^*$" (but it is more convenient to view it is a morphism). Similarly, a gauge field is a morphism $\alpha: \mathcal{B} \to \Omega^1$ where $\mathcal{B}$ is at least a coalgebra. Typically it might be a Hopf algebra in the category if this is braided, but such an assumption is again not needed for the basic level of gauge theory. One may think of α as a 1-form with values in the algebra $\mathcal{B}^*$, i.e., we do general possibly non-Abelian gauge theory here, but again it is more convenient to view α as a morphism. Finally, a gauge transformation is a morphism $\gamma: \mathcal{B} \to \mathcal{A}$ with inverse γ^{-1} in the sense

$$\cdot(\gamma \otimes \gamma^{-1})\Delta = \cdot(\gamma^{-1} \otimes \gamma)\Delta = 1 \circ \varepsilon$$

or in diagrams: if we split using the coproduct, apply γ, γ^{-1} and close up with a product Y, this composition is the same either way as the counit map ϵ into nothing, followed by the unit map 1 coming from nothing. The action of such gauge transformations is shown in Fig. 1(a). The basic covariant objects of interest namely the curvature and covariant derivative (the former is in a suitable sense the square of the latter) are shown in Fig. 1(b).

The fundamental lemmas of gauge theory are then shown in Figs. 1(c) and 1(d); we check that $F(\alpha^\gamma) = F(\alpha)^\gamma$ and that $\nabla(\sigma^\gamma) = (\nabla\sigma)^\gamma$. In Fig. 1(c), we expand d on the "conjugated" α using the Leibniz rule to obtain the first three terms. The next term is d applied to "$\gamma^{-1}\mathrm{d}\gamma$" again using the Leibniz rule, followed by $\mathrm{d}^2 = 0$. The remaining four terms are an expansion of "$(\alpha^\gamma)^2$." Of the various terms, the second and fifth (after canceling $\gamma\gamma^{-1}$ to obtain a unit and counit and "pruning" these as explained previously) give the transform of $F(\alpha)$ as required. The first (after inserting $\gamma\gamma^{-1}$) and seventh combine via Leibniz to give zero in view of $\mathrm{d}(1) = 0$. The fourth (inserting $\gamma\gamma^{-1}$) and eighth likewise give zero for the same reason. In (d) we compute ∇ using the transformed quantities. The second and fourth terms cancel (after canceling $\gamma\gamma^{-1}$) and we identify the required result.

This establishes "local gauge theory" at this diagrammatic level, cf. Ref. 14 (where the focus was on the universal calculus, not assumed here). For principal bundles etc at this level see Ref. 13. The latter contains explicit (associative) examples.

B. Algebraic construction of nonassociative gauge theory by twisting

The questions arise: how to obtain nonassociative examples of such a diagrammatic gauge theory and how does it look in explicit calculations? We will address the first in the remainder of the section, and the second in the remainder of the article.

We do this by extending the cochain twisting theory in Sec. II. Thus let A be an algebra with calculus covariant under a background symmetry H as in Sec. II. Here A could be functions on a classical manifold and H the enveloping algebra of an ordinary Lie algebra, for example. Let now B be an H-covariant coalgebra. It means that there is a coproduct $\Delta_B: B \to B \otimes B$ which is an intertwiner for the action of H. Also a counit ϵ_B. Suppose now that

$$\alpha: B \to \Omega^1(A), \quad \gamma: B \to A, \quad F(\alpha): B \to \Omega^2(A), \quad \sigma: V \to \Omega^1(A),$$

and ∇ are as in Sec. III A, i.e., a connection, gauge transformation etc. These form a gauge theory with the usual tensor product on the associative algebra A as in Sec. III A. This theory can also be written without diagrams by means of the "convolution product" $*$ of maps from a coalgebra to an algebra or module. Thus

$$\alpha * \alpha = \wedge(\alpha \otimes \alpha)\Delta_B, \quad F = \mathrm{d}\alpha + \alpha * \alpha, \quad \alpha^\gamma = \gamma^{-1} * \alpha * \gamma + \gamma^{-1} * \mathrm{d}\gamma$$

and so forth. If $B = \mathbb{C}.1$ with $\Delta_B 1 = 1 \otimes 1$, we have the simplest case of gauge theory mentioned in the preamble above. When $B = \mathbb{C}(G)$ the functions on a Lie group one has a general form of usual non-Abelian gauge theory. One can take here H to be trivial, otherwise one has an equivariant gauge theory.

Now let $F \in H \otimes H$ be a cochain and define $B_F = B$ as a vector space but with deformed coproduct

$$\Delta_\bullet = F \triangleright \Delta_B$$

and unchanged ϵ_B. First, it can be seen that B_F is covariant under the twisted H^F. Indeed,

$$h \triangleright (F \triangleright \Delta_B b) = F(\Delta h)F^{-1} \triangleright (F \triangleright \Delta_B b) = F \triangleright ((\Delta h) \triangleright \Delta_B b) = F \triangleright \Delta_B (h \triangleright b)$$

as the quasi-Hopf algebra H^F acts on tensor products by its twisted coproduct Δ_F as explained in Sec. II. Moreover, B_F is a coalgebra but only in the monoidal category of H^F-modules, i.e., a "quasicoalgebra" in the sense:

$$\Phi_{B,B,B}(\Delta_\bullet \otimes \mathrm{id})\Delta_\bullet = (\mathrm{id} \otimes \Delta_\bullet)\Delta_\bullet$$

as may be verified by direct computation. The theory is dual to that of twisting algebras so we omit the details. Similarly if $\Delta_V: V \to V \otimes B$ is a coaction covariant under H, we define V_F to be the same vector space but with deformed coaction $\Delta_{V\bullet} = F \triangleright \Delta_V$, and can check that it is covariant under H^F and a coaction of B_F in the monoidal category.

We now claim that the same maps viewed as morphisms

$$\alpha: B_F \to \Omega^1(A_F), \quad \gamma: B_F \to A_F, \quad F(\alpha): B_F \to \Omega^2(A_F), \quad \sigma: V_F \to A_F$$

form a gauge theory in the monoidal category of H^F-covariant objects, i.e., are an example of the constructions in Sec. III A and enjoy the same relationships as before twisting. For example, if we compute $\alpha *_\bullet \alpha$ where the subscript means in the deformed nonassociative theory,

$$\alpha *_\bullet \alpha = \bullet(\alpha \otimes \alpha)\Delta_\bullet = \bullet(F^{-1} \triangleright (\alpha \otimes \alpha) F \triangleright \Delta_B) = \wedge(\alpha \otimes \alpha)\Delta_B = \alpha * \alpha$$

because each α is an intertwiner, i.e., covariant under the action of H. We use $\bullet$ for the deformed product in the exterior algebra including wedge products. Similarly for all other expressions. In other words *the twisted nonassociative theory is fully equivalent to the original associative one*. This is an important requirement from a deformation-theoretic point of view; if one thinks of the

twisting as quantization, this is an extension of the correspondence principle from classical gauge theory to gauge theory on the quantum (possibly nonassociative) space.

On the other hand, computed entirely in the nonassociative deformed category, the gauge theory appears quite different. Remembering that the products are quasiassociative, we must fix brackettings when translating the diagrams into algebra and we do so by a convention to bracket by default to the left, inserting associators Φ according to Mac Lane's coherence theorem whenever a different bracketting is needed. Thus for example,

$$\alpha^\gamma_\bullet = ((\bullet)\otimes\bullet)((\gamma^{-1}\otimes\alpha)\otimes\gamma)(\Delta_\bullet\otimes\mathrm{id})\Delta_\bullet + \bullet(\gamma^{-1}\otimes\gamma)\Delta_\bullet$$

as a morphism $B_F\to\Omega^1(A_F)$. Provided one inserts Φ as specified (and where there is more than one way to do it one has the same result for any choice), the diagrammatic proof in Sec. III A becomes an algebraic proof that

$$F_\bullet(\alpha) = \mathrm{d}\alpha + \bullet(\alpha\otimes\alpha)\Delta_\bullet$$

obeys

$$F_\bullet(\alpha^\gamma_\bullet) = ((\bullet)\otimes\bullet)((\gamma^{-1}\otimes F_\bullet)\otimes\gamma)(\Delta_\bullet\otimes\mathrm{id})\Delta_\bullet$$

i.e., the fundamental lemma of (nonassociative) gauge theory. When there are matter fields we have similarly

$$\sigma^\gamma_\bullet(v) = \bullet(\sigma\otimes\gamma)\Delta_\bullet,\quad \nabla_\bullet\sigma(v) = \mathrm{d}\sigma(v) - \bullet(\sigma\otimes\alpha)\Delta_\bullet,\quad \nabla^\gamma_\bullet(\sigma^\gamma_\bullet) = (\nabla_\bullet\sigma)^\gamma.$$

C. Canonical example equivalent to *U*(1)-Yang–Mills

Finally, let us give a canonical example of an equivariant gauge theory and its twisting, that requires only the data for a cochain quantization as in Sec. II, i.e., there is a canonical choice of B.

Thus, let H be a Hopf algebra and A an algebra with calculus which is H-covariant. We then set $B=H$ as a coalgebra, $\Delta_B=\Delta$ (the coproduct of H, ignoring the algebra structure of H). This is automatically covariant under the action of H on B by left-multiplication:

$$h\triangleright\Delta_B(b) = \Delta_H(h)\triangleright\Delta_B(b) = \Delta_H(h)\Delta_H(b) = \Delta_H(hb) = \Delta_B(h\triangleright b).$$

On the other hand, since every element of B is obtained by acting by H on 1, and since α,γ,F etc. are morphisms, they are fully determined by their values on 1, i.e., by

$$\alpha(1)\in\Omega^1(A),\quad \gamma(1)\in A,\quad F(\alpha)(1)\in\Omega^2(A).$$

Here $\alpha(1),\gamma(1)$ etc. are chosen freely and form a usual gauge theory of the simplest $U(1)$-Yang–Mills type described in the preamble on any algebra. This is because $\Delta(1)=1\otimes 1$ so all the coproducts in Fig. 1 disappear when specialized to acting on 1, so

$$\alpha^\gamma(1) = \gamma^{-1}(1)\alpha(1)\gamma(1) + \gamma^{-1}(1)\mathrm{d}\gamma(1),\quad F(1) = \mathrm{d}\alpha(1) + \alpha(1)\wedge\alpha(1),$$

etc. Our construction "amplifies" this standard $U(1)$-Yang–Mills gauge theory on an algebra to an H-equivariant one for any H by $\alpha(b)=\alpha(b\triangleright 1)=b\triangleright\alpha(1)$ and $\gamma(b)=\gamma(b\triangleright 1)=b\triangleright\gamma(1)$.

For matter fields, the requirement that the coaction: $V\to V\otimes B$ is a morphism makes V into some form of "Hopf module," i.e. a vector space on which H both acts and coacts in a suitably compatible manner, namely here

$$\Delta_V(h\triangleright v) = (\Delta h)\triangleright\Delta_V(v).$$

Hopf modules are fully determined by their space

$$V^H = \{v \in V | \Delta_V(v) = v \otimes 1\}$$

of elements invariant under the coaction. The Hopf module-lemma ensures that these invariant elements $v \in V^H$ generate all of V through the action. Note that this is usually done for action and coaction in the same side but with care works also in our case where the action is a left one and the coaction a right one. Indeed, we have

$$H \otimes V^H \to V, \quad h \otimes v \to h \triangleright v, \quad V \to H \otimes V^H, \quad v \mapsto v^{(2)}{}_{(2)} \otimes S^{-1} v^{(2)}{}_{(1)} \triangleright v^{(1)},$$

where the antipode S of the Hopf algebra is assumed to be invertible and where $\Delta_V(v) \equiv v^{(1)} \otimes v^{(2)}$ and $\Delta h \equiv h_{(1)} \otimes h_{(2)}$ are standard Hopf algebra notations. It is straightforward to see then that these two maps are mutually inverse, so $V \cong H \otimes V^H$ and that the second map indeed lands in $H \otimes V^H$ (this is not obvious but can be checked using routine Hopf algebra methods). Conversely, given any vector space W we can define $V = H \otimes W$ with action and coaction of H

$$h \triangleright (g \otimes w) = hg \otimes v, \quad \Delta_V(h \otimes w) = (h_{(1)} \otimes w) \otimes h_{(2)}, \quad h, g \in H,\ w \in W,$$

and check that $W = V^H$; the previous discussion tells us that any crossed module V is equivalent to one of this standard type. In short, the input data for matter fields in the theory boils down to choosing a vector space.

Moreover, since $\sigma: V \to A$ is assumed to be H-covariant, it is fully determined by its values on this vector space V^H, since $\sigma(\Sigma_p h_p \triangleright v_p) = \Sigma_p h_p \triangleright \sigma(v_p)$ for any basis $\{v_p\}$ of V^H. So the gauge theory above is equivalent to specifying a map $\sigma: V^H \to A$ or a multiplet of matter fields $\sigma(v_p)$ if we fix a basis of V^H. Thus our theory becomes equivalent to usual $U(1)$-theory with a multitplet of matter fields. Indeed, $\sigma(v_p) \in A$ obeys

$$\sigma^\gamma(v_p) = \sigma(v_p)\gamma(1), \quad (\nabla\sigma)(v_p) = \mathrm{d}\sigma(v_p) - \sigma(v_p)\alpha(1)$$

as would be expected for $U(1)$ fields.

We now are ready simply to twist this theory using the method in Sec. III B. B_F now has "deformed coproduct" $\Delta_\bullet = F\Delta$. A gauge field is again determined by $\alpha(1)$ but $\Delta_\bullet(1) = F \in H \otimes H$ so

$$F_\bullet(\alpha)(1) = \mathrm{d}\alpha(1) + (\alpha *_\bullet \alpha)(1) = \mathrm{d}\alpha(1) + \bullet(\alpha \otimes \alpha)(F),$$

$$\alpha^\gamma_\bullet(1) = ((\bullet)\bullet)((\gamma^{-1} \otimes \alpha) \otimes \gamma)((\Delta \otimes \mathrm{id})F) + \bullet(\gamma^{-1} \otimes \mathrm{d}\gamma)(F)$$

in terms of the deformed bullet product on $\Omega(A_F)$. As previously, our convention is to read the diagrams with brackets accumulating to the left, with Φ to be inserted as needed for any other bracketting that may be required. The expressions above will be equal as linear maps to $F(\alpha(1)), \alpha^\gamma(1)$, etc. as explained in Sec. III B, so the deformed theory is in correspondence with the original theory before twisting, but is well-formed in its own right.

Finally, if we have matter fields and elements v_p that are invariant under the coaction, then the deformed coaction and hence gauge transform of matter fields is

$$\Delta_{V\bullet}(v_p) = F^{(1)} \triangleright v_p \otimes F^{(2)}, \quad \sigma^\gamma_\bullet(v) = \sigma(F^{(1)} \triangleright v_p)\gamma(F^{(2)}), \quad F \equiv F^{(1)} \otimes F^{(2)}.$$

Here we see that as with the gauge fields mentioned previously, it is the entire "amplified" theory that twists into a nonassociative one. It remains, however, equivalent to the $U(1)$-gauge theory with matter.

IV. DIFFERENTIALS AND GAUGE THEORY ON QUASI-$\mathbb{R}^n$

In this section we illustrate the above formalism on the example of quasi-$\mathbb{R}^n$. To be concrete, we focus calculations on the main example where $f = (1 + \lambda\Box/m)^{-m}$ in Sec. II A, but the same methods apply for the other versions of quasi-$\mathbb{R}^n$. We start with the algebra and differentials in more detail, and then turn to the gauge theory.

A. Algebra and differentials on quasi-$\mathbb{R}^n$

From Sec. II A, we have

$$a \bullet b = \sum_{r=0}^{m} \binom{m}{r} \left(\frac{\lambda}{m}\right)^r (\partial^{i_1} \cdots \partial^{i_r} a)(\partial_{i_1} \cdots \partial_{i_r} b),$$

where we use η_{ij} to lower indices. We call this algebra $\mathbb{R}^n_{m,\lambda}$; the case in string theory is with $\lambda = 1/m$. For example, with the usual coordinates x_μ of $\mathbb{R}^n$ we have the bullet product

$$x_\mu \bullet x_\nu = x_\mu x_\nu + \lambda \delta_{\mu,\nu}$$

which is a simplified version[20] of higher-dimensional so-called "fuzzy spheres" that arise from the truncated matrix product in certain string matrix models. Here m is a truncation order and the algebra becomes associative as $m \to \infty$.

For our purposes we also need a differential calculus and we use the same F built from f but now with the ∂^i acting by Lie derivative on differential forms. Then the usual $\Omega(\mathbb{R}^n)$ deforms to a (nonassociative) $\Omega(\mathbb{R}^n_{m,\lambda})$. Notice that Lie derivative commutes with exterior d, so the classical differential calculus is indeed covariant as required. Then

$$a \bullet \mathrm{d}b = \sum_{r=0}^{m} \binom{m}{r} \left(\frac{\lambda}{m}\right)^r (\partial^{i_1} \cdots \partial^{i_r} a) \mathrm{d}\partial_{i_1} \cdots \partial_{i_r} b$$

$$\mathrm{d}a \bullet \mathrm{d}b = \sum_{r=0}^{m} \binom{m}{r} \left(\frac{\lambda}{m}\right)^r \mathrm{d}(\partial^{i_1} \cdots \partial^{i_r} a) \mathrm{d}\partial_{i_1} \cdots \partial_{i_r} b$$

for functions a, b. For example,

$$x_\mu \bullet \mathrm{d}x_\nu = x_\mu \mathrm{d}x_\nu, \quad x_\mu \bullet \mathrm{d}(x_\nu \bullet x_\rho) = x_\mu \bullet \mathrm{d}(x_\mu x_\nu) = x_\mu \mathrm{d}(x_\nu x_\rho) + \lambda(\delta_{\mu,\nu}\mathrm{d}x_\rho + \delta_{\mu,\rho}\mathrm{d}x_\nu),$$

$$\mathrm{d}x_\mu \bullet \mathrm{d}x_\nu = \mathrm{d}x_\mu \wedge \mathrm{d}x_\nu = -\mathrm{d}x_\nu \wedge \mathrm{d}x_\mu = -\mathrm{d}x_\nu \bullet \mathrm{d}x_\mu,$$

and so forth. This deformed 'quasidifferential calculus' is the classical one at lowest order but differentials of functions of degree p will be modified by descendants of lower degree. Because $\mathrm{d}1 = 0$ the relations involving $\mathrm{d}x_\mu$ are necessarily unchanged,

$$\mathrm{d}a = (\partial^\mu a)\mathrm{d}x_\mu = (\partial^\mu a) \bullet \mathrm{d}x_\mu, \quad a \bullet \mathrm{d}x_\mu = a\mathrm{d}x_\mu = (\mathrm{d}x_\mu)a = \mathrm{d}x_\mu \bullet a.$$

B. Gauge fields on quasi-$\mathbb{R}^n$

We are now ready to construct gauge theory on the above-mentioned quasi-$\mathbb{R}^n$ using the general construction in Sec. III C.

First of all, we recall that here $H = U(\mathbb{R}^n) = \mathbb{C}[\partial^1, \ldots, \partial^n]$ has coproduct $\Delta\partial^i = \partial^i \otimes 1 + 1 \otimes \partial^i$ on the generators. We take for B the same coalgebra, but to avoid confusion we denote this second copy $B = U(\mathbb{R}^n) = \mathbb{C}[f^1, \ldots, f^n]$ with polynomial generators f^i. As before, we use a fixed (say Euclidean) η_{ij} to lower indices. A gauge field is a covariant map $\alpha: B \to \Omega^1(\mathbb{R}^n)$ so it is first of all a collection of 1-forms $\alpha(1)$, $\alpha(f^i)$, $\alpha(f^i f^j)$ etc. in $\Omega^1(\mathbb{R}^n)$. However, that α is a morphism requires

$$\alpha(f^i) = \mathcal{L}_i(\alpha(1)) = \partial^i \alpha(1)^\mu \mathrm{d}x_\mu, \ldots, \quad \alpha(f^{i_1} \cdots f^{i_p}) = \mathcal{L}_{i_i} \cdots \mathcal{L}_{i_p}(\alpha(1)) = \partial^{i_1} \cdots \partial^{i_p} \alpha(1)^\mu \mathrm{d}x_\mu,$$

where $\mathcal{L}_i$ denotes the Lie derivative by the vector field ∂^i acting here on 1-forms. This is just action by ∂^i on the components $\alpha(1)^\mu$ in the coordinate basis. This is how $\alpha(b)$ is determined from $\alpha(1) \in \Omega^1(\mathbb{R}^n)$. Similarly

$$\gamma(f^i)=\partial^i\gamma(1),\ldots,\quad \gamma(f^{i_1}\cdots f^{i_p})=\partial^{i_1}\cdots\partial^{i_p}\gamma(1)$$

and similarly for γ^{-1}. This inverse is defined by the "convolution product," which involves the coproduct above, so for example

$$\gamma^{-1}(1)\gamma(1)=1,\quad \gamma^{-1}(f^i)\gamma(1)+\gamma(1)\gamma(f^i)=0,$$

$$\gamma^{-1}(f^if^j)\gamma(1)+\gamma^{-1}(f^i)\gamma(f^j)+\gamma^{-1}(f^j)\gamma(f^i)+\gamma^{-1}(1)\gamma(f^if^j)=0,$$

etc., which agrees with $\gamma^{-1}(f^i)=\partial^i\gamma^{-1}(1)$ etc., as required by covariance. Similarly, we know that $\alpha^\gamma(1)=\alpha(1)^{\gamma(1)}=\alpha(1)+\gamma^{-1}(1)\mathrm{d}\gamma(1)$. For higher order we compute the convolution product as

$$\begin{aligned}\alpha^\gamma(f^i)&=\gamma^{-1}(f^i)\alpha(1)\gamma(1)+\gamma^{-1}(1)\alpha(f^i)\gamma(1)+\gamma^{-1}(1)\alpha(1)\gamma(f^k)+\gamma^{-1}(f^i)\mathrm{d}\gamma(1)+\gamma^{-1}(1)\mathrm{d}\gamma(f^i)\\&=\alpha(f^i)+\gamma^{-1}(1)\mathrm{d}\gamma(f^i)-\gamma^{-2}(1)\gamma(f^i)\mathrm{d}\gamma(1)=\alpha(f^i)+\mathrm{d}(\gamma^{-1}(1)\gamma(f^i))=\mathcal{L}_i(\alpha^\gamma(1))\end{aligned}$$

as it should as all our constructions are covariant under H. Likewise, we know that $F(\alpha)(1)=F(\alpha(1))=\mathrm{d}\alpha(1)$. At next order we have

$$F(\alpha)(f^i)=\mathrm{d}\alpha(f^i)+\alpha(f^i)\wedge\alpha(1)+\alpha(1)\wedge\alpha(f^i)=\mathrm{d}\alpha(f^i)=\mathcal{L}_i(F(\alpha)(1))$$

as it should. Thus the higher $\alpha(f^i)$ etc., behave like further auxiliary classical $U(1)$-gauge fields but are in fact determined from the $\alpha(1)$ gauge theory. This gives the flavor of the amplified theory and its equivalence with usual $U(1)$ theory on $\mathbb{R}^n$.

Next we deform to the coproduct of B_F,

$$\Delta_\bullet f^i=\left(1+\frac{\lambda}{m}f^j\otimes f_j\right)^{-m}(f^i\otimes 1+1\otimes f^i)=f^i\otimes 1+1\otimes f^i-\lambda f^if^j\otimes f_j-\lambda f^j\otimes f_jf^i+\cdots .$$

The action of H on B is multiplication by $\partial^i=f^i$.

As explained in Sec. III C a gauge field still means an H-covariant map determined by $\alpha(1)\in\Omega^1(\mathbb{R}^n_{m,\lambda})$, i.e., some differential form $\alpha(1)=\alpha^\mu\bullet\mathrm{d}x_\mu$. Its curvature from Sec. III C is

$$\begin{aligned}F_\bullet(\alpha)(1)&=\mathrm{d}\alpha(1)+\bullet(\alpha\otimes\alpha)(F)\\&=\mathrm{d}\alpha(1)+F^{(1)}\triangleright\alpha(1)\bullet F^{(2)}\triangleright\alpha(1)\\&=\mathrm{d}\alpha(1)+\sum_{r=0}^{\infty}\binom{m+r-1}{r}\left(-\frac{\lambda}{m}\right)^r(\partial^{i_1}\cdots\partial^{i_r}\alpha^\mu\bullet\mathrm{d}x_\mu)\bullet(\partial_{i_1}\cdots\partial_{i_r}\alpha^\nu\bullet\mathrm{d}x_\nu).\end{aligned}$$

We know from the equivalence with the classical gauge theory that this will in fact equal $\mathrm{d}\alpha(1)$ but this is a nontrivial computation from the point of view of the nonassociative theory. Similarly, we have

$$(\Delta\otimes\mathrm{id})(F)=\left(1+\frac{\lambda}{m}(\square_{13}+\square_{23})\right)^{-m}$$

and hence

$$\begin{aligned}\alpha^\gamma_\bullet(1)=((\bullet)\bullet)&\left(1+\frac{\lambda}{m}(\square_{13}+\square_{23})\right)^{-m}(\gamma^{-1}(1)\otimes\alpha(1)\otimes\gamma(1))+\sum_{r=0}^{\infty}\binom{m+r-1}{r}\\&\times\left(-\frac{\lambda}{m}\right)^r\partial^{i_1}\cdots\partial^{i_r}\gamma^{-1}(1)\bullet\mathrm{d}\partial_{i_1}\cdots\partial_{i_r}\gamma(1),\end{aligned}$$

where the first term can again be expanded as a powerseries as we have done for the second term. The action of a ∂^i on α is understood here to be via the Lie derivative. The second term is "pure gauge" and we know by the equivalence with the untwisted theory that it is equal to $\gamma^{-1}(1)\mathrm{d}\gamma(1)$

and hence its curvature is zero, as promised. From the point of view of the nonassociative theory, however, these are nontrivial powerseries in the $\bullet$ product. Matter fields if present can similarly be included according to the theory at the end of Sec. III C.

V. OCTONIONS AS A FINITE QUASIGEOMETRY AND GAUGE THEORY

Here we illustrate the formalism of Sec. III on the octonions viewed as a nonassociative coordinate ring obtained by quantizing the classical space $\mathbb{Z}_2^3$. The first section makes this point of view precise and is a main result of the article. We then consider gauge theory on this space.

A. Octonions as quantization and their differentials

The "classical" algebra of functions in the form of the group algebra $A=\mathbb{C}\mathbb{Z}_2^3$ before deformation is generated by commuting u, v, w say with $u^2=v^2=w^2=1$. A general basis element is

$$e_{\vec{a}}=u^{a_1}v^{a_2}w^{a_3}.$$

The deformed product has relations

$$u\bullet u=v\bullet v=w\bullet w=-1,\quad u\bullet v=-v\bullet u,\quad u\bullet w=-uw=-w\bullet u,\quad v\bullet w=-wv=-w\bullet v$$

which is indeed the usual octonions if one puts $i=u$, $j=v$ and $k=u\bullet v$. Here

$$F(\vec{a},\vec{a})=(-1)^{a_1+a_2+a_3+a_1a_2+a_1a_3+a_2a_3+a_1a_2a_3}=\begin{cases}1 & \text{if } \vec{a}=0\\ -1 & \text{else,}\end{cases}$$

which ensures that $k^2=-1$ as it should. Similarly one may check that

$$k\bullet i=(u\bullet v)\bullet u=-(v\bullet u)\bullet u=-v\bullet(u\bullet u)=v=j$$

and so forth. Note from Sec. II B that

$$e_{\vec{a}}\bullet(e_{\vec{b}}\bullet e_{\vec{c}})=(e_{\vec{a}}\bullet e_{\vec{b}})\bullet e_{\vec{c}}$$

whenever $\vec{a}$, $\vec{b}$, and $\vec{c}$ are linearly dependent over $\mathbb{Z}_2$. This expresses the "alternativity" property of the octions in our formulation.

Next, the classical differential calculus on A is fixed as follows. By Fourier transform $A=\mathbb{C}(\hat{\mathbb{Z}}_2^3)$ where $\hat{\mathbb{Z}}_2^3$ is position space if the previous $\mathbb{Z}_2^3$ above was momentum space. Each $\hat{\mathbb{Z}}_2$ of position space is a finite set of two points and it has only one possible differential calculus, the universal one. It is then natural to take the three copies commuting (direct product calculus), giving

$$\mathrm{d}u u=-u\mathrm{d}u,\quad \mathrm{d}u v=v\mathrm{d}u,\quad \mathrm{d}u w=w\mathrm{d}u$$

and cyclic rotations. The wedge product is then fixed by the graded Leibniz rule as

$$\mathrm{d}u\mathrm{d}u=0,\quad \mathrm{d}u\mathrm{d}v=-\mathrm{d}v\mathrm{d}u,\quad \mathrm{d}u\mathrm{d}w=-\mathrm{d}w\mathrm{d}v$$

and cyclic rotations of this. Notice that the more important objects here are the left-invariant closed 1-forms

$$\tau_1=-\frac{1}{2}u^{-1}\mathrm{d}u,\quad \tau_2=-\frac{1}{2}v^{-1}\mathrm{d}v,\quad \tau_3=-\frac{1}{2}w^{-1}\mathrm{d}w$$

and the geometrical picture is that of a 3-torus with the circle S^1 approximated by $\hat{\mathbb{Z}}_2$. Moreover, the calculus has noncommutative de Rahm cohomology generated by these τ_i, exactly as for a classical 3-torus. These τ_i anticommute among themselves in the wedge product and

$$\tau_i e_{\vec{a}} = (-1)^{a_i} e_{\vec{a}} \tau_i, \quad \mathrm{d}e_{\vec{a}} = -2e_{\vec{a}} a_i \tau_i.$$

We see that there is only a small amount of noncommutativity in our classical calculus attributable to the discrete nature of the underlying space.

The geometric picture here is clearer after making the above Fourier transform explicit. Thus, let

$$e_{\vec{a}}(x) = (-1)^{a_i x_i}, \quad u = (-1)^{x_1}, \quad v = (-1)^{x_2}, \quad w = (-1)^{x_3}$$

be the plane waves, where x is a point in position space (a $\mathbb{Z}_2$-valued vector). The exterior derivative here is

$$\mathrm{d}f = (\partial^i f)\tau_i, \quad \partial^i e_{\vec{a}} = -2a_i e_{\vec{a}},$$

where ∂^i is the finite-difference operator in the i-direction. We see that the differentials act by multiplication in momentum space.

In general, the Fourier transform of $f(x)$ is a function $f_{\vec{a}}$ on momentum space characterized by $f(x) = \Sigma_{\vec{a}} f_{\vec{a}} e_{\vec{a}}(x)$. The inverse is

$$f_{\vec{a}} = \frac{1}{8} \sum_x f(x) e_{\vec{a}}(x).$$

Now, we have given the $\bullet$ deformation of $\mathbb{Z}_2^3$ into the octonions in momentum space as multiplication by $F(\vec{a},\vec{b})$. Let $F(x,y)$ be the same function before Fourier transform. Then

$$(f \bullet g)(x) = \sum_{\vec{a},\vec{b}} f_{\vec{a}} g_{\vec{b}} F(\vec{a},\vec{b}) e_{\vec{a}+\vec{b}}(x) = \frac{1}{64} \sum_{y,z,\vec{a},\vec{b}} f(y) g(z) e_{\vec{a}}(y) e_{\vec{b}}(z) e_{\vec{a}+\vec{b}}(x) F(\vec{a},\vec{b})$$

$$= \frac{1}{64} \sum_{y,z} \sum_{y,z,\vec{a},\vec{b}} f(y) g(z) e_{\vec{a}}(x+y) e_{\vec{b}}(x+z) F(\vec{a},\vec{b}) = \frac{1}{64} \sum_{y,z} F(y,z) f(x+y) g(x+z).$$

Here

$$F(y,z) = \sum_{\vec{a},\vec{b}} (-1)^{a_1(b_1+b_2+b_3)+a_2(b_2+b_3)+a_3b_3+b_1a_2a_3+a_1b_2a_3+a_1a_2b_3+a_iy_i+b_iz_i}$$

$$= 2 \sum_{a_2,a_3,b_2,b_3} (-1)^{(z_1+a_2a_3+a_2)(b_2+b_3)+a_3b_3+(z_1+a_2a_3)(b_2a_3+a_2b_3)+(z_1+a_2a_3+z_1)y_1+a_2y_2+a_3y_3+b_2z_2+b_2z_3}$$

$$= 2^2 \sum_{a_3,b_3} (-1)^{(z_2+(z_1+z_2)a_3)b_3+a_3b_3+(z_1+z_2+a_3z_1)(z_1+a_3)b_3+y_1(z_1+a_3z_2)+y_2(z_1+z_2+a_2z_1)+y_3a_3+b_3z_3},$$

where we do the b_1 summation which gives a constraint $a_1+a_2a_3+z_1=0$ which eliminates a_1; then we do the b_2 summation to obtain a constraint $a_2+z_1+z_2+a_3z_1=0$ to eliminate a_2. We next do the b_3 summation to obtain a constraint $a_3+z_1+z_2+z_1z_2+z_3=0$, giving

$$y^T \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 1 & 1 & 1 \end{pmatrix} z + y_1z_2z_3 + z_1y_2z_3 + z_1z_2y_3.$$

$$F(y,z) = 8(-1)$$

We see that *the cochain F that defines the octonions has the remarkable property that up to a relabelling, it is its own Fourier transform*, i.e., $F(y,z)$ has just the same form in position space as $F(\vec{a},\vec{b})$ in momentum space after a rotation of the indices $1 \to 2 \to 3 \to 1$. Note that the factor 8 in

$F(y,z)$ is an artifact due to our use of $1/8$ on one side of each Fourier transform rather than a symmetrical $1/\sqrt{8}$.

Note also that $f(x+y)=(R_1^{y_1}R_2^{y_2}R_3^{y_3})f(x)$, where R_i is translation in the i direction. Since $\partial^i = R_i - 1$, we have $f(x+y)=((1+\partial^1)^{y_1}(1+\partial^2)^{y_2}(1+\partial^3)^{y_3}f)(x)$ which expresses the above-mentioned result as a finite "bidifferential" operator

$$
\begin{aligned}
f \bullet g = \cdot \Bigg(& \frac{1}{8}\sum_{y,z} (-1)^{y_1(z_1+z_2)+y_2z_2+y_3(z_1+z_2+z_3)+y_1z_2z_3+z_1y_2z_3+z_1z_2y_3} \\
& \times (1+\partial^1)^{y_1}(1+\partial^2)^{y_2}(1+\partial^3)^{y_3} \otimes (1+\partial^1)^{z_1}(1+\partial^2)^{z_2}(1+\partial^3)^{z_3} \Bigg)(f \otimes g) \\
= \cdot \Bigg(& 1 \otimes 1 - \frac{1}{2}(\partial^1 \otimes \partial^1 + \partial^2 \otimes \partial^1 + \partial^3 \otimes \partial^1 + \partial^2 \otimes \partial^2 + \partial^3 \otimes \partial^2 + \partial^3 \otimes \partial^3 + \partial^1\partial^2 \otimes \partial^1 + \partial^1\partial^3 \\
& \otimes \partial^1 + \partial^2\partial^3 \otimes \partial^1 + \partial^2\partial^3 \otimes \partial^2 + \partial^2 \otimes \partial^1\partial^2 + \partial^3 \otimes \partial^1\partial^3 + \partial^3 \otimes \partial^2\partial^3 + \partial^1\partial^2\partial^3 \otimes \partial^1 + \partial^2\partial^3 \otimes \partial^1\partial^2) \\
& - \frac{1}{4}(-\partial^1 \otimes \partial^2\partial^3 + \partial^2 \otimes \partial^1\partial^3 + \partial^3 \otimes \partial^1\partial^2 - \partial^1 \otimes \partial^1\partial^2\partial^3 + \partial^2 \otimes \partial^1\partial^2\partial^3 + \partial^3 \otimes \partial^1\partial^2\partial^3 + \partial^1\partial^2 \\
& \otimes \partial^1\partial^2 + \partial^1\partial^2 \otimes \partial^1\partial^3 - \partial^1\partial^2 \otimes \partial^2\partial^3 + \partial^1\partial^3 \otimes \partial^1\partial^3 + \partial^2\partial^3 \otimes \partial^1\partial^3 + \partial^2\partial^3 \otimes \partial^2\partial^3 + \partial^1\partial^2\partial^3 \otimes \partial^1\partial^2 \\
& + \partial^1\partial^2\partial^3 \otimes \partial^1\partial^3 + \partial^2\partial^3 \otimes \partial^1\partial^2\partial^3) - \frac{1}{8}\partial^1\partial^2\partial^3 \otimes \partial^1\partial^2\partial^3 \Bigg)(f \otimes g).
\end{aligned}
$$

These results have been obtained with MATHEMATICA. This makes precise the sense in which, in finite geometry, the octonions are a "quantization" of functions on $\hat{\mathbb{Z}}_2^3$.

For comparison, if we do the same for the cocycle that defines Clifford algebras as a simpler associative quantization of $\mathbb{Z}_2^n$, we have

$$F(a,b) = (-1)^{a_1(b_1+\cdots+b_n)+a_2(b_2+\cdots+b_n)+\cdots+a_nb_n},$$

$$F(y,z) = 2^n(-1)^{(y_1+y_2)z_1+(y_2+y_3)z_2+\cdots+(y_{n-1}+y_n)z_{n-1}+y_nz_n}.$$

The derivation of the latter is rather simpler than the above; we compute

$$
\begin{aligned}
F(y,z) &= (-1)^{a_1(b_1+\cdots+b_n)+a_2(b_2+\cdots+b_n)+\cdots+a_nb_n+\Sigma_{i=1}^n a_iy_i+\Sigma_{i=1}^n b_iz_i} \\
&= 2(-1)^{z_1(y_1+y_2)}(-1)^{a_2(b_2+\cdots+b_n)+a_3(b_3+\cdots+b_n)+\cdots+a_nb_n+\Sigma_{i=2}^n a_iy_i+\Sigma_{i=2}^n b_iz_i},
\end{aligned}
$$

where we do the b_1 integral to obtain the constraint $a_1+z_1=0$, and change variables $a_2+z_1 \to a_2$ in the result. What we obtain is $F(y,z)$ for $\mathbb{Z}_2^{n-1}$ in the remaining variables. The result then follows by induction. The $\bullet$-product description of the Clifford algebra in n-dimensions is then given as a quantization of $\mathbb{Z}_2^n$ by this $F(y,z)$ by a similar formula as previously. For example, for $n=3$ we have

$$
\begin{aligned}
f \bullet g = \cdot \Bigg(& \frac{1}{8}\sum_{y,z} (-1)^{(y_1+y_2)z_1+(y_2+y_3)z_2+y_3z_3}(1+\partial^1)^{y_1}(1+\partial^2)^{y_2}(1+\partial^3)^{y_3} \otimes (1+\partial^1)^{z_1}(1+\partial^2)^{z_2}(1+\partial^3)^{z_3} \Bigg) \\
& \times (f \otimes g) = \cdot \Bigg(1 \otimes 1 - \frac{1}{2}(\partial^1 \otimes \partial^1 + \partial^2 \otimes \partial^2 + \partial^3 \otimes \partial^3 + \partial^3 \otimes \partial^2 + \partial^2\partial^3 \otimes \partial^2 + 1 \otimes \partial^1\partial^2 \\
& + \partial^1 \otimes \partial^1\partial^2 + \partial^2 \otimes \partial^1\partial^2 + \partial^3 \otimes \partial^1\partial^2 + \partial^3 \otimes \partial^2\partial^3 + \partial^2\partial^3 \otimes \partial^1\partial^2) - \frac{1}{4}(\partial^3 \otimes \partial^1\partial^2\partial^3 \\
& + \partial^1\partial^2 \otimes \partial^1\partial^2 + \partial^1\partial^3 \otimes \partial^1\partial^2 - \partial^1\partial^3 \otimes \partial^1\partial^3 + \partial^2\partial^3 \otimes \partial^2\partial^3 + \partial^2\partial^3 \otimes \partial^1\partial^2\partial^3 + \partial^1\partial^2\partial^3 \otimes \partial^1\partial^2)
\end{aligned}
$$

$$-\frac{1}{8}\partial^1\partial^2\partial^3\otimes\partial^1\partial^2\partial^3\Big)(f\otimes g).$$

Finally, we turn to the differential geometry of the octonions. As a cochain twist we have that the relations involving the left-invariant forms τ_i are unchanged (because F acts trivially on them).

Hence

$$\mathrm{d}e_{\vec{a}}=(\partial^i e_{\vec{a}})\tau_i=(\partial^i e_{\vec{a}})\bullet\tau_i,\quad e_{\vec{a}}\bullet\tau_i=e_{\vec{a}}\tau_i=(-1)^{a_i}\tau_i e_{\vec{a}}=(-1)^{a_i}\tau_i\bullet e_{\vec{a}}$$

in this basis. For a more algebraic picture within the octonions, let us also consider

$$E_{\vec{a}}=(u^{a_1}\bullet v^{a_2})\bullet w^{a_3}=(-1)^{a_1a_2a_3}u^{a_1}\bullet(v^{a_2}\bullet w^{a_3})=(-1)^{a_1a_2+a_1a_3+a_2a_3}e_{\vec{a}}$$

after a short computation using F and Φ. Since the $e_{\vec{a}}$ have square 1 with their initial product, and from the form of $F(\vec{a},\vec{a})$ above, we know that $E_{\vec{a}}\bullet E_{\vec{a}}=e_{\vec{a}}\bullet e_{\vec{a}}=-1$ with the exception of $E_0=1$. So these are all 'unit octonions'. Moreover, from the previous,

$$\mathrm{d}E_{\vec{a}}=-2E_{\vec{a}}\bullet a_i\tau_i,\quad E_{\vec{a}}\bullet\tau_i=(-1)^{a_i}\tau_i\bullet E_{\vec{a}}$$

in this basis. We can then deduce

$$\tau_1=\tfrac{1}{2}u^{-1}\bullet\mathrm{d}u,\quad \tau_2=\tfrac{1}{2}v^{-1}\bullet\mathrm{d}v,\quad \tau_3=\tfrac{1}{2}w^{-1}\bullet\mathrm{d}w,$$

where inverse is in the octonions or bullet product algebra and eventually that

$$\mathrm{d}u\bullet u=-u\bullet\mathrm{d}u,\quad \mathrm{d}u\bullet v=-v\bullet\mathrm{d}u,\quad \mathrm{d}u\bullet w=-w\bullet\mathrm{d}u,$$

$$\mathrm{d}u\bullet\mathrm{d}u=0,\quad \mathrm{d}u\bullet\mathrm{d}v=\mathrm{d}v\bullet\mathrm{d}u,\quad \mathrm{d}u\bullet\mathrm{d}w=\mathrm{d}w\bullet\mathrm{d}u$$

and cyclic rotations of this. The latter are obtained by applying d and the graded-Leibniz rule which still holds. One can also obtain these results by direct computation from the action of F and the initial calculus on $\hat{\mathbb{Z}}_2^3$ as in Ref. 1.

B. Gauge fields on the octonions

We have a basis of H given by the δ-functions $\{\delta_{\vec{a}}\}$ on momentum space, with coalgebra

$$\Delta\delta_{\vec{a}}=\sum_{\vec{b}+\vec{c}=\vec{a}}\delta_{\vec{b}}\otimes\delta_{\vec{c}}.$$

Their action on $A=\mathbb{C}\mathbb{Z}_2^3=\mathbb{C}(\hat{\mathbb{Z}}_2^3)$ is

$$\delta_{\vec{a}}\triangleright f(x)=f_{\vec{a}}e_{\vec{a}}(x),\quad \delta_{\vec{a}}\triangleright(fg)=\sum_{\vec{b}+\vec{c}=\vec{a}}(\delta_{\vec{b}}\triangleright f)(\delta_{\vec{c}}\triangleright g),$$

i.e., it projects out the corresponding term in the Fourier expansion and behaves as shown on products. We use the same coalgebra B with the same basis element $\delta_{\vec{a}}$ denoted $f^{\vec{a}}$ to avoid confusion and the same form of coproduct as the above. The action of H is by $\delta_{\vec{a}}\triangleright f_{\vec{b}}=\delta_{\vec{a},\vec{b}}f_{\vec{b}}$. A gauge field is then a covariant map $\alpha:B\to\Omega^1(\hat{\mathbb{Z}}_2^3)$, i.e., a collection of 1-forms

$$\alpha(f_{\vec{a}})=\alpha(\delta_{\vec{a}}\triangleright 1)=\delta_{\vec{a}}\triangleright\alpha(1)=(\delta_a\triangleright\alpha(1)^i)\tau_i,$$

where the H acts trivially on the τ_i as explained in Sec. V A. Thus the collection is fully determined from $\alpha(1)=\Sigma_{\vec{a}}\alpha(f_{\vec{a}})$. Similarly the collection

$$\gamma(f_{\vec a}) = \delta_{\vec a} \triangleright \gamma(1), \quad \gamma(1) = \sum_{\vec a} \gamma(f_{\vec a})$$

is determined from the point-wise invertible function $\gamma(1)(x)$ in $\mathbb{C}(\hat{\mathbb{Z}}_2^3)$. The inverse $\gamma^{-1}(1) = \gamma(1)^{-1}$. More generally

$$\sum_{\vec b+\vec c=\vec a} \gamma^{-1}(f_{\vec b})\gamma(f_{\vec c}) = \delta_{\vec a,0}$$

which is consistent with $\gamma^{-1}(f_{\vec a}) = \delta_{\vec a} \triangleright \gamma^{-1}(1)$. A gauge transform of $\alpha(1)$ is as usual

$$\begin{aligned}\alpha^\gamma(1) &= \alpha(1)^{\gamma(1)} = \gamma^{-1}(1)\alpha(1)\gamma(1) + \gamma^{-1}(1)\mathrm{d}\gamma(1)\\ &= \gamma(1)^{-1}(R_i\gamma(1))\alpha(1)^i\tau_i + \gamma(1)^{-1}\partial^i\gamma(1)\tau_i = \alpha(1) + (\gamma(1)^{-1}\partial^i\gamma(1))\phi(1)^i\tau_i,\end{aligned}$$

where there is a sum over i and $\phi(1)^i = \alpha(1)^i + 1$. Note that unlike the quasi-$\mathbb{R}^n$ case the initial $U(1)$ theory already has a nontrivial conjugation because functions do not commute with the τ_i basic 1-forms. The change of variables to ϕ is quite useful (see Sec. V C) and ϕ transforms by conjugation. For other components we have

$$\begin{aligned}\alpha^\gamma(f_{\vec a}) &= \sum_{\vec b+\vec c+\vec d=\vec a} \gamma^{-1}(f_{\vec b})\alpha(f_{\vec c})\gamma(f_{\vec d}) + \sum_{\vec b+\vec c=\vec a} \gamma^{-1}(f_{\vec b})\mathrm{d}\gamma(f_{\vec c})\\ &= \sum_i \sum_{\vec b+\vec c+\vec d=\vec a} \gamma^{-1}(f_{\vec b})R_i(\gamma(f_{\vec d}))\alpha(f_{\vec c})^i\tau_i + \delta_{\vec c,0}\gamma^{-1}(f_{\vec b})\partial^i\gamma(f_{\vec d})\tau_i\\ &= \alpha(f_{\vec a}) + \sum_i \sum_{\vec b+\vec c+\vec d=\vec a} (\gamma^{-1}(f_{\vec b})\partial^i\gamma(f_{\vec d}))(\alpha(f_{\vec c})^i + \delta_{\vec c,0})\tau_i = \delta_{\vec a} \triangleright (\alpha^\gamma(1))\end{aligned}$$

as it should. For the last step we identify $\delta_{\vec c,0} = \delta_{\vec c} \triangleright 1$ as $1 = e_0(x)$ and use the action of $\delta_{\vec a}$ on triple products along the lines of its action on a product explained previously. Thus the theory looks like a collection of 1-forms with gauge-like transformation properties but determined consistently from the single theory for $\alpha(1)$. Similarly, for the curvature we have

$$\begin{aligned}F(\alpha)(1) = F(\alpha(1)) &= \mathrm{d}\alpha(1) + \alpha(1)\wedge\alpha(1) = \sum_{i,j} (\partial^i\alpha(1)^j + \alpha(1)^i R_i\alpha(1)^j)\tau_i\wedge\tau_j\\ &= \sum_{ij} (\partial^i\alpha(1)^j + \alpha(1)^i\partial^i\alpha(1)^i + \alpha(1)^i\alpha(1)^j)\tau_i\wedge\tau_j = \sum_{ij} \phi(1)^i\partial^i\phi(1)^j\tau_i\wedge\tau_j,\end{aligned}$$

where $\alpha(1)^i\alpha(1)^j\tau_i\wedge\tau_j = 0$ as the τ_i anticommute. This is a standard form for the $U(1)$-Yang–Mills curvature on a discrete space in noncommutative geometry. The other components may similarly be computed as

$$F(\alpha)(f_{\vec a}) = \mathrm{d}\alpha(f_{\vec a}) + \sum_{\vec b+\vec c=\vec a} \alpha(f_{\vec b})\wedge\alpha(f_{\vec c}) = \sum_{ij} \sum_{\vec b+\vec c=\vec a} \phi(f_{\vec b})^i\partial^i\phi(f_{\vec c})^j\tau_i\wedge\tau_j = \delta_{\vec a} \triangleright F(\alpha(1))$$

as it should, where $\delta_{\vec a}$ acts on the coefficients of $\tau_i\wedge\tau_j$, i.e., the other components have a similar form but are determined by $F(\alpha(1))$.

The above "amplification" of $\alpha(1)$ to a collection of gauge fields can be made even more explicit by a different basis $e_y \equiv \Sigma_{\vec a} e_y(\vec a)\delta_{\vec a}$ of H where $e_y(\vec a) = e_{\vec a}(y) = (-1)^{y_i a_i}$. These elements have $\Delta e_y = e_y \otimes e_y$ (this is the isomorphism $\mathbb{C}(\mathbb{Z}_2^3) \cong \mathbb{C}\hat{\mathbb{Z}}_2^3$). They act on functions by $(e_y \triangleright f)(x) = f(x+y)$ and $\alpha(e_{\vec x})$ behave more explicitly like $\alpha(1)$, which is one of the collection via $e_0 = 1$.

We now turn to the twisted nonassociative theory. The coproduct of B_F is

$$\Delta_\bullet f_{\vec a}=\sum_{\vec b+\vec c=\vec a} F(\vec b,\vec c) f_{\vec b}\otimes f_{\vec c},\quad \Delta_\bullet E_x=\frac{1}{64}\sum_{y,z} F(y,z)E_{x+y}\otimes E_{x+z};\quad E_y\equiv\sum_{\vec a} e_y(\vec a) f_{\vec a},$$

where the cochain and its Fourier transform are (if we want the octonions) as in Sec. V A. As explained in Sec. III C a gauge field still means an H-covariant map determined by $\alpha(1)\in\Omega^1(\mathbb{O})$, i.e., some differential form $\alpha(1)=\alpha^i\bullet\tau_i=(\phi^i-1)\bullet\tau_i$ (sum over i). The curvature according to Sec. III C is

$$F_\bullet(\alpha)(1)=\mathrm{d}\alpha(1)+\bullet(\alpha\otimes\alpha)(F)=\mathrm{d}\alpha(1)+\sum_{\vec b,\vec c} F(\vec b,\vec c)(\delta_{\vec b}\triangleright\alpha(1))\bullet(\delta_{\vec c}\triangleright\alpha(1)).$$

Similarly, we have

$$(\Delta\otimes\mathrm{id})(F)=\sum_{\vec a,\vec b,\vec c} F(\vec a+\vec b,\vec c)\delta_{\vec a}\otimes\delta_{\vec b}\otimes\delta_{\vec c}=\sum_{\vec a,\vec b,\vec c} F(\vec a,\vec c)F(\vec b,\vec c)\delta_{\vec a}\otimes\delta_{\vec b}\otimes\delta_{\vec c}=F_{13}F_{23}$$

for the particular form of F for the octonions (which is linear in the exponent with respect to the first argument). Then

$$\alpha^\gamma_\bullet(1)=\sum_{\vec a,\vec b,\vec c} F(\vec a,\vec c)F(\vec b,\vec c)((\delta_{\vec a}\triangleright\gamma^{-1}(1)\bullet\delta_{\vec b}\triangleright\alpha(1))\bullet\delta_{\vec c}\triangleright\gamma(1))+\sum_{\vec b,\vec c} F(\vec b,\vec c)\delta_{\vec b}\triangleright\gamma^{-1}(1)\bullet\mathrm{d}\delta_{\vec c}\triangleright\gamma(1).$$

Matter fields can similarly be included from the general theory in Sec. III C

Next, although our view of the octonions as a nonassociative quantization of functions on the cube is the "geometrical one," it remains very convenient to work with our original plane-wave basis $\{e_{\vec a}\}$ for calculations. Here $f\in H$ acts diagonally as multiplication by $f(\vec a)$ on an element of degree $\vec a$. Here the degree is multiplicative and d does not change degree, so for example $e_{\vec a}\mathrm{d}e_{\vec b}$ has degree $|e_{\vec a}\mathrm{d}e_{\vec b}|=\vec a+\vec b$. Similarly after deformation with the $E_{\vec a}$. Here for example $E_{\vec a}\bullet\mathrm{d}E_{\vec b}=F(\vec a,\vec b)e_{\vec a}de_{\vec b}$ etc. The hard part from this point of view is to find the inverse in the underformed algebra of a general gauge transformation $\gamma=\Sigma_{\vec a}\gamma_{\vec a}e_{\vec a}$. The answer is to construct $\gamma^{-1}=\Sigma_{\vec a}\gamma_{\vec a}^{-1}e_a$ by Fourier transform of the inversion operation:

$$\gamma_{\vec a}^{-1}=\frac{1}{8}\sum_x\frac{e_{\vec a}}{\gamma(x)}=\frac{1}{8}\sum_x\frac{e_{\vec a}}{\sum_{\vec b}\gamma_{\vec b}e_{\vec b}(x)},$$

where we require the $\gamma(x)$ (the sum in the denominator) to be nonzero for each x, i.e., all signed sums of the $\gamma_{\vec b}$ coefficients should be non-zero. Otherwise, since the action of $\delta_{\vec a}$ on any expression in the exterior algebra is to pick out the degree $\vec a$ part, we have more simply in this basis:

$$F_\bullet(\alpha)=\mathrm{d}\alpha+\sum F(|\alpha|,|\alpha'|)\alpha\bullet\alpha',$$

$$\alpha^\gamma_\bullet=\sum F(|\gamma^{-1}|,|\gamma|)F(|\alpha|,|\gamma|)(\gamma^{-1}\bullet\alpha)\bullet\gamma+\sum F(|\gamma^{-1}|,|\gamma|)\gamma^{-1}\bullet\mathrm{d}\gamma,$$

where the sum is over the different graded components of each object and to this end α' denotes a second independent copy of α. Also, we omit writing that these are the gauge and other fields at 1, i.e., $\alpha\equiv\alpha(1)$ etc. Even though the amplification to the collection of fields is needed for the diagrammatic picture of Sec. III A, all formulas are by now referred back to their values on 1. If one wants to be more explicit and write the homogeneous degree components explicitly, we have

$$F_\bullet(\alpha)=\mathrm{d}\alpha+\sum_{\vec a,\vec b} F(\vec a,\vec b)\alpha_{\vec a}\bullet\alpha_{\vec b},$$

$$\alpha^{\gamma}_{\bullet} = \sum F(\vec{a},\vec{c})F(\vec{b},\vec{c})(\gamma^{-1}_{\vec{a}}E_{\vec{a}} \bullet \alpha_{\vec{a}}) \bullet \gamma_{\vec{c}}E_{\vec{c}} + \sum_{\vec{a},\vec{b}} F(\vec{a},\vec{b})\gamma^{-1}_{\vec{a}}E_{\vec{a}}\mathrm{d}\gamma_{\vec{b}}E_{\vec{b}},$$

where $\alpha=\Sigma_{\vec{a}}\alpha_{\vec{a}}$ is the decomposition into homogeneous components (this is a slightly different notation from the Fourier decomposition of γ into components $\gamma_{\vec{a}}E_{\vec{a}}$). The quasi-$\mathbb{R}^n$ example in Sec. IV B can likewise be computed more simply in this "momentum space" point of view.

Finally, we demonstrate this gauge theory with an example of a completely explicit computation. Thus, let

$$\gamma = \lambda u + \mu v, \quad \gamma^{-1} = \frac{1}{\lambda^2 - \mu^2}(\lambda\mu - \mu v),$$

where $u=e_{(1,0,0)}$, $v=e_{(0,1,0)}$ are two of the octonion generators as explained in Sec. V A, and $\lambda \neq \pm\mu$. These are necessarily also inverse in the convolution-algebra $\gamma^{-1}*_{\bullet}\gamma=1$ as one may verify directly. Similarly, since $F(|u|,|u|)=F(|v|,|v|)=F(|u|,|v|)=-1, F(|v|,|u|)=1$, we have

$$\gamma^{-1}*_{\bullet}\mathrm{d}\gamma = \frac{1}{\lambda^2 - \mu^2}(-\lambda^2 u \bullet \mathrm{d}u - \lambda\mu(u \bullet \mathrm{d}v + v \bullet \mathrm{d}u) + \mu^2 v \bullet \mathrm{d}v).$$

Let us check that the curvature of this pure gauge part is zero:

$$\mathrm{d}(\gamma^{-1}*_{\bullet}\mathrm{d}\gamma) = -\frac{\lambda\mu}{\lambda^2 - \mu^2}(\mathrm{d}u \bullet \mathrm{d}v + \mathrm{d}v \bullet \mathrm{d}u) = -2\frac{\lambda\mu}{\lambda^2 - \mu^2}\mathrm{d}u \bullet \mathrm{d}v$$

using the relations in the octonion calculus from Section V A. Meanwhile, when we square $\gamma^{-1}*_{\bullet}\gamma$ in the convolution product we must insert the factors $F(\vec{a},\vec{b})$ when multiplying components of degrees $\vec{a},\vec{b}$ as explained above. Here $|u\bullet\mathrm{d}v| = |v\bullet\mathrm{d}u| = (1,1,0)$ while $u\bullet\mathrm{d}u$ and $v\bullet\mathrm{d}v$ have degree 0. Hence of the 16 terms only four come in with a negative sign. Moreover, when we multiply out the 16 terms we can, in these particular expressions, associate, because the degree vectors for $u, v, u\bullet\mathrm{d}v, v\bullet\mathrm{d}u$ are linearly dependent, so Φ for them is trivial. This results in all but four of the terms zero or cancelling pairwise. For example

$$(u \bullet \mathrm{d}v) \bullet (u \bullet \mathrm{d}v) = u \bullet ((\mathrm{d}v \bullet u) \bullet \mathrm{d}v) = -u \bullet (u \bullet (\mathrm{d}v \bullet \mathrm{d}v)) = 0,$$

$$\begin{aligned}(u \bullet \mathrm{d}v) \bullet (v \bullet \mathrm{d}u) &= u \bullet ((\mathrm{d}v \bullet v) \bullet \mathrm{d}u) = -u \bullet (v \bullet (\mathrm{d}v \bullet \mathrm{d}u)) = -(u \bullet v) \bullet (\mathrm{d}u \bullet \mathrm{d}v) \\ &= (v \bullet u) \bullet (\mathrm{d}u \bullet \mathrm{d}v) = -(v \bullet \mathrm{d}u) \bullet (u \bullet \mathrm{d}v)\end{aligned}$$

using the relations from Sec. V A (the last step is analogous to the first sequence). What remains is

$$\begin{aligned}(\gamma^{-1}*_{\bullet}\mathrm{d}\gamma)*_{\bullet}(\gamma^{-1}*_{\bullet}\mathrm{d}\gamma) = \frac{\lambda\mu}{(\lambda^2 - \mu^2)^2}(\lambda^2((u \bullet \mathrm{d}u) \bullet (u \bullet \mathrm{d}v) + (u \bullet \mathrm{d}v) \bullet (u \bullet \mathrm{d}u)) \\ - \mu^2((v \bullet \mathrm{d}v) \bullet (v \bullet \mathrm{d}u) + (v \bullet \mathrm{d}u) \bullet (v \bullet \mathrm{d}v))) = 2\frac{\lambda\mu}{\lambda^2 - \mu^2}\mathrm{d}u \bullet \mathrm{d}v\end{aligned}$$

by similar computations

$$(u \bullet \mathrm{d}u) \bullet (u \bullet \mathrm{d}v) = u \bullet ((\mathrm{d}u \bullet u) \bullet \mathrm{d}v) = -u \bullet ((u \bullet \mathrm{d}u) \bullet \mathrm{d}v) = -(u \bullet u) \bullet (\mathrm{d}u \bullet \mathrm{d}v) = \mathrm{d}u \bullet \mathrm{d}v,$$

etc., using the relations of the octonion calculus. Hence the curvature of this pure gauge part is zero as promised.

C. Moduli of zero-curvature $U(1)$-Yang–Mills connections on $\mathbb{Z}_2^n$ and octonions

By construction the above mentioned example of gauge theory on the octonions (not the only possible one, depending on the choice of gauge group coalgebra), is equivalent to that in the classical object $\mathbb{Z}_2^3$. Maxwell theory on $\mathbb{Z}_2^n$ (but not Yang–Mills) has been covered in Ref. 17 and also quantum Yang–Mills theory on $\mathbb{Z}_2^2$ but the analysis for classical $U(1)$-Yang–Mills and in particular the moduli space of zero curvature solutions has not to our knowledge been given even for $\mathbb{Z}_2^2$. We fill this gap now. As to be expected on a torus, this moduli space is nontrivial. We work with $\mathbb{Z}_2^n$ as position space.

We use the classical calculus on $\mathbb{Z}_2^n$ as described in Sec. V A before deformation to the octonions when $n=3$. The exterior algebra is generated by the plane-wave functions $e_{\vec{a}}(x)$ (now $\vec{a}$ an n-vector) and $\tau_i, i=1,\ldots,n$ as in Sec. V A but now for general n. They anticommute among themselves, etc.

A $U(1)$-Yang–Mills gauge field means $\alpha=\alpha^i\tau_i\in\Omega^1(\mathbb{Z}_2^n)$ where the $\alpha^i(x)$ are the component functions. The curvature $F=\mathrm{d}\alpha+\alpha\wedge\alpha$ is

$$F=\sum_{i<j}F^{ij}\tau_i\wedge\tau_j,\quad F^{ij}=\partial^i\alpha^i-\partial^j\alpha^i+\alpha^iR_i\alpha^j-\alpha^jR_j\alpha^i.$$

We change variables to $\phi^i=1+\alpha^i$ or $\alpha=\phi-\vartheta$, where $\phi=\phi^i\tau_i$ and $\vartheta=\Sigma_i\tau_i$ is a zero curvature "reference" connection that is closed, not exact and squares to zero. The moduli of flat connections contains at least this nonzero gauge-invariant element. Indeed, let γ be a pointwise invertible function on position space. The gauge transformation of α and the expression for the curvature in terms of ϕ^i are

$$(\phi^\gamma)^i=\frac{\gamma}{R_i\gamma}\phi^i,\quad F^{ij}=\rho_i\phi^j-\rho_j\phi^i,$$

where $\rho_i\equiv\phi^iR_i$. Finally, to be physical, we fix unitarity conditions. As in Ref. 18 we require the τ_i to be invariant under a $*$-operation extending the point-wise complex conjugation operation on position space. We then require the α to be Hermitian, which translates in view of the commutation relations between the τ_i and functions to

$$\overline{\phi^i}=R_i\phi^i,\quad \gamma=e^{\iota\xi},\quad (\phi^\gamma)^i=e^{-\iota\partial^i\xi}\phi^i.$$

The middle equation is because if the reality of all the ϕ^i is preserved one may deduce that $\partial^i(\bar{\gamma}\gamma)=0$ so γ is without loss of generality pointwise unitary. We then put this into the transformation of ϕ^i.

By a similar argument to the proof for S_3 in Ref. 18 we have for all i,j in the case of a zero-curvature solution:

$$\rho_i\rho_i\phi^j=\phi^iR_i(\phi^iR_i\phi^j)=\lambda_i^2\phi^j=\rho_i\rho_j\phi^i=\phi^iR_i(\phi^jR_j\phi^i)=\rho_i(\phi^j)R_jR_i\phi^i=\rho_j(\phi^i)R_iR_j\phi^i=\phi^jR_j(\lambda_i^2),$$

where

$$\phi^i=\lambda_ie^{\iota\theta_i},\quad \lambda_i^2=|\phi^i|^2=\phi^iR_i\phi^i$$

is a polar decomposition. We conclude that at each point $R_i\lambda_i=\lambda_i$ by the reality and at each point either $\lambda_i=0$ or $R_i\lambda_j=\lambda_j$ by the above-mentioned computation, i.e.,

$$\lambda_i\partial^i\lambda_j=0,\quad \forall\, i,j,\quad \partial^i\lambda_i=0,\quad \forall\, i.$$

These λ_i are gauge-invariant and we now use them to analyze the possible solutions.

Case 1: $\exists$ *a point with all* $\lambda_i\neq 0$ *(constant maximal case).* In this case each λ_j will be unchanged moving in every direction to an adjacent point. Hence at each adjacent point they will all be nonzero. We conclude that all the λ_i are constant functions.

Moreover, in this case the zero-curvature equations become

$$e^{\iota\theta_i}e^{\iota R_i\theta_j}e^{-\iota R_j\theta_i}e^{-\iota\theta_j}=1$$

after canceling $\lambda_i\lambda_j$ from both sides. If we think of $e^{\iota\theta_i(x)}$ to be a factor for parallel transport along the edge in direction i from x, then this says that the holonomy around the plaquet with bottom left corner x and edges in the i and j directions is trivial. In this case, from such a solution we construct the following gauge transform:

$$\gamma(0)=1,\quad \gamma(x)=e^{\iota\Sigma_a i\theta.\mathrm{d}a},$$

where we take any path a from 0 to x and multiply the parallel transports on the edges of the path. As in usual gauge theory, this transforms all the $\phi^i\to\lambda_i$, i.e., eliminates all the phases as gauge degrees. Hence the solutions up to gauge equivalence in this case are of the form

$$\alpha=\lambda_i\tau_i-\vartheta,\quad \lambda_i\in\mathbb{R}_{>0},\quad i=1,\ldots,n.$$

Case 2: $\exists$ *a point with exactly one* $\lambda_i=0$ *(split case).* In this case all $\lambda_j\neq 0$ for $j\neq i$, at the point in question. Therefore moving in all directions other than i, we have the same value for all λ_j, i.e., a constant maximal solution on the subspace $\mathbb{Z}_2^{n-1}$. We also have the same value of $\lambda_i=0$ throughout this subspace. Moreover, moving in the i direction from any point in the subspace keeps $\lambda_i=0$ (hence $\lambda_i\equiv 0$ everywhere) but says nothing about the values of any of the $\lambda_j, j\neq i$. Hence the solution is two independent copies of $n-1$-dimensional solutions, in which the first copy is maximal by assumption and the second copy is unconstrained.

For example, if the second copy is also maximal on the subspace, we have

$$\alpha=x_i\lambda_j\tau_j+(1-x_i)\mu_j\tau_j-\vartheta,\quad \lambda_j,\mu_j\in\mathbb{R}_{>0},\quad j\neq i$$

and again any solution in this case is equivalent to something of this form (one may gauge away the phases in each $\mathbb{Z}_2^{n-1}$ space separately). The value of $\partial^j\xi$ between the two copies could produce a gauge phase factor but this is irrelevant as $\lambda_i\equiv 0$ everywhere.

Case $2'$*:* What arises naturally here is the weaker assumption just that there is some i with $\lambda_i\equiv 0$ throughout the space. In this case the solution necessarily splits into independent solutions of one dimension lower, of whatever type. This is therefore covered by induction. Hence it remains only to classify the remaining cases under the assumption that the solution is not split in any direction.

Case 3: $\exists$ *a point with exactly two* $\lambda_i=\lambda_j=0$ *and no splitting.* Here as before there is a $\mathbb{Z}_2^{n-2}$ subset containing the point with $\lambda_k\neq 0$ for all $k\neq i,j$, and $\lambda_i=\lambda_j=0$ throughout. Moreover, stepping in the i direction carries over $\lambda_i=0$ to the entire adjacent quadrant, but none of the other information. Similarly stepping in the j direction carries over $\lambda_j=0$ to that quadrant. We then relate the quadrants by further analysis; see the following example.

One may proceed in this way to classify the cases with more and more assumed degeneracy. Among the solutions are those of the same form as the constant maximal case above but allowing any of the $\lambda_i=0$. These are multiply-split solutions and include each τ_i alone as a zero-curvature flat connection, as well as $\alpha=-\vartheta$.

To be concrete we now offer a complete classification for $n=2$ and $n=3$ which demonstrates the method. The $n=3$ case is in correspondence with solutions on the octonions by twisting as we have mentioned.

For $n=2$ we have two cases: (i) the constant maximal solution is

$$\alpha=\lambda_1\tau_1+\lambda_2\tau_2-\vartheta,\quad \lambda_i\in\mathbb{R}_{>0}.$$

(ii) We have a splitting $\lambda_1\equiv 0$, with λ_2 unconstrained other than being constant in the 2-direction, i.e.

$$\alpha=\lambda\tau_2-\vartheta,\quad \partial^2\lambda=0,$$

where λ is a function just in the x_1 variable and up to gauge equivalence can be taken real and non-negative in its values. Similarly for a splitting $\lambda_2\equiv 0$:

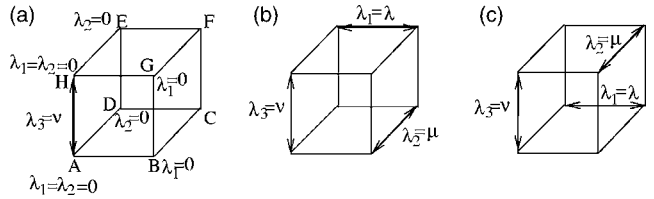

FIG. 2. Flat connections of type (iii) in the cube: (a) Initial assumption, (b) solution, and (c) its mirror image as the only possible. In (b) and (c) only the nonzero λ_i are shown.

$$\alpha = \lambda\tau_1 - \vartheta, \quad \partial^1\lambda = 0$$

for a real and nonnegative function λ of x_2 alone.

For $n=3$ we have three cases: (i) the constant maximal solution

$$\alpha = \lambda_1\tau_1 + \lambda_2\tau_2 + \lambda_3\tau_3 - \vartheta, \quad \lambda_i \in \mathbb{R}_{>0}.$$

(ii) We have a splitting $\lambda_1 \equiv 0$:

$$\alpha = x_1\phi + (1-x_1)\psi - \vartheta,$$

where ϕ, ψ correspond to two independent solutions on the $\mathbb{Z}_2^2$ subsets (faces) with $x_1=0$ and $x_1=1$ respectively. Up to gauge transformation they can be taken real and positive, i.e., without phases. Similarly in the other two directions.

(iii) we suppose that there does not exist a splitting, but there does exist a point with, say, $\lambda_1=\lambda_2=0$ and $\lambda_3=\nu\neq 0$. To be concrete let this point be A the origin in the standard cube shown in Fig. 2. These are also the values at H by the above argument; the equal value of λ_3 is shown in Fig. 2(a) by labeling the arrowed edge, and such a nonzero edge "transports" the other values from A to H by the previous arguments. We also see that $\lambda_1=0$ at B and G, whereas $\lambda_2=0$ at D and E, by the reality condition.

Now suppose that $\lambda_2=\mu\neq 0$ at corners B and C (the two must be the same value) as shown by the arrowed edge in Fig. 2(b). Then at B we must have $\lambda_3=0$ to avoid a split (to avoid the existence of a point with two nonzero λ_i). In this case $\lambda_1=\lambda_3=0$ also at C. Hence $\lambda_1=0$ at D. We conclude also that $\lambda_3=0$ at D (and hence all $\lambda_i=0$ at D) for if not, we could deduce the same values at E and hence that $\lambda_1=0$ at F, which would be a split with $\lambda_1\equiv 0$. Then $\lambda_1=\lambda\neq 0$ at E and F (to avoid a split with $\lambda_1\equiv 0$). Hence $\lambda_2=\lambda_3=0$ at E and F. Hence $\lambda_2=0$ also at G, and since $\lambda_3=0$ at A it must also vanish at G, i.e., all three λ_i vanish at G. The solution is then fully determined by the three nonzero values λ, μ, ν and all three λ_i vanishing at D, G as shown in Fig. 2(b). We mark only the nonzero edges, which imply those value on their endpoints; all other values are zero.

Alternatively, if $\lambda_2=0$ at B and C, then $\lambda_2=\mu\neq 0$ at F and G (the arrowed edge shown in Figure 2 part (c)) to avoid a split with $\lambda_2\equiv 0$. Hence $\lambda_3=0$ at G to avoid a maximal solution, and hence also at B (so all three $\lambda_i=0$ at B). Moreover, the values $\lambda_1=\lambda_3=0$ are transported to F. Hence $\lambda_3=0$ at C also, and $\lambda_1=0$ at E also. Finally, $\lambda_1=\lambda\neq 0$ at C, D (the final arrowed edge shown in part (c)) to avoid a split $\lambda_1\equiv 0$. This transports $\lambda_3=0$ also to D and hence to E, therefore we deduce the mirror image solution to the one above, where the $\lambda_i=0$ now at B, E as shown in part (c) of the figure.

The explicit formula in the first case, if A is the origin of a standard cube, is

$$\alpha = x_2x_3\lambda\tau_1 + x_1(1-x_3)\mu\tau_2 + (1-x_1)(1-x_2)\nu\tau_3 - \vartheta, \quad \lambda, \mu, \nu \in \mathbb{R}_{>0}.$$

Of course, we can rotate this solution by picking any other origin and initial non-zero edge, and we also have the mirror image solution. Finally, phases can be removed by gauge transformation in a similar manner to the above. This exhausts the moduli space for flat connections for the cube $n=3$ up to gauge equivalence.

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Noncommutative model with spontaneous time generation and Planckian bound

S. Majid[a)]
School of Mathematical Sciences, Queen Mary, University of London, 327 Mile End Rd., London E1 4NS, United Kingdom and Perimeter Institute for Theoretical Physics, 31 Caroline St. N., Waterloo, ON N2L 2Y5, Canada

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We illustrate the thesis that if time did not exist, we would have to create it if space is noncommutative, and extend functions by something like Schrödinger's equation. We propose that the phenomenon is a somewhat general mechanism within noncommutative geometry for "spontaneous time generation." We show in detail how this works for the su_2 algebra $[x_i,x_j]=2\imath\lambda\epsilon_{ij}{}^k x_k$ as noncommutative space, by explicitly adjoining the forced time variable. We find the natural induced noncommutative Schrödinger's equation and show that it has the correct classical limit for a particle of some mass $m\neq 0$, which is generated as a second free parameter by the theory. We show that plane waves exist provided $|\vec{p}|<\pi/2\lambda$, i.e., we find a Planckian bound on spatial momentum. We also propose dispersion relations $|\partial p^0/\partial\vec{p}|=|\tan(\lambda|\vec{p}|)|/m\lambda$ for the model and explore some elements of the noncommutative geometry. The model is complementary to our previous bicrossproduct one. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2084748]

I. INTRODUCTION

The origin of a time direction is a fundamental issue in any theory of quantum gravity, as likewise is the origin of mass for elementary particles. In this article we point out that previously known results on noncommutative differential calculi on quantum algebras can be viewed as evidence for a general phenomenon which we call "spontaneous time generation" in which both time and nonzero mass can be created by even a small amount of noncommutativity in space (or more precisely in its geometry). Put another way, a noncommutative deformation of space by a parameter λ can induce its own canonical evolution, forced by nothing other than the most minimal assumptions on existence of a differential structure on the space.

It is important that we use here the absolutely minimal and generally accepted notion of differential calculus or "exterior algebra" applicable to a noncommutative algebra A and common to all main approaches, i.e., we will not put in anything beyond this "by hand." This is to specify a bimodule of "1-forms" Ω^1 with left and right multiplication by a "function" in A, and a $\mathrm{d}:A\to\Omega^1$ operation obeying the Leibniz rule

$$\mathrm{d}(ab)=a\mathrm{d}b+(\mathrm{d}a)b.$$

One also requires that elements of the form $a\mathrm{d}b$ span Ω^1 and (a connectedness condition) that $\mathrm{d}a=0$ if and only if a is a constant. These are minimal properties that nevertheless suffice to do basic gauge theory on any algebra.

Next we note that for noncommutative algebras there is typically an element $\theta\in\Omega^1$ that generates the calculus in the sense

a)Electronic mail: s.majid@qmul.ac.uk

$$[\theta, a] = \lambda \mathrm{d}a$$

where λ is a parameter controlling the noncommutativity of the algebra A. Both sides go to zero when $\lambda \to 0$ (because classical 1-forms commute with functions), so this is a purely "quantum" phenomenon. The reason for the quotation marks here is that in our application λ is not related to $\hbar$ but is a new parameter in physics controlling a possible noncommutativity in space or space-time, or equivalently "cogravity" as curvature in momentum space.[18] The element θ must exist for example in the case of a semisimple Hopf algebra and a translation-covariant calculus, but also more generally whenever the geometry of A is fully noncommutative. On the other hand there is no reason at all to have such an element in the classical case as the equation above is empty. Therefore as we deform the classical algebra and its geometry, the constraints of noncommutative geometry will force the existence of a generating 1-form θ which *will have no reason to have any classical counterpart*. We are going to interpret this element θ as a time direction and the phenomenon then is that there may or may not be such a direction $\mathrm{d}t$ in our classical geometry with θ its deformation, but if there is not such a time direction it will have to be adjoined. This is what we propose here as "spontaneous generation" of time in our quantum groups approach to noncommutative geometry. Moreover, the partial derivative ∂^0 associated to this $\theta = \mathrm{d}t$ will generally have a classical limit for ∂^0/λ and this will be our induced *classical* Hamiltonian generated by the noncommutative geometry. Finally, we are free to change the normalization of θ in the previous discussion, which appears then as a new parameter induced at the same time.

In this article we will demonstrate this phenomenon in detail for one of the most basic noncommutative three-dimensional (3D) spaces, namely the angular momentum space

$$[x_i, x_j] = 2\imath\lambda \epsilon_{ij}{}^k x_k \tag{1}$$

of which the noncommutative geometry was studied in Ref. 5. This is the usual quantization of $\mathbb{R}^3$ as the coadjoint space su_2^* with its Kirillov–Kostant Poisson bracket, denoted $\mathbb{R}^3_\lambda$. The need for an extra direction θ in the calculus, as well as the link with Schrödinger's equation was proposed here, and in this sequel we develop it in detail. Section II is a reprise of the noncommutative differential geometry on (1) that we need from Ref. 5 except that we leave the normalization θ as a free nonzero parameter μ. Section III gives a quick account of quantum group Fourier transform and a direct derivation of formulae for the partial derivatives on 3D plane waves, which will also be needed.

In Section IV we proceed to explicitly adjoin a new variable t, commuting with x_i, such that $\theta = \mathrm{d}t$. In this extended space-time algebra the natural equation

$$\partial^t \psi(x,t) = 0 \tag{2}$$

(or that $\mathrm{d}\psi$ is purely spatial) is now our proposed noncommutative Schrödinger's equation (NCSE). We show that in the limit $\lambda \to 0$ this reproduces the usual Schrödinger equation for ψ for a particle of mass m with Compton wavelength $\mu = 1/m$. *We work throughout in units* $\hbar = c = 1$. In fact it turns out that as m approaches $1/\lambda$ we have to the next order a noncommutative version of the four-dimensional (4D) Euclidean wave equation for $e^{-\imath m t}\psi(x,t)$, suggesting a Euclidean aspect to the theory. Our construction is, however, very much tied to the nonrelativistic coordinate system consisting of x_i space and the induced t although it does not preclude the possibility of a Lorentz or 4D Euclidean (quantum) group action in the deformed theory. There is at least a full spatial Euclidean group of motions preserved in the construction, as the quantum group double $D(U(\mathrm{su}_2))$.[5] In Sec. V we finally solve the NCSE on plane waves, with solutions $e^{\imath \vec{p}\cdot x} e^{\imath p^0 t}$ of energy

$$p^0 = -\frac{1}{m\lambda^2} \ln(\cos(\lambda |\vec{p}|)) \tag{3}$$

provided $|\vec{p}| < \pi/2\lambda$. We also find the group velocity computed naively by differentiation of (3). It is a deformation of $|\vec{p}|/m$.

Our model comes out of noncommutative geometry and is not tied to specific values of λ, m. Our own view is that the theory could also be applicable in certain circumstances as an effective description of position "fuzziness" within quantum mechanics at the Compton wavelength scale of an ordinary particle, in the spirit of Ref. 21. However, if the theory appeared as a next-to-classical effective theory in a theory of quantum gravity, λ would be expected to be of the order of the Planck scale and hence we would have a Planckian spatial momentum cutoff for our particle. In fact it is known that the quantum double $D(U(\mathrm{su}_2))$ controls the tensor products of certain states in 2+1 quantum gravity,[3,22] therefore the result[5] that this quantum group acts covariantly on $\mathbb{R}^3_\lambda$ suggested that the latter should indeed be the effective noncommutative space in the next-to-classical approximation of 2+1 Chern–Simons quantum gravity. The algebra $\mathbb{R}^3_\lambda$ has also been proposed in string theory and in the reduction of certain matrix models but more usually in this context projected to a matrix algebra by setting the casmir equal to $j(j+1)$, which is to say a "fuzzy sphere."[1,4] However, we do not make such a projection here and we do not use the ad-hoc derivations-based matrix methods previously used for such objects. The noncommutative geometry in our case and with time adjoined is actually very rich and explored in Sec. VI where we show the existence of a closed radial polar coordinate system and some elements of gauge theory.

We note also that a Planckian cutoff is already a feature of the bicrossproduct spacetime[20] and we provide a comparison with this older model in the Appendix. In fact it has been known for some time that the zero-mass shell equation in the bicrossproduct model is deformed to

$$|\vec{p}| = \frac{1}{\lambda}(1 - e^{-\lambda p^0}) \quad \text{or} \quad p^0 = -\frac{1}{\lambda}\ln(1 - \lambda|\vec{p}|),$$

see (A2) in the Appendix, which (obviously) has the bound $|\vec{p}| < 1/\lambda$. Recently, some authors have dubbed models with such a Planckian cutoff as "doubly special" under the claim that the asymptotic feature of special relativity is now "doubled" by this additional asymptotic bound.[10] Although debatable, our own view is that such rebranding of the bicrossproduct model (which remains the main model in the theory) is unjustified as we also explain in the Appendix: What actually happens in our view is that the usual mass-shell hyperboloid is deformed nonlinearly and what used to be a 45° cone is now bent into a cylinder with vertical walls, rather than being a new bound. We also outline a different point of view on the cutoff in line with Ref. 13 (where p was viewed as position space rather than momentum) as an event-horizon-like coordinate singularity. In the present model part of the reason for a cutoff is rather more transparent: momentum space is compactified to a sphere $S^3 = \mathrm{SU}_2$ according to the quantum group Fourier transform.

Returning to the general phenomenon of spontaneous time creation, we note that for $\mathbb{C}_q[\mathrm{SU}_2]$ it is again known that the smallest bicovariant calculus is 4D not 3D and that the extra direction θ is linked to the Laplace operator, now on the quantum group as a noncommutative S^3. It is also already known that the local 4D cotangent bundle indeed has a natural q-Minkowski space metric, see Ref. 16 for a review and, for example, Ref. 8 for full calculations at q a root of unity (which is likely to be the physical case if such a deformation arises from quantum gravity in view of the well-known role of this quantum group in conformal field theory). The consistent addition of a time variable, however, and an analysis along the lines of the present paper is somewhat technical and will be presented elsewhere.

Finally, let us note that our proposal on time has no relation that we are aware of to the modular group in the theory of von-Neuman algebras; our results are purely algebraic and not connected with functional analysis. Briefly, Tomita and Takesaki in the 1970s showed that every von-Neumann algebra carries with it a 1-parameter automorphism group σ_t generated by the positive part Δ in the polar decomposition of the $*$-operation relative to a state. Translation by a finite imaginary interval in t is used to characterize KMS states in equilibrium quantum statistical mechanics on the algebra. Hence some authors, notably in Ref. 7, have proposed that t here should be viewed as time canonically associated to the von-Neumann algebra in a suitable setting. Although such a point of view is interesting, the phenomenon we propose in the "quantum groups approach" to noncommutative geometry is a rather more concrete one in which we shall show that a parameter t has to be adjoined and wave functions with respect to it naturally obey Schrödinger's

equation for some mass m. Our theory at the present level does not determine m, only that it must be nonzero, although $m=1/\lambda$ does present some simplifications in the mathematical structure as noted previously.

According to our analysis this mass and time generation is forced by the axioms of a differential calculus. We mention one alternative, which is to change these axioms by giving up associativity. At the semiclassical level it corresponds to curvature of an underlying Poisson-compatible preconnection.[6] (If one simply drops the θ terms in the calculus one would have such a situation with Poisson curvature and nonassociativity appearing at order λ^2). This gives an alternative idea of the nature of the obstruction involved. In physical terms one could say that the spatial translation group (as expressed in the differentials) is "anomalous" under the process of deformation quantization, with anomaly controlled by the above-mentioned Poisson curvature and nullified by adding an extra dimension.

II. REPRISE OF DIFFERENTIAL CALCULUS AND PLANE WAVES ON $\mathbb{R}^3_\lambda$

Since the calculus is crucial to our entire analysis, let us briefly reprise the construction in Ref. 5. For Lie groups it is well known that the translation-invariant differential structure is unique; for quantum groups there is a parallel theory for the weaker minimal axioms above that translation-invariant Ω^1 are freely generated over their space of invariant 1-forms and this latter space can be classified in terms of ideals in the augmentation ideal (the kernel of the counit) of the Hopf algebra. See Ref. 19 for a modern review of the theory. In general we refer to Ref. 16 for the notations and more basic theory of Hopf algebras.

Of course, $\mathbb{R}^3_\lambda$ is an additive Hopf algebra (in fact a classical enveloping algebra) with

$$\Delta x_i = x_i \otimes 1 + 1 \otimes x_i, \quad \epsilon x_i = 0, \quad S x_i = -x_i,$$

so we may use Hopf algebra or quantum group methods, and we do. The augmentation ideal in our case is the subalgebra $U(\mathrm{su}_2)^+$ generated by the x_i but not including 1. So left-invariant calculi (which will automatically be bicovariant in the present context) will be classified by ideals in here. These in turn are given by the kernels of matrix representations, more precisely by pairs (ρ, v) consisting of a representation and a ray in the representation space. The kernel of the map consisting of applying ρ to v is the ideal we need, and the left-invariant forms become identified with the orbit of v (which is the whole representation space for a cyclic vector). In our case, one can compute the differential calculi for the spin 0, 1/2, and 1 representations, of dimension 1,2,3, respectively. Especially, the last of these might be expected to be the correct calculus but in all these cases one may compute that d has a large kernel so these calculi are not successful. The next smallest is $\frac{1}{2}\otimes\frac{1}{2}$ which is to say the Pauli matrix representation on $M_2(\mathbb{C})$ where the algebra acts from the left and from the right (a 4D representation) by Pauli matrices. The canonical vector v is the identity matrix. This 4D calculus as shown to fulfill the connectedness property and is as we see the smallest such. We refer to Ref. 5 for details. We are assuming that $\lambda \neq 0$ (otherwise we could have the classical calculus).

The resulting calculus has commutation relations

$$\mathrm{d}x_i = \lambda \sigma_i, \quad x_i\theta - \theta x_i = \iota \frac{\lambda^2}{\mu} \mathrm{d}x_i,$$

$$(\mathrm{d}x_i)x_j - x_j \mathrm{d}x_i = \iota\lambda \varepsilon_{ij}{}^k \mathrm{d}x_k + \iota\mu\delta_{ij}\theta,$$

where θ is a multiple of the 2×2 identity matrix and, together with the Pauli matrices σ_i, completes the basis of left-invariant 1-forms. In the present paper relative to Ref. 5 we have put in a critical factor of ι and scale factor $\mu \neq 0$ in the normalization of θ to express explicitly that we are free to choose this normalization. One might expect $\mu \sim \lambda$ if both are generated by some deeper theory, or one might consider μ as second and independent length scale in the theory. The factor ι is justified as follows: to speak about unitarity all our algebras will be $*$-algebras and

thinking of the x_i as observables in the quantum algebra and real functions in the classical limit, we require

$$x_i^* = x_i,$$

which is consistent with λ real for the conventions used for $\mathbb{R}^3_\lambda$. Next, it is reasonable that $(\mathrm{d}x_i)^* = \mathrm{d}x_i$ if we want these also to be observables and to be identified with real 1-forms in the classical limit. The entire exterior algebra is generated by 1-forms, our case with the usual anticommutative wedge product, and we require this to be a $*$-algebra with

$$(\mathrm{d}\alpha)^* = (-1)^{|\alpha|}\mathrm{d}(\alpha^*)$$

for a form of degree $|\alpha|$. These conventions are not always adhered to in the literature (there are other equivalent ones in other contexts) but at least here, where there is a clear match with the classical limit, they are reasonable. For example, one of the main things one does with differential 1-forms is gauge theory. If u is unitary then

$$(u^{-1}\mathrm{d}u)^* = (\mathrm{d}u)^* u = (\mathrm{d}u^{-1})u = \mathrm{d}(1) - u^{-1}\mathrm{d}u = -u^{-1}\mathrm{d}u$$

is antihermitian. So connection 1-forms α are antihermitian. Then the curvature obeys

$$F(\alpha)^* = (\mathrm{d}\alpha + \alpha\wedge\alpha)^* = -\mathrm{d}\alpha^* + \alpha^*\wedge\alpha^* = F(\alpha)$$

which is to say behaves homogeneously under $*$. This justifies our reality conventions for the calculus. Indeed, a $U(1)$ connection in such a (trivial bundle) gauge theory would be $\imath$ times a real 1-form in classical geometry.

For our purposes we likewise require that $\theta^* = \theta$, i.e., a real 1-form in the classical limit, which determines the normalization used. An alternative is to require that $\theta^* = -\theta$ which would be more suitable for applications in which θ has the interpretation of a reference connection. The latter was the convention and application for θ in Ref. 5 for example.

Once one has fixed the differential calculus, the partial derivatives ∂^i as operators on $\mathbb{R}^3_\lambda$ are completely determined by

$$\mathrm{d}\psi(x) = (\partial^i\psi)\mathrm{d}x_i + (\partial^0\psi)\theta.$$

They are not derivations (that would be an older and widely discredited approach to noncommutative geometry); rather they are braided derivations with respect to a certain solution of the Yang–Baxter equations (induced from the quantum double).

Finally plane waves take the form of group elements in the enveloping algebra $\mathbb{R}^3_\lambda$,

$$\psi_{\vec{p}}(x) = e^{\imath\vec{p}\cdot x}, \quad \vec{p}\in\mathbb{R}^3.$$

The momenta p_i are nothing but local coordinates for the corresponding point $e^{\imath\lambda\vec{p}\cdot\sigma}\in \mathrm{SU}_2$ where $\lambda\sigma$ is the representation by Pauli matrices. It is really elements of this curved space SU_2 where momenta live, as evident in the addition law for momenta determined by the plane waves:

$$\psi_{\vec{p}}\cdot\psi_{\vec{p}'} = \psi_{C(\vec{p},\vec{p}')},$$

where $C(\vec{p},\vec{p}')$ is the Campbell–Baker–Hausdorf series. This is the general procedure for any enveloping algebra of a Lie algebra and the one we use here. Other coordinate systems are also possible, for example by Euler angles. We will show next that our plane waves are eigenfunctions of the ∂^i. The result is in Ref. 5 but the proof now is entirely different and self-contained.

III. QUANTUM GROUP FOURIER TRANSFORM AND ACTION ON PLANE WAVES

The algebra $\mathbb{R}^3_\lambda = U(\mathrm{su}_2)$ has dual $\mathbb{C}[\mathrm{SU}_2]$ and Hopf algebra Fourier transform (after suitable completion) takes one between these spaces. Thus, in one direction

$$\mathcal{F}(f)=\int_{\mathrm{SU}_2}\mathrm{d}u f(u)u\approx\int_{\mathbb{R}^3}\mathrm{d}^3pJ(\vec{p})f(\vec{p})e^{\imath\vec{p}\cdot x}$$

for f a function on SU_2. We use the Haar measure on SU_2. The local result on the right has J the Jacobian for the change to the local $\vec{p}$ coordinates and f is written in terms of these. Differential operators on $\mathbb{R}^3_\lambda$ are given by the action of elements of $\mathbb{C}[\mathrm{SU}_2]$ and are diagonal on these plane waves,

$$f\cdot\psi_{\vec{p}}=f(\vec{p})\psi_{\vec{p}},$$

which corresponds under Fourier transform simply to pointwise multiplication in $\mathbb{C}[\mathrm{SU}_2]$. This quantum group Fourier transform approach to noncommutative geometry whereby it becomes equivalent to a theory of classical but *curved* momentum space was introduced by the author in Ref. 17 more than a decade ago. We refer to Ref. 18 for a more recent review. Of course Fourier transform by other more conventional methods such as spherical harmonics is also possible but the quantum groups Fourier transform exactly takes us to noncommutative spaces such as $\mathbb{R}^3_\lambda$ which is what we need now.

Next, we show that the partial derivatives indeed act diagonally on plane waves as

$$\partial^i=\imath\frac{p^i}{\lambda|\vec{p}|}\sin(\lambda|\vec{p}|)=\frac{\imath}{2\lambda}\mathrm{Tr}(\sigma_i(\ \ )),\tag{4}$$

$$\partial^0=\frac{\imath\mu}{\lambda^2}(\cos(\lambda|p|)-1)=\frac{\imath\mu}{2\lambda^2}(\mathrm{Tr}-2).\tag{5}$$

The second expressions in each case are just the functions in $\mathbb{C}[\mathrm{SU}_2]$ whose evaluation on plane waves gives the first expression in each case. Thus

$$\mathrm{Tr}\,\psi_{\vec{p}}=\mathrm{Tr}(e^{\imath\lambda\vec{p}\cdot\sigma})\psi_{\vec{p}}=2\cos(\lambda|p|)\psi_{\vec{p}}$$

and so forth. It remains to prove the first expressions for the ∂^μ.

The full action of the ∂^μ are rather complicated but we need them only for functions of

$$X=\imath\vec{p}\cdot x.$$

Then from the relations for the calculus, we find the subcalculus

$$(\mathrm{d}X)\cdot X=X\mathrm{d}X-\imath\nu\theta,\quad \theta X=X\theta-\imath\nu'\mathrm{d}X,$$

where

$$\nu=\mu p^2,\quad \nu'=\frac{\lambda^2}{\mu}.$$

We let

$$\mathrm{d}X^n=f_n(X)\mathrm{d}X+g_n(X)\theta$$

and using the above-mentioned relations and the Leibniz rule we have

$$\begin{aligned}\mathrm{d}X^n&=(\mathrm{d}X^{n-1})X+X^{n-1}\mathrm{d}X=f_{n-1}\mathrm{d}X\cdot X+X^{n-1}\mathrm{d}X+g_{n-1}\theta X\\&=f_{n-1}X\mathrm{d}X-\imath\nu f_{n-1}\theta+X^{n-1}\mathrm{d}X+g_{n-1}X\theta-\imath\nu' g_{n-1}\mathrm{d}X\end{aligned}$$

hence, the recurrence relations

$$f_n = f_{n-1}X - \imath\nu' g_{n-1} + X^{n-1}, \quad g_n = g_{n-1}X - \imath\nu f_{n-1}, \quad f_1 = 1, \quad g_1 = 0.$$

These can be easily solved and yield

$$f_n = -\frac{\imath}{2\sqrt{\nu\nu'}}((X + \imath\sqrt{\nu\nu'})^n - (X - \imath\sqrt{\nu\nu'})^n),$$

$$g_n = -\frac{\imath}{\nu'}X^n + \frac{\imath}{2\nu'}((X + \imath\sqrt{\nu\nu'})^n + (X - \imath\sqrt{\nu\nu'})^n),$$

or

$$\mathrm{d}X^n = \frac{\imath}{2\lambda|\vec{p}|}\left((X - \imath\lambda|\vec{p}|)^n\left(\frac{\mu}{\lambda}|\vec{p}|\theta + \mathrm{d}X\right) + (X + \imath\lambda|\vec{p}|)^n\left(\frac{\mu}{\lambda}|\vec{p}|\theta - \mathrm{d}X\right)\right) - \frac{\imath\mu}{\lambda^2}X^n\theta.$$

In particular, we see that

$$e^{-X}\mathrm{d}e^X = \frac{\imath}{2\lambda|\vec{p}|}\left(e^{-\imath\lambda|\vec{p}|}\left(\frac{\mu}{\lambda}|\vec{p}|\theta + \mathrm{d}X\right) + e^{\imath\lambda|\vec{p}|}\left(\frac{\mu}{\lambda}|\vec{p}|\theta - \mathrm{d}X\right)\right) - \frac{\imath\mu}{\lambda^2}\theta$$

$$= \frac{\imath\mu}{\lambda^2}(\cos(\lambda|\vec{p}|) - 1)\theta + \frac{1}{\lambda|\vec{p}|}\sin(\lambda|\vec{p}|)\mathrm{d}X$$

which translates into ∂^μ acting as stated on plane waves. Through quantum group Fourier transform this allows one to compute them in principle on any $\psi(x)$. We will not need to do this explicitly, however.

IV. LAPLACIAN AND NONCOMMUTATIVE SCHRÖDINGER'S EQUATION

From the partial derivatives (4) and (5) on plane waves, we compute the 3D Laplacians on plane waves:

$$\nabla^2 = \partial_i\partial^i = -\frac{1}{\lambda^2}\sin^2(\lambda|\vec{p}|)$$

which has the correct classical limit $-|\vec{p}|^2$ as $\lambda \to 0$. Comparing with the expression in momentum space for ∂^0 we deduce that

$$\partial^0 = \frac{\imath\mu}{\lambda^2}(\sqrt{1 + \lambda^2\nabla^2} - 1) \tag{6}$$

on plane waves and hence in general for modes with $\nabla^2 \geqslant -1/\lambda^2$. Expanding this we find

$$\partial^0\psi = \imath\frac{\mu}{2}\nabla^2\psi + O(\lambda^2) \tag{7}$$

which is of the form of Schrödinger's equation with respect to an auxiliary "time" variable and a particle with Compton wavelength μ corresponding to mass m,

$$\mu = \frac{1}{m}. \tag{8}$$

Our point of view is that λ might be of the order of the Planck scale, so if μ is also of this scale then the effective mass of the particle being described is of the order of the Planck mass. We are not tied to such a value for either parameter, however.

We now proceed to develop this point of view. Thus let t be a time variable adjoined to the theory, commuting with the position generators and such that

$$\theta = \mathrm{d}t$$

which is consistent with our reality assumptions if $t^* = t$. For consistency with the relations in the differential calculus we need

$$0 = \mathrm{d}([t, x_i]) = \theta x_i + t\mathrm{d}x_i - (\mathrm{d}x_i)t - x_i\theta$$

so we require

$$[t, \mathrm{d}x_i] = \imath\frac{\lambda^2}{\mu}\mathrm{d}x_i$$

which implies that

$$(\mathrm{d}x_i)f(t) = f\left(t - \imath\frac{\lambda^2}{\mu}\right)\mathrm{d}x_i.$$

In this case for the Jacobi identity

$$0 = [\mathrm{d}x_i, [x_j, t]] + [x_j, [t, \mathrm{d}x_i]] + [t, [\mathrm{d}x_i, x_j]]$$

we need

$$[t, \theta] = \imath\frac{\lambda^2}{\mu}\theta.$$

Since $\theta = \mathrm{d}t$ we see that

$$f\left(t - \imath\frac{\lambda^2}{\mu}\right)\mathrm{d}t = (\mathrm{d}t)f(t)$$

holds as well, which in turn can be used to show that

$$\mathrm{d}f(t) = (\partial^t f(t))\mathrm{d}t, \quad \partial^t f(t) \equiv \frac{f(t) - f\left(t - \imath\frac{\lambda^2}{\mu}\right)}{\imath\frac{\lambda^2}{\mu}}$$

is necessarily a finite difference operator. Applying d again gives the usual anticommutation relations between $\mathrm{d}t$ and the $\mathrm{d}x_i$ (as among themselves). In summary, we can adjoin a t variable but for consistency with the spatial noncommuative calculus we will need its calculus to be a noncommutative finite difference one.

The differential on functions $a(x)$ just of x is unchanged:

$$\mathrm{d}a(x) = \partial^i a(x)\mathrm{d}x_i + \partial^0 a(x)\mathrm{d}t.$$

When we look in the extended algebra we will have functions generated by products of functions $a(x)$ and $f(t)$ and here we find, using the Leibniz rule,

$$\begin{aligned}\mathrm{d}(a(x)f(t)) &= (\partial^i a\mathrm{d}x_i)f + (\partial^0 a\mathrm{d}t)f + a\partial^t f\mathrm{d}t \\ &= (\partial^i a)f\left(t - \imath\frac{\lambda^2}{\mu}\right)\mathrm{d}x_i + \left((\partial^0 a)f\left(t - \imath\frac{\lambda^2}{\mu}\right) + a\partial^t f\right)\mathrm{d}t \equiv \tilde{\partial}^i(af)\mathrm{d}x_i + \tilde{\partial}^0(af)\mathrm{d}t.\end{aligned}$$

This defines the partial derivatives $\tilde{\partial}^\mu$ acting on general functions in the calculus. Here $\tilde{\partial}^0$ reduces to ∂^0 as before acting on $a(x)$ and to ∂^t acting on $f(t)$ alone. The braided Liebniz rule is evident here on products as the extra shift by $-i\lambda^2/\mu$ and is typical of noncommutative vector fields.

The calculus is clearly an unusual one in which the ∇^2 is built into $\tilde{\partial}^0$. Because we have adjoined the t the natural formulation of Schrödingers equation is now

$$\tilde{\partial}^0\psi(x,t)=0, \tag{9}$$

i.e., functions which are "constant" with respect to the extended differential calculus in the sense that $\mathrm{d}\psi$ is purely spatial. We can write this more explicitly using the above as

$$\frac{\imath\mu}{\lambda^2}\left(\psi(x,t)-\psi\left(x,t-\imath\frac{\lambda^2}{\mu}\right)\right)=\partial^0\psi\left(x,t-\imath\frac{\lambda^2}{\mu}\right) \tag{10}$$

exhibiting ∂^t as a finite difference operation in the continuous time variable t. Putting in our previous expression for ∂^0 this is

$$\psi(x,t)-\psi\left(x,t-\imath\frac{\lambda^2}{\mu}\right)=(\sqrt{1+\lambda^2\nabla^2}-1)\psi\left(x,t-\imath\frac{\lambda^2}{\mu}\right)$$

or

$$\psi\left(x,t+\imath\frac{\lambda^2}{\mu}\right)=(\sqrt{1+\lambda^2\nabla^2})\psi(x,t) \tag{11}$$

after a change of variable $t\to t+\imath\lambda^2/\mu$. Writing the left-hand side as the action of $e^{\imath(\lambda^2/\mu)(\partial/\partial t)}$ in terms of usual derivatives, and taking ln of the operators on both sides, we have formally (or not formally on plane waves),

$$\frac{\partial}{\partial t}\psi=-\imath\frac{\mu}{2\lambda^2}\ln(1+\lambda^2\nabla^2)=-\frac{\imath}{2m}\left(\nabla^2-\frac{\lambda^2}{2}\nabla^4+\frac{\lambda^4}{3}\nabla^6\cdots\right) \tag{12}$$

for small λ. Thus our equation explicitly deforms the usual Schrödingers equation with higher derivative terms.

Note that we can also expand the left-hand side of (11) in a Taylor series and the right-hand side in a binomial series so

$$\imath\frac{\partial}{\partial t}\psi-\frac{\lambda^2}{2\mu}\frac{\partial^2}{\partial t^2}\psi+\cdots=\frac{\mu}{2}\nabla^2\psi-\frac{\lambda^2\mu}{8}\nabla^4\psi+\cdots.$$

Now *if* we choose $\mu=\lambda$ and keep terms to $O(\lambda^2)$ then this reads in terms of m as

$$\frac{\partial}{\partial t}\psi=-\frac{\imath}{2m}\nabla^2\psi-\frac{\imath}{2m}\frac{\partial^2}{\partial t^2}\psi+O\left(\left(\frac{1}{m}\right)^3\right)$$

which is the 4D Euclidean wave equation for $\phi(x,t)=e^{-\imath mt}\psi(x,t)$ in terms of ψ. Here

$$\left(\frac{\partial^2}{\partial t^2}+\nabla^2+m^2\right)\phi=-2\imath me^{\imath mt}\dot{\psi}+e^{\imath mt}\ddot{\psi}+e^{\imath mt}\nabla^2\psi.$$

On the other hand, ∇ itself is a deformation and at least on plane waves brings its own corrections to the same order so that the above is a formal observation.

When $\mu=\lambda$ we also have a formal Euclidean aspect in the noncommutative wave operator. In fact we are not proposing an $SO_{1,3}$ or SO_4 symmetry in the noncommutative model (in our construction we have preserved spatial rotations only, and induced time from it). However, it is interesting to note that we have the following modified wave operator in the original (spatial) theory, from (4) and (5):

$$\Box^{(3)} = (\partial^0)^2 + \nabla^2 = \frac{2}{\lambda^2}(\cos(\lambda|p|) - 1) = \frac{1}{\lambda^2}(\mathrm{Tr} - 2) \tag{13}$$

which again has the usual limit $-|\vec{p}|^2$ as $\lambda \to 0$. The fact that this has such a nice description via the action of $\mathrm{Tr} \in \mathbb{C}[\mathrm{SU}_2]$ suggests that it is somewhat natural; if one takes instead $-(\partial^0)^2$ the result is similar but does not have such a simple expression. Here Tr−2 is the Casimir in $D(U(\mathrm{su}_2)) = \mathbb{C}[\mathrm{SU}_2] \rtimes U(\mathrm{su}_2)$ as explained in Ref. 5.

V. DISPERSION RELATIONS AND CUT-OFF

We can also immediately solve the NCSE on plane waves, using the results of Sec. III. We let $\psi(x,t) = e^{\imath\vec{p}\cdot x} f(t)$. Then from (11) and the value of ∂^0 on plane waves, we require

$$f\left(t + \imath\frac{\lambda^2}{\mu}\right) = \cos(\lambda|\vec{p}|) f(t)$$

which is solved by

$$\psi_{\vec{p}}(x,t) = e^{\imath\vec{p}\cdot x + \imath p^0 t}, \quad e^{-(\lambda^2/\mu)p^0} = \cos(\lambda|\vec{p}|), \quad |\vec{p}| < \frac{\pi}{2\lambda}. \tag{14}$$

Notice that the spatial momentum is bounded above for there to be a primary solution, which is a typical feature of quantum gravity as discussed in Sec. I. We also have unphysical solutions $5\pi/2 > |\vec{p}| > 3\pi/2\lambda$ etc. according to the periodicity of cos, which we consider an artefact of the local coordinate system. Recall that the p^i are local coordinates in momentum space which is actually here a sphere S^3 not flat, and this is also the reason for the cutoff in the first place.

Differentiating the p^0 equation immediately gives

$$e^{-(\lambda^2/\mu)p^0}\frac{\partial p^0}{\partial p^i} = \frac{\mu}{\lambda}\sin(\lambda|\vec{p}|)\frac{p^i}{|\vec{p}|}$$

and hence our proposed dispersion relation

$$\left|\frac{\partial p^0}{\partial \vec{p}}\right| = \frac{\mu}{\lambda}|\tan(\lambda|\vec{p}|)| = \frac{1}{m\lambda}|\tan(\lambda|\vec{p}|)|,$$

i.e., the group velocity is linear for small momentum as expected for a particle of mass m in our nonrelativistic coordinates, but blows up at the cutoff value. Note, however, that a detailed analysis of how plane waves in the noncommutative model might be measured experimentally and their group velocity is still needed in order to see if such a naive derivation is justified. In the bicrossproduct model calculation[2] this was somewhat justified by a natural normal-ordering postulate for the identification of noncommutative expressions with their classical counterparts. In the present model we can in principle do better; we can look at the plane waves in actual representations of the noncommutative algebra on the basis that it is such expectation values that are presumably observed. We propose to use here the coherent states $|j,\phi,\psi\rangle$ in which the coordinates behave with minimal uncertainty[5] and with expectation values

$$\langle x\rangle \equiv \langle j,\phi,\psi|\vec{x}|j,\phi,\psi\rangle = 2j\lambda(\sin\phi\cos\psi, \sin\phi\sin\psi, \cos\phi)$$

for a particle at angle ϕ,ψ and radius $2j\lambda$ (which we see is quantized). Explicitly,

$$|j,\phi,\psi\rangle = \sum_{k=0}^{2j} 2^{-j}\sqrt{\binom{2j}{k}}(1+\cos\phi)^{(2j-k)/2}(1-\cos\phi)^{k/2}e^{\imath k\psi}|j,j-k\rangle$$

in terms of usual spin j states and in the present conventions. In such a state our plane waves have a classical "shadow" as waves in polar coordinates. For example,

$$\left\langle \frac{1}{2},\phi,\psi \middle| e^{\imath\vec{p}\cdot x} \middle| \frac{1}{2},\phi,\psi \right\rangle = \cos\lambda|\vec{p}| + \imath\frac{\vec{p}\cdot\langle x\rangle}{\lambda|\vec{p}|}\sin\lambda|\vec{p}|$$

which should be compared with the classical value at this radius of

$$e^{\imath\lambda(p_1\sin\phi\cos\psi+p_2\sin\phi\sin\psi+p_3\cos\phi)} = e^{\imath\vec{p}\cdot\langle x\rangle}.$$

The approximation gets better for large spin. This suggests that the noncommutative plane waves would appear as something with comparable periodicity in the expectation values, and hence comparable group velocity to the extent that the expectation values appear wavelike. Note also that

$$|\langle j,\phi,\psi|j,\phi',\psi'\rangle|^2 = \left(\frac{1}{2}(1+\cos(\text{angle}(\phi,\psi|\phi',\psi')))\right)^{2j},$$

where the angle is the classical angle between vectors in directions (ϕ,ψ) and (ϕ',ψ') in polar coordinates. The point of view here is in the spirit of Ref. 21 but rather than a spin network we use noncommutative geometry. See also Ref. 9 concerning coherent states.

VI. POLAR COORDINATES AND GAUGE THEORY

The model with time adjoined has in fact a rich noncommutative geometry. Here we note that there is a closed algebra among the t and the Casimir $c=\vec{x}\cdot\vec{x}$. These from a commutative subalgebra of rotationally invariant functions varying in time, but as we show now with noncommutative differentials. First of all, we note that

$$\mathrm{d}c = x_i\mathrm{d}x_i + (\mathrm{d}x_i)x_i = 2x_i\mathrm{d}x_i + 3\imath\mu\theta \tag{15}$$

and $[c,x_i]=0$ implies that

$$\begin{aligned}
[\mathrm{d}c_i,x_i] &= -[c,\mathrm{d}x_i] = -x_j[x_j,\mathrm{d}x_i] - [x_j,\mathrm{d}x_i]x_j \\
&= \imath\lambda\epsilon_{ijk}x_j\mathrm{d}x_k + \imath\mu x_i\theta + \imath\lambda\epsilon_{ijk}(\mathrm{d}x_k)x_j + \imath\mu\theta x_i \\
&= 2\imath\lambda\epsilon_{ijk}x_j\mathrm{d}x_k - (\imath\lambda)^2\epsilon_{ijk}\epsilon_{kmj}\mathrm{d}x_m + \imath\mu(x_i\theta+\theta x_i) \\
&= 2\imath\lambda\epsilon_{ijk}x_j\mathrm{d}x_k + 2\lambda^2\mathrm{d}x_i + \imath\mu\left(2x_i\theta - \imath\frac{\lambda^2}{\mu}\mathrm{d}x_i\right) \\
&= 2\imath\lambda\epsilon_{ijk}x_j\mathrm{d}x_k + 3\lambda^2\mathrm{d}x_i + 2\imath\mu x_i\theta
\end{aligned}$$

using the relations in the calculus. From this and (15) we find that

$$\begin{aligned}
[\mathrm{d}c,c] &= [\mathrm{d}c,x_i]x_i + x_i[\mathrm{d}c,x_i] \\
&= -4\lambda^2x_i\mathrm{d}x_i + 3\lambda^2(\mathrm{d}x_i)x_i + 2\imath\mu x_i\theta x_i + x_i3\lambda^2\mathrm{d}x_i + 2\imath\mu c\theta \\
&= 4\lambda^2x_i\mathrm{d}x_i + 9\lambda^2\imath\mu\theta + 4\imath\mu c\theta = 2\lambda^2\mathrm{d}c + 4\imath\mu\left(c+\frac{3}{4}\lambda^2\right)\mathrm{d}t.
\end{aligned} \tag{16}$$

Meanwhile, from $[t,c]=0$ and $\theta=\mathrm{d}t$ as generator of d, we have

$$[\mathrm{d}c,t] = [\mathrm{d}t,c] = \frac{\lambda^2}{\imath\mu}\mathrm{d}c, \quad [\mathrm{d}t,t] = \frac{\lambda^2}{\imath\mu}\mathrm{d}t \tag{17}$$

to give a closed algebra (16) and (17) among the t, c, dt, and dc. As in Sec. IV we immediately conclude that

$$\mathrm{d}t.f(t)=f\left(t-\imath\frac{\lambda^2}{\mu}\right)\mathrm{d}t,\quad \mathrm{d}c.f(t)=f\left(t-\imath\frac{\lambda^2}{\mu}\right)\mathrm{d}c$$

for any function $f(t)$, whereas the commutation relations with some function $a(c)$ has to be determined by induction. Likewise $\mathrm{d}f(t)=\partial^t f\mathrm{d}t$ given by a finite difference as in Sec. IV, whereas $\mathrm{d}a(c)$ has to be determined by induction.

To this end, let

$$\begin{aligned}\mathrm{d}c^n &\equiv f_n\mathrm{d}c+g_n\mathrm{d}t=\mathrm{d}c^{n-1}.c+c^{n-1}\mathrm{d}c\\ &=f_{n-1}\mathrm{d}c.c+g_{n-1}\mathrm{d}t.c+c^{n-1}\mathrm{d}c\\ &=\left((c+2\lambda^2)f_{n-1}+c^{n-1}-\imath\frac{\lambda^2}{\mu}g_{n-1}\right)\mathrm{d}c+\left(cg_{n-1}+4\imath\mu\left(c+\frac{3}{4}\lambda^2\right)f_{n-1}\right)\mathrm{d}t\end{aligned}$$

which gives a recursion relation for f_n, g_n with $f_1=1$ and $g_1=0$. This can be solved to obtain $\mathrm{d}c^n$, or on any $a(c)$ to compute partial differentials ∂^c and $\partial^t{}_{|_c}$ defined by

$$\mathrm{d}a(c)\equiv(\partial^c a)\mathrm{d}c+(\partial^t_{|c}a)\mathrm{d}t.$$

Here the $|_c$ is to remind us that this is with respect to c and implicit angular coordinates being held constant, which is not quite the same as ∂^0 in Sec. IV where the x_i were being held constant. We find

$$\partial^c a(c)=\frac{a(c+\lambda^2+2\lambda\sqrt{c+\lambda^2})-a(c+\lambda^2-2\lambda\sqrt{2c+\lambda^2})}{4\lambda\sqrt{c+\lambda^2}}$$

$$\partial^t_{|c}a(c)=\frac{\mu}{\imath\lambda^2}\left(a(c)+\lambda^2\partial^c a(c)-\frac{a(c+\lambda^2+2\lambda\sqrt{c+\lambda^2})+a(c+\lambda^2-2\lambda\sqrt{c+\lambda^2})}{2}\right).$$

These extend to products by a braided derivation rule and by the same computation as in Sec. IV we find

$$\partial^c(af)=(\partial^c a)f\left(t-\imath\frac{\lambda^2}{\mu}\right),\quad \partial^t_{|c}(af)=(\partial^t_{|c}a)f\left(t-\imath\frac{\lambda^2}{\mu}\right)+a\partial^t f$$

for $a(c)f(t)$. This gives the partial derivatives and d on a general function $\psi(c,t)$ in polar coordinates.

As an application, we can write our NCSE in polar form as follows. The equation says that d is purely in the $\mathrm{d}x_i$ direction. Writing $\mathrm{d}a(c)=(\partial^i a)\mathrm{d}x_i+(\partial^0 a)\mathrm{d}t$ as in Sec. IV, we have in view of (15) that

$$\partial^i a(c)=(\partial^c a)2x_i,\quad \partial^0 a(c)=\partial^t_{|c}a+3\imath\mu\partial^c a.$$

The latter comes out as

$$\begin{aligned}\partial^0 a(c)=\frac{\imath\mu}{\lambda^2}\Bigg(&\frac{1}{2}\left(1+\frac{\lambda}{\sqrt{c+\lambda^2}}\right)a(c+\lambda^2+2\lambda\sqrt{c+\lambda^2})\\ &+\frac{1}{2}\left(1-\frac{\lambda}{\sqrt{c+\lambda^2}}\right)a(c+\lambda^2-2\lambda\sqrt{c+\lambda^2})-a(c)\Bigg)\end{aligned}\tag{18}$$

using the above results. This compares with (6) or (5) computed in our previous plane wave basis. We will not attempt to solve the NCSE here, for one thing one needs to have suitable proposals for a potential term for, say, a hydrogen atom. Suffice it to say that any such calculation is best done

in polar coordinates and (18) provides the radial part of the effective Laplacian to be used in (10), now on wave functions $\psi(c,t)$. One may compute for example that

$$\partial^0\left(\frac{1}{\sqrt{c+\lambda^2}}\right)=0$$

where $\rho=\sqrt{c+\lambda^2}$, makes for a reasonably nice answer and suggests that this is the appropriate analog of r in usual polar coordinates. This is the right answer when $\lambda\to 0$ (the radial Laplacian vanishes on $1/r$). Similarly one may check that

$$\partial^0 c=3\iota\mu,\quad \partial^0 c^2=\iota\mu(10c+9\lambda^2),\quad \partial^0\sqrt{c+\lambda^2}=\iota\mu\frac{1}{\sqrt{c+\lambda^2}}$$

as expected for $\iota\mu$ times $1/2$ the radial Laplacian as in (7) if c is understood as r^2 in the classical limit or more precisely ρ as r.

Another application of polar coordinates is for computations in the associated $U(1)$ gauge theory. As mentioned in Sec. II at the basic level a gauge field is a connection $\alpha=\alpha^\mu \mathrm{d}x_\mu$ with suitable reality properties. The curvature in the Maxwell theory is just

$$F_M(\alpha)=\mathrm{d}\alpha=\partial^\mu\alpha^\nu \mathrm{d}x_\mu\wedge\mathrm{d}x_\nu$$

which may be computed as usual using the partial derivatives. The theory is sensitive to cohomology and a gauge transformation is the addition of an exact differential. In the noncommutative case we also have the option of a nonlinear $U(1)$ Yang–Mills-type theory with curvature

$$F_{YM}(\alpha)=\mathrm{d}\alpha+\alpha\wedge\alpha=\partial^\mu\alpha^\nu \mathrm{d}x_\mu\wedge\mathrm{d}x_\nu+\alpha^\mu\mathrm{d}x_\mu\wedge\alpha^\nu\mathrm{d}x_\nu$$

and which detects homotopy. This needs also the commutation relations between functions and differentials. We look briefly at the electrostatic Maxwell case.

First, we look at gauge fields of the form

$$\alpha=a(c)\mathrm{d}t,$$

where $a(c)$ does not depend on t. This has

$$F_M=\partial^c a\mathrm{d}c\wedge\mathrm{d}t+\partial^t_{|c}a(\mathrm{d}t)^2=\partial^c a 2x_i\mathrm{d}x_i\wedge\mathrm{d}t$$

in view of (15) and $(\mathrm{d}t)^2=0$ in the calculus. We recall that the $\mathrm{d}x_\mu$ anticommute as usual. Thus we have an electric field

$$E_i=\partial^c a(c)2x_i$$

more or less as usual. For example, $a(c)=1/\sqrt{c+\lambda^2}$ gives

$$E_i=-\frac{x_i}{c\sqrt{c+\lambda^2}}$$

which is an inverse square law in the classical limit. Its divergence gives the corresponding charge density.

More surprisingly, we have also a different way of producing an electric field, namely

$$\alpha=a(c)2x_i\mathrm{d}x_i=a(c)\mathrm{d}c-3\iota\mu a(c)\mathrm{d}t$$

in view of (15). We have chosen α here to have purely spatial components in the $\mathrm{d}x_\mu$ basis but we have the same conclusion below (with a different coefficient) even if we do not include the second term. The curvature is

$$F_M = \partial^{\mathcal{F}} a(\mathrm{d}c)^2 + \partial^t_{|c} a \mathrm{d}t \wedge \mathrm{d}c - 3\imath\mu\partial^{\mathcal{F}} a \mathrm{d}c \wedge \mathrm{d}t$$

which we compute using

$$\begin{aligned}\mathrm{d}c \wedge \mathrm{d}c &= 4x_i \mathrm{d}x_i \wedge x_j \mathrm{d}x_j + 6\imath\mu x_i \mathrm{d}x_i \wedge \mathrm{d}t + 6\imath\mu \mathrm{d}t \wedge x_i \mathrm{d}x_i \\ &= 4x_i \mathrm{d}x_i \wedge x_j \mathrm{d}x_j = 2[x_i, x_j]\mathrm{d}x_i \wedge \mathrm{d}x_j + 4x_i[\mathrm{d}x_i, x_j] \wedge \mathrm{d}x_j \\ &= 4\imath\lambda\epsilon_{ijk} x_k \mathrm{d}x_i \wedge \mathrm{d}x_j + 4\imath\lambda x_i \epsilon_{ijk} \mathrm{d}x_k \wedge \mathrm{d}x_j + 4\imath\mu x_i \mathrm{d}t \wedge \mathrm{d}x_i \\ &= 2\imath\mu \mathrm{d}t \wedge \mathrm{d}c = -2\imath\mu \mathrm{d}c \wedge \mathrm{d}t\end{aligned}$$

using (15) and $(\mathrm{d}t)^2=0$ in the first line and that $[\mathrm{d}t, x_i] \propto \mathrm{d}x_i$ in the second line which produces nothing as $(\mathrm{d}x_i)^2=0$ for each i (and that $\mathrm{d}t, \mathrm{d}x_i$ anticommute as usual). We then use the commutation relations in the calculus and in the algebra. The same observations imply that $\mathrm{d}c, \mathrm{d}t$ anticommute. Hence

$$F_M = -(2\imath\mu\partial^{\mathcal{F}} a + \partial^0 a)\mathrm{d}c \wedge \mathrm{d}t = -(5\imath\mu\partial^{\mathcal{F}} a + \partial^t_{|c} a) 2x_i \mathrm{d}x_i \wedge \mathrm{d}t$$

which is again a radial electric field. Such a potential in the classical case would be absent as α would be pure gauge with zero curvature. There are clearly many other possibilities to be explored here including time dependent (such as standing wave) solutions. Also in this preliminary analysis we do not discuss source terms for the potentials since this would require a study of the suitable currents produced by matter fields. Finally, all of these remarks are more complicated for the Yang–Mills version.

APPENDIX: COMPARISON WITH BICROSSPRODUCT MODELS

The model above with noncommuting position and commuting t is complementary to the bicrossproduct model where the spacetime $\mathbb{R}^{1,3}_\lambda$ in Ref. 20 is

$$[t, x_i] = \imath\lambda x_i, \quad [x_i, x_j] = 0. \tag{A1}$$

Here the position coordinates commute and t is noncommutative, but we shall note similar features nevertheless. Some authors write $\kappa = 1/\lambda$ as a mass scale instead.

This time the relevant Lie algebra in (19) is the solvable one b_+ (say) and computations are rather easier using normal ordering as explained in Ref. 20. Hence we parametrize the plane waves as

$$\psi_{\vec{p}\cdot p^0} = e^{\imath\vec{p}\cdot x} e^{\imath p^0 t}, \quad \psi_{\vec{p},p^0}\psi_{\vec{p}',p^{0\prime}} = \psi_{\vec{p}+e^{-\lambda p^0}\vec{p}', p^0+p^{0\prime}}$$

which identifies the p^μ as the coordinates of a non-Abelian group B_+ with Lie algebra b_+. The group law in these coordinates is read off as usual from the above product of plane waves. The right-invariant Haar measure on B_+ in these coordinates is the usual $\mathrm{d}^4 p$ so the quantum group Fourier transform[17] reduces to the usual one but normal ordered,

$$\mathcal{F}(f) = \int_{\mathbb{R}^4} \mathrm{d}^4 p f(p) e^{\imath\vec{p}\cdot x} e^{\imath p^0 t}.$$

As before, the action of elements of $\mathbb{C}[B_+]$ define differential operators on $\mathbb{R}^{1,3}_\lambda$ and these act diagonally on plane waves.

There is also known to be a natural differential calculus with

$$(\mathrm{d}x_j)x_\mu = x_\mu \mathrm{d}x_j, \quad (\mathrm{d}t)x_\mu - x_\mu \mathrm{d}t = \imath\lambda \mathrm{d}x_\mu$$

which we see already has a generator with $\theta = \mathrm{d}t$; so we do not need to adjoin a further t in this model. The unitarity or $*$-structure is $x_i^* = x_i$, $t^* = t$ and the same for their differentials. The calculus recovers the partial derivatives[20]

$$\partial^i\psi =: \frac{\partial}{\partial x_i}\psi(x,t) := \imath p^i \,.\, \psi,$$

$$\partial^0\psi =: \frac{\psi(x,t+\imath\lambda)-\psi(x,t)}{\imath\lambda} := \frac{\imath}{\lambda}(1-e^{-\lambda p^0})\psi$$

for normal ordered polynomial functions ψ or as shown in terms of the action of the momenta p^μ. It was shown in Ref. 2 that by using adjusted derivatives $L^{-1/2}\partial^\mu$ where

$$L\psi =: \psi(x,t+\imath\lambda) := e^{-\lambda p^0}\psi$$

the 4D Laplacian $\Box = L^{-1}((\partial^0)^2 - \Sigma_i(\partial^i)^2)$ acts on plane waves as

$$\Box = -\frac{2}{\lambda^2}(\cosh(\lambda p^0)-1) + \vec{p}^2 e^{\lambda p^0} = e^{\lambda p^0}\left(\vec{p}^2 - \frac{1}{\lambda^2}(1-e^{-\lambda p^0})^2\right) \tag{A2}$$

which is the action of the Casimir of the bicrossproduct quantum group. The first expression should be compared with (13) in our previous model, as a hyperbolic version of it.

We recall that this bicrossproduct Poincaré quantum group $U(\mathrm{so}_{1,3})\triangleright\!\blacktriangleleft \mathbb{C}[B_+]$ in terms of translation generators p^μ, rotations M_i and boosts N_i, is[20]

$$[p^\mu,p^\nu]=0, \quad [M_i,M_j]=\imath\epsilon_{ij}{}^k M_k,$$

$$[N_i,N_j]=-\imath\epsilon_{ij}{}^k M_k, \quad [M_i,N_j]=\imath\epsilon_{ij}{}^k N_k,$$

$$[p^0,M_i]=0, \quad [p^i,M_j]=\imath\epsilon^i{}_{jk}p^k, \quad [p^0,N_i]=-\imath p_i,$$

as usual, and the modified relations and coproduct

$$[p^i,N_j]=-\frac{\imath}{2}\delta^i_j\left(\frac{1-e^{-2\lambda p^0}}{\lambda}+\lambda\vec{p}^2\right)+\imath\lambda p^i p_j,$$

$$\Delta N_i = N_i\otimes 1 + e^{-\lambda p^0}\otimes N_i + \lambda\epsilon_{ijk}p^j\otimes M_k,$$

$$\Delta p^i = p^i\otimes 1 + e^{-\lambda p^0}\otimes p^i$$

and the usual linear ones on p^0, M_i. We raise and lower i,j,k indices using the Euclidean metric. It follows from the general theory of bicrossproducts that this Hopf algebra acts on $U(b_+)=\mathbb{R}^{1,3}_\lambda$.

Part of the motivation for this model[20] consisting of noncommutative spacetime and associated bicrossproduct quantum group acting covariantly on it was a previous "κ-Poincaré" version of the Hopf algebra alone obtained[11] in another context (by contraction of $U_q(\mathrm{so}_{2,3})$). The bicrossproduct model should not be confused with this, however, because its generators and relations are fundamentally different and have very different physical content; for example the Lorentz generators in Ref. 11 do not close among themselves but mix with momentum. Moreover, prior to Ref. 20 there was either no action of κ-Poincaré on any spacetime or it was taken to act on classical Minkowski space with inconsistent results (there is no such covariant action).

Also key and fundamentally different in the bicrossproduct model from κ-Poincaré is that in the bicrossproduct case the Lorentz group is actually undeformed; rather the deformation is in a nonlinear but entirely geometrical action of it on the "curved" momentum group B_+. This is as part of the solution of a nonlinear set of "matched pair" equations[13] (the other part of the matched pair is a "backreaction" of B_+ on the manifold of the Lorentz group). Because of this fundamental difference it would be a mistake to view the bicrossproduct quantum group as merely a "change of basis" from κ-Poincaré. In particular, because of the classical geometry behind it one can see what

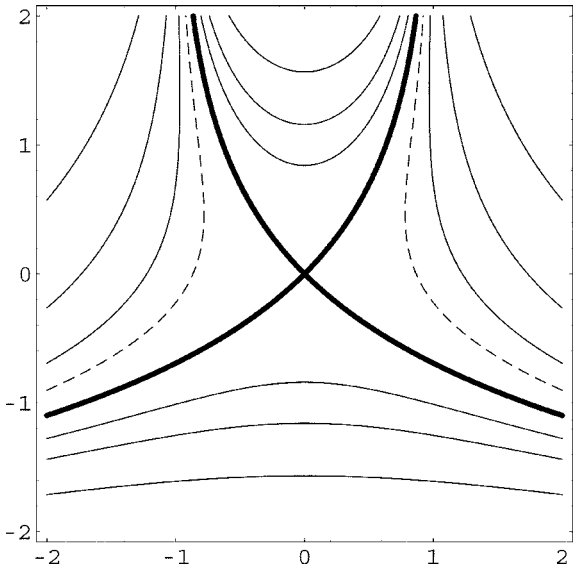

FIG. 1. Deformed mass-shell orbits in the bicrossproduct curved momentum space for $\lambda=1$.

is going on in terms of the curved momentum space, as shown in Fig. 1, which is a contour plot of p^0 against $|\vec{p}|$. The nonlinear action of the Lorentz group means that Lorentz group orbits in B_+ are now deformed hyperboloids. Because neither group here is compact one expects again from the general theory of bicrossproducts to have limiting accumulation regions and we see that indeed the $p^0>0$ mass shells are now cups with almost vertical walls, compressed into the vertical tube $|\vec{p}|<\lambda^{-1}$. In other words, the 3-momentum is bounded above by the Planck momentum scale (if λ is the Planck time), but this does not appear as a new "second bound" in addition to Einstein's postulate on the speed of light as sometimes claimed in the literature, but rather a deformation of it.

Such accumulation regions were already visible in the simplest "Planck-scale Hopf algebra"[13] from the 1980s under a different point of view. Under this point of view p^i above are position and not momentum coordinates and the quantum group is the algebra of obervables for a quantum particle moving on oribits under (in the present case Lorentz) group action. The flows for this action are geodesics on the orbits, which fit together to a natural 4D space that could be called a "pseudo-black hole." Here the physical region of Fig. 1 is the orbits that come in from spatial infinity and remain outside the tapered cylinder of radius $1/\lambda$. One such orbit comes in at large positions, bends upwards and asymptotically approaches the cylinder from the outside for large t (which points upwards), much as for an event horizon. Another orbit (dashed) crosses the asymptote and approaches it from the inside. The detailed geometry of this setup will be presented elsewhere. Such coordinate singularities are a generic feature of the nonlinear "matched pair" equations behind the model and is the reason that they were proposed in Ref. 13 as a toy version of Einstein's equations.

Finally, we point out what does not appear to be well known that the above-mentioned bicrossproduct is part of a family of which the 3D Euclidean bicrossproduct $\mathbb{C}[B_+]\blacktriangleright\!\!\triangleleft U(\mathrm{su}_2)$ was already obtained in the 1980s in Refs. 12, 14, and 15 actually as a Hopf–von-Neuman algebra and which has the following algebraic structure. First, B_+ is now a 3D version of the same solvable group, with Lie algebra

$$[x_3,x_i]=\imath\lambda x_i,\quad [x_i,x_j]=0 \tag{A3}$$

for $i=1,2$. This Lie algebra (with generators denoted $\{l_i\}$) and the required nonlinear solution of the matched pair equations are in Ref. 14. The original interpretation of $\mathbb{C}[B_+]\blacktriangleright\!\!\triangleleft U(\mathrm{su}_2)$ was different (namely particles moving in orbits in B_+ as position space) but there is of course nothing

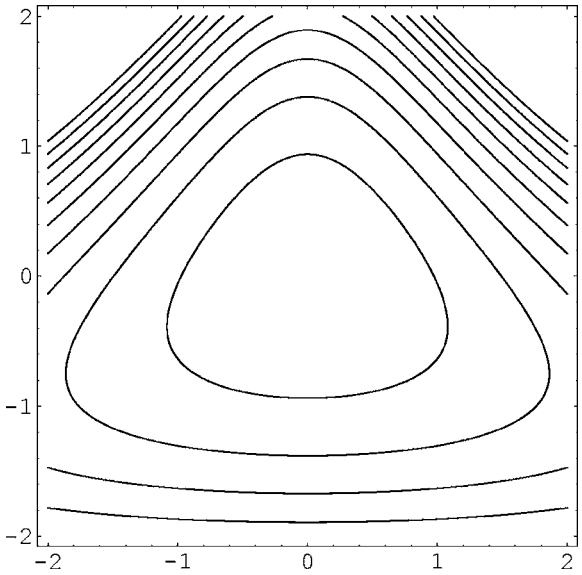

FIG. 2. Deformed spherical orbits in the 3D bicrossproduct model for $\lambda=1$.

stopping one considering it as a deformation of the group of motions on $\mathbb{R}^3$. The only difference is to denote the generators of $\mathbb{C}[B_+]$ by the symbols p^i, which we also combine with a cosmetic change to a logarithmic coordinate and explication of the deformation parameter, i.e.,

$$e^{-\lambda p_3}=\frac{1}{X_3+1},\quad \lambda p_i=\frac{X_i}{X_3+1}$$

in terms of the B_+ coordinates $\{X_i\}$ written in lower case in Refs. 16 and 17. We reserve x_i instead for the auxiliary noncommutative space (A3) on which the quantum group necessarily acts. Then the bicrossproduct has the form

$$[p_i,p_j]=0,\quad [M_i,M_j]=\imath\epsilon_{ij}{}^kM_k,$$

$$[M_3,p_j]=\imath\epsilon_{3j}{}^kp_k,\quad [M_i,p_3]=\imath\epsilon_{i3}{}^kp_k$$

as usual, for $i,j=1,2,3$, and the modified relations

$$[M_i,p_j]=\frac{\imath}{2}\epsilon_{ij}{}^3\left(\frac{1-e^{-2\lambda p_3}}{\lambda}-\lambda\vec{p}^2\right)+\imath\lambda\epsilon_{ij}{}^3p_jp_k$$

for $i,j=1,2$ and $\vec{p}^2=p_1^2+p_2^2$. The coproducts are

$$\Delta M_i=M_i\otimes e^{-\lambda p_3}+\lambda M_3\otimes p_i+1\otimes M_i,$$

$$\Delta p_i=p_i\otimes e^{-\lambda p_3}+1\otimes p_i$$

for $i=1,2$ and the usual linear ones for p_3, M_3.

The deformed spherical orbits under the nonlinear rotation in B_+ are constant values of the Casimir for the above algebra. This is found in Ref. 14 as

$$\frac{2}{\lambda^2}(\cosh(\lambda p_3) - 1) + \vec{p}^2 e^{\lambda p_3}$$

in our present coordinates, which is the Euclidean precursor to (A2). These deformed orbits are shown in Fig. 2. The model here is a Euclidean inhomogeneous one. The noncommutative differential geometry on (A3) is broadly similar to the 4D case.

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Analytic and contour representations in the unit disk based on SU(1,1) coherent states

C. Lei and A. Vourdas
Department of Computing, University of Bradford, Bradford BD7 1DP, United Kingdom

A. Wünsche
Institut für Physik, Humboldt-Universität, Newtonstrasse 15, 12489 Berlin, Germany

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A contour representation in the unit disk based on SU(1,1) coherent states is introduced. The scalar product is given by a contour integral. The regions of convergence of the functions representing ket and bra states are studied. An analytic representation in the unit disk is also considered, where the scalar product is represented by an integral over the unit disk, with the Lobachevsky measure. Various relations which connect these analytic functions with other phase-space quantities are derived. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2098527]

I. INTRODUCTION

Analytic representations are a powerful mathematical tool in quantum mechanics. The most familiar example is the Bargmann analytic representation in the Euclidean plane.[1] This is intimately connected to the Glauber coherent states.

Another analytic representation is the "elliptic analytic representation" in the extended complex plane (which is topologically equivalent to a sphere).[2] This is intimately connected to SU(2) coherent states.

Another analytic representation is the "hyperbolic analytic representation" in the unit disk (or half-plane).[3–11] This is intimately connected to SU(1,1) coherent states.

To each of these analytic representations corresponds a "contour representation." They represent the ket states with the same function as the corresponding analytic representation; but they represent the bra states with a different function so that the scalar product is given by a contour integral. Dirac[12] and later other authors[13,14] studied extensively the "Euclidean contour representation." The "elliptic contour representation" in the extended complex plane has been presented in Ref. 15. A preliminary work for the "hyperbolic contour representation" in the unit disk has been presented in Ref. 16 An important problem in this representation is the regions of convergence of the series that represent the ket and bra states.

The purpose of the present paper is to study analytic and contour representations in the unit disk, with emphasis on the relationship among them and also on their relationship with other phase-space quantities like the P, Q, and Wigner functions. In Sec. II we present briefly SU(1,1) coherent states and we define the notation. In Sec. III we study the analytic representation in the unit disk. The requirement for convergent scalar products leads to constraints on the growth of these functions near the unit circle. In Sec. IV we discuss the contour representation in the unit disk. We study carefully the regions of convergence of the functions representing ket and bra states. In order to express the scalar products as contour integrals, the region of convergence of the ket states should overlap with the region of convergence of the bra states. Although this is not always true, we find large subspaces within the full Hilbert space where this is the case. In Sec. V we derive relations which connect the analytic functions with other phase-space quantities. In Sec. VI we discuss briefly some physical applications. We give a Hamiltonian which is a combination of SU(1,1) generators and which is used to describe optical amplifiers. The time evolution of systems with this Hamiltonian can be studied using the contour representation in the unit disk. We conclude in Sec. VII with a discussion of our results. In the Appendix we present briefly the

elliptic contour representation in the extended complex plane in connection with the SU(2) group, so that the reader can compare and contrast the hyperbolic with the elliptic contour representation.

II. SU(1,1) COHERENT STATES

The representations of SU(1,1) have been studied in detail in Ref. 17 (see also Ref. 10). They are classified into the continuous series, the discrete series, and the supplementary. In this paper we are interested in the discrete series.

We consider the SU(1,1) generators K_0, K_+, K_- which obey the commutation relations

$$[K_0, K_\pm] = \pm K_\pm, \quad [K_-, K_+] = 2K_0,$$

$$K^2 = K_0^2 - \frac{1}{2}(K_+K_- + K_-K_+). \tag{1}$$

The operator K^2 is a Casimir operator. We also consider the standard basis $|k,n\rangle$

$$K^2|k,n\rangle = k(k-1)|k,n\rangle,$$

$$K_0|k,n\rangle = (k+n)|k,n\rangle,$$

$$K_-|k,n\rangle = [n(n+2k-1)]^{1/2}|k,n-1\rangle,$$

$$K_+|k,n\rangle = [(n+1)(n+2k)]^{1/2}|k,n+1\rangle, \quad k = 1/2, 1, 3/2, \ldots, \quad n = 0, 1, 2, \ldots, \tag{2}$$

where k characterizes the representation.

Coherent states in the unit disk $D(|z|<1)$ [which is related to $\mathrm{SU}(1,1)/U(1)$] are defined as follows:

$$|k,z\rangle = (1-|z|^2)^k \sum_{n=0}^{\infty} d(k,n) z^n |k,n\rangle, \tag{3}$$

$$d(k,n) = \left[\frac{\Gamma(n+2k)}{\Gamma(n+1)\Gamma(2k)}\right]^{1/2}. \tag{4}$$

An alternative equivalent definition is

$$S(k;\gamma,\theta,\lambda)|k,0\rangle = \exp(i\lambda k)|k,z\rangle, \tag{5}$$

where

$$S(k;\gamma,\theta,\lambda) \equiv S(k;z,\lambda) \equiv \exp\left[-\frac{1}{2}\gamma e^{-i\theta}K_+ + \frac{1}{2}\gamma e^{i\theta}K_-\right]\exp(i\lambda K_0), \tag{6}$$

$$z = -\tanh\frac{\gamma}{2}e^{-i(\lambda-\theta)}. \tag{7}$$

The overlap between two coherent states is given by

$$\langle k,z|k,w\rangle = \frac{(1-|z|^2)^k(1-|w|^2)^k}{(1-z^*w)^{2k}}. \tag{8}$$

The resolution of the identity of these states is given by

$$\frac{2k-1}{\pi}\int_D |k,z\rangle\langle k,z| d\mu(z) = \mathbf{1}; \quad d\mu(z) = (1-|z|^2)^{-2} d^2 z. \tag{9}$$

An interesting relation that involves the integration of $S(k;z,0)$ over the unit disk is

$$\frac{2k}{\pi}\int_D d\mu(z)(1-|z|^2)^{k+1} S(k;z,0) = |k,0\rangle\langle k,0|. \tag{10}$$

III. ANALYTIC REPRESENTATION IN THE UNIT DISK

A. Quantum states

We consider an arbitrary normalized state

$$|f\rangle = \sum_{n=0}^{\infty} f_n |k,n\rangle; \quad \langle f| = \sum_{n=0}^{\infty} f_n^* \langle k,n|; \quad \sum_{n=0}^{\infty} |f_n|^2 = 1. \tag{11}$$

This state is represented by the analytic function $f(z;k)$ defined as

$$f(z;k) = \sum_{n=0}^{\infty} f_n d(k,n) z^n = (1-|z|^2)^{-k} \langle k, z^*|f\rangle. \tag{12}$$

The scalar product of two such states is given by

$$\langle f|g\rangle = \sum_{N=0}^{\infty} f_N^* g_N = \frac{2k-1}{\pi}\int_D f^*(z;k) g(z;k)(1-|z|^2)^{2k} d\mu(z). \tag{13}$$

Convergence of this integral puts restrictions on the growth of the analytic functions near the unit circle. For an analytic function f in $\mathcal{D}$, we define its hyperbolic exponential type,[18]

$$t(f) = \lim_{|z|\to 1^-} \sup \frac{\log|f(z)|}{\log \dfrac{1}{1-|z|}}. \tag{14}$$

In our case $t(f) \leqslant k-1$.

Using Eq. (10), we prove that

$$\frac{2k}{\pi}\int_D d\mu(z)(1-|z|^2)^{2k+1} f(z;k) = f_0. \tag{15}$$

As examples, we easily show that

$$|k,n\rangle \to d(k,n) z^n, \tag{16}$$

$$|k,w\rangle \to \frac{(1-|w|^2)^k}{(1-zw)^{2k}}. \tag{17}$$

B. SU(1,1) transformations as Möbius mappings

SU(1,1) transformations in the unit disk are implemented through Mobius conformal mappings

$$w = \frac{az+b}{b^* z + a^*}; \quad |a|^2 - |b|^2 = 1. \tag{18}$$

The operators K_+, K_-, K_0 can be represented with the differential operators

$$K_+ = z^2\partial_z + 2kz, \quad K_0 = z\partial_z + k, \quad K_- = \partial_z. \tag{19}$$

Then, the transformations

$$|f\rangle \to S(k;\gamma,\theta,\lambda)|f\rangle, \tag{20}$$

are implemented as

$$f(z;k) \to f\left(\frac{az+b}{b^* z + a^*};k\right)(b^* z + a^*)^{-2k}, \tag{21}$$

where

$$a = e^{i\lambda}\cosh\frac{\gamma}{2}, \quad b = e^{i\theta}\sinh\frac{\gamma}{2}. \tag{22}$$

C. Parity transformations

We first consider reflections around some point w in the unit disk. A point ζ is transformed to the point

$$\xi = \frac{-(1+|w|^2)\zeta + 2w}{-2w^*\zeta + (1+|w|^2)}, \tag{23}$$

which is also in the unit disk.

The parity operator around the origin U_0 is defined as

$$U_0 = \sum_n (-1)^n |k,n\rangle\langle k,n|. \tag{24}$$

The displaced parity operator around a point w, is defined as

$$U(w) = S(k;\gamma,\theta,\lambda)U_0 S^\dagger(k;\gamma,\theta,\lambda); \quad w = -\tanh\frac{\gamma}{2}e^{-i(\lambda-\theta)}. \tag{25}$$

Acting on coherent states with it, we get[19]

$$U(w)|k,\zeta\rangle = |k,\xi\rangle. \tag{26}$$

For later use, we prove that

$$U(w;z_1,z_2) \equiv \langle k,z_1|U(w)|k,z_2\rangle = \frac{(1-|z_1|^2)^k(1-|z_2|^2)^k(1-|w|^2)^{2k}}{[(w-z_2)(w^*-z_1^*)+(1-w^* z_2)(1-wz_1^*)]^{2k}}. \tag{27}$$

Using the displaced parity operator, we can define the Wigner function of an arbitrary operator Θ as

$$W(\Theta;z) = \mathrm{Tr}(\Theta U(z)). \tag{28}$$

D. Operators

An arbitrary operator Θ

$$\Theta = \sum_{m,n=0}^{\infty} \Theta_{mn} |k,m\rangle\langle k,n|, \tag{29}$$

can be represented as follows:

$$A(z_1,z_2^*;\Theta) \equiv [(1-|z_1|^2)(1-|z_2|^2)]^{-k}\langle k,z_1^*|\Theta|k,z_2^*\rangle = \sum_{m,n=0}^{\infty} d(k,m)d(k,n)\Theta_{mn} z_1^m z_2^{*n}, \tag{30}$$

where A indicates "analytic" representation. The state $\Theta|f\rangle$ is then represented by the function

$$\frac{2k-1}{\pi}\int_D A(z,w^*;\Theta) f(w)(1-|w|^2)^{2k} d\mu(w). \tag{31}$$

Convergence of this integral implies that $t(A) \leqslant k-1$ [where $t(A)$ has been defined in Eq. (14)].

The product $\Theta = \Theta_1\Theta_2$ of two operators is given by

$$A(z_1,z_2^*;\Theta) = \frac{2k-1}{\pi}\int_D d\mu(z_3)(1-|z_3|^2)^{2k} A(z_1,z_3^*;\Theta_1)A(z_3,z_2^*;\Theta_2). \tag{32}$$

As an axample we consider the unit operator $\mathbf{1}$, $\Theta_{mn} = \delta_{mn}$ and

$$A(z_1,z_2;\mathbf{1}) = (1-z_1 z_2^*)^{-2k}. \tag{33}$$

We also consider the operators K_0, K_+, K_- which are represented by the kernels

$$A(z_1,z_2^*;K_0) = \frac{2k[-(z_1z_2^*)^2 + z_1z_2^* + 1]}{(1-z_1z_2^*)^{2k}},$$

$$A(z_1,z_2^*;K_+) = 2kz_1(1-z_1z_2^*)^{-(2k-1)},$$

$$A(z_1,z_2^*;K_-) = 2kz_2^*(1-z_1z_2^*)^{-(2k-1)}. \tag{34}$$

These integral representations are consistent with the differential representations of Eq. (19). Indeed, we can prove

$$\frac{2k-1}{\pi}\int_D d\mu(w)(1-|w|^2)^{2k} A(z,w^*;K_0) f(w) = (z\partial_z + k) f(z),$$

$$\frac{2k-1}{\pi}\int_D d\mu(w)(1-|w|^2)^{2k} A(z,w^*;K_+) f(w) = (z^2\partial_z + 2kz) f(z),$$

$$\frac{2k-1}{\pi}\int_D d\mu(w)(1-|w|^2)^{2k} A(z,w^*;K_-) f(w) = \partial_z f(z). \tag{35}$$

We first prove these relations for $f(w) = d(k,N)w^N$; then, summation proves the general result.

The trace of operator Θ can be expressed as

$$\mathrm{Tr}\Theta = \frac{2k-1}{\pi}\int_D d\mu(z)(1-|z|^2)^{2k} A(z,z^*;\Theta), \tag{36}$$

and the trace of product of two operators can be similarly expressed as

$$\mathrm{Tr}(\Theta_1\Theta_2)=\frac{(2k-1)^2}{\pi^2}\int_D d\mu(z)\int_D d\mu(z')(1-|z|^2)^{2k}(1-|z'|^2)^{2k}A(z,z'^*;\Theta_1)A(z',z^*;\Theta_2). \tag{37}$$

IV. HYPERBOLIC CONTOUR REPRESENTATION IN THE UNIT DISK

Dirac[12] introduced a contour representation in the Euclidean plane in which ket states are represented with analytic functions and bra states are represented with functions which are analytic in some region $|z|>R$ (where R depends on the state). In this representation the scalar product is a contour integral. Several authors[13,14] have discussed this method further in the Euclidean plane. The contour representation in the extended complex plane $C\cup\infty$ [which is topologically equivalent to a sphere, and is related to the SU(2)/U(1)], has been discussed in Ref. 15.

In this paper we study this method in the unit disk. We stress that in the unit disk there are convergence difficulties, and we need to define very carefully the regions of convergence of the various functions. This is the central problem in this paper. In contrast, in the SU(2) case we have polynomials and there are no convergence difficulties. In the Appendix we present briefly the contour representation for the SU(2) case so that the reader can compare and contrast it with the SU(1,1) case.

A. Quantum states

We consider the (arbitrary) normalized state of Eq. (11). In the contour representation it is represented as

$$|f\rangle\rightarrow f_k(z;k)=\sum_n f_n d(k,n)z^n, \tag{38}$$

$$\langle f|\rightarrow f_b(z;k)=\sum_n f_n^* d(k,n)^{-1}z^{-n-1}, \tag{39}$$

where the indices k and b refer to ket and bra, respectively. The function $f_k(z;k)$ is identical to that in Eq. (12). In order to study the convergence of the series associated with $f_k(z;k)$, we use the convergence criterion of the limit of the ratio of two successive terms. This ratio is

$$r_N=\frac{|f_{N+1}|}{|f_N|}\left[\frac{N+2k}{N+1}\right]^{1/2}|z|. \tag{40}$$

Since $\Sigma|f_N|^2=1$, the limit of the ratio $|f_{N+1}|/|f_N|$ does not exceed 1. Therefore, the $f_k(z;k)$ always converges in the unit disk. We next consider the case

$$\lim_{N\rightarrow\infty}\frac{|f_{N+1}|}{|f_N|}=1-\epsilon;\quad 0<\epsilon\leqslant 1. \tag{41}$$

Then, the $f_k(z;k)$ of the corresponding states also converges in the annulus $1<|z|<(1-\epsilon)^{-1}$ outside the unit disk. We call $\mathcal{H}_\epsilon$ the space

$$\mathcal{H}_\epsilon=\left\{|f\rangle:\lim_{N\rightarrow\infty}\frac{|f_{N+1}|}{|f_N|}\leqslant 1-\epsilon\right\}. \tag{42}$$

It is easily seen that when $\epsilon'>\epsilon$, then $\mathcal{H}_{\epsilon'}$ is a subspace of $\mathcal{H}_\epsilon$.

We next study the covergence of the series associated with $f_b(z;k)$. In this case the ratio of two successive terms is

$$r_N = \frac{|f_{N+1}|}{|f_N|}\left[\frac{N+1}{N+2k}\right]^{1/2}\frac{1}{|z|}. \tag{43}$$

Therefore, the $f_b(z;k)$ always converges in the exterior of the unit disk. For the states which satisfy Eq. (42) we easily see that the $f_b(z;k)$ also converges in the annulus $1>|z|>1-\epsilon$ within the unit disk. Therefore, for the states in the space $\mathcal{H}_\epsilon$ both the $f_k(z;k)$ and the $f_b(z;k)$ converge, at least within the annulus

$$\mathcal{R}_\epsilon = \left\{1-\epsilon<|z|<\frac{1}{1-\epsilon}\right\}. \tag{44}$$

Of course, there are many states for which the limit of the ratio $|f_{N+1}|/|f_N|$ is 1 and for which the $f_k(z;k)$ diverges outside the unit disk; also, the $f_b(z;k)$ diverges within the unit disk. Therefore, for any positive ϵ the space $\mathcal{H}_\epsilon$ is *not* dense in the full Hilbert space.

We consider the following example:

$$|k,n\rangle \to f_k(z;k) = d(k,n)z^n, \tag{45}$$

$$\langle k,n| \to f_b(z;k) = d(k,n)^{-1}z^{-n-1}. \tag{46}$$

In this example the $f_k(z;k)$ converges in the whole plane (it has singularity at infinity), and the $f_b(z;k)$ converges in the whole plane with a singularity at zero. The same result is true for any state which is a superposition of a *finite* number of $|k;k+N\rangle$ states.

We also consider the coherent states example

$$|k,\zeta\rangle \to f_k(z;k) = \frac{(1-|\zeta|^2)^k}{(1-z\zeta)^{2k}},$$

$$\langle k,\zeta| \to f_b(z;k) = (1-|\zeta|^2)^k\sum_{n=0}^{\infty}\frac{\zeta^n}{z^{n+1}} = \frac{(1-|\zeta|^2)^k}{z-\zeta}. \tag{47}$$

In this example the $f_k(z;k)$ converges in the disk $|z|<|\zeta|^{-1}$, which is larger than the unit disk (since $|\zeta|<1$). The $f_b(z;k)$ converges for $|z|>|\zeta|$.

We next show that for the states in the space $\mathcal{H}_\epsilon$

$$\oint_{c\in\mathcal{R}_\epsilon}\frac{dw}{2\pi i}f_b(w;k)(1-z^*w)^{-2k} = [f_k(z;k)]^*, \tag{48}$$

where c is an anticlockwise contour within the annulus $\mathcal{R}_\epsilon$ which does not enclose the singularity $w=1/z^*$.

The inverse formula is given by

$$\frac{2k-1}{z}\int_0^\infty\frac{dt}{(1+t)^{n+2k}}\left[f_k\left(\frac{t}{z^*};k\right)\right]^* = f_b(z;k), \quad k>\frac{1}{2}. \tag{49}$$

These two relations show how we calculate $f_k(z;k)$ if we know $f_b(z;k)$, and vice versa. In order to prove these relations we first perform the integrations for the case $f(w)=d(k,N)w^N$; summation then proves the general result.

We next consider two states $|f\rangle, |g\rangle$ in the space $\mathcal{H}_\epsilon$. The inner product is given by

$$\langle f|g\rangle = \oint_{c\in\mathcal{R}_\epsilon}\frac{dz}{2\pi i}f_b(z;k)g_k(z;k) = \sum_N f_N^* g_N, \tag{50}$$

where c is an anticlockwise contour within the annulus $\mathcal{R}_\epsilon$.

B. Operators

An arbitary operator

$$\Theta = \sum_{mn} \Theta_{mn} |k,m\rangle\langle k,n|, \tag{51}$$

is represented as follows:

$$C(z_1,z_2;\Theta) = \sum_{mn} \frac{\Theta_{mn} d(k,m) z_1^m}{d(k,n) z_2^{n+1}}, \tag{52}$$

where C indicates the "contour" representation. This function is useful if the double series converges in some region $\mathcal{A}_1(\Theta)\times\mathcal{A}_2(\Theta)$, where z_1 takes values in $\mathcal{A}_1(\Theta)$ and z_2 takes values in $\mathcal{A}_2(\Theta)$.

For a state in $\mathcal{H}_\epsilon$, the ket state $\Theta|f\rangle$ is given by

$$\oint_c \frac{d\zeta}{2\pi i} C(z,\zeta;\Theta) f_k(\zeta), \tag{53}$$

where c is an anticlockwise contour enclosing the singularities in $\mathcal{A}_2(\Theta)\cap\mathcal{R}_\epsilon$. The bra state $\langle f|\Theta$ is given by

$$\oint_c \frac{d(w)}{2\pi i} f_b(w;k) C(w,z;\Theta), \tag{54}$$

where c is an anticlockwise contour enclosing the singularities in $\mathcal{R}_\epsilon\cap\mathcal{A}_1(\Theta)$.

We next show that the product $\Theta=\Theta_1\Theta_2$ of two operators is given by

$$C(z_1,z_2;\Theta) = \oint_c \frac{dw}{2\pi i} C(z_1,w;\Theta_1) C(w,z_2;\Theta_2), \tag{55}$$

where c is an anticlockwise contour enclosing the singularities in $\mathcal{A}_2(\Theta_1)\cap\mathcal{A}_1(\Theta_2)$.

For the unit operator $\mathbf{1}$, $\Theta_{mn}=\delta_{mn}$ and

$$C(z_1,z_2;\mathbf{1}) = \frac{1}{z_2 - z_1} \quad |z_1| < |z_2|. \tag{56}$$

In the case $|z_1|\geqslant|z_2|$ the sum of Eq. (52) diverges. In this example $\mathcal{A}_1(\mathbf{1})=\{|z_1|<R\}$ and $\mathcal{A}_2(\mathbf{1})=\{|z_2|>R\}$ for arbitrary R.

Similarly, we calculate the representations of the operators K_0, K_+, K_-

$$C(z_1,z_2;K_0) = \frac{kz_2 + (1-k)z_1}{(z_2 - z_1)^2} \quad |z_1| < |z_2|, \tag{57}$$

$$C(z_1,z_2;K_+) = \frac{(1-2k)z_1^2 + 2kz_2z_1}{(z_2 - z_1)^2} \quad |z_1| < |z_2|, \tag{58}$$

$$C(z_1,z_2;K_-) = \frac{1}{(z_2 - z_1)^2} \quad |z_1| < |z_2|. \tag{59}$$

In these examples also $\mathcal{A}_1=\{|z_1|<R\}$ and $\mathcal{A}_2=\{|z_2|>R\}$ for arbitrary R. We note that the operators K_0, K_+, K_- can also be represented with the differential operators of Eq. (19); consistency between the two representations is proved with the following relations:

$$\oint_c \frac{d\zeta}{2\pi i} C(z,\zeta;K_0) f(\zeta) = (z\partial_z + k) f(z),$$

$$\oint_c \frac{d\zeta}{2\pi i} C(z,\zeta;K_+) f(\zeta) = (z^2\partial_z + 2kz) f(z),$$

$$\oint_c \frac{d\zeta}{2\pi i} C(z,\zeta;K_-) f(\zeta) = \partial_z f(z). \tag{60}$$

V. RELATIONSHIP BETWEEN THE VARIOUS REPRESENTATIONS

The Q and P representations of an arbitrary operator Θ are defined as follows:

$$Q(\Theta;z) = \langle k,z|\Theta|k,z\rangle, \tag{61}$$

$$\Theta = \frac{2k-1}{\pi} \int d\mu(z) P(\Theta;z) |k,z\rangle\langle k,z|. \tag{62}$$

It is easily seen that the trace of an operator is given by

$$\mathrm{Tr}\Theta = \frac{2k-1}{\pi} \int_D d\mu(z) Q(\Theta;z), \tag{63}$$

and also that the trace of the product of two operators is given by

$$\mathrm{Tr}(\Theta_1\Theta_2) = \frac{2k-1}{\pi} \int_D d\mu(z) P(\Theta_1;z) Q(\Theta_2;z). \tag{64}$$

In this section we derive relationships between $A(z_1,z_2;\Theta)$, $C(z_1,z_2;\Theta)$ and the $Q(\Theta;z)$ and $P(\Theta;z)$.

We first combine Eqs. (61) and (62) and prove easily that for $k>1/2$

$$Q(\Theta;z) = \frac{2k-1}{\pi} \int_D d\mu(w) P(\Theta;w) \frac{[(1-|z|^2)(1-|w|^2)]^{2k}}{|1-z^*w|^{4k}}. \tag{65}$$

We also combine Eqs. (30), (62), and (8), and prove that for $k>1/2$

$$A(z_1,z_2^*;\Theta) = \frac{2k-1}{\pi} \int_D d\mu(z) P(\Theta;z) \frac{(1-|z|^2)^{2k}}{(1-z_1z)^{2k}(1-z^*z_2^*)^{2k}}. \tag{66}$$

Equations (30) and (61) show easily that

$$Q(\Theta;z) = (1-|z|^2)^{2k} A(z^*,z;\Theta). \tag{67}$$

We next study the relatioship between the two analytic representations. Equations (48) and (52) show that

$$\oint_c \frac{dw}{2\pi i} C(\zeta,w;\Theta)(1-z^*w)^{-2k} = A(\zeta,z^*;\Theta), \tag{68}$$

where c is an anticlockwise contour within the annulus $\mathcal{A}_2(\Theta)$ which does not enclose the singularity $w=1/z^*$. From this, we easily see that

$$Q(\Theta;z)=(1-|z|^2)^{2k}\oint_c \frac{dw}{2\pi i}C(z^*,w;\Theta)(1-z^*w)^{-2k}, \tag{69}$$

The inverse of Eq. (68) is found by using Eqs. (49) and (52) to prove

$$\frac{2k-1}{z}\int_0^\infty \frac{dt}{(1+t)^{n+2k}}A\left(\zeta,\frac{t}{z};\Theta\right)=C(\zeta,z;\Theta),\quad k>\frac{1}{2}. \tag{70}$$

The relationship between $W(\Theta;z)$ and $P(\Theta;w)$ is found by using Eqs. (28) and (64) to prove

$$W(\Theta;z)=\frac{2k-1}{\pi}\int_D d\mu(w)P(\Theta;w)U(z;w,w). \tag{71}$$

Using Eqs. (37) and (30), we get the Wigner function $W(\Theta;z)$ in terms of the $A(z_1,z_2^*;\Theta)$

$$W(\Theta;z)=\frac{(2k-1)^2}{\pi^2}\int_D d\mu(z_1)\int_D d\mu(z_2)A(z_1,z_2^*;\Theta)U(z;z_2^*,z_1^*). \tag{72}$$

From this we easily prove that

$$W(\Theta;z)=\frac{(2k-1)^2}{\pi^2}\oint_c \frac{dz_3}{2\pi i}\int_D d\mu(z_1)\int_D d\mu(z_2)(1-z_2^*z_3)^{-2k}\times C(z_1,z_3;\Theta)U(z;z_2^*,z_1^*), \tag{73}$$

where c is an anticlockwise contour within the annulus $\mathcal{A}_2(\Theta)$ which does not enclose the singularity $z_3=1/z_2^*$.

VI. APPLICATIONS

In many quantum optics problems related to amplifiers, we have two-mode Hamiltonians of the type

$$h=\omega_1 a_1^\dagger a_1+\omega_2 a_2^\dagger a_2+\lambda a_1 a_2+\lambda^* a_1^\dagger a_2^\dagger, \tag{74}$$

where $a_1^\dagger, a_1$, and $a_2^\dagger, a_2$ are creation and annihilation operators. These Hamiltonians can be studied with the formalism developed in this paper.

We first point out the connection of the various terms in the Hamiltonian of Eq. (74) to the SU(1,1) generators

$$K_+=a_1^\dagger a_2^\dagger;\quad K_-=a_1 a_2,$$

$$K_0=\frac{1}{2}(a_1^\dagger a_1+a_2^\dagger a_2+1),$$

$$K^2=\frac{1}{4}K_C^2-\frac{1}{4};\quad K_C=a_1^\dagger a_1-a_2^\dagger a_2,$$

$$[K_C,K_0]=[K_C,K_+]=[K_C,K_-]=0. \tag{75}$$

The Hamiltonian can now be written as

$$h = (\omega_1 + \omega_2)\left(K_0 - \frac{1}{2}\right) + \frac{1}{2}(\omega_1 - \omega_2)K_C + \lambda K_- + \lambda^* K_+. \tag{76}$$

SU(1,1) techniques have been used extensively in the study of the time evolution of systems with this Hamiltonian (e.g., Ref. 20). The contour representation studied in this paper can be used for the study of these systems.

VII. DISCUSSION

We have studied an analytic representation in the unit disk, and the corresponding contour representation. They are both related to the SU(1,1) group and the corresponding coherent states.

The contour representation uses the functions $f_k(z;k)$ of Eq. (38) for ket states, and the functions $f_b(z;k)$ of Eq. (39) for bra states. The relationship between $f_k(z;k)$ and $f_b(z;k)$ is given in Eqs. (48) and (49). The analytic representation uses the functions $f(z;k)$ of Eq. (12), which are identical to $f_k(z;k)$. Therefore, Eqs. (48) and (49) also provide the relationship between the analytic representation and the contour representation.

An important task of the paper is to discuss carefully the regions of convergence for these functions, and to find annuli where both $f_k(z;k)$ and $f_b(z;k)$ converge, so that we can write the scalar product in the form of Eq. (50). The operators are represented with analytic functions of two complex variables; again, the regions of convergence are very important and have been discussed explicitly in Sec. IV B.

The relationship between these two representations and other phase-space quantities like the displaced parity operator and the P,Q,W functions has been discussed in Sec. V. The application of hyperbolic contour representation in the study of the time evolution of optical amplifiers with the Hamiltonian of Eq. (74) has been discussed in Sec. VI.

The work bridges the gap between the many phases space and analytic approaches to SU(1,1) systems.

APPENDIX: ELLIPTIC CONTOUR REPRESENTATIONS

In this appendix we discuss briefly the elliptic contour representation in the extended complex plane $C \cup \infty$, which is topologically equivalent to a sphere and is related to the $SU(2)/U(1)$.[15] The purpose is to compare and contrast the hyperbolic contour representation in the unit disk, which is the subject of this paper, with the elliptic contour representation in the extended complex plane.

In this case the Hilbert space is $2j+1$-dimensional, and we consider an orthonormal basis of angular momentum states $|j,n\rangle$. SU(2) coherent states are defined as

$$|z\rangle = (1+|z|^2)^{-j} \sum_{n=-j}^{j} d(j,n) z^{j+n} |j,n\rangle; \quad d(j,n) = \left[\frac{(2j)!}{(j+n)!(j-n)!}\right]^{1/2}. \tag{A1}$$

In the elliptic contour representation in the extended complex plane, an arbitrary ket state $|f\rangle$ is represented by the function

$$|f\rangle = \sum_{n=-j}^{j} f_n |j,n\rangle \to f_k(z) = \sum_{n=-j}^{j} d(j,n) f_n z^{j+n}, \tag{A2}$$

and the corresponding bra state $\langle f|$ is represented by the function $f_b(z)$

$$\langle f| = \sum_{n=-j}^{j} f_n^* \langle j,n| \to f_b(z) = \sum_{n=-j}^{j} \frac{f_n^*}{d(j,n) z^{j+n+1}}. \tag{A3}$$

The function $f_k(z)$ is a polynomial of z of order $2j$ and has singularity at ∞ (which is the north pole). The function $f_b(z)$ is a polynomial of z^{-1} of order $2j+1$ and has singularity at 0 (which is the south pole). We stress that all sums here are finite and there are no difficulties with convergence.

In this analytic representation the scalar product is given by

$$\langle f|g\rangle = \oint_C \frac{dz}{2\pi i} f_b(z) g_k(z) = \sum f_n^* g_n, \tag{A4}$$

where C is an anticlockwise contour around the origin, which is the singularity for $f_b(z)$. We stress that in the elliptic contour representation both functions $f_k(z)$ and $f_b(z)$ are well defined for $0 < |z| < \infty$, and we have no difficulty in choosing a contour C. In contrast, in the hyperbolic contour representation there is only the narrow annulus of Eq. (44), where both functions $f_k(z)$ and $f_b(z)$ converge, and the contour has to be restricted within it.

The following transformations take the bra representation to the ket representation and vice versa:[15]

$$\oint_C \frac{dw}{2\pi i} f_b(w)(1 + z^* w)^{2j} = [f_k(z)]^*, \tag{A5}$$

$$\frac{2j+1}{z} \int_0^\infty \frac{dt}{(1+t)^{2j+2}} \left[f_k\left(\frac{t}{z^*}\right) \right]^* = f_b(z). \tag{A6}$$

They should be compared and contrasted to Eqs. (48) and (49).

Relations between P, Q, and the other representations in the SU(2) case have been studied by various authors (e.g., Refs. 15, 21, and 22).

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A general treatment of deformation effects in Hamiltonians for inhomogeneous crystalline materials

B. Lassen and M. Willatzen
Mads Clausen Institute for Product Innovation, University of Southern Denmark, Grundtvigs Allé 150, DK-6400 Sønderborg, Denmark

R. Melnik
Mads Clausen Institute for Product Innovation, University of Southern Denmark, Grundtvigs Allé 150, DK-6400 Sønderborg, Denmark and CRC in Mathematical Modelling, Wilfrid Laurier University, 75 University Avenue West, Waterloo, ON, N2L 3C5 Canada

L. C. Lew Yan Voon
Department of Physics, Wright State University, 3640 Colonel Glenn Hwy., Dayton, OH 43435

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In this paper, a general method of treating Hamiltonians of deformed nanoscale systems is proposed. This method is used to derive a second-order approximation both for the strong and weak formulations of the eigenvalue problem. The weak formulation is needed in order to allow deformations that have discontinuous first derivatives at interfaces between different materials. It is shown that, as long as the deformation is twice differentiable away from interfaces, the weak formulation is equivalent to the strong formulation with appropriate interface boundary conditions. It is also shown that, because the Jacobian of the deformation appears in the weak formulation, the approximations of the weak formulation is not equivalent to the approximations of the strong formulation with interface boundary conditions. The method is applied to two one-dimensional examples (a sinusoidal and a quantum-well potential) and one two-dimensional example (a freestanding quantum wire), where it is shown that the energy eigenvalues of the second-order approximations lie within 1% of the exact energy eigenvalues for a linear strain of up to 9.8%, whereas the first-order approximation has an error of less than 1% for a linear strain of up to 5.5%. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Nanoscale semiconductor devices, such as quantum wells, wires, and dots, usually consist of materials with different lattice constants; hence, these structures will be strained. It is known that strain strongly affects the electronic and optical properties. This has for example been used in band structure engineering of quantum-well systems; see Ref. 1 for a review including theoretical and experimental results. Also, Johnson and Bose[2] have shown the necessity of including strain in the modeling of a system of coupled quantum dots, and it is known that the formation of pyramidal InAs quantum dots on GaAs substrates (self-assembled structures) is driven by the large lattice mismatch between the two semiconductors.[3] Thus, in order to be able to model these devices it is important to account for strain effects. It is well known how to incorporate homogeneous strain in electronic band structure calculations,[4] but in nanoscale heterostructures strain is no longer homogeneous. Zhang[5] and Suzuki[6] have proposed two different methods to include linear inhomogeneous strain terms in the Hamiltonian under certain assumptions for the strain and the potential. In this paper, a general method of treating Hamiltonians of deformed nanoscale systems (e.g., an inhomogeneous strained Hamiltonian) is proposed based on a Taylor series expansion. The advantage of this method is that fewer assumptions for the strain and the Hamiltonian are needed

compared to previous models[4–6] and, in addition, it is easily extended to a higher-order approximation. Finally, because the weak formulation of the problem is used, discontinuities in the gradient of the deformation are handled in an appropriate manner. Higher-order theories for Hamiltonian systems have previously been handled in the literature, e.g., in connection with Lagrangian systems for classical mechanics and field theory; see Ref. 7 and references therein.

In Sec. II, the problem is presented and the Hamiltonian appropriate for calculating the quantum-mechanical energy eigenvalues and corresponding eigenstates is specified. In Sec. II A, the mathematical tools needed to make a Taylor series expansion of the Hamiltonian with respect to a deformation of the system is presented. Section II B is concerned with the derivation of the second-order Taylor series expansion of the Hamiltonian and in Sec. II C the weak formulation of the problem is given, after which the second-order Taylor series expansion is derived for the weak formulation. Finally, in Sec. III, three examples of the application of the method are presented.

II. THEORY

The problem under investigation in this paper is how to model the behavior of an electron in a deformed system in general, and, more specifically, how to model the behavior of an electron in a deformed inhomogeneous crystal structure, based on the Schrödinger equation. Assuming that an undeformed domain $\mathcal{B}\subseteq\mathbb{R}^3$, e.g., a crystal volume, is given, a deformation ϕ: $\mathcal{B}\rightarrow\mathbb{R}^3$ of the undeformed domain $\mathcal{B}$ is defined to be a C^2 map satisfying certain requirements to be specified in the next section. Primed ($'$) coordinates, functions, and operators always refer to the domain $\mathcal{B}$ in the following, while unprimed coordinates, functions, and operators refer to the domain $\phi(\mathcal{B})$.

The deformation of a nanoscale system, as well as any material system in general, is found by minimizing the elastic energy of the system. There are basically two main approaches, an atomic approach[8] and a continuum approach.[9–11] If the deformation has been found using an atomic approach, it is necessary to use the information about how the individual atoms are shifted to construct a C^2 map, but this is outside the scope of this article, i.e., it will just be assumed that the deformation has been found using a continuum approach and that this results in a C^2 map (the C^2 demand will be weakened slightly in Sec. II C).

Assuming that an electron in a potential deformed by ϕ is subject to the potential $\tilde{V}_\phi$, the Hamiltonian of the deformed system, referred to as the deformed Hamiltonian, is given by the Schrödinger equation

$$\tilde{H}_\phi = -\frac{\hbar^2}{2m}\Delta + \tilde{V}_\phi.$$

It should be noted that the potential is a function of the deformed domain $\phi(\mathcal{B})$, i.e., $\tilde{V}_\phi(x)$, where x are coordinates on $\phi(\mathcal{B})$. The energies E and corresponding wave functions ψ are found by solving the eigenvalue equation

$$\tilde{H}_\phi\psi = E\psi, \tag{1}$$

subject to certain boundary conditions. For an electron in a crystal, the most important potential contributions are

$$\tilde{V}_\phi = V_\phi + \hat{H}^{\mathrm{SO}} = V_\phi - i\frac{\hbar^2}{2m^2c^2}(\nabla V_\phi \times \nabla)\cdot\sigma,$$

where V_ϕ is the potential of the deformed crystal without spin, $\hat{H}^{\mathrm{SO}}$ is the spin-orbit part, and σ are the Pauli spin matrices. This is the situation considered in this work, but it should be noted that the procedure can be used on any potential which is a differential function of ϕ in a sense to be defined later. In order to incorporate spin, operators on the function space $\mathcal{F}$ are extended to $\mathcal{F}\times\mathcal{F}$ by operating on each element of the pair separately, e.g., let $f\in\mathcal{F}\times\mathcal{F}$, i.e., $f=\binom{f_+}{f_-}$, where $f_+, f_-\in\mathcal{F}$; then

$$V_\phi f = V_\phi \begin{pmatrix} f_+ \\ f_- \end{pmatrix} = \begin{pmatrix} V_\phi f_+ \\ V_\phi f_- \end{pmatrix}.$$

The function f_+ corresponds to the spin-up state and f_- corresponds to the spin-down state.

The potential of the undeformed domain is usually better known than the potential of the deformed domain. Assuming that the deformation is known, it is therefore advantageous to express the deformed Hamiltonian with respect to the deformation and the undeformed potential. This can be achieved by making a Taylor series expansion of the deformed Hamiltonian with respect to the deformation. In order to do so, the deformed Hamiltonian is written with respect to coordinates on $\mathcal{B}$. This can be done as long as the deformation is invertible with twice differentiable inverse. The deformed Hamiltonian is, in that case, given by

$$\tilde{H}_\phi = -\frac{\hbar^2}{2m}\Delta + V_\phi - i\frac{\hbar^2}{2m^2c^2}(\nabla V_\phi \times \nabla)\cdot\sigma. \tag{2}$$

Changing to coordinates on $\mathcal{B}$, the deformed Hamiltonian takes the form

$$H_\phi = K_F + V_\phi \circ \phi + H_\phi^{\mathrm{SO}}, \tag{3}$$

where $F=\nabla'\phi$ and the kinetic and spin-orbit parts (K_F and H_ϕ^{SO}, respectively) are given by

$$K_F = -\frac{\hbar^2}{2m}[F^{-1}(\phi(\mathbf{r}'))]_{ji}\frac{\partial}{\partial x_j'}\left([F^{-1}(\phi(\mathbf{r}'))]_{ki}\frac{\partial}{\partial x_k'}\right), \tag{4}$$

and

$$H_\phi^{\mathrm{SO}} = -i\frac{\hbar^2}{4m^2c^2}([F^{-1}(\phi(\mathbf{r}'))]^T\nabla' V_\phi(\phi(\mathbf{r}')) \times [F^{-1}(\phi(\mathbf{r}'))]^T\nabla')\cdot\sigma. \tag{5}$$

Here and throughout the paper, Einstein's summation convention is applied, i.e., summation over repeated indices, e.g., $a_i b_i = \Sigma_{i=1}^3 a_1 b_i$. It should be noted that $\tilde{H}_\phi$ in Eq. (2) and H_ϕ in Eq. (3) are related by a unitary transformation (change of coordinates). It is possible to use other unitary transformations to write the Hamiltonian with respect to coordinates on $\mathcal{B}$, e.g., a transformation similar to the one used in Hislop *et al.*[12] in connection with spectral deformation theory, which take into account the determinant of the deformation gradient appearing in the probability distribution by solving for $\sqrt{\det F}\psi(\mathbf{r})$ instead of $\psi(\mathbf{r})$. The Taylor series expansion will of course reflect the choice of transformation, but the order of the approximation will stay the same.

The idea now is to make a Taylor series expansion of H_ϕ [Eq. (3)] with respect to the deformation ϕ. Hence, it is necessary to set up the mathematical theory required to handle the above situation. This will be done in the next section.

A. Mathematical tools

The first thing needed in order to use a Taylor series expansion is to define a derivative applicable in the given situation. The weakest notion of a derivative is the Gâteaux derivative, and this will be used in the present work. Let U and V be normed linear spaces, $S\subseteq U$ an open set, and P an operator from S to V. In addition, let $u_0\in S$, $\eta\in U$ nonzero, and $\mathcal{I}=(-\alpha,\alpha)$, where $\alpha\in\mathbb{R}$ is chosen such that $u_0+t\eta\in U$ for all $t\in\mathcal{I}$. The Gâteaux differential of P at u_0 in the direction η is then defined to be

$$DP(u_0)\cdot\eta \equiv \frac{d}{dt}(P(u_0+t\eta)) = \lim_{t\to 0}\frac{1}{t}(P(u_0+t\eta)-P(u_0)), \tag{6}$$

when the limit exists. An operator P which has a Gâteaux differential at each point in S in any direction is said to have a Gâteaux differential on S.[13] The higher-order differentials are introduced inductively in the usual manner. It should be noted that when the Gâteaux derivative fulfills certain

additional requirements it is equal to the stronger, and more widely used, concept of a derivative called Frechet differentiability.[14] This concept has, among other things, the advantage of being linear in η, which is not always the case for the Gâteaux derivative.

The version of Taylor's theorem that is relevant for this work is given as follows.

Theorem II.1. *Let U and V be normed linear spaces. Suppose that the space V is complete and that the region S of the space U is convex, and suppose that the function P from S to V has an nth Gâteaux differential on S. Suppose also that for every* u_1, u_2 *in S the function of r,* $D^n P(u_1+(u_2-u_1)r)\cdot(u_2-u_1)^n$, *is bounded on the interval (0, 1) and its set of discontinuities is of measure zero. Then, for every* u_1, u_2 *in S we have*

$$P(u_2) = P(u_1) + \sum_{i=1}^{n-1} \frac{D^i P(u_1)\cdot(u_2-u_1)^i}{i!} + R_n(u_1,u_2),$$

where

$$R_n(u_1,u_2) = \int_0^1 D^n P(u_1+(u_2-u_1)r)\cdot(u_2-u_1)^n \frac{(1-r)^{n-1}}{(n-1)!} dr.$$

The statement that a subset of an interval is of measure zero is equivalent to the statement that the total length of the subset is zero. For a proof of this theorem and a definition of the Riemann integral appearing in the theorem, refer to Ref. 13. In order to see how this theorem can be used in the situation given above, a more precise definition of a deformation, and of the corresponding deformed Hamiltonian, is necessary. This will be given in the following.

First, the overall normed linear space that a deformation belongs to is defined. Let f be a once differentiable function from $\mathcal{B}$ to $\mathbb{R}^3$, and define

$$\|f\|_{C^1} = \left\{ \sup_{\mathcal{B}} \left[f_1^2 + \sum_{i=1}^{3} \left(\frac{\partial f_1}{\partial x_i} \right)^2 + f_2^2 + \sum_{i=1}^{3} \left(\frac{\partial f_2}{\partial x_i} \right)^2 + f_3^2 + \sum_{i=1}^{3} \left(\frac{\partial f_3}{\partial x_i} \right)^2 \right] \right\}^{1/2}, \tag{7}$$

where $f=(f_1,f_2,f_3)$. Denote with $\hat{C}^2$ the normed linear space consisting of all the twice differentiable functions from $\mathcal{B}$ to $\mathbb{R}^3$ that have a finite norm given by (7). A deformation ϕ: $\mathcal{B}\to\mathbb{R}^3$ of the undeformed domain $\mathcal{B}$ is defined to be an injective $\hat{C}^2$ map satisfying $\inf(\det(\nabla'\phi))>0$. The last requirement is needed to ensure that the map has a twice differentiable inverse; this is guaranteed by the inverse function theorem. The existence of the inverse ensures that the deformation does not destroy parts of the domain, e.g., by collapsing or tearing parts of the domain. It is assumed that $\mathcal{B}$ is bounded; this ensures boundedness of considered operators. The space of all deformations of $\mathcal{B}$ is denoted $\mathcal{D}$. It can be shown that the function g: $\hat{C}^2\to\mathbb{R}$ given by $g(\phi)=\inf(\det(\nabla'\phi))$ is continuous, and $\mathcal{D}$ is, as a consequence, open in $\hat{C}^2$ (it is the inverse image of the open set $]\infty,0[$).

Next, the deformed Hamiltonian is shown to be a function from $\mathcal{D}$ to a normed linear space. The domain of the deformed Hamiltonian is, in this article, chosen to be the product of Sobolev spaces: $H^2(\phi(\mathcal{B}))\times H^2(\phi(\mathcal{B}))$. This is the largest space for which the deformed Hamiltonian is defined.[15] The deformation has, according to the inverse function theorem, a twice differentiable inverse. This ensures that H_ϕ can be written with respect to coordinates on $\mathcal{B}$, as it was done in Eq. (3). As a consequence, the deformed Hamiltonian can be viewed as an operator

$$\hat{H}:\mathcal{D}\to L(H^2(\mathcal{B})\times H^2(\mathcal{B}),\quad L^2(\mathcal{B})\times L^2(\mathcal{B})),$$

given by $\phi\mapsto H_\phi$, where $L(\mathcal{F},\mathcal{G})$ is the space of bounded linear mappings from $\mathcal{F}$ to $\mathcal{G}$ and $L^2(\mathcal{B})$ is the Lebesgue space. The Lebesgue space is needed here because of the definition of the Sobolev space.[15] It is also the appropriate space with respect to wave functions, because these give the probability that an electron is in a certain area, and, as a consequence, they only need to be defined

almost everywhere, i.e., up to sets of zero measure. The spaces $H^2(\mathcal{B})\times H^2(\mathcal{B})$ and $L^2(\mathcal{B})\times L^2(\mathcal{B})$ are equipped with the L^2 norm

$$\|\psi\|_{L^2}=\left(\int_{\mathcal{B}}\psi_+^*\psi_+ \mathrm{d}V\right)^{1/2}+\left(\int_{\mathcal{B}}(\psi_-^*\psi_-)\mathrm{d}V\right)^{1/2},$$

where $\psi=\binom{\psi_+}{\psi_-}$ and ψ_+,ψ_- are functions from $\mathcal{B}$ to $\mathbb{C}$. The space $L^2(\mathcal{B})\times L^2(\mathcal{B})$ equipped with this norm is a complete normed linear space. The space $L(H^2(\mathcal{B})\times H^2(\mathcal{B}),L^2(\mathcal{B})\times L^2(\mathcal{B}))$ is equipped with the operator norm

$$\|A\|_O=\sup\{\|A\psi\|_{L^2}|\psi\in H^2(\mathcal{B})\times H^2(\mathcal{B}),\quad \|\psi\|_{L^2}\leqslant 1\},$$

where $A\in L(H^2(\mathcal{B})\times H^2(\mathcal{B}),L^2(\mathcal{B})\times L^2(\mathcal{B}))$. This makes the space $L(H^2(\mathcal{B})\times H^2(\mathcal{B}),L^2(\mathcal{B})\times L^2(\mathcal{B}))$ into a complete normed linear space (see Theorem III.2.3 in Ref. 16).

The function to be approximated by a Taylor series expansion is the function $\hat{H}$, i.e., with respect to Theorem II.1: $P=\hat{H}$, $U=\hat{C}^2$, and $V=L(H^2(\mathcal{B})\times H^2(\mathcal{B}),L^2(\mathcal{B})\times L^2(\mathcal{B}))$. Depending on which element of $\mathcal{D}$ the deformed Hamiltonian is expanded about, the convexity requirement can be fulfilled by restricting the domain of $\hat{H}$ to the largest open ball with respect to the norm[7] that contains the element of expansion and is contained in $\mathcal{D}$. This restriction normally poses no problems because Taylor series expansions are in general only accurate within small deviations from the element of expansion. The restricted domain is the set S in Theorem II.1. That the Gâteaux derivatives exists and that $D^nP(u_1+(u_2-u_1)r)\cdot(u_2-u_1)^n$ fulfills the given requirements has to be verified for each specific potential V_ϕ.

B. Second-order deformed Hamiltonian

In this section, the second-order Taylor series expansion of the deformed Hamiltonian around the identity map *id* on $\mathcal{B}$ is presented. In order to find the second-order Taylor series expansion, it is necessary to find the first- and second-order Gâteaux derivatives. This is done in Appendix A. It is assumed that V_ϕ is well enough behaved such that Theorem II.1 can be used. The Taylor series expansion of the deformed Hamiltonian to the second order in ϕ around *id* is then given by

$$H_\phi\approx H_{id}+D^{(1)}(\phi-id)+D^{(1)}_{\mathrm{SO}}(\phi-id)+D^{(2)}(\phi-id,\phi-id)+D^{(2)}_{\mathrm{SO}}(\phi-id,\phi-id),\tag{8}$$

where

$$H_{id}=-\frac{\hbar^2}{2m}\nabla'^2+V_{id}-i\frac{\hbar^2}{4m^2c^2}(\nabla' V_{id}\times\nabla')\cdot\sigma,$$

$$D^{(1)}(\phi-id)=\frac{\hbar^2}{2m}\left\{[F+F^T-2I]_{jk}\frac{\partial}{\partial x_j'}\frac{\partial}{\partial x_k'}+\frac{\partial}{\partial x_i'}([F-I]_{ki})\frac{\partial}{\partial x_k'}\right\}+DV_{id}\cdot(\phi-id),$$

$$\begin{aligned}D^{(1)}_{\mathrm{SO}}(\phi-id)=&-i\frac{\hbar^2}{4m^2c^2}\{(\nabla'(DV_{id}\cdot(\phi-id))\times\nabla')\cdot\sigma-((F-I)^T\nabla' V_{id}\times\nabla')\cdot\sigma\\&-(\nabla' V_{id}\times(F-I)^T\nabla')\cdot\sigma\},\end{aligned}$$

$$D^{(2)}(\phi - id, \phi - id) = -\frac{\hbar^2}{2m}\Bigg\{[(F-I)(F-I)^T + (F-I)^2 + (F^T-I)^2]_{jk}\frac{\partial}{\partial x_j'}\frac{\partial}{\partial x_k'} + [(F-I)]_{ji}\frac{\partial}{\partial x_j'}([F-I]_{ki})\frac{\partial}{\partial x_k'} + \frac{\partial}{\partial x_i'}[(F-I)^2]_{ki}\frac{\partial}{\partial x_k'}\Bigg\} + \frac{1}{2}D^2V_{id}\cdot((\phi - id),(\phi - id)),$$

$$D_{\mathrm{SO}}^{(2)}(\phi - id, \phi - id) = -i\frac{\hbar^2}{4m^2c^2}\Bigg\{-((F-I)^T\nabla'(DV_{id}\cdot(\phi - id))\times\nabla')\cdot\sigma - (\nabla'(DV_{id}\cdot(\phi - id))\times(F-I)^T\nabla')\cdot\sigma + ((F-I)^T\nabla'V_{id}\times(F-I)^T\nabla')\cdot\sigma + \frac{1}{2}(\nabla'(D^2V_{id}\cdot((\phi - id),(\phi - id)))\times\nabla')\cdot\sigma + ((F^T-I)^2\nabla'V_{id}\times\nabla')\cdot\sigma + (\nabla'V_{id}\times(F^T-I)^2\nabla')\cdot\sigma\Bigg\},$$

and $F=\nabla'\phi$.

To connect these expressions with the strain tensor, note that the Green–Lagrange–St. Venant strain tensor is given by

$$\epsilon = \frac{1}{2}(F^TF - I),$$

and the linear strain tensor is given by

$$\epsilon^{\mathrm{lin}} = \frac{1}{2}(F + F^T - 2I). \tag{9}$$

In the case where F is symmetric, Eq. (9) becomes

$$\epsilon^{\mathrm{lin}} = F - I.$$

If only the first-order terms of the Taylor series expansion are used, and if the linear strain is used with a symmetric deformation gradient, then the herein derived first-order approximation to the deformed Hamiltonian is identical to the one proposed by Zhang.[5] In the case where the deformation is homogeneous, the first-order approximation is the same as the one derived by Bir *et al.*[4]

C. Weak formulation

The preceding sections are all concerned with deformations that are twice differentiable, but there are many situations where the deformations do not satisfy this. For example, in the quantum-well case the deformation is piecewise linear with different slopes inside and outside the well.[17] Therefore, to be able to handle this kind of deformations, an extension of the theory to a larger class of deformations is needed.

Let $\mathcal{A}$ be the set of injective functions from $\mathcal{B}$ to $\mathbb{R}^3$ that are once differentiable on $\mathcal{B}\backslash\Gamma$ with both a finite C^1 norm [Eq. (7)] and a positive Jacobian determinant, where Γ is a finite set of piecewise smooth surfaces (two-dimensional manifolds). This set of functions includes the deformations considered in quantum-well, as well as quantum-wire and quantum-dot structures (according to continuum mechanical models[9–11]). The problem with the functions belonging to $\mathcal{A}$ is that they are not necessarily once differentiable on $\mathcal{B}$ because the first derivative can have discon-

tinuities at interfaces. Therefore, caution is needed when "pulling back" the deformed Hamiltonian to coordinates on $\mathcal{B}$ [Eq. (3)]. The correct formalism to use in this case is the weak formalism, i.e., instead of solving the eigenvalue equation

$$H_\phi \tilde{\psi} = E\tilde{\psi},$$

subject to some boundary conditions (in this work either Dirichlet or periodic boundary conditions), a solution to the weak equation

$$\int_{\phi(\mathcal{B})} \xi_+^* (H_\phi \tilde{\psi})_+ \mathrm{d}V + \int_{\phi(\mathcal{B})} \xi_-^* (H_\phi \tilde{\psi})_- \mathrm{d}V = \int_{\phi(\mathcal{B})} \xi_+^* E\tilde{\psi}_+ \mathrm{d}V + \int_{\phi(\mathcal{B})} \xi_-^* E\tilde{\psi}_- \mathrm{d}V, \tag{10}$$

for all $\xi_+, \xi_- \in C_c^\infty(\phi(\mathcal{B}), \mathbb{C})$ (smooth functions with compact support; see, e.g., Ref. 16) is found, where $(H_\phi \tilde{\psi})_+$ is the first factor of $H_\phi \tilde{\psi}$ and $(H_\phi \tilde{\psi})_-$ is the last factor. The solution still has to satisfy the boundary conditions. Introducing

$$K_\phi^\pm(\eta_\pm, \zeta) = \frac{\hbar^2}{2m} \int_{\mathcal{B}\backslash\Gamma} [(F^{-1} \circ \phi)(F^{-1} \circ \phi)^T]_{ij} \frac{\partial(\eta_\pm)^*}{\partial x_i'} \frac{\partial \zeta_\pm}{\partial x_j'} \det F \mathrm{d}V', \tag{11}$$

$$V_\phi^\pm(\eta_\pm, \zeta) = \int_{\mathcal{B}} \eta_\pm^* V_\phi \circ \phi \zeta_\pm \det F \mathrm{d}V', \tag{12}$$

$$H_\phi^{\mathrm{SO},\pm}(\eta_\pm, \zeta) = -i \frac{\hbar^2}{4m^2c^2} \int_{\mathcal{B}\backslash\Gamma} \eta_\pm^* (F^T \sigma \times \nabla' V_\phi \circ \phi \cdot \nabla' \zeta)_\pm \mathrm{d}V', \tag{13}$$

$$W_\phi(\eta, \zeta; E) = K_\phi^+(\eta_\pm, \zeta) + V_\phi^+(\eta_\pm, \zeta) + H^{\mathrm{SO},+}{}_\phi(\eta_\pm, \zeta) - \int_{\mathcal{B}} \eta_+^* E\zeta_+ \det F \mathrm{d}V' + K_\phi^-(\eta_\pm, \zeta) + V_\phi^-(\eta_\pm, \zeta)$$

$$+ H^{\mathrm{SO},-}{}_\phi(\eta_\pm, \zeta) - \int_{\mathcal{B}} \eta_-^* E\zeta_- \det F \mathrm{d}V', \tag{14}$$

where $\eta = \binom{\eta_+}{\eta_-}$, $\zeta = \binom{\zeta_+}{\zeta_-}$, $\eta_+, \eta_- \in H^2(\mathcal{B})$, and $\zeta_+ \circ \phi^{-1}, \zeta_- \circ \phi^{-1} \in C_c^\infty(\phi(\mathcal{B}), \mathbb{C})$, the weak formulation [Eq. (10)] can be put in the form: Find $\tilde{\psi}$ and E such that

$$W_\phi(\xi \circ \phi, \tilde{\psi} \circ \phi; E) = 0,$$

for all $\xi_+, \xi_- \in C_c^\infty(\phi(\mathcal{B}), \mathbb{C})$. The expression for the kinetic part [Eq. (11)] is found by integrating by parts, using that ξ_+ and ξ_- have compact support, changing coordinates, and using the chain rule. The integral is restricted to $\mathcal{B}\backslash\Gamma$ for the chain rule to apply. This is possible because Γ has measure zero (zero volume). Finding the expression for the potential part [Eq. (12)] is straightforward, and the expression for the spin-orbit part [Eq. (13)] is found again by changing coordinates and using the chain rule; in addition, the rule that $Av_1 \times Av_2 \cdot Av_3 = \det(A) v_1 \times v_2 \cdot v_3$, for a 3×3 matrix A and $v_1, v_2, v_3 \in \mathbb{R}^3$ is used.

According to Theorem B.1 in the Appendix, the above weak formulation is equivalent to finding ψ and E such that

$$W_\phi(\eta, \psi; E) = 0, \tag{15}$$

for all $\eta_+, \eta_- \in C_c^\infty(\mathcal{B}, \mathbb{C})$, in which case $\tilde{\psi} = \psi \circ \phi^{-1}$. Equation (15) is a weak formulation of the problem with respect to the domain $\mathcal{B}$.

The operator W defined in Eq. (14) can be viewed as an operator $W: \mathcal{A} \to L(H^2(\mathcal{B}) \times H^2(\mathcal{B}), C_c^\infty(\mathcal{B}, \mathbb{C}) \times C_c^\infty(\mathcal{B}, \mathbb{C}); A(\mathbb{R}, \mathbb{R}))$, where $L(\mathcal{F}_1, \mathcal{F}_2; \mathcal{G})$ is the space of bilinear mappings

from $\mathcal{F}_1 \times \mathcal{F}_2$ to $\mathcal{G}$ and $A(\mathbb{R},\mathbb{R})$ is the space of affine mappings from $\mathbb{R}$ to $\mathbb{R}$. The space $A(\mathbb{R},\mathbb{R})$ is a finite-dimensional normed vector space, and because of this it is complete. It follows that the range of W is complete so, according to Theorem II.1, the Taylor series expansion of W exists, assuming that the Gâteaux derivative exists and fulfills given requirements. The domain of W can be restricted to an open convex set using similar arguments as in Sec. II A.

In Appendix B the derivatives needed to write out the second-order Taylor series expansion of W are found, giving

$$W_\phi \approx W_{id} + W^{(1)}(\phi - id) + W^{(1)}_{\mathrm{SO}}(\phi - id) + W^{(2)}(\phi - id, \phi - id) + W^{(2)}_{\mathrm{SO}}(\phi - id, \phi - id),$$

where

$$W^{(1)}(\phi - id)(\eta,\psi;E) = \sum_{s=+,-} \left\{ -\frac{\hbar^2}{2m}\int_{\mathcal{B}\setminus\Gamma} [F + F^T - 2I]_{ij} \frac{\partial(\eta_s)^*}{\partial x_i'}\frac{\partial \psi_s}{\partial x_j'} - \frac{\partial(\eta_s)^*}{\partial x_i'}\frac{\partial \psi_s}{\partial x_i'}\,\mathrm{Tr}(F-I)\mathrm{d}V' \right.$$
$$\left. + \int_{\mathcal{B}} \eta_s^*(DV_{id}\cdot(\phi - id) + (V_{id} - E)\mathrm{Tr}(F-I))\psi_s \mathrm{d}V' \right\},$$

$$W^{(2)}(\phi - id, \phi - id)(\eta,\psi;E) = \sum_{s=+,-} \left\{ \frac{\hbar^2}{2m}\int_{\mathcal{B}\setminus\Gamma} [(F-I)^2 + (F^T - I)^2 + (F-I)(F-I)^T]_{ij} \frac{\partial(\eta_s)^*}{\partial x_i'}\frac{\partial \psi_s}{\partial x_j'}\mathrm{d}V' \right.$$
$$- \frac{\hbar^2}{2m}\int_{\mathcal{B}\setminus\Gamma} [F + F^T - 2I]_{ij}\,\mathrm{Tr}(F-I)\frac{\partial(\eta_s)^*}{\partial x_i'}\frac{\partial \psi_s}{\partial x_j'}\mathrm{d}V'$$
$$+ \frac{\hbar^2}{2m}\int_{\mathcal{B}\setminus\Gamma} \frac{\partial(\eta_s)^*}{\partial x_i'}\frac{\partial \psi_s}{\partial x_i'}\,\mathrm{Tr}([F-I]_{co})\mathrm{d}V'$$
$$+ \frac{1}{2}\int_{\mathcal{B}} \eta_s^* D^2 V_{id}\cdot(\phi - id, \phi - id)\psi_s \mathrm{d}V,$$
$$\left. + \int_{\mathcal{B}} \eta_s^*(DV_{id}\cdot(\phi - id)\mathrm{Tr}(F-I) + (V_{id} - E)\mathrm{Tr}([F-I]_{co}))\psi_s \mathrm{d}V' \right\},$$

$$W^{(1)}_{\mathrm{SO}}(\phi - id)(\eta,\psi) = \sum_{s=+,-} -i\frac{\hbar^2}{4m^2c^2}\int_{\mathcal{B}\setminus\Gamma} \{\eta_s^*((F-I)^T\sigma \times \nabla' V_{id}\cdot\nabla'\psi)_s$$
$$+ \eta_s^*(\sigma\times\nabla'(DV_{id}\cdot(\phi - id))\cdot\nabla'\psi)_s\}\mathrm{d}V',$$

and

$$W^{(2)}_{\mathrm{SO}}(\phi - id, \phi - id)(\eta,\psi) = \sum_{s=+,-} \left\{ -i\frac{\hbar^2}{4m^2c^2}\int_{\mathcal{B}\setminus\Gamma} \eta_s^*((F-I)^T\sigma\times\nabla'(DV_{id}\cdot(\phi - id))\cdot\nabla'\psi)_s \mathrm{d}V' \right.$$
$$\left. - i\frac{\hbar^2}{4m^2c^2}\int_{\mathcal{B}\setminus\Gamma} \eta_s^*\left(\sigma\times\nabla'\left(\frac{1}{2}D^2V_{id}\cdot(\phi - id, \phi - id)\right)\cdot\nabla'\psi\right)_s \mathrm{d}V' \right\}.$$

In contrast to the previous deformed Hamiltonian models by Bir and Pikus,[4] Zhang,[5] and Suzuki,[6] the present model describes a general rigoristic mathematical model for incorporating nonsmooth (and of course, smooth) deformation fields in Hamiltonians.

1. Strong formulation with interface boundary conditions

The weak form can, as long as the deformations lie in $\mathcal{A}$ and are twice differentiable on $\mathcal{B}\backslash\Gamma$, be reformulated in a strong form with interface boundary conditions. This is done using integration by parts in the kinetic term [Eq. (11)]. Let $\mathbf{n}=(n_1,n_2,n_3)$ be a unit normal vector field on the interface Γ; then

$$K_{\phi}^{\pm}(\eta_{\pm},\zeta) = \frac{\hbar^2}{2m}\int_{\Gamma} n_i \Bigg\{ \left([(F^{-1}\circ\phi)(F^{-1}\circ\phi)^T]_{ij} (\eta_{\pm})^* \frac{\partial \zeta_{\pm}}{\partial x_j'} \det F \right)_{m1} - \left([(F^{-1}\circ\phi)(F^{-1}\circ\phi)^T]_{ij} (\eta_{\pm})^* \frac{\partial \zeta_{\pm}}{\partial x_j'} \det F \right)_{m2} \Bigg\} \mathrm{d}A' - \frac{\hbar^2}{2m}\int_{\mathcal{B}\backslash\Gamma} (\eta_{\pm})^* [F^{-1}\circ\phi]_{ji} \frac{\partial}{\partial x_j'} \left([F^{-1}\circ\phi]_{ki} \frac{\partial \zeta_{\pm}}{\partial x_k'} \right) \det F \mathrm{d}V', \tag{16}$$

where the subscripts $m1$ and $m2$ symbolize that the expression in brackets is found as the limit taken from the region that the normal vector points out of and into, respectively. To get this result, it has also been used that

$$\frac{\partial}{\partial x_i}(F^{-1}_{ik} \det F) = \frac{\partial}{\partial x_i}([F_{co}]_{ki}) = 0,$$

for $k=1,2,3$, where F_{co} is the matrix of cofactors of F. This result can easily be verified. From Eq. (16) it can be inferred that the weak formulation is equivalent to solving the eigenvalue equation

$$H_{\phi}\zeta = E\zeta,$$

on $\mathcal{B}\backslash\Gamma$, where H_{ϕ} is given in Eq. (3), subject to the interface boundary condition

$$n_i \left([(F^{-1}\circ\phi)(F^{-1}\circ\phi)^T]_{ij} \frac{\partial \zeta_{\pm}}{\partial x_j} \det F \right)_{m1} = n_i \left([(F^{-1}\circ\phi)(F^{-1}\circ\phi)^T]_{ij} \frac{\partial \zeta_{\pm}}{\partial x_j'} \det F \right)_{m2}. \tag{17}$$

Notice that the interface boundary condition should be satisfied simultaneously for both ζ_+ and ζ_- in order for the surface integral appearing in (16) to vanish.

The advantage of formulating the problem in strong form with interface boundary conditions [Eq. (17)] is that solution methods no longer are restricted to weak methods. Hence, it is possible to find solutions by any convenient numerical or exact method. This kind of procedure can be used in most situations involving derivatives of discontinuous quantities, e.g., $k\cdot p$ theory.

III. ONE- AND TWO-DIMENSIONAL EXAMPLES

A. Sinusoidal potential

The one-dimensional sinusoidal potential is chosen as a first example. This potential is given by

$$V_{id}(x') = V_0 + A\cos\left(\frac{2\pi}{a}x'\right),$$

for $x' \in \,]-Na, Na[$ (see Fig. 1). The real number a is the distance between the maximal value of the potential, and $N \in \mathbb{N}$ is a fixed number. In this example the values $V_0=0$ eV and $A=5$ eV are chosen. In addition, periodic boundary conditions are used. Assuming that the whole potential is deformed when subjected to some deformation ϕ, the deformed potential is given by

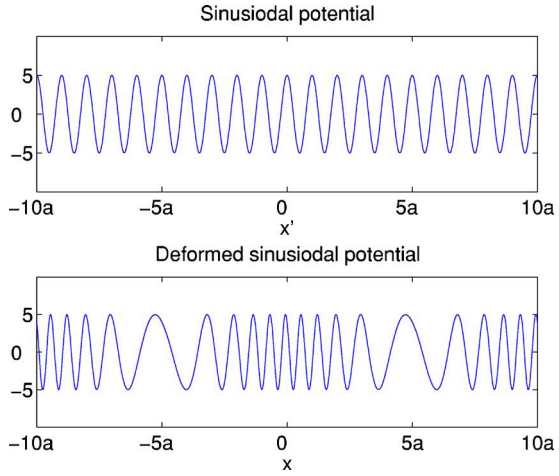

FIG. 1. (Color online) A figure showing the undeformed and deformed sinusoidal potential for $N=10$ and $\epsilon=0.1$.

$$V_\phi(x) = V_{id}(\phi^{-1}(x)) = V_0 + A\cos\left(\frac{2\pi}{a}\phi^{-1}(x)\right).$$

To get an idea of the influence of the deformation on the energies, the deformation is chosen such that

$$\phi^{-1}(x) = x + \epsilon a \sin\left(\frac{2\pi}{10a}x\right), \tag{18}$$

where it is assumed that $N/10 \in \mathbb{N}$ and $\epsilon \in \mathbb{R}$ is chosen such that $\partial\phi^{-1}/\partial x > 0$ for all $x \in [-Na, Na]$. In Fig. 1 the deformed potential is shown for $N=10$ and $\epsilon=0.1$. The inverse is specified because this insures that it is possible to solve the exact eigenvalue equation and, as a consequence, the first- and second-order approximations can be compared against the exact solution.

This example can be extended to a three-dimensional example by assuming that there is translational symmetry in the y' and z' directions, and that the system is only deformed in the x' direction. The undeformed region can, in this case, be chosen as $\mathcal{B}=]-Na, Na[\times]-Na, Na[\times]-Na, Na[$ with periodic boundary conditions. The potential can then be viewed as originating from a periodic array of plates perpendicular to the x' direction. The number a is, in this case, the period of the structure. Ignoring spin, the deformed Hamiltonian is given by

$$H_\phi = -\frac{\hbar^2}{2m}\Delta + V_\phi.$$

According to Eq. (8), the second-order Taylor series expansion is

$$H_\phi \approx H_{id} + D^{(1)}(\phi - id) + D^{(2)}(\phi - id, \phi - id).$$

Because of the translational symmetry, the solutions to the eigenvalue problem [Eq. (1)] can always be chosen such that

$$\tilde{\psi}(x', y', z') = \psi(x')e^{ik_{y'}y'}e^{ik_{z'}z'}.$$

Solving at the zone center, i.e., for $k_{y'}=0$ and $k_{z'}=0$, it is found that Eq. (8) takes the form

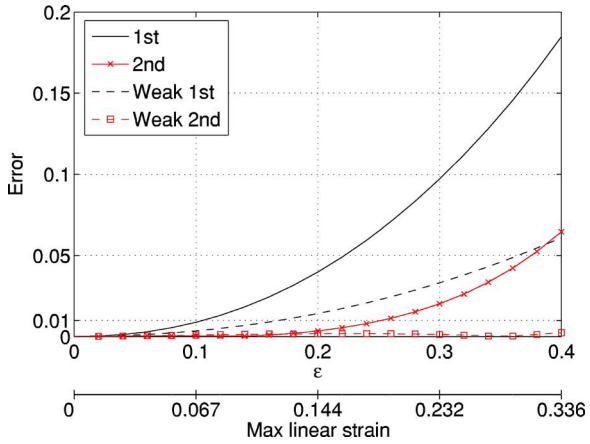

FIG. 2. (Color online) Graph showing the error in the energies for the sinusoidal potential when using the first- and second-order approximations.

$$H_\phi \approx -\frac{\hbar^2}{2m}\left\{\left(1-2\left(\frac{\partial\phi}{\partial x'}-1\right)+3\left(\frac{\partial\phi}{\partial x'}-1\right)^2\right)\frac{\partial^2}{\partial x'^2}+\left(-\frac{\partial^2\phi}{\partial x'^2}+3\left(\frac{\partial\phi}{\partial x'}-1\right)\frac{\partial^2\phi}{\partial x'^2}\right)\frac{\partial}{\partial x'}\right\}+V_{id}(x').$$

The reason why the Taylor series expansion of the potential is exact is that $V_\phi(x)=V_{id}(\phi^{-1}(x))=V_{id}(x')$. Another way of arriving at Eq. (19) is to derive a theory similar to the one in this article just for the one-dimensional case.

The eigenvalue equation has been solved numerically using FEMLAB, i.e., using a finite-element method, both for the first- and second-order approximation of the deformed Hamiltonian with respect to $((\partial\phi/\partial x')-1)$. The exact problem, i.e., without making the Taylor series expansion, was also solved using FEMLAB. In Fig. 2 a plot of the error in using the first- and second-order approximation as a function of ϵ and the maximum of the linear strain is presented (the solid lines), where the linear strain is given by $((\partial\phi/\partial x')-1)$. The errors of the first- and the second-order Hamiltonians are given by

$$\mathrm{Error}^x=\left|\frac{E_1^x-E_1^{\mathrm{Exact}}}{E_1^x}\right|,$$

$x=1\mathrm{st},2\mathrm{nd}$, respectively, where E_1^{Exact}, $E_1^{1\mathrm{st}}$, and $E_1^{2\mathrm{nd}}$ are the energy of the ground state calculated with the exact, first-order, and second-order Hamiltonians, respectively. From this graph it can be seen that the second-order approximation (crossed red line) is considerably more accurate then the first-order approximation (black line). The first-order approximation has an error of less than 1% for a max linear strain of up to 6.7%, whereas the second-order approximation is accurate to with in 1% up to a max linear strain of 18.6%.

Even though it is not necessary to use the weak formulation for the problem in this example (because the deformation is smooth over the whole domain), it is still interesting to see how accurate the results are using the weak approach. First of all, it should be noted that the exact results obtained with the weak formulation are identical to the exact results obtained with the strong formulation. This should also be the case because the formulations are equivalent when everything is smooth. Which formulation is used does however matter when the Taylor series expansion is made. In the weak formulation the Jacobian is present as a consequence of the coordinate transformation of the integral, and it is not present in the strong formulation. So, it is actually the influence of the Jacobian that is under investigation in the following.

According to Sec. II C, the second-order Taylor series expansion of the weak eigenvalues problem has the following form disregarding spin: Find $\tilde{\psi}$ and E such that

$$W(\phi)(\eta,\tilde{\psi},E)=0, \tag{19}$$

for all $\eta\in C_c^\infty(\mathcal{B},\mathbb{C})$, where

$$W(\phi)(\eta,\tilde{\psi},E)\approx\frac{\hbar^2}{2m}\int_{-Na}^{Na}\left[\left(1-\left(\frac{\partial\phi}{\partial x'}-1\right)+\left(\frac{\partial\phi}{\partial x'}-1\right)^2\right)\frac{\partial\hat{\eta}^*}{\partial x'}\frac{\partial\psi}{\partial x'}\right]\mathrm{d}x'$$
$$+\int_{-Na}^{Na}\left[(V_{id}-E)\frac{\partial\phi}{\partial x'}\hat{\eta}^*\psi\right]\mathrm{d}x',$$

and

$$\hat{\eta}=\int_{-Na}^{Na}\int_{-Na}^{Na}\eta\,\mathrm{d}y'\,\mathrm{d}z'.$$

The first- and second-order approximation of the eigenvalue equation (19) with respect to $((\partial\phi/\partial x')-1)$ is again solved using FEMLAB. The dashed lines in Fig. 2 show the error introduced by using the first- and second-order approximation (black and boxed red lines, respectively). From this figure, it is seen that the second-order approximation is again substantially better than the first-order approximation. In this case, the first-order approximation has an error of less then 1% for a max linear strain of up to 12%, and the second-order approximation is within an error of 1% in the whole interval shown, i.e., at least up to a max linear strain of 33.6%. It is also seen that the first- and second-order approximations of the weak problem are considerably more precise than the first- and second-order approximations of the strong problem. The reason for this goes back to the presence of the Jacobian in the weak formulation in the following way.

First, observe that $\partial\phi^{-1}/\partial x\circ\phi=1/(\partial\phi/\partial x')$ and $\det(\nabla'\phi)=\partial\phi/\partial x'$. From this it is seen that $\partial\phi^{-1}/\partial x\circ\phi\det(\nabla'\phi)=1$. Because of this, Eq. (14) reduces to

$$W(\phi)(\eta,\tilde{\psi},E)=\frac{\hbar^2}{2m}\int_{-Na}^{Na}\left[\frac{\partial\phi^{-1}}{\partial x}\circ\phi\frac{\partial\hat{\eta}^*}{\partial x}\frac{\partial\psi}{\partial x'}+(V_{id}-E)\frac{\partial\phi}{\partial x'}\hat{\eta}^*\psi\right]\mathrm{d}x'.$$

The reason why the Taylor approximations of this equation is more precise than the Taylor approximations of the strong problem is simply that the first- and second-order Taylor series expansion of $\partial\phi^{-1}/\partial x\circ\phi=1/(\partial\phi/\partial x')$ is more accurate than the first- and second-order Taylor series expansion of $((\partial\phi^{-1}/\partial x)\circ\phi)^2=(1/(\partial\phi/\partial x'))^2$. Hence, the reason why the approximations of the weak formulation are more accurate than the approximations of the strong formulation is that this example is, in essence, a one-dimensional problem. This will be confirmed in the quantum-wire example analyzed later.

B. Quantum well

In this section the influence of deformations on the quantum-well problem is investigated. This is done in order to give an example of a situation where the weak formulation is needed. The quantum-well problem is the one-dimensional problem where the undeformed potential is given by the step function

$$V_{id}(x')=\begin{cases}V_0, & x'\in\,]-d,-a[\\ V_1, & x'\in[-a,a]\\ V_0, & x'\in\,]a,d[\end{cases}.$$

To simplify matters, spin is again neglected. In this example the following values are used: $V_0=5$ eV, $V_1=0$ eV, $a=5$ nm, and $d=25$ nm, and Dirichlet boundary conditions are imposed. Again, it is assumed that the whole potential is deformed when it is subjected to a deformation ϕ, i.e., $V_\phi(x)=V_{id}(\phi^{-1}(x))$. In nanoscale semiconductor quantum wells, the well material will be de-

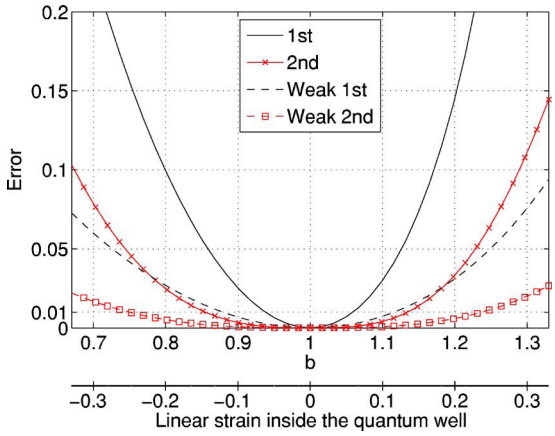

FIG. 3. (Color online) Graph showing the error in the energies for the quantum well when using the first- and second-order approximations.

formed homogeneously, whereas the barrier material will stay undeformed [see, e.g. (18)], i.e., the deformation will have the form

$$\phi(x') = \begin{cases} x' - a(b-1), & x' \in]-d,-a[\\ bx', & x' \in [-a,a] \\ x' + a(b-1), & x' \in]a,d[\end{cases},$$

for some $b>0$. The deformation is not differentiable at the interfaces and, as a consequence, the weak formulation is needed. Proceeding as in the sinusoidal example above, it is found that the second-order Taylor series expansion of the weak eigenvalue problem takes the form given in Eq. (19) and the equations that follow.

The first- and second-order approximations have again been solved using FEMLAB. The inverse of the deformation is easily found and, as a consequence, it is also possible to solve the exact weak eigenvalue problem, i.e., without making a Taylor series expansion. The error in the energy of the ground state in using the first- and second-order approximation is shown in Fig. 3 (dashed black and boxed red lines). Here, it is seen that the error introduced by using the first-order approximation is within 1% for a linear strain of up to 11.6%, whereas the error introduced by using the second-order approximation lies within 1% for a linear strain of up to 23.8%. Again, it is seen that the second-order approximation is substantially better than the first-order approximation.

In the sinusoidal example above, it was seen that the approximations of the weak formulation gave considerably more accurate results than the approximations of the strong formulation. In order to investigate whether this is the case for the quantum-well problem also, the strong form of the problem with interface boundary conditions (Sec. II C 1) has been solved, again using FEMLAB. It should be noted that the exact solution to the strong form with interface boundary conditions, i.e., without making a Taylor series expansion, is equal to the exact solution to the weak form. This has to be the case because the two formalisms are equivalent as long as no approximations have been made. The second-order approximation of the strong form is given by Eq. (19) above, and the interface boundary conditions are as follows:

$$\left(\frac{\partial \phi^{-1}}{\partial x} \circ \phi(x_0) \frac{\partial \psi}{\partial x'}(x_0)\right)_L = \left(\frac{\partial \phi^{-1}}{\partial x} \circ \phi(x_0) \frac{\partial \psi}{\partial x'}(x_0)\right)_R,$$

for $x_0 = -a, a$, where $L(R)$ indicates that the expression in brackets is taken in the limit from the left (right). The second-order Taylor series expansion of the interface boundary conditions takes the form

$$\left(\left(1-\left(\frac{\partial\phi}{\partial x'}(x_0)-1\right)+\left(\frac{\partial\phi}{\partial x'}(x_0)-1\right)^2\right)\frac{\partial\psi}{\partial x'}(x_0)\right)_L$$
$$=\left(\left(1-\left(\frac{\partial\phi}{\partial x'}(x_0)-1\right)+\left(\frac{\partial\phi}{\partial x'}(x_0)-1\right)^2\right)\frac{\partial\psi}{\partial x'}(x_0)\right)_R,$$

for $x_0=-a,a$.

The solid black and crossed red lines in Fig. 3 show the error introduced by using the first- and second-order approximation of the strong form with interface boundary conditions, denoted SForm-first and SForm-second, respectively. Here, we see that the error in using SForm-first is less than 1% for a linear strain of up to 5.9%, whereas the error introduced using SForm-second is within 1% for a linear strain of up to 13.5%. So again, it is seen that the second-order approximation is more accurate than the first-order approximation. In addition, it can be seen that the approximations of the weak form are substantially more accurate than the approximations of the strong form with interface boundary conditions. This is expected because this is also a one-dimensional problem, so the same reasoning as in the sinusoidal example can be applied.

C. Quantum wire

In this section a square-shaped, two-dimensional quantum-wire problem with infinite barrier is investigated. This is done in order to see whether or not the approximations of the weak problem are more accurate than the approximations of the strong form for a two-dimensional problem.

The undeformed two-dimensional domain under investigation is given by $]-5,5[\times]-5,5[$ (in nanometers) and the potential is zero. Dirichlet boundary conditions must be applied because of the infinite barrier. To simplify matters, the following homogeneous deformation is chosen:

$$\phi(\dot{x}',y')=\begin{pmatrix} b & b-1 \\ 0 & b \end{pmatrix}\begin{pmatrix} x' \\ y' \end{pmatrix},$$

where $b\neq 0$ (this ensures that the Jacobian determinant is positive). The second-order Taylor series expansion of the Strong formulation of the eigenvalue equation takes the form: Find ψ and E such that

$$H_\phi\psi=E\psi,$$

where

$$H_\phi\approx-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x'\partial x'}+\frac{\partial^2\psi}{\partial y'\partial y'}-2(b-1)\left(\frac{\partial^2\psi}{\partial x'\partial x'}+\frac{\partial^2\psi}{\partial y'\partial y'}+\frac{\partial^2\psi}{\partial x'\partial y'}\right)\right.$$
$$\left.+(b-1)^2\left(4\frac{\partial^2\psi}{\partial x'\partial x'}+3\frac{\partial^2\psi}{\partial y'\partial y'}+6\frac{\partial^2\psi}{\partial x'\partial y'}\right)\right).$$

This can either be derived in a similar manner to the three-dimensional case, or the quantum-wire problem can be extended to a three-dimensional problem by assuming translational symmetry in the third direction. If it is then solved at the zone center in the third direction, the second-order approximation of the deformed Hamiltonian will have the above form. In the latter case the problem is actually closer to a real problem, although a idealized version, because such quantum-wire structures can be grown in reality [see Ref. 18].

The solid lines in Fig. 4 show the error resulting from using the first- and second-order approximations (the black and crossed red lines, respectively). Here, it is seen that the first-order approximation is within an error of 1% for $b-1$ between -0.058 and 0.055, whereas the energies of the second-order approximation are within an error of 1% for $b-1$ between -0.197 and 0.098. Again, it can be seen that the second-order approximation gives substantially better results.

The second-order Taylor series expansion of the weak formulation of the problem takes the form: Find ψ and E such that

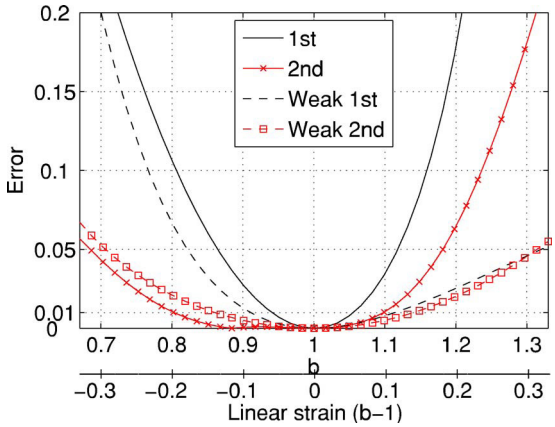

FIG. 4. (Color online) Graph showing the error in the energies for the quantum wire when using the first- and second-order approximations.

$$W(\phi)(\eta,\psi,E)=0,$$

for all $\eta\in C_c^\infty(]-5,5[\times]-5,5[,\mathbb{C})$, where

$$W(\phi)(\eta,\tilde{\psi},E)\approx\int_{-5}^{5}\int_{-5}^{5}\left\{\frac{\hbar^2}{2m}\left[\frac{\partial\eta^*}{\partial x'}\frac{\partial\psi}{\partial x'}+\frac{\partial\eta^*}{\partial x'}\frac{\partial\psi}{\partial x'}+(-(b-1)+(b-1)^2)\left(\frac{\partial\eta^*}{\partial x'}\frac{\partial\psi}{\partial y'}+\frac{\partial\eta^*}{\partial y'}\frac{\partial\psi}{\partial x'}\right)\right.\right.$$
$$\left.\left.+(b-1)^2\frac{\partial\eta^*}{\partial x'}\frac{\partial\psi}{\partial x'}\right]+(V_{id}-E)(1+2(b-1)+(b-1)^2)\hat{\eta}^*\psi\right\}\mathrm{d}x'\mathrm{d}y'.$$

From this, the energies can be calculated with respect to a first- and a second-order approximation of the weak form. The dashed lines in Fig. 4 show the error in the energy introduced by using the first- and the second-order approximation of the weak form as a function of both b and $b-1$ (black and boxed red lines, respectively). Here, it is seen that the first-order approximation of the weak form has an error of less than 1% for $b-1$ between −0.089 and 0.114, whereas the error of the second-order approximation of the weak form is within an error of 1% for $b-1$ between −0.139 and 0.14. It is seen, as expected, that the second-order approximation of the weak form is much better than the first-order approximation of the weak form. But, when the approximations of the weak form are compared to the approximations of the strong form, it is seen that the second-order approximation of the strong form is actually more accurate than the second-order approximation of the weak form in the negative direction, whereas it is the second-order approximation of the weak form which is more accurate in the positive direction. Hence, for this two-dimensional problem it is not easy to say which of the two formulations gives the best results. This differs from the observations made in the one-dimensional examples above, where it was seen that the approximations of the weak formulation always were more accurate than the approximations of the strong formulation.

IV. CONCLUSION

In this article a method to incorporate deformation effects in Hamiltonians has been presented based on a Taylor series expansion with respect to the deformation. This method was exemplified with a Hamiltonian of an inhomogeneous crystal structure including spin. For this Hamiltonian, the second-order Taylor series expansion of the eigenvalue problem was found both in a strong and a weak formulation. The weak formulation was needed in order to be able to handle deformations that might not be differentiable at interfaces. It was also shown that the weak formulation could be transformed into a strong formulation with interface boundary conditions.

One- and two-dimensional examples were presented, where it was shown that the Taylor series approximations give quite accurate results. In actual fact, an error in the energy within 1% for a linear strain of up to 5.5% for the first-order approximations and 9.8% for the second-order approximations was obtained. For the one-dimensional examples, it was also seen that the approximations of the weak formulation gave considerably more accurate results than the approximations of the strong formulation. But, for the two-dimensional example, this was not the case.

ACKNOWLEDGMENTS

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APPENDIX A: TAYLOR EXPANSION (STRONG FORMULATION)

First, it should be noted that all the functions under investigation in this appendix, except the potential V_ϕ, are Frechet differentiable. As a consequence, all the usual rules normally associated with derivatives can be applied.

In the course of finding the Gâteaux derivative of $\hat{H}$, the following lemma will be used:

Lemma A.1. Let F: $\mathcal{D}\to C(\mathcal{B},M(3,\mathbb{R}))$ *be given by* $F(\phi)=\nabla'\phi$, $G\in C(\mathcal{B},M(3,\mathbb{R}))$, *and* $\chi\in\hat{C}^2$, *where* $M(3,\mathbb{R})$ *is the set of* 3×3 *matrices with real coefficients; then*

$$DF(\phi)\cdot\chi=\nabla'\chi,$$

$$DF^{-1}(I)\cdot G=-G,$$

$$D\det F(I)\cdot G=\mathrm{Tr}(G)$$

where $I\in C(\mathcal{B},GL(3,\mathbb{R}))$ *is given by* $I(\mathbf{r}')_{ij}=\delta_{ij}$, F^{-1} *is the mapping* $F\mapsto F^{-1}$ *for* $F\in C(\mathcal{B},GL(3,\mathbb{R}))$, *and* $\det F$ *is the mapping* $F\mapsto\det F$. *In addition*

$$D^2F^{-1}(I)\cdot(G,G)=2(G)^2,$$

and

$$D^2\det F(I)\cdot(G,G)=2\,\mathrm{Tr}([G]_{co})=2(G_{11}G_{22}-G_{12}G_{21}+G_{11}G_{33}-G_{13}G_{31}+G_{22}G_{33}-G_{23}G_{32}),$$

where $[G]_{co}$ *is the matrix of cofactors of* G.

Proof of Lemma A.1. Using Eq. (6), it is seen that

$$DF(\phi)\cdot\chi=\frac{d}{dt}\{\nabla'(\phi+t\chi)\}\big|_{t=0}=\nabla'\chi.$$

Let F_0, $G\in C(\mathcal{B},M(3,\mathbb{R}))$, F_0 invertible, and let $\alpha\in\mathbb{R}$ be given such that F_0+tG is invertible for all $t\in(-\alpha,\alpha)$. Observe that

$$\frac{(F_0-tG)^{-1}-F_0^{-1}}{t}=\frac{F_0^{-1}}{t}((I+tGF_0^{-1})^{-1}-I)=-F_0^{-1}(I+tGF_0^{-1})^{-1}GF_0^{-1}.$$

From this it follows that the limit for $t\to 0$ exists and

$$DF^{-1}(F_0)\cdot G=-F_0^{-1}GF_0^{-1}. \tag{A1}$$

With $F_0=I$ the second result in Lemma A.1 is found. From Eq. (A1) it is also found that

$$D^2F^{-1}(F_0)\cdot(G,G) = D(-F^{-1}GF^{-1})(F_0)\cdot(G) = 2F_0^{-1}GF_0^{-1}GF_0^{-1}.$$

With $F_0=I$, the third result is obtained.

It is known that

$$\det F = F_1 \times F_2 \cdot F_3, \tag{A2}$$

where F_i is the ith column of F. From Eq. (A2), it is seen that

$$D\det F(F_0)\cdot G = G_1 \times [F_0]_2 \cdot [F_0]_3 + [F_0]_1 \times G_2 \cdot [F_0]_3 + [F_0]_1 \times [F_0]_2 \cdot G_3, \tag{A3}$$

i.e.,

$$D\det F(I)\cdot G = \mathrm{Tr}\, G.$$

Using Eq. (A3), it is found that

$$D^2\det F(F_0)\cdot G = 2(G_1 \times G_2 \cdot [F_0]_3 + [F_0]_1 \times G_2 \cdot G_3 + G_1 \times [F_0]_2 \cdot G_3),$$

giving

$$D^2\det F(I)\cdot G = 2\,\mathrm{Tr}\, G_{co}.$$

□

1. The kinetic part $K(F)$

The second-order Taylor series expansion is given by

$$K_F \approx K_I + DK_I\cdot(F-I) + \frac{1}{2}D^2K_I\cdot(F-I,F-I),$$

where K_F is given in Eq. (4). Using the chain rule, Lemma A.1, and the definition of the Gâteaux derivative, it can be shown that

$$DK_{F_0}\cdot G = \frac{\hbar^2}{2m}\left\{[DF^{-1}(F_0)\cdot G]_{ji}\frac{\partial}{\partial x_j'}\left([F_0^{-1}\circ\phi_0]_{ki}\frac{\partial}{\partial x_k'}\right) + [F_0^{-1}\circ\phi_0]_{ji}\frac{\partial}{\partial x_j'}\left([DF^{-1}(F_0)\cdot G]_{ki}\frac{\partial}{\partial x_k'}\right)\right\}, \tag{A4}$$

That is

$$DK_I\cdot G = \frac{\hbar^2}{2m}\left\{[G+G^T]_{jk}\frac{\partial}{\partial x_j'}\frac{\partial}{\partial x_k'} + \frac{\partial}{\partial x_i'}([G]_{ki})\frac{\partial}{\partial x_k'}\right\}.$$

The second derivative of the kinetic part $K(F)$ can be found from Eq. (A4) using that $D^2F(\phi_0)\cdot\chi=0$ for all χ and ϕ_0, giving

$$D^2K_I\cdot(G,G) = -\frac{\hbar^2}{m}\left\{[GG^T]_{jk}\frac{\partial}{\partial x_j'}\frac{\partial}{\partial x_k'} + [G]_{ji}\frac{\partial}{\partial x_j'}([G]_{ki})\frac{\partial}{\partial x_k'} + [G^2+[G^T]^2]_{jk}\frac{\partial}{\partial x_j'}\frac{\partial}{\partial x_k'} + \frac{\partial}{\partial x_i'}([G^2]_{ki})\frac{\partial}{\partial x_k'}\right\}.$$

2. The spin-orbit part, H_{SO}

The second-order Taylor series expansion of the spin-orbit part is given by

$$H_{\phi}^{SO} \approx H_{id}^{SO} + DH_{id}^{SO} \cdot (\phi - id) + \frac{1}{2} D^2 H_{id}^{SO} \cdot (\phi - id, \phi - id),$$

where H_{ϕ}^{SO} is given in Eq. (5). Again using (6), Lemma A.1, and the chain rule, it is straightforward to show that

$$\begin{aligned} DH_{\phi_0}^{SO} \cdot \chi = -i\frac{\hbar^2}{4m^2c^2}\{&([F_0^{-1} \circ \phi_0]^T \nabla'(DV_{\phi_0} \cdot \chi)) \times ([F_0^{-1} \circ \phi_0]^T \nabla') \cdot \sigma \\ &+ (D[F^{-1}]^T(F_0) \cdot (\nabla'\chi)\nabla' V_{\phi_0}) \times ([F_0^{-1} \circ \phi_0]^T \nabla') \cdot \sigma \\ &+ ([F_0^{-1} \circ \phi_0]^T \nabla' V_{\phi_0}) \times (D[F^{-1}]^T(F_0) \cdot (\nabla'\chi)\nabla') \cdot \sigma\}, \end{aligned} \tag{A5}$$

where $F_0 = \nabla' \phi_0$. That is

$$DH_{id}^{SO} \cdot \chi = -i\frac{\hbar^2}{4m^2c^2}\{(\nabla'(DV_{id} \cdot \chi)) \times \nabla' \cdot \sigma - (\nabla'\chi^T \nabla' V_{id}) \times \nabla' \cdot \sigma - (\nabla' V_{id}) \times \nabla' \chi^T \nabla' \cdot \sigma\}.$$

From Eq. (A5), the second derivative of H_{SO} is found, arriving at

$$\begin{aligned} D^2 H_{id}^{SO} \cdot (\chi, \chi) = -i\frac{\hbar^2}{2m^2c^2}\Bigg\{&-(\nabla'\chi^T \nabla'(DV_{id} \cdot \chi)) \times \nabla' \cdot \sigma - (\nabla'(DV_{id} \cdot \chi)) \times (\nabla'\chi^T \nabla') \cdot \sigma \\ &+ \frac{1}{2}(\nabla'(D^2 V_{id} \cdot (\chi, \chi))) \times (\nabla') \cdot \sigma + (\nabla'\chi^T \nabla' V_{id}) \times (\nabla'\chi^T \nabla') \cdot \sigma \\ &+ ([\nabla'\chi^T]^2 \nabla' V_{id}) \times \nabla p' \cdot \sigma + (\nabla' V_{id}) \times ([\nabla'\chi^T]^2 \nabla') \cdot \sigma \Bigg\}. \end{aligned}$$

APPENDIX B: TAYLOR EXPANSION (WEAK FORMULATION)

In the course of determining the weak formulation, Theorem B.1 was used. First, two problems are introduced.

(I) Find ζ and E such that

$$W(\phi)(\xi \circ \phi, \zeta, E) = 0,$$

for all $\xi_+, \xi_- \in C_c^{\infty}(\phi(\mathcal{B}), \mathbb{C})$.

(II) Find ζ and E such that

$$W(\phi)(\eta, \zeta, E) = 0,$$

for all $\eta_+, \eta_- \in C_c^{\infty}(\mathcal{B}, \mathbb{C})$.

Theorem B.1. *Problem I and II are equivalent.*

Proof. Let ζ and E be a solution to problem (II), and assume that there exists a $\xi = (\xi_+, \xi_-)^T$, with $\xi_+, \xi_- \in C_c^{\infty}(\phi(\mathcal{B}), \mathbb{C})$, such that $W(\phi)(\xi \circ \phi, \zeta, E) \neq 0$. It is easily seen, using a regularizer (see Ref. 19), that there exists two sequences of functions in $C_c^{\infty}(\mathcal{B}, \mathbb{C})$, denoted $\xi_{+\epsilon}$ and $\xi_{-\epsilon}$, such that $(\xi_{+\epsilon}, \xi_{-\epsilon})^T \to \xi \circ \phi$ for $\epsilon \to 0$. Using the dominated convergence theorem (see Ref. 16), it can be shown that

$$\lim_{\epsilon \to 0}(W(\phi)((\xi_{+\epsilon}, \xi_{-\epsilon})^T, \zeta, E)) = W(\phi)(\xi \circ \phi, \zeta, E);$$

at the same time using that ζ and E is a solution to problem (II), it is found that

$$\lim_{\epsilon\to 0}(W(\phi)((\xi_{+\epsilon},\xi_{-\epsilon})^T,\zeta,E))=0.$$

But, this contradicts the assumption that $W(\phi)(\xi\circ\phi,\zeta,E)\neq 0$. From this it is seen that $W(\phi)(\xi\circ\phi,\zeta,E)=0$ for all $\xi_+,\xi_-\in C_c^\infty(\phi(\mathcal{B}),\mathbb{C})$, showing that ζ and E is also a solution to problem (I).

That a solution to problem (I) is also a solution to problem (II) is shown in a similar manner by changing to coordinates on $\phi(\mathcal{B})$ in the integrals. □

1. The kinetic part, $K^{\pm}_{\phi}$

Using the expressions in Lemma A.1, it is found that

$$\begin{aligned}[DK^{\pm}_{\phi_0}\cdot\chi](\eta_\pm,\zeta)=\frac{\hbar^2}{2m}\int_{\mathcal{B}\setminus\Gamma}\Big\{&[(DF^{-1}(F_0)\cdot\nabla'\chi)(F_0^{-1}\circ\phi)^T]_{ij}\frac{\partial(\eta_\pm)^*}{\partial x_i'}\frac{\partial\zeta_\pm}{\partial x_j'}\det F_0\\&+[(F_0^{-1}\circ\phi)(DF^{-1}(F_0)\cdot\nabla'\chi)^T]_{ij}\frac{\partial(\eta_\pm)^*}{\partial x_i'}\frac{\partial\zeta_\pm}{\partial x_j'}\det F_0\,\mathrm{d}V'\\&+[(F_0^{-1}\circ\phi)(F_0^{-1}\circ\phi)^T]_{ij}\frac{\partial(\eta_\pm)^*}{\partial x_i'}\frac{\partial\zeta_\pm}{\partial x_j'}D\det F(F_0)\cdot\nabla'\chi\Big\}\mathrm{d}V',\end{aligned}\tag{B1}$$

where $F_0=\nabla'\phi_0$, giving

$$[DK^{\pm}_{id}\cdot\chi](\eta_\pm,\zeta)=-\frac{\hbar^2}{2m}\int_{\mathcal{B}\setminus\Gamma}[\nabla'\chi+\nabla'\chi^T]_{ij}\frac{\partial(\eta_\pm)^*}{\partial x_i'}\frac{\partial\zeta_\pm}{\partial x_j'}-\frac{\partial(\eta_\pm)^*}{\partial x_i'}\frac{\partial\zeta_\pm}{\partial x_i'}\mathrm{Tr}(\nabla'\chi)\mathrm{d}V'.$$

Continuing from Eq. (B1), it is seen that

$$\begin{aligned}[D^2K^{\pm}_{id}\cdot(\chi,\chi)](\eta_\pm,\zeta)=\frac{\hbar^2}{m}\int_{\mathcal{B}\setminus\Gamma}\Big\{&[(\nabla'\chi)^2+(\nabla'\chi^T)^2+(\nabla'\chi)(\nabla'\chi)^T]_{ij}\frac{\partial(\eta_\pm)^*}{\partial x_i'}\frac{\partial\zeta_\pm}{\partial x_j'}\mathrm{d}V'\\&-[\nabla'\chi+\nabla'\chi^T]_{ij}\frac{\partial(\eta_\pm)^*}{\partial x_i'}\frac{\partial\zeta_\pm}{\partial x_j'}\mathrm{Tr}(\nabla'\chi)\mathrm{d}V'+\frac{\partial(\eta_\pm)^*}{\partial x_i'}\frac{\partial\zeta_\pm}{\partial x_i'}\mathrm{Tr}([\nabla'\chi]_{co})\Big\}\mathrm{d}V'.\end{aligned}$$

2. The potential part, $V^{\pm}_{\phi}$

Again using Lemma A.1, it is found that

$$[DV^{\pm}_{\phi_0}\cdot\chi](\eta_\pm,\zeta)=\int_{\mathcal{B}}\eta_\pm^*(DV_{\phi_0}\cdot\chi\det F_0+V_{\phi_0}\circ\phi_0 D\det F(F_0)\cdot\nabla'\chi)\zeta_\pm\mathrm{d}V',\tag{B2}$$

that is

$$[DV^{\pm}_{id}\cdot\chi](\eta_\pm,\zeta)=\int_{\mathcal{B}}\eta_\pm^*(DV_{id}\cdot\chi+V_{id}\,\mathrm{Tr}(\nabla'\chi))\zeta_\pm\mathrm{d}V'.$$

The second-order derivative is found using Eq. (B2) and Lemma A.1, giving

$$[D^2V^{\pm}_{\phi_0}\cdot\chi](\eta_\pm,\zeta)=\int_{\mathcal{B}}\eta_\pm^*(D^2V_{id}\cdot(\chi,\chi)+2DV_{id}\cdot\chi\,\mathrm{Tr}(\nabla'\chi)+2V_{id}\,\mathrm{Tr}([\nabla'\chi]_{co}))\zeta_\pm\mathrm{d}V'.$$

3. The spin-orbit part, $H_{\phi}^{\mathrm{SO},\pm}$

Finding the derivatives of the spin-orbit part is straightforward, giving

$$[DH_{id}^{\mathrm{SO},\pm}\cdot\chi](\eta_{\pm},\zeta)=-i\frac{\hbar^2}{2m^2c^2}\int_{\mathcal{B}\setminus\Gamma}\eta_{\pm}^{*}(\nabla'\chi^{T}\sigma\times\nabla'V_{id}\cdot\nabla'\zeta+\sigma\times\nabla'(DV_{id}\cdot\chi)\cdot\nabla'\zeta)_{\pm}\mathrm{d}V'$$

and

$$\begin{aligned}[D^2H_{id}^{\mathrm{SO},\pm}\cdot(\chi,\chi)](\eta_{\pm},\zeta)=&-i\frac{\hbar^2}{2m^2c^2}\int_{\mathcal{B}\setminus\Gamma}\eta_{\pm}^{*}(2\nabla'\chi^{T}\sigma\times\nabla'(DV_{id}\cdot\chi)\cdot\nabla'\zeta)_{\pm}\mathrm{d}V'\\&-i\frac{\hbar^2}{2m^2c^2}\int_{\mathcal{B}\setminus\Gamma}\eta_{\pm}^{*}(\sigma\times\nabla'(D^2V_{id}\cdot(\chi,\chi))\cdot\nabla'\zeta)_{\pm}\mathrm{d}V'.\end{aligned}$$

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Remarks on the repulsive Wigner-Poisson system

Myeongju Chae[a)]
School of Mathematics, KIAS, Korea

Seung-Yeal Ha[b)] and Hyungjin Huh[c)]
Department of Mathematical Sciences, Seoul National University, Seoul 151-747, Korea

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We present an estimate for the space-time integral of classical solutions to the repulsive Wigner-Poisson system. We use Markowich's formalism between Wigner-Possion and Schrödinger-Poisson systems. Through this formalism and Morawetz interaction potentials, we derive the same *a priori* estimate given by Chae and Ha for the repulsive Vlasov-Poisson system. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2101068]

I. INTRODUCTION

In this paper, we are interested in the Wigner-Poisson (WP) system in the absence of collisions,

$$\partial_t w + v \cdot \nabla_x w - \frac{i}{\hbar}\Theta[V]w = 0, \quad x \in \mathbb{R}^3, \quad v \in \mathbb{R}^3, \quad t > 0,$$

$$\Delta V = -4\pi n, \quad n := \int_{\mathbb{R}^3} w(x,v,t)\mathrm{d}v,$$

$$w(x,v,t=0) = w_0(x,v), \tag{1.1}$$

where w and $\hbar$ denote the Wigner density distribution function of a system of quantum mechanical particles and a constant proportional to the Planck constant, respectively, and the pseudodifferential operator $\Theta[V]$ is given as

$$(\Theta[V]w)(x,v,t) := \frac{1}{(2\pi)^3}\int\int_{\mathbb{R}^3\times\mathbb{R}^3}\left(V\left(x+\frac{\hbar}{2}\eta,t\right)-V\left(x-\frac{\hbar}{2}\eta,t\right)\right)w(x,v',t)e^{i(v-v')\eta}\,\mathrm{d}v'\,\mathrm{d}\eta. \tag{1.2}$$

Here we have taken the mass of an electron to be unit for simplicity.

The quantum Liouville system (1.1) models the quantum mechanical motion of a large electron ensemble in a vacuum under the action of the Coulomb force generated by the charge of the electrons, and was first derived by Wigner[32] in 1932 from the Schrödinger equation as the quantum analog of the classical Liouville equation (see Refs. 3 and 24 for details). Recent miniaturization process of semiconductor devices has led to the need for a quantum transport model that can be used for numerical simulations.[12,13,26,31]

The global existence of one- and two-dimensional WP system was first established by Steinrück[30] and Anold-Nier,[2] respectively. For the case of three dimension, the global existence

[a)]Electronic mail: mchae@kias.re.kr
[b)]Electronic mail: syha@math.snu.ac.kr
[c)]Electronic mail: hjhuh3@math.snu.ac.kr

was obtained using the Markowich's reformulation[23] of the WP system as a system of infinitely many Schrödinger equations coupled with the Poisson system by Brezzi-Markowich[5] for the repulsive case. Ilner-Zweifel-Lange later extended the result of Ref. 5 to both repulsive and attractive potentials in Ref. 19 and also gave some dispersion estimates of the solutions.

On the other hand, the classical limit $\hbar \to 0$ from (1.1) to the Vlasov-Poisson system (1.3) was settled by Lions-Paul[21] and Markowich-Mauser,[24]

$$\begin{gathered} \partial_t f + v \cdot \nabla_x f - \nabla_x V \cdot \nabla_v f = 0, \quad x \in \mathbb{R}^3, \quad v \in \mathbb{R}^3, \quad t > 0, \\ \Delta V = -4\pi \int_{\mathbb{R}^3} f \, \mathrm{d}v, \quad f(x,v,t=0) = f_0(x,v), \end{gathered} \tag{1.3}$$

where $f(x,v,t)$ is the distribution function for charged particles at time t, at a phase space position (x,v). Recently Chae and Ha[8] derived an estimate for the space-time integral for the classical solutions to (1.3). More precisely, they explicitly constructed a Lyapunov functional which is nonincreasing along smooth solutions and satisfies the identity

$$\mathcal{D}(f(t)) + \int_0^t \int\int\int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3} f(x,v,s) f(x,v_*,s) \mathrm{d}v_* \, \mathrm{d}v \, \mathrm{d}x \, \mathrm{d}s = \mathcal{D}(f_0), \quad t \geqslant 0.$$

This yields

$$\int_0^\infty \int\int\int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3} f(x,v,t) f(x,v_*,t) \mathrm{d}v_* \, \mathrm{d}v \, \mathrm{d}x < \infty, \tag{1.4}$$

which might be useful to analyze the time-asymptotic behavior of solutions as in Ref. 16. The key ingredients of their constructions are the time decay of local density and detailed analysis of the characteristics, which is not useful to (1.1) due to the pseudodifferential operator $(\Theta[V]w)$.

The purpose of this paper is to derive the estimate (1.4), incorporating two key ingredients. First, we use *Markowich's formalism* which establishes the equivalence between the Wigner-Poisson system and Schrödinger-Poisson system under some reasonable initial data assumption. Second, we employ *Morawetz interaction potential* which has been widely used for the study on dispersive equations especially on the nonlinear defocusing Schrödinger equation as listed in Ref. 9. Below we briefly explain Markowich's formalism between WP system and countably many Schrödinger-Poisson systems following the presentation of Ref. 17. In the sequel we set the renormalized Planck constant to be unity ($\hbar = 1$).

Let $\mathcal{F}_v(f)$ be the Fourier transform of f in v variable and $\mathcal{F}_\eta^{-1}(f)$ be its inverse Fourier transform,

$$\mathcal{F}_v(f)(x,\eta) = \int_{\mathbb{R}^3} f(x,v) e^{-iv\cdot\eta} \, \mathrm{d}v \quad \text{and } \mathcal{F}_\eta^{-1}(g)(x,v) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} g(x,\eta) e^{iv\cdot\eta} \, \mathrm{d}\eta.$$

We take the Fourier transform of (1.1) to get

$$\partial_t \mathcal{F}_v(w) + i \nabla_\eta \cdot \nabla_x \mathcal{F}_v(w) - i \delta V \mathcal{F}_v(w) = 0, \tag{1.5}$$

where δV is the symbol of the pseudodifferential operator $(\Theta[V]w)(x,v,t)$,

$$\delta V := V\left(x + \frac{\eta}{2}, t\right) - V\left(x - \frac{\eta}{2}, t\right).$$

We now introduce a set of coordinates,

$$r = x + \frac{\eta}{2}, \quad s = x - \frac{\eta}{2},$$

and one-particle density matrix z defined as

$$z(r,s,t) := \frac{1}{(2\pi)^3}\mathcal{F}_v(w)(x,\eta,t).$$

Then (1.1) is transformed to the *Heisenberg equation*,

$$iz_t - \left(\tfrac{1}{2}\Delta_s + V(s,t)\right)z + \left(\tfrac{1}{2}\Delta_r + V(r,t)\right)z = 0. \tag{1.6}$$

Note that

$$n(x,t) = \int_{\mathbb{R}^3} w(x,v,t)\mathrm{d}v = \mathcal{F}_v(x,0,t) = (2\pi)^3 z(x,x,t).$$

Suppose that datum w_0 in (1.1) satisfies the following assumption.

$(\mathcal{A})$: $z(r,s,0) \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ is the kernel of a non-negative self-adjoint trace class operator in $L^2(\mathbb{R}^3)$,

$$\int_{\mathbb{R}^3} z(r,r,0) = 1 \text{ (trace class)}, \quad z(r,s,0) = \overline{z}(s,r,0) \text{ (self-adjoint)}.$$

Then it follows from the spectral theorem that

$$z(r,s,0) = \sum_{k=1}^{\infty} \lambda_k \overline{\varphi_k(r)}\varphi_k(s), \tag{1.7}$$

where λ_k and ϕ_k satisfy

$$\lambda_k \geqslant 0, \quad \sum_{k=1}^{\infty} \lambda_k = 1, \quad \varphi_k \in L^2(\mathbb{R}^3), \quad \|\varphi_k\|_{L^2} = 1, \quad \text{for } k \geqslant 1,$$

and the series converges in $L^2(\mathbb{R}^3_r \times \mathbb{R}^3_s)$. Hence it is easy to see that

$$z(r,s,t) := \sum_{k=1}^{\infty} \lambda_k \overline{\psi_k(r,t)}\psi_k(s,t) \tag{1.8}$$

is the solution of (1.6), when the functions $\{\psi_k(x,t)\}_{k\in\mathbb{N}}$ are solutions of the Schrödinger-Poisson system,

$$\begin{aligned} i\partial_t\psi_k + \tfrac{1}{2}\Delta\psi_k &= V\psi_k, \quad x \in \mathbb{R}^3, \quad t > 0, \\ \psi_k(x,t=0) &= \varphi_k(x), \end{aligned} \tag{1.9}$$

where V is an electric potential,

$$V(x,t) = \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{n(y,t)}{|x-y|}\mathrm{d}y$$

with the density n given by

$$n(x,t) = \sum_{k=1}^{\infty} \lambda_k |\psi_k(x,t)|^2. \tag{1.10}$$

The solution w of (1.1) is given by

$$w(x,v,t) = \mathcal{F}_{\eta}^{-1}\left(z\left(x + \frac{\eta}{2}, x - \frac{\eta}{2} \right) \right), \tag{1.11}$$

and local mass density $n(\cdot,t)$ defined by (1.10) is in $L^1(\mathbb{R}^3_x)$ and non-negative under the assumption $(\mathcal{A})$. The main result of this paper is as follows.

Theorem 1.1: *Suppose that initial datum $\omega_0 \in L^2(\mathbb{R}^3_x \times \mathbb{R}^3_v)$ is real-valued and its corresponding initial density matrix $z_0 = z(\cdot,\cdot,0)$ satisfies $(\mathcal{A})$ and*

$$\sum_{m=1}^{\infty} \lambda_m \|\varphi_m\|_{H^2(\mathbb{R}^3)} < \infty.$$

Then the classical solution of (1.1) *satisfies*

$$\int_0^{\infty} \int\int\int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3} w(x,v,t) w(x,v_*,t) \mathrm{d}v_* \, \mathrm{d}v \, \mathrm{d}x \, \mathrm{d}t < \infty. \tag{1.12}$$

Remark 1.1: (1) *The above covariance-type estimate has been obtained for other classical kinetic models such as the Boltzmann equation, Vlasov-Poisson system in Refs. 8 and 16 for small algebraically decaying initial data by using appropriate Lyapunov functionals. However, it seems that such a functional approach does not give an explicit time-decay rate for solutions of aforementioned models including the Wigner-Poisson system (1.1). For the Vlasov-Poisson system describing collisionless plasma, there are estimates yielding explicit time-decay rates of the electric field E and the local density ρ with smooth, compactly supported initial data in three dimensions.*[18,29]

(2) *The asymptotic behavior of the repulsive Wigner-Poisson system was studied in many literatures, for example, the explicit time-decay rates of solution, local density, and the potential were studied in Ref. 6 for initial data satisfying*

$$\sum_{m=1}^{\infty} \lambda_m (\|\varphi_m\|_{L^2(\mathbb{R}^3)} + \|x\varphi_m\|_{L^2(\mathbb{R}^3)}) < \infty. \tag{1.13}$$

The dispersion estimate was first considered in Ref. 19 for H^2-initial data with the second condition of (1.13) using the methods from Ref. 11. In particular, the following dispersion estimate for the local density $n(x,t)$ was obtained in Refs. 6 and 9.

$$\|n(\cdot,t)\|_{L^2(\mathbb{R}^3)} \leqslant C(1+t)^{-3/4}, \quad \text{for } t \geqslant 0,$$

hence this implies the space-time estimate (1.12), apart that the initial data in Theorem 1.1 does not need the one moment condition in x variable as above. On the other hand, there is a qualitative study on asymptotic behavior of the three-dimensional Schrödinger-Poisson equation (pure quantum state) using a scaling group,[22] *where the limit behavior of the solution is described by the solutions of the corresponding linear equation.*

The rest of this paper is organized in the following manner. In Sec. II, we address time-evolution estimate of Morawetz interaction potential for the defocusing Schrödinger-Poisson system. Finally in Sec. III, we present the proof of Theorem 1.1. In the Appendix we see that the inequality (2.7) also holds for Hartree-type equations and can provide a simpler proof of scattering result for Hatree-type equations.

Notations: Throughout the paper, we use the following notations:

$$f \lesssim g \Leftrightarrow f \leqslant Cg \quad \text{for some generic positive constant } C,$$

$$\|u(t)\|_{L^p} := \|u(\cdot,t)\|_{L^p(\mathbb{R}^3)}, \quad \|u(t)\|_{H^k} := \|u(\cdot,t)\|_{H^k(\mathbb{R}^3)}.$$

II. PRELIMINARIES

In this section we present the time-evolution estimate of the Morawetz interaction potential to Schrödinger-Poisson system (see Refs. 21, 23, and 26 for details).

Consider first *pure quantum state* or the Hartree equation which corresponds to the case $\lambda_1 = 1$, $\lambda_{m>1} = 0$ in the Schrödinger-Poisson system,

$$\begin{aligned} i\partial_t\psi + \tfrac{1}{2}\Delta\psi = V(|\psi|^2)\psi, \quad x \in \mathbb{R}^3, \quad t > 0, \\ \psi(x, t=0) = \psi_0(x), \end{aligned} \tag{2.1}$$

where $V(|\psi|^2)$ is the Newtonian potential of $|\psi|^2$, i.e.,

$$V(|\psi|^2) := \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{|\psi(y,t)|^2}{|x-y|}\mathrm{d}y.$$

More generally we set

$$V(|\psi|^2)(x,t) = \int v(x-y)|\psi(y,t)|^2\,\mathrm{d}y$$

for a non-negative function v with some integrability condition. We refer to Eq. (2.1) with such a general potential to be of Hartree type, which will be considered in the Appendix. In the sequel, we often drop the $|\psi|^2$ dependence in $V(|\psi|^2)$ for notational simplicity, i.e., $V := V(|\psi|^2)$. The conservation of L^2-norm and the energy defined as

$$E[t] := \int_{\mathbb{R}^3} (|\nabla\psi(t)|^2 + V|\psi(t)|^2)\mathrm{d}x$$

follow from the lemma below.

Lemma 2.1: Let ψ be a classical solution of (2.1) and decay fast enough at infinity. Then the following conservation laws hold:

$$\partial_t|\psi|^2 + \mathrm{div}(\mathrm{Im}\,\bar{\psi}\nabla\psi) = 0,$$

$$\partial_t(|\nabla\psi|^2 + V(\psi)|\psi|^2) + \mathrm{div}\left(2\,\mathrm{Re}(\nabla\bar{\psi}\partial_t\psi) - \frac{1}{2\pi}V\nabla\partial_t V - \frac{1}{4\pi}\partial_t(\nabla\cdot(V\nabla V))\right) = 0.$$

Proof: For the detailed proof, we refer to Ref. 7. □

We next turn to the Morawetz interaction potential introduced in Ref. 9. For given classical solution ψ of (2.1), define Morawetz interaction potential $M[\psi(t)]$ by

$$M[\psi(t)] := \int_{\mathbb{R}^3} |\psi(x,t)|^2 \underbrace{\left(\int_{\mathbb{R}^3} \mathrm{Im}[\bar{\psi}(y,t)\nabla\psi(y,t)]\cdot\frac{y-x}{|y-x|}\mathrm{d}y\right)}_{:=M_x[\psi(t)]}\mathrm{d}x. \tag{2.2}$$

We note that

$$|M_x[\psi(t)]| \leqslant \|\psi(t)\|_{L^2}\|\nabla\psi(t)\|_{L^2} \leqslant \|\psi_0\|_{L^2}E[0].$$

This yields *a priori* bound for $M[\psi(t)]$,

$$|M[\psi(t)]| \leqslant \|\psi_0\|_{L^2}^3 E[0].$$

We first study the time evolution of the weight $M_x[\psi(t)]$.

Lemma 2.2: Let ψ be the classical solution of (2.1). Then we have

$$(1) \quad \frac{d}{dt} M_x[\psi(t)] = 2\pi|\psi(x,t)|^2 + \int_{\mathbb{R}^3} \frac{|\nabla_x \psi(y,t)|^2}{|y-x|} dy + \int_{\mathbb{R}^3} \frac{1}{|y-x|} \left(\frac{y-x}{|y-x|} \cdot \nabla V(y,t) \right)^2 dy,$$

$$(2) \quad \nabla_x M_x[\psi(t)] = -2 \int_{\mathbb{R}^3} \frac{\mathrm{Im}[\bar{\psi}(y,t) \nabla \psi(y,t)]}{|y-x|} dy,$$

where $V(x,t) = V(|\psi|^2)$ and $\nabla_x \psi$ denotes the angular part of $\nabla \psi$, i.e.,

$$\nabla_x \psi = \nabla \psi - \frac{y-x}{|y-x|} \left(\frac{y-x}{|y-x|} \cdot \nabla \psi \right).$$

Proof: (1) We first rewrite

$$M_x[\psi(t)] = \mathrm{Im} \int_{\mathbb{R}^3} \bar{\psi}(y,t) \partial_r \psi(y,t) dy = \mathrm{Im} \int_{\mathbb{R}^3} \bar{\psi}(y,t) \left(\partial_r + \frac{1}{r} \right) \psi(y,t) dy = \mathrm{Im} \int_0^\infty \int_{\mathbb{S}^2} r \bar{\psi} \partial_r (r\psi) d\omega \, dr, \tag{2.3}$$

where we used

$$r = |y-x|, \quad \mathbb{S}^2 = \{y \in \mathbb{R}^3 : |y-x| = 1\} \quad \text{and} \quad \mathrm{Im} \int_{\mathbb{R}^3} \frac{1}{r} |\psi(y,t)|^2 \, dy = 0.$$

We use integration by parts and the equation (2.1) to see

$$\begin{aligned}
\frac{d}{dt} M_x(t) &= \mathrm{Im} \int_0^\infty \int_{\mathbb{S}^2} (\overline{r\psi}) \partial_r (r\psi_t) + (\overline{r\psi_t}) \partial_r (r\psi) d\omega \, dr \\
&= -2 \, \mathrm{Im} \int_0^\infty \int_{\mathbb{S}^2} \partial_r (\overline{r\psi}) (r\psi_t) d\omega \, dr \\
&= -2 \, \mathrm{Im} \int_0^\infty \int_{\mathbb{S}^2} \partial_r (\overline{r\psi}) \left(\frac{i}{2} \partial_r^2 (r\psi) + \frac{i}{2r} \Delta_\omega \psi - irV\psi \right) d\omega \, dr \\
&= -\mathrm{Re} \int_0^\infty \int_{\mathbb{S}^2} \partial_r (\overline{r\psi}) \partial_r^2 (r\psi) d\omega \, dr - \mathrm{Re} \int_0^\infty \int_{\mathbb{S}^2} \partial_r (\overline{r\psi}) \frac{1}{r} \Delta_\omega \psi \, d\omega \, dr \\
&\quad + 2 \, \mathrm{Re} \int_0^\infty \int_{\mathbb{S}^2} \partial_r (\overline{r\psi}) rV\psi \, d\omega \, dr := \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3,
\end{aligned}$$

where we used

$$\Delta \psi = \partial_r^2 \psi + \frac{2}{r} \partial_r \psi + \frac{1}{r^2} \Delta_w \psi.$$

By the same arguments given in Ref. 9, $\mathcal{I}_1$ and $\mathcal{I}_2$ satisfy

$$\mathcal{I}_1+\mathcal{I}_2=2\pi|\psi(x,t)|^2+\int_{\mathbb{R}^3}\frac{1}{|y-x|}|\nabla_x\psi(y,t)|^2\,\mathrm{d}y.$$

For the quantity $\mathcal{I}_3$, we have

$$\begin{aligned}2\,\mathrm{Re}\int_0^\infty\int_{\mathbb{S}^2}\partial_r(\overline{r\psi})rV\psi\,\mathrm{d}\omega\,\mathrm{d}r&=\int_0^\infty\int_{\mathbb{S}^2}\partial_r(r^2|\psi|^2)V\,\mathrm{d}\omega\,\mathrm{d}r\\&=\int_{\mathbb{R}^3}\frac{y-x}{|y-x|^3}\cdot\nabla(r^2|\psi|^2)V\,\mathrm{d}y\\&=-\int_{\mathbb{R}^3}|\psi|^2\frac{y-x}{|y-x|}\cdot\nabla V\,\mathrm{d}y=\int_{\mathbb{R}^3}\Delta V\frac{y-x}{|y-x|}\cdot\nabla V\,\mathrm{d}y,\end{aligned}$$

where we used

$$2\,\mathrm{Re}\{\partial_r(\overline{r\psi})rV\psi\}=\partial_r(r^2|\psi|^2)V\quad\text{and}\quad-|\psi(y,t)|^2=\Delta V.$$

Note that

$$\int_{\mathbb{R}^3}\Delta V\frac{y-x}{|y-x|}\cdot\nabla V(y,t)\mathrm{d}y=\int_{\mathbb{R}^3}\nabla_j\nabla_jV\frac{y_i-x_i}{|y-x|}\nabla_iV(y,t)\mathrm{d}y.$$

On the other hand, if $i\neq j$ we have

$$\int_{\mathbb{R}^3}\nabla_j\nabla_jV\frac{y_i-x_i}{|y-x|}\nabla_iV(y,t)\mathrm{d}y=\int_{\mathbb{R}^3}\frac{(y_i-x_i)(y_j-x_j)}{|y-x|^3}\nabla_iV\nabla_jV+\frac{1}{2}\left(\frac{1}{|y-x|}-\frac{(y_i-x_i)^2}{|y-x|^3}\right)\nabla_jV\nabla_jV\,\mathrm{d}y.\tag{2.4}$$

If $i=j$, then

$$\int_{\mathbb{R}^3}\nabla_i\nabla_iV\frac{y_i-x_i}{|y-x|}\nabla_iV(y,t)\mathrm{d}y=\int_{\mathbb{R}^3}-\frac{1}{2}\left(\frac{1}{|y-x|}-\frac{(y_i-x_i)^2}{|y-x|^3}\right)\nabla_iV\nabla_iV\,\mathrm{d}y.\tag{2.5}$$

Adding (2.4) and (2.5) and considering $i,j=1,2,3$ we obtain

$$-\int_{\mathbb{R}^3}|\psi(y,t)|^2\frac{y-x}{|y-x|}\cdot\nabla V(y,t)\mathrm{d}y=\int_{\mathbb{R}^3}\frac{1}{|y-x|}\left(\frac{y-x}{|y-x|}\cdot\nabla V(y,t)\right)^2\mathrm{d}y.$$

(2) We use

$$\nabla_x\cdot\left(\frac{y-x}{|y-x|}\right)=-\frac{2}{|y-x|}$$

to find

$$\nabla_xM_x[\psi(t)]=\nabla_x\left(\int_{\mathbb{R}^3}\mathrm{Im}(\bar{\psi}(y,t)\,\nabla\,\psi(y,t))\cdot\frac{y-x}{|y-x|}\mathrm{d}y\right)=-2\int_{\mathbb{R}^3}\frac{1}{|y-x|}\,\mathrm{Im}(\bar{\psi}(y,t)\,\nabla\,\psi(y,t))\mathrm{d}y.$$

□

Remark 2.1: (1) *The above Morawetz interaction potential was introduced to simplify the well-known Morawetz-type estimate by Lin-Strauss*[22] *for the nonlinear Schrödinger equation in Ref. 9.*

(2) *The Morawetz interaction potential is in spirit similar to the interaction potentials*[4,8,16] *in*

classical kinetic theory. As described in Ref. 10 when u satisfies a defocusing nonlinear Schrödinger equation

$$iu_t + \Delta u = |u|^{p-1}u, \quad p > 1,$$

we can define Morawetz interaction potential more generally by $M^a(t) := \partial_t V^a$, *where*

$$V^a(t) := \int\int_{\mathbb{R}^3\times\mathbb{R}^3} T_{00}(t,x)T_{00}(t,y)a(x-y)\mathrm{d}x\,\mathrm{d}y$$

with mass density $T_{00}=|u|^2$ *for an arbitrary real valued function* $a(x)$. *We let* $a(x)=|x|$ *for the above Morawetz interaction potential* $M(t)$.

Since the linear Schrödinger equation is transformed to the linear transport equation through Wigner transformation,

$$f(x,v,t) = \frac{1}{(2\pi)^n}\int_{\mathbb{R}^3} e^{-iv\cdot y}u\left(x+\frac{y}{2},t\right)\bar{u}\left(x-\frac{y}{2},t\right)\mathrm{d}y,$$

and mass density $|u|^2$ *corresponds to* $\int f(x,v,t)\mathrm{d}v$ *in the phase space, we would define*

$$M^a(t) := \partial_t \underbrace{\int\int\int\int}_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3} f(x,v,t)f(y,v_*,t)a(x-y)\mathrm{d}v\,\mathrm{d}v_*\,\mathrm{d}x\,\mathrm{d}y$$

for a phase space density function f. *If* f *satisfies the Boltzmann equation*,

$$\partial_t f(x,v,t) + v\cdot\nabla_x f(x,v,t) = Q(f,f)(x,v,t),$$

we have

$$M^a(t) = \underbrace{\int\int\int\int}_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3} (v-v_*)\cdot b(x-y)f(x,v,t)f(y,v_*,t)\mathrm{d}v\,\mathrm{d}v_*\,\mathrm{d}x\,\mathrm{d}y$$

with $b(x)=\nabla_x a(x)$, *employing conservation of mass and momentum. If we let* $b(\cdot)=\chi_{x\geqslant 0}(\cdot)$ *for the one-dimensional case, we obtain the celebrating Bony's interaction potential for the one-dimensional Boltzmann model*,

$$I[f](t) = \underbrace{\int\int}_{y<x}\int\int_{\mathbb{R}\times\mathbb{R}} (v-v_*)f(x,v,t)f(y,v_*,t)\mathrm{d}y\,\mathrm{d}x\,\mathrm{d}v\,\mathrm{d}v_*,$$

which enjoys

$$\partial_t I[f](t) = \frac{1}{2}\int\int\int_{\mathbb{R}\times\mathbb{R}\times\mathbb{R}} (v-v_*)^2 f(x,v,t)f(y,v_*,t)\mathrm{d}x\,\mathrm{d}v\,\mathrm{d}v_*.$$

The interaction potentials $\mathcal{D}(f(t))$ *in Refs. 8 and 16 can be considered as a generalization of Bony's potential*.

Proposition 2.1: Let ψ *be a classical solution of (2.1) with finite mass and energy. Then we have*

$$(1)\quad \frac{\mathrm{d}M[\psi(t)]}{\mathrm{d}t} \geqslant 2\pi\int_{\mathbb{R}^3}|\psi(x,t)|^4\,\mathrm{d}x + \int\int_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|\psi(x,t)|^2}{y-x}\left(\frac{y-x}{|y-x|}\cdot\nabla V(y,t)\right)^2\mathrm{d}y\,\mathrm{d}x,$$

$$(2)\quad \int_0^\infty \int_{\mathbb{R}^3} |\psi(x,t)|^4 \,\mathrm{d}x\,\mathrm{d}t \leqslant \|\psi_0\|^3_{L^2(\mathbb{R}^3)} E(0).$$

Proof: (1) We use Lemma 2.2 to see

$$\begin{aligned}\frac{d}{\mathrm{d}t}M[t] &= \int_{\mathbb{R}^3} [(\partial_t|\psi(x,t)|^2)M_x[t] + |\psi(x,t)|^2\partial_t M_x[t]]\mathrm{d}x = \int_{\mathbb{R}^3} [(\partial_t|\psi(x,t)|^2)M_x[t] \\ &+ 2\pi\int_{\mathbb{R}^3} |\psi(x,t)|^4 \,\mathrm{d}x + \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\psi(x,t)|^2|\nabla_x\psi(y,t)|^2}{|y-x|}\mathrm{d}y\,\mathrm{d}x \\ &+ \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\psi(x,t)|^2}{|y-x|}\left(\frac{y-x}{|y-x|}\cdot\nabla V(y,t)\right)^2 \mathrm{d}y\,\mathrm{d}x := \mathcal{J}_1[t] + \mathcal{J}_2[t] + \mathcal{J}_3[t] + \mathcal{J}_4[t].\end{aligned}$$

We next show

$$\mathcal{J}_1[t] + \mathcal{J}_3[t] \geqslant 0. \tag{2.6}$$

It follows from Lemma 2.1 that

$$\partial_t|\psi(x,t)|^2 = -\nabla_x\cdot(\mathrm{Im}[\bar{\psi}(x,t)\,\nabla\,\psi(x,t)]).$$

Then $\mathcal{J}_1[t]$ becomes

$$\mathcal{J}_1[t] = -\int\int_{\mathbb{R}^3\times\mathbb{R}^3} \nabla_x\cdot(\mathrm{Im}[\bar{\psi}(x,t)\nabla_x\psi(x,t)])\mathrm{Im}[\bar{\psi}(y)\nabla_x\psi(y,t)]\cdot\frac{y-x}{|y-x|}\mathrm{d}y\,\mathrm{d}x.$$

Define the momentum vector $\mathbf{P}(x,t)=\mathrm{Im}[\bar{\psi}(x,t)\nabla\psi(x,t)]$. We use integration by parts in y and the identity

$$\partial_{x_j}\left(\frac{y_i-x_i}{|y-x|}\right) = -\frac{\delta_{ji}}{|y-x|} + \frac{(y_j-x_j)(y_i-x_i)}{|y-x|^3}$$

to obtain

$$\begin{aligned}\mathcal{J}_1[t] &= -\int\int_{\mathbb{R}^3\times\mathbb{R}^3}\left[\mathbf{P}(x,t)\cdot\mathbf{P}(y,t) - \left(\mathbf{P}(x,t)\cdot\frac{y-x}{|y-x|}\right)\left(\mathbf{P}(y,t)\cdot\frac{y-x}{|y-x|}\right)\right]\frac{\mathrm{d}y\,\mathrm{d}x}{|y-x|} \\ &\geqslant -\int\int_{\mathbb{R}^3\times\mathbb{R}^3} |\psi(x,t)||\nabla_x\psi(x,t)||\psi(y,t)||\nabla_x\psi(y,t)|\frac{\mathrm{d}y\,\mathrm{d}x}{|y-x|}.\end{aligned}$$

We apply the inequality $|ab|\leqslant\frac{1}{2}(a^2+b^2)$ with $a=|\nabla_x\psi(x,t)||\psi(y,t)|$ and $b=|\psi(x,t)||\nabla_x\psi(y,t)|$ to see (2.6). Finally we have

$$\frac{d}{\mathrm{d}t}M[\psi(t)] \geqslant 2\pi\int_{\mathbb{R}^3}|\psi(x,t)|^4\,\mathrm{d}x + \int\int_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|\psi(x,t)|^2}{|y-x|}\left(\frac{y-x}{|y-x|}\cdot\nabla V(y,t)\right)^2\mathrm{d}y\,\mathrm{d}x.$$

(2) We integrate the above inequality from $t=0$ to $t=T$ to see

$$2\pi\int_0^T\int_{\mathbb{R}^3}|\psi(y,t)|^4\,\mathrm{d}y\,\mathrm{d}t \leqslant 2\sup_{t\in[0,T]}|M[\psi(t)]| \leqslant 2\|\psi_0\|^3_{L^2}E(0). \tag{2.7}$$

□

III. *A PRIORI* DISPERSION ESTIMATE

In this section, we present the proof of the Theorem 1.1 via Markowich's formalism between WP system and SP system and Morawetz's interaction potential in Sec. II.

Let w be the classical solutions to (1.1) with initial data satisfying the assumption of Theorem 1.1. Then we have

$$w(x,v,t)=\sum_{k=1}^{\infty}\lambda_k w[\psi_k],\quad \lambda_k\geqslant 0,$$

where $\psi_k(k=1,2,3,\ldots)$ is the solution of the Schrödinger-Poisson system

$$\begin{aligned} &i\partial_t\psi_k+\tfrac{1}{2}\Delta\psi_k=V\psi_k,\quad k\in\mathbb{N},\\ &\psi_k(x,t=0)=\varphi_k, \end{aligned} \tag{3.1}$$

where the electric potential V is defined by the Newtonian potential of n,

$$V=\frac{1}{4\pi}\int_{\mathbb{R}^3}\frac{n(y,t)}{|y-x|}\mathrm{d}y\quad\text{and } n(x,t)=\sum_{k=1}^{\infty}\lambda_k|\psi_k(x,t)|^2. \tag{3.2}$$

In the similar manner to the preceding section, we define a Morawetz interaction potential $\mathcal{M}[t]$ for (3.1),

$$\mathcal{M}[t]:=\sum_{k,m=1}^{\infty}\mathcal{M}_{km}[t],$$

$$\mathcal{M}_{km}[t]:=\int_{\mathbb{R}^3}(\lambda_k|\psi_k(x,t)|^2)(\lambda_m M_x[\psi_m(t)])\mathrm{d}x=\lambda_k\lambda_m\int_{\mathbb{R}^3}|\psi_k(x,t)|^2M_x[\psi_m(t)]\mathrm{d}x,$$

where $M_x[\psi_m(t)]$ is the functional defined in Sec. II. Then we have *a priori* estimates

$$|\mathcal{M}[t]|\leqslant\left(\sum_{k=1}^{\infty}\lambda_k\|\varphi_k\|^2_{L^2(\mathbb{R}^3)}\right)\left(\sum_{m=1}^{\infty}(\lambda_m\|\varphi_m\|^2_{L^2(\mathbb{R}^3)}+\lambda_m\|\nabla\varphi_m\|^2_{L^2(\mathbb{R}^3)})\right)\leqslant\left(\sum_{k=1}^{\infty}\lambda_k\|\varphi_k\|^2_{L^2(\mathbb{R}^3)}\right)E(0)<\infty. \tag{3.3}$$

Below we study the time evolution of $\mathcal{M}[t]$.

Lemma 3.1: Let $\psi_k,k=1,2,3,\ldots$ be a classical solutions of (3.1) decaying at infinity in x. Then we have

$$\begin{aligned} \frac{d}{\mathrm{d}t}\mathcal{M}[t]\geqslant{}&2\pi\sum_{k,m=1}^{\infty}\lambda_k\lambda_m\int_{\mathbb{R}^3}|\psi_k(x,t)|^2|\psi_m(x,t)|^2\,\mathrm{d}x\\ &+\sum_{k,m=1}^{\infty}\lambda_k\lambda_m\int\int_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|\psi_k(x,t)|^2}{|y-x|}\left(\frac{y-x}{|y-x|}\cdot\nabla V(y,t)\right)^2\mathrm{d}y\,\mathrm{d}x. \end{aligned}$$

Proof: Let $k,m\in\mathbf{N}$, then it follows from Proposition 2.1 that

$$\frac{d}{dt}\int_{\mathbb{R}^3}|\psi_k(x,t)|^2 M_x[\psi_m(t)]dx = \int_{\mathbb{R}^3}(\partial_t|\psi_k(x,t)|^2)M_x[\psi_m(t)]dx + \int_{\mathbb{R}^3}|\psi_k(x,t)|^2(\partial_t M_x[\psi_m(t)])dx$$

$$= \int_{\mathbb{R}^3}(\partial_t|\psi_k(x,t)|^2)M_x[\psi_m(t)]dx$$

$$+ \int\int_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|\psi_k(x,t)|^2|\nabla_x\psi_m(y,t)|^2}{|y-x|}dy\,dx$$

$$+ 2\pi\int_{\mathbb{R}^3}|\psi_k(x,t)|^2|\psi_m(x,t)|^2\,dx$$

$$+ \int\int_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|\psi_k(x,t)|^2}{|y-x|}\left(\frac{y-x}{|y-x|}\cdot\nabla V(y,t)\right)^2 dy\,dx.$$

We multiply the above inequality by $\lambda_k\lambda_m$ and sum up over k, m to find the desired result. □

The proof of Theorem 1.1: Define an interaction production functional $\Lambda[w]$ introduced in Ref. 8,

$$\Lambda[w(t)] := \int\int\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3} w(x,v,t)w(x,v_*,t)dv\,dv_*\,dx. \tag{3.4}$$

This can be regarded as functionals measuring *imaginary* collisions between quantum particles, although the physical situation is not clear unlike to the classical analogous case.[8] Then for given $T>0$, we have

$$\int_0^T\Lambda[w(t)]dt = \int_0^T\int\int\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3}\sum_{k,m=1}^{\infty}\lambda_k\lambda_m w[\psi_k](x,v,t)w[\psi_m](x,v_*,t)dv\,dv_*\,dx\,dt$$

$$= \sum_{k,m=1}^{\infty}\int_0^T\int_{\mathbb{R}^3}\lambda_k\lambda_m\int_{\mathbb{R}^3}w[\psi_k](x,v,t)dv\,dt\int_{\mathbb{R}^3}w[\psi_m](x,v_*,t)dv_*\,dx$$

$$= \sum_{k,m=1}^{\infty}\int_0^T\int_{\mathbb{R}^3}\lambda_k\lambda_m|\psi_k(x,t)|^2|\psi_m(x,t)|^2\,dx\,dt \leqslant \frac{1}{2\pi}(|\mathcal{M}[t]|+|\mathcal{M}[0]|)$$

$$\leqslant \left(\sum_{k=1}^{\infty}\lambda_k\|\psi_{k0}\|^2_{L^2(\mathbb{R}^3)}\right)E(0).$$

This completes the proof.

Remark 3.1: The computation in Secs. II and III is also valid assuming $\psi\in H^1(\mathbb{R}^3)$ for Hartree equation and $\psi_k\in H^1(\mathbb{R}^3)$, $k=1,2,3,\ldots$ such that $\{\psi_k:\Sigma_{k=1}^{\infty}\lambda_k\|\psi_k\|_{H^1(\mathbb{R}^3)}\}<\infty$ for the Schrödinger-Poisson system. In fact, the global well-posedness in $H^1(\mathbb{R}^3)$ space can be easily proved combining the energy conservation and the Stricharz estimate for the Schrödinger equation, as in the same manner in Ref. 6.

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APPENDIX: ENERGY SCATTERING FOR HARTREE-TYPE EQUATIONS

In this section we provide a simpler proof of the scattering result of Refs. 14 and 27 for Hartree-type equations in dimension 3,

$$\begin{aligned} i\partial_t u + \tfrac{1}{2}\Delta u = (v * |u|^2)u, \quad x \in \mathbb{R}^3, \quad t > 0, \\ u(x,t=0) = u_0(x). \end{aligned} \tag{A1}$$

More precisely we obtain the same space-time estimate in Proposition 2.1 for (A1) to prove the asymptotic completeness part of the scattering result. The initial value problem of (A1) is globally well-posed for data $u_0 \in H^1(\mathbb{R}^3)$ if $v \in L^{p_1}+L^{p_2}$ with $1 \leqslant p_1 \leqslant p_2 \leqslant \infty$ (Ref. 14).

Lemma A.1: Let u be the classical solution of (A1) *with* $v \in L^{p_1}+L^{p_2}$, $1 \leqslant p_1 \leqslant p_2 \leqslant \infty$, *and* $v(x)=v(|x|)$. *If we define the Morawetz interaction potential for u by* (2.2), *then we have*

$$\begin{aligned} (1) \quad \frac{d}{dt}M_x[u(t)] &= 2\pi|u(x,t)|^2 + \int_{\mathbb{R}^3} \frac{|\nabla_x u(y,t)|^2}{|y-x|}\,dy \\ &\quad - \frac{1}{2}\int\int_{\mathbb{R}^3\times\mathbb{R}^3} v'(|y-z|)\frac{y-z}{|y-z|}\cdot\left(\frac{y-x}{|y-x|}-\frac{z-x}{|z-x|}\right)|u(y)|^2|u(z)|^2\,dz\,dy, \end{aligned}$$

$$\begin{aligned} (2) \quad \frac{dM[u(t)]}{dt} &\geqslant 2\pi\int_{\mathbb{R}^3}|u(x,t)|^4\,dx - \frac{1}{2}\underbrace{\int\int\int}_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3} v'(|y-z|)\frac{y-z}{|y-z|}\cdot\left(\frac{y-x}{|y-x|}-\frac{z-x}{|z-x|}\right) \\ &\quad \times|u(x)|^2|u(y)|^2|u(z)|^2\,dz\,dy\,dx. \end{aligned}$$

We note that if $v(|x|)$ *is nonincreasing in* $|x|$, *then the third terms in the item* (1), (2) *are nonnegative since* $v' \leqslant 0$ *and*

$$\frac{y-z}{|y-z|}\cdot\left(\frac{y-x}{|y-x|}-\frac{z-x}{|z-x|}\right) \geqslant 0.$$

Proof: We only need to modify the estimate of the quantity $\mathcal{I}_3$ in Lemma 2.2 as

$$\begin{aligned} 2\,\mathrm{Re}\int_0^\infty\int_{S^2}\partial_r(\overline{ru})rVu\,d\omega\,dr &= \int_0^\infty\int_{S^2}\partial_r(r^2|u|^2)V\,d\omega\,dr \\ &= \int_{\mathbb{R}^3}\frac{y-x}{|y-x|^3}\cdot\nabla(r^2|u|^2)V\,dy = -\int_{\mathbb{R}^3}|u|^2\frac{y-x}{|y-x|}\cdot\nabla V\,dy \\ &= -\int_{\mathbb{R}^3}|u(y)|^2\frac{y_i-x_i}{|y-x|}\int_{\mathbb{R}^3}v'(|y-z|)\frac{y_i-z_i}{|y-z|}|u(z)|^2\,dz\,dy \\ &= -\frac{1}{2}\int\int v'(|y-z|)\frac{y-z}{|y-z|}\cdot\left(\frac{y-x}{|y-x|}-\frac{z-x}{|z-x|}\right)|u(y)|^2|u(z)|^2\,dz\,dy. \end{aligned}$$

□

The energy defined by

$$E[t] := \int_{\mathbb{R}^3}|\nabla u|^2 + (v * |u|^2)|u|^2\,dx$$

and $\|u(t)\|_{L^2}$ are conserved for Eq. (A1). Therefore under the same condition in the above lemma, we have

$$\int_0^\infty \int_{\mathbb{R}^3} |u|^4(x,t)\mathrm{d}x\,\mathrm{d}t \leqslant M[u(t)] \leqslant \|u(0)\|_{L^2}^3 E[0] \tag{A2}$$

if $v(|x|)$ is non-negative and nonincreasing in $|x|$.

Theorem A.1: *Assume that a non-negative* $v \in L^{p_1}+L^{p_2}$ *satisfying* $1 \leqslant p_1 \leqslant p_2 < 3/2$ *and* $v(x)=v(|x|)$ *with* $v(|x|)$ *nonincreasing in* $|x|$. *Then there is scattering for* H^1 *solutions. Precisely, for any solution* u *of* (A1) *with* $u(0) \in H^1(\mathbb{R}^3)$, *there exists a solution* w *of the free Schrödinger equation with* $w(0) \in H^1(\mathbb{R}^3)$ *such that* $\|u(t)-w(t)\|_{H^1} \to 0$ *as* $t \to \infty$. *In other words, the equation is asymptotically complete in* $H^1(\mathbb{R}^3)$. *Moreover, the correspondence* $u(0) \mapsto w(0)$ *defines a homeomorphism in* $H^1(\mathbb{R}^3)$.

According to Sec. 4 in Ref. 14, asymptotic completeness will follow once we establish that the global solution belongs to $X^1(\mathbb{R})$, where

$$X^1(\mathbb{R}) = \{u : u \text{ and } \nabla u \in X(\mathbb{R})\},$$

$$X(\mathbb{R}) = \{u : u \in C(\mathbb{R},L^2) \text{ and } u \in L^q(\mathbb{R},L^r) \text{ for admissible pair } (q,r)\}.$$

We refer to (q,r) as the admissible pair when $q,r \geqslant 2$, and

$$\frac{1}{q}+\frac{3}{2r}=\frac{3}{4}.$$

We recall the Strichartz estimates of the Schrödinger equation in three space dimension.

Proposition A.1: Suppose that (q,r), $(\tilde{q},\tilde{r})$ *are any two Schrödinger admissible pairs as the above. Suppose that* $u(x,t)$ *is a solution of the problem*

$$i\partial_t u(x,t) + \Delta u(x,t) = F(x,t), \quad (x,t) \in \mathbb{R}^3 \times [0,T],$$

for some data $u(0)$ *and* $T>0$. *Then we have the estimate*

$$\|u\|_{L_t^q L_x^r([0,T]\times\mathbb{R}^3)} \lesssim \|u(0)\|_{L^2(\mathbb{R}^3)} + \|F\|_{L_t^{\tilde{q}'} L_x^{\tilde{r}'}([0,T]\times\mathbb{R}^3)}, \tag{A3}$$

where

$$\frac{1}{\tilde{q}}+\frac{1}{\tilde{q}'}=1, \quad \frac{1}{\tilde{r}}+\frac{1}{\tilde{r}'}=1.$$

Let us define $Z(t)$ as

$$Z(t) = \sup_{(q,r)\ \text{admissible}} \|\langle\nabla\rangle u\|_{L_t^q L_x^r([0,t]\times\mathbb{R}^3)}. \tag{A4}$$

$\langle A\rangle = (1+A^2)^{1/2}$, and $\langle\nabla\rangle^s$ for the operator with Fourier multiplier $(1+|\xi|^2)^{s/2}$. We omit the index in case that $s=1$.

We claim that

$$Z(t) \leqslant C(\|u(0)\|_{H^1})$$

and this will settle the asymptotic completeness. Following the same manner in Ref. 9, we can decompose thanks to (A2) the time interval $(0,\infty)$ into a finite number of disjoint intervals $J_1, J_2, \ldots, J_K$ where for $i=1,\ldots,K$ we have

$$\|u\|_{L_{x,t}^4(J_i\times\mathbb{R}^3)} \leqslant \delta \tag{A5}$$

for a constant δ depending only on $\|u(0)\|_{H1}$ to be chosen later.

Choosing $\tilde{q}', \tilde{r}' = \frac{10}{7}$, the estimate (A3) gives for all $t \in J_1$,

$$Z(t) \lesssim \|u(0)\|_{H^1(\mathbb{R}^3)} + \|(v * |u|^2)u\|_{L_{t,x}^{10/7}([0,t]\times\mathbb{R}^3)} + \|\nabla((v * |u|^2)u)\|_{L_{t,x}^{10/7}([0,t]\times\mathbb{R}^3)}.$$

In the following we assume $p_1=p_2=3/(2+\varepsilon)$ for some $\varepsilon \in (0,1]$ and denote both by p without loss of generality.

(i) Estimate of $\|(v*\nabla|u|^2)u\|_{L_{t,x}^{\frac{10}{7}}}$.

By using the Hölder and Young inequality, we have

$$\|(v * \nabla|u|^2)u\|_{L_{t,x}^{\frac{10}{7}}([0,t]\times\mathbb{R}^3)} \leqslant \|v * \nabla|u|^2\|_{L_{t,x}^{\frac{20}{9}}([0,t]\times\mathbb{R}^3)}\|u\|_{L_{t,x}^4([0,t]\times\mathbb{R}^3)}.$$

When $0<\varepsilon<\frac{1}{4}$,

$$\|v * \bigtriangledown |u|^2\|_{L_{t,x([0,t]\times\mathbb{R}^3)}^{\frac{20}{9}}} \leqslant \|v\|_{L_x^{\frac{3}{2+\epsilon}}}\left(\int \|u \bigtriangledown u\|_{L_x^{\frac{60}{47-20\epsilon}}}^{\frac{20}{9}} dt\right)^{\frac{9}{20}}$$

$$\leqslant C(\|v\|_{L_x^{\frac{3}{2+\epsilon}}}, \|\bigtriangledown u\|_{L_t^\infty L_x^2([0,t]\times R^3)})\left(\int \|u\|_{L_x^{\frac{60}{17-20\epsilon}}}^{\frac{20}{9}} dt\right)^{\frac{9}{20}}$$

$$\leqslant C(\|v\|_{L_x^{\frac{3}{2+\epsilon}}}, \|\bigtriangledown u\|_{L_t^\infty L_x^2}([0,t]\times R^3), \|u\|_{L_t^\infty L_x^{\frac{12}{1-4\epsilon}}([0,t]\times R^3)})\|u\|_{L_t^{\frac{20}{9}}L_x^5([0,t]\times R^3)}$$

When $\frac{1}{4}\leqslant\epsilon\leqslant 1$,

$$\|v * \bigtriangledown |u|^2\|_{L_{t,x}^{\frac{20}{9}}([0,t]\times\mathbb{R}^3)} \leqslant \|v\|_{L_x^{\frac{3}{2+\epsilon}}}\|\nabla u\|_{L_t^{\frac{20}{9}}L_t^5([0,t]\times\mathbb{R}^3)}\|u\|_{L_t^\infty L_x^{\frac{12}{7-4\epsilon}}([0,t]\times\mathbb{R}^3)}.$$

Note that $\|u\|_{L_t^\infty L_x^m([0,\infty])\times R^3)}$ is bounded by $\|u(0)\|_{L_x^2}$ and the energy for any $2\leqslant m<\infty$, and that $(\frac{20}{9},5)$ is admissible. Thus we have

$$\|(v * \nabla|u|^2)u\|_{L_{t,x}^{\frac{10}{7}}([0,t]\times\mathbb{R}^3)} \lesssim \delta\|v\|_{L_x^p}Z(t).$$

(ii) Estimate of $\|(v*|u|^2)\nabla u\|_{L_{t,x}^{10/7}([0,t]\times\mathbb{R}^3)}$.

By using the Hölder and Young inequality, we have

$$\|(v * |u|^2)\nabla u\|_{L_{t,x}^{10/7}([0,t]\times\mathbb{R}^3)} \leqslant \|v * |u|^2\|_{L_{t,x}^{5/2}([0,t]\times\mathbb{R}^3)}\|\nabla u\|_{L_{t,x}^{10/3}([0,t]\times\mathbb{R}^3)}$$

$$\leqslant \|v * |u|^2\|_{L_{t,x}^{5/2}([0,t]\times\mathbb{R}^3)}Z(t) \leqslant \|v\|_{L_x^p}\|u\|_{L_t^5 L_x^{2\tilde{p}}([0,t]\times\mathbb{R}^3)}^2 Z(t),$$

where

$$\frac{1}{p}+\frac{1}{\tilde{p}}-1=\frac{2}{5}.$$

Note that $\tilde{p}=15/(11-5\varepsilon)$. By L^p interpolation and Hölder inequality, we have

$$\|u\|_{L_t^5 L_x^{2\tilde{p}}} \leqslant \left(\int_0^t \|u\|_{L_4^{5a}}^{5a}\|u\|_{L_x^q}^{5(1-a)}\,\mathrm{d}t\right)^{1/5} \leqslant \|u\|_{L_t^{5ac}L_x^4([0,t]\times\mathbb{R}^3)}^a \|u\|_{L_t^{5(1-a)c'}L_x^q([0,t]\times\mathbb{R}^3)}^{(1-a)},$$

where

$$\frac{1}{2\tilde{p}}=\frac{a}{4}+\frac{1-a}{q}, \quad 0\leqslant a\leqslant 1, \quad \frac{1}{c}+\frac{1}{c'}=1.$$

If we let $5ac=4$,

$$\|u\|_{L_t^5 L_x^{2\bar{p}}} \leqslant \|u\|^a_{L^4_{t,x}([0,t]\times\mathbb{R}^3)} \|u\|^{(1-a)}_{L_t^{[20(1-a)]/(4-5a)} L_x^q([0,t]\times\mathbb{R}^3)} \quad \text{for } 0 < a \leqslant \tfrac{4}{5}.$$

The pair $([20(1-a)]/(4-5a), r)$ is admissible for $3/r = 1+1/[10(1-a)]$. On the other hand, the norm $\|u\|_{L_x^q}$ is bounded by Sobolev embedding,

$$\|u\|_{L_x^q} \leqslant \|\langle\nabla\rangle^s u\|_{L_x^r} \quad \text{for } s = \frac{3}{r} - \frac{3}{q}.$$

Since

$$\frac{1}{q} = \frac{11-5\varepsilon}{30(1-a)} - \frac{a}{4(1-a)},$$

we have

$$s = 1 - \frac{4-3a-2\varepsilon}{4(1-a)}.$$

We locate $s \in (0,1)$ if a is smaller than min $[(4-2\varepsilon)/3, 2\varepsilon]$ so that

$$\|(v * |u|^2)\nabla u\|_{L^{10/7}_{t,x}([0,t]\times\mathbb{R}^3)} \lesssim \|v\|_{L_x^p} \delta^{2a} Z(t)^{3-2a}.$$

Thus we have

$$\|(v * |u|^2)u\|_{L^{10/7}_{t,x}([0,t]\times\mathbb{R}^3)} + \|(v * |u|^2)\nabla u\|_{L^{10/7}_{t,x}([0,t]\times\mathbb{R}^3)} \lesssim \delta^{\epsilon_1} Z(t)^{1+\epsilon_2}$$

for $\epsilon_1, \epsilon_2 > 0$ and finally

$$Z(t) \lesssim \|u(0)\|_{H^1} + \delta\|v\|_{L_x^p} Z(t) + \delta^{\epsilon_1} Z(t)^{1+\epsilon_2}. \tag{A6}$$

For sufficiently small choice of δ, the bound (A6) yields

$$Z(t) \leqslant C(\|u(0)\|_{H^1})$$

for all $t \in J_1$. Since $\|u(t)\|_{H^1}$ is bounded by the initial energy, we may repeat this argument to cover the whole intervals. (Also see Refs. 1, 15, 20, 25, 28, and 33.)

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Smoothness of wave functions in thermal equilibrium

Roderich Tumulka[a)]
Mathematisches Institut, Eberhard-Karls-Unversität, Auf der Morgenstelle 10, 72076 Tübingen, Germany.

Nino Zanghì[b)]
Dipartimento di Fisica dell'Università di Genova and INFN sezione di Genova, Via Dodecaneso 33, 16146 Genova, Italy

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We consider the thermal equilibrium distribution at inverse temperature β, or canonical ensemble, of the wave function Ψ of a quantum system. Since L^2 spaces contain more nondifferentiable than differentiable functions, and since the thermal equilibrium distribution is very spread out, one might expect that Ψ has probability zero to be differentiable. However, we show that for relevant Hamiltonians the contrary is the case: with probability 1, Ψ is infinitely often differentiable and even analytic. We also show that with probability 1, Ψ lies in the domain of the Hamiltonian. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2109767]

I. INTRODUCTION

We address the question whether the wave function Ψ of a typical system from the canonical ensemble of thermodynamics with inverse temperature β is differentiable. As pointed out in Ref. 7, the thermal equilibrium distribution of the wave function, corresponding to the canonical ensemble, is the "Gaussian adjusted projected measure" GAP(ρ), a probability measure on the unit sphere in Hilbert space whose definition we recall in Sec. II, for $\rho=\rho_\beta$, the density matrix of the canonical ensemble, given by (see, e.g., Refs. 8 and 10)

$$\rho_\beta = \frac{1}{Z(\beta,H)} \mathrm{e}^{-\beta H}, \text{ with } Z(\beta,H) = \mathrm{Tr}\, \mathrm{e}^{-\beta H}. \tag{1}$$

Thus, we take Ψ to be a random unit vector with distribution GAP(ρ_β). The surprising result is that in many relevant cases Ψ has probability 1 to be infinitely often differentiable and even analytic, i.e., $\mathrm{GAP}(\rho_\beta)(C^\infty)=\mathrm{GAP}(\rho_\beta)(C^\omega)=1$.

We explore four kinds of arguments concerning the smoothness of Ψ, each requiring somewhat different assumptions on the Hamiltonian H and leading to somewhat different conclusions. Some of the arguments do not depend on the special measure GAP(ρ_β) but show that, for suitable Hamiltonians H, every distribution whose density matrix is ρ_β will be concentrated on the smooth (respectively, analytic) functions; other arguments use the way the measure GAP(ρ) is constructed from a Gaussian measure. The measure GAP(ρ) is discussed in detail in Ref. 7. It has density matrix ρ and is stationary if ρ is.

The first argument aims at showing that the Fourier coefficients of Ψ go to zero so fast that they are still square summable after multiplication by any power of the wave number k. This can be easily applied to cases in which the eigenfunctions of H are plane waves, such as for the free Schrödinger equation in a box. The second argument is based on the assumption that the eigenfunctions of H are smooth, and the theorem asserting that, for a series of functions, summation and differentiation commute if the series of the derivatives converges uniformly. We formulate a condition on H that entails this kind of convergence almost surely (a.s.) for the expansion of Ψ in

[a)]Electronic mail: tumulka@everest.mathematik.uni-tuebingen.de
[b)]Electronic mail: zanghi@ge.infn.it

eigenfunctions of H. The third argument, which supposes that Ψ is a function on an interval $I \subseteq \mathbb{R}$, aims at showing that the increments are not too large, $|\Psi(q+\Delta q)-\Psi(q)| \lesssim \Delta q$, which suggests differentiability; however, the rigorous version of this argument provides only a very weak result. The fourth argument, the simplest and most elegant one, is of a more abstract nature: it concerns not the question $\Psi \in C^\infty$ but instead the related question $\Psi \in \mathrm{domain}(H^\ell)$ for $\ell \in \mathbb{N}$; indeed, we obtain without further assumptions on H that a.s. $\Psi \in C^\infty(H) := \cap_{\ell=1}^\infty \mathrm{domain}(H^\ell)$ for almost all β for which thermal equilibrium exists at all. We also provide a variant of this argument concerning the space of analytic vectors of H.

The paper is organized as follows. In Sec. II, we recall from Ref. 7 the definition of the measure $\mathrm{GAP}(\rho_\beta)$ representing the canonical ensemble. In Sec. III, we study as an example of H the Laplacian on the circle. We conclude smoothness and analyticity of Ψ from an analysis of the decay behavior of the Fourier coefficients of Ψ. In Sec. IV, we apply the same argument to the (relativistic or nonrelativistic) ideal gas in a box. In Sec. V, we take into account the symmetrization of the wave function for describing bosons or fermions. In Sec. VI, we give the second kind of argument, providing a general criterion on the Hamiltonian that is sufficient for concluding that Ψ is a.s. smooth. The criterion concerns bounds on the derivatives of the eigenfunctions of H. In Sec. VII, we discuss the third argument, which concerns the direct estimation of the difference quotients of Ψ. In Sec. VIII, we describe the fourth argument, which allows to conclude that Ψ lies in the domain of H and all its powers. In Sec. IX, we conclude, as an application of our results, that Ψ a.s. possesses a Bohmian velocity field.

II. CANONICAL ENSEMBLE

In this section we give the definition of the measure $\mathrm{GAP}(\rho)$ on the unit sphere $\mathcal{S}(\mathcal{H})$ of Hilbert space $\mathcal{H}$, as introduced in Ref. 7.

The measure $\mathrm{GAP}(\rho)$ is defined for every density matrix ρ (positive operator with $\mathrm{Tr}\rho=1$) on $\mathcal{H}$. We obtain the thermal equilibrium measure $\mathrm{GAP}(\rho_\beta)$ by using the canonical density matrix (1) for a self-adjoint operator H (the Hamiltonian) and a number $\beta>0$ (the inverse temperature) such that

$$Z(\beta,H) = \mathrm{Tr}\ \mathrm{e}^{-\beta H} < \infty. \tag{2}$$

The measure $\mathrm{GAP}(\rho)$ is defined as the distribution of the random vector

$$\Psi^{\mathrm{GAP}} = \Psi^{\mathrm{GA}}/\|\Psi^{\mathrm{GA}}\|, \tag{3}$$

where Ψ^{GA} is a random vector with distribution $\mathrm{GA}(\rho)$ (the "Gaussian adjusted measure") defined by

$$\mathrm{GA}(\rho)(\mathrm{d}\psi) = \|\psi\|^2 G(\rho)(\mathrm{d}\psi), \tag{4}$$

where $G(\rho)$ is the Gaussian measure on $\mathcal{H}$ with covariance matrix ρ.

More explicitly, for a random vector Ψ^G to be $G(\rho)$-distributed means that for any $\phi_1, \phi_2 \in \mathcal{H}$ the components $Z_1=\langle\phi_1|\Psi^G\rangle$ and $Z_2=\langle\phi_2|\Psi^G\rangle$ of Ψ^G are complex Gaussian random variables with mean zero and covariance

$$\mathbb{E}Z_1Z_2^* = \mathbb{E}\langle\phi_1|\Psi^G\rangle\langle\Psi^G|\phi_2\rangle = \langle\phi_1|\rho|\phi_2\rangle, \tag{5}$$

where $\mathbb{E}$ denotes expectation. In particular, if $\{|\varphi_n\rangle\}$ is an orthonormal basis of $\mathcal{H}$ consisting of eigenvectors of ρ with eigenvalues p_n, then the coefficients $\langle\varphi_n|\Psi^G\rangle$ of Ψ^G are independent complex Gaussian random variables with mean zero and variances

$$\mathbb{E}|\langle\varphi_n|\Psi^G\rangle|^2 = p_n. \tag{6}$$

If ρ is of the form (1) then the φ_n are also eigenvectors of H.

Although we are interested only in those ρ of the form (1) for physically relevant Hamiltonians, we will sometimes, when this makes the mathematics clearer and more elegant, formulate facts or conditions in terms of an arbitrary density matrix ρ.

For any probability measure μ on $\mathcal{S}(\mathcal{H})$, its density matrix is given by

$$\rho_\mu = \int_{\mathcal{S}(\mathcal{H})} \mu(\mathrm{d}\psi)|\psi\rangle\langle\psi|, \tag{7}$$

or $\rho_\mu = \mathbb{E}_\mu|\psi\rangle\langle\psi|$, where $\mathbb{E}_\mu$ denotes the expectation with respect to μ. In particular, $\mathbb{E}_\mu|\langle\varphi|\psi\rangle|^2 = \langle\varphi|\rho_\mu|\varphi\rangle$ for every fixed $\varphi \in \mathcal{H}$. [If a probability measure μ on $\mathcal{H}$ is not concentrated on $\mathcal{S}(\mathcal{H})$, the notion of density matrix of μ does not make sense any more; however (7), or $\mathbb{E}_\mu|\psi\rangle\langle\psi|$, is still the *covariance matrix* of μ.] As mathematically expressed by $\mathbb{E}_\mu\langle\psi|P|\psi\rangle = \mathrm{Tr}(\rho_\mu P)$ for every projection P, ρ_μ provides the distribution of outcomes of any quantum experiment on a system with μ-distributed random wave function. The density matrix of GAP(ρ) is indeed ρ. This and other fundamental properties of the measure GAP(ρ) are discussed in Ref. 7.

The following simple fact will sometimes be useful, as it reduces the task of showing smoothness of $\Psi = \Psi^{\mathrm{GAP}}$ to showing smoothness of the Gaussian random vector Ψ^G with distribution $G(\rho)$. For any subspace W of $\mathcal{H}$, we have that

$$\text{if } G(\rho)(W) = 1 \text{ then } \mathrm{GAP}(\rho)(W) = 1. \tag{8}$$

To see this, note that GA(ρ) has the same null sets as $G(\rho)$ [as it is absolutely continuous with respect to $G(\rho)$ with a density that vanishes only at one point], so that, if $G(\rho)(W)=1$, $0=G(\rho)(\mathcal{H}\backslash W)=\mathrm{GA}(\rho)(\mathcal{H}\backslash W)$and thus $\mathrm{GA}(\rho)(W)=1$; but, by definition (3), if $\Psi^{\mathrm{GA}} \in W$ then also $\Psi^{\mathrm{GAP}} \in W$.

III. CASE STUDY: LAPLACIAN ON THE CIRCLE

In this section we consider a single particle moving on a circle S^1 with the free Schrödinger Hamiltonian

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2}, \tag{9}$$

where m denotes the mass of the particle, q the angular coordinate on the circle, and wave functions are written as periodic functions of q. The result we derive is that relative to any measure μ on $\mathcal{S}(\mathcal{H})$ with density matrix ρ_β with $\beta > 0$ (or, in fact, any measure μ on $\mathcal{H}$ with covariance matrix ρ_β), almost every wave function ψ is smooth, $\psi \in C^\infty(\mathbb{R})$; we then go on to show that μ-almost every wave function is analytic, $\psi \in C^\omega(\mathbb{R})$.

We begin with considering, instead of differentiability, a closely related property: existence (in L^2) of the distributional derivative. In other words, we consider the property of a wave function ψ that $|k|\hat{\psi}(k)$ is still square integrable, where $\hat{\psi}$ is the Fourier transform of ψ. Since the functions we are considering are 2π-periodic in q, the appropriate property is that the Fourier coefficients c_k, defined by

$$\psi(q) = \sum_{k\in\mathbb{Z}} c_k \mathrm{e}^{\mathrm{i}kq}, \tag{10}$$

are still square summable after multiplication with $|k|$. Let W^ℓ denote the ℓth Sobolev space, i.e., the subspace of $L^2([0,2\pi])$ containing those functions whose Fourier coefficients c_k satisfy

$$|k|^\ell c_k \text{ is square summable, i.e., } \sum_{k\in\mathbb{Z}} |k|^{2\ell}|c_k|^2 < \infty. \tag{11}$$

We ask whether $\psi \in W^\ell$ for a random wave function ψ with distribution μ. Since the eigenfunctions of H are the plane waves

$$\varphi_n(q) = \frac{1}{\sqrt{2\pi}} e^{inq}, \quad n \in \mathbb{Z}, \tag{12}$$

the energy coefficients of a wave function are just the Fourier coefficients. The eigenvalues are

$$E_n = \frac{\hbar^2}{2m} n^2, \quad n \in \mathbb{Z}. \tag{13}$$

Thus, our question about ψ amounts to asking for which $\ell \in \mathbb{N}$ we have

$$\sum_{n\in\mathbb{Z}} n^{2\ell} |\langle \varphi_n | \psi \rangle|^2 < \infty. \tag{14}$$

This indeed holds μ-a.s. for all $\ell \in \mathbb{N}$ for every probability measure μ on $\mathcal{S}(\mathcal{H})$ with density matrix ρ_β; to see this, note that (with numbers on top of equality signs indicating which equation is being applied)

$$\mathbb{E}_\mu \sum_{n\in\mathbb{Z}} n^{2\ell} |\langle \varphi_n | \psi \rangle|^2 = \sum_{n\in\mathbb{Z}} n^{2\ell} \mathbb{E}_\mu |\langle \varphi_n | \psi \rangle|^2 \tag{15a}$$

$$\overset{(7)}{=} \sum_{n\in\mathbb{Z}} n^{2\ell} \frac{e^{-\beta E_n}}{Z(\beta,H)} \overset{(13)}{=} \frac{1}{Z(\beta,H)} \sum_{n\in\mathbb{Z}} n^{2\ell} e^{-(\beta\hbar^2/2m)n^2} < \infty, \tag{15b}$$

because for any constant $\gamma > 0$ and for sufficiently large $|n|$

$$(2\ell+2)\log|n| < \gamma |n|^2 \text{ and thus } |n|^{2\ell} e^{-\gamma|n|^2} < \frac{1}{|n|^2}. \tag{16}$$

If the expectation (15) of a $[0,\infty]$-valued random variable is finite, the variable is a.s. finite. Thus

$$\mu\left(\sum_{n\in\mathbb{Z}} n^{2\ell} |\langle \varphi_n | \psi \rangle|^2 = \infty \right) = 0 \text{ or } \mu(W^\ell) = 1, \tag{17}$$

for all $\ell \in \mathbb{N}$.

We now make the connection between W^ℓ and C^ℓ, i.e., with classical differentiability: by the Sobolev lemma (Ref. 9, p. 52), every function in W^ℓ is equal Lebesgue-almost-everywhere to a function in $C^{\ell-1}$. Hence, every function in $\cap_{\ell=1}^\infty W^\ell$ is equal Lebesgue-almost-everywhere to a function in C^∞. In particular, μ-a.s. there is a $\phi \in C^\infty$ such that $\psi(q) = \phi(q)$ Lebesgue-almost-everywhere.

We now turn to analyticity. By a similar argument as given in (15) and (16), one can see that

$$\mu\left(\sum_{n\in\mathbb{Z}} e^{2\alpha|n|} |\langle \varphi_n | \psi \rangle|^2 = \infty \right) = 0, \tag{18}$$

for every $\alpha > 0$, so that

$$e^{\alpha|k|} c_k \text{ is a.s. square summable.} \tag{19}$$

Regarding the variable q in (10) as complex, we observe that the right-hand side of (10) converges, as a consequence of (19), uniformly in every strip $-\alpha+\varepsilon < \operatorname{Im} q < \alpha-\varepsilon$ with $0 < \varepsilon < \alpha$. (To see this, we use that square-summable sequences are bounded, $e^{\alpha|k|}|c_k| \leqslant C$, so that for q in the strip, $|c_k e^{ikq}| = |c_k| e^{-k \operatorname{Im} q} < |c_k| e^{|k|(\alpha-\varepsilon)} \leqslant C e^{-|k|\varepsilon}$, which is summable over $k \in \mathbb{Z}$.) Since the uniform limit of analytic functions on an open set in the complex plane is analytic (by virtue of the Cauchy integral formula), ψ is analytic in the strip $-\alpha < \operatorname{Im} q < \alpha$; since α was arbitrary, ψ is entire (i.e., analytic on the whole complex plane). More precisely, μ-a.s. there is an entire function ϕ such that $\psi(q) = \phi(q)$ Lebesgue-almost-everywhere in $\mathbb{R}$.

IV. IDEAL GAS IN A BOX

In a similar way, we can treat any Hamiltonian whose eigenfunctions are plane waves. A particularly relevant case is that of the ideal gas: N noninteracting particles in a d-dimensional box $[0,\pi]^d$ with Hamiltonian

$$H = -\sum_{i=1}^{N} \frac{\hbar^2}{2m}\Delta_i, \tag{20}$$

with Dirichlet boundary conditions, where Δ_i is the Laplacian acting on the coordinates of the ith particle. Our conclusion will again be that $\mu(C^\infty)=\mu(C^\omega)=1$ for every measure μ on $\mathcal{H}$ whose covariance matrix is ρ_β, and in particular for $\mu=\mathrm{GAP}(\rho_\beta)$. For the moment, we ignore the symmetrization postulate; we will treat bosons and fermions in Sec. V.

The Hamiltonian H on $\mathcal{H}=L^2([0,\pi]^{Nd})$ has eigenfunctions (Ref. 3 p. 78)

$$\varphi_n(q) = \left(\frac{2}{\pi}\right)^{Nd/2} \prod_{i=1}^{N}\prod_{a=1}^{d} \sin(n_{i,a}q_{i,a}), \tag{21}$$

where $n=(n_{1,1},\ldots,n_{N,d})\in\mathbb{N}^{Nd}$ and $q=(q_{1,1},\ldots,q_{N,d})\in[0,\pi]^{Nd}$, and eigenvalues

$$E_n = \sum_{i=1}^{N}\sum_{a=1}^{d} \frac{\hbar^2}{2m} n_{i,a}^2 = \frac{\hbar^2}{2m}\|n\|^2. \tag{22}$$

The right-hand side of (21) extends in an obvious way to a function on $\mathbb{R}^{Nd}$ that is 2π-periodic in every variable, which we also call φ_n; using the coefficients $\langle\varphi_n|\psi\rangle$ of the energy expansion we have a natural extension of any $\psi\in\mathcal{H}$ to a function ϕ on $\mathbb{R}^{Nd}$ that is 2π-periodic in every variable, $\phi=\Sigma_n\langle\varphi_n|\psi\rangle\varphi_n$. Its Fourier coefficients are

$$c_k = (-i)^{Nd}\left(\prod_{i=1}^{N}\prod_{a=1}^{d}\mathrm{sign}(k_{i,a})\right)\langle\varphi_{|k_{1,1}|,\ldots,|k_{N,d}|}|\psi\rangle, \tag{23}$$

where $k=(k_{1,1},\ldots,k_{N,d})\in\mathbb{Z}^{Nd}$ and we set $\mathrm{sign}(0)=0$.

We begin with the existence in L^2 of the ℓ-fold distributional derivative. We assert that μ-a.s. for all $\ell\in\mathbb{N}$

$$\sum_{k\in\mathbb{Z}^{Nd}} \|k\|^{2\ell}|c_k|^2 < \infty. \tag{24}$$

This follows from

$$\mathbb{E}_\mu \sum_{k\in\mathbb{Z}^{Nd}} \|k\|^{2\ell}|c_k|^2 = 2^{Nd}\sum_{n\in\mathbb{N}^{Nd}} \|n\|^{2\ell}\mathbb{E}_\mu|\langle\varphi_n|\psi\rangle|^2 \tag{25a}$$

$$\overset{(7)}{=} \frac{2^{Nd}}{Z(\beta,H)}\sum_{n\in\mathbb{N}^{Nd}} \|n\|^{2\ell}\mathrm{e}^{-\beta E_n} \overset{(22)}{=} \frac{2^{Nd}}{Z(\beta,H)}\sum_{n\in\mathbb{N}^{Nd}} \|n\|^{2\ell}\mathrm{e}^{-(\beta\hbar^2/2m)\|n\|^2} \tag{25b}$$

$$\overset{(26)}{\leqslant} \frac{2^{Nd}}{Z(\beta,H)}\sum_{n\in\mathbb{N}^{Nd}} (1+n_{1,1})^{2\ell}\cdots(1+n_{N,d})^{2\ell}\mathrm{e}^{-(\beta\hbar^2/2m)\|n\|^2} \tag{25c}$$

$$= \frac{1}{Z(\beta,H)} \left(2 \sum_{\nu \in \mathbb{N}} (1+\nu)^{2\ell} \mathrm{e}^{-(\beta\hbar^2/2m)\nu^2} \right)^{Nd} \overset{(16)}{<} \infty, \tag{25d}$$

where we used

$$\|n\|^2 = \sum_{i,a} n_{i,a}^2 \leqslant \prod_{i,a} (1 + 2n_{i,a} + n_{i,a}^2) = \prod_{i,a} (1+n_{i,a})^2. \tag{26}$$

Inequality (24) means that ϕ lies in the Sobolev space W^ℓ, and by the Sobolev lemma (Ref. 9, p. 52) also in C^m for all $m < \ell - Nd/2$. Since ℓ was arbitrary, ϕ is μ-a.s. smooth, and thus so is ψ, its restriction to $[0,\pi]^{Nd}$.

The same argument can be applied to the relativistic case, in which the Hamiltonian is the free Dirac operator

$$H = -\sum_{i=1}^{N} (\mathrm{i}c\hbar\, \alpha_i \cdot \nabla_i + mc^2 \beta_i), \tag{27}$$

with c the speed of light, m the mass, and α_i and β_i the Dirac alpha and beta matrices acting on the ith spin index of the wave function. Again, one obtains that $\mu(C^\infty)=1$ for all μ with covariance matrix ρ_β.

We turn to analyticity, and to this end assert that μ-a.s. for all $\alpha > 0$

$$\sum_{k \in \mathbb{Z}^{Nd}} \mathrm{e}^{2\alpha\|k\|} |c_k|^2 < \infty. \tag{28}$$

This follows from the fact that, by the same reasoning as in (25),

$$\mathbb{E}_\mu \sum_{k \in \mathbb{Z}^{Nd}} \mathrm{e}^{2\alpha\|k\|} |c_k|^2 = \frac{2^{Nd}}{Z(\beta,H)} \sum_{n \in \mathbb{N}^{Nd}} \mathrm{e}^{2\alpha\|n\|} \mathrm{e}^{-(\beta\hbar^2/2m)\|n\|^2} < \infty,$$

because for any constant $\gamma > 0$ and for all but finitely many $n \in \mathbb{N}^{Nd}$, $2\alpha\|n\| - \gamma\|n\|^2 < -(\gamma/2)\|n\|^2$, while $\mathrm{e}^{-(\gamma/2)\|n\|^2}$ is summable over $\mathbb{N}^{Nd}$ by (16). By the same argument as in the last paragraph of Sec. III, one can conclude from (28) that ϕ is analytic in the cylinder $\{q \in \mathbb{C}^{Nd} : \|\mathrm{Im}\, q\| < \alpha\}$. Since α was arbitrary, ϕ is entire. Thus, μ-a.s. there is an entire function ϕ such that $\psi(q) = \phi(q)$ Lebesgue-almost-everywhere in $[0,\pi]^{Nd}$. (For the Dirac equation, since the energy eigenvalues grow like $c\hbar\|k\|$, ψ a.s. possesses an analytic continuation to the cylinder $\|\mathrm{Im}\, q\| < \beta c\hbar/2$.)

V. BOSONS AND FERMIONS

In the previous section, we ignored the symmetrization of the wave function for systems of bosons or fermions. If one takes the symmetrization into account, one reaches the same conclusion: smoothness is almost sure. But, instead of going through the calculation of the previous section again, we provide a simple argument why GAP(ρ_β) must be concentrated on C^∞ for indistinguishable particles (with symmetrized wave functions) if it is concentrated on C^∞ for distinguishable particles (with unsymmetrized wave functions).

The symmetric (respectively, antisymmetric) state vectors form a subspace of $\mathcal{H} = L^2([0,\pi]^{Nd})$; let P denote the projection to that subspace; the subspace can be written $P\mathcal{H}$. Since the Hamiltonian (20) is invariant under permutations, we have that $HP = PH = PHP$. Thus, the canonical density matrix for indistinguishable particles is

$$\rho_\beta(PH, P\mathcal{H}) = cP\rho_\beta(H,\mathcal{H})P, \tag{29}$$

where we have made explicit the dependence of ρ_β on the given Hamiltonian and Hilbert space, and $c = Z(\beta,H)/Z(\beta,PHP)$.

Now, observe that for a Gaussian measure with covariance ρ, we have that $G(P\rho P)=G(\rho)\circ P^{-1}$, where P^{-1} is understood as mapping subsets of $P\mathcal{H}$ to their preimages in $\mathcal{H}$, in other words $\Psi^{G(P\rho P)}=P\Psi^{G(\rho)}$ in distribution.

In our case, P is the symmetrization (respectively, antisymmetrization) operator, which maps smooth functions to smooth functions. Since Ψ^G is a.s. smooth (by the result of the previous section), so is $P\Psi^G$; with (8) we conclude that $\mathrm{GAP}(\rho_\beta(PH,P\mathcal{H}))(C^\infty)=1$. The same argument works with analyticity.

VI. GENERAL SUFFICIENT CONDITION FOR SMOOTHNESS

We now present a second kind of argument, different from the one used in the previous sections; it applies to the measure $\mathrm{GAP}(\rho)$ but not to all measures with density matrix ρ. The argument provides us with a condition [see (30) below] on any given density matrix ρ (and thus, for $\rho=\rho_\beta$, on the Hamiltonian) ensuring that $\mathrm{GAP}(\rho)(C^\infty)=1$.

Theorem 1: *Let $\mathcal{Q}$ be an open subset of $\mathbb{R}^d$. Suppose that the density matrix ρ on $\mathcal{H}=L^2(\mathcal{Q},\mathbb{C}^m)$ has C^∞ eigenfunctions $\varphi_n(q)$ with $\|\varphi_n\|=1$ and eigenvalues p_n, such that for all n and all $\ell=0,1,2,3,\ldots$, the ℓth derivative of φ_n is bounded*

$$\|\nabla^\ell\varphi_n\|_\infty=\sup_{q\in\mathcal{Q}}|\nabla^\ell\varphi_n(q)|<\infty,$$

where by absolute values we mean

$$|\nabla^\ell\psi(q)|^2=\sum_{i_1,\ldots,i_\ell=1}^{d}\sum_{s=1}^{m}\left|\frac{\partial^\ell\psi_s}{\partial q_{i_1}\cdots\partial q_{i_\ell}}(q)\right|^2.$$

If for all $\ell=0,1,2,3,\ldots$

$$\sum_n\|\nabla^\ell\varphi_n\|_\infty\sqrt{p_n}<\infty, \tag{30}$$

then $\mathrm{GAP}(\rho)(C^\infty(\mathcal{Q},\mathbb{C}^m))=1$.

Proof: To begin with, for a complex Gaussian random variable Z with $\mathbb{E}Z=0$ and $\mathbb{E}|Z|^2=\sigma^2$, one can determine that

$$\mathbb{E}|Z|=\int_{\mathbb{R}^2}\mathrm{d}x\,\mathrm{d}y\frac{\sqrt{x^2+y^2}}{\pi\sigma^2}\exp\left(-\frac{x^2+y^2}{\sigma^2}\right)=\frac{\sqrt{\pi}}{2}\sigma. \tag{31}$$

Setting $Z=\langle\varphi_n|\Psi^G\rangle$, we obtain that

$$\mathbb{E}\sum_n\|\nabla^\ell\varphi_n\langle\varphi_n|\Psi^G\rangle\|_\infty=\mathbb{E}\sum_n|\langle\varphi_n|\Psi^G\rangle|\|\nabla^\ell\varphi_n\|_\infty=\sum_n\mathbb{E}|\langle\varphi_n|\Psi^G\rangle|\|\nabla^\ell\varphi_n\|_\infty\overset{(31)}{=}\sum_n\frac{\sqrt{\pi}}{2}\sqrt{p_n}\|\nabla^\ell\varphi_n\|_\infty\overset{(30)}{<}\infty,$$

and therefore

$$\mathrm{Prob}\left(\sum_n\|\nabla^\ell\varphi_n\langle\varphi_n|\Psi^G\rangle\|_\infty<\infty\right)=1.$$

Since this is true of every ℓ, we have that in the expansion

$$\Psi^G(q)=\sum_n\varphi_n(q)\langle\varphi_n|\Psi^G\rangle \tag{32}$$

(having C^∞ partial sums), a.s. the ℓ*th* derivatives of the partial sums converge uniformly; and in particular (32) itself converges uniformly. It is a standard theorem (see, e.g., Ref. 4, p. 118) that, if a sequence f_n of functions converges pointwise and the derivatives ∇f_n uniformly, then the limit

function f is differentiable and has derivative $\nabla f = \lim \nabla f_n$. Therefore, a.s. $\Psi^G \in C^\infty(\mathcal{Q})$, and the derivatives are

$$\nabla^\ell \Psi^G(q) = \sum_n \nabla^\ell \varphi_n(q) \langle \varphi_n | \Psi^G \rangle. \tag{33}$$

By (8), a.s. $\Psi^{\mathrm{GAP}} \in C^\infty(\mathcal{Q})$, which completes the proof. □

By applying this proof to local coordinates, we can generalize the result to Riemannian manifolds and vector bundles as follows. *Let $\mathcal{Q}$ be a Riemannian C^∞ manifold, E a C^∞ complex vector bundle over $\mathcal{Q}$ with positive-definite C^∞ Hermitian inner products on the fiber spaces, and let ∇ be the covariant derivative operator corresponding to a C^∞ connection on E. Let $\mathcal{H} = L^2(E)$ be the Hilbert space of square-integrable (with respect to the Riemannian volume) measurable cross sections of E, and $C^\infty(E)$ the space of smooth cross sections. Suppose that the density matrix ρ on $\mathcal{H}$ has C^∞ eigen-cross sections $\varphi_n(q)$ with $\|\varphi_n\| = 1$ and eigenvalues p_n, such that for all n and all $\ell = 0, 1, 2, 3, \ldots$, the ℓth covariant derivative of φ_n is bounded*

$$\|\nabla^\ell \varphi_n\|_\infty = \sup_{q \in \mathcal{Q}} |\nabla^\ell \varphi_n(q)| < \infty, \tag{34}$$

where the absolute values are taken with respect to the Riemannian inner product on tangent spaces and the Hermitian inner product on fiber spaces. If for all $\ell = 0, 1, 2, 3, \ldots$

$$\sum_n \|\nabla^\ell \varphi_n\|_\infty \sqrt{p_n} < \infty, \tag{35}$$

then $\mathrm{GAP}(\rho)(C^\infty(E)) = 1$.

Another easy generalization of Theorem 1 concerns analyticity: *Let $\mathcal{Q}_{\mathbb{C}}$ be an open subset of $\mathbb{C}^d$ and $\mathcal{Q} := \{(q_1, \ldots, q_d) \in \mathcal{Q}_{\mathbb{C}} : q_1, \ldots, q_d \in \mathbb{R}\} \subseteq \mathbb{R}^d$. Suppose that the density matrix ρ on $\mathcal{H} = L^2(\mathcal{Q}, \mathbb{C}^m)$ has eigenvalues p_n with normalized eigenvectors $\varphi_n \in C^\omega(\mathcal{Q}_{\mathbb{C}})$, with $C^\omega(\mathcal{Q}_{\mathbb{C}})$ the space of L^2 functions on $\mathcal{Q}$ that possess analytic continuations to $\mathcal{Q}_{\mathbb{C}}$. If for every compact set $K \subseteq \mathcal{Q}_{\mathbb{C}}$*

$$\sum_n \|\varphi_n|_K\|_\infty \sqrt{p_n} < \infty \tag{36}$$

(writing also φ_n for the analytic continuation and $\varphi_n|_K$ for its restriction to K), then $\mathrm{GAP}(\rho)(C^\omega(\mathcal{Q}_{\mathbb{C}})) = 1$.

Proof: By (36) and (31)

$$\mathbb{E} \sum_n \|\varphi_n|_K\|_\infty |\langle \varphi_n | \Psi^G \rangle| = \sum_n \|\varphi_n|_K\|_\infty \frac{\sqrt{\pi}}{2} \sqrt{p_n} < \infty,$$

and thus a.s. $\Sigma_n \|\varphi_n|_K\|_\infty |\langle \varphi_n | \Psi^G \rangle| < \infty$. As a consequence, the expansion

$$\Psi^G(q) = \sum_n \varphi_n(q) \langle \varphi_n | \Psi^G \rangle, \tag{37}$$

converges not only for $q \in \mathcal{Q}$ but also for $q \in \mathcal{Q}_{\mathbb{C}}$, in fact uniformly on every compact set $K \subseteq \mathcal{Q}_{\mathbb{C}}$. Since uniform limits of analytic functions are analytic, Ψ^G and thus also Ψ^{GAP} are a.s. analytic. □

In order to demonstrate that the conditions (30), (35), and (36) are not unreasonably strong, we show that they are satisfied for the Laplacian on the circle. Here, the eigenfunctions are given by (12), and their derivatives, respectively, analytic continuations to disks $K = \{q \in \mathcal{Q}_{\mathbb{C}} = \mathbb{C} : |q| \leq \alpha\}$, have bounds

$$\|\nabla^\ell \varphi_n\|_\infty = \frac{|n|^\ell}{\sqrt{2\pi}}, \quad \|\varphi_n|_K\|_\infty = \frac{1}{\sqrt{2\pi}} e^{\alpha |n|}.$$

In this case, (30), respectively (35), is satisfied since

$$\sum_{n\in\mathbb{Z}} \|\nabla^\ell \varphi_n\|_\infty e^{-(1/2)\beta E_n} = \frac{1}{\sqrt{2\pi}} \sum_{n\in\mathbb{Z}} |n|^\ell e^{-(\beta\hbar^2/4m)n^2} < \infty,$$

by (16), and similarly (36), since

$$\sum_{n\in\mathbb{Z}} \|\varphi_n|_K\|_\infty e^{-(1/2)\beta E_n} = \frac{1}{\sqrt{2\pi}} \sum_{n\in\mathbb{Z}} e^{\alpha|n|} e^{-(\beta\hbar^2/4m)n^2} < \infty.$$

VII. ESTIMATING DIFFERENCE QUOTIENTS

In this section, we follow another line of reasoning for studying regularity properties of Ψ, based on a standard theorem on the regularity of sample paths of a Gaussian process. However, the result is much weaker than what we obtained in the previous section.

Assume for simplicity that the configuration space is an open interval $I\subseteq\mathbb{R}$, and that $\mathcal{H}=L^2(I,\mathbb{C})$. The idea in this section is to consider the increments $\Psi^G(q+\Delta q)-\Psi^G(q)$ of the Gaussian process Ψ^G, and to argue that for reasonable Hamiltonians they are of the order of magnitude of $\Delta q>0$

$$|\Psi^G(q+\Delta q)-\Psi^G(q)| \lesssim \Delta q, \tag{38}$$

which suggests that difference quotients converge to differential quotients as $\Delta q\to 0$, i.e., that Ψ^G be differentiable. However, what can rigorously be concluded from a statement about the variance of the increment analogous to (38) is less than differentiability, namely Hölder continuity with exponent $1-\varepsilon$.

We now describe the argument in detail. We pretend that Ψ^G is everywhere defined in I (although, strictly speaking, vectors in Hilbert space are equivalence classes of functions coinciding Lebesgue-almost-everywhere) in such a way that it is a Gaussian process in the sense that, for any choice of $q_1,\ldots,q_n\in I$, the joint distribution of $\Psi^G(q_1),\ldots,\Psi^G(q_n)$ in $\mathbb{C}^n$ is Gaussian. It follows that for any $\Delta q>0$, the increment $\Psi^G(q+\Delta q)-\Psi^G(q)$ is a Gaussian variable, and we can compute its variance

$$\mathbb{E}|\Psi^G(q+\Delta q)-\Psi^G(q)|^2 = \rho(q+\Delta q,q+\Delta q) - 2\,\mathrm{Re}\,\rho(q,q+\Delta q) + \rho(q,q), \tag{39}$$

where $\rho(q,q')=\langle q|\rho|q'\rangle$ are the "matrix elements" in the position representation of the density matrix $\rho=\rho_\beta$. Assuming that

$$\rho(q,q') \text{ is a smooth function}, \tag{40}$$

which would appear to be a reasonable assumption on the Hamiltonian, we can employ a Taylor expansion of ρ to the second order around (q,q) and obtain from (39) that

$$\mathbb{E}|\Psi^G(q+\Delta q)-\Psi^G(q)|^2 = \left.\frac{\partial^2\rho}{\partial q\partial q'}\right|_{q'=q} \Delta q^2 + O(\Delta q^3). \tag{41}$$

It is a standard result (Ref. 6, Theorem 8 of Chap. III) that for a Gaussian process Ψ^G with the following bound on the variances of the increments:

$$\mathbb{E}|\Psi^G(q+\Delta q)-\Psi^G(q)|^2 \leqslant K\Delta q^p, \tag{42}$$

where $K>0$ and $p>0$ are constants, the realization a.s. satisfies

$$|\Psi^G(q+\Delta q)-\Psi^G(q)| \leqslant K'\Delta q^{p/2}|\log\Delta q|^{1+\delta}, \tag{43}$$

for arbitrary $\delta>0$ and a suitable constant $K'=K'(\delta)>0$. Inserting (41) into (42), we obtain from (43), in the case $\partial^2\rho/\partial q\partial q'\neq 0$, that a.s.

$$|\Psi^G(q+\Delta q)-\Psi^G(q)| \leqslant K''\Delta q^{1-\varepsilon}, \tag{44}$$

for arbitrary $\varepsilon>0$, i.e., Hölder continuity of degree $1-\varepsilon$.

In order to obtain a stronger estimate than (44), one might hope that

$$\left.\frac{\partial^2\rho}{\partial q\partial q'}\right|_{q'=q} = 0 \text{ for all } q \in I. \tag{45}$$

This would allow us to replace the exponent in (44) by $3/2-\varepsilon$, which would give us in particular local Lipschitz continuity, so that Ψ^G would be differentiable Lebesgue-almost-everywhere. But, any exponent greater than 1 is too good to be true. Indeed, as we shall show presently (45) holds only for one particular density matrix ρ_0, the projection to the one-dimensional subspace of constant functions. For $\rho=\rho_0$, $\Psi(q)$ is constant with modulus determined by normalization and random phase.

To see $\rho=\rho_0$, write ρ in terms of its eigenfunctions $\varphi_n(q)$ and eigenvalues p_n, $\rho(q,q')=\Sigma_n p_n\varphi_n(q)\varphi_n^*(q')$, and observe that

$$\left.\frac{\partial^2\rho}{\partial q\partial q'}\right|_{q'=q} = \left.\sum_n p_n\varphi_n'(q)\varphi_n'^*(q')\right|_{q'=q} = \sum_n p_n|\varphi_n'(q)|^2,$$

where φ_n' denotes the derivative of φ_n. The only way this quantity can vanish for all q is that all φ_n have identically vanishing derivative and thus are constant, which implies $\rho=\rho_0$.

VIII. CONCENTRATION ON THE DOMAIN OF *H*

In this section we utilize a fourth kind of argument, different from those of the previous sections. It is our most elegant argument, particularly simple and direct, as it deals only with the eigenvalues and eigenvectors, but also more abstract. This argument applies not only to GAP(ρ_β) but to every probability measure μ on $\mathcal{S}(\mathcal{H})$ with density matrix ρ_β.

The question we address is whether $\mu(\text{domain}(H))=1$. The answer is yes. Even more, we show that, for any self-adjoint H and almost all β for which $Z(\beta,H)<\infty$, any μ with density matrix ρ_β is supported by the domain of H^ℓ for every $\ell\in\mathbb{N}$. [Whether $\psi\in\text{domain}(H)$ implies differentiability depends of course on H.] After that, we show further that GAP(ρ_β) for sufficiently large β is concentrated on the *subspace of analytic vectors*[1] of H.

Theorem 2: *Let ρ be a density matrix on the Hilbert space $\mathcal{H}$, μ a probability measure on $\mathcal{S}(\mathcal{H})$ with density matrix ρ, and $f:[0,1]\to\mathbb{R}$ a measurable function. If*

$$\text{Tr}(\rho f(\rho)^2) < \infty, \tag{46}$$

then $\mu(\text{domain}(f(\rho)))=1$, where the domain of $f(\rho)$ can be defined, in terms of an orthonormal basis $\{|\varphi_n\rangle\}$ of eigenvectors of ρ with eigenvalues p_n, by

$$\text{domain}(f(\rho)) = \left\{\psi\in\mathcal{H}: \sum_n |f(p_n)\langle\varphi_n|\psi\rangle|^2 < \infty\right\}. \tag{47}$$

Proof: From (46), it follows that

$$\mathbb{E}_\mu \sum_n |f(p_n)\langle\varphi_n|\psi\rangle|^2 = \sum_n f(p_n)^2\mathbb{E}_\mu|\langle\varphi_n|\psi\rangle|^2 = \sum_n f(p_n)^2 p_n < \infty.$$

Therefore, μ-a.s. $\Sigma_n|f(p_n)\langle\varphi_n|\psi\rangle|^2<\infty$, or $\mu(\text{domain}(f(\rho)))=1$. □

Corollary 1: Let H be a self-adjoint operator on the Hilbert space $\mathcal{H}$. Suppose $Z(\beta_0,H)<\infty$ for some $\beta_0>0$, which implies $Z(\beta,H)<\infty$ for every $\beta>\beta_0$. Then, for every $\beta>\beta_0$ and every probability measure μ on $\mathcal{S}(\mathcal{H})$ with density matrix ρ_β, $\mu(C^\infty(H))=1$, where $C^\infty(H)=\cap_{\ell=1}^\infty \text{domain}(H^\ell)$.

Proof: For ρ given by (1), we have that $H=-(1/\beta)\log\rho+E_0 id$ for some constant E_0. Define

$f(x)=(-(1/\beta)\log x+E_0)^\ell$ for $x>0$ and $f(x)=0$ for $x=0$. Since $f(\rho)=H^\ell$, Theorem 2 yields the claim if we can confirm the condition (46), which we do now.

Since $\mathrm{Tr}\exp(-\beta_0 H)<\infty$, there is a basis $\{|\varphi_n\rangle : n\in\mathbb{N}\}$ of eigenvectors of H with eigenvalues E_n. Furthermore, only finitely many of the eigenvalues lie below zero, so that the set $\mathcal{N}:=\{n\in\mathbb{N}: E_n>0\}$ contains all except finitely many numbers. Observe that for every $\beta>\beta_0$

$$\infty > \mathrm{Tr}\, \mathrm{e}^{-\beta_0 H} = \sum_{n\in\mathbb{N}} \mathrm{e}^{-\beta_0 E_n} \geqslant \sum_{n\in\mathcal{N}} \mathrm{e}^{-\beta_0 E_n} > \sum_{n\in\mathcal{N}} \mathrm{e}^{-\beta E_n},$$

and thus $Z(\beta,H)<\infty$. For $\varepsilon>0$ with $\varepsilon<\beta-\beta_0$, we find, for any $\ell\in\mathbb{N}$

$$\infty > \sum_{n\in\mathcal{N}} \mathrm{e}^{-(\beta-\varepsilon)E_n} = \sum_{n\in\mathcal{N}} \mathrm{e}^{-\beta E_n}\mathrm{e}^{\varepsilon E_n} > \sum_{n\in\mathcal{N}} \mathrm{e}^{-\beta E_n}\sum_{k=0}^{2\ell}\frac{\varepsilon^k E_n^k}{k!} = \sum_{k=0}^{2\ell}\frac{\varepsilon^k}{k!}\sum_{n\in\mathcal{N}} E_n^k \mathrm{e}^{-\beta E_n}.$$

In particular

$$\sum_{n\in\mathcal{N}} E_n^{2\ell}\mathrm{e}^{-\beta E_n} < \infty,$$

which implies $\mathrm{Tr}(\rho_\beta H^{2\ell})<\infty$. □

If $\beta>2\beta_0$ (with $Z(\beta_0,H)<\infty$), we obtain the stronger result for the measure $\mathrm{GAP}(\rho_\beta)$ that it is concentrated on the subspace $C^\omega(H)$ of analytic vectors of H, i.e., those vectors $\psi\in C^\infty(H)$ with

$$\sum_{\ell=0}^{\infty}\frac{\|H^\ell\psi\|\varepsilon^\ell}{\ell!}<\infty, \tag{48}$$

for some $\varepsilon>0$.[1] It is sufficient for $\psi\in C^\omega(H)$ that

$$\sum_n \mathrm{e}^{\varepsilon|E_n|}|\langle\varphi_n|\psi\rangle|<\infty, \tag{49}$$

because then

$$\sum_{\ell=0}^{\infty}\frac{\varepsilon^\ell}{\ell!}\|H^\ell\psi\| = \sum_{\ell=0}^{\infty}\frac{\varepsilon^\ell}{\ell!}\left\|\sum_n E_n^\ell|\varphi_n\rangle\langle\varphi_n|\psi\rangle\right\| \leqslant \sum_n\sum_{\ell=0}^{\infty}\frac{\varepsilon^\ell}{\ell!}|E_n|^\ell|\langle\varphi_n|\psi\rangle| = \sum_n \mathrm{e}^{\varepsilon|E_n|}|\langle\varphi_n|\psi\rangle|<\infty.$$

For $0<\varepsilon<\beta/2-\beta_0$ (49) is a.s. true of $\psi=\Psi^G$, and thus also of $\psi=\Psi^{\mathrm{GAP}}$, because, assuming without loss of generality that all $E_n>0$, we have by (31) that

$$\mathbb{E}\sum_n \mathrm{e}^{\varepsilon E_n}|\langle\varphi_n|\Psi^G\rangle| = \sum_n \mathrm{e}^{\varepsilon E_n}\frac{\sqrt{\pi}}{2\sqrt{Z(\beta)}}\mathrm{e}^{-\beta E_n/2} \leqslant \frac{\sqrt{\pi}}{2\sqrt{Z(\beta)}}\sum_n \mathrm{e}^{-\beta_0 E_n}<\infty.$$

IX. EXISTENCE OF BOHMIAN VELOCITIES

As a final remark, we mention an application of smoothness of the wave function: differentiability is needed in Bohmian mechanics,[2] a theory ascribing trajectories to the particles of nonrelativistic quantum mechanics. This is because the Bohmian law of motion, which for N particles with masses $m_1,\ldots,m_N$ at the configuration $Q(t)=(\boldsymbol{Q}_1(t),\ldots,\boldsymbol{Q}_N(t))$ reads

$$\frac{\mathrm{d}\boldsymbol{Q}_i}{\mathrm{d}t} = \boldsymbol{v}_i^\psi(Q) = \frac{\hbar}{m_i}\,\mathrm{Im}\,\frac{\psi^*\nabla_i\psi}{\psi^*\psi}(Q),$$

involves the derivative of the wave function. Suppose the wave function ψ is chosen at random according to the canonical distribution $\mathrm{GAP}(\rho_\beta)$ with inverse temperature β. Then, any condition on the Hamiltonian entailing that ψ is a.s. smooth also implies that the Bohmian velocity vector

field v^ψ on configuration space $\mathcal{Q}=\mathbb{R}^{3N}$, whose ith component is $\boldsymbol{v}_i^\psi$, is a.s. well defined everywhere outside the nodes of ψ.

The analogous conclusion holds, as we shall explain presently, for the numerous further variants of Bohmian mechanics that have been considered (such as Bohmian mechanics on curved spaces, on the configuration space of a variable number of particles,[5] for wave functions that are cross sections of a complex vector bundle, and variants suitable for the Dirac equation or for photons). The laws of motion of these variants

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = v^\psi(Q),$$

are defined by giving the appropriate expression for the velocity vector field v^ψ on the manifold $\mathcal{Q}$, and these definitions of v^ψ can be summarized by the formula[5]

$$v^\psi(q)\cdot\nabla f(q) = \mathrm{Re}\,\frac{\psi^*(q)\left(\frac{i}{\hbar}[H,f]\psi\right)(q)}{\psi^*(q)\psi(q)} \qquad \forall\, f\in C_0^\infty(\mathcal{Q}). \tag{50}$$

Here, $f:\mathcal{Q}\to\mathbb{R}$ is an arbitrary smooth function with compact support playing the role of a coordinate function, and numerator and denominator involve inner products in the value space of ψ (which may be a fiber space of a vector bundle of which ψ is a cross section). For $\psi\in\mathrm{domain}(H)$ and $f\in C_0^\infty(\mathcal{Q})$, the right-hand side of (50) will be well defined since multiplication by f maps the domain of H to itself, since H is the sum of a differential operator (of up to second order) and a multiplication operator. Since the f's from $C_0^\infty(\mathcal{Q})$ suffice for determining v^ψ (up to changes on a null set), one obtains indeed a vector field v^ψ, defined on $\mathcal{Q}\setminus\{q:\psi(q)=0\}$, for every ψ from the domain of H.

Hence, every wave function ψ from the domain of H is sufficiently regular to define a Bohm-type velocity field. By Corollary 1, the random wave function Ψ with the thermal equilibrium distribution $\mathrm{GAP}(\rho_\beta)$ possesses a velocity field v^Ψ with probability 1, provided that there is $\beta_0<\beta$ with $Z(\beta_0,H)<\infty$.

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Large-*D* expansion from variational perturbation theory

Sebastian F. Brandt[a)]
Department of Physics, Campus Box 1105, Washington University in St. Louis, Missouri 63130-4899

Axel Pelster[b)]
Fachbereich Physik, Campus Essen, Universität Duisburg-Essen, Universitätsstraße 5, 45117 Essen, Germany

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We derive recursively the perturbation series for the ground-state energy of the *D*-dimensional anharmonic oscillator and resum it using variational perturbation theory (VPT). From the exponentially fast converging approximants, we extract the coefficients of the large-*D* expansion to higher orders. The calculation effort is much smaller than in the standard field-theoretic approach based on the Hubbard-Stratonovich transformation. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The properties of nontrivial physical systems can only be calculated via efficient approximation schemes. Most easily accessible are perturbation expansions, but they are usually divergent and need resummation. To this end, a variational approach was developed by Feynman and Kleinert,[1] which has been systematically extended to an efficient nonperturbative approximation scheme called *variational perturbation theory* (VPT).[2–5] It allows the conversion of divergent weak-coupling into convergent strong-coupling expansions and has been applied successfully in various fields, such as quantum mechanics, quantum statistics, condensed matter physics, and critical phenomena. In fact, the most accurate critical exponents come from this theory,[6] as has been verified by recent satellite experiments.[7]

The convergence of VPT has been analyzed up to very high orders for the ground-state energy of the one-dimensional anharmonic oscillator,

$$V(x) = \tfrac{1}{2}\omega^2 x^2 + g x^4, \tag{1}$$

and was found to be exponentially fast.[8,9] This surprising result has been confirmed later by studying other physical systems and was proven to hold on general grounds.[3,4] Furthermore, the exponential convergence seems to be uniform with respect to other system parameters. In this manner, the variational resummation of perturbation series yields approximations which are generically reasonable for all temperatures,[10–12] space and time coordinates,[13–16] magnetic field strengths,[17] coupling constants,[18–20] etc.

In this paper, we show that the exponential convergence of VPT is uniform with respect to the space dimension *D*. To this end, we consider the *D*-dimensional generalization of the anharmonic oscillator (1), i.e.,

$$V(\mathbf{x}) = \tfrac{1}{2}\omega^2 \mathbf{x}^2 + g(\mathbf{x}^2)^2 \tag{2}$$

with $\mathbf{x}=(x_1,\cdots,x_D)$, and determine its ground-state energy as a function of the coupling constant *g*. In Sec. II, we derive the corresponding weak-coupling series by evaluating connected vacuum

[a)]Electronic mail: sbrandt@physics.wustl.edu
[b)]Electronic mail: pelster@uni-essen.de

diagrams. In Sec. III, we show how this perturbation series can be obtained more efficiently by means of Bender-Wu-type recursion relations.[21] In Sec. IV, we resum the weak-coupling series by applying VPT and examine the resulting convergence, which is again exponentially fast and improves uniformly with increasing dimension D. In Sec. V, we show that the latter observation is not surprising, since the ground-state energy of the anharmonic oscillator (2) can be determined with the help of a systematic large-D expansion. In Sec. VI, we apply VPT to extract the large-D expansion to higher orders, which have so far been inaccessible to other methods.

II. PERTURBATION THEORY

The perturbation series for the ground-state energy of the anharmonic oscillator (2) can be calculated from connected vacuum diagrams. Up to the second order in the coupling constant g, the ground-state energy is given by the Feynman diagrams

$$E = \frac{\omega}{2} - \lim_{\beta\to\infty}\frac{1}{\beta}\left\{ \frac{1}{8} \quad + \frac{1}{48} \quad + \frac{1}{16} \quad + \cdots \right\}, \tag{3}$$

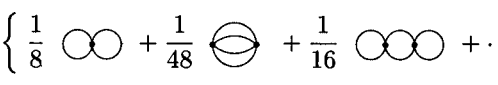

with the propagator

$$a \bullet \overset{i}{\longrightarrow} \bullet b \quad \equiv \quad \frac{\delta_{ij}}{2\omega} e^{-\omega|\tau_a-\tau_b|} \tag{4}$$

and the vertices

$$i \overset{j}{\underset{l}{\overset{|}{-}\!\bullet\!-}} k \quad \equiv \quad -\frac{g}{3}\,(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\int_0^\beta d\tau_a\,. \tag{5}$$

The connected vacuum diagrams (3) are derived most easily by an efficient graphical recursion method.[22] Evaluating these Feynman diagrams produces the following analytic expression for the ground-state energy:

$$E = \frac{D\omega}{2} + \frac{D(D+2)g}{4\omega^2} - \frac{D(2D^2+9D+10)g^2}{8\omega^5} + \cdots\,. \tag{6}$$

Only low perturbation orders are accessible by this procedure. If we want to study higher orders, we better use Bender-Wu-type recursion relations.[21]

III. BENDER-WU-TYPE RECURSION RELATIONS

The potential (2) of the D-dimensional anharmonic oscillator is rotationally symmetric. Hence, the ground-state wave function depends only on the distance $x=|\mathbf{x}|$. We solve the corresponding Schrödinger eigenvalue equation

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{D-1}{x}\frac{\partial}{\partial x}\right)+\frac{1}{2}\omega^2x^2+gx^4\right]\psi(x)=E\psi(x) \tag{7}$$

as follows. We write the wave function $\psi(x)$ as

$$\psi(x)=\left(\frac{\omega}{\pi}\right)^{1/4}\exp\left[-\frac{1}{2}\hat{x}^2+\phi(\hat{x})\right], \tag{8}$$

with the abbreviation $\hat{x}=x\sqrt{\omega}$, and expand the exponent in powers of the dimensionless coupling constant $\hat{g}=g/\omega^3$ by using

TABLE I. Expansion coefficients for the ground-state energy of the anharmonic oscillator (2) up to the fifth order.

k	ϵ_k
1	$D(D+2)/4$
2	$-D(2D^2+9D+10)/8$
3	$D(8D^3+59D^2+146D+120)/16$
4	$-D(168D^4+1773D^3+7144D^2+12960D+8840)/128$
5	$D(1024D^5+14325D^4+82222D^3+241464D^2+360736D+216960)/256$

$$\phi(\hat{x}) = \sum_{k=1}^{\infty} \phi_k(\hat{x}) \hat{g}^k. \tag{9}$$

The $\phi_k(\hat{x})$ are expanded in powers of the rescaled coordinate $\hat{x}$,

$$\phi_k(\hat{x}) = \sum_{m=1}^{k+1} c_m^{(k)} \hat{x}^{2m}. \tag{10}$$

For the ground-state energy we make the ansatz

$$E = \omega \left(\frac{D}{2} + \sum_{k=1}^{\infty} \epsilon_k \hat{g}^k \right). \tag{11}$$

Inserting (8)–(11) into (7), we obtain to first order

$$c_1^{(1)} = -\frac{D+2}{4}, \quad c_2^{(1)} = -\frac{1}{4}, \quad \epsilon_1 = \frac{D(D+2)}{4}. \tag{12}$$

For $k \geqslant 2$, we find the following recursion relation for the expansion coefficients in (10):

$$c_m^{(k)} = \frac{(m+1)(D+2m)}{2m} c_{m+1}^{(k)} + \sum_{l=1}^{k-1} \sum_{n=1}^{m} \frac{n(m+1-n)}{m} c_n^{(l)} c_{m+1-n}^{(k-l)}, \tag{13}$$

with $c_m^{(k)} \equiv 0$ for $m > k+1$. The expansion coefficients of the ground-state energy follow from

$$\epsilon_k = -D c_1^{(k)}. \tag{14}$$

Table I shows the resulting coefficients ϵ_k up to the fifth order. For $D=1$, they reduce to the well-known one-dimensional results.[21]

IV. VARIATIONAL RESUMMATION

Now we consider the strong-coupling limit of the perturbation series (11). Rescaling the coordinate according to $x \to x g^{-1/6}$, the Schrödinger equation (7) becomes

$$\left[-\frac{1}{2} \left(\frac{\partial^2}{\partial x^2} + \frac{D-1}{x} \frac{\partial}{\partial x} \right) + \frac{1}{2} g^{-2/3} \omega^2 x^2 + x^4 \right] \psi(x) = g^{-1/3} E \psi(x). \tag{15}$$

Expanding the wave function and the ground-state energy in powers of the coupling constant yields

$$\psi(x) = \psi_0(\hat{x}) + \psi_1(\hat{x}) \hat{g}^{-2/3} + \psi_2(\hat{x}) \hat{g}^{-4/3} + \cdots, \tag{16}$$

TABLE II. Numerical results for the leading strong-coupling coefficient b_0 of the ground-state energy (17).

$b_0(D=2)$	1.4771497535779972(31)
$b_0(D=3)$	2.3936440164822970(37)
$b_0(D=10)$	10.758265165443755(69)

$$E = \omega \hat{g}^{1/3}(b_0 + b_1 \hat{g}^{-2/3} + b_2 \hat{g}^{-4/5} + \cdots). \tag{17}$$

By considering (15) in the limit $g \to \infty$, we find that the leading strong-coupling coefficient b_0 equals the ground-state energy associated with the Hamilton operator

$$H = -\tfrac{1}{2}\boldsymbol{\Delta} + (\mathbf{x}^2)^2. \tag{18}$$

Precise numerical values for this ground-state energy for different dimensions D are listed in Table II.

The weak-coupling series (11) is of the form

$$E^{(N)}(g,\omega) = \omega\left[\frac{D}{2} + \sum_{k=1}^{N} \epsilon_k \left(\frac{g}{\omega^3}\right)^k\right]. \tag{19}$$

The alternating signs and fast growing coefficients in Table I suggest that (19) is a divergent Borel series which is resummable by VPT.[2–5] In order to perform the variational resummation, an artificial frequency parameter Ω is introduced in the perturbation series most easily by Kleinert's square-root trick,

$$\omega \to \Omega\sqrt{1 + gr}, \tag{20}$$

with

$$r = \frac{\omega^2 - \Omega^2}{g\Omega^2}. \tag{21}$$

One replaces the frequency ω in the weak-coupling series (19) according to (20) and reexpands the resulting expression in powers of g up to the order g^N. Afterwards, the parameter r is replaced according to (21). This procedure has the effect that the power series of order N for the ground-state energy becomes dependent on the variational parameter Ω,

$$E^{(N)}(g,\omega,\Omega) = \sum_{k=0}^{N} \epsilon_k g^k \Omega^{1-3k} \sum_{l=0}^{N-k} \binom{(1-3k)/2}{l} \left(\frac{\omega^2}{\Omega^2} - 1\right)^l. \tag{22}$$

The influence of Ω is then optimized according to the principle of minimal sensitivity,[23] the ground-state energy to Nth order is approximated by

$$E^{(N)} = E^{(N)}(g,\omega,\Omega^{(N)}), \tag{23}$$

where $\Omega^{(N)}$ denotes that value of the variational parameter for which $E^{(N)}(g,\omega,\Omega)$ has an extremum or a turning point.

As an example, consider the weak-coupling series (19) to first order,

$$E^{(1)} = \frac{D\omega}{2} + \frac{D(D+2)}{4\omega^2} g. \tag{24}$$

Inserting (20), reexpanding in g to first order, and taking into account (21), we find

$$E^{(1)}(g,\omega,\Omega)=\frac{D\Omega}{4}+\frac{D\omega^2}{4\Omega}+\frac{D(D+2)}{4\Omega^2}g. \tag{25}$$

Extremizing this and going to large coupling constants, we obtain the strong-coupling behavior of the variational parameter

$$\Omega^{(1)}=\omega\hat{g}^{1/3}(\Omega_0^{(1)}+\Omega_1^{(1)}\hat{g}^{-2/3}+\Omega_2^{(1)}\hat{g}^{-4/3}+\cdots), \tag{26}$$

with

$$\Omega_0^{(1)}=(2D+4)^{1/3},\quad \Omega_1^{(1)}=\frac{\omega^2}{3(2D+4)^{1/3}},\quad \Omega_2^{(1)}=\frac{\omega^4}{108(D+2)},\quad \cdots. \tag{27}$$

Inserting the result (26) and (27) into (25), we obtain the strong-coupling series (17) with the first-order coefficients

$$b_0^{(1)}=\frac{3D}{8}(2D+4)^{1/3},\quad b_1^{(1)}=\frac{D\omega^2}{4(2D+4)^{1/3}},\quad b_2^{(1)}=-\frac{D\omega^4}{48(D+2)},\quad \cdots. \tag{28}$$

For $D=1$, this reduces to earlier VPT results in Refs. 8 and 9.

In order to determine the strong-coupling coefficient b_0 in (17) to higher orders, we proceed as follows. We observe that the strong-coupling behavior of the variational parameter is for any order N of the form

$$\Omega^{(N)}=\omega\hat{g}^{1/3}(\Omega_0^{(N)}+\Omega_1^{(N)}\hat{g}^{-2/3}+\Omega_2^{(N)}\hat{g}^{-4/3}+\cdots), \tag{29}$$

which corresponds to (26). Inserting (29) into (22), the leading strong-coupling coefficient turns out to be given by

$$b_0^{(N)}(\Omega_0^{(N)})=\sum_{k=0}^{N}\sum_{l=0}^{N-k}\binom{(1-3k)/2}{l}(-1)^l\epsilon_k(\Omega_0^N)^{1-3k}, \tag{30}$$

where the inner sum can be further simplified by using[24]

$$\sum_{l=0}^{m}(-1)^l\binom{\alpha}{l}=(-1)^m\binom{\alpha-1}{m}. \tag{31}$$

Thus, the leading strong-coupling coefficient reduces to

$$b_0^{(N)}(\Omega_0^{(N)})=\sum_{k=0}^{N}\binom{(1-3k)/2-1}{N-k}(-1)^{N-k}\epsilon_k(\Omega_0^{(N)})^{1-3k}. \tag{32}$$

Determining the optimized $\Omega_0^{(N)}$ for which $b_0^{(N)}(\Omega_0^{(N)})$ has an extremum or a turning point then leads to the approximation $b_0^{(N)}(\Omega_0^{(N)})$ of the leading strong-coupling coefficient b_0.

By carrying the expansion to high orders, VPT yields approximations whose relative deviation from the exact value vanishes exponentially.[3,4] In our case, we have for large N

$$\frac{|b_0^{(N)}(D)-b_0(D)|}{b_0(D)}\sim\exp[A(D)-B(D)N^{1/3}], \tag{33}$$

where the exponent 1/3 is determined by the structure of the strong-coupling series (17). Due to the exponential convergence of VPT, it turns out that the accuracy of our numerical results for the leading strong-coupling coefficients b_0 in Table II is not sufficient for a useful examination of the convergence behavior of VPT in high orders. Therefore, we use our results from the 80th VPT order as a more precise approximation for b_0. Table III summarizes our high-precision VPT results, where in each case the uncertainty of b_0 has been estimated by examining the deviation

TABLE III. High-precision VPT results from the 80th order for the leading strong-coupling coefficient b_0 of the ground-state energy (17).

$b_0(D=2)$	1.4771497535779944356(33)
$b_0(D=3)$	2.39364401648230308 95(77)
$b_0(D=10)$	10.75826516544379740 8091(18)

from the result of the previous order. For $D=2$ and $D=10$, the VPT results lie within the error margins of the numerical results. However, this is not the case for $D=3$, where the VPT result lies just outside of the corresponding numerical error margins. We attribute this discrepancy to an overly optimistic error estimate for the numerical result. The precision of the results shown in Table III improves with increasing dimension, which already indicates that the calculation converges faster in higher dimensions. Figure 1 shows the convergence of the VPT results for the three different cases. Fitting the data to straight lines yields for the parameters $A(D)$ and $B(D)$ in (33),

$$A(D=2)=5.98(72), \quad B(D=2)=9.89(23), \tag{34}$$

$$A(D=3)=7.43(48), \quad B(D=3)=10.67(15), \tag{35}$$

$$A(D=10)=11.89(63), \quad B(D=10)=13.33(20). \tag{36}$$

Thus, we find that the convergence of the VPT result indeed improves uniformly with increasing dimension D. This tendency does not come as a surprise, since for $D\to\infty$ the ground-state energy of an oscillator with quartic anharmonicity can be determined exactly as we will see in the following section.

V. LARGE-*D* EXPANSION

Now, we elaborate the systematic large-D expansion for the ground-state energy of the anharmonic oscillator (2) based on standard field-theoretic methods (see, for instance, Refs. 3, 25, and 26).

A. Effective potential

We start with the path integral representation of the quantum-statistical partition function at finite temperature T,

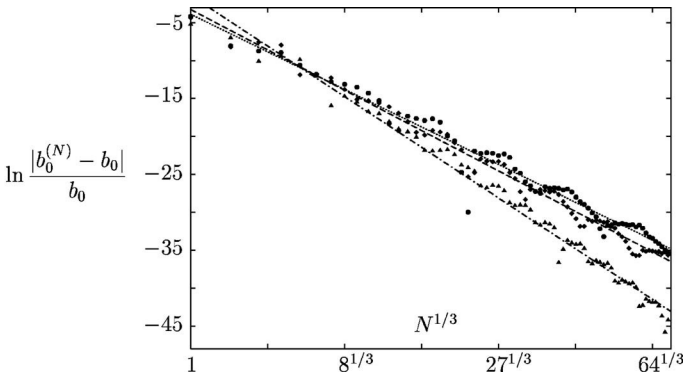

FIG. 1. Logarithm of the relative deviation of the VPT result for the leading strong-coupling coefficient $b_0(D)$ for $D=2$ (circles), $D=3$ (diamonds), and $D=10$ (triangles) plotted as a function of the cubic root of the perturbation order up to the 70th order. The dashed lines represent least squares fits of the data to straight lines.

$$Z = \oint \mathcal{D}\mathbf{x}\, e^{-\mathcal{A}[\mathbf{x}]}, \tag{37}$$

where the Euclidean action reads

$$\mathcal{A}[\mathbf{x}] = \int_0^\beta \mathrm{d}\tau \left\{ \frac{1}{2}\dot{\mathbf{x}}^2(\tau) + \frac{1}{2}\omega^2\mathbf{x}^2(\tau) + g[\mathbf{x}^2(\tau)]^2 \right\}. \tag{38}$$

The paths are periodic in the imaginary time τ with period $\beta \equiv 1/T$. Applying a Hubbard-Stratonovich transformation,

$$\oint \mathcal{D}\sigma \exp\left\{ -\int_0^\beta \mathrm{d}\tau \left[\frac{1}{g}\sigma^2(\tau) + 2i\mathbf{x}^2(\tau)\sigma(\tau) \right] \right\} = \exp\left\{ -g\int_0^\beta \mathrm{d}\tau [\mathbf{x}^2(\tau)]^2 \right\}, \tag{39}$$

the $\mathbf{x}(\tau)$-path integral (37) and (38) becomes harmonic and leads to

$$Z = \oint \mathcal{D}\sigma\, e^{-D\mathcal{A}[\sigma]}, \tag{40}$$

where we have introduced the Euclidean action

$$\mathcal{A}[\sigma] = \frac{1}{Dg}\int_0^\beta \mathrm{d}\tau\, \sigma^2(\tau) + \frac{1}{2}\mathrm{Tr}\ln\left[-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + \omega^2 + 4i\sigma(\tau) \right]. \tag{41}$$

The remaining path integral (40) and (41) over $\sigma(\tau)$ is then performed in the limit of large D by regarding the modified coupling constant $\tilde{g} = Dg$ as being independent of D, and by applying the background method.[3,27,28] Thus, we take into account order by order the effect of the fluctuations $\delta\sigma(\tau) \equiv \sigma(\tau) - \sigma_0$ of the paths $\sigma(\tau)$ from the background σ_0. This determines the effective potential

$$V_{\mathrm{eff}}(\sigma_0) = -\frac{1}{\beta}\ln Z \tag{42}$$

in the form of the loop expansion

$$V_{\mathrm{eff}}(\sigma_0) = \sum_{l=0}^{\infty} V_{\mathrm{eff}}^{(l)}(\sigma_0), \tag{43}$$

where the term of loop order l turns out to be of order D^{1-l}.

B. Loop orders $l=0$ and $l=1$

The leading term is the tree-level and follows from evaluating (41) for the background σ_0,

$$V_{\mathrm{eff}}^{(0)}(\sigma_0) = D\left[\frac{\sigma_0^2}{\tilde{g}} + \frac{1}{\beta}\ln\left(\sinh\frac{\beta\Omega}{2} \right) \right], \tag{44}$$

with the auxiliary frequency

$$\Omega = \sqrt{\omega^2 + 4i\sigma_0}. \tag{45}$$

The one-loop correction is given by

$$V_{\mathrm{eff}}^{(1)}(\sigma_0) = \frac{1}{2\beta}\mathrm{Tr}\ln G^{-1}(\tau_1, \tau_2), \tag{46}$$

where the operator

$$G^{-1}(\tau_1,\tau_2) = \left.\frac{\delta^2\mathcal{A}[\sigma]}{\delta\sigma(\tau_1)\delta\sigma(\tau_2)}\right|_{\sigma(\tau)=\sigma_0} \tag{47}$$

turns out to be

$$G^{-1}(\tau_1,\tau_2) = \frac{2}{\tilde{g}}\delta(\tau_1-\tau_2) + 8G_\Omega^2(\tau_1,\tau_2). \tag{48}$$

Here, the correlation function $G_\Omega(\tau_1,\tau_2)$ has the spectral representation

$$G_\Omega(\tau_1,\tau_2) = \sum_{m=-\infty}^{\infty} \frac{e^{-i\omega_m(\tau_1-\tau_2)}}{\beta(\omega_m^2+\Omega^2)}, \tag{49}$$

with the Matsubara frequencies $\omega_m = 2\pi m/\beta$. Inserting (49) in (48) yields

$$G^{-1}(\tau_1,\tau_2) = \frac{1}{\beta}\sum_{m=-\infty}^{\infty} G_m^{-1} e^{-i\omega_m(\tau_1-\tau_2)}, \tag{50}$$

with the coefficients

$$G_m^{-1} = \frac{2}{\tilde{g}} + \frac{8}{\beta}\sum_{m'=-\infty}^{\infty} \frac{1}{(\omega_{m'}^2+\Omega^2)(\omega_{m-m'}^2+\Omega^2)}. \tag{51}$$

For the quantum-mechanical ground-state energy to be calculated we only need the zero-temperature limit $\beta\to\infty$ of the above quantum statistical expressions. Thus, we obtain from (44),

$$V_{\text{eff}}^{(0)}(\sigma_0) \to D\left(\frac{\sigma_0^2}{\tilde{g}} + \frac{\Omega}{2}\right), \tag{52}$$

and the Matsubara sum (51) reduces to an integral,

$$\sum_{m=-\infty}^{\infty} f(\omega_m) \to \frac{\beta}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega_m\, f(\omega_m), \tag{53}$$

yielding

$$G_m^{-1} = \frac{2}{\tilde{g}} + \frac{8}{\Omega(\omega_m^2+4\Omega^2)}. \tag{54}$$

Correspondingly, Eq. (46) becomes

$$V_{\text{eff}}^{(1)}(\sigma_0) = \frac{1}{2\beta}\sum_{m=-\infty}^{\infty} \ln G_m^{-1} \to \frac{1}{4\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega_m \ln G_m^{-1} = \frac{\tilde{\Omega}}{2} - \Omega, \tag{55}$$

where

$$\tilde{\Omega} = 2\sqrt{\Omega^2 + \frac{\tilde{g}}{\Omega}} \tag{56}$$

denotes another auxiliary frequency.

C. Loop order $l=2$

The higher loop orders of the effective potential with $l \geqslant 2$ consist of all one-particle irreducible vacuum diagrams with the propagator

$$1 \text{ —— } 2 \quad \equiv \quad G(\tau_1, \tau_2) \tag{57}$$

defined by the identity

$$\int_0^\beta \mathrm{d}\tau_2\, G^{-1}(\tau_1, \tau_2) G(\tau_2, \tau_3) = \frac{1}{D}\delta(\tau_1 - \tau_3) \tag{58}$$

and the vertices

$$\begin{array}{ccc} & 2 & \\ 1 & \text{—}\bullet\text{—} & 3 \\ & n & \end{array} \quad \equiv -D \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \cdots \int_0^\beta d\tau_n \left. \frac{\delta^n \mathcal{A}[\sigma]}{\delta\sigma(\tau_1)\delta\sigma(\tau_2)\delta\sigma(\tau_3)\cdots\delta\sigma(\tau_n)} \right|_{\sigma(\tau)=\sigma_0} . \tag{59}$$

For instance, the two-loop contribution is given by the Feynman diagrams

$$V_{\text{eff}}^{(2)}(\sigma_0) = \frac{1}{8} \quad + \frac{1}{12} \quad . \tag{60}$$

In order to evaluate (60), we need the third and fourth functional derivatives of the Euclidean action (41). They are given by

$$\left. \frac{\delta^3 \mathcal{A}[\sigma]}{\delta\sigma(\tau_1)\delta\sigma(\tau_2)\delta\sigma(\tau_3)} \right|_{\sigma(\tau)=\sigma_0} = -64 i G_\Omega(\tau_1, \tau_2) G_\Omega(\tau_2, \tau_3) G_\Omega(\tau_3, \tau_1) \tag{61}$$

and

$$\begin{aligned} \left. \frac{\delta^4 \mathcal{A}[\sigma]}{\delta\sigma(\tau_1)\delta\sigma(\tau_2)\delta\sigma(\tau_3)\delta\sigma(\tau_4)} \right|_{\sigma(\tau)=\sigma_0} = -256 [& G_\Omega(\tau_1, \tau_2) G_\Omega(\tau_2, \tau_3) G_\Omega(\tau_3, \tau_4) G_\Omega(\tau_4, \tau_1) \\ & + G_\Omega(\tau_1, \tau_2) G_\Omega(\tau_2, \tau_4) G_\Omega(\tau_4, \tau_3) G_\Omega(\tau_3, \tau_1) \\ & + G_\Omega(\tau_1, \tau_3) G_\Omega(\tau_3, \tau_2) G_\Omega(\tau_2, \tau_4) G_\Omega(\tau_4, \tau_1)], \end{aligned} \tag{62}$$

where the explicit form of the correlation function $G_\Omega(\tau_1, \tau_2)$ at zero temperature follows from (49) and (53):

$$G_\Omega(\tau_1, \tau_2) = \frac{1}{2\Omega} e^{-\Omega|\tau_1 - \tau_2|}. \tag{63}$$

Furthermore, we must solve (58) for the propagator (57). Performing at arbitrary temperature the decomposition

$$G(\tau_1, \tau_2) = \frac{1}{\beta} \sum_{m=-\infty}^{\infty} G_m e^{-i\omega_m(\tau_1 - \tau_2)}, \tag{64}$$

the coefficient G_m turns out to be

$$G_m = \frac{1}{D G_m^{-1}}. \tag{65}$$

Using (54) and (65), we evaluate the Matsubara sum (64) at zero temperature according to (53) and obtain

$$G(\tau_1,\tau_2)=\frac{\tilde{g}}{2D}\left[\delta(\tau_1-\tau_2)-\frac{2\tilde{g}}{\Omega\tilde{\Omega}}e^{-\tilde{\Omega}|\tau_1-\tau_2|}\right]. \tag{66}$$

From (59) we read off that each vertex is of order D, whereas each propagator is of order $1/D$ due to (66). Thus both Feynman diagrams in (60) are, indeed, of order $1/D$. The first and second Feynman diagram in (60) lead to the expressions

$$V_{\mathrm{eff}}^{(2,1)}(\sigma_0)=\frac{1}{\beta D}\left\{-\frac{\tilde{g}^2}{2\Omega^4}[2I_2(2\Omega)+I_2(4\Omega)]+\frac{2\tilde{g}^3}{\Omega^5\tilde{\Omega}}[2I_3(\Omega,\Omega,\Omega+\tilde{\Omega})+I_3(2\Omega,2\Omega,\tilde{\Omega})]\right.$$
$$\left.-\frac{2\tilde{g}^4}{\Omega^6\tilde{\Omega}^2}[2I_4(\Omega+\tilde{\Omega},0,\Omega,\Omega,0,\Omega+\tilde{\Omega})+I_4(\tilde{\Omega},\Omega,\Omega,\Omega,\Omega,\tilde{\Omega})]\right\}, \tag{67}$$

$$V_{\mathrm{eff}}^{(2,2)}(\sigma_0)$$
$$=\frac{1}{\beta D}\left[\frac{2\tilde{g}^3}{3\Omega^6}I_3(2\Omega,2\Omega,2\Omega)-\frac{4\tilde{g}^4}{\Omega^7\tilde{\Omega}}I_4(\Omega,\Omega,\tilde{\Omega},2\Omega,\Omega,\Omega)\right.$$
$$\left.+\frac{8\tilde{g}^5}{\Omega^8\tilde{\Omega}^2}I_5(\Omega,\Omega,\tilde{\Omega},0,\Omega,0,\tilde{\Omega},\Omega,\Omega,\Omega)-\frac{16\tilde{g}^6}{3\Omega^9\tilde{\Omega}^3}I_6(\Omega,\Omega,\tilde{\Omega},0,0,\Omega,0,\tilde{\Omega},0,0,0,\tilde{\Omega},\Omega,\Omega,\Omega)\right], \tag{68}$$

respectively. Here we have introduced an abbreviation for multiple integrals with respect to imaginary times,

$$I_n(\Omega_{12},\ldots,\Omega_{1n},\Omega_{23},\ldots,\Omega_{2n},\ldots)=\int_0^\beta \mathrm{d}\tau_1\int_0^\beta \mathrm{d}\tau_2\cdots\int_0^\beta \mathrm{d}\tau_n\exp\left(-\sum_{i=1}^{n}\sum_{j=i+1}^{n}\Omega_{ij}|\tau_i-\tau_j|\right). \tag{69}$$

Considering the low-temperature limit $\beta\to\infty$, the first three of these integrals read in closed form[29]

$$I_2(\Omega_{12})=\frac{2\beta}{\Omega_{12}}, \tag{70}$$

$$I_3(\Omega_{12},\Omega_{13},\Omega_{23})=\frac{4\beta(\Omega_{12}+\Omega_{13}+\Omega_{23})}{(\Omega_{12}+\Omega_{13})(\Omega_{12}+\Omega_{23})(\Omega_{13}+\Omega_{23})}, \tag{71}$$

$$I_4(\Omega_{12},\Omega_{13},\Omega_{14},\Omega_{23},\Omega_{24},\Omega_{34})$$
$$=2\beta\times\left\{\frac{1}{\Omega_{12}+\Omega_{13}+\Omega_{24}+\Omega_{34}}\left[\frac{1}{\Omega_{12}+\Omega_{13}+\Omega_{14}}+\frac{1}{\Omega_{14}+\Omega_{24}+\Omega_{34}}\right]\right.$$
$$\times\left[\frac{1}{\Omega_{12}+\Omega_{23}+\Omega_{24}}+\frac{1}{\Omega_{13}+\Omega_{23}+\Omega_{34}}\right]+\frac{1}{\Omega_{12}+\Omega_{14}+\Omega_{23}+\Omega_{34}}$$
$$\times\left[\frac{1}{\Omega_{12}+\Omega_{23}+\Omega_{24}}+\frac{1}{\Omega_{14}+\Omega_{24}+\Omega_{34}}\right]\left[\frac{1}{\Omega_{12}+\Omega_{13}+\Omega_{14}}+\frac{1}{\Omega_{13}+\Omega_{23}+\Omega_{34}}\right]$$
$$\left.+\frac{1}{\Omega_{13}+\Omega_{14}+\Omega_{23}+\Omega_{24}}\left[\frac{1}{\Omega_{13}+\Omega_{23}+\Omega_{34}}+\frac{1}{\Omega_{14}+\Omega_{24}+\Omega_{34}}\right]\right.$$

$$\times\left[\frac{1}{\Omega_{12}+\Omega_{13}+\Omega_{14}}+\frac{1}{\Omega_{12}+\Omega_{23}+\Omega_{24}}\right]\Bigg\}. \tag{72}$$

Furthermore, in order to evaluate (68), we need one particular integral with respect to five and six imaginary times, respectively,

$$I_5(\Omega,\Omega,\tilde{\Omega},0,\Omega,0,\tilde{\Omega},\Omega,\Omega,\Omega)=\frac{\beta(3\tilde{\Omega}^5+42\tilde{\Omega}^4\Omega+227\tilde{\Omega}^3\Omega^2+568\tilde{\Omega}^2\Omega^3+656\tilde{\Omega}\Omega^4+288\Omega^5)}{2\Omega^2(\tilde{\Omega}+\Omega)^2(\tilde{\Omega}+2\Omega)^4(\tilde{\Omega}+4\Omega)}, \tag{73}$$

$$\begin{aligned}&I_6(\Omega,\Omega,\tilde{\Omega},0,0,\Omega,0,\tilde{\Omega},0,0,0,\tilde{\Omega},\Omega,\Omega,\Omega)\\&\quad=\frac{3\beta(\tilde{\Omega}^5+14\tilde{\Omega}^4\Omega+73\tilde{\Omega}^3\Omega^2+160\tilde{\Omega}^2\Omega^3+136\tilde{\Omega}\Omega^4+32\Omega^5)}{\tilde{\Omega}\Omega^2(\tilde{\Omega}+\Omega)^2(\tilde{\Omega}+2\Omega)^4(\tilde{\Omega}+4\Omega)}.\end{aligned} \tag{74}$$

From (44) and (67)–(74) we read off the effective potential for zero temperature up to the order $1/D$,

$$\begin{aligned}V_{\mathrm{eff}}(\sigma_0)=D\left(\frac{\sigma_0^2}{\tilde{g}}+\frac{\Omega}{2}\right)+\frac{\tilde{\Omega}}{2}-\Omega+\frac{1}{D}\Bigg[&-\frac{5\tilde{g}^2}{4\Omega^5}+\frac{\tilde{g}^3(\tilde{\Omega}^3+4\tilde{\Omega}^2\Omega+44\tilde{\Omega}\Omega^2+128\Omega^3)}{4\Omega^8\tilde{\Omega}(\tilde{\Omega}+2\Omega)^2}\\&-\frac{\tilde{g}^4(3\tilde{\Omega}^5+31\tilde{\Omega}^4\Omega+150\tilde{\Omega}^3\Omega^2+392\tilde{\Omega}^2\Omega^3+656\tilde{\Omega}\Omega^4+480\Omega^5)}{\Omega^9\tilde{\Omega}^2(\tilde{\Omega}+\Omega)(\tilde{\Omega}+2\Omega)^3(\tilde{\Omega}+4\Omega)}\\&+\frac{4\tilde{g}^5(3\tilde{\Omega}^5+42\tilde{\Omega}^4\Omega+227\tilde{\Omega}^3\Omega^2+568\tilde{\Omega}^2\Omega^3+656\tilde{\Omega}\Omega^4+288\Omega^5)}{\Omega^{10}\tilde{\Omega}^2(\tilde{\Omega}+\Omega)^2(\tilde{\Omega}+2\Omega)^4(\tilde{\Omega}+4\Omega)}\\&-\frac{16\tilde{g}^6(\tilde{\Omega}^5+14\tilde{\Omega}^4\Omega+73\tilde{\Omega}^3\Omega^2+160\tilde{\Omega}^2\Omega^3+136\tilde{\Omega}\Omega^4+32\Omega^5)}{\Omega^{11}\tilde{\Omega}^4(\tilde{\Omega}+\Omega)^2(\tilde{\Omega}+2\Omega)^4(\tilde{\Omega}+4\Omega)}\Bigg]+\mathcal{O}\left(\frac{1}{D^2}\right).\end{aligned} \tag{75}$$

The ground-state energy of the anharmonic oscillator (2) is found by extremizing the effective potential (75) with respect to the background σ_0 while taking into account the auxiliary frequencies (45) and (56).

D. Weak coupling

In order to cross-check our large-D result, we specialize now to the weak-coupling regime where the extremal background is expanded according to

$$\sigma_0=-i(s_1\tilde{g}+s_2\tilde{g}^2+s_3\tilde{g}^3+s_4\tilde{g}^4+s_5\tilde{g}^5+\cdots). \tag{76}$$

Inserting (76) into the vanishing first derivative of (75) and reexpanding in $\tilde{g}$, we obtain a system of equations which are solved by

$$s_1=\frac{1}{2\omega}, \tag{77}$$

$$s_2=-\frac{1}{2\omega^4}-\frac{1}{\omega^4 D}, \tag{78}$$

$$s_3=\frac{5}{4\omega^7}+\frac{45}{8\omega^7 D}+\frac{25}{4\omega^7 D^2}, \tag{79}$$

$$s_4 = -\frac{4}{\omega^{10}} - \frac{59}{2\omega^{10}D} - \frac{73}{\omega^{10}D^2}, \tag{80}$$

$$s_5 = \frac{231}{16\omega^{13}} + \frac{19503}{128\omega^{13}D} + \frac{9823}{16\omega^{13}D^2} + \frac{275}{2\omega^{13}D^3}, \quad \cdots . \tag{81}$$

Inserting (76)–(81) into (75) and reexpanding in $\tilde{g}=Dg$ yields again the weak-coupling series (11), where the weak-coupling coefficients ϵ_k of Table I are reproduced in the first three terms of order D^{k+1}, D^k, and D^{k-1}.

E. Strong coupling

We now derive the large-D expansion for the ground-state energy in the strong-coupling regime. There, we use for the extremal background the ansatz

$$\sigma_0 = -i\tilde{g}^{2/3}(S_1 + S_2\tilde{g}^{-2/3} + \cdots) \tag{82}$$

and find for the leading coefficient the expansion

$$S_1 = \frac{1}{2^{4/3}} + (2^{1/6}\times 3^{1/2} - 2^{5/3})\frac{1}{6D} + \left(27\times 6^{1/2} - \frac{73}{2}\right)^{1/3}\frac{1}{18D^2} + \mathcal{O}\left(\frac{1}{D^3}\right). \tag{83}$$

From (75), (82), and (83) we then obtain the strong-coupling series (17) where the leading strong-coupling coefficient has the large-D expansion

$$b_0 = \sum_{k=0}^{\infty} B_k D^{4/3-k}, \tag{84}$$

with

$$B_0 = \frac{3\times 2^{1/3}}{8}, \tag{85}$$

$$B_1 = \frac{3^{1/2} - 2^{1/2}}{2^{1/6}} \approx 0.283\,160\,794\,322\,179\,118\,844\,664\,604\,794\,882\,036\,512\,3, \tag{86}$$

$$B_2 = -\frac{239}{18\times 2^{2/3}(25 + 12\times 6^{1/2})} \approx -0.153\,776\,055\,939\,928\,491\,319\,576\,108\,549\,970\,570\,159\,0. \tag{87}$$

Figure 2 shows the leading strong-coupling coefficient (84)–(86) up to the first two orders plotted as a function of the dimension D.

VI. LARGE-D EXPANSION FROM VPT

In this section, we study how the large-D expansion (84) follows from VPT. Thereby, we numerically determine the large-D expansion coefficients up to B_6 with high precision.

A. Coefficients B_1 and B_2

To first order, VPT gives (28), and we obtain the expansion (84) simply by expanding the cubic root in (28) in powers of $1/D$. The first three coefficients in the expansion (84) read

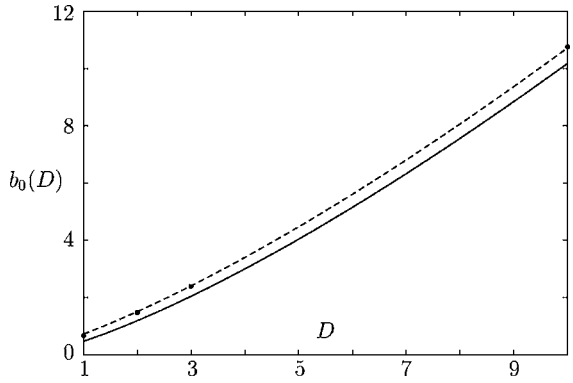

FIG. 2. Strong-coupling coefficient $b_0(D)$ versus dimension D. Solid and dashed lines represent leading and subleading results of the large-D expansion (84)–(86), respectively. For $D=1$, the dot represents the earlier result from Refs. 8 and 9; for $D=2,3,10$, the dots indicate the highly accurate VPT values obtained from the 80th order, as given in Table III.

$$B_0^{(1)} = \frac{3\times 2^{1/3}}{8}, \quad B_1^{(1)} = \frac{2^{1/3}}{4}, \quad B_2^{(1)} = -\frac{2^{1/3}}{6}. \tag{88}$$

The leading coefficient (85) is reproduced exactly, while the next two subleading coefficients B_1 and B_2 are missed by 11.2% and 36.6%, respectively. In the second order of VPT, Eq. (32) yields

$$b_0^{(2)}(\Omega_0^{(2)}) = \frac{3D\Omega_0^{(2)}}{16} + \frac{D(2+D)}{2(\Omega_0^{(2)})^2} - \frac{D(10+9D+2D^2)}{8(\Omega_0^{(2)})^5}, \tag{89}$$

which must be extremized with respect to the variational parameter $\Omega_0^{(2)}$. Setting the derivative of (89) to zero, the large-D expansion

$$\Omega_0^{(2)} = D^{1/3}\left(C_0^{(0,2)} + \frac{C_1^{(0,2)}}{D} + \frac{C_2^{(0,2)}}{D^2} + \cdots\right) \tag{90}$$

leads to a system of equations for the expansion coefficients whose solutions read

$$C_0^{(2)} = 2^{1/3}, \quad C_1^{(2)} = \frac{13\times 2^{1/3}}{12}, \quad C_2^{(2)} = -\frac{113\times 2^{1/3}}{288}, \quad \cdots. \tag{91}$$

Thus, by inserting the optimized variational parameter (90) and (91) into (89) and expanding in $1/D$ we obtain the first three coefficients in (84) to second order of VPT,

$$B_0^{(2)} = \frac{3\times 2^{1/3}}{8}, \quad B_1^{(2)} = \frac{7\times 2^{1/3}}{32}, \quad B_2^{(2)} = -\frac{71\times 2^{1/3}}{768}. \tag{92}$$

The leading large-D coefficient B_0 remains the same, whereas the error of the subleading coefficient $B_1^{(2)}$ is reduced to 2.67% and the next subleading coefficient $B_2^{(2)}$ now comes out with an error of 24.2%. Figure 3 shows that the VPT approximants $B_1^{(N)}$ and $B_2^{(N)}$ converge exponentially fast to their exact values B_1 and B_2 in (86) and (87). If we had not known the exact analytic result for the subleading coefficients B_1 and B_2, we could have extracted its value from the VPT approximants as follows. Figure 3 shows that the VPT approximants for odd and even orders converge towards the exact value independently. Extrapolating the values of $B_1^{(\mathrm{odd})}$ and $B_1^{(\mathrm{even})}$ for $N\to\infty$ leads to the limiting values

$$B_1^{(\mathrm{odd})} \approx 0.283\,160\,794\,322\,179\,118\,844\,664\,604\,794\,882\,038\,08, \tag{93}$$

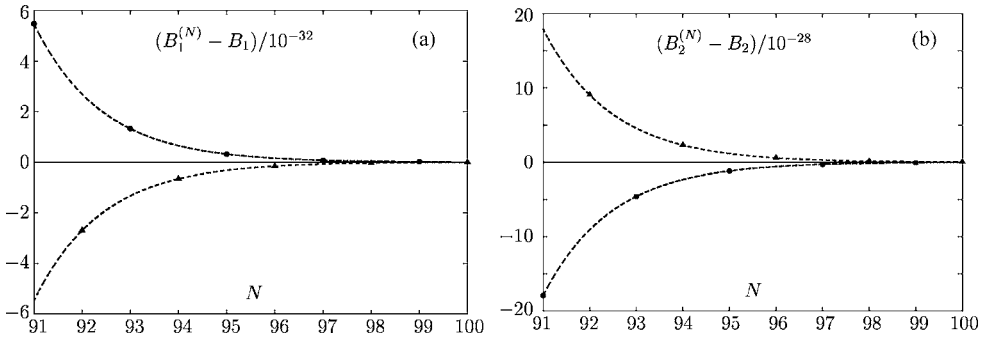

FIG. 3. Deviation of the VPT approximants for (a) $B_1^{(N)}$ and (b) $B_2^{(N)}$ from their exact values B_1 and B_2 in Eqs. (86) and (87), respectively. Odd orders are represented by circles; even orders by triangles. The dashed lines represent fits of the data to exponential functions.

$$B_1^{(\text{even})} \approx 0.283\,160\,794\,322\,179\,118\,844\,664\,604\,794\,882\,035\,75. \tag{94}$$

Assuming that the exact value lies within this interval, we obtain from this extrapolation method the result

$$B_1^{(\text{extrap})} = 0.283\,160\,794\,322\,179\,118\,844\,664\,604\,794\,882\,036\,9(24). \tag{95}$$

An analogous procedure can be applied to extract a numerical value for the subsequent coefficient B_2. Applying the extrapolation method for odd and even orders, we obtain the result

$$B_2^{(\text{extrap})} = -0.153\,776\,055\,939\,928\,491\,319\,576\,108\,549\,961(60). \tag{96}$$

B. Coefficients up to B_6

Figure 4 shows that the VPT approximants for B_1 and B_2 rapidly converge towards their exact values. For the large-D expansion coefficients of higher orders in $1/D$, however, the VPT approximants first fluctuate and then enter the regime of exponentially fast convergence. If we want to obtain the coefficients of the expansion (84) to higher orders and with good accuracy, we must therefore drive our VPT calculation to high orders. To this end, we specialize the expression for

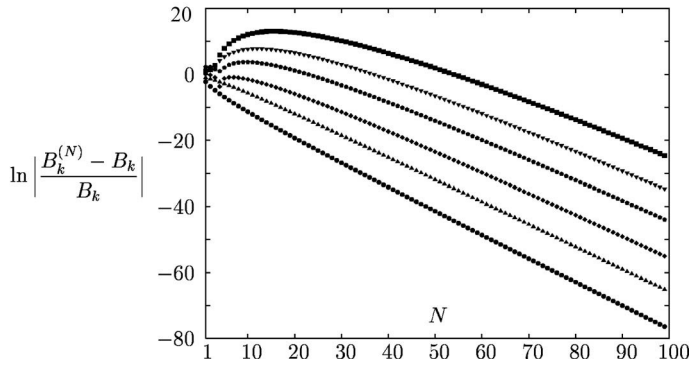

FIG. 4. Logarithm of the relative deviation of the VPT results $B_k^{(N)}$ for the coefficients B_1 through B_6 in the large-D expansion (84) versus the order N of VPT. The lowest curve (circles) is for $B_1^{(N)}$; the uppermost curve (squares) is for $B_6^{(N)}$; intermediate curves are for $B_2^{(N)}$ through $B_5^{(N)}$ ($B_2^{(N)}$, triangles; $B_3^{(N)}$, diamonds; $B_4^{(N)}$, pentagons; $B_5^{(N)}$, upside-down triangles). For $B_1^{(N)}$ and $B_2^{(N)}$ the exact values from (86) and (87) were used in order to determine the relative deviation. For $B_3^{(N)}$ through $B_6^{(N)}$ we used our extrapolation results from Table IV.

the leading strong-coupling coefficient as given in (32) in such a way that we can read off the corresponding large-D expansion. The weak-coupling coefficients for the ground-state energy ϵ_k can be expanded in powers of the spatial dimension D,

$$\epsilon_k = \sum_{j=1}^{k+1} \epsilon_j^{(k)} D^j, \tag{97}$$

whereas the variational parameter $\Omega_0^{(N)}$ can be expanded in $1/D$,

$$\Omega_0^{(N)} = D^{1/3} \sum_{j=0}^{M} C_j^{(0,N)} D^{-j}. \tag{98}$$

Here, M denotes the highest order to which we seek to drive the large-D expansion (84). Furthermore, recall the multinomial expansion

$$(x_1 + x_2 + \cdots + x_m)^n = \sum_{a_1=0}^{n} \sum_{a_2=0}^{n} \cdots \sum_{a_m=0}^{n} \delta\left(n, \sum_{k=1}^{m} a_k\right) \frac{n!}{a_1! a_2! \cdots a_m!} \prod_{l=1}^{m} x_l^{a_l}, \tag{99}$$

where n is an integer and where the Kronecker delta δ_{ij} is written as $\delta(i,j)$. This multinomial expansion can be generalized to hold for real exponents and infinite series as follows:

$$(1 + x_1 + x_2 + \cdots)^\alpha = \sum_{m=0}^{\infty} \left[\sum_{a_1=0}^{\infty} \sum_{a_2=0}^{\infty} \cdots \sum_{a_m=0}^{\infty} \delta\left(m, \sum_{l=1}^{m} l a_l\right) \times \frac{\Gamma(\alpha+1)}{\Gamma(\alpha - a_1 - a_2 - \cdots - a_m + 1) a_1! a_2! \cdots a_m!} \prod_{l=1}^{m} x_l^{a_l} \right]. \tag{100}$$

Using (97) and (98) in (32) and applying the multinomial expansion (100), we obtain

$$b_0^{(N)}(\Omega_0^{(N)}) = D^{1/3} \left\{ \frac{D}{2} \sum_{j=0}^{M} C_j^{(0,N)} D^{-j} + \sum_{k=1}^{N} \binom{(1-3k)/2 - 1}{N-k} (-1)^{N-k} D^{-k} (C_0^{(0,N)})^{1-3k} \times \left[\sum_{j=1}^{k+1} \epsilon_j^{(k)} D^j + \sum_{j=2}^{M+k} \sum_{m=1}^{\mathrm{Min}\{j-1, \lfloor (M+j-k)/2 \rfloor - 1\}} \epsilon_{j-m}^{(k)} K_{m,k}^{(N)} D^{j-2m} \right] \right\}, \tag{101}$$

where the coefficients $K_{m,k}^{(N)}$ are given by

$$K_{m,k}^{(N)} = \sum_{a_1=0}^{M} \sum_{a_2=0}^{M} \cdots \sum_{a_m=0}^{M} \delta\left(m, \sum_{l=1}^{m} l a_l\right) \frac{(3k - 2 + a_1 + a_2 + \cdots a_m)!}{(3k-2)! a_1! a_2! \cdots a_m!} (-1)^{a_1 + a_2 + \cdots + a_m} \prod_{l=1}^{m} \left(\frac{C_l^{(0,N)}}{C_0^{(0,N)}} \right)^{a_l}. \tag{102}$$

The summation boundaries in (101) are determined by the two conditions that (i) $\epsilon_j^{(k)} = 0$ for $j < 1 \vee j > k+1$ and (ii) we can neglect contributions containing coefficients $C_k^{(0,N)}$ with $k > M$. Note that a similar expansion holds for the derivative of the leading strong-coupling coefficient with respect to the variational parameter $\mathrm{d}b_0^{(N)}/\mathrm{d}\Omega_0^{(N)}$. Using (101) and (102) we can efficiently calculate the VPT approximants to high orders. In each order of VPT, the leading large-D coefficient B_0 comes out exactly. Furthermore, the expansion coefficients $C_k^{(0,N)}$ for the variational parameter are found by solving linear equations. Figure 4 shows the convergence behavior of our VPT approximants for B_1 through B_6 up to $N=100$. By extrapolating the VPT results $B_k^{(N)}$ for $k \geqslant 3$ in the limit $N \to \infty$, we are able to determine the coefficients in the large-D expansion to high accuracy. The numerical results are shown in Table IV.

TABLE IV. VPT results for the coefficients in the large-D expansion (84) of the leading strong-coupling coefficient b_0.

B_3	0.109850770164836799117922 4418(38)
B_4	−0.028863731985996976497 59(11)
B_5	−0.169597632126182899 3(92)
B_6	0.51902738902696(86)

VII. SUMMARY

We have determined the weak-coupling series of the ground-state energy for the D-dimensional anharmonic oscillator (2) and used variational perturbation theory to extract the coefficients of the large-D expansion to higher orders than accessible by standard field-theoretic methods based on the Hubbard-Stratonovich transformation.

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Existence of two-cluster threshold resonances and the *N*-body Efimov effect

Xue Ping Wang[a)]
Département de Mathématiques, UMR 6629 DU CNRS, Université de Nantes, 44322 Nantes Cedex 3, France

Yuefei Wang[b)]
Institute of Mathematics, The Chinese Academy of Sciences, 100871 Beijing, China

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We prove the existence of two-cluster threshold resonances in *N*-body problems and study their perturbation by intercluster interactions. As application, we construct concrete examples based on Yukawa potentials for which the *N*-body Efimov effect happens with $N \geqslant 4$. © *2005 American Institute of Physics.*
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I. INTRODUCTION

In Ref. 15, the first author of the present work proved the existence of the *N*-body Efimov effect for $N \geqslant 4$ which says that if the bottom of essential spectrum is attained by a unique three-cluster decomposition and if the three resulting two-cluster sub-Hamiltonians possess a threshold resonance at this threshold, then the number of discrete eigenvalues is always infinite even if the interaction potentials decay rapidly at the infinity. This phenomenon is similar to the famous three-body Efimov effect, discovered by the physicist. Efimov[4] and studied in mathematics literature by many authors. See, for example, Refs. 2, 8–12 and 17. For *N*-body quantum systems with $N \geqslant 4$, it has been unknown for a long time whether the Efimov effect exists. In Ref. 1, Amado and Greenwood argued that the zero eigenvalue and zero resonance of $(N-1)$-particle subsystems do not produce an infinite number of eigenvalues in *N*-body problems when $N \geqslant 4$. Note that in spite of the title, the result of Ref. 15 is not in discrepancy with Ref. 1, because it corresponds to a different spectral configuration, and that a mathematical proof of the affirmation of Ref. 1 is always lacking. After the work,[15] a question has then naturally been raised as how to give concrete examples such that all conditions acquired in Ref. 15 are satisfied, especially the existence of two-cluster threshold energy resonances with any number of particles. Trivial examples can be constructed from two-body zero resonance by adding some particles with independent variables. The goal of this work is to show the existence of two-cluster threshold resonances and the Efimov effect for a class of nontrivial interactions. We will show that mathematically, one can produce the *N*-body Efimov effect by adjusting parameters in Yukawa-type interactions of the form $-\alpha e^{-\epsilon\alpha|x|}/|x|$, α, $\epsilon > 0$. Yet, even for such concrete potentials, our proof for the existence of two-cluster *N*-body threshold resonance is abstract. We leave the interested reader to make numerical simulation or physical experiment.

Our example will be given in terms of atomic type four-body Schrödinger operators. This leads us to consider generalized *N*-body Schrödinger operators which include both atomic-type and regular *N*-body operators. Let *P* denote a generalized *N*-body Schrödinger operator of the form $P=-\Delta+\Sigma_{a\in\mathcal{A}}V_a(x^a)$ in $L^2(\mathbf{X})$, where $\mathcal{A}$ denotes the set of all cluster decompositions of the *N*-particle system labeled by $\{1,\ldots,N\}$, $x^a \in \mathbf{X}^a$ and $\{\mathbf{X}^a\}$ is a family of linear subspaces of $\mathbf{X}$

[a)]Electronic mail: xue-ping.wang@univ-nantes.fr
[b)]Electronic mail: yfwang@math.amss.ac.cn

satisfying some axioms. See Ref. 3. A typical example of such operators is regular N-body Schrödinger operator obtained by removing the mass-center from the operator

$$-\sum_{j=1}^{N}\frac{1}{2m_j}\Delta_{x_j}+\sum_{1\leqslant i\leqslant j\leqslant N}V_{ij}(x_i-x_j),\quad x_j\in\mathbb{R}^3, \tag{1.1}$$

where x_j and m_j denote the position and mass of the jth particle. P is regarded as a self-adjoint operator in $L^2(\mathbf{X})$, where $\mathbf{X}$ is the $3(N-1)$-dimensional real vectorial space, $\mathbf{X}=\{(x_1,\ldots,x_N)\in\mathbb{R}^{3N};\Sigma_{j=1}^{N}m_jx_j=0\}$. For $a\in\mathcal{A}$, let $\#a$ denote the number of clusters in a and P^a the sub-Hamiltonian associated with a. For $i,j\in\{1,\ldots,N\}$, $i\neq j$, we write $(ij)\in a$ if i and j belong to a same cluster in a. If a,b are two cluster decompositions, we write $b\subset a$ if b is a refinement of a. If a be a k-cluster decomposition $a=(a_1,\ldots,a_k)$, then $\mathbf{X}^a=\{x\in\mathbf{X};\Sigma_{l\in a_j}m_lx_l=0,j=1,\ldots,k\}$ the intracluster space and $\mathbf{X}_a=\{x\in\mathbf{X};x_i=x_j$ if $(ij)\in a_m$ for some $m\in\{1,\ldots,k\}\}$ the intercluster space. $\mathbf{X}^a$ and $\mathbf{X}_a$ give an orthogonal decomposition for $\mathbf{X}$ relative to the quadratic form $q(x)=\Sigma_j2m_j|x_j|^2$, $x\in\mathbf{X}$. For $x\in\mathbf{X}$, we have the orthogonal decomposition, $x=x^a+x_a$ with $x^a\in\mathbf{X}^a$ and $x_a\in\mathbf{X}_a$. The N-body Schrödinger operator, P, obtained above can be written in the form $P=P_0+V(x)$ where $P_0=-\Delta$ is the Laplace-Beltrami operator on the Euclidean space $(\mathbf{X},q)$ and $V(x)=\Sigma_{a\in\mathcal{A}}V_a(x^a)$ with $V_a(x^a)=V_{ij}(x_i-x_j)$ if a is an $(N-1)$-cluster decomposition and $(ij)\in a$; $V_a(x^a)=0$, otherwise. The atomic-type N-body operators can also be written in the form of generalized N-body operators. Let $-\Delta^a$ ($-\Delta_a$, respectively) denote the restriction of P_0 on $\mathbf{X}^a$ (on $\mathbf{X}_a$, respectively). For $a\in\mathcal{A}$, denote $P^a=-\Delta^a+\Sigma_{b\subseteq a}V_b(x^b),P_a=P^a-\Delta_a,I_a(x)=\Sigma_{b\nsubseteq a}V_b(x^b)$. P^a is the sub-Hamiltonian associated with the cluster decomposition a and I_a is the sum of all intercluster interactions. Assume that $V_a(x^a)$ is real and relatively form-compact with respect to $-\Delta^a$ in $L^2(\mathbf{X}^a)$, satisfying the decay

$$|V_a(x^a)|\leqslant C\langle x^a\rangle^{-\rho_0},\quad \rho_0>2, \tag{1.2}$$

for x^a outside some compact of $\mathbf{X}^a$. P is regarded as self-adjoint operator in $L^2(\mathbf{X})$ with form domain $H^1(\mathbf{X})$. Let $\mathcal{T}=\cup_{a\in\mathcal{A},\#a\geqslant2}\sigma_p(P^a)$ be the set of thresholds of P. The HVZ theorem says that the bottom of the essential spectrum, $E_0\triangleq\inf\sigma_{\mathrm{ess}}(P)$, of P is given by

$$E_0=\min_{a\in\mathcal{A},\#a\geqslant2}\inf\sigma(P^a)=\min_{a\in\mathcal{A},\#a=2}\inf\sigma(P^a).$$

Assume that E_0 is attained by a unique three-cluster decomposition, b, with $b=(b_1,b_2,b_3)$

$$\inf\sigma(P^b)=E_0=\inf\sigma_{\mathrm{ess}}(P). \tag{1.3}$$

Let $a_k=(b_i\cup b_j,b_k)$, where i, j, and k take different values in {1, 2, 3}. Throughout this paper, we suppose that $\dim\mathbf{X}^{a_j}\cap\mathbf{X}_b=3$, which is always satisfied for the operator obtained from (1.1). By HVZ theorem, one has $\sigma(P^{a_k})=[E_0,\infty[$. We assume that these are the only cluster decompositions attaining E_0,

$$\inf\sigma(P^a)=E_0,a\in\{b,a_1,a_2,a_3\},\quad \inf\sigma(P^a)>E_0,\quad a\notin\{b,a_1,a_2,a_3\},\#a\geqslant2. \tag{1.4}$$

Assume that the intercluster interactions related to b are attractive,

$$V_a(x^a)\leqslant0\quad\text{for } a\nsubseteq b. \tag{1.5}$$

Definition: Let Q be a generalized N-body Schrödinger operator with $N\geqslant3$. Let $E_0=\inf\sigma_{\mathrm{ess}}(Q)$. (a) Q is called *unique two-cluster* if there exits only one two-cluster decomposition a_0 such that $\inf\sigma(Q^{a_0})=E_0$. (b) E_0 is called a *threshold resonance* of Q if the equation $Qu=E_0u$ has a solution $u\in H^{1,-s}(\mathbf{X})\backslash L^2(\mathbf{X})$ for any $s>\frac{1}{2}$.

In our work, Q plays the role of one of the two-cluster sub-Hamiltonians P^{a_j} and $a_0=b$. Under the assumptions (1.2) and (1.4), the analysis of threshold resonances made in Ref. 14 is valid for P^{a_j}. One knows that if E_0 is a resonance of P^{a_j}, then it is simple and the corresponding resonant state u behaves like

$$u(x^{a_j}) = O(e^{-\delta|x^b|}|x_b^{a_j}|^{-1}), \quad |x^{a_j}| \to \infty, \quad \delta > 0. \tag{1.6}$$

Note the threshold resonances studied in Ref. 14 are two-cluster in nature and it is an interesting open question to study the many-cluster threshold resonances. See Ref. 16 for threshold resonances in geometric setting.

Theorem 1.1 (Ref. 15): *Let $N \geqslant 4$. Let the conditions (1.2) with $\rho > 2$, (1.4) and (1.5) be satisfied. Assume that each of the two-cluster sub-Hamiltonians P^{a_j}, $j=1,2,3$, have a threshold resonance at E_0. Let $N(\lambda)$ denote the number of the eigenvalues of P below $\lambda < E_0$. Then, there exists $C_0 > 0$ depending only on the reduced masses of b_1, b_2, b_3 such that*

$$N(\lambda) \geqslant C_0|\log|\lambda - E_0||, \quad \lambda \to E_0. \tag{1.7}$$

Assumption (1.4) may be realized when some particles are remarkably distinct from the others. In this work, we study the existence of two-cluster threshold resonances by varying some coupling constant. We will prove the following.

Theorem 1.2: *Let Q be an N-body operator with potentials V_c satisfying (1.2) and let a be a two-cluster decomposition. Assume that $V_c \leqslant 0$ for all $c \not\subseteq a$, $I_a = \Sigma_{c \not\subseteq a} V_c \neq 0$, $E_0 = \inf \sigma(Q^a) \in \sigma_d(Q^a)$. Denote $Q(g) = Q_a + gI_a$. Let g_0 be the critical coupling constant defined by*

$$g_0 = \sup\{g \geqslant 0; \inf \sigma(Q(g)) = \inf \sigma_{\mathrm{ess}}(Q(g)) = E_0\}. \tag{1.8}$$

Then, if $Q(g_0)$ is unique two-cluster, E_0 is a threshold resonance of $Q(g_0)$.

We will also give a sufficient condition to guarantee the unique two-cluster property of $Q(g_0)$ and study the perturbation of threshold resonance (Theorem 3.1), which is in some sense a converse of Theorem 1.2.

The idea of varying coupling constant limit is used in Ref. 7 for the study of absorption of discrete eigenvalues into a unique two-cluster threshold. In Ref. 7, the authors deduced their results by splitting some reduced operator into sum of a compact continuous part and a bounded holomorphic part. Our proof of Theorem 1.2 relies on the idea of Ref. 14, where the notion of N-body threshold resonance is introduced. In the proof of existence of resonant state (Proposition 2.3), the compactness of the whole reduced operator is essential.

Using Theorem 1.2, we will show that for appropriate constant $\alpha_1 > 0$, $\epsilon > 0$ small enough, there exists $g_j \in]0,1[$, $j=1,2,3$, such that Theorem 1.1 holds for the atomic-type four-body Schrödinger operator with Yukawa potentials

$$P = -\Delta_{x_1} - \Delta_{x_2} - \Delta_{x_3} - \frac{\alpha_1 e^{-\epsilon\alpha_1|x_1|}}{|x_1|} - g_1\frac{e^{-\epsilon|x_2-x_3|}}{|x_2-x_3|} - g_2\left(\frac{e^{-\epsilon|x_2|}}{|x_2|} + \frac{e^{-\epsilon|x_1-x_2|}}{|x_1-x_2|}\right) - g_3\left(\frac{e^{-\epsilon|x_3|}}{|x_3|} + \frac{e^{-\epsilon|x_1-x_3|}}{|x_1-x_3|}\right), \quad x_j \in \mathbb{R}^3. \tag{1.9}$$

The plan of this work is as follows. In Sec. II, we prove the existence of two-cluster threshold resonance. In Sec. III, we show that if E_0 is a two threshold resonance of $Q(g)$ for $g=g_0$, it is shifted to the left to become a nondegenerate discrete eigenvalue when g increases. These results are applied to the study of the N-body Efimov effect in Sec. IV; we give more explicit sufficient conditions under which Theorem 1.1 holds and establish a lower bound on the number of discrete eigenvalues of $P(g)$ as $g \to g_0$ and $g > g_0$, where $P = P(g_0)$ satisfies the assumptions of Theorem 1.1.

Notation: For $s \in \mathbb{R}$ and $k \in \mathbb{Z}$, we denote by $L^{2,s}$ and $H^{k,s}$ the weighted-L^2 and weighted-Sobolev spaces $L^2(\langle x\rangle^{2s}\,\mathrm{d}x)$ and $H^k(\langle x\rangle^{2s}\,\mathrm{d}x)$, respectively, and by $\mathcal{L}(s;s')$ and $\mathcal{L}(k,s;k',s')$ the space of bounded operators from $L^{2,s}$ to $L^{2,s'}$ and from $H^{k,s}$ to $H^{k',s'}$, respectively.

II. EXISTENCE OF TWO-CLUSTER THRESHOLD RESONANCES

The N-body Hamiltonian $Q = -\Delta + \Sigma_{c \in \mathcal{A}} V_c$ studied in Secs. II and III corresponds to a two-cluster sub-Hamiltonian in the Efimov effect with four or more particles. Thus let $N \geqslant 3$. Let a be

a two-cluster decomposition such that $\dim \mathbf{X}_a = 3$. Set $E_0 = \inf \sigma(Q^a)$. Assume that E_0 is in $\sigma_d(Q^a)$. Let φ_a be an associated eigenfunction, $Q^a\varphi_a = E_0\varphi_a$, $\|\varphi_a\| = 1$. We want to show that by varying the coupling constant g in $Q(g) = Q_a + gI_a(x)$, we can find a critical value g_0 such that E_0 is a threshold resonance of $Q(g_0)$. Let Π denote the orthogonal projection in $L^2(\mathbf{X})$ induced by φ_a,

$$\Pi u = (\varphi_a, u)_a \otimes \varphi_a, \quad u \in L^2(\mathbf{X}),$$

where $(,\cdot,\cdot)_a$ denotes the scalar product in x^a-variables. Let $\Pi' = 1 - \Pi$. Assume that for any $b \in \mathcal{A}$, $b \not\subseteq a$, $V_b \leqslant 0$, and V_b is $-\Delta$-form compact and outside some bounded set in $\mathbf{X}^b$,

$$|V_b(x^b)| \leqslant C|x^b|^{-\rho_0}, \quad \rho_0 > 2. \tag{2.1}$$

Assume that the intercluster interaction I_a is not identically zero. Set

$$Q(g) = Q^a - \Delta_a + gI_a, \quad Q'(g) = \Pi' Q(g) \Pi', \tag{2.2}$$

where $g > 0$ is a coupling constant. It is natural to expect that for g small, the bottom of the essential spectrum of $Q(g)$ remains to be E_0, while for g large, it may be shifted to the left.

Lemma 2.1: Let V_b be $-\Delta_{x^b}$-form compact. There exists $\mu_0 > 0$ such that if

$$g\|(-\Delta_{x^b} + 1)^{-1/2} V_b (-\Delta_{x^b} + 1)^{-1/2}\| \leqslant \mu_0, \tag{2.3}$$

then $\inf \sigma_{\mathrm{ess}}(Q(g)) = E_0$ *and a is the unique two-cluster decomposition which attains E_0: $\forall a' \in \mathcal{A}$, $\#a' = 2$ and $a' \neq a$, $\inf \sigma(Q^{a'}) > E_0$.*

Proof: Since E_0 is the discrete spectrum of Q^a, by HVZ theorem, for any $b \in \mathcal{A}$, $b \subset a$ (which means that b is a decomposition finer than a), one has

$$Q^b \geqslant E_0 + \epsilon_b$$

for some $\epsilon_b > 0$. Let a' be another two-cluster decomposition of the N-body system with $a' \neq a$. Take $b = a \cap a'$. Then, $b \subset a$ and the sub-Hamiltonian associated to a' can be decomposed as

$$Q_{a'}(g) = Q_b + g \sum_{c \subseteq a', c \not\subseteq a} V_c. \tag{2.4}$$

An argument of perturbation shows that if μ_0 is small enough, one has $Q_{a'} \geqslant E_0 + \epsilon_b/2$. By HVZ theorem, $\inf \sigma_{\mathrm{ess}}(Q(g)) = \min_{\#c=2} \inf \sigma(Q^c(g)) = \inf \sigma(Q^a) = E_0$. ∎

For potentials satisfying (2.1), with Lemma 2.1, one can apply the result on finiteness of discrete spectrum in N-body problems (Refs. 5 and 13) to conclude that $Q(g)$ has only a finite number of discrete eigenvalues for $g > 0$ small. In particular, if $g > 0$ is small enough, there is no discrete spectrum and $E(g) \triangleq \inf \sigma(Q(g))$ verifies $E(g) = \inf \sigma_{\mathrm{ess}}(Q(g)) = E_0$. Set

$$g_0 = \sup\{g > 0; E(g) = E_0, \inf \sigma_{\mathrm{ess}}(Q(g)) = E_0\}. \tag{2.5}$$

By Lemma 2.1, one has $g_0 > 0$. Since $I_a \leqslant 0$ and $I_a \neq 0$, one can show that for g large enough, there exists some sub-Hamiltonian $Q^{a'}(g)$, $a' \neq a$, such that $\inf \sigma(Q^{a'}(g)) < E_0$. Therefore $g_0 \epsilon]0, +\infty[$ is well defined. It may happen that when g increases from 0 to g_0, the bottom of the essential spectrum, E_0, of $Q(g_0)$ is attained by several two-cluster sub-Hamiltonians. In the following, we give the proof of Theorem 1.2, under the condition that $Q(g_0)$ is still unique two-cluster. By Theorem 3.3 (a) of Ref. 15, E_0 is not an eigenvalue of $Q(g_0)$. Therefore, to prove Theorem 1.2, we need only to construct a nontrivial solution for the equation $(Q(g_0) - E_0)u = 0$ with $u \in H^{1,-s}$ for any $s > \frac{1}{2}$. Then E_0 is a threshold resonance of $Q(g_0)$. The construction of a resonant state is based on the reduction made in Ref. 14.

According to whether or not E_0 is in $\sigma_p(Q'(g))$, the spectral property of $Q(g)$ at E_0 is determined either by an operator of the form $-\Delta_{x_a} + V_0$ or by an operator of the form

$$\begin{pmatrix} -\Delta_{x_a} + V_0 & C \\ C^* & 0 \end{pmatrix},$$

where V_0 is some effective potential and C some finite rank operator. Part (b) of the following lemma shows that we are actually in the first simpler situation.

Lemma 2.2: Assume that Q_a is the unique two-cluster Sub-Hamiltonian of $Q(g_0)$ which attains the bottom of its spectrum. There exists $\delta_0>0$ such that for $|g-g_0|<\delta_0$, one has

(a) $\inf \sigma_{\mathrm{ess}}(Q(g))=E_0$;
(b) $Q'(g)\geqslant(E_0+\epsilon_0)\Pi'$, *for some* $\epsilon_0>0$.

Proof: (a) By the unique two-cluster assumption for $Q(g_0)$, one has for any two-cluster decomposition $b\neq a Q_b(g_0)\geqslant(E_0+\epsilon_b)$ for some $\epsilon_b>0$. The same argument as in Lemma 2.1 shows that

$$\inf \sigma_{\mathrm{ess}}(Q(g) = \inf_{\#b=2} \sigma(Q^b(g)) = \inf \sigma(Q^a) = E_0$$

for g near g_0.

(b) We note that $E_0\notin\sigma_p(Q'(g_0))$. In fact, if $E_0\in\sigma_p(Q'(g_0))$, the associated eigenfunction ψ with $\|\psi\|=1$, would verify $\Pi'\psi=\psi$ and

$$E_0=\langle Q'(g_0)\psi,\psi\rangle=\langle Q(g_0)\psi,\psi\rangle.$$

Since $Q(g_0)\geqslant E_0$, this would imply $Q(g_0)\psi=E_0\psi$, which is impossible because by (a) of Theorem 3.3,[15] E_0 is not an eigenvalue of $Q(g_0)$. By Lemma 2.1 of Ref. 14, one has $\inf\sigma_{\mathrm{ess}}(Q'(g_0))\geqslant(E_0+\delta)$ for some $\delta>0$. Since $Q'(g_0)\geqslant E_0\Pi'$ and $E_0\notin\sigma_p(Q'(g_0))$, one sees that $Q'(g_0)\geqslant(E_0+\epsilon)\Pi'$ for some $\epsilon>0$. An easy argument of perturbation shows that for g sufficiently near g_0, $Q'(g)=Q'(g_0)+(g-g_0)\Pi' I_a\Pi'\geqslant(E_0+\epsilon/2)\Pi'$. ■

Lemma 2.2 (a) shows that for $g\in\,]g_0,g_0+\delta_0[$, $\delta_0>0$ small, $E(g)$ is in the discrete spectrum of $Q(g)$. It is clear that $E(g)\to E_0$ as $g\to g_0$.

With Lemma 2.2 (b), we can apply the reduction of Sec. III in Ref. 14 which says that for E near E_0, E is an eigenvalue (respectively, threshold resonance) of $Q(g)$ if and only if 0 is an eigenvalue (respectively, threshold resonance) of operator $\epsilon_{+-}(\lambda)$,

$$\epsilon_{+-}(\lambda,g)=\lambda-(-\Delta_{x_a}+V(\lambda,g)), \tag{2.6}$$

where $\lambda=E-E_0$, $R'(z,g)=(Q'(g)-z)^{-1}\Pi'$ and

$$V(\lambda,g)=([gI_a-g^2I_aR'(\lambda+E_0,g)I_a](\varphi_a\otimes\,\cdot\,),\varphi_a)_a.$$

Note that $I_a\leqslant 0$ and $R'(\lambda+E_0,g)\geqslant 0$ for λ near 0. $V(\lambda,g)$ is a negative self-adjoint operator, analytic in λ near 0 and g near g_0. Set

$$K(\lambda,g)=(-\Delta_{x_a}-\lambda)^{-1}V(\lambda,g). \tag{2.7}$$

Then, $K(\lambda,g):H^{1,-s}\to H^{1,-s}$ is compact operator-valued for $1/2<s<(\rho_0-1)/2$ and is continuous in λ near 0 and g near g_0. Clearly, u belongs to the kernel of $\epsilon_{+-}(\lambda,g)$ in $H^{1,-s}$ if and only if

$$(1+K(\lambda,g))u=0. \tag{2.8}$$

Proposition 2.3: One has $\dim\ker(1+K(0,g_0))_{H^{1,-s}}=1$.

Proof: By the assumption on $Q(g_0)$, for any $g>g_0$ sufficiently close to g_0, $E(g)$ is an eigenvalue of $Q(g)$ with $E(g)<E_0$ and $E(g)\to E_0$ as $g\to g_0$. Therefore, there exists a family of functions $u(g)\in H^1$ such that

$$u(g) = -K(\lambda(g), g)u(g), \quad \|u(g)\|_{H^{1,-s}} = 1, \quad \lambda(g) = E(g) - E_0.$$

The compactness of $K(\lambda(g), g)$ allows to extract a subsequence $\{u(g_k)\}$ of $\{u(g)\}$ such that $u(g_k) = -K(\lambda(g_k), g_k)u(g_k)$ converges (strongly) in $H^{1,-s}$. Let u_0 denote its limit. It is clear that $u_0 = -K(0, g_0)u_0$, $\|u_0\|_{H^{1,-s}} = 1$. This proves that 0 is an eigenvalue of $1 + K(0, g_0)$. Theorem 3.3 (a) of Ref. 15 implies that 0 is not an eigenvalue of $-\Delta_{x_a} + V_0$, where $V_0 = V(0, g_0)$. Therefore $u_0 \notin H^1$. Since the threshold resonance of $-\Delta_{x_a} + V_0$ at zero is at most simple,[6,14] one sees that $\ker(1 + K(0, g_0))$ in $H^{1,-s}$ is of dimension one and is spanned by u_0. ■

Proof of Theorem 1.2: Since $(-\Delta_{x_a} + V_0)u_0 = 0$, a direct calculation shows that

$$\psi_0 = \varphi_a \otimes u_0 - g_0 R'(E_0, g_0) I_a(\varphi_a \otimes u_0) \neq 0$$

verifies $(Q(g_0) - E_0)\psi_0 = 0$. See Ref. 14. Since $u_0 \in H^{1,-s}(\mathbf{X}_a) \backslash H^1(\mathbf{X}_a)$, $\psi_0 \in H^{1,-s}(\mathbf{X}) \backslash H^1(\mathbf{X})$ for any $s > 1/2$. E_0 is thus a threshold resonance of $Q(g_0)$. ■

Corollary 2.4: Let $Q = Q_a + I_a$, where a is a two-cluster decomposition, $I_a = \Sigma_{b \not\subset a} V_b$, $V_b \leqslant 0$, such that $E_0 \triangleq \inf \sigma(Q^a) \in \sigma_d(Q^a)$ and that $Q^{a'} > E_0$ for any other two-cluster decompositions $a' \neq a$. Assume in addition that Q has at least one discrete eigenvalue strictly below E_0. Then, E_0 is a threshold resonance of $Q(g_0)$.

Proof: It suffices to remark that g_0 defined by (2.5) is given by

$$g_0 = \inf\{g \in]0, 1\,]\,; \inf \sigma(Q(g)) < E_0, \tag{2.9}$$

and $g_0 \in]0, 1[$. $Q(g_0)$ is still unique two-cluster, because for any $a' \in \mathcal{A}$ with $\#a' = 2$ and $a' \neq a$, (2.4) shows that the sub-Hamiltonian of $Q(g_0)$ associated with a' satisfies $Q^{a'}(g_0) \geqslant Q^{a'}(1) > E_0$ for $g_0 \in]0, 1[$. Theorem 1.2 gives the desired result. ■

As an application of Corollary 2.4, we give a concrete example for the existence of two-cluster threshold resonance for three-body atomic-type Schrödinger operator with Yukawa-type potentials. Similar examples can be constructed for any number of particles.

Example: Consider an atomic-type three-body Schrödinger operator with Yukawa potentials,

$$Q(g) = -\Delta_{x_1} - \Delta_{x_2} - \frac{\alpha_1 e^{-\epsilon\alpha_1|x_1|}}{|x_1|} - g\left(\frac{\alpha_2 e^{-\epsilon\alpha_2|x_2|}}{|x_2|} + \frac{\alpha_3 e^{-\epsilon\alpha_3|x_1 - x_2|}}{|x_1 - x_2|}\right), \tag{2.10}$$

where the nucleus is fixed at the origin, $x_j \in \mathbb{R}^3$, α_i, ϵ, and g are suitable positive constants with $\alpha_1 > \max\{\alpha_2, \alpha_3\}$. We want to show Corollary 2.4 can be applied with $a = \{(01), (2)\}$. Consider first the two-body operator

$$Q(\alpha, \epsilon) = -\Delta - \frac{\alpha e^{-\alpha\epsilon|x|}}{|x|}, \quad x \in \mathbb{R}^3,$$

with $\alpha, \epsilon > 0$. By the change of variables $y = \alpha x$, one sees that $Q(\alpha, \epsilon)$ is unitarily equivalent with $\alpha^2 Q_1(\epsilon)$ where

$$Q_1(\epsilon) = -\Delta_y - \frac{e^{-\epsilon|y|}}{|y|}.$$

Using the perturbation theory around $Q_1(0) = -\Delta_y - (1/|y|)$, one sees that for $\epsilon > 0$ small,

$$\inf \sigma(Q_1(\epsilon)) = -\tfrac{1}{4} + c_0\epsilon + O(\epsilon^2).$$

This shows that there exists $\epsilon_0 > 0$ such that

$$\inf \sigma(Q(\alpha, \epsilon)) = \alpha^2\left(-\tfrac{1}{4} + c_0\epsilon + O(\epsilon^2)\right) < 0 \tag{2.11}$$

for all $0 < \epsilon < \epsilon_0, \alpha > 0$. For $g = 1$, let P_j denote the three two-body sub-Hamiltonians of $Q(1)$ associated with the cluster decompositions {(01), 2}, {(02), (1)}, {(12), (0)}, respectively. Using (2.11), one sees that their respective bottoms of spectrum are given by

$$E_j = a_j^2\left(-\tfrac{1}{4} + O(\epsilon)\right), \quad j = 1,2, \quad E_3 = \alpha_3^2\left(-\tfrac{1}{8} + O(\epsilon)\right),$$

which are all negative if $\epsilon > 0$ is small enough. So $Q(1)$ is unique two-cluster, since $\inf \sigma_{\mathrm{ess}}(Q(1)) = E_1 < \min\{E_2, E_3\}$. By minimax principle, one can easily check that $Q(1)$ has at least one discrete eigenvalue e_0 with $e_0 \leqslant E_1 + E_2 < E_1$. By Corollary 2.4, there exists some $g_0 \in]0,1[$ such that $E_0 = E_1$ is a two-cluster threshold resonance of $Q(g_0)$.

III. PERTURBATION OF TWO-CLUSTER THRESHOLD RESONANCES

In this section, we want to show that under intercluster perturbation, a two-cluster threshold resonance may be shifted to the left to produce discrete eigenvalue of the N-body system. Let $a \in \mathcal{A}$ be a two-cluster decomposition of an N-body system such that $\dim \mathbf{X}_a = 3$. With the notation of Sec. II, assume that

(i) $E_0 \triangleq \inf \sigma(Q^a) \in \sigma_d(Q^a)$;
(ii) for any $b \not\subseteq a$, $V_b(x^b) = O(\langle x^b \rangle^{-\rho_0})$, $\rho_0 > 2$, and $V_b \leqslant 0$ with $I_a \triangleq \Sigma_{b \not\subseteq a} V_a \neq 0$;
(iii) let $Q(g) = Q_a + gI_a$. Assume that there exists $g_0 > 0$ such that $Q(g_0)$ unique two-cluster at E_0, $Q(g_0) \geqslant E_0$ and that E_0 is a threshold resonance of $Q(g_0)$.

Note that different from Sec. II, here we do not assume that g_0 is the critical coupling constant such that $\inf \sigma(Q(g)) < E_0$ for any $g > g_0$.

Theorem 3.1: *Under the above assumptions, there exists* $\delta_0 > 0$ *such that for* $g \in]g_0, g_0 + \delta_0[$, $Q(g)$ *possesses only one eigenvalue* $E(g) \in]E_0 - \delta_0, E_0[$ *which is nondegenerated and satisfies*

$$E(g) = E_0 + E_1(g - g_0)^2 + o((g - g_0)^2), \tag{3.1}$$

as $g \to g_0$, *where* $E_1 < 0$.

Proof: We use the idea of Ref. 14 and only sketch the proof. Under the assumptions of Theorem 3.1, as in Sec. II, one has $Q'(g) \geqslant (E_0 + \epsilon_0/2)\Pi'$ for g near g_0. We can then apply the reduction made in Sec. III of Ref. 14 which implies that for $\delta_0 > 0$ small enough such that $E \in]E_0 - \delta_0, E_0 + \delta_0[$, $|g - g_0| < \delta_0$, E is an eigenvalue or threshold resonance of $Q(g)$ if and only if 0 is an eigenvalue or threshold resonance of $\epsilon_{+-}(\lambda, g)$ with the same multiplicity, where $\lambda = E - E_0$ and $\epsilon_{+-}(\lambda, g)$ is given by (2.6). Let

$$G_0 = \lim_{z \to 0, \Im z > 0} (-\Delta_{x_a} - z)^{-1} : H^{-1,s} \to H^{1,-s'}, s, s' > 1/2, s + s' > 2.$$

Denote $V_0 = V(0, g_0)$. The zero resonance of $\epsilon_{+-}(0, g_0)$ is simple[6,14] and Theorem 3.3 (a) of Ref. 15 shows that 0 is not an eigenvalue of $\epsilon_{+-}(0, g_0)$. Therefore the kernel of $\epsilon_{+-}(0, g_0)$ in $H^{1,-s}$ is of dimension one. Let u_0 be the resonant state of $\epsilon_{+-}(0, g_0)$ normalized by $\langle u_0^*, u_0 \rangle_a = 1$, where $u_0^* = -V_0 u_0$. Let $W(\lambda, g) = 1 + K(\lambda, g)$ with $K(\lambda, g)$ defined as in Sec. II. Study the Grushin problem associated with the operator

$$\mathcal{P}(\lambda, g) = \begin{pmatrix} W(\lambda, g) & T \\ S & 0 \end{pmatrix} : H^{1,-s} \times \mathbb{C} \to H^{1,-s} \times \mathbb{C},$$

where $s > 1/2$, $T : \mathbb{C} \ni c \to c u_0 \in H^{1,-s}$ and $S : H^{1,-s} \ni f \to \langle u_0^*, f \rangle \in \mathbb{C}$. Define $Q : H^{1,-s} \to H^{1,-s}$ by $Qf = \langle u_0^*, f \rangle_a u_0$. Denote $F = \mathrm{Range}(1 + G_0 V_0)$. Then, $Q' = 1 - Q$ is a projection from $H^{1,-s}$ onto F and $Q'(1 + G_0 V_0)Q'$ is invertible on F. For λ near 0 and g near g_0, one has

$$\begin{aligned} Q' W(\lambda, g) Q' (Q'(1 + G_0 V_0) Q')^{-1} Q' &= Q' + Q'(K(\lambda, g) - K(0, g_0)) Q' (Q'(1 + G_0 V_0) Q')^{-1} Q' \\ &= Q' + O(|\lambda|^{\epsilon} + |g - g_0|), \quad \epsilon > 0, \end{aligned} \tag{3.2}$$

in $\mathcal{L}(1, -s; 1, -s)$. We deduce that $Q' W(\lambda, g) Q'$ is invertible on F for $|\lambda|$ small and g near g_0. Let

$$D(\lambda,g) = (Q'W(\lambda,g)Q')^{-1}Q'.$$

Then for any $s>1/2$, one has

$$D(\lambda,g) = (Q'W(0,g_0)Q')^{-1}Q' + O(|\lambda|^{\epsilon} + |g-g_0|), \tag{3.3}$$

as operator on $H^{1,-s}$. Using $D(\lambda,g)$ to construct an approximate inverse, one can show that for λ near 0 and g near g_0, the operator $\mathcal{P}(\lambda,g)$ is invertible from $H^{1,-s}\times\mathbb{C}$ to $H^{1,-s}\times\mathbb{C}$ with the inverse given by

$$\mathcal{P}(\lambda,g)^{-1} = \begin{pmatrix} E(\lambda,g) & E_+(\lambda,g) \\ E_-(\lambda,g) & E_{+-}(\lambda,g) \end{pmatrix},$$

where

$$E(\lambda,g) = D(\lambda,g), \quad E_+(\lambda,g) = T - D(\lambda,g)Y, \tag{3.4}$$

$$E_-(\lambda,g) = S - SX, \quad E_{+-}(\lambda,g) = -SW(\lambda,g)T + SXY, \tag{3.5}$$

with

$$X = QW(\lambda,g)Q'D(\lambda,g), \quad Y = Q'W(\lambda,g)T.$$

Note that $E_{+-}(\lambda,g)$ is a scalar and that 0 is an eigenvalue of $1+K(\lambda,g)$ if and only if

$$E_{+-}(\lambda,g) = \langle V_0 u_0, (1 - W(\lambda,g)Q'D(\lambda,g)Q')W(\lambda,g)u_0\rangle = 0.$$

One has the asymptotic expansion

$$(-\Delta_a - \lambda)^{-1} = G_0 + i\lambda^{1/2}G_1 + O(|\lambda|^{1/2+\delta})$$

as operator from $H^{-1,s}$ to $H^{1,-s}$ with $s>3/2$, for some $\delta>0$. Set $\gamma=g-g_0$, $V_0=V(0,g_0)$. One has

$$V(\lambda,g) = V_0 + \gamma B_1 + \lambda C_1 + O((|\gamma| + |\lambda|)^2)$$

as operator from $H^{1,s}$ to $H^{1,s+\rho_0}$, where

$$B_1 = ([I_a - 2g_0 I_a R'(E_0,g_0)I_a](\varphi_a \otimes \cdot), \varphi_a)_a \tag{3.6}$$

$$+ (g_0^2 I_a R'(E_0,g_0))I_a R'\ (E_0,g_0)I_a(\varphi_a \otimes \cdot), \varphi_a)_a \leqslant 0 \tag{3.7}$$

as a sum of three negative self-adjoint operators in x_a variables. Since $u_0 \in H^{1,-s}$ for any $s>1/2$, $V_0u_0 \in H^{-1,s_0}$ for some $3/2<s_0<\rho_0-1/2$. By a direct calculation, one obtains

$$E_{+-}(\lambda,g) = b_1\gamma + c_1 i\lambda^{1/2} + O(\gamma^2 + \gamma|\lambda|^{1/2} + |\lambda|^{1/2+\delta_0}), \tag{3.8}$$

where

$$b_1 = -\langle u_0, B_1 u_0\rangle_a, \quad c_1 = \frac{1}{4\pi}|\langle V_0(u_0), 1\rangle_a|^2.$$

$c_1>0$ because u_0 is a resonant state so that $\langle V_0(u_0), 1\rangle_a \neq 0$ (Ref. 14), and

$$b_1 \geqslant -\langle I_a(\varphi_a \otimes u_0), (\varphi_a \otimes u_0)\rangle > 0,$$

because $I_a \leqslant 0$ and is not identically zero. It follows from (3.8) that for each $\gamma>0$ small enough, $\lambda \to E_{+-}(\lambda, g_0+\gamma)$ has a zero $\Lambda(g_0+\gamma)<0$ satisfying

$$\Lambda(g_0+\gamma)=E_1\gamma^2+O(\gamma^{2+\epsilon}), \tag{3.9}$$

where $E_1<0$. This shows that the generalized eigenvalue problem $(Q(g)-E)u=0$, $E\in]E-\delta_0,E+\delta_0[$, $u\in H^{1,-s}$, has only one solution $(E(g),u(g))$ with $E(g)=E_0+\Lambda(g)$. Since $E(g)<\inf\sigma_{\mathrm{ess}}(Q(g))$, by the method of *a priori* energy estimate, one can show that $u(g)\in H^1$. Thus, $E(g)$ is the unique eigenvalue of $Q(g)$ in $]E-\delta_0,E+\delta_0[$ and $E(g)$ is simple. This proves Theorem 3.1. ■

If g_0 be defined as in Sec. II, under the conditions of Theorem 1.2, one can apply Theorem 3.1 to conclude that $E(g)=\inf\sigma(Q(g))$ satisfies

$$E(g)=E_0+E_1(g-g_0)^2+o((g-g_0)^2), \tag{3.10}$$

as $g\to g_0$ and $g>g_0$. Equation (3.10) is known for C_0^∞ potentials.[7] If all potentials are dilation analytic, one can show that $E_{+-}(\lambda,g)$ has homomorphic extension for $\lambda\in\mathbb{C}$ in a small rotated half-disk around 0 and for g near g_0. From (3.8), we can derive that for $g<g_0$ and g near g_0, $\lambda\to E_{+-}(\lambda,g)$ has a zero $\Lambda(g)\in\mathbb{C}$ with $\Re\Lambda(g)>0$ and $\Im\Lambda(g)<0$. $E_0+\Lambda(g)$ is then a resonance of $Q(g)$ as pole of its resolvent.

IV. APPLICATIONS TO THE *N*-BODY EFIMOV EFFECT

Let $\mathcal{P}=-\Delta+\Sigma_a V_a(x^a)$ be an N-body Schrödinger operator, $N\geqslant 4$. Let $b\in\mathcal{A}$ with $\#b=3$, $E_0=\inf\sigma(\mathcal{P}^b)$. Assume that

(i) (1.5) is satisfied and $\inf\sigma(\mathcal{P}^a)>E_0$, $a\notin\{b,a_1,a_2,a_3\}$;
(ii) each $\mathcal{P}^{a_j}$ admits a discrete eigenvalue strictly below E_0.

Note that I_b can be decomposed as $I_b=I_1+I_2+I_3$ with $I_j=\Sigma_{c\not\subseteq b,c\subseteq a_j}V_c(x^c)$.

Theorem 4.1: *Under the above conditions, let* $\mathcal{P}^{a_j}(g)=\mathcal{P}^b-\Delta_{x_b^{a_j}}+gI_j$, *where* $-\Delta_{x_b^{a_j}}=-\Delta|_{\mathbf{x}^{a_j}\cap\mathbf{x}_b}$. *Then there exists* $g_j\in]0,1[$ *such that* E_0 *is a threshold resonance of* $P^{a_j}=\mathcal{P}^{a_j}(g_j)$, $j=1,2,3$. *In particular, Theorem 1.1 holds for the N-body operator* $P=\mathcal{P}_b+\Sigma_{j=1}^3 g_jI_j$.

Proof: Theorem 4.1 follows easily from Corollary 2.4. In fact, $\mathcal{P}^b$ can be regarded as a two-cluster sub-Hamiltonian of $\mathcal{P}^{a_j}=\mathcal{P}^b-\Delta_{x_b^{a_j}}+I_j$, $j=1,2,3$. The assumptions made on $\mathcal{P}^b$ imply that $\mathcal{P}^b$ is the only two-cluster sub-Hamiltonian of $\mathcal{P}^{a_j}$ such that $\inf\sigma(\mathcal{P}^c)=\inf\sigma_{\mathrm{ess}}(\mathcal{P}^{a_j})$, $c\subset a_j$, $c\neq a_j$, that is, $\mathcal{P}^{a_j}$ is unique two-cluster. Since $\mathcal{P}^{a_j}$ admits at least one discrete eigenvalue strictly below $E_0=\inf\sigma(P^b)$, Corollary 2.4 with $Q=\mathcal{P}^{a_j}$, $j=1,2,3$, says that there exists $g_j\in]0,1[$ such that $P^{a_j}=\mathcal{P}^{a_j}(g_j)=\mathcal{P}^b-\Delta_{x_b^{a_j}}+g_jI_j$ satisfies that $\inf\sigma(P^{a_j})=E_0$ and that E_0 is a threshold resonance of P^{a_j}. Now, for the N-body Hamiltonian $P=\mathcal{P}_b+\Sigma_{j=1}^3 g_jI_j$, one has $\inf\sigma(P^c)\geqslant\inf\sigma(\mathcal{P}^c)>E_0$ for $c\notin\{b,a_1,a_2,a_3\}$. Therefore, (1.4) is satisfied for P. It is clear that all conditions of Theorem 1.1 are verified for P. ■

Let us give an example of atomic-type four-body Schrödinger operator with Yukawa potentials such that all conditions of Theorem 1.1 are satisfied. Consider an atomic-type four-body quantum system labeled by {0, 1, 2, 3}, where the particle 0 denotes the nucleus with position at the origin in $\mathbb{R}^3$. Let $x_j\in\mathbb{R}^3$ denote the relative position between the jth electron and the nucleus. Consider the four-body Schrödinger operator with Yukawa potentials,

$$P(\alpha,\gamma,\epsilon)=\sum_{j=1}^{3}(-\Delta_{x_j}+V_j(x_j))+\sum_{1\leqslant j<k\leqslant 3}V_{jk}(x_j-x_k), \tag{4.1}$$

where

$$V_\beta(y)=-\frac{\gamma_\beta\alpha_\beta e^{-\epsilon_\beta\alpha_\beta|y|}}{|y|}$$

with $\alpha=(\alpha_\beta)$, $\gamma=(\gamma_\beta)$, $\epsilon=(\epsilon_\beta)$, the subscript β taking values in i or (jk) for $i,j,k\in\{1,2,3\}$, $j<k$. Here $\alpha_\beta,\epsilon_\beta>0$ and $\gamma_\beta\in]0,1]$. Let $b=\{(01),(2),(3)\}$ be the three-cluster decomposition of

the four-body system. The three resulting two-cluster decompositions are

$$a_1 = \{(01),(23)\}, \quad a_2 = \{(012),(3)\}, \quad a_3 = \{(013),(2)\}.$$

Let $Q(\alpha)$ be the four-body Schrödinger operator with Coulomb potentials

$$Q(\alpha) = \sum_{j=1}^{3} (-\Delta_{x_j} + W_j(x_j)) + \sum_{1 \leqslant j < k \leqslant 3} W_{jk}(x_j - x_k), \tag{4.2}$$

where

$$W_\beta(y) = -\frac{\alpha_\beta}{|y|}.$$

Let $E' = \min\{\inf(\sigma(Q^c(\alpha)) \ ; \ c \in \mathcal{A}, \#c = 2, c \not\supseteq b\}$. E' is independent of α_1. Take

$$\alpha_1 > 2\sqrt{-E'} \quad \text{and} \quad \gamma_1 = 1. \tag{4.3}$$

Denote

$$P^b = -\Delta_{x_1} - \frac{\alpha_1 e^{-\epsilon_1 \alpha_1 |x_1|}}{|x_1|}, \quad E_0 = \inf \sigma(P^b). \tag{4.4}$$

Let $\epsilon_\beta > 0$ be small enough such that the infimum of the spectrum of each two-particle sub-Hamiltonian,

$$-\Delta_y - \frac{\alpha_\beta e^{-\epsilon_\beta \alpha_\beta |y|}}{|y|}$$

is a negative eigenvalue. Then

$$E_0 = \inf \sigma(P^b) = \frac{\alpha_1^2}{4}(-1 + O(\epsilon_1)) \tag{4.5}$$

for ϵ_1 small enough. Since $P^a(\alpha, \gamma, \epsilon) \geqslant Q^a(\alpha)$ for any $a \in \mathcal{A}$ and for any $\gamma_\beta \in]0,1]$, one has

$$\inf \sigma(P^b) < E' \leqslant \min\{\inf(\sigma(P^c(\alpha, \gamma, \epsilon)); c \in \mathcal{A}, \# c = 2, c \not\supseteq b \}. \tag{4.6}$$

This shows that for any $\gamma_\beta \in]0,1]$, $\beta \neq 1$, $\inf \sigma_{\text{ess}}(P(\alpha, \gamma, \epsilon)) = E_0$ and that it can only be attained by the sub-Hamiltonians associated with $a \in \{b, a_1, a_2, a_3\}$. Note that $P^b(\alpha, \gamma, \epsilon)$ can be regarded as a two-cluster sub-Hamiltonian of $P^{a_j}(\alpha, \gamma, \epsilon)$. By the example given in Sec. II, for $k = 2, 3$, there exists $\gamma_k = \gamma_{1k} = g_k \in]0,1[$ such that

$$P^{a_k} = -\Delta_{x_1} - \Delta_{x_k} - \frac{\alpha_1 e^{-\epsilon_1 \alpha_1 |x_1|}}{|x_1|} - g_k \left(\frac{\alpha_k e^{-\epsilon_k \alpha_k |x_k|}}{|x_k|} + \frac{\alpha_{1k} e^{-\epsilon_{1k} \alpha_{1k} |x_1 - x_k|}}{|x_1 - x_k|} \right)$$

satisfies

$$\inf \sigma(P^{a_k}) = \inf \sigma(P^b) = E_0 \text{ and } E_0 \text{ is a threshold resonance of } P^{a_k}, \quad k = 2,3. \tag{4.7}$$

Using $y = x_2 - x_3$ as part of intracluster coordinates, one can write P^{a_1} as

$$P^{a_1} = -\Delta_{x_1} - 2\Delta_y - \frac{\alpha_1 e^{-\epsilon_1 \alpha_1 |x_1|}}{|x_1|} - \frac{\gamma_{23} \alpha_{23} e^{-\epsilon_{23} \alpha_{23} |y|}}{|y|}.$$

This is a particular case of the example of Sec. II. Let g_1 be defined

$$g_1 = \sup\left\{ \gamma_{23} > 0; -2\Delta_y - \frac{\gamma_{23}\alpha_{23}e^{-\epsilon_{23}\alpha_{23}|y|}}{|y|} \geqslant 0 \right\}.$$

Then, (4.7) is also satisfied for $k=1$ with $\gamma_{23}=g_1$. All assumptions of Theorem 1.1 are thus satisfied and Theorem 1.1 affirms that the Efimov effect takes place for $P(\alpha,\gamma,\epsilon)$ with the parameters adjusted as above. In particular, if $\alpha_\beta=1$ for $\beta\neq 1$, and $\epsilon_\beta=\epsilon$, our result claims that for any $\alpha_1>2\sqrt{-E'}$ and for any $\epsilon>0$ small enough, there exists $g_j\in\,]0,1[$, $j=1,2,3$, such that the Efimov effect happens at the energy $E_0=-(\alpha_1^2/4)+O(\epsilon)$ for the atomic-type four-body Schrödinger operator,

$$P = -\Delta_{x_1} - \Delta_{x_2} - \Delta_{x_3} - \frac{\alpha_1 e^{-\epsilon\alpha_1|x_1|}}{|x_1|} - g_1\frac{e^{-\epsilon|x_2-x_3|}}{|x_2-x_3|} - g_2\left(\frac{e^{-\epsilon|x_2|}}{|x_2|} + \frac{e^{-\epsilon|x_1-x_2|}}{|x_1-x_2|}\right) - g_3\left(\frac{e^{-\epsilon|x_3|}}{|x_3|} + \frac{e^{-\epsilon|x_1-x_3|}}{|x_1-x_3|}\right). \tag{4.8}$$

As application of Theorem 3.1, we give the following result which is an improvement of Theorem 5.1 of Ref. 15, where the additional condition $V_c\in C_0^\infty$ for $c\not\subset b$ was needed.

Theorem 4.2: *Let $b\in\mathcal{A}$ with $\#b=3$ and $P(g)=P_b+gI_b$. Assume the conditions of Theorem 1.1 satisfied for $P=P(g_0)$. Then for $g>g_0$ and g near g_0, the total number of discrete eigenvalues, $\mathcal{N}(g)$, of $P(g)$ is finite and satisfies*

$$\mathcal{N}(g) \geqslant 2C_0|\log(g-g_0)| - C_1, \tag{4.9}$$

as $g\to g_0$. Here $C_0>0$ is the same as in Theorem 1.1 and C_1 is a constant independent of g.

With the results of Secs. II and III, one has for $g>g_0$ and g near g_0,

$$\Sigma_3(g) \triangleq \min_{\#c=3} \inf \sigma(P^c(g)) = E_0$$

and

$$\Sigma_2(g) \triangleq \min_{\#c=2} \inf \sigma(P^c(g)) = \min_{1\leqslant j\leqslant 3} \inf \sigma(P^{a_j}(g)).$$

Applying Theorem 3.1 to $P^{a_j}(g)$ with P^a replaced by P^b, one has

$$\inf \sigma(P^{a_j}(g)) = E_0 + E_{1,j}(g-g_0)^2 + o((g-g_0)^2), \quad E_{1,j}<0.$$

This shows that

$$\Sigma_2(g) = E_0 + E_1(g-g_0)^2 + o((g-g_0)^2) < \Sigma_3(g),$$

where $E_1=\min_j\{E_{1,j}\}<0$. Since $\rho_0>2$, the number of discrete eigenvalues of $P(g)$ is finite. Noticing that $P(g)\leqslant P(g_0)$ for $g>g_0$, one has $\mathcal{N}(g)\geqslant N(\Sigma_2(g))$. Theorem 1.1 gives the desired result.

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Divergences in quantum electrodynamics on a graph

Nahomi Kan[a)]
Graduate School of Science and Engineering, Yamaguchi University, Yoshida, Yamaguchi-shi, Yamaguchi 753-8512, Japan

Kiyoshi Shiraishi[b)]
Faculty of Science, Yamaguchi University, Yoshida, Yamaguchi-shi, Yamaguchi 753-8512, Japan

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We consider a model of quantum electrodynamics (QED) on a graph as the generalization of dimensional deconstruction with the Abelian symmetry. Arbitrary structures of the theory space correspond to the graphs consisting of vertices and edges. The mass spectrum of the model is expressed in terms of eigenvalues of the Laplacian for the graph. We also find that physical massless scalar modes are associated with the fundamental tie set matrix on the graph. We further investigate the one-loop divergences in the model by use of the background field method. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2109687]

I. INTRODUCTION

One of the most important problems in modern particle physics is to understand the existence of largely different mass scales within a unified theory. On many occasions, we use the idea of supersymmetry (SUSY) to control the quantum correction in order to understand the mass hierarchy.

Recently, the scenario for the electroweak symmetry breaking without SUSY has been suggested and studied by many authors. The seminal paper in recent development is Ref. 1. The divergent diagrams are mutually canceled among contributions from a number of bosonic fields.

The basic idea of such a mechanism is now attributed to dimensional deconstruction,[2] where copies of a four-dimensional "theory" as well as a new set of fields linking pairs of these "theories" are considered. Then, the resulting whole theory given by the "theory space" may be equivalent to a higher-dimensional theory with discretized extra dimensions.

The present authors considered previously a generalization of the deconstruction.[3] A generalization of deconstruction is also argued in Ref. 4. We identify the theory space as a graph consisting of vertices and edges. In the present paper, we further investigate the divergences in the field theory on a graph, particularly focusing on an Abelian theory. Although the non-Abelian structure and alignment of fields in a certain representation may be essential for realistic models, the substantial behavior of divergences can be viewed from a simpler model. Recently, a model with extra massive vector boson was studied by Körs and Nath,[5] where the Stueckelberg formalism was utilized. Our model can be applied to a generalization of their work.

We organize the present paper in the following way. In Sec. II, we review graph theory and matrices associated with a graph, including the Laplacian of a graph. The Lagrangian for gauge fields on a graph is described in Sec. III. The Lagrangian for fermion fields is described in Sec. IV. In Sec. V, the one-loop logarithmical divergences in effective Lagrangian density are discussed. In

[a)]Electronic mail: b1834@sty.cc.yamaguchi-u.ac.jp
[b)]Electronic mail: shiraish@yamaguchi-u.ac.jp

Sec. VI, we study the one-loop finiteness of the effective potential for a constant background link scalar fields. Comment on the non-Abelian generalization is given in Sec. VII. We close with Sec. VIII, where summary and prospects are given.

II. GRAPH THEORY AND MATRICES ASSOCIATED WITH A GRAPH

In this section, after a brief description of "graph,"[6] some matrices associated with a graph are introduced.

Let $G(V,E)$ be a graph with vertex set V and edge set E. The set of edges connects the vertices. A graph which does not have multiple edges (edges connecting the same two vertices) and self-loops (edges from a vertex to itself) is called a simple graph. We only consider simple graphs in the present paper. The order of G, denoted by p in this paper, is the number of vertices in the graph, while the size of G, denoted by q in this paper, is the number of edges in the graph. A pair of vertices u and v is said to be adjacent, denoted $u \sim v$, if there exists an edge $e \in E$ which connects u and v. Such edge is denoted as $e=\{u,v\}$.

The adjacency matrix A is defined as

$$(A)_{vv'} = \begin{cases} 1 & \text{if } v \sim v' \ (v \text{ is adjacent to } v') \\ 0 & \text{otherwise} \end{cases} . \tag{1}$$

The degree of a vertex v, denoted $\deg(v)$, is the number of edges directly connected to (in other words, is incident with) v. The (diagonal) degree matrix D is defined as

$$(D)_{vv'} = \begin{cases} \deg(v) & \text{if } v = v' \\ 0 & \text{otherwise} \end{cases} . \tag{2}$$

The graph Laplacian (or combinatorial Laplacian) $\Delta(G)$ is defined[7] by

$$\Delta_{vv'} = (D-A)_{vv'} = \begin{cases} \deg(v) & \text{if } v = v' \\ -1 & \text{if } v \text{ and } v' \text{ are adjacent } (v \sim v') \\ 0 & \text{otherwise} \end{cases} , \tag{3}$$

where $v,v' \in V$, and $\deg(v)$ denotes the degree of v.

The $(\text{mass})^2$ matrix for vector fields in the Hill-Leibovich model[8] is proportional to Δ for a cycle graph[6] with N vertices (denoted as C_N).

Next, we consider a directed graph. An oriented edge $e=[u,v]$ $(u,v \in V(G))$ connects the origin $u=o(e)$ and the terminus $v=t(e)$ (and an unoriented edge does not distinguish its origin and terminus).

The incidence matrix (for a directed graph) E is defined by

$$(E)_{ve} = \begin{cases} 1 & \text{if } v = o(e) \\ -1 & \text{if } v = t(e) \\ 0 & \text{otherwise} \end{cases} . \tag{4}$$

Our important observation is

$$\Delta = EE^T, \tag{5}$$

for any given graph.

III. VECTOR FIELDS (+SCALAR FIELDS)

The simplest model with the Abelian symmetry is studied by Hill and Leibovich.[8] We consider here the extension of the model constructed on a general graph.

We associate vector fields with vertices of a graph G. Further, we introduce a link field U_e on each edge. We can write the Lagrangian density for vector fields whose $(\text{mass})^2$ matrix is $\Delta(G)$ as[5]

$$\mathcal{L}_V = -\frac{1}{4g^2}\sum_{v\in V} F_v^{\mu\nu}F_{v\mu\nu} + \frac{1}{2}v^2\sum_{e\in E}|D^\mu U_e|^2, \tag{6}$$

where g is a gauge coupling and $F_v^{\mu\nu}=\partial^\mu A_v^\nu-\partial^\nu A_v^\mu$ $(\mu,\nu=0,1,2,3)$ stands for the field strength. In this section the metric signature is $(+---)$. The covariant derivative is defined as $D^\mu U_e = \partial^\mu U_e - i(A^\mu_{o(e)}U_e - U_e A^\mu_{t(e)})$.

The Lagrangian is invariant under the following gauge transformations:

$$\begin{aligned} A_v^\mu &\to A_v^\mu + \partial^\mu \omega_v, \\ U_e &\to \exp(i\omega_{o(e)})U_e \exp(-i\omega_{t(e)}). \end{aligned} \tag{7}$$

Now, we assume that the absolute value of each link field $|U_k|$ has a common value 1. If we express U_e as $\exp(-i\chi_e)$, the Lagrangian (6) becomes

$$\begin{aligned} \mathcal{L}_V &= -\frac{1}{4g^2}\sum_{v\in V} F_v^{\mu\nu}F_{v\mu\nu} + \frac{1}{2}v^2\sum_{e\in E}(\partial^\mu\chi_e + A^\mu_{o(e)} - A^\mu_{t(e)})^2 \\ &= -\frac{1}{4g^2}\sum_{v\in V} F_v^{\mu\nu}F_{v\mu\nu} + \frac{1}{2}v^2\sum_{e\in E}(\partial^\mu\chi_e + (E^TA^\mu)_e)^2, \end{aligned} \tag{8}$$

where $(E^TA^\mu)_e$ is an abbreviated form of $\Sigma_{v\in V}(E^T)_{ev}A_v^\mu$.

We find that the term including χ_e resembles the gauge kinetic term of the extra "fifth" index, $\propto(F_{\mu 5})^2$, when we regard $gv(A^\mu_{t(e)}-A^\mu_{o(e)})$ as a discretization of differentiation and $A_5\propto\chi$. Then, the gauge transformation on χ_e is $\chi_e\to\chi_e+\delta\chi_e$, with

$$\delta\chi_e = \omega_{t(e)} - \omega_{o(e)} = -(E^T\omega)_e. \tag{9}$$

The degrees of freedom in this gauge transformation are $p-1$, and $(p-1)$ scalar fields can be gauged away from the Lagrangian. Therefore, there are $(q-p+1)$ physical, massless scalar fields. As explained in Ref. 8, the vector fields absorb massive modes of the link scalar fields, and the zero modes of the link fields survive as physical fields. Thus, except for the zero modes, the massive modes of link fields χ_e are nothing but the Stueckelberg fields.[9]

The physical massless scalar modes $\chi_0^{(i)}(i=1,\ldots,q-p+1)$ are orthogonal to the gauge transformation, i.e., $\Sigma_{e\in E}\chi_{0e}^{(i)}(E^T\omega)_e=0$. Thus, the zero modes satisfy $(E\chi_0^{(i)})_v=0$. Actually, the graph includes $(q-p+1)$ fundamental circuits, that is, independent (undirected) cycles as subgraphs. The number of fundamental circuit $n(G)$ is called the *cyclomatic number* of the graph G, or its *nullity*. For the ith fundamental circuit $C^{(i)}$

$$\chi_{0e}^{(i)} \propto \begin{cases} \pm 1 & \text{if } e\in E(C^{(i)}) \\ 0 & \text{otherwise} \end{cases}, \tag{10}$$

where the minus sign is chosen when the edge has the opposite direction to an orientation of the fundamental circuit, satisfies $(E\chi_0^{(i)})_v=0$. Then, $\chi_0^{(i)}$ is represented by rows of the *fundamental tie set matrix* F_f, since *rank* $F_f=n(G)$. For the definition of fundamental circuits and fundamental tie set matrix, in other words, fundamental circuit matrix, and for a related theorem, see Ref. 6. For example, for the graph including a (directed) fundamental circuit of length three, the incidence matrix includes

$$\begin{pmatrix} 1 & 0 & -1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix}, \tag{11}$$

as a submatrix. Then, $\chi_0\propto(1,1,1,0,\ldots,0)$ is a zero mode.

Now and then the part of the Lagrangian for the link fields gives a mass term for the vector fields. For example, we consider a cycle graph C_5. The (mass)^2 matrix for vector fields takes the form

$$(gv)^2\Delta(C_5) = (gv)^2\begin{pmatrix} 2 & -1 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & -1 & 2 \end{pmatrix}. \tag{12}$$

Up to the dimensionful coefficient g^2v^2, this matrix is identified with the Laplacian matrix for the graph C_p, the cycle graph with p vertices. We find, indeed, any theory space can be associated with the graph.

Next, we will manage to perform gauge fixing. We choose the gauge fixing term as

$$\mathcal{L}_{gf} = -\sum_{v\in V}\frac{1}{2g^2\xi}(\partial_\mu A_v^\mu - \xi(gv)^2(E\chi)_v)^2, \tag{13}$$

where $(E\chi)_v$ means $\Sigma_{e\in E}E_{ve}\chi_e$.

For this gauge choice, we introduce the ghost field and its Lagrangian

$$\mathcal{L}_{ghost} = \sum_{v\in V}\overline{c_v}[-(\partial^2 + \xi(gv)^2EE^T)c]_v, \tag{14}$$

because $\delta(\partial_\mu A_v^\mu - \xi(gv)^2(E\chi)_v) = \partial^2\omega_v + \xi(gv)^2(EE^T\omega)_v$.

The gauge-fixed Lagrangian $\mathcal{L}_{V\xi} = \mathcal{L}_V + \mathcal{L}_{gf} + \mathcal{L}_{ghost}$ becomes

$$\begin{aligned}\mathcal{L}_{V\xi} = &-\frac{1}{2g^2}\sum_{v\in V}\left[(\partial_\mu A_v^\nu)^2 - \left(1-\frac{1}{\xi}\right)(\partial_\mu A_v^\mu)^2\right] + \frac{1}{2}v^2\sum_{v\in V}A_v^\mu(EE^TA_\mu)_v + \frac{1}{2}\sum_{e\in E}(\partial^\mu X_e)^2 \\ &-\frac{1}{2}\xi(gv)^2\sum_{e\in E}X_e(E^TEX)_e + \sum_{v\in V}\overline{c_v}[-(\partial^2 + \xi(gv)^2EE^T)c]_v,\end{aligned} \tag{15}$$

where we rewrite the scalar fields as $X_e \equiv v\chi_e$. The massive scalar modes are the would-be Nambu-Goldstone bosons that become a longitudinal component of vector fields, while the massless modes are physical massless scalars. The massive scalar modes are associated with the *fundamental cutset matrix* C_f, since $F_fC_f^T = 0$.[10]

If we choose $\xi = 1$ gauge, we can apparently find that vector fields (physical and unphysical), scalar fields, and ghost fields have the same mass spectrum up to zero modes, since EE^T and E^TE have the same nonzero eigenvalues. Indeed, $\mathrm{Tr}\, e^{-EE^Tt} - \mathrm{Tr}\, e^{-E^TEt} = p - q$ is an "index theorem" in graph theory as well as the theory of non-negative matrices.

The treatment of the "unexpected" scalars in the phenomenological point of view will be discussed after considering the coupling to fermions in the successive section.

IV. FERMIONS ON A GRAPH

We associate right-handed fermion fields with vertices of a graph G, and left-handed fermion fields with edges of G. The Lagrangian density for Dirac fields associated with the directed graph can be written by

$$\mathcal{L}_f = \sum_{v\in V}\overline{\psi}_{Rv}i\gamma^\mu\partial_\mu\psi_{Rv} + \sum_{e\in E}\overline{\psi}_{Le}i\gamma^\mu\partial_\mu\psi_{Le} - m\left(\sum_{e\in E}\sum_{v\in V}\overline{\psi}_{Le}E_{ev}^T\psi_{Rv} + \mathrm{H.c.}\right). \tag{16}$$

The equations of motion are derived from this Lagrangian as

$$\partial^2 \psi_{Rv} + m^2 (EE^T \psi_R)_v = 0,$$
$$\partial^2 \psi_{Le} + m^2 (E^T E \psi_L)_e = 0. \tag{17}$$

Here, we already know that the graph Laplacian matrix $\Delta \equiv EE^T$ has a single zero eigenvalue for a simple connected graph.[7] Moreover, it is well known that the matrix $E^T E$ has the same eigenvalues as EE^T and $(q-p)$ zero modes. Therefore, the particle spectrum contains one right-handed Weyl fermion, $(q-p+1)$ left-handed Weyl fermions (or, one massless Dirac fermion and $(q-p)$ left-handed fermion), and $(p-1)$ massive Dirac fermions.

Now, we introduce the coupling between gauge and link fields. In addition to (7), we will impose the gauge symmetry and assume the following gauge transformation on fermions:

$$\psi_{Rv} \to \exp(i\omega_v)\psi_{Rv},$$
$$\psi_{Le} \to \exp(i\omega_{o(e)})\psi_{Le}. \tag{18}$$

The invariant Lagrangian is

$$\begin{aligned}\mathcal{L}_f &= \sum_{v\in V} \overline{\psi}_{Rv} i\gamma_\mu (\partial^\mu - iA_v^\mu)\psi_{Rv} + \sum_{e\in E} \overline{\psi}_{Le} i\gamma_\mu (\partial^\mu - iA_{o(e)}^\mu)\psi_{Le} - m\left(\sum_{e\in E} \overline{\psi}_{Le}(\psi_{Ro(e)} - U_e \psi_{Rt(e)}) + \text{H.c.}\right) \\ &= \sum_{v\in V} \overline{\psi}_{Rv} i\gamma_\mu D_v^\mu \psi_{Rv} + \sum_{e\in E} \overline{\psi}_{Le} i\gamma_\mu D_e^\mu \psi_{Le} - m\left(\sum_{e\in E}\sum_{v\in V} \overline{\psi}_{Le} \hat{E}_{ev}^\dagger \psi_{Rv} + \text{H.c.}\right),\end{aligned} \tag{19}$$

where the weighted incidence matrix $\hat{E}$ is defined as

$$(\hat{E})_{ve} = \begin{cases} 1 & \text{if } v = o(e) \\ -U_e^\dagger & \text{if } v = t(e) \\ 0 & \text{otherwise} \end{cases}. \tag{20}$$

The $(\text{mass})^2$ matrix, or modified graph Laplacian, can be read as

$$(\hat{\Delta})_{vv'} = (\hat{E}\hat{E}^\dagger)_{vv'} = \begin{cases} \deg(v) & \text{if } v = v' \\ -U_e^\dagger & e = [v', v] \in E(G) \\ -U_e & e = [v, v'] \in E(G) \\ 0 & \text{otherwise} \end{cases}. \tag{21}$$

Getting the gauge field Lagrangian in the previous section and the fermion Lagrangian together, we have a QED-like theory on a graph. When we investigate the model in view of quantum theory, we find that there appears chiral anomaly in general except for the $p=q$ case. The cancellation of anomaly requires more charged fermion species. We do not treat the problem of anomaly in the present paper. Another problem for phenomenologically viable models is the existence of exactly massless fermions. Even in the $p=q$ case a massless Dirac field appears. Of course, additional mass terms can be introduced into the model, but the origin of such a small "electron mass" is not discussed here.

Now, we study the coupling between zero-mode fields, which describes the low-energy physics $E \ll v, m$. The lowest-order interactions can be read as

$$\mathcal{L}_{\text{int}} = \sum_{v\in V} \overline{\psi}_{Rv} \gamma_\mu A_v^\mu \psi_{Rv} + \sum_{e\in E} \overline{\psi}_{Le} \gamma_\mu A_{o(e)}^\mu \psi_{Le} - \frac{m}{v}\left(\sum_{e\in E} \overline{\psi}_{Le} i X_e \psi_{Rt(e)} + \text{H.c.}\right). \tag{22}$$

We consider here the simplest case, $p=q$. Then, the graph contains one circuit $\tilde{C}_{\tilde{p}}$ with length $\tilde{p}(\leqslant p)$. The zero-mode fields of A^μ and ψ_R are expressed as

$$A_v^\mu = \frac{1}{\sqrt{p}} A_0^\mu, \quad \psi_{Rv} = \frac{1}{\sqrt{p}} \psi_{R0}, \quad \forall\, v \in V(G). \tag{23}$$

On the other hand, the zero-mode fields of X and ψ_L are expressed as

$$X_e = \frac{1}{\sqrt{\tilde{p}}} X_0, \quad \psi_{Le} = \frac{1}{\sqrt{\tilde{p}}} \psi_{L0}, \quad \forall\, e \in E(\tilde{C}_{\tilde{p}}). \tag{24}$$

Then, the zero-mode interactions can be written as

$$\mathcal{L}_{\text{int}0} = \frac{1}{\sqrt{p}} \bar{\psi}_{R0} \gamma_\mu A_0^\mu \psi_{R0} + \frac{1}{\sqrt{p}} \bar{\psi}_{L0} \gamma_\mu A_0^\mu \psi_{L0} - \frac{1}{\sqrt{p}} \frac{m}{v} (\bar{\psi}_{L0} i X_0 \psi_{R0} + \text{H.c.}). \tag{25}$$

The gauge coupling is $g/\sqrt{p}$, while the link scalar coupling is $(m/v)/\sqrt{p}$, which is the same order as the gauge coupling if the fermion mass equals the vector boson mass, $m=gv$.

We do not know the massless scalar interaction in the real world. One way to avoid the difficulty in the existence of scalars is to assume that the massless scalar interacts very weakly with matter fields. Unfortunately, here we found that the suppression of the scalar interaction due to the choice of a graph cannot be expected in general. We can only arrange the two scales m and v for this purpose.

A special case is the choice of a graph with $p=q+1$, called the tree (graph).[6] All link scalar fields are absorbed by massive vector bosons, leaving a massless vector field. The simplest tree graph, path graph P_p,[6] corresponds to the dimensional deconstruction of an orbifold S^1/Z_2.

Another method to discard the massless scalar is incorporation of the plaquette-type term, $\text{Re}(U_{e_1} \cdots U_{e_{q'}})$ where $e_1, \ldots, e_{q'} \in E(C)$ and C is a cycle in a graph, in the Lagrangian. The plaquette-type term will be studied elsewhere.

In the rest of the present paper, we will concentrate on the study of one-loop UV divergence of the model.

V. ONE-LOOP DIVERGENCES IN EFFECTIVE ACTION

We investigate the one-loop divergence in the model by calculating the effective action by the heat-kernel method with background fields.[11] In this section, we use the Euclidean signature for the metric. The gamma matrices satisfy $\{\gamma^\mu, \gamma^\nu\} = -2\delta^{\mu\nu}$. We assemble the fermion fields as

$$\Psi \equiv \begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix}, \tag{26}$$

and define a derivative operator

$$i\mathcal{D} \equiv \begin{pmatrix} iD_V & -m\hat{E} \\ -m\hat{E}^\dagger & iD_E \end{pmatrix}, \tag{27}$$

and

$$i\mathcal{D}^\dagger \equiv \begin{pmatrix} iD_V & m\hat{E} \\ m\hat{E}^\dagger & iD_E \end{pmatrix}, \tag{28}$$

where $D_V = \text{diag}(\gamma^\mu D_{v_1}^\mu, \gamma^\mu D_{v_2}^\mu, \ldots, \gamma^\mu D_{v_p}^\mu)$ and $D_E = \text{diag}(\gamma^\mu D_{e_1}^\mu, \gamma^\mu D_{e_2}^\mu, \ldots, \gamma^\mu D_{e_q}^\mu)$. Then, the Euclidean Lagrangian is expressed as $\mathcal{L}_f = \bar{\Psi}^\dagger i\mathcal{D}\Psi$.

As a preparation, we write the quadratic operator $\mathcal{D}^\dagger\mathcal{D}$ explicitly as

$$\mathcal{D}^\dagger\mathcal{D} = \begin{pmatrix} D_V^2 + m^2\hat{E}\hat{E}^\dagger & \mathrm{i}\,\mathrm{m}(D_V\hat{E} - \hat{E}D_E) \\ \mathrm{i}\,\mathrm{m}(D_E\hat{E}^\dagger - \hat{E}^\dagger D_V) & D_E^2 + m^2\hat{E}^\dagger\hat{E} \end{pmatrix}, \tag{29}$$

where

$$(D_V^2)_{vv'} = \begin{cases} -(D_v^\mu)^2 - \dfrac{i}{2}\gamma^\mu\gamma^\nu F_v^{\mu\nu} & \text{if } v = v' \\ 0 & \text{otherwise} \end{cases}, \tag{30}$$

$$(D_E^2)_{ee'} = \begin{cases} -(D_e^\mu)^2 - \dfrac{i}{2}\gamma^\mu\gamma^\nu F_{o(e)}^{\mu\nu} & \text{if } e = e' \\ 0 & \text{otherwise} \end{cases}, \tag{31}$$

$$(D_V\hat{E} - \hat{E}D_E)_{ve} = \begin{cases} -\gamma^\mu(D^\mu U_e)^\dagger & \text{if } v = t(e) \\ 0 & \text{otherwise} \end{cases}, \tag{32}$$

and

$$(D_E\hat{E}^\dagger - \hat{E}^\dagger D_V)_{ev} = \begin{cases} -\gamma^\mu(D^\mu U_e) & \text{if } v = t(e) \\ 0 & \text{otherwise} \end{cases}. \tag{33}$$

The effective action at the one-loop level can be written as (see Ref. 11 and references therein).

$$\Gamma = -\frac{1}{2}\mathrm{Tr}\,\ln(\mathcal{D}^\dagger\mathcal{D}) = \frac{1}{2}\int_0^\infty \frac{dt}{t}\mathrm{Tr}\,e^{-\mathcal{D}^\dagger\mathcal{D}t} = \frac{1}{2}\int_0^\infty \frac{dt}{t}\int d^4x\,\mathrm{Tr}\langle x|e^{-\mathcal{D}^\dagger\mathcal{D}t}|x\rangle. \tag{34}$$

Here, we use

$$\langle x|f(D_\mu)|x\rangle = \int \frac{d^4k}{(2\pi)^4}\langle x|f(D_\mu + ik_\mu)|0\rangle, \tag{35}$$

where $|0\rangle$ is a zero momentum state ($\langle x|0\rangle = 1$), to calculate the effective Lagrangian.[11]

To evaluate the t^2 term in the expansion of the integrand, we need the following explicit form:

$$\mathrm{Tr}(D_V^2)^2 = 2\sum_{v\in V}\left[(D_v^\mu)^2(D_v^\nu)^2 + \frac{1}{2}F_v^{\mu\nu}F_v^{\mu\nu}\right], \tag{36}$$

and

$$\mathrm{Tr}(D_E^2)^2 = 2\sum_{e\in E}\left[(D_e^\mu)^2(D_e^\nu)^2 + \frac{1}{2}F_{o(e)}^{\mu\nu}F_{o(e)}^{\mu\nu}\right], \tag{37}$$

where the coefficient 2 comes from the projection to the left/right-handed fermions.

Therefore, the logarithmically divergent part (with the Euclidean signature) turns out to be

$$\frac{1}{24\pi^2}\int\frac{dt}{t}\left[\sum_{v\in V}\frac{1}{4}(F_v^{\mu\nu})^2 + \sum_{e\in E}\frac{1}{4}(F_{o(e)}^{\mu\nu})^2 + \frac{3}{2}m^2\sum_{e\in E}|D^\mu U_e|^2 + \cdots\right]. \tag{38}$$

The coefficients of kinetic terms of gauge and link fields are logarithmically divergent.

In particular, the gauge coupling runs logarithmically. If every vertex is an origin of an edge for $p=q$ graph, the beta function is the same as the usual QED

$$\mu\frac{dg}{d\mu}=\frac{g^3}{12\pi^2}. \tag{39}$$

In the general case, if we define the individual gauge coupling for each gauge field on a vertex, such that the kinetic term becomes $\Sigma_{v\in V}(1/4g_v^2)F_{\mu\nu\,v}F_v^{\mu\nu}$, their beta functions are

$$\mu\frac{dg_v}{d\mu}=\frac{(1+d^+(v))g_v^3}{24\pi^2}, \tag{40}$$

where $d^+(v)$ is the *outgoing degree* of a vertex v, which is the number of edges whose origin is v. Note that the average of $d^+(v)$ is q/p.

The running of the individual gauge coupling is interesting for the possibility of variating the mass spectrum. However, the existence of zero modes is still unchanged, expressed as in (23). Thus, this running-coupling effect is not useful for symmetry breaking even when the model is generalized to the non-Abelian one.

For the non-Abelian case, the quantum fluctuation of the gauge fields and link fields also induces the logarithmic divergent contribution to the gauge and link field kinetic terms.

VI. ONE-LOOP FINITENESS IN EFFECTIVE POTENTIAL

The effective potential for constant background link field can be written as

$$\begin{aligned}V&=-\frac{1}{2}\int_0^\infty\frac{dt}{t}\int\frac{d^4k}{(2\pi)^4}e^{-k^2t}2[\mathrm{Tr}_p\exp(-m^2\hat{E}\hat{E}^\dagger t)+\mathrm{Tr}_q\exp(-m^2\hat{E}^\dagger\hat{E}t)]\\&=-\frac{1}{(4\pi)^2}\int_0^\infty\frac{dt}{t^3}[\mathrm{Tr}_p\exp(-m^2\hat{E}\hat{E}^\dagger t)+\mathrm{Tr}_q\exp(-m^2\hat{E}^\dagger\hat{E}t)],\end{aligned} \tag{41}$$

where Tr_M means the trace only on $(M\times M)$ matrices.

Since $\mathrm{Tr}_p(\hat{E}\hat{E}^\dagger)^n=\mathrm{Tr}_q(\hat{E}^\dagger\hat{E})^n$ for $n\geqslant 1$, the integrand can be expanded as

$$\frac{1}{2}[\mathrm{Tr}_p\exp(-m^2\hat{E}\hat{E}^\dagger t)+\mathrm{Tr}_q\exp(-m^2\hat{E}^\dagger\hat{E}t)]=\frac{p+q}{2}-m^2\,\mathrm{Tr}_p\,\hat{\Delta}t+\frac{1}{2}m^4\,\mathrm{Tr}_p\,\hat{\Delta}^2t^2+O(t^3). \tag{42}$$

Owing to $U_eU_e^\dagger=1$, $\mathrm{Tr}_p\,\hat{\Delta}=\mathrm{Tr}_p\,D$ obviously and $\mathrm{Tr}_p\,\hat{\Delta}^2=\mathrm{Tr}_p\,D^2+\mathrm{Tr}_p\,D$. In other words, the same relation as that on Δ holds. The expression (41) includes divergences, but they not depend on the background link fields.

This is the origin of the one-loop finiteness of the scalar potential in the deconstructed theory. This nature is preserved for non-Abelian generalization.

In the present Abelian case, the zero-mode field of the link variable acquires mass by the one-loop quantum effect. The explicit calculation for models with a cycle graph C_N can be carried out as in Refs. 8 and 12.

VII. GRAPH HOSOTANI MECHANISM?

If some non-Abelian gauge symmetry is introduced, a symmetry-breaking mechanism becomes possible in the theory on a graph, just as in the case of the Hosotani mechanism.[13]

Let the length of the shortest cycle $c=(e_1,\ldots,e_N)$ in G be $N(\geqslant 3)$. The trace of the kernel of $\hat{\Delta}$, $\mathrm{Tr}\exp(-\hat{\Delta}t)$, for matter fields coupled to the link fields, includes a term $\mathrm{Re}\,\mathrm{Tr}\,U_{e_1}\cdots U_{e_N}$ and its coefficient is $O(t^N)$. Therefore, the one-loop effective potential for the zero mode of link fields is finite (up to a field-independent divergence).

If we take a graph C_n into a model and consider the limit $n\to\infty$, the model reduces to the original Hosotani model[13] (it should be read $A_5\sim\chi$, where $U=e^{-i\chi}$).

The realization of non-Abelian symmetry breaking in the field theory on a graph may not be

so easy as in the Hosotani models. The simplest idea is that we abandon the *local symmetry on a whole graph*. Suppose that we dare to replace such a term $\overline{\psi_{Le}}(\psi_{Ro(e)}-U_e\psi_{Rt(e)})$ by $\overline{\psi_{Le}}(\psi_{Ro(e)}-\psi_{Rt(e)})$ on some edges. Then, the *local* symmetry on a graph disappears but *global* symmetry on a graph such as $\psi_{Rv}\to\exp(i\omega)\psi_{Rv}$, $\psi_{Le}\to\exp(i\omega)\psi_{Le}$ [where $\omega_v(x)=\omega(x)$ for all $v\in V$ and $\omega_e(x)=\omega(x)$ for all $e\in E$] remains. Thus, the model still has usual local gauge symmetry in space–time, at the classical level. In this case, the induced term like $\mathrm{Re}\,\mathrm{Tr}\,U_{e_1}\cdots U_{e_N}$, where some Us are replaced by unity, may lead to a novel phase structure of vacuum.

We will study the dynamical symmetry breaking in field theory on a graph which has edges with and without some weight functions elsewhere.

VIII. SUMMARY AND PROSPECTS

In conclusion, we clarified the divergences of the one-loop effective Lagrangian in the Abelian gauge field theory on graphs.

We must consider the following possibilities. To consider the generalization of the Hosotani model, we should investigate non-Abelian gauge theory on a graph. We also need adjoint matter fields or fields in other representations on vertices or edges. At the same time, we should study the possible inclusion of plaquette-like self-interaction of link fields in bare Lagrangian. By the way, to consider superfields on a graph is also an interesting subject.

We are interested also in the two-loop effective action. We still hope that the knowledge of algebraic graph theory may be useful to investigate higher-loop divergence as well as tree-level calculation of reaction amplitude mediated by the excited modes.

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Pure gravitational radiation with twisting rays in the linear approximation

Bogdan G. Nita[a)]
Department of Mathematics, Montclair State University, 1 Normal Avenue, Montclair, New Jersey 07043

Paul MacAlevey[b)] and Phillip T. Downes[c)]
Department of Physics, FO23, University of Texas at Dallas, PO Box 830688, Richardson, Texas 75083-0688

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Solutions of types N and III with twisting rays are derived in the linear approximation by means of complex coordinate transformations. Some solutions are shown to have Riemann tensors which vanish asymptotically and are everywhere regular. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2113412]

I. INTRODUCTION

Over the past 40 years, a great deal of progress has been made in studying the spacetimes with degenerate Weyl tensors.[2] For type III fields built around expanding and hypersurface orthogonal rays, the field equations reduce to a single one which specifies that, on each wavefront, the Laplacian of the Gaussian curvature should vanish. An example of this solution was given by Robinson and Trautman in 1962.[7] Stephani[8] has analyzed the symmetries of this equation and found that this method did not lead to any new solutions simply because the only known one, Robinson-Trautman, is a fixed point for the set of symmetry transformations.

For metrics with twisting rays, a class has been identified by Robinson and Robinson,[6] in which the system of field equations separate into a nonlinear background and a linear equation. The only known solution for this background equation is the old Robinson-Trautman solution; and since this is a stationary solution, so are all the spaces determined from it. Therefore these are examples of a rather restricted type of radiation. In any case, all solutions obtained this way appear to have directional singularities.

The lack of exact solutions and methods of discovering them increased the interest for approximate ones. For example, in the twisting type N case, only Kundt's solution was known until recently; Ivanov[1] found another one. However, both solutions are more difficult to understand, analyze or to work with than the regular approximate ones found by MacAlevey in Ref. 3.

In this paper we obtain approximate type III solutions in the case of pure radiation with twisting rays. The method we use was described and used by Trautman[9] to obtain solutions to linear special relativistic partial differential equations. One starts with a solution analytic in all four coordinates, continues it for complex values of the coordinates, makes a complex inhomogeneous Lorentz transformation and restricts the resulting solution to real values of the coordinates. Applying this method to Maxwell's equations and the linearized Einstein's equations one works throughout with the complex self-dual form of the field. The transformation then leaves invariant the algebraic structure of the field, i.e., the distinctness or coincidence of the principal

[a)]Electronic mail: nitab@mail.montclair.edu
[b)]Electronic mail: paulmac@utdallas.edu
[c)]Electronic mail: p2downes@hotmail.com

null directions. By these means Trautman obtained the null electromagnetic field built around the Robinson congruence given explicitly a year later. The method has also been applied extensively by Newman (see, e.g., Ref. 4).

We carry out this procedure explicitly starting with a linear approximation of a type III space-time built around the Robinson congruence. After complexifying and setting conditions for self-duality, we apply a complex transformation to obtain the most general expression for type III solutions built around what might be described as a generalized Kerr congruence. A large subclass of these solutions are shown to be regular using a scalar obtained from their Bel-Robinson tensor.

II. SELF-DUAL ROBINSON-TRAUTMAN SPACES

We can complexify the Robinson-Trautman metric given in Ref. 7, in a purely formal way, by taking the coordinates ρ, σ, ζ, $\tilde{\zeta}$ to be independent complex variables and the defining functions $m(\sigma)$ and $p(\sigma,\zeta,\tilde{\zeta})$ to be complex. It is easy to see that the Weyl tensor is self-dual if, and only if, $m=0$ and $p^{-1}p_{,\tilde{\zeta}\tilde{\zeta}}$ is a function of $\tilde{\zeta}$ only. By means of a coordinate transformation we can strengthen the last condition to $p_{,\tilde{\zeta}\tilde{\zeta}}=0$. The line element is then given by

$$\mathrm{d}s^2 = 2\,\mathrm{d}\rho\,\mathrm{d}\sigma + \left(K - 2\rho\frac{p_{,\sigma}}{p}\right)\mathrm{d}\sigma^2 - \frac{2\rho^2}{p^2}\mathrm{d}\zeta\,\mathrm{d}\tilde{\zeta}, \tag{1}$$

$$K = 2(AB_{,\zeta} - A_{,\zeta}B), \quad p = A + \tilde{\zeta}B, \tag{2}$$

where A and B are arbitrary functions of ζ and σ. The Weyl tensor is

$$C_{klmn} = \frac{p}{2\rho^2}K_{,\zeta}(M_{kl}N_{mn} + N_{kl}M_{mn}) - \frac{1}{2\rho^2}(p^2K_{,\zeta})_{,\zeta}N_{kl}N_{mn} + \frac{p^2}{\rho}(p^{-1}p_{,\zeta\zeta})_{,\sigma}N_{kl}N_{mn}, \tag{3}$$

where

$$N_{kl} = 2\frac{\rho}{p}\sigma_{,[k\zeta,l]}, \tag{4}$$

$$M_{kl} = 2\left(\sigma_{,[k\rho,l]} - \frac{\rho^2}{p^2}\zeta_{,[k\tilde{\zeta},l]}\right). \tag{5}$$

III. COMPLEX COORDINATE TRANSFORMATION

It is worth remarking that, at least in a special case, one can put this line element into the standard form for one with twisting rays. The special case is defined by $p=A(\zeta)+\tilde{\zeta}B(\zeta)$. The transformation

$$\rho = r - i\Sigma,$$

$$\zeta = z, \tag{6}$$

$$\tilde{\zeta} = \frac{r+ia}{r-ia}\tilde{z},$$

where

$$\Sigma = a\frac{A(z) - \tilde{z}B(z)}{P} \tag{7}$$

and

$$P = A(z) + \tilde{z}B(z), \tag{8}$$

a being a real parameter, transforms (1) into

$$ds'^2 = 2\lambda\nu - 2\mu\tilde{\mu}, \tag{9}$$

where

$$\lambda = d\sigma \mp 2L\, dz, \tag{10}$$

$$\mu = P^{-1}(r - i\Sigma)dz, \tag{11}$$

$$\tilde{\mu} = P^{-1}(r + i\Sigma)d\tilde{z}, \tag{12}$$

$$\nu = dr + i(\Sigma_z\, dz - \Sigma_{\tilde{z}}\, d\tilde{z}) + \tfrac{1}{2}K\lambda, \tag{13}$$

and

$$L = \frac{ai\tilde{z}}{P^2}. \tag{14}$$

In the coordinates, the bivectors N and M are given by

$$N_{kl} = \frac{r - ia}{r - i\Sigma}N'_{kl}, \tag{15}$$

$$M_{kl} = M'_{kl} + \frac{2PKL}{r - i\Sigma}N'_{kl}, \tag{16}$$

where

$$N'_{kl} = 2\frac{\rho}{p}\lambda_{[k\mu l]}, \tag{17}$$

(18)

$$M'_{kl} = 2\left(\lambda_{[k\nu l]} - \mu_{[k\tilde{\mu}l]}\right).$$

Making this transformation on the flat space line element

$$ds_0^2 = 2\, d\rho\, d\sigma \mp 2k\, d\sigma^2 - \frac{2\rho^2}{p_0^2}d\zeta\, d\tilde{\zeta}, \tag{19}$$

$$p_0 = 1 + k\zeta\tilde{\zeta}, \tag{20}$$

writing $\overline{z}$ for $\tilde{z}$ and setting

$$\sigma = u - ia\frac{z\overline{z}}{P_0} \tag{21}$$

with

$$P_0 = 1 + kz\overline{z} \tag{22}$$

we get

$$ds^2 = 2\lambda(dr + i\Sigma_z\, dz - i\Sigma_{\overline{z}}\, d\overline{z} + k\lambda) - \frac{2(r^2+\Sigma^2)}{P_0^2} dz\, d\overline{z}, \tag{23}$$

where

$$\lambda = du + iaP_0^{-2}(\overline{z}\, dz - z\, d\overline{z}) \tag{24}$$

and

$$\Sigma = a\frac{1 - kz\tilde{z}}{1 + kz\tilde{z}}. \tag{25}$$

For $k=0$, this is the transformation given in Trautman;[9] for $k>0$, it is equivalent to that of Newman.[4]

IV. LINEAR APPROXIMATION

Suppose that in the line element given by Eqs. (1) and (2), the function p is expanded as a power series

$$p = p_0 + \epsilon p_1 + \epsilon^2 p_2 + \cdots, \tag{26}$$

where p_0 is given by (20) and

$$p_1 = \alpha_{,\zeta} + \beta\overline{\zeta} + k\overline{\zeta}(\zeta\alpha_{,\zeta} - 2\alpha), \tag{27}$$

α and β being arbitrary functions of ζ and σ. In the expansion of the Weyl tensor we have

$$C_{0\ klmn} = 0, \tag{28}$$

$$C_{1\ klmn} = \frac{1}{\rho^2} p_0 \Phi(M_{kl}N_{mn} + N_{kl}M_{mn}) - \left[\frac{1}{\rho^2}\left(p_0^2\Phi\right)_{,\zeta} - \frac{1}{\rho} p_0\left(\Psi p_0 + \Phi_{,\sigma}\tilde{\zeta}\right)\right] N_{kl}N_{mn}, \tag{29}$$

where $\Phi = \beta_{,\zeta\zeta}$ and $\Psi = \alpha_{,\zeta\zeta\zeta\sigma}$.

Next we transform to the coordinates u, r, z, $\overline{z}$, restrict ourselves to the space-time in which u and r are real and in which z and $\overline{z}$ are complex conjugates. Consider the line element

$$ds^2 = ds_0^2 + \epsilon\left(ds_1^2 + d\vec{s}_1^2\right). \tag{30}$$

In the lowest approximation the line element is given by (23), (24), and (25). The next approximation to the line element is more complicated; fortunately, the Weyl tensor in the linear approximation is quite simple, using (29) and our expression for the transformed bivectors, we get

$$C_{klmn} = \epsilon[X(M'_{kl}N'_{mn} + N'_{kl}M'_{mn}) + YN'_{kl}N'_{mn}] + \text{complex conjugate}, \tag{31}$$

where

$$X = \frac{P}{(r - ia)(r - i\Sigma)}\Phi, \tag{32}$$

$$Y = -\frac{P}{(r - ia)^2}\left[\frac{2k\overline{z}(r + ia)}{r - i\Sigma}\Phi + P\Phi_{,z} - \Psi P(r - i\Sigma) - \Phi_{,\sigma}(r + ia)\overline{z}\right]. \tag{33}$$

The Bel-Robinson tensor can then be written as

$$\tfrac{1}{2}P_{abcd} = {}^{+}_{1}C_{amnc}\,{}^{-}_{1}C_{b}{}^{mn}{}_{d} = 4|\Gamma|^2[\lambda_{(a}\lambda_b\lambda_c\nu_{d)} + 3\lambda_{(a}\lambda_b\mu_c\overline{\mu}_{d)}] + 4\Gamma\overline{\Delta\lambda}_{(a}\lambda_b\lambda_c\overline{\mu}_{d)} + 4\overline{\Gamma}\Delta\lambda_{(a}\lambda_b\lambda_c\mu_{d)} + |\Delta|^2\lambda_a\lambda_b\lambda_c\lambda_d, \tag{34}$$

where

$$\Gamma = X\frac{r-ia}{r-i\Sigma}, \tag{35}$$

$$\Delta = \frac{2XPKL(r-ia)}{(r-i\Sigma)^2} + Y\left(\frac{r-ia}{r-i\Sigma}\right)^2. \tag{36}$$

V. THE GRAVITATIONAL DENSITY

A well-known measure of the strength of the gravitational field is the density

$$D = P_{abcd}t^a t^b t^c t^d, \tag{37}$$

where t^a is a unit timelike vector field. Here, we can reduce the arbitrariness of D by requiring that t^a should be covariantly constant with respect to the Minkowskian metric of the linear approximation. D then has the following interpretation: it is the sum of squares of the components of the Weyl tensor in Minkowskian coordinates with t_a as the time direction. For these components to be all regular and/or asymptotically vanishing, it is necessary and sufficient that D should have the same properties. We shall show that both these conditions can be satisfied by certain solutions with $k=0$. In this case the tetrad given by

$$\hat{\nu} = \nu, \tag{38}$$

$$\hat{\mu} = \mu + z\nu, \tag{39}$$

$$\hat{\lambda} = \lambda + \overline{z}\mu + z\overline{\mu} + z\overline{z}\nu \tag{40}$$

is constant. We may take, for example, $t_a = (1/\sqrt{2})(\hat{\lambda}_a + \hat{\mu}_a)$. Then

$$D = \tfrac{1}{2}(1+z\overline{z})^2[4|\Gamma|^2 + |4\overline{z}\Gamma - (1+z\overline{z})\Delta|^2] \tag{41}$$

and

$$\Gamma = \frac{\Phi}{(r-ia)^2}, \tag{42}$$

$$\Delta = Y|_{k=0} = -\frac{1}{(r-ia)^2}[\Phi_{,z} - \Psi(r-ia) - \Phi_{,\sigma}(r+ia)\overline{z}]. \tag{43}$$

Φ and Ψ are disposable functions of z and σ $(=u-iaz\overline{z})$. We may take, for example,

$$\Phi = c_1(\sigma - i)^{-n}, \quad \Psi = c_2(\sigma - i)^{-m}, \tag{44}$$

where $n \geqslant 2$, $m \geqslant 3$ and c_1, c_2 are constants. It is easy to verify that D is then regular and asymptotically vanishing.

VI. CONCLUSIONS

In this paper we have described the construction of pure radiative solutions of Einstein's field equations in the linear approximation. A large subclass of these (i.e., for $k=0$) were shown to be

regular and asymptotically vanishing using a scalar obtained from their Bel-Robinson tensor. The second approximation was also studied in Ref. 5 and, although only a partial result, it was shown to exhibit nice regularity properties. For solutions with $k>0$ the directional singularities were unavoidable (see Ref. 5).

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Volume elements and torsion

Ricardo A. Mosna[a] and Alberto Saa[b]
Instituto de Matemática, Estatística e Computação Científica, Universidade Estadual de Campinas, C.P. 6065, 13083-859, Campinas, SP, Brazil

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We reexamine here the issue of consistency of minimal action formulation with the minimal coupling procedure (MCP) in spaces with torsion. In Riemann-Cartan spaces, it is known that a proper use of the MCP requires that the trace of the torsion tensor be a gradient, $T_\mu = \partial_\mu \theta$, and that the modified volume element $\tau_\theta = e^\theta \sqrt{g} \mathrm{d}x^1 \wedge \cdots \wedge \mathrm{d}x^n$ be used in the action formulation of a physical model. We rederive this result here under considerably weaker assumptions, reinforcing some recent results about the inadequacy of propagating torsion theories of gravity to explain the available observational data. The results presented here also open the door to possible applications of the modified volume element in the geometric theory of crystalline defects. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The use of modified volume elements in physical models has been receiving considerable interest in recent years. In the context of the Einstein-Cartan theory of gravity,[1] for instance, the introduction of a new volume element gave rise to some models possessing several interesting characteristics, such as propagation of torsion,[2,3] interaction between torsion and gauge fields without violation of the gauge symmetry,[4] and a geometrical interpretation of string-theory inspired models of gravity.[5] Noncanonical volume elements have also proved to be useful in other contexts. For recent applications in field and string theory, see, for instance, Ref. 6.

Geometries with torsion, on the other hand, have a long tradition in Physics. For instance, in Einstein-Cartan theory of gravity,[1] space-time is assumed to be a Riemann-Cartan manifold, i.e., a manifold endowed with a Lorentzian metric and a nonsymmetrical metric-compatible linear connection. The anti-symmetrical part of the connection (the torsion tensor) is also relevant to field theory, mainly with respect to renormalization issues.[7] The very active area of defects in crystal microstructures also takes advantage of these non-Riemannian geometries: disclinations and dislocations in a crystal can be described by means of curvature and torsion (for a revision, see Refs. 8 and 9). Dislocations, in particular, are described by the Burgers vector, which has the torsion tensor as its surface density (see Fig. 1).

The motivation for the introduction of the modified volume element proposed in Ref. 10 was the observation that, in the presence of torsion, the minimal coupling procedure (MCP) performed at the action level is not equivalent to that performed directly at the corresponding field equations, a conflict known since long before, see, for instance, Ref. 11. The same volume element is shown in Ref. 12 to be mandatory in order to assure unitary evolution of a Klein-Gordon field in spaces with torsion. In Ref. 12, it is also shown that the introduction of a nonholonomic version of the minimal action principle can cure these problems. As shown in Ref. 10, in Riemann-Cartan spaces the equivalence between the MCP performed at the action and at the field equations can be

[a]Electronic mail: mosna@ime.unicamp.br
[b]Electronic mail: asaa@ime.unicamp.br

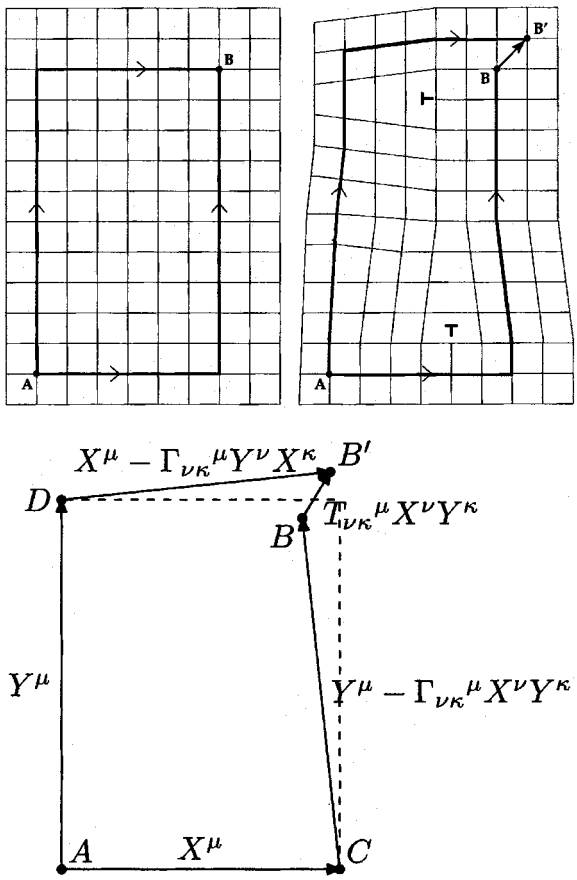

FIG. 1. We show, for illustrative purposes only, a lattice with two edge dislocation defects (upper right) and a reference one (upper left). A closed rectangular path in the reference lattice becomes unclosed in the presence of the defects. The vector $\overline{BB'}$, the so-called Burgers vector, measures how the path fails to close. In the associated geometrical description of the path generated by the (infinitesimal) vectors X^μ and Y^μ at the point A, the vector $\overline{CB}$ is obtained by parallel transport of Y^μ along X^μ, and $\overline{DB'}$ is obtained by transporting X^μ along Y^μ. The Burgers vector in this case is given by $\overline{BB'}=T_{\nu\kappa}{}^\mu X^\nu Y^\kappa$.

recovered, with the usual minimal action principle, provided that the trace of the torsion tensor be a gradient, $T_\mu=\partial_\mu\theta$, and that the usual volume element $\tau_0=\sqrt{g}\,\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^n$ be deformed to

$$\tau_\theta = e^\theta \tau_0. \tag{1}$$

In Ref. 3, Fiziev reinterpreted the model based in volume element (1) as a Transposed-Equi-Affine Theory of Gravity, since, as we will see, the covariant derivative of densities used in Ref. 10 can be related to a certain "transposed" connection. Such a transposed connection, however, is a highly artificial object, being generically not metric-compatible even when the initial connection is. Besides, at first glance, the very motivation of demanding equivalence between the MCP as applied to the action level and to the field equations may be contested on physical grounds. In fact, even in the case of General Relativity (where the connection is torsion-free), the naive minimal coupling between the electromagnetic field and gravity does not satisfy such equivalence requirement if one does not choose carefully in which set of equations the MCP should be applied. In such a case, the field equations contain partial derivatives of higher order, which renders the MCP, if applied directly to some field equations, ill-defined.[13] The usual solution for this kind of difficulty is to assume that the MCP should always be applied at the Lagrangian level.

The aim of this paper is to show that the modified volume element (1) follows from a more fundamental hypothesis, reinforcing its mathematical and physical relevance. We will show that the existence of the modified volume element (1) is a necessary and sufficient condition to render

the MCP well-defined even when considered solely at the action level. In particular, we will show that the results presented in Ref. 10 can be obtained without recourse to transposed connections. Our conclusions apply to any physical model where torsion is regarded as a dynamical entity that couples to the remaining fields via the MCP. In this way, one can expect that the results presented here can also be useful in the geometric theory of crystalline defects,[9,14] since the expressions for the free and interaction energies of defects and the equations for phonons and other test fields can be obtained by arguments very similar to the MCP.

We observe that the model proposed in Ref. 2 was carefully studied in Refs. 15 and 16. By considering solutions describing compact (neutron) stars and some solar system experiments, it was shown[15] that the predictions of the model[2] are in contradiction with General Relativity and, more important, with the available observational data. The propagating torsion model proposed in Ref. 2, therefore, is not a viable alternative to General Relativity. As we will see, the results presented here make the conclusions of Ref. 15 much stronger, since we will show that the existence of (1) is required to ensure the very consistency of the action formulation via the MCP. In other words, the results of Ref. 15 would allow us to conclude that the very reasonable requirement of consistency of the action formulation with the MCP *imply*, on account of the observational data, that the trace of the torsion tensor of space-time should vanish.

This work is organized as follows. The next section is a brief review of the mathematical framework necessary to set up the problem. Section III contains our main results, and the last section is devoted to some final remarks. Mathematical proofs are left to the Appendix, where we also discuss how the results presented here relate to the earlier approach of Refs. 2–5 and 10.

II. NOTATION

In order to introduce the problem, we briefly recall some definitions. For the sake of clarity, we employ here a more mathematically oriented notation, which slightly differs from that used in the original works.[2–5,10] Let $\mathcal{M}$ be an n-dimensional manifold. In the following, the components of the covariant derivative of a vector field $A=A^\nu e_\nu$, with respect to a local basis in $T\mathcal{M}$, are denoted by $D_\mu A^\nu$, so that $\nabla_\mu A=(D_\mu A^\nu)e_\nu$, with $D_\mu A^\nu=\partial_\mu A^\nu+\Gamma_{\mu\sigma}{}^\nu A^\sigma$. The components of the torsion tensor associated with the connection ∇,

$$T(X,Y)=\nabla_X Y-\nabla_Y X-[X,Y], \tag{2}$$

are given, in a coordinate basis, by

$$T_{\mu\nu}{}^\kappa=\Gamma_{\mu\nu}{}^\kappa-\Gamma_{\nu\mu}{}^\kappa. \tag{3}$$

Whenever the manifold $\mathcal{M}$ is endowed with a metric $g_{\mu\nu}$, the connection coefficients $\Gamma_{\mu\nu}{}^\kappa$ can be decomposed as

$$\Gamma_{\mu\nu}{}^\kappa=\left\{{\kappa\atop\mu\nu}\right\}+K_{\mu\nu}{}^\kappa+V_{\mu\nu}{}^\kappa, \tag{4}$$

where $\left\{{\kappa\atop\mu\nu}\right\}$ are the Christoffel symbols associated with the underlying Levi-Civita connection (uniquely defined metric-compatible connection without torsion on $(\mathcal{M},g)$),

$$K_{\mu\nu\kappa}=-\tfrac{1}{2}(T_{\nu\kappa\mu}+T_{\mu\kappa\nu}-T_{\mu\nu\kappa}) \tag{5}$$

is the contorsion tensor associated with ∇, and

$$V_{\mu\nu\kappa}=-\tfrac{1}{2}(D_\mu g_{\nu\kappa}+D_\nu g_{\kappa\mu}-D_\kappa g_{\mu\nu}) \tag{6}$$

provides a measure of the nonmetricity associated with ∇. Relevant quantities here are the trace of the above-defined tensors and their associated one-forms

$$\begin{aligned} T_\nu&=T_{\mu\nu}{}^\mu, \quad t=T_\nu\,\mathrm{d}x^\nu,\\ V_\nu&=V_{\mu\nu}{}^\mu, \quad v=V_\nu\,\mathrm{d}x^\nu. \end{aligned} \tag{7}$$

A volume element on an n-dimensional manifold $\mathcal{M}$ is a nowhere vanishing n-form on $\mathcal{M}$.[17] If $\mathcal{M}$ is endowed with a metric, an arbitrary volume element τ can be written as

$$\tau = f\tau_0, \tag{8}$$

where f is a nowhere vanishing smooth function on $\mathcal{M}$ and τ_0 is the canonical volume element

$$\tau_0 = \theta^1 \wedge \cdots \wedge \theta^n = \sqrt{g}\, \mathrm{d}x^1 \wedge \cdots \wedge \mathrm{d}x^n, \tag{9}$$

where $\{\theta^i\}$ is a local orthonormal basis.

III. MINIMAL COUPLING AND EQUIVALENT LAGRANGIANS

Let $\mathcal{L}$ be a Lagrangian density describing a given physical model defined on flat space or space-time $\mathcal{M}$. There is a natural equivalence relation $\sim$ on the set of such Lagrangians, defined by $\mathcal{L}_1 \sim \mathcal{L}_2$ if and only if $\mathcal{L}_1$ and $\mathcal{L}_2$ give rise to *identical* field equations on M. Except for scale transformations, we then have

$$\mathcal{L}_1 \sim \mathcal{L}_2 \Leftrightarrow \mathcal{L}_1 - \mathcal{L}_2 = \mathrm{div}(X) \tag{10}$$

for some vector field X, where, for flat $\mathcal{M}$,

$$\mathrm{div}(X) = \partial_\mu X^\mu. \tag{11}$$

This follows trivially from Gauss theorem, since integration of the Lagrangian density immediately yields

$$\int \mathrm{div}(X)\tau_0 = [\text{surface term}], \tag{12}$$

with no contribution to the Euler-Lagrange equations. We emphasize that, in the context of flat space (and of Special Relativity), *any choice* $\mathcal{L}$ in a given class $[\mathcal{L}]$ of Lagrangians leads to completely equivalent physical models.

Suppose now that the metric and connection on $\mathcal{M}$ become dynamical, describing in this way physical fields interacting with test particles or fields on $\mathcal{M}$. This would be the case, for instance, of General Relativity, in which gravity is described by a dynamical metric $g_{\mu\nu}$ with its associated Levi-Civita connection. Other examples are the Einstein-Cartan theory of gravity,[1] where torsion becomes an additional dynamical quantity, and the geometric theory of defects,[8,9] where curvature and torsion are related to the density of dislocations and disclinations of the crystalline lattice structure.

The MCP is the standard prescription to obtain the curved space equations from the flat space ones. It states that one needs merely to substitute ordinary derivatives by covariant ones and the Minkowskian metric tensor by its nonflat counterpart. It is worth noting that the MCP is used with success in nearly all physically relevant gauge theories, including General Relativity.[18]

Let us denote the Lagrangian density obtained from $\mathcal{L}$, via MCP, by $\mathcal{L}^*$. Similar to the flat-space case discussed above, the condition for $\mathcal{L}_1^*$ and $\mathcal{L}_2^*$ to be equivalent (i.e., to yield the same Euler-Lagrange equations) is given by

$$\mathcal{L}_1^* - \mathcal{L}_2^* = \mathrm{div}_\tau(X) \tag{13}$$

for some vector field X, with the definition of divergence now being given by[17]

$$(\mathrm{div}_\tau X)\tau = \pounds_X \tau, \tag{14}$$

where τ is a volume form on $\mathcal{M}$ and $\pounds_X$ denotes the Lie derivative along the vector field X. This is the most natural definition of divergence in this context, since $\pounds_X\tau = \mathrm{d}i_X\tau$ (where d denotes the exterior derivative and i_X the contraction by X)[17] leads directly to Gauss theorem

$$\int_{\mathcal{M}} \mathrm{div}_\tau(X)\tau = \int_{\partial\mathcal{M}} i_X\tau = [\text{surface term}]. \tag{15}$$

If $\mathcal{L}_1$ and $\mathcal{L}_2$ are equivalent Lagrangians in flat-space, we get, after applying the MCP,

$$\mathcal{L}_1 - \mathcal{L}_2 = \partial_\mu X^\mu \xrightarrow{\text{MCP}} \mathcal{L}_1^* - \mathcal{L}_2^* = D_\mu X^\mu. \tag{16}$$

Therefore, if the equivalence class of Lagrangians $[\mathcal{L}]$ is required to be preserved under the MCP, we need to have

$$D_\mu X^\mu = \mathrm{div}_\tau(X), \tag{17}$$

or, equivalently,

$$\pounds_X\tau = (D_\mu X^\mu)\tau. \tag{18}$$

The necessary and sufficient conditions to the existence of solutions for (17) can be obtained from the following proposition, whose (simple) proof is left to the Appendix.

Proposition 1: *Let $\mathcal{M}$ be a differentiable manifold endowed with a metric g and a connection ∇. Let $\tau=f\tau_0$ be a volume form on $\mathcal{M}$. Then, for every vector field X on $\mathcal{M}$,*

$$D_\mu X^\mu = \mathrm{div}_\tau X + t(X) + v(X) - X(\ln f),$$

where t and v are defined in Eq. (7).

MCP in affine manifolds

In order to illustrate the previous results, let us recall their application to the case of the metric-affine theory of gravity,[19] where space-time is represented by a manifold endowed with a connection with possibly nonzero curvature, torsion, and nonmetricity. We note that this contains, as a particular case, the Einstein-Cartan theory of gravity, where the associated connection presents curvature and torsion but is still metric-compatible (i.e., $D_\kappa g_{\mu\nu}=0$).

For this case, Proposition 1 implies that the canonical volume form τ_0 yields

$$D_\mu X^\mu - \mathrm{div}_{\tau_0} X = (T_\mu + V_\mu)X^\mu. \tag{19}$$

It follows from our previous discussion that equivalent Lagrangian densities of Special Relativity will be mapped, via MCP, to *nonequivalent* Lagrangian densities in the corresponding nonflat space-time. Therefore, since there is no canonical representative of $[\mathcal{L}]$ in Special Relativity, the MCP turns out to be essentially ill-defined in this context.

This difficulty can be circumvented with the help of Proposition 1 itself. The above-mentioned incompatibility arises only when $D_\mu X^\mu \neq \mathrm{div}_\tau X$. However, admitting a more general volume form $\tau=f\tau_0$ on $\mathcal{M}$, one can get $D_\mu X^\mu=\mathrm{div}_\tau X$ by choosing f such that

$$t(\partial_\mu) + v(\partial_\mu) - \partial_\mu \ln f = 0, \tag{20}$$

which is equivalent to

$$T_\mu + V_\mu = \partial_\mu\theta, \quad \tau = e^\theta\tau_0. \tag{21}$$

Therefore, the MCP is well defined (preserves equivalence classes of Lagrangians) precisely when:

1. $t+v$ is an exact form, say $t+v=d\theta$, and

2. the volume element on $\mathcal{M}$ is given by $\tau = e^{\theta}\tau_0$.

Again, since in the context of flat space (Special Relativity) there is no canonical choice of representative of a given class of Lagrangians, our results imply that the MCP is well defined only in the presence of the modified volume element (1).

This is our main result: in order to preserve a given class $[\mathcal{L}]$ of Lagrangians under the MCP, one must have $T_\mu + V_\mu = \partial_\mu \theta$ and, obligatorily, to use the modified volume element (1). If the sum of traces $T_\mu + V_\mu$ is not a gradient, the MCP turns out to be ill-defined, since it produces non-equivalent theories out of equivalent flat-space Lagrangians, even at the classical level.

The λ-symmetry

In an affine manifold, the Riemann tensor is invariant under the transformation

$$\Gamma_{\mu\nu}{}^{\kappa} \to \Gamma_{\mu\nu}{}^{\kappa} + \delta^{\kappa}_{\nu}\partial_\mu \lambda, \tag{22}$$

where λ is an arbitrary function. This is the so-called λ-symmetry,[20] introduced by Einstein in his pioneering work on unified field theory, which has been proved to be very useful in the analysis of affine theories of gravity.[21] In a λ-invariant theory, the function λ can be properly chosen in order to cancel some parts of the torsion tensor and/or of the nonmetricity, simplifying the overall analysis. Under (22), the torsion tensor and $V_{\mu\nu\kappa}$ are changed as

$$\begin{aligned} T_{\mu\nu\kappa} &\to T_{\mu\nu\kappa} + (g_{\kappa\nu}\partial_\mu \lambda - g_{\kappa\mu}\partial_\nu \lambda), \\ V_{\mu\nu\kappa} &\to V_{\mu\nu\kappa} + (g_{\kappa\nu}\partial_\mu \lambda + g_{\kappa\mu}\partial_\nu \lambda - g_{\mu\nu}\partial_\kappa \lambda), \end{aligned} \tag{23}$$

implying to their traces

$$T_\nu \to T_\nu - (n-1)\partial_\nu \lambda, \quad V_\nu \to V_\nu + n\partial_\nu \lambda. \tag{24}$$

One sees from (23) that a λ-transformation does not preserve the spaces of symmetric or metric-compatible connections. However, the condition ensuring the consistency of MCP, namely that $T_\mu + V_\mu$ be a gradient, is indeed preserved under (22). The Einstein-Hilbert action is, obviously, also preserved under (22). Hence, provided that the matter content action is also λ-invariant, the λ-transformation will map distinct solutions in a metric-affine theory of gravity governed by the Einstein-Hilbert action, preserving all the isometries if λ is properly chosen.

An interesting consequence arises from the transformation of the modified volume element under a λ-transformation,

$$e^{\theta}\tau_0 \to e^{\theta+\lambda}\tau_0. \tag{25}$$

Starting with, for instance, a Riemann-Cartan manifold with a gradient torsion trace and an Einstein-Hilbert action with the modified volume element, it is possible to choose $\lambda = -\theta$ and to get an equivalent theory, where the MCP is also well-defined, formulated in an affine manifold (the connection is not metric-compatible anymore) but with the usual volume element. In other words, in this new manifold, $D_\mu X^\mu = \mathrm{div}_{\tau_0} X$ for any vector field X.

IV. FINAL REMARKS

Before discussing possible applications of the results presented here to the study of crystalline defects, let us recall how they reinforce the results of Ref. 15 about the inadequacy of the propagating torsion model proposed in Ref. 2 to explain the available observational data. The modified volume element (1) was introduced in the model of Ref. 2 by means of exclusively geometrical arguments, and, hence, there is no free parameter associated with the field θ, which is responsible for the propagating components of the torsion. Moreover, by employing the MCP, no extra parameters, besides the Newtonian constant G, should arise in any gravitational model. Thus, the only way of fitting the available observational data described in Ref. 15 is to have θ constant,

leading to the already mentioned conclusion that the results of Ref. 15 would allow us to deduce that the observational data and the very reasonable requirement of consistency of the action formulation with the MCP *imply* that the trace of the torsion tensor of space-time should vanish.

Condensed matter is a vast subject but, to the best of our knowledge, the ideas presented here were not yet applied to the study of crystalline defects, which possess a geometrical description since the seminal works of Kondo in the fifties (see, for references, Ref. 8). The physics of crystalline defects is a promising arena to test experimentally the ideas of the last sections, with special emphasis on new effects that might be associated with the modified volume element (1). The first conclusion about the modified volume element in this context is that, in principle, it has no relation to the *real* volume (area, in this case) of the polygon depicted in Fig. 1. As discussed in Ref. 8, contributions to the elementary area coming from the Burgers vector are of higher order and should vanish in the linear continuum limit. Incidentally, for X^μ and Y^μ orthogonal in a Riemann-Cartan manifold ($D_\kappa g_{\mu\nu}=0$), the area of the polygon of Fig. 1 is given, up to higher order terms, by

$$A = |X||Y|\left(1 - \tfrac{1}{2}(X^\mu + Y^\mu)T_\mu\right), \tag{26}$$

from where one sees that, despite being unclosed, its area coincides with the area of the parallelogram with sides X^μ and Y^μ if $T_\mu=0$. However, the modified volume element (1) cannot represent a physical area since any geometrical property of the crystalline lattice should be invariant under a transformation of the type $\theta\rightarrow\theta+\Lambda$, with constant Λ, and the modified volume element, under this transformation, behaves as $\tau\rightarrow e^{\Lambda}\tau$. This behavior, on the other hand, is allowed in the minimal action formulation, since, as was already noted, a scale transformation of a Lagrangian preserves the dynamics. The dynamics of defects, on the other hand, are governed by their free energy, which can be expressed by means of a Lagrangian density related to the Einstein-Hilbert Lagrangian.[14,22] The use of the modified volume element in the action of the free energy would define a new dynamics to the torsion and metric tensors, analogous to that proposed in Ref. 2 in the context of Einstein-Cartan theory of gravity. An immediate consequence would be the propagation of the trace of the torsion tensor and, consequently, of the associated Burgers vector.

The free energy plays the role of the kinetic term in the geometrical action formulation of defects. However, kinetic terms are not, *a priori*, specified by the MCP. Our analysis seems more suitable to the study of fields/particles propagating on the crystalline lattice, such as phonons, impurities, and vacancies.[14] If the perturbation energy associated with these objects is small enough, their backreaction on the lattice may be ignored, and they can be considered *test* fields. Phonons are nothing more than small elastic (sound) excitations in the crystal; in the geometrical description, they correspond to gauge independent linearized perturbations of the metric.[9] On the other hand, one can also consider impurities or vacancies moving on the background medium defined by the solid with crystalline defects. The effect of the background on such test fields/particles can be gotten from the MCP by demanding that the corresponding equations for phonons, impurities, and vacancies be obtained, from the equations for the regular lattice, by changing the ordinary derivative to the covariant one and the Euclidean metric to the metric associated with the background medium. With use of MCP and the modified volume element, testable predictions for the propagation of phonons, impurities, and vacancies could arise. For instance, the modified volume element should affect the wave functions and energy spectrum of impurities and vacancies[14] in the presence of a crystalline defect. The occurrence of bound states due to dislocations[23] can also be studied in light of the present results. One probably, however, needs to go beyond the eikonal approximation for the test fields, since in this case the trajectory of the associated particle is assumed to be a geodesic curve,[14] a good approximation for high-frequency fields, but with no contributions from the torsion tensor. These points are now under investigation.

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APPENDIX

Let us first discuss how the results of this paper relate to the earlier approach of Refs. 2–5 and 10. Unlike the approach presented here, the analysis of these works explicitly uses the concept of covariant derivative of densities, which are defined as follows. Let h be a scalar density on $\mathcal{M}$. One can define the covariant derivative of h in two different ways:

$$D_\mu h = \partial_\mu h - \Gamma_{\mu\kappa}{}^{\kappa} h, \tag{A1}$$

or

$$\tilde{D}_\mu h = \partial_\mu h - \Gamma_{\kappa\mu}{}^{\kappa} h. \tag{A2}$$

The definition (A1) can be called the *usual* covariant derivative, since, as we show in the following,

$$\nabla_X(h\, \mathrm{d}x^1 \wedge \cdots \wedge \mathrm{d}x^n) = [X^\mu D_\mu h]\mathrm{d}x^1 \wedge \cdots \wedge \mathrm{d}x^n. \tag{A3}$$

The covariant derivative (A2), used also, for instance, in Ref. 24, is the so-called transposed derivative,[3] since it can be interpreted as the covariant derivative with respect to the transposed connection $\tilde{\Gamma}_{\mu\nu}{}^{\kappa} = \Gamma_{\nu\mu}{}^{\kappa}$ (see, in this context, the volume-preserving connection introduced in Ref. 19). Note that, according to Eq. (3), $\tilde{D}_\mu h = D_\mu h$ provided that the trace of the torsion tensor vanishes so that, in this case, no ambiguity concerning the definition of the covariant derivative of densities arises. The covariant derivative (A2) is closer to the *Lie derivative* on $\mathcal{M}$, since it satisfies, as we will see,

$$\pounds_X(h\, \mathrm{d}x^1 \wedge \cdots \wedge \mathrm{d}x^n) = [(D_\mu X^\mu)h + X^\mu(\tilde{D}_\mu h)]\mathrm{d}x^1 \wedge \cdots \wedge \mathrm{d}x^n. \tag{A4}$$

The mathematical property that distinguishes the volume element (1) in Ref. 10 is that, whereas the canonical volume element (9) is covariantly constant with respect to the usual derivative,

$$D_\mu \sqrt{g} = 0, \tag{A5}$$

the volume element (1) is covariantly constant with respect to the transposed derivative,

$$\tilde{D}_\mu(e^\theta \sqrt{g}) = 0, \tag{A6}$$

provided that

$$T_\mu + V_\mu = \partial_\mu \theta. \tag{A7}$$

By comparing with Eq. (A4), we see that (18) holds if and only if one chooses a volume form $\tau = f\tau_0$ such that

$$\tilde{D}_\mu(f\sqrt{g}) = 0, \tag{A8}$$

which has a solution only if $T_\mu + V_\mu = \partial_\mu \theta$ and $f = e^\theta$.[10] This shows how the earlier approach of Refs. 2–5 and 10 relates to the present work, which, as discussed in the previous sections, is based on weaker physical assumptions.

We end by providing proofs of identities (A3) and (A4), and of Proposition 1. Identity (A3) can be proved as follows:

$$\nabla_X(h\,\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^n)=(\nabla_X h)\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^n+h\sum\nolimits_\kappa \mathrm{d}x^1\wedge\cdots\wedge\nabla_X\mathrm{d}x^\kappa\wedge\cdots\wedge\mathrm{d}x^n$$
$$=X(h)\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^n+h\sum\nolimits_\kappa \mathrm{d}x^1\wedge\cdots\wedge(-X^\mu\Gamma_{\mu\nu}{}^\kappa\,\mathrm{d}x^\nu)\wedge\cdots\wedge\mathrm{d}x^n$$
$$=X^\mu(\partial_\mu h-\Gamma_{\mu\kappa}{}^\kappa)\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^n. \tag{A9}$$

As for (A4), since $\pounds_X$ and d commute, we have

$$\pounds_X\,\mathrm{d}x^\kappa=\mathrm{d}\pounds_X x^\kappa=\mathrm{d}X^\kappa=\partial_\nu X^\kappa\,\mathrm{d}x^\nu, \tag{A10}$$

which leads to

$$\pounds_X(h\,\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^n)=\pounds_X(h)\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^n+h\sum\nolimits_\kappa \mathrm{d}x^1\wedge\cdots\wedge\pounds_X\,\mathrm{d}x^\kappa\wedge\cdots\wedge\mathrm{d}x^n \tag{A11}$$

$$=[X(h)+h\partial_\kappa X^\kappa]\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^n \tag{A12}$$

$$=[hD_\mu X^\mu+X^\mu(\partial_\mu h-h\Gamma_{\kappa\mu}{}^\kappa)]\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^n. \tag{A13}$$

Finally, Proposition 1 can be proved as follows. We first notice that

$$D_\kappa X^\kappa=\partial_\kappa X^\kappa+\Gamma_{\kappa\mu}{}^\kappa X^\mu \tag{A14}$$

$$=\partial_\kappa X^\kappa+\left(\left\{{\kappa\atop\kappa\mu}\right\}+K_{\kappa\mu}{}^\kappa+V_{\kappa\mu}{}^\kappa\right)X^\mu \tag{A15}$$

$$=\partial_\kappa X^\kappa+\left(\partial_\kappa\ln\sqrt{g}+T_\kappa+V_\kappa\right)X^\kappa. \tag{A16}$$

On the other hand, it follows from Eq. (A12) that

$$\pounds_X\left(f\sqrt{g}\,\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^n\right)=\left(X^\kappa\partial_\kappa\ln(f\sqrt{g})+\partial_\kappa X^\kappa\right)\tau. \tag{A17}$$

Thus, from definition (14),

$$\mathrm{div}_\tau X=X^\kappa\partial_\kappa\ln(f\sqrt{g})+\partial_\kappa X^\kappa, \tag{A18}$$

which finally yields

$$D_\kappa X^\kappa=\mathrm{div}_\tau X+\left(T_\kappa+V_\kappa-\partial_\kappa\ln f\right)X^\kappa. \tag{A19}$$

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Soldered bundle background for the de Sitter top

J. Armenta
Departamento de Investigación en Física de la Universidad de Sonora, 83000 Hermosillo Sonora, México and Instituto Tecnológico y de Estudios Superiores de Monterrey, Campus Obregón, Apdo. Postal 622, 85000 Cd. Obregón Sonora, México

J. A. Nieto[a)]
Facultad de Ciencias Físico-Matemáticas de la Universidad Autónoma de Sinaloa, 80010 Culiacán Sinaloa, México

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We prove that the mathematical framework for the de Sitter top system is the de Sitter fiber bundle. In this context, the concept of soldering associated with a fiber bundle plays a central role. We comment on the possibility that our formalism may be of particular interest in different contexts including MacDowell-Mansouri theory, two time physics, and oriented matroid theory. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2121227]

In 1974, Hanson and Regge proposed a Lagrangian theory for a relativistic top.[1,2] One year later the importance and advantage of this formulation was shown when the equations of motion of a top in a gravitational field were derived by using the equivalence gravitational principle.[3] Furthermore, one of the original motivations for the Lagrangian formulation of the top was to quantize the system by means of Dirac's method for constraint Hamiltonian systems. Moreover, with the idea of making supersymmetric the Lagrangian of the system the square root of a bosonic top was proposed.[4] In this direction it was shown that the quantum top also allows a BFV[5] and BRST quantization.[6] It turned out that these pioneer developments motivated a generalization of the original theory to the so-called superstringtop theory[7,8] which combines, in a Lagrangian context, the concepts of string and top.

Recently, the de Sitter top theory[9] has been proposed (see also Ref. 10) which is a higher dimensional Lagrangian formulation of a special kind of a spherical relativistic top characterized by a Regge trajectory constraint of the de Sitter form $m^2+(1/2r^2)\Sigma^2+m_0^2=0$, where m is the mass of the top, Σ is the internal angular momentum, and r and m_0 are constants. One of the interesting aspects of the de Sitter top system is that by using the Kaluza-Klein mechanism[11,12] the equation of motion of the top in a gravitational field can be derived. Since Kaluza-Klein theory is closely linked to the fiber bundle concept[13,14] one should expect a geometric formulation of the de Sitter top in terms of such a concept. Although this idea has been outlined in Refs. 9 and 10 the precise connection between fiber bundle structure and the de Sitter top needs to be addressed. In this work, we claim that the soldered fiber bundle structure is the natural mathematical framework for a formal description of the de Sitter top. It turns out that the soldered bundle concept has been extensively used by Drechsler (see Ref. 15, and references therein) in particle physics. In particular, Drechsler has proposed a gauge theory for extended elementary objects based in the soldered bundle concept. These applications of the soldered bundle concept are, however, more focused on a gauge field scenario of the systems[16,17] rather than in a gravitational context. Moreover, part of the motivation of these applications are at the level of hadrons[18–21] and not a deeper level as is the case of the de Sitter top. Nevertheless, in this work we show that some of the mathematical tools in the soldered bundle theory can be used for describing the de Sitter top. We complement our

a)Electronic mail: nieto@uas.uasnet.mx

analysis of the de Sitter top by observing that the soldered bundle concept may provide the mathematical tool to clarify some aspects of the MacDowell-Mansouri formalism[22] (see also Ref. 23) and two time physics.[24]

Let us start writing the de Sitter top Lagrangian[9]

$$L = -m_0\left(-\tfrac{1}{2}\omega_M^{AB}\omega_{NAB}\dot{x}^M\dot{x}^N\right)^{1/2}, \tag{1}$$

where m_0 is a constant measuring the inertia of the system and $\dot{x}^M=(\mathrm{d}/\mathrm{d}\tau)x^M$, with M,N running from 0 to 9 and τ is an arbitrary parameter. Here, $\omega_M^{AB}=-\omega_M^{BA}$ denotes a connection associated with the de Sitter group SO(1,4) [or anti de Sitter group SO(2,3)]. Indeed, ω_M^{AB} is determined by the ansatz

$$\omega_M^{AB} = \begin{pmatrix} \omega_\mu^{5a}(x) & \omega_\mu^{ab}(x) \\ 0 & \omega_i^{ab}(y) \end{pmatrix}. \tag{2}$$

When writing (2) the coordinates x^M were separated in the form (x,y), with x corresponding to the four-dimensional base manifold M^4 and y parametrizing the group manifold SO(1,4). The Lagrangian (1) is interesting because it leads to a Regge trajectory constraint of the de Sitter form $m^2+(1/2r^2)\Sigma^2+m_0^2=0$ (see Refs. 1 and 2 and also Refs. 25 and 26) connecting the mass m and the spin Σ of the system.

Consider the antisymmetric pair $[ab]$ of the four valued indices a,b in the form $a'=([12],[13],[14],[23],[24],[34])$. Using this notation one discovers that if one makes the identifications ($\sim$),

$$\omega_\mu^{5a}(x) \sim e_\mu^a(x), \tag{3}$$

$$\omega_\mu^{ab}(x) \sim E_\mu^{a'}(x), \tag{4}$$

$$\omega_i^{ab}(y) \sim E_i^{a'}(y), \tag{5}$$

and

$$\omega_M^{AB} \to E_M^{\hat{A}}, \tag{6}$$

then the ansatz (2) becomes

$$E_M^{\hat{A}} = \begin{pmatrix} e_\mu^a(x) & E_\mu^{a'}(x) \\ 0 & E_i^{a'}(y) \end{pmatrix}, \tag{7}$$

which may be recognized as the typical form of the Kaluza-Klein ansatz.[11,12] This suggests introducing the metric

$$\gamma_{MN} = E_M^{\hat{A}}E_N^{\hat{B}}\eta_{\hat{A}\hat{B}}, \tag{8}$$

which according to (7) can be separated in the form

$$\gamma_{\mu\nu} = g_{\mu\nu} + E_\mu^{a'}E_\nu^{b'}\eta_{a'b'},$$

$$\gamma_{\mu i} = E_\mu^{a'}E_i^{b'}\eta_{a'b'}, \tag{9}$$

$$\gamma_{ij} = E_i^{a'}E_j^{b'}\eta_{a'b'} = g_{ij}(y),$$

where

$$g_{\mu\nu}(x) = e^a_\mu(x) e^b_\nu(x)\, \eta_{ab}. \tag{10}$$

Here, η_{ab} and $\eta_{a'b'}$ are flat metrics corresponding to M^4 and B, respectively.

From of the point of view of Kaluza-Klein theory the splitting (9) is the result of compactifying a $4+D$-dimensional space-time manifold M^{4+D} in the form $M^{4+D} \to M^4 \times B$, where M^4 is a four-dimensional base space manifold and B is a group manifold whose dimension is D. In the case of the de Sitter top it is not clear what the meaning of M^{4+D} and B is. Moreover, the meaning of the identification (3) is unclear. One may choose M^{4+D} as SO(1,4) and B as SO(1,3) but in this case M^4 will be completely determined without using the gravitational field equations. Thus, although the identifications (3)–(6) are suggestive they are not complete requiring a deeper analysis. We shall show that these aspects of the de Sitter top can be clarified through the so-called *soldered fiber bundle* notion. In order to achieve our goal we first observe that the object ω^{AB}_M may be identified with the fundamental one-form

$$\omega = g^{-1} dg + g^{-1} \Omega g, \tag{11}$$

where

$$\omega = \tfrac{1}{2} \omega^{AB}_M S_{AB} \mathrm{d}x^M \tag{12}$$

and

$$\Omega = \tfrac{1}{2} \omega^{AB}_\mu S_{AB} \mathrm{d}x^\mu. \tag{13}$$

Here, $g \in \mathrm{SO}(1,4)$ and S_{AB} are the generators of the de Sitter group SO(1,4) [or anti de Sitter group SO(2,3)]. In turn, (13) can be understood as a one-form connection in the cotangent space $T^*(P)$, where P is a principal bundle $P(M^4, \mathrm{SO}(1,4))$. Locally, $P(M^4, \mathrm{SO}(1,4))$ looks like $M^4 \times \mathrm{SO}(1,4)$ but once again this picture is incomplete in the sense that it leaves without answer the meaning of the relation (3). Nevertheless, this analysis motivates one to find a framework beyond the simple principal bundle $P(M^4, \mathrm{SO}(1,4))$.

In general, it is well known that given a principal bundle $P(M,G)$ one may construct an associated fiber bundle $E(M,F,G)$ where F is a fiber manifold and conversely, a fiber bundle $E(M,F,G)$ naturally induces a principal bundle $P(M,G)$ associated with it (see Ref. 27, Sec. 9.4.2, for details). Thus, the principal bundle $P(M^4, \mathrm{SO}(1,4))$ may have an associated fiber bundle $E(M^4, F, \mathrm{SO}(1,4))$. In principle F can be any vector space but in the case of the de Sitter top one may think of SO(1,4) as a group acting transitively over F. Moreover, by Inönü-Wigner contraction one should expect that de Sitter top is reduced to the usual relativistic top which is invariant under the Lorentz transformations determined by the Lorentz group SO(1,3) (see Ref. 2). Now, since SO(1,3) is an isotropy subgroup of SO(1,4) this suggests considering the coset space $\mathrm{SO}(1,4)/\mathrm{SO}(1,3)$. Applying a well-known theorem (see Ref. 28, Sec. 1.6, and see also Ref. 29) one can establish the homeomorphism $F \cong \mathrm{SO}(1,4)/\mathrm{SO}(1,3)$. Therefore, the fiber bundle which we are interested to relate to the de Sitter top is

$$E(M^4, F \cong \mathrm{SO}(1,4)/\mathrm{SO}(1,3), \mathrm{SO}(1,4)). \tag{14}$$

This is a fiber bundle of the Cartan type possessing as a fiber de Sitter space $dS_4 \equiv F$ which is homeomorphic to the noncompact coset space

$$\mathrm{SO}(1,4)/\mathrm{SO}(1,3).$$

Since $\dim G/H = \dim G - \dim H$ we find that

$$\dim \mathrm{SO}(1,4)/\mathrm{SO}(1,3) = \dim \mathrm{SO}(1,4) - \dim \mathrm{SO}(1,3) = 4$$

and therefore the dimension of dS_4 is four, the same as M^4. This result is an indication that the bundle (14) may admit a soldered fiber bundle structure. But before we present the definition of a

soldered fiber bundle let us motivate further the idea of soldering in connection with the de Sitter top.

Let us introduce a gauge parameter $\lambda=\frac{1}{2}\lambda^{AB}(x)S_{AB}$. The transformation associates with ω, given in (12), can be written as

$$\omega' = g\omega g^{-1} + g^{-1}dg, \tag{15}$$

which as an infinitesimal gauge transformation reads as

$$\delta\omega = \mathrm{d}\lambda + [\lambda, \omega]. \tag{16}$$

In components (16) leads to the expression

$$\delta\omega^{AB} = d\lambda^{AB} + \omega^{AC}\lambda^{B}_{C} + \omega^{AC}\lambda^{B}_{C}, \tag{17}$$

which can be separated in the form

$$\delta\omega^{5a} = D\lambda^{5a} + \omega^{5c}\lambda^{a}_{c} \tag{18}$$

and

$$\delta\omega^{ab} = D\lambda^{ab} + \omega^{a5}\lambda^{b}_{5} + \omega^{b5}\lambda^{a}_{5}. \tag{19}$$

Here, D means covariant derivative with ω^{ab} as a connection. Thus, if we set

$$\omega^{5a}_{\mu} = e^{a}_{\mu} \tag{20}$$

one sees that the expressions (18) and (19) lead to

$$\delta e^{a}_{\mu} = D_{\mu}\xi^{a} + e^{c}_{\mu}\lambda^{a}_{c} \tag{21}$$

and

$$\delta\omega^{ab}_{\mu} = D_{\mu}\lambda^{ab} + e^{a}_{\mu}\xi^{b} - e^{b}_{\mu}\xi^{a}, \tag{22}$$

respectively. But formulas (21) and (22) indicate that neither e^{a}_{μ} nor ω^{ab}_{μ} transform properly under Lorentz transformations SO(1,3) and therefore in general they cannot be identified with the Lorentz tetrad and connection, respectively. For this to be possible it is required that the parameter ξ^{a} vanishes in (21) and (22). In turn this implies that the de Sitter group SO(1,4) is broken leading to the Lorentz group SO(1,3). To set the parameter ξ^{a} equal to zero in a consistent way is not so simple and in fact requires one to introduce the soldering concept which we shall now formally define.

A bundle $E(M, F=G/H, G)$ over a base manifold M with homogeneous fiber $F=G/H$ and associated principle bundle $P(M, G)$ is soldered if[15]

(i) G acts transitively on F,
(ii) $\dim F = \dim M$,
(iii) E admits a global cross section σ and the structural group G of E can be reduced to H.
(iv) The tangent bundle $T(M)$ over M and the bundle $T(E)=T(F)$ of all tangent vectors to F at the section σ are isomorphic.

It is clear that the bundle $E(M^4, F\cong \mathrm{SO}(1,4)/\mathrm{SO}(1,3), \mathrm{SO}(1,4))$ which we try to associate to the de Sitter top satisfies (i), (ii), and (iii). The only remaining point is to impose condition (iv). It turns out that (iv) is equivalent to the two properties[15]

(a) $\theta(X')=0$ for $X' \in T(P'(M,H))$ if and only if X' is vertical.

(b) $\theta(dR_h X') = h^{-1} X' h$ for $X' \in T(P'(M,H))$ and $h \in H$,

which are satisfied for the so-called one-form of soldering θ. The reason to be interested in the one-form θ is because a connection ω in $P(M,G)$ can be written in terms of a connection in $P'(M,H)$ and the soldering one-form θ as follows:

$$\omega = \omega' + \theta. \tag{23}$$

Actually, the equivalence between (iv) and (a)–(b) is achieved when one assumes the reductive algebra

$$[\mathcal{L}(H), \Lambda] \subseteq \Lambda, \tag{24}$$

associated with the decomposition $\mathcal{L}(G) = \mathcal{L}(H) \oplus \Lambda$ of the Lie algebra of G, where $\mathcal{L}(H)$ corresponds to the subalgebra of H and Λ is required to be a vector subspace of G with dimension $\dim M = \dim G - \dim H$. In fact such equivalence is obtained when one assumes the existence of Λ-valued one-form θ satisfying (a) and (b) (see Refs. 15 and 30 for details). In connection with (23) two observations are necessary. First, the decomposition (23) does not require the additional condition

$$[\Lambda, \Lambda] \subseteq \mathcal{L}(H), \tag{25}$$

implying that $F \cong \mathrm{SO}(1,4)/\mathrm{SO}(1,3)$ is a symmetric space, and second, since ω is a $\mathcal{L}(G)$-valued one-form in the cotangent bundle $T^*(P)$ we can write $\omega = \omega(x,y)$, where the coordinates x and y parametrize locally M and F, respectively, and consequently, in general, we should have $\omega' = \omega'(x,y)$ and $\theta = \theta(x,y)$. However, (a) and (b) imply that we can write $\theta = \theta(x)$.

Let us now specialize (23) to the case of the de Sitter fiber bundle $E(M^4, F \cong \mathrm{SO}(1,4)/\mathrm{SO}(1,3), \mathrm{SO}(1,4))$. First let us observe that since S_{AB} are the generators of the de Sitter group SO(1,4) (or anti de Sitter group SO(2,3)) we can write the algebra

$$-i[S_{AB}, S_{CD}] = \eta_{AC} S_{BD} - \eta_{AD} S_{BC} + \eta_{BD} S_{AC} - \eta_{BC} S_{AD}, \tag{26}$$

where $\eta_{AC} = \mathrm{diag}(-1,1,1,1,1)$. From (26) we get

$$-i[S_{ab}, S_{cd}] = \eta_{ac} S_{bd} - \eta_{ad} S_{bc} + \eta_{bd} S_{ac} - \eta_{bc} S_{ad}, \tag{27}$$

$$-i[S_{5b}, S_{cd}] = \eta_{bd} S_{5c} - \eta_{bc} S_{5d}, \tag{28}$$

and

$$-i[S_{5b}, S_{5d}] = S_{bd}. \tag{29}$$

Thus, we conclude that S_{ab} are the generators of the subgroup SO(1,3) and that (28) is in agreement with (24). This in turn implies that the SO(1,4) valued one-form connection ω given in (12) can be written in terms of a SO(1,3) valued one-form connection ω^{ab} and the one-form ω^{5b} as

$$\omega = \tfrac{1}{2} \omega^{ab} S_{ab} + \omega^{5b} S_{5b}. \tag{30}$$

Comparing (30) with (23) one discovers that one can make the identifications $\omega'^{ab} = \omega^{ab}$ and $\theta^b = \omega^{5b}$. Since in general $\omega^{AB} = \omega^{AB}(x,y)$ [see expressions (11) and (12)], one finds that ω^{AB} can be split into the form

$$\theta^a = \omega_\mu^{5a} \mathrm{d}x^\mu + \omega_i^{5a} \mathrm{d}y^i \tag{31}$$

and

$$\omega^{ab} = \omega_{\mu}^{ab} \mathrm{d}x^{\mu} + \omega_{i}^{ab} \mathrm{d}y^{i}. \tag{32}$$

Now, the condition (a)–(b) for θ means that the soldering concept allows one to set $\omega_i^{5a}=0$ and therefore we have

$$\theta^{a} = \omega_{\mu}^{5a} \mathrm{d}x^{\mu}. \tag{33}$$

This is consistent with (iv) and in fact one should be able to write θ^a in terms of the base $e_\mu^a \in T(M^4)$. In particular one can set $\theta_\mu^a = e_\mu^a$, that is, $\omega_\mu^{5a} = e_\mu^a$. Consequently, one discovers that the complete connection ω_M^{AB} can be written as

$$\omega_M^{AB} = \begin{pmatrix} e_\mu^a(x) & \omega_\mu^{ab}(x,y) \\ 0 & \omega_i^{ab}(x,y) \end{pmatrix}, \tag{34}$$

which by using the Kaluza-Klein mechanism can be reduced to (2). Summarizing, we have explicitly shown that the geometrical framework for the de Sitter top is the de Sitter soldering fiber bundle $E(M^4, F \cong \mathrm{SO}(1,4)/\mathrm{SO}(1,3), \mathrm{SO}(1,4))$ as Fukuyama had anticipated.[9]

Until now we have focused more on the de Sitter top description determined by the line element (1) rather than in the dynamics of the background itself where the system moves. In other words, besides the mathematical framework for the de Sitter top one may be interested in the field equations which govern the evolution of the connection ω_M^{AB} given in (2). Since e_μ^a and $\omega_M^{ab}(x)$ are considered as independent variables one may think in Einstein-Cartan theory (linear in the curvature), as the more appropriate candidate. However, there exists another gravitational theory which seems to be closer to the spirit of the ansatz (2) than the Einstein-Cartan theory. We refer to the so-called MacDowell-Mansouri theory[22] (see also Ref. 23) which is one of the closest proposals for achieving a gauge theory for gravity. The idea in this theory is precisely to consider the field variables e_μ^a and $\omega_\mu^{ab}(x)$ as part of a bigger connection $\omega_\mu^{AB}(x)$ associated with the de Sitter group SO(1,4). In fact, by taking $e_\mu^a = \omega_\mu^{5a}(x)$ one verifies that the action

$$S = \int \mathrm{d}^4 x \varepsilon^{\mu\nu\alpha\beta} \mathcal{R}_{\mu\nu}^{ab} \mathcal{R}_{\alpha\beta}^{cd} \varepsilon_{abcd}, \tag{35}$$

where

$$\mathcal{R}_{\mu\nu}^{ab} = R_{\mu\nu}^{ab} + e_\mu^a e_\nu^b - e_\mu^b e_\nu^a, \tag{36}$$

with $R_{\mu\nu}^{ab}$ the curvature in terms of ω_μ^{ab}, leads to the two terms: the Euler-Pontrjagin topological invariant and the Einstein Hilbert action with a cosmological constant. One observes that the action (35) is intrinsically four dimensional and therefore there seems to be enough room for the additional part $\omega_i^{ab}(y)$. However, recently[31] in an effort to generalize the Ashtekar formalism to higher dimensions a generalization of (35) to eight dimensions has been proposed which may allow full background description of the connection (2). In fact, in Ref. 31 it was proposed the action

$$S = \int d^8 x \eta^{MNRS} \mathcal{R}_{MN}^{\hat{A}\hat{B}} \mathcal{R}_{MN}^{\hat{C}\hat{D}} \eta_{\hat{A}\hat{B}\hat{C}\hat{D}}, \tag{37}$$

where the object η^{MNRS} is connected with the algebra of octonions (see Ref. 31 for details). Our conjecture is that the background field equations, where the de Sitter top evolves, can be derived from the action (37). Assuming that the action (37) describes the evolution of the de Sitter connection $\omega_M^{\hat{A}\hat{B}}$ we observe that an interesting possibility arises. This has to do with the fact that a theory based on the action (30) would lead to a de Sitter vacuum solution for the base manifold M^4 rather than the Minkowski space. Consequently, the de Sitter soldering fiber bundle $E(M^4, F \cong \mathrm{SO}(1,4)/\mathrm{SO}(1,3), \mathrm{SO}(1,4))$ will be such that both M^4 and the fiber F are de Sitter (or anti-de Sitter) type spaces. Besides these observations our formalism may help one to understand

why the choice $e_\mu^a = \omega_\mu^{5a}(x)$ works in this context. In general this has been a mystery, but according to our discussion such a choice is the result of a soldering process associated with the fiber bundle

$$E(M^4, F \cong \mathrm{SO}(1,4)/\mathrm{SO}(1,3), \mathrm{SO}(1,4)).$$

Our observation that the de Sitter top may be described by the de Sitter soldering bundle may also be useful for a possible connection between the de Sitter top and two time physics. In fact, it turns out that two time physics is determined by the action[24]

$$S = \int_{\tau_i}^{\tau_f} \mathrm{d}\tau \left(\frac{1}{2} \varepsilon^{ab} \dot{x}_a^\mu x_b^\nu \eta_{\mu\nu} - \frac{1}{2} \lambda^{ab} (x_a^\mu x_b^\nu \eta_{\mu\nu} + m_{ab}^2) \right), \tag{38}$$

where $x_1^\mu = x_a^\mu$, $x_2^\mu = p^\mu$, $\lambda^{ab} = \lambda^{ba}$ is a Lagrange multiplier and m_{ab}^2 are constants which can be zero or different from zero. If $m_{ab}^2 = 0$ then the action (38) has the manifest $\mathrm{Sp}(2,R)$ (or $\mathrm{SL}(2,R)$) invariance and the action is consistent if the flat metric $\eta_{\mu\nu}$ admits signature with two time. However if $m_{ab}^2 \neq 0$ this symmetry is broken and the action leads to the constraint

$$\Omega_{ab} = x_a^\mu x_b^\nu \eta_{\mu\nu} + m_{ab}^2 = 0 \tag{39}$$

(see Ref. 32 for details). Choosing $m_{11}^2 = -R^2$, $m_{22}^2 = m_0^2$, and $m_{12}^2 = 0$ one discovers that (39) gives

$$x^\mu x_\mu - R^2 = 0, \tag{40}$$

$$x^\mu p_\mu = 0, \tag{41}$$

and

$$p^\mu p_\mu + m_0^2 = 0. \tag{42}$$

The formula (40) describes an anti-de Sitter space-time and therefore in a sense the system can be understood as a relativistic point particle moving in an anti-de Sitter background which is precisely the idea underlying the de Sitter top.

Finally, there are at least two possible interesting generalizations of our formalism for the de Sitter top. In the first case one may think in the de Sitter top as a result of Clifford geometry as presented by Castro (see Ref. 33, and references therein). The second possibility may arise from the so-called oriented matroid theory.[34] It has been shown that oriented matroid theory can be connected not only to string theory but also to any p-brane, supergravtiy and Chern-Simons theory.[35–39] These connections were possible thanks to the notion of *matroid bundle* introduced first by MacPherson[40] and generalized by Anderson and Davis[41] and Biss.[42] It turns out that matroid bundle is a generalization of the concept of a fiber bundle. Thus, it seems natural to associate with the bundle $E(M^4, F \cong \mathrm{SO}(1,4)/\mathrm{SO}(1,3), \mathrm{SO}(1,4))$ some kind of the de Sitter matroid bundle and therefore a de Sitter matroid top or a de Sitter "topoid." At present all these possibilities concerning the background (2) are under investigation and we expect to report our results somewhere in the not too distant future.

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Constrained reductions of two-dimensional dispersionless Toda hierarchy, Hamiltonian structure, and interface dynamics

J. Harnad[a)]
CRM, Universite de Montreal, C.P. 6128, succ. centre-ville, Montreal, Quebec, H3C 3J7, Canada

I. Loutsenko[b)]
Institute of Mathematics, University of Oxford, 24 - 29 St. Gilles', Oxford, OX1 3LB, United Kingdom

O. Yermolayeva[c)]
SISSA, Via Beirut 2-4, 34014, Trieste, Italy

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Finite-dimensional reductions of the two-dimensional dispersionless Toda hierarchy constrained by the "string equation" are studied. These include solutions determined by polynomial, rational, or logarithmic functions, which are of interest in relation to the "Laplacian growth" or Hele-Shaw problem governing interface dynamics. The consistency of such reductions is proved, and the Hamiltonian structure of the reduced dynamics is derived. The Poisson structure of the rationally reduced dispersionless Toda hierarchies is also derived. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2104307]

I. INTRODUCTION

This paper concerns rational and logarithmic reductions of the two-dimensional dispersionless Toda hierarchy of integrable equations (henceforth 2dToda). The subject is motivated by important applications to problems in interface dynamics and statistical physics.

Laplacian growth is a process that governs the dynamics of the boundary in the plane separating two disjoint, open regions $\mathcal{D}_+$ and $\mathcal{D}_-$ in which harmonic (scalar) fields are defined. These may be interpreted as the pressure fields for two incompressible viscous fluids (Hele-Shaw problem). The movement of the boundary is determined (according to Darcy's law, in the case of viscous fluids) by equating the normal velocity of the boundary to the boundary values of the gradients of the fields. In particular, one region (say, the "interior" region $\mathcal{D}_+$) may be chosen to be bounded and have constant harmonic field (corresponding to zero viscosity) with the boundary condition for the "exterior" $\mathcal{D}_+$ region at infinity such that there is a unit sink, implying that the area of the interior region grows linearly in time.[15] Denoting the harmonic field (e.g., the pressure) in the exterior region by $P(X,Y)$, this satisfies the conditions:

$$\Delta P(X,Y) = 0, \tag{1}$$

$$P \to (4\pi)^{-1} \ln(X^2 + Y^2) \text{ as } X^2 + Y^2 \to \infty \tag{2}$$

in the Cartesian coordinates (X,Y). The normalized exterior normal velocity at the boundary is given by

[a)]Electronic mail: harnad@crm.umonreal.ca
[b)]Electronic mail: loutsenk@maths.ox.ac.uk
[c)]Electronic mail: yermola@fm.sissa.it

$$v_n = -\nabla P. \tag{3}$$

In the case where the boundary is an analytic curve it is usual to use the Riemann mapping theorem to introduce a time-dependent conformal map from the exterior of the unit circle in the complex w plane to the exterior region $\mathcal{D}_-$ in the "physical" plane $z=X+iY$ taking the unit circle to the boundary $\partial\mathcal{D}_+$.

$$z = z(w,x), \quad w = \exp(i\phi), \quad 0 < \phi < 2\pi, \tag{4}$$

where x stands for the physical time of the Hele-Shaw problem. We choose this unusual notation for time for consistency with that used in the literature on the dispersionless integrable systems.

Simple considerations[14,4,11] show (see Appendix A) that Eqs. (1) and (3) are equivalent to

$$\mathrm{Im}\left(\frac{\partial z}{\partial \phi}\frac{\partial \bar{z}}{\partial x}\right) = w\left(\frac{\partial z(w,x)}{\partial w}\frac{\partial \bar{z}(1/w,x)}{\partial x} - \frac{\partial z(w,x)}{\partial x}\frac{\partial \bar{z}(1/w,x)}{\partial w}\right) = 1, \tag{5}$$

where bar stands for complex conjugation (and $\bar{w}=w^{-1}$ on the boundary curve). In our notations $\bar{z}(w)=\Sigma_i \bar{z}_i w^i$ if $z(w)=\Sigma_i z_i w^i$, while $\overline{z(w)}=\Sigma_i \bar{z}_i \bar{w}^i$.

Known as the Galin-Polubarinova equation[6,14] in the Hele-Shaw problem, Eq. (5) plays an essential role in the theory of infinite-dimensional integrable hierarchies in the dispersionless limit. The relation between the boundary dynamics above and the dispersionless limit of the integrable Toda hierarchy constrained by (5) was shown in Refs. 11 and 19.

Equation (5) may be interpreted as a constraint on an infinite commuting set of dynamical systems defined in the space $z(x,w)$ of one-parameter families of conformal maps. This constraint represents fixed points of an "additional symmetry"[12] and is called the "string equation" in the theory of integrable systems. The most interesting aspect of such constrained dToda flows is that they admit finite-dimensional reductions, which include so-called "multi-finger" solutions.[7] These solutions are of great importance in practical applications and describe numerous phenomena, such as viscous fingering in a Hele-Shaw cell[7,9,16] and pattern formation in the quantum Hall effect.[1]

In what follows, we consider finite-dimensional reductions of (5) in the context of the 2dToda hierarchy. We first study algebraic solutions of the problem, ignoring the real structure and treating $z,\bar{z}$ as independent functions, and w as a formal variable. Returning to the applications to interface dynamics we identify bar with complex conjugation.

II. 2DTODA HIERARCHY AND STRING EQUATION

The 2dToda hierarchy is a dispersionless limit[17] of the two-dimensional Toda hierarchy and is defined in terms of two functions $z(w,x)$ and $\bar{z}(w^{-1},x)$ of the form:

$$z(w,x) = r(x)w + \sum_{k=0}^{\infty} u_k(x)w^{-k}, \tag{6}$$

$$\bar{z}(w^{-1},x) = r(x)w^{-1} + \sum_{k=0}^{\infty} \bar{u}_k(x)w^{k}. \tag{7}$$

The 2dToda flow equations are

$$\partial_{t_k} z = \{H_k, z\}, \quad \partial_{\bar{t}_k}\bar{z} = \{\bar{H}_k, \bar{z}\},$$

$$\partial_{t_k} \bar{z} = \{H_k, \bar{z}\}, \quad \partial_{\bar{t}_k} z = \{\bar{H}_k, z\}, \tag{8}$$

where the "Poisson-Lax" bracket notation here denotes

$$\{f,g\} := w\frac{\partial f}{\partial w}\frac{\partial g}{\partial x} - w\frac{\partial f}{\partial x}\frac{\partial g}{\partial w} \tag{9}$$

and the coefficients $r(x), u_k(x), \bar{u}_k(x)$ are viewed as coordinate functions on the phase space. The evolution functions are defined as follows:

$$H_k = (z^k)_+ + 1/2(z^k)_0, \quad \bar{H}_k = (\bar{z}^k)_- + 1/2(\bar{z}^k)_0, \tag{10}$$

where subscripts $\pm, 0$ denote the negative/positive and zero parts of the formal Laurent expansion in w (i.e. $f_+ = \Sigma_{i>0} f_i w^i, f_- = \Sigma_{i<0} f_i w^i$ if $f = \Sigma_i f_i w^i$).

It is important to note that, despite the notation, (9) is not really a Poisson bracket defined on the infinite-dimensional phase space of the 2dToda system (8) (with coordinates $r, u_k, \bar{u}_k$), but rather a "quasiclassical" $\hbar \to 0$ limit of commutators in the Lax representation of the dispersive version of (8) (where $\hbar$ stands for the lattice spacing, see Ref. 17). Values (10) are dispersionless analogs of the upper or lower diagonal parts of the powers of Lax matrices.

The 2dToda system is nevertheless an integrable Hamiltonian system of PDEs for the functions $r(x, t_1, \ldots, \bar{t}_1 \ldots), u_k(x, t_1, \ldots, \bar{t}_1 \ldots), \bar{u}_k(x, t_1, \ldots, \bar{t}_1 \ldots)$, obtained by equating coefficients of (8) as Laurent polynomials in the dummy variable w. One can easily verify that vector fields (8) commute, i.e.,

$$\frac{\partial^2}{\partial t_i \partial t_j}\begin{pmatrix} z \\ \bar{z} \end{pmatrix} = \frac{\partial^2}{\partial t_j \partial t_i}\begin{pmatrix} z \\ \bar{z} \end{pmatrix}, \quad \frac{\partial^2}{\partial \bar{t}_i \partial t_j}\begin{pmatrix} z \\ \bar{z} \end{pmatrix} = \frac{\partial^2}{\partial t_j \partial \bar{t}_i}\begin{pmatrix} z \\ \bar{z} \end{pmatrix}, \quad \frac{\partial^2}{\partial \bar{t}_j \partial \bar{t}_i}\begin{pmatrix} z \\ \bar{z} \end{pmatrix} = \frac{\partial^2}{\partial \bar{t}_i \partial \bar{t}_j}\begin{pmatrix} z \\ \bar{z} \end{pmatrix}$$

due to the "zero curvature" condition

$$\frac{\partial H_i}{\partial t_j} - \frac{\partial H_j}{\partial t_i} - \{H_i, H_j\} = 0, \quad \frac{\partial H_i}{\partial \bar{t}_j} - \frac{\partial \bar{H}_j}{\partial t_i} - \{H_i, \bar{H}_j\} = 0, \quad \frac{\partial \bar{H}_i}{\partial \bar{t}_j} - \frac{\partial \bar{H}_j}{\partial \bar{t}_i} - \{\bar{H}_i, \bar{H}_j\} = 0,$$

which follows from equations of motion (8) and definitions (9) and (10).

The Galin-Polubarinova equation (5) for the Hele-Shaw problem written in terms of the Poisson-Lax bracket (9)

$$\{z(w,x), \bar{z}(w^{-1},x)\} = 1, \tag{11}$$

is the string equation.

It is fundamental that Eq. (11) is invariant under the flows generated by (8). Indeed

$$\partial_{t_k}\{z,\bar{z}\} = \{\partial_{t_k} z, \bar{z}\} + \{z, \partial_{t_k}\bar{z}\} = \{\{H_k, z\}, \bar{z}\} + \{z, \{H_k, \bar{z}\}\} = \{\{\bar{z}, z\}, H_k\} = 0, \tag{12}$$

where we have used (8) and (11), and the Jacobi identity for the Lax-Poisson bracket (9).

Thus the string equation (11) defines an invariant manifold under the Toda flows (8) and a reduction of the Toda hierarchy. On the other hand, the Toda flows may be viewed as symmetries generating new solutions of Eq. (11).

III. REDUCTIONS OF THE 2DTODA HIERARCHY CONSTRAINED BY THE STRING EQUATION

The reduction of the 2dToda hierarchy by the string equation is still a compatible set of infinite-dimensional dynamical systems.

Indeed, as seen from (6) and (7) the string equation (11) is a system of ODEs of the form

$$\mathrm{d}r/\mathrm{d}x = R(r, u_1, \ldots, \bar{u}_1, \ldots), \quad \mathrm{d}u_i/\mathrm{d}x = U_i(r, u_1, \ldots, \bar{u}_1, \ldots), \quad \mathrm{d}\bar{u}_i/\mathrm{d}x = \bar{U}_i(r, u_1, \ldots, \bar{u}_1, \ldots). \tag{13}$$

In what follows we will be interested in further "functional" reductions where $z, \bar{z}$ are polynomial, rational, or logarithmic functions of w. As shown in the following, such reductions are

consistent with (8) (i.e., the corresponding ansatz for z is preserved by the two-dimensional Toda flows) if the string equation (11) holds. Thus, for consistency we need a double ("functional" plus "string") reduction. These pairs of reductions define finite-dimensional invariant sub-manifolds in the phase space of the general 2dToda hierarchy. Indeed, functional reduction leaves a finite number of discrete indices in the ansatz for z as a function of w, while the string equation fixes the dependence of z on x, leaving finite number of degrees of freedom. These degrees of freedom are connected with the integration constants of system (13), which becomes finite-dimensional after functional reductions.

A. Polynomial reductions

We begin with polynomial reductions of the 2dToda hierarchy

$$z(w) = rw + \sum_{i=-N}^{0} u_i w^i, \tag{14}$$

$$\bar{z}(w^{-1}) = rw^{-1} + \sum_{i=0}^{N} \bar{u}_i w^i \tag{15}$$

constrained by the string equation (11).

The following proposition states the consistency of the polynomial reductions under the Toda flows:

Proposition 1: If the string equation (11) holds, then (14) and (15) is a finite dimensional reduction invariant under the t_i and $\bar{t}_i$ 2dToda flows, $0<i<N+2$ (8). This manifold has dimension $2N+3$ with local coordinates chosen as the initial values of the solutions $r=r(x), u_i=u_i(x), \bar{u}_i=\bar{u}_i(x)$ to the reduced string equation (13).

Proof: We must prove that z remains of the form (14), under the flows generated by $H_k, \bar{H}_k$ provided the string equation (11) holds. In other words, we have to show that the evolution does not change the highest and lowest degrees of the Laurent polynomial (14). The proof for $\bar{z}$ is analogous.

1. First we proceed with the projections to z of the flows which are identical to those appearing in 1dToda system, i.e., those generated by H_k. These flows will be referred to as the "proper" flows.

The lowest degree of w in z is $-N$. Since

$$H_k = (z^k)_+ + 1/2(z^k)_0 = h_k w^k + h_{k-1} w^{k-1} + \ldots + h_0 \tag{16}$$

is a Laurent polynomial of positive degree in w, the lowest degree of the bracket $\{z, H_k\}$ is not less than $-N$, as follows from (9). On the other hand, the complement $z^k - H_k$ of (16) is a polynomial in $1/w$ and so,

$$\{H_k, z\} = -\{z^k - H_k, z\}$$

is a Laurent polynomial whose highest degree in w does not exceed 1.

2. Unlike the H_k-flows, the form-invariance of z (14) under the flows generated by $\bar{H}_k$ requires extra restrictions on derivatives $\partial_x u_i$ (the string equation). These flows will be referred as the "cross-flows."

Since

$$\bar{H}_k = (\bar{z}^k)_- + 1/2(\bar{z}^k)_0$$

is a Laurent polynomial of nonpositive degree, it conserves the highest degree of $z(w)$ under the evolution (8), but not the lowest degree, in general. Indeed,

$$\bar{H}_k = \bar{z}^k - ((\bar{z}^k)_+ + 1/2(\bar{z}^k)_0)$$

is a difference between $\bar{z}^k$ and a polynomial of nonnegative degree, so that

$$\{\bar{H}_k, z\} = \{\bar{z}^k, z\} - \{((\bar{z}^k)_+ + 1/2(\bar{z}^k)_0), z\}.$$

The second bracket in the last expression preserves the lowest degree of z. Thus the lowest degree of $\{\bar{H}_k, z\}$ equals the lowest degree of $\{\bar{z}^k, z\} = k\bar{z}^{k-1}\{\bar{z}, z\}$. Imposing the extra restriction (11) (string equation), we see that the lowest degree does not exceed that of $\bar{z}^{k-1}$. Since the lowest degree of $\bar{z}$ is -1 and that of z is $-N$, it follows that $k < N+2$.

Therefore, the form of (14) is preserved by $t_i, \bar{t}_i$ Toda flows with $i = 1, \ldots, N+1$, provided the string equation (11) holds. This completes the proof.

It is easy to prove the converse to Proposition 1, i.e.,

Proposition 2: The string equation (11) is a necessary condition for the existence of integrable polynomial flows of the form (10), (14), and (15)

Proof: This essentially uses the same arguments as those leading to the result of Proposition 1. For the first $N+1$ z flows to be consistent with the polynomial reduction it is necessary that the Laurent expansion of $\{\bar{z}, z\}$ be of the form $\{\bar{z}, z\} = f(x) + \Sigma_{i>0} U_i(x)/w^i$. The corresponding condition for the $\bar{z}$ flows is $\{\bar{z}, z\} = \bar{f}(x) + \Sigma_{i>0} \bar{U}_i(x) w^i$. Both can be simultaneously satisfied only if

$$\{\bar{z}, z\} = f(x) = \bar{f}(x)$$

is independent of w. Differentiating with respect to t_i (or $\bar{t}_i$), i.e., along the flow lines, using the equations of motion (8), and the Jacobi identity we get

$$\frac{\partial f}{\partial t_i} = \{H_i, f\} = w \frac{\partial f}{\partial x} \frac{\partial H_i}{\partial w}.$$

Since $w(\partial H_i/\partial w)$ is w-dependent, while f is not, it follows that $\partial f/\partial x = \partial f/\partial t_i = 0$ and similarly $\partial f/\partial \bar{t}_i = 0$. Therefore f is a constant in x and also constant along the flows, implying (up to a constant scaling) that the string equation (11) holds.

In the following we consider rational and logarithmic reductions as well as their Hamiltonian structures. Polynomial solutions can then be viewed as a special case. Nevertheless the corresponding limiting procedures are rather cumbersome and it is easier to consider the polynomial case separately. A derivation of the canonical linearizing variables in the polynomial case is given in Appendix B. This closely follows the analogous procedure given in Sec. IV for the logarithmic case. Local canonical linearizing variables, which are constant and linear in the hierarchy times, turn out to be "Richardson's harmonic moments" of the Hele-Shaw (Laplacian growth) problem when $z(w)$ and $\bar{z}(\bar{w})$ are identified with the conformal mapping from the w to the z plane. This is a simple proof of the relation (originally established in Ref. 11) between the "times" of the 2dToda hierarchy and harmonic moments of the exterior Hele-Shaw problem.

An important consequence of the present section is the fact that the string equation (11) necessarily holds for reduced conformal mappings evolving under a sufficient number of 2dToda flows (i.e., sufficient for complete integrability). In the context of interface dynamics, *Darcy's law thus turns out to be a corollary of integrability* for reduced systems.

B. Rational reductions

We now consider a rational reduction for $z(w)$ and $\bar{z}(w), N > 1$ given by

$$z(w) = \frac{q_{N+1}(w)}{p_N(w)} = \frac{r w^{N+1} + \Sigma_{i=0}^{N} a_i w^i}{w^N + \Sigma_{i=0}^{N-1} b_i w^i}, \tag{17}$$

$$\bar{z}(w^{-1}) = \frac{\bar{q}_{N+1}(w^{-1})}{\bar{p}_N(w^{-1})} = \frac{rw^{-(N+1)} + \sum_{i=0}^{N} \bar{a}_i w^{-i}}{w^{-N} + \sum_{i=0}^{N-1} \bar{b}_i w^{-i}}. \tag{18}$$

The following Lemma states the consistency of such rational reductions under the t_i Toda flows for (17) and the $\bar{t}_i$ flows for (18).

Lemma 1: The form of the function $z(w)$ in (17) is invariant under the t_i flows and the form (18) of $\bar{z}(w^{-1})$ is invariant under the $\bar{t}_i$ flows for any $i>0$.

Proof: Consider the flows generated by H_k. Since

$$H_k = (z^k)_+ + 1/2(z^k)_0 \tag{19}$$

is a polynomial of non-negative degree in w, its complement $z^k - H_k$ is a polynomial in $1/w$. The Laurent expansion of brackets (9) $\{H_k, z\} = -\{z^k - H_k, z\}$ around infinity therefore has the following form:

$$\{H_k, z\} = k_1(T)w + k_0(T) + k_{-1}(T)w^{-1} + \cdots . \tag{20}$$

However the Lax bracket (9) also implies that it is rational of the form

$$\{H_k, z\} = Q(w)/p_N(w)^2.$$

It follows from (20) that the degree of polynomial $Q(w)$ does not exceed $2N+1$.

On the other hand,

$$\partial_{t_k} z = P(w)/{p_N}^2(w), \quad P(w) = p_N \partial_{t_k} q_{N+1} - q_{N+1} \partial_{t_k} p_N,$$

where the degree of the polynomial $P(w)$ also does not exceed $2N+1$. Equating the coefficients of polynomial $P(w) - Q(w)$ to zero, we get a system of differential equations for r, a, b. The number of equations is $2N+2$. Thus we get a compatible system of differential equations for $2N+2$ unknowns r, a, b. A similar argument shows the form invariance of (18) under the $\bar{t}_k$ flows.

The consistency of the rational reduction defined in (18) under the t_i flows and (17) under $\bar{t}_i$ flows, respectively, requires additional restrictions such as the string equation. But this only suffices to ensure form invariance under t_1 and $\bar{t}_1$ flows, respectively.

Lemma 2: The string equation (11) is a sufficient condition for $z(w)$ and $\bar{z}(w)$ [(17) and (18)] to be form invariant under the first two-Toda flows. Flows generated by $H_k, \bar{H}_k$ with $k>1$ are inconsistent with the rational reduction (17) and (18).

Remark: In the next section, we will show how to choose $4N+2$ independent commuting flows preserving the rational form of z (17) and $\bar{z}$ (18), generated by vector fields that are infinite linear combinations of those generating the 2dToda hierarchy.

Proof: In order to prove that z remains of the same form (17) under the $\bar{t}_i$ Toda flows we would have to find a compatibility condition for a system of differential equations for $r(T), a(T), b(T)$, induced by (8).

These "cross" flows are generated by $\bar{H}_k$. Again we write

$$\partial z/\partial \bar{t}_k = S(w)/{p_N}^2(w), \quad S(w) = p_N \partial_{\bar{t}_k} q_{N+1} - q_{N+1} \partial_{\bar{t}_k} p_N$$

with $S(w)$ a polynomial in w of order at most $2N+1$.

Since

$$\bar{H}_k = (\bar{z}^k)_- + 1/2(\bar{z}^k)_0 = \bar{h}_k w^{-k} + \bar{h}_{k-1} w^{-k+1} + \ldots + \bar{h}_0 \tag{21}$$

is a Laurent polynomial of non-positive degree in w, the Laurent expansion of the corresponding bracket has the following form:

$$\{\bar{H}_k, z\} = k_1(T)w + k_0(T) + k_{-1}(T)w^{-1} + \cdots .$$

The definition of the Lax bracket (9) and the expansion (21) implies that

$$\{\bar{H}_k, z\} = (U(w) + R(1/w))/p_N(w)^2,$$

where $U(w)$ is a polynomial of degree at most $2N+1$ and $R = w^{-1}(\eta_{k-1}(T)w^{-k+1} + \ldots + \eta_0)$ is a polynomial in w^{-1}. If $R(1/w) = 0$, the number of equations will not exceed the number of unknowns. However, as we show in the following, the string equation does not imply the vanishing of R.

Introduce the new variable $y = w^{-1}$. The vanishing of R is equivalent to the following form of expansion in y

$$\{\bar{H}_k, z\} = f_0(T) + f_{-1}(T)y^{-1} + \cdots . \tag{22}$$

Consider this as a function of y and, as before, express $\bar{H}_k$ as a difference of $\bar{z}_k$ and a polynomial of no-negative degree. Then

$$\{\bar{H}_k, z\} = \{\bar{z}^k, z\} - \{((\bar{z}^k)_+ + 1/2(\bar{z}^k)_0), z\} = k\bar{z}^{k-1}\{z, \bar{z}\} - \{((\bar{z}^k)_+ + 1/2(\bar{z}^k)_0), z\}. \tag{23}$$

Imposing the string equation (11) we see that the only flow that allows the above expansion (22) corresponds to $k=1$. A similar argument shows that only the t_1 flow preserves the form (18) of $\bar{z}$ even if the string equation is imposed.

As seen from the above-presented proof, there are only two flows generated by evolution operators of the form (10) compatible with the rational reduction. In fact, we should not expect more invariant flows associated with the simple poles at $w=0$ and $w=\infty$. In the polynomial case, the number of invariant flows was equal to the number of variables (polynomial coefficients), since one can associate n invariant flows to a pole of nth order, and the poles at zero and infinity are immovable.

However, in the following we introduce additional flows related to movable singularities of $z(w)$ and $\bar{z}(w^{-1})$ which do preserve the rational reduction (17) and (18), extending results of Krichever for the KP case.

C. Additional flows for rational reductions of dKP hierarchy

In this section we recall the theory of flows related to poles at a finite number of finite points applying an approach previously used by Krichever for dKP hierarchy. In the dispersionless limit, the dKP and 1dToda hierarchies are quite similar, while in 2dToda the existence of finite-dimensional reductions requires extra constraints.

Let us start by recalling[5] that on the phase space of extended Benney systems, i.e., rational dKP, there arise some new flows related to the pole structure of the corresponding maps. These additional flows were introduced by Krichever (see Ref. 8).

Consider the partial fraction expansion under the above-noted assumptions and the flows of the t_i type only. For the dKP hierarchy[5,18] these reductions have the form

$$z(w) = w + u_0 + \sum_{\alpha=1}^{N} \frac{u_\alpha}{w - w_\alpha}. \tag{24}$$

The new flows associated with the poles are defined similarly to the polynomial case

$$\partial_{t_{k,\alpha}} z = \{B_{k,\alpha}, z\}, \quad \alpha = \infty, 1, 2, \ldots, \quad k = 0, 1, 2, \ldots . \tag{25}$$

The evolution functions associated with the pole structure of z are as follows :

$$B_{k,\infty} = (z(w)^k)_{\geqslant 0}, \quad ()_{\geqslant 0} := ()_+ + ()_0$$

for an immovable pole at infinity, while for each finite-distance pole there appear additional flows with evolution functions:

$$B_{k,\alpha} = (z(w)^k)_\alpha, \quad B_{0,\alpha} = \log(w_\alpha - w).$$

Here $z(w)_\alpha$ denotes the negative part of a formal Laurent expansion of $z(w)$ near the pole w_α:

$$f(w)_\alpha = \sum_{i>0} \frac{f_i}{(w-w_\alpha)^i} \quad \text{if } f = \sum_{i\in Z} \frac{f_i}{(w-w_\alpha)^i}. \tag{26}$$

These additional flows commute amongst themselves and with the ordinary 1dToda or dKP flows (associated with poles at infinity).

D. Additional invariant flows of 2dToda system

In the following, we will look at reductions of the 2dToda systems analogous to the above-mentioned Benney-Krichever reductions of KP. We will thus choose the rational functions $z(w), \bar{z}(1/w)$ appearing in (17) and (18) to have only simple poles and express these in the partial fraction form

$$\begin{aligned} z(w) &= rw + u_0 + \textstyle\sum_{j=1}^n \frac{u_j}{w-w_j}, \\ \bar{z}(1/w) &= r/w + \bar{u}_0 + \textstyle\sum_{j=1}^n \frac{\bar{u}_j}{1/w-\bar{w}_j}. \end{aligned} \tag{27}$$

Now, introduce a new set of $4n+2$ evolution functions $H_{0,j}, H_{1,j}, H_{1,\infty}, \bar{H}_{0,j}, \bar{H}_{1,j}, \bar{H}_{1,\infty}$ defined by

$$H_{k,j}(w) = B_{k,j}(w) - \tfrac{1}{2}B_{k,j}(w=0), \quad \bar{H}_{k,j}(y) = \bar{B}_{k,j}(y) - \tfrac{1}{2}\bar{B}_{k,j}(y=0), \tag{28}$$

where $k=0,1, j=1,\ldots,n$ and

$$\begin{aligned} &B_{1,\infty}(w) = (z(w))_{\geqslant 0}, \quad B_{0,j} = \log(r(w_j - w)), \quad B_{1,j}(w) = (z(w))_j \\ &\bar{B}_{1,\infty}(y) = (\bar{z}(y))_{\geqslant 0}, \quad \bar{B}_{0,j} = \log(r(\bar{w}_j - y)), \quad \bar{B}_{1,j}(y) = (\bar{z}(y))_j, \quad y = 1/w. \end{aligned} \tag{29}$$

We denote the flow variables associated with $H_{0,j}$ as τ_{2j}, those associated with $H_{1,j}$ as τ_{2j-1}, and that associated with $H_{1,\infty}$ as τ_0. The flow variables associated with $\bar{H}_{0,j}\bar{H}_{1,j}$, and $\bar{H}_{0,\infty}$ are denoted $\bar{\tau}_{2j}, \bar{\tau}_{2j-1}, \bar{\tau}_0$, respectively. Correspondingly, we denote the evolution functions

$$h_0 = H_{1,\infty} = rw + u_0/2, \quad \bar{h}_0 = \bar{H}_{1,\infty} = r/w + \bar{u}_0/2,$$

$$h_{2j-1} = H_{1,j} = \tfrac{u_j}{w-w_j} + \tfrac{u_j}{2w_j}, \quad \bar{h}_{2j-1} = \bar{H}_{1,j} = \tfrac{\bar{u}_j}{\bar{w}_j - 1/w} + \tfrac{1}{2}\bar{u}_j/\bar{w}_j$$

$$h_{2j} = H_{0,j} = \log(w_j - w) + 1/2\,\log(r/w_j), \quad \bar{h}_{2j} = \bar{H}_{0,j} = \log(\bar{w}_j - 1/w) + 1/2\,\log(r/\bar{w}_j). \tag{30}$$

Then the following proposition holds

Proposition 3: The $4n+2$ commuting Toda-Krichever flows

$$\partial_{\tau_j} z = \{h_j, z\}, \quad \partial_{\bar{\tau}_j} z = \{\bar{h}_j, z\}$$
$$j = 0, \ldots, 2n \tag{31}$$
$$\partial_{\tau_j} \bar{z} = \{h_j, \bar{z}\}, \quad \partial_{\bar{\tau}_j} \bar{z} = \{\bar{h}_j, \bar{z}\}$$

preserve the rational form of $z(w)$ *and* $\bar{z}(1/w)$ *(27) [or equally (17) and (18)] provided the string equation (11) holds. The dimension of the reduced phase space equals* $4n+3$.

We defer the proof, since this follows as a limiting case of the more general logarithmic reduction introduced in Sec. III E.

As in the polynomial case, the total number of form invariant flows preserving the string equation equals the dimension of the reduced phase space minus one. In what follows we show that these flows are Hamiltonian. Since the dimension of the phase space is odd and equals $4n+3$, it is in fact a Poisson manifold whose symplectic leafs have dimension $4n+2$, which is exactly the number of commuting Toda-Krichever flows.

The above-presented result holds for a more general setting. In the following we introduce a logarithmic reduction of the 2dToda hierarchy and prove an analog of proposition 3 for logarithmic functions. Proposition 3 follows as a limiting case.

E. Logarithmic flows

It is easier to prove the consistency of the rational reductions with the dynamics of the 2dToda system by first considering the more general logarithmic functions and then taking limits in which the branch points degenerate in pairs. Let us set

$$z = r(x)w + u(x) + \sum_{i=1}^{n+1} a_i \log(w_i(x) - w),$$
$$\bar{z} = r(x)w^{-1} + \bar{u}(x) + \sum_{i=1}^{n+1} \bar{a}_i \log(\bar{w}_i(x) - w^{-1}), \tag{32}$$

where $a_i, \bar{a}_i$ are arbitrary constants, subject to the conditions

$$\sum_{i=1}^{n+1} a_i = 0, \quad \sum_{i=1}^{n+1} \bar{a}_i = 0, \tag{33}$$

which ensure absence of logarithmic singularities at infinity.

Introduce evolution functions as follows:

$$\mathcal{H}_0 = r(x)w + \tfrac{1}{2}u(x), \quad \bar{\mathcal{H}}_0 = \bar{r}(x)w^{-1} + \tfrac{1}{2}\bar{u}(x),$$
$$\mathcal{H}_j = \log(w_j(x) - w) + \tfrac{1}{2}\log(r(x)/w_j(x)), \quad j = 1, \ldots, n+1 \tag{34}$$
$$\bar{\mathcal{H}}_j = \log(\bar{w}_j(x) - w^{-1}) + \tfrac{1}{2}\log(r(x)/\bar{w}_j(x)).$$

We then have

Proposition 4: The string equation (11) is a necessary and sufficient condition for the existence of $2n+4$ *commuting flows on the* $2n+5$ *dimensional space of functions of the form (32)*

$$\partial_{\tau_i} z = \{\mathcal{H}_i, z\}, \quad \partial_{\bar{\tau}_i} z = \{\bar{\mathcal{H}}_i, z\},$$
$$i = 0, \ldots, n+1, \tag{35}$$

$$\partial_{\tau_i}\bar{z} = \{\mathcal{H}_i, \bar{z}\}, \quad \partial_{\bar{\tau}_i}\bar{z} = \{\bar{\mathcal{H}}_i \bar{z}\}.$$

In other words, the flows generated by (34) and (35) are tangential to the manifold of such logarithmic functions if the string condition is imposed (and conversely). We therefore have $2n+4$ flows leaving invariant a $2n+5$ dimensional sub-manifold of the 2dToda system. These will be shown to be infinite linear combinations of vector fields generating the 2dToda flows (8). See Eq. (46) and (47) in which we show how to express corresponding 2dToda times $t_i, \bar{t}_i$ in terms of the logarithmic flow parameters $\tau_i, \bar{\tau}_i$.

Proof:

1. *Commutativity* : This will be shown to follow as Corollary 1 to Proposition 5 below.

2. *Consistency of (32) with equations of motion (35):* As in the polynomial and rational cases the consistency of the $\partial_{\tau_i} z$ and $\partial_{\bar{\tau}_i}\bar{z}$ equations with the logarithmic reduction (32) follows from the fact that the structure of the Lax-Poisson brackets $\{\mathcal{H}_i, z\}, \{\bar{\mathcal{H}}_i, \bar{z}\}$ is identical to the infinitesimal deformations in z and $\bar{z}$ induced by ones in the functions $r, \bar{u}, u, \bar{w}_i, w_i$. However the consistency of the $\partial_{\tau_i}\bar{z}$ and $\partial_{\bar{\tau}_i} z$ equations with the logarithmic reduction requires an extra constraint, the string equation. First, we prove this for $\partial_{\bar{\tau}_i} z$.

Differentiating z in (32) with respect to $\bar{\tau}_i$ using the equation of motion (35), we get

$$\partial_{\bar{\tau}_i} z = w\partial_{\bar{\tau}_i} r + \partial_{\bar{\tau}_i} u + \sum_{j=1}^{n+1} \frac{a_i \partial_{\bar{\tau}_i} w_j}{w - w_j} = \{\bar{\mathcal{H}}_i, z\}. \tag{36}$$

The left-hand side of (36) may contain any terms that are linear in w at $w=\infty$ and simple poles at $w=w_j, j=1,\ldots,n+1$. Since the Lax-Poisson bracket (9) is a bi-derivation, the singularities in w that may occur in $\{\mathcal{H}_i, z\}$ consist either of simple poles at $w=w_j, j=1,\ldots,n+1$, linear terms at $w=\infty$ or a simple pole at $w=1/\bar{w}_i$. We show that the latter is absent.

Note that $\bar{z}$ can be represented as a sum over $\bar{\mathcal{H}}_i, i=0,\ldots,n+1$ plus a w-independent function $f(x)$;

$$\bar{z} = \sum_{i=0}^{n+1} \bar{a}_i \bar{\mathcal{H}}_i + f(x), \tag{37}$$

where $\bar{a}_0 := 1, f(x) = \frac{1}{2}(\bar{u}(x) - \Sigma_{i=1}^{n+1} a_i \log \bar{w}_i(x))$. Now, using (37) we get

$$\bar{a}_i\{\bar{\mathcal{H}}_i, z\} = \{\bar{z} - \sum_{j\neq i} \bar{a}_j \bar{\mathcal{H}}_j - f(x), z\} = \{\bar{z}, z\} - \sum_{j\neq i} \bar{a}_j \{\bar{\mathcal{H}}_j, z\} - \{f(x), z\}. \tag{38}$$

Since $f(x)$ is independent of w, the last term in (38) contains only linear terms in w plus simple poles at $w_j, j=1,\ldots,n+1$. The term $\Sigma_{j\neq i}\bar{a}_j\{\bar{\mathcal{H}}_j, z\}$ could, in principle, contain poles at $w=1/\bar{w}_j$ for $j\neq i$, but these must cancel since $\{\bar{\mathcal{H}}_i, z\}$ contains no such poles. Furthermore, this term contains no pole at $w=1/\bar{w}_i$, because $\bar{\mathcal{H}}_i$ is omitted in the sum. Since the string equation (11) holds by assumption, we see that the right-hand side of (36) only contains terms of the type induced by infinitesimal deformations in the functions r, u, w_j, showing that the $\partial_{\bar{\tau}_i} z$ equation, together with the string equation, is compatible with the reduction (32). The proof for the $\partial_{\tau_i}\bar{z}$ equation is similar.

The above proves the sufficiency of the string equation for the validity of Proposition 4. The necessity is proved similarly to Proposition 2. By Eq. (38), if the rational reduction (32) is preserved under the $\bar{\tau}_i$ flows, $\{\bar{z}, z\}$ can have no pole at $w=1/\bar{w}_i$ for any i or at zero. Similarly to preserve (32) under the τ_i flows it can have no poles at $w_i, i=1,\ldots,n+1$ or ∞. But since the only possible poles in $\{\bar{z}, z\}$ are at these points, we conclude that $\{\bar{z}, z\}$ is constant in w and hence can only be a function (say q) of $x, \tau, \bar{\tau}$,

$$\{\bar{z},z\}=q.$$

Differentiating the last equation with respect to τ_i (or $\bar{\tau}_i$) using the equation of motion (35), the Jacobi identity and the definition of the Lax-Poisson bracket we get

$$\frac{\partial q}{\partial \tau_i}=w\frac{\partial q}{\partial x}\frac{\partial \mathcal{H}_i}{\partial w}.$$

Since $w(\partial\mathcal{H}_i/\partial w)$ is w-dependent, while q is not, it follows that $\partial q/\partial x=\partial q/\partial\tau_i=0$ (similarly $\partial q/\partial\bar{\tau}_i=0$). Therefore $q=$const and the string equation (11) holds.

The demonstration that the reduced phase space is of dimension $2n+5$ is similar to the polynomial case. We view the string equation (11) together with the logarithmic reduction (32) as a set of $(2n+5)$ first-order ODEs for the $(2n+5)$ functions $r(x),u(x),\bar{u}(x),w_i(x),\bar{w}_i(x),i=1,\ldots,n+1$,

$$\frac{\mathrm{d}r}{\mathrm{d}x}=R(r,u,\bar{u},w_1,\ldots,\bar{w}_1,\ldots),\quad \frac{\mathrm{d}u}{\mathrm{d}x}=U(r,u,\bar{u},w_1,\ldots,\bar{w}_1,\ldots),\quad \frac{\mathrm{d}\bar{u}}{\mathrm{d}x}=\bar{U}(r,u,\bar{u},w_1,\ldots,\bar{w}_1,\ldots),$$

$$\frac{\mathrm{d}w_i}{\mathrm{d}x}=W_i(r,u,\bar{u},w_1,\ldots,\bar{w}_1,\ldots),\quad \frac{\mathrm{d}\bar{w}_i}{\mathrm{d}x}=\bar{W}_i(r,u,\bar{u},w_1,\ldots,\bar{w}_1,\ldots),\quad i=1,\ldots,n+1$$

which, at least locally, determine the dependence of these functions uniquely in terms of their values $r_0,u_0,\bar{u}_0,w_{i0},\bar{w}_{i0},i=1,\ldots,n+1$ at some initial value $x=x_0$,

$$r=r(r_0,u_0,\bar{u}_0,w_{1,0},\ldots,\bar{w}_{1,0},\ldots,x),\quad u=u(r_0,u_0,\bar{u}_0,w_{1,0},\ldots,\bar{w}_{1,0},\ldots,x),$$
$$\bar{u}=\bar{u}(r_0,u_0,\bar{u}_0,w_{1,0}\ldots\bar{w}_{1,0}\ldots,x),$$

$$w_i=w_i(r_0,u_0,\bar{u}_0,w_{10}\ldots,\bar{w}_{1,0}\ldots,x),\quad \bar{w}_i=\bar{w}_i(r_0,u_0,\bar{u}_0,w_{1,0},\ldots,\bar{w}_{1,0}\ldots,x),\quad i=1,\ldots,n+1.$$

The $2n+5$ initial values $r_0,u_0,\bar{u}_0,w_{i0},\bar{w}_{i0},i=1,\ldots,n+1$ may be viewed as coordinates of the reduced phase space.

Proof of Proposition 3: This follows from taking limits in which the logarithmic branch points w_{2i},w_{2i-1} coalesce in pairs.

Setting

$$\begin{aligned} &a_{2i-1}=1/\epsilon,\quad a_{2i}=-1/\epsilon,\quad w_{2i}=w_{2i-1}+\epsilon u_i,\\ &\bar{a}_{2i-1}=1/\epsilon,\quad \bar{a}_{2i}=-1/\epsilon,\quad \bar{w}_{2i}=\bar{w}_{2i-1}+\epsilon\bar{u}_i \end{aligned} \tag{39}$$

in (32) we get (27) in the $\epsilon\to 0$ limit.

The evolution functions (30), generating flows on the space of rational reduction (27), are then obtained as follows:

$$h_0=\lim_{\epsilon=0}\mathcal{H}_0,\quad \bar{h}_0=\lim_{\epsilon=0}\bar{\mathcal{H}}_0,$$

$$h_{2i-1}=\lim_{\epsilon=0}\tfrac{1}{\epsilon}(\mathcal{H}_{2i}-\mathcal{H}_{2i-1}),\quad \bar{h}_{2i}=\lim_{\epsilon=0}\tfrac{1}{\epsilon}(\bar{\mathcal{H}}_{2i}-\bar{\mathcal{H}}_{2i-1}),$$

$$h_{2i}=\lim_{\epsilon=0}\mathcal{H}_{2i-1},\quad \bar{h}_{2i-1}=\lim_{\epsilon=0}\bar{\mathcal{H}}_{2i-1}.$$

We thus obtain evolution functions for the rational reductions, where $z,\bar{z}$ have simple poles only, as a limiting degenerating logarithmic case. One may deduce structures related to general rational reductions by degenerating arbitrary numbers of logarithmic singularities at different finite points as well as at infinity.

IV. POISSON STRUCTURE OF LOGARITHMIC REDUCTIONS OF THE 2TODA HIERARCHY

In the following we study the Poisson structure of logarithmic reductions of the 2dToda hierarchy, which will be shown to define finite-dimensional completely integrable systems. We find explicit expressions leading to a canonical Hamiltonian structure on the phase space of rational reductions of the 2dToda system.

The Poisson structure of rational reductions of the 1dToda hierarchy (which are infinite-dimensional, having no string equation constraint) is described in Appendix C. It is related to the Poisson structure of the Benney system considered in Ref. 13.

Hamiltonians, action-angle variables. Let us now introduce the following $2n+5$ functions on the reduced phase space defined by (32) with $z,\bar{z}$ solutions to (11), extended by the auxiliary variable x,

$$r,u,\bar{u},w_1,\ldots,w_{n+1},\bar{w}_1,\ldots,\bar{w}_{n+1} \to Q,I_0,I_1,\ldots,I_{n+1},\bar{I}_0,\bar{I}_1,\ldots,\bar{I}_{n+1}, \tag{40}$$

where the new variables are defined as follows:

$$I_0 = \tfrac{1}{2i\pi}\oint_\infty \bar{z}\mathrm{d}\ln z, \quad \bar{I}_0 = \tfrac{1}{2i\pi}\oint_0 z\mathrm{d}\ln\bar{z},$$

$$I_j = \tfrac{1}{2i\pi}\oint_{w_j} \bar{z}\mathrm{d}z, \quad \bar{I}_j = \tfrac{1}{2i\pi}\oint_{1/\bar{w}_j} z\mathrm{d}\bar{z}, \quad j=1,\ldots,n+1$$

$$Q = \tfrac{1}{4i\pi}\sum_{i=0}^{n+1}\oint_{1/\bar{w}_i} z\mathrm{d}\bar{z} + \oint_{w_i}\bar{z}\mathrm{d}z.$$

Using (32), we may evaluate the contour integrals in the last equation, expressing these explicitly in terms of the old parametrization $r,u,\bar{u},w_j,\bar{w}_j,j=1,\ldots,n+1$,

$$I_0 = \bar{z}(1/w=0) = \bar{u} + \textstyle\sum_{j=1}^{n+1}\bar{a}_j\ln(\bar{w}_j), \quad \bar{I}_0 = z(0) = u + \sum_{j=1}^{n+1} a_j\ln(w_j),$$

$$\begin{aligned} I_j &= a_j\bar{z}(w_j^{-1}) = a_j\Big(rw_j^{-1} + \bar{u} + \textstyle\sum_{k=1}^{n+1}\bar{a}_k\ln(\bar{w}_k - w_j^{-1})\Big), \\ \bar{I}_j &= \bar{a}_j z(\bar{w}_j^{-1}) = \bar{a}_j\Big(r\bar{w}_j^{-1} + u + \textstyle\sum_{k=1}^{n+1} a_k\ln(w_k - \bar{w}_j^{-1})\Big), \quad j=1,\ldots,n+1, \end{aligned} \tag{41}$$

$$Q = \tfrac{1}{2}r\Big(\Big(\tfrac{\partial z(w)}{\partial w}\Big)_{w=0} + \Big(\tfrac{\partial\bar{z}(1/w)}{\partial(1/w)}\Big)_{1/w=0}\Big) - \tfrac{1}{2}\textstyle\sum_{j=1}^{n+1}(I_j+\bar{I}_j) = r^2 - \tfrac{1}{2}\sum_{j=1}^{n+1}\Big(r\Big(\tfrac{a_j}{w_j} + \tfrac{\bar{a}_j}{\bar{w}_j}\Big) + I_j + \bar{I}_j\Big). \tag{42}$$

Proposition 5:The functions $I_k,\bar{I}_k,Q$ (41) and (42) are linearizing variables of the system (35) satisfying

$$\partial_{\tau_j}Q = 0, \quad \partial_{\bar{\tau}_j}Q = 0,$$

$$\partial_{\tau_j} I_k = \delta_{jk}, \quad \partial_{\bar{\tau}_j} I_k = 0, \tag{43}$$

$$\partial_{\tau_j} \bar{I}_k = 0, \quad \partial_{\bar{\tau}_j} \bar{I}_k = -\delta_{jk}.$$

Proof: We first calculate derivatives of each I_k with respect to the times $\tau_j, j=0,\ldots,n+1$. Applying integration by parts, we get

$$2\pi i \frac{\partial I_k}{\partial \tau_j} = \frac{\partial}{\partial \tau_j} \oint_{w_k} \bar{z} \frac{\partial z}{\partial w} \mathrm{d}w = \oint_{w_k} \frac{\partial}{\partial w}\left(\bar{z}\frac{\partial z}{\partial \tau_j}\right)\mathrm{d}w + \oint_{w_k} \left(\frac{\partial \bar{z}}{\partial \tau_j}\frac{\partial z}{\partial w} - \frac{\partial z}{\partial \tau_j}\frac{\partial \bar{z}}{\partial w}\right)\mathrm{d}w.$$

By the equations of motion (35) and the definition of the Lax-Poisson brackets (9) this equals

$$\oint_{w_k} \frac{\partial}{\partial w}\left(\bar{z}\frac{\partial z}{\partial \tau_j}\right)\mathrm{d}w + \oint_{w_k} \left(\{\mathcal{H}_j, \bar{z}\}\frac{\partial z}{\partial w} - \{\mathcal{H}_j, z\}\frac{\partial \bar{z}}{\partial w}\right)\mathrm{d}w$$
$$= \oint_{w_k} \frac{\partial}{\partial w}\left(\bar{z}\frac{\partial z}{\partial \tau_j}\right)\mathrm{d}w + \oint_{w_k} \frac{\partial \mathcal{H}_j}{\partial w} w \left(\frac{\partial z}{\partial w}\frac{\partial \bar{z}}{\partial x} - \frac{\partial z}{\partial x}\frac{\partial \bar{z}}{\partial w}\right)\mathrm{d}w,$$

which by the string equation (11) reduces to

$$\oint_{w_k} \frac{\partial}{\partial w}\left(\bar{z}\frac{\partial z}{\partial \tau_j}\right)\mathrm{d}w + \oint_{w_k} \frac{\partial \mathcal{H}_j}{\partial w}\mathrm{d}w = 2\pi i \delta_{kj}, \quad \delta_{jk} = \begin{cases} 1, & j = k \\ 0, & j \neq k \end{cases}.$$

The first term on the left-hand side vanishes, because $\bar{z}(\partial z/\partial \tau_j)$ is univalent in a neighborhood of $w_k, k=1,\ldots,n+1$ [and at ∞ due to (33)] and the remaining integral is evaluated by substituting expression (34) for $\mathcal{H}_j$. We have thus proved that

$$\frac{\partial I_i}{\partial \tau_j} = \delta_{ij}.$$

The rest of the proposition is proved by similar computations.

Corollary 1:The vector fields defining (35) commute.

Proof: Since $z, \bar{z}$ are completely determined by the new coordinates $Q, I, \bar{I}$, infinitesimal deformations of the former under the τ_i flows can be expressed via the chain rule through the infinitesimal deformations of the latter. It follows from Proposition 5 that

$$\frac{\delta}{\delta \tau_i}\begin{pmatrix} z \\ \bar{z} \end{pmatrix} = \frac{\partial}{\partial I_i}\begin{pmatrix} z \\ \bar{z} \end{pmatrix}, \quad \frac{\delta}{\delta \bar{\tau}_i}\begin{pmatrix} z \\ \bar{z} \end{pmatrix} = \frac{\partial}{\partial \bar{I}_i}\begin{pmatrix} z \\ \bar{z} \end{pmatrix}$$

so we have

$$\left(\frac{\delta}{\delta \tau_i}\frac{\delta}{\delta \tau_j} - \frac{\delta}{\delta \tau_j}\frac{\delta}{\delta \tau_i}\right)\begin{pmatrix} z \\ \bar{z} \end{pmatrix} = \left(\frac{\partial}{\partial I_i}\frac{\partial}{\partial I_j} - \frac{\partial}{\partial I_j}\frac{\partial}{\partial I_i}\right)\begin{pmatrix} z \\ \bar{z} \end{pmatrix} = 0.$$

The commutativity of the other flows is seen to similarly follow from Proposition 5.

Choosing Poisson structure for Eq. (43) in a canonical way

$$\{I_i, \bar{I}_j\}_p = \delta_{ij}, \quad \{I_i, I_j\}_p = \{\bar{I}_i, \bar{I}_j\}_p = 0, \quad \{Q, \bar{I}_j\}_p = \{Q, I_j\}_p = 0 \tag{44}$$

we may interpret $I, \bar{I}$ as canonical linearizing variables and Q as a Casimir invariant. The equations of motion induced by the evolution operators $\mathcal{H}_i$ or $\bar{\mathcal{H}}_i$ are seen to be Hamiltonian and generated by the Hamiltonians

$$\mathrm{H}_i = \bar{I}_i, \quad \bar{\mathrm{H}}_i = I_i. \tag{45}$$

The Poisson brackets $\{,\}_p$ in (44) are different from $\{,\}$ in (9); they define a Poisson structure on the finite dimensional space of logarithmic reductions of the phase space satisfying the string equation, while the latter (the Lax-Poisson bracket) is a dispersionless limit of the commutator.

Remark: Linearizing coordinates similar to (41) appeared in Ref. 10 in connection with the Laplacian Growth problem as integrals of the Laplacian Growth (string) equation, without the introduction of the compatible τ_i and $\bar{\tau}_i$ flows considered here.

The following proposition makes explicit the fact that the string equation implies the finite dimensionality of the reduced phase space.

Proposition 6:The functions (41) form a set of integrals of the string equation (11). The string equation (11) implies

$$\frac{\partial I_i}{\partial x} = \frac{\partial \bar{I}_i}{\partial x} = 0, \quad \frac{\partial Q}{\partial x} = 1.$$

Equivalently, this may be integrated to

$$Q - x = c_0, \quad I_i = c_i, \quad \bar{I}_i = \bar{c}_i, \quad i = 0, \ldots, n = 1,$$

where c_i, c_i are constants in x, which may be interpreted as coordinates on the $2n+5$ dimensional reduced phase space.

Proof: This is similar to the proof of proposition (5); one simply differentiates with respect to x and evaluates corresponding residues.

As mentioned in Sec I, the Laplacian growth problem is recovered by identifying $\bar{z}$ as the complex conjugate of z. As seen from Proposition 6, the Casimir Q, which is proportional to the area of $\mathcal{D}_+$, grows with unit speed in physical time x, while $I_k, \bar{I}_k$ are functions of the harmonic moments of the boundary curve.

To obtain similar results for the rational case we take a limit as in (39).

Corollary 2: Let $z, \bar{z}$ be of the rational reduction form (27). Then the following $2n+3$ quantities

$$I_0 = \bar{u}_0 - \sum_{i=1}^n \bar{u}_i/\bar{w}_i, \quad \bar{I}_0 = u_0 - \sum_{i=1}^n u_i/w_i,$$

$$I_{2i-1} = r w_i^{-1} + \bar{u}_0 + \sum_{j=1}^n \frac{\bar{u}_j}{1/w_i - \bar{w}_j}, \quad \bar{I}_{2i-1} = r \bar{w}_i^{-1} + u_0 + \sum_{j=1}^n \frac{u_j}{1/\bar{w}_i - w_j}, \quad i = 1, \ldots, n$$

$$I_{2i} = \left(r - \sum_{j=1}^n \frac{\bar{u}_j}{(1/w_i - \bar{w}_j)^2} \right) \frac{u_i}{w_i^2}, \quad \bar{I}_{2i} = \left(r - \sum_{j=1}^N \frac{u_j}{(1/\bar{w}_i - w_j)^2} \right) \frac{\bar{u}_i}{\bar{w}_i^2},$$

$$Q = r^2 - \frac{1}{2} \sum_{i=1}^n \left(r \left(\frac{\bar{u}_i}{\bar{w}_i^2} + \frac{u_i}{w_i^2} \right) + \bar{I}_{2i} + I_{2i} \right)$$

the linearizing canonical variables for the rational reduction, i.e., variables in terms of which the equations of motion (31) for the rational reduction (27) have the canonical form (43).

The logarithmic or rational flows are infinite linear combinations of the 2dToda flows (8). As shown in Appendix B, harmonic moments of the conformal mapping $z(w)$ are linear in the 2dToda times. Therefore to express $t_i, \bar{t}_i, i=1, 2\ldots$ through $\tau_i, \bar{\tau}_i, i=0, \ldots, n+1$ one has to evaluate the integrals

$$M_k(z,\bar{z}) = \frac{1}{2k\pi i}\oint_{\infty} \bar{z}z^{-k}\frac{\partial z}{\partial w}\mathrm{d}w, \quad \bar{M}_k(z,\bar{z}) = \frac{1}{2k\pi i}\oint_{0} z\bar{z}^{-k}\frac{\partial \bar{z}}{\partial w}\mathrm{d}w, \tag{46}$$

which are functions of coordinates $z,\bar{z}$ of the reduced phase space (32), and then express $z,\bar{z}$ through $Q,I_i,\bar{I}_i, i=0,\ldots,n+1$. Then

$$M_k(Q,I,\bar{I}) = M_k(z(Q,I,\bar{I}),\bar{z}(Q,I,\bar{I})), \quad \bar{M}_k(Q,I,\bar{I}) = M_k(z(Q,I,\bar{I}),\bar{z}(Q,I,\bar{I})). \tag{47}$$

Since, modulo integration constants

$$M_i = t_i, \quad \bar{M}_i = \bar{t}_i, \quad i > 0,$$

$$I_i = \tau_i, \quad \bar{I}_i = \bar{\tau}_i, \quad i = 0,\ldots,n+1$$

and $Q=x$, it follows that Eq. (47) expresses $t_i,\bar{t}_i$ in terms of $\tau_i,\bar{\tau}_i$.

V. CONCLUSIONS

We have derived consistent finite dimensional logarithmic and rational reductions of certain flows related to the 2dToda hierarchy. The requirement for the consistency of these reductions was the string equation. Since the latter may also be viewed as the Galin-Polubarinova equation for the Hele-Shaw (Laplacian growth) process, this also established the latter as a compatible constraint for such reduced 2dToda flows.

More generally, it would be of interest to determine all finite dimensional reductions of the 2dToda hierarchy that imply fulfillment of the Darcy law in various forms.

Also, it would be useful to study integrable systems connected to various kinds of Hele-Shaw flows. This could include boundary conditions which are more general than a point sink at infinity. For instance, one can consider an exterior problem with a steady and uniform viscous flow at infinity. This can describe the evolution of a bubble surrounded by a viscous liquid moving through a wide channel, or a bubble within a viscous flow generated by a source and a sink of equal magnitude separated by a large distance. In such models, the constraint on $z,\bar{z}$ (6) and (7) has the form

$$\{z(w,x),\bar{z}(w^{-1},x)\} = (1/w + w)r(x).$$

This is an exterior analog of the interior problem with a dipole source inside the domain. In contrast to a monopole sink, this implies that the first harmonic moment changes with the time x, while the others (including area) remain unchanged. In general any combination of n-pole sources could be considered:

$$\{z(w,x),\bar{z}(w^{-1},x)\} = f(x,w),$$

where f is defined by the asymptotics of the hydrodynamic potential.

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APPENDIX A: STRING EQUATION AND DARCY LAW

We recall here the derivation of the Galin-Polubarinova equation. Consider evolution of the exterior $\mathcal{D}_-$ of a simply connected planar domain bounded by an analytic curve on z plane. The

curve is an image of the unit circle in the w plane under a conformal mapping (4). As stated in the introduction the pressure field $P(X,Y)$ is constant in the interior domain $\mathcal{D}_+$ and at the boundary $\partial\mathcal{D}_+$, so that at $\partial\mathcal{D}_+$,

$$0 = \mathrm{d}P/\mathrm{d}x = \partial P/\partial x + v_n \nabla P = \partial P/\partial x - (\nabla P)^2,$$

where we used Darcy law (3) and the pressure gradient is taken in the exterior vicinity of the curve. Since P is harmonic in $\mathcal{D}_-$ [cf. (1)], it is the real part of a homomorphic function (hydrodynamic potential) $P=\mathrm{Re}\,\phi(z)$. It follows that

$$0 = \mathrm{Re}\left(\frac{\partial\phi}{\partial x} - \frac{\partial\phi}{\partial z}\overline{\left(\frac{\partial\phi}{\partial z}\right)}\right).$$

The hydrodynamic potential can be chosen as $\phi(z,x)=1/2\pi \log w(z,x)$ due to the logarithmic asymptotic in (1). Then

$$0 = \mathrm{Re}\left(\overline{w(z,x)}\frac{\partial w(z,x)}{\partial x} - \frac{\partial w(z,x)}{\partial z}\overline{\left(\frac{\partial w(z,x)}{\partial z}\right)}\right),$$

where $w(z,x)$ stands for the map inverse to $z(w,x)$. Using the facts that $z=z(w(z,x),x)$, i.e.,

$$\frac{\partial z(w,x)}{\partial w}\frac{\partial w(z,x)}{\partial x} + \frac{\partial z(w,x)}{\partial x} = 0, \quad \frac{\partial w(z,x)}{\partial z} = 1 \Big/ \frac{\partial z(w,x)}{\partial w}$$

and $\bar{w}=1/w$ on $\partial\mathcal{D}_+$, we arrive at (5).

APPENDIX B: POISSON STRUCTURE OF POLYNOMIAL REDUCTIONS

Following steps similar to the proof of Proposition 5, one arrives at the following result for polynomial reductions (10), (14), and (15) of the 2dToda system.

Proposition 7: The following quantities

$$M_k = \frac{1}{2i\pi k}\oint_\infty \bar{z}z^{-k}\mathrm{d}z, \quad \bar{M}_i = \frac{1}{2i\pi k}\oint_0 z\bar{z}^{-k}\mathrm{d}\bar{z},$$

$$Q = \frac{1}{4i\pi}\left(\oint_\infty \bar{z}dz - \oint_0 zd\bar{z}\right)$$

are canonical linearizing variables of the (polynomially) reduced 2dToda system (8), (10), (14), and (15):

$$M_k(z,\bar{z}) = t_k + \mathrm{const}, \quad \bar{M}_k(z,\bar{z}) = \bar{t}_k + \mathrm{const}, \quad Q(z,\bar{z}) = x + \mathrm{const}.$$

Solutions to the string equation (11) are then defined by the set of algebraic equations

$$Q(z,\bar{z}) = x + c_0, \quad M_k(z,\bar{z}) = c_k, \quad \bar{M}_k(z,\bar{z}) = \bar{c}_k,$$

where $c_k,\bar{c}_k$ are arbitrary constants.

Proof: Evaluating $\partial M_j/\partial t_k, \partial M_j/\partial \bar{t}_k$ by arguments similar to those of Proposition 5, we get

$$\frac{\partial M_j}{\partial t_k} = -\frac{1}{2i\pi j}\oint_\infty \frac{\partial H_k}{\partial w}z^{-i}\mathrm{d}w, \quad \frac{\partial M_i}{\partial \bar{t}_j} = \frac{1}{2i\pi j}\oint_\infty \frac{\partial \bar{H}_k}{\partial w}z^{-i}\mathrm{d}w.$$

Using the fact that

$$H_k = (z(w)^k)_+ + \tfrac{1}{2}(z(w)^k)_0 = z(w)^k - (z(w)^k)_- - \tfrac{1}{2}(z(w)^k)_0$$

and the negative part of the Laurent expansion does not contribute to the integral, we obtain

$$\frac{\partial M_j}{\partial t_k} = \frac{1}{2i\pi j}\oint_\infty z(w)^{-i}\frac{\partial z(w)^j}{\partial w}\mathrm{d}w = \delta_{kj}.$$

Using the fact that the evolution functions $\bar{H}_j = (\bar{z}^j)_- + 1/2(\bar{z}^j)_0$ generating the $\bar{\tau}_i$ flows are polynomials of non-negative degrees in $1/w$, we obtain

$$\frac{\partial M_i}{\partial \bar{t}_j} = 0.$$

In the context of the Hele-Shaw problem, the first $N+1$ Richardson moments[15] equal the first $N+1$ dToda times. Indeed, in the Hele-Shaw problem $z(w)$ has the meaning of a conformal mapping from w to the z plane. In the exterior problem, the exterior of the unit circle (i.e., domain $|w|>1$) is mapped to the exterior $\mathcal{D}_-$ of the boundary curve $z(w)$. The exterior harmonic moments are, by Green's theorem,

$$\frac{1}{2j\pi i}\int_{|w|>1} z^{-j}\mathrm{d}z\,\mathrm{d}\bar{z} = \frac{1}{2j\pi i}\oint_{|w|=1}\bar{z}(1/w)z(w)^{-j}\mathrm{d}z.$$

Since the mapping $z(w)$ is univalent in $\mathcal{D}_-$, all zeros of $z(w)$ are located in $\mathcal{D}_+$ and we can move the integration contour to infinity if $i \geqslant 1$. Thus, we get

$$\frac{1}{2j\pi i}\oint_\infty \bar{z}(1/w)z(w)^{-j}\mathrm{d}z = M_i$$

which, by Proposition 7 equals t_i modulo an integration constant.

APPENDIX C: POISSON STRUCTURE OF 1DTODA HIERARCHY.

In this section we consider the Poisson structure of rational reductions of 1dToda system. Recall that for the 1dToda system one takes into account only the t_i flows,

$$\partial_{t_i} z = \{H_i, z\}, \quad H_i = (z(w)^i)_+ + 1/2(z(w)^i)_0, \quad i = 0, \ldots \infty. \tag{C1}$$

This system is bi-Hamiltonian (for general information, e.g., see Ref. 3) with two (linear and quadratic) compatible Poisson structures. For generic Toda system (6), the dispersionless linear Poisson brackets for the "field variables" $u_i, i=1,\ldots,\infty$ (6) have the following form:[2]

$$\{u_n(x), u_m(y)\}_1 = 2(c_n + c_m - 1)[(n+m)u_{n+m}(x)\delta'(x-y) + mu'_{n+m}(x)\delta(x-y)], \tag{C2}$$

where

$$c_k = \begin{cases} 1 & \text{if } k > 0 \\ 1/2 & \text{if } k = 0 \\ 0 & \text{if } k < 0 \end{cases}$$

while the quadratic brackets are

$$\{u_n(x), u_m(y)\}_2 = \left[\frac{1}{2}(n-m)u_n(x)u'_m(x) + \left(\sum_{k=1}^{1-n}(n-m+k)u_{n+k}(x)u'_{m-k}(x) + ku'_{n+k}(x)u_{m-k}(x)\right)\right] \times \delta(x-y) + \left[1/2(n-m)u_n u_m + \left(\sum_{k-1}^{1-n}(n-m+2k)u_{n+k}u_{m-k}\right)\right]\delta(x-y). \tag{C3}$$

As seen from Lemma 1, the rational functions

$$z(w) = \frac{q_{N+1}(w)}{p_N(w)} = \frac{w^{N+1} + \Sigma_{i=0}^{N} a_i w^i}{\Sigma_{i=0}^{N} b_i w^i} \tag{C4}$$

are form-invariant under all the 1dToda flows (C1), without any extra restriction (e.g., no string equation is needed).

We obtain corresponding Poisson structures for the variables a_i, b_i, by using result (C3), expressing u_i in terms of $a_i, b_i, i=0,\ldots N$. Both the linear (C2) and the quadratic (C3) Poisson structures lead to quadratic brackets for a_i, b_i . Namely, the second Poisson structure for (C4)) becomes

$$\{a_k(x), a_l(y)\}_2 = \left[\sum_{n=1} (l+n-k) a_{k-n}(x) a_{l+n}(y) + n a_{k-n}(y) a_{l+n}(x) + (l-N-1) a_k(x) a_l(y)\right] \delta'(x-y), \tag{C5}$$

$$\{b_k(x), b_l(y)\}_2 = \left[\sum_{n=1} (k-l-n) b_{k-n}(x) b_{l+n}(y) - n b_{k-n}(y) b_{l+n}(x) + \frac{k-\ell}{2} b_k(x) b_l(y)\right] \delta'(x-y), \tag{C6}$$

$$\{a_k(x), b_l(y)\}_2 = \frac{k-N-1}{2} a_k(x) b_l(y)\, \delta'(x-y). \tag{C7}$$

The first Poisson structure can be obtained from (C5)–(C7) with the help of a linear transformation (shift by constant)

$$a_i \to a_i + \lambda b_i, \quad z(w,x) \to z(w,x) + \lambda$$

and using a bi-Hamiltonian nature of (C2) and (C3),

$$\{a_k(x), a_l(y)\}_1 = \left[\sum_{n=1} (k-l-n)(a_{k-n}(x) b_{l+n}(y) + b_{k-n}(x) a_{l+n}(y)) - n(a_{k-n}(y) b_{l+n}(x) + b_{k-n}(y) a_{l+n}(x)) + \frac{N+1-l}{2} b_k(x) a_l(y) + \frac{k+N+1-2l}{2} a_k(x) b_l(y)\right] \delta'(x-y), \tag{C8}$$

$$\{a_k(x), b_l(y)\}_1 = \left[\sum_{n=1} ((k-l-n) b_{k-n}(x) b_{l+n}(y) - n b_{k-n}(y) b_{l+n}(x)) + \frac{N+1-l}{2} b_k(x) b_l(y)\right] \delta'(x-y), \tag{C9}$$

$$\{b_k(x), b_l(y)\}_1 = 0. \tag{C10}$$

In all the above expressions $a_{N+1}=1$ and $a_i=0$ if i goes beyond the range $i=0,\ldots N+1$ (and $b_j=0$ if $j \neq 0,\ldots,N$).

These brackets form a bi-Hamiltonian structure for rational reductions of 1dToda hierarchy:

$$\partial_{t_i} z = \{H_i, z\}_1 = \{H_{i-1}, z\}_2 \tag{C11}$$

with the following Hamiltonians:

$$\mathrm{H}_i = \frac{1}{i+1} \int (z^{i+1}(x))_0 dx \tag{C12}$$

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The effects of nonlocality on the evolution of higher order fluxes in nonequilibrium thermodynamics

V. A. Cimmelli[a)]
Department of Mathematics, University of Basilicata, Campus Macchia Romana, 85100 Potenza, Italy

P. Ván[b)]
Department of Chemical Physics, Budapest University of Technology and Economics, Budafoki út 8, 1521 Budapest, Hungary

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The role of gradient dependent constitutive spaces is investigated on the example of Extended Thermodynamics of rigid heat conductors. Different levels of nonlocality are developed and the different versions of extended thermodynamics are classified. The local form of the entropy density plays a crucial role in the investigations. The entropy inequality is solved under suitable constitutive assumptions. Balance form of evolution equations is obtained in special cases. Closure relations are derived on a phenomenological level. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Weakly nonlocal thermodynamic theories are those that introduce the space derivatives of the basic variables into constitutive functions.[1] Second law restricts considerably the form of the constitutive quantities and gives a genuine insight into the structure of the theories. Weakly nonlocal constitutive functions are mostly investigated in relation of material microstructure in mechanics[2,3] or to find nonlocal extensions of classical theories.[1]

In this paper we investigate nonlocal constitutive spaces with different levels of nonlocality, namely of different order of derivatives. However, we derive also the restrictions that are due to locality assumptions on different levels. In our analysis we assume a nonequilibrium entropy function that can be approximated by its values measured at the equilibrium. Such an assumption is referred to as *local state* hypothesis.[4]

We restrict ourselves to extended thermodynamic theories of rigid heat conductors[5–7] and introduce the heat flux together with a second order tensor as internal variables. The balance structure of the evolution equations is not postulated. Furthermore, the entropy current is regarded as a constitutive quantity and we are to give a complete solution of the thermodynamic constraints, i.e., both the equalities and the residual dissipation inequality.

In a previous work[8] the local theory has been developed in the details and the evolution equations for fluxes of higher tensorial order have been obtained. Also it was proved that under particular assumptions on the entropy density and the entropy current the balance form can be recovered. Moreover, the system of equations was closed, in that the evolution equations for the highest order variable in the hierarchy—ordinary differential equations—can be interpreted as a closure relation.

In the present paper we extend our investigation to the case of weakly nonlocal constitutive state spaces. The solutions are derived with the help of minimal assumptions on the form of the

[a)]Electronic mail: cimmelli@unibas.it
[b)]Author to whom correspondence should be addressed. Electronic mail: vpet@eik.bme.hu

entropy, on its flux or on the evolution equations of the internal variables. In this way the different solutions of the entropy inequality are clearly classified. The most general assumption, that covers all existing phenomenological theories lies on the concept of *current multipliers*, which represent some constitutive functions entering the entropy current. We will see that the final evolution equations are more general than the traditional balance ones. The conditions to recover the classical cases are clarified.

In Sec. II we investigate first order nonlocality by applying Liu procedure[9,10] for the exploitation of second law.

In Sec. III we solve the Liu equation in the case of local state and local evolution equations for the dynamic variables. These assumptions result in a set of rather unusual restrictions from which we argue that some kind of nonlocality, either of the constitutive space or of the evolution equations, seems to be unavoidable. On the other hand, if we face with nonlocal state but local evolution equations then the entropy current is local, provided that the entropy density does not depend on the gradient of the internal energy.

In Sec. IV we investigate the traditional assumptions of Extended Irreversible Thermodynamics based on the following form of the local entropy:[11]

$$s(e,q_i,\Phi_{ij}) = s_0 - \tfrac{1}{2}m_{ij}q_iq_j - \tfrac{1}{2}n_{ijkl}\Phi_{ij}\Phi_{kl}, \tag{1.1}$$

where the matrices m_{ij} and n_{ijkl} are constitutive functions and s_0 is the *equilibrium entropy*, that depends only on the internal energy. We first suppose the entropy current is given as[12]

$$j_i = A_{ij}q_j + B_{ijk}\Phi_{jk}, \tag{1.2}$$

where A_{ij} and B_{ijk} are constitutive functions, the so-called current multipliers. Then we explore the less general case,[13] too

$$j_i = \frac{\partial s}{\partial e}q_i + \frac{\partial s}{\partial q_k}\Phi_{ki}. \tag{1.3}$$

It is worth noticing that the general form of the entropy current (1.2) reduces to (1.3) when $A_{ij} = (\partial s/\partial e)\delta_{ij}$ and $B_{ijk} = (\partial s/\partial q_j)\delta_{ik}$. We investigate different assumptions that can be compatible with the balance form of the evolution equations.

In Sec. V we consider second order nonlocality but conserve the form (1.1) of the entropy density and the expression (1.2) of the entropy current. In such a case, due to the enlargement of the state space, the balance form can be obtained even if the general constitutive equation (1.2) holds true. We show that all previous examples can be recovered under simple special assumptions.

In Sec. VI we point out some nonlocal effects arising in thermal wave propagation at low temperature, which are described by the celebrated Guyer-Krumhansl equation.[14–16] Such an equation has been derived by the authors by solving a linearized Boltzmann equation for phonon gas hydrodynamic. Here we prove that it can be obtained in the classical macroscopic framework of nonlocal irreversible thermodynamics.

The previous results are discussed in Sec. VII, where a table shows the connections between the constitutive assumptions and the thermodynamic restrictions, as far as the locality and nonlocality are concerned.

II. FIRST ORDER NONLOCALITY—EXPLOITATION OF THE SECOND LAW

In a rigid heat conductor at rest we start from the following local balance equation of the internal energy:

$$\dot{e} + q_{i',i} = 0, \tag{2.1}$$

where e is the density of internal energy, q_i $i=1,2,3$ are the components of the heat flux, $\dot{f} \equiv \partial f/\partial t$, $f_{,i} \equiv \partial f/\partial x_i$, x_i $i=1,2,3$ are the Cartesian coordinates of the points of the body and the

Einstein convention of summation over the repeated indices has been applied. The only equilibrium variable will be the internal energy e, while the first dynamic variable is supposed to be the heat flux q_i. As a further dynamic variable let us choose a second order tensor, whose components will be denoted by Φ_{ij}, $i,j=1,2,3$. Hence the *basic state space* (the wanted fields) in our investigations will be spanned by the variables (e,q_i,Φ_{ij}). This is a 13 field theory, because the number of the independent fields is 13. However, some reductions are possible. For instance in Extended Thermodynamics tensor Φ_{ij} is identified with the symmetric momentum flux $N_{[ij]}$ coming from kinetic theory.[7] Then the unknown fields reduce to 10 and we are left with a 10-field theory. Furthermore it is possible to decompose $N_{[ij]}$ into an isotropic part, which is related to the internal energy, and a deviatoric part according to the equation $N_{[ij]}=\frac{1}{3}e\delta_{[ij]}+N_{\langle ij\rangle}$, where $N_{\langle ij\rangle}$ is symmetric and traceless.[17] In such a particular case the internal energy coincides with one of the six independent components of $N_{[ij]}$ and we deal with a 9-field theory. We are investigating a first order weak nonlocality in all variables of the basic state, therefore the *constitutive space* is spanned by the basic state and its spacial derivatives, that is the fields $(e,q_i,\Phi_{ij},e_{,i},q_{i'j},\Phi_{ij'k})$. We assume that the evolution equations for the heat current q_i and for Φ_{ij} can be written in the following rather general form:

$$\dot{q}_i = g_i, \tag{2.2}$$

$$\dot{\Phi}_{ij} = f_{ij}, \tag{2.3}$$

where g_i and f_{ij} are constitutive functions. With the assumption of first order nonlocality the spacial derivatives of the above equations give further restrictions,[18,19]

$$\dot{e}_{,i} + q_{j'ji} = 0, \tag{2.4}$$

$$\dot{q}_{i'j} - g_{i,j} = 0, \tag{2.5}$$

$$\dot{\Phi}_{ij'k} - f_{ij'k} = 0. \tag{2.6}$$

These equations are sometimes referred to as *prolonged forms* of the evolution equations (2.1)–(2.3).

The local balance of entropy is given by

$$\dot{s} + j_{i'i} = \sigma_s, \tag{2.7}$$

with s standing for the entropy density, j_i, $i=1,2,3$ for the components of the entropy current and σ_s for the density of entropy production. Second law of thermodynamics forces σ_s to be nonnegative.

In the following we will investigate the restrictions from the inequality of the second law with the general assumption that both the entropy and the entropy flux are constitutive quantities. The method of the exploitation is given by the Liu procedure.[9] However, according to our calculations, in the present case a generalized Coleman-Noll[20] procedure gives identical results.

Let us introduce the Lagrange-Farkas multipliers[9,10] Γ^1, Γ^2_i, and Γ^3_{ij} for the evolution equations (2.1)–(2.3), respectively. The multipliers Γ^4_i, Γ^5_{ij}, and Γ^6_{ijk} are for the prolonged evolution equations (2.4)–(2.6), respectively.

Now, Liu procedure gives

$$\begin{aligned}
&\partial_1 s\dot{e} + (\partial_2 s)_i\dot{q}_i + (\partial_3 s)_{ij}\dot{\Phi}_{ij} + (\partial_4 s)_i\dot{e}_{,i} + (\partial_5 s)_{ij}\dot{q}_{i'j} + (\partial_6 s)_{ijk}\dot{\Phi}_{ij'k} + (\partial_1 j_i)e_{,i} + (\partial_2 j_i)_j q_{j'i} + (\partial_3 j_i)_{jk}\Phi_{jk'i}\\
&\quad + (\partial_4 j_i)_j e_{,ij} + (\partial_5 j_i)_{jk} q_{j'ki} + (\partial_6 j_i)_{jkl}\Phi_{jk'li} - \Gamma^1(\dot{e} + q_{i'i}) - \Gamma^2_i(\dot{q}_i - g_i) - \Gamma^3_{ij}(\dot{\Phi}_{ij} - f_{ij}) - \Gamma^4_i(\dot{e}_{,i}\\
&\quad + q_{j'ji}) - \Gamma^5_{ij}(\dot{q}_{i'j} - (\partial_1 g_i)e_{,j} - (\partial_2 g_i)_k q_{k'j} - (\partial_3 g_i)_{kl}\Phi_{kl'j} - (\partial_4 g_i)_k e_{,kj} - (\partial_5 g_i)_{kl} q_{k'lj}
\end{aligned}$$

$$-(\partial_6 g_i)_{klm}\Phi_{kl'lmj}) - \Gamma^6_{ijk}(\dot{\Phi}_{ij'k} - (\partial_1 f_{ij})e_{,l} - (\partial_2 f_{ij})_l q_{l'k} - (\partial_3 f_{ij})_{lm}\Phi_{lm'k} - (\partial_4 f_{ij})_l e_{,lk}$$
$$-(\partial_5 f_{ij})_{lm} q_{l'mk} - (\partial_6 f_{ij})_{lmn}\Phi_{lm'nk}) \geqslant 0.$$

Here ∂_n, $n=1,2,3,4,5,6$ denotes the partial derivatives of the constitutive functions according to the variables $(e, q_i, \Phi_{ij}, e_{,i}, q_{i'j}, \Phi_{ij'k})$, respectively. After some rearrangements of the inequality one obtains the Lagrange-Farkas multipliers from the first set of the Liu equations. These are obtained by imposing that the coefficients of the time derivatives vanish,

$$\partial_1 s = \Gamma^1, \tag{2.8}$$

$$(\partial_2 s)_i = \Gamma^2_i, \tag{2.9}$$

$$(\partial_3 s)_{ij} = \Gamma^3_{ij}, \tag{2.10}$$

$$(\partial_4 s)_i = \Gamma^4_i, \tag{2.11}$$

$$(\partial_5 s)_{ij} = \Gamma^5_{ij}, \tag{2.12}$$

$$(\partial_6 s)_{ijk} = \Gamma^6_{ijk}. \tag{2.13}$$

The second set of Liu equations is obtained by taking equal to zero the multipliers of the second order space derivatives. By applying (2.8)–(2.13) one can write them as

$$(\partial_4 j_i)_j + (\partial_5 s)_{il}(\partial_4 g_l)_j + (\partial_6 s)_{kli}(\partial_4 f_{kl})_j = 0, \tag{2.14}$$

$$(\partial_5 j_i)_{jk} - (\partial_4 s)_i \delta_{jk} + (\partial_5 s)_{mi}(\partial_5 g_m)_{jk} + (\partial_6 s)_{mni}(\partial_5 f_{mn})_{jk} = 0, \tag{2.15}$$

$$(\partial_6 j_i)_{jkl} + (\partial_5 s)_{mi}(\partial_6 g_m)_{jkl} + (\partial_6 s)_{mni}(\partial_6 f_{mn})_{jkl} = 0. \tag{2.16}$$

Finally the residual dissipation inequality can be written in the following form:

$$[\partial_1 j_i + (\partial_5 s)_{ji}\partial_1 g_j + (\partial_6 s)_{jki}\partial_1 f_{jk}]e_{,i} + [(\partial_2 j_j)_i - \partial_1 s\,\delta_{ij} + (\partial_5 s)_{kj}(\partial_2 g_k)_i + (\partial_6 s)_{klj}(\partial_2 f_{kl})_i]q_{i'j} + [(\partial_3 j_k)_{ij}$$
$$+ (\partial_5 s)_{lk}(\partial_3 g_l)_{ij} + (\partial_6 s)_{lmk}(\partial_3 f_{lm})_{ij}]\Phi_{ij'k} + (\partial_2 s)_i g_i + (\partial_3 s)_{ij} f_{ij} \geqslant 0. \tag{2.17}$$

It is easily seen that the Liu system (2.14)–(2.16) is composed by 117 differential equations constraining the set of the 832 partial derivatives of the constitutive functions s, j_i, g_i, f_{ij} with respect to the elements of the constitutive space $(e, q_i, \Phi_{ij}, e_{,i}, q_{i'j}, \Phi_{ij'k})$. Without some simplifications there is no hope to solve such a system.

In the following sections we are looking for special simplifying assumptions to solve the Liu equations (2.14)–(2.16) and the dissipation inequality (2.17). First we will investigate cases where some of the constitutive functions are assumed to be local.

III. SOLUTIONS OF THE LIU EQUATIONS—LOCALITY ASSUMPTIONS

A. Local state

Let us start the assumption of the local state in the form that the entropy is independent of the gradients,

$$s := s(e, q_i, \Phi_{ij}). \tag{3.1}$$

In this case the Liu equations (2.14)–(2.16) are simplified considerably and as a solution we obtain a local entropy current,

$$j_i = j_i(e, q_i, \Phi_{ij}). \tag{3.2}$$

The dissipation inequality (2.17) also simplifies,

$$\begin{aligned}&\partial_1 j_i e_{,i} + [(\partial_2 j_j)_i - \partial_1 s\,\delta_{ij}] q_{i'j} + (\partial_3 j_k)_{ij} \Phi_{ij'k} + (\partial_2 s)_i g_i + (\partial_3 s)_{ij} f_{ij} \\ &\quad = (j_i)_{,i} - \partial_1 s q_{i'i} + (\partial_2 s)_i g_i + (\partial_3 s)_{ij} f_{ij} \geqslant 0. \end{aligned} \tag{3.3}$$

B. Local state and local evolution

Let us investigate now the case when the evolution equations of the internal variables are ordinary differential equations, that is we assume that the constitutive quantities g_i and f_{ij} take the local form,

$$g_i := g_i(e, q_j, \Phi_{jk}), \tag{3.4}$$

$$f_{ij} := f_{ij}(e, q_j, \Phi_{jk}). \tag{3.5}$$

Now the dissipation inequality simplifies further the possible constitutive functions, because the coefficients of the derivatives should disappear. These restrictions result in a rather unusual material, since we get

$$j_i = j_i(q_j), \quad \frac{\partial j_i}{\partial q_j} = \frac{\partial s}{\partial e}\delta_{ij}. \tag{3.6}$$

On the other hand, the dissipation inequality can be written in a force-current form and can be solved for the constitutive functions g_i and f_{ij},

$$(\partial_2 s)_i g_i + (\partial_3 s)_{ij} f_{ij} \geqslant 0.$$

By (3.6) it follows that the temperature of the material $\partial s/\partial e$ is independent of the internal energy. Such a property is in contrast with the physical reality. We conclude that some nonlocality is necessary in modelling rigid heat conductors.

C. Local evolution

Let us assume now that the evolution of the internal variables is local, but there is no local state, therefore we require (3.4) and (3.5), but (3.1) is not assumed. In this case the entropy current is nonlocal, but the nonlocality is rather reduced. The Liu equations (2.14) and (2.16) give that the entropy current does not depend on the gradients of e and Φ, and (2.15) simplifies to

$$\frac{\partial j_i}{\partial q_{j'k}} = \frac{\partial s}{\partial e_{,i}}\delta_{jk}.$$

The nonlocality in the q_i is due to balance form of the evolution equation of the internal energy (2.1). From the above constraint one can easily see, that the entropy current is local if we further assume that the entropy is local in the internal energy,

$$s := s(e, q_i, \Phi_{ij}, q_{i'j}, \Phi_{ij'k}).$$

IV. SOLUTIONS OF THE ENTROPY INEQUALITY IN CASE OF LOCAL STATE

As we have seen above, the Liu equations are trivially solvable in the local state. However, the solution of the dissipation inequality can be achieved only with further assumptions. Moreover, there are different assumptions to have physical models, to introduce suitable gradient dependencies. In Classical Irreversible Thermodynamics[5] and in Rational Thermodynamics[20] the mentioned requirement of nonlocality is achieved by introducing the gradient of temperature (or, equiva-

lently, of the internal energy) into the constitutive space. In Extended Thermodynamics[6,7] the constitutive space is local but the evolution equations are balances, they have a special nonlocal form. All kinds of theories of Extended Thermodynamics resulted in more or less satisfactory models of different phenomena, but they provide different solutions of the entropy inequality.

A. Local state and special nonlocal evolution: linear nonlocality

In this case the evolution equations depend linearly on the gradients,

$$g_i := A_{ij}e_{,j} + B_{ijk}q_{k'j} + C_{ijkl}\Phi_{kl'j}, \tag{4.1}$$

$$f_{ij} := D_{ijk}e_{,k} + E_{ijkl}q_{l'k} + F_{ijklm}\Phi_{lm'k}, \tag{4.2}$$

where $A_{ij}, B_{ijk}, C_{ijkl}, D_{ijk}, E_{ijkl}, F_{ijklm}$ are local constitutive functions.

Now the dissipation inequality (2.17) reduces to a solvable form as

$$(\partial_1 j_i + (\partial_2 s)_j A_{jk} + (\partial_3 s)_{jk} D_{jki}) e_{,i} \tag{4.3}$$

$$+ ((\partial_2 j_j)_i - \partial_1 s\,\delta_{ij} + (\partial_2 s)_k B_{kji} + (\partial_3 s)_{kl} E_{klji}) q_{i'j} \tag{4.4}$$

$$+ ((\partial_3 j_k)_{ij} + (\partial_2 s)_l C_{lkij} + (\partial_3 s)_{lm} F_{lmkij}) \Phi_{ij'k} \geqslant 0. \tag{4.5}$$

As the quantities in the parentheses are local functions they should be zero, respectively. Therefore we get

$$\partial_1 j_i = -(\partial_2 s)_j A_{jk} - (\partial_3 s)_{jk} D_{jki}, \tag{4.6}$$

$$(\partial_2 j_j)_i = \partial_1 s\,\delta_{ij} - (\partial_2 s)_k B_{kji} - (\partial_3 s)_{kl} E_{klji}, \tag{4.7}$$

$$(\partial_3 j_k)_{ij} = -(\partial_2 s)_l C_{lkij} - (\partial_3 s)_{lm} F_{lmkij}. \tag{4.8}$$

These equations cannot be solved without any further ado. However, we can see that even if we do not know anything on the entropy current j_i they result in strong correlations on the entropy derivatives and the evolution equation, as the mixed partial derivatives of j_i should be equal. On the other hand, let us observe that in this case the entropy production is zero, there is no dissipation.

B. Local state and special local evolution: balance form

In this case one assumes, that the evolution equations have a special balance form. Therefore there are potentials Q_{ij} and H_{ijk} of the fields $(A_{ij}, B_{ijk}, C_{ijkl})(e, q_i, \Phi_{ij})$ and $(D_{ijk}, E_{ijkl}, F_{ijklm}) \times (e, q_i, \Phi_{ij})$, respectively. The evolution equations can be written as

$$g_i := \partial_1 Q_{ij} e_{,j} + (\partial_2 Q_{ij})_k q_{k'j} + (\partial_3 Q_{ij})_{kl} \Phi_{kl'j}, \tag{4.9}$$

$$f_{ij} := \partial_1 H_{ijk} e_{,k} + (\partial_2 H_{ijk})_l q_{l'k} + (\partial_3 H_{ijk})_{lm} \Phi_{lk'k}. \tag{4.10}$$

The conditions (4.6)–(4.8) can be written as

$$\partial_1 j_i = -(\partial_2 s)_j \partial_1 Q_{ij} - (\partial_3 s)_{jk} \partial_1 H_{ijk}, \tag{4.11}$$

$$(\partial_2 j_j)_i = \partial_1 s\,\delta_{ij} - (\partial_2 s)_k (\partial_2 Q_{ij})_k - (\partial_3 s)_{kl} (\partial_2 H_{ijk})_l, \tag{4.12}$$

$$(\partial_3 j_k)_{ij} = -(\partial_2 s)_l (\partial_3 Q_{ij})_{kl} - (\partial_3 s)_{lm} (\partial_3 H_{ijk})_{lm}. \tag{4.13}$$

As a consequence the above system of equations can be solved, as the entropy current is a potential of the field (q_i, Q_{ij}, H_{ijk}), therefore it can be conveniently written as

$$j_i(e, q_i, \Phi_{ij}) = \tilde{j}_i(q_i, Q_{ij}, H_{ijk}). \tag{4.14}$$

This fact can be expressed also with differential forms, according to the traditions of thermodynamics

$$\mathrm{d}\tilde{j}_i = \partial_1 s \, \mathrm{d}q_i + (\partial_2 s)_j \, \mathrm{d}Q_{ji} + (\partial_3 s)_{jk} \, \mathrm{d}H_{jki} = \Gamma^1 \, \mathrm{d}q_i + \Gamma^2_j \, \mathrm{d}Q_{ji} + \Gamma^3_{jk} \, \mathrm{d}H_{jki}. \tag{4.15}$$

The derivatives of the entropy current are identical to the intensives, the derivatives of the entropy functions. However, the variables are different. This form results in serious restrictions of the entropic intensives, and the currents Q_{ij} and H_{ijk} because the mixed second partial derivatives should be equal in these variables, too. Expressed in the basic variables the above requirements are rather ugly

$$(\partial_{22} s)_{kj} \partial_1 Q_{ki} + (\partial_{23} s)_{lkj} \partial_1 H_{lki} = \partial_{11} s \, \delta_{ij} + (\partial_{12} s)_k (\partial_2 Q_{ik})_j + (\partial_{13} s)_{lk} (\partial_2 H_{lki})_j, \tag{4.16}$$

$$(\partial_{32} s)_{ljk} \partial_1 Q_{li} + (\partial_{33} s)_{lmjk} \partial_1 H_{lmi} = (\partial_{12} s)_l (\partial_3 Q_{li})_{jk} + (\partial_{13} s)_{lm} (\partial_3 H_{lmi})_{jk}, \tag{4.17}$$

$$(\partial_{31} s)_{kl} \delta_{ij} + (\partial_{32} s)_{mkl} (\partial_2 Q_{im})_j + (\partial_{33} s)_{mnkl} (\partial_2 H_{mni})_j = (\partial_{22} s)_{ml} (\partial_3 Q_{mi})_{jk} + (\partial_{32} s)_{mnl} (\partial_3 H_{mni})_{jk}. \tag{4.18}$$

The property (4.15) is an important consequence of the balance form of the evolution equations. It is independent of the choice of the basic variables. If one assumes, e.g., that the chosen internal variable is the current of the heat flux, $\Phi_{ij} = Q_{ij}$, as it is usual in extended thermodynamics, then the above system of requirements simplifies but does not disappear.

In Rational Extended Thermodynamics it was shown that the above result of the phenomenological theory can be in accordance with the kinetic theory of gases, at least with a classical formulation of kinetic physics. A crucial step in the different systems was the choice of the phenomenological variables (we will see that all of the currents cannot be chosen as internal variables without any further ado) and the use of source terms in the balances.

C. Local state and balance form evolution: isotropy

The system (4.16)–(4.18) does not have a general solution for the currents. Q_{ij} and H_{ijk} cannot be determined by the entropy function in general. Therefore we have lost one of the basic flavors of irreversible thermodynamics, that the requirements of the second law can be exploited constructively to find the appropriate evolution equations. Now the dissipation inequality was solved, but the evolution equations cannot be determined constitutively.

Jou *et al.* gave some simplifying conditions to have a solution of the conditions (4.16)–(4.18) on the phenomenological level.[21] They have assumed a local state, balance form evolution equations and a simpler set of variables, they introduced only q_i as an additional variable. Then only condition (4.16) applies in a simplified form as

$$(\partial_{22} s)_{kj} \partial_1 Q_{ki} = \partial_{11} s \, \delta_{ij} + (\partial_{12} s)_k (\partial_2 Q_{ik})_j.$$

Moreover they have assumed *isotropic materials*, when all scalar valued functions, including the entropy, depend only on $q^2 = q_i q_i$ and the flux of the heat current and the entropy current can be written as

$$Q_{ij} = \beta(e, q^2) + \psi(e, q^2) q_i q_j, \tag{4.19}$$

$$j_i = \Psi(e, q^2) q_i. \tag{4.20}$$

Now the requirement (4.15) results in the following system of equations, as (4.2)–(4.4) in Ref. 21:

$$\partial_e \Psi = 2\partial_{q^2} s(\partial_e \beta + \partial_e \psi q^2), \tag{4.21}$$

$$\Psi = \partial_{e^s} + 2\partial_{q^2} s \psi q^2, \tag{4.22}$$

$$\partial_{q^2} \Psi = 2\partial_{q^2} s(\partial_{q^2} \beta + \partial_{q^2} \psi q^2). \tag{4.23}$$

Therefore the entropy current can be written as

$$j_i = (\partial_e s + 2\partial_{q^2} s \psi q^2) q_i. \tag{4.24}$$

After further calculations, considering also the requirement (4.16), one can get explicit solutions for the functions β and ψ together with some additional restriction on the form of the entropy function.

V. LOCAL STATE AND SPECIAL ENTROPY CURRENT

A different solution of the dissipation inequality can be given with the help of the entropy current. As in our previous work[8] we consider the local entropy of the form (1.1). This general form is motivated by the requirement of the thermodynamic stability, or, equivalently the requirement of the concavity of the entropy function on the nonequilibrium part of the state space (spanned by q_i and Φ_{ij}). Therefore, m_{ij} and n_{ijkl} are positive definite constitutive functions. Moreover, let us assume the entropy current takes the form (1.2) and let us introduce the convenient notations $\hat{m}, \hat{n}, \tilde{n}, \tilde{m}$ as follows:

$$(\partial_2 s)_i = -m_{ij} q_j - \tfrac{1}{2}(\partial_2 m_{lj})_i q_l q_j - \tfrac{1}{2}(\partial_2 n_{rjkl})_i \Phi_{rj} \Phi_{kl} = -\hat{m}_{ij} q_j - (\partial_2 \tilde{n}_{jk})_i \Phi_{jk}, \tag{5.1}$$

$$(\partial_3 s)_{ij} = -\tfrac{1}{2}(\partial_3 m_{lk})_{ij} q_l q_k - n_{ijkl} \Phi_{kl} - \tfrac{1}{2}(\partial_3 n_{lkrs})_{ij} \Phi_{lk} \Phi_{rs} = -(\partial_3 \tilde{m}_k)_{ij} q_k - \hat{n}_{ijkl} \Phi_{kl}. \tag{5.2}$$

If m_{ij} and n_{ijkl} are constant, then $\hat{m}_{ij}=m_{ij}$, $\hat{n}_{ijkl}=n_{ijkl}$, $(\partial_3 \tilde{m}_k)_{ij}=0$, and $(\partial_2 \tilde{n}_{jk})_i=0$.

Let us emphasize again that the entropy, written in the Gyarmati form (1.1) and the entropy current, written in (1.2) are only convenient notations as long as the corresponding inductivities and current multipliers are general constitutive functions.

With the (1.2) form of the entropy current and using the notations of (5.1) and (5.2) the dissipation inequality (3.3) in local state can be written in the following form:

$$[A_{ji'j} - \hat{m}_{ij} g_j - (\partial_3 m)_{kji} f_{ik}] q_i + [A_{ij} - \partial_1 s \delta_{ij}] q_{j'i} + [B_{kij'k} - (\partial_2 n)_{kji} g_k - \hat{n}_{ijkl} f_{kl}] \Phi_{ij} + B_{ijk} \Phi_{jk'i} \geqslant 0. \tag{5.3}$$

Seemingly the system is a normal force-current system, because the coefficients of the thermodynamic forces $q_i, q_{i,j}, \Phi_{ij}, \Phi_{ijk}$ all contain undetermined constitutive quantities $A_{ij}, g_i, f_{ij}, B_{ijk}$, respectively. However, let us observe that in local state g_i and f_{ij} are nonlocal but all other terms are local in the above inequality. This fact introduces degeneracy since, although the coefficients of the derivatives $q_{i'j}$ and $\Phi_{ij'k}$ cannot disappear, their possible couplings are rather reduced, e.g., B_{ijk} is local, therefore cannot depend on its own force $\Phi_{ij'k}$.

In this degenerate case the solution of the dissipation inequality is not straightforward.

Fortunately we can avoid the treatment of degeneracy, e.g., by assuming that m_{ij} and n_{ijkl} depend only on the internal energy and introducing the form (1.3) of the entropy current with the assumptions $A_{ij}=\partial_1 s \delta_{ij}$ and $B_{ijk}=(\partial_2 s)_k \delta_{ij}$. In this particular case the dissipation inequality reduces to

$$((\partial_1 s)_{,i} - m_{ij}g_j - m_{ki}\Phi_{jk'j})q_i + (-m_{jl}q_{l'i} - n_{ijkl}f_{kl})\Phi_{ij} \geqslant 0. \tag{5.4}$$

This is a force-current system, with the following Onsagerian solution:

$$-m_{ij}(\dot{q}_j + \Phi_{kj'k}) + (\partial_1 s)_{,i} = L^{11}_{ij}q_j + L^{12}_{ijk}\Phi_{jk}, \tag{5.5}$$

$$-n_{ijkl}\dot{\Phi}_{kl} - m_{jl}q_{l'i} = L^{21}_{ijk}q_k + L^{22}_{ijkk}\Phi_{kl}. \tag{5.6}$$

The system above conserves the structure already obtained in Ref. 8 in the case of local state. One should emphasize the central role of the invertibility of the matrices m_{ij} and n_{ijkl} in order to obtain the balance form. Such a property is not trivial since there exist real materials for which it is not guaranteed. A classical example is given in Ref. 22, where an electric circuit described by dynamic variables is considered.

As it was observed in Ref. 8 the second equation is a phenomenological closure of the system (2.1) and (5.5). It is remarkable that we have recovered the usual phenomenological structure of extended irreversible thermodynamics keeping the entropy current of the form (1.3). The same is not true for the constitutive equation (1.2) which, in the case of first order nonlocality, seems to be much too general. However, the compatibility of the entropy current of Verhás (1.3) and the requirements of the balance form (4.15) is valid only with the restriction that the conductivities depend only on the internal energy. The mentioned solution of Jou *et al.* (4.24) clearly does not have the Verhás form and indicates the necessity of a more general treatment.

In the next section we study the same problem in the presence of second order nonlocality.

VI. SECOND ORDER NONLOCALITY—SOLUTION IN LOCAL STATE

Now we will extend our investigations to consider second order nonlocalities. However, for the sake of simplicity we will investigate only the case of local entropy, i.e., systems in local state. The basic state is spanned by the variables (e, q_i, Φ_{ij}) as previously. However, the constitutive space contains the second order space derivatives and is spanned by $(e, q_i, \Phi_{ij}, e_{,i}, q_{i'j}, \Phi_{ij'k}, e_{,ij}, q_{i'jk}, \Phi_{ij'kl})$. Therefore, in the exploitation of the entropy inequality (2.7) we should consider as constraints the evolution equations (2.1)–(2.3), their first prolongations (2.4)–(2.6) and also their second prolongations as follows:

$$\dot{e}_{,ij} + q_{j'jik} = 0, \tag{6.1}$$

$$\dot{q}_{i'jk} - g_{i,jk} = 0, \tag{6.2}$$

$$\dot{\Phi}_{ij'kl} - f_{ij'kl} = 0. \tag{6.3}$$

Our simplifying condition of local entropy can be written as

$$s = s(e, q_i, \Phi_{ij}).$$

Let us introduce again the Lagrange-Farkas multipliers Γ^1, Γ^2_i, Γ^3_{ij}, Γ^4_i, Γ^5_{ij}, and Γ^6_{ijk} for the evolution equations (2.1)–(2.3) and their prolonged forms (2.4)–(2.6), respectively. The multipliers Γ^7_{ij}, Γ^8_{ijk}, and Γ^9_{ijkl} stand for the second prolongations (6.1)–(6.3), respectively. The Liu procedure gives

$$\begin{aligned}
&\partial_1 s\dot{e} + (\partial_2 s)_i\dot{q}_i + (\partial_3 s)_{ij}\dot{\Phi}_{ij} + (\partial_1 j_i)e_{,i} + (\partial_2 j_i)_j q_{j'i} + (\partial_3 j_i)_{jk}\Phi_{jk'i} + (\partial_4 j_i)_j e_{,ij} + (\partial_5 j_i)_{jk}q_{j'ki} \\
&\quad + (\partial_6 j_i)_{jkl}\Phi_{jk'li} + (\partial_7 j_i)_{jk}e_{,ijk} + (\partial_8 j_i)_{jkl}q_{j'kli} + (\partial_9 j_i)_{jklm}\Phi_{jk'lmi} - \Gamma^1(\dot{e} + q_{i'i}) - \Gamma^2_i(\dot{q}_i - g_i) \\
&\quad - \Gamma^3_{ij}(\dot{\Phi}_{ij} - f_{ij}) - \Gamma^4_i(\dot{e}_{,i} + q_{j'ji}) - \Gamma^5_{ij}[\dot{q}_{i'j} - (\partial_1 g_i)e_{,j} - (\partial_2 g_i)_k q_{k'j} - (\partial_3 g_i)_{kl}\Phi_{kl'j} - (\partial_4 g_i)_k e_{,kj}
\end{aligned}$$

$$
\begin{aligned}
&-(\partial_5 g_i)_{kl} q_{k'lj} - (\partial_6 g_i)_{klm} \Phi_{kl'mj} - (\partial_7 g_i)_{kl} e_{,klj} - (\partial_8 g_i)_{klm} q_{k'lmj} - (\partial_9 g_i)_{klmn} \Phi_{kl'mnj}] - \Gamma^6_{ijk} [\dot{\Phi}_{ij'k} \\
&- (\partial_1 f_{ij}) e_{,k} - (\partial_2 f_{ij})_l q_{l'k} - (\partial_3 f_{ij})_{lm} \Phi_{lm'k} - (\partial_4 f_{ij})_l e_{,lk} - (\partial_5 f_{ij})_{lm} q_{l'mk} - (\partial_6 f_{ij})_{lmn} \Phi_{lm'nk} \\
&- (\partial_7 f_{ij})_{lm} e_{,lmk} - (\partial_8 f_{ij})_{lmn} q_{l'mnk} - (\partial_9 f_{ij})_{lmno} \Phi_{lm'nok}] - \Gamma^7_{ij} (\dot{e}_{ij} + q_{k'kij}) - \Gamma^8_{ijk} (\dot{q}_{i'jk} - g_{i'jk}) \\
&- \Gamma^9_{ijkl} (\dot{\Phi}_{ij'kl} - f_{ij'kl}) \geqslant 0.
\end{aligned}
$$

Here ∂_n, $n=1,2,3,4,5,6,7,8,9$ denotes the partial derivatives of the constitutive functions according to the variables of the constitutive space $(e, q_i, \Phi_{ij}, e_{,i}, q_{i'j}, \Phi_{ij'k}, e_{,ij}, q_{i'jk}, \Phi_{ij'kl})$, respectively. The first set of Liu equations defines the Lagrange-Farkas multipliers as the derivatives of the entropy and gives that the last six multipliers are zero, due to the local state,

$$\partial_1 s = \Gamma^1, \tag{6.4}$$

$$(\partial_2 s)_i = \Gamma^2_i, \tag{6.5}$$

$$(\partial_3 s)_{ij} = \Gamma^3_{ij}, \tag{6.6}$$

$$\Gamma^4_i = 0, \tag{6.7}$$

$$\Gamma^5_{ij} = 0, \tag{6.8}$$

$$\Gamma^6_{ijk} = 0, \tag{6.9}$$

$$\Gamma^7_{ij} = 0, \tag{6.10}$$

$$\Gamma^8_{ijk} = 0, \tag{6.11}$$

$$\Gamma^9_{ijkl} = 0. \tag{6.12}$$

Considering (6.7)–(6.12) the second set of Liu equations are also simple,

$$(\partial_7 j_i)_{jk} = 0, \tag{6.13}$$

$$(\partial_8 j_i)_{jkl} = 0, \tag{6.14}$$

$$(\partial_9 j_i)_{jklm} = 0. \tag{6.15}$$

Therefore the entropy current presents only first order nonlocalities

$$j_i = j_i(e, q_i, \Phi_{ij}, e_{,i}, q_{i'j}, \Phi_{ij'k}).$$

Considering the above conditions the dissipation inequality can be written exactly in the same form as it was in case of first order nonlocal constitutive space (3.3),

$$(j_i)_{,i} - \partial_1 s q_{i'i} + (\partial_2 s)_i g_i + (\partial_3 s)_{ij} f_{ij} \geqslant 0. \tag{6.16}$$

On the other hand, now the constitutive quantities are higher orderly nonlocal, the entropy current is a first order nonlocal quantity and g_i and f_{ij} are second order nonlocal quantities. Let us introduce the same assumptions on the form of the entropy and of the entropy current as previ-

ously with assuming (1.1) and (1.2) with the notations (5.1) and (5.2) but letting the current multipliers A_{ij} and B_{ijk} to contain first order nonlocalities. The dissipation inequality can be written in the same form as above

$$[A_{ji'j} - \hat{m}_{ij}g_j - (\partial_3 m)_{kji}f_{ik}]q_i + [A_{ij} - \partial_1 s\delta_{ij}]q_{j'i} + [B_{kij'k} - (\partial_2 n)_{kji}g_k - \hat{n}_{ijkl}f_{kl}]\Phi_{ij} + B_{ijk}\Phi_{jk'i} \geqslant 0. \tag{6.17}$$

However, in this case it is a nondegenerate force-current system, due to the extension of the constitutive state space. All additive terms contain unknown functions. Therefore one can give an Onsagerian solution as follows:

$$-\hat{m}_{ij}g_j - (\partial_3 m)_{ijk}f_{jk} + A_{ji'j} = L^{11}_{ij}q_j + L^{12}_{ijk}q_{j'k} + L^{13}_{ijk}\Phi_{jk} + L^{14}_{ijkl}\Phi_{jk'l}, \tag{6.18}$$

$$A_{ij} - \partial_1 s\delta_{ij} = L^{21}_{ijk}q_k + L^{22}_{ijkl}q_{k'l} + L^{23}_{ijkl}\Phi_{kl} + L^{24}_{ijklm}\Phi_{kl'm}, \tag{6.19}$$

$$-(\partial_2 n)_{kji}g_k - \hat{n}_{ijkl}f_{kl} + B_{kij'k} = L^{31}_{ijk}q_k + L^{32}_{ijkl}q_{k'l} + L^{33}_{ijkl}\Phi_{kl} + L^{34}_{ijklm}\Phi_{kl'm}, \tag{6.20}$$

$$B_{ijk} = L^{41}_{ijkl}q_l + L^{42}_{ijklm}q_{l'm} + L^{43}_{ijklm}\Phi_{lm} + L^{44}_{ijklmn}\Phi_{lm'n}. \tag{6.21}$$

Here $L^{11}, L^{12}, L^{13}, L^{14}, L^{21}, L^{22}, L^{23}, L^{24}, L^{31}, L^{32}, L^{33}, L^{34}, L^{41}, L^{42}, L^{43}, L^{44}$ are constitutive functions with the suitable definiteness restrictions. Moreover (6.18) and (6.20) are the candidates of balances under suitable restrictions. It is worth noticing, that the current multipliers A_{ij} and B_{ijk} are given explicitly. Therefore, they can be easily eliminated from the above system substituting (6.19) into (6.18) and (6.21) into (6.20). The resulting set of equations is closed and contains first and second order derivatives of the basic state,

$$\begin{aligned} &-\hat{m}_{ij}\dot{q}_j - (\partial_3 m)_{ijk}\dot{\Phi}_{jk} + [\partial_1 s\delta_{ij} + L^{21}_{ijk}q_k + L^{22}_{ijkl}q_{k'l} + L^{23}_{ijkl}\Phi_{kl} + L^{24}_{ijklm}\Phi_{kl'm}]_{,j} \\ &\quad = L^{11}_{ij}q_j + L^{12}_{ijk}q_{j'k} + L^{13}_{ijk}\Phi_{jk} + L^{14}_{ijkl}\Phi_{jk'l}, \end{aligned} \tag{6.22}$$

$$\begin{aligned} &-(\partial_2 n)_{kji}\dot{q}_k - \hat{n}_{ijkl}\dot{\Phi}_{kl} + [L^{41}_{ijkl}q_l + L^{42}_{ijklm}q_{l'm} + L^{43}_{ijklm}\Phi_{lm} + L^{44}_{ijklmn}\Phi_{lm'n}]_{,k} \\ &\quad = L^{31}_{ijk}q_k + L^{32}_{ijkl}q_{k'l} + L^{33}_{ijkl}\Phi_{kl} + L^{34}_{ijklm}\Phi_{kl'm}. \end{aligned} \tag{6.23}$$

As one can see, the evolution equations are rather general. They are more general than those given with the help of the entropy currents (1.3). On the other hand, the entropy current (4.24) is also a special case of the general (1.2). However, the compatibility to the current potential structure, expressed by (4.15), cannot be expressed explicitly in general. Equation (1.2) is definitely more general regarding the nonlocality, moreover, (4.24) proves, that it can be compatible with the potential structure in special cases. However, it definitely restricts the functional form of the current multipliers A_{ij} and B_{ijk}.

Moreover, the potential structure is unavoidable requiring locality and balance form evolution equations. If m_{ij} and n_{ijkl} are constant a balance structure similar to that obtained in Ref. 8 is recovered. This fact represents the main effect of the enlargement of the state space since the balance structure is compatible with more general entropy fluxes.

VII. NONLOCAL SECOND SOUND: THE GUYER-KRUMHANSL EQUATION

Thermal wave propagation, sometime referred to as second sound, is a low temperature phenomenon which can be observed, for instance, in dielectric crystals such as sodium fluoride (NaF) and bismuth (Bi).[23,24,17] It requires an extension of the classical Fourier's theory in order to remove the paradox of infinite speed of propagation of thermal disturbances.[25] Phonon gas hydrodynamics[26,27] supplies a satisfactory explanation of heat transport at low temperature.

Phonons are quasiparticles which obey the Bose-Einstein statistics. In a solid crystal they form a rarefied gas whose kinetic equation can be derived similarly to that of an ordinary gas. Phonons may interact among themselves and with lattice imperfections through two different types of processes:

(i) normal (N) processes, that conserve the phonon momentum;
(ii) resistive (R) processes, in which the phonon momentum is not conserved.

The frequencies ν_N and ν_R of normal and resistive processes determine the characteristic relaxation times $\tau_N=1/\nu_N$ and $\tau_R=1/\nu_R$. Diffusive processes take over when there are many more R processes than N processes. If instead there are only a few R processes and many more N processes, then a wavelike energy transport may occur.

Such a phenomenology is satisfactorily described by the Guyer-Krumhansl equation,[14] Eq. (57) (see also Refs. 28 and 15).

$$\dot{q}_i+\frac{1}{\tau_R}q_i+\frac{1}{3}c^2c_V T_{,i}=\frac{1}{5}\tau_N c^2(q_{i'jj}+2q_{j'ji}), \tag{7.1}$$

where $T=\hat{T}-T_0$ is the temperature variation (T is the temperature and T_0 is the average temperature). c_V is the specific heat and c means the Debye phonons velocity. Such an equation, which generalizes the Maxwell-Cattaneo-Vernotte equation[25]

$$\tau_R\dot{q}_i+q_i=-\tau_R\tfrac{1}{3}c^2c_V T_{,i}, \tag{7.2}$$

was the first in the literature to include both relaxation times. It can be obtained by the linearized Boltzman equation for phonons in the Debye approximation, if one maintains terms $O(\tau_N)$.[14] The material coefficients τ_N, τ_R, and c_V are all dependent on the temperature. According to experimental observations[16] one can get

$$c_V=aT^3,\quad \tau_R=de^{-\alpha/T},\quad \tau_N=bT^{-m}.$$

Here a,b,d,α are constant coefficients and $m\in\{3,4,5\}$ depending on the material. Let us remark that the last function, a temperature dependent τ_N is clearly contradictory to the assumptions made by Guyer and Krumhansl,[14] and did not consider, that (7.1) is a linearized equation.

In extended thermodynamics the Guyer-Krumhansl equation can be recovered in a 4-field theory provided one assumes weakly nonlocal constitutive equations for the internal energy e and for the momentum flux.[17]

However, such an approach seems to be questionable because

(i) a nonlocal constitutive space is in contrast with the basic assumptions of extended thermodynamics,
(ii) a nonlocal internal energy does not assure that the specific heat $c_V=\partial e/\partial T$ is positive,
(iii) a nonlocal internal energy would modify also the energy balance.

The last observation was pointed out also by Dreyer and Struchtrup and they suggested to consider higher order moments.[6,7] The other important question is the temperature dependency of the coefficients. A phenomenological theory cannot predict the exact form to the constitutive functions, but gives restrictions and interrelations. These restrictions on the temperature dependencies are frequently treated rather loosely to get the compatibility with the *linearized* kinetic theory.[14,6]

These problems do not arise in the present theory. In fact, we can obtain the equation (7.1) by considering a 4-field model with second order nonlocality, namely the balance equation (6.22) with $\Phi_{ij}=0$ and m_{ij} depending only on the internal energy. It yields

$$-m_{ij}\dot{q}_j+\left[\partial_1 s\,\delta_{ij}+L^{21}_{ijk}q_k+L^{22}_{ijkl}q_{k'l}\right]_{,j}=L^{11}_{ij}q_j+L^{12}_{ijk}q_{j'k}. \tag{7.3}$$

It is convenient to choose as equilibrium thermodynamic variable the absolute temperature T_a instead of the internal energy e. Let us assume the constitutive equations $L^{21}_{ijk}=L^{12}_{ijk}=0$. We may exploit the thermodynamic relation $1/T_a=\partial s/\partial e$ and introduce the temperature perturbation T by $T_a=T_0+T$, where T_0 is a background (average) temperature. Now, Eq. (7.3) reduces to

$$m_{ij}\dot{q}_j+L^{11}_{ij}q_j+\frac{1}{T^2}T_{,i}=L^{22}_{ijkl}q_{k'lj}. \tag{7.4}$$

Here m_{ij}, L^{11}_{ij}, and L^{22}_{ijkl} can depend on the background temperature T_0. Finally, equation (7.1) is easily obtained by (7.4) under the further constitutive assumptions,

$$m_{ij}=\frac{3}{c^2aT^5}\delta_{ij}, \tag{7.5}$$

$$L^{11}_{ij}=\frac{3}{c^2aT^5}e^{\alpha/T}\delta_{ij}, \tag{7.6}$$

$$L^{22}_{ijkl}=\frac{3b}{5aT^{5+m}}\delta_{ij}\delta_{kl}. \tag{7.7}$$

That way, the Guyer-Krumhansl theory may be obtained in a classical macroscopic framework. Let us remark, that the previous phenomenological linearization is only a last step in the calculation based on the linearization of the Boltzmann equation [Eq. (57)–Eq. (59) in Ref. 14]. A similar result has been obtained in Ref. 29.

VIII. CONCLUSIONS

We have shown that Classical Irreversible Thermodynamics supplemented with dynamic degrees of freedom is consistent with the idea of higher order fluxes as independent thermodynamic variables. In such a framework the balance form of the evolution equations can be obtained under suitable constitutive assumptions. The locality of the entropy density, i.e., the local state assumption, plays a central role. Moreover, the nonlocality of the constitutive functions results in a wide class of materials including the classical Cattaneo and Guyer-Krumhansl heat conductors, which normally are derived from kinetic theory. Let us observe that the model above encompasses all extended thermodynamic models, since the balance structure represents a very particular form of nonlocal evolution equations (2.2) and (2.3).

Considering that the balance is not the only possible form of the evolution equations, the nomination of the internal variable as a "higher order flux" can be misleading. However, if the tensorial order of the internal variables increases and we are in a local state, the evolution equations are close to a balance form (except the closure) and the flux interpretation is straightforward. However, the exploitation method of the second law reveals applications far beyond the heat conduction problem. An internal variable can be responsible for different microstructural effects with a well-defined microphysical interpretation where one must consider the most general expression of the entropy current (and sometimes it is not enough). Here we only want to call the attention to the role of the entropy current in the thermodynamic derivations of the Ginzburg-Landau equation where the microstructure have a definite meaning.[3,30,31,19]

Although in the present investigations the highest order flux is only the flux of the heat flux (Φ_{ij}), there is no principal reason of restricting ourselves to the second order case. One can easily extend the ideas of the recent investigation to the higher order cases and to derive, e.g., closure relations at a higher level of the hierarchy.

Figure 1 shows the connections between the constitutive assumptions and the thermodynamic restrictions, as far as the locality and nonlocality are concerned. The last column refers to the

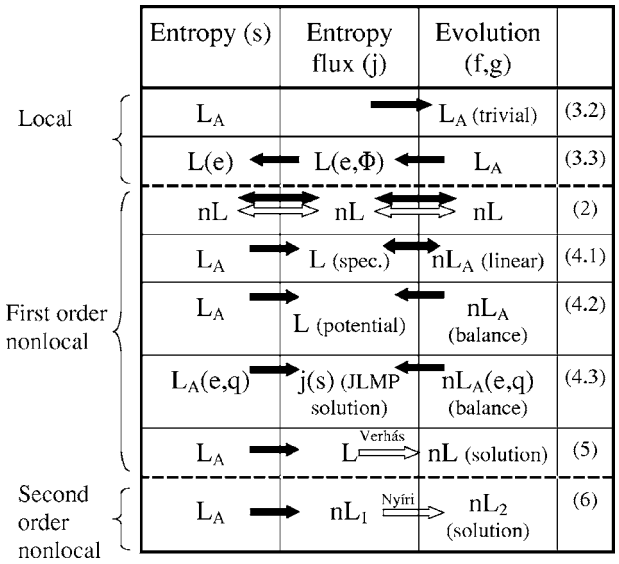

FIG. 1. Logical relations of nonlocality assumptions in nonequilibrium thermodynamics. Interplay of nonlocality in entropy (s), in entropy flux (j) and in the evolution of higher order fluxes (f,g) (2.2)–(2.2). Notations, L, local; nL, nonlocal; $L(e)$, local in the variable e; L_A, assumed locality; L_i, ith order nonlocal, black arrow, consequence of the Liu equations, white arrow, consequence of the dissipation inequality.

corresponding section of the paper. L_A denotes a locality assumption. The double-headed arrows denote specific interrelations, e.g., the black double-headed arrows in the first row denote equations (2.14)–(2.16), that give conditions between the entropy and entropy current functions and evolution equations. The fifth row refers to Rational Extended Thermodynamics and the sixth row to the specific solution of the potential restriction given by Jou *et al.* As in Extended Thermodynamics the dissipations inequality is fulfilled as an equality, we cannot conclude anything on the dissipative constitutive functions (that is why there are no white arrows in these rows). Let us observe, that assumptions on the form of the entropy current makes possible to build all requirements of the second law into the evolution equations in general (last two rows). In this case the second law becomes a material property, satisfied independently of the initial conditions and the resulted constitutive functions depend only on the material.

It is worth noticing that the potential form of the entropy current and the balance structure is compatible with the general form of the entropy current, such as that proposed by Nyíri, which yields (1.3) when $A_{ij}=\partial_1 s\,\delta_{ij}$ and $B_{ijk}=(\partial_2 s)_k\delta_{ij}$. In this case the balance structure results in restrictions for the current multipliers from the potential requirement (4.15).

We obtained closure relations both with local and nonlocal entropy current and in the first case the closure for the highest order flux was an ordinary differential equation. The obtained thermodynamic closure of the hierarchical structure stresses some deeper relations between the thermodynamic and the more detailed kinetic structure, similar to that recognized, e.g., in Ref. 32.

We reinspected the thermal wave propagation at low temperature and proved that the Guyer-Krumhansl theory of second sound can be derived in the framework of macroscopic nonlocal irreversible thermodynamics.

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An invariant variational principle for canonical flows on Lie groups

Zoltán Muzsnay[a)]
Department of Mathematics, University of Debrecen, Debrecen, H-4032, Hungary

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In this paper we examine the existence of Lie groups, whose canonical geodesic flows are variational with respect to a left-invariant regular—but not necessarily quadratic (i.e., metric)—Lagrange function. We give effective necessary and sufficient conditions for the existence of an invariant variational principle generating the canonical flow. With these results, taken in conjunction with the classification of Lie algebras, we solve the inverse problem of invariant Lagrangian dynamics in dimensions up to four. © *2005 American Institute of Physics.*
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I. INTRODUCTION

One of the basic objects of classical physics is the equation of motion of a system. In the most relevant cases it can be derived as the Euler-Lagrange equation of a regular Lagrange function. An old, and in the general case still unsolved problem, posed first in 1887 by Helmholtz, is the determination and classification of second order differential equations derivable from a variational principle. This is the inverse problem of the calculus of variations. Moreover, since the Euler-Lagrange equation inherits the symmetries of the Lagrangian, one can also consider the invariant version of the inverse problem of the calculus of variations, determine if an equation of motion possessing some symmetry property can be derived as the Euler-Lagrange equation of a regular Lagrangian having the same symmetry.

There are interesting examples of this phenomena in the cases of motions on Lie groups governed by the canonical symmetric, linear connections of the Lie group.[1] We remark that the corresponding canonical flow occurs in the one-dimensional reductions of well-known models of theoretical physics, like the σ or chiral models. One can say that all possible situations occur in these deceptively simple systems. This claim is illustrated by the following examples: (1) on a semisimple Lie group the canonical flow can be derived from the Lagrangian corresponding to the bi-invariant Killing metric of the Lie algebra. In this case the Lagrangian is obviously invariant; (2) on the Heisenberg group or on the affine group of the line the canonical flows are variational, but the Lagrangians are not invariant with respect to the natural action of the groups (see paragraph 5); (3) on the four-dimensional Lie groups $A_{4,7}$, $A_{4,9b}$, and $A_{4,11a}$ the canonical flows are not variational.[9]

Moreover, one can investigate the unicity of the Lagrangian (up to an inessential total derivative term). The unicity problem and the existence of invariant variational principle might be related to each other in some cases, as if the equation of motion has some symmetry, but the Lagrangian does not possess that one, then the Lagrangian is necessarily nonunique, as a new Lagrangian obtained from the old one by a symmetry transformation must give the same Euler-Lagrange equation.

In this paper we examine the existence of Lie groups, other than the semisimple groups, where the geodesic flow associated to the canonical connection is variational with respect to a left-invariant regular (but not necessarily quadratic, i.e., metric) Lagrange function. In this case we

[a)]Electronic mail: muzsnay@math.klte.hu

will say that there exists a G-invariant variational principle for the canonical flow of the group G. We give an effective necessary and sufficient condition for the existence of a G-invariant variational principle for the canonical flow. Using this result, we determine the Lie groups up to four dimensions for which the canonical flow is variational with respect to a nondegenerate left-invariant Lagrangian.

II. INVERSE PROBLEM OF THE CALCULUS OF VARIATIONS ON LIE GROUPS

On a Lie group G there are three kinds of natural linear connections, the plus, minus, and zero connections introduced first by Cartan and Schouten.[1] A simple way to define these connections is to give their values on left-invariant vector-fields X, Y by

$$\nabla^+_X Y = [X,Y], \quad \nabla^-_X Y = 0, \quad \nabla^0_X Y = \tfrac{1}{2}[X,Y],$$

and extend them to arbitrary vector fields by making them tensorial in the X argument and satisfy the Leibniz rule in the Y argument. The curvature tensors of the minus and plus connections are zero, but in general, the corresponding torsion tensors are nonvanishing. All three of the natural connections have the same geodesics. We shall denote ∇^0 simply by ∇ and refer to it as the canonical symmetric, linear connection.

Let $E: TG \to \mathbb{R}$ be a smooth function on the tangent bundle of a Lie group G, called the Lagrange function. For an arbitrary curve $g(t): [t_0, t_1] \to G$ one can consider the functional $I[g] := \int_{t_0}^{t_1} E(g(t), \dot{g}(t))\mathrm{d}t$. A standard argument shows that the functions $g(t)$ giving extrema of this functional (in the class of variations preserving the endpoints) satisfy the Euler-Lagrange equations. In standard local coordinates $\{g^i\}$ on G they are

$$\frac{d}{\mathrm{d}t}\left(\frac{\partial E}{\partial \dot{g}^i}\right) - \frac{\partial E}{\partial g^i} = 0. \tag{1}$$

If the Lagrangian E is regular, then (1) is a second order ordinary differential equation.

In a series of papers, Thompson and his co-workers investigated the inverse problem of Lagrangian dynamics for the geodesic flow associated to ∇ (see Refs. 2, 7, and 9). Here one wishes to decide if there exists a Lagrangian function defined on an open subset of the tangent bundle of the Lie group whose Euler-Lagrange equations coincide with the geodesic equations of ∇. In this paper we consider the invariant version of this problem. We examine the existence of Lie groups, whose canonical geodesic flows are variational with respect to a left-invariant regular—but not necessarily quadratic—Lagrange function.

III. DIFFERENTIAL GEOMETRIC BACKGROUND OF THE INVERSE PROBLEM OF THE CALCULUS OF VARIATIONS

We present here the basic objects that play a role in the theory. More details can be found in Refs. 5 and 7

If M is a manifold TM denotes its tangent space and π the natural submersion. Let $J: TTM \to TTM$ be the canonical vertical endomorphism, and let $C \in \mathfrak{X}(TM)$ be the Liouville vector field, if (x^α) is a local coordinate system on M and (x^α, y^α) is the induced coordinate system on TM, then

$$J = \mathrm{d}x^\alpha \otimes \frac{\partial}{\partial y^\alpha}, \quad C = y^\alpha \frac{\partial}{\partial y^\alpha}. \tag{2}$$

A *(non-linear) connection* on M is a tensor field of type (1-1) Γ on TM such that $J\Gamma = J$ and $\Gamma J = -J$ (see Ref. 4). If Γ is a connection, then $\Gamma^2 = id_{TTM}$ and the eigenspace corresponding to the eigenvalue -1 is the vertical space V_z. Then, at any $z \in TM$, we have the splitting $T_z TM = H_z \oplus V_z$, where H_z is the eigenspace corresponding to $+1$. The subspace H_z is called the horizontal space. In the sequel we will write

$$h := \tfrac{1}{2}(I+\Gamma), \quad v := \tfrac{1}{2}(I-\Gamma),$$

for the *horizontal* and *vertical* projectors.

Definition 1: A Lagrangian is a map $E: TM \to \mathbb{R}$ *that is smooth on at least an open subset of* TM. *The Lagrangian* E *is said to be regular if*

$$\det\left(\frac{\partial^2 E}{\partial y^\alpha \partial y^\beta}\right) \neq 0. \tag{3}$$

The Lagrangian E is regular if and only if the 2-form $\Omega_E := \mathrm{d}d_J E$ has maximal rank. In this case, the vector field S on TM defined by the equation

$$i_S \Omega_E = d(E - \mathcal{L}_C E) \tag{4}$$

is a spray (that is $JS=C$), and the paths of S are the solutions of the Euler-Lagrange equations,[3]

$$\frac{d}{\mathrm{d}t}\frac{\partial E}{\partial \dot{x}^\alpha} - \frac{\partial E}{\partial x^\alpha} = 0, \quad \alpha = 1, \ldots, n. \tag{5}$$

Let us fix a second order differential equation, or in other words a spray S on the manifold M. Then, to every Lagrangian E a scalar 1-form ω_E can be associated by

$$\omega_E := i_S \Omega_E + \mathrm{d}\mathcal{L}_C E - \mathrm{d}E, \tag{6}$$

which is called *Euler-Lagrange* form. According to Eq. (4) we have $\omega_E \equiv 0$ if and only if the path of the spray is the solution of the Euler-Lagrange equation (5) associated to E. (See Refs. 5 and 7.)

IV. LEFT-INVARIANT VARIATIONAL PRINCIPLE FOR THE CANONICAL CONNECTION

In the sequel we will consider the case, where $M := G$ is a Lie group. We will denote by $L_x g$ or simply by xg the left translation of $g \in G$ by $x \in G$. Let (x) be coordinates on G, and let (x,y) be the standard associated coordinate system on TG. We will also use the "left invariant" coordinates (x,α) on $TG \simeq G \times \mathfrak{g}$, where $\alpha = (L_{x^{-1}})_* y$ is the Maurer-Cartan form. The corresponding coordinates on TTG are (x,α,X,A), that is,

$$(x,\alpha,X,A) = X \left.\frac{\partial}{\partial x}\right|_{(x,\alpha)} + A \left.\frac{\partial}{\partial \alpha}\right|_{(x,\alpha)}.$$

Since the coordinates $\alpha=(\alpha_i)$ and $A=(A_i)$ are left-invariant coordinates, we find that the left translation by a group element g induces on TTG the following action:

$$L_g(x,\alpha,X,A) = (gx,\alpha,gX,A) = gX \left.\frac{\partial}{\partial x}\right|_{(gx,\alpha)} + A \left.\frac{\partial}{\partial \alpha}\right|_{(gx,\alpha)}.$$

The canonical projection $\pi: TG \to G$ is $(x,\alpha) \to x$, therefore $\pi_*: TTG \to TG$ is given by $(x,\alpha,X,A) \to (x,x^{-1}X)$ and the vertical subspace on $(x,\alpha) \in TG$ is

$$V_{(x,\alpha)}TG := \mathrm{Ker}\ \pi_* = \{(x,\alpha,0,b) | b \in \mathfrak{g}\}.$$

Second order differential equations are described by vector-fields S (called spray) on the tangent space, that have the characteristic property $JS=C$. On a Lie group the geodesic flow of the canonical connection is described by the system

$$\ddot{x} = \dot{x}x^{-1}\dot{x}, \tag{7}$$

and the vector field on the tangent space, corresponding to the geodesic flow of the canonical connection is the spray S where

$$S_{(x,\alpha)} = (x,\alpha,x\alpha,0) = x\alpha \left.\frac{\partial}{\partial x}\right|_{(x,\alpha)}. \tag{8}$$

Then γ_t is a geodesic of ∇ if and only if the equation $S_{\dot\gamma} = \ddot\gamma$ holds. The horizontal and vertical projections of the connection $\Gamma := [J,S]$ associated the spray S are h and v where

$$v(x,b,xa,c) = \left(x,b,0,\frac{1}{2}[a,b]+c\right) = \left(\frac{1}{2}[a,b]+c\right) \left.\frac{\partial}{\partial\alpha}\right|_{(x,b)},$$

$$h(x,b,xa,c) = \left(x,b,xa,-\frac{1}{2}[a,b]\right) = xa \left.\frac{\partial}{\partial x}\right|_{(x,b)} - \frac{1}{2}[a,b] \left.\frac{\partial}{\partial\alpha}\right|_{(x,b)},$$

therefore the horizontal and vertical lifts of a left-invariant vector field $X=(x,a)$ are

$$X^h_{(x,\alpha)} = \left(x,\alpha,xa,-\frac{1}{2}[a,\alpha]\right) = xa \left.\frac{\partial}{\partial x}\right|_{(x,\alpha)} - \frac{1}{2}[a,\alpha] \left.\frac{\partial}{\partial\alpha}\right|_{(x,\alpha)}, \tag{9}$$

$$X^v_{(x,\alpha)} = (x,\alpha,0,a) = a \left.\frac{\partial}{\partial\alpha}\right|_{(x,\alpha)}. \tag{10}$$

Moreover, with (x,α) as a local coordinate system, the vertical endomorphism and the Liouville vector fields are

$$J = (x^{-1}\,\mathrm{d}x)\otimes\frac{\partial}{\partial\alpha}, \quad C = \alpha\frac{\partial}{\partial\alpha}.$$

Indeed,

$$C_{(x,\alpha)} = \left.\frac{d}{\mathrm{d}t}\right|_{t=0} (x,e^t\alpha) = (x,\alpha,0,\alpha),$$

$$J(x,\alpha,A,B) = \left.\frac{d}{\mathrm{d}t}\right|_{t=0} (x,\alpha+tx^{-1}A) = (x,\alpha,0,x^{-1}A).$$

For more details see Ref. 7.

Let us examine the existence of a left-invariant variational principle for the canonical flow of Lie groups. We have the following.

Proposition 2: The canonical flow of the Lie group G is variational with respect a left-invariant Lagrangian if and only if there exists an ad-invariant function $\mathcal{E}:\mathfrak{g}\to\mathbb{R}$ with nondegenerate Hessian.

To prove the proposition, we compute the Euler-Lagrange equation for the canonical flow of G. Using the notation introduced in (6), the Euler-Lagrange partial differential equation associated to a spray S can be written as

$$\omega_E \equiv 0, \tag{11}$$

where the unknown is the Lagrangian E. Let us compute explicitly the equation (11). If $X=(x,a)$ denotes a left-invariant vector field on G corresponding to $a\in\mathfrak{g}$, and X^v, X^h are its vertical and horizontal lifts, then we have $\omega_E(X^v)\equiv 0$, since ω_E is semibasic. Moreover, we have

$$\begin{aligned}\omega_E(X^h) &= (i_S\,\mathrm{d}d_J E + \mathrm{d}\mathcal{L}_C\,E - \mathrm{d}E)(X^h) = \mathrm{d}d_J\,E(S,X^h) + \mathrm{d}\mathcal{L}_C\,E(X^h) - \mathrm{d}E(X^h)\\ &= S(JX^h(E)) - X^h(JS(E)) - J[S,X^h]E + X^h(C(E)) - X^hE\\ &= S(X^v(E)) - J[S,X^h]E - X^hE.\end{aligned}$$

Taking into account (8) and the local expression (9) of X^h we have

$$[X^h,S] = \left[xa\frac{\partial}{\partial x} - \frac{1}{2}[a,\alpha]\frac{\partial}{\partial\alpha}, x\alpha\frac{\partial}{\partial x}\right] = \frac{1}{2}x[a,\alpha]\frac{\partial}{\partial x},$$

$$J[X^h,S] = \frac{1}{2}J\left(x[a,\alpha]\frac{\partial}{\partial x}\right) = \frac{1}{2}[a,\alpha]\frac{\partial}{\partial\alpha},$$

and

$$\begin{aligned}\omega_E(X^h) &= x\alpha\frac{\partial}{\partial x}\left(a\frac{\partial}{\partial\alpha}(E)\right) - \frac{1}{2}[a,\alpha]\frac{\partial}{\partial\alpha}(E) - \left(xa\frac{\partial}{\partial x} - \frac{1}{2}[a,\alpha]\frac{\partial}{\partial\alpha}\right)E\\ &= x\alpha a\frac{\partial^2E}{\partial x\partial\alpha} + \frac{1}{2}[a,\alpha]\frac{\partial E}{\partial\alpha} - xa\frac{\partial E}{\partial x} + \frac{1}{2}[a,\alpha]\frac{\partial E}{\partial\alpha}\\ &= [a,\alpha]\frac{\partial E}{\partial\alpha} + x\alpha a\frac{\partial^2E}{\partial x\partial\alpha} - xa\frac{\partial E}{\partial x}.\end{aligned}$$

If the Lagrangian is left-invariant, then $\partial E/\partial x=0$ and we obtain that

$$\omega(X^h) = [a,\alpha]\frac{\partial E}{\partial\alpha},$$

consequently the canonical connection of the group G is variational with respect to a left-invariant regular Lagrangian E if and only if

$$\frac{\partial E}{\partial x} = 0, \tag{12}$$

$$[a,\alpha]\frac{\partial E}{\partial\alpha} = 0, \quad \forall\, a \in \mathfrak{g}, \tag{13}$$

where (12) expresses the fact that E is left-invariant and (13) expresses that E is a solution of the Euler-Lagrange equation (11). Therefore the canonical flow is variational with respect to an invariant Lagrangian if and only if the Frobenius differential system (12) and (13) has a solution $E: TG \simeq G\times\mathfrak{g}\to\mathbb{R}$ satisfying the regularity condition, or equivalently, there exists a function $\mathcal{E}:\mathfrak{g}\to\mathbb{R}$ satisfying the equation

$$[a,\alpha]\frac{\partial\mathcal{E}}{\partial\alpha} = 0, \tag{14}$$

for all $a\in\mathfrak{g}$, such that the Hessian matrix $(\partial^2\mathcal{E}/\partial\alpha_i\partial\alpha_j)$ is nondegenerate. The equation (14) is identically satisfied if and only if $\mathcal{E}$ is constant on the orbit of the *ad* representation of $\mathfrak{g}$.

□

Let $\{e_1,\ldots,e_n\}$ be a basis of $\mathfrak{g}$. Then the structure constants $C^\gamma_{\alpha\beta}$ of the Lie algebra $\mathfrak{g}$ are defined by

$$[e_\alpha,e_\beta] = C^\gamma_{\alpha\beta}e_\gamma. \tag{15}$$

We denote by (α_i) the coordinate of $\alpha\in\mathfrak{g}$. We have the following.

Theorem 3: *There exists a left-invariant variational principle for the canonical flow of the Lie group G in a neighborhood of a generic element $\alpha \in \mathfrak{g}$ if and only if the linear system*

$$C_{ij}^k \alpha_j x_k = 0, \quad i = 1, \ldots, n, \tag{16}$$

$$C_{ij}^k x_k + C_{jm}^k \alpha_m x_{ik} = 0, \quad i,j = 1, \ldots, n, \tag{17}$$

has a solution $\{x_i = \epsilon_i,\ x_{ij} = \epsilon_{ij}\}$ satisfying the condition $\det(\epsilon_{ij}) \neq 0$.

Proof: Let us consider the distribution Δ in the tangent space of $\mathfrak{g}$ defined as

$$\Delta_\alpha := \left\{ X_a := [a,\alpha] \left.\frac{\partial}{\partial \alpha}\right|_\alpha \middle| a \in \mathfrak{g} \right\},$$

for $\alpha \in \mathfrak{g}$. If a and b are two elements of the Lie algebra $\mathfrak{g}$, then

$$\left[[a,\alpha]\frac{\partial}{\partial \alpha}, [b,\alpha]\frac{\partial}{\partial \alpha} \right] = [[\alpha,a],b]\frac{\partial}{\partial \alpha} - [[\alpha,b],a]\frac{\partial}{\partial \alpha} = [\alpha,[a,b]]\frac{\partial}{\partial \alpha},$$

that is for every $X_a \in \Delta$ and $X_b \in \Delta$ we have $[X_a, X_b] = X_{[a,b]} \in \Delta$. This shows that Δ is involutive and the system (14) is integrable.

Let us denote by $J_1(\mathfrak{g},\mathbb{R})$ and by $J_2(\mathfrak{g},\mathbb{R})$ the first and second order jet spaces of real valued functions on $\mathfrak{g}$. As usual, a local coordinates system on $J_1(\mathfrak{g},\mathbb{R})$ and $J_2(\mathfrak{g},\mathbb{R})$ can be given as follows: if $\mathcal{E}: \mathfrak{g} \to \mathbb{R}$, then

$$j_{1,\alpha}(\mathcal{E}) = (\alpha, \epsilon, \epsilon_i), \quad j_{2,\alpha}(\mathcal{E}) = (\alpha, \epsilon, \epsilon_i, \epsilon_{ij}),$$

where

$$\epsilon = \mathcal{E}(\alpha), \quad \epsilon_i = \left.\frac{\partial \mathcal{E}}{\partial \alpha_i}\right|_\alpha, \quad \epsilon_{ij} = \left.\frac{\partial^2 \mathcal{E}}{\partial \alpha_i \partial \alpha_j}\right|_\alpha.$$

Since (14) is integrable, the first prolongation of (14) is also integrable. Therefore for every initial condition $j_{2,\alpha} \in J_2(\mathfrak{g},\mathbb{R})$ at α, there exists a solution $\mathcal{E}: \mathfrak{g} \to \mathbb{R}$ in the neighborhood of α such that $j_2(\mathcal{E}) = j_{2,\alpha}$. On the other hand, the jet $j_{2,\alpha} = \{\alpha, \epsilon, \epsilon_i, \epsilon_{ij}\}$ is a second order initial condition of the prolongated system if and only if $\{\epsilon_i, \epsilon_{ij}\}$ is a solution of the system composed by (16) and (17). Moreover the solution $\mathcal{E}$ corresponding to $j_{2,\alpha}$ is nondegenerate if and only if $\det(\epsilon_{ij}) \neq 0$.

□

Corollary 1: The canonical connection of a commutative Lie group is variational with respect to a left-invariant Lagrangian.

In that case $C_{ij}^k = 0$ for all $i,j,k = 1, \ldots, n$, and there is no obstruction to choose a nondegenerate initial condition for the system (14). □

Corollary 2: If the derived Lie algebra is one dimensional, then there is no left-invariant variational principle for the canonical flow.

In that case all the solutions $\{x_i = \epsilon_i,\ x_{ij} = \epsilon_{ij}\}$ of the system composed by (16) and (17) are degenerate, and therefore there is no nondegenerate initial condition for the differential system (14). □

Remark: The Lagrangian $E(\alpha) = K(\alpha,\alpha)$, where K is the Killing form of G, is always a solution to the equations (12) and (13). *That way we rediscover the well-known property of semisimple Lie groups: the canonical connection is variational with respect to a left-invariant Lagrangian.*

Indeed, E is left-invariant, it is not dependent on the x coordinates in the (x,α) system, and (12) is satisfied. Moreover, at every $\alpha \in \mathfrak{g}$ and $a \in \mathfrak{g}$ we have

$$[a,\alpha]\frac{\partial E}{\partial \alpha} = \left.\frac{d}{dt}\right|_{t=0} K(\alpha + t[a,\alpha]; \alpha + t[a,\alpha]) = K([a,\alpha],\alpha) + K(\alpha,[a,\alpha]) = 0$$

and Eq. (13) is satisfied. □

V. SOLUTION OF THE GROUP-INVARIANT INVERSE PROBLEM IN DIMENSIONS UP TO FOUR

The variationality of the geodesic flow of the canonical connection of Lie groups was studied in Refs. 9 and 2, where the inverse problem for Lie groups up to dimension 4 were solved. Here we determine if there exits group-invariant variational principle for canonical geodesic flows. Theorem 3 formulates a necessary and sufficient condition for the Lie algebra so that the canonical flow is variational with respect to a group-invariant Lagrangian.

Jacobson in Ref. 6 gives the classification of Lie algebras of dimension 3 or less. The classification of Lie algebras of dimensions 4 and 5 can be found in Ref. 8.

A. Two-dimensional Lie groups

There are, up to isomorphism, two algebras distinguished according to whether or not $[,]$ is trivial or not. In the former case we have the Abelian Lie algebra, and according to Corollary 1 it is variational with respect to a G-invariant Lagrangian.

The latter one is the Lie algebra of the affine group of the line. Up to isomorphism the Lie algebra of the affine group of the line is the only non-Abelian two-dimensional Lie algebra. A representation of the group G is given by $g=\left(\begin{smallmatrix} x & y \\ 0 & 1 \end{smallmatrix}\right)$ where $x \neq 0$. The corresponding Lie algebra is given by the 2×2 matrices $\left(\begin{smallmatrix} x & y \\ 0 & 0 \end{smallmatrix}\right)$. Let us consider the basis $\{e_1, e_2\}$, where $e_1 := \left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right)$ and $e_2 := \left(\begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix}\right)$. Then $[e_1, e_2] = e_2$, i.e., the nonzero structure constants are $C^2_{12} = -C^2_{21} = 1$. If (a_1, a_2) and (α_1, α_2) denote the coordinates of a and α with respect to this basis, then Eq. (13) is $[a,\alpha] = (a_1\alpha_2 - a_2\alpha_1)e_2$ which gives $\partial E/\partial \alpha_2 = 0$. Since any solution of the prolongations is nonregular we conclude that there is no invariant variational principle for the canonical connection of the affine group of the line.

B. Three-dimensional Lie groups

In Ref. 9, Thompson proved that all the canonical connections on Lie groups of dimension 3 have variational locally geodesic equations. On the other hand, Jacobson's classification of the three-dimensional Lie algebras depends primarily on the dimension of the first derived algebra $g^{(1)}$ where g is the original algebra. We have the following possibilities.

If $\dim(g^{(1)}) = 0$, then g is Abelian and, according to Corollary 1, the canonical connection of a commutative Lie group is variational with respect to a left-invariant Lagrangian. If $\dim(g^{(1)}) = 3$, then g is simple and we have $g = s\ell(2,\mathbb{R})$ or $g = so(3)$. In both cases the Killing form provides a metric and so the connections are variational.

If $\dim(g^{(1)}) = 1$ there are, up to isomorphism, two algebras distinguished according to whether $g^{(1)}$ lies inside the center of g. In the former case g may be realized as the Lie algebra of the group of matrices of the form $\begin{bmatrix} 1 & x & y \\ 0 & 1 & z \\ 0 & 0 & 1 \end{bmatrix}$, $(x,y,z \in \mathbb{R})$ and $\mathfrak{g}$ is the Heisenberg algebra. Its canonical connection is a flat connection and so it is variational. The latter case g is isomorphic to the Lie algebra of the group of nonsingular 2×2 upper triangular matrices and so it is again variational.

Let us consider the Heisenberg group. A basis of the Lie algebra is given by $\{e_1, e_2, e_3\}$, where

$$e_1 := \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad e_2 := \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad e_3 := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}.$$

If (a_1, a_2, a_3) and $(\alpha_1, \alpha_2, \alpha_3)$ denotes the coordinates of a and α with respect to this basis, then

$$(a_1\alpha_3 - a_3\alpha_1)\frac{\partial E}{\partial \alpha_2} = 0$$

and Eq. (13) gives $\partial E/\partial \alpha_2 = 0$. Since any solution of the prolongations is nonregular we conclude that there is no invariant variational principle for the canonical connection of the Heisenberg group.

Next we consider the Lie group of 2×2 upper triangular matrices $\left(\begin{smallmatrix} x & y \\ 0 & z \end{smallmatrix}\right)$ where $xz \neq 0$. Here $\{e_1, e_2, e_3\}$ is a basis of the Lie algebra, where

$$e_1 := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad e_2 := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad e_3 := \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

If (a_1, a_2, a_3) and $(\alpha_1, \alpha_2, \alpha_3)$ are the coordinates of a and α, then

$$(a_1\alpha_2 + a_2\alpha_3 - a_1\alpha_2 - a_3\alpha_3)\frac{\partial E}{\partial \alpha_2} = 0,$$

and Eq. (14) gives again $\partial E/\partial \alpha_2 = 0$. Therefore any solution will be nonregular. Consequently there is no invariant variational principle in this case.

C. Four-dimensional Lie groups

There are 12 classes of Lie algebras in dimension 4 denoted in Ref. 8 as $A_{4,i}$, $i = 1, \ldots, 12$. The generators of the algebras are listed as $\{e_1, e_2, e_3, e_4\}$ and in each case we list the nonzero Lie brackets. Several of the Lie algebras have parameters denoted by a or b or both. The generic solution of the linear system (16) at a point $\alpha = \alpha_i e_i$ will be denoted by $\epsilon := \{\epsilon_i, \epsilon_{ij}\}$.

In Ref. 2, Thompson and his co-workers computed all the canonical connections on Lie groups of dimension 4 and determined whether the connection is variational or not. He has shown that the Lie groups with Lie algebras $A_{4,7}$, $A_{4,9b}$, and $A_{4,11a}$, where the brackets are defined as

$$A_{4,7}, \quad [e_2, e_3] = e_1, \quad [e_1, e_4] = 2e_1, \quad [e_2, e_4] = e_2, \quad [e_3, e_4] = e_2 + e_3,$$

$$A_{4,9b}, \quad [e_2, e_3] = e_1, \quad [e_1, e_4] = (1+b)e_1, \quad [e_2, e_4] = e_2, \quad [e_3, e_4] = be_3,$$

$$A_{4,11a}, \quad [e_2, e_3] = e_1, \quad [e_1, e_4] = 2ae_1, \quad [e_2, e_4] = ae_2 - e_3, \quad [e_3, e_4] = e_2 + ae_3,$$

$-1 < b < 1$ and $0 < a$, are not variational.

$A_{4,2a}$, the brackets are

$$[e_1, e_4] = ae_1, \quad [e_2, e_4] = e_2, \quad [e_3, e_4] = e_2 + e_3, \quad a \neq 0.$$

Equation (16) leads to a solution $\{\epsilon_i, \epsilon_{ij}\}$, where $\epsilon_{ij} = 0$ for every $(i, j) \neq (4, 4)$. Therefore the condition (13) entails that the matrix ϵ_{ij} is singular, whatever is the value of a. Therefore the canonical flow is variational, but there is no left-invariant regular Lagrangian for its geodesics.

In the case of the Lie groups with Lie algebras $A_{4,1}$, $A_{4,3}$, $A_{4,4}$, $A_{4,9}$, and $A_{4,12}$, the nontrivial brackets of the algebras are determined as

$$A_{4,1}, \quad [e_2, e_4] = e_1, \quad [e_3, e_4] = e_2,$$

$$A_{4,3}, \quad [e_1, e_4] = e_1, \quad [e_3, e_4] = e_2,$$

$$A_{4,4}, \quad [e_1, e_4] = e_1, \quad [e_2, e_4] = e_1 + e_2, \quad [e_3, e_4] = e_2 + e_3,$$

$$A_{4,9}, \quad [e_2, e_3] = e_1, \quad [e_1, e_4] = 2e_1, \quad [e_2, e_4] = e_2, \quad [e_3, e_4] = e_3,$$

$$A_{4,12}, \quad [e_1,e_3]=e_1, \quad [e_2,e_3]=e_2, \quad [e_1,e_4]=-e_2, \quad [e_2,e_4]=e_1.$$

We can find that the general solution of Eq. (16) can be described as follows: $\epsilon_{33},\epsilon_{34},\epsilon_{44}$ are arbitrary numbers and the other components are all zero. Therefore

$$\epsilon_{ij}=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \epsilon_{33} & \epsilon_{34} \\ 0 & 0 & \epsilon_{34} & \epsilon_{44} \end{pmatrix}.$$

Since ϵ_{ij} is singular, there is no left-invariant regular Lagrangian for the geodesics of the canonical connection. The situation is analogous in the following.

$\mathbf{A_{4,5ab}}$, the Lie algebra relations are

$$[e_1,e_4]=e_1, \quad [e_2,e_4]=ae_2, \quad [e_3,e_4]=be_3.$$

Depending on the value of a and b we have four cases,

$$\text{if } a=0, \quad b=0, \text{ then } \epsilon_{ij}=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \epsilon_{22} & \epsilon_{23} & \epsilon_{24} \\ 0 & \epsilon_{23} & \epsilon_{33} & \epsilon_{34} \\ 0 & \epsilon_{24} & \epsilon_{34} & \epsilon_{44} \end{pmatrix},$$

$$\text{if } a=0, \quad b\neq 0, \text{ then } \epsilon_{ij}=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \epsilon_{22} & 0 & \epsilon_{24} \\ 0 & 0 & 0 & 0 \\ 0 & \epsilon_{24} & 0 & \epsilon_{44} \end{pmatrix},$$

$$\text{if } a\neq 0, \quad b=0, \text{ then } \epsilon_{ij}=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \epsilon_{33} & \epsilon_{34} \\ 0 & 0 & \epsilon_{34} & \epsilon_{44} \end{pmatrix},$$

$$\text{if } a\neq 0, \quad b\neq 0, \text{ then } \epsilon_{ij}=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \epsilon_{44} \end{pmatrix}.$$

In all three cases the Lagrangian must be nonregular, and therefore there is no left-invariant regular Lagrangian for the geodesics of the canonical connection.

$\mathbf{A_{4,6ab}}$, the Lie algebra relations are

$$[e_1,e_4]=ae_1, \quad [e_2,e_4]=be_2-e_3, \quad [e_3,e_4]=be_3,$$

with $a\neq 0$, $b\geqslant 0$. Depending on the value of a and b we have two cases,

$$\text{if } b \neq 0, \text{ then } \epsilon_{ij} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \epsilon_{44} \end{pmatrix},$$

$$\text{if } b = 0, \text{ then } \epsilon_{ij} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \epsilon_{22} & 0 & \epsilon_{24} \\ 0 & 0 & 0 & 0 \\ 0 & \epsilon_{24} & 0 & \epsilon_{44} \end{pmatrix}.$$

In both cases the Lagrangian must be degenerate and therefore there is no left-invariant regular Lagrangian for the geodesics of the canonical connection.

$\mathbf{A_{4,8}}$, the Lie algebra relations are

$$[e_2, e_3] = e_1, \quad [e_2, e_4] = e_2, \quad [e_3, e_4] = -e_3.$$

$\epsilon_3, \epsilon_4, \epsilon_{3,2}, \epsilon_{4,1}, \epsilon_{4,4}$ are free and the matrix (ϵ_{ij}) is

$$\begin{pmatrix} \frac{\alpha_4^2(\alpha_2\epsilon_{32} - \epsilon_3)}{\alpha_2^2\alpha_3} & -\frac{\alpha_4(\alpha_2\epsilon_{23} - \epsilon_3)}{\alpha_2^2} & -\frac{\alpha_4(\alpha_2\epsilon_{32} - \epsilon_3)}{\alpha_2\alpha_3} & \epsilon_{14} \\ -\frac{\alpha_4(\alpha_2\epsilon_{23} - \epsilon_3)}{\alpha_2^2} & \frac{\alpha_3(\alpha_2\epsilon_{32} - \epsilon_3)}{\alpha_2^2} & \epsilon_{23} & -\frac{\alpha_3(\alpha_2\epsilon_{14} + \epsilon_3)}{\alpha_2\alpha_4} \\ -\frac{\alpha_4(\alpha_2\epsilon_{32} - \epsilon_3)}{\alpha_2\alpha_3} & \epsilon_{23} & \frac{\alpha_2\epsilon_{23} - \epsilon_3}{\alpha_3} & -\frac{\alpha_2\epsilon_{41} + \epsilon_3}{\alpha_4} \\ \epsilon_{14} & -\frac{\alpha_3(\alpha_2\epsilon_{14} + \epsilon_3)}{\alpha_2\alpha_4} & -\frac{\alpha_2\epsilon_{41} + \epsilon_3}{\alpha_4} & \epsilon_{44} \end{pmatrix}.$$

In Ref. 9 Thompson showed that $A_{4,8}$ admits a bi-invariant metric. In order to give a regular initial condition we can choose the free components as

$$\epsilon_3 := \alpha_2\epsilon_{32}, \quad \epsilon_{4,1} := -\epsilon_{23},$$

ϵ_4, $\epsilon_{4,4}$ arbitrary, $\epsilon_{3,2}$ arbitrary nonzero and compute the other components. Then we obtain a solution $\epsilon = \{\epsilon_i, \epsilon_{ij}\}$ of the system (16),

$$\begin{pmatrix} 0 & 0 & 0 & -\epsilon_{23} \\ 0 & 0 & \epsilon_{23} & 0 \\ 0 & \epsilon_{23} & 0 & 0 \\ -\epsilon_{23} & 0 & 0 & \epsilon_{44} \end{pmatrix},$$

where $\det(\epsilon_{ij}) = (\epsilon_{23})^4 \neq 0$. According to Theorem 3 there exists an invariant regular Lagrangian generating the canonical geodesic flow.

$\mathbf{A_{4,10}}$, the Lie algebra relations are

$$[e_2,e_3]=e_1, \quad [e_2,e_4]=-e_3, \quad [e_3,e_4]=e_2.$$

The ϵ_3, ϵ_4, $\epsilon_{3,3}$, $\epsilon_{4,2}$, and $\epsilon_{4,4}$ are free components and the matrix (ϵ_{ij}) is

$$\begin{pmatrix} \frac{\alpha_4^2(\alpha_3\epsilon_{33}-\epsilon_3)}{\alpha_3^3} & \frac{\alpha_2\alpha_4(\alpha_3\epsilon_{33}-\epsilon_3)}{\alpha_3^3} & \frac{\alpha_4(\alpha_3\epsilon_{33}-\epsilon_3)}{\alpha_3^2} & \frac{\alpha_4\alpha_3\epsilon_{24}+\alpha_2\epsilon_3}{\alpha_2\alpha_3} \\ \frac{\alpha_2\alpha_4(\alpha_3\epsilon_{33}-\epsilon_3)}{\alpha_3^3} & \frac{\alpha_2^2\alpha_3\epsilon_{33}+(\alpha_3^2-\alpha_2^2)\epsilon_3}{\alpha_3^3} & \frac{\alpha_2(\alpha_3\epsilon_{33}-\epsilon_3)}{\alpha_3^2} & \epsilon_{4,2} \\ \frac{\alpha_4(\alpha_3\epsilon_{33}-\epsilon_3)}{\alpha_3^2} & \frac{\alpha_2(\alpha_3\epsilon_{33}-\epsilon_3)}{\alpha_3^2} & \epsilon_{33} & \frac{\alpha_3\epsilon_{24}}{\alpha_2} \\ \frac{\alpha_4\alpha_3\epsilon_{24}+\alpha_2\epsilon_3}{\alpha_2\alpha_3} & \epsilon_{24} & \frac{\alpha_3\epsilon_{24}}{\alpha_2} & \epsilon_{44} \end{pmatrix}.$$

A nondegenerate initial condition can be chosen as follows:

$$\epsilon_3 := x_3\epsilon_{33}, \quad \epsilon_{4,2} := 0,$$

ϵ_4, $\epsilon_{4,1}$, $\epsilon_{4,4}$ arbitrary, $\epsilon_{3,2}$ arbitrary nonzero and the other components zero. We have

$$\begin{pmatrix} 0 & 0 & 0 & \epsilon_{33} \\ 0 & \epsilon_{33} & 0 & 0 \\ 0 & 0 & \epsilon_{33} & 0 \\ \epsilon_{33} & 0 & 0 & \epsilon_{44} \end{pmatrix}$$

and $\det(\epsilon_{ij})=-(\epsilon_{33})^4\neq 0$. As in the previous case, Theorem 3 guarantees the existence of an invariant regular Lagrangian generating the canonical geodesic flow.

We remark that in Ref. 9 Thompson has already shown that a Lie group with $A_{4,8}$ or $A_{4,10}$ as Lie algebra has a bi-invariant metric which generates its canonical geodesic flow.

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Hamiltonian multivector fields and Poisson forms in multisymplectic field theory

Michael Forger[a)]
Departamento de Matemática Aplicada, Instituto de Matemática e Estatística, Universidade de São Paulo, Caixa Postal 66281, BR-05315-970 São Paulo, S.P., Brazil

Cornelius Paufler[b)]
Matematisk Fysik/Alba Nova, Kungliga Tekniska Högskolan, SE-10691 Stockholm, Sweden

Hartmann Römer[c)]
Fakultät für Mathematik und Physik, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg im Breisgau, Hermann-Herder-Strasse 3, D-79104 Freiburg i.Br., Germany

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We present a general classification of Hamiltonian multivector fields and of Poisson forms on the extended multiphase space appearing in the geometric formulation of first order classical field theories. This is a prerequisite for computing explicit expressions for the Poisson bracket between two Poisson forms. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2116320]

I. INTRODUCTION AND GENERAL SETUP

The present paper is a continuation of previous work on Poisson brackets of differential forms in the multiphase space approach to classical field theory.[1,2] Our aim is to specialize the general constructions of Ref. 2 from abstract (exact) multisymplectic manifolds to the extended multiphase spaces of field theory, which at present seem to be the only known examples of multisymplectic manifolds, to clarify the structure of Hamiltonian multivector fields, of Hamiltonian forms and of Poisson forms on these spaces and to give explicit formulas for the Poisson bracket between the latter introduced in Refs. 1 and 2.

The structure of this paper is as follows. In the remainder of this introduction, we briefly review the geometric constructions needed in the paper. We put particular emphasis on the consequences that arise from the existence of a certain vector field, the scaling or Euler vector field. Also, we fix the notation to be used in what follows. In Sec. II, we present an explicit classification of locally Hamiltonian multivector fields on extended multiphase space in terms of adapted local coordinates and, following the logical inclusion from locally Hamiltonian to (globally) Hamiltonian to exact Hamiltonian multivector fields, show how the last two are situated within the first. Sec. III is devoted to the study of Hamiltonian forms and Poisson forms that are associated with (globally) Hamiltonian multivector fields. In Sec. IV, we use the outcome of our previous analysis to derive expressions for the Poisson bracket between two Poisson forms. In Sec. V, we summarize our main conclusions and comment on the relation of our results to other approaches, as well as on perspectives for future research. Finally, in order to make the paper self-contained, we include in an appendix a proposition that is not new but is needed in some of the proofs.

We begin with a few comments on the construction of the extended multiphase space of field theory,[3–7] which starts out from a given general fiber bundle over space-time, with base space

[a)]Electronic mail: forger@ime.usp.br
[b)]Electronic mail: pcp@theophys.kth.se
[c)]Electronic mail: hartmann.roemer@physik.uni-freiburg.de

M ($\dim M=n$), total space E, bundle projection $\pi: E \to M$ and typical fiber Q ($\dim Q=N$). It is usually referred to as the configuration bundle since its sections constitute the possible field configurations of the system. (Of course, the manifold M represents space-time, whereas the manifold Q plays the role of a configuration space.) The extended multiphase space, which we shall simply denote by P, is then the total space of a larger fiber bundle over M and in fact the total space of a vector bundle over E which can be defined in several equivalent ways, e.g., by taking the twisted affine dual $J^{\circledast}E$ of the first order jet bundle JE of E or by taking the bundle $\Lambda^n_{n-1}T^*E$ of $(n-1)$-horizontal n-forms on E; see Refs. 2, 5, and 7 for details. Therefore, there is a natural class of local coordinate systems on P, namely those that arise from combining fiber bundle charts of E over M with vector bundle charts of P over E: these so-called adapted local coordinates (x^μ, q^i, p^μ_i, p) are completely fixed by specifying local coordinates x^μ for M (the space-time coordinates), local coordinates q^i for Q (the position variables) and a local trivialization of E over M, and are such that the induced local coordinates p^μ_i (the multimomentum variables) and p (the energy variable) are linear along the fibers of P over E. For details, we refer to Ref. 2, where one can also find the explicit transformation law for the multimomentum variables and the energy variable induced by a change of the space-time coordinates, of the position variables and of the local trivialization.

A first important feature of the extended multiphase space P is that it carries a naturally defined multicanonical form θ whose exterior derivative is, up to a sign, the multisymplectic form ω,

$$\omega = -\,\mathrm{d}\theta. \tag{1}$$

The global construction can be found in Refs. 2, 5, and 7, so we shall just state their explicit form in adapted local coordinates,

$$\theta = p^\mu_i\, \mathrm{d}q^i \wedge \mathrm{d}^n x_\mu + p\mathrm{d}^n x. \tag{2}$$

$$\omega = \mathrm{d}q^i \wedge \mathrm{d}p^\mu_i \wedge \mathrm{d}^n x_\mu - \mathrm{d}p \wedge \mathrm{d}^n x. \tag{3}$$

Here, we have already employed part of the following conventions concerning local differential forms defined by a system of adapted local coordinates, which will be used systematically throughout this paper,

$$\mathrm{d}^n x = \mathrm{d}x^1 \wedge \cdots \wedge \mathrm{d}x^n, \quad \mathrm{d}^n x_{\mu_1 \ldots \mu_r} = i_{\partial_{\mu_r}} \cdots i_{\partial_{\mu_1}} \mathrm{d}^n x.$$

For later use, we also recall the definition of the Lie derivative of a differential form α along an r-multivector field X,

$$L_X \alpha = \mathrm{d} i_X \alpha - (-1)^r i_X\, \mathrm{d}\alpha, \tag{4}$$

which leads to the following relations, valid for any differential form α and any two multivector fields X and Y of tensor degrees r and s, respectively,

$$\mathrm{d}L_X \alpha = (-1)^{r-1} L_X\, \mathrm{d}\alpha, \tag{5}$$

$$i_{[X,Y]}\alpha = (-1)^{(r-1)s} L_X i_Y \alpha - i_Y L_X \alpha, \tag{6}$$

$$L_{[X,Y]}\alpha = (-1)^{(r-1)(s-1)} L_X L_Y \alpha - L_Y L_X \alpha, \tag{7}$$

$$L_{X\wedge Y}\alpha = (-1)^s i_Y L_X \alpha + L_Y i_X \alpha, \tag{8}$$

where $[X,Y]$ denotes the Schouten bracket of X and Y. For decomposable multivector fields $X = X_1 \wedge \cdots \wedge X_r$ and $Y = Y_1 \wedge \cdots \wedge Y_s$, it can be defined in terms of the Lie bracket of vector fields according to the formula

$$[X,Y]=\sum_{i=1}^{r}\sum_{j=1}^{s}(-1)^{i+j}[X_i,X_j]\wedge X_1\wedge\cdots\hat{X}_i\cdots\wedge X_r\wedge Y_1\wedge\cdots\hat{Y}_j\cdots\wedge Y_s,$$

where as usual the hat over a symbol denotes its omission. We shall also write

$$L_X Y=[X,Y],$$

for any two multivector fields X and Y. For properties of the Schouten bracket, we refer to Ref. 8. A proof of the above identities relating the Schouten bracket and the Lie derivative of forms along multivector fields can be found in the appendix of Ref. 2.

A second property of the extended multiphase space P which provides additional structures for tensor calculus on this manifold is that it is the total space of a fiber bundle, which implies that we may speak of vertical vectors and horizontal covectors. In fact, it is so in no less than three different ways. Namely, P is the total space of a fiber bundle over M (with respect to the so-called source projection), the total space of a vector bundle over E (with respect to the so-called target projection) and the total space of an affine line bundle over the ordinary multiphase space P_0.[2] Therefore, the notions of verticality for multivector fields and of horizontality for differential forms on P admit different interpretations, depending on which projection is used. In any case, one starts by defining tangent vectors to the total space of a fiber bundle to be vertical if they are annihilated by the tangent map to the bundle projection, or what amounts to the same thing, if they are tangent to the fibers. Dually, a k-form on the total space of a fiber bundle is said to be l-horizontal if it vanishes whenever one inserts at least $k-l+1$ vertical tangent vectors; the standard horizontal forms are obtained by taking $l=k$. Finally, an r-multivector on the total space of a fiber bundle is said to be s-vertical if its contraction with any $(r-s+1)$-horizontal form vanishes. It is not difficult to show that these definitions are equivalent to requiring that, locally, an l-horizontal k-form should be a sum of exterior products of k one-forms, among which there are at least l horizontal ones, and that an s-vertical r-multivector field should be a sum of exterior products of r tangent vectors, among which there are at least s vertical ones. Using this rule, properties of verticality for multivectors or horizontality for forms are easily derived from the corresponding properties for vectors or one-forms, respectively. In what follows, the terms "vertical" and "horizontal" will usually refer to the source projection, except when explicitly stated otherwise.

A third important feature of the extended multiphase space P is that it carries a naturally defined vector field Σ, the scaling vector field or Euler vector field, which exists on any manifold that is the total space of a vector bundle. In adapted local coordinates,

$$\Sigma=p_i^\mu\frac{\partial}{\partial p_i^\mu}+p\frac{\partial}{\partial p}.$$

It is then easy to verify the following relations (see Proposition 2.1 of Ref. 2):

$$i_\Sigma\theta=0,\quad i_\Sigma\omega=-\theta,\quad L_\Sigma\theta=\theta,\quad L_\Sigma\omega=\omega. \tag{9}$$

The main utility of Σ is that taking the Lie derivative L_Σ along Σ provides a device for controlling the dependence of functions and, more generally, of tensor fields on P on the multimomentum variables and the energy variable, that is, along the fibers of P over E: L_Σ has only integer eigenvalues, and eigenfunctions of L_Σ with eigenvalue k are homogeneous polynomials of degree k in these variables.

As we shall see soon, homogeneity under L_Σ plays a central role in the analysis of various classes of multivector fields and differential forms on P.

Let us recall a few definitions. An r-multivector field X on P is called *locally Hamiltonian* if $i_X\omega$ is closed, or equivalently, if

$$L_X\omega=0. \tag{10}$$

It is called *globally Hamiltonian* if $i_X\omega$ is exact, that is, if there exists an $(n\text{-}r)$-form f on P such that

$$i_X\omega = \mathrm{d}f. \tag{11}$$

In this case, f is said to be a *Hamiltonian form associated with* X. Finally, it is called *exact Hamiltonian* if

$$L_X\theta = 0. \tag{12}$$

Of course, exact Hamiltonian multivector fields are globally Hamiltonian [to show this, set $f=(-1)^{r-1}i_X\theta$ and apply Eqs. (4) and (1)], and globally Hamiltonian multivector fields are obviously locally Hamiltonian. Conversely, an $(n\text{-}r)$-form f on P is called a *Hamiltonian form* if there exists an r-multivector field X on P such that Eq. (11) holds; in this case, X is said to be a *Hamiltonian multivector field associated with* f. Moreover, f is called a *Poisson form* if in addition, it vanishes on the kernel of ω, that is, if for any multivector field Z, we have

$$i_Z\omega = 0 \Rightarrow i_Zf = 0. \tag{13}$$

A trivial example of a Poisson form is the multisymplectic form ω itself. Another example is provided by the multicanonical form θ, since it can be written as $\theta=-i_\Sigma\omega$.

Concerning stability under the Lie derivative along the scaling vector field Σ, we have the following.

Proposition 1.1: The space $\mathfrak{X}^\wedge_{LH}(P)$ *of locally Hamiltonian multivector fields, the space* $\mathfrak{X}^\wedge_{H}(P)$ *of globally Hamiltonian multivector fields, the space* $\mathfrak{X}^\wedge_{EH}(P)$ *of exact Hamiltonian multivector fields and the space* $\mathfrak{X}^\wedge_{0}(P)$ *of multivector fields taking values in the kernel of* ω *are all invariant under the Lie derivative along the scaling vector field* Σ,

$$L_X\omega = 0 \;\Rightarrow\; L_{[\Sigma,X]}\omega = 0, \tag{14}$$

$$i_X\omega = \mathrm{d}f \;\Rightarrow\; i_{[\Sigma,X]}\omega = \mathrm{d}(L_\Sigma f - f), \tag{15}$$

$$L_X\theta = 0 \;\Rightarrow\; L_{[\Sigma,X]}\theta = 0, \tag{16}$$

$$i_\xi\omega = 0 \;\Rightarrow\; i_{[\Sigma,\xi]}\omega = 0. \tag{17}$$

Proof: All these relations can be shown by direct calculation. □

Dually, we have the following.

Proposition 1.2: The space $\Omega_H(P)$ *of Hamiltonian forms, the space* $\Omega_0(P)$ *of forms that vanish on the kernel of* ω *and the space* $\Omega_P(P)$ *of Poisson forms are all invariant under the Lie derivative along the scaling vector field* Σ,

$$\mathrm{d}f = i_X\omega \;\Rightarrow\; \mathrm{d}(L_\Sigma f) = i_{X+[\Sigma,X]}\omega. \tag{18}$$

Proof: The first statement is a consequence of Eq. (18), which follows directly from combining Eqs. (5) and (6) with Eq. (9). For the second statement, assume that f vanishes on the kernel of ω. Then if ξ is any multivector field ϑ taking values in the kernel of ω, the multivector field $[\Sigma,\xi]$ takes values in the kernel of ω as well [cf. Eq. (17)], so that according to Eq. (6),

$$i_\xi(L_\Sigma f) = L_\Sigma i_\xi f - i_{[\Sigma,\xi]}f = 0.$$

But this means that $L_\Sigma f$ vanishes on the kernel of ω. Finally, the third statement follows by combining the first two. □

A special class of multivector fields and of differential forms on P which will be of particular importance in what follows is that of *fiberwise polynomial multivector fields* and of *fiberwise polynomial differential forms* on P: their coefficients are polynomials along the fibers of P over E,

or in other words, polynomials in the multimomentum variables and the energy variable. The main advantage of working with tensor fields on the total space of a vector bundle which are fiberwise polynomial is that they allow a unique and globally defined (or in other words, coordinate independent) decomposition into homogeneous components, according to the different eigenspaces of the Lie derivative L_Σ along Σ; the corresponding eigenvalue will in what follows be called the *scaling degree* (to distinguish it from the ordinary tensor degree). In doing so, it must be borne in mind that, in an expansion with respect to an adapted local coordinate system, the scaling degree receives contributions not only from the coefficient functions but also from some of the coordinate vector fields and differentials since the vector fields $\partial/\partial x^\mu$, $\partial/\partial q^i$, $\partial/\partial p_i^\mu$, and $\partial/\partial p$ carry scaling degree 0, 0, −1, and −1, respectively, while the differentials dx^μ, dq^i, dp_i^μ, and dp carry scaling degree 0, 0, +1, and +1, respectively; moreover, the scaling degree is additive under the exterior product, since L_Σ is a derivation. Therefore, a fiberwise polynomial r-multivector field on P admits a globally defined decomposition into a finite sum

$$X = \sum_{s \geqslant -r} X_s,$$

where X_s is its homogeneous component of scaling degree s,

$$L_\Sigma X_s = s X_s.$$

Each X_s can be obtained from X by applying a projector which is itself a polynomial in L_Σ,

$$X_s = \prod_{\substack{s' \geqslant -r \\ s' \neq s}} \frac{1}{s - s'} (L_\Sigma - s') X.$$

Similarly, a fiberwise polynomial $(n\text{-}r)$-form f on P admits a globally defined decomposition into a finite sum

$$f = \sum_{s \geqslant 0} f_s,$$

where f_s is its homogeneous component of scaling degree s,

$$L_\Sigma f_s = s f_s.$$

Again, the f_s can be obtained from f,

$$f_s = \prod_{\substack{s' \geqslant 0 \\ s' \neq s}} \frac{1}{s - s'} (L_\Sigma - s') f.$$

The relevance of these decompositions for locally Hamiltonian multivector fields and for Hamiltonian forms on the extended multiphase space P stems from the following theorem, whose proof will follow from statements to be derived in the course of the next two sections, by means of explicit calculations in adapted local coordinates.

Theorem 1.3: *For $0 < \tau < n$ and up to trivial contributions (τ-multivector fields taking values in the kernel of ω and closed $(n-r)$-forms, respectively), locally Hamiltonian τ-multivector fields and Hamiltonian $(n-\tau)$-forms on P are fiberwise polynomial and have non-trivial homogeneous components of scaling degree s only for $s = -1, 0, \ldots, r-1$ and for $s = 0, 1, \ldots, r$, respectively. More precisely, we have*

(i) *Every fiberwise polynomial locally Hamiltonian (Hamiltonian, exact Hamiltonian) r-multivector field X on P, admits a unique, globally defined decomposition into homogeneous components with respect to scaling degree, which can be written in the form (we abbreviate X_{-1} as X_-)*

$$X = X_- + X_+ + \xi \quad \text{with } X_+ = \sum_{s=0}^{r-1} X_s, \tag{19}$$

where each X_s is locally Hamiltonian (Hamiltonian, exact Hamiltonian) and

$$\xi = \sum_{-r \leqslant s \leqslant -2} \xi_s + \sum_{s \geqslant r} \xi_s \tag{20}$$

is a fiberwise polynomial r-multivector field on P taking values in the kernel of ω.

(ii) *Every fiberwise polynomial Hamiltonian form (Poisson form) f of degree $n-r$ on P, admits a unique, globally defined decomposition into homogeneous components with respect to scaling degree, which can be written in the form*

$$f = f_0 + f_+ + f_c \quad \text{with } f_+ = \sum_{s=1}^{r} f_s, \tag{21}$$

where each f_s is Hamiltonian (Poisson) and

$$f_c = \sum_{s \geqslant r+1} (f_c)_s \tag{22}$$

is a fiberwise polynomial closed $(n-r)$-form on P.

The cases $r=0$ and $r=n$ are exceptional and must be dealt with separately; see Propositions 2.2 and 3.2 for $r=0$ and Propositions 2.3 and 3.1 for $r=n$.

In view of this theorem, it is sufficient to study locally Hamiltonian multivector fields and Hamiltonian forms which are homogeneous under the Lie derivative along the scaling vector field Σ. This condition of homogeneity is also compatible with the correspondence between globally Hamiltonian multivector fields X and Hamiltonian forms f established by the fundamental relation (11), because ω itself is homogeneous: according to Eq. (9), ω has scaling degree 1. Indeed, except for the ambiguity inherent in this correspondence (f determines X only up to a multivector field taking values in the kernel of ω and X determines f only up to a closed form), Eq. (11) preserves the scaling degree, up to a shift by 1: X is homogeneous with scaling degree $s-1$ if and only if f is homogeneous with scaling degree s,

$$\begin{array}{c} L_\Sigma X = (s-1)X \\ \text{modulo multivector fields} \\ \text{taking values in the kernel of } \omega \end{array} \quad \Leftrightarrow \quad \begin{array}{c} L_\Sigma f = sf \\ \text{modulo closed forms} \end{array}. \tag{23}$$

For a proof, note that the condition on the left-hand side (lhs) amounts to requiring that $i_{[\Sigma,X]}\omega = (s-1) i_X \omega$, while the condition on the right-hand side (rhs) amounts to requiring that $\mathrm{d} L_\Sigma f = s\, \mathrm{d}f$, so the equivalence stated in Eq. (23) is an immediate consequence of Eq. (18). A particular case occurs when $s=1$, since the locally Hamiltonian multivector fields which are homogeneous of scaling degree 0 are precisely the exact Hamiltonian multivector fields: for $L_X\omega = 0$,

$$\begin{array}{c} L_\Sigma X = 0 \\ \text{modulo multivector fields} \\ \text{taking values in the kernel of } \omega \end{array} \quad \Leftrightarrow \quad L_X \theta = 0. \tag{24}$$

Indeed, the properties of θ and ω give

$$L_X \theta = -L_X i_\Sigma \omega = (-1)^r (i_{[X,\Sigma]}\omega - i_\Sigma L_X \omega) = (-1)^{r-1} i_{[\Sigma,X]}\omega. \tag{25}$$

More generally, the fundamental relation (11) preserves the property of being fiberwise polynomial, in the following sense: If X is a fiberwise polynomial Hamiltonian r-multivector field and f is a Hamiltonian $(n-r)$-form associated with X, then modifying f by addition of an appropriate

closed $(n-r)$-form if necessary, we may always assume, without loss of generality, that f is fiberwise polynomial as well. Conversely, if f is a fiberwise polynomial Hamiltonian $(n-r)$-form and X is a Hamiltonian r-multivector field associated with f, then modifying X by addition of an appropriate r-multivector field taking values in the kernel of ω if necessary, we may always assume, without loss of generality, that X is fiberwise polynomial as well.

II. HAMILTONIAN MULTIVECTOR FIELDS

Our aim in this section is to determine the explicit form, in adapted local coordinates, of locally Hamiltonian r-multivector fields on the extended multiphase space P, where $0 \leqslant r \leqslant n+1$. (Multivector fields of tensor degree $>n+1$ are uninteresting since they always take their values in the kernel of ω.)

As a first step towards this goal, we shall determine the explicit form, in adapted local coordinates, of the multivector fields on P taking values in the kernel of ω; this will also serve to identify, in the next section, the content of the kernel condition (13) that characterizes Poisson forms. To this end, note first that ω being a homogeneous differential form (of degree $n+1$), its kernel is graded, that is, if an inhomogeneous multivector field takes values in the kernel of ω, so do all its homogeneous components.

Proposition 2.1: Every r-multivector field X on P admits, in adapted local coordinates, a unique decomposition of the form

$$X = \frac{1}{r!} X^{\mu_1 \cdots \mu_r} \frac{\partial}{\partial x^{\mu_1}} \wedge \cdots \wedge \frac{\partial}{\partial x^{\mu_r}} + \frac{1}{(r-1)!} X^{i,\mu_2 \cdots \mu_r} \frac{\partial}{\partial q^i} \wedge \frac{\partial}{\partial x^{\mu_2}} \wedge \cdots \wedge \frac{\partial}{\partial x^{\mu_r}}$$
$$+ \frac{1}{r!} X_i^{\mu_1 \cdots \mu_r} \frac{\partial}{\partial p_i^{\mu_1}} \wedge \frac{\partial}{\partial x^{\mu_2}} \wedge \cdots \wedge \frac{\partial}{\partial x^{\mu_r}} + \frac{1}{(r-1)!} \tilde{X}^{\mu_2 \cdots \mu_r} \frac{\partial}{\partial p} \wedge \frac{\partial}{\partial x^{\mu_2}} \wedge \cdots \wedge \frac{\partial}{\partial x^{\mu_r}} + \xi, \tag{26}$$

where all coefficients are totally antisymmetric in their space-time indices and ξ takes values in the kernel of ω.

Proof: This is an immediate consequence of the particular form of ω in adapted local coordinates, Eq. (3). For more details, see Ref. 9. □

With this local coordinate representation at hand, we are in a position to analyze the restrictions imposed on the coefficients $X^{\mu_1 \cdots \mu_r}$, $X^{i,\mu_2 \cdots \mu_r}$, $X_i^{\mu_1 \cdots \mu_r}$, and $\tilde{X}^{\mu_2 \cdots \mu_r}$ by requiring X to be locally Hamiltonian. (Of course, it makes no sense to discuss the question which locally Hamiltonian multivector fields are also globally Hamiltonian when working in local coordinates.) As a warm-up exercise, we shall settle the extreme cases of tensor degree 0 and $n+1$.

Proposition 2.2: A function on P, regarded as a 0-multivector field, is locally Hamiltonian if and only if it is constant; it is then also exact Hamiltonian. Similarly, an $(n+1)$-multivector field on P, with standard local coordinate representation

$$X = \tilde{X} \frac{\partial}{\partial p} \wedge \frac{\partial}{\partial x^1} \wedge \cdots \wedge \frac{\partial}{\partial x^n} + \xi, \tag{27}$$

where ξ takes values in the kernel of ω, is locally Hamiltonian if and only if the coefficient function $\tilde{X}$ is constant and is exact Hamiltonian if and only if it vanishes.

Proof: For functions, we use the fact that the operator i_1 corresponding to the constant function 1 on a manifold is defined to be the identity, so that the operator i_f corresponding to an arbitrary function f on a manifold is simply multiplication by f. Therefore, we have for any differential form α

$$L_f \alpha = \mathrm{d}(i_f \alpha) - i_f \, \mathrm{d}\alpha = \mathrm{d}(f\alpha) - f \, \mathrm{d}\alpha = \mathrm{d}f \wedge \alpha,$$

implying that if f is constant, $L_f \alpha = 0$ no matter what α one chooses. On the other hand, an explicit calculation in adapted local coordinates shows that the condition $L_f \omega = 0$ forces all partial deriva-

tives of f to vanish; see Ref. 9. Similarly, for multivector fields of degree $n+1$, it is clear that, as r equals $n+1$, the first three terms in Eq. (26) also take values in the kernel of ω and can thus be incorporated into ξ. Therefore, by setting $\widetilde{X}^{\mu_1\cdots\mu_n}=\epsilon^{\mu_1\cdots\mu_n}\widetilde{X}$, we see that $i_X\omega=-\widetilde{X}$. But $L_X\omega=\mathrm{d}(i_X\omega)-(-1)^n i_X\,\mathrm{d}\omega=\mathrm{d}(i_X\omega)$ and $L_X\theta=\mathrm{d}(i_X\theta)-(-1)^{n+1}i_X\,\mathrm{d}\theta=(-1)^{n+1}i_X\omega$, so the proposition follows. □

The intermediate cases $(0<r\leqslant n)$ are much more interesting. However, the situation for tensor degree n is substantially different from that for tensor degree $<n$ and hence will be dealt with first. To simplify the notation, we write

$$X^{\mu_1\cdots\mu_n}=\epsilon^{\mu_1\cdots\mu_n}\widetilde{X},\quad X^{i,\mu_2\cdots\mu_n}=\epsilon^{\mu_2\cdots\mu_n\mu}X^i_\mu,$$

$$X^{\mu_1\cdots\mu_n}_i=\epsilon^{\mu_1\cdots\mu_n}X_i,\quad \widetilde{X}^{\mu_2\cdots\mu_n}=\epsilon^{\mu_2\cdots\mu_n\mu}X_\mu,$$

so that we obtain

$$i_X\omega=(-1)^{n-1}\widetilde{X}\,\mathrm{d}p+X^i_\mu\,\mathrm{d}p^\mu_i-(-1)^{n-1}X_i\,\mathrm{d}q^i-X_\mu\,\mathrm{d}x^\mu, \tag{28}$$

and

$$i_X\theta=p\widetilde{X}+(-1)^{n-1}p^\mu_iX^i_\mu,$$

respectively.

Proposition 2.3: An n-multivector field X on P is locally Hamiltonian if and only if, locally and modulo terms taking values in the kernel of ω, it can be written in terms of a single function f, as follows:

$$\begin{aligned}X=&-\frac{1}{(n-1)!}\epsilon^{\mu_2\cdots\mu_n\mu}\left(\frac{\partial f}{\partial x^\mu}\frac{\partial}{\partial p}-\frac{1}{n}\frac{\partial f}{\partial p}\frac{\partial}{\partial x^\mu}\right)\wedge\frac{\partial}{\partial x^{\mu_2}}\wedge\cdots\wedge\frac{\partial}{\partial x^{\mu_n}}\\&+\frac{1}{(n-1)!}\epsilon^{\mu_2\cdots\mu_n\mu}\left(\frac{\partial f}{\partial p^\mu_i}\frac{\partial}{\partial q^i}-\frac{1}{n}\frac{\partial f}{\partial q^i}\frac{\partial}{\partial p^\mu_i}\right)\wedge\frac{\partial}{\partial x^{\mu_2}}\wedge\cdots\wedge\frac{\partial}{\partial x^{\mu_n}}.\end{aligned} \tag{29}$$

Moreover, X is exact Hamiltonian if and only if f is a linear function of the multimomentum variables p^ρ_r and the energy variable p.

Proof: Obviously, X is locally Hamiltonian if and only if, locally, $i_X\omega=\mathrm{d}f$ for some function f, which in view of Eq. (28) leads to the following system of equations for the coefficients $\widetilde{X}$, X^i_μ, X_i, and X_μ of X:

$$\widetilde{X}=(-1)^{n-1}\frac{\partial f}{\partial p},\quad X^i_\mu=\frac{\partial f}{\partial p^\mu_i},\quad X_i=(-1)^n\frac{\partial f}{\partial q^i},\quad X_\mu=-\frac{\partial f}{\partial x^\mu}.$$

Inserting this back into X, we arrive at Eq. (29). Note also that then,

$$i_X\theta=(-1)^{n-1}p\frac{\partial f}{\partial p}+(-1)^{n-1}p^\mu_i\frac{\partial f}{\partial p^\mu_i}=(-1)^{n-1}L_\Sigma f.$$

Next, X will be exact Hamiltonian if and only if, in addition,

$$f=(-1)^{n-1}i_X\theta,$$

which in view of the preceding equation means that f must be an eigenfunction of the scaling operator L_Σ with eigenvalue 1, this is well known to be the case if and only if f is linear in the multimomentum variables p^ρ_r and the energy variable p. □

Now we turn to multivector fields of tensor degree $<n$. Here, the main result is the following.

Theorem 2.4: *An r-multivector field X on P, with $0<r<n$, is locally Hamiltonian if and only*

if the coefficients $X^{\mu_1\cdots\mu_r}$, $X^{i,\mu_2\cdots\mu_r}$, $X_i^{\mu_1\cdots\mu_r}$, *and* $\widetilde{X}^{\mu_2\cdots\mu_r}$ *in its standard local coordinate representation (26) satisfy the following conditions:*

(1) *The coefficients* $X^{\mu_1\cdots\mu_r}$ *depend only on the local coordinates* x^ρ *for* M *and, in the special case* $N=1$, *also on the local fiber coordinates* q^r *for* E,

(2) *The coefficients* $X^{i,\mu_2\cdots\mu_r}$ *are "antisymmetric polynomials in the multimomentum variables" of degree* $r-1$, *i.e., they can be written in the form*

$$X^{i,\mu_2\cdots\mu_r}=\sum_{s=1}^{r}X_{s-1}^{i,\mu_2\cdots\mu_r}, \tag{30}$$

with

$$X_{s-1}^{i,\mu_2\cdots\mu_r}=\frac{1}{(s-1)!}\frac{1}{(r-s)!}\sum_{\pi\in S_{r-1}}(-1)^\pi p_{i_2}^{\mu_{\pi(2)}}\cdots p_{i_s}^{\mu_{\pi(s)}}Y_{s-1}^{ii_2\cdots i_s,\mu_{\pi(s+1)}\cdots\mu_{\pi(r)}}, \tag{31}$$

where S_{r-1} *denotes the permutation group of* $\{2,\ldots,r\}$ *and the coefficients* $Y_{s-1}^{ii_2\cdots i_s,\mu_{s+1}\cdots\mu_r}$ *depend only on the local coordinates* x^ρ *for* M *as well as the local fiber coordinates* q^r *for* E *and are totally antisymmetric in* $i,i_2,\ldots,i_s$ *as well as in* $\mu_{s+1},\ldots,\mu_r$.

(3) *The remaining coefficients* $X_i^{\mu_1\cdots\mu_r}$ *and* $\widetilde{X}^{\mu_2\cdots\mu_r}$ *can be expressed in terms of the previous ones and of new coefficients* $X_-^{\mu_1\cdots\mu_r}$ *depending only on the local coordinates* x^ρ *for* M *as well as the local fiber coordinates* q^r *for* E *and are totally antisymmetric in* $\mu_1,\ldots,\mu_r$, *according to*

$$\begin{aligned}X_i^{\mu_1\cdots\mu_r}=&-p\frac{\partial X^{\mu_1\cdots\mu_r}}{\partial q^i}+p_i^\mu\frac{\partial X^{\mu_1\cdots\mu_r}}{\partial x^\mu}-\sum_{s=1}^{r}p_i^{\mu_s}\frac{\partial X^{\mu_1\cdots\mu_{s-1}\nu\mu_{s+1}\cdots\mu_r}}{\partial x^\nu}\\&-\Sigma^{-1}\left(\sum_{s=1}^{r}(-1)^{s-1}p_j^{\mu_s}\frac{\partial X^{j,\mu_1\cdots\mu_{s-1}\mu_{s+1}\cdots\mu_r}}{\partial q^i}\right)+\frac{\partial X_-^{\mu_1\cdots\mu_r}}{\partial q^i},\end{aligned} \tag{32}$$

(the first term being absent as soon as $N>1$*) and*

$$\begin{aligned}\widetilde{X}^{\mu_2\cdots\mu_r}=&(-1)^r p\frac{\partial X^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu}-\Sigma^{-1}\left(p_i^\mu\frac{\partial X^{i,\mu_2\cdots\mu_r}}{\partial x^\mu}-\sum_{s=2}^{r}p_i^{\mu_s}\frac{\partial X^{i,\mu_2\cdots\mu_{s-1}\nu\mu_{s+1}\cdots\mu_r}}{\partial x^\nu}\right)\\&-(-1)^r\frac{\partial X_-^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu}.\end{aligned} \tag{33}$$

It is exact Hamiltonian if and only if, in addition, the coefficents $X^{i,\mu_2\cdots\mu_r}$ *depend only on the local coordinates* x^ρ *for* M *as well as the local fiber coordinates* q^r *for* E *and the coefficients* $X_-^{\mu_1\cdots\mu_r}$ *vanish.*

Proof: The proof will be carried out by "brute force" computation.[9] We obtain for the Lie derivative of ω along X the expression

$$\begin{aligned}L_X\omega=&-\frac{1}{(r-2)!}\frac{\partial\widetilde{X}^{\mu_3\cdots\mu_r\nu}}{\partial x^\nu}\mathrm{d}^n x_{\mu_3\cdots\mu_r}-\frac{1}{(r-1)!}\left(\frac{\partial\widetilde{X}^{\mu_2\cdots\mu_r}}{\partial q^i}-(-1)^{r-1}\frac{\partial X_i^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu}\right)\mathrm{d}q^i\wedge\mathrm{d}^n x_{\mu_2\cdots\mu_r}\\&-\frac{1}{(r-1)!}\left(\frac{\partial\widetilde{X}^{\mu_2\cdots\mu_r}}{\partial p_i^\mu}+\frac{\partial X^{i,\mu_2\cdots\mu_r}}{\partial x^\mu}-\sum_{s=2}^{r}\delta_\mu^{\mu_s}\frac{\partial X^{i,\mu_2\cdots\mu_{s-1}\nu\mu_{s+1}\cdots\mu_r}}{\partial x^\nu}\right)\mathrm{d}p_i^\mu\wedge\mathrm{d}^n x_{\mu_2\cdots\mu_r}\\&-\frac{1}{(r-1)!}\left(\frac{\partial\widetilde{X}^{\mu_2\cdots\mu_r}}{\partial p}+(-1)^{r-1}\frac{\partial X^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu}\right)\mathrm{d}p\wedge\mathrm{d}^n x_{\mu_2\cdots\mu_r}\\&-\frac{(-1)^r}{r!}\left(\frac{\partial X^{\mu_1\cdots\mu_r}}{\partial q^i}+\frac{\partial X_i^{\mu_1\cdots\mu_r}}{\partial p}\right)\mathrm{d}q^i\wedge\mathrm{d}p\wedge\mathrm{d}^n x_{\mu_1\cdots\mu_r}\end{aligned}$$

$$
\begin{aligned}
&-\frac{(-1)^r}{r!}\left(\frac{\partial X^{\mu_1\cdots\mu_r}}{\partial p_i^\mu}-\sum_{s=1}^r(-1)^{s-1}\delta_\mu^{\mu_s}\frac{\partial X^{i,\mu_1\cdots\mu_{s-1}\mu_{s+1}\cdots\mu_r}}{\partial p}\right)\mathrm{d}p_i^\mu\wedge\mathrm{d}p\wedge\mathrm{d}^nx_{\mu_1\cdots\mu_r}\\
&+\frac{(-1)^r}{r!}\left(\delta_i^k\delta_\kappa^\mu\frac{\partial X^{\mu_1\cdots\mu_r}}{\partial x^\mu}-\sum_{s=1}^r\delta_i^k\delta_\kappa^{\mu_s}\frac{\partial X^{\mu_1\cdots\mu_{s-1}\nu\mu_{s+1}\cdots\mu_r}}{\partial x^\nu}\right.\\
&\left.-\sum_{s=1}^r(-1)^{s-1}\delta_\kappa^{\mu_s}\frac{\partial X^{k,\mu_1\cdots\mu_{s-1}\mu_{s+1}\cdots\mu_r}}{\partial q^i}-\frac{\partial X_i^{\mu_1\cdots\mu_r}}{\partial p_k^\kappa}\right)\mathrm{d}q^i\wedge\mathrm{d}p_k^\kappa\wedge\mathrm{d}^nx_{\mu_1\cdots\mu_r}\\
&-\frac{(-1)^r}{r!}\frac{\partial X_i^{\mu_1\cdots\mu_r}}{\partial q^j}\mathrm{d}q^i\wedge\mathrm{d}q^j\wedge\mathrm{d}^nx_{\mu_1\cdots\mu_r}+\frac{(-1)^{r-1}}{(r-1)!}\frac{\partial X^{l,\mu_2\cdots\mu_r}}{\partial p_k^\kappa}\mathrm{d}p_k^\kappa\wedge\mathrm{d}p_l^\lambda\wedge\mathrm{d}^nx_{\lambda\mu_2\cdots\mu_r}\\
&-\frac{1}{r!}\frac{\partial X^{\mu_1\cdots\mu_r}}{\partial q^j}\mathrm{d}q^i\wedge\mathrm{d}q^j\wedge\mathrm{d}p_i^\mu\wedge\mathrm{d}^nx_{\mu\mu_1\cdots\mu_r}-\frac{1}{r!}\frac{\partial X^{\mu_1\cdots\mu_r}}{\partial p_k^\kappa}\mathrm{d}q^l\wedge\mathrm{d}p_k^\kappa\wedge\mathrm{d}p_l^\lambda\wedge\mathrm{d}^nx_{\lambda\mu_1\cdots\mu_r}\\
&+\frac{1}{r!}\frac{\partial X^{\mu_1\cdots\mu_r}}{\partial p}\mathrm{d}q^i\wedge\mathrm{d}p_i^\mu\wedge\mathrm{d}p\wedge\mathrm{d}^nx_{\mu\mu_1\cdots\mu_r}.
\end{aligned}
$$

(Note that the last three terms would have to be omitted if $r=n$.)

Let us number the terms in this equation from 1 to 12. As we shall see, each of these terms must vanish separately.

Term No. 12: After contraction with a suitably chosen $(n-r+2)$-multivector field, we see that $X^{\kappa_1\cdots\kappa_r}$ cannot depend on p.

Term No. 11: Given indices i, μ and mutually different indices $\kappa_1,\ldots,\kappa_r$, we choose indices j and $\nu\notin\{\kappa_1,\ldots,\kappa_r\}$ (here we use the hypothesis that $r<n$) such that either $j\neq i$ or $\nu\neq\mu$ and, when $r<n-1$, a complementary set of indices $\nu_1,\ldots,\nu_{n-r-1}$ to contract this term with the multivector field $\partial_j\wedge\partial_\mu^i\wedge\partial_\nu^j\wedge\partial_{\nu_1}\wedge\cdots\wedge\partial_{\nu_{n-r-1}}$ (no sum over j), concluding that $X^{\kappa_1\cdots\kappa_r}$ cannot depend on p_i^μ. Obviously, there is one case where this argument does not work, namely when $N=1$, $r=n-1$, and $\mu\notin\{\kappa_1,\ldots,\kappa_r\}$. This situation will however be covered in the next item.

Term No. 6: Given indices k, κ and mutually different indices $\kappa_1,\ldots,\kappa_r$ such that $\kappa\notin\{\kappa_1,\ldots,\kappa_r\}$, we choose a complementary set of indices $\nu_1,\ldots,\nu_{n-r-1}$ to contract this term with the multivector field $\partial_\kappa^k\wedge\partial_0\wedge\partial_\kappa\wedge\partial_{\nu_1}\wedge\cdots\wedge\partial_{\nu_{n-r-1}}$, concluding that $X^{\kappa_1\cdots\kappa_r}$ cannot depend on p_k^κ, since in this case the second term in the bracket gives no contribution. In particular, this settles the remaining case of the previous item.

Term No. 10: After contraction with a suitably chosen $(n-r+2)$ - multivector field, we see that $X^{\kappa_1\cdots\kappa_r}$ cannot depend on q^l if $N>1$. For $N=1$, the whole term vanishes identically, and no conclusion can be drawn.

This proves the statements in item (1) of the theorem. Moreover, it allows to simplify *term No. 6*, as follows:

$$
-\frac{(-1)^{r-1}}{(r-1)!}\frac{\partial X^{i,\mu_2\cdots\mu_r}}{\partial p}\mathrm{d}p_i^\mu\wedge\mathrm{d}p\wedge\mathrm{d}^nx_{\mu\mu_2\cdots\mu_r}.
$$

As before, contraction with a suitably chosen $(n-r+2)$-multivector field shows that $X^{k,\kappa_2\cdots\kappa_r}$ cannot depend on p.

Next we analyze *term No. 9*, which will give an important restriction on the coefficients $X^{i,\mu_2\cdots\mu_r}$. Given indices i,j,μ,ν and mutually different indices $\kappa_2,\ldots,\kappa_r$, we choose a set of indices $\nu_1,\ldots,\nu_{n-r}$ such that $\{\kappa_2,\ldots,\kappa_r\}\cap\{\nu_1,\ldots,\nu_{n-r}\}=\emptyset$ to contract this term with the multivector field $\partial_\mu^i\wedge\partial_\nu^j\wedge\partial_{\nu_1}\wedge\cdots\wedge\partial_{\nu_{n-r}}$, obtaining

$$\frac{\partial X^{j,\mu_2\cdots\mu_r}}{\partial p_i^\mu}\epsilon_{\nu\mu_2\cdots\mu_r\nu_1\cdots\nu_{n-r}}=\frac{\partial X^{i,\mu_2\cdots\mu_r}}{\partial p_j^\nu}\epsilon_{\mu\mu_2\cdots\mu_r\nu_1\cdots\nu_{n-r}}. \tag{34}$$

Now assume the index ν to be chosen such that $\nu\notin\{\kappa_2,\ldots,\kappa_r,\nu_1,\ldots,\nu_{n-r}\}$. Then if $\mu\notin\{\kappa_2,\ldots,\kappa_r\}$, we can take $\mu=\nu_1$, say, to conclude that $X^{j,\kappa_2\cdots\kappa_r}$ cannot depend on p_i^μ,

$$\frac{\partial X^{j,\mu_2\cdots\mu_r}}{\partial p_i^\mu}=0 \quad \text{if } \mu\notin\{\mu_2,\ldots,\mu_r\}. \tag{35}$$

Moreover, if $\mu\in\{\kappa_2,\ldots,\kappa_r\}$, this result implies that applying an operator $\partial_\mu^{i'}$ (with arbitrary i') to Eq. (34) gives zero since on the right-hand side (rhs), the ϵ-tensor kills all terms in the sum over the indices $\mu_2,\ldots,\mu_r$ in which the index μ appears among them,

$$\frac{\partial^2 X^{j,\mu_2\cdots\mu_r}}{\partial p_{i_1}^\mu\partial p_{i_2}^\mu}=0 \quad \text{if } \mu\in\{\mu_2,\ldots,\mu_r\} \quad (\text{no sum over } \mu). \tag{36}$$

The general solution to Eqs. (35) and (36) can be written in the form

$$X^{j,\mu_2\cdots\mu_r}=\sum_{s=1}^{r}\frac{1}{(s-1)!}\frac{1}{(r-s)!}\sum_{\pi\in S_{r-1}}(-1)^\pi p_{j_2}^{\mu_{\pi(2)}}\cdots p_{j_s}^{\mu_{\pi(s)}}Y_{s-1}^{j,j_2\cdots j_s,\mu_{\pi(s+1)}\cdots\mu_{\pi(r)}},$$

where S_{r-1} denotes the permutation group of $\{2,\ldots,r\}$ and the newly introduced coefficients $Y_{s-1}^{i,j_2\cdots j_s,\mu_{s+1}\cdots\mu_r}$ are local functions on E, they do not depend on the multimomentum variables p_k^κ or the energy variable p and are totally antisymmetric both in $j_2,\ldots,j_s$ and in $\mu_{s+1},\ldots,\mu_r$. Differentiating this expression with respect to p_i^μ with $\mu=\mu_2$ gives

$$\begin{aligned}&\frac{\partial X^{j,\mu\mu_3\cdots\mu_r}}{\partial p_i^\mu}\epsilon_{\nu\mu\mu_3\cdots\mu_r\nu_1\cdots\nu_{n-r}} \quad (\text{no sum over } \mu)\\ &=\sum_{s=2}^{r}\frac{1}{(s-2)!}\frac{1}{(r-s)!}\sum_{\pi\in S_{r-2}}(-1)^\pi p_{j_3}^{\mu_{\pi(3)}}\cdots p_{j_s}^{\mu_{\pi(s)}}Y_{s-1}^{j,ij_3\cdots j_s,\mu_{\pi(s+1)}\cdots\mu_{\pi(r)}}\epsilon_{\nu\mu\mu_3\cdots\mu_r\nu_1\cdots\nu_{n-r}},\end{aligned}$$

where S_{r-2} denotes the permutation group of $\{3,\ldots,r\}$, which shows that Eq. (34) will hold provided that

$$Y_{s-1}^{j,ij_3\cdots j_s,\mu_{\pi(s+1)}\cdots\mu_{\pi(r)}}=-Y_{s-1}^{i,jj_3\cdots j_s,\mu_{\pi(s+1)}\cdots\mu_{\pi(r)}}.$$

This proves the statements in item (2) of the theorem.

We proceed with *terms Nos. 4 and 5* which imply

$$\frac{\partial\widetilde{X}^{\mu_2\cdots\mu_r}}{\partial p}=(-1)^r\frac{\partial X^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu}, \quad \frac{\partial X_i^{\mu_1\cdots\mu_r}}{\partial p}=-\frac{\partial X^{\mu_1\cdots\mu_r}}{\partial q^i}. \tag{37}$$

We observe first of all that the rhs of both equations does not depend on the energy variable, so they can be immediately integrated with respect to p.

From *term No. 3* we infer

$$\frac{\partial\widetilde{X}^{\mu_2\cdots\mu_r}}{\partial p_i^\mu}=-\frac{\partial X^{i,\mu_2\cdots\mu_r}}{\partial x^\mu}+\sum_{s=2}^{r}\delta_\mu^{\mu_s}\frac{\partial X^{i,\mu_2\cdots\mu_{s-1}\nu\mu_{s+1}\cdots\mu_r}}{\partial x^\nu}. \tag{38}$$

An explicit calculation shows that the rhs of this equation does not depend on the p_j^μ, not only when $\mu\notin\{\mu_2,\ldots,\mu_r\}$ but even when $\mu\in\{\mu_2,\ldots,\mu_r\}$. (Of course, it also does not depend on p.) Thus, according to Lemma A.2 formulated in the appendix, we can integrate Eq. (38) explicitly to obtain (recall that Σ^{-1} is the operator that acts on polynomials in the multimomentum variables

and the energy variable without constant term by multiplying the homogeneous component of degree s by $1/s$)

$$\widetilde{X}^{\mu_2\cdots\mu_r} = (-1)^r p \frac{\partial X^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu} - \Sigma^{-1}\left(p_i^\mu \frac{\partial X^{i,\mu_2\cdots\mu_r}}{\partial x^\mu} - \sum_{s=2}^{r} p_i^{\mu_s} \frac{\partial X^{i,\mu_2\cdots\mu_{s-1}\nu\mu_{s+1}\cdots\mu_r}}{\partial x^\nu} \right) + \widetilde{Y}^{\mu_2\cdots\mu_r}, \tag{39}$$

where the $\widetilde{Y}^{\mu_2\cdots\mu_r}$ are local functions on E: they do not depend on the multimomentum variables or on the energy variable.

The same procedure works for *term No. 7*. There, we are left with

$$\frac{\partial X_i^{\mu_1\cdots\mu_r}}{\partial p_k^\kappa} = \delta_i^k \delta_\kappa^\mu \frac{\partial X^{\mu_1\cdots\mu_r}}{\partial x^\mu} - \sum_{s=1}^{r} \delta_i^k \delta_\kappa^{\mu_s} \frac{\partial X^{\mu_1\cdots\mu_{s-1}\nu\mu_{s+1}\cdots\mu_r}}{\partial x^\nu} - \sum_{s=1}^{r} (-1)^{s-1} \delta_\kappa^{\mu_s} \frac{\partial X^{k,\mu_1\cdots\mu_{s-1}\mu_{s+1}\cdots\mu_r}}{\partial q^i}. \tag{40}$$

Using the same argument as before, we show that the rhs does not depend on the p_l^κ, not only when $\kappa \notin \{\mu_1, \ldots, \mu_r\}$ but even when $\kappa \in \{\mu_1, \ldots, \mu_r\}$, and neither does it depend on p. Therefore, we can integrate Eq. (40) explicitly to obtain

$$\begin{aligned} X_i^{\mu_1\cdots\mu_r} = &- p \frac{\partial X^{\mu_1\cdots\mu_r}}{\partial q^i} + p_i^\mu \frac{\partial X^{\mu_1\cdots\mu_r}}{\partial x^\mu} - \sum_{s=1}^{r} p_i^{\mu_s} \frac{\partial X^{\mu_1\cdots\mu_{s-1}\nu\mu_{s+1}\cdots\mu_r}}{\partial x^\nu} \\ &- \Sigma^{-1}\left(\sum_{s=1}^{r} (-1)^{s-1} p_k^{\mu_s} \frac{\partial X^{k,\mu_1\cdots\mu_{s-1}\mu_{s+1}\cdots\mu_r}}{\partial q^i} \right) + Y_i^{\mu_1\cdots\mu_r}, \end{aligned} \tag{41}$$

where the $Y_i^{\mu_1\cdots\mu_r}$ are local functions on E: they do not depend on the multimomentum variables or on the energy variable.

Finally, we turn to *terms Nos. 1, 2, and 8*. They imply

$$\frac{\partial \widetilde{X}^{\mu_3\cdots\mu_r\nu}}{\partial x^\nu} = 0, \quad \frac{\partial \widetilde{X}^{\mu_2\cdots\mu_r}}{\partial q^i} = (-1)^{r-1} \frac{\partial X_i^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu}, \quad \frac{\partial X_i^{\mu_1\cdots\mu_r}}{\partial q^j} = \frac{\partial X_j^{\mu_1\cdots\mu_r}}{\partial q^i},$$

respectively. With the help of (39), these reduce to

$$\frac{\partial \widetilde{Y}^{\mu_3\cdots\mu_r\nu}}{\partial x^\nu} = 0, \quad \frac{\partial \widetilde{Y}^{\mu_2\cdots\mu_r}}{\partial q^i} = (-1)^{r-1} \frac{\partial Y_i^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu}, \quad \frac{\partial Y_i^{\mu_1\cdots\mu_r}}{\partial q^j} = \frac{\partial Y_j^{\mu_1\cdots\mu_r}}{\partial q^i},$$

which is easily solved by setting

$$\widetilde{Y}^{\mu_2\cdots\mu_r} = (-1)^{r-1} \frac{\partial X_-^{\mu_2\cdots\mu_r\mu}}{\partial x^\mu}, \quad Y_i^{\mu_1\cdots\mu_r} = \frac{\partial X_-^{\mu_1\cdots\mu_r}}{\partial q^i}. \tag{42}$$

Here, the $X_-^{\mu_1\cdots\mu_r}$ are local functions on E: they do not depend on the multimomentum variables or on the energy variable. This completes the proof of the statements in item (3) of the theorem.

All that remains to be shown are the final statements concerning exact Hamiltonian multivector fields. To this end, we calculate

$$
\begin{aligned}
L_X\theta = \frac{1}{(r-1)!}\Bigg(&\frac{\partial X^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu}p - (-1)^r\frac{\partial X^{i,\mu_2\cdots\mu_r}}{\partial x^\mu}p_i^\mu \\
&+ (-1)^r\sum_{s=2}^{r}\frac{\partial X^{i,\mu_2\cdots\mu_{s-1}\nu\mu_{s+1}\cdots\mu_r}}{\partial x^\nu}p_i^{\mu_s} - (-1)^r\widetilde{X}^{\mu_2\cdots\mu_r}\Bigg)\mathrm{d}^n x_{\mu_2\cdots\mu_r} \\
&- \frac{1}{r!}\Bigg(\frac{\partial X^{\mu_1\cdots\mu_r}}{\partial x^\mu}p_i^\mu - \sum_{s=1}^{r}\frac{\partial X^{\mu_1\cdots\mu_{s-1}\nu\mu_{s+1}\cdots\mu_r}}{\partial x^\nu}p_i^{\mu_s} - \frac{\partial X^{\mu_1\cdots\mu_r}}{\partial q^i}p \\
&- \sum_{s=1}^{r}(-1)^{s-1}\frac{\partial X^{j,\mu_1\cdots\mu_{s-1}\mu_{s+1}\cdots\mu_r}}{\partial q^i}p_j^{\mu_s} - X_i^{\mu_1\cdots\mu_r}\Bigg)\mathrm{d}q^i\wedge\mathrm{d}^n x_{\mu_1\cdots\mu_r} \\
&+ \frac{1}{r!}\Bigg(\frac{\partial X^{\mu_1\cdots\mu_r}}{\partial p_j^\nu}p + \sum_{s=1}^{r}(-1)^{s-1}\frac{\partial X^{i,\mu_1\cdots\mu_{s-1}\mu_{s+1}\cdots\mu_r}}{\partial p_j^\nu}p_i^{\mu_s}\Bigg)\mathrm{d}p_j^\nu\wedge\mathrm{d}^n x_{\mu_1\cdots\mu_r} \\
&+ \frac{1}{r!}\Bigg(\frac{\partial X^{\mu_1\cdots\mu_r}}{\partial p}p + \sum_{s=1}^{r}(-1)^{s-1}\frac{\partial X^{i,\mu_1\cdots\mu_{s-1}\mu_{s+1}\cdots\mu_r}}{\partial p}p_i^{\mu_s}\Bigg)\mathrm{d}p\wedge\mathrm{d}^n x_{\mu_1\cdots\mu_r},
\end{aligned}
$$

where we have omitted four terms that vanish because X is locally Hamiltonian. Moreover, using the expressions derived above for locally Hamiltonian multivector fields, we see that the other terms vanish as well if and only if we have

$$
(\Sigma^{-1}-1)\Bigg(\sum_{s=1}^{r}(-1)^{s-1}p_j^{\mu_s}\frac{\partial X^{j,\mu_1\cdots\mu_{s-1}\mu_{s+1}\cdots\mu_r}}{\partial q^i}\Bigg) = 0,
$$

$$
(\Sigma^{-1}-1)\Bigg(p_i^\mu\frac{\partial X^{i,\mu_2\cdots\mu_r}}{\partial x^\mu} - \sum_{s=2}^{r}p_i^{\mu_s}\frac{\partial X^{i,\mu_2\cdots\mu_{s-1}\nu\mu_{s+1}\cdots\mu_r}}{\partial x^\nu}\Bigg) = 0,
$$

and

$$
\frac{\partial X_-^{\mu_1\cdots\mu_r}}{\partial q^i} = 0, \quad \frac{\partial X_-^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu} = 0.
$$

But this means that the coefficients of the multimomentum variables in the above expressions must be independent of the multimomentum variables and that the coefficients $X_-^{\mu_1\cdots\mu_r}$ can without loss of generality be assumed to vanish, which completes the proof of the theorem. □

Proof of Theorem 1.3, part 1: The statements of Theorem 1.3 about multivector fields are, in their local form, based on the local decomposition given in Proposition 2.1, taking into account the scaling behavior of the coefficient functions that follows from Theorem 2.4, together with that of the coordinate vector fields. The global version of these statements can be obtained by glueing together such local decompositions using appropriate partitions of unity. To see that the homogeneous components X_s, $s=-1,\ldots,r-1$, of a fiberwise polynomial locally Hamiltonian r-multivector field X are locally Hamiltonian, we compute

$$
0 = (L_\Sigma)^k\,\mathrm{d}i_X\,\omega = \sum_{s=0}^{r-1}(s+1)^k\,\mathrm{d}i_{X_s}\,\omega, \quad k=1,\ldots,r-1.
$$

Together with $\mathrm{d}i_X\omega=0$, this leads to a Vandermonde matrix equation with entries $0,2,3,\ldots,r-1$ annihilating the vector $(\mathrm{d}i_{X_{-1}}\omega,\ldots,\mathrm{d}i_{X_{r-1}}\omega)^T$. As the determinant of a Vandermonde matrix does not vanish, the above vector must vanish. □

The following proposition clarifies the interpretation of homogeneous locally Hamiltonian multivector fields.

Proposition 2.5: Let X be a locally Hamiltonian r-multivector field on P. Then

(1) X is exact Hamiltonian iff $[\Sigma, X]$ *takes values in the kernel of* ω.

(2) If $[\Sigma, X] - sX$ *takes values in the kernel of* ω, *for some integer s between 0 and* $r-1$, *then X is globally Hamiltonian with associated Poisson form*

$$\frac{(-1)^{r-1}}{s+1} i_X \theta.$$

(3) If $[\Sigma, X] + X$ *takes values in the kernel of* ω, *then* $i_X \theta = 0$.

Proof: The first statement follows immediately from Eq. (25). Similarly, the second claim can be proved by multiplying Eq. (25) by $(-1)^{r-1}/(s+1)$ and combining it with Eq. (1) and Eq. (4) to give

$$\mathrm{d}\left(\frac{(-1)^{r-1}}{s+1} i_X \theta\right) = \frac{(-1)^{r-1}}{s+1} L_X \theta + \frac{1}{s+1} i_X \omega = \frac{1}{s+1} i_{[\Sigma,X]+X} \omega,$$

which equals $i_X \omega$ since, by hypothesis, $i_{[\Sigma,X]-sX}\omega = 0$. Finally, the third statement follows by observing that the kernel of ω is contained in the kernel of θ and hence according to the hypothesis made,

$$0 = i_{[\Sigma,X]+X}\theta = L_\Sigma i_X \theta - i_X L_\Sigma \theta + i_X \theta = L_\Sigma i_X \theta,$$

where we have used the invariance of θ under Σ. Therefore, according to Proposition A.1, $i_X \theta$ is the pull-back to P of an n-form on E via the projection that defines P as a vector bundle over E, which in turn can be obtained as the pull-back to E of $i_X \theta$ via the zero section of P over E. But this pull-back is zero, since θ vanishes along the zero section of P over E. □

It may be instructive to spell all this out more explicitly for locally Hamiltonian vector fields $(r=1)$.

We begin by writing down the general form of a locally Hamiltonian vector field X: in adapted local coordinates, it has the representation

$$X = X^\mu \frac{\partial}{\partial x^\mu} + X^i \frac{\partial}{\partial q^i} + X^\mu_i \frac{\partial}{\partial p^\mu_i} + \widetilde{X} \frac{\partial}{\partial p},$$

where according to Theorem 2.4, the coefficient functions X^μ and X^i depend only on the local coordinates x^ρ for M and on the local fiber coordinates q^r for E (the X^μ being independent of the latter as soon as $N > 1$), whereas the coefficient functions X^μ_i and $\widetilde{X}$ are explicitly given by

$$X^\mu_i = -p \frac{\partial X^\mu}{\partial q^i} + p^\nu_i \frac{\partial X^\mu}{\partial x^\nu} - p^\mu_i \frac{\partial X^\nu}{\partial x^\nu} - p^\mu_j \frac{\partial X^j}{\partial q^i} + \frac{\partial X^\mu_-}{\partial q^i} \tag{43}$$

(the first term being absent as soon as $N > 1$) and

$$\widetilde{X} = -p \frac{\partial X^\nu}{\partial x^\nu} - p^\mu_i \frac{\partial X^i}{\partial x^\mu} + \frac{\partial X^\nu_-}{\partial x^\nu} \tag{44}$$

with coefficient functions X^μ_- that once again depend only on the local coordinates x^ρ for M and on the local fiber coordinates q^r for E. Regarding the decomposition (19), the situation here is particularly interesting and somewhat special since ω is nondegenerate on vector fields, so there are no nontrivial vector fields taking values in the kernel of ω and hence the decomposition (19) can be improved.

Corollary 2.6: Any locally Hamiltonian vector field X on P can be uniquely decomposed into the sum of two terms,

$$X = X_- + X_+, \tag{45}$$

where

(i) *X_- has scaling degree -1, i.e., $[\Sigma, X_-] = -X_-$, and is vertical with respect to the projection onto E.*

(ii) *X_+ has scaling degree 0, i.e., $[\Sigma, X_+] = 0$, is exact Hamiltonian, is projectable onto E and coincides with the canonical lift of its projection onto E.*

Proof: In adapted local coordinates, the two contributions to X are, according to Eqs. (43) and (44), given by

$$X_- = \frac{\partial X_-^\mu}{\partial q^i}\frac{\partial}{\partial p_i^\mu} + \frac{\partial X_-^\nu}{\partial x^\nu}\frac{\partial}{\partial p}$$

and

$$X_+ = X^\mu \frac{\partial}{\partial x^\mu} + X^i \frac{\partial}{\partial q^i} - \left(\frac{\partial X^j}{\partial q^i} p_j^\mu - \frac{\partial X^\mu}{\partial x^\nu} p_i^\nu + \frac{\partial X^\nu}{\partial x^\nu} p_i^\mu + \frac{\partial X^\mu}{\partial q^i} p\right)\frac{\partial}{\partial p_i^\mu} - \left(\frac{\partial X^i}{\partial x^\mu} p_i^\mu + \frac{\partial X^\nu}{\partial x^\nu} p\right)\frac{\partial}{\partial p}.$$

Thus all statements of the corollary follow from what has already been shown, except for the very last one, which is based on the following remark. □

Remark: Every bundle automorphism of E (as a fiber bundle over M) admits a canonical lift to a bundle automorphism of its first order jet bundle JE (as an affine bundle over E) and, by appropriate (twisted affine) dualization, to the extended multiphase space P (as a vector bundle over E). Similarly, passing to generators of one-parameter groups, one sees that every vector field X_E on E that is projectable to a vector field X_M on M admits a canonical lift to a vector field X_{JE} on JE and, by appropriate (twisted affine) dualization, to a vector field X_P on P. (See, for example, Ref. 7, Sec. 4B.) When $N=1$, lifting to P is even possible for arbitrary diffeomorphisms of E and arbitrary vector fields on E, since in this case P can be identified with the nth exterior power of the cotangent bundle of E. Explicitly, in terms of adapted local coordinates (x^μ, q^i, p_i^μ, p), we may write

$$X_M = X^\mu \frac{\partial}{\partial x^\mu} \quad \text{and } X_E = X^\mu \frac{\partial}{\partial x^\mu} + X^i \frac{\partial}{\partial q^i},$$

where, except for $N=1$, the X^μ do not depend on the q^r; then the coordinate expression for the lifted vector field, X_P, is precisely given by the expression for X_+ above. Obviously, X_P has scaling degree 0 and hence is not only locally but even exact Hamiltonian. Conversely, starting with an exact Hamiltonian vector field X_+, we can obtain X_M and X_E by projection onto M and E, respectively. Thus, the coordinate expression for X_+ shows that *precisely all exact Hamiltonian vector fields are obtained by this lifting procedure*. Similarly, one can show that all diffeomorphisms of P that preserve the multicanonical form θ are obtained by lifting of automorphisms or, for $N=1$, diffeomorphisms of E, this is the field theoretical analog of a well-known theorem in geometric mechanics, according to which all diffeomorphisms of a cotangent bundle that preserve the canonical form θ are induced by diffeomorphisms of its base manifold.

To conclude this section, let us note that the definition of projectability of vector fields can be immediately generalized to multivector fields: an r-multivector field X_E on the total space E of a fiber bundle over a manifold M with bundle projection $\pi: E \to M$ is called *projectable* if for any two points e_1 and e_2 in E,

$$\Lambda^r T_{e_1}\pi \cdot X_E(e_1) = \Lambda^r T_{e_2}\pi \cdot X_E(e_2) \quad \text{if } \pi(e_1) = \pi(e_2),$$

or in other words, if there exists an r-multivector field X_M on M such that

$$\Lambda^r T\pi \circ X_E = X_M \circ \pi.$$

In adapted local coordinates, this amounts to requiring that if we write

$$X_E = \frac{1}{r!} X^{\mu_1 \cdots \mu_r} \frac{\partial}{\partial x^{\mu_1}} \wedge \cdots \wedge \frac{\partial}{\partial x^{\mu_r}} + \cdots ,$$

where the dots denote 1-vertical terms, the coefficients $X^{\mu_1 \cdots \mu_r}$ should depend only on the local coordinates x^ρ for M but not on the local fiber coordinates q^r for E. Now we introduce the following terminology.

Definition 2.7: An r-multivector field on P is called projectable if it is projectable with respect to any one of the three projections from P: to P_0, to E, and to M.

With this terminology, Theorem 2.4 states that for $0 < r < n$, locally Hamiltonian r-multivector fields on P are projectable as soon as $N > 1$ and are projectable to E but not necessarily to P_0 or to M when $N = 1$. [Inspection of Eq. (32) shows, however, that they are projectable to P_0 if and only if they are projectable to M.]

Considering the special case of vector fields ($r = 1$), we believe that vector fields on the total space of a fiber bundle over space-time which are not projectable should be regarded as pathological, since they generate transformations which do not induce transformations of space-time. It is hard to see how such transformations might be interpreted as candidates for symmetries of a physical system. By analogy, we shall adopt the same point of view regarding multivector fields of higher degree, since although these do not generate diffeomorphisms of E as a manifold, they may perhaps allow for an interpretation as generators of superdiffeomorphisms of an appropriate supermanifold built over E as its even part.

III. POISSON FORMS AND HAMILTONIAN FORMS

Our aim in this section is to give an explicit construction of Poisson $(n-r)$-forms and, more generally, of Hamiltonian $(n-r)$-forms on the extended multiphase space P, where $0 \leqslant r \leqslant n$. [Note that Eq. (11) only makes sense for r in this range.] A special role is played by closed forms, since closed forms are always Hamiltonian and closed forms that vanish on the kernel of ω are always Poisson, these are in a sense the trivial examples. In other words, the main task is to understand the extent to which general Hamiltonian forms deviate from closed forms and general Poisson forms deviate from closed forms that vanish on the kernel of ω.

As a warm-up exercise, we shall settle the extreme cases of tensor degree 0 and n. The case $r = n$ has already been analyzed in Ref. 2, so we just quote the result.

Proposition 3.1: A function f on P, regarded as a 0-form, is always Hamiltonian and even Poisson. Moreover, its associated Hamiltonian n-multivector field X is, in adapted local coordinates and modulo terms taking values in the kernel of ω, given by Eq. (29).

The case $r = 0$ is equally easy.

Proposition 3.2: An n-form f on P is Hamiltonian or Poisson if and only if it can be written as the sum of a constant multiple of θ with a closed form which is arbitrary if f is Hamiltonian and vanishes on the kernel of ω if f is Poisson.

Indeed, if f is a Hamiltonian n-form, the multivector field X that appears in Eq. (11) will in fact be a function which must be locally Hamiltonian and hence, by Proposition 2.2, constant. Thus $\mathrm{d}f$ must be proportional to ω and so f must be the sum of some constant multiple of θ and a closed form.

The intermediate cases $(0 < r < n)$ are much more interesting. To handle them, the first step is to identify the content of the kernel condition (13) in adapted local coordinates (for completeness, we also include the two extreme cases).

Proposition 3.3: An $(n-r)$-form f on P, with $0 \leqslant r \leqslant n$, vanishes on the kernel of ω if and only if, in adapted local coordinates, it can be written in the form

$$f = \frac{1}{r!} f^{\mu_1 \cdots \mu_r} \mathrm{d}^n x_{\mu_1 \cdots \mu_r} + \frac{1}{(r+1)!} f_i^{\mu_0 \cdots \mu_r} \, \mathrm{d}q^i \wedge \mathrm{d}^n x_{\mu_0 \cdots \mu_r} + \frac{1}{r!} f^{i, \mu_1 \cdots \mu_r} \, \mathrm{d}p_i^\mu \wedge \mathrm{d}^n x_{\mu \mu_1 \cdots \mu_r}$$
$$+ \frac{1}{(r+1)!} f'^{\mu_0 \cdots \mu_r} (\mathrm{d}p \wedge \mathrm{d}^n x_{\mu_0 \cdots \mu_r} - \mathrm{d}q^i \wedge \mathrm{d}p_i^\mu \wedge \mathrm{d}^n x_{\mu_0 \cdots \mu_r \mu}), \tag{46}$$

where the second term in the last parentheses is to be omitted if $r=n-1$ *whereas only the first term remains if* $r=n$.

Note that for one-forms (just as for functions), the kernel condition (13) is void, since ω is nondegenerate. Also, it is in this case usually more convenient to replace Eq. (46) by the standard local coordinate representation

$$f = f_\mu \, \mathrm{d}x^\mu + f_i \, \mathrm{d}q^i + f^i_\mu \, \mathrm{d}p^\mu_i + f_0 \, \mathrm{d}p. \tag{47}$$

Proof: From the particular expression for ω in adapted local coordinates, we see first of all that forms of degree $n-r$ vanishing on the kernel of ω must be $(n-r-2)$-horizontal (since they vanish on 3-vertical multivector fields) and that the only term which is not $(n-r-1)$-horizontal is

$$\mathrm{d}q^i \wedge \mathrm{d}p^\kappa_k \wedge \mathrm{d}^n x_{\mu_0 \cdots \mu_r \mu}.$$

Furthermore, f must vanish on the bivectors

$$\frac{\partial}{\partial q^i} \wedge \frac{\partial}{\partial p^\kappa_k} + \delta^k_i \frac{\partial}{\partial p} \wedge \frac{\partial}{\partial x^\kappa} \quad \text{and} \quad \frac{\partial}{\partial p^\mu_i} \wedge \frac{\partial}{\partial x^\nu} + \frac{\partial}{\partial p^\nu_i} \wedge \frac{\partial}{\partial x^\mu}$$

which yields the statement of the proposition. For more details, see Ref. 9 □

The proposition above can be used to prove the following interesting and useful fact.

Proposition 3.4: An $(n-r)$*-form* f *on* P, *with* $0 \leqslant r \leqslant n$, *vanishes on the kernel of* ω *if and only if there exists an* $(r+1)$*-multivector field* X *on* P *such that*

$$f = i_X \omega. \tag{48}$$

Then obviously,

$$\mathrm{d}f = L_X \omega. \tag{49}$$

In particular, f *is closed if and only if* X *is locally Hamiltonian*.

At every point of P, the statement that the inclusion of the kernel of ω in the kernel of f implies that there is a multivector Y such that $i_Y \omega = f$ at this point, can be shown without reference to the particular form of ω.[10] However, the expression for ω in adapted local coordinates shows that we can even obtain a multivector field Y with this property.

Proof: The "if" part being obvious, observe that it suffices to prove the "only if" part locally, in the domain of definition of an arbitrary system of adapted local coordinates, by constructing the coefficients of X from those of f. [Indeed, since the relation between f and X postulated in Eq. (48) is purely algebraic, i.e., it does not involve derivatives, we can construct a global solution patching together local solutions with a partition of unity.] A comparison of $i_X \omega$, where X is an $(r+1)$-multivector field [!] given by Eq. (26), with (46) shows that when $r < n$, this can be achieved by setting

$$X^{\mu_0 \cdots \mu_r} = (-1)^r f'^{\mu_0 \cdots \mu_r}, \quad X^{i,\mu_1 \cdots \mu_r} = (-1)^r f^{i,\mu_1 \cdots \mu_r}, \tag{50}$$

$$X^{\mu_0 \cdots \mu_r}_i = (-1)^{r+1} f^{\mu_0 \cdots \mu_r}_i, \quad \widetilde{X}^{\mu_1 \cdots \mu_r} = -f^{\mu_1 \cdots \mu_r}, \tag{51}$$

while for $r=n$, only the last equation is pertinent [for $r=n-1$, the same conclusion can also be reached by comparing (28) and (47)]. □

Corollary 3.5: An $(n-r)$*-form* f *on* P, *with* $0 \leqslant r \leqslant n$, *is a Hamiltonian form if and only if* $\mathrm{d}f$ *vanishes on the kernel of* ω *and is a Poisson form if and only if both* $\mathrm{d}f$ *and* f *vanish on the kernel of* ω.

With these preliminaries out of the way, we can proceed to the construction of Poisson forms which are not closed. As we shall see, there are two such constructions which, taken together, will be sufficient to handle the general case.

The first construction is a generalization of the universal multimomentum map of Ref. 2, which to each exact Hamiltonian r-multivector field F on P associates a Poisson $(n-r)$-form $J(F)$ on P defined by Eq. (52) below. What remained unnoticed in Ref. 2 is that this construction works even when X is only locally Hamiltonian. In fact, we have the following generalization of Proposition 4.3 of Ref. 2.

Proposition 3.6: For every locally Hamiltonian r-multivector field F on P, with $0 \leqslant r \leqslant n$, *the formula*

$$J(F) = (-1)^{r-1} i_F \theta \tag{52}$$

defines a Poisson $(n-r)$*-form* $J(F)$ *on* P *whose associated Hamiltonian multivector field is* $F+[\Sigma,F]$, *that is, we have*

$$\mathrm{d}(J(F)) = i_{F+[\Sigma,F]}\omega. \tag{53}$$

Proof: Obviously, $J(F)$ vanishes on the kernel of ω since this is contained in the kernel of θ. Moreover, since $L_F\omega$ is supposed to vanish, we can use the algebraic relations for the Lie derivative along multivector fields and $\theta = -i_\Sigma \omega$ to compute

$$\mathrm{d}(J(F)) = (-1)^{r-1}\mathrm{d}(i_F\theta) = (-1)^{r-1}L_F\theta - i_F\,\mathrm{d}\,\theta = (-1)^r L_F i_\Sigma\omega + i_\Sigma L_F\omega + i_F\omega = -i_{[F,\Sigma]}\omega + i_F\omega.$$

□

The second construction uses differential forms on E, pulled back to differential forms on P via the target projection $\tau: P \to E$. Characterizing which of these are Hamiltonian forms and which are Poisson forms is a simple exercise.

Proposition 3.7: Let f_0 *be an* $(n-r)$*-form on* E, *with* $0 < r < n$. *Then*

(i) $\tau^* f_0$ *is a Hamiltonian form on P if and only if* $\mathrm{d}f_0$ *is* $(n-r)$*-horizontal.*

(ii) $\tau^* f_0$ *is a Poisson form on P if and only if* f_0 *is* $(n-r-1)$*-horizontal and* $\mathrm{d}f_0$ *is* $(n-r)$*-horizontal.*

Proof: In adapted local coordinates (x^μ, q^i) for E and (x^μ, q^i, p_i^μ, p) for P, we can write

$$f_0 = \frac{1}{r!} f_0^{\mu_1\cdots\mu_r}\mathrm{d}^n x_{\mu_1\cdots\mu_r} + \frac{1}{(r+1)!}(f_0)_i^{\mu_0\cdots\mu_r}\,\mathrm{d}q^i \wedge \mathrm{d}^n x_{\mu_0\cdots\mu_r} + \cdots, \tag{54}$$

where the dots denote higher order terms containing at least two $\mathrm{d}q$'s. Now applying Proposition 3.3 to $\tau^* f_0$, we see that $\tau^* f_0$ will vanish on the kernel of ω if and only if the terms denoted by the dots all vanish, i.e., if f_0 can be written in the form

$$f_0 = \frac{1}{r!} f_0^{\mu_1\cdots\mu_r}\mathrm{d}^n x_{\mu_1\cdots\mu_r} + \frac{1}{(r+1)!}(f_0)_i^{\mu_0\cdots\mu_r}\,\mathrm{d}q^i \wedge \mathrm{d}^n x_{\mu_0\cdots\mu_r}. \tag{55}$$

But this is precisely the condition for the $(n-r)$-form f_0 to be $(n-r-1)$-horizontal. (Note that this equivalence holds even when $r=n-1$, provided we understand the condition of being 0-horizontal to be empty.) Similarly, since Proposition 3.4 implies that a form on P is Hamiltonian if and only if its exterior derivative vanishes on the kernel of ω, the same argument applied to $\mathrm{d}(\tau^* f_0) = \tau^*\,\mathrm{d}f_0$ shows that, irrespectively of whether $\tau^* f_0$ itself vanishes on the kernel of ω or not and hence whether we use Eq. (54) or Eq. (55) as our starting point, $\tau^* f_0$ will be Hamiltonian if and only if

$$\mathrm{d}f_0 = \frac{1}{(r-1)!}\frac{\partial f_0^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu}\mathrm{d}^n x_{\mu_2\cdots\mu_r} + \frac{1}{r!}\left(\frac{\partial f_0^{\mu_1\cdots\mu_r}}{\partial q^i} - \frac{\partial (f_0)_i^{\mu_1\cdots\mu_r\nu}}{\partial x^\nu}\right)\mathrm{d}q^i \wedge \mathrm{d}^n x_{\mu_1\cdots\mu_r}.$$

But this is precisely the condition for the $(n-r+1)$-form $\mathrm{d}f_0$ to be $(n-r)$-horizontal. Moreover, it is easy to write down an associated Hamiltonian r-multivector field X_0,

$$X_0 = \frac{(-1)^r}{r!}\left(\frac{\partial f_0^{\mu_1\cdots\mu_r}}{\partial q^i} - \frac{\partial (f_0)_i^{\mu_1\cdots\mu_r\nu}}{\partial x^\nu}\right)\frac{\partial}{\partial p_i^{\mu_1}} \wedge \frac{\partial}{\partial x^{\mu_2}} \wedge \cdots \wedge \frac{\partial}{\partial x^{\mu_r}}$$
$$- \frac{1}{(r-1)!}\frac{\partial f_0^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu}\frac{\partial}{\partial p} \wedge \frac{\partial}{\partial x^{\mu_2}} \wedge \cdots \wedge \frac{\partial}{\partial x^{\mu_r}}.$$

□

Note also that if f_0 is $(n-r-1)$-horizontal and thus has the form stated in Eq. (55), $\mathrm{d}f_0$ would contain just one additional higher order term, namely

$$\frac{1}{(r+1)!}\frac{\partial (f_0)_j^{\mu_0\cdots\mu_r}}{\partial q^i}\mathrm{d}q^i \wedge \mathrm{d}q^j \wedge \mathrm{d}^n x_{\mu_0\cdots\mu_r}.$$

Its absence means that

$$\frac{\partial (f_0)_j^{\mu_0\cdots\mu_r}}{\partial q^i} = \frac{\partial (f_0)_i^{\mu_0\cdots\mu_r}}{\partial q^j},$$

so there exist local functions $f_0^{\mu_0\cdots\mu_r}$ on E such that

$$(f_0)_i^{\mu_0\cdots\mu_r} = \frac{\partial f_0^{\mu_0\cdots\mu_r}}{\partial q^i}.$$

This implies that f_0 can be written as the sum

$$f_0 = f_h + f_c \tag{56}$$

of a horizontal form f_h and a closed form f_c, defined by setting

$$f_h = \frac{1}{r!}\left(f_0^{\mu_1\cdots\mu_r} - \frac{\partial f_0^{\mu_1\cdots\mu_r\nu}}{\partial x^\nu}\right)\mathrm{d}^n x_{\mu_1\cdots\mu_r}$$

and

$$f_c = \frac{1}{r!}\frac{\partial f_0^{\mu_1\cdots\mu_r\nu}}{\partial x^\nu}\mathrm{d}^n x_{\mu_1\cdots\mu_r} + \frac{1}{(r+1)!}\frac{\partial f_0^{\mu_0\cdots\mu_r}}{\partial q^i}\mathrm{d}q^i \wedge \mathrm{d}^n x_{\mu_0\cdots\mu_r}.$$

The same kind of local decomposition into the sum of a horizontal form and a closed form can also be derived if f_0 is arbitrary and thus has the form stated in Eq. (54); this case can be handled by decreasing induction on the number of $\mathrm{d}q$'s that appear in the higher order terms denoted by the dots in Eq. (54). We shall refrain from working this out in detail, since unfortunately the decomposition (56) depends on the system of adapted local coordinates used in its construction: under coordinate transformations, the terms f_h and f_c mix. Therefore, this decomposition has no coordinate independent meaning and is in general valid only locally.

Finally, we note that in the above discussion, we have deliberately excluded the extreme cases $r=0$ (n-forms) and $r=n$ (functions). For n-forms, the equivalences stated above would be incorrect since if f_0 has tensor degree n and hence X_0 has tensor degree 0, $i_{X_0}\omega$ would by Proposition 2.2 be a constant multiple of ω whereas $\mathrm{d}(\tau^* f_0)$ would be reduced to a linear combination of terms of the form $\mathrm{d}q^i \wedge \mathrm{d}^n x$, implying that $\tau^* f_0$ can only be Hamiltonian if it is closed. For functions, the construction is uninteresting since according to Proposition 3.1, all functions on P are Poisson, and not just the ones lifted from E.

Now we are ready to state our main decomposition theorem. (In what follows, we shall simply write f_0 instead of $\tau^* f_0$ when there is no danger of confusion, the main exception being the proof of Theorem 3.8 below.)

Theorem 3.8: *Any Hamiltonian $(n-r)$-form and, in particular, any Poisson $(n-r)$-form f on P, with $0<r<n$, admits a unique decomposition*

$$f = f_0 + f_+ + f_c \quad \text{with } f_+ = \sum_{s=1}^{r} f_s, \tag{57}$$

where

(1) *f_0 is (the pull-back to P of) an $(n-r)$-form on E whose exterior derivative is $(n-r)$-horizontal and which is otherwise arbitrary if f is Hamiltonian whereas it is restricted to be $(n-r-1)$-horizontal iff f is Poisson.*

(2) *f_+ is of the form*

$$f_+ = J(F) = (-1)^{r-1} i_F \theta \quad \text{with } F = (1 + L_\Sigma)^{-1} X_+, \tag{58}$$

and correspondingly, for $s = 1, \ldots, r$, f_s is of the form

$$f_s = \frac{(-1)^{r-1}}{s} i_{X_{s-1}} \theta, \tag{59}$$

where X is any fiberwise polynomial Hamiltonian r-multivector field associated with f, decomposed according to Eq. (19).

(3) *f_c is a closed $(n-r)$-form on P which vanishes on the zero section of P (as a vector bundle over E) and which is otherwise arbitrary if f is Hamiltonian whereas it is restricted to vanish on the kernel of ω iff f is Poisson.*

We shall refer to Eq. (57) and to Eq. (60) below as the canonical decomposition of Hamiltonian forms or Poisson forms on P.

Proof: Let f be a Poisson $(n-r)$-form and X be a Hamiltonian r-multivector field associated with f. As already mentioned in the introduction, we may without loss of generality assume X to be fiberwise polynomial and decompose it into homogeneous components with respect to scaling degree, according to Eq. (19),

$$X = X_- + X_+ + \xi \quad \text{with } X_+ = \sum_{s=1}^{r} X_{s-1}.$$

Then defining F as in the theorem, or equivalently, by

$$F = \sum_{s=1}^{r} F_{s-1} \quad \text{with } F_{s-1} = \frac{1}{s} X_{s-1},$$

we obtain

$$F + [\Sigma, F] = X_+,$$

and hence according to Eq. (53), the exterior derivative of the difference $f - J(F)$ is given by

$$\mathrm{d}(f - J(F)) = \mathrm{d}f - \mathrm{d}(J(F)) = i_X \omega - i_{X_+} \omega = i_{X_-} \omega.$$

Applying the equivalence stated in Eq. (23), we see that since X_- has scaling degree -1, $i_{X_-}\omega$ must have scaling degree 0 and hence, according to Proposition A.1, is the pull-back to P of some $(n-r)$-form f_0' on E,

$$\mathrm{d}(f - J(F)) = i_{X_-} \omega = \tau^* f_0'.$$

Next, we define f_0 to be the restriction of $f - J(F)$ to the zero section of P, or more precisely, its pull-back to E with the zero section $s_0 : E \to P$,

$$f_0 = s_0^*(f - J(F)),$$

and set

$$f_c = f - \tau^* f_0 - J(F).$$

Then

$$\mathrm{d}f_c = \mathrm{d}(f - J(F)) - \mathrm{d}(\tau^* s_0^*(f - J(F))) = \mathrm{d}(f - J(F)) - \tau^* s_0^* \mathrm{d}(f - J(F)) = \tau^* f_0' - \tau^* s_0^* \tau^* f_0' = 0,$$

and

$$s_0^* f_c = s_0^*(f - J(F)) - s_0^* \tau^* f_0 = f_0 - s_0^* \tau^* f_0 = 0,$$

showing that indeed, f_c is closed and vanishes on the zero section of P. □

Proof of Theorem 1.3, part 2: The statements of Theorem 1.3 about differential forms are immediate consequences of Theorem 3.8. □

Remark: It should be noted that despite appearances, the decompositions (57) of Theorem 3.8 and (21) of Theorem 1.3 are not necessarily identical: for $s = 1, \ldots, r$, the f_s of Eq. (57) and the f_s of Eq. (21) may differ by homogeneous closed $(n-r)$-forms of scaling degree s. But the decomposition (57) of Theorem 3.8 seems to be the more natural one.

Theorem 3.8 implies that Poisson forms have a rather intricate local coordinate representation, involving two locally Hamiltonian multivector fields. Indeed, if we take f to be a general Poisson $(n-r)$-form on P, with $0 < r < n$, we can apply Propositions 3.4 and 3.6 to rewrite Eq. (57) in the form

$$f = f_0 + (-1)^{r-1} i_F \theta + (-1)^r i_{F_c} \omega, \tag{60}$$

where f_0 is as before while F and F_c are two locally Hamiltonian multivector fields on P of tensor degree r and $r+1$, respectively, satisfying $F_- = 0$ and $(F_c)_- = 0$. [The condition $(F_c)_- = 0$ will guarantee that $i_{F_c}\omega$ vanishes on the zero section of P.] In terms of the standard local coordinate representations (46) for f, (55) for f_0, (26) for F and for F_c, and for θ and ω, Eqs. (2) and (3), we obtain

$$f^{\mu_1 \cdots \mu_r} = (-1)^{r-1} p F^{\mu_1 \cdots \mu_r} + \sum_{s=1}^{r} (-1)^{r-s} p_i^{\mu_s} F^{i, \mu_1 \cdots \mu_{s-1} \mu_{s+1} \cdots \mu_r} + f_0^{\mu_1 \cdots \mu_r} + (-1)^{r-1} (\widetilde{F}_c)^{\mu_1 \cdots \mu_r}, \tag{61}$$

$$f_i^{\mu_0 \cdots \mu_r} = -\sum_{s=0}^{r} (-1)^s p_i^{\mu_s} F^{\mu_0 \cdots \mu_{s-1} \mu_{s+1} \cdots \mu_r} + (f_0)_i^{\mu_0 \cdots \mu_r} - (F_c)_i^{\mu_0 \cdots \mu_r}, \tag{62}$$

$$f^{i, \mu_1 \cdots \mu_r} = (F_c)^{i, \mu_1 \cdots \mu_r}, \tag{63}$$

$$f'^{\mu_0 \cdots \mu_r} = (F_c)^{\mu_0 \cdots \mu_r}, \tag{64}$$

where the coefficients of F and of F_c are subject to the constraints listed in Theorem 2.4; in particular, the coefficients $(F_c)_i^{\mu_0 \cdots \mu_r}$ and $(\widetilde{F}_c)^{\mu_1 \cdots \mu_r}$ can be completely expressed in terms of the coefficients $(F_c)^{\mu_0 \cdots \mu_r}$ and $(F_c)^{i, \mu_1 \cdots \mu_r}$, according to Eqs. (32) and (33) (with r replaced by $r+1$, X replaced by F_c, and X_- replaced by 0). In particular, we see that the coefficients $f^{\mu_1 \cdots \mu_r}$ are "antisymmetric polynomials in the multimomentum variables" of degree r. More explicitly, we can rewrite Eq. (61) in the form

$$f^{\mu_1\cdots\mu_r} = (-1)^{r-1} pF^{\mu_1\cdots\mu_r} + \sum_{s=1}^{r} f_s^{\mu_1\cdots\mu_r} + f_0^{\mu_1\cdots\mu_r} + (-1)^{r-1}(\widetilde{F}_c)^{\mu_1\cdots\mu_r},$$

where inserting the expansion (31) [with X replaced by F, X_{s-1} replaced by F_{s-1} and Y_{s-1} replaced by $G_{s-1}=(1/s)g_s$] gives, after a short calculation,

$$f_s^{\mu_1\cdots\mu_r} = (-1)^{r-1}\frac{1}{s!}\frac{1}{(r-s)!}\sum_{\pi\in S_r}(-1)^{\pi} p_{i_1}^{\mu_{\pi(1)}}\cdots p_{i_s}^{\mu_{\pi(s)}} g_s^{i_1\cdots i_s,\mu_{\pi(s+1)}\cdots\mu_{\pi(r)}}.$$

Finally, we want to clarify the relation between Poisson forms and Hamiltonian multivector fields in terms of their standard local coordinate representations.

Theorem 3.9: *Let f be a Poisson $(n-r)$-form and X be a Hamiltonian r-multivector field on P associated with f. Assume that, in adapted local coordinates, f and X are given by Eqs* (46) and (26), *respectively. Then*

$$X^{\mu_1\cdots\mu_r} = (-1)^{r-1}\left(\frac{\partial f^{\mu_1\cdots\mu_r}}{\partial p} - \frac{\partial f'^{\mu_1\cdots\mu_r\nu}}{\partial x^\nu}\right), \tag{65}$$

$$X^{i,\mu_2\cdots\mu_r} = \frac{1}{n-r+1}\frac{\partial f^{\mu_2\cdots\mu_r\mu}}{\partial p_i^\mu}, \tag{66}$$

$$X_i^{\mu_1\cdots\mu_r} = (-1)^{r}\left(\frac{\partial f^{\mu_1\cdots\mu_r}}{\partial q^i} - \frac{\partial f_i^{\mu_1\cdots\mu_r\nu}}{\partial x^\nu}\right), \tag{67}$$

$$\widetilde{X}^{\mu_2\cdots\mu_r} = -\frac{\partial f^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu}, \tag{68}$$

that is, locally and modulo terms taking values in the kernel of ω, X is given by

$$\begin{aligned} X = &-\frac{1}{(r-1)!}\left(\frac{\partial f^{\mu_2\cdots\mu_r\mu}}{\partial x^\mu}\frac{\partial}{\partial p} - \frac{1}{r}\frac{\partial f^{\mu_2\cdots\mu_r\mu}}{\partial p}\frac{\partial}{\partial x^\mu} + \frac{1}{r}\frac{\partial f'^{\mu_2\cdots\mu_r\mu\nu}}{\partial x^\nu}\frac{\partial}{\partial x^\mu}\right)\wedge\frac{\partial}{\partial x^{\mu_2}}\wedge\cdots\wedge\frac{\partial}{\partial x^{\mu_r}} \\ &+\frac{1}{(r-1)!}\left(\frac{1}{n-r+1}\frac{\partial f^{\mu_2\cdots\mu_r\mu}}{\partial p_i^\mu}\frac{\partial}{\partial q^i} - \frac{1}{r}\frac{\partial f^{\mu_2\cdots\mu_r\mu}}{\partial q^i}\frac{\partial}{\partial p_i^\mu} + \frac{1}{r}\frac{\partial f_i^{\mu_2\cdots\mu_r\mu\nu}}{\partial x^\nu}\frac{\partial}{\partial p_i^\mu}\right)\wedge\frac{\partial}{\partial x^{\mu_2}}\wedge\cdots\wedge\frac{\partial}{\partial x^{\mu_r}}. \end{aligned} \tag{69}$$

If, in the canonical decomposition (57) and (60) *of f, the closed term $f_c=(-1)^r i_{F_c}\omega$ is absent, then $f'^{\mu_0\cdots\mu_r}=0$. If f is horizontal with respect to the projection onto M, then $f_i^{\mu_0\cdots\mu_r}=0$. In these cases, the above formulas simplify accordingly.*

Proof: There are several methods for proving this, with certain overlaps. Let us begin with the "trivial" case of closed forms f, for which we must have $X=0$. Assuming f to be of the form $f_c=(-1)^r i_{F_c}\omega$ and using Eqs. (61)–(64) to rewrite the expressions on the rhs of the above equations in terms of the components of F_c, we must show that

$$\frac{\partial(\widetilde{F}_c)^{\mu_1\cdots\mu_r}}{\partial p} + (-1)^r\frac{\partial(F_c)^{\mu_1\cdots\mu_r\nu}}{\partial x^\nu} = 0, \quad \frac{\partial(\widetilde{F}_c)^{\mu_2\cdots\mu_r\mu}}{\partial p_i^\mu} = 0,$$

$$\frac{\partial(\tilde{F}_c)^{\mu_1\cdots\mu_r}}{\partial q^i}-(-1)^r\frac{\partial(F_c)_i^{\mu_1\cdots\mu_r\nu}}{\partial x^\nu}=0,\quad \frac{\partial(\tilde{F}_c)^{\mu_2\cdots\mu_r\nu}}{\partial x^\nu}=0.$$

But this follows directly from the pertinent relations for locally Hamiltonian multivector fields derived in the proof of Theorem 1.3 which hold since F_c is locally Hamiltonian. To handle the remaining cases where f is of the form $f=f_0+(-1)^{r-1}i_F\theta$, it is easier to proceed by direct inspection of Eq. (11). Indeed, we may for a general Poisson form f apply the exterior derivative to Eq. (46) and compare the result with the expression for $i_X\omega$. In this way, Eqs. (68), (67), and (65) can be obtained directly by equating the coefficients of $\mathrm{d}^n x_{\mu_2\cdots\mu_r}$, of $\mathrm{d}q^i\wedge\mathrm{d}^n x_{\mu_1\cdots\mu_r}$ and of $\mathrm{d}p\wedge\mathrm{d}^n x_{\mu_1\cdots\mu_r}$, respectively. The only case which requires an additional argument is Eq. (66), since collecting terms proportional to $\mathrm{d}p_i^\mu\wedge\mathrm{d}^n x_{\mu_1\cdots\mu_r}$ leads to

$$\begin{aligned}&\frac{(-1)^{r-1}}{(r-1)!}X^{i,\mu_2\cdots\mu_r}\,\mathrm{d}p_i^\mu\wedge\mathrm{d}^n x_{\mu\mu_2\cdots\mu_r}\\&\quad=\frac{1}{r!}\frac{\partial f^{\mu_1\cdots\mu_r}}{\partial p_i^\mu}\mathrm{d}p_i^\mu\wedge\mathrm{d}^n x_{\mu_1\cdots\mu_r}-\frac{1}{(r-1)!}\frac{\partial f^{i,\mu_2\cdots\mu_r\nu}}{\partial x^\nu}\mathrm{d}p_i^\mu\wedge\mathrm{d}^n x_{\mu\mu_2\cdots\mu_r}\\&\quad-\frac{(-1)^r}{r!}\frac{\partial f^{i,\mu_1\cdots\mu_r}}{\partial x^\mu}\mathrm{d}p_i^\mu\wedge\mathrm{d}^n x_{\mu_1\cdots\mu_r}.\end{aligned}$$

But when f is of the form $f=f_0+(-1)^{r-1}i_F\theta$, Eq. (63) implies that the last two terms on the rhs of the equation above vanish. Moreover, since F is Hamiltonian, we know from Theorem 2.4 that the $F^{\mu_1\cdots\mu_r}$ depend on the p_i^μ only if $\mu\in\{\mu_1,\ldots,\mu_r\}$, and hence according to Eq. (61), the same is true for the $f^{\mu_1\cdots\mu_r}$. This reduces the first term on the rhs of the above equation to an expression which, when compared with the lhs, leads to the conclusion that for any choice of mutually different indices μ and $\mu_2,\ldots,\mu_r$, we have

$$X^{i,\mu_2\cdots\mu_r}=\frac{\partial f^{\mu_2\cdots\mu_r\mu}}{\partial p_i^\mu}\quad\text{if }\mu\notin\{\mu_2,\ldots,\mu_r\}\quad(\text{no sum over }\mu).$$

Summing over μ gives Eq. (66). □

IV. POISSON BRACKETS

In the characterization of locally Hamiltonian multivector fields and of Poisson forms derived in the preceding two sections, the decomposition into homogeneous terms with respect to scaling degree plays a central role. It is therefore natural to ask how this decomposition complies with the Schouten bracket of Hamiltonian multivector fields and with the Poisson bracket of Poisson forms. To this end, let us first recall the definition of the Poisson bracket between Poisson forms given in Ref. 1 for $(n-1)$-forms and in Ref. 2 for forms of arbitrary degree.

Definition 4.1: Let f and g be Poisson forms of tensor degree $n-r$ and $n-s$ on P, respectively. Their Poisson bracket is the Poisson form of tensor degree $n-r-s+1$ on P defined by

$$\{f,g\}=(-1)^{r(s-1)}i_Yi_X\omega+\mathrm{d}((-1)^{(r-1)(s-1)}i_Yf-i_Xg-(-1)^{(r-1)s}i_Yi_X\theta),\tag{70}$$

where X and Y are Hamiltonian multivector fields associated with f and g, respectively.

We find the following properties of the two mentioned bracket operations with respect to scaling degree.

Proposition 4.2: Let X and Y be homogeneous multivector fields on P of scaling degree k and l, respectively. Then their Schouten bracket $[X,Y]$ is of scaling degree $k+l$,

$$L_\Sigma X=kX,\quad L_\Sigma Y=lY\quad\Rightarrow\quad L_\Sigma[X,Y]=(k+l)[X,Y].\tag{71}$$

Proof: The proposition is a consequence of the graded Jacobi identity for multivector fields,[8]

which can be rewritten as the statement that the Schouten bracket with a given multivector field Z of odd/even tensor degree acts as an even/odd superderivation,

$$[Z,[X,Y]] = [[Z,X],Y] + (-1)^{(t-1)(r-1)}[X,[Z,Y]].$$

In particular, since Σ has tensor degree 1,

$$[\Sigma,[X,Y]] = [[\Sigma,X],Y] + [X,[\Sigma,Y]],$$

from which the proposition follows immediately. □

Corollary 4.3: Let X and Y be locally Hamiltonian multivector fields on P of scaling degree -1. *Then their Schouten bracket* $[X,Y]$ *takes values in the kernel of* ω.

Proof: From the preceding proposition, $[X,Y]$ is a locally Hamiltonian multivector field of scaling degree -2. and hence, by Theorem 1.3, must take values in the kernel of ω. □

For the Poisson bracket of Poisson forms, we have the following property.

Proposition 4.4: Let f and g be homogeneous Poisson forms on P of scaling degree k and l, respectively. Then their Poisson bracket $\{f,g\}$ *is of scaling degree* $k+l-1$*:*

$$L_\Sigma f = kf, \quad L_\Sigma g = lg \quad \Rightarrow \quad L_\Sigma\{f,g\} = (k+l-1)\{f,g\}. \tag{72}$$

Proof: As explained in the last paragraph of Sec. I [see, in particular, Eq. (23)], we can find homogeneous Hamiltonian multivector fields X of scaling degree $k-1$ and Y of scaling degree $l-1$ such that $i_X\omega = \mathrm{d}f$ and $i_Y\omega = \mathrm{d}g$. We shall consider each of the terms in the definition of the Poisson bracket separately. We find

$$L_\Sigma(i_Y i_X \omega) = i_Y L_\Sigma i_X \omega + i_{[\Sigma,Y]} i_X \omega = i_Y i_X L_\Sigma \omega + i_Y i_{[\Sigma,X]}\omega + i_{[\Sigma,Y]} i_X \omega = (k+l-1) i_Y i_X \omega.$$

The same calculation works with ω replaced by θ, so that, since L_Σ commutes with d,

$$L_\Sigma(\mathrm{d}(i_Y i_X \theta)) = (k+l-1)\mathrm{d}(i_Y i_X \theta).$$

Moreover,

$$L_\Sigma(\mathrm{d}(i_Y f)) = \mathrm{d}(L_\Sigma i_Y f) = \mathrm{d}(i_Y L_\Sigma f + i_{[\Sigma,Y]} f) = (k+l-1)\mathrm{d}(i_Y f),$$

and similarly $L_\Sigma(\mathrm{d}(i_X g)) = (k+l-1)\mathrm{d}(i_X g)$. Putting the pieces together, the proposition follows. □

Having shown in what sense both the Schouten bracket and the Poisson bracket respect scaling degree, let us use the canonical decomposition of Poisson forms to express their Poisson bracket in terms of known operations on the simpler objects from which they can be constructed. To start with, we settle the case of homogeneous Poisson forms of positive scaling degree.

Proposition 4.5: Let X_{k-1} *be a homogeneous locally Hamiltonian r-multivector field on P of scaling degree* $k-1$, *with* $1 \leqslant k \leqslant r$, *and* Y_{l-1} *be a homogeneous locally Hamiltonian s-multivector field on P of scaling degree* $l-1$, *with* $1 \leqslant l \leqslant s$. *Set*

$$f_k = \frac{(-1)^{r-1}}{k} i_{X_{k-1}}\theta, \quad g_l = \frac{(-1)^{s-1}}{l} i_{Y_{l-1}}\theta.$$

Then

$$\{f_k, g_l\} = \frac{(-1)^{r+s}}{k+l-1} i_{[Y_{l-1},X_{k-1}]}\theta - (-1)^{(r-1)s}\frac{(k-1)(l-1)(k+l)}{kl(k+l-1)}\mathrm{d}(i_{X_{k-1}} i_{Y_{l-1}}\theta).$$

Proof: From the defining equation (70) for the Poisson bracket, we find

$$\{f_k,g_l\} = (-1)^{r(s-1)} i_{Y_{l-1}} i_{X_{k-1}} \omega + \mathrm{d}\left(\frac{(-1)^{(r-1)s}}{k} i_{Y_{l-1}} i_{X_{k-1}} \theta - \frac{(-1)^{(s-1)}}{l} i_{X_{k-1}} i_{Y_{l-1}} \theta - (-1)^{(r-1)s} i_{Y_{l-1}} i_{X_{k-1}} \theta \right)$$

$$= (-1)^{r(s-1)} i_{Y_{l-1}} i_{X_{k-1}} \omega + (-1)^{(r-1)s} \left(\frac{1}{k} + \frac{1}{l} - 1 \right) \mathrm{d}(i_{Y_{l-1}} i_{X_{k-1}} \theta).$$

On the other hand, one verifies that $\mathrm{d} i_{X_{k-1}} \theta = k(-1)^{r-1} i_{X_{k-1}} \omega$ and hence

$$i_{[Y_{l-1},X_{k-1}]}\theta = (-1)^{(s-1)r} L_{Y_{l-1}} i_{X_{k-1}} \theta - i_{X_{k-1}} L_{Y_{l-1}} \theta$$

$$= (-1)^{(s-1)r} \mathrm{d} i_{Y_{l-1}} i_{X_{k-1}} \theta + (-1)^{s(r-1)} (k+l-1) i_{Y_{l-1}} i_{X_{k-1}} \omega.$$

Thus,

$$\{f_k,g_l\} = \frac{(-1)^{r+s}}{k+l-1} i_{[Y_{l-1},X_{k-1}]}\theta - \frac{(-1)^{(r-1)s}}{k+l-1} \mathrm{d}(i_{Y_{l-1}} i_{X_{k-1}} \theta) + (-1)^{(r-1)s} \left(\frac{1}{k} + \frac{1}{l} - 1 \right) \mathrm{d}(i_{Y_{l-1}} i_{X_{k-1}} \theta), \tag{73}$$

which implies the asserted relation. □

As a special case, consider homogeneous Poisson forms of scaling degree 1, which arise by contracting θ with a Hamiltonian multivector field of scaling degree 0, that is, with an exact Hamiltonian multivector field (see the first statement in Proposition 2.5). These Poisson forms have been studied in Ref. 2 under the name "universal multimomentum map."

Corollary 4.6: The space of homogeneous Poisson forms on P of scaling degree 1 closes under the Poisson bracket.

Obviously, it also follows from the proposition that no such statement holds for homogeneous Poisson forms of scaling degree >1, since the second term in the expression in Proposition 4.5 vanishes only for $k=1$ or $l=1$.

Turning to homogeneous Poisson forms on P of scaling degree 0, which come from forms on E by pull-back, we have the following.

Proposition 4.7: The space of homogeneous Poisson forms on P of scaling degree 0 is Abelian under the Poisson bracket,

$$\{f_0,g_0\} = 0. \tag{74}$$

Proof: Without loss of generality, we may assume the Hamiltonian multivector fields X_- and Y_- associated with f_0 and with g_0, respectively, to be homogeneous of scaling degree -1. Therefore, using the fact that if a multivector field X is homogeneous of scaling degree k and a differential form α is homogeneous of scaling degree l, then the differential form $i_X\alpha$ is homogeneous of scaling degree $k+l$,

$$L_\Sigma X = kX, \quad L_\Sigma \alpha = l\alpha \quad \Rightarrow \quad L_\Sigma i_X \alpha = (k+l) i_X \alpha,$$

which follows immediately from the formula $L_\Sigma i_X \alpha = i_X L_\Sigma \alpha + i_{[\Sigma,X]}\alpha$, we see that all four terms in the definition (70) of the Poisson bracket between f_0 and g_0 are differential forms of scaling degree -1 and hence must vanish. □

For the mixed case of the Poisson bracket between a homogeneous Poisson form of strictly positive scaling degree with one of scaling degree zero, we find the following result.

Proposition 4.8: Let X_{k-1} be a homogeneous locally Hamiltonian r-multivector field on P of scaling degree $k-1$, with $1 \leqslant k \leqslant r$, and let g_0 be a homogeneous Poisson $(n-s)$-form on P of scaling degree zero, with associated Hamiltonian s-multivector field Y_-. Set

$$f_k = \frac{(-1)^{r-1}}{k} i_{X_{k-1}} \theta. \tag{75}$$

Then

$$\{f_k, g_0\} = -L_{X_{k-1}} g_0. \tag{76}$$

Proof: By Proposition 2.5, $i_{Y\_}\theta$ vanishes. Hence only two of the four terms in the defining equation (70) for the Poisson bracket survive,

$$\{f_k, g_0\} = (-1)^{r(s-1)} i_{Y\_} i_{X_{k-1}} \omega - \mathrm{d} i_{X_{k-1}} g_0 = -(\mathrm{d} i_{X_{k-1}} g_0 - (-1)^r i_{X_{k-1}} \mathrm{d} g_0) = -L_{X_{k-1}} g_0.$$

□

Finally, let us consider closed Poisson forms, whose associated Hamiltonian multivector fields vanish. Still, the Poisson bracket of a closed Poisson form with an arbitrary Poisson form does not vanish, but it is once again a closed Poisson form.

Proposition 4.9: Let f be a Poisson $(n-r)$-form on P, with associated Hamiltonian r-multivector field X, and let g be a closed Poisson $(n-s)$-form on P. Set

$$g = (-1)^s i_{G_c} \omega. \tag{77}$$

Then

$$\{f, g\} = (-1)^{r+s-1} i_{[G_c, X]} \omega. \tag{78}$$

Proof: As the Hamiltonian multivector field associated with g vanishes, only one of the four terms in the defining equation (70) for the Poisson bracket survives,

$$\{f, g\} = -\mathrm{d}(i_X g) = (-1)^{s-1} \mathrm{d}(i_X i_{G_c} \omega) = (-1)^{rs-1} i_{[X, G_c]} \omega = (-1)^{r+s-1} i_{[G_c, X]} \omega.$$

(For the penultimate equation, see, e.g., Proposition 3.3 of Ref. 2.) □

In view of the canonical decomposition for Poisson forms stated in Theorem 3.8, the above propositions exhaust the possible combinations for the computation of Poisson brackets.

V. CONCLUSIONS AND OUTLOOK

In this paper, we have achieved three goals. First, we have determined the general structure of locally Hamiltonian multivector fields on the extended multiphase space of classical first order field theories. According to Theorem 2.4, the basic structure that arises from explicit calculations in adapted local coordinates is the decomposition of any such multivector field X, of tensor degree r $(0<r<n)$, into a sum of terms of homogeneous scaling degree plus a remainder ξ which is a multivector field taking values in the kernel of ω,

$$X = X_{-1} + X_0 + \cdots + X_{r-1} + \xi \quad \text{with } L_\Sigma X_k = k X_k. \tag{79}$$

Moreover, according to Proposition 2.5, all homogeneous locally Hamiltonian multivector fields of non-negative scaling degree are in fact globally Hamiltonian, and they are exact Hamiltonian if and only if they have zero scaling degree. At the level of local coefficient functions, this decomposition arises because the coefficient functions must be antisymmetric polynomials in the multimomentum variables; see Eqs. (30) and (31).

Second, we have extended the scaling degree analysis to the study of Hamiltonian forms by means of the formula

$$L_\Sigma i_X \omega = i_{X + [\Sigma, X]} \omega.$$

As shown in Theorem 3.8, this leads to a canonical decomposition of any Hamiltonian $(n-r)$-form f $(0<r<n)$ into a sum of terms of homogeneous scaling degree plus a remainder f_c which is a closed form,

$$f = f_0 + f_1 + \cdots + f_r + f_c \quad \text{with } L_\Sigma f_s = s f_s. \tag{80}$$

Moreover, if X is a Hamiltonian multivector field associated with f, then

$$f_s = \frac{(-1)^{r-1}}{s} i_{X_{s-1}} \theta \quad \text{for } s > 0, \tag{81}$$

where the X_{s-1} are the homogeneous components of X of non-negative scaling degree as described before, whereas f_0 arises by pull-back from a form on the total space of the configuration bundle of the theory. Locally, this form can be decomposed into the sum of a horizontal form and a closed form (we prove this explicitly only for Poisson forms), but this decomposition has no global, coordinate invariant meaning. The canonical decomposition of Poisson forms is also useful for deriving local formulas for X in terms of f; these are given in Theorem 3.9. They clearly show that the situation in multisymplectic geometry resembles that encountered in symplectic geometry but exhibits a significantly richer structure. In particular, the notion of conjugate variables requires a conceptual extension.

Third, we have used the canonical decomposition of Poisson forms to derive explicit formulas for the Poisson bracket between Poisson forms. The resulting Lie algebra shows an interesting and nontrivial structure. It has a trivial part, namely the space of closed Poisson forms, which constitutes an ideal that one might wish to divide out; this ideal is Abelian but not central. It commutes with the most interesting and useful part, namely the subalgebra of homogeneous Poisson forms of scaling degree 1, which by means of Eq. (81), specialized to the case $s=1$, correspond to the exact Hamiltonian multivector fields, and in such a way that the Poisson bracket on this subalgebra corresponds to the Schouten bracket for exact Hamiltonian multivector fields (up to signs). The nontrivial mixing occurs through the spaces of homogeneous Poisson forms of scaling degree 0 and of scaling degree >1, they close under the operation of taking the Poisson bracket with a homogeneous Poisson forms of scaling degree 1 but not under the operation of taking mutual Poisson brackets, since these contain contributions lying in the ideal of closed Poisson forms.

An important aspect of our results is that they confirm, once again, the apparently unavoidable appearance of strong constraints on the dependence of Hamiltonian multivector fields and Hamiltonian forms on the multimomentum variables and the energy variable in extended multiphase space, expressed through the "antisymmetric polynomial" structure of their coefficient functions. This strongly suggests that there should be some product structure complementing the Poisson bracket operation. So far, such a structure seems to exist only for a very restricted class of Poisson forms, namely the horizontal forms studied by Kanatchikov.[11] Also, one might wonder whether the structural properties derived here still hold in the multisymplectic formulation of higher order field theories.[6]

Finally, a central question that remains is how the various proposals of Poisson brackets in the multisymplectic formalism that can be found in the literature, including the one proposed in Refs. 1 and 2, relates to the Peierls-DeWitt bracket that comes from the functional approach based on the concept of covariant phase space. Briefly, covariant phase space is defined as the space $\mathcal{S}$ of solutions of the equations of motion and, formally viewed as an infinite-dimensional manifold, carries a naturally defined symplectic form Ω.[12–14] A systematic general investigation of the Peierls-DeWitt bracket in the multisymplectic framework, including a proof of the fact that it is precisely the canonical Poisson bracket for functionals on $\mathcal{S}$ derived from the symplectic form Ω on $\mathcal{S}$, has been carried out recently.[15,16] In order to establish the desired relation, we must restrict this bracket to a certain class of functionals, namely functionals F obtained by using fields to pull Hamiltonian forms or Poisson forms f on extended multiphase space back to space-time and then integrate over submanifolds Σ of the corresponding dimension. Explicitly, using the notation of Ref. 16, we have

$$\mathsf{F}[\phi] = \int_{\Sigma} (\mathbb{F}\mathcal{L} \circ (\varphi, \partial\varphi))^* f \tag{82}$$

in the Lagrangian framework and

$$\mathsf{F}[\phi] = \int_{\Sigma} (\mathcal{H} \circ (\varphi, \pi))^* f \tag{83}$$

in the Hamiltonian framework. Now using the classification of Hamiltonian vector fields and Hamiltonian $(n-1)$-forms obtained in this paper, it has been shown recently that the Peierls-DeWitt bracket $\{\mathsf{F},\mathsf{G}\}$ between two functionals F and G derived from Hamiltonian $(n-1)$-forms f and g, respectively, is the functional derived from the Hamiltonian $(n-1)$-form $\{f,g\}$;[17] details will be published elsewhere. The question of how to extend this result to Poisson forms of other degree is currently under investigation.

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APPENDIX

Proposition A.1: Let V be a vector bundle over a manifold M with projection π and let Σ be the scaling or Euler vector field on V. A differential form α on the total space V will be the pull-back of a differential form α_0 on the base space M to V via π if and only if it is scale invariant,

$$\alpha = \pi^* \alpha_0 \quad \Leftrightarrow \quad L_\Sigma \alpha = 0.$$

Proof: Assume first that the form α on V is the pull-back of a form α_0 on M; then $\alpha = \pi^* \alpha_0$ and hence $\mathrm{d}\alpha = \pi^* \mathrm{d}\alpha_0$. Therefore, α and $\mathrm{d}\alpha$ are both horizontal. This means that for any vertical vector field X on V, including Σ, we have $i_X \alpha = 0$ as well as $i_X \mathrm{d}\alpha = 0$, so $L_X \alpha = 0$.

Conversely, assume that the form α on V, of degree r, say, satisfies $L_\Sigma \alpha = 0$, so α is invariant under the flow F of Σ,[9]

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} F_\lambda^* \alpha = 0.$$

This means that given $v \in V$ and $w_1, \ldots, w_r \in T_v V$, the expression

$$(F_\lambda^* \alpha)_v (w_1, \ldots, w_r) = \alpha_{F_\lambda(v)} (T_v F_\lambda \cdot w_1, \ldots, T_v F_\lambda \cdot w_r)$$

does not depend on λ, so its value $\alpha_v(w_1, \ldots, w_r)$ at $\lambda = 0$ is equal to its value $\alpha_{v_0}((w_1)_0, \ldots, (w_r)_0)$ obtained in the limit $\lambda \to -\infty$, where v_0 denotes the zero vector in the fiber of v. But this means that α is equal to $\pi^* \alpha_0$ where α_0 is defined with the help of the zero section $i_0 : M \to V$ of V as $\alpha_0 = i_0^* \alpha$. □

The following lemma is used in the proof of Theorem 2.4.

Lemma A.2: Let f be a polynomial of degree s in a set of variables x^μ. Let f_r, $0 \leq r \leq s$, be the homogeneous component of degree r of f. Then

$$f = \sum_{r=1}^{s} \frac{1}{r} x^\mu \frac{\partial f_r}{\partial x^\mu} + f_0.$$

Proof: For the operator $x^\mu (\partial / \partial x^\mu)$, the homogeneous polynomials f_r are eigenvectors with eigenvalue r. Writing this as $f_r = (1/r) x^\mu (\partial f_r / \partial x^\mu)$ for $0 < r \leq s$, we obtain

$$f = \sum_{r=0}^{s} f_r = f_0 + \sum_{r=1}^{s} \frac{1}{r} x^\mu \frac{\partial f_r}{\partial x^\mu}.$$

□

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Ideality criterion for unilateral constraints in time-dependent impulsive mechanics

Stefano Pasquero[a)]
Dipartimento di Matematica dell'Università di Parma, Parco Area delle scienze 53/A, 43100 Parma (Italia)

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We construct a new geometric framework based on the concepts of left and right jet-bundles of a classical space-time $\mathcal{V}$ in order to analyze the impulsive behavior of a unilateral constraint $\mathcal{S}$. The setup allows deep insights into how one can choose an ideality criterion for the constraint $\mathcal{S}$ when the hypothesis of conservation of kinetic energy is assumed. We show that the conservation of kinetic energy alone univocally determines the impulsive reaction when the codimension of $\mathcal{S}$ is 1, and that it leaves the impulsive reaction partially undetermined when the codimension of $\mathcal{S}$ is greater than 1. If the codimension of $\mathcal{S}$ is greater than 1, we prove that an additional minimality requirement determines a physically meaningful constitutive characterization of $\mathcal{S}$. We show that both the Newton-like and the Poisson-like approaches to the description of the reactive impulse are equivalent, in the sense that both give the same results about the ideality criterion. Moreover, we prove that the same results hold using the classical approach based on reflection operators, possible only in case of codimension 1. We present also several physically meaningful examples. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2121247]

I. INTRODUCTION

The geometric approach to Impulsive Mechanics played a role of minor interest in the study of Classical Mechanics until the last decade of the last century. There were essentially two main reasons for this: first, the difficulty, due to the intrinsic nonsmoothness of its problems, of framing Impulsive Mechanics in a differential geometric context without involving the technicalities of Functional Analysis or Differential Geometry of manifolds with boundary. This difficulty effectively stopped, with very few exceptions, the evolution of the geometric studies of Impulsive Mechanics at the level of the first half of the last century, while Analytical Mechanics fruitfully and continuously applied the techniques of smooth Differential Geometry along the years (see, for example, among the many resources, Refs. 1–5, and references therein). The second reason for the minor role of the geometric approach is the deep and fruitful insights in Impulsive Mechanics obtained by the standard local approach (see, for example, once again among the many resources, Refs. 6–11, and the references therein).

However, in recent years, a clever use of classical differential geometric techniques (see Refs. 12–16) and, later, the introduction of new differential geometric setups particularly suited for Impulsive Mechanics (see Refs. 17–19), have shed new light on the potential effectiveness of a formal geometric approach. Such an approach could allow a deeper understanding and produce significant results about the concept of free impulse,[17] the classification of constraints,[14,18] and the energy balance[15,19] in both time-independent and time-dependent cases.

This paper goes precisely in this direction: we embody in the geometric setup of the (left and right) jet-bundles associated to the classical space-time bundle $\mathcal{V}$ of a time-dependent mechanical system the presence of a unilateral constraint $\mathcal{S}$, viewed as a subbundle of $\mathcal{V}$. The fibered immer-

a)Electronic mail: stefano.pasquero@unipr.it

sion $i:\mathcal{S}\to\mathcal{V}$ allows the construction, using the concept of pull-back bundle, of a new environment suitable for a strictly geometric study of the concepts of impulsive reaction and of constitutive characterization of the constraint. The new environment inherits several structures and properties of the jet-extensions of $\mathcal{V}$. Among them are the affine or vector structures of the bundles, the vertical metric, the nonrigid frames of reference viewed as special vector fields, and the corresponding concepts of relative velocity and relative kinetic energy associated to a frame. Moreover, the immersion $i:\mathcal{S}\to\mathcal{V}$ produces natural splits of the velocity spaces of the system. This enriches the structure with projection operators that turn out to be related to the classical Gauss minimality requirement (see, for example, Refs. 20 and 21).

Due to the explicit time dependence of the context, the condition of conservation of kinetic energy, naturally required in order to determine ideality criterion for $\mathcal{S}$, selects a special class $\mathcal{H}$ of frames of reference. This class coincides with the class of frames of reference tangent to $\mathcal{S}$, that, together with an obvious geometric meaning, also has a clear physical meaning: it is the set of all possible frames "of rest" of the constraint or, what is the same, the set of all possible "internal motions" of $\mathcal{S}$. Heuristically speaking, the requirement of conservation of kinetic energy in the impact process for all the frames in $\mathcal{H}$ parallels the well-known situation that the reactive behavior of a bilateral smooth surface constraining a point mass is not affected by the internal motions of the surface itself.

The main result of the paper is essentially based on this idea: we prove that the requirement of conservation of kinetic energy for all the frames in $\mathcal{H}$ drastically reduces the possible ideal constitutive characterizations of $\mathcal{S}$. In particular, when $\mathrm{codim}(\mathcal{S})=1$ (as submanifold of $\mathcal{V}$) the condition selects a unique possible constitutive characterization. This case covers almost all the physically meaningful situations, such as point masses or balls bouncing on walls, rods impacting with the floor and so on.

Some specific, but somewhat artificial, problems, such as the simultaneous impact of a ball with two different walls, or a point mass moving in three-dimensional space and impacting with a thread, give rise to constraints for which $\mathrm{codim}(\mathcal{S})>1$. In this case the condition on kinetic energy alone does not determine a unique constitutive characterization but splits the reaction into two well-defined parts. An additional, but natural, requirement of minimality of one of these parts of the reaction once again univocally determines a physically meaningful constitutive characterization.

In the paper, the main analysis of the impulsive problem is based on a Newton-type approach, i.e., considering the impulsive reaction as a single object. Nevertheless, it is also shown that the same results can be obtained following a Poisson-type approach, based on the separation of the impulsive reaction into two parts with different physical meaning. Moreover, when $\mathrm{codim}(\mathcal{S})=1$, the geometric formulation of the problem allows yet another approach based on reflection operators. We show that even this third possibility gives the same results.

Before concluding the introduction, a brief remark should be made about the geometric approach to Impulsive Mechanics. In Analytical Mechanics the correspondence between the physical problem in study (such as point particles moving on a surface, or balls moving respecting rolling conditions) and the geometric objects involved in its description (such as manifolds, bundles, and smooth maps) is clearly stated and formalized. In Impulsive Mechanics we are great at the beginning of our understanding of this correspondence, even for very simple mechanical problems, such as nonconvex rigid bodies impacting with walls, balls impacting with threads, or in case of articulated mechanical systems.

This problem of correspondence will not be analyzed in detail in this paper. However in Sec. V some examples (one is the ball impacting with the thread) will be briefly presented in order to illustrate this problem.

The paper is divided into four main sections: Section II contains the basic ideas and results about the geometric approach to time-dependent Mechanics, both in the Lagrangian and in the Impulsive cases. This is a well-known material that we recall in order to fix notation and to keep the paper self-contained.

Section III presents the construction of the geometric setup for unilateral constraints in Im-

pulsive Mechanics, in both the coordinate-free and the coordinate-dependent cases. It contains the kinematical aspects of the problem, such as the splits of the velocity spaces, the corresponding projectors and their relations with assigned frames of reference.

Section IV introduces the concept of constitutive characterization in the Newton-type approach and presents the results about the choice of an ideality criterion, in both the $\mathrm{codim}(\mathcal{S})=1$ and the $\mathrm{codim}(\mathcal{S})>1$ cases. Moreover, it presents the discussion about the Poisson-type and the "reflection operators" approaches.

Section V is devoted to examples. Four physically meaningful examples are presented, all of them with some peculiarities: the first is a disk moving in the plane and impacting with a straight line; the second is a rod moving in the plane and impacting with a straight line; the third is a ball moving in the space and impacting with a thread; the last is an articulated system with three different possible kinds of impact.

II. PRELIMINARIES

In the following we recall, also in order to fix notation, the structures and the principal properties of the geometric environments of Lagrangian and Impulsive Mechanics. The following contains standard material that is presented, very briefly, to keep the paper self-contained. More ample discussions can easily be found in literature (see, for example, Refs. 22–24, 5, and 25, and references therein for additional commentary on Lagrangian Mechanics and Refs. 17 and 18 for additional background on Impulsive Mechanics).

A. The classical Lagrangian environment

The geometric setup generally used to study the time-dependent Lagrangian Mechanics of a system with a finite number n of degrees of freedom is constructed starting from the *configuration space-time* bundle, i.e., an $(n+1)$-dimensional fiber bundle $\pi:\mathcal{V}\to\mathbb{E}_1$ where $\mathbb{E}_1$ denotes the one-dimensional Euclidean space, and the first and second jet-extensions of this bundle.[4,21,24,5] All the fibers of $\pi:\mathcal{V}\to\mathbb{E}_1$ are diffeomorphic to an n-dimensional manifold $\mathcal{M}$, usually thought of as the *configuration space* of the system. The configuration space-time takes into account, intrinsically, the positional bilateral constraints acting on the mechanical system. Its first jet-extension $\pi:J_1(\mathcal{V})\to\mathcal{V}$ represents the *absolute velocity bundle* of the system, which takes into account the restrictions on the velocities of the mechanical system due to the positional bilateral constraints. Since Impulsive Mechanics mainly deals with velocities, it is not necessary, in this paper, to introduce higher jet-extensions.

The following properties and notation (see Refs. 21, 24, 22, and 25) will be extensively used throughout.

i) The composition $t\circ\pi:\mathcal{V}\to\mathbb{R}$ of the projection $\pi:\mathcal{V}\to\mathbb{E}_1$ and the Cartesian coordinate t defined on $\mathbb{E}_1$ is the absolute time function, expressing the Absolute Time Axiom of Classical Mechanics in this context. With a mild abuse of language, it will be briefly denoted by $t:\mathcal{V}\to\mathbb{R}$. It selects *admissible* coordinate systems $(t,x^1,\ldots,x^n)$ having t as first coordinate. The rules of variation of such a system

$$\begin{cases}\bar{t}=t,\\ \bar{x}^i=\bar{x}^i(t,x^k), \quad i=1,\ldots,n,\end{cases}$$

distinguish $\mathcal{V}$ from $\mathbb{R}\times\mathcal{M}$ (see Ref. 25). Henceforth, the restriction to admissible coordinates will be always assumed.

ii) The velocity bundle $\pi:J_1(\mathcal{V})\to\mathcal{V}$ is an affine bundle modeled on the *vertical* vector bundle $\pi:V(\mathcal{V})\to\mathcal{V}$ of the tangent vectors $X\in T(\mathcal{V})$ satisfying the condition $t_*(X)=0$. Admissible coordinates (t,x^i) in $\mathcal{V}$ determine admissible jet-coordinates $(t,x^i,\dot{x}^i)$, in $J_1(\mathcal{V})$, whose use will be always assumed. Both $J_1(\mathcal{V})$ and $V(\mathcal{V})$ can be viewed as subbundles of the tangent bundle $T(\mathcal{V})$ as follows:

$$J_1(\mathcal{V}) = \{\mathbf{X} \in T(\mathcal{V}) | \langle \mathrm{d}t, \mathbf{X} \rangle = 1\},$$
$$V(\mathcal{V}) = \{\mathbf{X} \in T(\mathcal{V}) | \langle \mathrm{d}t, \mathbf{X} \rangle = 0\}, \tag{1}$$

where $\langle , \rangle$ denotes the usual pairing between one-forms and tangent vectors. The elements $\mathbf{x} \in J_1(\mathcal{V})$ then admit a representation of the form $\mathbf{x} = \partial/\partial t + \dot{x}^i(\partial/\partial x^i)$, while the elements $\mathbf{U} \in V(\mathcal{V})$ have the form $\mathbf{U} = U^i \partial/\partial x^i$.

iii) The Absolute Space Axiom is introduced in this context by assigning a Riemannian metric on each fiber of $t: \mathcal{V} \to \mathbb{R}$, i.e., we introduce a differentiable positive definite scalar product $\Phi: V(\mathcal{V}) \times_{\mathcal{V}} V(\mathcal{V}) \to \mathbb{R}$, where $\times_{\mathcal{V}}$ denotes the usual fiber product of bundles on $\mathcal{V}$. The scalar product Φ will be called the *vertical* scalar product of $\mathcal{V}$. As usual, we denote by g_{ij} the functions

$$g_{ij}(p) = \Phi\left(\left(\frac{\partial}{\partial x^i}\right)_p, \left(\frac{\partial}{\partial x^j}\right)_p\right), \quad p \in \mathcal{V}, \tag{2}$$

and we recall that the g_{ij} take intrinsically into account the mass properties of the system (see Ref. 24).

iv) Each global section $\mathbf{H}: \mathcal{V} \to J_1(\mathcal{V})$ can be represented as a vector field $\mathbf{H} = \partial/\partial t + H^i(t, x^j)\partial/\partial x^i$ and, due to the affine structure (1) of the velocity bundle $J_1(\mathcal{V})$, it determines a diffeomorphism $\Delta_{\mathbf{H}}$ defined by

$$\Delta_{\mathbf{H}}: J_1(\mathcal{V}) \to V(\mathcal{V}) \text{ such that } \Delta_{\mathbf{H}}(\mathbf{x}) = \mathbf{x} - \mathbf{H}(\pi(\mathbf{x})). \tag{3}$$

A global section $\mathbf{H}: \mathcal{V} \to J_1(\mathcal{V})$ represents a frame of reference for the system (without any assumption of rigidity. See Refs. 25 and 5). Given a frame $\mathbf{H}$, the vertical vector ${}^{\mathbf{H}}\mathbf{v}(\mathbf{x}) = \Delta_{\mathbf{H}}(\mathbf{x})$ is the *relative velocity* of $\mathbf{x} \in J_1(\mathcal{V})$ with respect to $\mathbf{H}$. Moreover, the function

$${}^{\mathbf{H}}\mathcal{K}: J_1(\mathcal{V}) \to \mathbb{R} \text{ such that } {}^{\mathbf{H}}\mathcal{K}(\mathbf{x}) = \tfrac{1}{2}\Phi({}^{\mathbf{H}}\mathbf{v}(\mathbf{x}), {}^{\mathbf{H}}\mathbf{v}(\mathbf{x})) \tag{4}$$

is the *kinetic energy* of the system with respect to $\mathbf{H}$.

Additional positional constraints acting on the system can be introduced in this context by assigning a globally time-fibered subbundle $i: \mathcal{S} \to \mathcal{V}$, where the manifold $\mathcal{S}$ has dimension $(r+1)$, $r < n$. Of course, the bundle $t: \mathcal{S} \to \mathbb{R}$ is the space-time bundle of the system that takes into account the constraint $\mathcal{S}$ acting bilaterally on the system. As with the bundle $t: \mathcal{V} \to \mathbb{R}$, the bundle $t: \mathcal{S} \to \mathbb{R}$ admits its own admissible coordinates $(t, q^1, \ldots, q^r)$. Moreover, it determines its own first jet-extension $\pi: J_1(\mathcal{S}) \to \mathcal{S}$, that is described by admissible jet-coordinates $(t, q^\alpha, \dot{q}^\alpha)$, $\alpha = 1, \ldots, r$ and that is an affine bundle modeled on the vertical bundle $\pi: V(\mathcal{S}) \to \mathcal{S}$. The elements $\mathbf{q}$ of $J_1(\mathcal{S})$ admit the vector representation $\mathbf{q} = \partial/\partial t + \dot{q}^\alpha \partial/\partial q^\alpha$, while the elements $\mathbf{V} \in V(\mathcal{V})$ have the form $\mathbf{V} = V^\alpha \partial/\partial q^\alpha$.

The restrictions of the tangent map $i_*: T(\mathcal{S}) \to T(\mathcal{V})$ determine the fibered immersions $i_*: J_1(\mathcal{S}) \to J_1(\mathcal{V})$ and $i_*: V(\mathcal{S}) \to V(\mathcal{V})$. As a consequence, the vertical scalar product Φ of $\mathcal{V}$ can be pulled back to $V(\mathcal{S})$, defining the vertical scalar product φ of $\mathcal{S}$.

The entire geometric context can be summarized with the following diagram:

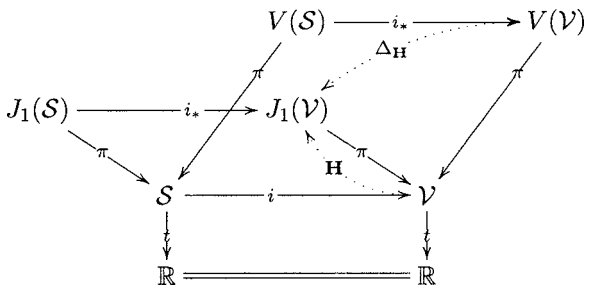

(5)

B. The bilateral impulsive environment

The explicit construction of the velocity bundle $J_1(\mathcal{V})$ made by considering the equivalence classes of sections $\gamma:\mathbb{R}\to\mathcal{V}$ having a first-order contact in a point $p\in\mathcal{V}$ (see, for example, Ref. 22) can be repeated using the left and the right derivatives of γ in p separately.[17] This procedure gives rise to the bundles $\pi:L_1(\mathcal{V})\to\mathcal{V}$ of the left velocities of the system and $\pi:R_1(\mathcal{V})\to\mathcal{V}$ of the right velocities which are each canonically isomorphic to $J_1(\mathcal{V})$ in the geometric sense, but whose physical interpretation is slightly different from that of $J_1(\mathcal{V})$. The following properties are straightforward consequences of the definitions of $L_1(\mathcal{V})$ and $R_1(\mathcal{V})$.

i) $\pi:L_1(\mathcal{V})\to\mathcal{V}$ and $\pi:R_1(\mathcal{V})\to\mathcal{V}$ are affine bundles modeled on the vertical bundle $V(\mathcal{V})$. The canonical isomorphisms with $J_1(\mathcal{V})$ will be denoted by Id_L and Id_R, respectively, and their action will be from now on implicitly understood when necessary. We use the jet-coordinates $(t,x^i,\dot{x}^i_L)$ to describe $L_1(\mathcal{V})$ and the jet-coordinates $(t,x^i,\dot{x}^i_R)$ to describe $R_1(\mathcal{V})$. The elements $\mathbf{x}_L$ of $L_1(\mathcal{V})$ can then be represented in the vector form $\mathbf{x}_L=\partial/\partial t+\dot{x}^i_L\partial/\partial x^i$ and, analogously, $\mathbf{x}_R\in R_1(\mathcal{V})$ can be written as $\mathbf{x}_R=\partial/\partial t+\dot{x}^i_R\partial/\partial x^i$.

ii) The natural action of the modeling vector bundle $V(\mathcal{V})$ on the affine bundle $J_1(\mathcal{V})$ and the natural isomorphisms Id_L, Id_R allow the definition of fibered maps

$$\begin{aligned}&\Xi:\ L_1(\mathcal{V})\times_{\mathcal{V}}V(\mathcal{V})\to R_1(\mathcal{V})\ \text{such that}\ \Xi(\mathbf{x}_L,\mathbf{U})=\mathbf{x}_L+\mathbf{U},\\&\Delta:\ L_1(\mathcal{V})\times_{\mathcal{V}}R_1(\mathcal{V})\to V(\mathcal{V})\ \text{such that}\ \Delta(\mathbf{x}_L,\mathbf{x}_R)=\mathbf{x}_R-\mathbf{x}_L.\end{aligned}\tag{6}$$

The entire geometric context can be summarized by the following diagram:

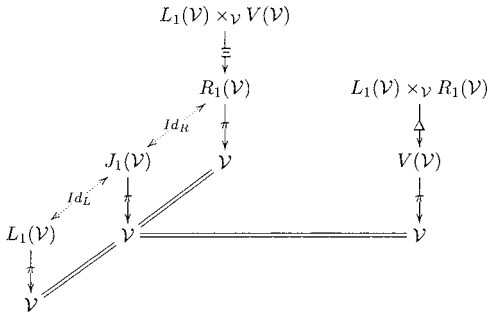

(7)

III. THE UNILATERAL IMPULSIVE ENVIRONMENT

In the following we construct a geometric setup adapted to the study of the impulsive behavior of the system due to the presence of a unilateral constraint acting on the system itself. From the geometric point of view, the following do not present new ideas, since the setup is constructed through the standard concept of pull-back. However, from the point of view of Impulsive Mechanics of unilateral constraints, the setup allows a different approach from those usually found in literature (see, for example, Refs. 14 and 15, and references therein).

Section III A presents the coordinate free construction of the setup and the coordinate free description of its properties. Section III B shows, using admissible coordinates, the explicit coordinate representations of the spaces and the properties of the setup itself.

A. The coordinate free description

The geometric framework of unilateral problems can be constructed, starting from the bundle $\mathcal{V}$ and the assignment of an additional positional constraint $\mathcal{S}$, through the concept of pull-back bundle.[26,27]

The standard pull-back bundle construction applied to $J_1(\mathcal{V})$, $L_1(\mathcal{V})$, $R_1(\mathcal{V})$, gives three affine bundles $i^*(J_1(\mathcal{V}))$, $i^*(L_1(\mathcal{V}))$, $i^*(R_1(\mathcal{V}))$ locally described by admissible coordinates $(t,q^\alpha,\dot{x}^i)$,

$((t,q^\alpha,\dot{x}^i_L)$, $(t,q^\alpha,\dot{x}^i_R)$. By construction $\pi:i^*(J_1(\mathcal{V}))\to\mathcal{S}$ is the bundle of all possible velocities of the system in a configuration of $\mathcal{S}$, and analogously the bundles $\pi:i^*(L_1(\mathcal{V}))\to\mathcal{S}$ and $\pi:i^*(R_1(\mathcal{V}))\to\mathcal{S}$ are the bundles of all possible left and right velocities of the system in a configuration of $\mathcal{S}$.

The pull-back bundle construction can also be applied to the vertical bundle $V(\mathcal{V})$ giving rise to the bundle $\pi:i^*(V(\mathcal{V}))\to\mathcal{S}$ of the vectors that are vertical with respect to $\mathcal{V}$ and with base point in $\mathcal{S}$. The vertical scalar product (2) of $\mathcal{V}$ can be pulled back to a vertical scalar product $\Phi:i^*(V(\mathcal{V}))\times_{\mathcal{S}}i^*(V(\mathcal{V}))\to\mathbb{R}$.

The immersion $i_*:J_1(\mathcal{S})\to J_1(\mathcal{V})$ can be split into two maps $J_1(\mathcal{S})\to i^*(J_1(\mathcal{V}))\to J_1(\mathcal{V})$, that (with a mild abuse of language) will both be called i_*. The image $i_*(J_1(\mathcal{S}))$ is an affine subbundle of $i^*(J_1(\mathcal{V}))$. The same splitting can also be applied to the maps $i_*:L_1(\mathcal{S})\to L_1(\mathcal{V})$, $i_*:R_1(\mathcal{S})\to R_1(\mathcal{V})$ and $i_*:V(\mathcal{S})\to V(\mathcal{V})$. The images $i_*(L_1(\mathcal{S}))$ and $i_*(R_1(\mathcal{S}))$ are then affine subbundles of $i^*(L_1(\mathcal{V}))$ and $i^*(R_1(\mathcal{V}))$, respectively, while $i_*(V(\mathcal{S}))$ is a vector subbundle of $i^*(V(\mathcal{V}))$.

Any assigned frame of reference $\mathbf{H}$ of $\mathcal{V}$, viewed as a section of the velocity bundle $J_1(\mathcal{V})$, can be restricted to a section $\mathbf{H}:\mathcal{S}\to i^*(J_1(\mathcal{V}))$ and gives a diffeomorphism $\Delta_{\mathbf{H}}:i^*(J_1(\mathcal{V}))\to i^*(V(\mathcal{V}))$. The kinetic energy (4) relative to a frame $\mathbf{H}$ can be restricted to a kinetic energy function ${}^{\mathbf{H}}\mathcal{K}:i^*(J_1(\mathcal{V}))\to\mathbb{R}$.

The whole construction, taking into account diagrams (5) and (7) can be synthesized by the following diagram

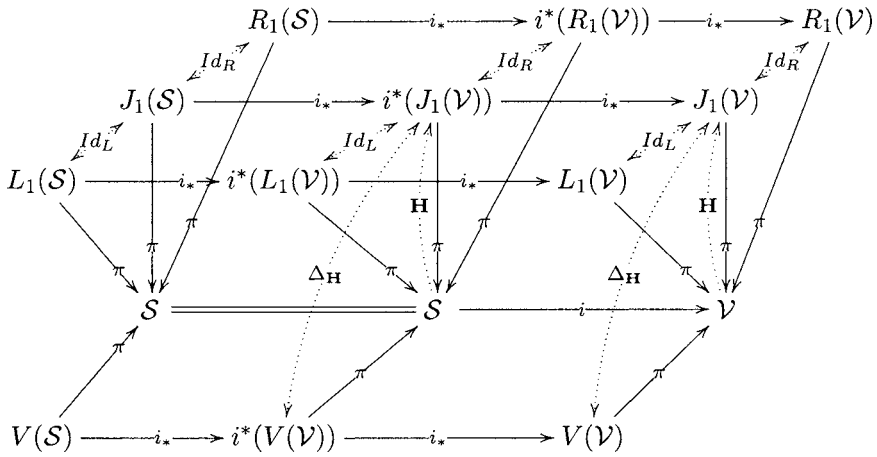

(8)

The slice in the middle of diagram (8), together with its own subbundles given by the slice in the left part of the diagram, is, in a very natural way, the correct geometric environment for the study of the impulsive behavior of $\mathcal{S}$ viewed as unilateral constraint acting on the system. Therefore, in the next part of this section, we focus our attention on these parts of the diagram. We recall once again that, using the (restrictions of the) isomorphisms between $i^*(J_1(\mathcal{V}))$, $i^*(L_1(\mathcal{V}))$, and $i^*(R_1(\mathcal{V}))$, all the geometric properties of the bundle $i^*(J_1(\mathcal{V}))$ have corresponding properties in $i^*(L_1(\mathcal{V}))$ and $i^*(R_1(\mathcal{V}))$.

The simultaneous presence of the vertical metric Φ and of the vector subbundle $i_*(V(\mathcal{S}))$ allows the splitting of the vector bundle $i^*(V(\mathcal{V}))$ into

$$i^*(V(\mathcal{V}))=i_*(V(\mathcal{S}))\oplus(i_*(V(\mathcal{S})))^\perp. \tag{9}$$

The vertical scalar product Φ can then be decomposed into the sum of a scalar product φ acting on $i_*(V(\mathcal{S}))$ and a scalar product ψ acting on $(i_*(V(\mathcal{S})))^\perp$, so that

$$\Phi=\varphi\otimes\psi. \tag{10}$$

Recalling that both $i_*(J_1(\mathcal{S}))$ and $i^*(J_1(\mathcal{V}))$ have an affine nature, an analogous splitting can be performed on the affine bundle $i^*(J_1(\mathcal{V}))$, so that

$$i^*(J_1(\mathcal{V})) = i_*(J_1(\mathcal{S})) \oplus (i_*(V(\mathcal{S})))^\perp, \tag{11}$$

where in this case the meaning of the symbol $\oplus$ is related to the action of the modeling bundle $i^*(V(\mathcal{V}))$ on the affine bundle $i^*(J_1(\mathcal{V}))$ and will be clarified by the coordinate expression in Sec. III B. The decompositions (9) and (11) allow the definitions of projection operators

$$\begin{gathered}\mathcal{P}_{\mathcal{V}}\colon i^*(V(\mathcal{V})) \to i_*(V(\mathcal{S})), \quad \mathcal{P}^\perp_{\mathcal{V}}\colon i^*(V(\mathcal{V})) \to (i_*(V(\mathcal{S})))^\perp, \\ \mathcal{P}\ \colon i^*(J_1(\mathcal{V})) \to i_*(J_1(\mathcal{S})), \quad \mathcal{P}^\perp\colon i^*(J_1(\mathcal{V})) \to (i_*(V(\mathcal{S})))^\perp.\end{gathered} \tag{12}$$

Note that (see, for example, Refs. 21 and 14), from the computational point of view, the operators $\mathcal{P}$ and $\mathcal{P}^\perp$ can be determined through a minimum principle, since, for every point $\mathbf{x} \in i^*(J_1(\mathcal{V}))$, the projection $\mathcal{P}\ (\mathbf{x})$ realizes the minimum of the scalar function

$$f_{\mathbf{x}}\colon i_*(J_1(\mathcal{S})) \to \mathbb{R} \text{ such that } f_{\mathbf{x}}(\mathbf{y}) = \Phi(\mathbf{x}-\mathbf{y}, \mathbf{x}-\mathbf{y}).$$

Proposition 3.1: For each $\mathbf{x}_1, \mathbf{x}_2 \in i^*(J_1(\mathcal{V}))$, *for each* $\mathbf{v} \in i^*(V(\mathcal{V}))$, *the following properties hold*:

(i) $\mathcal{P}_{\mathcal{V}}(\mathbf{x}_1 - \mathbf{x}_2) = \mathcal{P}\ (\mathbf{x}_1) - \mathcal{P}\ (\mathbf{x}_2)$,
(ii) $\mathcal{P}^\perp_{\mathcal{V}}(\mathbf{x}_1 - \mathbf{x}_2) = \mathcal{P}^\perp(\mathbf{x}_1) - \mathcal{P}^\perp(\mathbf{x}_2)$,
(iii) $\mathcal{P}\ (\mathbf{x}_1 + \mathbf{v}) = \mathcal{P}\ (\mathbf{x}_1) + \mathcal{P}_{\mathcal{V}}(\mathbf{v})$,
(iv) $\mathcal{P}^\perp(\mathbf{x}_1 + \mathbf{v}) = \mathcal{P}^\perp(\mathbf{x}_1) + \mathcal{P}^\perp_{\mathcal{V}}(\mathbf{v})$.

Proof: Obviously *(iii)* implies *(i)* and *(iv)* implies *(ii)* choosing $\mathbf{v} = \mathbf{x}_2 - \mathbf{x}_1$. The proof of *(iii)* and *(iv)* is straightforward using admissible coordinates (see also Sec. III B) and is left to the reader. □

The vertical vector $\mathcal{P}^\perp(\mathbf{x}) \in (i_*(V(\mathcal{S})))^\perp$ associated to a velocity $\mathbf{x} \in i^*(J_1(\mathcal{V}))$ is the natural candidate for the orthogonal component of the velocity $\mathbf{x}$ with respect to the constraint $\mathcal{S}$. Unfortunately, the concept of velocity as vertical vector is intrinsically related to the knowledge of a frame of reference $\mathbf{H}$: the following discussion shows that $\mathcal{P}^\perp(\mathbf{x})$ actually is the orthogonal component of the relative velocity $\Delta_{\mathbf{H}}(\mathbf{x})$, not only for a single frame, but even for all the frames in a wide (and geometrically important) class.

Proposition 3.2: Given a frame of reference $\mathbf{H}$, *the following conditions are equivalent*

a) $\exists \mathbf{K}\colon \mathcal{S} \to J_1(\mathcal{S})$ *such that* $\mathbf{H} = i_*(\mathbf{K})$,
b) $\mathcal{P}\ (\mathbf{H}) = \mathbf{H}$,
c) $\mathcal{P}^\perp(\mathbf{H}) = 0$.

Proof: The equivalence *b)* $\Leftrightarrow$ *c)* and the arrow *a)* $\Rightarrow$ *b)* are obvious. The arrow *b)* $\Rightarrow$ *a)* is a consequence of the fact that i_* is an isomorphism between $T(\mathcal{S})$ and its image, so that $\mathbf{K} = (i_*)^*(\mathbf{H})$. □

Definition 1: A frame of reference $\mathbf{H}\colon \mathcal{S} \to i^*(J_1(\mathcal{V}))$ *will be called tangent to* $\mathcal{S}$ *if it obeys one of the equivalent conditions of Proposition (3.2). The set of frames tangent to* $\mathcal{S}$ *will be denoted by* $\mathcal{H}$.

Taking into account the splitting (9), for each velocity $\mathbf{x} \in i^*(J_1(\mathcal{V}))$ and frame $\mathbf{H}$ we have (with the obvious meaning of the symbol $\mathbf{v}^{\|}$) the decomposition

$$\Delta_{\mathbf{H}}(\mathbf{x}) = {}^{\mathbf{H}}\mathbf{v}(\mathbf{x}) = \mathcal{P}_{\mathcal{V}}({}^{\mathbf{H}}\mathbf{v}(\mathbf{x})) + \mathcal{P}^\perp_{\mathcal{V}}({}^{\mathbf{H}}\mathbf{v}(\mathbf{x})) = {}^{\mathbf{H}}\mathbf{v}^{\|}(\mathbf{x}) + {}^{\mathbf{H}}\mathbf{v}^{\perp}(\mathbf{x}). \tag{13}$$

At first glance, there appears to be no relation between the relative "orthogonal" velocity ${}^{\mathbf{H}}\mathbf{v}^{\perp}(\mathbf{x})$, that is, in general, dependent on $\mathbf{H}$, and the vertical vector $\mathcal{P}^\perp(\mathbf{x})$. The following result shows however that the class of frames for which the identity ${}^{\mathbf{H}}\mathbf{v}^{\perp}(\mathbf{x}) = \mathcal{P}^\perp(\mathbf{x})$ holds coincides with the class of the frames tangent to $\mathcal{S}$.

Theorem 3.1: *Given a frame* $\mathbf{H}$, *the condition* ${}^{\mathbf{H}}\mathbf{v}^{\perp}(\mathbf{x}) = \mathcal{P}^\perp(\mathbf{x})\ \forall\, \mathbf{x} \in i^*(J_1(\mathcal{V}))$ *holds if and only if* $\mathbf{H}$ *obeys one of the equivalent conditions of Proposition (3.2).*

Proof: The proof follows easily from property *(ii)* of Proposition (3.1) applied to the vector ${}^{\mathbf{H}}\mathbf{v}(\mathbf{x})=\Delta_{\mathbf{H}}(\mathbf{x})=\mathbf{x}-\mathbf{H}$. □

Definition 3.2: For each $\mathbf{x}\in i^*(J_1(\mathcal{V}))$, *the vertical vector* $\mathcal{P}^{\perp}(\mathbf{x})\in(i_*(V(\mathcal{S})))^{\perp}$ *will be called the orthogonal velocity of* $\mathbf{x}$ *with respect to* $\mathcal{S}$, *and will be denoted by* $\mathbf{v}^{\perp}(\mathbf{x})$ *(or briefly* $\mathbf{v}^{\perp}$ *when no confusion can arise*).

The set $\mathcal{H}$ will play a crucial role in the choice of an ideal constitutive characterization of the reactive impulse of $\mathcal{S}$. We will see that in Sec. IV. Moreover, note that a meaningful definition of the concept of frame of rest of the constraint $\mathcal{S}$ must involve the set $\mathcal{H}$ (see Ref. 25).

B. The coordinate description

All the immersions, projection operators, and properties described in Sec. III A can be rewritten using local admissible coordinates.

The immersion $i:\mathcal{S}\to\mathcal{V}$ can be described in local admissible coordinates as

$$\begin{cases} t=t, \\ x^i=x^i(t,q^\alpha) \end{cases} \tag{14}$$

or by its Cartesian representation

$$g_A(t,x^1,\ldots,x^n)=0, \quad A=1,\ldots,n-r. \tag{15}$$

Using the vector representation (in admissible coordinates), the bundles of the slice in the middle of diagram (8) are described by

$$\begin{aligned} i^*(J_1(\mathcal{V}))&=\left\{\mathbf{x}=\left(\frac{\partial}{\partial t}\right)_{(t,q^\alpha)}+\dot{x}^i\left(\frac{\partial}{\partial x^i}\right)_{(t,q^\alpha)}\right\}, \\ i^*(V(\mathcal{V}))&=\left\{\mathbf{U}=u^i\left(\frac{\partial}{\partial x^i}\right)_{(t,q^\alpha)}\right\}, \end{aligned} \tag{16}$$

and similar expressions hold for the bundles $i^*(L_1(\mathcal{V}))$ and $i^*(R_1(\mathcal{V}))$, substituting $\dot{x}^i$ with $\dot{x}^i_L$ and $\dot{x}^i_R$, respectively.

The corresponding subbundles obtained through the map i_*, omitting the coordinates of the application point of the vectors, are described by

$$\begin{aligned} i_*(J_1(\mathcal{S}))&=\left\{\mathbf{q}=\frac{\partial}{\partial t}+\left(\frac{\partial x^i}{\partial t}+\dot{q}^\alpha\frac{\partial x^i}{\partial q^\alpha}\right)\frac{\partial}{\partial x^i}\right\}, \\ i_*(V(\mathcal{S}))&=\left\{\mathbf{V}=\dot{q}^\alpha\frac{\partial x^i}{\partial q^\alpha}\frac{\partial}{\partial x^i}\right\}, \end{aligned} \tag{17}$$

and similar expressions hold for the bundles $i_*(L_1(\mathcal{S}))$ and $i_*(R_1(\mathcal{S}))$, substituting $\dot{q}^i$ with $\dot{q}^i_L$ and $\dot{q}^i_R$, respectively.

Note that expression (17) points out the affine nature of the injection $i_*:i_*(J_1(\mathcal{S}))\to i^*(J_1(\mathcal{V}))$ and the linear nature of $i_*:i_*(V(\mathcal{S}))\to i^*(V(\mathcal{V}))$.

The vertical metric Φ in $i^*(V(\mathcal{V}))$ is described by the functions $g_{ij}(t,q^\alpha)=g_{ij}(t,x^k(t,q^\alpha))$, while its restriction φ to $i_*(V(\mathcal{S}))$ is described by

$$\gamma_{\alpha\beta}=g_{ij}\frac{\partial x^i}{\partial q^\alpha}\frac{\partial x^j}{\partial q^\beta}. \tag{18}$$

As usual, we denote by g^{ij} and $\gamma^{\alpha\beta}$ the inverse matrices of g_{ij} and $\gamma_{\alpha\beta}$, respectively.

The projection operator $\mathcal{P}_{\mathcal{V}}:i^*(V(\mathcal{V}))\to i_*(V(\mathcal{S}))$ has the (linear) coordinate description

$$\mathcal{P}_{\mathcal{V}}\colon i^*(V(\mathcal{V})) \to i_*(V(\mathcal{S})),$$
$$U^i\frac{\partial}{\partial x^i} \rightsquigarrow \gamma^{\xi\eta} g_{rs}\frac{\partial x^r}{\partial q^\xi}\frac{\partial x^i}{\partial q^\eta}U^s\frac{\partial}{\partial x^i} := A^i_s U^s\frac{\partial}{\partial x^i}. \tag{19}$$

Using (for conciseness) the matrix $A^i_s = \gamma^{\xi\eta} g_{rs}(\partial x^r/\partial q^\xi)(\partial x^i/\partial q^\eta)$, the other projection operators (12) are described by

$$\mathcal{P}^\perp_{\mathcal{V}}\colon i^*(V(\mathcal{V})) \to (i_*(V(\mathcal{S})))^\perp,$$
$$U^i\frac{\partial}{\partial x^i} \rightsquigarrow (\delta^i_s - A^i_s)U^s\frac{\partial}{\partial x^i};$$

$$\mathcal{P}\ :\ i^*(J_1(\mathcal{V})) \to i_*(J_1(\mathcal{S})),$$
$$\frac{\partial}{\partial t} + \dot{x}^i\frac{\partial}{\partial x^i} \rightsquigarrow \frac{\partial}{\partial t} + \left(\frac{\partial x^i}{\partial t} + A^i_s\left(\dot{x}^s - \frac{\partial x^s}{\partial t}\right)\right)\frac{\partial}{\partial x^i}; \tag{20}$$

$$\mathcal{P}^\perp\colon i^*(J_1(\mathcal{V})) \to (i_*(V(\mathcal{S})))^\perp,$$
$$\frac{\partial}{\partial t} + \dot{x}^i\frac{\partial}{\partial x^i} \rightsquigarrow (\delta^i_s - A^i_s)\left(\dot{x}^s - \frac{\partial x^s}{\partial t}\right)\frac{\partial}{\partial x^i}.$$

These expressions allow a tedious but straightforward check of properties *(iii)* and *(iv)* of Proposition 3.1. Moreover, the computation $\mathcal{P} + \mathcal{P}^\perp = \text{Ident}$ clarifies the decomposition (11).

Once a frame **H** is assigned, relations (20) allow an easy check of the condition

$${}^{\mathbf{H}}\mathbf{v}^\perp(\mathbf{x}) = \mathcal{P}^\perp(\mathbf{x})\ \forall\ \mathbf{x} \in i^*(J_1(\mathcal{V})) \Leftrightarrow \mathcal{P}^\perp(\mathbf{H}) = 0.$$

This gives an alternative proof of Theorem (3.1).

IV. IMPULSIVE MECHANICS

In the following the environment previously introduced is applied to give a constitutive characterization of $\mathcal{S}$, based on the simplest criterion of conservation of kinetic energy, particularly suitable to be assumed as an ideality criterion for $\mathcal{S}$. Although very simple, the criterion is strong enough to be directly applied to the wide class of constraints of codimension 1. The case of codimension greater than 1 is, in general, very artificial and physically irrelevant, but can also be treated by adding a very natural requirement of minimality of the impulsive reaction. The discussion is presented following a Newton-type approach, but it is proved that the Poisson-type approach gives the same results. Also the classical approach using reflection operators is applicable to the particular case of constraints of codimension 1. Once again it is proved that it is equivalent to the Newton-type and Poisson-type approaches.

From now on, unless otherwise specified, each frame of reference **H** will be considered as tangent to $\mathcal{S}$.

A. Ideality criterion

A constitutive characterization of the impulsive action of the constraint $\mathcal{S}$ is a map $\tilde{I}: i^*(L_1(\mathcal{V})) \to i^*(R_1(\mathcal{V}))$ assigning to each "entrance" or left velocity $\mathbf{x}_L \in i^*(L_1(\mathcal{V}))$ of the system in the constraint $\mathcal{S}$ a corresponding "exit" or right velocity $\mathbf{x}_R = \tilde{I}(\mathbf{x}_L) \in i^*(R_1(\mathcal{V}))$. Alternatively, and preferably in order to preserve some structural analogies with the force acting on the system (see Refs. 24 and 17), a constitutive characterization of $\mathcal{S}$ is a map $\mathbf{I}: i^*(J_1(\mathcal{V})) \to i^*(V(\mathcal{V}))$ assigning to each velocity $\mathbf{x}$ a corresponding jump $\mathbf{I}(\mathbf{x})$.

The equivalence of the definitions is obtained through the isomorphisms Id_L, Id_R, noting that $\mathbf{x}_L=\mathrm{Id}_L(\mathbf{x})$ and $\mathbf{x}_R=\mathrm{Id}_R(\mathbf{x}+\mathbf{I}(\mathbf{x}))$. Alternatively, recalling (6), we have that $\mathbf{I}(\mathbf{x})=\Delta(\mathbf{x}_L,\tilde{I}(\mathbf{x}_L))$. We will often use the brief (mild abuse of) notation $\mathbf{x}_R=\mathbf{x}_L+\mathbf{I}$.

Usually, an "impenetrability" condition of the form $\Phi(\mathbf{v}^{\perp}(\mathbf{x}_L),\mathbf{v}^{\perp}(\tilde{I}(\mathbf{x}_L)))\leqslant 0\,\forall\,\mathbf{x}_L \in i^*(L_1(\mathcal{V}))$, or equivalently $\Phi(\mathbf{v}^{\perp}(\mathbf{x}),\mathbf{I}(\mathbf{x}))\leqslant 0\,\forall\,\mathbf{x}\in i^*(J_1(\mathcal{V}))$, is further assumed to ensure the unilaterality of $\mathcal{S}$. Even with this condition, a trivial constitutive characterization $\mathbf{I}_0: i^*(J_1(\mathcal{V})) \to i^*(V(\mathcal{V}))$ assigning to each velocity $\mathbf{x}$ the null jump $\mathbf{I}_0(\mathbf{x})\equiv 0$ is theoretically admissible, but its physical meaning is that $\mathcal{S}$ is not a constraint for the system.

In order to define an ideal constitutive characterization of the impulsive reaction, two requirements are very natural. The first, parallelizing the analogous problem in Analytical Mechanics, is that the ideality criterion should have a geometric nature: something like orthogonality with respect to some natural spaces, maybe in addition with a "minimality" criterion (see, for example, Refs. 21, 24, 14, and 15). This requirement then suggests that one avoids the introduction of additional structures, such as, for example, the frame of reference of the rest of the constraint. To clarify this idea, consider for example a point particle bilaterally constrained to the surface of a sphere. The ideal constitutive characterization does not take into account the internal motion of the points of the sphere, on condition that the shape of the sphere does not vary. Moreover, the reaction is orthogonal to the constraint and it has minimum norm. Differently, a constitutive characterization taking into account the presence of friction implies the necessity of knowing the velocity of the point particle with respect to the points of the sphere, and then the knowledge of the frame of the rest of the sphere.

The second natural requirement for an ideal characterization is the conservation of kinetic energy before and after impact. Unfortunately, in contrast to the time-independent approach where an intrinsic choice of a frame of reference is done *a priori* (see Refs. 25 and 19), in a time-dependent environment, kinetic energy is indissolubly related to the knowledge of a frame of reference.

It can be easily proved that is not possible to impose the conservation of kinetic energy in the impact process for every frame of reference, due to the law of variation of kinetic energy with the frame (see Refs. 25 and 18). The conservation of kinetic energy could be imposed in a specific frame of reference tangent to $\mathcal{S}$ chosen as the frame of rest of the constraint, but in this case we should select (arbitrarily) one of the tangent frames. This is in contradiction with the first requirement.

We analyze, then, the consequences of imposing the conservation of kinetic energy before and after the impact in every frame of reference in the class $\mathcal{H}$. With this aim, we state the following.

Lemma 4.1: Let V be a finite dimensional vector space, Φ *a positive definite scalar product on V, and let* $\theta: V\to V$ *be a map such that*

$$\Phi(v+\theta(v),v+\theta(v))=\Phi(v,v),\quad \forall\, v\in V. \tag{21}$$

Let $\|\,\|$ *denote the norm induced on V by* Φ *and let* $\mathcal{B}(u,\epsilon)$ *the ball with center u and radius* ϵ *in V. Then the following conditions hold:*

1) $\theta(v)\in\partial\mathcal{B}(-v,\sqrt{\Phi(v,v)})\,\forall\, v\in V$;
2) there exists a map $\xi_\theta: V\to V$ *obeying the conditions*

$$\begin{cases}\theta(v)=-2v+\xi_\theta(v),\\ \Phi(\theta(v),\xi_\theta(v))=0,\end{cases}\quad \forall\, v\in V, \tag{22}$$

3) the map $\theta_{\min}$ *obeying (21) and having minimum norm is* $\theta_{\min}(v)\equiv 0$;
4) the map $\theta_{\max}$ *obeying (21) and having maximum norm is* $\theta_{\max}(v)=-2v$.

Proof:

1) Using the norm function $\|\,\|$, condition (21) can be rewritten as

$$\|v + \theta(v)\|^2 = \|v\|^2,$$

that is the thesis.

2) Condition (21) can be rewritten as

$$\Phi(2v + \theta(v), \theta(v)) = 0,$$

so that $\xi_\theta(v) := 2v + \theta(v)$ obeys condition $\Phi(\theta(v), \xi_\theta(v)) = 0$.

3,4) Independent of the fact that 3) is obvious, and of the geometric meaning of the first statement of the lemma, conditions 3,4) can be simultaneously proved using coordinates in V. We have

$$\Phi(\theta(v), \theta(v)) = \|\theta(v)\|^2 = g_{ij}\theta^i\theta^j,$$

$$\Phi(2v + \theta(v), \theta(v)) = 0 \Leftrightarrow g_{ij}(2v^i + \theta^i)\theta^j = 0.$$

The standard Lagrange multipliers minimization procedure applied to the function $F(\theta^i, \lambda) = g_{ij}\theta^i\theta^j + \lambda g_{ij}(2v^i + \theta^i)\theta^j$ gives the conditions

$$\begin{cases} \theta^j = -\dfrac{\lambda}{1+\lambda}v^i, \\ \lambda = 0 \text{ or } \lambda = -2 \end{cases}$$

and then both the conclusions. □

We can now prove the following:

Theorem 4.1: *Let* $\mathbf{I}: i^*(J_1(\mathcal{V})) \to i^*(V(\mathcal{V}))$ *be a nontrivial constitutive characterization of* $\mathcal{S}$ *satisfying the condition*

$$^{\mathbf{H}}\mathcal{K}(\mathbf{x} + \mathbf{I}(\mathbf{x})) = {}^{\mathbf{H}}\mathcal{K}(\mathbf{x}), \quad \forall\, \mathbf{x} \in i^*(J_1(\mathcal{V})), \quad \forall\, \mathbf{H} \in \mathcal{H}. \tag{23}$$

Then:

1) $\mathcal{P}_{\mathcal{V}}(\mathbf{I}(\mathbf{x})) = 0\ \forall\, \mathbf{x} \in i^*(J_1(\mathcal{V}))$ *or, equivalently,* $\mathbf{I}(\mathbf{x}) = \mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I}(\mathbf{x}))\ \forall\, \mathbf{x} \in i^*(J_1(\mathcal{V}))$.

2) there exists a map $\mathbf{Z}: i^*(J_1(\mathcal{V})) \to (i_*(V(\mathcal{S})))^{\perp}$ *satisfying the conditions*

$$\begin{cases} \mathbf{I}(\mathbf{x}) = -2\mathbf{v}^{\perp}(\mathbf{x}) + \mathbf{Z}(\mathbf{x}), \\ \Phi(\mathbf{I}(\mathbf{x}), \mathbf{Z}(\mathbf{x})) = 0. \end{cases} \quad \forall\, \mathbf{x} \in i^*(J_1(\mathcal{V})), \tag{24}$$

Proof: 1) By definition, recalling the decomposition (10) and omitting the dependence on $\mathbf{x}$, we have

$$\begin{aligned} {}^{\mathbf{H}}\mathcal{K}(\mathbf{x} + \mathbf{I}) &= \tfrac{1}{2}\Phi(\mathbf{x} - \mathbf{H} + \mathbf{I}, \mathbf{x} - \mathbf{H} + \mathbf{I}) = \tfrac{1}{2}\Phi({}^{\mathbf{H}}\mathbf{v} + \mathbf{I}, {}^{\mathbf{H}}\mathbf{v} + \mathbf{I}) \\ &= \tfrac{1}{2}\Phi({}^{\mathbf{H}}\mathbf{v}^{\|} + \mathbf{v}^{\perp} + \mathcal{P}_{\mathcal{V}}(\mathbf{I}) + \mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I}), {}^{\mathbf{H}}\mathbf{v}^{\|} + \mathbf{v}^{\perp} + \mathcal{P}_{\mathcal{V}}(\mathbf{I}) + \mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I})) \\ &= \tfrac{1}{2}\varphi({}^{\mathbf{H}}\mathbf{v}^{\|} + \mathcal{P}_{\mathcal{V}}(\mathbf{I}), {}^{\mathbf{H}}\mathbf{v}^{\|} + \mathcal{P}_{\mathcal{V}}(\mathbf{I})) + \tfrac{1}{2}\psi(\mathbf{v}^{\perp} + \mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I}), \mathbf{v}^{\perp} + \mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I})) \end{aligned}$$

and analogously

$$^{\mathbf{H}}\mathcal{K}(\mathbf{x}) = \tfrac{1}{2}\Phi(\mathbf{x} - \mathbf{H}, \mathbf{x} - \mathbf{H}) = \tfrac{1}{2}\varphi({}^{\mathbf{H}}\mathbf{v}^{\|}, {}^{\mathbf{H}}\mathbf{v}^{\|}) + \tfrac{1}{2}\psi(\mathbf{v}^{\perp}, \mathbf{v}^{\perp}).$$

By comparison, Eq. (23) implies

$$\varphi({}^{\mathbf{H}}\mathbf{v}^{\|}, \mathcal{P}_{\mathcal{V}}(\mathbf{I})) + \tfrac{1}{2}\varphi(\mathcal{P}_{\mathcal{V}}(\mathbf{I}), \mathcal{P}_{\mathcal{V}}(\mathbf{I})) + \psi(\mathbf{v}^{\perp}, \mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I})) + \tfrac{1}{2}\psi(\mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I}), \mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I})) = 0.$$

Since both $\mathbf{x} \in i^*(J_1(\mathcal{V}))$ and $\mathbf{H} \in \mathcal{H}$ are arbitrary, the vector ${}^{\mathbf{H}}\mathbf{v}^{\|} \in i_*(V(\mathcal{S}))$ is also arbitrary. Therefore we have that

$$\begin{cases} \varphi({}^{\mathbf{H}}\mathbf{v}^{\parallel}, \mathcal{P}_{\mathcal{V}}(\mathbf{I})) = 0, \\ \frac{1}{2}\varphi(\mathcal{P}_{\mathcal{V}}(\mathbf{I}), \mathcal{P}_{\mathcal{V}}(\mathbf{I})) + \psi(\mathbf{v}^{\perp}, \mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I})) + \frac{1}{2}\psi(\mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I}), \mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I})) = 0 \end{cases}$$

and then

$$\begin{cases} \mathcal{P}_{\mathcal{V}}(\mathbf{I}) = 0 \Leftrightarrow \mathbf{I} = \mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I}), \\ \psi(\mathbf{v}^{\perp}, \mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I})) + \frac{1}{2}\psi(\mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I}), \mathcal{P}^{\perp}_{\mathcal{V}}(\mathbf{I})) = 0. \end{cases}$$

The conclusion follows immediately from Lemma (4.1). □

The theorem has an immediate application to the class of constraints $\mathcal{S}$ of codimension 1.

Corollary 4.1: Let $\mathcal{S}$ be such that codim$(\mathcal{S})=1$ and let $\mathbf{I}: i^*(J_1(\mathcal{V})) \to i^*(V(\mathcal{V}))$ be a nontrivial constitutive characterization for $\mathcal{S}$ satisfying the hypotheses of Theorem (4.1). Then

$$\mathbf{I}(\mathbf{x}) = -2\mathbf{v}^{\perp}(\mathbf{x}), \quad \forall\, \mathbf{x} \in i^*(J_1(\mathcal{V})). \tag{25}$$

Proof: Since $\dim((i_*(V(\mathcal{S})))^{\perp})=1$, conditions (24) imply that $\mathbf{Z}(\mathbf{x})=0\,\forall\,\mathbf{x} \in i^*(J_1(\mathcal{V}))$. Moreover, the impenetrability condition $\Phi(\mathbf{v}^{\perp}(\mathbf{x}), \mathbf{I}(\mathbf{x})) \leqslant 0\,\forall\,\mathbf{x} \in i^*(J_1(\mathcal{V}))$ has a straightforward verification. □

The case codim$(\mathcal{S})>1$ is not particularly significant from the physical point of view: a simple example is given by a point particle moving in a three-dimensional space and colliding with a one-dimensional straight line. Anyway, Theorem (4.1) allows a simple treatment of such cases by requiring an additional "minimality" criterion. Of course, due to results 3,4) of Lemma (4.1), the minimality must be required for the part $\mathbf{Z}(\mathbf{x})$ of the reactive impulse $\mathbf{I}(\mathbf{x})$ or, alternatively, a "maximality" condition must be required for $\mathbf{I}(\mathbf{x})$. A minimality requirement on $\mathbf{I}(\mathbf{x})$ would give in fact the trivial (null) reaction.

The described procedure applied to a point particle moving in a three-dimensional space and colliding with a one-dimensional straight line gives a very natural result: the impulsive reaction belongs to the plane determined by $\mathbf{v}^{\perp}$ and the constraint. The detailed calculation will not be presented in the following, since we prefer to discuss more significant examples.

B. The Poisson-type approach

The Poisson-type approach to impulsive problems divides the reactive impulse $\mathbf{I}$ due to $\mathcal{S}$ into two parts $\mathbf{I}_{\text{in}}$ and $\mathbf{I}_{\text{out}}$ with different physical meanings (see, for example, Ref. 28, and references therein).

The part $\mathbf{I}_{\text{in}}: i^*(J_1(\mathcal{V})) \to i^*(V(\mathcal{V}))$ is related to the "entrance" of the system in the constraint $\mathcal{S}$ viewed, roughly speaking, as a "suddenly appearing positional constraint." Then, with the previous discussion about the natural requirements to ask of an ideal constitutive characterization kept in mind, we see that $\mathbf{I}_{\text{in}}$ must satisfy the property

$$\mathbf{x} + \mathbf{I}_{\text{in}}(\mathbf{x}) \in i_*(J_1(\mathcal{S})), \quad \forall\, \mathbf{x} \in i^*(J_1(\mathcal{V})) \tag{26}$$

and $\mathbf{I}_{\text{in}}$ should be dependent only on the geometric objects of the setup. The most natural choice of a constitutive characterization for $\mathbf{I}_{\text{in}}$ follows from the requirement $\mathbf{x}+\mathbf{I}_{\text{in}}(\mathbf{x})=\mathcal{P}\ (\mathbf{x})$. Moreover, this is the same result given by the application of the usual minimality principle. The requirement $\mathbf{x}+\mathbf{I}_{\text{in}}(\mathbf{x})=\mathcal{P}\ (\mathbf{x})$ implies $\mathbf{I}_{\text{in}}(\mathbf{x})=-\mathbf{v}^{\perp}(\mathbf{x})$.

The part $\mathbf{I}_{\text{out}}: i^*(J_1(\mathcal{V})) \to i^*(V(\mathcal{V}))$ is related to the "exit" of the system from the constraint $\mathcal{S}$, and it is subject to additional requirements, which, in general, express mechanical properties of the impulsive problem. For example, one such property could be the conservation of kinetic energy. Once again the conservation of energy cannot be required for every frame of reference and should not be required for a single rest frame. The discussion of a constitutive characterization for $\mathbf{I}_{\text{out}}$ can be phrased in terms of the properties of the total reactive impulse $\mathbf{I}_{\text{tot}}=\mathbf{I}_{\text{in}}+\mathbf{I}_{\text{out}}$ as presented in Theorem 4.1. Alternatively, it can be presented *ex novo* starting from the condition

$$^{\mathbf{H}}\mathcal{K}(\mathbf{x}-\mathbf{v}^{\perp}(\mathbf{x})+\mathbf{I}_{\text{out}}(\mathbf{x}))=\,^{\mathbf{H}}\mathcal{K}(\mathbf{x}),\quad \forall\,\mathbf{x}\in i^{*}(J_1(\mathcal{V})),\quad \forall\,\mathbf{H}\in\mathcal{H}$$

and repeating the procedure of Theorem 4.1. In both cases it easily follows that

$$\mathbf{I}_{\text{out}}(\mathbf{x})+\mathbf{v}^{\perp}(\mathbf{x})=\mathbf{Z}(\mathbf{x}),\quad \forall\,\mathbf{x}\in i^{*}(J_1(\mathcal{V})). \tag{27}$$

The latter gives results completely analogous to the ones of the Newton-type approach both when $\text{codim}(\mathcal{S})=1$ and when $\text{codim}(\mathcal{S})>1$.

C. The reflection operator approach

The case $\text{codim}(\mathcal{S})=1$ can be approached in a classical, but different, way through the use of reflection operators.

We recall that once a scalar product Φ is known in a vector space V, it is possible to associate to each assigned vector $N\in V$, with $\|N\|=1$, a reflection operator

$$\mathbf{R}_N\colon V\to V \text{ such that } v\rightsquigarrow \mathbf{R}_N(v)=v-2\Phi(v,N)N. \tag{28}$$

When $\text{codim}(\mathcal{S})=1$ we can introduce a unitary generator $\mathbf{N}$ of $(i_*(V(\mathcal{S})))^{\perp}$ and then we can define its associated reflection operator $\mathbf{R}_{\mathbf{N}}\colon i^{*}(V(\mathcal{V}))\to i^{*}(V(\mathcal{V}))$, that will be denoted simply by $\mathbf{R}$.

Recalling that each frame of reference $\mathbf{H}$ determines the diffeomorphism $\Delta_{\mathbf{H}}\colon i^{*}(J_1(\mathcal{V}))\to i^{*}(V(\mathcal{V}))$, a possible choice of a constitutive characterization of $\mathcal{S}$ can be given by the rule

$$\tilde{I}_{\mathbf{R}}\colon i^{*}(L_1(\mathcal{V}))\to i^{*}(R_1(\mathcal{V})) \text{ such that } \mathbf{x}_L\rightsquigarrow \mathbf{x}_R=\Delta_{\mathbf{H}}^{-1}(\mathbf{R}(^{\mathbf{H}}\mathbf{v}(\mathbf{x}_L))). \tag{29}$$

A straightforward calculation shows that this characterization is the same as

$$\mathbf{I}_{\mathbf{R}}\colon i^{*}(J_1(\mathcal{V}))\to i^{*}(V(\mathcal{V})) \text{ such that } \mathbf{x}\rightsquigarrow \mathbf{I}_{\mathbf{R}}(\mathbf{x})=-2\Phi(\mathbf{x}-\mathbf{H},\mathbf{N})\mathbf{N}. \tag{30}$$

Unfortunately, following this line of argument brings us to the same difficulty we mentioned earlier, since any constitutive characterization of type (30) depends on the frame $\mathbf{H}$. The relation with the constitutive characterization of Sec. IV A is clarified by the following.

Corollary 4.2: The constitutive characterization $\mathbf{I}_{\mathbf{R}}$ *does not depend on the frame* $\mathbf{H}$ *if and only if* $\mathbf{H}$ *is chosen in the class* $\mathcal{H}$ *of the frames tangent to* $\mathcal{S}$. *In this case, the characterization* $\mathbf{I}_{\mathbf{R}}$ *coincides with the characterization* $\mathbf{I}$ *of Sec. IV A.*

Proof: Since the single vector $\mathbf{N}$ forms a unitary basis of $(i_*(V(\mathcal{S})))^{\perp}$, the vector $\Phi(\mathbf{x}-\mathbf{H},\mathbf{N})\mathbf{N}$ is the component $^{\mathbf{H}}\mathbf{v}^{\perp}\in(i_*(V(\mathcal{S})))^{\perp}$ of the velocity $\mathbf{x}$. Then Theorem (3.1) gives the first statement of the corollary. Once $\mathbf{H}\in\mathcal{H}$, then

$$\begin{aligned}\mathbf{I}_{\mathbf{R}}(\mathbf{x})&=-2\Phi(\mathbf{x}-\mathbf{H},\mathbf{N})\mathbf{N}\\&=-2\Phi(\mathbf{v}^{\perp}(\mathbf{x}),\mathbf{N})\mathbf{N}=-2\psi(\mathbf{v}^{\perp}(\mathbf{x}),\mathbf{N})\mathbf{N}=-2\mathbf{v}^{\perp}\end{aligned}$$

from which the result follows. □

V. EXAMPLES

The main reason for the choice of the examples in the following is to show in detail the application of the ideal constitutive characterization for impulsive constraints acting on some significant mechanical systems. Secondarily, in order to prove the naturalness of the ideal characterization, our choice of examples is based on the intention of illustrating the clear physical interpretation of some peculiar results regarding specific mechanical systems. A third reason is the possibility of returning to some arguments, such as the geometric representation of constraints in Impulsive Mechanics, that were only skimmed in the previous discussions.

For these reasons, the simplest example of a point particle moving in a plane and impacting with a straight line is left to the reader.

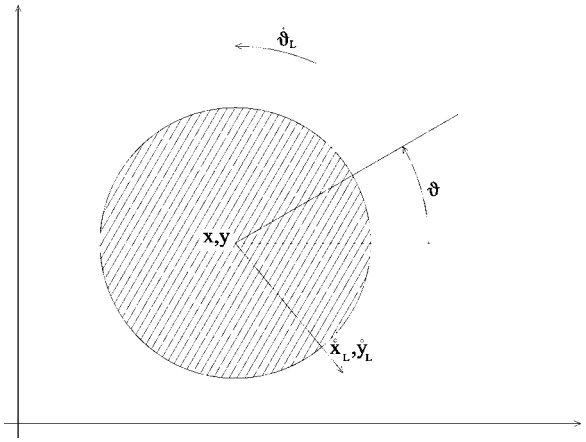

FIG. 1. Example 1.

A. Example 1

A homogeneous disk of mass m and radius R is moving in a plane and impacts with a smooth straight line.

The space-time bundle $\mathcal{V}$ is a four-dimensional manifold. Local admissible coordinates can be chosen as (t,x,y,ϑ) where x,y are the Cartesian coordinates of the center of the disk in the plane of the motion and ϑ is the orientation of the disk (see Fig. 1). The configuration space is $\mathbb{R}^2 \times \mathbb{S}^1$. The vertical scalar product Φ on $\mathcal{V}$ is described by the matrix $g_{ij}=\mathrm{diag}(m,m,A)$ with $A=\frac{1}{2}mR^2$. The constraint $\mathcal{S}$ can be described by the condition $y=R$ or, choosing admissible coordinates (t,x,ϑ) in $\mathcal{S}$, by the injection

$$i:\mathcal{S}\to\mathcal{V} \text{ such that } (t,x,\vartheta)\rightsquigarrow(t,x,R,\vartheta). \tag{31}$$

Therefore in this example $\mathrm{codim}(\mathcal{S})=1$. The scalar product φ on $\mathcal{S}$ is described by the matrix $\gamma_{\alpha\beta}=\mathrm{diag}(m,A)$. The velocity and vertical spaces are:

$$i^*(J_1(\mathcal{V}))=\left\{\mathbf{x}=\frac{\partial}{\partial t}+\dot{x}\frac{\partial}{\partial x}+\dot{y}\frac{\partial}{\partial y}+\dot{\vartheta}\frac{\partial}{\partial\vartheta}\right\},$$

$$i^*(V(\mathcal{V}))=\left\{\mathbf{U}=\dot{x}\frac{\partial}{\partial x}+\dot{y}\frac{\partial}{\partial y}+\dot{\vartheta}\frac{\partial}{\partial\vartheta}\right\},$$

$$i_*(J_1(\mathcal{S}))=\left\{\mathbf{q}=\frac{\partial}{\partial t}+\dot{x}\frac{\partial}{\partial x}+\dot{\vartheta}\frac{\partial}{\partial\vartheta}\right\},$$

$$i_*(V(\mathcal{S}))=\left\{\mathbf{V}=\dot{x}\frac{\partial}{\partial x}+\dot{\vartheta}\frac{\partial}{\partial\vartheta}\right\},$$

$$(i_*(V(\mathcal{S})))^\perp=\left\{\mathbf{W}=w\frac{\partial}{\partial y}\right\}.$$

A unit vector generating $(i_*(V(\mathcal{S})))^\perp$ is $\mathbf{N}=(1/\sqrt{m})\partial/\partial y$.

Given a left velocity $\mathbf{x}_L=\partial/\partial t+\dot{x}_L\partial/\partial x+\dot{y}_L\partial/\partial y+\dot{\vartheta}_L\partial/\partial\vartheta$, we have $\mathbf{v}^\perp(\mathbf{x}_L)=\mathcal{P}^\perp(\mathbf{x}_L)=\dot{y}_L\partial/\partial y$ and the corresponding ideal reactive impulse is $\mathbf{I}(\mathbf{x}_L)=-2\mathbf{v}^\perp(\mathbf{x}_L)=-2\dot{y}_L\partial/\partial y$. It follows that

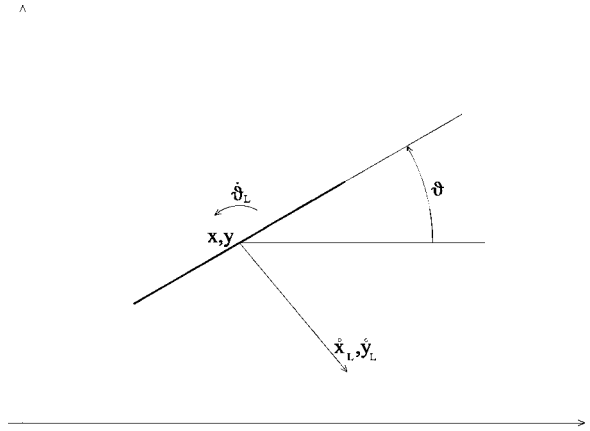

FIG. 2. Example 2.

$$\mathbf{x}_R = \mathbf{x}_L + \mathbf{I}(\mathbf{x}_L) = \frac{\partial}{\partial t} + \dot{x}_L \frac{\partial}{\partial x} - \dot{y}_L \frac{\partial}{\partial y} + \dot{\vartheta}_L \frac{\partial}{\partial \vartheta}. \tag{32}$$

The result has a clear physical interpretation: both the velocity along the x axis and the angular velocity of the disk do not vary with the impact, while the velocity of the disk along the y axis simply reverses. This is of course in perfect agreement with the reflection operator approach.

B. Example 2

A homogeneous rod of mass m and length $2L$ is moving in a plane and one of its ends impacts with a smooth straight line.

The space-time bundle $\mathcal{V}$ is again a four-dimensional manifold with local admissible coordinates (t,x,y,ϑ), where x,y are the Cartesian coordinates of the center of mass of the rod in the plane of the motion and ϑ is the angle formed by the rod with the x axis (see Fig. 2). Once again, the configuration space is $\mathbb{R}^2 \times \mathbb{S}^1$. The vertical scalar product Φ on $\mathcal{V}$ is described by the matrix $g_{ij}=\mathrm{diag}(m,m,A)$ with $A=\frac{1}{3}mL^2$. The constraint $\mathcal{S}$ can be described by the condition $y-L\sin\vartheta=0$ or, choosing admissible coordinates (t,x,ϑ) in $\mathcal{S}$, by the injection

$$i:\mathcal{S} \to \mathcal{V} \text{ such that } (t,x,\vartheta) \rightsquigarrow (t,x,L\sin\vartheta,\vartheta). \tag{33}$$

Therefore $\mathrm{codim}(\mathcal{S})=1$. We avoid the possibility that all the points of the rod simultaneously impact with $\mathcal{S}$ by requiring $\vartheta \in (0,\pi)$. The scalar product φ on $\mathcal{S}$ is described by the matrix $\gamma_{\alpha\beta}=\mathrm{diag}(m,A(1+3\cos^2\vartheta))$. The velocity and vertical spaces are:

$$i^*(J_1(\mathcal{V})) = \left\{ \mathbf{x} = \frac{\partial}{\partial t} + \dot{x}\frac{\partial}{\partial x} + \dot{y}\frac{\partial}{\partial y} + \dot{\vartheta}\frac{\partial}{\partial \vartheta} \right\},$$

$$i^*(V(\mathcal{V})) = \left\{ \mathbf{U} = \dot{x}\frac{\partial}{\partial x} + \dot{y}\frac{\partial}{\partial y} + \dot{\vartheta}\frac{\partial}{\partial \vartheta} \right\},$$

$$i_*(J_1(\mathcal{S})) = \left\{ \mathbf{q} = \frac{\partial}{\partial t} + \dot{x}\frac{\partial}{\partial x} + L\dot{\vartheta}\cos\vartheta\frac{\partial}{\partial y} + \dot{\vartheta}\frac{\partial}{\partial \vartheta} \right\},$$

$$i_*(V(\mathcal{S})) = \left\{ \mathbf{V} = \dot{x}\frac{\partial}{\partial x} + L\dot{\vartheta}\cos\vartheta\frac{\partial}{\partial y} + \dot{\vartheta}\frac{\partial}{\partial \vartheta} \right\},$$

$$(i_*(V(\mathcal{S})))^{\perp} = \left\{ \mathbf{W} = w\left(\frac{\partial}{\partial y} - \frac{3}{L}\cos\vartheta \frac{\partial}{\partial \vartheta} \right) \right\}.$$

Given a left velocity $\mathbf{x}_L = \partial/\partial t + \dot{x}_L \partial/\partial x + \dot{y}_L \partial/\partial y + \dot{\vartheta}_L \partial/\partial \vartheta$, we have

$$\mathbf{v}^{\perp}(\mathbf{x}_L) = \left(\dot{y}_L - \frac{mL\dot{y}_L \cos\vartheta + A\dot{\vartheta}_L}{A(1+3\cos^2\vartheta))} L\cos\vartheta \right) \frac{\partial}{\partial y} + \left(\dot{\vartheta}_L - \frac{mL\dot{y}_L \cos\vartheta + A\dot{\vartheta}_L}{A(1+3\cos^2\vartheta))} \right) \frac{\partial}{\partial \vartheta}.$$

It follows that

$$\mathbf{x}_R = \mathbf{x}_L + \mathbf{I}(\mathbf{x}_L) = \frac{\partial}{\partial t} + \dot{x}_L \frac{\partial}{\partial x} + \left(2\frac{mL\dot{y}_L \cos\vartheta + A\dot{\vartheta}_L}{A(1+3\cos^2\vartheta))} L\cos\vartheta - \dot{y}_L \right) \frac{\partial}{\partial y}$$
$$+ \left(2\frac{mL\dot{y}_L \cos\vartheta + A\dot{\vartheta}_L}{A(1+3\cos^2\vartheta))} - \dot{\vartheta}_L \right) \frac{\partial}{\partial \vartheta}.$$

A simple test of reasonableness of the result follows from the analysis of the particular case of impact configuration with the rod orthogonal to the constraint, that is when $\vartheta = \pi/2$. A straightforward substitution gives $\mathbf{v}^{\perp}(\mathbf{x}_L) = \dot{y}_L \partial/\partial y$, from which follows the expected result $\mathbf{x}_R = \partial/\partial t + \dot{x}_L \partial/\partial x - \dot{y}_L \partial/\partial y + \dot{\vartheta}_L \partial/\partial \vartheta$.

Another possible test follows from an analysis of the dependence on the "impact angle" ϑ of the behavior of the rod when the rod collides with left velocity $\mathbf{x}_L = \partial/\partial t + \dot{x}_L \partial/\partial x + \dot{y}_L \partial/\partial y$, that is with null angular velocity. A first result, once again easily predicted, is that the component $\dot{x}_R$ of the right velocity along the x axis coincides with $\dot{x}_L$, that is the component of the velocity of the center of mass along the x axis is not affected by the impact. A second result is the existence of two symmetric angles, determined by the condition $\dot{y}_R = 0$ and given by $\cos^2\vartheta = \frac{1}{3}$. It can be easily seen that, for impact angles ϑ with $\cos^2\vartheta < \frac{1}{3}$, the component $\dot{y}_R$ of the right velocity along the y axis has the opposite sign of $\dot{y}_L$ (the rod "rebounds" off the constraint) while for impact angles ϑ with $\cos^2\vartheta > \frac{1}{3}$, the component $\dot{y}_R$ of the right velocity along the y axis has the same sign of $\dot{y}_L$ (the center of mass of the rod "continues its approach" to the constraint). However in both cases an angular velocity $\dot{\vartheta}_R \neq 0$ appears (with a sign correctly determined by the impact angle).

C. Example 3

A homogeneous sphere of mass m and radius R is moving in a three-dimensional space and impacts with a smooth straight line (see Fig. 3).

In this example the space-time bundle $\mathcal{V}$ is a seven-dimensional manifold with local admissible coordinates $(t,x,y,z,\psi,\vartheta,\phi)$, where x,y,z are the Cartesian coordinates of the center of mass of the sphere and ψ,ϑ,ϕ are the usual Euler angles. The configuration space is $\mathbb{R}^3 \times \mathbf{SO(3)}$. The vertical scalar product Φ on $\mathcal{V}$ is described by the matrix

$$g_{ij} = \begin{pmatrix} m & 0 & 0 & 0 & 0 & 0 \\ 0 & m & 0 & 0 & 0 & 0 \\ 0 & 0 & m & 0 & 0 & 0 \\ 0 & 0 & 0 & A & 0 & A\cos\vartheta \\ 0 & 0 & 0 & 0 & A & 0 \\ 0 & 0 & 0 & A\cos\vartheta & 0 & A \end{pmatrix}$$

with $A = \frac{2}{5}mR^2$. The constraint $\mathcal{S}$ can be described by the condition $y^2 + z^2 = R$ or, choosing admissible coordinates $(t,x,\alpha,\psi,\vartheta,\phi)$ in $\mathcal{S}$, by the injection

$$i:\mathcal{S} \to \mathcal{V} \text{ such that } (t,x,\alpha,\psi,\vartheta,\phi) \rightsquigarrow (t,x,R\cos\alpha,R\sin\alpha,\psi,\vartheta,\phi). \tag{34}$$

Again $\operatorname{codim}(\mathcal{S}) = 1$. With the additional condition $\sin\vartheta \neq 0$, the velocity and vertical spaces are:

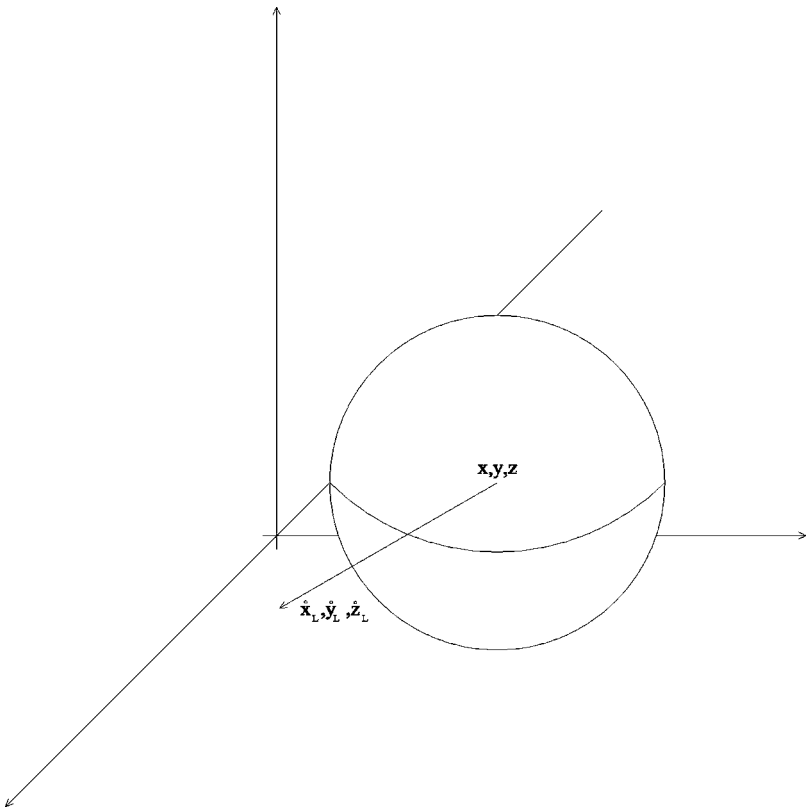

FIG. 3. Example 3.

$$i^*(J_1(\mathcal{V})) = \left\{ \mathbf{x} = \frac{\partial}{\partial t} + \dot{x}\frac{\partial}{\partial x} + \dot{y}\frac{\partial}{\partial y} + \dot{z}\frac{\partial}{\partial z} + \dot{\psi}\frac{\partial}{\partial \psi} + \dot{\vartheta}\frac{\partial}{\partial \vartheta} + \dot{\phi}\frac{\partial}{\partial \phi} \right\},$$

$$i^*(V(\mathcal{V})) = \left\{ \mathbf{U} = \dot{x}\frac{\partial}{\partial x} + \dot{y}\frac{\partial}{\partial y} + \dot{z}\frac{\partial}{\partial z} + \dot{\psi}\frac{\partial}{\partial \psi} + \dot{\vartheta}\frac{\partial}{\partial \vartheta} + \dot{\phi}\frac{\partial}{\partial \phi} \right\},$$

$$i_*(J_1(\mathcal{S})) = \left\{ \mathbf{q} = \frac{\partial}{\partial t} + \dot{x}\frac{\partial}{\partial x} - \dot{\alpha}R\sin\alpha\frac{\partial}{\partial y} + \dot{\alpha}R\cos\alpha\frac{\partial}{\partial z} + \dot{\psi}\frac{\partial}{\partial \psi} + \dot{\vartheta}\frac{\partial}{\partial \vartheta} + \dot{\phi}\frac{\partial}{\partial \phi} \right\},$$

$$i_*(V(\mathcal{S})) = \left\{ \mathbf{V} = \dot{x}\frac{\partial}{\partial x} - \dot{\alpha}R\sin\alpha\frac{\partial}{\partial y} + \dot{\alpha}R\cos\alpha\frac{\partial}{\partial z} + \dot{\psi}\frac{\partial}{\partial \psi} + \dot{\vartheta}\frac{\partial}{\partial \vartheta} + \dot{\phi}\frac{\partial}{\partial \phi} \right\},$$

$$(i_*(V(\mathcal{S})))^\perp = \left\{ \mathbf{W} = w\left(\cos\alpha\frac{\partial}{\partial y} + \sin\alpha\frac{\partial}{\partial z} \right) \right\}.$$

Given a left velocity $\mathbf{x}_L = \partial/\partial t + \dot{x}_L\partial/\partial x + \dot{y}_L\partial/\partial y + \dot{z}_L\partial/\partial z + \dot{\psi}_L\partial/\partial \psi + \dot{\vartheta}_L\partial/\partial \vartheta + \dot{\phi}_L\partial/\partial \phi$, we have

$$\mathbf{v}^\perp(\mathbf{x}_L) = [(\dot{y}_L\cos\alpha + \dot{z}_L\sin\alpha)\cos\alpha]\frac{\partial}{\partial y} + [(\dot{y}_L\cos\alpha + \dot{z}_L\sin\alpha)\sin\alpha]\frac{\partial}{\partial z}.$$

It follows that

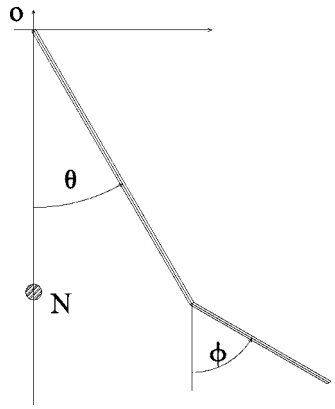

FIG. 4. Example 4.

$$\mathbf{x}_R = \mathbf{x}_L + \mathbf{I}(\mathbf{x}_L) = \frac{\partial}{\partial t} + \dot{x}_L \frac{\partial}{\partial x} + (\dot{y}_L - 2\cos\alpha(\dot{y}_L \cos\alpha + \dot{z}_L \sin\alpha))\frac{\partial}{\partial y}$$
$$+ (\dot{z}_L - 2\sin\alpha(\dot{y}_L \cos\alpha + \dot{z}_L \sin\alpha))\frac{\partial}{\partial z} + \dot{\psi}_L \frac{\partial}{\partial \psi} + \dot{\vartheta}_L \frac{\partial}{\partial \vartheta} + \dot{\phi}_L \frac{\partial}{\partial \phi}.$$

Once again, simple tests of reasonableness of the result follow from the analysis of particular cases of impact configurations. For example, an impact with $\dot{y}_L < 0$, $\dot{z}_L = 0$, $\alpha = \pi/4$ gives $\dot{y}_R = 0$, $\dot{z}_R = -\dot{y}_L$ and leaves invariant the other component of the left velocity.

However, one important peculiarity of this example is that it points out the fact, only alluded to in the introduction of the paper, that the translation of the physical problem with its constraints (the ball impacting with the line) into the geometric context can transform the thread $y = z = 0$, that is a constraint with codimension greater than 1, into a constraint with codimension 1 (the "cylinder" $\mathcal{S}$).

D. Example 4

A mechanical system is formed by two rods of mass $2m$ and m and length $2L$ and L, respectively, moving in a plane. The first rod has one of its ends fixed at a point O of the plane (so that it can only rotate around O), the second rod has one of its ends fixed at the second end of the first rod. A nail N is fixed in the plane at a distance $\sqrt{3}L$ from O (see Fig. 4). Then there are three different kinds of impact: the first rod impacts with the nail while the second rod is far from the nail; the second rod impacts with the nail while the first rod is far from the nail; both the rods impact simultaneously with the nail.

In this example the space-time bundle $\mathcal{V}$ is a three-dimensional manifold with local admissible coordinates (t, ϑ, ϕ), where ϑ is the angle formed by the first rod and the straight line determined by O and N while ϕ is the angle formed by the second rod and the direction of the straight line ON. The configuration space of the system is the two-dimensional torus $\mathbb{T}^2$ and the vertical scalar product Φ on $\mathcal{V}$ is described by the matrix

$$g_{ij} = \begin{pmatrix} \frac{10}{3}mL^2 & mL^2\cos(\vartheta - \phi) \\ mL^2\cos(\vartheta - \phi) & \frac{1}{6}mL^2 \end{pmatrix}.$$

The constraint $\mathcal{S}$ is the union of the zero sets described by the two conditions $\mathcal{S}_1, \mathcal{S}_2$, where

$$\mathcal{S}_1 : \vartheta = 0,$$

$$\mathcal{S}_2:\begin{cases}\phi=\dfrac{3\pi}{2}+\arctan\left(\dfrac{\frac{\sqrt{3}}{2}-\cos\vartheta}{\sin\vartheta}\right) & \text{if } \vartheta\in\left[0,\dfrac{\pi}{6}\right)\\ \phi=\dfrac{\pi}{2}+\arctan\left(\dfrac{\frac{\sqrt{3}}{2}-\cos\vartheta}{\sin\vartheta}\right) & \text{if } \vartheta\in\left(\dfrac{11\pi}{6},2\pi\right].\end{cases}$$

The codimension of the constraint requires a discussion, due to the three different kinds of impact: the impact with $\mathcal{S}_1$, the impact with $\mathcal{S}_2$, and the impact with $\mathcal{S}_1\cap\mathcal{S}_2$.

We leave it to the reader to verify that in the first two situations the codimension of the constraint is 1 and the behavior of the system is very natural. In the third case the codimension of the constraint is 2 and Corollary 4.1 cannot be applied.

One might hope that to analyze the third case it would be enough to first consider Case 1 and then follow it by Case 2 (or vice versa). Unfortunately, the conclusion one obtains depends on the order in which we consider the cases. Consequently, the hope remains unrealized. On the contrary, the additional "minimality" requirement discussed at the end of Sec. IV A applied to the third case gives rise to a well-defined and naturally interpretable right velocity.

VI. OUTLOOKS AND WISHES

The results and techniques described in the paper to approach the study of time-dependent unilateral constraints could be (we hope…) useful tools to investigate several other aspects of Impulsive Mechanics. The most natural step in the direction traced out by the paper seems to be the study of the so-called kinetically constrained impulsive motion, i.e., the impulsive motion of a mechanical system subject to kinetic constraints, possibly of permanent or instantaneous nature. The most classical example is the billiard ball, rolling on a rough plane (and then subject to a permanent kinetic constraint) and impacting with a rough wall (and then subject to the unilateral impulsive constraint given by the wall and the instantaneous kinetic impulsive constraint due to the roughness of the wall).

Another possible application of the results of the paper is the study of impacts between different parts of the same mechanical system (or between two different systems, such as two billiard balls), and the analysis of the conservation of linear and angular momenta.

It goes without saying that the most interesting development of this geometric approach to Impulsive Mechanics consists in the study of the behavior of time-dependent systems subject to nonideal unilateral impulsive constraints. Surely, at the present time, this problem is almost totally open, but, in our opinion, a possible first step is a consistent definition of the coefficient of restitution, that, in the time-dependent case, seems to be strictly related to the concept of frame of rest of the constraint.

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The Gauss-Landau-Hall problem on Riemannian surfaces

Manuel Barros[a] and Alfonso Romero[b]
Departamento de Geometría y Topología, Facultad de Ciencias, Universidad de Granada, 18071-Granada, Spain

José L. Cabrerizo[c] and Manuel Fernández[d]
Departamento de Geometría y Topología, Facultad de Matematicas Universidad de Sevilla, 41012-Sevilla, Spain

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We introduce the notion of Gauss-Landau-Hall magnetic field on a Riemannian surface. The corresponding Landau-Hall problem is shown to be equivalent to the dynamics of a massive boson. This allows one to view that problem as a globally stated, variational one. In this framework, flowlines appear as critical points of an action with density depending on the proper acceleration. Moreover, we can study global stability of flowlines. In this equivalence, the massless particle model corresponds with a limit case obtained when the force of the Gauss-Landau-Hall magnetic field increases arbitrarily. We also obtain properties related with the completeness of flowlines for general magnetic fields. The paper also contains results relative to the Landau-Hall problem associated with a uniform magnetic field. For example, we characterize those revolution surfaces whose parallels are all normal flowlines of a uniform magnetic field. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Classically, the Landau-Hall problem consists of the motion study of a charged particle in the presence of a static magnetic field, H. In this setting, free of any electric field, a particle, of charge e and mass m, evolves with velocity v satisfying the Lorentz force law,[1]

$$\frac{\mathrm{d}P}{\mathrm{d}t} = \frac{e}{c} v \times H,$$

where c denotes the light speed, $P=(\epsilon/c^2)v$ stands for the momentum of the particle, and $\epsilon = mc^2[1-(\|v\|^2/c^2)]^{-1/2}$ is its energy. Since $\mathrm{d}P/\mathrm{d}t$ is orthogonal to P, then $(d/\mathrm{d}t)(\|P\|^2)=0$. This implies the constancy of both $\|v\|$ and ϵ. Assume H is stationary, i.e., H is a time-independent vector of the Euclidean space $\mathbb{R}^3$. With the choice of a suitable orthonormal reference system, we may assume that $H=h(0,0,1)$, for some $h \in \mathbb{R}$. In this framework, we have

$$\frac{d}{\mathrm{d}t} v_1(t) = \omega v_2(t), \quad \frac{d}{\mathrm{d}t} v_2(t) = -\omega v_1(t), \quad \frac{d}{\mathrm{d}t} v_3(t) = 0,$$

where $\omega=(ehc)/\epsilon$ is constant. Then

[a]Electronic mail: mbarros@ugr.es
[b]Electronic mail: aromero@ugr.es
[c]Author to whom correspondence should be addressed. Electronic mail: jaraiz@us.es
[d]Electronic mail: mafernan@us.es

$$x_1(t) = x_1^0 + r\sin(\omega t + \alpha), \quad x_2(t) = x_2^0 + r\cos(\omega t + \alpha), \quad x_3(t) = x_3^0 + v_3^0 t,$$

where $r = \|v\|/\omega$. In particular, if $v_3^0 = 0$, then the particle describes a circle in the plane $x_3 = x_3^0$, with center (x_1^0, x_2^0, x_3^0) and radius r. Now, in this plane we consider the 2-form F defined by $F(X,Y) = \varepsilon\langle X \times Y, H\rangle$, where $\varepsilon = \pm 1$ is the sign of h/ω. It is clear that F is covariantly constant, and therefore it is a constant multiple of the area element, indeed $F = \varepsilon h\, \mathrm{d}x_1 \wedge \mathrm{d}x_2$. Now, consider the metric g on the plane defined by $g := \varepsilon(h/\omega)g^0$, where $g^0 = \langle , \rangle$ denotes the Riemannian metric on the plane induced by the usual one of $\mathbb{R}^3$. Define the operator Φ, g-equivalent to F, by $g(\Phi(X), Y) = F(X,Y)$. Then, the Lorentz force law can be expressed in terms of this form by

$$\frac{d}{\mathrm{d}t} v(t) = \Phi(v(t)). \tag{1}$$

This approach to the classical picture can be obviously extended to a more general setting. In fact, it seems natural to define a *magnetic field* on a $n(\geqslant 2)$-dimensional Riemannian manifold (M,g), as a closed 2-form F on M. The *Lorentz force* of a magnetic background (M,g,F) is defined to be the skew-symmetric operator, Φ, given by

$$g(\Phi(X), Y) = F(X,Y), \tag{2}$$

for any couple of vector fields X, Y on M. Let us remark that Φ is metrically equivalent to F, so no information is lost when Φ is considered instead of F. In classical terminology, it is said that Φ is obtained from F by raising its second index, and Φ and F are then said to be physically equivalent. On the other hand, there exists another operator Φ' defined from F via g in a similar way, namely $g(X, \Phi'(Y)) = F(X,Y)$, but it is easily seen that $\Phi' = -\Phi$. So, the choice from among Φ or Φ' to represent F, using g, is not relevant. Along this paper, we will use Φ to denote the Lorentz force induced from (M,g,F).

A (smooth) curve γ in (M,g) is called a *flowline* of the dynamical system associated with the magnetic field F [or simply a flowline of F, or a *magnetic curve* of (M,g,F)], if its velocity vector field, γ', satisfies the following (Landau-Hall) differential equation:

$$\text{(LH)} \quad \nabla_{\gamma'} \gamma' = \Phi(\gamma'),$$

where ∇ is the Levi-Civita connection of g [compare with Eq. (1)].

For the trivial magnetic field, $F = 0$, the case without the force of a magnetic field, magnetic curves correspond with the geodesics of (M,g). As it is well known, they are nicely characterized as critical points of an energy action and so they represent the trajectories for free fall particles (moving under the influence of only gravity). In the general case, however, magnetic flows are important examples of dynamical systems on Riemannian manifolds whose flowlines, being the trajectories of charged particles in (nontrivial) magnetic fields, are not geodesics (Proposition 2.1) but, as we will see later, they are closely related with the Riemannian structure.

Nevertheless, the magnetic curves of (M,g,F) can be also viewed, at least locally, as the solutions of a variational principle. In fact, let U be an open subset of M where $F = \mathrm{d}\omega$ for some potential 1-form ω [this open subset could be the whole M when $H^2(M) = 0$]. For any two fixed points p, $q \in U$, we consider the space Γ_{pq} of smooth curves in U that connect these two points. Now, we choose the action $\mathcal{LH}: \Gamma_{pq} \to \mathbb{R}$ defined by

$$\mathcal{LH}(\gamma) = \frac{1}{2}\int_\gamma g(\gamma', \gamma')\mathrm{d}t - \int_\gamma \omega(\gamma')\mathrm{d}t. \tag{3}$$

The tangent space of Γ_{pq} in γ is made up of the smooth vector fields, V, along γ that vanish at the endpoints p, $q \in U$. A standard computation involving integration by parts allows one to compute the first variation of this action to be

$$\delta(\mathcal{LH})(\gamma)[V] = -\int_{\gamma} g(\nabla_{\gamma'}\gamma' - \Phi(\gamma'), V)\mathrm{d}t.$$

As a consequence, we get

$$\delta(\mathcal{LH})(\gamma)[V] = 0, \quad \text{for any } V \in T_{\gamma}\Gamma_{pq} \quad \text{if and only if } \gamma \text{ is a solution of (LH)}.$$

This argument shows that the differential equation (LH) is indeed the Euler-Lagrange equation associated with the functional $\mathcal{LH}$.

However, it seems natural to realize the old idea of characterizing magnetic curves from a global variational principle. In other words, to obtain the magnetic trajectories of (M,g,F) as solutions of a variational problem that neither it does not involve any local potential nor it does not constraint the topology of M. This is, in general, an interesting open problem. One of the main aims of this paper is just to solve it for certain magnetic fields on surfaces.

To be precise, we introduce the notion of a Gauss-Landau-Hall magnetic field (in brief, GMF) on an oriented Riemannian surface (M,g). First, we do it in the natural context that surfaces are immersed in Euclidean space $\mathbb{R}^3$ using the Gauss map. However, we notice that the notion of GMF is absolutely intrinsic so it can be considered on surfaces even if they are not regarded in $\mathbb{R}^3$. Then, we are able to obtain an amazing result which characterizes the normal flowlines of a GMF as the solutions of a variational principle globally stated. Therefore, those flowlines appear as critical points of an action whose Lagrangian density involves the proper acceleration of particles (relativistic particles with rigidity of order one, in the sense of Plyushchay[2,3]). *A priori*, these actions describe a massive relativistic boson. However, massless particles with arbitrary helicity are obtained as a limit case, just when the Lorentz force of the GMG increases arbitrarily.

Other details on the paper are the following. We first provide in Sec. II an analysis of the existence, uniqueness, extendibility, and completeness of the magnetic curves associated with a given (M,g,F). Section III deals with uniform magnetic fields on Riemannian surfaces, while the particular case when (M,g) is a revolution surface is studied in Sec. IV. In Sec. V, a one-parameter family $\mathcal{F}_m$ of functionals is considered on an appropriate space of curves Λ in the surface. The Euler-Lagrange equation associated to the variational problem is then obtained. In Sec. VI we define a Gauss-Landau-Hall magnetic field on a surface, first in $\mathbb{R}^3$, and then in general. In this section, we obtain the main result, Theorem 6.1, which asserts that the normal flowlines of a GMF coincide with the critical points of the appropriate functional $\mathcal{F}_m$. Stability of the field equation solutions is also studied. In Sec. VII, we show a characterization theorem for those revolution surfaces whose parallels are all normal magnetic curves associated to a GMF. We close the section studying some particular examples.

II. COMPLETENESS OF MAGNETIC CURVES AND MORE

An early property of the magnetic curves is the following conservation's law. Particles evolve with constant speed, and so constant energy, along the magnetic trajectories

$$\frac{d}{\mathrm{d}t}g(\gamma',\gamma') = 2g(\Phi(\gamma'),\gamma') = 0. \tag{4}$$

In particular, a magnetic curve γ is said to be *normal* if it has unit energy, i.e., $\|\gamma'\|^2 \equiv 1$.

The existence and uniqueness of geodesics, remains true when one considers magnetic curves. Thus, for each $p \in M$ and $v \in T_pM$ there is exactly one inextendible (i.e., maximal) magnetic curve, $\gamma:(-a,a)\to M$, of (M,g,F) with $\gamma(0)=p$ and $\gamma'(0)=v$ (see for instance Ref. 4, p. 91). Since the proof of this result does not make use of neither the definiteness of g nor the skew-symmetry of Φ, one has a *present determines the future* type result for an indefinite metric, Lorentzian in particular, and for any smooth operator. Even more, the result also works for solutions of a differential equation that extends that of Landau-Hall in the following terms:[5]

$$\nabla_{\gamma'}\gamma' = \Phi(\gamma') + X \circ \gamma,$$

where X is a vector field on a semi-Riemannian manifold. This setting includes the important case in Mechanics where $X=-\nabla V$, and V standing for smooth function on M (Ref. 6, Proposition 3.7.4).

Nevertheless, the well-known homogeneity result for geodesics, works quite different in nontrivial magnetic fields. Therefore, if γ is the inextendible magnetic curve of (M,g,F) determined from the initial data (p,v), the curve β, defined by $\beta(t)=\gamma(\lambda t)$, $\lambda \in \mathbb{R}\backslash\{0\}$, is a magnetic trajectory of $(M,g,\lambda F)$ and also, when $\lambda>0$, of $(M,(1/\lambda)g,F)$, in both cases determined from initial data $(p,\lambda v)$. Furthermore, the whole families of magnetic curves of (M,g,F) and $(M,\lambda g,\lambda F)$ coincides, for any constant $\lambda>0$. Consequently, we have the following.

Proposition 2.1: Let F be a nontrivial magnetic field on a Riemannian manifold (M,g). *Then, there exists no affine connection on M whose geodesics are the magnetic curves of* (M,g,F).

A magnetic field (M,g,F) with Lorentz force Φ, provides, in a similar way as in Ref. 7, Proposition 3.28, with a unique vector field Q_Φ on the tangent bundle TM. This is defined to have integral curves being the lifting to TM of the magnetic curves, that is, $t\mapsto(\gamma(t),\gamma'(t))$, where γ is a magnetic curve of (M,g,F) (compare with Ref. 8). Certainly this vector field is nothing but the geodesic flow when $F=0$. Once more, neither the definiteness of g nor the skew symmetry of Φ is needed to define Q_Φ.[5] On the other hand, the fact that any integral curve of Q_Φ is the velocity of its projection on M, allows us to think of Q_Φ as a nice example of the classically so-called *second order differential equation* on M. Because the comment previous to Proposition 2.1, Q_Φ is not a *spray*, in general.

A dynamical system with complete trajectories is often thought in Physics to be persisting eternally. But in many circumstances one must deal with incompleteness. So, because of its importance, we next give criteria to assert when it holds true. An important tool to study the completeness of the inextendible magnetic curves, i.e., under what assumptions all the inextendible magnetic curves are defined on all $\mathbb{R}$, is the vector field Q_Φ. By using Lemma 1.56 in Ref. 7, it is easily seen as the following result.

Proposition 2.2: Let (M,g) *be a Riemannian manifold*, F *a magnetic field on* M, *and* $\gamma:[a,b)\to M$, $a<b$, *a magnetic curve of F. The following are equivalent:*

(a) γ *is extendible to b as a magnetic curve*.
(b) *There exists a sequence* $\{t_n\}\to b$, $t_n\in[a,b)$ *such that the sequence of velocities* $\{\gamma'(t_n)\}$ *converges in TM*.

Accordingly, a magnetic curve $\gamma:(a,b)\to M$, a, $b\in\mathbb{R}$, $a<b$, of (M,g,F) can be extended to some open interval I, $(a,b)\subset I$, if and only if $\gamma(a,b)$ is contained in a compact subset of M. Therefore, we get (compare with Theorem 2.1.18 in Ref. 6) the following.

Proposition 2.3: Let γ *be an inextendible magnetic curve of* (M,g,F) *such that* $\gamma(a,b)$ *lies in a compact subset of* M, *for every finite interval* (a,b) *in its domain. Then,* γ *must be complete*.

In particular, if M is assumed to be compact, then we get that any inextendible magnetic curve of (M,g,F) must be complete. This fact can be also obtained as a consequence of Corollary 2.4, and it will be stated in Remark 2.5 (a), from a different approach.

Now, let $\gamma:[a,b)\to M$ be a magnetic curve. Its length $L(\gamma)$ satisfies $L(\gamma)\leqslant(b-a)\sqrt{e}$, where e is the (constant) energy of γ. For each $t\in[a,b)$, the distance between $\gamma(a)$ and $\gamma(t)$ satisfies $d(\gamma(a),\gamma(t))\leqslant L(\gamma|_{[a,t]})\leqslant(b-a)\sqrt{e}$, which shows that $\gamma([a,b))$ is contained in the closed metric ball B centered at $\gamma(a)$ and with radius $(b-a)\sqrt{e}$. Therefore,

$$\gamma'([a,b)) \subset \{(p,v)\in TM : p\in B,\ g(v,v)=e\} \subset TM.$$

Then, we have the following:

Corollary 2.4: Let F be any magnetic field on a geodesically complete Riemannian manifold (M,g). *Then, all the inextendible magnetic curves of* (M,g,F) *are complete*.

Proof: If (M,g) is assumed to be geodesically complete, then the Hopf-Rinow theorem implies that B must be compact. Hence $\{(p,v)\in TM : p\in B,\ g(v,v)=e\}$ is a compact subset of TM.

Take now a sequence $\{t_n\}\to b$, $t_n\in[a,b)$, then $\{\gamma'(t_n)\}$ lies in a compact subset of TM. So, by passing to a subsequence of $\{t_n\}$, we are under the assumption (b) of Proposition 2.2, concluding that γ is extendible to b as a magnetic curve.

Remark 2.5:

(a) If M is assumed to be compact [therefore (M,g) is geodesically complete for any Riemannian metric g on M], then we can give an alternative proof of Corollary 2.4. In fact, the previous conservation's law [Eq. (4)] for the length of velocity vectors of magnetic curves, implies that the vector field Q_Φ on TM can be restricted to each spherical tangent bundle $U_eM\{(p,v)\in TM: g(v,v)=e\}\subset TM$, $e>0$. But U_eM is compact whenever M is compact, and hence the restriction of Q_Φ to U_eM is a complete vector field. This proves that all the inextendible magnetic curves of F are complete.

(b) Proposition 2.1 has shown a remarkable difference between magnetic curves and geodesics. The following nonconnectness fact complements that result. Let us consider the unit 2-sphere $\mathbb{S}^2(1)$ endowed with its standard round metric g, and let F be the magnetic field $F=\mu\Omega_2$, where Ω_2 is the area 2-form and $\mu\in\mathbb{R}$, $\mu\neq 0$. As we will show later (see the comment after Proposition 3.2), the associated magnetic curves with energy e are circles on $\mathbb{S}^2(1)$ with radius $r=[1+(\mu^2/e)]^{-1/2}$. Then, as $r<1$, any two antipodal points cannot be connected by a magnetic curve of $(\mathbb{S}^2,g,F)$. Moreover, for any $p\in\mathbb{S}^2$, all the inextendible magnetic curves γ of $(\mathbb{S}^2\backslash\{-p\},g,F)$ such that $\gamma(0)=p$ are complete.

(c) Let (M,g) be a Riemannian manifold where g is an incomplete metric. If F is a magnetic field on (M,g), then there exists a pointwise conformal metric f^2g such that the inextendible magnetic curves of (M,f^2g,F) are complete. In fact, there exists $f\in C^\infty(M)$, $f>0$, such that f^2g is geodesically complete.[9] Therefore, Corollary 2.4 gives that the magnetic curves of (M,f^2g,F) are complete.

(d) It should be observed that the closedness assumption on the 2-form F in Corollary 2.4 was not used. On the other hand, the skew symmetry of the tensor field F has played a crucial role [recall the conservation's law (4)]. In fact, consider the tensor field $F=-2x\,\mathrm{d}x^2$ on the Euclidean plane $(\mathbb{R}^2,g^0=\mathrm{d}x^2+\mathrm{d}y^2)$. If Φ denotes the operator defined from F using Eq. (2), then $\Phi(\partial/\partial x)=-2x(\partial/\partial x)$ and $\Phi(\partial/\partial y)=0$. Therefore, $\gamma(t)=(x(t),y(t))$ satisfies the equation (LH) if and only if $x''(t)+2x(t)x'(t)=0$ and $y''(t)=0$. So, $\gamma(t)=(1/t,t)$ is an inextendible incomplete trajectory of $(\mathbb{R}^2,g^0,F)$.

(e) Finally, let us point out that Corollary 2.4 cannot be also extended to the indefinite case. In fact, consider $\mathbb{R}^2$ endowed with the Lorentzian metric $g_L=\mathrm{d}x^2-\mathrm{d}y^2$, and define the magnetic field $F=-x\,\mathrm{d}x\wedge\mathrm{d}y$. A curve $(x(t),y(t))$ is a magnetic curve of $(\mathbb{R}^2,g_L,F)$ if and only if it satisfies $x''(t)=x(t)y'(t)$, $y''(t)=x(t)x'(t)$. Then, $\gamma(t)=(2/t,-2/t)$ is an inextendible magnetic curve which is defined on $(0,\infty)$.

III. UNIFORM MAGNETIC FIELDS

From now on, M will be an oriented Riemannian surface with standard complex structure J, and area element Ω_2 so that $\Omega_2(X,JX)=1$ for any unit vector field X in M.

Given a curve γ in M such that $g(\gamma',\gamma')=e>0$ is constant, its Frenet apparatus is $\{T=(1/\sqrt{e})\gamma', N=JT\}$. If κ denotes the curvature function, we have the following well-known Frenet equations

$$\nabla_{\gamma'}T=\kappa\sqrt{e}N,\quad \nabla_{\gamma'}N=-\kappa\sqrt{e}T.$$

Obviously, any magnetic field on a surface, M, is determined from a smooth function, f (the *strength*), by $F=f\Omega_2$. Therefore, the matrix of Φ in any orthonormal frame, $\{X,JX\}$ is given by

$$\begin{pmatrix} 0 & -f \\ f & 0 \end{pmatrix}.$$

In particular, along a magnetic curve γ of (M,g,F), with energy e, and relative to its Frenet frame, the Lorentz force is obtained to be

$$\begin{pmatrix} 0 & -\kappa\sqrt{e} \\ \kappa\sqrt{e} & 0 \end{pmatrix}.$$

Therefore, we get the following.

Proposition 3.1: The curvature of the magnetic curves with energy e is given by $\kappa = f/\sqrt{e}$. *So, the curvature of the normal magnetics curves completely determines the Lorentz force, i.e.,* $f = \kappa$ *along these flowlines*.

A parallel magnetic field F, i.e., a magnetic field with constant strength $f = \mu$, is called a *uniform magnetic field*. This class of magnetic fields has been extensively considered in the literature from different points of view (Refs. 8 and 10–16, etc.). The geometric partner of the Landau-Hall problem, for uniform magnetic fields, is nothing but the computation of curves with constant curvature. To be precise, we have the following.

Proposition 3.2: Let $F = \mu\Omega_2$ *be a uniform magnetic field, with constant strength* μ, *on a Riemannian surface* (M,g). *A curve* γ *in* M, *with constant energy* e, *is a magnetic curve of* (M,g,F) *if and only if it has constant curvature* $\kappa = \mu/\sqrt{e}$.

On surfaces of constant Gauss curvature, the feature of the normal flowlines of a nontrivial uniform magnetic field $F = \mu\Omega_2$ is well known for any uniform magnetic field. On the Euclidean plane, $\mathbb{R}^2$, they are circles with radius $1/|\mu|$. On the 2-sphere of radius r, $\mathbb{S}^2(r)$, flowlines with energy e are circles with radius $(r\sqrt{e})/\sqrt{e + r^2\mu^2} (< r)$. In these two backgrounds, the flowlines are always closed.

On the other hand, the situation in a hyperbolic plane is quite different. Let $\mathbb{H}^2(-G)$ be the upper half-plane (in $\mathbb{R}^2$) endowed with the Lobatchevski metric of curvature $-G$, $G > 0$, that is, the Poincaré plane. We use Proposition 3.2 with the basic knowledge of the curves of constant curvature in $\mathbb{H}^2(-G)$ (see any basic text of Riemannian geometry) to make trivial the following description of the flowlines which is due to Comtet,[11] and has been mentioned along a large list of references. The behavior of normal magnetic curves changes according to the ratio between the strength, μ, and the curvature of $\mathbb{H}^2(-G)$. Namely,

(i) If $|\mu|/\sqrt{G} > 1$, then the trajectories are geodesic circles, and therefore they are closed curves.
(ii) If $|\mu|/\sqrt{G} \leqslant 1$, then the trajectories are nonclosed curves which intersect the boundary line, $\partial\mathbb{H}^2(-G)$, of the upper half-plane. In particular, they are tangent to this boundary, and so they are horocycles when $|\mu| = \sqrt{G}$.

Remark 3.3:

(a) Let γ be a curve with constant geodesic curvature $\kappa \neq 0$ in any of the three previous constant curvature surfaces. Then, for a given uniform magnetic field $F = \mu\Omega_2$, a suitable fitting of the constant speed (and hence, the energy) of γ makes this curve to be a magnetic curve of F.
(b) Let (M,g) be again one of the three above space forms and $F = \mu\Omega_2$ a uniform magnetic field on (M,g). Then, any magnetic curve γ with energy e of (M,g,F) can be then considered as a *normal* magnetic curve of $(M,(1/e)g,(1/e)F)$ (see the comment previous to Proposition 2.1).

IV. THE LANDAU-HALL PROBLEM IN A SURFACE OF REVOLUTION

Let $\alpha(s)=(f(s),h(s))$, $a<s<b$, $f(s)>0$, be a parameterization by the arclength of a curve, C, contained in the $\{xz\}$-plane of $\mathbb{R}^3$. We rotate C around the z-axis to obtain a surface of revolution, say M_α, with canonical parametrization in $\mathbb{R}^3$,

$$X(s,v)=(f(s)\cos v, f(s)\sin v, h(s)), \quad 0 \leqslant v \leqslant 2\pi. \tag{5}$$

Of course we consider that M_α is endowed with the induced metric g of the Euclidean one of $\mathbb{R}^3$.

Each point of C describes a parallel, γ_s, which can be parametrized by arclength in the following way:

$$\gamma_s(t)=\left(f(s)\cos\frac{t}{f(s)},\ f(s)\sin\frac{t}{f(s)},\ h(s)\right),$$

where $0\leqslant t\leqslant 2\pi f(s)$.

The curvature, κ_s, of γ_s in M_α, is computed to be

$$\kappa_s(t)=\|\nabla_{T_s}T_s\|=\frac{f'(s)}{f(s)},$$

where $T_s=\gamma_s'$ and ∇ is the Levi-Civita connection of M_α. In particular, κ_s is constant along γ_s, and so this curve is a good candidate to be a flowline of a suitable uniform magnetic field on M_α.

Let $F=\mu\Omega_2$ be a uniform magnetic field on M_α with constant strength μ. Then γ_s is a normal magnetic flowline of $(M_\alpha,g,F=\mu\Omega_2)$ if and only if $\kappa_s=\mu$ (Proposition 3.2). Therefore, the set of magnetic parallels of $(M_\alpha,g,F=\mu\Omega_2)$ can be identified with the following subset of the interval (a,b):

$$\Gamma_\mu=\{s\in(a,b): f'(s)=\mu f(s)\}.$$

To determine those surfaces of revolution whose parallels are all normal magnetic curves of a given uniform magnetic field [that is, those with $\Gamma_\mu=(a,b)$] we need to solve the ordinary differential equation

$$f'(s)=\mu f(s).$$

Obviously, we have two possibilities. The trivial one, corresponding with the case of a trivial magnetic field (the strength vanishes), the flowlines are then geodesics, and the surface of revolution is a right circular cylinder. Otherwise, since the Gauss curvature of a surface of revolution (in the canonical parametrization) is given by

$$G(s,t)=-\frac{f''(s)}{f(s)}, \tag{6}$$

we get that $G(s,t)=-\mu^2$, and hence the surface has constant negative curvature. In particular, we have the following.

Proposition 4.1: The parallels of a surface of revolution, M_α, are all normal magnetic flowlines of a uniform magnetic field, $F=\mu\Omega_2$, if and only if either

(1) *M_α is a right circular cylinder (when $\mu=0$), or*
(2) *M_α is a bugle surface with Gaussian curvature $-\mu^2$.*

Let us consider the torus of revolution, $\mathbf{T}(r,R)$, obtained by rotating the circle, $\mathbf{C}$, centered at $(R,0,0)$ and with radius $r(R>r)$, around the z axis. The circle can be arclength parametrized by $\alpha(s)=(R+r\cos(s/r),0,r\sin(s/r))$. Therefore, $f(s)=R+r\cos(s/r)$, with $0\leqslant s\leqslant 2\pi r$.

Given a uniform magnetic field $F=\mu\Omega_2$ on $\mathbf{T}(r,R)$, the set of normal magnetic parallels is identified to

$$\Gamma_\mu = \{s \in [0,2\pi r]: H_\mu(s) = 0\},$$

where

$$H_\mu(s) = R\mu + r\mu \cos\left(\frac{s}{r}\right) + \sin\left(\frac{s}{r}\right).$$

To study $\Gamma_\mu = H_\mu^{-1}(0)$, we use elemental calculus. First, we assume that $\mu \neq 0$, otherwise $\Gamma_0 = H_0^{-1}(0)$ is made up of the two parallels that are geodesics in $\mathbf{T}(r,R)$. In this setting, we see that H_μ has exactly two critical points on $\mathbf{C}$ (the maximum and the minimum) which are antipodal. In fact, $H'_\mu(s)=0$ if and only if $\cot(s/r)=r\mu$ and it happens just in the following two antipodal points:

$$p_\mu = \left(\cos\frac{s}{r},\ \sin\frac{s}{r}\right) = \left(\frac{r\mu}{\sqrt{1+r^2\mu^2}},\ \frac{1}{\sqrt{1+r^2\mu^2}}\right),$$

$$q_\mu = \left(\cos\frac{s}{r},\ \sin\frac{s}{r}\right) = -\left(\frac{r\mu}{\sqrt{1+r^2\mu^2}},\ \frac{1}{\sqrt{1+r^2\mu^2}}\right).$$

The values of H_μ in p_μ and q_μ are

$$H_\mu(p_\mu) = R\mu + \sqrt{1+r^2\mu^2}, \quad \text{the maximum of } H_\mu,$$

$$H_\mu(q_\mu) = R\mu - \sqrt{1+r^2\mu^2}, \quad \text{the minimum of } H_\mu.$$

We call D_μ the diameter in $\mathbf{C}$ determined by p_μ and q_μ, and let $\rho=(R^2-r^2)^{-1/2}$. We distinguish two cases.

(A) If $\mu>0$, then the point p_μ, where H_μ gets its maximum, lies in the first quadrant of the circle $\mathbf{C}$. Since $H_\mu(p_\mu)>0$, then $\Gamma_\mu \neq \emptyset$ if and only if $H_\mu(q_\mu)\leqslant 0$ (the minimum is nonpositive) that is $\mu \leqslant \rho$. Certainly if the equality holds, then H_ρ vanishes only at $q_\rho=(-r/R,-1/(\rho R))$. Otherwise, H_μ vanishes exactly in two points, say z_μ and w_μ, which are separated by D_μ so they lie in different half circles.

(B) If $\mu<0$, then the point p_μ, where H_μ gets its maximum, lies in the second quadrant of the circle $\mathbf{C}$. Since the minimum is negative, $H_\mu(q_\mu)<0$, then $\Gamma_\mu \neq \emptyset$ if and only if $H_\mu(p_\mu)\geqslant 0$ and it happens if and only if $\mu \geqslant -\rho$. It is clear that when the equality holds, then H_ρ vanishes just at $p_\rho=(-r/R,1/(\rho R))$. However, if $\mu>-\rho$, then H_μ has exactly two zeroes, say z'_μ and w'_μ, which are obviously separated by D_μ so they lie in different half circles.

All this information can be summarized in the following statement.

Proposition 4.2: Let $F=\mu\Omega_2$ be a uniform magnetic field on a torus of revolution, $\mathbf{T}(r,R)$. Then $(\mathbf{T}(r,R),g,\mu\Omega_2)$ has normal magnetic parallels if and only if $\mu \in [-\rho,\rho]$. Furthermore,

(1) *If $\mu=-\rho$, then there is one normal magnetic parallel obtained by rotating the point $(R+(r^2/R),r/(\rho R)) \in \mathbf{C}$.*
(2) *If $\mu=\rho$, then there is one normal magnetic parallel obtained by rotating the point $(R-(r^2/R),-r/(\rho R)) \in \mathbf{C}$.*
(3) *If $\mu \in (-\rho,\rho)$, then H_μ has exactly two normal magnetic parallels obtained by rotating two points of $\mathbf{C}$ that are separated by D_μ.*

Example 4.3: Let C be the cathenoid generated by revolving the cathenary curve $\alpha(t)=(\cosh t,0,t)$, $t \in \mathbb{R}$ around the z axis. Let F be a uniform magnetic field with constant strength $\mu \neq 0$, defined on C. Then, it can be shown that there exist magnetic parallels if and only if $\mu \in [-1/2,1/2]$. Moreover, we have the following.

(1) If $\mu=1/2$ (respectively, $\mu=-1/2$), there exists only a normal magnetic parallel corresponding to $t=\ln(1+\sqrt{2})$ [respectively, $t=-\ln(1+\sqrt{2})$].

(2) If $\mu \in (-1/2,0)$ [respectively, $\mu \in (0,1/2)$], then C has two normal magnetic parallels which are located in the region $t>0$ (respectively, $t<0$).

Example 4.4: Let S be the revolution surface obtained by rotating the cycloid curve $\alpha(t) = (a(1-\cos t),0,a(t-\sin t))$, $t \in (0,2\pi)$ around the z axis. It is easy to see the following.

(1) If $\mu>0$, then S has only a normal magnetic parallel corresponding to the parameter value $t_0 = 2\arccos[(-1+\sqrt{1+16a^2\mu^2})/(4a\mu)]$.
(2) If $\mu<0$, then S has also only a normal magnetic parallel corresponding to $t_1 = 2\pi - t_0$.

Example 4.5: Finally, let us consider the cone M generated by the line $\alpha(t)=(at,0,bt)$, $a^2+b^2=1$, $t>0$ around the z axis. Then, it can be seen that for any $\mu>0$, there exists a unique normal magnetic parallel given by $t=1/\mu$.

V. RELATIVISTIC PARTICLES WITH RIGIDITY OF ORDER ONE

The search for Lagrangians describing spinning particles (both massive and massless) has a long history. An interesting and unconventional approach is to provide the necessary extra degrees of freedom by actions whose densities depend on higher order geometrical invariants. In particular, this means that those extra bosonic variables must be encoded in the geometry of the world trajectories. The simplest models are those involving density Lagrangians that depend on the curvature, κ, of the worldlines (Refs. 17–19, etc.). In particular, actions that depend linearly from κ (Refs. 2 and 18–22, etc.) will be considered in this section. These models describing a massive relativistic boson.[3]

Suppose that Λ is a suitable space of curves (closed curves or clamped curves, for instance) in a Riemannian surface (M,g). Define a one-parameter family of functionals $\mathcal{F}_m: \Lambda \to \mathbb{R}$, $m \in \mathbb{R}$, by

$$\mathcal{F}_m(\gamma) = \int_\gamma (\kappa + m)\mathrm{d}s, \tag{7}$$

where s stands for the arclength parameter of curves $\gamma \in \Lambda$. In order to obtain the first variation of these actions, we use the following standard machinery (see for instance Ref. 20). For a curve $\gamma:[0,L]\to M$, we take variations $\Theta = \Theta(t,r):[0,L]\times(-\varepsilon,\varepsilon)\to M$ with $\Theta(t,0)=\gamma(t)$. Then, we have the variation vector field $W=W(t)=(\partial\Theta/\partial r)(t,0)$ along the curve γ. We also set $V=V(t,r) = (\partial\Theta/\partial t)(t,r)$, $W=W(t,r)$, $v=v(t,r)=\|V(t,r)\|$, $T=T(t,r)$, $N=N(t,r)$, with the obvious meanings. The corresponding reparametrizations will be denoted by $V(s,r)$, $W(s,r)$, etc. The variations of v and κ in γ, in the direction of W, can be obtained to be

$$W(v) = g(\nabla_T W, T)v, \tag{8}$$

$$W(\kappa) = g(\nabla_T^2, W, N) - 2g(\nabla_T, W, T)\kappa + Gg(W,N), \tag{9}$$

here G denotes the Gauss curvature of (M,g) and ∇ its Levi-Civita connection.

To obtain the first derivative of $\mathcal{F}_m$, we use (8) and (9) and proceed as follows:

$$\delta\mathcal{F}_m(\gamma)[W] = \int_\gamma W(\kappa)\mathrm{d}s + \int_0^L (\kappa+m)W(v)\mathrm{d}t = \int_\gamma W(\kappa)\mathrm{d}s + \int_\gamma (\kappa+m)g(\nabla_T W,T)\mathrm{d}s$$

$$= \int_\gamma [g(\nabla_T^2 W,N) - (\kappa-m), g(\nabla_T W,T) + Gg(W,N)]\mathrm{d}s.$$

Then, we use, as usual, suitable integrations by parts to get

$$\delta\mathcal{F}_m(\gamma)[W] = \int_\gamma g(\Omega(\gamma), W)\mathrm{d}s + [\mathcal{B}(\gamma, W)]_0^L, \tag{10}$$

where $\Omega(\gamma)$ and $\mathcal{B}(\gamma, W)$ denote the Euler-Lagrange and the boundary operators and they are, respectively, given by

$$\Omega(\gamma) = (G - m\kappa)N,$$

$$\mathcal{B}(\gamma, W) = g(\nabla_T W, N) + mg(W, T).$$

Proposition 5.1 (Clamped curves): Given points q_1, $q_2 \in M$ *and unit vectors* $x_1 \in T_{q_1}M$ *and* $x_2 \in T_{q_2}M$, *define the space of curves*

$$\Lambda = \{\gamma:[t_1, t_2] \to M: \gamma(t_i) = q_i,\ T(t_i) = x_i,\ N(t_i) = Jx_i,\ 1 \leqslant i \leqslant 2\}.$$

Then, the critical points of the functional $\mathcal{F}_m: \Lambda \to \mathbb{R}$ *are characterized by the following Euler-Lagrange equation:*

$$G|_\gamma = m\kappa,$$

where $G|_\gamma$ *denotes the Gauss curvature of* (M, g) *along* γ.

Proof: Let $\gamma \in \Lambda$ and $W \in T_\gamma\Lambda$, then W defines a curve in Λ associated with a variation Θ of γ. Since $V = \mathrm{d}\Theta(\partial_t)$ and $W = \mathrm{d}\Theta(\partial_r)$, then $[V, W] = 0$ along Θ. Furthermore, we use $V = vT$ to have

$$\nabla_T W = W(\ln v)T + \nabla_W T,$$

along Θ. We evaluate this formula along γ by making $r = 0$ and use that Θ is a curve in the space Λ to obtain

$$[\mathcal{B}(\gamma, W)]_{t_1}^{t_2} = 0.$$

Therefore, using Eq. (10), we have that γ is a critical point of $\mathcal{F}_m: \Lambda \to \mathbb{R}$, that is $\delta\mathcal{F}_m(\gamma)[W] = 0$ for any $W \in T_\gamma\Lambda$ if and only if $\Omega(\gamma) = 0$ which proves the statement.

Similarly, we can obtain the following.

Proposition 5.2 (Closed curves): Let $\mathcal{C}$ *be the space of immersed closed curves in* (M, g). *The critical points of the functional* $\mathcal{F}_m: \mathcal{C} \to \mathbb{R}$ *are those closed curves that are solutions of the following Euler-Lagrange equation:*

$$G|_\gamma = m\kappa.$$

VI. GAUSSIAN MAGNETIC FIELDS

Let M be a surface immersed in the Euclidean three-space, $\mathbb{R}^3$, so the metric, g is the induced one. We denote by $N: M \to \mathbb{S}^2$ its Gauss map and $\mathrm{d}\sigma^2$ will stand for the area element on the unit round sphere $\mathbb{S}^2$. The two form $N^*(d\sigma^2)$ on M can be used, for example, to measure areas of the spherical images or topological total charges of solitons in the $O(3)$ nonlinear sigma model (see for instance Refs. 23 and 24, and references therein). In this section we will consider magnetic fields of the type

$$F = \frac{1}{m}N^*(\mathrm{d}\sigma^2),$$

where m is a nonzero constant. We call them *Gaussian magnetic fields* (GMF). It is well known that $N^*(\mathrm{d}\sigma^2) = G\Omega_2$, G denoting the Gaussian curvature of (M, g) and this, in particular, implies that we can consider these kinds of magnetic fields with no mention to the surrounding space. Namely, a GMF is always of the type

$$F = \frac{G}{m}\Omega_2. \tag{11}$$

The Lorentz force of a GMF is computed to be $\Phi=(G/m)J$, where J is the standard complex structure in M. In particular, for any unit vector field, X, on M, the matrix of Φ, in the terminology of Sec. III, with respect to an orthonormal frame $\{X, JX\}$ is given by

$$\begin{pmatrix} 0 & -\frac{G}{m} \\ \frac{G}{m} & 0 \end{pmatrix}.$$

In this framework, we can combine Proposition 3.1 and the field equations of the particle models defined from $\mathcal{F}_m$, see Eq. (7), to obtain the following amazing relationship between the flow of a GMF and the worldline trajectories of relativistic particles with order one. To be precise, we have the following.

Theorem 6.1: *Let* $\gamma \in \Lambda$ *be a curve* (clamped or closed) *in* (M, g). *Then it is a normal flowline of* $(M, g, F=(G/m)\Omega_2)$ *if and only if it is a critical point* (worldline) *of the action* $\mathcal{F}_m : \Lambda \to \mathbb{R}$ *given by*

$$\mathcal{F}_m(\gamma) = \int_\gamma (\kappa + m)\mathrm{d}s.$$

At this point, we can take advantage of the variational approach to study stability of the GMF flowlines. Therefore, we need the second derivative of $\mathcal{F}_m$ in a critical point, say γ in a suitable space of curves, Λ (recall closed or clamped curves). After some long computations (see Ref. 17 for details) one can obtain the following expression:

$$\delta^2\mathcal{F}_m(\gamma)[W] = \int_\gamma g\,(W, \nabla_W \Psi)\big|_\gamma \,\mathrm{d}s, \tag{12}$$

where Ψ denotes the vector field, along a variation of γ, given by $\Psi=(G-m\kappa)N$. Now, we choose $W=\Phi N$ to obtain

$$g\,(W, \nabla_W \Psi)\big|_\gamma = \Phi^2 N(G - m\kappa),$$

where the right-hand term is restricted to γ. However the variation of κ was given in Eq. (9); so, in particular, we have $N(\kappa)=\kappa^2+G$. Then, one gets from Eq. (12),

$$\delta^2\mathcal{F}_m(\gamma)[W] = \int_\gamma \Phi^2\left(N(G) - \frac{1}{m}(G^2 + m^2 G)\right)\mathrm{d}s.$$

Hence, we have the following useful test of stability.

Proposition 6.2: A critical point, $\gamma \in \Lambda$, *of* $\mathcal{F}_m$ *is stable if and only if the function* $N(G) - (1/m)(G^2+m^2G)$ *is signed along* γ.

It should be observed that the previous test has the following geometrical meaning. Set $\varphi = G - m\kappa$, then $\gamma \subset \varphi^{-1}(0)$, because it is a critical point of $\mathcal{F}_m$, and then stability means that γ is made up of regular points of φ. Moreover, observe that this happens if 0 is a regular value of φ.

Now, let us use all this information in the following elemental setting. We consider $M = \mathbb{S}^2(1)$ the unit round sphere. Then any GMF, $F=(G/m)\Omega_2=(1/m)\Omega_2$, is uniform. However, when studying uniform magnetic fields on a round sphere, we cannot talk about stability of magnetic trajectories. This is not the case of our approach.

In this setting, the magnetic curves are, according to Theorem 6.1, the critical points of the functional

$$\mathcal{F}_m(\gamma) = \int_\gamma (\kappa + m)\mathrm{d}s = \int_\gamma \kappa\, \mathrm{d}s + mL(\gamma),$$

and they are nothing but those curves that satisfy $1 = m\kappa$, that is geodesic circles with geodesic curvature $\kappa = 1/m$.

On the other hand, we can use the Gauss-Bonnet formula to see that this variational problem is equivalent to that associated with the action $\mathcal{D}_m : \mathbf{D} \to \mathbb{R}$ defined by

$$\mathcal{D}_m(\Delta) = \int_\Delta G\Omega_2 + m\int_{\partial\Delta} \mathrm{d}s = \mathrm{Area}(\Delta) + mL(\partial\Delta),$$

acting on the space (D) of simply connected domains, Δ in $\mathbb{S}^2$, with the same boundary $\gamma = \partial\Delta$. This is nothing but the isoperimetric problem in the round sphere. The solution is a couple of domains Δ_1 and Δ_2 (the maximum and the minimum) with common boundary a geodesic circle, γ, of curvature $\kappa = 1/m$. Since $N(G) = 0$ then, $-(1+m^2)/m$ has obvious sign for any choice of the coupling constant m. Consequently, calling to Proposition 6.2, the solutions are stable.

The case where $m = 0$ deserves a few words. First of all GMF with $m = 0$ could be considered as a limiting case, however, after our variational approach, it can be identified with the massless Plyushchay model,[21] which is governed by the Lagrangian

$$\mathcal{F}_0(\gamma) \equiv \int_\gamma \kappa\, \mathrm{d}s.$$

This model has been considered with detail in Ref. 18. For example, the sphere does not admit, non-only minima (maxima) for this model but also critical points. However, an anchor ring has two critical points corresponding to the two parallels of parabolic points.

VII. GMF FLOWLINES ON SOME NONCONSTANT GAUSS CURVATURE SURFACES

In this section we would like to analyze when certain relevant curves on some nonconstant Gauss curvature surfaces are in fact magnetic.

We recalled the explicit expression of the Gauss curvature, $G(s,v)$, of a surface of revolution, M_α, see Eq. (6). Consequently, we can assert now that a parallel, γ_s, is a normal flowline of the GMF given by $(G/m)\Omega_2$ on M_α if and only if

$$f''(s) + mf'(s) = 0. \tag{13}$$

Next, we will obtain the surfaces of revolution whose parallels are all normal flowline of a GMF. In contrast to the case of a uniform magnetic field, where only the bugle surface appeared as a solution (see Proposition 4.1), now the general solution is made up of a three parameter family of surfaces which includes the bugle surface too.

Theorem 7.1: *The normal flow of a GMF,* $(G/m)\Omega_2$, *in a surface of revolution,* M_α, *is invariant under rotations if and only if the profile curve of* M_α *lies in the following three parameter family of arclength parametrized plane curves:*

$$\alpha(s) = \left(f(s), \int_0^s \sqrt{1 - f'(s)^2}\, \mathrm{d}s \right),$$

where

$$f(s) = \frac{1}{m}[a + c\exp(-ms + b)], \quad a,b,c \in \mathbb{R} \text{ with } a > 0.$$

Observe that the general solution of the ordinary differential equation (13) has the form $f(s)=[a+c\exp(-ms+b)]/m$, so the proof of the last result becomes obvious. Observe also that the above characterized class of surfaces of revolution includes the bugle surface ($a=0$) and the right circular cylinder ($c=0$) too.

It should be noticed the following coupling phenomenon in a surface of revolution, M_α, between the GMF, $F_1=(G/m)\Omega_2$ and the uniform magnetic field $F_2=-m\Omega_2$, for some values of the coupling constant m. Suppose, for example, that $M_\alpha=\mathbf{T}(r,R)$ is a torus of revolution and $\rho=(R^2-r^2)^{-1/2}$ (notation as in Sec. IV). Then, F_1 always has two parallels being normal magnetic curves, no matter the value of m. Now, we use Proposition 4.2 to obtain the following statement.

Proposition 7.2: If $-m\in(-\rho,\rho)$, then both F_1 and F_2 have two normal magnetic parallels coming from points alternatively placed in the profile circle. Moreover they collapse when $-m$ goes to $-\rho$ or ρ.

Proof: For any value of m in $\mathbb{R}$, $(\mathbf{T}(r,R),g,F_1)$ has two normal magnetic parallels obtained by rotation of the two antipodal points in $\mathbf{C}$, defined by $\cot(s/r)=-rm$. These two points are just those determining the diameter D_{-m} that separates the two magnetic parallel of $(\mathbf{T}(r,R),g,F_2)$ when $-m\in(-\rho,\rho)$. The second part of this statement follows similarly when we use points 1 and 2 of Proposition 4.2.

We finish the paper showing several examples.

Example 7.3: Let $\beta(s)$ be an arclength parametrized curve contained in a plane, Π (with unit normal vector B_0), in $\mathbb{R}^3$. We denote by $\{T(s),N(s)\}$ a Frenet frame along $\beta(s)$, so that $T(s)\wedge N(s)=B_0$, and $\kappa(s)$ will stand for its curvature function. For a suitable $r>0$, we define a tube of radius r, say $T_\beta(r)$, as the surface given by

$$X(s,v)=\beta(s)+r(\cos(v)N(s)+\sin(v)B_0).$$

We denote by $\Lambda_\beta=\{\gamma_v,:v\in[0,2\pi]\}$ the family of curves in the tube obtained when we make v constant. The curvature of these curves in $T_\beta(r)$ can be obtained, from a direct computation, to be

$$\kappa_v(s)=\frac{\kappa(s)\sin(v)}{1-r\kappa(s)\cos(v)}.$$

Notice that it is not constant unless $\beta(s)$ is chosen to be constant curvature.

On the other hand, the Gauss curvature of the tube $T_\beta(r)$ is computed to be

$$G(s,v)=-\frac{\kappa(s)\cos(v)}{r(1-r\kappa(s)\cos(s))}.$$

Now, we can apply these formulas together with the Euler-Lagrange equations associated with the GMF, $F=(G/m)\Omega_2$ (Propositions 5.1 and 5.2), to see that there exist exactly two curves (clamped or closed) in Λ_β that are normal magnetic trajectories. They are obtained for $\cot(v)=-rm$ and this is, formally, the same result that we have obtained for a torus of revolution (Proposition 4.2) which can be regarded as a tube around a circle.

Example 7.4: Similarly, for a curve, $\beta(s)$, in $\mathbb{R}^3$ with Frenet frame $\{T(s),N(s),B(s)\}$, curvature $\kappa(s)$ and torsion $\tau(s)$, one can define the tube $T_\beta(r)$ by

$$X(s,v)=\beta(s)+r(\cos(v)N(s)+\sin(v)B(s)).$$

In particular, if $\beta(s)$ is a helix (κ and τ are both constant) then the curvature function, $\kappa_v(s)$ of the curves in $\Lambda_\beta=\{\gamma_v,:v\in[0,2\pi]\}$ satisfy

$$\kappa_v^2=\frac{\kappa^2\sin^2(v)}{(1-r\kappa\cos(v))^2+r^2\tau^2}.$$

Now, the curves in Λ_β that are normal flowlines of $(G/m)\Omega_2$ on the helicoidal tube $T_\beta(r)$ correspond with the zeroes of the function $\vartheta:\mathbb{S}^1\to\mathbb{R}$ defined by

$$\vartheta(v) = (1 - r\kappa\cos(v))^2(\cos^2(v) - r^2m^2\sin^2(v)) + r^2\tau^2\cos^2(v).$$

However, we have

$$\vartheta(0) = \vartheta(\pi) = (1 - r\kappa)^2 + r^2\tau^2 > 0 \quad \text{and} \quad \vartheta\left(\frac{\pi}{2}\right) = \vartheta\left(\frac{3\pi}{2}\right) = -r^2m^2 < 0.$$

Therefore, there exist four curves of Λ_β in the flow of $(G/m)\Omega_2$.

Example 7.5: On the cathenoid (Example 4.3), the GMF given by $(G/m)\Omega_2$ has a unique normal magnetic parallel for all m. If $m>0$, it is obtained for a $t_0<0$. If $m<0$, then it is obtained for a $t_0'=-t_0>0$.

Example 7.6: On the hyperboloid of revolution obtained from Eq. (5) by setting $f(t)=\cosh t$ and $h(t)=\sinh t$, the GMF given by $(G/m)\Omega_2$ has also a unique normal magnetic parallel for all m, analogously to the previous case.

Example 7.7: On the cicloidal surface (Example 4.4), the GMF given by $(G/m)\Omega_2$ has a unique normal magnetic parallel for $m\in(-\infty,-1/(4a))\cup(1/(4a),\infty)$. If $m>0$, $t_0=\arccos((1/(4am))$, whereas if $m<0$, then $t_0'=2\pi-t_0$.

VIII. CONCLUSIONS

Oriented surfaces, M, in $\mathbb{R}^3$ admit two natural 2-forms. First, the area element, Ω_2, associated with the induced metric, g. Second, the area element, $N^*(\mathrm{d}\sigma^2)$, of its spherical image under the Gauss map, $N:M\to\mathbb{S}^2$. It is well known that these 2-forms are nicely related by

$$N^*(\mathrm{d}\sigma^2) = G\Omega_2,$$

where G denotes the Gaussian curvature of g. In particular, both 2-forms are intrinsic and then they are defined once we know a Riemannian metric, g, on M. Associated with these 2-forms appear two classes of magnetic fields on (M,g).

(1) The class made up of the constant multiples of the former one, $\mathcal{C}_1=\{\mu\Omega_2:\mu\in\mathbb{R}\}$, provides that of uniform magnetic fields, with strength μ, on (M,g). The corresponding Landau-Hall problem has been widely studied along the literature. Even in this paper, we have obtained some new information relative to uniform magnetic field essentially in a surface of revolution. For example, we have characterized right circular cylinders and bugle surfaces as the only surfaces of revolution whose parallels are all normal magnetic flowlines of uniform magnetic fields.

(2) The class of the constant multiples of the latter one, $\mathcal{C}_2=\{\mu N^*(\mathrm{d}\sigma_2):\mu\in\mathbb{R}\}$, constitutes a class of magnetic fields that in this paper are introduced under the terminology of Gauss-Landau-Hall magnetic fields. In this case the strength is given by μG and obviously both classes coincide when (M,g) has constant curvature.

In this paper, we wish to state the importance and nice interest of GMF on surfaces. In fact, the chief result of the paper appears when we study the Landau-Hall problem associated with a GMF (which we call the Gauss-Landau-Hall problem). Then, we are able to show that this problem is equivalent to the dynamics of a massive relativistic boson. This provides an amazing relationship between two, *a priori*, quite different physical phenomena.

Therefore, we can use two points of view to study each of the two involved problems. On the one hand, one can study completeness, homogeneity and so on, in the dynamical study of bosonic worldlines. By the way, we have introduced a section with results on these topics. But on the other hand, the Gauss-Landau-Hall problem can be regarded as a variational problem globally stated. In this setting, flowlines are critical points of an action which has been used to model relativistic particles with order one rigidity. In particular, we can talk about, and so we study, global stability of normal flowlines of a GMF. Say finally that under this equivalence, the model to describe a massless particle with arbitrary helicity corresponds with a limit case obtained when the force of the GMF increases arbitrarily.

We believe that this point of view in the study of GMF is physically remarkable and it could be extended to other classes of magnetic fields.

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Fluid-dynamic equations for granular particles in a host medium

M. Bisi and G. Spiga[a)]
Dipartimento di Matematica, Università di Parma, Parco Area delle Scienze 53/A, 43100 Parma, Italy

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A kinetic model for a granular gas interacting with a given background by binary dissipative collisions is analyzed, with particular reference to the derivation of macroscopic equations for the fundamental observables. Particles are modelled as inelastic hard spheres under the assumption of collision dominated regime (small mean free path). Closure of the relevant moment equations is achieved by resorting to a maximum entropy principle, and two specific entropy functionals have been worked out in detail, in the class of the admissible ones for the relevant linear extended Boltzmann equation. Considered macroscopic fields include density, mass velocity, and granular temperature. In the hydrodynamic limit when the mean free path tends to zero, a single drift-diffusion equation of Navier-Stokes type is recovered for the only hydrodynamic variable of the physical problem. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2118468]

I. INTRODUCTION

In the last few years, kinetic models for granular materials have attracted significant interest in the mathematical and physical communities.[13,8] The largest attention has been devoted to nonlinear models for dilute flows based on generalizations of the Boltzmann-Enskog equation describing energy dissipation in binary encounters. Most of the analytic investigation has been performed in the frame of the so-called pseudo-Maxwellian inelastic particles,[6] both in the free case in which granular temperature decays to zero, and in the driven case in which there is an external energy supply. Some results are available also for the more realistic, but much more difficult to deal with, inelastic hard sphere model.[7]

Very important for practical applications are also linear kinetic equations for dissipative interactions of dilute granular matter with a given background, though this kind of inelastic process has been much less addressed. The relevant physical problem may be considered as limiting case of a binary mixture made up by species with different masses and densities, and describes typically the diffusion of fine polluting powders in a much denser medium (like air).

Though grains are in principle macroscopic objects, and their interaction with background molecules is a complex process that would require an adequate treatment,[23] we shall stick here to the standard approximation of extremely tiny grains undergoing localized and instantaneous mechanical encounters with a single partner. Collision integrals in the kinetic equation describe then binary interactions of a test particle of the granular gas with a field particle of the fixed background. The most significant recent results, together with the general existence and stability analysis by Pettersson,[24] concern the unique determination of collision equilibria as Maxwellian distributions, with number density as the only free parameter, whereas mass velocity coincides with the background drift, and granular temperature is smaller than the temperature of the host medium, with a reduction factor depending on the crucial control parameters, namely mass ratio and coefficient of inelasticity.[21,25,1,19] It has also been possible to prove[19] an essential ingredient of

[a)]Electronic mail: giampiero.spiga@unipr.it

any kinetic-type approach, namely a space homogeneous H-theorem, in terms of an entire class of different possible entropy functionals, each of them being determined by a suitable convex function, as indeed typical in linear kinetic theory.[20]

On the other hand, what people are interested in for practical applications is mainly availability of consistently derived and justified macroscopic equations for the observable fields, moments of the distribution function. Peculiar feature of the linear Boltzmann equation, both elastic and inelastic, is that there exists only one collision invariant, and consequently only one hydrodynamic variable (number density). With respect to the nonlinear case of rarefied gas dynamics, "conservation" equations for momentum and energy become balance equations, with nonvanishing collision contributions describing exchange rates with the background. Hydrodynamic closure at the Navier-Stokes level may be still achieved by a Chapman-Enskog asymptotic expansion in the collision dominated regime, and results in a single drift-diffusion equation for density, available already also in the inelastic frame,[25] but only, to our knowledge, for the simplified pseudo-Maxwellian model.[6] However, it would be obviously desirable to include also drift velocity and temperature as unknown fields into the macroscopic equations, though they are not conserved quantities, as they would be in the nonlinear case. Such equations should then be regarded as moment equations for higher order moments, and would play a role similar to that of Grad's equations[16] of gas dynamics,[10,17] where the additional nonhydrodynamic moments are instead viscous stress tensor and heat flux vector. To our knowledge, first numerical results in this respect have been worked out, and not yet published, in very recent times.[12] This is the problem that will be dealt with in the present paper, by resorting to a suitable expansion technique in a neighborhood of the collision equilibrium. We consider in fact a hard sphere granular gas, inelastically scattering with a given background, and with a mean free path much smaller than the macroscopic scale. The investigation will be developed in the spirit of the maximum entropy principle (MEP)[18,22,15] as moment closure strategy. In addition, using the Knudsen number (ratio of the mean free path to the macroscopic length) as small parameter, a standard Chapman-Enskog algorithm allows to achieve in the simplest way the pertinent hard-sphere diffusive hydrodynamic equation with first order corrections (thus, at the Navier-Stokes level).

The paper is organized as follows. The governing kinetic Boltzmann-type equation and its main features are presented and discussed in Sec. II, where also previous results needed in the subsequent investigation are recalled. Then, the existence of an infinite number of admissible entropy functionals implies of course an ample choice of disparate normal form expansions satisfying a MEP to be used for closing the exact nonclosed set of moment equations. For the sake of simplicity, in this work we shall confine ourselves to the consideration of the most important moments, the first five (density, the three components of mass velocity, and temperature), though additional fields, like the viscous stress tensor (completing the second order moments), could be treated with only technical extra difficulties. Also, only two (the most common) entropy functionals will be worked out, the quadratic entropy, probably the simplest one, in Sec. III, and the very popular logarithmic entropy in Sec. IV. The resulting closed moment equations differ of course from each other, though exhibiting a common structure. Other macroscopic equations would follow of course from other functionals. Such indeterminacy is obvious consequence of the existence, in the linear framework, of an infinite set of entropies, as mentioned above. Clearly, an immediate question arises: which of the closed sets of partial differential equations gives the best approximations with respect to the kinetic results? A detailed comparative analysis, including numerical calculations, is scheduled as future work. However, the relevant hydrodynamic equations in the asymptotic limit coincide exactly up to the first order corrections. Of course, this is not surprising, since Navier-Stokes equations could be determined, independently from any chosen entropy, by the Chapman-Enskog algorithm applied directly to the kinetic equation. Unfortunately we have not been able to prove yet a universality result in this respect, namely that the hydrodynamic limit of the closed set of moment equations is the same for any admissible entropy functional, and this also will be the matter of further studies. When needed, manipulations whose length and heaviness could compromise presentation and clarity are shifted to the Appendix.

II. KINETIC EQUATION

We start from the linear dissipative Boltzmann equation for granular test particles (tp) subjected to hard-sphere collisions against the field particles (fp) of a fixed (in general, nonuniform) background, labelled by a superscript B in the following notation. The host medium is supposed in local thermodynamical equilibrium with given density n^B, drift velocity $\mathbf{u}^B$, and temperature T^B, thus with a Maxwellian distribution function $f^B=n^BM^B$, where $M^B=M(\mathbf{v};m^B,\mathbf{u}^B,T^B)$ and M is a normalized Gaussian. Symbols m and d are used to denote particle mass and diameter, and (tp,tp) interactions are negligible. All (binary) (tp,fp) encounters, with ingoing velocities $(\mathbf{v},\mathbf{w})$, preserve momentum but dissipate kinetic energy of the relative motion according to the rule (a prime denotes post-collision values)

$$\mathbf{g}'\cdot\hat{\mathbf{n}}=-e(\mathbf{g}\cdot\hat{\mathbf{n}}),\quad \mathbf{g}'-(\mathbf{g}'\cdot\hat{\mathbf{n}})\hat{\mathbf{n}}=\mathbf{g}-(\mathbf{g}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}}, \tag{1}$$

where $\mathbf{g}=\mathbf{v}-\mathbf{w}$ is the relative velocity, $\hat{\mathbf{n}}$ the unit vector of the apse line, and e, with $0<e\leqslant 1$, is the so-called restitution coefficient (supposed to be constant in this paper), which measures the amount of inelasticity. As is well known, test particles exchange momentum and energy with the background even in the elastic case $e=1$. The collision mechanism and the apse line determine uniquely the post-collision velocities associated to $\mathbf{v}$ and $\mathbf{w}$ as

$$\mathbf{v}'=\mathbf{v}-2\alpha(1-\beta)(\mathbf{g}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}},\quad \mathbf{w}'=\mathbf{w}+2(1-\alpha)(1-\beta)(\mathbf{g}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}}, \tag{2}$$

where the dimensionless parameters α and β, with $0<\alpha<1$, $0\leqslant\beta<\frac{1}{2}$, are defined as

$$\alpha=\frac{m^B}{m+m^B},\quad \beta=\frac{1-e}{2} \tag{3}$$

and represent, respectively, mass ratio and degree of inelasticity. Dissipation implies that the dual collision associated to $(\mathbf{v},\mathbf{w})$ (i.e., the one which produces $\mathbf{v}$ and $\mathbf{w}$ as final output) may not be obtained starting from $(\mathbf{v}',\mathbf{w}')$, and in fact the precollision velocities associated to $\mathbf{v}$ and $\mathbf{w}$ turn out to be

$$\mathbf{v}''=\mathbf{v}-2\alpha\frac{1-\beta}{1-2\beta}(\mathbf{g}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}},\quad \mathbf{w}''=\mathbf{w}+2(1-\alpha)\frac{1-\beta}{1-2\beta}(\mathbf{g}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}}. \tag{4}$$

A standard phase-space balance, under the usual assumptions underlying the Boltzmann equation, leads to the linear integro-differential equation

$$\frac{\partial f}{\partial t}+\mathbf{v}\cdot\nabla_{\mathbf{x}}f=n^B\left(\frac{d+d^B}{2}\right)^2\int_{\mathbb{R}^3}\int_{S_+^2}(\mathbf{g}\cdot\hat{\mathbf{n}})\left[\frac{1}{e^2}f(\mathbf{v}'')M^B(\mathbf{w}'')-f(\mathbf{v})M^B(\mathbf{w})\right]d_3\mathbf{w}d_2\hat{\mathbf{n}}, \tag{5}$$

where explicit dependence on $\mathbf{x}$ and t is not shown just for simplicity, and S_+^2 is the positive unit sphere, defined by $\mathbf{g}\cdot\hat{\mathbf{n}}>0$. As usual, it is convenient to introduce suitable scalings and make (5) dimensionless. Assuming the Strouhal number of order unity, and measuring distances in units of a characteristic length L, if $\bar{n}^B$ denotes a typical value of background density, manipulations single out in a spontaneous way the mean free path

$$\lambda=\left[\bar{n}^B\pi\left(\frac{d+d^B}{2}\right)^2\right]^{-1} \tag{6}$$

and the Knudsen number

$$Kn=\frac{\lambda}{L}\equiv\varepsilon, \tag{7}$$

where the symbol ε is used as a reminder of the fact that we are mainly interested here in the continuum limit $Kn\ll 1$, in which the process is dominated by collisions. If the same dimensional

symbol is retained for all scaled quantities, the kinetic equation may be rewritten as

$$\frac{\partial f}{\partial t}+\mathbf{v}\cdot\nabla_{\mathbf{x}}f=\frac{n^B}{2\pi\varepsilon}\int_{\mathbb{R}^3}\int_{S^2}|\mathbf{g}\cdot\hat{\mathbf{n}}|\left[\frac{1}{e^2}f(\mathbf{v}'')M^B(\mathbf{w}'')-f(\mathbf{v})M^B(\mathbf{w})\right]d_3\mathbf{w}d_2\hat{\mathbf{n}}=\frac{n^B}{\varepsilon}Q(f), \tag{8}$$

where ε labels the importance of the collision integral, n^B may be set equal to unity for a homogeneous steady background, and

$$M^B(\mathbf{v})=\left(\frac{m^B}{2\pi T^B}\right)^{3/2}\exp\left[-\frac{m^B}{2T^B}(\mathbf{v}-\mathbf{u}^B)^2\right]. \tag{9}$$

The macroscopic parameters n^B, $\mathbf{u}^B$, T^B fulfill the classical Euler equations valid in local thermodynamical equilibrium,[9]

$$\frac{\partial n^B}{\partial t}+\frac{\partial(n^Bu_k^B)}{\partial x_k}=0,$$

$$\frac{\partial u_i^B}{\partial t}+u_k^B\frac{\partial u_i^B}{\partial x_k}=-\frac{1}{n^Bm^B}\frac{\partial(n^BT^B)}{\partial x_i}, \tag{10}$$

$$\frac{\partial T^B}{\partial t}+u_k^B\frac{\partial T^B}{\partial x_k}=-\frac{2}{3}T^B\frac{\partial u_k^B}{\partial x_k}.$$

The most convenient tool of investigation is the weak form associated to (8). Taken any smooth test function $\varphi=\varphi(\mathbf{v})$, if $\langle\cdot,\cdot\rangle$ denotes the usual dual product with respect to the kinetic variable $\mathbf{v}$, under standard smoothness assumptions we may write

$$\frac{\partial}{\partial t}\langle\varphi,f\rangle+\nabla_{\mathbf{x}}\cdot\langle\mathbf{v}\varphi,f\rangle=\frac{n^B}{\varepsilon}\langle\varphi,Q(f)\rangle \tag{11}$$

with

$$\langle\varphi,Q(f)\rangle=\frac{1}{2\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{S^2}|\mathbf{g}\cdot\hat{\mathbf{n}}|f(\mathbf{v})M^B(\mathbf{w})[\varphi(\mathbf{v}')-\varphi(\mathbf{v})]d_3\mathbf{v}d_3\mathbf{w}d_2\hat{\mathbf{n}}. \tag{12}$$

This expression of the weak form of the collision operator, where the effects of collisions are accounted for only by the test function evaluated at the post-collision velocity $\mathbf{v}'$, is crucial for future developments. It is easy to see that $\varphi(\mathbf{v})=1$ is the only collision invariant, and thus density n is the only conserved quantity. Moreover, macroscopic fields in which we are interested are simply amenable to the first power moments of f, namely

$$n=\langle 1,f\rangle=\int_{\mathbb{R}^3}f(\mathbf{v})d_3\mathbf{v},$$

$$n\mathbf{u}=\langle\mathbf{v},f\rangle=\int_{\mathbb{R}^3}\mathbf{v}f(\mathbf{v})d_3\mathbf{v},$$

$$n\left(u^2+\frac{3T}{m}\right)=\langle v^2,f\rangle=\int_{\mathbb{R}^3}v^2f(\mathbf{v})d_3\mathbf{v}, \tag{13}$$

hence transport equations for the first five moments of the distribution function are nothing but the specialization of (11) to $\varphi=1,\mathbf{v},v^2$. Unfortunately, power moments of $Q(f)$ are not amenable to

the corresponding power moments of f, as it would occur for pseudo-Maxwellian molecules,[6,25] and not even to higher order moments. More precisely, collision contributions (12) relevant to the weights $\varphi=\mathbf{v},v^2$ involve the differences:

$$\begin{aligned}\mathbf{v}'-\mathbf{v}&=-2\alpha(1-\beta)(\mathbf{g}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}},\\ (v')^2-v^2&=-4\alpha(1-\beta)(\mathbf{g}\cdot\hat{\mathbf{n}})(\mathbf{v}\cdot\hat{\mathbf{n}})+4\alpha^2(1-\beta)^2(\mathbf{g}\cdot\hat{\mathbf{n}})^2.\end{aligned} \tag{14}$$

They exhibit simple dependencies on the unit vector $\hat{\mathbf{n}}$, so that the required angular integrations may be performed explicitly as

$$\begin{aligned}\int_{S^2}|\mathbf{g}\cdot\hat{\mathbf{n}}|(\mathbf{g}\cdot\hat{\mathbf{n}})^2d_2\hat{\mathbf{n}}&=\pi g^3,\\ \int_{S^2}|\mathbf{g}\cdot\hat{\mathbf{n}}|(\mathbf{g}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}}d_2\hat{\mathbf{n}}&=\pi g\mathbf{g},\end{aligned} \tag{15}$$

where $g=|\mathbf{g}|$. By collecting such results, the macroscopic equations for the first five moments may be finally cast, in indicial notation, as

$$\frac{\partial n}{\partial t}+\frac{\partial}{\partial x_k}(nu_k)=0,$$

$$\begin{aligned}&\frac{\partial}{\partial t}(nu_i)+\frac{\partial}{\partial x_k}\left(nu_ku_i+\frac{P_{ki}}{m}\right)\\ &\quad=-\frac{n^B}{\varepsilon}\alpha(1-\beta)\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}gg_if(\mathbf{v})M^B(\mathbf{w})d_3\mathbf{v}d_3\mathbf{w},\ i=1,2,3,\end{aligned}$$

$$\begin{aligned}&\frac{\partial}{\partial t}\left(nu^2+\frac{3nT}{m}\right)+\frac{\partial}{\partial x_k}\left[u_k\left(nu^2+\frac{3nT}{m}\right)+\frac{2}{m}P_{kj}u_j+\frac{2}{m}q_k\right]=-\frac{n^B}{\varepsilon}2\alpha(1-\beta)\\ &\quad\times\left[\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}gg_iv_if(\mathbf{v})M^B(\mathbf{w})d_3\mathbf{v}d_3\mathbf{w}-\alpha(1-\beta)\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}g^3f(\mathbf{v})M^B(\mathbf{w})d_3\mathbf{v}d_3\mathbf{w}\right],\end{aligned} \tag{16}$$

where $\mathbf{P}$ is the pressure tensor, and $\mathbf{q}$ the heat flux. As anticipated, only the first, the continuity equation, represents a conservation law, and the complete set is not closed because of the presence of viscous stress $p_{ij}=P_{ij}-nT\delta_{ij}$ and heat flux q_i in the streaming terms, and because of the three collision integrals on the right-hand sides, describing exchange of momentum and energy with the background. They are affected by the inelasticity parameter β, but would be nonzero even in the elastic case $\beta=0$. For future convenience, macroscopic equations (16) can be rewritten in convective form, by taking into account in each equation the ones relevant to lower moments, in order to single out exactly the time derivatives of $n,\mathbf{u},T$,

$$\frac{\partial n}{\partial t}+\frac{\partial}{\partial x_k}(nu_k)=0,$$

$$n\frac{\partial u_i}{\partial t}+nu_k\frac{\partial u_i}{\partial x_k}+\frac{1}{m}\frac{\partial nT}{\partial x_i}+\frac{1}{m}\frac{\partial p_{ij}}{\partial x_j}=-\frac{n^B}{\varepsilon}\alpha(1-\beta)\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}gg_if(\mathbf{v})M^B(\mathbf{w})d_3\mathbf{v}d_3\mathbf{w},$$

$$n\frac{\partial T}{\partial t}+nu_k\frac{\partial T}{\partial x_k}+\frac{2}{3}nT\frac{\partial u_k}{\partial x_k}+\frac{2}{3}p_{hk}\frac{\partial u_h}{\partial x_k}+\frac{2}{3}\frac{\partial q_k}{\partial x_k}$$
$$=-\frac{n^B}{\varepsilon}\alpha(1-\beta)\frac{2}{3}m\left\{\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}gg_i(v_i-u_i)f(\mathbf{v})M^B(\mathbf{w})d_3\mathbf{v}d_3\mathbf{w}\right.$$
$$\left.-\alpha(1-\beta)\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}g^3f(\mathbf{v})M^B(\mathbf{w})d_3\mathbf{v}d_3\mathbf{w}\right\}. \tag{17}$$

Concerning well posedness of the mathematical problem, existence and uniqueness have been established in general in Ref. 24. In order to proceed further towards closed macroscopic equations, two important theorems, that we quote from the literature, mainly from Ref. 19, are essential. More precisely we will resort to the following result, which extends to hard-sphere collisions a theorem already established for the pseudo-Maxwellian model.[25]

Theorem 1: *The Maxwellian distribution*

$$M^*(\mathbf{v})=M(\mathbf{v};m,\mathbf{u}^B,T^*)=\left(\frac{m}{2\pi T^*}\right)^{3/2}\exp\left[-\frac{m}{2T^*}(\mathbf{v}-\mathbf{u}^B)^2\right] \tag{18}$$

with temperature

$$T^*=\frac{(1-\alpha)(1-\beta)}{1-\alpha(1-\beta)}T^B \tag{19}$$

is collision equilibrium for (8), i.e., $f=nM^*$ solves the integral equation $Q(f)(\mathbf{v})=0$, $\forall\mathbf{v}\in\mathbb{R}^3$.

The proof goes through a clever exploitation of the Fourier transformed collision operator Q and of Bobylev's lemma,[5] and quantifies the fact that the granular gas is in equilibrium under collisions if, irrespective of density, it has a Gaussian distribution at the background velocity and at a suitable temperature ranging in the interval $(0,T^B)$. Such temperature T^* is determined by the control parameters α and β, as a balance of the competing processes of energy dissipation (driving granular temperature to 0) and of energy exchange with the medium by scattering (driving granular temperature to T^B). The other result is the H-theorem appropriate in this context.

Theorem 2: *Take the space-homogeneous version of (8). Let $\phi:\mathbb{R}^+\to\mathbb{R}$ be any convex C^1 function and define the functional*

$$H_\phi(f)=\int_{\mathbb{R}^3}M^*(\mathbf{v})\phi\left[\frac{f(\mathbf{v})}{M^*(\mathbf{v})}\right]d_3\mathbf{v}. \tag{20}$$

Consider the initial value problem in a stationary background, with initial datum f_0 such that $H_\phi(f_0)<\infty$, and let $f(\mathbf{v},t)$ be its (unique) solution, necessarily with constant number density $n(t)=n_0$. Then $H_\phi(f)$ is a Lyapunov functional, in the sense that

(a) $H_\phi(f)>H_\phi(n_0M^*)$ *for* $f\neq n_0M^*$,

(b) $\frac{d}{dt}H_\phi(f(t))\leqslant 0$, $\forall t\geqslant 0$.

The proof resorts to suitable applications and generalizations of typical convexity arguments. A simple corollary is that n_0M^* is the unique stationary solution of the considered initial value problem, and the whole theorem implies, as discussed in Ref. 19, that the overall effect of collisions is pushing the shape of test particle distribution function towards the normal distribution M^* defined by (18) and (19). This will strongly affect of course the hydrodynamic description of the space-dependent problem (8) in the continuum limit, since collisions are the dominant process governing evolution in such a regime.

In the next sections we shall deal with the closure problem and the asymptotic limit for the moment equations (17) on the basis of the previously established collision equilibria and entropy functionals.

III. QUADRATIC ENTROPY

The simplest choice in (20) to get a Lyapunov functional is of course $\phi(z)=z^2/2$, and its opposite provides then a suitable entropy for the MEP. Since our approximate distribution function $\bar{f}$ must reproduce the actual density, velocity, and temperature fields, we introduce Lagrange multipliers and apply the variational principle to

$$U_q(f) = -\frac{1}{2}\int_{\mathbb{R}^3} \frac{f(\mathbf{v})^2}{M^*(\mathbf{v})} d_3\mathbf{v} + \lambda_1\left(\int_{\mathbb{R}^3} f(\mathbf{v}) d_3\mathbf{v} - n\right) + \boldsymbol{\lambda_2}\cdot\left(\int_{\mathbb{R}^3} \mathbf{v} f(\mathbf{v}) d_3\mathbf{v} - n\mathbf{u}\right) + \lambda_3\left(\int_{\mathbb{R}^3} v^2 f(\mathbf{v}) d_3\mathbf{v} - nu^2 - \frac{3nT}{m}\right). \tag{21}$$

Standard manipulations yield then

$$\bar{f}(\mathbf{v}) = M^*(\mathbf{v})(\lambda_1 + \boldsymbol{\lambda_2}\cdot\mathbf{v} + \lambda_3 v^2), \tag{22}$$

where the Lagrange multipliers are uniquely determined in terms of $n, \mathbf{u}, T$ by the constraints

$$\langle 1, \bar{f}\rangle = n, \quad \langle \mathbf{v}, \bar{f}\rangle = n\mathbf{u}, \quad \langle v^2, \bar{f}\rangle = nu^2 + \frac{3nT}{m}. \tag{23}$$

It is now only a matter of some algebra to obtain

$$\lambda_1 = n - \frac{m}{T^*} n(\mathbf{u}-\mathbf{u}^B)\cdot\mathbf{u}^B + \frac{m^2}{6(T^*)^2} n\left[(\mathbf{u}-\mathbf{u}^B)^2 + \frac{3(T-T^*)}{m}\right]\left((u^B)^2 - \frac{3T^*}{m}\right),$$

$$\boldsymbol{\lambda_2} = \frac{m}{T^*} n(\mathbf{u}-\mathbf{u}^B) - \frac{m^2}{3(T^*)^2} n\mathbf{u}^B\left[(\mathbf{u}-\mathbf{u}^B)^2 + \frac{3(T-T^*)}{m}\right],$$

$$\lambda_3 = \frac{m^2}{6(T^*)^2} n\left[(\mathbf{u}-\mathbf{u}^B)^2 + \frac{3(T-T^*)}{m}\right], \tag{24}$$

so that we end up with

$$\bar{f}(\mathbf{v}) = nM^*(\mathbf{v})\left\{1 + \frac{m}{T^*}(\mathbf{u}-\mathbf{u}^B)\cdot(\mathbf{v}-\mathbf{u}^B) + \frac{m}{3T^*}\left[(\mathbf{u}-\mathbf{u}^B)^2 + \frac{3(T-T^*)}{m}\right]\left[\frac{m}{2T^*}(\mathbf{v}-\mathbf{u}^B)^2 - \frac{3}{2}\right]\right\}. \tag{25}$$

As for Grad's 13-moments expansion, this polynomial correction to the collision equilibrium does not fulfill positivity, but may be considered as a complete polynomial expansion truncated after few addends, where correction terms are small in the considered hydrodynamic regime, since, out of initial and boundary layers, $\mathbf{u}$ and T are close to their equilibrium values $\mathbf{u}^B$ and T^*. Now, as regards the streaming contributions to (17), higher order moments can be computed easily by using (25) in their definitions

$$\mathbf{P} = m\int_{\mathbb{R}^3} (\mathbf{v}-\mathbf{u})\otimes(\mathbf{v}-\mathbf{u}) f(\mathbf{v}) d_3\mathbf{v}, \quad \mathbf{q} = \frac{1}{2} m\int_{\mathbb{R}^3} |\mathbf{v}-\mathbf{u}|^2 (\mathbf{v}-\mathbf{u}) f(\mathbf{v}) d_3\mathbf{v}. \tag{26}$$

It turns out convenient to translate the integration variable $\mathbf{v}-\mathbf{u}^B \to \mathbf{v}$, so that, neglecting the terms whose integration vanishes simply by parity arguments, the pressure tensor corresponding to $\bar{f}$ is provided by

$$\begin{aligned} P_{ij} = mn\left(\frac{m}{2\pi T^*}\right)^{3/2} \Bigg\{ & \left[1 - \frac{1}{2T^*}[m(\mathbf{u}-\mathbf{u}^B)^2 + 3(T-T^*)]\right] \int_{\mathbb{R}^3} [v_i v_j + (u_i - u_i^B)(u_j - u_j^B)] \\ & \times \exp\left[-\frac{m}{2T^*} v^2\right] d_3\mathbf{v} - \frac{m}{T^*}(u_h - u_h^B) \int_{\mathbb{R}^3} [(u_i - u_i^B) v_j v_h + (u_j - u_j^B) v_i v_h] \exp\left[-\frac{m}{2T^*} v^2\right] d_3\mathbf{v} \\ & + \frac{m}{6(T^*)^2}[m(\mathbf{u}-\mathbf{u}^B)^2 + 3(T-T^*)] \int_{\mathbb{R}^3} [v^2 v_i v_j + v^2 (u_i - u_i^B)(u_j - u_j^B)] \exp\left[-\frac{m}{2T^*} v^2\right] d_3\mathbf{v} \Bigg\}. \end{aligned}$$

By resorting now to the Gaussian integrals (A1) reported in the Appendix, we get

$$P_{ij} = nT\delta_{ij} - \rho\left[(u_i - u_i^B)(u_j - u_j^B) - \tfrac{1}{3}\delta_{ij}|\mathbf{u}-\mathbf{u}^B|^2\right], \tag{27}$$

where $\rho = mn$ denotes mass density and δ is the Kronecker symbol. Analogous computations allow the evaluation of the heat flux vector, which results in

$$q_i = n(u_i - u_i^B)\left[\tfrac{1}{6} m|\mathbf{u}-\mathbf{u}^B|^2 - \tfrac{5}{2}(T-T^*)\right]. \tag{28}$$

As remarked in the preceding section, the scattering contributions appearing on the right-hand sides of (17) are in general not directly amenable to macroscopic fields. However, with the particular assumption (25) for the distribution function, all collision integrals may be solved explicitly, and we shall end up with a closed set of five (approximated) macroscopic evolution equations. More precisely, in (17) we must evaluate three integrals of the form

$$n^B \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \Phi(\mathbf{g},\mathbf{G}) \bar{f}(\mathbf{v}) M^B(\mathbf{w}) d_3\mathbf{v} d_3\mathbf{w}, \tag{29}$$

where $\mathbf{g} = \mathbf{v}-\mathbf{w}$ is the relative velocity, while $\mathbf{G} = (1-\alpha)\mathbf{v} + \alpha\mathbf{w}$ represents the center of mass velocity. Let us perform again the usual translation $\mathbf{v}-\mathbf{u}^B \to \mathbf{v}$, $\mathbf{w}-\mathbf{u}^B \to \mathbf{w}$; consequently, the integral (29) becomes

$$\begin{aligned} & \frac{nn^B}{(2\pi)^3}\left(\frac{mm^B}{T^* T^B}\right)^{3/2} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \hat{\Phi}(\mathbf{g},\mathbf{G}) \exp\left[-\frac{m}{2T^*} v^2\right] \exp\left[-\frac{m^B}{2T^B} w^2\right] \\ & \times \left\{1 + \frac{m}{T^*}(\mathbf{u}-\mathbf{u}^B)\cdot\mathbf{v} + [m(\mathbf{u}-\mathbf{u}^B)^2 + 3(T-T^*)]\left[\frac{m}{6(T^*)^2} v^2 - \frac{1}{2T^*}\right]\right\} d_3\mathbf{v} d_3\mathbf{w}, \end{aligned} \tag{30}$$

and the three functions $\hat{\Phi}$ involved in our macroscopic equations are $\hat{\Phi}(\mathbf{g},\mathbf{G}) = g g_i, g^3, g g_i (G_i + \alpha g_i - (u_i - u_i^B))$. At this point, it seems convenient to use $(\mathbf{g},\mathbf{G})$ as integration variables; bearing in mind also the relation (19) between T^* and T^B we have

$$\begin{aligned} & \exp\left[-\frac{m}{2T^*} v^2\right] \exp\left[-\frac{m^B}{2T^B} w^2\right] \\ & \quad = \exp\left\{-\frac{m}{2T^*}\frac{1}{1-\alpha(1-\beta)}[G^2 + \alpha(\alpha\beta + (1-\alpha)(1-\beta)) g^2 + 2\alpha\beta \mathbf{G}\cdot\mathbf{g}]\right\}. \end{aligned} \tag{31}$$

Since a little algebra yields

$$G^2+\alpha[\alpha\beta+(1-\alpha)(1-\beta)]g^2+2\alpha\beta\mathbf{G}\cdot\mathbf{g}=(\mathbf{G}+\alpha\beta\mathbf{g})^2+\alpha(1-\beta)[1-\alpha(1-\beta)]g^2,$$

setting $\tilde{\mathbf{g}}=\mathbf{g}$ and $\tilde{\mathbf{G}}=\mathbf{G}+\alpha\beta\mathbf{g}$ the integral (30) can be finally cast as

$$\begin{aligned}&\frac{nn^B}{(2\pi)^3}\left(\frac{mm^B}{T^*T^B}\right)^{3/2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\tilde{\Phi}(\tilde{\mathbf{g}},\tilde{\mathbf{G}})\exp\left[-\frac{m}{2T^*}\frac{1}{1-\alpha(1-\beta)}\tilde{G}^2\right]\exp\left[-\frac{m}{2T^*}\alpha(1-\beta)\tilde{g}^2\right]\\&\quad\times\left\{1+\frac{m}{T^*}(\mathbf{u}-\mathbf{u}^B)\cdot[\tilde{\mathbf{G}}+\alpha(1-\beta)\tilde{\mathbf{g}}]+[m(\mathbf{u}-\mathbf{u}^B)^2+3(T-T^*)]\right.\\&\quad\left.\times\left[\frac{m}{6(T^*)^2}[\tilde{\mathbf{G}}+\alpha(1-\beta)\tilde{\mathbf{g}}]^2-\frac{1}{2T^*}\right]\right\}d_3\tilde{\mathbf{G}}d_3\tilde{\mathbf{g}}.\end{aligned}\tag{32}$$

Now we can make it explicit for the three weight functions $\tilde{\Phi}$ appearing in our collision contributions. For $\tilde{\Phi}(\tilde{\mathbf{g}},\tilde{\mathbf{G}})=\tilde{g}\tilde{g}_i$, the unique term in (32) that provides a nonvanishing result is

$$\begin{aligned}&\frac{nn^B}{(2\pi)^3}\left(\frac{mm^B}{T^*T^B}\right)^{3/2}\frac{m}{T^*}\alpha(1-\beta)(u_h-u_h^B)\\&\quad\times\int_{\mathbb{R}^3}\tilde{g}\tilde{g}_i\tilde{g}_h\exp\left[-\frac{m}{2T^*}\alpha(1-\beta)\tilde{g}^2\right]d_3\tilde{\mathbf{g}}\int_{\mathbb{R}^3}\exp\left[-\frac{m}{2T^*}\frac{1}{1-\alpha(1-\beta)}\tilde{G}^2\right]d_3\tilde{\mathbf{G}}.\end{aligned}$$

By resorting to the integrals (A2) reported in the Appendix we get

$$n^B\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}gg_i\bar{f}(\mathbf{v})M^B(\mathbf{w})d_3\mathbf{v}d_3\mathbf{w}=\frac{1}{\sqrt{\alpha(1-\beta)}}\frac{8}{3}nn^B\sqrt{\frac{2T^*}{m\pi}}(u_i-u_i^B),\tag{33}$$

that shows a linear dependence on the macroscopic unknown fields n and $\mathbf{u}$. Analogous computations lead to the evaluation of the contributions relevant to $\tilde{\Phi}(\tilde{\mathbf{g}},\tilde{\mathbf{G}})=\tilde{g}^3$ and $\tilde{\Phi}(\tilde{\mathbf{g}},\tilde{\mathbf{G}})=\tilde{g}\tilde{g}_i[\tilde{G}_i+\alpha(1-\beta)\tilde{g}_i-(u_i-u_i^B)]$. Skipping further technical details, they finally result in

$$\begin{aligned}n^B\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}g^3\bar{f}(\mathbf{v})M^B(\mathbf{w})d_3\mathbf{v}d_3\mathbf{w}&=\left[\frac{1}{\alpha(1-\beta)}\right]^{3/2}\frac{4}{m}nn^B\sqrt{\frac{2T^*}{m\pi}}\\&\quad\times\{2T^*+\alpha(1-\beta)[m(\mathbf{u}-\mathbf{u}^B)^2+3(T-T^*)]\},\end{aligned}\tag{34}$$

$$\begin{aligned}n^B\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}g\mathbf{g}\cdot(\mathbf{v}-\mathbf{u})\bar{f}(\mathbf{v})M^B(\mathbf{w})d_3\mathbf{v}d_3\mathbf{w}&=\sqrt{\frac{1}{\alpha(1-\beta)}}\frac{8}{m}nn^B\sqrt{\frac{2T^*}{m\pi}}\\&\quad\times\left\{T+\frac{1}{6}\alpha(1-\beta)[m(\mathbf{u}-\mathbf{u}^B)^2+3(T-T^*)]\right\},\end{aligned}\tag{35}$$

presenting both a linear dependence on the variables n, T and a quadratic dependence on the velocity $\mathbf{u}$.

In conclusion, by inserting the results (27), (28), and (33)–(35) into the macroscopic equations (17) we obtain the following closed set of evolution equations:

$$\frac{\partial n}{\partial t}+\frac{\partial}{\partial x_k}(nu_k)=0,$$

$$n\frac{\partial u_i}{\partial t}+nu_k\frac{\partial u_i}{\partial x_k}+\frac{1}{m}\frac{\partial}{\partial x_i}(nT)+\frac{1}{3}\frac{\partial}{\partial x_i}[n(\mathbf{u}-\mathbf{u}^B)^2]-\frac{\partial}{\partial x_k}[n(u_i-u_i^B)(u_k-u_k^B)]$$
$$=-\frac{1}{\varepsilon}\sqrt{\alpha(1-\beta)}\frac{8}{3}nn^B\sqrt{\frac{2T^*}{m\pi}}(u_i-u_i^B),\quad i=1,2,3,$$

$$n\frac{\partial T}{\partial t}+nu_k\frac{\partial T}{\partial x_k}+\frac{2}{3}nT\frac{\partial u_k}{\partial x_k}+\frac{2}{9}nm(\mathbf{u}-\mathbf{u}^B)^2\frac{\partial u_k}{\partial x_k}-\frac{2}{3}nm(u_h-u_h^B)(u_k-u_k^B)\frac{\partial u_h}{\partial x_k}$$
$$+\frac{1}{9}m\frac{\partial}{\partial x_k}[n(u_k-u_k^B)(\mathbf{u}-\mathbf{u}^B)^2]-\frac{5}{3}\frac{\partial}{\partial x_k}[n(u_k-u_k^B)(T-T^*)]$$
$$=-\frac{1}{\varepsilon}\sqrt{\alpha(1-\beta)}\frac{16}{3}nn^B\sqrt{\frac{2T^*}{m\pi}}\left\{[1-\alpha(1-\beta)](T-T^*)-\frac{1}{3}\alpha(1-\beta)m(\mathbf{u}-\mathbf{u}^B)^2\right\}. \quad (36)$$

They are five equations for the fundamental moments $n,\mathbf{u},T$ appearing in the expression of $\bar{f}$. The option $\beta=0$ corresponds to elastically scattering hard spheres: as anticipated above, even in this particular frame collision contributions do not vanish. As for classical Grad's equations,[14,2] the macroscopic system (36) is of course approximated, since in the whole procedure the distribution function f has been replaced by the truncated polynomial expansion $\bar{f}$, but it provides a "robust" approximation of the evolution, in the sense that the right-hand sides of (36) are vanishing if and only if $\mathbf{u}=\mathbf{u}^B$ and $T=T^*$, which reproduce the macroscopic moments of the Maxwellian equilibrium M^*. In space homogeneous conditions the equilibrium $(\mathbf{u}^B,T^*)$ is asymptotically stable, and the relaxation to the equilibrium values is as fast as the convergence of the distribution function towards M^*. It is easily checked in fact that eigenvalues of the relevant Jacobian matrix are all negative, and that the asymptotic trend is exponential with relaxation times of order ε for both $\mathbf{u}$ and T.[26] This behavior differs from other nonconservative kinetic frames, for instance chemical reacting mixtures,[2] in which the distribution evolves very rapidly towards a local Maxwellian, whose macroscopic parameters reach more slowly the corresponding equilibrium values. Indeed, we can even show that the dynamical system originated by (36) in space homogeneous conditions admits a Lyapunov function (finite dimensional entropy), proving convergence to equilibrium $(n_0,\mathbf{u}^B,T^*)$ from any initial datum $(n_0,\mathbf{u}_0,T_0)$. With $n=\text{constant}=n_0$ it is sufficient in fact to consider, for the evolution of $\mathbf{u}$ and T by effects of collisions, the function

$$V_q(\mathbf{u},T)=\frac{m}{T^*}(\mathbf{u}-\mathbf{u}^B)^2+\frac{1}{6}\left[\frac{m}{T^*}(\mathbf{u}-\mathbf{u}^B)^2+3\frac{T-T^*}{T^*}\right]^2. \quad (37)$$

It is immediately seen that V_q is positive definite with respect to $\mathbf{u}=\mathbf{u}^B$ and $T=T^*$, and some simple algebra provides its time derivative along solutions

$$\dot{V}_q(\mathbf{u},T)=\nabla_{\mathbf{u}}V_q\cdot\dot{\mathbf{u}}+\frac{\partial V_q}{\partial T}\dot{T}=-\frac{16}{3}\frac{\sqrt{\alpha(1-\beta)}}{\varepsilon}n^B\sqrt{\frac{2T^*}{\pi m}}$$
$$\times\left\{\frac{m}{T^*}(\mathbf{u}-\mathbf{u}^B)^2+\frac{1-\alpha(1-\beta)}{3}\left[\frac{m}{T^*}(\mathbf{u}-\mathbf{u}^B)^2+3\frac{T-T^*}{T^*}\right]^2\right\}. \quad (38)$$

This function is everywhere nonpositive, and vanishes only when both its nonpositive addends vanish, which leads again to the unique point $(\mathbf{u}^B,T^*)$. Therefore $\dot{V}_q$ is negative definite and Lyapunov's theorem is proved.

In order to achieve a hydrodynamic equation at the Navier-Stokes level for the unique hydrodynamic variable n, we shall perform an asymptotic analysis of Chapman-Enskog type to the system (36), following the main steps outlined in Refs. 9 and 11 and already applied in Refs. 3 and 4 in different (dissipative) physical contexts. The small parameter is the Knudsen number *Kn*

$\equiv \varepsilon$, that appears in the kinetic equation (5) as a consequence of the adimensionalization. As already pointed out in the literature,[17] it is not necessary to apply the classical Chapman-Enskog procedure directly to the kinetic level, expanding f in powers of ε and determining the relevant coefficients, since we already have a polynomial expansion $\bar{f}$ for f, hence the corresponding macroscopic system (36) may be considered as a useful intermediate step between the kinetic and the hydrodynamic level. Keeping unexpanded n, the field corresponding to the unique collision invariant, we expand the other macroscopic variables in powers of ε,

$$\mathbf{u} = \boldsymbol{\nu}^0 + \varepsilon \boldsymbol{\nu}^1, \quad T = \Upsilon^0 + \varepsilon \Upsilon^1, \tag{39}$$

and we insert these expansions into the equations (36). Neglecting $O(\varepsilon^2)$ terms, the continuity equation becomes

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_k}(n\nu_k^0) + \varepsilon \frac{\partial}{\partial x_k}(n\nu_k^1) = 0. \tag{40}$$

To close this equation, we must determine the first two coefficients of the expansion of $\mathbf{u}$. Going on in the asymptotic analysis of (36), from the evolution law for $\mathbf{u}$ the leading order ($O(\varepsilon^{-1})$) terms provide the equality

$$-\sqrt{\alpha(1-\beta)}\frac{8}{3} n n^B \sqrt{\frac{2T^*}{m\pi}}(\nu_i^0 - u_i^B) = 0 \quad \forall\, i, \tag{41}$$

hence

$$\boldsymbol{\nu}^0 = \mathbf{u}^B. \tag{42}$$

Then, taking into account this result, equating the coefficients of the power ε^0 we get

$$\nu_i^1 = -\frac{1}{\sqrt{\alpha(1-\beta)}} \frac{3}{8nn^B} \sqrt{\frac{m\pi}{2T^*}} \left[n \frac{\partial u_i^B}{\partial t} + n u_k^B \frac{\partial u_i^B}{\partial x_k} + \frac{1}{m} \frac{\partial}{\partial x_i}(n\Upsilon^0) \right] \quad \forall\, i. \tag{43}$$

Therefore the determination of the coefficient $\boldsymbol{\nu}^1$ requires also the evaluation of Υ^0. Leading terms of the equation for temperature in (36) give

$$-\sqrt{\alpha(1-\beta)}[1-\alpha(1-\beta)]\frac{16}{3} n n^B \sqrt{\frac{2T^*}{m\pi}}(\Upsilon^0 - T^*) = 0, \tag{44}$$

that yields immediately

$$\Upsilon^0 = T^*. \tag{45}$$

Finally, bearing in mind that the host medium fulfills the Euler equations (10), the mass velocity of granular test particles turns out to be, up to $O(\varepsilon)$ accuracy,

$$\mathbf{u} = \mathbf{u}^B - \varepsilon \frac{1}{\sqrt{\alpha(1-\beta)}} \frac{3}{8n^B} \sqrt{\frac{m\pi}{2T^*}} \left[\frac{1}{nm} \nabla_{\mathbf{x}}(nT^*) - \frac{1}{n^B m^B} \nabla_{\mathbf{x}}(n^B T^B) \right]. \tag{46}$$

By inserting this expression into the continuity equation (40), we find the hydrodynamic "Navier-Stokes" equation for the number density of hard spheres inelastically (elastically only for $\beta = 0$) colliding with a fixed background

$$\frac{\partial n}{\partial t} + \nabla_{\mathbf{x}} \cdot (n\mathbf{u}^B) = \varepsilon \frac{3}{8} \sqrt{\frac{m\pi}{2}} \nabla_{\mathbf{x}} \cdot \left\{ \frac{1}{n^B \sqrt{T^* \alpha(1-\beta)}} \left[\frac{1}{m} \nabla_{\mathbf{x}}(nT^*) - \frac{n}{n^B m^B} \nabla_{\mathbf{x}}(n^B T^B) \right] \right\}. \tag{47}$$

The time evolution of n involves spatial derivatives (up to the second order) of n itself, together with gradients of the known (but in general nonconstant) background macroscopic fields

$n^B, \mathbf{u}^B, T^B$. Equation (47) is of "drift-diffusion" type, the convective term depends on the mean velocity of the host medium, while the diffusive part involves the two (different) kinetic temperatures T^* (equilibrium temperature) and T^B.

In the particular case of spatially homogeneous background, if in the adimensionalization we assume n^B as typical density, then (46) simplifies to

$$\mathbf{u} = \mathbf{u}^B - \varepsilon \frac{1}{\sqrt{\alpha(1-\beta)}} \frac{3}{8n} \sqrt{\frac{\pi T^*}{2m}} \nabla_{\mathbf{x}} n, \tag{48}$$

while the drift-diffusion equation (47) becomes

$$\frac{\partial n}{\partial t} + \mathbf{u}^B \cdot \nabla_{\mathbf{x}} n = \varepsilon \frac{3}{8} \sqrt{\frac{\pi}{2m}} \sqrt{\frac{T^*}{\alpha(1-\beta)}} \nabla_{\mathbf{x}}^2 n. \tag{49}$$

The main difference with respect to the corresponding hydrodynamic equation relevant to pseudo-Maxwellian particles, derived in detail in Ref. 25, is the factor $\sqrt{T^*/\alpha(1-\beta)}$ instead of $T^*/\alpha(1-\beta)$, as typical for the temperature dependence of transport coefficients relevant to the two different collision models.[11]

Finally, it is worth to remark that considering $O(1)$ terms of the temperature equation in (36), and recalling again Euler equations (10), we get

$$\Upsilon^1 = 0, \tag{50}$$

hence the granular temperature T in the hydrodynamic description coincides with its equilibrium value T^* apart from $O(\varepsilon^2)$ corrections.

In low inelasticity regimes, with the inelasticity parameter β of the same order of magnitude as the Knudsen number ($\beta = \gamma\varepsilon$), the hydrodynamic diffusive equation (47) does not contain any more inelastic corrections, that would appear only at the Burnett level, namely to the second order accuracy.

IV. LOGARITHMIC ENTROPY

The most popular choice in kinetic theory to get a Lyapunov functional out of (20) is $\phi(z) = z \log z$, from which the familiar relative entropy of the linear framework follows. Again, taking into account the same constraints of the preceding section, the variational principle in order to enforce the MEP closure concerns the functional

$$U_l(f) = -\int_{\mathbb{R}^3} f(\mathbf{v}) \log \frac{f(\mathbf{v})}{M^*(\mathbf{v})} d_3\mathbf{v} + \lambda_1 \left(\int_{\mathbb{R}^3} f(\mathbf{v}) d_3\mathbf{v} - n \right) + \boldsymbol{\lambda_2} \cdot \left(\int_{\mathbb{R}^3} \mathbf{v} f(\mathbf{v}) d_3\mathbf{v} - n\mathbf{u} \right)$$
$$+ \lambda_3 \left(\int_{\mathbb{R}^3} v^2 f(\mathbf{v}) d_3\mathbf{v} - nu^2 - \frac{3nT}{m} \right). \tag{51}$$

Now manipulations lead to an approximate distribution $\tilde{f}$ of the form ($\lambda_1 - 1 \to \lambda_1$),

$$\tilde{f}(\mathbf{v}) = M^*(\mathbf{v}) \exp(\lambda_1 + \boldsymbol{\lambda_2} \cdot \mathbf{v} + \lambda_3 v^2), \tag{52}$$

so that one immediately realizes that the requirement of recovering from $\tilde{f}$ the exact fundamental fields amounts simply to

$$\tilde{f}(\mathbf{v}) = n \left(\frac{m}{2\pi T} \right)^{3/2} \exp\left[-\frac{m}{2T} (\mathbf{v} - \mathbf{u})^2 \right] = n M_{\mathrm{loc}}(\mathbf{v}), \tag{53}$$

where by $M_{\mathrm{loc}}(\mathbf{v}) = M(\mathbf{v}; m, \mathbf{u}, T)$ we denote the well-known local Maxwellian associated to the distribution function f. This entropy leads then to a 5-moments closure in terms of the local Maxwellian. The exponential form of (52) implies also positivity for the approximate normal form

distribution (53). It remains a perturbation of collision equilibrium when $\mathbf{u}$ and T are close to $\mathbf{u}^B$ and T^*, as in the physical situation we are interested in. Immediate implication of the Maxwellian shape is then that viscous stress and heat flux vanish, so that (27) and (28) may be simply replaced by

$$P_{ij} = nT\delta_{ij}, \quad q_i = 0. \tag{54}$$

As concerns the scattering contributions, we consider at first the general form

$$n^B \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \Phi(\mathbf{g},\mathbf{G}) \tilde{f}(\mathbf{v}) M^B(\mathbf{w}) d_3\mathbf{v} d_3\mathbf{w}, \tag{55}$$

specializing then the function Φ to the ones appearing in (17). Unlike the corresponding integral (29) of the preceding section, now the two integration variables are not affected by the same translation in the exponentials, since the mean value of the Gaussian function $\tilde{f}$ is the granular drift velocity $\mathbf{u}$ instead of the background velocity $\mathbf{u}^B$. It is again convenient to resort to the change of variables $(\mathbf{v},\mathbf{w}) \to (\mathbf{G},\mathbf{g})$, providing

$$\frac{nn^B}{(2\pi)^3}\left(\frac{mm^B}{TT^B}\right)^{3/2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \Phi(\mathbf{g},\mathbf{G}) \exp\left[-\frac{m}{2T}(\mathbf{G}+\alpha\mathbf{g}-\mathbf{u})^2\right]$$
$$\times \exp\left[-\frac{m^B}{2T^B}(\mathbf{G}-(1-\alpha)\mathbf{g}-\mathbf{u}^B)^2\right] d_3\mathbf{G} d_3\mathbf{g}. \tag{56}$$

Setting now

$$\mathbf{s} = a(\mathbf{G}+\alpha\mathbf{g}-\mathbf{u}) + b(\mathbf{u}-\mathbf{u}^B-\mathbf{g}), \tag{57}$$

where

$$a = \sqrt{\frac{mT^B + m^B T}{TT^B}} \text{ and } b = \frac{m^B}{T^B}\sqrt{\frac{TT^B}{mT^B + m^B T}},$$

simple manipulations show that the integral (56) takes the form

$$\frac{nn^B}{(2\pi)^3}\left[\frac{\alpha m}{(1-\alpha)T^B + \alpha T}\right]^{3/2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \tilde{\Phi}(\mathbf{g},\mathbf{s}) \exp\left(-\frac{1}{2}s^2\right)$$
$$\times \exp\left[-\frac{1}{2}\frac{\alpha m}{(1-\alpha)T^B + \alpha T}(\mathbf{g}+\mathbf{u}^B-\mathbf{u})^2\right] d_3\mathbf{g} d_3\mathbf{s}. \tag{58}$$

At this point, the contributions corresponding to the weight functions $\tilde{\Phi}(\mathbf{g},\mathbf{s}) = gg_i, g^3$ can be easily made explicit by using the integrals (A3a) and (A3b), respectively, getting

$$n^B \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} gg_i \tilde{f}(\mathbf{v}) M^B(\mathbf{w}) d_3\mathbf{v} d_3\mathbf{w} = nn^B \frac{4}{3}\sqrt{\frac{2}{\pi}}\sqrt{\frac{\alpha m}{(1-\alpha)T^B + \alpha T}}\left[2\frac{(1-\alpha)T^B + \alpha T}{\alpha m} + \frac{1}{5}(\mathbf{u}-\mathbf{u}^B)^2\right]$$
$$\times (u_i - u_i^B), \tag{59}$$

$$n^B \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} g^3 \tilde{f}(\mathbf{v}) M^B(\mathbf{w}) d_3\mathbf{v} d_3\mathbf{w} = nn^B \frac{1}{5}\sqrt{\frac{2}{\pi}}\sqrt{\frac{\alpha m}{(1-\alpha)T^B + \alpha T}}\left\{(\mathbf{u}-\mathbf{u}^B)^4 + 20\frac{(1-\alpha)T^B + \alpha T}{\alpha m}(\mathbf{u}\right.$$
$$\left. - \mathbf{u}^B)^2 + 40\left[\frac{(1-\alpha)T^B + \alpha T}{\alpha m}\right]^2\right\}. \tag{60}$$

Similar computations allow to evaluate the other collision term in the evolution equation (17) for

granular temperature: its weight function can be rearranged in terms of the variables $(\mathbf{g},\mathbf{s})$ as

$$\tilde{\Phi}(\mathbf{g},\mathbf{s}) = g\mathbf{g}\cdot\left\{\frac{1}{a}\mathbf{s}+\frac{b}{a}[\mathbf{g}-(\mathbf{u}-\mathbf{u}^B)]\right\},$$

so that by resorting again to (A3a) and (A3b) it finally results in

$$\begin{aligned} n^B\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} g\mathbf{g}\cdot(\mathbf{v}-\mathbf{u})\tilde{f}(\mathbf{v})M^B(\mathbf{w})d_3\mathbf{v}d_3\mathbf{w} \\ = nn^B\sqrt{\frac{2\alpha m}{\pi}}\frac{\alpha T}{[(1-\alpha)T^B+\alpha T]^{3/2}} \\ \times\left\{-\frac{1}{15}(\mathbf{u}-\mathbf{u}^B)^4+\frac{4}{3}\frac{(1-\alpha)T^B+\alpha T}{\alpha m}(\mathbf{u}-\mathbf{u}^B)^2+8\left[\frac{(1-\alpha)T^B+\alpha T}{\alpha m}\right]^2\right\}. \end{aligned} \tag{61}$$

All integrals (59)–(61) depend, obviously, on $n,\mathbf{u},T$, in particular, they present a polynomial dependence on the drift velocity $\mathbf{u}$, which may be cast in terms of the scaled variable $\alpha m(\mathbf{u}-\mathbf{u}^B)^2/((1-\alpha)T^B+\alpha T)$.

By inserting the results (54) and (59)–(61) into the equations (17), we find the following closed set of balance laws for the macroscopic fields $n,\mathbf{u},T$:

$$\frac{\partial n}{\partial t}+\frac{\partial}{\partial x_k}(nu_k)=0,$$

$$\begin{aligned} n\frac{\partial u_i}{\partial t}+nu_k\frac{\partial u_i}{\partial x_k}+\frac{1}{m}\frac{\partial}{\partial x_i}(nT) = -\frac{\alpha(1-\beta)}{\varepsilon}\frac{4}{3}nn^B\sqrt{\frac{2}{\pi}}\sqrt{\frac{\alpha m}{(1-\alpha)T^B+\alpha T}} \\ \times\left[\frac{1}{5}(\mathbf{u}-\mathbf{u}^B)^2+2\frac{(1-\alpha)T^B+\alpha T}{\alpha m}\right](u_i-u_i^B), \quad i=1,2,3, \end{aligned} \tag{62}$$

$$\begin{aligned} n\frac{\partial T}{\partial t}+nu_k\frac{\partial T}{\partial x_k}+\frac{2}{3}nT\frac{\partial u_k}{\partial x_k} = \frac{\alpha(1-\beta)}{\varepsilon}\frac{2}{3}mnn^B\sqrt{\frac{2}{\pi}}\sqrt{\frac{\alpha m}{(1-\alpha)T^B+\alpha T}} \\ \times\left\{\frac{1}{5}\left[\alpha(1-\beta)+\frac{1}{3}\frac{\alpha T}{(1-\alpha)T^B+\alpha T}\right](\mathbf{u}-\mathbf{u}^B)^4+4\frac{(1-\alpha)T^B+\alpha T}{\alpha m}\right. \\ \times\left[\alpha(1-\beta)-\frac{1}{3}\frac{\alpha T}{(1-\alpha)T^B+\alpha T}\right](\mathbf{u}-\mathbf{u}^B)^2+8\left[\frac{(1-\alpha)T^B+\alpha T}{\alpha m}\right]^2 \\ \left.\times\left[\alpha(1-\beta)-\frac{\alpha T}{(1-\alpha)T^B+\alpha T}\right]\right\}. \end{aligned}$$

Like (36), this system is in general not exact, since it has been achieved assuming that during the evolution the granular medium is accomodated at a local thermodynamical equilibrium (LTE) configuration. Notice that (62) is more difficult than (36) to be studied analytically, since collision contributions depend on $\mathbf{u}$ and T in a more complicated fashion. In space homogeneous conditions, collision equilibria of equations (62) reproduce the results of the kinetic level, namely $\mathbf{u}=\mathbf{u}^B$ and $T=T^*$, as in the preceding section. Again this is a good indication of robustness, and also shows that equilibrium can be reached through LTE states. In fact, convergence to the equilibrium $(\mathbf{u}^B,T^*)$ from any initial point $(\mathbf{u}_0,T_0)$ in the space homogeneous case can be proved again by means of Lyapunov's theorem. As a tentative entropy we may select $H[\tilde{f}]$, which, upon discarding inessential constants, turns out to be

$$V_l(\mathbf{u},T)=\frac{m}{2T^*}(\mathbf{u}-\mathbf{u}^B)^2+\frac{3}{2}\frac{T-T^*}{T^*}-\frac{3}{2}\log\frac{T}{T^*}. \tag{63}$$

It is clearly positive definite with respect to $\mathbf{u}=\mathbf{u}^B$ and $T=T^*$ as sum of two separate positive definite functions of a single variable. The computation of time derivative along trajectories $\dot{V}_l=\nabla_{\mathbf{u}}V_l\cdot\dot{\mathbf{u}}+(\partial V_l/\partial T)\dot{T}$ requires some patient manipulations, due to the heavy structure of the right-hand sides of equations (62). A careful rearrangement yields

$$\dot{V}_l(\mathbf{u},T)=-\frac{2}{3}\sqrt{\frac{2}{\pi}}\frac{\alpha(1-\beta)}{\varepsilon}n^B\sqrt{\frac{\alpha m}{(1-\alpha)T^B+\alpha T}}$$
$$\times[A(T,T^*)|\mathbf{u}-\mathbf{u}^B|^4+B(T,T^*)|\mathbf{u}-\mathbf{u}^B|^2+C(T,T^*)(T-T^*)^2], \tag{64}$$

where $A(T,T^*)$ is proportional, by a positive factor, to

$$3\alpha(1-\beta)[1-\alpha(1-\beta)]\left(\frac{T}{T^*}\right)^2+2[2-3\alpha(1-\beta)+3\alpha^2(1-\beta)^2]\frac{T}{T^*}+3\alpha(1-\beta)[1-\alpha(1-\beta)],$$

which in turn is positive for any pair (T,T^*) since also the prefactor of T/T^* can be easily seen to be positive. Therefore we have $A(T,T^*)>0$. Analogously, $B(T,T^*)$ is given by a positive quantity times the quadratic term

$$3\alpha(1-\beta)[1-\alpha(1-\beta)]\left(\frac{T}{T^*}\right)^2+2[1-3\alpha(1-\beta)+3\alpha^2(1-\beta)^2]\frac{T}{T^*}+3\alpha(1-\beta)[1-\alpha(1-\beta)],$$

and the same reasoning holds for this slightly different expression, so that also $B>0$. Finally we get simply

$$C(T,T^*)=12\frac{[1-\alpha(1-\beta)][T^*+\alpha(1-\beta)(T-T^*)]}{\alpha m(1-\beta)TT^*},$$

which is clearly positive $\forall T$, T^*, and therefore $\dot{V}_l$, as given by (64), is the sum of three nonpositive addends, and vanishes if and only if $\mathbf{u}=\mathbf{u}^B$ and $T=T^*$. This completes the required proof that V_l is a strict entropy function for (62).

Let us apply now a Chapman-Enskog asymptotic procedure to the system (62), in order to build up a fluid-dynamic Navier-Stokes equation for the number density n. Proceeding as in the preceding section, we substitute into (62) the expansions of the nonhydrodynamic variables $\mathbf{u}$ and T in powers of the chosen small parameter $Kn\equiv\varepsilon$, as given in (39). In order to close the continuity equation we must determine the coefficients $\boldsymbol{\nu}^0$ and $\boldsymbol{\nu}^1$. The main difference with respect to the previous closure approach is the presence in (62) of quantities of the kind $[(1-\alpha)T^B+\alpha T]^{-\kappa}$ (with $\kappa=1,\ 1/2$) which, containing T, must be expanded in powers of ε,

$$[(1-\alpha)T^B+\alpha T]^{-\kappa}=[(1-\alpha)T^B+\alpha\Upsilon^0]^{-\kappa}\left[1-\kappa\frac{\alpha\Upsilon^1}{(1-\alpha)T^B+\alpha\Upsilon^0}\varepsilon+O(\varepsilon^2)\right].$$

Hence, by considering $O(\varepsilon^{-1})$ terms appearing in the equation for $\mathbf{u}$ we have

$$-\alpha(1-\beta)\frac{4}{3}nn^B\sqrt{\frac{2}{\pi}}\sqrt{\frac{\alpha m}{(1-\alpha)T^B+\alpha\Upsilon^0}}\left[\frac{1}{5}(\boldsymbol{\nu}^0-\mathbf{u}^B)^2+2\frac{(1-\alpha)T^B+\alpha\Upsilon^0}{\alpha m}\right]$$
$$\times(\nu_i^0-u_i^B)=0\quad\forall\, i, \tag{65}$$

thus we get again

$$\boldsymbol{\nu}^0=\mathbf{u}^B. \tag{66}$$

Then, the next step [$O(1)$ terms] of the asymptotic procedure yields

$$\nu_i^1 = -\frac{1}{\alpha(1-\beta)}\frac{3}{8nn^B}\sqrt{\frac{\pi}{2}}\sqrt{\frac{\alpha m}{(1-\alpha)T^B+\alpha\Upsilon^0}}\left[n\frac{\partial u_i^B}{\partial t}+nu_k^B\frac{\partial u_i^B}{\partial x_k}+\frac{1}{m}\frac{\partial}{\partial x_i}(n\Upsilon^0)\right], \tag{67}$$

so that we need also the coefficient Υ^0. As before, we must consider the leading order of the temperature evolution equation, and this provides

$$\alpha^2(1-\beta)\frac{16}{3}nn^Bm\sqrt{\frac{2}{\pi}}\left[\frac{(1-\alpha)T^B+\alpha\Upsilon^0}{\alpha m}\right]^{3/2}\left[(1-\beta)-\frac{\Upsilon^0}{(1-\alpha)T^B+\alpha\Upsilon^0}\right]=0, \tag{68}$$

hence

$$\Upsilon^0=\frac{(1-\alpha)(1-\beta)}{1-\alpha(1-\beta)}T^B=T^*. \tag{69}$$

By inserting this result into (67) and recalling the Euler equations (10) for the background medium, finally we get for the drift velocity $\mathbf{u}$ the same approximation (46), accurate to $O(\varepsilon)$, achieved in the previous approach. Consequently, the present fluid-dynamic equation for the number density n coincides with (47). Moreover, equating zero order terms in the equation for T, we find again, after some algebra, $\Upsilon^1=0$, hence $T=T^*+O(\varepsilon^2)$.

V. DISCUSSION AND CONCLUSIONS

The two different closure strategies performed in this work have provided then, as anticipated, different moment equations but the same fluid-dynamic limit, at least up to the first order in the small parameter ε. Both closures are approximations justified by a maximum entropy principle applied to a specific choice of entropy functional, and, in the considered collision dominated regime, describe relaxation towards collision equilibrium, which maximizes all possible entropies. The different entropies imply different constraints on the evolutions, which explain the different macroscopic equations. However, in the hydrodynamic limit, it is conceivable that closeness to collision equilibrium, valid outside initial and boundary layers, implies the same fluid-dynamic equation of drift-diffusion type at the Navier-Stokes level. This matter will be the object of future separate investigations. Validation of the trends provided by the different closures by comparison with kinetic calculations will also be one of the first steps in the scheduled future work. This will be essential in order to ascertain which macroscopic equations best approximate the solution of the kinetic problem, and to possibly investigate whether there exists an optimal entropy in this sense, among the infinite possible ones. For now, it is worth concluding this paper with some observations arising from the general structure of the analytical results and from the simple numerical experiments that are easily performed in space homogeneous conditions. A sample of them is reported here just for illustrative purposes, with randomly selected numerical values of the involved parameters, chosen on their physically pertinent ranges. The presented results are relevant to physical situations in which the discrepancies between the two entropies are large enough to be seen in the figures. No discrepancy would occur for the pseudo-Maxwellian model, since moment equations would be exact in the absence of spatial gradients. In any case, evolution reduces now to relaxation to (the correct) equilibrium, which is reached after few collision times, so that differences can be seen only in such small initial layer. Computed velocities and temperatures are shown in Figs. 1 and 2 for $m=1$, $\mathbf{u}^B=(1,2,3)$, $T^B=2$, starting from initial conditions $\mathbf{u}_0=\mathbf{0}$, $T_0=3$. The Knudsen number Kn is only a scaling factor and does not affect the evolution if time is measured in mean collision times. For this reason results are plotted versus the microscopic time scale t/Kn and are universal with respect to Kn. A quantity like n^B is also merely a scaling factor and its value may be considered as included into Kn. Crucial control parameters are here mass ratio α and inelasticity coefficient β, that in fact have been varied in Figs. 1 and 2, respectively. Increasing α for fixed β amounts to enhancing the rate of exchange of momentum and energy with the background, and at the same time makes the equilibrium temperature T^* lower and lower. In fact, a faster relaxation of both $\mathbf{u}$ to $\mathbf{u}^B$ and T to T^*, accompanied by a slight decrease of T^*, may

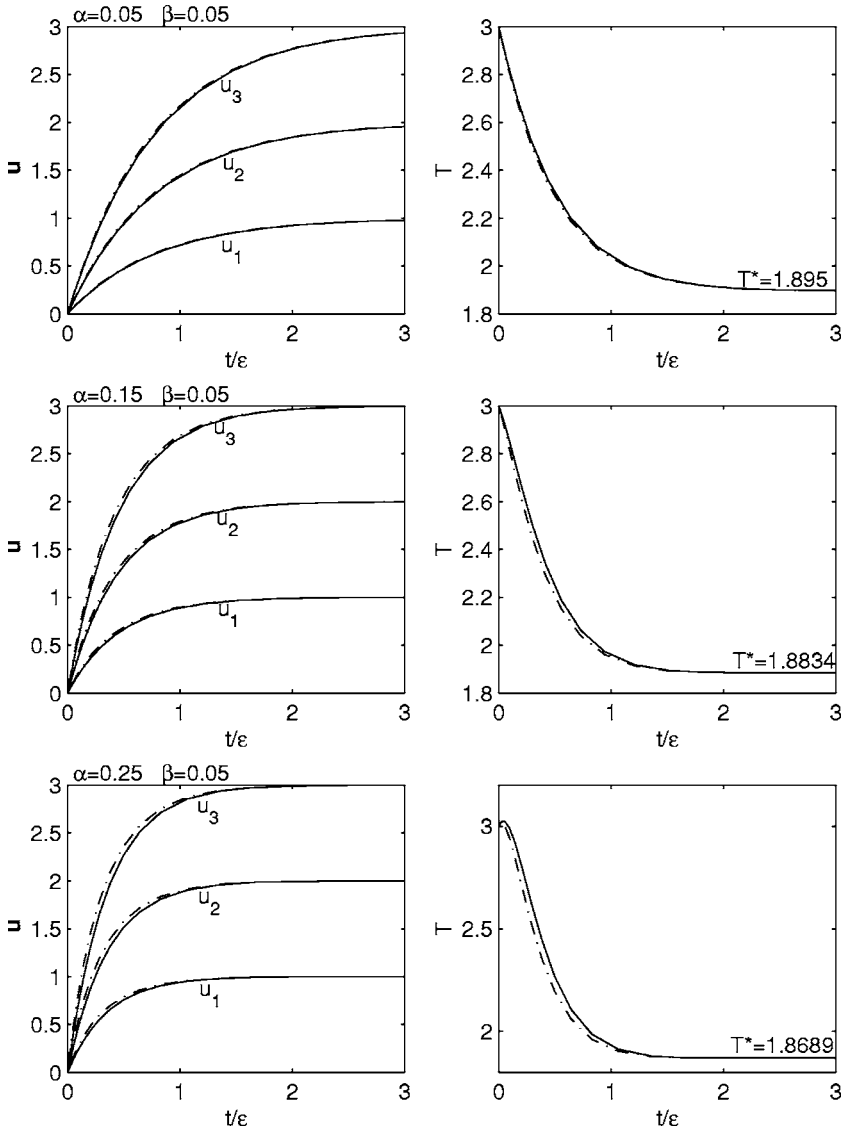

FIG. 1. Evolution of mass velocity **u** and temperature T for varying α in the microscopic time scale t/ε for the values of parameters given in the text: quadratic entropy (solid line) versus logarithmic entropy (dashed dotted line).

be observed in Fig. 1. Notice that, just because a higher α implies a stronger impact of collisions, discrepancies in the plots become larger and larger for increasing α. Similar arguments apply to the effects of the parameter β, based again on physical grounds, and quantitatively described by collision contributions in Eqs. (36) and (62). Results are shown in Fig. 2. Now increasing β makes the relaxation rate slightly smaller, and at the same time causes a sensible decrease of the equilibrium temperature. A general feature that has been observed systematically is that the logarithmic entropy produces a faster relaxation than the quadratic one. Of course it will be interesting to compare these trends with kinetic computations.

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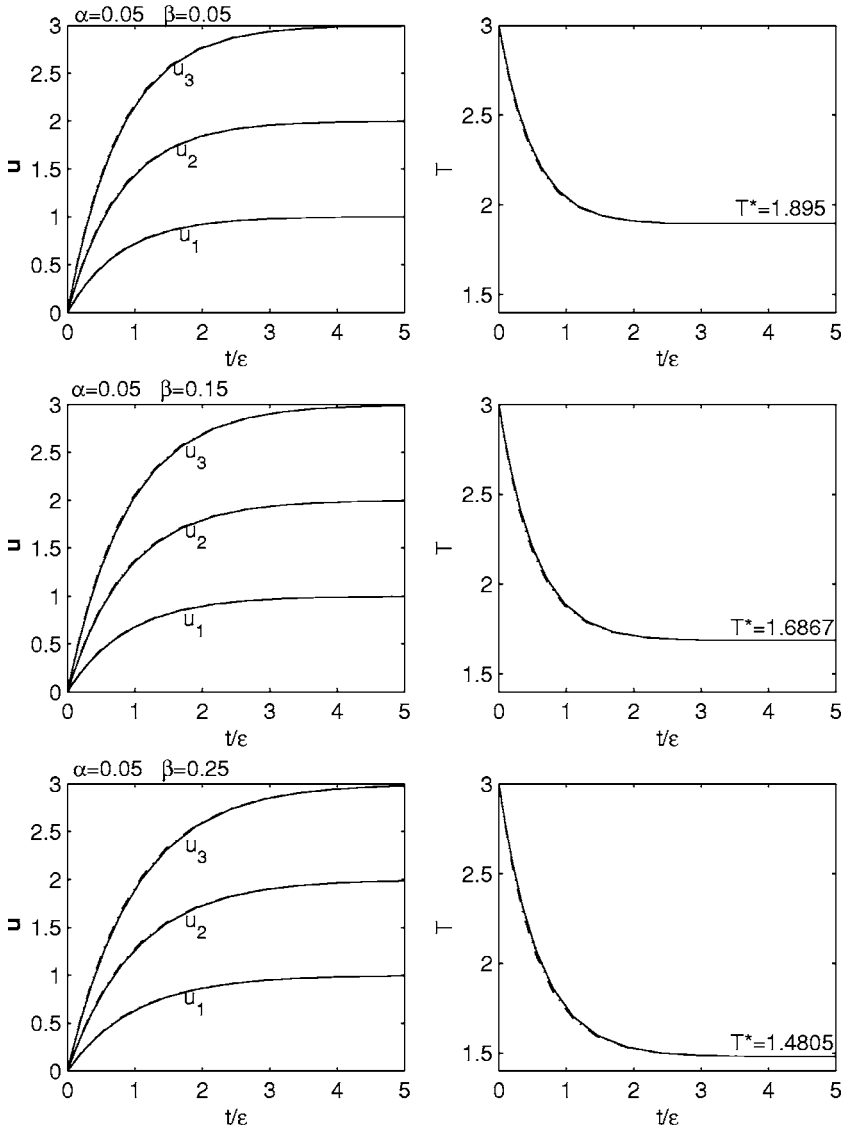

FIG. 2. Evolution of mass velocity **u** and temperature T for varying β in the microscopic time scale t/ε for the values of parameters given in the text: quadratic entropy (solid line) versus logarithmic entropy (dashed dotted line).

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APPENDIX

We collect here for convenience some Gaussian integrals needed in the evaluation of collision contributions performed in Secs. III and IV. With $\gamma>0$ we have

$$\int_{\mathbb{R}^3} \exp(-\gamma x^2) d_3\mathbf{x} = \left(\frac{\pi}{\gamma}\right)^{3/2}, \tag{A1a}$$

$$\int_{\mathbb{R}^3} x_i^2 \exp(-\gamma x^2) d_3\mathbf{x} = \left(\frac{\pi}{\gamma}\right)^{3/2} \frac{1}{2\gamma}, \tag{A1b}$$

$$\int_{\mathbb{R}^3} x_i^2 x_j^2 \exp(-\gamma x^2) d_3\mathbf{x} = \left(\frac{\pi}{\gamma}\right)^{3/2} \left(\frac{1}{2\gamma}\right)^2, \quad i \neq j, \tag{A1c}$$

$$\int_{\mathbb{R}^3} x_i^4 \exp(-\gamma x^2) d_3\mathbf{x} = \left(\frac{\pi}{\gamma}\right)^{3/2} 3\left(\frac{1}{2\gamma}\right)^2, \tag{A1d}$$

$$\int_{\mathbb{R}^3} x x_i x_h \exp(-\gamma x^2) d_3\mathbf{x} = \frac{4}{3}\pi \frac{1}{\gamma^3} \delta_{ih} \quad \forall\, i,h, \tag{A2a}$$

$$\int_{\mathbb{R}^3} x^5 \exp(-\gamma x^2) d_3\mathbf{x} = 12\pi \frac{1}{\gamma^4}, \tag{A2b}$$

$$\int_{\mathbb{R}^3} x x_i \exp[-\gamma(\mathbf{x}+\mathbf{a})^2] d_3\mathbf{x} = -\frac{8\pi}{3\gamma} a_i \left(\frac{1}{\gamma} + \frac{1}{5}a^2\right), \tag{A3a}$$

$$\int_{\mathbb{R}^3} x^3 \exp[-\gamma(\mathbf{x}+\mathbf{a})^2] d_3\mathbf{x} = \frac{2\pi}{5\gamma}\left(a^4 + \frac{10}{\gamma}a^2 + \frac{10}{\gamma^2}\right). \tag{A3b}$$

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Random multi-overlap structures for optimization problems

Luca De Sanctis[a)]
Department of Condensed Matter, ICTP, Strada Costiera 11, Trieste, Italy

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We extend to the K-SAT and *p*-XOR-SAT optimization problems the results recently achieved, by introducing the concept of random multi-overlap structure, for the Viana-Bray model of diluted mean field spin glass. More precisely we can prove a generalized bound and an extended variational principle for the free energy per site in the thermodynamic limit. Moreover a trial function implementing ultrametric breaking of replica symmetry is exhibited. The ultrametric structure exhibits the same factorization property as the optimal structures for the Viana-Bray model and the Sherrington-Kirkpatrick nondiluted model. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2121267]

I. INTRODUCTION

In the case of nondiluted spin glasses, Aizenman, Sims, and Starr[1] introduced the idea of random overlap structure (ROSt) to express in a very elegant manner the free energy of the model as an infimum over a rich probability space, to exhibit an optimal structure (the so-called Boltzmann one), to write down a general trial function through which one can formulate various ansatzs for the free energy of the model. It was also described how to formulate in particular the Parisi ansatz within this formalism. In Refs. 2 and 3 we extended those results to the case of diluted spin glass (Viana-Bray model). Here we extend the same results to optimization problems, the K-SAT and the *p*-XOR-SAT. The latter is the simple extension to *p*-body interactions of the Viana-Bray model, which is the diluted version of the famous model of Sherrington and Kirkpatrick (SK) of mean field spin glass. We also prove that the optimal structures must enjoy a certain factorization property, known as invariance with respect to the cavity step, that was first found by Guerra in Ref. 5 for the SK model, and that turned out to be valid also for the Viana-Bray dilute spin glass model.[2] The ultrametric ansatz we propose verifies such a property.

Many of the calculations in the present paper are quite simple and standard, and as a general reference with many details the reader can take for instance Refs. 4 and 7.

II. MODEL, NOTATIONS, DEFINITIONS

Consider configurations of Ising spins σ: $i \to \sigma_i = \pm 1$, $i = 1, \ldots, N$. Let P_ζ be a Poisson random variable of mean ζ, and $\{i_\nu^\mu\}$ be independent identically distributed random variables, uniformly distributed over points $\{1, \ldots, N\}$. If $\{J_\nu^\mu\}$ are independent identically distributed copies of a symmetric random variable $J = \pm 1$, then the Hamiltonian of random K-SAT is

a)Electronic mail: lde@math.princeton.edu

$$H = -\sum_{\nu=1}^{P_{\alpha N}} \frac{1}{2}(1 + J_\nu^1 \sigma_{i_\nu^1}) \cdots \frac{1}{2}(1 + J_\nu^K \sigma_{i_\nu^K}).$$

Here $\alpha \geqslant 0$ is the degree of connectivity and K is assumed to be even. We do not consider the presence of an external field, but all the results trivially extend to this case as well. By ω we mean the Bolztmann-Gibbs average

$$\omega(\mathcal{O}) = Z_N^{-1} \sum_{\{\sigma\}} \mathcal{O}(\sigma) \exp(-\beta H), \quad Z_N = \sum_{\{\sigma\}} \exp(-\beta H).$$

We will denote by $\mathbb{E}$ the average over all the other (quenched) random variables, and the free energy f_N per site and its thermodynamic limit are defined by

$$-\beta f_N = \frac{1}{N} \mathbb{E} \ln Z_N, \quad f = \lim_{N \to \infty} f_N.$$

The existence of the above-mentioned limit has been proven in Ref. 4 (see also Ref. 2 for the proof in the framework of overlap structures). We will use the notation Ω for the product of the needed number of independent copies (replicas) of ω and $\langle \cdot \rangle$ for the composition of an $\mathbb{E}$-type average over some quenched variables and some sort of Boltzmann-Gibbs average over the spin variables, which will be clear from the context. The multi-overlaps are defined (using replicas) by

$$q_{1,\cdots,n} = \frac{1}{N} \sum_{i=1}^{N} \sigma_i^{(1)} \cdots \sigma_i^{(n)}.$$

Definition 1: A random multi-overlap structure (*RaMOSt*) $\mathcal{R}$ *is a triple* $(\Sigma, \{\tilde{q}_n\}, \xi)$ *where*

1. Σ *is a discrete space*;
2. ξ: $\Sigma \to \mathbb{R}_+$ *is a system of random weights*;
3. $\tilde{q}_{r_1,\cdots,r_{2l}}$: $\Sigma_{r_1} \times \cdots \times \Sigma_{r_l} \to [0,1]$, $l \in \mathbb{N}$, $|\vec{q}| \leqslant 1$ *is a positive definite* multi-overlap kernel.

III. THE STRUCTURE OF THE MODEL

In order to understand what is the underlying structure of the model, it is well known that it is useful to compute the derivative of the free energy with respect to the somewhat basic parameter. In the case of nondiluted spin glasses such a parameter is the strength of the couplings (and it is equivalent to differentiating with respect to the inverse temperature). In the case of diluted spin glasses such a parameter is the connectivity.

It is very easy to show (see, e.g., Ref. 4) by pretty standard calculation that

$$\frac{\mathrm{d}}{\mathrm{d}\alpha} \frac{1}{N} \mathbb{E} \ln \sum_{\sigma} \exp(-\beta H) = \sum_{n>0} \frac{(-1)^{n+1}}{n} \left(\frac{e^{-\beta} - 1}{2^K} \right)^n \langle (1 + Q_n(q))^K \rangle, \tag{1}$$

where

$$Q_n(q) = \sum_{l=1}^{[n/2]} \sum_{r_1 < \cdots < r_{2l}}^{1,n} q_{r_1,\ldots,r_{2l}}.$$

The fundamental quantities governing the model are therefore the multi-overlaps, like for diluted spin glasses.[2,3] That is why we use RaMOSt in this context as well. The main difference is that here the function $1 + Q_n$ takes the place of the mere multi-overlaps.

As should be clear from Refs. 1–3 we must therefore introduce also two random variables $\tilde{H}(\gamma, \alpha; \tilde{J})$ and $\hat{H}(\gamma, \alpha; \hat{J})$ such that

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\mathbb{E}\ln\sum_{\gamma}\xi_{\gamma}\exp(-\beta\tilde{H}_{\cdot})=K\sum_{n>0}\frac{(-1)^{n+1}}{n}\left(\frac{e^{-\beta}-1}{2^{K-1}}\right)^{n}\langle(1+Q_n(\tilde{q}))^{K-1}\rangle, \tag{2}$$

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\frac{1}{N}\mathbb{E}\ln\sum_{\gamma}\xi_{\gamma}\exp(-\beta\hat{H})=(K-1)\sum_{n>0}\frac{(-1)^{n+1}}{n}\left(\frac{e^{-\beta}-1}{2^{K}}\right)^{n}\langle(1+Q_n(\tilde{q}))^{K}\rangle. \tag{3}$$

Finally, we introduce as expected the following trial function:

$$G_N(\mathcal{R},\tilde{H},\hat{H})=\frac{1}{N}\mathbb{E}\ln\frac{\Sigma_{\sigma,\gamma}\xi_{\gamma}\exp\left(-\beta\Sigma_{i=1}^{N}\tilde{H}_i\frac{1}{2}(1+J_i\sigma_i)\right)}{\Sigma_{\gamma}\xi_{\gamma}\exp(-\beta\hat{H})},$$

where $\tilde{H}_i$ are independent copies of $\tilde{H}_{\cdot}$. We will construct explicitly $\tilde{H}_{\cdot}$ and $\hat{H}$ in the next sections. Lastly, let us define

$$\tilde{H}=\sum_{i=1}^{N}\tilde{H}_i\frac{1}{2}(1+J_i\sigma_i).$$

IV. GENERAL THEOREMS

Let us state the extension to the K-SAT model of the results presented in Refs. 1, 5, and 2. The first result is a general bound for the free energy per spin.

Theorem 1 (Generalized Bound):

$$-\beta f_N\leqslant\inf_{\mathcal{R}}G_N.$$

Proof: Consider the interpolating Hamiltonian

$$H_{\gamma}(t)=H(t)+\tilde{H}(1-t)+\hat{H}(t),\quad t\in[0,1],$$

where t is understood to multiply the connectivity, and consider also

$$R(t)=\frac{1}{N}\mathbb{E}\ln\frac{\Sigma_{\gamma,\sigma}\xi_{\gamma}\exp(-\beta H_{\gamma}(t))}{\Sigma_{\gamma}\xi_{\gamma}\exp(-\beta\hat{H}_{\gamma})}.$$

Now observe that $R(1)=-\beta f_N$, $R(0)=G_N$, and compute the t-derivative of $R(t)$ using the expressions in Sec. III,

$$\frac{\mathrm{d}}{\mathrm{d}t}R(t)=-\alpha\sum_{n>0}\frac{1}{n}\left(\frac{e^{-\beta}-1}{2^{K}}\right)^{n}$$
$$\times\langle(1+Q_n(q))^{K}-K(1+Q_n(q))(1+Q_n(\tilde{q}))^{K-1}+(K-1)(1+Q_n(\tilde{q}))^{K}\rangle.$$

Therefore the derivative above is nonpositive since the function $x^K-Kxy^{K-1}+(K-1)y^K$ of x and y is non-negative. This completes the proof of the theorem. □

The second result is the explicit construction of a RaMOSt which provides the proof of the existence of such structures and a reversed bound to the one in the previous theorem. This RaMOSt is called Boltzmann, and it is equivalent to the existence of the thermodynamic limit for the free energy per site.[6]

Definition 2 (Boltzmann RaMOSt): The Boltzmann RaMOSt $\mathcal{R}_B(M)$ is the triple

1. $\Sigma=\{-1,1\}^M\ni\tau$,
2. $\xi_{\tau}=\exp(-\beta H_M(\tau))$,

3. $\tilde{q}_{r_1\cdots r_l}=1/M\Sigma_j \tau_j^{(r_1)}\cdots\tau_j^{(r_l)}$.

We choose

$$\tilde{H}_\tau = -\sum_{\nu=1}^{P_{K\alpha N}} \frac{1}{2}(1+\tilde{J}_\nu^1 \tau_{j_\nu^1})\cdots\frac{1}{2}(1+\tilde{J}_\nu^{K-1}\tau_{j_\nu^{K-1}})\frac{1}{2}(1+J_\nu^K\sigma_{i_\nu}),$$

$$\hat{H}_\tau = -\sum_{\nu=1}^{P_{(K-1)\alpha N}} \frac{1}{2}(1+\hat{J}_\nu^1 \tau_{j_\nu^1})\cdots\frac{1}{2}(1+\hat{J}_\nu^K\tau_{j_\nu^K}),$$

where the independent random variables $j_\cdot^\cdot$ are uniformly distributed over $1,\ldots,M$ and $\tilde{J}_\cdot^\cdot, \hat{J}_\cdot^\cdot$ are independent copies of J.

Theorem 2 (Reversed Bound):

$$-\beta f \geqslant \lim_{N\to\infty}\liminf_{M\to\infty} G_N(\mathcal{R}_B(M)).$$

Proof: It is clearly enough to show

$$-\beta f = \mathbf{C}\lim_M \frac{1}{N}\mathbb{E}\ln\frac{Z_{M+N}}{Z_M} \geqslant \liminf_N \liminf_M G_N(\mathcal{R}_B(M)), \tag{4}$$

where the limit **C** lim is in the Cesàro sense. We can rewrite G_N as

$$\frac{1}{N}\mathbb{E}\ln\left[\frac{\Sigma_{\tau,\sigma}e^{-\beta(H_M+\tilde{H})}}{Z_{N+M}(\alpha')}\frac{Z_{N+M}(\alpha')}{Z_{N+M}(\alpha)}\frac{Z_{N+M}(\alpha)}{Z_M(\alpha)}\frac{Z_M(\alpha)}{\Sigma_\tau e^{-\beta(H_M+\hat{H})}}\right]$$

and therefore we have four terms. If we now take

$$\alpha' = \alpha\left(1+(K-1)\frac{N}{M}\right)$$

we see that the fourth fraction is the same as $Z_M(\alpha)/Z_M(\alpha')$, and it cancels out with the second in the limit of large M (just like in Ref. 2). We also know that the third fraction tends to $-\beta f$.

Now we keep proceeding like in Ref. 2. In the denominator of the first fraction we can split the mean $\alpha'(N+M)$ into the sum of three means such that H_{N+M} splits into the sum of three Hamiltonians with the first depending only on cavity spins τ, the second containing exactly one spin from the original system in its interactions, the third has the interactions with at least two spins σ. Hence the three coefficients of the connectivities, up to corrections vanishing when M is large, will be M^K, KM^{K-1}, and a negligible third (of order M^{K-2}), respectively. Incidentally, this means that when the cavity is large the added spins do not interact with one another (asymptotically).

The choice of α' we made guarantees that numerator and denominator contain two (up to a negligible third in the denominator) identical Hamiltonians with the same connectivities. As a consequence, the first fraction in G_N vanishes in the limit and the theorem is proven. □

An immediate consequence of the two bounds is clearly the following

Theorem 3 (Extended Variational Principle):

$$-\beta f = \lim_{N\to\infty}\inf_{\mathcal{R}} G_N.$$

All the RaMOSts yielding the correct value of the free energy per site in the thermodynamic limit are called optimal, and they enjoy the same factorization property that is found for both nondilute spin glasses and the Viana-Bray model of dilute spin glass.[2] This statement is made precise by factorizing the cavity part of the trial free energy[2]

$$c_1 \cdots c_N = \sum_{\sigma} \exp(-\beta \tilde{H}), \tag{5}$$

in the next

Theorem 4: *In the whole region where the parameters are uniquely defined, the following Cesàro limit is linear in N and* $\bar{\alpha}$:

$$\mathbf{C} \lim_{M} \mathbb{E} \ln \Omega_M \left\{ \sum_{\sigma} c_1 \cdots c_N \exp[-\beta(\hat{H}(\bar{\alpha}/N))] \right\} = N(-\beta f + \alpha A) + \bar{\alpha} A, \tag{6}$$

where

$$A = \sum_{n>0} \frac{(-1)^{n+1}}{n} \left(\frac{e^{-\beta} - 1}{2^K} \right)^n \langle (1 + Q_n(q))^K \rangle.$$

Proof: As expected, the proof is similar to that of the analogous theorem in Ref. 2 and to that of Theorem 2 above, except here we will choose

$$\alpha' = \alpha + (K-1)\frac{1}{M}(\alpha N + \bar{\alpha})$$

and use only three fractions, re-writing the left-hand side of (6) as

$$\frac{1}{N} \mathbb{E} \ln \left[\frac{\Sigma_{\tau,\sigma} \exp(-\beta(H_M + \tilde{H}))}{Z_{N+M}(\alpha')} \frac{Z_{N+M}(\alpha')}{Z_{N+M}(\alpha)} \frac{Z_{N+M}(\alpha)}{Z_M(\alpha)} \right].$$

Notice that this choice of α' reduces to the previous one of Theorem 2 for $\bar{\alpha}=0$, as it should do. □

V. REPLICA SYMMETRY BREAKING AND ULTRAMETRIC RaMOSt

Now we are equipped with the main theorems about the random multi-overlap structures in the case of the K-SAT problem, and we are about to extend the results of Ref. 3 to the K-SAT. We want to construct a trial function depending on ultrametric trial multi-overlaps, that fulfills the generalized bound and obeys the factorization property of the optimal structures.

Definition 3 (Ultrametric RaMOSt): The R-level replica symmetry breaking ultrametric RaMOSt $\mathcal{R}_U$ *is the triple*

1. $\Sigma = \mathbb{N}^R \ni \gamma = (\gamma_1, \ldots, \gamma_R)$;
2. $\xi_\gamma(m_1, \ldots, m_R)$ *from the random probability cascades*;
3. $\tilde{q}_{r_1 \cdots r_l} = (\tilde{q}^{(1)}_{r_1,\cdots,r_l} - \tilde{q}^{(0)}_{r_1 \cdots r_l}) \delta_{\gamma_1^{r_1},\cdots,\gamma_1^{r_l}} + \cdots + (\tilde{q}^{(R)}_{r_1,\cdots,r_l} - \tilde{q}^{(R-1)}_{r_1,\cdots,r_l}) \delta_{\gamma_1^{r_1} \cdots \gamma_1^{r_l}} \cdots \delta_{\gamma_R^{r_1} \cdots \gamma_R^{r_l}}$ *is the ultrametric multi-overlap, given partitions* $q^{(a)}_{r_1,\cdots,r_l}$, $0 \leqslant a \leqslant R$ *of the interval [0,1].*

Denoting by X the map

$$X: \tilde{\alpha}_a \to m_a$$

satisfying (7), we can consider the trial function $G(\mathcal{R}_U)$ as a function $G(X)$ of X.

Theorem 5: *There exist* $\tilde{H}$, $\hat{H}$ *satisfying* (2) and (3) *with* $\tilde{q}$ *ultrametric and the ultrametric trial function* $G(X)$ *satisfying the bound*

$$-\beta f(\beta, \alpha) \leqslant \inf_X G(X)$$

as a special case of the generalized bound. Moreover, the Ultrametric RaMOSt enjoys the same factorization property as in Theorem 4.

Proof: Take

$$\tilde{H}_\gamma = \sum_{\nu=1}^{P_{KaN}} \tilde{u}_\nu^\gamma \frac{1}{2}(1 + J_\nu \sigma_{i_\nu}) - \frac{1}{\beta} \ln \cosh(\beta \tilde{u}_\nu^\gamma),$$

$$\hat{H}_\gamma = \sum_{\nu=1}^{P_{(K-1)aN}} \hat{u}_\nu^\gamma - \frac{1}{\beta} \ln \cosh(\beta \hat{u}_\nu^\gamma)$$

with $\tilde{u}_\gamma$, $\hat{u}_\gamma$ defined by

$$\tanh(\beta \tilde{u}_\gamma) = (e^{-\beta} - 1)\tfrac{1}{2}(1 + \tilde{J}^1 W_\gamma^1) \cdots \tfrac{1}{2}(1 + \tilde{J}^{K-1} W_\gamma^{K-1}),$$

$$\tanh(\beta \hat{u}_\gamma) = (e^{-\beta} - 1)\tfrac{1}{2}(1 + \hat{J}^1 W_\gamma^1) \cdots \tfrac{1}{2}(1 + \hat{J}^K W_\gamma^K)$$

in which W_γ is the same as in Ref. 3

$$W_\gamma = \tilde{\omega}_{\tilde{\alpha}_1}(\rho_{k_\nu}) \bar{J}_{\gamma_1} + \cdots + \tilde{\omega}_{\tilde{\alpha}_R}(\rho_{k_\nu}) \bar{J}_{\gamma_1, \cdots, \gamma_R},$$

where $\tilde{\omega}_{\tilde{\alpha}}(\rho_{k_\nu})$ is the infinite volume limit of the Boltzmann-Gibbs average of a random spin from an auxiliary system with a Viana-Bray one-body interaction Hamiltonian at connectivity $\tilde{\alpha}^3$ and $\bar{J} = \pm 1$ is symmetric. Notice that

$$\mathbb{E}\tilde{\omega}_{\tilde{\alpha}}^n(\rho_k) = \langle \tilde{q}_n \rangle_{\tilde{\alpha}} = \tilde{q}_n(\tilde{\alpha}).$$

The indices, the bar, the tilde, and the caret mean independent copies of the corresponding variables. Let us now report a comment from Ref. 2. Given any partition $\{x^a\}_{a=0}^R$ of the interval [0, 1], there exists a sequence $\{\tilde{\alpha}_a\}_{a=0}^R \in [0, \infty]$ such that $\tilde{q}_{1,\cdots,n}(\tilde{\alpha}_a) = x_a - x_{a-1}$. In other words, a sequence $\{\tilde{\alpha}_a\}_{a=0}^R \in [0, \infty]$ generates for each $n \in \mathbb{N}$ a partition of [0, 1] considered as the set of trial values of $\tilde{q}_{1,\cdots,n}$, provided the $\tilde{\alpha}_a$ are not too large

$$\sum_{a \leqslant R} \tilde{q}_{1,\cdots,n}(\tilde{\alpha}_a) \leqslant 1. \tag{7}$$

We limit our trial multi-overlaps to belong to partitions generated in this way. This implies that the points of the generated partitions tend to get closer to zero as n increases. This is good, since in any probability space $\langle \tilde{q}_n \rangle$ decreases as n increases and therefore the probability integral distribution functions tend to grow faster near zero. Now put inductively

$$\mathbb{E}\tilde{\Omega}_{\tilde{\alpha}_a}(\tau_{k_\nu}^{(r_1)} \cdots \tau_{k_\nu}^{(r_l)}) = \tilde{q}_{r_1,\cdots,r_l}(\tilde{\alpha}_a) = \tilde{q}_{r_1,\cdots,r_l}^{(a)} - \tilde{q}_{r_1,\cdots,r_l}^{(a-1)}, \quad \tilde{q}_{r_1,\cdots,r_l}^{(0)} = 0,$$

then an elementary calculation shows that

$$\mathbb{E}\tanh^n(\beta \tilde{u}_\gamma) = \left(\frac{e^{-\beta} - 1}{2^{K-1}}\right)^n (1 + Q_n(\tilde{q}))^{K-1},$$

$$\mathbb{E}\tanh^n(\beta \hat{u}_\gamma) = \left(\frac{e^{-\beta} - 1}{2^K}\right)^n (1 + Q_n(\tilde{q}))^K$$

with $\tilde{q}$ ultrametric,[3] i.e.,

$$\tilde{q}_{r_1,\cdots,r_l} = (\tilde{q}_{r_1,\cdots,r_l}^{(1)} - \tilde{q}_{r_1,\cdots,r_l}^{(0)}) \delta_{\gamma_1^{r_1} \cdots \gamma_1^{r_l}} + \cdots + (\tilde{q}_{r_1,\cdots,r_l}^{(R)} - \tilde{q}_{r_1,\cdots,r_l}^{(R-1)}) \delta_{\gamma_1^{r_1} \cdots \gamma_1^{r_l}} \cdots \delta_{\gamma_R^{r_1} \cdots \gamma_R^{r_l}}.$$

Hence we reproduced the setting of the generalized bound in the particular case of ultrametric multi-overlap, and therefore we just proved that

$$-\beta f \leqslant \inf_X G(X).$$

At this point we only need to make sure that the ultrametric RaMOSt passes the invariance test prescribed by Theorem 4. Notice that $G(X)$ does not depend on N (see Lemma 1 in Appendix A of Ref. 3). Moreover $\tilde{W}$ and $\hat{W}$ are chosen to be independent, therefore the factorization property of the optimal RaMOSts holds:

$$\mathbb{E} \ln \Omega_{\xi}[c_1 \cdots c_N \exp(-\beta \hat{H}(\bar{\alpha}/N))] = NB + \bar{\alpha}A$$

for some B, and we are again using the definition (5). □

VI. CONCLUSIONS

The RaMOSt is the minimal generalization of the ROSt, and what we showed here and in Ref. 2 is that the minimal generalization is enough to formulate the variational principle and also exhibit a concrete RaMOSt analogous to the Parisi one for SK. As a consequence, it is enough to restrict the space of trial functions to those expressible in terms of fixed multi-overlaps (i.e., a set of numbers, not random variables to be averaged).

Unfortunately the case of odd K still escapes our approach.

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APPENDIX: THE *p*-XOR-SAT

The Hamiltonian of the random p-XOR-SAT coincides with the one of the diluted p-spin glass

$$H = -\sum_{\nu=1}^{P_{\alpha N}} J_\nu \sigma_{i_\nu^1} \cdots \sigma_{i_\nu^p}.$$

It is therefore elementary, assuming p even, to extend all the results of Refs. 2 and 3 to this case, also when in the presence of an external field. Since it is easy to show[2]

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\frac{1}{N}\mathbb{E} \ln \sum_{\sigma} \exp(-\beta H) = \sum_{n>0} \frac{1}{2n}\mathbb{E} \tanh^{2n}(\beta J)(1 - \langle q_{2n}^p \rangle),$$

the structure of the model is the same RaMOSt valid for the case of the Viana-Bray model, but the above-mentioned equality suggests to try and get the non-negative convex function $x^p - pxy^{p-1} + (p-1)y^p$ whenever we got the square $x^2 - 2xy + y^2$ in the Viana-Bray case. That is why here $\tilde{H}$ and $\hat{H}$ are chosen such that

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\mathbb{E} \ln \sum_{\gamma} \xi_\gamma \exp(-\beta \tilde{H}_\cdot) = p \sum_{n>0} \frac{1}{2n}\mathbb{E} \tanh^{2n}(\beta J)(1 - \langle \tilde{q}_{2n}^{p-1} \rangle),$$

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\frac{1}{N}\mathbb{E} \ln \sum_{\gamma} \xi_\gamma \exp(-\beta \hat{H}) = (p-1) \sum_{n>0} \frac{1}{2n}\mathbb{E} \tanh^{2n}(\beta J)(1 - \langle \tilde{q}_{2n}^{p} \rangle)$$

and plugged into

$$G_N(\mathcal{R},\tilde{H},\hat{H}) = \frac{1}{N}\mathbb{E}\ln\frac{\Sigma_{\sigma,\gamma}\xi_\gamma \exp\left(-\beta\Sigma_{i=1}^N \tilde{H}_i\sigma_i\right)}{\Sigma_\gamma \xi_\gamma \exp(-\beta\hat{H})}.$$

The generalized bound clearly holds, the Boltzmann RaMOSt is the one with $\xi_\tau=\exp(-\beta H_M)$ and

$$\tilde{H}_\tau = -\sum_{\nu=1}^{P_{p\alpha N}} \tilde{J}_\nu \tau_{j_\nu^1}\cdots\tau_{j_\nu^{p-1}}\sigma_{i_\nu}, \quad \hat{H}_\tau = -\sum_{\nu=1}^{P_{(p-1)\alpha N}} \hat{J}_\nu \tau_{j_\nu^1}\cdots\tau_{j_\nu^p}$$

(same couplings as the original system) and it is optimal so that we can also state the extended variational principle. The broken replica symmetry ultrametric RaMOSt (which includes as a trivial case the replica symmetric one) relies on the weights ξ_γ of the random probability cascades as in Ref. 7 and on

$$\tilde{H}_\gamma = -\sum_{\nu=1}^{P_{p\alpha N}} \left(\frac{1}{\beta}\ln\frac{\cosh(\beta J)}{\cosh(\beta\tilde{J}_\nu^\gamma)} + \tilde{J}_\nu^\gamma\sigma_{i_\nu}\right),$$

$$\hat{H}_\gamma = -\sum_{\nu=1}^{P_{(p-1)\alpha N}} \left(\frac{1}{\beta}\ln\frac{\cosh(\beta J)}{\cosh(\beta\hat{J}_\nu^\gamma)} + \hat{J}_\nu^\gamma\right)$$

with

$$\tanh(\beta\tilde{J}_\gamma) = \tanh(\beta J)\tilde{W}_\gamma^1\cdots\tilde{W}_\gamma^{p-1},$$

$$\tanh(\beta\hat{J}_\gamma) = \tanh(\beta J)\tilde{W}_\gamma^1\cdots\tilde{W}_\gamma^{p},$$

where $\tilde{W}_\gamma$ are independent copies of

$$\tilde{W}_\gamma(\bar{J},k_\nu) = \tilde{\omega}_{\tilde{\alpha}_1}(\rho_{k_\nu})\bar{J}_{\gamma_1} + \cdots + \tilde{\omega}_{\tilde{\alpha}_R}(\rho_{k_\nu})\bar{J}_{\gamma_1,\cdots,\gamma_R}$$

with $\bar{J}_\cdot = \pm 1$ symmetric.

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Harmonic fields on the extended projective disk and a problem in optics

Thomas H. Otway[a)]
Department of Mathematics, Yeshiva University, New York, New York 10033

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The Hodge equations for 1-forms are studied on Beltrami's projective disk model for hyperbolic space. Ideal points lying beyond projective infinity arise naturally in both the geometric and analytic arguments. An existence theorem for weakly harmonic 1-fields, changing type on the unit circle, is derived under Dirichlet conditions imposed on the noncharacteristic portion of the boundary. A similar system arises in the analysis of wave motion near a caustic. A class of elliptic-hyperbolic boundary-value problems is formulated for those equations as well. For both classes of boundary-value problems, an arbitrarily small lower-order perturbation of the equations is shown to yield solutions which are strong in the sense of Friedrichs. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2098529]

I. INTRODUCTION

The projective disk was introduced by Beltrami[3] in 1868. His construction was an early example of a Euclidean model for a non-Euclidean space, in this case, a space having curvature equal to −1. The projective disk has the striking property that even points infinitely distant from the origin are enclosed by the Euclidean unit circle centered at the origin of $\mathbb{R}^2$. This implies the possibility of points in projective space which lie beyond the curve at infinity. It is known that such *ideal points* arise naturally in the process of constructing normal and translated lines for chords of the projective disk. In this sense ideal points may be said to be intrinsic to the model, rather than only a theoretical possibility allowed by the model. We call the union of the conventional projective disk $\mathbb{P}^2$ and its ideal points the *extended projective disk*.

Hua[9] considered a second-order partial differential equation for scalar functions on the extended projective disk. He proved the existence of solutions to certain boundary-value problems of *Tricomi type*, in which data are given on characteristic curves, which represent trajectories of generalized wavefronts. Hua's work was extended to other problems of Tricomi type by Ji and Chen.[10,11] The existence of a class of weak solutions to the Hodge equations for harmonic 1-fields on extended $\mathbb{P}^2$, with data prescribed only on the noncharacteristic part of the boundary, was proven in Ref. 23. Locally, the Hodge equations reduce in the smooth scalar case to the equation studied by Hua.

This communication provides a geometric and analytic context for such results (Sec. I). In addition, we prove an existence theorem for weakly harmonic 1-fields which includes the results of Ref. 23 as a special case (Sec. II A), and consider a similar system that arises in optics (Secs. III A and III B). Boundary-value problems are formulated for both systems, in which the boundary contains points in both the elliptic and hyperbolic regions of the equations. These problems are shown in Secs. II B and III C to be an arbitrarily small, lower-order perturbation away from problems possessing a unique, strong solution.

a)Electronic mail: otway@ymail.yu.edu

Because both scalar equations and systems are discussed, we distinguish a vector-valued solution by writing it in boldface. However, for typographic simplicity, coefficient matrices and operators are not written in boldface.

A. A geometric classification of linear second-order operators

The highest-order terms of any linear second-order partial differential equation on a domain $\Omega \subset \mathbb{R}^2$ can be written in the form

$$Lu = \alpha(x,y)u_{xx} + 2\beta(x,y)u_{xy} + \gamma(x,y)u_{yy},$$

where (x,y) are coordinates on Ω and α, β, and γ are given functions. (A subscripted variable denotes partial differentiation in the direction of the variable.)

If the discriminant

$$\Delta(x,y) = \alpha\gamma - \beta^2$$

is positive, then the equation associated with the operator L is said to be of *elliptic type*. The simplest example is Laplace's equation, for which $\alpha=\gamma=1$ and $\beta=0$. If the discriminant is negative, then the equation associated with the operator L is said to be of *hyperbolic type*. The simplest example is the normalized wave equation, for which $\alpha=1$, $\gamma=-1$, $\beta=0$; other forms are $\alpha=-1$, $\gamma=1$, $\beta=0$, or $\alpha=\gamma=0$, $\beta=1$. If $\Delta=0$, then the equation associated with the operator L is said to be of *parabolic type;* examples are equations which model diffusion. If the discriminant is positive on part of Ω and negative elsewhere on Ω, then the equation associated with the operator L is said to be of *mixed elliptic-hyperbolic type*. A simple example of an elliptic-hyperbolic equation is the Lavrent'ev–Bitsadze equation, for which $\alpha=\mathrm{sgn}(y)$, $\beta=0$, and $\gamma=1$.

If we take Ω to be a smooth but curved surface, then we may not be able to cover Ω by a single system of Cartesian coordinates. However, we can always introduce Cartesian coordinates (x^1,x^2) *locally* on any smooth surface, in the neighborhood of a point on the surface. In terms of such coordinates, the distance element $\mathrm{d}s$ on Ω can be written in the form

$$\mathrm{d}s^2 = \sum_{i=1}^{2}\sum_{j=1}^{2} g_{ij}(x^1,x^2)\mathrm{d}x^i\,\mathrm{d}x^j,$$

where g_{ij} is a symmetric 2×2 matrix, the *metric tensor* on Ω. [In the sequel we will understand repeated indices to have been summed from 1 to $\dim(\Omega)$ without writing out the summation notation each time.] A natural differential operator on functions u defined on such a space is the *Laplace-Beltrami operator*

$$Lu = \frac{1}{\sqrt{|g|}}\frac{\partial}{\partial x^i}\left(g^{ij}\sqrt{|g|}\frac{\partial u}{\partial x^j}\right),$$

where g^{ij} is the inverse of the matrix g_{ij} and g is its determinant.

Laplace's equation can be associated with the Laplace-Beltrami operator on the Euclidean metric for which g_{ij} is the identity matrix. The wave equation for $\beta=0$ can be associated with the Laplace-Beltrami operator on the two-dimensional Minkowski metric $g_{11}=1$, $g_{22}=-1$, $g_{12}=g_{21}=0$. The Lavrent'ev–Bitsadze equation can be associated with the Laplace-Beltrami operator on a metric which is Euclidean above the x-axis and Minkowskian below the x-axis.

In this classification, the type of a linear second-order equation is not a function of the associated linear operator at all; that operator is always the Laplace-Beltrami operator. Rather, the type of the equation is a feature of the metric tensor on an underlying surface. A Riemannian metric, in which the distance between distinct points of Ω is always positive, corresponds to an elliptic equation, whereas a pseudo-Riemannian metric, for which the distance between distinct points may be zero, corresponds to a hyperbolic equation. The Laplace-Beltrami operator on a surface for which the metric is Riemannian on part of a surface and pseudo-Riemannian elsewhere

will be of mixed elliptic-hyperbolic type. However, any *sonic*—or *parabolic*—curve on which the change of type occurs will necessarily represent a singularity of the metric tensor, as the determinant g will vanish along that curve. (The term *sonic curve* is borrowed from compressible fluid dynamics, in which the equations for the velocity field of a steady ideal flow change from elliptic to hyperbolic type at the speed of sound. The underlying pseudo-Riemannian metric in that case is called the *flow metric*.[4])

One definition of the *signature* of a metric is the sign of the diagonal entries of the metric tensor. Any change in the signature which results in a change in sign of the determinant g will change the Laplace-Beltrami operator on the metric from elliptic to hyperbolic type. The Laplace-Beltrami operator on surface metrics for which such a change occurs along a smooth curve will correspond to planar elliptic-hyperbolic operators in local coordinates.

If we consider the distance element

$$\mathrm{d}s_L^2 \equiv \alpha(x,y)\mathrm{d}y^2 - 2\beta(x,y)\mathrm{d}x\,\mathrm{d}y + \gamma(x,y)\mathrm{d}x^2,$$

then *null geodesics* on the corresponding surface are solutions of the ordinary differential equation

$$\mathrm{d}s_L^2 = 0.$$

The graphs of these solutions are called *characteristic curves* of the equation $Lu=0$. Hyperbolic operators, which are associated with wave propagation, always have real-valued *characteristics,* or null geodesics.

In determining the qualitative behavior of solutions to partial differential equations we often ignore lower-order terms, but this neglect is only justified when considering purely second-order properties such as the nature of the sonic curve. The importance to this paper of lower-order terms is related to the fact that the Laplace-Beltrami equations on the extended projective disk are not of *real principal type* in the sense of Ref. [6]; see Ref. 27 for an accessible discussion of scalar elliptic-hyperbolic operators of real principal type and their properties.

B. The geometry and analysis of ideal points

Here we review basic properties of Laplace-Beltrami equations on Beltrami's hyperbolic metric on the projective disk:

$$\mathrm{d}s^2 = \frac{(1-y^2)\mathrm{d}x^2 + 2xy\,\mathrm{d}x\,\mathrm{d}y + (1-x^2)\mathrm{d}y^2}{(1-x^2-y^2)^2}$$

(see, e.g., Ref. 32, Vol. I, Sec. 65 and Vol. II, Sec. 138, for a derivation). In this metric the unit circle is the *absolute:* the locus of points at infinity.

The existence of points lying beyond the curve at infinity on the projective disk is natural from a geometric point of view. For example, choose a point p in the interior of the projective disk and draw a vertical line ℓ_v through it. A *hyperbolic line* in the Beltrami metric is any open chord of the unit circle, so ℓ_v is a hyperbolic line plus two points at infinity and an *ideal extension* to points outside the unit circle. Denote by $F(p)$ the family of hyperbolic lines created by rotating ℓ_v about p. Move p along the horizontal line ℓ_h through p, and consider the effect of this motion on the family $F(p)$. As p passes through the boundary of the unit circle κ into the $\mathbb{R}^2$ complement of κ, the family of hyperbolic rotations becomes a family of hyperbolic translations. For this reason, hyperbolic translations inside the unit disk can be interpreted as rotations about a point in $\mathbb{R}^2$ lying beyond the unit disk.

As another example, consider that the *pole* of a hyperbolic line ℓ is the intersection of those two tangents to the unit circle which intersect ℓ at the two points of its contact with the unit circle. (We call these the *polar lines* of ℓ.) Thus, any two hyperbolic lines ℓ_1 and ℓ_2 are orthogonal if and only if the pole of ℓ_2 lies on the ideal extension of ℓ_1 and vice versa.

These and other geometric constructions on extended $\mathbb{P}^2$ are described in more detail in Chap. 4 of Ref. 28.

In order to see that ideal points also arise naturally in analysis, consider the Laplace-Beltrami operator on the projective disk with Beltrami's metric. We have

$$L[u] = (1 - x^2 - y^2)[(1 - x^2)u_{xx} - 2xyu_{xy} + (1 - y^2)u_{yy} + \text{lower order terms}].$$

The characteristics of the equation $L[u]=0$ satisfy the ordinary differential equation

$$(1 - y^2)\mathrm{d}x^2 + 2xy\ \mathrm{d}x\ \mathrm{d}y + (1 - x^2)\mathrm{d}y^2 = 0. \tag{1}$$

This equation has solutions

$$x\cos\theta + y\sin\theta = 1, \tag{2}$$

where, as is conventional, we take θ to be the angle between the radial vector and the positive x-axis. Solutions of Eq. (2) correspond geometrically to the family of tangent lines to the unit circle centered at the origin of $\mathbb{R}^2$.

Thus the characteristic lines always include ideal points, and wave propagation can only occur on regions composed of such points.

The Laplace-Beltrami equations on extended $\mathbb{P}^2$ come with a natural gauge theory in the following sense: The characteristic equation is obviously invariant under the projective group. So although the equations in the form in which we study them change type on the unit circle in $\mathbb{R}^2$, they are projectively equivalent to a system which changes type on any conic section. Note that whereas classical gauge theories are invariant under groups of Euclidean motions, which are inertial transformations, this kind of gauge invariance is with respect to a group of non-Euclidean motions, which are noninertial. Also, the gauge theories which are familiar from particle physics act "upstairs" on a fiber bundle of physical states. The transformation group under which the Laplace-Beltrami equations are invariant acts "downstairs" on the underlying metric, in the manner of the gauge group of general relativity. Indeed, analysis of wave motion on extended $\mathbb{P}^2$ has certain similarities to the analysis of wave motion in the vicinity of a light cone (cf. Ref. 30). The timelike and spacelike regions are inverted, and characteristic lines for the Laplace-Beltrami equation are analogous to the paths of photons.

II. HARMONIC 1-FIELDS ON THE EXTENDED PROJECTIVE DISK

We can solve, instead of the Laplace-Beltrami equation, a system of two first-order equations of the form

$$|g|^{-1/2}\partial_i(g^{ij}\sqrt{|g|}u_j) = 0, \tag{3}$$

$$\frac{1}{2}(\partial_i u_j - \partial_j u_i) = 0, \tag{4}$$

where $u_i = u_i(x^1, x^2)$, $i = 1, 2$. As in the second-order equation, g_{ij} is a metric tensor on the underlying surface. Solutions $\mathbf{u} = (u_1, u_2)$ of this first-order system are (locally) *harmonic 1-fields*. Notice that if the scalar function $\varphi(x^1, x^2)$ satisfies $\varphi_{x^1} = u_1$ and $\varphi_{x^2} = u_2$, then φ satisfies the Laplace-Beltrami equations. But there are solutions φ of the Laplace-Beltrami system for which the pair $(\varphi_{x^1}, \varphi_{x^2})$ is not a harmonic 1-field.

Consider a system of first-order equations on $\mathbb{R}^2$ having the form

$$L\mathbf{u} = \mathbf{f}, \tag{5}$$

where

$$L = (L_1, L_2), \quad \mathbf{f} = (f_1, f_2),$$

$$\mathbf{u} = (u_1(x,y), u_2(x,y)), \quad (x,y) \in \Omega \Subset \mathbb{R}^2.$$

Let $\mathbf{u}$ satisfy (5) with

$$(L\mathbf{u})_1 = [(1-x^2)u_1]_x - 2xyu_{1y} + [(1-y^2)u_2]_y + k_1xu_1 + k_2yu_2, \tag{6}$$

and

$$(L\mathbf{u})_2 = (1-y^2)(u_{1y} - u_{2x}) + k_3xu_1 + k_4yu_2, \tag{7}$$

where Ω is chosen so that $y^2 \neq 1$ there. Here k_1, k_2, k_3, and k_4 are constants representing lower-order coefficients. In this section we consider three particular distributions of lower-order terms, studied in Ref. 23:

Case 1: $k_1=k_2=-2$, $k_3=k_4=0$. The domain of Eqs. (5)–(7) in this case will be called Ω_1.

Case 2: $k_1=-2$, $k_2=k_3=0$, $k_4=2$. The domain of Eqs. (5)–(7) in this case will be called Ω_2.

Case 3: $k_1=k_2=k_3=k_4=0$. The domain of Eqs. (5)–(7) in this case will be called Ω_3. This case corresponds to Eqs. (3) and (4).

The union of the domains Ω_1, Ω_2, and Ω_3 will be called Ω.

A system of first-order equations can also be said to be of elliptic or hyperbolic type, and thus may change type along a singular curve. See, e.g., Ref. 5, Chap. III.2. The higher-order terms of the preceding system can be written in the form $A^1\mathbf{u}_x + A^2\mathbf{u}_y$, where

$$A^1 = \begin{bmatrix} 1-x^2 & 0 \\ 0 & -(1-y^2) \end{bmatrix} \tag{8}$$

and

$$A^2 = \begin{bmatrix} -2xy & 1-y^2 \\ 1-y^2 & 0 \end{bmatrix}. \tag{9}$$

If $y^2 \neq 1$, the characteristic equation

$$|A^1 - \lambda A^2| = -(1-y^2)[(1-y^2)\lambda^2 + 2xy\lambda + (1-x^2)]$$

possesses two real roots λ_1, λ_2 on Ω precisely when $x^2+y^2>1$. Thus the system is elliptic in the intersection of Ω with the open unit disk centered at (0, 0) and hyperbolic in the intersection of Ω with the complement of the closure of this disk. The boundary of the unit disk, along which this change in type occurs, is the line at infinity on the projective disk and a line singularity of the tensor g_{ij}.

Denote by Ω a region of the plane for which part of the boundary $\partial\Omega$ consists of a family of curves Γ composed of points satisfying Eq. (1) and the remainder $C=\partial\Omega\backslash\Gamma$ of the boundary consists of points (x,y) which do not satisfy Eq. (1). We seek solutions of Eqs. (5)–(7) which satisfy the boundary condition

$$u_1\frac{dx}{ds} + u_2\frac{dy}{ds} = 0, \tag{10}$$

where s denotes arc length, on the noncharacteristic part C of the domain boundary. Because the tangent vector $\mathbf{T}$ on C is given by

$$\mathbf{T} = \frac{dx}{ds}\mathbf{i} + \frac{dy}{dx}\mathbf{j},$$

a geometric interpretation of this boundary condition is that the dot product of the vector $\mathbf{u} = (u_1, u_2)$ and the tangent vector to C vanishes, i.e., $\mathbf{u}$ is normal to the boundary $\partial\Omega$ on the boundary section C. We call these *homogeneous Dirichlet conditions*.

A. Weak solutions

In Ref. 23, weak solutions to (5)–(7) and (10) are shown to exist in certain weighted L^2 spaces on a class of domains. Here we extend that result to the case in which the domain is formed by the polar lines of a hyperbolic line ℓ and a smooth curve C extending between the two polar lines of ℓ. The curve C must have the property that $\mathrm{d}y_{|C} \leqslant 0$ when $\partial\Omega$ is traversed in a counterclockwise direction. However, as long as this condition is met, C need not intersect the polar lines of ℓ at their points of tangency with the unit circle. Thus C may extend into both the elliptic and the hyperbolic regions.

This domain is the analog of the "ice-cream cone"-shaped domain associated to the *Tricomi equation*[31]

$$yu_{xx} + u_{yy} = 0,$$

where in our case the curve C is the boundary of the ice-cream part and the polar lines, which are characteristics of Eqs. (5)–(7), are the boundary of the cone part. The unit circle is the analog of the x-axis, which is the sonic curve for the Tricomi equation.

We initially consider the distribution of lower-order terms in case 1 of Eqs. (6) and (7). Let θ lie in the interval $[0, \pi/4]$, and denote by Ω_1 the region of the first and fourth quadrants bounded by the characteristic line

$$\Gamma_1 : x \cos\theta + y \sin\theta = 1,$$

the characteristic line

$$\Gamma_2 : x \cos\theta - y \sin\theta = 1,$$

and a smooth curve C. Let C intersect the lines Γ_1, Γ_2 at two distinct points c_1, c_2, respectively. Assume that $\forall (x,y) \in \Omega_1$, $1/\sqrt{2} \leqslant x < \sqrt{2}$ and $-1/\sqrt{2} \leqslant y \leq 1/\sqrt{2}$ and that $\mathrm{d}y \leqslant 0$ on C. A cusp is permitted for $\theta = \pi/4$ at the points $c_1, c_2 = (1/\sqrt{2}, \pm 1/\sqrt{2})$. Otherwise, the boundary will have piecewise continuous tangent (so that Green's theorem can be applied to it). Note that the domain considered in Sec. 3 of Ref. 23 is equivalent to this domain in the degenerate special case $\theta = 0$.

Define U to be the vector space consisting of all pairs of measurable functions $\mathbf{u} = (u_1, u_2)$ for which the weighted L^2 norm

$$\|\mathbf{u}\|_* = \left[\int \int_{\Omega_1} (|2x^2 - 1| u_1^2 + |2y^2 - 1| u_2^2) \mathrm{d}x \, \mathrm{d}y \right]^{1/2}$$

is finite. Notice that this expression vanishes at the intersection of ℓ with its polar lines at the value $\theta = \pi/4$. Denote by W the linear space defined by pairs of functions $\mathbf{w} = (w_1, w_2)$ having continuous derivatives and satisfying:

$$w_1 \mathrm{d}x + w_2 \, \mathrm{d}y = 0 \tag{11}$$

on $\Gamma = \Gamma_1 \cup \Gamma_2$;

$$w_1 = 0 \tag{12}$$

on C; and

$$\int \int_{\Omega_1} [|2x^2 - 1|^{-1} (L^* \mathbf{w})_1^2 + |2y^2 - 1|^{-1} (L^* \mathbf{w})_2^2] \mathrm{d}x \, \mathrm{d}y < \infty.$$

Here

$$(L^* \mathbf{w})_1 = [(1 - x^2) w_1]_x - 2xy w_{1y} + [(1 - y^2) w_2]_y + 2x w_1,$$

and

$$(L^*\mathbf{w})_2 = (1-y^2)(w_{1y} - w_{2x}) + 2yw_1.$$

Define the Hilbert space H to consist of pairs of measurable functions $\mathbf{h}=(h_1,h_2)$ for which the norm

$$\|\mathbf{h}\|^* = \left[\int\int_{\Omega_1} (|2x^2-1|^{-1}h_1^2 + |2y^2-1|^{-1}h_2^2)\mathrm{d}x\,\mathrm{d}y\right]^{1/2}$$

is finite.

We say that $\mathbf{u}$ is a *weak solution* of the system (5)–(7) and (10) in case 1 on Ω_1 if $\mathbf{u}\in U$ and for every $\mathbf{w}\in W$

$$-(\mathbf{w},\mathbf{f}) = (L^*\mathbf{w},\mathbf{u}),$$

where

$$(\mathbf{w},\mathbf{f}) = \int\int_{\Omega_1} (w_1 f_1 + w_2 f_2)\mathrm{d}x\,\mathrm{d}y.$$

In case 2, we restrict the domain Ω_2 to lie in the fourth quadrant of the Cartesian plane. Define $\Gamma_1,\Gamma_2\subset\Gamma$ to be characteristic lines which are tangent to the unit circle at distinct points in the fourth quadrant and which intersect at a point in the complement of the unit disk in $\mathbb{R}^2$. The curve C is defined analogously to the corresponding curve of Ω_1. In particular, $\mathrm{d}y_{|C}\leqslant 0$ on Ω_2 when C is traversed in a counterclockwise direction. Replace U by the space U' of all pairs $\mathbf{u}$ of measurable functions (u_1,u_2) for which the weighted L^2 norm

$$\|\mathbf{u}\|'_* = \left[\int\int_{\Omega_2} (xu_1^2 + |y|u_2^2)\mathrm{d}x\,\mathrm{d}y\right]^{1/2}$$

is finite. Replace W by the space W' defined by pairs of continuously differentiable functions $\mathbf{w}=(w_1,w_2)$ satisfying Eq. (11) on Γ, Eq. (12) on C, and

$$\int\int_{\Omega_2} [x^{-1}(L^*\mathbf{w})_1^2 + |y|^{-1}(L^*\mathbf{w})_2^2]\mathrm{d}x\,\mathrm{d}y < \infty.$$

In this case

$$(L^*\mathbf{w})_1 = [(1-x^2)w_1]_x - 2xyw_{1y} + [(1-y^2)w_2]_y + 2xw_1,$$

and

$$(L^*\mathbf{w})_2 = (1-y^2)(w_{1y} - w_{2x}) - 2yw_2.$$

Finally, we replace H by the space H' of measurable functions $\mathbf{h}=(h_1,h_2)$ for which the norm

$$\|\mathbf{h}\|'^* = \left[\int\int_{\Omega_2} (x^{-1}h_1^2 + |y|^{-1}h_2^2)\mathrm{d}x\,\mathrm{d}y\right]^{1/2}$$

is finite.

Because k_4 is nonzero in case 2, the consistency condition (4) is violated and $\mathbf{u}$ cannot be the gradient of a scalar potential, even locally. Harmonic fields in which condition (4) is violated arise in various contexts—see Sec. 4 of Ref. 25 for a nonlinear example—and correspond physically to stationary fields having sources.

In case 3, we restrict the domain, Ω_3, to lie in the first quadrant. Define $\Gamma_1,\Gamma_2\subset\Gamma$ to be characteristic lines which are tangent to the unit circle at distinct points in the first quadrant, and which intersect at a point in the complement of the unit disk in $\mathbb{R}^2$. In this case we replace U and

H by L^2. We replace W by the space of pairs of L^2 functions (w_1, w_2) which satisfy (11) on Γ and (12) on C. Note that L is self-adjoint in case 3. In addition, we fix positive numbers $\delta \ll 1/2$ and $\varepsilon \ll 1/2$, and require Ω_3 to lie in the semi-infinite rectangle

$$\frac{1}{\sqrt{2}} < x, \quad \frac{1}{\sqrt{2-\delta}} < y \leqslant \sqrt{1-\varepsilon}.$$

Weak solutions in cases 2 and 3 are defined exactly analogously to case 1, with appropriate replacement of the domain and function spaces.

Theorem 1: *Let the lower-order terms in Eqs. (6) and (7) be distributed as in cases 1, 2, or 3, on the domains* Ω_1, Ω_2, *or* Ω_3, *respectively. Then there exists a weak solution of the boundary-value problem (5)–(7) and (10) for every* $\mathbf{f} \in H$.

Proof: The proof is an extension of the arguments in Ref. 23, so we will be brief. We derive a *basic inequality*, that there is a $K \in \mathbb{R}^+$ such that $\forall \mathbf{w} \in W$

$$K\|\mathbf{w}\|_* \leqslant \|L^*\mathbf{w}\|^*$$

(with the norms appropriately adjusted in cases 2 and 3). We derive this inequality by choosing a scalar multiplier a, computing the L^2 inner product $(L^*\mathbf{w}, a\mathbf{w})$, and integrating by parts. Denoting the coefficients of w_1^2 off the boundary by α, those of w_2^2 by γ, and those of $w_1 w_2$ by 2β, we choose, in case 1, $a = x^2$ and obtain

$$\alpha = x(3x^2 - 1), \quad \gamma = x(1 - y^2),$$

and

$$\beta = yx^2,$$

where

$$2\beta w_1 w_2 \geqslant -2x|xw_1||yw_2| \geqslant -(x^3 w_1^2 + xy^2 w_2^2).$$

In case 2 we choose $a = 1$ and obtain

$$\alpha = 2x, \quad \gamma = -2y,$$

and $\beta = 0$.

In case 3 we choose $a = xy$ and obtain

$$\alpha = \frac{y}{2}(3x^2 - 1), \quad \gamma = \frac{y}{2}(1 - y^2),$$

and

$$2\beta = -(1 - y^2)x.$$

The quadratic form $\alpha\gamma - \beta^2$ can be shown to be non-negative in case 3 by noticing that the argument in Sec. 6.2 of Ref. 23 does not use the restriction $x \leqslant 1$ and thus extends to our more general case.

The remainder of the proof is essentially the same for all three cases. Applying Green's theorem to derivatives of products in $(L^*\mathbf{w}, a\mathbf{w})$, we obtain a boundary integral I having the form

$$\int_{\partial\Omega} \frac{a}{2}[(1 - x^2)w_1^2\, dy + 2xyw_1^2\, dx] - \int_{\partial\Omega} a\left[(1 - y^2)w_1 w_2\, dx + \frac{1}{2}(1 - y^2)w_2^2\, dy\right].$$

Because w_1 vanishes identically on C, the boundary integral is non-negative on C by the hypothesis on $dy_{|C}$. On the characteristic curves, we no longer have the property that $dx = 0$, which we used in deriving the basic inequality of Ref. 23. However,

$$I_{|\Gamma} = \int_{\Gamma} \frac{a}{2}\{(1-x^2)w_1^2\,\mathrm{d}y + [2xyw_1^2 - (1-y^2)w_1w_2]\mathrm{d}x\},$$

where we have used the fact that

$$w_2\,\mathrm{d}y = -w_1\,\mathrm{d}x$$

on characteristic lines. In fact, we have

$$\begin{aligned} I_{|\Gamma} &= \int_{\Gamma} \frac{a}{2}\left[(1-x^2)w_1^2\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right) + 2xyw_1^2 - (1-y^2)w_1w_2\right]\mathrm{d}x \\ &= \int_{\Gamma} \frac{a}{2}\left[-(1-x^2)w_1w_2\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2 + 2xyw_1^2 - (1-y^2)w_1w_2\right]\mathrm{d}x, \end{aligned}$$

by the same identity. Equation (1) implies that

$$-(1-x^2)\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2 = 2xy\frac{\mathrm{d}y}{\mathrm{d}x} + 1 - y^2,$$

so we can write

$$I = \int_{\Gamma} \frac{a}{2}\left[2xy\frac{\mathrm{d}y}{\mathrm{d}x} + 1 - y^2\right]w_1w_2\,\mathrm{d}x + \int_{\Gamma} \frac{a}{2}\left[2xyw_1\left(-w_2\frac{\mathrm{d}y}{\mathrm{d}x}\right) - (1-y^2)w_1w_2\right]\mathrm{d}x = 0.$$

This establishes the basic inequality.

Proceeding as in Ref. 19, we use the basic inequality to apply the Riesz representation theorem and obtain an element $\mathbf{h} \in H$ for which

$$-(\mathbf{w},\mathbf{f}) = -(L^*\mathbf{w},\mathbf{h})^*,$$

where the product on the right is the inner product on H (or on H' or L^2 in cases 2 or 3, respectively). Writing h_1 and h_2 of $\mathbf{h}$ in terms of appropriate rescalings of u_1 and u_2,[23] we obtain

$$-(L^*\mathbf{w},\mathbf{h})^* = (L^*\mathbf{w},\mathbf{u}),$$

which completes the proof.

B. Strong solutions

By a *strong solution* of the boundary-value problem (5) and (10) we mean an element $\mathbf{u} \in L^2(\Omega)$ for which there exists a sequence $\mathbf{u}^\nu$ of continuously differentiable vectors satisfying the boundary condition (10), for which

$$\lim_{\nu\to\infty} \|\mathbf{u}^\nu - \mathbf{u}\|_{L^2} = 0,$$

and

$$\lim_{\nu\to\infty} \|L\mathbf{u}^\nu - \mathbf{f}\|_{L^2} = 0.$$

For $\mathbf{u}=(u_1(x,y),u_2(x,y))$, $(x,y) \in \Omega \Subset \mathbb{R}^2$, define the operator $L=(L_1,L_2)$ by the matrix equation

$$L\mathbf{u} = A^1\mathbf{u}_x + A^2\mathbf{u}_y + B\mathbf{u}, \tag{13}$$

for matrices A^1, A^2, and B. We say that L is *symmetric positive*[7,15,16] if the matrices A^1 and A^2 are symmetric and the matrix

$$Q \equiv 2B^* - A_x^1 - A_y^2$$

is bounded below by a positive multiple of the identity matrix. Here

$$B^* = \frac{1}{2}(B + B^t),$$

where for a matrix $W=[w_{ij}]$, $W^t=[w_{ji}]$.

In cases for which L is not symmetric positive, there may be a nonsingular matrix E such that EL is symmetric positive. In that case we replace the equation

$$L\mathbf{u} = \mathbf{f}$$

by the equation

$$EL\mathbf{u} = E\mathbf{f},$$

and try to show that the operator EL is symmetric positive. (The conversion of L into a symmetric-positive operator by the construction of a suitable multiplier E will not be used in this section, but will be used in Sec. III C.)

Suppose that $N(x,y)$, $(x,y) \in \partial\Omega$, is a linear subspace of the vector space V, where $\mathbf{u}$ is regarded as a mapping $\mathbf{u}:\Omega \cup \partial\Omega \to V$, and that $N(x,y)$ depends smoothly on x and y. Define the matrix

$$\beta = n_1 A^1_{|\partial\Omega} + n_2 A^2_{|\partial\Omega},$$

where $\mathbf{n}=(n_1,n_2)$ is the outward-pointing normal vector to $\partial\Omega$. The boundary condition that u lie in N is said to be *admissible*[15] if N is a maximal subspace of V and if the quadratic form $(\mathbf{u},\beta\mathbf{u})$ is non-negative on $\partial\Omega$.

A sufficient condition[7] for admissibility is that there exist a decomposition

$$\beta = \beta_+ + \beta_-,$$

for which the direct sum of the null spaces for β_+ and β_- spans the restriction of V to the boundary, the intersection of the ranges of β_+ and β_- have only the vector $\mathbf{u}=0$ in common, and the matrix $\mu=\beta_+-\beta_-$ satisfies

$$\mu^* = \frac{\mu + \mu^t}{2} \geqslant 0.$$

In this case the boundary condition

$$\beta_-\mathbf{u} = 0 \text{ on } \partial\Omega$$

is admissible for the boundary-value problem

$$L\mathbf{u} = f \text{ in } \Omega.$$

Moreover, the boundary condition

$$\beta_+^t\mathbf{w} = 0 \text{ on } \partial\Omega$$

is admissible for the adjoint problem

$$L^*\mathbf{w} = \mathbf{h} \text{ in } \Omega.$$

These two problems possess unique, strong solutions whenever the differential operators are symmetric positive and the boundary conditions are admissible.[7,15]

In this section we give sufficient conditions for the existence of certain strong solutions arising from an arbitrarily small lower-order perturbation of the Laplace-Beltrami equations on extended $\mathbb{P}^2$. We do so by showing that the differential operator L given by (5)–(7) with $k_1=k_2=k_3=k_4=0$ is arbitrarily close to a symmetric-positive operator and by stating an admissible boundary condition. The existence of strong solutions to a different perturbation on an explicit domain will be shown in Sec. III C.

If the matrices A^1 and A^2 of Eq. (13) are given by Eqs. (8) and (9), and the matrix B is given by

$$\begin{pmatrix} -2x & -2y \\ 0 & 0 \end{pmatrix},$$

then the quantity Q is zero. Thus we replace the matrix B by a matrix B_ε, which differs from B by an arbitrarily small perturbation and takes the form

$$B_\varepsilon = \begin{pmatrix} -2x+\varepsilon_1 & -2y+\varepsilon_2 \\ (1-y^2)\varepsilon_3 & (1-y^2)\varepsilon_4 \end{pmatrix}, \tag{14}$$

where $\varepsilon_1>0$, $\varepsilon_4>0$, and $\varepsilon_2+(1-y^2)\varepsilon_3>0$. If we choose the domain of L in such a way that $y^2<1$ there, then this replacement converts Q into a positive-definite matrix and L into a symmetric-positive operator.

Denote by Ω_4 a domain having C^2 boundary $\partial\Omega_4=E\cup F$ such that $y^2<1$ on Ω_4. Let the components of the normal vector $\mathbf{n}$ on $\partial\Omega_4$ be given by (n_1,n_2). Assume that n_1 and n_2 never vanish at the same point of $\partial\Omega_4$. We place conditions on n_1,n_2, and $\partial\Omega_4$ sufficient to guarantee admissibility of the boundary condition

$$u_1n_2-u_2n_1=0 \tag{15}$$

on F, with no condition given on E.

Let $n_1\geqslant 0, n_2\leqslant 0$ on F and $n_1\leqslant 0, n_2\geqslant 0$ on E. Defining the adjoint space as in Sec. II A, for $\mathbf{w}\in V^*$ we take $\mathbf{w}=(0,w_2)$ on F and

$$w_1n_2-w_2n_1=0$$

on E. Define

$$\alpha=[-(1-y^2)n_2/n_1+2xy-(1-x^2)n_1/n_2]n_2.$$

Assume that $\alpha=0$ on E, and that $\alpha\leqslant 0$ on F.

Theorem 2: *The boundary-value problem*

$$L\mathbf{u}=A^1\mathbf{u}_x+A^2\mathbf{u}_y+B_\varepsilon\mathbf{u}=\mathbf{f},$$

for $(x,y)\in\Omega_4$, *with* A^1, A^2, *and* B_ε *given by Eqs. (8), (9), and (14), respectively, and with condition (15) imposed on the curve F of* $\partial\Omega_4$, *possesses a unique, strong solution* $\mathbf{u}(x,y)$ *for every* $\mathbf{f}\in L^2(\Omega_4)$.

Proof: Because the matrix B_ε has been constructed in such a way that L is symmetric positive, it remains only to show that the boundary condition (15) is admissible on Ω_4.

We have

$$\beta=\begin{pmatrix} -\alpha-(1-y^2)n_2^2/n_1 & (1-y^2)n_2 \\ (1-y^2)n_2 & -(1-y^2)n_1 \end{pmatrix}.$$

Note that the apparent singularities in β at $n_1=0$ and in α at $n_2=0$ are removable.

On F, choose

$$\beta_+ = \begin{pmatrix} -\alpha & 0 \\ 0 & 0 \end{pmatrix}$$

and

$$\beta_- = (1-y^2)n_2 \begin{pmatrix} -n_2/n_1 & 1 \\ 1 & -n_1/n_2 \end{pmatrix}.$$

On E, choose

$$\beta_+ = (1-y^2)n_2 \begin{pmatrix} -n_2/n_1 & 1 \\ 1 & -n_1/n_2 \end{pmatrix}$$

and

$$\beta_- = \begin{pmatrix} -\alpha & 0 \\ 0 & 0 \end{pmatrix}.$$

If $\mathbf{u} \in V_{|F}$, then (15) implies that $\beta_-\mathbf{u}=0$. The properties of V^* imply that $\mathbf{w}^t\beta_+=0$ for $\mathbf{w} \in V^*_{|F}$. If $\mathbf{u} \in V_{|E}$, then $\beta_-\mathbf{u}=0$ for all values of $\mathbf{u}$ and $\mathbf{w}^t\beta_+=0$ by the properties of V^* and α. So the direct sum of the null spaces of β_- and β_+ spans V on $\partial\Omega_4$. Moreover, the hypotheses guarantee that the ranges of β_- and β_+ have only the zero vector in their intersection. Finally,

$$\beta_+ - \beta_- = \mu^* \geqslant 0$$

on both E and F.

This completes the proof of Theorem 2.

III. AN ANALOGOUS PROBLEM FROM OPTICS

Geometrical optics is a zero-wavelength approximation to classical wave mechanics in which the governing differential equations are replaced by the Euclidean geometry of rays. The limitations of the geometrical optics approximation are apparent in the neighborhood of *caustics*, which are envelopes of a family of rays. It is not simply that geometrical optics predicts infinite intensity in such regions, whereas diffractive effects reduce the predicted intensity to a finite number. Even in applications for which the agreement between the predictions of geometrical optics and experiment is generally good, the former may predict singularities, e.g., cusps, which are entirely smoothed out by diffraction. A dramatic example of this for the case of water waves is illustrated in Figs. 5.6.1 and 5.6.2 of Ref. 29. This is, of course, far from the only drawback of the geometrical optics approximation. See, for example, the discussion of the rainbow caustic in Sec. 6.3 of Ref. 22.

The accuracy of the geometrical optics approximation can be improved by considering waves of arbitrarily high frequency obtained by uniform asymptotic approximation of solutions to the Helmholtz equation (Sec. III A). While the older of these approximations also fail at caustics, an asymptotic formula introduced independently by Kravtsov[12] and Ludwig[17] retains its meaning even in the neighborhood of a caustic; see Ref. 13 for a review.

Recently, Magnanini and Talenti studied a nonlinear elliptic-hyperbolic equation, implied by the Ludwig-Kravtsov approximation, having the form[18]

$$(|\nabla v|^4 - v_y^2)v_{xx} + 2v_x v_y v_{xy} + (|\nabla v|^4 - v_x^2)v_{yy} = 0, \tag{16}$$

where $v=v(x,y)$, $(x,y) \in \mathbb{R}^2$. Those authors were able to show the existence of weak solutions to the full Dirichlet problem for the linear elliptic-hyperbolic equation

$$[(p^2+q^2)^2 - p^2]V_{pp} - 2pqV_{pq} + [(p^2+q^2)^2 - q^2]V_{qq} = 0, \tag{17}$$

which is related to Eq. (16) by the *Legendre transformation*

$$V_L(p,q) = xp + yq - v(x,y). \tag{18}$$

Magnanini and Talenti's result is remarkable in that it is difficult to formulate a full Dirichlet problem which is well-posed for a given elliptic-hyperbolic equation, even in the weak sense. (By *full* we mean that data are prescribed on the entire boundary.) Morawetz's proof of the existence of weak solutions to the full Dirichlet problem for the Tricomi equation, the most intensively studied elliptic-hyperbolic equation, required a delicate argument.[20,27] The full Dirichlet problems for other important elliptic-hyperbolic equations remain unknown. For example, the full Dirichlet problem has not been correctly formulated even for weak solutions to a scalar elliptic-hyperbolic equation associated to electromagnetic wave propagation in cold plasma, although a well-posed Dirichlet problem for weak solutions has been formulated for data prescribed only on part of the boundary.[24]

The existence of a well-posed Dirichlet problem is important because physical reasoning often suggests that the full Dirichlet problem is the correct problem even in the case of equations for which mathematical reasoning suggests otherwise.

Two questions suggested by Magnanini and Talenti's paper are

(i) The transformation (18) itself fails at caustics (which are not generally identical to the caustics of the physical model). One would like to characterize regions at which this linearization method fails and the nature of the singularities that arise in such regions. See, for example, Proposition 2 of Ref. 26.

(ii) The result proven in Ref. 18 requires the domain boundary to lie entirely within the elliptic region of the equation. It is an important quality of Eq. (17) that the elliptic region surrounds the hyperbolic region, a property not shared by other elliptic-hyperbolic equations. Thus there is some mathematical interest in asking whether solutions of (17) exist with boundary points lying in both the elliptic and hyperbolic regions, a situation in which this special condition is no longer applicable. We consider this question in Sec. III C.

Equation (16) is a special case of the system

$$[(p^2+q^2)^2 - q^2]p_x + 2pqp_y + [(p^2+q^2)^2 - p^2]q_y = 0, \tag{19}$$

$$p_y - q_x = 0. \tag{20}$$

This system is equivalent to Eq. (16) if there is a continuously differentiable scalar function $v(x,y)$ for which $v_x = p$ and $v_y = q$. [Such a function always exists locally, by Eq. (20).]

Consider any two-dimensional quasilinear system of two equations having the form

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \frac{\partial}{\partial x}\begin{pmatrix} p \\ q \end{pmatrix} + \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} \frac{\partial}{\partial y}\begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{21}$$

where the entries of the coefficient matrices depend only on p and q. Then the coordinate transformation $(x,y) \to (p,q)$ takes Eq. (21) into the linear form

$$\begin{bmatrix} b_{12} & -a_{12} \\ b_{22} & -a_{22} \end{bmatrix} \frac{\partial}{\partial p}\begin{pmatrix} x \\ y \end{pmatrix} + \begin{bmatrix} -b_{11} & a_{11} \\ -b_{21} & a_{21} \end{bmatrix} \frac{\partial}{\partial q}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

provided the Jacobian of the transformation

$$J = \frac{\partial(x,y)}{\partial(p,q)} = \frac{\partial x}{\partial p}\frac{\partial y}{\partial q} - \frac{\partial y}{\partial p}\frac{\partial x}{\partial q}$$

is nonzero. This special case of the Legendre transformation is called a *hodograph map*, and the space having coordinates (p,q) is called the *hodograph plane;* see, e.g., Sec. V.2.2 of Ref. 5.

The coordinate systems (p,q) and (x,y) are related by Eq. (18), where

$$(x,y)=\left(\frac{\partial V}{\partial p},\frac{\partial V}{\partial q}\right)$$

and

$$(p,q)=\left(\frac{\partial v}{\partial x},\frac{\partial v}{\partial y}\right).$$

Applying a hodograph transformation to Eqs. (19) and (20) yields the system

$$[(p^2+q^2)^2-p^2]x_p-2pqx_q+[(p^2+q^2)^2-q^2]y_q=0, \tag{22}$$

$$x_q-y_p=0. \tag{23}$$

This system is equivalent to Eq. (17) if there is a continuously differentiable scalar function $V(x,y)$ for which $V_p=x$ and $V_q=y$. (Again, this can always be arranged locally.)

As in Sec. II, we write the second-order terms of Eqs. (22) and (23) in the form $A^1\mathbf{u}_x+A^2\mathbf{u}_y$, where $\mathbf{u}=\mathbf{u}(x,y)$ and in this case

$$A^1=\begin{bmatrix}(x^2+y^2)^2-x^2 & 0\\ 0 & -1\end{bmatrix}$$

and

$$A^2=\begin{bmatrix}-2xy & (x^2+y^2)^2-y^2\\ 1 & 0\end{bmatrix}.$$

The characteristic equation

$$|A^1-\lambda A^2|=-\{[(x^2+y^2)^2-y^2]\lambda^2+2xy\lambda+[(x^2+y^2)^2-x^2]\}$$

possesses two real roots λ_1,λ_2 precisely when $x^2+y^2>(x^2+y^2)^2$, that is, when $x^2+y^2<1$. Thus the system is hyperbolic at points lying inside the open unit disk centered at $(x,y)=(0,0)$ and elliptic outside the closure of this disk. The circle $x^2+y^2=1$, along which the change in type occurs, is the parabolic region of the system.

A. Uniform asymptotic approximations

Substitution of the simplest formula for an oscillatory wave into the wave equation results in the *Helmholtz equation*

$$\Delta U(\mathbf{x})+k^2\nu^2U(\mathbf{x})=0, \tag{24}$$

where we take $\mathbf{x}$ to be a vector in $\mathbb{R}^2$, and where k and ν are physical constants. In the standard application, ν is the refractive index of the medium and k is inversely proportional to wavelength. In the region of visible light, the wavelength is sufficiently small that k dominates over all other mathematically relevant parameters, an undesirable property known as *stiffness*.

For this reason, short-wave solutions of (24) are usually approximated by *uniform asymptotic expansions*[12,17] which satisfy (24) to arbitrarily high order in k^{-1}. These approximations are valid in regions which contain smooth and convex caustics such as a circular caustic. The size of the region of validity is independent of k. Take $\nu\equiv 1$ and approximate the solution to (24) by an expansion having the form

$$U_{\text{approx}}(x,y)=\left\{Z(k^{2/3}u)\left(\sum_{j=0}^{\infty}W_j(\mathbf{r})\cdot(ik)^{-j}\right)+\frac{i}{k^{1/3}}Z'(k^{2/3}u)\left(\sum_{j=0}^{\infty}X_j(\mathbf{r})\cdot(ik)^{-j}\right)\right\}\times\exp[ikv(x,y)],$$

where $u(x,y)$, $v(x,y)$, $W_j(\mathbf{r})$, and $X_j(\mathbf{r})$ are functions which do not depend on k and which are to

be determined with the solution; the function $Z(t)$ is a solution of the *Airy equation*

$$Z''(t) - tZ(t) = 0,$$

with initial conditions

$$Z(0) = \frac{3^{-2/3}}{\Gamma(2/3)}$$

and

$$Z'(0) = -\frac{3^{-1/3}}{\Gamma(1/3)},$$

where $\Gamma(\,)$ is the gamma function.

This model implies the following system of equations for u and v:

$$u(u_x^2 + u_y^2) - (v_x^2 + v_y^2) + 1 = 0,$$

$$u_x v_x + u_y v_y = 0.$$

In Ref. 18 three possible solutions of this system are enumerated:

$$u = 0, \quad |\nabla v|^2 = 1;$$

$$|\nabla u| = 0, \quad |\nabla v|^2 = 1;$$

the third possibility is that Eq. (16) is satisfied.

Obviously, the third alternative is the most interesting, and this case is studied in Ref. 18. This case is linearized to Eq. (17) by a hodograph transformation.

B. A first-order system

Thus we are led to a system resembling Eqs. (5)–(7):

$$L\mathbf{u} = \mathbf{g}, \tag{25}$$

where

$$L = (L_1, L_2), \quad \mathbf{g} = (g_1, g_2),$$

$$\mathbf{u} = (u_1(x,y), u_2(x,y)), \quad (x,y) \in \Omega \Subset \mathbb{R}^2,$$

$$(L\mathbf{u})_1 = [f(x,y) - x^2]u_{1x} - 2xyu_{1y} + [f(x,y) - y^2]u_{2y}, \tag{26}$$

and

$$(L\mathbf{u})_2 = [f(x,y) - y^2](u_{1y} - u_{2x}), \tag{27}$$

for

$$f(x,y) = (x^2 + y^2)^2. \tag{28}$$

The domain is chosen so that

$$f(x,y) - y^2 \neq 0,$$

under which system (25)–(28) becomes an inhomogeneous generalization of Eqs. (22) and (23). If, in particular, $g_1 = g_2 = 0$, $u_1 = V_x$, and $u_2 = V_y$, where $V(x,y)$ is a scalar function, then Eqs. (25)–(28) reduce to Eq. (17).

As in the preceding sections, the second-order terms of Eqs. (25)–(28) can be written in the form $A^1\mathbf{u}_x + A^2\mathbf{u}_y$, where

$$A^1 = \begin{bmatrix} f(x,y) - x^2 & 0 \\ 0 & -(f(x,y) - y^2) \end{bmatrix}$$

and

$$A^2 = \begin{bmatrix} -2xy & f(x,y) - y^2 \\ f(x,y) - y^2 & 0 \end{bmatrix}.$$

We find that the system is hyperbolic in the intersection of Ω with the open unit disk centered at (0,0) and elliptic in the intersection of Ω with the complement of the closure of this disk.

C. Strong solutions in an annulus

Writing Eq. (17) in polar coordinates $(r,\theta), r \geqslant 0, -\pi < \theta \leqslant \pi$, we obtain[18]

$$(r^2 - 1)V_{rr} + rV_r + V_{\theta\theta} = 0. \tag{29}$$

Letting $u_1 = V_r$ and $u_2 = V_\theta$ transforms Eq. (29) into a first-order system of the form

$$L\mathbf{u} = A^1\mathbf{u}_r + A^2\mathbf{u}_\theta + B\mathbf{u} = \mathbf{f}, \tag{30}$$

with $\mathbf{u} = (u_1(r,\theta), u_2(r,\theta))$, $\mathbf{f} = (0,0)$,

$$A^1 = \begin{pmatrix} r^2 - 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad A^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{31}$$

and

$$B = \begin{pmatrix} r & 0 \\ 0 & 0 \end{pmatrix}.$$

As in Sec. II B, the matrices are symmetric and we find that $Q = 2B^* - A^1_r - A^2_\theta$ is exactly zero, suggesting that an arbitrarily small perturbation of the matrix B will result in a symmetric-positive operator. However we find that we can retain the consistency condition $u_{1\theta} - u_{2r} = 0$ if we employ a multiplier E as described in Sec. II B. Thus we define

$$E = \begin{pmatrix} a & c(1 - r^2) \\ c & a \end{pmatrix},$$

where $a = a(r,\theta)$ and $c = c(r,\theta)$ are continuously differentiable functions to be chosen. We replace B by the matrix

$$B_\varepsilon = \begin{pmatrix} r + \varepsilon_1 & \varepsilon_2 \\ 0 & 0 \end{pmatrix}, \tag{32}$$

where $\varepsilon_1, \varepsilon_2$ are arbitrarily small, strictly negative constants.

Replacing Eq. (30) by the system

$$EL = EA^1\mathbf{u}_r + EA^2\mathbf{u}_\theta + EB_\varepsilon\mathbf{u} = E\mathbf{f}, \tag{33}$$

with A^1, A^2, and B_ε given by Eqs. (31) and (32), we find that EL is a symmetric-positive operator provided we choose $0<\varepsilon_0\leqslant r\leqslant R<\infty$, $a=-r$, and

$$c = -\left(\frac{M}{r} + \theta\right),$$

where M is a large, positive constant.

We will solve Eq. (33) in the annulus Ω_5 given by $\varepsilon_0\leqslant r\leqslant R$, where $R>1$, imposing Dirichlet conditions on the outer boundary and composite boundary conditions on the inner boundary. Annular domains are natural when numerical methods are used to study an equation, such as Eq. (17), which is known to be singular at the origin, with the singular point excluded. The problem is also of some historical interest. An equation differing from (17) only in its lower-order terms was one of the first elliptic-hyperbolic equations to be studied, more than 75 years ago, by Bateman (Sec. 9 of Ref. 1). That equation arose from the solution of Laplace's equation in toroidal coordinates.[2] At the time, Bateman raised the question of the existence and uniqueness of solutions in an annular region containing the unit circle, in which the outer boundary lies in the elliptic region and the inner boundary lies in the hyperbolic region of the equation. Finally, the boundary-value problem in an annulus highlights the similarity between Eqs. (25)–(28) and (5)–(7), as we will use virtually the same argument to solve annular boundary-value problems in the two cases.

Although the system that we consider is a small perturbation of the one studied in Ref. 18, we note that the original equation is itself an approximation, as described in Sec. III A.

Theorem 3: *Equation (33), with boundary conditions*

$$\tau(\theta)u_1 + \sigma(\theta)u_2 = 0, \tag{34}$$

where $\tau(\theta)\sigma(\theta)>0$ *at* $r=\varepsilon_0$ *and* $\sigma=0$, $\tau=1$ *at* $r=R$, *possesses a unique, strong solution on the annulus* Ω_5.

Proof: Although the equations are different, the argument is similar to the proof by Torre[30] of the corresponding assertion for the helically reduced wave equation.

The matrices E and B_ε have been constructed in such a way that the operator EL is manifestly symmetric positive (for large M), and the proof again reduces to a demonstration that the boundary conditions are admissible. At the inner boundary, choose

$$\mathbf{n}_{\text{inner}} = (\varepsilon_0^2 - 1)^{-1}\mathrm{d}r.$$

Then

$$\beta_{\text{inner}} = \begin{pmatrix} a & c \\ c & -(\varepsilon_0^2-1)^{-1}a \end{pmatrix}\mathrm{d}r.$$

Choose

$$\beta_{\text{inner}^-} = \frac{1}{\sigma^2+\tau^2}\begin{pmatrix} \sigma\tau c + \tau^2 a & \sigma^2 c + \sigma\tau a \\ -\sigma\tau(\varepsilon_0^2-1)^{-1}a + \tau^2 c & -\sigma^2(\varepsilon_0^2-1)^{-1}a + \sigma\tau c \end{pmatrix}\mathrm{d}r.$$

Then

$$\beta_{\text{inner}^+} = \frac{1}{\sigma^2+\tau^2}\begin{pmatrix} -\sigma\tau c + \sigma^2 a & \tau^2 c - \sigma\tau a \\ \sigma\tau(\varepsilon_0^2-1)^{-1}a + \sigma^2 c & -\tau^2(\varepsilon_0^2-1)^{-1}a - \sigma\tau c \end{pmatrix}\mathrm{d}r.$$

Notice that $\beta_{\text{inner}^+}+\beta_{\text{inner}^-}=\beta_{\text{inner}}$ and that $\beta_{\text{inner}^-}\mathbf{u}=0$, as (34) implies that $u_2=-(\tau/\sigma)u_1$ on the circle $r=\varepsilon_0$. Moreover,

$$\mu = \frac{1}{\sigma^2+\tau^2}\begin{pmatrix} (\sigma^2-\tau^2)a - 2\sigma\tau c & (\tau^2-\sigma^2)c - 2\sigma\tau a \\ (\sigma^2-\tau^2)c + 2\sigma\tau(\varepsilon_0^2-1)^{-1}a & (\sigma^2-\tau^2)(\varepsilon_0^2-1)^{-1}a - 2\sigma\tau c \end{pmatrix} \mathrm{d}r,$$

implying that

$$\mu^* = \frac{1}{\sigma^2+\tau^2}\begin{pmatrix} (\sigma^2-\tau^2)a - 2\sigma\tau c & \sigma\tau a[(\varepsilon_0^2-1)^{-1}-1] \\ \sigma\tau a[(\varepsilon_0^2-1)^{-1}-1] & (\sigma^2-\tau^2)(\varepsilon_0^2-1)^{-1}a - 2\sigma\tau c \end{pmatrix} \mathrm{d}r.$$

But this matrix is non-negative for our choices of a and c, given that $0<\varepsilon_0<1, \sigma\tau>0$, provided that we choose M sufficiently large.

On the upper boundary we choose

$$\mathbf{n}_{\text{outer}} = (R^2-1)^{-1}\mathrm{d}r.$$

Then

$$\beta_{\text{outer}} = \begin{pmatrix} a & c \\ c & -(R^2-1)^{-1}a \end{pmatrix} \mathrm{d}r.$$

Choose

$$\beta_{\text{outer}^-} = \begin{pmatrix} a & 0 \\ c & 0 \end{pmatrix} \mathrm{d}r.$$

Then

$$\beta_{\text{outer}^+} = \begin{pmatrix} 0 & c \\ 0 & -(R^2-1)^{-1}a \end{pmatrix} \mathrm{d}r.$$

Applying (34) with the Dirichlet condition $\sigma=0$, $\tau=1$, we find that $\beta_{\text{outer}^-}\mathbf{u}=0$ on the circle $r=R$. Moreover,

$$\mu = \begin{pmatrix} -a & c \\ -c & -(R^2-1)^{-1}a \end{pmatrix} \mathrm{d}r,$$

so

$$\mu^* = \begin{pmatrix} -a & 0 \\ 0 & -(R^2-1)^{-1}a \end{pmatrix} \mathrm{d}r.$$

This matrix is positive, as $a<0$ and $R>1$.

Because conditions have been imposed on all of $\partial\Omega_5$, in this case the null space of β_- alone spans V on the boundary.

This completes the proof of Theorem 3.

As expected, this proof fails if the outer boundary is taken to lie inside the unit circle.

We note that we can prove an analogous result for a generalization to systems of an arbitrarily small perturbation of the Laplace-Beltrami equations on extended $\mathbb{P}^2$. As in the case of Theorem 3, we do not need to perturb the compatibility equations in order to obtain strong solutions on the annulus Ω_5. A similar problem was considered in the scalar case by Hua (Sec. III, heuristic consideration 2, of the supplement to Ref. 9); that scalar problem was solved using Fourier expansions.

Write the second-order form of Eqs. (3) and (4) in the polar form

$$r^2(1-r^2)\varphi_{rr} + r(1-2r^2)\varphi_r + \varphi_{\theta\theta} = 0.$$

Let $u_1 = r^2\varphi_r$ and $u_2 = \varphi_\theta$ on the annulus Ω_5. We obtain a first-order system of the form (30) with $\mathbf{f}=0$,

$$A^1 = \begin{pmatrix} 1-r^2 & 0 \\ 0 & -r^2 \end{pmatrix}, \quad A^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{35}$$

and

$$B = \begin{pmatrix} -1/r & 0 \\ 0 & 0 \end{pmatrix}.$$

This operator L is symmetric, but fails to be symmetric positive for $r \leqslant 1$. So we replace B by the matrix

$$B_\varepsilon = \begin{pmatrix} \varepsilon_1 - 1/r & \varepsilon_2 \\ 0 & 0 \end{pmatrix}, \tag{36}$$

for $\varepsilon_1 > 0$ and $\varepsilon_2 > 0$.

Theorem 4: *Define the matrices A^1, A^2, B_ε, as in Eqs. (35) and (36). Impose boundary condition (34), taking $\sigma\tau > 0$ on the outer boundary and $\sigma = 0$, $\tau = 1$ on the inner boundary. Then there exists a unique, strong solution to Eq. (33) on Ω_5 for every $\mathbf{f} \in L^2(\Omega_5)$.*

Proof: Choose

$$E = \begin{pmatrix} a & c(1-r^2)/r^2 \\ c & a \end{pmatrix},$$

where $a = 1/r$ and $c = (M/r) + \theta$, for a sufficiently large constant M. Because ε_1 and ε_2 are positive, the operator EL is symmetric positive.

Choose

$$n_{\text{inner}} = (\varepsilon_0^2 - 1)^{-1} \mathrm{d}r$$

and

$$n_{\text{outer}} = (R^2 - 1)^{-1} \mathrm{d}r.$$

Then

$$\beta(r) = \begin{pmatrix} -a(r) & -c(r,\theta) \\ -c(r,\theta) & [r^2/(1-r^2)]a \end{pmatrix} \mathrm{d}r,$$

where $r = \varepsilon_0$ on the inner radius and $r = R$ on the outer radius. Choose β_{inner^+}, β_{inner^-}, β_{outer^+}, and β_{outer^-} analogously to the choices made in the proof of Theorem 3, with coefficients of the form $r^2 - 1$ in those matrices replaced by coefficients of the form $r^2/(1-r^2)$. The proof is then completed as in the proof of Theorem 3.

We note that if the outer boundary is taken to lie within the elliptic region, then the proof of Theorem 4 will work with Dirichlet conditions imposed on both the inner and outer boundaries, as expected.[14]

IV. A REMARK ON TERMINOLOGY AND NOTATION

Hodge[8] originally considered a p-form ω to be harmonic if it satisfies the first-order equations

$$\mathrm{d}\omega = \delta\omega = 0, \tag{37}$$

where $\mathrm{d}: \Lambda^p \to \Lambda^{p+1}$ is the exterior derivative and $\delta: \Lambda^{p+1} \to \Lambda^p$ is the adjoint of d. If the underlying space is $\mathbb{R}^2$ and ω is a 1-form given by

$$\omega = p\,\mathrm{d}x + q\,\mathrm{d}y,$$

where p and q are continuously differentiable functions, then the Hodge equations (37) reduce to the Cauchy-Riemann equations for p and $-q$. However, although d is independent of the underlying metric, its adjoint δ has a different local form for different metrics. Thus for a surface having metric tensor g_{ij}, the Hodge equations for 1-forms are equivalent to the system (3) and (4). A discussion of exterior forms and their properties is given in, e.g., Ref. 21.

The standard definition of a *harmonic form* is given in terms of a second-order operator: it is a solution of the form-valued Laplace-Beltrami equations

$$(\mathrm{d}\delta + \delta\mathrm{d})\omega = 0.$$

If the domain has *zero boundary* (either no boundary or the prescribed value $\omega \equiv 0$ on the boundary), then the definitions in terms of first- and second-order operators are equivalent. Otherwise, one distinguishes them by calling a form that satisfies Eq. (37) a *harmonic field*. In words, the Hodge equations assert that a harmonic field ω is both *closed* ($\mathrm{d}\omega = 0$) and *coclosed* ($\delta\omega = 0$) under the exterior derivative d. Obviously, every harmonic field is a harmonic form, but the converse is false.

Notice that in Eqs. (6) and (7), $L_1 \neq \delta$ and $L_2 \neq \mathrm{d}$. For example, L_2 includes a factor of $1 - y^2$ whereas d does not, and δ includes determinants of the metric tensor, whereas L_1 does not. In addition, cases 1 and 2 of (6) and (7) include additional lower-order terms. Thus for example δ and d are self-adjoint, whereas L_1 and L_2 are not unless $k_1 = k_2 = k_3 = k_4 = 0$.

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Integrable quasiclassical deformations of cubic curves

Y. Kodama
Department of Mathematics, Ohio State University, Columbus, Ohio 43210

B. Konopelchenko
Dipartimento di Fisica, Universitá di Lecce and Sezione INFN, 73100 Lecce, Italy

L. Martínez Alonso
Departamento de Física Teórica II, Universidad Complutense, E28040 Madrid, Spain

E. Medina
Departamento de Matemáticas, Universidad de Cádiz, E11510 Puerto Real, Cádiz, Spain

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A general scheme for determining and studying hydrodynamic type systems describing integrable deformations of algebraic curves is applied to cubic curves. Lagrange resolvents of the theory of cubic equations are used to derive and characterize these deformations. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The theory of algebraic curves is a fundamental ingredient in the analysis of integrable nonlinear differential equations as it is shown, for example, by its relevance in the description of the finite-gap solutions or the formulation of the Whitham averaging method.[1–8] A particularly interesting problem is characterizing and classifying integrable deformations of algebraic curves. Indeed, as it is shown in a series of recent papers,[9–12] these deformations lie at the crossroads of intricate connections between the theory of random matrices and several models of Laplacian growth processes. It turns out that the integrable models underlying these applications are members of the Whitham hierarchies of dispersionless integrable models introduced by Krichever in Refs. 6 and 7. Moreover, the corresponding solutions are usually characterized in terms of solutions of hydrodynamic systems.

Natural deformations of algebraic curves arise in the dynamics of the *algebraic orbits*[7] of the Whitham hierarchies. For example, algebraic orbits of the Zabolotskaya-Khokhlov dispersionless KP (dKP) hierarchy

$$\frac{\partial k}{\partial t_n} = \{Q_n, k\}, \quad n \geqslant 1, \tag{1}$$

where

$$k = p + \sum_{n=1}^{\infty} \frac{a_n(x,t)}{p^n}, \quad Q_n := (k^n)_{\geqslant 0}, \quad t := (t_1, t_2, \dots) \tag{2}$$

are deformations of algebraic curves

$$f(k) = E(p,x,t), \tag{3}$$

where $E=E(p,x,t)$ is a meromorphic function of p, such that (3) determines a reduction of the dKP hierarchy. In the Gelfand-Dikii case the function E depends on the variables (x,t) through a finite number of functions which evolve according to a system of hydrodynamic type. Neverthe-

less, other deformations of algebraic curves have been formulated which do not correspond to algebraic orbits of the standard dispersionless hierarchies. For example, the integrable hierarchy associated to the *energy-dependent* Schrödinger problem[13] admits a dispersionless limit which leads to a family of deformations of the curves[14,15]

$$p^2 = k^{2N+1} + \sum_{n=1}^{N} u_n k^{2n-1}. \tag{4}$$

These curves do not constitute any reduction of the dKP hierarchy and, as it is shown in Ref. 14, their deformations must be formulated in terms of the singular sectors of a dKdV Grassmannian structure.

A different approach for determining integrable deformations of general algebraic curves $\mathcal{C}$ defined by monic polynomial equations,

$$\mathcal{C}: F(p,k) := p^N - \sum_{n=1}^{N} u_n(k) p^{N-n} = 0, \quad u_n \in \mathbb{C}[k], \tag{5}$$

was proposed in Refs. 14 and 15. It applies for finding deformations $\mathcal{C}(x,t)$ of $\mathcal{C}$ with the deformation parameters (x,t), such that the multiple-valued function $\mathbf{p}=\mathbf{p}(k)$ determined by (5) obeys an equation of the form of conservation laws

$$\partial_t \mathbf{p} = \partial_x \mathbf{Q}, \tag{6}$$

where the flux $\mathbf{Q}$ is given by an element from $\mathbb{C}[k,p]/\mathcal{C}$,

$$\mathbf{Q} = \sum_{r=1}^{N} a_r(k,x,t)\mathbf{p}^{r-1}, \quad a_r \in \mathbb{C}[k].$$

Starting with (6), changing to the dynamical variables u_n and using Lenard-type relations (see Ref. 15) one gets a scheme for finding consistent deformations of (5). One should also note that (6) provides an infinite number of conservation laws, when one expands $\mathbf{p}$ and $\mathbf{Q}$ in Laurent series in z with $k=z^r$ for some r. In this sense, we say that Eq. (6) is integrable.

Our strategy can be applied to the *generic case* where the coefficients (*potentials*) u_n of (5) are general polynomials in k,

$$u_n(k) = \sum_{i=0}^{d_n} u_{n,i} k^i,$$

with all the coefficients $u_{n,i}$ being considered as independent dynamical variables, i.e., $u_{n,i} = u_{n,i}(x,t)$. However, with appropriate modifications, the scheme can be also applied to cases in which constraints on the potentials are imposed. A complete description of these deformations for the generic case of hyperelliptic curves ($N=2$) was given in Ref. 15.

The present paper is devoted to the deformations of cubic curves ($N=3$),

$$p^3 - wp^2 - vp - u = 0, \quad u,v,w \in \mathbb{C}[k], \tag{7}$$

and it considers not only the generic case but also the important constrained case $w \equiv 0$. Although some of the curves may be conformally equivalent (with, for example, the dispersionless Miura transformation), we will not discuss the classification problem under this equivalence in this paper (we will discuss the details of the problem elsewhere). In Sec. II a general approach to construct integrable deformations of algebraic curves is reported briefly. Section III is devoted to the analysis of the cubic case (7). We emphasize the role of Lagrange resolvents, describe the Hamiltonian structure of integrable deformations and present several illustrative examples including Whitham-type deformations.

II. SCHEMES OF DEFORMATIONS OF ALGEBRAIC CURVES

In order to describe deformations of the curve $\mathcal{C}$ defined by (5), one may use the potentials u_n, as well as the N branches $p_i=p_i(k)$ $(i=1,\dots,N)$ of the multiple-valued function $\mathbf{p}=\mathbf{p}(k)$ satisfying

$$F(p,k)=\prod_{i=1}^{N}(p-p_i(k)). \tag{8}$$

The potentials can be expressed as elementary symmetric polynomials s_n (Refs. 16–18) of the branches p_i,

$$u_n=(-1)^{n-1}s_n(p_1,p_2,\dots)=(-1)^{n-1}\sum_{1\leqslant i_1<\cdots<i_n\leqslant N}p_{i_1}\cdots p_{i_n}. \tag{9}$$

However, notice that, according to the famous Abel theorem,[16] for $N>4$ the branches p_i of the generic equation (5) cannot be written in terms of the potentials u_n by means of rational operations and radicals.

There is an important result concerning the branches p_i which is useful in our analysis. Let $\mathbb{C}((\lambda))$ denote the field of Laurent series in λ with at most a finite number of terms with positive powers,

$$\sum_{n=-\infty}^{N}c_n\lambda^n,\quad N\in\mathbb{Z}.$$

Then we have the following.[19,20]

Theorem 1 (Newton theorem): *There exists a positive integer l such that the N branches*

$$p_i(z):=(p_i(k))|_{k=z^l}, \tag{10}$$

are elements of $\mathbb{C}((z))$. Furthermore, if $F(p,k)$ is irreducible as a polynomial over the field $\mathbb{C}((k))$ then $l_0=N$ is the least permissible l and the branches $p_i(z)$ can be labelled so that

$$p_i(z)=p_N(\epsilon^i z),\quad \epsilon:=\exp\frac{2\pi i}{N}.$$

Notation convention: Henceforth, given an algebraic curve $\mathcal{C}$ we will denote by z the variable associated with the least positive integer l_0 for which the substitution $k=z^{l_0}$ implies $p_i\in\mathbb{C}((z))$, $\forall\, i$.The number l_0 will be referred to as the Newton exponent of the curve.

For the generic case the method proposed in Ref. 15 may be summarized as follows: Given an algebraic curve (5), we define an evolution equation for $\mathbf{u}:=(u_1,\dots,u_N)$ in the form

$$\partial_t\mathbf{u}=J_0(T\nabla_{\mathbf{u}}R)_+,\quad R(z,\mathbf{p})=\sum_i f_i(z)p_i, \tag{11}$$

where $(\cdot)_+$ indicates the part of non-negative powers of a Laurent series in k and

$$f_i\in\mathbb{C}((z)),\quad \nabla_{\mathbf{u}}R:=\left(\frac{\partial R}{\partial u_1}\dots\frac{\partial R}{\partial u_N}\right)^{\mathsf{T}},$$
$$J_0:=T^{\mathsf{T}}V^{\mathsf{T}}\partial_x V, \tag{12}$$

$$T := \begin{pmatrix} 1 & -u_1 & \cdots & -u_{N-1} \\ 0 & 1 & \cdots & -u_{N-2} \\ & & \cdots & \\ 0 & & \cdots & 1 \end{pmatrix}, \quad V := \begin{pmatrix} 1 & p_1 & \cdots & p_1^{N-1} \\ & & \cdots & \\ & & \cdots & \\ 1 & p_N & \cdots & p_N^{N-1} \end{pmatrix}. \tag{13}$$

Let d_{nm} and d_n be the degrees of the matrix elements $(J_0)_{nm}$ and the potentials u_n as polynomials in k, respectively. Then (11) defines a deformation of the curve, if d_{nm} and d_n satisfy the consistency conditions

$$\max\{d_{nm}, m = 1,2,3\} \leqslant d_n + 1, \quad n = 1,2,3, \tag{14}$$

and the components of $\nabla_{\mathbf{u}} R$ are in $\mathbb{C}((k))$ with $k = z^{l_0}$.

Equivalently, in terms of branches

$$\mathbf{p} := (p_1, \ldots, p_N)^{\mathsf{T}},$$

the system (11) can be written as

$$\partial_t \mathbf{p} = \partial_x (V \mathbf{r}_+), \tag{15}$$

where

$$\mathbf{r} := T \nabla_{\mathbf{u}} R(z, \mathbf{p}) = V^{-1} \mathbf{f}(z), \tag{16}$$

with $\mathbf{f}(z) := (f_1(z), \ldots, f_N(z))^{\mathsf{T}}$. Notice that $\mathbf{r}$ is a solution of the Lenard relation

$$J_0 \mathbf{r} = 0. \tag{17}$$

Although there is not a general procedure for analyzing constrained cases, one may try a similar strategy. First, we start from the equation for branches (6) and then, by expressing the potentials in terms of the independent branches only, we look for a formulation of the flows as

$$\partial_t \mathbf{u} = J_0 \mathbf{a}, \quad \mathbf{a} := (a_1, \ldots, a_N)^{\mathsf{T}}, \tag{18}$$

for a certain operator J_0. Finally, we use solutions $\mathbf{r}$ of Lenard relations (17) and set $\mathbf{a} = \mathbf{r}_+$.

Another scheme for defining integrable deformations of algebraic curves of genus *zero* (i.e., rational curve) is implicit in the theory of integrable systems of dispersionless type developed in Refs. 7 and 8 which we refer to them as the Whitham deformations. It is concerned with algebraic curves characterized by equations of the form

$$k = p^N + v_{N-2} p^{N-2} + \cdots + v_0 + \sum_{r=1}^{M} \sum_{i=1}^{n_r} \frac{v_{r,i}}{(p - w_r)^i}, \tag{19}$$

where v_n, $v_{r,i}$, w_r are k-independent coefficients. These curves arise in the theory of algebraic orbits of the genus-zero Whitham hierarchy,[7,8] where the function k represents the Landau-Ginzburg potential of the associated topological field theory. We may rewrite the equation of the curve (19) in the polynomial form (5) with potentials u_n of degrees $d_n \leqslant 1$ and satisfying a certain system of constraints.

To describe the deformations of (19) determined by Whitham flows we introduce local coordinates $\{z_0, z_1, \ldots, z_M\}$ of the extended p-plane at the punctures $\{w_0 := \infty, w_1, \ldots, w_M\}$ such that

$$k = z_0^N = z_1^{n_1} = \cdots = z_{n_M}^{n_M}. \tag{20}$$

It is clear that there are N branches of $\mathbf{p}$ which have expansions in powers of $k^{1/N}$ and that, for each puncture w_r, $(r = 1, \ldots, M)$, there are n_r branches of $\mathbf{p}$ having expansions in powers of k^{1/n_r}. Therefore, the Newton exponent l_0 is given by the least common multiple of the set of integers

$\{N, n_1, \ldots, n_M\}$. Furthermore, it is clear that only in the absence of finite punctures ($M=0$) the curve (19) is irreducible over $\mathbb{C}((k))$.

At each puncture in $\{\infty, w_1, \ldots, w_M\}$, there is an infinite family of Whitham deformations of (19). They can be expressed by equations of the form (see Refs. 7 and 8)

$$\partial_t \mathbf{p} = \partial_x \mathbf{Q}_{\alpha,n}, \tag{21}$$

where

$$\mathbf{Q}_{\alpha,n} = (z_\alpha^n)_\oplus(\mathbf{p}), \quad \alpha = 0,1,\ldots,M,\ n \geqslant 1,$$

$$\mathbf{Q}_{r,0} = \ln(\mathbf{p} - w_r), \quad r = 1,\ldots,M.$$

Here $(z_\alpha^n)_\oplus$ stands for the singular part of $z_\alpha^n(p)$ at the puncture w_α, with $(z_r^n)_\oplus(\infty)=0$ for $1 \leqslant r \leqslant M$. There exist also commuting flows for the negative n in (21) with logarithmic terms which correspond to the descendant flows of $Q_{r,0}$ (see Ref. 8 for the details).

In the absence of finite punctures ($M=0$), Whitham deformations become the dispersionless Gelfand-Dikii flows. They can be described by our scheme[15] as the reductions $u_1 \equiv 0$, $u_N = k - v_0$ of the generic case corresponding to $d_n = \delta_{Nn}$. However, for $M \geqslant 1$ it can be seen that, in general, Whitham deformations of (19) are not reductions of the flows (11) provided by our method. Some examples of this situation for cubic curves are shown below.

III. DEFORMATIONS OF CUBIC CURVES

For our subsequent analysis we introduce a basic tool of the theory of third order polynomial equations,[16] the so-called *Lagrange resolvents*, defined by

$$\mathcal{L}_i := \sum_{j=1}^{3} (\epsilon^i)^j p_j, \quad i = 1,2,3, \quad \epsilon := e^{2\pi i/3}, \tag{22}$$

or, equivalently,

$$\mathcal{L}_1 := \epsilon p_1 + \epsilon^2 p_2 + p_3,$$

$$\mathcal{L}_2 := \epsilon^2 p_1 + \epsilon p_2 + p_3,$$

$$\mathcal{L}_3 := p_1 + p_2 + p_3.$$

They can be expressed in terms of the potentials $\mathbf{u} = (w, v, u)^{\mathsf{T}}$ by using the identities

$$\mathcal{L}_1 \cdot \mathcal{L}_2 = 3v + w^2, \quad \mathcal{L}_3 = w,$$

$$\mathcal{L}_1^3 + \mathcal{L}_2^3 = 27u + 9vw + 2w^3,$$

which lead to

$$2\mathcal{L}_1^3 = 27u + 9vw + 2w^3 + \sqrt{(27u + 9vw + 2w^3)^2 - 4(3v + w^2)^3},$$

$$2\mathcal{L}_2^3 = 27u + 9vw + 2w^3 - \sqrt{(27u + 9vw + 2w^3)^2 - 4(3v + w^2)^3}.$$

The fundamental advantage of Lagrange resolvents is that they provide explicit expressions of the branches p_i in terms of the potentials according to Cardano formulas

$$3p_i = \sum_{j=1}^{3} (\epsilon^{-i})^j \mathcal{L}_j, \quad i = 1,2,3, \tag{23}$$

or, equivalently,

$$3p_1 = \epsilon^2 \mathcal{L}_1 + \epsilon \mathcal{L}_2 + \mathcal{L}_3,$$

$$3p_2 = \epsilon \mathcal{L}_1 + \epsilon^2 \mathcal{L}_2 + \mathcal{L}_3,$$

$$3p_3 = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3.$$

As we will prove below, the Lagrange resolvents are essential to determine consistent deformations of cubic equations.

A. Generic case

As it was found in, Ref. 15 for $N=3$ the operator J_0 reads

$$J_0 = \begin{pmatrix} 3\partial_x & w\partial_x + w_x & (2v + w^2)\partial_x + (2v + w^2)_x \\ -2w\partial_x & 2v\partial_x + v_x & (3u + vw)\partial_x + 2u_x + 2vw_x \\ -v\partial_x & 3u\partial_x + u_x & uw\partial_x + 2uw_x \end{pmatrix}. \tag{24}$$

Thus if d_1, d_2, and d_3 are the degrees in k of the potential functions w, v, and u, respectively, the consistency conditions (14) are

$$d_1 \leqslant 1, \quad d_2 \leqslant d_1 + 1,$$

$$d_3 \leqslant d_2 + 1, \quad d_2 \leqslant d_3 + 1,$$

which lead to the following 12 nontrivial choices for (d_1, d_2, d_3):

$$\begin{gathered} (0,0,1), \quad (0,1,0), \quad (0,1,1), \quad (0,1,2), \\ (1,0,0), \quad (1,0,1), \quad (1,1,0), \quad (1,1,1), \\ (1,1,2), \quad (1,2,1), \quad (1,2,2), \quad (1,2,3). \end{gathered} \tag{25}$$

By using (23) and (24) it is straightforward to determine the Newton exponent l_0 for each of the cases (25). Thus one finds three categories

l_0	3	2	1
	(0,0,1), (0,1,2)	(0,1,0), (0,1,1,)	(1,0,1), (1,1,0)
		(1,0,0), (1,1,2)	(1,1,1), (1,2,1)
			(1,2,2), (1,2,3)

Only the cases with $l_0=3$ correspond to irreducible curves over the field $\mathbb{C}((k))$. We also note here that our deformations for the trigonal curves (5) in the generic case allow one to have only the curves with genus less than or equal to 1 (the details will be discussed elsewhere).

Once the Newton exponent l_0 is known, in order to derive the associated hierarchy of integrable deformations according to our scheme, two steps are still required:

(1) To determine the functions $R(z,\mathbf{p})=\Sigma_i f_i(z)p_i$ such that the components of $\nabla_{\mathbf{u}}R$ are in $\mathbb{C}((k))$ with $k=z^{l_0}$.
(2) To find the explicit form of the gradients $\nabla_{\mathbf{u}}R$ in terms of the potentials.

Both problems admit a convenient treatment in terms of Lagrange resolvents. Thus by introducing the following element σ_0 of the Galois group of the curve:

$$\sigma_0(p_i)(z) := p_i(\epsilon_0 z), \quad \epsilon_0 := e^{2\pi i/l_0}, \tag{26}$$

we see that our first problem can be fixed by determining functions R invariants under σ_0, i.e., $R(\epsilon_0 z, \sigma_0 \mathbf{p}) = R(z, \mathbf{p})$. In this way, we have the following forms of R.

For the case $l_0=3$, the element σ_0 is given by the permutation

$$\sigma_0 = \begin{pmatrix} p_1 & p_2 & p_3 \\ p_2 & p_3 & p_1 \end{pmatrix}, \tag{27}$$

or, in terms of Lagrange resolvents,

$$\sigma_0 = \begin{pmatrix} \mathcal{L}_1 & \mathcal{L}_2 & \mathcal{L}_3 \\ \epsilon^2 \mathcal{L}_1 & \epsilon \mathcal{L}_2 & \mathcal{L}_3 \end{pmatrix}. \tag{28}$$

Thus we get the invariant functions

$$R = z f_1(z^3)\mathcal{L}_1 + z^2 f_2(z^3)\mathcal{L}_2 + f_3(z^3)\mathcal{L}_3, \tag{29}$$

with $f_i(z^3)$ being arbitrary functions in $\mathbb{C}((z^3))$.

For the case $l_0=2$, σ_0^2 is the identity permutation, so that under the action of σ_0 two branches are interchanged while the other remains invariant. If we label the branches in such a way that

$$\sigma_0 = \begin{pmatrix} p_1 & p_2 & p_3 \\ p_2 & p_1 & p_3 \end{pmatrix}, \tag{30}$$

then

$$\sigma_0 = \begin{pmatrix} \mathcal{L}_1 & \mathcal{L}_2 & \mathcal{L}_3 \\ \mathcal{L}_2 & \mathcal{L}_1 & \mathcal{L}_3 \end{pmatrix}, \tag{31}$$

and we obtain the invariant functions

$$R = f_1(z^2)(\mathcal{L}_1 + \mathcal{L}_2) + z f_2(z^2)(\mathcal{L}_1 - \mathcal{L}_2) + f_3(z^2)\mathcal{L}_3, \tag{32}$$

where $f_i(z^2)$ are arbitrary functions in $\mathbb{C}((z^2))$.

For the case $l_0=1$, we have $z=k$ and σ_0 is the identity, so that any function $R(k, \mathbf{p})$ is invariant under σ_0.

Now the problem of finding the gradients of R reduces to determine the gradients of the Lagrange resolvents. To this end we differentiate (23) and obtain

$$\mathcal{L}_2 \nabla_{\mathbf{u}} \mathcal{L}_1 + \mathcal{L}_1 \nabla_{\mathbf{u}} \mathcal{L}_2 = (2w, 3, 0)^{\mathsf{T}},$$

$$\mathcal{L}_1^2 \nabla_{\mathbf{u}} \mathcal{L}_1 + \mathcal{L}_2^2 \nabla_{\mathbf{u}} \mathcal{L}_2 = (2w^2 + 3v, 3w, 9)^{\mathsf{T}},$$

so that

$$(\mathcal{L}_1^3 - \mathcal{L}_2^3)\nabla_{\mathbf{u}} \mathcal{L}_1 = ((2w^2 + 3v)\mathcal{L}_1 - 2w\mathcal{L}_2^2, 3(w\mathcal{L}_1 - \mathcal{L}_2^2), 9\mathcal{L}_1)^{\mathsf{T}},$$

$$(\mathcal{L}_2^3 - \mathcal{L}_1^3)\nabla_{\mathbf{u}} \mathcal{L}_2 = ((2w^2 + 3v)\mathcal{L}_2 - 2w\mathcal{L}_1^2, 3(w\mathcal{L}_2 - \mathcal{L}_1^2), 9\mathcal{L}_2)^{\mathsf{T}}.$$

Hence the gradients of the generic density R for (29) and (32) are given as follows.

For $l_0=3$, we have

$$\nabla_{\mathbf{u}}R = \frac{zf_1(z^3)}{\mathcal{L}_1^3 - \mathcal{L}_2^3}\begin{pmatrix} (2w^2+3v)\mathcal{L}_1 - 2w\mathcal{L}_2^2 \\ 3(w\mathcal{L}_1 - \mathcal{L}_2^2) \\ 9\mathcal{L}_1 \end{pmatrix} - \frac{z^2 f_2(z^3)}{\mathcal{L}_1^3 - \mathcal{L}_2^3}\begin{pmatrix} (2w^2+3v)\mathcal{L}_2 - 2w\mathcal{L}_1^2 \\ 3(w\mathcal{L}_2 - \mathcal{L}_1^2) \\ 9\mathcal{L}_2 \end{pmatrix} + f_3(z^3)\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

For $l_0=2$, we get

$$\nabla_{\mathbf{u}}R = \frac{f_1(z^2)}{\mathcal{L}_1^3 - \mathcal{L}_2^3}\begin{pmatrix} (2w^2+3v)(\mathcal{L}_1 - \mathcal{L}_2) + 2w(\mathcal{L}_1^2 - \mathcal{L}_2^2) \\ 3(w\mathcal{L}_1 - \mathcal{L}_2^2) - 3(w\mathcal{L}_2 - \mathcal{L}_1^2) \\ 9(\mathcal{L}_1 - \mathcal{L}_2) \end{pmatrix}$$
$$+ \frac{zf_2(z^2)}{\mathcal{L}_1^3 - \mathcal{L}_2^3}\begin{pmatrix} (2w^2+3v)(\mathcal{L}_1 + \mathcal{L}_2) - 2w(\mathcal{L}_1^2 + \mathcal{L}_2^2) \\ 3(w\mathcal{L}_1 - \mathcal{L}_2^2) + 3(w\mathcal{L}_2 - \mathcal{L}_1^2) \\ 9(\mathcal{L}_1 + \mathcal{L}_2) \end{pmatrix} + f_3(z^2)\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

From these expressions and (28) and (31) it follows that the corresponding components of $\nabla_{\mathbf{u}}R$ are in $\mathbb{C}((k))$.

Example 1: The case $l_0=3$ with $(d_1,d_2,d_3)=(0,0,1)$. Taking into account (24) and (23) it is clear that there are two trivial equations corresponding to w_0 and u_1. Then, we take for the potentials

$$w = 1, \quad v = v_0(x,t), \quad u = k + u_0(x,t).$$

Thus, by using (29) with

$$f_1 \equiv f_3 \equiv 0, \quad f_2(z^3) = \frac{27(1-\sqrt{3}i)}{4}z^3,$$

we obtain

$$v_{0t} = \tfrac{5}{3}(2 + 27u_0 + 9v_0)u_{0x} + \tfrac{5}{18}(7 + 54u_0 + 36v_0 + 27v_0^2)v_{0x},$$

$$u_{0t} = \tfrac{5}{18}(-1 - 54u_0 + 27v_0{}^2)u_{0x} + \tfrac{5}{9}v_0(2 + 27u_0 + 9v_0)v_{0x}.$$

It can be checked that this system corresponds to the one obtained by setting $M=0$, $N=3$ in (19), and $\alpha=0$, $n=5$ in (21).

Example 2: The case $l_0=2$ with $(d_1,d_2,d_3)=(0,1,0)$, $(l_0=2)$. From (24) and (23) we see that $v_{1t}=0$. We then take

$$w = w_0(x,t), \quad v = k + v_0(x,t), \quad u = u_0(x,t),$$

and

$$f_1(z^2) = z^4, \quad f_2 \equiv f_3 \equiv 0.$$

Thus it follows

$$w_{0t} = 4(w_0u_{0x} + v_0v_{0x} + u_0w_{0x}),$$

$$v_{0t} = -2(w_0^2u_{0x} - 2u_0v_{0x} + u_0w_0w_{0x}) + 2v_0(2u_{0x} - w_0v_{0x}),$$

$$u_{0t} = -2(v_0w_0u_{0x} + u_0(-2u_{0x} + w_0v_{0x} + v_0w_{0x})).$$

It turns out that this system can also be found among the Whitham deformations, by setting $M=1$, $N=2$ in (19), and $\alpha=0$, $n=4$ in (21).

Example 3: The case $l_0=2$ with $(d_1,d_2,d_3)=(1,0,0)$. From (23) and (24) it is easy to see that $(u_0/w_1)_t=0$. If we choose

$$w(k,x,t)=w_1(x,t)k+w_0(x,t),\quad v(k,x,t)=v_0(x,t),$$

$$u(k,x,t)=w_1(x,t),$$

and set

$$f_1(z^2)=z^4,\quad f_2\equiv f_3\equiv 0$$

in (32), then the following system arises:

$$w_{1t}=2w_1^{-2}(w_1w_{0x}-w_0w_{1x}),$$

$$w_{0t}=2w_1^{-3}(w_1(v_{0x}+w_0w_{0x})-(2v_0+w_0^2)w_{1x}),$$

$$v_{0t}=w_1^{-3}(-4w_1w_{1x}+2v_0(w_1w_{0x}-w_0w_{1x})).$$

This is one of the flows in the dispersionless Dym hierarchy corresponding to the curve, $w_1k=p-w_0-v_0p^{-1}-w_1p^{-2}$. Also note that the linear flow, i.e., $w_{1t}=cw_{1x}$, etc., with $c=$constant, can be obtained by the choice $f_2\propto z^{-2}$ with $f_1=f_3=0$.

Example 4: The case $l_0=1$ with $(d_1,d_2,d_3)=(1,0,1)$. From (23) and (24) one finds that $(u_1/w_1)_t=0$. By setting

$$w(k,x,t)=w_1(x,t)k+w_0(x,t),\quad v(k,x,t)=v_0(x,t),$$

$$u(k,x,t)=w_1(x,t)k+u_0(x,t),$$

and

$$R=\frac{2(1+\sqrt{3}i)}{\sqrt{3}}k\mathcal{L}_1,$$

we obtain

$$w_{1t}=u_{0x}+w_{0x},$$

$$w_{0t}=w_1^{-2}(w_1(v_{0x}+u_0w_{0x})-(3+v_0)w_{1x}-w_0^2w_{1x}+w_0(w_1(u_{0x}+2w_{0x})-u_0w_{1x})),$$

$$v_{0t}=w_1^{-2}(w_1(2(2+v_0)u_{0x}+u_0v_{0x}+w_0v_{0x}+2v_0w_{0x})-2(u_0(3+v_0)-(1-v_0)w_0)w_{1x}),$$

$$u_{0t}=w_1^{-2}(-w_0w_1u_{0x}-3u_0^2w_{1x}+v_0(w_1v_{0x}+(1-v_0)w_{1x})+u_0(w_1(4u_{0x}+w_{0x})+w_0w_{1x})).$$

We also note that the linear flow is obtained by choosing $R\propto\mathcal{L}_1$, and the higher flows in the hierarchy can be obtained by $R\propto k^n\mathcal{L}_1$.

Example 5: The case $l_0=1$ with $(d_1,d_2,d_3)=(1,1,0)$. From (23) and (24) we deduce that $(v_1/w_1)_t=0$. Now we take

$$w(k,x,t)=w_1(x,t)k+w_0(x,t),\quad v(k,x,t)=w_1(x,t)k+v_0(x,t),$$

$$u(k,x,t)=u_0(x,t)$$

and set

$$R = \frac{\sqrt{3}+i}{2\sqrt{3}} k\mathcal{L}_2.$$

Then the following system is obtained:

$$w_{1t} = 2u_{0x} - v_{0x},$$

$$w_{0t} = w_1^{-2}(w_1((3+2w_0)u_{0x} - (2+w_0)v_{0x} + (2u_0 - v_0)w_{0x}) + (v_0(2+w_0) - u_0(3+2w_0))w_{1x}),$$

$$v_{0t} = w_1^{-2}(w_1((-2+4v_0-2w_0)u_{0x} + (2u_0 - 3v_0 + w_0)v_{0x}) + (v_0(2v_0 - w_0) + u_0(3-4v_0+2w_0))w_{1x}),$$

$$u_{0t} = w_1^{-2}((-2v_0 + w_0)w_1u_{0x} - 6u_0^2w_{1x} + u_0(w_1(8u_{0x} - 3v_{0x} + w_{0x}) + 2(2v_0 - w_0)w_{1x})).$$

B. Hamiltonian structures

The general structure of integrable deformations (11) does not exhibit a direct Hamiltonian form. However, the analysis of particular cases reveals the presence of certain Hamiltonian structures. We look for a Hamiltonian operator J such that for certain appropriate densities R it verifies

$$J_0(T\nabla_{\mathbf{u}}R)_+ = J(\nabla_{\mathbf{u}}R)_+, \tag{33}$$

where

$$T := \begin{pmatrix} 1 & -w & -v \\ 0 & 1 & -w \\ 0 & 0 & 1 \end{pmatrix}.$$

Thus, if (33) holds then the flows (11) can be written in the pre-Hamiltonian form

$$\partial_t \mathbf{u} = J(\nabla_{\mathbf{u}}R)_+. \tag{34}$$

To achieve our aim we require a k-independent operator T_0 verifying

$$T\nabla_{\mathbf{u}}R = T_0\nabla_{\mathbf{u}}R, \tag{35}$$

so that $J := J_0 \cdot T_0$ is a Hamiltonian operator.

Let us consider first the case $l_0=3$. It involves two classes of cubic curves.

For the case with $(d_1,d_2,d_3)=(0,0,1)$, the potentials are of the form

$$w = w_0(x), \quad v(x) = v_0(x), \quad u = u_0(x) + ku_1(x).$$

The matrix T is k independent so that by setting $J=J_0 \cdot T$ we find the Hamiltonian operator

$$J = \begin{pmatrix} 3\partial_x & -2\partial_x \cdot w & -\partial_x \cdot v \\ -2w\partial_x & 2w\partial_x \cdot w + 2v\partial_x + v_x & (3u+vw)\partial_x + 2u_x + wv_x \\ -v\partial_x & (3u+vw)\partial_x + vw_x + u_x & v\partial_x \cdot v - 2uw\partial_x - (uw)_x \end{pmatrix}. \tag{36}$$

It represents the dispersionless limit of the Hamiltonian structure of the Boussinesq hierarchy.

For the case with (0,1,2) the potentials now are

$$w = w_0(x), \quad v(x) = v_0(x) + kv_1(x),$$

$$u = u_0(x) + ku_1(x) + k^2u_2(x).$$

From (33) one deduces

$$T\nabla_{\mathbf{u}}\mathcal{L}_i = T_0\nabla_{\mathbf{u}}\mathcal{L}_i, \quad i=1,2,$$

$$T\nabla_{\mathbf{u}}\mathcal{L}_3 = \mathcal{L}_3, \tag{37}$$

where T_0 is the k-independent matrix

$$T_0 = \begin{pmatrix} -2 & w & 0 \\ 0 & 1 & -w \\ 0 & 0 & 1 \end{pmatrix}. \tag{38}$$

Moreover $J := J_0 \cdot T_0$ takes the Hamiltonian form

$$J = \begin{pmatrix} -6\partial_x & 4\partial_x \cdot w & 2\partial_x \cdot v \\ 4w\partial_x & -2w\partial_x \cdot w + 2v\partial_x + v_x & (3u - vw)\partial_x + 2u_x - wv_x \\ 2v\partial_x & (3u - vw)\partial_x - vw_x + u_x & -2uw\partial_x - (uw)_x \end{pmatrix}. \tag{39}$$

Thus by setting

$$R = zf_1(z^3)\mathcal{L}_1 + z^2 f_2(z^3)\mathcal{L}_2,$$

equation (11) reduces to the form (34).

For the remaining cases of $l_0=2$ and $l_0=1$, the situation is as follows:

(1) For the sets of degrees (0,1,0) and (0,1,1) for $l_0=2$, the identities (37) with the same operator (38) hold, so that by setting

$$R = f_1(z^2)(\mathcal{L}_1 + \mathcal{L}_2) + zf_2(z^2)(\mathcal{L}_1 - \mathcal{L}_2),$$

Eq. (11) reduces to the form (34) with the Hamiltonian operator (39).

(2) For the sets of degrees (two cases of $l_0=2$ and all the cases of $l_0=1$),

$$(1,0,0),\ (1,0,1),\ (1,1,0),\ (1,1,1),$$

$$(1,1,2),\ (1,2,1),\ (1,2,2),\ (1,2,3),$$

there is no k-independent operator T_0 satisfying (36) for $\nabla_{\mathbf{u}}\mathcal{L}_i$, $(i=1,2)$.

C. Deformations of cubic curves with $w=0$

Deformations of cubic curves of the form

$$p^3 - vp - u = 0, \tag{40}$$

cannot be obtained simply by setting $w=0$ in the above analysis. Indeed, as it is clear from the expression (24) for J_0, the constraint $w=0$ does not constitute a reduction of the flows (11). Therefore, we must apply our deformation scheme to (40) directly.

In terms of the branches p_i the condition $w=0$ reads

$$p_1 + p_2 + p_3 = 0,$$

which is preserved by deformations

$$\partial_t p_i = \partial_x(a_1 + a_2 p_i + a_3 p_i^2) \tag{41}$$

satisfying

$$3a_1 = -(p_1^2 + p_2^2 + p_3^2)a_3. \tag{42}$$

By expressing the potentials as functions of the branches p_1 and p_2,

$$v = p_1^2 + p_2^2 + p_1p_2, \quad u = -(p_1^2p_2 + p_1p_2^2), \tag{43}$$

and using (41) and (42), we obtain

$$\partial_t \mathbf{u} = \mathcal{J}_0 \mathbf{a}, \quad \mathbf{u} := (v\ u)^{\mathsf{T}}, \quad \mathbf{a} := (a_1\ a_2)^{\mathsf{T}}, \tag{44}$$

where

$$\mathcal{J}_0 = \begin{pmatrix} 2p_1 + p_2 & 2p_2 + p_1 \\ -2p_1p_2 - p_2^2 & -2p_1p_2 - p_1^2 \end{pmatrix} \partial_x \begin{pmatrix} p_1 & \frac{1}{3}p_1^2 - \frac{2}{3}(p_2^2 + p_1p_2) \\ p_2 & \frac{1}{3}p_2^2 - \frac{2}{3}(p_1^2 + p_1p_2) \end{pmatrix} = \begin{pmatrix} 2v\partial_x + v_x & 3u\partial_x + 2u_x \\ 3u\partial_x + u_x & \frac{1}{3}(2v^2\partial_x + 2vv_x) \end{pmatrix}. \tag{45}$$

According to our strategy for finding consistent deformations, we use Lenard-type relations

$$\mathcal{J}_0 \mathbf{R} = 0, \quad \mathbf{R} := (r_1\ r_2)^{\mathsf{T}}, \quad r_i \in \mathbb{C}((k)),$$

to generate systems of the form

$$\mathbf{u}_t = \mathcal{J}_0 \mathbf{a}, \quad \mathbf{a} := \mathbf{R}_+. \tag{46}$$

Here $(\cdot)_+$ and $(\cdot)_-$ indicate the parts of non-negative and negative powers in k, respectively. Now from the identity

$$\mathcal{J}_0 \mathbf{a} = \mathcal{J}_0 \mathbf{R}_+ = -\mathcal{J}_0 \mathbf{R}_-,$$

it is clear that a sufficient condition for the consistency of (46) is that the degrees d_2 and d_3 of v and u as polynomials of k satisfy

$$d_3 \leqslant d_2 + 1, \quad 2d_2 \leqslant d_3 + 1.$$

Hence only four nontrivial cases arise for (d_2, d_3)

$$(0,1), \quad (1,1), \quad (1,2), \quad (2,3). \tag{47}$$

We notice that they represent the dispersionless versions of the standard Boussinesq hierarchy and all three hidden hierarchies found by Antonowicz, Fordy, and Liu for the third-order spectral problem.[21]

Solutions of the Lenard relation can be generated by noticing that the operator $\mathcal{J}_0$ admits the factorization

$$\mathcal{J}_0 = U^{\mathsf{T}} \cdot \frac{1}{3} \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \partial_x \cdot U, \tag{48}$$

where

$$U := \begin{pmatrix} 2p_1 + p_2 & -2p_1p_2 - p_2^2 \\ 2p_2 + p_1 & -2p_1p_2 - p_1^2 \end{pmatrix} = \begin{pmatrix} \dfrac{\partial v}{\partial p_1} & \dfrac{\partial u}{\partial p_1} \\ \dfrac{\partial v}{\partial p_2} & \dfrac{\partial u}{\partial p_2} \end{pmatrix}. \tag{49}$$

This shows two things,

(i) $\mathcal{J}_0$ is a Hamiltonian operator.
(ii) The gradients $\nabla_{\mathbf{u}} p_i$ of the branches p_1 and p_2 solve the Lenard relations.

Thus our candidates to deformations are the equations of the form

$$\partial_t \mathbf{u} = \mathcal{J}_0(\nabla_{\mathbf{u}} R)_+, \quad R(z,\mathbf{p}) = f_1(z)p_1 + f_2(z)p_2. \tag{50}$$

At this point one applies the same strategy as that used for the curves (7) Sec. III A. We first determine the Newton exponents of the four cases (47) which turn out to be given by

l_0	3	2	1
	(0,1) (1,2)	(1,1)	(2,3)

Then, with the help of Lagrange resolvents, we characterize the functions $R(z,\mathbf{p})$ verifying $\nabla_{\mathbf{u}} R \in \mathbb{C}((k))$ with $k=z^{l_0}$. In summary, one finds the following.

For the case $l_0=3$,

$$R = zf_1(z^3)\mathcal{L}_1 + z^2 f_2(z^3)\mathcal{L}_2, \quad k = z^3. \tag{51}$$

For the case $l_0=2$,

$$R = f_1(z^2)(\mathcal{L}_1 + \mathcal{L}_2) + zf_2(z^2)(\mathcal{L}_1 - \mathcal{L}_2), \quad k = z^2. \tag{52}$$

For the case $l_0=1$, we have $z=k$, so that any function $R(k,\mathbf{p})=f_1(k)\mathcal{L}_1+f_2(k)\mathcal{L}_2$ is appropriate.

Example 1: The case $l_0=3$ with $(d_2,d_3)=(1,2)$. From (44) and (45) we have that $u_{2t}=0$. Then if one takes

$$u(k,x,t) = k^2 + u_1(x,t)k + u_0(x,t), \quad v(k,x,t) = v_1(x,t)k + v_0(x,t),$$

and sets

$$f_1(z^3) = \tfrac{1}{2}(1 + i\sqrt{3})z^3, \quad f_2 \equiv 0,$$

in (51), one gets

$$v_{1t} = -2u_{1x} + \tfrac{5}{9}v_1^2 v_{1x},$$

$$v_{0t} = \tfrac{1}{9}(-18u_{0x} + v_1^2 v_{0x} + 4v_0 v_1 v_{1x}),$$

$$u_{1t} = \tfrac{1}{9}(v_1^2 u_{1x} - 6v_0 v_{1x} - 6v_1 v_{0x} + 6v_1 u_1 v_{1x}),$$

$$u_{0t} = \tfrac{1}{9}(v_1^2 u_{0x} - 6v_0 v_{0x} + 6u_0 v_1 v_{1x}),$$

i.e., the dispersionless version of the *coupled Boussinesq system* (3.20b) in Ref. 21.

Example 2: The case $l_0=2$ with $(d_2,d_3)=(1,1)$. Now, one can see that $v_{1t}=0$. By setting

$$u(k,x,t) = u_1(x,t)k + u_0(x,t), \quad v(k,x,t) = -k + v_0(x,t),$$

and

$$f_1(z^2) = -z^2, \quad f_2 \equiv 0,$$

in (52), we find the system,

$$v_{0t} = -2u_{0x} - 2v_0 u_{1x} - u_1 v_{0x},$$

$$u_{1t} = -4u_1 u_{1x} + \tfrac{2}{3}v_{0x},$$

$$u_{0t} = -u_1 u_{0x} - 3u_0 u_{1x} - \tfrac{2}{3} v_0 v_{0x}.$$

This is the dispersionless version of the system (4.13) in Ref. 21.

D. Whitham deformations of cubic curves

There are four types of cubic curves of the form (19) given by the following equations:

M	0	1	2
	$k=p^3+v_1p+v_0$	$k=p^2+v_0+\dfrac{v_1}{p-w_1}$	$k=p+\dfrac{v_{1,1}}{p-w_1}+\dfrac{v_{2,1}}{p-w_2}$
		$k=p+\dfrac{v_1}{p-w_1}+\dfrac{v_2}{(p-w_1)^2}$	

Note here that the Newton exponent l_0 is given by $l_0=3-M$. Also in Ref. 18, two cases in $M=1$ are shown to be conformally equivalent, i.e., $p=\infty \leftrightarrow p=w_1$.

For $M=0$ the Whitham deformations are reductions of our flows with $w\equiv 0$. But, in general, other Whitham deformations are not of that form. To illustrate this point let us take the class with $M=1$ and $N=2$. The corresponding Newton exponent is $l_0=2$ and there the branches of $\mathbf{p}$ have the following asymptotic behavior as $z\to\infty$:

$$p_1(z) = z + \mathcal{O}\left(\frac{1}{z}\right),$$

$$p_2(z) = p_1(-z) = -z + \mathcal{O}\left(\frac{1}{z}\right),$$

$$p_3(z) = w_1 + \mathcal{O}\left(\frac{1}{z}\right).$$

Let us consider now the Whitham flows (21) associated with the puncture at $p=\infty$,

$$\mathbf{Q}_{0,n} = (z^n)_{\oplus}(\mathbf{p}).$$

In terms of the potentials $\mathbf{u}=(w,v,u)^{\mathsf{T}}$ they read

$$\partial_t \mathbf{u} = J_0 \mathbf{a}, \tag{53}$$

where

$$\mathbf{a} = \left(V^{-1} \begin{pmatrix} (z^n)_{\oplus}(p_1) \\ (z^n)_{\oplus}(p_2) \\ (z^n)_{\oplus}(p_3) \end{pmatrix} \right)_{+}.$$

One easily sees that all matrix elements of V^{-1} are of order $\mathcal{O}(1/z)$ with the exception of

$$(V^{-1})_{13} = 1 + \mathcal{O}\left(\frac{1}{z}\right).$$

On the other hand, we have

$$(z^n)_{\oplus}(p_1) = z^n + \mathcal{O}\left(\frac{1}{z}\right),$$

$$(z^n)_\oplus(p_2) = (-z)^n + \mathcal{O}\left(\frac{1}{z}\right),$$

$$(z^n)_\oplus(p_3) = (z^n)_\oplus(w_1) + \mathcal{O}\left(\frac{1}{z}\right).$$

Therefore one gets

$$\mathbf{a} = \left(z^n V^{-1} \begin{pmatrix} 1 \\ (-1)^n \\ 0 \end{pmatrix} \right)_+ + (z^n)_\oplus(w_1)\mathbf{e}_3,$$

where $\mathbf{e}_3 = (0,0,1)^\mathsf{T}$, so that Eq. (53) becomes

$$\partial_t \mathbf{u} = J_0(T\nabla_\mathbf{u}[z^n(p_1 + (-1)^n p_2)])_+ + J_0((z^n)_\oplus(w_1)\mathbf{e}_3). \tag{54}$$

Similar expressions can be obtained for the deformations generated by the Whitham flows (21) for $\alpha = 1$ and $n \geqslant 1$.

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Ince's limits for confluent and double-confluent Heun equations

B. D. Bonorino Figueiredo[a)]
Instituto de Cosmologia, Relatividade e Astrofísica (ICRA-BR), Centro Brasileiro de Pesquisas Físicas (CBPF), Rua Dr. Xavier Sigaud, 150 - 22290-180 - Rio de Janeiro, RJ, Brasil

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We find pairs of solutions to a differential equation which is obtained as a special limit of a generalized spheroidal wave equation (this is also known as confluent Heun equation). One solution in each pair is given by a series of hypergeometric functions and converges for any finite value of the independent variable z, while the other is given by a series of modified Bessel functions and converges for $|z|>|z_0|$, where z_0 denotes a regular singularity. For short, the preceding limit is called Ince's limit after Ince who have used the same procedure to get the Mathieu equations from the Whittaker-Hill ones. We find as well that, when z_0 tends to zero, the Ince limit of the generalized spheroidal wave equation turns out to be the Ince limit of a double-confluent Heun equation, for which solutions are provided. Finally, we show that the Schrödinger equation for inverse fourth- and sixth-power potentials reduces to peculiar cases of the double-confluent Heun equation and its Ince's limit, respectively. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2104267]

I. INTRODUCTION

First, we construct two linear differential equations whose solutions behave at infinity as the so-called subnormal Thomé solutions, in contrast to solutions of a confluent and double-confluent Heun equations,[1] from which the former equations are obtained by a limit process. Second, we provide solutions which afford the expected asymptotic behavior for these equations. Finally, we find that the Schrödinger equation with inverse fourth- and sixth-power potentials reduces to particular instances of the double-confluent Heun equation and its Ince limit, respectively.

In the first place, let us introduce the two equations under consideration. Our starting point is the generalized spheroidal wave equation (GSWE) in the form used by Leaver,[2] namely,

$$z(z-z_0)\frac{\mathrm{d}^2U}{\mathrm{d}z^2}+(B_1+B_2z)\frac{\mathrm{d}U}{\mathrm{d}z}+\left[B_3-2\eta\omega(z-z_0)+\omega^2z(z-z_0)\right]U=0,\quad(\omega\neq0),\tag{1}$$

where B_i, η, and ω are constants (notice that, if $\omega=0$ and η is fixed, the equation may be transformed into a hypergeometric equation). The points $z=0$ and $z=z_0$ are regular singularities with indices $(0,1+B_1/z_0)$ and $(0,1-B_2-B_1/z_0)$, respectively, while the infinity is an irregular singularity in which the behavior of $U(z)$, inferred from the normal Thomé solutions,[3] is given by

$$\lim_{z\to\infty}U(z)\sim e^{\pm i\omega z}z^{\mp i\eta-(B_2/2)}.\tag{2}$$

Since its parameters are not specified, the above noted GSWE is equivalent to the confluent Heun equation,[1] an equation that is more general than the original Wilson GSWE.[4] Furthermore, as noted by Leaver, for $z_0=0$ we obtain a double-confluent Heun equation (DCHE) having five parameters, rather than four as in other contexts,[5,6] namely,

[a)]Electronic mail: barto@cbpf.br

$$z^2\frac{d^2U}{dz^2}+(B_1+B_2z)\frac{dU}{dz}+\left[B_3-2\eta\omega z+\omega^2z^2\right]U=0,\quad(\omega\neq0,B_1\neq0),\tag{3}$$

where the singular points $z=0$ and $z=\infty$ are both irregular. For $\omega=0$ and/or $B_1=0$ (with η fixed) this equation degenerates into confluent hypergeometric equations (see Appendix A). At infinity, the behavior of $U(z)$ is again given by (2), while at $z=0$ we find in the usual way[3] that

$$\lim_{z\to0}U(z)\sim1\ \text{or}\ \lim_{z\to0}U(z)\sim e^{B_1/z}z^{2-B_2}.\tag{4}$$

The Leaver procedure also allows us to obtain solutions to the DCHE from solutions to the GSWE when z_0 goes to zero. The known Leaver-type solutions[2,7] are appropriate to solve, for instance, the Teukolsky equations for the extreme upper limit of the rotation parameter,[2] the time dependence of Dirac test fields in dust-dominated Friedmann-Robertson-Walker spacetimes, and the Schrödinger equation with asymmetric double-Morse potentials.[7] They are suitable for handling the Schrödinger equation with inverse fourth-power potentials, as we will see.

Now, to get the equations we are interested in, the Leaver limit is combined with a limit that Ince[8] had used to derive the Mathieu equation from the Whittaker-Hill equation. The Ince limit is obtained by taking

$$\omega\to0,\quad\eta\to\infty,\quad\text{such that}\ 2\eta\omega=-q,\tag{5}$$

where q is a constant. Thus, the Ince limit of the GSWE is

$$z(z-z_0)\frac{d^2U}{dz^2}+(B_1+B_2z)\frac{dU}{dz}+[B_3+q(z-z_0)]U=0,\quad(q\neq0).\tag{6}$$

This is a generalization of the Mathieu equation, for by setting

$$z_0=1,\quad B_1=-1/2,\quad B_2=1,\quad z=\cos^2(\sigma u),\quad W(u)=U(z),\tag{7a}$$

we obtain

$$\frac{d^2W}{du^2}+\sigma^2[2q-4B_3-2q\cos(2\sigma u)]W=0,\tag{7b}$$

that is, the Mathieu equation if $\sigma=1$, and the modified Mathieu equation if $\sigma=i$.[9] In fact, inserting $z_0=1, B_1=-1/2$, and $B_2=1$ into Eq. (6), one recovers the algebraic Lindemann form for the Mathieu equation.[10] Nevertheless, the trigonometric form (7b) with $4B_3=2q-a$ is useful to verify that our solutions for the Ince limit of the GSWE give solutions already known for the Mathieu equation.

On the other hand, the Ince limit of the DCHE—or Leaver limit of Eq. (6)—is

$$z^2\frac{d^2U}{dz^2}+(B_1+B_2z)\frac{dU}{dz}+(B_3+qz)U=0,\quad(q\neq0,B_1\neq0),\tag{8}$$

which degenerates into simpler equations if $q=0$ and/or $B_1=0$ (see Appendix A). Solutions are obtained for this special DCHE by taking the Leaver limit of solutions for Eq. (6). By the way, we shall see that the Schrödinger equation for an inverse sixth-power potential is a particular case of Eq. (8), as stated in the first paragraph.

We emphasize that the Ince limits of the GSWE and DCHE, unlike the original GSWE and DCHE, require solutions behaving according to the subnormal Thomé solutions,[3] that is,

$$\lim_{z\to\infty}U(z)\sim e^{\pm2i\sqrt{qz}}z^{(1/4)-(B_2/2)}.\tag{9}$$

Despite this, our main mathematical issue consists in deriving pairs of series solutions to Eqs. (6) and (8)—having the behavior stipulated above at the singular points—from pairs of solutions to

the GSWE. For this we shall again employ the Ince and Leaver limits. The solutions in each pair have the same series coefficients and these satisfy three-term recurrence relations.

In Sec. II, a pair of solutions for the Ince limit of the GSWE is obtained by taking the Ince limit (5) of a known pair of solutions for the GSWE. One solution is given by an expansion in series of hypegeometric functions and converges for any finite z; the other solution is given by an expansion in series of modified Bessel functions and converges for $|z|>|z_0|$. Other pairs are generated by using transformation rules. These rules result from variable substitutions that preserve the form of the differential equations but modify their parameters and/or arguments.

In Sec. III, we find pairs of solutions for the Ince limit of the DCHE by taking the Leaver limit $(z_0\to 0)$ of solutions for the Ince limit of the GSWE. Solutions in series of irregular confluent hypergeometric functions result from expansions in series of hypergeometric functions and converge for any finite z. The other solution in each pair is given by a series of modified Bessel functions and converges for $|z|>0$.

In both of these sections we deal with solutions with and without a phase parameter ν. In general, this ν is introduced in order to assure the convergence of the series when there is no free constant in the differential equation, as in some scattering problems or in equations where z is a variable related to the time.[2,7] Solutions with a phase parameter are two-sided in the sense that the summation index n runs from $-\infty$ to ∞. However, if there is an arbitrary parameter in the equation, we can truncate the series by requiring that $n\geqslant 0$. In this manner, we obtain ν in terms of parameters of the differential equation.

In Sec. IV, we show that the Schrödinger equation with inverse fourth- and sixth-power potentials in fact leads to the DCHE and its Ince limit. Some additional considerations are provided in Sec. V, while in Appendix A we discuss the degenerate cases of the DCHEs, in Appendix B we present an alternative derivation of the expansions in Bessel functions, and in Appendix C we rewrite the Leaver-type solutions for the DCHE in a form appropriate to solve the Schrödinger equation with an inverse fourth-power potential.

II. INCE'S LIMITS FOR THE GENERALIZED SPHEROIDAL WAVE EQUATION

In the following we use transformation rules that permit us to generate new solutions from a given solution for the Ince limit of the GSWE. The rules T_1, T_2, and T_3 in the following are derived from the ones valid for the GSWE[7] and can be checked by substitution of variables. If $U(z)=U(B_1,B_2,B_3;z_0,q;z)$ denotes one solution for Eq. (6), the effects of these rules are as follows

$$T_1U(z)=z^{1+B_1/z_0}U(C_1,C_2,C_3;z_0,q;z),\quad z_0\neq 0,$$

$$T_2U(z)=(z-z_0)^{1-B_2-B_1/z_0}U(B_1,D_2,D_3;z_0,q;z),\quad z_0\neq 0, \tag{10a}$$

$$T_3U(z)=U(-B_1-B_2z_0,B_2,B_3-qz_0;z_0,-q;z_0-z),$$

where

$$C_1=-B_1-2z_0,\quad C_2=2+B_2+\frac{2B_1}{z_0},\quad C_3=B_3+\left(1+\frac{B_1}{z_0}\right)\left(B_2+\frac{B_1}{z_0}\right),$$

$$D_2=2-B_2-\frac{2B_1}{z_0},\quad D_3=B_3+\frac{B_1}{z_0}\left(\frac{B_1}{z_0}+B_2-1\right). \tag{10b}$$

We use only T_1 and T_2. The rule T_3 exchange the position of the regular singular points $z=z_0\leftrightarrow z=0$ and may be used to get an alternative representation for the solutions, but these are not proper for getting the limit $z_0\to 0$.

In Sec. II A we derive two pairs of solutions for the Ince limit of the GSWE—denoted by $(U^0_{i\nu},U^\infty_{i\nu}),i=1,2$—with a phase parameter ν. The superscript "zero" indicates that the series con-

verges in any finite part of the complex plane, while the superscript "infinity" indicates convergence for $|z|>|z_0|$. The second pair of solutions results from the first by means of the rule T_2. In Sec. II B, we truncate these series by taking $n \geqslant 0$ and obtain four pairs of solutions without phase parameter.

A. Solutions with a phase parameter

Denoting by b_n the series coefficients of a solution, their recurrence relations will have the general form

$$\alpha_n b_{n+1} + \beta_n b_n + \gamma_n b_{n-1} = 0, \quad (-\infty < n < \infty), \tag{11a}$$

where $\alpha_n, \beta_n, \gamma_n$, and b_n depend on a phase parameter ν which may be determined from a characteristic equation given as a sum of two infinite continued fractions, namely,

$$\beta_0 = \frac{\alpha_{-1}\gamma_0}{\beta_{-1}-}\frac{\alpha_{-2}\gamma_{-1}}{\beta_{-2}-}\frac{\alpha_{-3}\gamma_{-2}}{\beta_{-3}-}\cdots + \frac{\alpha_0\gamma_1}{\beta_1-}\frac{\alpha_1\gamma_2}{\beta_2-}\frac{\alpha_2\gamma_3}{\beta_3-}\cdots . \tag{11b}$$

For a specific pair of solutions we add a superscript in each of these quantities.

The first pair of solutions for the Ince limit of the GSWE comes from the following pair of solutions of the GSWE[7]

$$U^0_{1\nu}(z) = e^{i\omega z}\sum_{n=-\infty}^{\infty} b_n^{(1)} F\left(\frac{B_2}{2} - n - \nu - 1, n + \nu + \frac{B_2}{2}; B_2 + \frac{B_1}{z_0}; 1 - \frac{z}{z_0}\right),$$

$$U^\infty_{1\nu}(z) = e^{i\omega z} z^{1-(B_2/2)} \sum_{n=-\infty}^{\infty} b_n^{(1)} (-2i\omega z)^{n+\nu} \Psi(n + \nu + 1 + i\eta, 2n + 2\nu + 2; -2i\omega z), \tag{12a}$$

where $F(a,b;c;y)$ and $\Psi(a,b;y)$ denote, respectively, the hypergeometric functions and the irregular confluent hypergeometric functions.[11,12] The solution $U^0_{1\nu}$ converges for any finite z, whereas $U^\infty_{1\nu}$ converges for $|z|>|z_0|$. In the recurrence relations (11a) for $b_n^{(1)}$ we have

$$\alpha_n^{(1)} = i\omega z_0 \frac{\left(n + \nu + 2 - \frac{B_2}{2}\right)\left(n + \nu + 1 - \frac{B_2}{2} - \frac{B_1}{z_0}\right)(n + \nu + 1 - i\eta)}{2(n + \nu + 1)\left(n + \nu + \frac{3}{2}\right)},$$

$$\beta_n^{(1)} = -B_3 - \eta\omega z_0 - \left(n + \nu + 1 - \frac{B_2}{2}\right)\left(n + \nu + \frac{B_2}{2}\right) - \frac{\eta\omega z_0\left(\frac{B_2}{2} - 1\right)\left(\frac{B_2}{2} + \frac{B_1}{z_0}\right)}{(n + \nu)(n + \nu + 1)}, \tag{12b}$$

$$\gamma_n^{(1)} = -i\omega z_0 \frac{\left(n + \nu + \frac{B_2}{2} - 1\right)\left(n + \nu + \frac{B_2}{2} + \frac{B_1}{z_0}\right)(n + \nu + i\eta)}{2\left(n + \nu - \frac{1}{2}\right)(n + \nu)}.$$

Note that ν cannot be integer or half-integer in order to avoid vanishing denominators in the coefficients of the recurrence relations. Moreover, for an integer or half-integer ν, we would have two equal hypergeometric or confluent hypergeometric functions (for different values of n), contrary to the hypothesis that all the terms of the series are independent. On the other hand, the hypergeometric functions are not defined if $B_2+(B_1/z_0)$ is zero or a negative integer. Nonetheless, a transformation rule supplies another solution which is valid for these values of $B_2+(B_1/z_0)$.

The three-term recurrence relations (11a) constitute an infinite system of homogeneous linear equations for which nontrivial solutions for the coefficients b_n demand that the determinant of respective tridiagonal matrix vanishes. Equivalently, the characteristic equation must be satisfied and this is a condition necessary also to assure the convergence of the series by means of a Poincaré-Perron theorem.[13] However, there are two possibilities to satisfy this requirement.

On the one hand, if there is some free constant in the differential equation, that constant must be determined so that the characteristic equation is fulfilled for the admissible values of ν (that is, neither integer nor half-integer). In this case, the freedom of choosing ν may be used in two different ways: (i) to obtain two-sided solutions $(-\infty<n<\infty)$ by ascribing appropriate values for ν, or (ii) to obtain one-sided solutions by choosing ν such that $n\geqslant 0$. At the end of the present section, we use the first alternative to rederive some Poole's solutions[14,15] for the Mathieu equation, having period $2\pi m$, where m is any integer equal or greater than 2. In Sec. II B, we use the second alternative for the general case. These latter solutions afford solutions with period π or 2π for the Mathieu equation, in contrast to the solutions obtained in the first alternative.

On the other hand, if there is no arbitrary parameter in the differential equation, the parameter ν takes the role of free parameter in the sense that it must be adjusted to ensure the validity of the characteristic equation and, consequently, the convergence of the series. For this reason, ν is also called characteristic index or parameter.[16] Examples of equations requiring a phase parameter are discussed in Sec. IV.

From the above-noted pair of solutions for the GSWE, by using the Ince limit (5), we readily find the solution $U_{1\nu}^{0}(z)$ written in the first pair in the following. To get the Ince limit of the solution $U_{1\nu}^{\infty}(z)$, we define c_n as

$$b_n^{(1)}=(i\eta)^{n+\nu}\Gamma(i\eta-n-\nu)c_n.$$

This implies that

$$U_{1\nu}^{\infty}(z)=e^{i\omega z}z^{1-(B_2/2)}\sum_{n=-\infty}^{\infty}c_n\Gamma(i\eta-n-\nu)(-qz)^{n+\nu}\Psi\left(n+\nu+1+i\eta,2n+2\nu+2;-\frac{qz}{i\eta}\right),$$

where $q=-2\eta\omega$. The recurrence relations for c_n are

$$\bar{\alpha}_n c_{n+1}+\beta_n^{(1)}c_n+\bar{\gamma}_n c_{n-1}=0,\quad (-\infty<n<\infty)$$

with

$$\bar{\alpha}_n=\frac{i\eta}{i\eta-n-\nu-1}\alpha_n^{(1)},\quad \bar{\gamma}_n=\frac{i\eta-\nu-1}{i\eta}\gamma_n^{(1)}.$$

On the other hand, we have[12]

$$\lim_{a\to\infty}[\Gamma(a+1-c)\Psi(a,c;x/a)]=2x^{(1-c)/2}K_{c-1}(2\sqrt{x}),\tag{13}$$

where $K_\lambda(\xi)$ denotes the modified Bessel function of the second kind[17] whose definition in terms of irregular confluent hypergeometric functions is[12]

$$K_\lambda(\xi)=K_{-\lambda}(\xi)=\sqrt{\pi}e^{-\xi}(2\xi)^{\lambda}\Psi\left(\lambda+\tfrac{1}{2},2\lambda+1;2\xi\right).\tag{14}$$

Then, using (13) we find that for $i\eta\to\infty$ (n fixed and q=constant)

$$\Gamma(i\eta-n-\nu)(-qz)^{n+\nu}\Psi\left(n+\nu+1+i\eta,2n+2\nu+2;-\frac{qz}{i\eta}\right)$$
$$\to 2(-qz)^{1/2}K_{2n+2\nu+1}(\pm 2i\sqrt{qz}),\quad \lim\bar{\alpha}_n\to\lim\alpha_n^{(1)},\lim\bar{\gamma}_n\to\lim\gamma_n^{(1)}\Rightarrow\lim c_n\to\lim b_n^{(1)}.$$

Using these results, we find the Ince limit of $U_{1\nu}^{\infty}$, written in the first pair in the following. Although this is a formal derivation, the solution may be checked by inserting it into Eq. (6) (see Appendix B). In addition, from the relation[17]

$$\lim_{|\xi|\to\infty} K_\lambda(\xi) \sim \sqrt{\frac{\pi}{2\xi}} e^{-\xi}, \quad -\frac{3\pi}{2} < \arg\,\xi < \frac{3\pi}{2} \tag{15}$$

we see that the expansions in series of Bessel functions have the behavior given by

$$\lim_{z\to\infty} U^{\infty}_{j\nu}(z) \sim e^{\pm 2i\sqrt{qz}} z^{(1/4)-(B_2/2)}, \quad -\frac{3\pi}{2} < \arg(\pm 2i\sqrt{qz}) < \frac{3\pi}{2}, \quad (j=1,2)$$

in accordance with Eq. (9). The second pair of solutions follows from the first one through the rule T_2, as mentioned before. Moreover, solutions for the Mathieu equation are obtained by using Eq. (7a) and by noting that in this case the hypergeometric functions can be rewritten in terms of trigonometric functions.

First pair:

$$U^0_{1\nu}(z) = \sum_{n=-\infty}^{\infty} b_n^{(1)} F\left(\frac{B_2}{2} - n - \nu - 1, n + \nu + \frac{B_2}{2}; B_2 + \frac{B_1}{z_0}; 1 - \frac{z}{z_0}\right),$$

$$U^{\infty}_{1\nu}(z) = z^{(1-B_2)/2} \sum_{n=-\infty}^{\infty} b_n^{(1)} K_{2n+2\nu+1}(\pm 2i\sqrt{qz}), \tag{16a}$$

where in the recurrence relations (11a)

$$\alpha_n^{(1)} = qz_0 \frac{\left(n+\nu+2-\frac{B_2}{2}\right)\left(n+\nu+1-\frac{B_2}{2}-\frac{B_1}{z_0}\right)}{(n+\nu+1)\left(n+\nu+\frac{3}{2}\right)},$$

$$\beta_n^{(1)} = 4B_3 - 2qz_0 + 4\left(n+\nu+1-\frac{B_2}{2}\right)\left(n+\nu+\frac{B_2}{2}\right) - 2qz_0 \frac{\left(\frac{B_2}{2}-1\right)\left(\frac{B_2}{2}+\frac{B_1}{z_0}\right)}{(n+\nu)(n+\nu+1)}, \tag{16b}$$

$$\gamma_n^{(1)} = qz_0 \frac{\left(n+\nu+\frac{B_2}{2}-1\right)\left(n+\nu+\frac{B_2}{2}+\frac{B_1}{z_0}\right)}{\left(n+\nu-\frac{1}{2}\right)(n+\nu)}.$$

If $B_2+(B_1/z_0)$ is zero or a negative integer we have the solution $U^0_{2\nu}$ instead of $U^0_{1\nu}$.

For the Mathieu equation we use Eq. (7a) and the formula[11]

$$F\left[-a, a; (1/2); \sin^2(\sigma u)\right] = \cos(2a\sigma u).$$

Then, we obtain even solutions with respect to u, namely,

$$W^0_{1\nu}(u) = \sum_{n=-\infty}^{\infty} b_n^{(1)} \cos[(2n+2\nu+1)\sigma u], \quad |\cos(\sigma u)| < \infty,$$

$$W^{\infty}_{1\nu}(u) = \sum_{n=-\infty}^{\infty} b_n^{(1)} K_{2n+2\nu+1}[\pm 2i\sqrt{q}\cos(\sigma u)], \quad |\cos(\sigma u)| > 1, \tag{17a}$$

with the simplified recurrence relations ($a=2q-4B_3$)

$$qb_{n+1}^{(1)} + \left[(2n+2\nu+1)^2 - a\right] b_n^{(1)} + qb_{n-1}^{(1)} = 0. \tag{17b}$$

Second pair:

$$U_{2\nu}^{0}(z)=(z-z_0)^{1-B_2-B_1/z_0}z^{1+B_1/z_0}\sum_{n=-\infty}^{\infty}b_n^{(2)}$$
$$\times F\left(-n-\nu-\frac{B_2}{2}+1,n+\nu+2-\frac{B_2}{2};2-B_2-\frac{B_1}{z_0};1-\frac{z}{z_0}\right),$$

$$U_{2\nu}^{\infty}(z)=(z-z_0)^{1-B_2-B_1/z_0}z^{B_1/z_0+B_2/2-\frac{1}{2}}\sum_{n=-\infty}^{\infty}b_n^{(2)}K_{2n+2\nu+1}(\pm 2i\sqrt{qz}), \tag{18a}$$

where

$$\alpha_n^{(2)}=qz_0\frac{\left(n+\nu+\frac{B_2}{2}\right)\left(n+\nu+1+\frac{B_2}{2}+\frac{B_1}{z_0}\right)}{(n+\nu+1)\left(n+\nu+\frac{3}{2}\right)},\quad \beta_n^{(2)}=\beta_n^{(1)},$$
$$\gamma_n^{(2)}=qz_0\frac{\left(n+\nu+1-\frac{B_2}{2}\right)\left(n+\nu-\frac{B_2}{2}-\frac{B_1}{z_0}\right)}{\left(n+\nu-\frac{1}{2}\right)(n+\nu)}, \tag{18b}$$

in the recurrence relations (11a) for $b_n^{(2)}$. If $B_2+(B_1/z_0)$ is a positive integer equal or greater than 2 we have the solution $U_{1\nu}^{0}$ instead of $U_{2\nu}^{0}$. Note that, in writing the solution $U_{2\nu}^{0}$, we have used

$$F(a,b;c;y)=(1-y)^{c-a-b}F(c-a,c-b;c;y). \tag{19}$$

For the Mathieu equation we use[11]

$$F\left(a,1-a;\frac{3}{2};\sin^2(\sigma u)\right)=\frac{\sin[(2a-1)\sigma u]}{(2a-1)\sin(\sigma u)}$$

and, in addition, define c_n as $b_n^{(2)}=(2n+2\nu+1)c_n$. So, we find that the recurrence relations for c_n become identical to the ones for $b_n^{(1)}$, giving the odd solutions

$$W_{2\nu}^{0}(u)=\sum_{n=-\infty}^{\infty}b_n^{(1)}\sin[(2n+2\nu+1)\sigma u],$$
$$W_{2\nu}^{\infty}(u)=\tan(\sigma u)\sum_{n=-\infty}^{\infty}(2n+2\nu+1)b_n^{(1)}K_{2n+2\nu+1}[\pm 2i\sqrt{q}\cos(\sigma u)], \tag{20}$$

where $|\cos(\sigma u)|<\infty$ and $|\cos(\sigma u)|>1$, respectively.

As we have explained earlier, if there is a free parameter in the differential equation, it is possible to satisfy the characteristic equation for any noninteger or half-integer ν. We use this fact to rederive some Poole's solutions[14,15] to the Mathieu equation. For this, in the previous $W_{1\nu}^{0}(u)$ and $W_{1\nu}^{0}(u)$ we take

$$2\nu+1=l/m,\quad \sigma=1, \tag{21}$$

where l and m are integers prime to one another, $l<m$. Then, we find the two-sided Poole solutions $W_1^P(u)$ and $W_1^P(u)$ given by

$$W_1^P(u) = \sum_{n=-\infty}^{\infty} b_n^{(1)} \cos\left[\left(2n + \frac{l}{m}\right)u\right] \quad , W_2^P(u) = \sum_{n=-\infty}^{\infty} b_n^{(1)} \sin\left[\left(2n + \frac{l}{m}\right)u\right]. \tag{22}$$

The first is even with respect to u and the second is odd, and both of them have period $2\pi m, m > 1$. Since they have the same series coefficients, we can combine them to find another Poole solution, that is,

$$W^P(u) = \sum_{n=-\infty}^{\infty} b_n^{(1)} \exp\left[i\left(2n + \frac{l}{m}\right)u\right]. \tag{23}$$

Furthermore, for an arbitrary ν we find

$$W(u) = \sum_{n=-\infty}^{\infty} b_n^{(1)} \exp[i(2n + 2\nu + 1)u], \tag{24}$$

which is also a solution already known in the literature.[11,15]

B. Solutions without phase parameter

Now we truncate the solutions obtained in Sec. II A by taking $n \geqslant 0$. This gives ν in terms of some parameters of the differential equation. The resulting solutions are convergent only if there is a free parameter to be determined from the characteristic equation.

This truncation reverses the procedure by which the solution $U_{1\nu}^0(z)$ for the GSWE, given in Eq. (12a), was obtained. Indeed, that solution was constructed[18] as a generalization of a one-sided series of Jacobi polynomials, constructed by Fackerell and Crossman[19] to solve the angular Teukolsky equations of the relativistic astrophysics. Despite this, the truncated solutions found in Ref. 7 are more general than the Fackerell-Crossman ones because no particular values are attached to the parameters of the GSWE and also because the truncation was extended to the Leaver expansion $U_{1\nu}^{\infty}(z)$. In addition, these one-sided series are suitable to get solutions in finite series, the so called quasi-polynomial solutions. In effect, a solution whose coefficients b_n obey recurrence relations as

$$\alpha_n b_{n+1} + \beta_n b_n + \gamma_n b_{n-1} = 0, \quad n \geqslant 0, \quad b_{-1} = 0$$

becomes a quasi-polynomial solution with $0 \leqslant n \leqslant N-1$ whenever $\gamma_N = 0$ for some $n = N$.[20]

For the truncated solutions—denoted by $(U_i^0, U_i^{\infty}), i = 1,2,3,4$—the recurrence relations and the characteristic equations have one of the three forms written in the following. The first case ($\alpha_{-1} = 0$) is the general one and the others ($\alpha_{-1} \neq 0$) may occur only for special cases,

$$\left.\begin{array}{c} \alpha_0 b_1 + \beta_0 b_0 = 0 \\ \alpha_n b_{n+1} + \beta_n b_n + \gamma_n b_{n-1} = 0 (n \geqslant 1) \end{array}\right\} \Rightarrow \beta_0 = \frac{\alpha_0\gamma_1}{\beta_1 -} \frac{\alpha_1\gamma_2}{\beta_2 -} \frac{\alpha_2\gamma_3}{\beta_3 -} \cdots . \tag{25}$$

$$\left.\begin{array}{c} \alpha_0 b_1 + \beta_0 b_0 = 0 \\ \alpha_1 b_2 + \beta_1 b_1 + [\alpha_{-1} + \gamma_1] b_0 = 0 \\ \alpha_n b_{n+1} + \beta_n b_n + \gamma_n b_{n-1} = 0 (n \geqslant 2) \end{array}\right\} \Rightarrow \beta_0 = \frac{\alpha_0[\alpha_{-1} + \gamma_1]}{\beta_1 -} \frac{\alpha_1\gamma_2}{\beta_2 -} \frac{\alpha_2\gamma_3}{\beta_3 -} \cdots . \tag{26}$$

$$\left.\begin{array}{c} \alpha_0 b_1 + [\beta_0 + \alpha_{-1}] b_0 = 0 \\ \alpha_n b_{n+1} + \beta_n b_n + \gamma_n b_{n-1} = 0 (n \geqslant 1) \end{array}\right\} \Rightarrow \beta_0 + \alpha_{-1} = \frac{\alpha_0\gamma_1}{\beta_1 -} \frac{\alpha_1\gamma_2}{\beta_2 -} \frac{\alpha_2\gamma_3}{\beta_3 -} \cdots . \tag{27}$$

Note that we have $n \geqslant -1$ in $\alpha_n, n \geqslant 0$ in β_n and $n \geqslant 1$ in γ_n.

These forms for the recurrence relations are the same that appear in truncation of the expansions (12a) for the GSWE.[7] As a matter of fact, the solutions of the present section are the Ince

limit of solutions for the GSWE given in Sec. 3 of Ref. 7. However, in order to illustrate how these recurrence relations are obtained, we insert the solution $U_{1\nu}^{\infty}$ given in (16a) into the Ince limit of the GSWE. Then, for $n \geqslant 0$, from Eq. (B4) we find that

$$\sum_{n=0}^{\infty} \alpha_{n-1}^{(1)} b_n^{(1)} K_{2n+2\nu-1}(\xi) + \sum_{n=0}^{\infty} \beta_n^{(1)} b_n^{(1)} K_{2n+2\nu+1}(\xi) + \sum_{n=0}^{\infty} \gamma_{n+1}^{(1)} b_n^{(1)} K_{2n+2\nu+3}(\xi) = 0.$$

Setting $m=n-1, m=n$, and $m=n+1$ in the first, second, and third terms, respectively, this equation becomes

$$\alpha_{-1} b_0 K_{2\nu-1}(\xi) + [\alpha_0 b_1 + \beta_0 b_0] K_{2\nu+1}(\xi) + [\alpha_1 b_2 + \beta_1 b_1 + \gamma_1 b_0] K_{2\nu+3}(\xi) + \sum_{n=2}^{\infty} [\alpha_n b_{n+1} + \beta_n b_n + \gamma_n b_{n-1}] K_{2n+2\nu+1}(\xi) = 0, \tag{28}$$

where we have dropped the upper suffixes. Therefore, if we can choose ν so that $\alpha_{-1}=0$, we find the first set of recurrence relations. However, notice that

$$\alpha_{-1} = \frac{q z_0 \left(\nu + 1 - \frac{B_2}{2}\right)\left(\nu - \frac{B_1}{z_0} - \frac{B_2}{2}\right)}{2\nu(\nu + 1/2)} = 0 \quad \text{if} \begin{cases} \nu = \frac{B_2}{2} - 1 \text{ for } B_2 \neq 1,2; \\ \nu = \frac{B_1}{z_0} + \frac{B_2}{2} \text{ for } \frac{B_1}{z_0} + \frac{B_2}{2} \neq 0, \frac{1}{2}. \end{cases}$$

Hence we see that there are two possible choices for ν and, for each of them we have two cases in which α_{-1} may differ from zero. Let us consider only the case $\nu=(B_2/2)-1$. Then, for the exceptional case $B_2=1(\nu=-1/2)$, we find $K_{2\nu-1}=K_{2\nu+3}=K_2$ (since $K_\lambda=K_{-\lambda}$) and therefore the Bessel functions in the first and third terms of Eq. (28) are equal, giving the recurrence relations (26). Similarly, if $B_2=2(\nu=0)$ we find $K_{2\nu-1}=K_{2\nu+1}=K_1$ and this leads to the recurrence relations (27). In this manner we obtain the first pair given in the following. The remaining can be derived from this by using the transformations rules T_1 and T_2 as

$$(U_1^0, U_1^{\infty}) \overset{T_1}{\leftrightarrow} (U_2^0, U_2^{\infty}) \overset{T_2}{\leftrightarrow} (U_3^0, U_3^{\infty}) \overset{T_1}{\leftrightarrow} (U_4^0, U_4^{\infty}) \overset{T_2}{\leftrightarrow} (U_1^0, U_1^{\infty}).$$

The condition on each pair is imposed in order to assure that the special functions are independent in both solutions; it guarantees that there is no vanishing denominator in the recurrence relations. Furthermore, we have additional restrictions on the parameters of the solutions U_i^0. Thus, if $B_2 + (B_1/z_0)$ is zero or a negative integer, the hypergeometric functions are not defined in U_1^0 and U_2^0 but are defined in U_3^0 and U_4^0, and vice versa. The results for the Mathieu equations are already known,[9] but note that the recurrence relations for this case come from the three equations (25)–(27) above.

First pair: $B_2 \neq 0, -1, -2, \ldots$. This first pair corresponds to $\nu=(B_2/2)-1$ in $(U_{1\nu}^0, U_{1\nu}^{\infty})$,

$$U_1^0(z) = \sum_{n=0}^{\infty} b_n^{(1)} F\left(-n, n + B_2 - 1; B_2 + \frac{B_1}{z_0}; 1 - \frac{z}{z_0}\right),$$

$$U_1^{\infty}(z) = z^{(1-B_2)/2} \sum_{n=0}^{\infty} b_n^{(1)} K_{2n+B_2-1}(\pm 2i\sqrt{qz}), \tag{29a}$$

with the following coefficients

$$\alpha_n^{(1)} = \frac{q z_0 (n+1)\left(n - \frac{B_1}{z_0}\right)}{\left(n + \frac{B_2}{2}\right)\left(n + \frac{B_2}{2} + \frac{1}{2}\right)},$$

$$\beta_n^{(1)} = 4B_3 - 2qz_0 + 4n(n+B_2-1) - \frac{2qz_0\left(\frac{B_2}{2}-1\right)\left(\frac{B_2}{2}+\frac{B_1}{z_0}\right)}{\left(n+\frac{B_2}{2}-1\right)\left(n+\frac{B_2}{2}\right)}, \tag{29b}$$

$$\gamma_n^{(1)} = \frac{qz_0(n+B_2-2)\left(n+B_2+\frac{B_1}{z_0}-1\right)}{\left(n+\frac{B_2}{2}-\frac{3}{2}\right)\left(n+\frac{B_2}{2}-1\right)},$$

in the recurrence relations for the $b_n^{(1)}$, namely: Eq. (25) if $B_2 \neq 1, 2$; Eq. (26) if $B_2=1$; Eq. (27) if $B_2=2$.

For the Mathieu equation we find solutions

$$W_1^0(u) = \sum_{n=0}^{\infty} b_n^{(1)} \cos(2n\sigma u), \quad |\cos(\sigma u)| < \infty,$$
$$W_1^{\infty}(u) = \sum_{n=0}^{\infty} b_n^{(1)} K_{2n}[\pm 2i\sqrt{q}\,\cos(\sigma u)], \quad |\cos(\sigma u)| > 1, \tag{30a}$$

with the simplified recurrence relations

$$qb_1^{(1)} - ab_0^{(1)} = 0, \quad qb_2^{(1)} + [4-a]b_1^{(1)} + 2qb_0^{(1)} = 0,$$
$$qb_{n+1}^{(1)} + [4n^2 - a]b_n^{(1)} + qb_{n-1}^{(1)} = 0 (n \geqslant 2). \tag{30b}$$

These solutions are even with respect to u and, for $\sigma=1$, the solution $W_1^0(u)$ has period π.

Second pair: $(B_2/2)+(B_1/z_0) \neq -1, -3/2, -2, -5/2 \cdots$. This pair of solutions can also be obtained by taking $\nu=(B_2/2)+(B_1/z_0)$ in $(U_{1\nu}^0, U_{1\nu}^0)$,

$$U_2^0(z) = z^{1+(B_1/z_0)} \sum_{n=0}^{\infty} b_n^{(2)} F\left(-n, n+1+B_2+\frac{2B_1}{z_0}; B_2+\frac{B_1}{z_0}; 1-\frac{z}{z_0}\right),$$
$$U_2^{\infty}(z) = z^{(1-B_2)/2} \sum_{n=0}^{\infty} b_n^{(2)} K_{2n+1+B_2+(2B_1/z_0)}(\pm 2i\sqrt{qz}), \tag{31a}$$

where

$$\alpha_n^{(2)} = \frac{qz_0(n+1)\left(n+2+\frac{B_1}{x_0}\right)}{\left(n+1+\frac{B_2}{2}+\frac{B_1}{z_0}\right)\left(n+\frac{3}{2}+\frac{B_2}{2}+\frac{B_1}{z_0}\right)},$$

$$\beta_n^{(2)} = 4B_3 - 2qz_0 + 4\left(n+1+\frac{B_1}{x_0}\right)\left(n+B_2+\frac{B_1}{x_0}\right) - \frac{2qz_0\left(\frac{B_2}{2}-1\right)\left(\frac{B_2}{2}+\frac{B_1}{z_0}\right)}{\left(n+\frac{B_2}{2}+\frac{B_1}{x_0}\right)\left(n+1+\frac{B_2}{2}+\frac{B_1}{x_0}\right)},$$

$$\gamma_n^{(2)} = \frac{qz_0\left(n+B_2+\frac{B_1}{x_0}-1\right)\left(n+B_2+\frac{2B_1}{z_0}\right)}{\left(n-\frac{1}{2}+\frac{B_2}{2}+\frac{B_1}{z_0}\right)\left(n+\frac{B_2}{2}+\frac{B_1}{z_0}\right)}, \tag{31b}$$

in the recurrence relations for $b_n^{(2)}$: Eq. (25) if $(B_2/2)+(B_1/z_0) \neq 0, -1/2$; Eq. (26) if $(B_2/2)+(B_1/z_0)=-1/2$; Eq. (27) if $(B_2/2)+(B_1/z_0)=0$.

For the Mathieu equation we again have even solutions

$$W_2^0(u) = \sum_{n=0}^{\infty} b_n^{(2)} \cos[(2n+1)\sigma u], \quad |\cos(\sigma u)| < \infty,$$

$$W_2^{\infty}(u) = \sum_{n=0}^{\infty} b_n^{(2)} K_{2n+1}[\pm 2i\sqrt{q}\,\cos(\sigma u)], \quad |\cos(\sigma u)| > 1, \tag{32a}$$

with the recurrence relations

$$qb_1^{(2)} + [q+1-a]b_0^{(2)} = 0,$$

$$qb_{n+1}^{(2)} + [(2n+1)^2 - a]b_n^{(2)} + qb_{n-1}^{(2)} = 0 (n \geqslant 1). \tag{32b}$$

If $\sigma=1$ the solution $W_2^0(u)$ has period 2π.

Third pair: $B_2 \neq 4, 5, 6, \cdots$. This corresponds to $\nu = 1-(B_2/2)$ in $(U_{2\nu}^0, U_{2\nu}^{\infty})$,

$$U_3^0(z) = (z-z_0)^{1-B_2-B_1/z_0} z^{1+B_1/z_0} \sum_{n=0}^{\infty} b_n^{(3)} F\left(-n, n+3-B_2; 2-B_2-\frac{B_1}{z_0}; 1-\frac{z}{z_0}\right),$$

$$U_3^{\infty}(z) = (z-z_0)^{1-B_2-B_1/z_0} z^{B_1/z_0+B_2/2-1/2} \sum_{n=0}^{\infty} b_n^{(3)} K_{2n+3-B_2}(\pm 2i\sqrt{qz}), \tag{33a}$$

with the coefficients

$$\alpha_n^{(3)} = \frac{qz_0(n+1)\left(n+2+\frac{B_1}{z_0}\right)}{\left(n+2-\frac{B_2}{2}\right)\left(n+\frac{5}{2}-\frac{B_2}{2}\right)},$$

$$\beta_n^{(3)} = 4B_3 - 2qz_0 + 4(n+1)(n+2-B_2) - \frac{2qz_0\left(\frac{B_2}{2}-1\right)\left(\frac{B_2}{2}+\frac{B_1}{z_0}\right)}{\left(n+1-\frac{B_2}{2}\right)\left(n+2-\frac{B_2}{2}\right)}, \tag{33b}$$

$$\gamma_n^{(3)} = \frac{qz_0(n+2-B_2)\left(n+1-B_2-\frac{B_1}{z_0}\right)}{\left(n+\frac{1}{2}-\frac{B_2}{2}\right)\left(n+1-\frac{B_2}{2}\right)}.$$

in the recurrence relations: Eq. (25) if $B_2 \neq 2, 3$; Eq. (26) if $B_2=3$; Eq. (27) if $B_2=2$.

For the Mathieu equation we redefine the coefficients $b_n^{(3)}$ as $b_n^{(3)} \to (2n+2)b_n^{(3)}$. Then we find the odd solutions

$$W_3^0(u) = \sum_{n=0}^{\infty} b_n^{(3)} \sin[(2n+2)\sigma u], \quad |\cos(\sigma u)| < \infty,$$

$$W_3^{\infty}(u) = \tan(\sigma u) \sum_{n=0}^{\infty} (2n+2) b_n^{(3)} K_{2n+2}[\pm 2i\sqrt{q}\cos(\sigma u)], \quad |\cos(\sigma u)| > 1, \tag{34a}$$

with the recurrence relations

$$qb_1^{(3)} + [4-a]b_0^{(3)} = 0,$$

$$qb_{n+1}^{(3)} + [4(n+1)^2 - a]b_n^{(3)} + qb_{n-1}^{(3)} = 0, \quad (n \geqslant 1). \tag{34b}$$

For $\sigma=1$ the solution $W_3^0(u)$ has period π.

Fourth pair: $(B_2/2)+(B_1/z_0)\neq 1,3/2,2,5/2\cdots$. This can also be obtained by setting $\nu=-(B_2/2)-(B_1/z_0)$ in $(U^0_{2\nu},U^\infty_{2\nu})$,

$$U_4^0=(z-z_0)^{1-B_2-B_1/z_0}\sum_{n=0}^{\infty}b_n^{(4)}F\left(-n,n+1-B_2-\frac{2B_1}{z_0};2-B_2-\frac{B_1}{z_0};1-\frac{z}{z_0}\right),$$

$$U_4^\infty=(z-z_0)^{1-B_2-B_1/z_0}z^{B_1/z_0+B_2/2-\frac{1}{2}}\sum_{n=0}^{\infty}b_n^{(4)}K_{2n+1-B_2-(2B_1/z_0)}(\pm 2i\sqrt{qz}), \tag{35a}$$

with coefficients

$$\alpha_n^{(4)}=\frac{qz_0(n+1)\left(n-\frac{B_1}{z_0}\right)}{\left(n+1-\frac{B_2}{2}-\frac{B_1}{z_0}\right)\left(n+\frac{3}{2}-\frac{B_2}{2}-\frac{B_1}{z_0}\right)},$$

$$\beta_n^{(4)}=4B_3-2qz_0+4\left(n-\frac{B_1}{z_0}\right)\left(n-B_2+1-\frac{B_1}{z_0}\right)-\frac{2qz_0\left(\frac{B_2}{2}-1\right)\left(\frac{B_2}{2}+\frac{B_1}{z_0}\right)}{\left(n-\frac{B_2}{2}-\frac{B_1}{z_0}\right)\left(n+1-\frac{B_2}{2}-\frac{B_1}{z_0}\right)}, \tag{35b}$$

$$\gamma_n^{(4)}=\frac{qz_0\left(n+1-B_2-\frac{B_1}{z_0}\right)\left(n-B_2-\frac{2B_1}{z_0}\right)}{\left(n-\frac{1}{2}-\frac{B_2}{2}-\frac{B_1}{z_0}\right)\left(n-\frac{B_2}{2}-\frac{B_1}{z_0}\right)},$$

in the recurrence relations: Eq. (25) if $(B_2/2)+(B_1/z_0)\neq 0,1/2$; Eq. (26) if $(B_2/2)+(B_1/z_0)=1/2$; Eq. (27) if $(B_2/2)+(B_1/z_0)=0$.

For the Mathieu equation we redefine $b_n(4)$ according to $b_n^{(4)}\to(2n+1)b_n^{(4)}$ and find the odd solutions

$$W_4^0(u)=\sum_{n=0}^{\infty}b_n^{(4)}\sin[(2n+1)\sigma u],\quad |\cos(\sigma u)|<\infty,$$

$$W_4^\infty(u)=\tan(\sigma u)\sum_{n=0}^{\infty}(2n+1)b_n^{(4)}K_{2n+1}[\pm 2i\sqrt{q}\cos(\sigma u)],\quad |\cos(\sigma u)|>1, \tag{36a}$$

with the recurrence relations

$$qb_4^{(4)}+[1-q-a]b_0^{(4)}=0,$$

$$qb_{n+1}^{(4)}+[(2n+1)^2-a]b_n^{(4)}+qb_{n-1}^{(4)}=0(n\geqslant 1). \tag{36b}$$

Now, for $\sigma=1$, $W_4^0(u)$ has period 2π.

III. INCE'S LIMITS FOR THE DOUBLE-CONFLUENT HEUN EQUATION

As in the case of the Ince limit of the GSWE, we have found no solution in the literature for the Ince limit of the DCHE. The solutions in the following are obtained by taking the limit $z_0\to 0$ (Leaver limit) of the solutions given in Sec. II for the Ince limit of the GSWE. For this we use the formulas[12]

$$\lim_{c\to\infty}F\left(a,b;c;1-\frac{c}{y}\right)=y^a\Psi(a,a+1-b;y), \tag{37a}$$

$$\lim_{\alpha\to\infty}\left(1+\frac{y}{\alpha}\right)^{\alpha}=e^{y}\Rightarrow\lim_{z_0\to 0}\left(1-\frac{z_0}{z}\right)^{-B_1/z_0}=e^{B_1/z}. \tag{37b}$$

Actually, it is not necessary to use the second equation above, since we can get one pair of solutions as the limit of the first pair of Sec. II A and, then, generate the other pair by means of the transformation rule

$$\tau U(z)=e^{B_1/z}z^{2-B_2}U(-B_1,4-B_2,B_3+2-B_2;q;z), \tag{38}$$

where $U(z)=U(B_1,B_2,B_3;q;z)$ denotes known solutions of Eq. (8). On the other hand, to check that the solutions $U_i^0(z)$ exhibit the behavior given in Eq. (4) when $z\to 0$, we may use the relation[12]

$$\lim_{|y|\to\infty}\Psi(a,b;y)\sim y^{-a}[1+O(|y|^{-1}],\quad -\frac{3\pi}{2}<\arg y<\frac{3\pi}{2}. \tag{39}$$

A. Solutions with a phase parameter

For the solution $U_{1\nu}^0$ of Sec. II A, we find that the limit of the hypergeometric functions when z_0 tends to zero, B_2 and B_1 being fixed ($c=B_2+B_1/z_0\to\infty$), is given by

$$\lim_{z_0\to 0}F\left(n+\nu+\frac{B_2}{2},-n-\nu-1+\frac{B_2}{2};B_2+\frac{B_1}{z_0};1-\frac{z}{z_0}\right)$$
$$\propto z^{-\nu-\frac{B_2}{2}}\left(\frac{B_1}{z}\right)^{n}\Psi\left(n+\nu+\frac{B_2}{2},2n+2\nu+2;\frac{B_1}{z}\right).$$

Then, considering also the solution $U_{1\nu}^{\infty}$ and the limits for the coefficients in the recurrence relations, we get the first pair of solutions with a phase parameter ν (different of integer or half-integer). The rule τ leads to the second pair.

First pair:

$$U_{1\nu}^0(z)=z^{-\nu-B_2/2}\sum_{n=-\infty}^{\infty}b_n^{(1)}\left(\frac{B_1}{z}\right)^{n}\Psi\left(n+\nu+\frac{B_2}{2},2n+2\nu+2;\frac{B_1}{z}\right),$$
$$U_{1\nu}^{\infty}(z)=z^{(1-B_2)/2}\sum_{n=-\infty}^{\infty}b_n^{(1)}K_{2n+2\nu+1}(\pm 2i\sqrt{qz}), \tag{40a}$$

where in the recurrence relations (11a))

$$\alpha_n^{(1)}=-\frac{qB_1\left(n+\nu+2-\frac{B_2}{2}\right)}{(n+\nu+1)\left(n+\nu+\frac{3}{2}\right)},$$

$$\beta_n^{(1)}=4B_3+4\left(n+\nu+1-\tfrac{B_2}{2}\right)\left(n+\nu+\tfrac{B_2}{2}\right)-\frac{qB_1(B_2-2)}{(n+\nu)(n+\nu+1)},$$

$$\gamma_n^{(1)}=\frac{qB_1\left(n+\nu+\frac{B_2}{2}-1\right)}{\left(n+\nu-\frac{1}{2}\right)(n+\nu)}. \tag{40b}$$

Second pair:

$$U_{2\nu}^0(z)=e^{B_1/z}z^{-\nu-B_2/2}\sum_{n=-\infty}^{\infty}b_n^{(2)}\left(-\frac{B_1}{z}\right)^{n}\Psi\left(n+\nu+2-\frac{B_2}{2},2n+2\nu+2;-\frac{B_1}{z}\right), \tag{41a}$$

$$U_{2\nu}^{\infty}(z) = e^{B_1/z} z^{(1-B_2)/2} \sum_{n=-\infty}^{\infty} b_n^{(2)} K_{2n+2\nu+1}(\pm 2i\sqrt{qz}),$$

where

$$\alpha_n^{(2)} = \frac{qB_1\left(n+\nu+\frac{B_2}{2}\right)}{(n+\nu+1)\left(n+\nu+\frac{3}{2}\right)}, \quad \beta_n^{(2)} = \beta_n^{(1)}, \quad \gamma_n^{(2)} = -\frac{qB_1\left(n+\nu+1-\frac{B_2}{2}\right)}{\left(n+\nu-\frac{1}{2}\right)(n+\nu)}, \tag{41b}$$

in the recurrence relations (11a) for $b_n^{(2)}$.

B. Solutions without phase parameter

These solutions may be derived by truncating the solutions of Sec. III A. In this case, we see that there is only one choice for ν in each pair. Alternatively, the solutions can be found by applying the Leaver procedure to the first and third pairs of Sec. II B.

First pair: $B_2 \neq 0, -1, -2, \cdots$. This corresponds to $\nu=(B_2/2)-1$ in $(U_{1\nu}^0, U_{1\nu}^{\infty})$.

$$U_1^0(z) = z^{1-B_2} \sum_{n=0}^{\infty} b_n^{(1)} \left(\frac{B_1}{z}\right)^n \Psi\left(n + B_2 - 1, 2n + B_2; \frac{B_1}{z}\right),$$

$$U_1^{\infty}(z) = z^{(1-B_2)/2} \sum_{n=0}^{\infty} b_n^{(1)} K_{2n+B_2-1}(\pm 2i\sqrt{qz}), \tag{42a}$$

with the following coefficients:

$$\alpha_n^{(1)} = -\frac{qB_1(n+1)}{\left(n+\frac{B_2}{2}\right)\left(n+\frac{B_2}{2}+\frac{1}{2}\right)},$$

$$\beta_n^{(1)} = 4B_3 + 4n(n+B_2-1) - \frac{qB_1(B_2-2)}{\left(n+\frac{B_2}{2}-1\right)\left(n+\frac{B_2}{2}\right)}, \tag{42b}$$

$$\gamma_n^{(1)} = \frac{qB_1(n+B_2-2)}{\left(n+\frac{B_2}{2}-\frac{3}{2}\right)\left(n+\frac{B_2}{2}-1\right)}.$$

in the recurrence relations for the $b_n^{(1)}$: Eq. (25) if $B_2 \neq 1, 2$; Eq. (26) if $B_2=1$; Eq. (27) if $B_2=2$.

Second pair: $B_2 \neq 4, 5, 6, \cdots$. It corresponds to $\nu=1-(B_2/2)$ in $(U_{2\nu}^0, U_{2\nu}^{\infty})$ but can also be obtained from the first pair via the rule τ.

$$U_2^0(z) = e^{B_1/z} z^{-1} \sum_{n=0}^{\infty} b_n^{(2)} \left(-\frac{B_1}{z}\right)^n \Psi\left(n + 3 - B_2, 2n + 4 - B_2; -\frac{B_1}{z}\right),$$

$$U_2^{\infty}(z) = e^{B_1/z} z^{(1-B_2)/2} \sum_{n=0}^{\infty} b_n^{(2)} K_{2n+3-B_2}(\pm 2i\sqrt{qz}), \tag{43a}$$

where

$$\alpha_n^{(3)} = \frac{qB_1(n+1)}{\left(n+2-\frac{B_2}{2}\right)\left(n+\frac{5}{2}-\frac{B_2}{2}\right)},$$

$$\beta_n^{(3)} = 4B_3 + 4(n+1)(n+2-B_2) - \frac{qB_1(B_2-2)}{\left(n+1-\frac{B_2}{2}\right)\left(n+2-\frac{B_2}{2}\right)}, \tag{43b}$$

$$\gamma_n^{(3)} = -\frac{qB_1(n+2-B_2)}{\left(n+\frac{1}{2}-\frac{B_2}{2}\right)\left(n+1-\frac{B_2}{2}\right)}.$$

in the recurrence relations for $b_n^{(2)}$: Eq. (25) if $B_2 \neq 2,3$; Eq. (26) if $B_2=3$; Eqs. (27) if $B_2=2$.

IV. POTENTIAL APPLICATIONS

As we have mentioned, the Schrödinger equation with inverse fourth- and sixth-power potentials can be reduced, respectively, to the double-confluent Heun equation (3) and its Ince limit (8). Singular potentials like these have appeared in the description of intermolecular forces[21] and in the scattering of ions by polarizable atoms. For the sake of illustration, we consider the last problem.

Before discussing these examples, let us present the so-called normal forms of the DCHE, that is, the forms in which there is no first-order derivative terms in the differential equations. The general procedure for this, consists in writing the equation as

$$\frac{\mathrm{d}^2U}{\mathrm{d}z^2} + p(z)\frac{\mathrm{d}U}{\mathrm{d}z} + q(z)U = 0.$$

Then, the substitution

$$U(z) = F(z)\exp\left(-\frac{1}{2}\int p(z)\mathrm{d}z\right)$$

gives a first normal form, namely,

$$\frac{\mathrm{d}^2F}{\mathrm{d}z^2} + I(z)F = 0, \quad I(z) = q(z) - \frac{1}{2}\frac{\mathrm{d}p(z)}{\mathrm{d}z} - \frac{1}{4}[p(z)]^2.$$

From this, other normal forms are obtained by the transformations

$$z = h(\vartheta), \quad F(z) = \sqrt{\frac{\mathrm{d}h}{\mathrm{d}\vartheta}}G(\vartheta)$$

which yield

$$\frac{\mathrm{d}^2G}{\mathrm{d}\vartheta^2} + J(\vartheta)G = 0, \quad J(\vartheta) = I[h(\vartheta)]\left(\frac{\mathrm{d}h}{\mathrm{d}\vartheta}\right)^2 + \frac{1}{2}\frac{\mathrm{d}^3h}{\mathrm{d}\vartheta^3}\Big/\frac{\mathrm{d}h}{\mathrm{d}\vartheta} - \frac{3}{4}\left(\frac{\mathrm{d}^2h}{\mathrm{d}\vartheta^2}\Big/\frac{\mathrm{d}h}{\mathrm{d}\vartheta}\right)^2.$$

By employing this procedure, Lemieux and Bose[22] have derived several normal forms for the general Heun equation and its confluent cases, excepting the triconfluent equation. These forms are useful to recognize whether a given equation belongs to the Heun class. Nevertheless, to find the solutions for the equation, we have to come back to the form for which the solutions were established, as in the following. The three Lemieux-Bose normal forms for the DCHE, together with the transformations of variables, are the following:

$$\begin{gathered} U(z) = z^{-B_2/2}e^{B_1/(2z)}F(z), \\ \frac{\mathrm{d}^2F}{\mathrm{d}z^2} + \left[\omega^2 - \frac{2\eta\omega}{z} + \frac{1}{z^2}\left(B_3 - \frac{B_2^2}{4} + \frac{B_2}{2}\right) + \frac{B_1}{z^3}\left(1 - \frac{B_2}{2}\right) - \frac{B_1^2}{4z^4}\right]F = 0; \end{gathered} \tag{44}$$

$$\begin{gathered} z = \rho^2, \quad U(z) = \rho^{(1-2B_2)/2}e^{B_1/(2\rho^2)}G(\rho) \Leftrightarrow G(\rho) = z^{(2B_2-1)/4}e^{-B_1/(2z)}U(z), \\ \frac{\mathrm{d}^2G}{\mathrm{d}\rho^2} + \left[4\omega^2\rho^2 - 8\eta\omega + \frac{4}{\rho^2}\left(B_3 - \frac{B_2^2}{4} + \frac{B_2}{2} - \frac{3}{16}\right) + \frac{4B_1}{\rho^4}\left(1 - \frac{B_2}{2}\right) - \frac{B_1^2}{\rho^6}\right]G = 0; \end{gathered} \tag{45}$$

$$z=e^{\lambda u},\quad U(z)=H(u)\exp\left[\frac{1}{2}\lambda(1-B_2)u+\frac{B_1}{2}e^{-\lambda u}\right]\Leftrightarrow H(u)=z^{(B_2-1)/2}e^{-B_1/(2z)}U(z),$$
$$\frac{\mathrm{d}^2H}{\mathrm{d}u^2}+\lambda^2\left[B_3-\left(\frac{1-B_2}{2}\right)^2-\frac{B_1^2}{4}e^{-2\lambda u}-B_1\left(\frac{B_2}{2}-1\right)e^{-\lambda u}-2\eta\omega e^{\lambda u}+\omega^2e^{2\lambda u}\right]H=0, \tag{46}$$

where λ is a constant at our disposal, for example, $\lambda=1$ or $\lambda=i$. Note that, since these transformations involve neither η nor ω, their Ince limits are obtained by putting $\omega^2=0$ and $2\eta\omega=-q$.

Now we proceed with the scattering problem. The radial part $R(r)=\chi(r)/r$ of the wave function for the Schrödinger equation in three dimensions, for a particle with mass μ and energy E, is

$$\frac{\mathrm{d}^2\chi(r)}{\mathrm{d}r^2}+\left[k^2-\frac{l(l+1)}{r^2}-\frac{2\mu}{\hbar^2}V(r)\right]\chi(r)=0, \tag{47}$$

where $k^2=2\mu E/\hbar^2$, l is the angular momentum, and $V(r)$ is the potential. Now, according to Kleinman, Hahn, and Spruch,[23] for the interaction of a light particle of charge e' with a fixed atom of charge $Z\bar{e}$ containing z' electrons, we have

$$V(r)=\frac{(Z-z')\bar{e}e'}{r}-\frac{\alpha_1'(e')^2}{2r^4}-(\alpha_2'-6a_0\beta_1')\frac{(e')^2}{2r^6}, \tag{48}$$

where r is the distance from the incident ion to the atom, $a_0=\hbar^2/(\mu\bar{e}^2)$ is the Bohr radius, α_1', and α_2' are, respectively, the electric dipole and quadrupole polarizabilities of the atom and β_1' is a parameter resulting from a nonadiabatic correction (α_1',α_2', and β_1' are constants which describe the properties of the target only). For this potential, the Schrödinger equation becomes

$$\frac{\mathrm{d}^2\chi}{\mathrm{d}r^2}+\left[k^2-\frac{2\mu(Z-z')\bar{e}e'}{\hbar^2r}-\frac{l(l+1)}{r^2}+\frac{\mu\alpha_1'(e')^2}{\hbar^2r^4}+\frac{\mu(\alpha_2'-6a_0\beta_1')(e')^2}{\hbar^2r^6}\right]\chi=0. \tag{49}$$

Therefore, for neutral targets ($Z=z'$) this is a particular case of the Ince limit of the DCHE, as we see from Eq. (45) with $\omega^2=0,2\eta\omega=-q$, and $z=\rho^2=r^2$. On the other hand, if the inverse sixth-power term vanishes ($\alpha_2'=6a_0\beta_1'$), this radial Schrödinger equation is a particular case of the DCHE as seen from Eq. (44) with $B_2=2$, for neutral or ionized targets. In both cases the energy of the incident particle (k^2) is given and, consequently, there is no free parameter in these equations since the other constants are also fixed. Then, convergent solutions require a phase parameter ν, analogous to the scattering by the field of an electric dipole.[2] To obtain the radial dependence $R(r)$ we must convert Eq. (49) into the DCHE (3) and its limit (8). In the following we discuss only the asymptotic behaviors of solutions for each case. For this reason, we do not write the recurrence relations for the coefficients.

Potential with inverse fourth- and sixth-power terms. Equation (45) suggests the substitutions

$$z=r^2,\quad \chi(r)=e^{-B_1/(2r^2)}r^{B_2-(1/2)}U(z=r^2)\ \text{with}$$

$$B_1=\pm\frac{e'}{\hbar}\sqrt{\mu(6a_0\beta_1'-\alpha_2')},\quad B_2=2-\frac{\alpha_1'(e')^2}{2\hbar^2B_1},\quad (6a_0\beta_1'\neq\alpha_2'),$$

which transform the Schrödinger equation (49) into

$$z^2\frac{\mathrm{d}^2U}{\mathrm{d}z^2}+(B_1+B_2z)\frac{\mathrm{d}U}{\mathrm{d}z}+\left[\left(\frac{B_2}{2}-\frac{1}{4}\right)\left(\frac{B_2}{2}-\frac{3}{4}\right)-\frac{l(l+1)}{4}+\frac{k^2}{4}z-\frac{\mu}{2}(Z-z')\sqrt{z}\right]U=0.$$

Then, for $Z\neq z'$, the Schrödinger equation is more general than the Ince limit of DCHE. However, assuming a neutral target, we may form two pairs of solutions according to

$$R_{i\nu}(r) = \frac{1}{r}\chi_{i\nu}(r) = e^{-B_1/(2r^2)} r^{B_2-(3/2)} U_{i\nu}(z=r^2) \quad (i=1,2), \tag{50}$$

where on the right-hand side the $U_{i\nu}$ represent the solutions with a phase parameter for the Ince limit of the DCHE, given in Sec. III A. Then, taking into account that for this case $q=k^2/4 = \mu E/(2\hbar^2)$ and $z=r^2$, we find

$$R^0_{1\nu}(r) = e^{-B_1/(2r^2)} r^{-2\nu-3/2} \sum_{n=-\infty}^{\infty} b_n^{(1)} \left(\frac{B_1}{r^2}\right)^n \Psi\left(n+\nu+\frac{B_2}{2}, 2n+2\nu+2; \frac{B_1}{r^2}\right),$$

$$R^\infty_{1\nu}(r) = e^{-B_1/(2r^2)} r^{-1/2} \sum_{n=-\infty}^{\infty} b_n^{(1)} K_{2n+2\nu+1}(\pm ikr); \tag{51}$$

$$R^0_{2\nu}(r) = e^{B_1/(2r^2)} r^{-2\nu-3/2} \sum_{n=-\infty}^{\infty} b_n^{(2)} \left(-\frac{B_1}{r^2}\right)^n \Psi\left(n+\nu+2-\frac{B_2}{2}, 2n+2\nu+2; -\frac{B_1}{r^2}\right),$$

$$R^\infty_{2\nu}(r) = e^{B_1/(2r^2)} r^{-1/2} \sum_{n=-\infty}^{\infty} b_n^{(2)} K_{2n+2\nu+1}(\pm ikr). \tag{52}$$

From these expressions we obtain

$$\lim_{r\to\infty} R^\infty_{1\nu}(r) \propto \lim_{r\to\infty} R^\infty_{2\nu}(r) \sim \frac{e^{\mp ikr}}{r}, \quad -\frac{3\pi}{2} < \arg(\pm ikr) < \frac{3\pi}{2}, \tag{53}$$

where we have employed the limit (15) for the modified Bessel functions. Thus, when $r\to\infty$, the solutions $R^\infty_{i\nu}$ are bounded even if k is a pure imaginary, since in this case $\exp(ikr)$ or $\exp(-ikr)$ goes to zero. At $r=0$, Eq. (39) implies that

$$\lim_{r\to 0} R^0_{1\nu}(r) \sim e^{-B_1/r^2} r^{B_2-(3/2)}, \quad -\frac{3\pi}{2} < \arg\frac{B_1}{r^2} < \frac{3\pi}{2},$$

$$\lim_{r\to 0} R^0_{2\nu}(r) \sim e^{B_1/r^2} r^{(5/2)-B_2}, \quad -\frac{3\pi}{2} < \arg\left(-\frac{B_1}{r^2}\right) < \frac{3\pi}{2}. \tag{54}$$

Then, if B_1 is a positive real number, the first limit goes to zero; if B_1 is a negative real number, the second limit goes to zero. However, if B_1 is a pure imaginary, we write

$$B_1 = iC, \quad B_2 = 2 + \frac{i\alpha_1'(e')^2}{2\hbar^2 C},$$

where C is real. Thus we find

$$|R^0_{1\nu}(r)| \propto |R^0_{2\nu}(r)| \sim \sqrt{r} \to 0.$$

Therefore, it is possible to find at least one pair of solutions for which both the solutions are bounded at the singularities.

Potential without inverse sixth-power term. From Eq. (44) we find that the substitutions

$$z = r, \quad \chi(r) = e^{-B_1/(2r)} r^{B_2/2} U(z=r) \quad \text{with } \hbar^2 B_1^2 = -4\mu(e')^2, \quad B_2 = 2$$

transform the Schrödinger equation (49) into

$$r^2\frac{\mathrm{d}^2U}{\mathrm{d}r^2}+(B_1+2r)\frac{\mathrm{d}U}{\mathrm{d}r}+\left[-l(l+1)-\frac{2\mu}{\hbar^2}(Z-z')\bar{e}e'r+k^2r^2+\frac{\mu(\alpha_2'-6a_0\beta_1')(e')^2}{\hbar^2r^4}\right]U=0. \tag{55}$$

Thus, in the absence of the inverse sixth-power term, the radial Schrödinger equation, even if we have a Coulomb term in the potential, may be solved by

$$R_{i\nu}(r)=e^{-B_1/(2r)}U_{i\nu}(z=r), \tag{56}$$

where $U_{i\nu}(z=r)$ are solutions with a phase parameter for the DCHE with $z=r$ and $B_2=2$ (see Appendix B). As

$$\omega=\pm k\leftrightarrow\pm\eta=\pm\frac{\mu}{k\hbar^2}(Z-z')\bar{e}e',\quad k=\frac{\sqrt{2\mu E}}{\hbar}, \tag{57}$$

those solutions give

$$\begin{aligned}R_{1\nu}^0(r)&=e^{\pm ikr-B_1/2r}\sum_{n=-\infty}^{\infty}b_n\left(\frac{B_1}{r}\right)^{n+\nu+1}\Psi\left(n+\nu+1,2n+2\nu+2;\frac{B_1}{r}\right),\\ R_{1\nu}^{\infty}(r)&=e^{\pm ikr-B_1/2r}\sum_{n=-\infty}^{\infty}b_n(\mp 2ikr)^{n+\nu}\Psi(n+\nu+1\pm i\eta,2n+2\nu+2;\mp 2ikr);\end{aligned} \tag{58}$$

$$\begin{aligned}R_{2\nu}^0(r)&=e^{\pm ikr+B_1/2r}\sum_{n=-\infty}^{\infty}b_n\left(-\frac{B_1}{r}\right)^{n+\nu+1}\Psi\left(n+\nu+1,2n+2\nu+2;-\frac{B_1}{r}\right),\\ R_{2\nu}^{\infty}(r)&=e^{\pm ikr+B_1/2r}\sum_{n=-\infty}^{\infty}b_n(\mp 2ikr)^{n+\nu}\Psi(n+\nu+1\pm i\eta,2n+2\nu+2;\mp 2ikr).\end{aligned} \tag{59}$$

Using Eq. (39), we find

$$\lim_{r\to\infty}R_{1\nu}^{\infty}(r)\propto\lim_{r\to\infty}R_{2\nu}^{\infty}(r)\sim r^{\mp i\eta}\frac{e^{\pm ikr}}{r},\quad -\frac{3\pi}{2}<\arg(\mp ikr)<\frac{3\pi}{2}. \tag{60}$$

Thus, when $r\to\infty$, the solutions $R_{i\nu}^{\infty}$ are bounded even if k is a pure imaginary number, since in this case the behavior of $\exp(ikr)$ or $\exp(-ikr)$ predominates over the other factor. At $r=0$, by using Eq. (39) we get

$$\begin{aligned}\lim_{r\to 0}R_{1\nu}^0(r)&\sim e^{-B_1/(2r)},\quad -\frac{3\pi}{2}<\arg\frac{B_1}{r}<\frac{3\pi}{2},\\ \lim_{r\to 0}R_{2\nu}^0(r)&\sim e^{B_1/(2r)},\quad -\frac{3\pi}{2}<\arg\left(-\frac{B_1}{r}\right)<\frac{3\pi}{2}.\end{aligned} \tag{61}$$

As B_1 is a pure imaginary number, we find that

$$|R_{1\nu}^0(r)|\propto|R_{2\nu}^0(r)|\sim 1.$$

Therefore, in this case we can form two pairs of solutions which are regular at the singular points, both pairs having the same series coefficients. For neutral targets ($\eta=0$) the previous results have already been found by Bühring who has treated the Schrödinger equation as a DCHE.[16,24] Before this author, the Schrödinger equation (for neutral targets and an inverse fourth-power polarization potential) had been transformed into a Mathieu equation.[25,26] Thus, the Bühring approach is

profitable since it works for ionized targets, too. In addition, as we have seen, for inverse sixth-power polarization potential, the Schrödinger equation may be transformed to the Ince limit of the DCHE, provided that the target is neutral.

V. FINAL REMARKS

We have constructed the differential equation (6) by applying the Ince limit, defined in Eq. (5), to a generalized spheroidal wave equation (GSWE). The Leaver limit ($z_0 \to 0$) of that equation has afforded Eq. (8) that turns out to be the Ince limit of a double-confluent Heun equation (DCHE) as well. The subnormal Thomé behavior at $z=\infty$, for the solutions of the these Ince limits of the GSWE and DCHE, distinguishes such equations from the original GSWE and DCHE hitherto considered in the literature.

In sec. II, a pair of solutions (with a phase parameter) for the Ince limit of the GSWE have been found as the Ince limit of a pair of solutions for the original GSWE. One solution is given by a series of hypergeometric functions and the other by a series of modified Bessel functions of the second kind. Both solutions in that pair have the same series coefficients but different regions of convergence, as in solutions for the Mathieu equations. Another pair has followed from the first one by means of a transformation rule. Hence, four pairs of solutions without phase parameter have resulted from the truncation of the series with a phase parameter, that is, by restricting the summation index of the series to $n \geqslant 0$.

In Sec. III, solutions for the Ince limit of the DCHE have been established by taking the Leaver limit of solutions for the Ince limit of the GSWE. These solutions, given by series of irregular confluent hypergeometric functions and modified Bessel functions, present the appropriate behavior at the irregular singularities $z=0$ and $z=\infty$. Note, nonetheless, that in Secs. III and IV we have dealt with expansions in series of modified Bessel functions only. Other possibilities may be investigated, especially solutions in series of Bessel function products, as these could have important properties as regards the convergence of the series.

In the solutions without phase parameter for the Ince limits of the GSWE and DCHE, there are three possible forms to the recurrence relations for the series coefficients. This fact is relevant in itself and, in particular, is essential to recover solutions for the Mathieu equation from the ones for the Ince limit of the GSWE.

The solutions we have obtained for the Mathieu equation are already known and exhibit the usual parity and periodicity properties. This includes also the solutions found by Poole, given by two-sided series ($-\infty < n < \infty$) and having period $2\pi m$, where m is any integer greater than 1. However, we note that other types of solutions for the Mathieu equations (and also for the Whittaker-Hill equations) are possible, since these equations may be considered as particular cases of both the GSWE and double-confluent Heun equations as well.[27]

At last, notice that we have pointed out no application for Ince limit of the GSWE. Nevertheless, in Sec. IV we have seen that the Schrödinger equation (49) for the scattering of low-energy particles by polarizable targets leads to a DCHE and its Ince limit. The exception is the Schrödinger equation with Coulomb and inverse sixth-power terms which requires solutions for a more general equation, possibly similar to an equation considered by Kurth and Schmidt in Ref. 28.

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APPENDIX A: DEGENERATE DCHEs

Let us show that DCHE

$$z^2\frac{d^2U}{dz^2}+(B_1+B_2z)\frac{dU}{dz}+(B_3-2\eta\omega z+\omega^2z^2)U=0,\quad (B_1\neq 0,\omega\neq 0),$$

for $B_1=0$ and/or $\omega=0$ degenerates into a confluent hypergeometric equation or an equation with constant coefficients. Thus, if $B_1=0$ and $\omega\neq 0$, the substitutions

$$y=-2i\omega z,\quad U(z)=e^{-y/2}y^{\alpha}f(y),\quad \alpha^2-(1-B_2)\alpha+B_3=0$$

give the confluent hypergeometric equation

$$y\frac{d^2f}{dy^2}+[(2\alpha+B_2)-y]\frac{df}{dy}-\left(i\eta+\alpha+\frac{B_2}{2}\right)f=0.$$

If $B_1\neq 0$ and $\omega=0$, the change of variables

$$y=B_1/z,\quad U(z)=y^{\beta}g(y),\quad \beta^2-(B_2-1)\beta+B_3=0$$

leads to

$$y\frac{d^2g}{dy^2}+[(2\beta+2-B_2)-y]\frac{dg}{dy}-\beta g=0.$$

If $B_1=\omega=0$, we find an equation with constant coefficients by taking $z=\exp y$.

Now let us show that the Ince limit of the DCHE

$$z^2\frac{d^2U}{dz^2}+(B_1+B_2z)\frac{dU}{dz}+(B_3+qz)U=0,\quad (q\neq 0,B_1\neq 0)$$

also gives degenerate cases if $q\neq 0$ and/or $B_1\neq 0$. In fact, if $q=0$ and $B_1\neq 0$, this equation is equivalent to the DCHE with $\omega=0$ and $B_1\neq 0$. If $q\neq 0$ and $B_1=0$, the substitutions

$$\xi=\pm 2i\sqrt{qz},\quad U(z)=\xi^{1-B_2}T(\xi)$$

reduce the equation to the modified Bessel equation

$$\xi^2\frac{d^2T}{d\xi^2}+\xi\frac{dT}{d\xi}-[(1-B_2)^2-4B_3+\xi^2]T=0.$$

Finally, for $q=B_1=0$, we find again an equation with constant coefficients by taking $z=\exp y$.

APPENDIX B: THE SOLUTIONS IN SERIES OF BESSEL FUNCTIONS

The solution $U_{1\nu}^{\infty}(z)$ in series of Bessel functions can also be constructed as follows. We perform the substitutions

$$\xi=\pm 2i\sqrt{qz},\quad U(z)=\xi^{1-B_2}Y(\xi) \tag{B1}$$

in the Ince limit of the GSWE (6). This yields

$$\xi^2\frac{d^2Y}{d\xi^2}+\xi\frac{dY}{d\xi}-\xi^2Y=-4qz_0\frac{d^2Y}{d\xi^2}-\frac{4q(z_0-2B_1-2B_2z_0)}{\xi}\frac{dY}{d\xi}+\left[4q(1-B_2)\frac{2B_1+B_2z_0+z_0}{\xi^2}+(1-B_2)^2+4qz_0-4B_3\right]Y. \tag{B2}$$

Now we expand $Y(\xi)$ according to

$$Y(\xi)=\sum_{n=-\infty}^{\infty} b_n^{(1)} K_\lambda(\xi), \quad \lambda=2n+2\nu+1, \tag{B3}$$

where $K_\lambda(\xi)$ denotes the modified Bessel function of the second kind.[17] The last equation and (B1) afford the solution $U_{1\nu}^{\infty}(z)$.

When we insert (B3) into (B2), we use some difference-differential relations derived from the properties of K_λ.[17] Thus, we have

$$\xi^2\frac{\mathrm{d}^2K_\lambda(\xi)}{\mathrm{d}\xi^2}+\xi\frac{\mathrm{d}K_\lambda(\xi)}{\mathrm{d}\xi}-\xi^2K_\lambda(\xi)=\lambda^2K_\lambda(\xi)$$

on the left-hand side and

$$4\frac{\mathrm{d}^2K_\lambda(\xi)}{\mathrm{d}\xi^2}=K_{\lambda+2}(\xi)+2K_\lambda(\xi)+K_{\lambda-2}(\xi), \quad \frac{4}{\xi}\frac{\mathrm{d}K_\lambda(\xi)}{\mathrm{d}\xi}=-\frac{4\lambda}{\xi^2}K_\lambda(\xi)+\frac{2}{\lambda-1}[K_{\lambda-2}(\xi)-K_\lambda(\xi)]$$

on the right-hand side. This gives

$$\begin{aligned} qz_0\sum_{n=-\infty}^{\infty}\left[1+\frac{2[1-2B_2-(2B_1/z_0)]}{\lambda-1}\right]b_n^{(1)}K_{\lambda-2}(\xi)+\sum_{n=-\infty}^{\infty}\Bigg[\lambda^2+4B_3-2qz_0-(1-B_2)^2 \\ -\frac{2qz_0[1-2B_2-(2B_1/z_0)]}{\lambda-1}\Bigg]b_n^{(1)}K_\lambda(\xi)+qz_0\sum_{n=-\infty}^{\infty}b_n^{(1)}K_{\lambda+2}(\xi) \\ =qz_0\sum_{n=-\infty}^{\infty}\left[\left(1-2B_2-\frac{2B_1}{z_0}\right)\lambda+(1-B_2)\left(1+B_2+\frac{2B_1}{z_0}\right)\right]b_n^{(1)}\frac{4K_\lambda(\xi)}{\xi^2}. \end{aligned}$$

To remove the term $4K_\lambda(\xi)/\xi^2$ on the right-hand side we use the relation

$$\frac{4K_\lambda(\xi)}{\xi^2}=\frac{K_{\lambda-2}(\xi)}{\lambda(\lambda-1)}-\frac{2K_\lambda(\xi)}{(\lambda-1)(\lambda+1)}+\frac{K_{\lambda+2}(\xi)}{\lambda(\lambda+1)}.$$

Then, recalling that $\lambda=2n+2\nu+1$, we find

$$\sum_{n=-\infty}^{\infty}\alpha_{n-1}^{(1)}b_n^{(1)}K_{2n+2\nu-1}(\xi)+\sum_{n=-\infty}^{\infty}\beta_n^{(1)}b_n^{(1)}K_{2n+2\nu+1}(\xi)+\sum_{n=-\infty}^{\infty}\gamma_{n+1}^{(1)}b_n^{(1)}K_{2n+2\nu+3}(\xi)=0, \tag{B4}$$

where the coefficients $\alpha_n^{(1)},\beta_n^{(1)}$, and $\gamma_n^{(1)}$ are just the ones given in Eq. (16b)). To get the recurrence relations with the form given in (11a), we change $n\to m+1$ and $n\to m-1$ in the first and third terms, respectively. After this, we equate to zero the coefficients of each independent $K_{2m+2\nu+1}(\xi)$.

On the other hand, to study the convergence of the series, we apply a Perron-Kreuser theorem[13] for the minimal solutions of the recurrence relations for $b_n^{(1)}$ and obtain (if $z_0\neq 0$)

$$\lim_{n\to\infty}\frac{b_{n+1}^{(1)}}{b_n^{(1)}}=\lim_{n\to-\infty}\frac{b_{n-1}^{(1)}}{b_n^{(1)}}=-\frac{qz_0}{4n^2}. \tag{B5}$$

Using also the relation[17]

$$\lim_{\lambda\to\infty}K_\lambda(\xi)=\frac{1}{2}\Gamma(\lambda)\left(\frac{\xi}{2}\right)^{-\lambda}$$

and $K_{-\lambda}(\xi)=K_\lambda(\xi)$, we get

$$\lim_{n\to\infty}\frac{K_{2n+2\nu+3}(\xi)}{K_{2n+2\nu+1}(\xi)}=\lim_{n\to-\infty}\frac{K_{2n+2\nu-1}(\xi)}{K_{2n+2\nu+1}(\xi)}=-\frac{4n^2}{qz}.$$

Hence, we have

$$\lim_{n\to\infty}\frac{b_{n+1}^{(1)}K_{2n+2\nu+3}(\xi)}{b_n^{(1)}K_{2n+2\nu+1}(\xi)}=\lim_{n\to-\infty}\frac{b_{n-1}^{(1)}K_{2n+2\nu-1}(\xi)}{b_n^{(1)}K_{2n+2\nu+1}(\xi)}=\frac{z_0}{z}.$$

Therefore, by the ratio test the series converges for $|z|>|z_0|$. In (B5) we have supposed that $z_0\neq 0$ but, if $z_0=0$, we find

$$\lim_{n\to\infty}\frac{b_{n+1}^{(1)}}{b_n^{(1)}}=\lim_{n\to-\infty}\frac{b_{n-1}^{(1)}}{b_n^{(1)}}=-\frac{B_1}{4n^3}\Rightarrow\lim_{n\to\infty}\frac{b_{n+1}^{(1)}K_{2n+2\nu+3}(\xi)}{b_n^{(1)}K_{2n+2\nu+1}(\xi)}=\lim_{n\to-\infty}\frac{b_{n-1}^{(1)}K_{2n+2\nu-1}(\xi)}{b_n^{(1)}K_{2n+2\nu+1}(\xi)}=\frac{B_1}{nz}.$$

Thus, in this limit the series converges for $|z|>0$ and per se this result is already included in $|z|>|z_0|$.

APPENDIX C: SOLUTIONS FOR THE DCHE OF SEC. IV

The Leaver-type solutions for the DCHE (3) present some simplifications for $B_2=2$. The solutions given in Ref. 7 are expansions in series of regular and irregular confluent hypergeometric functions. However, to obtain the expected behavior at the singular points $z=0$ and $z=\infty$, we have to choose the irregular functions. Then, by using the same notation of Secs. II A and III A, we find that for $B_2=2$ the first pair of solutions with a phase parameter is given by

$$U_{1\nu}^{0}(z)=e^{i\omega z}\sum_{n=-\infty}^{\infty}b_n\left(\frac{B_1}{z}\right)^{n+\nu+1}\Psi\left(n+\nu+1,2n+2\nu+2;\frac{B_1}{z}\right),$$

$$U_{1\nu}^{\infty}(z)=e^{i\omega z}\sum_{n=-\infty}^{\infty}b_n(-2i\omega z)^{n+\nu}\Psi(n+\nu+1+i\eta,2n+2\nu+2;-2i\omega z), \tag{C1}$$

and the second pair takes the form

$$U_{2\nu}^{0}(z)=e^{i\omega z+B_1/z}\sum_{n=-\infty}^{\infty}b_n\left(-\frac{B_1}{z}\right)^{n+\nu+1}\Psi\left(n+\nu+1,2n+2\nu+2;-\frac{B_1}{z}\right),$$

$$U_{2\nu}^{\infty}(z)=e^{i\omega z+B_1/z}\sum_{n=-\infty}^{\infty}b_n(-2i\omega z)^{n+\nu}\Psi(n+\nu+1+i\eta,2n+2\nu+2;-2i\omega z). \tag{C2}$$

Then, we see that the two pairs have the same series coefficients b_n and the coefficients in the recurrence relations (11a) are simply

$$\alpha_n=i\omega B_1\left(\frac{n+\nu+1-i\eta}{2n+2\nu+3}\right),\quad \beta_n=B_3+(n+\nu)(n+\nu+1),\gamma_n=i\omega B_1\left(\frac{n+\nu+i\eta}{2n+2\nu-1}\right). \tag{C3}$$

In these solutions ν cannot be integer or half-integer and the $U_{i\nu}^{0}$ converge for any finite z, whereas the $U_{i\nu}^{\infty}$ converge for $|z|>0$. Note, moreover, that the irregular confluent hypergeometric functions that appear in $U_{i\nu}^{0}$ could be rewritten in terms of modified Bessel of the second kind by using the definition (14). In the solutions $U_{i\nu}^{\infty}$ the confluent hypergeometric functions could be rewritten in terms of the Hankel functions $H_{\nu}^{(1)}$ but only if $\eta=0$ (neutral target, in the problem of Sec. IV. For this we have to use the relation[12]

$$\Psi\left(\rho+\frac{1}{2},2\rho+1;-2ix\right)=\frac{i}{2\sqrt{\pi}}e^{i(\rho\pi-x)}H_{\rho}^{(1)}(x),\rho=n+\nu+\frac{1}{2}.$$

The asymptotic behaviors of the solutions given in (C1) and (C2) may be found by using Eq. (39).

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A classification of generalized quantum statistics associated with basic classical Lie superalgebras

N. I. Stoilova[a] and J. Van der Jeugt[b]
Department of Applied Mathematics and Computer Science, University of Ghent, Krijgslaan 281-S9, B-9000 Gent, Belgium

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Generalized quantum statistics such as para-statistics is usually characterized by certain triple relations. In the case of para-Fermi statistics these relations can be associated with the orthogonal Lie algebra $B_n=so(2n+1)$; in the case of para-Bose statistics they are associated with the Lie superalgebra $B(0|n)=osp(1|2n)$. In a previous paper, a mathematical definition of "a generalized quantum statistics associated with a classical Lie algebra G" was given, and a complete classification was obtained. Here, we consider the definition of "a generalized quantum statistics associated with a basic classical Lie *superalgebra* G." Just as in the Lie algebra case, this definition is closely related to a certain $\mathbb{Z}$-grading of G. We give in this paper a complete classification of all generalized quantum statistics associated with the basic classical Lie superalgebras $A(m|n), B(m|n), C(n)$, and $D(m|n)$. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2104287]

I. INTRODUCTION

A historically important extension of Bose and Fermi statistics has been known for 50 years, namely the para-Bose and para-Fermi statistics as developed by Green.[1] In para-statistics, the usual bilinear commutators or anti-commutators for bosons and fermions are replaced by certain trilinear or triple relations. For example, for n pairs of para-Bose creation and annihilation operators B_i^{ξ} ($\xi=\pm$ and $i=1,\ldots,n$), the defining relations are

$$[\{B_j^{\xi},B_k^{\eta}\},B_l^{\epsilon}]=(\epsilon-\xi)\delta_{jl}B_k^{\eta}+(\epsilon-\eta)\delta_{kl}B_j^{\xi}, \quad \xi,\eta,\epsilon=\pm \text{ or } \pm 1; \quad j,k,l=1,\ldots,n. \tag{1.1}$$

Similar triple relations hold for the para-Fermi operators F_i^{ξ},[1] see (1.1) in Ref. 2. Both for para-Bose and para-Fermi statistics, there is a group theoretical setting. It was shown[3] that the Lie algebra generated by the $2n$ elements F_i^{ξ}, with $\xi=\pm$ and $i=1,\ldots,n$, subject to the para-Fermi relations is $B_n=so(2n+1)$ (as a Lie algebra defined by means of generators and relations).

Twenty years after the connection between para-Fermi statistics and the Lie algebra $so(2n+1)$, a new connection, between para-Bose statistics and the orthosymplectic Lie superalgebra $B(0|n)=osp(1|2n)$[4] was discovered.[5] The Lie superalgebra generated by $2n$ odd elements B_i^{ξ}, with $\xi=\pm$ and $i=1,\ldots,n$, subject to the triple relations (1.1), is $osp(1|2n)$ (as a Lie superalgebra defined by means of generators and relations). Moreover, there is a certain representation of $osp(1|2n)$, the so-called Bose representation $\mathcal{B}$, that yields the classical Bose relations, i.e., where the representatives $\mathcal{B}(B_i^{\xi})$ satisfy the relations of classical Bose statistics. For more general para-Bose statistics, a class of infinite dimensional $osp(1|2n)$ representations needs to be investigated.

These examples show that para-statistics, as introduced by Green[1] and further developed by others (see Ref. 6 and references therein), can be associated with representations of the Lie (super)algebras of class B [namely B_n and $B(0,n)$]. Whether alternative types of generalized

[a]Permanent address: Institute for Nuclear Research and Nuclear Energy, Boul. Tsarigradsko Chaussee 72, 1784 Sofia, Bulgaria; electronic mail: neli.stoilova@ugent.be
[b]Electronic mail: joris.vanderjeugt@ugent.be

quantum statistics can be found in the framework of other classes of simple Lie algebras or superalgebras has been considered in particular by Palev.[7–15] Building upon his examples and inspired by the definition of creation and annihilation operators in Ref. 11, a mathematical definition of "generalized quantum statistics" was given in Ref. 2. Furthermore, a complete classification was given of all the classes of generalized quantum statistics for the classical Lie algebras A_n, B_n, C_n, and D_n,[2] by means of their algebraic relations. In the present paper we make a similar classification for the basic classical Lie superalgebras.

For certain examples of quantum statistics associated with Lie superalgebras, see Refs. 14 and 15. However, a complete classification was never made. A particularly interesting example was described for the Lie superalgebra $sl(1|n)=A(0|n-1)$.[15] For this superalgebra, a set of odd creation and annihilation operators was given,[11] and it was shown that these n pairs of operators a_i^{ξ}, with $\xi=\pm$ and $i=1,\ldots,n$, subject to the defining relations

$$[\{a_i^+,a_j^-\},a_k^+]=\delta_{jk}a_i^+-\delta_{ij}a_k^+,$$

$$[\{a_i^+,a_j^-\},a_k^-]=-\delta_{ik}a_j^-+\delta_{ij}a_k^-,$$

$$\{a_i^+,a_j^+\}=\{a_i^-,a_j^-\}=0, \tag{1.2}$$

$(i,j,k=1,\ldots,n)$, generate the special linear Lie superalgebra $sl(1|n)$ (as a Lie superalgebra defined by means of generators and relations). Just as in the case of para-Bose relations, (1.2) has two interpretations. On the one hand, it describes the algebraic relations of a new kind of generalized statistics, in this case A-superstatistics or a statistics related to the Lie superalgebra $A(0|n-1)$. On the other hand, (1.2) yields a set of defining relations for the Lie superalgebra $A(0|n-1)$ in terms of generators and relations. Observe that certain microscopic and macroscopic properties of this statistics have already been studied.[15]

A description similar to (1.2) for the Lie algebra A_n was given for the first time by Jacobson[16] in the context of "Lie triple systems." Therefore, this type of generator is often referred to as "Jacobson generators." In this context, we shall mainly use the terminology "creation and annihilation operators (CAOs) for $sl(1|n)$."

Following the mathematical definition of "generalized quantum statistics associated with a Lie algebra," given in Ref. 2, this notion will be extended to Lie superalgebras G. This definition, and the corresponding classification method, are described in Sec. II. Just as for the case of Lie algebras, the method leads to a classification of certain gradings of G, and to regular subalgebras of G. In this process, Dynkin diagram techniques play a crucial role. For the basic classical Lie superalgebras however, the description by means of a Dynkin diagram is not unique: besides the so-called distinguished Dynkin diagram, other nonequivalent Dynkin diagrams exist.[4,17] This feature will make it harder to obtain a complete classification of all generalized quantum systems. In the remaining sections, the classification results are presented for all basic classical Lie superalgebras. A final section discusses some possible applications.

For the basic classical Lie superalgebras,[4] we use the notation $A(m|n)=sl(m+1|n+1)$, $B(m|n)=osp(2m+1|2n)$, $C(n)=osp(2|2n-2)$, and $D(m|n)=osp(2m|2n)$. The algebra $B(0|n)=osp(1|2n)$ has a different structure and is usually considered separately (also here). For the classical simple Lie algebras, we use the notation $A_n=sl(n+1)$, $B_n=so(2n+1)$, $C_n=sp(2n)$ and $D_n=so(2n)$; note the difference between C_n and $C(n)$. Note also that for trivial values of m or n, a Lie superalgebra coincides with a Lie algebra: $sl(r|0)=sl(0|r)=sl(r)$, $B(m|0)=B_m$, $D(m|0)=D_m$, $D(0|n)=C_n$.

II. DEFINITION AND CLASSIFICATION METHOD

Let G be a basic classical Lie superalgebra. G has a $\mathbb{Z}_2$-grading $G=G_{\bar{0}}\oplus G_{\bar{1}}$; an element x of $G_{\bar{0}}$ is an even element $[\deg(x)=0]$, an element y of $G_{\bar{1}}$ is an odd element $[\deg(y)=1]$. The elements which are purely even or odd are called homogeneous elements. The Lie superalgebra bracket is denoted by $[\![x,y]\!]$. In the universal enveloping algebra of G, this stands for

$$[\![x,y]\!]=xy-(-1)^{\deg(x)\deg(y)}yx,$$

if x and y are homogeneous. So the bracket can be a commutator or an anti-commutator.

Just as for a Lie algebra,[2] a generalized quantum statistics associated with G is determined by a set of N creation operators x_i^+ and N annihilation operators x_i^-. Following the ideas of para-Bose statistics and those of Ref. 2, these $2N$ operators should generate the Lie superalgebra G, subject to certain triple relations. Let G_{+1} and G_{-1} be the subspaces of G spanned by these elements:

$$G_{+1}=\mathrm{span}\{x_i^+;i=1,\ldots,N\},\quad G_{-1}=\mathrm{span}\{x_i^-;i=1,\ldots,N\}. \tag{2.1}$$

We do not require that these subspaces are homogeneous. The space $[\![G_{+1},G_{+1}]\!]$ can be zero [in which case the creation operators mutually supercommute, as in (1.2)] or nonzero [as in (1.1)]. A similar statement holds for the annihilation operators and $[\![G_{-1},G_{-1}]\!]$. Putting $G_{\pm 2}=[\![G_{\pm 1},G_{\pm 1}]\!]$ and $G_0=[\![G_{+1},G_{-1}]\!]$, the condition that G is generated by the $2N$ elements subject to triple relations only, leads[2] to the requirement that $G=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$, and this must be a $\mathbb{Z}$-grading of G. Since these subspaces are not necessarily homogeneous, this $\mathbb{Z}$-grading is in general not consistent with the $\mathbb{Z}_2$-grading.

Just as in Ref. 2, we shall impose two further requirements: first of all, the generating elements $x_i^\pm$ must be root vectors of G. Second, $\omega(x_i^+)=x_i^-$, where ω is the standard antilinear anti-involutive mapping of G [in terms of root vectors e_α,ω satisfies $\omega(e_\alpha)=e_{-\alpha}$]. This leads to the following definition, completely analogous as in Ref. 2:

Definition 1: Let G be a basic classical Lie superalgebra, with antilinear anti-involutive mapping ω. A set of $2N$ root vectors $x_i^\pm(i=1,\ldots,N)$ is called a set of creation and annihilation operators for G if:

- $\omega(x_i^\pm)=x_i^\mp$,
- $G=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$ *is a* $\mathbb{Z}$*-grading of* G, *with* $G_{\pm 1}=\mathrm{span}\{x_i^\pm,i=1,\ldots,N\}$ *and* $G_{j+k}=[\![G_j,G_k]\!]$.

The algebraic relations $\mathcal{R}$ satisfied by the operators $x_i^\pm$ are the relations of a generalized quantum statistics (GQS) associated with G.

This is a *mathematical* generalization of quantum statistics. Whether all such GQS actually lead to physically acceptable quantum statistics remains to be seen; in this sense one should interpret our GQS as "candidates for generalizations of quantum statistics."

A GQS is characterized by a set $\{x_i^\pm\}$ of CAOs and the set of algebraic relations $\mathcal{R}$ they satisfy. A consequence of this definition is that G is generated by G_{-1} and G_{+1}, i.e., by the set of CAOs, and since $G_{j+k}=[\![G_j,G_k]\!]$, it follows that

$$G=\mathrm{span}\{x_i^\xi,[\![x_i^\xi,x_j^\eta]\!];\quad i,j=1,\ldots,N,\xi,\eta=\pm\}. \tag{2.2}$$

This implies that it is necessary and sufficient to give all relations of the following type:
(R1) The set of all linear relations between the elements $[\![x_i^\xi,x_j^\eta]\!](\xi,\eta=\pm,i,j=1,\ldots,N)$.
(R2) The set of all triple relations of the form $[\![[\![x_i^\xi,x_j^\eta]\!],x_k^\zeta]\!]$=linear combination of x_l^θ.
So $\mathcal{R}$ consists of a set of quadratic relations and a set of triple relations. Also, as a Lie superalgebra defined by generators and relations, G is uniquely characterized by the set of generators $x_i^\pm$ subject to the relations $\mathcal{R}$.

A consequence of this definition is that G_0 itself is a subalgebra of G spanned by root vectors of G.[2] It follows that G_0 is a regular subalgebra containing the Cartan subalgebra H of G. By the adjoint action, the remaining G_i's are G_0-modules. Thus the technique of Ref. 2 can be used in order to obtain a complete classification of all GQS associated with G:

1. Determine all regular subalgebras G_0 of G. If not yet contained in G_0, replace G_0 by G_0+H.
2. For each regular subalgebra G_0, determine the decomposition of G into simple G_0-modules g_k $(k=1, 2,\ldots)$.
3. Investigate whether there exists a $\mathbb{Z}$-grading of G of the form

$$G = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}, \tag{2.3}$$

where each G_i is either directly a module g_k or else a sum of such modules $g_1 \oplus g_2 \oplus \cdots$, such that $\omega(G_{+i})=G_{-i}$.

If the $\mathbb{Z}$-grading is of the form (2.3) with $G_{\pm 2} \neq 0$, we shall say that it has *length* 5; if $G_{+2}=0$ (then $G_{-2}=0$, but $G_{\pm 1} \neq 0$), then the $\mathbb{Z}$-grading is of length 3.

To find regular subalgebras one can use the method of (extended) Dynkin diagrams.[18] The second stage is straightforward by means of representation theoretical techniques. The third stage requires most of the work: one must try out all possible combinations of the G_0-modules g_k, and see whether it is possible to obtain a grading of the type (2.3). In this process, if one of the simple G_0-modules g_k is such that $\omega(g_k)=g_k$, then it follows that this module should be part of G_0. In other words, such a case reduces essentially to another case with a larger regular subalgebra.

In the following sections we shall give a summary of the classification process for the basic classical Lie superalgebras $A(m|n), B(m|n), B(0|n), D(m|n)$, and $C(n)$. Note that, in order to identify a GQS associated with G, it is sufficient to give only the set of CAOs, or alternatively, to give the subspace G_{-1} [then the x_i^- are the root vectors of G_{-1}, and $x_i^+=\omega(x_i^-)$]. The set $\mathcal{R}$ then consists of all quadratic relations (i.e., the linear relations between the elements $[[x_i^{\xi}, x_j^{\eta}]]$) and all triple relations, and all of these relations follow from the known supercommutation relations in G. Because, in principle, $\mathcal{R}$ can be determined from the set $\{x_i^{\pm}; i=1,\ldots,N\}$, we will not always give it explicitly.

Finally, observe that two different sets of CAOs $\{x_i^{\pm}; i=1\ldots,N\}$ and $\{y_i^{\pm}; i=1\ldots,N\}$ (same N) are said to be isomorphic if, for a certain permutation τ of $\{1,2,\ldots,N\}$, the relations between the elements $x_{\tau(i)}^{\pm}$ and $y_i^{\pm}$ are the same. In that case, the regular subalgebra G_0 spanned by $\{[[x_i^+, x_j^-]]\}$ is isomorphic (as a Lie superalgebra) to the regular subalgebra spanned by $\{[[y_i^+, y_j^-]]\}$.

III. THE LIE SUPERALGEBRA $A(m|n)$

Let G be the special linear Lie superalgebra $A(m|n) \equiv sl(m+1|n+1)$, consisting of traceless $(m+n+2)\times(m+n+2)$ matrices. The Cartan subalgebra H of G is the subspace of diagonal matrices. The root vectors of G are known to be the elements $e_{jk}(j \neq k=1,\ldots,m+n+2)$, where e_{jk} is a matrix with zeros everywhere except a 1 on the intersection of row j and column k. The $\mathbb{Z}_2$-grading is such that $\deg(e_{jk})=\theta_{jk}=\theta_j+\theta_k$, where

$$\theta_j = \begin{cases} 0 & \text{if } j = 1, \ldots, m+1 \\ 1 & \text{if } j = m+2, \ldots, m+n+2. \end{cases} \tag{3.1}$$

The root corresponding to $e_{jk}(j,k=1,\ldots,m+1)$ is given by $\epsilon_j-\epsilon_k$; for $e_{m+1+j,m+1+k}(j,k=1,\ldots,n+1)$ it is $\delta_j-\delta_k$; and for $e_{j,m+1+k}$, respectively, $e_{m+1+k,j}(j=1,\ldots,m+1, k=1,\ldots,n+1)$, it is $\epsilon_j-\delta_k$, respectively, $\delta_k-\epsilon_j$. The anti-involution is such that $\omega(e_{jk})=e_{kj}$. The distinguished set of simple roots and the distinguished Dynkin diagram of $A(m|n)$ are given in Table I, and so is the extended distinguished Dynkin diagram.

To find regular subalgebras of $G=A(m|n)$, one should delete nodes from the Dynkin diagrams of $A(m|n)$ (first the ordinary, and then the extended). This goes in systematic steps. For each step, we shall investigate whether it leads to a grading of type (2.3).

TABLE I. Classical Lie superalgebras, their (extended) Dynkin diagrams with a labeling of the nodes and the corresponding simple roots.

LSA	Dynkin diagram and extended Dynkin diagram
$A(m\|n)$	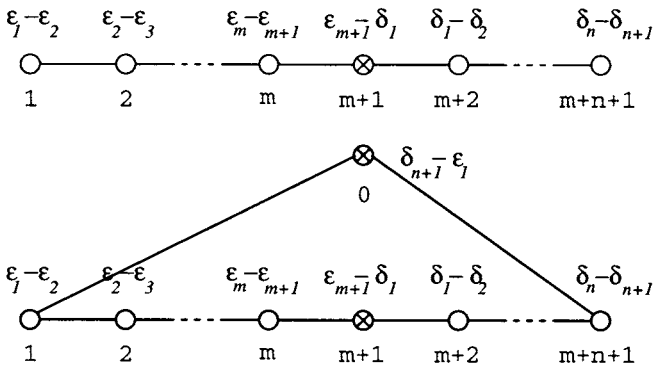
$B(m\|n)$	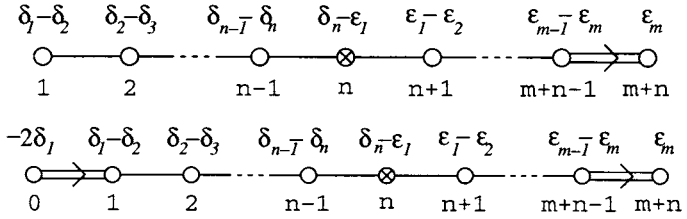
$B(0\|n)$	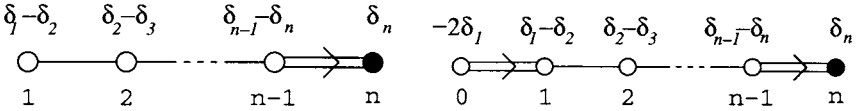
$D(m\|n)$	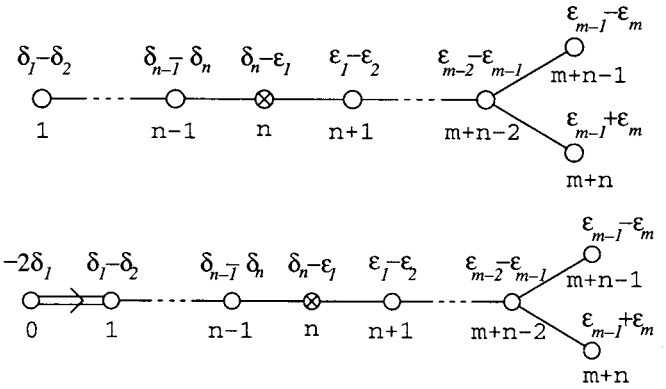
$C(n)$	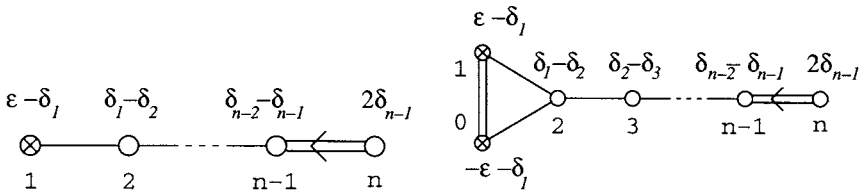

Step 1. Delete node i from the distinguished Dynkin diagram. Then the corresponding diagram is the Dynkin diagram of $G_0=sl(i)\oplus sl(m+1-i|n+1)$ for $i=1,\ldots,m+1$ and of $G_0=sl(m+1|i-m-1)\oplus sl(n+m+2-i)$ for $i=m+2,\ldots,m+n+1$. There are only two G_0-modules and

$$G_{-1}=\text{span}\{e_{kl};k=1,\ldots,i,\quad l=i+1,\ldots,m+n+2\},\tag{3.2}$$

$$G_{+1}=\text{span}\{e_{lk};k=1,\ldots,i,\quad l=i+1,\ldots,m+n+2\}.\tag{3.3}$$

Therefore $A(m|n)$ has a grading of length 3, $A(m|n)=G_{-1}\oplus G_0\oplus G_{+1}$, and the number of creation and annihilation operators is $N=i(m+n+2-i)$.

The most interesting realizations are those with $i=1, i=m+n+1, i=2$ and $i=m+n$. We shall give the explicit supercommutation relations between the CAOs for some of these cases.

For $i=1, N=m+n+1$. Putting

$$a_j^-=e_{1,j+1},\quad a_j^+=e_{j+1,1},\quad j=1,\ldots,m+n+1,$$

the relations $\mathcal{R}$ are

$$\begin{aligned}&[\![a_j^+,a_k^+]\!]=[\![a_j^-,a_k^-]\!]=0,\\ &[\![[\![a_j^+,a_k^-]\!],a_l^+]\!]=(-1)^{\theta_{j+1}}\delta_{jk}a_l^+ +\delta_{kl}a_j^+,\\ &[\![[\![a_j^+,a_k^-]\!],a_l^-]\!]=-(-1)^{\theta_{j+1}}\delta_{jk}a_l^- -(-1)^{\theta_{j+1,k+1}\theta_{l+1}}\delta_{jl}a_k^-.\end{aligned}\tag{3.4}$$

For $m=0$, these are the relations of A-superstatistics,[11,15] see (1.2). Also for general m and n, these relations have been considered in another context.[14]

For $i=m+n+1, N=m+n+1$. Putting

$$a_j^-=e_{j,m+n+2},\quad a_j^+=e_{m+n+2,j},\quad j=1,\ldots,m+n+1$$

one finds:

$$\begin{aligned}&[\![a_j^+,a_k^+]\!]=[\![a_j^-,a_k^-]\!]=0,\\ &[\![[\![a_j^+,a_k^-]\!],a_l^+]\!]=\delta_{jk}a_l^+ -(-1)^{\theta_k}\delta_{kl}a_j^+,\\ &[\![[\![a_j^+,a_k^-]\!],a_l^-]\!]=-\delta_{jk}a_l^- -(-1)^{(\theta_j+1)(\theta_k+1)}\delta_{jl}a_k^-.\end{aligned}\tag{3.5}$$

The relations (3.4) and (3.5) are similar; however the corresponding GQS are not isomorphic. For instance, in (3.4) there are m even and $n+1$ odd pairs of CAOs, and in (3.5) there are n even and $m+1$ odd pairs of CAOs.

For $i=2, N=2(m+n)$. One puts

$$a_{-,j}^-=e_{1,j+2},\quad a_{+,j}^-=e_{2,j+2},\quad j=1,\ldots,m+n,$$

$$a_{-,j}^+=e_{j+2,1},\quad a_{+,j}^+=e_{j+2,2},\quad j=1,\ldots,m+n.$$

Then the corresponding relations read ($\xi,\eta,\epsilon=\pm;j,k,l=1,\ldots,m+n$):

$$[\![a_{\xi j}^+,a_{\eta k}^+]\!]=[\![a_{\xi j}^-,a_{\eta k}^-]\!]=0,$$

$$[\![a_{\xi j}^+,a_{-\xi k}^-]\!]=0,\quad j\neq k,$$

$$[\![a_{-j}^+,a_{-k}^-]\!]=[\![a_{+j}^+,a_{+k}^-]\!],\quad j\neq k,$$

$$[\![a^+_{+j},a^-_{-j}]\!]=[\![a^+_{+k},a^-_{-k}]\!],\quad \text{for } \theta_j=\theta_k,$$

$$[\![a^+_{-j},a^-_{+j}]\!]=[\![a^+_{-k},a^-_{+k}]\!],\quad \text{for } \theta_j=\theta_k,$$

$$[\![[\![a^+_{\xi j},a^-_{\eta k}]\!],a^+_{\epsilon l}]\!]=(-1)^{\deg(a^+_{\xi j})\deg(a^-_{\eta k})+\delta_{\xi,-\eta}\theta_{12}\deg(a^+_{\epsilon l})}\delta_{\eta\epsilon}\delta_{jk}a^+_{\xi l}+\delta_{\xi\eta}\delta_{kl}a^+_{\epsilon j},$$

$$[\![[\![a^+_{\xi j},a^-_{\eta k}]\!],a^-_{\epsilon l}]\!]=-(-1)^{\deg(a^+_{\xi j})\deg(a^-_{\eta k})}\delta_{\xi\epsilon}\delta_{jk}a^-_{\eta l}-(-1)^{\theta_{j+2,k+2}\deg(a^-_{\epsilon l})}\delta_{\xi\eta}\delta_{jl}a^-_{\epsilon k}. \tag{3.6}$$

Such relations are definitely more complicated than (3.4) or (3.5). However, they are still proper defining relations for $A(m|n)$.

Step 2. Delete node i and j from the distinguished Dynkin diagram. We have $G_0=H+sl(i)\oplus sl(j-i)\oplus sl(m+1-j|n+1)$ for $1\leqslant i<j\leqslant m+1$, $G_0=H+sl(i)\oplus sl(m+1-i|j-m-1)\oplus sl(m+n+2-j)$ for $1\leqslant i\leqslant m+1, m+2\leqslant j\leqslant m+n+1$ and $G_0=H+sl(m+1|i-m-1)\oplus sl(j-i)\oplus sl(m+n+2-j)$ for $m+2\leqslant i<j\leqslant m+n+1$. There are six simple G_0-modules. All the possible combinations of these modules give rise to gradings of length 5. There are essentially three different ways in which these G_0-modules can be combined. To characterize these three cases, it is sufficient to give only G_{-1}:

$$G_{-1}=\text{span}\{e_{kl},e_{lp};\quad k=1,\ldots,i,\quad l=i+1,\ldots,j,\quad p=j+1,\ldots,m+n+2\},$$
$$\text{with } N=(j-i)(m+n+2-j+i); \tag{3.7}$$

$$G_{-1}=\text{span}\{e_{kl},e_{pk};\quad k=1,\ldots,i,\quad l=i+1,\ldots,j,\quad p=j+1,\ldots,m+n+2\},$$
$$\text{with } N=i(m+n+2-i); \tag{3.8}$$

$$G_{-1}=\text{span}\{e_{kl},e_{lp};\quad k=1,\ldots,i,\quad p=i+1,\ldots,j,\quad l=j+1,\ldots,m+n+2\},$$
$$\text{with } N=j(m+n+2-j). \tag{3.9}$$

Note that a part of the solutions in (3.8) and (3.9) is isomorphic to some of those given by (3.7). The isomorphic cases can be recognized as those having the same Dynkin diagram of G_0 and the same N-value.

For reasons explained earlier, we shall no longer give the corresponding set of relations explicitly for all possible cases. As an example, we consider here the case $j-i=1$ and (3.7). Then there are $N=m+n+1$ pairs of CAOs, which we can label as follows:

$$a^-_k=e_{k,i+1},\quad a^+_k=e_{i+1,k},\quad k=1,\ldots,i;$$

$$a^-_k=e_{i+1,k+1},\quad a^+_k=e_{k+1,i+1},\quad k=i+1,\ldots,m+n+1.$$

Using

$$\langle k\rangle=\begin{cases}0 & \text{if } k=1,\ldots,i\\ 1 & \text{if } k=i+1,\ldots,m+n+1,\end{cases} \tag{3.10}$$

the quadratic and triple relations now read:

$$[\![a^+_k,a^+_l]\!]=[\![a^-_k,a^-_l]\!]=0,\quad k,l=1,\ldots,i \text{ or } k,l=i+1,\ldots,m+n+1,$$

$$[\![a^-_k,a^+_l]\!]=[\![a^+_k,a^-_l]\!]=0,\quad k=1,\ldots,i,\quad l=i+1,\ldots,m+n+1,$$

$$[[[a_k^+,a_l^-],a_p^+]] = (-1)^{\langle l\rangle+\langle p\rangle+\langle k\rangle\theta_{k+1,i+1}}\delta_{kl}a_p^+ + (-1)^{\langle l\rangle+\langle p\rangle+(1-\langle l\rangle)\theta_{l,i+1}(\theta_{lk}+\theta_{k,i+1})}\delta_{lp}a_k^+, \quad k,l=1,\cdots,i,$$
$$\text{or } k,l=i+1,\ldots,m+n+1,$$

$$[[[a_k^+,a_l^-],a_p^-]] = -(-1)^{\langle l\rangle+\langle p\rangle+\deg(a_k^+)[\langle k\rangle\theta_{k+1,l+1}+(1-\langle l\rangle)\theta_{l,i+1}]}\delta_{kp}a_l^- - (-1)^{\langle l\rangle+\langle p\rangle+\langle k\rangle\theta_{k+1,i+1}}\delta_{kl}a_p^-,$$
$$k,l=1,\ldots,i, \text{or } k,l=i+1,\ldots,m+n+1,$$

$$[[[a_k^\xi,a_l^\xi]],a_p^{-\xi}]] = -(-1)^{\frac{1}{2}\theta_{p,i+1}[(1+\xi)\theta_{l+1,i+1}+(1-\xi)\theta_{k,l+1}]}\delta_{kp}a_l^\xi + (-1)^{\frac{1}{2}(1+\xi)\theta_{l+1,i+1}(\theta_{k,i+1}+\theta_{k,l+1})}\delta_{lp}a_k^\xi,$$
$$k=1,\ldots,i, \quad l=i+1,\ldots,m+n+1,$$

$$[[[a_k^\xi,a_l^\xi]],a_p^\xi]] = 0, \quad \xi=\pm; \quad k,l,p=1,\ldots,m+n+1. \tag{3.11}$$

Step 3. If we delete three or more nodes from the distinguished Dynkin diagram, the resulting $\mathbb{Z}$-gradings of $A(m|n)$ are no longer of the form (2.3). So these cases are not relevant for our classification.

Step 4. Next, we move on to the extended distinguished Dynkin diagram, also given in Table I. If we delete node i from this extended diagram, the remaining diagram is again (a nondistinguished Dynkin diagram) of type $A(m|n)$, so $G_0=G$, and there are no CAOs.

Step 5. If we delete node i and j $(i<j)$ from the extended distinguished Dynkin diagram, then $A(m|n)=G_{-1}\oplus G_0\oplus G_{+1}$ with $G_0=H+sl(m|n+1)$ or $H+sl(m+1|n)$ when the nodes are adjacent, and $G_0=H+sl(k|l)\oplus sl(p|q)$ with $k+p=m+1$ and $l+q=n+1$ when the nodes are nonadjacent. Note that p or q can be zero: $sl(r|0)=sl(0|r)=sl(r)$. Now

$$G_{-1}=\text{span}\{e_{kl}; \quad k=i+1\ldots,j, \quad l\neq i+1,\ldots,j\}. \tag{3.12}$$

The number of annihilation operators is $N=(j-i)(n+m+2-j+i)$. A part of these solutions is isomorphic to some of those of Step 1. The isomorphic cases are again characterized by the fact that their G_0's are isomorphic Lie superalgebras and their N-values coincide.

Step 6. If we delete nodes i,j, and k from the extended distinguished Dynkin diagram $(i<j<k)$, then the corresponding $\mathbb{Z}$-gradings are of the form (2.3). If the three nodes are adjacent $G_0=H+sl(m-1|n+1),H+sl(m|n)$, or $H+sl(m+1|n-1)$. When two adjacent and one nonadjacent nodes are deleted, $G_0=H+sl(l|p)\oplus sl(q|r)$ with $l+q=m,p+r=n+1$ or $l+q=m+1,p+r=n$. If all three nodes are nonadjacent then $G_0=H+sl(l|p)\oplus sl(q|r)\oplus sl(s|t)$ with $l+q+s=m+1,p+r+t=n+1$. One or two of these three Lie superalgebras is $sl(r|0)=sl(0|r)=sl(r)$. There are three different ways in which the corresponding G_0-modules can be combined. We give here only G_{-1}:

$$G_{-1}=\text{span}\{e_{ps},e_{sq}; \quad p=1,\ldots,i,k+1,\ldots,n+m+2, \quad s=i+1,\ldots,j, \quad q=j+1,\ldots,k\},$$
$$\text{with } N=(j-i)(n+m+2-j+i); \tag{3.13}$$

$$G_{-1}=\text{span}\{e_{ps},e_{qp}; \quad p=1,\ldots,i,k+1,\ldots,n+m+2, \quad s=i+1,\ldots,j, \quad q=j+1,\ldots,k\},$$
$$\text{with } N=(k-i)(n+m+2+i-k); \tag{3.14}$$

$$G_{-1}=\text{span}\{e_{pq},e_{qs}; \quad p=1,\ldots,i,k+1,\ldots,n+m+2, \quad s=i+1,\ldots,j, \quad q=j+1,\ldots,k\}$$
$$\text{with } N=(k-j)(n+m+2+j-k). \tag{3.15}$$

Again a part of these solutions is isomorphic to some of those in Step 2 (characterized by an isomorphic G_0 and the same N).

Step 7. If we delete four or more nodes from the extended distinguished Dynkin diagram, the corresponding $\mathbb{Z}$-grading of $A(m|n)$ no longer has the required properties (i.e., there are non zero subspaces G_i with $|i|>2$).

Step 8. Next, one should repeat the process for all non distinguished Dynkin diagrams of G

and their extensions. This is what makes the work harder than the corresponding classification for Lie algebras (which have only one Dynkin diagram and one extension). A general Dynkin diagram is determined by a general simple root system. All the systems of simple roots $\Pi_{S,T}$ of $A(m|n)$ are determined by two increasing sequences[4,17]

$$S=\{s_1<s_2<\ldots\} \text{ and } T=\{t_1<t_2<\ldots\}$$

and a sign:

$$\Pi_{S,T}=\pm\{\epsilon_1-\epsilon_2,\epsilon_2-\epsilon_3,\ldots,\epsilon_{s_1}-\delta_1,\delta_1-\delta_2,\ldots,\delta_{t_1}-\epsilon_{s_1+1},\ldots\}.$$

The Dynkin diagram itself looks like

where each dot can be a white or gray circle (depending upon whether the corresponding simple root is even or odd). Let $\pm(\eta_i-\eta'_j)$ be the last element of $\Pi_{S,T}$ (η and η' can be ϵ or δ). Then the zero node of the extended Dynkin diagram corresponds to $\pm(\eta'_j-\epsilon_1)$ and it is uniquely determined.

If we repeat the whole procedure with the nondistinguished Dynkin diagrams (ordinary and extended), the only new result corresponds to Step 6 deleting three nonadjacent nodes from the extended Dynkin diagram. We have $G_0=H+sl(l|p)\oplus sl(q|r)\oplus sl(s|t)$ with $l+q+s=m+1, p+r+t=n+1$ and in some cases none of the three algebras is $sl(r|0)=sl(0|r)=sl(r)$. Just as in Step 2 or 6, there are three different ways in which the G_0-modules can be combined; the explicit expression is left to the reader.

IV. THE LIE SUPERALGEBRAS $B(m|n)$

$G=B(m|n)\equiv osp(2m+1|2n)$ is the subalgebra of $sl(2m+1|2n)$ consisting of matrices of the form:

$$\begin{pmatrix} a & b & u & x & x_1 \\ c & -a^t & v & y & y_1 \\ -v^t & -u^t & 0 & z & z_1 \\ y_1^t & x_1^t & z_1^t & d & e \\ -y^t & -x^t & -z^t & f & -d^t \end{pmatrix}, \tag{4.1}$$

where a is any $(m\times m)$-matrix, b and c are antisymmetric $(m\times m)$-matrices, u and v are $(m\times 1)$-matrices, x,y,x_1,y_1 are $(m\times n)$-matrices, z and z_1 are $(1\times n)$-matrices, d is any $(n\times n)$-matrix, and e and f are symmetric $(n\times n)$-matrices. The even elements have $x=y=x_1=y_1=0, z=z_1=0$ and the odd elements are those with $a=b=c=0, u=v=0, d=e=f=0$. We shall consider $m=0$ separately in the next section. The Cartan subalgebra H of G is again the subspace of diagonal matrices D. Putting $\epsilon_i(D)=D_{ii}, i=1,\cdots,m$ and $\delta_i(D)=D_{2m+i+1,2m+i+1}, i=1,\ldots,n$, the even root vectors and corresponding roots of G are given by,

$$e_{jk}-e_{k+m,j+m}\leftrightarrow\epsilon_j-\epsilon_k,\quad j\neq k=1,\ldots,m,$$

$$e_{j,k+m}-e_{k,j+m}\leftrightarrow\epsilon_j+\epsilon_k,\quad j<k=1,\ldots,m,$$

$$e_{j+m,k}-e_{k+m,j}\leftrightarrow-\epsilon_j-\epsilon_k,\quad j<k=1,\ldots,m,$$

$$e_{j,2m+1}-e_{2m+1,j+m}\leftrightarrow\epsilon_j,\quad j=1,\ldots,m,$$

$$e_{j+m,2m+1} - e_{2m+1,j} \leftrightarrow -\epsilon_j, \quad j = 1,\ldots,m,$$

$$e_{2m+1+j,2m+1+k} - e_{n+2m+1+k,n+2m+1+j} \leftrightarrow \delta_j - \delta_k, \quad j \neq k = 1,\ldots,n,$$

$$e_{2m+1+j,2m+1+k+n} + e_{2m+1+k,2m+1+j+n} \leftrightarrow \delta_j + \delta_k, \quad j \leqslant k = 1,\ldots,n,$$

$$e_{2m+1+n+j,2m+1+k} + e_{2m+1+n+k,2m+1+j} \leftrightarrow -\delta_j - \delta_k, \quad j \leqslant k = 1,\ldots,n,$$

and the odd ones by

$$e_{j,2m+1+k} - e_{2m+1+n+k,j+m} \leftrightarrow \epsilon_j - \delta_k, \quad j = 1,\ldots,m, \quad k = 1,\ldots,n,$$

$$e_{m+j,2m+1+k} - e_{2m+1+n+k,j} \leftrightarrow -\epsilon_j - \delta_k, \quad j = 1,\ldots,m, \quad k = 1,\ldots,n,$$

$$e_{2m+1,2m+1+k} - e_{2m+1+n+k,2m+1} \leftrightarrow -\delta_k, \quad k = 1,\ldots,n,$$

$$e_{j,2m+1+n+k} + e_{2m+1+k,m+j} \leftrightarrow \epsilon_j + \delta_k, \quad j = 1,\ldots,m, \quad k = 1,\ldots,n,$$

$$e_{m+j,2m+1+n+k} + e_{2m+1+k,j} \leftrightarrow -\epsilon_j + \delta_k, \quad j = 1,\ldots,m, \quad k = 1,\ldots,n,$$

$$e_{2m+1,2m+1+n+k} + e_{2m+1+k,2m+1} \leftrightarrow \delta_k, \quad k = 1,\ldots,n.$$

The distinguished set of simple roots and the corresponding Dynkin diagram of $B(m|n)$ are given in Table I.

Step 1. Delete node i from the distinguished Dynkin diagram. The corresponding diagram is the Dynkin diagram of $G_0 = H + sl(i) \oplus B(m|n-i)$ for $i = 1,\ldots,n$ and of $G_0 = H + sl(j|n) \oplus B_{m-j}$ for $i = n+j, j = 1,\ldots,m$. There are four simple G_0-modules and $B(m|n) = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}$, where for $i = 1,\ldots n$:

$$\begin{aligned} G_{-1} = \text{span}\{&e_{2m+1,2m+1+n+k} + e_{2m+1+k,2m+1}, e_{2m+1+k,2m+1+n+l} + e_{2m+1+l,2m+1+n+k}, e_{2m+1+k,2m+1+l} \\ &- e_{n+2m+1+l,n+2m+1+k}, e_{p,2m+1+n+k} + e_{2m+1+k,m+p}, e_{m+p,2m+1+n+k} + e_{2m+1+k,p}; \\ &k = 1,\ldots,i, \quad l = i+1,\ldots,n, \quad p = 1,\ldots,m\}, \quad \text{with } N = 2i(m+n) - i(2i-1); \end{aligned} \tag{4.2}$$

and for $i = n+j, j = 1,\ldots m$:

$$\begin{aligned} G_{-1} = \text{span}\{&e_{2m+1,2m+1+n+k} + e_{2m+1+k,2m+1}, e_{p,2m+1} - e_{2m+1,m+p}, e_{p,m+q} - e_{q,m+p}, e_{pq} \\ &- e_{m+q,m+p}, e_{q,2m+1+n+k} + e_{2m+1+k,m+q}, e_{m+q,2m+1+n+k} + e_{2m+1+k,q}; \\ &k = 1,\ldots,n, \quad p = 1,\ldots,j, \quad q = j+1,\ldots,m\}, \quad \text{with } N = 2i(m+n) - i(2i-1). \end{aligned} \tag{4.3}$$

It is interesting to give $\mathcal{R}$ for $i = n+m$, because then the number of creation or annihilation operators is $N = n+m$. One can label (and rescale) the CAOs as follows:

$$\begin{aligned} b_j^- \equiv B_j^- &= -\sqrt{2}(e_{2m+1,2m+1+n+j} + e_{2m+1+j,2m+1}), \quad j = 1,\ldots,n, \\ b_j^+ \equiv B_j^+ &= \sqrt{2}(e_{2m+1,2m+1+j} - e_{2m+1+n+j,2m+1}), \quad j = 1,\ldots,n, \\ b_{n+j}^- \equiv F_j^- &= \sqrt{2}(e_{j,2m+1} - e_{2m+1,m+j}), \quad j = 1,\ldots,m, \end{aligned} \tag{4.4}$$

$$b_{n+j}^{+} \equiv F_j^{+} = \sqrt{2}(e_{2m+1,j} - e_{m+j,2m+1}), \quad j = 1,\ldots,m. \tag{4.5}$$

Note that

$$\deg(b_j^{\pm}) = \langle j \rangle = \begin{cases} 1 & \text{if } j = 1,\ldots,n \\ 0 & \text{if } j = n+1,\ldots,n+m. \end{cases} \tag{4.6}$$

There are no quadratic relations, and $\mathcal{R}$ consists of triple relations only:

$$\begin{gathered} [[[b_j^{\xi}, b_k^{\eta}], b_l^{\epsilon}]] = -2\delta_{jl}\delta_{\epsilon,-\xi}\epsilon^{\langle l \rangle}(-1)^{\langle k \rangle \langle l \rangle} b_k^{\eta} + 2\epsilon^{\langle l \rangle}\delta_{kl}\delta_{\epsilon,-\eta} b_j^{\xi}, \\ \xi, \eta, \epsilon = \pm \text{ or } \pm 1; \quad j,k,l = 1,\ldots,n+m. \end{gathered} \tag{4.7}$$

Note that $B_j^{\pm}, j=1,\ldots,n$ (respectively, $F_k^{\pm}, k=1,\ldots,m$) are para-Bose (respectively, para-Fermi) CAOs, namely

$$\begin{gathered} [\{B_j^{\xi}, B_k^{\eta}\}, B_l^{\epsilon}] = (\epsilon - \xi)\delta_{jl} B_k^{\eta} + (\epsilon - \eta)\delta_{kl} B_j^{\xi}, \\ \xi, \eta, \epsilon = \pm \text{ or } \pm 1; \quad j,k,l = 1,\ldots,n; \end{gathered} \tag{4.8}$$

$$\begin{gathered} [[F_j^{\xi}, F_k^{\eta}], F_l^{\epsilon}] = \tfrac{1}{2}(\epsilon - \eta)^2 \delta_{kl} F_j^{\xi} - \tfrac{1}{2}(\epsilon - \xi)^2 \delta_{jl} F_k^{\eta}, \\ \xi, \eta, \epsilon = \pm \text{ or } \pm 1; \quad j,k,l = 1,\ldots,m. \end{gathered} \tag{4.9}$$

The fact that $B(m|n)$ can be generated by n pairs of para-Bose and m pairs of para-Fermi operators has been discoved in Ref. 19.

Step 2. If we delete two or more nodes from the distinguished Dynkin diagram, the resulting $\mathbb{Z}$-gradings of $B(m|n)$ are no longer of the form (2.3).

Step 3. Now we continue with the extended Dynkin diagram, also given in Table I. Delete node $i=0,1,\ldots,n+m$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $G_0 = B(m|n), A_1 \oplus B(m|n-1), C_2 \oplus B(m,n-2), \ldots, C_{n-1} \oplus B(m|1), C_n \oplus B_m, C(n+1) \oplus B_{m-1}, D(2|n) \oplus B_{m-2}, \ldots, D(m-1|n) \oplus A_1, D(m|n)$. In all these cases there is only one G_0-module, so there are no contributions to the classification.

Step 4. Delete the adjacent nodes $(i-1)$ and i, $i=2,3,\ldots,n$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $\widetilde{G}_0 = A_1 \oplus B(m|n-2)$ for $i=2$, of $\widetilde{G}_0 = C_{i-1} \oplus B(m|n-i)$ for $i=3,\ldots,n-1$ and of $\widetilde{G}_0 = C_{n-1} \oplus B_m$ for $i=n$. In each case there are seven $\widetilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0 = H + \widetilde{G}_0 + g_1$, and in each case one finds $G_0 \equiv H + B(m|n-1)$. Now there are four G_0-modules and $B(m|n) = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}$ with

$$\begin{aligned} G_{-1} = \operatorname{span}\{ & e_{2m+1,2m+1+n+i} + e_{2m+1+i,2m+1}, e_{2m+1+i,2m+1+n+j} + e_{2m+1+j,2m+1+n+i}, e_{2m+1+i,2m+1+j} \\ & - e_{n+2m+1+j,n+2m+1+i}, \quad i \neq j = 1,\ldots,n; e_{k,2m+1+n+i} + e_{2m+1+i,m+k}, e_{m+k,2m+1+n+i} + e_{2m+1+i,k}, \\ & k = 1,\ldots,m\}, \end{aligned}$$

and $N = 2(m+n)-1$. Observe that in this case $G_{-2} = \operatorname{span}\{e_{2m+1+i,2m+1+n+i}\}$, and all these cases are isomorphic to that of Step 1 with $i=1$.

Step 5. Delete the adjacent nodes $(i-1)$ and i, $i=n+j$, $j=1,2,\ldots,m$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $\widetilde{G}_0 = C_n \oplus B_{m-1}$ for $j=1$, of $\widetilde{G}_0 = C(n+1) \oplus B_{m-2}$ for $j=2$, of $\widetilde{G}_0 = D(j-1|n) \oplus B_{m-j}$ for $j=3,\ldots,m-2$, of $\widetilde{G}_0 = D(m-2|n) \oplus A_1$ for $j=m-1$, and of $\widetilde{G}_0 = D(m-1|n)$ for $j=m$. In each case there are five $\widetilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0 = H + \widetilde{G}_0 + g_1$, and in each case one finds $G_0 \equiv H + B(m-1|n)$. Now there are two G_0-modules and $B(m|n) = G_{-1} \oplus G_0 \oplus G_{+1}$ with

$$G_{-1}=\mathrm{span}\{e_{j,2m+1}-e_{2m+1,j+m},e_{j,k+m}-e_{k,j+m},e_{jk}-e_{k+m,j+m},\quad j\neq k=1,\ldots,m;e_{j,2m+1+n+l}+e_{2m+1+l,m+j},e_{j,2m+1+l}-e_{2m+1+n+l,j+m},\quad l=1,\ldots,n\},\tag{4.10}$$

and $N=2(m+n)-1$. All these cases are mutually isomorphic.

Step 6. Delete the nonadjacent nodes i,j, $i<j-1$, $j=3,\ldots,n$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=C_i\oplus sl(j-i)\oplus B(m|n-j)$ (for $i=1$ instead of C_i we have A_1). In each case there are seven $\tilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0=H+\tilde{G}_0+g_1$, and in each case one finds $G_0\equiv H+sl(j-i)\oplus B(m|n-j+i)$. Now there are four G_0-modules and $B(m|n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$. All these cases are isomorphic to those in Step 1 with $i=2,\ldots,n-1$.

Step 7. Delete the nonadjacent nodes i,j, $i=1,\ldots,n$, $j=n+1,\ldots,n+m$ [but $(i,j)\neq(n,n+1)$] from the extended distinguished Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=C_i\oplus sl(j-n|n-i)\oplus B_{n+m-j}$ (for $i=1$ instead of C_i we have A_1). In each case there are seven $\tilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0=H+\tilde{G}_0+g_1$, and one always finds $G_0\equiv H+sl(j-n|n-i)\oplus B(n+m-j|i)$. Now there are four G_0-modules and $B(m|n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$, where

$$\begin{aligned}G_{-1}=\mathrm{span}\{&e_{k,2m+1}-e_{2m+1,k+m},e_{2m+1,2m+1+n+l}+e_{2m+1+l,2m+1},e_{k,2m+1+n+p}+e_{2m+1+p,m+k},e_{k,2m+1+p}\\&-e_{2m+1+n+p,m+k},e_{2m+1+l,2m+1+n+p}+e_{2m+1+p,2m+1+n+l},e_{2m+1+l,2m+1+p}\\&-e_{2m+1+n+p,2m+1+n+l},e_{s,2m+1+n+l}+e_{2m+1+l,m+s},e_{m+s,2m+1+n+l}+e_{2m+1+l,s},\\&k=1,\ldots,j-n,\quad l=i+1,\ldots,n,\quad p=1,\ldots,i,\quad s=j+1-n,\ldots,m\},\end{aligned}\tag{4.11}$$

with $N=2(j-i)(m+n)-(j-i)(2(j-i)-1)$. All these cases are new (i.e., not isomorphic to an earlier case).

Step 8. Delete the nonadjacent nodes i,j, $i<j-1$, $i=n+1,\ldots,n+m-2$, $j=n+3,n+4,\ldots,n+m$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=D(i-n|n)\oplus sl(j-i)\oplus B_{n+m-j}$ [for $i=n+1$ instead of $D(i-n|n)$ we have $C(n+1)$]. In each case there are seven $\tilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0=H+\tilde{G}_0+g_1$, and one finds $G_0\equiv H+sl(j-i)\oplus B(m-j+i|n)$. Now there are four G_0-modules, and $B(m|n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$, where

$$\begin{aligned}G_{-1}=\mathrm{span}\{&e_{k,2m+1}-e_{2m+1,k+m},e_{k,m+l}-e_{l,m+k},e_{kl}-e_{m+l,m+k},e_{k,2m+1+n+p}+e_{2m+1+p,m+k},e_{k,2m+1+p}\\&-e_{2m+1+n+p,m+k},\\&k=i-n+1,i-n+2,\ldots,j-n,\quad l=1,2,\ldots,i-n,j-n+1,j-n+2,\ldots,m,\quad p=1,2,\ldots,n\},\end{aligned}\tag{4.12}$$

with $N=2(j-i)(m+n)-(j-i)(2(j-i)-1)$. All these cases are isomorphic to cases of Step 7.

Step 9. If we delete three or more nodes from the extended distinguished Dynkin diagram, the corresponding $\mathbb{Z}$-grading of $B(m|n)$ no longer has the required properties (i.e., there are non zero subspaces G_i with $|i|>2$).

The next step consists of repeating this procedure for the nondistinguished Dynkin diagrams and their extensions. Following Ref. 17 one can obtain all such Dynkin diagrams of $B(m|n)$. We have repeated this procedure for all of them, leading to a lot of case studies but not leading to any new results (i.e., each case is isomorphic to one described already by means of the distinguished diagram).

V. THE LIE SUPERALGEBRAS $B(0|n)$

We consider the Lie superalgebra $B(0|n)$ separately because the distinguished choice of the simple roots for $B(0|n)$ is different than that of $B(m|n)$. In Table I the distinguished simple roots, the distinguished Dynkin diagram, and the extended distinguished Dynkin diagram are given.

Step 1. Delete node i, $i=1,\ldots,n$ from the distinguished Dynkin diagram. The corresponding diagram is the Dynkin diagram of $G_0=H+sl(i)\oplus B(0|n-i)$. There are four simple G_0-modules and $B(0|n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$, where

$$G_{-1}=\mathrm{span}\{e_{1,1+n+k}+e_{1+k,2m+1},e_{1+k,1+n+l}+e_{1+l,1+n+k},e_{1+k,1+l}-e_{n+1+l,n+1+k},\\ k=1,\ldots,i,\quad l=i+1,\ldots,n,\}, \tag{5.1}$$

with $N=2i(n-i)+i$. We give $\mathcal{R}$ for $i=n$, because then the number of creation or annihilation operators is $N=n$. One can label the CAOs as follows:

$$B_j^-=-\sqrt{2}(e_{1,1+n+j}+e_{1+j,1}),\quad j=1,\ldots,n,\\ B_j^+=\sqrt{2}(e_{1,1+j}-e_{1+n+j,1}),\quad j=1,\ldots,n. \tag{5.2}$$

These are all odd generators of $B(0|n)$ and the relations $\mathcal{R}$ consist of the triple para-Bose relations given already in (4.8).

Step 2. If we delete two or more nodes from the distinguished Dynkin diagram, the resulting $\mathbb{Z}$-gradings of $B(0|n)$ are no longer of the form (2.3).

Step 3. Delete node i, $i=0,1,\ldots,n$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $G_0=B(0|n),A_1\oplus B(0|n-1),C_2\oplus B(0,n-2),\ldots,C_{n-1}\oplus B(0|1),C_n$. In all these cases there is only one G_0-module, so there are no contributions to the classification.

Step 4. Delete the adjacent nodes $(i-1)$ and i, $i=2,3,\ldots,n$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=A_1\oplus B(0|n-2)$ for $i=2$, of $\tilde{G}_0=C_{i-1}\oplus B(0|n-i)$ for $i=3,\ldots,n-1$, and of $\tilde{G}_0=C_{n-1}$ for $i=n$. In each case there are seven $\tilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0=H+\tilde{G}_0+g_1$, and in each case one finds $G_0\equiv H+B(0|n-1)$. Now there are four G_0-modules and $B(0|n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$ with

$$G_{-1}=\mathrm{span}\{e_{1,1+n+i}+e_{1+i,1},e_{1+i,1+n+j}+e_{1+j,1+n+i},e_{1+i,1+j}-e_{n+1+j,n+1+i},\quad i\neq j=1,\ldots,n\},$$

$N=2n-1$, and $G_{-2}=\mathrm{span}\{e_{1+i,1+n+i}\}$. All these cases are isomorphic to those of Step 1 with $i=1$.

Step 5. Delete the nonadjacent nodes i,j from the extended distinguished Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=C_i\oplus sl(j-i)\oplus B(0|n-j)$ [for $i=1,\tilde{G}_0=A_1\oplus sl(j-1)\oplus B(0|n-j)$; for $j=n,\tilde{G}_0=C_i\oplus sl(n-i)$]. In each case there are seven $\tilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0=H+\tilde{G}_0+g_1$, and in each case one finds $G_0\equiv H+sl(j-i)\oplus B(0|n-j+i)$. Now there are four G_0-modules and $B(0|n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$. All these cases are isomorphic to those in Step 1 with $i=2,\ldots,n-1$.

Step 6. If we delete three or more nodes from the extended distinguished Dynkin diagram, the corresponding $\mathbb{Z}$-grading of $B(0|n)$ no longer has the required properties (i.e., there are nonzero subspaces G_i with $|i|>2$).

In the case of $B(0|n)$ any other choice of simple roots is equivalent to the distinguished choice, so there are no more cases to study.

VI. THE LIE SUPERALGEBRAS $D(m|n)$

$G=D(m|n)\equiv osp(2m|2n)$ is the subalgebra of $sl(2m|2n)$ consisting of matrices of the form (4.1) with the middle row and column deleted. The Cartan subalgebra H of G is again the subspace of diagonal matrices D. Putting $\epsilon_i(D)=d_{ii},i=1,\ldots,m,\delta_i(D)=d_{2m+i,2m+i},i=1,\ldots,n$, the even root vectors and corresponding roots of G are given by

$$e_{jk}-e_{k+m,j+m}\leftrightarrow\epsilon_j-\epsilon_k,\quad j\neq k=1,\ldots,m,$$

$$e_{j,k+m} - e_{k,j+m} \leftrightarrow \epsilon_j + \epsilon_k, \quad j < k = 1,\ldots,m,$$

$$e_{j+m,k} - e_{k+m,j} \leftrightarrow -\epsilon_j - \epsilon_k, \quad j < k = 1,\ldots,m,$$

$$e_{2m+j,2m+k} - e_{n+2m+k,n+2m+j} \leftrightarrow \delta_j - \delta_k, \quad j \neq k = 1,\ldots,n,$$

$$e_{2m+j,2m+k+n} + e_{2m+k,2m+j+n} \leftrightarrow \delta_j + \delta_k, \quad j \leqslant k = 1,\ldots,n,$$

$$e_{2m+n+j,2m+k} + e_{2m+n+k,2m+j} \leftrightarrow -\delta_j - \delta_k, \quad j \leqslant k = 1,\ldots,n,$$

and the odd root vectors and roots by

$$e_{j,2m+k} - e_{2m+n+k,j+m} \leftrightarrow \epsilon_j - \delta_k, \quad j = 1,\ldots,m, \quad k = 1,\ldots,n,$$

$$e_{m+j,2m+k} - e_{2m+n+k,j} \leftrightarrow -\epsilon_j - \delta_k, \quad j = 1,\ldots,m, \quad k = 1,\ldots,n,$$

$$e_{j,2m+n+k} + e_{2m+k,m+j} \leftrightarrow \epsilon_j + \delta_k, \quad j = 1,\ldots,m, \quad k = 1,\ldots,n,$$

$$e_{m+j,2m+n+k} + e_{2m+k,j} \leftrightarrow -\epsilon_j + \delta_k, \quad j = 1,\ldots,m, \quad k = 1,\ldots,n.$$

The distinguished set of simple roots, the corresponding Dynkin diagram and its extension are given in Table I.

Step 1. Delete node i, $i=1,\ldots,m+n-2$ from the distinguished Dynkin diagram. The corresponding diagram is that of $G_0=H+D(m|n-1)$ for $i=1$, of $G_0=H+sl(i)\oplus D(m|n-i)$ for $i=2,\ldots,n-1$, of $G_0=H+sl(n)\oplus D_m$ for $i=n$, of $G_0=H+sl(i-n|n)\oplus D_{m+n-i}$ for $i=n+1,\ldots,m+n-3$, and of $G_0=H+sl(m-2|n)\oplus A_1\oplus A_1$ for $i=m+n-2$. There are four simple G_0-modules and $D(m|n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$, where for, $i=1,\ldots,n$:

$$G_{-1} = \mathrm{span}\{e_{2m+j,2m+n+k} + e_{2m+k,2m+j+n}, e_{2m+j,2m+k} - e_{n+2m+k,n+2m+j}, e_{l,2m+n+j} + e_{2m+j,m+l}, e_{m+l,2m+n+j} + e_{2m+j,l}; \quad j = 1,\ldots,i, \quad k = i+1,\ldots,n, \quad l = 1,\ldots,m\} \tag{6.1}$$

with $N=2i(m+n-i)$; whereas for $i=n+1,\ldots,m+n-2$:

$$G_{-1} = \mathrm{span}\{e_{k,2m+n+j} + e_{2m+j,m+k}, e_{m+k,2m+n+j} + e_{2m+j,k}, e_{l,m+k} - e_{k,m+l}, e_{lk} - e_{m+k,m+l}; \quad j = 1,\ldots,n, \quad k = i-n+1,\ldots,m, \quad l = 1,\ldots,i-n,\}, \tag{6.2}$$

with $N=2i(m+n-i)$.

Step 2. Delete node $m+n-1$ or $m+n$ from the distinguished Dynkin diagram. The corresponding diagram is the Dynkin diagram of $G_0=H+sl(m|n)$. There are two simple G_0-modules and $D(m|n)=G_{-1}\oplus G_0\oplus G_{+1}$, where, for $m+n-1$:

$$G_{-1} = \mathrm{span}\{e_{j,m+k} - e_{k,m+j}, \quad j < k = 1,\ldots,m-1, \quad e_{2m+q,2m+n+s} + e_{2m+s,2m+n+q}, \quad q \leqslant s = 1,\ldots,n, \quad e_{lm} + e_{2m,m+l}, e_{l,2m+n+p} + e_{2m+p,m+l}, e_{2m,2m+n+p} + e_{2m+p,m}, \quad l = 1,\ldots,m-1, \quad p = 1,\ldots,n\}; \tag{6.3}$$

and for $m+n$:

$$G_{-1} = \mathrm{span}\{e_{j,m+k} - e_{k,m+j}, \quad j < k = 1,\ldots,m, \quad e_{2m+p,2m+n+s} + e_{2m+s,2m+n+p}, \quad p \leqslant s = 1,\ldots,n, \quad e_{j,2m+n+l} + e_{2m+l,m+j}, \quad j = 1,\ldots,m, \quad l = 1,\ldots,n\}. \tag{6.4}$$

Both cases have $N=(m+n)(m+n+1)/2-m$, and they are isomorphic.

Step 3. Upon deleting two nodes i and j (except $i=m+n-1, j=m+n$) or more from the

distinguished Dynkin diagram of $D(m|n)$, the corresponding $\mathbb{Z}$-gradings no longer have the required property (there are nonzero G_i with $|i|>2$).

Step 4. Delete node $m+n-1$ and $m+n$ from the distinguished Dynkin diagram. We have $G_0=H+sl(m-1|n)$. There are six simple G_0-modules. All the possible combinations of these modules give rise to gradings of the form (2.3). There are essentially three different ways in which these G_0-modules can be combined. To characterize these three cases, it is sufficient to give only G_{-1}:

$$G_{-1}=\mathrm{span}\{e_{jm}-e_{2m,m+j},e_{j,2m}-e_{m,m+j},e_{m,2m+k}-e_{2m+n+k,2m},e_{m,2m+n+k}+e_{2m+k,2m};\\ j=1,\ldots,m-1,\quad k=1,\ldots,n\},\tag{6.5}$$

with $N=2(m+n-1)$;

$$G_{-1}=\mathrm{span}\{e_{jm}-e_{2m,m+j},e_{2m,2m+n+k}+e_{2m+k,m},e_{m+j,l}-e_{m+l,j},e_{m+j,2m+k}-e_{2m+n+k,j},e_{2m+n+k,2m+p}\\ +e_{2m+n+p,2m+k};\quad j=1,\ldots,m-1,\quad k=1,\ldots,n,\quad j<l=1,\ldots,m-1,\quad k\leqslant p=1,\ldots,n\},\tag{6.6}$$

with $N=(m+n)(m+n+1)/2-m$;

$$G_{-1}=\mathrm{span}\{e_{j,m+l}-e_{l,m+j},e_{j,2m+n+k}+e_{2m+k,m+j},e_{2m+k,2m+n+p}+e_{2m+p,2m+n+k},e_{m+j,m}-e_{2m,j},e_{2m,2m+k}\\ -e_{2m+n+k,m};\quad j=1,\ldots,m-1,\quad k=1,\ldots,n,\quad j<l=1,\ldots,m-1,\quad k\leqslant p=1,\ldots,n\},\tag{6.7}$$

with $N=(m+n)(m+n+1)/2-m$. The cases (6.6) and (6.7) are isomorphic.

Step 5. Delete node i, $i=0,1,\ldots,n+m$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $G_0=D(m|n),A_1\oplus D(m|n-1),C_2\oplus D(m|n-2),\ldots,C_{n-1}\oplus D(m|1),C_n\oplus D_m,C(n+1)\oplus D_{m-1},D(2|n)\oplus D_{m-2},\ldots,D(m-2|n)\oplus A_1\oplus A_1,D(m|n),D(m|n)$. In all these cases there is only one G_0-module, so there are no contributions to the classification.

Step 6. Delete the adjacent nodes $(i-1)$ and i, $i=2,3,\ldots,n$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=A_1\oplus D(m|n-2)$ for $i=2$, of $\tilde{G}_0=C_{i-1}\oplus D(m|n-i)$ for $i=3,\ldots,n-1$ and of $\tilde{G}_0=C_{n-1}\oplus D_m$ for $i=n$. In each case there are seven $\tilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0=H+\tilde{G}_0+g_1$, and in each case one finds $G_0\equiv H+D(m|n-1)$. Now there are four G_0-modules and $D(m|n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$ with

$$G_{-1}=\mathrm{span}\{e_{2m+k,2m+n+i}+e_{2m+i,2m+n+k},e_{2m+i,2m+k}-e_{2m+n+k,2m+n+i},\quad i\neq k=1,\ldots,n,\\ e_{l,2m+n+i}+e_{2m+i,m+l},e_{m+l,2m+n+i}+e_{2m+i,l},\quad l=1,\ldots,m\},$$

$N=2(m+n-1)$ and $G_{-2}=\mathrm{span}\{e_{2m+i,2m+n+i}\}$. All these cases are isomorphic to that of Step 1 with $i=1$.

Step 7. Delete the adjacent nodes $(i-1)$ and i, $i=n+1,\ldots,m+n-1$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=C_n\oplus D_{m-1}$ for $i=n+1$, of $\tilde{G}_0=C(n+1)\oplus D_{m-2}$ for $i=n+2$, of $\tilde{G}_0=D(i-n-1|n)\oplus D_{m+n-i}$ for $i=n+3,\ldots,m+n-3$, of $\tilde{G}_0=D(m-3|n)\oplus A_1\oplus A_1$ for $i=m+n-2$ and of $\tilde{G}_0=D(m-2|n)\oplus A_1$ for $i=m+n-1$. In each case there are five $\tilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0=H+\tilde{G}_0+g_1$, and in each case one finds $G_0\equiv H+D(m-1|n)$. Now there are two G_0-modules and $D(m|n)=G_{-1}\oplus G_0\oplus G_{+1}$ with

$$G_{-1}=\mathrm{span}\{e_{i-n,2m+n+j}+e_{2m+j,m+i-n},e_{i-n,2m+j}-e_{2m+n+j,m+i-n},\quad j=1,\ldots,n,\\ e_{k,m+i-n}-e_{i-n,m+k},e_{i-n,k}-e_{m+k,m+i-n},\quad i-n\neq k=1,\ldots,m\}\tag{6.8}$$

and $N=2(m+n-1)$. All these cases are mutually isomorphic.

Step 8. Delete the adjacent nodes $m+n-1$ and $m+n$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $G_0 \equiv D(m-1|n)$. There are two G_0-modules and $D(m|n)=G_{-1}\oplus G_0\oplus G_{+1}$ with

$$G_{-1}=\mathrm{span}\{e_{m,2m+n+j}+e_{2m+j,2m},e_{m,2m+j}-e_{2m+n+j,2m},\quad j=1,\ldots,n,$$
$$e_{k,2m}-e_{m,m+k},e_{m,k}-e_{m+k,2m},\quad k=1,\ldots,m-1\},\tag{6.9}$$

with $N=2(m+n-1)$. This case and all cases from Step 7 are isomorphic.

Step 9. Delete the nonadjacent nodes $i,j,\quad i<j-1,\ j=3,\ldots,n$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=C_i\oplus sl(j-i)\oplus D(m|n-j)$ (for $i=1$ instead of C_i we have A_1). In each case there are seven $\tilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0=H+\tilde{G}_0+g_1$, and in each case one finds $G_0 \equiv H+sl(j-i)\oplus D(m|n-j+i)$. Now there are four G_0-modules and $D(m|n)=G_{-2}\oplus G_{-1}\oplus G_0 \oplus G_{+1}\oplus G_{+2}$. All these cases are isomorphic to those of Step 1 with $i=2,\ldots,n-1$.

Step 10. Delete the nonadjacent nodes $i,j,\ i=1,\ldots,n,\ j=n+1,\ldots,n+m-2$ [but $(i,j)\neq(n,n+1)$] from the extended distinguished Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=C_i \oplus sl(j-n|n-i)\oplus D_{m+n-j}$ (for $j=n+m-2$ instead of D_{n+m-j} we have $A_1\oplus A_1$). In each case there are seven $\tilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0=H+\tilde{G}_0+g_1$, and in each case one finds $G_0\equiv H+sl(j-n|n-i)\oplus D(m+n-j|i)$. Now there are four G_0-modules and $D(m|n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$ with

$$G_{-1}=\mathrm{span}\{e_{kl}-e_{m+l,m+k},e_{k,m+l}-e_{l,m+k},e_{r,2m+n+s}+e_{2m+s,m+r},e_{m+l,2m+n+p}+e_{2m+p,l},$$
$$e_{k,2m+q}-e_{2m+n+q,m+k},e_{2m+q,2m+n+p}+e_{2m+p,2m+n+q},e_{2m+p,2m+q}-e_{2m+n+q,2m+n+p},$$
$$k=1,\ldots,j-n,\quad l=j-n+1,\ldots,m,\quad r=1,\ldots,m,\quad s=1,\ldots,n,\quad q=1,\ldots,i,\quad p=i+1,\ldots,n\},\tag{6.10}$$

with $N=2(j-i)(m+n-j+i)$.

Step 11. Delete the nonadjacent nodes $i,j,\quad i=1,\ldots,n$, and $j=n+m-1$ or $n+m$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $G_0=C_i\oplus sl(m|n-i)$. There are four G_0-modules and $D(m|n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$ with

$$G_{-1}=\mathrm{span}\{e_{k,2m+p}-e_{2m+n+p,m+k},e_{k,2m+n+p}+e_{2m+p,m+k},e_{2m+p,2m+n+q}+e_{2m+q,2m+n+p},e_{2m+q,2m+p}$$
$$-e_{2m+n+p,2m+n+q};\quad k=1,\ldots,m,\quad p=1,\ldots,i,\quad q=i+1,\ldots,n\}\tag{6.11}$$

for $j=m+n$ and a similar expression for $j=m+n-1$. Naturally, both cases are isomorphic and $N=2i(m+n-i)$.

Step 12. Delete the nonadjacent nodes $i,j,\ i=n+1,\ldots,m+n-2,\ j=n+m-1$ or $n+m$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $G_0=D(i-n|n)\oplus sl(m+n-i)$ (if $i=n+1$ instead of $D(i-n|n)$ we have $C(n+1)$). There are four G_0-modules and $D(m|n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$ with

$$G_{-1}=\mathrm{span}\{e_{kl}-e_{m+l,m+k},e_{m+k,l}-e_{m+l,k},e_{m+l,2m+n+p}+e_{2m+p,l};e_{m+l,2m+p}-e_{2m+n+p,l},$$
$$k=1,\ldots,i-n,\quad l=i-n+1,\ldots,m,\quad p=1,\ldots,n\},\tag{6.12}$$

for $j=m+n$ and a similar expression for $j=m+n-1$, both having $N=2i(m+n-i)$. The cases here and in Step 10 with one and the same G_0 and N are isomorphic.

Step 13. Delete the nonadjacent nodes $i,j,\ i<j-1,\ i=n+1,\ldots,n+m-4,\ j=n+3,\ldots,n+m-2$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $\tilde{G}_0=D(i-n|n)\oplus sl(j-i)\oplus D_{m+n-j}$ [for $i=n+1$ instead of $D(i-n|n)$ we have $C(n+1)$, for $j=m+n-2$ instead of D_{m+n-j} we have $A_1\oplus A_1$]. In each case there are seven $\tilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0=H+\tilde{G}_0+g_1$, and in each case one finds G_0

$\equiv H+sl(j-i)\oplus D(m-j+i|n)$. Now there are four G_0-modules and $D(m|n)=G_{-2}\oplus G_{-1}\oplus G_0 \oplus G_{+1}\oplus G_{+2}$ with

$$G_{-1}=\mathrm{span}\{e_{kl}-e_{m+l,m+k},e_{m+k,l}-e_{m+l,k},e_{m+l,2m+n+q}+e_{2m+q,l},e_{m+l,2m+q}-e_{2m+n+q,l},$$
$$k=1,\ldots,i-n,j-n+1,\ldots,m,\quad l=i-n+1,\ldots,j-n,\quad q=1,\ldots,n\}$$

with $N=2(j-i)(m+n-j+i)$. All of these are isomorphic to cases in Step 12.

Step 14. If we delete three or more nodes from the extended distinguished Dynkin diagram, the corresponding $\mathbb{Z}$-grading of $D(m|n)$ has no longer the required properties (i.e., there are non-zero subspaces G_i with $|i|>2$).

Step 15. Also here, we have considered all the nondistinguished Dynkin diagrams and their extensions, following Ref. 17. Repeating our procedure for all of them leads again to a lot of case studies, most of which are isomorphic to results of the previous steps. There is, however, one extra case that is not covered in the previous steps, and that we shall briefly describe. Consider the nondistinguished Dynkin diagrams of $D(m|n)$ of the following form:

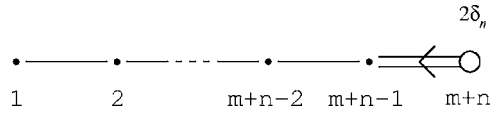

In this diagram, each dot stands for a white or gray circle, depending upon whether the corresponding simple root is even or odd. All these other simple roots are of the form $\eta-\eta'$, where η and η' can be a ϵ_i or a δ_j. For example, root $m+n-1$ is either $\delta_{n-1}-\delta_n$ (in which case the circle is white) or $\epsilon_m-\delta_n$ (in which case it is gray). Deleting node i ($i=1,\ldots,m+n-2$) yields the (nondistinguished) Dynkin diagram of $G_0=sl(k|l)\oplus D(m-k|n-l)$. Most of these cases are isomorphic to those already found in Step 10 or 11. However, the case $G_0=H+sl(m-1|l)\oplus D(1|n-l)=H+sl(m-1|l)\oplus C(n-l+1)$ ($l=0,\ldots,n-1$) did not occur before. This adds a new case to the classification, for which the length of the grading is 5. From a detailed analysis, it follows that this is the only extra case that can be obtained from the nondistinguished Dynkin diagrams (extended or not).

VII. THE LIE SUPERALGEBRAS $C(n)$

Let $G=C(n)=D(1|n-1)=osp(2|2n-2)$. For a description of the root vectors, we refer to Sec. VI. The even roots are of the form $\pm\delta_j\pm\delta_k(j,k=1,\ldots,n-1)$ and the odd roots are $\pm\epsilon\pm\delta_k(k=1,\ldots,n-1)$. This Lie superalgebra is treated separately from $D(m|n)$ because its distinguished Dynkin diagram is different (see Table I), and its structure is also different (it is a type I Lie superalgebra[4]).

Step 1. Delete node 1 from the distinguished Dynkin diagram. Then the corresponding diagram is that of $G_0=C_{n-1}$. There are only two G_0-modules and $C(n)$ has the grading $C(n)=G_{-1}\oplus G_0\oplus G_{+1}$, where

$$\begin{aligned}G_{-1}&=\mathrm{span}\{e_{1,i+2}-e_{n+1+i,2},e_{1,n+1+i}+e_{i+2,2},\quad i=1,\ldots,n-1\},\\ G_{+1}&=\mathrm{span}\{e_{2,n+1+i}+e_{i+2,1},e_{2,i+2}-e_{n+1+i,1},\quad i=1,\ldots,n-1\},\end{aligned}\tag{7.1}$$

with $N=2(n-1)$. Putting

$$c^-_{-,i}=e_{1,2+i}-e_{n+1+i,2},\quad c^-_{+,i}=e_{1,n+1+i}+e_{2+i,2},$$

$$c^+_{-,i}=e_{2,n+1+i}+e_{2+i,1},\quad c^+_{+,i}=e_{2,2+i}-e_{n+1+i,1},$$

the operators $c^{\pm}_{\xi i},\xi=\pm,i=1,\ldots,n-1$, satisfy the following relations:

$$[\{c^-_{\xi i},c^+_{\eta j}\},c^+_{\epsilon k}]=\xi\delta_{\xi\eta}\delta_{ij}c^+_{\epsilon k}-\epsilon\delta_{\xi\epsilon}\delta_{ik}c^+_{\eta j}+\eta\delta_{-\eta\epsilon}\delta_{jk}c^+_{-\xi i},$$

$$[\{c^-_{\xi i},c^+_{\eta j}\},c^-_{\epsilon k}]=-\xi\delta_{\xi\eta}\delta_{ij}c^-_{\epsilon,k}+\eta\delta_{\eta\epsilon}\delta_{jk}c^-_{\xi i}+\epsilon\delta_{-\xi\epsilon}\delta_{ik}c^-_{-\eta j},$$

$$\{c^-_{-i},c^+_{+j}\}=\{c^-_{-j},c^+_{+i}\},\quad \{c^-_{+i},c^+_{-j}\}=\{c^-_{+j},c^+_{-i}\},$$

$$\{c^-_{\xi i},c^-_{\eta j}\}=\{c^+_{\xi i},c^+_{\eta j}\}=0. \tag{7.2}$$

(Here and throughout, by convention, ξ,η,ϵ are written as $\pm$ when used as subscripts, and as ±1 when used algebraically as multipliers.)

Step 2. Delete node i, $i=2,\ldots,n-1$, from the distinguished Dynkin diagram. The corresponding diagram is the Dynkin diagram of $G_0=H+sl(1|i-1)\oplus C_{n-i}$ (if $i=n-1, C_{n-i}=A_1$). There are four simple G_0-modules and $C(n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$ where

$$G_{-1}=\mathrm{span}\{e_{j+2,k+2}-e_{n+1+k,n+1+j},e_{j+2,n+1+k}+e_{k+2,n+1+j},e_{1,k+2}-e_{n+1+k,2},e_{1,n+1+k}+e_{k+2,2},;$$
$$j=1,\ldots,i-1,\ k=i,\ldots,n-1\}, \tag{7.3}$$

with $N=2i(n-i)$. An interesting case is that with $i=n-1$ and $N=2(n-1)$.

Step 3. Delete node n from the distinguished Dynkin diagram. Then the corresponding diagram is that of $G_0=sl(1|n-1)$. There are only two G_0-modules and $C(n)$ has grading $C(n)=G_{-1}\oplus G_0\oplus G_{+1}$, where

$$G_{-1}=\mathrm{span}\{e_{k+2,n+1+l}+e_{l+2,n+1+k},\quad k\leqslant l=1,\ldots,n-1,\quad e_{1,n+1+j}+e_{j+2,2},\quad j=1,\ldots,n-1\}. \tag{7.4}$$

This is also an interesting case, since there are

$$N=\frac{n(n+1)}{2}-1$$

supercommuting annihilation (respectively, creation) operators.

Step 4. Upon deleting two nodes i and j (except $i=1,j=n$) or more from the distinguished Dynkin diagram of $C(n)$, the corresponding $\mathbb{Z}$-gradings no longer have the required property (there are nonzero G_i with $|i|>2$).

Step 5. Delete node 1 and n from the distinguished Dynkin diagram. We have $G_0=H+sl(n-1)$. There are six simple G_0-modules. All the possible combinations of these modules give rise to gradings of the form $C(n)=G_{-2}\oplus G_{-1}\oplus G_0\oplus G_{+1}\oplus G_{+2}$. There are essentially three different ways in which these G_0-modules can be combined. To characterize these three cases, it is sufficient to give only G_{-1}:

$$G_{-1}=\mathrm{span}\{e_{j+2,n+k+1}+e_{k+2,n+j+1},\quad j\leqslant k=1,\ldots,n-1,\quad e_{1,i+2}-e_{n+i+1,2},\ i=1,\ldots,n-1\}, \tag{7.5}$$

with $N=n(n+1)/2-1$;

$$G_{-1}=\mathrm{span}\{e_{1,k+2}-e_{n+k+1,2},e_{2,k+2}-e_{n+k+1,1},\quad k=1,\ldots,n-1\}, \tag{7.6}$$

with $N=2(n-1)$;

$$G_{-1}=\mathrm{span}\{e_{1,n+k+1}+e_{k+2,2},\quad k=1,\ldots,n-1,\ e_{n+l+1,p+2}+e_{n+p+1,l+2},\quad l\leqslant p=1,\ldots,n-1\}, \tag{7.7}$$

with $N=n(n+1)/2-1$. It is interesting to give the algebraic relations for (7.6), since the number of creation and annihilation operators is $N=2(n-1)$. One can label the CAOs as follows ($k=1,\ldots,n-1$):

$$c^-_{-k}=e_{1,k+2}-e_{n+k+1,2},\quad c^-_{+k}=e_{2,k+2}-e_{n+k+1,1},$$

$$c^+_{-k} = e_{2,n+k+1} + e_{k+2,1}, \quad c^+_{+k} = e_{1,n+k+1} + e_{k+2,2}.$$

The CAOs $c^{\pm}_{\xi k}, \xi = \pm, k = 1, \ldots, n-1$, satisfy the relations ($\xi, \eta, \epsilon = \pm$ or $\pm 1; j, k, l = 1, \ldots, n-1$):

$$\{c^{\eta}_{\xi j}, c^{\eta}_{\xi k}\} = \{c^-_{-j}, c^+_{+k}\} = \{c^-_{+j}, c^+_{-k}\} = 0,$$

$$\{c^-_{+j}, c^+_{+k}\} = \{c^-_{-j}, c^+_{-k}\}, \quad j \neq k,$$

$$\{c^{\xi}_{\xi j}, c^{\xi}_{-\xi k}\} = \{c^{\xi}_{\xi k}, c^{\xi}_{-\xi j}\},$$

$$[\{c^{\gamma}_{\xi j}, c^{\gamma}_{\eta k}\}, c^{\gamma}_{\epsilon l}] = 0,$$

$$[\{c^{\xi}_{\xi j}, c^{\xi}_{-\xi k}\}, c^{-\xi}_{\epsilon l}] = -\xi \delta_{kl} c^{\xi}_{-\epsilon j} - \xi \delta_{jl} c^{\xi}_{-\epsilon k},$$

$$[\{c^-_{\xi j}, c^+_{\xi k}\}, c^-_{\eta l}] = -\delta_{kl} c^-_{\eta j} - (-1)^{\delta_{\xi\eta}} \delta_{jk} c^-_{\eta l},$$

$$[\{c^-_{\xi j}, c^+_{\xi k}\}, c^+_{\eta l}] = (-1)^{\delta_{\xi\eta}} \delta_{jk} c^+_{\eta l} + \delta_{jl} c^+_{\eta k}. \tag{7.8}$$

Step 6. Delete node i, $i = 0, 1, \ldots, n$, from the extended distinguished Dynkin diagram. The remaining diagram is that of $G_0 = C(n), C(n), sl(2|1) \oplus C_{n-2}, C(3) \oplus C_{n-3}, \ldots, C_{n-1} \oplus A_1, C(n)$. In all these cases there is only one G_0-module, so there are no contributions to the classification.

Step 7. Delete the adjacent nodes i and $i+1$, $i = 2, 3, \ldots, n-2$, from the extended distinguished Dynkin diagram. The remaining diagram is that of $\widetilde{G}_0 = H + sl(2|1) \oplus C_{n-3}$ for $i = 2$ and of $\widetilde{G}_0 = H + C(i) \oplus C_{n-i-1}$ for $i = 3, \ldots, n-2$. In each case there are seven $\widetilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0 = H + \widetilde{G}_0 + g_1$, and in each case one finds $G_0 \equiv H + C(n-1)$. Now there are four G_0-modules and $C(n) = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}$ with

$$G_{-1} = \operatorname{span}\{e_{i+2,n+k+1} + e_{k+2,n+i+1}, e_{i+2,k+2} - e_{n+k+1,n+i+1}, e_{1,n+i+1} + e_{i+2,2}, e_{2,n+i+1} + e_{i+2,1};$$
$$k \neq i = 1, \ldots, n-1\} \tag{7.9}$$

and $N = 2(n-1)$. All these cases are mutually isomorphic.

*Step 8.*Delete the adjacent nodes $n-1$ and n from the extended distinguished Dynkin diagram. The remaining diagram is that of $G_0 \equiv H + C(n-1)$. This case turns out to be isomorphic to those of Step 7.

Step 9. Delete the nonadjacent nodes i, $i = 2, 3, \ldots, n-2$, and $j = n$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $G_0 = H + C(i) \oplus sl(n-i)$ [for $i = 2$ instead of $C(i)$ we have $sl(2|1)$]. In each case there are four G_0-modules and $C(n) = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}$ with

$$G_{-1} = \operatorname{span}\{e_{k+2,l+2} - e_{n+1+l,n+1+k}, e_{n+1+k,l+2} + e_{n+l+1,k+2}, e_{1,l+2} - e_{n+l+1,2}, e_{2,l+2} - e_{n+l+1,1};$$
$$l = i, \ldots, n-1, \quad k = 1, \ldots, i-1\} \tag{7.10}$$

and $N = 2i(n-i)$. These are all new cases.

Step 10. Delete the nonadjacent nodes $i < j-1$, $i = 2, 3, \ldots, n-2$, $j = 4, \ldots, n-1$ from the extended distinguished Dynkin diagram. The remaining diagram is that of $\widetilde{G}_0 = H + C(i) \oplus sl(j-i) \oplus C_{n-j}$ [for $i = 2$ instead of $C(i)$ we have $sl(2|1)$, for $j = n-1$ instead of C_{n-j} we have A_1]. In each case there are seven $\widetilde{G}_0$-modules g_k, one of which is invariant under ω (say g_1). Then one has to put $G_0 = H + \widetilde{G}_0 + g_1$, and in each case one finds $G_0 \equiv H + sl(j-i) \oplus C(n-j+i)$. Now there are four G_0-modules and $C(n) = G_{-2} \oplus G_{-1} \oplus G_0 \oplus G_{+1} \oplus G_{+2}$ with

$$G_{-1} = \mathrm{span}\{e_{k+2,l+2} - e_{n+1+l,n+1+k}, e_{n+1+k,l+2} + e_{n+l+1,k+2}, e_{1,l+2} - e_{n+l+1,2}, e_{2,l+2} - e_{n+l+1,1};$$
$$l = i,\ldots,j-1, \quad k = 1,\ldots,i-1, \quad j,\ldots,n-1\} \tag{7.11}$$

and $N=2(j-i)(n-j+i)$. All these cases are amongst those of Step 10.

Step 11. Upon deleting three or more nodes from the extended distinguished Dynkin diagram of $C(n)$, the corresponding $\mathbb{Z}$-gradings no longer have the required property (there are nonzero G_i with $|i|>2$).

The other nondistinguished choices for the simple root systems give no new results.

VIII. SUMMARY AND CONCLUSIONS

Our analysis has led to a complete classification of all GQS associated with the basic classical Lie superalgebras. Some cases in our classification have appeared earlier as examples, e.g., para-Bose statistics (5.1), A-superstatistics (3.4) in Refs. 11 and 15, and the combined para-Bose/para-Fermi case (4.7) in Ref. 19. Some other examples are also rather simple, e.g., the alternatives to A-superstatistics in (3.5), a statistics with two kinds of particles in (3.6), and the statistics related to $C(n)$ superalgebras (7.2) and (7.8).

Although the detailed analysis in the previous sections was necessary to present the complete solution, it is convenient to summarize the final results in a table. Table II recapitulates the classification of all GQS. From this table, it follows that many of the earlier cases can be somewhat unified in a simple form, provided one makes use of the common isomorphisms for Lie algebras and Lie superalgebras [such as $D_1=C_1=A_1, D_2=A_1\oplus A_1, B(m|0)=B_m, D(1|1)=C(2)=sl(1|2)$ etc.]. For $A(m|n)$, there are essentially two distinct cases. Either $G_0=H+sl(k|l)\oplus sl(p|q)$, in which case the grading has length 3 and $G_{\pm1}$ is fixed by G_0. Or else $G_0=H+sl(k|l)\oplus sl(p|q)\oplus sl(r|s)$, in which case the grading has length 5. In this second case, there are always three ways of combining the G_0-modules in order to give some G_{-1}. For $B(m|n)$, all the cases are characterized by a G_0 of the form $G_0=H+sl(k|l)\oplus B(m-k,n-l)$. This includes cases such as $sl(l)\oplus B(m|n-l), sl(k|n)\oplus B_{m-k}$ (Step 1), $B(m|n-1)$ (Step 4) and $B(m-1|n)$ (Step 5). Also the results for the remaining Lie superalgebras can be neatly summarized. Note that for $D(m|n)$ [and for $C(n)=D(1|n-1)$] there is one G_0 which gives rise not only to different possibilities for G_{-1} but even for N.

A striking property, see Table II, is that all basic classical Lie superalgebras, except $B(0|n)$, allow a GQS with a grading of length 3; in other words, a GQS with supercommuting creation and annihilation operators.

Note that a set of CAOs together with a complete set of relations $\mathcal{R}$ unambiguously describes the Lie superalgebra. So each case of our classification also gives the description of a Lie superalgebra in terms of a number of generators subject to certain relations. This can also be reformulated in terms of the notion of Lie supertriple systems.[20] In fact, in our case the subspace $G_{-1}\oplus G_{+1}$ (i.e., the subspace spanned by all CAOs) is a Lie supertriple system for the universal enveloping algebra $U(G)$.

Just as in Ref. 2, we have dealt only with a mathematical definition of generalized quantum statistics. In order to talk about a quantum statistics in the physical sense, one should take into account additional requirements for the CAOs, related to certain quantization postulates.[8] These conditions are related to the existence of state spaces (Fock spaces), in which the CAOs act in such a way that the corresponding observables are Hermitian operators. We refer to Sec. VII of Ref. 2 for a discussion on this. We hope that some cases of our classification will yield interesting GQS also from this point of view.

As a second application, we mention the possible solutions of Wigner quantum systems.[21] Roughly speaking, the compatibility conditions (CCs) to be satisfied by a Wigner quantum oscillator system [see formula (3.7) in Ref. 22) are written in terms of certain odd operators $A_i^{\pm}$; furthermore, these CCs are special triple relations. So it is of importance to investigate which triple relations $\mathcal{R}$ of our current classification of GQS could provide special solutions of these CCs. It is known, for instance, that there is a $sl(1|n)$ solution[21–23] or a $sl(n|3)$ solution.[24] Obvi-

TABLE II. Summary of the classification: all nonisomorphic GQS associated with a classical Lie superalgebra (LSA) are given. For each GQS, we list: the subalgebra G_0 (each G_0 contains the complete Cartan subalgebra H, so we only list the remaining part of $G_0=H+\cdots$); the length ℓ of the Z-grading; the number N of annihilation operators; the equation in the text where (an example of) G_{-1} can be found.

LSA	$G_0=H+\cdots$	ℓ	N	G_{-1}
$A(m\|n)$	$sl(k\|l)\oplus sl(p\|q)$ $(k+p=m+1, l+q=n+1, k+l\neq 0, p+q\neq 0)$	3	$(k+l)(p+q)$	(3.2) and (3.12)
	$sl(k\|l)\oplus sl(p\|q)\oplus sl(r\|s)$	5	$(k+l)(p+q+r+s)$	(3.7) and (3.13)
	$(k+p+r=m+1$	5	$(p+q)(k+l+r+s)$	(3.8) and (3.14)
	$l+q+s=n+1, k+l\neq 0, p+q\neq 0, r+s\neq 0)$	5	$(r+s)(k+l+p+q)$	(3.9) and (3.15)
$B(m\|n)$	$sl(k\|l)\oplus B(m-k\|n-l)$ $(k=0,\ldots,m; l=0,\ldots,n; (k,l)\notin\{(0,0),(1,0)\})$	5	$(k+l)(2m-2k+2n-2l+1)$	(4.2) and (4.3), (4.11) and (4.12)
	$B(m-1\|n)[(k,l)=(1,0)]$	3	$2m+2n-1$	(4.10)
$B(0\|n)$	$sl(i)\oplus B(0\|n-i)$ $(i=1,\ldots,n)$	5	$i(2n-2i+1)$	(5.1)
$D(m\|n)$	$sl(k\|l)\oplus D(m-k\|n-l)$ $(k=0,1,\ldots,m; l=0,1,\ldots,n; (k,l)\notin\{(0,0),(1,0),(m-1,n),(m,n)\})$	5	$2(k+l)(m+n-k-l)$	(6.10) and (6.11), (6.1) and (6.2), (6.12)
	$D(m-1\|n)[(k,l)=(1,0)]$	3	$2(m+n-1)$	(6.8) and (6.9)
	$sl(m\|n)[(k,l)=[m,n)]$	3	$(m+n)(m+n+1)/2-m$	(6.3) and (6.4)
	$sl(m-1\|n)[(k,l)=(m-1,n)]$	5	$(m+n)(m+n+1)/2-m$	(6.6) and (6.7)
	$sl(m-1\|n)[(k,l)=(m-1,n)]$	5	$2(m+n-1)$	(6.5)
$C(n)$	$sl(k\|l)\oplus D(1-k\|n-1-l)$ $(k=0,1; l=1,\ldots,n-2)$	5	$2(k+l)(n-k-l)$	(7.3) and (7.9), (7.10) and (7.11)
	$C_{n-1}[(k,l)=(1,0)]$	3	$2(n-1)$	(7.1)
	$sl(1\|n-1)[(k,l)=(1,n-1)]$	3	$n(n+1)/2-1$	(7.4)
	$sl(n-1)[(k,l)=(0,n-1)]$	5	$n(n+1)/2-1$	(7.5) and (7.7)
	$sl(n-1)[(k,l)=(0,n-1)]$	5	$2(n-1)$	(7.6)

ously, for a possible candidate solution all the CAOs of $\mathcal{R}$ should be odd operators. Let us briefly describe the GQSs of the current classification which have only odd CAOs. Then G_{-1} and G_{+1} are odd subspaces, and by the grading condition it follows automatically that the GQS grading (2.3) is *consistent* with the $\mathbb{Z}_2$-grading. So our problem reduces to selecting those GQS from our classification with a consistent $\mathbb{Z}$-grading. This is not too difficult.

For $A(m|n)$, one can consider $i=m+1$ in Step 1. Then all elements of G_{-1} in (3.2) are odd; $G_0=H+sl(m+1)\oplus sl(n+1)$, and the grading has length 3 (the case $m=0$ corresponds to Refs. 11 and 21–23). Alternatively, one can consider the cases $(i,j)=(i,m+1)$ or $(i,j)=(m+1,j)(i<j)$ of Step 2. In the case $(i,j)=(i,m+1)$, the elements of G_{-1} given by (3.9) are all odd, and $G_0=H+sl(i)\oplus sl(m+1-i)\oplus sl(n+1)$. In the case $(i,j)=(m+1,j)$, the elements of G_{-1} given by (3.8) are all odd, and $G_0=H+sl(m+1)\oplus sl(k)\oplus sl(n+1-k)$ with $k=j-m-1$. For $B(m|n)$, the case $i=n$ in Step 1 leads to a G_{-1} with only odd elements in (4.2). Note that in this case $G_0=H+sl(n)\oplus B_m$. For $B(0|n)$, this corresponds to taking $i=n$ in Step 1, so that G_{-1} in (5.1) has odd elements only and $G_0=H+sl(n)$ (this is the para-Bose case). For $D(m|n)$, the case $i=n$ in Step 1 leads to a G_{-1} in (6.1) with odd elements only, and with $G_0=H+sl(n)\oplus D_m$. There is a second solution here, namely the case $i=n$ in Step 11; then G_{-1}, given by (6.11) has odd elements only and $G_0=H+sl(m)\oplus C_n$. Finally for $C(n)$ the solution provided in Step 1 has only odd elements for G_{-1}, see (7.1),

with $G_0=H+C_{n-1}$. Also here there is a second solution given in Step 5 with G_{-1} of the form (7.6) and $G_0=H+sl(n-1)$. To conclude, all the basic classical Lie superalgebras have GQSs with odd CAOs only. Whether all these cases provide special solutions to the CCs of the Wigner quantum oscillator will be treated elsewhere.

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Nilpotent representations of classical quantum groups at roots of unity[a)]

Yuuki Abe[b)] and Toshiki Nakashima[c)]
Department of Mathematics, Sophia University, Chiyoda-ku-Kioicho 7-1, Tokyo 102-8554, Japan

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Properly specializing the parameters in "Schnizer modules," for types A,B,C, and D, we get its unique primitive vector. Then we show that the module generated by the primitive vector is an irreducible highest weight module of finite dimensional classical quantum groups at roots of unity. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2107307]

I. INTRODUCTION

The representation theory of quantum groups at roots of unity are divided into the following two types: one is for U_ε defined by DeConcini-Kac (=nonrestricted type)[3] and the other is for $U_\varepsilon^{\mathrm{res}}$ defined by Lusztig(=restricted type).[6] In the latter case, the classification of irreducible modules is the same as the generic case, that is, they are classified by highest weights.[6,7] In the former case, however, most irreducible modules are no longer highest or lowest weight modules and they are characterized by several continuous parameters.[3] For type A, such modules are constructed very explicitly in Ref. 2, which are called maximal cyclic representations. For any simple Lie algebra, Schnizer introduced an alternative construction of such modules in Refs. 9 and 10, which we also call maximal cyclic representations or "Schnizer modules."

In Ref. 8, T. N. found that for type A_n-case if the continuous parameters in a maximal cyclic representation are specialized properly, then there exists a unique primitive vector and the submodule generated by the primitive vector is irreducible as a module of finite dimensional quantum group at roots of unity(denoted by $U_\varepsilon^{\mathrm{fin}}$). In this paper, we shall show that this method is applicable to the Schnizer modules of types A_n, B_n, C_n, and D_n.

In order to explain what we shall do in this paper, let us see A_n-case explicitly: Let $N=\frac{1}{2}n(n+1)$ be the number of positive roots, l be an odd integer greater than 3, and ε be the primitive lth root of unity. Set $V:=(\mathbb{C}^l)^{\otimes N}$ and for each $a\in(\mathbb{C}^\times)^N, b\in\mathbb{C}^N$, and $\lambda\in\mathbb{C}^n$, we can define a $U_\varepsilon(\mathsf{sl}(n+1,\mathbb{C}))$-module structure on V as follows.

Theorem 1.1 (Ref. 10): *For any* $a=(a_{i,j})_{1\leqslant i\leqslant j\leqslant n}\in(\mathbb{C}^\times)^N, b=(b_{i,j})_{1\leqslant i\leqslant j\leqslant n}\in\mathbb{C}^N, \lambda=(\lambda_1,\cdots,\lambda_n)\in\mathbb{C}^n$, *we obtain a* $U_\varepsilon(sl(n+1,\mathbb{C}))$*-module structure on* $V:\Phi_\lambda: U_\varepsilon(sl(n+1,\mathbb{C}))\to End(V)$. *For any* $i\in I$,

$$\Phi_\lambda(f_i)(u(m))=\sum_{j=i}^{n}[m_{i,j}-m_{i+1,j}+b_{i,j}-b_{i+1,j}-\mu_{i,j-1}^{m,b}]u(m+\epsilon_{i,j}),$$

$$\Phi_\lambda(t_i)(u(m))=\varepsilon^{\mu_{i,n}^{m,b}}u(m),$$

[a)] In memory of W. A. Schnizer

[b)] Electronic Mail: yu-abe@hoffman.cc.sophia.ac.jp

[c)] Supported in part by JSPS Grants in Aid for Scientific Research, electronic-mail: toshiki@mm.sophia.ac.jp

$$\Phi_\lambda(e_i)(u(m)) = \sum_{j=1}^{i} [m_{j-1,n-i+j} - m_{j,n-i+j} + b_{j-1,n-i+j} - b_{j,n-i+j}]$$
$$\times a_{j,n-i+j}^{-1} \prod_{k=j+1}^{i} (a_{k-1,n-i+k} a_{k,n-i+k}^{-1}) u(m + \sum_{k=j+1}^{i} (\epsilon_{k-1,n-i+k} - \epsilon_{k,n-i+k}) - \epsilon_{j,n-i+j}),$$

where

$$\mu_{i,j}^{m,b} = \lambda_i + m_{i-1,i-1} + b_{i-1,i-1} + \sum_{k=i}^{j} (m_{i-1,k} - 2m_{i,k} + m_{i+1,k} + b_{i-1,k} - 2b_{i,k} + b_{i+1,k}),$$

$$(1 \leqslant i \leqslant n, i-1 \leqslant j \leqslant n),$$

and we understand that $m_{i,j} := 0$ *if the index* (i,j) *is out of range and* $\Sigma_{j=k}^{i}(\cdots) := 0, \Pi_{j=k}^{i}(\cdots) := 1$ *for* $k > i$.

Let us define $a^{(0)} = (a_{i,j}^{(0)})_{1 \leqslant i \leqslant j \leqslant n} \in (\mathbb{C}^\times)^N, b^{(0)} = (b_{i,j}^{(0)})_{1 \leqslant i \leqslant j \leqslant n} \in \mathbb{C}^N$, by

$$a_{i,j}^{(0)} = 1, \quad b_{i,j}^{(0)} = 0, \quad (1 \leqslant i \leqslant j \leqslant n).$$

For any $\lambda \in \mathbb{C}^n$, let us denote by $V(\lambda)$ the $U_\varepsilon(\mathsf{sl}(n+1,\mathbb{C}))$-module defined by $(\Phi_{a^{(0)},b^{(0)},\lambda}, V)$.

Proposition 1.2: For any $\lambda \in \mathbb{C}^n$, *there exists a unique (up to nonzero scalar multiplication) nonzero vector* $u_{\mathbf{0}}$, *such that* $e_i u = 0$ *in* $V(\lambda)$ *for any* $i \in I$.

Finally, it turns out that the submodule $U_\varepsilon u_{\mathbf{0}} \subset V(\lambda)$ is an irreducible highest weight $U_\varepsilon^{\mathrm{fin}}$-module. By this method, we obtain all finite dimensional irreducible $U_\varepsilon^{\mathrm{fin}}$-modules:

Theorem 1.3: *Let* $\lambda \in \mathbb{Z}_l^n (\mathbb{Z}_l := \{0,1,\cdots,l-1\})$. *Then* $U_\varepsilon u_{\mathbf{0}}$ *is a finite dimensional irreducible* $U_\varepsilon^{\mathrm{fin}}(sl(n+1,\mathbb{C}))$*-module of type* 1 *with highest weight* λ.

The proofs of the above-noted statements are done in a similar way to the ones in Ref. 8.

The organization of the paper is as follows: in Sec. II, we prepare notations and review the theory of quantum groups at roots of unity briefly. In Sec. III, we introduce Schnizer modules and show the uniqueness of primitive vectors. In the last two sections, we show that the submodule generated by the primitive vector is regarded as a module for the finite dimensional quantum group at roots of unity $U_\varepsilon^{\mathrm{fin}}$ of types (A), B, C, and D. At last, we obtain that such submodule is an irreducible $U_\varepsilon^{\mathrm{fin}}$-module and all finite dimensional irreducible $U_\varepsilon^{\mathrm{fin}}$-modules are obtained as such modules.

II. QUANTUM ENVELOPING ALGEBRA $U_q(\ )$

A. Definition of quantum enveloping algebra

In this section, we define the quantum enveloping algebra $U_q(\mathfrak{g})$ for a generic q. Let $\mathbb{C}(q)$ be the rational function field in an indeterminate q. Define

$$[a]_{q^d} := \frac{q^{da} - q^{-da}}{q^d - q^{-d}}, \quad [a] := [a]_q,$$

$$[a]_{q^d}! := [a]_{q^d}[a-1]_{q^d} \cdots [1]_{q^d}, \quad [0]! := 1,$$

for any $a, d \in \mathbb{Z}_+ := \{0,1,2,\ldots\}$. Let $\mathfrak{g}$ be a finite dimensional simple Lie algebra over $\mathbb{C}$ of rank n and $\{\alpha_1,\ldots,\alpha_n\}$ be the set of simple roots, $I := \{1,2,\ldots,n\}, \Delta$ be the set of roots (respectively, Δ_+ be the set of positive roots). Define the root lattice $Q = \oplus_{i=1}^n \mathbb{Z}\alpha_i$ (respectively, $Q_+ = \oplus_{i=1}^n \mathbb{Z}_+\alpha_i$). Let $(\mathsf{a}_{ij})_{i,j=1}^n$ be the Cartan matrix associated with $\mathfrak{g}$, and $d = (d_1,\ldots,d_n)$ be an element in $\mathbb{N}^n$ such that $d_i \mathsf{a}_{i,j} = d_j \mathsf{a}_{j,i}$ for any $i,j \in I$ and g.c.d $(d_1,\cdots,d_n) = 1$. In particular, $d = (1,\cdots,1)$ for $\mathfrak{g} = \mathsf{sl}(n+1,\mathbb{C}), \mathsf{so}(2n,\mathbb{C}), d = (1,\ldots,1,2)$ for $\mathfrak{g} = \mathsf{sp}(2n,\mathbb{C}), d = (2,\cdots,2,1)$ for $\mathfrak{g} = \mathsf{so}(2n+1,\mathbb{C})$, We denote

the Weyl group of $\mathfrak{g}$ by W which is generated by the simple reflections $\{s_1,\ldots,s_n\}$. Now, we define the quantum enveloping algebra $U_q(\mathfrak{g})$ over $\mathbb{C}(q)$.

Definition 2.1.: Quantum enveloping algebra $U_q(\mathfrak{g})$ is an associative $\mathbb{C}(q)$-algebra generated by $\{e_i,f_i,t_i^{\pm 1}\,|\,i\in I\}$ with the relations

$$t_it_i^{-1}=t_i^{-1}t_i=1,\quad t_it_j=t_jt_i,$$

$$t_ie_jt_i^{-1}=q_i^{\mathsf{a}_{ij}}e_j,$$

$$t_if_jt_i^{-1}=q_i^{-\mathsf{a}_{ij}}e_j,$$

$$e_if_j-f_je_i=\delta_{ij}\{t_i\}_{q_i},$$

$$\sum_{k=0}^{1-\mathsf{a}_{ij}}(-1)^k e_i^{(k)}e_je_i^{(1-\mathsf{a}_{ij}-k)}=\sum_{k=0}^{1-\mathsf{a}_{ij}}(-1)^k f_i^{(k)}f_jf_i^{(1-\mathsf{a}_{ij}-k)}=0\quad (i\neq j),$$

where

$$q_i:=q^{d_i},e_i^{(k)}:=\frac{1}{[k]_{q^{d_i}}!}e_i^k,f_i^{(k)}:=\frac{1}{[k]_{q^{d_i}}!}f_i^k,\{t_i\}_{q_i}:=\frac{t_i-t_i^{-1}}{q_i-q_i^{-1}}.$$

Let $U_q^+(\mathfrak{g})$ [respectively, $U_q^-(\mathfrak{g}),U_q^0(\mathfrak{g})$] be the $\mathbb{C}(q)$-subalgebra of $U_q(\mathfrak{g})$ generated by $\{e_i\}_{i=1}^n$ (respectively, $\{f_i\}_{i=1}^n,\{t_i^{\pm 1}\}_{i=1}^n$).

B. Non restricted specialization

In this section, we define the non restricted specializations U_ε for a root of unity ε.

Definition 2.2.: Let $A:=\mathbb{C}[q,q^{-1}]$ be the Laurent polynomial ring, U_A be the A-subalgebra of $U_q(\mathfrak{g})$ generated by $\{e_i,f_i,t_i^{\pm 1},\{t_i\}_{q_i}\}_{i=1}^n,l$ be an odd integer greater than 3, and ε be a primitive lth root of unity such that $\varepsilon^{2d_i}\neq 1$ for any $i\in I$. We regard $\mathbb{C}$ as A-algebra by $f(q)c:=f(\varepsilon)\cdot c$ for any $f(q)\in A,c\in\mathbb{C}$ and we denote it by $\mathbb{C}_\varepsilon$. Now we define

$$U_\varepsilon:=U_A\otimes_A\mathbb{C}_\varepsilon,$$

and we call U_ε "non-restricted specialization of $U_q(\mathfrak{g})$." By a similar manner to Definition 2.1, we define $U_\varepsilon^+,U_\varepsilon^-$, and U_ε^0, and we denote $u\otimes 1$ as u for any $u\in U_A$.

Remark. (Ref. 3): One can also describe U_ε in terms of generators and relations. That is, U_ε is an associative $\mathbb{C}$-algebra generated by $\{e_i,f_i,t_i^{\pm 1}\}_{i=1}^n$ with the relations of Definition 2.1 replacing q by ε.

C. Root vectors

In this section, we introduce the root vectors and their properties.

Proposition 2.3 (Refs. 3 and 4): (i) For any $i\in I$, there exists an automorphism of U_ε, denoted by T_i, such that

$$T_i(e_i)=-f_it_i,\quad T_i(e_j)=\sum_{s=0}^{-a_{ij}}(-1)^{s-a_{ij}}q_i^{-s}e_i^{(-a_{ij}-s)}e_je_i^{(s)}\quad (i\neq j),$$

$$T_i(f_i)=-t_i^{-1}e_i,\quad T_i(f_j)=\sum_{s=0}^{-a_{ij}}(-1)^{s-a_{ij}}q_i^{s}f_i^{(s)}f_jf_i^{(-a_{ij}-s)}\quad (i\neq j),$$

$$T_i(t_j)=t_jt_i^{-a_{ij}}.$$

(ii) For $w\in W$, let $w=s_{i_1}\cdots s_{i_r}$ be a reduced expression of w, and set $T_w:=T_{i_1}\cdots T_{i_r}$. Then T_w

is well-defined (that is, T_w does not depend on a choice of reduced expression of w).

Definition 2.4.: Let w_0 be the longest element of $W, w_0=s_{i_1}\cdots s_{i_N}$ be a reduced expression of w_0, and we set

$$\beta_1 := \alpha_{i_1}, \beta_2 := s_{i_1}(\alpha_{i_2}), \ldots, \beta_N := s_{i_1}\cdots s_{i_{N-1}}(\alpha_{i_N})$$

(by the theory of the classical Lie algebra, $\Delta_+=\{\beta_1,\cdots,\beta_N\}$) and

$$e_{\beta_k} := T_{i_1}\cdots T_{i_{k-1}}(e_{i_k}), f_{\beta_k} := T_{i_1}\cdots T_{i_{k-1}}(f_{i_k}) \quad (1 \leqslant k \leqslant N).$$

We call these e_{β_k}, f_{β_k} "root vectors of U_ε."

Definition 2.5.: Set $\deg(e_i) := \alpha_i, \deg(f_i) := -\alpha_i, \deg(t_i) := 0$.

These are compatible with the relations of U_ε. Therefore, we can regard U_ε as Q-graded algebra and we have

$$U_\varepsilon = \bigoplus_{\alpha\in Q} (U_\varepsilon)_\alpha, \quad (U_\varepsilon)_\alpha (U_\varepsilon)_{\alpha'} \subset (U_\varepsilon)_{\alpha+\alpha'},$$

for any $\alpha, \alpha' \in Q$, where $(U_\varepsilon)_\alpha := \{u \in U_\varepsilon \,|\, \deg(u)=\alpha\}$. We also use the following propositions later.

Proposition 2.6: (Ref. 4): We have $e_\alpha \in U_\varepsilon^+ \cap (U_\varepsilon)_\alpha, f_\alpha \in U_\varepsilon^- \cap (U_\varepsilon)_{-\alpha}$ $(\alpha \in \Delta_+)$.

Proposition 2.7 (Ref. 3):Let $Z(U_\varepsilon)$ be the center of U_ε. We have $e_\alpha^l, f_\alpha^l, t_i^l \in Z(U_\varepsilon)$ for any $\alpha \in \Delta_+, 1 \leqslant i \leqslant n$.

Next, we introduce the PBW theorem and the triangular decomposition. They will be used in the subsequent sections. Let $\{\beta_1,\ldots,\beta_N\}$ be as in Definition 2.4, then $\Delta_+=\{\beta_1,\ldots,\beta_N\}$.

Theorem 2.8 (Ref. 3): *(i) $\{e_{\beta_1}^{m_1}\cdots e_{\beta_N}^{m_N} | m_1,\ldots,m_N \in \mathbb{Z}_+\}$ is a $\mathbb{C}$-basis of U_ε^+.*

(ii) $\{f_{\beta_1}^{m_1}\cdots f_{\beta_N}^{m_N} | m_1,\ldots,m_N \in \mathbb{Z}_+\}$ is a $\mathbb{C}$-basis of U_ε^-.

(iii) $\{k_1^{m_1}\cdots k_n^{m_n} | m_1,\ldots,m_n \in \mathbb{Z}\}$ is a $\mathbb{C}$-basis of U_ε^0.

(iv) Let ϕ be the multiplication map $\phi: U_\varepsilon^- \otimes U_\varepsilon^0 \otimes U_\varepsilon^+ \to U_\varepsilon (u_- \otimes u_0 \otimes u_+ \mapsto u_- u_0 u_+)$. Then ϕ is an isomorphism of $\mathbb{C}$-vector space.

III. PRIMITIVE VECTORS

We keep the settings and notations as in Sec. II.

A. Schnizer modules

In this section, we introduce the Schnizer modules of $U_\varepsilon(\mathsf{sp}(2n,\mathbb{C}))$, $U_\varepsilon(\mathsf{so}(2n+1,\mathbb{C}))$ and $U_\varepsilon(\mathsf{so}(2n,\mathbb{C}))$.

First, we fix the following notations. Let N be the number of positive roots, that is, $N=n^2$ for $\mathfrak{g}=\mathsf{sp}(2n,\mathbb{C}), \mathsf{so}(2n+1,\mathbb{C})$, and $N=(n-1)n$ for $\mathfrak{g}=\mathsf{so}(2n,\mathbb{C})$. We set

$$M := \{m=(m_{i,j})_{1\leqslant i\leqslant (N/n), 1\leqslant j\leqslant n} \in \mathbb{Z}^N | 0 \leqslant m_{i,j} \leqslant l-1 \text{ for any } i,j\}.$$

Let V be the l^N-dimensional $\mathbb{C}$-vector space with the basis $\{u(m) | m \in M\}$ and $\epsilon_{i,j} (1 \leqslant i \leqslant N/n, 1 \leqslant j \leqslant n)$ be an element in $\mathbb{Z}^N$ such that the (i,j)-component of $\epsilon_{i,j}$ is 1 and the other components of $\epsilon_{i,j}$ are 0. [We regard $u(-\epsilon_{i,j})$ as $u((l-1)\epsilon_{i,j})$.] For any $a=(a_{i,j})_{i,j} \in (\mathbb{C}^\times)^N, b=(b_{i,j})_{i,j} \in \mathbb{C}^N$, and $m=(m_{i,j})_{i,j} \in \mathbb{Z}^N$, we define

$$a(m) = \prod_{i,j} a_{i,j}^{m_{i,j}}, \quad m^b = (m_{i,j}^b)_{i,j} := (m_{i,j}+b_{i,j})_{i,j}. \tag{3.1}$$

Theorem 3.1 (Ref. 9 Theorem 3.8): *Let $\mathfrak{g}=sp(2n,\mathbb{C})$ $(n \geqslant 2)$. For any $a=(a_{i,j})_{i,j=1}^n \in (\mathbb{C}^\times)^N, b=(b_{i,j})_{i,j=1}^n \in \mathbb{C}^N$, and $\lambda=(\lambda_1,\ldots,\lambda_n) \in \mathbb{C}^n$, we obtain the U_ε-module structure on V by*

the following algebra homomorphism $\Phi_{a,b,\lambda}: U_\varepsilon \to End(V)$. *We call these modules "Schnizer module." For any* $m=(m_{i,j})_{i,j=1}^n \in M$,

$$\begin{aligned}\Phi_{a,b,\lambda}(e_j)u(m) = a(\alpha_{j,j})[-m^b_{j,j}]_{\varepsilon_j} u(m+\alpha_{j,j}) + \sum_{i=1}^{j-1} a(\alpha_{i,j})\{[m^b_{i,j-1}-m^b_{i,j}]_{\varepsilon_j} u(m+\alpha_{i,j}) \\ + a_{i,j-1}a_{j,i}^{-1}[m^b_{j+1,i}-m^b_{j,i}]_{\varepsilon_j} u(m+\alpha_{i,j}+\epsilon_{i,j-1}-\epsilon_{j,i})\} \quad (1\le j\le n-1),\end{aligned} \tag{3.2}$$

$$\begin{aligned}\Phi_{a,b,\lambda}(e_n)u(m) = a(\alpha_{n,n})[-m^b_{n,n}]_{\varepsilon_n} u(m+\alpha_{n,n}) + \sum_{i=1}^{n-1} a(\alpha_{i,n})\{[m^b_{i,n}-m^b_{n,i}]_{\varepsilon_n} u(m+\alpha_{i,n}) \\ + a_{i,n-1}a_{n,i}^{-1}[m^b_{i,n-1}-m^b_{n,i}]_{\varepsilon_n} u(m+\alpha_{i,n}+\epsilon_{i,n-1}-\epsilon_{n,i}) \\ + a^2_{i,n-1}a^{-2}_{n,i}[m^b_{i,n}-m^b_{n,i}]_{\varepsilon_n} u(m+\alpha_{i,n}+2\epsilon_{i,n-1}-2\epsilon_{n,i})\},\end{aligned} \tag{3.3}$$

$$\Phi_{a,b,\lambda}(t_j)u(m) = \varepsilon_j^{-\mu^{m^b}_{1,j}+\lambda_j} u(m) \quad (1\le i\le n), \tag{3.4}$$

$$\begin{aligned}\Phi_{a,b,\lambda}(f_j)u(m) = \sum_{i=1}^{j}\{a_{i,j}[\eta^{m^b}_{i,j}+\mu^{m^b}_{i+1,j}-\lambda_j]_{\varepsilon_j} u(m+\epsilon_{i,j}) \\ + a_{j+1,i}[\eta^{m^b}_{j+1,i}+\mu^{m^b}_{i+1,j}-\lambda_j]_{\varepsilon_j}\}u(m+\epsilon_{j+1,i}) \quad (1\le j\le n-1),\end{aligned} \tag{3.5}$$

$$\Phi_{a,b,\lambda}(f_n)u(m) = \sum_{i=1}^{n} a_{i,n}[\eta^{m^b}_{i,n}+\mu^{m^b}_{i+1,n}-\lambda_n]_{\varepsilon_n} u(m+\epsilon_{i,n}). \tag{3.6}$$

Here we set

$$\begin{aligned}\alpha_{i,j} &= -\epsilon_{i,j} + \sum_{k=1}^{i-1}(-\epsilon_{j,k}+\epsilon_{j+1,k}-\epsilon_{k,j}+\epsilon_{k,j-1}) \quad (1\le i\le j\le n-1), \\ \alpha_{i,n} &= -\epsilon_{i,n} + 2\sum_{k=1}^{i-1}(-\epsilon_{n,k}+\epsilon_{k,n-1}) \quad (1\le i\le n),\end{aligned} \tag{3.7}$$

$$\mu^{m^b}_{i,j} = \sum_{k=i}^{j} \nu^{m^b}_{k,j} \quad (1\le i\le j\le n), \tag{3.8}$$

where

$$\begin{aligned}\nu^{m^b}_{i,j} &= -m^b_{i,j-1}+2m^b_{i,j}-m^b_{i,j+1}-m^b_{j+2,i}+2m^b_{j+1,i}-m^b_{j,i} \quad (1\le i<j\le n-2), \\ \nu^{m^b}_{j,j} &= 2m^b_{j,j}-m^b_{j,j+1}-m^b_{j+2,j}+2m^b_{j+1,j}-m^b_{j+1,j+1}-m^b_{j+2,j+1} \quad (1\le j\le n-2), \\ \nu^{m^b}_{i,n-1} &= -m^b_{i,n-2}+2m^b_{i,n-1}-2m^b_{i,n}-2m^b_{n,i}-m^b_{n-1,i} \quad (1\le i<n-1), \\ \nu^{m^b}_{n-1,n-1} &= 2m^b_{n-1,n-1}-2m^b_{n-1,n}+2m^b_{n,n-1}-2m^b_{n,n},\end{aligned} \tag{3.9}$$

$$\nu^{m^b}_{i,n} = -m^b_{i,n-1} + 2m^b_{i,n} - m^b_{n,i} \quad (1 \leqslant i < n) \quad \nu^{m^b}_{n,n} = 2m^b_{n,n},$$

$$\eta^{m^b}_{i,j} = -m^b_{i,j+1} - m^b_{j+2,i} + 2m^b_{j+1,i} - m^b_{j,i} + m^b_{i,j},$$

$$\eta^{m^b}_{j+1,i} = -m^b_{j,i} + m^b_{j+1,i} \quad (1 \leqslant i < j \leqslant n-2),$$

$$\eta^{m^b}_{j,j} = m^b_{j,j} - m^b_{j,j+1} - m^b_{j+2,j} + 2m^b_{j+1,j} - m^b_{j+1,j+1} - m^b_{j+2,j+1},$$
$$\eta^{m^b}_{j+1,j} = m^b_{j+1,j} - m^b_{j+1,j+1} - m^b_{j+2,j+1} \quad (1 \leqslant j \leqslant n-2), \tag{3.10}$$

$$\eta^{m^b}_{i,n-1} = -2m^b_{i,n} - m^b_{i,n-1} + 2m^b_{n,i} - m^b_{n-1,i}, \quad \eta^{m^b}_{n,i} = -m^b_{n-1,i} + m^b_{n,i} \quad (1 \leqslant i < n-1),$$

$$\eta^{m^b}_{n-1,n-1} = m^b_{n-1,n-1} - 2m^b_{n-1,n} + 2m^b_{n,n-1} - 2m^b_{n,n}, \quad \eta^{m^b}_{n,n-1} = m^b_{n,n-1} - 2m^b_{n,n},$$

$$\eta^{m^b}_{i,n} = m^b_{i,n} - m^b_{n,i}, \quad (1 \leqslant i < n), \quad \eta^{m^b}_{n,n} = m^b_{n,n},$$

where we understand that $\mu_{i,j} = \eta_{i,j} = 0$ if the index (i,j) is out of the range.

Theorem 3.2 (Ref. 9 Theorem 3.10): *Let* $\mathfrak{g} = so(2n+1, \mathbb{C})$ $(n \geqslant 3)$. *For any* $a = (a_{i,j})^n_{i,j=1} \in (\mathbb{C}^\times)^N, b = (b_{i,j})^n_{i,j=1} \in \mathbb{C}^N$, *and* $\lambda = (\lambda_1, \ldots, \lambda_n) \in \mathbb{C}^n$, *we obtain the* U_ε*-module structure on* V *by the following algebra homomorphisms* $\Phi_{a,b,\lambda}: U_\varepsilon \to End(V)$. $\Phi_{a,b,\lambda}(e_j), (1 \leqslant j \leqslant n-1), \Phi_{a,b,\lambda}(t_j), \Phi_{a,b,\lambda}(f_j), (1 \leqslant j \leqslant n)$, *as in (3.2) and (3.4)–(3.6)), and for any* $m = (m_{i,j})^n_{i,j=1} \in M$,

$$\Phi_{a,b,\lambda}(e_n)u(m) = a(\alpha_{n,n})[-m^b_{n,n}]_{\varepsilon_n} u(m + \alpha_{n,n}) + \sum_{i=1}^{n-1} a(\alpha_{i,n})\{[2m^b_{i,n-1} - m^b_{i,n}]_{\varepsilon_n} u(m + \alpha_{i,n})$$
$$+ a_{i,n-1}a^{-1}_{n,i}[m^b_{i,n} - 2m^b_{n,i}]_{\varepsilon_n} u(m + \alpha_{i,n} + \epsilon_{i,n-1} - \epsilon_{n,i})\}, \tag{3.11}$$

where, $\alpha_{i,j} (1 \leqslant i \leqslant j \leqslant n-1)$, *as in (3.7), and*

$$\alpha_{i,n} = -\epsilon_{i,n} + \sum_{k=1}^{i-1} (-\epsilon_{n,k} + \epsilon_{k,n-1}) \quad (1 \leqslant i \leqslant n), \tag{3.12}$$

$\mu^{m^b}_{i,j} (1 \leqslant i \leqslant j \leqslant n), \nu^{m^b}_{i,j} (1 \leqslant i \leqslant j \leqslant n-2)$ *as in (3.8) and (3.9), and*

$$\nu^{m^b}_{i,n-1} = -m^b_{i,n-2} + 2m^b_{i,n-1} - m^b_{i,n} - 2m^b_{n,i} - m^b_{n-1,i} \quad (1 \leqslant i \leqslant n-1),$$

$$\nu^{m^b}_{n-1,n-1} = 2m^b_{n-1,n-1} - m^b_{n-1,n} + 2m^b_{n,n-1} - m^b_{n,n}, \tag{3.13}$$

$$\nu^{m^b}_{i,n} = -m^b_{i,n-1} + m^b_{i,n} - m^b_{n,i} \quad (1 \leqslant i \leqslant n-1) \quad \nu^{m^b}_{n,n} = m^b_{n,n},$$

$\eta^{m^b}_{i,j}, \eta^{m^b}_{j+1,i} (1 \leqslant i \leqslant j \leqslant n-2)$, *as in (3.10), and*

$$\eta^{m^b}_{i,n-1} = -m^b_{i,n} + m^b_{i,n-1} + 2m^b_{n,i} - m^b_{n-1,i}, \quad \eta^{m^b}_{n,i} = -m^b_{n-1,i} + m^b_{n,i} \quad (1 \leqslant i < n-1),$$
$$\eta^{m^b}_{n-1,n-1} = m^b_{n-1,n-1} - m^b_{n-1,n} + 2m^b_{n,n-1} - m^b_{n,n}, \quad \eta^{m^b}_{n,n-1} = m^b_{n,n-1} - m^b_{n,n}, \tag{3.14}$$

$$\eta^{m^b}_{i,n} = m^b_{i,n} - 2m^b_{n,i} \quad (1 \leqslant i < n), \quad \eta^{m^b}_{n,n} = m^b_{n,n},$$

where we understand that $\mu_{i,j} = \eta_{i,j} = 0$ *if the index* (i,j) *is out of the range.*

Theorem 3.3 (Ref. 9 Theorem 3.11): *Let* $\mathfrak{g}=so(2n,\mathbb{C})$ $(n\geqslant 4)$. *For any* $a=(a_{i,j})_{1\leqslant i\leqslant n-1,1\leqslant j\leqslant n}\in(\mathbb{C}^{\times})^N, b=(b_{i,j})_{1\leqslant i\leqslant n-1,1\leqslant j\leqslant n}\in\mathbb{C}^N$, *and* $\lambda=(\lambda_1,\ldots,\lambda_n)\in\mathbb{C}^n$, *we obtain the* U_ε*-module structure on* V *by the following algebra homomorphisms* $\Phi_{a,b,\lambda}: U_\varepsilon\to End(V)$.

$\Phi_{a,b,\lambda}(e_j),(1\leqslant j\leqslant n-2),\Phi_{a,b,\lambda}(t_j),\Phi_{a,b,\lambda}(f_j),(1\leqslant j\leqslant n)$, *as in (3.2) and (3.4)–(3.6), and for any* $m=(m_{i,j})_{1\leqslant i\leqslant n-1,1\leqslant j\leqslant n}\in M$, *if* $n=2n'(n'\in\mathbb{Z})$, *then*

$$\begin{aligned}\Phi_{a,b,\lambda}(e_{n-1}) &= a(\alpha_{2n'-1,n-1})[-m^b_{n-1,n-1}]_{\varepsilon_{n-1}}u(m+\alpha_{2n'-1,n-1})+\sum_{i=1}^{n'-1}\{a(\alpha_{2i-1,n-1})[m^b_{2i-1,n-2}\\ &\quad -m^b_{2i-1,n-1}]_{\varepsilon_{n-1}}u(m+\alpha_{2i-1,n-1})+a_{2i-1,n-2}a^{-1}_{n-1,2i-1}a(\alpha_{2i-1,n-1})[m^b_{2i-1,n}-m^b_{n-1,2i-1}]_{\varepsilon_{n-1}}\\ &\quad\times u(m+\alpha_{2i-1,n-1}+\epsilon_{2i-1,n-2}-\epsilon_{n-1,2i-1})+a(\alpha_{2i,n})[m^b_{2i,n-2}-m^b_{2i,n}]_{\varepsilon_{n-1}}u(m+\alpha_{2i,n})\\ &\quad+a_{2i,n-2}a^{-1}_{n-1,2i}a(\alpha_{2i,n})[m^b_{2i,n-1}-m^b_{n-1,2i}]_{\varepsilon_{n-1}}u(m+\alpha_{2i,n}+\epsilon_{2i,n-2}-\epsilon_{n-1,2i})\},\end{aligned}\tag{3.15}$$

$$\begin{aligned}\Phi_{a,b,\lambda}(e_n)u(m) &= a(\alpha_{2n'-1,n})[-m^b_{n-1,n}]_{\varepsilon_n}u(m+\alpha_{2n'-1,n})+\sum_{i=1}^{n'-1}\{a(\alpha_{2i,n-1})[m^b_{2i,n-2}-m^b_{2i,n-1}]_{\varepsilon_n}u(m\\ &\quad+\alpha_{2i,n-1})+a_{2i,n-2}a^{-1}_{n-1,2i}a(\alpha_{2i,n-1})[m^b_{2i,n}-m^b_{n-1,2i}]_{\varepsilon_n}u(m+\alpha_{2i,n-1}+\epsilon_{2i,n-2}-\epsilon_{n-1,2i})\\ &\quad+a(\alpha_{2i-1,n})[m^b_{2i-1,n-2}-m^b_{2i-1,n}]_{\varepsilon_n}u(m+\alpha_{2i-1,n})+a_{2i-1,n-2}a_{n-1,2i-1}a(\alpha_{2i-1,n})\\ &\quad\times[m^b_{2i-1,n-1}-m^b_{n-1,2i-1}]_{\varepsilon_n}u(m+\alpha_{2i-1,n}+\epsilon_{2i-1,n-2}-\epsilon_{n-1,2i-1})\}.\end{aligned}\tag{3.16}$$

If $n=2n'+1(n'\in\mathbb{Z})$, *then*

$$\begin{aligned}\Phi_{a,b,\lambda}(e_{n-1})u(m) &= a(\alpha_{2n',n})[-m^b_{n-1,n}]_{\varepsilon_{n-1}}u(m+\alpha_{2n',n})\\ &\quad+\sum_{i=1}^{n'}a(\alpha_{2i-1,n-1})\{[m^b_{2i-1,n-2}-m^b_{2i-1,n-1}]_{\varepsilon_{n-1}}u(m+\alpha_{2i-1,n-1})\\ &\quad+a_{2i-1,n-2}a^{-1}_{n-1,2i-1}[m^b_{2i-1,n}-m^b_{n-1,2i-1}]_{\varepsilon_{n-1}}\\ &\quad\times u(m+\alpha_{2i-1,n-1}+\epsilon_{2i-1,n-2}-\epsilon_{n-1,2i-1})\}\\ &\quad+\sum_{i=1}^{n'-1}a(\alpha_{2i,n})\{[m^b_{2i,n-2}-m^b_{2i,n}]_{\varepsilon_{n-1}}u(m+\alpha_{2i,n})\\ &\quad+a_{2i,n-2}a^{-1}_{n-1,2i}[m^b_{2i,n-1}-m^b_{n-1,2i}]_{\varepsilon_{n-1}}u(m+\alpha_{2i,n}+\epsilon_{2i,n-2}-\epsilon_{n-1,2i})\},\end{aligned}\tag{3.17}$$

$$\begin{aligned}\Phi_{a,b,\lambda}(e_n)u(m) &= a(\alpha_{2n',n-1})[-m^b_{n-1,n-1}]_{\varepsilon_n}u(m+\alpha_{2n',n-1})+\sum_{i=1}^{n'-1}a(\alpha_{2i,n-1})\{[m^b_{2i,n-2}-m^b_{2i,n-1}]_{\varepsilon_n}u(m\\ &\quad+\alpha_{2i,n-1})+a_{2i,n-2}a^{-1}_{n-1,2i}[m^b_{2i,n}-m^b_{n-1,2i}]_{\varepsilon_n}u(m+\alpha_{2i,n-1}+\epsilon_{2i,n-2}-\epsilon_{n-1,2i})\}\\ &\quad+\sum_{i=1}^{n'}a(\alpha_{2i-1,n})\{[m^b_{2i-1,n-2}-m^b_{2i-1,n}]_{\varepsilon_n}u(m+\alpha_{2i-1,n})+a_{2i-1,n-2}a^{-1}_{n-1,2i-1}[m^b_{2i-1,n-1}\\ &\quad-m^b_{n-1,2i-1}]_{\varepsilon_n}\times u(m+\alpha_{2i-1,n}+\epsilon_{2i-1,n-2}-\epsilon_{n-1,2i-1})\},\end{aligned}\tag{3.18}$$

where $\alpha_{i,j},(1\leqslant j\leqslant n-2)$, *as in (3.7), and*

$$\alpha_{2i-1,n-1}=\beta_{2i-1,n-1}+\beta_{2i,n}-\epsilon_{2i-1,n-1},$$

$$\alpha_{2i,n-1} = \beta_{2i,n-1} + \beta_{2i+1,n} - \epsilon_{2i,n-1},$$
$$\alpha_{2i-1,n} = \beta_{2i,n-1} + \beta_{2i-1,n} - \epsilon_{2i-1,n},$$
$$\alpha_{2i,n} = \beta_{2i+1,n-1} + \beta_{2i,n} - \epsilon_{2i,n}, \quad (1 \leqslant 2i, 2i-1 \leqslant n),$$
$$\beta_{2i-1,n-1} = \sum_{k=1}^{i-1} (\epsilon_{2k-1,n-2} - \epsilon_{2k-1,n-1} + \epsilon_{2k-1,n} - \epsilon_{n-1,2k-1}),$$
$$\beta_{2i,n-1} = \sum_{k=1}^{i-1} (\epsilon_{2k,n-2} - \epsilon_{2k,n-1} + \epsilon_{2k,n} - \epsilon_{n-1,2k}),$$
$$\beta_{2i-1,n} = \sum_{k=1}^{i-1} (\epsilon_{2k-1,n-2} - \epsilon_{2k-1,n-1} + \epsilon_{2k-1,n} - \epsilon_{n-1,2k-1}),$$
$$\beta_{2i,n} = \sum_{k=1}^{i-1} (\epsilon_{2k,n-2} - \epsilon_{2k,n-1} + \epsilon_{2k,n} - \epsilon_{n-1,2k}), \tag{3.19, 3.20}$$

$\mu_{i,j}^{m^b} (1 \leqslant i \leqslant j \leqslant n)$, $\nu_{i,j}^{m^b} (1 \leqslant i \leqslant j \leqslant n-3)$, *as in (3.8) and (3.9), and*

$$\nu_{i,n-2}^{m^b} = -m_{i,n-3}^b + 2m_{i,n-2}^b - m_{i,n-1}^b - m_{i,n}^b + 2m_{n-1,i}^b - m_{n-2,i}^b, \quad (1 \leqslant i < n-2),$$
$$\nu_{n-2,n-2}^{m^b} = 2m_{n-2,n-2}^b - m_{n-2,n-1}^b - m_{n-2,n}^b + 2m_{n-1,n-2}^b - m_{n-1,n-1}^b - m_{n-1,n}^b,$$
$$\nu_{i,n-1}^{m^b} = -m_{i,n-2}^b + 2m_{i,n-1}^b - m_{n-1,i}^b, \quad (1 \leqslant i < n-1), \quad \nu_{n-1,n-1}^{m^b} = 2m_{n-1,n-1}^b,$$
$$\nu_{i,n}^{m^b} = -m_{i,n-2}^b + 2m_{i,n}^b - m_{n-1,i}^b, \quad (1 \leqslant i < n-1), \quad \nu_{n-1,n}^{m^b} = 2m_{n-1,n}^b. \tag{3.21}$$

$\eta_{i,j}^{m^b}$, $\eta_{j+1,i}^{m^b} (1 \leqslant i \leqslant j \leqslant n-3)$, *as in (3.10), and*

$$\eta_{i,n-2}^{m^b} = m_{i,n-2}^b - m_{i,n-1}^b - m_{i,n}^b + 2m_{n-1,i}^b - m_{n-2,i}^b,$$
$$\eta_{n-1,i}^{m^b} = m_{n-1,i}^b - m_{n-2,i}^b, \quad (1 \leqslant i \leqslant n-3),$$
$$\eta_{n-2,n-2}^{m^b} = m_{n-2,n-2}^b - m_{n-2,n-1}^b - m_{n-2,n}^b + 2m_{n-1,n-2}^b - m_{n-1,n-1}^b - m_{n-1,n}^b,$$
$$\eta_{n-1,n-2}^{m^b} = m_{n-1,n-2}^b - m_{n-1,n-1}^b - m_{n-1,n}^b,$$
$$\eta_{i,n-1}^{m^b} = m_{i,n-1}^b - m_{n-1,i}^b, \quad \eta_{n-1,n-1}^{m^b} = m_{n-1,n-1}^b,$$
$$\eta_{i,n}^{m^b} = m_{i,n}^b - m_{n-1,i}^b, \quad (1 \leqslant i \leqslant n-2), \quad \eta_{n-1,n}^{m^b} = m_{n-1,n}^b, \tag{3.22}$$

where we understand that $\mu_{i,j} = \eta_{i,j} = 0$ *if the index* (i,j) *is out of the range.*

B. Existence and uniqueness of primitive vector in *V*

In this section, we show the existence and uniqueness of primitive vector in the specialized Schnizer modules.

We define $a^{(0)}=(a_{i,j}^{(0)})_{i,j}\in(\mathbb{C}^{\times})^N, b^{(0)}=(b_{i,j}^{(0)})_{i,j}\in\mathbb{C}^N$, by

$$a_{i,j}^{(0)}=1,\quad b_{i,j}^{(0)}=0\quad (1\leqslant i\leqslant N/n, 1\leqslant j\leqslant n). \tag{3.23}$$

Obviously, by (3.1), for any $c\in\mathbb{Z}^N$ and $m\in M$, we have

$$a^{(0)}(c)=1,\quad m^b=m,\quad m_{i,j}^b=m_{i,j}. \tag{3.24}$$

For any $\lambda\in\mathbb{C}$, we denote the U_ε-module defined by $(\Phi_{a^{(0)},b^{(0)},\lambda},V)$ by $V(\lambda)$.

Proposition 3.4: Let $\mathfrak{g}=sp(2n,\mathbb{C})(n\geqslant 2)$ *and* $\lambda=(\lambda_1,\ldots,\lambda_n)\in\mathbb{C}^n$. *A vector* $u\in V(\lambda)$ *satisfies that* $e_iu=0$ *for any* $i\in I$ *if and only if* $u\in\mathbb{C}u_0$, *where* $u_0=u(0,\ldots,0)\in V(\lambda)$. *(We call these vectors "primitive vectors.")*

Proof: "If part" is obvious by (3.2) and (3.3). So we prove "only if part." First, we define $\{r_i\}_{1\leqslant i\leqslant n^2}(=I\times I)$ inductively as follows: $r_1:=(1,1)$ and if $r_s=(i,j)$, then

$$\begin{aligned} r_{s+1}&:=(n,i)\quad (1\leqslant i<j=n),\\ r_{s+1}&:=(i-1,j)\quad (1\leqslant j<i\leqslant n,\text{and } i-1\neq j),\\ r_{s+1}&:=(i,j+1)\quad (\text{otherwise}). \end{aligned} \tag{3.25}$$

And we define $M_s:=\{m\in M\,|\,m_{r_1}=m_{r_2}\cdots=m_{r_s}=0\}(1\leqslant s\leqslant n^2)$. So we have

$$\{(0)\}=M_{n^2}\subset M_{n^2-1}\subset\cdots\subset M_1\subset M.$$

Now, assume that $e_iu=0$ for any $i\in I$ and set $u=\Sigma_{m\in M}c_mu(m)\in V(c_m\in\mathbb{C})$. We shall prove that $u=\Sigma_{m\in M_s}c_mu(m)$ for any $1\leqslant s\leqslant n^2$ by the induction on s. Indeed, if we can prove this, then we have $u=\Sigma_{m\in M_{n^2}}c_mu(m)=c_0u_0\in\mathbb{C}u_0$.

Since $e_1u=0$, by (3.2), we have $0=\Sigma_{m\in M}c_m[-m_{1,1}]u(m-\epsilon_{1,1})$. Since the vectors $\{u(m-\epsilon_{1,1})\,|\,m\in M\}$ are linearly independent, $c_m[-m_{1,1}]=0$ for any $m\in M$. Therefore if $0\neq m_{1,1}(=m_{r_1})$, then $c_m=0$. Hence $u=\Sigma_{m\in M_1}c_mu(m)$. Now we assume that $u=\Sigma_{m\in M_s}c_mu(m)$ for $1\leqslant s<n^2$, and $r_s=(i_s,j_s)$.

Case 1: $1\leqslant i_s\leqslant j_s\leqslant n-2$: In this case $r_{s+1}=(i_s,j_s+1)$. Let $m\in M_s$ then

$$m_{i,j_s}=m_{i,j_s+1}=m_{j_s+2,i}=m_{j_s+1,i}=0(1\leqslant i\leqslant i_s-1).$$

Hence, by (3.2), we have

$$\begin{aligned} 0=e_{j_s+1}u&=\sum_{m\in M_s}c_m[-m_{j_s+1,j_s+1}]_{\varepsilon_{j_s+1}}u(m+\alpha_{j_s+1,j_s+1})+\sum_{m\in M_s}\sum_{i=i_s}^{j_s}c_m[m_{i,j_s}-m_{i,j_s+1}]_{\varepsilon_{j_s+1}}u(m+\alpha_{i,j_s+1})\\ &+\sum_{m\in M_s}\sum_{i=i_s}^{j_s}c_m[m_{j_s+2,i}-m_{j_s+1,i}]_{\varepsilon_{j_s+1}}u(m+\alpha_{i,j_s+1}+\epsilon_{i,j_s}-\epsilon_{j_s+1,i}). \end{aligned} \tag{3.26}$$

On the other hand, by (3.7), for any $m\in M_s$, we have

$$\begin{aligned} (m+\alpha_{j_s+1,j_s+1})_{i_s,j_s}&=\left(m-\epsilon_{j_s+1,j_s+1}+\sum_{k=1}^{j_s}(-\epsilon_{j_s+1,k}+\epsilon_{j_s+2,k}-\epsilon_{k,j_s+1}+\epsilon_{k,j_s})\right)_{i_s,j_s}\\ &=(m+\epsilon_{i_s,j_s})_{i_s,j_s}=m_{i_s,j_s}+1=1. \end{aligned}$$

Similarly , for any $i(i_s\leqslant i\leqslant j_s)$, we have

$$(m+\alpha_{i,j_s+1})_{i_s,j_s}=(m-\epsilon_{i,j_s+1}+\sum_{k=1}^{i-1}(-\epsilon_{j_s+1,k}+\epsilon_{j_s+2,k}-\epsilon_{k,j_s+1}+\epsilon_{k,j_s}))_{i_s,j_s}=1-\delta_{i,i_s},$$

$$(m+\alpha_{i,j_s+1}+\epsilon_{i,j_s}-\epsilon_{j_s+1,i})_{i_s,j_s}=(1-\delta_{i,i_s})+\delta_{i,i_s}=1,$$

where $\delta_{i,j}$ is the Kronecker's delta. Thus

$$\sum_{m\in M_s}\sum_{i=i_s}^{j_s+1}\mathbb{C}u(m+\alpha_{i,j_s+1})+\sum_{m\in M_s}\sum_{i=i_s}^{j_s}\mathbb{C}u(m+\alpha_{i,j_s+1}+\epsilon_{i,j_s}-\epsilon_{j_s+1,i})$$
$$=\{\bigoplus_{m\in M_s}\mathbb{C}u(m+\alpha_{i_s,j_s+1})\}$$
$$\oplus\{\sum_{m\in M_s}\sum_{i=i_s+1}^{j_s+1}\mathbb{C}u(m+\alpha_{i,j_s+1})+\sum_{m\in M_s}\sum_{i=i_s}^{j_s}\mathbb{C}u(m+\alpha_{i,j_s+1}+\epsilon_{i,j_s}-\epsilon_{j_s+1,i})\}.$$

Then, by (3.26), we have that

$$0=c_m[m_{i_s,j_s}-m_{i_s,j_s+1}]=c_m[-m_{i_s,j_s+1}]$$

for any $m\in M_s$, which implies if $0\neq m_{i_s,j_s+1}=m_{r_{s+1}}$ then $c_m=0$. Therefore $u=\Sigma_{m\in M_{s+1}}c_m u(m)$.
Case 2—$1\leqslant i_s\leqslant j_s=n-1$: In this case , $r_{s+1}=(i_s,n)$. Let $m\in M_s$ then

$$m_{i,n}=m_{n,i}=m_{i,n-1}=0\quad(1\leqslant i\leqslant i_s-1).$$

Thus, by (3.3),

$$0=e_n u=\sum_{m\in M_s}c_m[-m_{n,n}]_{\varepsilon_n}u(m+\alpha_{n,n})+\sum_{m\in M_s}\sum_{i=i_s}^{n-1}c_m[m_{i,n}-m_{n,i}]_{\varepsilon_n}u(m+\alpha_{i,n})+\sum_{m\in M_s}\sum_{i=i_s}^{n-1}c_m[m_{i,n-1}$$
$$-m_{n,i}]_{\varepsilon_n}u(m+\alpha_{i,n}+\epsilon_{i,n-1}-\epsilon_{n,i})+\sum_{m\in M_s}\sum_{i=i_s}^{n-1}c_m[m_{i,n}-m_{n,i}]_{\varepsilon_n}u(m+\alpha_{i,n}+2\epsilon_{i,n-1}-2\epsilon_{n,i}).$$

On the other hand, in a similar way to Case 1, for any $i(i_s\leqslant i\leqslant n)$, we have

$$(m+\alpha_{i,n})_{i_s,n-1}=2-2\delta_{i,i_s},\quad(m+\alpha_{i,n}+\epsilon_{i,n-1}-\epsilon_{n,i})_{i_s,n-1}=2-\delta_{i,i_s},$$

$$(m+\alpha_{i,n}+2\epsilon_{i,n-1}-2\epsilon_{n,i})_{i_s,n-1}=2.$$

Thus, $(m+\alpha_{i_s,n})_{i_s,n-1}=0,(m+\alpha_{i_s,n}+\epsilon_{i_s,n-1}-\epsilon_{n,i_s})_{i_s,n-1}=1$, and the others are 2. Hence, by the linearly independence, we have that

$$0=c_m[m_{i_s,n}-m_{n,i_s}]_{\varepsilon_n}=c_m[m_{i_s,n-1}-m_{n,i_s}]_{\varepsilon_n}=c_m[-m_{n,i_s}]_{\varepsilon_n}$$

for any $m\in M_s$. Therefore $u=\Sigma_{m\in M_{s+1}}c_m u(m)=\Sigma_{m\in M_{s+2}}c_m u(m)$.

Case 3—$1\leqslant i_s\leqslant j_s=n$. This case is already shown in Case 2.

Case 4—$1\leqslant j_s<i_s\leqslant n$ and $j_s\neq i_s-1$: In this case $r_{s+1}=(i_s-1,j_s)$. For $m\in M_s$, we have

$$m_{j,i_s-2}=m_{j,i_s-1}=0\quad(1\leqslant j\leqslant j_s),\quad m_{i_s,j}=m_{i_s-1,j}=0\quad(1\leqslant j\leqslant j_s-1).$$

Thus, by (3.2),

$$0 = e_{i_s-1}u = \sum_{m\in M_s} c_m[-m_{i_s-1,i_s-1}]_{\varepsilon_{i_s-1}} u(m+\alpha_{i_s-1,i_s-1})$$
$$+ \sum_{m\in M_s}\sum_{j=j_s+1}^{i_s-2} c_m[m_{j,i_s-2}-m_{j,i_s-1}]_{\varepsilon_{i_s-1}} u(m+\alpha_{j,i_s-1})$$
$$+ \sum_{m\in M_s}\sum_{j=j_s}^{i_s-2} c_m[m_{i_s,j}-m_{i_s-1,j}]_{\varepsilon_{i_s-1}} u(m+\alpha_{j,i_s-1}+\epsilon_{j,i_s-2}-\epsilon_{i_s-1,j}).$$

On the other hand,

$$(m+\alpha_{j,i_s-1})_{i_s,j_s} = 1 \quad (j_s+1 \leqslant j \leqslant i_s-1),$$

$$(m+\alpha_{j,i_s-1}+\epsilon_{j,i_s-2}-\epsilon_{i_s-1,j})_{i_s,j_s} = 1-\delta_{j,j_s} \quad (j_s \leqslant j \leqslant i_s-2).$$

Thus, by the linearly independence, $0=c_m[m_{i_s,j_s}-m_{i_s-1,j_s}]=c_m[-m_{i_s-1,j_s}]=0$ for any $m\in M_s$. Therefore $u=\Sigma_{m\in M_{s+1}}c_m u(m)$.

Case 5—$1\leqslant j_s<i_s\leqslant n$ and $j_s=i_s-1$: In this case $r_{s+1}=(i_s,i_s)$. For any $m\in M_s$, we have

$$m_{j,i_s-1}=m_{j,i_s}=m_{i_s,j}=m_{i_s+1,j}=0 \quad (1\leqslant j\leqslant i_s-1).$$

Thus, by (3.2) and (3.3),

$$0 = e_{i_s}u = \sum_{m\in M_s} c_m[-m_{i_s,i_s}]_{\varepsilon_{i_s}} u(m+\alpha_{i_s,i_s}).$$

Hence, $c_m[-m_{i_s,i_s}]=0$ for any $m\in M_s$. Therefore $u=\Sigma_{m\in M_{s+1}}c_m u(m)$. □

In a similar way to the proof of Proposition 3.4, we can prove the following propositions.

Proposition 3.5: Let $\mathfrak{g}=so(2n+1,\mathbb{C}), so(2n,\mathbb{C})$, *and* $\lambda=(\lambda_1,\cdots,\lambda_n)\in\mathbb{C}^n$. *A vector* $u=\Sigma_{m\in M}c_m u(m)\in V(\lambda)(c_m\in\mathbb{C})$ *satisfies the condition* $e_i u=0$ *for any* $i\in I$ *if and only if* $u\in\mathbb{C}u_0$.

In the case of $\mathfrak{g}=\mathsf{so}(2n,\mathbb{C})$, the proof of Proposition 3.5 is slightly different from the one of Proposition 3.4.

Proof: ($\mathsf{so}(2n,\mathbb{C})$-*case*): "If part" is obvious from (3.2) and (3.15)–(3.18). So we prove "only if part." We define $\{r_i\}_{i=1}^{(n-1)n}$ by a similar way to the previous cases: $r_1:=(1,1)$ and if $r_s=(i,j)$, then

$$r_{s+1}:=(n-1,i) \quad (1\leqslant i<j=n),$$

$$r_{s+1}:=(i-1,j) \quad (1\leqslant j<i\leqslant n-1, i-1\neq j),$$

$$r_{s+1}:=(i,j+1) \quad (\text{otherwise}).$$

We set $M_s=\{m\in M\,|\,m_{r_1}=\cdots=m_{r_s}=0\}$ for any $s(1\leqslant s\leqslant(n-1)n)$.

Now we shall prove that $u=\Sigma_{m\in M_s}c_m u(m)$ for any $1\leqslant s\leqslant(n-1)n$ by the induction on s. By using $e_1u=0$, we can prove $u=\Sigma_{m\in M_1}c_m u(m)$. Next, we assume that $u=\Sigma_{m\in M_s}c_m u(m)$ for $s(1\leqslant s<(n-1)n)$, and $r_s=(i_s,j_s)$. Then we prove by a similar manner to the proof of Proposition 3.4.

In case $j_s\neq n-2,n-1,n$, we only use $e_{j_s}(1\leqslant j\leqslant n-2)$ to prove $u=\Sigma_{m\in M_{s+1}}c_m u(m)$. Since the action of e_j is the same as the one of $\mathfrak{g}=\mathsf{sp}(2n,\mathbb{C})$ for $1\leqslant j\leqslant n-2$, the proof is also the same. So we prove the case of $j_s=n-2,n-1,n$.

Let $1\leqslant i_s\leqslant j_s=n-2$. In this case, $r_{s+1}=(i_s,n-1), r_{s+2}=(i_s,n)$ and $r_{s+3}=(n-1,i_s)$. We assume that $i_s=2i_s'-1, n=2n'(i',n'\in\mathbb{Z})$. Then, for any $m\in M_s$,

$$m_{2i-1,n-2}-m_{2i-1,n-1}=m_{2i-1,n}-m_{n-1,2i-1}=m_{2i,n-2}-m_{2i,n}=m_{2i,n-1}-m_{n-1,2i}=0 \quad (1\leqslant i<i_s').$$

Thus, by (3.15),

$$e_{n-1}u = \sum_{m\in M_s} c_m[-m_{n-1,n-1}]u(m+\alpha_{2n'-1,n-1}) + \sum_{m\in M_s}\sum_{i=i'_s}^{n'-1} c_m\{[m_{2i-1,n-2}-m_{2i-1,n-1}]u(m+\alpha_{2i-1,n-1})$$
$$+[m_{2i-1,n}-m_{n-1,2i-1}]u(m+\alpha_{2i-1,n-1}+\epsilon_{2i-1,n-2}-\epsilon_{n-1,2i-1})+[m_{2i,n-2}-m_{2i,n}]u(m+\alpha_{2i,n})$$
$$+[m_{2i,n-1}-m_{n-1,2i}]u(m+\alpha_{2i,n}+\epsilon_{2i,n-2}-\epsilon_{n-1,2i})\},$$

On the other hand, by (3.20),

$$(\beta_{2i-1,n-1})_{2i'_s-1,n-2}=1-\delta_{i,i'_s},\quad (\beta_{2i,n})_{2i'_s-1,n-2}=0,\quad (i'_s\leqslant i\leqslant n').$$

Hence, by (3.19),

$$(\alpha_{2i-1,n-1})_{2i'_s-1,n-2}=1-\delta_{i,i'_s},\quad (\alpha_{2i-1,n-1}+\epsilon_{2i-1,n-2}-\epsilon_{n-1,2i-1})_{2i'_s-1,n-2}=1,$$

$$(\alpha_{2i,n})_{2i'_s-1,n-2}=1,\quad (\alpha_{2i,n}+\epsilon_{2i,n-2}-\epsilon_{n-1,2i})_{2i'_s-1,n-2}=1,\quad (i'_s\leqslant i\leqslant n').$$

So $(\alpha_{2i'_s-1,n-1})_{2i'_s-1,n-1}=0$, and the others are 1. Thus, for any $m\in M_s$ we have

$$0=c_m[m_{2i'_s-1,n-2}-m_{2i'_s-1,n-1}]=c_m[m_{i_s,n-2}-m_{i_s,n-1}]=c_m[-m_{i_s,n-1}].$$

Therefore $u=\Sigma_{m\in M_{s+1}}c_m u(m)$.

Furthermore, for any $m\in M_s$, we have

$$m_{2i,n-2}-m_{2i,n-1}=m_{2i,n}-m_{n-1,2i}=m_{2i-1,n-2}-m_{2i-1,n}=m_{2i-1,n-1}-m_{n-1,2i-1}=0\quad (1\leqslant i<i'_s).$$

Thus, by (3.16),

$$e_n u = \sum_{m\in M_s} c_m[-m_{n-1,n}]u(m+\alpha_{2n'-1,n}) + \sum_{m\in M_s}\sum_{i=i'_s}^{n'-1} c_m\{[m_{2i,n-2}-m_{2i,n-1}]u(m+\alpha_{2i,n-1})+[m_{2i,n}$$
$$-m_{n-1,2i}]u(m+\alpha_{2i,n-1}+\epsilon_{2i,n-2}-\epsilon_{n-1,2i})+[m_{2i-1,n-2}-m_{2i-1,n}]u(m+\alpha_{2i-1,n})+[m_{2i-1,n-1}$$
$$-m_{n-1,2i-1}]u(m+\alpha_{2i-1,n}+\epsilon_{2i-1,n-2}-\epsilon_{n-1,2i-1})\}.$$

On the other hand, by (3.20),

$$(\beta_{2i,n-1})_{2i'_s-1,n-2}=0,\quad (\beta_{2i-1,n})_{2i'_s-1,n-2}=1-\delta_{i,i'_s},\quad (i'_s\leqslant i\leqslant n').$$

Hence, by (3.19),

$$(\alpha_{2i,n-1})_{2i'_s-1,n-2}=1,\quad (\alpha_{2i,n-1}+\epsilon_{2i,n-2}-\epsilon_{n-1,2i})_{2i'_s-1,n-2}=1,$$

$$(\alpha_{2i-1,n})_{2i'_s-1,n-2}=1-\delta_{i,i'_s},\quad (\alpha_{2i-1,n}+\epsilon_{2i-1,n-2}-\epsilon_{n-1,2i-1})_{2i'_s-1,n-2}=1,\quad (i'_s\leqslant i\leqslant n').$$

So $(\alpha_{2i'_s-1,n})_{2i'_s-1,n-2}=0$, and the others are 1. Thus, for any $m\in M_s$ we have

$$0=c_m[m_{2i'_s-1,n-2}-m_{2i'_s-1,n}]=c_m[m_{i_s,n-2}-m_{i_s,n}]=c_m[-m_{i_s,n}].$$

Therefore $u=\Sigma_{m\in M_{s+2}}c_m u(m)$. Then,

$$e_n u = \sum_{m\in M_{s+2}} c_m[-m_{n-1,n}]u(m+\alpha_{2n'-1,n}) + \sum_{m\in M_{s+2}} \sum_{i=i'_s}^{n'-1} c_m\{[m_{2i,n-2}-m_{2i,n-1}]u(m+\alpha_{2i,n-1})$$
$$+[m_{2i,n}-m_{n-1,2i}]u(m+\alpha_{2i,n-1}+\epsilon_{2i,n-2}-\epsilon_{n-1,2i})+[m_{2i-1,n-1}-m_{n-1,2i-1}]u(m+\alpha_{2i-1,n}$$
$$+\epsilon_{2i-1,n-2}-\epsilon_{n-1,2i-1})\}+\sum_{m\in M_{s+2}}\sum_{i=i'_s+1}^{n'-1} c_m[m_{2i-1,n-2}-m_{2i-1,n}]u(m+\alpha_{2i-1,n}).$$

On the other hand, by (3.20),

$$(\beta_{2i,n-1})_{2i'_s-1,n}=0,\quad (\beta_{2i-1,n})_{2i'_s-1,n}=1-\delta_{i,i'_s},\quad (i'_s\leqslant i\leqslant n').$$

Hence, by (3.19),

$$(\alpha_{2i,n-1})_{2i'_s-1,n}=1,\quad (\alpha_{2i,n-1}+\epsilon_{2i,n-2}-\epsilon_{n-1,2i})_{2i'_s-1,n}=1,$$

$$(\alpha_{2i-1,n}+\epsilon_{2i-1,n-2}-\epsilon_{n-1,2i-1})_{2i'_s-1,n}=1-2\delta_{i,i'_s},\quad (i'_s\leqslant i\leqslant n'),$$

$$(\alpha_{2i-1,n})_{2i'_s-1,n}=1,\quad (i_s+1\leqslant i\leqslant n').$$

So $(\alpha_{2i'_s-1,n}+\epsilon_{2i'_s-1,n-2}-\epsilon_{n-1,2i'_s-1})_{2i'_s-1,n}=-1$, and the others are 1. Thus, for any $m\in M_{s+2}$ we have

$$0=c_m[m_{2i'_s-1,n-1}-m_{n-1,2i'_s-1}]=c_m[m_{i_s,n-1}-m_{n-1,i_s}]=c_m[-m_{n-1,i_s}].$$

Therefore $u=\Sigma_{m\in M_{s+3}}c_m u(m)$. So we also obtain the case $1\leqslant i_s\leqslant n-2, j_s=n-1,n, (n=2n', i_s=2i'_s-1)$.

Similarly, we can prove the cases $(n=2n', i_s=2i'_s), (n=2n'+1, i_s=2i'_s-1)$ and $(n=2n'+1, i_s=2i'_s)$.

The remaining cases are $(i_s,j_s)=(n-1,n-2),(n-1,n-1)$. But these cases are proved similarly. □

IV. IRREDUCIBLE $U_\varepsilon^{\mathrm{fin}}$-MODULE $U_\varepsilon u_0$

We keep the settings and notations as in Secs. II and III.

A. Restricted specializations

In this section, we introduce the restricted specializations and their properties.

Definition 4.1: Let $A:=\mathbb{C}[q,q^{-1}]$ and U_A^{res} be the A-subalgebra of $U_q(\mathsf{g})$ generated by $\{e_i^{(k)}, f_i^{(k)}, t_i^{\pm 1} \mid i\in I, k\in\mathbb{Z}_+\}$. Let l be an odd integer greater than 3 and ε be a primitive lth root of unity such that $\varepsilon^{2d_i}\neq 1$ for any $i\in I$. We regard $\mathbb{C}$ as A-algebra by $f(q).c:=f(\varepsilon)\cdot c$ for any $f(q)\in A, c\in\mathbb{C}$ and we denote it by $\mathbb{C}_\varepsilon$. We define

$$U_\varepsilon^{\mathrm{res}} := U_A^{\mathrm{res}}\otimes_A \mathbb{C}_\varepsilon,$$

which is called "restricted specialization of $U_q(\mathsf{g})$." Similarly, we define $(U_\varepsilon^{\mathrm{res}})^+, (U_\varepsilon^{\mathrm{res}})^-, (U_\varepsilon^{\mathrm{res}})^0$. We denote $u\otimes 1$ by u for any $u\in U_A^{\mathrm{res}}$. Let $U_\varepsilon^{\mathrm{fin}}$ be the subalgebra of $U_\varepsilon^{\mathrm{res}}$ generated by $\{e_i, f_i, t_i^{\pm 1}\}_{i=1}^n$. (Similarly, we define $(U_\varepsilon^{\mathrm{fin}})^+, (U_\varepsilon^{\mathrm{fin}})^-$ and $(U_\varepsilon^{\mathrm{fin}})^0$).

Next we review the representation theory of $U_\varepsilon^{\mathrm{res}}$.

Definition 4.2: Let L be a finite dimensional $U_\varepsilon^{\mathrm{res}}$-module. If $t_i^l v=v$ for any $v\in L, i\in I$ (that is, t_i^l is the identity map), we call L "$U_\varepsilon^{\mathrm{res}}$-module of type 1."

Remark (Ref. 1): In general, finite dimensional irreducible $U_\varepsilon^{\mathrm{res}}$-modules are divided into 2^n types according to $\{\sigma: Q\to\{\pm 1\}$; homomorphism of group $\}$. Without a loss of generality, we may assume that finite dimensional irreducible $U_\varepsilon^{\mathrm{res}}$-modules are of type 1.

Definition 4.3: For $\lambda=(\lambda_1,\ldots,\lambda_n)\in\mathbb{Z}_+^n$, let I_λ be the left ideal of $U_q(\mathfrak{g})$ generated by $\{e_i, f_i^{\lambda_i+1}, t_i-q_i^{\lambda_i} \mid i\in I\}$ and $L(\lambda):=U_q(\mathfrak{g})/\mathsf{I}_\lambda$. We set $v_\lambda=1+\mathsf{I}_\lambda\in L(\lambda)$. Let $V_A^{\mathrm{res}}(\lambda)$ be the U_A^{res}-submodule of $L(\lambda)$ generated by v_λ, $V_\varepsilon^{\mathrm{res}}(\lambda):=V_A^{\mathrm{res}}(\lambda)\otimes_A\mathbb{C}_\varepsilon$, and $W_\varepsilon^{\mathrm{res}}(\lambda)$ be the maximal proper $U_\varepsilon^{\mathrm{res}}$-submodule of $V_\varepsilon^{\mathrm{res}}(\lambda)$. We define

$$L_\varepsilon^{\mathrm{res}}(\lambda):=V_\varepsilon^{\mathrm{res}}(\lambda)/W_\varepsilon^{\mathrm{res}}(\lambda).$$

Theorem 4.4 (Refs. 6 and 7): *(i) For any $\lambda\in\mathbb{Z}_+^n$, $L_\varepsilon^{\mathrm{res}}(\lambda)$ is a finite dimensional irreducible $U_\varepsilon^{\mathrm{res}}$-module of type 1 (We call λ "highest weight of $L_\varepsilon^{\mathrm{res}}(\lambda)$").*

(ii) Let L be a finite dimensional irreducible $U_\varepsilon^{\mathrm{res}}$-module of type 1. Then, there exists a unique element $\lambda\in\mathbb{Z}_+^n$ such that $L\cong L_\varepsilon^{\mathrm{res}}(\lambda)$.

(iii) Let $\lambda'=(\lambda_1',\ldots,\lambda_n')\in\mathbb{Z}_l^n(\mathbb{Z}_l:=\{0,1,\ldots,l-1\})$, $\lambda''\in\mathbb{Z}_+^n$, and $\lambda:=\lambda'+l\lambda''$. Then we have

$$L_\varepsilon^{\mathrm{res}}(\lambda)\cong L_\varepsilon^{\mathrm{res}}(\lambda')\otimes L_\varepsilon^{\mathrm{res}}(l\lambda'').$$

Next, we give the relation between the representations of $U_\varepsilon^{\mathrm{res}}$ and $U_\varepsilon^{\mathrm{fin}}$.

Proposition 4.5 (Ref. 6 and 7): (i) For any $\lambda=(\lambda_1,\ldots,\lambda_n)\in\mathbb{Z}_l^n$, we regard $L_\varepsilon^{\mathrm{res}}(\lambda)$ as $U_\varepsilon^{\mathrm{fin}}$-module and denote it by $L_\varepsilon^{\mathrm{fin}}(\lambda)$. Then $L_\varepsilon^{\mathrm{fin}}(\lambda)$ is a finite dimensional irreducible $U_\varepsilon^{\mathrm{fin}}$-module of type 1. Conversely, let L be any finite dimensional irreducible $U_\varepsilon^{\mathrm{fin}}$-module of type 1, then there exists a unique element $\lambda=(\lambda_1,\ldots,\lambda_n)\in\mathbb{Z}_l^n$ such that $L\cong L_\varepsilon^{fin}(\lambda)$.

(ii) Let $U(\mathfrak{g})$ be the universal enveloping algebra of $\mathfrak{g}$. Then for any $\lambda\in\mathbb{Z}_+^n$, we can regard $L_\varepsilon^{\mathrm{res}}(l\lambda)$ as a finite dimensional irreducible $U(\mathfrak{g})$-module of the highest weight λ.

B. Finite dimensional quantum algebra $U_\varepsilon^{\mathrm{fin}}$

In this section, we introduce the properties of $U_\varepsilon^{\mathrm{fin}}$ to prove Theorem 4.10 below. First, we introduce PBW theorem and the triangular decomposition of $U_\varepsilon^{\mathrm{fin}}$.

Theorem 4.6 (Ref. 7): Let $\beta_1,\ldots,\beta_N$ *be as in Definition 2.4* ($\Delta_+=\{\beta_1,\ldots,\beta_N\}$). *We assume that $l\not\equiv 0$ (mod 3) if $\mathfrak{g}$ is type G_2. Then we have*

(i) $\{e_{\beta_1}^{m_1}\cdots e_{\beta_N}^{m_N} \mid 0\le m_i\le l-1$ *for any* $1\le i\le N\}$ *is a $\mathbb{C}$-basis of* $(U_\varepsilon^{\mathrm{fin}})^+$.
(ii) $\{f_{\beta_1}^{m_1}\cdots f_{\beta_N}^{m_N} \mid 0\le m_i\le l-1$ *for any* $1\le i\le N\}$ *is a $\mathbb{C}$-basis of* $(U_\varepsilon^{\mathrm{fin}})^-$.
(iii) $\{t_1^{m_1}\cdots t_n^{m_n} \mid 0\le m_i\le 2l-1$ *for any* $1\le i\le n\}$ *is a $\mathbb{C}$-basis of* $(U_\varepsilon^{\mathrm{fin}})^0$.
(iv) *Let ϕ be the multiplication map*

$$\phi:(U_\varepsilon^{\mathrm{fin}})^-\otimes(U_\varepsilon^{\mathrm{fin}})^0\otimes(U_\varepsilon^{\mathrm{fin}})^+\to U_\varepsilon^{\mathrm{fin}}\quad u_-\otimes u_0\otimes u_+\quad\mapsto\quad u_-u_0u_+.$$

Then ϕ is an isomorphism of $\mathbb{C}$-vector space.

By Theorem 4.6, we know that the dimension of $U_\varepsilon^{\mathrm{fin}}$ is $2^n l^{n+2N}$.

Proposition 4.7(Ref. 1): We have $e_\alpha^l=f_\alpha^l=0$ *in* $U_\varepsilon^{\mathrm{fin}}$ *for any* $\alpha\in\Delta_+$, *and* $t_i^{2l}=1$ *in* $U_\varepsilon^{\mathrm{fin}}$ *for any* $i\in I$.

Lemma 4.8: We assume that $l\not\equiv 0$ (mod 3) if $\mathfrak{g}$ is type G_2. Let J be the two-sided ideal of U_ε generated by $\{e_\alpha^l, f_\alpha^l \mid \alpha\in\Delta_+\}\cup\{t_i^{2l}-1 \mid i\in I\}$. Then we have $U_\varepsilon^{\mathrm{fin}}\cong U_\varepsilon/\mathrm{J}$.

Proof: By the definition of $U_\varepsilon^{\mathrm{fin}}$, $(e_i,f_i,t_i^{\pm1})$ satisfies the relations in U_ε. Therefore, there exists the following surjective $\mathbb{C}$-algebra homomorphism π,

$$\pi:U_\varepsilon\to U_\varepsilon^{\mathrm{fin}}\quad(e_i,f_i,t_i^{\pm1})\mapsto(e_i,f_i,t_i^{\pm1}).$$

By Proposition 4.7, we obtain the surjective $\mathbb{C}$-algebra homomorphism π',

$$\pi':U_\varepsilon/\mathrm{J}\to U_\varepsilon^{\mathrm{fin}}\quad(e_i,f_i,t_i^{\pm1})\mapsto(e_i,f_i,t_i^{\pm1}).$$

On the other hand, by Proposition 2.7 and Theorem 2.8, U_ε/J is spanned by

$$\{e_{\beta_1}^{m_1}\cdots e_{\beta_N}^{m_N}f_{\beta_1}^{m_{N+1}}\cdots f_{\beta_N}^{m_{2N}}t_1^{m_{2N+1}}\cdots t_n^{m_{2N+n}}|0\leqslant m_i\leqslant l-1(1\leqslant i\leqslant 2N),0\leqslant m_i\leqslant 2l-1(2N+1\leqslant i\leqslant 2N+n)\}.$$

So, by Theorem 4.6, π' is an injective homomorphism. Therefore π' is an isomorphism of algebra. □

C. $U_\varepsilon^{\mathrm{fin}}$-module structure on the $U_\varepsilon u_0$

In this section, we construct $U_\varepsilon^{\mathrm{fin}}$-module by using the Schnizer modules.

Lemma 4.9: Let $\mathfrak{g}=sp(2n,\mathbb{C}),so(2n+1,\mathbb{C})$ *or* $so(2n,\mathbb{C})$. *For any* $\lambda=(\lambda_1,\cdots,\lambda_n)\in\mathbb{Z}^n$, *we denote the* U_ε*-submodule of* $V(\lambda)$ *generated by* u_0 *by* $U_\varepsilon u_0$. *Then we have*

(i) $e_\alpha^l=0$ *on* $U_\varepsilon u_0$ *for any* $\alpha\in\Delta_+$.
(ii) $t_i^l=1$ *on* $U_\varepsilon u_0$ *for any* $i\in I$.
(iii) $f_\alpha^l=0$ *on* $U_\varepsilon u_0$ *for any* $\alpha\in\Delta_+$.

Proof: We prove the case of $\mathfrak{g}=\mathsf{sp}(2n,\mathbb{C})$. The other cases are shown similarly.

By Proposition 2.7, it is enough to prove that $e_\alpha^l u_0=f_\alpha^l u_0=(t_i^l-1)u_0=0$.

(i) By Proposition 3.4, $e_i u_0=0$ for any $i\in I$. On the other hand, by Proposition 2.6, $e_\alpha\in U_\varepsilon^+\cap(U_\varepsilon)_\alpha$ for any $\alpha\in\Delta_+$. Therefore $e_\alpha u_0=e_\alpha^l u_0=0$.

(ii) By (3.4), (3.8), and (3.9)), $t_i u_0=\varepsilon_i^{\lambda_i}u_0$ in $V(\lambda)$. Since $\lambda_i\in\mathbb{Z}, t_i^l u_0=u_0$. We shall prove (iii) in the next section. □

We call the U_ε-modules such that $e_i^l=f_i^l=0$ "nilpotent module." By Lemma 4.9, $U_\varepsilon u_0$ is a nilpotent module. In general, Schnizer modules are not necessarily nilpotent unless we specialize their parameters properly.

Theorem 4.10: *Let* $\mathfrak{g}=sp(2n,\mathbb{C}),so(2n+1,\mathbb{C})$ *or* $so(2n,\mathbb{C})$, *and* $\lambda\in\mathbb{Z}_l^n$. *Then we have*

(i) $U_\varepsilon u_0$ *is a* $U_\varepsilon^{\mathrm{fin}}$*-module*.
(ii) $U_\varepsilon u_0$ *is isomorphic to* $L_\varepsilon^{fin}(\lambda)$ *as* $U_\varepsilon^{\mathrm{fin}}$*-module. That is,* $U_\varepsilon u_0$ *is a finite dimensional irreducible* $U_\varepsilon^{\mathrm{fin}}$*-module of type* 1 *with highest weight* λ.

Proof: We prove the case of $\mathfrak{g}=sp(2n,\mathbb{C})$. The other cases are shown similarly. By Lemma 4.8, 4.9, we obtain (i).

(ii) Finite dimensionality of $U_\varepsilon u_0$ is obvious. $U_\varepsilon u_0$ is type 1 with the highest weight λ by Lemma 4.9 (ii) and its proof. So we shall prove the irreducibility of $U_\varepsilon u_0$.

We can regard $U_\varepsilon^{\mathrm{fin}}$ as a well-defined Q-graded algebra by the following way (cf. Definition 2.5).

$$(U_\varepsilon^{\mathrm{fin}})_d:=\{u+\mathrm{J}|u\in(U_\varepsilon)_d\}(d\in Q),$$

where J is the two-sided ideal as in Lemma 4.8. Hence

$$e_{i_1}\cdots e_{i_r}\in(U_\varepsilon^{\mathrm{fin}})_{\alpha_{i_1}+\cdots+\alpha_{i_r}}\quad(i_1,\ldots,i_r\in I).$$

On the other hand, by Proposition 4.7, if $(U_\varepsilon^{\mathrm{fin}})_d\neq 0$ then

$$d\leqslant(l-1)\sum_{\beta\in\Delta_+}\beta$$

for any $d\in Q$, where $d\geqslant d'\Leftrightarrow d-d'\in Q_+$. So, there exists $r_0\in\mathbb{Z}_+$ such that $e_{i_1}e_{i_2}\cdots e_{i_r}=0$ for any $r\geqslant r_0$ and $i_1,i_2\cdots,i_r\in I$. Thus, for any nonzero $U_\varepsilon^{\mathrm{fin}}$-submodule L of $U_\varepsilon u_0$, there exists a nonzero element $v\in L$ such that $e_i v=0$ for any $i\in I$. Therefore, by the uniqueness of primitive vector of Proposition (3.4), $U_\varepsilon u_0\subset L$. Then we have $L\supseteq U_\varepsilon^{\mathrm{fin}}u_0=U_\varepsilon u_0\supseteq L$. Therefore, $U_\varepsilon u_0$ is irreducible. □

Comment: We expect that we can treat infinitesimal Verma modules for orthogonal and symplectic cases in a similar way to Ref. 5.

V. PROOF OF LEMMA 4.9(III)

A. Case of λ_{l-1}

In this section we shall show Lemma 4.9 (iii) for the special case : $\lambda=\lambda_{l-1}:=(l-1,\cdots,l-1)$. For $\lambda=(\lambda_1,\ldots,\lambda_n)\in\mathbb{Z}_l^n$, in case $\mathfrak{g}=\mathsf{sp}(2n,\mathbb{C})$, we define $m^\lambda=(m^\lambda_{i,j})^n_{i,j=1}\in M$ by

$$m^\lambda_{i,i}=\lambda_i \quad (1\leqslant i\leqslant n),$$

$$m^\lambda_{i,j}=\lambda_i+\cdots+\lambda_j \quad (1\leqslant i<j\leqslant n),$$

$$m^\lambda_{j,i}=\lambda_i+\cdots+\lambda_{j-1}+2\lambda_j+\cdots+2\lambda_n \quad (1\leqslant i<j\leqslant n).$$

Obviously, we have

$$m^\lambda_{i,j+1}-m^\lambda_{i,j}=\lambda_{j+1} \quad (1\leqslant i\leqslant j<n),$$

$$m^\lambda_{n,i}-m^\lambda_{i,n}=\lambda_n \quad (1\leqslant i<n), \tag{5.1}$$

$$m^\lambda_{j,i}-m^\lambda_{j+1,i}=\lambda_j \quad (1\leqslant i\leqslant j<n-1).$$

Similarly, in case $\mathfrak{g}=\mathsf{so}(2n+1,\mathbb{C})$, for $\lambda=(\lambda_1,\ldots,\lambda_n)\in\mathbb{Z}_l^n$, we define $m^\lambda=(m^\lambda_{i,j})^n_{i,j=1}\in M$ by

$$m^\lambda_{i,i}:=\lambda_i \quad (1\leqslant i\leqslant n),$$

$$m^\lambda_{i,j}:=\lambda_i+\cdots+\lambda_j \quad (1\leqslant i<j\leqslant n-1),$$

$$m^\lambda_{i,n}:=2\lambda_i+\cdots+2\lambda_{n-1}+\lambda_n \quad (1\leqslant i\leqslant n-1),$$

$$m^\lambda_{j,i}:=\lambda_i+\cdots+\lambda_{j-1}+2\lambda_j+\cdots+2\lambda_{n-1}+\lambda_n \quad (1\leqslant i<j\leqslant n-1),$$

$$m^\lambda_{n,i}:=\lambda_i+\cdots+\lambda_n \quad (1\leqslant i\leqslant n-1),$$

and in case $\mathfrak{g}=\mathsf{so}(2n,\mathbb{C})$, we define $m^\lambda=(m^\lambda_{i,j})^n_{1\leqslant i\leqslant n-1,1\leqslant j\leqslant n}\in M$ by

$$m^\lambda_{i,i}:=\lambda_i \quad (1\leqslant i\leqslant n-1),$$

$$m^\lambda_{n-1,n}:=\lambda_n,$$

$$m^\lambda_{i,j}:=\lambda_i+\cdots+\lambda_j \quad (1\leqslant i<j\leqslant n-2),$$

$$m^\lambda_{i,n-1}:=\lambda_i+\cdots+\lambda_{n-2}+\lambda_n \quad (1\leqslant i\leqslant n-2),$$

$$m^\lambda_{i,n}:=\lambda_i+\cdots+\lambda_{n-2}+\lambda_{n-1} \quad (1\leqslant i\leqslant n-2),$$

$$m^\lambda_{j,i}:=\lambda_i+\cdots+\lambda_{j-1}+2\lambda_j+\cdots+2\lambda_{n-2}+\lambda_{n-1}+\lambda_n \quad (1\leqslant i<j\leqslant n-2),$$

$$m^\lambda_{n-1,i}:=\lambda_i+\cdots+\lambda_n \quad (1\leqslant i\leqslant n-2).$$

Lemma 5.1: (i) For any $\lambda\in\mathbb{Z}_l^n$ and $\alpha\in\Delta_+$, we have $f_\alpha u(m^\lambda)=0$ in $V(\lambda)$.
(ii) For any $\alpha\in\Delta_+$ and $v\in V(\lambda_{l-1})$, write

$$f_\alpha v = \sum_{m\in M} c_\alpha(m)u(m) \quad in\ V(\lambda_{l-1}) \quad (c_\alpha(m)\in\mathbb{C}).$$

Then $c_\alpha(0)=0$, *i.e., the vector* u_0 *never occurs in* $f_\alpha v$.

Proof: We only show for $\mathfrak{g}=\mathsf{sp}(2n,\mathbb{C})$. The other cases are shown similarly. By Proposition 2.6, $f_\alpha\in U_\varepsilon^-\cap(U_\varepsilon)_\alpha$. So, it is enough to prove the case of $\alpha=\alpha_j(j\in I)$.

(i) For any $1\leqslant i<j\leqslant n-2$, by (3.9) and (5.1),

$$\begin{aligned}\nu_{i,j}^{m_\lambda} &= -m_{i,j-1}^\lambda + 2m_{i,j}^\lambda - m_{i,j+1}^\lambda - m_{j+2,i}^\lambda + 2m_{j+1,i}^\lambda - m_{j,i}^\lambda\\ &= (m_{i,j}^\lambda - m_{i,j-1}^\lambda) - (m_{i,j+1}^\lambda - m_{i,j}^\lambda) + (m_{j+1,i}^\lambda - m_{j+2,i}^\lambda) - (m_{j,i}^\lambda - m_{j+1,i}^\lambda)\\ &= \lambda_j - \lambda_{j+1} + \lambda_{j+1} - \lambda_j = 0.\end{aligned}$$

Similarly, we obtain

$$\nu_{i,n-1}^{m_\lambda} = 0 \quad (1\leqslant i\leqslant n-2), \quad \nu_{i,n}^{m_\lambda} = 0 \quad (1\leqslant i\leqslant n-1).$$

Furthermore, for any $1\leqslant i\leqslant n-2$,

$$\begin{aligned}\nu_{j,j}^{m_\lambda} &= 2m_{j,j}^\lambda - m_{j,j+1}^\lambda - m_{j+1,j+1}^\lambda - m_{j+2,j}^\lambda + 2m_{j+1,j}^\lambda - m_{j+2,j+1}^\lambda\\ &= 2\lambda_j - (\lambda_j+\lambda_{j+1}) - \lambda_{j+1} - (\lambda_j+\lambda_{j+1}+2\lambda_{j+2}+\cdots 2\lambda_n) + 2(\lambda_j+2\lambda_{j+1}+2\lambda_{j+2}+\cdots 2\lambda_n)\\ &\quad - (\lambda_{j+1}+2\lambda_{j+2}+\cdots 2\lambda_n) = 2\lambda_j\end{aligned}$$

Similarly, we obtain

$$\nu_{n-1,n-1}^{m_\lambda} = 2\lambda_{n-1}, \quad \nu_{n,n}^{m_\lambda} = 2\lambda_n.$$

Thus, it follows from (3.8) that for any $1\leqslant i,j\leqslant n$,

$$\mu_{i,j}^{m^\lambda} = \sum_{k=i}^{j} \nu_{k,j}^{m^\lambda} = \nu_{j,j}^{m^\lambda} = 2\lambda_j.$$

Hence, for any $1\leqslant i<j\leqslant n-2$, by (3.10),

$$\begin{aligned}\eta_{i,j}^{m^\lambda} + \mu_{i+1,j}^{m^\lambda} - \lambda_j &= -(m_{i,j+1}^\lambda - m_{i,j}^\lambda) + (m_{j+1,i}^\lambda - m_{j+2,i}^\lambda) - (m_{j,i}^\lambda - m_{j+1,i}^\lambda) + \lambda_j\\ &= -\lambda_{j+1} + \lambda_{j+1} - \lambda_j + \lambda_j = 0,\end{aligned}$$

$$\eta_{j+1,i}^{m^\lambda} + \mu_{i+1,j}^{m^\lambda} - \lambda_j = -(m_{j,i}^\lambda - m_{j+1,i}^\lambda) + \lambda_j = -\lambda_j + \lambda_j = 0,$$

$$\begin{aligned}\eta_{j,j}^{m^\lambda} - \lambda_j &= m_{j,j}^\lambda - m_{j,j+1}^\lambda - m_{j+1,j+1}^\lambda + (m_{j+1,j}^\lambda - m_{j+2,j}^\lambda) + (m_{j+1,j}^\lambda - m_{j+2,j+1}^\lambda) - \lambda_j\\ &= \lambda_j - (\lambda_j+\lambda_{j+1}) - \lambda_{j+1} + \lambda_{j+1} + (\lambda_j+\lambda_{j+1}) - \lambda_j = 0,\end{aligned}$$

$$\eta_{j+1,j}^{m^\lambda} - \lambda_j = -m_{j+1,j+1}^\lambda + (m_{j+1,j}^\lambda - m_{j+2,j+1}^\lambda) - \lambda_j = -\lambda_{j+1} + (\lambda_j+\lambda_{j+1}) - \lambda_j = 0.$$

So, $f_j u(m^\lambda)=0$ in $V(\lambda)(1\leqslant j\leqslant n-2)$. Similarly, we obtain $f_{n-1}u(m^\lambda)=f_n u(m^\lambda)=0$.

(ii) Let $\lambda\in\mathbb{Z}_l^n$. Since for any $1\leqslant i<j\leqslant n-2, m_{i,j}$ does not appear in $\mu_{i+1,j}^m$ and $(i,j)\neq(i,j+1),(j+2,i),(j+1,i),(j,i)$, for any $c(m)\in\mathbb{C}$, we have

$$\sum_{m\in M} c(m)[\eta_{i,j}^m + \mu_{i+1,j}^m - \lambda_j] = \sum_{m\in M} c(m)[m_{i,j} - m_{i,j+1} - m_{j+2,i} + 2m_{j+1,i} - m_{j,i} + \mu_{i+1,j}^m - \lambda_j]u(m+\epsilon_{i,j})$$
$$= \sum_{m\in M} c(m-\epsilon_{i,j})[(m_{i,j}-1) - m_{i,j+1} - m_{j+2,i} + 2m_{j+1,i} - m_{j,i} + \mu_{i+1,j}^m - \lambda_j]u(m).$$

By (3.8) and (3.9), if $m\equiv 0$, we have $\mu_{i+1,j}^m=0$. Thus, we obtain that the coefficient of u_0 is equal to

$$c(-\epsilon_{i,j})[-1-\lambda_j].$$

Hence, if $\lambda=\lambda_{l-1}$, then this is 0. Similarly, we obtain that the coefficient of u_0 in $f_j v$ is equal to $c[-\lambda_j-1]$ (for some $c\in\mathbb{C}$). So, if $\lambda=\lambda_{l-1}$, then it is equal to 0. □

Lemma 5.2: We have $f_\alpha^l u_0=0$ in $V(\lambda_{l-1})$ for any $\alpha\in\Delta_+$.

Proof: By Proposition 2.7, for any $\alpha\in\Delta_+, f_\alpha^l$ is a central element of U_ε. Thus,

$$e_i(f_\alpha^l u_0) = f_\alpha^l(e_i u_0) = 0 \quad (i\in I).$$

So, $f_\alpha^l u_0$ is a primitive vector. Therefore, by the uniqueness of primitive vector (see Proposition 3.4), $f_\alpha^l u_0\in\mathbb{C}u_0$. On the other hand, by Lemma 5.1(ii), the coefficient of u_0 in $f_\alpha^l u_0$ is 0. Hence $f_\alpha^l u_0=0$. □

B. Proof of $e_\alpha^l=0$ on $V(\lambda)$

Definition 5.3: Let $\lambda=(\lambda_1,\ldots,\lambda_n)\in\mathbb{Z}_l^n, I_\lambda$ be the left ideal of U_ε generated by $\{e_i, t_i-\varepsilon_i^{\lambda_i}, f_\alpha^l | i\in I, \alpha\in\Delta_+\}$. We set $M(\lambda):=U_\varepsilon/I_\lambda$.

Proposition 5.4 (Ref. 3, Proposition 3.2, Corollary 3.2(b)):

(i) *If $\lambda=\lambda_{l-1}$, then $M(\lambda)$ is an irreducible U_ε-module.*

(ii) *For any $\lambda\in\mathbb{Z}_l^n, dimM(\lambda)=l^{n^2}$ $(=dimV(\lambda))$.*

Proposition 5.5: If $\lambda=\lambda_{l-1}$, then $M(\lambda)\cong V(\lambda)$ (as U_ε-module).

Proof: By Lemma 5.2 and the property of u_0, we have

$$e_i u_0 = 0, \quad t_i u_0 = \varepsilon_i^{\lambda_i} u_0, \quad f_\alpha^l u_0 = 0 \quad (i\in I, \alpha\in\Delta_+).$$

So, by the universality of $M(\lambda)$, there exists an U_ε-module homomorphism $\phi: M(\lambda)\to V(\lambda)$ such that $\phi(1+I_\lambda)=u_0$. By Proposition 5.4(i), $M(\lambda)$ is an irreducible U_ε-module if $\lambda=\lambda_{l-1}$, and $\phi\not\equiv 0$. Hence ϕ is injective.

On the other hand, by Proposition 5.4(ii), $\dim M(\lambda)=\dim V(\lambda)$. Thus ϕ is surjective. Therefore ϕ is an isomorphism of U_ε-module. □

Lemma 5.6: For any $\lambda\in\mathbb{Z}_l^n$ and $\alpha\in\Delta_+, e_\alpha^l=0$ on $V(\lambda)$.

Proof: By Proposition 5.5 and Proposition 5.4(i), $V(\lambda_{l-1})$ is an irreducible U_ε-module and then we have $U_\varepsilon u_0=V(\lambda_{l-1})$. Thus,

$$e_\alpha^l V(\lambda_{l-1}) = e_\alpha^l(U_\varepsilon u_0) = U_\varepsilon(e_\alpha^l u_0) = \{0\}.$$

Hence $e_\alpha^l=0$ on $V(\lambda_{l-1})$. Due to (3.2) and (3.3), we know that the action of e_i on $V(\lambda)$ does not depend on λ. Therefore, for any $\lambda\in\mathbb{Z}_l^n, e_\alpha^l=0$ on $V(\lambda)$. □

C. General case

Lemma 5.7: For any $\lambda\in\mathbb{Z}_l^n$ and $v\in V(\lambda)(v\neq 0)$, there exists $u^+\in U_\varepsilon^+$ such that $u^+v=u_0$.

Proof: By Lemma 5.6, we can regard $V(\lambda)$ as a $(U_\varepsilon^{\mathrm{fin}})^+$-module (see proof of Lemma 4.8). So, by the similar manner to the proof of Theorem 4.10(ii), we can take $u^+\in U_\varepsilon^+$ such that u^+v is a nonzero primitive vector. Therefore, by the uniqueness of the primitive vector, we have $u^+v\in\mathbb{C}^\times u_0$. □

Proof of Lemma 4.9(iii): Let us show that for any $\lambda \in \mathbb{Z}_l^n$ and $\alpha \in \Delta_+, f_\alpha^l u_0 = 0$ in $V(\lambda)$. By Lemma 5.7, there exists $u^+ \in U_\varepsilon^+$ such that $u^+ u(m^\lambda) = u_0$. Since $f_\alpha u(m^\lambda) = 0$, by Lemma 5.1(i), we obtain

$$f_\alpha^l u_0 = f_\alpha^l (u^+ u(m^\lambda)) = u^+ (f_\alpha^l u(m^\lambda)) = 0.$$

□

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Discrete and continuous cosine transform generalized to Lie groups SU(3) and G(2)

J. Patera[a] and A. Zaratsyan[b]
Centre de Recherches Mathématiques, Université de Montréal, C.P. 6128 Succ. Centre-ville, Montréal, Québec H3C 3J7, Canada

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In the paper we complete the development and description of the four variants of two-dimensional generalization of the cosine transform started in [Patera and Zaratsyan, J. Math Phys. **46**, 053514 (2005)]. Each variant is based on a compact semisimple Lie group G of rank 2. Here, the groups are SU(3) and G(2). The cosines are generalized as the corresponding C-functions of the Lie group. A C-function is the contribution to an irreducible character from one orbit of the appropriate Weyl group. An explicit description is provided for expansions of functions given on the fundamental region F of the two compact simple Lie groups into series of C-functions. The fundamental region F is an equilateral triangle for SU(3) and half of such a triangle for G(2). Expansion coefficients are calculated using orthogonality of C-functions on F. Discrete expansions are set up on a grid $F_M \subset F$. The grid is defined group theoretically for all positive integers M. It consists of points in F that represent conjugacy classes of elements of the finite maximal Abelian subgroup of G generated by its elements of order M. The C-functions are orthogonal on such a grid; hence, coefficients of discrete expansions are calculated independently of the continuous expansions. Processing digital data, sampled on triangular lattices, is the motivating application here. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2109707]

I. INTRODUCTION

This is the second of a series of three articles.[1,2] In this paper we complete our consideration of the four versions of generalization of cosine transform (discrete and continuous ones), each based on one semisimple compact Lie group of rank 2. The third paper of the series is devoted to two-dimensional discrete and continuous generalizations of the sine transform for the four groups.

In the first paper,[1] the cases of the group $SU(2) \times SU(2)$ and O(5) or Sp(4) were considered. Traditional cosine transform would be the discrete version of our SU(2) case. It was discovered some 30 years ago and has been extensively used ever since. Its straightforward generalization to two dimensions is, in our notation, the case of $A_1 \times A_1$ [equivalently, $SU(2) \times SU(2)$]; see Refs. [3,4]. The O(5) case is apparently not found elsewhere in the literature other than in Ref. 1. We use Lie algebraic notation for the cases, respectively, $A_1 \times A_1$ and C_2. The two cases have in common the fact that the discrete transforms are played on square lattices.

In the present paper, the cases of SU(3) and G(2) groups are considered in an analogous way. Equivalently, we call the cases A_2 and G_2. Here, the discrete transforms exploit triangular lattices.

For general comments, motivation, and additional remarks, as well as for uniform description of the four cases, we refer the reader to Ref. 1. Also, the rank 1 case of SU(2) group (equivalently A_1) is found there, as well as in Ref. 5.

[a]Electronic mail: patera@crm.umontreal.ca
[b]Electronic mail: zaratsyan@crm.umontreal.ca

The discrete general version of the method was laid down in Ref. 6. Subsequently, it was used to solve some challenging eight-dimensional decomposition problems.[7–9] Most recently, two of the discrete lowest cases were described in Ref. 10. The continuous version of the method was apparently ignored in the literature until Ref. 1.

Useful properties of the continuous extensions of the discrete method were noticed in Ref. 5 and further exploited in Refs. 11, 1, and 12, as well as here.

Lattices in physics are often taken as computationally manageable models of a continuous space. Increasing density of lattice points, one often rightfully expects to approach the continuous reality. In doing that, it hardly matters what type of lattice one chooses, the square one usually being easier to deal with. However, there are problems where such choice is not available. Indeed, recognition of the need to work on triangular lattices is not new (cf. Ref. 13). As a specific argument, one may point to the analysis of data from existing major installations of hexagonal batteries of particle counters in high-energy experimental astrophysics and/or particle physics.[11]

The method we describe here is a versatile approach to the treatment of such data, which has been mostly unexplored so far, although it originates in the general case of Ref. 6. Apparently, the first exploitation of the case A_2 [equivalently SU(3)] is quite recent.[10–12] The G(2) case is not found in the literature. One of our objectives is to make our approach as ready to use as possible also for triangular lattices.

Finally, let us point out some notations used throughout the paper. The symbols $\mathbb{R}$, $\mathbb{Z}$, and $\mathbb{N}$ denote real numbers, integers, and positive integers, respectively. The scalar product of $a,b \in \mathbb{R}^2$ in a real Euclidean space $\mathbb{R}^2$ of dimension 2 is denoted by $\langle a|b\rangle$. We denote the Hermitian product of class functions in the functional space spanned by irreducible characters (or C-functions) in a similar way. We will frequently refer to equations already given in Ref. 1, and therefore not repeated here. When we need to make such a reference, we use a notation [paper, (equation)]. For example, [1, (4.8)] is a reference to Eq. (4.8) of Ref. 1. In general, this paper should be read with Ref. 1 at hand.

In the following sections we consider the expansion of class functions on the two compact Lie groups of rank two in terms of their C-functions, and the inversion of such expansions. In both cases triangular lattices of weights and roots are involved. For more about our goal in general, as well as for more technical details, see Refs. 1, Secs. II–IV. Since similar applications of C-functions are very recent[14,15,5,11,12] for A_2 and are apparently nowhere to be found for G_2, we describe also other properties of C-functions, which do not serve our immediate goals.

Secs. II and III of this paper contain, respectively, all the details for exploitation of the method for the cases A_2 and G_2. Discretization of these cases is the subject of Sec. IV. Some motivating examples are shown in Sec. V, and concluding remarks and related problems are brought forward in Sec. VI.

II. THE CONTINUOUS CASE OF A_2

A. Root and weight lattices

All roots of A_2 are of the same length. The two simple roots with the relative angle 120° between them are given by the scalar products in $\mathbb{R}^2$:

$$\langle \alpha_1|\alpha_2\rangle = -1, \quad \langle \alpha_1|\alpha_1\rangle = \langle \alpha_2|\alpha_2\rangle = 2.$$

Consequently, the A_2 Cartan matrix and its inverse are the following:

$$C = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}, \quad C^{-1} = \frac{1}{3}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}.$$

The α- and ω-bases are defined through

$$\langle \alpha_j|\omega_k\rangle = \delta_{j,k}, \quad \text{where } j,k = 1,2,$$

which amounts to the explicit relations

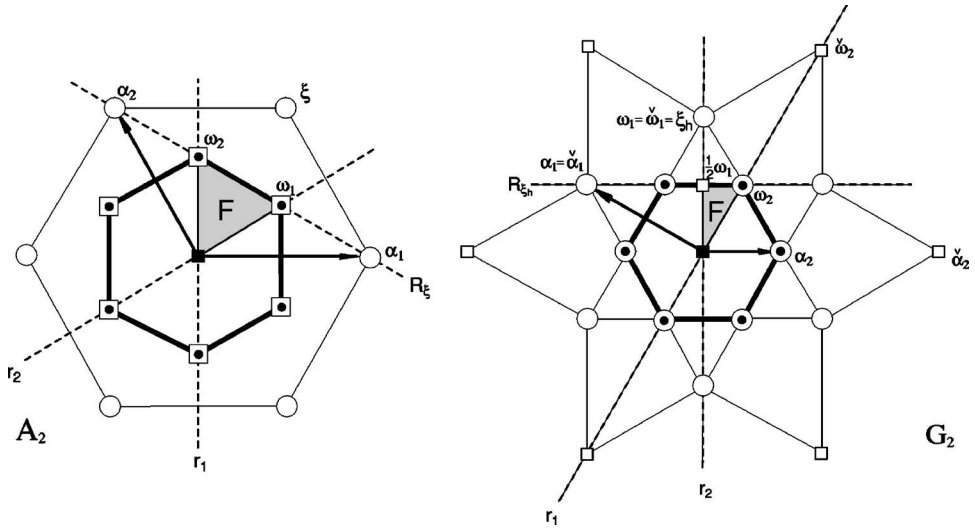

FIG. 1. The simple roots, the fundamental weights, along with their duals, and the fundamental region for the cases A_2 and G_2. The thick line hexagon encloses the proximity cell to origin of the dual root lattice in each case.

$$\alpha_1 = 2\omega_1 - \omega_2, \quad \omega_1 = \frac{1}{3}(2\alpha_1 + \alpha_2),$$

$$\alpha_2 = -\omega_2 + 2\omega_2, \quad \omega_2 = \frac{1}{3}(\alpha_1 + 2\alpha_2).$$

The root system $\Delta = \{\pm(\alpha_1+\alpha_2), \pm\alpha_1, \pm\alpha_2\}$ geometrically represents vertices of a regular hexagon. The highest root $\xi_h = \alpha_1 + \alpha_2$ (see Fig. 1).

The weight lattice P consists of three copies of the root lattice Q shifted relative to each other. Both P and Q are triangular. One has

$$P = Q \cup (Q + \omega_1) \cup (Q + \omega_2).$$

By P^+ one denotes the "positive chamber" of P, containing all the points $a\omega_1 + b\omega_2$ with $a, b \in \mathbb{Z}^{\geq 0}$.

B. Fundamental region

The fundamental region of A_2 is an equilateral triangle with vertices in 0, ω_1, and ω_2, as shown in Fig. 1. Equivalently

$$F = \{x\omega_1 + y\omega_2 \mid 0 \leqslant x, y \text{ and } x + y \leqslant 1\}.$$

Each of its sides is orthogonal either to α_1 or α_2, or to the highest root $\xi_h = \alpha_1 + \alpha_2$ (see Fig. 1).

C. Weyl group orbits of A_2

Set $\lambda = a\omega_1 + b\omega_2 = (a, b) \in P^+$. Then, A_2-Weyl group orbit $W_\lambda \equiv W_{(a,b)}$ consists of either 1, 3, or 6 points generated from λ by repeated action of the reflections r_1 and r_2, according to: [1, (4.4)]

$$W_{(a,b)} = \begin{cases} \{(0,0)\}, & \text{if } a=b=0, \\ \{(a,0),(-a,a),(0,-a)\}, & \text{if } a\neq 0 \text{ and } b=0, \\ \{(0,b),(b,-b),(-b,0)\}, & \text{if } a=0 \text{ and } b\neq 0, \\ \{(a,b),(-a,a+b),(a+b,-b),(-b,-a),(b,-a-b),(-a-b,a)\}, & \text{if } a,b\neq 0. \end{cases}$$

Each weight/point of P belongs to precisely one W-orbit.

D. C-functions of A_2

C-functions $\Omega_{(a,b)}(x,y)$, with $\lambda=a\omega_1+b\omega_2\in P^+$ and $z=x\omega_1+y\omega_2\in\mathbb{R}^2$, are defined in [1, (4.7)] In the A_2-case they are in general complex valued. Only for $a=b$ they are real

$$\begin{aligned} \Omega_{(0,0)}(x,y) &= 1, \\ \Omega_{(a,0)}(x,y) &= e^{(2\pi i/3)(2x+y)a} + e^{(2\pi i/3)(y-x)a} + e^{-(2\pi i/3)(x+2y)a}, \\ \Omega_{(0,b)}(x,y) &= e^{-(2\pi i/3)(2x+y)b} + e^{(2\pi i/3)(x-y)b} + e^{(2\pi i/3)(x+2y)b}, \\ \Omega_{(a,b)}(x,y) &= e^{(2\pi i/3)((2a+b)x+(a+2b)y)} + e^{(2\pi i/3)((b-a)x+(a+2b)y)} + e^{(2\pi i/3)((2a+b)x+(a-b)y)} \\ &\quad + e^{-(2\pi i/3)((a-b)x+(b+2a)y)} + e^{-(2\pi i/3)((a+2b)x+(b-a)y)} + e^{-(2\pi i/3)((2b+a)x+(b+2a)y)}, \\ \Omega_{(a,a)}(x,y) &= 2\cos(2\pi ax) + 2\cos(2\pi ay) + 2\cos(2\pi a(x+y)), \end{aligned} \tag{2.1}$$

assuming that $0<a,b\in\mathbb{Z}$ and $x,y\in\mathbb{R}$.

In Ref. 1 we introduced a convenient normalization of C-functions, which simplifies the calculations. The normalized C-functions, as defined in [1, (4.8)], are given for the case A_2 for all $a,b\in\mathbb{Z}^{\geq 0}$ in one expression

$$\begin{aligned} \Phi_{(a,b)}(x,y) &= e^{(2\pi i/3)((2a+b)x+(a+2b)y)} + e^{(2\pi i/3)((b-a)x+(a+2b)y)} + e^{(2\pi i/3)((2a+b)x+(a-b)y)} \\ &\quad + e^{-(2\pi i/3)((a-b)x+(b+2a)y)} + e^{-(2\pi i/3)((a+2b)x+(b-a)y)} + e^{-(2\pi i/3)((2b+a)x+(b+2a)y)}. \end{aligned} \tag{2.2}$$

E. Decomposition of products of C-functions

Products of C-functions are decomposable into finite sums of C-functions

$$\begin{aligned} \Omega_{(1,0)}\Omega_{(1,0)} &= \Omega_{(2,0)} + 2\Omega_{(0,1)}, \\ \Omega_{(1,0)}\Omega_{(0,1)} &= \Omega_{(1,1)} + 3\Omega_{(0,0)}, \\ \Omega_{(1,1)}\Omega_{(1,1)} &= \Omega_{(2,2)} + 2\Omega_{(0,3)} + 2\Omega_{(3,0)} + 2\Omega_{(1,1)} + 6\Omega_{(0,0)}, \\ &\vdots \end{aligned}$$

In general,

$$\Omega_{(a,b)}\Omega_{(c,d)} = \Omega_{(a+c,b+d)} + \cdots + \Omega_{(a-d,b-c)}.$$

The weight $(a-d,b-c)$ may not be from P^+. Nevertheless, it belongs to just one C-function. Hence, it can be used to label the C-function.

It is possible to build up recursively the C-functions of A_2, starting from the three lowest ones: $\Omega_{(1,0)}$, $\Omega_{(0,1)}$, and $\Omega_{(0,0)}=1$.

F. Weyl group symmetries of C-functions of A_2

The affine Weyl group W^{aff}, generated by the reflections $r_1 \equiv r_{\alpha_1}$, $r_2 \equiv r_{\alpha_2}$, and $R_{N\xi} \equiv R_{N(\alpha_1+\alpha_2)}$, describes the symmetries of C-functions

$$\Omega_\lambda(r_1 z) \equiv \Omega_{(a,b)}(r_1(x\omega_1 + y\omega_2)) = \Omega_{(a,b)}((-x\omega_1 + (x+y)\omega_2\ ),$$

$$\Omega_\lambda(r_2 z) \equiv \Omega_{(a,b)}(r_2(x\omega_1 + y\omega_2)) = \Omega_{(a,b)}((x+y)\omega_1 - y\omega_2), \tag{2.3}$$

$$\Omega_\lambda(R_{N\xi} z) \equiv \Omega_{(a,b)}(R_{N\xi}(x\omega_1 + y\omega_2)) = \Omega_{(a,b)}((N-y)\omega_1 + (N-x)\omega_2).$$

G. Laplace operator

Direct calculation verifies that $\Omega_\lambda(z)$ is an eigenfunction of the Laplace operator L

$$\begin{aligned} L\Omega_\lambda(z) &\overset{\text{def}}{=} (\alpha_1\partial_x + \alpha_2\partial_y)^2\Omega_\lambda(z) = 2(\partial_{xx} - \partial_{xy} + \partial_{yy})\Omega_\lambda(z) \\ &= -4\pi\langle\lambda|\lambda\rangle\Omega_\lambda(z) = -\frac{8\pi}{3}(a^2 + ab + b^2)\Omega_\lambda(z), \end{aligned} \tag{2.4}$$

where $z = x\omega_1 + y\omega_2$ and $\lambda = a\omega_1 + b\omega_2$.

As a consequence of (2.3), C-functions satisfy the Neumann condition at the boundary of F, i.e., their normal derivatives vanish.

H. Orthogonality of C-functions of A_2

The C-functions are orthogonal when integrated over the fundamental region F of A_2

$$\begin{aligned} \int_F \Omega_{(a,b)}(x,y)\overline{\Omega_{(c,d)}(x,y)}\mathrm{d}F &= \frac{1}{\sqrt{3}}\int_0^1 \mathrm{d}x \int_0^{1-x} \Omega_{(a,b)}(x,y)\Omega_{(d,c)}(x,y)\mathrm{d}y \\ &= \begin{cases} 0, & \text{if } a \neq c \text{ or } b \neq d, \\ \dfrac{1}{2\sqrt{3}}, & \text{if } a = b = c = d = 0, \\ \dfrac{\sqrt{3}}{2}, & \text{if } a = c > 0 \text{ and } b = d = 0, \\ & \text{or } a = c = 0 \text{ and } b = d > 0, \\ \sqrt{3}, & \text{if } a = c > 0 \text{ and } b = d > 0. \end{cases} \end{aligned} \tag{2.5}$$

In the case of A_2, the complex conjugation, denoted here by an overbar, is also achieved by interchange of the subscripts, $\Omega_{(d,c)}(x,y) = \overline{\Omega_{(c,d)}(x,y)}$.

Note the special case (2.5), namely $c = d = 0$ and $a + b \neq 0$

$$\int_F \Omega_{(a,b)}(x,y)\mathrm{d}F = \frac{1}{\sqrt{3}}\int_0^1 \mathrm{d}x \int_0^{1-x} \Omega_{(a,b)}(x,y)\mathrm{d}y = 0. \tag{2.6}$$

I. Decomposition of class functions

Finally, a decomposition

$$f(x,y) = \sum_{\lambda \in P^+} a_\lambda \Omega_\lambda(x,y),$$

can be inverted using (2.5), i.e., expansion coefficients a_λ can be found

$$a_\lambda = \frac{1}{\langle \Omega_\lambda | \Omega_\lambda \rangle} \int_F f(x,y) \overline{\Omega_\lambda(x,y)} \mathrm{d}x\, \mathrm{d}y,$$

with the scalar product of orbit functions, already defined in Ref. 1

$$\langle \Omega_\lambda | \Omega_\lambda \rangle = \int_F \Omega_\lambda(x,y) \overline{\Omega_\lambda(x,y)} \mathrm{d}x\, \mathrm{d}y.$$

J. Branching rules for C-functions of A_2

Reduction of C-functions with respect to a subgroup of the same rank is achieved by a corresponding change of basis and by subsequently rearranging the exponential functions according to *W*-orbits of the subgroup. In general, a C-function of the group splits into a sum of C-functions of the subgroup. The splitting is called the branching rule.

There is only one subgroup of rank 2 in A_2, namely $U_1 \times A_1$. General structure of its C-functions is particularly simple

$$\Omega_\lambda(v) = 2e^{2\pi i m_1 \theta_1} \cos \pi m_2 \theta_2, \quad m_1 \in \mathbb{Z}; \quad m_2 \in \mathbb{Z}^{\geqslant 0}; \quad \theta_1, \theta_2 \in \mathbb{R}.$$

Here, $\lambda = m_1 \nu_1 + m_2 \nu_2$ and $v = \theta_1 \nu_1 + \theta_2 \nu_2$ are given relative to an orthogonal basis $\{\nu_1, \nu_2\}$, where ν_2 is the "ω-basis" of A_1 (compare with [1, (2.2)] and [1, (3.2)]).

An A_2-weight $a\omega_1 + b\omega_2 \equiv (a\ b)$ is transformed into a weight of the subgroup in $\{\nu_1, \nu_2\}$-basis by the matrix multiplication

$$(a \quad b)\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = (a+b \quad a-b).$$

Consequently, the scalar product $\langle \lambda | z \rangle$ is

$$\begin{aligned} \langle \lambda | z \rangle &= \langle (a \quad b) | (x \quad y) \rangle \\ &= \langle (a+b \quad a-b) | (x+y \quad x-y) \rangle = (a+b)(x+y) + (a-b)(x-y) = 2ax + 2by \end{aligned}$$

III. THE CONTINUOUS CASE OF G_2

A. Root and weight lattices

Relative length and angles of the simple roots are given by

$$\langle \alpha_1 | \alpha_2 \rangle = -1, \quad \langle \alpha_1 | \alpha_1 \rangle = 2, \quad \langle \alpha_2 | \alpha_2 \rangle = \frac{2}{3}.$$

The Cartan matrix and its inverse are

$$C = \begin{pmatrix} 2 & -3 \\ -1 & 2 \end{pmatrix}, \quad C^{-1} = \begin{pmatrix} 2 & 3 \\ 1 & 2 \end{pmatrix}.$$

Consequently

$$\alpha_1 = 2\omega_1 - 3\omega_2, \quad \omega_1 = 2\alpha_1 + 3\alpha_2, \quad \check{\alpha}_1 = \alpha_1, \quad \check{\omega}_1 = \omega_1,$$

$$\alpha_2 = -\omega_1 + 2\omega_2, \quad \omega_2 = \alpha_1 + 2\alpha_2, \quad \check{\alpha}_2 = 3\alpha_2, \quad \check{\omega}_2 = 3\omega_2.$$

Note that in this case, $\alpha_1, \alpha_2 \in P$. Hence, the root and weight lattices coincide: $P=Q$.

There are 12 roots in $\Delta(\mathrm{G}_2)$, namely the following:

$$\Delta = \{\pm(2\alpha_1 + 3\alpha_2), \pm(\alpha_1 + 3\alpha_2), \pm(\alpha_1 + 2\alpha_2), \pm(\alpha_1 + \alpha_2), \pm\alpha_1, \pm\alpha_2\}.$$

Geometrically the roots are vertices of a regular hexagonal star (see Fig. 1). The long roots are $\pm\alpha_1$, $\pm(\alpha_1+3\alpha_2)$, and $\pm(2\alpha_1+3\alpha_2)$, and the short roots are $\pm\alpha_2$, $\pm(\alpha_1+\alpha_2)$, and $\pm(\alpha_1+2\alpha_2)$. The highest root of G_2 is $\xi_h=2\alpha_1+3\alpha_2$.

B. Fundamental region

The fundamental region F of G_2 is a triangle with vertices 0, $\frac{1}{2}\check{\omega}_1$, and $\frac{1}{3}\check{\omega}_2$. Geometrically F is half of an equilateral triangle. It is shown in Fig. 1. One has the fundamental region $F(\mathrm{G}_2)$

$$F(\mathrm{G}_2) = \{x\check{\omega}_1 + y\check{\omega}_2 \mid 0 \leqslant x,y; 1 \geqslant 2x + 3y\}.$$

C. Weyl group orbits of G_2

Consider the weight lattice P and its subset P^+ of weights $\mathbb{Z}^{\geqslant 0}\omega_1+\mathbb{Z}^{\geqslant 0}\omega_2$, called dominant chamber. Let

$$\lambda = a\omega_1 + b\omega_2 \equiv (a,b) \in P^+. \tag{3.1}$$

A Weyl group orbit $W_\lambda = W_{(a,b)}$ consists of 1, 6, or 12 weights that are generated by the reflections [1, (4.4)] and therefore are equidistant from the origin

$$W_{(a,b)} = \begin{cases} \{(0,0)\}, & \text{if } a=b=0, \\ \{\pm(a,0), \pm(-a,3a), \pm(2a,-3a)\}, & \text{if } a\neq 0 \text{ and } b=0, \\ \{\pm(0,b), \pm(b,-b), \pm(-b,2b)\}, & \text{if } a=0 \text{ and } b\neq 0, \\ \{\pm(a,b), \pm(-a,3a+b), \pm(a+b,-b) & \\ \pm(2a+b,-3a-b), \pm(-a-b,3a+2b), & \\ \pm(2a+b,-3a-2b)\} & \text{if } a,b\neq 0. \end{cases}$$

In particular, the root system of G_2 is a union of two W-orbits, namely the orbit of long roots with $\lambda=(1,0)$ and the orbit of short roots with $\lambda=(0,1)$

D. C-functions of G_2

In the G_2 case, any C-function with $\lambda=a\omega_1+b\omega_2$ and $z=x\check{\omega}_1+y\check{\omega}_2$ is real because for each weight $\mu \in W_\lambda$ one finds also $-\mu \in W_\lambda$, so that corresponding exponential functions in $\Omega_\lambda(z)$ combine into $2\cos 2\pi\langle\mu|z\rangle$.

$$\Omega_{(0,0)}(x,y) = 1,$$

$$\Omega_{(a,0)}(x,y) = 2\cos(2\pi a(2x+3y)) + 2\cos(2\pi ax) + 2\cos(2\pi a(x+3y)),$$

$$\Omega_{(0,b)}(x,y) = 2\cos(2\pi b(x+y)) + 2\cos(2\pi by) + 2\cos(2\pi b(x+2y)), \tag{3.2}$$

$$\begin{aligned}\Omega_{(a,b)}(x,y) = {} & 2\cos(2\pi((a+b)x+by)) + 2\cos(2\pi(ax+(3a+b)y)) + 2\cos(2\pi((2a+b)x \\ & + (3a+b)y)) + 2\cos(2\pi((2a+b)x+(3a+2b)y)) + 2\cos(2\pi(ax-by)) \\ & + 2\cos(\pi((a+b)x+(3a+2b)y)).\end{aligned}$$

The C-functions, normalized as defined in [1, (4,8)], are given for G_2 for all $a,b \in \mathbb{Z}^{\geqslant 0}$ in one expression

$$\begin{aligned}\Phi_{(a,b)}(x,y) = {} & 2\cos(2\pi((a+b)x+by)) + 2\cos(2\pi(ax+(3a+b)y)) + 2\cos(2\pi((2a+b)x \\ & + (3a+b)y)) + 2\cos(2\pi((2a+b)x+(3a+2b)y)) + 2\cos(2\pi(ax-by)) \\ & + 2\cos(\pi((a+b)x+(3a+2b)y)). \end{aligned} \tag{3.3}$$

E. Weyl group symmetries of C-functions of G_2

The affine Weyl group W^{aff}, generated by the reflections $r_1 \equiv r_{\alpha_1}$, $r_2 \equiv r_{\alpha_2}$, and $R_{N\xi_h} \equiv R_{N(2\alpha_1+3\alpha_2)}$, describes the symmetries of C-functions

$$\Omega_\lambda(r_1 z) \equiv \Omega_{(a,b)}(r_1(x\check{\omega}_1 + y\check{\omega}_2)) = \Omega_{(a,b)}((-x\check{\omega}_1 + (x+y)\check{\omega}_2)\ ,$$

$$\Omega_\lambda(r_2 z) \equiv \Omega_{(a,b)}(r_2(x\check{\omega}_1 + y\check{\omega}_2)) = \Omega_{(a,b)}((x+3y)\check{\omega}_1 - y\check{\omega}_2), \tag{3.4}$$

$$\Omega_\lambda(R_{N\xi_h} z) \equiv \Omega_{(a,b)}(R_{N\xi_h}(x\check{\omega}_1 + y\check{\omega}_2)) = \Omega_{(a,b)}((N-x-3y)\check{\omega}_1 + y\check{\omega}_2).$$

Note that variable z is given relative to a dual basis $\{\check{\omega}_1, \check{\omega}_2\}$. Its lengths are interchanged.

F. Laplace operator

Direct calculation verifies that $\Omega_\lambda(z)$ is an eigenfunction of the Laplace operator L

$$\begin{aligned} L\Omega_\lambda(z) &\overset{\text{def}}{=} (\alpha_1\partial_x + \alpha_2\partial_y)^2\Omega_\lambda(z) = 2\left(\partial_{xx} - \partial_{xy} + \frac{1}{3}\partial_{yy}\right)\Omega_\lambda(z) \\ &= -4\pi\langle\lambda|\lambda\rangle\Omega_\lambda(z) = -8\pi\left(a^2 + ab + \frac{1}{3}b^2\right)\Omega_\lambda, \end{aligned} \tag{3.5}$$

where $z = x\check{\omega}_1 + y\check{\omega}_2$ and $\lambda = a\omega_1 + b\omega_2$. The operator L is positive definite. By a change of variables it can be brought to a sum of second derivative with coefficients of the same sign. That justifies its name.

G. Orthogonality of C-functions of G_2

Orthogonality property of the C-functions in the case of G_2

$$\int_F \Omega_{(a,b)}(x,y)\Omega_{(c,d)}(x,y)\mathrm{d}F = \sqrt{3}\int_0^{1/2} dx \int_0^{1/3-2/3x} \Omega_{(a,b)}(x,y)\Omega_{(c,d)}(x,y)\mathrm{d}y$$
$$= \begin{cases} 0, & \text{if } a \neq c \text{ or } b \neq d, \\ \dfrac{1}{4\sqrt{3}}, & \text{if } a=b=c=d=0, \\ \dfrac{\sqrt{3}}{2}, & \text{if } a=c>0 \text{ and } b=d=0, \\ & \text{or } a=c=0 \text{ and } b=d>0, \\ \sqrt{3}, & \text{if } a=c>0 \text{ and } b=d>0. \end{cases} \tag{3.6}$$

H. Decomposition of products of C-functions of G_2

Since a product of W-orbits is a union of W-orbits, one has a corresponding decomposition of C-functions. Here are some G_2-examples:

$$\Omega_{(0,1)}\Omega_{(0,1)} = \Omega_{(0,2)} + 2\Omega_{(1,0)} + 2\Omega_{(0,1)} + 6\Omega_{(0,0)},$$

$$\Omega_{(1,0)}\Omega_{(0,1)} = \Omega_{(1,1)} + 2\Omega_{(0,2)} + 2\Omega_{(0,1)},$$

$$\Omega_{(1,0)}\Omega_{(1,0)} = \Omega_{(2,0)} + 2\Omega_{(0,3)} + 2\Omega_{(1,0)} + 6\Omega_{(0,0)}.$$

There is a possibility to calculate C-functions one by one by judiciously choosing the sequence of products, starting from the lowest three: $\Omega_{(0,0)}=1$, $\Omega_{(0,1)}$, and $\Omega_{(1,0)}$.

I. Branching rules for C-functions of G_2 to the subgroups $A_1\times A_1$ and A_2

A branching rule is the reduction of a C-function of G_2 to a sum of C-functions of a subgroup. In order to do that, one needs to write any $\lambda \in P(G_2)$ in a basis of P of the subgroups. The transformations are performed as follows, relative to respective ω-bases:

$$(a \quad b)_{G_2}\begin{pmatrix} 1 & 3 \\ 1 & 1 \end{pmatrix} = (a+b \quad 3a+b)_{A_1\times A_1},$$

$$(a \quad b)_{G_2}\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} = (a+b \quad a)_{A_2}.$$

Each C-function of G_2 then splits into C-functions of the subgroup. The following relations describe all the branching rules:

$$G_2 \supset A_1 \times A_1: \quad [\Omega_{(a,0)}(z)]_{G_2} = [\Omega_{(a,3a)} + \Omega_{(2a,0)}]_{A_1\times A_1},$$

$$[\Omega_{(0,b)}(z)]_{G_2} = [\Omega_{(b,b)} + \Omega_{(0,2b)}]_{A_1\times A_1},$$

$$[\Omega_{(a,b)}(z)]_{G_2} = [\Omega_{(2a+b,3a+b)} + \Omega_{(2a+b,b)} + \Omega_{(a,3a+2b)}]_{A_1\times A_1},$$

$$G_2 \supset A_2: \quad [\Omega_{(a,0)}(z)]_{G_2} = [\Omega_{(a,a)}]_{A_2},$$

$$[\Omega_{(0,b)}(z)]_{G_2} = [\Omega_{(b,0)} + \Omega_{(0,b)}]_{A_2},$$

$$[\Omega_{(a,b)}(z)]_{G_2} = [\Omega_{(a+b,a)} + \Omega_{(a,a+b)}]_{A_2}.$$

IV. DISCRETIZATION OF A_2- AND G_2-TRANSFORMS

In this section we specialize the general results of Ref. 6 to A_2 and G_2, and follow it by their continuous extensions. For more information about discretization in the case of rank $n=2$, we refer to Sec. VII of Ref. 1 Here, only a minimum is recalled to make the paper reasonably self-contained.

In general, we proceed as follows. First, we set up a triangular lattice of points of any density. The set of its points in the fundamental region F is denoted F_M. Action of the affine Weyl group W^{aff} on F allows one to tile the entire space $\mathbb{R}^2$ by copies of F. By the same action, F_M is transformed into a lattice in $\mathbb{R}^2$. Density of points in F_M is chosen by fixing a positive integer M. Subsequently, the set F_M is used in two roles: (i) it is the stage on which digital data are given; (ii) it identifies the set S_M of pairwise orthogonal C-functions on F_M.

Second, we consider any function $f(s)$ sampled digitally on the points $s \in F_M$ and its expansion in terms of normalized C-functions

$$f(s) = \sum_{\lambda \in S_M} d_\lambda \Phi_\lambda(s), \quad s \in F_M, \quad M \in \mathbb{Z}^{>0}. \tag{4.1}$$

Expansion (4.1) is inverted using the discrete orthogonality of C-functions

$$\langle \Phi_{(a,b)} | \Phi_{(a',b')} \rangle_M = \sum_{s \in F_M} c_s \Phi_{(a,b)}(s) \overline{\Phi_{(a',b')}(s)} = \delta_{a,a'} \delta_{b,b'} \langle \Phi_{(a,b)} | \Phi_{(a,b)} \rangle_M. \tag{4.2}$$

Thus, we calculate the coefficients d_λ of the expansion according to

$$d_\lambda = \frac{1}{\langle \Phi_\lambda | \Phi_\lambda \rangle_M} \sum_{s \in F_M} c_s f_\lambda(s) \cdot \overline{\Phi_\lambda(s)}. \tag{4.3}$$

Here, c_s and $\langle \Phi_\lambda | \Phi_\lambda \rangle_M$ are constants specific for each Lie group.

Our final step is the continuous extension of (4.1). It is accomplished very simply: the discrete variable $s \in F_M$ is replaced by a continuous one, $z \in F$

$$f(z) = \sum_{\lambda \in S_M} d_\lambda \Phi_\lambda(z), \quad z \in F \subset \mathbb{R}^2. \tag{4.4}$$

Coefficients d_λ and the set S_M remain as in (4.1). Through them, the continuous extension depends on the discrete expansion.

A. Discretization in the case of A_2

The density of points $s \in F_M$ is chosen by fixing a positive integer M. Individual points $s \in F_M$ are given by triplets $s=[s_0,s_1,s_2] \equiv (s_1/M, s_2/M)$ of non-negative integers, which must not be all zero simultaneously and have to satisfy the following A_2-sum rule:

$$M = s_0 + s_1 + s_2 > 0, \quad s_0, s_1, s_2 \in \mathbb{Z}^{\geq 0}. \tag{4.5}$$

All points of $F_M \subset F$ are obtained by letting the three non-negative integers run through all the values compatible with (4.5). Equivalently

$$F_M \overset{\text{def}}{=} \left\{ \frac{s_1}{M}\omega_1 + \frac{s_2}{M}\omega_2 \mid s_0, s_1, s_2 \in \mathbb{Z}^{\geq 0}, \quad s_0 + s_1 + s_2 = M > 0 \right\}. \tag{4.6}$$

For example, the vertices of F belong to F_M for all M in the case of A_2. More precisely, the three vertices are

$$[M,0,0]=(0,0),\quad [0,M,0]=(1,0),\quad [0,0,M]=(0,1),$$

for any positive integer M. Every side of the equilateral triangle F contains $M+1$ equidistant points of F_M. See Fig. 3.

Discrete orthogonality of C-functions (4.2) is valid for a finite number of C-functions. More precisely, C-functions Φ_λ and $\Phi_{\lambda'}$ are orthogonal provided $\lambda,\lambda' \in S_M \subset P^+$, where

$$S_M=\left\{ s_1\omega_1+s_2\omega_2 \,\middle|\, \frac{s_1}{M}\omega_1+\frac{s_2}{M}\omega_2 \in F_M \right\}. \tag{4.7}$$

Coefficients c_s in (4.3) and (4.2) take the following values in the case of A_2:

$$c_s \equiv c_{(s_1/M,s_2/M)}=\begin{cases} 1, & \text{if } s_1=s_2=0,\\ & \text{or } s_1=0 \text{ and } s_2=M,\\ & \text{or } s_1=M \text{ and } s_2=0,\\ 3, & \text{if } s_1=0 \text{ and } 0<s_2<M,\\ & \text{or } s_2=0 \text{ and } 0<s_1<M,\\ & \text{or } s_1,s_2>0 \text{ and } s_1+s_2=M,\\ 6, & \text{if } s_1,s_2>0 \text{ and } s_1+s_2<M. \end{cases} \tag{4.8}$$

From (4.2) we have

$$\langle \Phi_{(a,b)} | \Phi_{(a',b')} \rangle_M = 0, \quad \text{if } a\neq a' \text{ and } b\neq b';$$

otherwise, for the set of the lowest pairwise orthogonal normalized C-functions

$$\langle \Phi_{(a,b)} | \Phi_{(a,b)} \rangle_M = 18M^2 \times \begin{cases} 1, & \text{if } 0<a,b \text{ and } a+b<M,\\ 2, & \text{if } a=0 \text{ and } 0<b<M,\\ & \text{or } 0<a<M \text{ and } b=0,\\ & \text{or } 0<a,b \text{ and } a+b=M,\\ 6, & \text{if } a=b=0,\\ & \text{or } a=0 \text{ and } b=M,\\ & \text{or } a=M \text{ and } b=0, \end{cases} \tag{4.9}$$

with the higher C-functions repeating the values of the lowest ones.

Example. $F_2(A_2)$ consists of the following six points given as $[s_0,s_1,s_2]\equiv(s_1/M,s_2/M)$:

$$F_2=\left\{ [2,0,0]=(0,0),\quad [0,2,0]=(1,0),\quad [0,0,2]=(0,1),\quad [1,1,0]=\left(\tfrac{1}{2},0\right),\right.$$
$$\left. [1,0,1]=\left(0,\tfrac{1}{2}\right),\quad [0,1,1]=\left(\tfrac{1}{2},\tfrac{1}{2}\right) \right\}. \tag{4.10}$$

In Table I the values of several normalized C-functions are shown at the points of $F_2(A_2)$. The first six belong to $S_2(A_2)$. However, a closer inspection reveals the presence of another orthogonal set obtained from $S_2(A_2)$ by affine reflection $R_{(2,2)}$ applied to all its elements. See Fig. 2.

Using the entries of Table I, let us calculate several examples in the discretized A_2-case

$$\langle \Omega_{(2,0)} | \Omega_{(0,0)} \rangle_2 = \langle \Omega_{(0,0)} | \Omega_{(0,2)} \rangle_2 = 3(1+3\eta^4+3\eta^2+\eta^2+3+\eta^4)=0;$$

$$\langle \Omega_{(1,1)} | \Omega_{(1,2)} \rangle_2 = 12(3-\eta^5-\eta+3\eta^4+1+3\eta^2)=0;$$

$$\langle \Omega_{(2,1)} | \Omega_{(2,1)} \rangle_2 = 6\cdot 6+3\cdot 2\eta^5\cdot 2\eta+3\cdot 2\eta\cdot 2\eta^5+6\eta^4\cdot 6\eta^2+3\cdot(-2)\cdot(-2)+6\eta^2\cdot 6\eta^4=144.$$

TABLE I. Values of several normalized C-functions of A_2 at the points of the grid F_2. Note that only the first six C-functions are pairwise orthogonal. The higher ones repeat the values of the lowest six. The c_s are the coefficients from (4.8). Here, $\eta=e^{2\pi i/6}$.

s	(0,0)	$\left(\frac{1}{2},0\right)$	$\left(0,\frac{1}{2}\right)$	(1,0)	$\left(\frac{1}{2},\frac{1}{2}\right)$	(0,1)
$\Phi_{(0,0)}(s)$	6	6	6	6	6	6
$\Phi_{(1,0)}(s)$	6	$2\eta^5$	2η	$6\eta^4$	−2	$6\eta^2$
$\Phi_{(0,1)}(s)$	6	2η	$2\eta^5$	$6\eta^2$	−2	$6\eta^4$
$\Phi_{(2,0)}(s)$	6	$6\eta^4$	$6\eta^2$	$6\eta^2$	6	$6\eta^4$
$\Phi_{(1,1)}(s)$	6	−2	−2	6	−2	6
$\Phi_{(0,2)}(s)$	6	$6\eta^2$	$6\eta^4$	$6\eta^4$	6	$6\eta^2$
$\Phi_{(3,0)}(s)$	6	−2	−2	6	−2	6
$\Phi_{(4,2)}(s)$	6	$6\eta^4$	$6\eta^2$	$6\eta^2$	6	$6\eta^4$
$\Phi_{(1,2)}(s)$	6	2η	$2\eta^5$	$6\eta^2$	−2	$6\eta^4$
$\Phi_{(2,1)}(s)$	6	$2\eta^5$	2η	$6\eta^4$	−2	$6\eta^2$
$\Phi_{(2,2)}(s)$	6	6	6	6	6	6
c_s	1	3	3	1	3	1

The sesquilinear form $\langle f|g\rangle_M$ can be used to multiply any class functions f and g sampled on F_M of A_2. Moreover, dependence of (4.2) on A_2 comes only through F_M, S_M, and the sum rule for M. Otherwise, the discrete orthogonality does not change from one group to another.

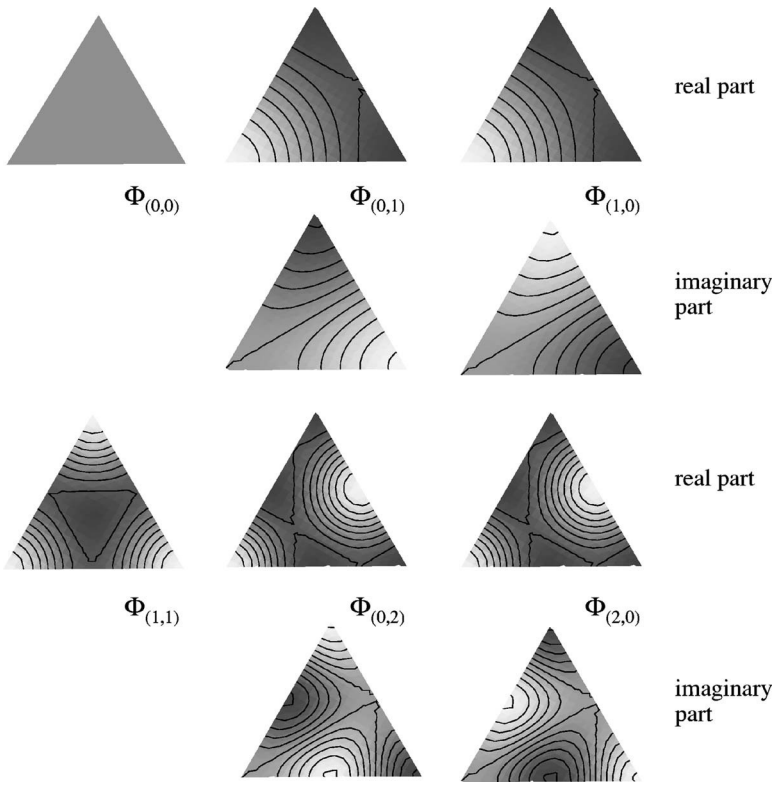

FIG. 2. The set of six lowest normalized C-functions of A_2 which are pairwise orthogonal on the grid F_2.

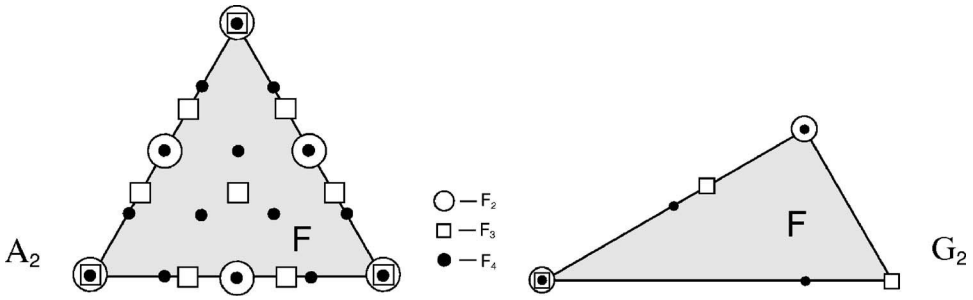

FIG. 3. The lattice points of F_2, F_3, and F_4 on the fundamental region F for A_2 and G_2.

B. Discretization in the case of G_2

Similarly as before, M is the positive integer fixing the density of the discrete points $s \in F_M \subset F$. The fundamental region F is a triangle, half of an equilateral one (see Fig. 1). The G_2 sum rule differs from that of A_2 of (4.5)

$$M = s_0 + 2s_1 + 3s_2 > 0, \quad s_0, s_1, s_2 \in \mathbb{Z}^{\geq 0}. \tag{4.11}$$

It restricts the choice of the triples $[s_0, s_1, s_2]$ to a finite set of possible values. Each triple stands for one point $s \in F_M$, where $s = [s_0, s_1, s_2] \equiv (s_1/M, s_2/M)$. In particular, origin belongs to F_M for any M, while $(1, 0)$ and $(0, 1) \in F_M$ only if M is divisible by 2 and 3, respectively. See Fig. 3.

A few more examples are the sets

$$F_8{:}[6,1,0] = \left(\tfrac{1}{8}, 0\right), \quad [5,0,1] = \left(0, \tfrac{1}{8}\right), \quad [3,1,1] = \left(\tfrac{1}{8}, \tfrac{1}{8}\right), \quad [1,2,1] = \left(\tfrac{1}{4}, \tfrac{1}{8}\right), \quad + \text{points of } F_4;$$

$$F_5{:}[5,0,0] = (0,0), \quad [2,0,1] = \left(0, \tfrac{1}{5}\right), \quad [3,1,0] = \left(\tfrac{1}{5}, 0\right), \quad [0,1,1] = \left(\tfrac{1}{5}, \tfrac{1}{5}\right), \quad [1,2,0] = \left(\tfrac{2}{5}, 0\right);$$

$$F_4{:}[1,0,1] = \left(0, \tfrac{1}{4}\right), \quad [2,1,0] = \left(\tfrac{1}{4}, 0\right), \quad + \text{points of } F_2;$$

$$F_3{:}[3,0,0] = (0,0), \quad [0,0,1] = \left(0, \tfrac{1}{3}\right), \quad [1,1,0] = \left(\tfrac{1}{3}, 0\right).$$

Discrete orthogonality (4.2) holds for the set of C-functions $\Omega_\lambda(z)$ of G_2 with λ in the set (4.7), where M is now given by the sum rule (4.11). The set of pairwise orthogonal C-functions of G_2 is again given by (4.7). Hence, we have (4.1) and (4.3), where coefficients c_s in the G_2 case are the following ones:

$$c_s \equiv c_{(s_1/M, s_2/M)} = \begin{cases} 1, & \text{if } s_1 = s_2 = 0, \\ 2, & \text{if } s_1 = 0 \text{ and } s_2 = \dfrac{M}{3}, \\ 3, & \text{if } s_1 = \dfrac{M}{2} \text{ and } s_2 = 0, \\ 6, & \text{if } s_1 = 0 \text{ and } 0 < s_2 < \dfrac{M}{3}, \\ & \text{or } s_2 = 0 \text{ and } 0 < s_1 < \dfrac{M}{2}, \\ & \text{or } s_1, s_2 > 0 \text{ and } 2s_1 + 3s_2 = M, \\ 12, & \text{if } s_1, s_2 > 0 \text{ and } 2s_1 + 3s_2 < M. \end{cases}$$

The discrete orthogonality is

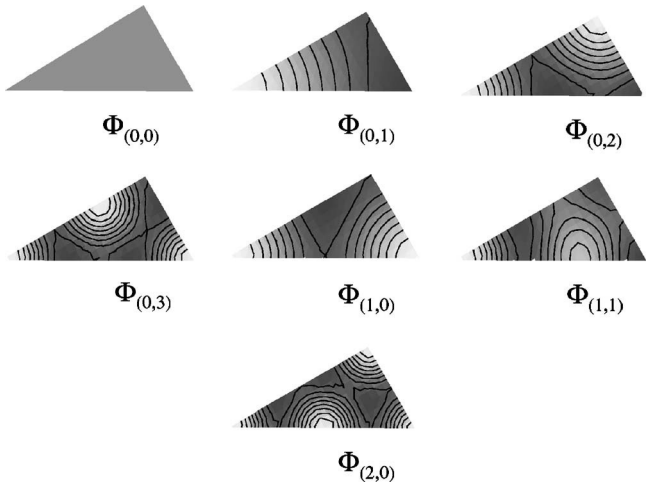

FIG. 4. The set of seven lowest normalized C-functions of G_2 which are pairwise orthogonal on the grid F_6.

$$\langle \Phi_{(a,b)} | \Phi_{(a',b')} \rangle_M = 0, \quad \text{if } a \neq a' \text{ and } b \neq b';$$

otherwise, for the set of the lowest pairwise orthogonal normalized C-functions

$$\langle \Phi_{(a,b)} | \Phi_{(a,b)} \rangle_M = 12M^2 \times \begin{cases} 1, & \text{if } 0 < a,b \text{ and } 3a + 2b < M, \\ 2, & \text{if } a = 0 \text{ and } 0 < b < \dfrac{M}{2}, \\ & \text{or } 0 < a < \dfrac{M}{3} \text{ and } b = 0, \\ & \text{or } 0 < a,b \text{ and } 3a + 2b = M, \\ 4, & \text{if } a = 0 \text{ and } b = \dfrac{M}{2}, \\ 6, & \text{if } a = \dfrac{M}{3} \text{ and } b = 0, \\ 12, & \text{if } a = b = 0, \end{cases} \tag{4.12}$$

with the higher C-functions repeating the values of the lowest ones. See Fig. 4.

V. MOTIVATING EXAMPLES

Comparison of expansions of class functions into series of C-functions of both groups considered here, as well as the two additional groups of Ref. 1, will require further study. Related results/questions are illustrated by the following examples.

There are two examples shown in this section, involving decomposition of the same function $f(x,y)$ into series of C-functions of A_2 and G_2. Goal of the examples is (i) to illustrate discrete decomposition of a given function followed by the continuous extension, and (ii) to compare the continuous extensions in both cases.

In order to make the comparison, we set up the vertices of the two fundamental regions as follows (relative to an orthonormal basis):

$$F(A_2) = \left\{ (0,0), (1,0), \left(\frac{1}{2}, \frac{\sqrt{3}}{2} \right) \right\}, \tag{5.1}$$

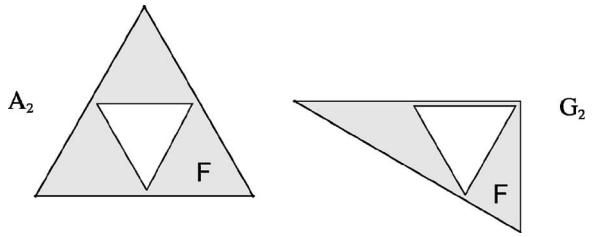

FIG. 5. The triangular step function (5.3) placed in the fundamental regions of A_2 and G_2.

$$F(G_2) = \left\{ \left(-\frac{1}{4}, \frac{\sqrt{3}}{4} \right), \left(\frac{3}{4}, \frac{\sqrt{3}}{4} \right), \left(\frac{3}{4}, \frac{\sqrt{3}-2}{4} \right) \right\}. \tag{5.2}$$

Thus, the area of $F(G_2)$ is exactly half of the area of $F(A_2)$.

We choose for $f(x,y)$ a triangular step function with sharp edges with vertices in $(1/4, \sqrt{3}/4)$, $(3/4, \sqrt{3}/4)$, and $(1/2, 0)$

$$f(x,y) = \begin{cases} 1 & \text{for } (x,y) \in \left\{ \left(\frac{1}{4}, \frac{\sqrt{3}}{4} \right), \left(\frac{3}{4}, \frac{\sqrt{3}}{4} \right), \left(\frac{1}{2}, 0 \right) \right\}, \\ 0 & \text{elsewhere in } F. \end{cases} \tag{5.3}$$

Chosen as such, $f(x,y)$ fits into the fundamental regions F of the two groups as shown in Fig. 5. Furthermore, in order to have the same density of grid points, the orders of the grids are taken with the ratio $M_{G_2} = 2M_{A_2}$. Figure 3 demonstrates the difference of densities of the grids of the same order for the two cases. It also helps to demonstrate the reason of the choice of $f(x,y)$ and its placement into the fundamental region of G_2 in order to ensure a fair comparison of the two cases.

Figures 6 and 7 contain results of our two examples. The values of the function $f(x,y)$ are sampled at the points s of the grids F_M [1, (7.2)] and taken as our digital data $f(s)$. Then, the functions are expanded [1, (7.7)] into C-functions of A_2 and of G_2 on the corresponding grid F_M, i.e., expansion coefficients are calculated [1, (7.8)]. After that, continuous extensions of the discrete expansions of $f(s)$ are made [1, (7.9)] by replacing the C-functions of the discrete argument s in the expansions by the same functions of the continuous argument, while keeping the expansion coefficients unchanged. Each figure shows the function $f_{\text{cont}}(x,y)$ resulting from the continu-

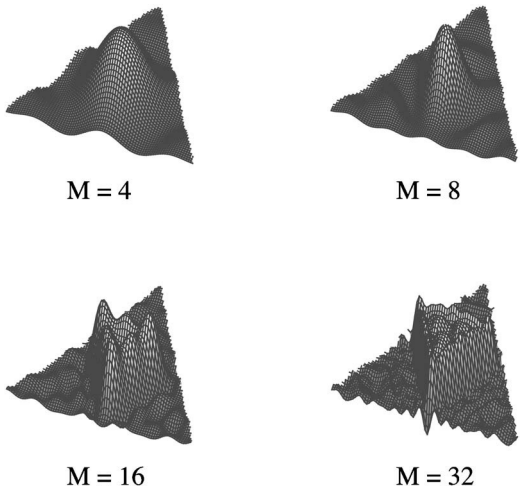

FIG. 6. Decomposition and continuous extension of a triangular step function placed in the fundamental region of A_2 on the grids of orders $M = 4$, 8, 16, and 32.

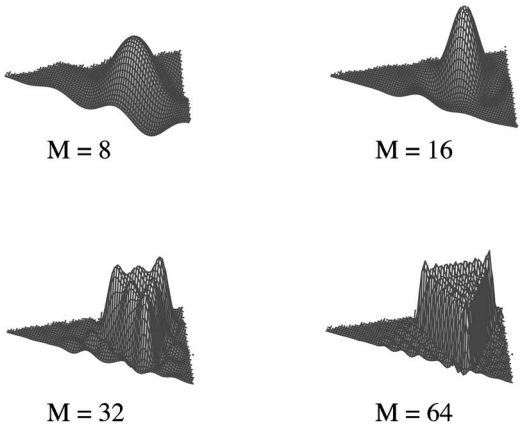

FIG. 7. Decomposition and continuous extension of a triangular step function placed in the fundamental region of G_2 on the grids of orders $M=8$, 16, 32, and 64.

ous extension of discrete expansions. More precisely, four different continuous extensions are shown in each figure. They differ by the densities of the grid F_M, namely $M_{A_2}=4$, 8, 16, 32, and $M_{G_2}=8$, 16, 32, and 64, from which the continuous extension is made. For these values the densities of grid points of A_2 and G_2 in the sample function are the same. The points of the grids are not shown in the figures.

Inspecting and comparing the two results, one readily observes the following:

(i) As in Ref. 1, increasing density of the grid, i.e., increasing the value of M, makes the continuous extension match more closely the given model function $f(x,y)$ of (5.3).

(ii) Quality of the extension, i.e., the match between the continuous extension $f_{\text{cont}}(x,y)$ and the original function $f(x,y)$, is comparable for the same density of the grid in both cases, though G_2 expansion may be slightly superior, as noticeable by comparing the two at $M_{A_2}=32$ and $M_{G_2}=64$.

(iii) The calculations of complex-valued functions in the case of A_2 took a much longer time compared to the case of G_2, which gives G_2 an obvious advantage in the discretization of real-valued functions, while A_2 is more useful for processing complex-valued information.

VI. CONCLUDING REMARKS

A number of concluding comments of Ref. 1 are equally pertinent for us here. In addition to those, we would like to point out the following:

(1) The versatile way of setting up the triangular grid F_M in the fundamental region, and, consequently, a lattice of corresponding symmetry in $\mathbb{R}^2$, should prove useful in other applications where lattices are essential. Note that the density of the lattice is chosen by a single natural number $0<M<\infty$. Also, general results of Ref. 6 allow one to set up a grid F_M and the corresponding lattice in any dimension n, using a semisimple Lie groups of rank n.

(2) Practically the most interesting question that remains is the characterization of functions $f(z)$, $z\in\mathbb{R}^2$, which are most advantageously expanded in C-functions of each of the four groups of rank 2.

(3) In general, one may expect that triangular lattices offer advantages in comparable problems due to their higher density of points. Indeed, given an equal distance between first neighbors, the ratio of densities of points (sphere packing densities) of square and triangular lattices is $1:\sqrt{2}$.

(4) There are other curious properties of C-functions we did not exploit either here or in Ref. 1. For example, the following assertion is valid for any compact semisimple Lie group.
Among the infinity of possible grid points in F, i.e., points with rational coordinates relative

to the ω-basis, there are finitely few, say $z_1, \ldots, z_k$, such that all C-functions take integer values on them

$$\Omega_\lambda(z_j) \in \mathbb{Z} \quad 1 \leqslant j \leqslant k, \quad \text{for all } \lambda \in P^+.$$

Such grid points identify the conjugacy classes of elements of the group G consisting of elements called rational.[16] For rank 2 groups, the rational conjugacy classes were found in Ref. 17.

(5) The last of the concluding remarks in Ref. 1 identifies the C-functions of that paper as two infinite families of orthogonal polynomials in two variables. Similar substitution of variables allows one to interpret the C-functions here as another two families of orthogonal polynomials in two variables. A distinguishing feature of the four families is the structure of their polynomials. Indeed, their degrees grow without limits, but the number of monomials comprising such a polynomial is equal to the order $|W|$ of the corresponding Weyl group or to one of the divisors of $|W|$. More precisely, an $\Omega_{(a,b)}(z)$ is identified as the polynomial consisting of monomials with degrees varying between $a+b$ and $-a-b$. The number of terms in such a polynomial is equal to $|W|$ precisely if $a \neq 0$ and $b \neq 0$. Recall that $|W|=4,6,8,12$, respectively, for $A_1 \times A_1$, A_2, C_2, and G_2.

(6) A systematic comparison of the quality and computational efficiency of continuous extensions, as described here and in Ref. 1 with the current methods of interpolation of digital data (for example, Refs. 18 and 19) is of considerable practical interest, but it is outside of the scope of this series of papers.

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Ergodic property of Markovian semigroups on standard forms of von Neumann algebras

Yong Moon Park[a)]
Department of Mathematics, Yonsei University, Seoul 120-749, Korea

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We give sufficient conditions for ergodicity of the Markovian semigroups associated to Dirichlet forms on standard forms of von Neumann algebras constructed by the method proposed by Park. We apply our result to show that the diffusion type Markovian semigroups for quantum spin systems are ergodic in the region of high temperatures where the uniqueness of the KMS state holds. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2113067]

I. INTRODUCTION

The purpose of this work is to investigate ergodic property of the Markovian semigroups associated to Dirichlet forms on the standard form of a von Neumann algebra[1,2] $\mathcal{M}$ acting on a Hilbert space $\mathcal{H}$ with a cyclic and separating vector ξ_0. Denote by $\sigma_t, t \in \mathbb{R}$, the modular automorphism on $\mathcal{M}$ associated with the pair $(\mathcal{M}, \xi_0)$ and $\mathcal{M}_{1/2}$ the dense subset of $\mathcal{M}$ consisting of every σ_t-analytic element on a domain containing the strip $\{z \in \mathbb{C}: |\mathrm{Im}\, z| \leqslant 1/2\}$.[3] Let $\{x_k : k \in I\}$ be a (finite or countable) family of elements in $\mathcal{M}_{1/2}$ which generates $\mathcal{M}$. Let $(\mathcal{E}, D(\mathcal{E}))$ be the Dirichlet form constructed with $\{x_k : k \in I\}$ and an admissible function by means of Refs. 1 and 2. For the details, see Sec. II. Denote by $T_t, t \geqslant 0$, the Markovian semigroup associated to $(\mathcal{E}, D(\mathcal{E}))$. Let $\mathcal{N}$ be the fixed point space of T_t,

$$\mathcal{N} = \{\eta \in \mathcal{H} : T_t \eta = \eta, \forall\, t \geqslant 0\}.$$

We show that $\mathcal{N} = [\mathcal{Z}(\mathcal{M})\xi_0]$, where $\mathcal{Z}(\mathcal{M})$ is the center of $\mathcal{M}$; $\mathcal{Z}(\mathcal{M}) = \mathcal{M} \cap \mathcal{M}'$, and $[\mathcal{Z}(\mathcal{M})\xi_0]$ is the closure of $\mathcal{Z}(\mathcal{M})\xi_0$. As a consequence, T_t is ergodic if and only if $\mathcal{M}$ is a factor. We apply our result to the translation invariant Markovian semigroups for quantum spin systems,[1] and show that the semigroups are ergodic in the region of high temperatures where the uniqueness of the KMS state holds.

Let us describe the background of this study briefly. The need to construct Markovian semigroups on von Neumann algebras, which are (KMS) symmetric with respect to nontracial states, is clear for various applications to open systems,[4] quantum statistical mechanics[3] and quantum probability.[5,6] Although on the abstract level we have quite well-developed theory,[7–9] the progress in concrete applications is relatively slow. For construction of Dirichlet forms and associated Markovian semigroups, we refer to Refs. 1 and 10–14 and the references there in.

During the last 10 years, systematic methods to construct Dirichlet forms and associated Markovian semigroups of jump and diffusion types have been developed. Nontrivial translation invariant symmetric semigroups of jump type for quantum spin systems have been constructed and the strong ergodicity of the semigroups has been established in Refs. 12 and 13. See also Ref. 14 and the references therein. In Ref. 1, we gave a general construction method of Dirichlet forms of diffusion type in the framework of the general theory of Dirichlet forms and Markovian semigroups on standard forms of von Neumann algebras developed by Cipriani.[7] The method has been used successfully to construct Dirichlet forms and associated Markovian semigroups for quantum

[a)]Electronic mail: ympark@yonsei.ac.kr

spin systems,[1] CCR and CAR algebras with respect to quasifree states,[10,11,15] and quantum mechanical systems.[16] Recently, in Ref. 2 we have shown that the symmetric embedding of a general Lindblad type (bounded) generator of a quantum dynamical semigroup satisfying KMS symmetry can be written in the form of a Dirichlet operator associated to a Dirichlet form given in Ref. 1.

The next step in this research area would be the investigation of detailed properties of Markovian semigroups, such as ergodicity, mixing property and convergence to the equilibrium, etc. In the case of CCR and CAR algebras with respect to quasifree states, the spectrum of the generators of the Markovian semigroups constructed in Refs. 17, 10, 11, and 15 has been analyzed. However, in general the detail properties of the Markovian semigroups associated to Dirichlet forms in Refs. 1 and 2 are hard to be established. Thus it would be nice to have a simple criteria whether the Markovian semigroup under study is ergodic or not in the sense of Cipriani.[18]

We organize the paper as follows: In Sec. II, we introduce notations and terminologies, and then list our results (Theorem 2.1 and Corollary 2.1). We also give comments (Remark 2.1) on possible applications of our results. Section III is devoted to the proof of Theorem 2.1. We first describe the basic ideas of the proof and then establish some technical lemmas (Lemma 3.1–Lemma 3.5) which are needed in the sequel. Using the lemmas we complete the proof of Theorem 2.1. In Sec. IV, we apply our main results to prove that the diffusion type translation invariant Markovian semigroups for quantum spin systems constructed in Ref. 1 are ergodic in the region of high temperature where the uniqueness of the KMS state holds.

II. NOTATION, TERMINOLOGIES AND MAIN RESULTS

We first introduce necessary terminologies in the theory of Dirichlet forms and Markovian semigroups on standard form of von Neumann algebras.[7] Next we give a brief review on the construction of Dirichlet forms developed in Ref. 1 and then list our main results.

Let $\mathcal{M}$ be a σ-finite von Neumann algebra acting on a complex Hilbert space $\mathcal{H}$ with an inner product $\langle\cdot,\cdot\rangle$ which is conjugate linear in the first and linear in the second variable. Let ξ_0 be a cyclic and separating vector for $\mathcal{M}$. We use Δ and J to denote, respectively, the modular operator and the modular conjugation associated with the pair $(\mathcal{M},\xi_0)$.[3] The associated modular automorphism is denoted by $\sigma_t{:}\sigma_t(A)=\Delta^{it}A\Delta^{-it}$, $A\in\mathcal{M}$. Finally, $j{:}\mathcal{M}\to\mathcal{M}'$ is the antilinear $*$-isomorphism defined by $j(A)=JAJ$, $A\in\mathcal{M}$, where $\mathcal{M}'$ is the commutant of $\mathcal{M}$. By the Tomita-Takesaki theorem (Theorem 2.5.14 of Ref. 3), it follows that $\sigma_t(\mathcal{M})=\mathcal{M}$ and $j(\mathcal{M})=\mathcal{M}'$.

The natural positive cone $\mathcal{P}$ associated with the pair $(\mathcal{M},\xi_0)$ is the closure of the set

$$\{Aj(A)\xi_0{:}A\in\mathcal{M}\}.$$

By a general result, the closed convex cone $\mathcal{P}$ can be obtained by the closure of the set

$$\{\Delta^{1/4}AA^*\xi_0{:}A\in\mathcal{M}\}$$

and this cone $\mathcal{P}$ is self-dual in the sense that

$$\{\xi\in\mathcal{H}{:}\langle\xi,\eta\rangle\geqslant 0,\ \forall\ \eta\in\mathcal{P}\}=\mathcal{P}.$$

For the details we refer to Ref. 19 and Sec. 2.5 of Ref. 3.

The form $(\mathcal{M},\mathcal{H},\mathcal{P},J)$ is the standard form associated with the pair $(\mathcal{M},\xi_0)$. We shall use the fact that $\mathcal{H}$ is the complexification of the real subspace $\mathcal{H}^J=\{\xi\in\mathcal{H}{:}\langle\xi,\eta\rangle\in\mathbb{R},\forall\,\eta\in\mathcal{P}\}$, whose elements are called *J-real*: $\mathcal{H}=\mathcal{H}^J\oplus i\mathcal{H}^J$. The cone $\mathcal{P}$ gives rise to a structure of ordered Hilbert space on $\mathcal{H}^J$ (denoted by $\leqslant$) and to an antilinear involution J on $\mathcal{H}$, which preserves $\mathcal{P}$ and $\mathcal{H}^J$: $J(\xi+i\eta)=\xi-i\eta$, $\forall\xi,\ \eta\in\mathcal{H}^J$. Also note that any J-real element $\xi\in\mathcal{H}^J$ can be decomposed uniquely as a difference of two mutually orthogonal, positive and negative part of ξ, respectively, $\xi=\xi_+-\xi_-$, $\xi_+,\xi_-\in\mathcal{P}$, and $\langle\xi_+,\xi_-\rangle=0$.

A bounded operator A on $\mathcal{H}$ is called *J-real* if $AJ=JA$ and *positive preserving* if $A\mathcal{P}\subset\mathcal{P}$. A semigroup $\{T_t\}_{t\geqslant 0}$ is said to be *J-real* if T_t is J-real for any $t\geqslant 0$ and it is called *positive preserving* if T_t is positive preserving for any $t\geqslant 0$. A bounded operator $A{:}\mathcal{H}\to\mathcal{H}$ is called *sub-Markovian*

(with respect to ξ_0) if $0 \leqslant \xi \leqslant \xi_0$ implies $0 \leqslant A\xi \leqslant \xi_0$. A is called *Markovian* if it is sub-Markovian and also $A\xi_0 = \xi_0$. A semigroup $\{T_t\}_{t \geqslant 0}$ is said to be *sub-Markovian* (with respect to ξ_0) if T_t is sub-Markovian for every $t \geqslant 0$. A semigroup $\{T_t\}_{t \geqslant 0}$ is called *Markovian* if T_t is Markovian for every $t \geqslant 0$.

Next, we consider a sesquilinear form on some linear manifold of $\mathcal{H}$: $\mathcal{E}(\cdot,\cdot): D(\mathcal{E}) \times D(\mathcal{E}) \to \mathbb{C}$. We also consider the associated quadratic form: $\mathcal{E}[\cdot]: D(\mathcal{E}) \to \mathbb{C}$, $\mathcal{E}[\xi] := \mathcal{E}(\xi, \xi)$. A real valued quadratic form $\mathcal{E}[\cdot]$ is said to be *semibounded* (or *bounded below*) if $\inf\{\mathcal{E}[\xi]: \xi \in D(\mathcal{E}), \|\xi\| = 1\} = -b > -\infty$. A quadratic form $(\mathcal{E}, D(\mathcal{E}))$ is said to be *J-real* if $JD(\mathcal{E}) \subset D(\mathcal{E})$ and $\mathcal{E}[J\xi] = \overline{\mathcal{E}[\xi]}$ for any $\xi \in D(\mathcal{E})$. For a semibounded quadratic form $\mathcal{E}$, one considers the inner product given by $\langle \xi, \eta \rangle_\lambda := \mathcal{E}(\xi, \eta) + \lambda \langle \xi, \eta \rangle$, for $\lambda > b$. The form $(\mathcal{E}, D(\mathcal{E}))$ is *closed* if $D(\mathcal{E})$ is a Hilbert space for some of the above inner products. The form $(\mathcal{E}, D(\mathcal{E}))$ is called *closable* if it admits a closed extension.

Associated to a semibounded closed form $(\mathcal{E}, D(\mathcal{E}))$, there are a self-adjoint operator $(H, D(H))$ and a strongly continuous, symmetric semigroup $\{T_t\}_{t \geqslant 0}$. Each of the above objects determines uniquely the others according to well-known relations (see Ref. 20 and Sec. 3.1 of Ref. 3).

Let us denoted by $\mathrm{Proj}(\xi, Q)$ the projection of the vector $\xi \in \mathcal{H}^J$ onto the closed, convex cone $Q \subset \mathcal{H}^J$. For $\xi, \eta \in \mathcal{H}^J$, define

$$\xi \vee \eta := \mathrm{Proj}(\xi, \eta + \mathcal{P}),$$

$$\xi \wedge \eta := \mathrm{Proj}(\xi, \eta - \mathcal{P}).$$

A J-real, real-valued, densely defined quadratic form $(\mathcal{E}, D(\mathcal{E}))$ is called *Markovian* with respect to $\xi_0 \in \mathcal{P}$ if

$$\xi \in D(\mathcal{E})^J \text{ implies } \xi \wedge \xi_0 \in D(\mathcal{E}) \text{ and } \mathcal{E}[\xi \wedge \xi_0] \leqslant \mathcal{E}[\xi],$$

where $D(\mathcal{E})^J := D(\mathcal{E}) \cap \mathcal{H}^J$. A closed Markovian form is called a *Dirichlet form*.

Next, we collect main results of Ref. 7. Let $(\mathcal{E}, D(\mathcal{E}))$ be a J-real, real valued, densely defined closed form. Assume that the following properties hold:

$$\text{(a)} \quad \xi_0 \in D(\mathcal{E}),$$

$$\text{(b)} \quad \mathcal{E}(\xi, \xi) \geqslant 0 \quad \text{for } \xi \in D(\mathcal{E}), \tag{2.1}$$

$$\text{(c)} \quad \xi \in D(\mathcal{E})^J \quad \text{implies } \xi_\pm \in D(\mathcal{E}) \quad \text{and } \mathcal{E}(\xi_+, \xi_-) \leqslant 0.$$

Then $(\mathcal{E}, D(\mathcal{E}))$ is a Dirichlet form if and only if $\mathcal{E}(\xi, \xi_0) \geqslant 0$ for all $\xi \in D(\mathcal{E}) \cap \mathcal{P}$. The above result follows from Proposition 4.5 (b) and Proposition 4.10 (ii) of Ref. 7. The following is one of main results (Theorem 4.11) of Ref. 7: Let $\{T_t\}_{t \geqslant 0}$ be a J-real, strongly continuous, symmetric semigroup on $\mathcal{H}$ and let $(\mathcal{E}, D(\mathcal{E}))$ be the associated densely defined J-real, real valued quadratic form. Then the following are equivalent:

$$\text{(a)} \quad \{T_t\}_{t \geqslant 0} \text{ is sub-Markovian.}$$

$$\text{(b)} \quad (\mathcal{E}, D(\mathcal{E})) \quad \text{is a Dirichlet form.}$$

We refer the reader to Ref. 7 for the details.

Next, we describe the construction of Dirichlet forms developed in Ref. 1. See also Ref. 2. For any $\lambda > 0$, denote by I_λ the closed strip given by

$$I_\lambda = \{z: z \in \mathbb{C}, |\mathrm{Im}\, z| \leqslant \lambda\}. \tag{2.2}$$

Recall that an analytic function $f: D \to \mathbb{C}$ on a domain D containing the strip $I_{1/4}$ is called *admissible* if the following properties hold:

$$\text{(a)} \quad f(t) \geqslant 0 \quad \text{for } \forall\, t \in \mathbb{R},$$

$$\text{(b)} \quad f(t+i/4) + f(t-i/4) \geqslant 0 \quad \text{for } \forall\, t \in \mathbb{R},$$

$$\text{(c)} \quad \text{there exist } M > 0 \text{ and } p > 1 \text{ such that the bound} \tag{2.3}$$

$$|f(t+is)| \leqslant M(1+|t|)^{-p}$$

holds uniformly in $s \in [-1/4, 1/4]$.

We also consider the function $f_0 : \mathbb{R} \to \mathbb{R}$ given by

$$f_0(t) = 2(e^{2\pi t} + e^{-2\pi t})^{-1}. \tag{2.4}$$

One can see that f_0 has an analytic extension, denoted by f_0 again, to the interior of $I_{1/4}$.

For any $\lambda > 0$, denote by $\mathcal{M}_\lambda$ the dense subset of $\mathcal{M}$ consisting of every σ_t-analytic element with a domain containing I_λ. By Proposition 2.5.21 of Ref. 3, any $A \in \mathcal{M}_\lambda$ is strongly analytic on I_λ. We denote by $\mathcal{M}_0$ the dense subset of $\mathcal{M}$ consisting of every σ_t-entire analytic element, i.e., $\mathcal{M} = \cap_\lambda \mathcal{M}_\lambda$.

Let I be a finite or countable (index) set. For given family $\{x_k : k \in I\} \subset \mathcal{M}_{1/2}$ of self-adjoint elements in $\mathcal{M}_{1/2}$ and an admissible function f or $f = f_0$, define a sesquilinear form by

$$D(\mathcal{E}) = \left\{ \xi \in \mathcal{H} : \sum_{k \in I} \mathcal{E}_k(\xi, \xi) < \infty \right\}, \tag{2.5}$$

$$\mathcal{E}(\eta, \xi) = \sum_{k \in I} \mathcal{E}_k(\eta, \xi), \tag{2.6}$$

where for each $k \in I$,

$$\mathcal{E}_k(\eta, \xi) = \int \langle (\sigma_{t-i/4}(x_k) - j(\sigma_{t-i/4}(x_k)))\eta, (\sigma_{t-i/4}(x_k) - j(\sigma_{t-i/4}(x_k)))\xi \rangle f(t) \mathrm{d}t. \tag{2.7}$$

For each $k \in I$, the above form is positive and bounded. In fact, the form $(\mathcal{E}_k, \mathcal{H})$ is a Dirichlet form for each $k \in I$ by Theorem 3.1 of Ref. 1. See also Theorem 2.1 of Ref. 2 for $f = f_0$. Moreover, if $D(\mathcal{E})$ is dense in $\mathcal{H}$, then the form $(\mathcal{E}, D(\mathcal{E}))$ given in (2.6) is a Dirichlet form by Theorem 5.2 of Ref. 7.

Before proceeding further, we would like to make a few remarks. The function f_0 given in (2.5) played a special role in Ref. 2. The symmetric embedding of a general Lindblad type (bounded) generator of a quantum dynamical semigroup (satisfying KMS symmetry) on $\mathcal{M}$ can be written as the Dirichlet operator associated to a Dirichlet form in (2.6) with $f = f_0$. Next, we would like to mention that it is not necessary to assume that each x_k in $\{x_k : k \in I\}$ is self-adjoint if one defines the Dirichlet form $(\mathcal{E}_k, \mathcal{H})$ in (2.7) appropriately as in (2.6) of Ref. 2. Note that, by a simple transformation, one can write $\mathcal{E}_k(\eta, \xi)$ as a sum of two Dirichlet forms corresponding with two self-adjoint elements. See Remark 2.1 (a) in Ref. 2. Thus without loss of the generality, we assume that each x_k is self-adjoint.

A family $\{x_k : k \in I\}$ is said to *generate* $\mathcal{M}$ if the $*$-algebra generated by $\{x_k : k \in I\}$ is dense in $\mathcal{M}$. For given $\{x_k : k \in I\} \subset \mathcal{M}_{1/2}$ of self-adjoint elements and either an admissible function f or else $f = f_0$, let $(\mathcal{E}, D(\mathcal{E}))$ be the Dirichlet form defined as in (2.5)–(2.7). Denote by $(H, D(H))$ and $\{T_t\}_{t \geqslant 0}$ the Dirichlet operator and Markovian semigroup associated to $(\mathcal{E}, D(\mathcal{E}))$, i.e., $T_t = e^{-tH}$. We denote by $\mathcal{N}$ the fixed point space of T_t,

$$\mathcal{N} := \{\eta \in \mathcal{H} : T_t\eta = \eta\} = \{\eta \in \mathcal{H} : H\eta = 0\}. \tag{2.8}$$

The following is the main result in this paper.

Theorem 2.1: *For a family* $\{x_k : k \in I\} \subset \mathcal{M}_{1/2}$ *of self-adjoint elements and an admissible function* f *or else* $f = f_0$, *let* $(\mathcal{E}, D(\mathcal{E}))$ *be the densely defined Dirichlet form given as in (2.5)–(2.7). Assume that* $\{x_k : k \in I\}$ *generates* $\mathcal{M}$. *Then the equality*

$$\mathcal{N} = [\mathcal{Z}(\mathcal{M})\xi_0]$$

holds, where $\mathcal{Z}(\mathcal{M})$ *is the center of* $\mathcal{M}$, *i.e.*, $\mathcal{Z}(\mathcal{M}) = \mathcal{M} \cap \mathcal{M}'$, *and* $[\mathcal{Z}(\mathcal{M})\xi_0]$ *is the closure of* $\mathcal{Z}(\mathcal{M})\xi_0$.

Recall that a symmetric, strongly continuous, positive preserving semigroup $\{T_t\}_{t\geqslant 0}$ on $\mathcal{H}$ is called *ergodic* if for each $\xi, \eta \in \mathcal{P}, \xi, \eta \neq 0$, there exists $t > 0$ such that $\langle \xi, T_t\eta \rangle > 0$.[18] Assume that $\inf \sigma(H)$ is an eigenvalue of the generator H of $\{T_t\}_{t\geqslant 0}$. Then the ergodicity of $\{T_t\}_{t\geqslant 0}$ is equivalent to that $\inf \sigma(H)$ is a simple eigenvalue of H with a strictly positive (cyclic and separating) eigenvector (Theorem 4.3 of Ref. 18). As a consequence of Theorem 2.1, we have the following.

Corollary 2.1: Let $\mathcal{M}$ *be a factor, i.e.*, $\mathcal{Z}(\mathcal{M}) = \mathbb{C}\mathbf{1}$. *Let* $(\mathcal{E}, D(\mathcal{E}))$ *be the densely defined Dirichlet form as in Theorem 2.1 and* T_t *the associated Markovian semigroup. Under the assumptions as in Theorem 2.1,* $\{T_t\}_{t\geqslant 0}$ *is ergodic in the sense that zero is a simple eigenvalue of the generator* H *of* T_t *with eigenvector* ξ_0.

Proof: Under the assumptions, $\mathcal{N} = \mathbb{C}\xi_0$ by Theorem 2.1. Since $j(\sigma_{t-i/4}(x))\xi_0 = \sigma_{t-i/4}(x)\xi_0$, it follows from (2.7) that $\mathcal{E}_k(\xi_0, \xi_0) = 0$ for each $k \in I$ and so $\mathcal{E}(\xi_0, \xi_0) = 0$, which implies that $H\xi_0 = 0$. See also Theorem 3.1 (a) of Ref. 1. Hence zero is a simple eigenvalue of H with eigenvector ξ_0.

□

We will produce the proof of Theorem 2.1 in the next section. Before closing this section, it may be worth to give comments on possible applications of Theorem 2.1.

Remark 2.1: (a) In order to apply Theorem 2.1 (and Corallary 2.1) to concrete models, one must choose a family $\{x_k : k \in I\} \subset \mathcal{M}_{1/2}$ *which generates* $\mathcal{M}$. *Recall that the condition* $x_k \in \mathcal{M}_{1/2} \subset \mathcal{M}_{1/4}$ *for each* x_k *is needed for* $(\mathcal{E}_k, \mathcal{H})$ *to be well defined. If* $\mathcal{H}$ *is a finite dimensional Hilbert space, then the modular operator* Δ *is bounded and so every element* x *of* $\mathcal{M}$ *is* σ_t*-entire analytic. In general, it would be not easy to choose a generating family* $\{x_k : k \subset I\}$ *from* $\mathcal{M}_{1/2}$ *directly*.

(b) For quantum spin systems in the region of high temperatures, every local observable belongs to $\mathcal{M}_{1/2}$. *In this case, the choice of* $\{x_k : k \in I\}$ *is easy. See Sec. IV for the details*.

(c) Let $\{f_n : n \in \mathbb{N}\}$ *be an orthonormal basis for* $L^2(\mathbb{R}^d)$ *and let* $a^*(f_n)$ *and* $a(f_n)$, $n \in \mathbb{N}$, *be the creation and annihilation operators which generate a CAR algebra* $\mathcal{A}$. *Let* ω *be a quasifree state on* $\mathcal{A}$ *and* $(\mathcal{H}_\omega, \pi_\omega(\mathcal{A}), \Omega_\omega)$ *be the cyclic representation associated to* $(\mathcal{A}, \omega)$. *Let* $\mathcal{M} = \pi_\omega(\mathcal{A})''$ *and* $\xi_0 = \Omega_\omega$. *Then for each* $n \in \mathbb{N}$, $\pi_\omega(a(f_n))$ *and* $\pi_\omega(a^*(f_n))$ *are* σ_t*-entire analytic element.*[11] *Thus one can apply Theorem 2.1 and Corollary 2.1 directly in this case*.

(d) In applications to open systems[4] *and quantum statistical mechanics,*[3] *one may need to construct a Dirichlet form for a given* $\{x_k : k \in I\}$, *where each* x_k *is unbounded (self-adjoint) operator affiliated with* $\mathcal{M}$. *By employing appropriate approximation procedures, one may be able to construct the Dirichlet form associated to* $\{x_k : k \in I\}$ *(Refs. 16 and 10) and then extend Theorem 2.1 by modifying the method used in this paper*.

III. PROOF OF THEOREM 2.1

Before producing the proof of Theorem 2.1, we first describe the basic ideas used in the proof, and then establish necessary technical lemmas which will be needed in the proof. Using the lemmas, we complete the proof at the last part of this section.

The inclusion $[\mathcal{Z}(\mathcal{M})\xi_0] \subset \mathcal{N}$ is easy to check. See the proof of Theorem 2.1. Thus we concentrate to the inclusion $\mathcal{N} \subset [\mathcal{Z}(\mathcal{M})\xi_0]$. Note that $\eta \in \mathcal{N}$ if and only if $\mathcal{E}[\eta] = \langle H^{1/2}\eta, H^{1/2}\eta \rangle$

$=0$. Since $\mathcal{E}_k[\eta]\geqslant 0$ for $\eta\in\mathcal{H}$, $k\in I$, $\eta\in\mathcal{N}$ if and only if $\mathcal{E}_k[\eta]=0$ for any $k\in I$. Since f is an admissible function or else $f=f_0$, it is easy to show that $\mathcal{E}_k[\eta]=0$ if and only if

$$\|(\sigma_{t-i/4}(x_k)-j(\sigma_{t-i/4}(x_k)))\eta\|=0$$

for any $t\in\mathbb{R}$ and $k\in I$. See Lemma 3.1. The above implies that

$$\|(\sigma_{-i/4}(x_k)-j(\sigma_{-i/4}(x_k)))\eta\|=0,\quad k\in I. \tag{3.1}$$

Suppose that η is of the form $\eta=\Delta^{1/4}Q\xi_0$, $Q\in\mathcal{M}$. Then the above equality implies that

$$[x_k,Q]\xi_0=0,\quad \forall\, k\in I$$

and so

$$[x_k,Q]A'\xi_0=0,\quad \forall\, k\in I$$

for any $A'\in\mathcal{M}'$. Since $\mathcal{M}'\xi_0$ is dense in $\mathcal{H}$, we conclude that $[x_k,Q]=0$ for $k\in I$. Since $\{x_k:k\in I\}$ generates $\mathcal{M}$, $Q\in\mathcal{M}'$. Thus $Q\in\mathcal{M}\cap\mathcal{M}'$ and $\eta=\Delta^{1/4}Q\xi_0=Q\xi_0$. However, in general $\eta\in\mathcal{N}$ cannot be written as $\eta=\Delta^{1/4}Q\xi_0$, $Q\in\mathcal{M}$.

Note that H is J-real, $JH=HJ$, and so $J\mathcal{N}=\mathcal{N}$. Any $\eta\in\mathcal{H}$ can be written as $\eta=\eta_r+i\eta_i$, where $\eta_r=(\eta+J\eta)/2$ and $\eta_i=-i(\eta-J\eta)/2$. Thus $\eta\in\mathcal{N}$ implies η_r, $\eta_i\in\mathcal{N}$. Hence we may suppose that $\eta\in\mathcal{N}\cap\mathcal{H}^J$. Because of the Dirichlet property, (2.1) (c), of $\mathcal{E}[\eta]$, it can be shown that $\eta\in\mathcal{N}\cap\mathcal{H}^J$ implies η_+, $\eta_-\in\mathcal{N}\cap\mathcal{P}$ [Lemma 3.2 (d)]. Thus the problem is reduced to the case $\eta\in\mathcal{N}\cap\mathcal{P}$.

Any $\eta\in D(\Delta^{-1/4})\cap\mathcal{P}$ can be written as $\eta=\Delta^{1/4}Q\xi_0$ where Q is positive self-adjoint operator affiliated with $\mathcal{M}$ (Lemma 3.4). For any $\eta\in D(\Delta^{-1/4})\cap(\mathcal{N}\cap\mathcal{P})$, $\eta=\Delta^{1/4}Q\xi_0$, we use (3.1) to show that

$$(x_kQ-Qx_k)\xi_0=0.$$

Using the facts that $\mathcal{M}'\xi_0$ is dense in $\mathcal{H}$ and that $\{x_k:k\in I\}$ generates $\mathcal{M}$, we will show that Q is affiliated with $\mathcal{M}'$. Since $\Delta\xi=\xi$ for any $\xi\in[\mathcal{Z}(\mathcal{M})\xi_0]$, we conclude that $\eta\in[\mathcal{Z}(\mathcal{M})\xi_0]$. Next, we use the fact that $D(\Delta^{-1/4})\cap(\mathcal{N}\cap\mathcal{P})$ is dense in $(\mathcal{N}\cap\mathcal{P})$ (Lemma 3.3) to complete the proof of Theorem 2.1.

Next, we collect technical lemmas which will be used in the sequel. In the rest of this section, we assume that the conditions in the theorem hold.

Lemma 3.1: A vector $\eta\in\mathcal{H}$ belongs to $\mathcal{N}$ if and only if the equality

$$(\sigma_{t-i/4}(x_k)-j(\sigma_{t-i/4}(x_k)))\eta=0$$

holds for any $t\in\mathbb{R}$ and $k\in I$.

Proof: Since

$$\langle\eta,H\eta\rangle=\mathcal{E}(\eta,\eta)=\sum_{k\in I}\mathcal{E}_k(\eta,\eta),$$

and $\mathcal{E}_k(\eta,\eta)\geqslant 0$ for $\eta\in\mathcal{H}$ and $k\in I$, $H\eta=0$ if and only if $\mathcal{E}_k(\eta,\eta)=0$. Recall the expression of $\mathcal{E}_k(\eta,\eta)$ in (2.7). Notice that $f_0(t)>0$ for any $t\in\mathbb{R}$ by (2.4). If f is an admissible function, $f(t)\geqslant 0$ by (2.3) (a). Since f is analytic on a domain containing $I_{1/4}$, $f(t)>0$ except on a countable set with no accumulation points. Thus the left-hand side of the expression in the lemma is zero except on a countable set of $t\in\mathbb{R}$. Since $\sigma_{t-i/4}(x_k)$ is strongly continuous with respect to $t\in\mathbb{R}$, we proved the lemma. □

Lemma 3.2: (a) $\mathcal{N}$ is a closed subspace of $\mathcal{H}$.

(b) $\Delta^{it}\mathcal{N}=\mathcal{N}$, $\forall t\in\mathbb{R}$.

(c) $J\mathcal{N}=\mathcal{N}$.

(d) $\eta\in\mathcal{N}\cap\mathcal{H}^J$ implies η_+, $\eta_-\in\mathcal{N}\cap\mathcal{P}$.

Proof: (a) Since H is self-adjoint (closed), (a) is obvious.

(b) Notice that

$$H\Delta^{-is}\eta = \Delta^{-is}(\Delta^{is}H\Delta^{-is})\eta$$

and $\Delta^{is}H\Delta^{-is}$ is the Dirichlet operator associated to the Dirichlet form constructed with $\{\sigma_s(x_k): k \in I\}$. Note that $\sigma_{t-i/4}(\sigma_s(x_k)) = \sigma_{t+s-i/4}(x_k)$. Thus, if $\eta \in \mathcal{N}$, $\Delta^{-is}\eta \in \mathcal{N}$ by Lemma 3.1. Hence $\Delta^{-is}\mathcal{N} \subset \mathcal{N}$ for any $s \in \mathbb{R}$, which also implies $\mathcal{N} \subset \Delta^{is}\mathcal{N}$ for any $s \in \mathbb{R}$.

(c) Since each $\mathcal{E}_k$ is J-real [Theorem 2.1 (b) of Ref. 2], it is easy to check that H is J-real, $JH = HJ$. Thus $HJ\eta = JH\eta = 0$ if $\eta \in \mathcal{N}$ and so $J\mathcal{N} \subset \mathcal{N}$. Since $J^2 = \mathbf{1}$, we also have that $\mathcal{N} \subset J\mathcal{N}$.

(d) Let $\eta \in \mathcal{N} \cap \mathcal{H}^J$, and $\eta = \eta_+ - \eta_-$. Notice that

$$0 = \mathcal{E}(\eta, \eta) = \mathcal{E}(\eta_+, \eta_+) - 2\mathcal{E}(\eta_+, \eta_-) + \mathcal{E}(\eta_-, \eta_-).$$

Here we have used the fact that $\eta \in D(\mathcal{E})$ implies $\eta_+, \eta_- \in D(\mathcal{E})$. Since $\mathcal{E}(\eta_+, \eta_-) \leqslant 0$ by (2.1) (c) [Theorem 2.1 (c) of Ref. 2], we have that $\mathcal{E}(\eta_+, \eta_+) = \mathcal{E}(\eta_-, \eta_-) = 0$, which imply $H\eta_+ = H\eta_- = 0$.

□

Lemma 3.3: (a) For any bounded, positive definite, continuous function $f: \mathbb{R} \to \mathbb{R}$,

$$f(\log \Delta)(\mathcal{N} \cap \mathcal{P}) \subset \mathcal{N} \cap \mathcal{P}.$$

(b) $(\cap_{\alpha \in \mathbb{R}} D(\Delta^\alpha)) \cap (\mathcal{N} \cap \mathcal{P})$ is dense in $\mathcal{N} \cap \mathcal{P}$.

Proof: (a) Let f be a bounded, positive definite, continuous function on $\mathbb{R}$. Then f can be written as

$$f(x) = \int e^{itx}\, \mathrm{d}\mu(t),$$

where μ is a positive finite Borel measure on $\mathbb{R}$. Thus

$$f(\log \Delta) = \int \Delta^{it}\, \mathrm{d}\mu(t).$$

The inclusion

$$f(\log \Delta)\mathcal{P} \subset \mathcal{P}$$

holds by the fact that $\Delta^{it}\mathcal{P} \subset \mathcal{P}$ (Proposition 2.5.26 of Ref. 3). Due to Lemma 3.2 (b), the inclusion

$$f(\log \Delta)\mathcal{N} \subset \mathcal{N}$$

also holds. This proved the part (a) of the lemma.

(b) Let

$$f_n(x) := e^{-x^2/2n^2}.$$

Then by the part (a) of the lemma,

$$f_n(\log \Delta)(\mathcal{N} \cap \mathcal{P}) \subset \mathcal{N} \cap \mathcal{P}.$$

For any $\eta \in \mathcal{N} \cap \mathcal{P}$, $f_n(\log \Delta)\eta \in D(\Delta^\alpha)$ for any $\alpha \in \mathbb{R}$, and $f_n(\log \Delta)\eta \to \eta$ as $n \to \infty$. This proved the part (b).

□

Lemma 3.4: Let $\eta \in D(\Delta^{-1/4}) \cap \mathcal{P}$. Then there is a positive self-adjoint operator Q affiliated with $\mathcal{M}$ such that $Q\xi_0 \in D(\Delta^{1/4})$ and $\eta = \Delta^{1/4}Q\xi_0$.

Proof: We use the method similar to that employed in the proof of Proposition 2.5.27 (1) of Ref. 3. Let $\eta \in D(\Delta^{-1/4}) \cap \mathcal{P}$. For any $A \in \mathcal{M}$, $\Delta^{-1/4}j(A^*)j(A)\xi_0 \in \mathcal{P}$ and so

$$\langle \Delta^{-1/4} j(A^*) j(A) \xi_0, \eta \rangle \geqslant 0, \quad \forall A \in \mathcal{M},$$

which implies

$$\langle j(A^*) j(A) \xi_0, \Delta^{-1/4} \eta \rangle \geqslant 0, \quad \forall A \in \mathcal{M}.$$

Define an operator $\tilde{Q}$, $D(\tilde{Q}) = \mathcal{M}'\xi_0$, by

$$\tilde{Q} j(B) \xi_0 = j(B) \Delta^{-1/4} \eta, \quad \forall B \in \mathcal{M}.$$

Then for any unitary $U' \in \mathcal{M}'$,

$$U' \tilde{Q} j(B) \xi_0 = U' j(B) \Delta^{-1/4} \eta = \tilde{Q} U' j(B) \xi_0,$$

and so

$$U'^* \tilde{Q} U' = \tilde{Q}.$$

For any $A \in \mathcal{M}$,

$$\langle j(A)\xi_0, \tilde{Q} j(A) \xi_0 \rangle = \langle j(A)\xi_0, j(A)\Delta^{-1/4}\eta \rangle = \langle \Delta^{-1/4} j(A^*) j(A) \xi_0, \eta \rangle \geqslant 0.$$

Thus $\tilde{Q}$ is a positive symmetric operator. Notice that for any unitary $U' \in \mathcal{M}'$, $U' D(\tilde{Q}) \subset D(\tilde{Q})$. Let Q be the Friedrichs extension of $\tilde{Q}$. By the uniqueness of Friedrichs extension

$$U'^* Q U' = Q$$

for any unitary $U' \in \mathcal{M}'$. Thus Q is affiliated with $\mathcal{M}$. Since $Q\xi_0 = \Delta^{-1/4}\eta$, $Q\xi_0 \in D(\Delta^{1/4})$, and $\eta = \Delta^{1/4} Q \xi_0$.

□

Lemma 3.5: Let $\eta \in D(\Delta^{-1/4}) \cap (\mathcal{N} \cap \mathcal{P})$ *and* $\eta = \Delta^{1/4} Q \xi_0$ *as in Lemma 3.4. Then* $x_k \xi_0 \in D(Q)$ *and* $x_k Q \xi_0 = Q x_k \xi_0$ *for any* $k \in I$.

Proof: Since $\eta \in \mathcal{N}$, it follows from Lemma 3.1 that

$$[\sigma_{-i/4}(x_k) - j(\sigma_{-i/4}(x_k))] \Delta^{1/4} Q \xi_0 = 0, \quad k \in I.$$

Recall that $\mathcal{M}_0$ is the dense subset of $\mathcal{M}$ consisting of σ_t-entire analytic elements. For any $A \in \mathcal{M}_0$,

$$\begin{aligned} 0 = \langle \sigma_{i/4}(A)\xi_0, [\sigma_{-i/4}(x_k) - j(\sigma_{-i/4}(x_k))]) \Delta^{1/4} Q \xi_0 \rangle &= \langle \sigma_{i/4}(x_k)\sigma_{i/4}(A)\xi_0, \Delta^{1/4} Q \xi_0 \rangle \\ &- \langle j(\sigma_{i/4}(x_k))\sigma_{i/4}(A)\xi_0, \Delta^{1/4} Q \xi_0 \rangle. \end{aligned} \tag{3.2}$$

For any $A \in \mathcal{M}_0$,

$$\sigma_{i/4}(x_k)\sigma_{i/4}(A)\xi_0 = \sigma_{i/4}(x_k A)\xi_0 = \Delta^{-1/4} x_k A \xi_0 \tag{3.3}$$

and

$$j(\sigma_{i/4}(x_k))\sigma_{i/4}(A)\xi_0 = j(\sigma_{i/4}(x_k)) j(\sigma_{-3i/4}(A^*))\xi_0 = \Delta^{-1/4} j(\sigma_{i/2}(x_k)) j(\sigma_{-i/2}(A))\xi_0 = \Delta^{-1/4} j(\sigma_{i/2}(x_k)) A \xi_0. \tag{3.4}$$

Substituting (3.3) and (3.4) into (3.2), we have

$$\langle A\xi_0, [x_k - j(\sigma_{-i/2}(x_k))] Q \xi_0 \rangle = 0$$

for any $A \in \mathcal{M}_0$ and $k \in I$. Since $\mathcal{M}_0 \xi_0$ is dense in $\mathcal{H}$,

$$[x_k - j(\sigma_{-i/2}(x_k))]Q\xi_0 = 0.$$

Since Q is affiliated with $\mathcal{M}$, $j(\sigma_{-i/2}(x_k))Q\xi_0 = Qj(\sigma_{-i/2}(x_k))\xi_0 = Qx_k\xi_0$, and so $x_k\xi_0 \in D(Q)$ and $x_kQ\xi_0 = Qx_k\xi_0$.

□

Next, we use Lemma 3.4 and Lemma 3.5 to prove the following result.

Proposition 3.1: Let $\eta \in D(\Delta^{-1/4}) \cap (\mathcal{N} \cap \mathcal{P})$. *Then there is a positive self-adjoint operator* Q *affiliated with* $\mathcal{Z}(\mathcal{M})$ *such that* $\eta = Q\xi_0$.

Proof: Let $\eta = \Delta^{1/4}Q\xi_0$ as in Lemma 3.4. Due to Lemma 3.5,

$$x_kQ\xi_0 = Qx_k\xi_0, \quad \forall\, k \in I.$$

Since $x_k \in \mathcal{M}_{1/2} \subset \mathcal{M}$ and Q is affiliated with $\mathcal{M}$,

$$x_kQj(A)\xi_0 = j(A)x_kQ\xi_0 = j(A)Qx_k\xi_0 = Qx_kj(A)\xi_0$$

for any $A \in \mathcal{M}$, and so

$$x_kQj(A)\xi_0 = Qx_kj(A)\xi_0, \quad \forall\, A \in \mathcal{M}.$$

Notice that for any $x_{k_1}, x_{k_2} \in \{x_k : k \in I\}$

$$x_{k_1}x_{k_2}Qj(A)\xi_0 = x_{k_1}Qx_{k_2}j(A)\xi_0 = x_{k_1}Qj(A)j(\sigma_{-i/2}(x_{k_2}))\xi_0 = Qx_{k_1}j(A)j(\sigma_{-i/2}(x_{k_2}))\xi_0 = Qx_{k_1}x_{k_2}j(A)\xi_0. \tag{3.5}$$

Let $\tilde{\mathcal{M}}$ be the $*$-algebra generated by $\{x_k : k \in I\}$. Then $\tilde{\mathcal{M}}$ is dense in $\mathcal{M}$ by the assumption in Theorem 2.1. The relation (3.5) implies that for any $x \in \tilde{\mathcal{M}}$,

$$xQj(A)\xi_0 = Qxj(A)\xi_0, \quad \forall\, A \in \mathcal{M}.$$

For given $x \in \mathcal{M}$, choose a sequence $x_n \in \tilde{\mathcal{M}}$ such that $x_n \to x$ strongly. Then

$$Qx_nj(A)\xi_0 = x_nQj(A)\xi_0 \to xQj(A)\xi_0 \quad \text{as } n \to \infty.$$

Due to the closedness of Q and the fact that $x_nj(A)\xi_0 \to xj(A)\xi_0$ as $n \to \infty$, we conclude that $xj(A)\xi_0 \in D(Q)$ and

$$xQj(A)\xi_0 = Qxj(A)\xi_0 \tag{3.6}$$

for any $x, A \in \mathcal{M}$.

Denote by

$$(\mathcal{M} \times \mathcal{M}')\xi_0 := \{AA'\xi_0 : A \in \mathcal{M}, A' \in \mathcal{M}'\}.$$

By (3.6), $(\mathcal{M} \times \mathcal{M}')\xi_0 \in D(Q)$ and for any $A_1, A_2 \in \mathcal{M}$ and $A_1', A_2' \in \mathcal{M}'$,

$$A_1QA_2A_2'\xi_0 = A_1A_2QA_2'\xi_0 = QA_1A_2A_2'\xi_0 \tag{3.7}$$

and

$$A_1'QA_2A_2'\xi_0 = QA_2A_1'A_2'\xi_0 = QA_1'A_2A_2'\xi_0. \tag{3.8}$$

Let Q_0 be the restriction of Q on $(\mathcal{M} \times \mathcal{M}')\xi_0$. Then Q_0 is a positive symmetric operator. It follows from (3.7) and (3.8) that for any unitary $U \in \mathcal{M}$, $U' \in \mathcal{M}'$,

$$U^*Q_0U = Q_0,$$

$$U'^{*}Q_0U' = Q_0. \tag{3.9}$$

Notice that U and U' leave $(\mathcal{M}\times\mathcal{M}')\xi_0$ invariant. Let $\hat{Q}$ be the Friedrichs of Q_0. By the uniqueness of Friedrichs extension,

$$U^{*}\hat{Q}U = \hat{Q},$$

$$U'^{*}\hat{Q}U' = \hat{Q},$$

for any unitary $U\in\mathcal{M}$, $U'\in\mathcal{M}'$. Thus $\hat{Q}$ is affiliated with $\mathcal{Z}(\mathcal{M})$. By the inclusions $\mathcal{M}'\xi_0\subset(\mathcal{M}\times\mathcal{M}')\xi_0\subset D(Q)$ and the uniqueness of the Friedrichs extension, $\hat{Q}=Q$. Since $\Delta\xi=\xi$ for any $\xi\in[\mathcal{Z}(\mathcal{M})\xi_0]$, $\eta=\Delta^{1/4}Q\xi=Q\xi_0$. This completes the proof of the proposition.

□

We are ready to prove Theorem 2.1.

Proof of Theorem 2.1: The inclusion

$$[\mathcal{Z}(\mathcal{M})\xi_0]\subset\mathcal{N} \tag{3.10}$$

is easy to prove as follows: Let $\xi\in\mathcal{Z}(\mathcal{M})\xi_0$. Then $\xi=A\xi_0$ for some $A\in\mathcal{Z}(\mathcal{M})$. Thus

$$[\sigma_{t-i/4}(x_k)-j(\sigma_{t-i/4}(x_k))]A\xi_0 = A[\sigma_{t-i/4}(x_k)-j(\sigma_{t-i/4}(x_k))]\xi_0 = 0.$$

By Lemma 3.1, $\xi\in\mathcal{N}$. Since $\mathcal{N}$ is closed by Lemma 3.2 (a), the closure of $\mathcal{Z}(\mathcal{M})\xi_0$ is a subspace of $\mathcal{N}$. This proved the inclusion (3.10).

Next, we prove the inclusion

$$\mathcal{N}\subset[\mathcal{Z}(\mathcal{M})\xi_0]. \tag{3.11}$$

Any $\eta\in\mathcal{N}$ can be written as $\eta=\eta_r+i\eta_i$, where $\eta_r=(\eta+J\eta)/2$ and $\eta_i=-i(\eta-J\eta)/2$. By Lemma 3.2 (c), $\eta_r,\eta_i\in\mathcal{N}$. Note that $\|\eta\|^2=\|\eta_r\|^2+\|\eta_i\|^2$. Thus we may assume that η is J-real, $\eta\in\mathcal{N}\cap\mathcal{H}^J$. η is decomposed uniquely as $\eta=\eta_+-\eta_-$, $\eta_+,\eta_-\in\mathcal{P}$ and $\eta_+\perp\eta_-$. See Proposition 2.5.28 (3) of Ref. 3. By Lemma 3.2 (d), $\eta_+,\eta_-\in\mathcal{N}\cap\mathcal{P}$. Lemma 3.3 (b) implies that $D(\Delta^{-1/4})\cap(\mathcal{N}\cap\mathcal{P})$ is dense in $\mathcal{N}\cap\mathcal{P}$. Thus Lemma 3.3 (b) and Proposition 3.1 imply that η_+, $\eta_-\in[\mathcal{Z}(\mathcal{M})\xi_0]$, and so $\eta\in[\mathcal{Z}(\mathcal{M})\xi_0]$. This completes the proof of Theorem 2.1.

□

IV. ERGODICITY OF MARKOVIAN SEMIGROUPS FOR QUANTUM SPIN SYSTEMS

In this section, we first describe the translation invariant Markovian semigroups for quantum spin systems constructed in Ref. 1, and then apply Theorem 2.1 (and Corollary 2.1) to show the ergodicity of the semigroups in the region of high temperatures where the uniqueness of the KMS state holds.

Let us describe quantum spin systems briefly. For details, we refer to Sec. 6.2 of Ref. 3. Let $\mathbb{Z}^d$ be a d-dimensional lattice space and let $\mathcal{F}$ denote the family of all finite subsets of $\mathbb{Z}^d$. Let $\mathcal{A}$ be a C^*-algebra with norm $\|\cdot\|$ defined as the inductive limit over a finite-dimensional matrix algebra $\mathbb{M}$. For any $X\in\mathcal{F}$, let $\mathcal{A}_X$ denote the subalgebra localized in X, i.e., the subalgebra in $\mathcal{A}$ isomorphic to $\mathbb{M}^X$. An element $A\in\mathcal{A}$ will be called *local* if there is some $Y\in\mathcal{F}$ such that $A\in\mathcal{A}_Y$. By $\mathcal{A}_0$ we denote the subset of all local elements, i.e., $\mathcal{A}_0=\cup_{X\in\mathcal{F}}\mathcal{A}_X$.

Let $\Phi:=\{\Phi_X\}_{X\in\mathcal{F}}$ be an interaction, i.e., a family of self-adjoint element in $\mathcal{A}$. Suppose that

$$\|\Phi\|_\lambda := \sup_{i\in\mathbb{Z}^d}\sum_{X\in\mathcal{F}:i\in X} e^{\lambda|X|}\|\Phi_X\| < \infty \tag{4.1}$$

for some $\lambda>0$, where $|X|=\mathrm{card}(X)$. Define a derivation δ by

$$D(\delta) = \mathcal{A}_0,$$
$$\delta(A) = -i \sum_{X \cap \Lambda \neq \emptyset} [\Phi_X, A], \quad A \in \mathcal{A}_\Lambda. \tag{4.2}$$

Then $\mathcal{A}_0$ is a norm-dense $*$-subalgebra of analytic element of the closure $\bar{\delta}$ of δ. Thus $\bar{\delta}$ generates one-parameter group of $*$-automorphism τ of $\mathcal{A}$. Let ω be a τ-KMS state corresponding to the interaction Φ.

Let $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ be the GNS representation of $(\mathcal{A}, \omega)$. For the standard form, we choose $\mathcal{H}=\mathcal{H}_\omega$, $\mathcal{M}=\pi_\omega(\mathcal{A})''$, and $\xi_0=\Omega_\omega$. By the uniqueness of the modular automorphism (see Theorem 5.3.10 of Ref. 3), one may identify $\sigma_t=\tau_t$, $t \in \mathbb{R}$, on $\mathcal{M}$. In this section, we denote by $\mathcal{M}_0$ the algebra of local elements, i.e., $\mathcal{M}_0=\pi_\omega(\mathcal{A}_0)$. Every element $A \in \mathcal{M}_0$ is an analytic element for σ_t. For a given $\lambda > 0$, set $\gamma=\lambda/2\|\Phi\|_\lambda$. Then for any $s \in (-\gamma, \gamma)$ the series

$$\sigma_{is}(A) = \sum_{n=0}^{\infty} \frac{(-is)^n}{n!} \delta^n(A), \quad A \in \mathcal{M}_0, \tag{4.3}$$

converges absolutely, where δ is the derivation given by (4.2). See the proof of Theorem 5.2.4 of Ref. 3. From now on, we assume that Φ is chosen sufficiently small so that $\gamma > 1/2$.

We now turn to Dirichlet form for quantum spin systems.[1] Let $\{\tau_j\}_{j \in \mathbb{Z}^d}$ be the translational automorphism on $\mathcal{M}$ corresponding to the translation of the lattice by vectors $j \in \mathbb{Z}^d$. Let $x^a \in \pi_\omega(\mathbb{M})$, $a=1,2,\ldots,D$, be a basis of $\pi_\omega(\mathbb{M})$ consisting of self-adjoint elements of norm one and let $x_j^a=\tau_j(x^a)$, $j \in \mathbb{Z}^d$. For the family $\{x_j^a : j \in \mathbb{Z}^d, a=1,2,\ldots,D\}$ and an admissible function f (or else f_0), let $(\mathcal{E}, D(\mathcal{E}))$ be the quadratic form defined as in (2.5)–(2.7),

$$D(\mathcal{E}) = \left\{ \xi \in \mathcal{H} : \sum_{j \in \mathbb{Z}^d} \sum_{a=1}^{D} \mathcal{E}_{a,j}[\xi] < \infty \right\},$$
$$\mathcal{E}[\xi] = \sum_{j \in \mathbb{Z}^d} \sum_{a=1}^{D} \mathcal{E}_{a,j}[\xi], \quad \xi \in D(\mathcal{E}), \tag{4.4}$$

where

$$\mathcal{E}_{a,j}[\xi] = \int \|(\sigma_{t-i/4}(x_j^a) - j(\sigma_{t-i/4}(x_j^a)))\xi\|^2 f(t) \mathrm{d}t. \tag{4.5}$$

The following is Theorem 5.1 of Ref. 1.

Theorem 4.1 (Theorem 5.1 of Ref. 1): *Let f be an admissible function such that p in (2.3) (c) is greater than $d+1$, i.e., $p > d+1$. Let the interaction Φ be of finite range and translation invariant. Then the form $(\mathcal{E}, D(\mathcal{E}))$ defined as in (4.4) and (4.5) is a densely defined Dirichlet form which generates a translation invariant, symmetric, Markovian semigroup.*

Remark 4.1: The strongly decay property of i.e., $p > d+1$, has been used to show that $D(\mathcal{E})$ is dense in $\mathcal{H}$. See the proof of Theorem 5.1 of Ref. 1. The function f_0 given in (2.4) decays exponentially fast and so the conclusion in Theorem 4.1 holds for $f=f_0$.

In order to describe the main result, we need to replace Φ by $\beta\Phi$, where β is the inverse temperature. Then the condition $\gamma > 1/2$ is equivalent to $(\lambda/2\beta\|\Phi\|_\lambda) > \frac{1}{2}$. This is, $\beta\|\Phi\|_\lambda < \lambda$. The following is the main result in this section.

Theorem 4.2: *Let f be either an admissible function satisfying the decay property in Theorem 4.1 or else $f=f_0$. Let the interaction Φ be of finite range and translation invariant. For $\{x_j^a : j \in \mathbb{Z}^d, a=1,2,\ldots,D\}$, let $\{T_t\}_{t \geq 0}$ be the translation invariant Markovian semigroup associated to the Dirichlet form defined as in (4.4) and (4.5). Assume that $\beta\|\Phi\|_\lambda$ is sufficiently small so that (τ, β)-KMS state for Φ is unique. Then the Markovian semigroup $\{T_t\}_{t \geq 0}$ is ergodic.*

Remark 4.2: The region of high temperatures where the uniqueness of (τ,β)*-KMS state holds can be given explicitly. For an instance, see Proposition 6.2.25 of Ref. 3. For one-dimensional models with uniform bounded surface energies, the uniqueness of* (τ,β)*-KMS state is independent of temperature (Theorem 6.2.47 of Ref. 3). However, we still need the condition* $\beta\|\Phi\|_\lambda<\lambda$.

Proof of Theorem 4.2: By the condition $\beta\|\Phi\|_\lambda<\lambda$, the series (4.3) converges absolutely on a region containing $[-\beta/2,\beta/2]$. Thus it is easy to see that $\{x_j^a: j\in\mathbb{Z}^d, a=1,2,\ldots,D\}\subset\mathcal{M}_{\beta/2}$. Since the $*$-algebra generated by the family is $\mathcal{M}_0$, which is dense in $\mathcal{M}$, the condition in Theorem 2.1 hold. The uniqueness of the (τ,β)-KMS state ω implies that ω is an extremal (τ,β)-KMS state, and hence a factor state by Theorem 5.3.30 of Ref. 3. Thus $\mathcal{M}$ is a factor, and so $\{T_t\}_{t\geqslant 0}$ is ergodic by Corollary 2.1.

□

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On-diagonal singularities of the Green functions for Schrödinger operators

Jochen Brüning
Institut für Mathematik, Humboldt-Universität zu Berlin, Rudower Chaussee 25, 12489 Berlin, Germany

Vladimir Geyler
Mathematical Faculty, Mordovian State University, 430000 Saransk, Russia

Konstantin Pankrashkin[a)]
Institut für Mathematik, Humboldt-Universität zu Berlin, Rudower Chaussee 25, 12489 Berlin, Germany

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We investigate the behavior of the Green functions of Schrödinger operators near the diagonal. The only nontrivial cases, where the on-diagonal singularities are nonzero and do not depend on the spectral parameter, are two and three dimensions. In the case of two dimensions we show that the singularity is independent of both the scalar and the gauge potentials. In dimension three, we obtain conditions for preserving the singularity under perturbations by nonregular potentials. Some examples illustrating dependence of the singularity on general scalar and gauge potentials are presented. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Singularities of the Green functions of quantum-mechanical operators play a crucial role in many branches of theoretical and mathematical physics, from which one should mention first the renormalization procedure of the quantum field theory.[1,2] From the point of view of the high-derivative quantum gravity, the corresponding problem was considered, e.g., in Ref. 3. In particular, in the case of nonminimal coupling of quantum matter to the gravitational background with conical singularities, an operator of the form $H=-\Delta+V$ arises on a Riemannian manifold X. Here Δ is the Laplace-Beltrami operator on X and V represents the nonminimal coupling term $\xi\mathcal{R}$ with the Ricci scalar $\mathcal{R}$. The scalar curvature possesses a distributional behavior at conical singularities,[4] $\mathcal{R}=\mathcal{R}_{\mathrm{reg}}+4\pi(1-\alpha)\delta_M$, where δ_M is a Dirac δ-like potential supported by a submanifold $M\subset X$ and $2\pi(1-\alpha)$ is the angle deficit. As a result, an operator

$$H_M=-\Delta+U+a\delta_M \tag{1.1}$$

arises where $U=\xi\mathcal{R}_{\mathrm{reg}}$ and the coupling constant $a=4\pi\xi(1-\alpha)$ characterizes the interaction with the background field concentrated on M. Operators of such form appear in the investigation of scalar fields with nonminimal coupling on the cosmic string background, in the Euclidean approach to the black hole thermodynamics, in the study of the particle scattering at the Planck scale (see Ref. 4 and references therein). Moreover, in the context of the scattering theory, the potential U can have singularity (e.g., of the Coulomb type) even in the case of a flat manifold X.

We are interested here in the question how to add the singular term δ_M concentrated on a zero-dimensional submanifold M of X to the operator $H_U=-\Delta+U$ (this case covers not only quantum fields with point interactions, but also the case when X is a Cartesian product of two

a)Author to whom correspondence should be addressed. Electronic mail: const@mathematik.hu-berlin.de

manifolds, $X=X_0\times Y$, and M has the form $M_0\times Z$ with M_0 being a discrete subset of X_0). If M is a uniformly discrete subset of X and $\dim X\leqslant 3$, then the Green function $G_M(x,y;\zeta)$ of H_M can be obtained through the Krein resolvent formula in terms of the Green function $G_U(x,y;\zeta)$ for H_U.[5,6] An important ingredient of this formula is the so-called "Krein $\mathcal{Q}$-matrix" (a kind of the Dirichlet-to-Neumann map) $Q_{mn}(z)$, $m,n\in M$; under the name "Wigner $\mathcal{R}$-matrix" it appears in the scattering theory[7] and is used in the charge transport theory.[8] To define the diagonal elements of Q for $\dim X>1$ a renormalization procedure is needed. For smooth U, the renormalized Green function $G_U^{\mathrm{ren}}(x,y;\zeta)$, which must be continuous in the whole $X\times X$, is defined as

$$G_U^{\mathrm{ren}}(x,y;\zeta)=G_U(x,y;\zeta)-S(x,y), \tag{1.2}$$

where the "standard singularity" S has the form $S(x,y)=-(1/2\pi)\log d(x,y)$ if $\dim X=2$, and $S(x,y)=1/4\pi d(x,y)$ if $\dim X=3$ [here $d(x,y)$ is the geodesic distance on X]. Now one can set $Q_{mm}(\zeta)=G_U^{\mathrm{ren}}(m,m;\zeta)$. The corresponding renormalization procedure in the Euclidean case is known long ago, see, e.g., Refs. 9 and 10 for the history and the quantum mechanical treatment. It is important to note that usually one obtains $G_U^{\mathrm{ren}}(x,y;\zeta)$ by a momentum cutoff (an ultraviolet regularization procedure); the result is equivalent to that obtained with the help of a dimensional regularization. In the case of brane coupling to gravity or to a gauge field it is necessary to use a dimensional regularization.[11] It is worthy to add that the strict mathematical treatment of the operators (1.1) has its origins in the paper[12] by Berezin and Faddeev. In the case $\dim X\geqslant 4$ there is no regularization procedure involving a singularity independent of the energy parameter ζ (see Example 7 below). Moreover, if U has a Coulomb-type singularity or if an interaction with a gauge field is present, then the function S in (1.2) is different from the standard one, i.e., $S(x,y)\neq 1/4\pi d(x,y)$ (see Examples 12 and 14 below); similar phenomena related to propagation of waves in strongly inhomogeneous media have been studied recently in Ref. 13.

The main goal of our paper is to investigate in detail the singularity of the Green function for the operator $H_U=H_0+U$ where H_0 is the Bochner-Laplace operator on a Riemannian manifold of dimension $\leqslant 3$ and U is a scalar potential from a wide class of measurable functions. As an important consequence we conclude that the operator of the form (1.1) is well defined in this case. It should be stressed that the operators of this form are used not only in the quantum field theory but they occur often in the single-electron theory of condensed matter physics where H_0 represents the Hamiltonian of an electron in the presence of a time-independent magnetic field, U is a confinement electric potential, and δ_M is an additional potential (e.g., the potential of impurities or of a crystal lattice). The Riemannian manifold with nontrivial curvature can appear in this situation, e.g., as a result of the reduction of a few-electron problem to the single-electron one.[14] Another example of using nontrivial three-dimensional Riemannian manifolds is the simulation of the confinement potential of a quantum dot.[15] The defects in solids were investigated previously by methods of quantum gravity in Ref. 16. New technologies of manufacturing two-dimensional nanostructures with nontrivial geometry[17,18] caused the appearance of mathematical models of such structures where, in particular, the Hamiltonian has the form (1.1) with the δ-term simulating the potential of a short range impurity[19] [if the nanostructure is placed in a magnetic field we must replace Δ in (1.1) by the Bochner Laplacian as above]. Moreover, the properties of the Green function G_U are needed for investigation of explicitly solvable models of the geometric scattering theory[20] or spectral theory of periodic hybrid manifolds.[21]

Our analysis of the singularity for the Green function G_U shows that in dimension two the singular term has the standard form even in the presence of an additional $\mathbf{U}(1)$-gauge potential (Theorem 15). On the other hand, in dimension three, S depends on U modulo a Lebesgue class of functions on X (see Theorem 16) and is defined up only to a continuous additive term (the situation here is completely similar to that for the Krein $\mathcal{Q}$-functions, they are defined up to an additive constant). The concrete value of this term is subject of analysis of a given physical problem and is out of the scope of the present work. We mention only that a possible way to fix the corresponding additive constant is to compare the integrated density of states with the trace of G_U^{ren}. At last but not at least we stress that our main results are new *even for the case of Euclidean spaces* $X=\mathbb{R}^n$.

II. DEFINITIONS AND PRELIMINARIES

Throughout the paper we denote by X a complete connected Riemannian manifold of bounded geometry, which means that the injectivity radius r_{inj} of X is positive and every covariant derivative of the Riemann curvature tensor is bounded. Examples are provided by homogeneous spaces with invariant metrics (in particular, Euclidean spaces), compact Riemannian manifolds and their covering manifolds; for discussion of various properties of such manifolds in the context of differential operators we refer to Ref. 22. The dimension of X we denote by ν; the geodesic distance between $x,y\in X$ will be denoted by $d(x,y)$. For $x\in X$ and $r\geqslant 0$ we use the notation $B(x,r)=\{y\in X: d(x,y)<r\}$; throughout the paper, we suppose $r<r_{\mathrm{inj}}$ for radiuses r of all considered sufficiently small balls. For a measurable function f on X, we denote by $\|f\|_p$ the L^p-norm of f. If K is a bounded operator from $L^p(X)$ to $L^q(X)$, $1\leqslant p,q\leqslant\infty$, then its norm will be denoted by $\|K\|_{p,q}$.

Let $A=A_j\,\mathrm{d}x^j$ be a 1-form on X, for simplicity we suppose here $A_j\in C^\infty(X)$. The functions A_j can be considered as the components of the vector potential of a magnetic field on X. On the other hand, A defines a connection ∇_A in the trivial line bundle $X\times\mathbb{C}\to X$, $\nabla_A u=\mathrm{d}u+iuA$; by $-\Delta_A=\nabla_A^*\nabla_A$ we denote the corresponding Bochner Laplacian. In addition, we consider a real-valued scalar potential U of an electric field on X. This potential will be assumed to satisfy the following conditions:

$$U_+ := \max(U,0)\in L^{p0}_{\mathrm{loc}}(X),\quad U_- := \max(-U,0)\in\sum_{i=1}^{n} L^{pi}(X),$$

$$2\leqslant p_i\leqslant\infty \quad \text{if } \nu\leqslant 3,\quad \nu/2<p_i\leqslant\infty \quad \text{if } \nu\geqslant 4,\quad 0\leqslant i\leqslant n;$$

we stress that p_i as well as n are not fixed and depend on U. The class of such potentials will be denoted by $\mathcal{P}(X)$. Below we will need an approximation of singular potentials by smooth ones; for this purpose the following lemma is useful.

Lemma 1: Let $f\in L^p_{\mathrm{loc}}(X)$, *where* $1\leqslant p<\infty$, *and* $f\geqslant 0$. *Then there is* $g\in C^\infty(X)$ *such that* $g\geqslant 0$ *and* $f-g\in L^q(X)$ *for all* $1\leqslant q\leqslant p$.

Proof: Fix $a\in X$ and for integers n, $n\geqslant 1$, denote $Y_n=B(a,n)\setminus\overline{B}(a,n-1)$. Fix a real sequence a_n, $a_n>0$ such that $\Sigma a_n\leqslant 1$ and denote by f_n the restriction of f to the set Y_n. Since the measure of Y_n is finite, for every n we can find a function g_n, $g_n\in C_0^\infty(X)$, such that $g_n\geqslant 0$, $\mathrm{supp}(g_n)\subset Y_n$, and $\max(\|f_n-g_n\|_p^p,\|f_n-g_n\|_1)\leqslant a_n$. Since the family (Y_n) is locally finite, the pointwise sum $g=\Sigma g_n$ exists and $g\in C_0^\infty(X)$. It is clear that $g\geqslant 0$ and $\max(\|f-g\|_p,\|f-g\|_1)\leqslant 1$, i.e., $f-g\in L^p(X)\cap L^1(X)$. □

We denote by $H_{A,U}$ the operator acting on functions $\phi\in C_0^\infty(X)$ by the rule $H_{A,U}\phi=-\Delta_A\phi+U\phi$. This operator is essentially self-adjoint in $L^2(X)$ and semibounded below,[23] its closure will be also denoted by $H_{A,U}$. By $\mathrm{spec}(H_{A,U})$ we denote the spectrum of $H_{A,U}$ and by $\mathrm{res}(H_{A,U})$ the set of regular points: $\mathrm{res}(H_{A,U})=\mathbb{C}\setminus\mathrm{spec}(H_{A,U})$. Let us denote the resolvent of $H_{A,U}$ by $R_{A,U}(\zeta)$, i.e., $R_{A,U}(\zeta)=(H_{A,U}-\zeta)^{-1}$.

Here we introduce two classes of integral kernels used in the paper. First class, $\mathcal{K}_{\mathrm{cont}}(p)$, $1\leqslant p\leqslant\infty$, consists of all continuous on $X\times X$ functions $K(x,y)$ satisfying for any $r>0$ the condition

$$\lfloor K\rfloor_{p,r} := \max(\sup\mathrm{ess}_{x\in X}\|\chi_{X\setminus B(x,r)}K(x,\cdot)\|_p,\sup\mathrm{ess}_{y\in X}\|\chi_{X\setminus B(y,r)}K(\cdot,y)\|_p)<\infty, \tag{2.1}$$

where χ_A stands for the characteristic function of the set $A\subset X$. The second class, $\mathcal{K}(\alpha,p)$, $0\leqslant\alpha<\nu$, $1\leqslant p\leqslant\infty$, consists of all measurable functions K on $X\times X$ obeying the condition (2.1) and

$$|K(x,y)|\leqslant c\max(1,d(x,y)^{-\alpha}) \quad \text{for a constant } c=c(K)>0. \tag{2.2}$$

We set $\mathcal{K}_{\mathrm{cont}}(\alpha,p):=\mathcal{K}(\alpha,p)\cap C(X\times X\setminus D)$, where D is the diagonal $\{(x,y)\in X\times X: x=y\}$.

The above introduced classes of integral kernels are important due to their relations to the properties of the resolvents $R_{A,U}(\zeta)$; these relationships are stated in the following theorem which is our starting point (see Ref. 23, for the proof).

Theorem 2: *For any* $\zeta \in \mathrm{res}(H_{A,U})$ *the resolvent* $R_{A,U}(\zeta)$ *has an integral kernel* $G_{A,U}(x,y;\zeta)$, *the Green function, which belongs to* $\mathcal{K}_{\mathrm{cont}}(\lambda,q)$, *where* q, $1 \leqslant q \leqslant \infty$, *is arbitrary, and* $\lambda = \nu - 2$ *for* $\nu > 2$, $\lambda \in (0,\nu)$ *is arbitrary for* $\nu = 2$, $\lambda = 0$ *for* $\nu = 1$; *moreover,* $G_{A,U}$ *is continuous in* $X \times X$ *for* $\nu = 1$.

We should point out that the Green function of a Schrödinger operator can violate the conditions (2.1) and (2.2), if the potential U is not from the class $\mathcal{P}(X)$. Even the decay of the Green function for large distances between x and y (the off-diagonal behavior) can be different from the "standard" exponential one coming from the comparison with the Laplacian; a good example is delivered by the one-dimensional inverse harmonic oscillator, whose Green function has only a polynomial decay at infinity (see Appendix A).

Our further calculations will involve a couple of operations with integral kernels introduced above; here we collect some useful estimates which will be used very intensively.

The well-known Gelfand-Dunford-Pettis theorem claims that if K is a bounded operator from $L^p(X)$ to $L^\infty(X)$ with some p, $1 \leqslant p < \infty$, then it is an integral operator and its kernel $K(x,y)$ satisfies the estimate

$$\sup \mathrm{ess}_{x \in X} \|K(x,\cdot)\|_q < \infty, \quad q = (1 - p^{-1})^{-1}. \tag{2.3}$$

Conversely, if a kernel $K(x,y)$ satisfies (2.3), then it is an integral kernel of a bounded operator from $L^p(X)$ to $L^\infty(X)$.

Lemma 3: Let $K_j : L^{q_j}(X) \to L^\infty(X)$, $1 \leqslant q_j < \infty$, *be bounded linear operators with integral kernels* $K_j(x,y)$, $j = 1,2$, *and* $W \in L^{q_1}(X)$, *then for a.e.* $(x,y) \in X \times X$ *the integral* $J(x,y) = \int_X K_1(x,z) W(z) K_2(z,y) \mathrm{d}z$ *exists and* $J(x,y)$ *is an integral kernel of the operator* $K_1 W K_2$.

Proof: The operator $K_1 W K_2$ is bounded from $L^{q_2}(X)$ to $L^\infty(X)$, therefore, it is an integral operator. Let $f \in L^{q_2}(X) \cap C(X)$ such that $f(x) > 0$ for all $x \in X$. Then there holds

$$K_1 W K_2 f(x) = \int_X K_1(x,z) W(z) \int_X K_2(z,y) f(y) \mathrm{d}y \, \mathrm{d}z. \tag{2.4}$$

From the other side, according to the estimates (2.3) for K_1 and K_2, there holds

$$\int_X |K_2(\cdot,y) f(y)| \mathrm{d}y \in L^\infty(X), \quad |W(\cdot)| \int_X |K_2(\cdot,y) f(y)| \mathrm{d}y \in L^{q_1}(X),$$

hence,

$$\int_X |K_1(x,z)| \left(|W(z)| \int_X |K_2(z,y) f(y)| \mathrm{d}y \right) \mathrm{d}z < \infty.$$

By the Fubini

$$\int_X \left(\int_X |K_1(x,z) W(z) K_2(z,y)| \mathrm{d}z \right) f(y) \mathrm{d}y < \infty,$$

and since $f(x) > 0$, the inner integral exists for a.e. $(x,y) \in X \times X$.

Let now f be an arbitrary function from $L^{q_2}(X)$. Repeating the arguments above, we get

$$K_1 W K_2 f(x) = \int_X \left(\int_X K_1(x,z) W(z) K_2(z,y) \mathrm{d}z \right) f(y) \mathrm{d}y \tag{2.5}$$

for a.e. $x \in X$. Therefore J is an integral kernel for $K_1 W K_2$. □

We will often use the estimate given by the lemma below (cf. Ref. 23).

Lemma 4: There exists $r_0>0$ *such that for any* α, r *with* $0<r<r_0$, $0\leqslant\alpha<\nu$, *and* $a,x\in X$ *there holds*

$$\int_{B(a,r)}\frac{\mathrm{d}y}{d(x,y)^{\alpha}}\leqslant cr^{\nu-\alpha} \tag{2.6}$$

with some $c>0$ *depending only on* α.

Our next auxiliary result is the following lemma.

Lemma 5: Let $K\in\mathcal{K}(\alpha,p)$, $1\leqslant p<\infty$, $p\alpha<\nu$, *and* $1/p+1/q=1$, *then* K *is an integral kernel of a bounded operator from* $L^q(X)$ *to* $L^{\infty}(X)$.

Proof: According to the Gelfand-Dunford-Pettis theorem we must prove

$$\sup\operatorname{ess}_{x\in X}\int_X|K(x,y)|^p\,\mathrm{d}y<\infty.$$

Fix r, $0<r<r_0$, and for $x\in X$ expand the integral into two parts,

$$\int_X|K(x,y)|^p\,\mathrm{d}y=\int_{B(x,r)}|K(x,y)|^p\,\mathrm{d}y+\int_{X\setminus B(x,r)}|K(x,y)|^p\,\mathrm{d}y.$$

The first term is estimated by Lemma 4, and the second one is majorated by $\lfloor K\rfloor_{p,r}^p$. □

Lemma 6: Let three measurable functions $K_1(x,y)$, $K_2(x,y)$ *and* $W(x)$ *be given, where* $x,y\in X$. *Denote* $F(x,y,z):=K_1(x,z)W(z)K_2(z,y)$, *and if the integral* $\int_X F(x,y,z)\mathrm{d}z$ *exists, denote it by* $J(x,y)$.

(A) *Let* $K_j\in\mathcal{K}_{\mathrm{cont}}(\alpha_j,p_j)$, $j=1,2$, *and* $W\in L^p(X)$, *such that* $1/p_1+1/p_2+1/p=1$ *and* $p>\nu/(\nu-\max(\alpha_1,\alpha_2))$. *Then* $F(x,y,\cdot)\in L^1(X)$ *for* $x\neq y$, *hence* J *is well defined. Moreover,* $J\in\mathcal{K}_{\mathrm{cont}}(\alpha,\infty)$, *where* $\alpha=\max(p'(\alpha_1+\alpha_2)-\nu,0)$ *with* $1/p+1/p'=1$, *if* $p'(\alpha_1+\alpha_2)\neq\nu$, *and* α *is an arbitrary number from* $(0,\nu)$ *otherwise*.

(B) *Let the conditions of the item* (A) *be satisfied. Assume additionally that* $\alpha_1+\alpha_2<\nu$ *and* $W\in L^q_{\mathrm{loc}}(X)$ *with* $q>\nu/(\nu-\alpha_1-\alpha_2)$. *Then* $F(x,y,\cdot)\in L^1(X)$ *for any* $x,y\in X$ *and* $J\in C(X\times X)$.

(C) *Let* $W\in L^p(X)$, *and* $K_1\in\mathcal{K}_{\mathrm{cont}}(p_1)$, $K_2\in\mathcal{K}_{\mathrm{cont}}(\alpha,p_2)$ *or* $K_1\in\mathcal{K}_{\mathrm{cont}}(\alpha,p_1)$, $K_2\in\mathcal{K}_{\mathrm{cont}}(p_2)$. *Assume additionally that* $1/p+1/p_1+1/p_2=1$ *and* $p>\nu/(\nu-\alpha)$. *Then* $F(x,y,\cdot)\in L^1(X)$ *for any* $x,y\in X$, *and* $J\in C(X\times X)$.

Proof: The proof of the items (A) and (B) is given in Ref. 23.

(C) We give a proof for the case $K_1\in\mathcal{K}_{\mathrm{cont}}(p_1)$ and $K_2\in\mathcal{K}_{\mathrm{cont}}(\alpha,p_2)$; the second case can be considered exactly in the same way.

Let $x,y\in X$; we show first that $F(x,y,\cdot)\in L^1(X)$. Let $r>0$, then for $z\in B(y,r)$ we have

$$|F(x,y,z)|\leqslant ck_1(x,y)W(z)d(y,z)^{-\alpha},\quad k_1(x,y):=\sup_{z\in B(y,r)}K_1(x,z)<\infty,\quad c>0, \tag{2.7}$$

therefore, $F(x,y,\cdot)\in L^1(B(y,r))$ due to the Hölder inequality and our conditions on p. For $z\notin B(y,r)$ due to the Hölder inequality we have the estimate

$$\int_{X\setminus B(y,r)}|F(x,y,z)|\mathrm{d}z\leqslant\left(\int_{X\setminus B(y,r)}|K_1(x,z)|^{p_1}\,\mathrm{d}z\right)^{1/p_1}\lfloor K_2\rfloor_{p_2,r}\|W\|_p,$$

and

$$\int_{X\setminus B(y,r)}|K_1(x,z)|^{p_1}\,\mathrm{d}z\leqslant\int_X|K_1(x,z)|^{p_1}\,\mathrm{d}z=\int_{B(x,r)}|K_1(x,z)|^{p_1}\,\mathrm{d}z+\int_{X\setminus B(x,r)}|K_1(x,z)|^{p_1}\,\mathrm{d}z,$$

where the first term on the right-hand where the first term on the right-hand side is finite due to the continuity of K_1, and the second one is estimated by (2.1). This proves the inclusion $F(x,y,\cdot)\in L^1(X)$.

Now let $x_0, y_0 \in X$, $0<r<R$, and $x \in B(x_0, r/2)$, $y \in B(y_0, r/2)$, then

$$|J(x,y)-J(x_0,y_0)| \leqslant \int_{B(y_0,r)} |F(x,y,z)|\mathrm{d}z + \int_{B(y_0,r)} |F(x_0,y_0,z)|\mathrm{d}x + \int_{X\setminus B(y_0,R)} |F(x,y,z)|\mathrm{d}z + \int_{X\setminus B(y_0,R)} |F(x_0,y_0,z)|\mathrm{d}z + \int_{B(y_0,R)\setminus B(y_0,r)} |F(x,y,z)-F(x_0,y_0,z)|\mathrm{d}z. \tag{2.8}$$

Take $\epsilon>0$ and assume $r<r_0$. For $z \in B(y_0,r)$ we estimate $F(x,y,z)$ as in (2.7), then we get using Lemma 4

$$\int_{B(y_0,r)} |F(x,y,z)|\mathrm{d}z \leqslant c \sup_{\substack{x\in B(x_0,r),\\ y\in B(y_0,r)}} K_1(x,y) \|W\|_p \left[\int_{B(y_0,r)} d(y,z)^{p\alpha/(1-p)}\,\mathrm{d}z\right]^{(p-1)/p} \leqslant Cr^{\nu-\alpha-(1/p)} = o(1)$$

as $r\to 0$. On the other hand,

$$\int_{X\setminus B(x_0,R)} |F(x,y,z)|\mathrm{d}z \leqslant \lfloor K_1\rfloor_{p_1,r} \lfloor K_2\rfloor_{p_2,r} \|\chi_{X\setminus B(x_0,R)} W\|_p = o(1) \quad \text{as } R\to\infty.$$

Finally, we conclude that r can be taken sufficiently small and R sufficiently large, such that the sum of the first four terms on the right-hand side of (2.8) is less than $\epsilon/2$. Now it is sufficient to prove that at these fixed r and R the function

$$\int_{B(y_0,R)\setminus B(y_0,r)} F(x,y,z)\mathrm{d}z$$

is continuous as $x \in B(x_0,r/2)$ and $y \in B(y_0,r/2)$. To do this, we note that with some $C'>0$ the following estimate $|F(x,y,z)| \leqslant C'|W(z)|$ takes place for all $x \in B(x_0,r/2)$, $y \in B(y_0,r/2)$, and $z \in B(y_0,R)\setminus B(y_0,r)$. Since $W \in L^1(B(y_0,R)\setminus B(y_0,r))$, the requested continuity follows from the Lebesgue majorization theorem. □

As it was mentioned in the Introduction, we are going to present the Green function in the form

$$G_{A,U}(x,y;\zeta) = S_{A,U}(x,y) + G^{\mathrm{ren}}_{A,U}(x,y;\zeta),$$

where the second term must be continuous in $X\times X$. Such a representation is trivial in the one-dimensional case, the Green function is continuous, and one can set $S_{A,U}\equiv 0$. In dimensions $\nu \geqslant 4$ the problem makes no sense, as the following example shows.

Example 7 (four-dimensional Laplace operator): Consider the simplest case of the Laplacian in $L^2(\mathbb{R}^4)$. The Green function takes the form

$$G(x,y;\zeta) = \frac{\sqrt{-\zeta}}{4\pi^2|x-y|} K_1(\sqrt{-\zeta}|x-y|),$$

where K_1 is the modified Bessel function of the first order. Near the diagonal $x=y$ one has

$$G(x,y;\zeta) = \frac{1}{4\pi^2|x-y|^2} - \frac{\zeta \log|x-y|}{8\pi^2} + k(x,y;\zeta)$$

with a continuous k. Therefore, for $\zeta_1, \zeta_2 \in \mathrm{res}(-\Delta)$, $\zeta_1 \neq \zeta_2$, the difference

$$G(x,y;\zeta_1) - G(x,y;\zeta_2) \sim \frac{\zeta_2 - \zeta_1}{8\pi^2} \log|x-y|$$

is a discontinuous function, so that the singularity cannot be chosen independent of the spectral parameter.

Therefore, the only nontrivial cases remain $\nu=2$ and $\nu=3$, which we will consider in the present paper.

Example 8 (on-diagonal singularity for the Laplace operator): Here we consider the case $A=0$ and $U=0$, i.e., the case of the Laplace-Beltrami operator $-\Delta$ on the manifold X with $\nu=2$ or $\nu=3$. Denote the Green function of $-\Delta$ by $G(x,y;\zeta)$. Take $y \in X$ and introduce polar coordinates (r_y,ω), $r_y=d(x,y)$, $\omega \in \mathbb{S}^{\nu-1}$, centered at y, then we have in a normal neighborhood W_y of y,

$$-\Delta\psi = -\frac{\partial^2\psi}{\partial r_y^2} + \left(\frac{\nu-1}{r_y} + \theta_y^{-1}\frac{\partial\theta_y}{\partial r_y}\right)\frac{\partial\psi}{\partial r_y},$$

where the function $\theta_y=\theta_y(r_y,\omega)$ is defined in such a way that in W_y, we have $\mathrm{d}x = r_y^{\nu-1}\theta_y(r_y,\omega)\mathrm{d}r_y\,\mathrm{d}\omega$. Since $r_y^{\nu-1}\theta(r_y,\omega)$ is the Jacobian for the inverse to the exponential map in W_y, there holds $\theta_y(0,\omega)\geqslant c_y>0$ and $(\partial/\partial r)\theta_y(0,\omega)=0$ for all $\omega\in\mathbb{S}^{\nu-1}$. Moreover, $\inf c_y>0$ as y runs over a compact set in X.

Denote now

$$S(x,y) = \begin{cases} \dfrac{1}{2\pi}\log\dfrac{1}{d(x,y)}, & \nu=2, \\ \dfrac{1}{4\pi d(x,y)}, & \nu=3, \end{cases}$$

and for a fixed $\zeta\in\mathrm{res}(-\Delta)$ denote $K(x,y) := G(x,y;\zeta) - S(x,y)$. Then there holds

$$(-\Delta-\zeta)K(\cdot,y) = \theta_y^{-1}\frac{\partial\theta_y}{\partial r_y}\frac{\partial}{\partial r_y}S(\cdot,y) - \zeta S(\cdot,y) =: L(x,y). \tag{2.9}$$

It is clear that $L(\cdot,y)\in L^2(W_y)$, hence due to the Sobolev embedding theorem, $x\mapsto K(x,y)$ is continuous in W_y. Let us show that really $K(x,y)$ is continuous in (x,y). To do this, we fix $y_0\in X$ and take $r_0>0$ such that $B(y_0,2r_0)\subset W_{y_0}$. We prove the following assertion:

(CM) *the map* $B(y_0,r_0)\ni y\mapsto L(\cdot,y)\in L^2(B(y_0,r_0))$ *is continuous with respect to the norm topology of the space* $L^2(B(y_0,r_0))$.

Let $\chi\in C^\infty(X)$ such that $\mathrm{supp}\,\chi\subset B(y_0,2r_0)$, $\chi(x)=1$ for $x\in B(y_0,r_0)$, and $0\leqslant\chi(x)\leqslant 1$ for all $x\in X$. Note that $B(y_0,2r_0)$ is a normal neighborhood of y for all $y\in B(y_0,2r_0)$, therefore we can assume that $L(x,y)$ is defined for all $x\in X$ and $y\in B(y_0,2r_0)$. Extend L by zero for $y\notin B(y_0,2r_0)$ and set $T(x,y)=\chi(x)\chi(y)L(x,y)$. It is clear that $T\in\mathcal{K}_{\mathrm{cont}}(\alpha,p)$ where p is arbitrary number with $1\leqslant p\leqslant\infty$, and $\alpha=1$ for $\nu=3$, α is any strictly positive number for $\nu=2$. Using items (A) and (B) of Lemma 6 we can easily show that for every $f\in L^2(X)$ the mapping $B(y_0,r_0)\ni y\to\int_{B(y_0,r_0)}L(x,y)f(y)\mathrm{d}y$ is continuous and the mapping $B(y_0,r_0)\ni y\to\int_{B(y_0,r_0)}|L(x,y)|^2\,\mathrm{d}y$ is also continuous. This proves the assertion (CM). Returning to Eq. (2.9) we see that $K(\cdot,y)$ tends to $K(\cdot,y_0)$ with respect to the topology of $W_2^2(B(y_0,r_0))$. Due to the Sobolev embedding theorem, this implies a uniform convergence in the ball $B(y_0,r)$, i.e.,

$$\lim_{y\to y_0}\sup_{x\in B(y_0,r_0)}|K(x,y)-K(x,y_0)| = 0.$$

This together with the continuity in x proves the required joint continuity in (x,y). Therefore, the functions $S(x,y)$ are suitable on-diagonal singularities of the Laplace operator.

Note that the proof of the separate continuity of the function $K(x,y)$ is considerably simpler and can be found, e.g., in Ref. 24.

III. ON-DIAGONAL BEHAVIOR FOR SINGULAR SCALAR POTENTIALS

Below we will use the notation $L^{p+}_{\mathrm{loc}}(X)=\cup_{q>p}L^q_{\mathrm{loc}}(X)$.

Lemma 9 (singularity is independent of the spectral parameter): Let $\nu=2$ *or* 3, $A\in[C^\infty(X)]^\nu$, $U\in\mathcal{P}(X)$, $\zeta_1,\zeta_2\in\mathrm{res}(H_{A,U})$, *then the difference* $G_{A,U}(x,y;\zeta_1)-G_{A,U}(x,y;\zeta_2)$ *is continuous in* $X\times X$.

Proof: The proof follows from the Hilbert resolvent identity for the kernels, $R_{A,U}(\zeta_1)-R_{A,U}(\zeta_2)=(\zeta_1-\zeta_2)R_{A,U}(\zeta_1)R_{A,U}(\zeta_2)$. The integral kernel $\int_X G_{A,U}(x,z;\zeta_1)G_{A,U}(z,y;\zeta_2)\mathrm{d}z$ of $R_{A,U}(\zeta_1)R_{A,U}(\zeta_2)$ is continuous due to Lemma 6(B). □

The preceding lemma shows that for fixed A and U, the on-diagonal singularity in question exists; for example, as a singularity one can take $G_{A,U}(x,y;\zeta_0)$ for a fixed $\zeta_0\in\mathrm{res}(H_{A,U})$. Our aim is to understand how the singularity depends on A and U.

The following lemma shows that Green functions of Schrödinger operators with smooth potentials have the same on-diagonal singularity.

Lemma 10 (singularity for operator with smooth potentials): Let $\nu=2$ *or* 3, $A\in[C^\infty(X)]^\nu$, $U,V\in\mathcal{P}(X)\cap C^\infty(\Omega)$, *where* Ω *is a domain in* X, *then the difference* $G_{A,U}(x,y;\zeta)-G_{A,V}(x,y;\zeta)$ *has a continuous extension to all points* (x,x), $x\in\Omega$. *In particular, if* $\Omega=X$, *then* $G_{A,U}(x,y;\zeta)-G_{A,V}(x,y;\zeta)\in\mathcal{K}_{\mathrm{cont}}(p)$ *with arbitrary* $p\geqslant 1$.

Proof: Fix a real E sufficiently close to $-\infty$ and take $x_0\in\Omega$. We show that in a neighborhood of (x_0,x_0) in $X\times X$, the difference $F(x,y;E)=G_{A,U}(x,y;E)-G_{A,V}(x,y;E)$ is the restriction of a continuous function in this neighborhood. Due to Lemma 9 the same will hold for all values of the spectral parameter.

Let Ω_0 be a bounded subdomain of Ω and contain x_0; denote $W=U+\chi_{\Omega_0}(V-U)$; it is clear that $W\in\mathcal{P}(X)$. Since $W-U$ is bounded with compact support, one has $R_{A,U}(\zeta)-R_{A,W}(\zeta)=R_{A,U}(\zeta)(W-U)R_{A,W}(\zeta)$, so that the difference

$$G_{A,U}(x,y;E)-G_{A,W}(x,y;E)=\int_X G_{A,U}(x,z;E)(W(z)-U(z))G_{A,W}(z,y;E)\mathrm{d}z$$

is continuous in $X\times X$ according to Lemma 6(B). It remains to show that the function $L(x,y)=G_{A,V}(x,y;E)-G_{A,W}(x,y;E)$ is continuous on $\Omega_0\times\Omega_0$. To do this, let us note that in the sense of distributions the following equality holds:

$$((H_{A,V})_x-E+\overline{(H_{A,V})_y}-E)L(x,y)=(W(x)-V(x))G_{A,W}(x,y;E)+(W(y)-V(y))G_{A,W}(x,y;E), \tag{3.1}$$

where $(H_{A,V})_x$ [respectively, $(H_{A,V})_y$] means that $H_{A,V}$ acts on the first (respectively, the second) argument in L; the bar means that we change the coefficients in $H_{A,V}$ by the complex conjugate ones. The operator in the left-hand side of (3.1) is elliptic in $\Omega_0\times\Omega_0$ with smooth coefficients, while the right-hand term vanishes in $\Omega_0\times\Omega_0$. According to the elliptic regularity theorem L is continuous in $\Omega_0\times\Omega_0$. □

The following Proposition contains our main result on the dependence of the on-diagonal singularity on singularities of the scalar potential.

Proposition 11 (preserving the on-diagonal singularity under singular perturbations): Let $\nu=2$ *or* 3, $A\in[C^\infty(X)]^\nu$, *and* $U_1,U_2\in\mathcal{P}(X)$. *If* $\nu=3$, *assume additionally that* $U_1-U_2\in L^{3+}_{\mathrm{loc}}(X)$. *Then the difference* $G_{A,U_1}(x,y;\zeta)-G_{A,U_2}(x,y;\zeta)$ *is continuous in* $X\times X$ *for any* $\zeta\in\mathrm{res}(H_{A,U_1})\cap\mathrm{res}(H_{A,U_2})$.

Proof: For the sake of brevity we fix A and remove it from the notation, i.e., instead of $G_{A,U}$ we will write G_U, etc.

First of all, using Lemma 1 we choose functions $V_1,V_2\in C^\infty(X)$ semibounded below such that $W_j:=U_j-V_j=\Sigma_{s=1}^{n_j}W_{j,s}$, where $W_{j,s}\in L^{p_{j,s}}$ with $2\leqslant p_{j,s}<\infty$, $s=1,\ldots,n_j$, $j=1,2$.

For $\zeta \in \mathrm{res}(H_{U_1}) \cap \mathrm{res}(H_{U_2})$ the sets $\mathcal{D}_j := (H_{U_j} - \zeta) C_0^\infty(X)$ are dense in $L^2(X)$, because $C_0^\infty(X)$ is an essential domain of both H_{U_1} and H_{U_2}. As $\psi \in \mathcal{D}_j$, one has

$$R_{U_j}(\zeta)\psi - R_{V_j}(\zeta)\psi = R_{V_j}(\zeta) W_j R_{U_j}(\zeta)\psi. \tag{3.2}$$

As the operators on both sides of (3.2) are bounded and coincide on a dense subset, they coincide everywhere, i.e., (3.2) holds for any $\psi \in L^2(X)$. Combining Lemma 3 and Lemma 6(B) we conclude that in the dimension two, the operator on the right-hand side of (3.2) has a continuous integral kernel, which together with Lemma 10 implies the conclusion of the proposition.

Let us consider the dimension three more carefully. To be shorter, we remove the dependence of the resolvents on ζ from the notation. We have the following chain of equalities:

$$\begin{aligned} R_{U_1} - R_{U_2} &= R_{V_1} - R_{V_2} + R_{V_1} W_1 R_{U_1} - R_{V_2} W_2 R_{U_2} = R_{V_1} - R_{V_2} + R_{V_1} W_1 R_{U_1} + R_{V_2} W_2 (R_{U_1} - R_{U_2}) \\ &\quad - R_{V_2} W_2 R_{U_1} = R_{V_1} - R_{V_2} + R_{V_2} W_2 (R_{U_1} - R_{U_2}) + R_{V_2} (W_1 - W_2) R_{U_1} + (R_{V_1} - R_{V_2}) W_1 R_{U_1}. \end{aligned}$$

Therefore, $(1 - R_{V_2} W_2)(R_{U_1} - R_{U_2}) =: L = A + B + C$, where $A := R_{V_1} - R_{V_2}$, $B := R_{V_2}(W_1 - W_2) R_{U_1}$, $C := (R_{V_1} - R_{V_2}) W_1 R_{U_1}$.

Due to Lemma 10, the operator A has an integral kernel from $\mathcal{K}_{\mathrm{cont}}(p)$ with arbitrary p, $p \geqslant 1$. Since $W_1 - W_2 \in L^{3+}_{\mathrm{loc}}(X)$, the operator B has an integral kernel from $\mathcal{K}_{\mathrm{cont}}(\infty)$ due to Theorem 2 and the items (A), (B) of Lemma 6. As $R_{V_2} - R_{V_1} \in \mathcal{K}_{\mathrm{cont}}(p)$ with arbitrary $p \geqslant 1$ (Lemma 10), the integral kernel for C is from $\mathcal{K}_{\mathrm{cont}}(\infty)$ due to Theorem 2 again and the items (A), (C) of Lemma 6. Therefore, the operator L has an integral kernel $L(x,y) = L(x,y;\zeta) \in \mathcal{K}_{\mathrm{cont}}(\infty)$. Now we note that the multiplication by $W_{2,s}$ is a continuous mapping from $L^\infty(X)$ to $L^{p_{2,s}}(X)$. At the same time, as $G_{V_2} \in \mathcal{K}_{\mathrm{cont}}(1,p)$, $p \geqslant 1$, the resolvent R_{V_2} is a bounded operator from each $L^{p_{2,s}}(X)$ to $L^\infty(X)$ due to Lemma 5. Since $L = (1 - R_{V_2} W_2)(R_{U_1} - R_{U_2})$, we can combine Theorem 2 and Lemma 5 to show that the operator L is a bounded map from $L^p(X)$ to $L^\infty(X)$ for any p with $3/2 < p < \infty$. Since $|L(x,y;\zeta)| = |L(y,x;\bar{\zeta})|$, we see from (2.3) that $L(x,y) \in \mathcal{K}_{\mathrm{cont}}(q)$ for any q with $1 < q < 3$.

One can find ζ such that $\|R_{V_2}(\zeta) W_2\|_{\infty,\infty} =: \alpha < 1$ (see Ref. 23), therefore, the operator $1 - R_{V_2} W_2$ acting in $L^\infty(X)$ is invertible and for any $n \in \mathbb{N}$ there holds

$$R_{U_1} - R_{U_2} = \sum_{k=0}^{n-1} (R_{V_2} W_2)^k L + (1 - R_{V_2} W_2)^{-1} (R_{V_2} W_2)^n L. \tag{3.3}$$

Applying iteratively Lemmas 3 and 6(A) and taking into account Theorem 2, we can show that the operators $(R_{V_2} W_2)^k R_{V_2}$ have integral kernels from $\mathcal{K}_{\mathrm{cont}}(\beta_k, \infty)$ with $\beta_k \leqslant 1$. At the same time, all these operators are bounded from $L^p(X)$ to $L^\infty(X)$ for any p with $3/2 < p < \infty$. Using the same arguments as for L above, we conclude that these kernels are in $\mathcal{K}_{\mathrm{cont}}(\beta_k, q)$ for any q with $1 < q < 3$. Applying now Lemma 6 (C) one proves that the first term on the right-hand side has a continuous integral kernel.

Denote $T_n := (1 - R_{V_2} W_2)^{-1} (R_{V_2} W_2)^{n-1} R_{V_2}$; this operator is bounded from each $L^{p_{j,s}}(X)$ to $L^\infty(X)$; due to the Gelfand-Dunford-Pettis theorem, this is an integral operator with an integral kernel $T_n(x,y)$. The second term in (3.3) takes the form $T_n W_2 L$, and by virtue of Lemma 3 this is also an integral operator with the kernel $S_n(x,y) := \int_X T_n(x,z) W_2(z) L(z,y) \mathrm{d}z$. From the other side, one can write $S_n(x,y) = T_n W_2 l_y(x)$, where $l_y(x) := L(x,y)$. Note that for each $y \in X$ there holds $l_y \in L^\infty(X)$, and the operator $T_n W_2$ is a bounded mapping from $L^\infty(X)$ to $L^\infty(X)$ with the norm $\|T_n W_2\|_{\infty,\infty} \leqslant \|(1 - R_{V_2} W_2)^{-1}\|_{\infty,\infty} \cdot \|R_{V_2} W_2\|^n_{\infty,\infty} \leqslant \alpha^n / (1 - \alpha)$.

Now let us fix $x_0 \in X$ and take a bounded open neighborhood Ω of x_0. It is clear that $\|l_y\|_\infty \leqslant c_\Omega$ for all $y \in \Omega$ with a certain $c_\Omega > 0$. Therefore $\sup_{x,y \in \Omega} |S_n(x,y;\zeta)| \leqslant c_\Omega \alpha^n / (1 - \alpha)$. Take $\epsilon > 0$ and choose n such that $c_\Omega \alpha^n / (1 - \alpha) < \epsilon$. From Eq. (3.3) we have in $\Omega \times \Omega$ the relation $G_{U_1}(x,y;\zeta) - G_{U_2}(x,y;\zeta) = K_n(x,y) + \tau_n(x,y)$, where K_n is continuous and $|S_n| < \epsilon$. As ϵ is arbitrary, this means that $G_{U_1}(x,y;\zeta) - G_{U_2}(x,y;\zeta)$ is continuous in $\Omega \times \Omega$. Since $x_0 \in X$ is arbitrary, the lemma is proven. Due to Lemma 9, this holds for all $\zeta \in \mathrm{res}(H_{V_1}) \cap \mathrm{res}(H_{V_2})$. □

The following example shows that the condition $U_1-U_2\in L^{3+}_{\mathrm{loc}}(X)$ cannot be omitted in dimension three.

Example 12 (Coulomb potential in three dimensions): Let $X=\mathbb{R}^3$, $A=0$, and $U=q/|x|$, i.e., $H\equiv H_{A,U}=-\Delta+q/|x|$. Clearly, $U\notin L^{3+}_{\mathrm{loc}}(\mathbb{R}^3)$. The Green function can be calculated explicitly,[25]

$$G(x,y;\zeta)=\frac{\Gamma(1-\kappa)}{4\pi|x-y|}[W_{\kappa,1/2}(\sqrt{-\zeta}\xi)M'_{\kappa,1/2}(\sqrt{-\zeta}\eta)-W'_{\kappa,1/2}(\sqrt{-\zeta}\xi)M_{\kappa,1/2}(\sqrt{-\zeta}\eta)], \tag{3.4}$$

where $\xi:=|x|+|y|+|x-y|$, $\eta:=|x|+|y|-|x-y|$, $\kappa=-q/\sqrt{-4\zeta}$, $M_{\kappa,1/2}$ and $W_{\kappa,1/2}$ are the Whittaker functions,

$$M_{\kappa,1/2}(x)=e^{x/2}x\Phi(a,2;x),\quad W_{\kappa,1/2}(x)=e^{x/2}x\Psi(a,2;x). \tag{3.5}$$

Here $\Phi(a,c;x)$ and $\Psi(a,c;x)$ are the Kummer function and the Tricomi function, respectively. We prove in Appendix B the asymptotics

$$G(x,0;\zeta)=\frac{1}{4\pi|x|}+\frac{q}{4\pi}\log|x|-\frac{\sqrt{-\zeta}}{4\pi}+\frac{q}{4\pi}\left(\psi\left(1+\frac{q}{2\sqrt{-\zeta}}\right)+\log\sqrt{-\zeta}+\log(2/e)+2C_E\right)$$
$$+O(|x|\log|x|). \tag{3.6}$$

Therefore, the singularity for $G(x,y;\zeta)$ contains an unavoidable logarithmic term and is different from the standard three-dimensional singularity.

IV. DEPENDENCE OF THE SINGULARITY ON THE MAGNETIC FIELD

Lemma 13 (singularity due to the magnetic field in two dimensions): Let $\nu=2$, then for any $A\in[C^\infty(X)]^\nu$ the difference $G_{A,0}(x,y;\zeta)-G_{0,0}(x,y;\zeta)$ is continuous in $X\times X$ if $\zeta\in\mathrm{res}(H_{A,0})\cap\mathrm{res}(H_{0,0})$.

Proof: Let x_0 be an arbitrary point of X. We show that the difference $G_{A,0}(x,y;\zeta)-G_{0,0}(x,y;\zeta)$ is continuous in a neighborhood of (x_0,x_0) for at least one value of the spectral parameter ζ; due to Lemma 9 this difference is continuous for all admissible spectral parameters.

Take two sufficiently small numbers r and r_0 with $0<r<r_0$. Fix a function $\phi\in C^\infty_0(X)$ such that $\mathrm{supp}\,\phi\subset B(x_0,r_0)$, $\phi(x)=1$ as $x\in B(x_0,r)$. Denote for brevity $H_0:=H_{0,0}$, $H_1:=H_{A,0}$, $H_2:=H_{\phi A,0}$; the corresponding Green functions will be denoted by G_0, G_1, and G_2, respectively.

In $B(x_0,r)\times B(x_0,r)$ for real ζ sufficiently close to $-\infty$ one has in the sense of distributions

$$(((H_1)_x-\zeta)+((\overline{H_2})_y-\zeta))(G_1(x,y;\zeta)-G_2(x,y;\zeta))=0,$$

therefore, due to the elliptic regularity, the difference $G_1(x,y;\zeta)-G_2(x,y;\zeta)$ is continuous in $B(x_0,r)\times B(x_0,r)$. Now we are going to show that $G_2(x,y;\zeta)-G_0(x,y;\zeta)$ is continuous. Since H_0 and H_2 are uniformly elliptic operators with C^∞-bounded coefficients, we are able to use estimates for the Green functions and their derivatives obtained in Ref. 22. First of all,

$$G_0(x,y;\zeta),\quad G_2(x,y;\zeta)\in\mathcal{K}_{\mathrm{cont}}(\lambda,q) \tag{4.1}$$

for arbitrary $\lambda>0$ and $q\in[1,\infty]$ (see Theorem 2). Moreover, for ζ close to $-\infty$ both these kernels are smooth outside the diagonal $x=y$, and according to (Ref. 22, Theorem A1.3.7) we have

$$|\partial_x G_0(x,y;\zeta)|\leqslant C\left(1+\frac{|\log d(x,y)|}{d(x,y)}\right)e^{-\omega d(x,y)},\quad j=1,2,$$

where ∂ is any first order derivative taken in canonical coordinates, and $C,\omega>0$. Additionally, by (Ref. 22, Theorem A1.2.3) for any $p\geqslant 1$ there exist $\epsilon,C'>0$ such that

$$\sup_x \int_{d(x,y)>r} |\partial_x G_0(x,y;\zeta)|^p e^{\epsilon d(x,y)}\, \mathrm{d}y + \sup_y \int_{d(x,y)>r} |\partial_x G_0(x,y;\zeta)|^p e^{\epsilon d(x,y)}\, \mathrm{d}x \leqslant C', \quad j=1,2.$$

This implies the inclusion

$$\partial_x G_0(x,y;\zeta) \in \mathcal{K}_{\mathrm{cont}(1+\lambda,q),} \tag{4.2}$$

with the same λ and q as in (4.1).

In canonical coordinates in $B(x_0,r_0)$ both H_0 and H_2 are given by symmetric second-order elliptic expressions with the same principal symbol, in particular, the difference $T:=H_2-H_0$ is defined by a first order differential expression, $T=b_1(x)\partial_1+b_2(x)\partial_2+c(x)$, where b_1, b_1, c are compactly supported smooth functions. For the functions of the form $\psi=(H_0-\zeta)\phi$ with $\phi \in C_0^\infty(X)$ we have $(H_2-\zeta)\phi=(H_0+T-\zeta)R_0(\zeta)\psi=(1+TR_0(\zeta))\psi$, therefore, $R_0(\zeta)\psi-R_2(\zeta)\psi = R_2(\zeta)TR_0(\zeta)\psi$. In terms of integral kernels this means

$$\begin{aligned}\int_X G_0(x,y;\zeta)\psi(y)\mathrm{d}y - \int_X G_2(x,y;\zeta)\psi(y)\mathrm{d}y &= \int_X G_2(x,z;\zeta)[b_1(z)\partial_1 + b_2(z)\partial_2 + c(z)] \\ &\quad \times \int_X G_0(z,y;\zeta)\psi(y)\mathrm{d}y\, \mathrm{d}z \\ &= \int_X G_2(x,z;\zeta) \int_X [b_1(z)K_1(z,y;\zeta) + b_2(z)K_2(z,y;\zeta) \\ &\quad + c(z)G_0(z,y;\zeta)]\psi(y)\mathrm{d}y\, \mathrm{d}z, \end{aligned} \tag{4.3}$$

where

$$K_1(z,y;\zeta) := \partial_{z_1} G_0(z,y;\zeta), \quad K_2(z,y;\zeta) := \partial_{z_2} G_0(z,y;\zeta).$$

According to the general theory of elliptic operators, the set $(H_0-\zeta)C_0^\infty(X)$ is dense in all $L^p(X)$ with any p, $1 \leqslant p < \infty$, if ζ is sufficiently close to $-\infty$ (Ref. 22, Sec. A1.2). Due to the estimates (4.1) and (4.2), and Lemma 5, the kernels K_1 and K_2 define bounded operators from $L^q(X)$ to $L^\infty(X)$ for arbitrary $q>2$; denote these operators by $K_1(\zeta)$ and $K_2(\zeta)$. In this notation, the expression on the right-hand side of (4.3) can be rewritten as

$$R_0(\zeta)\psi - R_2(\zeta)\psi = [R_2(\zeta)b_1K_1(\zeta) + R_2(\zeta)b_2K_2(\zeta) + R_2(\zeta)cR(\zeta)]\psi.$$

The operators in both sides are bounded from $L^q(X)$ to $L^\infty(X)$ with any $q>2$ and coincide on a dense subset, therefore, the corresponding kernels coincide, i.e.,

$$\begin{aligned} G_0(x,y;\zeta) - G_2(x,y;\zeta) &= \int_X G_2(x,z;\zeta)b_1(z)K_1(z,y;\zeta)\mathrm{d}z + \int_X G_2(x,z;\zeta)b_2(z)K_2(z,y;\zeta)\mathrm{d}z \\ &\quad + \int_X G_2(x,z;\zeta)c(z)G_0(z,y;\zeta)\mathrm{d}z. \end{aligned} \tag{4.4}$$

By Lemma 6 (B), the function on the right-hand side of (4.4) is continuous. □

The three-dimensional analog of Lemma 13 is not true as the following example shows.

Example 14 (three-dimensional Landau Hamiltonian): Consider in $L^2(\mathbb{R}^3)$ the vector potential of a nonzero uniform magnetic field. By a suitable choice of coordinates one can assume that the field is directed along the x_3 axis, i.e., the magnetic strength vector is $\mathbf{B}=(0,0,2\pi\xi x_3)$, where $\xi > 0$ is the density of the magnetic flux through the plane (x_1,x_2). Choose the symmetric gauge for the magnetic vector potential, $\mathbf{A}(\mathbf{x})=\frac{1}{2}\mathbf{B}\times\mathbf{x}$, then $H:=H_{\mathbf{A},0}$ takes the form

$$H=\left(i\frac{\partial}{\partial x_1}-\pi\xi x_2\right)^2+\left(i\frac{\partial}{\partial x_2}+\pi\xi x_1\right)^2-\frac{\partial^2}{\partial x_3^2},$$

and the corresponding Green function is $G(\mathbf{x},\mathbf{y};\zeta)=\Phi(\mathbf{x},\mathbf{y})F(\mathbf{x}-\mathbf{y};\zeta)$, where

$$F(\mathbf{x};\zeta)=\int_0^\infty \frac{\exp[-\pi|\xi|(\mathbf{x}_\perp^2(e^t-1)^{-1}+\mathbf{x}_\parallel^2 t^{-1}]}{(1-e^{-t})\exp\left[\left(\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)t\right]\sqrt{t}}\mathrm{d}t, \tag{4.5}$$

$\mathbf{x}_\perp=(x_1,x_2,0)$ and $\mathbf{x}_\parallel=(0,0,x_3)$.[26] In Appendix C we prove the asymptotics

$$G(\mathbf{x},\mathbf{y};\zeta)=\frac{e^{i\pi\xi(\mathbf{x}_\perp\wedge\mathbf{y}_\perp)}}{4\pi|\mathbf{x}-\mathbf{y}|}+\frac{1}{4}\left(\frac{|\xi|}{\pi}\right)^{1/2}Z\left(\frac{1}{2};\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)+o(|\mathbf{x}-\mathbf{y}|) \tag{4.6}$$

as $|\mathbf{x}-\mathbf{y}|\to 0$; here $Z(z;u)$ is the generalized Riemann ζ-function (also known as the Hurwitz ζ-function). Therefore, the on-diagonal asymptotics is

$$S(\mathbf{x},\mathbf{y})=\frac{e^{i\pi\xi(\mathbf{x}_\perp\wedge\mathbf{y}_\perp)}}{4\pi|\mathbf{x}-\mathbf{y}|}=\frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\exp\left(\frac{i\mathbf{B}(\mathbf{x}\times\mathbf{y})}{2}\right).$$

V. SUMMARY OF RESULTS

We summarize some corollaries from the proven assertions in the following two theorems.

Theorem 15 (on-diagonal singularities of the Green functions in dimension two): *On a two-dimensional manifold of bounded geometry X, for any vector potential $A\in[C^\infty(X)]^2$ and scalar potential $U\in\mathcal{P}(X)$, the Green function $G_{A,U}$ of the Schrödinger operator $H_{A,U}=-\Delta_A+U$ has the same on-diagonal singularity as that for the Laplace-Beltrami operator, i.e.,*

$$G_{A,U}(x,y;\zeta)=\frac{1}{2\pi}\log\frac{1}{d(x,y)}+G_{A,U}^{\mathrm{ren}}(x,y;\zeta),$$

where $G_{A,U}^{\mathrm{ren}}$ is continuous on $X\times X$.

Proof: Proposition 11 shows that the singularity does not depend on the scalar potential $U\in\mathcal{P}(X)$, and Lemma 13 shows that it is independent of the magnetic potential. Therefore, the singularity coincides with that for the Laplacian, see Example 8. □

Theorem 16 (on-diagonal singularities of the Green functions in dimension three): *Let X be a three-dimensional manifold of bounded geometry. For $U\in\mathcal{P}(X)$ and $A\in[C^\infty(X)]^3$ consider the Schrödinger operator $H_{A,U}=-\Delta_A+U$ and its Green function $G_{A,U}(x,y;\zeta)$. If $U_1,U_2\in\mathcal{P}(X)$ and $U_1-U_2\in L^{3+}_{\mathrm{loc}}(X)$, then the Green functions G_{A,U_1} and G_{A,U_2} have the same on-diagonal singularity (i.e., $G_{A,U_1}-G_{A,U_2}$ is continuous in $X\times X$). In particular, for any $U\in\mathcal{P}(X)\cap L^{3+}_{\mathrm{loc}}(X)$ there holds*

$$G_{0,U}(x,y;\zeta)=\frac{1}{4\pi d(x,y)}+G_{0,U}^{\mathrm{ren}}(x,y;\zeta), \tag{5.1}$$

where $G_{0,U}^{\mathrm{ren}}$ is continuous in $X\times X$.

Proof: The theorem is a simple corollary of Proposition 11, and the formula (5.1) follows from Example 8. □

Remark 17: Contrary to the two-dimensional case, the singular term of the Green function for the three-dimensional Schrödinger operator $H_{A,U}$ *does* depend on the scalar potential U as well as on the magnetic vector potential A. In particular, if A is the vector potential of a uniform magnetic field $\mathbf{B}$ in $X=\mathbb{R}^3$, then instead of (5.1) we have

$$G_{A,0}(\mathbf{x},\mathbf{y};\zeta)=\frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\exp\left(\frac{i\mathbf{B}(\mathbf{x}\times\mathbf{y})}{2}\right)+G^{\mathrm{ren}}_{A,0}(\mathbf{x},\mathbf{y};\zeta),$$

see Example 14. On the other hand, the dependence on scalar potentials is shown in Example 12.

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APPENDIX A: OFF-DIAGONAL ASYMPTOTICS FOR THE INVERSE HARMONIC OSCILLATOR IN DIMENSION ONE

The Green function $G(x,y;\zeta)$ for the inverse harmonic oscillator $H=-d^2/\mathrm{d}x^2-\omega^2x^2/4$, has the form

$$G(x,y;\zeta)=\frac{e^{i\pi/4}\Gamma\left(\frac{1}{2}-i\zeta\right)}{\sqrt{2\pi\omega}}\times U(-i\zeta/\omega,e^{-i\pi/4}\omega^{1/2}\max(x,y))\times U(-i\zeta/\omega,e^{-i\pi/4}\omega^{1/2}\max(-x,-y)),\tag{A1}$$

where $\Im\zeta>0$ and $U(a,x)$ is the Weber function, see (Ref. 27, Chap. 19). Using (Ref. 27, No. 19.8.1), for large z one obtains $U(a,z)=e^{-z^2/4}z^{-1/2-a}u(z)$, where $\lim_{z\to\infty}u(z)=1$. Returning to the Green function we see that for fixed x and large y one has (assuming $y>x$)

$$G(x,y;\zeta)=\frac{e^{i\pi/4}\Gamma\left(\frac{1}{2}-i\zeta\right)}{\sqrt{2\pi\omega}}U(-i\zeta/\omega,-e^{-i\pi/4}\omega^{1/2}x)\frac{e^{i\omega y^2/4}}{(e^{-i\pi/4}\omega^{1/2}y)^{-i\zeta/\omega+(1/2)}}v(y),$$

where $\lim_{y\to\infty}v(y)\neq 0$. Therefore, for large $|x-y|$ the Green function has only a polynomial decay.

APPENDIX B: ON-DIAGONAL SINGULARITY FOR THE COULOMB HAMILTONIAN

Here we prove the asymptotics (3.6).

We are interested in asymptotics of the functions $x\mapsto G(x,x_0;\zeta)$ as $x\to x_0$ at fixed $\zeta\in\mathrm{res}(H)$ and $x_0\in\mathbb{R}^3$. As the potential is smooth outside the origin, the Green function has the standard on-diagonal asymptotics if $x_0\neq 0$. We consider the case $x_0=0$. We have $M_{\kappa,1/2}(0)=0$, $M'_{\kappa,1/2}(0)=1$, therefore,

$$G(x,0;\zeta)=\frac{\Gamma(1-\kappa)}{4\pi|x|}W_{\kappa,1/2}(2\sqrt{-\zeta}|x|).$$

Consider the following expansions [cf. items 6.1(1) and 6.8(13) in Ref. 28]:

$$\Phi(a,2;x)=1+\frac{a}{2}x+\frac{a(a+1)}{12}x^2+\cdots,$$

$$\begin{aligned}\Psi(a,2;x)&=\frac{1}{x\Gamma(a)}+\Phi(a,2;x)\log x+\sum_{k=0}^{\infty}\frac{\Gamma(a+k)[\psi(a+k)-\psi(1+k)-\psi(2+k)]}{\Gamma(a)(k+1)!k!}x^k\\&=A_{-1}x^{-1}+A_0+A_1x+A_2x^2+\cdots+B_0\log x+B_1x\log x+B_2x^2\log x+\cdots,\end{aligned}$$

where

$$A_{-1}=\frac{1}{\Gamma(a)},\quad A_0=\frac{\psi(a)-\psi(1)-\psi(2)}{\Gamma(a-1)},\quad A_1=\frac{a(\psi(a+1)-\psi(2)-\psi(3))}{2\Gamma(a-1)},$$

$$A_2=\frac{a(a+1)(\psi(a+2)-\psi(3)-\psi(4))}{12\Gamma(a-1)},\quad B_0=\frac{1}{\Gamma(a-1)},\quad B_0=\frac{a}{2\Gamma(a-1)},\quad B_2=\frac{a(a+1)}{12\Gamma(a-1)}.$$

Using (3.5), we get

$$\begin{aligned}W_{\kappa,1/2}(x)&=A_{-1}+\left(A_0-\frac{1}{2}A_{-1}\right)x+B_0x\log x+O(|x^2\log x|)\\&=\frac{1}{\Gamma(a)}+\left(\frac{\psi(a)-\psi(1)-\psi(2)}{\Gamma(a-1)}-\frac{1}{2\Gamma(a)}\right)x+\frac{1}{\Gamma(a-1)}x\log x+O(|x^2\log x|).\end{aligned}$$

Since $\psi(1)=-C_E$, $\psi(2)=1-C_E$, where C_E is the Euler constant, we get (3.6) after some trivial algebra.

APPENDIX C: ON-DIAGONAL SINGULARITY OF THE THREE-DIMENSIONAL LANDAU HAMILTONIAN

In this appendix, we are going to prove the asymptotics (4.6).

Set in the integral (4.5) $\mathbf{x}_\perp=0$ and denote $\mathbf{x}_\parallel=z$. Then after the change of variables $t\to t^2$ in this integral, we obtain

$$G(0,0,z;0,0,0;\zeta)=\frac{|\xi|^{1/2}}{2\pi}\int_0^\infty\frac{\exp(-az^2t^{-2}-ct^2)}{1-e^{-t^2}}\mathrm{d}t,\tag{C1}$$

where $a=\pi|\xi|$ and $c=(1/2)-(\zeta/4\pi|\xi|)$. Represent now $G(0,0,z;0,0,0;\zeta)=f_1(z;\zeta)+f_2(z;\zeta)$, where

$$f_1(z;\zeta)=\frac{|\xi|^{1/2}}{2\pi}\int_0^\infty\frac{\exp(-az^2t^{-2}-ct^2)}{t^2}\mathrm{d}t,$$

$$f_2(z;\zeta)=\frac{|\xi|^{1/2}}{2\pi}\int_0^\infty\left(\frac{1}{1-e^{-t^2}}-\frac{1}{t^2}\right)\exp(-az^2t^{-2}-ct^2)\mathrm{d}t.\tag{C2}$$

Changing the variable $t\to t^{-1}$ and using the relation

$$\int_0^\infty\exp(-bt^2-c/t^2)\mathrm{d}t=\frac{1}{2}(\pi/b)^{1/2}\exp(-2(bc)^{1/2})$$

(see Ref. 29, Sec. V. I, formula 2.3.16.3), we obtain $f_1(z;\zeta)=\exp(-(2\pi|\xi|-\zeta)^{1/2}|z|)/(4\pi|z|)$, or $G(0,0,z;0,0,0;\zeta)=(4\pi|z|)^{-1}+g(z;\zeta)$, where

$$g(z;\zeta)=-\frac{1}{4\pi}(2\pi|\xi|-\zeta)^{1/2}+f_2(z;\zeta).\tag{C3}$$

It is clear that the function g is continuous with respect to z and analytic with respect to ζ, $\zeta\in\mathrm{res}(H_{A,0})$. We can rewrite (C1) in the form

$$\frac{|\xi|^{1/2}}{2\pi}\int_0^\infty\frac{\exp(-\pi|\xi|z^2t^{-1})}{(1-e^{-t})\exp\left(\left(\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)t\right)\sqrt{t}}\mathrm{d}t=\frac{1}{4\pi|z|}+g(z;\zeta).\tag{C4}$$

Let $h(t)=(e^t-1)^{-1}-t^{-1}$; the function h is real analytic on the whole line, $h(t)\to0$ as $t\to+\infty$ and $h(t)\to-1$ as $t\to-\infty$. Therefore, h is bounded on $\mathbb{R}$. Let us represent $F(\mathbf{x};\zeta)$ in the form

$$F(\mathbf{x};\zeta)=\int_0^\infty \frac{\exp(-\pi|\xi|\mathbf{x}^2t^{-1})}{(1-e^{-t})\exp\left[\left(\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)t\right]\sqrt{t}}\mathrm{d}t+\int_0^\infty \frac{\exp(-\pi|\xi|\mathbf{x}^2t^{-1})}{(1-e^{-t})\exp\left[\left(\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)t\right]\sqrt{t}}$$
$$\times\{\exp[-\pi|\xi|\mathbf{x}_\perp h(t)]-1\}\mathrm{d}t\equiv I_1(\mathbf{x},\zeta)+I_2(\mathbf{x},\zeta). \tag{C5}$$

It is easy to show that I_2 is a continuous function in the domain $\mathbf{x}\in\mathbb{R}^3$, $\mathrm{Re}\,\zeta<2\pi|\xi|$. Let us show that $I_2(\mathbf{x},\zeta)\to 0$ locally uniformly with respect to ζ, $\mathrm{Re}\,\zeta<2\pi|\xi|$, as $\mathbf{x}\to 0$. It is sufficient to show that

$$A(\mathbf{x},\zeta)\equiv\int_0^\infty \frac{\exp(-\pi|\xi|\mathbf{x}^2t^{-1})}{(1-e^{-t})\exp\left[\left(\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)t\right]\sqrt{t}}|\exp[-\pi|\xi|\mathbf{x}_\perp^2h(t)]-1|\mathrm{d}t\to 0$$

locally uniformly with respect to $\zeta\in\mathbb{R}$, $\zeta<2\pi|\xi|$, as $\mathbf{x}\to 0$. Fix $\zeta\in\mathbb{R}$, $\zeta<2\pi|\xi|$. Since $\mathbf{x}_\perp^2\leqslant\mathbf{x}^2$, we have $|\exp[-\pi|\xi|\mathbf{x}_\perp^2h(t)]-1|\leqslant\mathrm{const}\,\mathbf{x}^2$ in a neighborhood of the point $(0,0,z)$. Therefore, using (C4), we get

$$A(\mathbf{x},\zeta)\leqslant c\mathbf{x}^2\int_0^\infty \frac{\exp(-\pi|\xi|\mathbf{x}^2t^{-1})}{(1-e^{-t})\exp\left[\left(\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)t\right]\sqrt{t}}\mathrm{d}t\leqslant\frac{|\mathbf{x}|}{|\xi|^{1/2}}+\frac{c\mathbf{x}^2}{|\xi|^{1/2}}f(|\mathbf{x}|,\zeta),$$

and we get the required limit. Using (C4) again, we obtain

$$I_1(|\mathbf{x}|,\zeta)=\frac{1}{|\xi|^{1/2}|\mathbf{x}|}+f(|\mathbf{x}|,\zeta). \tag{C6}$$

Using (C5) and (C6) we get

$$G(\mathbf{x},\mathbf{y};\zeta)=\frac{1}{4\pi}\frac{\exp[\pi i\xi(\mathbf{x}_\perp\wedge\mathbf{y}_\perp)]}{|\mathbf{x}-\mathbf{y}|}+\tilde{F}(\mathbf{x},\mathbf{y};\zeta),$$

where $\tilde{F}(\mathbf{x},\mathbf{y};\zeta)$ is jointly continuous with respect to $(\mathbf{x},\mathbf{y})\in\mathbb{R}^3\times\mathbb{R}^3$ for all $\zeta\in\mathrm{res}(H_{\mathbf{A},0})$.

Denote $Q(\zeta)=\lim_{|\mathbf{x}-\mathbf{y}|\to 0}\tilde{F}(\mathbf{x},\mathbf{y};\zeta)$; this limit is independent of $\mathbf{x}$ and $\mathbf{y}$ since $\tilde{F}(\mathbf{x},\mathbf{y};\zeta)$ is invariant with respect to magnetic translations $T_\mathbf{a}$, $\mathbf{a}\in\mathbb{R}^3$: $T_\mathbf{a}f(\mathbf{x})=\exp[\pi i\xi(\mathbf{a}_\perp\wedge\mathbf{x}_\perp)]f(\mathbf{x}-\mathbf{a})$. From (4.5) we obtain

$$\frac{\partial}{\partial\zeta}Q(\zeta)=\frac{1}{16\pi^2|\xi|^{1/2}}\int_0^\infty \exp\left[\left(\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)t\right](1-e^{-t})^{-1}\sqrt{t}\,\mathrm{d}t.$$

Using Eq. (1.10.4) from Ref. 28 we get $\int_0^\infty t^{s-1}e^{-vt}(1-e^{-t})^{-1}\,\mathrm{d}t=\Gamma(s)\mathrm{Z}(s,v)$ and the obvious relation $\partial Z(s,v)/\partial v=-sZ(s+1,v)$ implies immediately

$$Q(\zeta)=\frac{1}{4}\left(\frac{|\xi|}{\pi}\right)^{1/2}Z\left(\frac{1}{2};\frac{1}{2}-\frac{\zeta}{4\pi|\xi|}\right)+C \tag{C7}$$

with a constant $C\in\mathbb{R}$. To determine C we compare (C7) with (C3) in the limit $\Re\zeta\to-\infty$. Since $Q(\zeta)=g(0;\zeta)$, we have from (C3) and (C2),

$$Q(\zeta)-\frac{1}{4\pi}(2\pi|\xi|-\zeta)^{1/2}\to 0\quad\text{as }\Re\zeta\to-\infty.$$

On the other hand, by the Hermite relation [see (1.10.7) from Ref. 28] there holds $Z(1/2,v)+2v^{1/2}\to 0$ as $\Re v\to+\infty$. Comparing the two last relations with (C7), we get $C=0$. Thus, (4.6) is

proven. Note that the expression for $Q(\zeta)$ was obtained at the physical level of rigor in Ref. 30 and can be found also in Ref. 9.

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On the Cauchy problem for the integrable system of Lie minimal surfaces

E. Musso[a)]
Dipartimento di Matematica Pura ed Applicata, Università degli Studi di L'Aquila, via Vetoio, I-67010 Coppito (L'Aquila), Italy

L. Nicolodi[b)]
Dipartimento di Matematica, Università degli Studi di Parma, Parco Area Delle Scienze 53/A, I-43100 Parma, Italy

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In this paper we apply the Cartan-Kähler theory of exterior differential systems to solve the Cauchy problem for the integrable system of Lie minimal surfaces and discuss the underlying geometry. One purpose for this work is to show how methods and language from the theory of exterior differential systems may prove to be useful in the study of real analytic initial value problems, especially for gaining insight into the geometric aspects of the initial conditions and the solutions.
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I. INTRODUCTION

The study of surfaces in the framework of Lie sphere geometry was developed to a large extent during the 1920s, mainly by Blaschke and Thomsen. A great deal of material about it can be found in Ref. 1. Over the past years, there has been some renewed interest in the subject due to the fact that many classes of surfaces in Lie geometry have been recognized as integrable systems.[11,12,5] Examples include, among others, diagonally cyclidic surfaces and Lie minimal surfaces.

To put our discussion in context, we recall some facts about Lie geometry. Consider the set of oriented spheres in Euclidean space. If we add to this set the set of oriented planes, the set of point spheres, and the point at infinity, we obtain the space of Lie sphere geometry. This space can be identified with the standard projective quadric $\mathcal{Q}\subset\mathbb{P}^5$ of signature (3,1)—the conformal completion of Minkowski 4-space. Any smooth immersion of an oriented surface in Euclidean space has a contact lift to the unit sphere bundle of $\mathbb{R}^3$ called the Legendre lift. The unit sphere bundle embeds as an open and dense subset into the five-dimensional space Λ of lines lying on $\mathcal{Q}$. Thus the Lie transformation group, that is the projective transformations of $\mathbb{P}^5$ fixing $\mathcal{Q}$, acts on the set of Legendre surfaces. Lie geometry studies the properties of immesions which are invariant under this action. One way to do this is to think of the surface as an envelope of an appropriate congruence of invariant model surfaces. In this case, one attaches to each point p of the surface a Dupin cyclide $D(p)$ having second order contact with the immersion, a so-called Lie cyclide. The map D plays the role of a generalized Gauss map and is the analogue of the conformal Gauss map (central sphere congruence) in Möbius geometry. It defines an immersion into the space $\mathfrak{D}$ of Dupin cyclides, which is identified with the pseudo-Riemannian symmetric space given by the Grassmannian of three-dimensional subspaces of signature (2, 1) in $\mathbb{R}^{4,2}$. The geometric invariants of D are exactly the Lie invariants of the original surface. In particular, its area defines a Lie invariant functional, whose critical points are called Lie minimal surfaces. Actually, the critical points of this functional are characterized by the harmonicity of the generalized Gauss map D,[5] so

[a)]Electronic mail: musso@univaq.it
[b)]Electronic mail: lorenzo.nicolodi@unipr.it

as Willmore surfaces in Möbius geometry are characterized by the harmonicity of the central sphere congruence[3] and L-minimal surfaces in Laguerre geometry by the harmonicity of the middle sphere congruence.[15]

In this paper we discuss the Cauchy problem for Lie minimal surfaces. Application of the Cartan-Kähler theory leads to a description of the space of local real analytic Lie minimal surfaces in terms of six functions in one variable. In addition to the existence and uniqueness result for Lie minimal surfaces satisfying given initial conditions, our main contribution here is that of clarifying the geometry of the Cauchy problem, providing a neat geometric description of the real analytic initial data and of the corresponding solution surface. To do this we use the method of moving frames[9] and the theory of exterior differential systems.[4]

We turn now to a more detailed description of the main result of the paper. Consider an oriented Legendre surface $X \subset \mathbb{R}^3 \times S^2$. Under suitable nondegeneracy conditions, we can introduce on X a canonical Lie-invariant coframe α^1, α^2 (see Ref. 1 and 11). This induces two distinguished geometric structures on the surface, namely the Lorentzian metric $\Phi = \alpha^1 \cdot \alpha^2$ and the 3-web (we refer to Ref. 8 for more details on web geometry) formed by the two families of curvature lines and the family of *cyclidic curves*, defined, respectively, by the equations

$$\alpha^1 = 0, \quad \alpha^2 = 0, \quad \alpha^1 - \alpha^2 = 0.$$

Let $\Gamma \subset \mathbb{R}^3 \times S^2$ be a Legendrian curve, and $\sigma: \Gamma \to \mathcal{Q}$ a one-parameter family of osculating spheres along Γ. For each $(P, \vec{b}) \in \Gamma$, $\sigma(P, \vec{b})$ denotes the sphere in oriented contact at P with the plane through P orthogonal to $\vec{b}$. We are now in a position to state the following.

Theorem 1.1: Let $\Gamma \subset \mathbb{R}^3 \times S^2$ be a real-analytic Legendre curve, σ a generic real-analytic one-parameter family of osculating spheres along Γ, and $k, K: \Gamma \to \mathbb{R}$ real-analytic functions. Then, there exists a unique real-analytic Lie minimal surface $X \subset \mathbb{R}^3 \times S^2$ containing Γ such that

(i) Γ is anticyclidic, i.e., intersects the cyclidic curves of X orthogonally;
(ii) k is the web-curvature of Γ [the web-curvature of Γ is the function $k_\Gamma: \Gamma \to \mathbb{R}$ defined by $k_\Gamma = \Phi(D^w_{\Gamma'}(\Gamma'), \Gamma')$, where D^w denotes the covariant derivative operator associated with the connection of the 3-web and Γ' is a unit tangent vector along Γ];
(iii) $\sigma(\xi)$ is a curvature sphere of X at ξ, for each $\xi \in \Gamma$;
(iv) $K(\xi)$ is the curvature of the 3-web of X at the point ξ, for each $\xi \in \Gamma$.

According to this theorem, the appropriate Cauchy data for the problem are

(i) a curve γ of $\mathbb{R}^3$ and a field $\vec{b}: \gamma \to S^2$ of unit normals along γ;
(ii) a smooth function $r: \gamma \to \mathbb{R}$ which gives the signed radii of the osculating spheres;
(iii) other two additional functions $k, K: \gamma \to \mathbb{R}^3$.

The paper is organized as follows. In Sec. II, we briefly overview some general facts about surface theory in Lie geometry. In Sec. III, we set up an exterior differential system whose integral manifolds can be regarded as framed Lie minimal surfaces. Then, we apply the techniques of the Cartan-Kähler theory to prove the main theorem. In the Appendix we provide the details of the construction of the canonical frames used in the proof of the theorem.

II. SURFACE THEORY IN LIE SPHERE GEOMETRY

In this section, we briefly recall some background material about Lie sphere geometry and develop the method of moving frames for immersed surfaces in this context. A complete treatment of Lie sphere geometry can be found in the classical treatise of Blaschke and Thomsen[1] or in the more recent monograph of Cecil.[6]

A. Basic definitions

Let $\mathbb{R}^{4,2}$ be the vector space $\mathbb{R}^6$ endowed with the nondegenerate scalar product

$$\langle X,Y\rangle = -(x^0y^5 + x^5y^0) - (x^1y^4 + x^4y^1) + x^2y^2 + x^3y^3 = X^t gY, \tag{2.1}$$

where $x^0,\ldots,x^5$ and $y^0,\ldots,y^5$ are the coordinates of the vectors X and Y with respect to the standard basis $(\epsilon_0,\ldots,\epsilon_5)$ of $\mathbb{R}^6$. Let SO(4,2) be the identity component of the group that preserves (2.1) and let G be the quotient of SO(4,2) by its center $\mathbb{Z}_2=\{\pm\mathrm{Id}\}$. For each $A\in \mathrm{SO}(4,2)$, we denote by $A_J=A\cdot\epsilon_J, J=0,\ldots,5$, the column vectors of A. Thus $(A_0,\ldots,A_5)$ is a positive, time-oriented basis of $\mathbb{R}^{4,2}$ such that

$$\langle A_I,A_J\rangle = g_{IJ}, \quad I,J=0,\ldots,5.$$

Expressing the exterior derivatives $\mathrm{d}A_J$ in terms of the basis $(A_0,\ldots,A_5)$, we obtain

$$\mathrm{d}A_J = A_I\otimes\omega^I_J, \quad J=0,\ldots,5, \tag{2.2}$$

where $\omega=(\omega^I_J)$ is the $\mathfrak{o}(4,2)$-valued Maurer-Cartan form $A^{-1}\,\mathrm{d}A$. Taking the exterior derivative of (2.2) yields the structure equations

$$\mathrm{d}\omega + \omega\wedge\omega = 0. \tag{2.3}$$

The elements of $G=\mathrm{SO}(4,2)/\mathbb{Z}_2$ are equivalence classes $[A]$ of matrices $A\in\mathrm{SO}(4,2)$. Since the Maurer-Cartan form ω is bi-invariant under the action of $\mathbb{Z}_2$, we identify the Lie algebra $\mathfrak{g}$ of G with $\mathfrak{o}(4,2)$ and we think of ω as the Maurer-Cartan form of G.

The group G acts transitively on the following three spaces:

(i) the four-dimensional space $\mathcal{Q}\subset\mathbb{RP}^5$ of isotropic one-dimensional linear subspaces of $\mathbb{R}^{4,2}$; $\mathcal{Q}$ is known as the Lie quadric;
(ii) the five-dimensional Grassmannian $\Lambda\subset G_2(\mathbb{R}^6)$ of two-dimensional totally isotropic linear subspaces of $\mathbb{R}^{4,2}$;
(iii) the nine-dimensional Grassmannian $\mathfrak{D}=G_{2,1}(\mathbb{R}^{4,2})$ of all theree-dimensional linear subspaces of signature (2,1) in $\mathbb{R}^{4,2}$.

The geometric meaning of these spaces is the following.

(i) The Lie quadric $\mathcal{Q}$ identifies with the set of oriented spheres in $\mathbb{R}^3$, including point spheres, oriented planes and the "point at infinity." Given a point $P=(p^1,p^2,p^3)\in\mathbb{R}^3$ and a real number r, let $\sigma(P,r)$ denote the oriented sphere with center P and signed radius r. Similarly, for each $P\in\mathbb{R}^3$ and every unit vector $\vec{n}\in S^2$, let $\pi(P,\vec{n})$ denote the oriented plane through P orthogonal to $\vec{n}$. The correspondence between the points of $\mathcal{Q}$ and oriented spheres is given by

$$\sigma(P,r)\mapsto\left[\left(1,\frac{r+p^1}{\sqrt{2}},p^2,p^3,\frac{r-p^1}{\sqrt{2}},\frac{\|P\|^2-r^2}{2}\right)\right],$$

$$\pi(P,\vec{n})\mapsto\left[\left(0,\frac{1+n^1}{2},\frac{n^2}{\sqrt{2}},\frac{n^3}{\sqrt{2}},\frac{1-n^1}{2},\frac{\vec{n}\cdot P}{\sqrt{2}}\right)\right],$$

$$\infty\mapsto\epsilon_5.$$

(ii) To each contact element $\xi=(P,\vec{n})\in\mathbb{R}^3\times S^2$ we associate the null plane

$$\ell(\xi)=[F_0(P)\wedge F_1(P,\vec{n})]$$

generated by the null vectors

$$F_0(P)=\left(1,\frac{1}{\sqrt{2}}p^1,p^2,p^3,-\frac{1}{\sqrt{2}}p^1,\frac{\|P\|}{2}\right),$$

$$F_1(P,\vec{n}) = \left(0, \frac{1+n^1}{\sqrt{2}}, n^2, n^3, \frac{1-n^1}{\sqrt{2}}, \vec{n}\cdot P\right). \tag{2.4}$$

The mapping

$$\xi \in \mathbb{R}^3 \times S^2 \to \ell(\xi) \in \Lambda$$

embeds $\mathbb{R}^3 \times S^2$ as an open and dense subset of $\Lambda \cong T_1 S^3$. Thus, Λ is obtained from $\mathbb{R}^3 \times S^2$ by adding the 2-sphere of null planes through $[\epsilon_5]$ at infinity. Correspondingly, the Lie sphere group G can be viewed as a pseudogroup of contact transformations acting on $\mathbb{R}^3 \times S^2$. (See also Ref. 14)

(iii) Let $V \in \mathfrak{D}$ and consider the two-dimensional torus

$$T(V) = \{([x],[y]) \in \mathbb{P}(V) \times \mathbb{P}(V^\perp) : \|x\|^2 = \|y\|^2 = 0\} \cong S^1 \times S^1.$$

The map $([x],[y]) \in T(V) \mapsto [x \wedge y] \in \Lambda$ is a Legendre immersion and determines a *cyclide of Dupin* in $\mathbb{R}^3$. (We recall that a surface is called a cyclide of Dupin if each principal curvature is constant along its own line of curvature. A torus of revolution is a Dupin cyclide. Dupin cyclides are algebraic surfaces of the fourth order. For more details we refer to Ref. 6.) In the framework of Lie-geometry any cyclide of Dupin arises in this way. Thus, the manifold $\mathfrak{D}$ can be viewed as the space of all Dupin cyclides of $\mathbb{R}^3$. Note that $\mathfrak{D}$ is a pseudo-Riemannian symmetric space G/K of the group G, whose G-invariant pseudo-Riemannian metric $g_{\mathfrak{D}}$ is represented by the tensorial quadratic form

$$2\omega_0^1\omega_1^0 + 2\omega_0^4\omega_4^0 + 2\omega_0^2\omega_2^0 + 2\omega_3^1\omega_1^3 - \omega_2^3\omega_2^3. \tag{2.5}$$

B. Legendre surfaces

Definition 2.1: An oriented immersed surface $X \subset \mathbb{R}^3 \times S^2$ is said to be *Legendre* if $\mathrm{d}f \cdot \vec{n} = 0$, where $f: X \to \mathbb{R}^3$ and $\vec{n}: X \to S^2$ denote the restrictions to X of the natural projections.

Remark 2.2: The basic examples are the contact lifts of oriented immersed surfaces $\widetilde{X} \subset \mathbb{R}^3$. In this case $\vec{n}$ is the usual Gauss map and the embedding is given by $\widetilde{X} \ni P \mapsto (P, \vec{n}|_P) \in \mathbb{R}^3 \times S^2$.

Given a Legendre surface, we consider the quadratic forms

$$\mathrm{I} = \mathrm{d}f \cdot \mathrm{d}f, \quad \mathrm{III} = \mathrm{d}\vec{n} \cdot \mathrm{d}\vec{n}.$$

Definition 2.3: We say that X has no umbilical points if $\mathrm{I}|_\xi$ and $\mathrm{III}|_\xi$ are linearly independent, for every $\xi \in X$.

Remark 2.4: If X is the contact lift of an oriented surface $\widetilde{X} \subset \mathbb{R}^3$, then I and III are the first and the third fundamental forms, respectively. Thus, X has no umbilical points if and only if $\widetilde{X}$ is umbilic free in the usual sense.

If X is umbilic free, there exist *curvature line* coordinates, that is, positive-oriented charts $(\mathcal{U}, x^1, x^2)$ with respect to which I and III are in diagonal form. We have

$$\mathrm{d}f = \phi_1\, \mathrm{d}x^1 \vec{e}_1 + \phi_2\, \mathrm{d}x^2 \vec{e}_2,$$

$$\mathrm{d}\vec{n} = \nu_1\, \mathrm{d}x^1 \vec{e}_1 + \nu_2\, \mathrm{d}x^2 \vec{e}_2, \tag{2.6}$$

where $(\vec{e}_1, \vec{e}_2, \vec{n})$ is a positive-oriented frame field and $\phi_i, \nu_i, i = 1, 2$, are smooth functions such that $(\nu_1\phi_2 - \nu_2\phi_1)|_p \neq 0$, for every $p \in X$.

Definition 2.5: The *curvature spheres* at the point $\xi = (P, \vec{n})$ of X are the oriented spheres $\sigma_i(\xi) \in \mathcal{Q}, i = 1, 2$, represented by the null vectors

$$S_i(\xi) = \phi_i F_0(P) + \nu_i F_1(P, \vec{n}), \quad i = 1, 2.$$

Remark 2.6: If X is the contact lift of an immersed surface $\widetilde{X} \subset \mathbb{R}^3$, then $\sigma_i(P, \vec{n}|_P), i = 1, 2$, give

back the curvature spheres of $\widetilde{X}$ at P corresponding to the principal curvatures.

Definition 2.7 (nondegeneracy condition): We say that a Legendre surface X is *nondegenerate* if it is umbilic free and both the *curvature sphere mappings*

$$\sigma_i: X \ni \xi \mapsto \sigma_i(\xi) \in \mathcal{Q}, \quad i = 1,2$$

are immersions into the Lie quadric $\mathcal{Q}$.

For each $\xi \in X$ there are two *osculating Dupin cyclides* $D_i(\xi), i=1, 2$ (the Lie cyclides) represented by the three-dimensional linear subspaces,

$$D_i(\xi) = [S_i|_\xi \wedge \partial_i S_i|_\xi \wedge \partial_{ii}^2 S_i|_\xi] \in \mathfrak{D}.$$

Definition 2.8: The map $D: \xi \in X \mapsto D_1(\xi) \in \mathfrak{D}$ is called the *generalized Gauss map* of the Legendre surface (see Ref. 1 and 5).

C. Moving frames

Following the usual practice in the method of moving frames, we can construct a canonical lift to the group G for any nondegenerate Legendre surface.

Theorem 2.9: Let $X \subset \mathbb{R}^3 \times S^2 \subset \Lambda$ be a nondegenerate Legendre surface. Then there exists a unique lift $[A]: X \to G$ satisfying the Pfaffian equations

$$\alpha_0^4 = \alpha_0^2 = \alpha_1^3 = \alpha_2^3 = \alpha_0^1 - \alpha_1^2 = \alpha_1^0 - \alpha_0^3 = \alpha_2^0 = \alpha_3^1 = 0, \tag{2.7}$$

with the independence condition

$$\alpha_0^3 \wedge \alpha_1^2 > 0. \tag{2.8}$$

(The proof of this theorem is given in the Appendix. Our canonical frame is related the "Wilczynski frame" introduced by Blaschke[1] and reconsidered by Ferapontov in Ref. 11 and 12. The main difference is a final normalization, which makes our frame independent of the choice of the curvature line coordinates.)

We call $\alpha^1 := \alpha_0^3, \alpha^2 := \alpha_1^2$ canonical or Blaschke's coframe of X (Ref. 1 and 11). It is given by

$$\alpha^1 = \sqrt[3]{3\beta^2\gamma}\, \mathrm{d}x^1, \quad \alpha^2 = \sqrt[3]{3\beta^2\gamma}\, \mathrm{d}x^2, \tag{2.9}$$

where

$$\beta = \frac{\phi_1 \partial_1 \nu_1 - \partial_1 \phi_1 \nu_1}{\phi_2 \partial_2 \nu_2 - \partial_2 \phi_2 \nu_2}, \quad \gamma = \frac{\partial_2 \phi_2 \nu_2 - \phi_2 \partial_2 \nu_2}{\phi_2 \partial_2 \nu_2 - \partial_2 \phi_2 \nu_2}.$$

Remark 2.10: Geometrically, the equations $\alpha^1 = 0$ and $\alpha^2 = 0$ define the curvature lines of the surface. The curvature spheres of the surface at $\xi \in X$ are represented by the null lines $[A_0(\xi)]$ and $[A_1(\xi)]$, respectively, while the two Lie cyclides are represented by the three-dimensional subspaces $[A_0(\xi) \wedge A_3(\xi) \wedge A_5(\xi)]$ and $[A_1(\xi) \wedge A_2(\xi) \wedge A_4(\xi)]$, respectively. Note also that $\Phi := D^*(g_{\mathfrak{D}}) = \alpha^1 \cdot \alpha^2$.

The only nonzero components of the Maurer-Cartan form α of the canonical frame are $\alpha^1 = \alpha_0^3, \alpha^2 = \alpha_1^2$, and $\alpha_0^0, \alpha_1^1, \alpha_2^1, \alpha_1^1, \alpha_3^0, \alpha_4^0$. From the exterior differentiation of (2.7) and the structure equations, it follows that there exist smooth functions q_1, q_2, p_1, p_2, and r_1, r_2 such that

$$\alpha_0^0 = -2q_1\alpha^1 + q_2\alpha^2, \quad \alpha_1^1 = -q_1\alpha^1 + 2q_2\alpha^2,$$

$$\alpha_3^0 = r_1\alpha^1 + p_2\alpha^2, \quad \alpha_2^1 = p_1\alpha^1 + r_2\alpha^2,$$

$$\alpha_4^0 = -r_2\alpha^1 + r_1\alpha^2. \tag{2.10}$$

We call q_1, q_2, p_1, p_2 and r_1, r_2 the *invariant functions* of the Legendre surface. Again using the structure equations, we obtain

$$\mathrm{d}\alpha^1 = \alpha_0^0 \wedge \alpha^1, \quad \mathrm{d}\alpha^2 = \alpha_1^1 \wedge \alpha^2, \quad \mathrm{d}\alpha_2^1 = -\alpha_1^1 \wedge \alpha_2^1, \quad \mathrm{d}\alpha_3^0 = -\alpha_0^0 \wedge \alpha_3^0, \tag{2.11}$$

$$\mathrm{d}\alpha_0^0 = (\alpha^2 - \alpha_3^0) \wedge \alpha^1, \quad \mathrm{d}\alpha_1^1 = (\alpha^1 - \alpha_2^1) \wedge \alpha^2, \quad \mathrm{d}\alpha_4^0 = -(\alpha_0^0 + \alpha_1^1) \wedge \alpha_4^0, \tag{2.12}$$

which in terms of the invariant functions read

$$\mathrm{d}\alpha^1 = -q_2 \alpha^1 \wedge \alpha^2, \quad \mathrm{d}\alpha^2 = -q_1 \alpha^1 \wedge \alpha^2, \tag{2.13}$$

$$\begin{aligned} -2\,\mathrm{d}q_1 \wedge \alpha^1 + \mathrm{d}q_2 \wedge \alpha^2 &= (p_2 - q_1 q_2 - 1)\alpha^1 \wedge \alpha^2, \\ -\mathrm{d}q_1 \wedge \alpha^1 + 2\,\mathrm{d}q_2 \wedge \alpha^2 &= (-p_1 + q_1 q_2 + 1)\alpha^1 \wedge \alpha^2, \\ \mathrm{d}r_1 \wedge \alpha^1 + \mathrm{d}p_2 \wedge \alpha^2 &= (2q_2 r_1 + 3q_1 p_2)\alpha^1 \wedge \alpha^2, \\ \mathrm{d}p_1 \wedge \alpha^1 + \mathrm{d}r_2 \wedge \alpha^2 &= (2q_1 r_2 + 3q_2 p_1)\alpha^1 \wedge \alpha^2, \\ -\mathrm{d}r_2 \wedge \alpha^1 + \mathrm{d}r_1 \wedge \alpha^2 &= 4(q_1 r_1 - q_2 r_2)\alpha^1 \wedge \alpha^2. \end{aligned} \tag{2.14, 2.15}$$

We may consider (2.13)–(2.15) as the Lie sphere analogues of the *Gauss* and *Codazzi-Mainardi* equations.

Remark 2.11: If (x^1, x^2) are curvature line coordinates, then

$$q_1 = -\frac{1}{3\sqrt[3]{\beta^2 \gamma}}(\partial_1(\log \beta) + 2\partial_1(\log \gamma)),$$

$$q_2 = \frac{1}{3\sqrt[3]{\beta \gamma^2}}(2\partial_2(\log \beta) + \partial_2(\log \gamma)),$$

$$p_1 = -\frac{1}{\beta\gamma}\partial_{12}(\log \beta) + 1,$$

$$p_2 = -\frac{1}{\beta\gamma}\partial_{12}(\log \gamma) + 1.$$

From this and from (2.15), we infer that the invariant functions p_1, p_2, r_1, r_2 coincide, up to unessential normalizations, with the local differential invariants k, l, a, b defined by Ferapontov in Ref. 11.

Remark 2.12: With respect to the Blaschke coframe, the connection form of the 3-web is represented by the 1-form

$$\zeta_w = -q_1 \alpha^1 + q_2 \alpha^2,$$

while the Levi-Civita connection of the Lorentzian metric $\Phi = \alpha^1 \cdot \alpha^2$ is given by the 1-form

$$\zeta_\Phi = q_1 \alpha^1 + q_2 \alpha^2.$$

Computing the exterior derivatives of ζ_w and ζ_Φ, we obtain

$$\mathrm{d}\zeta_w = \tfrac{1}{3}(p_2 - p_1)\alpha^1 \wedge \alpha^2, \quad \mathrm{d}\zeta_\Phi = (2 - p_1 - p_2)\alpha^1 \wedge \alpha^2.$$

The respective *sectional curvatures* K_w and K_Φ are given by

$$K_w = \tfrac{1}{3}(p_2 - p_1), \quad K_\Phi = 2 - p_1 - p_2.$$

Definition 2.13: Let $\Gamma \subset X$ be a nonisotropic curve and Γ' a unit vector field tangent to Γ. The *web-curvature* of Γ is the function $k_\Gamma : \Gamma \to \mathbb{R}$ defined by

$$k_\Gamma := \Phi(D^w_{\Gamma'}(\Gamma'), \Gamma'),$$

where D^w denotes the covariant derivative operator associated to the connection of the 3-web.

Remark 2.14: If Γ is an *anticyclidic* curve, that is a solution of the Pfaffian equation $\alpha^1 + \alpha^2 = 0$, then

$$k_\Gamma = \left. \frac{1}{\sqrt{2}}(q_1 + q_2) \right|_\Gamma .$$

D. Lie minimal surfaces

Following Blaschke (see Ref. 1, Sec. 94), we say that a nondegenerate Legendre surface $X \subset \mathbb{R}^3 \times S^2$ is a *Lie minimal surface* (K-Minimalfläche) if the differential equations

$$\mathrm{d}r_1 \wedge \alpha^2 - 4q_1 r_1 \alpha^1 \wedge \alpha^2 = 0,$$

$$\mathrm{d}r_2 \wedge \alpha^1 - 4q_2 r_2 \alpha^1 \wedge \alpha^2 = 0 \tag{2.16}$$

are satisfied. Actually, due to the integrability conditions (2.15), either one of the above differential equations implies the other. Lie minimal surfaces are characterized as critical points of the area functional defined by the generalized Gauss map D (see Ref. 1, Sec. 94, and also Ref. 20).

Recently, this result has been taken up by Burstall and Hertrich-Jeromin,[5] who proved that a nondegenerate Legendre surface X is Lie minimal if and only if its generalized Gauss map D is a conformal harmonic map into the pseudo-Riemannian symmetric space $\mathfrak{D} = G/K$. In the same article, the authors apply the theory of harmonic maps of surfaces to explain the integrable structure of Lie minimal surfaces that was first recognized by Ferapontov in Ref. 11.

Remark 2.15: Note that the canonical frame field $[A] : X \to G$ is also a frame along the generalized Gauss map D. Following Ref. 5, we write $\alpha = \alpha_\mathfrak{k} + \alpha_\mathfrak{p}$ according to the symmetric decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ of the Lie algebra $\mathfrak{g}$ and set

$$\alpha_p = \alpha'_\mathfrak{p} + \alpha''_\mathfrak{p},$$

where $\alpha'_\mathfrak{p}$ and $\alpha''_\mathfrak{p}$ are the components of $\alpha_\mathfrak{p}$ along the null directions of the quadratic form Φ. The key observation (this follows from the characterization of conformal harmonic maps of Riemannian or Lorentzian surfaces into pseudo-Riemannian symmetric spaces, see for instance Refs. 17, 21, and 22) is that D is conformal and harmonic if and only if the one-parameter family of $\mathfrak{g}$-valued 1-forms

$$\alpha_\mu := \alpha_\mathfrak{k} + e^\mu \alpha'_\mathfrak{p} + e^{-\mu} \alpha''_\mathfrak{p}, \quad \mu \in \mathbb{R},$$

satisfies the Maurer-Cartan equations

$$\mathrm{d}\alpha_\mu + \alpha_\mu \wedge \alpha_\mu = 0. \tag{2.17}$$

It is now an easy matter to check that (2.17) holds true if and only if the invariant functions, in addition to the Gauss-Codazzi-Mainardi equations (2.13)–(2.15), satisfy also the equations (2.16).

Example 2.16: Examples of Lie-minimal surfaces include the analogues of Demoulin surfaces in projective differential geometry (see Refs. 13 and 11). These surfaces are defined by the equations $r_1 = r_2 = 0$. From a geometrical viewpoint, they are characterized by the property that D

has only two distinct enveloping surfaces, the original surface X and the dual surface $\hat{X}$ parametrized by the Legendre map $X \ni \ell \mapsto [A_4(\ell) \wedge A_5(\ell)] \in \Lambda$. Locally, with respect to curvature line coordinates (x_1, x_2), such surfaces satisfy

$$\partial_{12}^2(\log \beta) = \beta\gamma + \frac{1}{\beta}, \quad \partial_{12}^2(\log \gamma) = \beta\gamma + \frac{1}{\gamma}.$$

If, in addition, we require that the 3-web is exagonal (i.e., $K^w=0$), then $\beta=\gamma$ and β is a solution of *Tzitzéica equation*,

$$\partial_{12}^2(\log \beta) = \beta^2 + \frac{1}{\beta}. \tag{2.18}$$

Equation (2.18) possesses finite-gap solutions that can be written in terms of Baker-Akhiezer functions.[7,19] It is interesting to notice that (2.18) appears in various contexts such as affine spheres,[18] classical projective geometry,[2] hypercomplex four-manifolds[10] and minimal Legendre tori in S^5.[19]

Another remarkable class of Lie minimal surfaces is represented by the contact lifts of surfaces in $\mathbb{R}^3$ with plane curvature lines (see Ref. 16). These surfaces can be characterized by having curvature line coordinates (x^1, x^2) such that $\beta=\gamma$, where β is a solution of the *Liouville equation*

$$\partial_{12}^2(\log \beta) = \beta^2.$$

III. THE CAUCHY PROBLEM

A. Setting up the system

Let $P=G\times\mathbb{R}^6$ and let $(q_1, q_2, p_1, p_2, r_1, r_2)$ denote the coordinates on $\mathbb{R}^6$. On P we consider the differential ideal $\mathcal{I} \subset \Omega^*(P)$ generated by the differential 1-forms

$$\eta^1 = \omega_0^4, \quad \eta^2 = \omega_0^2, \quad \eta^3 = \omega_1^3,$$

$$\eta^4 = \omega_2^3, \quad \eta^5 = \omega_0^1 - \omega^2, \quad \eta^6 = \omega_1^0 - \omega^1,$$

$$\eta^7 = \omega_2^0, \quad \eta^8 = \omega_3^1, \tag{3.1}$$

$$\eta^9 = \omega_0^0 + 2q_1\omega^1 - q_2\omega^2,$$

$$\eta^{10} = \omega_1^1 + q_1\omega^1 - 2q_2\omega^2, \tag{3.2}$$

$$\eta^{11} = \omega_3^0 - r_1\omega^1 - p_2\omega^2,$$

$$\eta^{12} = \omega_2^1 - p_1\omega^1 - r_2\omega^2,$$

$$\eta^{13} = \omega_4^0 + r_2\omega^1 - r_1\omega^2, \tag{3.3}$$

and by the exterior differential 2-forms

$$\Theta^1 = \mathrm{d}r_1 \wedge \alpha^2 - 4q_1r_1\alpha^1 \wedge \alpha^2, \quad \Theta^2 = \mathrm{d}r_2 \wedge \alpha^1 - 4q_2r_2\alpha^1 \wedge \alpha^2, \tag{3.4}$$

with the independence condition $\Omega=\omega^1\wedge\omega^2$, where $\omega^1=\omega_0^3$ and $\omega^2=\omega_1^2$. Taking the exterior derivatives of (3.1)–(3.3) and using the structural equations of G, we obtain the *quadratic equations*

$$\mathrm{d}\eta^1 \equiv \cdots \equiv \mathrm{d}\eta^8 \equiv \cdots \equiv \mathrm{d}\eta^{13} \equiv 0 \bmod\{\mathcal{I}\}, \tag{3.5}$$

$$\begin{cases} \mathrm{d}\eta^9 \equiv 2\pi^1\wedge\omega^1 - \pi^2\wedge\omega^2 + (-1+p_2-q_1q_2)\omega^1\wedge\omega^2 \\ \mathrm{d}\eta^{10} \equiv \pi^1\wedge\omega^1 - 2\pi^2\wedge\omega^2 + (1-p_1+q_1q_2)\omega^1\wedge\omega^2 \\ \mathrm{d}\eta^{11} \equiv \zeta^1\wedge\omega^1 + \upsilon^2\wedge\omega^2 - (2r_1q_2+3q_1p_2)\omega^1\wedge\omega^2 \\ \mathrm{d}\eta^{12} \equiv \upsilon^1\wedge\omega^1 + \zeta^2\wedge\omega^2 - (3p_1q_2+2r_2q_1)\omega^1\wedge\omega^2 \end{cases} \mod\{\mathcal{I}\}, \tag{3.6}$$

where $\{\mathcal{I}\}$ denotes the algebraic ideal generated by $\eta^1,\ldots,\eta^{13},\Theta^1,\Theta^2$ and where

$$\pi^i = \mathrm{d}q_i, \quad \upsilon^i = \mathrm{d}p_i, \quad \zeta^i = \mathrm{d}r_i \quad (i=1,2).$$

If we set

$$\begin{aligned} \Omega^1 &= 2\pi^1\wedge\omega^1 - \pi^2\wedge\omega^2 + (-1+p_2-q_1q_2)\omega^1\wedge\omega^2, \\ \Omega^2 &= \pi^1\wedge\omega^1 - 2\pi^2\wedge\omega^2 + (1-p_1+q_1q_2)\omega^1\wedge\omega^2, \\ \Omega^3 &= \zeta^1\wedge\omega^1 + \upsilon^2\wedge\omega^2 - (2r_1q_2+3q_1p_2)\omega^1\wedge\omega^2, \\ \Omega^4 &= \upsilon^1\wedge\omega^1 + \zeta^2\wedge\omega^2 - (3p_1q_2+2r_2q_1)\omega^1\wedge\omega^2, \end{aligned} \tag{3.7}$$

then

$$\{\eta^1,\ldots,\eta^{13},\Theta^1,\Theta^2,\Omega^1,\Omega^2,\Omega^3,\Omega^4,\mathrm{d}\Theta^1,\mathrm{d}\Theta^2\} \tag{3.8}$$

is a set of algebraic generators of the differential ideal $\mathcal{I}$.

An integral manifold of this system is a two-dimensional submanifold $\widetilde{X}\subset P$ such that

$$\eta^a = 0, \quad \Theta^1=\Theta^2=\Omega^1=\Omega^2=\Omega^3=\Omega^4=0, \quad \Omega\neq 0.$$

Thus, if $\widetilde{X}$ is an integral manifold, the map

$$F{:}([A],q_1,q_2,p_1,p_2,r_1,r_2)\in\widetilde{X}\mapsto[A_1\wedge A_2]\in\Lambda \tag{3.9}$$

defines a Lie minimal surface. Conversely, if $X\subset\mathbb{R}^3\times S^2$ is a Lie minimal surface with normal frame field $[A]{:}X\to G$ and invariant functions $q_1,\ldots,r_2$, then

$$([A],q_1,q_2,p_1,p_2,r_1,r_2){:}X\to P, \tag{3.10}$$

is an integral manifold of the differential system $(\mathcal{I},\Omega)$. Thus we have the following.

Proposition 3.1: Lie minimal surfaces may be regarded as the integral submanifolds of the exterior differential system $(\mathcal{I},\Omega)$.

On P, consider the parallelization

$$\left(\frac{\partial}{\partial\omega^i},\frac{\partial}{\partial\eta^a},\frac{\partial}{\partial\pi^i},\frac{\partial}{\partial\upsilon^i},\frac{\partial}{\partial\zeta}\right) \quad (i=1,2;a=1,\ldots,13)$$

dual to the coframe $(\omega^i,\eta^a,\pi^i,\upsilon^i,\zeta^i)$. The one-dimensional integral elements of $(\mathcal{I},\Omega)$ are of the form

$$E_1 = \left[a^1\frac{\partial}{\partial\omega^1} + a^2\frac{\partial}{\partial\omega^2} + y^i\frac{\partial}{\partial\pi^i} + u^i\frac{\partial}{\partial\upsilon^i} + v^i\frac{\partial}{\partial\zeta^i}\right],$$

where $(a^1)^2+(a^2)^2\neq 0$. Contracting $\Theta^1,\Theta^2,\Omega^1,\ldots,\Omega^4$ with E_1, we deduce the polar equations

$$\eta^a = 0 \quad (a=1,\ldots,13),$$

$$2a^1\pi^1 - a^2\pi^2 - (2y^1 + a^2(1-p_2+q_1q_2))\omega^1 + (y^2 + a^1(1-p_2+q_1q_2))\omega^2 = 0,$$

$$a^1\pi^1 - 2a^2\pi^2 - (y^1 - a^2(1 - p_1 + q_1q_2))\omega^1 + (2y^2 - a^1(1 - p_1 + q_1q_2))\omega^2 = 0,$$

$$a^1\upsilon^1 + a^2\zeta^2 - (u^1 + a^2(3p_1q_2 + 2r_2q_1))\omega^1 - (v^2 - a^1(3p_1q_2 + 2r_2q_1))\omega^2 = 0,$$

$$a^2\upsilon^2 + a^1\zeta^1 - (v^1 + a^2(2r_1q_2 + 3q_1p_2))\omega^1 - (u^2 - a^1(2r_1q_2 + 3q_1p_2))\omega^2 = 0,$$

$$a^2\zeta^1 - 4a^2q_1r_1\omega^1 + (4a^1q_1r_1 + v^1)\omega^2 = 0,$$

$$a^1\zeta^2 - (4a^2q_2r_2 + v^2)\omega^1 + 4a^1q_2r_2\omega^2 = 0.$$

From this we see that if E_1 is noncharacteristic (i.e., $a^1a^2 \neq 0$), then the polar space $H(E_1)$ is two dimensional. Thus, from the Cartan-Kähler theorem we obtain the following.

Proposition 3.2: If $\widetilde{\Gamma}$ is a real-analytic integral curve of $(\mathcal{I}, \Omega)$ such that $\omega^1\omega^2|_{\widetilde{\Gamma}} \neq 0$, then there exists a unique real-analytic integral manifold $\widetilde{X}$ such that $\widetilde{\Gamma} \subset \widetilde{X}$.

B. Proof of Theorem 1.1

Let $\Gamma \subset \mathbb{R}^3 \times S^2 \subset \Lambda$ be a Legendre curve and $\sigma: \Gamma \to \mathcal{Q}$ a one-parameter family of osculating spheres along Γ. Then we may parametrize the curve by $\Gamma \ni \ell \mapsto [V_0(\ell) \wedge V_1(\ell)]$, where $V_0, V_1: \Gamma \to \mathbb{R}^{4,2}$ are smooth maps such that

$$\|V_0\| = \|V_1\| = \langle V_0, V_1\rangle = 0, \quad \langle V_0, \mathrm{d}V_1\rangle = 0, \quad \sigma = [V_0]. \tag{3.11}$$

If (we use the notation $\mathrm{d}V = V'\zeta$, where ζ is a nowhere vanishing 1-form on Γ)

$$V_0(\ell) \wedge V_1(\ell) \wedge V_0'(\ell) \wedge V_1'(\ell) \wedge V_0''(\ell) \wedge V_1''(\ell) \neq 0,$$

$$V_0(\ell) \wedge V_0'(\ell) \wedge \cdots \wedge V_0^{(v)}(\ell) \neq 0, \tag{3.12}$$

for every $\ell \in \Gamma$, then $[V_0(\ell) \wedge V_0'(\ell) \wedge V_0''(\ell)] \subset \mathbb{R}^{4,2}$ is a three-dimensional linear subspace of signature (2, 1), for every $\ell \in \Gamma$.

Definition 3.3: If, in addition to (3.12), the map $\delta: \ell \in \Gamma \mapsto [V_0(\ell) \wedge V_0'(\ell) \wedge V_0''(\ell)] \in \mathfrak{D}$ is nonisotropic [i.e., $\delta^*(g_{\mathfrak{D}}) \neq 0$], then σ is said to be *generic*.

Using standard moving frame techniques, we obtain (see the Appendix for a proof of this statement) the following.

Lemma 3.4: Let Γ and σ be as above, then there exists a unique map $[B]: \Gamma \to G$ such that

$$\ell = [B_0(\ell) \wedge B_1(\ell)], \quad \sigma(\ell) = [B_0(\ell)], \quad \forall\, \ell \in \Gamma \tag{3.13}$$

and that

$$B^{-1}\,\mathrm{d}B = (\mathcal{B}_{-1} + k_0\mathcal{B}_0 + k_1\mathcal{B}_1 + k_2\mathcal{B}_2 + k_3\mathcal{B}_3)\mu, \tag{3.14}$$

where μ is a nowhere vanishing 1-form, k_0, k_1, k_2, k_3 are real-valued functions and the matrices $\mathcal{B}_J \in \mathfrak{g}$ are given by $\mathcal{B}_{-1} = -E_{1,0} + E_{3,0} + E_{0,1} - E_{2,1} - E_{4,2} + E_{5,3} + E_{5,4} - E_{4,5}$, $\mathcal{B}_0 = E_{0,0} - E_{1,1} + E_{4,4} - E_{5,5}$, $\mathcal{B}_1 = E_{0,3} + E_{3,5}$, $\mathcal{B}_2 = E_{1,2} + E_{2,4}$, $\mathcal{B}_3 = E_{0,4} - E_{1,5}$, being $E_{i,j}$ $(0 \leqslant i, j \leqslant 5)$ the matrix with 1 in the (i, j) place and 0 elsewhere.

Proof of Theorem 1.1: Let Γ and σ as above and let $[B]: \Gamma \to G$ be the canonical frame constructed in Lemma 3.4. We set $h = -3\sqrt{2}k$ and we let $[C]: \Gamma \to G$ be defined by

$$C = \mathrm{Id}_{6\times 6} + \frac{h}{2}\mathcal{C}_1 + \frac{h^2}{8}\mathcal{C}_2, \tag{3.15}$$

where $\mathcal{C}_1 = E_{1,2} - E_{0,3} + E_{0,4} + E_{2,4} - E_{1,5} - E_{3,5}$ and $\mathcal{C}_2 = E_{1,4} + E_{0,5}$. We then consider the frame field $[\widetilde{B}] = [B] \cdot C$. It is now a computational matter to check that

$$\widetilde{B}^{-1}\,\mathrm{d}\widetilde{B}=\left(\mathcal{B}_{-1}+k_0\mathcal{B}_0+\hat{k}_1\mathcal{B}_1+\hat{k}_2\mathcal{B}_2+\hat{k}_3\mathcal{B}_3+\frac{h}{2}\mathcal{B}_4\right)\mu, \tag{3.16}$$

where $\mathcal{B}_4=E_{0,0}+E_{1,1}-E_{4,4}-E_{5,5}$, $\hat{k}_2=k_2+\frac{1}{2}h'-\frac{1}{2}(hk_0-\frac{1}{4}h^2)$, $\hat{k}_1=k_1-\frac{1}{2}h'-\frac{1}{2}(hk_0+\frac{1}{4}h^2)$ and $\hat{k}_3=k_3-\frac{1}{2}h'-\frac{1}{4}h^2$. We then define the function $\bar{q}_i,\bar{p}_i,\bar{r}_i:\Gamma\to\mathbb{R}$ as follows:

$$\bar{q}_1=-\hat{k}_0-\tfrac{1}{6}h,$$

$$\bar{q}_2=\hat{k}_0-\tfrac{1}{6}h,$$

$$\bar{p}_1=-\tfrac{1}{2}\left(\hat{k}_1-\hat{k}_2-\hat{k}_3-3K\right),$$

$$\bar{p}_2=-\tfrac{1}{2}\left(\hat{k}_1-\hat{k}_2+\hat{k}_3+3K\right),$$

$$\bar{r}_1=\tfrac{1}{2}\left(\hat{k}_1+\hat{k}_2-\hat{k}_3-3K\right),$$

$$\bar{r}_2=-\tfrac{1}{2}\left(\hat{k}_1+\hat{k}_2+\hat{k}_3-3K\right). \tag{3.17}$$

Consider now the embedding $\widetilde{\Gamma}=([\widetilde{B}],\bar{q},\bar{p},\bar{r}):\Gamma\to P$. From (3.16) and (3.17) it follows that $\widetilde{\Gamma}$ is a one-dimensional integral manifold of the differential system $(\mathcal{I},\Omega)$. If we set $\mathrm{d}\bar{q}_j=\bar{q}_j^*\mu$, $\mathrm{d}\bar{p}_j=\bar{p}_j^*\mu$, and $\mathrm{d}\bar{r}_j=\bar{r}_j^*\mu$, then (3.16) implies that

$$\frac{\partial}{\partial\omega^1}-\frac{\partial}{\partial\omega^2}+\bar{q}_i^*\frac{\partial}{\partial\pi^i}+\bar{p}_i^*\frac{\partial}{\partial v^i}+\bar{r}_i^*\frac{\partial}{\partial\zeta^i} \tag{3.18}$$

is a tangent vector field along $\widetilde{\Gamma}$. This yields that $\widetilde{\Gamma}$ is a noncharacteristic K-regular integral curve of $(\mathcal{I},\Omega)$. Therefore, there exists a unique two-dimensional integral manifold $\widetilde{X}\subset P$ such that $\widetilde{\Gamma}\subset\widetilde{X}$. Consider the Legendre immersion

$$F:([A],q,p,r)\in\widetilde{X}\mapsto[A_0\wedge A_1]\in\Lambda. \tag{3.19}$$

Since our reasoning is of local nature, we may suppose that F is one-to-one and that $X=F(\widetilde{X})$ is contained in $\mathbb{R}^3\times S^2\subset\Lambda$. If we identify $\widetilde{X}$ and X, $([A],q,p,r)\in X\mapsto[A]\in G$ is the canonical frame and q_1,q_2,p_1,p_2,r_1,r_2 are the invariant functions of X. From this we deduce that X is a Lie minimal surface. By construction, the curve Γ is contained in X and

$$\alpha^1|_\Gamma=-\alpha^2|_\Gamma=\mu,\quad \bar{q}_i=q_i|_\Gamma,\quad \bar{p}_i=p_i|_\Gamma,\quad \bar{r}_i=r_i|_\Gamma,\quad i=1,2. \tag{3.20}$$

In particular, the 1-form $\alpha^1+\alpha^2$ vanishes identically along Γ. This implies that Γ is an anti-cyclidic curve of X. Combining (3.17) and (3.20) we obtain

$$K=\frac{1}{3}(p_1-p_2)|_\Gamma=K_w|_\Gamma,\quad k=\frac{1}{\sqrt{2}}(q_1+q_2)|_\Gamma=k_\Gamma,\quad \sigma=[A_0]|_\Gamma=\sigma_1|_\Gamma.$$

From this we infer that X satisfies the required properties. The uniqueness of X follows from the uniqueness of the real-analytic integral manifold $\widetilde{X}$ containing $\widetilde{\Gamma}$.

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APPENDIX: THE FRAME CONSTRUCTIONS

Proof of Theorem 2.9

Consider the fiber bundle

$$\mathcal{F}_0(X) = \{(\ell, A) \in X \times G : \ell = [A_0 \wedge A_1]\} \to X.$$

Local cross sections of $\mathcal{F}_0(X)$ are called *local frame fields* along X. They can be considered as smooth maps $[A]: U \to G$, where U is an open subset of X, such that $\ell = [A_0(\ell) \wedge A_1(\ell)]$, for every $\ell \in U$. For every local frame field $[A]: U \to G$ we let $\alpha = (\alpha^I_J)$ be the pull-back of the Maurer-Cartan form. Any other local frame field $[\widetilde{A}]$ on U is given by $[\widetilde{A}] = [A] \cdot [B]$, where $[B]: U \to G_0$ is a smooth map into the isotropy subgroup

$$G_0 = \{[A] \in G : [A_0 \wedge A_1] = [\epsilon_0 \wedge \epsilon_1]\}.$$

Thus, the 1-forms α and $\widetilde{\alpha}$ are related by the gauge transformation

$$\widetilde{\alpha} = B^{-1}\, \mathrm{d}B + B^{-1} \alpha B. \tag{A1}$$

A frame field $[A]: U \to G$ is of *first order* if

$$\alpha^3_0 \wedge \alpha^2_0 > 0, \quad \alpha^2_0 = \alpha^3_1 = 0. \tag{A2}$$

From (A1) it follows that first order frames exist on a neighborhood of any point of X. The totality of first order frames is a principal G_1-bundle $\mathcal{F}_1(X) \to X$ where

$$G_1 = \left\{ [X(D,S,Y,b)] \in G_0 : S = \epsilon \mathrm{Id}_{2\times 2},\ D = \begin{pmatrix} r & 0 \\ 0 & s \end{pmatrix},\ \epsilon = \pm 1,\ rs > 0 \right\}.$$

Notation: The elements of G_1 will be denoted by $[Y_\epsilon(r,s,Y,b)]$, where $\epsilon = \pm 1, Y \in \mathfrak{gl}(2,\mathbb{R}), b, r, s \in \mathbb{R}$ and $rs > 0$.

If $[A]: U \to G$ is a first order frame then, the linear differential forms $\alpha^1 = \alpha^3_0$ and $\alpha^2 = \alpha^2_1$ give a positive-oriented coframing on U so that we may write

$$\alpha = P_1 \alpha^1 + P_2 \alpha^2,$$

where $P_1, P_2 : U \to \mathfrak{g}$ are smooth maps. The components of P_a are denoted by P^I_{Ja}, where $a = 1, 2$ and where $I, J = 0, \ldots, 5$. If $[A], [\widetilde{A}] : U \to G$ are first order frames on U and if the corresponding transition function is of the form $[Y_\epsilon(r,s,Y,b)] : U \to G_1$, then

$$\widetilde{\alpha}^1 = \epsilon r \alpha^1, \quad \widetilde{\alpha}^2 = \epsilon s \alpha^2,$$

$$\widetilde{\alpha}^1_0 = r(s^{-1}\alpha^1_0 - Y^2_1 \alpha^1), \quad \widetilde{\alpha}^0_1 = s(r^{-1}\alpha^0_1 - Y^1_2 \alpha^2). \tag{A3}$$

This implies

$$\widetilde{P}^1_{01} = \epsilon(s^{-1} P^1_{01} - Y^2_1), \quad \widetilde{P}^1_{02} = \epsilon r s^{-2} P^1_{02},$$

$$\widetilde{P}^0_{12} = -\epsilon(r^{-1}P^0_{12} + Y^1_2), \quad \widetilde{P}^0_{11} = \epsilon s r^{-2} P^0_{11}. \tag{A4}$$

From (A4) we see that for every point $\ell \in X$ there exist a first order frame field $A: U \to G$ defined on an open neighborhood U of ℓ with respect to which $P^1_{01} = P^0_{12} = 0$. Such first order frame fields are said to be of *second order*. In addition, any other second order frame field on U is of the form $[\widetilde{A}] = [A] \cdot [B]$, where $[B]: U \to G_2$ is a smooth map and

$$G_2 = \left\{ [Y_\epsilon(r,s,Y,b)] \in G_1 : Y = \begin{pmatrix} p & 0 \\ 0 & q \end{pmatrix}, p,q \in \mathbb{R} \right\}.$$

Notation: The elements of G_2 will be denoted by $Y_\epsilon(r,s,p,q,b)$, where $\epsilon = \pm 1, p,q,r,s,b \in \mathbb{R}$ and $rs > 0$.

Second order frame fields are the cross sections of a reduced sub-bundle $\mathcal{F}_2(X)$ of $\mathcal{F}_1(X)$ with structural group G_2. Differentiating $\alpha^2_0 = \alpha^3_1 = 0$ and applying the structure equations and Cartan's lemma, we have that $\alpha^3_2 = 0$, for every second order frame field A. Taking the exterior derivative of $\alpha^3_2 = 0$ and using again the structure equations and the Cartan's lemma we have $\alpha^0_2 \wedge \alpha^1 - \alpha^1_3 \wedge \alpha^2 = 0$. This implies $P^0_{22} = -P^1_{31}$ and hence we may write

$$\alpha^0_2 = P^0_{21}\alpha^1 + P^0_{22}\alpha^2, \quad \alpha^1_3 = -P^0_{22}\alpha^1 + P^1_{32}\alpha^2. \tag{A5}$$

If $[A]$ and $[\widetilde{A}]$ are second order frame fields on $U \subset X$ and if $[Y_\epsilon(r,s,p,q,b)]: U \to G_2$ is the corresponding transition function, we then have

$$\widetilde{\alpha}^0_2 = \epsilon r^{-1} s p \alpha^0_1 + \epsilon r^{-1}\alpha^0_2 - sb\alpha^2, \quad \widetilde{\alpha}^1_3 = \epsilon s^{-1} r q \alpha^1_0 + \epsilon s^{-1}\alpha^1_3 + rb\alpha^1. \tag{A6}$$

From this we obtain

$$\widetilde{P}^0_{21} = r^{-2}(P^0_{21} + spP^0_{11}), \quad \widetilde{P}^0_{22} = \frac{1}{rs}P^0_{22} - \epsilon b, \quad \widetilde{P}^1_{32} = s^{-2}(P^1_{32} + rqP^1_{02}). \tag{A7}$$

Thus, for every point $\ell \in X$ there exist a second order frame field $U \to G$ defined on an open neighborhood of ℓ with respect to which

$$P^0_{22} = P^1_{31} = 0. \tag{A8}$$

Such frame fields are said to be of *third order*. Now, (A7) implies that these frame fields are the local cross sections of a reduced sub-bundle $\mathcal{F}_3(X)$ of $\mathcal{F}_2(X)$. The structure group of $\mathcal{F}_3(X)$ is

$$G_3 = \{[Y_\epsilon(r,s,p,q,b)] \in G_2 : b = 0\}.$$

Since X is nondegenerate, then the functions P^1_{02} and P^0_{11} are nowhere vanishing. Thus, from (A4) we infer that for every $\ell \in M$ there exist a third order frame field $[A]: U \to G$ defined on an open neighborhood U of ℓ such that

$$\alpha^0_1 = \alpha^1, \quad \alpha^1_0 = \alpha^2. \tag{A9}$$

A third order frame field satisfying (A9) is said to be of *fourth order*. If $[A]$ is a fourth order frame field on U, then any other is given by $[\widetilde{A}] = [A][B]$, where $[B]: U \to G_4$ and

$$G_4 = \{[Y_\epsilon(r,s,p,q,0)] \in G_3 : r = s = \epsilon\}.$$

The elements of G_4 are denoted by $[Y_\epsilon(p,q)]$, where $p,q \in \mathbb{R}$. From this we immediately see that the fourth order frame fields define a G_4 sub-bundle $\mathcal{F}_4(X)$ of $\mathcal{F}_3(X)$. Now, using (A7) we see that for every $\ell \in X$ there exist a unique fourth order frame $[A]: X \to G$ such that

$$\alpha^0_2 = \alpha^1_3 = 0.$$

Then, $[A]$ is the unique frame along X satisfying the required properties.

Proof of Lemma 3.4

Let G_0 be the fiber bundle defined by

$$\mathcal{R}_0 = \{(\ell, R) \in \Gamma \times G : \ell = [R_0 \wedge R_1], [R_0] = \sigma(\ell)\} \to \Gamma.$$

The cross sections of $\mathcal{R}_0$ are smooth maps $R : U \to G$ defined on an open subset $U \subset \Gamma$, such that

$$\ell = [R_0(\ell) \wedge R_1(\ell)], \quad [R_0(\ell)] = \sigma(\ell), \quad \forall\, \ell \in U.$$

For each frame field $R : U \to G$ we let ρ be the $\mathfrak{g}$-valued 1-form $R^{-1}\, \mathrm{d}R$. We say that $R : U \to G$ is of *first order* if

$$\rho_0^3 \neq 0, \quad \rho_0^2 = \rho_1^3 = \rho_0^3 + \rho_1^2 = \rho_0^4 = 0. \tag{A10}$$

Since Γ satisfies (3.11) and (3.12) then, first order frames do exist near any point of Γ and they define a sub-bundle $\mathcal{R}_1$ of $\mathcal{R}_0$ with fiber

$$H_1 = \{X \in G_0 : X = X(r\epsilon I, \epsilon I, Y, b), \epsilon = \pm 1, r, b \in \mathbb{R}, r \neq 0, Y \in \mathfrak{gl}(2, \mathbb{R})\}.$$

If R and $\widetilde{R}$ are first order frames related by $\widetilde{R} = RX(r\epsilon I, \epsilon I, Y, b)$ then

$$\widetilde{\rho}_1^0 = \rho_1^0 + rY_1^2\rho_0^3, \quad \widetilde{\rho}_0^1 = \rho_0^1 - rY_2^1\rho_0^3, \quad \widetilde{\rho}_2^3 = \rho_2^3 + \epsilon r(Y_2^1 + Y_1^2)\rho_0^3. \tag{A11}$$

This shows that near any point of Γ there exist first order frames such that

$$\rho_0^1 + \rho_1^0 = \rho_2^3 = 0. \tag{A12}$$

Frame fields satisfying (A12) are said to be of *second order*. From (A11) it follows that the totality of second order frames defines a fiber bundle $\mathcal{R}_2$ with fiber

$$H_2 = \{X = X(r\epsilon I, \epsilon I, Y, b) \in H_1 : Y_2^1 = Y_1^2 = 0\}.$$

Notice that the 1-form ρ_1^0 is independent of the choice of the second order frame and hence there exist $\mu \in \Omega^1(\Gamma)$ such that $\mu|_U = \rho_1^0$. Since $\delta : \Gamma \to \mathfrak{D}$ is nonisotropic and since $\delta^*(g_{\mathfrak{D}}) = -\mu^2$ we may conclude that μ is nowhere vanishing. From (A11) it follows that, locally, there exist second order frames such that

$$\rho_0^3 = -\rho_1^2 = -\rho_0^1 = \rho_1^0 = \mu. \tag{A13}$$

Frame fields satisfying (A13) are of *third order*. The totality of third order frames originates a principal fiber bundle $\mathcal{R}_3$ with structural group

$$H_3 = \{X = X(r\epsilon I, \epsilon I, Y, b) \in H_2 : r = 1\}.$$

If $\widetilde{R}$ and R are third order frame fields then

$$\widetilde{\rho}_0^0 = \rho_0^0 - \epsilon Y_2^2\rho_0^3, \quad \widetilde{\rho}_1^1 = \rho_1^1 + \epsilon Y_1^1\rho_0^3.$$

Therefore, near any point of Γ there exist a third order frame field R such that

$$\rho_1^1 + \rho_0^0 = 0. \tag{A14}$$

Frame fields satisfying (A14) define a reduced sub-bundle $\mathcal{R}_4$ with structure group

$$H_4 = \{X = X(\epsilon I, \epsilon I, Y, b) \in H_3 : Y_1^1 = Y_2^2\}.$$

Consider two local cross sections R and $\widetilde{R}$ of $\mathcal{R}_4$, we then have

$$\widetilde{\rho}_2^0 = \rho_2^0 + \epsilon\left(Y_1^1 + \frac{b}{2}\right)\mu, \quad \widetilde{\rho}_3^1 = \rho_3^1 - \epsilon\left(Y_1^1 - \frac{b}{2}\right)\mu. \tag{A15}$$

This implies that there exist fourth order frame fields with respect to which

$$\rho_2^0 = \rho_3^1 = 0. \tag{A16}$$

Fourth order frame fields satisfying (A16) are said to be of *fifth order*. The totality of fifth order frames generates a reduced sub-bundle $\mathcal{R}_5$ with fiber $\mathbb{Z}_2=\{\pm I\}$ and henceforth $\mathcal{R}_5$ is generated by a unique map $[B]:\Gamma\to G$ satisfying the required properties.

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Integrable equations on time scales

Metin Gürses
Department of Mathematics, Faculty of Sciences, Bilkent University, 06800 Ankara, Turkey

Gusein Sh. Guseinov
Department of Mathematics, Atilim University, 06836 Incek, Ankara, Turkey

Burcu Silindir
Department of Mathematics, Faculty of Sciences, Bilkent University, 06800 Ankara, Turkey

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Integrable systems are usually given in terms of functions of continuous variables (on $\mathbb{R}$), in terms of functions of discrete variables (on $\mathbb{Z}$), and recently in terms of functions of q-variables (on $\mathbb{K}_q$). We formulate the Gel'fand-Dikii (GD) formalism on time scales by using the delta differentiation operator and find more general integrable nonlinear evolutionary equations. In particular they yield integrable equations over integers (difference equations) and over q-numbers (q-difference equations). We formulate the GD formalism also in terms of shift operators for all regular-discrete time scales. We give a method allowing to construct the recursion operators for integrable systems on time scales. Finally, we give a trace formula on time scales and then construct infinitely many conserved quantities (Casimirs) of the integrable systems on time scales. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Integrable systems are well studied and well understood in $1+1$ dimensions.[1–3] Here one of the dimensions denotes the time (evolution) variable and the other one denotes the space variable which is usually taken as continuous. There are also important examples where this variable takes values in $\mathbb{Z}$, i.e., integer values. In both cases the Gel'fand-Dikii (GD) approach is quite effective. One can generate hierarchies of integrable evolution equations, both on $\mathbb{R}$ and on $\mathbb{Z}$ (see Ref. 3 for GD applications and related references). In addition one can construct the conserved quantities, Hamilton operators, and recursion operators. Investigation of integrable systems on q-discrete intervals started in Refs. 4–6. They considered GD formalism on $\mathbb{K}_q$ and found q-integrable hierarchies including the q-KdV equation.

In this work we extend the Gel'fand-Dikii approach to time scales where $\mathbb{R}$, $\mathbb{Z}$, and $\mathbb{K}_q$ are special cases. In the next section we give a brief review of time scales calculus. See Refs. 7–13 for a more detailed review of the subject. In GD formalism, in obtaining integrable systems the essential tools are the differential and shift operators and their inverses. For extending the GD formulation to time scales we give the necessary means to construct in the sequel the algebra of pseudo-Δ-differential operators and the algebra of shift operators. In Sec. III we assume Δ-differential Lax operators and derive the Δ-Burgers hierarchy with its recursion operator. We present special cases of the Burgers equation for $\mathbb{T}=h\mathbb{Z}$ and $\mathbb{T}=\mathbb{K}_q$. In Sec. IV, we consider the *regular* time scales where the inverse of jump operators can be defined. Here we assume a pseudo-Δ-differential algebra and give the corresponding GD formulation. As an example we present a Δ-KdV hierarchy. We first find $n=1$ member of the hierarchy and write out it explicitly for $\mathbb{T}=\mathbb{R},\mathbb{Z},\mathbb{K}_q$ and for $\mathbb{T}=(-\infty,0)\cup\mathbb{K}_q$. Then we give the $n=3$ member and call it as the Δ-KdV system. We call it Δ-KdV equation, because the corresponding Lax operator is a second order Δ-differential operator. It involves two fields u and v, but the second field v can be expressed in

terms of the first filed u. When $\mathbb{T}=\mathbb{R}$, this system reduces to the standard KdV equation. In Sec. V, we consider the *regular-discrete* time scales and introduce the algebra of shift operators on them and give the corresponding GD formulation for all such time scales. Here several examples are presented. We first generalize the examples of discrete systems on $\mathbb{Z}$ given in Ref. 3 (one field, two fields, and four fields examples in Ref. 3) to arbitrary discrete time scales. In all these examples when $\mathbb{T}=\mathbb{Z}$ we get the discrete evolutions given in Ref. 3. We construct the recursion operators of these systems on time scales. We generalize the Frenkel's KdV system[4] introduced on $\mathbb{K}_q$ to arbitrary discrete time scales and we construct its recursion operator. In this section, we finally give an example of the KP hierarchy on discrete time scales. In Sec. VI, we extend the standard way of constructing the conserved quantities of integrable systems to time scales by introducing a *trace form* on the algebra of Δ-pseudo-differential operators. The trace form introduced in this section reduces, in particular cases, to the standard trace forms on $\mathbb{R}$ and $\mathbb{Z}$. In the Appendix we give the recursion operators of two *four-fields systems* introduced in Sec. V. We end up with a conclusion.

II. TIME SCALE CALCULUS

The time scale calculus is developed mainly to unify differential, difference, and q-calculus. A time scale ($\mathbb{T}$) is an arbitrary nonempty closed subset of the real numbers. The calculus of time scales was initiated by Aulbach and Hilger[7,8] in order to create a theory that can unify and extend discrete and continuous analysis. The real numbers ($\mathbb{R}$), the integers ($\mathbb{Z}$), the natural numbers ($\mathbb{N}$), the non-negative integers ($\mathbb{N}_0$), the h-numbers ($h\mathbb{Z}=\{hk:k\in\mathbb{Z}\}$, where $h>0$ is a fixed real number), and the q-numbers ($\mathbb{K}_q=q^{\mathbb{Z}}\cup\{0\}\equiv\{q^k:k\in\mathbb{Z}\}\cup\{0\}$, where $q>1$ is a fixed real number) are examples of time scales, as are $[0,1]\cup[2,3]$,$[0,1]\cup\mathbb{N}$, and the Cantor set, where $[0,1]$ and $[2,3]$ are real number intervals. In Refs. 7 and 8 Aulbach and Hilger introduced also dynamic equations on time scales in order to unify and extend the theory of ordinary differential equations, difference equations, and quantum equations[9] (h-difference and q-difference equations based on h-calculus and q-calculus, respectively). For a general introduction to the calculus on time scales we refer the reader to the textbooks by Bohner and Peterson.[10,11] Here we give only those notions and facts connected to time scales which we need for our purpose in this paper.

Any time scale $\mathbb{T}$ is a complete metric space with the metric (distance) $d(x,y)=|x-y|$ for $x,y\in\mathbb{T}$. Consequently, according to the well-known theory of general metric spaces, we have for $\mathbb{T}$ the fundamental concepts such as open balls (intervals), neighborhood of points, open sets, closed sets, compact sets, and so on. In particular, for a given number $r>0$, the r-neighborhood $U_r(x)$ of a given point $x\in\mathbb{T}$ is the set of all points $y\in\mathbb{T}$ such that $d(x,y)<r$. By a neighborhood of a point $x\in\mathbb{T}$ is meant an arbitrary set in $\mathbb{T}$ containing an r-neighborhood of the point x. Also we have for functions $f:\mathbb{T}\to\mathbb{R}$ the concepts of the limit, continuity, and properties of continuous functions on general complete metric spaces (note that, in particular, any function $f:\mathbb{Z}\to\mathbb{R}$ is continuous at each point of $\mathbb{Z}$). The main task is to introduce and investigate the concept of derivative for functions $f:\mathbb{T}\to\mathbb{R}$. This proves to be possible due to the special structure of the metric space $\mathbb{T}$. In the definition of derivative, the so-called forward and backward jump operators play special and important roles.

Definition 1: For $x\in\mathbb{T}$ we define the forward jump operator $\sigma:\mathbb{T}\to\mathbb{T}$ by

$$\sigma(x)=\inf\{y\in\mathbb{T}:y>x\}, \tag{1}$$

while the backward jump operator $\rho:\mathbb{T}\to\mathbb{T}$ is defined by

$$\rho(x)=\sup\{y\in\mathbb{T}:y<x\}. \tag{2}$$

In this definition we set in addition $\sigma(\max\mathbb{T})=\max\mathbb{T}$ if there exists a finite $\max\mathbb{T}$, and $\rho(\min\mathbb{T})=\min\mathbb{T}$ if there exists a finite $\min\mathbb{T}$. Obviously both $\sigma(x)$ and $\rho(x)$ are in $\mathbb{T}$ when $x\in\mathbb{T}$. This is because of our assumption that $\mathbb{T}$ is a closed subset of $\mathbb{R}$.

Let $x\in\mathbb{T}$. If $\sigma(x)>x$, we say that x is *right-scattered*, while if $\rho(x)<x$ we say that x is *left-scattered*. Also, if $x<\max\mathbb{T}$ and $\sigma(x)=x$, then x is called *right-dense*, and if $x>\min\mathbb{T}$ and

$\rho(x)=x$, then x is called *left-dense*. Points that are right-scattered and left-scattered at the same time are called *isolated*. Finally, the *graininess functions* $\mu,\nu:\mathbb{T}\to[0,\infty)$ are defined by

$$\mu(x)=\sigma(x)-x, \quad \text{and } \nu(x)=x-\rho(x) \quad \text{for all } x\in\mathbb{T}. \tag{3}$$

Example 1: If $\mathbb{T}=\mathbb{R}$, then $\sigma(x)=\rho(x)=x$ and $\mu(x)=\nu(x)=0$. If $\mathbb{T}=h\mathbb{Z}$, then $\sigma(x)=x+h$, $\rho(x)=x-h$, and $\mu(x)=\nu(x)=h$. On the other hand, if $\mathbb{T}=\mathbb{K}_q$ then we have

$$\sigma(x)=qx, \quad \rho(x)=q^{-1}x, \quad \mu(x)=(q-1)x, \quad \text{and } \nu(x)=(1-q^{-1})x. \tag{4}$$

Let $\mathbb{T}^\kappa$ denote Hilger's above truncated set consisting of $\mathbb{T}$ except for a possible left-scattered maximal point. Similarly, $\mathbb{T}_\kappa$ denotes the below truncated set obtained from $\mathbb{T}$ by deleting a possible right-scattered minimal point.

Definition 2: Let $f:\mathbb{T}\to\mathbb{R}$ be a function and $x\in\mathbb{T}^\kappa$. Then the delta derivative of f at the point x is defined to be the number $f^\Delta(x)$ (provided it exists) with the property that for each $\varepsilon>0$ there exists a neighborhood U of x in $\mathbb{T}$ such that

$$|f(\sigma(x))-f(y)-f^\Delta(x)[\sigma(x)-y]|\leqslant\varepsilon|\sigma(x)-y|, \tag{5}$$

for all $y\in U$.

Remark 1: If $x\in\mathbb{T}\backslash\mathbb{T}^\kappa$, then $f^\Delta(x)$ is not uniquely defined, since for such a point x, small neighborhoods U of x consist only of x and besides we have $\sigma(x)=x$. Therefore (5) holds for an arbitrary number $f^\Delta(x)$. This is a reason why we omit a maximal left-scattered point.

We have the following: (i) If f is delta differentiable at x, then f is continuous at x. (ii) If f is continuous at x and x is right-scattered, then f is delta differentiable at x with

$$f^\Delta(x)=\frac{f(\sigma(x))-f(x)}{\mu(x)}. \tag{6}$$

(iii) If x is right-dense, then f is delta differentiable at x iff the limit

$$\lim_{y\to x}\frac{f(x)-f(y)}{x-y} \tag{7}$$

exists as a finite number. In this case $f^\Delta(x)$ is equal to this limit. (iv) If f is delta differentiable at x, then

$$f(\sigma(x))=f(x)+\mu(x)f^\Delta(x). \tag{8}$$

Definition 3: If $x\in\mathbb{T}_\kappa$, then we define the nabla derivative of $f:\mathbb{T}\to\mathbb{R}$ at x to be the number $f^\nabla(x)$ (provided it exists) with the property that for each $\varepsilon>0$ there is a neighborhood U of x in $\mathbb{T}$ such that

$$|f(\rho(x))-f(y)-f^\nabla(x)[\rho(x)-y]|\leqslant\varepsilon|\rho(x)-y|, \tag{9}$$

for all $y\in U$.

We have the following: (i) If f is nabla differentiable at x, then f is continuous at x. (ii) If f is continuous at x and x is left-scattered, then f is nabla differentiable at x with

$$f^\nabla(x)=\frac{f(x)-f(\rho(x))}{\nu(x)}. \tag{10}$$

(iii) If x is left-dense, then f is nabla differentiable at x if and only if the limit

$$\lim_{y\to x}\frac{f(x)-f(y)}{x-y} \tag{11}$$

exists as a finite number. In this case $f^{\nabla}(x)$ is equal to this limit. (iv) If f is nabla differentiable at x, then

$$f(\rho(x))=f(x)-\nu(x)f^{\nabla}(x). \tag{12}$$

Example 2: If $\mathbb{T}=\mathbb{R}$, then $f^{\Delta}(x)=f^{\nabla}(x)=f'(x)$, the ordinary derivative of f at x. If $\mathbb{T}=h\mathbb{Z}$, then

$$f^{\Delta}(x)=\frac{f(x+h)-f(x)}{h} \quad \text{and } f^{\nabla}(x)=\frac{f(x)-f(x-h)}{h}. \tag{13}$$

If $\mathbb{T}=\mathbb{K}_q$, then

$$f^{\Delta}(x)=\frac{f(qx)-f(x)}{(q-1)x} \quad \text{and } f^{\nabla}(x)=\frac{f(x)-f(q^{-1}x)}{(1-q^{-1})x}, \tag{14}$$

for all $x\neq 0$, and

$$f^{\Delta}(0)=f^{\nabla}(0)=\lim_{y\to 0}\frac{f(y)-f(0)}{y} \tag{15}$$

provided that this limit exists.

Among the important properties of the delta differentiation on $\mathbb{T}$ we have the Leibnitz rule, if $f,g:\mathbb{T}\to\mathbb{R}$ are delta differentiable functions at $x\in\mathbb{T}^{\kappa}$, then so is their product fg and

$$(fg)^{\Delta}(x)=f^{\Delta}(x)g(x)+f(\sigma(x)g^{\Delta}(x) \tag{16}$$

$$=f(x)g^{\Delta}(x)+f^{\Delta}(x)g(\sigma(x)). \tag{17}$$

Also, if $f,g:\mathbb{T}\to\mathbb{R}$ are nabla differentiable functions at $x\in\mathbb{T}_{\kappa}$, then so is their product fg and

$$(fg)^{\nabla}(x)=f^{\nabla}(x)g(x)+f(\rho(x)g^{\nabla}(x), \tag{18}$$

$$=f(x)g^{\nabla}(x)+f^{\nabla}(x)g(\rho(x)). \tag{19}$$

In the next proposition we give a relationship between the delta and nabla derivatives (see Ref. 12).

Proposition 4: (i) Assume that $f:\mathbb{T}\to\mathbb{R}$ is delta differentiable on $\mathbb{T}^{\kappa}$. Then f is nabla differentiable at x and

$$f^{\nabla}(x)=f^{\Delta}(\rho(x)), \tag{20}$$

for $x\in\mathbb{T}_{\kappa}$ such that $\sigma(\rho(x))=x$. If, in addition, f^{Δ} is continuous on $\mathbb{T}^{\kappa}$, then f is nabla differentiable at x and (20) holds for any $x\in\mathbb{T}_{\kappa}$.

(ii) Assume that $f:\mathbb{T}\to\mathbb{R}$ is nabla differentiable on $\mathbb{T}_{\kappa}$. Then f is delta differentiable at x and

$$f^{\Delta}(x)=f^{\nabla}(\sigma(x)), \tag{21}$$

for $x\in\mathbb{T}^{\kappa}$ such that $\rho(\sigma(x))=x$. If, in addition, f^{∇} is continuous on $\mathbb{T}_{\kappa}$, then f is delta differentiable at x and (21) holds for any $x\in\mathbb{T}^{\kappa}$.

Now we introduce the concept of integral for functions $f:\mathbb{T}\to\mathbb{R}$.

Definition 5: A function $F:\mathbb{T}\to\mathbb{R}$ is called a Δ-antiderivative of $f:\mathbb{T}\to\mathbb{R}$ provided $F^{\Delta}(x)=f(x)$ holds for all x in $\mathbb{T}^{\kappa}$. Then we define the Δ-integral from a to b of f by

$$\int_a^b f(x)\Delta x = F(b) - F(a) \quad \textit{for all } a,b \in \mathbb{T}. \tag{22}$$

Definition 6: A function $\Phi:\mathbb{T}\to\mathbb{R}$ *is called a* ∇*-antiderivative of* $f:\mathbb{T}\to\mathbb{R}$ *provided* $\Phi^{\nabla}(x) = f(x)$ *holds for all* x *in* $\mathbb{T}_{\kappa}$*. Then we define the* ∇*-integral from* a *to* b *of* f *by*

$$\int_a^b f(x)\,\nabla x = \Phi(b) - \Phi(a) \quad \textit{for all } a,b \in \mathbb{T}. \tag{23}$$

If $a,b \in \mathbb{T}$ with $a \leqslant b$ we define the closed interval $[a,b]$ in $\mathbb{T}$ by

$$[a,b] = \{x \in \mathbb{T}: a \leqslant x \leqslant b\}. \tag{24}$$

Open and half-open intervals, etc., are defined accordingly. Below all our intervals will be time scale intervals

Example 3: Let $a,b \in \mathbb{T}$ with $a < b$. Then we have the following.

(i) If $f:\mathbb{T}=\mathbb{R}$ then

$$\int_a^b f(x)\Delta x = \int_a^b f(x)\,\nabla x = \int_a^b f(x)\mathrm{d}x, \tag{25}$$

where the integral on the right-hand side is the ordinary integral.

(ii) If $[a,b]$ consists of only isolated points, then

$$\int_a^b f(x)\Delta x = \sum_{x\in[a,b)} \mu(x)f(x) \quad \text{and} \quad \int_a^b f(x)\,\nabla x = \sum_{x\in(a,b]} \nu(x)f(x). \tag{26}$$

In particular, if $\mathbb{T}=\mathbb{Z}$, then

$$\int_a^b f(x)\Delta x = \sum_{k=a}^{b-1} f(k) \quad \text{and} \quad \int_a^b f(x)\,\nabla x = \sum_{k=a+1}^{b} f(k). \tag{27}$$

If $\mathbb{T}=h\mathbb{Z}$, then

$$\int_a^b f(x)\Delta x = h\sum_{x\in[a,b)} f(x) \quad \text{and} \quad \int_a^b f(x)\,\nabla x = h\sum_{x\in(a,b]}^{b} f(x) \tag{28}$$

and if $\mathbb{T}=\mathbb{K}_q$, then

$$\int_a^b f(x)\Delta x = (1-q)\sum_{x\in[a,b)} xf(x) \quad \text{and} \quad \int_a^b f(x)\,\nabla x = (1-q^{-1})\sum_{x\in(a,b]} xf(x). \tag{29}$$

The following relationship between the delta and nabla integrals follows from Definitions 5 and 6 by using Proposition 4.

Proposition 7: If the function $f:\mathbb{T}\to\mathbb{R}$ *is continuous, then for all* $a,b \in \mathbb{T}$ *with* $a<b$ *we have*

$$\int_a^b f(x)\Delta x = \int_a^b f(\rho(x))\,\nabla x \quad \textit{and} \quad \int_a^b f(x)\,\nabla x = \int_a^b f(\sigma(x))\Delta x. \tag{30}$$

Indeed, if $F:\mathbb{T}\to\mathbb{R}$ is a Δ-antiderivative for f, then $F^{\Delta}(x)=f(x)$ for all $x\in\mathbb{T}^{\kappa}$, and by Proposition 4 we have $f(\rho(x))=F^{\Delta}(\rho(x))=F^{\nabla}(x)$ for all $x\in\mathbb{T}_{\kappa}$, so that F is a ∇-antiderivative for $f(\rho(x))$. Therefore

$$\int_a^b f(\rho(x))\,\nabla x = F(b) - F(a) = \int_a^b f(x)\Delta x. \tag{31}$$

From (16)–(21) and (30) we have the following integration by parts formulas: If the functions $f, g: \mathbb{T} \to \mathbb{R}$ are delta and nabla differentiable with continuous derivatives, then

$$\int_a^b f^{\Delta}(x)g(x)\Delta x = f(x)g(x)\Big|_a^b - \int_a^b f(\sigma(x))g^{\Delta}(x)\Delta x, \tag{32}$$

$$\int_a^b f^{\nabla}(x)g(x)\,\nabla x = f(x)g(x)\Big|_a^b - \int_a^b f(\rho(x))g^{\nabla}(x)\,\nabla x, \tag{33}$$

$$\int_a^b f^{\Delta}(x)g(x)\Delta x = f(x)g(x)\Big|_a^b - \int_a^b f(x)g^{\nabla}(x)\,\nabla x, \tag{34}$$

$$\int_a^b f^{\nabla}(x)g(x)\,\nabla x = f(x)g(x)\Big|_a^b - \int_a^b f(x)g^{\Delta}(x)\Delta x. \tag{35}$$

For more general treatment of the delta integral on time scales (Riemann and Lebesgue delta integrals on time scales) see Ref. 13 and Chap. 5 of Ref. 11.

III. BURGERS EQUATION ON TIME SCALES

The Gel'fand-Dikii approach is very effective in studying the symmetries, bi-Hamiltonian formulation, and in constructing the recursion operators of integrable nonlinear partial differential equations. In this approach one takes the Lax operator L in an algebra like a differential or pseudodifferential algebra, a matrix algebra, a polynomial algebra, or the Moyal algebra. In this section we take L in the algebra of delta-differential operators.

Let $\mathbb{T}$ be a time scale. We say that a function $f: \mathbb{T} \to \mathbb{R}$ is Δ-smooth if it is infinitely Δ-differentiable (and hence infinitely ∇-differentiable). By Δ we denote the *delta-differentiation operator* which assigns to each Δ-differentiable function $f: \mathbb{T} \to \mathbb{R}$ its delta derivative $\Delta(f)$ defined by

$$[\Delta(f)](x) = f^{\Delta}(x) \quad \text{for } x \in \mathbb{T}^{\kappa}. \tag{36}$$

The *shift operator* E is defined by the formula

$$(Ef)(x) = f(\sigma(x)) \tag{37}$$

for $x \in \mathbb{T}$, where $\sigma: \mathbb{T} \to \mathbb{T}$ is the forward jump operator. It is convenient, in the operator relations to denote the delta-differentiation operator by δ rather than by Δ. For example, δf will denote the composition (product) of the delta-differentiation operator δ and the operator of multiplication by the function f. According to formula (16) we have

$$\delta f = f^{\Delta} + E(f)\delta. \tag{38}$$

Consider the Nth order δ-differential operator given by

$$L = a_N \delta^N + a_{N-1}\delta^{N-1} + \cdots + a_1\delta + a_0, \tag{39}$$

where the coefficients a_i $(i=0,1,\ldots,N)$ are some Δ-smooth functions of the variable $x \in \mathbb{T}$. These functions are assumed to depend also on a continuous variable $t \in \mathbb{R}$, however, we will not (for simplicity) indicate explicitly the dependence on t.

Proposition 8: Let L be given as in (39) and $A_n = (L^n)_{>0}$ *be the operator* L^n *missing the* δ^0

term. Then the Lax equation

$$\frac{dL}{dt_n} = [A_n, L] = A_n L - L A_n \tag{40}$$

for $n = 1, 2, \ldots$ *produces a consistent hierarchy of coupled nonlinear evolutionary equations.*

Example 4. Burgers equation on time scale: Let $L = v\delta + u$, where u and v are functions of $x \in \mathbb{T}$ and $t \in \mathbb{R}$. Then for an appropriate operator A the Lax equation

$$\frac{dL}{dt} = [A, L] \tag{41}$$

defines a system of two differential equations for the functions u and v. We find the operator A by using the Gelfand-Dikii formalism. Let us start with the second power of L and assume $A = (L^2)_{>0}$, where

$$L^2 = vE(v)\delta^2 + [vv^{\Delta} + vE(u) + uv]\delta + vu^{\Delta} + u^2. \tag{42}$$

We can assume $A = -(L^2)_0$ (the part of $-L^2$ without the δ terms). With this choice, (41) gives

$$\frac{dv}{dt} = \mu v(vu^{\Delta} + u^2)^{\Delta}, \tag{43}$$

$$\frac{du}{dt} = v(vu^{\Delta} + u^2)^{\Delta}, \tag{44}$$

where $\mu(x) = \sigma(x) - x$ for $x \in \mathbb{T}$.

Equations (43) and (44) given above are not independent of each other. It is easy to see that $v = \mu u + \lambda$, where λ is an arbitrary real function depending only on $x \in \mathbb{T}$. Then these two equations reduce to a single equation, a Burgers equation on time scales,

$$\frac{du}{dt} = (\mu u + \lambda)[u^2 + (\mu u + \lambda)u^{\Delta}]^{\Delta}. \tag{45}$$

Let us present some special cases: (i) When $\mathbb{T} = \mathbb{R}$ then $\mu = 0$ and $\delta = D$, the usual differentiation. Hence we can let $\lambda = 1$ and (45) reduces to the standard Burgers equation on $\mathbb{R}$. (ii) When $\mathbb{T} = h\mathbb{Z}$ then $\mu(m) = h$ and $f^{\Delta}(m) = (1/h)[f(m+h) - f(m)]$ for any f. Then taking $\lambda = 0$ in (45) we find

$$\frac{du(m)}{dt} = u(m)u(m+h)[u(m+2h) - u(m)], \tag{46}$$

where $m \in h\mathbb{Z}$. The evolution equation given above in (46) represents a difference version of the Burgers equation. (iii) Let $\mathbb{T} = q^{\mathbb{Z}}$, where $q \neq 1$ and $q > 0$. Then we have $\mu(x) = (q-1)x$ and $f^{\Delta}(x) = [f(qx) - f(x)]/(q-1)x$ and taking $\lambda = 0$ we get from (45)

$$\frac{du(x)}{dt} = u(x)u(qx)[u(q^2x) - u(x)]. \tag{47}$$

Taking $A_n = -(L^n)_0$ with L given as in Example 4 we get a hierarchy of evolution equations (Burgers hierarchy on time scales) from

$$\frac{dL}{dt_n} = -[(L^n)_0, v\delta + u] \tag{48}$$

for all $n = 1, 2, 3, \ldots$. Since $(L^n)_0$ is a scalar function, letting $(L^n)_0 = \rho_n$ we obtain

$$\frac{dv}{dt_n} = \mu v(\rho_n)^{\Delta}, \tag{49}$$

$$\frac{du}{dt_n} = v(\rho_n)^{\Delta}, \tag{50}$$

where the first three ρ_n are given by

$$\rho_1 = u, \tag{51}$$

$$\rho_2 = vu^{\Delta} + u^2, \tag{52}$$

$$\rho_3 = vE(v)u^{\Delta\Delta} + [vv^{\Delta} + vE(u) + uv]u^{\Delta} + (vu^{\Delta} + u^2)u. \tag{53}$$

The above hierarchy reduces to a single evolution equation with $v = \mu u + \lambda$,

$$\frac{du}{dt_n} = (\mu u + \lambda)(\tilde{\rho}_n)^{\Delta}, \quad n = 1,2, \dots , \tag{54}$$

where $\tilde{\rho}_n$ is equal to ρ_n with $v = \mu u + \lambda$. When $\mathbb{T}$ is a regular-discrete time scale, the first three $\tilde{\rho}_n$ are given for $\lambda = 0$ by

$$\tilde{\rho}_1 = u, \tag{55}$$

$$\tilde{\rho}_2 = uE(u), \tag{56}$$

$$\tilde{\rho}_3 = uE(u)E^2(u). \tag{57}$$

It is possible to construct the recursion operator $\mathcal{R}$ by using the Lax representation.[14–16] The hierarchy satisfies a recursion relation like

$$\frac{dL}{dt_{n+1}} = L\frac{dL}{dt_n} + [R_n, L], \quad n = 1,2, \dots , \tag{58}$$

where R_n is the remainder operator which has the same degree as the Lax operator L. We shall construct this operator for the Burgers equation with $\lambda = 0$ on regular-discrete time scales. Choosing $R_n = \alpha_n \delta$ we get [by choosing $v(x) = \mu(x)u(x)$]

$$\mathcal{R} = uE + [u(E(u) - u)](E - 1)^{-1}\frac{E}{E(u)}. \tag{59}$$

One can generate the hierarchy (54) by application of the recursion operator $\mathcal{R}$ to the lowest order symmetry $u_1 = u(E(u) - u)$,

$$\frac{du}{dt_n} = \mathcal{R}^{n-1}u_1, \quad n = 1,2, \dots . \tag{60}$$

IV. ALGEBRA OF PSEUDO-DELTA-DIFFERENTIAL OPERATORS ON REGULAR TIME SCALES

Let us define the notion of regular time scales.

Definition 9: We say that a time scale $\mathbb{T}$ is regular if the following two conditions are satisfied simultaneously:

$$\text{(i) } \sigma(\rho(x)) = x \quad \textit{for all } x \in \mathbb{T} \tag{61}$$

and

$$\text{(ii) } \rho(\sigma(x)) = x \quad \textit{for all } x \in \mathbb{T}, \tag{62}$$

where σ and ρ denote the forward and backward jump operators, respectively.

From (61) it follows that the operator $\sigma:\mathbb{T}\to\mathbb{T}$ is "onto" while (62) implies that σ is "one-to-one." Therefore σ is invertible and $\sigma^{-1}=\rho$. Similarly, the operator $\rho:\mathbb{T}\to\mathbb{T}$ is invertible and $\rho^{-1}=\sigma$ if $\mathbb{T}$ is regular.

Let us set $x_*=\min\mathbb{T}$ if there exists a finite $\min\mathbb{T}$, and set $x_*=-\infty$ otherwise. Also set $x^*=\max\mathbb{T}$ if there exists a finite $\max\mathbb{T}$, and $x^*=\infty$ otherwise. It is not difficult to see that the following statement holds.

Proposition 10: A time scale $\mathbb{T}$ is regular if and only if the following two conditions hold:

(i) *The point $x_*=\mathbb{T}$ is right-dense and the point $x^*=\max\mathbb{T}$ is left-dense.*
(ii) *Each point of $\mathbb{T}\backslash\{x_*,x^*\}$ is either two-sided dense or two-sided scattered.*

In particular, $\mathbb{R}$, $h\mathbb{Z}$, and $\mathbb{K}_q$ are regular time scales, as are $[0,1]$, $[-1,0]\cup\{1/k:k\in\mathbb{N}\}\cup\{k/(k+1):k\in\mathbb{N}\}\cup[1,2]$, and $(-\infty,0]\cup\{1/k:k\in\mathbb{N}\}\cup\{2k:k\in\mathbb{N}\}$, where $[-1,0]$, $[0,1]$, $[1,2]$, $(-\infty,0]$ are real line intervals.

If $f:\mathbb{T}\to\mathbb{R}$ is a function we define the functions $f^\sigma:\mathbb{T}\to\mathbb{R}$ and $f^\rho:\mathbb{T}\to\mathbb{R}$ by

$$f^\sigma(x) = f(\sigma(x)) \quad \text{and } f^\rho(x) = f(\rho(x)) \quad \text{for all } x\in\mathbb{T}. \tag{63}$$

Defining the shift operator E by the formula $Ef=f^\sigma$ we have

$$(Ef)(x) = f^\sigma(x) = f(\sigma(x)) \quad \text{for all } x\in\mathbb{T}. \tag{64}$$

The inverse E^{-1} exists only in case of regular time scales and is defined by

$$(E^{-1}f)(x) = f(\sigma^{-1}(x)) = f(\rho(x)) \quad \text{for all } x\in\mathbb{T}. \tag{65}$$

In the operator relations, for convenience, we will denote the shift operator by $\mathcal{E}$ rather than by E. For example, $\mathcal{E}f$ will denote the composition (product) of the shift operator $\mathcal{E}$ and the operator of multiplication by the function f. Obviously, for any integer $m\in\mathbb{Z}$, we have

$$\mathcal{E}^m f = (E^m f)\mathcal{E}^m. \tag{66}$$

Remember that δ denotes the delta-differentiation operator acting in the operator relations by $\delta f=f^\Delta+E(f)\delta$. The following proposition is an immediate consequence of the formulas (8) and (16).

Proposition 11: The operator formulas

$$\mathcal{E} = I + \mu\delta \tag{67}$$

and

$$\delta f = f^\Delta + E(f)\delta \tag{68}$$

hold, where the function $\mu:\mathbb{T}\to\mathbb{R}$ is defined by $\mu(x)=\sigma(x)-x$ for all $x\in\mathbb{T}$, and I denotes the identity operator.

In this section we will assume that all our considered functions from $\mathbb{T}$ to $\mathbb{R}$ are Δ-smooth and tend to zero sufficiently rapidly together with their Δ-derivatives as x goes to x_* or x^*, where $x_*=\min\mathbb{T}$ if there exists a finite $\min\mathbb{T}$ and $x_*=-\infty$ otherwise, $x^*=\max\mathbb{T}$ if there exists a finite $\max\mathbb{T}$ and $x^*=\infty$ otherwise. The inverse operator δ^{-1} exists on such functions. If $g:\mathbb{T}\to\mathbb{T}$ is such a function, then

$$[\Delta^{-1}(g)](x) = \int_{x_*}^{x} g(y)\Delta y. \tag{69}$$

Proposition 12: Let $f:\mathbb{T}\to\mathbb{R}$ be a Δ-smooth function such that f and all its Δ-derivatives vanish rapidly at x_* and x^*. Then the operator $\delta^{-1}f$ being the composition (product) of δ^{-1} and f has the form of the formal series in powers of δ^{-1},

$$\delta^{-1}f = \alpha_0\delta^{-1} + \alpha_1\delta^{-2} + \cdots, \tag{70}$$

where $\alpha_0 = E^{-1}f$, and $\alpha_k = (-1)^k(E^{-1}f)^{\nabla^k}$ for $k=1,2,\ldots$.

Proof: Multiplying (68) on the left and right by δ^{-1} we obtain

$$\delta^{-1}E(f) = f\delta^{-1} - \delta^{-1}f^{\Delta}\delta^{-1}. \tag{71}$$

Replacing here f by $E^{-1}f$ we get

$$\delta^{-1}f = (E^{-1}f)\delta^{-1} - \delta^{-1}(E^{-1}f)^{\Delta}\delta^{-1}. \tag{72}$$

Further, applying this rule to the function $(E^{-1}f)^{\Delta}$ and taking into account that by Proposition 4(i)

$$E^{-1}(E^{-1}f)^{\Delta} = (E^{-1}f)^{\nabla}, \tag{73}$$

we find

$$\delta^{-1}(E^{-1}f)^{\Delta} = (E^{-1}f)^{\nabla}\delta^{-1} - \delta^{-1}((E^{-1}f)^{\nabla})^{\Delta}\delta^{-2}. \tag{74}$$

Substituting this into the second term on the right-hand side of (72) we obtain

$$\delta^{-1}f = (E^{-1}f)\delta^{-1} - (E^{-1}f)^{\nabla}\delta^{-2} + \delta^{-1}((E^{-1}f)^{\Delta})^{\nabla}\delta^{-2}. \tag{75}$$

Continuing this procedure repeatedly we arrive at the statement of the proposition.

Definition 13: By Λ we denote the algebra of pseudo-delta-differential operators. Any operator $K\in\Lambda$ of order k has the form

$$K = \sum_{\ell=-\infty}^{k} a_\ell\delta^{\ell}, \tag{76}$$

where a_ℓ's are Δ-smooth functions of $x\in\mathbb{T}$. For K given by (76) we will use the following notations:

$$K_{\geqslant 0} = \sum_{\ell=0}^{k} a_\ell\delta^{\ell} \quad \text{and } K_{<0} = \sum_{-\infty}^{-1} a_\ell\delta^{\ell}. \tag{77}$$

As an example we let

$$L = a_N\delta^N + a_{N-1}\delta^{N-1} + \cdots + a_1\delta + a_0, \tag{78}$$

where $a_i (i=0,1,\ldots,N)$ are some Δ-smooth functions on $\mathbb{T}$. Then we have the following.

Proposition 16: Let L be given in (78). For each fixed N the Lax equation

$$\frac{\mathrm{d}L}{\mathrm{d}t_n} = [A_n, L], \quad A_n = (L^{n/N})_{\geqslant 0}, \tag{79}$$

for $n=1,2,\ldots$ not divisible by N, produces a (consistent) hierarchy of evolution equations (a KdV hierarchy on time scales).

Proof: Since $(L^{n/N})_{\geqslant 0} = L^{n/N} - (L^{n/N})_{<0}$, we get

$$\frac{dL}{dt_n} = [(L^{n/N})_{\geqslant 0}, L] = -[L^{n/N})_{<0}, L]. \tag{80}$$

Evidently the commutator $[(L^{n/N})_{\geqslant 0}, L]$ involves only non-negative powers of δ, while the commutator $[(L^{n/N})_{<0}, L]$ has the form $\Sigma_{j=-\infty}^{N-1} b_j \delta^j$. Therefore, we get by (80) that, for all n not divisible by N, (79) produces nontrivial consistent $N+1$-number of evolutionary coupled Δ-differential equations for a_i, $i=0,1,\ldots,N$. Note that a_N turns out to be a fixed (i.e., time independent) function of x.

Example 5: A KdV hierarchy on time scales. Let

$$L = \delta^2 + v\delta + u, \tag{81}$$

where u and v are Δ-smooth functions. It is straightforward to find that

$$L^{1/2} = \delta + \alpha_0 + \alpha_1 \delta^{-1} + \alpha_2 \delta^{-2} + \cdots, \tag{82}$$

where

$$E(\alpha_0) + \alpha_0 = v, \tag{83}$$

$$E(\alpha_1) + \alpha_1 + (\alpha_0)^{\Delta} + (\alpha_0)^2 = u, \tag{84}$$

$$E(\alpha_2) + \alpha_2 + \alpha_1 E^{-1}(\alpha_0) + (\alpha_1)^{\Delta} = 0. \tag{85}$$

Choosing $n=1,3,\ldots$ we get the members of the KdV hierarchy.

(1) Let $n=1$. Then Lax equation (79) becomes

$$\frac{dv}{dt}\delta + \frac{du}{dt} = [(L^{1/2})_{\geqslant 0}, L] \tag{86}$$

and gives coupled equations for u and v,

$$\frac{du}{dt} = u^{\Delta} - v(\alpha_0)^{\Delta} - (\alpha_0)^{\Delta\Delta}, \tag{87}$$

$$\frac{dv}{dt} = v^{\Delta} + E(u) - u - v[E(\alpha_0) - \alpha_0] - E(\alpha_0^{\Delta}) - E(\alpha_0)^{\Delta} = \mu(u^{\Delta} - v(\alpha_0)^{\Delta} - (\alpha_0)^{\Delta\Delta}). \tag{88}$$

Comparing the above equations we get

$$\frac{dv}{dt} - \mu\frac{du}{dt} = 0, \tag{89}$$

and therefore

$$v = \mu u + \lambda, \tag{90}$$

where λ is an arbitrary real function depending only on $x \in \mathbb{T}$. Thus, two equations (87) and (88) reduce to the following single equation:

$$\frac{du}{dt} = u^{\Delta} - (\mu u + \lambda)(\alpha_0)^{\Delta} - (\alpha_0)^{\Delta\Delta}, \tag{91}$$

where α_0 is expressed, according to (83), from

$$E(\alpha_0) + \alpha_0 = \mu u + \lambda. \tag{92}$$

If we take $\lambda = 0$, then (91) and (92) become

$$\frac{du}{dt} = u^{\Delta} - \mu u(\alpha_0)^{\Delta} - (\alpha_0)^{\Delta\Delta}, \tag{93}$$

$$E(\alpha_0) + \alpha_0 = \mu u. \tag{94}$$

We shall now give α_0, for illustration, for particular cases of $\mathbb{T}$.

(i) In the case $\mathbb{T} = \mathbb{R}$ we have $\mu = 0$ and (94) gives $\alpha_0 = 0$ and (93) becomes

$$\frac{du}{dt} = \frac{du}{dx}, \tag{95}$$

which is a linear equation explicitly solvable,

$$u(x,t) = \varphi(x+t), \tag{96}$$

where φ is an arbitrary differentiable function.

(ii) In the case $\mathbb{T} = \mathbb{Z}$ we have $\mu = 1$ and (94) is satisfied by

$$\alpha_0(n) = -\sum_{k=-\infty}^{n-1} (-1)^{n+k} u(k), \quad n \in \mathbb{Z} \tag{97}$$

and therefore the Eq. (93) becomes

$$\frac{du(n)}{dt} = -u^2(n) + 2u(n) + 2(-1)^n [2 + u(n)] \sum_{k=-\infty}^{n-1} (-1)^k u(k), \tag{98}$$

for $n \in \mathbb{Z}$.

(iii) In the case $\mathbb{T} = \mathbb{K}_q$ we have $\mu(x) = (q-1)x$ and (94) is satisfied by $\alpha_0(0) = 0$ and

$$\alpha_0(x) = -(q-1) \sum_{y \in (0, q^{-1}x]} (-1)^{\log_q(xy)} y u(y) \tag{99}$$

for $x \in \mathbb{K}_q$ and $x \neq 0$. Substituting (99) into (93) we can get an evolution equation for u.

(iv) Let $\mathbb{T} = (-\infty, 0) \cup \mathbb{K}_q = (-\infty, 0] \cup q^{\mathbb{Z}}$. In this case $\mu(x) = 0$ if $x \in (-\infty, 0]$ and $\mu(x) = (q-1)x$ if $x \in q^{\mathbb{Z}}$. The equation (94) is satisfied by the function α_0 given by

$$\alpha_0(x) = \begin{cases} 0 & x \in (-\infty, 0], \\ -(q-1)\Sigma_{y \in (0, q^{-1}x]} (-1)^{\log_q(xy)} y u(y) & x \in q^{\mathbb{Z}}. \end{cases} \tag{100}$$

Therefore (93) will yield an evolution equation coinciding on $(-\infty, 0]$ and $q^{\mathbb{Z}}$ with the evolution equations described in the examples (i) and (iii), respectively. Now an essential complementary point is that the solution u must satisfy at $x = 0$ the smoothness conditions

$$u(0^-) = u(0^+), \quad u'(0^-) = u^{\Delta}(0^+). \tag{101}$$

(2) Letting $n = 3$, first we get

$$L^{3/2} = \delta^3 + p\delta^2 + q\delta + r + (\text{terms with negative powers of } \delta), \tag{102}$$

where

$$p = \alpha_0 + E(v), \tag{103}$$

$$q = v^{\Delta} + E(u) + \alpha_0 v + \alpha_1, \tag{104}$$

$$r = u^{\Delta} + \alpha_0 u + \alpha_1 E^{-1}(v) + \alpha_2, \tag{105}$$

and the Lax equation

$$\frac{\mathrm{d}v}{\mathrm{d}t}\delta + \frac{\mathrm{d}u}{\mathrm{d}t} = [(L^{3/2})_{\geqslant 0}, L], \tag{106}$$

gives the coupled equations for u and v,

$$\frac{\mathrm{d}u}{\mathrm{d}t} = u^{\Delta\Delta\Delta} + pu^{\Delta\Delta} + qu^{\Delta} - r^{\Delta\Delta} - vr^{\Delta}, \tag{107}$$

$$\frac{\mathrm{d}v}{\mathrm{d}t} = v^{\Delta\Delta\Delta} + E(u^{\Delta\Delta}) + (E(u^{\Delta}))^{\Delta} + E(u)^{\Delta\Delta} + p[v^{\Delta\Delta} + E(u^{\Delta}) + E(u)^{\Delta}] + q(v^{\Delta} + E(u) - u) + rv - q^{\Delta\Delta}$$
$$- E(r^{\Delta}) - E(r)^{\Delta} - vq^{\Delta} - vE(r). \tag{108}$$

As in the first member of the hierarchy ($n=1$ case), the above Δ-KdV equations reduce to a single equation for the function u. Below in Corollary 23 we found that $v=\mu(x)u+\lambda(x)$. Letting $\lambda=$ constant we get

$$\frac{\mathrm{d}u}{\mathrm{d}t} = u^{\Delta\Delta\Delta} + pu^{\Delta\Delta} + qu^{\Delta} - r^{\Delta\Delta} - vr^{\Delta}. \tag{109}$$

It is possible to write the above equation more explicitly in terms of u for $\mathbb{T}=\mathbb{R}$, $\mathbb{T}=\mathbb{Z}$, and for $\mathbb{T}=\mathbb{K}_q$ but they are quite lengthy. For the discrete case we give a KdV hierarchy in Example 8, next section.

V. SHIFT LAX OPERATORS ON REGULAR-DISCRETE TIME SCALES

Let $\mathbb{T}$ be a time scale. Let us set $x_*=\min\mathbb{T}$ if there exists a finite $\min\mathbb{T}$ and $x_*=-\infty$ otherwise. Also set $x^*=\max\mathbb{T}$ if there exists a finite $\max\mathbb{T}$ and $x^*=\infty$ otherwise. We will briefly write $x_*=\min\mathbb{T}$ and $x^*=\max\mathbb{T}$.

Definition 17: We say that a time scale $\mathbb{T}$ is regular-discrete if the following two conditions are satisfied:

(i) *The point x_* is right-dense and the point x^* is left-dense.*
(ii) *Each point of $\mathbb{T}\backslash\{x_*,x^*\}$ is two-sided scattered (isolated).*

The shift operator E is defined on functions $f:\mathbb{T}\to\mathbb{R}$ by the formula

$$(Ef)(x) = f(\sigma(x)) \quad \text{for } x \in \mathbb{T}, \tag{110}$$

where $\sigma:\mathbb{T}\to\mathbb{T}$ is the forward jump operator.

In this section we deal only with regular-discrete time scales $\mathbb{T}$. For such time scales $\mathbb{T}$ we have

$$\mu(x) = \sigma(x) - x \neq 0 \quad \text{for all } x \in \mathbb{T}\setminus\{x_*,x^*\} \tag{111}$$

and, therefore, on functions given on $\mathbb{T}\backslash\{x_*,x^*\}$ we have the operator relationship

$$\delta = \frac{1}{\mu}(\mathcal{E} - 1). \tag{112}$$

All our functions will be assumed to be defined on $\mathbb{T}\backslash\{x_*,x^*\}$ and tends to zero sufficiently rapidly as x goes to x_* or x^*.

This shift operator $\mathcal{E}$, should be quite useful in the application of the Gel'fand-Dikii formalism. The reason is that for any integer m we have the simple product rule

$$\mathcal{E}^m u = (E^m u)\mathcal{E}^m. \tag{113}$$

Hence, for regular-discrete time scales, we can define an algebra of $\mathcal{E}$ operators.

Definition 18: An algebra, Λ_ϵ, of $\mathcal{E}$ operators satisfying the operator equation (113) is defined as follows: Any operator K in Λ_ϵ with degree k is of the form

$$K = \sum_{-\infty}^{k} a_\ell \mathcal{E}^\ell, \tag{114}$$

where a_ℓ are functions of $x \in \mathbb{T}$ that depend also on $t \in \mathbb{R}$.

Hence we can form Lax operators in Λ_ϵ, and produce integrable equations on regular-discrete time scales. Following[3] we obtain two classes of Lax representations.

Proposition 19: The Lax equation

$$\frac{\mathrm{d}L}{\mathrm{d}t_\ell} = [(L^\ell)_{\geqslant k}, L], \quad k = 0, 1 \tag{115}$$

produces consistent hierarchy of equations for $\ell = 1, 2, \ldots$ with the following suitable Lax operators:

$$L = \mathcal{E}^{\alpha+n} + u_{\alpha+n-1}\mathcal{E}^{\alpha+n-1} + \cdots + u_\alpha \mathcal{E}^\alpha, \tag{116}$$

$$L = v_{\alpha+n}\mathcal{E}^{\alpha+n} + v_{\alpha+n-1}\mathcal{E}^{\alpha+n-1} + \cdots + v_{\alpha+1}\mathcal{E}^{\alpha+1} + E^\alpha, \tag{117}$$

for $k=0$ and $k=1$, respectively. Here u_i and v_i are functions defined on $\mathbb{T}$ and the integer α is restricted to satisfy the inequality $-n < \alpha \leqslant -1$.

Remark: Lax operators above and the following examples are given on any regular-discrete time scale $\mathbb{T}$ (we can take in particular $\mathbb{T}=\mathbb{Z}$ or $\mathbb{K}_q$). This means that for any function u on such a time scale $E(u)=u(\sigma(x))$ where σ is the jump operator defined in the second section. Hence our examples and results should be considered as more general than those considered in Ref. 3. In the case of Ref. 3 time scale is just the integers ($\mathbb{T}=\mathbb{Z}$) where $E(u(n))=u(n+1)$.

Example 6: Two field equations. Let $k=0$, $\alpha=-1$ and

$$L = u_{-1}\mathcal{E}^{-1} + u_0 + \mathcal{E} \equiv v\mathcal{E}^{-1} + u + \mathcal{E}. \tag{118}$$

Then we find

$$\ell = 1 \quad \frac{\mathrm{d}v}{\mathrm{d}t_1} = v(u - E^{-1}(u)), \tag{119}$$

$$\frac{\mathrm{d}u}{\mathrm{d}t_1} = E(v) - v, \tag{120}$$

$$\ell = 2 \quad \frac{\mathrm{d}v}{\mathrm{d}t_2} = u^2 v + E(v)v - vE^{-1}(v) - vE^{-1}(u^2), \tag{121}$$

$$\frac{\mathrm{d}u}{\mathrm{d}t_2} = uE(v) + E(u)E(v) - vE^{-1}(u) - uv, \tag{122}$$

$$\ell = 3, \quad \frac{dv}{dt_3} = uv^2 + u^3 v - vE^{-1}(v)E^{-2}(u) - 2vE^{-1}(u)E^{-1}(v) - vE^{-1}(u^3) + 2uvE(v) - v^2E^{-1}(u) + vE(u)E(v), \tag{123}$$

$$\frac{du}{dt_3} = E(v)[u^2 + uE(u) + E(u^2) + E(v) + (E^2(v))] - v[E^{-1}(v) + E^{-1}(u^2) + uE^{-1}(u) + u^2 + v]. \tag{124}$$

This is a Toda hierarchy on discrete time scales. The recursion relation between the $n+1$th and nth elements of the hierarchy is given by

$$v_{n+1} = uv_n + vu_n + vE^{-1}(u_n) + v(E^{-1}(u) - u)(1-E)^{-1}\frac{v_n}{v}, \tag{125}$$

$$u_{n+1} = E(v_n) + uu_n + v(1-E)^{-1}\frac{v_n}{v} - E(v)(1-E)^{-1}E\frac{v_n}{v}. \tag{126}$$

From this recursion relation the recursion operator of the hierarchy follows.

Example 7: Four-field system on time scale. We give two examples which are studied in Ref. 3 for the case $\mathbb{T}=\mathbb{Z}$.

(1) Let $k=0$ and $\alpha=-2$ and

$$L = \mathcal{E}^2 + w\mathcal{E} + v + u\mathcal{E}^{-1} + p\mathcal{E}^{-2}. \tag{127}$$

Then we get the four-field equations

$$\ell = 1 \quad \frac{dp}{dt_1} = vp - pE^{-2}(v), \tag{128}$$

$$\frac{du}{dt_1} = vu + wE(p) - pE^{-2}(w) - uE^{-1}(v), \tag{129}$$

$$\frac{dv}{dt_1} = wE(u) + E^2(p) - uE^{-1}(w) - p, \tag{130}$$

$$\frac{dw}{dt_1} = E^2(u) - u. \tag{131}$$

(2) Let $k=1$ and $\alpha=-2$ and

$$L = \bar{q}\mathcal{E}^2 + \bar{w}\mathcal{E} + \bar{v} + \bar{u}\mathcal{E}^{-1} + \mathcal{E}^{-2}. \tag{132}$$

Then we get another four-field equations,

$$\ell = 1 \quad \frac{d\bar{u}}{dt_1} = \bar{w} - E^{-2}(\bar{w}), \tag{133}$$

$$\frac{d\bar{v}}{dt_1} = \bar{w}E(\bar{u}) + \bar{q} - E^{-2}(\bar{q}) - \bar{u}E^{-1}(\bar{w}), \tag{134}$$

$$\frac{\mathrm{d}\bar{w}}{\mathrm{d}t_1} = \bar{w}E(\bar{v}) + \bar{q}E^2(\bar{u}) - \bar{u}E^{-1}(\bar{q}) - \bar{v}\bar{w}, \tag{135}$$

$$\frac{\mathrm{d}\bar{q}}{\mathrm{d}t_1} = \bar{q}E^2(\bar{v}) - \bar{v}\bar{q}. \tag{136}$$

So far we considered the hierarchies coming from Proposition 19 with integer powers of the Lax operators. Now we consider the rational powers of the Lax operator.

Proposition 22: Let

$$L = w\mathcal{E}^N + u_{N-1}\mathcal{E}^{N-1} + \cdots + u_0, \tag{137}$$

where $w(x)$ *is a function of* x *which is not a dynamical variable* $\mathrm{d}w/\mathrm{d}t=0$, u_i, $i=0,1,\ldots,N-1$ *are functions of* t *and* $x \in \mathbb{T}$. *Then*

$$\frac{\mathrm{d}L}{\mathrm{d}t_n} = [(L^{n/N})_{\geqslant 0}, L], \quad n = 1,2,\ldots \tag{138}$$

produces hierarchies of integrable systems. Here n *is a positive integer not divisible by* N. *Furthermore the function* u_0 *is also not dynamical, i.e.,* $u_0=u_0(x)$, *not depending on* t.

Corollary 23: When $N=2$ *and* $w=(1/\mu)E(1/\mu)$ *then the* Δ*-KdV Lax operator (81) reduces to the above form with*

$$u_0 = -\frac{v}{\mu} + \frac{1}{\mu^2} + u, \tag{139}$$

$$u_1 = -\frac{1}{\mu}\left[E\left(\frac{1}{\mu}\right) + \frac{1}{\mu}\right] + \frac{v}{\mu}. \tag{140}$$

Hence in part (2) of Example 5 we have a single equation with $v=-\mu u_0+(1/\mu)+\mu u$.

In the following example we study the $N=2$ case in more detail.

Example 8: KdV on discrete time scales. Let

$$L = wE(w)\mathcal{E}^2 + u\mathcal{E} + v. \tag{141}$$

Then

$$L^{1/2} = w\mathcal{E} + \alpha_0 + \alpha_1\mathcal{E}^{-1} + \alpha_2\mathcal{E}^{-2} + \cdots, \tag{142}$$

where first three α_i are given as

$$w(E(\alpha_0) + \alpha_0) = u, \tag{143}$$

$$wE(\alpha_1) + E^{-1}(w)\alpha_1 = v - (\alpha_0)^2, \tag{144}$$

$$wE(\alpha_2) + E^{-2}(w)\alpha_2 = -\frac{\alpha_1 E^{-1}(u)}{E^{-1}(w)}. \tag{145}$$

Then we calculate $L^{3/2}$ by

$$L^{3/2} = wE(w)E^2(w)\mathcal{E}^3 + p_2\mathcal{E}^2 + p_1\mathcal{E} + p_0 + \text{negative powers of } \mathcal{E}, \tag{146}$$

where

$$p_2 = E(w)[wE^2(\alpha_0) + u], \tag{147}$$

$$p_1 = wE(w)E^2(\alpha_1) + uE(\alpha_0) + wv, \tag{148}$$

$$p_0 = wE(w)E^2(\alpha_2) + uE(\alpha_1) + v\alpha_0, \tag{149}$$

$$= wE^{-1}(w)[E^{-1}(w) + E(w)E]^{-1}\left(E(\alpha_1)\frac{u}{w}\right) + v(1+E)^{-1}\frac{u}{w}. \tag{150}$$

Then (138) with $N=2$ produces a hierarchy of evolution equations. It turns out that v becomes a constant in the whole hierarchy. We give the first two members of the hierarchy (for $n=1$ and $n=3$),

$$u_{t_1} = u(1-E)(1+E)^{-1}\frac{u}{w}, \tag{151}$$

$$u_{t_3} = u(1-E)p_0, \tag{152}$$

where p_0 is given above. The next members of the hierarchy can be found by taking $n=5$ in (138) or by applying the recursion operator $\mathcal{R}$ to u_{t_3}. For $\mathbb{T}=\mathbb{K}_q$ and $w=1$ the above hierarchy and its Hamilton formulation were given by Frenkel.[4] The recursion operator of this hierarchy with $w=1$ can be found by using (58) with $R_n=\alpha_n\mathcal{E}+\beta_n$. We find that

$$(E^2-1)\alpha_n = E^2(u_n), \tag{153}$$

$$(E^2-1)\beta_n = uE(u_n) + E(u)\alpha_n - uE(\alpha_n) \tag{154}$$

and the equation which determines the recursion operator is

$$u_{n+1} = vu_n - u(E-1)\beta_n, \quad n = 0,1,2,\ldots\ . \tag{155}$$

We find that

$$\mathcal{R} = v - u(E+1)^{-1}[-u + E(u)E](E^2-1)^{-1}E. \tag{156}$$

When the Lax operator is of degree one and has an infinite power series in operator $\mathcal{E}^{-1}$ the corresponding system is called the KP hierarchy.

Proposition 24: Let

$$L = \mathcal{E} + u_0 + u_1\mathcal{E}^{-1} + u_2\mathcal{E}^{-2} + \cdots\ . \tag{157}$$

Then

$$\frac{dL}{dt_n} = [(L^n)_{\geqslant 0}, L], \quad n = 1,2,\ldots\ , \tag{158}$$

produces the following hierarchy:

$$n=1 \quad \frac{du_0}{dt_1} = (E-1)u_1, \tag{159}$$

$$\frac{du_1}{dt_1} = (E-1)u_2 + u_1[u_0 - E^{-1}(u_0)], \tag{160}$$

$$\frac{du_k}{dt_1} = (E-1)u_{k+1} + u_k[u_0 - E^{-k}(u_0)], \quad k = 0,1,\ldots\ . \tag{161}$$

$$n=2 \quad \frac{du_0}{dt_2}=(E^2-1)u_2-u_1E^{-1}(E+1)u_0+E(u_1)(E(u_0)+u_0), \tag{162}$$

$$\frac{du_1}{dt_2}=(E^2-1)u_3+\alpha_1E(u_2)-u_2E^{-2}(\alpha_1)+\alpha_0u_1-u_1E^{-1}(\alpha_0), \tag{163}$$

$$\frac{du_k}{dt_2}=(E^2-1)u_{k+2}+\alpha_1E(u_{k+1})-u_{k+1}E^{-k-1}(\alpha_1)+\alpha_0u_k-u_kE^{-k}(\alpha_0), \quad k=0,1,\dots, \tag{164}$$

where $\alpha_0=(E+1)u_1+(u_0)^2$ and $\alpha_1=(E+1)u_0$. The case $\mathbb{T}=\mathbb{Z}$ of this hierarchy is discussed in Ref. 3 (see also the references therein) and the case $\mathbb{T}=\mathbb{K}_q$ is discussed in Refs. 4 and 5.

VI. TRACE FUNCTIONAL AND CONSERVATION LAWS

Let $\mathbb{T}$ be a regular time scale and Λ be the algebra of pseudo-delta-differential operators. Any operator $F\in\Lambda$ of order k has the form

$$F=a_k\delta^k+a_{k-1}\delta^{k-1}+\cdots+a_1\delta+a_0+a_{-1}\delta^{-1}+a_{-2}\delta^{-2}+\cdots, \tag{165}$$

where a_ℓ's are Δ-smooth functions of $x\in\mathbb{T}$ (they are also functions of $t\in\mathbb{R}$). The coefficients a_0 and a_{-1} we call, respectively, the *free term* (zero order term) and the *residue* of F associated with its "δ-expansion" (165) and write

$$\mathrm{Free}_\delta F=a_0(x) \quad \text{and } \mathrm{Res}_\delta F=a_{-1}(x). \tag{166}$$

In case of regular-discrete time scales $\mathbb{T}$ we have

$$\delta=\frac{1}{\mu}(\mathcal{E}-I)=\frac{1}{\mu}\mathcal{E}-\frac{1}{\mu} \tag{167}$$

and therefore the same operator F can be expanded in series with respect to the powers of $\mathcal{E}$ of the form

$$F=b_k\mathcal{E}^k+b_{k-1}\mathcal{E}^{k-1}+\cdots+b_1\mathcal{E}+b_0+b_{-1}\mathcal{E}^{-1}+b_{-2}\mathcal{E}^{-2}+\cdots. \tag{168}$$

We write

$$\mathrm{Free}_\mathcal{E} F=b_0(x) \quad \text{and } \mathrm{Res}_\mathcal{E} F=b_{-1}(x). \tag{169}$$

Substituting (167) and

$$\delta^{-1}=(\mathcal{E}-I)^{-1}\mu=(\mathcal{E}^{-1}+\mathcal{E}^{-2}+\cdots)\mu=E^{-1}(\mu)\mathcal{E}^{-1}+E^{-2}(\mu)\mathcal{E}^{-2}+\cdots, \tag{170}$$

into (165) and taking into account that

$$E^{-1}(\mu)=\mu(\rho(x))=\sigma(\rho(x))-\rho(x)=x-\rho(x)=\nu(x), \tag{171}$$

we find that

$$\mathrm{Res}_\mathcal{E} F=\nu\,\mathrm{Res}_\delta F. \tag{172}$$

Definition 25: The trace of an operator $F\in\Lambda$ is defined by

$$\mathrm{Tr}(F)=\int_\mathbb{T}\mathrm{Res}_\delta\{F(I+\mu\delta)^{-1}\}\nabla x, \tag{173}$$

where the nabla integral is defined according to Sec. II.

Proposition 26: Let F be given as in (165). In case of regular-discrete time scales we have

$$\mathrm{Res}_\delta\{F(I+\mu\delta)^{-1}\}=\frac{1}{\nu(x)}\mathrm{Free}_{\mathcal{E}}F \tag{174}$$

for $x\in\mathbb{T}\backslash\{x_*,x^*\}$, *where* $x_*=\min\mathbb{T}$ *and* $x^*=\max\mathbb{T}$. *Therefore in this case*

$$\mathrm{Tr}(F)=\int_{\mathbb{T}}(\mathrm{Free}_{\mathcal{E}}F)\frac{\nabla x}{\nu(x)}=\sum_{x\in\mathbb{T}}b_0(x). \tag{175}$$

Proof: Since $I+\mu\delta=\mathcal{E}$ we have, by using (172) and (168),

$$\begin{aligned}\nu\,\mathrm{Res}_\delta\{F(I+\mu\delta)^{-1}\}&=\mathrm{Res}_{\mathcal{E}}\{F(I+\mu\delta)^{-1}\}=\mathrm{Res}_{\mathcal{E}}(F\mathcal{E}^{-1})=\mathrm{Res}_{\mathcal{E}}(b_k\mathcal{E}^{k-1}+\cdots+b_1+b_0\mathcal{E}^{-1}+\cdots)\\&=b_0=\mathrm{Free}_{\mathcal{E}}(F).\end{aligned} \tag{176}$$

Proposition 27: For all $F_1,F_2\in\Lambda$,

$$\mathrm{Tr}([F_1,F_2])=\mathrm{Tr}(F_1F_2-F_2F_1)=0, \tag{177}$$

in other words the pairing $(F_1,F_2)=\mathrm{Tr}(F_1F_2)$ *is symmetric.*

We prove (177) only for particular cases of time scales $\mathbb{T}$. They indicate a way to the proof in the general case of regular time scales.

(i) If $\mathbb{T}=\mathbb{R}$, then $\delta=\partial=(d/\mathrm{d}x)\cdot$ and $\mu(x)=0$,

$$F=a_k\partial^k+\cdots+a_1\partial+a_0+a_{-1}\partial^{-1}+\cdots \tag{178}$$

and

$$\mathrm{Tr}(F)=\int_{\mathbb{R}}\mathrm{Res}(F)\mathrm{d}x=\int_{\mathbb{R}}a_{-1}(x)\mathrm{d}x. \tag{179}$$

It is well known that (for example, see Ref. 3) for such functional $\mathrm{Tr}(F)$ the statement (177) holds.

(ii) Let $\mathbb{T}$ be a regular-discrete time scale. Then by Proposition 26 we have

$$\mathrm{Tr}([F_1,F_2])=\int_{\mathbb{T}}\mathrm{Res}_\delta\{[F_1,F_2](I+\mu\delta)^{-1}\}\nabla x=\int_{\mathbb{T}}(\mathrm{Free}_{\mathcal{E}}[F_1,F_2])\frac{\nabla x}{\nu(x)}=0. \tag{180}$$

It is enough to check (180) for monomials $F_1=A\mathcal{E}^k$ and $F_2=B\mathcal{E}^\ell$. By the use of the property (113) of $\mathcal{E}$ we have

$$F_1F_2=A(E^kB)\mathcal{E}^{k+\ell}\quad\text{and}\quad F_2F_1=B(E^\ell A). \tag{181}$$

Therefore $\mathrm{Free}_{\mathcal{E}}[F_1,F_2]$ is either zero or

$$\mathrm{Free}_{\mathcal{E}}[F_1,F_2]=A(E^kB)-B(E^{-k}A)=(E^k-I)(E^{-k}A)B$$

$$=(I-E^{-1})(E^k+E^{k-1}+\cdots+E)(E^{-k}A)B=\nu(x)[\Phi(A,B)]^\nabla,$$

where $\Phi(A,B)=(E^k+E^{k-1}+\cdots+E)(E^{-k}A)B$. Hence

$$\int_{\mathbb{T}}\mathrm{Free}_{\mathcal{E}}[F_1,F_2]\frac{\nabla x}{\nu(x)}=\int_{\mathbb{T}}[\Phi(A,B)]^\nabla\nabla x=\Phi(A,B)\Big|_{x_*}^{x^*}=0 \tag{182}$$

so that (177) is proved for regular-discrete time scales.

(iii) Let $\mathbb{T}$ be a mixed time scale, say, of the form $\mathbb{T}=(-\infty,0)\cup\mathbb{K}_q$, where $(-\infty,0)$ denotes the real line interval. Then for any $F_1,F_2\in\Lambda$ we have, taking into account Proposition 26, that

$$\mathrm{Tr}([F_1,F_2])=\int_{\mathbb{T}}\mathrm{Res}_{\delta}\{[F_1,F_2](I+\mu\delta)^{-1}\}\nabla x=\int_{-\infty}^{0}\left(\mathrm{Res}_{\partial}([F_1,F_2])\mathrm{d}x+\int_{\mathbb{K}_q}(\mathrm{Free}_{\mathcal{E}}[F_1,F_2])\frac{\nabla x}{\nu(x)}.\right. \tag{183}$$

Take for instance $F_1=A\delta$ and $F_2=B\delta^{-1}$. Then

$$\mathrm{Res}_{\partial}[F_1,F_2]=\mathrm{Res}_{\partial}[A\partial,B\partial^{-1}]=AB'+A'B=(AB)',\mathrm{Free}_{\mathcal{E}}[F_1,F_2]=\mathrm{Free}_{\mathcal{E}}\left[\frac{A}{\mu}(\mathcal{E}-I),B(\mathcal{E}-I)^{-1}\mu\right]$$
$$=AE(B)-BE^{-1}(A). \tag{184}$$

Therefore

$$\int_{-\infty}^{0}(\mathrm{Res}_{\partial}[F_1,F_2])\mathrm{d}x=\int_{-\infty}^{0}(AB)'\,\mathrm{d}x=A(0^-)B(0^-), \tag{185}$$

$$\int_{\mathbb{K}_q}\mathrm{Free}_{\mathcal{E}}[F_1,F_2]\frac{\nabla x}{\nu(x)}=\int_{\mathbb{K}_q}[AE(B)-BE^{-1}(A)]\frac{\nabla x}{\nu(x)}$$
$$=\sum_{x\in\mathbb{K}_q}[A(x)B(qx)-A(q^{-1}x)B(x)]=-A(0^+)B(0^+). \tag{186}$$

Hence

$$\mathrm{Tr}([F_1,F_2])=A(0^-)B(0^-)-A(0^+)B(0^+)=0, \tag{187}$$

where A and B are Δ-smooth functions on $\mathbb{T}$ and hence they are continuous at $x=0$.

Proposition 28: Equation (79) implies that

$$\frac{d}{\mathrm{d}t_n}L^k=[A_n,L^k],\quad A_n=(L^{n/N})_{\geqslant 0}, \tag{188}$$

for all $k=\ell/N$, where ℓ is any positive integer.

Propositions 27 and 28 imply the next proposition.

Proposition 29: For all $\ell=0,1,\ldots$ the functionals

$$H_\ell=\mathrm{Tr}(L^{\ell/N}), \tag{189}$$

are common constants of motion for the hierarchy (79) and (115).

Note that in proof of Proposition 29 it is, in particular, used the fact that the flows (vector fields) defined by the different members of the hierarchy all commute with each other (see Refs. 2 and 17).

VII. CONCLUSION

We have developed the Gel'fand-Dikii approach to time scales. So far the integrable systems were studied on $\mathbb{R},\mathbb{Z}$ or on $\mathbb{K}_q$. Here we gave a unified and extended approach. In particular cases when $\mathbb{T}=\mathbb{R},\mathbb{Z},\mathbb{K}_q$ we find several examples of the integrable systems. We developed the algebra of Δ-pseudo differential and $\mathcal{E}$-shift operators. We established the GD formalism on these algebras and introduced several Lax representations on these algebras. All these Lax representations are straightforward generalizations of the Lax representations on pseudodifferential algebras of integrable systems on $\mathbb{R}$ and the Lax representations of the algebra of shift operators on $\mathbb{Z}$. The Burgers and KdV hierarchies on time scales that we found are the special cases of these Lax representations. We also generalized the Frenkel KdV hierarchy introduced on $\mathbb{K}_q$ to arbitrary

discrete time scales. We constructed the recursion operators of each example considered in this paper and gave a way of constructing the constants of motions by introducing an appropriate trace form on time scales.

In this work we did not consider the r-matrix construction and the Hamiltonian formulation of integrable systems on time scales. The trace form on a general time scale needs a little care. Such a work is in progress and will be communicated in a separate paper.

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APPENDIX: RECURSION OPERATORS OF FOUR-FIELD SYSTEMS

We give the recursion operator of the four-field systems on time scale which are studied in example 7.

(1) For the case $k=0$, $\alpha=-2$, we obtain the recursion relation between the $n+1$th and nth elements of the hierarchy as follows:

$$\begin{aligned} w_{n+1} &= w(E+1)^{-1}E(v_n) + E(v)(E^2-1)^{-1}E^2(w_n) - v(E^2-1)^{-1}w_n \\ &\quad + w(E+1)^{-1}(1-E)w(E^2-1)^{-1}E(w_n) + E^2(u_n) + (1-E^2)\eta_n, \end{aligned} \tag{A1}$$

$$\begin{aligned} v_{n+1} &= wE(u_n) + vv_n - u(E^2-1)^{-1}E^{-1}(w_n) + E(u)(E^2-1)^{-1}E^2(w_n) \\ &\quad + (1-E^2)p(1-E^2)^{-1}\frac{p_n}{p} + E^2(p_n) + (E^{-1}(w) - wE)\eta_n, \end{aligned} \tag{A2}$$

$$\begin{aligned} u_{n+1} &= wE(p_n) + u(E+1)^{-1}(E+1+E^{-1})v_n - p(E^2-1)^{-1}E^{-2}(w_n) \\ &\quad + u(E+1)^{-1}(E-1)E^{-1}(w)(E^2-1)^{-1}w_n + E(p)(E^2-1)^{-1}E^2(w_n) \\ &\quad + (E^{-2}(w) - wE)p(1-E^2)^{-1}\frac{p_n}{p} + vu_n + (E^{-1}(v) - v)\eta_n, \end{aligned} \tag{A3}$$

$$\begin{aligned} p_{n+1} &= uE^{-1}(u_n) + p(1+E^{-2})v_n + p(E^{-1}-E^{-2})w(E^2-1)^{-1}E(w_n) \\ &\quad + (E^{-2}(v) - v)p(1-E^2)^{-1}\frac{p_n}{p} + vp_n + (E^{-1}(u) - uE^{-1})\eta_n, \end{aligned} \tag{A4}$$

where

$$\eta_n = (E^2(p) - E(p)E^2)^{-1}\left[E^2(u)E(p_n) + E^2(p)u_n + (uE^2(p) - E^2(u)E(p)E^{-1})(1-E^2)^{-1}E^2\left(\frac{p_n}{p}\right)\right].$$

(2) For the case $k=1$, $\alpha=-2$, the recursion relation between the $n+1$th and nth elements of the hierarchy is given by

$$\begin{aligned} \bar{u}_{n+1} &= E^{-2}(\bar{w}_n) + \bar{u}(1+E)^{-1}(E-1)\bar{u}(1-E^2)^{-1}E(\bar{u}_n) + \bar{v}\bar{u}_n + \bar{u}(1+E)^{-1}\bar{v}_n \\ &\quad + (E^{-1}(\bar{v}) - \bar{v})(1-E^2)^{-1}\bar{u}_n + (1-E^{-2})\bar{\zeta}_n, \end{aligned} \tag{A5}$$

$$\begin{aligned} \bar{w}_{n+1} &= \bar{u}E^{-1}(\bar{q}_n) + \bar{w}(1+E)^{-1}(E^2+E+1)\bar{v}_n + (E^{-1}(\bar{q}) - \bar{q}E^4)(1-E^2)^{-1}\bar{u}_n + \bar{w}(1+E)^{-1}(1-E)E(\bar{u}) \\ &\quad \times(1-E^2)^{-1}E^2(\bar{u}_n) + \bar{v}\bar{w}_n + (E(\bar{v}) - \bar{v})\bar{\zeta}_n + (E^2(\bar{u}) - \bar{u}E^{-1})\bar{q}(E^2-1)^{-1}E^2\left(\frac{\bar{q}_n}{\bar{q}}\right), \end{aligned} \tag{A6}$$

$$\bar{q}_{n+1} = \bar{v}\bar{q}_n + \bar{w}E(\bar{w}_n) + \bar{q}(1+E^2)\bar{v}_n + (E^2(\bar{v}) - \bar{v})\bar{q}(E^2-1)^{-1}E^2\left(\frac{\bar{q}_n}{\bar{q}}\right)$$
$$+ \bar{q}(1+E)^{-1}(1-E^2)E(\bar{u})(1-E^2)^{-1}E^2(\bar{u}_n) + (E(\bar{w}) - \bar{w}E)\bar{\zeta}_n, \tag{A7}$$

$$\bar{v}_{n+1} = E^{-2}(\bar{q}_n) + \bar{u}E^{-1}(\bar{w}_n) + (E^{-1}(\bar{w}) - \bar{w}E^3)(1-E^2)^{-1}\bar{u}_n + \bar{v}\bar{v}_n + (E(\bar{u}) - \bar{u}E^{-1})\bar{\zeta}_n$$
$$+ (1-E^{-2})\bar{q}(E^2-1)^{-1}E^2\left(\frac{\bar{q}_n}{\bar{q}}\right), \tag{A8}$$

where

$$\bar{\zeta}_n = (\bar{q}E^2 - E(\bar{q}))^{-1}\left[\bar{q}E^2(\bar{w}_n) + (E^2(\bar{w})\bar{q}E - \bar{w}E(\bar{q}))(E^2-1)^{-1}E\left(\frac{\bar{q}_n}{\bar{q}}\right)\right]. \tag{A9}$$

From the recursion relations obtained in both cases, we can construct the recursion operators of the hierarchies.

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Eigenfunctions of the curl in cylindrical geometry

Edward C. Morse
University of California, Berkeley, California 94720

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Eigenfunctions of the equation $\vec{\nabla}\times\vec{B}=\lambda\vec{B}$ are found for finite cylindrical geometry with normal boundary condition $\vec{B}\cdot\hat{n}=0$ and nonaxisymmetric modes $\sim e^{im\theta}, m\neq 0$. The vector field $\vec{B}$ can be represented by a scalar generating function of the Chandrasekhar-Kendall type with radial Bessel functions for the nondegenerate cases. A general set of solutions can also be generated by transformation of variables. A series solution in terms of radial Bessel functions is found which has excellent convergence properties ($a_n \sim 1/n^4$) and a robust method of locating eigenvalues is described. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The equation $\vec{\nabla}\times\vec{B}=\lambda\vec{B}$ appears in many treatments of hydrodynamics and magnetohydrodynamics. It was first noted by Beltrami[1] in 1889 and the form with $\lambda=$constant was used by Trkal[2] in 1919. In the context of magnetohydrodynamics it was identified as a special force-free magnetic field by Woltjer[3] and was associated with a variational principle by Taylor[4] and thus acquired the name "Taylor state" when describing its lowest eigenvalue in a magnetostatic equilibrium. The eigenfields $\vec{B}_n$ of the nth eigenmode λ_n of this equation form a complete Hilbert space for decomposition of divergence-free vector fields,[5] such as the magnetic field or the velocity field in an incompressible fluid. The decomposition of magnetic and velocity field components into the eigenfunctions of the curl has proven useful as a method of studying magnetohydrodynamics using a Galerkin spectral representation of these fields in dynamic simulations.[6,7]

In this paper the solution of the eigenfunction equation $\vec{\nabla}\times\vec{B}=\lambda\vec{B}$ is discussed for the case of finite cylindrical geometry with boundary conditions $\vec{B}\cdot\hat{n}=0$ for nonaxisymmetric modes. A brief treatment of the symmetric $m=0$ case is given for completeness as a special case.

II. SYMMETRIC CASE, $m=0$

The solution of the curl-eigenfunction equation in cylindrical geometry for symmetrical ($m=0$) modes is relatively straightforward. Using a scalar generating function first shown by Chandrasekhar and Kendall,[8] the vector field $\vec{B}$ can be generated by

$$\vec{B}=\vec{\nabla}\times(\hat{z}\psi(R,Z))+(1/\lambda)\vec{\nabla}\times\vec{\nabla}\times(\hat{z}\psi(R,Z))$$

and these solutions are eigenfunctions of the curl provided that $\psi(R,Z)$ is a solution of the Helmholtz equation

$$\nabla^2\psi(R,Z)+\lambda^2\psi(R,Z)=0.$$

For these axisymmetric modes, the magnetic field components are given in cylindrical coordinates (R,θ,Z) by

$$B_R = (1/\lambda)\frac{\partial^2 \psi(R,Z)}{\partial R \partial Z},$$

$$B_\theta = -\frac{\partial \psi(R,Z)}{\partial R},$$

$$B_Z = \lambda \psi(R,Z) + (1/\lambda)\frac{\partial^2 \psi(R,Z)}{\partial Z^2}.$$

Normal boundary conditions $\vec{B}\cdot\hat{n}=0$ with boundaries $R=a$ and $Z=\pm 1/2$ imply that $B_R(a,Z)=0$ and $B_Z(R,\pm 1/2)=0$. Separable solutions to the scalar Helmholtz equation in this geometry which fit the boundary condition on B_Z are

$$\psi(R,Z) = J_0(\sqrt{\lambda^2 - ((2n'-1)\pi)^2}R)\cos((2n'-1)\pi Z)$$

and

$$\psi(R,Z) = J_0(\sqrt{\lambda^2 - (2n\pi)^2}R)\sin(2n\pi Z)$$

and the radial boundary condition $B_R(a,Z)=0$ is then given by

$$J_0'(k'a) = 0,$$

where $k' = (\sqrt{\lambda^2-(2n\pi)^2}, \sqrt{\lambda^2-((2n'-1)\pi)^2})$ for the modes. (The use of both sines and cosines to describe the modes may seem artificial but will simplify the description of the $m\neq 0$ modes later on.) For these modes, the general eigenvalue equation is then written as

$$\lambda_{pq}^2 = (1/a)^2(z_p')^2 + q^2\pi^2,$$

where p and q are integers and z_p' is the pth root of the derivative of the zeroth order Bessel function, $J_0'(z_p')=0$. The integer q simply replaces the set of even integers $2n$ and odd integers $2n'-1$ given above.

III. NONSYMMETRIC CASE, $m \neq 0$

The equation $\vec{\nabla}\times\vec{B}=\lambda\vec{B}$ can be recursively applied to obtain the "squared" version $\vec{\nabla}\times\vec{\nabla}\times\vec{B}=\lambda^2\vec{B}$. The eigenfunctions of this equation are not directly applicable to the first-order equation because the eigenfunctions of $\vec{\nabla}\times\vec{\nabla}\times\vec{B}=\lambda^2\vec{B}$ contain the eigenfunctions of $\vec{\nabla}\times\vec{B}=-\lambda\vec{B}$ as well as the eigenfunctions of $\vec{\nabla}\times\vec{B}=+\lambda\vec{B}$. However examination of the system $\vec{\nabla}\times\vec{\nabla}\times\vec{B}=\lambda^2\vec{B}$ is useful because it reveals the underlying elliptic nature of the equation, with the first-order equation forming connections between the three dependent variables in the vector $\vec{B}$.

We note that the equation $\vec{\nabla}\times\vec{\nabla}\times\vec{B}=\lambda^2\vec{B}$ can be manipulated for solenoidal fields with $\vec{\nabla}\cdot\vec{B}=0$ into the form

$$LB_R = \frac{+2im}{R^2}B_\theta,$$

$$LB_\theta = \frac{-2im}{R^2}B_R,$$

$$LB_Z = -\frac{1}{R^2}B_Z,$$

where

$$L = \frac{\partial^2}{\partial R^2} + \frac{1}{R}\frac{\partial}{\partial R} + \frac{\partial^2}{\partial Z^2} - \frac{(m^2+1)}{R^2} + \lambda^2.$$

The equations are of the form $Lu=Cu$, with the matrix C being nondiagonal. Following Ref. 9, we then perform a Jordan decomposition on C by finding a unitary transformation such that $C=pC'p^{-1}$ with C' diagonal. Applying the operator matrix p^{-1} to both sides of the equation, we have

$$p^{-1}Lu = p^{-1}Cu = p^{-1}(pC'p^{-1})u,$$

$$L(p^{-1}u) - [L,p^{-1}]u = C'(p^{-1}u).$$

The transformation matrix p^{-1} is given by

$$p^{-1} = \begin{pmatrix} 0 & 0 & 1 \\ i/2 & 1/2 & 0 \\ -i/2 & 1/2 & 0 \end{pmatrix}$$

and the commutator $[L,p^{-1}]=0$ for this system. Introducing a set of variables $w=p^{-1}u$ then gives $Lw=C'w$ with the matrix C' given by

$$C' = \begin{pmatrix} -1/R^2 & 0 & 0 \\ 0 & -2m/R^2 & 0 \\ 0 & 0 & +2m/R^2 \end{pmatrix}.$$

We can relabel the variables w in a more suggestive way. We write

$$B_Z(R,\theta,Z) = w_m(R,Z)e^{im\theta},$$

$$B_\theta(R,\theta,Z) = \left(\frac{w_{m+1}(R,Z) - w_{m-1}(R,Z)}{2i}\right)e^{im\theta},$$

$$B_R(R,\theta,Z) = \left(\frac{w_{m+1}(R,Z) + w_{m-1}(R,Z)}{2}\right)e^{im\theta}.$$

The transformed equations then become

$$L_{m+1}w_{m+1} = 0,$$

$$L_m w_m = 0,$$

$$L_{m-1}w_{m-1} = 0$$

with

$$L_n = \frac{\partial^2}{\partial R^2} + \frac{1}{R}\frac{\partial}{\partial R} + \frac{\partial^2}{\partial Z^2} - \frac{n^2}{R^2} + \lambda^2.$$

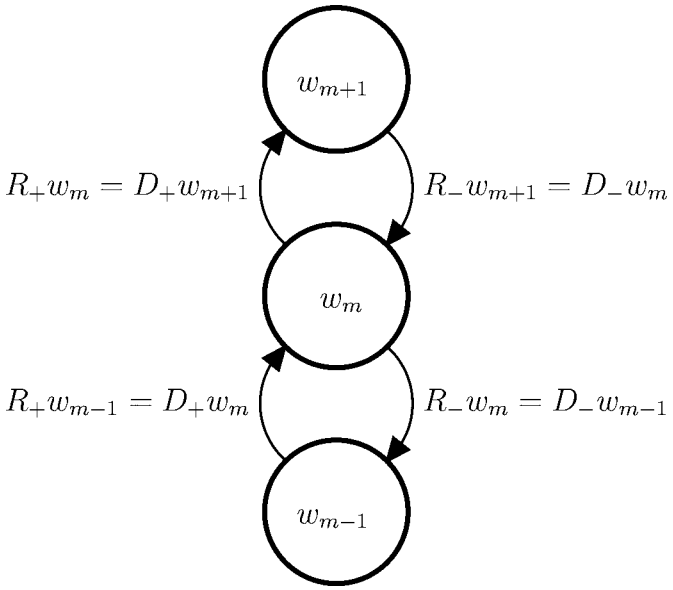

FIG. 1. Connection diagram for $m \neq 0$ transformed variables.

The first-order equations $\vec{\nabla} \times \vec{B} = \lambda \vec{B}$ and $\vec{\nabla} \cdot B = 0$ then can be manipulated into a set of first-order relations between the variables w. These relations can be written in a suggestive form of raising and lowering operators with the definitions

$$D_- = i\lambda - \partial/\partial Z,$$

$$D_+ = i\lambda + \partial/\partial Z,$$

$$R_-^n = (-1)^{n+m+1}(n/R + \partial/\partial R),$$

$$R_+^n = (-1)^{n+m+1}(n/R - \partial/\partial R).$$

The first-order equations then form a set of connection relations between the components w_n which each must satisfy the elliptic conditions given above. The connection diagram is shown in Fig. 1.

The Chandrasekhar-Kendall form may be employed to generate solutions to the $m \neq 0$ eigenequation[10], although this method does not directly translate the vector problem into a scalar problem. The Chandrasekhar-Kendall fields for $m \neq 0$ are given by

$$B_R = \left(\frac{im}{R} \psi(R,Z) + (1/\lambda) \frac{\partial^2 \psi(R,Z)}{\partial R \partial Z} \right) e^{im\theta},$$

$$B_\theta = \left(\frac{im}{\lambda R} \frac{\partial \psi(R,Z)}{\partial Z} - \frac{\partial \psi(R,Z)}{\partial R} \right) e^{im\theta},$$

$$B_Z = \left(\lambda \psi(R,Z) + (1/\lambda) \frac{\partial^2 \psi(R,Z)}{\partial Z^2} \right) e^{im\theta}.$$

For the $m \neq 0$ case, the radial boundary condition is complicated by the additional term $(im/R)\psi$, which is of course zero in the symmetric case. The radial boundary condition,

$$\left(\frac{im}{R}\psi(R,Z)+(1/\lambda)\frac{\partial^2\psi(R,Z)}{\partial R\partial Z}\right)\Bigg|_{R=a}=0,$$

is not a standard boundary condition for an elliptic equation and in fact cannot yield distinct eigenmodes without some additional restriction. The generating function $\psi=R^m\exp(-i\lambda Z)\exp(im\theta)$ solves the boundary equations independent of λ, although it does so trivially by generating zero vector field. While the Chandrasekhar-Kendall form does not compose a proper elliptic scalar problem, the Chandrasekhar-Kendall eigenfields can be used to solve the vector eigenproblem, which is well posed.[5]

Partial-term solutions to the boundary problem can be found by expansion of ψ into modes with radial Bessel functions and axial sines and cosines in the usual manner for cylindrical problems. It is important to note, however, that an alternative to the Bessel-function solution to the cylindrical Helmholtz equation exists, and this is the set of Sonine polynomials,

$$S(n,m,R,Z)=R^m e^{im\theta}e^{i\lambda Z}\frac{(-1)^n}{\Gamma(n+2)}L(n,m,i\lambda(\sqrt{R^2+Z^2}-Z))L(n,m,-i\lambda(\sqrt{R^2+Z^2}+Z)).$$

Here $L(n,m,x)$ represents the Laguerre polynomial. For integer n and m, the above expression generates solutions to the Helmholtz equation which are expressed in polynomials in R and Z times an exponential $e^{i(m\theta+\lambda Z)}$. As an example, the $n=0$ term is anharmonic in Z and satisfies $B_Z=0$ everywhere,

$$\psi=R^m\exp(i\lambda Z)\exp(im\theta).$$

The Sonine polynomials become important for calculation of degenerate solutions to the eigenequation, as shall be shown later.

IV. SERIES SOLUTION FOR $m\neq 0$ MODES

As discussed above, the transformation of the vector problem into a scalar problem using the Chandrasekhar-Kendall form generates a radial boundary condition which is perhaps unusual for elliptic equations but it has a suggestive form. The appearance of this operator $(i\cdots+(\partial/\partial Z\cdots))$ suggests that we seek a solution of form

$$\psi=\exp(im\theta)(F(R,Z)+iG(R,Z)),$$

where $F(R,Z)$ and $G(R,Z)$ are real functions and where, say, $F(R,Z)$ is an even function of Z and $G(R,Z)$ is an odd function of Z. The boundary condition can then be written as a separate pair of conditions,

$$\left(\frac{a}{m\lambda}\right)\frac{\partial^2F(R,Z)}{\partial R\partial Z}\Bigg|_{R=a}=G(a,Z),$$

$$\left(\frac{a}{m\lambda}\right)\frac{\partial^2G(R,Z)}{\partial R\partial Z}\Bigg|_{R=a}=-F(a,Z).$$

Using this form for a solution, and noting that the anharmonic term already has this form, we have a general series expression for the generating function $\psi=e^{im\theta}\psi(R,Z)$,

$$\psi(R,Z) = R^m e^{i\lambda Z} + \sum_{n'=1}^{\infty} b_{n'} \frac{J_m(R\sqrt{\lambda^2 - (2n'-1)^2\pi^2})}{J_m(a\sqrt{\lambda^2 - (2n'-1)^2\pi^2})} \cos((2n'-1)\pi Z)$$
$$+ i\sum_{n=1}^{\infty} a_n \frac{J_m(R\sqrt{\lambda^2 - 4n^2\pi^2})}{J_m(a\sqrt{\lambda^2 - 4n^2\pi^2})} \sin(2n\pi Z).$$

Here we have normalized the Bessel functions to their value at $R=a$ because at some n and n' the argument of the Bessel function becomes imaginary and thus the Bessel functions become exponentially large, since $J_m(ix)=I_m(x)\sim\exp(x)$ when $x\gg 1$. (This normalization produces spurious poles in the matrix representation at values of λ which reflect zeroes in the low-order Bessel functions. This has been found not to interfere with the calculation near an eigenvalue, which is not typically near one of these zeroes. In any case, it would be possible to leave this normalization off for the first few Bessel functions with a real argument.)

The Z derivative appearing in the boundary condition causes some complication in the Fourier decomposition. The odd-integer cosine terms when differentiated become terms in $\sin((2n'-1)\pi Z)$, and these are not independent of the functions $\sin(2n\pi Z)$. A Fourier decomposition of these terms into terms in $\sin(2n\pi Z)$ thus is done in order to generate a set of matching equations which are orthogonal to one another. The Z derivatives of the even-integer sine terms also are mapped into the basis of odd-integer cosine terms. Similarly, the anharmonic term $(\sim\cos(\lambda Z) + i\sin(\lambda Z))$ is mapped into the appropriate basis, the real part into the basis of odd-integer cosines and the imaginary part into the basis of even-integer sines.

This strategy then generates a set of $2N$ matching equations for the boundary condition, where N is the number of even-integer terms in the expansion, typically taken equal to the number of odd-integer terms. The radial differentiation operator and the Z differentiation and basis remapping operator are given here separately. (Note that in the notation that follows, the superscripts "odd" and "even" relate to the integer appearing in the trigonometric expression, not to the Z-parity of ψ. In fact the "odd" terms have even Z-parity and vice versa.) It is interesting to note that by combining the Z-differentiation and basis remapping operations a symmetrical expression for this operator is obtained, as can be demonstrated by integrating by parts.

An expression for the radial differentiation operator is

$$Q_p = \frac{\sqrt{\lambda^2 - p^2\pi^2}(J_{m-1}(a\sqrt{\lambda^2 - p^2\pi^2}) - J_{m+1}(a\sqrt{\lambda^2 - p^2\pi^2}))}{2J_m(a\sqrt{\lambda^2 - p^2\pi^2})}$$

Here p takes on even values $2n$ and odd values $2n'-1$.

The Z-differentiation and basis remapping ("sine-to-cosine") operator is given by

$$\mathbf{SC}(n,n') = \frac{8(-1)^{n'+n}(1-2n')n}{(2n'-1)^2 - 4n^2}.$$

We can now construct a set of matrix equations which form the $2N$ total boundary conditions. We write this equation in the form

$$\mathbf{M}\cdot\mathbf{x} = \mathbf{u},$$

where the forcing vector $\mathbf{u}$ is given by the Fourier decomposition of the anharmonic term as described above. The operator corresponding to the term $(a/m\lambda)\partial^2/\partial R\partial Z$ is given by

$$\mathbf{M}^{\text{even}}_{n,n'} = \frac{a\,\mathbf{SC}(n,n')Q^{\text{even}}_n}{m\lambda}$$

and

$$\mathbf{M}^{\text{odd}}_{n',n} = \frac{a\,\mathbf{SC}(n,n')Q^{\text{odd}}_{n'}}{m\lambda}.$$

The forcing vector $\mathbf{u}$ is then given by

$$\mathbf{u} = \{u^{\text{even}}_1, u^{\text{even}}_2, \ldots, u^{\text{even}}_N, u^{\text{odd}}_1, u^{\text{odd}}_2, \ldots, u^{\text{odd}}_N\},$$

where

$$u^{\text{even}}_n = \frac{8(-1)^n n\pi \sin(\lambda/2)}{(2n\pi)^2 - \lambda^2}$$

and

$$u^{\text{odd}}_{n'} = \frac{4(-1)^{n'}(1-2n')\pi\cos(\lambda/2)}{(1-2n')^2\pi^2 - \lambda^2}.$$

The vector $\mathbf{x}$ is the union of a_n and $b_{n'}$,

$$\mathbf{x} = (\mathbf{a},\mathbf{b}) = (a_1, a_2, \ldots, a_N, b_1, b_2, \ldots, b_N)$$

and the matrix $\mathbf{M}$ is given by

$$\mathbf{M} = \begin{pmatrix} \mathbf{M}^{\text{even}} & \mathbf{I} \\ \mathbf{I} & \mathbf{M}^{\text{odd}} \end{pmatrix}.$$

Some comments about the structure of the matrix equation $\mathbf{M}\cdot\mathbf{x}=\mathbf{u}$ are in order. The radial operator generates terms which are proportional to n as they become large. The terms near the diagonal of the sine-to-cosine matrix $\mathbf{SC}$ also are proportional to n, and thus the matrices $\mathbf{M}^{\text{even}}$ and $\mathbf{M}^{\text{odd}}$ have terms that increase as n^2. The alternating nature of the terms $(-1)^{n+n'}$ does result in less difficulty in inverting the matrix $\mathbf{M}$ than would be required otherwise. However, the matrix equations can become better conditioned by inverting the individual components $\mathbf{M}^{\text{even}}$ and $\mathbf{M}^{\text{odd}}$. This can be done since each can be decomposed into the product of a diagonal matrix and the basis transformation matrix $\mathbf{SC}$. The $\mathbf{SC}$ matrix has an inverse which is given by

$$\mathbf{SC}^{-1}(n',n) = \frac{-8(-1)^{n+n'}n'}{(-1+2n)((1-2n)^2 - 4n'^2)\pi^2}.$$

(This expression can be arrived at by considering that differentiating a function $f(x)$ [and obtaining function $g(x)$] in basis $|n\rangle$ and transforming into a new basis $|n'\rangle$ must have the inverse operator formed by integrating the function $g(x)$ termwise in basis $|n'\rangle$ and transforming the result into basis $|n\rangle$.) Also, upon multiplication and substitution, the matrix equations can be separated into two matrix equations each of rank N rather than $2N$. If we form auxiliary matrices $\mathbf{z}_1$ and $\mathbf{z}_2$ which are the inverses of $\mathbf{M}^{\text{even}}$ and $\mathbf{M}^{\text{odd}}$,

$$\mathbf{z}_1(n,n') = \mathbf{M}^{\text{even}^{-1}} = \frac{m\lambda}{a}\mathbf{SC}^{-1}(n,n')/Q_{\text{even}}(n),$$

$$\mathbf{z}_2(n',n) = \mathbf{M}^{\text{odd}^{-1}} = \frac{m\lambda}{a}\mathbf{SC}^{-1}(n,n')/Q_{\text{odd}}(n'),$$

$$\mathbf{Z}^{\text{even}} = \mathbf{I} - \mathbf{z}_1\cdot\mathbf{z}_2, \quad \mathbf{u}'_1 = \mathbf{z}_1\cdot\mathbf{u}_1 - \mathbf{z}_1\cdot\mathbf{z}_2\cdot\mathbf{u}_2,$$

$$\mathbf{Z}^{\text{odd}} = \mathbf{I} - \mathbf{z}_2 \cdot \mathbf{z}_1, \quad \mathbf{u}_2' = \mathbf{z}_2 \cdot \mathbf{u}_2 - \mathbf{z}_2 \cdot \mathbf{z}_1 \cdot \mathbf{u}_1,$$

then the transformed set of matrix equations is

$$\begin{aligned} \mathbf{Z}^{\text{even}} \cdot \mathbf{a} &= \mathbf{u}_1', \\ \mathbf{Z}^{\text{odd}} \cdot \mathbf{b} &= \mathbf{u}_2'. \end{aligned} \tag{4.1}$$

When these are solved for some finite N as a function of λ, a proper eigenfield is obtained only when the coefficients a_n and b_n form a convergent series representation of the field components B_R, B_θ, and B_Z. Since the operator $\mathbf{M}$ for the field components has terms proportional to n^2, it would seem that the minimum convergence criterion for the a_n and b_n is that $n^2(a_n, b_n) \to 0$ as $n \to \infty$. However, because of the additional constraints imposed by the connection relations outlined above, the a_n and $b_n \propto 1/n^4$ when λ is an eigenvalue. In fact the eigenvalue problem can be defined as solutions to (4.1) above with the limiting forms $\lim_{n\to\infty} n^3(a_n, b_n) = 0$. However, a stronger eigenvalue criterion can be formed by observing that solutions to the odd series b_n always have a $1/n^4$ characteristic independent of λ and the terms a_n have a $1/n^2$ characteristic when λ is not an eigenvalue and a $1/n^4$ characteristic as λ approaches an eigenvalue. The reason for this unequal behavior arises from the following observation regarding the trigonometric series of terms produced by the odd and even Fourier series when differentiation is included. To wit, the series of terms in $\cos((2n-1)\pi Z)$, $n = 1, 2, \ldots, \infty$ form a complete space on $(-1/2, 1/2)$ for even functions of Z, as do the terms $\sin(2n\pi Z)$, $n = 1, 2, \ldots, \infty$ for odd functions of z. These are used as the Z-basis functions for the functions ψ used as the generator. However, the derivatives of these series are also used in the method outlined above, and whereas $\sin((2n-1)\pi Z)$, $n = 1, 2, \ldots, \infty$ is complete for odd functions, the series $\cos(2n\pi Z)$, $n = 1, 2, \ldots, \infty$ is not complete for even functions on $(-1/2, 1/2)$ since the $n = 0$ term, i.e., a constant function, would be necessary to make this series complete. Since this function is not generated by the differentiation operation, a constraint for the convergence of the series solution is that the even function $F(R, Z)$ does not contain a constant part in the Fourier decomposition, i.e., $\int_{-1/2}^{1/2} F(a, Z)\mathrm{d}Z = 0$. The function F is represented by the anharmonic term $\propto \cos(\lambda Z)$ and by the Fourier terms in $b_n \cos((2n-1)\pi Z)$ and thus the eigenvalue criterion becomes

$$\epsilon(\lambda) = \sum_{n=1}^{\infty} \frac{b_n(-1)^n}{2n-1} - \pi \frac{\sin(\lambda/2)}{\lambda} = 0. \tag{4.2}$$

The summation appearing in this equation contains terms decreasing as $1/n^5$ independent of λ, so that this equation has robust convergence as a function N, the total terms used in the series expansion. The error term caused by truncation is thus proportional to $1/N^4$. It is also important to note that for eigenvalue-only studies, only one of the matrix equations need be solved, since only the b_n are needed in (4.2). In practice the matrix $\mathbf{Z}^{\text{odd}}$ is diagonally dominant (with the possible exception of the first few entries in the upper left-hand corner) and so the linear solve operation is rapidly convergent.

V. NUMERICAL STUDIES

The eigenvalues λ can be located by solving the eigenvalue equation $\epsilon(\lambda) = 0$ with a finite series of terms b_n using a linear matrix solution. Figure 2 shows a numerical solution of the eigenequation (4.2) given above for a length-to-radius ratio $1/a$ of unity with 100 terms kept in the orthonormal expansion, and Fig. 3 shows the spectrum of partial terms a_n and b_n for the lowest eigenmode at $\lambda = 1.734\,26\pi$. Note that the smooth zero crossings of $\epsilon(\lambda)$ at values of the eigenvalue parameter λ which are not integer multiples of π represent actual eigenvalues for the system. Spurious zeroes of the eigenequation occur at $\lambda = p\pi$, with p integer, because at these points the anharmonic solution used as the forcing term is identical to one of the partial eigenfields, and this redundancy forces a trivial solution which has vector fields $\vec{B} = 0$ everywhere.

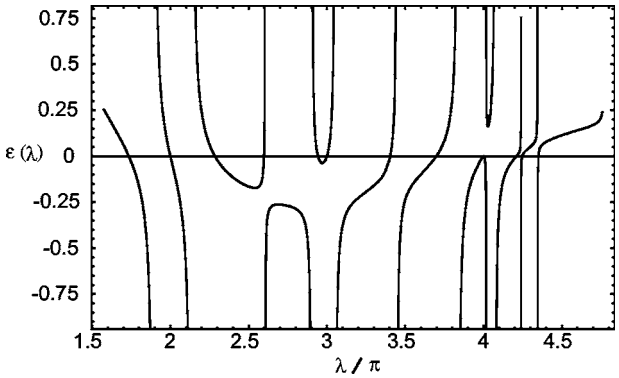

FIG. 2. Behavior of the eigenvalue parameter $\epsilon(\lambda)$ for $m=1$ mode at $1/a=1$ for a 100-term expansion of the eigenvalue solution as a function of eigenvalue parameter λ.

(Details of the construction of an eigenfield for degenerate cases where λ actually attains an integer value are discussed later.) It is a simple matter to vary the number of terms N kept in the expansion of ψ, and thus an extrapolated value λ_∞ can be calculated by applying this technique to a series of N values. The error in eigenvalue $\lambda_N-\lambda_\infty$ can then be computed. Figure 4 shows that the error in λ is of order $1/N^4$ using this approach. The robust characteristics of the matrices involved allow computation to machine accuracy on a personal computer. For example, iterative calculations with $N=2000$ can be performed on a machine with 256 MB memory that yield the eigenvalue to machine accuracy ($\approx$15 digits) in a matter of minutes. A numerical predictor for the error term remainder, $\epsilon(N)-\epsilon(\infty)$, can be added, and this has been found to speed convergence somewhat.

VI. SPECIAL CASES

It is interesting to explore the range of parameter space in the aspect ratio $1/a$ and in azimuthal mode number m in order to find simple analytical models for the behavior of the eigenproblem in extreme cases. First we examine the behavior of the eigenvalue problem when $a \rightarrow \infty$, i.e., for a "thin disk" case. Here the eigenvalues $\lambda \sim p\pi$, with integer p. For this case, a single Bessel function plus the anharmonic term can be used to approximate the solution

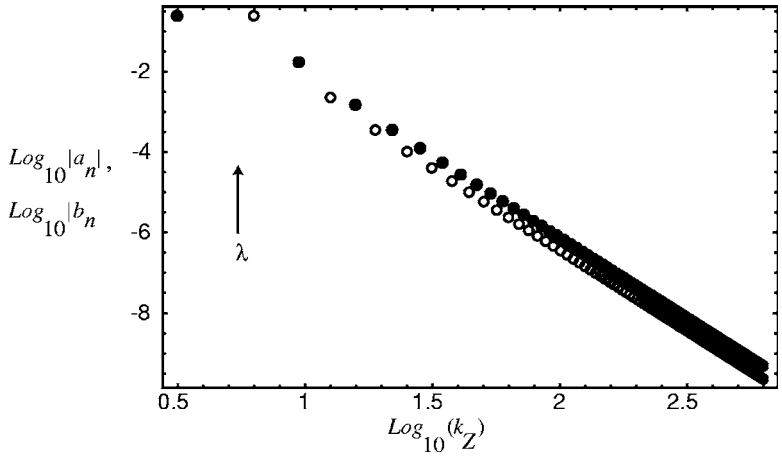

FIG. 3. Spectral plot of $|a_n|$ and $|b_n|$ vs axial wave number k_Z for the lowest $m=1$ mode with aspect ratio $1/a=1.0$. Eigenvalue λ is marked.

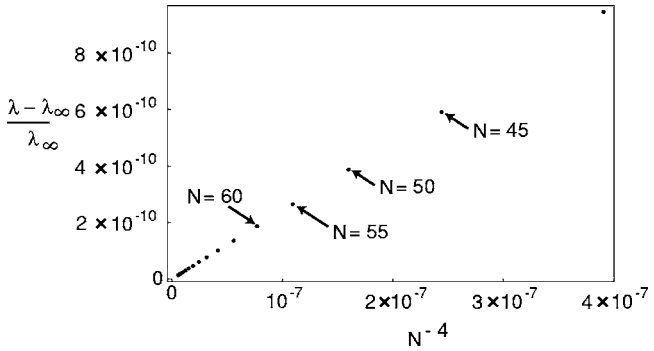

FIG. 4. Convergence study of computed eigenvalue λ as a function of number or terms N.

$$\psi(R,Z) \approx (R/a)^m e^{i\lambda Z} - J_m(\sqrt{\lambda^2 - p^2\pi^2}R)/J_m(\sqrt{\lambda^2 - p^2\pi^2}a)\begin{pmatrix}\cos\\ i\sin\end{pmatrix}(p\pi Z)$$

with the cos (sin) term used when p is odd (even). The expression automatically satisfies the boundary condition at $Z=\pm 1/2$ and the radial boundary condition is approximately satisfied when

$$\frac{m}{a}J_m(\sqrt{\lambda^2 - p^2\pi^2}a) = \sqrt{\lambda^2 - p^2\pi^2}J'_m(\sqrt{\lambda^2 - p^2\pi^2}a).$$

As an example, for the $m=1$, $p=1$ case, this is satisfied when the argument of the Bessel function is $r_1=5.135\,62$ and thus the eigenvalue equation becomes

$$\lambda^2 \approx \pi^2 + \left(\frac{5.135\,62}{a}\right)^2.$$

For the opposite extreme where $a\to 0$, the "long tube" case, we first consider the case when there is no Z-boundary, i.e., the infinitely long tube. In this case we ignore the anharmonic term and look at a complex solution of the form

$$\psi(R,Z) = e^{ik_Z Z}J_m(\sqrt{\lambda^2 - k_Z^2}R).$$

The radial boundary condition is satisfied when

$$m/aJ_m(\sqrt{\lambda^2 - k_Z^2}a) + k_Z/\lambda(\sqrt{\lambda^2 - k_Z^2}a)J'_m(\sqrt{\lambda^2 - k_Z^2}a) = 0.$$

This equation has roots in k_Z which depend on λa. There is a critical value of λa above which two distinct real roots in k_Z appear, and thus a continuum of eigenvalues are possible. For the $m=1$ case, the critical root $\lambda_c a \approx 3.112\,36$. The eigenvalue spectrum becomes discrete in the finite-length case. The asymptotic value of the lowest eigenvalue for finite $a\to 0$ is thus λ_c. A refined estimate of the lowest eigenvalue for small a becomes apparent when the spectrum of the partial terms a_n and b_n is examined numerically. Figure 5 shows the partial term spectrum for the $m=1$ case with $1/a=20$. One notes that there is a large spectral content around the eigenvalue λ which effectively cancels the contribution for the anharmonic term. There is also a large contribution from spectral terms at the two values of k_Z which satisfy the equation above when the eigenvalue is slightly above the critical value of λ_c. The significance of the separated modes can be seen by examining the Z-boundary condition. Since the radial argument $\sqrt{\lambda^2 - k_Z^2}R$ appearing in the Bessel function is nearly the same for $k_Z=k_Z^+$ and for $k_Z=k_Z^-$ when a is small, the modes corresponding to the two roots k_Z^+ and k_Z^- have nearly identical radial structure. The Z-boundary equation is satisfied approximately when the two terms cancel at $Z=\pm 1/2$. Since

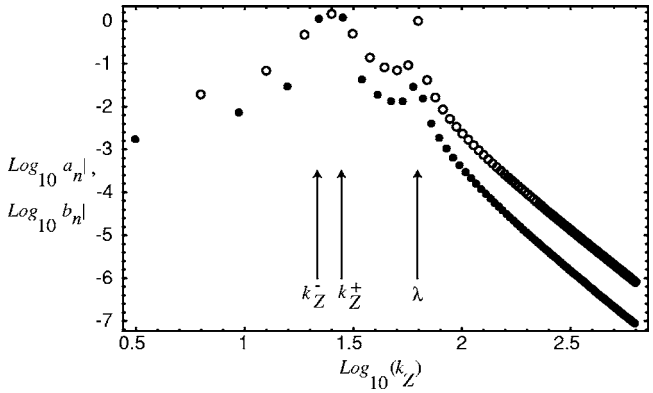

FIG. 5. Spectral plot of $|a_n|$ and $|b_n|$ vs axial wave number k_Z for the lowest $m=1$ mode with $1/a=20$. Upper and lower infinite-cylinder eigenmodes are marked. $(k_Z^+-k_Z^-)/(2\pi)=1.000\,96$ for this case.

$$e^{ik_Z^+Z}+e^{ik_Z^-Z}=2\cos((k_Z^+-k_Z^-)Z/2)e^{i[(k_Z^++k_Z^-)/2]Z},$$

we have cancellation of these terms when $\cos((k_Z^+-k_Z^-)/4)=0$. Thus the eigenvalue equation for the lowest mode becomes $k_Z^+-k_Z^-=2\pi$. Since the roots k_Z appear close to a parabolic minimum, the separation of these roots is proportional to the square root of $(\lambda-\lambda_c)$. For the $m=1$ case, one finds the approximate form

$$(k_Z^+-k_Z^-)^2\approx 9.523(\lambda-\lambda_c).$$

We wish to fit this approximate expression into a canonical form $\lambda^2=r_3^2+r_2^2/a^2$, i.e., the usual hyperbolic relationship between λ and $1/a$, and then for an approximate expression for the lowest $m=1$ eigenvalue with $a\ll 1$ we find $r_2=3.1126$, $r_3^2=2r_2(2\pi)^2/9.523$ and thus

$$\lambda^2=(3.1126/a)^2+25.8454.$$

Figure 6 shows a plot of the lowest $m=1$ eigenvalue for cylinders with aspect ratio $1/a$ ranging from 10^{-2} to 10^3 with these two asymptotic limits drawn. One sees that the eigenvalue λ is somewhat lower than either estimate near length-to-radius ratios $1/a$ near unity, as expected from physical arguments.

It is also interesting to note the special case formed by $m\to\infty$. In this case the term containing $\partial/\partial R\partial Z$ becomes small compared to the other term in the boundary equation. Thus the solutions become similar to the solution of the scalar Helmholtz equation with Dirichlet boundary condi-

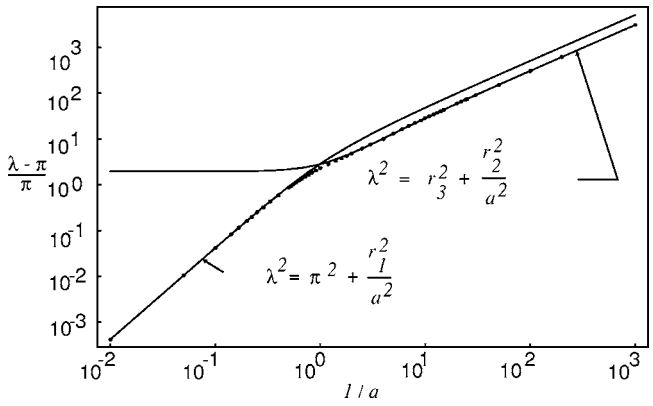

FIG. 6. Lowest $m=1$ eigenvalue as a function of aspect ratio $1/a$, with asymptotic values. Parameters $r_1=5.135\,62$, $r_2=3.112\,36$, $r_3=5.083\,83$.

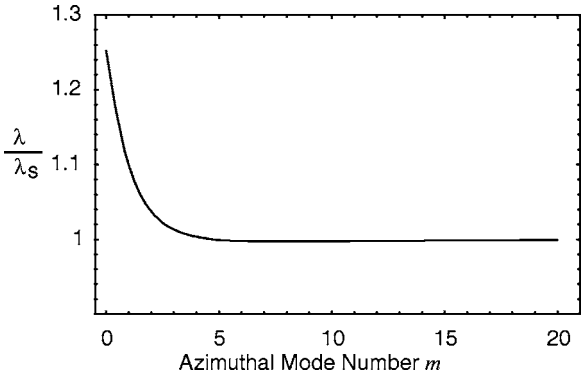

FIG. 7. Ratio of lowest eigenvalue λ to the lowest eigenvalue λ_s for the scalar Helmholtz equation with Dirichlet boundary conditions, as a function of azimuthal mode number m, for aspect ratio $1/a=1.0$.

tions as $m\rightarrow\infty$. This is illustrated by Fig. 7, where a plot of the ratio of the eigenvalue λ for the curl-eigenfunction problem to the scalar Helmholtz eigenvalue λ_s is shown for all values from $m=0$ to $m=20$. This figure shows that the ratio approaches unity rather quickly, and also illustrates that noninteger values of m can be accounted for.

Last, we treat the case where the eigenvalue $\lambda=p\pi$, $p=2,3,\ldots$. This is a degenerate case for the algorithm described above because the "anharmonic" term $\propto e^{i\lambda Z}$ is equivalent to one of the basis functions when $\lambda=n\pi$ and thus the matrix equation, while nonsingular, returns a trivial solution $\psi=0$. To avoid this situation, we observe that in this case there is a special mode which is a curl eigenfunction and has $B_Z=0$ at $Z=\pm 1/2$ that can be constructed starting with the fundamental solutions $B_Z=w_m=R^m e^{i\lambda Z}$ and $B_Z=w_m=R^m e^{-i\lambda Z}$. This solution is not obtainable from the Chandrasekhar-Kendall form with solutions of the elliptic equation with separation of variables in (R,Z) but can be derived from the connection diagram shown in Fig. 1 with the use of Sonine polynomials as solutions to the elliptic equations, or by use of the $n=2$ Sonine polynomial $S(2,m,R,Z)$ in the Chandrasekhar-Kendall form. For example, for the $m=1$ case, with $\lambda=2\pi,4\pi,\ldots$, i.e., for even p, a curl eigenfunction satisfying the Z boundary condition is

$$B_R=-4\cos(\lambda Z)-(4i\lambda Z+2\lambda^2R^2)e^{i\lambda Z}-\lambda^2R^2e^{-i\lambda Z},$$

$$B_\theta=-4i\cos(\lambda Z)+(4\lambda Z-2i\lambda^2R^2)e^{i\lambda Z}+i\lambda^2R^2e^{-i\lambda Z},$$

$$B_Z=8\lambda R\sin(\lambda Z).$$

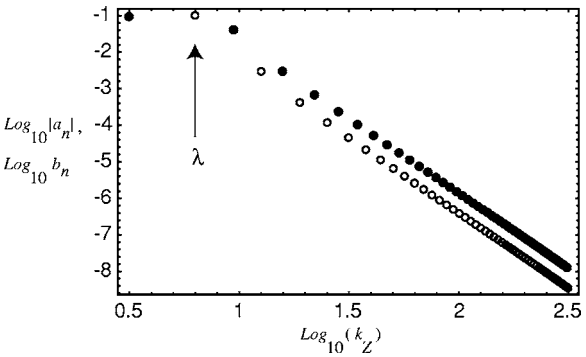

FIG. 8. Spectral plot of $|a_n|$ and $|b_n|$ vs axial wave number k_Z for the degenerate $m=1$ eigenmode with $\lambda=2\pi$. The aspect ratio $1/a=1.3272$ for this case.

Here the $e^{i\theta}$ dependence has been suppressed. The $B_R(R=a)$ component of this eigenfield is then decomposed into Fourier terms in $\sin(2n\pi Z)$ and $\cos((2n-1)\pi Z)$ as before, and this column of Fourier components is substituted into the matrix **M** at the appropriate column to replace the redundant mode. Convergence of this algorithm is obtained for the choice of radius a corresponding to the degenerate eigenvalue. Figure 8 shows the partial term spectrum for the case $m=1$, $p=2$.

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An interpolation between the wave and diffusion equations through the fractional evolution equations Dirac like

T. Pierantozzi[a)]
Departamento de Matemática Aplicada, Facultad de Informática, Universidad Complutense de Madrid, Madrid E-28040, Spain

L. Vázquez[b)]
Departamento de Matemática Aplicada, Facultad de Informática, Universidad Complutense de Madrid, Madrid E-28040, Spain and Centro de Astrobiología (CSIC-INTA), Torrejón de Ardoz, Madrid 28850, Spain

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Through fractional calculus and following the method used by Dirac to obtain his well-known equation from the Klein-Gordon equation, we analyze a possible interpolation between the Dirac and the diffusion equations in one space dimension. We study the transition between the hyperbolic and parabolic behaviors by means of the generalization of the D'Alembert formula for the classical wave equation and the invariance under space and time inversions of the interpolating fractional evolution equations Dirac like. Such invariance depends on the values of the fractional index and is related to the nonlocal property of the time fractional differential operator. For this system of fractional evolution equations, we also find an associated conserved quantity analogous to the Hamiltonian for the classical Dirac case. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2121167]

I. INTRODUCTION

Following the well-known Dirac's approach,[19] the free Dirac equation can be considered as the square root of the Klein-Gordon equation. In a more general context Morinaga and Nono[11] analyzed the integer s-root of the partial differential equations of the form

$$\sum_{|I|=s} a_I \frac{\partial^{|I|}}{\partial x^I}\phi = \phi, \tag{1}$$

by defining them as the first-order system

$$\sum_{i=1}^{n} \alpha_i \frac{\partial \Phi}{\partial x_i} = \Phi, \tag{2}$$

where $\alpha_1, \ldots, \alpha_n$ are matrices. From the physical point of view the α_k describe internal degrees of freedom of the associated system.

In the above-mentioned context, Vázquez *et al.* recently considered in Refs. 21 and 22 the fractional diffusion equations with internal degrees of freedom. They can be obtained as the s-roots of the standard scalar linear diffusion equation. Thus, a possible definition of the square root of the standard diffusion equation (SDE) in one space dimension, $u_t - u_{xx} = 0$, is the following:

[a)]Electronic mail: Teresa_Pierantozzi@mat.ucm.es
[b)]Electronic mail: lvazquez@fdi.ucm.es

$$\left(A\frac{\partial^{1/2}}{\partial t^{1/2}}+B\frac{\partial}{\partial x}\right)\psi(x,t)=0, \tag{3}$$

where A and B are 2×2 matrices satisfying Pauli's algebra

$$A^2=I,\quad B^2=-I,\quad AB+BA=0, \tag{4}$$

I being the identity operator.

It is worthy of mention that Oldham and Spanier[12,13] were the first authors to derive a formulation involving the mathematical operation of semidifferentiation in replacement of Fick's laws in a work of 1970.

Here $\psi(x,t)$ is a multicomponent function with at least two scalar space-time components. Also, each scalar component satisfies the SDE. Such solutions can be interpreted as *probability distributions with internal structure associated to internal degrees of freedom of the system*. They are named *diffunors* in analogy with the spinors in Quantum Mechanics.

In this paper we deal with a further generalization of Dirac's method, considering the system of fractional evolution equations

$$(A\partial_t^{\alpha}+B\partial_x)\psi(t,x)=0,\quad \psi(t,x)=\begin{pmatrix}u_1(t,x)\\ u_2(t,x)\end{pmatrix}, \tag{5}$$

with $0<\alpha<1$, A and B satisfying (4), as the square root of the time fractional diffusion-wave equation

$$\partial_t^{2\alpha}u(t,x)-\partial_{xx}u(t,x)=0. \tag{6}$$

Equation (6), associated with anomalous diffusion, has been widely studied in the literature by many authors, including Schneider and Wyss,[18] Metzler *et al.*,[7,9,23] Mainardi *et al.*,[4–6] Sokolov *et al.*,[20] Saichev *et al.*[16] A more physical discussion of this equation was given by Metzler and Klafter in Ref. 8 and it is worthwhile mentioning that they proved that the resulting probability density is bimodal in character. In this sense, Schneider and Wyss[18] showed that, for dimensions higher than 1, the character of the solution of the fractional wave equation (when $1/2<\alpha\leqslant 1$) as a proper probability density is lost.

Each component of $\psi(t,x)$ satisfies (6) while the index property $\partial_t^{\alpha}\partial_t^{\alpha}u=\partial_t^{2\alpha}u$ holds. Thus, in the interval $1/2<\alpha<1$, the decomposition (5) of (6), expressed in terms of fractional evolution equations of Dirac-type, represents a fractional interpolation between the diffusion ($\alpha=1/2$) and wave ($\alpha=1$) equations.

The applications of the fractional calculus range in a wide spectrum of areas like material sciences (viscoelasticity, polymers, etc.), circuits, diffusion processes, Biology, Economy, Geology, traffic problems, data analysis, and others, as illustrated, for example, in the textbooks by Hilfer,[2] Ross,[15] and Samko *et al.*[17] Many of the associated models amount to replacing the time derivative in an evolution equation with a fractional derivative of real order.

The fractional derivative operator ∂_t^{α} appearing in (5) can be specified according to several definitions available in the literature (see, for example, Refs. 17 and 14); we will refer to the two commonly used definitions of Riemann-Liouville and Caputo.

The Riemann-Liouville derivative of order $\alpha>0$ is defined as

$$({}_a^{\mathrm{RL}}D_x^{\alpha}f)(x)=\frac{\mathrm{d}^n}{\mathrm{d}x^n}\frac{1}{\Gamma(n-\alpha)}\int_a^x(x-t)^{n-\alpha-1}f(t)\mathrm{d}t, \tag{7}$$

with $x>a$, $n=-[-\alpha]$, whereas the Caputo fractional derivative, usually considered as a regularized version of the Riemann-Liouville fractional differential operator, takes the form

$$({}_x^{C}D_x^{\alpha}f)(x)=\frac{1}{\Gamma(n-\alpha)}\int_a^x\frac{f^n(\tau)}{(x-\tau)^{\alpha-n+1}}\mathrm{d}\tau. \tag{8}$$

There exists the following relation between the above-noted definitions:

$$({}_a^C D_x^\alpha f)(x) = {}_a^{\mathrm{RL}} D_x^\alpha \left[f(x) - \sum_{j=0}^{n-1} f^{(j)}(a+) \frac{(x-a)^j}{j!} \right], \tag{9}$$

and, a condition under which both derivatives hold is that $f \in AC^{n-1}(a,\infty)$. Equivalence (9) allows one to use only initial conditions of the classical type when dealing with fractional equations involving Riemann-Liouville or Caputo derivatives. The integral approach pursued by Schneider and Wyss in Ref. 18 is probably the most physical way of incorporating these initial values to the corresponding equation.

Definitions (7) and (8) reproduce the classical derivative $\mathrm{d}^n/\mathrm{d}x^n$ when $\alpha=n$ ($n \in \mathbb{N}$) and the identity operator for $\alpha=0$, and they are *nonlocal* operators being given by a definite integral.

It is important to highlight that, in general (see Refs. 10 and 14, for example) the index property ${}_a D_x^\alpha {}_a D_x^\beta f = {}_a D_x^{\alpha+\beta} f$ does not hold using the definitions of fractional derivative of Riemann-Liouville (7) or Caputo (8), unless the function f verifies

$$f^{(j)}(a+) = 0, \quad j = 0,1,2,\ldots,m-1, \tag{10}$$

whenever $f(x) \in AC^{m-1}(a,\infty)$ and $f^m(x) \in L^1_{\mathrm{loc}}(a,\infty)$, $m-1 < \beta \leqslant m$.

Reference 10, Chap. 4 analyzes a restricted class of functions C for which the Riemann-Liouville fractional derivative satisfies the cited index property. Some examples of functions in C are: x^λ with $\lambda > -1$, the polynomials, the exponentials, the sine and cosine functions, and all the linear combinations of them.

The structure of the paper is as follows. In Sec. II, a physical meaning to the solutions of (5) is given, showing how they generalize the behavior of the solutions of the Dirac system, recovered when $\alpha=1$, in relation with the D'Alembert solution. Following the analogy with the classical Dirac case, the internal symmetries of the system (5) under inversions and translations in time and/or space, and Galileo transform are considered in Sec. III, whereas in Sec. IV a conserved quantity for (5), analogous to the Hamiltonian for the classical Dirac equation, is found.

II. PHYSICAL MEANING OF THE SOLUTIONS OF THE SYSTEM OF FRACTIONAL EVOLUTION EQUATIONS

It is well known that the general solution of the wave equation with zero initial velocity,

$$\begin{cases} \partial_{tt} u(t,x) - c^2 \partial_{xx} u(t,x) = 0, \\ u(0,x) = \varphi(x), \ \varphi \in \mathcal{C}^2, \\ u_t(0,x) = 0, \end{cases} \tag{11}$$

is given by the D'Alembert Formula

$$u(t,x) = \tfrac{1}{2}[\varphi(x-ct) + \varphi(x+ct)]. \tag{12}$$

From a physical point of view, we can interpret this fact as that the amplitude at time t of a perturbation created by a given starting deformation at rest, $\varphi(x)$, is the superposition of two waves, $\varphi(x+ct)$ and $\varphi(x-ct)$, whose shape is identical to the starting one's and traveling in opposite directions. The two waves are solutions of the following first-order problems:

$$\begin{cases} \partial_t u(t,x) - c \partial_x u(t,x) = 0, \\ u(0,x) = \varphi(x), \ \varphi \in \mathcal{C}^2, \end{cases} \tag{13}$$

and

$$\begin{cases} \partial_t u(t,x) + c\partial_x u(t,x) = 0, \\ u(0,x) = \varphi(x),\ \varphi \in \mathcal{C}^2, \end{cases} \tag{14}$$

and the D'Alembert solution is a linear combination of them with coefficients equal to $1/2$.

Now, if we only shrink the study to the pure real matrices leading to a system (5) of separated equations, then we have two possible choices:

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{15}$$

and the second pair of matrices given by the same A and $-B$.

Substituting (15) in (5), it reduces to the following system of equations:

$$\begin{cases} \partial_t^\alpha u_1(t,x) - \partial_x u_1(t,x) = 0, \\ \partial_t^\alpha u_2(t,x) + \partial_x u_2(t,x) = 0, \end{cases} \tag{16}$$

where $0<\alpha<1$, and the equations appearing in (13) and (14) are devolved for the limiting case of $\alpha=1$ and $c=1$.

We want to show that the solution $u(t,x)$ of the time fractional diffusion equation (6) is still a linear combination of the solutions $u_1(t,x)$ and $u_2(t,x)$ of (16), for each $0<\alpha<1$ and, therefore, that the relation existing between the Dirac solutions and the D'Alembert expression is extended to the fractional case.

In Ref. 3 the following initial value problem

$$\begin{gathered} ({}^C D_t^\alpha u)(t,x) = \lambda \partial_x u(t,x) \quad (t>0, x \in \mathbb{R};\ 0<\alpha<1), \\ \lim_{|x|\to\infty} u(t,x) = 0, \quad u(0+,x) = g(x), \end{gathered} \tag{17}$$

has been solved and the general solution, expressed in terms of the inverse of its Fourier transform, is given by

$$u(t,x) = u_{g,\lambda}(t,x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} E_{\alpha,1}(-i\lambda k t^\alpha) G(k) e^{-ikx} \mathrm{d}k, \tag{18}$$

where $E_{\alpha,\beta}(z)$ is the biparametric Mittag-Leffler special function.[1] This solution is said to be *localized* due to the property $\lim_{|x|\to\infty} u(t,x)=0$.

On the other hand, the general localized solution of the Cauchy problem for the time fractional diffusion equation,

$$\begin{gathered} ({}^C D_t^{2\alpha} f)(t,x) = \lambda^2 \partial_{xx} f(t,x), \\ \lim_{|x|\to\infty} f(t,x) = 0, \quad f(0+,x) = g(x), \quad [\partial_t f(t,x)]_{t=0} = 0 \quad (t>0, x \in \mathbb{R}), \end{gathered} \tag{19}$$

where $0<\alpha<1$, can be found in Ref. 5 and it reads

$$f(t,x) = f_g(t,x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} E_{2\alpha,1}(-(\lambda k)^2 t^{2\alpha}) G(k) e^{-ikx} \mathrm{d}k. \tag{20}$$

Now, if we apply the duplication formula[1] for the Mittag-Leffler function,

$$E_{2\alpha,1}(z) = \tfrac{1}{2}[E_{\alpha,1}(+z^{1/2}) + E_{\alpha,1}(-z^{1/2})], \tag{21}$$

then we can rewrite (20) as follows:

$$f_g(t,x) = \tfrac{1}{2}[u_{g,-\lambda}(t,x) + u_{g,\lambda}(t,x)], \tag{22}$$

where $u_{g,\lambda}$ is given in (18).

So, we can conclude that the general solution of the Cauchy problem (19) for the time fractional diffusion equation turns out to be a linear combination, with coefficients equals to 1/2, of the two general solutions of the Cauchy problems for the fractional Dirac-type equations represented by (17) and by the problem obtained when λ is replaced by $-\lambda$ in (17).

In particular, the fundamental solution of (19), when $g(x)=\delta(x)$, turns out to be

$$f(t,x) = \frac{1}{2\lambda t^{\alpha}} W\left(-\frac{|x|}{t^{\alpha}\lambda}; -\alpha, 1-\alpha\right) \quad (0<\alpha<1), \tag{23}$$

where $W(z;\alpha,\beta)$ is the Wright special function (Ref. 1, [18.1(27)].

Therefore, if we assume $\lambda=1$ in (19), we obtain

$$f(t,x) = \frac{1}{2t^{\alpha}} W\left(-\frac{|x|}{t^{\alpha}}; -\alpha, 1-\alpha\right) = \frac{1}{2}[u_1(t,x) + u_2(t,x)], \tag{24}$$

where

$$u_1(t,x) = \begin{cases} \dfrac{1}{t^{\alpha}} W\left(\dfrac{x}{t^{\alpha}}; -\alpha, 1-\alpha\right), & x \leqslant 0 \\ 0, & x > 0 \end{cases} \tag{25}$$

and

$$u_2(t,x) = \begin{cases} 0, & x < 0 \\ \dfrac{1}{t^{\alpha}} W\left(-\dfrac{x}{t^{\alpha}}; -\alpha, 1-\alpha\right), & x \geqslant 0 \end{cases} \tag{26}$$

are the functions appearing in (16), fundamental solutions of (17) when $\lambda=1$ and $\lambda=-1$, respectively (see Ref. 3).

III. INVARIANCE WITH RESPECT TO INVERSIONS AND TRANSLATIONS IN TIME AND/OR SPACE

The aim of this section is to establish whether the system (5) turns out to be invariant under inversions and translations in time and/or space, and Galileo transform, and how the nonlocal property of the time fractional differential operator affects these results.

Let us first consider the spatial inversion $P: x' = -x$ of the system (5), and set

$$\psi'(t,x') = S\psi(t,x(x')). \tag{27}$$

We look for a matrix S so that the transformed multicomponent function $\psi'(t,x')$ is still a solution of the system (5), this is:

$$A\partial_t^{\alpha}\psi'(t,x') + B\partial_{x'}\psi'(t,x') = 0, \quad \psi'(t,x') = S\begin{pmatrix} u_1(t,x(x')) \\ u_2(t,x(x')) \end{pmatrix}, \tag{28}$$

where the fractional derivative ∂_t^{α} could be specified in this context either through (7) or (8).

We calculate

$$\partial_{x'}\psi'(t,x') = S\partial_{x'}\psi(t,x(x')) = -S\partial_x\psi(t,x) \tag{29}$$

and this allows us to write:

$$A\partial_t^{\alpha}\psi'(t,x') + B\partial_{x'}\psi'(t,x') = AS\partial_t^{\alpha}\psi(t,x) - BS\partial_x\psi(t,x).$$

Therefore, in order for (28) to be verified, it has to turn out

$$S^{-1}AS\partial_t^\alpha \psi(t,x) - S^{-1}BS\partial_x \psi(t,x) = 0,$$

and, according to (4), when $S=A$, this requirement is fulfilled, being $\psi(t,x)$ solution of (5). Thus, the system of fractional evolution equations (5) is invariant under spatial inversion, as well as the time fractional diffusion equation (6) with respect to this transformation.

Let us now consider the time inversion $T: t^* = -t$ and set

$$\psi^*(t^*,x) = T\psi(t(t^*),x). \tag{30}$$

Then, as for the spatial inversion, we have to find a matrix T such that $\psi^*(t^*,x)$ is solution of the system of equations (5), where now it is necessary to specify the used definition of fractional derivative ∂_t^α.

If we assume the Caputo fractional derivative (8) in (5), then we have

$$A\,{}_a^C D_{t^*}^\alpha \psi^*(t^*,x) + B\partial_x \psi^*(t^*,x) = 0, \quad \psi^*(t^*,x) = T\begin{pmatrix} u_1(t(t^*),x) \\ u_2(t(t^*),x) \end{pmatrix}. \tag{31}$$

It results

$${}_a^C D_{t^*}^\alpha \psi^*(t^*,x) = T(-1)^\alpha\, {}_{-a}^C D_t^\alpha \psi(t,x). \tag{32}$$

and, in particular, when $a=0$:

$${}_0^C D_{t^*}^\alpha \psi^*(t^*,x) = T(-1)^\alpha\, {}_0^C D_t^\alpha \psi(t,x). \tag{33}$$

Therefore, in general, the left-hand side of the equation in (31) takes the form

$$(-1)^\alpha AT\, {}_{-a}^C D_t^\alpha \psi(t,x) + BT\partial_x \psi(t,x),$$

and we only can have invariance of (5), with respect to time inversion, if $a=0$ and the matrix T verifies

$$\begin{cases} (-1)^\alpha AT = TA, \\ BT = TB. \end{cases}$$

The matrix $T=B$ fulfills the above-noted conditions while $(-1)^\alpha = -1$, which means

$$(-1)^\alpha = e^{i(\pi+2n\pi)\alpha} = -1 = e^{i(\pi+2k\pi)},$$

with $n,k \in \{\mathbb{N} \cup \{0\}\}$, and this implies

$$\alpha = \frac{1+2k}{1+2n}, \quad k = 0,1,2,\ldots, \quad n = k+1, k+2, k+3, \ldots,$$

as the hypothesis $0 < \alpha < 1$ has to be preserved.

Some particular values of α, for which the invariance of the system (5) under time inversion holds, are the following:

$$\alpha = \tfrac{1}{3}, \tfrac{1}{5}, \tfrac{1}{7}, \ldots, \tfrac{3}{5}, \tfrac{3}{7}, \tfrac{3}{9}, \ldots, \tfrac{5}{7}, \tfrac{5}{9}, \tfrac{5}{11}, \ldots .$$

Note that the time fractional diffusion equation (6) is invariant under time inversion while $(-1)^{2\alpha} = 1$, which holds and it is well defined for

$$\alpha = \frac{k}{1+2n}, \quad n = 1,2,3,\ldots, \quad k = 1,2,\ldots,2n,$$

this is,

$$\alpha = \tfrac{1}{3}, \tfrac{2}{3}, \tfrac{1}{5}, \tfrac{2}{5}, \tfrac{3}{5}, \tfrac{4}{5}, \tfrac{1}{7}, \tfrac{2}{7}, \ldots, \tfrac{6}{7}, \tfrac{1}{9}, \ldots,$$

in agreement with known results for the classical one-dimensional time diffusion equation ($\alpha = 1/2$).

The invariance properties under time inversion of systems (5) and (6) are a partial characterization of the transition between the parabolic ($\alpha = 1/2$) and hyperbolic ($\alpha = 1$) behaviors.

If we repeat the computations when $\partial t^{\alpha} = {}_{a}^{\mathrm{RL}}D_{t^*}^{\alpha}$ in (5), we obtain the same results so that we can deal in this context with any of the two definitions of fractional derivative without losing generality.

Now, if we consider the space-time inversion $PT: t^* = -t$, $x' = -x$ and we assume

$$\bar{\psi}(t^*, x') = R\psi(t(t^*), x(x')), \tag{34}$$

over the system of equations (5), repeating exactly the same calculations as above the system turns out to be invariant under space-time inversion if we still restrict our study to the case of $a = 0$ in the lower extreme of integration of the fractional derivative and when the matrix R fulfills

$$\begin{cases} (-1)^{\alpha} AR = RA, \\ BR + RB = 0. \end{cases}$$

Therefore it must be distinguished between two cases:

(1) If $(-1)^{\alpha} = -1$ that means

$$\alpha = \frac{1+2k}{1+2n}, \quad k = 0,1,2, \ldots, \quad n = k+1, k+2, k+3, \ldots,$$

then for $R = AB = -BA$ the system (5) is invariant under space-time inversion.

(2) If $(-1)^{\alpha} = 1$, that means

$$\alpha = \frac{2k}{1+2n}, \quad k = 1,2,3, \ldots, \quad n = k, k+1, k+2, \ldots,$$

then the space-time invariance only holds when $R = A$.

The invariance property of system (5) fails, in general, with respect to space-time translation and Galileo transform. In fact, if we operate with a space-time translation on the system (5), assuming the changes of variable $t^* = t + t_0$, $x' = x + x_0$, where t_0 and x_0 are constants, and setting

$$\tilde{\psi}(t^*, x') = V\psi(t(t^*), x(x')), \tag{35}$$

the system turns out to be invariant under this space-time transformation just for the trivial case of $t_0 = 0$ and $V = I$. Actually, for the Caputo derivative, for example, it results

$${}_{a}^{C}D_{t^*}^{\alpha}\tilde{\psi}(t^*, x') = V\,{}_{a-t_0}^{C}D_{t}^{\alpha}\psi(t,x).$$

In the case of the Galileo transform: $x' = x + vt$, $t' = t$, with $v > 0$ constant, we set

$$\hat{\psi}(t, x') = W\psi(t, x(x', t)) \tag{36}$$

in (5). In general, we do not have invariance of system (5) with respect to Galileo transform, as well as it occurs with the classical Dirac equation. Indeed, it is

$${}_{a}^{C}D_{t}^{\alpha}\hat{\psi}(t,x') = W\,{}_{a}^{C}D_{t}^{\alpha}\psi(t,x) - vW\,{}_{a}I_{t}^{1-\alpha}\psi_x(t,x),$$

where I_t^{α} is the Riemann-Liouville fractional integral defined as

$$({}_aI_x^\alpha f)(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-t)^{\alpha-1} f(t) \mathrm{d}t,$$

with $x > a$, $\alpha > 0$, $f \in L^1_{\mathrm{loc}}(a,\infty)$ and $({}_aI_t^0 f)(x) = f(x)$.

Then, the transformed multicomponent function $\hat{\psi}(t,x')$ is still a solution of (5) if the system

$$A\,{}_a^C D_t^\alpha \hat{\psi}(t,x') + B\partial_{x'}\hat{\psi}(t,x') = AW\,{}_a^C D_t^\alpha \psi(t,x) - vAW\,{}_aI_t^{1-\alpha}\psi_x(t,x) + BW\partial_x\psi(t,x) \tag{37}$$

is equal to the zero vector, which implies

$$AW\,{}_aI_t^{1-\alpha}\psi_x(t,x) = 0. \tag{38}$$

Therefore, in general, we do not have invariance of the system (5) with respect to Galileo transform because, in view of the evaluation of the beta integral,[1] valid for all $p > 0$ and $q > 0$ (or $\mathrm{Re}(p) > 0$ and $\mathrm{Re}(q) > 0$), namely

$$B(p,q) := \int_0^1 u^{p-1}(1-u)^{q-1}\mathrm{d}u = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)},$$

the following property for the Riemann-Liouville fractional integral can be proved

$${}_aI_t^\alpha (t-a)^\beta = \frac{\Gamma(\beta+1)}{\Gamma(\beta+\alpha+1)}(t-a)^{\beta+\alpha} \tag{39}$$

when $\beta > -1$. As a consequence, it results ${}_aI_t^{1-\alpha}\psi_x(t,x) = 0$ just in case $\psi_x(t,x) = 0$ for any $0 < \alpha < 1$, which means $\psi(t,x) = \psi(t)$, constant function in x. If this condition is not fulfilled, as occurs in general, then, being $A = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ in our case, we can obtain a restricted class of functions u_1 and u_2 for which (5) is invariant under Galileo transform.

Given $W = \left(\begin{smallmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{smallmatrix}\right)$, the system (38) can be reduced to

$$\begin{cases} w_{21}\,{}_aI_t^{\alpha-1}\dfrac{\partial}{\partial x}u_1(t,x) + w_{22}\,{}_aI_t^{\alpha-1}\dfrac{\partial}{\partial x}u_2(t,x) = 0, \\ w_{11}\,{}_aI_t^{\alpha-1}\dfrac{\partial}{\partial x}u_1(t,x) + w_{12}\,{}_aI_t^{\alpha-1}\dfrac{\partial}{\partial x}u_2(t,x) = 0 \end{cases}$$

and, if $\det(W) = 0$, which means $w_{12}w_{21} - w_{11}w_{22} = 0$, then it has the solution $(\partial/\partial x)u_1(t,x) = -(w_{22}/w_{21})(\partial/\partial x)u_2(t,x)$ which implies $u_1(t,x) = -(w_{22}/w_{21})u_2(t,x) + c(t)$, where $c(t)$ is a constant function in x.

The general noninvariance of the fractional evolution equations under time translation and Galileo transform is due to the nonlocal property of the time fractional derivative and it is in contrast with the invariance results holding for the Dirac equation, with respect to the time translation, as a fundamental requirement to be the relativity principle verified.[19]

IV. A CONSERVED QUANTITY: THE FRACTIONAL HAMILTONIAN

The invalidity of the invariance of the fractional Dirac-type system (5) under time translation does not prevent it from possessing a fractional conserved quantity, analogous to the Hamiltonian for the classical Dirac system.

It is well known (see, for example, Ref. 19) that the Lagrangian density for the classical Dirac equation obtained from (5) when $\alpha = 1$ is given by

$$\mathcal{L}(t,x) = \bar{\psi}A\partial_t\psi + \bar{\psi}B\partial_x\psi,$$

with $\psi = \psi(t,x) = (u_1(t,x), u_2(t,x))^T$, $\bar{\psi} = \bar{\psi}(t,x) = \psi^+ A$, and $\psi^+ = \psi^+(t,x) = (u_1^*(t,x), u_2^*(t,x))$, complex conjugate of ψ that verifies the conjugated equation of (5) with $\alpha = 1$:

$$\partial_t \psi^+ A^+ + \partial_x \psi^+ B^+ = 0.$$

Therefore, the Hamiltonian density will be

$$\mathcal{H}(t,x) = \frac{\partial \mathcal{L}(t,x)}{\partial(\partial_t \psi)} \partial_t \psi - \mathcal{L}(t,x) = \bar{\psi} A \partial_t \psi - \mathcal{L}(t,x) = -\psi^+ C \partial_x \psi, \tag{40}$$

with $C=AB=-BA$, the Hamiltonian

$$H(t,x) = \int_{-\infty}^{+\infty} \mathcal{H}(t,x)\mathrm{d}x = -\int_{-\infty}^{+\infty} \psi^+ C \partial_x \psi \mathrm{d}x, \tag{41}$$

and, its time derivative,

$$\frac{\mathrm{d}}{\mathrm{d}t} H(t,x) = \int_{-\infty}^{+\infty} \partial_x [\psi^+ \partial_x \psi] \mathrm{d}x, \tag{42}$$

provided that we restrict ourselves to the pure real matrices A and B so that the equivalence $\partial_t \psi^+ = -\partial_x \psi^+ C$ is verified. In this case, if we assume, for example, the initial condition $\psi^+ \partial_x \psi \to 0$ when $|x| \to \infty$, we can conclude that there exists a conserved quantity associated with Eq. (5) with $\alpha=1$, given by the Hamiltonian (41).

In what follows, we want to show that, as well as we did earlier, it is possible to find a conserved quantity associated with the system of fractional Dirac-type equations (5) for general $0<\alpha<1$, even if it does not present invariance with respect to time translation.

We start defining, by analogy with the classical Dirac case, a formal "fractional Lagrangian density" related to (5),

$$\mathcal{L}^\alpha(t,x) = \bar{\psi} A \partial_t^\alpha \psi + \bar{\psi} B \partial_x \psi, \tag{43}$$

and a formal "fractional Hamiltonian density,"

$$\mathcal{H}_\alpha(t,x) = \frac{\partial \mathcal{L}^\alpha(t,x)}{\partial(\partial_t^\alpha \psi)} \partial_t^\alpha \psi - \mathcal{L}^\alpha(t,x) = \bar{\psi} A \partial_t^\alpha \psi - \mathcal{L}^\alpha(t,x) = -\psi^+ C \partial_x \psi. \tag{44}$$

The final expression in (44) is equivalent to (40) and can be simplified observing that, A and B being pure real matrices, if ψ is a solution of (5), then also ψ^+ has to solve it, the reason why a pure real solution of (5) can always be found. Therefore, we will assume that ψ is a pure real solution of (5) and this allows us to write the "fractional Hamiltonian" as

$$H_\alpha(t,x) = \int_{-\infty}^{+\infty} \mathcal{H}_\alpha(t,x)\mathrm{d}x = -\int_{-\infty}^{+\infty} \psi^T C \partial_x \psi \, \mathrm{d}x \tag{45}$$

and, consequently,

$$\frac{\mathrm{d}}{\mathrm{d}t} H_\alpha(t,x) = -\int_{-\infty}^{+\infty} [\partial_t \psi^T C \partial_x \psi + \psi^T C \partial_x \partial_t \psi] \mathrm{d}x = -\int_{-\infty}^{+\infty} \partial_x [\psi^T C \partial_t \psi] \mathrm{d}x. \tag{46}$$

The equivalence $\partial_t \psi^T C \partial_x \psi = \partial_x \psi^T C \partial_t \psi$, due to the fact that the matrix $C=AB$, with pure real A and B, can only be of two types:

$$C_1 = \begin{pmatrix} c_{11} & 0 \\ 0 & -c_{11} \end{pmatrix}, \quad C_2 = \begin{pmatrix} 0 & c_{12} \\ c_{12} & 0 \end{pmatrix},$$

where c_{11} and c_{12} take the values ± 1.

At this point it is necessary to specify the definition of the fractional derivative in use.

When $0<\alpha<1$ the Riemann-Liouville fractional derivative $\partial_t^\alpha = {}^{\mathrm{RL}}D_t^\alpha$, according to (9), fulfills the following identity:

$$({}^{\mathrm{RL}}D_t^\alpha \psi)(t,x) = (I_t^{1-\alpha}\partial_t\psi)(t,x) + \frac{t^{-\alpha}}{\Gamma(1-\alpha)}\psi(0,x), \tag{47}$$

being $({}^{\mathrm{RL}}D_t^\alpha \psi(0,x))(t,x) = t^{-\alpha}/[\Gamma(1-\alpha)]\psi(0,x)$ and $({}^{C}D_t^\alpha \psi)(t,x) = (I_t^{1-\alpha}\partial_t\psi)(t,x)$ by definition (8).

Now, if we introduce the Riemann-Liouville fractional derivative in (5), using the fact that this derivative is the left inverse operator of the Riemann-Liouville fractional integral, we can write

$$(\partial_t\psi)(t,x) = -C\partial_x({}^{\mathrm{RL}}D_t^{1-\alpha}\psi)(t,x) - A\left({}^{\mathrm{RL}}D_t^{1-\alpha}\frac{t^{-\alpha}}{\Gamma(1-\alpha)}\psi(0,x)\right)(t,x) = -C\partial_x({}^{\mathrm{RL}}D_t^{1-\alpha}\psi)(t,x)$$
$$-A\partial_t\psi(0,x) = -C\partial_x({}^{\mathrm{RL}}D_t^{1-\alpha}\psi)(t,x). \tag{48}$$

In a similar straightforward way it can be proved that result (48) holds exactly the same when the Caputo derivative appears in (5).

Therefore, when $\alpha=1/2$ both derivatives verify

$$(\partial_t\psi)(t,x) = C^2(\partial_x^2\psi)(t,x) = (\partial_x^2\psi)(t,x). \tag{49}$$

In agreement with (48), the expression for the Hamiltonian time derivative (46) takes the form:

$$\frac{\mathrm{d}}{\mathrm{d}t}H_\alpha(t,x) = -\int_{-\infty}^{+\infty}\partial_x[\psi^T C\partial_t\psi]\mathrm{d}x = \int_{-\infty}^{+\infty}\partial_x[\psi^T\partial_x{}^{\mathrm{RL}}D_t^{1-\alpha}\psi], \tag{50}$$

when $0<\alpha<1$ and, in particular,

$$\frac{\mathrm{d}}{\mathrm{d}t}H_{1/2}(t,x) = \int_{-\infty}^{+\infty} -\partial_x[\psi^T C\partial_x^2\psi]\mathrm{d}x, \tag{51}$$

for $\alpha=1/2$, when the fractional derivative is either of the Riemann-Liouville or of the Caputo type.

Therefore, we can conclude that, when $0<\alpha<1$, if the condition

$$\frac{\mathrm{d}}{\mathrm{d}t}H_\alpha(t,x) = \int_{-\infty}^{+\infty}\partial_x[\psi^T\partial_x{}^{\mathrm{RL}}D_t^{1-\alpha}\psi]\mathrm{d}x = [u_1\partial_x{}^{\mathrm{RL}}D_t^{1-\alpha}u_1 + u_2\partial_x{}^{\mathrm{RL}}D_t^{1-\alpha}u_2]|_{x=-\infty}^{x=+\infty} = 0, \tag{52}$$

is fulfilled, then a conserved quantity exists associated with Eq. (5) and it is given by the fractional Hamiltonian (45).

For the particular case of $\alpha=1/2$, we deduce from (51) an alternative condition, equivalent to (52), to provide the existence of the conserved quantity $H_{1/2}(t,x)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}H_{1/2} = \int_{-\infty}^{+\infty} -\partial_x[\psi^T C\partial_x^2\psi]\mathrm{d}x = -\psi^T C\partial_x^2\psi|_{x=-\infty}^{x=+\infty} = 0,$$

which means

$$(u_1\partial_x^2u_1 - u_2\partial_x^2u_2)|_{x=-\infty}^{x=+\infty} = 0, \tag{53}$$

when $C=C_1$, and

$$(u_1\partial_x^2u_2 + u_2\partial_x^2u_1)|_{x=-\infty}^{x=+\infty} = 0, \tag{54}$$

when $C=C_2$. Both conditions (53) and (54) come true when, for example, $|u_h|\to 0$ and $\partial_x^2u_h$ is bounded when $|x|\to\infty$, for $h=1,2$.

We can conclude this section recalling some results obtained in Ref. 3

If we consider the system of fractional equations of Dirac-type (5) when $\partial_t^{\alpha} = {}^{C}D_t^{\alpha}$, when A and B are given by (15) so that it turns out to be

$$C = C_1 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},$$

and we complete (5) with the initial conditions

$$\lim_{|x|\to\infty} \psi(t,x) = 0, \quad \psi(0+,x) = \delta(x),$$

then the localized fundamental solutions are given by (25) and (26).

In Ref. 6 the asymptotic behavior of the Wright function $W(z;\alpha,\beta)$, for the case of $\alpha=-\nu$ and $\beta=1-\nu$, has been studied. In particular, if the function $M(z;\nu)=W(-z;-\nu,1-\nu)$ is introduced, when the argument $z=r>0$ is real and positive and $r\to+\infty$, it holds

$$M\left(\frac{r}{\nu};\nu\right) \sim a(\nu) r^{(\nu-1/2)/(1-\nu)} \exp[-b(\nu) r^{1/(1-\nu)}], \tag{55}$$

where $a(\nu)=1/\sqrt{2\pi(1-\nu)}$, $b(\nu)=(1-\nu)/\nu$.

This implies an asymptotic exponential decay of our solutions u_1 and u_2, and, consequently, that $|u_h|\to 0$ when $|x|\to\infty$ for $h=1,2$.

In order to ensure the existence of the conserved quantity (45) when $0<\alpha<1$, we also have to analyze the asymptotic behavior of $\partial_x {}^{\mathrm{RL}}D_t^{1-x}u_h$ for $h=1,2$.

It turns out to be

$$\begin{aligned} {}^{\mathrm{RL}}D_t^{1-\alpha}\left(\frac{1}{t^{\alpha}}W\left(-\frac{|x|}{t^{\alpha}};-\alpha,1-\alpha\right)\right) &= \partial_t I_t^{\alpha}\left[\sum_{k=0}^{+\infty}\frac{-(|x|)^k t^{-\alpha k-\alpha}}{k!\Gamma(-\alpha k+1-\alpha)}\right] = \partial_t\left[\sum_{k=0}^{+\infty}\frac{-(|x|)^k t^{-\alpha k}}{k!\Gamma(1-\alpha k)}\right] \\ &= \left[\sum_{k=0}^{+\infty}\frac{-(|x|)^k t^{-\alpha k-1}}{k!\Gamma(-\alpha k)}\right] = \frac{1}{t}W\left(-\frac{|x|}{t^{\alpha}};-\alpha,0\right) \\ &= \frac{\alpha|x|}{t^{\alpha+1}}W\left(-\frac{|x|}{t^{\alpha}};-\alpha,1-\alpha\right) \end{aligned}$$

if we use the property $W(-z;-\nu,1-\nu)=(1/\nu z)W(-z;-\nu,0)$; therefore, (55) implies that ${}^{\mathrm{RL}}D_t^{1-\alpha}u_h$, as well as $\partial_x {}^{\mathrm{RL}}D_t^{1-\alpha}u_h$, will also decay exponentially when $|x|\to\infty$ for $h=1,2$.

V. CONCLUSIONS

We have treated a generalization of the classical free Dirac equations, namely the *fractional evolution equations of Dirac-type*. For the localized solutions of these equations we have derived their relation with the corresponding solution of the *fractional diffusion equation*, showing how the latter turns out to be a linear combination of the formers, similarly to the D'Alembert solution of the classical wave equation is a linear combination of the solutions of the first-order equations derived from the decomposition of the second-order wave operator into its corresponding square-root operators.

Following the analogy existing between the fractional evolution equations and the classical Dirac equation, we have studied their internal symmetries with respect to certain transformations in space and/or time. The system of fractional Dirac-type equations is invariant under spatial inversion for each $0<\alpha<1$, whereas it possesses invariance under time inversion only for certain values of the fractional index α, so enclosing the hyperbolic behavior of the classical Dirac equation or of the time fractional diffusion equation (6) when $\frac{1}{2}<\alpha\leqslant 1$ (including the classical wave equation corresponding to $\alpha=1$), and the parabolic one of the time fractional diffusion equation (6) when $0<\alpha\leqslant\frac{1}{2}$ (including the classical diffusion equation corresponding to $\alpha=1/2$).

In keeping with the joint space-time inversion, a range of validity for the invariance is located, still depending on the index α, but wilder than the one corresponding to time inversion only.

The system proves to be never invariant under time translation and Galileo transform due to the nonlocal property of the time fractional derivative. This lack of invariance of the fractional evolution equations under time translation is in contrast to the invariance results holding for the classical Dirac equation, with respect to the same transformation, as a fundamental requirement to be the relativity principle verified, but does not prevent the fractional Dirac-type system from possessing a fractional conserved quantity, analogous to the Hamiltonian for the classical Dirac system.

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Uniqueness for Dissipative Schrödinger-Poisson Systems

H. Neidhardt[a] and J. Rehberg[b]
Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstrasse 39, D-10117 Berlin, Germany

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The paper is devoted to the dissipative Schrödinger-Poisson system. We indicate conditions in terms of the Schrödinger-Poisson data which guarantee that there is a unique solution. Moreover, it is shown that if the system is sufficiently small shrunken, then it always admits a unique solution. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2121187]

I. INTRODUCTION

Schrödinger-Poisson systems describe for instance the nonlinear interaction between an electric field and charged carriers (electrons and holes) in a semiconductor device, within this electric field. We investigate a model which intrinsically allows—in contrast to self-adjoint Schrödinger-Poisson systems, see Refs. 8, 19–21, 27, and 28—an interaction with the environment. In particular, in the open quantum system under consideration here (see also Refs. 10 and 29) a nontrivial current is possible. In Ref. 20 non-self-adjoint boundary conditions for the Schrödinger operators (3) were proposed which are induced by a potential flow acting on the boundary of the domain Ω which is occupied by the quantum system. The spectral theory for the associated non-self-adjoint Schrödinger-type operators has been developed in Ref. 16. For a one-dimensional device this ansatz—called dissipative Schrödinger-Poisson system—was analyzed in detail in Refs. 2, 16–18. While the existence of a solution was shown in Ref. 2 it is the aim of this paper to prove uniqueness of the solution under certain conditions. This result should be interpreted from the physical point of view as follows: it is known that uniqueness cannot be expected in general because there are physical situations where the existence of several solutions explains well observed hysteresis phenomena[14,30]. However, if the parameters of the system are chosen in accordance with our uniqueness condition of Theorem 5.4, then hysteresis phenomena cannot occur. In particular, hysteresis is absent if the device is sufficiently small, cf. Theorem 5.6. By the way, this situation is quite parallel to that of self-adjoint Schrödinger-Poisson systems with exchange correlation potentials, see Ref. 31.

In the form considered in this paper a Schrödinger-Poisson system can be regarded as a nonlinear Poisson equation

$$-\nabla\cdot(\epsilon\nabla\varphi) = C + \mathcal{N}^+(V_0^+ + \varphi) - \mathcal{N}^-(V_0^- - \varphi) \tag{1}$$

on an interval (a,b) of the real axis, combined with Dirichlet boundary conditions

$$\varphi(a) = \varphi_a, \quad \varphi(b) = \varphi_b. \tag{2}$$

By ϵ and C the dielectric permittivity and the doping profile are denoted, respectively, while $V_0^\pm$ are fixed potentials for a given device. The particle densities $\mathcal{N}^\pm(V)$ are associated to one-electron Hamiltonians in effective mass approximation (Ben-Daniel-Duke form)

[a]Electronic mail: neidhard@wias-berlin.de
[b]Electronic mail: rehberg@wias-berlin.de

$$H^{\pm}[V]\psi = -\frac{1}{2}\nabla\cdot\left(\frac{1}{m^{\pm}}\nabla\psi\right) + V\psi, \tag{3}$$

acting on $L^2(a,b)$ and supplemented by dissipative boundary conditions of the form

$$\frac{1}{2m^{\pm}(a)}\psi'(a) = -\kappa_a^{\pm}\psi(a), \quad \frac{1}{2m^{\pm}(b)}\psi'(b) = \kappa_b^{\pm}\psi(b), \tag{4}$$

$\kappa_a^{\pm}, \kappa_b^{\pm} \in \mathbb{C}_+ := \{z \in \mathbb{C} : \Im\mathrm{m}(z) > 0\}$. By $m^{\pm}$ the position dependent effective masses of holes and electrons are denoted (Planck's constant $\hbar$ and the elementary charge q are scaled to one).

The collective behavior of holes and electrons [and, hence, the particle densities $\mathcal{N}^{\pm}(V)$] is described by density operators $\varrho^{\pm}[V]$ which are given in case of closed quantum systems by equilibrium states, i.e., non-negative trace class operators of the form

$$\varrho^{\pm}[V] = f^{\pm}(H^{\pm}[V]).$$

In the case of open quantum systems, which is of interest here, the density operators are obtained as follows: one finds—by an explicit construction, see Ref. 17—a so-called (self-adjoint) dilation $K^{\pm}[V]$ of $H^{\pm}[V]$ on a larger Hilbert space $\supseteq L^2(a,b)$. As density operators now serve certain non-negative self-adjoint operators $\varrho[V]$, commuting with $K^{\pm}[V]$ and enjoying the property that their product with the orthogonal projection $P_{L^2(a,b)}$ from the dilation space onto the original Hilbert space $L^2(a,b)$ is of trace class. [In fact, these operators $\varrho[V]$ are induced by density matrices $\rho^{\pm} \in L^{\infty}(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ with certain decaying properties.] Thus, the definition

$$\int_{\omega} \mathrm{d}x \mathcal{N}^{\pm}(V)(x) := \mathrm{tr}(P_{L^2(a,b)}^{\mathfrak{K}} \varrho^{\pm}[V]\chi_{\omega}), \quad \omega \text{ any Borel subset of } (a,b)$$

gives rise to the carrier density operators $\mathcal{N}^{\pm}$ which assigns to each electrostatic potential $V \in L^{\infty}_{\mathbb{R}}(a,b)$ carrier densities from $L^1_{\mathbb{R}}(a,b)$, see Refs. 2, 3, and 18.

The main technical tool for our uniqueness proof is to show that the carrier density operators do depend in fact locally Lipschitz continuous on the potentials—and not only continuously as proven in Ref. 3. The proof of this property relies on the theory of Kato-smooth operators, see Refs. 22 and 23. We show that the orthogonal projection $P_{L^2(a,b)}$ is Kato-smooth with respect to the minimal self-adjoint dilations $K^{\pm}[V]$ and we calculate their smoothness constants, which allows us to compute the local Lipschitz constants for the carrier density operators. For this purpose we have to strengthen the assumptions on the effective masses $m^{\pm}$. In Ref. 3 it was assumed that $m^{\pm} + (1/m^{\pm}) \in L^{\infty}_{\mathbb{R}}(\Omega)$. In addition, we demand now that $m^{\pm}$ has a finite total variation. This admits countably many discontinuities, what is sufficient for applications to heterogeneous material compositions. At the end, the solution becomes unique, if the local Lipschitz constants of the carrier density operators are small enough.

It turns out that uniqueness always takes place if we shrink the dissipative Schrödinger-Poisson system to a sufficiently small subdevice $\Omega' \subseteq \Omega$. That means, we consider the same boundary conditions (4) and (2), the same density matrices $\rho^{\pm}$ but replace the mass functions $m^{\pm}$ by $m^{\pm} \restriction \Omega'$, the potentials $V_0^{\pm}$ by $V_0^{\pm} \restriction \Omega'$, the dielectric permittivity ϵ by $\epsilon \restriction \Omega'$ and the doping profile C by $C \restriction \Omega'$. If Ω' will be sufficiently small, then the shrunken Schrödinger-Poisson systems admits a unique solution.

This has implications for dissipative hybrid models considered in Ref. 4 which use a mixed description by a drift-diffusion model and a dissipative Schrödinger-Poisson system. In more detail, one divides the device $\Delta = [a_0, b_0]$ into two regions $\Omega_c = (a_0, a) \cup (b, b_0)$ and $\Omega_q = (a,b)$, which are called "classical zone" and "quantum zone," respectively. On the "classical zone" Ω_c, which is disconnected, one uses a classical drift diffusion description, cf. Refs. 11, 25, and 32, while on the "quantum zone" Ω_q a dissipative Schrödinger-Poisson system is considered. The length $|\Omega_q|$ of the quantum zone Ω_q is crucial for the hybrid model. Indeed, if Ω_q is very large, then we have nearly a quantum description of the device which increases the costs of the numeri-

cal treatment of the model. If the quantum zone Ω_q is very small, then by the above-noted result it can happen that the hybrid model has only one solution in contradiction to a pure classical description which usually allows several solutions. This shows us that one has to very carefully choose the quantum zone in hybrid models.

The paper is organized as follows. In Sec. II we introduce constants repeatedly used in the following. If the Schrödinger-Poisson data are fixed, then the constants are fixed. The dissipative Schrödinger-type operator is introduced and in detail investigated in Sec. III. Crucial are the notions of the characteristic function, see Sec. III C, and the phase shift, see Sec. III D. The self-adjoint dilations and Lax-Phillips scattering theory are recalled in Secs. III F and III G. The carrier density operator is defined in Sec. IV. Its local Lipschitz continuity is verified in Sec. IV B. The dissipative Schrödinger-Poisson system is considered in Sec. V. The existence proof is sketched in Sec. V B, the uniqueness is proven in Sec. V C, the uniqueness for a sufficiently small shrunken Schrödinger-Poisson system is established in Sec. V D. We end with some remarks in Sec. VI.

II. NOTATION, ASSUMPTIONS, AND CONSTANTS

By $L^p(\Omega,X,m)$, $1\leqslant p<\infty$, $\Omega=(a,b)$, we denote the space of $\mathfrak{m}$-measurable and p-integrable functions over Ω with values in a Banach space X. By $L^\infty(\Omega,X,\mathfrak{m})$ the space of essentially bounded functions is denoted. If $\mathfrak{m}$ is the Lebesgue measure, then we write $L^p(\Omega)=L^p(\Omega,\mathbb{C},\mathfrak{m})$ and $L^p_{\mathbb{R}}(\Omega):=L^p(\Omega,\mathbb{R},\mathfrak{m})$, $1\leqslant p\leqslant\infty$. The Lebesgue measure of a set is denoted by $|\cdot|$.

The norm of a Banach or Hilbert space X is indicated by $\|\cdot\|_X$ or simply by $\|\cdot\|$, the scalar product of a Hilbert space X by $(\cdot,\cdot)_X$ or simply by $(\cdot,\cdot)$ where the first argument is the linear one. The dual space is indicated by X^*. By $\mathcal{B}(X,Y)$ the space of all linear bounded operators from the Banach space X to the Banach space Y is denoted with norm $\|\cdot\|_{\mathcal{B}(X,Y)}$. If $X=Y$, then $\mathcal{B}(X,X)=\mathcal{B}(X)$ and $\|\cdot\|_{\mathcal{B}(X,Y)}=\|\cdot\|_{\mathcal{B}(X)}$. If X is a Hilbert spaces, then $\mathcal{B}_1(X)$ and $\mathcal{B}_2(X)$ denote the spaces of trace class and Hilbert-Schmidt operators, respectively. For a densely defined linear operator $A:X\to Y$ we denote by A^*, $\mathrm{spec}(A)$ and $\mathrm{res}(A)$ its adjoint, spectrum, and resolvent set, respectively. We write $X[V]$ if we have in mind a parameter dependence on V and $X(V)$ if a functional dependence on V is considered. Of course, it is quite possible that a parameter dependence becomes a functional one and vice versa.

Furthermore, we denote by $W^{1,2}(\Omega)$ the usual Sobolev spaces of complex-valued functions on Ω. The subspace of elements with homogeneous Dirichlet boundary conditions at the end points of the interval $\Omega\subseteq\mathbb{R}$ is denoted by $W^{1,2}_0(\Omega)$. Its dual with respect to the L^2-pairing is denoted by $W^{-1,2}_0(\Omega)=(W^{1,2}_0(\Omega))^*$. If we have in mind only real-valued functions, then we write $W^{1,2}_{\mathbb{R}}(\Omega)$ and $W^{1,2}_{0,\mathbb{R}}(\Omega)$.

With respect to the Schrödinger-type operators we made the following assumptions.

Assumptions 2.1 (Schrödinger assumptions):

(Q_1) There are constants $\underline{m}^\pm>0$ and $\bar{m}^\pm>0$ such that $\underline{m}^\pm\leqslant m^\pm(x)\leqslant\bar{m}^\pm$ for $x\in\Omega$.

($Q2$) $\kappa^\pm_a,\kappa^\pm_b\in\mathbb{C}_+=\{z\in\mathbb{C}:\Im\mathrm{m}(z)>0\}$.

($Q3$) $V^\pm_0\in L^\infty_{\mathbb{R}}(\Omega)$.

($Q4$) The matrix valued-functions $\rho^\pm(\cdot)\in L^\infty(\mathbb{R},\mathcal{B}(\mathbb{C}^2))$ obey $0\leqslant\rho^\pm(\lambda)=\rho^\pm(\lambda)^*$. There are real, continuous differentiable, even functions $g^\pm(\cdot):\mathbb{R}\to\mathbb{R}_+$ such that

$$0\leqslant\rho^\pm(\lambda)\leqslant g^\pm(\lambda)I_{\mathbb{C}^2},\quad \lambda\in\mathbb{R}, \tag{5}$$

$$\mathrm{sign}(\lambda)\frac{\mathrm{d}}{\mathrm{d}\lambda}g^\pm(\lambda)\leqslant 0,\quad \lambda\in\mathbb{R}, \tag{6}$$

$$\int_0^\infty \mathrm{d}\lambda\frac{g^\pm(\lambda)}{\sqrt{\lambda}}<\infty, \tag{7}$$

and

$$\left|\frac{\mathrm{d}}{\mathrm{d}\lambda}g^{\pm}(\lambda)\right| \leqslant {}^{\pm}g^{\pm}(\lambda), \quad \lambda \in \mathbb{R}, \tag{8}$$

where ${}^{\pm}$ are given real constants. In particular, the functions

$$g^{\pm}(\lambda) = {}^{\pm}_{0}(1+\lambda^2)^{-1/2}, \quad \lambda \in \mathbb{R},$$

used in Ref. 2 satisfy assumptions (6)–(8) with $\mathfrak{c}^{\pm}=\mathfrak{c}^{\pm}_{0}$.

The parameter set $:=\{m^{\pm},\kappa^{\pm}_{a},\kappa^{\pm}_{b},V^{\pm}_{0},\rho^{\pm}\}$ is called the Schrödinger data of the device Ω. The Schrödinger data are fixed in the following.

With respect to the Poisson equation we made the following assumptions.

Assumptions 2.2 (Poisson assumptions):

($P1$) The doping profile C is from $W^{-1,2}_{0}(\Omega)$.

($P2$) The dielectric permittivity ϵ is positive and satisfies $\epsilon+(1/\epsilon)\in L^{\infty}_{\mathbb{R}}(\Omega)$.

The quadruple $:=\{C,\epsilon,\varphi_a,\varphi_b\}$ is called the Poisson data of the device Ω which are also fixed through the paper. The union $:= \cup$ is called the Schrödinger-Poisson data of the device Ω.

For the convenience of the reader we collect here important constants which are composed of the Schrödinger-Poisson data and which are needed in the following. We set

$$B^{\pm}_{0} := 2g^{\pm}(0) + \frac{1}{2\pi}\sqrt{|\Omega|\bar{m}^{\pm}}\int_{0}^{\infty}\mathrm{d}\lambda\frac{g^{\pm}(\lambda)}{\sqrt{\lambda}} \tag{9}$$

and

$$B^{\pm}_{1} := \frac{1}{\pi}g(0)\sqrt{|\Omega|\bar{m}^{\pm}}. \tag{10}$$

We note that the quantities $B^{\pm}_{0}$ and $B^{\pm}_{1}$ depend only on the Schrödinger data and on the length $|\Omega|$ of the device.

The embedding operators from $W^{1,2}_{0}(\Omega)$ into $L^{\infty}(\Omega)$ and $L^{1}(\Omega)$ into $W^{-1,2}_{0}(\Omega)$ are denoted by E_{∞} and E_1, respectively. We note that $E_1=E^{*}_{\infty}\restriction L^{1}(\Omega)$. Their norms are equal and are denoted by ε_1 in the sequel. A straightforward computation shows that $\varepsilon_1\leqslant\sqrt{|\Omega|}$. Let $\hat{\varphi}$ be the function

$$\Omega \ni x \to \frac{1}{\displaystyle\int_{a}^{b}\mathrm{d}t\frac{1}{\epsilon(t)}}\left\{\varphi_a\int_{a}^{x}\mathrm{d}t\frac{1}{\epsilon(t)}+\varphi_b\int_{x}^{b}\mathrm{d}t\frac{1}{\epsilon(t)}\right\}. \tag{11}$$

Clearly, $\hat{\varphi}\in W^{1,2}(\Omega)\hookrightarrow L^{\infty}(\Omega)$. We set

$$D_0 := \varepsilon_1\|1/\epsilon\|_{L^{\infty}}\sqrt{1+|\Omega|}\{\|C\|_{W^{-1,2}_{0}}+\varepsilon_1(B^{+}_{0}+B^{-}_{0}+B^{+}_{1}\sqrt{\|V^{+}_{0}+\hat{\varphi}\|_{L^{\infty}}}+B^{-}_{1}\sqrt{\|V^{-}_{0}-\hat{\varphi}\|_{L^{\infty}}})\} \tag{12}$$

and

$$D_1 := \varepsilon^{2}_{1}\|1/\epsilon\|_{L^{\infty}}\sqrt{1+|\Omega|}(B^{+}_{1}+B^{-}_{1}). \tag{13}$$

Using D_0 and D_1 we introduce the radii

$$r_0 := \frac{1}{2}(D_1+\sqrt{D^{2}_{1}+4D_0}) \tag{14}$$

and

$$r_1^{\pm} := \|V_0^{\pm} + \hat{\varphi}\|_{L^\infty} + r_0. \tag{15}$$

If $h:[a,b]\to\mathbb{R}$ is a function of finite total variation and $x,y\in[a,b]$, then the total variation of $h|_{[x,y]}$ is denoted by $\mathsf{V}_x^y h$. If $1/m^{\pm}$ has a finite total variation, then we set

$$^{\pm} := \sqrt{\bar{m}^{\pm}} \exp\left\{ \frac{\bar{m}^{\pm}}{2} \mathsf{V}_a^b \frac{1}{m^{\pm}} \right\}. \tag{16}$$

Next we introduce the functions

$$R_j^{\pm}(y) := \quad ^{\pm}\left(1 + |\kappa_j^{\pm}| \sqrt{\frac{2}{\underline{m}^{\pm}}} \right) \exp\left\{ y|\Omega|(\quad ^{\pm})^2 \sqrt{\frac{2}{\underline{m}^{\pm}}} \right\} \tag{17}$$

for $y\geqslant 0$ and $j=a,b$. Further we set

$$L^{\pm}(y) := \sqrt{\frac{2}{\pi}} \left\{ \frac{R_a^{\pm}[2y+2+\gamma_0^{\pm}]^2}{(\alpha_a^{\pm})^2} + \frac{R_b^{\pm}[2y+2+\gamma_0^{\pm}]^2}{(\alpha_b^{\pm})^2} \right\}^{1/2} \tag{18}$$

for $y\geqslant 0$ where the representation

$$\kappa_a^{\pm} = q_a^{\pm} + i\frac{(\alpha_a^{\pm})^2}{2}, \quad \kappa_b^{\pm} = q_b^{\pm} + i\frac{(\alpha_b^{\pm})^2}{2} \tag{19}$$

is used. The constants $\gamma_0^{\pm}$ are given by

$$\gamma_0^{\pm} := 2\bar{m}^{\pm}(\quad ^{\pm})^2 \left\{ \frac{1}{2} + \frac{1}{^{\pm}|\Omega|\bar{m}^{\pm}} + \sqrt{\frac{1}{4} + \frac{1}{^{\pm}|\Omega|\bar{m}^{\pm}}} \right\}, \tag{20}$$

where

$$^{\pm} := \max\{0, q_a^{\pm}, q_b^{\pm}\}. \tag{21}$$

We define

$$^{\pm}(y) = \sqrt{B_0^{\pm} + B_1^{\pm}\sqrt{y}}, \quad y\geqslant 0. \tag{22}$$

and

$$^{\pm}(x,y) := \ ^{\pm}(\quad ^{\pm}(x) + \quad ^{\pm}(y))^2 + 4\pi|\Omega|L^{\pm}(x)L^{\pm}(y) \quad ^{\pm}(x) \quad ^{\pm}(y), \tag{23}$$

for $x,y\geqslant 0$. Finally, we introduce the constant

$$:= \quad ^{+}(r_1^{+}, r_1^{+}) + \quad ^{-}(r_1^{-}, r_1^{-}). \tag{24}$$

and we set

$$:= \varepsilon_1^2 \|1/\epsilon\|_{L^\infty} \sqrt{1+|\Omega|} \quad . \tag{25}$$

We note again that the introduced constants (9)–(25) depend only on the Schrödinger-Poisson data which means that they are fixed for fixed Schrödinger-Poisson data.

III. SCHRÖDINGER-TYPE OPERATORS

Since it is unimportant in the following whether we have to do with electrons or with holes we admit the superscript ± in this section. Further, throughout we assume that Schrödinger data $=\{m,\kappa_a,\kappa_b,V_0,\rho\}$ satisfy the Schrödinger assumptions mutatis mutandis.

A. Definitions

Following the suggestion of Refs. 20 and 21 we consider the non-self-adjoint Schrödinger-type operator $H[V]$ on the Hilbert space defined by

$$\mathrm{dom}(H[\kappa_a,\kappa_b,V]) = \left\{ \begin{array}{c} \\ f \in W^{1,2}: \\ \\ \end{array} \begin{array}{c} \dfrac{1}{m(x)} f'(x) \in W^{1,2}(\Omega), \\ \dfrac{1}{2m(a)} f'(a) = -\kappa_a f(a), \\ \dfrac{1}{2m(b)} f'(b) = \kappa_b f(b) \end{array} \right\}$$

and

$$(H[\kappa_a,\kappa_b,V]g)(x) = (l[V]g)(x), \quad g \in \mathrm{dom}(H[\kappa_a,\kappa_b,V]),$$

where

$$(l[V]g)(x) := -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{m(x)}\frac{\mathrm{d}}{\mathrm{d}x}g(x) + V(x)g(x),$$

cf. Refs. 16 and 17, where $V \in L^\infty_{\mathbb{R}}(\Omega)$ and $\kappa_a, \kappa_b \in \overline{\mathbb{C}_+} := \{z \in \mathbb{C}: \Im\mathrm{m}(z) \geqslant 0\}$, are called the boundary coefficients. The operator $H[\kappa_a,\kappa_b,V]$ is maximal dissipative if either $\kappa_a \in \mathbb{C}_+$ or $\kappa_b \in \mathbb{C}_+$. In both cases the operator is completely non-self-adjoint, see Ref. 16. In the following we consider the case $\kappa_a, \kappa_b \in \mathbb{C}_+$. In this case we usually write $H[V]$ instead of $H[\kappa_a,\kappa_b,V]$. The spectrum of $H[V]$ consists of isolated eigenvalues in the lower half-plane with the only accumulation point at infinity, i.e., $\mathrm{spec}\,(H[V]) \subseteq \overline{\mathbb{C}_-} := \{z \in \mathbb{C}: \Im\mathrm{m}(z) \leqslant 0\}$. Since the operator $H[V]$ is completely non-self-adjoint, its eigenvalues are non-real.

Besides the operator $H[V]$ we consider the operator $H_{\mathfrak{R}}[V] := H[q_a,q_b,V]$, $V \in L^\infty_{\mathbb{R}}(\Omega)$, $q_a, q_b \in \mathbb{R}$. The operator $H_{\mathfrak{R}}[V]$ is self-adjoint and semi-bounded from below. In some sense the operator $H_{\mathfrak{R}}[V]$ can be regarded as the real part of the maximal dissipative $H[V]$. By $\gamma[V]$ we denote the bottom of the spectrum of $H_{\mathfrak{R}}[V]$, i.e., $\gamma[V] := \inf \mathrm{spec}(H_{\mathfrak{R}}[V])$.

Lemma 3.1: Let the Schrödinger assumptions Q_1 be satisfied. If $q_a, q_b \in \mathbb{R}$, then

$$\gamma[V] \geqslant -\gamma_0 - \|V_-\|_{L^\infty}, \tag{26}$$

where $V_-(x) := \frac{1}{2}\{|V(x)| - V(x)\}$, $x \in \Omega$, *and* γ_0 *is given by* (20).

Proof: We consider the quadratic form $[q_a,q_b](\cdot,\cdot)$,

$$[q_a,q_b](f,f) := -q_a|f(a)|^2 - q_b|f(b)|^2 + \int_a^b \frac{1}{2m(x)}|f'(x)|^2\mathrm{d}x,$$

$f \in \mathrm{dom}([q_a,q_b,V]) = W^{1,2}(\Omega)$, which is associated with the self-adjoint operator $H[q_a,q_b,0]$. The quadratic form $[q_a,q_b](\cdot,\cdot)$ admits the estimate

$$[q_a,q_b](f,f) \geqslant \hat{}(f,f) := -\{|f(a)|^2 + |f(b)|^2\} + \frac{1}{2\bar{m}}\int_a^b |f'(x)|^2\mathrm{d}x,$$

where $:= \max\{0,q_a,q_b\}$, cf. (21). The quadratic form $\hat{}$ corresponds to the self-adjoint operator $\hat{H}$,

$$(\hat{H}f)(x) = -\frac{1}{2\bar{m}}\frac{\mathrm{d}^2}{\mathrm{d}x^2}f(x), \quad f \in \mathrm{dom}(\hat{H}),$$

$$\mathrm{dom}(\hat{H}) = \left\{ f \in W^{2,2}(\Omega) : \frac{1}{2\bar{m}} f'(a) = -\quad f(a),\ \frac{1}{2\bar{m}} f'(b) = \quad f(b) \right\}.$$

A straightforward computation shows that $\lambda = -\mu^2$, $\mu \geqslant \mathfrak{q}\sqrt{2\bar{m}}$, is an eigenvalue of $\hat{H}$ if and only if μ satisfies

$$\mu|\Omega|\sqrt{2\bar{m}} = \ln\left(\frac{\mu + \quad \sqrt{2\bar{m}}}{\mu - \quad \sqrt{2\bar{m}}} \right).$$

Hence, if $\lambda = -\mu^2$ is an eigenvalue, then the estimate

$$\mu|\Omega|\sqrt{2\bar{m}} \leqslant \frac{2 \quad \sqrt{2\bar{m}}}{\mu - \quad \sqrt{2\bar{m}}}$$

holds. This yields

$$\lambda = -\mu^2 \geqslant -2\bar{m} \quad {}^2\left\{ \frac{1}{2} + \frac{1}{|\Omega|\bar{m}} + \sqrt{\frac{1}{4} + \frac{1}{|\Omega|\bar{m}}} \right\}.$$

Using this estimate we immediately verify (26). □

B. Elementary solutions and estimates

An important tool to investigate the dissipative operator $H[V]$ is the so-called elementary solutions defined by

$$l[V](v_a(x,z)) = z v_a(x,z), \quad v_a(a,z) = 1, \quad \frac{1}{2m(a)} v_a'(a,z) = -\kappa_a, \tag{27}$$

$$l[V](v_b(x,z)) = z v_b(x,z), \quad v_b(b,z) = 1, \quad \frac{1}{2m(b)} v_a'(b,z) = \kappa_b. \tag{28}$$

The existence of these solutions for each $z \in \mathbb{C}$ can be proved by writing (27) and (28) in integral form

$$v_a(x,z) = 1 - 2\kappa_a M_a(x) + 2\int_a^x \mathrm{d}t (M_a(x) - M_a(t))(V(t) - z) v_a(t,z) \tag{29}$$

and

$$v_b(x,z) = 1 - 2\kappa_b M_b(x) + 2\int_x^b \mathrm{d}t (M_b(x) - M_b(t))(V(t) - z) v_b(t,z) \tag{30}$$

where

$$M_a(x) := \int_a^x \mathrm{d}t\, m(t), \quad M_b(x) := \int_x^b \mathrm{d}t\, m(t).$$

Since (29) and (30) are Volterra-type equations they have always solutions for any $z \in \mathbb{C}$, in particular, for $z = \lambda \in \mathbb{R}$. Moreover, one gets that v_a and v_b as well as $(1/m)v_a'$ and $(1/m)v_b'$ are absolutely continuous.

In the following the estimates are based on Gronwall's lemma which we need in a slightly generalized form.

Lemma 3.2 (Gronwall's lemma): Let μ be a finite Borel measure on $[a,b]$. If the non-negative continuous function $g(\cdot):[a,b] \to \mathbb{R}$ obeys

$$0 \leqslant g(x) \leqslant C + \int_{[a,x]} g(t)\mathrm{d}\mu(t), \quad x \in [a,b], \quad C > 0, \tag{31}$$

then the estimate

$$g(x) \leqslant C \exp\left\{ \int_{[a,x]} \mathrm{d}\mu(t) \right\}, \quad x \in [a,b], \tag{32}$$

holds.

The proof follows immediately from Lemma 5 of Ref. 15. Using Gronwall's lemma we are going to establish bounds for the elementary solutions if $\lambda > 0$. At first we prove this for the special case $V=0$ and later on we extend the result to $V \neq 0$.

Let $V=0$. We consider the boundary value problem

$$l[0]w(x,\lambda) = \lambda w(x,\lambda), \quad w(a,\lambda) = p, \quad \frac{1}{2m(a)} w'(a,\lambda) = q,$$

where $p, q \in \mathbb{C}$.

Lemma 3.3: Let the Schrödinger assumption Q_1 be satisfied. If m has a finite total variation, then

$$|w(x,\lambda)| \leqslant \sqrt{|p|^2 + \frac{2}{\lambda m(a)}|q|^2} \quad , \tag{33}$$

for $x \in [a,b]$ and $\lambda > 0$, where is defined by (16).

Proof: We note that

$$-\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{m(x)}\frac{\mathrm{d}}{\mathrm{d}x} w(x,\lambda) = \lambda w(x,\lambda)$$

is satisfied for a.e. $x \in [a,b]$ with respect of the Lebesgue measure. Multiplying by $(1/m(x)w'(x,\lambda)$ we get

$$-\frac{1}{2}\overline{\frac{1}{m(x)} w'(x,\lambda)}\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{m(x)} w'(x,\lambda) = \lambda w(x,\lambda)\overline{\frac{1}{m(x)} w'(x,\lambda)}$$

which yields

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\left| \frac{1}{m(x)} w'(x,\lambda) \right|^2 = -\frac{\lambda}{m(x)}\frac{\mathrm{d}}{\mathrm{d}x}|w(x,\lambda)|^2$$

for a.e. $x \in [a,b]$. Since $(1/m(x))w'(x,\lambda)$ is absolutely continuous we obtain

$$\frac{1}{2}\left| \frac{1}{m(x)} w'(x,\lambda) \right|^2 = \frac{1}{2}\left| \frac{1}{m(a)} w'(a,\lambda) \right|^2 - \lambda \int_a^x \frac{1}{m(t)}\frac{\mathrm{d}}{\mathrm{d}t}|w(t,\lambda)|^2 \mathrm{d}t$$

for $x \in [a,b]$. Since m has a finite total variation, the limits $m(x-0) := \lim_{y \uparrow x} m(y)$ for $x \in (a,b]$ and $m(x+0) := \lim_{y \downarrow x} m(y)$ for $x \in [a,b)$ exist. Further, we set $m(a-0) := m(a)$ and $m(b+0) := m(b)$. Notice that $m(x)$ and $m(x-0)$ are different only on a countable set. Hence we can replace $1/m(t)$ by $1/m(t-0)$ above. Using the boundary conditions we get

$$\left|\frac{1}{m(x)}w'(x,\lambda)\right|^2 = 4|q|^2 - 2\lambda\int_{[a,x]}\frac{1}{m(t-0)}\mathrm{d}|w(t,\lambda)|^2$$

for all $x\in[a,b]$ where the integral on the right-hand side is regarded as a Lebesgue-Stieltjes integral. If m has a finite total variation, then by assumption Q_1 the function $1/m$ has a finite total variation, too. By Theorem 21.67 and Remark 21.68 of Ref. 13 we get

$$\left|\frac{1}{m(x)}\frac{\mathrm{d}}{\mathrm{d}x}w(x,\lambda)\right|^2 + \frac{2\lambda}{m(x+0)}|w(x,\lambda)|^2 = 4|q|^2 + \frac{2\lambda}{m(a)}|w(a,\lambda)|^2 + 2\lambda\int_{[a,x]}|w(t,\lambda)|^2\mathrm{d}\mu(t), \tag{34}$$

where μ is the signed measure associated with $1/m$. Since $1/m$ is of bounded variation, the functions $\varpi(x) := \mathrm{V}_a^x(1/m)$ and $\nu(x) := \varpi(x) - 1/m(x)$, $x\in[a,b]$, are non-decreasing. Notice that $1/m(x) = \varpi(x) - \nu(x)$. Thus we find

$$\int_{[a,x]}|w(t,\lambda)|^2\mathrm{d}\mu(t) = \int_{[a,x]}|w(t,\lambda)|^2\mathrm{d}\mu_\varpi(t) - \int_{[a,x]}|w(t,\lambda)|^2\mathrm{d}\mu_\nu(t),$$

where μ_ϖ and μ_ν the measures associated with ϖ and ν, respectively. Hence

$$\int_{[a,x]}|w(t,\lambda)|^2\mathrm{d}\mu(t) \leqslant \int_{[a,x]}|w(t,\lambda)|^2\mathrm{d}\mu_\varpi(t), \quad x\in[a,b].$$

Inserting this estimate into (34) and using the boundary condition $w(a,\lambda)=p$ we get

$$\frac{1}{m(x+0)}|w(x,\lambda)|^2 \leqslant \frac{2}{\lambda}|q|^2 + \frac{1}{m(a)}|p|^2 + \int_{[a,x]}|w(t,\lambda)|^2\mathrm{d}\mu_\varpi(t), \quad x\in[a,b],$$

which yields

$$|w(x,\lambda)|^2 \leqslant m(x+0)\left(\frac{2}{\lambda}|q|^2 + \frac{1}{m(a)}|p|^2\right) + m(x+0)\int_{[a,x]}|w(t,\lambda)|^2\mathrm{d}\mu_\varpi(t)$$

for $x\in[a,b]$. Since $m(x)\leqslant\bar{m}$, $x\in[a,b]$, we obtain

$$|w(x,\lambda)|^2 \leqslant \bar{m}\left(\frac{2}{\lambda}|q|^2 + \frac{1}{m(a)}|p|^2\right) + \bar{m}\int_{[a,x]}|w(t,\lambda)|^2\mathrm{d}\mu_\varpi(t).$$

Applying Lemma 3.2, we immediately get

$$|w(x,\lambda)|^2 \leqslant \left(\frac{2}{\lambda}|q|^2 + \frac{1}{m(a)}|p|^2\right)\exp\left\{\bar{m}\int_{[a,x]}\mathrm{d}\mu_\varpi(t)\right\}$$

for $x\in[a,b]$. Hence

$$|w(x,\lambda)| \leqslant \sqrt{|p|^2 + \frac{2}{\lambda m(a)}|q|^2}\sqrt{\bar{m}}\exp\left\{\frac{\bar{m}}{2}\int_{[a,x]}\mathrm{d}\mu_\varpi(t)\right\}$$

for $x\in[a,b]$. Finally, taking into account

$$\int_{[a,x]}\mathrm{d}\mu_\varpi(t) \leqslant \int_{[a,b]}\mathrm{d}\mu_\varpi(t) \leqslant \mathop{\mathrm{V}}_a^b\frac{1}{m}$$

we prove (33). □

We note that a similar lemma holds if the end point a is replaced by b.

In the following we consider the solutions $w_0(x,\lambda)$ and $w_1(x,\lambda)$ of the boundary value problems

$$(l[0]w_1)(x) = \lambda w_1(x,\lambda), \quad w_1(a,\lambda) = 1, \quad \frac{1}{2m(a)} w_1'(a,\lambda) = 0,$$

$$(l[0]w_0)(x) = \lambda w_0(x,\lambda), \quad w_0(a,\lambda) = 0, \quad \frac{1}{2m(a)} w_0'(a,\lambda) = 1.$$

By Lemma 3.3 we have the estimates

$$|w_1(x,\lambda)| \leqslant \quad , \quad |w_0(x,\lambda)| \leqslant \sqrt{\frac{2}{\lambda m(a)}} \quad , \quad x \in [a,b], \quad \lambda > 0.$$

Lemma 3.4: Let the Schrödinger assumption Q_1 be satisfied and let $V \in L^\infty_{\mathbb{R}}(\Omega)$. If m has a finite total variation, then

$$|v_j(x,\lambda)| \leqslant \begin{cases} R_j(\|V\|_{L^\infty}), & \lambda \geqslant 1, \\ R_j(\|V+1-\lambda\|_{L^\infty}), & \lambda < 1, \end{cases} \quad , \quad j = a,b, \quad x \in \Omega, \tag{35}$$

where $R_j(\cdot)$ is defined by (17)

Proof: The solution $v_a(x,\lambda)$ satisfies the integral equation

$$v_a(x,\lambda) = w_1(x,\lambda) - \kappa_a w_0(x,\lambda) + \int_a^x \mathrm{d}t \, \{w_0(x,\lambda)w_1(t,\lambda) - w_0(t,\lambda)w_1(x,\lambda)\} V(t) v_a(t,\lambda),$$

$x \in \Omega$ and $\lambda \in \mathbb{R}$. Therefore, we have the estimate

$$|v_a(x,\lambda)| \leqslant \quad \left(1 + |\kappa_a| \sqrt{\frac{2}{\lambda m(a)}}\right) + \quad {}^2\sqrt{\frac{2}{\lambda m(a)}} \int_a^x \mathrm{d}t \, |V(t)||v_a(t,\lambda)|,$$

$x \in \Omega$ and $\lambda > 0$. Applying Gronwall's lemma we find

$$|v_a(x,\lambda)| \leqslant \quad \left(1 + |\kappa_a| \sqrt{\frac{2}{\lambda m(a)}}\right) \exp\left\{ \quad {}^2\sqrt{\frac{2}{\lambda m(a)}} \int_a^x \mathrm{d}t \, |V(t)| \right\}$$

for $x \in \Omega$ and $\lambda > 0$. If $\lambda \geqslant 1$, then we immediately verify the first part of (35).

If $\lambda < 1$, then $v_j(x,\lambda)$ satisfies the equation $l[V+1-\lambda]v_a(x,\lambda) = v_a(x,\lambda)$. Taking into account the first estimate of (35) we prove the second estimate. The proof for $j=b$ is similar. □

C. Characteristic function

Let us introduce the operator-valued function $T(z): \mathcal{H} \to \mathbb{C}^2$,

$$T[V](z)f := \begin{pmatrix} \alpha_b((H[V]-z)^{-1}f)(b) \\ -\alpha_a((H[V]-z)^{-1})f(a) \end{pmatrix}, \quad \alpha_a, \alpha_b > 0,$$

for $z \in \mathrm{res}(H[V])$ and $f \in L^2(\Omega)$. Using Theorem 2.1 of Ref. 17, we find

$$T[V](z)f = \frac{1}{W(z)} \begin{pmatrix} -\alpha_b \int_a^b \mathrm{d}y \, v_a(y,z) f(y) \\ \alpha_a \int_a^b \mathrm{d}y \, v_b(y,z) f(y) \end{pmatrix}$$

for $f \in L^2(\Omega)$ where $W(z)$ denotes the Wronskian of the solutions $v_a(x,z)$ and $v_b(x,z)$,

$$W(z) := v_a(x,z)\frac{1}{2m(x)}v_b'(x,z) - v_b(x,z)\frac{1}{2m(x)}v_a'(x,z),$$

which is independent from $x \in \Omega$. The adjoint operator is given by

$$(T[V](z)^*\xi)(x) = \frac{1}{W(z)}(-\alpha_b\overline{v_a(x,z)}, \alpha_a\overline{v_b(x,z)})\xi, \tag{36}$$

$x \in \Omega$, where

$$\xi = \begin{pmatrix} \xi^b \\ \xi^a \end{pmatrix} \in \mathbb{C}^2. \tag{37}$$

and the right-hand side is regarded as a matrix multiplication. Similarly, we set

$$T_*[V](z)f := \begin{pmatrix} \alpha_b((H[V]^* - z)^{-1}f)(b) \\ -\alpha_a((H[V]^* - z)^{-1}f)(a) \end{pmatrix}$$

for $z \in \mathrm{res}(H^*)$ and $f \in L^2(\Omega)$. Using again Theorem 2.1 of Ref. 17 we find

$$T_*[V](z)f = \frac{1}{W_*(z)}\begin{pmatrix} -\alpha_b\int_a^b \mathrm{d}y\, v_{*a}(y,z)f(y) \\ \alpha_b\int_a^b \mathrm{d}y\, v_{*b}(y,z)f(y) \end{pmatrix},$$

where $W_*(z)$ is the Wronskian of the solutions $v_{*a}(x,z) := \overline{v_a(x,\bar{z})}$ and $v_{*b}(x,z) := \overline{v_b(x,\bar{z})}$,

$$W_*(z) := v_{*a}(x,z)\frac{1}{2m(x)}v_{*b}'(x,z) - v_{*b}(x,z)\frac{1}{2m(x)}v_{*a}'(x,z),$$

which also independent from $x \in \Omega$. The adjoint operator has the representation

$$(T_*[V](z)^*\xi)(x) = \frac{1}{W_*(z)}(-\alpha_b\overline{v_{*a}(x,z)}, \alpha_a\overline{v_{*b}(x,z)})\xi,$$

$x \in \Omega$, $\xi \in \mathbb{C}^2$.

The operator $H[V]$ can be (up to unitary equivalence) characterized by its characteristic function $z \to \Theta[V](z)$, with $z \in \mathrm{res}(H[V]) \cap \mathrm{res}(H[V]^*)$, cf. Ref. 9. The characteristic function $\Theta[V](\cdot)$ of the maximal dissipative operator $H[V]$ is a two-by-two matrix-valued function which satisfies the relation

$$\Theta[V](z)T[V](z)f = T_*[V](z)f, \quad z \in \mathrm{res}(H[V]) \cap \mathrm{res}(H[V]^*),$$

$f \in \mathfrak{h}$. In terms of the adjoint elementary solutions the characteristic function can be expressed as follows:

$$\Theta[V](z) = I_{\mathbb{C}^2} + i\frac{1}{W_*(z)}\begin{pmatrix} \alpha_b^2 v_{*a}(b,z) & -\alpha_b\alpha_a \\ -\alpha_b\alpha_a & \alpha_a^2 v_{*b}(a,z) \end{pmatrix},$$

which can be written as

$$\Theta[V](z) = I_{\mathbb{C}^2} - i\alpha T[V](\bar{z})^*,$$

$z \in \mathrm{res}(H[V]) \cap \mathrm{res}(H[V]^*)$, where the operator $\alpha: L^2(\Omega) \to \mathbb{C}$, is defined by

$$\alpha f := \begin{pmatrix} \alpha_b f(b) \\ -\alpha_a f(a) \end{pmatrix}, \quad f \in \mathrm{dom}(\alpha) := C(\bar{\Omega}).$$

Notice that the operator α is not closed and not closable. The characteristic function $\Theta[V](\lambda)$ is a holomorphic on $\mathrm{res}(H[V]) \cap \mathrm{res}(H[V]^*)$ and contractive on $\mathbb{C}_- \cup \mathbb{R}$, i.e., it satisfies

$$\|\Theta[V](z)\| \leqslant 1 \quad \text{for} \quad z \in \mathbb{C}_- \cup \mathbb{R}.$$

In particular, it is well-defined and continuous on $\mathbb{R}$, cf. Ref. 17. We note that by Lemma 2.2 of Ref. 26 one has $\lim_{\lambda \to -\infty} \|\Theta[V](\lambda) - I_{\mathbb{C}^2}\|_{\mathcal{B}(\mathbb{C}^2)} = 0$.

D. Phase shift

The phase shift $\omega[V]$ is defined by

$$e^{2\pi i \omega[V](\lambda)} := \det(\Theta[V](\lambda)), \quad \lambda \in \mathbb{R},$$

where it is assumed that $\omega[V](\cdot) : \mathbb{R} \to \mathbb{R}$ is continuous. Notice that the phase shift is determined modulo $\mathbb{Z}$. Since $\lim_{\lambda \to -\infty} \det(\Theta[V](\lambda)) = 1$ by Lemma 2.2 of Ref. 26 we fix the phase shift by the condition

$$\lim_{\lambda \to -\infty} \omega[V](\lambda) = 0.$$

Lemma 3.5: [Ref. 26, Lemma 4.1] Let the Schrödinger assumptions Q_1 and Q_2 be satisfied. If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then the phase shift is holomorphic in a neighborhood of $\mathbb{R}$ and satisfies

$$\omega'[V](\lambda) := \frac{\mathrm{d}}{\mathrm{d}\lambda} \omega[V](\lambda) = -\frac{1}{2\pi} \mathrm{tr}(T[V](\lambda) T[V](\lambda)^*) \leqslant 0 \tag{38}$$

for $\lambda \in \mathbb{R}$.

Lemma 3.5 shows that the phase shift is non-increasing. Moreover, since $\omega[V](-\infty) = 0$ the phase shift is always non-positive, i.e., $\omega[V](\lambda) \leqslant 0$ for $\lambda \in \mathbb{R}$. Let us introduce the counting function

$$\Phi[V](\lambda) := \mathrm{card}\{s \leqslant \lambda : \det(\Theta[V](s)) = 1\}, \quad \lambda \in \mathbb{R}.$$

It turns out that the $\Phi[V](\cdot)$ is comparable with the counting function $N_D[V](\cdot)$,

$$N_D[V](\lambda) := \mathrm{card}\{s \leqslant \lambda : s \in \mathrm{spec}(H_D[V])\}, \quad \lambda \in \mathbb{R}.$$

where $H_D[V]$ denotes the Schrödinger-type operator with Dirichlet boundary conditions.

Theorem 3.6: *[Ref. 26, Theorem 4.7] Let the Schrödinger assumption Q_1 and Q_2 be satisfied. If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then*

$$N_D[V](\lambda) \leqslant \Phi[V](\lambda) \leqslant N_D[V](\lambda) + 1, \quad \lambda \in \mathbb{R}.$$

Corollary 3.7: Let the Schrödinger assumption Q_1 and Q_2 be satisfied. If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then

$$0 \leqslant -\omega[V](\lambda) \leqslant 2 + \frac{1}{\pi} \sqrt{2\bar{m}|\Omega|} \sqrt{(\lambda + \|V_-\|_{L^\infty})_+} \tag{39}$$

for $\lambda \in \mathbb{R}$.

Proof: Since $-\omega[V](\lambda)$ is non-decreasing by Lemma 3.5 the estimate $-\omega[V](\lambda) \leqslant 1 + \Phi[V](\lambda)$, $\lambda \in \mathbb{R}$, holds. By Remark 4.8 of Ref. 26 and Theorem 3.6 one gets

$$N_D[V](\lambda) \leqslant \frac{1}{\pi}\sqrt{2\overline{m}|\Omega|}\sqrt{(\lambda + \|V_-\|_{L^\infty})_+}, \quad \lambda \in \mathbb{R},$$

which yields (39). □

E. Lipschitz continuity of the phase shift

We are going to verify the Lipschitz continuity of the phase shift by giving bounds for the derivative of $\omega[V]$.

Proposition 3.8: Let the Schrödinger assumptions Q_1 and Q_2 be satisfied and let $V \in L^\infty_{\mathbb{R}}(\Omega)$. If m has a finite total variation, then

$$|\omega[V](\lambda) - \omega[V](\lambda')| \leqslant |\Omega| L(\|V\|_{L^\infty})^2 |\lambda - \lambda'|, \tag{40}$$

$\lambda, \lambda' \in \mathbb{R}$ *where* $L(\cdot)$ *is defined by* (18).

Proof: Since the phase shift is continuously differentiable it is sufficient to show $-\omega'[V](\lambda) \leqslant |\Omega| L(\|V\|_{L^\infty})^2$, $\lambda \in \mathbb{R}$. Taking into account Lemma 3.5 we get

$$\omega'[V](\lambda) = -\frac{1}{2\pi}\sum_{j=1}^{2} \|T[V](\lambda)^* e_j\|^2_{L^2}, \quad \lambda \in \mathbb{R}, \tag{41}$$

where

$$e_1 := \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad e_2 := \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

By (36) we find

$$\|T[V](\lambda)^* e_1\|^2_{L^2} = \frac{\alpha_b^2}{|W(\lambda)|^2}\int_a^b \mathrm{d}x |v_a(x,\lambda)|^2.$$

Let

$$E := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

We note that $\|E\Theta[V](\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} \leqslant 1$, $\lambda \in \mathbb{R}$, and

$$\mathrm{tr}(E\Theta[V](\lambda)) = -2i\frac{\alpha_a \alpha_b}{W(\lambda)}, \quad \lambda \in \mathbb{R},$$

which yields

$$\frac{\alpha_a \alpha_b}{|W(\lambda)|} \leqslant 1, \quad \lambda \in \mathbb{R}.$$

Hence

$$\|T[V](\lambda)^* e_1\|^2_{L^2} \leqslant \frac{1}{\alpha_a^2}\int_a^b \mathrm{d}x |v_a(x,\lambda)|^2, \quad \lambda \in \mathbb{R}.$$

Applying Lemma 3.4 we get the estimate

$$\|T[V](\lambda)^* e_1\|_{L^2}^2 \leqslant |\Omega| \frac{R_a[\|V+2-\lambda_0\|_{L^\infty}]^2}{\alpha_a^2}, \quad \lambda \in [\lambda_0 - 1, \infty). \tag{42}$$

where $\lambda_0 := -\|V\|_{L^\infty} - \gamma_0$ and γ_0 is given by (20). By Lemma 3.1 one immediately gets that $(-\infty, \lambda_0) \subseteq \mathrm{res}(H[V])$. Using the resolvent formula

$$(H[V]-\lambda)^{-1} = (H[V]-\lambda_0)^{-1}\{I + (\lambda-\lambda_0)(H[V]-\lambda)^{-1}\},$$

$\lambda \in (-\infty, \lambda_0)$, we find the representation

$$T[V](\lambda) = T[V](\lambda_0)\{I + (\lambda-\lambda_0)(H[V]-\lambda)^{-1}\}, \tag{43}$$

$\lambda \in (-\infty, \lambda_0)$. By $\Gamma[V]$ we denote the numerical range of $H[V]$. One easily verifies that $\Gamma[V] \subseteq \{z \in \mathbb{C} : \mathfrak{Re}(z) \geqslant \lambda_0\}$. Applying Theorem 3.1 of Ref. 16 we get the estimate

$$\|(H[V]-\lambda)^{-1}\|_{\mathcal{B}(L^2(\Omega))} \leqslant \frac{1}{\mathrm{dist}(\Gamma[V], \lambda)} \leqslant \frac{1}{|\lambda - \lambda_0|} \leqslant 1$$

for $\lambda \in (-\infty, \lambda_0 - 1)$. Hence we find the estimate

$$\|I + (\lambda-\lambda_0)(H[V]-\lambda)^{-1}\|_{\mathcal{B}(L^2(\Omega))} \leqslant 1 + \frac{|\lambda-\lambda_0|}{|\lambda-\lambda_0|} = 2$$

for $\lambda \in (-\infty, \lambda_0 - 1)$. Further, from (43) we get

$$T[V](\lambda)^* e_1 = \{I + (\lambda-\lambda_0)(H[V]^* - \lambda)^{-1}\} T[V](\lambda_0)^* e_1$$

for $\lambda \in (-\infty, \lambda_0 - 1)$. Using (42)

$$\|T[V](\lambda)^* e_1\|_{L^2}^2 \leqslant 4\|T[V](\lambda_0)^* e_1\|_{L^2}^2 \leqslant 4|\Omega| \frac{R_a[\|V+2-\lambda_0\|_{L^\infty}]^2}{\alpha_a^2}, \tag{44}$$

$\lambda \in (-\infty, \lambda_0 - 1)$. Taking into account (42) and (44) we finally get

$$\|T[V](\lambda)^* e_1\|_{L^2}^2 \leqslant 4|\Omega| \frac{R_a[\|V+2-\lambda_0\|_{L^\infty}]^2}{\alpha_a^2}, \quad \lambda \in \mathbb{R}. \tag{45}$$

Similarly, we prove

$$\|T[V](\lambda)^* e_2\|_{L^2}^2 \leqslant 4|\Omega| \frac{R_b[\|V+2-\lambda_0\|_{L^\infty}]^2}{\alpha_b^2}, \quad \lambda \in \mathbb{R}. \tag{46}$$

From (41), (45), and (46) we obtain

$$-\omega'[V](\lambda) \leqslant \frac{2}{\pi}|\Omega| \left\{ \frac{R_a[\|V+2-\lambda_0\|_{L^\infty}]^2}{\alpha_a^2} + \frac{R_b[\|V+2-\lambda_0\|_{L^\infty}]^2}{\alpha_b^2} \right\}$$

for $\lambda \in \mathbb{R}$. Inserting $\lambda_0 = -\|V\|_{L^\infty} - \gamma_0$ into this formula and using the definition (18) we obtain (40). □

F. Dilations

Since $H[V]$ is a maximal dissipative operator there is a larger Hilbert space $\supseteq$ and a self-adjoint operator $K[V]$ on such that

$$P\ \ (K[V]-z)^{-1}\restriction\quad =(H[V]-z)^{-1},\quad \Im\mathrm{m}(z)>0, \tag{47}$$

see Ref. 9. The operator $K[V]$ is called a self-adjoint dilation of the maximal dissipative operator $H[V]$. Obviously, from the condition (47) one gets

$$P\ \ (K[V]-z)^{-1}\restriction\quad =(H[V]^{*}-z)^{-1},\quad \Im\mathrm{m}(z)<0.$$

If the condition

$$\mathrm{clospan}\{z\in\mathbb{C}\setminus\mathbb{R}:(K[V]-z)^{-1}\quad\}=$$

is satisfied, then $K[V]$ is called a minimal self-adjoint dilation of $H[V]$. Minimal self-adjoint dilations of maximal dissipative operators are determined up to an isomorphism, in particular, all minimal self-adjoint dilations are unitarily equivalent. The self-adjoint operator $K[V]$ is absolutely continuous and its spectrum coincides with the real axis, i.e., $\mathrm{spec}(K)=\mathbb{R}$. The multiplicity of its spectrum is two. For more details the reader is referred to Ref. 17.

Definition 3.9: (cf. Ref. 22) Let K be a self-adjoint, absolutely continuous operator on a Hilbert space $\mathcal{H}$ and A be a bounded operator on $\mathcal{H}$. Then A is called K-smooth if there is a constant $C_A>0$ such that

$$\int_{-\infty}^{+\infty}\mathrm{d}t\|Ae^{-itK}\vec{f}\|_{\mathcal{H}}^{2}\leqslant 2\pi C_A^{2}\|\vec{f}\|_{\mathcal{H}}^{2} \tag{48}$$

for all $\vec{f}\in\mathcal{H}$. The smallest constant C_A is denoted by $\|A\|_K$.

Let us verify that the projection $P\quad$ is $K[V]$-smooth. To this end we need the following lemma which was proved in Ref. 26.

Lemma 3.10: [Ref. 26, Lemma 5.3] Let the Schrödinger assumptions Q_1 and Q_2 be satisfied. If $V\in L^{\infty}_{\mathbb{R}}(\Omega)$, then

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}(E_{K[V]}(\lambda)P\ \ \vec{f},P\ \ \vec{g})\ \ =(T[V](\lambda)P\ \ \vec{f},T[V](\lambda)P\ \ \vec{g})_{\mathbb{C}^2}$$

for a.e $\lambda\in\mathbb{R}$ and $\vec{f},\vec{g}\in$ where $E_{K[V]}(\cdot)$ denotes the spectral measure of the the self-adjoint dilation $K[V]$.

Proposition 3.8 and Lemma 3.10 imply the smoothness of $P\ \ $:

Theorem 3.11: *Let the Schrödinger assumptions Q_1 and Q_2 be satisfied and let $V\in L^{\infty}_{\mathbb{R}}(\Omega)$. If m has a finite total variation, then the projection $P\quad$ is $K[V]$-smooth and the estimate*

$$\|P\ \ \|_{K[V]}\leqslant\sqrt{|\Omega|}L(\|V\|_{L^{\infty}}) \tag{49}$$

holds where $L(\cdot)$ is defined by (18).

Proof: In accordance with Ref. 22 we set

$$a_2:=\sup_{\Delta\subseteq\mathbb{R},\vec{f}\in\ \ \vec{f}\neq 0}\frac{\|E_{K[V]}(\Delta)P\ \ \vec{f}\|^{2}}{|\Delta|\,\|\vec{f}\|^{2}},$$

where $\Delta=(\lambda_1,\lambda_2)\subseteq\mathbb{R}$ are bounded intervals of $\mathbb{R}$ and $|\Delta|:=\lambda_2-\lambda_1$ denotes their length. Then Theorem 5.1 of Ref. 22 states $\|P\ \ \|_{K[V])}=\sqrt{a_2}$. Thus, the $K[V]$-smoothness of the projection P including the estimate (49) is shown if we verify

$$a_2\leqslant|\Omega|L(\|V\|_{L^{\infty}})^{2}.$$

Using Lemma 3.10 we get that

$$\|E_{K[V]}(\Delta)P\ \vec{f}\|^2 = \frac{1}{2\pi}\int_\Delta d\lambda \|T[V](\lambda)f\|^2 .$$

We note that

$$\|T[V](\lambda)f\|^2 \leqslant \|f\|^2 \operatorname{tr}(T[V](\lambda)^* T[V](\lambda)) = \|f\|^2 \operatorname{tr}(T[V](\lambda)T[V](\lambda)^*),$$

$\lambda \in \mathbb{R}$. Hence

$$\|E_{K[V]}(\Delta)P\ \vec{f}\|^2 \leqslant \|\vec{f}\|^2 \frac{1}{2\pi}\int_\Delta d\lambda \operatorname{tr}(T[V](\lambda)T[V](\lambda)^*).$$

Taking into account Lemma 3.5 we obtain the estimate

$$\|E_{K[V]}(\Delta)P\ \vec{f}\|^2 \leqslant -\|\vec{f}\|^2 \int_\Delta d\lambda\ \omega'[V](\lambda).$$

Hence we obtain

$$\frac{\|E_{K[V]}(\Delta)P\ \vec{f}\|^2}{\|\vec{f}\|^2} \leqslant (\omega[V](\lambda_1) - \omega[V](\lambda_2))$$

Using (40) we find the estimate

$$\frac{\|E_{K[V]}(\Delta)P\ \vec{f}\|^2}{|\Delta|\ \|f^2} \leqslant |\Omega| L(\|V\|_{L^\infty})^2.$$

□

G. Lax-Phillips scattering theory

The dilation space admits the decomposition

$$= \mathcal{D}_- \oplus \quad \oplus \mathcal{D}_+.$$

where $\mathcal{D}_\pm = L^2(\mathbb{R}_\pm, \mathbb{C}^2)$, see Ref. 17. Since

$$e^{-itK[V]}\mathcal{D}_- \subseteq \mathcal{D}_-, \quad t \leqslant 0,$$

$$e^{-itK[V]}\mathcal{D}_+ \subseteq \mathcal{D}_+, \quad t \geqslant 0$$

as well as

$$\begin{aligned} &\bigcap_{t\in\mathbb{R}} e^{-itK[V]}\mathcal{D}_- = \bigcap_{t\in\mathbb{R}} e^{-itK[V]}\mathcal{D}_+ = \{0\}, \\ &\overline{\bigcup_{t\in\mathbb{R}} e^{-itK[V]}\mathcal{D}_-} = \overline{\bigcup_{t\in\mathbb{R}} e^{-itK[V]}\mathcal{D}_+} = \end{aligned} \tag{50}$$

the subspaces $\mathcal{D}_-$ and $\mathcal{D}_+$ are called incoming and outgoing subspaces with respect to $e^{-itK[V]}$, cf. Ref. 1, Chap. XII or Ref. 24. Further, introducing the Hilbert space $_0$,

$$_0 = L^2(\mathbb{R}, \mathbb{C}^2) = \mathcal{D}_- \oplus \mathcal{D}_+ \subseteq \quad = \mathcal{D}_- \oplus \quad \oplus \mathcal{D}_+,$$

and the self-adjoint differentiation operator K_0,

$$(K_0 f)(x) = -i\frac{\mathrm{d}}{\mathrm{d}x}f(x), \quad f \in \mathrm{dom}(K_0) = W^{1,2}(\mathbb{R},\mathbb{C}^2),$$

one easily verifies that $\mathcal{D}_-$ and $\mathcal{D}_+$ are incoming and outgoing subspaces with respect to e^{-itK_0}. The Lax-Phillips wave operators are defined by

$$W_\pm(K[V],K_0;J_\pm) := s - \lim_{t\to\pm\infty} e^{itK[V]}J_\pm e^{-itK_0},$$

where the identification operators $J_\pm$: $_0 \to$ are given by

$$\vec{f} = J_- f := P_{\mathcal{D}_-^0} f \oplus 0 \oplus 0, \quad f \in \ _0,$$

$$\vec{f} = J_+ f := 0 \oplus 0 \oplus P_{\mathcal{D}_+^0} f, \quad f \in \ _0.$$

Since

$$e^{-itK[V]}|\mathcal{D}_- = e^{-itK_0}|\mathcal{D}_-, \quad t \leqslant 0,$$

$$e^{-itK[V]}|\mathcal{D}_+ = e^{-itK_0}|\mathcal{D}_+, \quad t \geqslant 0,$$

the wave operators $W_\pm(K[V],K_0;J_\pm)$ exist. Using (50) one proves the completeness of the wave operators, i.e., $\mathrm{ran}(W_\pm(K[V],K_0;J_\pm)) =$. For details see Ref. 1, Chap. XII or Ref. 24. Defining the Fourier transform F: $_0 \to \hat{}_0 = L^2(\mathbb{R},\mathbb{C}^2)$ by

$$(Ff)(\lambda) := \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \mathrm{d}x\, e^{-ix\lambda} f(x), \quad f \in \ _0, \quad \lambda \in \mathbb{R},$$

one defines the generalized Fourier transform $\Phi[V]$: $\to \hat{}_0$ by

$$\Phi[V] := FW_-(K[V],K_0;J_-)^*, \tag{51}$$

cf. Remark 5.2 of Ref. 18, which is an isometry. Moreover, if M is the multiplication operator defined by

$$(M\hat{f}) = \lambda\hat{f}(\lambda), \quad \hat{f} \in \mathrm{dom}(M) = \{\hat{f} \in \hat{}_0 : \lambda\hat{f}(\lambda) \in \hat{}_0\}.$$

on the Hilbert space $_0$, then $M = \Phi[V]K[V]\Phi[V]^{-1}$.

Lemma 3.12: Let the Schrödinger assumptions Q_1 and Q_2 be satisfied and let $V, W \in L^\infty_{\mathbb{R}}(\Omega)$. If m has a finite total variation, then the estimate

$$\|(W_-(K[W],K[V]) - I\ )\|_{\mathcal{B}(\ )} \leqslant 2\pi|\Omega|L(\|V\|_{L^\infty})L(\|W\|_{L^\infty})\|V - W\|_{L^\infty} \tag{52}$$

holds where $L(\cdot)$ is given by (18).

Proof: Similar to formula (X.3.24) of Ref. 22 one has

$$((W_-(K[W],K[V]) - I\ )\vec{f},\vec{g})\ = -i\int_{-\infty}^{0} \mathrm{d}t([W - V]P\ \ e^{-itK[V]}\vec{f}, P\ \ e^{-itK[W]}\vec{g}),$$

for $\vec{f},\vec{g} \in \mathrm{dom}(K[V]) = \mathrm{dom}(K[W])$. Hence, we obtain the estimate

$$|((W_-(K[W],K[V]) - I\ )\vec{f},\vec{g})\ | \leqslant \|V - W\|_{L^\infty}\left(\int_{\mathbb{R}} \mathrm{d}t\|P\ \ e^{-itK[V]}\vec{f}\|^2\right)^{1/2}\left(\int_{\mathbb{R}} \mathrm{d}t\|P\ \ e^{-itK[W]}\vec{g}\|^2\right)^{1/2},$$

$\vec{f},\vec{g} \in$. Applying (48) and (49) we obtain

$$|((W_-(K[W],K[V])-I\ )\vec{f},\vec{g})\ | \leqslant 2\pi|\Omega|L(\|V\|_{L^\infty})L(\|W\|_{L^\infty})\|V-W\|_{L^\infty}\|\vec{f}\|\ \|\vec{g}$$

for $\vec{f},\vec{g}\in$ which proves (52). □

IV. CARRIER DENSITY OPERATOR AND CONTINUITY

A. Carrier density operator

In the following an operator $\varrho:\ \rightarrow$ is called a density operator if ϱ is a bounded, nonnegative, self-adjoint operator. The operator ϱ is called a steady state, if ϱ commutes with $K[V]$, see Ref. 18. Thus any steady state ϱ is unitarily equivalent to a multiplication operator $\hat{\rho}$ on the Hilbert space $L^2(\mathbb{R},\mathbb{C}^2)$ induced by a density matrix $\rho(\cdot)\in L^\infty(\mathbb{R},\mathcal{B}(\mathbb{C}^2))$. In the following we assume that the function $\rho(\cdot)$ is fixed. This leads to a steady state of the form

$$\varrho[V]=\Phi[V]^{-1}\hat{\rho}\Phi[V], \tag{53}$$

which depends on V. The reduced density operator $\varrho\ [V]\in\mathcal{B}(\ )$ is defined

$$\varrho\ [V]:=P\ \ \varrho[V]\restriction\ .$$

Similarly, we define the reduced density operator $g\ (K[V])\in\mathcal{B}(\ )$ by

$$g\ (K[V]):=P\ \ g(K[V])\restriction\ .$$

Notice that by the Schrödinger assumption (5) one has

$$0\leqslant\varrho\ [V]\leqslant g\ (K[V]). \tag{54}$$

Lemma 4.1; Let the Schrödinger assumptions Q_1, Q_2, and Q_4 be satisfied. If $V\in L^\infty_{\mathcal{R}}(\Omega)$, then $g\ (K[V])$ is a trace class operator such that

$$0\leqslant\mathrm{tr}(g\ (K[V]))\leqslant\ (\|V_-\|_{L^\infty})^2 \tag{55}$$

where $(\cdot)$ is defined by (22).

Proof: Let $\{\psi_k\}_{k=1}^\infty$ be an orthonormal basis in . By the spectral theorem

$$\sum_{k=1}^n(g\ (K[V])\psi_k,\psi_k)=\sum_{k=1}^n(g(K[V])\psi_k,\psi_k)=\int_{\mathbb{R}}\mathrm{d}\lambda\ g(\lambda)\sum_{k=1}^n\frac{\mathrm{d}}{\mathrm{d}\lambda}(E_{K[V]}(\lambda)\psi_k,\psi_k),$$

where we have used that the spectral measure $E_{K[V]}(\cdot)$ of $K[V]$ is absolutely continuous with respect to the Lebesgue measure. Applying Lemma 3.10 we find

$$\int_{\mathbb{R}}\mathrm{d}\lambda\ g(\lambda)\frac{\mathrm{d}}{\mathrm{d}\lambda}(E_{K[V]}(\lambda)\psi_k,\psi_k)=\frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}\lambda\ g(\lambda)(T[V](\lambda)\psi_k,T[V](\lambda)\psi_k),\quad k\in\mathbb{N},$$

which yields

$$\sum_{k=1}^n(g(K[V])\psi_k,\psi_k)=\frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}\lambda\ g(\lambda)\sum_{k=1}^n(T[V](\lambda)\psi_k,T[V](\lambda)\psi_k).$$

Hence we obtain

$$\sum_{k=1}^n(g(K[V])\psi_k,\psi_k)\leqslant\frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}\lambda\ g(\lambda)\mathrm{tr}(T[V](\lambda)^*T[V](\lambda))$$

or

$$\sum_{k=1}^{n} (g(K[V])\psi_k, \psi_k) \leqslant \frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\mathrm{tr}_{\mathbb{C}^2}(T[V](\lambda)T[V](\lambda)^*). \tag{56}$$

By (38) we get

$$\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\mathrm{tr}_{\mathbb{C}^2}(T[V](\lambda)T[V](\lambda)^*) = -\int d\lambda\, g(\lambda)\omega'[V](\lambda), \quad \lambda \in \mathbb{R},$$

which yields

$$\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\mathrm{tr}_{\mathbb{C}^2}(T[V](\lambda)T[V](\lambda)^*) = -g(\lambda)\omega[V](\lambda)|_{\lambda=-\infty}^{\lambda=+\infty} + \int_{\mathbb{R}} d\lambda\, g'(\lambda)\omega[V](\lambda).$$

By Corollary 3.7 we have

$$-\omega[V](\lambda) \leqslant 2 + \frac{1}{\pi}\sqrt{\bar{m}|\Omega|}\sqrt{(\lambda + \|V_-\|_{L^\infty})_+}$$

for $\lambda \in \mathcal{R}$. We note that the conditions (6) and (7) imply

$$\lim_{\lambda\to\infty} \sqrt{\lambda} g(\lambda) = 0.$$

Taking into account this property we obtain

$$\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\mathrm{tr}_{\mathbb{C}^2}(T[V](\lambda)T[V](\lambda)^*) = \int_{\mathbb{R}} d\lambda\, g'(\lambda)\omega[V](\lambda).$$

Since $g'(\lambda) \geqslant 0$ for $\lambda \leqslant 0$ and $g'(\lambda) \leqslant 0$ for $\lambda \geqslant 0$ as well as $\omega[V](\lambda) \leqslant 0$, $\lambda \in \mathbb{R}$, we get

$$\begin{aligned}\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\mathrm{tr}_{\mathbb{C}^2}(T[V](\lambda)T[V](\lambda)^*) &\leqslant \int_0^{+\infty} d\lambda\, g'(\lambda)\omega[V](\lambda) \\ &\leqslant -\int_0^{\infty} d\lambda\, g'(\lambda)\left(2 + \frac{1}{\pi}\sqrt{\bar{m}|\Omega|}\sqrt{\lambda + \|V_-\|_{L^\infty}}\right).\end{aligned}$$

Integrating by parts we find

$$\begin{aligned}\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\mathrm{tr}_{\mathbb{C}^2}(T[V](\lambda)T[V](\lambda)^*) &\leqslant g(0)\left(2 + \frac{1}{\pi}\sqrt{\bar{m}|\Omega|}\sqrt{\|V_-\|_{L^\infty}}\right) \\ &\quad + \frac{1}{2\pi}\sqrt{\bar{m}|\Omega|}\int_0^{\infty} d\lambda \frac{g(\lambda)}{\sqrt{\lambda + \|V_-\|_{L^\infty}}},\end{aligned}$$

which yields the estimate

$$\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, g(\lambda)\mathrm{tr}_{\mathbb{C}^2}(T[V](\lambda)T[V](\lambda)^*) \leqslant \left(2g(0) + \frac{1}{2\pi}\sqrt{\bar{m}|\Omega|}\int_0^{\infty} d\lambda \frac{g(\lambda)}{\sqrt{\lambda}}\right) + \frac{1}{\pi}g(0)\sqrt{\bar{m}|\Omega|}\sqrt{\|V_-\|_{L^\infty}}.$$

From (56) we get the estimate

$$\sum_{k=1}^{n} (g(K[V])\psi_k, \psi_k) \leqslant \left(2g(0) + \frac{1}{2\pi}\sqrt{\bar{m}|\Omega|}\int_0^{\infty} d\lambda \frac{g(\lambda)}{\sqrt{\lambda}}\right) + \frac{1}{\pi}g(0)\sqrt{\bar{m}|\Omega|}\sqrt{\|V_-\|_{L^\infty}}$$

for $n \in \mathcal{N}$ which shows that $\Sigma_{k=1}^{\infty}(g(K[V])\psi_k, \psi_k)$ is finite for any orthonormal basis of . Hence, the restriction g $(K[V])$ is a trace class operator. Using the notation (9), (10), and (22) we obtain

(55). □

In the Hilbert space let us introduce the multiplication operator

$$(M(h)f)(x) := h(x)f(x), \quad f \in \mathrm{dom}(M(h)) = \quad ,$$

for functions $h \in L^\infty(\Omega)$. Since $\varrho\ [V]$ is a trace class operator the functional Ξ_ρ given by $h \to \mathrm{tr}(\varrho\ [V]M(h))$ is well-defined on $L^\infty(\Omega)$. Moreover, setting $\nu_\rho(\Delta) := \Xi(\chi_\Delta)$ for Borel subsets Δ of Ω one defines a Borel measure on Ω which is absolutely continuous with respect to the Lebesgue measure, cf. Ref. 18. Its Radon-Nikodym derivative $u_\rho[V] \in L^1(\Omega)$ obeys the relation

$$\mathrm{tr}(\varrho[V]M(h)) = \int_a^b \mathrm{d}x\, u_\rho[V](x)h(x), \quad h \in L^\infty(\Omega). \tag{57}$$

The function $u_\rho[V](\cdot)$ is not negative and is called the carrier density for a given potential $V \in L^\infty$. The operator $\mathcal{N}_\rho(V): L^\infty_{\mathbb{R}}(\Omega) \to L^1_{\mathbb{R}}(\Omega)$ defined by

$$\mathcal{N}_\rho(V) := u_\rho[V], \quad V \in \mathrm{dom}(\mathcal{N}_\rho) := L^\infty_{\mathbb{R}}(\Omega),$$

is called the carrier density operator.

Proposition 4.2: Let the Schrödinger assumptions Q_1, Q_2, and Q_4 be satisfied. If $V \in L^\infty_{\mathbb{R}}(\Omega)$, then

$$\|\mathcal{N}_\rho(V)\|_{L^1} \leqslant \quad (\|V_-\|_{L^\infty})^2 \tag{58}$$

where $(\cdot)$ *is defined by* (22).

Proof: From (57) one gets the estimate

$$\|u_\rho[V]\|_{L^1} \leqslant \|\varrho\ [V]\|_{\mathcal{B}_1(\ )} = \mathrm{tr}(\varrho\ [V]).$$

Using (54) we obtain the estimate

$$\|u_\rho[V]\|_{L^1} \leqslant \mathrm{tr}(g\ \ (K[V])).$$

Finally, taking into account Lemma 4.1 we verify (58). □

B. Lipschitz continuity

Further, it was shown that the carrier density operator is continuous, i.e., if $V_n \overset{L^\infty}{\to} V$, then $\mathcal{N}_\rho(V_n) \overset{L^1}{\to} \mathcal{N}_\rho(V)$. We are going to show that the continuity of the carrier density operator can be improved to bounded Lipschitz continuity, cf. Definition III.1.2 of Ref. 12.

At first let us prove the following lemma.

Lemma 4.3: Let $g(\cdot)$ be non-negative, continuously differentiable even functions obeying (6). *The condition* (8) *is satisfied if and only if*

$$|g(\lambda) - g(\mu)| \leqslant \quad \max\{g(\lambda), g(\mu)\}|\lambda - \mu| \tag{59}$$

holds for $\lambda, \mu \in \mathcal{R}$.

Proof: We assume $\lambda \leqslant \mu$. Obviously, we have

$$g(\mu) - g(\lambda) = \int_\lambda^\mu g'(t)\mathrm{d}t, \quad \lambda, \mu \in \mathbb{R},$$

which yields

$$|g(\mu)-g(\lambda)| \leqslant \int_{\lambda}^{\mu} g(t)\mathrm{d}t$$

where we have used (8). Let $\lambda \in \mathbb{R}_+$. Since $g(\lambda)$, $\lambda \in \mathbb{R}_+$, is decreasing by (6) we find

$$|g(\mu)-g(\lambda)| \leqslant g(\lambda)(\mu-\lambda), \quad 0 \leqslant \lambda \leqslant \mu,$$

which yields (59). If $\lambda \leqslant 0 \leqslant \mu$, then

$$|g(\mu)-g(\lambda)| = |g(\mu)-g(-\lambda)| \leqslant \max\{g(\mu),g(-\lambda)\}|\mu+\lambda| \leqslant \max\{g(\mu),g(\lambda)\}|\mu-\lambda|$$

which also yields (59). The case $\lambda \leqslant \mu \leqslant 0$ follows from the case $0 \leqslant \lambda \leqslant \mu$.

Conversely, if (59) is satisfied, then tending μ to λ we obtain

$$|g'(\lambda)| \leqslant \max\{g(\lambda),g(\lambda)\} = g(\lambda), \quad \lambda \in \mathbb{R},$$

which proves (8). □

Next we consider the operator $G[V] := \sqrt{g(K[V])}\restriction$ acting from into .

Lemma 4.4: Let the Schrödinger assumptions Q_1, Q_2, and Q_4 be satisfied. If $V \in L^{\infty}_{\mathbb{R}}(\Omega)$, then $G[V] \in \boldsymbol{\mathcal{B}}_2(\ ,\ )$ and

$$\|G[V]\|_{\mathcal{B}_2(\ ,\ )} \leqslant (\|V_-\|_{L^\infty}), \tag{60}$$

where $(\cdot)$ is defined by (22). If $V, W \in L^{\infty}_{\mathbb{R}}(\Omega)$, then

$$\|G[V]-G[W]\|_{\mathcal{B}_2(\ ,\ )} \leqslant (\ (\|V_-\|_{L^\infty}) + (\|W_-\|_{L^\infty}))\|V-W\|_{L^\infty}. \tag{61}$$

Proof: By

$$\|G[V]\|^2_{\mathcal{B}_2(\ ,\ )} = \mathrm{tr}(G[V]^* G[V]) = \mathrm{tr}(g\ (K[V]))$$

and Lemma 4.1 one gets (60). Further, from (8) and Lemma 4.3 we obtain that

$$|g(\lambda)-g(\mu)| \leqslant \max\{g(\lambda),g(\mu)\}|\lambda-\mu| \leqslant (g(\lambda)+g(\mu))|\lambda-\mu|, \quad \lambda,\mu \in \mathbb{R},$$

which yields

$$|\sqrt{g(\lambda)}-\sqrt{g(\mu)}|(\sqrt{g(\lambda)}+\sqrt{g(\mu)}) \leqslant (\sqrt{g(\lambda)}+\sqrt{g(\mu)})^2|\lambda-\mu|. \quad \lambda,\mu \in \mathbb{R}.$$

Therefore we get

$$|\sqrt{g(\lambda)}-\sqrt{g(\mu)}| \leqslant (\sqrt{g(\lambda)}+\sqrt{g(\mu)})|\lambda-\mu|, \quad \lambda,\mu \in \mathbb{R}.$$

Hence, if we put

$$h(\lambda,\mu) := \frac{\sqrt{g(\lambda)}-\sqrt{g(\mu)}}{(\lambda-\mu)(\sqrt{g(\lambda)}+\sqrt{g(\mu)})}, \quad \lambda,\mu \in \mathbb{R},$$

then $|h(\lambda,\mu)| \leqslant c$, $\lambda,\mu \in \mathbb{R}$. Since the operators V and W act only on the subspace we get $\sqrt{G[V]}(V-W)+(V-W)\sqrt{G[W]} \in \mathcal{B}_2(\ )$. Applying the technique of double operator spectral integrals[5–7] we find the representation

$$\sqrt{g(K[V])}-\sqrt{g(K[W])} = \int_{\mathbb{R}}\int_{\mathbb{R}} h(\lambda,\mu)\mathrm{d}E_{K[V]}(\lambda)\{G[V](V-W)+(V-W)G[W]^*\}\mathrm{d}E_{K[W]}(\mu),$$

which yields $\sqrt{g(K[V])}-\sqrt{g(K[W])} \in \mathcal{B}_2(\ )$. Moreover, we find the estimate

$$\|\sqrt{g(K[V])}-\sqrt{g(K[W])}\|_{\mathcal{B}_2(\ ,\ )} \leqslant \ \{\|G[V]\|_{\mathcal{B}_2(\ ,\ )}+\|G[W]\|_{\mathcal{B}_2(\ ,\ )}\}\|V-W\|_{\mathcal{B}(\ )}.$$

Since $G[V]:=\sqrt{g(K[V])}\restriction$ and $G[W]:=\sqrt{g(K[W])}\restriction$ we obtain

$$\|G[V]-G[W]\|_{\mathcal{B}_2(\ ,\ )} \leqslant \ \{\|G[V]\|_{\mathcal{B}_2(\ ,\ )}+\|G[W]\|_{\mathcal{B}_2(\ ,\ )}\}\|V-W\|_{\mathcal{B}(\ )}.$$

Using (60) we finally get (61). □

Proposition 4.5: Let the Schrödinger assumptions Q_1, Q_2, and Q_4 be satisfied. If m has a finite total variation and $V,W\in L^\infty_{\mathbb{R}}(\Omega)$, then

$$\|\mathcal{N}_\rho(V)-\mathcal{N}_\rho(W)\|_{L^1} \leqslant \quad (\|V\|_{L^\infty},\|W\|_{L^\infty})\|V-W\|_{L^\infty} \tag{62}$$

where $(\cdot,\cdot)$ *is given by* (23).

Proof: By (57) we get

$$\int_a^b \mathrm{d}x(u_\rho[V](x)-u_\rho[W](x))h(x)=\mathrm{tr}((\varrho\ [V]-\varrho\ [W])M(h))$$

for any $h\in L^\infty(\Omega)$ where $\varrho[V]$ and $\varrho[W]$ are defined in accordance with (53). By (51) we have

$$\varrho[V]=W_-(K[V],K_0)F^*\hat{\rho}FW_-(K[V],K_0)^*$$

and

$$\varrho[W]=W_-(K[W],K_0)F^*\hat{\rho}FW_-(K[W],K_0)^*.$$

The wave operators $W_-(K[V],K_0)$ and $W_-(K[W],K_0)$ exist and are complete; consequently, the wave operator $W_-(K[W],K[V])$ exists and is complete. Moreover, the representation

$$W_-(K[W],K_0)=W_-(K[W],K[V])W_-(K[V],K_0)$$

holds. For brevity we set $W_-[W,V]:=W_-(K[W],K[V])$ as well as $W_-[W]:=W_-(K[W],K_0)$ and $W_-[V]:=W_-(K[V],K_0)$. Let us introduce the matrix valued function

$$\rho_0(\lambda):=g(\lambda)^{-1}\rho(\lambda),\quad \lambda\in\mathbb{R}.$$

By assumption Q_4 one has

$$0\leqslant\rho_0(\lambda)\leqslant I_{\mathbb{C}^2},\quad \lambda\in\mathbb{R}.$$

Using this notation we find the representation

$$\begin{aligned}\varrho\ [V]-\varrho\ [W]&=G[V]^*\varrho_0[V]G[V]-G[W]^*\varrho_0[W]G[W]=(G[V]^*-G[W]^*)\varrho_0[V]G[V]\\&\quad+G[W]^*\varrho_0[V](G[V]-G[W])+G[W](\varrho_0[V]-\varrho_0[W])G[W].\end{aligned}$$

Hence, we get the estimate

$$\begin{aligned}\|\varrho\ [V]-\varrho\ [W]\|_{\mathcal{B}_1(\ ,\ )}&\leqslant\{\|G[V]\|_{\mathcal{B}_2(\ ,\ )}+\|G[W]\|_{\mathcal{B}_2(\ ,\ )}\}\|G[V]-G[W]\|_{\mathcal{B}_2(\ ,\ )}\\&\quad+\|G[W]\|_{\mathcal{B}_2(\ ,\ )}\|G[W]\|_{\mathcal{B}_2(\ ,\ )}\|\varrho_0[V]-\varrho_0[W]\|_{\mathcal{B}(\ )}.\end{aligned}$$

By the representation

$$\begin{aligned}\varrho_0[V]-\varrho_0[W]&=\varrho_0[V]-W_-[W,V]\varrho_0[V]W_-[W,V]^*\\&=(I\ -W_-[W,V])\varrho_0[V]W_-[W,V]^*+\varrho_0[V](I\ -W_-[W,V]^*)\end{aligned}$$

and Lemma 3.12 we obtain the estimate

$$\|\varrho_0[V]-\varrho_0[W]\|_{\mathcal{B}(\ )} \leqslant 4\pi|\Omega|L[V]L[W]\|V-W\|_{L^\infty}.$$

By Lemma 4.4 we get

$$\|\varrho\ [V]-\varrho\ [W]\|_{\mathcal{B}_1(\ ,\ )} \leqslant (\ (\quad(\|V\|_{L^\infty})+\quad(\|W\|_{L^\infty}))^2 + 4\pi|\Omega|L(\|V\|_{L^\infty})L(\|W\|_{L^\infty})\quad(\|V\|_{L^\infty})\quad(\|W\|_{L^\infty}))\|V-W\|_{L^\infty}$$

which proves (62). Taking into account the definition (23) we verify (62). □

V. DISSIPATIVE SCHRÖDINGER-POISSON SYSTEM

A. Rigorous definition

By $W_0^{1,2}(\Omega)$ we denote the subspace of $W^{1,2}(\Omega)$ given by $W_0^{1,2}(\Omega) := \{f \in W^{1,2}(\Omega) : f(a)=f(b)=0\}$. Its dual space with respect to the scalar product $\langle\cdot,\cdot\rangle$ of $L^2(\Omega)$ is denoted by $W_0^{-1,2}(\Omega)$.

At first we will give a rigorous definition of Poisson's equation and afterwards define what we will call a solution of the dissipative Schrödinger Poisson system. We define the Poisson operator $\mathcal{P}: W_{\mathbb{R}}^{1,2}(\Omega) \to W_{0,\mathbb{R}}^{-1,2}(\Omega)$ as usual by

$$\langle \mathcal{P}\upsilon, \varsigma\rangle = \int_a^b \mathrm{d}x\ \epsilon \frac{\mathrm{d}\upsilon}{\mathrm{d}x}\frac{\mathrm{d}\varsigma}{\mathrm{d}x}, \quad \upsilon \in W_{\mathbb{R}}^{1,2}(\Omega), \quad \varsigma \in W_{0,\mathbb{R}}^{1,2}(\Omega).$$

Further, we set $\mathcal{P}_0 := \mathcal{P} \restriction W_{0,\mathbb{R}}^{1,2}(\Omega)$. The operators $\mathcal{P}$ and $\mathcal{P}_0$ are linear and bounded. We have

$$|\langle \mathcal{P}\upsilon, \varsigma\rangle| \leqslant \|\epsilon\|_{L^\infty}\|\upsilon\|_{W^{1,2}}\|\varsigma\|_{W_0^{1,2}}.$$

Hence $\mathcal{P}$ is continuous. Furthermore, one has the estimate

$$\|\varphi\|_{W_0^{1,2}} \leqslant \sqrt{1+|\Omega|}\|\varphi'\|_{L^2}, \quad \varphi \in W_0^{1,2}(\Omega).$$

Thus, we get by (5.1)

$$\|\varphi\|_{W_0^{1,2}}^2 \leqslant \|1/\epsilon\|_{L^\infty}\sqrt{1+|\Omega|}\langle \mathcal{P}_0\varphi, \varphi\rangle, \quad \varphi \in W_0^{1,2}(\Omega).$$

By the Lax-Milgram lemma the inverse operator $\mathcal{P}_0^{-1}$ exists and its norm does not exceed $\|1/\epsilon\|_{L^\infty}\sqrt{1+|\Omega|}$, i.e.,

$$\|\mathcal{P}_0^{-1}\|_{\mathcal{B}(W_0^{-1,2}, W_0^{1,2})} \leqslant \|1/\epsilon\|_{L^\infty}\sqrt{1+|\Omega|}. \tag{63}$$

Definition 5.1: Let $u^\pm \in L^1$. We say that $\varphi \in W_{\mathbb{R}}^{1,2}$ satisfies Poisson's equation with boundary conditions $\varphi(a)=\varphi_a$ and $\varphi(b)=\varphi_b$ if $\zeta := \varphi - \hat{\varphi} \in W_0^{1,2}(\Omega)$ and the equation

$$\mathcal{P}_0\zeta = C + E_1 u^+ - E_1 u^-$$

is fulfilled, where $\hat{\varphi}$ is defined by (11).

Definition 5.2: We say that $\varphi \in W_{\mathbb{R}}^{1,2}(\Omega)$ is a solution of the dissipative Schrödinger-Poisson system if

1. the carrier densities $u^\pm \in L^1(\Omega)$ are given by $u^\pm = \mathcal{N}_{\rho^\pm}^{\pm}(V_0^\pm \pm \hat{\varphi} \pm E_\infty\zeta)$, $\zeta := \varphi - \hat{\varphi}$, and
2. φ satisfies the Poisson equation with boundary conditions $\varphi(a)=\varphi_a$ and $\varphi(b)=\varphi_b$.

B. Existence of solutions and estimates

Let us introduce the non-linear mappings $\mathcal{Q}: L_{\mathbb{R}}^\infty(\Omega) \to W_{0,\mathbb{R}}^{1,2}(\Omega)$,

$$\mathcal{Q}(\psi) := \mathcal{P}_0^{-1}(C + E_1\mathcal{N}_{\rho^+}^+(V_0^+ + \hat{\varphi} + \psi) - E_1\mathcal{N}_{\rho^-}^-(V_0^- - \hat{\varphi} - \psi)), \tag{64}$$

$\psi \in \mathrm{dom}(\mathcal{Q}) = L^\infty_{\mathbb{R}}(\Omega)$, and $\mathcal{Q}_\infty : L^\infty_{\mathbb{R}}(\Omega) \to L^\infty_{\mathbb{R}}(\Omega)$,

$$\mathcal{Q}_\infty(\psi) = E_\infty \mathcal{Q}(\psi),$$

$\psi \in \mathrm{dom}(\mathcal{Q}_\infty) = L^\infty_{\mathbb{R}}(\Omega)$. It was shown in Ref. 2 that the dissipative Schrödinger-Poisson system admits a solution if and only if $\mathcal{Q}_\infty$ admits a fixed point. Moreover, if $\zeta_\infty \in L^\infty_{\mathbb{R}}(\Omega)$ is a fixed point, i.e., $\mathcal{Q}_\infty(\zeta_\infty) = \zeta_\infty$, then $\varphi := \hat{\varphi} + \mathcal{Q}(\zeta_\infty)$ is a solution of the dissipative Schrödinger-Poisson system. If $\zeta_\infty \in L^\infty_{\mathbb{R}}(\Omega)$ is a fixed point, i.e., $\zeta_\infty = \mathcal{Q}_\infty(\zeta_\infty)$, then one has the estimate

$$\begin{aligned}\|\zeta_\infty\|_{L^\infty} = \|\mathcal{Q}_\infty(\zeta_\infty)\|_{L^\infty(\Omega)} \leqslant \varepsilon_1 \|\mathcal{P}_0^{-1}\|_{\mathcal{B}(W_0^{-1,2}, W_0^{1,2})} \times (\|C\|_{W_0^{-1,2}} + \varepsilon_1 \|\mathcal{N}_{\rho^+}^+(V_0^+ + \hat{\varphi} + \zeta_\infty)\|_{L^1} \\ + \varepsilon_1 \|\mathcal{N}_{\rho^-}^-(V_0^- - \hat{\varphi} - \zeta_\infty)\|_{L^1}).\end{aligned}$$

Taking into account (63) we obtain

$$\begin{aligned}\|\zeta_\infty\|_{L^\infty} = \|\mathcal{Q}_\infty(\zeta_\infty)\|_{L^\infty(\Omega)} \leqslant \varepsilon_1 \|1/\epsilon\|_{L^\infty} \sqrt{1 + |\Omega|} \times (\|C\|_{W_0^{-1,2}} + \varepsilon_1 \|\mathcal{N}_{\rho^+}^+(V_0^+ + \hat{\varphi} + \zeta_\infty)\|_{L^1} \\ + \varepsilon_1 \|\mathcal{N}_{\rho^-}^-(V_0^- - \hat{\varphi} - \zeta_\infty)\|_{L^1}).\end{aligned} \tag{65}$$

Applying Proposition 4.2 we find

$$\|\mathcal{N}_{\rho^+}^+(V_0^+ + \hat{\varphi} + \zeta_\infty)\|_{L^1} \leqslant B_0^+ + B_1^+ \sqrt{\|(V_0^+ + \hat{\varphi} + \zeta_\infty)_-\|_{L^\infty}},$$

which yields

$$\|\mathcal{N}_{\rho^+}^+(V_0^+ + \hat{\varphi} + \zeta_\infty)\|_{L^1} \leqslant B_0^+ + B_1^+ \sqrt{\|V_0^+ + \hat{\varphi}\|_{L^\infty}} + B_1^+ \sqrt{\|\zeta_\infty\|_{L^\infty}}.$$

Similarly, we obtain

$$\|\mathcal{N}_{\rho^-}^-(V_0^- - \hat{\varphi} - \zeta_\infty)\|_{L^1} \leqslant B_0^- + B_1^- \sqrt{\|V_0^- - \hat{\varphi}\|_{L^\infty}} + B_1^- \sqrt{\|\zeta_\infty\|_{L^\infty}}.$$

Inserting these estimates into (65) we find

$$\|\zeta_\infty\|_{L^\infty} \leqslant D_0 + D_1 \sqrt{\|\zeta_\infty\|_{L^\infty}}, \tag{66}$$

where D_0 and D_1 are given by (12) and (13). From (66) we obtain the estimate

$$\|\zeta_\infty\|_{L^\infty} \leqslant r_0 \tag{67}$$

for any fixed point of the map $\mathcal{Q}_\infty$ where r_0 is defined by (14). So the following theorem is proven:

Theorem 5.3: *[Ref. 3, Theorem 4.8] If the Schrödinger and Poisson assumptions are satisfied, then the dissipative Schrödinger-Poisson system always admits a solution. Moreover, for any solution* $\varphi \in W^{1,2}_{\mathbb{R}}(\Omega)$ *the estimate* $\|\varphi_\infty - \hat{\varphi}\|_{L^\infty} \leqslant r_0$ *holds.*

We note that the radius r_0 depends only on the Schrödinger and Poisson data. Therefore, if the Schrödinger and Poisson data are fixed, then the radius r_0 is fixed.

However, Theorem 5.3 does not answer the question whether this solution is unique.

C. Uniqueness

Now we are going to give conditions under which the solution of the dissipative Schrödinger-Poisson system is unique.

Theorem 5.4: *Let the Schrödinger and Poisson assumptions be satisfied. If* $m^\pm$ *have finite total variations and the condition* < 1 *is valid, where* *is given by* (25), *then the dissipative Schrödinger-Poisson system admits only one solution.*

Proof: Let ζ_∞ and ζ'_∞ be two fixed points of $\mathcal{Q}_\infty$. From (64) we get the representation

$$\zeta_\infty - \zeta'_\infty = E_\infty \mathcal{P}_0^{-1} E_1 \{(\mathcal{N}^+_{\rho^+}(V^+) - \mathcal{N}^+_{\rho^+}(W^+)) - (\mathcal{N}^-_{\rho^-}(V^-) - \mathcal{N}^-_{\rho^-}(W^-))\}$$

where

$$V^+ := V_0^+ + \hat{\varphi} + \zeta_\infty \text{ and } W^+ := V_0^+ + \hat{\varphi} + \zeta'_\infty$$

and

$$V^- := V_0^- + \hat{\varphi} + \zeta_\infty \text{ and } W^- := V_0^- + \hat{\varphi} + \zeta'_\infty.$$

Hence we find

$$\|\zeta_\infty - \zeta'_\infty\|_{L^\infty} \leqslant \varepsilon_1^2 \|\mathcal{P}_0^{-1}\|_{\mathcal{B}(W_0^{-1,2}, W_0^{1,2})} \times \{\|\mathcal{N}^+_{\rho^+}(V^+) - \mathcal{N}^+_{\rho^+}(W^+)\|_{L^1} + \|\mathcal{N}^-_{\rho^-}(V^-) - \mathcal{N}^-_{\rho^-}(W^-)\|_{L^1}\}.$$

Using (63) we obtain

$$\|\zeta_\infty - \zeta'_\infty\|_{L^\infty} \leqslant \varepsilon_1^2 \|1/\epsilon\|_{L^\infty} \sqrt{1 + |\Omega|} \times \{\|\mathcal{N}^+_{\rho^+}(V^+) - \mathcal{N}^+_{\rho^+}(W^+)\|_{L^1} + \|\mathcal{N}^-_{\rho^-}(V^-) - \mathcal{N}^-_{\rho^-}(W^-)\|_{L^1}\}.$$

Applying Proposition 4.5 we get

$$\|\zeta_\infty - \zeta'_\infty\|_{L^\infty} \leqslant \varepsilon_1^2 \|1/\epsilon\|_{L^\infty} \sqrt{1 + |\Omega|} \times \{ \quad ^+(\|V^+\|_{L^\infty}, \|W^+\|^{L^\infty}) + \quad ^-(\|V^-\|_{L^\infty}, \|W^-\|^{L^\infty})\} \|\zeta_\infty - \zeta'_\infty\|_{L^\infty}.$$

We have

$$\|V^+\|_{L^\infty} \leqslant \|V_0^+ + \hat{\varphi}\|_{L^\infty} + \|\zeta_\infty\|_{L^\infty} \leqslant r_1^+,$$

where we have used the estimate (67) and r_1^+ is defined by (15). Similarly we prove that

$$\|W^+\|_{L^\infty} \leqslant r_1^+$$

and

$$\|V^-\|_{L^\infty} \leqslant r_1^- \text{ and } \|W^-\|_{L^\infty} \leqslant r_1^-,$$

where we have used the definitions (15). Since

$$^\pm(\|V^\pm\|_{L^\infty}, \|W^\pm\|_{L^\infty}) \leqslant \quad ^\pm(r_1^\pm, r_1^\pm)$$

we obtain

$$\|\zeta_\infty - \zeta'_\infty\|_{L^\infty} \leqslant \varepsilon_1^2 \|1/\epsilon\|_{L^\infty} \sqrt{1 + |\Omega|} \quad \|\zeta_\infty - \zeta'_\infty\|_{L^\infty},$$

where given by (24). Hence, if condition (25) is satisfied, then $\|\zeta_\infty - \zeta'_\infty\|_{L^\infty}$ has to be zero which proves the uniqueness. □

D. Uniqueness and shrinking

Our next aim is to show that a dissipative Schrödinger-Poisson system admits always a solution if $|\Omega|$ is small. To this end we introduce the following

Definition 5.5: Let $\Omega' \subseteq \Omega$ and let = ∩ be Schrödinger-Poisson data of the device Ω. We say ′ := ′ ∩ ′ are shrunken Schrödinger-Poisson data of if

$$' := \{m^\pm \restriction \Omega', \kappa_a^\pm, \kappa_b^\pm, V_0^\pm \restriction \Omega', \rho^\pm\} \text{ and } ' := \{C \restriction \Omega', \epsilon \restriction \Omega', \varphi_a, \varphi_b\}.$$

The corresponding dissipative Schrödinger-Poisson system is called a shrunken dissipative Schrödinger-Poisson system.

Definition 5.5 means that we leave unchanged the boundary coefficients $\kappa_a^\pm, \kappa_b^\pm$ of the dissipative Schrödinger operators and the density matrices as well as the boundary values of the

inhomogeneous Poisson equation but we restrict the effective masses $m^{\pm}$, the external potentials $V_0^{\pm}$, the doping profile C, and dielectric permittivity ϵ to the subinterval Ω'.

We note that the quantities (9)–(25) except (19) in fact depend on the interval Ω. We express this fact by adding in notation the term $[\Omega]$, for instance, $B_0^{\pm}[\Omega]$, $B_1^{\pm}[\Omega]$, $\hat{\varphi}[\Omega](x), \ldots,$ $[\Omega]$.

Theorem 5.6: *Let the Schrödinger and Poisson assumptions be satisfied and let $m^{\pm}$ have finite total variations. A shrunken dissipative Schrödinger-Poisson system admits a unique solution if $|\Omega'|$, $\Omega' \subseteq \Omega$, is sufficiently small.*

Proof. By Theorem 4 it is sufficiently to show that $\limsup_{|\Omega'|\to 0} \quad [\Omega']=0$. Since

$$\underline{m}^{\pm} \leqslant m^{\pm}(x) \leqslant \bar{m}^{\pm}, \quad x \in \Omega',$$

we obtain from (9) and (10) that

$$\lim_{|\Omega'|\to 0} B_0^{\pm}[\Omega'] = 2g^{\pm}(0) \text{ and } \lim_{|\Omega'|\to 0} B_1^{\pm}[\Omega'] = 0.$$

Since

$$\|\hat{\varphi}[\Omega']\|_{L^{\infty}(\Omega')} \leqslant \max\{|\varphi_a|, |\varphi_b|\}$$

we find

$$\|V_0^{\pm} \restriction \Omega' + \hat{\varphi}[\Omega']\|_{L^{\infty}(\Omega')} \leqslant \|V_0^{\pm}\|_{L^{\infty}(\Omega)} + \max\{|\varphi_a|, |\varphi_b|\}.$$

Taking into account this estimate and using $\|C \restriction \Omega'\|_{W^{-1,2}} \leqslant \|C\|_{W^{-1,2}}$, $\varepsilon_1[\Omega'] \leqslant \sqrt{|\Omega'|}$ we obtain

$$\lim_{|\Omega'|\to 0} D_0^{\pm}[\Omega'] = 0 \text{ and } \lim_{|\Omega'|\to 0} D_1^{\pm}[\Omega'] = 0$$

which yields

$$\lim_{|\Omega'|\to 0} r_0^{\pm}[\Omega'] = 0$$

and

$$\limsup_{|\Omega'|\to 0} r_1^{\pm}[\Omega'] \leqslant \|V_0^{\pm}\|_{L^{\infty}(\Omega)} + \max\{|\varphi_a|, |\varphi_b|\}. \tag{68}$$

Since $\vee_{a'}^{b'}(1/m^{\pm} \restriction \Omega') \leqslant \vee_a^b 1/m^{\pm}$, $\Omega' = (a', b')$, we get

$$\limsup_{|\Omega'|\to 0} \quad {}^{\pm}[\Omega'] \leqslant \quad {}^{\pm}[\Omega].$$

Further, we have

$$\limsup_{|\Omega'|\to 0} R_j^{\pm}(r_1^{\pm}[\Omega']) \leqslant \quad {}^{\pm}[\Omega]\left(1 + |\kappa_j^{\pm}| \sqrt{\frac{2}{\underline{m}^{\pm}}}\right), \quad j = a, b.$$

Using Lemma 3.1, (20) and (68) one gets

$$\lim_{|\Omega'|\to 0} \{2r_1^{\pm}[\Omega'] + 2\gamma_0[\Omega']\}|\Omega| = 4 \ {}^{\pm}\bar{m}^{\pm}$$

which yields

$$\lim_{|\Omega'|\to 0} \sup R_j^{\pm}(2r_1^{\pm}[\Omega'] + 2\gamma_0[\Omega']) \leqslant \quad {}^{\pm}[\Omega]\left(1 + |\kappa_j^{\pm}|\sqrt{\frac{2}{\underline{m}^{\pm}}}\right) \times \exp\left\{4 \ {}^{\pm}\bar{m}^{\pm}(\quad {}^{\pm}[\Omega])^2\sqrt{\frac{2}{\underline{m}^{\pm}}}\right\}, \quad j = a,b.$$

Using that we obtain

$$\lim_{|\Omega'|\to 0} \sup L^{\pm}(r^{\pm}[\Omega']) \leqslant \quad {}^{\pm}[\Omega]\exp\left\{4 \ {}^{\pm}\bar{m}^{\pm}(\quad {}^{\pm}[\Omega])^2\sqrt{\frac{2}{\underline{m}^{\pm}}}\right\} \times \left\{\frac{1}{(\alpha_a^{\pm})^2}\left(1 + |\kappa_a^{\pm}|\sqrt{\frac{2}{\underline{m}^{\pm}}}\right) + \frac{1}{(\alpha_b^{\pm})^2}\left(1 + |\kappa_b^{\pm}|\sqrt{\frac{2}{\underline{m}^{\pm}}}\right)\right\}.$$

By

$$\lim_{|\Omega'|\to 0} \quad {}^{\pm}(r_1^{\pm}[\Omega']) = \sqrt{2g^{\pm}(0)}.$$

we have

$$\lim_{|\Omega'|\to 0} \quad {}^{\pm}(r^{\pm}[\Omega'], r^{\pm}[\Omega']) = 8 \ {}^{\pm}g^{\pm}(0).$$

Therefore, we finally obtain

$$\lim_{|\Omega'|\to 0} \quad [\Omega'] = 8(\ {}^{+}g^{+}(0) + \ {}^{-}g^{-}(0))$$

where

$$[\Omega'] := \quad {}^{+}(r_1^{+}[\Omega'], r_1^{+}[\Omega']) + \quad {}^{-}(r_1^{-}[\Omega'], r_1^{-}[\Omega']).$$

Since $\lim_{|\Omega'|\to 0}\varepsilon_1[\Omega']=0$ we find $\lim_{|\Omega'|\to 0} \ [\Omega']=0$ where

$$[\Omega'] := \varepsilon_1^2[\Omega']\sqrt{1 + |\Omega'|} \ \ [\Omega'].$$

Applying Theorem 5.4 we see that for sufficiently small domains $\Omega' \subseteq \Omega$ the solution of the dissipative Schrödinger-Poisson system is unique. □

VI. REMARKS

Let us comment on the results.

1. Comparing the existence Theorem 5.3 with Theorem 4.8 of Ref. 2 one observes that Theorem 5.3 proves the existence under weaker assumptions. In particular, the Schrödinger assumption Q_4 is weaker than Assumption 4.2 $A_4^{\pm}$ of Ref. 2. The assumption Q_4 is close to a necessary condition. However, both proofs use the Schauder fixed point theorem.
2. In contrast to Ref. 2 the proof of the crucial estimate (58) of Proposition 4.2, cf. Theorem 3.1 of Ref. 2 is now based on the phase shift and its asymptotic behavior at $-\infty$ and $+\infty$.
3. The asymptotic properties of the phase shift are established by a detailed investigation in Ref. 26.
4. The uniqueness proof is essentially based on the Lipschitz continuity of the carrier density operator, cf. Proposition 4.5 which heavily rests on the Lipschitz continuity of the Lax-Phillips wave operators, cf. Sec. III C. This continuity relies on Kato's theory of smooth operators, cf. Refs. 22 and 23.
5. The results of the paper, in particular the results of Sec. V D, suggest the possibility that the solution of the dissipative hybrid model, cf., Ref. 4, is also unique provided the quantum zone is sufficiently small.

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Polyhedral realizations of crystal bases for quantum algebras of finite types

Ayumu Hoshino[a)]
Department of Mathematics, Sophia University, Tokyo 102-8554, Japan

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Polyhedral realization of crystal bases is one of the methods for describing the crystal base $B(\infty)$ of a quantized enveloping algebra explicitly. This method can be applied to symmetrizable Kac-Moody types. We can also apply this method to the crystal bases $B(\lambda)$ of integrable highest weight modules and of modified quantum algebras. But, the explicit forms of the polyhedral realizations of crystal bases $B(\infty)$ and $B(\lambda)$ are only given in the case of arbitrary rank 2, of A_n and of $A_n^{(1)}$. So, we will give the polyhedral realizations of crystal bases $B(\infty)$ and $B(\lambda)$ for all simple Lie algebras in this paper. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The quantum algebra $U_q(\mathfrak{g}) := \langle e_i, f_i, q^h \rangle_{i \in I} (I = \{1, 2, \ldots, n\})$ which was introduced in the study of solvable lattice models is applied to the several kinds of study of mathematical physics and plays important roles. The nilpotent part $U_q^-(\mathfrak{g}) (= \langle f_i \rangle_{i \in I})$ of $U_q(\mathfrak{g})$ has a crystal base $B(\infty)$ which was constructed by Kashiwara[1] and the irreducible integrable highest weight representaion of $U_q(\mathfrak{g})$ also has crystal base $B(\lambda)$.

The crystal base has been realized by several methods but it is not so easy to obtain the explicit form. Polyhedral realization of crystal bases is one of the methods for realizing crystal bases explicitly, which was introduced by Nakashima and Zelevinsky.[2] We can describe a vector in the crystal base $B(\infty)$ as a lattice point of certain convex polyhedron in an infinite $\mathbb{Z}$-lattice by this method. This method can be applied to symmetrizable Kac-Moody types and applied to the crystal base $B(\lambda)$ of the irreducible integrable highest weight module. In Ref. 2, polyhedral realizations of $B(\infty)$ are given when $\mathfrak{g}$ is arbitrary of rank 2, when $\mathfrak{g}$ is of type A_n and when $\mathfrak{g}$ is of type $A_{n-1}^{(1)}$ and in Ref. 3, Nakashima gave the polyhedral realizations of the crystal base $B(\lambda)$ $(\lambda \in P_+)$ of irreducible integrable highest weight module when $\mathfrak{g}$ is the same cases as the mentioned earlier. He and the author[4] applied this method to the modified quantum algebras and gave the polyhedral realizations of $B(U_q(\mathfrak{g})a_\lambda)$ and also for some specific connected component $B_0(\lambda)$ $(\lambda \in P)$ containing $u_\infty \otimes t_\lambda \otimes u_{-\infty}$ for $\mathfrak{g}$ of type A_n under certain assumptions on the weight λ and for $\mathfrak{g}$ of type $A_1^{(1)}$ on positive level λ and in Ref. 5 the author gave polyhedral realization for $B_0(\lambda)$ for arbitrary rank 2 cases on positive level λ. After Nakashima and Zelevinsky's work, Littelmann[6] described the crystal base $B(\infty)$ by some inequalities (which are called "cones") for all simple Lie algebras and $B(\lambda)$ for classical Lie algebras for a special choice of a reduced word for a longest element of Weyl group. Gleizer and Postnikov[7] described the canonical base for A_n and any reduced word. They also obtained Littlewood-Richardson coefficients $C_{\lambda,\mu}^{\nu}$. Berenstein and Zelevinsky[8] described the canonical bases for any reduced word and $C_{\lambda,\mu}^{\nu}$ for B_n, C_n, and D_n explicitly, which imply that the weight multiplicity formula of $B(\lambda)$ is given. As a result, they described the canonical bases and the crystal base $B(\lambda)$ by similar expression to our results, but it

a)Electronic mail: a-hoshin@mm.sophia.ac.jp

seems to be different from ours. In this paper, we will give the polyhedral realizations of crystal bases $B(\infty)$ and $B(\lambda)$ for all simple Lie algebras. In order to treat the cases, we improve the Theorem in Ref. 3 and obtain the polyhedral realizations.

This paper is organized as follows: in Sec. II, we review the theory of crystal base and methods of polyhedral realizations of $B(\infty)$ and $B(\lambda)$. In Sec. III, we improve the method which is given in Ref. 2 and obtain the explicit forms of the polyhedral realizations of $B(\infty)$ and $B(\lambda)$ for all simple Lie algebras. But, we do not write in this paper about the $B(\lambda)$ for E_7 and E_8 since numerous inequalities appear.

II. PRELIMINARIES

A. Crystal bases and crystals

In this section, we review the theory of crystal bases and crystals. We fix a finite index set I and let $A=(a_{ij})_{i,j\in I}$ be a generalized symmetrizable Cartan matrix, $(\mathfrak{t},\{\alpha_i\}_{i\in I},\{h_i\}_{i\in I})$ the associated Cartan data, and $\mathfrak{g}$ the associated Kac-Moody Lie algebra where α_i (respectively, h_i) is called a simple root (respectively, simple coroot). Let P be a weight lattice with a $\mathbb{Q}$-valued symmetric bilinear form $(\cdot,)$, P^* a dual lattice including $\{h_i\}_{\in I}$, and $Q:=\oplus_{i\in I}\mathbb{Q}(q)\alpha_i$ a root lattice. The quantum algebra $U_q(\mathfrak{g})$ is the associative algebra with 1 over $\mathbb{Q}(q)$ generated by e_i,f_i,q^h $(i\in I,h\in P^*)$ with the usual relations. Let $U_q^-(\mathfrak{g}):=\langle f_i\rangle_{i\in I}$ be the subalgebra of $U_q(\mathfrak{g})$ and $V(\lambda)$ be the irreducible integrable highest weight module. $U_q^-(\mathfrak{g})$ [respectively, $V(\lambda)$] have a crystal base $(L(\infty),B(\infty))$ [respectively, $(L(\lambda),B(\lambda))$] satisfying some properties. Let $\pi_\lambda: U_q^-(\mathfrak{g})\to V(\lambda)\cong U_q^-(\mathfrak{g})/\Sigma_i U_q^-(\mathfrak{g})f_i^{1+\langle h_i,\lambda\rangle}$ be the canonical projection and $\hat{\pi}_\lambda: L(\infty)/qL(\infty)\to L(\lambda)/qL(\lambda)$ be the induced map from π_λ. We note that $\hat{\pi}_\lambda(B(\infty))=B(\lambda)\sqcup\{0\}$.

The notion of crystal is obtained by abstracting the combinatorial properties of crystal bases. A crystal B has maps $wt: B\to P,\varepsilon_i,\varphi_i: B\to\mathbb{Z}\sqcup\{-\infty\}$ and $\tilde{e}_i,\tilde{f}_i: B\sqcup\{0\}\to B\sqcup\{0\}$ with some axioms. In fact, crystal bases $B(\infty)$ and $B(\lambda)$ are also crystals. The tensor product of the crystal bases is again crystal base and so we can consider the tensor product of crystals.

B. Polyhedral realization of $B(\infty)$

In this section, we review the polyhedral realization of the crystal $B(\infty)$ (see Ref. 3).

First, we recall the crystal structure of $\mathbb{Z}^\infty$. We consider the following additive groups:

$$\mathbb{Z}^\infty := \{(\cdots,x_k,\cdots,x_2,x_1)\,|\,x_k\in\mathbb{Z} \text{ and } x_k=0 \text{ for } k\gg 0\}.$$

We will denote by $\mathbb{Z}^\infty_{\geqslant 0}\subset\mathbb{Z}^\infty$ the semigroup of non-negative sequences. Take an infinite sequence of indices $\iota=(\ldots,i_k,\ldots,i_2,i_1)$ from I such that

$$i_k\neq i_{k+1} \text{ for any } k, \quad \text{and} \quad \sharp\{k>0: i_k=i\}=\infty \text{ for any } i\in I. \tag{2.1}$$

The crystal structure on $\mathbb{Z}^\infty$ associated with ι is defined as follows. Let $\vec{x}=(\ldots,x_2,x_1)\in\mathbb{Z}^\infty$. We set for $k\geqslant 1$

$$\sigma_k(\vec{x}) := x_k+\sum_{j>k}\langle h_{i_k},\alpha_{i_j}\rangle x_j. \tag{2.2}$$

Since $x_j=0$ for $j\gg 0$, σ_k is well-defined. Let $\sigma^{(i)}(\vec{x}):=\max_{k:i_k=i}\sigma_k(\vec{x})$ and

$$M^{(i)}=M^{(i)}(\vec{x}) := \{k: i_k=i,\sigma_k(\vec{x})=\sigma^{(i)}(\vec{x})\}. \tag{2.3}$$

Note that $\sigma^{(i)}(\vec{x})\geqslant 0$, and that $M^{(i)}=M^{(i)}(\vec{x})$ is finite set if and only if $\sigma^{(i)}(\vec{x})>0$. Now, we define the map $\tilde{e}_i:\mathbb{Z}^\infty\to\mathbb{Z}^\infty\sqcup\{0\}$, $\tilde{f}_i:\mathbb{Z}^\infty\to\mathbb{Z}^\infty$, by $\tilde{e}_i(0)=\tilde{f}_i(0)=0$ and

$$(\tilde{f}_i(\vec{x}))_k=x_k+\delta_{k,\min M^{(i)}}, \tag{2.4}$$

$$(\tilde{e}_i(\vec{x}))_k = x_k - \delta_{k,\max M^{(i)}} \text{ if } \sigma^{(i)}(\vec{x}) > 0 \quad \text{otherwise } \tilde{e}_i(\vec{x}) = 0, \tag{2.5}$$

where $\delta_{i,j}$ is Kronecker's delta. We also define the weight function and the function ε_i and φ_i on $\mathbb{Z}^\infty$ as follows:

$$wt(\vec{x}) := -\sum_{j=-\infty}^{\infty} x_j \alpha_{i_j}, \quad \varepsilon_i(\vec{x}) := \sigma^{(i)}(\vec{x}), \quad \varphi_i(\vec{x}) := \langle h_i, wt(\vec{x}) \rangle + \varepsilon_i(\vec{x}). \tag{2.6}$$

We denote this crystal by $\mathbb{Z}^\infty_\iota$.

Proposition 2.1 (Ref. 9): There is a unique embedding of crystals according to ι,

$$\Psi_\iota : B(\infty) \hookrightarrow \mathbb{Z}^\infty_{\geqslant 0} \subset \mathbb{Z}^\infty_\iota \ (u_\infty \mapsto (\cdots, 0, 0)). \tag{2.7}$$

This embedding is called *Kashiwara embedding*.

Next, we review the polyhedral realization of $B(\infty)$ for describing the image of *Kashiwara embedding*. We consider the following infinite dimensional vector spaces and their dual spaces:

$$\mathbb{Q}^\infty := \{\vec{x} = (\ldots, x_k, \ldots, x_2, x_1) : x_k \in \mathbb{Q} \text{ and } x_k = 0 \text{ for } k \gg 0\},$$

$$(\mathbb{Q}^\infty)^* := \mathrm{Hom}(\mathbb{Q}^\infty, \mathbb{Q}).$$

We will write a linear form $\varphi \in (\mathbb{Q}^\infty)^*$ as $\varphi(\vec{x}) = \sum_{k \geqslant 1} \varphi_k x_k$ $(\varphi_j \in \mathbb{Q})$. For the sequence $\iota = (i_k)_{k \geqslant 1}$ and $k \geqslant 1$, we set

$$k^{(+)} := \min\{l : l > k \text{ and } i_k = i_l\},$$

$$k^{(-)} := \max\{l : l < k \text{ and } i_k = i_l\} \text{ if it exists} \quad \text{otherwise } k^{(-)} = 0.$$

We define a linear form β_k $(k \geqslant 1)$ on $\mathbb{Q}^\infty$ by

$$\beta_k(\vec{x}) = \sigma_k(\vec{x}) - \sigma_{k^{(+)}}(\vec{x}) = x_k + \sum_{k < j < k^{(+)}} \langle h_{i_k}, \alpha_{i_j} \rangle x_j + x_{k^{(+)}}. \tag{2.8}$$

By using these linear forms, let us define a piecewise-linear operator $S_k = S_{k,\iota}$ on $(\mathbb{Q}^\infty)^*$ as follows:

$$S_k(\varphi) := \begin{cases} \varphi - \varphi_k \beta_k & \text{if } \varphi_k > 0, \\ \varphi - \varphi_k \beta_{k^{(-)}} & \text{if } \varphi_k \leqslant 0, \end{cases} \tag{2.9}$$

for $\varphi(\vec{x}) = \sum \varphi_k x_k \in (\mathbb{Q}^\infty)^*$. Here we set

$$\Xi_\iota := \{S_{j_l} \cdots S_{j_2} S_{j_1}(x_{j_0}) \mid l \geqslant 0, j_0, j_1, \ldots, j_l \geqslant 1\}, \tag{2.10}$$

$$\Sigma_\iota := \{\vec{x} \in \mathbb{Z}^\infty \subset \mathbb{Q}^\infty \mid \varphi(\vec{x}) \geqslant 0 \text{ for any } \varphi \in \Xi_\iota\}. \tag{2.11}$$

We impose on ι the following "positivity assumption" (P):

$$\text{(P) for } \iota, \quad \text{if } k^{(-)} = 0 \text{ then } \varphi_k \geqslant 0 \text{ for any } \varphi(\vec{x}) = \sum_k \varphi_k x_k \in \Xi_\iota. \tag{2.12}$$

Theorem 2.2 (Ref. 2): *Let* ι *be the sequence of indices satisfying (2.1) and the positivity assumption* (*P*). *Let* $\Psi_\iota : B(\infty) \hookrightarrow \mathbb{Z}^\infty_\iota$ *be the Kashiwara embedding. Then, we have* $\mathrm{Im}(\Psi_\iota)(\cong B(\infty)) = \Sigma_\iota$.

We call Σ_ι the polyhedral realization of $B(\infty)$.

C. Polyhedral realization of $B(\lambda)$

In this section, we review the polyhedral realization of the crystal $B(\lambda)$ (see Ref. 3).

Let $R_\lambda := \{r_\lambda\}$ be the crystal for $\lambda \in P_+$ (P_+: set of dominant integral weights) defined in Ref. 3. For the crystal $B(\infty)\otimes R_\lambda$, we define the following map:

$$\Phi_\lambda : (B(\infty)\otimes R_\lambda) \sqcup \{0\} \to B(\lambda) \sqcup \{0\} \tag{2.13}$$

by $\Phi_\lambda(0)=0$ and $\Phi_\lambda(b\otimes r_\lambda)=\hat{\pi}_\lambda(b)$ for $b\in B(\infty)$. We set

$$\widetilde{B}(\lambda) := \{b\otimes r_\lambda \in B(\infty)\otimes R_\lambda : \Phi_\lambda(b\otimes r_\lambda)\neq 0\}.$$

Theorem 2.3 (Ref. 3): *(i) The map* Φ_λ *becomes a surjective strict morphism of crystals* $B(\lambda)\otimes R_\lambda \to B(\lambda)$.

(ii) $\widetilde{B}(\lambda)$ *is a subcrystal of* $B(\lambda)\otimes R_\lambda$, *and* Φ_λ *induces the isomorphism of crystals* $\widetilde{B}(\lambda) \simeq B(\lambda)$.

Let us denote $\mathbb{Z}_\iota \otimes R_\lambda$ by $\mathbb{Z}_\iota[\lambda]$. Here note that we can identify $\mathbb{Z}_\iota[\lambda]$ with $\mathbb{Z}_\iota^\infty$ as a set since the crystal R_λ has only one element but their crystal structures are different. By Theorem 2.3, we have the strict embedding of crystals $\Omega_\lambda : B(\lambda)(\cong \widetilde{B}(\lambda)) \hookrightarrow B(\infty)\otimes R_\lambda$. Combining Ω_λ and Kashiwara embedding Ψ_ι, we obtain the following:

Theorem 2.4 (Ref. 3): *There exists the unique strict embedding of crystals*

$$\Psi_\iota^{(\lambda)} : B(\lambda) \hookrightarrow B(\infty)\otimes R_\lambda \hookrightarrow \mathbb{Z}_\iota^\infty \otimes R_\lambda =: \mathbb{Z}_\iota^\infty[\lambda]$$

such that $\Psi_\iota^{(\lambda)}(u_\lambda)=(\ldots,0,0)\otimes r_\lambda$.

We fix an infinite sequence of indices $\iota=(\ldots,i_k,\ldots,i_2,i_1)$ satisfying (2.1) and $\lambda\in P_+$. We define a linear form $\beta_k^{(\pm)}(k\geqslant 1)$ on $\mathbb{Q}^\infty$ by

$$\beta_k^{(+)}(\vec{x}) = x_k + \sum_{k<j<k^{(+)}} \langle h_{i_k}, \alpha_{i_j}\rangle x_j + x_{k^{(+)}}, \tag{2.14}$$

$$\beta_k^{(-)}(\vec{x}) = \begin{cases} x_{k^{(-)}} + \displaystyle\sum_{k^{(-)}<j<k} \langle h_{i_k}, \alpha_{i_j}\rangle x_j + x_k & \text{if } k^{(-)}>0 \\ -\langle h_{i_k}, \lambda\rangle + \displaystyle\sum_{1<j<k} \langle h_{i_k}, \alpha_{i_j}\rangle x_j + x_k & \text{if } k^{(-)}=0. \end{cases} \tag{2.15}$$

Here note that $\beta_k^{(+)}=\beta_k$ and $\beta_k^{(-)}=\beta_{k^{(-)}}$ if $k^{(-)}>0$. By using these linear forms, let us define a piecewise-linear operator $\hat{S}_k=\hat{S}_{k,\iota}$ on $(\mathbb{Q}^\infty)^*$ as follows:

$$\hat{S}_k(\varphi) := \begin{cases} \varphi - \varphi_k \beta_k^{(+)} & \text{if } \varphi_k > 0 \\ \varphi - \varphi_k \beta_k^{(-)} & \text{if } \varphi_k \leqslant 0, \end{cases} \tag{2.16}$$

for $\varphi(\vec{x})=c+\Sigma\varphi_k x_k$ ($c,\varphi_k\in\mathbb{Q}$) on $\mathbb{Q}^\infty$. For the fixed sequence $\iota=(i_k)$, in case $k^{(-)}=0$ for $k\geqslant 1$, there exists unique $i\in I$ such that $i_k=i$. We denote such k by $\iota^{(i)}$, namely, $\iota^{(i)}$ is the first number k such that $i_k=i$. Here we set for $\lambda\in P_+$ and $i\in I$,

$$\lambda^{(i)}(\vec{x}) := -\beta_{\iota^{(i)}}^{(-)}(\vec{x}) = \langle h_i, \lambda\rangle - \sum_{1<j<\iota^{(i)}} \langle h_i, \alpha_{i_j}\rangle x_j - x_{\iota^{(i)}}. \tag{2.17}$$

For ι and $\lambda\in P_+$, let $\Xi_\iota[\lambda]$ be the set of all linear functions generated by $\hat{S}_k$ from the functions x_j ($j\geqslant 1$) and $\lambda^{(i)}$ ($i\in I$), namely,

$$\Xi_\iota[\lambda] := \{\hat{S}_{j_l}\cdots\hat{S}_{j_2}\hat{S}_{j_1}(x_{j_0}) : l\geqslant 0, j_0, j_1, \ldots, j_l \geqslant 1\}$$
$$\cup \{\hat{S}_{j_k}\cdots\hat{S}_{j_2}\hat{S}_{j_1}(\lambda^{(i)}(x)) : k\geqslant 0, i\in I, j_0, j_1, \ldots, j_k \geqslant 1\}.$$

Now we set

$$\Sigma_\iota := \{\vec{x} \in \mathbb{Z}_\iota^\infty[\lambda] \subset \mathbb{Q}^\infty : \varphi(\vec{x}) \geqslant 0 \text{ for any } \varphi \in \Xi_\iota[\lambda]\}. \tag{2.18}$$

For ι and $\lambda \in P_+$, a pair (ι,λ) is called *ample* if $\Sigma_\iota[\lambda] \ni \vec{0} = (\cdots,0,0)$.

Theorem 2.5 (Ref. 3): *Suppose that* (ι,λ) *is ample. Let* $\Psi_\iota^\lambda : B(\lambda) \hookrightarrow \mathbb{Z}_\iota^\infty[\lambda]$ *be the embedding as in Theorem 2.4. Then we have* $\mathrm{Im}(\Psi_\iota^{(\lambda)})(\cong B(\lambda)) = \Sigma_\iota[\lambda]$.

We call $\Sigma_\iota[\lambda]$ the polyhedral realization of $B(\lambda)$.

In the rest of this section, we discuss $\hat{S}_k$ and S_k. We define the linear form $\xi^{(i)}$ $(i \in I)$ on $\mathbb{Q}$ by

$$\xi^{(i)}(\vec{x}) := -\sum_{1<j<\iota^{(i)}} \langle h_i, \alpha_{i_j} \rangle x_j - x_{\iota^{(i)}} = -\langle h_i, \lambda \rangle + \lambda^{(i)}(\vec{x}) \tag{2.19}$$

and set of linear forms $\Xi_\iota^{(i)}$ by

$$\Xi_\iota^{(i)} := \{S_{j_l} \cdots S_{j_2} S_{j_1} \xi^{(i)} : l \geqslant 0, j_0, j_1, \ldots, j_l \geqslant 1\}. \tag{2.20}$$

Here we introduce the *strict positivity assumption* for ι as follows:

$$\text{if } k^{(-)} = 0 \text{ then } \varphi_k \geqslant 0 \text{ for any } \varphi(\vec{x}) = \sum_k \varphi_k x_k \in (\Xi_\iota \cup \cup_{j \in I} \Xi_\iota^{(j)}) \setminus \{\xi^{(i)} : i \in I\}, \tag{2.21}$$

where Ξ_ι is defined by (2.10). Then we have the following Lemma:

Lemma 2.6 (Ref. 3): Under the strict positivity assumption for ι, *we have*

$$\hat{S}_{j_l} \cdots \hat{S}_{j_2} \hat{S}_{j_1} x_{j_0} = S_{j_l} \cdots S_{j_2} S_{j_1} x_{j_0}, \tag{2.22}$$

for any $l \geqslant 0$, $j_0, j_1, \ldots, j_l \geqslant 1$, *and*

$$\hat{S}_{j_l} \cdots \hat{S}_{j_2} \hat{S}_{j_1} \lambda^{(i)}(\vec{x}) = \langle h_i, \lambda \rangle + S_{j_l} \cdots S_{j_2} S_{j_1} \xi^{(i)}(\vec{x}), \tag{2.23}$$

for any $l \geqslant 0$, $j_0, j_1, \ldots, j_l \geqslant 1$ *and* $i \in I$, *if the left-hand side of* (2.23) *is nonzero*.

III. EXPLICIT FORMS OF POLYHEDRAL REALIZATION OF $B(\infty)$ AND $B(\lambda)$

The polyhedral realizations of $B(\infty)$ and $B(\lambda)$ are already known in the case of all rank 2 Kac-Moody types, of A_n and of $A_{n-1}^{(1)}$.[2,3] In this section, we treat other simple types. We obtain the following Theorem by Nakashia and Zelevinsky.

Theorem 3.1: *Let* Ξ_ι' *be a set of the linear forms in* $(\mathbb{Q}^\infty)^*$ *and set*

$$\Sigma_\iota' := \{\vec{x} \in \mathbb{Z}_\iota^\infty | \varphi(\vec{x}) \geqslant 0 \text{ for any } \varphi \in \Xi_\iota'\}$$

satisfying the following conditions:

(i) Ξ_ι' *is closed under the action of* S_k*'s,*
(ii) ι *satisfies the positivity assumption* (P),
(iii) all entries of $\vec{x} = (\cdots, x_2, x_1) \in \Sigma_\iota'$ *are non-negative.*

Then we have

$$\mathrm{Im}(\Psi_\iota)(\cong B(\infty)) = \Sigma_\iota'.$$

Proof: We recall that the following two facts for certain $\Sigma_\iota(\subset \mathbb{Z}_\iota^\infty)$ (see Nakashia and Zelevinsky's Theorem 3.1):

A) If Σ_ι is closed under the action of $\tilde{f}_i$, then $\mathrm{Im}(\Psi_\iota) \subset \Sigma_\iota$.

B) If Σ_ι is closed under the action of $\tilde{e}_i$ and all the entries of $\vec{x} \in \Sigma_\iota$ are non-negative, then $\Sigma_\iota \subset \mathrm{Im}(\Psi_\iota)$ since every $\vec{x} \in \Sigma_\iota$ can be transformed to $\vec{0}$ by the action of $\tilde{e}_i$'s $(i \in I)$.

We assume condition (i). Condition (i) means that Σ_ι' is closed under the action of $\tilde{e}_i$'s. Using (ii), we obtain that Σ_ι' is closed under the action of $\tilde{f}_i$'s and this shows $\mathrm{Im}(\Psi_\iota) \subset \Sigma_\iota'$. Using (iii), we

obtain that $\Sigma'_\iota \subset \mathrm{Im}(\Psi_\iota)$. □

Remark 3.2: Theorem 3.1 implies that we need not consider a set of linear functions Ξ_ι which is closed under the action of the S_k's to x_j for any $j>0$. We only need to find a set of linear functions Ξ_ι which is closed under the action of the S_k's to x_j for some $j>0$ and which satisfies the two conditions (*ii*), (*iii*).

It will be convenient for us to change the indexing set for $\mathbb{Z}^\infty$ from $\mathbb{Z}_{\geqslant 1}$ to $\mathbb{Z}_{\geqslant 1}\times[1,n]$. We will do this with the help of the bijection $\mathbb{Z}_{\geqslant 1}\times[1,n]\to\mathbb{Z}_{\geqslant 1}$ given by $((j;i)\mapsto(j-1)n+i)$. Thus, we will write an element $\vec{x}\in Z^\infty$ as doubly indexed family $(x_{j;i})_{j\geqslant 1, i\in[1,n]}$ of non-negative integers. Therefore, we can write that $\vec{x}\in\mathbb{Z}^\infty$ as $(\ldots,x_{1;2},x_{1;1})$. We will adopt the convention that $x_{j;i}=0$ unless $i\in[1,n]$. Hereafter, we fix the infinite sequence ι as follows:

$$\iota := (\cdots,\underbrace{n,n-1,\cdots,2,1},\cdots,\underbrace{n,n-1,\cdots,2,1},\underbrace{n,n-1,\cdots,2,1}),$$

where n is the size of Cartan matrix. We use the same Cartan data as the one in Ref. 10 except for the cases F_4 and E_7.

A. B_n case

We consider the case of type B_n and give the explicit forms of Σ_ι and $\Sigma_\iota[\lambda]$. First, we give the polyhedral realization Σ_ι. We define for any $j\geqslant 1, 0\leqslant k\leqslant 2n-1$,

$$\varphi_{j;k} := \begin{cases} id & (k=0) \\ S_{j;k}S_{j;k-1}\cdots S_{j;2}S_{j;1} & (1\leqslant k\leqslant n-1) \\ S_{j+k-n;2n-k}S_{j+k-1-n;2n-k+1}\cdots S_{j+1;n-1}S_{j;n}\varphi_{j;n-1} & (n\leqslant k\leqslant 2n-1). \end{cases} \tag{3.1}$$

Lemma 3.3:

$$\varphi_{j;k}(x_{j;1}) = \begin{cases} x_{j;k+1}-x_{j+1;k} & (0\leqslant k\leqslant n-1) \\ x_{j+k-n+1;2n-k-1}-x_{j+k-n+1;2n-k} & (n\leqslant k\leqslant 2n-1). \end{cases} \tag{3.2}$$

Proof: By the induction on k. The case of $k=0$ is trivial.

Case I) $1\leqslant k\leqslant n-1$.

If $k=1$, we have

$$S_{j;1}(x_{j;1}) = x_{j;1}-(x_{j;1}-x_{j;2}+x_{j+1;1}) = x_{j;2}-x_{j+1;1} = \varphi_{j;1}(x_{j;1}).$$

If $1<k\leqslant n-1$, we assume that $\varphi_{j;k-1}(x_{j;1})=x_{j;k}-x_{j+1;k-1}$. Then we have

$$\begin{aligned} S_{j;k}\varphi_{j;k-1}(x_{j;1}) = S_{j;k}(x_{j;k}-x_{j+1;k-1}) &= x_{j;k}-x_{j+1;k-1}-(x_{j;k}-x_{j;k+1}-x_{j+1;k-1}+x_{j+1;k}) \\ &= x_{j;k+1}-x_{j+1;k} = \varphi_{j;k}(x_{j;1}). \end{aligned}$$

Case II) $n\leqslant k\leqslant 2n-1$.

If $k=n$, using the result of Case I), we have

$$\begin{aligned} S_{j;n}\varphi_{j;n-1}(x_{j;1}) = S_{j;n}(x_{j;n}-x_{j+1;n-1}) &= x_{j;n}-x_{j+1;n-1}-(x_{j;n}-2x_{j+1;n-1}+x_{j+1;n}) \\ &= x_{j+1;n-1}-x_{j+1;n} = \varphi_{j;n}(x_{j;1}). \end{aligned}$$

If $n<k\leqslant 2n-1$, we assume that $\varphi_{j;k-1}(x_{j;1})=x_{j+k-n;2n-k}-x_{j+k-n;2n-k+1}$. Then we have

$$\begin{aligned} S_{j+k-n;2n-k}\varphi_{j;k-1}(x_{j;1}) &= S_{j+k-n;2n-k}(x_{j+k-n;2n-k}-x_{j+k-n;2n-k+1}) \\ &= x_{j+k-n;2n-k}-x_{j+k-n;2n-k+1}-(x_{j+k-n;2n-k}-x_{j+k-n;2n-k+1}-x_{j+k-n+1;2n-k-1} \\ &\quad +x_{j+k-n+1;2n-k}) \\ &= x_{j+k-n+1;2n-k-1}-x_{j+k-n+1;2n-k} = \varphi_{j;k}(x_{j;1}). \end{aligned}$$

□

Lemma 3.4: The set $\{\varphi_{j;k}(x_{j;1}): 1 \leqslant j, 0 \leqslant k \leqslant 2n-1\}$ *is closed under the actions of all transformations* $S_{m;l}$ *for any* $m \geqslant 1, l \geqslant 1$.

Proof: Using the definition of $\varphi_{j;k}$ (3.1) and the formula (3.2) in Lemma 3.3, if $k=0$, $\varphi_{j;0} = id$ and we have

$$S_{m;l}(\varphi_{j;0}(x_{j;1})) = \begin{cases} \varphi_{j;1}(x_{j;1}) & \text{if } (m;l) = (j;1) \\ x_{j;1} & \text{otherwise.} \end{cases}$$

If $1 \leqslant k \leqslant n-1$, we have

$$S_{m;l}(\varphi_{j;k}(x_{j;1})) = \begin{cases} \varphi_{j;k-1}(x_{j;1}) & \text{if } (m;l) = (j;k) \\ \varphi_{j;k+1}(x_{j;1}) & \text{if } (m;l) = (j;k+1) \\ \varphi_{j;k}(x_{j;1}) & \text{otherwise.} \end{cases}$$

If $n \leqslant k \leqslant 2n-1$, we have

$$S_{m;l}(\varphi_{j;k}(x_{j;1})) = \begin{cases} \varphi_{j;k-1}(x_{j;1}) & \text{if } (m;l) = (j+k-n;2n-k), \\ \varphi_{j;k+1}(x_{j;1}) & \text{if } (m;l) = (j+k-n+1;2n-k-1), \\ \varphi_{j;k}(x_{j;1}) & \text{otherwise.} \end{cases}$$

□

Now, we define

$$\Xi_\iota := \{\varphi_{j;k}(x_{j;1}): j \geqslant 1, 0 \leqslant k \leqslant 2n-1\},$$

$$\Sigma_\iota := \{\vec{x} \in \mathbb{Z}_\iota^\infty : \varphi(\vec{x}) \geqslant 0 \text{ for any } \varphi \in \Xi_\iota\}.$$

Theorem 3.5: *The polyhedral realization* Σ_ι *of* $B(\infty)$ *for type* B_n *is described as follows:*

$$x_{j;i} = 0 \text{ for } j,i \notin [1,n], \tag{3.3}$$

$$x_{1;i} \geqslant x_{2;i-1} \geqslant \cdots \geqslant x_{i;1} \geqslant 0 \text{ for } 1 \leqslant i \leqslant n-1, \tag{3.4}$$

$$x_{j;n} \geqslant x_{j+1;n-1} \geqslant \cdots \geqslant x_{n;j} \geqslant 0 \text{ for } 1 \leqslant j \leqslant n, \tag{3.5}$$

$$x_{j;n-j+1} \geqslant x_{j;n-j+2} \geqslant \cdots \geqslant x_{j;n} \geqslant 0 \text{ for } 2 \leqslant j \leqslant n. \tag{3.6}$$

Proof: First, we show that Σ_ι is the polyhedral realization of $B(\infty)$, so we shall check the conditions of Theorem 3.1. Ξ_ι is closed under the action of S_k by Lemma 3.4. The coefficients of $x_{1;i}$ $(i=1,2,\ldots,n)$ are positive for $\varphi \in \Xi_\iota$ by Lemma 3.3, and this shows that ι satisfies the "positivity assumption."

We will show that all entries of $\vec{x} \in \Sigma_\iota$ are non-negative. In the case of $m \geqslant 1$, $0 \leqslant l \leqslant n-1$ for $\varphi_{m;l}(x_{m;1})$, we have

$$x_{m;l+1} \geqslant x_{m+1;l} \tag{3.7}$$

and we consider the cases that $(m;l) = (j;i-1), (j+1;i-2), \ldots, (j+i-2;1), (j+i-1;0)$ for any $j \geqslant 1$, $1 \leqslant i \leqslant n$. We obtain

$$x_{j;i} \geqslant x_{j+1;i-1} \geqslant \cdots \geqslant x_{j+i-2;2} \geqslant x_{j+i-1;1} \geqslant 0.$$

This shows that $x_{j;i} \geqslant 0$ for any $j \geqslant 1$, $1 \leqslant i \leqslant n$. Therefore, Σ_ι is the polyhedral realization of $B(\infty)$.

Next we show that Σ_ι has the form of Theorem 3.5. We determine when $x_{j;i} \equiv 0$ for $j \geqslant 1$, $1 \leqslant i \leqslant n$. In the case of $m \geqslant 1$, $n \leqslant l \leqslant 2n-1$ for $\varphi_{m;l}(x_{m;1})$ we have

$$x_{m+l-n+1;2n-l-1} \geqslant x_{m+l-n+1;2n-l} \tag{3.8}$$

and consider the cases that $(m;l)=(j;2n-1),(j+1;2n-2),\ldots,(j+n-1;n)$. Then we have

$$0 \geqslant x_{j+n;1} \geqslant x_{j+n;2} \geqslant \cdots \geqslant x_{j+n;n-1} \geqslant x_{j+n;n} \geqslant 0$$

and $x_{j+n;i} \equiv 0$ for any $j \geqslant 1$, $1 \leqslant i \leqslant n$. We shall show (3.4). In (3.7), by setting $(m;l)=(1;i-1),(2;i-2),\ldots,(i;0)$ for any $1 \leqslant i \leqslant n-1$ then we obtain (3.4). Similarly, in (3.7) if $(m;l)=(j;n-1),(j+1;n-2),\ldots,(n;j-1)$ for any $1 \leqslant j \leqslant n$, then we have (3.5). Let us see (3.6). In (3.8), we consider the cases that $(m;l)=(1;n+j-2),(2;n+j-3),\ldots,(j-1;n)$ for any $2 \leqslant j \leqslant n$. Then we have (3.6). □

Next, we give the polyhedral realization $\Sigma_\iota[\lambda]$ for $\lambda := \sum_{k=1}^n \lambda_k \Lambda_k$, where $\lambda_k \in \mathbb{Z}_{\geqslant 0}$, Λ_k are the fundamental weights. Here we set

$$\Xi_\iota^{(1,n-1)} := \{S_{j_k} \cdots S_{j_2} S_{j_1} \xi^{(i)}(\vec{x}) : k \geqslant 0, 1 \leqslant i \leqslant n-1, j_1, \ldots, j_k \geqslant 1\},$$

$$\Xi_\iota^{(n)} := \{S_{j_k} \cdots S_{j_2} S_{j_1} \xi^{(n)}(\vec{x}) : k \geqslant 0, j_1, \ldots, j_k \geqslant 1\},$$

$$\Xi_\iota^{(1,n-1)}[\lambda] := \{\hat{S}_{j_k} \cdots \hat{S}_{j_2} \hat{S}_{j_1} \lambda^{(i)}(\vec{x}) : k \geqslant 0, 1 \leqslant i \leqslant n-1, j_1, \ldots, j_k \geqslant 1\},$$

$$\Xi_\iota^{(n)}[\lambda] := \{\hat{S}_{j_k} \cdots \hat{S}_{j_2} \hat{S}_{j_1} \lambda^{(n)}(\vec{x}) : k \geqslant 0, j_1, \ldots, j_k \geqslant 1\},$$

$$\Xi_\iota[\lambda] := \Xi_\iota \cup \Xi_\iota^{(1,n-1)}[\lambda] \cup \Xi_\iota^{(n)}[\lambda] = \{\varphi_{j;k}(x_{j;1}) : j \geqslant 1, 0 \leqslant k \leqslant 2n-1\} \cup \{\hat{S}_{j_k} \cdots \hat{S}_{j_2} \hat{S}_{j_1} \lambda^{(i)}(\vec{x}) : k \geqslant 0, 1 \leqslant i \leqslant n-1, j_1, \ldots, j_k \geqslant 1\} \cup \{\hat{S}_{j_k} \cdots \hat{S}_{j_2} \hat{S}_{j_1} \lambda^{(n)}(\vec{x}) : k \geqslant 0, j_1, \ldots, j_k \geqslant 1\},$$

$$\Sigma_\iota[\lambda] := \{\vec{x} \in \mathbb{Z}_\iota[\lambda] : \varphi(\vec{x}) \geqslant 0 \text{ for any } \varphi \in \Xi_\iota[\lambda]\}.$$

In order to show that $\Sigma_\iota[\lambda]$ is the polyhedral realization of $B(\lambda)$, we give the explicit forms of $\Xi_\iota^{(1,n-1)}[\lambda]$ and $\Xi_\iota^{(n)}[\lambda]$. Since the Dynkin diagrams for A_n and B_n are the same for $1 \geqslant i \geqslant n-1$, we give the explicit form of $\Xi_\iota^{(1,n-1)}$ by the result in Ref. 2 as follows:

$$\Xi_\iota^{(1,n-1)} = \{x_{j;i-j} - x_{j;i-j+1} : 1 \leqslant i \leqslant n-1, 1 \leqslant j \leqslant i\}. \tag{3.9}$$

For giving the explicit form of $\Xi_\iota^{(n)}$, we say that an integer sequence $\mu_1, \mu_2, \ldots, \mu_n$ is an admissible pattern if:

$$\begin{cases} 1 \leqslant \mu_1 \leqslant n, \\ 0 \leqslant \mu_2 \leqslant \mu_1 - 1, \\ \qquad \cdots, \\ 0 \leqslant \mu_k \leqslant \mu_{k-1} - 1, \\ \qquad \cdots, \end{cases} \tag{3.10}$$

where if μ_k does not exist, we define $\mu_k = 0$, and

$$S^{(\mu_1)} := \begin{cases} id & (\mu_1 = 1) \\ S_{\mu_1;n-\mu_1} \cdots S_{2;n-2} S_{1;n-1} & (\mu_1 \geqslant 2), \end{cases}$$

$$S^{(\mu_k)} := \begin{cases} id & (\mu_k = 0) \\ S_{\mu_k+k-2;n-\mu_k+1} \cdots S_{k;n-1} S_{k-1;n} & (\mu_k \geqslant 1) \end{cases} \quad \text{for } k \geqslant 2,$$

$$\varphi^{(\mu)} := S^{(\mu_k)} \cdots S^{(\mu_2)} S^{(\mu_1)} \text{ for } \mu = (\mu_1, \mu_2, \ldots, \mu_k, 0, 0, \ldots).$$

We prepare the symbol X as follows:

$$X := 2x_{1;n-1} - x_{1;n} (= \xi^{(n)}(\vec{x})). \tag{3.11}$$

For convenience, we define

$$X_{j;i} := \begin{cases} 2x_{j;i} & \text{if } i \neq n \\ x_{j;n} & \text{if } i = n. \end{cases} \tag{3.12}$$

Theorem 3.6: *Let* $\mu = (\mu_1, \mu_2, \ldots, \mu_k, 0, 0, \ldots)$ *be an admissible pattern.*
(*i*) *The forms* $\varphi^{(\mu)}X$ *are given by*

$$\varphi^{(\mu)}X = \sum_{k=1}^{l} (X_{\mu_k+k-1;n-\mu_k} - X_{\mu_k+k-1;n-\mu_k+1}), \tag{3.13}$$

where

$$L := \max\{k : \mu_k \neq 0\},$$

$$l := \begin{cases} L & \text{if } \mu_L = 1, \\ L+1 & \text{if } \mu_L \geqslant 2. \end{cases}$$

(*ii*) $\Xi_{\iota}^{(n)}$ *is the set of all linear forms which are of the form* $\varphi^{(\mu)}X$, *where* μ *are the admissible patterns.*

Proof: (i) First, we give a remark. When $\mu_k - \mu_{k+1} = 1$, the terms $X_{\mu_k+k-1;n-\mu_k+1}$ and $X_{\mu_{k+1}+k;n-\mu_{k+1}}$ in the sum (3.13) are canceled as $-X_{\mu_k+k-1;n-\mu_k+1} + X_{\mu_{k+1}+k;n-\mu_{k+1}} = 0$. We show the theorem by induction on $|\mu| = \mu_1 + \mu_2 + \cdots + \mu_i$ for $\mu = (\mu_1, \mu_2, \ldots, \mu_i, 0, 0, \ldots)$.

If $|\mu| = 1$, then $l = 1$ and the sum of the right-hand side of (3.13) is $X_{1;n-1} - X_{1;n} = 2x_{1;n-1} - x_{1;n}$ and equal to $\varphi^{(\mu)}X$ by (3.11). We assume that $|\mu| = \mu_1 + \mu_2 + \cdots + \mu_i = k-1$ for $\mu = (\mu_1, \mu_2, \ldots, \mu_i, 0, 0, \ldots)$. We consider the two cases: I) $\mu_i \to \mu_i + 1$, II) "$\mu_{i+1} = 0$" $\to$ "$\mu_{i+1} = 1$".

I) $\mu_i \to \mu_i + 1$.

In this case, $l = i+1$ and we note that $1 \leqslant \mu_i \leqslant \mu_{i-1} - 2$ since μ is an admissible pattern and the term $X_{\mu_i+i-1;n-\mu_i}$ in the sum (3.13) is not canceled. We set $\mu' := (\mu_1, \mu_2, \ldots, \mu_i + 1, 0, 0, \ldots)$. We have

$$\varphi^{(\mu')}X = S_{\mu_i+i-1;n-\mu_i} \varphi^{(\mu)}X.$$

The right-hand side of (3.13) is

$$S_{\mu_i+i-1;n-\mu_i} \left(\sum_{k=1}^{l} (X_{\mu_k+k-1;n-\mu_k} - X_{\mu_k+k-1;n-\mu_k+1}) \right) = \sum_{k=1}^{l} (X_{\mu_k+k-1;n-\mu_k} - X_{\mu_k+k-1;n-\mu_k+1}) - (X_{\mu_i+i-1;n-\mu_i}$$
$$- X_{\mu_i+i-1;n-\mu_i+1} - X_{\mu_i+i;n-\mu_i-1} + X_{\mu_i+i;n-\mu_i}) = \varphi^{(\mu')}X.$$

II) "$\mu_{i+1} = 0$" $\to$ "$\mu_{i+1} = 1$".

We set $\mu' := (\mu_1, \mu_2, \ldots, \mu_i, 1, 0, \ldots)$ (i.e., $\mu_{i+1} = 1$) and then $l = i+1$. By the admissible pattern of μ, we have $0 \leqslant \mu_{i+1} \leqslant \mu_i - 1$. This shows that $\mu_i \geqslant 2$ and the term $X_{i;n}$ in the sum (3.13) is not canceled. We have

$$\varphi^{(\mu')}X = S_{i;n} \varphi^{(\mu)}X.$$

The right-hand side of (3.13) is

$$S_{i;n}\left(\sum_{k=1}^{l}(X_{\mu_k+k-1;n-\mu_k}-X_{\mu_k+k-1;n-\mu_k+1})\right)=\sum_{k=1}^{l}(X_{\mu_k+k-1;n-\mu_k}-X_{\mu_k+k-1;n-\mu_k+1})-(X_{i;n}-X_{i+1;n-1}+X_{i+1;n})=\varphi^{(\mu')}X.$$

(ii) It is sufficient to show that $\{\varphi^{(\mu)}X \mid \mu:\text{admissible pattern}\}$ is closed under the actions of all $S_{j;i}$. We set for $1\leqslant k\leqslant l+1$,

$$\mu=(\mu_1,\mu_2,\dots,\mu_l,0,0,\dots),\quad \mu^+=(\mu_1,\mu_2,\dots,\mu_k+1,\dots,\mu_l,0,0,\dots),$$

$$\mu^-=(\mu_1,\mu_2,\dots,\mu_k-1,\dots,\mu_l,0,0,\dots).$$

Then we have

$$S_{j;i}\varphi^{(\mu)}X=\begin{cases}\varphi^{(\mu^+)}X & \text{if } (j;i)=(\mu_k+k-1;n-\mu_k) \text{ and } \mu_{k-1}-\mu_k\neq 1\\ \varphi^{(\mu^-)}X & \text{if } (j;i)=(\mu_k+k-1;n-\mu_k+1) \text{ and } \mu_k-\mu_{k+1}\neq 1\\ \varphi^{(\mu)}X & \text{otherwise.}\end{cases}$$

□

Therefore, ι satisfies the strict positivity assumption by the explicit forms of $\Xi_\iota^{(1,n-1)}$ and $\Xi_\iota^{(n)}$. By Lemma 2.6, this shows that

$$\Xi_\iota^{(1,n-1)}[\lambda]=\{\lambda_i+x_{j;i-j}-x_{j;i-j+1}:1\leqslant i\leqslant n-1,1\leqslant j\leqslant i\},$$

$$\Xi_\iota^{(n)}[\lambda]=\left\{\lambda_n+\sum_{k=1}^{l}(X_{\mu_k+k-1;n-\mu_k}-X_{\mu_k+k-1;n-\mu_k+1}):\mu \text{ are the admissible patterns}\right\}$$

by (3.9), (3.13) and $\Sigma_\iota[\lambda]$ is the polyhedral realization of $B(\lambda)$.

B. C_n case

We consider the case of type C_n. First, we give the polyhedral realization Σ_ι of $B(\infty)$. We define for $j\geqslant 1$, $0\leqslant k\leqslant 2n-1$

$$\varphi_{j;k}:=\begin{cases}id & (k=0)\\ S_{j;k}S_{j;k-1}\cdots S_{j;2}S_{j;1} & (1\leqslant k\leqslant n-1)\\ S_{j+k-n;2n-k}S_{j+k-1-n;2n-k+1}\cdots S_{j+1;n-1}S_{j;n}\varphi_{j;n-1} & (n\leqslant k\leqslant 2n-1).\end{cases}$$

Lemma 3.7:

$$\varphi_{j;k}(x_{j;1})=\begin{cases}x_{j;k+1}-x_{j+1;k} & (0\leqslant k\leqslant n-2)\\ 2x_{j;n}-x_{j+1;n-1} & (k=n-1)\\ x_{j+1;n-1}-2x_{j+1;n} & (k=n)\\ x_{j+k-n+1;2n-k-1}-x_{j+k-n+1;2n-k} & (n+1\leqslant k\leqslant 2n-1).\end{cases}$$

Proof: By the induction on k. The case of $k=0$ is trivial.
Case I) $1\leqslant k\leqslant n-2$.
If $k=1$, we have

$$S_{j;1}(x_{j;1})=x_{j;1}-(x_{j;1}-x_{j;2}+x_{j+1;1})=x_{j;2}-x_{j+1;1}=\varphi_{j;1}(x_{j;1}).$$

If $1<k\leqslant n-2$, we assume that $\varphi_{j;k-1}(x_{j;1})=x_{j;k}-x_{j+1;k-1}$. Then we have

$$S_{j;k}\varphi_{j;k-1}(x_{j;1}) = S_{j;k}(x_{j;k} - x_{j+1;k-1}) = x_{j;k} - x_{j+1;k-1} - (x_{j;k} - x_{j;k+1} - x_{j+1;k-1} + x_{j+1;k})$$
$$= x_{j;k+1} - x_{j+1;k} = \varphi_{j;k}(x_{j;1}).$$

Case II) $k=n-1,n$.

If $k=n-1$, using the result of Case I), we have

$$S_{j;n-1}\varphi_{j;n-2}(x_{j;1}) = S_{j;n-1}(x_{j;n-1} - x_{j+1;n-2})$$
$$= x_{j;n-1} - x_{j+1;n-2} - (x_{j;n-1} - 2x_{j;n} - x_{j+1;n-2} + x_{j+1;n-1})$$
$$= 2x_{j;n} - x_{j+1;n-1} = \varphi_{j;n-1}(x_{j;1}),$$

and then if $k=n$,

$$S_{j;n}\varphi_{j;n-1}(x_{j;1}) = S_{j;n}(2x_{j;n} - x_{j+1;n-1}) = 2x_{j;n} - x_{j+1;n-1} - 2(x_{j;n} - x_{j+1;n-1} + x_{j+1;n})$$
$$= x_{j+1;n-1} - 2x_{j+1;n} = \varphi_{j;n}(x_{j;1}).$$

Case III) $n+1 \leqslant k \leqslant 2n-1$.

If $k=n+1$, using the result of the case of $k=n$, we have[11,12]

$$S_{j+1;n-1}\varphi_{j;n}(x_{j;1}) = S_{j+1;n-1}(x_{j+1;n-1} - 2x_{j+1;n})$$
$$= x_{j+1;n-1} - 2x_{j+1;n} - (x_{j+1;n-1} - 2x_{j+1;n} - x_{j+2;n-2} + x_{j+2;n-1})$$
$$= x_{j+2;n-2} - x_{j+2;n-1} = \varphi_{j;n+1}(x_{j;1}).$$

If $n+1 < k \leqslant 2n-1$, we assume that $\varphi_{j;k-1}(x_{j;1}) = x_{j+k-n;2n-k} - x_{j+k-n;2n-k+1}$. Then we have

$$S_{j+k-n;2n-k}\varphi_{j;k-1}(x_{j;1}) = S_{j+k-n;2n-k}(x_{j+k-n;2n-k} - x_{j+k-n;2n-k+1})$$
$$= x_{j+k-n;2n-k} - x_{j+k-n;2n-k+1} - (x_{j+k-n;2n-k} - x_{j+k-n;2n-k+1} - x_{j+k-n+1;2n-k-1}$$
$$+ x_{j+k-n+1;2n-k})$$
$$= x_{j+k-n+1;2n-k-1} - x_{j+k-n+1;2n-k} = \varphi_{j;k}(x_{j;1}).$$

□

Lemma 3.8. *The set* $\{\varphi_{j;k}(x_{j;1}) : 1 \leqslant j, 0 \leqslant k \leqslant 2n-1\}$ *is closed under the actions of all transformations* $S_{m;l}$ *for any* $m \geqslant 1$, $l \geqslant 1$.

Proof. Using the definition of $\varphi_{j;k}$ (3.14) and the formula (3.14) in Lemma 3.7, if $k=0$, $\varphi_{j;0} = id$ and we have

$$S_{m;l}(\varphi_{j;0}(x_{j;1})) = \begin{cases} \varphi_{j;1}(x_{j;1}) & \text{if } (m;l) = (j;1) \\ x_{j;1} & \text{otherwise.} \end{cases}$$

If $1 \leqslant k \leqslant n-1$, we have

$$S_{m;l}(\varphi_{j;k}(x_{j;1})) = \begin{cases} \varphi_{j;k-1}(x_{j;1}) & \text{if } (m;l) = (j;k) \\ \varphi_{j;k+1}(x_{j;1}) & \text{if } (m;l) = (j;k+1) \\ \varphi_{j;k}(x_{j;1}) & \text{otherwise.} \end{cases}$$

If $n \leqslant k \leqslant 2n-1$, we have

$$S_{m;l}(\varphi_{j;k}(x_{j;1})) = \begin{cases} \varphi_{j;k-1}(x_{j;1}) & \text{if } (m;l) = (j+k-n;2n-k) \\ \varphi_{j;k+1}(x_{j;1}) & \text{if } (m;l) = (j+k-n+1;2n-k-1) \\ \varphi_{j;k}(x_{j;1}) & \text{otherwise.} \end{cases}$$

□

Now, we define

$$\Xi_\iota := \{\varphi_{j;k}(x_{j;1}) : j \geqslant 1, 0 \leqslant k \leqslant 2n-1\},$$

$$\Sigma_\iota := \{\vec{x} \in \mathbb{Z}_\iota^\infty \mid \varphi(\vec{x}) \geqslant 0 \text{ for any } \varphi \in \Xi_\iota\}.$$

Theorem 3.9: *The polyhedral realization Σ_ι of $B(\infty)$ for type C_n is described as follows:*

$$x_{j;i} = 0 \text{ for } j,i \notin [1,n], \tag{3.14}$$

$$x_{1;i} \geqslant x_{2;i-1} \geqslant \cdots \geqslant x_{i;1} \geqslant 0 \text{ for } 1 \leqslant i \leqslant n-1, \tag{3.15}$$

$$2x_{j;n} \geqslant x_{j+1;n-1} \geqslant \cdots \geqslant x_{n;j} \geqslant 0 \text{ for } 1 \leqslant j \leqslant n-1, \tag{3.16}$$

$$x_{j;n-j+1} \geqslant x_{j;n-j+2} \geqslant \cdots \geqslant x_{j;n-1} \geqslant 2x_{j;n} \geqslant 0 \text{ for } 2 \leqslant j \leqslant n. \tag{3.17}$$

Proof: We shall show that Σ_ι is the polyhedral realization of $B(\infty)$ and check the conditions of Theorem 3.1. Ξ_ι is closed under the action of S_k by Lemma 3.8. The coefficients of $x_{1;i}$ $(i=1,2,\ldots,n)$ are positive for $\varphi \in \Xi_\iota$ by Lemma 3.7. This shows that ι satisfies the positivity assumption.

We shall show that all entries of $\vec{x} \in \Sigma_\iota$ are non-negative. In the case of $m \geqslant 1$, $0 \leqslant l \leqslant n-2$ for $\varphi_{m;l}(x_{m;1})$, we have

$$x_{m;l+1} \geqslant x_{m+1;l} \tag{3.18}$$

and we consider the cases that $(m;l)=(j;i-1),(j+1;i-2),\ldots,(j+i-2;1),(j+i-1;0)$. We obtain

$$x_{j;i} \geqslant x_{j+1;i-1} \geqslant \cdots \geqslant x_{j+i-2;2} \geqslant x_{j+i-1;1} \geqslant 0. \tag{3.19}$$

This shows that $x_{j;i} \geqslant 0$ for any $j \geqslant 1$, $1 \leqslant i \leqslant n-1$. Similarly, for any $j \geqslant 1$ and $l=n-1$, we have

$$2x_{j;n} \geqslant x_{j+1;n-1} (\geqslant 0). \tag{3.20}$$

This shows $x_{j;n} \geqslant 0$ for any $j \geqslant 1$. Therefore, Σ_ι is the polyhedral realization of $B(\infty)$.

We show that Σ_ι has the form of Theorem 3.9. In the case of $(m;l)=(j+n-1;n)$ for $\varphi_{m;l}(x_{m;1})$, we obtain

$$x_{j+n;n-1} \geqslant 2x_{j+n;n} \tag{3.21}$$

and in the case of $m \geqslant 1$, $n+1 \leqslant l \leqslant 2n-1$, we have

$$x_{m+l-n+1;2n-l-1} \geqslant x_{m+l-n+1;2n-l}. \tag{3.22}$$

We consider the cases that $(m;l)=(j;2n-1),(j+1;2n-2),\ldots,(j+n-2;n+1)$, then we have

$$0 \geqslant x_{j+n;1} \geqslant x_{j+n;2} \geqslant \cdots \geqslant x_{j+n;n-2} \geqslant x_{j+n;n-1} \geqslant 2x_{j+n;n} \geqslant 0.$$

This shows that $x_{j+n;i} \equiv 0$ for any $j \geqslant 1$, $1 \leqslant i \leqslant n$. We shall show (3.15). In (3.18), by setting $(m;l)=(1;i-1),(2;i-2),\ldots,(i;0)$ for any $1 \leqslant i \leqslant n-1$ then we have (3.15). Let us see (3.16). In (3.18), we consider the cases that $(m;l)=(j+1;n-2),(j+2;n-3),\ldots,(n;j-1)$ for any $1 \leqslant j \leqslant n$. Combining (3.20), we have (3.16). We shall show (3.17). We consider the cases that $(m;l)=(1;n+j-2),(2;n+j-3),\ldots,(j-2;n+1)$ for any $2 \leqslant j \leqslant n$ in (3.22) and the case $k=n$ for $2 \leqslant j$ in Lemma 3.14. Then we obtain (3.17). □

Next, we give the polyhedral realization $\Sigma_\iota[\lambda]$ of $B(\lambda)$. We prepare the following symbols:

$$X := x_{1;n-1} - x_{1;n} (= \xi^{(n)}(\vec{x})), \tag{3.23}$$

$$X_{j;i} := \begin{cases} x_{j;i} & \text{if } i \neq n \\ 2x_{j;n} & \text{if } i = n. \end{cases} \tag{3.24}$$

Then, we can show that the polyhedral realization $\Sigma_\iota[\lambda]$ is given by replacing $x_{j;i}$ of B_n with $X_{j;i}$.

C. D_n case

We consider the case of type D_n. First, we give the polyhedral realization Σ_ι of $B(\infty)$. We define for $j \geqslant 1$, $0 \leqslant k \leqslant 2n-2$,

$$\varphi_{j;k} := \begin{cases} id & (k=0) \\ S_{j;k}S_{j;k-1}\cdots S_{j;2}S_{j;1} & (0 \leqslant k \leqslant n) \\ S_{j+k-n;2n-k-1}S_{j+k-1-n;2n-k}\cdots S_{j+2;n-3}S_{j+1;n-2}\varphi_{j;n} & (n+1 \leqslant k \leqslant 2n-2). \end{cases}$$

$$\varphi'_{j;k} := \begin{cases} id & (k=0) \\ S_{j;k}S_{j;k-1}\cdots S_{j;2}S_{j;1} & (1 \leqslant k \leqslant n-2) \\ S_{j;n}\varphi'_{j;n-2} & (k=n-1) \\ S_{j;n-2}\varphi'_{j;n-1} & (k=n) \\ S_{j+k-n;2n-k-1}S_{j+k-1-n;2n-k}\cdots S_{j+2;n-3}S_{j+1;n-2}\varphi'_{j;n} & (n+1 \leqslant k \leqslant 2n-2). \end{cases}$$

Lemma 3.10:

$$\varphi_{j;k}(x_{j;1}) = \begin{cases} x_{j;k+1} - x_{j+1;k} & (0 \leqslant k \leqslant n-3) \\ x_{j;n-1} + x_{j;n} - x_{j+1;n-2} & (k=n-2) \\ x_{j;n} - x_{j+1;n-1} & (k=n-1) \\ x_{j+1;n-2} - x_{j+1;n-1} - x_{j+1;n} & (k=n) \\ x_{j+k-n+1;2n-k-2} - x_{j+k-n+1;2n-k-1} & (n+1 \leqslant k \leqslant 2n-2), \end{cases}$$

$$\varphi'_{j;k}(x_{j;1}) = \begin{cases} x_{j;n-1} - x_{j+1;n} & (k=n-1) \\ \varphi_{j;k}(x_{j;1}) & \text{otherwise}. \end{cases}$$

Proof: We shall prove the case $\varphi_{j;k}$ by the induction on k since the other case can be proved by the same argument. The case of $k=0$ is trivial.

Case I) $1 \leqslant k \leqslant n-3$.

If $k=1$, we have

$$S_{j;1}(x_{j;1}) = x_{j;1} - (x_{j;1} - x_{j;2} + x_{j+1;1}) = x_{j;2} - x_{j+1;1} = \varphi_{j;1}(x_{j;1}).$$

If $1 < k \leqslant n-3$, we assume that $\varphi_{j;k-1}(x_{j;1}) = x_{j;k} - x_{j+1;k-1}$. Then we have

$$\begin{aligned} S_{j;k}\varphi_{j;k-1}(x_{j;1}) = S_{j;k}(x_{j;k} - x_{j+1;k-1}) &= x_{j;k} - x_{j+1;k-1} - (x_{j;k} - x_{j;k+1} - x_{j+1;k-1} + x_{j+1;k}) \\ &= x_{j;k+1} - x_{j+1;k} = \varphi_{j;k}(x_{j;1}). \end{aligned}$$

Case II) $k = n-2, n-1, n$.

If $k=n-2$, using the result of Case I), we have

$$\begin{aligned} S_{j;n-2}\varphi_{j;n-3}(x_{j;1}) &= S_{j;n-2}(x_{j;n-2} - x_{j+1;n-3}) \\ &= x_{j;n-2} - x_{j+1;n-3} - (x_{j;n-2} - x_{j;n-1} - x_{j;n} - x_{j+1;n-3} + x_{j+1;n-2}) \\ &= x_{j;n-1} + x_{j;n} - x_{j+1;n-2} = \varphi_{j;n-2}(x_{j;1}), \end{aligned}$$

and then if $k=n-1$,

$$S_{j;n-1}\varphi_{j;n-2}(x_{j;1}) = S_{j;n-1}(x_{j;n-1}+x_{j;n}-x_{j+1;n-2}) = x_{j;n-1}+x_{j;n}-x_{j+1;n-2}-(x_{j;n-1}-x_{j+1;n-2}+x_{j+1;n-1})$$
$$= x_{j;n}-x_{j+1;n-1} = \varphi_{j;n-1}(x_{j;1}).$$

If $k=n$, then we have

$$S_{j;n}\varphi_{j;n-1}(x_{j;1}) = S_{j;n}(x_{j;n}-x_{j+1;n-1}) = x_{j;n}-x_{j+1;n-1}-(x_{j;n}-x_{j+1;n-2}+x_{j+1;n})$$
$$= x_{j+1;n-2}-x_{j+1;n-1}-x_{j+1;n} = \varphi_{j;n}(x_{j;1}).$$

Case III) $n+1\leqslant k\leqslant 2n-2$.

If $k=n+1$, using the result of the case of $k=n$, we have

$$S_{j+1;n-2}\varphi_{j;n}(x_{j;1}) = S_{j+1;n-2}(x_{j+1;n-2}-x_{j+1;n-1}-x_{j+1;n})$$
$$= x_{j+1;n-2}-x_{j+1;n-1}-x_{j+1;n}-(x_{j+1;n-2}-x_{j+1;n-1}-x_{j+1;n}-x_{j+2;n-3}+x_{j+2;n-2})$$
$$= x_{j+2;n-3}-x_{j+2;n-2} = \varphi_{j;n+1}(x_{j;1}).$$

If $n+1<k\leqslant 2n-2$, we assume that $\varphi_{j;k-1}(x_{j;1})=x_{j+k-n;2n-k-1}-x_{j+k-n;2n-k}$. Then we have

$$S_{j+k-n;2n-k-1}\varphi_{j;k-1}(x_{j;1}) = S_{j+k-n;2n-k-1}(x_{j+k-n;2n-k-1}-x_{j+k-n;2n-k})$$
$$= x_{j+k-n;2n-k-1}-x_{j+k-n;2n-k}-(x_{j+k-n;2n-k-1}-x_{j+k-n;2n-k}-x_{j+k-n+1;2n-k-2}$$
$$+x_{j+k-n+1;2n-k-1})$$
$$= x_{j+k-n+1;2n-k-2}-x_{j+k-n+1;2n-k-1}) = \varphi_{j;k}(x_{j;1}).$$

□

Lemma 311: The set $\{\varphi_{j;k}(x_{j;1}):1\leqslant j,0\leqslant k\leqslant 2n-2\}\cup\{\varphi'_{j;k}(x_{j;1}):1\leqslant j,0\leqslant k\leqslant 2n-2\}$ *is closed under the actions of all transformations* $S_{m;l}$ *for any* $m\geqslant 1$, $l\geqslant 1$.

Proof: First, we consider the action of $S_{m;l}$ to $\varphi_{j;k}(x_{j;1})$. If $k=0$, $\varphi_{j;0}=id$ and we have

$$S_{m;l}(\varphi_{j;0}(x_{j;1})) = \begin{cases} \varphi_{j;1}(x_{j;1}) & \text{if } (m;l)=(j;1) \\ x_{j;1} & \text{otherwise.} \end{cases}$$

If $1\leqslant k\leqslant n-3$, we have

$$S_{m;l}(\varphi_{j;k}(x_{j;1})) = \begin{cases} \varphi_{j;k-1}(x_{j;1}) & \text{if } (m;l)=(j;k) \\ \varphi_{j;k+1}(x_{j;1}) & \text{if } (m;l)=(j;k+1) \\ \varphi_{j;k}(x_{j;1}) & \text{otherwise.} \end{cases}$$

If $k=n-2$, we have

$$S_{m;l}(\varphi_{j;n-2}(x_{j;1})) = \begin{cases} \varphi_{j;n-3}(x_{j;1}) & \text{if } (m;l)=(j+1;n-2) \\ \varphi_{j;n-1}(x_{j;1}) & \text{if } (m;l)=(j;n-1) \\ \varphi'_{j;n-1}(x_{j;1}) & \text{if } (m;l)=(j;n) \\ \varphi_{j;n-2}(x_{j;1}) & \text{otherwise.} \end{cases} \tag{3.25}$$

If $k=n-1$, we have

$$S_{m;l}(\varphi_{j;n-1}(x_{j;1})) = \begin{cases} \varphi_{j;n-2}(x_{j;1}) & \text{if } (m;l)=(j+1;n-1) \\ \varphi_{j;n}(x_{j;1}) & \text{if } (m;l)=(j;n) \\ \varphi_{j;n-1}(x_{j;1}) & \text{otherwise.} \end{cases}$$

If $k=n$, we have

$$S_{m;l}(\varphi_{j;n}(x_{j;1})) = \begin{cases} \varphi_{j;n-1}(x_{j;1}) & \text{if } (m;l) = (j+1;n) \\ \varphi'_{j;n-1}(x_{j;1}) & \text{if } (m;l) = (j+1;n-1) \\ \varphi_{j;n+1}(x_{j;1}) & \text{if } (m;l) = (j+1;n-2) \\ \varphi_{j;n}(x_{j;1}) & \text{otherwise.} \end{cases} \tag{3.26}$$

If $n+1 \leqslant k \leqslant 2n-2$, we have

$$S_{m;l}(\varphi_{j;k}(x_{j;1})) = \begin{cases} \varphi_{j;k-1}(x_{j;1}) & \text{if } (m;l) = (j+k-n+1;2n-k-1) \\ \varphi_{j;k+1}(x_{j;1}) & \text{if } (m;l) = (j+k-n+1;2n-k-2) \\ \varphi_{j;k}(x_{j;1}) & \text{otherwise.} \end{cases}$$

Next, we consider the action of $S_{m;l}$ to $\varphi'_{j;k}(x_{j;1})$. Since the difference of $\varphi_{j;k}(x_{j;1})$ and $\varphi'_{j;k}(x_{j;1})$ is only the case of $k=n-1$ and by (3.25) and (3.26), we consider the case of $k=n-1$,

$$S_{m;l}(\varphi'_{j;n-1}(x_{j;1})) = \begin{cases} \varphi'_{j;n-2}(x_{j;1})(=\varphi_{j;n-2}(x_{j;1})) & \text{if } (m;l) = (j+1;n) \\ \varphi'_{j;n}(x_{j;1})(=\varphi_{j;n}(x_{j;1})) & \text{if } (m;l) = (j;n-1) \\ \varphi'_{j;n-1}(x_{j;1}) & \text{otherwise.} \end{cases}$$

□

Now, we define

$$\Xi'_\iota := \{\varphi_{j;k}(x_{j;1}) : j \geqslant 1, 0 \leqslant k \leqslant 2n-2\} \cup \{\varphi'_{j;k}(x_{j;1}) : j \geqslant 1, 0 \leqslant k \leqslant 2n-2\},$$

$$\Xi''_\iota := \{x_{j;n-1} : j \geqslant 1\} \cup \{x_{j;n} : j \geqslant 1\},$$

$$\Xi_\iota := \Xi'_\iota \cup \Xi''_\iota,$$

$$\Sigma_\iota := \{\vec{x} \in \mathbb{Z}_\iota^\infty : \varphi(\vec{x}) \geqslant 0 \text{ for any } \varphi \in \Xi_\iota\}.$$

Theorem 3.12: *The polyhedral realization Σ_ι of $B(\infty)$ for type D_n is described as follows:*

$$x_{j;i} = 0 \text{ for } j \notin [1,n-1] \text{ or } i \notin [1,n], \tag{3.27}$$

$$x_{1;i} \geqslant x_{2;i-1} \geqslant \cdots \geqslant x_{i;1} \geqslant 0 \text{ for } 1 \leqslant i \leqslant n-2, \tag{3.28}$$

$$x_{j;n-1} + x_{j;n} \geqslant x_{j+1;n-2} \geqslant x_{j+2;n-3} \cdots \geqslant x_{n-1;j} \geqslant 0 \text{ for } 1 \leqslant j \leqslant n-2, \tag{3.29}$$

$$x_{j;n-j} \geqslant x_{j;n-j+1} \geqslant \cdots \geqslant x_{j;n-2} \geqslant x_{j;n-1} + x_{j;n} \geqslant 0 \text{ for } 2 \leqslant j \leqslant n-1, \tag{3.30}$$

$$\begin{cases} x_{1;n-1} \geqslant x_{2;n} \geqslant x_{3;n-1} \geqslant x_{4;n} \geqslant \cdots \geqslant x_{n-1;n} \geqslant 0 \\ x_{1;n} \geqslant x_{2;n-1} \geqslant x_{3;n} \geqslant x_{4;n-1} \geqslant \cdots \geqslant x_{n-1;n-1} \geqslant 0 \end{cases} \quad (n\text{:odd}) \tag{3.31}$$

$$\left(\begin{cases} x_{1;n-1} \geqslant x_{2;n} \geqslant x_{3;n-1} \geqslant x_{4;n} \geqslant \cdots \geqslant x_{n-1;n-1} \geqslant 0 \\ x_{1;n} \geqslant x_{2;n-1} \geqslant x_{3;n} \geqslant x_{4;n-1} \geqslant \cdots \geqslant x_{n-1;n} \geqslant 0 \end{cases} \quad (\textit{respectively}, n\text{:even}) \right). \tag{3.32}$$

Proof: Since Ξ_ι is not closed under the action of S_k, we shall show that

(i) Σ_ι is closed under the action of $\tilde{f}_i$,
(ii) Σ_ι is closed under the action of $\tilde{e}_i$,

(iii) all the entries of $\vec{x} \in \Sigma_\iota$ are non-negative
(These show that Σ_ι is the polyhedral realization of $B(\infty)$),
(iv) Σ_ι has the form of Theorem 3.12.

(*i*) We show that Σ_ι is closed under the action of $\tilde{f}_i$.
Note that ι satisfies the positivity assumption by Lemma 3.11. Let $\vec{x}=(\ldots,x_2,x_1) \in \Sigma_\iota$ and $i \in I$, and suppose that $\tilde{f}_i\vec{x}=(\ldots,x_k+1,\ldots,x_2,x_1)$ for $i_k=i$. We need to show that

$$\varphi(\tilde{f}_i\vec{x}) \geqslant 0$$

for any $\varphi=\Sigma\varphi_j x_j \in \Xi_\iota$. First, we consider the case of $\varphi \in \Xi'_\iota$. Since $\varphi(\tilde{f}_i\vec{x})=\varphi(\vec{x})+\varphi_k$, it is enough to consider the case when $\varphi_k<0$. Since ι satisfies the positivity assumption, we have $k^{(-)} \geqslant 1$. By (2.4), we have $\sigma_k(\vec{x}) > \sigma_{k^{(-)}}(\vec{x})$ and by (2.9), we conclude that

$$\beta_{k^{(-)}}(\vec{x}) = \sigma_{k^{(-)}}(\vec{x}) - \sigma_k(\vec{x}) \leqslant -1.$$

It follows that

$$\varphi(\tilde{f}_i\vec{x}) = \varphi(\vec{x}) + \varphi_k \geqslant \varphi(\vec{x}) - 1 \cdot \beta_{k^{(-)}}(\vec{x}) = (S_k\varphi)(\vec{x}) \tag{3.33}$$

$$\geqslant 0 \tag{3.34}$$

since $S_k\varphi \in \Xi'_\iota$. This shows that Σ_ι is closed under the action of $\tilde{f}_i$ for $\varphi \in \Xi'_\iota$. Next, we consider the case of $\varphi=x_{j;n-1} \in \Xi''_\iota$. We have

$$\varphi(\tilde{f}_i\vec{x}) = x_{j;n-1} + 1 \geqslant 0.$$

The case of $\varphi=x_{j;n} \in \Xi''_\iota$ can be proved by the same argument.
(*ii*) We show that Σ_ι is closed under the action of $\tilde{e}_i$.
We need to show that

$$\varphi(\tilde{e}_i\vec{x}) \geqslant 0$$

for any $\varphi \in \Xi_\iota$. First, we consider the case of $\varphi \in \Xi'_\iota$. Since $\varphi(\tilde{e}_i\vec{x})=\varphi(\vec{x})-\varphi_k$, it is enough to consider the case when $\varphi_k>0$. By (2.5), $\sigma_k(\vec{x}) > \sigma_{k^{(+)}}(\vec{x})$ and by (2.9) we conclude that

$$\beta_k(\vec{x}) = \sigma_k(\vec{x}) - \sigma_{k^{(+)}}(\vec{x}) \geqslant 1.$$

It follows that

$$\varphi(\tilde{e}_i\vec{x}) = \varphi(\vec{x}) - \varphi_k \geqslant \varphi(\vec{x}) - 1 \cdot \beta_k(\vec{x}) = (S_k\varphi)(\vec{x}) \geqslant 0$$

since $S_k\varphi \in \Xi'_\iota$. This shows that Σ_ι is closed under the action of $\tilde{e}_i$ for $\varphi \in \Xi'_\iota$. Next, we consider the case of $\varphi=x_{j;n-1} \in \Xi''_\iota$. It follows that

$$\begin{aligned}\varphi(\tilde{e}_i\vec{x}) = x_{j;n-1}(\vec{x}) - 1 &\geqslant x_{j;n-1}(\vec{x}) - 1 \cdot \beta_{j;n-1}(\vec{x}) = (S_{j;n-1}x_{j;n-1})(\vec{x}) \\ &= (x_{j+1;n-2} - x_{j+1;n-1})(\vec{x}) \geqslant x_{j+1;n}(\vec{x}) \text{ (by Lemma 3.10)} \\ &\geqslant 0 \ (by\ x_{j+1;n} \in \Xi''_\iota).\end{aligned}$$

The case of $\varphi=x_{j;n} \in \Xi''_\iota$ can be proved by the same argument.
(*iii*) We show that all the entries of $\vec{x} \in \Sigma_\iota$ are non-negative.
In the case of $1 \leqslant m$, $0 \leqslant l \leqslant n-3$ for $\varphi_{m;l}(x_{m;1})$, we have

$$x_{m;l+1} \geqslant x_{m+1;l}, \tag{3.35}$$

and we consider the cases that $(m;l)=(j;i-1),(j+1;i-2),\cdots,(j+i-2;1),(j+i-1;0)$. We obtain

$$x_{j;i} \geqslant x_{j+1;i-1} \geqslant \cdots \geqslant x_{j+i-2;2} \geqslant x_{j+i-1;1} \geqslant 0.$$

This shows that $x_{j;i} \geqslant 0$ for any $j \geqslant 1$, $1 \leqslant i \leqslant n-2$. By the definition of Ξ''_ι, we have $x_{j;n-1}$ and $x_{j;n} \geqslant 0$ for $j \geqslant 1$ and these show $x_{j;n} \geqslant 0$ for any $j \geqslant 1$.
(*iv*) We show that Σ_ι has the form of Theorem 3.12.
We determine when $x_{j;i} \equiv 0$ for $j \geqslant 1$, $1 \leqslant i \leqslant n$. In the case of $1 \leqslant m$, $n+1 \leqslant l \leqslant 2n-2$ for $\varphi_{m;l}(x_{m;1})$, we have

$$x_{m+l-n+1;2n-l-2} \geqslant x_{m+l-n+1;2n-l-1} \tag{3.36}$$

and in the case of $0 \leqslant m$, $l=n$,

$$x_{m+1;n-2} \geqslant x_{m+1;n-1} + x_{m+1;n} \geqslant 0 \text{ (since } x_{m+1;n-1} \geqslant 0 \text{ and } x_{m+1;n} \geqslant 0). \tag{3.37}$$

We consider the cases that $(m;l)=(j;2n-2),(j+1;2n-3),\ldots,(j+n-2;n)$, then we have

$$0 \geqslant x_{j+n-1;1} \geqslant x_{j+n-1;2} \geqslant \cdots \geqslant x_{j+n-1;n-3} \geqslant x_{j+n-1;n-2} \geqslant x_{j+n-1;n-1} + x_{j+n-1;n} \geqslant 0.$$

Combining $x_{j+n-1;n-1} \geqslant 0, x_{j+n-1;n} \geqslant 0$ this shows that $x_{j+n-1;i} \equiv 0$ for any $j \geqslant 1$, $1 \leqslant i \leqslant n$. We shall show (3.28). In (3.35), by setting $(m;l)=(1;i-1),(2;i-2),\ldots,(i;0)$ for $1 \leqslant i \leqslant n-2$ then we have (3.28). Let us show (3.29). We consider the cases that $(m;l)=(j+1;n-3),(j+2;n-4),\ldots,(n-1;j-1)$ for $1 \leqslant j \leqslant n-2$ in (3.35) and the case $k=n-2$ in Lemma 3.10. We have (3.29). We shall show (3.30). We consider the cases that $(m;l)=(1;n+j-2),(2;n+j-3),\ldots,(j-2;n+1)$ for $2 \leqslant j \leqslant n-1$ in (3.36) and $(m;l)=(j-1;n)$ for $2 \leqslant j \leqslant n-1$ in (3.37). This shows (3.30). Let us see (3.31). We consider the cases that $k=n-1$ for $\varphi_{j;k}$, $\varphi'_{j;k}$ in Lemma 3.10. We obtain (3.31). Here, (3.32) can be proved by the same argument as (3.31). Therefore, Σ_ι has the form of Theorem 3.12. □

Next, we give the polyhedral realization $\Sigma_\iota[\lambda]$ of $B(\lambda)$ for $\lambda := \sum_{k=1}^n \lambda_k \Lambda_k$, where $\lambda_k \in \mathbb{Z}_{\geqslant 0}$, Λ_k are the fundamental weights. Here we set

$$\Xi_\iota^{(1,n-2)} := \{S_{j_k} \cdots S_{j_2} S_{j_1} \xi^{(i)}(\vec{x}) : k \geqslant 0, 1 \leqslant i \leqslant n-2, j_1, \ldots, j_k \geqslant 1\},$$

$$\Xi_\iota^{(n-1)} := \{S_{j_k} \cdots S_{j_2} S_{j_1} \xi^{(n-1)}(\vec{x}) : k \geqslant 0, j_1, \ldots, j_k \geqslant 1\},$$

$$\Xi_\iota^{(n)} := \{S_{j_k} \cdots S_{j_2} S_{j_1} \xi^{(n)}(\vec{x}) : k \geqslant 0, j_1, \ldots, j_k \geqslant 1\},$$

$$\Xi_\iota^{(1,n-2)}[\lambda] := \{\hat{S}_{j_k} \cdots \hat{S}_{j_2} \hat{S}_{j_1} \lambda^{(i)}(\vec{x}) : k \geqslant 0, 1 \leqslant i \leqslant n-2, j_1, \ldots, j_k \geqslant 1\},$$

$$\Xi_\iota^{(n-1)}[\lambda] := \{\hat{S}_{j_k} \cdots \hat{S}_{j_2} \hat{S}_{j_1} \lambda^{(n-1)}(\vec{x}) : k \geqslant 0, j_1, \ldots, j_k \geqslant 1\},$$

$$\Xi_\iota^{(n)}[\lambda] := \{\hat{S}_{j_k} \cdots \hat{S}_{j_2} \hat{S}_{j_1} \lambda^{(n)}(\vec{x}) : k \geqslant 0, j_1, \ldots, j_k \geqslant 1\},$$

$$\begin{aligned}
\Xi_\iota[\lambda] &:= \Xi_\iota \cup \Xi_\iota^{(1,n-2)}[\lambda] \cup \Xi_\iota^{(n-1)}[\lambda] \cup \Xi_\iota^{(n)}[\lambda] \\
&= \{\varphi_{j;k}(x_{j;1}) : j \geqslant 1, 0 \leqslant k \leqslant 2n-1\} \\
&\quad \cup \{\hat{S}_{j_k} \cdots \hat{S}_{j_2} \hat{S}_{j_1} \lambda^{(i)}(\vec{x}) : k \geqslant 0, 1 \leqslant i \leqslant n-2, j_1, \ldots, j_k \geqslant 1\} \\
&\quad \cup \{\hat{S}_{j_k} \cdots \hat{S}_{j_2} \hat{S}_{j_1} \lambda^{(n-1)}(\vec{x}) : k \geqslant 0, j_1, \cdots, j_k \geqslant 1\} \cup \{\hat{S}_{j_k} \cdots \hat{S}_{j_2} \hat{S}_{j_1} \lambda^{(n)}(\vec{x}) : k \geqslant 0, j_1, \ldots, j_k \geqslant 1\},
\end{aligned}$$

$$\Sigma_\iota[\lambda] := \{\vec{x} \in \mathbb{Z}_\iota[\lambda] : \varphi(\vec{x}) \geqslant 0 \text{ for any } \varphi \in \Xi_\iota[\lambda]\}.$$

In order to show that $\Sigma_\iota[\lambda]$ is the polyhedral realization of $B(\lambda)$, we give the explicit forms of $\Xi_\iota^{(1,n-2)}[\lambda]$, $\Xi_\iota^{(n-1)}[\lambda]$, and $\Xi_\iota^{(n)}[\lambda]$. Since the Dynkin diagrams for A_n and D_n are the same for $1 \leqslant i \leqslant n-2$, we give the explicit form of $\Xi_\iota^{(1,n-2)}$ as follows:

$$\Xi_\iota^{(1,n-2)} = \{x_{j;i-j} - x_{j;i-j+1} : 1 \leqslant i \leqslant n-2, 1 \leqslant j \leqslant i\}. \tag{3.38}$$

For giving the explicit form of $\Xi_\iota^{(n-1)}$ and $\Xi_\iota^{(n)}$, we say that an integer sequence $\mu_1, \mu_2, \ldots, \mu_n$ is an admissible pattern if:

$$\begin{cases} 1 \leqslant \mu_1 \leqslant n-1, \\ 0 \leqslant \mu_2 \leqslant \mu_1 - 1, \\ \cdots, \\ 0 \leqslant \mu_k \leqslant \mu_{k-1} - 1, \\ \cdots, \end{cases} \tag{3.39}$$

where if μ_k does not exist, we define $\mu_k = 0$, and

$$S^{(\mu_1)} := \begin{cases} id & (\mu_1 = 1) \\ S_{\mu_1 - 1;n-\mu_1} \cdots S_{2;n-3} S_{1;n-2} & (\mu_1 \geqslant 2), \end{cases}$$

$$S^{(\mu_k)} := \begin{cases} id & (\mu_k = 0) \\ S_{\mu_k+k-2;n-\mu_k} \cdots S_{k+1;n-3} S_{k;n-2} S_{k-1;n} & (\mu_k \geqslant 1 \text{ and } k\text{:even}) \\ S_{\mu_k+k-2;n-\mu_k} \cdots S_{k+1;n-3} S_{k;n-2} S_{k-1;n-1} & (\mu_k \geqslant 1 \text{ and } k\text{:odd}) \end{cases} \quad \text{for } k \geqslant 2,$$

$$S^{(\mu'_k)} := \begin{cases} id & (\mu_k = 0) \\ S_{\mu_k+k-2;n-\mu_k} \cdots S_{k+1;n-3} S_{k;n-2} S_{k-1;n} & (\mu_k \geqslant 1 \text{ and } k\text{:odd}) \\ S_{\mu_k+k-2;n-\mu_k} \cdots S_{k+1;n-3} S_{k;n-2} S_{k-1;n-1} & (\mu_k \geqslant 1 \text{ and } k\text{:even}) \end{cases} \quad \text{for } k \geqslant 2,$$

$$\varphi^{(\mu)} := S^{(\mu_k)} \cdots S^{(\mu_2)} S^{(\mu_1)} \text{ for } \mu = (\mu_1, \mu_2, \ldots, \mu_k, 0, 0, \ldots),$$

$$\varphi'^{(\mu')} := S^{(\mu'_k)} \cdots S^{(\mu'_2)} S^{(\mu_1)} \text{ for } \mu = (\mu_1, \mu'_2, \ldots, \mu'_k, 0, 0, \ldots).$$

We prepare the symbol X as follows:

$$X := x_{1;n-2} - x_{1;n-1} (= \xi^{(n-1)}(\vec{x})), \tag{3.40}$$

$$X' := x_{1;n-2} - x_{1;n} (= \xi^{(n)}(\vec{x})). \tag{3.41}$$

For convenience, we define

$$X_{j;i} := \begin{cases} x_{j;n} & \text{if } j\text{:even and } i = n-1 \\ x_{j;n-1} & \text{if } j\text{:even and } i = n \\ x_{j;i} & \text{otherwise}, \end{cases} \tag{3.42}$$

$$X'_{j;i} := \begin{cases} x_{j;n} & \text{if } j\text{:odd and } i = n-1 \\ x_{j;n-1} & \text{if } j\text{:odd and } i = n \\ x_{j;i} & \text{otherwise}. \end{cases} \tag{3.43}$$

Theorem 3.13: *Let* $\mu=(\mu_1,\mu_2,\ldots,\mu_k,0,0,\ldots)$ *be an admissible pattern.*

(i) *The forms* $\varphi^{(\mu)}X$ *are given by*

$$\varphi^{(\mu)}X=\begin{cases}\displaystyle\sum_{k=1}^{l}(X_{\mu_k+k-1;n-\mu_k-1}-X_{\mu_k+k-1;n-\mu_k}) & \text{if } \mu_l=1\\ \displaystyle\sum_{k=1}^{l}(X_{\mu_k+k-1;n-\mu_k-1}-X_{\mu_k+k-1;n-\mu_k})+X_{l;n} & \text{if } \mu_l\geqslant 2.\end{cases}\tag{3.44}$$

where $l:=\max\{k:\mu_k\neq 0\}$.

(ii) *The forms* $\varphi'^{(\mu')}X'$ *are given by*

$$\varphi'^{(\mu')}X'=\begin{cases}\displaystyle\sum_{k=1}^{l}(X'_{\mu_k+k-1;n-\mu_k-1}-X'_{\mu_k+k-1;n-\mu_k}) & \text{if } \mu'_l=1\\ \displaystyle\sum_{k=1}^{l}(X'_{\mu_k+k-1;n-\mu_k-1}-X'_{\mu_k+k-1;n-\mu_k})+X'_{l;n} & \text{if } \mu'_l\geqslant 2.\end{cases}\tag{3.45}$$

where $l:=\max\{k:\mu'_k\neq 0\}$.

(iii) $\Xi_\iota^{(n-1)}$ *(respectively,* $\Xi_\iota^{(n)}$*) is the set of all linear forms which are of the form* $\varphi^{(\mu)}X$ *(respectively,* $\varphi'^{(\mu')}X'$*), where* μ *(respectively,* μ'*) are the admissible patterns.*

Proof: We shall show (i), the case (ii) can be proved by the same argument. First, we give a remark. When $\mu_k-\mu_{k+1}=1$, the terms $X_{\mu_k+k-1;n-\mu_k}$ and $X_{\mu_{k+1}+k;n-\mu_{k+1}-1}$ in the sum (3.44) are canceled as $-X_{\mu_k+k-1;n-\mu_k}+X_{\mu_{k+1}+k;n-\mu_{k+1}-1}=0$. We show the theorem by induction on $|\mu|=\mu_1+\mu_2+\cdots+\mu_i$ for $\mu=(\mu_1,\mu_2,\cdots,\mu_i,0,0,\ldots)$.

If $|\mu|=1$, then $l=1$ and the sum of the right-hand side of (3.44) is $X_{1;n-2}-X_{1;n-1}=x_{1;n-2}-x_{1;n-1}$ and equal to $\varphi^{(\mu)}X$ by (3.41). We assume that $|\mu|=\mu_1+\mu_2+\cdots+\mu_i=k-1$ for $\mu=(\mu_1,\mu_2,\ldots,\mu_i,0,0,\ldots)$. We consider the two cases: I) $\mu_i\to\mu_i+1$, II) "$\mu_{i+1}=0$" $\to$ "$\mu_{i+1}=1$".

I) $\mu_i\to\mu_i+1$.

We shall prove the case $\mu_i=1$, the case $\mu_i\geqslant 2$ can be proved by the same argument. We have $l=i$ and note that $1\leqslant\mu_i\leqslant\mu_{i-1}-2$ by the fact that μ is admissible pattern and the term $X_{\mu_i+i-1;n-\mu_i-1}$ in the sum (3.13) is not canceled. We set $\mu':=(\mu_1,\mu_2,\ldots,\mu_i+1,0,0,\ldots)$. We have

$$\varphi^{(\mu')}X=S_{\mu_i+i-1;n-\mu_i-1}\varphi^{(\mu)}X.$$

The right-hand side of (3.44) is

$$\begin{aligned}S_{\mu_i+i-1;n-\mu_i-1}\left(\sum_{k=1}^{l}(X_{\mu_k+k-1;n-\mu_k-1}-X_{\mu_k+k-1;n-\mu_k})\right)&=\sum_{k=1}^{l}(X_{\mu_k+k-1;n-\mu_k-1}-X_{\mu_k+k-1;n-\mu_k})\\&\quad-(X_{\mu_i+i-1;n-\mu_i-1}-X_{\mu_i+i-1;n-\mu_i}-X_{\mu_i+i;n-\mu_i-2}\\&\quad+X_{\mu_i+i;n-\mu_i-1})=\varphi^{(\mu')}X.\end{aligned}$$

II) "$\mu_{i+1}=0$" $\to$ "$\mu_{i+1}=1$."

We set $\mu':=(\mu_1,\mu_2,\ldots,\mu_i,1,0,\ldots)$ (*i.e.* $\mu_{i+1}=1$) and then $l=i+1$. By the fact that μ is admissible pattern, we have $0\leqslant\mu_{i+1}\leqslant\mu_i-1$. This shows that $\mu_i\geqslant 2$ and the term $X_{i;n}$ in the sum (3.44) is not canceled. If i is odd, then we have

$$\varphi^{(\mu')}X=S_{i;n}\varphi^{(\mu)}X.$$

The right-hand side of (3.44) is

$$S_{i;n}\left(\sum_{k=1}^{l}(X_{\mu_k+k-1;n-\mu_k-1}-X_{\mu_k+k-1;n-\mu_k})+X_{i;n}\right)=\sum_{k=1}^{l}(X_{\mu_k+k-1;n-\mu_k-1}-X_{\mu_k+k-1;n-\mu_k})$$
$$+X_{i;n}-(X_{i;n}-X_{i+1;n-2}+X_{i+1;n})=\varphi^{(\mu')}X.$$

If i is even, we can prove II) by the same argument.

(iii) It is sufficient to show that $\{\varphi^{(\mu)}X|\,\mu$:admissible pattern$\}$ is closed under the actions of all $S_{j;i}$, the other case can be proved by the same argument. We set for $1\leqslant k\leqslant l+1$, $\mu=(\mu_1,\mu_2,\ldots,\mu_k,\ldots,\mu_l,0,0,\ldots)$, $\mu^+=(\mu_1,\mu_2,\ldots,\mu_k+1,\ldots,\mu_l,0,0,\ldots)$, $\mu^-=(\mu_1,\mu_2,\ldots,\mu_k-1,\ldots,\mu_l,0,0,\ldots)$.

Then we have

$$S_{j;i}\varphi^{(\mu)}X=\begin{cases}\varphi^{(\mu^+)}X & \text{if } (j;i)=(\mu_k+k-1;n-\mu_k) \text{ and } \mu_{k-1}-\mu_k\neq 1\\ \varphi^{(\mu^-)}X & \text{if } (j;i)=(\mu_k+k-1;n-\mu_k+1) \text{ and } \mu_k-\mu_{k+1}\neq 1\\ \varphi^{(\mu)}X & \text{otherwise.}\end{cases}$$

□

Therefore, ι satisfies the strict positivity assumption by the explicit forms of $\Xi_\iota^{(1,n-2)}$, $\Xi_\iota^{(n-1)}$, and $\Xi_\iota^{(n)}$. By the Lemma 2.6, this shows that

$$\Xi_\iota^{(1,n-2)}[\lambda]=\{\lambda_i+x_{j;i-j}-x_{j;i-j+1}:1\leqslant i\leqslant n-1,1\leqslant j\leqslant i\},$$

$$\Xi_\iota^{(k)}[\lambda]=\{\lambda_k+\varphi(\vec{x}):\varphi(\vec{x})\in\Xi_\iota^{(k)}:\mu \text{ are the admissible patterns}\} \text{ for } k=n-1,n$$

by (3.38) and (3.44) and $\Sigma_\iota[\lambda]$ is the polyhedral realization of $B(\lambda)$.

D. F_4 case

We use the different Cartan data from the one in Ref. 10, where the Cartan matrix $(a_{ij})_{1\leqslant i,j\leqslant 4}$ is given by

$$a_{ij}:=\begin{cases}2 & \text{if } i=j\\ -1 & \text{if } |i-j|=1 \text{ and } (i,j)\neq(2,3)\\ -2 & \text{if } (i,j)=(2,3)\\ 0 & \text{otherwise.}\end{cases}$$

We fix ι as follows:

$$\iota:=(\ldots,\underbrace{4,3,2,1},\ldots,\underbrace{4,3,2,1},\underbrace{4,3,2,1}).$$

We define

$$\Xi_\iota:=\{S_{m_l}\cdots S_{m_2}S_{m_1}(x_{j;1}):l\geqslant 0,m_1,\ldots,m_l\geqslant 1,1\leqslant j\leqslant 6\},$$

$$\Sigma_\iota:=\{\vec{x}\in\mathbb{Z}_\iota^\infty|\varphi(\vec{x})\geqslant 0 \text{ for any } \varphi\in\Xi_\iota\}.$$

Using Theorem 3.3, we shall give the polyhedral realization of $B(\infty)$. We give the explicit form of Ξ_ι by direct calculation and show that the polyhedral realization of $B(\infty)$ is equal to Σ_ι using the following three steps:

(i) We check the positivity assumption,
(ii) For $\vec{x}=(\ldots,x_{1;2},x_{1;1})\in\Sigma_\iota$, we check that $x_{j;i}\geqslant 0$ for all $i,j\geqslant 1$, ((i), (ii) shows that Σ_ι is the polyhedral realization of $B(\infty)$),
(iii) We determine when $x_{j;i}\equiv 0$ for convenience.

Theorem 3.14: *We give the explicit form of* Ξ_ι *as follows*:

$$\left\{\begin{array}{ccc}
x_{j;1} & x_{j;2}-x_{j+1;1} & 2x_{j;3}-x_{j+1;2} \quad 2x_{j;4}-x_{j+3;1} \\
x_{j+1;2}-2x_{j+1;4} & x_{j+2;2}-x_{j+3;2} & x_{j+2;1}-x_{j+4;1} \quad 2x_{j+2;4}-x_{j+4;2} \\
x_{j+3;1}-x_{j+3;4} & x_{j+4;2}-2x_{j+4;3} & x_{j+5;1}-x_{j+5;2} \quad -x_{j+6;1} \\
2x_{j;4}+x_{j+1;2}-2x_{j+1;3} & 2x_{j;4}-x_{j+2;1}-x_{j+2;2} & 2x_{j+1;3}-2x_{j+1;4}-x_{j+3;1} \\
x_{j+2;1}+x_{j+2;2}-2x_{j+2;3} & 2x_{j+2;2}-2x_{j+2;3}-x_{j+3;1} & x_{j+2;1}+x_{j+3;1}-x_{j+3;2} \\
2x_{j+2;3}+x_{j+3;1}-2x_{j+3;2} & 2x_{j+2;4}+x_{j+3;1}-2x_{j+3;3} & 2x_{j+2;3}-x_{j+3;2}-x_{j+4;1} \\
x_{j+2;2}-x_{j+3;1}-x_{j+4;1} & x_{j+3;2}-2x_{j+3;4}-x_{j+4;1} & 2x_{j+3;3}-2x_{j+3;4}-x_{j+4;2} \\
2x_{j+1;3}+x_{j+2;1}-2x_{j+1;4}-x_{j+2;2} & 2x_{j+2;4}+x_{j+3;2}-2x_{j+3;3}-x_{j+4;1}
\end{array}\right\}.$$

Proof: (i) By the form of Σ_ι, coefficients of $x_{1;1}, x_{1;2}, x_{1;3}, x_{1;4}$ are positive. This shows that the "positivity assumption" is satisfied.

(ii) We assume $x_{j;1} \geqslant 0$ for any $j \geqslant 1$. We show that $x_{j;2}, x_{j;3}, x_{j;4} \geqslant 0$ for any $j \geqslant 1$. By the results of (i), we have

$$x_{j;2} \geqslant x_{j+1;1}, \quad 2x_{j;3} \geqslant x_{j+1;2}, \quad 2x_{j;4} \geqslant x_{j+3;1}.$$

Then we have $x_{j;2} \geqslant 0$ for $j \geqslant 1$ since $x_{j;2} \geqslant x_{j+1;1}$. Similarly, we obtain $x_{j;3} \geqslant 0$, $x_{j;4} \geqslant 0$ for $j \geqslant 1$ since $2x_{j;3} \geqslant x_{j+1;2}$, $2x_{j;4} \geqslant x_{j+3;1}$, respectively. (i) and (ii) show that Σ_ι is the polyhedral realization of $B(\infty)$.

(iii) We determine when $x_{j;i} \equiv 0$. By the forms of Σ_ι and (ii), we have

$$0 \geqslant x_{j+6;1} \geqslant 0.$$

This shows $x_{m;1} \equiv 0$ for $m \geqslant 7$. Similarly, we obtain

$$x_{m;2} \equiv 0, \quad x_{m;3} \equiv 0, \quad x_{m;4} \equiv 0 \quad \text{for } m \geqslant 7$$

since $x_{j+5;1} \geqslant x_{j+5;2}$, $x_{j+4;1} \geqslant x_{j+4;3}$, $x_{j+3;1} \geqslant x_{j+3;4}$, respectively. In particular, the parameter j in Ξ_ι runs over $1 \leqslant j \leqslant 6$. □

Next, we give the polyhedral realization of $B(\lambda)$ for $\lambda := \lambda_1\Lambda_1 + \ldots + \lambda_4\Lambda_4$. Here we set for $1 \leqslant i \leqslant 4$,

$$\Xi_\iota^{(i)} := \{S_{j_k} \cdots S_{j_2} S_{j_1} \xi^{(i)}(\vec{x}) : k \geqslant 0, j_1, \ldots, j_k \geqslant 1\},$$

$$\Xi_\iota^{(i)}[\lambda] := \{\hat{S}_{j_k} \cdots \hat{S}_{j_2} \hat{S}_{j_1} \lambda^{(i)}(\vec{x}) : k \geqslant 0, j_1, \ldots, j_k \geqslant 1\},$$

$$\Xi_\iota[\lambda] := \Xi_\iota \cup \Xi_\iota^{(1)}[\lambda] \cup \cdots \cup \Xi_\iota^{(4)}[\lambda]$$

$$\Sigma_\iota[\lambda] := \{\vec{x} \in \mathbb{Z}_\iota[\lambda] : \varphi(\vec{x}) \geqslant 0 \text{ for any } \varphi \in \Xi_\iota[\lambda]\}.$$

In order to show that $\Sigma_\iota[\lambda]$ is the polyhedral realization of $B(\lambda)$, we give the explicit forms of $\Xi_\iota^{(i)}$ for $1 \leqslant i \leqslant 4$ by direct calculation as follows:

$$\Xi_\iota^{(1)} = \{-x_{1;1}\},$$

$$\Xi_\iota^{(2)} = \{x_{1;1} - x_{1;2}, -x_{2;1}\},$$

$$\Xi_\iota^{(3)} = \left\{ \begin{array}{ccccc} x_{1;2}-x_{1;3} & x_{1;3}-x_{3;1} & x_{2;1}-x_{2;4} & x_{2;3}-x_{3;3} \\ x_{1;4}-x_{3;4} & x_{2;4}-x_{5;1} & x_{4;1}-x_{4;3} & x_{4;3}-x_{5;2} \\ & x_{4;4}-x_{5;3} & -x_{5;4} & \\ x_{1;3}+x_{2;1}-x_{2;2} & x_{1;4}+x_{2;1}-x_{2;3} & x_{1;4}+x_{2;3}-x_{3;2} & \\ x_{1;4}+x_{2;4}-x_{3;3} & x_{2;4}+x_{3;2}-2x_{3;3} & x_{2;4}+x_{4;1}-x_{4;2} & \\ x_{2;2}-x_{2;4}-x_{3;1} & 2x_{2;3}-x_{2;4}-x_{3;2} & x_{3;2}-x_{3;3}-x_{3;4} & \\ x_{2;3}-x_{2;4}-x_{3;4} & x_{3;3}-x_{3;4}-x_{5;1} & x_{4;2}-x_{4;3}-x_{5;1} & \\ x_{1;4}+x_{2;2}-x_{2;3}-x_{3;1} & x_{3;3}+x_{4;1}-x_{3;4}-x_{4;2} & & \end{array} \right\},$$

$$\Xi_\iota^{(4)} = \left\{ \begin{array}{ccccc} x_{1;3}-x_{1;4} & x_{2;2}-x_{2;3} & x_{2;3}-x_{4;1} & x_{3;1}-x_{3;4} \\ x_{3;3}-x_{4;3} & x_{2;4}-x_{4;4} & x_{3;4}-x_{6;1} & x_{5;1}-x_{5;3} \\ & x_{5;3}-x_{6;2} & x_{5;4}-x_{6;3} & -x_{6;4} \\ x_{2;3}+x_{3;1}-x_{3;2} & x_{2;4}+x_{3;1}-x_{3;3} & x_{2;4}+x_{3;3}-x_{4;2} & \\ x_{2;4}+x_{3;4}-x_{4;3} & x_{3;4}+x_{4;2}-2x_{4;3} & x_{3;4}+x_{5;1}-x_{5;2} & \\ x_{3;2}-x_{3;4}-x_{4;1} & 2x_{3;3}-x_{3;4}-x_{4;2} & x_{4;2}-x_{4;3}-x_{4;4} & \\ x_{3;3}-x_{3;4}-x_{4;4} & x_{4;3}-x_{4;4}-x_{6;1} & x_{5;2}-x_{5;3}-x_{6;1} & \\ x_{2;4}+x_{3;2}-x_{3;3}-x_{4;1} & x_{4;3}+x_{5;1}-x_{4;4}-x_{5;2} & & \end{array} \right\}.$$

Therefore, ι satisfies the strict positivity assumption by the explicit forms of $\Xi_\iota^{(i)}$ for $1 \leqslant i \leqslant 4$. This shows that

$$\Xi_\iota^{(1)}[\lambda] = \{\lambda_1 - x_{1;1}\},$$

$$\Xi_\iota^{(2)}[\lambda] = \{\lambda_2 + x_{1;1} - x_{1;2}, \lambda_2 - x_{2;1}\},$$

$$\Xi_\iota^{(k)}[\lambda] = \{\lambda_k + \varphi_k(\vec{x}) : \varphi_k(\vec{x}) \in \Xi_\iota^{(k)}\} \text{ for } k = 3,4$$

by Lemma 2.6 and $\Sigma_\iota[\lambda]$ is the polyhedral realization of $B(\lambda)$.

E. E_6 case

We fix ι as follows:

$$\iota := (\ldots, \underline{6,5,4,3,2,1}, \ldots, \underline{6,5,4,3,2,1}, \underline{6,5,4,3,2,1}).$$

We define

$$\Xi_\iota := \{S_{m_l} \cdots S_{m_2} S_{m_1}(x_{j;1}) : l \geqslant 0, m_1, \ldots, m_l \geqslant 1, 1 \leqslant j \leqslant 8\},$$

$$\Sigma_\iota := \{\vec{x} \in Z_\iota^\infty : \varphi(\vec{x}) \geqslant 0 \text{ for any } \varphi \in \Xi_\iota\}.$$

We give the explicit form of Ξ_ι by direct calculation and show that the polyhedral realization of $B(\infty)$ is equal to Σ_ι using the following steps similar to the case of F_4:

(i) We check the positivity assumption.
(ii) For $\vec{x} = (\ldots, x_{1;2}, x_{1;1}) \in \Sigma_\iota$, we check that $x_{j;i} \geqslant 0$ for all $i, j \geqslant 1$.
(iii) We determine when $x_{j;i} \equiv 0$ for convenience.

Theorem 3.15: *We give the explicit form of* Ξ_ι *as follows*:

$$\left\{\begin{array}{c} x_{j;1} \quad x_{j;2}-x_{j+1;1} \quad x_{j;3}-x_{j+1;2} \quad x_{j;4}-x_{j+1;6} \\ x_{j;6}-x_{j+1;5} \quad x_{j+2;2}-x_{j+2;4} \quad x_{j;5}-x_{j+4;1} \quad x_{j+3;1}-x_{j+3;6} \\ x_{j+2;6}-x_{j+2;2} \quad x_{j+3;4}-x_{j+4;3} \quad x_{j+3;5}-x_{j+4;4} \quad -x_{j+4;5} \\ x_{j;4}+x_{j;6}-x_{j+1;3} \quad x_{j;5}+x_{j;6}-x_{j+1;4} \quad x_{j;5}+x_{j+2;2}-x_{j+2;3} \\ x_{j;5}+x_{j+3;1}-x_{j+3;2} \quad x_{j+2;6}+x_{j+3;1}-x_{j+3;3} \quad x_{j+1;3}-x_{j+1;5}-x_{j+1;6} \\ x_{j+1;4}-x_{j+1;5}-x_{j+4;1} \quad x_{j+2;3}-x_{j+2;4}-x_{j+4;1} \quad x_{j+3;2}-x_{j+3;6}-x_{j+4;1} \\ x_{j+3;3}-x_{j+3;6}-x_{j+4;2} \quad x_{j;5}+x_{j+1;3}-x_{j+1;4}-x_{j+1;6} \\ x_{j+1;4}+x_{j+2;2}-x_{j+1;5}-x_{j+2;3} \quad x_{j+1;4}+x_{j+3;1}-x_{j+1;5}-x_{j+3;2} \\ x_{j+2;3}+x_{j+3;1}-x_{j+2;4}-x_{j+3;2} \quad x_{j+2;6}+x_{j+3;2}-x_{j+3;3}-x_{j+4;1} \end{array}\right\}.$$

Proof: (i) By the form of Σ_ι, coefficients of $x_{1;1}$, $x_{1;2}$, $x_{1;3}$, $x_{1;4}$, $x_{1;5}$, $x_{1;6}$ are positive. This shows that the "positivity assumption" is satisfied.

(ii) We assume $x_{j;1} \geqslant 0$ for any $j \geqslant 1$. We show that $x_{j;2}, x_{j;3}, x_{j;4}, x_{j;5}, x_{j;6} \geqslant 0$ for any $j \geqslant 1$. By the form of Σ_ι, we have

$$x_{j;2} \geqslant x_{j+1;1}, \quad x_{j;3} \geqslant x_{j+1;2}, \quad x_{j;5} \geqslant x_{j+4;1}, \quad x_{j;6} \geqslant x_{j+1;5}, \quad x_{j;4} \geqslant x_{j+1;6}.$$

This shows $x_{j;2} \geqslant 0$ for $j \geqslant 1$ since $x_{j+1;1} \geqslant 0$ and similarly, we have $x_{j;3} \geqslant 0$, $x_{j;5} \geqslant 0$, $x_{j;6} \geqslant 0$, $x_{j;4} \geqslant 0$ for $j \geqslant 1$ since $x_{j;3} \geqslant x_{j+1;2}$, $x_{j;5} \geqslant x_{j+4;1}$, $x_{j;6} \geqslant x_{j+1;5}$, $x_{j;4} \geqslant x_{j+1;6}$, respectively.

(iii) We determine when $x_{j;i} \equiv 0$. We have

$$0 \geqslant x_{j+4;5} \geqslant 0.$$

This shows $x_{m;5} \equiv 0$ for $m \geqslant 5$. Similarly, we have $x_{m;4} \equiv 0$ for $m \geqslant 6$, $x_{m;3} \equiv 0$ for $m \geqslant 7$, $x_{m;6} \equiv 0$ for $m \geqslant 7$, $x_{m;2} \equiv 0$ for $m \geqslant 8$, $x_{m;1} \equiv 0$ for $m \geqslant 9$ since $x_{j+3;4} \geqslant x_{j+4;3}$, $x_{j+3;5} \geqslant x_{j+4;4}$, $x_{j;4} \geqslant x_{j+1;6}$, $x_{j;3} \geqslant x_{j+1;2}$, $x_{j;2} \geqslant x_{j+1;1}$, respectively. In particular, the parameter j in Ξ_ι runs over $1 \leqslant j \leqslant 8$. □

Next, we give the polyhedral realization of $B(\lambda)$ for $\lambda := \lambda_1\Lambda_1 + \ldots + \lambda_6\Lambda_6$. Here we set for $1 \leqslant i \leqslant 6$

$$\Xi_\iota^{(i)} := \{S_{j_k} \cdots S_{j_2} S_{j_1} \xi^{(i)}(\vec{x}) : k \geqslant 0, j_1, \ldots, j_k \geqslant 1\},$$

$$\Xi_\iota^{(i)}[\lambda] := \{\hat{S}_{j_k} \cdots \hat{S}_{j_2} \hat{S}_{j_1} \lambda^{(i)}(\vec{x}) : k \geqslant 0, j_1, \ldots, j_k \geqslant 1\},$$

$$\Xi_\iota[\lambda] := \Xi_\iota \cup \Xi_\iota^{(1)}[\lambda] \cup \cdots \cup \Xi_\iota^{(6)}[\lambda]$$

$$\Sigma_\iota[\lambda] := \{\vec{x} \in \mathbb{Z}_\iota[\lambda] : \varphi(\vec{x}) \geqslant 0 \text{ for any } \varphi \in \Xi_\iota[\lambda]\}.$$

In order to show that $\Sigma_\iota[\lambda]$ is the polyhedral realization of $B(\lambda)$, we give the explicit forms of $\Xi_\iota^{(i)}$ for $1 \leqslant i \leqslant 6$ by direct calculation as follows:

$$\Xi_\iota^{(1)} = \{-x_{1;1}\},$$

$$\Xi_\iota^{(2)} = \{x_{1;1} - x_{1;2}, -x_{2;1}\},$$

$$\Xi_\iota^{(3)} = \{x_{1;2} - x_{1;3}, x_{2;1} - x_{2;2}, -x_{3;1}\},$$

$$\Xi_\iota^{(4)} = \left\{ \begin{array}{cccccccc} x_{1;3}-x_{1;4} & x_{2;2}-x_{2;6} & x_{1;6}-x_{4;1} & x_{3;1}-x_{3;5} & x_{2;4}-x_{4;2} & x_{2;5}-x_{4;6} & x_{3;6}-x_{4;4} & \\ & & x_{5;2}-x_{5;3} & x_{6;1}-x_{6;2} & -x_{7;1} & & & \\ x_{1;6}+x_{2;2}-x_{2;3} & x_{1;6}+x_{3;1}-x_{3;2} & x_{2;4}+x_{3;1}-x_{3;3} & x_{2;5}+x_{3;1}-x_{3;4} & & & & \\ & & x_{2;5}+x_{3;6}-x_{4;3} & & & & & \\ x_{2;3}-x_{2;6}-x_{4;1} & x_{3;2}-x_{3;5}-x_{4;1} & x_{3;3}-x_{3;5}-x_{4;2} & x_{3;4}-x_{3;5}-x_{4;6} & & & & \\ & & x_{4;3}-x_{4;4}-x_{4;6} & & & & & \\ x_{2;3}+x_{3;1}-x_{2;6}-x_{3;2} & x_{2;4}+x_{3;2}-x_{3;3}-x_{4;1} & x_{2;5}+x_{3;2}-x_{3;4}-x_{4;1} & & & & & \\ x_{2;5}+x_{3;3}-x_{3;4}-x_{4;2} & x_{3;4}+x_{3;6}-x_{3;5}-x_{4;3} & & & & & & \end{array} \right\},$$

$$\Xi_\iota^{(5)} = \left\{ \begin{array}{cccccccc} x_{1;4}-x_{1;5} & x_{2;3}-x_{2;4} & x_{3;2}-x_{3;6} & x_{2;6}-x_{5;1} & x_{4;1}-x_{4;5} & x_{3;4}-x_{5;2} & x_{3;5}-x_{5;6} & \\ & & x_{4;6}-x_{5;4} & x_{6;2}-x_{6;3} & x_{7;1}-x_{7;2} & -x_{8;1} & & \\ x_{2;6}+x_{3;2}-x_{3;3} & x_{2;6}+x_{4;1}-x_{4;2} & x_{3;4}+x_{4;1}-x_{4;3} & x_{3;5}+x_{4;1}-x_{4;4} & & & & \\ x_{3;5}+x_{4;6}-x_{5;3} & x_{3;3}-x_{3;6}-x_{5;1} & x_{4;2}-x_{4;5}-x_{5;1} & x_{4;3}-x_{4;5}-x_{5;2} & & & & \\ & & x_{4;4}-x_{4;5}-x_{5;6} & x_{5;3}-x_{5;4}-x_{5;6} & & & & \\ x_{3;3}+x_{4;1}-x_{3;6}-x_{4;2} & x_{3;4}+x_{4;2}-x_{4;3}-x_{5;1} & x_{3;5}+x_{4;2}-x_{4;4}-x_{5;1} & & & & & \\ x_{3;5}+x_{4;3}-x_{4;4}-x_{5;2} & x_{4;4}+x_{4;6}-x_{4;5}-x_{5;3} & & & & & & \end{array} \right\},$$

$$\Xi_\iota^{(6)} = \left\{ \begin{array}{cccccccc} x_{1;3}-x_{1;6} & x_{2;2}-x_{2;5} & x_{1;4}-x_{4;1} & x_{3;3}-x_{4;3} & x_{3;1}-x_{6;1} & x_{2;6}-x_{4;6} & x_{1;5}-x_{4;5} & \\ & & x_{5;1}-x_{5;4} & x_{3;5}-x_{6;2} & x_{5;6}-x_{6;3} & -x_{6;1} & & \\ x_{1;4}+x_{2;2}-x_{2;3} & x_{1;5}+x_{2;2}-x_{2;4} & x_{1;4}+x_{3;1}-x_{3;2} & x_{1;5}+x_{3;1}-x_{3;6} & & & & \\ x_{2;6}+x_{3;1}-x_{2;4} & x_{1;5}+x_{2;6}-x_{4;2} & x_{2;1}+x_{4;2}-x_{4;3} & x_{1;5}+x_{3;4}-x_{4;3} & & & & \\ x_{3;1}+x_{5;1}-x_{5;2} & x_{2;6}+x_{3;6}-x_{4;3} & x_{1;5}+x_{3;5}-x_{4;4} & x_{3;5}+x_{5;1}-x_{5;3} & & & & \\ x_{2;3}-x_{2;5}-x_{4;1} & x_{3;2}-x_{4;1}-x_{6;1} & x_{3;3}-x_{3;6}-x_{4;6} & x_{2;4}-x_{2;5}-x_{4;5} & & & & \\ x_{3;3}-x_{4;2}-x_{6;1} & x_{3;3}-x_{3;4}-x_{4;5} & x_{4;2}-x_{4;5}-x_{4;6} & x_{3;4}-x_{4;6}-x_{6;1} & & & & \\ x_{3;6}-x_{4;5}-x_{6;1} & x_{5;2}-x_{5;4}-x_{6;1} & x_{4;4}-x_{4;5}-x_{6;2} & x_{5;3}-x_{5;4}-x_{6;2} & & & & \\ x_{2;3}+x_{3;1}-x_{2;5}-x_{3;2} & x_{1;5}+x_{2;3}-x_{2;4}-x_{4;1} & x_{2;4}+x_{3;1}-x_{2;5}-x_{3;6} & & & & & \\ x_{1;5}+x_{3;2}-x_{3;6}-x_{4;1} & x_{3;1}+x_{3;3}-x_{3;4}-x_{3;6} & x_{2;6}+x_{3;2}-x_{3;4}-x_{4;1} & & & & & \\ x_{2;4}+x_{2;5}-x_{2;6}-x_{4;2} & x_{1;5}+x_{3;3}-x_{3;6}-x_{4;2} & x_{2;6}+x_{3;3}-x_{3;4}-x_{4;2} & & & & & \\ x_{3;2}+x_{4;2}-x_{4;1}-x_{4;3} & x_{2;4}+x_{3;4}-x_{2;5}-x_{4;3} & x_{3;2}+x_{5;1}-x_{4;1}-x_{5;2} & & & & & \\ x_{2;4}+x_{3;5}-x_{2;5}-x_{4;4} & x_{3;4}+x_{4;2}-x_{4;3}-x_{4;6} & x_{3;3}+x_{4;2}-x_{5;1}-x_{5;2} & & & & & \\ x_{3;3}+x_{3;5}-x_{3;4}-x_{4;4} & x_{3;6}+x_{4;2}-x_{4;3}-x_{4;5} & x_{3;5}+x_{4;2}-x_{4;4}-x_{4;6} & & & & & \\ x_{3;4}+x_{5;1}-x_{4;6}-x_{5;2} & x_{3;4}+x_{3;6}-x_{4;3}-x_{6;1} & x_{3;6}+x_{5;1}-x_{4;5}-x_{5;2} & & & & & \\ x_{3;5}+x_{3;6}-x_{4;4}-x_{6;1} & x_{4;4}+x_{5;1}-x_{4;5}-x_{5;3} & x_{3;5}+x_{5;2}-x_{5;3}-x_{6;1} & & & & & \\ x_{1;5}+x_{2;6}+x_{3;1}-x_{3;3} & x_{3;4}+x_{3;6}+x_{4;2}-2x_{4;3} & 2x_{3;3}-x_{3;4}-x_{3;6}-x_{4;2} & & & & & \\ & & x_{4;3}-x_{4;5}-x_{4;6}-x_{6;1} & & & & & \\ x_{2.4}+x_{2;6}+x_{3;2}-x_{2;5}-x_{3;3}-x_{4;1} & x_{3;5}+x_{4;3}+x_{5;1}-x_{4;4}-x_{4;6}-x_{5;2} & & & & & & \\ x_{1;5}+x_{2;3}+x_{3;1}-x_{2;4}-x_{3;2} & x_{2;4}+x_{2;6}+x_{3;1}-x_{2;5}-x_{3;3} & & & & & & \\ x_{1;5}+x_{2;6}+x_{3;2}-x_{3;3}-x_{4;1} & x_{3;5}+x_{3;6}+x_{4;2}-x_{4;3}-x_{4;4} & & & & & & \\ x_{3;4}+x_{3;6}+x_{5;1}-x_{4;3}-x_{5;2} & x_{3;5}+x_{3;6}+x_{5;1}-x_{4;4}-x_{5;2} & & & & & & \\ x_{2;4}+x_{3;2}-x_{2;5}-x_{3;6}-x_{4;1} & x_{3;2}+x_{3;3}-x_{3;4}-x_{3;6}-x_{4;1} & & & & & & \\ x_{2;4}+x_{3;3}-x_{2;5}-x_{3;6}-x_{4;2} & x_{4;3}+x_{5;1}-x_{4;5}-x_{4;6}-x_{5;2} & & & & & & \\ x_{3;5}+x_{4;3}-x_{4;4}-x_{4;6}-x_{6;1} & x_{4;4}+x_{5;2}-x_{4;5}-x_{5;3}-x_{6;1} & & & & & & \end{array} \right\}.$$

Therefore, ι satisfies the strict positivity assumption by the explicit forms of $\Xi_\iota^{(i)}$ for $1 \leqslant i \leqslant 6$. This shows that

$$\Xi_\iota^{(1)}[\lambda] = \{\lambda_1 - x_{1,1}\},$$

$$\Xi_\iota^{(2)}[\lambda] = \{\lambda_2 + x_{1;1} - x_{1;2},\ \lambda_2 - x_{2;1}\},$$

$$\Xi_\iota^{(3)}[\lambda] = \{\lambda_3 + x_{1;2} - x_{1;3},\ \lambda_2 + x_{2;1} - x_{2;2},\ \lambda_3 - x_{3;1}\},$$

$$\Xi_\iota^{(k)}[\lambda] = \{\lambda_k + \varphi_k(\vec{x}) : \varphi_k(\vec{x}) \in \Xi_\iota^{(k)}\} \quad \text{for } k = 4,5,6$$

by Lemma 2.6 and $\Sigma_\iota[\lambda]$ is the polyhedral realization of $B(\lambda)$.

F. E_7 case

We use the different Cartan data from the one in Ref. 10, where the Cartan matrix $(a_{ij})_{1 \leqslant i,j \leqslant 7}$ is given by

$$a_{ij} := \begin{cases} 2 & \text{if } i = j \\ -1 & \text{if } |i-j| = 1 \text{ and } (i,j) \neq (6,7),(7,6), \text{ or } (i,j) = (4,7),(7,4) \\ 0 & \text{otherwise.} \end{cases}$$

We fix ι as follows:

$$\iota := (\cdots, \underline{7,6,5,4,3,2,1,} \cdots, \underline{7;6;5;4;3;2;1,} \underline{7;6;5;4;3;2;1).}$$

We define

$$\Xi_\iota := \{S_{m_l} \cdots S_{m_2} S_{m_1}(x_{j;1}) ; l \geqslant 0,\ m_1, \cdots, m_l \geqslant 1,\ 1 \leqslant j \leqslant 9\},$$

$$\Sigma_\iota := \{\vec{x} \in \mathbb{Z}_\iota^\infty : \varphi(\vec{x}) \geqslant 0 \text{ for any } \varphi \in \Xi_\iota\}.$$

Theorem 3.16: *We give the explicit form of* Ξ_ι *as follows*:

$$\left\{\begin{array}{c}
x_{j;1}\quad x_{j;2}-x_{j+1;1}\quad x_{j;3}-x_{j+1;2}\quad x_{j;4}-x_{j+1;3}\\
x_{j;5}-x_{j+1;7}\quad x_{j;7}-x_{j+1;6}\quad x_{j+2;3}-x_{j+2;5}\quad x_{j;6}-x_{j+5;1}\\
x_{j+3;2}-x_{j+3;7}\quad x_{j+2;7}-x_{j+5;2}\quad x_{j+4;1}-x_{j+4;6}\quad x_{j+3;5}-x_{j+5;3}\\
x_{j+3;6}-x_{j+5;7}\quad x_{j+4;7}-x_{j+5;5}\quad x_{j+6;3}-x_{j+6;4}\quad x_{j+7;2}-x_{j+7;3}\\
x_{j+8;1}-x_{j+8;2}\quad -x_{j+9;1}\\
x_{j;5}+x_{j;7}-x_{j+1;4}\quad x_{j;6}+x_{j;7}-x_{j+1;5}\quad x_{j;6}+x_{j+2;3}-x_{j+2;4}\\
x_{j;6}+x_{j+3;2}-x_{j+3;3}\quad x_{j;6}+x_{j+4;1}-x_{j+4;2}\quad x_{j+2;7}+x_{j+3;2}-x_{j+3;4}\\
x_{j+2;7}+x_{j+4;1}-x_{j+4;3}\quad x_{j+3;5}+x_{j+4;1}-x_{j+4;4}\quad x_{j+3;6}+x_{j+4;1}-x_{j+4;5}\\
x_{j+3;6}+x_{j+4;7}-x_{j+5;4}\quad x_{j+1;4}-x_{j+1;6}-x_{j+1;7}\quad x_{j+1;5}-x_{j+1;6}-x_{j+5;1}\\
x_{j+2;4}-x_{j+2;5}-x_{j+5;1}\quad x_{j+3;3}-x_{j+3;7}-x_{j+5;1}\quad x_{j+3;4}-x_{j+3;7}-x_{j+5;2}\\
x_{j+4;2}-x_{j+4;6}-x_{j+5;1}\quad x_{j+4;3}-x_{j+4;6}-x_{j+5;2}\quad x_{j+4;4}-x_{j+4;6}-x_{j+5;3}\\
x_{j+4;5}-x_{j+4;6}-x_{j+5;7}\quad x_{j+5;4}-x_{j+5;5}-x_{j+5;7}\\
x_{j;6}+x_{j+1;4}-x_{j+1;5}-x_{j+1;7}\quad x_{j+1;5}+x_{j+2;3}-x_{j+1;6}-x_{j+2;4}\\
x_{j+1;5}+x_{j+3;2}-x_{j+1;6}-x_{j+3;3}\quad x_{j+2;4}+x_{j+3;2}-x_{j+2;5}-x_{j+3;3}\\
x_{j+1;5}+x_{j+4;1}-x_{j+1;6}-x_{j+4;2}\quad x_{j+2;4}+x_{j+4;1}-x_{j+2;5}-x_{j+4;2}\\
x_{j+3;3}+x_{j+4;1}-x_{j+3;7}-x_{j+4;2}\quad x_{j+2;7}+x_{j+3;3}-x_{j+3;4}-x_{j+5;1}\\
x_{j+3;4}+x_{j+4;1}-x_{j+3;7}-x_{j+4;3}\quad x_{j+2;7}+x_{j+4;2}-x_{j+4;3}-x_{j+5;1}\\
x_{j+3;5}+x_{j+4;2}-x_{j+4;4}-x_{j+5;1}\quad x_{j+3;6}+x_{j+4;2}-x_{j+4;5}-x_{j+5;1}\\
x_{j+3;5}+x_{j+4;3}-x_{j+4;4}-x_{j+5;2}\quad x_{j+3;6}+x_{j+4;3}-x_{j+4;5}-x_{j+5;2}\\
x_{j+3;6}+x_{j+4;4}-x_{j+4;5}-x_{j+5;3}\quad x_{j+4;5}+x_{j+4;7}-x_{j+4;6}-x_{j+5;4}\\
x_{j+2;7}+x_{j+3;3}+x_{j+4;1}-x_{j+3;4}-x_{j+4;2}\quad x_{j+3;4}+x_{j+4;2}-x_{j+3;7}-x_{j+4;3}-x_{j+5;1}
\end{array}\right\}.$$

Proof: (*i*) By the form of Σ_ι, coefficients of $x_{1;1}$, $x_{1;2}$, $x_{1;3}$, $x_{1;4}$, $x_{1;5}$, $x_{1;6}$, $x_{1;7}$ are positive. This shows that the "positivity assumption" is satisfied.

(*ii*) We assume $x_{j;1}\geqslant 0$ for any $j\geqslant 1$. We show that $x_{j;2}$, $x_{j;3}$, $x_{j;4}$, $x_{j;5}$, $x_{j;6}$, $x_{1;7}\geqslant 0$ for any $j\geqslant 1$. By the form of Σ_ι, we have

$$x_{j;2}\geqslant x_{j+1;1},\quad x_{j;3}\geqslant x_{j+1;2},\quad x_{j;4}\geqslant x_{j+1;3},\quad x_{j;6}\geqslant x_{j+5;1},\quad x_{j;7}\geqslant x_{j+1;6},\quad x_{j;5}\geqslant x_{j+1;7}.$$

This shows $x_{j;2}\geqslant 0$ for $j\geqslant 1$ since $x_{j+1;1}\geqslant 0$ and similarly, we have $x_{j;3}\geqslant 0$, $x_{j;4}\geqslant 0$, $x_{j;6}\geqslant 0$, $x_{j;7}\geqslant 0$, $x_{j;5}\geqslant 0$ for $j\geqslant 1$ since $x_{j;3}\geqslant x_{j+1;2}$, $x_{j;4}\geqslant x_{j+1;3}$, $x_{j;6}\geqslant x_{j+5;1}$, $x_{j;7}\geqslant x_{j+1;6}$, $x_{j;5}\geqslant x_{j+1;7}$, respectively.

(*iii*) We determine when $x_{j;i}\equiv 0$. We have

$$0\geqslant x_{j+9;1}\geqslant 0.$$

This shows $x_{m;1}\equiv 0$ for $m\geqslant 10$. Similarly, we have $x_{m;2}\equiv 0$, $x_{m;3}\equiv 0$, $x_{m;4}\equiv 0$, $x_{m;5}\equiv 0$, $x_{m;6}\equiv 0$, $x_{m;7}\equiv 0$ for $m\geqslant 10$ since $x_{j+8;1}\geqslant x_{j+8;2}$, $x_{j+7;2}\geqslant x_{j+7;3}$, $x_{j+6;3}\geqslant x_{j+6;4}$, $x_{j+2;3}\geqslant x_{j+2;5}$, $x_{j+4;1}\geqslant x_{j+4;6}$, $x_{j+3;2}\geqslant x_{j+3;7}$, respectively. In particular, the parameter j in Ξ_ι runs over $1\leqslant j\leqslant 9$. □

G. E_8 case

We fix ι as follows:

$$\iota := (\ldots,\underline{8,7,6,5,4,3,2,1},\ldots,\underline{8,7,6,5,4,3,2,1},\underline{8,7,6,5,4,3,2,1}).$$

We define

$$\Xi_\iota := \{S_{m_l}\cdots S_{m_2}S_{m_1}(x_{j;1}) : l\geqslant 0, m_1,\ldots,m_l\geqslant 1, 1\leqslant j\leqslant 15\},$$

$$\Sigma_\iota := \{\vec{x} \in \mathbb{Z}_\iota^\infty : \varphi(\vec{x}) \geqslant 0 \text{ for any } \varphi \in \Xi_\iota\}.$$

Theorem 3.17: *We give the explicit form of* Ξ_ι *as follows:*

$$x_{j;1} \quad x_{j;2} - x_{j+1;1} \quad x_{j;3} - x_{j+1;2} \quad x_{j;4} - x_{j+1;3} \quad x_{j;5} - x_{j+1;4}$$

$$x_{j;6} - x_{j+1;8} \quad x_{j;7} - x_{j+6;1} \quad x_{j;8} - x_{j+1;7} \quad x_{j+2;4} - x_{j+2;6} \quad x_{j+2;8} - x_{j+6;2}$$

$$x_{j+3;3} - x_{j+3;8} \quad x_{j+3;6} - x_{j+6;3} \quad x_{j+3;7} - x_{j+6;7} \quad x_{j+4;2} - x_{j+4;7} \quad x_{j+4;8} - x_{j+6;8}$$

$$x_{j+5;1} - x_{j+10;1} \quad x_{j+5;5} - x_{j+6;5} \quad x_{j+5;7} - x_{j+10;2} \quad x_{j+7;3} - x_{j+7;6} \quad x_{j+7;8} - x_{j+10;3}$$

$$x_{j+8;2} - x_{j+8;8} \quad x_{j+8;6} - x_{j+10;4} \quad x_{j+8;7} - x_{j+10;8} \quad x_{j+9;1} - x_{j+9;7} \quad x_{j+9;8} - x_{j+10;6}$$

$$x_{j+11;4} - x_{j+11;5} \quad x_{j+12;3} - x_{j+12;4} \quad x_{j+13;2} - x_{j+13;3} \quad x_{j+14;1} - x_{j+14;2} \quad - x_{j+15;1}$$

$$2x_{j+5;5} - x_{j+5;6} - x_{j+5;8} - x_{j+6;4} \quad x_{j+6;5} - x_{j+6;7} - x_{j+6;8} - x_{j+10;1}$$

$$x_{j+3;7} + x_{j+4;8} + x_{j+5;1} - x_{j+5;5} \quad x_{j+5;6} + x_{j+5;8} + x_{j+6;4} - 2x_{j+6;5}$$

$$x_{j;6} + x_{j;8} - x_{j+1;5} \quad x_{j;7} + x_{j;8} - x_{j+1;6} \quad x_{j;7} + x_{j+2;4} - x_{j+2;5}$$

$$x_{j;7} + x_{j+3;3} - x_{j+3;4} \quad x_{j;7} + x_{j+4;2} - x_{j+4;3} \quad x_{j;7} + x_{j+5;1} - x_{j+5;2}$$

$$x_{j+2;8} + x_{j+3;3} - x_{j+3;5} \quad x_{j+2;8} + x_{j+4;2} - x_{j+4;4} \quad x_{j+2;8} + x_{j+5;1} - x_{j+5;3}$$

$$x_{j+3;6} + x_{j+4;2} - x_{j+4;5} \quad x_{j+3;6} + x_{j+5;1} - x_{j+5;4} \quad x_{j+3;7} + x_{j+4;2} - x_{j+4;6}$$

$$x_{j+3;7} + x_{j+4;8} - x_{j+6;4} \quad x_{j+3;7} + x_{j+5;1} - x_{j+5;8} \quad x_{j+3;7} + x_{j+5;6} - x_{j+6;5}$$

$$x_{j+3;7} + x_{j+5;7} - x_{j+6;6} \quad x_{j+4;8} + x_{j+5;1} - x_{j+5;6} \quad x_{j+4;8} + x_{j+5;8} - x_{j+6;5}$$

$$x_{j+5;1} + x_{j+6;4} - x_{j+6;5} \quad x_{j+5;1} + x_{j+7;3} - x_{j+7;4} \quad x_{j+5;1} + x_{j+8;2} - x_{j+8;3}$$

$$x_{j+5;1} + x_{j+9;1} - x_{j+9;2} \quad x_{j+5;7} + x_{j+7;3} - x_{j+7;5} \quad x_{j+5;7} + x_{j+8;2} - x_{j+8;4}$$

$$x_{j+5;7} + x_{j+9;1} - x_{j+9;3} \quad x_{j+7;8} + x_{j+8;2} - x_{j+8;5} \quad x_{j+7;8} + x_{j+9;1} - x_{j+9;4}$$

$$x_{j+8;6} + x_{j+9;1} - x_{j+9;5} \quad x_{j+8;7} + x_{j+9;1} - x_{j+9;6} \quad x_{j+8;7} + x_{j+9;8} - x_{j+10;5}$$

$$x_{j+1;5} - x_{j+1;7} - x_{j+1;8} \quad x_{j+1;6} - x_{j+1;7} - x_{j+6;1} \quad x_{j+2;5} - x_{j+2;6} - x_{j+6;1}$$

$$x_{j+3;4} - x_{j+3;8} - x_{j+6;1} \quad x_{j+3;5} - x_{j+3;8} - x_{j+6;2} \quad x_{j+4;3} - x_{j+4;7} - x_{j+6;1}$$

$$x_{j+4;4} - x_{j+4;7} - x_{j+6;2} \quad x_{j+4;5} - x_{j+4;7} - x_{j+6;3} \quad x_{j+4;6} - x_{j+4;7} - x_{j+6;7}$$

$$x_{j+5;2} - x_{j+6;1} - x_{j+10;1} \quad x_{j+5;3} - x_{j+6;2} - x_{j+10;1} \quad x_{j+5;4} - x_{j+6;3} - x_{j+10;1}$$

$$x_{j+5;5}-x_{j+5;6}-x_{j+6;7}\quad x_{j+5;5}-x_{j+6;4}-x_{j+10;1}\quad x_{j+5;5}-x_{j+5;8}-x_{j+6;8}$$

$$x_{j+5;6}-x_{j+6;8}-x_{j+10;1}\quad x_{j+5;8}-x_{j+6;7}-x_{j+10;1}\quad x_{j+6;4}-x_{j+6;7}-x_{j+6;8}$$

$$x_{j+6;6}-x_{j+6;7}-x_{j+10;2}\quad x_{j+7;4}-x_{j+7;6}-x_{j+10;1}\quad x_{j+7;5}-x_{j+7;6}-x_{j+10;2}$$

$$x_{j+8;3}-x_{j+8;8}-x_{j+10;1}\quad x_{j+8;4}-x_{j+8;8}-x_{j+10;2}\quad x_{j+8;5}-x_{j+8;8}-x_{j+10;3}$$

$$x_{j+9;2}-x_{j+9;7}-x_{j+10;1}\quad x_{j+9;3}-x_{j+9;7}-x_{j+10;2}\quad x_{j+9;4}-x_{j+9;7}-x_{j+10;3}$$

$$x_{j+9;5}-x_{j+9;7}-x_{j+10;4}\quad x_{j+9;6}-x_{j+9;7}-x_{j+10;8}\quad x_{j+10;5}-x_{j+10;6}-x_{j+10;8}$$

$$x_{j+3;5}+x_{j+4;3}+x_{j+5;1}-x_{j+3;8}-x_{j+4;4}-x_{j+5;2}\quad x_{j+3;6}+x_{j+4;4}+x_{j+5;2}-x_{j+4;5}-x_{j+5;3}-x_{j+6;1}$$

$$x_{j+3;7}+x_{j+4;4}+x_{j+5;2}-x_{j+4;6}-x_{j+5;3}-x_{j+6;1}\quad x_{j+3;7}+x_{j+4;5}+x_{j+5;2}-x_{j+4;6}-x_{j+5;4}-x_{j+6;1}$$

$$x_{j+3;7}+x_{j+4;5}+x_{j+5;3}-x_{j+4;6}-x_{j+5;4}-x_{j+6;2}\quad x_{j+4;6}+x_{j+4;8}+x_{j+5;2}-x_{j+4;7}-x_{j+5;5}-x_{j+6;1}$$

$$x_{j+4;6}+x_{j+4;8}+x_{j+5;3}-x_{j+4;7}-x_{j+5;5}-x_{j+6;2}\quad x_{j+4;6}+x_{j+4;8}+x_{j+5;4}-x_{j+4;7}-x_{j+5;5}-x_{j+6;3}$$

$$x_{j+5;7}+x_{j+6;5}+x_{j+7;3}-x_{j+6;6}-x_{j+6;8}-x_{j+7;4}\quad x_{j+5;7}+x_{j+6;5}+x_{j+8;2}-x_{j+6;6}-x_{j+6;8}-x_{j+8;3}$$

$$x_{j+5;7}+x_{j+6;5}+x_{j+9;1}-x_{j+6;6}-x_{j+6;8}-x_{j+9;2}\quad x_{j+6;6}+x_{j+7;4}+x_{j+8;2}-x_{j+6;7}-x_{j+7;5}-x_{j+8;3}$$

$$x_{j+6;6}+x_{j+7;4}+x_{j+9;1}-x_{j+6;7}-x_{j+7;5}-x_{j+9;2}\quad x_{j+6;6}+x_{j+8;3}+x_{j+9;1}-x_{j+6;7}-x_{j+8;4}-x_{j+9;2}$$

$$x_{j+7;5}+x_{j+8;3}+x_{j+9;1}-x_{j+7;6}-x_{j+8;4}-x_{j+9;2}\quad x_{j+7;8}+x_{j+8;4}+x_{j+9;2}-x_{j+8;5}-x_{j+9;3}-x_{j+10;1}$$

$$x_{j+7}+x_{j+1;5}-x_{j+1;6}-x_{j+1;8}\quad x_{j+1;6}+x_{j+2;4}-x_{j+1;7}-x_{j+2;5}\quad x_{j+1;6}+x_{j+3;3}-x_{j+1;7}-x_{j+3;4}$$

$$x_{j+1;6}+x_{j+4;2}-x_{j+1;7}-x_{j+4;3}\quad x_{j+1;6}+x_{j+5;1}-x_{j+1;7}-x_{j+5;2}\quad x_{j+2;5}+x_{j+2;6}-x_{j+3;3}-x_{j+3;4}$$

$$x_{j+2;5}+x_{j+4;2}-x_{j+2;6}-x_{j+4;3}\quad x_{j+2;5}+x_{j+5;1}-x_{j+2;6}-x_{j+5;2}\quad x_{j+2;8}+x_{j+3;4}-x_{j+3;5}-x_{j+6;1}$$

$$x_{j+2;8}+x_{j+4;3}-x_{j+4;4}-x_{j+6;1}\quad x_{j+2;8}+x_{j+5;2}-x_{j+5;3}-x_{j+6;1}\quad x_{j+3;4}+x_{j+4;2}-x_{j+3;8}-x_{j+4;3}$$

$$x_{j+3;4}+x_{j+5;1}-x_{j+3;8}-x_{j+5;2}\quad x_{j+3;5}+x_{j+4;2}-x_{j+3;8}-x_{j+4;4}\quad x_{j+3;5}+x_{j+5;1}-x_{j+3;8}-x_{j+5;3}$$

$$x_{j+3;6}+x_{j+4;3}-x_{j+4;5}-x_{j+6;1}\quad x_{j+3;6}+x_{j+4;4}-x_{j+4;5}-x_{j+6;2}\quad x_{j+3;6}+x_{j+5;2}-x_{j+5;4}-x_{j+6;1}$$

$$x_{j+3;6}+x_{j+5;3}-x_{j+5;4}-x_{j+6;2}\quad x_{j+3;7}+x_{j+4;3}-x_{j+4;6}-x_{j+6;1}\quad x_{j+3;7}+x_{j+4;4}-x_{j+4;6}-x_{j+6;2}$$

$$x_{j+3;7}+x_{j+4;5}-x_{j+4;6}-x_{j+6;3}\quad x_{j+3;7}+x_{j+5;2}-x_{j+5;8}-x_{j+6;1}\quad x_{j+3;7}+x_{j+5;3}-x_{j+5;8}-x_{j+6;2}$$

$$x_{j+3;7}+x_{j+5;4}-x_{j+5;8}-x_{j+6;3}\quad x_{j+3;7}+x_{j+5;5}-x_{j+5;8}-x_{j+6;4}\quad x_{j+4;3}+x_{j+5;1}-x_{j+4;7}-x_{j+5;2}$$

$$x_{j+4;4}+x_{j+5;1}-x_{j+4;7}-x_{j+5;3} \quad x_{j+4;5}+x_{j+5;1}-x_{j+4;7}-x_{j+5;4} \quad x_{j+4;6}+x_{j+4;8}-x_{j+4;7}-x_{j+6;4}$$

$$x_{j+4;6}+x_{j+5;1}-x_{j+4;7}-x_{j+5;8} \quad x_{j+4;6}+x_{j+5;6}-x_{j+4;7}-x_{j+6;5} \quad x_{j+4;6}+x_{j+5;7}-x_{j+4;7}-x_{j+6;6}$$

$$x_{j+4;8}+x_{j+5;2}-x_{j+5;6}-x_{j+6;1} \quad x_{j+4;8}+x_{j+5;3}-x_{j+5;6}-x_{j+6;2} \quad x_{j+4;8}+x_{j+5;4}-x_{j+5;6}-x_{j+6;3}$$

$$x_{j+4;8}+x_{j+5;5}-x_{j+5;6}-x_{j+6;4} \quad x_{j+5;1}+x_{j+5;5}-x_{j+5;6}-x_{j+5;8} \quad x_{j+5;2}+x_{j+6;4}-x_{j+6;1}-x_{j+6;5}$$

$$x_{j+5;2}+x_{j+7;3}-x_{j+6;1}-x_{j+7;4} \quad x_{j+5;2}+x_{j+8;2}-x_{j+6;1}-x_{j+8;3} \quad x_{j+5;2}+x_{j+9;1}-x_{j+6;1}-x_{j+9;2}$$

$$x_{j+5;3}+x_{j+6;4}-x_{j+6;2}-x_{j+6;5} \quad x_{j+5;3}+x_{j+7;3}-x_{j+6;2}-x_{j+7;4} \quad x_{j+5;3}+x_{j+8;2}-x_{j+6;2}-x_{j+8;3}$$

$$x_{j+5;3}+x_{j+9;1}-x_{j+6;2}-x_{j+9;2} \quad x_{j+5;4}+x_{j+6;4}-x_{j+6;3}-x_{j+6;5} \quad x_{j+5;4}+x_{j+7;3}-x_{j+6;3}-x_{j+7;4}$$

$$x_{j+5;4}+x_{j+8;2}-x_{j+6;3}-x_{j+8;3} \quad x_{j+5;4}+x_{j+9;1}-x_{j+6;3}-x_{j+9;2} \quad x_{j+5;5}+x_{j+5;7}-x_{j+5;6}-x_{j+6;6}$$

$$x_{j+5;5}+x_{j+7;3}-x_{j+6;4}-x_{j+7;4} \quad x_{j+5;5}+x_{j+8;2}-x_{j+6;4}-x_{j+8;3} \quad x_{j+5;5}+x_{j+9;1}-x_{j+6;4}-x_{j+9;2}$$

$$x_{j+5;6}+x_{j+5;8}-x_{j+6;5}-x_{j+10;1} \quad x_{j+5;6}+x_{j+6;4}-x_{j+6;5}-x_{j+6;8} \quad x_{j+5;6}+x_{j+7;3}-x_{j+6;8}-x_{j+7;4}$$

$$x_{j+5;6}+x_{j+8;2}-x_{j+6;8}-x_{j+8;3} \quad x_{j+5;6}+x_{j+9;1}-x_{j+6;8}-x_{j+9;2} \quad x_{j+5;7}+x_{j+5;8}-x_{j+6;6}-x_{j+10;1}$$

$$x_{j+5;7}+x_{j+6;4}-x_{j+6;6}-x_{j+6;8} \quad x_{j+5;7}+x_{j+7;4}-x_{j+7;5}-x_{j+10;1} \quad x_{j+5;7}+x_{j+8;3}-x_{j+8;4}-x_{j+10;1}$$

$$x_{j+5;7}+x_{j+9;2}-x_{j+9;3}-x_{j+10;1} \quad x_{j+5;8}+x_{j+6;4}-x_{j+6;5}-x_{j+6;7} \quad x_{j+5;8}+x_{j+7;3}-x_{j+6;7}-x_{j+7;4}$$

$$x_{j+5;8}+x_{j+8;2}-x_{j+6;7}-x_{j+8;3} \quad x_{j+5;8}+x_{j+9;1}-x_{j+6;7}-x_{j+9;2} \quad x_{j+6;6}+x_{j+7;3}-x_{j+6;7}-x_{j+7;5}$$

$$x_{j+6;6}+x_{j+8;2}-x_{j+6;7}-x_{j+8;4} \quad x_{j+6;6}+x_{j+9;1}-x_{j+6;7}-x_{j+9;3} \quad x_{j+7;4}+x_{j+8;2}-x_{j+7;6}-x_{j+8;3}$$

$$x_{j+7;4}+x_{j+9;1}-x_{j+7;6}-x_{j+9;2} \quad x_{j+7;5}+x_{j+8;2}-x_{j+7;6}-x_{j+8;4} \quad x_{j+7;5}+x_{j+9;1}-x_{j+7;6}-x_{j+9;3}$$

$$x_{j+7;8}+x_{j+8;3}-x_{j+8;5}-x_{j+10;1} \quad x_{j+7;8}+x_{j+8;4}-x_{j+8;5}-x_{j+10;2} \quad x_{j+7;8}+x_{j+9;2}-x_{j+9;4}-x_{j+10;1}$$

$$x_{j+7;8}+x_{j+9;3}-x_{j+9;4}-x_{j+10;2} \quad x_{j+8;3}+x_{j+9;1}-x_{j+8;8}-x_{j+9;2} \quad x_{j+8;4}+x_{j+9;1}-x_{j+8;8}-x_{j+9;3}$$

$$x_{j+8;5}+x_{j+9;1}-x_{j+8;8}-x_{j+9;4} \quad x_{j+8;6}+x_{j+9;2}-x_{j+9;5}-x_{j+10;1} \quad x_{j+8;6}+x_{j+9;3}-x_{j+9;5}-x_{j+10;2}$$

$$x_{j+8;6}+x_{j+9;4}-x_{j+9;5}-x_{j+10;3} \quad x_{j+8;7}+x_{j+9;2}-x_{j+9;6}-x_{j+10;1} \quad x_{j+8;7}+x_{j+9;3}-x_{j+9;6}-x_{j+10;2}$$

$$x_{j+8;7}+x_{j+9;4}-x_{j+9;6}-x_{j+10;3} \quad x_{j+8;7}+x_{j+9;5}-x_{j+9;6}-x_{j+10;4} \quad x_{j+9;6}+x_{j+9;8}-x_{j+9;7}-x_{j+10;5}$$

$$x_{j+2;8}+x_{j+3;4}+x_{j+4;2}-x_{j+3;5}-x_{j+4;3} \quad x_{j+2;8}+x_{j+3;4}+x_{j+5;1}-x_{j+3;5}-x_{j+5;2}$$

$$x_{j+2;8}+x_{j+4;3}+x_{j+5;1}-x_{j+4;4}-x_{j+5;2} \quad x_{j+3;6}+x_{j+4;3}+x_{j+5;1}-x_{j+4;5}-x_{j+5;2}$$

$$x_{j+3;6}+x_{j+4;4}+x_{j+5;1}-x_{j+4;5}-x_{j+5;3} \quad x_{j+3;7}+x_{j+4;3}+x_{j+5;1}-x_{j+4;6}-x_{j+5;2}$$

$$x_{j+3;7}+x_{j+4;4}+x_{j+5;1}-x_{j+4;6}-x_{j+5;3} \quad x_{j+3;7}+x_{j+4;5}+x_{j+5;1}-x_{j+4;6}-x_{j+5;4}$$

$$x_{j+3;7}+x_{j+4;8}+x_{j+5;2}-x_{j+5;5}-x_{j+6;1} \quad x_{j+3;7}+x_{j+4;8}+x_{j+5;3}-x_{j+5;5}-x_{j+6;2}$$

$$x_{j+3;7}+x_{j+4;8}+x_{j+5;4}-x_{j+5;5}-x_{j+6;3} \quad x_{j+4;6}+x_{j+4;8}+x_{j+5;1}-x_{j+4;7}-x_{j+5;5}$$

$$x_{j+5;6}+x_{j+5;8}+x_{j+7;3}-x_{j+6;5}-x_{j+7;4} \quad x_{j+5;6}+x_{j+5;8}+x_{j+8;2}-x_{j+6;5}-x_{j+8;3}$$

$$x_{j+5;6}+x_{j+5;8}+x_{j+9;1}-x_{j+6;5}-x_{j+9;2} \quad x_{j+5;7}+x_{j+5;8}+x_{j+6;4}-x_{j+6;5}-x_{j+6;6}$$

$$x_{j+5;7}+x_{j+5;8}+x_{j+7;3}-x_{j+6;6}-x_{j+7;4} \quad x_{j+5;7}+x_{j+5;8}+x_{j+8;2}-x_{j+6;6}-x_{j+8;3}$$

$$x_{j+5;7}+x_{j+5;8}+x_{j+9;1}-x_{j+6;6}-x_{j+9;2} \quad x_{j+5;7}+x_{j+7;4}+x_{j+8;2}-x_{j+7;5}-x_{j+8;3}$$

$$x_{j+5;7}+x_{j+7;4}+x_{j+9;1}-x_{j+7;5}-x_{j+9;2} \quad x_{j+5;7}+x_{j+8;3}+x_{j+9;1}-x_{j+8;4}-x_{j+9;2}$$

$$x_{j+7;8}+x_{j+8;3}+x_{j+9;1}-x_{j+8;5}-x_{j+9;2} \quad x_{j+7;8}+x_{j+8;4}+x_{j+9;1}-x_{j+8;5}-x_{j+9;3}$$

$$x_{j+3;5}+x_{j+4;3}-x_{j+3;8}-x_{j+4;4}-x_{j+6;1} \quad x_{j+3;5}+x_{j+5;2}-x_{j+3;8}-x_{j+5;3}-x_{j+6;1}$$

$$x_{j+4;4}+x_{j+5;2}-x_{j+4;7}-x_{j+5;3}-x_{j+6;1} \quad x_{j+4;5}+x_{j+5;2}-x_{j+4;7}-x_{j+5;4}-x_{j+6;1}$$

$$x_{j+4;5}+x_{j+5;3}-x_{j+4;7}-x_{j+5;4}-x_{j+6;2} \quad x_{j+4;6}+x_{j+5;2}-x_{j+4;7}-x_{j+5;8}-x_{j+6;1}$$

$$x_{j+4;6}+x_{j+5;3}-x_{j+4;7}-x_{j+5;8}-x_{j+6;2} \quad x_{j+4;6}+x_{j+5;4}-x_{j+4;7}-x_{j+5;8}-x_{j+6;3}$$

$$x_{j+4;6}+x_{j+5;5}-x_{j+4;7}-x_{j+5;8}-x_{j+6;4} \quad x_{j+5;2}+x_{j+5;5}-x_{j+5;6}-x_{j+5;8}-x_{j+6;1}$$

$$x_{j+5;3}+x_{j+5;5}-x_{j+5;6}-x_{j+5;8}-x_{j+6;2} \quad x_{j+5;4}+x_{j+5;5}-x_{j+5;6}-x_{j+5;8}-x_{j+6;3}$$

$$x_{j+5;7}+x_{j+6;5}-x_{j+6;6}-x_{j+6;8}-x_{j+10;1} \quad x_{j+6;5}+x_{j+7;3}-x_{j+6;7}-x_{j+6;8}-x_{j+7;4}$$

$$x_{j+6;5}+x_{j+8;2}-x_{j+6;7}-x_{j+6;8}-x_{j+8;3} \quad x_{j+6;5}+x_{j+9;1}-x_{j+6;7}-x_{j+6;8}-x_{j+9;2}$$

$$x_{j+6;6}+x_{j+7;4}-x_{j+6;7}-x_{j+7;5}-x_{j+10;1} \quad x_{j+6;6}+x_{j+8;3}-x_{j+6;7}-x_{j+8;4}-x_{j+10;1}$$

$$x_{j+6;6}+x_{j+9;2}-x_{j+6;7}-x_{j+9;3}-x_{j+10;1} \quad x_{j+7;5}+x_{j+8;3}-x_{j+7;6}-x_{j+8;4}-x_{j+10;1}$$

$$x_{j+7;5}+x_{j+9;2}-x_{j+7;6}-x_{j+9;3}-x_{j+10;1} \quad x_{j+8;4}+x_{j+9;2}-x_{j+8;8}-x_{j+9;3}-x_{j+10;1}$$

$$x_{j+8;5}+x_{j+9;2}-x_{j+8;8}-x_{j+9;4}-x_{j+10;1} \quad x_{j+8;5}+x_{j+9;3}-x_{j+8;8}-x_{j+9;4}-x_{j+10;2}$$

Proof: (*i*) By the form of Σ_ι, coefficients of $x_{1;1}$, $x_{1;2}$, $x_{1;3}$, $x_{1;4}$, $x_{1;5}$, $x_{1;6}$, $x_{1;7}$, $x_{1;8}$ are positive. This shows that the "positivity assumption" is satisfied.

(*ii*) We assume $x_{j;1} \geqslant 0$ for any $j \geqslant 1$. We show that $x_{j;2}, x_{j;3}, x_{j;4}, x_{j;5}, x_{j;6}, x_{1;7}, x_{1;8} \geqslant 0$ for any $j \geqslant 1$. By the form of Σ_ι, we have

$$x_{j,2} \geqslant x_{j+1;1}, \quad x_{j,3} \geqslant x_{j+1;2}, \quad x_{j;4} \geqslant x_{j+1;3}, \quad x_{j;5} \geqslant x_{j+1;4},$$

$$x_{j;7} \geqslant x_{j+6;1}, \quad x_{j;8} \geqslant x_{j+1;7}, \quad x_{j;6} \geqslant x_{j+1;8}.$$

This shows $x_{j;2} \geqslant 0$ for $j \geqslant 1$ since $x_{j+1;1} \geqslant 0$ and similarly, we have $x_{j;3} \geqslant 0$, $x_{j;4} \geqslant 0$, $x_{j;5} \geqslant 0$, $x_{j;7} \geqslant 0$, $x_{j;8} \geqslant 0$, $x_{j;6} \geqslant 0$ for $j \geqslant 1$ since $x_{j;3} \geqslant x_{j+1;2}$, $x_{j;4} \geqslant x_{j+1;3}$, $x_{j;5} \geqslant x_{j+1;4}$, $x_{j;7} \geqslant x_{j+1;6}$, $x_{j;8} \geqslant x_{j+1;7}$, $x_{j;6} \geqslant x_{j+1;8}$, respectively.

(iii) We determine when $x_{j;i} \equiv 0$. We have

$$0 \geqslant x_{j+15;1} \geqslant 0.$$

This shows $x_{m;1} \equiv 0$ for $m \geqslant 16$. Similarly, we have $x_{m;2} \equiv 0$, $x_{m;3} \equiv 0$, $x_{m;4} \equiv 0$, $x_{m;5} \equiv 0$, $x_{m;6} \equiv 0$, $x_{m;7} \equiv 0$, $x_{m;8} \equiv 0$ for $m \geqslant 16$ since $x_{j+14;1} \geqslant x_{j+14;2}$, $x_{j+13;2} \geqslant x_{j+13;3}$, $x_{j+12;3} \geqslant x_{j+12;4}$, $x_{j+11;4} \geqslant x_{j+11;5}$, $x_{j+7;3} \geqslant x_{j+7;6}$, $x_{j+9;1} \geqslant x_{j+9;7}$, $x_{j+8;2} \geqslant x_{j+8;8}$, respectively. In particular, the parameter j in Ξ_ι runs over $1 \leqslant j \leqslant 15$. □

Remark 3.18: For all simple Lie algebras, the number of $x_{j;i}$'s such that $x_{j;i} \neq 0$ is equal to the length of the longest element of Weyl group.

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Comment on "Central potentials on spaces of constant curvature: The Kepler problem on the two-dimensional sphere S^2 and the hyperbolic plane H^2" [J. Math. Phys. 46, 052702 (2005)]

A. V. Shchepetilov[a)]
Department of Physics, Moscow State University, 119992 Moscow, Russia

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Cariñena, Rañada, and Santander consider a classical Kepler problem in constant curvature spaces and related theory of conics in these spaces. Here we point out that earlier results exist in the literature. Some of these results date back to the nineteenth and the beginning of the twentieth century. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2107267]

In Ref. 1, Cariñena, Rañada, and Santander deal with a classical Kepler problem on constant curvature spaces. In the Introduction they cite Refs. 2–9 concerning quantum-mechanical version of this problem and related topics. After that they note: "since then, a certain number of authors have studied this question from both the classical (Kepler problem) and the quantum (hydrogen atom) point of view" (here they cite 16 papers from 1985 to 2003). It should be pointed out however that the classical Kepler problem on constant curvature spaces is naturally much older than its quantum analog.

Indeed, the analog of Newton force for the hyperbolic space $\mathbf{H}^3$ was proposed already by Lobachevski (in 1835–1838)[10] as the value $F(\rho)$ which is inverse to the area of the sphere of radius ρ in the space $\mathbf{H}^3$ with an attractive body in the center. An analytical expression for the Newtonian potential in $\mathbf{H}^3$ was written in 1870 by Schering[11] (see also his paper[12] of 1873).

In 1873 Lipschitz considered a one-body motion in a central potential on the sphere $\mathbf{S}^2$.[13] Although he knew the central potential, satisfying the Laplace equation in the space $\mathbf{S}^3$, he preferred to consider another central potential $V(\rho) \sim \sin^{-1}(\rho/R)$, where R is the curvature radius. He found a general solution to this problem in terms of elliptic functions.

In 1885 Killing found a generalization of all three Kepler laws to the case of a sphere $\mathbf{S}^3$.[14] He considered an attractive force as an inverse area of a two-dimensional sphere in $\mathbf{S}^3$, as Lobachevski did before. In 1886, similar results were published by Neumann.[15]

The extension of these results to the hyperbolic case was carried out by Liebman in Ref. 16 in 1902, and later in 1905 in his book on non-Euclidean geometry.[17] Note that he started from ellipses in $\mathbf{S}^3$ or $\mathbf{H}^3$, and derived a potential in such a way that the first Kepler law would be valid. He also derived the generalization of the oscillator potential for these spaces from the requirement that a particle motion occur along the ellipse with its center coinciding with the center of the potential.

The well-known Bertrand theorem[18] states that there are only two central potentials in Euclidean space that make all bounded trajectories of a one-particle problem closed. Its generalization for spaces $\mathbf{S}^2$ and $\mathbf{H}^2$ was proved by Liebman in 1903.[19]

One may regard classical mechanics in spaces of constant curvature as a predecessor of special and general relativity. After the rise of these theories the above-mentioned papers of Schering, Killing, and Liebmann were almost completely forgotten. Note that the description of a particle motion in central potentials in spaces $\mathbf{S}^3$ and $\mathbf{H}^3$ was shortened in the second and third

[a)]Electronic mail: quant@phys.msu.su

editions of the Liebman book[17] with respect to the first one in favor of special relativity. Similar models attracted attention later from the point of view of quantum mechanics and theory of integrable systems.

Equation (4) from Ref. 1, which is used there for an analysis of trajectories, is not a new one. Its equivalent form for different types of trajectories is presented in Ref. 16 (hyperbolic case) and later in Ref. 20 (spherical case).

Two ideas appearing in Ref. 1—the description of the spherical, hyperbolic and Euclidean cases in a uniform way with the sectional curvature κ as a parameter, and the conic nature of trajectories for the Kepler problem in constant curvature spaces—can be found in earlier literature. The first one is presented in Ref. 21, where one can also find a history of the problem prior to Schrödinger's paper.[2] The second idea was explored in Liebmann's paper,[16] and is also presented in Ref. 21.

Section V of Ref. 1 describes a theory of conics in constant curvature two-dimensional spaces, but the authors do not provide references. Note that this theory was developed as early as 1883.[22] A lot of relevant information on this theory can be found also in Refs. 16, 17, 21, and 23.

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Response to "Comment on 'Central potentials on spaces of constant curvature: The Kepler problem on the two-dimensional sphere S^2 and the hyperbolic plane H^2' " [J. Math. Phys. 46, 052702 (2005)]

J. F. Cariñena and M. F. Ranada
Departamento de Física Teórica, Universidad de Zaragoza, 50009 Zaragoza, Spain

M. Santander
Departamento de Física Teórica, Universidad de Valladolid, 47011 Valladolid, Spain

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published online 10 November 2005)

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Shchepetilov starts pointing out that many references in Ref. 3 are related to Quantum Mechanics. Nevertheless this is a characteristic, not only of Ref. 3, but of many of the research papers written along the second half of the twentieth century, because it is well known that, in the study of integrable systems, classical and quantum properties are very closely related.

The first part of the comment provides historical precision on research made on the Kepler problem in the second half of the nineteenth century. This is interesting information that, unfortunately, has remained as completely forgotten for many years (we are talking of Mathematical Physics, perhaps the situation is different in the History of Science circles). This is indeed a matter of fact. Look at the paper *"Dynamical symmetries in a spherical geometry I"*[8] by Higgs that has been considered, since its publication 25 years ago, as one of the most important and cited papers on this matter: it has 20 references but no mention of any of the old papers of Lobachevski, Schering, Lipschitz, Killing, etc. Moreover, we did not find any of these references in Rosenfeld's book.[14] In any case, this question seems more related with the history of mathematics than with the actual mathematics or physics.

It seems that corresponds to Dombrowski and Zitterbarth's "rediscovery" of all these nineteenth century results in Ref. 6 that seems to be a summary of the Ph. D. thesis[16] of the second author (the comment by Shchepetilov is very closely related with the first part of this paper). These authors start with a fully detailed survey, quoting results by Bolyai, Dirichlet, Lipschitz, Beltrami, Schering, Killing, and Liebmann (spanning from 1848 to 1905), and then write "In many cases these statements are … rather incomplete, sometimes not presented in an optimal form, or their proofs are not quite sufficient resp. rather 'out of date' since several appropriate tools … were not available … . So we thought it to be worthwhile to make these (wonderful, classical) results and proofs of them accessible in a rather rigid and complete version … ." The situation they describe is thus the following: whereas some old results on the non-Euclidean Kepler problem were stated or demonstrated at different places in the literature prior to 1905, no complete, accessible and modern presentation was available when Ref. 6 was written.

Concerning the last three paragraphs, focused on three particular aspects of Ref. 3, we must first say that Ref. 3 has, roughly speaking, two parts (as mentioned in the paper's title): the first one devoted to the geodesic motion, the theory of symmetries and the general theory of central potentials with constant curvature $\kappa \neq 0$, and the second one, more specific, devoted to the Kepler problem as a particular case. We consider Secs. II and III as important, not only from the structure of the paper but also because of the results obtained (the equation of Binet is obtained for all the central potentials and for all the values of κ and not just for the Kepler problem on a particular

space). Shchepetilov restricts his comments to the second part of Ref. 3 and completely ignores the first one; we think that this can give a partial image of Ref. 3. Next we consider the last three paragraphs.

(i) All the mathematical expressions are presented using the curvature κ as a parameter. Thus, some previous results, obtained in some cases for the sphere and in others for the hyperbolic plane, arise now as particular cases of this more general κ-dependent situation. Section II of Ref. 9 contains some equations that coincide (after the appropriate changes of notation) with the $\kappa=1$ value of κ-dependent expressions in Ref. 3 (by the way, Ref. 9 has five references and none of them are related with the above-mentioned mathematicians of the second half of the nineteenth century).

(ii) The technique of introducing the curvature κ as a parameter for the joint analysis of the dynamics in the three manifolds $(S^2_\kappa, E^2, H^2_\kappa)$ has been systematically used in some of our previous papers (see, e.g., Refs. 11–13) not only for the Kepler problem but for other superintegrable systems. Moreover, in some previous papers of one of the authors, which are related to the Cayley-Klein geometries (they start with Refs. 1 and 2 and continue until recent papers such as Refs. 7 and 10), this technique is used, not just with one single parameter κ, but with *two parameters*, κ_1, κ_2, which correspond to a space M_{κ_1,κ_2} with constant curvature κ_1 and signature $(+1, \kappa_2)$. This formalism is more general and it includes the κ-dependent formalism used in Ref. 3 as the particular case $\kappa_1=\kappa$ and $\kappa_2=1$ (the "Lorentzian" version of the Kepler problem depending on the two parameters, κ_1 and κ_2, is studied in Ref. 4).

(iii) It is true that Sec. V does not have references but it is also true that the total number of references in Ref. 3 is 44 (not only the references mentioned by Shchepetilov in his introductory paragraph). The article of Story is written from a geometrical projective viewpoint and without any mechanical application, and its approach is very different from the metric approach to conics presented in Ref. 3. The situation is similar to the book by Coolidge,[5] so it seems out of place to quote them. The Liebmann books include a study of hyperbolic conics, but, aside from its role in the history of geometry, Dombrowski and Zitterbarth suggest that the list of types of Kepler orbits given by Liebmann for the hyperbolic plane was not known for sure to be complete (we recall that they consider this book as important but *"rather incomplete, sometimes not presented in an optimal form, …"* for the present time reader). Finally, we note that Dombrowski and Zitterbarth, in spite of their interest in old references, do not mention either the paper by Story[15] or the book of Klein.

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Constraints on the mixing of bipartite states

Hao Chen[a)]
Department of Computing and Information Technology, Fudan University, Shanghai 200433, People's Republic of China

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A mixed state may be represented in many different ways as a mixture of pure states $\rho=\Sigma p_i|\psi_i\rangle\langle\psi_i|$. The mixing problem in quantum mechanics asks the characterization of the probability distribution (p_i) and the mixed states (ρ_i) such that $\rho=\Sigma p_i\rho_i$ for any given mixed state ρ. Some constraints based on eigenvalues of the mixed states are established in uni-party case [see Nielsen, Phys. Rev. A. **63**, 052308 (2000), **63**, 022144 (2000), Nielsern and Vidal Quantum Inf. Comput. **1** 76 (2001)]. We develop some new invariant sets for bipartite mixed states under local unitary operations, which are independent of eigenvalues, and prove some strong constraints based on these invariant sets for the mixing problem in bipartite case. This exhibits a remarkable difference from the uni-party case. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2138048]

I. INTRODUCTION

A feature of quantum mechanics is that every mixed state can be represented as an ensemble of pure states $\{p_i,|\psi_i\rangle\}$ in many different ways. An important problem in quantum mechanics is the following mixing problem: for any given mixed state ρ to characterize the probability distribution (p_i) and the mixed states (ρ_i) such that $\rho=\Sigma p_i\rho_i$. In the context of quantum information processing, the action of mixing $\{p_i,\rho_i\}\rightarrow\rho=\Sigma p_i\rho_i$ corresponds to the erasure of information concerning the identity of a member of the ensemble (see Refs. 1 and 2). Thus it is interesting to characterize this process of mixing of quantum states. In the uni-party case there is the so-called "ensemble classification theorem" of Schrödinger, which established a connection via a unitary matrix between two ensembles representing the same mixed state(Refs. 1 and 3). From the work in Refs. 4, 5, and 1, we know the constraint $(p_i)\prec\lambda(\rho)$ on the ensemble $\{p_i,|\psi_i\rangle\}$ such that $\rho=\Sigma p_i|\psi_i\rangle\langle\psi_i|$, where $\lambda(\rho)$ is the eigenvalue vector of the mixed state ρ and $\prec$ is the majorization. Here we recall the definition of the majorization (Refs. 4, 5, and 1). (p_i) and $\lambda(\rho)$ are rearranged in decreasing order as $(p_1^{\downarrow},\ldots,p_d^{\downarrow})$ and $(\lambda_1^{\downarrow},\ldots,\lambda_d^{\downarrow})$, we say $(p_i)\prec\lambda(\rho)$ if

$$\begin{aligned} p_1^{\downarrow} &\leqslant \lambda_1^{\downarrow}, \\ p_1^{\downarrow}+\cdots+p_k^{\downarrow} &\leqslant \lambda_1^{\downarrow}+\cdots+\lambda_k^{\downarrow} \\ p_1^{\downarrow}+\cdots+p_d^{\downarrow} &= \lambda_1^{\downarrow}+\cdots+\lambda_d^{\downarrow}. \end{aligned} \tag{1}$$

For the process of mixing of general quantum states $\{p_i,\rho_i\}\rightarrow\rho=\Sigma p_i\rho_i$ the constraint $\lambda(\rho)\prec\Sigma p_i\lambda(\rho_i)$ must be hold. Further analysis about the ensemble $\{p_i,|\psi_i\rangle\}$ representing ρ was presented in Ref. 6.

It is natural to consider the mixing problem in bipartite (or general multipartite) case from the theoretical view and the motivation of quantum information processing. As is well known, much of the difficulty for a complete understanding of the bipartite mixed state entanglement can be

[a)]Electronic mail: chenhao1964cn@yahoo.com.cn

traced to the basic fact that there are infinitely many ways of viewing a bipartite mixed state ρ as an ensemble of pure states $\rho=\Sigma p_i|\psi_i\rangle\langle\psi_i|$. For the purpose of understanding the entanglement of the bipartite mixed state ρ it is always useful to know the constraints on the pure states $|\psi_i\rangle$'s in the ensemble. Thus we hope to find as many constraints as possible on the mixing process of bipartite quantum states $\{p_i,\rho_i\}\rightarrow\rho=\Sigma p_i\rho_i$, where p_i is a probability distribution and $(\rho_i),\rho$ are mixed states on $H_A^m\otimes H_B^n$.

We can have some constraints of the mixing problem for bipartite states from some previous known results and invariants. First we can trace over A or B for the mixing of bipartite states $\rho=\Sigma p_i\rho_i$ and then apply the known constraints in the uni-party case to get the constraints in the bipartite case. On the other hand, it is clear that there is at least one entangled pure state $|\psi_i\rangle$ in the ensemble $\{p_i,|\psi_i\rangle\}$ representing an entangled bipartite mixed state ρ. For a bipartite mixed state ρ, it has Schmidt number k if and only if for any decomposition $\rho=\Sigma_i p_i|v_i\rangle\langle v_i|$ for positive real number p_i's and pure state $|v_i\rangle$'s, at least one the of $|v_i\rangle$'s has its Schmidt rank at least k, and there exists such a decomposition with all pure state $|v_i\rangle$'s Schmidt rank at most k (see Ref. 7). Generally speaking if the Schmidt number of ρ is k, then there is at least one pure state $|\psi_i\rangle$ with Schmidt rank at least k for the ensemble $\{p_i,|\psi_i\rangle\}$ representing ρ. This kind of constraint is a feature of the bipartite case. Of course people can have more constraints on the mixing of bipartite states based on, e.g., formation of entanglement, etc. However it is difficult to calculate invariants such as Schmidt number and formation of entanglement, thus these kinds of constraints in the bipartite case are quite restrictive in application.

For the mixing process $\{p_i,\rho_i\}\rightarrow\rho=\Sigma p_i\rho_i$, it is clear $U\rho U^\dagger=\Sigma p_i U\rho_i U^\dagger$ ($\dagger$ is the adjoint) for any unitary operation U on the system. Thus the mixing problem in the uni-party case is actually about the equivalence classes of mixed states under unitary operations, and the constraints should be based on the invariants of mixed states under unitary operations. It is clear that for bipartite mixed states $\rho=\Sigma p_i\rho_i$ is equivalent to $(U_1\otimes U_2)\rho(U_1\otimes U_2)^\dagger=\Sigma p_i(U_1\otimes U_2)\rho_i(U_1\otimes U_2)^\dagger$ for any local unitary operation $U_1\otimes U_2$ on the bipartite system. Thus when the mixing problem is considered in the bipartite case, it is actually about the equivalence classes of mixed states under local unitary operations, and the constraints should be based on the invariants of bipartite mixed states under local unitary operations. In the uni-party case it is well known that there are exactly $n-1$ invariants (i.e., n eigenvalues sum up to 1) of a mixed state on H^n under the group of unitary operations [i.e., $n-1=$dim (the space of all mixed states)-dim(the group of unitary operations) $=n(n+1)/2-1-n(n-1)/2$]. Thus it is natural that the previous known constraints in Refs. 4, 5, and 1 are based on these invariants. For bipartite mixed states on $H_A^m\otimes H_B^n$, it is known that there are $m^2n^2-m^2-n^2+1$ nonlocal invariants under local unitary operations.[8] These nonlocal invaraints have not been constructed explicitly, however we can speculate that there would be many constraints on the mixing of bipartite states based on the nonlocal invariants.

In this paper we develop some new invariant sets of bipartite mixed states under local unitary operations, which are independent of eigenvalues. These invariant sets are natural from the physical consideration of measuring mixed states by separable pure states. Some strong constraints (thus independent of eigenvalues) on the mixing of bipartite states based on these invariant sets are proved. From these constraints based on invariant sets it is easy to have constraints based on numerical quantities derived from these invariant sets (here we note that these numerical quantities are invariant under local unitary operations). Since these invariants can be computed easily it is convenient to use these constraints as illustrated in the examples to follow. Moreover the constraints are imposed on each member ρ_i appearing in $\rho=\Sigma p_i\rho_i$ and are independent of the probability distribution (p_i). Therefore they are essentially a feature of the bipartite case.

II. CONSTRAINTS BASED ON $L_A(\rho)$ AND $L_B(\rho)$

For any given bipartite mixed state ρ on $H_A^m\otimes H_B^n$, we can define $L_A(\rho)$ [respectively, $L_B(\rho)$] (the subspaces of H_A^m and H_B^n) as follows.

Definition 1:

$$L_A(\rho)=\{|a\rangle\in H_A^m:\langle a\otimes x|\rho|a\otimes x\rangle=0,\ \forall\ |x\rangle\in H_B^n\},\tag{2}$$

$$L_B(\rho) = \{|b\rangle \in H_B^n : \langle x \otimes b|\rho|x \otimes b\rangle = 0, \forall\, |x\rangle \in H_A^m\}. \tag{3}$$

It is clear $\langle a\otimes x|\rho|a\otimes x\rangle=0$ if and only if $|a\rangle\otimes|x\rangle$ is orthogonal to the range of ρ since ρ is Hermitian. Thus $L_A(\rho)$ [respectively, $L_B(\rho)$] is the linear subspace of H_A^m (respectively, H_B^m). We should note that $L_A(\rho)$ [respectively, $L_B(\rho)$] is completely determined by the range of the mixed state ρ, thus it only depends on the eigenstates of ρ and does not depend on the nonzero eigenvalues of ρ.

Since

$$\langle a \otimes b|(U_A \otimes U_B)\rho(U_A \otimes U_B)^\dagger|a \otimes b\rangle = \langle \left(U_A^\dagger a\right) \otimes \left(U_B^\dagger b\right)|\rho|\left(U_A^\dagger a\right) \otimes \left(U_B^\dagger b\right)\rangle, \tag{4}$$

we have

$$L_A((U_A \otimes U_B)\rho(U_A \otimes U_B)^\dagger) = U_A^\dagger(L_A(\rho)). \tag{5}$$

Similarly $L_B((U_A\otimes U_B)\rho(U_A\otimes U_B)^\dagger)=U_B^\dagger(L_B(\rho)))$, i.e., the dimensions of $L_A(\rho)$ and $L_B(\rho)$ are invariant under local unitary operations. It is easy to verify that $L_A(\rho)=\ker(\mathrm{Tr}_B(\rho))$ and $L_B(\rho)=\ker(\mathrm{Tr}_A(\rho))$. These subspaces have been used to give lower bound for Schmidt numbers of low-rank bipartite mixed states in Ref. 9.

For a pure state $\rho=|\psi\rangle\langle\psi|$, from the invariance under local unitary operations, we can compute $L_A(\rho)$ and $L_B(\rho)$ from the Schmidt decomposition of $|\psi\rangle=\Sigma_{i=1}^k p_i|a_i\rangle\otimes|b_i\rangle$. We have $\langle a\otimes b|\rho|a\otimes b\rangle=\Sigma_{i=1}p_i^2|\langle a|a_i\rangle\langle b|b_i\rangle|^2=0$ implies that $L_A(\rho)$ [respectively, $L_B(\rho)$] is the orthogonal complementary in H_A^m of the space span by pure states $|a_i\rangle$'s (respectively, $|b_i\rangle$'s). Thus the Schmidt rank k of the pure state ρ is just the codimensions of the linear subspaces of $L_A(\rho)$ and $L_B(\rho)$.

If $\rho=\Sigma p_i|\psi_i\rangle\langle\psi_i|$ with $p_i>0$, we have the following equation $\langle a\otimes x|\rho|a\otimes x\rangle=\Sigma p_i|\langle a\otimes x|\psi_i\rangle|^2$. Thus

$$\begin{aligned} L_A(\rho) &= \cap L_A(|\psi_i\rangle\langle\psi_i|), \\ L_B(\rho) &= \cap L_B(|\psi_i\rangle\langle\psi_i|). \end{aligned} \tag{6}$$

The following result is the main result of this section.

Theorem 1: *For any given mixed state ρ on $H_A^m\otimes H_B^n$ and an ensemble $\{p_i,|\psi_i\rangle\}$ such that $\rho=\Sigma p_i|\psi_i\rangle\langle\psi_i|$, we have:*

1) *Let $s(|v\rangle)$ be the Schmidt rank of the pure state $|v\rangle$,*

$$s(|\psi_i\rangle) \leqslant \min\{m - \dim(L_A(\rho)), n - \dim(L_B(\rho))\}. \tag{7}$$

2) *For any $r=\mathrm{rank}(\rho)$ linearly independent pure states $|\psi_{i_1}\rangle,\ldots,|\psi_{i_r}\rangle$ in the ensemble,*

$$\sum_{j=1}^r s(|\psi_{i_j}) \geqslant \max\{m - \dim(L_A(\rho)), n - \dim(L_B(\rho))\}. \tag{8}$$

Proof: We have $L_A(\rho)=\cap L(|\psi_i\rangle\langle\psi_i|)$, thus $\dim(L_A(\rho))\leqslant\dim(L_A(|\psi_i\rangle\langle\psi_i|))$ and the Schmidt rank $s(|\psi_i\rangle)=m-\dim(L_A(|\psi_i\rangle\langle\psi_i|)\leqslant m-\dim(L_A(\rho))$. Similarly we have the Schmidt rank $s(|\psi_i\rangle)\leqslant n-\dim(L_B(\rho))$. The conclusion of 1 is proved.

Because $|\psi_{i_1}\rangle,\ldots,|\psi_{i_r}\rangle$ are linearly independent, they span the range of ρ. From the fact that $\langle a\otimes x|\rho|a\otimes x\rangle=0$ is equivalent to the fact that $|a\rangle\otimes|x\rangle$ is orthogonal to the range of ρ, we have $L_A(\rho)=\cap_{j=1}^r L_A(|\psi_{i_j}\rangle\langle\psi_{i_j}|)$. Thus $\mathrm{codim}(L_A(\rho))\leqslant\Sigma_{j=1}^r\mathrm{codim}(L_A(|\psi_{i_j}\rangle\langle\psi_{i_j}|))$, then $m-\dim(L_A(\rho))\leqslant\Sigma_{j=1}^r s(|\psi_{i_j})$. Similarly we have $n-\dim(L_B(\rho))\leqslant\Sigma_{j=1}^r s(|\psi_{i_j})$. The conclusion is proved.

We can have another proof of conclusion 1 of Theorem 1 from the previous known constraint in uni-party case (see Ref. 5 and 1). First by the trace over B of $\rho=\Sigma p_i|\psi_i\rangle\langle\psi_i|$, we get $\mathrm{Tr}_B(\rho))=\Sigma p_i\mathrm{Tr}_B(|\psi_i\rangle\langle\psi_i|)$. Thus $\lambda(\mathrm{Tr}_B(\rho))\prec\Sigma p_i\lambda(\mathrm{Tr}_B(|\psi_i\rangle\langle\psi_i|))$ from the constraint in the uni-party case. If the codimension of $L_A(|\psi_i\rangle\langle\psi_i|)=\ker(Tr_B(|\psi_i\rangle\langle\psi_i|))$ is bigger than the codimension of $L_A(\rho)=\ker(Tr_B(\rho))$, there are more non zeros in the vector $\Sigma p_i\lambda(\mathrm{Tr}_B(|\psi_i\rangle\langle\psi_i|))$ than in the vector

$\lambda(\mathrm{Tr}_B(\rho))$. This is a contradiction to the fact $\lambda(\mathrm{Tr}_B(\rho)) < \Sigma p_i \lambda(\mathrm{Tr}_B(|\psi_i\rangle\langle\psi_i|))$. Thus Theorem 1.1 can be derived from the previous known constraint, however our proof here is more transparent.

Example 1: We consider the mixed state $\rho = T_1 \otimes T_2$ on $H_A^m \otimes H_B^n$, where T_1 and T_2 are the mixed states on H_A^m and H_B^n, respectively, satisfying the condition that the rank of T_1 is 1 (or the rank of T_2 is 1). It is clear that ρ is separable. However we know from Theorem 1.1 that for any ensemble $\{p_i, |\psi_i\rangle\}$ representing ρ, the pure states $|\psi_i\rangle$'s are separable. It is easy to verify that the rank of $\mathrm{Tr}_B(\rho)$ [or of $\mathrm{Tr}_A(\rho)$] is 1, thus the conclusion follows from Theorem 1.1 immediately.

Example 2: Let $\rho = \frac{1}{2}(|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|)$ be a mixed state of rank 2 on $H_A^m \otimes H_B^n$ (assume $m \leqslant n$ without loss of generality), where $|\psi_1\rangle$ is a pure state with Schmidt rank m and $|\psi_2\rangle$ is an arbitrary pure state not equal to $|\psi_1\rangle$. From the fact $L_A(|\psi_1\rangle\langle\psi_1|) = \{0\}$ we know $L_A(\rho) = \{0\}$. From Theorem 1.2), for any ensemble $\{p_i, |\phi_i\rangle\}$ representing ρ, we know that the sum of the Schmidt ranks of any two distinct pure states in the ensemble is at least m, that is, except for one pure state, all other pure states in the ensemble have their Schmidt ranks at least $m/2$. This implies that the Schmidt number of ρ is at least $m/2$.

III. CONSTRAINTS BASED ON $L_A^k(\rho)$ AND $L_B^k(\rho)$

We can see that the invariance of the dimensions of the linear subspaces $L_A(\rho)$ and $L_B(\rho)$ under the local unitary operations is derived from the symmetry of the bilinear form $\langle a \otimes x|\rho|a \otimes x\rangle$ under local unitary operations. Thus the idea about $L_A(\rho)$ [respectively, $L_B(\rho)$] can be extended as follows.

Definition 2: Let ρ be a mixed state on $H_A^m \otimes H_B^n$. For non-negative integers $k = 0, 1, \ldots, n-1$, we define $L_A^k(\rho)$ to be the set $|a\rangle \in H_A^m$, such that the Hermitian semi-positive bilinear form $\langle a \otimes x|\rho|a \otimes x\rangle$ ($|x\rangle \in H_B^n$ is considered as the variable, $|a\rangle$ is fixed) has its rank at most k. That is

$$L_A^k(\rho) = \{|a\rangle \in H_A^m : \mathrm{rank}(\langle a \otimes x|\rho|a \otimes x\rangle) \leqslant k\}. \tag{9}$$

Here $\langle a \otimes x|\rho|a \otimes x\rangle$ for a fixed $|a\rangle$ is considered as a bilinear form on H_B^n.

Similarly the set $L_B^k(\rho) \subseteq H_B^n$ can be defined for $k = 0, 1, \ldots, m-1$. It is clear that $L_A^0(\rho) = L_A(\rho)$ and $L_B^0(\rho) = L_B(\rho)$. From (4) we have $L_A^k((U_A \otimes U_B)(\rho)(U_A \otimes U_B)^\dagger) = U_A^\dagger(L_A^k(\rho))$ [respectively, $L_B^k((U_A \otimes U_B)(\rho)(U_A \otimes U_B)^\dagger) = U_B^\dagger(L_B^k(\rho))$]. $L_A^k(\rho)$ [respectively, $L_B^k(\rho)$] is the subset of H_A^m (respectively, H_B^n), which is invariant (up to unitary transformations of the ambient space) under local unitary operations.

Now we want to see how to calculate these invariant subsets by coordi nate forms. We use the standard basis $\{|11\rangle, |12\rangle, \ldots |1n\rangle, \ldots, |m1\rangle, \ldots, |mn\rangle\}$ of $H = H_A^m \otimes H_B^n$. Take

$$\rho = \sum_{l=1}^{t} p_l |v_l\rangle\langle v_l| \tag{10}$$

to be any given representation of ρ as a convex combination of projections with $p_1 > 0, \ldots, p_t > 0$. Suppose

$$|v_l\rangle = \sum_{i,j=1}^{m,n} a_{ijl} |ij\rangle. \tag{11}$$

Consider

$$A = (a_{ijl})_{1 \leqslant i \leqslant m, 1 \leqslant j \leqslant n, 1 \leqslant l \leqslant t} \tag{12}$$

as the $mn \times t$ matrix with mn rows corresponding to the standard basis $\{|11\rangle, \ldots, |1n\rangle, \ldots, |m1\rangle, \ldots, |mn\rangle\}$ and t columns corresponding to the expansions of $|v_1\rangle, \ldots |v_t\rangle$ with respect to this basis as in (11). It is clear that the matrix of ρ with respect to the standard basis is $APA^\dagger$, where P is the $t \times t$ diagonal matrix with diagonal entries $p_1, \ldots, p_t$.

Let A_i be the ith block $n \times t$ submatrix of A corresponding to the $A|i1\rangle, \ldots, |in\rangle$ rows. For any $|a\rangle = \Sigma_{i=1}^m r_i |i\rangle \in H_A^m$, we have

$$\langle a\otimes x|\rho|a\otimes x\rangle=\langle x|\Big(\sum_{i=1}^{m} r_iA_i\Big)P\Big(\sum_{j=1}^{m} r_jA_j\Big)^{\dagger}|x\rangle. \tag{13}$$

Thus for any fixed $|a\rangle=\Sigma_{i=1}^{m}r_i|i\rangle\in H_A^m$ the matrix of the bilinear form $\langle a\otimes x|\rho|a\otimes x\rangle$ (considered as a bilinear form on $|x\rangle\in H_B^n$, with respect to the base $\{|1\rangle,\ldots,|n\rangle\}$) is $\Sigma_{i,j=1}^{m}r_ir_j^{\dagger}A_iPA_j^{\dagger}=(\Sigma_{i=1}^{m}r_iA_i)P(\Sigma_{i=1}^{m}r_iA_i)^{\dagger}$. On the other hand, we know that $\mathrm{rank}((\Sigma_{i=1}^{m}r_iA_i)P(\Sigma_{i=1}^{m}r_iA_i)^{\dagger}))\leqslant k$ is equivalent to $\mathrm{rank}(\Sigma_{i=1}^{m}r_iA_i)\leqslant k$ because P is strictly positive definite. Therefore

$$L_A^k(\rho)=\Big\{r_1|1\rangle+\cdots+r_m|m\rangle\in H_A^m:\mathrm{rank}\Big(\sum_{i=1}^{m} r_iA_i\Big)\leqslant k\Big\}. \tag{14}$$

Thus $L_A^k(\rho)=\{\ r_1|1\rangle+\ldots+r_m|m\rangle\in H_A^m$: the determinants of all $(k+1)\times(k+1)$ submatrices of $(\Sigma_{i=1}^{m}r_iA_i)$ are zero$\}$. Similarly we have

$$L_B^k(\rho)=\Big\{r_1|1\rangle+\cdots+r_n|n\rangle\in H_B^n:\mathrm{rank}\Big(\sum_{i=1}^{n} r_iB_i\Big)\leqslant k\Big\}. \tag{15}$$

Thus $L_B^k(\rho)=\{\ r_1|1\rangle+\cdots+r_n|n\rangle\in H_B^n$: the determinants of all $(k+1)\times(k+1)$ submatrices of $(\Sigma_{i=1}^{n}r_iB_i)$ are zero $\}$, where $B_i, i=1,\ldots,n$, are defined similarly. In this way we can see that $L_A^k(\rho)$'s and $L_B^k(\rho)$'s are the zero locus of some homogeneous polynomials in H_A^m and H_B^n.

These kinds of subsets can be understood as subsets in the complex projective spaces $P(H_A^m)=CP^{m-1}$ and $P(H_B^n)=CP^{n-1}$ since their defining equations are homogeneous, and are called determinantal varieties in Algebraic Geometry (see Ref. 10). We should emphasize that these homogeneous polynomials are independent of these positive real numbers p_i's and only dependent on the pure states $|v_l\rangle$'s. In the case $k=0$ the defining homogeneous polynomials of $L_A^0(\rho)$ and $L_B^0(\rho)$ are of degree 1, thus they are subspaces. For general $k, L_A^k(\rho)$ and $L_B^k(\rho)$ are just (algebraic) subsets of H_A^m and H_B^n defined as the zero locus of some homogeneous polynomials. From the invariance under local unitary operations we know that the geometric properties of $L_A^k(\rho)$ [respectively, $L_B^k(\rho)$, considered as subset of the complex projective spaces], such as their volumes, dimensions, etc., are invariants of the mixed states under local unitary operations.

If we take the spectral decomposition of $\rho=\Sigma_i\lambda_i|\phi_i\rangle\langle\phi_j|$, where λ_i's and $|\phi_i\rangle$'s are eigenvalues and eigenstates, and then compute $L_A^k(\rho), k=0,1,\ldots n-1$ [respectively, $L_B^k(\rho), k=0,1,\ldots,m-1$] as above, it is clear that these invariant sets under local unitary operations are computed from the eigenstates and thus independent of eigenvalues of the mixed state. Therefore the following constraints on the mixing of bipartite mixed states are independent of eigenvalues.

Theorem 2: *Let ρ,ρ_i be bipartite mixed states on $H_A^m\otimes H_B^n$ and p_i's be positive real numbers. Suppose $\rho=\Sigma p_i\rho_i$. Then $L_A^k(\rho)\subseteq L_A^k(\rho_i), k=0,1,\ldots,n-1$ and $L_B^k(\rho)\subseteq L_B^k(\rho_i), k=0,1,\ldots,m-1$ for any possible index i.*

Proof: Let $\rho_i=\Sigma\lambda_j^i|\psi_j^i\rangle\langle\psi_j^i|$ be the spectral decomposition of the mixed state ρ_i. Then $\rho=\Sigma p_i\rho_i=\Sigma_{i,j}p_i\lambda_j|\psi_j^i\rangle\langle\psi_j^i|$ with $p_i\lambda_j>0$. We know that $L_A^k(\rho)$ can be computed from the matrix Σr_iA_i, where A_i's are defined from the pure states $|\psi_j^i\rangle$'s as in (13). On the other hand $L_A^k(\rho_i)$ can be computed from the matrix $\Sigma r_iA_i'$, where A_i''s are defined from the pure states $|\psi_j^i\rangle$'s for the fixed i as in (13). Thus it is clear that the matrix $\Sigma r_iA_i'$ is the submatrix of $\Sigma_i r_iA_i$ and $\mathrm{rank}(\Sigma r_iA_i)\leqslant k$ implies $\mathrm{rank}(\Sigma r_iA_i')\leqslant k$. We have $L_A^k(\rho)\subseteq L_A^k(\rho_i)$. The conclusion $L_B^k(\rho)\subseteq L_B^k(\rho_i)$ can be proved similarly.

If we consider the $L_A(\rho)$'s as algebraic subsets of the projective space, then the constraints

$$\begin{aligned}\mathrm{volume}\big(L_A^k(\rho)\big)&\leqslant\mathrm{volume}\big(L_A^k(\rho_i)\big),\\ \mathrm{dimension}\big(L_A^k(\rho)\big)&\leqslant\mathrm{dimension}\big(L_A^k(\rho_i)\big)\end{aligned} \tag{16}$$

[respectively, about $L_B^k(\rho)$] if $\rho=\Sigma p_i\rho_i$ with $p_i>0$ follows from Theorem 2 directly. Here we should note that the volume and dimension of $L_A^k(\rho)$ [respectively, $L_B^k(\rho)$] are invariants of the mixed states ρ under local unitary operations.

Example 3: Let $\rho_{BP}=\frac{1}{4}(|\psi_1\rangle\langle\psi_1|+\cdots+|\psi_4\rangle\langle\psi_4|)$ be a mixed state on $H_A^3\otimes H_B^3$ of rank 4, where

$$|\psi_1\rangle=m|11\rangle+s|31\rangle+n|22\rangle,$$

$$
\begin{aligned}
|\psi_2\rangle &= b|12\rangle + a|21\rangle + c|32\rangle,\\
|\psi_3\rangle &= n^*|11\rangle + t|13\rangle - m^*|22\rangle,\\
|\psi_4\rangle &= -a^*|12\rangle + b^*|21\rangle + d|23\rangle
\end{aligned}
\tag{17}
$$

for suitable chosen parameters. This is just the mixed states constructed in Ref. 11. It is proved there that for randomly chosen parameters ρ_{BP} is PPT entangled mixed state.

From the above noted computation we know that $L_A^2(\rho_{BP})$ is defined by the condition $\mathrm{rank}(\Sigma r_i A_i) \leqslant 2$, where $\Sigma r_i A_i$ can be computed from the above four pure states as the following:

$$
\begin{pmatrix}
mr_1 + sr_3 & ar_2 & n^* r_1 & b^* r_2\\
nr_2 & br_1 + cr_3 & -m^* r_2 & -a^* r_1\\
0 & 0 & tr_1 & dr_2
\end{pmatrix}.
\tag{18}
$$

We can check that the point $(r_1, r_2, r_3) = (0, 1, -1)$ is not in $L_A^2(\rho_{BP})$ for randomly chosen parameters.

Consider the following five pure states $|\phi_1\rangle, \ldots, |\phi_5\rangle$ in $H_A^3 \otimes H_B^3$, where

$$
\begin{aligned}
|\phi_1\rangle &= \frac{1}{\sqrt{2}}(|11\rangle - |12\rangle),\\
|\phi_2\rangle &= \frac{1}{\sqrt{2}}(|13\rangle - |23\rangle),\\
|\phi_3\rangle &= \frac{1}{\sqrt{2}}(|32\rangle - |33\rangle),\\
|\phi_4\rangle &= \frac{1}{\sqrt{2}}(|21\rangle - |31\rangle),\\
|\phi_5\rangle &= \tfrac{1}{3}(|1\rangle + |2\rangle + |3\rangle) \otimes (|1\rangle + |2\rangle + |3\rangle).
\end{aligned}
\tag{19}
$$

They form an UPB (Unextendible Product Base) as shown in Ref. 12. Let T be the orthogonal complementary space and $\rho_{\mathrm{UPB}} = (1/D)P_T$, where D is a normalizing constant and P_T is the projection to T. It is known that ρ_{UPB} is PPT entangled mixed state from the UPB context (Ref. 12).

Generally speaking we need four orthogonal pure states in T to compute $L_A^2(\rho_{\mathrm{UPB}})$. However for any four linearly independent pure states in T, it is observed that the corresponding $\Sigma r_i A_i$ and $\Sigma r_i A_i'$ defined from these two sets of pure states only differ with a non-singular 4×4 matrix on the right side, thus the conditions $\mathrm{rank}(\Sigma r_i A_i) \leqslant 2$ and $\mathrm{rank}(\Sigma r_i A_i') \leqslant 2$ are equivalent. This makes our computation simpler. Let $|v_1\rangle, \ldots, |v_4\rangle$ be the following four linearly independent pure states in T:

$$
\begin{aligned}
|v_1\rangle &= \tfrac{1}{2}(|11\rangle + |12\rangle - |21\rangle - |31\rangle),\\
|v_2\rangle &= \tfrac{1}{2}(|11\rangle + |12\rangle - |13\rangle - |23\rangle),\\
|v_3\rangle &= \tfrac{1}{2}(|11\rangle + |12\rangle - |32\rangle - |33\rangle),
\end{aligned}
\tag{20}
$$

$$|v_4\rangle = \frac{1}{\sqrt{20}}(|11\rangle + |12\rangle + |13\rangle + |23\rangle - 4|22\rangle).$$

Therefore $L_A^2(\rho_{\mathrm{UPB}})$ as defined by the rank of the following matrix is at most 2:

$$\begin{pmatrix} r_1 - r_2 - r_3 & r_1 & r_1 & r_1 \\ r_1 & r_1 & r_1 - r_3 & r_1 - 4r_2 \\ 0 & -r_1 - r_2 & -r_3 & r_1 + r_2 \end{pmatrix}. \tag{21}$$

It is easy to check that the point $(r_1, r_2, r_3) = (0, 1, -1)$ is in $L_A^2(\rho_{\mathrm{UPB}})$. Thus $L_A^2(\rho_{\mathrm{UPB}})$ is not a subset of $L_A^2(\rho_{BP})$, and from Theorem 2 we know that it is impossible to find positive real p_i's and mixed state ρ_i's with $\rho_1 = \rho_{BP}$ on $H_A^3 \otimes H_B^3$ such that $\rho_{\mathrm{UPB}} = \Sigma p_i \rho_i$.

Example 4: Let $\rho' = \frac{1}{3}(|v_1\rangle\langle v_1| + |v_2\rangle\langle v_2| + |v_4\rangle\langle v_4|)$ be a mixed state on $H_A^3 \otimes H_B^3$ where $|v_1\rangle, |v_2\rangle, |v_4\rangle$ are as above. This is a rank 3 mixed state. We want to know if there exist positive real p_i's and mixed state ρ_i's with $\rho_1 = \rho'$ such that $\rho_{BP} = \Sigma p_i \rho_i$. It is easy to check the point (0; 1; 0) is in the set $L_A^2(\rho_{BP})$ (for randomly chosen parameters). From the above-described computation the set $L_A^2(\rho')$ is defined by the condition that the following matrix has its rank at most 2:

$$\begin{pmatrix} r_1 - r_2 - r_3 & r_1 & r_1 \\ r_1 & r_1 & r_1 - 4r_2 \\ 0 & -r_1 - r_2 & r_1 + r_2 \end{pmatrix}. \tag{22}$$

Thus it is easy to check that the point (0; 1; 0) is not in the set $L_A^2(\rho')$. From Theorem 2 we know that it is impossible to find positive real p_i's and mixed state ρ_i's with $\rho_1 = \rho'$ such that $\rho_{BP} = \Sigma p_i \rho_i$.

From these examples we can see that it is not necessary to locate the set $L_A^k(\rho)$ [or $L_B^k(\rho)$] exactly when we use Theorem 2 to decide whether a mixed state is mixed by some special mixed states. Because Theorem 2 gives *strong* constraints on the mixing problem of bipartite states, it is convenient to use it to get the negative result for mixing problem in bipartite case.

In conclusion, we have developed new invariant sets of bipartite mixed states under local unitary operations and proved some strong constraints on the mixing problem of bipartite states based on these new invariant sets. The invariant sets and the constraints based on them are independent of the eigenvalues of the mixed states. This exhibits the feature that the mixing problem in bipartite case is *essentially* different from the uni-party case. These constraints can be used easily to decide if a given bipartite mixed state is mixed by some other mixed states.

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Ladder operators and coherent states for the Jaynes-Cummings model in the rotating-wave approximation

V. Hussin[a] and L. M. Nieto[b]
Departamento de Física Teórica, Atómica y Óptica, Universidad de Valladolid, 47071 Valladolid, Spain

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Using algebraic techniques, we realize a systematic search of different types of ladder operators for the Jaynes-Cummings model in the rotating-wave approximation. The link between our results and previous studies on the diagonalization of the associated Hamiltonian is established. Using some of the ladder operators obtained before, examples are given on the possibility of constructing a variety of interesting coherent states for this Hamiltonian. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The Jaynes-Cummings model describes the interaction between one mode of a quantized electromagnetic field and a simplified version of an atomic system with two levels.[1,2] It is a nonlinear model of great interest in atomic physics and quantum optics, where it is the fundamental theoretical tool in the study of cavity QED for analyzing ion traps.[3] Hence, it has become very valuable for researchers working in the quickly developing domain of quantum information processing.[4] The solution of the complete system (including the counter-rotating terms) is not yet known in a closed form, although there has been some conjectures never proved.[5] Using the so-called rotating-wave approximation, the Hamiltonian remains nonlinear, but it turns out to be exactly solvable; its eigenvalues and eigenvectors can be computed in a closed form.[6] In this work we are going to focus on the possibility of constructing ladder operators for this simplified model, using some of them to obtain the associated coherent states.

In Sec. II, we will recall the essential features of the Jaynes-Cummings Hamiltonian in the rotating-wave approximation using a notation which is well adapted to the purpose of this presentation. When solving this quantum mechanical problem, we will see that two "towers" of eigenstates appear. The explicit construction of ladder operators will be given in Sec. III. They are assumed to act on the eigenstates to move them up or down in one of the "towers" of eigenstates but do not mix them. We will prove that this condition is not enough to determine them completely, and some extra requirements are needed to fully accomplish our goal. Therefore, in Sec. IV, the commutator of these operators will be fixed to be either the identity operator or the Jaynes-Cummings Hamiltonian itself. In this context, some of the solutions are related with already known results on the diagonalization of the Jaynes-Cummings Hamiltonian in the rotating-wave approximation. In Sec. V we will assume the factorization of the Jaynes-Cummings Hamiltonian by these ladder operators, analyzing two of such possible factorizations. In all the cases considered in Secs. IV and V we will also study two situations of particular interest, the case in which the field and the atom are uncoupled and the case when they are in resonance. In Sec. VI,

[a]Electronic mail: veronique.hussin@umontreal.ca; On leave of absence from Centre de Recherches Mathématiques et Département de Mathématiques et de Statistique, Université de Montréal, C.P. 6128, succ. Centre-ville, Montréal (Québec), H3C 3J7 Canada.
[b]Electronic mail: luismi@metodos.fam.cie.uva.es

using some of the ladder operators obtained in the preceding sections, examples are given on the possibility of constructing a wide variety of coherent states for the Jaynes-Cummings Hamiltonian. Finally, some concluding remarks will be given in Sec. VII.

II. THE JAYNES-CUMMINGS HAMILTONIAN AND ITS ENERGY SPECTRUM

We begin with the Hamiltonian of the Jaynes-Cummings model in the rotating-wave approximation[6–9]

$$\mathcal{H}_{\mathrm{JC}} = \hbar\omega\left(a^{+}a + \tfrac{1}{2}\right)\mathbb{I} + \tfrac{1}{2}\hbar\omega_0\sigma_3 + \hbar\kappa(a^{+}\sigma_{-} + a\sigma_{+}). \tag{2.1}$$

In this expression, a^{+} and a are the photon creation and annihilation operators (the usual ladder operator for the harmonic oscillator), $\mathbb{I}$ is the 2×2 identity matrix, $\{\sigma_1,\sigma_2,\sigma_3\}$ are the Pauli matrices, and $\sigma_{\pm}=\sigma_1\pm i\sigma_2$. The parameters that appear in Eq. (2.1) are the following: ω is the field mode frequency, ω_0 is the atomic frequency and κ is the coupling constant between the radiation and the atom. It must be noticed that the rotating-wave approximation is reliable only if[9]

$$|\omega_0 - \omega| \ll \omega_0, \omega. \tag{2.2}$$

In a realistic experiment we can imagine that the atomic frequency ω_0 is fixed (the atomic species do not change, and the same is true for the transition levels we are considering) and that we can modulate the field mode frequency ω. Hence, let us introduce the following "detuning" parameter ϵ, which can be positive or negative, and is such that

$$\omega = \omega_0(1+\epsilon). \tag{2.3}$$

In terms of it, the rotating-wave approximation condition (2.2) is thus

$$|\epsilon| \ll 1, 1+\epsilon, \quad \text{or } |\epsilon| \approx 0. \tag{2.4}$$

For simplicity, in the sequel we will use the following dimensionless form of the Hamiltonian (2.1), in which we use ϵ and a new parameter $\lambda=\kappa/\omega_0$,

$$\mathcal{H}_{\lambda,\epsilon} = \frac{\mathcal{H}_{\mathrm{JC}}}{\hbar\omega_0} = (1+\epsilon)\left(a^{+}a + \frac{1}{2}\right)\mathbb{I} + \frac{1}{2}\sigma_3 + \lambda(a^{+}\sigma_{-} + a\sigma_{+}). \tag{2.5}$$

As we already pointed out, this model is exactly solvable. The main results can be presented in a quite elegant form if we use the following Fock space, built as the tensor product of the Hilbert space associated to the field, times the Hilbert space associated to the spin,

$$F = F_b \otimes F_f = \left\{ |n,-\rangle = \begin{pmatrix} 0 \\ |n\rangle \end{pmatrix}, |n,+\rangle = \begin{pmatrix} |n\rangle \\ 0 \end{pmatrix}, n = 0,1,\ldots \right\}, \tag{2.6}$$

with $\{|n\rangle\}$ the eigenstates of the photon number operator

$$N = a^{+}a. \tag{2.7}$$

Working in the Fock space F given in (2.6), we can find the following matrix representation of the dimensionless Jaynes-Cummings Hamiltonian $\mathcal{H}_{\lambda,\epsilon}$:

$$\mathcal{H}_{\lambda,\epsilon}=\begin{pmatrix}(1+\epsilon)a^{+}a+1+\dfrac{\epsilon}{2} & \lambda a\\ \lambda a^{+} & (1+\epsilon)a^{+}a+\dfrac{\epsilon}{2}\end{pmatrix}=\begin{pmatrix}(1+\epsilon)N+1+\dfrac{\epsilon}{2} & \lambda a\\ \lambda a^{+} & (1+\epsilon)N+\dfrac{\epsilon}{2}\end{pmatrix}. \tag{2.8}$$

It is very easy to see that this Hamiltonian leaves invariant the following subspaces of F: the one-dimensional subspace F_0 generated by the vector $\{|0,-\rangle\}$ and the two-dimensional subspaces F^n_{n+1} generated by the vectors $\{|n,+\rangle,|n+1,-\rangle\}_{n=0}^{\infty}$. Therefore,

$$F=F_0\overset{\infty}{\underset{n=0}{\oplus}}F^n_{n+1}. \tag{2.9}$$

Taking this fact into account, it is easy to prove that the normalized energy eigenstates of $\mathcal{H}_{\lambda,\epsilon}$ are

$$|E_*\rangle=|0,-\rangle, \tag{2.10}$$

$$|E^+_n\rangle=\sin\,\vartheta(n)|n,+\rangle+\cos\,\vartheta(n)|n+1,-\rangle, \tag{2.11}$$

$$|E^-_n\rangle=\cos\,\vartheta(n)|n,+\rangle-\sin\,\vartheta(n)|n+1,-\rangle, \tag{2.12}$$

where we have set

$$\sin\,\vartheta(n)=\xi_\lambda\sqrt{\frac{q(n+1)-\dfrac{\epsilon}{2}}{2q(n+1)}},\quad \cos\,\vartheta(n)=\sqrt{\frac{q(n+1)+\dfrac{\epsilon}{2}}{2q(n+1)}}, \tag{2.13}$$

that satisfy the usual identity $\cos^2\vartheta(n)+\sin^2\vartheta(n)=1$. In the previous expressions, ξ_λ denotes the sign of the coupling constant λ and we have introduced the following auxiliary function of n:

$$q(n)=\sqrt{\left(\frac{\epsilon}{2}\right)^2+\lambda^2 n}=\frac{|\epsilon|}{2}\sqrt{1+\left(\frac{2\lambda}{\epsilon}\right)^2 n}. \tag{2.14}$$

In all these formulas and in the following, if no indication is given in another sense, it is understood that $n=0,1,\ldots$. Morevover, we will frequently make use of the following limits:

$$\lim_{\epsilon\to 0}q(n)=|\lambda|\sqrt{n},\quad \lim_{\lambda\to 0}q(n)=\frac{|\epsilon|}{2}=q(0), \tag{2.15}$$

$$\lim_{\epsilon\to 0}\sin\,\vartheta(n)=\frac{\xi_\lambda}{\sqrt{2}},\quad \lim_{\epsilon\to 0}\cos\,\vartheta(n)=\frac{1}{\sqrt{2}}, \tag{2.16}$$

and

$$\lim_{\lambda\to 0}\sin\,\vartheta(n)=\xi_\lambda H(-\epsilon)=\sin\,\vartheta(-1),\quad \lim_{\lambda\to 0}\cos\,\vartheta(n)=H(\epsilon)=\cos\,\vartheta(-1), \tag{2.17}$$

where $H(\epsilon)$ is the Heaviside function. Note that in (2.17), there is a trace of the sign of λ after taking the limit.

The "dimensionless energy" eigenvalues corresponding to the eigenstates in Eqs. (2.10)–(2.12) are

$$E_*=\frac{\epsilon}{2}, \tag{2.18}$$

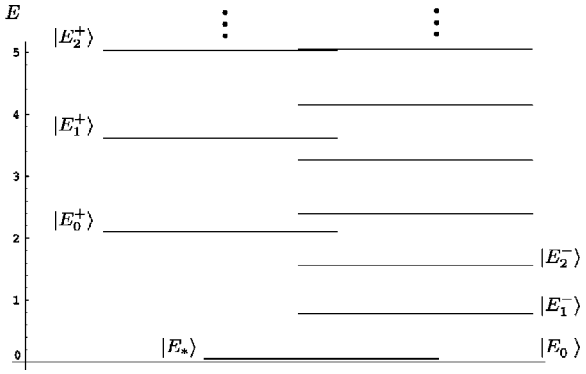

FIG. 1. The two towers of states in the Jaynes-Cummings Hamiltonian for $\epsilon=0.1$, $\lambda=1$

$$E_n^+ = (1+\epsilon)(n+1) + q(n+1), \tag{2.19}$$

$$E_n^- = (1+\epsilon)(n+1) - q(n+1). \tag{2.20}$$

We also introduce the diagonalized version of the Hamiltonian in $\mathcal{H}_{\lambda,\epsilon}$, which may be realized as

$$\mathbb{H}_{\lambda,\epsilon} = \mathcal{U}_{\lambda,\epsilon}^{+}\mathcal{H}_{\lambda,\epsilon}\mathcal{U}_{\lambda,\epsilon} = \begin{pmatrix} (1+\epsilon)(N+1)+q(N+1) & 0 \\ 0 & (1+\epsilon)(N+1)-q(N+1) \end{pmatrix}, \tag{2.21}$$

where $q(N+1)$ is the function defined in (2.14), changing the number n for the number operator N, the operator $\mathcal{U}_{\lambda,\epsilon}$ is given by

$$\mathcal{U}_{\lambda,\epsilon} = \begin{pmatrix} \sin\vartheta(N) & \cos\vartheta(N) \\ a^{+}\dfrac{\cos\vartheta(N)}{\sqrt{N+1}} & -a^{+}\dfrac{\sin\vartheta(N)}{\sqrt{N+1}} \end{pmatrix} \tag{2.22}$$

and $\mathcal{U}_{\lambda,\epsilon}^{+}$ is its adjoint. The eigenstates of (2.21) are $|n,\pm\rangle$, with $\mathbb{H}_{\lambda,\epsilon}|n,\pm\rangle = E_n^{\pm}|n,\pm\rangle$, justifying the notation used for the energy eigenstates (2.11) and (2.12). They are related to the states $|E_n^{\pm}\rangle$ by the following formulas

$$|E_n^{\pm}\rangle = \mathcal{U}_{\lambda,\epsilon}|n,\pm\rangle, \quad |n,\pm\rangle = \mathcal{U}_{\lambda,\epsilon}^{+}|E_n^{\pm}\rangle, \quad n=0,1,\ldots\ . \tag{2.23}$$

Note that the eigenstate $|E_*\rangle$ is not included in this scheme, and it satisfies

$$\mathcal{U}_{\lambda,\epsilon}^{+}|E_*\rangle = 0. \tag{2.24}$$

Due to this fact, the operator $\mathcal{U}_{\lambda,\epsilon}$ is not unitary in the whole space F, but only when it is restricted to the subspace $F-F_0$.

Let us now make some comments concerning the energy spectrum. First, the eigenstates can be arranged in two groups or "towers" denoted by $\{|E_k^+\rangle\}_{k=0}^{\infty}$ and $\{|E_k^-\rangle\}_{k=0}^{\infty}$, defined in (2.11) and (2.12), as shown in Figs. 1 and 2. Second, we see that the energies E_k^+ are strictly increasing with $k\in\mathbb{N}$ while for the energies E_k^-, there can be some values of λ and ϵ for which the spectrum is not strictly increasing and even may present some degeneracies.[10,11] Our definition of raising and lowering operators will require that both energy spectra will be strictly increasing. It is easy to show that, for example, when $\epsilon=0$, this is always true if we take $\lambda<1+\sqrt{2}$. The two examples shown in Figs. 1 and 2 correspond precisely to strictly increasing energy spectra. A more detailed analysis of the spectrum is carried out in Ref. 11.

Let us analyze now two limit cases which are significant.

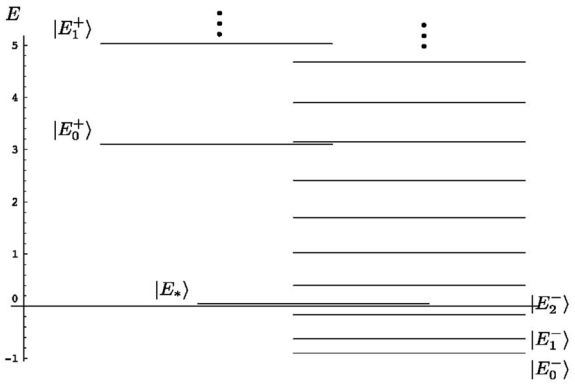

FIG. 2. The two towers of states in the Jaynes-Cummings Hamiltonian for $\epsilon=0.1$, $\lambda=2$

A. Uncoupled system

If we first take the limit for $\lambda \to 0$ of the Jaynes-Cummings Hamiltonian $\mathcal{H}_{\lambda,\epsilon}$, we get immediately, from (2.8),

$$\mathcal{H}_{0,\epsilon}=\begin{pmatrix} (1+\epsilon)N+1+\dfrac{\epsilon}{2} & 0 \\ 0 & (1+\epsilon)N+\dfrac{\epsilon}{2} \end{pmatrix}=(1+\epsilon)\left(N+\frac{1}{2}\right)\mathbb{I}+\frac{1}{2}\sigma_3, \tag{2.25}$$

which is the usual diagonal supersymmetric harmonic oscillator Hamiltonian. The limit process goes properly in the formulas (2.11) and (2.12) and (2.19) and (2.20),

$$|E_n^+\rangle = \xi_\lambda H(-\epsilon)|n,+\rangle + H(\epsilon)|n+1,-\rangle), \quad E_n^+=(1+\epsilon)(n+1)+\frac{|\epsilon|}{2}, \tag{2.26}$$

$$|E_n^-\rangle = H(\epsilon)|n,+\rangle - \xi_\lambda H(-\epsilon)|n+1,-\rangle), \quad E_n^-=(1+\epsilon)(n+1)-\frac{|\epsilon|}{2}, \tag{2.27}$$

even if the operator $\mathcal{U}_{0,\epsilon}$ is not the identity. Indeed, the Hamiltonian $\mathbb{H}_{0,\epsilon}$ is given by

$$\mathbb{H}_{0,\epsilon}=\begin{pmatrix} (1+\epsilon)(N+1)+\dfrac{|\epsilon|}{2} & 0 \\ 0 & (1+\epsilon)(N+1)-\dfrac{|\epsilon|}{2} \end{pmatrix} \tag{2.28}$$

and, using (2.17), the operator $\mathcal{U}_{0,\epsilon}$ is

$$\mathcal{U}_{0,\epsilon}=\begin{pmatrix} \xi_\lambda H(-\epsilon) & H(\epsilon) \\ a^+\dfrac{H(\epsilon)}{\sqrt{N+1}} & -\xi_\lambda a^+\dfrac{H(-\epsilon)}{\sqrt{N+1}} \end{pmatrix}. \tag{2.29}$$

B. Zero detuning

The second special case is obtained when $\epsilon \to 0$, i.e., when the detuning between the atom and the field is zero. The Hamiltonian in (2.8) thus becomes

$$\mathcal{H}_{\lambda,0}=\begin{pmatrix} N+1 & \lambda a \\ \lambda a^{+} & N \end{pmatrix}. \tag{2.30}$$

Using (2.17), we easily find, from (2.10)–(2.12), the eigenstates and eigenvalues of $\mathcal{H}_{\lambda,0}$ as

$$|E_{*}\rangle=|0,-\rangle, \quad E_{*}=0, \tag{2.31}$$

$$|E_{n}^{+}\rangle=\frac{\sqrt{2}}{2}(\xi_{\lambda}|n,+\rangle+|n+1,-\rangle), \quad E_{n}^{+}=n+1+|\lambda|\sqrt{n+1}, \tag{2.32}$$

$$|E_{n}^{-}\rangle=\frac{\sqrt{2}}{2}(|n,+\rangle-\xi_{\lambda}|n+1,-\rangle), \quad E_{n}^{-}=n+1-|\lambda|\sqrt{n+1}. \tag{2.33}$$

The diagonalized version of $\mathcal{H}_{\lambda,0}$ is now

$$\mathbb{H}_{\lambda,0}=\mathcal{U}_{\lambda,0}^{+}\mathcal{H}_{\lambda,0}\mathcal{U}_{\lambda,0}=\begin{pmatrix} N+1+|\lambda|\sqrt{N+1} & 0 \\ 0 & N+1-|\lambda|\sqrt{N+1} \end{pmatrix} \tag{2.34}$$

and the operator $\mathcal{U}_{\lambda,0}$ is given by

$$\mathcal{U}_{\lambda,0}=\frac{\sqrt{2}}{2}\begin{pmatrix} \xi_{\lambda} & 1 \\ a^{+}\dfrac{1}{\sqrt{N+1}} & -a^{+}\dfrac{1}{\sqrt{N+1}}\xi_{\lambda} \end{pmatrix}. \tag{2.35}$$

Let us mention finally that the iteration of the two limits $\lambda\to 0$ and $\epsilon\to 0$ is consistent since we have

$$\lim_{\epsilon\to 0}\mathbb{H}_{0,\epsilon}=\lim_{\lambda\to 0}\mathbb{H}_{\lambda,0}=(N+1)\mathbb{I}\equiv\mathbb{H}_{0,0} \tag{2.36}$$

and

$$\lim_{\epsilon\to 0}\mathcal{H}_{0,\epsilon}=\lim_{\lambda\to 0}\mathcal{H}_{\lambda,0}=\begin{pmatrix} N+1 & 0 \\ 0 & N \end{pmatrix}\equiv\mathcal{H}_{0,0}. \tag{2.37}$$

$\mathbb{H}_{0,0}$ and $\mathcal{H}_{0,0}$ can be related through the operator given in (2.29). Let us mention that the limit Hamiltonian $\mathcal{H}_{0,0}$ admits a degenerated energy spectrum, since in this particular case we have $E_{n}^{+}=E_{n}^{-}=n+1$.

III. RAISING AND LOWERING OPERATORS FOR THE JAYNES-CUMMINGS MODEL

A. General results

Since the energy eigenstates are organized in two towers, we want to find ladder operators which move them up or down without mixing them. This means that a lowering operator $\mathcal{M}_{\lambda,\epsilon}^{-}$ will satisfy the following relations:

$$\mathcal{M}_{\lambda,\epsilon}^{-}|E_{*}\rangle=0, \tag{3.1}$$

and

$$\mathcal{M}_{\lambda,\epsilon}^{-}|E_{n}^{\pm}\rangle=k_{\pm}(n)|E_{n-1}^{\pm}\rangle, \quad n\in\mathbb{N}. \tag{3.2}$$

We are assuming that $k_{\pm}(0)=0$ as a kind of initial condition for determining $k_{\pm}(n)$. The corresponding raising operator $\mathcal{M}^{+}_{\lambda,\epsilon}$ will be the adjoint of the lowering operator. To realize this task, it is useful to work with the diagonalized version of the model since the corresponding lowering operator $\mathbb{M}^{-}_{\lambda,\epsilon}=\mathcal{U}^{+}_{\lambda,\epsilon}\mathcal{M}^{-}_{\lambda,\epsilon}\mathcal{U}_{\lambda,\epsilon}$ satisfies

$$\mathbb{M}^{-}_{\lambda,\epsilon}|n,\pm\rangle = k_{\pm}(n)|n-1,\pm\rangle, \quad n\in\mathbb{N}. \tag{3.3}$$

Let us mention that the condition (3.1) may be written as

$$\mathcal{M}^{-}_{\lambda,\epsilon}|E_{*}\rangle = \mathcal{U}_{\lambda,\epsilon}\mathbb{M}^{-}_{\lambda,\epsilon}\mathcal{U}^{+}_{\lambda,\epsilon}|E_{*}\rangle = 0, \tag{3.4}$$

which is identically satisfied due to the relation (2.24).

Using the well-known relationships

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^{+}|n\rangle = \sqrt{n+1}|n+1\rangle, \tag{3.5}$$

$$g(N)a = ag(N-1), \quad g(N)a^{+} = a^{+}g(N+1), \tag{3.6}$$

it is easy to get, from (3.3),

$$\mathbb{M}^{-}_{\lambda,\epsilon} = \begin{pmatrix} \dfrac{k_{+}(N+1)}{\sqrt{N+1}}a & 0 \\ 0 & \dfrac{k_{-}(N+1)}{\sqrt{N+1}}a \end{pmatrix}. \tag{3.7}$$

The expression of $\mathcal{M}^{-}_{\lambda,\epsilon}$ in the original model will be

$$\mathcal{M}^{-}_{\lambda,\epsilon} = \mathcal{U}_{\lambda,\epsilon}\mathbb{M}^{-}_{\lambda,\epsilon}\mathcal{U}^{+}_{\lambda,\epsilon} = \begin{pmatrix} m_1(N)a & m_2(N)a^2 \\ m_3(N) & m_4(N)a \end{pmatrix}, \tag{3.8}$$

where the functions $m_i(n)$ are given by

$$m_1(n) = \frac{\sin\vartheta(n)\sin\vartheta(n+1)k_{+}(n+1) + \cos\vartheta(n)\cos\vartheta(n+1)k_{-}(n+1)}{\sqrt{n+1}}, \tag{3.9}$$

$$m_2(n) = \frac{\sin\vartheta(n)\cos\vartheta(n+1)k_{+}(n+1) - \cos\vartheta(n)\sin\vartheta(n+1)k_{-}(n+1)}{\sqrt{n+1}\sqrt{n+2}}, \tag{3.10}$$

$$m_3(n) = \cos\vartheta(n-1)\sin\vartheta(n)k_{+}(n) - \sin\vartheta(n-1)\cos\vartheta(n)k_{-}(n), \tag{3.11}$$

$$m_4(n) = \frac{\cos\vartheta(n-1)\cos\vartheta(n)k_{+}(n) + \sin\vartheta(n-1)\sin\vartheta(n)k_{-}(n)}{\sqrt{n+1}}. \tag{3.12}$$

Note that the relations on the functions $m_3(n)$ and $m_4(n)$ are, in principle, valid only for $n>0$, due to the presence of $\cos\vartheta(n-1)$ and $\sin\vartheta(n-1)$. Nevertheless, the quantities $\cos\vartheta(-1)$ and $\sin\vartheta(-1)$, make also sense, as it was shown in (2.17).

B. Particular cases

In the special case $\lambda=0$, we easily find

$$\mathcal{M}^{-}_{0,\epsilon}=\begin{pmatrix} \dfrac{H(\epsilon)k_{-}(N+1)+H(-\epsilon)k_{+}(N+1)}{\sqrt{N+1}}a & 0 \\ 0 & \dfrac{H(\epsilon)k_{+}(N)+H(-\epsilon)k_{-}(N)}{\sqrt{N+1}}a \end{pmatrix}. \tag{3.13}$$

When we take $\epsilon=0$, the annihilator $\mathcal{M}^{-}_{\lambda,0}$ is

$$\mathcal{M}^{-}_{\lambda,0}=\begin{pmatrix} \dfrac{k_{+}(N+1)+k_{-}(N+1)}{2\sqrt{N+1}}a & \xi_{\lambda}\dfrac{k_{+}(N+1)-k_{-}(N+1)}{2\sqrt{N+1}\sqrt{N+2}}a^{2} \\ \xi_{\lambda}\dfrac{k_{+}(N)-k_{-}(N)}{2} & \dfrac{k_{+}(N)+k_{-}(N)}{2\sqrt{N+1}}a \end{pmatrix}. \tag{3.14}$$

The results presented up to now are completely general, but the two functions $k_{\pm}(n)$ are not fixed at all. Therefore, in order to solve this problem, in the next section some extra requirements will be imposed to determine the functions $k_{\pm}(n)$, which are supposed to be complex in general. These will be related to conditions on the products of the ladder operators which we write as

$$\mathbb{M}^{+}_{\lambda,\epsilon}\mathbb{M}^{-}_{\lambda,\epsilon}=\begin{pmatrix} |k_{+}(N)|^{2} & 0 \\ 0 & |k_{-}(N)|^{2} \end{pmatrix}, \quad \mathbb{M}^{-}_{\lambda,\epsilon}\mathbb{M}^{+}_{\lambda,\epsilon}=\begin{pmatrix} |k_{+}(N+1)|^{2} & 0 \\ 0 & |k_{-}(N+1)|^{2} \end{pmatrix}. \tag{3.15}$$

IV. CONDITIONS ON THE COMMUTATOR OF THE LADDER OPERATORS

In this section, ladder operators are obtained by imposing two different constraints on the value of the commutator of the two ladder operators. First, the commutator is assumed to be the identity operator, and second, it is assumed to be the Hamiltonian itself.

A. The commutator is the identity operator

That situation will be the most similar to the harmonic oscillator, and taking

$$[\mathbb{M}^{-}_{\lambda,\epsilon},\mathbb{M}^{+}_{\lambda,\epsilon}]=\mathbb{I}, \tag{4.1}$$

we get the following relations:

$$|k_{\pm}(n+1)|^{2}-|k_{\pm}(n)|^{2}=1, \tag{4.2}$$

together with the initial condition $k_{\pm}(0)=0$. The general solution is thus

$$k_{\pm}(n)=e^{i\varphi_{\pm}(n)}\sqrt{n}, \tag{4.3}$$

where the phases $\varphi_{\pm}(n)$ are not yet fixed. Therefore the annihilation operator (3.7) is nothing else than

$$\mathbb{M}^{-}_{\lambda,\epsilon}=\begin{pmatrix} e^{i\varphi_{+}(N+1)}a & 0 \\ 0 & e^{i\varphi_{-}(N+1)}a \end{pmatrix}. \tag{4.4}$$

The explicit expression of the original operator $\mathcal{M}^{-}_{\lambda,\epsilon}$ is thus given by (3.8) where the functions $m_{i}(N)$ are now

$$m_1(N)=\frac{1}{2}\frac{e^{i\varphi_+(N+1)}\sqrt{q(N+1)-\frac{\epsilon}{2}}\sqrt{q(N+2)-\frac{\epsilon}{2}}+e^{i\varphi_-(N+1)}\sqrt{q(N+1)+\frac{\epsilon}{2}}\sqrt{q(N+2)+\frac{\epsilon}{2}}}{\sqrt{q(N+1)q(N+2)}},$$

$$m_2(N)=\frac{\xi_\lambda}{2}\frac{e^{i\varphi_+(N+1)}\sqrt{q(N+1)-\frac{\epsilon}{2}}\sqrt{q(N+2)+\frac{\epsilon}{2}}-e^{i\varphi_-(N+1)}\sqrt{q(N+1)+\frac{\epsilon}{2}}\sqrt{q(N+2)-\frac{\epsilon}{2}}}{\sqrt{N+2}\sqrt{q(N+1)q(N+2)}},$$

$$m_3(N)=\frac{\xi_\lambda}{2}\sqrt{N}\frac{e^{i\varphi_+(N)}\sqrt{q(N)+\frac{\epsilon}{2}}\sqrt{q(N+1)-\frac{\epsilon}{2}}-e^{i\varphi_-(N)}\sqrt{q(N)-\frac{\epsilon}{2}}\sqrt{q(N+1)+\frac{\epsilon}{2}}}{\sqrt{q(N)q(N+1)}},$$

$$m_4(N)=\frac{1}{2}\sqrt{\frac{N}{N+1}}\frac{e^{i\varphi_+(N)}\sqrt{q(N)+\frac{\epsilon}{2}}\sqrt{q(N+1)+\frac{\epsilon}{2}}+e^{i\varphi_-(N)}\sqrt{q(N)-\frac{\epsilon}{2}}\sqrt{q(N+1)-\frac{\epsilon}{2}}}{\sqrt{q(N)q(N+1)}}.$$

Let us also mention that, due to (4.4), we have $\mathbb{M}^+_{\lambda,\epsilon}\mathbb{M}^-_{\lambda,\epsilon}=N\mathbb{I}$ and $\mathbb{M}^-_{\lambda,\epsilon}\mathbb{M}^+_{\lambda,\epsilon}=(N+1)\mathbb{I}$. The original annihilation and creation operators thus satisfy

$$\mathcal{M}^+_{\lambda,\epsilon}\mathcal{M}^-_{\lambda,\epsilon}=\begin{pmatrix}N & 0\\ 0 & N-1\end{pmatrix},\quad \mathcal{M}^-_{\lambda,\epsilon}\mathcal{M}^+_{\lambda,\epsilon}=\begin{pmatrix}N+1 & 0\\ 0 & N\end{pmatrix}. \tag{4.5}$$

In the absence of coupling between the atom and the field ($\lambda=0$), using (3.13) and (4.3) we get the following diagonal annihilation operator:

$$\mathcal{M}^-_{0,\epsilon}=\begin{pmatrix}G_-(N+1)a & 0\\ 0 & \sqrt{\frac{N}{N+1}}G_+(N)a\end{pmatrix}, \tag{4.6}$$

where

$$G_+(N)=e^{i\varphi_+(N)}H(\epsilon)+e^{i\varphi_-(N)}H(-\epsilon),\quad G_-(N)=e^{i\varphi_-(N)}H(\epsilon)+e^{i\varphi_+(N)}H(-\epsilon). \tag{4.7}$$

Moreover, we have

$$\mathcal{H}_{0,\epsilon}=(1+\epsilon)\mathcal{M}^+_{0,\epsilon}\mathcal{M}^-_{0,\epsilon}+\begin{pmatrix}1+\frac{\epsilon}{2} & 0\\ 0 & 1+\frac{3\epsilon}{2}\end{pmatrix}=(1+\epsilon)\mathcal{M}^-_{0,\epsilon}\mathcal{M}^+_{0,\epsilon}+\begin{pmatrix}-\frac{\epsilon}{2} & 0\\ 0 & \frac{\epsilon}{2}\end{pmatrix}. \tag{4.8}$$

In the case of zero detuning ($\epsilon=0$), using (3.14) and (4.3), we easily get

$$\mathcal{M}^-_{\lambda,0}=\begin{pmatrix}\frac{1}{2}(e^{i\varphi_+(N+1)}+e^{i\varphi_-(N+1)})a & \frac{\xi_\lambda}{2\sqrt{N+2}}(e^{i\varphi_+(N+1)}-e^{i\varphi_-(N+1)})a^2\\ \frac{\xi_\lambda}{2}\sqrt{N}(e^{i\varphi_+(N)}-e^{i\varphi_-(N)}) & \frac{1}{2}\sqrt{\frac{N}{N+1}}(e^{i\varphi_+(N)}+e^{i\varphi_-(N)})a\end{pmatrix}. \tag{4.9}$$

B. The commutator is the Hamiltonian

An alternative choice for $k_\pm(n)$ is obtained when we take

$$[\mathcal{M}^-_{\lambda,\epsilon},\mathcal{M}^+_{\lambda,\epsilon}]=\mathcal{H}_{\lambda,\epsilon} \tag{4.10}$$

or equivalently

$$[\mathbb{M}^-_{\lambda,\epsilon},\mathbb{M}^+_{\lambda,\epsilon}]=\mathbb{H}_{\lambda,\epsilon}. \tag{4.11}$$

We thus must solve

$$|k_\pm(n+1)|^2-|k_\pm(n)|^2=E^\pm_n. \tag{4.12}$$

The general solution is

$$k_\pm(0)=0,\quad k_\pm(n)=e^{i\varphi_\pm(n)}\sqrt{\sum_{\ell=0}^{n-1}E^\pm_\ell},\quad n>0. \tag{4.13}$$

The last expresssion can also be written as follows:

$$\begin{aligned}k_\pm(n)&=e^{i\varphi_\pm(n)}\sqrt{\frac{1}{2}(1+\epsilon)n(n+1)\pm\sum_{\ell=0}^{n-1}q(\ell+1)}\\&=e^{i\varphi_\pm(n)}\sqrt{\frac{1}{2}(1+\epsilon)n(n+1)\pm|\lambda|\sum_{\ell=0}^{n-1}\sqrt{\delta+\ell+1}}\\&=e^{i\varphi_\pm(n)}\sqrt{\frac{1}{2}(1+\epsilon)n(n+1)\pm|\lambda|\left(\zeta\left(-\frac{1}{2},\delta\right)-\zeta\left(-\frac{1}{2},\delta+n\right)\right)},\end{aligned} \tag{4.14}$$

where $\delta=(\epsilon/2\lambda)^2$ and $\zeta(s,a)$ is the generalized Riemann zeta function.

In the case $\lambda=0$, the annihilation operator takes the form (3.13) with

$$(\mathcal{M}^-_{0,\epsilon})_{11}=\frac{1}{\sqrt{2}}G_-(N+1)\sqrt{(1+\epsilon)(N+1)+1}a, \tag{4.15}$$

$$(\mathcal{M}^-_{0,\epsilon})_{22}=\frac{1}{\sqrt{2}}G_+(N)\sqrt{(1+\epsilon)N+\frac{N\epsilon}{N+1}}a, \tag{4.16}$$

where $G_\pm(N)$ were defined in (4.7).

In the case where $\epsilon=0$, we get, from (4.14), the following expressions for $k_\pm(n)$:

$$k_\pm(n)=e^{i\varphi_\pm(n)}\sqrt{\tfrac{1}{2}(n+1)n+1\pm|\lambda|H_n^{(-1/2)}},\quad n>0, \tag{4.17}$$

where $H_n^{\left(-\frac{1}{2}\right)}=\Sigma_{\ell=1}^n\ell^{\frac{1}{2}}$ is a harmonic number of order $\left(-\frac{1}{2}\right)$.

V. FACTORIZATION OF THE JAYNES-CUMMINGS HAMILTONIAN

Another special set of ladder operators, which will be consider next, is the one that leads to the factorization of the Hamiltonian.

A. First type of factorization

Assuming that we have first

$$\mathbb{M}^-_{\lambda,\epsilon}\mathbb{M}^+_{\lambda,\epsilon}=\mathbb{H}_{\lambda,\epsilon}-\begin{pmatrix}\mu_+ & 0\\ 0 & \mu_-\end{pmatrix},\quad \mu_+,\mu_-\in\mathbb{R}, \tag{5.1}$$

we immediately get from (3.15),

$$k_{\pm}(n+1) = e^{i\varphi_{\pm}(n+1)}\sqrt{E_n^{\pm} - \mu_{\pm}}, \quad k_{\pm}(0) = 0. \tag{5.2}$$

If we now take the special case $\lambda = 0$, the annihilator takes the form (3.13), with

$$(\mathcal{M}^-_{0,\epsilon})_{11} = \left[H(\epsilon) e^{i\varphi_-(N+1)} \sqrt{1 + \epsilon - \frac{\epsilon + 2\mu_-}{2(N+1)}} + H(-\epsilon) e^{i\varphi_+(N+1)} \sqrt{1 + \epsilon - \frac{\epsilon + 2\mu_+}{2(N+1)}} \right] a,$$

$$(\mathcal{M}^-_{0,\epsilon})_{22} = \left[H(\epsilon) e^{i\varphi_+(N)} \sqrt{1 + \epsilon - \frac{\epsilon + 2 + 2\mu_+}{2(N+1)}} + H(-\epsilon) e^{i\varphi_-(N)} \sqrt{1 + \epsilon - \frac{\epsilon + 2 + 2\mu_-}{2(N+1)}} \right] a,$$

which leads to the following factorization of the original Hamiltonian:

$$\mathcal{H}_{0,\epsilon} = \mathcal{M}^-_{0,\epsilon}\mathcal{M}^+_{0,\epsilon} + \begin{pmatrix} H(\epsilon)\mu_- + H(-\epsilon)\mu_+ & 0 \\ 0 & H(\epsilon)\mu_+ + H(-\epsilon)\mu_- \end{pmatrix}. \tag{5.3}$$

We also have in this case

$$[\mathcal{M}^-_{0,\epsilon}, \mathcal{M}^+_{0,\epsilon}] = (1+\epsilon)\mathbb{I}. \tag{5.4}$$

Let us observe that if we choose $\mu_+ = \mu_- = -(1+\epsilon)$, then the Hamiltonian is exactly factorized as $\mathcal{H}_{0,\epsilon} = \mathcal{M}^+_{0,\epsilon}\mathcal{M}^-_{0,\epsilon}$, and we get

$$(\mathcal{M}^-_{0,\epsilon})_{11} = G_-(N+1)\sqrt{1 + \epsilon + \frac{1 + \epsilon/2}{N+1}}\, a, \tag{5.5}$$

$$(\mathcal{M}^-_{0,\epsilon})_{22} = G_+(N)\sqrt{1 + \epsilon + \frac{\epsilon/2}{N+1}}\, a, \tag{5.6}$$

with $G_{\pm}(N)$ given in (4.7)

When $\epsilon > 0$, the special choice $\mu_- = -\epsilon/2$ and $\mu_+ = -[1 + (\epsilon/2)]$ gives rise to a particularly simple form of the annihilator, i.e.,

$$\mathcal{M}^-_{0,\epsilon>0} = \sqrt{1+\epsilon}\begin{pmatrix} e^{i\varphi_-(N+1)}a & 0 \\ 0 & e^{i\varphi_+(N)}a \end{pmatrix}. \tag{5.7}$$

Something similar can be done when $\epsilon < 0$, choosing now $\mu_- = -[1 + (\epsilon/2)]$ and $\mu_+ = -\epsilon/2$. In both cases, we can thus write the Hamiltonian as

$$\mathcal{H}_{0,\epsilon} = \mathcal{M}^-_{0,\epsilon}\mathcal{M}^+_{0,\epsilon} - \begin{pmatrix} \frac{\epsilon}{2} & 0 \\ 0 & \left(1 + \frac{\epsilon}{2}\right) \end{pmatrix} = \mathcal{M}^+_{0,\epsilon}\mathcal{M}^-_{0,\epsilon} + \begin{pmatrix} \left(1 + \frac{\epsilon}{2}\right) & 0 \\ 0 & \frac{\epsilon}{2} \end{pmatrix}. \tag{5.8}$$

We get here a result similar to the one obtained in the preceding section when we ask for the commutator of the ladder operators to be the identity. It is expected due to the relation (5.4) but the ladder operators are essentially different because of the presence of the operator $\sqrt{N/(N+1)}$ in (4.6).

When we take $\epsilon = 0$, we get, from (5.2),

$$k_{\pm}(n+1) = e^{i\varphi_{\pm}(n+1)}\sqrt{n + 1 - \mu_{\pm} \pm |\lambda|\sqrt{n+1}}, \tag{5.9}$$

and the form of $\mathcal{M}^-_{\lambda,0}$ is obtained from (3.14). Since we are interested in a factorization of the original Hamiltonian which is nondiagonal in this case, further constraints must be imposed on the unknown quantities $\mu_{\pm}$. Indeed, a diagonal matrix does not remain diagonal, in general, when we

transform it by the operator $\mathcal{U}_{\lambda,0}$. The simplest choice is to take $\mu_{\pm}=0$. Thus we get an exact factorization

$$\mathcal{H}_{\lambda,0}=\mathcal{M}^{-}_{\lambda,0}\mathcal{M}^{+}_{\lambda,0}. \tag{5.10}$$

Changing the order of the factors, we get a new Hamiltonian $\mathcal{H}'_{\lambda,0}=\mathcal{M}^{+}_{\lambda,0}\mathcal{M}^{-}_{\lambda,0}$, whose explicit form in the subspace $F-F_0$ is

$$\mathcal{H}'_{\lambda,0}=\mathcal{M}^{+}_{\lambda,0}\mathcal{M}^{-}_{\lambda,0}=\begin{pmatrix} N & \lambda\sqrt{\dfrac{N}{N+1}}a \\ a^{\dagger}\lambda\sqrt{\dfrac{N}{N+1}} & N-1 \end{pmatrix}. \tag{5.11}$$

The Hamiltonian $\mathcal{H}'_{\lambda,0}$ is in fact isospectral[12] to $\mathcal{H}_{\lambda,0}$. Indeed, its eigenstates are $\mathcal{M}^{+}_{\lambda,0}|E^{\pm}_n\rangle$ with eigenvalues $E^{\pm}_n$ and also the state $E_*\rangle=|0,-\rangle$ with eigenvalue 0. Note that $\mathcal{M}^{+}_{\lambda,0}|E_*\rangle=0$ and therefore it is not an eigenstate of $\mathcal{H}'_{\lambda,0}$.

B. Second type of factorization

It is obtained when we take

$$\mathbb{M}^{+}_{\lambda,\epsilon}\mathbb{M}^{-}_{\lambda,\epsilon}=\mathbb{H}_{\lambda,\epsilon}-\begin{pmatrix}\nu_+ & 0\\ 0 & \nu_-\end{pmatrix}. \tag{5.12}$$

Indeed, the diagonal matrix is now fixed due to the initial condition on the $k_{\pm}(n)$. From (3.15), we get

$$k_{\pm}(n)=e^{i\varphi_{\pm}(n)}\sqrt{E^{\pm}_n-E^{\pm}_0},\quad \nu_{\pm}=E^{\pm}_0, \tag{5.13}$$

so that $k_{\pm}(0)=0$ as expected, although the phases $\varphi_{\pm}(n)$ are not yet fixed.

Here again, if we take $\lambda=0$, we easily get the annihilator $\mathcal{M}^{-}_{0,\epsilon}$ of (3.13) on the form

$$(\mathcal{M}^{-}_{0,\epsilon})_{11}=\sqrt{(1+\epsilon)}G_{-}(N+1)a,\quad (\mathcal{M}^{-}_{0,\epsilon})_{22}=\sqrt{(1+\epsilon)\frac{N}{N+1}}G_{+}(N)a.$$

We thus have

$$\mathcal{H}_{0,\epsilon}=\mathcal{M}^{+}_{0,\epsilon}\mathcal{M}^{-}_{0,\epsilon}+\begin{pmatrix}1+\dfrac{\epsilon}{2} & 0\\ 0 & 1+\dfrac{3\epsilon}{2}\end{pmatrix}=\mathcal{M}^{-}_{0,\epsilon}\mathcal{M}^{+}_{0,\epsilon}+\begin{pmatrix}-\dfrac{\epsilon}{2} & 0\\ 0 & \dfrac{\epsilon}{2}\end{pmatrix}. \tag{5.14}$$

When $\epsilon=0$, we have $E^{\pm}_n-E^{\pm}_0=n\pm|\lambda|(\sqrt{n+1}-1)$ and

$$\mathbb{M}^{-}_{\lambda,0}=\begin{pmatrix} e^{i\varphi_+(N+1)}\sqrt{\dfrac{N+1+|\lambda|(\sqrt{N+2}-1)}{N+1}}a & 0\\ 0 & e^{i\varphi_-(N+1)}\sqrt{\dfrac{N+1-|\lambda|(\sqrt{N+2}-1)}{N+1}}a\end{pmatrix}, \tag{5.15}$$

but the original Hamiltonian cannot be factorized in this case (except when λ is also equal to zero) since the transformation by the operator $\mathcal{U}_{\lambda,0}$ affects the constant diagonal matrix appearing in (5.12).

Note that the exact factorization for the zero detuning $\epsilon=0$ and strong coupling $\lambda=1$ encountered in the literature[13] does not contradict our result. Indeed, we can show that for $\lambda=1+\epsilon$ the Jaynes-Cummings Hamiltonian can be written as

$$\mathcal{H}_{(1+\epsilon),\epsilon}=(1+\epsilon)\mathcal{A}^{+}\mathcal{A}^{-}-\frac{\epsilon}{2}\sigma_3 \tag{5.16}$$

with

$$\mathcal{A}^{-}=\begin{pmatrix} a & 0 \\ 1 & a \end{pmatrix}. \tag{5.17}$$

The operators $\mathcal{A}^{+}$ and $\mathcal{A}^{-}$ have been introduced as some ladder operators for supersymmetric harmonic oscillator.[13,14] The operator $\mathcal{A}^{-}$ has a form similar to the general $\mathcal{M}^{-}_{\lambda,\epsilon}$ in (3.8). Nevertheless, it is not an annihilation operator for our model, as it could be easily checked from (3.2), even if $\epsilon=0$.

VI. GENERAL SETS OF COHERENT STATES

Our annihilation operators $\mathcal{M}^{-}_{\lambda,\epsilon}$ may be used to construct new sets of coherent states for the Jaynes-Cummings system. A detailed analysis of these sets and the corresponding physical properties is beyond the scope of this paper and will be presented elsewhere. Nevertheless, we will insist here on the general construction taking place into the Gazeau-Klauder scheme[15] and also its vector coherent states generalization.[16] We will also illustrate it with some specific examples which connect the new states with preceding approaches.[7,10,17]

A. General results

Let us introduce the following notation for the coherent states: $|z;\boldsymbol{\alpha};\boldsymbol{\theta}\rangle_{\lambda,\epsilon}$, where $z\in\mathbb{C}$ is the usual label for a coherent state, $\boldsymbol{\alpha}=(\alpha_+,\alpha_-)$ and $\boldsymbol{\theta}=(\theta,\phi)$ are two sets of real parameters that will be specified later, $\boldsymbol{\alpha}$ related to the temporal evolution and $\boldsymbol{\theta}$ related to the normalization. As usual, these states are defined as the eigenstates of the annihilator, that is

$$\mathcal{M}^{-}_{\lambda,\epsilon}|z;\boldsymbol{\alpha};\boldsymbol{\theta}\rangle_{\lambda,\epsilon}=z|z;\boldsymbol{\alpha};\boldsymbol{\theta}\rangle_{\lambda,\epsilon}. \tag{6.1}$$

Once we decompose $|z;\boldsymbol{\alpha};\boldsymbol{\theta}\rangle_{\lambda,\epsilon}$ in the basis of the eigenstates (2.10)–(2.12) of $\mathcal{H}_{\lambda,\epsilon}$ as

$$|z;\boldsymbol{\alpha};\boldsymbol{\theta}\rangle_{\lambda,\epsilon}=C_{*}(z)|E_{*}\rangle+\sum_{n=0}^{\infty}\left(C_n^{+}(z)|E_n^{+}\rangle+C_n^{-}(z)|E_n^{-}\rangle\right) \tag{6.2}$$

and insert this expression in (6.1), using (3.1) and (3.2), we find $C_{*}(z)=0$ and

$$C_n^{\pm}(z)=\frac{z^n}{\rho_{\pm}(n)}C_0^{\pm}(z),\quad n>0, \tag{6.3}$$

with

$$\rho_{\pm}(n)=k_{\pm}(1)k_{\pm}(2)\cdots k_{\pm}(n). \tag{6.4}$$

The coherent states take the form

$$|z;\boldsymbol{\alpha};\boldsymbol{\theta}\rangle_{\lambda,\epsilon}=\sum_{n=0}^{\infty}z^n\left(\frac{C_0^{+}(z)}{\rho_{+}(n)}|E_n^{+}\rangle+\frac{C_0^{-}(z)}{\rho_{-}(n)}|E_n^{-}\rangle\right), \tag{6.5}$$

if we set $\rho_{\pm}(0)=1$. Let us mention now that there are three coherent states associated to the value $z=0$, $|E_{*}\rangle$, $|E_0^{+}\rangle$, and $|E_0^{+}\rangle$.

Taking into account that from (2.5) the time-dependent Schrödinger equation for the Hamiltonian $\mathcal{H}_{\lambda,\epsilon}$ is

$$\mathcal{H}_{\lambda,\epsilon}|\psi\rangle = -i\frac{\partial}{\partial(\omega_0 t)}|\psi\rangle, \tag{6.6}$$

the temporal evolution of these coherent states is obtained as

$$\begin{aligned} U(t)|z;\boldsymbol{\alpha};\boldsymbol{\theta}\rangle_{\lambda,\epsilon} &= e^{-i\omega_0 t\mathcal{H}_{\lambda,\epsilon}}|z;\boldsymbol{\alpha};\boldsymbol{\theta}\rangle_{\lambda,\epsilon} \\ &= \sum_{n=0}^{\infty} z^n\left(\frac{C_0^+(z)}{\rho_+(n)}e^{-i\omega_0 tE_n^+}|E_n^+\rangle + \frac{C_0^-(z)}{\rho_-(n)}e^{-i\omega_0 tE_n^-}|E_n^-\rangle\right). \end{aligned} \tag{6.7}$$

Additional constraints can now be imposed to fix the undetermined functions appearing in such states. First, let us recall that the functions $k_\pm(n)$ in (6.4) have been determined up to a phase $\varphi_\pm(n)$, and a way to fix them is to ask for the temporal stability[15] of the coherent states (6.5), which in our case means that

$$U(t)|z;\boldsymbol{\alpha};\boldsymbol{\theta}\rangle_{\lambda,\epsilon} = U(t)|z;\alpha_+,\alpha_-;\boldsymbol{\theta}\rangle_{\lambda,\epsilon} = |z;\alpha_+ + t,\alpha_- + t;\boldsymbol{\theta}\rangle_{\lambda,\epsilon}. \tag{6.8}$$

Indeed, taking into account what has been done in the two preceding sections, we first write

$$k_\pm(n) = e^{i\varphi_\pm(n)}k_\pm^0(n), \tag{6.9}$$

where $k_\pm^0(n)$ are now real functions, and then, from (6.4), we get

$$\rho_\pm(n) = e^{i\Sigma_{\ell=1}^n\varphi_\pm(\ell)}\prod_{\ell=1}^n k_\pm^0(\ell) = e^{i\Sigma_{\ell=1}^n\varphi_\pm(\ell)}\rho_\pm^0(n),\ \rho_\pm(0) = 1, \tag{6.10}$$

$\rho_\pm^0(n)$ being real functions. The states (6.5) may be written as

$$|z;\alpha_+,\alpha_-;\boldsymbol{\theta}\rangle_{\lambda,\epsilon} = C_0^+(z)|E_0^+\rangle + C_0^-(z)|E_0^-\rangle + \sum_{n=1}^{\infty} z^n\left(\frac{C_0^+(z)}{\rho_+^0(n)}e^{-i\Sigma_{\ell=1}^n\varphi_+(\ell)}|E_n^+\rangle + \frac{C_0^-(z)}{\rho_-^0(n)}e^{-i\Sigma_{\ell=1}^n\varphi_-(\ell)}|E_n^-\rangle\right), \tag{6.11}$$

where the presence of the phases is now explicit. It can be proved that the temporal stability (6.8) is assured by choosing the, up to now, arbitrary phases to be linear functions of the real parameters $\alpha_\pm$, more precisely,

$$\varphi_\pm(\ell) = \omega_0\alpha_\pm(E_\ell^\pm - E_{\ell-1}^\pm) = \omega_0(1 + \epsilon \pm [q(\ell+1) - q(\ell)])\alpha_\pm, \tag{6.12}$$

so that

$$\sum_{\ell=1}^{n}\varphi_\pm(\ell) = \omega_0\alpha_\pm(E_n^\pm - E_0^\pm). \tag{6.13}$$

If we redefine

$$K_0^\pm(z) = C_0^\pm(z)e^{i\omega_0\alpha_\pm E_0^\pm}, \tag{6.14}$$

the coherent states (6.11) will now take the form

$$|z;\alpha_+,\alpha_-;\boldsymbol{\theta}\rangle_{\lambda,\epsilon} = \sum_{n=0}^{\infty} z^n\left(\frac{K_0^+(z)}{\rho_+^0(n)}e^{-i\omega_0\alpha_+E_n^+}|E_n^+\rangle + \frac{K_0^-(z)}{\rho_-^0(n)}e^{-i\omega_0\alpha_-E_n^-}|E_n^-\rangle\right). \tag{6.15}$$

Note first that, due to the form of the eigenstates $|E_n^{\pm}\rangle$ in the Fock space F, we deal with vector coherent states.[16] More precisely, using (2.23), we can observe that the states (6.15) may be written using similar matrix decomposition as in Ref. 16, i.e.,

$$|z;\alpha_+,\alpha_-;\boldsymbol{\theta}\rangle_{\lambda,\epsilon}=\sum_{n=0}^{\infty}\mathcal{U}_{\lambda,\epsilon}\begin{pmatrix}\dfrac{1}{\rho_+^0(n)} & 0\\ 0 & \dfrac{1}{\rho_-^0(n)}\end{pmatrix}\begin{pmatrix}z & 0\\ 0 & z\end{pmatrix}^n \exp\left[-i\begin{pmatrix}\omega_0\alpha_+E_n^+ & 0\\ 0 & \omega_0\alpha_+E_n^-\end{pmatrix}\right]$$
$$\times\left\{K_0^+(z)\begin{pmatrix}|n\rangle\\ 0\end{pmatrix}+K_0^-(z)\begin{pmatrix}0\\ |n\rangle\end{pmatrix}\right\}, \tag{6.16}$$

where $\mathcal{U}_{\lambda,\epsilon}$ is the operator given in (2.22).

Second, the normalization to unity of the states (6.15) leads to the following condition on the quantities $K_0^{\pm}(z)$:

$$|K_0^+(z)|^2\left(\sum_{n=0}^{\infty}\frac{|z|^{2n}}{(\rho_+^0(n))^2}\right)+|K_0^-(z)|^2\left(\sum_{n=0}^{\infty}\frac{|z|^{2n}}{(\rho_-^0(n))^2}\right)=1. \tag{6.17}$$

Introducing now the positive real functions $K^+(z)$ and $K^-(z)$, defined as

$$K^{\pm}(z)=\left(\sum_{n=0}^{\infty}\frac{|z|^{2n}}{(\rho_{\pm}^0(n))^2}\right)^{-1/2}, \tag{6.18}$$

where

$$K_0^+(z)=K^+(z)\cos\,\theta,\quad K_0^-(z)=K^-(z)e^{i\phi}\sin\,\theta,\quad \theta\in[0,\pi],\quad \phi\in[0,2\pi). \tag{6.19}$$

We can write the final form of the general coherent states (6.15), which now contain the variables $\boldsymbol{\theta}=(\theta,\phi)\in S^2$ parametrizing the unit sphere, as

$$|z;\alpha_+,\alpha_-;\theta,\phi\rangle_{\lambda,\epsilon}=K^+(z)\cos\,\theta\left(\sum_{n=0}^{\infty}\frac{z^n}{\rho_+^0(n)}e^{-i\omega_0\alpha_+E_n^+}|E_n^+\rangle\right)+K^-(z)e^{i\phi}\sin\,\theta\left(\sum_{n=0}^{\infty}\frac{z^n}{\rho_-^0(n)}e^{-i\omega_0\alpha_-E_n^-}|E_n^-\rangle\right). \tag{6.20}$$

At this moment it is important to insist on the fact that the coherent states we have do not depend only on the complex number z, as it is usual, but also on the variables $\boldsymbol{\theta}\in S^2$. Therefore, the space parametrizing our coherent states is $\mathbb{C}\times S^2$.

Let us mention also that the mean value of the Jaynes-Cummings energy in those states is given by

$$\langle\mathcal{H}_{\lambda,\epsilon}\rangle=(K^+(z))^2\cos^2\,\theta\left(\sum_{n=0}^{\infty}E_n^+\frac{|z|^{2n}}{(\rho_+^0(n))^2}\right)+(K^-(z))^2\sin^2\,\theta\left(\sum_{n=0}^{\infty}E_n^-\frac{|z|^{2n}}{(\rho_-^0(n))^2}\right). \tag{6.21}$$

To be more precise on the results, it is necessary to fix the values of the functions $K^{\pm}(z)$; and to do that, it is necessary to consider the particular examples studied in the previous section, some of which are studied next.

B. Examples

Example 1: The commutator of the ladder operators is the identity. Let us take the ladder operators such that the commutator is the identity. In this case, from (6.3), (6.9), and (6.10), we find

$$\rho_{\pm}^{0}(n)=\sqrt{n!},\quad K^{\pm}(z)=e^{-|z|^2/2} \tag{6.22}$$

and the coherent states (6.20) may be written as

$$|z;\alpha_+,\alpha_-;\theta,\phi\rangle_{\lambda,\epsilon}=e^{-|z|^2/2}\left[\cos\,\theta\left(\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}e^{-i\omega_0\alpha_+E_n^+}|E_n^+\rangle\right)+\sin\,\theta e^{i\phi}\left(\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}e^{-i\omega_0\alpha_-E_n^-}|E_n^-\rangle\right)\right]. \tag{6.23}$$

Taking into account the explicit form (2.19) and (2.20) of the energies $E_n^{\pm}$, the mean value (6.21) is thus

$$\langle\mathcal{H}_{\lambda,\epsilon}\rangle=(1+\epsilon)(1+|z|^2)+e^{-|z|^2}\left(\sum_{n=0}^{\infty}q(n+1)\frac{|z|^{2n}}{n!}\right)\cos 2\theta. \tag{6.24}$$

For a large number of photons, i.e., $|z|\to\infty$, it has been shown[7] that we get

$$\langle\mathcal{H}_{\lambda,0}\rangle\to 1+|z|^2+|\lambda||z|\cos 2\theta. \tag{6.25}$$

Note that the coherent states given in Ref. 7 are a special case of (6.30) when $\alpha_{\pm}=0$. This means that they do not satisfy the temporal stability given in (6.8). Let us mention that other relevant mean values have been given also in Ref. 7.

For the special case when $\lambda=0$ and $\epsilon>0$ (the case $\epsilon<0$ will be similar), we get explicitly the annihilation operator (6.6),

$$\mathcal{M}_{0,\epsilon}^{-}=\begin{pmatrix} e^{i(1+\epsilon)\omega_0\alpha_-}a & 0 \\ 0 & e^{i(1+\epsilon)\omega_0\alpha_+}\sqrt{\dfrac{N}{N+1}}a \end{pmatrix}. \tag{6.26}$$

Moreover, since we have $E_n^{\pm}=(1+\epsilon)(n+1)\pm(\epsilon/2)$ and the energy eigenstates are given by $\{|E_n^+\rangle=|n+1,-\rangle,|E_n^-\rangle=|n,+\rangle\}$, we get

$$|z;\alpha_+,\alpha_-;\theta,\phi\rangle_{0,\epsilon}=e^{-|z|^2/2}\left[\cos\,\theta e^{-i\omega_0[1+(3\epsilon/2)]\alpha_+}\left(\sum_{n=0}^{\infty}\frac{(ze^{-i\omega_0(1+\epsilon)\alpha_+})^n}{\sqrt{n!}}|n+1,-\rangle\right)\right.$$
$$\left.+\sin\,\theta e^{i\phi}e^{-i\omega_0[1+(\epsilon/2)]\alpha_-}\left(\sum_{n=0}^{\infty}\frac{(ze^{-i\omega_0(1+\epsilon)\alpha_-})^n}{\sqrt{n!}}|n,+\rangle\right)\right]. \tag{6.27}$$

These are generalized coherent states of the supersymmetric harmonic oscillator $\mathcal{H}_{0,\epsilon}$ and the mean value of the energy is directly obtained through (6.24) [or through the factorization (6.8)] as

$$\langle\mathcal{H}_{0,\epsilon}\rangle=(1+\epsilon)(1+|z|^2)+\frac{\epsilon}{2}\cos 2\theta. \tag{6.28}$$

For the special case when $\epsilon=0$ the eigenstates and eigenvalues are given in (2.31)–(2.33) and using (6.12)

$$\varphi_{\pm}(n)=\omega_0(1\pm|\lambda|(\sqrt{n+1}-\sqrt{n}))\alpha_{\pm}. \tag{6.29}$$

The annihilator is given as (4.9) and the coherent states (6.23) thus take the form

$$|z;\alpha_+,\alpha_-;\theta,\phi\rangle_{\lambda,0}=\frac{\sqrt{2}}{2}e^{-|z|^2/2}\left[\cos\,\theta e^{-i\omega_0\alpha_+}\left(\sum_{n=0}^{\infty}\frac{(ze^{-i\omega_0\alpha_+})^n}{\sqrt{n!}}e^{-i\omega_0|\lambda|\sqrt{n+1}\alpha_+}(\xi_\lambda|n,+\rangle+|n+1,-\rangle)\right)\right.$$
$$\left.+\sin\,\theta e^{i(\phi-\omega_0\alpha_-)}\left(\sum_{n=0}^{\infty}\frac{(ze^{-i\omega_0\alpha_-})^n}{\sqrt{n!}}e^{i\omega_0|\lambda|\sqrt{n+1}\alpha_-}(|n,+\rangle-\xi_\lambda|n+1,-\rangle)\right)\right] \quad (6.30)$$

and the mean value of the energy is given as

$$\langle\mathcal{H}_{\lambda,0}\rangle=1+|z|^2+|\lambda|e^{-|z|^2}\cos 2\theta\left(\sum_{n=0}^{\infty}\sqrt{n+1}\frac{|z|^{2n}}{n!}\right). \quad (6.31)$$

Example 2: The Hamiltonian is factorized. Next, some annihilators dealing with the factorization of the Jaynes-Cummings Hamiltonian will be considered. Indeed, we first take the annihilator (5.7) which led to the factorization (5.8). In this case, we have $\varphi_\pm(\ell)=\omega_0(1+\epsilon)\alpha_\pm$. Thus, from (5.2) with $\mu_-=-\epsilon/2$ and $\mu_+=-[1+(\epsilon/2)]$, we get

$$k_+(n)=e^{i\omega_0(1+\epsilon)\alpha_+}\sqrt{(1+\epsilon)(n+1)},\quad k_-(n)=e^{i\omega_0(1+\epsilon)\alpha_-}\sqrt{(1+\epsilon)n} \quad (6.32)$$

and

$$\rho_+^0(n)=(1+\epsilon)^{n/2}\sqrt{(n+1)!},\quad \rho_-^0(n)=(1+\epsilon)^{n/2}\sqrt{n!}. \quad (6.33)$$

Moreover, we have

$$K^+(z)=\left(\frac{|\zeta|^2}{e^{|\zeta|^2}-1}\right)^{1/2},\quad K^-(z)=e^{-|\zeta|^2/2}, \quad (6.34)$$

introducing the new variable $\zeta=z/\sqrt{1+\epsilon}$. The coherent states are explicitly given as

$$|z;\alpha_+,\alpha_-;\theta,\phi\rangle_{0,\epsilon}=\left(\frac{\bar{\zeta}\zeta}{e^{|\zeta|^2}-1}\right)^{1/2}\cos\,\theta e^{-i\omega_0(\epsilon/2)\alpha_+}\left(\sum_{n=1}^{\infty}\frac{(\zeta e^{-i\omega_0(1+\epsilon)\alpha_+})^n}{\sqrt{n!}}|n,-\rangle\right)$$
$$+e^{-|z|^2/2}\sin\,\theta e^{i\phi}e^{-i\omega_0[1+(\epsilon/2)]\alpha_-}\left(\sum_{n=0}^{\infty}\frac{(\zeta e^{-i\omega_0(1+\epsilon)\alpha_-})^n}{\sqrt{n!}}|n,+\rangle\right), \quad (6.35)$$

which are closely related to the usual harmonic oscillator coherent states. The mean value of the energy in these coherent states is easily obtained through the factorization (5.8),

$$\langle\mathcal{H}_{0,\epsilon}\rangle=|z|^2+\frac{1+\epsilon}{2}-\frac{1}{2}\cos 2\theta. \quad (6.36)$$

Let us finally mention that when the ladder operators factorize the diagonalized Hamiltonian $\mathbb{H}_{\lambda,\epsilon}$, as in (5.12), we find the coherent states constructed in Ref. 10. In this case, we have $k_\pm^0(n)=\sqrt{E_n^\pm-E_0^\pm}$ and

$$\rho_\pm^0(n)=\sqrt{\prod_{\ell=1}^{n}(E_\ell^\pm-E_0^\pm)}. \quad (6.37)$$

C. The resolution of the identity

To end this section, we will analyze the completeness (in fact, the overcompleteness) of the systems of coherent states we have studied before. In order to accomplish this goal, we must compute the resolution of the identity,[10,12,15] which can be written here as

$$I = |E_*\rangle\langle E_*| + \int (|z;\boldsymbol{\alpha};\boldsymbol{\theta}\rangle_{\lambda,\epsilon})({}_{\lambda,\epsilon}\langle z;\boldsymbol{\alpha};\boldsymbol{\theta}|)\mathrm{d}\mu(z;\boldsymbol{\alpha};\boldsymbol{\theta}), \tag{6.38}$$

where the measure $\mathrm{d}\mu(z;\boldsymbol{\alpha};\boldsymbol{\theta})$ could be determined through different special cases. The matrix operator appearing here can be written as follows:

$$(|z;\boldsymbol{\alpha};\boldsymbol{\theta}\rangle_{\lambda,\epsilon})({}_{\lambda,\epsilon}\langle z;\boldsymbol{\alpha};\boldsymbol{\theta}|) = (K^+(z))^2\cos^2\theta\sum_{n=0}^{\infty}\frac{|z|^{2n}}{(\rho_+^0(n))^2}|E_n^+\rangle\langle E_n^+| \tag{6.39}$$

$$+ (K^-(z))^2\sin^2\theta\sum_{n=0}^{\infty}\frac{|z|^{2n}}{(\rho_-^0(n))^2}|E_n^-\rangle\langle E_n^-| \tag{6.40}$$

$$+ (K^+(z))^2\cos^2\theta\sum_{n\neq m}^{\infty}\frac{z^n\overline{z}^m}{\rho_+^0(n)\rho_+^0(m)}e^{-i\omega_0\alpha_+(E_n^+-E_m^+)}|E_n^+\rangle\langle E_m^+| \tag{6.41}$$

$$+ (K^-(z))^2\sin^2\theta\sum_{n\neq m}^{\infty}\frac{z^n\overline{z}^m}{\rho_-^0(n)\rho_-^0(m)}e^{-i\omega_0\alpha_-(E_n^--E_m^-)}|E_n^-\rangle\langle E_m^-| \tag{6.42}$$

$$+ K^+(z)K^-(z)e^{-i\phi}\cos\theta\sin\theta\sum_{n,m=0}^{\infty}\frac{z^n\overline{z}^m}{\rho_+^0(n)\rho_-^0(m)}e^{-i\omega_0(\alpha_+E_n^+-\alpha_-E_m^-)}|E_n^+\rangle\langle E_m^-| \tag{6.43}$$

$$+ K^+(z)K^-(z)e^{i\phi}\cos\theta\sin\theta\sum_{n,m=0}^{\infty}\frac{z^n\overline{z}^m}{\rho_-^0(n)\rho_+^0(m)}e^{-i\omega_0(\alpha_-E_n^--\alpha_+E_m^+)}|E_n^-\rangle\langle E_m^+|. \tag{6.44}$$

The integration of this operator with respect to the measure $\mathrm{d}\mu(z;\boldsymbol{\alpha};\boldsymbol{\theta})$ should include an integration over the complex plane ($z\in\mathbb{C}$) and also an integration over the sphere S^2 with respect to $\theta\in[0,\pi]$ and $\phi\in[0,2\pi)$, as indicated in (6.19), with the usual measure $\mathrm{d}\Omega=\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$. To be precise, $\mathrm{d}\mu(z;\boldsymbol{\alpha};\boldsymbol{\theta})=\mathcal{W}(|z|)\mathrm{d}z\,\mathrm{d}\Omega$, where $\mathcal{W}(|z|)$ is an appropriate "weight matrix" to be determined later. The integration with respect to $\mathrm{d}\Omega$ completely eliminates the terms in (6.43) and (6.44). Moreover, we can show that the terms (6.41) and (6.42) also disappear. Indeed, using polar coordinates $(r=|z|,\varphi)$ on the complex plane and assuming that $K^{\pm}(z)$ depends only on r (as it happens in the two examples considered in the preceding section), that is, $K^{\pm}(z)\equiv K^{\pm}(r)$, it is very easy to see that the integration on $\varphi\in[0,2\pi)$ eliminates all the terms in which $n\neq m$. Therefore, we get

$$\int (|z;\boldsymbol{\alpha};\boldsymbol{\theta}\rangle_{\lambda,\epsilon})({}_{\lambda,\epsilon}\langle z;\boldsymbol{\alpha};\boldsymbol{\theta}|)\mathrm{d}\mu(z;\boldsymbol{\alpha};\boldsymbol{\theta}) = \frac{8\pi^2}{3}\sum_{n=0}^{\infty}\frac{1}{(\rho_+^0(n))^2}|E_n^+\rangle\langle E_n^+|\int_0^{\infty}(K^+(r))^2\mathcal{W}(r)r^{2n+1}\,\mathrm{d}r \tag{6.45}$$

$$+ \frac{16\pi^2}{3}\sum_{n=0}^{\infty}\frac{1}{(\rho_-^0(n))^2}|E_n^-\rangle\langle E_n^-|\int_0^{\infty}(K^-(r))^2\mathcal{W}(r)r^{2n+1}\,\mathrm{d}r. \tag{6.46}$$

To go further, we remark that in the diagonal basis the operators $|E_n^+\rangle\langle E_n^+|$ and $|E_n^-\rangle\langle E_n^-|$ are proportional to the matrices

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

respectively. Hence, the "weight matrix" $\mathcal{W}(r)$ should be taken diagonal, in the form

$$\mathcal{W}(r) = \begin{pmatrix} W^+(r) & 0 \\ 0 & W^-(r) \end{pmatrix}, \tag{6.47}$$

and then Eqs. (6.45) and (6.46) take the form

$$\int (|z;\boldsymbol{\alpha};\boldsymbol{\theta}\rangle_{\lambda,\epsilon})(_{\lambda,\epsilon}\langle z;\boldsymbol{\alpha};\boldsymbol{\theta}|)\mathrm{d}\mu(z;\boldsymbol{\alpha};\boldsymbol{\theta}) = \sum_{n=0}^{\infty} \frac{\int_0^\infty h^+(u)u^n\,\mathrm{d}u}{(\rho_+^0(n))^2}|E_n^+\rangle\langle E_n^+| + \sum_{n=0}^{\infty} \frac{\int_0^\infty h^-(u)u^n\,\mathrm{d}u}{(\rho_-^0(n))^2}|E_n^-\rangle\langle E_n^-|, \tag{6.48}$$

where $u=r^2$ and

$$h^+(r^2) = \frac{4\pi^2}{3}(K^+(r))^2W^+(r), \quad h^-(r^2) = \frac{8\pi^2}{3}(K^-(r))^2W^-(r). \tag{6.49}$$

Therefore, in order to have a resolution of the identity on the subspace $F-F_0$, we must have the following conditions:

$$\int_0^\infty h^\pm(u)u^n\,\mathrm{d}u = (\rho_\pm^0(n))^2, \tag{6.50}$$

where the functions $\rho_\pm^0(n)$ are known (in particular, they can be some of the functions determined in the preceding section). What we have here is a couple of "moment problems," i.e., given $(\rho_\pm^0(n))^2$ we must find the functions $h^\pm(u)$ satisfying (6.50).

To show that this construction admits explicit solutions, let us consider now the two examples considered in the preceding section.

Example 1: The commutator of the ladder operators is the identity. In this case, the functions $\rho_\pm^0(n)$ and $K^\pm(r)$ were given in (6.22). Hence, the momentum problem is unique,

$$\int_0^\infty h^\pm(u)u^n\,\mathrm{d}u = b^n n!, \quad b=1. \tag{6.51}$$

We have introduced here the constant b in order to give a solution to the momentum problem which will be useful for the next example too. Indeed, the solution of (6.51) is well known,

$$h^\pm(u) = \left.\frac{1}{b}e^{-u/b}\right|_{b=1} = e^{-u}, \tag{6.52}$$

and therefore

$$W^+(r) = \frac{3}{4\pi^2}, \quad W^-(r) = \frac{3}{8\pi^2}. \tag{6.53}$$

Example 2: The Hamiltonian is factorized. In the present case, the functions $\rho_\pm^0(n)$ are given in (6.33) and the functions $K^\pm(r)$ in (6.34). The two momentum problems are now different,

$$\int_0^\infty h^-(u)u^n\,\mathrm{d}u = b^n n!, \quad \int_0^\infty h^+(u)u^n\,\mathrm{d}u = b^n(n+1)!, \tag{6.54}$$

where in both cases $b=1+\epsilon$. The solutions are

$$h^{-}(u) = \left.\frac{1}{b}e^{-u/b}\right|_{b=1+\epsilon} = \frac{1}{1+\epsilon}e^{-u/(1+\epsilon)}, \tag{6.55}$$

$$h^{+}(u) = \left.\frac{u}{b^2}e^{-u/b}\right|_{b=1+\epsilon} = \frac{u}{(1+\epsilon)^2}e^{-u/(1+\epsilon)}. \tag{6.56}$$

The weight matrix elements are then

$$W^{-}(r) = \frac{3}{8\pi^2}\frac{1}{1+\epsilon}, \quad W^{+}(r) = \frac{3}{4\pi^2}\frac{1-e^{-r^2/(1+\epsilon)}}{1+\epsilon}. \tag{6.57}$$

The two examples previously considered show that in every particular case, it is possible to obtain the "weight matrix" associated to the measure $\mathrm{d}\mu(z;\boldsymbol{\alpha};\boldsymbol{\theta})$ in such a way that the resolution of the identity (6.38) is satisfied by the corresponding family of coherent states.

VII. FINAL REMARKS

The main objective of this paper was to make a systematic study of the ladder operators associated to the Jaynes-Cummings model. We notice that several authors have considered some factorization of the corresponding Hamiltonian and then used the factor operators to build up coherent states, for example. Sometimes, these factors turned out to be either special cases of our ladder operators[10] or, sometimes, they had no relation with our work because they are not raising or lowering operators at all.[13,17]

Let us recall that the ladder operators $\mathcal{M}^{+}_{\lambda,\epsilon}$ and $\mathcal{M}^{-}_{\lambda,\epsilon}$ have been defined so they move up and down the energy eigenstates $\{|E^{-}_n\rangle\}$ and $\{|E^{+}_n\rangle\}$ without mixing them. We see in Figs. 1 and 2 that the energy levels are in fact intercalated into each other and the way they are mixed depends on the values of λ and ϵ. Using the fact that for the diagonalized Hamiltonian $\mathbb{H}_{\lambda,\epsilon}$ in (2.21), the energy eigenstates are given by the two sets $\{|n,-\rangle\}$ and $\{|n,+\rangle\}$, the operator which exchanges the two sets is nothing else but the matrix σ_1 and the corresponding operator for the original Hamiltonian $\mathcal{H}_{\lambda,\epsilon}$ in (2.8) is

$$\Sigma_{\lambda,\epsilon} = \mathcal{U}_{\lambda,\epsilon}\sigma_1\mathcal{U}^{+}_{\lambda,\epsilon} = \begin{pmatrix} \lambda\dfrac{\sqrt{N+1}}{q(N+1)} & \dfrac{\epsilon/2}{q(N+1)\sqrt{N+1}}a \\ a^{\dagger}\dfrac{\epsilon/2}{q(N+1)\sqrt{N+1}} & -\lambda\dfrac{\sqrt{N}}{q(N)} \end{pmatrix}. \tag{7.1}$$

The limit when $\lambda \to 0$ gives the operator

$$\Sigma_{0,\epsilon} = \begin{pmatrix} 0 & \dfrac{\epsilon/|\epsilon|}{\sqrt{N+1}}a \\ a^{\dagger}\dfrac{\epsilon/|\epsilon|}{\sqrt{N+1}} & 0 \end{pmatrix}, \tag{7.2}$$

while for $\epsilon \to 0$, we get $\Sigma_{\lambda,0} = \xi_\lambda\sigma_3$. Let us mention that it acts correctly on the eigenstates, i.e.,

$$\Sigma_{\lambda,0}|E^{\pm}_n\rangle = |E^{\mp}_n\rangle, \quad \Sigma_{\lambda,0}|E_*\rangle = 0. \tag{7.3}$$

Using the operators $\Sigma_{\lambda,\epsilon}$, $\mathcal{M}^{+}_{\lambda,\epsilon}$, and $\mathcal{M}^{-}_{\lambda,\epsilon}$, we can connect all the different eigenstates of the system, as it is shown in Fig. 3. With all of them it will be possible to make a comprehensive analysis of the Jaynes-Cummings model using in particular our new sets of coherent states. This work is in progress.

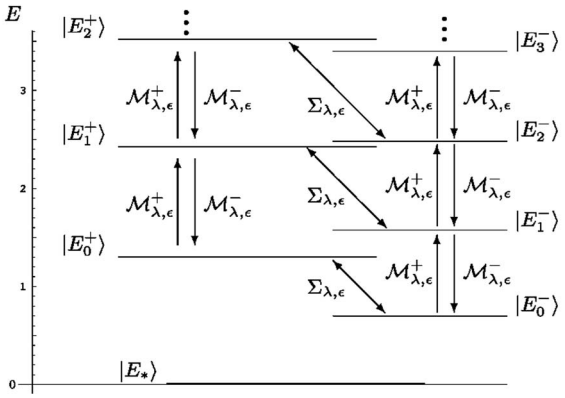

FIG. 3. The eigenstates of the Jaynes-Cummings Hamiltonian for ($\epsilon=0$, $\lambda=0.3$) are interconnected by means of the operators $\Sigma_{\lambda,\epsilon}$ $\mathcal{M}^+_{\lambda,\epsilon}$ and $\mathcal{M}^-_{\lambda,\epsilon}$

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Quantitative estimates on the enhanced binding for the Pauli-Fierz operator

Jean-Marie Barbaroux[a)]
Centre de Physique Théorique, Luminy Case 907, 13288 Marseille Cedex 9, France and Département de Mathématiques, Université du Sud-Toulon-Var, Avenue de l'Université, 83957 La Garde Cedex, France

Helmut Linde[b)]
Facultad de Fìsica, P. Universidad Católica de Chile, Casilla 306, Santiago 22, Chile

Semjon Vugalter[c)]
Mathematisches Institut, Ludwig-Maximilians-Universität München, Theresienstrasse 39, 80333 München, Germany and Institut für Analysis, Dynamik und Modelierung, Universität Stuttgart, Stuttgart, Germany

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For a quantum particle interacting with a short-range potential, we estimate from below the shift of its binding threshold, which is due to the particle interaction with a quantized radiation field. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Recently, the question of enhanced binding in nonrelativistic QED has been extensively studied in several presentations.[10,9,6,4,2,3] Dressing a charged particle with photons increases the ability of a potential to confine it. For the Pauli-Fierz operator which describes a nonrelativistic particle interacting with a radiation field, this effect was proved for small values of the fine structure constant α, first under the simplifying assumption that the spin of the particle is absent,[9] and later generalized to the case of a particle with spin.[6,4] In Ref. 2, it was shown that the effect of the enhanced binding is asymptotically small in α in the sense that the binding threshold for the Pauli-Fierz operator tends to the binding threshold for the corresponding Schrödinger operator as α tends to zero. Some quantitative estimates on this effect were obtained in Ref. 3 where it was proved that the difference between the binding threshold for the Schrödinger operator and the corresponding Pauli-Fierz operator with spin zero is at least of the order α. In the work at hand, using a different method, we prove similar results for the more general case of a particle with spin zero or one-half. Notice that studying the enhanced binding effect in the case of a particle with spin requires recovering one more term of the energy's expansion in powers of α than in the spinless case.

The method of the proof is a further development of a method used in Refs. 9 and 6. We prove that the Pauli-Fierz operator has a ground state even for some value of the potential coupling constant that is smaller than the binding threshold for the corresponding Schrödinger operator. To do so, we construct a trial function for which the quadratic form of the Pauli-Fierz operator with this coupling constant takes a value strictly less than the self-energy. Then we apply (Ref. 8, Theorem 2.1) which tells us that this implies the existence of a ground state. The trial function we

[a)]Electronic mail: barbarou@univ-tln.fr
[b)]Electronic mail: Helmut.Linde@gmx.de
[c)]Electronic mail: wugalter@mathematik.uni-muenchen.de

use is similar to the one in Ref. 6 with some modifications necessary to obtain quantitative estimates in the case with spin. It is constructed using the ground state of the self-energy operator with total momentum zero.

As in all previous papers,[9,6,4,2,3] our method is asymptotic in α. Therefore, the problem of establishing the enhanced binding effect and estimating its strength for the physical value of $\alpha \approx 1/137$ still remains open.

II. DEFINITIONS AND MAIN RESULT

The Pauli-Fierz Hamiltonian H for a charged particle with or without spin in an external electrostatic potential and coupled to the quantized electromagnetic radiation field is defined by

$$H = (-i\nabla_x \otimes I_f + \sqrt{\alpha}A(x))^2 + g\sqrt{\alpha}\sigma \cdot B(x) + \lambda W(x) \otimes I_f + I_{el} \otimes H_f - c_{\text{n.o.}}\alpha. \tag{1}$$

The operator H acts on the Hilbert space $\mathfrak{H} := \mathfrak{H}^{\text{el}} \otimes \mathfrak{F}$. The Hilbert space $\mathfrak{H}^{\text{el}}$ of the nonrelativistic particle is $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$ in the case $g=1$ and $L^2(\mathbb{R}^3)$ in the case $g=0$. Here $\mathbb{R}^3$ is the configuration space of a single particle, while $\mathbb{C}^2$ accommodates its spin in the case $g=1$.

We will describe the quantized electromagnetic field by use of the Coulomb gauge condition. Accordingly, the one-photon Hilbert space is given by $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$, where $\mathbb{R}^3$ denotes either the photon momentum or configuration space, and $\mathbb{C}^2$ accounts for the two independent transversal polarizations of the photon. The photon Fock space is then defined by

$$\mathfrak{F} = \bigoplus_{n=0}^{\infty} \mathfrak{F}_s^{(n)},$$

where the n-photons space $\mathfrak{F}_s^{(n)} = \otimes_s^n (L^2(\mathbb{R}^3) \otimes \mathbb{C}^2)$ is the symmetric tensor product of n copies of $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$.

We use units such that $\hbar = c = 1$, and where the mass of the particle equals $m = 1/2$. The particle charge is then given by $e = \sqrt{\alpha}$. As usual, we will consider α as a small parameter.

The operator that couples a particle to the quantized vector potential is given by

$$A(x) = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \frac{\zeta(|k|)}{2\pi|k|^{1/2}} \varepsilon_\lambda(k)[e^{ikx} \otimes a_\lambda(k) + e^{-ikx} \otimes a_\lambda^*(k)]\mathrm{d}k$$

$$=: D(x) + D^*(x),$$

where $\operatorname{div} A = 0$ by the Coulomb gauge condition. The operators a_λ, a_λ^* satisfy the usual commutation relations

$$[a_\nu(k), a_\lambda^*(k')] = \delta(k-k')\delta_{\lambda,\nu}, \quad [a_\nu(k), a_\lambda(k')] = 0.$$

The vectors $\varepsilon_\lambda(k) \in \mathbb{R}^3$ are the two orthonormal polarization vectors perpendicular to k,

$$\varepsilon_1(k) = \frac{(k_2, -k_1, 0)}{\sqrt{k_1^2 + k_2^2}} \quad \text{and } \varepsilon_2(k) = \frac{k}{|k|} \wedge \varepsilon_1(k). \tag{2}$$

The function $\zeta(|k|)$ describes the *ultraviolet cutoff* on the wave numbers k. We assume ζ to be of class C^1 and to have compact support.

The constant $c_{\text{n.o.}}$ is

$$c_{\text{n.o.}} = [D, D^*] = \frac{2}{\pi} \int_0^\infty r|\zeta(r)|^2 \, \mathrm{d}r,$$

and subtraction of the constant $c_{\text{n.o.}}\alpha$ amounts to normal ordering of the operator A^2.

The operator that couples a particle to the magnetic field $B = \operatorname{curl} A$ is given by

$$B(x) = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \frac{\zeta(|k|)}{2\pi|k|^{1/2}} k \times i\varepsilon_\lambda(k)[e^{ikx} \otimes a_\lambda(k) - e^{-ikx} \otimes a_\lambda^*(k)]\mathrm{d}k$$

$$=: K(x) + K^*(x).$$

In Eq. (1), $\sigma=(\sigma_1,\sigma_2,\sigma_3)$ is the three-component vector of Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The photon field energy operator H_f is given by

$$H_f = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} |k| a_\lambda^*(k) a_\lambda(k) \mathrm{d}k.$$

The multiplicative potential W is assumed to be short range and in $L^4_{\mathrm{loc}}(\mathbb{R}^3)$, and λ is a positive coupling constant. If the negative part of W is nontrivial, then there exists a critical value λ_0 such that the Schrödinger operator $-\Delta+\lambda W$ has discrete spectrum for all $\lambda>\lambda_0$, but does not have any discrete spectrum for $0\leqslant\lambda<\lambda_0$. Analogously, the Pauli-Fierz operator also has a critical coupling constant λ_1, which depends on the fine structure constant α. It is known[2] that λ_1 converges to λ_0 from below as α goes to zero.

Before stating our main result, let us introduce some notations. For v a measurable function in $\mathbb{R}^3$, we define

$$d_v = \frac{1}{2\pi}\left(\int \frac{|v(x)||v(y)|}{|x-y|^2} \mathrm{d}x\, \mathrm{d}y \right)^{1/2}, \tag{3}$$

if v is not spherically symmetric and

$$d_v = \min\left\{ \frac{1}{2\pi}\left(\int \frac{|v(x)||v(y)|}{|x-y|^2} \mathrm{d}x\, \mathrm{d}y \right)^{1/2}, \int_0^\infty t|v(t)|\mathrm{d}t \right\} \tag{4}$$

if v is spherically symmetric.

Our main result is the following.

Theorem 2.1: *Assume that $W(x)$ satisfies the following conditions: $W\in L^4_{\mathrm{loc}}(\mathbb{R}^3)$ and there exists $a>0$, $c>0$, and $\delta>0$, such that for all $|x|>a$, $|W(x)|\leqslant c(1+|x|)^{-2-\delta}$. Then*

$$\lambda_1 \leqslant \lambda_0(1 - \alpha\eta^2 + \mathcal{O}(\alpha^{5/4}))$$

with

$$\eta^2 = \frac{1}{6\pi^2} \int_{\mathbb{R}^3} \frac{\zeta(|k|)}{|k|(k^2+|k|+C_W)} \mathrm{d}k,$$

and

$$C_W = \lambda_0^2(1+\lambda_0 d_{W_+}) d_{W^2} \quad \textit{and } W_+ = (|W|+W)/2.$$

III. PROOF OF THE MAIN THEOREM

In this section, we will prove the main theorem in the case of particle with spin $g=1$. The proof for $g=0$ can easily be deduced with several simplifications.

We start with establishing some useful preliminary estimates.

A. Properties of the self-energy operator $T(0)$ with zero total momentum

This section addresses the main properties of the self-energy operator $T(0)$. Let us consider the case of a free particle coupled to the quantized electromagnetic field. The self-energy operator T is given by

$$T = (-i\nabla_x \otimes I_f + \sqrt{\alpha}A(x))^2 + g\sqrt{\alpha}\sigma \cdot B(x) + I_{\mathrm{el}} \otimes H_f - c_{\mathrm{n.o.}}\alpha.$$

We note that this system is translationally invariant, that is, T commutes with the operator of total momentum,

$$P_{\mathrm{tot}} = p_{\mathrm{el}} \otimes I_f + I_{\mathrm{el}} \otimes P_f,$$

where p_{el} and $P_f = \Sigma_{\lambda=1,2} \int k a_\lambda^*(k) a_\lambda(k) \mathrm{d}k$ denote the particle and the photon momentum operators.

Let $\mathfrak{H}_P \cong \mathbb{C}^2 \otimes \mathfrak{F}$ denote the fiber Hilbert space corresponding to conserved total momentum P. For any fixed value P of the total momentum, the restriction of T to the fiber space $\mathfrak{H}_P$ is given by (see, e.g., Ref. 5)

$$T(P) = (P - P_f + \sqrt{\alpha}A(0))^2 + g\sqrt{\alpha}\sigma \cdot B(0) + H_f - c_{\mathrm{n.o.}}\alpha. \tag{5}$$

We denote $\Sigma_0 := \inf \sigma(T(0))$.

For the reader convenience, we first collect in the following theorem different known facts regarding the ground state of the operator $T(0)$, which will be used in the proof of the main theorem.

From now on, we will denote by Π_n the projection onto the subspace of $\mathbb{C}^2 \otimes \mathfrak{F}$ corresponding to vectors which have all components zero except the n-photon components. We also define $\Pi_n^{\geqslant} = 1 - \Sigma_{i=1}^{n-1} \Pi_n$.

For vectors in $\mathbb{C}^2 \otimes \mathfrak{F}$, the norm $\|.\|$ will refer to the standard norm in $\mathbb{C}^2 \otimes \mathfrak{F}$.

Theorem 3.1: (Refs. 7, 5, 6, and 1) *For α sufficiently small we have*

Σ_0 is an eigenvalue bordering to continuous spectrum of $T(0)$ and $\Sigma_0 = \inf \sigma(T)$.

For any $\Omega_0 \in \mathrm{Ker}(T(0) - \Sigma_0)$, its projection $\Pi_0\Omega_0$ onto the zero-photon sector of $\mathbb{C}^2 \otimes \mathfrak{F}$ fulfills $\|\Pi_0\Omega_0\| \neq 0$. If Ω_0 is normalized by $\|\Pi_0\Omega_0\| = 1$, then the following inequalities are satisfied: $\|\Omega_0\| = 1 + \mathcal{O}(\alpha^{1/2})$, $\|D(0)\Omega_0\| = \mathcal{O}(\alpha^{1/2})$, and $\|H_f^{1/2}\Omega_0\| = \mathcal{O}(\alpha^{1/2})$.

For the photon number operator $N_f := \Sigma_{\lambda=1,2} \int a_\lambda^*(k) a_\lambda(k) \mathrm{d}k$, we have $\|N_f^{1/2}\Omega_0\| = \mathcal{O}(\alpha^{1/2})$.

Corollary 3.2: For any vector $\Omega_0 \in \mathrm{Ker}(T(0) - \Sigma_0)$ normalized by $\|\Pi_0\Omega_0\| = 1$, we have $\|\Omega_0\| = 1 + \mathcal{O}(\alpha)$, $\|D^*(0)\Pi_1^{\geqslant}\Omega_0\| = \mathcal{O}(\alpha^{1/2})$ and $\|\sigma \cdot K^*(0)\Pi_1^{\geqslant}\Omega_0\| = \mathcal{O}(\alpha^{1/2})$.

In the following, we consider two 4-vectors in $\mathbb{C}^2 \otimes (L^2(\mathbb{R}^3) \otimes \mathbb{C}^2)$, of the form $(\xi(\uparrow,k,\lambda_1), \xi(\uparrow,k,\lambda_2), \xi(\downarrow,k,\lambda_1), \xi(\downarrow,k,\lambda_2))$, where $\uparrow$ and $\downarrow$ refer to the spin-up and spin-down of the particle, and λ_1, λ_2 refer to the two polarizations of the transverse photons,

$$\Gamma_{a,b} := \begin{pmatrix} \Gamma(\uparrow,k,\lambda_1) \\ \Gamma(\uparrow,k,\lambda_2) \\ \Gamma(\downarrow,k,\lambda_1) \\ \Gamma(\downarrow,k,\lambda_2) \end{pmatrix} := \begin{pmatrix} \dfrac{\zeta_\Lambda(k)}{|k|^{1/2}} \left(-a\sqrt{k_1^2 + k_2^2} + b\dfrac{(k_1 - ik_2)k_3}{\sqrt{k_1^2 + k_2^2}} \right) \\ b\zeta_\Lambda(k) \dfrac{-k_2 - ik_1}{\sqrt{k_1^2 + k_2^2}} |k|^{1/2} \\ \dfrac{\zeta_\Lambda(k)}{|k|^{1/2}} \left(b\sqrt{k_1^2 + k_2^2} + a\dfrac{(k_1 + ik_2)k_3}{\sqrt{k_1^2 + k_2^2}} \right) \\ a\zeta_\Lambda(k) \dfrac{-k_2 + ik_1}{\sqrt{k_1^2 + k_2^2}} |k|^{1/2} \end{pmatrix}.$$

Let

$$\varphi_{a,b} = \sqrt{\alpha} \frac{i}{2\pi|k|(1 + |k|)} \Gamma_{a,b}. \tag{6}$$

Proposition 3.3 (approximate ground state of the Pauli-Fierz operator): *For a and b in* $\mathbb{C}$ *such that* $|a|^2+|b|^2=1$, *we consider the family of real-valued functionals* $L_{a,b}$ *defined on* $\mathbb{C}^2\otimes L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$ *by*

$$L_{a,b}(\xi)=\left\langle (k^2+|k|)\xi,\xi\right\rangle+2\sqrt{\alpha}\,\mathcal{R}e\left\langle \xi,\Pi_1\sigma\cdot K^*(0)\left(\begin{pmatrix}a\\b\end{pmatrix}0,0,\cdots\right)\right\rangle,$$

where as before $B(0)=K(0)+K^*(0)$. *Then we have*

(i) *The vector* $\varphi_{a,b}$ *defined by* (6) *is the unique minimizer of* $L_{a,b}$.
(ii) $|\Sigma_0-\inf L_{a,b}(\xi)|=\mathcal{O}(\alpha^{3/2})$.
(iii) *Let* $\Omega_0\in\mathrm{Ker}(T(0)-\Sigma_0)$ *be normalized by* $\|\Pi_0\Omega_0\|=1$. *Let us denote by* $(a,b):=\Pi_0\Omega_0$. *We define the scalar product* $\langle .,.\rangle_1$ *onto the one-photon sector* $\Pi_1(\mathbb{C}^2\otimes\mathfrak{F})=\mathbb{C}^2\otimes L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$ *by* $\langle f,g\rangle_1=\langle(k^2+|k|)f,g\rangle_{\Pi_1(\mathbb{C}^2\otimes\mathfrak{F})}$. *Then for* $\gamma\in\mathbb{R}$ *and* $R\in\mathbb{C}^2\otimes L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$ *such that*

$$\Pi_1\Omega_0=\gamma\varphi_{a,b}+R$$

and $\langle\varphi_{a,b},R\rangle_1=0$, *we have*

$$\langle R,R\rangle_1=\mathcal{O}(\alpha^{3/2})\quad\text{and}\quad|\gamma-1|=\mathcal{O}(\alpha^{3/4}).\tag{7}$$

Remark 3.4: In the above proposition, and in the sequel, we use the same notation for $\Pi_1\Omega_0$ *as a vector in* $\mathbb{C}^2\otimes\mathfrak{F}$ *which has all components zero except its one-photon component* $(\Pi_1\Omega_0)^{(1)}$, *as well as for the vector* $(\Pi_1\Omega_0)^{(1)}$ *in* $\mathbb{C}^2\otimes L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$.

Proof: In this proof, for the sake of simplicity of notations, we will drop the argument 0 in the operators $A(0)$, $B(0)$, $D(0)$, $K(0)$ and their adjoint. We first prove (i). Denoting

$$g_{a,b}:=\frac{1}{(k^2+|k|)}\Pi_1\sigma\cdot K^*\left(\begin{pmatrix}a\\b\end{pmatrix},0,0,\ldots\right),$$

we have

$$L_{a,b}(\xi)=\langle\xi,\xi\rangle_1+2\sqrt{\alpha}\,\mathcal{R}e\langle\xi,g_{a,b}\rangle_1=\left\|\xi+\sqrt{\alpha}g_{a,b}\right\|_1^2-\left\|\sqrt{\alpha}g_{a,b}\right\|_1^2,\tag{8}$$

where $\|.\|_1$ is the norm associated to the scalar product $\langle .,.\rangle_1$. Therefore, the minimizer of $L_{a,b}$ is $-\sqrt{\alpha}g_{a,b}$. A straightforward computation shows that $-\sqrt{\alpha}g_{a,b}=\varphi_{a,b}$. This implies that

$$\inf L_{a,b}=L_{a,b}(\varphi_{a,b})=-\left\|\varphi_{a,b}\right\|_1^2.\tag{9}$$

We now prove (ii). We have

$$\begin{aligned}\langle T(0)\Omega_0,\Omega_0\rangle&=\langle P_f^2\Omega_0,\Omega_0\rangle-\sqrt{\alpha}2\,\mathcal{R}e\langle P_f\Omega_0,A\Omega_0\rangle+\alpha\langle A^2\Omega_0,\Omega_0\rangle\\&\quad+\sqrt{\alpha}\langle\sigma\cdot B\Omega_0,\Omega_0\rangle+\langle H_f\Omega_0,\Omega_0\rangle-c_{\mathrm{n.o.}}\alpha.\end{aligned}\tag{10}$$

Let us estimate the terms in the above equality in order to identify those who are of order $\alpha^{3/2}$ and higher,

$$\begin{aligned}\langle P_f^2\Omega_0,\Omega_0\rangle&=\langle P_f^2\Pi_0\Omega_0,\Pi_0\Omega_0\rangle+\langle P_f^2\Pi_1\Omega_0,\Pi_1\Omega_0\rangle+\langle P_f^2\Pi_2^{\geqslant}\Omega_0,\Pi_2^{\geqslant}\Omega_0\rangle\\&=\langle P_f^2\Pi_1\Omega_0,\Pi_1\Omega_0\rangle+\langle P_f^2\Pi_2^{\geqslant}\Omega_0,\Pi_2^{\geqslant}\Omega_0\rangle,\end{aligned}\tag{11}$$

$$\begin{aligned}\langle H_f\Omega_0,\Omega_0\rangle&=\langle H_f\Pi_0\Omega_0,\Pi_0\Omega_0\rangle+\langle H_f\Pi_1\Omega_0,\Pi_1\Omega_0\rangle+\langle H_f\Pi_2^{\geqslant}\Omega_0,\Pi_2^{\geqslant}\Omega_0\rangle\\&=\langle H_f\Pi_1\Omega_0,\Pi_1\Omega_0\rangle+\langle H_f\Pi_2^{\geqslant}\Omega_0,\Pi_2^{\geqslant}\Omega_0\rangle.\end{aligned}\tag{12}$$

Now, using the fact that n-photon sectors are invariant under P_f, $P_f\Pi_0\Omega_0=0$, and $\langle P_f\Omega_0,A\Omega_0\rangle=\langle AP_f\Pi_1^{\geqslant}\Omega_0,\Omega_0\rangle=\langle A\Pi_1^{\geqslant}\Omega_0,P_f\Omega_0\rangle=\langle A\Pi_1^{\geqslant}\Omega_0,P_f\Pi_1^{\geqslant}\Omega_0\rangle$, we get

$$
\begin{aligned}
\left|\langle P_f\Omega_0, A\Omega_0\rangle\right| &= \left|\langle P_f\Pi_1^{\geqslant}\Omega_0, A\Pi_1^{\geqslant}\Omega_0\rangle\right| \\
&\leqslant \left|\langle P_f\Pi_1^{\geqslant}\Omega_0, D\Pi_2^{\geqslant}\Omega_0\rangle\right| + \left|\langle P_f\Pi_2^{\geqslant}\Omega_0, D^*\Pi_1^{\geqslant}\Omega_0\rangle\right| \\
&\leqslant \left|\langle P_f\Pi_1\Omega_0, D\Pi_2\Omega_0\rangle\right| + \left|\langle P_f\Pi_2^{\geqslant}\Omega_0, D\Pi_3^{\geqslant}\Omega_0\rangle\right| \\
&\quad + \left|\langle P_f\Pi_2^{\geqslant}\Omega_0, D^*\Pi_1^{\geqslant}\Omega_0\rangle\right| \\
&\left|\left|\left|P_f\Pi_1\Omega_0\right|\right|\right| \left\|D\Pi_2\Omega_0\right\| + \tfrac{1}{2}\left\|P_f\Pi_2^{\geqslant}\Omega_0\right\|^2 \\
&\quad + 2\left\|D\Pi_3^{\geqslant}\Omega_0\right\|^2 + 2\left\|D^*\Pi_1^{\geqslant}\Omega_0\right\|^2.
\end{aligned}
$$

Using Theorem 3.1 and Corollary 3.2 and the fact that $\|P_f\Pi_1\Omega_0\| \leqslant c(\Lambda)\|\Pi_1\Omega_0\| = \mathcal{O}(\alpha^{1/2})$, where $c(\Lambda)$ depends only on the ultraviolet cutoff, yields

$$
\left|\langle P_f\Omega_0, A\Omega_0\rangle\right| \leqslant \tfrac{1}{2}\left\|P_f\Pi_2^{\geqslant}\Omega_0\right\|^2 + \mathcal{O}(\alpha). \tag{13}
$$

We also have

$$
\begin{aligned}
&\langle A^2\Omega_0, \Omega_0\rangle \\
&= \langle (D + D^*)^2\Omega_0, \Omega_0\rangle \\
&= 2\,\mathcal{R}e\langle DD\Omega_0, \Omega_0\rangle + 2\|D\Omega_0\|^2 + \|[D, D^*]\|\|\Omega_0\|^2 \\
&= \mathcal{O}(\alpha^{1/2}) + \mathcal{O}(\alpha) + \|[D, D^*]\|(1 + \mathcal{O}(\alpha)),
\end{aligned}
$$

where we used from Theorem 3.1 that $\|\Omega_0\| = 1 + \mathcal{O}(\alpha)$ and $\|D\Omega_0\| = \mathcal{O}(\alpha^{1/2})$. Since the commutator $[D, D^*]$ equals $c_{\text{n.o.}}$ we arrive at

$$
\langle A^2\Omega_0, \Omega_0\rangle = c_{\text{n.o.}} + \mathcal{O}(\alpha^{1/2}). \tag{14}
$$

Finally we have, writing $B = K + K^*$,

$$
\begin{aligned}
\langle \sigma \cdot B\Omega_0, \Omega_0\rangle &= \langle \sigma \cdot K\Pi_1\Omega_0, \Pi_0\Omega_0\rangle + \langle \sigma \cdot K\Pi_2^{\geqslant}\Omega_0, \Pi_1^{\geqslant}\Omega_0\rangle \\
&\quad + \langle \sigma \cdot K^*\Pi_0\Omega_0, \Pi_1\Omega_0\rangle + \langle \sigma \cdot K^*\Pi_1^{\geqslant}\Omega_0, \Pi_2^{\geqslant}\Omega_0\rangle \\
&= 2\,\mathcal{R}e\langle \sigma \cdot K\Pi_1\Omega_0, \Pi_0\Omega_0\rangle + 2\,\mathcal{R}e\langle \sigma \cdot K^*\Pi_1^{\geqslant}\Omega_0, \Pi_2^{\geqslant}\Omega_0\rangle
\end{aligned}
$$

using Theorem 3.1 and Corollary 3.2 we obtain

$$
\langle \sigma \cdot B\Omega_0, \Omega_0\rangle = 2\,\mathcal{R}e\langle \sigma \cdot K\Pi_1\Omega_0, \Pi_0\Omega_0\rangle + \mathcal{O}(\alpha). \tag{15}
$$

Collecting (10)–(15) and using $\langle H_f\Pi_2^{\geqslant}\Omega_0, \Pi_2^{\geqslant}\Omega_0\rangle \geqslant 0$ we obtain

$$
\langle T(0)\Omega_0, \Omega_0\rangle \geqslant \langle P_f^2\Pi_1\Omega_0, \Pi_1\Omega_0\rangle + \langle H_f\Pi_1\Omega_0, \Pi_1\Omega_0\rangle + 2\sqrt{\alpha}\,\mathcal{R}e\langle \sigma \cdot K\Pi_1\Omega_0, \Pi_0\Omega_0\rangle + \mathcal{O}(\alpha^{3/2}). \tag{16}
$$

Since on the one-photon sector the operator P_f^2 reduces to multiplication by k^2, and the operator H_f reduces to multiplication by $|k|$, we obtain

$$\Sigma_0 = \frac{\langle T(0)\Omega_0, \Omega_0\rangle}{\|\Omega_0\|^2} \geqslant L_{a,b}(\Pi_1\Omega_0) + \mathcal{O}(\alpha^{3/2}) \geqslant \inf L_{a,b} + \mathcal{O}(\alpha^{3/2}). \tag{17}$$

On the other hand, using (i), and for $\psi_{a,b}=\binom{a}{b}, \varphi_{a,b}, 0, 0, \ldots)$ we have

$$\inf L_{a,b} = L_{a,b}(\varphi_{a,b}) = \langle T(0)\psi_{a,b}, \psi_{a,b}\rangle \geqslant \Sigma_0\|\psi_{a,b}\|^2 = \Sigma_0(1 + \mathcal{O}(\alpha)) \geqslant \Sigma_0 + \mathcal{O}(\alpha^2). \tag{18}$$

Inequalities (17) and (18) conclude the proof of (ii).

Eventually, we prove (iii). Due to the inequalities (17) and (18), we have $\inf L_{a,b}+\mathcal{O}(\alpha^{3/2}) = L_{a,b}(\Pi_1\Omega_0)$. Using (8), the fact that $-\sqrt{\alpha}g_{a,b}=\varphi_{a,b}$, and (9), we thus get

$$\inf L_{a,b} + \mathcal{O}(\alpha^{3/2}) = L_{a,b}(\Pi_1\Omega_0) = \|\gamma\varphi_{a,b} + R - \varphi_{a,b}\|_1^2 - \|\varphi_{a,b}\|_1^2 = (\gamma-1)^2\|\varphi_{a,b}\|_1^2 + \|R\|_1^2 + \inf L_{a,b}, \tag{19}$$

which proves (7). □

B. Proof of Theorem 2.1

As it was mentioned in the Introduction, we prove the theorem by constructing a trial function Ψ for which the quadratic form of H takes a value strictly smaller than $\Sigma_0\|\Psi\|^2$.

Let us start by proving an auxiliary result. For $\gamma \in (0,1)$, we define $f_\gamma \in L^2(\mathbb{R}^3)$ to be a normalized real valued eigenfunction, with associated eigenvalue e_γ, of the Schrödinger operator:

$$h_\gamma := -(1-\gamma)\Delta + \lambda_0 W(x).$$

Here λ_0 is the critical coupling constant defined in Sec. II.

Lemma 3.5: Then for $\lambda \leqslant \lambda_0$, *we have*

$$\sum_i \left\langle (-\Delta + \lambda W)\frac{\partial f_\gamma}{\partial x_i}, \frac{\partial f_\gamma}{\partial x_i}\right\rangle \leqslant C_W\|\nabla f_\gamma\|^2 + o_\gamma(1)\|\nabla f_\gamma\|^2,$$

with $C_W := \lambda_0^2(1+\lambda_0 d_{W_+})d_{W^2}$, *where* $W_+ = (W+|W|)/2$ *and* d_{W^2} *and* d_{W_+} *are defined by* (3) *and* (4).

Proof: For a potential V such that $V \in L^2_{\mathrm{loc}}$ and short range we have

$$|\langle V\psi, \psi\rangle| \leqslant d_V\|\nabla\psi\|^2.$$

Moreover, we know that f_γ is an eigenfunction of $-(1-\gamma)\Delta+\lambda_0 W$ and that the associated eigenvalue e_γ tends to zero as γ tends to zero, since λ_0 is the critical coupling constant. Therefore we obtain the following sequence of inequalities:

$$\begin{aligned}
\sum_i \left\langle (-\Delta + \lambda W)\frac{\partial f_\gamma}{\partial x_i}, \frac{\partial f_\gamma}{\partial x_i}\right\rangle &\leqslant \sum_i \left\langle (-\Delta + \lambda W_+)\frac{\partial f_\gamma}{\partial x_i}, \frac{\partial f_\gamma}{\partial x_i}\right\rangle \\
&\leqslant \sum_i \left\langle (-\Delta + \lambda_0 W_+)\frac{\partial f_\gamma}{\partial x_i}, \frac{\partial f_\gamma}{\partial x_i}\right\rangle \leqslant \sum_i \left\langle -\Delta\frac{\partial f_\gamma}{\partial x_i}, \frac{\partial f_\gamma}{\partial x_i}\right\rangle (1 + d_{\lambda_0 W_+}) \\
&= (1 + d_{\lambda_0 W_+})\langle -\Delta f_\gamma, -\Delta f_\gamma\rangle = (1 + d_{\lambda_0 W_+})\left\langle \frac{e_\gamma - \lambda_0 W}{1-\gamma} f_\gamma, -\Delta f_\gamma\right\rangle \\
&= \frac{e_\gamma(1 + d_{\lambda_0 W_+})}{1-\gamma}\langle f_\gamma, -\Delta f_\gamma\rangle - \frac{\lambda_0(1 + d_{\lambda_0 W_+})}{1-\gamma}\langle W f_\gamma, -\Delta f_\gamma\rangle.
\end{aligned} \tag{20}$$

We estimate the last term on the right-hand side by

$$-\langle Wf_\gamma, -\Delta f_\gamma\rangle = \left\langle Wf_\gamma, \frac{\lambda_0 W - e_\gamma}{1-\gamma} f_\gamma \right\rangle$$

$$\leqslant -\frac{e_\gamma d_{W_+}}{1-\gamma}\|\nabla f_\gamma\|^2 + \frac{\lambda_0}{1-\gamma} d_{W^2}\|\nabla f_\gamma\|^2. \tag{21}$$

The inequalities (20) and (21) imply for $\lambda \leqslant \lambda_0$,

$$\sum_i \left\langle (-\Delta + \lambda W)\frac{\partial f_\gamma}{\partial x_i}, \frac{\partial f_\gamma}{\partial x_i}\right\rangle \leqslant (\lambda_0^2(1+\lambda_0 d_{W_+})d_{W^2} + o_\gamma(1))\|\nabla f_\gamma\|^2. \tag{22}$$

□

In the rest of this section, we will mainly work in the space representation for both particle and photons. Following,[6] let us introduce, for given $x \in \mathbb{R}^3$, the shift operator on the photon space variables $\tau_x : \mathbb{C}^2 \otimes \mathfrak{F} \to \mathbb{C}^2 \otimes \mathfrak{F}$. For $\phi = (\phi_0, \phi_1, \ldots, \phi_n, \ldots) \in \mathbb{C}^2 \otimes \mathcal{F}$, we have writing by abuse of notation $\tau_x \phi = (\tau_x \phi_0, \tau_x \phi_1, \ldots)$,

$$\tau_x \phi_n(s; y_1, \ldots, y_n; \lambda_1, \ldots, \lambda_n) = \phi_n(s; y_1 - x, \ldots, y_n - x; \lambda_1, \ldots, \lambda_n),$$

where s is the spin of the particle and takes value in $\{\uparrow, \downarrow\}$.

We denote by Ω_0^x the ground state Ω_0 written in space representation and shifted by x, i.e.,

$$\Omega_0^x := \tau_x \mathcal{F}^{-1} \Omega_0,$$

where $\mathcal{F}$ stands for the Fourier transform.

Recall that $D^*(0)$ is an operator valued vector with three components which we denote by $D^*(0)_i$ $(i = 1, 2, 3)$. Then we consider the functions

$$\theta_i = (0, \theta_i^{(1)}, 0, \ldots) \in \mathbb{C}^2 \otimes \mathfrak{F} \tag{23}$$

with

$$\theta_i^{(1)} = \left(k^2 + |k| + C_W\right)^{-1} \Pi_1 D^*(0)_i \left(\begin{pmatrix} a \\ b \end{pmatrix}, 0, \ldots\right) \tag{24}$$

and

$$\theta_i^x = \tau_x \mathcal{F}^{-1} \theta_i. \tag{25}$$

We first state some properties of θ_i.

Lemma 3.6:

(i) *For $i \neq j$ we have*

$$\langle \theta_i, \theta_j \rangle = 0 \quad \textit{and} \ \langle \theta_i, \theta_j \rangle_1 = 0.$$

(ii) *For $i = 1, 2, 3$ holds*

$$\|\theta_i \sqrt{k^2 + |k| + C_W}\|^2 = \frac{1}{6\pi^2} \int_{\mathbb{R}^3} \frac{\zeta(|k|)}{|k|(k^2 + |k| + C_W)} \mathrm{d}k.$$

(iii) *For $i = 1, 2, 3$ $\langle k_i \varphi_{a,b}, \Pi_1 \theta_i \rangle = 0$.*

Proof: To prove this lemma we remind that θ_i has only a nonzero component $\Pi_1 \theta_i$ in the one-photon sector, and

$$\Pi_1\theta_i=\begin{pmatrix} a\dfrac{\varepsilon_{1,i}(k)\zeta(|k|)}{|k|^{1/2}(k^2+|k|+C_W)} \\ a\dfrac{\varepsilon_{2,i}(k)\zeta(|k|)}{|k|^{1/2}(k^2+|k|+C_W)} \\ b\dfrac{\varepsilon_{1,i}(k)\zeta(|k|)}{|k|^{1/2}(k^2+|k|+C_W)} \\ b\dfrac{\varepsilon_{2,i}(k)\zeta(|k|)}{|k|^{1/2}(k^2+|k|+C_W)} \end{pmatrix},$$

where the two polarization vectors $\varepsilon_1(k)$ and $\varepsilon_2(k)$ are defined in (2). The properties stated in the lemma follow straightforwardly from computations of the corresponding integrals. □

We consider the trial function $\Psi\in L^2(\mathbb{R}^3)\otimes\mathbb{C}^2\otimes\mathfrak{F}$,

$$\Psi:=\Psi_1+\Psi_2:=f_\gamma(x)\Omega_0^x+i\sqrt{\alpha}\sum_{i=1}^{3}\theta_i^x\frac{\partial f_\gamma(x)}{\partial x_i}. \tag{26}$$

Now we compute the expectation value of H in the state Ψ. We have

$$\langle H\Psi,\Psi\rangle=\langle H\Psi_1,\Psi_1\rangle+\langle H\Psi_2,\Psi_2\rangle+2\,\mathcal{R}e\langle H\Psi_1,\Psi_2\rangle.$$

As usual,[6] due to the orthogonality $\langle f,\partial f/\partial x_i\rangle=0$, we have

$$\langle H\Psi_1,\Psi_1\rangle=\Sigma_0\|\Psi_1\|^2+\langle(-\Delta+\lambda W(x))f_\gamma,f_\gamma\rangle\|\Omega_0\|^2. \tag{27}$$

Since Ψ_2 has only a nonzero component in the one photon sector, in the quadratic form $\langle H\Psi_2,\Psi_2\rangle$, all the terms involving $A(0)$ or $B(0)$ vanish. Moreover, using Lemma 3.6 and the orthogonalities $\langle\partial f_\gamma/\partial x_i,\partial f_\gamma/\partial x_j\rangle=0$ and $\langle\partial f_\gamma/\partial x_i,\partial^2 f_\gamma/\partial x_i\partial x_j\rangle=0$, for $i\neq j$, we arrive at

$$\begin{aligned}\langle H\Psi_2,\Psi_2\rangle=&\alpha\sum_l\|\theta_l^x\|^2\left\langle(-\Delta+\lambda W)\frac{\partial f_\gamma}{\partial x_l},\frac{\partial f_\gamma}{\partial x_l}\right\rangle+\mathcal{O}(\alpha^2)\|\nabla f_\gamma\|^2\\&+\alpha\sum_l\left\|\frac{\partial f_\gamma}{\partial x_l}\right\|^2\langle(|k|+k^2)\Pi_1\theta_l^x,\Pi_1\theta_l^x\rangle.\end{aligned} \tag{28}$$

To compute the last term $\langle H\Psi_1,\Psi_2\rangle$, we first note that

$$\left\langle(-\Delta+\lambda W)f_\gamma,\frac{\partial f_\gamma}{\partial x_i}\right\rangle=\left\langle(-(1-\gamma)\Delta+\lambda W)f_\gamma,\frac{\partial f_\gamma}{\partial x_i}\right\rangle-\gamma\left\langle\Delta f_\gamma,\frac{\partial f_\gamma}{\partial x_i}\right\rangle$$

$$=e_\gamma\left\langle f_\gamma,\frac{\partial f_\gamma}{\partial x_i}\right\rangle+\gamma\sum_j\left\langle\frac{\partial^2 f_\gamma}{\partial x_j^2},\frac{\partial f_\gamma}{\partial x_i}\right\rangle=0.$$

The last equality holds since f_γ is a real function vanishing at infinity. Moreover, all other terms in the quadratic form $\langle H\Psi_1,\Psi_2\rangle$ which contain $\langle f_\gamma,\partial f_\gamma/\partial x_i\rangle$ vanish also. So we arrive at

$$2\,\mathcal{R}e\langle H\Psi_1,\Psi_2\rangle=-2\,\mathcal{R}e\langle P\cdot(P_f-\sqrt{\alpha}A(0))\Psi_1,\Psi_2\rangle=2\sqrt{\alpha}\sum_i\left\|\frac{\partial f_\gamma}{\partial x_i}\right\|^2\mathcal{R}e\langle(P_f-\sqrt{\alpha}A(0))_i\Omega_0,\theta_i\rangle. \tag{29}$$

The term with P_f on the right-hand side is estimated as follows:

$$\begin{aligned}\mathcal{R}e\langle (P_f)_i\Omega_0,\theta_i\rangle_{\mathbb{C}^2\otimes\mathfrak{F}} &= \mathcal{R}e\langle \Pi_1(P_f)_i(\gamma\varphi_{a,b}+R),\Pi_1\theta_i\rangle_{\mathbb{C}^2\otimes L^2(\mathbb{R}^3)\otimes\mathbb{C}^2}\\ &= \mathcal{R}e\langle k_i(\gamma\varphi_{a,b}+R),\Pi_1\theta_i\rangle_{\mathbb{C}^2\otimes L^2(\mathbb{R}^3)\otimes\mathbb{C}^2}\\ &\leqslant \|R\|_1\||k|^{1/2}\Pi_1\theta_i\| + \gamma\,\mathcal{R}e\langle k_i\varphi_{a,b},\Pi_1\theta_i\rangle_{\mathbb{C}^2\otimes L^2(\mathbb{R}^3)\otimes\mathbb{C}^2}. \end{aligned} \tag{30}$$

Using Proposition 3.3 yields the following bound for the first term on the right-hand side of (30):

$$\|R\|_1\||k|^{1/2}\Pi_1\theta_i\| = \mathcal{O}(\alpha^{3/4}). \tag{31}$$

According to Lemma 3.6 (iii), the second term on the right-hand side of (30) equals zero. Therefore, collecting (29)–(31), we arrive at

$$2\,\mathcal{R}e\langle H\Psi_1,\Psi_2\rangle = -2\alpha\sum_i \left\|\frac{\partial f_\gamma}{\partial x_i}\right\|^2 \mathcal{R}e\langle A(0)_i\Omega_0,\theta_i\rangle + \mathcal{O}(\alpha^{5/4})\|\nabla f_\gamma\|^2. \tag{32}$$

Now we have, using Theorem 3.1 and the fact that $D(0)$ restricted to the two-photon sector is a bounded operator,

$$\begin{aligned}\mathcal{R}e\langle A(0)_i\Omega_0,\theta_i\rangle &= \mathcal{R}e\langle D(0)_i\Pi_2\Omega_0,\theta_i\rangle + \mathcal{R}e\langle D^*(0)_i\Pi_0\Omega_0,\theta_i\rangle\\ &= \mathcal{O}(\alpha^{1/2}) + \mathcal{R}e\langle D^*(0)_i\Pi_0\Omega_0,\theta_i\rangle. \end{aligned} \tag{33}$$

Due to the definition (24) of θ_i, the second term on the right-hand side of (33) is $\|\theta_i\sqrt{k^2+|k|+C_W}\|^2$. Therefore, collecting the equalities (27), (28), (32), and (33) we obtain

$$\begin{aligned}\langle H\Psi,\Psi\rangle = \Sigma_0\|\Psi_1\|^2 + \|\Omega_0\|^2\langle(-\Delta+\lambda W)f_\gamma,f_\gamma\rangle + \alpha\sum_l \|\theta_l\|^2\left\langle(-\Delta+\lambda W)\frac{\partial f_\gamma}{\partial x_l},\frac{\partial f_\gamma}{\partial x_l}\right\rangle\\ -2\alpha\sum_l\left\|\frac{\partial f_\gamma}{\partial x_l}\right\|^2\|\theta_i\sqrt{k^2+|k|+C_W}\|^2 + \mathcal{O}(\alpha^{5/4})\|\nabla f_\gamma\|^2 + \alpha\sum_l\left\|\frac{\partial f_\gamma}{\partial x_l}\right\|^2\|\theta_l\|_1^2. \end{aligned} \tag{34}$$

From Lemma 3.6, we know that $\|\theta_l\sqrt{k^2+|k|+C_W}\|^2$ is independent of l. We denote this constant by η^2. With Lemma 3.5 we thus arrive at

$$\begin{aligned}\langle H\Psi,\Psi\rangle \leqslant \Sigma_0\|\Psi\|^2 - \Sigma_0\|\Psi_2\|^2 + \|\Omega_0\|^2(\|\nabla f_\gamma\|^2 + \langle\lambda W f_\gamma,f_\gamma\rangle)\\ -\alpha\sum_l\left\|\frac{\partial f_\gamma}{\partial x_l}\right\|^2\eta^2 + \alpha o_\gamma(1)\|\nabla f_\gamma\|^2 + \mathcal{O}(\alpha^{1/2})\|\nabla f_\gamma\|^2. \end{aligned} \tag{35}$$

Note that $\Sigma_0\|\psi_2\|^2 = \mathcal{O}(\alpha^2)\|\nabla f_\gamma\|^2$. We thus obtain

$$\begin{aligned}&\langle H\Psi,\Psi\rangle - \Sigma_0\|\Psi\|^2\\ &\leqslant \|\Omega_0\|^2\left(\left(1-\frac{\alpha}{\|\Omega_0\|^2}\eta^2 + \frac{\alpha}{\|\Omega_0\|^2}(o_\gamma(1)+\mathcal{O}(\alpha^{1/4}))\right)\|\nabla f_\gamma\|^2 + \langle\lambda W f_\gamma,f_\gamma\rangle\right). \end{aligned} \tag{36}$$

Using from Corollary 3.2 that $\|\Omega_0\|^2 = 1+\mathcal{O}(\alpha)$, we obtain

$$\begin{aligned}&\langle H\Psi,\Psi\rangle - \Sigma_0\|\Psi\|^2\\ &\leqslant \|\Omega_0\|^2((1-\alpha\eta^2 + \alpha o_\gamma(1) + \mathcal{O}(\alpha^{5/4}))\|\nabla f_\gamma\|^2 + \langle\lambda W f_\gamma,f_\gamma\rangle). \end{aligned} \tag{37}$$

Therefore

$$\langle H\Psi,\Psi\rangle - \Sigma_0\|\Psi\|^2 \leqslant \|\Omega_0\|^2(1-\alpha\eta^2+\alpha o_\gamma(1)+\mathcal{O}(\alpha^{5/4}))$$

$$\times(\|\nabla f_\gamma\|^2+(1+\alpha\eta^2+\alpha o_\gamma(1)+\mathcal{O}(\alpha^{5/4}))^{-1}\langle\lambda W f_\gamma,f_\gamma\rangle). \tag{38}$$

If $\lambda>\lambda_0(1-\alpha\eta^2+\mathcal{O}(\alpha^{5/4}))$, choosing γ (depending on α) small enough, we arrive at $\langle H\Psi,\Psi\rangle - \Sigma_0\|\Psi\|^2<0$. Due to Griesemer *et al.*,[8] this implies the existence of a ground state for H.

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Analytic Coulomb matrix elements in a three-dimensional geometry

Jaime Zaratiegui García[a)]
Department of Physical Sciences, P.O. Box 3000, FIN-90014 University of Oulu, Finland

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Using a complete basis set we have obtained an analytic expression for the matrix elements of the Coulomb interaction. These matrix elements are written in a closed form. We have used the basis set of the three-dimensional isotropic quantum harmonic oscillator in order to develop our calculations, which can be useful when treating interactions in localized systems. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Having an analytic expression for the Coulomb matrix elements is an important step for several numerical methods, like, for example, exact diagonalization method. In order to describe the Coulomb interaction in three dimensions, we have chosen the basis set of the isotropic harmonic oscillator for the single-particle wave functions, which, in one dimension, is written as

$$\psi_{n_x}(x) = (a\sqrt{\pi}2^{n_x}n_x!)^{-1/2}e^{-(1/2)x^2/a^2}H_{n_x}(x/a), \tag{1}$$

where $a=\sqrt{\hbar/m\omega}$ is taken as the characteristic unit length. One of the reasons for the election of this particular basis set is the Gaussian Product Theorem, which guarantees that the product of two Gaussian type orbitals (a linear combination of them in our case) centered on two different atoms is a finite sum of Gaussians centered on a point along the axis connecting them.

In previous works, several ways to evaluate the two-dimensional matrix elements using different approaches have been studied,[1–3] such as restricting to the lowest Landau level due to simplicity reasons.[4,5]

The purpose of this paper is to report an analytic formula for the Coulomb interaction written in closed form. It can be easily implemented by computer means and could help to improve the performance of solid state simulations in which interactions are taken into account.

II. MATRIX ELEMENTS

In order to derive an analytical expression for the Coulomb interaction matrix elements we will proceed starting with the same approach as the one used in Ref. 6, i.e., writing the single-electron wave function and the Coulomb potential as their Fourier transform integrals:

$$\psi_\lambda(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}}\int \phi_\lambda(\boldsymbol{q})e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\mathrm{d}\boldsymbol{q}, \tag{2}$$

$$V(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}}\int \tilde{V}(\boldsymbol{q})e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\mathrm{d}\boldsymbol{q}, \tag{3}$$

where λ stands for a set of quantum numbers $\{n_i\}$ and $V(\boldsymbol{r}_1-\boldsymbol{r}_2)=r_{12}^{-1}$ is the Coulomb potential. Now, the two-particle matrix element, which, in real space is written as

[a)]Electronic mail: jaime.zaratiegui@oulu.fi

$$\mathcal{V}^{\lambda_1\lambda_2}_{\lambda_3\lambda_4} = \int \psi^*_{\lambda_1}(\boldsymbol{r}_1)\psi^*_{\lambda_2}(\boldsymbol{r}_2)V(\boldsymbol{r}_1-\boldsymbol{r}_2) \times \psi_{\lambda_3}(\boldsymbol{r}_2)\psi_{\lambda_4}(\boldsymbol{r}_1)\mathrm{d}\boldsymbol{r}_1\boldsymbol{r}_2, \tag{4}$$

is now expressed, in momentum space, as

$$\mathcal{V}^{\lambda_1\lambda_2}_{\lambda_3\lambda_4} = \frac{1}{(2\pi)^{3/2}} \int \phi^*_{\lambda_1}(\boldsymbol{q}_1)\phi_{\lambda_4}(\boldsymbol{q}_1-\boldsymbol{q}) \times \phi^*_{\lambda_2}(\boldsymbol{q}_2)\phi_{\lambda_3}(\boldsymbol{q}_2+\boldsymbol{q})\widetilde{V}(\boldsymbol{q})\mathrm{d}\boldsymbol{q}_1\mathrm{d}\boldsymbol{q}_2\mathrm{d}\boldsymbol{q}. \tag{5}$$

Equation (5) can be rewritten in a more convenient and compact form. Let us define $C^{\lambda}_{\lambda'}(\boldsymbol{q})$ and $D^{\lambda}_{\lambda'}(\boldsymbol{q})$ as the following convolution integrals:

$$C^{\lambda}_{\lambda'}(\boldsymbol{q}) = \int \phi^*_{\lambda}(\boldsymbol{k})\phi_{\lambda'}(\boldsymbol{k}-\boldsymbol{q})\mathrm{d}\boldsymbol{k} \tag{6}$$

$$= \int \psi^*_{\lambda}(\boldsymbol{r})\psi_{\lambda'}(\boldsymbol{r})e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\mathrm{d}\boldsymbol{r}, \tag{7}$$

$$D^{\lambda}_{\lambda'}(\boldsymbol{q}) = \int \phi^*_{\lambda}(\boldsymbol{k})\phi_{\lambda'}(\boldsymbol{k}+\boldsymbol{q})\mathrm{d}\boldsymbol{k} \tag{8}$$

$$= \int \psi^*_{\lambda}(\boldsymbol{r})\psi_{\lambda'}(\boldsymbol{r})e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\mathrm{d}\boldsymbol{r} \tag{9}$$

$$= C^{\lambda}_{\lambda'}(-\boldsymbol{q}). \tag{10}$$

Substituting Eqs. (6) and (8) into Eq. (5) we obtain

$$\mathcal{V}^{\lambda_1\lambda_2}_{\lambda_3\lambda_4} = \frac{1}{(2\pi)^{3/2}} \int C^{\lambda_1}_{\lambda_4}(\boldsymbol{q})D^{\lambda_2}_{\lambda_3}(\boldsymbol{q})\widetilde{V}(\boldsymbol{q})\mathrm{d}\boldsymbol{q}. \tag{11}$$

Now, it is straightforward to perform the integral appearing in Eq. (7).[7] Using Cartesian coordinates, it is possible to separate all three variables and integrate independently. For simplicity reasons, let us integrate only along the x variable, the result then reads:

$$C^{n^1_x}_{n^4_x}(q_x) = \left(\frac{2^{n^{14}_{x+}}}{n^{14}_{x+}!}\frac{n^{14}_{x-}!}{2^{n^{14}_{x-}}}\right)^{1/2} i^{n^1_x+n^4_x}(-1)^{n^{14}_{x+}} \times e^{-q_x^2a^2/4}\left(\frac{aq_x}{2}\right)^{|n^1_x-n^4_x|} L^{|n^1_x-n^4_x|}_{n^{14}_{x-}}(a^2q_x^2/2), \tag{12}$$

where n^j_i is the quantum number referring to the i axis of the particle j. We have also used the terms n^{jk}_{i+} and n^{jk}_{i-}, which are defined as $\max(n^j_i, n^k_i)$ and $\min(n^j_i, n^k_i)$ respectively. The final form for $C^{\lambda_1}_{\lambda_4}(\boldsymbol{q})$ will be

$$C^{n^1_x n^1_y n^1_z}_{n^4_x n^4_y n^4_z}(\boldsymbol{q}) = \prod_{i\in\{x,y,z\}} C^{n^1_i}_{n^4_i}(q_i). \tag{13}$$

Using the relation between D and C shown in Eq. (10), it is trivial to find out the value of the former convolution integral.

It still remains to calculate the Fourier transform $\tilde{V}(\boldsymbol{q})$ of the spherically symmetric interaction potential $V(\boldsymbol{r})$,

$$\tilde{V}(q) = \sqrt{\frac{2}{\pi}}\frac{1}{q^2}. \tag{14}$$

But it will be more convenient to substitute it by

$$\tilde{V}(q) = \sqrt{\frac{2}{\pi}}\int_0^\infty e^{-(q_x^2+q_y^2+q_z^2)u}\mathrm{d}u. \tag{15}$$

The integration over variables q_x, q_y, and q_z can be performed all in the same fashion. Using the symmetry of the problem we only need to integrate over one variable, i.e., q_x and then use the same result for q_y and q_z. Therefore, integrating over q_x yields

$$\int_{-\infty}^{\infty} e^{-(u+a^2/2)q_x^2}\left(\frac{aq_x}{2}\right)^{|n_x^1-n_x^4|+|n_x^2-n_x^3|} \times L_{n_{x-}^{14}}^{|n_x^1-n_x^4|}(a^2q_x^2/2)L_{n_{x-}^{23}}^{|n_x^2-n_x^3|}(a^2q_x^2/2)\mathrm{d}q_x. \tag{16}$$

This integral does not vanish if and only if

$$|n_x^1 - n_x^4| + |n_x^2 - n_x^3| = 2s_x, \tag{17}$$

where $s_x=0,1,2,\ldots$. Therefore, using the previous selection rule and the power series for the associated Laguerre polynomial

$$L_n^l(x) = \sum_{k=0}^{n}\frac{1}{k!}\binom{n+l}{n-k}(-x)^k, \tag{18}$$

we can write Eq. (16) as

$$\sum_{k_x=0}^{n_{x-}^{14}}\frac{(-1)^{k_x}}{k_x!}\binom{n_{x+}^{14}}{n_{x-}^{14}-k_x}\sum_{k_x=0}^{n_{x-}^{14}}\frac{(-1)^{k_x'}}{k_x'!}\binom{n_{x+}^{23}}{n_{x-}^{23}-k_x'} \times 2^{k_x+k_x'}\left(\frac{a}{2}\right)^{2s_x+2k_x+2k_x'} \times \frac{(2s_x+2k_x+2k_x'-1)!!}{(2u+a^2)^{s+k_x+k_x'+1/2}}\sqrt{2\pi}. \tag{19}$$

Taking into account only the u-dependent part in Eq. (19) and its symmetric extension for y and z variables, we end up with the last integral which will lead to the final result. This last integral is expressed as:

$$\int_0^\infty (2u+a^2)^{-\Omega-3/2}\mathrm{d}u = \frac{1}{1+2\Omega}\frac{1}{a^{1+2\Omega}}, \tag{20}$$

where $\Omega=s_x+s_y+s_z+k_x+k_y+k_z+k_x'+k_y'+k_z'$.

Finally, collecting all the terms, we end up with the analytic expression for the Coulomb interaction matrix elements:

$$\mathcal{V}^{n_x^1 n_y^1 n_z^1 n_x^2 n_y^2 n_z^2}_{n_x^3 n_y^3 n_z^3 n_x^4 n_y^4 n_z^4} = \frac{1}{a}\sqrt{\frac{2}{\pi}}(-1)^{n_x^1+n_y^1+n_z^1+n_x^4+n_y^4+n_z^4-s_x-s_y-s_z}$$
$$\times \left(\frac{2^{n_{x+}^{14}}}{n_{x+}^{14}!}\frac{n_{x-}^{14}!}{2^{n_{x-}^{14}}}\frac{2^{n_{y+}^{14}}}{n_{y+}^{14}!}\frac{n_{y-}^{14}!}{2^{n_{y-}^{14}}}\frac{2^{n_{z+}^{14}}}{n_{z+}^{14}!}\frac{n_{z-}^{14}!}{2^{n_{z-}^{14}}}\right)^{1/2}\left(\frac{2^{n_{x+}^{23}}}{n_{x+}^{23}!}\frac{n_{x-}^{23}!}{2^{n_{x-}^{23}}}\frac{2^{n_{y+}^{23}}}{n_{y+}^{23}!}\frac{n_{y-}^{23}!}{2^{n_{y-}^{23}}}\frac{2^{n_{z+}^{23}}}{n_{z+}^{23}!}\frac{n_{z-}^{23}!}{2^{n_{z-}^{23}}}\right)^{1/2}$$
$$\times \sum_{k_x=0}^{n_{x-}^{14}}\frac{(-1)^{k_x}}{k_x!}\binom{n_{x+}^{14}}{n_{x-}^{14}-k_x}\sum_{k_x'=0}^{n_{x-}^{23}}\frac{(-1)^{k_x'}}{k_x'!}\binom{n_{x+}^{23}}{n_{x-}^{23}-k_x'}\frac{(2s_x+2k_x+2k_x'-1)!!}{2^{2s_x+k_x+k_x'}}$$
$$\times \sum_{k_y=0}^{n_{y-}^{14}}\frac{(-1)^{k_y}}{k_y!}\binom{n_{y+}^{14}}{n_{y-}^{14}-k_y}\sum_{k_y'=0}^{n_{y-}^{23}}\frac{(-1)^{k_y'}}{k_y'!}\binom{n_{y+}^{23}}{n_{y-}^{23}-k_y'}\frac{(2s_y+2k_y+2k_y'-1)!!}{2^{2s_y+k_y+k_y'}}$$
$$\times \sum_{k_z=0}^{n_{z-}^{14}}\frac{(-1)^{k_z}}{k_z!}\binom{n_{z+}^{14}}{n_{z-}^{14}-k_z}\sum_{k_z'=0}^{n_{z-}^{23}}\frac{(-1)^{k_z'}}{k_z'!}\binom{n_{z+}^{23}}{n_{z-}^{23}-k_z'}\frac{(2s_z+2k_z+2k_z'-1)!!}{2^{2s_z+k_z+k_z'}}$$
$$\times \frac{1}{1+2(s_x+s_y+s_z+k_x+k_x'+k_y+k_y'+k_z+k_z')}. \tag{21}$$

III. RECURRENCE

Due to the six summatories appearing in Eq. (21), if the indices start to grow to values say, just of the order of tenths, the process for calculating a single matrix element can be quite time-consuming, and thus, a real bottleneck for any numerical simulation. Using the recurrence relations that the Hermite polynomials obey, it is possible to find a simple iterative formula for the matrix elements which will accelerate the process of calculating the matrix elements.

Let $\{n_-,n_+\}$ be any pair of quantum numbers $\{n_{i-}^{jk},n_{i+}^{jk}\}$ with $i\in\{x,y,z\}$ and $jk\in\{14,23\}$, satisfying $n_+\geqslant n_-$. Then, the Coulomb matrix elements will satisfy (remaining indices ommitted for clarity)

$$\mathcal{V}_{n_-}^{n_+} = \sqrt{\frac{n_++1}{n_-}}\mathcal{V}_{n_--1}^{n_++1} + \sqrt{\frac{n_+}{n_-}}\mathcal{V}_{n_--1}^{n_+-1} - \sqrt{\frac{n_--1}{n_-}}\mathcal{V}_{n_--2}^{n_+}, \tag{22}$$

for $n_->0$. If we consider the unnormalized matrix elements

$$\bar{\mathcal{V}}^{n_x^1 n_y^1 n_z^1 n_x^2 n_y^2 n_z^2}_{n_x^3 n_y^3 n_z^3 n_x^4 n_y^4 n_z^4} = \prod_{i\in\{1,2,3,4\}}(2^{n_x^i}n_x^i!2^{n_y^i}n_y^i!2^{n_z^i}n_z^i!)^{1/2}$$
$$\times \mathcal{V}^{n_x^1 n_y^1 n_z^1 n_x^2 n_y^2 n_z^2}_{n_x^3 n_y^3 n_z^3 n_x^4 n_y^4 n_z^4}, \tag{23}$$

Eq. (22) can be transformed to

$$\bar{\mathcal{V}}_{n_-+1}^{n_+} = \bar{\mathcal{V}}_{n_-}^{n_++1} + 2n_+\bar{\mathcal{V}}_{n_-}^{n_+-1} - 2n_-\mathcal{V}_{n_--1}^{n_+}. \tag{24}$$

Another interesting recurrence relation which, this time involves four indices $\{0,n_+\}$ and $\{m_-,m_+\}$, is the following:

$$\bar{\mathcal{V}}_{0,m_-}^{n_+,m_++1} = \bar{\mathcal{V}}_{0,m_-}^{n_++1,m_+} + \bar{\mathcal{V}}_{0,m_--1}^{n_+,m_+}. \tag{25}$$

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A combinatorial approach for studying local operations and classical communication transformations of multipartite states

Sudhir Kumar Singh[a)]
Department of Electrical Engineering, University of California, Los Angeles, California 90095

Sudebkumar Prasant Pal[b)]
Department of Computer Science and Engineering, Indian Institute of Technology, Kharagpur-721302, India

Somesh Kumar[c)]
Department of Mathematics, Indian Institute of Technology, Kharagpur-721302, India

R. Srikanth[d)]
Raman Research Institute, Sadashiva Nagar, Bangalore-560080, Karnataka, India

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We develop graph theoretic methods for analyzing maximally entangled pure states distributed between a number of different parties. We introduce a technique called bicolored merging, based on the monotonicity feature of entanglement measures, for determining combinatorial conditions that must be satisfied for any two distinct multiparticle states to be comparable under local operations and classical communication. We present several results based on the possibility or impossibility of comparability of pure multipartite states. We show that there are exponentially many such entangled multipartite states among n agents. Further, we discuss a new graph theoretic metric on a class of multipartite states, and its implications. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2142840]

I. INTRODUCTION

Given the extensive use of quantum entanglement as a resource for quantum information processing,[6,19,23] the theory of entanglement, in particular, entanglement quantification, is a topic important to quantum information theory. However, apart from a limited number of cases like low dimension Hilbert spaces and for pure states, the mathematical structure of entanglement is not yet fully understood. The entanglement properties of bipartite states have been widely explored (see Refs. 8 and 12 for a comprehensive review). This has been aided by the fact that bipartite states possess the nice mathematical property in the form of the Schmidt decomposition,[19] the Schmidt coefficients encompassing all their nonlocal properties. No such simplifying structure is known in the case of larger systems. Approaches using certain generalizations of Schmidt decomposition[4,14,20] and group theoretic or algebraic methods,[15–17] have been taken in this direction. A number of methods for comparing or quantifying or qualifying entanglement have been proposed for bipartite systems and/or pure states such as entanglement of formation,[3] entanglement cost,[3,26] distillable entanglement,[3,21] relative entropy of entanglement,[11] negativity,[27]

[a)]Electronic mail: suds@ee.ucla.edu
[b)]Electronic mail: spp@cse.iitkgp.ernet.in
[c)]Electronic mail: smsh@maths.iitkgp.ernet.in
[d)]Electronic mail: srik@rri.res.in

concurrence,[28] and entanglement witnesses.[13] However, these quantifications do not always lend themselves to being computed, except in some restricted situations. As such, a general formulation is still an open problem.

It is known that state transformations under local operations and classical communication (LOCC) are very important to quantifying entanglement because LOCC can at the best increase only classical correlations. Therefore a good measure of entanglement is expected not to increase under LOCC. A necessary and sufficient condition for the possibility of such transformations in the case of bipartite states was given by Nielsen.[18] An immediate consequence of his result was the existence of *incomparable* states (the states that cannot be obtained by LOCC from one another). Bennett *et al.*,[4] formalized the notions of reducibility, equivalence and incomparability to multipartite states and gave a sufficient condition for incomparability based on *partial* entropic criteria.

In this work, our principal aim is not to quantify entanglement, but to develop graph theoretic techniques to analyze the comparability of maximally entangled multipartite states of several qubits distributed between a number of different parties. We obtain various qualitative results concerning reversibility of operations and comparability of states by observing the combinatorics of multiparitite entanglement. For our purpose, it is sufficient to consider the graph theoretic representation of various maximally entangled states (represented by specific graphs built from EPR, GHZ, and so on). Although this might at first seem overly restrictive, we will in fact be able to demonstrate a number of new results. Furthermore, being based only on the monotonicity principle, it can be adapted to any specific quantification of entanglement. Therefore, our approach is quite generic, in principle applicable to all entanglement measures. Since the entanglement of maximally entangled states is usually represented by integer values, it turns out that we can analyze entangled systems simply by studying the combinatorial properties of graphs and set systems representing the states. The basic definitions and concepts are introduced through the framework set in Sec. II. We introduce a technique called *bicolored merging* in Sec. III, which is essentially a combinatorial way of quantifying maximal entanglment between two parts of the system, and inferring transformation properties to be satisfied by the states.

In Sec. IV, we present our first result: the impossibility of obtaining two Einstein-Podolsky-Rosen (EPR) pairs among three players starting from a Greenberger-Horne-Zeilinger (GHZ) state (Theorem 2). We then show that this can be used to establish the impossibility of implementing a two-pronged teleportation (called *selective teleportation*) given preshared entanglement in the form of a GHZ state. We then demonstrate various classes of incomparable multipartite states in Sec. V. Finally, we discuss the minimum number of copies of a state required to prepare another state by LOCC and present bounds on this number in terms of the *quantum distance* between the two states in Sec. VII.

We believe that our combinatorial approach vastly simplifies the study of entanglement in very complex systems. Moreover, it opens up the road for further analysis, for example, to interpret entanglement topologically. In future works, we intend to apply and extend these insights to nonmaximal and mixed multipartite states, and to combine our approach with a suitable measure of entanglement.

II. THE COMBINATORIAL FRAMEWORK

In this section we introduce a number of basic concepts useful to describe combinatorics of entanglement. First, an *EPR graph* $G(V,E)$ is a graph whose vertices are the players ($\in V$) and edges ($\in E$) represent shared entanglement in the form of an EPR pair. Formally, we have the following.

Definition 1: EPR graph. For n agents $A_1,A_2,\ldots,A_n$ *an undirected graph* $G=(V,E)$ *is constructed as follows:* $V=\{A_i: i=1,2,\ldots,n\}$, $E=\{\{A_i,A_j\}: A_i$ *and* A_j *share an EPR pair,* $1\leqslant i,j.\leqslant n; i\neq j\}$. *The graph* $G=(V,E)$ *thus formed is called the EPR graph of the n agents.*

A spanning tree is a graph which connects all vertices without forming cycles (i.e., loops). Accordingly, we have the following.

Definition 2: Spanning EPR tree. A spanning tree *is a connected, undirected graph linking all vertices without forming cycles. An EPR graph* $G=(V,E)$ *is called a* spanning EPR tree *if the*

undirected graph $G=(V,E)$ is a spanning tree.

The above notions are generalized to more general multipartite entanglement by means of the concept of a *hypergraph.* A usual graph is built up from edges, where a normal edge links precisely two vertices. A hyperedge is a generalization that links r vertices, where $r \geqslant 2$. A graph endowed with at least one hyperedge is called a hypergraph. From the combinatorial viewpoint, a simple and interesting connection can be made between entanglement and hyperedges, an n-cat state (also sometimes called an n-GHZ state) corresponds to a hyperedge of size n. In particular, an EPR state corresponds to a simple edge connecting only two vertices. Formally, we have the following.

Definition 3: Entangled hypergraph. Let S be the set of n agents and $F=\{E_1,E_2,\ldots,E_m\}$, where $E_i \subseteq S; i=1,2,\ldots,m$ and E_i is such that its elements (agents) are in $|E_i|$-CAT state. The hypergraph (set system) $H=(S,F)$ is called an entangled hypergraph of the n agents.

A graph is connected if there is a path (having a length of one or more edges) between any two vertices. Accordingly, we have the following.

Definition 4: Connected entangled hypergraph. A sequence of j hyperedges $E_1,E_2,\ldots,E_j$ in a hypergraph $H=(S,F)$ is called a hyperpath (path) from a vertex a to a vertex b if

(1) *E_i and E_{i+1} have a common vertex for all $1 \leqslant i \leqslant j-1$,*
(2) *a and b are agents in S,*
(3) *$a \in E_1$, and*
(4) *$b \in E_j$.*

If there is a hyperpath between every pair of vertices of S in the hypergraph H, we say that H is connected.

Analogous to a spanning EPR tree we have the following.

Definition 5: Entangled hypertree. A connected entangled hypergraph $H=(S,F)$ is called an entangled hypertree if it contains no cycles, that is, there do not exist any pair of vertices from S such that there are two distinct paths between them.

Further, we have the following.

Definition 6: r-uniform entangled hypertree: An entangled hypertree is called an r-uniform entangled hypertree if all of its hyperedges are of size r for $r \geqslant 2$.

In ordinary graphs, a vertex that terminates, i.e., has precisely a single edge linked to it is called a terminal or pendent vertex. This concept is extended to the case of hypergraphs.

Definition 7: Pendant vertex. A vertex of a hypergraph $H=(S,F)$ such that it belongs to only one hyperedge of F is called a pendant vertex in H. Vertices which belong to more than one hyperedge of H are called nonpendant.

In the paper we use polygons for pictorially representing an entangled hypergraph of multipartite states. (There should be no confusion with a closed loop of EPR pairs because we consider only tree structured states.) A hyperedge representing an n-CAT amongst the parties $\{i_1,i_2,\ldots,i_n\}$ is pictorially represented by an n-gon with vertices distinctly numbered by $i_1,i_2,\ldots,i_n$. We write these vertices $i_1,i_2,\ldots,i_n$ corresponding to the n vertices of the n-gon in the pictorial representation in arbitrary order. This only means that out of n qubits of the n-CAT, one qubit is with each of the n parties.

A result we will require frequently is that there exist teleportation[2] protocols to produce n-partite entanglement starting from pairwise entanglement shared along any spanning tree connecting the n parties. That is, there exist LOCC protocols to turn a n-party spanning EPR tree into an n-regular hypergraph consisting of a single hyperedge of size n. The protocol is detailed in Refs. 24 and 23, but the basic idea is readily described. It is essentially a scheme to deterministically create a maximally entangled n-cat state from $n-1$ EPR pairs shared along a spanning tree. Briefly, the protocol consists in teleporting entanglement along a spanning tree. Players not on terminal vertices along the tree execute the following subroutine. Suppose player Alice shares an m-cat with $(m-1)$ preceding players along the tree and wishes to create an $(m+1)$-cat state including Bob, the next player down the tree. First she entangles an auxiliary particle with her

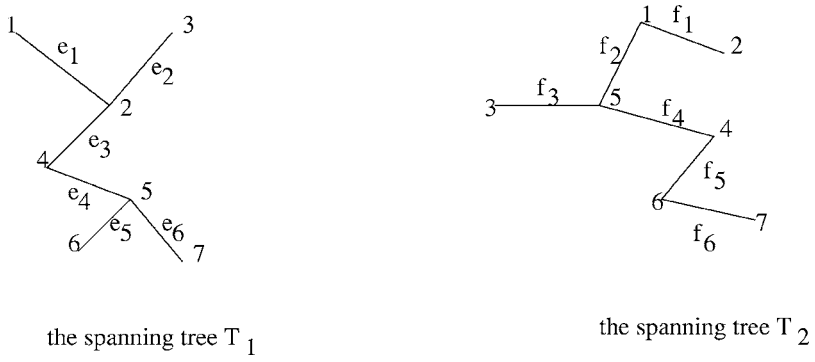

FIG. 1. Spanning EPR trees T_1 and T_2.

particle in the m-cat state by means of local operation. She then uses her EPR pair shared with Bob to teleport the state of the auxiliary particle to Bob. The $(m+1)$ players, including Alice and Bob, now share an $(m+1)$-cat state, as desired.

Another result we will require in some of our proofs, given as the theorem below, is that the spanning EPR tree mentioned above is also a necessary condition to prepare an n-CAT state starting from shared EPR pairs.

Theorem 1: *Given a communication network of n agents with only EPR pairs permitted for pairwise entanglement between agents, a necessary condition for creation of a n-CAT state is that the EPR graph of the n agents must be connected.*

Proof of the theorem is given in Appendix A using our method of bicolored merging developed in Sec. III.

III. BICOLORED MERGING

Monotonicity is easily the most natural characteristic that should be satisfied by all entanglement measures.[12] It requires that any appropriate measure of entanglement must not change under local unitary operations and more generally, the expected entanglement must not increase under LOCC. We should note here that in LOCC, LO involves unitary transformations, additions of ancillas (that is, enlarging the Hilbert space), measurements, and throwing away parts of the system, each of these actions performed by one party on his or her subsystem. CC between the parties allows local actions by one party to be conditioned on the outcomes of the earlier measurements performed by the other parties.

Apart from monotonicity, there are certain other characteristics required to be satisfied by entanglement measures. However, monotonicity itself vastly restricts the choice of entanglement measures (for example, marginal entropy as a measure of entanglement for bipartite pure states or entanglement of formation for mixed states). In the present work, we find that monotonicity, where proven for a particular entanglement measure candidate, restricts a large number of state transformations and gives rise to several classes of incomparable (multipartite) states. So, in order to study the possible state transformations of (multipartite) states under LOCC, it would be interesting to look at the kind of state transforms under LOCC which monotonicity does not allow. We can observe that monotonicity does not allow the preparation of $n+1$ or more EPR pairs between two parties starting from only n EPR pairs between them. In particular, it is not possible to prepare two or more EPR pairs between two parties starting only with a single EPR pair and only LOCC. This is an example of impossible state transformation in the bipartite case as dictated by the monotonicity postulate. We anticipate that a large class of multipartite states could also be shown to be incomparable by using impossibility results for the bipartite case through suitable reductions. For instance, consider transforming (under LOCC) the state represented by a spanning EPR tree, say T_1, to that of the state represented by another spanning EPR tree, say T_2 (see Fig. 1). This transformation can be shown to be impossible by reducing to the bipartite case as follows: We

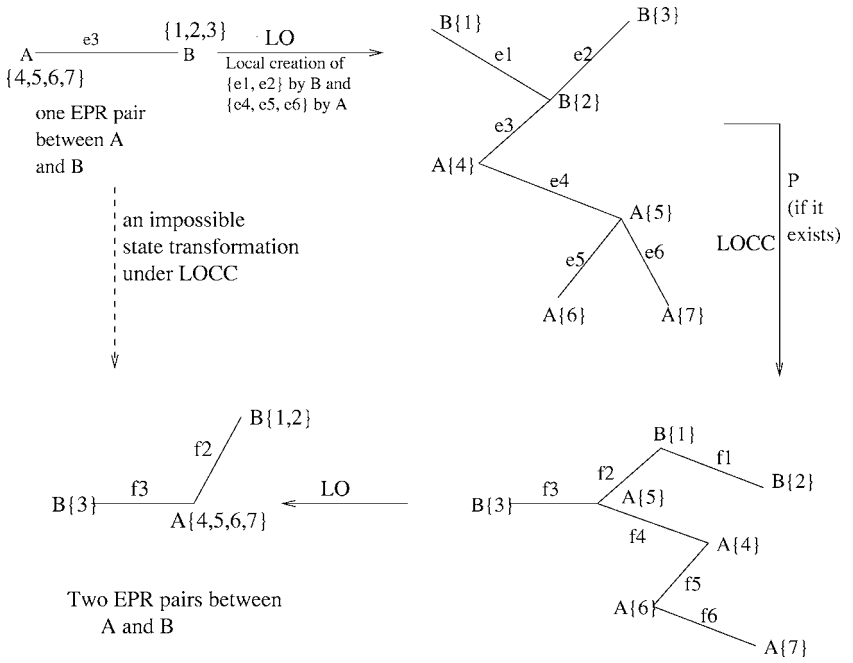

FIG. 2. Converting T_1 to T_2 under LOCC.

assume for the sake of contradiction that there exists a protocol P which can perform the required transformation. It is easy to see that the protocol P is also applicable in the case when a party A possesses all the qubits of parties 4, 5, 6, and 7 and another party B possesses all the qubits of the parties 1, 2, and 3. This means that party A is playing the role of parties 4, 5, 6, and 7 and B is playing the role of parties 1, 2, and 3. Clearly, any LOCC actions done within group {1, 2, 3} ({4, 5, 6, 7}) is a subset of LO available to B (A) and any CC done between one party from {1, 2, 3} and the other from {4, 5, 6, 7} is managed by CC between B and A.

Therefore, starting only with one edge (e_3) they eventually construct T_1 just by LO (by local creation of EPR pairs representing the edges e_1, e_2, e_4, e_5, and e_6 ($\{e_1,e_2\}$ by B and $\{e_4,e_5,e_6\}$ by A). They then apply protocol P to obtain T_2 with the edges f_1, f_2, f_3, f_4, f_5, and f_6 (refer to Fig. 2). All edges except f_2 and f_3 are local EPR pairs (that is, both qubits are with the same party, A or B). Now the parties A and B share two EPR pairs in the form of the edges f_2 and f_3, even though they started sharing only one EPR pair. But this is in contradiction with monotonicity, that expected entanglement should not increase under LOCC. Hence, we can conclude that such a protocol P cannot exist.

The approach we took in the above example could also be motivated from the marginal entropic criterion (noting that this criterion in essence is also a direct implication of monotonicity). As clear from the above example, the above scheme aims to create a bipartition among the n players in such a way that the marginal entropy of each partition is different for the two states. In many cases, this difference will simply correspond to different number of EPR pairs shared between the two partitions. Given two multipartite states, the relevant question is, "is there a bipartition such that the marginal entropy for the two states is different?" If yes, then the state (configuration of entanglement) corresponding to the higher entropy cannot be obtained from that to lower entropy by means of LOCC. It is convenient to imagine the two partitions being colored distinctly to identify the partitions which they make up.

In general, suppose we want to show that the multipartite state $|\psi\rangle$ cannot be converted to the multipartite state $|\phi\rangle$ by LOCC. This can be done by showing an assignment of the qubits (of all parties) to only two parties such that $|\psi\rangle$ can be obtained from n ($n=0,1,2,\ldots$) EPR pairs between the two parties by LOCC while $|\phi\rangle$ can be converted to more than n EPR pairs between

the two parties by LOCC. This is equivalent to saying that each party is given either of two colors (say A or B). Finally all qubits with parties colored with color A are assigned to the first party (say A) and that with parties colored with the second color to the second party (say B). This coloring is done in such a way that the state $|\psi\rangle$ can be obtained by LOCC from less number of EPR pairs between A and B than that obtained from $|\phi\rangle$ by LOCC. Local preparation (or throwing away) of EPR pairs is what we call merging in combinatorial sense. Keeping this idea in mind, we now formally introduce the idea of bicolored merging for such reductions in the case of the multipartite states represented by EPR graphs and entangled hypergraphs.

Suppose that there are two EPR graphs $G_1=(V,E_1)$ and $G_2=(V,E_2)$ on the same vertex set V (this means that these two multipartite states are shared amongst the same set of parties) and we want to show the impossibility of transforming G_1 to G_2 under LOCC, then this is reduced to a bipartite LOCC transformation which violates monotonicity, as follows:

(1) Bicoloring, assign either of the two colors A or B to every vertex, that is, each element of V.
(2) Merging, for each element $\{v_i,v_j\}$ of E_1, merge the two vertices v_i and v_j if and only if they have been assigned the same color during the bicoloring stage and assign the same color to the merged vertex. Call this graph obtained from G_1 as BCM (bicolored-merged) EPR graph of G_1 and denote it by G_1^{bcm}. Similarily, obtain the BCM EPR graph G_2^{bcm} of G_2.
(3) The bicoloring and merging is done in such a way that the graph G_2^{bcm} has more number of edges than that of G_1^{bcm}.
(4) Give all the qubits possessed by the vertices with color A to the first party (say, party A) and all the qubits possessed by the vertices with color B to the second party (say, party B). Combining this with the previous steps, it is ensured that in the bipartite reduction of the multipartite state represented by G_2, the two parties A and B share more number of EPR pairs (say, state $|\psi_2\rangle$) than that for G_1 (say, state $|\psi_1\rangle$).

We denote this reduction as $G_1 \not> G_2$. Now if there exits a protocol P which can transform G_1 to G_2 by LOCC, then P can also transform $|\psi_1\rangle$ to $|\psi_2\rangle$ just by LOCC as follows: A (B) will play the role of all vertices in V which were colored as A (B). The edges which were removed due to merging can easily be created by local operations (local preparation of EPR pairs) by the party A (B) if the color of the merged end vertices of the edge was assigned color A (B). This means that starting from $|\psi_1\rangle$ and only LO, G_1 can be created. This graph is virtually amongst $|V|$ parties even though there are only two parties. The protocol P then, can be applied to G_1 to obtain G_2 by LOCC. Subsequently $|\psi_2\rangle$ can be obtained by the necessary merging of vertices by LO, that is by throwing away the local EPR pair represented by the edges between the vertices being merged. Since the preparation of $|\psi_2\rangle$ from $|\psi_1\rangle$ by LOCC violates the monotonocity postulate, such a protocol P cannot exist. An example of bicolored merging for EPR graphs has been illustrated in Fig. 3.

The bicolored merging in the case of entangled hypergraphs is essentially the same as that for EPR graphs. For the sake of completeness, we present it here. Suppose there are two entangled hypergraphs $H_1=(S,F_1)$ and $H_2=(S,F_2)$ on the same vertex set S (that is, the two multipartite states are shared amongst the same set of parties) and we want to show the impossibility of transforming H_1 to H_2 under LOCC. Transformation of H_1 to H_2 can be reduced to a bipartite LOCC transformation which violates monotonicity thus proving the impossibility. The reduction is done as follows:

(1) Bicoloring, assign either of the two colors A or B to every vertex, that is, each element of S.
(2) Merging, for each element $E=\{v_{i1},v_{i2},\ldots,v_{ij}\}$ of $F_1(F_2)$, merge all vertices with color A to one vertex and those with color B to another vertex and give them colors A and B, respectively. This merging collapses each hyperedge to either a simple edge or a vertex and thus the hypergraph reduces to a simple graph with vertices assigned with either of the two colors A or B. Call this graph obtained from H_1 as BCM EPR graph of H_1 and denote it by H_1^{bcm}. Similarily obtain the BCM EPR graph H_2^{bcm} of H_2.
(3) The bicoloring and merging is done in such a way that the graph H_2^{bcm} has more number of edges than that of H_1^{bcm}.

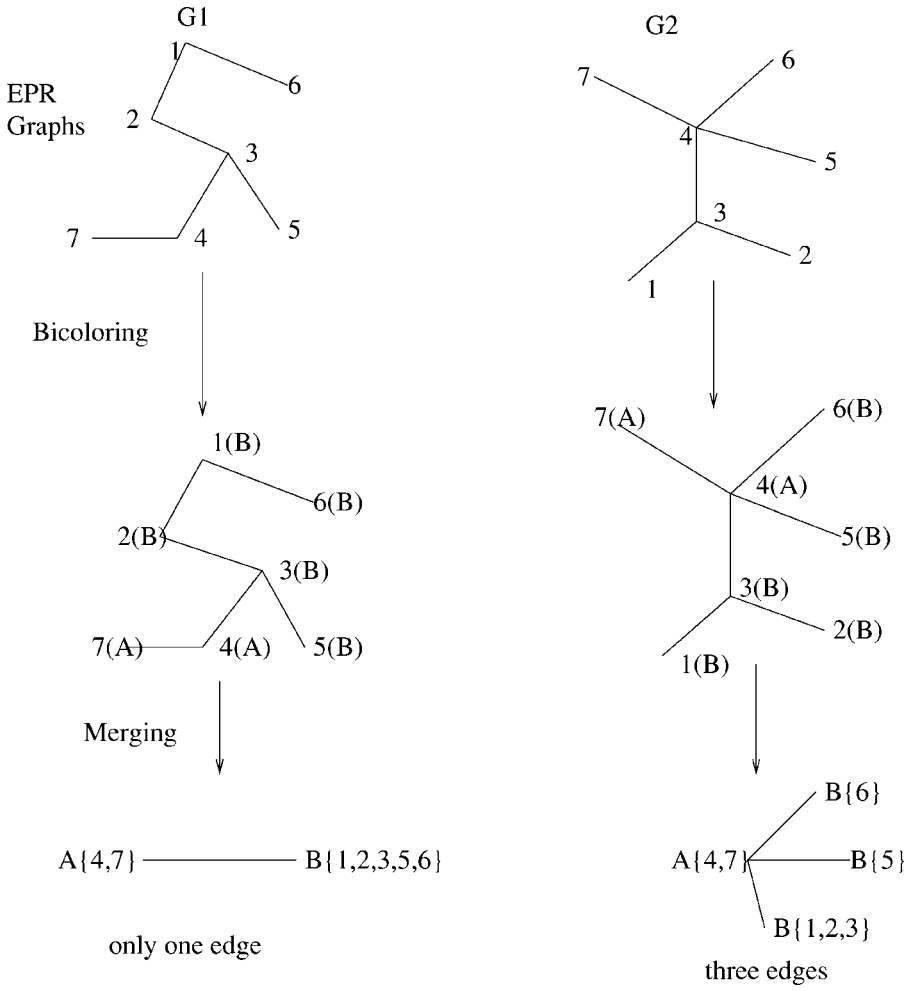

FIG. 3. Bicolored merging of EPR graphs.

(4) Give all the qubits possessed by the vertices with color A to the party one (say party A) and all the qubits possessed by the vertices with color B to the second party (say party B).

We denote the above reduction as $H_1 \succ H_2$. The rest of the discussion is similar to that for the case of EPR graphs given before. In Fig. 4, we demostrate the bicolored merging of entangled hypergraphs. Note that the two entangled hypergraphs H_1 and H_2 are LOCC comparable only if one of $H_1 \succ H_2$ and $H_2 \succ H_1$ is not true. Equivalently, if both of $H_1 \succ H_2$ and $H_2 \succ H_1$ hold, then the entangled hypergraphs H_1 and H_2 are incomparable.

It is also interesting to note at this point that LOCC incomparability shown by using the method of bicolored merging is in fact *strong incomparability* as defined in Ref. 1. We would also like to stress that any kind of reduction (in particular, various possible extensions of bicolored merging) which leads to the violation of *any* of the properties of a potential entanglement measure, is pertinent to show the impossibility of many multipartite state transformations under LOCC. Since the bipartite case has been extensively studied, such reductions can potentially provide many ideas about multipartite case by just exploiting the results from the bipartite case. In particular, the definitions of EPR graphs and entangled hypergraphs could also be suitably extended to capture more types of multipartite pure states and even mixed states and a generalization of the idea of bicolored merging as a suitable reduction for this case could also be worked out.

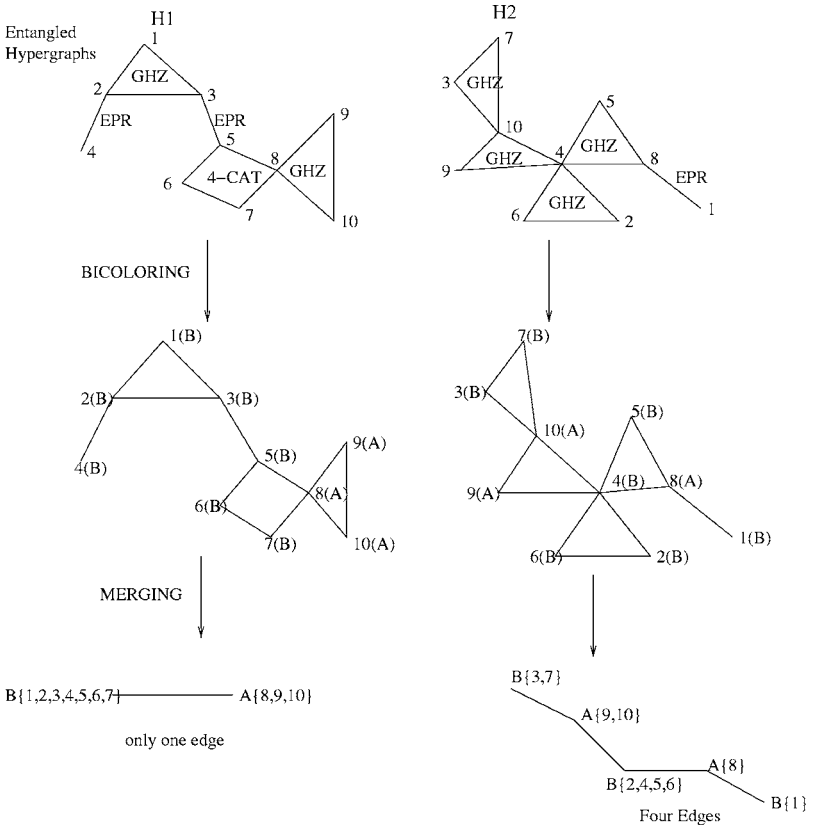

FIG. 4. Bicolored merging of entangled hypergraphs.

IV. LOCC INCOMPARABILITY AND SELECTIVE TELEPORTATION

We know that a GHZ state amongst three agents A, B, and C can be prepared from EPR pairs shared between any two pairs of the three agents using only LOCC.[24,7,29,30] We consider the problem of *reversing* this operation, that is, whether it is possible to construct two EPR pairs between any two pairs of the three agents from a GHZ state amongst the three agents, using only LOCC. By using the method of bicolored merging, we answer this question in the negative by establishing the following theorem.

Theorem 2: *Starting from a GHZ state shared amongst three parties in a communication network, two EPR pairs cannot be created between any two sets of two parties using only LOCC.*

Proof: Suppose there exists a protocol P for *reversing* a GHZ state into two EPR pairs using only LOCC. In particular, suppose protocol P starts with a GHZ state amongst the agents A, B, and C, and prepares EPR pairs between any two pairs of A, B, and C (say, $\{A,C\}$, and $\{B,C\}$, corresponding to configuration G_1 as shown in Fig. 5). Since we can prepare the GHZ state from EPR pairs between any two pairs of the three agents, we can prepare the GHZ state starting from EPR pairs between A and B, and A and C. Once the GHZ state is prepared, we can apply protocol P to construct EPR pairs between A and C and between B and C using only LOCC (i.e., configuration $G_2 \equiv \{\{A,C\},\{B,C\}\}$). So, we can use only LOCC to convert a configuration where EPR pairs exist between A and C and between A and B, to a configuration where EPR pairs are shared between A and C and between B and C. The possibility of P means that the marginal entropy of C can be increased using only LOCC, which is known to be impossible. □

The same result could also be achieved by similar bicolored merging directly applied on the GHZ state and any of G_1 or G_2 but we prefer the above proof for stressing the argument on the symmetry of G_1 and G_2 with respect to the GHZ. Moreover, this proof gives an intuition about

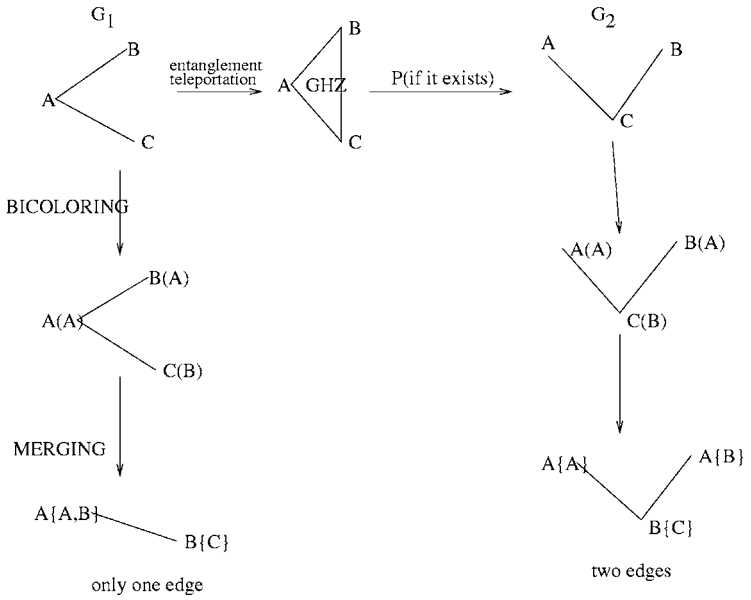

FIG. 5. LOCC irreversibility of the process [2 EPR $\rightarrow$ GHZ].

possibility of incomparability amongst spanning EPR trees as G_1 and G_2 are two distinct spanning EPR trees on three vertices. We prove this general result in the Theorem 8.

The above theorem motivates us to propose some kind of comparison between a GHZ state and two pairs of EPR pairs in terms of the nonlocal correlations they possess. In this sense, therefore, a GHZ state may be viewed as less than two EPR pairs. It is easy to see that an EPR pair between any two parties can be obtained starting only from a GHZ state shared amongst the three parties and LOCC. The third party will just do a measurement in the diagonal basis and send the result to the other two. By applying the corresponding suitable operations they get the required EPR pair. From Theorem 1, we observe that a single EPR pair, between any two of the three parties, is not sufficient for preparing a GHZ state amongst the three parties using only LOCC. These arguments can be summarized in the following theorem.

Theorem 3: *1-EPR pair* $<_{LOCC}$ *a GHZ state* $<_{LOCC}$ *2-EPR pairs.*

An interesting problem in quantum information theory is that of *selective teleportation*.[22] Given three agents A, B, and C, and two qubits of unknown quantum states $|\psi_1\rangle$ and $|\psi_2\rangle$ with A, the problem is to send $|\psi_1\rangle$ to B and $|\psi_2\rangle$ to C selectively, using only LOCC and *a priori* entanglement between the three agents. A simple solution to this problem is applying standard teleportation,[2] in the case where A shares EPR pairs with both B and C. An interesting question is whether any other form of *a priori* entanglement can help achieving selective teleportation. In particular, is it possible to perform selective teleportation where the *a priori* entanglement is in the form of a GHZ state amongst the three agents? The following theorem answers this question using the result of the Theorem 2.

Theorem 4: *With a priori entanglement given in the form of a GHZ state shared amongst three agents, two qubits cannot be selectively teleported by ane of the three parties to the other two parties.*

Proof: Suppose there exists a protocol P which can enable one of the three parties (say A) to teleport two qubits $|\psi_1\rangle$ and $|\psi_2\rangle$ selectively to the other two parties (say B and C). Now A takes four qubits; she prepares two EPR pairs one from the first and second qubits and the other from the third and fourth qubits. He then teleports the first and third qubits selectively to B and C using P (consider first qubit as $|\psi_1\rangle$ and the third qubit as $|\psi_2\rangle$). We can note here that in this way A is able to share one EPR pair each with B and C. But this is impossible because it allows A to prepare two EPR pairs starting from a GHZ state and only using LOCC. This contradicts Theorem 2. Hence follows the result. □

V. COMBINATORIAL CONDITIONS FOR LOCC INCOMPARABILITY OF EPR GRAPHS

An immediate result comparing an n-CAT state with EPR pairs follows from noting that, given a spanning EPR tree among n parties, an n-CAT state can be constructed using only LOCC using the teleportation protocol described in Sec. II. The result we present below generalizes Theorem 3.

Theorem 5: *1-EPR pair* $<_{LOCC}$ *n-CAT* $<_{LOCC}$ $(n-1)$*-spanning EPR tree.*

We can argue in a similar manner that an n-CAT state amongst n-parties cannot be converted by just using LOCC to any form of entanglement structure which possesses EPR pairs between any two or more different sets of two parties. Assume this is possible for the sake of contradiction. Then the two edges could be in either of the two forms: (1) $\{i_1,i_2\}$ and $\{j_1,j_2\}$ and (2) $\{i_1,i_2\}$ and $\{i_2,j_2\}$, where i_1,i_2,j_1,j_2 are all distinct. In bicolored-merging assign the colors as follows. In case (1), give color A to i_2 and j_2 and give the color B to the rest of the vertices. In case (2), give color A to i_2 and color B to the rest of the vertices. Since both the cases are contrary to our assumption, the assertion follows. Moreover, from Theorem 1 (see Appendix A for proof), no disconnected EPR graph would be able to yield n-CAT just by LOCC. These two observations combined together lead to the following theorem which signifies the fact that these two multipartite states cannot be compared.

Theorem 6: *A CAT state amongst n agents in a communication network is LOCC incomparable to any disconnected EPR graph associated with the n agents having more than one edge.*

The above result indicates that there are many possible forms of entanglement structures (multipartite states) which cannot be compared at all in terms of nonlocal correlations they may have. This simple result is just an implication of the necessary combinatorics required for the preparation of CAT states. One more interesting question with respect to this combinatorics is to compare a spanning EPR tree and a CAT state. A spanning EPR tree is combinatorially sufficient for preparing the CAT state and thus seems to entail more nonlocal correlations than in a CAT state. The question whether this ordering is strict needs to be further investigated. It is easy to see that an EPR pair between any two parites can be obtained starting from a CAT state shared amongst the n agents just by LOCC (Theorem 5). Therefore, given $n-1$ copies of the CAT state we can build all the $n-1$ edges of any spanning EPR tree just by LOCC. But whether this is the lower bound on the number of copies of n-CAT required to obtain a spanning EPR tree is even more interesting. The following theorem shows that this is indeed the lower bound.

Theorem 7: *Starting with only* $n-2$ *copies of n-CAT state shared amongst its n agents, no spanning EPR tree of the n agents can be obtained just by LOCC.*

Proof: Suppose it is possible to create a spanning EPR tree T from $(n-2)$ copies of n-CAT states. As we know, an n-CAT state can be prepared from any spanning EPR tree by LOCC.[24,7,29,30] Thus, if $(n-2)$ copies of n-CAT can be converted to T, then $(n-2)$ copies of any spanning EPR tree can be converted to T just by LOCC. In particular, $(n-2)$ copies of a chain EPR graph (which is clearly a spanning EPR tree, Fig. 6) can be converted to T just by LOCC. Now, we know that any tree is a bipartite connected graph with $n-1$ edges across the two parts. Let vertices $i_1,i_2,\ldots,i_m$ be the members of the first group and the rest be in the other group. Construct a chain EPR graph where the first m vertices are $i_1,i_2,\ldots,i_m$ in the sequence, and the rest of the vertices are from the other group in the sequence (Fig. 6). In bicolored merging, we give the color A to the parties $\{i_1,i_2,\ldots,i_m\}$ and the rest of the parties are given the color B. This way we are able to create $(n-1)$ EPR pairs (note that there are $n-1$ edges in T across the two groups) between A and B starting from only $(n-2)$ EPR pairs (considering the $n-2$ chainlike spanning EPR trees). So, we conclude that $(n-2)$ copies of n-CAT cannot be converted to any spanning EPR tree just by LOCC. See Fig. 6 for illustration of the required bicolored merging. The proof could also be acheived by similar kind of bicolored merging directly applied on n-CAT and T. □

In the preceding results we have compared spanning EPR trees with CAT states. We discuss the comparability/incomparability of two distinct spanning EPR trees in the next theorem and corollary.

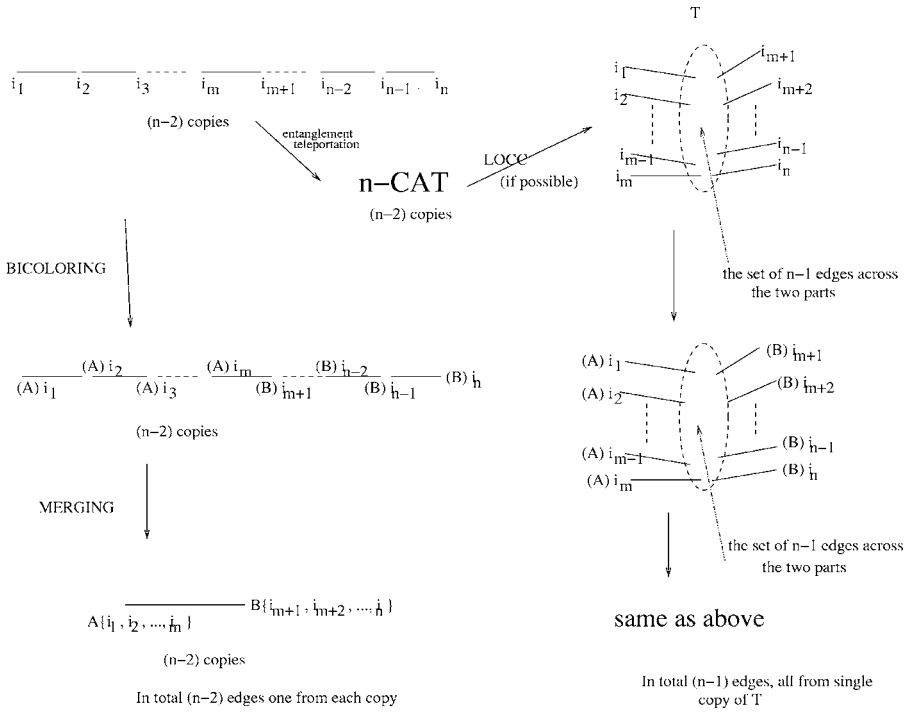

FIG. 6. $n-2$ copies of n-CAT are not sufficient to prepare a spanning EPR tree.

Theorem 8: *Any two distinct spanning EPR trees are LOCC incomparable.*

Proof: Let T_1 and T_2 be the two distinct spanning EPR trees on the same n vertices. Clearly, there exist two vertices (say i and j) which are connected by an edge in T_2 but not in T_1. Also by virtue of connectedness of spanning trees, there will be a path between i and j in T_1. Let this path be $ik_1k_2\cdots k_mj$ with $m>0$ (see Fig. 7). Since $m>0$, k_1 must exist.

Let $T_i^1 \equiv$ subtree in T_1 rooted at i except for the branch which contains the edge $\{i,k_1\}$, $T_j^1 \equiv$ subtree in T_1 rooted at j except for the branch which contains the edge $\{j,k_m\}$, $T_{k_r} \equiv$ subtree in T_1 rooted at k_r except for the branches which contain either of the edges $\{k_{r-1},k_r\}$ and $\{k_r,k_{r+1}\}$ ($k_0=i$, $k_{m+1}=j$), $T_i^2 \equiv$ subtree in T_2 rooted at i except for the branch which contains the edge $\{i,j\}$, and $T_j^2 \equiv$ subtree in T_2 rooted at j except for the branch which contains the edge $\{i,j\}$.

It is easy to see that the set $T_i^2 \cup T_j^2$ is nonempty as T_1 and T_2, being distinct, must contain more than two vertices. Also T_i^2 and T_j^2 must be disjoint; for, otherwise there will be a path between i and j in T_2 which does not contain the edge $\{i,j\}$. Thus there will be two paths between i and j in T_2 contradicting the fact that T_2 is a spanning EPR tree (Fig. 7). With these two charactistics of T_i^2 and T_j^2, it is clear that k_1 will lie either in T_i^2 or in T_j^2. Without loss of generality, let us assume that $k_1 \in T_i^2$. Now we do bicolored merging where the color A is assigned to i and all vertices in T_i^1 and the color B is assigned to the rest of the vertices (refer to Fig. 7 for illustration). Since T_1 and T_2 were chosen arbitrarily, the same arguments also imply that there cannot exist a method which converts T_2 to T_1. This leads to the conclusion that any two distinct spanning EPR trees are LOCC incomparable.

Corollary 1: There are at least exponentially many LOCC-incomparable classes of pure multipartite entangled states.

Proof: We know from results in graph theory[9] that on a labelled graph on n vertices, there are n^{n-2} posible distinct spanning trees. Hence there are n^{n-2} distinct spanning EPR trees in a network of n agents. From Theorem 8 all these spanning EPR trees are LOCC incomparable. It can be noted here that the most general local operation of n qubits is an element of the group $U(2)^n$ (local unitary rotations on each qubit alone). So, if two states are found incomparable, this means that there are actually two incomparable equivalence classes of states [where members in a class are

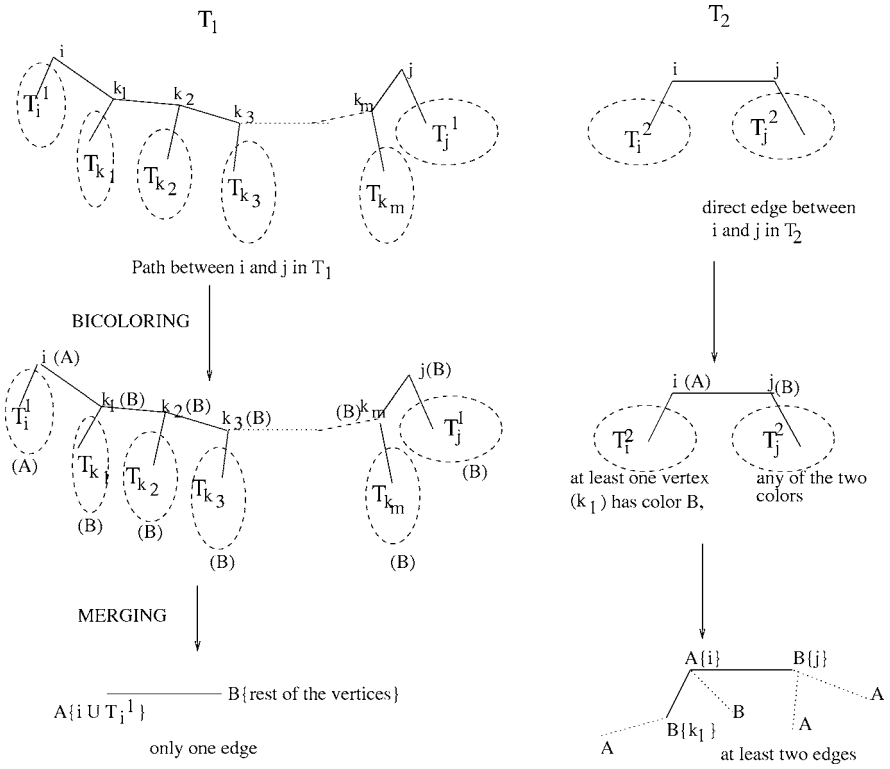

FIG. 7. Spanning EPR trees are LOCC incomparable.

related by a $U(2)^n$ transformation]. Thus we have at least exponentially many LOCC-incomparable classes of multipartite entangled states. □

VI. COMBINATORIAL CONDITIONS FOR LOCC INCOMPARABILITY OF ENTANGLED HYPERGRAPHS

Since entangled hypergraphs represent more general entanglement structures than those represented by the EPR graphs (in particular spanning EPR trees are nothing but 2-uniform entangled hypertrees), it is likely that there will be even more classes of incomparable multipartite states and this motivates us to generalize Theorem 8 for entangled hypertrees. However, remarkably this intuition does not work directly and there are entangled hypertrees which are not incomparable. But there are a large number of entangled hypertrees which do not fall under any such partial ordering and thus remain incomparable. To this end we present our first imcomparability result on entangled hypergraphs.

Theorem 9: *Let $H_1=(S,F_1)$ and $H_2=(S,F_2)$ be two entangled hypertrees. Let P_1 and P_2 be the set of pendant vertices of H_1 and H_2, respectively. If the sets $P_1\backslash P_2$ and $P_2\backslash P_1$ are both nonempty then the multipartite states represented by H_1 and H_2 are necessarily LOCC incomparable.*

Proof: Using bicolored merging we first show that H_1 cannot be converted to H_2 under LOCC. Impossibility of the reverse conversion will also be immediate. Since $P_1\backslash P_2$ is nonempty, there exists $u \in S$ such that $u \in P_1\backslash P_2$. That is, u is pendant in H_1 but nonpendant in H_2 (Fig. 8).

In the bicolored merging assign the color A to the vertex u and the color B to all other vertices. This reduces H_1 to a single EPR pair shared between the two parties A and B whereas H_2 reduces to at least two EPR pairs shared between A and B. The complete bicolored merging is shown in Fig. 8. □

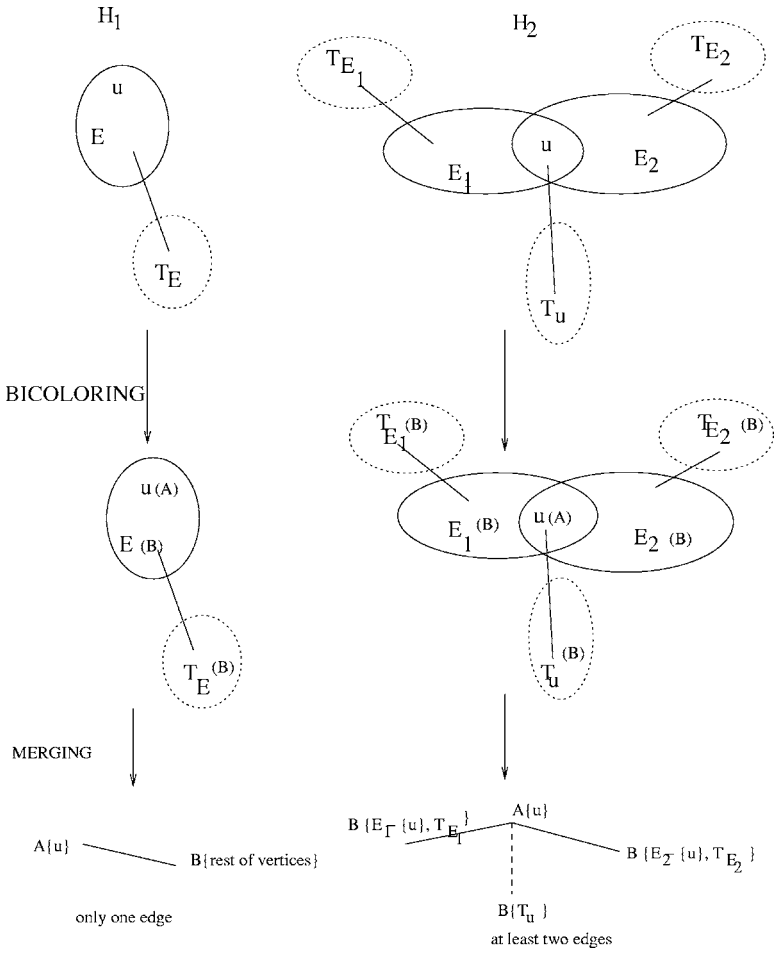

FIG. 8. Entangled hypergraphs with $P_1 \backslash P_2$ nonempty.

We note that this proof does not utilize the fact that H_1 and H_2 are entangled hypertrees, and thus the theorem is indeed true even for entangled hypergraphs satisfying the conditions specified on the set of pendant vertices.

The conditions specified on the set of pendant vertices in Theorem 9 cover a very small fraction of the entangled hypergraphs. However, these conditions are not necessary and it may be possible to find further characterizations of incomparable classes of entangled hypergraphs. We present two examples where the conditions of Theorem 9 are not satisfied.

Example 1: (Figs. 9 and 10) $P_1 \neq P_2$ but either $P_1 \subset P_2$ or $P_2 \subset P_1$.

Example 2: (Fig. 11) $P_1 = P_2$.

In the first example, the entangled hypergraphs H_1 and H_2 staisfy $P_1 \neq P_2$ and $P_1 \subset P_2$. H_1 and H_2 are comparable in Fig. 9 but incomparable in Fig. 10. In Fig. 10, the incomparability has been proved by showing that H_1 is not convertible to H_2 under LOCC because the impossibility of reverse conversion follows from the proof of Theorem 9 ($P_2 \backslash P_1 \neq \phi$). Figure 11 gives examples of comparable and incomparable entangled hypergraphs with condition $P_1 = P_2$.

Theorem 8 shows that two distinct EPR spanning trees are LOCC incomparable and the spanning EPR trees are nothing but 2-uniform entangled hypertrees. Therefore, a natural generalization of this theorem would be to r-uniform entangled hypertrees for any $r \geqslant 3$. As we show below, the generalization indeed holds. It should be noted that Theorem 9 does not necessarily capture such entanglement structures (multipartite states) (Fig. 12). However, in order to prove

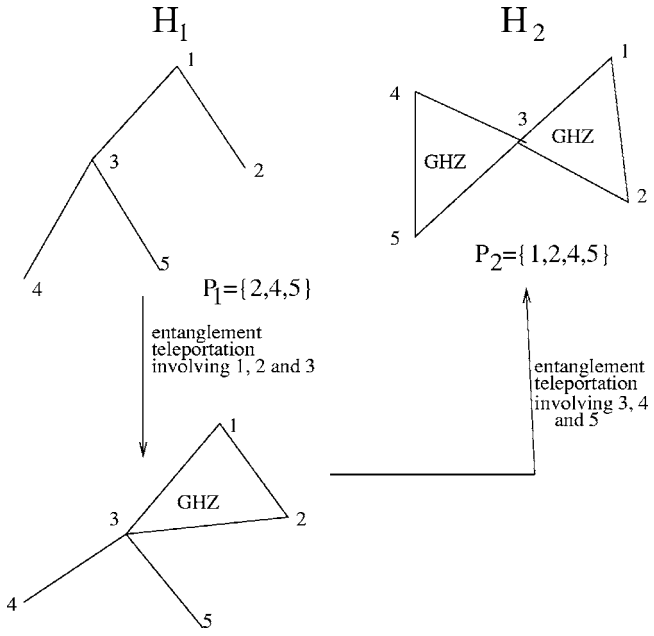

FIG. 9. Comparable with $P_1 \neq P_2$ and $P_1 \subset P_2$.

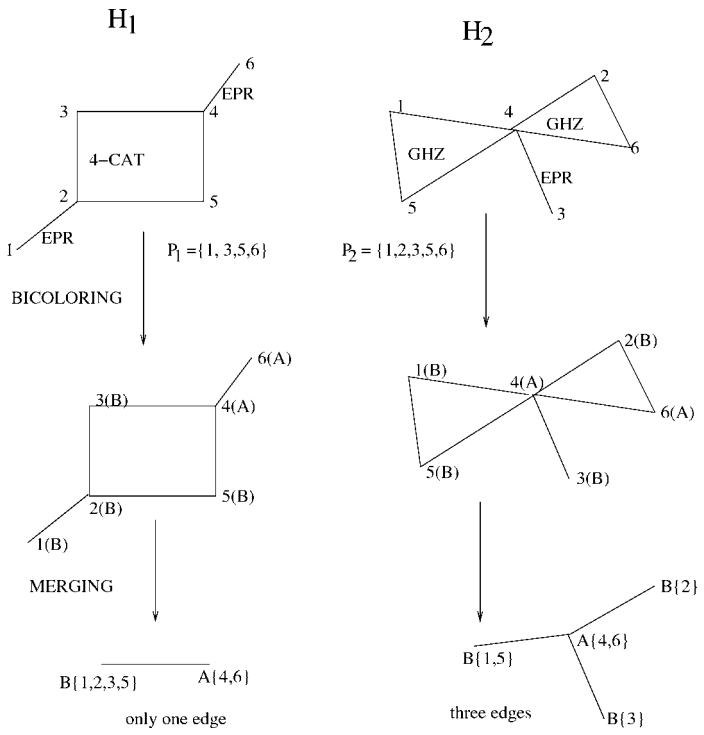

FIG. 10. Incomparable with $P_1 \neq P_2$ and $P_1 \subset P_2$.

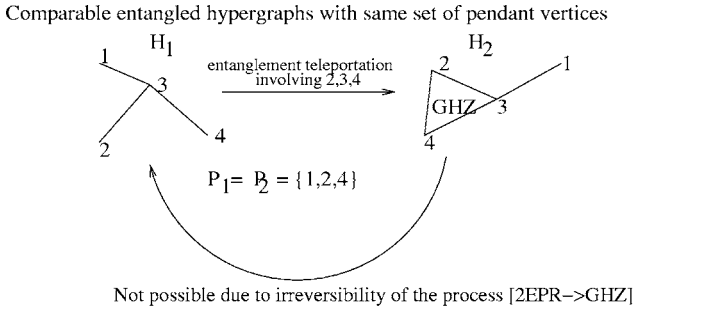

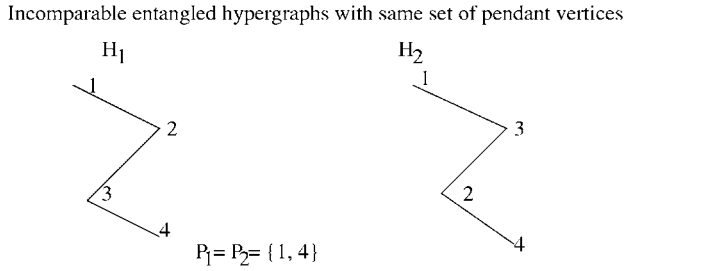

FIG. 11. $P_1 = P_2$.

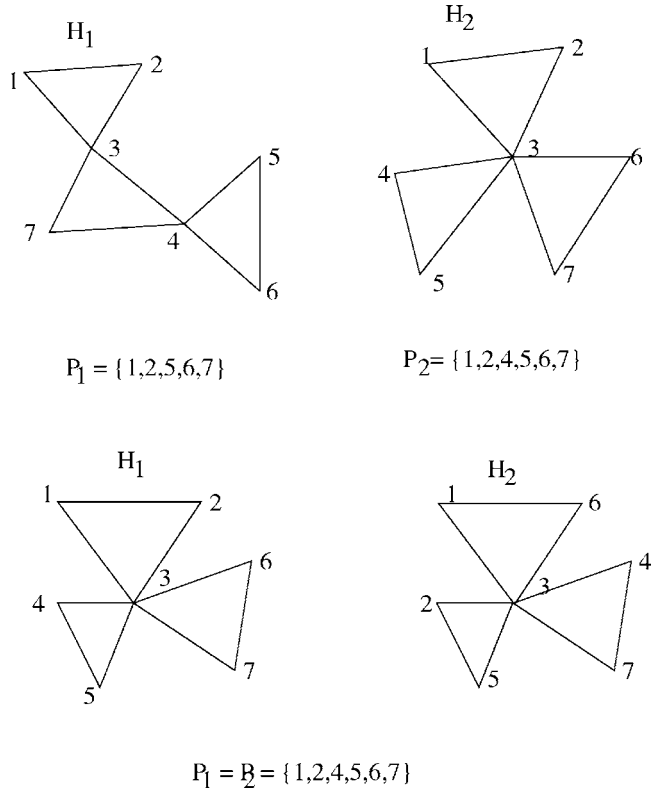

FIG. 12. r-uniform entangled hypertrees not captured in Theorem 9.

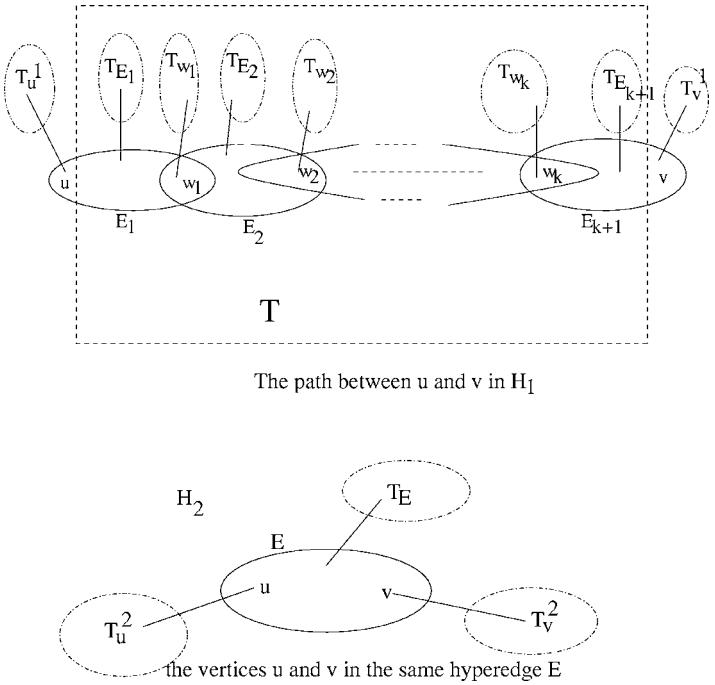

FIG. 13. Two distinct r-uniform entangled hypertrees.

that two distinct r-uniform entangled hypertrees are LOCC incomparable, we need the following important result about r-uniform hypertrees. See Appendix B for the proof.

Theorem 10: *Given two distinct r-uniform hypertrees* $H_1=(S,F_1)$ *and* $H_2=(S,F_2)$ *with* $r \geqslant 3$, *there exist vertices* $u,v \in S$ *such that u and v belong to the same hyperedge in* H_2 *but necessarily to different hyperedges in* H_1.

Now we state one of our main results on LOCC incomparability of multipartite entangled states in the following theorem.

Theorem 11: *Any two distinct r-uniform entangled hypertrees are LOCC incomparable.*

Proof: Let $H_1=(S,F_1)$ and $H_2=(S,F_2)$ be the two r-uniform entangled hypertrees. If $r=2$ then H_1 and H_2 happen to be two distinct spanning EPR trees and the proof follows from Theorem 8. Therefore, let $r \geqslant 3$.

Now from Theorem 10, there exist $u,v \in S$ such that u and v belong to the same hyperedge in H_2 but necessarily to different hyperedges in H_1. Let the same hyperedge in H_2 be $E \in F_2$. Also, since H_1, being hypertree, is *connected*, there exists a path between u and v in H_1. Let this path be $uE_1E_2 \cdots E_{k+1}v$. Clearly $k>0$ because u and v necessarily do not belong to the same hyperedge in H_1.

We introduce the following notations (Fig. 13).

T_u^1, subhypertree rooted at u in H_1 except the branch that contains E_1. T_v^1, subhypertree rooted at v in H_1 except the branch that contains E_{k+1}. T_{w_i}, subhypertree rooted at w_i in H_1 except branches containing E_i and E_{i+1}. T_{E_i}, Collection of all subhypertrees in H_1 rooted at some vertices in E_i other than w_{i-1} and w_i (where $w_0=u$ and $w_{k+1}=v$) except for the branches which contain E_i. $T=((E_1 \cup E_2 \cup \cdots \cup E_{k+1}) \cup (T_{E_1} \cup T_{E_2} \cup \cdots \cup T_{E_{k+1}}) \cup (T_{w_1} \cup T_{w_2} \cup \cdots \cup T_{w_k}))\backslash\{u,v\}$=set of all vertices from $S\backslash\{u,v\}$ which are not contained in $T_u \cup T_v$. T_u^2, subhypertree rooted at u in H_2 except the branch that contains E. T_v^2, subhypertree rooted at v in H_2 except the branch that contains E. T_E, collection of all subhypertrees in H_2 rooted at some vertices in $E\backslash\{u,v\}$ except for the branches which contain E.

In order to complete the proof we consider the following cases.

Case 1: $\exists w \in T$ such that $w \in (T_u^2 \cup T_v^2)$.

Without loss of generality let us take $w \in T_u^2$. Now since $w \in T$, $w \in$ exactly one of E_i, T_{w_i}, or T_{E_i} for some i. Accordingly there will be three subcases. *Case 1.1*, $w \in E_i$ for some i (take such minimum i).

Do bicolored merging where the vertex u along with all the vertices in

$$T_u^1, E_1, E_2, \ldots, E_{i-1}, T_{w_1}, T_{w_2}, \ldots, T_{w_{i-1}}, T_{E_1}, T_{E_2}, \ldots, T_{E_{i-1}}$$

are given the color A and the rest of the vertices are given the color B.

Case 1.2: $w \in T_{w_i}$ for some i.

Do the bicolored merging while assigning the colors as in the above case.

Case 1.3: $w \in T_{E_i}$ for some i.

Bicolored merging in this case is also the same as in Case 1.1.

Case 2: There does not exist any $w \in T$ such that $w \in T_u^2 \cup T_v^2$.

Clearly, $T_u^2 \cup T_v^2 \subset T_u^1 \cup T_v^1$ and $T \subset T_E \cup (E \setminus \{u,v\})$. Note that whenever we are talking of set relations like union, containment, etc., we are considering the trees, edges, etc., as sets of appropriate vertices from S which make them. First we establish the following claim.

Claim: $\exists t \in (E_1 \setminus \{u, w_1\}) \cup (E_2 \setminus \{w_1, w_2\})$ such that $t \in T_E$.

We have $k > 0$. Therefore, both E_1 and E_2 exist and since H_1 is r-uniform $|E_1| = |E_2| = r$. Also $(E_1 \setminus \{u, w_1\}) \cap (E_2 \setminus \{w_1, w_2\})$ is empty, for, otherwise there will be a cycle in H_1 which is not possible as H_1 is a hypertree.[5,10] Therefore,

$$|(E_1 \setminus \{u,w_1\} \cup (E_2 \setminus \{w_1,w_2\})| = |(E_1 \setminus \{u,w_1\}| + |E_2 \setminus \{w_1,w_2\}| = (r-2) + (r-2) = 2r-4.$$

Also $|E| = r$ implies that $|E \setminus \{u,v\}| = (r-2)$.

It is clear that $u, v \notin (E_1 \setminus \{u, w_1\}) \cup (E_2 \setminus \{w_1, w_2\})$. Therefore,

$$|(E_1 \setminus \{u,w_1\}) \cup (E_2 \setminus \{w_1,w_2\})| - |E \setminus \{u,v\}| = (2r-4) - (r-2) = r - 2 \geqslant 1$$

since $r \geqslant 3$.

Also $(E_1 \setminus \{u, w_1\}) \cup (E_2 \setminus \{w_1, w_2\}) \subset T \subset T_E \cup (E \setminus \{u,v\})$, and so by pigeonhole principle,[25]

$$\exists t \in (E_1 \setminus \{u,w_1\}) \cup (E_2 \setminus \{w_1,w_2\}) \text{ and } t \in T_E (\notin (E \setminus \{u,v\}))$$

Hence our claim is true.

Now we have $t \in (E_1 \setminus \{u, w_1\}) \cup (E_2 \setminus \{w_1, w_2\})$ such that $t \in T_E$. Since $t \in T_E$, by the definition of T_E it is clear that there must exist $w \in E \setminus \{u,v\}$ such that $t \in T_w$, the subhypertree in H_2 rooted at w except for the branch containing E. Depending on whether $t \in E_1 \setminus \{u, w_1\}$ or $t \in E_2 \setminus \{w_1, w_2\}$, we break this case into several subcases and futher in sub-subcases depending on the part in H_1 where w lies.

Case 2.1: $t \in E_1 \setminus \{u, w_1\}$ (Fig. 14).

Case 2.1.1: $w \in T_u^1$.

Do the bicolored merging where u and the vertices in T_u^1 are assigned the color A and the rest of the vertices from S are given the color B.

Case 2.1.2: $w \in T_v^1$.

Bicolored merging is done where v as well as all the vertices in T_v^1 are assigned the color B and rest of the vertices from S are given the color A.

Case 2.1.3: $w \in T$.

Here in this case, depending on whether w is in T_t or not, there can be two cases.

Case 2.1.3.1: $w \in T_t$.

Bicolored merging is done where all the vertices in T_t are given the color A and the rest of the vertices are assigned the color B.

Case 2.1.3.2: $w \notin T_t$.

$w \notin T_t$ implies that either $w \in E_i$ for some i, or $w \in T_q$, where $q \in E_i$ for some i and $q \neq t$. For both of these possibilities, bicolored merging is the same and is done as follows.

Assign the color A to u as well as all vertices in

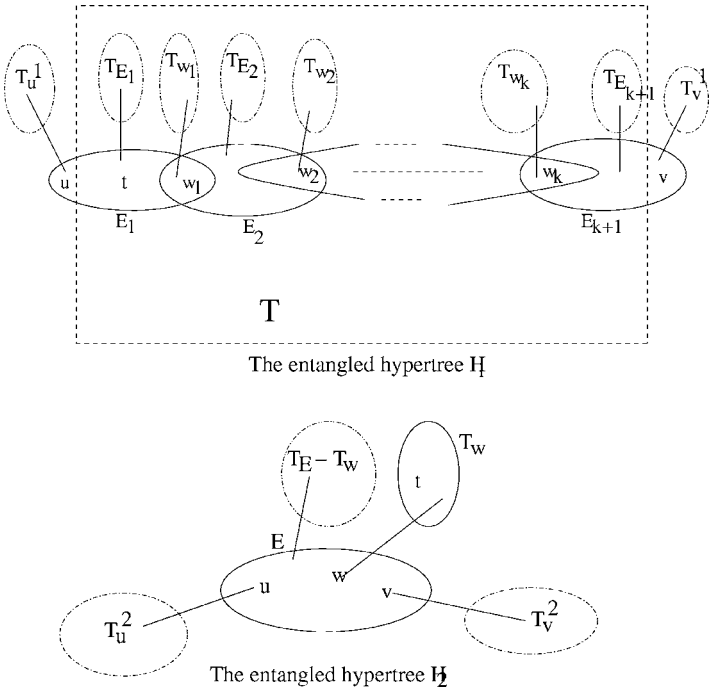

FIG. 14. Case 2.1.

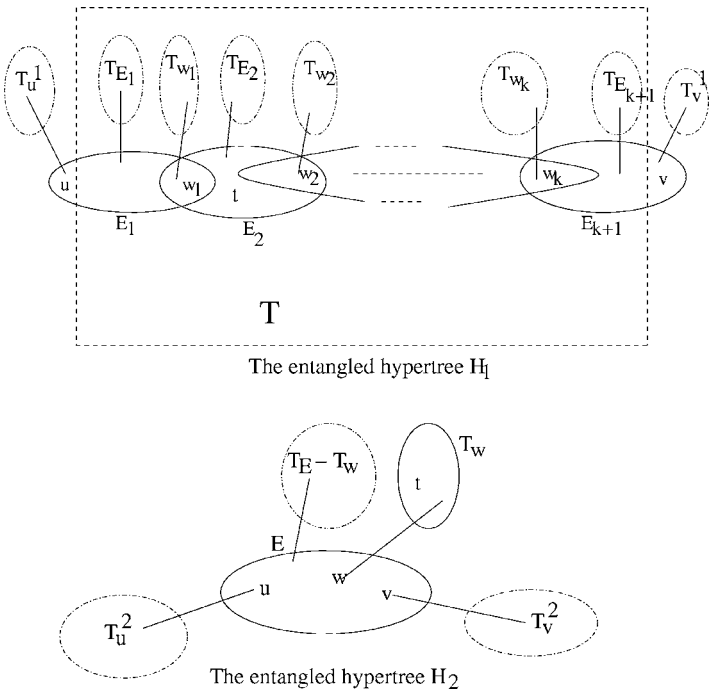

FIG. 15. Case 2.2.

$$T_u^1 \cup E_1 \cup T_{E_1} \cup T_{w_1} \cup \cdots \cup E_{i-1} \cup T_{E_{i-1}} \cup T_{w_{i-1}} \cup (E_i \setminus \{q,w,w_i\}) \cup (T_{E_i} \setminus T_q)$$

and assign the color B to rest of the vertices.

Case 2.2: $t \in E_2 \setminus \{w_1, w_2\}$ (Fig. 15).

Case 2.2.1: $w \in T_u^1 \cup E_1 \cup T_{E_1} \cup T_{w_1}$.

Do the bicolored merging where all the vertices in $T_u^1 \cup E_1 \cup T_{E_1} \cup T_{w_1}$ including u are given the color A and rest of the vertices are assigned the color B.

Case 2.2.2: $w \in T_v^1 \cup T_{E_{k+1}} \cup E_{k+1} \cup T_{w_k} \cup \cdots \cup T_{E_3} \cup E_3 \cup T_{w_2}$.

In bicolored merging give the color B to all the vertices (including v) in $T_v^1 \cup T_{E_{k+1}} \cup E_{k+1} \cup T_{w_k} \cup \cdots \cup T_{E_3} \cup E_3 \cup T_{w_2}$ and color A to the rest of the vertices.

Case 2.2.3: $w \in E_2 \cup T_{E_2}$.

In this case depending on whether $w \in T_t$, or $w \notin T_t$ the bicolored merging will be different.

Case 2.2.3.1: $w \in T_t$.

Bicolored merging is done where all the vertices in T_t are given the color A and rest of the vertices are assigned the color B.

Case 2.2.3.2: $w \notin T_t$.

$w \notin T_t$ implies that either $w \in E_2$, or $w \in T_q$ for some $q(\neq t) \in E_2$. In any case do the bicolored merging where the color A is assigned to all the vertices in

$$T_u^1 \cup E_1 \cup T_{E_1} \cup T_{w_1} \cup (E_2 \setminus \{w,q,w_2\}) \cup (T_{E_2} \setminus T_q)$$

and the rest of the vertices are assigned the color B.

Now that we have exhausted all possible cases and shown by the method of bicolored merging that the r-uniform entangled hypertree H_1 cannot be LOCC converted to the r-uniform entangled hypertree H_2. The same arguments also work for showing that H_2 can not be LOCC converted to H_1 by interchanging the roles of H_1 and H_2. Hence the theorem follows. □

Before ending our section on LOCC incomparability of multipartite states represented by EPR graphs and entangled hypergraphs, we note that partial entropic criteria of Bennett *et al.*[4] which gives a sufficient condition for LOCC incomparability of multipartite states, does not capture the LOCC incomparability of spanning EPR trees or entangled hypertrees in general. Consider two spanning EPR trees T_1 and T_2 on three vertices (say 1, 2, 3). T_1 is such that the vertex pairs 1, 2 and 1, 3 are forming the two edges where as in T_2 the vertex pairs 1, 3 and 2, 3 are forming the two edges. It is easy to see that T_1 and T_2 are not marginally isentropic.

VII. QUANTUM DISTANCE BETWEEN MULTIPARTITE ENTANGLED STATES

In the proof of Theorem 8, we have utilized the fact that there exist at least two vertices which are connected by an edge in T_2 but not in T_1. This follows as T_1 and T_2 are different and they also have equal number of edges (namely $n-1$, if there are n vertices). In fact, in general there may exist several such pairs of vertices depending on the structures of T_1 and T_2. Fortunately, the number of such pair of vertices has some nice features giving rise to a metric on the set of spanning (EPR) trees with fixed vertex set and thus giving a concept of distance.[9] The distance between any two spanning (EPR) trees T_1 and T_2 denoted by QD_{T_1,T_2} on the same vertex set is defined as the number of edges in T_1 which are not in T_2. Let us call this distance to be the *quantum distance* between T_1 and T_2. We have proved in Theorem 8 that obtaining T_2 from T_1 is not possible just through LOCC, so we need to do quantum communication. The minimum number of qubit required to be communicated for this purpose should be an interesting parameter related to state transformations amongst multipartite states represented by spanning EPR trees; let us denote this number by q_{T_1,T_2}. We note that $q_{T_1,T_2} \leqslant QD_{T_1,T_2}$. This is because each edge not present in T_2 can be created by only one qubit communication. The exact value of q_{T_1,T_2} will depend on the structures of T_1 and T_2 and, as we can note, on the number of edge disjoint paths in T_1 between the vertex pairs which form an edge in T_2 but not T_1.

We can say more about quantum distance. Recall Theorem 7 where we show that a lower bound on the number of copies of n-CAT to prepare a spanning EPR tree by LOCC, is $n-1$. Can

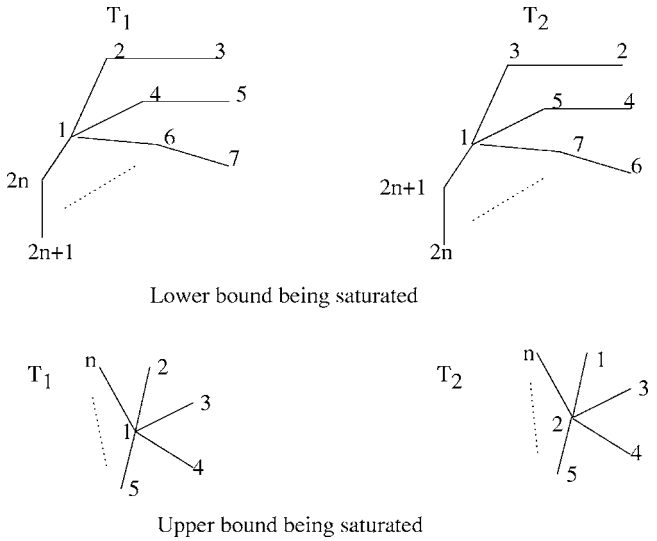

FIG. 16. Saturating bounds on copies required to go from one EPR spanning tree to another via LOCC.

we obtain a similar lower bound in the case of two spanning EPR trees and relate it to the quantum distance? The answer is indeed yes. Let C_{T_1,T_2} denote the minimum number of copies of the spanning EPR tree T_1 required to obtain T_2 just by LOCC. We claim that $2 \leqslant C_{T_1,T_2}$, $C_{T_2,T_1} \leqslant QD_{T_1,T_2}+1$. The lower bound follows from Theorem 8. The upperbound is also true because of the following reason. QD_{T_1,T_2} is the number of (EPR pairs) edges present in T_2 but not in T_1. For each such edge in T_2 (let u, v be the vertices forming the edge), while converting many copies of T_1 to T_2 by LOCC an edge between u and v must be created. Since T_1 is a spanning tree and therefore connected, there must be a path between u and v in T_1 and this path can be well converted (using entanglement swapping) to an edge between them (i.e., EPR pair between them) only using LOCC. Hence one copy each will suffice to create each such edges in T_2. Thus QD_{T_1,T_2} copies of T_1 will be sufficient to create all such QD_{T_1,T_2} edges in T_2. One more copy will supply all the edges common in T_1 and T_2. Even more interesting point is that both these bounds are saturated. This means to say that there do exist spanning EPR trees satifying these bounds (Fig. 16).

It is important to note that a similar concept of distance also holds in the case of r-uniform entangled hypertrees.

ACKNOWLEDGMENTS

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APPENDIX A

Proof of Theorem 1: We use the method of bicolored merging to prove the fact that any disconnected EPR graph G on n-vertices cannot be converted to an n-CAT state on those vertices under LOCC. We first note that the BCM EPR graph of an n-CAT state, irrespective of the bicoloring done, is always a graph which contains exactly one edge. Now as G is disconnected it will have more than one connected components. Let these components be $C_1, C_2 \vdots C_k$, where $k \geqslant 2$. The bicoloring is done as follows: assign the color A to all the vertices in the component C_1 and the color B to all other vertices, i.e., all vertices in $G \backslash C_1$. After merging, therefore, G reduces to a disconnected graph with no edges, i.e., the BCM EPR graph of G is a graph with k isolated vertices and no edges. Now if we are able to prepare an n-CAT state from G just using LOCC, we could also prepare an EPR pair between two parties who were never sharing an EPR pair just using LOCC. This violates monotonicity and hence the theorem is proved. □

APPENDIX B

Proof of Theorem 10: We first establish the following claim.

Claim: $\exists E_1 \in F_1, E_2 \in F_2$ such that $E_1 \cap E_2 \neq \phi$ and $E_2 \notin F_1 \cap F_2$.

Proof of the claim: We first show that on the same vertex set, the number of hyperedges in any r-uniform hypertree is always same. Let n and m be the number of vertices and hyperedges in a r-uniform hypertree. We show by induction on m that $n=m*(r-1)+1$.

For $m=1$, $n=1*(r-1)+1=r$ which is true because all possible vertices (since no one can be isolated) fall in the single hyperedge and it has exactly r vertices.

Let us assume that this relation between n and m for a fixed r holds for all values of the induction variable up to $m-1$. We show that it holds good for m.

Now take a r-uniform hypertree with m hyperedges. Remove any of the hyperedges to get another hypergraph (which may not be connected) having only $m-1$ edges. This removal may introduce k connected components (subhypertrees); $1 \leqslant k \leqslant r$. Let these components have, respectively, $m_1, m_2, \ldots, m_k$ number of hyperedges. Therefore, $\Sigma_{i=1}^{k} m_i = m-1$. The total number of vertices in the new hypergraph (with the k subhypertrees as components), $n^1 = \Sigma n_i$ where n_i is the number of vertices in the component i. Therefore, $n^1 = \Sigma n_i = \Sigma_{i=1}^{k} \{m_i(r-1)+1\} = (m-1)(r-1)+k$ (under induction assumption).

Now the number of vertices in the original hypertree, $n=n^1+(r-k)$ because k vertices were already covered, one each in the k components. Therefore, $n=(m-1)(r-1)+k+(r-k)=(m-1)(r-1)+r=(m-1)(r-1)+(r-1)+1=m(r-1)+1$. The result is thus true for m and hence for any number of hyperedges by induction. This result implies that any r-uniform hypertree on the same vertex set will always have the same number of hyperedges.

Let $F=F_1 \cap F_2$ and $m=|F_1|=|F_2|$. Obviously $m>|F|$ otherwise $H_1=H_2$. This implies that $\exists E \in F_2$ such that $E \notin F$.

Take any vertex say $w \in E$. Since $w \in S$ and H_1 is a hypertree therefore connected, w can not be an isolated vertex and therefore $\exists E^1 \in F_1$ such that $w \in E^1$. Take $E_1=E^1$ and $E_2=E$. This proves our claim.

Now we prove the theorem. Choose E_1 and E_2 so as to satify the above claim.

Let $E_1=\{u_1, u_2, \ldots, u_l, w_{l+1}, w_{l+2}, \ldots, w_r\}$ and $E_2=\{u_1, u_2, \ldots, u_l, v_{l+1}, v_{l+2}, \ldots, v_r\}$.

Since $E_1 \cap E_2 \neq \phi$, $l \geqslant 1$ and $E_1 \neq E_2$ implies that $l \leqslant r-1$.

Hence $1 \leqslant l \leqslant r$.

Now based on the value of l, we have the following different cases.

Case 1: $l>1$.

Case 1.1: $\exists v_i$ such that u_1 and v_i are not in the same hyperedge in H_1.

Take $u=u_1$ and $v=v_i$ in the statement of the theorem.

Case 1.2: Each v_i is in some hyperedge in H_1 in which u_1 also lies.

None of these v_i's can belong to the hyperedges in H_1 in which u_2 lies.

This is due to the fact that if, say, v_j happens to be in same hyperedge as of u_2 in H_1 then $u_1 u_2 v_j u_1$ will be a cycle in H_1, which is absurd as H_1 is a hypertree.

Note that at least one such v_i must exist as $l<r$. Take $u=u_2$ and $v=$any v_i.

Case 2: $l=1$.

Case 2.1: $\exists v_i$ such that u_1 and v_i are not in same hyperedge in H_1.

Take $u=u_1$ and $v=v_i$.

Case 2.2: Each v_i is in some hyperedge in H_1 in which u_1 also lies.

Since v_i's are $r-1$ in number and $E_2 \notin F_1 \cap F_2$, these v_i's will be distributed in at least two distinct hyperedges in H_1 in which u_1 also lies.

Therefore, $\exists v_i$, v_j such that they are in the same hyperedge in H_2 (namely in E_2) but in necessarily different edges in H_1, otherwise (that is, if they lie in the same hyperedge in H_1) $u_1 v_i v_j u_1$ will be a cycle in H_1, which is absurd as H_1 is a hypertree.

Also note that both v_i and v_j will exist as $r \geqslant 3$.

Take $u=v_i$ and $v=v_j$.

Thus we have proved Theorem 10 in all possible cases. □

We would like to point out that the result of Theorem 10 could follow from some standard results in combinatorics. We have however not found literature proving this result.

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Generalized coherent states and the control of quantum systems

Holger Teismann[a)]
Acadia University, University Avenue, Wolfville, Nova Scotia B4P 2R6, Canada

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The control problem for linear and nonlinear Schrödinger equations is considered. The controls are given by applying a spatially homogeneous field or varying the frequency of a quadratic trapping potential. It is demonstrated that the existence of (exact or approximate) coherent-state-type solutions may severely limit the degree to which the system can be controlled. © *2005 American Institute of Physics.*
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I. INTRODUCTION

In 1926 Erwin Schrödinger[1] discovered harmonic-oscillator quantum states with quasiclassical, particle-like properties, which have become known as coherent states. Schrödinger's original idea has since been generalized in many ways; in this paper we will focus on one of these generalizations, called "trajectory-coherent states."[2] Later, in the 1980s, questions of controlling quantum systems and engineering quantum states began to be addressed systematically.[3] The purpose of this paper is to expose a link between these developments.

Our main thesis is that the existence of coherent structures in quantum systems may limit the degree of controllability with respect to control by means of spatially homogeneous external fields (coherent control). Roughly speaking, (generalized) coherent states present "obstacles" to the control process which can be difficult to overcome.[4] The basic mechanism is that, in a first-order approximation, the application of a homogeneous field will only affect the position $\langle x \rangle$ of a wave packet, but will leave its higher moments, and hence its shape, (essentially[5]) unaffected. To illustrate this phenomenon we will consider Bose–Einstein condensates (BEC) in a quadratic trap, whose dynamics is described by a nonlinear Schrödinger equation, the *Gross–Pitaevskii equation*, and we will discuss *trajectory-coherent states*, which are Gaussian-shaped *approximate* solutions to the (linear) Schrödinger equation with a general potential.

Specifically, we will show that (a) the Gross–Pitaevskii equation supports (generalized) coherent states, which restrict the set of states that, given an initial state, can be "engineered" (by manipulating the spatially homogeneous control field) to a finite-dimensional manifold (see "Observation I" below); (b) the dominant effect of varying the frequency of a quadratic trap is a rescaling of the wave packet ("Observation II"); (c) access to the inherently *quantum* (nonclassical) degrees of freedom can only be gained indirectly by means of higher-order effects involving the external potential ("Observation III"); (d) the existence of trajectory-coherent states may render the time required to reach (or approximate) a given target state very large—essentially infinite—if the control field is not designed very carefully ("Observation IV").

These observations seem to provide a rather poor prognosis for the "dream"[6] of quantum control. However, it should be noted that the existence of "exact" coherent states is a rather exceptional occurrence,[7] very intimately linked to the harmonic oscillator potential (or, more generally, to the fact that the Hamiltonian is quadratic in its variables). For instance, the definition of coherent states for other quantum systems, such as the hydrogen atom, remains difficult,

[a)]Electronic mail: hteisman@acadiau.ca

contrary to Schrödinger's belief that quasiclassical states analogous to the ones he found for the harmonic oscillator could certainly be defined for other quantum systems as well.[1]

In this sense, this paper does not undermine the notion that coherent control of quantum systems is feasible for "the majority" of quantum systems, as they will typically not possess exact coherent states.[8] However, the existence of trajectory-coherent states for general, not necessarily quadratic, potentials shows that special care must be taken in designing the control fields if unrealistically large control times are to be avoided.

This paper is organized as follows: In Sec. II we give the basic definitions and introduce the quantum control problem. Section III presents two transformations designed to capture the dominant effects of the linear (in x) and quadratic control terms $E(t)x$ and $\frac{1}{2}\Omega(t)|x|^2$. In Sec. IV we investigate the consequences of these transformations for the control problem; this section includes Observations I–III mentioned earlier. In Sec. V we introduce trajectory-coherent states and study their effect on the control process (Observation IV). We conclude the paper with a number of remarks (Sec. VI). Many of the calculations we present here have appeared elsewhere (if often not for nonlinear equations such as the GPE); our objective here is to present them under unifying aspects, in particular concerning their significance for the quantum control problem.

II. QUANTUM CONTROL

We consider quantum systems whose dynamics can be described by (possibly nonlinear) Schrödinger equations of the form

$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\Delta\psi + V(x)\psi + \frac{1}{2}\Omega(t)|x|^2\psi + (E(t)\cdot x)\psi + f(|\psi|^2)\psi \tag{1}$$

($\psi=\psi(t,x)\in\mathbb{C}$, $t\in[0,T]\subset\mathbb{R}$, $x\in\mathbb{R}^D$, $D=1, 2, 3$, $V=V(x)\in\mathbb{R}$) where the time-dependent fields $E=E(t)\in\mathbb{R}^D$ and $\Omega=\Omega(t)\in\mathbb{R}$ will play the role of *controls*. We will assume that Eq. (1) is globally well-posed in some reasonable function space $\mathcal{H}\subset L^2(\mathbb{R}^D)$, such as $\mathcal{H}:=\{\varphi(x)\in H^2(\mathbb{R}^D)\,|\,|x|^2\varphi(x)\in L^2(\mathbb{R}^D)\}$, where $L^2(\mathbb{R}^D)$ and $H^2(\mathbb{R}^D)$ denote the usual Lebesgue and Sobolev spaces.[9] The nonlinearity $f(|\psi|^2)\in\mathbb{R}$ may be local or nonlocal as we have the following examples in mind.

(a) *BEC in a quadratic trap*. Here (1) is the Gross–Pitaevskii equation with the nonlinearity $f(|\psi^2|)=\pm a^2|\psi|^2$ ($a\in\mathbb{R}$).[10] The time-independent part, V, of the external potential, will typically be zero or a periodic function or may contain an additional quadratic term.[11] Obviously, in the case $V\equiv 0$ and $f\equiv 0$ Eq. (1) reduces to the well-known quantum-mechanical *time-dependent, driven harmonic oscillator*. The functions $E(t)$ and $\Omega(t)$ model the manipulation of the system by "shaking" the trap (i.e., changing its position) and varying its frequency, respectively.

(b) *Molecular dynamics*. Here we set $\Omega\equiv 0$ as the external potential will typically be nonconfining; V may be thought of as something like the Coulomb potential. Equation (1) may be linear or nonlinear. An important example is the *Hartree equation* with the (nonlocal) nonlinearity $\kappa\Delta^{-1}|\psi|^2(\kappa\in\mathbb{R})$. Molecular systems are usually controlled by means of laser light; hence E represents an electric field. The special form of the control term $(E(t)\cdot x)$ in (1) is due to the dipole approximation.

The *control problem*[12] associated with Eq. (1) consists of the question of whether, given an *initial state* ψ_0 and a *target state* ψ_T, control fields $E(t)$ and/or $\Omega(t)$ can be found that will steer the system from ψ_0 to ψ_T, i.e., whether there exist functions $E=E(t)$ and/or $\Omega=\Omega(t)$ such that the solution $\psi=\psi(t,x)$ of (1) satisfies

$$\psi(0,x)=\psi_0(x) \quad \text{and} \quad \psi(T,x)=\psi_T(x).$$

Note that, in this formulation of the control problem, the control time—or *horizon*—, T, is finite. Note also that Eq. (1) conserves the L^2 norm, i.e.,

$$\|\psi(t)\|_{L^2}^2 = \int_{\mathbb{R}^D} |\psi(t,x)|^2 \mathrm{d}x = \int_{\mathbb{R}^D} |\psi(0,x)|^2 \mathrm{d}x = \|\psi(0)\|_{L^2}^2.$$

The appropriate state manifold is therefore given by the sphere $\mathcal{S}=\{\varphi \in \mathcal{H} \,|\, \|\varphi\|_{L^2}=1\}$, and the control problem will have to be restricted to this state manifold. The degree to which the system is controllable for a given initial state $\psi_0 \in \mathcal{S}$ is measured by the "size" of the set, $R_T(\psi_0) \subset \mathcal{S}$, of states that are reachable from ψ_0:

$$R_T(\psi_0) := \{\psi_T \in \mathcal{S} \,|\, \exists\, E(t), \Omega(t) : \psi(0) = \psi_0, \psi(T) = \psi_T\}$$

III. TWO TRANSFORMATIONS

Our point of departure is a generalized Wentzel–Kramers–Brillouin-style ansatz

$$\psi(t,x) = e^{iS(t,x)}\phi(t,x) \quad (S = S(t,x) \in \mathbb{R}, \phi = \phi(t,x) \in \mathbb{C}) \tag{2}$$

for solutions ψ of (1)—"generalized" because the function ϕ is allowed to take on complex values. For convenience we set $\hbar = m = 1$ until further notice. Then ψ is a solution to (1) iff the pair (S, ϕ) is a solution to the system

$$S_t + \tfrac{1}{2}(\nabla S)^2 = -V_1(t,x) - \tfrac{1}{2}\Omega(t)|x|^2 - E(t)\cdot x, \tag{3a}$$

$$i[\phi_t + (\nabla\phi)\cdot(\nabla S)] = -\frac{1}{2}\Delta\phi + V_2(t,x)\phi + f(|\phi|^2)\phi - \frac{i}{2}(\Delta S)\phi, \tag{3b}$$

where $V(t,x) = V_1(t,x) + V_2(t,x)$ is an arbitrary decomposition of V.

A linear (with respect to x) ansatz for the phase function S will allow us to capture the dominant effect of the linear control term $E(t)\cdot x$ by essentially removing the control field from the equation; a quadratic ansatz for S will have a similar effect for the quadratic control term $\Omega(t)|x|^2$.

A. Linear phase function

In this section we assume that

$$\Omega \equiv 0.$$

Equation (3a) is the Hamilton–Jacobi equation for the Hamiltonian function

$$H^c(t,x,p) = \tfrac{1}{2}p^2 + V_1(t,x) + E(t)\cdot x; \tag{4}$$

we denote by $(x^c, p^c) = (x^c(t), p^c(t)) \in \mathbb{R}^{2D}$ the solution of the corresponding Hamiltonian system

$$\dot{x}^c(t) = \frac{\partial H^c}{\partial p}(t, x^c(t), p^c(t)), \quad \dot{p}^c(t) = -\frac{\partial H^c}{\partial x}(t, x^c(t), p^c(t)), \quad x^c(0) = x_0, \quad p^c(0) = p_0. \tag{5}$$

Now we define the phase function $S = S^c$ by

$$S^c(t,x) = \int_0^t [\dot{x}^c(s)\cdot p^c(s) - H^c(s)]\mathrm{d}s + p^c(t)\cdot(x - x^c(t)) \tag{6}$$

(where $H^c(t) := H^c(t, x^c(t), p^c(t))$); we write $\phi(t,x) = \chi^c(t, x - x^c(t))$, and obtain *coherent-state-type* solutions $\psi = \psi^c$ of (1),

$$\psi^c(t,x) = e^{iS^c(t,x)}\chi^c(t, x - x^c(t)) \tag{7}$$

(The superscript "c" stands for "controlled;" it will be applied to quantities that depend on the control field $E(t)$.)

Then it is easy to see that ψ^c is a solution to (1) iff the function $\chi^c=\chi^c(t,x)$ is a solution to

$$i\chi_t^c = -\tfrac{1}{2}\Delta\chi^c + V_2(t,x+x^c(t))\chi^c + W^c(t,x)\chi^c + f(|\chi^c|^2)\chi^c, \tag{8}$$

where

$$W^c(t,x) := V_1(t,x+x^c(t)) - V_1(t,x^c(t)) - \nabla V_1(t,x^c(t))\cdot x.$$

There are two obvious choices for the decomposition $V(t,x)=V_1(t,x)+V_2(t,x)$.

1. $V_1\equiv 0$, $V_2\equiv V$. In this case, the equation for the classical trajectory, x^c, reads

$$\ddot{x}^c(t) = -E(t),$$

i.e., the "classical particle," x^c, only feels the control field $E(t)$ but no other external potential. Equation (8) takes the form

$$i\chi_t^c = -\tfrac{1}{2}\Delta\chi^c + V(t,x+x^c(t))\chi^c + f(|\chi^c|^2)\chi^c. \tag{9}$$

As mentioned earlier, this means that the effect of the control term $E(t)\cdot x$ is to move ("shake") the external potential V by $-x^c(t)$.

2. $V_2\equiv 0$, $V_1\equiv V$. Here the classical trajectory, x^c, satisfies

$$\ddot{x}^c(t) = -\nabla V(t,x^c(t)) - E(t), \tag{10}$$

i.e., the classical particle, x^c, feels the control field $E(t)$ *and* the external potential V. Equation (8) reads

$$i\chi_t^c = -\tfrac{1}{2}\Delta\chi^c + W^c(t,x)\chi^c + f(|\chi^c|^2)\chi^c. \tag{11}$$

Remarks:

(a) The term *(generalized) coherent states* for solutions of the form (7) is motivated by the (time-independent, undriven) harmonic-oscillator case given by

$$f\equiv 0, \quad E\equiv 0, \quad V\equiv 0, \quad \Omega\equiv 1.$$

If the solution χ of Eq. (8) are chosen to be stationary solutions $\chi(t,x)=e^{i\epsilon t}\varphi(x)$, where $\varphi(x)$ is the ground state of the harmonic oscillator Hamiltonian $\frac{1}{2}(-\Delta+|x|^2)$, then the solutions ψ in (7) coincide with the quasiclassical states discovered by Schrödinger that are now called *coherent states*.

(b) All formulas would remain the same if we were to allow the potential V to be time-dependent as well.

B. Quadratic phase function

We assume

$$E\equiv 0$$

and choose the phase function as

$$S(t,x) = \tfrac{1}{2}Q(t)x^2 \tag{12}$$

where $Q:[0,T^*)\to\mathbb{R}$ is the solution of the ODE

$$\dot{Q}(t) + Q^2(t) + \Omega(t) = 0, \quad Q(0)=0. \tag{13}$$

Then the equation for ϕ takes the form

$$i[\phi_t + Q(t)(\nabla\phi)\cdot x] = -\frac{1}{2}\Delta\phi + V(x)\phi + f(|\phi|^2)\phi - \frac{iD}{2}Q(t)\phi, \tag{14}$$

which can be transformed further by writing

$$\phi(t,x) = e^{-(D/2)R(t)}\chi(\Lambda(t), e^{-R(t)}x), \tag{15}$$

where the functions $R=R(t)$ and $\Lambda=\Lambda(t)$ satisfy the ODEs

$$\dot{R}(t) = Q(t), \quad \dot{\Lambda}(t) = e^{-2R(t)}, \quad R(0) = \Lambda(0) = 0, \tag{16}$$

and χ is a solution to

$$i\chi_t = -\tfrac{1}{2}\Delta\chi + e^{2R(\tau)}V(e^{R(\tau)}x)\chi + e^{2R(\tau)}f(e^{-DR(\tau)}|\chi|^2)\chi, \ \tau := \Lambda^{-1}(t). \tag{17}$$

To summarize, the solution ψ of (1) (with $E\equiv 0$) can be written as

$$\psi(t,x) = e^{(1/2)[iQ(t)x^2 - DR(t)]}\chi(\Lambda(t), e^{-R(t)}x), \tag{18}$$

where the functions Q, R, Λ, and χ are defined as above.

Remarks:

(a) The solution $Q(t)$ of the ODE (13) may not exist for all $t>0$ (i.e., $T^*<\infty$). For instance, for $\Omega(t)\equiv\omega>0$ the solution can be found explicitly:

$$Q(t) = -\sqrt{\omega}\tan(\sqrt{\omega}t) \Rightarrow T^* = \frac{\pi}{2\sqrt{\omega}}.$$

The above noted transformation is therefore only valid on the interval $[0, T^*)$.

(b) It is easy to see that the solution $Q(t)$ *does* exist for all $t>0$ (i.e., $T^*=\infty$) if $\Omega(t)\leqslant 0$ for all $t\geqslant 0$.

(c) Even if Q does blow up in finite time T^*, due to the dispersive properties of the function χ, the solution ψ may still be regular at $t=T^*$. As an example, consider the case $\Omega\equiv\omega$, $V\equiv 0$, $f\equiv 0$, and $\psi_0(x)=e^{-x^2/2}$.

(d) It can be shown that Eq. (13) possesses global solutions if they are allowed to be complex-valued and satisfy $\mathrm{Im}(Q(0))>0$. This fact will become important in the construction of trajectory-coherent states.

Critical power nonlinearity. If we assume that

$$f(|\psi|^2) = \kappa|\psi|^{4/D} \quad (\kappa\in\mathbb{R}),$$

Eq. (17) takes the form

$$i\chi_t = -\tfrac{1}{2}\Delta\chi + e^{2R(\tau)}V(e^{R(\tau)}x)\chi + \kappa|\chi|^{4/D}\chi. \tag{19}$$

IV. IMPLICATIONS FOR THE CONTROL PROBLEM

A. Homogeneous control field and quadratic exterior potential

In the following we consider a general quadratic potential, which we write as

$$\Omega\equiv 0, \quad V(x) = \tfrac{1}{2}x^T A x, \tag{20}$$

where A is a symmetric $D\times D$ matrix. This includes the Gross–Pitaevskii equation with a time-independent quadratic trapping potential,

$$i\psi_t = -\frac{1}{2}\Delta\psi + \frac{\omega}{2}x^2\psi + (E(t)\cdot x)\psi \pm a^2|\psi|^2\psi$$

$(\omega, a \in \mathbb{R})$. Since

$$W^c(t,x) := V(x+x^c(t)) - V(x^c(t)) - \nabla V(x^c(t))\cdot x = V(x),$$

Eq. (11) is *independent of the control field E*,

$$i\chi_t = -\tfrac{1}{2}\Delta\chi + V(x)\chi + f(|\chi|^2)\chi. \tag{21}$$

This has the following important consequence.

Observation I: *Let $\psi_0 \in \mathcal{S}$ and $x_0 = p_0 = 0$.*[13] *Then, for any control field $E = E(t)$, the solution $\psi^c = \psi^c(t,x)$ of Eq. (1) (with (20)) satisfying $\psi(0,x) = \psi_0(x)$ is given by $\psi^c(t,x) = e^{iS^c(t,x)}\chi(t, x - x^c(t))$, where χ is the unique solution of (the control-independent) Eq. (21) that satisfies the initial condition $\chi(0,x) = \psi_0(x)$. As a result, the set of reachable states, $R_T(\psi_0)$, is given by*

$$R_T(\psi_0) = \{e^{i\lambda}e^{i\pi\cdot(x-\xi)}\chi(T, x-\xi) \,|\, \lambda \in \mathbb{R}; \pi, \xi \in \mathbb{R}^D\}. \tag{22}$$

and thus finite-dimensional.

Remarks:

(a) In terms of the controllability problem, the significance of the "coherent-state transformation" (7) lies in the fact that it transforms the control problem (1) (with (20)) into the control-independent equation (21). The controlled state ψ^c can therefore essentially (i.e., up to the classical degrees of freedom—see the following) be precomputed by solving Eq. (21). Specifically, since the "shape," $|\psi^c(T,x)|$, of the terminal state is given by $|\chi(T, x - x^c(T))|$ it cannot be changed by the application of the control field E. All that can be affected by the homogeneous exterior field is a shift of the function $|\chi(T,x)|$.

(b) In physical terms, one might interpret this by saying that the centre-of-mass degrees of freedom are decoupled from the remaining degrees of freedom. This was previously observed in Refs. 14 and 15.

(c) The terminal state $\psi_T = \psi^c(T)$ is given by

$$\psi^c(T,x) = e^{iL_T^c}e^{ip^c(T)\cdot(x-x^c(T))}\chi(T, x - x^c(T)),$$

where $L_T^c := \int_0^T [\dot{x}^c(t)\cdot p^c(t) - H^c(t)]\mathrm{d}t$ denotes the classical action. The set of reachable states may therefore be parametrized by the classical degrees of freedom (cf. (22)).

(d) It is illuminating to look at the special case where the function χ is chosen to be a *stationary* solution of (21),

$$\chi(t,x) := e^{i\mu t}\varphi_\mu(x),$$

where φ_μ is a (real) solution to the nonlinear eigenvalue problem

$$\left[-\mu + \tfrac{1}{2}(\Delta - x^2) - f(\varphi^2)\right]\varphi = 0. \tag{23}$$

(here we assume $V(x) = \frac{1}{2}x^2$). For $\psi_0 = \varphi_\mu$ the set of reachable states then has the form

$$R_T(\varphi_\mu) = \{e^{i(\lambda + T\mu)}e^{i\pi\cdot(x-\xi)}\varphi_\mu(x-\xi) \,|\, \lambda \in \mathbb{R}; \pi, \xi \in \mathbb{R}^D\},$$

in particular,

$$\psi(x) \in R_T(\varphi_\mu) \Rightarrow |\psi(x)| = |\varphi_\mu(x-\xi)|, \tag{24}$$

which again highlights the fact that the shape of the state cannot be influenced by the (spatially homogeneous) control fields E.

(e) It is not difficult to show that *no transitions between nonlinear eigenstates* (corresponding to different values of μ) can be affected by the spatially homogeneous control field $E(t)$. This

is even more obvious in the linear case as the node structure of the eigenstates for the harmonic oscillator Hamiltonian $\frac{1}{2}(-\Delta+x^2)$ cannot be changed.

(f) The fact that the manifold of controllable states, $R_T(\psi_0)$, is finite-dimensional is well-known in the *linear case* (quantum-mechanical driven harmonic oscillator DHO). It is a consequence of an important result in (geometric) control theory due to Huang, Tarn, and Clark.[16,17]
This "noncontrollability property" of the DHO was also observed in Ref. 18, using essentially the transformation (7). The DHO is a classical problem in quantum mechanics. As a result, the amount of literature on the DHO is enormous. To the best of the author's knowledge, the first version of the transformation (7), applied to the DHO, appeared in Ref. 19; see also Ref 20.

(g) Let $\langle x\rangle_\psi$ denote the expectation value of the position operator with respect to the state ψ, i.e.,

$$\langle x\rangle_\psi = \int_{\mathbb{R}^D} x|\psi(x)|^2 \mathrm{d}x.$$

Then we have

$$\langle x\rangle^c(t) := \langle x\rangle_{\psi^c(t)} = x^c(t) + \langle x\rangle_{\chi(t)}.$$

Ehrenfest relations give

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle x\rangle_{\chi(t)} = -\langle \nabla V\rangle_{\chi(t)} = -\nabla V(\langle x\rangle_{\chi(t)}) \tag{25a}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle x\rangle_{\psi^c(t)} = -\langle \nabla V - E(t)\rangle_{\psi^c(t)} = -\nabla V(\langle x\rangle_{\psi^c(t)}) - E(t) \tag{25b}$$

and so

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}x^c(t) = -\nabla V(x^c(t)) - E(t)$$

(since $\nabla V(x)=Ax$), which is consistent with (10).

B. Time-dependent trap frequency and critical nonlinearity

We now consider the situation in which the control is applied by varying the trap frequency, $\Omega=\Omega(t)$. We assume that the external potential, V, has the right scaling, i.e., satisfies

$$\lambda^2 V(\lambda x) = V(x), \quad \lambda > 0,$$

which obviously includes $V\equiv 0$ as well as the inverse square potential $V(x)=\beta/|x|^2(\beta\in\mathbb{R})$. So our control problem is

$$i\psi_t = -\tfrac{1}{2}\Delta\psi + V(x)\psi + \tfrac{1}{2}\Omega(t)x^2\psi + \kappa|\psi|^{4/D}\psi \quad (\kappa\in\mathbb{R}). \tag{26}$$

As seen in Sec. III B, applying the transformation (18) results in (19), which is *independent of the control* $\Omega(t)$ due to the scaling invariance of the potential,

$$i\chi_t = -\tfrac{1}{2}\Delta\chi + V(x)\chi + \kappa|\chi|^{4/D}\chi. \tag{27}$$

We are therefore in the position to make the following observation.

Observation II: *Let $\psi_0\in\mathcal{S}$ be given. Then, for any control $\Omega(t)$, the unique solution of Eq. (26) is given by*

$$\psi(t,x) = e^{(i/2)Q(t)x^2}e^{-DR(t)/2}\chi(\Lambda(t), e^{-R(t)}x) \tag{28}$$

(for $t \in [0,T^*)$), where Q, R, and Λ are given by (13) and (16), and χ is the unique solution of (control-independent) Eq. (27) satisfying $\chi(0,x)=\psi_0(x)$. As a result, on the interval $[0,T^*)$ all the states that can be reached from ψ_0 have the form

$$\psi(t,x) = e^{(i/2)Qx^2}\frac{1}{\sigma^{D/2}}\chi\left(\Lambda, \frac{x}{\sigma}\right), \quad Q,\sigma,\Lambda \in \mathbb{R},\ \sigma > 0. \tag{29}$$

Remarks:

(a) In terms of the controllability problem, the main point here is that the solution trajectory, $\gamma := \chi(\mathbb{R}) \subset \mathcal{S}$, for Eq. (27) can be determined independently of the control Ω. Thus, the states $\psi(t) \in \mathcal{S}$ that are engineered by varying the trap frequency coincide, up to a phase factor, with *rescaled* versions of states on γ.

(b) More specifically, the geometric meaning of the function

$$\sigma(t) := e^{R(t)}$$

is readily revealed by computing the appropriate expectation values. From

$$|\psi(t,x)|^2 = \frac{1}{[\sigma(t)]^D}\left|\chi\left(\Lambda(t), \frac{x}{\sigma(t)}\right)\right|^2,$$

we get

$$\langle x\rangle_{\psi(t)} = \int_{\mathbb{R}^D} x|\psi(t,x)|^2 \mathrm{d}x = \sigma(t)\langle x\rangle_{\chi(\Lambda(t))}, \tag{30a}$$

$$\langle |x|^2\rangle_{\psi(t)} = \int_{\mathbb{R}^D} |x|^2|\psi(t,x)|^2 \mathrm{d}x = \sigma(t)^2\langle |x|^2\rangle_{\chi(\Lambda(t))}. \tag{30b}$$

Moreover, it is easy to see from (13) that $\sigma(t)$ satisfies the second-order initial value problem

$$\ddot{\sigma}(t) + \Omega(t)\sigma(t) = 0, \quad \sigma(0) = 1, \quad \dot{\sigma}(0) = 0. \tag{31}$$

(c) Our conclusion is that varying the trap frequency allows us to control the spread, $\langle |x|^2\rangle_{\psi(t)}$, of a wave packet (see (30b)); Eq. (31) can be used to determine an appropriate control function $\Omega(t)$. However, in general we do not have control over the position, $\langle x\rangle_{\psi(t)}$, of the wave packet, as, for instance, $\langle x\rangle_{\chi(\Lambda(t))}$ in (30a) may be zero so that the control of $\langle x\rangle_{\psi(t)}$ is lost completely.

(d) It should be kept in mind that the transformation is only valid *locally in time* as $Q(t)$ may blow up.

(e) It has been noticed before that time-independent quadratic potentials can be removed from the critical nonlinear Schrödinger equation by the transformation (28); see Refs. 21 and 22 and the literature therein (see also Refs. 23 and 24).

C. Homogeneous control field and general external potential (second-order approximation)

For simplicity we restrict our attention to the 1D linear case:

$$i\psi_t = -\tfrac{1}{2}\psi_{xx} + V(x)\psi + (E(t)x)\psi \quad (x \in \mathbb{R}). \tag{32}$$

Applying the coherent-state-transformation (7), $\psi(t,x) = e^{iS^c(t,x)}\chi^c(t, x-x^c(t))$, yields

$$i\chi^c_t = -\tfrac{1}{2}\chi^c_{xx} + W^c(t,x)\chi^c, \tag{33}$$

where

$$W^c(t,x) = V(x+x^c(t)) - V(x^c(t)) - V'(x^c(t))x = \frac{1}{2}V''(x^c(t))x^2 + \sum_{\alpha\geqslant 3}\frac{V^{(\alpha)}(x^c(t))}{\alpha!}x^\alpha$$

by Taylor expansion. If we truncate the Taylor series after the quadratic term and set $\Omega = \Omega^c(t) := V''(x^c(t))$, we can apply the transformation in Sec. III B to obtain the *approximate* solution

$$\chi(t,x) \approx e^{(i/2)Q^c(t)x^2}e^{-(1/2)DR^c(t)}\widetilde{\chi}(\Lambda^c(t), e^{-R^c(t)}x),$$

$$\psi^\varepsilon(t,x) \approx \widetilde{\psi}^\varepsilon(t,x) = e^{i[S^c(t,x)+(1/2)Q^c(t)(x-x^c(t))^2]}e^{-1/2DR^c(t)}\widetilde{\chi}(\Lambda^c(t), e^{-R^c(t)}[x-x^c(t)]), \tag{34}$$

where the functions $x^c(t)$, $S^c(t,x)$, $Q^c(t)$, $R^c(t)$, and $\Lambda^c(t)$ are defined by (5), (6), (13), and (16), respectively (with $\Omega(t) = \Omega^c(t) = V''(x^c(t))$), and $\widetilde{\chi}$ is a solution to the free Schrödinger equation $i\widetilde{\chi}_t = -\frac{1}{2}\widetilde{\chi}_{xx}$. From

$$|\widetilde{\psi}^\varepsilon(t,x)|^2 = \frac{1}{[\sigma^c(t)]^D}\left|\widetilde{\chi}\left(\Lambda^c(t), \frac{x-x^c(t)}{\sigma^c(t)}\right)\right|^2,$$

the expectation values are readily computed.

$$\langle x\rangle^c(t) := \langle x\rangle_{\psi^\varepsilon(t)} \approx \int_{\mathbb{R}^D} x|\widetilde{\psi}^\varepsilon(t,x)|^2 \mathrm{d}x = x^c(t) + \sigma^c(t)\langle x\rangle_{\widetilde{\chi}(\Lambda^c(t))}, \tag{35a}$$

$$(\Delta x^c)^2(t) := \langle (x-x^c(t))^2\rangle_{\psi^\varepsilon(t)} \approx \int_{\mathbb{R}^D}(x-x^c(t))^2|\widetilde{\psi}^\varepsilon(t,x)|^2\mathrm{d}x = \sigma^c(t)^2\langle x^2\rangle_{\widetilde{\chi}(\Lambda^c(t))}, \tag{35b}$$

$$\begin{aligned}[(\Delta x)^c]^2(t) &:= \langle (x-\langle x\rangle^c(t))^2\rangle_{\psi^\varepsilon(t)} \approx \langle (x-x^c(t)-\sigma^c(t)\langle x\rangle_{\widetilde{\chi}(\Lambda^c(t))})^2\rangle_{\psi^\varepsilon(t)} \\ &\approx \sigma^c(t)^2\langle x^2\rangle_{\widetilde{\chi}(\Lambda^c(t))} - \sigma^c(t)^2\langle x\rangle^2_{\widetilde{\chi}(\Lambda^c(t))} = \sigma^c(t)^2[(\Delta x)_{\widetilde{\chi}(\Lambda^c(t))}]^2.\end{aligned} \tag{35c}$$

The functions $x^c(t)$ and $\sigma^c(t)$ depend on the control $E(t)$ by way of the system

$$\ddot{x}^c(t) = -V'(x^c(t)) - E(t), \quad x^c(0) = x_0, \quad \dot{x}^c(0) = p_0, \tag{36a}$$

$$\ddot{\sigma}^c(t) = -V''(x^c(t))\sigma^c(t), \quad \sigma^c(0) = 1, \quad \dot{\sigma}^c(0) = 0. \tag{36b}$$

Remarks:

(a) If we choose the initial conditions for (36a) to be

$$x_0 = \langle x\rangle_{\psi(0)} \quad \text{and } p_0 = \langle p\rangle_{\psi(0)},$$

we get $\langle x\rangle_{\widetilde{\chi}(\Lambda^c(t))} \equiv 0$ and hence

$$\langle x\rangle^c(t) = \langle x\rangle_{\psi^\varepsilon(t)} \approx \langle x\rangle_{\widetilde{\psi}^\varepsilon(t)} = x^c(t),$$

i.e., the position of the wave packet coincides with the classical trajectory $x^c(t)$.

(b) Note that, although Eq. (36b) may have global solutions, in view of (35c) (and the definition of $\sigma^c(t)$ as an exponential), its solutions $\sigma^c(t)$ are only relevant as long as they are positive.

(c) Note also that $(\Delta x)_{\widetilde{\chi}(\Lambda^c(t))}$ is known in principle. The spread, $(\Delta x)^c(t)$, of the wave packet is therefore essentially given by the function $\sigma^c(t)$.

(d) Clearly "everything" is accurate (i.e., we may replace "≈" with "=" everywhere) if the potential V is a quadratic function.

Observation III. *Let $\psi_0 \in \mathcal{S}$. In a second-order approximation and for times $t < T^*$, the solution is given by (34) and is therefore, up to a phase factor, a translated and rescaled version of the*

state $\tilde{\chi}(t)=U(t)\tilde{\psi}_0$, *where* $\tilde{\psi}_0(x):=e^{-ip_0\cdot x}\psi_0(x+x_0)$ *and* $U(t)$ *denotes the Schrödinger evolution group. In this approximation, the effect of the control term* $E(t)x$ *is "direct" control of the position,* $\langle x\rangle^c$, *of the wave packet (cf. (36a)); the influence on the spread,* $(\Delta x)^c(t)\approx\sigma^c(t)(\Delta x)_{\tilde{\chi}(\Lambda^c(t))}$, *is indirect and depends on the properties of* V'' *(cf. (36b)). In particular, if* $V''=const$, $(\Delta x)^c$ *cannot be controlled, which is consistent with "Observation I."*

V. TRAJECTORY-COHERENT STATES

We now turn to a class of approximate solutions to the Schrödinger equation with quasiclassical and particle-like properties, introduced by Bagrov *et al.*,[2] which are closely related to the approximate solutions constructed in Sec. IV C. Trajectory-coherent states (TCS) have actually been constructed for arbitrary dimension and even for certain nonlinear equations.[25–29] However, to demonstrate the implications for the control problem, it will be sufficient to consider the simplest case: "vacuum TCS" for the 1D linear Schrödinger equation. After reintroducing the physical constants $\hbar$ and m, our control problem reads

$$\mathcal{L}\psi:=i\hbar\psi_t+\frac{\hbar^2}{2m}\psi_{xx}-V(x)\psi-(E(t)x)\psi=0\ (x\in\mathbb{R}). \tag{37}$$

A. Construction of vacuum TCS

We proceed exactly as in Sec. IV C to obtain approximate, second-order accurate, solutions, given by (34),

$$\tilde{\psi}^c(t,x)=e^{(i/\hbar)[S^c(t,x)+(1/2)Q^c(t)(x-x^c(t))^2]}e^{-R^c(t)/2}\tilde{\chi}(\Lambda^c(t),e^{-R^c(t)}[x-x^c(t)]). \tag{38}$$

As in Sec. IV C, the functions $x^c(t)$, $S^c(t,x)$, $R^c(t)$, $\Lambda^c(t)$, and $\Omega^c(t)=V''(x^c(t))$ are defined by (5), (6), and (16), respectively, and $\tilde{\chi}$ is a solution to the free Schrödinger equation $i\hbar\tilde{\chi}_t=-(\hbar^2/2m)\tilde{\chi}_{xx}$. The main shortcoming of the construction consists of the fact that the function $Q^c(t)$, given by (13), may not be defined globally. We remedy this by allowing $Q^c(t)$ to take on complex values. Specifically, the function $Q^c=Q^c(t)\in\underline{\mathbb{C}}$ is now defined as the solution of the IVP

$$\dot{Q}(t)+Q(t)^2+\Omega^c(t)=0,\quad \mathrm{Re}(Q(0))=0,\quad \mathrm{Im}(Q(0))=b>0, \tag{39}$$

where $b>0$ is a positive number which we will keep fixed. It can be shown that the solution, $Q^c=Q^c(t)\in\mathbb{C}$, of (39) exists globally and satisfies $\mathrm{Im}(Q(t))>0$ for all $t\geqslant 0$. Note that the functions $\Lambda^c(t)$, $R^c(t)$, and $\sigma^c(t)$ are now complex-valued as well; we write $Q^c=Q_1^c+iQ_2^c$, $R^c=R_1^c+iR_2^c$, etc. for the decompositions in real and imaginary parts. Moreover, the functions $\Lambda^c(t)$ and $R^c(t)$ now exist globally and the function $\sigma^c(t)$ is nonzero everywhere. The function $\tilde{\psi}^c$ satisfies

$$\mathcal{L}\tilde{\psi}^c=-[V(x)-V(x^c(t))-V'(x^c(t))(x-x^c(t))-\tfrac{1}{2}V''(x^c(t))(x-x^c(t))^2]\tilde{\psi}^c=:r. \tag{40}$$

Now "vacuum" TCS are constructed by simply choosing the function $\tilde{\chi}$ to be constant—with the constant to be chosen such that the resulting state is normalized, $\tilde{\chi}\equiv[b/\pi\hbar]^{1/4}$,

$$\begin{aligned}\tilde{\psi}^c(t,x)&=\tilde{\chi}e^{(i/\hbar)[S^c(t,x)+(1/2)Q^c(t)(x-x^c(t))^2]}e^{-R^c(t)/2}\\&=\tilde{\chi}\,[\sigma^c(t)]^{-1/2}e^{(i/\hbar)[S^c(t,x)+(1/2)Q_1^c(t)(x-x^c(t))^2]}e^{-(1/2\hbar)Q_2^c(t)(x-x^c(t))^2}.\end{aligned} \tag{41}$$

These are Gaussian-shaped states,

$$|\tilde{\psi}^c(t,x)|^2=\tilde{\chi}^2|\sigma^c(t)|^{-1}e^{-(1/\hbar)Q_2^c(t)(x-x^c(t))^2},$$

which satisfy

$$\|\tilde{\psi}^c(t)\|_{L^2}^2 = \frac{|\tilde{\chi}|^2\sqrt{\pi\hbar}}{|\sigma^c(t)|\sqrt{Q_2(t)}\sqrt{b}} = 1, \tag{42a}$$

$$\langle x\rangle_{\tilde{\psi}^c(t)} = x^c(t), \tag{42b}$$

$$\langle(\Delta x)^2\rangle_{\tilde{\psi}^c(t)} = \langle(x - \langle x\rangle_{\tilde{\psi}^c(t)})^2\rangle_{\tilde{\psi}^c(t)} = \frac{\hbar}{2Q_2(t)}. \tag{42c}$$

Lemma: *Assume that* $V'''(x)$ *is bounded,* $\sup_{x\in\mathbb{R}}|V'''(x)| \leqslant M$, *and let* $\psi_0(x) := \tilde{\psi}(0,x) = e^{-(b/2\hbar)x^2}$. *Then*

(i) (Ref. 2)

$$\|r(t)\|_{L^2}^2 \leqslant \frac{5M^2\hbar^3}{96[Q_2^c(t)]^3}.$$

(ii) *If* ψ *is the (actual) solution of (37) corresponding to the initial condition* ψ_0 *and* $\underline{Q}^c := \min_{t\in[0,t]}Q_2^c(t)$, *then*

$$\|\psi(t) - \tilde{\psi}(t)\|_{L^2} \leqslant \frac{M\hbar^{1/2}T}{2[\underline{Q}^c]^{3/2}}.$$

Proof.

(i) (Ref. 2). (The estimate may also be derived directly from (40).)

(ii) Let $\delta\psi := \psi - \tilde{\psi}$, hence

$$\mathcal{L}\,\delta\psi = -r.$$

Then, by standard calculations,

$$\|\delta\psi(t)\|_{L^2}^2 = -\frac{2}{\hbar}\,\mathrm{Im}\int_0^t \langle r(s), \delta\psi(s)\rangle_{L^2}\mathrm{d}s \leqslant \frac{2}{\hbar}\int_0^t \|r(s)\|_{L^2}\|\delta\psi(s)\|_{L^2}\mathrm{d}s$$
$$\overset{(i)}{\leqslant} 2\frac{\sqrt{5}M\hbar^{1/2}}{2\sqrt{6}[\underline{Q}^c]^{3/2}}\int_0^t \|\delta\psi(s)\|_{L^2}\mathrm{d}s$$

and so, by Gronwall's lemma,

$$\|\delta\psi(t)\|_{L^2} \leqslant t\frac{\sqrt{5}M\hbar^{1/2}}{2\sqrt{6}[\underline{Q}^c]^{3/2}} \leqslant \frac{M\hbar^{1/2}T}{2[\underline{Q}^c]^{3/2}} \qquad \square$$

B. Consequences for the control problem

We now demonstrate a mechanism by which TCS might "hamper" the control process. To this end, we choose a target state $\psi_T \in \mathcal{S}$ such that

$$|\langle\sigma^{-1/2}e^{i[\pi\cdot(x-\xi)+(1/2)Q(x-\xi)^2]}, \psi_T(x)\rangle_{L^2}| \leqslant \tfrac{1}{2} \quad \text{for all } \xi,\pi\in\mathbb{R}, \sigma, Q\in\mathbb{C}^*, \mathrm{Im}(Q) > 0, |\sigma|\sqrt{\mathrm{Im}(Q)} = 1. \tag{43}$$

Our task is to try to steer the system from the initial state $\psi_0(x) := \tilde{\psi}(0,x) = e^{-(b/2\hbar)x^2}$ to the target state ψ_T. If we are successful, i.e., if we do find a control field $E(t)$ such that $\psi(T) = \psi_T$, we obviously have

$$\langle \psi(T), \psi_T \rangle_{L^2} = 1 .$$

This suggests to estimate the overlap, $\langle \psi(T), \psi_T \rangle_{L^2}$, between the states $\psi(T)$ and ψ_T. Note that assumption (43) implies that $|\langle \tilde{\psi}(T), \psi_T \rangle_{L^2}| \leqslant \frac{1}{2}$. Thus,

$$|\langle \psi(T), \psi_T \rangle_{L^2}| \leqslant |\langle \tilde{\psi}(T), \psi_T \rangle_{L^2}| + |\langle \psi(T) - \tilde{\psi}(T), \psi_T \rangle_{L^2}| \overset{(ii)}{\leqslant} \frac{1}{2} + \frac{M\hbar^{1/2}T}{2[\underline{Q}^c]^{3/2}} .$$

Note that the right hand side of this inequality contains the factor $\hbar^{1/2}$.

$$|\langle \psi(T), \psi_T \rangle_{L^2}| < 1 \Rightarrow \psi_T \notin R_T(\psi_0),$$

we obtain an estimate for the control time, which can be unreasonably large if the control field is not designed carefully.

Observation IV: *There are states $\psi_T \in \mathcal{S}$ which cannot be attained in times T less than*

$$\frac{[\underline{Q}^c]^{3/2}}{M\hbar^{1/2}} .$$

To obtain realistic control times the control field $E(t)$ should thus be designed such that

$$\underline{Q}^c = \mathcal{O}(\hbar^{1/3}) .$$

Remarks:

(a) The dependence of $Q_2(t)$ on the control $E(t)$ is given by the system

$$\dot{Q}_1^c(t) = \frac{1}{m}[Q_2^c(t)]^2 - \frac{1}{m}[Q_1^c(t)]^2 - V''(x^c(t)), \quad Q_1^c(0) = 0, \tag{44a}$$

$$\dot{Q}_2^c(t) = -\frac{2}{m} Q_1^c(t) Q_2^c(t), \qquad Q_2^c(0) = b > 0, \tag{44b}$$

where the controlled classical trajectory $x^c(t)$ is determined by Eq. (36a). The properties of this system and strategies for accomplishing the condition $\underline{Q}^c = \mathcal{O}(\hbar^{1/3})$, such as resonance, will be discussed elsewhere.

(b) In view of (42c), the geometric interpretation of the condition $\underline{Q}^c = \mathcal{O}(\hbar^{1/3})$ is that we have to make the state spread out in order to be able to access the nonclassical degrees of freedom.

VI. CONCLUDING REMARKS

1. The discussion in Secs. III A and IV A can be extended to include homogeneous *magnetic* fields[30] and *rotating* condensates. For spherically symmetric external potentials, this will produce the "missing degrees of freedom" (angular momentum) in the parametrization (22).
2. It has been shown recently[31] that the "particle-in-the-box problem," i.e., the control problem (37) with potential

$$V(x) = \begin{cases} 0, & |x| < \frac{1}{2} \\ \infty, & |x| \geqslant \frac{1}{2} \end{cases}$$

is locally controllable in the vicinity of the ground state. On the other hand, the present paper shows that (37) is certainly *not* controllable (not even locally) if V is the harmonic oscillator potential $V = (\omega/2)x^2$. This raises the very interesting (and difficult) question of how the controllability properties of Eq. (37) depend on the external potential. There is evidence to suggest that the harmonic oscillator potential may be some sort of threshold. One might

conjecture that (local) controllability holds for potentials that are steeper than the HO potential, whereas it fails for potentials that are shallower.

3. In a first approximation, the presence of a nonlinear term of the form $f(|\psi|^2)$ does not change the controllability properties with respect to spatially homogeneous control fields. This is due to the translation invariance of $f(|\psi|^2)$.
4. While the linear potential V is the dominant factor in the *bilinear* control problem with the control $E(t)x$, the nonlinear term turns out to be the main difficulty in control problems with *additive* control. See Ref. 32 for a small-data result in this direction.
5. Solitons may be interpreted as "nonlinear coherent structures." Continuing the theme of this paper, it will be shown elsewhere that they, too, constitute obstacles to the control process.[33]

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[5] This is actually exact for quadratic Hamiltonians.
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[7] As mentioned above, trajectory-coherent states are only approximate solutions to the Schrödinger equation; they become exact solutions for quadratic Hamiltonians.
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[9] This is an assumption on the various parameters in Eq. (1).
[10] Depending on the character of the two-body pair interaction, the nonlinearity may also be nonlocal. The local cubic form is appropriate for short-range interactions.
[11] For instance, if the quadratic trap is time-independent altogether, we will set $\Omega \equiv 0$.
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Decomposition of time-covariant operations on quantum systems with continuous and/or discrete energy spectrum

Dominik Janzing[a)]
IAKS, Arbeitsgruppe Quantum Computing, Universität Karlsruhe, Am Fasanengarten 5, D-76 131 Karlsruhe, Germany

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Every completely positive map G that commutes with the Hamiltonian time evolution is an integral or sum over (densely defined) CP-maps G_σ where σ is the energy that is transferred to or taken from the environment. If the spectrum is non-degenerate each G_σ is a *dephasing* channel followed by an *energy shift*. The dephasing is given by the Hadamard product of the density operator with a (formally defined) positive operator. The Kraus operator of the energy shift is a partial isometry which defines a translation on $\mathbb{R}$ with respect to a non-translation-invariant measure. As an example, this decomposition is explicitly calculated for the rotation invariant Gaussian channel on a single mode. The question of under what conditions a covariant channel destroys superpositions between mutually orthogonal states on the same orbit is addressed. For channels which allow mutually orthogonal output states on the same orbit, a lower bound on the quantum capacity is derived using the Fourier transform of the CP-map-valued measure (G_σ). © *2005 American Institute of Physics.* [DOI: 10.1063/1.2142839]

I. INTRODUCTION

It was an important insight in the early days of quantum computing and quantum cryptography research that quantum theory should not be considered as a purely physical theory, but it rather defines a new kind of information, called quantum information. The decisive feature is its fragility since quantum information is destroyed whenever one tries to copy it.[1]

The question of which physical processes and information channels preserve quantum information therefore plays a crucial role in the theory of quantum communication. A central concept for addressing this issue is the notion of a *channel*. Here we consider a channel or ("operation") to be a completely positive trace preserving map $\rho \mapsto G(\rho)$ where ρ and $G(\rho)$ are positive operators of trace one acting on Hilbert spaces $\mathcal{H}_{\text{in}}$ and $\mathcal{H}_{\text{out}}$, respectively.[2] Analyzing quantum or classical channel capacities is in general a difficult task. Here we consider a certain kind of channels or operations, namely those which are *time-covariant*. For simplicity, we will assume that the input and the output state is a state of the same physical system. Then we have $\mathcal{H}_{\text{in}} = \mathcal{H}_{\text{out}} =: \mathcal{H}$. Furthermore we have a Hamiltonian time evolution on $\mathcal{H}$ generated by a densely defined self-adjoint operator H which reads

$$\alpha_t(\rho) := e^{-iHt} \rho e^{iHt}, \tag{1}$$

where ρ is a positive operator with trace one. We call a channel G time-covariant if it satisfies

$$\alpha_t \circ G = G \circ \alpha_t. \tag{2}$$

[a)]Electronic mail: janzing@ira.uka.de

(Note that in the context of classical linear systems the corresponding property is usually referred to as time-"invariance.") It is a special case of the requirement

$$G(U_g \rho U_g^\dagger) = U_g G(\rho) U_g^\dagger, \tag{3}$$

where $g \mapsto U_g$ is an arbitrary unitary group representation.

For compact groups, each covariant CP-map G has a representation (see Ref. 3, which refers partly to Ref. 4)

$$G(\rho) = \sum_j L_j \rho L_j^\dagger,$$

where the Kraus operators L_j satisfy

$$U_g L_j U_g^\dagger = \sum_k d_{jk}(g) L_k, \tag{4}$$

and $g \mapsto [d_{jk}(g)]_{j,k \leqslant d}$ is a d-dimensional unitary representation with arbitrary d (in Ref. 3 it is mainly focused on the case that $g \mapsto U_g$ is an irreducible representation). Note that the time evolution can only be described by a compact group if it is periodic, which cannot be guaranteed even in the finite dimensional case. In Ref. 5 the case is considered that G is replaced by a whole dynamical semigroup $(G_t)_{t \in \mathbb{R}^+}$ which is covariant with respect to a group representation.

Condition (2) appears naturally, for instance, in the following situations:

1. *Theory of timing information:* Assume that the density matrix ρ is subjected to an arbitrary quantum operation G at a completely unknown time instant. Then the statistical description of this operation leads to a map G' which necessarily satisfies (2). This is the key idea in Ref. 6 where condition (2) defines a "quasiorder of clocks," which classifies systems with respect to their timing information. The time-covariant maps are exactly those which can be implemented without using external clocks. Given a nonstationary state ρ, the set of states that can be obtained from ρ using time-covariant operations are those which have at most as much timing information as ρ.
2. *Decoherence:* Dephasing of systems is described by a decay of the off-diagonal entries with respect to the energy eigenbasis. This channels satisfy clearly condition (2).
3. *Scattering processes/quantum generalization of transfer functions:* Time-covariant operations appear naturally in the description of scattering processes. Then G generalizes the scattering operator by including classical or quantum stochastic fluctuations. Here *scattering* is understood in a rather general sense. Apart from the situation that a particle is scattered by the potential of another particle, one may, for instance, also think of a light beam that passes a filter. One may consider time-covariant maps as quantum generalization of classical time-invariant linear devices which are described by their transfer functions.

The paper is organized as follows. In Sec. II we recall briefly how to describe classical time-invariant linear systems in signal processing by a transfer function.[7] Figuring out the extent to which this concept can be generalized to the quantum stochastic setting is the key motivation of this paper. In Sec. III we recall abstract scattering theory in Hilbert spaces and explain in Sec. IV why time-covariant channels are also considered as a natural generalization of scattering theory. In Sec. V we consider CP-maps which are given by the Hadamard product of the density matrix with a positive matrix. These maps will turn out as a building block of our decomposition. In Sec. VI we derive the general form of a time-covariant CP-map. The main result is that every time-covariant CP-map acting on a system with nondegenerate Hamiltonian has a (densely defined) decomposition as an integral or sum over (densely defined) CP-maps G_σ is a dephasing followed by an energy shift. In Sec. VII we address the question of whether and to what extent covariant channels can destroy superpositions between states on the same orbit (with respect to the time-evolution). We use the general decomposition to derive a lower bound on the quantum capacity of

a specific type of time-covariant channels, namely those which have as output mutually orthogonal density operators on the same orbit. In Sec. VIII we apply the decomposition to a single mode Gaussian channel.

II. CLASSICAL TIME-INVARIANT LINEAR SYSTEMS

To show the differences and the analogies to the theory of classical linear time-invariant channels we briefly rephrase the concept of transfer functions, which is among the most important tools in classical signal processing.

Consider a classical channel with an incoming and an outgoing signal. These may, for instance, be light pulses or electrical pulses, acoustical or other signals. Let $t \mapsto Y(t)$ be the incoming signal where $Y(t)$ is the value of an arbitrary physical quantity at the time instant t. Let $Y'(t)$ denote the outgoing signal. In order to avoid problems with undefined Fourier transforms we assume that Y and Y' are vectors in $L^2(\mathbb{R})$, the Hilbert space of square-integrable functions on $\mathbb{R}$. We assume that the system is described by a linear bounded operator A on $L^2(\mathbb{R})$ with

$$Y' = AY.$$

Assuming time-invariance of the channel we have $Y'(t+s)=(AY)(t+s)$. Defining the group of shifts $(S_t)_{t\in\mathbb{R}}$ by

$$(S_t Y)(s) = Y(t-s) \tag{5}$$

we have

$$S_t A = A S_t, \quad \forall\, t \in \mathbb{R}.$$

The implications of this condition can easily be derived by applying Fourier transformation to both sides of the equation: The shift operators S_t act then as the multiplication operators M_t,

$$\hat{Y} \mapsto M_t \hat{Y}$$

with

$$(M_t \hat{Y})(\omega) = e^{i\omega t}\hat{Y}(\omega).$$

A linear operator commuting with all operators M_t is necessarily a multiplication operator as well (see Ref. 8, 12.1.5). Therefore A can be characterized by a so-called transfer function a with

$$\hat{Y}'(\omega) = a(\omega)\hat{Y}(\omega). \tag{6}$$

Note that it is essential that the quantity $Y(t)$ is a scalar. If $Y(t)$ is a vector of dimension d greater than 1 the spectrum of the time-evolution group S_t is degenerate and $\hat{Y}(\omega)$ is an element of a vector space $\mathbb{C}^d$ or $\mathbb{R}^d$ and the transfer function a had to be replaced by a $d\times d$-matrix. It is straightforward to ask whether time-covariant quantum operations allow a natural generalization of the transfer function. However, one should recall that the situation with nondegenerate spectrum is possible on the Hilbert space level (this is well-known in abstract scattering theory, as will be rephrased in Sec. III) but not on the level of density matrices, where the dynamics is generated by the super-operator $-i[H,.]$. The latter always has degenerate spectrum.

III. ABSTRACT SCATTERING THEORY

A similar approach as presented earlier applies to a scattering process of a quantum mechanical particle: a particle which comes from the infinity and passes a scattering potential. After it has left the potential it disappears to infinity. Here we only recall some standard results of scattering theory[8,9] which are essential for this paper. Let $H=H_i+H_0$ be the total Hamiltonian of the system which consists of the free Hamiltonian H_0 and the interactions term H_i. One assumes that the

particle moves approximatively according to its free Hamiltonian H_0 for $t \to \pm\infty$. For potentials which decay sufficiently with the distance between particle and the scattering center, the limits

$$|\psi^{\pm}\rangle := \lim_{t\to\pm\infty} \exp(iHt)\exp(-iH_0t)|\psi\rangle \tag{7}$$

exist[9] on an appropriate subspace of wave functions $|\psi\rangle$. There is a rich literature addressing the question under which circumstances and on which subspaces one can define a unitary scattering operator

$$|\psi^-\rangle \mapsto |\psi^+\rangle =: S|\psi_-\rangle.$$

(It is usual to denote the scattering operator with S. On the other hand, it is usual to denote shifts by S_t with some index t. It is hoped that this will not lead to confusion.) However, if it exists it commutes with the free Hamiltonian evolution $\exp(-iH_0t)$. Therefore the free time evolution and the scattering operator S can simultaneously be described by multiplication operators. The analogy to Sec. II can even be closer in a scattering process with so-called Lax-Phillips evolution.[8] Assume that there exist subspaces $\mathcal{H}_- \leqslant \mathcal{H}$ and $\mathcal{H}_+ \leqslant \mathcal{H}$ ("incoming and outgoing subspaces," respectively) such that

$$e^{-iHt}\mathcal{H}_- \subset \mathcal{H}_-$$

for all negative t (the particle comes from the infinity) and

$$e^{-iHt}\mathcal{H}_+ \subset \mathcal{H}_+$$

for all positive t (the particle disappears to the infinity). Assume furthermore that the intersection

$$\cap_{t\in\mathbb{R}} \exp(-iHt)\mathcal{H}_{\pm}$$

vanishes and that the span of all spaces $\exp(-iHt)\mathcal{H}_+$ as well as the span of all $\exp(-iHt)\mathcal{H}_-$ is dense in $\mathcal{H}$. Then one can assume without loss of generality that $\mathcal{H}$ is the set of square integrable functions on $\mathbb{R}$ with respect to the Lebesgue measure, and H is the multiplication operator $(H\psi)\times(\omega) = \omega\psi(\omega)$. The scattering operator is then (like the transfer function in Sec. II) given by $(S\psi)(\omega) = s(\omega)\psi(\omega)$ with an appropriate function s.

IV. QUANTUM CHANNELS FROM SCATTERING PROCESSES

The unitary scattering operator S in Sec. III defines a channel $G(\rho) = S\rho S^{\dagger}$ which satisfies obviously the time-covariance condition (2) with respect to the *free* evolution $\alpha_t(\rho) = \exp(-iH_0t)\rho\exp(iH_0t)$ due to $SH_0 = H_0S$. It is clear that scattering with an unknown potential could lead to an operation which is a statistical mixture of maps $S\rho S^{\dagger}$. But not only classical fluctuations of the scattering potential lead to a mixture of output wave functions; due to quantum fluctuations of the potential one may also have a CP-map which is not a mixture of unitary scattering processes. To see this, consider a bipartite quantum system with Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ that evolves according to a joint Hamiltonian H_{AB}. Assume that the joint evolution coincides asymptotically with the separate evolution generated by $H_A + H_B$ and that the limits

$$|\psi^{\pm}\rangle := \lim_{t\to\infty} \exp(itH_{AB})\exp(-iH_At)\exp(-iH_Bt)|\psi\rangle$$

exist in an appropriate sense. Then we have formally the same situation as in Sec. III with the substitution

$$H_0 \mapsto H_A + H_B, \quad H \mapsto H_{AB}.$$

If a scattering operator U on $\mathcal{H}_A \otimes \mathcal{H}_B$ exists we have

$$[U, H_A + H_B] = 0. \tag{8}$$

Let ρ_A be an arbitrary initial density matrix of system A. Then the scattering process defines a completely positive map on the system B by

$$G(\rho_B) := \mathrm{tr}_A(U(\rho_A \otimes \rho_B)U^\dagger).$$

Due to Eq. (8) it is easy to verify that G is time-covariant if the initial state ρ_A is stationary with respect to the time evolution $\exp(-iH_A t)$. Here we do not address the difficult question in which situation the above-noted limits exist. The problem of the existence of scattering operators in the quantum stochastic setting is addressed in Ref. 10. This will not be our subject. The above-presented remarks were only to show that time-covariant channels appear naturally also in the description of (possibly inelastic) scattering processes. Another situation where time-covariance appears is when the energy spectrum is discrete and a weak interaction with the environment is switched on. Then the interaction implements clearly a unitary U on system + environment such that U satisfies (8).

V. QUANTUM CHANNELS FROM HADAMARD-PRODUCTS

Here we consider a simple type of time-covariant CP-maps which will play a crucial role in the description of general time-covariant CP-maps.

The Hadamard product $A*B$ of two $n \times n$- matrices A, B is defined as the entry-wise product $(A*B)_{ij} := A_{ij}B_{ij}$. Remarkably, the Hadamard product between a density matrix ρ with any positive matrix M of the same size n defines a completely positive map:

If $M := \Sigma_j r_j |d_j\rangle\langle d_j|$ is a spectral decomposition of M then we may define diagonal matrices D_j which have the coefficients of the vector $d_j \in \mathbb{C}^n$ as diagonal entries. Then the map

$$\rho \mapsto D_j \rho D_j^\dagger = (|d_j\rangle\langle d_j|) * \rho \tag{9}$$

is obviously completely positive. So is the positive linear combination of those maps. Channels of this type have already be considered in Ref. 11. Also Ref. 12 has already used them to describe decoherence. It is clear that they commute with the Hamiltonian time evolution if the Hadamard product is calculated with respect to the energy basis. In the finite dimensional case, we also obtain time-covariant channels by the following construction: Let $\Sigma := \{\omega_1, \ldots, \omega_n\}$ be the eigenvalues of H acting on $\mathbb{C}^n$. Let $|\omega_j\rangle$ be the corresponding eigenstates. For any $\sigma \in \mathbb{R}$ let $j_1, \ldots, j_k$ be all indices j such that $\omega_j + \sigma$ is in the spectrum Σ. Define the "partial shift" by

$$S_\sigma := \sum |\omega_{j_i} + \sigma\rangle\langle\omega_{j_i}|, \tag{10}$$

where the sum runs over all spectral values ω with $\omega + \sigma \in \Sigma$.

The map $\rho \mapsto S_\sigma \rho S_\sigma^\dagger$ is time-covariant and also every map of the form

$$\rho \mapsto \sum_\sigma S_\sigma (M_\sigma * \rho) S_\sigma^\dagger, \tag{11}$$

where the sum runs over all σ for which a nonzero partial shift exists. Each M_σ is an arbitrary positive matrix. It is easy to check that this map is trace-preserving if and only if

$$\sum_\sigma M_\sigma(\omega, \omega) = 1, \quad \forall\ \omega \in \Sigma, \tag{12}$$

where the sum runs over all values σ for which there exist an $\omega \in \Sigma$ such that $\omega + \sigma \in \Sigma$.

In the following we will show that this is the most general form of time-covariant CP-maps. As will be shown, this holds in principle even for the infinite dimensional case with continuous spectrum when the sum is replaced by an integral over a potentially uncountable number of energy shifts.

VI. THE GENERAL FORM OF TIME-COVARIANT CHANNELS

To understand our construction it is helpful to consider the finite dimensional case first. Using the Kraus representation[2]

$$G(\rho) = \sum_j A_j \rho A_j^\dagger, \tag{13}$$

one may choose A_j such that they are eigenvectors of α_t. [Since the derivation for the finite dimensional case follows actually from the general derivation later in this section we only mention briefly that this can be derived as follows. One shows that the representations $t \mapsto [d_{kj}(t)]$ of $(\mathbb{R}, +)$ in Eq. (4) corresponding to time-translations can be chosen such that they are irreducible, i.e., one-dimensional]. The eigenvalue is $\exp(-i\sigma_j t)$, where σ_j may be any possible frequency difference $\omega - \omega'$. For each possible value σ we obtain a CP-map

$$G_\sigma(\rho) := \sum_{\sigma=\sigma_j} A_j \rho A_j^\dagger.$$

Let $A_j = U_j |A_j|$ be the polar decomposition of A_j where the partial isometry U_j is computed from the pseudo-inverse $|A_j|^{-1}$ by

$$U_j := A_j |A_j|^{-1}.$$

One has $\alpha_t(U_j) = \exp(-i\sigma_j t) U_j$ and equivalently

$$[H, U_j] = \sigma_j U_j, \quad [H, |A_j|] = 0, \tag{14}$$

since $|A_j|$ is α_t-invariant according to $\alpha_t(A_j)\alpha_t(A_j^\dagger) = e^{-i\sigma_j t} e^{i\sigma_j t}$. Using Eq. (14) one checks easily that

$$U_j |\omega\rangle = V_j |\omega + \sigma\rangle, \quad \forall\, \omega \in \Sigma,$$

where V_j is an appropriate diagonal operator. Hence we can write

$$A_j = S_{\sigma_j} D_j$$

with the diagonal matrix $D_j := |A_j| V_j$. Using the remarks of Sec. V we may write

$$G_\sigma(\rho) = S_\sigma (M_\sigma * \rho) S_\sigma^\dagger,$$

where $M_\sigma = \Sigma_j |d_j\rangle\langle d_j|$ is defined as in Sec. V from the vectors $|d_j\rangle$ of diagonal entries of D_j.

We conclude:

Theorem 1 (Decomposition in finite dimensions): *Let G be a CP-map on $\mathbb{C}^n$ which commutes with the time evolution α_t corresponding to a nondegenerate diagonal Hamiltonian. Then G has the form*:

$$G(\rho) = \sum_\sigma S_\sigma (M_\sigma * \rho) S_\sigma^\dagger, \tag{15}$$

where the sum runs over all possible energy differences σ. Here S_σ denotes partial shifts and M_σ positive matrices.

The map $\rho \mapsto (M_\sigma * \rho)$ preserves the energy of every state and destroys to some extent the coherent superpositions between them. This is shown by the following two extreme cases: $M_\sigma = \mathbf{1}$ where $\mathbf{1}$ denotes the identity matrix. Then we have complete dephasing and obtain a mixture of energy eigenstates. If M_σ has only 1 as entries it is the trivial channel which does not affect the state at all. The map G consists of decohering channels followed by different energy shifts.

To see the relation of our decomposition to the transfer function note that all rank-one operators $|\omega + \sigma\rangle\langle\omega|$ span the eigenspace of $[H, .]$ with eigenvalue σ. A time-covariant operation has to

leave this subspace invariant. Therefore one could decompose G into a direct sum of linear maps B_σ acting on these eigenspaces. However, in this decomposition one would have restrictions on the family B_σ in order to yield a *completely positive map*. Therefore we have preferred a decomposition where each component is completely positive. However, the Hadamard multiplication for each frequency pair (ω,ω') reminds to the multiplication with the value of the transfer function for each frequency ω.

To generalize the decomposition to infinite dimensions we will need several vector-valued measures. Therefore we recall the precise definition:[13]

Definition 1 (Vector-valued measures and densities):

1. *Let Ω be a set and M the σ-algebra of measurable subsets of Ω. For a Banach space B a mapping $\gamma: M \to B$ is called a vector measure if*

$$\gamma(\cup_j m_j) = \sum_j \gamma(m_j)$$

for all finite collections of mutually disjoint sets m_j. It is called countably additive when the same holds for countable sums.

2. *Let ν be a measure on the measure space (Ω, M). A measurable function $f: \Omega \to B$ is the Radon-Nikodym derivative of γ with respect to ν if*

$$\int_m f \mathrm{d}\nu = \gamma(m), \quad \forall\, m \in M.$$

We also say that f is the (vector-valued) density of γ with respect to ν.

For trace-class operator-valued measures we will have countable additivity in the weak sense, i.e., that the scalar measure that is given by evaluation on observables is countably additive. For CP-map valued measures we demand countable additivity only after applying the maps to states and evaluating them on observables.

In order to construct the infinite dimensional analog of G_σ we define a function

$$f_{K,\rho}(t) := \mathrm{tr}(KG(\rho e^{-iHt})e^{iHt}) \tag{16}$$

for every observable K and state ρ. First consider the simple case that $G = A\rho A^\dagger$, where A is an operator satisfying $\alpha_t(A) = e^{-i\sigma t}A$. Then we have

$$f_{K,\rho}(t) = e^{i\sigma t} f_{K,\rho}(0).$$

If G is defined by several Kraus operators A_j which are eigenvectors with different eigenvalues σ_j the function $f_{K,\rho}$ would consist of harmonic functions with all these frequencies σ_j. Even though we do not expect in the infinite dimensional case that we have Kraus operators which are eigenvectors of α_t it will turn out that we can nevertheless construct a decomposition of G based on the Fourier transform of $f_{K,\rho}$. We show that for each positive bounded operator K and density operator ρ the function $f_{K,\rho}$ is positive semidefinite, i.e., it satisfies

$$\sum_{k,l} x_k \bar{x}_l f_{K,\rho}(t_k - t_l) \geqslant 0$$

for all vectors $x \in \mathbb{C}^m$ and m-tuples $t_1, \ldots, t_m \in \mathbb{R}$ with arbitrary m:

$$f_{K,\rho}(t_k - t_l) = \mathrm{tr}\left(K \sum_j A_j \rho e^{-iH(t_k - t_l)} A_j^\dagger e^{-iH(t_l - t_k)} \right) = \sum_j \mathrm{tr}(K e^{iHt_k} A_j e^{-iHt_k} \rho e^{iHt_l} A_j^\dagger e^{-iHt_l}),$$

where we have used

$$\sum_j A_j \rho e^{-iHt_k} A_j^\dagger e^{iHt_k} = \sum_j e^{iHt_k} A_j e^{-iHt_k} \rho A_j^\dagger,$$

which is just another version of the time-invariance condition. We have therefore

$$\sum_{k,l} x_k \bar{x}_l f(t_k - t_l) = \sum_j \mathrm{tr}\left(K\left(\sum_k x_k e^{iHt_k} A_j e^{-iHt_k} \right) \rho \left(\sum_l \bar{x}_l e^{iHt_l} A_j^\dagger e^{-iHt_l} \right) \right) = \sum_j \mathrm{tr}(K C_j \rho C_j^\dagger) \geqslant 0$$

with the abbreviation

$$C_j := \sum_k x_k e^{iHt_k} A_j e^{-iHt_k}.$$

Since $f_{K,\rho}$ is positive semidefinite it defines a unique positive scalar measure $\nu_{K,\rho}$ on $\mathbb{R}$ by Bochner's theorem.[14] For every measurable set $m \subset \mathbb{R}$ the map $K \mapsto \nu_{K,\rho}(m)$ is a positive linear functional. It is norm-continuous (with respect to the operator norm) since the norm of a positive functional is given by its value on the identity,[15] i.e., by $\nu_{\mathbf{1},\rho}(m)$. Now we restrict the functional to the set of compact operators where every norm-continuous functional is given by a trace-class operator.[16] Therefore we may define a positive trace-class operator ρ_m by

$$\mathrm{tr}(\rho_m K) = \nu_{K,\rho}(m).$$

Hence the map G_m defined by $G_m(\rho) := \rho_m$ is a positive map on the trace-class operators. One can easily check that G_m is also *completely* positive: one substitutes G and e^{-iHt} by an arbitrary tensor product extension $G \otimes id$ by and $e^{-iHt} \otimes \mathbf{1}$ and considers ρ and K as operators on the extended space. Then it is obvious that the above-noted positivity argument works similarly. We have $G_{\mathbb{R}} = G$ due to

$$\mathrm{tr}(K\rho_{\mathbb{R}}) = \nu_{K,\rho}(\mathbb{R}) = f_{K,\rho}(0) = \mathrm{tr}(K\rho).$$

Since the trace of each $G_m(\rho)$ is at most $\mathrm{tr}(G(\rho)) = \mathrm{tr}(\rho) = 1$, each map G_m is a bounded operator on T, the set of trace-class operators. Since $G_{\mathbb{R}}$ is trace-preserving the map $m \mapsto G_m$ is formally an *instrument* in the sense of Davies (see Ref. 17, Chap. 4). Think of $G_m(\rho)/\mathrm{tr}(G_m(\rho))$ as the post-measurement state given the knowledge that the measurement outcome σ is in m. Then $\rho \mapsto G(\rho)$ is formally the effect of the measurement if the measured outcome is completely ignored. Even though this interpretation refers to a virtual measurement the virtual result σ has an observable interpretation: Assume one observes the energy of the environment before and after it has interacted with the system. Due to energy conservation σ is the energy loss of the environment. Note that the initial energy of the environment can be observed without disturbing its state since we have assumed that it is in a stationary state. [The idea to observe the environment in order to have a less mixed output state (which increases information capacities) can already be found in Refs. 18 and 19]. We shall call the probability measure $\nu_{\rho,\mathbf{1}}$ the "energy shift probabilities" in the state ρ.

Each map G_m is also time-covariant: The obvious equation

$$f_{K,\rho} = f_{\alpha_t(K),\alpha_t(\rho)}$$

implies that it is irrelevant for the measure $\nu_{K,\rho}$ if α_t is applied to ρ and α_{-t} to the output state (which is equivalent to applying α_t to K).

We summarize the results:

Theorem 2: *For each time-covariant channel G there is a unique CP-map-valued-measure*

$$m \mapsto G_m$$

such that

1. *Each G_m is a time-covariant bounded operator on T.*
2. *The Fourier transform of $m \mapsto G_m$ is the function $t \mapsto \hat{G}_t$ with*

$$\hat{G}_t(\rho) := G(\rho e^{-iHt})e^{iHt}$$

in the sense that

$$t \mapsto \mathrm{tr}(K\hat{G}_t(\rho))$$

is for all $K>0$ *and all states* ρ *the Fourier transform of the (non-negative) measure*

$$m \mapsto \mathrm{tr}(KG_m(\rho)).$$

The positive-map-valued measure defines a positive operator-valued-measure (POVM)[17] $m \mapsto Q_m$ by

$$\mathrm{tr}(Q_m\rho) := \mathrm{tr}(G_m(\rho)).$$

In contrast to CP-map valued measures, POVMs describe only the probabilities for the measurement outcome without referring to the post-measurement state. The Fourier transform of this POVM will play a crucial role later.

In order to have a stronger analogy to Theorem 1 we would like to write G as an integral

$$G = \int G_\sigma \mathrm{d}\,\nu(\sigma)$$

with an appropriate measure ν. Then the function $\sigma \mapsto G_\sigma$ would be the CP-map valued Radon-Nikodym derivative of the measure $m \mapsto G_m$, i.e., G_σ would be the *density* of the measure with respect to the measure ν. The general problem of Radon-Nikodym derivatives of *instruments* (CP-map valued measures) has already been considered in Ref. 20. It is shown that it exists in the following sense:

There is a σ-finite measure ν, a dense domain $\mathcal{D} \in \mathcal{H}$, and a countable family of functions

$$\sigma \mapsto A_k^\sigma$$

defined for ν-almost all σ such that A_k^σ are linear operators $\mathcal{D} \to \mathcal{H}$ (not necessarily closable) such that

$$\int \sum_k \|A_k^\sigma|\psi\rangle\|^2 = \||\psi\rangle\|^2, \quad \forall\, |\psi\rangle \in \mathcal{D} \tag{17}$$

and

$$\mathrm{tr}(KG_m(\rho)) = \int_m \sum_k \langle A_k^\sigma\psi|KA_k^\sigma\psi\rangle \mathrm{d}\,\nu(\sigma), \quad \forall\, |\psi\rangle \in \mathcal{D}. \tag{18}$$

Note that A_k^σ could formally be considered as the Kraus operators of a CP-map G_σ with the "only" difference being that Kraus operators are not only closable but even bounded.

Equation (17) states implicitly that

$$\sum_k \langle A_k^\sigma\psi|KA_k^\sigma\psi\rangle < \infty \tag{19}$$

for ν-almost all σ. Since it even converges for $K=\mathbf{1}$, expression (19) defines a bounded positive functional on the operators K. We can find a unique positive trace-class operator ρ_σ such that

$$\mathrm{tr}(K\rho_\sigma) = \int_m \sum_k \langle A_k^\sigma \psi | K A_k^\sigma \psi \rangle$$

for all compact K. The proof in Ref. 20 states furthermore that $\mathcal{D}$ can be the finite span of any orthogonal system of $\mathcal{H}$. Summarizing these results, we have:

Theorem 3 (Radon-Nikodym derivative of the instrument): *For every orthonormal system* $(|x_j\rangle)$ *of* $\mathcal{H}$ *there is a family of CP-maps* G_σ *defined on the finite span of all rank-one operators* $|x_i\rangle\langle x_j|$ *such that*

$$G_m(\rho) = \int_m G_\sigma(\rho)\mathrm{d}\nu(\sigma) \tag{20}$$

for all ρ *in the domain of* G_σ *and an appropriate* σ*-finite measure* ν.

However, the domain of the maps G_σ can be extended:

Lemma 1 (Extended domains): Let $\rho \in T$ *be arbitrary and* ν *be an arbitrary measure. If the trace-class operators* $G_\sigma(\rho)$ *are consistently defined (in the sense that they define the density of the measure* $m \mapsto G_m(\rho)$*) then we have:*

1. *The domain of* G_σ *can consistently be extended to* ρe^{-iHt} *by*

$$G_\sigma(\rho e^{-iHt}) := G_\sigma(\rho) e^{-iHt} e^{i\sigma t}.$$

Consistency means that it is the density of the measure $m \mapsto G_m(\rho e^{-iHt})$. *Similarly, we may define* $G_\sigma(\exp(iHt)\rho) := \exp(-i\sigma t)\exp(iHt)G_\sigma(\rho)$.

2. *Let* l *be a measurable subset of* $\mathbb{R}$ *and* P_l *be the projection onto the space of functions vanishing on the complement of* l. *Then one may extend the domain of* G_σ *consistently to* ρP_l *by setting*

$$G_\sigma(\rho P_l) := G_\sigma(\rho) P_{l+\sigma},$$

and similarly $G_\sigma(P_l\rho) := P_{l+\sigma} G_\sigma(\rho)$.

Proof: The Fourier transform of the measure

$$m \mapsto \mathrm{tr}(K G_m(\rho e^{-iHt}))$$

is given by

$$f(r) := \mathrm{tr}(K\hat{G}_r(\rho e^{-iHt})) = \mathrm{tr}(K\hat{G}_{t+r}(\rho)e^{-iHt}) \tag{21}$$

$$= \int \mathrm{tr}(K G_\sigma(\rho) e^{-iHt}) e^{i(r+t)\sigma} \mathrm{d}\nu(\sigma). \tag{22}$$

The last equality holds since $\hat{G}_{r+t}$ is the Fourier transform of $m \mapsto G_m$ evaluated at $r+t$. Set $\rho_\sigma := G_\sigma(\rho)$. We write (22) as

$$\int \mathrm{tr}(K\rho_\sigma e^{-iHt} e^{it\sigma}) e^{ir\sigma} \mathrm{d}\nu(\sigma),$$

which is the Fourier transform of a measure with density

$$\sigma \mapsto tr(K\rho_\sigma e^{-iHt} e^{it\sigma}).$$

This proves statement (1).

To prove (2) we have to show that

$$\mathrm{tr}(KG_m(\rho P_l)) = \int_m G_\sigma(\rho) P_{l+\sigma} \mathrm{d}\nu(\sigma) \tag{23}$$

holds for all K and measurable m. Consider the scalar complex-valued measure

$$l \mapsto \mathrm{tr}(KG_m(\rho P_l)).$$

Its Fourier transform is

$$f(t) := \mathrm{tr}(KG_m(\rho e^{iHt})) = \int_m \mathrm{tr}(K\rho_\sigma e^{-iHt} e^{it\sigma}) \mathrm{d}\nu(\sigma),$$

where the last equality is due to statement (1). By

$$e^{-iHt} e^{it\sigma} = e^{i(H+\sigma \mathbf{1})t}$$

the last expression is the Fourier transform of the measure

$$l \mapsto \int_m G_\sigma(\rho) P_{l+\sigma} \mathrm{d}\nu(\sigma).$$

This proves that both sides of Eq. (23) coincide. □

We would like to characterize the maps G_σ more explicitly. We already have done this in Theorem 1 for the finite dimensional case when the spectrum of H is nondegenerate. Now we assume that $\mathcal{H}$ is the set of square integrable functions on $\mathbb{R}$,

$$\mathcal{H} := L^2(\mathbb{R}, \mu),$$

where μ is an arbitrary measure on $\mathbb{R}$ defined on the Lebesgue measurable sets. To formalize the assumption of nondegenerate spectrum we define H as the multiplication operator

$$(H\psi)(\omega) = \omega\psi(\omega), \quad \forall\, \omega \in \mathbb{R}. \tag{24}$$

Note that the Hadamard product can be generalized to infinite dimensions since every density operator ρ has a representation $\rho = \sum_j p_j |\phi_j\rangle\langle\phi_j|$ with eigenvectors $|\phi_j\rangle$. Then we may interpret

$$\rho(\omega, \omega') := \sum_j p_j \phi_j(\omega) \bar{\phi}_j(\omega')$$

as the entries of ρ. This is also the representation of ρ by its integral kernel, i.e.,

$$(\rho\psi)(\omega) = \int \rho(\omega, \omega')\psi(\omega') \mathrm{d}\mu(\omega').$$

Accordingly, we define:

Definition 2 (Hadamard product in infinite dimensions): For two trace-class operators ρ, ρ' and a function $M: \mathbb{R} \times \mathbb{R} \to \mathbf{C}$ we write

$$\rho' = M * \rho \tag{25}$$

if

$$\rho'(\omega, \omega') = M(\omega, \omega')\rho(\omega, \omega'). \tag{26}$$

To generalize the concept of partial shifts to $L^2(\mathbb{R}, \mu)$ is less straightforward. Since they should be partial isometries, the problem is twofold: Assume first that μ is given by a nonconstant and nonzero density with respect to the Lebesgue measure. Then it is intuitively clear that the generalized "shift" rescales the function to compensate the different densities at different points in order to be isometric. Assume, second, that H has discrete and continuous spectrum, i.e., μ

consists of singular and absolutely continuous parts with respect to the Lebesgue measure. Then one cannot expect that the discrete part of the wave function can be shifted to the continuous part and vice versa. The part of the wave function where this is the case has to be mapped to zero.

Despite these difficulties, the following lemma shows that our concept makes sense even in the general situation:

Lemma 2 (Partial shifts): For every $\sigma \in \mathbb{R}$ there is a unique partial isometry S_σ with the following properties:

1. *For all $f \in \mathcal{H}$ we have*

$$(S_\sigma f)(\omega) := s_\sigma(\omega - \sigma) f(\omega - \sigma), \tag{27}$$

   where s_σ is an appropriate measurable "scaling" function.

2. *Under all partial isometries $\widetilde{S}_\sigma$ which have a representation as in (1) with an appropriate scaling function $\widetilde{s}_\sigma$ the operator S_σ has minimal kernel, i.e., its kernel is contained in the kernel of all those $\widetilde{S}_\sigma$.*

Proof: Define the translated measure $\mu_\sigma(m) := \mu(m+\sigma)$. Then there is a unique decomposition

$$\mu = \mu_c + \mu_s, \tag{28}$$

where μ_c is absolutely continuous with respect to μ_σ and μ_s is orthogonal to μ_σ.[21] Here, orthogonality means that there is a measurable set B such that $\mu_s(B)=0$ and $\mu_\sigma(\bar{B})=0$ where $\bar{B}$ denotes the complement of B. Let p be the density of μ_c with respect to μ_σ. Set $s_\sigma := \sqrt{p}$. First we show that S_σ is an isometry of the subspace $\mathcal{H}_c$ given by all functions f with $f(\omega)=0$ for $\omega \in \bar{B}$:[22,23]

$$\int |s_\sigma(\omega-\sigma) f(\omega-\sigma)|^2 \mathrm{d}\mu(\omega) = \int |s_\sigma(\omega)|^2 |f(\omega)|^2 \mathrm{d}\mu_\sigma(\omega) = \int |f(\omega)|^2 p(\omega) \mathrm{d}\mu_\sigma(\omega) = \int |f(\omega)|^2 \mathrm{d}\mu_c. \tag{29}$$

This integral is equal to $\int |f(\omega)|^2 \mathrm{d}\mu$ if f vanishes on $\bar{B}$. On the other hand, it is zero if f vanishes on B. This shows that the space can be decomposed into the kernel of S_σ and a subspace where S_σ is an isometry. Hence we have $\|S_\sigma f\| \leq \|f\|$ on the whole space. Note that the equations showing this inequality show furthermore that S_σ is well-defined with respect to the equivalence classes in $L^2(\mathbb{R}, \mu)$.

Let $\widetilde{S}_\sigma$ be another isometry satisfying condition (1) with the scaling function $\widetilde{s}_\sigma$. Set $D := \widetilde{s}^{-1}(0)$. Clearly, condition (1) implies $[H, \widetilde{S}_\sigma] = \sigma \widetilde{S}_\sigma$ and $[H, \widetilde{S}_\sigma^\dagger] = -\sigma \widetilde{S}_\sigma^\dagger$. Hence the initial projection $\widetilde{S}_\sigma^\dagger \widetilde{S}_\sigma$ commutes with H and is therefore the multiplication operator with the characteristic function χ_D of a measurable set D. Let f vanish on $\bar{D}$. Since $\widetilde{S}_\sigma$ preserves its norm we have

$$\int |f(\omega)|^2 \mathrm{d}\mu(\omega) = \int |f(\omega)|^2 \widetilde{s}_\sigma^2(\omega) \mathrm{d}\mu_\sigma(\omega).$$

Since this holds for all functions which vanish on $\bar{D}$ μ-almost everywhere it shows that the restriction of μ to D is absolutely continuous with respect to μ_σ (with the density $\widetilde{s}_\sigma^2$). Hence the singular part of μ (with respect to μ_σ) vanishes on D and we have

$$\int |f(\omega)|^2 \mathrm{d}\mu(\omega) = \int |f(\omega)|^2 \mathrm{d}\mu_c(\omega).$$

As can be seen in Eq. (29), this shows that the norm of f is also preserved by S_σ. Hence the isometric subspace of $\widetilde{S}_\sigma$ is a subspace of the isometric subspace of S_σ and the kernel of S_σ is a subspace of the kernel of $\widetilde{S}_\sigma$. □

Fortunately, these shifts have the following property:

Lemma 3: The partial shift of Lemma 2 satisfies

$$S_\sigma^\dagger = S_{-\sigma}. \tag{30}$$

Proof: Rewriting the inner product of $\mathcal{H}$ as an integral one checks easily that $S_\sigma^\dagger$ has to be a translation by $-\sigma$ with an appropriate scaling function. It is easy to see that $S_{-\sigma}S_\sigma = S_\sigma^\dagger S_\sigma$: On the kernel of S_σ both products coincide trivially. On its orthogonal complement, i.e., the isometric subscape of S_σ the operator $S_\sigma^\dagger S_\sigma$ is the identity. But this must also be true for $S_{-\sigma}S_\sigma$ because the isometric subspace of $S_{-\sigma}$ must contain the isometric subspace of $S_\sigma^\dagger$ since $S_{-\sigma}$ has minimal kernel in the set of all partially isometric translations [see property (2) in Lemma 2]. Using general properties of partial isometries[22,23] the image of $S_\sigma^\dagger$ satisfies therefore

$$\mathrm{Im}\, S_\sigma^\dagger = \mathrm{Im}(S_\sigma^\dagger S_\sigma) = \mathrm{Im}(S_{-\sigma}S_\sigma) \leqslant \mathrm{Im}\, S_{-\sigma}.$$

Reversing this inequality by taking the orthogonal complement we obtain

$$\ker S_\sigma \geqslant \ker S_{-\sigma}^\dagger.$$

Because this holds for all $\sigma \in \mathbb{R}$ we have

$$\ker S_{-\sigma} \geqslant \ker S_\sigma^\dagger.$$

Since $S_{-\sigma}$ has minimal kernel we conclude

$$\ker S_{-\sigma} = \ker S_\sigma^\dagger.$$

Due to the uniqueness of the maximal element in the set of all partially isometric translations we have

$$S_\sigma^\dagger = S_{-\sigma}.$$

□

Note that we can only write $G_\sigma(\rho)$ in the form $S_\sigma(M_\sigma * \rho)S_\sigma^\dagger$ if the density operator $G_\sigma(\rho)$ acts only on the image of S_σ (which coincides with the image of the projection $S_\sigma S_\sigma^\dagger$). But this is indeed the case:

Lemma 4: If ρ is in the domain of G_σ its output $\rho_\sigma := G_\sigma(\rho)$ satisfies

$$S_\sigma S_\sigma^\dagger \rho_\sigma S_\sigma S_\sigma^\dagger = \rho_\sigma. \tag{31}$$

Proof: We will show $G_\sigma(\rho)S_\sigma S_\sigma^\dagger = G_\sigma(\rho)$. The statement $S_\sigma S_\sigma^\dagger G_\sigma(\rho) = G_\sigma(\rho)$ follows similarly. Due to Lemma 3 we have $S_\sigma S_\sigma^\dagger = S_{-\sigma}^\dagger S_{-\sigma}$, which is the projection onto the isometric subspace of $S_{-\sigma}$. It can explictly be given as follows (see proof of Lemma 2): Let $\mu := \mu_c \oplus \mu_s$ be the decomposition into the absolutely continuous and singular part of μ with respect to $\mu_{-\sigma}$. Let C be a set such that $\mu_{-\sigma}(\bar{C}) = 0$ and $\mu_s(C) = 0$. Then $S_{-\sigma}^\dagger S_{-\sigma} = P_C$. Due to $\mu(\bar{C} - \sigma) = \mu_{-\sigma}(\bar{C}) = 0$ we have $P_{\bar{C}-\sigma} = 0$. This implies

$$G_\sigma(\rho)P_{\bar{C}} = G_\sigma(\rho P_{\bar{C}-\sigma}) = 0.$$

□

For the construction in the sequel we choose the ONS in Theorem 3 such that its finite span contains a vector $|\psi\rangle$ with $\psi(\omega) \neq 0$ for μ-almost all ω.

Now we can define a function

$$M_\sigma : \mathbb{R} \times \mathbb{R} \to \mathbf{C}$$

by

$$M_\sigma(\omega,\omega') := \frac{k(\omega,\omega')}{\psi(\omega)\bar{\psi}(\omega')}, \tag{32}$$

where the function k represents the trace-class operator $S_\sigma^\dagger \rho_\sigma S_\sigma$. Even though this function is not well-defined, the calculations to follow show that the freedom of choosing M_σ is irrelevant.

By construction and using Lemma 4, we have

$$G_\sigma(\rho) = \rho_\sigma = S_\sigma(M_\sigma * \rho_\sigma)S_\sigma^\dagger.$$

We conclude

$$G(|\psi\rangle\langle\psi|) = \int S_\sigma(M_\sigma * (|\psi\rangle\langle\psi|))S_\sigma^\dagger \mathrm{d}\nu(\sigma)$$

with $|\psi\rangle$ as above. Using Lemma 1, part (1), we have

$$\int G_\sigma(e^{-iHt}|\psi\rangle\langle\psi|e^{iHs})\mathrm{d}\nu(\sigma) = \int S_\sigma(M_\sigma * (e^{-iHt}|\psi\rangle\langle\psi|e^{iHs}))S_\sigma^\dagger \mathrm{d}\nu(\sigma),$$

for all $s,t \in \mathbb{R}$. The finite span of these rank-one operators is dense in T since H is the multiplication with the identity and the span of all $\exp(-iHt)|\psi\rangle$ is therefore dense in $\mathcal{H}$. We conclude:

Theorem 4 (Dephasing—energy shift representation): *There is a family of functions* $(M_\sigma)_{\sigma\in\mathbb{R}}$,

$$M_\sigma : \mathbb{R}\times\mathbb{R} \to \mathbf{C}, \tag{33}$$

and a σ*-finite measure* ν *on* $\mathbb{R}$ *such that for a dense set of density operators* ρ *the decompostion*

$$G(\rho) = \int S_\sigma(M_\sigma * \rho)S_\sigma^\dagger \mathrm{d}\nu(\sigma)$$

holds.

We would like to have an analogy to the statement that M_σ is in the finite dimensional case a *positive* matrix. However, we have specified M_σ only as a function and not as an operator. It seems straightforward to consider it as an operator by

$$(M_\sigma\psi)(\omega) := \int M_\sigma(\omega,\omega')\psi(\omega')\mathrm{d}\mu(\omega').$$

But it is easy to see that this is not in general well-defined. Let, for instance, G be the identity on the density operators on $l^2(\mathbb{Z})$. Then the decomposition of G reduces to $G(\rho)=M_0*\rho$ with $M_0(\omega,\omega')=1$. The formal matrix multiplication of this "all-one" matrix with any square-integrable sequence leads to infinite coefficients. However, formally it is like a positive operator in the following sense.

$$M_\sigma * (|\psi\rangle\langle\psi|)$$

is by construction the trace-class operator ρ_σ. Translated to finite dimensions this expression to

$$DM_\sigma D^\dagger,$$

where D is a nonsingular diagonal matrix [in analogy to the statement that $\psi(\omega)$ vanishes almost nowhere]. Such a matrix can only be positive if M_σ is itself positive. In this sense we consider M_σ as positive even though it is not an operator. In analogy to the finite dimensional case, an exact measurement of the energy of the environment (before and after the interaction has taken place) would lead to a map

$$S_\sigma(M_\sigma * \rho)S_\sigma^\dagger,$$

which is only a dephasing channel up to the known energy shift.

It should be noted that (depending on ν) the integral may represent a finite, or countable infinite sum, or a continuous integral even though the Kraus representation of G is always possible with a countable sum.[2]

VII. SUPERPOSITIONS BETWEEN STATES IN THE SAME ORBIT

The "Hadamard-channel" $\rho \mapsto M * \rho$ with a positive matrix M allows perfect classical information transfer by using energy eigenstates as logical states. Its quantum capacity depends on the destruction of off-diagonal elements, i.e., whether the output states are more or less stationary states. Explicitly one has the following lower bound on the quantum capacity:

Lemma 5: In dimension n, the quantum capacity Q of the channel $\rho \mapsto M * \rho$ *with* $M(\omega, \omega) = 1$ *for all* $\omega \in \Omega$ *satisfies*

$$Q \geqslant \log_2(n) - S(M/n),$$

where S(.) denotes the von-Neumann entropy.

Proof: Let

$$M := \sum_j |m_j\rangle\langle m_j| \tag{34}$$

be a decomposition into mutually orthogonal rank-one operators with non-normalized vectors $|m_j\rangle$. Let D_j be the diagonal matrices having the coefficients of $|m_j\rangle$ as entries. Then we have

$$G(\rho) = \sum_j D_j \rho D_j^\dagger.$$

The quantum capacity is given by the supremum of the coherent information[24] over all input states for arbitrarily many copies of the channel. Let $|\phi\rangle\langle\phi|$ be a state on $\mathbb{C}^n \otimes \mathbb{C}^n$ and ρ its restriction to the right component. Then the coherent information is defined as

$$S(G(\rho)) - S((\mathrm{id} \otimes G)(|\phi\rangle\langle\phi|)),$$

where S denotes the von Neumann entropy. Consider the maximally entangled state

$$|\phi\rangle := \frac{1}{\sqrt{n}} \sum_j |j\rangle \otimes |j\rangle. \tag{35}$$

Note that ρ is the maximally mixed state and that it is preserved by the channel. Hence we have $G(S(\rho)) = \log_2(n)$ and

$$(\mathrm{id} \otimes G)(|\phi\rangle\langle\phi|) = \sum_j (1 \otimes D_j)|\phi\rangle\langle\phi|(1 \otimes D_j^\dagger). \tag{36}$$

Furthermore we have

$$\langle\phi|(1 \otimes D_j^\dagger)(1 \otimes D_i)|\phi\rangle = \mathrm{tr}(D_j^\dagger D_i) = \langle m_j|m_i\rangle = 0.$$

Therefore the sum (36) is already the spectral decomposition of $(\mathrm{id} \otimes G)(|\phi\rangle\langle\phi|)$. The eigenvalues are the square of the length of each vector $(1 \otimes D_j)|\phi\rangle$. It is given by $\langle m_j|m_j\rangle/n$. Hence the entropy of the output state is the von Neumann entropy $S(M/n)$. □

Here the destruction of quantum information coincides with the destruction of timing information in the sense that states on the same orbit of α_t become less distinguishable. It is obvious that decoherence with respect to the energy eigenbasis leads always destroys *timing* information in this sense. Here we want to address the question of what happens when one considers orthogonal

states on the same orbit of the time evolution as reference basis. Is it possible that a time-covariant channel destroys superpositions between them without affecting the basis states? Consider two vector states $|\phi_0\rangle$ and $|\phi_s\rangle := \exp(-iHs)|\phi_0\rangle$. Clearly, $G(|\phi_0\rangle\langle\phi_0|) = |\phi_0\rangle\langle\phi_0|$ implies

$$S_\sigma(M_\sigma * (|\phi_0\rangle\langle\phi_0|))S_\sigma^\dagger = 0$$

for all $\sigma \neq 0$. This follows from the observation that the output state can only be pure if all output operators are linearly dependent. Every $\sigma \neq 0$ would lead to a different output state. Furthermore we have

$$M_0 * (|\phi_0\rangle\langle\phi_s|) = M_0 * (|\phi_0\rangle\langle\phi_0|)e^{iHs} = |\phi_0\rangle\langle\phi_s|.$$

One can conclude easily that every density operator acting on the subspace spanned by $|\phi_0\rangle$ and $|\phi_s\rangle$ is preserved by G. A little bit more general, one has:

Theorem 5: *Let G be a time-covariant CP-map on a system with nondegenerate Hamiltonian. If there is any pure state* $|\phi\rangle\langle\phi|$ *with*

$$G(|\phi\rangle\langle\phi|) = |\phi\rangle\langle\phi|$$

then G leaves all density operators invariant which act on the Hilbert subspace spanned by all $\exp(-iHt)|\phi\rangle$.

The essential argument above is that there exist no states which are invariant with respect to S_σ for some $\sigma \neq 0$. An analog statement would not be true for covariance with respect to a discretized time evolution:

Consider the Hilbert space $l^2(\mathbb{Z})$ of square summable two-sided sequences and the discrete time evolution given by the translation $(U\psi)(n) := \psi(n+1)$. Let $(|e_n\rangle)_{n\in\mathbb{Z}}$ be the canaonical basis of $l^2(\mathbb{Z})$. Then the channel

$$\rho \mapsto \sum_{n\in\mathbb{Z}} |e_n\rangle\langle e_n|\rho|e_n\rangle\langle e_n|$$

leaves all basis states $|e_n\rangle$ invariant but destroys all superpositions.

The assumption that a pure state is preserved by G is rather strong. Actually we want to figure out whether *distiguishability* of different states in the same orbit may be conserved even though their *superpositions* are destroyed. We consider the following extreme case:

Definition 3 (Reliable timing): A time-covariant channel G has the "reliable timing property" (with respect to the time s) if there exists an input density operator ρ *and a real number s such that for* $\rho_s := \alpha_s(\rho)$ *the outputs* $G(\rho)$ *and* $G(\rho_s)$ *are perfectly distinguishable, i.e., the density matrices are mutually orthogonal.*

It is easy to verify that the input state ρ can be chosen to be pure. To justify the definition, we show that this property appears in the following situation: Assume a sender, say Alice, wants to send a signal to a receiver, say Bob. Assume furthermore that it should be guaranteed that Bob receives the signal in the time interval $[t_1, t_2]$. This requires that the physical state ρ of the signal (when it is sent) is perfectly distinguishable from the time evolved state ρ_s with $s := t_1 - t_2$. This is due to the fact that the following "measurement" distinguishes between them: wait the time t_1 and ask Bob whether he has already received the signal. If the medium between Alice and Bob modifies the signal, we may model this by a time-covariant operation G which has clearly to preserve the distinguishability of the states ρ and ρ_s.

It is clear that reliable transfer of classical information requires two states ρ and γ such that $G(\rho)$ and $G(\gamma)$ are mutually orthogonal. The above-noted remark shows that there are situations in classical information processing where two orthogonal output states should exist *on the same orbit* since reliable timing requires this feature. To see that nontrivial channels with this property exist one may construct a channel of the form

$$\rho \mapsto \sum_j p_j S_{\sigma_j} \rho S_{\sigma_j}^\dagger,$$

where the σ_j are chosen such that $\langle \phi | S_{\sigma_i}^\dagger S_{\sigma_j} \phi \rangle = 0$ for $i \neq j$. This condition is, for instance, satisfied if the minimal distance between the values σ_j exceeds the spectral bandwidth of the input state. Real physical channels will satisfy condition 3 at most approximately.

In order to consider the quantum capacity of reliable timing channels we choose ρ and $\rho_s = U_s \rho U_s^\dagger$ with $U_s := \exp(-iHs)$ such that ρ and ρ_s are mutually orthogonal. For simplicity we assume that the dynamical evolution of $G(\rho)$ is periodic. We obtain a set

$$G(\rho_0), G(\rho_s), G(\rho_{2s}), \ldots, G(\rho_{s(N-1)})$$

of N mutually perfectly distinguishable density matrices. Let P be the support of $G(\rho)$, i.e., the smallest projection with $PG(\rho) = G(\rho)$. Then the projections $U_{sj} P U_{sj}^\dagger$ with $j = 0, \ldots, N-1$ are mutually orthogonal.

Now we consider the channel with input

$$\mathbb{C}^N \equiv \mathrm{span}\{|\phi_{sj}\rangle\}_{j=0,\ldots,N-1}.$$

It is clear that there exist pure input states $|\psi_0\rangle, \ldots, |\psi_{s(N-1)}\rangle$ for which the orthogonality of the output states is satisfied. By sending either of these N states G can transfer $\log_2 N$ bits of classical information. We want to derive sufficient conditions under which G allows one to send superpositions between the chosen basis states. For doing so, we restrict G to a channel K on $N \times N$-density matrices as follows.

The input is restricted to the span of all $|\psi_{sj}\rangle$ with $j = 0, \ldots, N-1$. The corresponding output space is

$$\mathcal{H}_r := \oplus_{j=0}^{N-1} U_{sj} P U_{sj}^\dagger \mathcal{H}. \tag{37}$$

We may consider this space as the tensor product

$$\mathcal{H}_r = \mathbb{C}^N \otimes P\mathcal{H}$$

if we identify the spaces $U_{sj} P U_{sj}^\dagger \mathcal{H}$ for $j \neq 0$ with $P\mathcal{H}$ via arbitrary unitaries. It is straightforward and convenient to choose the isomorphisms U_{sj} with $j = 0, \ldots, N-1$. For any output density operator γ acting on $\mathcal{H}_r$ the entry corresponding to $|j\rangle\langle k|$ of its restriction to $\mathbb{C}^N$ is given by

$$\mathrm{tr}(U_{sk} P U_{sj}^\dagger \gamma).$$

To determine the channel K we have to compute all values

$$\mathrm{tr}(U_{sk} P U_{sj}^\dagger G(|\phi_{sl}\rangle\langle\phi_{sm}|)),$$

for $k, j, l, m \in \{0, \ldots, N-1\}$. Due to the reliable timing property we know that each state $|\phi_{sj}\rangle\langle\phi_{sj}|$ leads to the output state $|j\rangle\langle j|$. Furthermore the operator $|\phi_{sl}\rangle\langle\phi_{sm}|$ leads with certainty to a multiple of $|l\rangle\langle m|$. Roughly speaking, the reason is that a CP-map which maps the states $|m\rangle\langle m|$ and $|l\rangle\langle l|$ onto itself maps also $|l\rangle\langle m|$ onto multiples of itself. This could, for instance, be shown by reformulating the CP-map as the restriction of an appropriate unitary map (see Ref. 15). Hence we have only to determine which factors the off-diagonal terms obtain. Due to the symmetry of the channel with respect to time translations U_{sj} we have only to evaluate

$$v(j) := \mathrm{tr}(U_{sj} P G(|\phi_0\rangle\langle\phi_{sj}|)) = \mathrm{tr}(P G(|\phi_0\rangle\langle\phi_{sj}| U_{sj})).$$

Then K is explicitly given by

$$K\left(\sum_{jk} c_{jk}|j\rangle\langle k|\right) = \sum_{jk} c_{jk} v(j-k)|j\rangle\langle k|.$$

This shows that the channel K is a "Hadamard channel" even though we have not chosen the energy states as reference basis but the states $|\phi_{sj}\rangle$ instead. Furthermore, K is given by Hadamard multiplication with a *circulant* matrix V with entries $V_{ij} := v(i-j)$. In order to calculate v we use the explicit form of G according to Theorem 3. Using Lemma 1 this yields

$$v(j) = \int \mathrm{tr}(G_\sigma(|\phi_0\rangle\langle\phi_0|)e^{-i\sigma sj}\mathrm{d}\nu(\sigma) = f_{|\phi_0\rangle\langle\phi_0|,\mathbf{1}}(-sj),$$

i.e., the Fourier transform of the energy shift probability measure $\nu_{|\phi_0\rangle\langle\phi_0|,\mathbf{1}}$ evaluated at the points $-sj$. The eigenvalues $q_0,\ldots,q_{M-1}$ of V/n are given by the inverse Fourier transform of v:

$$q_k := \frac{1}{N}\sum_{j=0}^{N-1} v(j)e^{-ijk}.$$

Using Lemma 5 we conclude:

Theorem 6 (Q-capacity of channels with reliable timing): *Let G be a time-covariant channel with reliable timing property with respect to the time s and the initial state $|\phi_0\rangle$. Let the dynamics be periodic with period length sN. Then the quantum capacity can only be zero if the Fourier transform $\hat{p}$ of the probability measure $p(m) := \mathrm{tr}(G_m(|\phi_0\rangle\langle\phi_0|))$ has zeros at sj for $j = 1,\ldots,N-1$. Otherwise the quantum capacity is at least*

$$\log_2 N - \sum_k q_k \log_2 q_k,, \tag{38}$$

where $q=(q_0,\ldots,q_{N-1})$ is the discrete Fourier transform of the evaluation of $f_{|\phi_0\rangle\langle\phi_0|,\mathbf{1}}$ on the N points $0, -s, -2s, \ldots, -(N-1)s$.

Of course there are many possibilities to define finite dimensional channels from the original one. However, to study whether G destroys superpositions between different states in the orbit ("different pointer states of a clock") one has always to consider

$$G(|\phi_0\rangle\langle\phi_{sj}|) = \hat{G}_{-sj}(|\phi_0\rangle\langle\phi_0|)e^{iHsj}.$$

This shows that the Fourier transform of the measure (G_m) is decisive. For deriving the lower bound above we have evaluated it for the observable $\mathbf{1}$ which leads to the Fourier transform of the POVM (Q_m) defined in the last section. However, $\mathbf{1}$ is not necessarily optimal for detecting superpositions between the output states.

VIII. GAUSSIAN CHANNEL ON A SINGLE MODE

The Hilbert space of a single mode in quantum optics is $l^2(\mathbb{N}_0)$, the set of square summable sequences. It can also be interpreted as the energy levels of a harmonic oscillator. A time-covariant channel which is often considered is the following. As usual, we introduce the creation operator $a^\dagger$ and the annihilation operator a by $a|j\rangle := \sqrt{j}|j-1\rangle$ for $j \geqslant 1$ and $a|0\rangle = 0$. Using position and momentum observables X and P, respectively, we define a translation $(a_1,a_2) \in \mathbb{R}^2$ by the unitary transformation $\exp(i(a_1X+a_2P))$, where $X := a^\dagger + a$ and $P := (a^\dagger - a)/i$. It is convenient to introduce variables $r \in \mathbb{R}_0^+$ and z on the complex unit circle Γ by $a_1 + ia_2 = rz$. Rewriting the translation with operators $a^\dagger$ and a and the parameters z,r we obtain the translation operator (compare Ref. 25) by

$$D(z,r) := \exp(r(\bar{z}a^\dagger - za)) = e^{ir^2/2}e^{r\bar{z}a^\dagger}e^{-rza}.$$

Since the global phase factor is irrelevant we will, in abuse of notation, use $D(z,r)$ for the term without this factor.

Let the Gaussian channel be given by a random displacement rz according to the two-dimensional rotation invariant Gauss distribution. Note that rotation symmetry is necessary in order to obtain a time-covariant channel since the Hamiltonian $H:=diag(0,1,2,\ldots)$ corresponds to a rotation in the "phase space." Note that the possible energy shifts are in $\mathbb{Z}$, hence we expect a countable sum of G_σ which are (in contrary to the general case) not only densely defined.

The whole channel is given by (see Ref. 26)

$$G(\rho)=\int\int_{\Gamma} D(z,r)\rho D(\bar{z},r)\mathrm{d}z p(r)\mathrm{d}r$$

with $p(r):=\exp(-r^2/(2s^2))r/s^2$ and s denotes the standard deviation.

Then we write $D(z,r)$ as the power series

$$D(z,r)=e^{r\bar{z}a^\dagger}e^{-rza}=\sum_{m\geqslant 0}\frac{(r\bar{z})^n(a^\dagger)^m}{m!}\sum_{n\geqslant 0}\frac{(-rz)^n a^n}{n!}. \tag{39}$$

It decomposes canonically into terms $D_\sigma(z,r)$ with $\sigma\in\mathbb{Z}$ satisfying the commutation relation $[H,D_\sigma(z,r)]=\sigma D_\sigma(z,r)$ if we define

$$D_\sigma(z,r):=\sum_{n\geqslant -\sigma,0}\frac{(r\bar{z})^{n+\sigma}(a^\dagger)^{n+\sigma}}{(n+\sigma)!}\frac{(-rz)^n a^n}{n!}=\bar{z}^\sigma r^\sigma\sum_{n\geqslant -\sigma,0}(-1)^n\frac{(a^\dagger)^{n+\sigma}}{(n+\sigma)!}\frac{a^n}{n!}(r^2)^n.$$

Note that $D_\sigma(z,r)$ maps states with energy j onto states with energy $j+\sigma$. This suggests already that they may correspond to the maps G_σ of Sec. VI. The operator

$$D_\sigma(r):=D_\sigma(z,r)z^\sigma\sqrt{2\pi}$$

is independent of z. We conclude therefore that terms of the form $D_\sigma(\bar{z},r)\rho D_{\sigma'}(z,r)$ cancel for $\sigma\neq\sigma'$ after integration over all $z\in\Gamma$. We obtain

$$G(\rho)=\sum_{\sigma\in\mathbb{Z}}\int D_\sigma(r)\rho D_\sigma(r)p(r)\mathrm{d}r.$$

Consider the case $\sigma\geqslant 0$ first. Then we have

$$(a^\dagger)^{n+\sigma}a^n|j\rangle=\sqrt{(j+\sigma)\ldots(j+1)}j(j-1)\ldots(j-n+1)|j+\sigma\rangle=\frac{1}{\sqrt{(j+1)\ldots(j+\sigma)}}\frac{(j+\sigma)!}{(j-n)!}|j+\sigma\rangle,$$

for all $n\leqslant j$. For the case $\sigma<0$ we obtain

$$(a^\dagger)^{n+\sigma}a^n|j\rangle=\sqrt{j(j-1)\ldots(j+\sigma+1)}\frac{(j+\sigma)!}{(j-n)!}|j+\sigma\rangle.$$

For $\sigma\geqslant 0$ we conclude

$$\begin{aligned}D_\sigma(r)|j\rangle&=\frac{r^\sigma}{\sqrt{(j+1)\ldots(j+\sigma)}}\sum_{n=0}^{j}(-1)^n\frac{(j+\sigma)!}{(j-n)!\,(n+\sigma)!\,n!}(r^2)^n|j+\sigma\rangle\\&=\frac{r^\sigma}{\sqrt{(j+1)\ldots(j+\sigma)}}L_j^\sigma(r^2)|j+\sigma\rangle,\end{aligned}$$

where

$$L_j^{(\sigma)}(x):=\sum_{n=0}^{j}(-1)^n\frac{(j+\sigma)!}{(j-n)!\,(n+\sigma)!\,n!}(x)$$

is a Laguerre polynomial.[27]

Hence we have

$$M_\sigma(j,j') = \int \frac{(r^2)^\sigma}{\sqrt{(j+1)\ldots(j+\sigma)(j'+1)\ldots(j'+\sigma)}} L_j^{(\sigma)}(r^2) L_{j'}^{(\sigma)}(r^2) p(r) \mathrm{d}r.$$

For negative σ we may express M_σ similarly by Laguerre polynomials together with a different factor. Hence the decomposition of the single mode Gaussian channel can be given in a closed form even though it leads to a less familiar representation.

IX. CONCLUSIONS

We have shown that every time-covariant CP-map has a representation as an integral over a family of CP-maps. If the spectrum of the system Hamiltonian is nondegenerate, each of these components consists of a Hadamard multiplication with a positive operator followed by an energy shift. Formally, the output of the channel is an unselected post-measurement state. The measured (and ignored) quantity is the energy which has been transferred to or from the environment. Conditional to the measurement outcome a different dephasing channel is applied.

Furthermore we have addressed the question to what extent covariant channels can destroy superpositions between N mutually orthogonal states on the same orbit of the time evolution. For a specific type of channels (with "reliable timing property") we have shown that the general decomposition helps to derive lower bounds on the quantum capacity.

The decomposition presented here may be a helpful approach to describe a rather general type of decoherence and relaxation phenomena.

We have calculated the decomposition explicitly for a rotation invariant Gaussian channel acting on the state space of a single mode Fock space. The dephasing operations can then be described using Laguerre polynomials.

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A de Finetti representation for finite symmetric quantum states

Robert König[a] and Renato Renner[b]
Swiss Federal Institute of Technology (ETH) Zurich, 8092 Zurich, Switzerland

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Consider a *symmetric* quantum state on an n-fold product space, that is, the state is invariant under permutations of the n subsystems. We show that, conditioned on the outcomes of an informationally complete measurement applied to a number of subsystems, the state in the remaining subsystems is close to having product form. This immediately generalizes the so-called de Finetti representation to the case of finite symmetric quantum states. © *2005 American Institute of Physics.*
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I. INTRODUCTION

The analysis of physical experiments is often based on the assumption that the same experiment can be repeated many times independently. In particular, one usually assumes that the results $Z_1,\ldots,Z_n$ obtained from n repetitions of the same experiment are distributed according to some product distribution, i.e., $P_{Z_1\cdots Z_n}=(P_Z)^n$. In practical situations, however, the independence of the individual outcomes Z_i can usually not be guaranteed.

The so-called de Finetti representation theorem[6] can be seen as a solution to this problem. (See Ref. 15 for a collection of de Finetti's original papers.) Basically, it states that the assumption on the product structure of $P_{Z_1\cdots Z_n}$ can be replaced by a seemingly weaker assumption, namely that the distribution of the outcomes of infinitely many repetitions of the experiment is invariant under reordering. For instance, this is the case if the n samples $Z_1,\ldots,Z_n$ are randomly chosen from infinitely many repetitions of the experiment.

Let us briefly explain this result on a more formal level. We say that an n-partite probability distribution $P_{Z_1\cdots Z_n}$ is *symmetric* if it is invariant under any permutation of the random variables $Z_1,\ldots,Z_n$. If $P_{Z_1\cdots Z_n}$ is the marginal of a symmetric distribution $P_{Z_1\cdots Z_m}$ of $m\geqslant n$ random variables, then $P_{Z_1\cdots Z_n}$ is called *m-exchangeable.* Moreover, $P_{Z_1\cdots Z_n}$ is *infinitely exchangeable* if it is m-exchangeable for all $m\geqslant n$. The result of de Finetti now states that any infinitely exchangeable probability distribution $P_{Z_1\cdots Z_n}$ can be written as a convex combination of products $(P_Z)^n$ of n identical distributions.

This result has been generalized in different directions. Diaconis and Freedman[7] analyzed the structure of m-exchangeable probability distributions of n random variables, for $n\leqslant m<\infty$. This is of particular interest for practical applications, where the number of experiments is only finite. They found that, for appropriate values of n and m, these distributions are still close to the convex hull of the set of product distributions $(P_Z)^n$.

The result of de Finetti has also been extended to quantum states, to which the notion of symmetry and exchangeability can be adapted in an obvious way. Hudson and Moody[13] showed that any infinitely exchangeable quantum state $\rho^{\bar{n}}$ over n subsystems is a convex combination of product states, i.e., $\rho^{\bar{n}}=\Sigma_{\mathbf{z}}p_{\mathbf{z}}(\rho_{\mathbf{z}})^{\otimes n}$, for appropriate weights $p_{\mathbf{z}}$ (see also Ref. 11). An alternative proof of this claim has recently been presented by Caves, Fuchs, and Schack[4] (see also Ref. 8), relying on the original result of de Finetti.

[a]Electronic mail: rkoenig@inf.ethz.ch
[b]Electronic mail: renner@inf.ethz.ch

In this paper, we analyze the structure of m-exchangeable quantum states over n subsystems, for $n \leqslant m < \infty$. In a sense, our result combines the two mentioned directions of generalizing de Finetti's result. Note that any m-exchangeable state $\rho^{\bar{n}}$ over n subsystems can be extended to an m-exchangeable state $\rho^{\overline{n+k}}$ over $n+k$ subsystems, for $n+k \leqslant m$. We show that the state $\rho_{\mathbf{z}}^{\bar{n}}$ of the first n subsystems, conditioned on the outcomes $\mathbf{z}=(z_1,\ldots,z_k)$ of an informationally complete measurement applied to each of the remaining k subsystems, is close to the n-fold product state $(\rho_{\mathbf{z}}^{\bar{1}})^{\otimes n}$, where $\rho_{\mathbf{z}}^{\bar{1}}$ is the state $\rho_{\mathbf{z}}^{\bar{n}}$ restricted to one subsystem. (The density operator $\rho_{\mathbf{z}}^{\bar{1}}$ is obtained from $\rho_{\mathbf{z}}^{\bar{n}}$ by taking the trace over $n-1$ subsystems.) In particular, since $\rho^{\bar{n}}$ can be written as a convex combination of the states $\rho_{\mathbf{z}}^{\bar{n}}$, i.e., $\rho^{\bar{n}}=\Sigma_{\mathbf{z}} p_{\mathbf{z}} \rho_{\mathbf{z}}^{\bar{n}}$, this immediately implies that $\rho^{\bar{n}}$ is close to the convex combination $\Sigma_{\mathbf{z}} p_{\mathbf{z}} (\rho_{\mathbf{z}}^{\bar{1}})^{\otimes n}$. As in the classical case, the distance between the m-exchangeable state $\rho^{\bar{n}}$ and the convex hull of the set of product states depends on the values m and n. In particular, for any fixed m, as n tends to infinity, we recover the result of Refs. 13 and 4. [A somewhat different generalization of the de Finetti theorem has been proposed in Ref. 16, where it is shown that the set of states on an infinite tensor product satisfying a weaker symmetry condition than exchangeability is identical to the convex hull of m-dependent states (which corresponds to product states if $m=0$).]

Quantum de Finetti-style theorems are crucial for a Bayesian interpretation of quantum mechanics (see Ref. 8). Moreover, they can be used in various applications such as entanglement purification[3] and the study of entanglement in general.[12] In fact, many information-theoretic tasks, e.g., entanglement purification or quantum key distillation, are well understood in the special case where the states to be considered have product form. According to the de Finetti theorem, this is equivalent to saying that the state is a part of a state on infinitely many subsystems which is invariant under reordering of the subsystems. Our result relaxes this requirement to a finite number of subsystems only. This is important for realistic situations, where such a symmetry can be obtained by applying a randomly chosen permutation. [A remarkable example illustrating the power of the quantum de Finetti theorem is in the context of quantum cryptography.[1] Many security proofs for quantum key distribution (QKD) schemes only hold against so-called *collective* attacks,[2] where one assumes that the states generated by an adversary have product form. On the other hand, the ultimate goal is to prove security against the most general, so-called *coherent,* attacks. Because any state on a product system can be turned into a symmetric state by applying a random permutation, the finite quantum de Finetti representation theorem can be used to show that coherent attacks are not stronger than collective attacks.]

Outline of the paper: In Sec. II, we introduce some basic notation and definitions, including the notion of symmetry and exchangeability. Additionally, we briefly review the properties of the variational distance between probability distributions, as well as its quantum analogue, the trace distance between density operators. Sections III–VI are devoted to the proof of our main results on the structure of symmetric quantum states. Generally speaking, our proof is based on the analysis of the statistics obtained when applying informationally complete POVMs to symmetric quantum states. We will thus be interested in good POVMs in the sense that the measurement statistics gives maximal information about the measured state. Constructing such POVMs is the main purpose of Sec. III, which is somehow independent of the remaining part of the paper. In Sec. IV, we analyze classical symmetric probability distributions and derive bounds on their distance to product distributions. In Sec. V, it is shown how to deduce structural properties of quantum states from the corresponding properties of the measurement statistics, using the POVMs constructed in Sec. III. Finally, in Sec. VI, we combine these results to obtain our main statements, including a de Finetti representation for finitely exchangeable quantum states. Additionally, in the Appendix, we present an alternative version of these statements which might be more suitable for certain applications.

II. PRELIMINARIES

A. Density operators, POVMs, and probability distributions

Throughout this paper, we will restrict our attention to finite-dimensional Hilbert spaces, denoted by $\mathcal{H}$ or $\mathcal{H}_A$, for some index A. Let $\mathrm{Herm}(\mathcal{H})$ the set of Hermitian endomorphisms on $\mathcal{H}$.

An element $\rho \in \mathrm{Herm}(\mathcal{H})$ is called a *density operator* or, equivalently, a *quantum state* on $\mathcal{H}$ if it is positive semidefinite, $\rho \geqslant 0$, and has trace one, $\mathrm{tr}(\rho)=1$. We denote by $\mathrm{S}(\mathcal{H})$ the set of density operators on $\mathcal{H}$. A *positive operator valued measure (POVM)* on $\mathcal{H}$ is a family $\mathfrak{Z}=\{F_z\}_{z\in\mathcal{Z}}$ of non-negative operators $F_z \in \mathrm{Herm}(\mathcal{H})$, $F_z \geqslant 0$, such that $\Sigma_{z\in\mathcal{Z}} F_z = \mathrm{id}_{\mathcal{H}}$. The POVM $\mathfrak{Z}$ is called *informationally complete* if it is a basis of $\mathrm{Herm}(\mathcal{H})$.

To improve the readability of formulas involving density operators on product spaces, we use superscripts to indicate which subsystems an operator acts on, e.g., we write ρ^{ABC} for a density operator on $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$. Operators with the same name but different superscripts are related to each other by the partial trace. For example, ρ^{AB} is the partial state obtained from ρ^{ABC} by tracing over $\mathcal{H}_C$, i.e., $\rho^{AB}=\mathrm{Tr}_C(\rho^{ABC})$, and, similarly, $\rho^{A}=\mathrm{Tr}_{BC}(\rho^{ABC})$. This notation is consistent since partial traces over different subsystems commute, e.g., we have $\rho^A=\mathrm{Tr}_B(\rho^{AB})=\mathrm{Tr}_C(\rho^{AC})=\mathrm{Tr}_{BC}(\rho^{ABC})$.

A similar formalism can be used to denote conditional quantum states. Let ρ^{AB} be a density operator on $\mathcal{H}_A \otimes \mathcal{H}_B$ and let $\mathfrak{Z}=\{F_z\}_{z\in\mathcal{Z}}$ be a POVM on $\mathcal{H}_B$. Then $\rho^A{}_{|\mathfrak{Z}=z}$ denotes the quantum state on $\mathcal{H}_A$ conditioned on the event that the outcome of the measurement $\mathfrak{Z}$ applied to the subsystem $\mathcal{H}_B$ equals $z \in \mathcal{Z}$, i.e.,

$$\rho^A{}_{|\mathfrak{Z}=z} := \frac{1}{\mathrm{tr}((\mathrm{id}_A \otimes F_z)\rho^{AB})} \mathrm{Tr}_B((\mathrm{id}_A \otimes F_z)\rho^{AB}).$$

The notation can be extended to density operators over three and more subsystems in an obvious way. Note that, since the partial trace and the operation of conditioning on a measurement result commute, this is compatible with our notation for partial states. For instance, if ρ^{ABC} is a tripartite density operator, then the conditional states $\rho^A{}_{|\mathfrak{Z}=z}$ and $\rho^{AC}{}_{|\mathfrak{Z}=z}$ are related by the partial trace, i.e., $\rho^A{}_{|\mathfrak{Z}=z}=\mathrm{Tr}_C(\rho^{AC}{}_{|\mathfrak{Z}=z})$.

We will use a similar formalism to denote the probability distributions resulting from measurements of quantum states. Let ρ^A be a density operator and let $\mathfrak{Y}=\{E_y\}_{y\in\mathcal{Y}}$ be a POVM on $\mathcal{H}_A$. Then $\rho^A_{\mathfrak{Y}}$ denotes the distribution of the outcome of the measurement $\mathfrak{Y}$ applied to ρ^A, i.e.,

$$\rho^A_{\mathfrak{Y}}(y) = \mathrm{tr}(E_y\rho), \quad \text{for all } y \in \mathcal{Y}.$$

This can easily be generalized to product systems. For example, if $\mathfrak{Y}$ and $\mathfrak{Z}$ are POVMs on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, then $\rho^{AB}_{\mathfrak{Y}\mathfrak{Z}}$ is the probability distribution of the outcome of the product measurement $\mathfrak{Y}\otimes\mathfrak{Z}$ applied to ρ^{AB}.

Note that the operation of taking the partial trace of a density operator has a classical analogue, namely taking the marginal distribution. Similarly, the operation of conditioning a quantum state on a measurement result corresponds to conditioning a probability distribution on the value of a random variable. Our formalism is consistent with respect to these operations in the sense that the following diagram commutes:

$$\begin{array}{ccccc}
\rho^A{}_{|\mathfrak{Z}=z} & \xleftarrow{\text{cond.}} & \rho^{AB} & \xrightarrow{\text{trace}} & \rho^A \\
\text{meas.}\downarrow & & \text{meas.}\downarrow & & \text{meas.}\downarrow \\
\rho^A_{\mathfrak{Y}|\mathfrak{Z}=z} & \xleftarrow{\text{cond.}} & \rho^{AB}_{\mathfrak{Y}\mathfrak{Z}} & \xrightarrow{\text{marginal}} & \rho^A_{\mathfrak{Y}}
\end{array}$$

Let P be a probability distribution on $\mathcal{Z}$ and let, for each $z \in \mathcal{Z}$, ρ_z be a density operator on $\mathcal{H}$. We will often write the weighted sum of ρ_z as an expectation value, i.e.,

$$\mathop{\mathbb{E}}_{z\leftarrow P}[\rho_z] := \sum_{z\in\mathcal{Z}} P(z)\rho_z.$$

If the probability distribution is clear from the context, we only write $\mathbb{E}_z[\rho_z]$. For example, using our formalism, we have

$$\mathop{\mathbb{E}}_{z\leftarrow\rho_3^B}[\rho^A_{|3=z}]=\rho^A, \tag{1}$$

for any bipartite quantum state ρ^{AB} on $\mathcal{H}_A\otimes\mathcal{H}_B$. This is a simple reformulation of the fact that the partial state ρ^A on $\mathcal{H}_A$ does not change when a measurement is applied to the subsystem $\mathcal{H}_B$.

B. Distance measures

Let $\mathrm{Distr}(\mathcal{Z})$ be the set of probability distributions on the set $\mathcal{Z}$. The *variational distance* between two probability distributions $P,Q\in\mathrm{Distr}(\mathcal{Z})$ is defined by

$$\delta(P,Q):=\frac{1}{2}\sum_{z\in\mathcal{Z}}|P(z)-Q(z)|.$$

The variational distance is a metric on $\mathrm{Distr}(\mathcal{Z})$. In particular, $\delta(P,Q)=0$ if and only if $P=Q$, δ is symmetric, $\delta(P,Q)=\delta(Q,P)$, and the triangle inequality holds, $\delta(P,R)\leqslant\delta(P,Q)+\delta(Q,R)$. For two bipartite distributions P_{XY} and$P_{X'Y'}$, the variational distance cannot increase when taking the marginals,

$$\delta(P_X,P_{X'})\leqslant\delta(P_{XY},P_{X'Y'}). \tag{2}$$

If P_{XY} and $P_{X'Y'}$ have the same marginals $P_X=P_{X'}$, their distance can be expressed as the expectation value of the distance between their conditional probability distributions,

$$\delta(P_{XY},P_{X'Y'})=\mathop{\mathbb{E}}_{x\leftarrow P_X}[\delta(P_{Y|X=x},P_{Y'|X'=x})]:=\sum_x P_X(x)\delta(P_{Y|X=x},P_{Y'|X'=x}). \tag{3}$$

In particular, if the distributions have product form

$$\delta(P_X\times P_Y,P_X\times P_{Y'})=\delta(P_Y,P_{Y'}). \tag{4}$$

A similar distance measure can be defined on the set $\mathrm{Herm}(\mathcal{H})$ of Hermitian operators on $\mathcal{H}$, using the trace norm $\|\cdot\|_1$ on $\mathrm{Herm}(\mathcal{H})$, which is defined as $\|W\|_1:=\mathrm{tr}(|W|)$ for every $W\in\mathrm{Herm}(\mathcal{H})$. [For an operator $T\in\mathrm{Herm}(\mathcal{H})$, the operator norm of T is the value $\|T\|:=\sup_{v\in\mathcal{H}:\|v\|\leqslant 1}\|Tv\|$, where $\|v\|:=\sqrt{\langle v|v\rangle}$ for every $v\in\mathcal{H}$. It is easy to see that

$$\|W\|_1=\sup_{T:\|T\|\leqslant 1}|\mathrm{tr}(WT)|, \tag{5}$$

where the supremum is over all operators $T\in\mathrm{Herm}(\mathcal{H})$ with $\|T\|\leqslant 1$. From (5), it follows that $\|\cdot\|_1$ is a norm, as the right-hand side (rhs) of (5) is the norm of the linear functional $\mathrm{tr}(W\cdot)$ in the dual space $\mathrm{Herm}(\mathcal{H})^*$ and the embedding $W\mapsto\mathrm{tr}(W\cdot)$ is an isomorphism of $\mathrm{Herm}(\mathcal{H})$ to its dual.] The *trace distance* between two operators $U,V\in\mathrm{Herm}(\mathcal{H})$ is then given by

$$\delta(U,V):=\tfrac{1}{2}\|U-V\|_1.$$

Many properties of the variational distance also hold for the trace distance. In particular, the trace distance is a metric on $\mathrm{Herm}(\mathcal{H})$. Moreover, similarly to (2), the trace distance cannot increase when taking the partial trace, i.e., for $U,V\in\mathrm{Herm}(\mathcal{H}_A\otimes\mathcal{H}_B)$,

$$\delta(\mathrm{Tr}_B(U),\mathrm{Tr}_B(V))\leqslant\delta(U,V). \tag{6}$$

[More generally, $\delta(\mathcal{E}(U),\mathcal{E}(V))\leqslant\delta(U,V)$ for any trace-preserving quantum operation $\mathcal{E}:\mathrm{Herm}(\mathcal{H})\to\mathrm{Herm}(\mathcal{H}')$, which can most generally be written as $\mathcal{E}(U):=\sum_k E_kUE_k^\dagger$ for operators $E_k:\mathcal{H}\to\mathcal{H}'$. To prove this, it suffices to show that $\|\mathcal{E}(W)\|_1\leqslant\|W\|_1$, for every $W\in\mathrm{Herm}(\mathcal{H})$. Note that the operator norm of an operator $T\in\mathrm{Herm}(\mathcal{H})$ can equivalently be written as $\|T\|=\sup_{\sigma\in\mathrm{S}(\mathcal{H})}\mathrm{tr}(T\sigma)$. Defining the operation $\mathcal{E}^\dagger:\mathrm{Herm}(\mathcal{H}')\to\mathrm{Herm}(\mathcal{H})$ by $\mathcal{E}^\dagger(T'):=\sum_k E_k^\dagger T'E_k$ for $T'\in\mathrm{Herm}(\mathcal{H}')$, we have the identity $\mathrm{tr}(\mathcal{E}^\dagger(T')W)=\mathrm{tr}(T'\mathcal{E}(W))$ for any operators W

$\in \mathrm{Herm}(\mathcal{H}), T' \in \mathrm{Herm}(\mathcal{H}')$. Hence $\|\mathcal{E}^\dagger(T')\| = \sup_{\sigma\in \mathrm{S}(\mathcal{H})} \mathrm{tr}(\mathcal{E}^\dagger(T')\sigma) = \sup_{\sigma\in \mathrm{S}(\mathcal{H})} \mathrm{tr}(T'\mathcal{E}(\sigma)) \leqslant \|T'\|$ since $\mathcal{E}(\sigma) \in \mathrm{S}(\mathcal{H}')$ for any $\sigma \in \mathrm{S}(\mathcal{H})$. Using (5), this implies that $\|\mathcal{E}(W)\|_1 = \sup_{T':\|T'\|\leqslant 1} |\mathrm{tr}(\mathcal{E}(W)T')| = \sup_{T':\|T'\|\leqslant 1} |\mathrm{tr}(W\mathcal{E}^\dagger(T'))| \leqslant \sup_{T:\|T\|\leqslant 1} \mathrm{tr}(WT) = \|W\|_1$, as required.] We will also use the strong convexity of the trace distance, which follows directly from the triangle inequality of $\|\cdot\|_1$, i.e., for any $U, U', V, V' \in \mathrm{Herm}(\mathcal{H})$ and $p, q \in [0,1]$ with $p+q=1$,

$$\delta(pU + qU', pV + qV') \leqslant p\,\delta(U,V) + q\,\delta(U',V').$$

The following lemma gives a simple expression for the trace distance between two product operators $U \otimes V$ and $U' \otimes V$ with a common factor V.

Lemma II.1: Let $U, U' \in \mathrm{Herm}(\mathcal{H}_A)$ *and* $V \in \mathrm{Herm}(\mathcal{H}_B)$. *Then*

$$\delta(U \otimes V, U' \otimes V) = \delta(U,U') \cdot \mathrm{tr}(|V|).$$

Proof: By definition,

$$\delta(U \otimes V, U' \otimes V) = \mathrm{tr}|(U - U') \otimes V|. \tag{7}$$

We use the following general fact, which can be verified easily using the appropriate definitions. Let $f: \mathbb{C} \to \mathbb{C}$ be a function satisfying

$$f(a \cdot b) = f(a) \cdot f(b) \quad \text{for all } a,b \in \mathbb{C}.$$

Then

$$f(A \otimes B) = f(A) \otimes f(B)$$

for all $A, B \in \mathrm{Herm}(\mathcal{H})$. Applying this to Eq. (7) yields

$$|(U - U') \otimes V| = |(U - U')| \otimes |V|.$$

The assertion then follows from the identity $\mathrm{tr}(A \otimes B) = \mathrm{tr}(A) \cdot \mathrm{tr}(B)$. □

As an immediate consequence of Lemma II.1, we obtain the equation

$$\delta(\rho \otimes \sigma, \rho' \otimes \sigma) = \delta(\rho, \rho'), \tag{8}$$

for states $\rho, \rho' \in \mathrm{S}(\mathcal{H}_A)$ and $\sigma \in \mathrm{S}(\mathcal{H}_B)$, which is the quantum analogue of (4). The trace distance between two density operators ρ and σ on $\mathcal{H}$ corresponds to the variational distance between the probability distributions $\rho_{\mathfrak{Z}}$ and $\sigma_{\mathfrak{Z}}$ of the outcomes of a measurement applied to ρ and σ, respectively, for an optimal POVM $\mathfrak{Z}$ on $\mathcal{H}$, i.e.,

$$\delta(\rho,\sigma) = \max_{\mathfrak{Z}} \delta(\rho_{\mathfrak{Z}}, \sigma_{\mathfrak{Z}}). \tag{9}$$

C. Symmetry and exchangeability

1. Symmetric probability distributions and symmetric functions

Let $\mathbf{z} = (z_1, \ldots, z_n) \in \mathcal{Z}^n$ and $\mathbf{z}' = (z'_1, \ldots, z'_m) \in \mathcal{Z}^m$ be tuples of elements from a set $\mathcal{Z}$. We denote by $(\mathbf{z}, \mathbf{z}')$ the $(n+m)$-tuple obtained by concatenating $\mathbf{z}$ and $\mathbf{z}'$, i.e., $(\mathbf{z}, \mathbf{z}') := (z_1, \ldots, z_n, z'_1, \ldots, z'_m)$.

The *frequency distribution* $Q_{\mathbf{z}}$ of an n-tuple $\mathbf{z} = (z_1, \ldots, z_n) \in \mathcal{Z}^n$ is the function with domain $\mathcal{Z}$ defined by (we denote by $[n]$ the set of natural numbers between 1 and n, i.e., $[n] := \{1, \ldots, n\}$)

$$Q_{\mathbf{z}}(z) := \frac{1}{n} |\{i \in [n] : z_i = z\}|, \quad \text{for every } z \in \mathcal{Z},$$

i.e., $Q_{\mathbf{z}}(z)$ is the relative number of occurrences of the symbol z in $\mathbf{z}$. Note that $Q_{\mathbf{z}}$ is a probability distribution on $\mathcal{Z}$, $Q_{\mathbf{z}} \in \mathrm{Distr}(\mathcal{Z})$.

A symmetric function f on $\mathcal{Z}^n$ is a function such that $f(\mathbf{z})$ is invariant under permutations of the entries in $\mathbf{z}$. The value $f(\mathbf{z})$ then only depends on the frequency distribution $Q_{\mathbf{z}}$ of $\mathbf{z}$. For a formal definition, let S_n be the set of permutations on $[n]$, and let, for any $\pi \in S_n$, $\pi_{\mathcal{Z}}$ be the bijection on $\mathcal{Z}^n$ defined by

$$\pi_{\mathcal{Z}}:(z_1, \ldots, z_n) \mapsto (z_{\pi(1)}, \ldots, z_{\pi(n)}), \quad \text{for all } (z_1, \ldots, z_n) \in \mathcal{Z}^n.$$

Definition II.2: A function f with domain $\mathcal{Z}^n$ is called symmetric *if*

$$f = f \circ \pi_{\mathcal{Z}}, \quad \textit{for all } \pi \in S_n.$$

In particular, a probability distribution $P_{\mathbf{Z}} \in \mathrm{Distr}(\mathcal{Z}^n)$ on $\mathcal{Z}^n$ is called *symmetric* if $P_{\mathbf{Z}}$ is a symmetric function. The following lemma is an immediate consequence of these definitions.

Lemma II.3: Let $\mathbf{Z}$ be an n-tuple of random variables over a set $\mathcal{Z}$ such that $P_{\mathbf{Z}}$ is symmetric, and let Y be a random variable over $\mathcal{Y}$ defined by a channel $P_{Y|\mathbf{Z}}$ such that for every $y \in \mathcal{Y}$, the function $\mathbf{z} \mapsto P_{Y|\mathbf{Z}=\mathbf{z}}(y)$ is symmetric. Then, for every $y \in \mathcal{Y}$, the conditional probability distribution $P_{\mathbf{Z}|Y=y}$ is symmetric.

In particular, if $f: \mathcal{Z}^n \to \mathcal{Y}$ is a symmetric function and $P_{\mathbf{Z}}$ is symmetric, then, for any $y \in \mathcal{Y}$, $P_{\mathbf{Z}|f(\mathbf{Z})=y}$ is symmetric. An example is the function mapping any n-tuple $\mathbf{z}$ to the frequency distribution $Q_{\mathbf{z}}$, i.e., $P_{\mathbf{Z}|Q_{\mathbf{Z}}=q}$ is symmetric. [$Q_{\mathbf{Z}}$ is the random variable defined by $Q_{\mathbf{z}}$, for $\mathbf{z}$ randomly chosen according to $P_{\mathbf{Z}}$, that is, $P_{Q_{\mathbf{Z}}}(q) := \mathbb{P}_{\mathbf{z} \leftarrow P_{\mathbf{Z}}}[Q_{\mathbf{z}} = q]$.] The following lemma is an immediate consequence of this fact.

Lemma II.4: Let $\mathbf{Z} = (Z_1, \ldots, Z_n)$ be an n-tuple of random variables over a set $\mathcal{Z}$ such that $P_{\mathbf{Z}}$ is symmetric. Then, for any $q \in \mathrm{Distr}(\mathcal{Z})$,

$$P_{Z_i|Q_{\mathbf{Z}}=q} = q, \quad \textit{for every } i \in [n].$$

2. Symmetric and exchangeable density operators

For any permutation $\pi \in S_n$, let $\pi_{\mathcal{H}}$ be the unique endomorphism on $\mathcal{H}^{\otimes n}$ satisfying

$$\pi_{\mathcal{H}}(|\phi_1\rangle \otimes \cdots \otimes |\phi_n\rangle) = |\phi_{\pi(1)}\rangle \otimes \cdots \otimes |\phi_{\pi(n)}\rangle, \quad \text{for all } |\phi_1\rangle, \ldots, |\phi_n\rangle \in \mathcal{H}.$$

It is easy to verify that $\pi_{\mathcal{H}}$ is unitary. Let $\rho^{B_1 \cdots B_n}$ be a density operator on $\mathcal{H}_{B_1} \otimes \cdots \otimes \mathcal{H}_{B_n}$ where, for all $i \in [n]$, $\mathcal{H}_{B_i} = \mathcal{H}$, i.e., $\rho^{B_1 \cdots B_n} \in \mathrm{S}(\mathcal{H}^{\otimes n})$. The state $\rho^{B_1 \cdots B_n}$ is called *symmetric* if $\rho^{B_1 \cdots B_n} = \pi_{\mathcal{H}} \rho^{B_1 \cdots B_n} \pi_{\mathcal{H}}^{\dagger}$ for every $\pi \in S_n$. The following definition generalizes this concept to include an additional system $\mathcal{H}_A$.

Definition II.5: A density operator $\rho^{AB_1 \cdots B_n} \in \mathrm{S}(\mathcal{H}_A \otimes \mathcal{H}^{\otimes n})$ is called symmetric relative to $\mathcal{H}_A$ *if*

$$\rho^{AB_1 \cdots B_n} = (\mathrm{id}_A \otimes \pi_{\mathcal{H}}) \rho^{AB_1 \cdots B_n} (\mathrm{id}_A \otimes \pi_{\mathcal{H}}^{\dagger}), \quad \textit{for all } \pi \in S_n.$$

Let $\rho^{AB_1 \cdots B_n} \in \mathrm{S}(\mathcal{H}_A \otimes \mathcal{H}^{\otimes n})$ be symmetric relative to $\mathcal{H}_A$. Then, for any choice of r distinct indices $i_1, \ldots, i_r \in [n]$, $r \in [n]$, the state $\rho^{AB_{i_1} \cdots B_{i_r}}$ is symmetric relative to $\mathcal{H}_A$. Since it only depends on the number r of distinct indices, we will write $\rho^{A\overline{r}}$ instead of $\rho^{AB_{i_1} \cdots B_{i_r}}$.

Similarly, for every $\mathbf{z} \in \mathcal{Z}^s$, the density operator $\rho^{AB i_1 \cdots B_{i_{n-s}}}_{|\mathfrak{Z}^{\otimes s} = \mathbf{z}}$ obtained by conditioning a symmetric state $\rho^{A\overline{n}} = \rho^{AB_1 \cdots B_n}$ on the outcomes of a POVM $\mathfrak{Z} = \{F_z\}_{z \in \mathcal{Z}}$ applied to s subsystems is independent of the indices $i_1, \ldots, i_{n-s}$. Additionally, as an immediate consequence of Lemma II.6 below, this conditional state is still symmetric relative to $\mathcal{H}_A$. We will thus use the abbreviation $\rho^{A\overline{n-s}}_{|\mathfrak{Z}^s = \mathbf{z}}$.

Lemma II.6: Let $\rho^{AB\overline{n}} \in \mathrm{S}(\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}^{\otimes n})$ be symmetric relative to $\mathcal{H}_A \otimes \mathcal{H}_B$. Then, for any POVM $\mathfrak{N} = \{E_y\}_{y \in \mathcal{Y}}$ on $\mathcal{H}_A$ and every $y \in \mathcal{Y}$, $\rho^{B\overline{n}}_{|\mathfrak{N}=y}$ is symmetric relative to $\mathcal{H}_B$.

Proof: It suffices to show that, for any $\pi \in S_n$ and any $y \in \mathcal{Y}$

$$(\mathrm{id}_B \otimes \pi_{\mathcal{H}})\mathrm{Tr}_A((E_y \otimes \mathrm{id}_{B\bar{n}})\rho^{AB\bar{n}})(\mathrm{id}_B \otimes \pi_{\mathcal{H}}^\dagger) = \mathrm{Tr}_A((E_y \otimes \mathrm{id}_{B\bar{n}})\rho^{AB\bar{n}}),$$

where $\mathrm{id}_{B\bar{n}} := \mathrm{id}_B \otimes \mathrm{id}_{\mathcal{H}}^{\otimes n}$. We use the general identity,

$$U\,\mathrm{Tr}_A(W)U' = \mathrm{Tr}_A((\mathrm{id}_A \otimes U)W(\mathrm{id}_A \otimes U'))$$

for endomorphisms U, U' on $\mathcal{H}_B$ and W on $\mathcal{H}_A \otimes \mathcal{H}_B$, which follows from the fact that the identity is trivial for product operators $W = S \otimes T$ and the linearity of the partial trace. Setting $U := \mathrm{id}_B \otimes \pi_{\mathcal{H}}$, $U' := \mathrm{id}_B \otimes \pi_{\mathcal{H}}^\dagger$, and $W := (E_y \otimes \mathrm{id}_{B\bar{n}})\rho^{AB\bar{n}}$ leads to

$$\begin{aligned}(\mathrm{id}_B \otimes \pi_{\mathcal{H}})\mathrm{Tr}_A((E_y \otimes \mathrm{id}_{B\bar{n}})\rho^{AB\bar{n}})(\mathrm{id}_B \otimes \pi_{\mathcal{H}}^\dagger) &= \mathrm{Tr}_A((\mathrm{id}_{AB} \otimes \pi_{\mathcal{H}})(E_y \otimes \mathrm{id}_{B\bar{n}})\rho^{AB\bar{n}}(\mathrm{id}_{AB} \otimes \pi_{\mathcal{H}}^\dagger)) \\ &= \mathrm{Tr}_A((E_y \otimes \mathrm{id}_{B\bar{n}})(\mathrm{id}_{AB} \otimes \pi_{\mathcal{H}})\rho^{AB\bar{n}}(\mathrm{id}_{AB} \otimes \pi_{\mathcal{H}}^\dagger)).\end{aligned}$$

The assertion then follows since $\rho^{AB\bar{n}}$ is symmetric relative to $\mathcal{H}_A \otimes \mathcal{H}_B$, that is,

$$(\mathrm{id}_{AB} \otimes \pi_{\mathcal{H}})\rho^{AB\bar{n}}(\mathrm{id}_{AB} \otimes \pi_{\mathcal{H}}^\dagger) = \rho^{AB\bar{n}}.$$

□

The notation for symmetric quantum states introduced above can also be used to denote symmetric probability distributions resulting from measuring a symmetric quantum state. Let, for instance, $\rho^{A\bar{n}} = \rho^{AB_1\cdots B_n} \in \mathrm{S}(\mathcal{H}_A \otimes \mathcal{H}^{\otimes n})$ be symmetric relative to $\mathcal{H}_A$. Then, for POVMs $\mathcal{Y}$ and $\mathcal{Z}$ on $\mathcal{H}_A$ and $\mathcal{H}$, respectively, we write $p_{\mathcal{Y}\mathcal{Z}^n}^{A\bar{n}}$ instead of $p_{\mathcal{Y}\mathcal{Z}\cdots\mathcal{Z}}^{A B_1\cdots B_n}$.

To formulate our theorems in a compact way, we will make use of the notion of exchangeability. A symmetric density operator $\rho^{\bar{n}} \in \mathrm{S}(\mathcal{H}^{\otimes n})$ is said to be *m-exchangeable,* for $m \geqslant n$, if there exists a symmetric density operator $\sigma^{\bar{m}} \in \mathrm{S}(\mathcal{H}^{\otimes m})$ such that $\rho^{\bar{n}}$ is the partial trace of $\sigma^{\bar{m}}$, i.e., $\rho^{\bar{n}} = \sigma^{\bar{n}}$. Similarly to Definition II.5, the definition of exchangeability can be generalized to include an additional system $\mathcal{H}_A$.

Definition II.7: A density operator $\rho^{A\bar{n}} \in \mathrm{S}(\mathcal{H}_A \otimes \mathcal{H}^{\otimes n})$ which is symmetric relative to $\mathcal{H}_A$ is called m-exchangeable relative to $\mathcal{H}_A$ *if there exists a density operator $\sigma^{A\bar{m}} \in \mathrm{S}(\mathcal{H}_A \otimes \mathcal{H}^{\otimes m})$ such that $\sigma^{A\bar{n}}$ is symmetric relative to $\mathcal{H}_A$ and $\rho^{A\bar{n}} = \sigma^{A\bar{n}}$. We refer to $\sigma^{A\bar{m}}$ as an* extension of $\rho^{A\bar{n}}$.

In the following, we will often use the same label for an extension of a state. For example, we will denote an extension of $\rho^{A\bar{n}}$ to m systems (for $m \geqslant n$) by $\rho^{A\bar{m}}$.

D. Dual basis and quantum tomography

Let $\{e_i\}_{i\in\mathcal{N}}$ be a family of vectors in a Hilbert space $\mathcal{H}$. A family $\{f_i\}_{i\in\mathcal{N}}$ is called a *dual* of $\{e_i\}_{i\in\mathcal{N}}$ if $v = \sum_{i\in\mathcal{N}}\langle f_i|v\rangle e_i$ for all $v \in \mathcal{H}$, where $\langle f_i|v\rangle$ denotes the inner product of f_i and v.

Note that the set of endomorphisms on $\mathcal{H}$ forms a complex Hilbert space with inner product $(U,V) \mapsto \mathrm{tr}(UV^\dagger)$. Similarly, the set $\mathrm{Herm}(\mathcal{H})$ of Hermitian operators on $\mathcal{H}$ is a real Hilbert space with inner product $(U,V) \mapsto \mathrm{tr}(UV)$. Hence, a family $\{F_z\}_{z\in\mathcal{Z}}$ of elements from $\mathrm{Herm}(\mathcal{H})$ is a dual of a family $\{F_z^*\}_{z\in\mathcal{Z}}$ if

$$U = \sum_{z\in\mathcal{Z}} \mathrm{tr}(F_z U)F_z^*, \quad \text{for all } U \in \mathrm{Herm}(\mathcal{H}). \tag{10}$$

In particular, expression (10) states that the operator U is fully determined by the values of the traces $\mathrm{tr}(F_z U)$. The following lemma generalizes this fact to product spaces.

Lemma II.8: Let $\{F_z\}_{z\in\mathcal{Z}}$ and $\{F_z^*\}_{z\in\mathcal{Z}}$ be families of elements from $\mathrm{Herm}(\mathcal{H}_B)$ *such that $\{F_z\}_{z\in\mathcal{Z}}$ is the dual of $\{F_z^*\}_{z\in\mathcal{Z}}$. Then, for any $W \in \mathrm{Herm}(\mathcal{H}_A \otimes \mathcal{H}_B)$,*

$$W = \sum_{z\in\mathcal{Z}} W_z \otimes F_z^*,$$

where $W_z := \mathrm{Tr}_B((\mathrm{id}_A \otimes F_z)W)$, *for all* $z \in \mathcal{Z}$.

Proof: It is easy to verify that $\mathrm{Herm}(\mathcal{H}_A \otimes \mathcal{H}_B) = \mathrm{Herm}(\mathcal{H}_A) \otimes \mathrm{Herm}(\mathcal{H}_B)$. Hence there exist operators $U_i \in \mathrm{Herm}(\mathcal{H}_A)$ and $V_i \in \mathrm{Herm}(\mathcal{H}_B)$ such that $W = \sum_i U_i \otimes V_i$. By the linearity of the sum and the trace operator, it thus suffices to show that

$$U \otimes V = \sum_{z \in \mathcal{Z}} \mathrm{Tr}_B((\mathrm{id}_A \otimes F_z)(U \otimes V)) \otimes F_z^*$$

for any $U \in \mathrm{Herm}(\mathcal{H}_A)$ and $V \in \mathrm{Herm}(\mathcal{H}_B)$. Since Tr_B can be written as $\mathrm{Tr}_B = \mathrm{id}_A \otimes \mathrm{tr}_B$ (where $\mathcal{H}_A \otimes \mathbb{C}$ is identified with $\mathcal{H}_A$) we find

$$\mathrm{Tr}_B((\mathrm{id}_A \otimes F_z)(U \otimes V)) = \mathrm{Tr}_B(U \otimes (F_z V)) = \mathrm{tr}(F_z V)U,$$

and thus

$$\sum_{z \in \mathcal{Z}} \mathrm{Tr}_B((\mathrm{id}_A \otimes F_z)(U \otimes V)) \otimes F_z^* = U \otimes \left(\sum_{z \in \mathcal{Z}} \mathrm{tr}(F_z V) F_z^* \right).$$

The assertion then follows from (10). □

Let $\mathfrak{Z} = \{F_z\}_{z \in \mathcal{Z}}$ be a POVM on $\mathcal{H}_B$ and let $\{F_z^*\}_{z \in \mathcal{Z}}$ be a family of elements from $\mathrm{Herm}(\mathcal{H}_B)$ such that $\{F_z\}_{z \in \mathcal{Z}}$ is the dual of $\{F_z^*\}_{z \in \mathcal{Z}}$. Definition 10 directly implies that any density operator ρ^B on $\mathcal{H}_B$ can be written as

$$\rho^B = \mathop{\mathbb{E}}_{z \leftarrow \rho^B_{\mathfrak{Z}}} [F_z^*], \tag{11}$$

i.e., ρ^B is fully determined by the probability distribution $\rho^B_{\mathfrak{Z}}$ of the outcomes when applying the measurement $\mathfrak{Z}$ on ρ^B. On the other hand, it is an immediate consequence of Lemma II.8 that, for any density operator ρ^{AB} on $\mathcal{H}_A \otimes \mathcal{H}_B$,

$$\rho^{AB} = \mathop{\mathbb{E}}_{z \leftarrow \rho^B_{\mathfrak{Z}}} [\rho^A{}_{|\mathfrak{Z}=z} \otimes F_z^*]. \tag{12}$$

The above formulas are useful for quantum state tomography, that is, the reconstruction of an unknown quantum state ρ given only the statistics of measurement applied to identical copies of ρ. For example, it follows from (11), the strong convexity of the trace distance and Lemma II.1 that the estimate $\tilde{\rho}^B := \mathbb{E}_{z \leftarrow \tilde{P}_Z}[F_z^*]$ is close to ρ^B,

$$\delta(\rho^B, \tilde{\rho}^B) \leqslant \sum_{z \in \mathcal{Z}} |P_Z(z) - \tilde{P}_Z(z)| \cdot \mathrm{tr}|F_z^*|. \tag{13}$$

In particular, in order to obtain good estimates, one should choose a POVM $\mathfrak{Z}$ such that the traces $\mathrm{tr}|F_z^*|$ are small.

III. INFORMATIONALLY COMPLETE POVMs AND DUALS

A. Symmetric informationally complete POVMs

Intuitively, a POVM $\mathfrak{Z} = \{F_z\}_{z \in \mathcal{Z}}$ is useful for tomography if the distance between any two operators F_z and $F_{z'}$ is large. This is for instance the case for symmetric POVMs as defined below, where the operators F_z are symmetrically distributed over the space of positive operators.

Definition III.1: Let $\mathcal{H}$ *be a d-dimensional Hilbert space. A* symmetric *informationally complete POVM* $\mathfrak{Z} = \{F_z\}_{z \in [d^2]}$ *on* $\mathcal{H}$ *is an informationally complete POVM that consists of rank-one projectors*

$$F_z := \frac{1}{d} |\psi_z\rangle\langle\psi_z| \quad \textit{for all } z \in [d^2]$$

with the property that

$$\mathrm{tr}(F_z F_{z'}) = \theta_d \quad \textit{for all } z \neq z'.$$

for some $\theta_d \in \mathbb{C}$.

Analytic constructions of symmetric informationally complete POVMs are known for dimensions $d=2,3,4,6,8$ (see, e.g., Refs. 17 and 9). It can be shown that if a symmetric informationally complete POVM exists in dimension d, then θ_d is a universal constant which is independent of the particular symmetric informationally complete POVM. It equals

$$\theta_d = \frac{1}{d^2(d+1)}.$$

Lemma III.2: Let $\mathfrak{Z}=\{F_z\}_{z\in[d^2]} \in \mathrm{POVM}_{\mathcal{H}}$ *be a symmetric informationally complete POVM on a d-dimensional Hilbert space* $\mathcal{H}$. *Then there is a set of operators* $\{F_z^*\}_{z\in[d^2]} \subset \mathrm{Herm}(\mathcal{H})$ *that satisfies*

(i) $\mathfrak{Z}$ *is a dual of* $\{F_z^*\}_{z\in[d^2]}$.
(ii) *For every* $z \in [d^2]$, *the eigenvalues of* F_z^* *and their multiplicities are*

$$\lambda_0 := d, \quad n_0 := 1,$$

$$\lambda_1 := -1, \quad n_1 := d-1.$$

Proof: Let us define $\alpha := d^2+d-1$. It is straightforward to verify that the operators

$$F_z^* := \alpha F_z - \sum_{z'\neq z} F_{z'}, \quad z \in [d^2]$$

satisfy $\mathrm{tr}(F_z^* F_{z'}) = \delta_{zz'}$, where $\delta_{zz'}$ denotes the Kronecker delta, which equals one if $z=z'$ and 0 otherwise. This implies property (i). To obtain their eigenvalues, consider the matrix

$$B := F_z^* + \mathrm{id} = (\alpha+1)F_z.$$

Because $F_z = (1/d)|\psi_z\rangle\langle\psi_z|$, the eigenvalues of B are $(\alpha+1)/d$ and 0, occurring with multiplicities 1 and $d-1$, respectively. Hence statement (ii) follows. □

B. A construction for arbitrary dimensions

As mentioned in the preceding section, symmetric informationally complete POVMs are suitable for tomography. Unfortunately, their existence is only proven for certain dimensions. In this section, we will give a construction of informationally complete POVMs for any dimension. It is, however, not symmetric in the sense of Definition III.1, but still useful for tomography. Our construction is motivated by a general group-theoretic technique for finding such POVMs (see e.g., Ref. 5).

Note that a construction of an informationally complete POVM in any dimension is also given and applied in Ref. 4. Ours is more symmetric and allows us to construct a family of operators such that the informationally complete POVM is a dual of the family.

Let $\mathcal{H}$ be a d-dimensional Hilbert space and let $\omega := e^{2\pi i/d}$ be the dth primitive root of unity. Define the operators

$$D_{jk} := \omega^{j\odot k/2} \sum_{m\in\mathbb{Z}_d} \omega^{jm} |k\oplus m\rangle\langle m| \quad \text{for all } (j,k) \in \mathbb{Z}_d \times \mathbb{Z}_d,$$

where $\oplus$, $\odot$ denotes addition and multiplication modulo d, respectively. Furthermore, define

$$c((j,k),(l,m)) := jm - kl \quad \text{for all } (j,k),(l,m) \in \mathbb{Z}_d \times \mathbb{Z}_d.$$

We will use the simple identity

$$\sum_{\beta\in\mathbb{Z}_d\times\mathbb{Z}_d} \omega^{c(\alpha,\beta)} = d^2\cdot\delta_{\alpha,0} \quad \text{for all } \alpha\in\mathbb{Z}_d\times\mathbb{Z}_d, \tag{14}$$

where $\delta_{\alpha,\beta}$ denotes the Kronecker delta, which equals 1 if $\alpha=\beta$ and 0 otherwise. Note that this identity directly follows from

$$\sum_{m\in\mathbb{Z}_d} \omega^{km} = d\cdot\delta_{k,0} \quad \text{for all } k\in\mathbb{Z}_d. \tag{15}$$

Lemma III.3: The operators $\{D_\alpha\}_{\alpha\in\mathbb{Z}_d\times\mathbb{Z}_d}$ *have the following properties:*

(i) D_α *is unitary for every* $\alpha\in\mathbb{Z}_d\times\mathbb{Z}_d$.
(ii) *For every* $\rho\in\mathrm{S}(\mathcal{H})$, $\Sigma_{\alpha\in\mathbb{Z}_d\times\mathbb{Z}_d} D_\alpha\rho D_\alpha^\dagger = d\cdot\mathrm{id}$.
(iii) $D_\alpha D_\beta D_\alpha^\dagger = \omega^{c(\alpha,\beta)} D_\beta$, *for all* $\alpha,\beta\in\mathbb{Z}_d\times\mathbb{Z}_d$.
(iv) $D_\alpha^\dagger = D_{-\alpha}$, *for all* $\alpha\in\mathbb{Z}_d\times\mathbb{Z}_d$.
(v) $\mathrm{tr}(D_\alpha^\dagger D_\beta) = d\cdot\delta_{\alpha,\beta}$.

Proof: These properties are well known (see e.g., Ref. 5) and can also be verified by direct calculation. The proof is omitted here. □

Lemma III.4: Define

$$\rho := \frac{d}{d^2+1}\mathrm{id} + \frac{1}{2d(d^2+1)} \sum_{\beta\in\mathbb{Z}_d\times\mathbb{Z}_d} (D_\beta + D_\beta^\dagger).$$

Then ρ *is a state, i.e.,* $\rho\in\mathrm{S}(\mathcal{H})$.

Proof: To show that the operator ρ is non-negative, we make use of the following operators. Let

$$|\psi_{km}^\nu\rangle := \frac{1}{\sqrt{2}}(\omega^{\nu/2}|k\oplus m\rangle + \omega^{-\nu/2}|m\rangle)$$

and

$$\rho_{km}^\nu := |\psi_{km}^\nu\rangle\langle\psi_{km}^\nu| \quad \text{for } \nu\in\mathbb{R}, k,m\in\mathbb{Z}_d, \quad k\neq 0,$$

$$\rho_{0m}^\nu := \left(1+\frac{\omega^\nu+\omega^{-\nu}}{2}\right)|m\rangle\langle m|.$$

Note that ρ_{0m}^ν is not normalized, but non-negative [if $(\nu \bmod d) = d/2$ it equals 0].

With the definition

$$\nu(j,k,m) := \frac{j\odot k}{2} + jm,$$

it is easy to verify that

$$\sum_m \rho_{km}^{\nu(j,k,m)} = \mathrm{id} + \tfrac{1}{2}(D_{jk} + D_{jk}^\dagger),$$

and hence

$$\rho = \frac{1}{d(d^2+1)} \sum_{j,k}\sum_m \rho_{km}^{\nu(j,k,m)}.$$

This implies that ρ is indeed positive. Let us show that ρ given by this expression is correctly normalized. Note that

$$\sum_{j,k,m} \mathrm{tr}(\rho_{km}^{\nu(j,k,m)}) = \sum_{j,m} \sum_{k\neq 0} \mathrm{tr}(\rho_{km}^{\nu(j,k,m)}) + \sum_{j,m} \mathrm{tr}(\rho_{0m}^{\nu(j,0,m)}) = d^2(d-1) + \sum_{j,m} \left(1 + \frac{\omega^{\nu(j,0,m)} + \omega^{-\nu(j,0,m)}}{2}\right).$$

Because of

$$\sum_{j,m} \omega^{\nu(j,0,m)} = \sum_{j,m} \omega^{jm} = d,$$

where the second equation follows from (15), we obtain

$$\sum_{j,k,m} \mathrm{tr}(\rho_{km}^{\nu(j,k,m)}) = d(d^2+1).$$

This concludes the proof. □

Lemma III.5: Let

$$\Delta_\alpha := \frac{1}{d^2+1}\mathrm{id} + \frac{1}{2d^2(d^2+1)} \sum_{\beta\in\mathbb{Z}_d\times\mathbb{Z}_d} (\omega^{c(\alpha,\beta)} D_\beta + \omega^{-c(\alpha,\beta)} D_\beta^\dagger).$$

Then $\mathfrak{Z} := \{\Delta_\alpha\}_{\alpha\in\mathbb{Z}_d\times\mathbb{Z}_d}$ *is a POVM on* $\mathcal{H}$.

Proof: We show that $\Delta_\alpha := (1/d) D_\alpha \rho D_\alpha^\dagger$ where $\rho \in \mathrm{S}(\mathcal{H})$ is the state given in Lemma III.4. The statement then follows from Lemma III.3 (i) and (ii) because these imply that the operators are non-negative and resolve the identity.

We claim that

$$D_\alpha D_\beta^\dagger D_\alpha^\dagger = \omega^{-c(\alpha,\beta)} D_\beta^\dagger. \tag{16}$$

This can be verified as follows using the fact that the operators are unitary, Lemma III.3 (iii), and the identity $c(\alpha,\beta) = -c(\beta,\alpha)$,

$$D_\alpha D_\beta^\dagger D_\alpha^\dagger = D_\beta^\dagger D_\beta D_\alpha D_\beta^\dagger D_\alpha^\dagger = D_\beta^\dagger \omega^{c(\beta,\alpha)} D_\alpha D_\alpha^\dagger = \omega^{-c(\alpha,\beta)} D_\beta^\dagger.$$

By inserting the state ρ given in Lemma III.4, we obtain

$$\frac{1}{d} D_\alpha \rho D_\alpha^\dagger = \frac{1}{d^2+1}\mathrm{id} + \frac{1}{2d^2(d^2+1)} \sum_{\beta\in\mathbb{Z}_d\times\mathbb{Z}_d} (D_\alpha D_\beta D_\alpha^\dagger + D_\alpha D_\beta^\dagger D_\alpha^\dagger).$$

Using Lemma III.3 (iii) again as well as the identity (16) establishes the fact that this equals Δ_α.□

To simplify the notation, let us introduce the Hermitian operators

$$\Lambda_\alpha := \frac{1}{2d} \sum_{\beta\in\mathbb{Z}_d\times\mathbb{Z}_d} (\omega^{c(\alpha,\beta)} D_\beta + \omega^{-c(\alpha,\beta)} D_\beta^\dagger).$$

With these operators, the POVM in question has the simple form

$$\Delta_\alpha := \frac{1}{d^2+1} \cdot \left(\mathrm{id} + \frac{1}{d} \cdot \Lambda_\alpha\right) \quad \text{for all } \alpha \in \mathbb{Z}_d \times \mathbb{Z}_d. \tag{17}$$

Let us first compute two useful identities concerning the trace of these operators.

Lemma III.6: For all $\alpha, \beta \in \mathbb{Z}_d \times \mathbb{Z}_d$,

$$\mathrm{tr}(\Lambda_\alpha) = 1,$$

$$\mathrm{tr}(\Lambda_\alpha^\dagger \Lambda_\beta) = d \cdot \delta_{\alpha,\beta}.$$

Proof: As $D_0=\mathrm{id}$, we have from Lemma III.3 (v) the identity $\mathrm{tr}(D_\beta)=d\cdot\delta_{\beta,0}$. With

$$\mathrm{tr}(A^\dagger)=\overline{\mathrm{tr}(A)} \tag{18}$$

this gives

$$\mathrm{tr}(\Lambda_\alpha)=\tfrac{1}{2}(\omega^{c(\alpha,0)}+\omega^{-c(\alpha,0)})=1\,.$$

Because of

$$\Lambda_\alpha^\dagger\Lambda_\beta=\frac{1}{4d^2}\left(\sum_\gamma \omega^{-c(\alpha,\gamma)}D_\gamma^\dagger+\omega^{c(\alpha,\gamma)}D_\gamma\right)\left(\sum_\delta \omega^{c(\beta,\delta)}D_\delta+\omega^{-c(\beta,\delta)}D_\delta^\dagger\right)$$

and identity (18) we have

$$\mathrm{tr}(\Lambda_\alpha^\dagger\Lambda_\beta)=\frac{1}{4d^2}\sum_{\gamma,\delta}(\omega^{c(\beta,\delta)-c(\alpha,\gamma)}\,\mathrm{tr}(D_\gamma^\dagger D_\delta)+\omega^{c(\alpha,\gamma)+c(\beta,\delta)}\,\mathrm{tr}(D_\gamma D_\delta))+\mathrm{H.c.}\,,$$

where H.c. denotes the complex conjugate of the previous expression. Applying Lemma III.3 (iv) and (v) gives

$$\mathrm{tr}(\Lambda_\alpha^\dagger\Lambda_\beta)=\frac{1}{4d}\cdot\sum_\gamma(\omega^{c(\beta,\gamma)-c(\alpha,\gamma)}+\omega^{c(\alpha,\gamma)+c(\beta,-\gamma)})+\mathrm{H.c.}$$

But $c(\beta,-\gamma)=-c(\beta,\gamma)$ and $c(\beta,\gamma)-c(\alpha,\gamma)=c(\beta-\alpha,\gamma)$, hence we obtain

$$\mathrm{tr}(\Lambda_\alpha^\dagger\Lambda_\beta)=\frac{1}{4d}\cdot\sum_\gamma(\omega^{c(\beta-\alpha,\gamma)}+\omega^{c(\alpha-\beta,\gamma)})+\mathrm{H.c.}$$

and thus finally

$$\mathrm{tr}(\Lambda_\alpha^\dagger\Lambda_\beta)=d\cdot\delta_{\alpha,\beta},$$

as a consequence of Eq. (14). □

Lemma III.7: The POVM $\mathfrak{Z}$ *is a dual of the family of Hermitian operators*

$$\Theta_\alpha:=-d\left(\mathrm{id}-\frac{d^2+1}{d}\cdot\Lambda_\alpha\right),\quad \alpha\in\mathbb{Z}_d\times\mathbb{Z}_d.$$

Proof: The operators Θ_α are Hermitian since, by definition, the operators Λ_α are Hermitian. The fact that $\mathfrak{Z}$ is a dual of the family of operators Θ_α follows from the representation (17) of the POVM operators and Lemma III.6. □

Lemma III.8: For every $\alpha\in\mathbb{Z}_d\times\mathbb{Z}_d$, $\mathrm{tr}(|\Theta_\alpha|)\leqslant d\cdot\sqrt{d^4+d^2-1}$.

Proof: Let $\lambda_1,\ldots,\lambda_d$ be the eigenvalues of Θ_α (including multiplicities). Then using Cauchy-Schwartz,

$$\mathrm{tr}(|\Theta_\alpha|)=\sum_{i=1}^d|\lambda_i|\leqslant d^{1/2}\sqrt{\sum_{i=1}^d|\lambda_i|^2}=d^{1/2}\sqrt{\mathrm{tr}(\Theta_\alpha^\dagger\Theta_\alpha)}.$$

But $\mathrm{tr}(\Theta_\alpha^\dagger\Theta_\alpha)=d(d^4+d^2-1)$ as can be computed directly using Lemma III.6. □

IV. ANALYSIS OF SYMMETRIC PROBABILITY DISTRIBUTIONS

In this section, we derive a number of useful properties of symmetric probability distributions. These results will later be applied to probability distributions resulting from measurements of a symmetric quantum state.

It is worth noting that our proof of the finite quantum de Finetti representation does not rely on a classical de Finetti-style theorem (as opposed to Ref. 4). It is, however, straightforward to obtain a de Finetti representation for (classical) probability distributions based on the results presented in the sequel.

A. Estimating the frequency distribution of a subsequence

Let $(\mathbf{z},\bar{\mathbf{z}})$ be the concatenation of an n-tuple $\mathbf{z}$ and a k-tuple $\bar{\mathbf{z}}$ of elements from $\mathcal{Z}$. We show that, if $(\mathbf{z},\bar{\mathbf{z}})$ is randomly chosen according to a symmetric probability distribution $P_{(\mathbf{Z},\bar{\mathbf{Z}})}$, then the frequency distribution $Q_{\bar{\mathbf{z}}}$ of the subtuple $\bar{\mathbf{z}}$ is a good estimate for the frequency distribution $Q_{\mathbf{z}}$ of the remaining subsequence $\mathbf{z}$.

We need the following simple relation between the distances of frequency distributions of subsequences obtained from a sequence of elements from $\mathcal{Z}$.

Lemma IV.1: Let $\mathcal{Z}$ be a set and let $\mathbf{z}$ and $\bar{\mathbf{z}}$ be elements of $\mathcal{Z}^n$ and $\mathcal{Z}^k$, respectively. Then

$$\delta(Q_{\mathbf{z}},Q_{\bar{\mathbf{z}}}) \leqslant \frac{n+k}{n}\delta(Q_{\bar{\mathbf{z}}},Q_{(\mathbf{z},\bar{\mathbf{z}})}).$$

Proof: By the definition of the frequency distribution,

$$(n+k)Q_{(\mathbf{z},\bar{\mathbf{z}})} = nQ_{\mathbf{z}} + kQ_{\bar{\mathbf{z}}}.$$

Hence, using the convexity of the variational distance,

$$\delta(Q_{(\mathbf{z},\bar{\mathbf{z}})},Q_{\mathbf{z}}) = \delta\left(\frac{n}{n+k}Q_{\mathbf{z}} + \frac{k}{n+k}Q_{\bar{\mathbf{z}}},Q_{\mathbf{z}}\right) \leqslant \frac{k}{n+k}\delta(Q_{\bar{\mathbf{z}}},Q_{\mathbf{z}}).$$

The triangle inequality then leads to

$$\delta(Q_{\bar{\mathbf{z}}},Q_{\mathbf{z}}) \leqslant \delta(Q_{\bar{\mathbf{z}}},Q_{(\mathbf{z},\bar{\mathbf{z}})}) + \delta(Q_{(\mathbf{z},\bar{\mathbf{z}})},Q_{\mathbf{z}}) \leqslant \delta(Q_{\bar{\mathbf{z}}},Q_{(\mathbf{z},\bar{\mathbf{z}})}) + \frac{k}{n+k}\delta(Q_{\bar{\mathbf{z}}},Q_{\mathbf{z}}),$$

from which the assertion follows.

We now show that $Q_{\mathbf{z}}$ is close to $Q_{\bar{\mathbf{z}}}$ by showing that the expression on the rhs of the inequality in Lemma IV.1 is small in expectation.

Lemma IV.2: Let $\mathbf{Z}$ be an n-tuple and $\bar{\mathbf{Z}}$ a k-tuple of random variables over a set $\mathcal{Z}$ of size $|\mathcal{Z}|=t$ such that $P_{(\mathbf{Z},\bar{\mathbf{Z}})}$ is symmetric. Then, for $(\mathbf{z},\bar{\mathbf{z}}) \leftarrow P_{(\mathbf{Z},\bar{\mathbf{Z}})}$,

$$\mathop{\mathbb{E}}_{(\mathbf{z},\bar{\mathbf{z}})}[\delta(Q_{\bar{\mathbf{z}}},Q_{(\mathbf{z},\bar{\mathbf{z}})})] \leqslant \frac{1}{2}\sqrt{\frac{t}{k}}.$$

Proof: Let $\mathbf{Z} := (Z_1,\ldots,Z_n)$ and $\bar{\mathbf{Z}} := (\bar{Z}_1,\ldots,\bar{Z}_k)$. It suffices to show that, for all probability distributions $q \in \mathrm{Distr}(\mathcal{Z})$,

$$\mathop{\mathbb{E}}_{\bar{\mathbf{z}}\leftarrow P_{\bar{\mathbf{Z}}|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q}}[\delta(Q_{\bar{\mathbf{z}}},q)] \leqslant \frac{1}{2}\sqrt{\frac{t}{k}}. \tag{19}$$

The assertion then follows from

$$\mathop{\mathbb{E}}_{(\mathbf{z},\bar{\mathbf{z}})\leftarrow P_{(\mathbf{Z},\bar{\mathbf{Z}})}}[\delta(Q_{\bar{\mathbf{z}}},Q_{(\mathbf{z},\bar{\mathbf{z}})})] = \mathop{\mathbb{E}}_{q\leftarrow P_{Q_{(\mathbf{Z},\bar{\mathbf{Z}})}}}\left[\mathop{\mathbb{E}}_{\bar{\mathbf{z}}\leftarrow P_{\bar{\mathbf{Z}}|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q}}[\delta(Q_{\bar{\mathbf{z}}},q)]\right].$$

Let thus $q \in \mathrm{Distr}(\mathcal{Z})$ be fixed. For every $z \in \mathcal{Z}$, let χ_z be the function from $\mathcal{Z}$ to $\{0,1\}$ defined by $\chi_z(z')=1$ if $z'=z$ and $\chi_z(z')=0$ otherwise. Then

$$\delta(Q_{\bar{\mathbf{z}}}, q) = \frac{1}{2} \sum_{z \in \mathcal{Z}} |d_z(\bar{\mathbf{z}})|, \tag{20}$$

where, for any $\bar{\mathbf{z}} = (\bar{z}_1, \ldots, \bar{z}_k) \in \mathcal{Z}^k$,

$$d_z(\bar{\mathbf{z}}) := \frac{1}{k} \sum_{i=1}^{k} (\chi_z(\bar{z}_i) - q(z)).$$

Using Jensen's inequality,

$$\mathop{\mathbb{E}}_{\bar{\mathbf{z}} \leftarrow P_{\bar{\mathbf{Z}}|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q}} [|d_z(\bar{\mathbf{z}})|] \leq \sqrt{\mathop{\mathbb{E}}_{\bar{\mathbf{z}} \leftarrow P_{\bar{\mathbf{Z}}|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q}} [d_z(\bar{\mathbf{z}})^2]}. \tag{21}$$

We claim that for any $i \neq j$,

$$\mathop{\mathbb{E}}_{(\bar{z}_i,\bar{z}_j) \leftarrow P_{(\bar{Z}_i,\bar{Z}_j)|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q}} [(\chi_z(\bar{z}_i) - q(z))(\chi_z(\bar{z}_j) - q(z))] \leq 0. \tag{22}$$

To prove this identity, first note that the expectation value can be written in the form

$$\mathop{\mathbb{E}}_{\bar{z}_i \leftarrow P_{\bar{Z}_i|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q}} [\mathop{\mathbb{E}}_{\bar{z}_j \leftarrow P_{\bar{Z}_j|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q, \bar{Z}_i=\bar{z}_i}} [(\chi_z(\bar{z}_i) - q(z))(\chi_z(\bar{z}_j) - q(z))]].$$

Since $0 \leq q(z) \leq 1$, it suffices to show that

$$\mathop{\mathbb{E}}_{\bar{z}_j \leftarrow P_{\bar{Z}_j|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q, \bar{Z}_i=\bar{z}_i}} [\chi_z(\bar{z}_j) - q(z)] \begin{cases} \leq 0 & \text{if } \bar{z}_i = z, \\ \geq 0 & \text{otherwise.} \end{cases} \tag{23}$$

Because of Lemma II.3, the probability distribution $P_{\bar{\mathbf{Z}}|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q, \bar{Z}_i=\bar{z}_i}$ is symmetric. Hence by the definition of the frequency distribution, we have

$$\mathop{\mathbb{E}}_{\bar{z}_j \leftarrow P_{\bar{Z}_j|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q, \bar{Z}_i=\bar{z}_i}} [\chi_z(\bar{z}_j)] = P_{\bar{Z}_j|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q, \bar{Z}_i=\bar{z}_i}(z) = \begin{cases} \dfrac{nq(z)-1}{n-1} & \text{if } z = \bar{z}_i, \\ \dfrac{nq(z)}{n-1} & \text{otherwise.} \end{cases}$$

This proves (23) and thus (22).

Using (22) and Lemma II.4, we obtain

$$\mathop{\mathbb{E}}_{\bar{\mathbf{z}} \leftarrow P_{\bar{\mathbf{Z}}|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q}} [d_z(\bar{\mathbf{z}})^2] \leq \frac{1}{k^2} \sum_{i=1}^{k} \mathop{\mathbb{E}}_{\bar{z}_i \leftarrow P_{\bar{Z}_i|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q}} [(\chi_z(\bar{z}_i) - q(z))^2] = \frac{1}{k^2} \sum_{i=1}^{k} (q(z) - q(z)^2) \leq \frac{q(z)}{k}. \tag{24}$$

Combining (20), (21), and (24) leads to

$$\mathop{\mathbb{E}}_{\bar{\mathbf{z}} \leftarrow P_{\bar{\mathbf{Z}}|Q_{(\mathbf{Z},\bar{\mathbf{Z}})}=q}} [\delta(Q_{\bar{\mathbf{z}}}, q)] = \frac{1}{2} \sum_{z \in \mathcal{Z}} \sqrt{\frac{q(z)}{k}}.$$

The bound (19) then follows from the Cauchy-Schwartz inequality, which concludes the proof.□

B. The product structure of symmetric probability distributions

Let $\mathbf{z}$ be an n-tuple over $\mathcal{Z}$ randomly chosen according to a probability distribution $P_{\mathbf{Z}}$ and let $q \in \mathrm{Distr}(\mathcal{Z})$ be an estimate for the frequency distribution $Q_{\mathbf{z}}$ of $\mathbf{z}$. To quantify the quality of this estimate, it is convenient to introduce the abbreviation $D_q(P_{\mathbf{Z}})$ for the expected distance between the actual frequency distribution $Q_{\mathbf{z}}$ and the estimate q, that is

$$D_q(P_{\mathbf{Z}}) := \mathop{\mathbb{E}}_{\mathbf{z} \leftarrow P_{\mathbf{Z}}} [\delta(Q_{\mathbf{z}}, q)].$$

The main result of Sec. IV A can then be rephrased as follows.

Lemma IV.3: Let $\mathbf{Z}$ *be an n-tuple and* $\overline{\mathbf{Z}}$ *a k-tuple of random variables over a set* $\mathcal{Z}$ *of size* $|\mathcal{Z}| = t$, *for* $k \leq n$, *such that* $P_{(\mathbf{Z},\overline{\mathbf{Z}})}$ *is symmetric. Then, for* $\overline{\mathbf{z}} \leftarrow P_{\overline{\mathbf{Z}}}$,

$$\mathop{\mathbb{E}}_{\overline{\mathbf{z}}} [D_{Q_{\overline{\mathbf{z}}}}(P_{\mathbf{Z}|\overline{\mathbf{Z}}=\overline{\mathbf{z}}})] \leq \sqrt{\frac{t}{k}}.$$

Proof: From Lemma IV.2 and Lemma IV.1,

$$\mathop{\mathbb{E}}_{(\mathbf{z},\overline{\mathbf{z}}) \leftarrow P_{(\mathbf{Z},\overline{\mathbf{Z}})}} [\delta(Q_{\mathbf{z}}, Q_{\overline{\mathbf{z}}})] \leq \sqrt{\frac{t}{k}}.$$

The assertion then follows from the definition of $D_{\cdot}(\cdot)$.

□

Lemma IV.4 establishes a connection between the quantity $D_q(P_{\mathbf{Z}})$ and the product structure of symmetric probability distributions.

Lemma IV.4: Let Y *be a random variable over* $\mathcal{Y}$ *and let* $\mathbf{Z} = (Z_1, \ldots, Z_r)$ *be an r-tuple of random variables over* $\mathcal{Z}$, *such that the conditional probability distribution* $P_{\mathbf{Z}|Y=y}$ *is symmetric for every* $y \in \mathcal{Y}$. *Then, for all* $q \in \mathrm{Distr}(\mathcal{Z})$,

$$\delta(P_{YZ_i}, P_Y \times q) \leq D_q(P_{\mathbf{Z}}), \quad \textit{for every } i \in [r].$$

Proof: Using the strong convexity of the variational distance, we have

$$\delta(P_{YZ_i}, P_Y \times q) \leq \mathop{\mathbb{E}}_{\tilde{q} \leftarrow P_{Q_{\mathbf{Z}}}} [\delta(P_{YZ_i|Q_{\mathbf{Z}}=\tilde{q}}, P_{Y|Q_{\mathbf{Z}}=\tilde{q}} \times q)]. \tag{25}$$

Since $P_{\mathbf{Z}|Y=y}$ is symmetric, Lemma II.4 implies $P_{Z_i|Y=y,Q_{\mathbf{Z}}=\tilde{q}} = \tilde{q}$, for every $y \in \mathcal{Y}$. In particular, conditioned on $Q_{\mathbf{z}} = \tilde{q}$, Z_i is independent of Y. Hence,

$$\delta(P_{YZ_i|Q_{\mathbf{Z}}=\tilde{q}}, P_{Y|Q_{\mathbf{Z}}=\tilde{q}} \times q) = \delta(P_{Y|Q_{\mathbf{Z}}=\tilde{q}} \times \tilde{q}, P_{Y|Q_{\mathbf{Z}}=\tilde{q}} \times q) = \delta(\tilde{q}, q), \tag{26}$$

where the last equality follows from (4). Combining (25) and (26) leads to

$$\delta(P_{YZ_i}, P_Y \times q) \leq \mathop{\mathbb{E}}_{\tilde{q} \leftarrow P_{Q_{\mathbf{Z}}}} [\delta(\tilde{q}, q)] = \mathop{\mathbb{E}}_{\mathbf{z} \leftarrow P_{\mathbf{Z}}} [\delta(Q_{\mathbf{z}}, q)] = D_q(P_{\mathbf{Z}}).$$

V. ANALYSIS OF SYMMETRIC QUANTUM STATES

The goal of this section is to derive results on symmetric quantum states, based on the corresponding results on symmetric probability distributions given in the preceding section. In Sec. V A, we first show how certain properties of the measurement statistics imply structural properties of the corresponding quantum states. Then, in Sec. V B, we combine these results with those of Sec. IV B in order to prove statements about the structure of symmetric quantum states.

A. Deducing the state structure from measurement results

Consider a state of a bipartite system conditioned on a measurement on one of the systems. We first prove an upper bound on the amount of dependence between this conditional state and the measurement outcome.

Lemma V.1: Let $\rho^{AB} \in \mathrm{S}(\mathcal{H}_A \otimes \mathcal{H}_B)$ *and let* $\mathfrak{Z}=\{F_z\}_{z\in\mathcal{Z}}$ *be a POVM on* $\mathcal{H}_B$. *Then, for all* $q \in \mathrm{Distr}(\mathcal{Z})$ *and* $z \in \mathcal{Z}$,

$$\delta(\rho^A{}_{|\mathfrak{Z}=z}, \rho^A) \leqslant \frac{2}{\rho^B_{\mathfrak{Z}}(z)} \max_{\mathfrak{Y}} \delta(\rho^{AB}_{\mathfrak{Y}\mathfrak{Z}}, \rho^A_{\mathfrak{Y}} \times q),$$

where the maximization is over all POVMs $\mathfrak{Y}$ *on* $\mathcal{H}_A$.

Proof: Let $\mathfrak{Y} := \{E_y\}_{y\in\mathcal{Y}}$ be a POVM on $\mathcal{H}_A$. Then, from the triangle inequality, (2) and (4),

$$\delta(\rho^{AB}_{\mathfrak{Y}\mathfrak{Z}}, \rho^A_{\mathfrak{Y}} \times \rho^B_{\mathfrak{Z}}) \leqslant \delta(\rho^{AB}_{\mathfrak{Y}\mathfrak{Z}}, \rho^A_{\mathfrak{Y}} \times q) + \delta(\rho^A_{\mathfrak{Y}} \times q, \rho^A_{\mathfrak{Y}} \times \rho^B_{\mathfrak{Z}}) = \delta(\rho^{AB}_{\mathfrak{Y}\mathfrak{Z}}, \rho^A_{\mathfrak{Y}} \times q) + \delta(q, \rho^B_{\mathfrak{Z}}) \leqslant 2D, \tag{27}$$

where

$$D := \max_{\mathfrak{Y}'} \delta(\rho^{A\,B}_{\mathfrak{Y}'\,\mathfrak{Z}}, \rho^A_{\mathfrak{Y}'} \times q),$$

with the maximization ranging over all POVMs $\mathfrak{Y}'$ on $\mathcal{H}_A$. Using Eq. (3), we have

$$\rho^B_{\mathfrak{Z}}(z) \cdot \delta(\rho^A_{\mathfrak{Y}|\mathfrak{Z}=z}, \rho^A_{\mathfrak{Y}}) \leqslant \mathop{\mathbb{E}}_{z\leftarrow\rho^B_{\mathfrak{Z}}} [\delta(\rho^A_{\mathfrak{Y}|\mathfrak{Z}=z}, \rho^A_{\mathfrak{Y}})] = \delta(\rho^{AB}_{\mathfrak{Y}\mathfrak{Z}}, \rho^A_{\mathfrak{Y}} \times \rho^B_{\mathfrak{Z}}).$$

With (27), it follows that

$$\delta(\rho^A_{\mathfrak{Y}|\mathfrak{Z}=z}, \rho^A_{\mathfrak{Y}}) \leqslant \frac{2D}{\rho^B_{\mathfrak{Z}}(z)}$$

for every $z \in \mathcal{Z}$ and every POVM $\mathfrak{Y}$ on $\mathcal{H}_A$. Therefore, using (9), we conclude that

$$\delta(\rho^A{}_{|\mathfrak{Z}=z}, \rho^A) = \max_{\mathfrak{Y}} \delta(\rho^A_{\mathfrak{Y}|\mathfrak{Z}=z}, \rho^A_{\mathfrak{Y}}) \leqslant \frac{2D}{\rho^B_{\mathfrak{Z}}(z)}.$$

□

For a POVM $\mathfrak{Z}=\{F_z\}_{z\in\mathcal{Z}}$ on a Hilbert space $\mathcal{H}$, we define the constants

$$C_1(\mathfrak{Z}) := \min_{\{F^*_z\}_{z\in\mathcal{Z}}} 2 \cdot \left(\sum_{z\in\mathcal{Z}} \mathrm{tr}(|F^*_z|) \right),$$

$$C_2(\mathfrak{Z}) := \sqrt{|\mathcal{Z}|} \cdot C_1(\mathfrak{Z}),$$

where the minimum ranges over all families $\{F^*_z\}_{z\in\mathcal{Z}}$ of elements from $\mathrm{Herm}(\mathcal{H})$ such that $\mathfrak{Z}$ is the dual of $\{F^*_z\}_{z\in\mathcal{Z}}$. If no such family $\{F^*_z\}_{z\in\mathcal{Z}}$ exists, we set $C_i(\mathfrak{Z}) := \infty$, for $i=1,2$.

It is clear (from linear algebra, it is well known that whenever a family $\{f_i\}_{i\in\mathcal{N}}$ forms a basis of $\mathcal{H}$, there exists a unique family $\{e_i\}_{i\in\mathcal{N}}$ such that $\{f_i\}_{i\in\mathcal{N}}$ is a dual of $\{e_i\}_{i\in\mathcal{N}}$) that $C_i(\mathfrak{Z}) < \infty$, for $i=1,2$, if $\mathfrak{Z}$ is an informationally complete POVM. By the interpretation given to the values $\mathrm{tr}(|F^*_z|)$ in Sec. II D, the value $C_1(\mathfrak{Z})$ can be seen as a measure for the resulting accuracy when estimating an unknown state ρ given the statistics obtained by the measurement $\mathfrak{Z}$.

For a d-dimensional Hilbert space $\mathcal{H}$, let $\bar{C}_i(d)$ be the minimum of $C_i(\mathfrak{Z})$, minimized over all POVMs $\mathfrak{Z}$ on $\mathcal{H}$, that is

$$\bar{C}_i(d) := \min_{\mathfrak{Z}} C_i(\mathfrak{Z}) \quad \text{for } i = 1,2.$$

The following corollary is a direct consequence of Lemma III.2 and Lemma III.8.

Corollary V.2: Let $\mathcal{H}$ be a d-dimensional Hilbert space. Then

$$\bar{C}_1(d) \leqslant 2\sqrt{2} \cdot d^5,$$

$$\bar{C}_2(d) \leqslant 2\sqrt{2} \cdot d^6.$$

If symmetric informationally complete POVMs exist in dimension d, then

$$\bar{C}_1(d) \leqslant 2d^2(2d-1).$$

$$\bar{C}_2(d) \leqslant 2d^3(2d-1).$$

The main result of this section expresses the intuitive fact that a bipartite state has product form if every bipartite measurement yields a product distribution.

Theorem V.3: *Let $\rho^{AB} \in \mathrm{S}(\mathcal{H}_A \otimes \mathcal{H}_B)$ and let $\mathfrak{Z}$ be a POVM on $\mathcal{H}_B$. Then, for any $q \in \mathrm{Distr}(\mathcal{Z})$,*

$$\delta(\rho^{AB}, \rho^A \otimes \rho^B) \leqslant C_1(\mathfrak{Z}) \cdot \max_{\mathfrak{Y}} \delta(\rho^{A\,B}_{\mathfrak{Y}\mathfrak{Z}}, \rho^A_{\mathfrak{Y}} \times q).$$

In particular, if $\mathcal{H}_B$ is d-dimensional, then

$$\delta(\rho^{AB}, \rho^A \otimes \rho^B) \leqslant \bar{C}_1(d) \cdot \max_{\mathfrak{Y},\mathfrak{Z}} \delta(\rho^{A\,B}_{\mathfrak{Y}\mathfrak{Z}}, \rho^A_{\mathfrak{Y}} \times \rho^B_{\mathfrak{Z}}).$$

(*The maxima are taken over all POVMs $\mathfrak{Y}$ on $\mathcal{H}_A$ and $\mathfrak{Z}$ on $\mathcal{H}_B$, respectively.*)

Proof: Let $\{F_z^*\}_{z \in \mathcal{Z}}$ be a family of elements from $\mathrm{Herm}(\mathcal{H}_B)$ such that $\mathfrak{Z}=\{F_z\}_{z \in \mathcal{Z}}$ is the dual of $\{F_z^*\}_{z \in \mathcal{Z}}$. Then, according to (12),

$$\rho^{AB} = \mathop{\mathbb{E}}_{z \leftarrow \rho^B_{\mathfrak{Z}}} [\rho^A{}_{|\mathfrak{Z}=z} \otimes F_z^*] \quad \text{and} \quad \rho^B = \mathop{\mathbb{E}}_{z \leftarrow \rho^B_{\mathfrak{Z}}} [F_z^*].$$

Using these identities, the strong convexity of the trace distance, and Lemma II.1, we obtain

$$\begin{aligned}\delta(\rho^{AB}, \rho^A \otimes \rho^B) &= \delta\Big(\mathop{\mathbb{E}}_{z \leftarrow \rho^B_{\mathfrak{Z}}} [\rho^A{}_{|\mathfrak{Z}=z} \otimes F_z^*], \mathop{\mathbb{E}}_{z \leftarrow \rho^B_{\mathfrak{Z}}} [\rho^A \otimes F_z^*]\Big) \leqslant \mathop{\mathbb{E}}_{z \leftarrow \rho^B_{\mathfrak{Z}}} [\delta(\rho^A{}_{|\mathfrak{Z}=z} \otimes F_z^*, \rho^A \otimes F_z^*)] \\ &= \mathop{\mathbb{E}}_{z \leftarrow \rho^B_{\mathfrak{Z}}} [\delta(\rho^A{}_{|\mathfrak{Z}=z}, \rho^A) \cdot \mathrm{tr}(|F_z^*|)].\end{aligned}$$

The assertion then follows from Lemma V.1 and the definition of $C_1(\mathfrak{Z})$. □

B. The product structure of symmetric quantum states

We now combine the results of Sec. IV and Sec. V A. We start with a quantum analogue of Lemma IV.4.

Lemma V.4: Let $\rho^{A\bar{r}} \in \mathrm{S}(\mathcal{H}_A \otimes \mathcal{H}^{\otimes r})$ be symmetric relative to $\mathcal{H}_A$ and let $\mathfrak{Z}=\{F_z\}_{z \in \mathcal{Z}}$ be a POVM on $\mathcal{H}$. Then, for any $q \in \mathrm{Distr}(\mathcal{Z})$,

$$\delta(\rho^{A\bar{1}}, \rho^A \otimes \rho^{\bar{1}}) \leqslant C_1(\mathfrak{Z}) D_q(\rho^{\bar{r}}_{\mathfrak{Z}^r})$$

and

$$\delta(\rho^{\bar{1}}_{\mathfrak{Z}}, q) \leqslant D_q(\rho^{\bar{r}}_{\mathfrak{Z}^r}).$$

Proof: Let $\mathcal{Y}$ be a POVM on $\mathcal{H}_A$. Since, by Lemma II.6, $\rho^{\bar{r}}_{|\mathcal{Y}=y}$ is symmetric, the probability distribution $\rho^{\bar{r}}_{\mathcal{Z}^r|\mathcal{Y}=y}$ is also symmetric, for all $y \in \mathcal{Y}$. Lemma IV.4 thus implies

$$\delta(\rho^{A\bar{1}}_{\mathcal{Y}\mathcal{Z}}, \rho^{A}_{\mathcal{Y}} \times q) \leq D_q(\rho^{\bar{r}}_{\mathcal{Z}^r}). \tag{28}$$

The first assertion of the lemma then follows from Theorem V.3.

The second assertion of the lemma follows directly from (28) and property (2) of the variational distance, i.e., $\delta(\rho^{\bar{1}}_{\mathcal{Z}}, q) \leq \delta(\rho^{A\bar{1}}_{\mathcal{Y}\mathcal{Z}}, \rho^{A}_{\mathcal{Y}} \times q)$. □

The next lemma shows that symmetry imposes severe constraints on the structure of quantum states. More precisely, if a symmetric quantum state has (almost) product structure with respect to one of its subsystems, this directly implies that the state has (almost) product structure with respect to all its subsystems.

Lemma V.5: Let $\rho^{A\bar{n}} \in \mathrm{S}(\mathcal{H}_A \otimes \mathcal{H}^{\otimes n})$ *be symmetric relative to* $\mathcal{H}_A$. *Then*

$$\delta(\rho^{A\bar{n}}, \rho^{A} \otimes (\rho^{\bar{1}})^{\otimes n}) \leq n \cdot \delta(\rho^{A\bar{n}}, \rho^{A\overline{n-1}} \otimes \rho^{\bar{1}}).$$

Proof: Using the triangle inequality for the trace distance, we get

$$\delta(\rho^{A\bar{n}}, \rho^{A} \otimes (\rho^{\bar{1}})^{\otimes n}) \leq \sum_{i=0}^{n-1} \delta(\rho^{A\overline{n-1}} \otimes (\rho^{\bar{1}})^{\otimes i}, \rho^{A\overline{n-i-1}} \otimes (\rho^{\bar{1}})^{\otimes (i+1)}). \tag{29}$$

Since, by Eq. (8), the trace distance does not change when tracing out the product state $(\rho^{\bar{1}})^{\otimes i}$, we have, for any $i \in [n]$,

$$\delta(\rho^{A\overline{n-i}} \otimes (\rho^{\bar{1}})^{\otimes i}, \rho^{A\overline{n-i-1}} \otimes (\rho^{\bar{1}})^{\otimes (i+1)}) = \delta(\rho^{A\overline{n-i}}, \rho^{A\overline{n-i-1}} \otimes \rho^{\bar{1}}). \tag{30}$$

Using the fact that the trace distance can only decrease when taking a partial trace [see (6)], we get

$$\delta(\rho^{A\overline{n-i}}, \rho^{A\overline{n-i-1}} \otimes \rho^{\bar{1}}) \leq \delta(\rho^{A\bar{n}}, \rho^{A\overline{n-1}} \otimes \rho^{\bar{1}}). \tag{31}$$

Combining (30) with (31) and inserting this into (29) concludes the proof. □

Combined with Lemma V.4, we obtain an upper bound on the distance between a symmetric state on n subsystems and an n-fold product state.

Corollary V.6: Let $\rho^{A\overline{n+m}} \in \mathrm{S}(\mathcal{H}_A \otimes \mathcal{H}^{\otimes n+m})$ *be symmetric relative to* $\mathcal{H}_A$ *and let* $\mathcal{Z} = \{F_z\}_{z \in \mathcal{Z}}$ *be a POVM on* $\mathcal{H}$. *Then, for any* $q \in \mathrm{Distr}(\mathcal{Z})$,

$$\delta(\rho^{A\bar{n}}, \rho^{A} \otimes (\rho^{\bar{1}})^{\otimes n}) \leq n C_1(\mathcal{Z}) D_q(\rho^{\overline{m+1}}_{\mathcal{Z}^{m+1}}).$$

Proof: Obviously, the density operator $\rho^{A\overline{n+m}}$ is symmetric relative to $\mathcal{H}_{A'} := \mathcal{H}_A \otimes \mathcal{H}^{\otimes n-1}$. Thus, with $r := m+1$, we can write $\rho^{A'\bar{r}}$ instead of $\rho^{A\overline{n+m}}$, and, similarly, $\rho^{A\bar{n}} = \rho^{A'\bar{1}}$ and $\rho^{A\overline{n-1}} = \rho^{A'}$. Hence, by Lemma V.4,

$$\delta(\rho^{A\bar{n}}, \rho^{A\overline{n-1}} \otimes \rho^{\bar{1}}) = \delta(\rho^{A'\bar{1}}, \rho^{A'} \otimes \rho^{\bar{1}}) \leq C_1(\mathcal{Z}) D_q(\rho^{\bar{r}}_{\mathcal{Z}^r}).$$

Applying Lemma V.5 concludes the proof. □

Finally, we give an upper bound on the expected value of the quantity appearing on the rhs. in Corollary 6. For this, we need a quantum analogue of Lemma IV.3.

Lemma V.7: Let $\rho^{\overline{n+k}} \in S(\mathcal{H}^{\otimes n+k})$, *for* $k \leq n$, *be symmetric and let* $\mathcal{Z} = \{F_z\}_{z \in \mathcal{Z}}$ *be a POVM on* $\mathcal{H}$ *with* $|\mathcal{Z}| = t$. *Then, for* $\bar{\mathbf{z}} \leftarrow \rho^{\bar{k}}_{\mathcal{Z}^k}$,

$$\mathop{\mathbb{E}}_{\bar{\mathbf{z}}}[D_{Q_{\mathbf{z}}}(\rho^{\bar{n}}_{\mathcal{Z}^n|\mathcal{Z}^k=\bar{\mathbf{z}}})] \leq \sqrt{\frac{t}{k}}.$$

Proof: The assertion follows directly from Lemma IV.3 and the fact that the probability

distribution $\rho^{\bar{n}}_{\mathfrak{Z}^n}{}^{\bar{k}}_{\mathfrak{Z}^k}=\rho^{\overline{n+k}}_{\mathfrak{Z}^{n+k}}$ is symmetric. □

VI. MAIN RESULTS

Our main results immediately follow from the characterizations of symmetric quantum states given in the preceding section. Basically, we consider the quantum state $\rho^{A\bar{n}}_{\bar{\mathbf{z}}}:=\rho^{A\bar{n}}{}_{|\mathfrak{Z}^k=\bar{\mathbf{z}}}$ on $\mathcal{H}_A \otimes \mathcal{H}^{\otimes n}$ obtained by conditioning an exchangeable state $\rho^{A\overline{n+k}}$ on the outcomes $\bar{\mathbf{z}}=(z_1,\ldots,z_k)$ of a POVM $\mathfrak{Z}$ applied to k subsystems. We show that $\rho^{A\bar{n}}_{\bar{\mathbf{z}}}$ is close to a product state $\rho^{A}_{\bar{\mathbf{z}}}\otimes(\rho^{\bar{1}}_{\bar{\mathbf{z}}})^{\otimes n}$ where $\rho^{\bar{1}}_{\bar{\mathbf{z}}}$ is a density operator on a single subsystem $\mathcal{H}$. Moreover, $\rho^{\bar{1}}_{\bar{\mathbf{z}}}$ is almost determined by the observed measurement statistics.

Theorem VI.1: *Let $\rho^{A\overline{n+k}}\in S(\mathcal{H}_A\otimes\mathcal{H}^{\otimes n+k})$ be $(n+2k-1)$-exchangeable relative to $\mathcal{H}_A$ and let $\mathfrak{Z}=\{F_z\}_{z\in\mathcal{Z}}$ be a POVM on $\mathcal{H}$ with $|\mathcal{Z}|=t$. For every $\bar{\mathbf{z}}\in\mathcal{Z}^k$, let $\rho^{A\bar{n}}_{\bar{\mathbf{z}}}:=\rho^{A\bar{n}}{}_{|\mathfrak{Z}^k=\bar{\mathbf{z}}}$. Then for $\overline{\mathbf{z}}\leftarrow\rho^{\bar{k}}_{\mathfrak{Z}^k}$,*

$$\mathop{\mathbb{E}}_{\bar{\mathbf{z}}}[\delta(\rho^{A\bar{n}}_{\bar{\mathbf{z}}},\rho^{A}_{\bar{\mathbf{z}}}\otimes(\rho^{\bar{1}}_{\bar{\mathbf{z}}})^{\otimes n})]\leqslant C_2(\mathfrak{Z})\frac{n}{\sqrt{k}}$$

where $\rho^{\bar{1}}_{\bar{\mathbf{z}}}=\rho^{\bar{1}}{}_{|\mathfrak{Z}^k=\bar{\mathbf{z}}}$ is determined by

$$\mathop{\mathbb{E}}_{\bar{\mathbf{z}}}[\delta(\rho^{\bar{1}}_{\mathfrak{Z}|\mathfrak{Z}^k=\bar{\mathbf{z}}},Q_{\bar{\mathbf{z}}})]\leqslant\sqrt{\frac{t}{k}}.$$

Proof: Let $m:=k-1$. According to the definition of exchangeability, there exists an extension $\rho^{A\overline{n+k+m}}\in S(\mathcal{H}_A\otimes\mathcal{H}^{\otimes n+k+m})$ of $\rho^{A\overline{n+k}}$ which is symmetric relative to $\mathcal{H}_A$. For every $\bar{\mathbf{z}}\in\mathcal{Z}^k$, let $[\rho_{\bar{\mathbf{z}}}]^{A\overline{n+m}}:=\rho^{A\overline{n+m}}{}_{|\mathfrak{Z}^k=\bar{\mathbf{z}}}$.

By Lemma II.6, $[\rho_{\bar{\mathbf{z}}}]^{A\overline{n+m}}$ is symmetric relative to $\mathcal{H}_A$. Hence, from the second bound of Lemma V.4, with $r:=m+1$,

$$\delta([\rho_{\bar{\mathbf{z}}}]^{\bar{1}}_{\mathfrak{Z}},Q_{\bar{\mathbf{z}}})\leqslant D_{Q_{\bar{\mathbf{z}}}}([\rho_{\bar{\mathbf{z}}}]^{\overline{m+1}}_{\mathfrak{Z}^{m+1}}) \tag{32}$$

and, from Corollary V.6,

$$\delta([\rho_{\bar{\mathbf{z}}}]^{A\bar{n}},[\rho_{\bar{\mathbf{z}}}]^{A}\otimes([\rho_{\bar{\mathbf{z}}}]^{\bar{1}})^{\otimes n})\leqslant nC_1(\mathfrak{Z})D_{Q_{\bar{\mathbf{z}}}}([\rho_{\bar{\mathbf{z}}}]^{\overline{m+1}}_{\mathfrak{Z}^{m+1}}). \tag{33}$$

Since $k=m+1$, we can apply Lemma V.7 to the state $\rho^{\overline{(m+1)+k}}$, i.e.,

$$\mathop{\mathbb{E}}_{\bar{\mathbf{z}}}[D_{Q_{\bar{\mathbf{z}}}}([\rho_{\bar{\mathbf{z}}}]^{\overline{m+1}}_{\mathfrak{Z}^{m+1}})]\leqslant\sqrt{\frac{t}{k}}.$$

The assertion follows by taking the expectation on both sides of (32) and (33), respectively. □

Using Markov's inequality, it is straightforward to turn Theorem VI.1, which expresses closeness in terms of expected distance, into a statement providing a bound on the probability that the distance is larger than a given value ε. However, by adapting the auxiliary results derived so far and using a tail inequality by Hoeffding, we obtain a tighter bound. The interested reader is referred to the Appendix for a derivation of an alternative version of Theorem VI.1.

Finally, as a simple corollary of Theorem VI.1, we obtain the following representation for finitely exchangeable quantum states.

Corollary VI.2 (finite quantum de Finetti representation): Let $\mathcal{H}$ be a d-dimensional Hilbert space and let $\rho^{\bar{n}}\in S(\mathcal{H}^{\otimes n})$ be $(n+s)$-exchangeable. Then $\rho^{\bar{n}}$ is ε-close to the convex hull of the set of n-fold product states $\{\sigma^{\otimes n}:\sigma\in S(\mathcal{H})\}$, for $\varepsilon=\sqrt{2}\bar{C}_2(d)n/\sqrt{s}$.

Proof: Let $k:=\lceil s/2\rceil$ and let $\rho^{\overline{n+k}}\in S(\mathcal{H}^{\otimes n+k})$ be an $(n+2k-1)$-exchangeable extension of $\rho^{\bar{n}}$. Let $\mathfrak{Z}$ be an informationally complete POVM on $\mathcal{H}$ and let, for any $\bar{\mathbf{z}}\in\mathcal{Z}^k$, $\rho^{\bar{n}}_{\bar{\mathbf{z}}}:=\rho^{\bar{n}}{}_{|\mathfrak{Z}^k=\bar{\mathbf{z}}}$. We show that

$$\delta(\rho^{\bar{n}}, \mathop{\mathbb{E}}_{\bar{\mathbf{z}}}[(\rho_{\bar{\mathbf{z}}}^{\bar{1}})^{\otimes n}]) \leqslant \sqrt{2}\bar{C}_2(d)\frac{n}{\sqrt{s}}, \tag{34}$$

where $\bar{\mathbf{z}} \leftarrow \rho_{\bar{\mathfrak{Z}}^k}^{\bar{k}}$. Since, by (1),

$$\mathop{\mathbb{E}}_{\bar{\mathbf{z}}}[\rho_{\bar{\mathbf{z}}}^{\bar{n}}] = \rho^{\bar{n}},$$

we obtain, using the strong convexity of the trace distance

$$\delta(\rho^{\bar{n}}, \mathop{\mathbb{E}}_{\bar{\mathbf{z}}}[(\rho_{\bar{\mathbf{z}}}^{\bar{1}})^{\otimes n}]) = \delta(\mathop{\mathbb{E}}_{\bar{\mathbf{z}}}[\rho_{\bar{\mathbf{z}}}^{\bar{n}}], \mathop{\mathbb{E}}_{\bar{\mathbf{z}}}[(\rho_{\bar{\mathbf{z}}}^{\bar{1}})^{\otimes n}]) \leqslant \mathop{\mathbb{E}}_{\bar{\mathbf{z}}}[\delta(\rho_{\bar{\mathbf{z}}}^{\bar{n}}, (\rho_{\bar{\mathbf{z}}}^{\bar{1}})^{\otimes n})]. \tag{35}$$

Inequality (34) then follows directly from Theorem VI.1. □

While this result is of interest in its own right, we point out that taking the limit $s \to \infty$ directly gives the well-known quantum de Finetti representation for *infinitely* exchangeable quantum states,[13] thus providing yet another new (compare Ref. 4) and conceptually simple proof.

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APPENDIX: MARKOV-STYLE VERSION OF THEOREM VI.1

While Theorem VI.1 provides a bound on the expected distance between the conditional state $\rho_{\bar{\mathbf{z}}}^{A\bar{n}}$ and the product state $\rho_{\bar{\mathbf{z}}}^{A} \otimes (\rho_{\bar{\mathbf{z}}}^{\bar{1}})^{\otimes n}$, Theorem A.1 below gives an expression for the minimum probability such that this distance is smaller than some given value.

Theorem A.1: *Let* $\rho^{A\overline{n+k}} \in S(\mathcal{H}_A \otimes \mathcal{H}^{\otimes n+k})$ *be* $(n+2k-1)$*-exchangeable relative to* $\mathcal{H}_A$ *and let* $\mathfrak{Z}=\{F_z\}_{z\in\mathcal{Z}}$ *be a POVM on* $\mathcal{H}$ *with* $|\mathcal{Z}|=t$. *For every* $\bar{\mathbf{z}} \in \mathcal{Z}^k$, *let* $\rho_{\bar{\mathbf{z}}}^{A\bar{n}} := \rho^{A\bar{n}}_{|\mathfrak{Z}^k=\bar{\mathbf{z}}}$. Then, for all $\lambda \geqslant 0$, *and for* $\bar{\mathbf{z}} \leftarrow \rho_{\bar{\mathfrak{Z}}^k}^{\bar{k}}$, *with probability at least* $1-2ke^{-\lambda^2/8}$,

$$\delta(\rho_{\bar{\mathbf{z}}}^{A\bar{n}}, \rho_{\bar{\mathbf{z}}}^{A} \otimes (\rho_{\bar{\mathbf{z}}}^{\bar{1}})^{\otimes n}) < \frac{n\lambda}{\sqrt{k}} C_2(\mathfrak{Z})$$

and

$$\delta(\rho_{\bar{\mathfrak{Z}}|\mathfrak{Z}^k=\bar{\mathbf{z}}}^{\bar{1}}, Q_{\bar{\mathbf{z}}}) < \sqrt{\frac{t}{k}}\lambda.$$

The proof of this theorem essentially follows the lines of the proof of Theorem VI.1. The main difference is that Lemma IV.2 is replaced by a statement based on a tail inequality due to Hoeffding[10] which applies to hypergeometric distributions as defined below (for more details, see, e.g., Ref. 14).

Definition A.2: The hypergeometric distribution $\mathrm{Hyp}(n,m,k)$ *with parameters* n, m, and k *is defined as the probability distribution of the random variable* $S := |\Gamma \cap [m]|$ *where* Γ *is a randomly chosen subset of* $[n]$ *of size* $|\Gamma|=k$.

Lemma A.3. Hoeffding: Let S *be a random variable with* $P_S=\mathrm{Hyp}(n,m,k)$. *Then, for all* $\ell \geqslant 0$,

$$\mathop{\mathbb{P}}_{s}\left[s \leqslant k\frac{m}{n} - \ell \right] \leqslant e^{-\ell^2 n/2km}.$$

Lemma A.4 and Lemma A.5 are adapted versions of Lemma IV.2 and Lemma IV.3, proven in Sec. IV A and Sec. IV B, respectively.

Lemma A.4: Let $\mathbf{Z}$ *be an n-tuple and* $\overline{\mathbf{Z}}$ *a k-tuple of random variables over a set* $\mathcal{Z}$ *of size* $|\mathcal{Z}|=t$ *such that* $P_{(\mathbf{Z},\overline{\mathbf{Z}})}$ *is symmetric. Then, for any* $\varepsilon \geqslant 0$ *and for* $(\mathbf{z},\overline{\mathbf{z}}) \leftarrow P_{(\mathbf{Z},\overline{\mathbf{Z}})}$,

$$\mathop{\mathbb{P}}_{(\mathbf{z},\overline{\mathbf{z}})}[\delta(Q_{\overline{\mathbf{z}}},Q_{(\overline{\mathbf{z}},\mathbf{z})}) \geqslant \varepsilon] \leqslant te^{-k\varepsilon^2/2t}.$$

Proof: It suffices to show that, for all probability distributions $q \in \mathrm{Distr}(\mathcal{Z})$,

$$\mathop{\mathbb{P}}_{\overline{\mathbf{z}}\leftarrow P_{\overline{\mathbf{Z}}|Q_{(\mathbf{Z},\overline{\mathbf{Z}})}=q}}[\delta(Q_{\overline{\mathbf{z}}},q) \geqslant \varepsilon] \leqslant te^{-k\varepsilon^2/2t}. \tag{A1}$$

The assertion of the lemma then follows from

$$\mathop{\mathbb{P}}_{(\mathbf{z},\overline{\mathbf{z}})\leftarrow P_{(\mathbf{Z},\overline{\mathbf{Z}})}}[\delta(Q_{\overline{\mathbf{z}}},Q_{(\mathbf{z},\overline{\mathbf{z}})}) \geqslant \varepsilon] = \mathop{\mathbb{E}}_{q\leftarrow P_{Q_{(\mathbf{Z},\overline{\mathbf{Z}})}}}\Big[\mathop{\mathbb{P}}_{\overline{\mathbf{z}}\leftarrow P_{\overline{\mathbf{Z}}|Q_{(\mathbf{Z},\overline{\mathbf{Z}})}=q}}[\delta(Q_{\overline{\mathbf{z}}},q) \geqslant \varepsilon]\Big].$$

Let thus $q \in \mathrm{Distr}(\mathcal{Z})$ with $P_{Q_{(\mathbf{Z},\overline{\mathbf{Z}})}}(q)>0$ be fixed. The variational distance between $Q_{\overline{\mathbf{z}}}$ and q can be written as

$$\delta(Q_{\overline{\mathbf{z}}},q) = \sum_{z\in\mathcal{Z}'} \max(q(z) - Q_{\overline{\mathbf{z}}}(z),0), \tag{A2}$$

where $\mathcal{Z}' := \{z \in \mathcal{Z}: q(z)>0\}$. It is easy to see that, for any $z \in \mathcal{Z}$, the random variable $S_z := k \cdot Q_{\overline{\mathbf{Z}}}(z)$, conditioned on the event $Q_{(\mathbf{Z},\overline{\mathbf{Z}})}=q$, is distributed according to $\mathrm{Hyp}(n+k,(n+k)q(z),k)$. For any $z \in \mathcal{Z}'$, let $\varepsilon_z := \varepsilon\sqrt{q(z)/t}$. Lemma A.3 (with $\ell = k\varepsilon_z$) then implies

$$\mathop{\mathbb{P}}_{\overline{\mathbf{z}}\leftarrow P_{\overline{\mathbf{Z}}|Q_{(\mathbf{Z},\overline{\mathbf{Z}})}=q}}[q(z) - Q_{\overline{\mathbf{z}}}(z) \geqslant \varepsilon_z] \leqslant e^{-k\varepsilon_z^2/2q(z)} = e^{-k\varepsilon^2/2t},$$

and thus, using the union bound,

$$\mathop{\mathbb{P}}_{\overline{\mathbf{z}}\leftarrow P_{\overline{\mathbf{Z}}|Q_{(\mathbf{Z},\overline{\mathbf{Z}})}=q}}\left[\forall z \in \mathcal{Z}': q(z) - Q_{\overline{\mathbf{Z}}}(z) < \varepsilon\sqrt{\frac{q(z)}{t}}\right] \geqslant 1 - te^{k\varepsilon^2/2t}. \tag{A3}$$

Since, by the Cauchy-Schwartz inequality,

$$\sum_{z\in\mathcal{Z}'} \varepsilon\sqrt{\frac{q(z)}{t}} \leqslant \varepsilon,$$

the event in (A3) implies that the sum on the rhs of (A2) is smaller than ε, that is, $\delta(Q_{\overline{\mathbf{z}}},q)<\varepsilon$. Inequality (A1) thus follows directly from the bound (A3). □

Lemma A.5: Let $\mathbf{Z}$ *be an n-tuple and* $\overline{\mathbf{Z}}$ *a k-tuple of random variables over a set* $\mathcal{Z}$ *of size* $|\mathcal{Z}|=t$, *for* $k \leqslant n$, *such that* $P_{(\mathbf{Z},\overline{\mathbf{Z}})}$ *is symmetric. Then, for all* $\varepsilon \geqslant 0$ *and for* $\overline{\mathbf{z}} \leftarrow P_{\overline{\mathbf{Z}}}$,

$$\mathop{\mathbb{P}}_{\overline{\mathbf{z}}}[D_{Q_{\overline{\mathbf{z}}}}(P_{\mathbf{Z}|\overline{\mathbf{Z}}=\overline{\mathbf{z}}}) \geqslant \varepsilon] \leqslant 2ke^{-k\varepsilon^2/8t}.$$

Proof: Let $\tau := t/k$ and $\bar{\varepsilon} := \varepsilon - \tau$. Note that, if $\varepsilon \leqslant \tau$, the rhs of the inequality in the lemma becomes larger than 1 because $\varepsilon \leqslant 1$, i.e., the assertion is trivially true. Thus we can assume that $\bar{\varepsilon}>0$. For all $\overline{\mathbf{z}} \in \mathcal{Z}^k$, let

$$p_{\overline{\mathbf{z}}} := \mathop{\mathbb{P}}_{\mathbf{z}\leftarrow P_{\mathbf{Z}|\overline{\mathbf{Z}}=\overline{\mathbf{z}}}}[\delta(Q_{\mathbf{z}},Q_{\overline{\mathbf{z}}}) \geqslant \bar{\varepsilon}].$$

We then have, by Lemma A.4 and Lemma IV.1,

$$\mathop{\mathbb{E}}_{\bar{\mathbf{z}}\leftarrow P_{\bar{\mathbf{Z}}}}[p_{\bar{\mathbf{z}}}] = \mathop{\mathbb{P}}_{(\mathbf{z},\bar{\mathbf{z}})\leftarrow P_{(\mathbf{Z},\bar{\mathbf{Z}})}}[\delta(Q_{\mathbf{z}},Q_{\bar{\mathbf{z}}}) \geqslant \bar{\varepsilon}] \leqslant \mathop{\mathbb{P}}_{(\mathbf{z},\bar{\mathbf{z}})\leftarrow P_{(\mathbf{Z},\bar{\mathbf{Z}})}}\left[\delta(Q_{\bar{\mathbf{z}}},Q_{(\mathbf{z},\bar{\mathbf{z}})}) \geqslant \frac{\bar{\varepsilon}}{2}\right] \leqslant te^{-k\bar{\varepsilon}^2/8t},$$

and, by Markov's inequality,

$$\mathop{\mathbb{P}}_{\bar{\mathbf{z}}\leftarrow P_{\bar{\mathbf{Z}}}}[p_{\bar{\mathbf{z}}} \geqslant \tau] \leqslant \frac{t}{\tau}e^{-k\bar{\varepsilon}^2/8t}. \tag{A4}$$

With the definition

$$\Lambda := \{\bar{\mathbf{z}} \in \mathcal{Z}^k : p_{\bar{\mathbf{z}}} < \tau\},$$

the bound (A4) can be rewritten as

$$\mathop{\mathbb{P}}_{\bar{\mathbf{z}}\leftarrow P_{\bar{\mathbf{Z}}}}[\bar{\mathbf{z}} \notin \Lambda] \leqslant \frac{t}{\tau}e^{-k\bar{\varepsilon}^2/8t} \leqslant 2ke^{-k\varepsilon^2/8t},$$

where the second inequality follows from the observation that $\bar{\varepsilon}^2=(\varepsilon-\tau)^2 \geqslant \varepsilon^2-2\tau$ and $\tau=t/k$.

It thus remains to be shown that, for any $\bar{\mathbf{z}} \in \Lambda$,

$$D_{Q_{\bar{\mathbf{z}}}}(P_{\mathbf{Z}|\bar{\mathbf{Z}}=\bar{\mathbf{z}}}) = \mathop{\mathbb{E}}_{\mathbf{z}\leftarrow P_{\mathbf{Z}|\bar{\mathbf{Z}}=\bar{\mathbf{z}}}}[\delta(Q_{\mathbf{z}},Q_{\bar{\mathbf{z}}})] < \varepsilon. \tag{A5}$$

Let thus $\bar{\mathbf{z}} \in \Lambda$ be fixed. Then

$$\mathop{\mathbb{E}}_{\mathbf{z}\leftarrow P_{\mathbf{Z}|\bar{\mathbf{Z}}=\bar{\mathbf{z}}}}[\delta(Q_{\mathbf{z}},Q_{\bar{\mathbf{z}}})] = \sum_{\substack{\mathbf{z}\in\mathcal{Z}^n \\ \delta(Q_{\mathbf{z}},Q_{\bar{\mathbf{z}}})<\bar{\varepsilon}}} P_{\mathbf{Z}|\bar{\mathbf{Z}}=\bar{\mathbf{z}}}(\mathbf{z})\,\delta(Q_{\mathbf{z}},Q_{\bar{\mathbf{z}}}) + \sum_{\substack{\mathbf{z}\in\mathcal{Z}^n \\ \delta(Q_{\mathbf{z}},Q_{\bar{\mathbf{z}}})\geqslant\bar{\varepsilon}}} P_{\mathbf{Z}|\bar{\mathbf{Z}}=\bar{\mathbf{z}}}(\mathbf{z})\,\delta(Q_{\mathbf{z}},Q_{\bar{\mathbf{z}}}) < \bar{\varepsilon} + p_{\bar{\mathbf{z}}}$$

from which the bound (A5) follows by the definition of Λ and $\bar{\varepsilon}+\tau=\varepsilon$. □

Finally, using Lemma A.5, we directly obtain Lemma A.6 below which corresponds to Lemma A.7 of Sec. V B.

Lemma A.6: Let $\rho^{\overline{n+k}} \in S(\mathcal{H}^{\otimes n+k})$, *for* $k \leqslant n$, *be symmetric and let* $\mathfrak{Z}=\{F_z\}_{z\in\mathcal{Z}}$ *be a POVM on* $\mathcal{H}$ *with* $|\mathcal{Z}|=t$. *Then, for all* $\varepsilon \geqslant 0$ *and for* $\bar{\mathbf{z}} \leftarrow \rho_{\mathfrak{Z}^k}^{\bar{k}}$,

$$\mathop{\mathbb{P}}_{\bar{\mathbf{z}}}[D_{Q_{\bar{\mathbf{z}}}}(\rho_{\mathfrak{Z}^n|\mathfrak{Z}^k=\bar{\mathbf{z}}}^{\bar{n}}) \geqslant \varepsilon] \leqslant 2ke^{-k\varepsilon^2/8t}.$$

The proof of Theorem A.1 is now similar to the proof of Theorem VI.1, where, instead of Lemma V.7, Lemma A.6 is used to bound the rhs of (32) and (33).

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Non-Abelian Chern-Simons action is topological invariant on 3 simple knot

Tieyan Si[a)]
Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing, 100080, China

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Under SU(2) gauge transformation, the non-Abelian Chern-Simons action is invariant on a class of three dimensional manifold—3 simple knot. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2137721]

I. INTRODUCTION

The Chern-Simons gauge theory provides a topological field theoretic framework for the study of knots and links in a given three manifold.[1,2] It was Schwarz who first conjectured[3] that the now famous Jones polynomial[4] may be related to Chern-Simons theory. Witten in his pioneering paper[5] set up the general framework to study knots and links through Chern-Simons field theories. Wilson loop operators are the topological operators of this theory. Expectation value of these operators are the topological invariants for knots and links. It is well known that the Abelian Chern-Simons action

$$I = \frac{1}{4\pi}\int_M A \wedge F = \frac{1}{8\pi}\int_M \epsilon^{ijk} A_i F_{jk} d^3x \tag{1}$$

is the topological invariant on one-dimensional knots.[5,6] As for the non-Abelian Chern-Simons action

$$\Omega = \frac{1}{8\pi^2}\,\mathrm{Tr}\left(A \wedge F - \frac{2}{3} A \wedge A \wedge A\right), \tag{2}$$

although mathematical development suggests that the link invariants provide a method of obtaining topological invariants for three-manifold,[7,8] there is still no work which can give the relation between the non-Abelian Chern-Simons action and 3-knot manifold (it is three-dimensional knot, and is totally different from the knots in Jones polynomial and in the mathematical method mentioned above).

The 3-knot has a very important application in modern physics. According to the closed universe model, our universe can also be treated as a 3-sphere in modern cosmology theory, since our universe is viewed as embedding in a higher dimensional world, in which, the observed elementary particles are the light particles trapped on the $(3+1)$-dimensional defect. Since the 3-sphere S^3 is the most trivial 3-knot, it is natural to generalize the closed and oriented manifold which are homeomorphic to S^3. This may provide us with insight into modern cosmology.

In knot theory, a knotted (closed, oriented) n-manifold M, i.e., n-knot is a smoothly embedded n-sphere in S^{n+2}, $K=f(S^n)\subset S^{n+2}$. Obviously the 3-knot is a knotted three-dimensional manifold $M=f(S^3)\subset S^5$. It is well known that every classical knot bounds a compact orientable surface, known as a Seifert surface for the knot.[9] A Seifert surface for a 3-knot K is defined to be a compact orientable four-manifold W in S^5, such that

[a)]Electronic mail: sity@itp.ac.cn

$$\partial W = K. \tag{3}$$

The simple n-knots[10] are those for which $\pi_i(\overline{X})=0$ (Ref. 11) for $i<m$ with $n=2m$ or $n=2m-1$.

On the mathematical side, odd dimensional simple knots have a tendency to look like classical knots. We will show that the non-Abelian Chern-Simons action is invariant under SU(2) gauge transformation on the simple 3-knot, just like the Abelian Chern-Simons action which is invariant on one-dimensional knots under U(1) transformation.[6]

Our discussion is based on Levine's theorem,[10] which states, for any simple knot $K\subset S^{2m+1}$, with a $(m-1)$-connected Seifert surface W, as dim $W=2m$ the only nontrivial homology group of W is $H_m(W)$, where the coefficient is integer.

Applying this theorem to 3-knot, for which $m=2$, we arrive that the only nontrivial homology group of Seifert surface W of 3-knot is $H_2(W.z)$. Therefore, we have $H_4(W.z)=\emptyset$.

If we denote the non-Abelian Chern-Simons action under SU(2) gauge transformation as Ω^S, we arrive at the quantity $I=\Omega^S-\Omega$ which appeared in the many topological field theory.[12] As pointed out by many physicists, this quantity just represents the second Chern number C_2.[12] While according to the characteristic class theory, the nonzero Chern class must follow[12]

$$C_i(p) \in H^{2i}(M), \tag{4}$$

this immediately leads to $C_2(p)\in H^4(W)$. As we know, on the Seifert surface W of 3-knot, $H_4(W.z)=\emptyset$. Recall the De Rahm cohomology theory,[13] the cohomology groups $H^4(W)$ are isomorphic to homology groups $H_4(W)$, so we have $C_2(p)=0$. It means $\Omega^S-\Omega=0$, therefore the non-Abelian Chern-Simons action is an invariant under gauge transformation. It must be pointed out here that this conclusion only holds for a special class of knot—3 simple knot, which is defined by Levine.[10]

In the following we will present a more exhaustive discussion.

II. THE NON-ABELIAN CHERN-SIMONS IS AN INVARIANT ON 3 SIMPLE KNOT

Under SU(2) gauge transformation, the non-Abelian Chern-Simons action,

$$I = \int \Omega = \frac{1}{8\pi^2}\int_K \mathrm{Tr}\left(A\wedge \mathrm{d}A - \frac{2}{3}A\wedge A\wedge A\right) \tag{5}$$

can be denoted as

$$I^s = \frac{1}{8\pi^2}\int_K \mathrm{Tr}\left(A^s\wedge F^s + \frac{1}{3}A^s\wedge A^s\wedge A^s\right), \tag{6}$$

in which $A^s=SAS^{-1}+\mathrm{d}S\,S^{-1}$ and $F^s=SFS^{-1}$, S is an element of SU(2). After some algebra, one can arrive at[12]

$$I^s - I = \frac{1}{24\pi^2}\int_K \mathrm{Tr}[\mathrm{d}S\,S^{-1}\wedge \mathrm{d}S\,S^{-1}\wedge \mathrm{d}S\,S^{-1}]. \tag{7}$$

Here K is a 3 simple knot. It is well known that the right-hand side of Eq. (7) just represents the second Chern class which describes the winding number of the manifold.

Since $S\in$ SU(2) and Spin(3) is homeomorphic to SU(2), we can replace S with an element of Spin(3); n; it can be expressed in terms of Clifford algebra[14] as $n=n^a\tau_a$ $(a=0,1,2,3)$, where $\tau=(I,i\vec{\sigma})$, $\tau^\dagger=(I,-i\vec{\sigma})$ with $\vec{\sigma}$ denotes the Pauli matrices. It is easily seen that n is just the element of Spin(3) in terms of geometric algebra. Obviously $nn^\dagger=1$, from the formula $n^\dagger\,\mathrm{d}n=-\mathrm{d}n^\dagger\,n$, Eq. (7) can be written as

$$I^s - I = -\frac{1}{24\pi^2}\int_K \mathrm{Tr}[\mathrm{d}n \wedge \mathrm{d}n^\dagger \wedge \mathrm{d}n\, n^\dagger]. \tag{8}$$

Considering $\partial W = K$, following Duan's work on second Chern class,[15] it can be proved that

$$C_2 = I^s - I = \frac{1}{24\pi^2}\int_W \mathrm{Tr}[\mathrm{d}n \wedge \mathrm{d}n^\dagger \wedge \mathrm{d}n \wedge \mathrm{d}n^\dagger]. \tag{9}$$

Now we see, for the non-Abelian Chern-Simons action on a 3 simple knot, after the SU(2) gauge transformation, it becomes $I^s = I + C_2$, where C_2 is the second Chern number on the Seifert surface W of the 3 simple knot.

It will be shown in the following that, the second Chern number on the Seifert surface W of the 3 simple knot is zero. This conclusion can be deduced from Levine's theorem.[10] For any simple knot $K \subset S^{2m+1}$, a $(m-1)$-connected Seifert surface W, as $\dim W = 2m$ the only nontrivial homology group of W is $H_m(W)$, where the coefficient is integer.

For 3 knot, $m=2$. Levine's theorem suggests the only nontrivial homology group of the Seifert surface of a 3 simple knot $H_2(W.z)$. The other homology group must be empty, then $H_4(W.z) = \emptyset$.

Recall the De Rahm cohomology theory,[13] the cohomology groups are isomorphic to homology groups, i.e.,

$$b^k = \dim H^k(M) = b_k = \dim H_k(M), \tag{10}$$

where $b^k = \dim H^k(M)$ is the co-Betti number, and $b_k = \dim H_k(M)$ is the Betti number. From $H_4(W.z) = \emptyset$ and (10), one sees that

$$b^4 = \dim H^4(W) = \dim H_4(W) = 0. \tag{11}$$

According to the characteristic class theory, the possible nonzero Chern class must follow[12]

$$C_i(p) \in H^{2i}(M). \tag{12}$$

For the second Chern class C_2, we have $C_2(p) \in H^4(W)$. Considering Eq. (11), we arrive at

$$C_2(p) = 0. \tag{13}$$

So the second Chern number on the 3-knot's Seifert surface is

$$I^s - I = 0. \tag{14}$$

Therefore, the non-Abelian Chern-Simons action is invariant over 3-knot. In fact, according to Duan's ϕ-mapping topological current theory, it is easy to prove that[15] $C_2(p) = \Sigma_{\alpha=1}^{l} W_\alpha$, where W_α is the winding number around instantons in space-time; this may provide us with a deep understanding of the 3-brane world theory.[16]

Now we can conclude that the non-Abelian Chern-Simons action is invariant under SU(2) gauge transformation over a 3 simple knot.

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[11] Let N be an open tubular neighborhood of K and set $X=S^5-N$, If V is radial inside N and $W=V\cap X$, Let Y be the manifold with boundary obtained by cutting X along W. Let $Y_i(i\in Z)$ be a collection of copies of Y, then $\overline{X}$ is the quotient of the disjoint union $\cup Y_i|_{i\in Z}$ by the obvious identification of W_- and W_+.
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On Chern-Simons theory with an inhomogeneous gauge group and BF theory knot invariants

Gad Naot[a)]
Department of Mathematics, University of Toronto, Toronto, Ontario, Canada M5S2E4

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We study the Chern-Simons topological quantum field theory with an inhomogeneous gauge group, a non-semi-simple group obtained from a semisimple one by taking its semidirect product with its Lie algebra. We find that the standard knot observable (i.e., trace of the holonomy along the knot) essentially vanishes, and yet, the non-semi-simplicity of the gauge group allows us to consider a class of unorthodox observables which breaks gauge invariance at one point and leads to a nontrivial theory on long knots in $\mathbb{R}^3$. We have two main morals. (1) In the non-semi-simple case there is more to observe in Chern-Simons theory. There might be other interesting non-semi-simple gauge groups to study in this context beyond our example. (2) In the case of an inhomogeneous gauge group, we find that Chern-Simons theory with the unorthodox observable is actually the same as three-dimensional BF theory with the Cattaneo-Cotta-Ramusino-Martellini knot observable. This leads to a simplification of their results and enables us to generalize and solve a problem they posed regarding the relation between BF theory and the Alexander-Conway polynomial. We prove that the most general knot invariant coming from pure BF topological quantum field theory is in the algebra generated by the coefficients of the Alexander-Conway polynomial. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2146190]

I. INTRODUCTION

We would like to address the question of the most general knot invariant coming from BF topological quantum field theory (TQFT). In the mid-1990s, Cattaneo *et al.*[9–12] showed that while BF theory with cosmological constant produces the same invariants of knots as the Chern-Simons (CS) theory, the BF theory with no cosmological constant (pure BF theory) and SU(2) gauge group produces invariants that lie in the algebra generated by the coefficients of the Alexander-Conway polynomial. The BF TQFT is completely equivalent to CS theory, however, while the equivalence with nonzero cosmological constant maintains the semisimplicity property of the gauge group, the equivalence when the cosmological constant is set to zero shifts us to a CS theory with a non-semi-simple gauge group. Thus, starting with a gauge group G in the pure BF theory we end up on the CS side with a semidirect product of the group with its Lie algebra $G \ltimes \mathcal{G}$, also known as the inhomogeneous group of G (denoted IG). Eventually, the question we want to address is as follows: *What is the most general knot invariant (or knot observable) in a CS theory with an inhomogeneous gauge group*?

The natural thing to begin with is the standard gauge invariant observable, the trace of the holonomy of the gauge connection along the knot, in some chosen representation. As we shall see in Sec. II, this observable gives us no information regarding the knot (except for framing information that can be normalized to zero anyway). This fact seems to pose a contradiction since in

[a)]Electronic mail: gnaot@math.toronto.edu

the equivalent pure BF theory one can extract some nontrivial information regarding the knot [at least in the case of SU(2) gauge]. Therefore, there must be a procedure that will give us nontrivial information regarding the knot in this setting.

In this paper we will introduce the following procedure (Sec. III A): We take an observable which is not gauge invariant at one single point on the knot (holonomy along the knot without the trace). By doing that, we get a CS theory on S^3 with broken gauge symmetry at one point on the knot. Then, we declare this point to be infinity by taking the point out of our space (i.e., puncturing S^3 at that point). Since the gauge transformations are taken to vanish at infinity, we get a completely invariant CS theory on $\mathbb{R}^3$ with a long knot embedded in it. Since knot theory in S^3 and long knot theory in $\mathbb{R}^3$ are "isomorphic" theories we lose no information as far as knot theory is concerned and we get "legal" CS theory in which we can consider a new and wider class of observables.

Using perturbation theory, we will show that our observable gives nontrivial information about the knot (Sec. III B). Continuing with perturbation theory in our setting (CS with IG gauge group and the new observable) we will be able to prove that the most general knot invariant coming from such a construction is in the algebra generated by the coefficients of the Alexander-Conway polynomial (Sec. III C). Returning to BF theory (Chap. IV) we will create an observable that reproduces the Cattaneo *et al.* result for SU(2) and generalize it to every metrizable gauge group and representation thereof used in the construction of the pure BF theory.

Our construction detects, in some sense, the difference between the invariant subspace of the universal enveloping algebra of the non-semi-simple gauge group and the coinvariant quotient of the universal enveloping algebra. This enables us to extract nontrivial information regarding the knot (a difference which does not exist in the semisimple case). We discuss this issue in Chap. V.

II. PERTURBATION THEORY FOR THE STANDARD OBSERVABLE WITH AN INHOMOGENEOUS GAUGE GROUP

In this section we will show that the perturbation theory of Chern-Simons (CS) theory with an inhomogeneous gauge group and the standard knot observable is almost trivial. We start (2.1) with some reminders about perturbation theory (in CS context). Unfortunately, due to the size of the topic this reminder is not meant to teach the theory. For recent detailed pedagogic reviews see Refs. 19 and 18. This will be followed by introduction of the inhomogeneous gauge group and our notations for it (Sec. II B). We continue with giving more details about perturbation theory using this gauge group (Sec. II C). Section II C will describe the consequences of using such a gauge group on the knot invariants coming from the standard observable. Finally, in Sec. II D, we will show that the standard construction in this setting is trivial, leading to (almost) trivial knot invariants.

A. Some reminders about perturbation theory and Chern-Simons theory

We recall the setting for knot invariants in the framework of CS theory (in this section a knot is an embedding of S^1 into S^3). We take S^3 to be the three-dimensional manifold on which the CS theory is defined. We choose any gauge group G whose Lie algebra is metrizable (e.g., semisimple gauge group). Denote the metric on the Lie algebra by $\langle,\rangle$ and let A be a G-connection. We consider the following action functional:

$$\text{Chern - Simons action } \mathrm{CS}(A) = k \cdot 2\pi \int_{S^3} \left\langle A \wedge \mathrm{d}A + \frac{2}{3} A \wedge A \wedge A \right\rangle,$$

where k is a coupling constant which satisfies a quantization condition (e.g., for semisimple gauge groups it must be an integer). In what follows, however, we will work perturbatively with formal power series in k^{-1}.

Now, recall the standard knot observable, $\mathrm{Tr}_R\,\mathrm{hol}(A)$ where $\mathrm{hol}(A)$ stands for the holonomy of the connection A along the knot (the path-ordered exponent of the integral of A along the knot) and the trace is taken in some chosen representation R of the gauge group.

One obtains a knot invariant by taking the path integral over all connections with the observable plugged into the integrand,

$$Z(\text{knot}) = \int \mathcal{D}\mathcal{A} e^{i\text{CS}(A)} \operatorname{Tr}_R \operatorname{hol}(A).$$

This integral is usually referred to as the expectation value of the standard observable and it is viewed as a function from knots to the base field (the complex numbers from now on). One is usually interested in $Z(\text{knot})/Z(\emptyset)$, where $Z(\emptyset)$ is the path integral with no observable plugged in (no knot).

Calculating the integral using perturbation theory we get the following sum:

$$\sum_{D \in D_{\text{CS}}} k^{-\deg D} \cdot \zeta^{\text{CS}}(D) \cdot W_{\mathcal{G}}(D),$$

where D_{CS} is defined to be the set of all trivalent connected graphs based on S^1 (Feynman diagrams based on a Wilson loop), ζ^{CS} is the integration of the corresponding propagators over the diagram (that is, the integration over the appropriate configuration space) and $W_{\mathcal{G}}$ is the Lie-algebraic part of the expectation value which holds all the information coming from the Lie group G and its representation R (that is, the weight system, reviewed quickly below).

In the CS perturbation theory calculation, every internal edge contributes $1/k$ and every internal vertex contributes k to the total power of k of the diagram (recall that an internal edge/vertex is an edge/vertex which is not on the Wilson loop). The total power of $1/k$ is called the *degree* of the diagram. A convenient way of counting the degree is labeling each internal vertex with -1 and each edge with $+1$ and then summing all the labels to get the degree of the diagram. This number is denoted $\deg D$.

We want to factorize the perturbation theory calculation in order to get a better hold on the above knot invariant. As a first step, we can drop the weight system and replace it with the diagram D on which it is calculated. We get the following invariant:

$$\sum_{D \in D_{\text{CS}}} k^{-\deg D} \cdot \zeta^{\text{CS}}(D) \cdot D.$$

This invariant is viewed as taking values in $\mathcal{A}(S^1)$, where we define $\mathcal{A}(S^1)$ as follows.

Definition 2.1: $\mathcal{A}(S^1)$ is the algebra of all connected trivalent graphs based on a circle (i.e., D_{CS}) quotient by the IHX relation

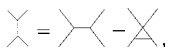

the STU relation

and the antisymmetry relation

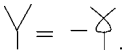

When we apply the weight system $W_{\mathcal{G}}$ to this invariant we get the first sum. Next we will apply the weight system by parts, in order to get a further factorization.

Weight systems are described and explored in Ref. 6. We recall the main construction of a weight system coming from a Lie algebra, which includes three parts, labeling, contracting, and the trace part. In the labeling part, after choosing a basis for the Lie algebra, one labels each internal edge of a given diagram (i.e., edges that are not contained in the base circle) with a different index on each end of the edge. In the second part, one writes the structure constants

tensor for each internal vertex and the metric tensor for each internal edge (using the indices on these vertices/edges and the chosen basis) and proceeds to contract matching indices (using the metric to raise and lower indices). At that point, one is left with an invariant tensor in the enveloping algebra of $\mathcal{G}$ whose indices are the ones on the vertices on the base loop. In the final part, the trace part, one represents this tensor using a chosen representation of $\mathcal{G}$ and takes the trace. This concludes the construction of the weight system.

Taking a diagram (more precisely a class representative but we will not make these distinctions throughout the paper) in $\mathcal{A}(S^1)$ and applying to it the labeling and contracting parts of the weight system gives us a tensor in the universal enveloping algebra. This tensor is invariant under the adjoint action (all the tensors used in building it are invariant under the action and contractions are $\mathcal{G}$-maps) and therefore it is in the invariant subspace of the universal enveloping algebra $U(\mathcal{G})^{\mathcal{G}}$. Although we did not apply the trace part of the weight system yet, we still have a trace of the trace that appears in the standard observable we started with, which comes about diagrammatically in the fact that we are looking at diagrams based on S^1. The ability to move legs around cyclically (which is the trace property) forces us to quotient the resulting tensor in $U(\mathcal{G})^{\mathcal{G}}$ into the coinvariant quotient of the algebra, thus getting an invariant in $(U(\mathcal{G})^{\mathcal{G}})_{\mathcal{G}}$. Finally, one can apply the trace part to get elements of $\mathbb{C}$.

To summarize, when we use perturbation theory for the standard observable, we get a knot invariant in the form of a series (in $1/k$) with coefficients in $\mathbb{C}$, which factorize in the following way:

$$\{\text{knots}\} \to \mathcal{A}(S^1)[[k^{-1}]] \to (U(\mathcal{G})^{\mathcal{G}})_{\mathcal{G}}[[k^{-1}]] \to \mathbb{C}[[k^{-1}]]. \tag{1}$$

Although there is much more to say about Chern-Simons theory and the use of perturbation theory in this context, we will stop at this point. We recommend Refs. 5, 4, 3, 2, 1, and 15 for various approaches (physically and/or mathematically inclined) in addition to the reviews cited above. The fact that we actually get a knot invariant in every step of the factorization above is an example of an important issue which we completely ignored here.

B. The inhomogeneous gauge group

We now present a specific type of gauge group that we wish to focus on in the context of perturbation theory of CS theory.

Start with a semisimple gauge group G and take a semidirect product of it with its Lie algebra (the semidirect action is the adjoint action). Look at the Lie algebra of this semidirect product and denote it L_0. As a vector space, L_0 is a double copy of the original algebra, $\mathcal{G} \oplus \bar{\mathcal{G}}$, where we use upper bar notation to distinguish the second copy. For any $X \in \mathcal{G}$ let $X \mapsto \bar{X}$ be the identity map between the two copies. Thus $\bar{X}$ is the element X in the second copy of $\mathcal{G}$. Let X_i be a basis for $\mathcal{G}$, $\overline{X_i}$ the corresponding basis for $\bar{\mathcal{G}}$ and $[.,.]$ the original bracket structure on $\mathcal{G}$. We have the following bracket structure on L_0:

$$[X_i, X_j]_{L_0} = [X_i, X_j], \quad [X_i, \overline{X_j}]_{L_0} = \overline{[X_i, X_j]}, \quad [\overline{X_i}, \overline{X_j}]_{L_0} = 0.$$

We see now that the second copy is the Abelianization of the original algebra.

Letting the metric on $\mathcal{G}$ be $\langle , \rangle$ (the one coming from the trace of the adjoint representation, say) we take the following (invariant) metric on L_0:

$$\langle X_i, X_j \rangle_{L_0} = 0 = \langle \overline{X_i}, \overline{X_j} \rangle_{L_0}, \quad \langle X_i, \overline{X_j} \rangle_{L_0} = \langle X_i, X_j \rangle.$$

C. The structure of the perturbation theory expansion with the inhomogeneous gauge group

Let us look at the perturbation theory expansion using the inhomogeneous gauge group L_0. As we will show, the factorization (1) factors even further as the weight system using this type of Lie algebra is more refined. We will define the space of directed "legal" diagrams and construct a factorization of the weight system W_{L_0} through a map into it.

As known from standard perturbation theory of quantum gauge theories, the algebraic contributions of vertices and edges in a Feynman diagram are determined by the structure constants and the metric on the Lie algebra. These contributions are encoded in the weight system, as described earlier.

Given a diagram, choose a basis X_i to $\mathcal{G}$, take the corresponding basis $\overline{X_i}$ to $\bar{\mathcal{G}}$ (obtaining a basis to the entire algebra) and apply the weight system using the following steps.

1(pre). Sum over all the ways of labeling the ends of the edges of the diagram with different indices i and $\bar{i}$ representing the basis for $\mathcal{G}$ and $\bar{\mathcal{G}}$, respectively. Therefore, instead of labeling with one type of indices running over the entire basis of the algebra, label with two types of indices, each running over one summand in the direct sum that forms the algebra.

2(pre). Write the structure constants tensor and the metric tensor (as before) with indices according to the labeling, and contract the matching indices [thus in each summand of step 1(pre) only a part of the algebra basis is contracted].

Since the summations are finite, one can see that this way of applying the labeling and contraction parts of the weight system (i.e., in two summation steps having two types of algebra indices instead of one) is equivalent to the usual way of applying the weight system.

Furthermore, we know that certain combinations of indices vanish in the second step. By looking at the metric we observe that the only edges which are nonzero are the ones that have a nonbar index on one end and a bar index at the other end. By looking at the bracket structure we observe that the only combination of indices on a vertex that will not be zero at step 2(pre) is a combination of two nonbar indices and one bar index. This allows us to revise step 1(pre) above into the following.

1(revised). Sum over all ways of labeling the ends of the edges of the diagram with indices i and $\bar{i}$, representing the basis for $\mathcal{G}$ and $\bar{\mathcal{G}}$, respectively, in such a way that each edge has one bar index and one nonbar index at its ends, and each vertex has two nonbar indices and one bar index at its legs.

Let us introduce a notation. Wherever we have an edge after step 1(revised) we direct the edge (by setting an arrow head) from the nonbar index to the bar index and drop the bar on top of the bar index. Thus the two steps for applying the weight system of L_0 on a diagram can be finalized into the following form.

(1) Sum over all ways of directing the edges of the diagram (internal edges only) in such a way that each vertex has two outgoing legs and one ingoing leg (we call it a "legal" directing and it looks like ).

(2) Set a different index on each end of all the directed edges, write down the appropriate tensors and contract indices according to the arrow convention above (i.e., the arrow's direction indicates if the index is considered bar or nonbar, and we use the appropriate basis accordingly).

Step (1) is a map from the space of all Feynman diagrams D^{CS} to the space of all directed Feynman diagrams $\overrightarrow{D^{\mathrm{CS}}}$, defined to be all trivalent connected graphs based on a circle with arrows on the internal edges (the edges which are not a part of the base circle) such that each vertex is "legal" in the above sense. This map takes a diagram to the sum of all possible "legal" directing of it. In order to extend this map to $\mathcal{A}(S^1)$ we need to treat the STU/IHX/AS relations. For that purpose we define the directed STU, directed IHX, and directed AS relations which we will use in taking a quotient of $\overrightarrow{D^{\mathrm{CS}}}$. These relations reflect the algebraic structure of L_0 and can be read directly from the bracket structure.

Definition 2.2: The directed STU relations in $\overrightarrow{D^{\mathrm{CS}}}$ are the following relations:

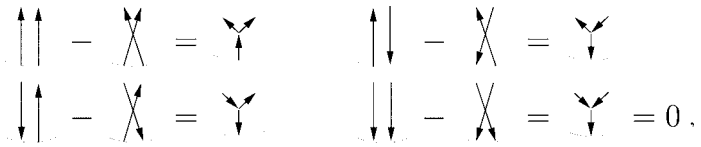

where the bottom nondirected arc is a part of the base circle.

The directed IHX relations are actually a consequence of the directed STU relations in $\overrightarrow{D^{\mathrm{CS}}}$, just as in Ref. 6. We draw one example here and the rest are just rotations thereof

The directed AS relation is defined just as the usual AS relation,

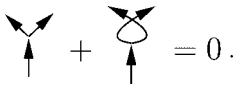

Definition 2.3: The space of all "legally" directed diagrams modulo the directed STU/IHX and AS relations, denoted $\overrightarrow{\mathcal{A}(S^1)}$, is the space of all trivalent connected graphs based on a circle (the Wilson loop) with arrows on the internal edges such that each vertex looks like

(i.e., the space $\overrightarrow{D_{\mathrm{CS}}}$ defined above), quotient by the directed STU, directed IHX and directed AS relations defined above.

Armed with these definitions we can see that step (1) of the factorization above is well defined as a map $\mathcal{A}(S^1)\to\overrightarrow{\mathcal{A}(S^1)}$. Composed with step (2) above (labeling and contracting of indices) and with taking the trace of the resulting tensor in some chosen representation, we get the following factorization of the perturbation theory expansion of CS theory with an inhomogeneous gauge group and the standard observable:

$$\{\text{knots}\}\to\mathcal{A}(S^1)[[k^{-1}]]\to\overrightarrow{\mathcal{A}(S^1)}[[k^{-1}]]\to(U(L_0)^{L_0})_{L_0}[[k^{-1}]]\to\mathbb{C}[[k^{-1}]]. \tag{2}$$

Note that the directed STU relations (which reflect the structure of L_0) tell us that two adjacent legs which touch the base circle and have arrows pointed towards it, are commutative (as the bar indices are commutative). On the other hand, if they originate from one vertex they are anticommutative according to the AS relation. Thus one gets an important relation in $\overrightarrow{\mathcal{A}(S^1)}$:

This relation will be used in the arguments presented in the next section.

D. But $\vec{\mathcal{A}}(S^1)$ is (almost) empty

We will now prove that there are only few nonzero diagrams in $\overrightarrow{\mathcal{A}(S^1)}$ and the ones that are not zero encode a very specific type of information regarding the knot—the framing. This information can actually be normalized to zero showing that the entire weight system W_{L_0} is trivial. We will prove that the only primitive element which is nonzero in $\overrightarrow{\mathcal{A}(S^1)}$ is the directed single chord diagram $\ominus$ (drawn without the arrow here) and thus the only degree n diagram which is nonzero in $\overrightarrow{\mathcal{A}(S^1)}$ is $\ominus^n$. We will do that by first showing that the only primitive elements that are possibly

nonzero are the wheel diagrams (e.g. , ) and $\ominus$. We will then present an argument as to why the wheel diagrams are actually zero. We remind the reader that whenever we mention a diagram we mean a (representative of) diagram class.

Lemma 2.4: Every degree n diagram in $\overrightarrow{\mathcal{A}(S^1)}$ has at least n external vertices (vertices that are on the base loop).

Proof: As already mentioned, to every diagram we attach a power of $1/k$ which is called the degree. A convenient way of counting the degree is labeling each internal vertex with -1 and each edge with $+1$ and then summing up all the labels to get the degree of the diagram. Given a degree n diagram in $\overrightarrow{\mathcal{A}(S^1)}$, label it with $+1$ and -1 according to the above. "Push" the labels on the edges in the direction of the arrows. Whenever a label hits a vertex it stops and the labels at the vertex are added. An example of this procedure for a degree 3 diagram is given by

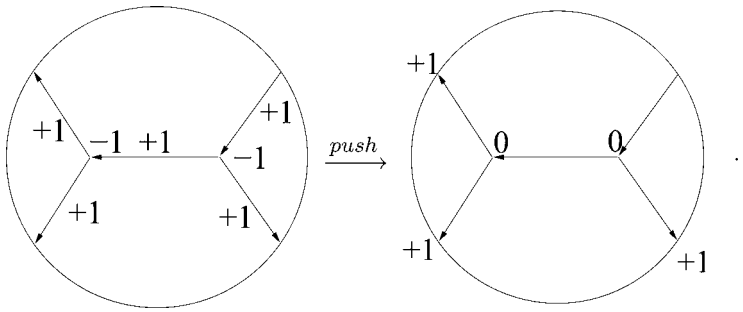

According to the "legal" directing rules, each internal vertex will have one label $+1$ hitting the vertex label -1 thus summing to a zero label. All other labels are pushed to the external vertices (on the Wilson loop). Since the total sum of labels is conserved and equal to the degree of the diagram, what we have just proven is that a degree n diagram in $\overrightarrow{\mathcal{A}(S^1)}$ has at least n vertices on the Wilson loop (in other words at least n external legs).

This lemma has immediate consequences in terms of the primitive elements that generate the algebra $\overrightarrow{\mathcal{A}(S^1)}$. The primitive elements of the nondirected algebra $\mathcal{A}(S^1)$ are these diagrams which remain connected when the Wilson loop is removed from them. Let $\mathcal{P}_n$ be the space of primitive diagrams in $\mathcal{A}(S^1)$ of degree n. Filter the primitive spaces (of different degrees) according to the number of external legs and write $\mathcal{P}_{n,d}$ for the space of primitive diagrams in $\mathcal{A}(S^1)$ of degree n and at most d external legs.

Lemma 2.5 (Refs. 14 and 13): If n is even, then $\mathcal{P}_n=\mathcal{P}_{n,n}$ and the quotient space $\mathcal{P}_{n,n}/\mathcal{P}_{n,n-1}$ is one dimensional generated by the n-degree wheel. If n is odd, then $\mathcal{P}_n=\mathcal{P}_{n,n-1}$ (with the exception of $\mathcal{P}_1$ being generated by $\ominus$).

Proof: See Refs. 14, 13, and 6 for proof and much more details on the subject. Again, we mention that a wheel diagram looks like the following: the two wheel  the four wheel  and so on.

This lemma transfers over to $\overrightarrow{\mathcal{A}(S^1)}$ where the primitives are the primitives of $\mathcal{A}(S^1)$ directed in all possible ways. Combining the previous two lemmas we obtain the following.

Corollary 2.6: The only primitive diagrams that might possibly be nonzero are the wheel diagrams and $\ominus$.

However, we have the following.

Lemma 2.7: The wheel diagrams are zero in $\overrightarrow{\mathcal{A}(S^1)}$.

Proof: We start by looking at a directed wheel diagram. There are only two directed wheel diagrams of each degree, one for each of the two ways of directing the inner loop, and it does not matter which one we choose to look at. Due to the "legal" directing rules, it is not hard to see that the external legs are always pointing towards the base loop. We apply a directed STU relation on

one of these legs 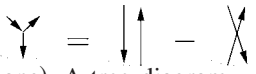 obtaining two tree diagrams (i.e., diagrams which contain no internal loops). A tree diagram will always have exactly one leg pointing from the base loop inwards. The tree diagram that corresponds to the first summand on the right-hand side of the relation has a vertex which looks like  This means the tree diagram is equal to zero (see the comment at the end of Sec. II C). The second tree diagram, corresponding to the second summand on the right-hand side of the directed STU relation, is "leg crossed." This crossing can be untangled by moving the crossed leg around the base circle using the directed AS relation when necessary and the commutativity of outward pointing legs. Moving the leg around the circle will yield a diagram which again has a vertex which looks like  (up to a sign) and thus equals to zero. Apply this argument to any n-wheel diagram and the lemma is proven.

We demonstrate the entire argument on the four wheel:

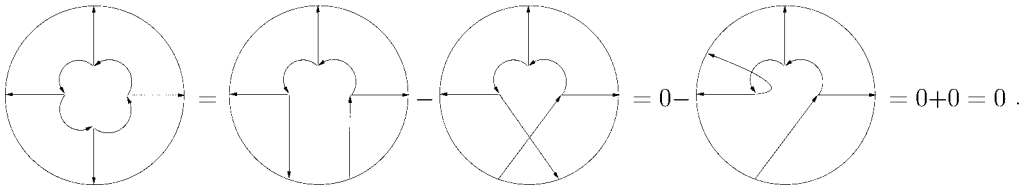

Combining all of the above lemmas we finally get the following.

Proposition 2.8: The only possible nonzero primitive element in $\widehat{\mathcal{A}(S^1)}$ *is the directed single-chord diagram* $\ominus$. *Thus, the only diagrams of degree n that are possibly nonzero in* $\widehat{\mathcal{A}(S^1)}$ *are directed* $\ominus$.

Proof: The proof is a corollary of all the above lemmas. The only primitive element which is nonzero is $\ominus$ and it generates powers of itself and sums of such powers.

In CS perturbation theory it is well known that the single-chord diagram has the framing (self-linking) of the knot as its integral $\zeta^{\mathrm{CS}}(\ominus)$ (see, for example, Ref. 15). Higher degree diagrams, which are merely power of the single-chord diagram, will hold information encoded in powers of the framing of the knot. Moreover, this framing number can be normalized as we wish, including normalization to zero, thus we can summarize this chapter with the following proposition.

Proposition 2.9: CS topological quantum field theory with an inhomogeneous gauge group and the standard knot observable (expectation value of the trace, in some representation, of the holonomy along the knot) holds no more than the framing information (which can be trivialized anyway).

CS theory with an inhomogeneous gauge group and the standard observable fail to recognize knotting in S^3. As a gauge theory, CS theory with inhomogeneous gauge group is equivalent to pure BF theory and should therefore "see" knots at least for ISU(2) gauge group, as was shown by Cattaneo *et al.*[10–12] Therefore, we need a procedure that will extract some nontrivial information regarding the knot in our setting. This is what we will be presenting in the next section.

III. EXTRACTING NONTRIVIAL INFORMATION REGARDING THE KNOT

A. Breaking gauge symmetry at one point—puncturing the space

As seen in the preceding section, the reason we got zero information when the standard observable is used is the "emptiness" of $\widehat{\mathcal{A}(S^1)}$. Working with the inhomogeneous gauge group allows us to factor through the "legally" directed diagrams space when applying perturbation theory thus there is no way of avoiding the consequences of Lemmas 2.3 and 2.4 of the preceding section which state that the only possible nonvanishing contribution in perturbation theory comes from the wheel diagrams. The best we can do is try and avoid the reasons Lemma 2.5 is true. When we look at the proof of Lemma 2.5 we can realize that the cause for the vanishing contribution of the wheel diagrams is the fact that legs can be moved around the Wilson loop (the base

circle of the diagram). Dealing with the loop translates (observablewise) to dealing with the trace (and its cyclic properties) in the standard observable. In diagrammatic terms (perturbationwise) this means trying to cut the base circle open.

Assume first that we just remove the trace from the standard observable of a knot in S^3. We get an expectation value which is formally a tensor in the universal enveloping algebra $\int \mathcal{D}\mathcal{A} e^{i\mathrm{CS}(A)}\,\mathrm{hol} \in U(L_0)$. This expression, though, is not well defined since the holonomy by itself is not well defined and transforms nontrivially by conjugation under gauge transformation $\chi(x)$. Choosing (in advance) one point on the knot, say x_0, the conjugation is done by the gauge element at that point $[\mathrm{hol} \to \chi(x_0)\mathrm{hol}\,\chi^{-1}(x_0)]$. The remedy for that would be to view this (not well defined) invariant in the coinvariant quotient $U(L_0)_{L_0}$. The way this is done (observablewise) is of course by bringing back the trace. We have done nothing then.

This leads us to try and have special considerations for x_0 (the chosen point on the knot) and the gauge symmetry at that point. Let us break the gauge symmetry at x_0. There are a few equivalent ways of looking at that process. The first is by declaring that the gauge transformation at x_0 is always the identity element. This might seem to be a bit artificial but an equivalent way of doing it is taking x_0 out of the space on which the theory is defined by puncturing S^3 on x_0. In other words, "send" x_0 to infinity where gauge transformations are taken to vanish. This shifts us to a theory on a long knot (embedding of $\mathbb{R}$) in $\mathbb{R}^3$ with an invariant $\int \mathcal{D}\mathcal{A} e^{i\mathrm{CS}(A)}\,\mathrm{hol} \in U(L_0)$ which is well defined in the framework of CS theory.

To summarize, we move from a CS theory on S^3 and a knot (embedding of S^1) in it to a CS theory on $\mathbb{R}^3$ and a long knot (embedding of $\mathbb{R}$) in it. This is done by choosing a special point on the knot, puncturing the space there and declaring the puncture as infinity. The standard observable $\mathrm{Tr}_R\,\mathrm{hol}$ *is replaced by a more general observable hol.*

As far as knots are concerned, "regular" knots and long knots are equivalent and we do not lose any information regarding the knot in the process above. Moreover, hol (and functions of it) is actually the most general observable in this framework since the connection can always be recovered (up to gauge transformations) from the holonomy information. Thus we work in the setting which allows us to extract maximum information regarding the knot when using the inhomogeneous gauge group.

We take now $\int \mathcal{D}\mathcal{A} e^{i\mathrm{CS}(A)}\,\mathrm{hol}$ and apply the same perturbation theory factorization as in Sec. II. There are several differences to note.

First, we work with a long knot. Thus, all the Feynman diagrams are not based on a loop but on an interval (representing the embedding of our long knot $\mathbb{R}$). The other properties of the diagrams do not change, though. We define the following.

Definition 3.1: $\mathcal{A}(I)$ is the algebra of all connected trivalent graphs based on an interval, modulo the STU, IHX and AS relations [i.e., $\mathcal{A}(S^1)$ with the circle replaced by an interval]. $\widehat{\mathcal{A}(I)}$ is defined the same way as $\widehat{\mathcal{A}(S^1)}$, except that the diagrams are based on an interval and not on a circle.

Second, the knot invariant factors through the invariant subspace of the universal enveloping algebra $U(L_0)^{L_0}$. This time there is no necessity in taking the coinvariant quotient of that space, a necessity that came about because of the base circle (or the trace in the observable). Note that the fact that we indeed get a tensor in the invariant subspace tells us that the construction was independent of the choice of the special point x_0.

Third, we do not have a map to $\mathbb{C}$ yet.

All together we get the following factorization for the perturbation theory of CS theory on $\mathbb{R}^3$ with a long knot in it (we denote by l the last map):

$$\{\mathrm{knots}\} \to \mathcal{A}(I)[[k^{-1}]] \to \widehat{\mathcal{A}(I)}[[k^{-1}]] \xrightarrow{l} U(L_0)^{L_0}[[k^{-1}]]. \tag{3}$$

B. Building an observable and extracting nontrivial information

We have not shown so far that the algebra $\widehat{\mathcal{A}(I)}$ is nonzero and that our construction is indeed nontrivial in the sense that it fixes the problems encountered with the standard observable. We

have also not defined a scalar observable, i.e., a map $U(L_0)^{L_0}\to\mathbb{C}$ which completes the perturbation theory factorization. We will now achieve both goals by finding an explicit functional from $\widetilde{\mathcal{A}(I)}$ to $\mathbb{C}$ that does not vanish when composed with the above factorization. We will give a formula for a scalar function $U(L_0)^{L_0}\to\mathbb{C}$ that is not zero on the part of $U(L_0)^{L_0}$ which comes from wheel diagrams in $\widetilde{\mathcal{A}(I)}$. This observable cannot possibly be any trace of hol in some representation, since that will bring us back to the case of Sec. II. Thus we need to find some other scalar function of hol.

Start with an n-dimensional representation of $\mathcal{G}$ and denote it B. Define the following representation R of L_0:

$$R(g)=\begin{pmatrix} B(g) & 0 \\ 0 & B(g) \end{pmatrix},\quad g\in\mathcal{G},\quad R(\bar{g})=\begin{pmatrix} 0 & B(g) \\ 0 & 0 \end{pmatrix},\quad \bar{g}\in\bar{\mathcal{G}}. \tag{4}$$

It is straightforward to verify that the commutation relation for R is indeed compatible with the commutation relations of the semidirect product and that R is indeed a representation of L_0. We extend R to $U(L_0)$ in the usual way.

Definition 3.2: We have the following.

(1) Let Δ denote the comultiplication of the universal enveloping algebra $U(L_0)$ and let Δ^m denote the map $U(L_0)\to U(L_0)^{\otimes m}$ we get by composing $m-1$ times the map Δ.

(2) Given the representation R above, denote by $R^{\otimes m}$ the m-tensored representation $U(L_0)^{\otimes m}\to\mathrm{End}(\mathbb{C}^{2n})^{\otimes m}$ defined by $u_1\otimes\cdots\otimes u_m\mapsto R(u_1)\otimes\cdots\otimes R(u_m)$.

(3) Define a transformation λ, $\mathrm{End}(\mathbb{C}^{2n})^{\otimes m}\to\mathrm{End}(\mathbb{C}^{2n})$ by $\tau_1\otimes\tau_2\otimes\cdots\otimes\tau_m\mapsto\tau_1\cdot C\cdot\tau_2\cdot C\cdot\cdots\cdot\tau_m\cdot C$, where C is the following $2n\times 2n$ matrix:

$$\begin{pmatrix} 0 & 0 \\ I & 0 \end{pmatrix}$$

and $\cdot$ is matrix multiplication.

(4) The "half-trace," denoted $\mathrm{Tr}_{1/2}$, is the trace over the upper-left $n\times n$ block of a $2n\times 2n$ matrix,

$$\mathrm{Tr}_{1/2}\begin{pmatrix} A & B \\ C & D \end{pmatrix}=\mathrm{Tr}(A).$$

Armed with the above definitions and notations we can finally build the following.

Definition 3.3: Let Σ_m denote the following composition of maps ($\circ$ is used for composition):

$$\mathrm{Tr}_{1/2}\circ\lambda\circ R^{\otimes m}\circ\Delta^m: U(L_0)^{L_0}\xrightarrow{\Sigma_m}\mathbb{C}.$$

Lemma 3.4: The map $\Sigma_m\circ l$ is nonzero on the m-wheel diagram for at least one choice of gauge group L_0 and representation R.

Proof: We start by looking at a directed wheel diagram [i.e., a wheel in $\widetilde{\mathcal{A}(I)}$]. All the external legs (the ones that touch the base interval) point towards the interval, as we have already seen. This means that after applying l, the tensor w that we get in $U(L_0)$ will have all its components in $\bar{\mathcal{G}}$. After applying Δ^m to w we get a tensor in $U(L_0)^{\otimes m}$ such that each of its summands actually looks like $u_1\otimes\cdots\otimes u_m\in U(\bar{\mathcal{G}})^{\otimes m}\subset U(L_0)^{\otimes m}$.

Now, the only type of tensors $u_1\otimes\cdots\otimes u_m\in U(\bar{\mathcal{G}})^{\otimes m}$ that will possibly not result in zero after applying $\lambda\circ R^{\otimes m}$ to it, is the type in which each component u_i is actually an element of $\bar{\mathcal{G}}$ [i.e., tensors of length one in $U(L_0)$ with entry from $\bar{\mathcal{G}}$]. This is immediate from the definition of R (4) on $U(\bar{\mathcal{G}})$, the definition of λ and the definition of C.

We summarize then—given a wheel diagram we apply l to it and get a tensor w in $U(L_0)$. $\Delta^m(w)$ is a tensor in $U(L_0)^{\otimes m}$ but the only nonzero contributions to $\lambda\circ R^{\otimes m}(\Delta^m(w))$ come from the summands of $\Delta^m(w)$ that look like w or any permutations of its entries,

$$w = l(\text{directed } m-\text{wheel}) = \sum_{i_1,\ldots,i_m=1}^{\dim \mathcal{G}} C^{i_1,\ldots,i_m} \bar{X}_{i_1} \otimes \cdots \otimes \bar{X}_{i_m},$$

$$\lambda \circ R^{\otimes m}(\Delta^m(w)) = \lambda \circ R^{\otimes m}\left(\sum_{i_1,\ldots,i_m=1}^{\dim \mathcal{G}} \sum_{\sigma \in S_m} C^{i_1,\ldots,i_m} \bar{X}_{i_{\sigma(1)}} \otimes \cdots \otimes \bar{X}_{i_{\sigma(m)}} \right),$$

where we made a distinction between the tensor product $\otimes$ of $U(L_0)$ and the product $\bigotimes$ of $U(L_0)^{\otimes m}$ for the sake of clarity.

The calculation of $\mathrm{Tr}_{1/2} \circ \lambda \circ R^{\otimes m} \circ \Delta^m \circ l(\text{directed } m-\text{wheel})$ is almost the same as the calculation of the weight system $W_{\mathcal{G},B}$ on the nondirected m-wheel diagram (i.e., the directed m-wheel with its arrows forgotten). The only difference is the summation over all permutations of the components of the tensor w above, but that can be done on the diagram level by permuting all external legs of the nondirected diagram. Thus we have

$$\mathrm{Tr}_{1/2} \circ \lambda \circ R^{\otimes m} \circ \Delta^m \circ l(\text{directed } m-\text{wheel}) = W_{\mathcal{G},B}(\chi(m-\text{wheel})),$$

where $\chi(D)$ is defined to be the sum over all diagrams which differ from D by permutation of the external legs.

In order to show that $\Sigma_m \circ l(\text{directed } m-\text{wheel})$ is nonzero for at least one choice of L_0 and representation R we let $L_0 = gl(n) \oplus \overline{gl(n)}$ with B taken to be the defining representation and calculate the highest order in n of $W_{gl(n),B}(\chi(m-\text{wheel}))$. Using simple counting arguments one may show that all the highest order contributions are positive and sum up to a nonzero contribution: $\Sigma_m \circ l(\text{directed } m-\text{wheel}) = mn^{m+1} + \text{lower order terms (in } n)$. We leave the exact calculation and arguments to the interested reader. These can be done using exercise 6.36 in Ref. 6.

Proposition 3.5: In $\widetilde{\mathcal{A}(I)}$, *the wheel diagrams (and possibly the directed* $\ominus$*) are nonzero.*

Proof: We already know that the only possible nonzero directed generators in $\widetilde{\mathcal{A}(I)}$ are the wheel diagrams and possibly $\ominus$ [following the exact same arguments for $\widetilde{\mathcal{A}(S^1)}$ as in Sec. II]. Applying the lemma above for all possible m implies the proposition.

The actual observable: The proposition and lemma above tell us that the perturbation theory (3) for the long knot in $\mathbb{R}^3$ factors through a nontrivial space, and that there is a way of extracting nontrivial information regarding the knot. We can now build an actual quantum observable (function of hol) to plug in the path integral such that the map $\mathrm{Tr}_{1/2} \lambda R^{\otimes m} \Delta^m$ will be the last part of the factorization $(U(L_0)^{L_0} \to \mathbb{C})$ in its perturbation theory calculation of the expectation value. This observable is $\mathrm{Tr}_{1/2}((R(\mathrm{hol}) \cdot C)^m)$, where $R(\mathrm{hol})$ stands for representing the holonomy using the representation R as defined above.

The expectation value $\int \mathcal{D}\mathcal{A} e^{i\mathrm{CS}} \mathrm{Tr}_{1/2}((R(\mathrm{hol}) \cdot C)^m)$ has a perturbation theory factorization (with Σ_m as the last map),

$$\{\text{knots}\} \to \mathcal{A}(I)[[k^{-1}]] \to \widetilde{\mathcal{A}(I)}[[k^{-1}]] \xrightarrow{l} U(L_0)^{L_0}[[k^{-1}]] \xrightarrow{\Sigma_m} \mathbb{C}[[k^{-1}]]. \tag{5}$$

C. The most general knot invariant in this setting—the Alexander-Conway polynomial

We have just seen in the preceding section that we can extract all the information contained in the wheel diagrams by using CS theory with the inhomogeneous gauge group on long knots in $\mathbb{R}^3$ (with the new class of observables). This is opposed to the fact that the standard observable in CS theory with the inhomogeneous gauge group will not see these knots in S^3. We now turn to the task of recognizing the nontrivial information we extracted.

Theorem 1: *The most general knot invariant coming from Chern-Simons topological quantum field theory with an inhomogeneous gauge group is nontrivial and is in the algebra generated by the coefficients of the Alexander-Conway polynomial (together with possible framing information).*

Proof: In Ref. 16, following motivations from Refs. 17 and 7, it is proven that any weight system which is zero on the kernel of the deframing operator and zero on all the primitive spaces which are not wheels, belongs to a knot invariant which is in the algebra generated by the coefficients of the Alexander-Conway polynomial. Since we showed that the only diagrams that contribute to our weight system are the wheel diagrams, and since we can always choose our knot to be of (standard) zero framing, the theorem follows. Other choices of framing will show up through $\ominus$.

Notice that it is possible to take the semidirect product of G with $\mathcal{G}^*$, the dual of the Lie algebra. We can follow the exact same considerations and get the same results, this time without the need of the metric on $\mathcal{G}$ (just use the natural dual pairing to get a metric on L_0). Therefore our results are true for any Lie algebra $\mathcal{G}$, not necessarily a metrizable one.

IV. PURE BF THEORY AND THE ALEXANDER-CONWAY POLYNOMIAL

Recall that the pure BF theory has the following action $S_{\mathrm{BF}}=\int_{S^3}\mathrm{Tr}(B\wedge F)$, where F is the curvature of the G-connection A and B is a one form taking values in the algebra $\mathcal{G}$. In Refs. 10–12 Cattaneo *et al.* took $\mathrm{Tr}_R(\mathrm{Exp}(\lambda\gamma_1))$ as the most general observable one can consider in pure BF theory, as long as the standard (zero) framing of the knot is chosen. Here R is any representation of G, γ_1 is $\oint_x \mathrm{Hol}(A)B(x)\mathrm{Hol}(A)$ [the first degree element in the Taylor expansion of $\mathrm{Hol}(A+\kappa B)$ around $\kappa=0$] and λ is a "coupling" constant counting orders.

Using this observable, QFT techniques and the Melvin-Morton conjecture (MMR, see Ref. 7), it was proven[10] that the set of unframed knot invariants we get from the pure BF theory, using SU(2) gauge group, is generated by the coefficients of the Alexander-Conway polynomial.

In this paper we proved the following.

Theorem 2: *The most general knot invariant coming from pure BF topological quantum field theory with any gauge group whose Lie algebra is metrizable and with any representation, is in the algebra generated by the coefficients of the Alexander-Conway polynomial.*

Proof: Using the fact that the pure BF theory with gauge group G is just CS theory with gauge group IG (Ref. 8) this theorem is just a corollary of Theorem 1.

The same generalization for nonmetrizable Lie algebras, as right after Theorem 1, applies here as well.

A closer look at our observable $\mathrm{Tr}_{1/2}((R(\mathrm{hol})\cdot C)^m)$ shows that it is actually the mth degree in the expansion of the BF observable $\mathrm{Tr}_R(\mathrm{Exp}(\lambda\gamma_1))$ (up to numerical factors coming from the exponent expansion). The fact that the BF observable also breaks the gauge symmetry of the pure BF theory at one point (it must be assumed that the special BF gauge symmetry is identity at one point on the knot) was not emphasized much before (though observed of course in Refs. 10–12). Our setting gives a natural explanation as to why this is indeed the most general observable for BF theory without any need for taking various limits or referring to MMR. We also get a somewhat clearer explanation as to why one can ignore the γ_0 part of the Taylor expansion above.

One can now say that as far as knot theory and three-dimensional BF topological quantum field theory (with or without cosmological constant) are concerned, there is nothing new beyond Chern-Simons theory, which can reproduce the same knot theoretical results.

V. DISCUSSION: NON-SEMI-SIMPLICITY

Algebraically, the main difference between our construction and the standard one is getting invariants in the invariant subspace $U(L_0)^{L_0}$ instead of the coinvariant quotient space $(U(L_0)^{L_0})_{L_0}$ of the universal enveloping algebra.

Our construction gives no new extra information if we work with a semisimple gauge group instead of L_0. This is true because for semisimple groups, $U(\mathcal{G})^{\mathcal{G}}$ is isomorphic to $(U(\mathcal{G})^{\mathcal{G}})_{\mathcal{G}} \cong U(\mathcal{G})_{\mathcal{G}}$. We get no new information from applying our procedure and working in $\mathcal{A}(I)$ instead of $\mathcal{A}(S^1)$, since these spaces are isomorphic (the diagram-space way of expressing the previous isomorphism). Our construction seems to detect the difference between the invariant subspace and

the coinvariant quotient of the non-semi-simple Lie algebra we have worked with. In other words, it uses the fact that $\overrightarrow{\mathcal{A}(I)}$ is not isomorphic to $\overrightarrow{\mathcal{A}(S^1)}$ [the map $\overrightarrow{\mathcal{A}(I)} \to \overrightarrow{\mathcal{A}(S^1)}$ that closes the base interval into the base circle has a kernel].

We saw that there is more to observe in Chern-Simons theory when dealing with a non-semi-simple gauge group. A question to be raised is whether other non-semi-simple gauge groups can hold the same property as the inhomogeneous group—meaning that the above procedure can extract more information about the knot than what was given by the standard observables.

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Noncommutative unification of general relativity and quantum mechanics

Michael Heller[a)]
Vatican Observatory, Vatican City, V-00120 Vatican City, Rome

Leszek Pysiak and Wiesław Sasin
Department of Mathematics and Information Science, Warsaw University of Technology, Plac Politechniki 1, 00-661 Warsaw, Poland

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We present a model unifying general relativity and quantum mechanics based on a noncommutative geometry. This geometry is developed in terms of a noncommutative algebra $\mathcal{A}$ which is defined on a transformation groupoid Γ given by the action of a noncompact group G on the total space E of a principal fiber bundle over space-time M. The case is important since to obtain physical effects predicted by the model we should assume that G is a Lorentz group or some of its representations. We show that the generalized Einstein equation of the model has the form of the eigenvalue equation for the generalized Ricci operator, and all relevant operators in the quantum sector of the model are random operators; we study their dynamics. We also show that the model correctly reproduces general relativity and the usual quantum mechanics. It is interesting that the latter is recovered by performing the measurement of any observable. In the act of such a measurement the model "collapses" to the usual quantum mechanics. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2137720]

I. INTRODUCTION

Noncommutative geometry plays an increasingly important role in the present search for quantum gravity (from a host of papers let us quote at least a few[3,4,2,1,6,14–16,19]). It has also recently been recognized that it is a useful tool in superstring theory (the classical paper is Ref. 18, and a book, Ref. 13). In a series of papers,[10–12] we have proposed our own approach to the unification of general relativity and quantum mechanics based on noncommutative geometry. Our starting point is the standard method of changing a differential manifold (space-time) M into a noncommutative space (Ref. 5, p. 86). It is done by implementing the following steps: (1) we represent M as a quotient space N/R where N is a suitable space and R a suitable equivalence relation; (2) then we change from N/R to a suitably organized subset $\mathcal{R}$ of $N\times N$; we call this the "pairing process;" (3) we define a suitable algebra on $\mathcal{R}$; and finally, (4) we extract information about N/R from this algebra.

We implement this strategy as follows. Let M be a space-time manifold. The natural way to present M as a quotient space is with the help of the frame bundle over M. Let $\pi_M: E\to M$ be the frame bundle with the structure group G, then $M=E/G$. To perform the "pairing process" let us notice that the group G acts (to the right) on E (along the fibers), $E\times G\to E$. We can equip $E\times G$ with the groupoid structure. This groupoid is called a *transformation groupoid*, and will be denoted by Γ (its description is given in Sec. II). Now, we define a (noncommutative) compactly supported, smooth, complex valued algebra $\mathcal{A}$ on Γ with convolution as multiplication. Then we construct, in terms of this algebra, the (noncommutative) geometry of the groupoid Γ which is a

[a)]Author to whom correspondence should be addressed: ul. Powstańców Warszawy 13/94, 33-110 Tarnów, Poland. Electronic mail: mheller@wsd.tarnow.pl

generalization of the usual space-time geometry (on M). The regular representation of the algebra $\mathcal{A}$ on a bundle of Hilbert spaces gives us the "quantum sector" of the model.

To smooth out some inaccuracies and avoid conceptual traps in which our previous work was involved we have tested the method on a simpler model in which the group G was finite.[8,9,17] It has turned out that this simplified model works well. Let us notice, however, that if a finite group G acts freely on a space E then G must be a cyclic group isomorphic with $\mathbb{Z}^n$ where $n=|G|$. Indeed, for $G \ni g \neq e$ the set $\{gp, g^2p, \ldots, g^np\}$ is bijective with G and, as it can be easily seen, $g^n=e$. However, we should notice that the fact that the group G is Abelian does not entail the commutativity of the groupoid algebra $\mathcal{A}$. Therefore, our model with a finite group G could serve well as an "exercise model," but to have a more physically realistic approach we must change to an infinite group G. This is exactly what we do in the present paper. Throughout this paper it is assumed that G is a noncompact group. This is an important case since to obtain physical effects predicted by our model we should assume that G is a Lorentz group or some of its representations.

In Sec. II, we briefly present the groupoid Γ and its algebra $\mathcal{A}$, and we establish notation. The geometry of the groupoid Γ is based on the module of derivations of the algebra $\mathcal{A}$. In Sec. III, we study the structure of this module and, in Secs. IV and V, we develop the differential geometry of the groupoid Γ. This enables us to formulate, in Sec. VI, generalized Einstein's equation. It turns out that it has the form of the eigenvalue equation for the generalized Ricci operator. We also show that the standard space-time geometry is obtained by suitably "averaging" elements of $\mathcal{A}$. In Sec. VII, we study the quantum sector of the model, and show that all relevant operators are random operators. We also investigate their generalized dynamics. The transition from our model to the usual quantum mechanics is presented in Sec. VIII. Interestingly, it is the act of measurement of any observable that reduces our model to the usual quantum mechanics. We thus can say that from the perspective of our model quantum mechanics is but a theory of making measurements.

The present paper focuses on mathematical aspects of the proposed model; its physical aspects will be discussed in a forthcoming paper.

II. PRELIMINARIES

Let $\Gamma=E\times G$, where E is the frame bundle over space-time M with the structural group G, such that G is a noncompact semisimple Lie group (let us notice that the Lorentz group is noncompact and semisimple) acting on E, be a transformation groupoid, and $\mathcal{A}=C_c^\infty(\Gamma,\mathbf{C})$ the noncommutative algebra of smooth, compactly supported, complex valued functions on Γ with convolution as multiplication. Let further $\gamma_1=(p_1,g_1)$, $\gamma_2=(p_2,g_2)\in\Gamma$, and $p_2=p_1g$. We assume the convention $\gamma_1\circ\gamma_2=(p_1,g_1g_2)$, and consequently

$$(f_1 * f_2)(\gamma) = \int_{\Gamma_{d(\gamma)}} f_1(\gamma_1) f_2(\gamma_1^{-1}\gamma)\mathrm{d}\gamma_1$$

for $f_1,f_2\in\mathcal{A}$, where $d(\gamma)=d(p,g)=p$.

Let us notice that the center of the algebra $\mathcal{A}$ vanishes, $\mathcal{Z}(\mathcal{A})=\{0\}$, but $\mathcal{A}$ is a module over $Z=\pi_M^*(C^\infty(\mathrm{M}))$ (here $\pi_M:E\to M$ is the bundle projection). Functions of Z, in general, are not compactly supported. However, they do act on $\mathcal{A}$ in the following way: $\alpha:Z\times\mathcal{A}\to\mathcal{A}$ by

$$\alpha(f,a)(p,q) = f(p)a(p,g),$$

$f\in Z$, $a\in\mathcal{A}$. Now, let us define the distribution

$$\tilde{f}(p,g) = f(p)\,\delta_e(g),$$

where δ is the Dirac distribution, $g\in G$, and e is the unit of G. $\tilde{f}$ convolutes well with functions of $\mathcal{A}$. Indeed, let $a\in\mathcal{A}$; we have

$$(\tilde{f} * a)(p,g) = \int_G \tilde{f}(p,g_1)a(pg_1,g_1^{-1}g)\mathrm{d}g_1 = f(p)a(p,g) \in \mathcal{A}.$$

(Here we have used the integral notation for the distribution action on test functions.)

Let $\mathcal{G}=E\times E$ be the space of the pair groupoid, where E is, as before, the total space of the frame bundle over space-time M, i.e., $\mathcal{G}=\{(x,p_1,p_2): p_1,p_2 \in E \text{ and } \pi_M(p_1)=(\pi_M(p_2))=x\}$, and the algebra $\tilde{\mathcal{A}}=C^\infty(\mathcal{G},\mathbf{C})$ with convolution as multiplication. The composition law reads $(x,p_1,p_2)\circ(x,p_2,p_3)=(x,p_1,p_3), p_1,p_2,p_3 \in E_x, x \in M$, and the convolution is defined accordingly.

Proposition 1: The mapping $J:\tilde{\mathcal{A}}\to\mathcal{A}$, given by

$$J(f)(\gamma) = f(\pi_M(p),p,pg),$$

for $f \in \tilde{\mathcal{A}}$, $\gamma=(p,g)$, is an isomorphism of algebras.

Proof: Let $\tilde{f}_1,\tilde{f}_2 \in \tilde{\mathcal{A}}$, we have

$$(\tilde{f}_1 * \tilde{f}_2)(x,p_1,p_2) = \int_{E_x} \tilde{f}_1(x,p_1,p_3)\tilde{f}_2(x,p_3,p_2)\mathrm{d}p_3.$$

We notice that the fiber E_x, for every $x \in M$, is diffeomorphic with the group G, and consequently there is a measure on E_x induced from the Haar measure on G. After making the substitution $p_3=p_1g_1$, $p_2=p_1g$, we obtain

$$(\tilde{f}_1 * \tilde{f}_2)(x,p_1,g) = \int_G \tilde{f}_1(x,p_1,p_1g_1)\tilde{f}_2(x,p_1g_1,p_1g)\mathrm{d}g_1$$

which can be rewritten as

$$(f_1 * f_2)(\gamma) = \int_{\Gamma_{d(\gamma)}} f_1(\gamma_1)f_2(\gamma_1^{-1}\circ\gamma)\mathrm{d}\gamma_1.$$

□

III. MODULE OF DERIVATIONS

Among derivations of the algebra $\mathcal{A}$ on the groupoid $\Gamma=E\times G$ we can distinguish three types, horizontal derivations, vertical derivations, and inner derivations of $\mathcal{A}$; we denote them by $\mathrm{Der}_{\mathrm{Hor}}\mathcal{A}$, $\mathrm{Der}_{\mathrm{Ver}}\mathcal{A}$, and $\mathrm{Inn}\,\mathcal{A}$, respectively. We shall study them in turn.

Lemma 1: Let $\bar{X} \in \mathcal{X}(E)$ be a right invariant vector field (on a principal bundle), i.e., $(\mathcal{R}_g)_{*p}\bar{X}(p)=\bar{X}(pg)$ for every $g \in G$. Its lifting to Γ, $\bar{\bar{X}}(p,g)=(\iota_g)_{*p}\bar{X}(p)$, where the inclusion $\iota_g: E\hookrightarrow E\times G$ is defined by $\iota_g(p)=(p,g)$, is a derivation of the algebra $(\mathcal{A},*)$.

Proof:

$$\begin{aligned}
\bar{\bar{X}}\,(p,g)(f*h)](p,g) &= [\bar{X}(p)(f*h)](\iota_g(p)) \\
&= \int_G [\bar{X}(p)f(p,g_1)]h(pg_1,g_1^{-1}g)\mathrm{d}g_1 + \int_G f(p,g_1)[(\bar{X})(p)h(pg_1,g_1^{-1}g)]\mathrm{d}g_1 \\
&= \int_G [\ (\bar{\bar{X}}))(p,g_1)f](p,g_1)h(pg_1,g_1^{-1}g)\mathrm{d}g_1 \\
&\quad + \int_G f(p,g_1)[\bar{\bar{X}}(pg_1,g_1^{-1}g)]h(pg_1,g_1^{-1}g)\mathrm{d}g_1 \\
&= (\bar{\bar{X}}f * h + f * \bar{\bar{X}}h)(p,g).
\end{aligned}$$

We have employed here the right invariance property. □

A. Horizontal derivations

The group G acts freely and transitively on the fibers of E. Consequently, the G-right-invariant vector fields on E are determined by their values at a single point of every fiber. Therefore, they can be identified with the cross sections of the bundle $\Sigma = TE/G$. Let us consider the mapping

$$(\pi_M)_*: TE \to TM.$$

Since $(\pi_M)_*$ is G-invariant, it induces the mapping

$$\pi_M: \Sigma \to TM.$$

Let us denote $\rho = (\bar{\pi}_M)_*$, and consider the exact sequence of vector bundles

$$0 \to \ker \rho \xrightarrow{j} \Sigma \underset{\sigma}{\overset{\rho}{\rightleftarrows}} TM \to 0.$$

The mappings j and ρ are homomorphisms of vector bundles, and j is an inclusion. The homomorphism of vector bundles $\sigma: TM \to \Sigma$ is a connection in the principal bundle $\pi_M: E \to M$ if it splits this sequence, i.e., if $\rho \circ \sigma = \mathrm{id}_{TM}$. In our case, such σ always exists although it is not unique. With the help of σ we lift a vector field $X \in \mathcal{X}(M)$ from M to Σ, i.e., $\bar{X}(p) = \sigma(X(\pi_M(p)), \pi_M(p) = x \in M$, and we consider $\bar{X}$ as a G-right-invariant vector field on E. Finally, we lift this field, with the help of the inclusion ι_g, to the groupoid Γ. We thus obtain

$$\bar{\bar{X}}(p,g) = (\iota_g)_{*p} \bar{X}(p) \in \mathcal{X}(E \times G)$$

for every $(p,g) \in \Gamma$. Vector fields $\bar{\bar{X}} \in \mathcal{X}(\Gamma)$, obtained in this way, inherit from σ the right invariance property. Lemma 1 evidently applies to such vector fields. Moreover, we have the following proposition.

Proposition 2: Vector fields $\bar{\bar{X}} \in \mathcal{X}(\Gamma)$ *form a Z-submodule of the Z-module* Der $\mathcal{A}$ *of derivations of the algebra* $\mathcal{A}$. *They will be called* horizontal *derivations of* $\mathcal{A}$ *and denoted by* $\mathrm{Der}_{\mathrm{Hor}}\, \mathcal{A}$.

Proof: Let $a, b \in \mathcal{A}$. One readily checks, taking into account the right invariance of $\bar{\bar{X}}$, that $f\bar{\bar{X}}(a * b)$, $f \in Z, a, b \in \mathcal{A}$, satisfies the Leibniz rule. We shall show that $f\bar{\bar{X}} \in \mathrm{Der}_{\mathrm{Hor}}\, \mathcal{A}$. Indeed, let $f_0 \in C^\infty(M)$ be such that $f = \pi_M^* f_0$, and $X' := f_0 X$, $X \in \mathcal{X}(M)$. We have

$$\bar{X}' = \pi_M^* f_0 \bar{X} = f\bar{X},$$

and by acting on both sides with ι_g we obtain $\bar{\bar{X}}' = f\bar{\bar{X}}$. □

B. Vertical derivations

Let us consider all right invariant vertical vector fields on E, i.e., all right invariant vector fields $\bar{X} \in \mathcal{X}(E)$ such that $(\pi_M)_*(\bar{X}) = 0$. Such vector fields lifted to Γ are, on the strength of Lemma 1, derivations of the algebra $(\mathcal{A}, *)$; we shall call them vertical derivations of this algebra, i.e.,

$$\bar{\bar{X}}(p,g) = (\iota_g)_{*p} \bar{X}(p) \in \mathrm{Der}_{\mathrm{Ver}}\, \mathcal{A}$$

for every $g \in G$.

Let us notice that $\bar{X} \in \mathcal{X}(E)$ can be regarded as cross sections of the vector bundle $\ker \rho$ and, as it can be easily seen, $\mathrm{Der}_{\mathrm{Ver}}\, \mathcal{A}$ is a Z-submodule of the Z-module Der $\mathcal{A}$.

C. Inner derivations

The set of inner derivations of the algebra $\mathcal{A}$ is defined as follows:

$$\mathrm{Inn}\,\mathcal{A} = \{\mathrm{ad}\,a : a \in \mathcal{A}\},$$

where $(\mathrm{ad}\,a)(b) := a*b - b*a$.

Lemma 2: The mapping $\Phi : A \to \mathrm{Inn}\,\mathcal{A}$, *given by* $\Phi(a) = \mathrm{ad}\,a$, *is an isomorphism of Lie algebras (and also of Z-moduli).*

Proof: It can be easily seen that

$$[\mathrm{ad}\,a, \mathrm{ad}\,b] = \mathrm{ad}[a,b] \in \mathcal{A},$$

i.e., $\mathrm{Inn}\,\mathcal{A}$ is a Lie algebra and Φ is a Lie algebra homomorphism. Then we have $\Phi(a) = \Phi(b) \Rightarrow [a,c] = [b,c]$, for every $c \in \mathcal{A}$. Hence $[a-b,c]=0$ since $a-b \in \mathcal{Z}(\mathcal{A}) = \{0\}$. Therefore, $a = b$. We also see that

$$\Phi(fa) = \mathrm{ad}(fa) = f\,\mathrm{ad}\,a = f\Phi(a)$$

for every $f \in Z$. □

As we have seen in the proof of this lemma, the fact that $\mathcal{Z}(\mathcal{A}) = \{0\}$ plays an important role in the entire structure.

D. Some properties of derivations

By *differential algebra* we understand a pair $(\mathcal{A}, \mathrm{Der}\,\mathcal{A})$ where $\mathcal{A}$ is a not necessarily commutative algebra and $\mathrm{Der}\,\mathcal{A}$ a (sub)module of its derivations. In the following, we will base the construction of a noncommutative geometry of the transformation groupoid Γ on the differential algebra $(\mathcal{A}, \mathrm{Der}\,\mathcal{A})$ where $\mathcal{A}$ is, as above, $C_c^\infty(\Gamma, \mathbf{C})$, and

$$\mathrm{Der}\,\mathcal{A} = \mathrm{Der}_{\mathrm{Hor}}\,\mathcal{A} \oplus \mathrm{Der}_{\mathrm{Ver}}\,\mathcal{A} \oplus \mathrm{Inn}\,\mathcal{A}.$$

Let $\bar{\bar{X}}_1, \bar{\bar{Y}}_1 \in \mathrm{Der}_{\mathrm{Hor}}\,\mathcal{A}$, $\bar{\bar{X}}_2, \bar{\bar{Y}}_2 \in \mathrm{Der}_{\mathrm{Ver}}\,\mathcal{A}$, $\mathrm{ad}\,a$, $\mathrm{ad}\,b \in \mathrm{Inn}\,\mathcal{A}$. We have the following properties:

(1) $[\bar{\bar{X}}_1, \bar{\bar{Y}}_1] = \overline{\overline{[X_1, Y_1]}}$. This follows from the fact that $\bar{X} = \sigma(X)$ which implies that $[\bar{X}_1, \bar{Y}_1] = \overline{[X_1, Y_1]}$.
(2) $[\bar{\bar{X}}_2, \bar{\bar{Y}}_2] = \overline{\overline{[X_2, Y_2]}}$.
(3) $[\mathrm{ad}\,a, \mathrm{ad}\,b] = \mathrm{ad}[a,b] \in \mathrm{Inn}\,\mathcal{A}$, see proof of Lemma 2.
(4) $[\bar{\bar{X}}_1, \bar{\bar{X}}_2] = 0$, since cross sections of the vector bundle Σ form a Lie algebra which splits into the sum of two Lie subalgebras, and the fields $\bar{X}_1$ and $\bar{X}_2$ belong to different subalgebras.
(5) $[\bar{\bar{X}}_1, \mathrm{ad}\,a] = \mathrm{ad}\,\bar{\bar{X}}_1(a)$, by simple computations.
(6) $[\bar{\bar{X}}_2, \mathrm{ad}\,a] = \mathrm{ad}\,\bar{\bar{X}}_2(a)$, by simple computations.

IV. GEOMETRY OF $\mathrm{Der}_{\mathrm{Ver}}\,\mathcal{A}$ AND $\mathrm{Inn}\,\mathcal{A}$

Because of the decomposition of the Z-module $\mathrm{Der}\,\mathcal{A}$ into three parts, the metric on $\mathrm{Der}\,\mathcal{A}$,

$$\mathcal{G} : \mathrm{Der}\,\mathcal{A} \times \mathrm{Der}\,\mathcal{A} \to Z$$

also decomposes into three parts. If $u = u_1 + u_2 + u_3$, and $u_1 \in \mathrm{Der}_{\mathrm{Hor}}\,\mathcal{A}$, $u_2 \in \mathrm{Der}_{\mathrm{Ver}}\,\mathcal{A}$, $u_3 \in \mathrm{Inn}\,\mathcal{A}$, and analogously for $v = v_1 + v_2 + v_3$, then

$$\mathcal{G}(u,v) = \bar{g}(u_1,v_1) + \bar{k}(u_2,v_2) + h(u_3,v_3),$$

where $\bar{g}:\mathrm{Der}_{\mathrm{Hor}}\mathcal{A}\times\mathrm{Der}_{\mathrm{Hor}}\mathcal{A}\to Z$ is evidently the lifting of the metric $g:\mathcal{X}(M)\times\mathcal{X}(M)\to C^\infty(M)$ on space-time M, i.e.,

$$\bar{g}(u_1,v_1) = \pi_M^*(g(x,y)),$$

where $x,y\in\mathcal{X}(M)$. We assume that the metrics $\bar{k}:\mathrm{Der}_{\mathrm{Ver}}\mathcal{A}\times\mathrm{Der}_{\mathrm{Ver}}\mathcal{A}\to Z$ and $h:\mathrm{Inn}\,\mathcal{A}\times\mathrm{Inn}\,\mathcal{A}\to Z$ are of the Killing type. Their form will be determined below.

The preconnection is given by the Koszul formula,

$$(\nabla_u^* v)w = \tfrac{1}{2}[u(\mathcal{G}(v,w)) + v(\mathcal{G}(u,w)) - w(\mathcal{G}(u,v)) + \mathcal{G}(w,[u,v]) + \mathcal{G}(v,[w,u]) - \mathcal{G}(u,[v,w])]. \tag{1}$$

Let us now consider a more general situation which will later be specified to that in our model. Let $(\mathcal{A},*)$ be an algebra over $\mathbf{C}$, $Z=\mathcal{Z}(\mathcal{A})$ its center, and $\mathcal{V}$ a Z-module of derivations of the algebra $\mathcal{A}$. What follows is also valid if $\mathcal{Z}(\mathcal{A})=\{0\}$ and $Z=\pi_M^*(C^\infty(M))$ as in our model. We further assume that elements of Z play the role of constants for derivations of $\mathcal{V}$, i.e., $\mathcal{V}(Z)=\{v(f)=0: v\in\mathcal{V}, f\in Z\}$. Let us consider a metric $g:\mathcal{V}\times\mathcal{V}\to Z$; we assume the $Z-2$ linearity and symmetry of g, but not necessarily its nondegeneracy. Let us denote $\mathcal{V}^*=\mathrm{Hom}(\mathcal{V},Z)$, and $u^*=g(u,\cdot)=\Phi_g(u)$ is a one-form corresponding to the derivation $v\in\mathcal{V}$.

The symmetric two-form g determines the preconnection $\nabla^*:\mathcal{V}\times\mathcal{V}\to\mathcal{V}^*$ by the Koszul formula (1) (with $\mathcal{G}$ replaced by g). Since, by assumption, $\mathcal{V}(Z)=\{0\}$, one has $\nabla_u^*(fv)=f\nabla_u^* v$, and ∇^* is a $Z-2$ linear mapping, i.e., a tensor of (2,1) type. Moreover, from the Koszul formula it follows (even if g is degenerate) that

$$w(g(u,v)) = (\nabla_w^* u)(v) + (\nabla_w^* v)(u).$$

In the Koszul formula the first three terms vanish, and if we assume that

$$g(v,[w,u]) = g(u,[v,w]), \tag{2}$$

which—as we shall see below—is valid in our case, we obtain an interesting result

$$(\nabla_u^* v)(w) = g\left(\tfrac{1}{2}[u,v],w\right)$$

showing that there is a strict dependence between the (pre)connection and the metric. We should only look for a mapping $\nabla:\mathcal{V}\times\mathcal{V}\to\mathcal{V}$ that would be g-consistent with $\nabla^*:\mathcal{V}\times\mathcal{V}\to\mathcal{V}^*$, i.e., satisfying the condition

$$(\nabla_u^* v)(w) = g(\nabla_u v, w)$$

for every $u,v,w\in\mathcal{V}$. By comparison with (2), it immediately follows that

$$\nabla_u v = \tfrac{1}{2}[u,v]$$

for every $u,v\in\mathcal{V}$. Moreover, for a nondegenerate tensor g the mapping ∇, g-consistent with ∇^*, is unique. Indeed, since from

$$(\nabla_u^* v)(w) = g(\overset{1}{\nabla}_u v, w) = g(\overset{2}{\nabla}_u v, w),$$

for every $u,v\in\mathcal{V}$, it follows that

$$\overset{1}{\nabla}_u v = \overset{2}{\nabla}_u v.$$

It turns out that if g is nondegenerate, it has all properties required for connection. Let us check, for instance,

$$(\nabla^*_{u_1+u_2}v)(w) = (\nabla^*_{u_1}v)(w) + (\nabla^*_{u_2}v)(w) = g(\nabla_{u_1}v + \nabla_{u_2}v, w) = g(\nabla_{u_1+u_2} - \nabla_{u_1}v - \nabla_{u_2}v, w) = 0,$$

and, from the nondegeneracy of g, one has

$$\nabla_{u_1+u_2}v = \nabla_{u_1}v + \nabla_{u_1}v.$$

Therefore, we have proved the following proposition.

Proposition 3: Let $\mathcal{V}$ be a Z-module of derivations of an algebra $(\mathcal{A},*)$ such that $\mathcal{V}(Z)=\{0\}$. For every symmetric nondegenerate tensor $g:\mathcal{V}\times\mathcal{V}\to Z$, there exists one and only one connection g-consistent with the preconnection ∇^*. It is given by

$$\nabla_u v = \tfrac{1}{2}[u,v].$$

□

In the following, we shall assume the metric of the Killing form

$$g(u,v) = \mathrm{Tr}(u\circ v).$$

It satisfies the g-consistency condition. Indeed, from the trace definition we have

$$\mathrm{Tr}[w\circ u, v\circ u] = \mathrm{Tr}([w,u]\circ v) + \mathrm{Tr}([w,v]\circ u) = 0.$$

We now return to our model, and assume the above kind of metric for both $\mathrm{Der}_{\mathrm{Ver}}\,\mathcal{A}$ and $\mathrm{Inn}\,\mathcal{A}$, but in both these cases the trace should be defined differently.

We first define the metric for $\mathrm{Der}_{\mathrm{Ver}}\,\mathcal{A}$. We assume that G is a semisimple group. In this case, the Killing form reads

$$\mathcal{B}(V,W) = \mathrm{Tr}(\mathrm{ad}\,V\circ \mathrm{ad}\,W),$$

for $V,W\in \underline{g}$, where $\underline{g}$ is the Lie algebra of the group G, and $\mathcal{B}$ is nondegenerate. The tangent space to any fiber $E_x, x\in M$, is isomorphic to $\underline{g}$. Therefore, the metric $\bar{k}:\mathrm{Der}_{\mathrm{Ver}}\,\mathcal{A}\times\mathrm{Der}_{\mathrm{Ver}}\,\mathcal{A}\to Z$ is given by

$$\bar{k}(\bar{\bar{X}},\bar{\bar{Y}}) = \mathcal{B}(X(\pi_M(p)),\quad Y\ (\pi_M(p))).$$

To define the metric for $\mathrm{Inn}\,\mathcal{A}$, let us first define the trace for the algebra $\tilde{\mathcal{A}}$ (which, by Proposition 1, is isomorphic to the algebra $\mathcal{A}$), $\mathrm{Tr}:\mathcal{A}\to Z$, by

$$(\mathrm{Tr}\,a)(x) = \int_G a(x,g,g)\mathrm{d}g.$$

It has the following properties: (i) $\mathrm{Tr}(a+b)=\mathrm{Tr}\,a+\mathrm{Tr}\,b$, (ii) $\mathrm{Tr}(fa)=f\,\mathrm{Tr}\,a$, (iii) $\mathrm{Tr}(a*b)=\mathrm{Tr}(b*a)$, for $a,b\in\mathcal{A}$, $f\in Z$. From the last property it follows that

$$\mathrm{Tr}([a,b]) = 0,$$

and, of course, $\mathrm{Tr}\circ\mathrm{ad}\,a=0$.

Let us now turn to the submodule $\mathrm{Inn}\,\mathcal{A}$. We should notice that, on the strength of Lemma 2, we also have the connection $\tilde{\nabla}:\mathcal{A}\times\mathcal{A}\to\mathcal{A}$ on $\mathcal{A}$ given by

$$\tilde{\nabla}_a b = \tfrac{1}{2}[a,b].$$

We define the metric $h:\mathrm{Inn}\,\mathcal{A}\times\mathrm{Inn}\,\mathcal{A}\to Z$ by

$$h(\mathrm{ad}\,a,\mathrm{ad}\,b) = \mathrm{Tr}(a*b),$$

and the corresponding connection is

$$\nabla_{\mathrm{ad}\, a}\, \mathrm{ad}\, b = \tfrac{1}{2}[\mathrm{ad}\, a, \mathrm{ad}\, b].$$

We shall show that the metric h is nondegenerate. Indeed, let us assume that

$$\mathrm{Tr}(a * b) = \int_G \int_G a(x, g_{1,} g_2) b(x, g_2, g_1) \mathrm{d}g_2\, \mathrm{d}g_1 = 0.$$

If $a \neq 0$, then the support of this function is not of the measure zero, and by choosing the function $b(x, g_2, g_1) = a(x, g_1, g_2)$, we obtain

$$\int_G \int_G a^2(x, g_1, g_2) \mathrm{d}g_2\, \mathrm{d}g_1 \neq 0.$$

We conclude that if the metric is of the trace type (either $\mathcal{B}$ or Tr), the formula (2) is valid (for $g = \bar{k}$, or $g = h$).

V. CURVATURE

Let us introduce the following abbreviations:

$$V_1 = \mathrm{Der}_{\mathrm{Hor}}\, \mathcal{A}, \quad V_2 = \mathrm{Der}_{\mathrm{Ver}}\, \mathcal{A}, \quad V_3 = \mathrm{Inn}\, \mathcal{A}.$$

We continue to develop the geometry for $V_i, i = 1, 2, 3$. The curvature is

$$\overset{i}{R}: V_i \times V_i \times V_i \to V_i,$$

$$\overset{i}{R}(u, v)w = \overset{i}{\nabla}_u \overset{i}{\nabla}_v w - \overset{i}{\nabla}_v \overset{i}{\nabla}_u w - \overset{i}{\nabla}_{[u,v]} w.$$

If $j = 2, 3$, we have

$$\overset{j}{R}(u, v)w = \tfrac{1}{2}\big[u, \tfrac{1}{2}[v, w]\big] - \tfrac{1}{2}\big[v, \tfrac{1}{2}[u, w] - \tfrac{1}{2}[[u, v], w] = -\tfrac{1}{4}[[u, v], w].$$

Here we have made use of the Jacobi identity.

For every endomorphism $T: V_i \to V_i$, $i = 1, 2$, there exists $\mathrm{Tr}\, T \in Z$ satisfying the usual trace conditions. We thus can define

$$\overset{i}{R^m}_{uwm}: V_i \to V_i,$$

$$\overset{i}{R}_{uw}(v) = \overset{i}{R}(u, v)w,$$

and

$$\overset{i}{\mathbf{ric}}: V_i \times V_i \to Z$$

$$\overset{i}{\mathbf{ric}}(u, v) = \mathrm{Tr}\, \overset{i}{R}_{uw}.$$

We also define the *adjoint Ricci operator*,

$$\overset{i}{\mathbf{ric}}(u,w) = \overset{i}{\mathcal{G}}(\overset{i}{\mathcal{R}}(u),w), \tag{3}$$

where we have introduced the notation $\bar{g}=\overset{1}{\mathcal{G}}$, $\bar{k}=\overset{2}{\mathcal{G}}$. If the metric $\overset{i}{\mathcal{G}}$ is nondegenerate, there exists the unique $\overset{i}{\mathcal{R}}$ satisfying Eq. (3) for every $v \in V_i$.

The *curvature scalar* is

$$\overset{i}{r} = \operatorname{Tr} \overset{i}{\mathcal{R}} \in Z.$$

In the module V_2 there exists the usual trace operator which, in the local basis, can be written as the trace of the operator matrix. Therefore,

$$\overset{2}{R}_{uv}(w) = \tfrac{1}{4}[w,[u,v]] = \tfrac{1}{4}(\operatorname{ad} w \circ \operatorname{ad} u)(v),$$

and we have

$$\overset{2}{R}_{uw} = \tfrac{1}{4}(\operatorname{ad} w \circ \operatorname{ad} u)$$

for every $u,w \in V_2$, and

$$\operatorname{Tr} \overset{2}{R}_{uw} = \tfrac{1}{4}\operatorname{Tr}(\operatorname{ad} w \circ \operatorname{ad} u).$$

Hence,

$$\overset{2}{\mathbf{ric}}(u,w) = \tfrac{1}{4}\bar{k}(u,w) \tag{4}$$

for every $u,w \in V_2$, which can be regarded as a generalized Killing form. By analogy, we postulate

$$\overset{3}{\mathbf{ric}}(u,w) = \alpha h(u,w), \tag{5}$$

$\alpha \in Z$, for every $u,w \in V_3$.

The "Ricci scalar" can be determined from the generalized Einstein equation

$$\overset{3}{\mathbf{ric}}(u,v) - \tfrac{1}{2} r h(u,v) = 0$$

or

$$\alpha h(u,v) - \tfrac{1}{2} r h(u,v) = 0.$$

Hence we obtain

$$\left(\alpha - \tfrac{1}{2} r\right) h(u,v) = 0,$$

and

$$\alpha = \tfrac{1}{2} r.$$

We can symbolically regard $r \in Z$ as a trace of the Ricci operator $\mathcal{R}$. The Ricci 2-form is thus proportional to the metric tensor h, and the proportionality coefficient (up to factor 2) is a counterpart of the Ricci curvature scalar.

A counterpart of Eq. (3) for V_3 is

$$\overset{3}{\mathbf{ric}}(u,v) = h(\overset{3}{\mathcal{R}}(u),v). \tag{6}$$

Hence

$$\alpha h(u,v) = h(\overset{3}{\mathcal{R}}(u),v),$$

or

$$h(\alpha u,v) = h(\overset{3}{\mathcal{R}}(u),v),$$

and finally,

$$\overset{3}{\mathcal{R}}(u) = \alpha u.$$

Let us notice that for a commutative algebra we have $\alpha=0$, and the sector corresponding to V_3 vanishes. Therefore, the coefficient α could be regarded as a "measure" of noncommutativity.

This concludes the construction of the noncommutative groupoid geometry. The transition from this geometry to the usual space-time geometry can be done by the following "averaging" procedure. If $a \in \mathcal{A}$ then we have the isomorphism $a(p,g)=\tilde{a}(x,g_1,g_2)$, and we define

$$\langle\tilde{a}\rangle(x) = \int_G \tilde{a}(x,g,g)\mathrm{d}g.$$

It is clear that $\langle\tilde{a}\rangle \in C_c^\infty(M)$, and from the algebra $C_c^\infty(M)$ one can reconstruct the usual space-time geometry together with the usual Einstein equations.[7]

VI. GENERALIZED EINSTEIN'S EQUATION

We have all geometric quantities necessary to write the counterpart of Einstein's equation on the groupoid Γ. We stipulate that in the noncommutative regime at the fundamental level, there is only a "pure noncommutative geometry," and all necessary "matter terms" will somehow emerge out of it. We thus assume that there is no counterpart of the energy-momentum tensor and, consequently, the generalized Einstein's equation is of the form

$$\mathcal{R} - \tfrac{1}{2} r\,\mathrm{id}_V = 0, \tag{7}$$

where $\mathcal{R}$ is the Ricci operator defined by Eq. (3) (superscipt $i=1,2$ is omitted but presupposed), and $r=\mathrm{Tr}\,\mathcal{R}$.

It is clear that Eq. (7), for $V=V_1$, is a "lifting" of the usual Einstein equation on space-time M to the groupoid Γ, and if g solves this equation on M then $\bar{g}$ solves Eq. (7).

Let us now consider the case $V=V_2$. By comparing Eq. (3) with Eq. (4) and noticing that $\frac{1}{4}\bar{k}(u,v)=\bar{k}(\frac{1}{4}u,v)$, one obtains

$$\overset{2}{\mathcal{R}} = \tfrac{1}{4}\mathrm{id}_{V_2}.$$

Similarly, for $V=V_3$, by taking into account Eq. (5) and comparing it with Eq. (4), we obtain

$$\overset{3}{\mathcal{R}} = \alpha\,\mathrm{id}_{V_3}.$$

Let us consider the $\mathcal{G}$-orthogonal sum $V=V_1\oplus V_2\oplus V_3$. For the Ricci operator $\mathcal{R}:V\to V$ we have $\mathcal{R}(V_i)\subseteq V_i$, $i=1,2,3$, and $\mathcal{R}\,|\,V_i=\overset{i}{\mathcal{R}}$. This leads to the eigenvalue equation

$$\mathcal{R}(u) = \lambda u$$

for $u \in V$. This eigenvalue problem has the following solutions:

(1) $\lambda_1 = \frac{1}{2}r$ where r is the Ricci scalar curvature for the metric tensor $\bar{g}$. We thus have the equation

$$\mathcal{R}(u) - \tfrac{1}{2}ru = 0$$

for $u \in V_1$, and each such u satisfies this equation. It can be easily checked that this equation reduces to the equation $\mathcal{R}=0$ on space-time M.

(2) $\lambda_2 = \frac{1}{4}$ which leads to the equation

$$\mathcal{R}(u) - \tfrac{1}{4}u = 0$$

for $u \in V_2$.

(3) $\lambda_3 = \alpha$ leading to the equation

$$\mathcal{R}(u) - \alpha u = 0$$

for $u \in V_3$. In the commutative case $\alpha=0$ and we obtain $\mathcal{R}(u)=0$ (on the groupoid Γ).

VII. QUANTUM SECTOR

The quantum sector of our model is obtained by the regular representation of the groupoid algebra $\mathcal{A}$ in a Hilbert space $\mathcal{H}^p = L^2(\Gamma^p)$, $p \in E$,

$$\pi_p : \mathcal{A} \to \mathcal{B}(\mathcal{H}^p),$$

where $\mathcal{B}(\mathcal{H}^p)$ denotes the algebra of bounded operators on $\mathcal{H}^p$, given by

$$(\pi_p(a)\psi)(\gamma) = \int_{\Gamma_{d(\gamma)}} a(\gamma_1)\psi(\gamma_1^{-1} \circ \gamma)\mathrm{d}\gamma_1,$$

where $a \in \mathcal{A}$, $\psi \in \mathcal{H}^p$, γ, $\gamma_1 \in \Gamma$. Let us notice that the Haar measure on the group G, transferred to the fibers of Γ, forms a Haar system on Γ.[16]

We shall show that every element $a \in \mathcal{A}$ generates a random operator r_a on $(\mathcal{H}^p)_{p \in E}$. By a *random operator* r we mean a family of operators $(r_p)_{p \in E}$, i.e., a function

$$r : E \to \bigsqcup_{p \in E} \mathcal{B}(\mathcal{H}^p)$$

such that

(1) the function r is measurable in the following sense: if $\xi_p, \eta_p \in \mathcal{H}^p$ then the function

$$E \ni p \mapsto (r(p)\xi_p, \eta_p) \in \mathbf{C}$$

is measurable with respect to the manifold measure on E;

(2) the function r is bounded with respect to the norm,

$$\|r\| = \operatorname{ess\,sup}\|r(p)\|,$$

where ess sup means the "supremum modulo zero measure sets."

Random operator r acts, in fact, on cross sections of the Hilbert bundle $\mathcal{H} = \sqcup_{p \in E}\mathcal{H}^p$.

It can be easily seen that the family of operators $r_a = (\pi_p(a))_{p \in E}$ is a random operator. Indeed, if $\xi_p, \eta_p \in L^2(\Gamma^p)$ then we have the scalar product

$$\left(\int_{\Gamma^p} \pi_p(a)\xi_p, \eta_p\right) = \int_{\Gamma^p} \left(\int_{\Gamma_{d(\gamma)}} a(\gamma_1)\xi_p(\gamma_1^{-1}\circ\gamma)\mathrm{d}\gamma_1\right)\overline{\eta_p(\gamma)}\mathrm{d}\gamma,$$

and the Haar measure is transferred from G to Γ^p for each $p \in E$. Therefore, condition (1) is satisfied.

To check condition (2) let us introduce the isomorphisms of Hilbert spaces $I_p: L^2(G) \to \mathcal{H}^p$ given by the formula

$$(I_p\psi)(pg^{-1}, g) = \psi(g)$$

for $\psi \in L^2(G)$. Let us consider the operators $\tilde{\pi}_p(a) = I_p^{-1} \circ \pi_p(a) \circ I_p$. It is clear that $\|\pi_p(a)\| = \|\tilde{\pi}_p(a)\|$. Let us also notice that

$$\tilde{\pi}_{pg}(a) = R_{g^{-1}} \circ \tilde{\pi}_p(a) \circ R_g$$

[where R_g denotes the right translation operator in the space $L^2(G)$], which entails the (unitary) invariance of the norm

$$\|\pi_{pg}(a)\| = \|\pi_p(a)\|.$$

Hence, the norm $\|\pi_p(a)\|$ depends only on $x = \pi_M(p) \in M$; therefore, the function $x \mapsto \|\pi_p(a)\|$ is well defined, compactly supported, and continuous (in its dependence on x) on M.

Let $\mathcal{M}$ denote the set of all equivalence classes (modulo equality almost everywhere) of random operators $r_a, a \in \mathcal{A}$. It forms a von Neumann algebra; we shall call it the *algebra of random operators of the groupoid* Γ, or simply the *von Neumann algebra of the groupoid* Γ. We shall show that $\mathcal{M}$ is a semifinite algebra and, consequently, that it admits a "modular evolution," just like in the model with a finite group G.[17] To this end, let us first recall some important concepts.

A von Neumann algebra $\mathcal{M}$ is *semifinite* if there exists a faithful, normal, semifinite weight φ on $\mathcal{M}$ which is a trace.

(i) A linear functional $\varphi: \mathcal{M} \to \mathbf{C}$ is a *state* on $\mathcal{M}$ if $\varphi(r) \geqslant 0$ for every $r \in \mathcal{M}_+$, where $\mathcal{M}_+ = \{x \cdot x^* : x \in \mathcal{M}\}$ is the subset of positive elements of $\mathcal{M}$ and $\varphi(1) = 1$.

(ii) A functional $\varphi: \mathcal{M}_+ \to [0, \infty]$ is a *weight* if φ is additive, i.e., $\varphi(x+y) = \varphi(x) + \varphi(y)$, and positively homogeneous, i.e., $\varphi(\lambda x) = \lambda\varphi(x)$, for $\mathbf{R} \ni \lambda \geqslant 0, x, y \in \mathcal{M}$. We additionally assume $\lambda + \infty = \infty$, $\lambda \cdot \infty = \infty$ if $\lambda \neq 0$, and $\lambda \cdot \infty = 0$ if $\lambda = 0$. Let us notice that every state defines a weight.

(iii) A weight φ is *faithful* if for $r \in \mathcal{M}_+$ one has $\varphi(r) = 0 \Rightarrow r = 0$.

(iv) The sufficient and necessary condition for a weight φ to be *normal* is $\varphi(x) = \Sigma_i \omega_i$ for a family $\{\omega_i\}$ of normal states, i.e., $\omega(r) = \mathrm{Tr}(\rho r)$, $\mathrm{Tr}\{\rho\} = 1$.[20]

(v) Let us define $D_\varphi := \{x \in \mathcal{M}_+ : \varphi(x) < \infty\}$ and $\mathcal{M}_\varphi := \mathrm{Span}_{\mathbf{C}}(D_\varphi)$, i.e., $\mathcal{M}_\varphi$ is the space of $\mathbf{C}$-linear combinations of elements of D_φ. A weight φ is *semifinite* if $\mathcal{M}_\varphi$ is σ weakly dense in $\mathcal{M}$ (Ref. 20, p. 56).

(vi) A weight φ is a trace if $\varphi(r^* \cdot r) = \varphi(r \cdot r^*)$, for every $r \in \mathcal{M}$.

Proposition 4: The von Neumann algebra $\mathcal{M}$ *of the groupoid* Γ *is semifinite.*

Proof: We can consider the von Neumann algebra $\mathcal{M}$ as an algebra of bounded operators on the Hilbert space $H = L^2_G(E, \mathcal{H})$ of G-covariant square-integrable sections of the bundle $\mathcal{H}$. H is isomorphic to $L^2_G(E, L^2(G)) \simeq L^2(M \times G)$. The latter space is separable ($M \times G$ is a locally compact manifold). We choose the Hilbert basis $\{\psi_k\}_{k=1}^{\infty}$ in H, and define the weight $\varphi: \mathcal{M}_+ \to [0, \infty]$ by

$$\varphi(r) = \sum_{k=1}^{\infty} (r\psi_k, \psi_k).$$

This weight is clearly faithful and trace. It is also normal since $\varphi_i = \Sigma_{i=1}^{\infty} \omega_i$ where ω_i is given by $\omega_i(r) = \mathrm{Tr}(r\rho_i)$ with ρ_i being the projection onto the basis vector $\psi_i \in H$.

To show that φ is semifinite, let us notice that we have the net of finite-dimensional projections P_α such that $\varphi(P_\alpha)<\infty$ and $\lim P_\alpha=\mathbf{1}$, in strong topology, i.e., for every $h\in H$ one has $P_\alpha h=h$. And this is the necessary and sufficient condition for φ to be semifinite (Ref. 20, p. 57).□

The fact that the von Neumann algebra $\mathcal{M}$ is semifinite ensures that it admits a modular group of automorphisms (Ref. 20, Chap. 2). In our case, this group can be defined for a state (the assumption that φ is a weight was necessary only to prove that $\mathcal{M}$ is semifinite). Let us consider a functional of the form

$$\varphi(r)=\int_E \mathrm{tr}(\hat{\rho}(p)r(p))\mathrm{d}\mu_E(p),$$

where $\hat{\rho}(p)$ is a positive operator of trace class in $\mathcal{B}(\mathcal{H}^p)$, for every $p\in E$. Let $\{e_i\}$ be a basis in $\mathcal{H}^p$ such that $\hat{\rho}(p)e_i=\lambda_i(p)e_i$, $\lambda_i>0$. We also postulate

$$\sum_{i=0}^{\infty}\lambda_i(p)=\lambda(p)<\infty$$

for almost every $p\in E$, and $\lambda(\cdot)\in L^1(E)$ with

$$\int_E \lambda(p)\mathrm{d}\mu_E(p)=1.$$

With these conditions the functional φ is a state, and it satisfies all conditions of the Tomita-Takesaki theorem. We thus can write the state dependent evolution of random operators $r\in\mathcal{M}$ as

$$\sigma_s^{\varphi}(r(p))=e^{isH^{\varphi}(p)}r(p)e^{-isH^{\varphi}(p)},$$

where $H(p)=\ln\hat{\rho}(p)$ and $\ln\hat{\rho}(p)e_i=(\ln\lambda_i(p))e_i$. After differentiating the above equation it can be rewritten as

$$\left.\frac{d}{\mathrm{d}s}\right|_{s=0} r_a(p,s)=i[H^{\varphi}(p),r_a(p)]. \tag{8}$$

This is a generalization of the Heisenberg equation of the standard quantum mechanics with the only difference that now the dynamics depends on the state φ. The fact we have just proved that the von Neumann algebra $\mathcal{M}$ is semifinite, has serious consequences in this respect. The Dixmier-Takesaki theorem (Ref. 5, p. 470) states that if $\mathcal{M}$ is semifinite then every state-dependent evolution is inner equivalent to the trivial one, i.e.,

$$U_s\sigma_s^{\varphi}(r(p))U_s^*=r(p)$$

for every $s\in\mathbf{R}$, where U_s is a unitary element of $\mathcal{M}$. This means that the state-independent evolution, obtained by the Connes-Nikodym-Radon construction (Ref. 20, p. 74), is trivial. To overcome this difficulty we should assume that the group G is a locally compact nonunimodular group. We will return to this problem in a forthcoming paper.

However, a dependence of dynamics on a state need not be a drawback when we are dealing with the Planck level. The theory of von Neumann algebras can be regarded as a noncommutative counterpart of the measure theory. In the commutative case there is only one interesting measure (the Lebesgue measure), whereas in the noncommutative case there is a great variety of measures (see, for instance Ref. 21). Each pair $(\mathcal{M},\varphi)$, where $\mathcal{M}$ is a von Neumann algebra and φ a state on $\mathcal{M}$ (usually assumed to be faithful and normal), is both a dynamic object and a probabilistic object. In this context, the fact that there are as many φ-dependent dynamics as are generalized probabilistic measures φ seems quite natural.

VIII. TRANSITION TO QUANTUM MECHANICS

Let $a^*(\gamma)=\overline{a(\gamma^{-1})}$, $a\in\mathcal{A}$, $\gamma\in\Gamma$, and let us denote by $\mathcal{A}_H$ the subset of all Hermitian elements of $\mathcal{A}$, i.e., such that $a^*=a$. If $a\in\mathcal{A}_H$ then $\pi^p(a)\in(\mathcal{B}(\mathcal{H}^p))_H$ since π_p is a $*$-representation of the algebra $\mathcal{A}$. In the following we shall consider the random operators of the form $r_a(p)=\pi_p(a)$. Such operator is Hermitian if $(r_a(p)\psi,\varphi)=(\psi,r_a(p)\varphi)$. Moreover, it is a compact operator for $a\in\mathcal{A}$, since a has compact support. On the strength of the spectral theorem for Hermitian compact operators in a separable Hilbert space, there exists in $\mathcal{H}^p$ an orthonormal countable Hilbert basis of eigenvectors $\{\psi_i\}_{i\in I}$ of the Hermitian operator $r_a(p)$. We can write its eigenvalue equation as

$$r_a(p)\psi_i(p)=\lambda_i(p)\psi_i(p).$$

Let us notice that this equation is valid "for every $p\in E$" which reflects the fact that the random operator r_a is a family of functions indexed by $p\in E$. Therefore, with respect to a random operator it is meaningful to speak only about its eigenfunction $\lambda_i:E\to\mathbf{R}$ (not about its eigenvalue). However, every concrete measurement is always performed in a given local frame $p\in E$, and when such a measurement has been done the eigenfunction λ_i collapses to the eigenvalue $\lambda_i(p)$. Let us observe that from the perspective of the local measurement it looks as if the measurement result were a random effect, but in fact it is but a value of a well determined function $\lambda_i(p)$ at a given p. Its "randomness" comes from a subtler source, namely from the fact that r_a is a random operator. This is our model's version of the so often discussed "collapse of the wave function."

Let us also notice that a very act of measurement, performed at p, singles out the isomorphism $\Gamma_p^{-1}:\mathcal{H}^p\to L^2(G)$ which reproduces the usual quantum mechanics (on G). For instance, to obtain the quantum evolution for $a\in\mathcal{A}$, we apply Γ_p^{-1} to the left-hand side of Eq. (8), and I_p to its right-hand side. In this way, we obtain

$$\left.\frac{d}{dt}\right|_{t=o}\tilde{\pi}(a(t))=i[\tilde{H}^{\varphi},\tilde{\pi}(a(t))],$$

where $\tilde{\pi}(a)=\Gamma_p^{-1}\circ\pi_p\circ I_p$ and $\tilde{H}^{\varphi}=\Gamma_p^{-1}\circ H_p^{\varphi}\circ I_p$, we have also set $s=t$. This is the Heisenberg equation of the standard quantum mechanics with the only difference that it depends on the state φ. In more realistic models, to which the Connes-Nikodym-Radon construction applies, even this difference disappears (see remarks at the end of the preceding section).

The above results seem to be important as far as the interpretation of quantum mechanics is concerned. Its peculiarities are largely due to the fact that it is but a part of a larger structure, out of which it is cut off by every act of measurement. When such an act is performed the larger structure "collapses" to its substructure known as quantum mechanics. Quantum mechanics turns out to be but a theory of making measurements within our model.

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Causal sites as quantum geometry

J. Daniel Christensen[a)]
Department of Mathematics, University of Western Ontario, London, Ontario, N6A 5B7 Canada

Louis Crane[b)]
Mathematics Department, Kansas State University, Manhattan, Kansas 66506

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We propose a structure called a causal site to use as a setting for quantum geometry, replacing the underlying point set. The structure has an interesting categorical form, and a natural "tangent 2-bundle," analogous to the tangent bundle of a smooth manifold. Examples with reasonable finiteness conditions have an intrinsic geometry, which can approximate classical solutions to general relativity. We propose an approach to quantization of causal sites as well. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2138043]

I. INTRODUCTION AND PHYSICAL MOTIVATION

This paper is part of a program to found quantum gravity in relational topology, more precisely, to replace point set topology with a special type of category as the underlying structure on which to put geometrodynamics.

Physically, the idea is that what we actually observe are interactions between bounded regions of space-time. These could be either material systems or regions of empty space whose causal effects can be directly or indirectly distinguished by material systems. There should be a direct mathematical description of the flow of information between the regions, and points should appear only relative to an observer, as minimal distinguished regions. We will propose a specific axiomatic structure for a type of category which would contain the regions as objects and the relationships between them as different types of morphisms. The hope is that this would lead to a description of quantum physics free from ultraviolet divergences, by eliminating the underlying point set continuum.

Since categories as generalizations of topological spaces are well known in mathematics, where they are referred to as *sites* (Artin, 1962; Mac Lane and Moerdijk, 1992), we are calling our new structures *causal sites*. Strictly speaking, a site is a category together with a structure called a "Grothendieck topology," which is the analog of a topology for an ordinary space. We will explain below that our axioms also involve a structure very similar to a Grothendieck topology.

This paper will mainly discuss the "topological" side of the problem, i.e., the structure of the causal sites themselves. We discover that, unlike manifolds, causal sites with suitable finiteness conditions have an intrinsic geometry. Thus the distinction between topology and geometry is bridged over in our new picture. Examples are described which reproduce the classical solutions to general relativity above the Planck scale. We briefly consider the possibility of directly quantizing causal sites, thus directly producing a quantum theory of general relativity.

We will then briefly consider the appropriate classes of presheaves over causal sites, namely unitary and bisimplicial prestacks. We hope this can serve as a bridge between the topological aspects of causal site theory and the problem of constructing quantum physics over them. We will make some remarks as to how to construct a model for quantum gravity at the end.

[a)]Electronic mail: jdc@uwo.ca
[b)]Electronic mail: crane@math.ksu.edu

A very important feature of the topology of causal sites is that they have a tangent 2-bundle, which is analogous to the tangent bundle of a manifold. We believe this will serve as a setting for applications to quantum geometry and physics.

The structure of *causal sites* is a synthesis of two constructions, one well known from homotopy theory and algebraic geometry, the other familiar in the relativity literature. A *site* (Artin, 1962) is a category thought of as a generalization of the lattice of open sets of a topological space, with a distinguished family of covers for objects. (We warn the reader that our construction does not fully conform to the accepted definition of a site, since the covers in it do not satisfy the axioms of a Grothendieck topology, as explained below.) The morphisms of the category represent an abstract version of containment. Doing sheaf theory over such generalized spaces is an important part of modern mathematics.

On the other hand, a *causal set* (Sorkin, 2003; Hawkins *et al.*, 2003), or partially ordered set, is a discrete point set approximating the causal structure of a space-time manifold.

Now, since up to this point nobody has tried to use sites as a foundation for relativity, the natural structure that occurs when we combine the two ideas has never been considered. We will show that it is surprisingly rich and elegant.

Since causal sets are well known as models for general relativity, let us mention some of their similarities and differences with causal sites. Causal sites with a suitable finiteness condition have an intrinsic metric structure, as mentioned above. It is defined by counting the length of a maximal causal chain. This is quite similar to the intrinsic metric of a discrete causal set (Sorkin, 2003). We believe the greater flexibility of the families of regions in a causal site will mean they give much better approximations to the geometry of space-times than causal sets do. There can be infinitely many regions intermediate between two given ones in a causal site, and yet causal paths can have a finite maximal length, as we show in examples below. While random causal sets which approximate Minkowski space are believed to reproduce Lorentz invariance in the infinite volume limit, examples of causal sites which approximate Minkowski space have an invariance under germs of the Lorentz group on bounded regions as well. As models for general relativity, causal sites can be studied in many of the same ways as causal sets. Mathematically, causal sites are a "categorification" of causal sets.

The fundamental mathematical observation is that both the containment structure of a site and the causal structure of a causal set can be described as partial orders. As we will explain in Sec. V, these two partial orders give rise to a natural bisimplicial set which we call the elementary classifying space of the causal site. From this point of view, certain collections of regions can be viewed as products of simplices, and these products are glued together in a well-defined way.

We also construct another bisimplicial set, which we call the physical classifying space. This turns out to be a "special" bisimplicial set, a type of bisimplicial set which corresponds to a weak 2-category (Tamsamani, 1995). This means that causal sites fall into a class of structure which is already studied, and that the family of simplicial presheaves over it is well understood.

We will argue at the end that this suggests an approach to doing quantum general relativity over causal sites, by putting state sum models on their tangent 2-bundles.

This paper is meant to open a number of lines of research. The contents are as follows: in Sec. II we present the axioms for a causal site and some simple consequences. In Sec. III we show how a causal site with suitable finiteness conditions can have an intrinsic geometry. In Sec. IV, we briefly discuss quantization of sites, and in Sec. V we discuss the simplicial and bisimplicial structures inherent in a causal site. In Sec. VI, we translate this into a bicategorical structure. Sections VII and VIII discuss the structure of the tangent spaces and tangent bundle, while Sec. IX discusses the general analog of a bundle for a causal site, namely a prestack. In Secs. X and XI we discuss how state sum models could emerge in a causal site. Section XII contains conclusions and outlook.

Categorical background: We freely make use of terminology and ideas from category theory. In particular, we assume basic familiarity with weak 2-categories, which are also called bicategories. Good references for this topic are Leinster, 2004, Chap. 1; Leinster, 1998; and Bénabou, 1967. We also give more specific references as needed.

II. THE AXIOMATIC STRUCTURE OF CAUSAL SITES

We are now going to axiomatize the structure of regions in a causal space-time.

Example 2.1: Let M be a Lorentzian manifold with no closed timelike curves and a global time orientation. For points p and r in M, write $p \ll r$ if there is a future-directed timelike curve from p to r, and let $D(p,r)$ be the set of all points q with $p \ll q \ll r$. We call $D(p,r)$ a *diamond*, and we say that a subset A of M is *bounded* if it is contained in a finite union of diamonds. For A and B bounded regions, write $A \subseteq B$ when A is a subset of B, and write $A \prec B$ when every point in region A is in the causal past of every point in region B. That is, for each a in A and b in B, $a \ll b$.

The motivation for the above definition of "bounded" is the following. If a subset A has compact closure, then it is bounded in the above sense. And if the manifold M is globally hyperbolic, then the converse holds. So for globally hyperbolic manifolds, bounded is equivalent to compact closure. However, in general, our completion axiom below is only satisfied if one allows regions without compact closure.

Below we list some properties that this set of regions has. We then want to consider more general systems satisfying the axioms. We believe the interesting examples will actually have fewer regions than the example above coming from a Lorentzian manifold.

Definition 2.2: A *causal site* is a set of "regions" with two binary relations denoted $\subseteq$ and $\prec$ satisfying the axioms below. If $A \subseteq B$ we say that A is a *subset* of B or that B *contains* A. If $A \prec B$ we say that A *precedes* B.

(1) $\subseteq$ is a partial order on the set of regions. This means that for all regions A, B, and C,
   (a) $A \subseteq B$ and $B \subseteq C$ implies $A \subseteq C$,
   (b) $A \subseteq A$,
   (c) $A \subseteq B$ and $B \subseteq A$ implies $A = B$.

(2) The partial order $\subseteq$ has a minimum element ϕ. This means that ϕ is contained in every region A. This uniquely determines ϕ, and ϕ is called the *empty region*.

(3) The partial order $\subseteq$ has *unions*. This means that for all regions A and B, there exists a region $A \cup B$ such that
   (a) $A \subseteq A \cup B$ and $B \subseteq A \cup B$;
   (b) if $A \subseteq C$ and $B \subseteq C$ then $A \cup B \subseteq C$.

   These requirements uniquely determine $A \cup B$, and the binary operation $\cup$ is automatically associative and commutative.

(4) $\prec$ induces a strict partial order on the nonempty regions. This means that for all nonempty regions A, B, and C,
   (a) $A \prec B$ and $B \prec C$ implies $A \prec C$,
   (b) A does not precede A.

(5) For all regions A, B, and C, $A \subseteq B$ and $B \prec C$ implies $A \prec C$.

(6) For all regions A, B, and C, $A \subseteq B$ and $C \prec B$ implies $C \prec A$.

(7) For all regions A, B, and C, $A \prec C$ and $B \prec C$ implies $A \cup B \prec C$.

(8) For all regions A and B, there exists a region B_A such that
   (a) $B_A \prec A$ and $B_A \subseteq B$,
   (b) if $D \prec A$ and $D \subseteq B$ then $D \subseteq B_A$.

   These requirements uniquely determine B_A, and B_A is called the *cutting* of A by B. Note that B_A can be empty.

(9) If A and C are nonempty regions such that $A \prec C$, and there exists a D with $A \prec D \prec C$, then there exists a B complete with respect to $A \prec C$. The definition of "complete" is below (Definition 2.5).

Definition 2.3: Regions A and B in a causal site are *disjoint* if the only region which is

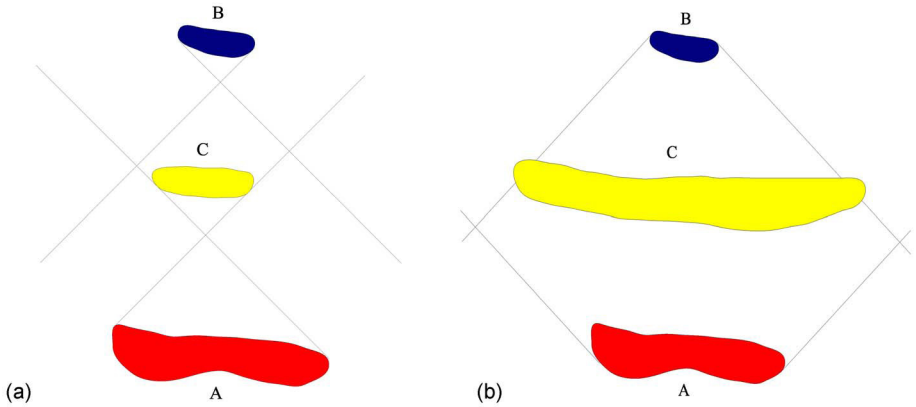

FIG. 1. (Color online) Comparing completions. (a) Completion. (b) Strong completions.

contained in both A and B is the empty region. More generally, a set of regions is *disjoint* if each pair of regions it contains is disjoint.

Note that if $A \prec B$ then A and B are disjoint.

Definition 2.4: Suppose S and T are sets of disjoint regions. If every region in S contains some region in T, we say that T is a *refinement* of S. That is, T is obtained from S by shrinking some regions and adding new regions.

A *causal path* P is a sequence $A_1 \prec A_2 \prec \cdots \prec A_m$ of nonempty regions. If $A \prec A_1$ and $A_m \prec B$, we say that P is a *causal path from A to B* and has *length* $m+1$. There is exactly one causal path of length 1.

A *refinement* of the causal path $A_1 \prec A_2 \prec \cdots \prec A_m$ is a causal path $C_1 \prec C_2 \prec \cdots \prec C_n$ such that $\{C_j\}$ is a refinement of $\{A_i\}$.

If P is a causal path from A to B, and $A' \prec A$, then P is also a causal path from A' to B. Analogous statements can be made when $A' \subseteq A$, $B \prec B'$ and $B' \subseteq B$. See Sec. VIII for more details.

Definition 2.5: If $A \prec B \prec C$, we say that B is *complete* for the causal pair $A \prec C$ if every causal path from A to C can be refined to a causal path from A to C one of whose members is contained in B. B is called a *completion of* $A \prec C$.

See Fig. 1 for an example of a completion. The final axiom of a causal site requires that completions exist. But note that they are rarely unique.

There are some elementary consequences whose proofs we leave to the reader.

Proposition 2.6: The following are true in any causal site.

(1) *For every region* A, $\phi \prec A$ *and* $A \prec \phi$.
(2) $B_A = B$ *iff* $B \prec A$.
(3) $B \subseteq C$ *implies* $B_A \subseteq C_A$.
(4) $B_A \cup C_A \subseteq (B \cup C)_A$. (*The reverse inclusion fails for some of our examples*.)
(5) *The collection of regions of a causal site which precedes a region B forms another causal site. When B is nonempty, this causal site is called the* local site *of B*.

Example 2.7: Let M be as in Example 2.1. Then the bounded regions in M, with the relations $\subseteq$ and $\prec$ defined earlier, satisfy the axioms.

We will check the nontrivial axioms. For the cutting axiom (Axiom 8), let B_A be the set of all points p such that $\{p\} \prec A$ and $p \in B$. This is bounded (contained in a finite union of diamonds) since B is.

For the completion axiom (Axiom 9 and Definition 2.5), a completion of $A \prec C$ can be taken

to be the set of all points p such that $A \prec \{p\} \prec C$. This is bounded because it is a subset of the diamond $D(a,c)$ for any points $a \in A$ and $c \in C$. (In general, this completion may not have compact closure.)

The remaining axioms are straightforward.

Example 2.8: Let $(M, \preccurlyeq)$ be any poset (partially ordered set) and let $\mathcal{P}(M)$ be the set of all subsets of M. We define $\subseteq$ to be the usual subset relation, and for A and B subsets of M, we say that $A \prec B$ iff $\forall a \in A \, \forall b \in B \; a < b$. (Note that we use the strict inequality $a < b$.) Then $\mathcal{P}(M)$, $\subseteq$, and $\prec$ form a causal site. A completion of $A \prec B$ can be taken to be $\{m \in M \,|\, \forall a \in A \, \forall b \in B \; a < m < b\}$.

Example 2.9: Let $(M, \preccurlyeq)$ be a poset such that $\{n \in M \,|\, m \preccurlyeq n \preccurlyeq m'\}$ is finite for each m and m' in M. Such a poset is called *locally finite* or a *causal set* (Sorkin, 2003). Let $\mathcal{P}'(M)$ be the set of finite subsets of M. Then $\mathcal{P}'(M)$ is a causal site using relations defined as in the previous example. The hypothesis on M ensures that completions exist.

While the axioms for a causal site were modelled on the example where regions are bounded subsets of a causally well-behaved Lorentzian manifold, and $A \prec B$ iff every element of A is in the causal past of every element of B, we can use the structure we have to define a weaker relation.

Definition 2.10: For regions A and B, write $A \preccurlyeq B$ if there exist nonempty subsets $A' \subseteq A$ and $B' \subseteq B$ with $A' \prec B'$ or $A' = B'$. We say that A *weakly precedes* B.

In the example of a Lorentzian manifold (Example 2.1), $A \preccurlyeq B$ iff some point of A is in the causal past of some point of B.

Note that $\preccurlyeq$ is not transitive. That is, $A \preccurlyeq B$ and $B \preccurlyeq C$ does not imply $A \preccurlyeq C$.

Definition 2.11: For regions A and B with $A \prec B$, we say that C is *strongly complete* for A and B if for all nonempty $A' \subseteq A$ and $B' \subseteq B$, any causal path from A' to B' can be refined to a causal path from A' to B' one of whose members is contained in C.

Note that we do not require that $A \prec C \prec B$, since a strong completion will rarely satisfy this. A strong completion is "wider" than an ordinary completion. See Fig. 1.

Definition 2.12: A region B is a *cover* of a region A if $B \prec A$ and if every causal path ending in A can be refined to a causal path ending in A one of whose elements is contained in B.

A finite set of regions $\{B_i\}$ is a *cover* of A if the union is a cover of A.

Remark 2.13: We can regard a causal site as a category whose objects are the regions by saying that there is one morphism from A to B if $A \prec B$ or $A = B$, and no morphisms otherwise. The collection of covers defined above has the feel of being a Grothendieck topology (Mac Lane and Moerdijk, 1992). But even if pullbacks exist in this category (they do, for example, in the case of Example 2.1), the pullback of a cover is not necessarily a cover.

Below we shall define a 2-category whose 1-arrows are all composable strings of arrows in this category, i.e., causal paths.

Definition 2.14: A causal site is *Noetherian* if every chain of strictly descending regions $A_1 \supset A_2 \supset A_3 \supset \cdots$ is finite. It is *locally Noetherian* if every local site is Noetherian.

Noetherian implies locally Noetherian.

The causal site $\mathcal{P}'(M)$ described in Example 2.9 is always Noetherian. If $M = \mathbb{N}$ with the usual order, then the causal site $\mathcal{P}(M)$ described in Example 2.8 is locally Noetherian but not Noetherian.

Definition 2.15: A nonempty region A in a causal site is an *absolute point* if it contains no subregions besides ϕ and A. If A and B are nonempty regions in a causal site, we say that A is a *relative point* for B if $A \prec B$ and for any C with $C \prec B$ either $A = A_C$ (i.e., $A \prec C$) or $A_C = \phi$.

If A is an absolute point and $A \prec B$, then A is a relative point for B. And if A is a relative point for B, then any nonempty subregion of A is also a relative point for B.

In Example 2.1, an absolute point is just a point in the usual sense, and every relative point is an absolute point.

In Examples 2.8 and 2.9, the absolute points are just the elements of the poset, but the relative points can be larger. For example, let Q be the poset $\{a, b, b', c\}$ with $a < b < c$, $a < b' < c$ and with b and b' unrelated. Then in the causal site $\mathcal{P}(Q)$, the subset $B = \{b, b'\}$ is a relative point for $C = \{c\}$. It is a union of the absolute points $\{b\}$ and $\{b'\}$.

We believe that because of the theorems that only a finite dimensional space of information can flow across horizons in general relativity (Flanagan *et al.*, 2000) there should be causal sites associated to Lorentzian manifolds which have interesting examples of relative points. The information contained in the relative position of a finite set of regions should exhaust what an external observer can see.

Definition 2.16: If A and B are regions in a causal site, we say that A is *amply pointed* with respect to B if $A \prec B$ and if $C, D \subseteq A$ then either C or D contains a relative point for B which the other does not, or $C=D$. A causal site is *amply pointed* if all causal pairs in it are.

Definition 2.17: A causal site which is locally Noetherian and amply pointed is a *grained world*.

In addition to the examples coming from causal sets, we believe that the family of Noetherian causal sites described in Sec. III produces grained worlds whenever there are no pairs of points connected by more than one Planck-scale geodesic. This still needs proof.

Although one can think of the regions in a causal site as like the bounded subsets of a causal space-time, we believe the interesting cases will be very different from such classical examples. The Noetherian property discussed above is an approach to imposing a Planck scale cutoff on the structure of a causal site.

III. THE INTRINSIC GEOMETRY OF CAUSAL SITES

It turns out that a causal site can contain more information than just the causal structure of a manifold. The reason is that a causal site may have a fundamental graininess which sets a length and time scale. Physically, this graininess is expected to occur at the Planck scale, and serves as a measuring rod or clock. Heuristically, a measurement at a smaller scale would result in the formation of black hole, so the maximum possible number of successive measurements along a timelike path gives its duration in Planck units.

Definition 3.1: A causal site is *causally finite* if for any two regions $A \prec B$, the length of any causal path from A to B is bounded above by a constant $M_{A,B}$.

We now want to interpret the least upper bound for the length of a causal path between two causally related regions as the discretized timelike separation between them in Planck units. This is quite similar to the notion of length in a discrete causal set in Sorkin, 2003.

We now give examples to show that the resulting geometry can be quite interesting.

Example 3.2: Consider Minkowski space. Recall from Example 2.1 that a diamond is a region $D(p,r)=\{q \mid p \ll q \ll r\}$. Define a *fundamental diamond* to be a region $D(p,r)$ where the proper time from p to r is 1. Consider the set of bounded regions which are unions of fundamental diamonds. Define $\subseteq$ and $\prec$ as in Example 2.1. This forms a causal site.

Let us check the nontrivial axioms. For the cutting axiom (Axiom 8), let B_A be the union of all fundamental diamonds D such that $D \prec A$ and $D \subseteq B$. This is bounded (contained in a finite union of diamonds) since B is. Note that it can happen that B_A is empty even though there are points of B which are in the past of A.

For the completion axiom (Axiom 9 and Definition 2.5), a completion of $A \prec C$ can be taken to be the union of all fundamental diamonds D such that $A \prec D \prec C$. This is bounded because it is a subset of the diamond $D(a,c)$ for any points $a \in A$ and $c \in C$.

The remaining axioms are straightforward.

Figure 2 gives two examples of fundamental diamonds. The timelike vectors shown have proper length 1.

The following theorem explains how this causal site captures the geometry of Minkowski space.

Theorem 3.3: *Let γ be a finite timelike geodesic segment in Minkowski space, starting at the point s and ending at t. In the causal site of Example 3.2, consider the causal paths $A_1 \prec \cdots \prec A_m$ with $s \in A_1$ and $t \in A_m$. Then the proper length of γ, rounded up to an integer, is equal to the least upper bound of the lengths of these causal paths.*

The key element of the proof is the observation that using fundamental diamonds in any other

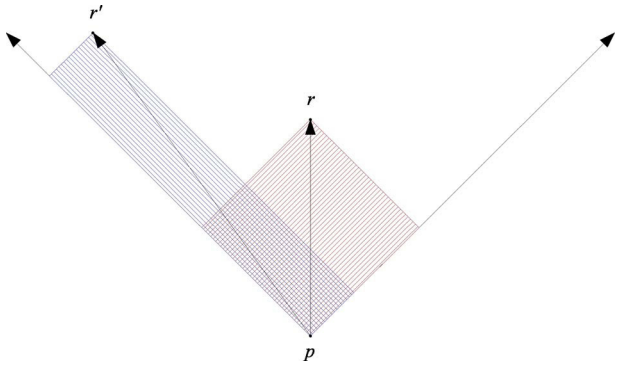

FIG. 2. (Color online) Fundamental diamonds.

rest frame than the one determined by the geodesic produces a shorter chain. This is clear from the above picture. In physical applications we would use units in which the Planck time is 1.

To handle curved space-times, we need to introduce the concept of stable causality. A Lorentzian manifold M is *stably causal* if it has no closed timelike curves, and every small perturbation of the metric g also has this property. This can be expressed by saying that there exists a metric h whose light cones are wider than those of g and such that h has no closed timelike curves. This condition is more physical than simply requiring no closed timelike curves, since measurements have only finite accuracy.

It is a nontrivial result (Hawking and Ellis, 1973, Prop. 6.4.9) that stable causality is equivalent to the existence of a global time function. In particular, a stably causal space-time is automatically time orientable.

Suppose that M is stably causal and we have chosen a time orientation. It is shown in Penrose, 1972 that since M is stably causal, the diamonds $D(p,r)$ determine the topology of M.

Example 3.4: Generalizing the previous example, let M be a stably causal Lorentzian manifold. Define a *fundamental diamond* to be a region $D(p,r)$ such that there is a future-directed timelike geodesic of length 1 from p to r. Consider the set of bounded regions which are unions of fundamental diamonds. Define $\subseteq$ and $\prec$ as in Example 2.1. This forms a causal site. The proof is the same as Example 3.2.

The following conjecture explains how these causal sites capture the large-scale geometric information of the manifold.

Conjecture 3.5: *Let M be a stably causal Lorentzian manifold whose sectional curvatures are much less than 1, and let* γ *be a timelike curve from s to t in M whose radius of curvature and length are large. In the causal site of Example 3.4, consider the causal paths* $A_1 \prec \cdots \prec A_m$ *such that each region* A_i *intersects* γ*. Then the proper length of* γ *is well approximated by the least upper bound of the lengths of these causal paths, with an error which is small compared to the length of* γ*.*

Of course, the precise statement of the error of the approximation in terms of the curvatures will require a more delicate analysis.

We believe this causal site reflects classical geometry more accurately than a causal set can. This is because we have enough relative points to adjust to any direction to get the best fit.

It is well known that the lengths of timelike curves (clock times), are enough to describe the geometry of a Lorentzian manifold completely. Thus our conjecture implies that any solution to general relativity whose sectional curvature is small compared to the Planck scale, with any type of matter whatsoever, can be approximated by the intrinsic geometry of a causally finite causal site with accuracy on the order of the Planck scale.

The causal sites discussed in this section have a fundamental graininess, but are nevertheless not Noetherian or locally Noetherian. It is not hard to invent modifications of our examples which would have stronger finiteness conditions and still recover interesting geometrodynamics. For

example, fix a discrete closed subspace L of Minkowski space and a discrete closed subspace S of the hyperboloid of unit timelike vectors. Now consider bounded regions R in Minkowski space which are unions of fundamental diamonds $D(l-s/2,l+s/2)$ centered on points l of L and pointing in directions s in S. Since R is bounded, it contains only finitely many points in L. Moreover, in any sufficiently boosted coordinate system, it would be too contracted to contain a fundamental diamond. Thus it only contains finitely many fundamental diamonds whose directions are contained in S and which are centered on points of L. Therefore this collection of regions forms a Noetherian causal site which reproduces the space-time geometry of Minkowski space at a large scale. Such a model is computationally accessible, and is a good candidate for quantization, as discussed below.

The discrete subspace L of Minkowski space could be chosen to be a random sprinkling of points, or a lattice. In a general manifold, L would have to be an irregular collection of points. If the manifold is globally hyperbolic, then one again obtains a Noetherian causal site.

Note that the use of fundamental diamonds is not crucial to any of the discussion in this section. One could use other shapes, such as "fundamental cylinders," which are regions formed by working in normal coordinates and taking the Cartesian product of a timelike interval of length 1 with a ball of radius 1 in the hyperplane orthogonal to the chosen timelike direction.

As yet, we do not know how to impose Einstein's equation on a causal site purely intrinsically.

IV. QUANTUM SITES

A causal site can be thought of as a large number of answers to questions, either telling us one region is inside another, or that one region can observe another.

The answers to these questions can be grouped together in certain good examples and reinterpreted as describing physically interesting geometries.

Therefore it is natural to reinterpret the statements that define a causal site as quantum observables and attempt to extract a quantum geometry from them. This could be a new avenue of attack on the problem of quantizing gravity.

It is not hard to see how to begin such a program. We could tensor together a finite dimensional Hilbert space for each pair of regions, and construct operators for containment and causal relatedness on each. The interesting part would be to see if suitable commutation relations could be found on the operators to reproduce Einstein's equation in the classical limit for suitable families of causal sites. We have not yet investigated this.

V. SIMPLICIAL STRUCTURES AND CAUSAL SITES

We first remind the reader of the relationship between partial orders and simplicial sets. A good reference for simplicial sets is Goerss and Jardine, 1999.

Roughly speaking, a *simplicial set* is a set of abstract simplices (points, edges, triangles, tetrahedra, etc.) with the faces of the simplices of dimension n identified with simplices of dimension $n-1$, thus gluing the simplices together into a combinatorial model of a space. The mathematically natural definition of a simplex includes an ordering of its vertices, and includes "degenerate" simplices in which some vertices are repeated. If X is a simplicial set, we write X_n for the set of n-simplices.

Associated to a given partially ordered set is a simplicial set which contains all of the information. An n-simplex of this simplicial set is a weakly ascending chain of length $n+1$. The face maps come from omitting one member of the chain, and the degeneracies from repeating one member.

Since the regions of a causal site have two partial orders on them, they have a natural description as the vertices of a bisimplicial set. Roughly speaking, a bisimplicial set is a collection of abstract cartesian products of pairs of simplices, with attachments along face maps corresponding to both simplicial factors separately. The product of a triangle with a tetrahedron, for example, has three faces which are edge $\times$ tetrahedron, and four which are triangle $\times$ triangle. If X is a bisimplicial set, we write $X_{m,n}$ for the set of (m,n)-bisimplices.

Let us give an explicit description of the bisimplicial set of a causal site. An (m,n)-bisimplex is a family $A_{i,j}$ of regions in the site, $i=0,\ldots,m$, $j=0,\ldots,n$, such that if $a<b$ then $A_{a,j}<A_{b,j}$ or $A_{a,j}=A_{b,j}$ and if $c<d$ then $A_{i,c}\subseteq A_{i,d}$. The two types of face maps come from omitting one value of i or j, and the two types of degeneracies from repeating items in the sequences.

Definition 5.1: The bisimplicial set associated to a causal site above is called its *elementary classifying space*.

Note that if X is any bisimplicial set, and we fix m, then there is a natural simplicial set $X_{m,\cdot}$ whose n-simplices are the (m,n)-bisimplices of X. We call $X_{m,\cdot}$ the *simplicial set of m-simplices*.

It is now an important observation that the elementary classifying space of a causal site satisfies the *Segal condition* (Leinster, 2002, Defn. Ta; Tamsamani, 1995). The Segal condition for a bisimplicial set has two parts. Translated into our situation, the first part states that the simplicial set of m-simplices is the subset of the product of m copies of the simplicial set of 1-simplices, where the adjacent 0-simplex objects are equal. More explicitly, it says that for each m and n, the natural map

$$X_{m,n}\to X_{m,1}\times_{X_{m,0}}\cdots\times_{X_{m,0}}X_{m,1}$$

must be a bijection. This is true for the elementary classifying space essentially because giving a chain $A_{i,0}\subseteq\cdots\subseteq A_{i,n}$ is the same as giving n chains $A_{i,0}\subseteq A_{i,1}$, $A_{i,1}\subseteq A_{i,2},\ldots,A_{i,n-1}\subseteq A_{i,n}$.

The second part of the Segal condition for bisimplicial sets is more subtle in general. The first part of the Segal condition tells us that for each m, the simplicial set $X_{m,\cdot}$ can be regarded as a category. The second part of the Segal condition then requires that for each m, the natural map

$$X_{m,\cdot}\to X_{1,\cdot}\times_{X_{0,\cdot}}\cdots\times_{X_{0,\cdot}}X_{1,\cdot}$$

must be an equivalence of categories. In our case, something stronger is true: for each m and n, the natural map

$$X_{m,n}\to X_{1,n}\times_{X_{0,n}}\cdots\times_{X_{0,n}}X_{1,n}$$

is a bijection. The reason this is true is similar to the reason that the first part of the Segal condition holds. And from this it follows that the categories above are equivalent.

Now let us describe the *Segal condition* for a simplicial set A. It simply states that there is exactly one n-simplex for each chain of n 1-simplices with the second vertex of the ith 1-simplex equal to the first vertex of the $i+1$st. That is, it states that the natural map

$$A_n\to A_1\times_{A_0}A_1\cdots\times_{A_0}A_1$$

is a bijection. This is true, for example, for the simplicial set associated to any partially ordered set. We will explain the importance of this condition below, when we study the relationship with category theory.

One point of all this is that we can completely capture the structure of a causal site as a combinatorially described space. This allows us to translate the problem of constructing physical theories on a causal site into the construction of presheaves over such a space, a problem which is well understood. Another is to join the concept of causal sites to the field of higher category theory.

Now we need to construct a modification of the elementary classifying space of a causal site. The modification will allow us to associate to a causal site a "special" bisimplicial set; see Tamsamani, 1995, where it is referred to as axiom C1, and Leinster, 2002, Defn. Ta.

Definition 5.2: A bisimplicial set X is *special* if the simplicial set $X_{0,\cdot}$ of 0-simplices is a disjoint union of points. In other words, all of the face and degeneracy maps between sets of the form $X_{0,n}$ are bijections.

This condition is important in category theory, because it is necessary for a bisimplicial set to be the nerve of a weak 2-category. As we shall see, this condition also plays a natural role when we try to construct models for quantum physical systems.

Now we want to define a new version of the classifying space of a causal site.

Definition 5.3: The *physical classifying space* of a causal site is the bisimplicial set whose (m,n)-bisimplices correspond to the following data:

(a) a sequence $A_0,\ldots,A_m$ of regions with $A_i \prec A_{i+1}$
(b) for each $i=0,\ldots,m-1$ and $j=0,\ldots,n$ a causal path C_i^j from A_i to A_{i+1}

such that for each i and j, the causal path C_i^j is a refinement of C_i^{j+1}. The two types of face maps are given by composition of rows and columns, respectively.

In this definition, refinements of causal paths play a central role. The physical motivation for this is the goal of writing discrete analogs of Feynman path integrals by summing effects of propagation along causal paths with the same beginning and end. Mathematically, we will see below that the (m,n)-bisimplices of the physical classifying space fit together to form a weak 2-category, because the initial and final paths of a refinement share a common initial and final region.

We would like to formulate the idea that all the information of a causal site is contained in its physical classifying space. We therefore make the following tentative definition.

Definition 5.4: A causal site is *tractable* if its elementary and physical classifying spaces are homotopy equivalent.

We do not know which causal sites are tractable, or whether this will prove to be a useful way to formulate the idea that the physical classifying space "suffices."

Proposition 5.5: *The physical classifying space of a causal site is a special bisimplicial set satisfying the Segal condition*.

The proof is similar to the argument given for the elementary classifying space, including the fact that a stronger form of the second part of the Segal condition holds.

Thus, as we explain below, the physically natural idea of focussing on the causal paths of a causal site supplies the missing mathematical ingredient to replace a space-time with a weak 2-category. We think this is suggestive for our program of applying higher categorical ideas of topology to quantum physics.

VI. THE WEAK 2-CATEGORY STRUCTURE OF A CAUSAL SITE

There is a very strong connection between simplicial and multisimplicial sets and higher categories. We begin with a standard theorem about (1-)categories (Leinster, 2002, p. 34; Tamsamani, 1995).

Theorem 6.1: *There is a one-to-one correspondence between categories and simplicial sets satisfying the Segal condition*.

The connection can be described by taking the nerve of the category. This is a simplicial set with one n-simplex for each string of n composable morphisms in the category, with face maps given by compositions of pairs of adjacent morphisms and degeneracies given by inserting identity maps.

This theorem has recently been extended from categories to 2-categories by Tamsamani (Leinster, 2002, Defn. Ta; Tamsamani, 1995); he proved that there is a natural one-to-one correspondence between special bisimplicial sets satisfying the Segal condition and weak 2-categories.

The connection proceeds by taking the "2-nerve" of the 2-category. This is the bisimplicial set with $(0,0)$-bisimplices the objects of the 2-category, $(1,0)$-bisimplices the 1-morphisms in the 2-category, $(1,1)$-bisimplices the 2-morphisms in the 2-category. A general (m,n)-bisimplex is a doubly indexed array of mn 2-morphisms along with some additional data.

The analogy with the structure of the physical classifying space prompts the following definition.

Definition 6.2: If the causal path $A \prec P_1 \prec P_2 \prec \cdots \prec P_p \prec B$ is a refinement of the causal path $A \prec Q_1 \prec Q_2 \prec \cdots \prec Q_q \prec B$ then we say that there is a *chain inclusion* from the causal path $\{Q_j\}$ to the causal path $\{P_i\}$.

The *inclusion 2-category* of a causal site is the 2-category whose objects are regions, 1-morphisms are causal paths, and 2-morphisms are chain inclusions.

The inclusion 2-category of a causal site connects regions, processes between regions, and inclusions of processes. These are the elements which would go into a description of an experiment. A 2-functor on this 2-category would then give us a mathematical language in which to associate calculations to an experiment, by associating concrete mathematical structures and relations to the objects and processes.

As we shall discuss below, the state sum models for quantum gravity have a natural formulation in terms of 1- or 2-categories. Any two 2-categories are connected by a 2-category of functors, natural transformations and modifications. This means the categorical structure we have described gives us a sort of calculus for constructing physical models over causal sites using the state sum models as local physical data.

To put things simply, one could easily feel that passing from point sets to regions leads to a mathematical wilderness. The structure we have discovered has geometric, categorical and algebraic aspects which make available to us a large framework of definitions and theorems which can guide us to natural constructions of physical models. The natural definition of a physical model on a causal site is a type of functor on it. The definition could in principle be found without the categorical language, but it is a foolish cave explorer who throws away a light.

VII. BISIMPLICIAL PATCHES

The geometrical and physical applications of smooth manifolds largely grow out of the fact that to every smooth manifold we can naturally associate a tangent bundle. This develops from the more elementary fact that every point of a manifold has a neighborhood which can be described as a space of a fixed and familiar kind. In this section we propose such a neighborhood structure. In the next, we show how to construct an analog of the tangent bundle, but a relational, or 2-categorical one.

Definition 7.1: If A is a region in a causal site, the bisimplicial set of regions contained in it is its *bisimplicial patch*. This bisimplicial set sits naturally inside the elementary classifying space (Definition 5.1).

With this definition in place, it is possible to treat causal sites in a manner analogous to manifolds, by working on the local bisimplicial patches thought of as coordinate patches.

Simplicial and bisimplicial sets have a homotopy theory equivalent to the homotopy theory of topological spaces. This subtle mathematical fact should allow us to use the combinatorics of the bisimplicial patch as an approximation to the local topology of a region.

Definition 7.2: Let $R \subseteq R'$ be regions. The *bisimplicial patch* of the complement is the bisimplicial set of regions A which are contained in R' and disjoint from R. The *relative homotopy type* of R in R' means the homotopy type of the pair (X, Y) where X is the bisimplicial patch of R' and Y is the bisimplicial patch of the complement of R in R'.

Definition 7.3: A region R is an *n-ball* if it is contained in a region R' such that the relative homotopy type is that of an n-sphere.

A causal site is a *grained n-manifold* if every region is contained in a union of a finite number of n-balls.

VIII. THE TANGENT 2-BUNDLE

In a physical model on a causal site, we would like to think of information being transferred along causal paths. We will now describe a construction of a version of a tangent bundle for causal sites in which the regions contain just such information as can be observed along the causal paths, while the compositions and inclusions of causal paths have a natural action.

8.1. Causal paths: For $A \prec B$ we define $\mathrm{Path}(A, B)$ to be the set of causal paths from A to B. For any $A \prec B \prec C$ there is a natural composition map $\mathrm{Path}(A, B) \times \mathrm{Path}(B, C) \to \mathrm{Path}(A, C)$ which sends $A \prec P_1 \prec \cdots P_m \prec B$ and $B \prec Q_1 \prec \cdots Q_n \prec C$ to $A \prec P_1 \prec \cdots P_m \prec B \prec Q_1 \prec \cdots Q_n \prec C$. The composition map is injective.

For a region A, define the *future cone* of A to be $A\uparrow = \{B \,|\, A \prec B\}$ and define the *future tangent space* of A to be $A\Uparrow = \{A'\uparrow \,|\, A' \subseteq A\}$, the poset of future cones of subregions of A, ordered by

inclusion. The future cone $A\uparrow$ is a minimum element of $A\Uparrow$. For a region B, define the *past cone* of B to be $B\downarrow=\{A\,|\,A\prec B\}$ and define the *past tangent space* of B to be $B\Downarrow=\{B'\downarrow\,|\,B'\subseteq B\}$, ordered by inclusion. The past cone $B\downarrow$is a minimum element of $B\Downarrow$.

The relevance of these cones is that if $A_1\uparrow=A_2\uparrow$, then $\mathrm{Path}(A_1,B)=\mathrm{Path}(A_2,B)$ for any B. (This is an equality rather than a bijection because a path from A to B doesn't include the regions A and B.) More generally, if $A_1\uparrow\subseteq A_2\uparrow$, then $\mathrm{Path}(A_1,B)\subseteq\mathrm{Path}(A_2,B)$ for any B. Similarly, $B_1\downarrow\subseteq B_2\downarrow$ implies that $\mathrm{Path}(A,B_1)\subseteq\mathrm{Path}(A,B_2)$ for any A. Writing Fut for the poset $\{A\uparrow\}$ of all future cones and Past for the poset $\{B\downarrow\}$ of all past cones, this says that $\mathrm{Path}(-,-)$ is an order preserving map from the poset Fut$\times$Past to the poset Inc of sets and inclusions. In fancier language, $\mathrm{Path}(-,-)$ is a functor.

This has various consequences. For example, if $A'\subseteq A$, then $A'\uparrow\supseteq A\uparrow$ and so $\mathrm{Path}(A',B)\supseteq\mathrm{Path}(A,B)$ for any B. And if $A'\prec A$, then $A'\uparrow\supseteq A\uparrow$ and so again $\mathrm{Path}(A',B)\supseteq\mathrm{Path}(A,B)$ for any B. Similar reasoning shows that if $B'\subseteq B$ or $B'\succ B$ (note the reversal), then $B'\uparrow\supseteq B\uparrow$ and so $\mathrm{Path}(A,B')\supseteq\mathrm{Path}(A,B)$ for any A.

8.2. Causal paths subordinate to a given path: If we are given a causal path P from A to B, we can assign to any pair of subregions $A'\subseteq A$ and $B'\subseteq B$ the set $\mathrm{Path}_P(A',B')$ of causal paths from A' to B' which are refinements of P. As above, this defines a functor, in this case from $A\Uparrow\times B\Downarrow$ to Inc.

We next describe a 2-category which is a natural target for this construction.

Definition 8.1: Define a weak 2-category $\mathcal{PP}$ in the following way. The objects are pairs (F,P) of posets with minimum elements m_F and m_P. A 1-morphism from (F_1,P_1) to (F_2,P_2) is a functor from $F_1\times P_2$ to Inc. The composite of $S:F_1\times P_2\to\mathrm{Inc}$ with $T:F_2\times P_3\to\mathrm{Inc}$ is the functor $TS:F_1\times P_3\to\mathrm{Inc}$ defined by $TS(f,p)=S(f,m_{P_2})\times T(m_{F_2},p)$. If S and T are 1-morphisms from (F_1,P_1) to (F_2,P_2), i.e., functors from $F_1\times P_2$ to Inc, a 2-morphism from S to T is a natural family of injections $S(f,p)\to T(f,p)$.

Note that the composites $(TS)R$ and $T(SR)$ of 1-morphisms are in general not equal. Instead, there is a natural bijection between them. Thus $\mathcal{PP}$ is a *weak* 2-category. This also explains why the 2-morphisms allow arbitrary injections rather than just inclusions.

The horizontal and vertical compositions of the 2-morphisms of $\mathcal{PP}$ are given by Cartesian product and composition of injections, respectively. The coherence of $\mathcal{PP}$ is natural.

The discussion above can be summarized by saying that there is a weak 2-functor from the inclusion 2-category of our causal site to the weak 2-category $\mathcal{PP}$. This can be thought of as a prestack. It sends a region A to the pair $(A\Uparrow,A\Downarrow)$ of posets. It sends a causal path P from A to B to the functor $\mathrm{Path}_P(-,-)$ from $A\Uparrow\times B\Downarrow$ to Inc. And it sends a chain inclusion from P' to P (which means that P and P' are both causal paths from A to B, and P' is a refinement of P) to the natural family of inclusions $\mathrm{Path}_{P'}(A',B')\subseteq\mathrm{Path}_P(A',B')$. If P is a causal path from A to B and Q is a causal path from B to C, there is a natural injection $\mathrm{Path}_P(A',B)\times\mathrm{Path}_Q(B,C')\to\mathrm{Path}_{Q\circ P}(A',C')$, where $Q\circ P$ denotes the composite of P and Q.

Definition 8.2: We call this weak 2-functor the *tangent 2-bundle* of the causal site.

The tangent 2-bundle contains information about how causal paths can link the observable tangent spaces together. Since we can also refine causal paths, expansions into discretized path sums will be possible by decomposing intermediate regions into unions and summing over the families of refined paths which occur.

We think the analogy between smooth manifolds and causal sites may be a good guide to applications. We use the tangent bundle as a setting in order to apply calculus to the geometry of manifolds. Similarly, the local simplicial or bisimplicial structures on a site may enable us to apply the calculus of categorical state sums to quantum geometry on them. In constructing a quantum theory over a causal site, it should be possible to use the connecting complexes as discretized analogs of a Feynman path integral, and their 2-categorical structure should help constrain such a construction, allowing us to find interesting models just from the requirement of 2-functoriality.

IX. UNITARY PRESTACKS ON A CAUSAL SITE

In the next few sections, we investigate a more conventional approach to constructing geometrical or physical models on causal sites, namely, putting suitable presheaves and prestacks over them.

We will begin with a preliminary investigation of the type of physical model which the mathematical structure of a causal site suggests. We will not attempt to construct specific physically realistic models in this paper.

The original idea of a site was motivated by the fact that a presheaf over a topological space X is equivalent to a contravariant functor from the category of open subsets of X.

Since a bundle, including the tangent bundle of a manifold, can be regarded as a type of sheaf, we have a language for describing analogs of the basic structures underlying Yang-Mills theory and general relativity available for sites, although we will probably need stronger regularity assumptions to be able to create more precise analogs.

It is interesting that including a causal structure in our model, which traditionally is expressed by changing from a Riemannian to a Lorentzian metric, is expressed here by passage from a 1-category to a 2-category, a process which has been called categorification (Crane and Frenkel, 1994; Baez-Dolan, 1998).

This has the immediate consequence that rather than looking for models over a causal site within an ordinary category, such as the category of Hilbert spaces, we must turn to a 2-category, such as the category of 2-Hilbert spaces (Baez, 1996). Instead of a presheaf of Hilbert spaces, we work with a prestack of 2-Hilbert spaces. A prestack is a weak 2-functor from our causal site to a 2-category (Breen, 1994). In a prestack, a triangle of restriction morphisms only needs to commute up to a 2-morphism.

This means that rather than thinking of an assignment of a single Hilbert space to a region (something like the space of quantum states propagating through it), we assign to it a category of Hilbert spaces. Physically, we can think of this as related to the idea that the state space of a region has dimension related to the area of its boundary, so that if the geometry is itself a quantum variable, then the Hilbert space itself cannot be unique.

Indeed, if we tried to construct a physical theory over a causal site, we would quickly discover that we couldn't find a natural linear map to associate to containment, because of the nonlocal correlations in quantum theories. We would be trapped trying to map pure states to mixed states.

It actually provides an interesting new slant on the interpretation of quantum mechanics rewriting this process in terms of the different choices of Hilbert spaces in the categories corresponding to two regions, one of which contains the other.

Let us explain in a very simple situation, using the category 2-Vect (Kapranov and Voevodsky, 1994) rather than 2-Hilb, how this would look. Objects in 2-Vect are n-vector spaces, i.e., the category of all n-tuples of vector spaces for some n. Arrows in 2-Vect are functors defined by tensoring by some column of vector spaces. Thus, a (contravariant) functor from a causal site to 2-Vect would find the vector spaces which could appear on a subregion being combined into tensor products of vector spaces associated to a larger region.

Now there is neither a natural map $A \to A \otimes B$ nor $A \otimes B \to A$, so there would be no way to represent inclusion as a map on individual Hilbert spaces. This is a mathematically elegant way to express the existence of nonlocal correlations in compound systems in quantum mechanics. The overall rule which tells us how the different Hilbert spaces associated to regions are related has an elegant functorial form, which cannot be recovered on the individual Hilbert spaces. In Hawkins *et al.*, 2003, a similar problem was studied for models on causal sets, and it was discovered that maps between causally related points must be expressed as completely positive maps on spaces of mixed states (i.e., Hermitian operators over the Hilbert spaces, rather than the Hilbert spaces themselves). The setting we are exploring, combining both causality and containment, should contain examples of this, but set in a broader algebraic context.

Now we can ask ourselves which of the models which have appeared in mathematical physics would be good candidates for extending to a causal site. An obvious choice would be 2-Yang-

Mills theory (Baez, 2002; Girelli and Pfeiffer, 2003), which is a theory which puts a nonlinear partial differential operator on a 2-form, by analogy with the Yang-Mills equation on a 1-form.

Since 2-Yang-Mills theory has the interpretation of physics on the curvature of a gerbe, which is really a special type of stack of categories, it will have a direct generalization to causal sites.

X. A BRIEF REVIEW OF CATEGORICAL STATE SUM MODELS

Categorical state sums (Crane *et al.*, 1994; Barrett and Crane, 1998; Crane and Yetter, 2003; Noui and Roche, 2003; Crane *et al.*, 2001) are models of quantum geometry on simplicial complexes. They are constructed out of unitary representations of Lie groups or quantum groups, intertwining maps of these representations, and in some cases, 2-intertwiners. The maps are composed in closed patterns related to the combinatorics of the simplicial complex, traced, and summed over. The result is a discrete version of a path integral for quantum geometry, with the unitary representations acting as Hilbert spaces on which geometric quantities are represented as operators.

For example, in the model of Barrett and Crane, 1998, we have a four-dimensional simplicial complex. The 2-simplices (triangles) are labelled with unitary representations of the Lorentz group. We think of these as quantizations of the oriented area elements a geometry would assign to the faces, because oriented area elements can be identified with elements of the Lie algebra of the Lorentz group.

In fact, in order to impose the necessary constraints on the geometry, we restrict ourselves to a class of representations called the balanced ones. We then label the tetrahedra with a sum over the balanced intertwining maps between the four representations, trace over each 4-simplex, multiply, then sum over all possible choices of representations.

There are a number of models of this type, differing by the dimension, choice of symmetry group, constraints, etc. These amount to different choices of the geometry to be quantized.

This type of model is closely related to the ideas discussed above describing simplicial sets as categories. They can be written as sums of functors from the category associated to the complex to the category of representations of the geometrical symmetry group or quantum group.

In short, the categorical state sum picture makes it natural to assign a quantum geometry to a simplicial complex.

In the context of causal sites, this can be thought of as a candidate for local quantum geometry on a tangent space, analogously to the use of inner products on tangent spaces in classical Riemannian geometry.

One of the reasons that manifold theory was so important to the development of relativity was that it gives a natural concrete expression for the equivalence principle: laws must be expressed in tensor form. The categorical underpinning of the structure of causal sites suggests a similar principle in quantum gravity: laws must be expressed in functorial form. This simple and attractive principle will cut down the possibilities greatly.

Given that we already have subcategories which express the relational world seen by an observer, it is also a natural expression of the idea behind the equivalence principle, if we take the point of view that coordinate systems are idealized observers.

XI. STATE SUM MODELS ON CAUSAL SITES

The physically interesting examples of Sec. III all possess local symmetries. (Since a bounded region which is boosted too far no longer contains fundamental diamonds, a mathematical formalization of this would need to use actions of germs of the Lorentz or Poincare groups. We will not work this out in this paper.)

It therefore seems that the Hilbert spaces in a quantum site would group together in unitary representations of the Lorentz group.

Now one of the great challenges for our proposal is to find a way to derive Einstein's equation as a classical limit for some formulation of the dynamics on a quantum site. Categorical state sum models are interesting because the laws of combination of the representations produce a classical

limit which implies Einstein's equation. In other words, Einstein's equation is actually determined by the symmetry of the model, expressed in the tensor category of unitary representations of the Lorentz group.

Now is it possible that we can introduce categorical state sum models into a suitable family of causal sites with local symmetries? Let us try to imagine how that could arise.

In order to define a class of causal sites which would be physically realistic near the Planck scale, we have defined "grained worlds" above as locally Noetherian, amply pointed causal sites. We think of this as a way to embed facts about the limited amount of information which can flow between regions in general relativity into the fabric of spacetime itself.

The combination of these two properties means that given a causally related pair of regions $A \prec B$, we can find a finite set of relational points for B in A which in some sense exhaust the information which B can see in A. This would mean that the relational tangent space would be adequately described by a simplicial set, assuming the set of points did not contain one another.

This suggests that the state sum model of Barrett and Crane, 1998, or some similar model, might appear as a good approximation to the quantum theory of the part of a quantum site contained in a region.

This is probably a better setting for state sum models than direct application to a whole universe, since the finiteness of the simplicial set becomes better motivated.

Then, when we wanted to express the flow of information from one region, described by a state sum on a simplicial set, to another, along a given causal path, we would know that the map which described it would have to behave well when we included one causal path in another.

This includes the information flow law in a 2-categorical structure, which might be rich enough to allow us to determine it.

So a program suggests itself, to make a suitable set of assumptions on a prestack over a grained world, so that if we pass to a set of relational points the relative position information ends up containing all the transferred information, and takes the form of a state sum model.

At this point, we realize that our new point of view is making us ask a series of new questions about state sums which had no motivation in the past when they were thought of as stand alone models. We need to express the relationship between two state sum models when the complex of one is embedded in the other, we need to work out expressions for causal flows of information between state sums, and we need to investigate in what sense they approximate points with quantum variables between them as they grow far apart. If nothing else, the causal sites proposal has widened our perspective on state sum models.

XII. CONCLUSIONS AND FUTURE DIRECTIONS

We now have defined a new class of mathematical objects, which are not point sets, but which can function as a topological foundation for classical general relativity. We have families of examples corresponding to classical space-times, which include descriptions of the geometrodynamics of classical spacetimes above the Planck scale, without the inclusion of a metric tensor as a mathematical datum separate from the underlying space-time structure.

The representation of geometry by a causal site is analogous to the representation by a discrete causal set, but as we have discussed, it seems to give a much closer approximation. Our relative and absolute points should not be confused with ordinary points, either in manifolds or causal sets. They are not "atomic." For example, a union of a finite family of fundamental diamonds in a Lorentzian manifold can contain an infinite number of other fundamental diamonds. Nevertheless, the causality relationship between them gives rise to a finiteness or discreteness in the structure. It therefore makes a bridge between continuous and discrete structures in a new way. The hypothesis of overlapping minimal regions seems more physically natural to us than the discrete point sets of causal sets or categorical state sum models. It also means that the continuous or discrete symmetry properties of a causal site can be more robust than a causal set. In the examples we have constructed, the symmetry with respect to the Lorentz group is not broken, because we have fundamental diamonds in all reference frames. In the theory of causal sets, by contrast, it is only possible to recover the symmetry on the average in the infinite volume of Minkowski space

(Sorkin, 2003). The fact that we are able to produce a mathematical construction which combines a fundamental graininess with symmetry in local regions gives our construction added interest.

We think it will be interesting to try to find further families of examples, for instance to try to construct quantum n-manifolds neither related to causal sets nor directly derived from manifolds. Different classes of these might give new examples of "space-time textures," which could be explored as new settings for physical models. It may well be that the physical intuition expressed in the phrase "space-time foam" can find better expression in our setting that when constrained by the necessity of considering only families of smooth manifolds.

Causality and time are integrated into the mathematical structure of a causal site in a striking fashion: space-time appears as a categorification of space. The fact that causal sites can be considered either as bisimplicial sets or as 2-categories means we have a number of well-understood tools at our disposal for constructing examples.

In addition, the structure of a causal site seems to lend itself readily to quantization. We have not yet examined this in any detail.

We have, at this point, many more questions than answers. Can the geometric picture of Example 3.4 be generalized to more intrinsic models, i.e., models which have definitions not so directly dependent on a classical space-time? Can it be quantized? Since it seems natural to approach quantization by beginning with the family of containments of a particular causal site, it will be easier to find semiclassical states in this approach than in other approaches to quantum gravity.

It would seem that the Hilbert spaces arising from quantization of a causal site with local symmetries would decompose into unitary representations of the Lorentz group. Do the state sum models arise in such a picture? We should remind ourselves that Einstein's equation is almost determined by symmetry considerations. Would a quantization of a causal site with Lorentz symmetry which was required to respect the symmetry be nearly determined as well?

We also have not yet studied the description of curvature in causal sites, nor searched for a geometric way to impose Einstein's equation.

General relativity is intimately bound up with our ideas about space-time and geometry. Changing the foundation of these creates a situation in which all the questions of classical and quantum relativity can be reexamined. The large family of accessible examples we have constructed means that a fairly broad program can be practically implemented.

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Universal homogeneous causal sets

Manfred Droste[a)]
Institut für Informatik, Universität Leipzig, D-04109 Leipzig, Germany

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Causal sets are particular partially ordered sets which have been proposed as a basic model for discrete space-time in quantum gravity. We show that the class $\mathfrak{C}$ of all countable past-finite causal sets contains a unique causal set $(U, \leqslant)$ which is universal (i.e., any member of $\mathfrak{C}$ can be embedded into $(U, \leqslant)$) and homogeneous (i.e., $(U, \leqslant)$ has maximal degree of symmetry). Moreover, $(U, \leqslant)$ can be constructed both probabilistically and explicitly. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2147607]

I. INTRODUCTION

The causal set hypothesis asserts that the ultimate structure of space-time in quantum gravity is discrete, and that a fundamental relationship between points in space-time is causality, enabling us to say that x is in the past of y. Such a structure can be naturally modeled by partially ordered sets $(S, \leqslant)$ which are locally finite (i.e., any interval $[x,y]$ between two points x,y is finite) or which are even past-finite (i.e., the past of each point x is finite). Locally finite partially ordered sets are called causal sets and have been investigated in detail, cf. e.g., Refs. 3,14 and 16. Moreover, an interesting sequential growth dynamics for finite causal sets was investigated in Refs. 15, 5, and 4: a finite causal set can be extended by a single element z by adding it to the given partial order as a new maximal element (naturally, z cannot be in the past of any given element). Continuing in this way, one obtains a countable past-finite causal set. Conversely, any countable past-finite causal set can be built up this way. For further work on this dynamics, see, e.g., Refs. 1,10 and 12.

It is the goal of this paper to investigate the class of countable past-finite causal sets. We will show that there is a countable past-finite causal set $(U, \leqslant)$ which is universal and homogeneous. Here, *universal* means that $(U, \leqslant)$ contains an isomorphic copy of any countable past-finite causal set as a natural substructure. *Homogeneous* means that any isomorphism between two finite substructures (stems) of $(U, \leqslant)$ extends to an automorphism of $(U, \leqslant)$. Thus homogeneity intuitively says that $(U, \leqslant)$ has the highest possible degree of structural symmetry. Moreover, with these two properties, universality and homogeneity, $(U, \leqslant)$ is unique up to isomorphism in the class of all countable past-finite causal sets. Our proof employs the Fraïssé-Jónsson theorem well-known in model theory for constructions of homogeneous relational structures. We also give an explicit order-theoretic construction of the universal homogeneous past-finite causal set, and we show that the larger class of all countable causal sets (not requiring "past-finite"), in contrast, does not contain a universal object.

In our second result, we will describe a probabilistic construction of the universal homogeneous past-finite causal set $(U, \leqslant)$. Probabilistic procedures for constructing one-point extensions of finite causal sets were crucial for Refs. 15 and 10 and investigated in detail. Here we also propose a probabilistic construction. It is motivated by a classical construction of Erdös and Rényi[8] of the random graph (which is universal and homogeneous in the class of all countable graphs). More recently, a similar construction of the universal homogeneous countable partial

[a)]Electronic mail: droste@informatik.uni-leipzig.de

order was given in Ref. 7. If we employ the present probabilistic one-point extensions of finite causal sets successively, we obtain an infinite sequence of causal sets whose union is a countable past-finite causal set, the *random* past-finite causal set. Then we show that with probability 1, this random causal set is universal and homogeneous (hence unique up to isomorphism). Our construction of one-point extensions differs from the ones investigated in Ref. 15 in technical details, which we discuss briefly, and it would be interesting to investigate the relationship further. Finally, we describe a simple explicit number-theoretic construction of $(U,\leqslant)$. This is motivated by a classical construction of the random graph.[13] We close with a short discussion.

II. UNIVERSAL CAUSAL SETS

First we establish some terminology. For a fuller introduction to causal sets, see Ref. 16.

A partially ordered set (poset) is a pair $(S,\leqslant)$ where S is a set and $\leqslant$ is a binary relation on S which is reflexive, antisymmetric, and transitive. Let $(S,\leqslant)$ be a poset. For $x,y\in S$ we write $x<y$ to denote that $x\leqslant y$ and $x\neq y$. If $x<y$, we let $[x,y]=\{s\in S\,|\,x\leqslant s\leqslant y\}$, and for $x\in S$ let $\mathrm{past}_S(x)=\{s\in S\,|\,s\leqslant x\}$. Then $(S,\leqslant)$ is called *locally finite*, if each interval $[x,y]$ $(x,y\in S, x<y)$ is finite, and *past-finite*, if $\mathrm{past}_S(x)$ is finite for each $x\in S$. Clearly, any past-finite poset is locally finite (but not conversely as seen by the set of negative integers with their natural order). A *causal set* (or *causet*) is a locally finite poset. If $X\subseteq S$ is a subset, let $\mathrm{past}_S(X)=\cup_{x\in X}\mathrm{past}(x)$. If S is clear from the context, we also write $\mathrm{past}(x)$ and $\mathrm{past}(X)$. Then X is called a *stem of* S, denoted $(X,\leqslant)\lhd(S,\leqslant)$ or $X\lhd S$, if $\mathrm{past}(X)\subseteq X$ (note that here, in slight generalization of Ref. 16, we do not require X to be finite).

In Refs. 15 and 16, constructions of countable causal sets $(S,\leqslant)$ are given as unions of chains of finite posets $(A_1,\leqslant_1)\lhd(A_2,\leqslant_2)\lhd\ldots$. Indeed, given such a chain, let $S=\cup_{i\in\mathbb{N}}A_i$, and for $x,y\in S$ put $x\leqslant y$ if for some $i\in\mathbb{N}$ we have $x,y\in A_i$ and $x\leqslant_i y$. Then $(S,\leqslant)$ is a past-finite countable poset and $A_i\lhd S$ for each $i\in\mathbb{N}$. Such constructions will also be crucial for this paper.

Let $(S,\leqslant)$ and $(S',\leqslant)$ be two posets. A mapping $f:S\to S'$ is called an (*order-*) *embedding of* $(S,\leqslant)$ *into* $(S',\leqslant)$, if for any $x,y\in S$ we have $x\leqslant y$ iff $f(x)\leqslant f(y)$. Clearly, any embedding is one-to-one. An embedding $f:(S,\leqslant)\to(S',\leqslant)$ is called an *isomorphism*, if f is onto, and a *stem-embedding*, if $f(S)\lhd S'$. So, f is a stem-embedding iff f is an isomorphism from $(S,\leqslant)$ onto a stem of $(S',\leqslant)$. An isomorphism of $(S,\leqslant)$ onto itself is called an *automorphism* of $(S,\leqslant)$.

Let $\mathfrak{C}$ be a class (collection) of posets. A poset $(S,\leqslant)\in\mathfrak{C}$ will be called *stem-universal* in $\mathfrak{C}$, if each poset $(C,\leqslant)\in\mathfrak{C}$ is isomorphic to some stem in $(S,\leqslant)$, i.e., there exists a stem-embedding $f:(C,\leqslant)\to(S,\leqslant)$. We call $(S,\leqslant)$ *homogeneous*, if each isomorphism $f:(A,\leqslant)\to(B,\leqslant)$ between two finite stems of $(S,\leqslant)$ extends to an automorphism of $(S,\leqslant)$; equivalently, for any finite poset $(A,\leqslant)$ and any two stem-embeddings $f,f':(A,\leqslant)\to(S,\leqslant)$ there exists an automorphism g of $(S,\leqslant)$ such that $f'=g\circ f$. (We mention that in the literature there are other concepts called homogeneity. Our homogeneity, for instance, does *not* mean that $\mathrm{Aut}(S)$, the automorphism group of $(S,\leqslant)$, acts transitively on S).

We say that $(S,\leqslant)$ *realizes all one-point stem-extensions of finite stems of* S, if whenever $(A,\leqslant),(B,\leqslant)$ are finite posets such that $(A,\leqslant)\lhd(S,\leqslant),(A,\leqslant)\lhd(B,\leqslant)$ and $|B|=|A|+1$, then there exists a stem-embedding $g:(B,\leqslant)\to(S,\leqslant)$ such that $g|_A=\mathrm{id}_A$, the identity on A (this condition includes the case $A=\emptyset$).

The first main goal of this paper will be the following result.

Theorem 2.1: *Let* $\mathfrak{C}$ *be the class of all past-finite countable causal sets.*

(a) *A poset* $(U,\leqslant)\in\mathfrak{C}$ *is stem-universal and homogeneous in* $\mathfrak{C}$ *iff* $(U,\leqslant)$ *realizes all one-point stem-extensions of finite stems of* U.

(b) *There exists a stem-universal homogeneous past-finite causet* $(U,\leqslant)$ *in* $\mathfrak{C}$. *Moreover,* $(U,\leqslant)$ *is unique up to isomorphism with these properties.*

One approach to the proof of Theorem 2.1 would be to use a category-theoretic generalization of the Fraïssé-Jónsson theorem from model theory, see Ref. 6, and to argue directly for past-finite

causal sets and stem embeddings. In order to avoid the category-theoretic machinery needed for this, here we will base our argument on a more classical version of the Fraïssé-Jónsson theorem, cf. Refs. 9, 2, and 11, which describes the existence of universal homogeneous objects for various classes of, e.g., relational structures. This also has the advantage of showing how to regard past-finite causal sets and stem-embeddings as relational structures and relational embeddings. For the convenience of the reader, we recall these notions. Let $\sigma=(n_i)_{i\in I}$ be a fixed I-indexed sequence of natural numbers $n_i\geqslant 1$ (a relational signature) denoting prescribed arities of relations. A tuple $\mathcal{A}=(A,(R_i)_{i\in I})$ is called a *σ-structure*, if A is a set (possibly empty) and R_i is an n_i-ary relation on A, i.e., $R_i\subseteq A^{n_i}$, for each $i\in I$. Given two σ-structures $\mathcal{A}=(A,(R_i)_{i\in I})$ and $\mathcal{B}=(B,(Q_i)_{i\in I})$, a mapping $f:A\to B$ is called an *embedding* of $\mathcal{A}$ into $\mathcal{B}$, if f is one-to-one and for each $i\in I$ and $x_1,\ldots,x_{n_i}\in A$ we have $(x_1,\ldots,x_{n_i})\in R_i$ iff $(f(x_1),\ldots,f(x_{n_i}))\in Q_i$. An embedding which is onto is called an *isomorphism*. An isomorphism of $\mathcal{A}$ onto itself is called an *automorphism of $\mathcal{A}$*. Further, $\mathcal{A}$ is said to be a *substructure* of $\mathcal{B}$, if $A\subseteq B$ and $R_i=Q_i\cap A^{n_i}$ for each $i\in I$, i.e., $A\subseteq B$ and the identity mapping $\mathrm{id}:A\to B$ is an embedding of $\mathcal{A}$ into $\mathcal{B}$; this is denoted by $\mathcal{A}\subseteq\mathcal{B}$.

Now let $\mathfrak{C}$ be a class (collection) of σ-structures. A structure $\mathcal{U}\in\mathfrak{C}$ is called *universal* in $\mathfrak{C}$, if for each $\mathcal{A}\in\mathfrak{C}$ there exists an embedding $f:\mathcal{A}\to\mathcal{U}$. Further, $\mathcal{U}$ is *homogeneous*, if each isomorphism $f:\mathcal{A}\to\mathcal{B}$ between two finite substructures $\mathcal{A},\mathcal{B}$ of $\mathcal{U}$ with $\mathcal{A},\mathcal{B}\in\mathfrak{C}$ extends to an automorphism of $\mathcal{U}$. The structure $\mathcal{U}$ *realizes all finite extensions of finite substructures*, if whenever $\mathcal{A},\mathcal{B}\in\mathfrak{C}$ are finite structures such that $\mathcal{A}\subseteq\mathcal{U}$ and $\mathcal{A}\subseteq\mathcal{B}$, then there exists an embedding $g:\mathcal{B}\to\mathcal{U}$ such that $g|_A=\mathrm{id}_A$. The class $\mathfrak{C}$ is said to be an *ω-class*, if it satisfies the following conditions:

(0) Any $\mathcal{A}\in\mathfrak{C}$ is countable.
(1) Whenever $\mathcal{A}\in\mathfrak{C}$ and $\mathcal{B}$ is a structure isomorphic to $\mathcal{A}$, then $\mathcal{B}\in\mathfrak{C}$.
(2) If $\mathcal{A}_1\subseteq\mathcal{A}_2\subseteq\ldots$ are finite structures from $\mathfrak{C}$, forming a chain of substructures under inclusion, then their union $\mathcal{A}=\cup_{i\in\mathbb{N}}\mathcal{A}_i$ (whose domain and relations are defined as the union of the domain respectively corresponding relations of the structures $\mathcal{A}_i$) also belongs to $\mathfrak{C}$.
(3) If $\mathcal{A}\in\mathfrak{C}$ and F is a finite subset of the domain of $\mathcal{A}$, then there exists a finite substructure $\mathcal{S}\subseteq\mathcal{A}$ with $\mathcal{S}\in\mathfrak{C}$ whose domain contains F.

An object $\mathcal{A}\in C$ is called *weakly initial in* $\mathfrak{C}$, if for each $\mathcal{B}\in\mathfrak{C}$ there exists an embedding $f:\mathcal{A}\to\mathcal{B}$. (Often, this is the empty or a singleton structure.) The class $\mathfrak{C}$ is said to have

- the *joint embedding property*, if for any $\mathcal{A},\mathcal{B}$ there exists $\mathcal{C}\in\mathfrak{C}$ and embeddings $f:\mathcal{A}\to\mathcal{C},g:\mathcal{B}\to\mathcal{C}$

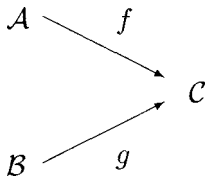

- the *amalgamation property*, if for any $\mathcal{A},\mathcal{B}_1,\mathcal{B}_2\in\mathfrak{C}$ and embeddings $f_i:\mathcal{A}\to\mathcal{B}_i$ $(i=1,2)$ there exists $\mathcal{C}\in\mathfrak{C}$ and embeddings $g_i:\mathcal{B}_i\to\mathcal{C}$ $(i=1,2)$ such that $g_1\circ f_1=g_2\circ f_2$, i.e., the subsequent diagram "commutes."

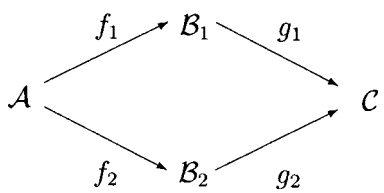

Theorem 2.2 (Refs. 2, 9, and 11): *Let σ be a relational signature and $\mathfrak{C}$ an ω-class of σ-structures.*

(a) *Let $\mathfrak{C}$ contain a weakly initial structure. Then a structure $\mathcal{U} \in \mathfrak{C}$ is universal and homogeneous in $\mathfrak{C}$ if and only if $\mathcal{U}$ realizes all finite extensions of finite substructures.*

(b) *The following are equivalent:*

(1) *$\mathfrak{C}$ contains a universal homogeneous structure $\mathcal{U}$.*

(2) *$\mathfrak{C}_{\mathrm{fin}}$, the class of all finite structures in $\mathfrak{C}$, has the joint embedding and the amalgamation property and contains up to isomorphism only countably many structures.*

Moreover, in this case $\mathcal{U}$ is unique up to isomorphism.

We just note that the proof of Theorem 2.2(a) as well as of the uniqueness of $\mathcal{U}$ in part (b) employs a standard "back-and-forth argument." The construction of the universal homogeneous structure $\mathcal{U}$ given condition (2) of part (b) uses a suitable enumeration of all possible embeddings of the finite structures in $\mathfrak{C}$.

In order to be able to apply Theorem 2.2 to causal sets, we have to enrich them to relational structures such that stem-embeddings become relational embeddings as above. Given a poset $(A, \leqslant)$, we define its *relational expansion* to be $(A, \leqslant, \mathcal{R})$ where $\mathcal{R}=(R_i)_{i\geqslant 1}$ and $R_i=\{ x \in A \,|\, |\mathrm{past}(x)|=i\}$ $(i \geqslant 1)$. Hence $\leqslant$ is a binary and each R_i a unary relation on A, so $(A, \leqslant, \mathcal{R})$ is a σ-structure for the signature $\sigma=(2,1,1,1,\ldots)$. Observe that if A is finite, then each of the relations R_i where $i>|A|$ is empty. Next we show that for past-finite causal sets, this expansion achieves our first goal:

Proposition 2.3: Let $(A, \leqslant)$ and $(B, \leqslant)$ be two past-finite causal sets and let $(A, \leqslant, \mathcal{R})$ respectively $(B, \leqslant, \mathcal{Q})$ be their relational expansions.

(a) *$(A, \leqslant)$ is a stem of $(B, \leqslant)$ iff $(A, \leqslant, \mathcal{R})$ is a substructure of $(B, \leqslant, \mathcal{Q})$.*

(b) *Let $f: A \to B$ be a mapping. Then $f: (A, \leqslant) \to (B, \leqslant)$ is a stem-embedding iff $f: (A, \leqslant, \mathcal{R}) \to (B, \leqslant, \mathcal{Q})$ is an embedding of relational structures.*

Proof: (a) We have $\mathcal{R}=(R_i)_{i\geqslant 1}$ and $\mathcal{Q}=(Q_i)_{i\geqslant 1}$ with $R_i=\{ x \in A \,|\, |\mathrm{past}_A(x)|=i\}$ and $Q_i=\{ y \in B \,|\, |\mathrm{past}_B(y)|=i\}$ $(i \geqslant 1)$.

First, let $A \lhd B$. Let $x \in A$. By $A \lhd B$ we get $\mathrm{past}_A(x)=\mathrm{past}_B(x)$, so $x \in R_i$ iff $x \in Q_i$, for each $i \geqslant 1$. Hence $(A, \leqslant, \mathcal{R}) \subseteq (B, \leqslant, \mathcal{Q})$. Conversely, assume the latter. Let $x \in A$ and $y \in B$ with $y \leqslant x$. By assumption, we have $\mathrm{past}_A(x) \subseteq \mathrm{past}_B(x)$ and $|\mathrm{past}_A(x)|=|\mathrm{past}_B(x)| \in \mathbb{N}$, so $\mathrm{past}_A(x) = \mathrm{past}_B(x) \ni y$ showing $y \in A$. Hence $A \lhd B$.

(b) Straightforward by (a), using that the image of A under f is an isomorphic copy of A and a stem respectively a substructure of B. □

This result allows us to translate all notions concerning stem-embeddings (like universality, homogeneity, etc.) into corresponding ones for the relational expansions and their embeddings.

Let $\mathfrak{C}$ be the class of all countable past-finite causal sets and let $\mathfrak{C}_{\mathrm{rel}}$ be the collection of all relational expansions $(A, \leqslant, \mathcal{R})$ where $(A, \leqslant) \in \mathfrak{C}$. Next we give an easy application of Proposition 2.3 to show how this translation of notions works:

Remark 2.4: $\mathfrak{C}_{\mathrm{rel}}$ is an ω-class of σ-structures.

Proof: Conditions (0) and (1) of the definition of ω-class are trivial. For (2), let $(A_1, \leqslant, \mathcal{R}_1) \subseteq (A_2, \leqslant, \mathcal{R}_2) \subseteq \ldots$ be a chain of finite structures from $\mathfrak{C}_{\mathrm{rel}}$, and let $(A, \leqslant, \mathcal{R}')$ be their union. Then $(A_1, \leqslant) \lhd (A_2, \leqslant) \lhd \ldots$ is a sequence of stems by Propositions 2.3 (a), and $(A, \leqslant)$ is a past-finite causal set whose expansion $(A, \leqslant, \mathcal{R})$ coincides with $(A, \leqslant, \mathcal{R}')$. Hence $(A, \leqslant, \mathcal{R}') \in \mathfrak{C}_{\mathrm{rel}}$. To check (3), let $(A, \leqslant, \mathcal{R}) \in \mathfrak{C}_{\mathrm{rel}}$ and let F be a finite subset of A. Then $\mathrm{past}(F)$ is a finite stem of $(A, \leqslant)$, so by Proposition 2.3 (a) its relational expansion is a finite substructure of $(A, \leqslant, \mathcal{R})$ belonging to $\mathfrak{C}_{\mathrm{rel}}$. □

Next we show:

Lemma 2.5: Let $(A,\leqslant),(B,\leqslant)$ *be two finite posets such that* $A\lhd B$. *Then there is a sequence of stems*

$$A=A_0\lhd A_1\lhd\ldots\lhd A_m=B$$

such that $|A_{i+1}|=|A_i|+1$ *for each* $i=0,\ldots,m-1$.

Proof: By induction on $|B\backslash A|$. Choose a minimal element x of $B\backslash A$, and put $A_1=A\cup\{x\}$. Then $A\lhd A_1\lhd B$, and by induction we obtain a sequence of stems and one-point extensions from A_1 to B. □

Now we can give the

Proof of Theorem 2.1: By Remark 2.4, $\mathfrak{C}_{\mathrm{rel}}$ is an ω-class of σ-structures.

(a) The empty structure is a weakly initial object of $\mathfrak{C}_{\mathrm{rel}}$. Lemma 2.5 shows that if $\mathcal{U}$ realizes all one-point extensions of finite stems, it also realizes all finite stem-extensions of finite stems. Now the result is a translation of Theorem 2.2 (a).

(b) Again we use Proposition 2.3. We check condition (2) of Theorem 2.2 (b). It is clear that $\mathfrak{C}_{\mathrm{rel}}$ contains up to isomorphism only countably many finite structures $(A,\leqslant,\mathcal{R})$, since if A is finite, only finitely many of the relations R_i are nonempty. It remains to show that the collection of finite posets satisfies the joint embedding and the amalgamation properties with respect to stem-embeddings. Since this collection contains the empty poset, it suffices to check the amalgamation property. For this, let $(A_i,\leqslant_i)$ $(i=0,1,2)$ be three finite posets such that $(A_0,\leqslant_0)\lhd(A_i,\leqslant_i)$ for $i=1,2$. We may assume that $A_0=A_1\cap A_2$. Put $A=A_1\cup A_2$ and $\leqslant=\leqslant_1\cup\leqslant_2$, i.e., for $x,y\in A$ let $x\leqslant y$ iff either $x,y\in A_1$ and $x\leqslant_1 y$ or $x,y\in A_2$ and $x\leqslant_2 y$. Then $\leqslant$ is transitive, since if, e.g., $x\leqslant_1 y$ and $y\leqslant_2 z$, we have $y\in A_1\cap A_2=A_0$ and $x\in A_1$. Since $A_0\lhd A_1$, we get $x\in A_0$ and $x\leqslant_0 y$, so $x\leqslant_2 y\leqslant_2 z$ which implies $x\leqslant z$. Hence $\leqslant$ is a partial order on A. Observe that if $x\in A_1\backslash A_0$ and $y\in A_2\backslash A_0$, then neither $x\leqslant y$ nor $y\leqslant x$. Also note that if $x,y\in A_1\cap A_2$ and $x\leqslant_1 y$, say, then this implies $x\leqslant_0 y$, hence also $x\leqslant_2 y$. We claim that $(A_i,\leqslant_i)\lhd(A,\leqslant)$ for $i=1,2$. By the remark just made, $\leqslant_i$ is just the restriction of $\leqslant$ to A_i. So, it only remains to show that A_i is a stem of $(A,\leqslant)$.

Indeed, let $x\in A$ and $y\in A_1$ with $x\leqslant y$. We claim that $x\in A_1$. This is trivial if $x\leqslant_1 y$. So let $x\leqslant_2 y$. Then $x,y\in A_2$ and $y\in A_0$. Now A_0 is a stem of $(A_2,\leqslant)$, so $x\in A_0\subseteq A_1$. Hence A_1 is a stem of $(A,\leqslant)$ and for A_2 we argue analogously. This proves the amalgamation property.

Now the result follows from Theorem 2.2 (b). □

Next we wish to describe the structure of the universal homogeneous past-finite causet $(U,\leqslant)$ further. A poset $(S,\leqslant)$ is called *directed*, if for any $a,b\in S$ there is $c\in S$ with $a\leqslant c$ and $b\leqslant c$. Two elements $a,b\in S$ are *incomparable*, if neither $a\leqslant b$ nor $b\leqslant a$; this is denoted by $a\|b$. A subset $A\subseteq S$ is called an *antichain*, if any two elements of A are incomparable. An element $x\in S$ is called *maximal*, if there is no $y\in S$ with $x<y$. Together with Theorem 2.1 (a), the following provides an order-theoretic characterization of the structure of the universal homogeneous past-finite causal set.

Proposition 2.6: Let $(U,\leqslant)$ *be a past-finite causal set. The following are equivalent*:

(1) $(U,\leqslant)$ *realizes all one-point stem-extensions of finite stems of* U.

(2)

- *(i)* $(U,\leqslant)$ *is directed, and*
- *(ii)* *For any finite antichain* $A\subseteq U$ *(including the case that* $A=\emptyset$*) and any* $y\in U\backslash A$ *with* $A\subseteq\mathrm{past}(y)$ *there is* $x\in U\backslash A$ *such that* $x\|y$ *and* $\mathrm{past}(x)=\mathrm{past}(A)\cup\{x\}$.

In this case, no element of $(U,\leqslant)$ *is maximal.*

Note that the condition $\mathrm{past}(x)=\mathrm{past}(A)\cup\{x\}$ means that $a\leqslant x$ for each $a\in A$, and whenever $u\in U$ with $u<x$, then $u\leqslant a$ for some $a\in A$.

Proof: (1)$\rightarrow$(2): To show (i), let $a,b\in U$. We claim that there is $c\in U$ with $a\leqslant c$ and $b\leqslant c$. Clearly, we may assume that $a\|b$. Let $A=\mathrm{past}(\{a,b\})$, choose an element $z\notin A$, and put $B=A\cup\{z\}$. We define a partial order $\leqslant^*$ on B such that it extends the order $\leqslant$ on A and $a\leqslant^* z, b\leqslant^* z$, so z is the greatest element of $(B,\leqslant^*)$. Then $(A,\leqslant)\lhd(B,\leqslant^*)$, a one-point extension of the finite stem A of U. Hence, there exists a stem-embedding $g:(B,\leqslant^*)\rightarrow(U,\leqslant)$ with $g|_A=\mathrm{id}_A$. Now put $c=g(z)$ to obtain the claim.

For (ii), choose a finite antichain $A\subseteq U$ and $u\in U\backslash A$ with $A\subseteq\mathrm{past}_U(y)$. Put $A'=\mathrm{past}_U(y)$, choose an element $z\notin A'$, and put $B=A'\cup\{z\}$. Define a partial order $\leqslant^*$ on B such that it extends the order $\leqslant$ on A, such that each $x\in\mathrm{past}_U(A)$ satisfies $x\leqslant^* z$, but each $x\in A'\backslash\mathrm{past}_U(A)$ is incomparable to z in $(B,\leqslant^*)$. Then $(A',\leqslant)\lhd(B,\leqslant^*)$, a one-point extension of the finite stem A' of U. Again, there is a stem-embedding $g:(B,\leqslant^*)\rightarrow(U,\leqslant)$ with $g|_{A'}=\mathrm{id}_{A'}$. Then $x=g(z)$ satisfies $x\notin A'$ and $x\|y$, and by $g(B)\lhd U$ we obtain

$$\begin{aligned}\mathrm{past}_U(x)&=\mathrm{past}_{g(B)}(x)=g(\mathrm{past}_B(z))=g(\mathrm{past}_B(A)\cup\{z\})\\&=\mathrm{past}_{g(B)}(A)\cup\{x\}=\mathrm{past}_U(A)\cup\{x\},\end{aligned}\tag{1}$$

as required.

(2)$\rightarrow$(1): We first show that no element of $(U,\leqslant)$ is maximal. Let $y\in U$. Applying assumption (ii) to the empty antichain, we obtain $x\in U$ with $x\|y$. Now by (i) there is $z\in U$ with $x\leqslant z$ and $y\leqslant z$. Then $y<z$.

Now let $(A',\leqslant)$ and $(B,\leqslant')$ be finite posets such that $(A',\leqslant)\lhd(U,\leqslant),(A',\leqslant)\lhd(B,\leqslant')$, and $B=A'\cup\{z\}$, say. Let A comprise all elements $a\in A'$ maximal with respect to $a<'z$ in $(B,\leqslant')$. So, A is an antichain and $\mathrm{past}_B(z)=\mathrm{past}_B(A)\cup\{z\}$. Since $(U,\leqslant)$ is directed and A' is finite, there exists $y\in U$ with $a\leqslant y$ for each $a\in A'$. Choose $y'\in U$ with $y<y'$; then $y'\notin A'$. Now by assumption (ii), there is $x\in U\backslash A$ such that in $(U,\leqslant)$ we have $x\|y'$ and $\mathrm{past}_U(x)=\mathrm{past}_U(A)\cup\{x\}$. Define $g:B\rightarrow U$ by $g|_{A'}=\mathrm{id}_{A'}$ and $g(z)=x$. By $x\|y'$, we obtain $x\notin A'$, and moreover, x is incomparable to each element of $A'\backslash\mathrm{past}_U(A)$. Hence g is an embedding, and we show that $g(B)\lhd U$. We have $A'\lhd U$, and so $\mathrm{past}_U(x)=\mathrm{past}_U(A)\cup\{x\}\subseteq A'\cup\{x\}=g(B)$. Thus g is a stem-embedding. □

Next we wish to use Theorem 2.2 (a) and Proposition 2.6 to give a direct construction (avoiding Theorem 2.2 (b)) of the universal homogeneous past-finite causal set $(U,\leqslant)$.

Construction 2.7 (of the universal homogeneous past-finite causal set $(U,\leqslant)$): We construct a sequence of finite posets $(A_1,\leqslant_1)\lhd(A_2,\leqslant_2)\lhd\ldots$ as follows. Let $(A_1,\leqslant_1)$ be any singleton set, with the trivial order. Now let $i\in\mathbb{N}$ and assume we have constructed a finite poset $(A_i,\leqslant_i)$. Let $\mathcal{A}$ comprise all antichains in $(A_i,\leqslant_i)$, and choose pairwise different elements $x_A(A\in\mathcal{A})$ not belonging to A_i. Then put $A_{i+1}=A_i\cup\{x_A|A\in\mathcal{A}\}$, and define a partial order $\leqslant_{i+1}$ on A_{i+1} such that it extends $\leqslant_i$ and for any $z\in A_{i+1}$, if $z\in\mathrm{past}_{A_i}(A)\cup\{x_A\}$ then $z\leqslant_{i+1}x_A$, but if $z\notin\mathrm{past}_{A_i}(A)\cup\{x_A\}$ then z and x_A are incomparable in $(A_{i+1},\leqslant_{i+1})$. Hence each element $x_A(A\in\mathcal{A})$ is maximal in $(A_{i+1},\leqslant_{i+1})$, and thus $(A_i,\leqslant_i)\lhd(A_{i+1},\leqslant_{i+1})$. Finally, let $(U,\leqslant)=\cup_{i\in\mathbb{N}}(A_{i+1},\leqslant_{i+1})$. Clearly, $(A_i,\leqslant_i)\lhd(U,\leqslant)$ for each $i\in\mathbb{N}$, and $(U,\leqslant)$ is a countable past-finite causal set.

Claim: $(U,\leqslant)$ is universal and homogeneous.

Proof: We show that $(U,\leqslant)$ satisfies condition (2) of Proposition 2.6; then this proposition and Theorem 2.1 (a) imply the result. For condition (2)(i), let $a,b\in U$ with $a\|b$. Then $A=\{a,b\}\subseteq A_i$ for some $i\in\mathbb{N}$, and $x_A\in A_{i+1}$ satisfies $a\leqslant x_A$ and $b\leqslant x_A$. For condition (2)(ii), let $A\subset U$ be a finite antichain and $y\in U\backslash A$ with $A\subseteq\mathrm{past}_U(y)$. Again, $A\cup\{y\}\subseteq A_i$ for some $i\in\mathbb{N}$. Then $x_A\in A_{i+1}$ and by $A_{i+1}\lhd U$ and construction of $\leqslant_{i+1}$ we obtain

$$\mathrm{past}_U(x_A) = \mathrm{past}_{A_{i+1}}(x_A) = \mathrm{past}_{A_{i+1}}(A) \cup \{x_A\} = \mathrm{past}_U(A) \cup \{x_A\}.$$

Furthermore, since $y \notin \mathrm{past}_{A_{i+1}}(A)$, we get $x_A \| y$ in $(A_{i+1}, \leqslant_{i+1})$ and in $(U, \leqslant)$, as required. Our claim follows. □

This argument is more direct and intuitive than the previous one using Theorem 2.2 (b) with its proof. However, Theorem 2.2 puts the result into a general context, and checking the amalgamation property required for condition (2) of Theorem 2.2 (b) was also uncomplicated.

Next we mention two further structural properties of the universal homogeneous past-finite causet $(U, \leqslant)$.

Corollary 2.8: Let $(U, \leqslant)$ *be the universal homogeneous countable past-finite causet.*

(a) *For any finite subset* $F \subseteq U$, $(U, \leqslant)$ *is isomorphic to the poset* $(U \backslash F, \leqslant)$. *In particular,* $(U, \leqslant) \cong (U \backslash \mathrm{past}(z), \leqslant)$ *for each* $z \in U$.

(b) *For each* $z \in U$, $(U, \leqslant)$ *is isomorphic to* $(\{u \in U | z < u\}, \leqslant)$, *the proper future of* z.

Proof: (a) We may assume that $F \neq \emptyset$. Trivially, $(U \backslash F, \leqslant)$ is a countable past-finite causet. We wish to check that $(U \backslash F, \leqslant)$ satisfies condition (2) of Proposition 2.6; then the result is immediate by Proposition 2.6 and Theorem 2.1. Since $(U, \leqslant)$ is directed and contains no maximal element, $(U \backslash F, \leqslant)$ is directed. So, let $A \subseteq U \backslash F$ be a finite antichain and $y \in (U \backslash F) \backslash A$ with $A \subseteq \mathrm{past}_{U \backslash F}(y)$. Again, since $(U, \leqslant)$ is directed and contains no maximal element, there is $y' \in U \backslash F$ with $F \cup \{y\} \subseteq \mathrm{past}_U(y')$. By Proposition 2.6, for $(U, \leqslant)$, there is $x \in U \backslash A$ such that $x \| y'$ and $\mathrm{past}_U(x) = \mathrm{past}_U(A) \cup \{z\}$. Then $x \notin F$ and neither $x \leqslant y$ nor $y \leqslant x$, and clearly $\mathrm{past}_{U \backslash F}(x) = \mathrm{past}_{U \backslash F}(A) \cup \{x\}$, as required for condition (ii). The final claim is immediate, since past(z) is finite for each $z \in U$.

(b) Let $z \in U$ and $U' = \{u \in U | z < u\}$. Again we show that $(U', \leqslant)$ satisfies condition (2) of Proposition 2.6. If the antichain A chosen is empty, replace it by $\{z\}$. Then, and also in case A is nonempty, apply condition (ii) for $(U, \leqslant)$ to obtain the element $x \in U'$ as required. □

Finally, we wish to show that the restriction to *past-finite* causets in Theorem 2.1 is essential:

Proposition 2.9: The class of all countable causets does not *contain a universal causet.*

Proof: We will exploit that this class also contains posets which are not past-finite. Suppose there was a countable causet $(U, \leqslant)$ such that each countable causet can be stem-embedded into $(U, \leqslant)$. Let $-\mathbb{N}$ denote the set of negative integers. We denote the natural partial order on $-\mathbb{N}$ by $\leqslant$, so $n-1 < n$ for each $n \in -\mathbb{N}$. For each subset $A \subseteq -\mathbb{N}$ let $(S_A, \leqslant)$ be the causet obtained from $(-\mathbb{N}, \leqslant)$ by replacing each element $n \in A$ by a 2-element antichain $\{n, n^*\}$. That is, $S_A = -\mathbb{N} \cup \{n^* | n \in A\}$, n and n^* are incomparable for each $n \in A$, and $m < n^*$ iff $m < n$ iff $m < n$ $(m \in -\mathbb{N}, n \in A)$, likewise for $m^* < n^*$, respectively, $m^* < n$. By assumption, there is a stem-embedding $f_A : (S_A, \leqslant) \to (U, \leqslant)$. Let $x_A = f_A(-1)$. Then $f_A(S_A)$ is a stem of U, and $f_A(S_A) = \mathrm{past}(x_A)$.

As is easily seen, for $A, A' \subseteq -\mathbb{N}$ we have $(S_A, \leqslant) \cong (S_{A'}, \leqslant)$ iff $A = A'$. Hence there are uncountably many nonisomorphic causets of the form $(S_A, \leqslant)$; these are isomorphic to the posets $(\mathrm{past}(x_A), \leqslant)$. But U is countable and contains only countably many posets of the form $\mathrm{past}(x)(x \in U)$, a contradiction. □

III. PROBABILISTIC CONSTRUCTIONS

In this section, we wish to provide probabilistic constructions of the universal homogeneous causal set $(U, \leqslant)$ of Sec. II. Probabilistic constructions of causal sets were already investigated in Refs. 10 and 15. This employed successive one-point extensions ("generalized percolations") of finite posets; such extensions will also be used here. Suppose we are given a finite poset $(A, \leqslant)$

and want to extend it to a poset $(B,\leqslant)$ such that $B=A\cup\{z\}$, say, and $(A,\leqslant)$ is a stem in $(B,\leqslant)$. Then we just have to define the order relations between z and the elements of A; moreover, since A should become a stem of B, z has to become a maximal element of $(B,\leqslant)$, thus for each $a\in A$ we can only put $a<z$ or $a\|z$, and this can be decided probabilistically. Let us now give the details of this construction for our case. We will discuss a technical difference to Refs. 10 and 15 afterwards. For sake of concreteness, we will take the underlying set of our causet to be $\mathbb{N}$ (as in Ref. 15, but the construction would work for any countably enumerated set). Hence we will construct a partial order $\leqslant$ on $\mathbb{N}$. Recall that we write $x<y$ if $x\leqslant y$ and $x\neq y$. We denote the natural order on $\mathbb{N}$ by $\leqslant$, i.e., $n\prec n+1$ for each $n\in\mathbb{N}$. Our basic construction will depend on a parameter $p\in[0,1]$.

Construction 3.1 (Probabilistic one-point extension of an enumerated finite poset): Let $p\in[0,1]$. Let $(A,\leqslant)$ be a finite poset with $A=\{1,\ldots,n\}$ for some $n\geqslant 1$, and let $B=A\cup\{n+1\}$. Furthermore, letting $A_j=\{1,\ldots,j\}$ for $1\leqslant j\leqslant n$, assume that $A_1\lhd\ldots\lhd A_n=A$. As noted before, we wish to extend the order $\leqslant$ to a partial order $\leqslant'$ on B such that $(A,\leqslant)$ is a stem of $(B,\leqslant')$. We proceed as follows. First choose, with equal probability, some $j\in\{1,\ldots,n\}$. If j was chosen, this means that we will restrict ourselves to having $\mathrm{past}_B(n+1)\subseteq A_j\cup\{n+1\}$. We define a binary relation R in $\{1,\ldots,n\}\times\{n+1\}$ as follows. Decide independently for each $i\in\{1,\ldots,j\}$ with probability p that $(i,n+1)\in R$, and with probability $1-p$ that $(i,n+1)\notin R$. Now let $\leqslant'$ on B be the reflexive transitive closure of the relation $\leqslant\cup R$. That is, we have $n+1\leqslant' n+1$, for $x,y\in A$ we have $x\leqslant' y$ iff $x\leqslant y$, and for any $x\in A$ we have $x\leqslant' n+1$ iff there is $i\in\{1,\ldots,j\}$ such that $x\leqslant i$ and $(i,n+1)\in R$; in this case $x\in A_j$ by $A_j\lhd A$. Clearly, $(B,\leqslant')$ is a partial order, $n+1$ is maximal in $(B,\leqslant')$, $\mathrm{past}_B(n+1)\subseteq A_j\cup\{n+1\}$, and $(A,\leqslant)\lhd(B,\leqslant')$.

Next we wish to construct our random past-finite countable causal set structure on $\mathbb{N}$.

Construction 3.2 (of a probabilistic order $\leqslant$ on $\mathbb{N}$): Let $p\in[0,1]$. Let $A_n=\{1,2,\ldots,n\}$ $(n\in\mathbb{N})$. For $n=1$, put $1\leqslant 1$. Now use Construction 3.1 to successively extend the order $\leqslant$ from A_n to A_{n+1}. We obtain a sequence of stems $A_1\lhd A_2\lhd\ldots\lhd A_n\lhd\ldots$, and we put $(\mathbb{N},\leqslant)=\cup_{n\in N}(A_n,\leqslant)$. Then each A_n is a stem of $(\mathbb{N},\leqslant)$ and $(\mathbb{N},\leqslant)$ is a past-finite causal set.

Next we will show:

Theorem 3.3: Let $p\in(0,1)$. *With probability 1, the above construction produces a partial order $\leqslant$ on $\mathbb{N}$ such that $(\mathbb{N},\leqslant)$ is a stem-universal homogeneous past-finite causal set.*

Proof: As noted before, $(\mathbb{N},\leqslant)$ is a past-finite causal set. By Theorem 2.1 (a), it suffices to show that with probability 1, $(\mathbb{N},\leqslant)$ realizes all one-point stem-extensions of finite stems of $(\mathbb{N},\leqslant)$. There are countably many such stem-extensions. Since the intersection of countably many events of probability 1 again has probability 1, it suffices to consider an arbitrary fixed one-point stem-extension $A\lhd(B,\leqslant')$ with $B=A\cup\{y\}$, A finite and $A\lhd(\mathbb{N},\leqslant)$. We claim that with probability 1 there exists $z\in\mathbb{N}$ such that the mapping $g:B\to\mathbb{N}$ with $g|_A=\mathrm{id}_A$ and $g(y)=z$ is a stem-embedding, i.e., for each $a\in A$ we have $a\leqslant' y$ in B iff $a\leqslant z$ in $\mathbb{N}$ and $A\cup\{z\}\lhd(\mathbb{N},\leqslant)$.

For each $j\in\mathbb{N}$ let $A_j=\{1,2,\ldots,j\}$. Since A is finite, there is $m\in\mathbb{N}$ such that $A\subseteq A_m$. Then $A\lhd A_m$. Now choose any integer $n\geqslant m$ and consider the extension of the order $\leqslant$ from A_n to A_{n+1} given by Construction 3.1. We wish to compute a lower bound for the probability that we can put $z=n+1$ to obtain the required stem $A\cup\{z\}\lhd(\mathbb{N},\leqslant)$. First, the probability that we choose the number m from $\{1,\ldots,n\}$ is $1/n$. Then by Construction 3.1 for each $i\in A$, if $i<' y$ in $(B,\leqslant')$ we put $(i,n+1)\in R$ with probability p, and if $i\|' y$ we put $(i,n+1)\notin R$ with probability $1-p$; further with probability $1-p$ we put $(i,n+1)\notin R$ for each $i\in A_m\backslash A$. Hence, given m, there is a (small but) fixed $r>0$, depending only on the structure of $(A_m,\leqslant)$, on $A\lhd B$ and on y (but not on n), such that at least with probability r all $i\in A_m$ satisfy the above conditions, so $A\cup\{n+1\}\lhd A_m\cup\{n+1\}\lhd A_{n+1}$ and $n+1$ realizes the one-point stem extension of A as required.

Thus the probability that in $(A_{n+1},\leqslant)$, the structure of $(A_m\cup\{n+1\},\leqslant)$ is as required is at least $r\cdot 1/n$. Hence the probability that $n+1$ and $(A_m\cup\{n+1\},\leqslant)$ do not satisfy these conditions is at most $1-r/n$. Consequently, the probability that for *no* integer $n\geqslant m,n+1$ and

$(A_m \cup \{n+1\})$ realize this one-point extension of A is $\Pi_{n=m}^{\infty}(1-r/n)$. Since the series $\Sigma_{n=m}^{\infty}(r/n)$ diverges, we obtain $\Pi_{n=m}^{\infty}(1-r/n)=0$. Hence with probability 1, this one-point extension of A is realized inside $(\mathbb{N}, \leqslant)$ as required, and the result follows. □

We just note that the above "intuitive" probabilistic statements can easily be made exact by a precise (but technical) definition of the employed probability space; this can be done analogously to the case of the random graph, cf. Refs. 8 and 11, or to the procedure in Refs. 15, 5, and 4 for constructing the probability space of completed labeled causets: The sample space of this probability space is the collection of all past-finite causets $(\mathbb{N}, \leqslant)$ (hence the underlying set, $\mathbb{N}$, is fixed, but the order $\leqslant$ can vary), and Construction 3.1 yields a corresponding probability measure. Theorem 3.3 can then be rephrased by saying that in this probability space the collection of all causets which are universal and homogeneous has measure 1.

The above construction would work also for other probability distributions on $\{1, \ldots, n\}$, in Construction 3.1, than the uniform one. However, they would have to be chosen with some care in order to ensure the final argument in the proof of Theorem 3.3.

Our construction of $(U, \leqslant)$ uses and depends on the given enumeration of $\mathbb{N}$, respectively, in Construction 3.1, of the poset $A=\{1, \ldots, n\}$, and not only on the structure of the poset $(A, \leqslant)$: After choosing $j \in \{1, \ldots, n\}$, we decided to possibly put $(i, n+1) \in R$ only for elements $i \in \{1, \ldots, j\}$. This is a bit unfortunate, since, in the notions of Ref. 15, it would correspond to some externally given time. Apart from this, our construction is very similar to the ones proposed in Refs. 10 and 15. It even shares with it a property of the "gregarious child transition," cf. Ref. 15, Lemma 2:

Remark 3.4: Let $p \in [0,1]$, let $(A, \leqslant)$ be a finite poset with $A=\{1, \ldots, n\}$, and let $B=A \cup \{n+1\}$. The probability to obtain by Construction 3.1 the poset $(B, \leqslant)$ with $(A, \leqslant) \lhd (B, \leqslant)$ and $n+1 \| a$ for each $a \in A$ depends only on the cardinality of A.

Proof: Given $j \in \{1, \ldots, n\}$, for each $i \in \{1, \ldots, j\}$ we have to put $(i, n+1) \notin R$. The probability of this equals $1/n \cdot \Sigma_{j=1}^{n}(1-p)^j$. □

Furthermore, our construction apparently satisfies a weak form of the Bell causality condition, but not the condition of discrete general covariance of Refs. 10 and 15. It would be interesting to investigate this further. Also, this raises the question whether the universal homogeneous past-finite causet $(U, \leqslant)$ can be constructed without referring as in Construction 3.1 to a given enumeration, with positive probability, say. This would require a more intricate analysis of the probabilities of the finite posets occurring.

Finally, we wish to present also a number-theoretic representation of the universal homogeneous past-finite causet $(U, \leqslant)$. As underlying set, we take again the natural numbers $\mathbb{N}$.

Construction 3.5 (of a partial order $\leqslant$ on $\mathbb{N}$): We define a binary relation R on $\mathbb{N}$ as follows. For any $j, n \in N$, put $(j, n) \in R$ iff $j \prec n$ and in the unique ternary expansion of n as a sum of distinct powers of 3, 3^j occurs with coefficient 1. That is, $(j, n) \in R$ iff

$$n = 3^j + \sum_{\substack{0 \leqslant i \leqslant n \\ i \neq j}} x_i \cdot 3^i$$

for some $x_i \in \{0, 1, 2\}$. Then let $\leqslant$ be the transitive reflexive closure of R.

Since $(j, n) \in R$ implies $j \prec n$, clearly $(N, \leqslant)$ is a past-finite causal set, for $A_n=\{1, \ldots, n\}$ we have $A_n \lhd \mathbb{N}$, and n is a maximal element of $(A_n, \leqslant)$. We show:

Theorem 3.6: *The poset $(N, \leqslant)$ constructed above is a stem-universal homogeneous past-finite causal set.*

Proof: By Theorem 2.1 (a), it suffices to show that $(N, \leqslant)$ realizes all one-point extensions.

So let $(A,\leqslant)\lhd(\mathbb{N},\leqslant)$, with A finite, $(A,\leqslant)\lhd(B,\leqslant')$ and $B=A\cup\{y\}$, say, with $y\notin A$. We claim that there exists $z\in\mathbb{N}$ such that the mapping $g:B\to\mathbb{N}$ with $g|_A=\mathrm{id}_A$ and $g(y)=z$ is a stem-embedding. Choose $m\in\mathbb{N}$ such that $A\subseteq A_m$. Put

$$z=\sum_{\substack{a\in A\\ a<'y}} 3^a+2\cdot 3^m.$$

Then $z\notin A$ and z is maximal in $(A\cup\{z\},\leqslant)$. The construction of $\leqslant$ shows that if $a\in A$ with $a<'y$, then $(a,z)\in R$, so $a<z$. Conversely, let $a\in\mathbb{N}$ and $a<z$. Since $\leqslant$ is the transitive reflexive closure of R, there is $a'\in\mathbb{N}$ such that $a\leqslant a'$ and $(a',z)\in R$. By definition of R and of z, we immediately get $a'\in A$ and $a'<'y$. Since $A\lhd\mathbb{N}$, we obtain $a\in A$ and $a<'y$. It follows that g, defined as above, is an order-embedding of $(B,\leqslant')$ into $(\mathbb{N},\leqslant)$ and that $g(B)$ is a stem of $\mathbb{N}$, as required. □

IV. DISCUSSION

We studied the class of all countable causal sets. In algebra, many classes of structures have been investigated with respect to the existence of universal or homogeneous objects. Most often, this completely depends on the given class of structures. Here, we could show that the class of all countable past-finite causets, in contrast to the class of all causets, contains a universal object. Somehow surprisingly, a random (intuitively: "chaotic") construction produces, in the end, almost surely a universal causet bearing maximal degree of symmetry.

A basic idea behind causal set theory is that a manifold M may emerge from a causal set $(S,\leqslant)$ by some sprinkling of a coarse-grained version of $(S,\leqslant)$ densely into M (cf. Ref. 16). Then it would be interesting to see how symmetry properties of $(S,\leqslant)$ are reflected in the structure of M. It is tempting to recall, in this context, Noether's close correspondence between symmetries and conservation laws. A bold question: Can conservation laws be founded on symmetry properties of causal sets and, ultimately, traced to some random constructions of causal sets?

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Nonstandard connections in *k*-cosymplectic field theory

Miguel-C. Muñoz-Lecanda[a)]
Departamento de Matemática Aplicada IV, Edificio C-3, Campus Norte UPC, C/Jordi Girona 1, E-08034 Barcelona, Spain

Modesto Salgado[b)]
Departamento de Xeometría e Topoloxía, Facultade de Matemáticas, Universidade de Santiago de Compostela, 15706-Santiago de Compostela, Spain

Silvia Vilariño[c)]
Departamento de Xeometría e Topoloxía, Facultade de Matemáticas, Universidade de Santiago de Compostela, 15706-Santiago de Compostela, Spain

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In the jet-bundle description of time-dependent mechanics there are some elements, such as the Lagrangian energy and the construction of the Hamiltonian formalism, which require the prior choice of a connection. This situation is analyzed by Echeverría-Enríquez *et al.* [J. Phys. A **28**, 5553–5567 (1995)]. The aim of this paper is to extend the results in that paper to first order field theory, using the *k*-cosymplectic formalism described by de León and co-workers [J. Math. Phys. **39**, 876–893 (1998); **42**, 2092–2104 (2001)]. If the trivial configuration bundle of a Lagrangian system is endowed with one connection, different from the trivial one given by the product structure, we study the consequences on the geometric elements of the theory, the dynamical equations and the variational principles. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2146191]

I. INTRODUCTION

There are several ways to state first order classical field theories in a geometrical setting. All of them are a generalization of time-dependent mechanics in its different formulations, see Ref. 1 for a detailed account of these formulations. These formulations come from contact formulation, that is from symplectic or presymplectic approaches.

In the jet bundle description of time depending mechanics, one begins with the configuration bundle over $\mathbb{R}$, that is a trivial bundle $\pi:\mathbb{R}\times Q\to\mathbb{R}$, being $\mathbb{R}$ the "time." In the case of field theory, the most similar to this description is the *k*-cosymplectic formulation. Here, the base manifold of mechanics is changed by $\mathbb{R}^k$, described as "several times," and the configuration bundle is a trivial one, $\pi:\mathbb{R}^k\times Q\to\mathbb{R}^k$. See Refs. 2 and 3 for details.

The consideration of a trivial bundle hides the use of a connection in several parts of the theory: there is a natural one given by the product structure. It is natural to ask about the changes needed in the development of the theory if one takes another connection. In the case of mechanical systems, these changes are analyzed in Ref. 4.

In this paper we try to give insight into the consequences of taking another different connection in the configuration bundle to build the *k*-cosymplectic approach to classical field theory. On the one hand, the Lagrangian energy, and hence the Hamiltonian, are connection depending. But the dynamical equations are the same for different connections.

[a)]Electronic mail: matmcml@ma4.upc.edu
[b)]Electronic mail: modesto@zmat.usc.es
[c)]Electronic mail: svfernan@usc.es

On the other hand, it is usual to find the theory on a variational principle, both in Lagrangian and Hamiltonian settings, and we study what are the changes to be introduced in these principles in order to get the dynamical equations.

The structure of the work is as follows.

Sections II and III are devoted to the elements of the theory. In particular, in Sec. II, we review the k-cosymplectic formalism in field theory introduced in Refs. 2 and 3. The relationship between these formalisms and the multisymplectic formalism has been studied in Ref. 5 and it will be commented at the end of this section.

In Sec. III, we introduce first the basic ideas about connections in the configuration bundle $\pi_{\mathbb{R}^k}:\mathbb{R}^k\times Q\to\mathbb{R}^k$ and the definition and properties of the Lagrangian energy function, E_L^∇, associated with a Lagrangian L and a connection ∇. Under some assumptions, we obtain that E_L^∇ is constant along the solutions of the classical Euler-Lagrange equations. Some of the results obtained have as a particular case the results of Ref. 4.

Sections IV and V are devoted to the analysis of the deformed dynamical equations and solutions, both in Hamiltonian and Lagrangian settings. In Sec. IV, we construct the Hamiltonian formalism depending on the choice of an arbitrary connection ∇, and we show that if the curvature of the connection vanishes then the Hamilton equations of the modified Hamiltonian and classical Hamiltonian equations have the same solutions. In Sec. V we begin by constructing the vertical endomorphisms associated to a connection, which enables us to the construction of the Lagrangian formalism depending on the connection ∇. If the Lagrangian L is regular, we obtain again that if the curvature of ∇ vanishes then the Lagrangian equations of the modified Lagrangian and classical Lagrangian equations have the same solutions.

In Sec. VI, by means of other new geometrical elements in $\mathbb{R}^k\times Q$, we establish a characterization of the Lagrangian energy function based on variational principles. We conclude that the energy function E_L^∇ is the only function that performs the equivalence between the Hamiltonian principle of minimal action and the Hamilton-Jacobi principle. Section V in Ref. 4 is a particular case of this section.

Manifolds are real, paracompact, connected and C^∞. Maps are C^∞. Sum over crossed repeated indices is understood.

II. THE *k*-COSYMPLECTIC FORMALISMS IN FIELD THEORY

The concepts and results of this section are given in Refs. 2 and 3.

A. The Hamiltonian approach (Ref. 2)

1. The geometric elements

Let Q be a differentiable manifold, $\dim Q=n$, and $\tau_Q^*:T^*Q\to Q$ its cotangent bundle.

Denote by $(T^1_k)^*Q=T^*Q\overset{k}{\oplus}\dots\oplus T^*Q$, the Whitney sum of k copies of T^*Q. The manifold $(T^1_k)^*Q$ can be identified with the manifold $J^1(Q,\mathbb{R}^k)_0$ of 1-jets of mappings from Q to $\mathbb{R}^k$ with target at $0\in\mathbb{R}^k$, that is

$$J^1(Q,\mathbb{R}^k)_0\equiv T^*Q\overset{k}{\oplus}\dots\oplus T^*Q,$$

$$j^1_{q,0}\sigma\equiv(d\sigma^1(q),\dots,d\sigma^k(q)),$$

where $\sigma^A=\pi^A\circ\sigma:Q\to\mathbb{R}$ is the Ath component of σ, and $\pi^A:\mathbb{R}^k\to\mathbb{R}$ is the canonical projection onto the A component, for $1\leqslant A\leqslant k$. $(T^1_k)^*Q$ is called *the bundle of k^1-covelocities of the manifold Q*, see Ref. 6.

The manifold $J^1\pi_Q$ of 1-jets of sections of the trivial bundle $\pi_Q:\mathbb{R}^k\times Q\to Q$ is diffeomorphic to $\mathbb{R}^k\times(T^1_k)^*Q$, via the diffeomorphism given by

$$J^1\pi_Q\to\mathbb{R}^k\times(T^1_k)^*Q,$$

$$j^1_q\phi=j^1_q(\phi_Q,Id_Q)\mapsto(\phi_Q(q),\alpha^1_q,\ldots,\alpha^k_q),$$

where $\phi_Q:Q\overset{\phi}{\to}\mathbb{R}^k\times Q\overset{\pi_{\mathbb{R}^k}}{\to}\mathbb{R}^k$, $\alpha^A_q=d(\phi_Q)^A(q)$, $1\leqslant A\leqslant k$ and $(\phi_Q)^A:Q\overset{\phi_Q}{\to}\mathbb{R}^k\overset{\pi^A}{\to}\mathbb{R}$ is the Ath component of ϕ_Q.

Throughout the paper we shall use the following notation for the canonical projections:

$$\mathbb{R}^k\times(T^1_k)^*Q\xrightarrow{(\pi_Q)_{1,0}}\mathbb{R}^k\times Q\xrightarrow{(\pi_Q)}Q$$

and $(\pi_Q)_1=\pi_Q\circ(\pi_Q)_{1,0}$, where

$$\pi_Q(t,q)=q,\quad(\pi_Q)_{1,0}(t,\alpha^1_q,\ldots,\alpha^k_q)=(t,q),\quad(\pi_Q)_1(t,\alpha^1_q,\ldots,\alpha^k_q)=q,$$

with $t\in\mathbb{R}^k$, $q\in Q$ and $(\alpha^1_q,\ldots,\alpha^k_q)\in(T^1_k)^*Q$.

If (q^i) are local coordinates on $U\subseteq Q$, then the induced local coordinates (q^i,p_i), $1\leqslant i\leqslant n$, on $(\tau^*_Q)^{-1}(U)=T^*U\subset T^*Q$, are given by

$$q^i(\alpha_q)=q^i(q),\quad p_i(\alpha_q)=\alpha_q\left(\left.\frac{\partial}{\partial q^i}\right|_q\right),\tag{1}$$

and, in the same way, the induced local coordinates (t^A,q^i,p^A_i) on $[(\pi_Q)_1]^{-1}(U)=\mathbb{R}^k\times(T^1_k)^*U$ are given by

$$t^A(j^1_q\phi)=(\phi_Q(q))^A,\quad q^i(j^1_q\phi)=q^i(q),\quad p^A_i(j^1_q\phi)=d(\phi_Q)^A(q)\left(\left.\frac{\partial}{\partial q^i}\right|_q\right),$$

or equivalently

$$t^A(t,\alpha^1_q,\ldots,\alpha^k_q)=t^A,\quad q^i(t,\alpha^1_q,\ldots,\alpha^k_q)=q^i(q),\quad p^i_A(t,\alpha^1_q,\ldots,\alpha^k_q)=\alpha^A_q\left(\left.\frac{\partial}{\partial q^i}\right|_q\right),$$

where $1\leqslant i\leqslant n$, $1\leqslant A\leqslant k$.

On $\mathbb{R}^k\times(T^1_k)^*Q$, we define the differential forms

$$\eta^A_0=(\pi^A_1)^*\,\mathrm{d}t^A,\quad\theta^A_0=(\pi^A_2)^*\theta_0,\quad\omega^A_0=(\pi^A_2)^*\omega_0,\quad 1\leqslant A\leqslant k,\tag{2}$$

where $\pi^A_1:\mathbb{R}^k\times(T^1_k)^*Q\to\mathbb{R}$ and $\pi^A_2:\mathbb{R}^k\times(T^1_k)^*Q\to T^*Q$ are the projections defined by

$$\pi^A_1(t,(\alpha^1_q,\ldots,\alpha^k_q))=t^A,\quad\pi^A_2(t,(\alpha^1_q,\ldots,\alpha^k_q))=\alpha^A_q,\quad 1\leqslant A\leqslant k,$$

and $\omega_0=-\mathrm{d}\theta_0=\mathrm{d}q^i\wedge\mathrm{d}p_i$ is the canonical symplectic form on T^*Q and $\theta_0=p_i\,\mathrm{d}q^i$ is the Liouville 1-form on T^*Q. Obviously $\omega^A_0=-\mathrm{d}\theta^A_0$.

In local coordinates we have

$$\eta^A_0=\mathrm{d}t^A,\quad\theta^A_0=\sum_{i=1}^n p^A_i\mathrm{d}q^i,\quad\omega^A_0=\sum_{i=1}^n\mathrm{d}q^i\wedge\mathrm{d}p^A_i,\quad 1\leqslant A\leqslant k.\tag{3}$$

Moreover, let $V_0=\ker T(\pi_Q)_{1,0}$. Then

$$V=\left\langle \frac{\partial}{\partial p_i^1},\ldots,\frac{\partial}{\partial p_i^k}\right\rangle_{i=1,\ldots,n}.$$

A simple inspection of their expressions in local coordinates shows that the forms η_0^A and ω_0^A are closed and the following relation hold:

(1) $\eta_0^1\wedge\cdots\wedge\eta_0^k\neq 0$, $(\eta_0^A)_{|V}=0$ $(\omega_0^A)_{|V\times V}=0$,
(2) $(\cap_{A=1}^k \ker \eta_0^A)\cap(\cap_{A=1}^k \ker \omega_0^A))=\{0\}$, $\dim(\cap_{A=1}^k \ker \omega_0^A)=k$.

Remark: From the above geometrical model, the following definition is introduced in Ref. 2.

Definition 2.1: Let M be a differentiable manifold of dimension $k(n+1)+n$. A family $(\eta_A,\omega_A,V;1\leqslant A\leqslant k)$, where each η_A is a 1-form, each ω_A is a 2-form and V is an nk-dimensional distribution on M, such that

(1) $\eta_1\wedge\cdots\wedge\eta_k\neq 0$, $\eta_{A_{|V}}=0$, $\omega_{A_{|V\times V}}=0$,
(2) $(\cap_{A=1}^k \ker \eta_A)\cap(\cap_{A=1}^k \ker \omega_A)=\{0\}$, $\dim(\cap_{A=1}^k \ker \omega_A)=k$,

is called an almost k-cosymplectic structure, and the manifold M an almost k-cosymplectic manifold.

The following theorem has been proved in Ref. 2.

Theorem 2.2 (*Darboux theorem*)**:** *If the forms η_A and ω_A are closed and V is integrable then around each point of M there exist local coordinates $(t^A,q^i,p_i^A;1\leqslant A\leqslant k,1\leqslant i\leqslant n)$ such that*

$$\eta_A=\mathrm{d}t^A,\quad \omega_A=\mathrm{d}q^i\wedge\mathrm{d}p_i^A,\quad V=\left\langle \frac{\partial}{\partial p_i^1},\ldots,\frac{\partial}{\partial p_i^k}\right\rangle_{i=1,\ldots,n}.$$

In this case M will be called a k-cosymplectic manifold.

The canonical model of these geometrical structures is $(\mathbb{R}^k\times(T_k^1)^*Q,\eta_0^A,\omega_0^A,V_0)$.

For any k-cosymplectic structure (η_A,ω_A,V) on M, there exists a family of k vector fields $\{R_A,1\leqslant A\leqslant k\}$ characterized by the following conditions:

$$\iota_{R_A}\eta_B=\delta_{AB},\quad \iota_{R_A}\omega_B=0,\quad 1\leqslant A,B\leqslant k. \tag{4}$$

They are called the *Reeb vector fields* associated to the k-cosymplectic structure. In the canonical model $R_A=\partial/\partial t^A$, $1\leqslant A\leqslant k$.

2. k-vector fields and integral sections

Let M be an arbitrary manifold, T_k^1M the Whitney sum $TM\overset{k}{\oplus}\ldots\oplus TM$ of k copies of TM and $\tau:T_k^1M\to M$ its canonical projection. $\tau:T_k^1M\to M$ is usually called the tangent bundle of k^1 velocities of M, the reason for this name will be explained in Sec. II B 1.

*Definition 2.3: A section $\mathbf{X}:M\to T_k^1M$ of the projection τ will be called a k-*vector field *on M.*

Since T_k^1M is the Whitney sum $TM\overset{k}{\oplus}\ldots\oplus TM$ of k copies of TM, we deduce that to give a k-vector field $\mathbf{X}$ is equivalent to giving a family of k vector fields $X_1,\ldots,X_k$ on M by projecting $\mathbf{X}$ onto every factor. For this reason we will denote a k-vector field by $(X_1,\ldots,X_k)$.

Definition 2.4: An integral section of the k-vector field $(X_1,\ldots,X_k)$ passing through a point $x\in M$ is a map $\phi:U_0\subset\mathbb{R}^k\to M$, defined on some neighborhood U_0 of $0\in\mathbb{R}^k$, such that

$$\phi(0)=x,\quad \phi_*(t)\left(\left.\frac{\partial}{\partial t^A}\right|_t\right)=X_A(\phi(t))\quad \text{for all } t\in U_0,\ 1\leqslant A\leqslant k. \tag{5}$$

We say that a k-vector field $(X_1,\ldots,X_k)$ on M is integrable if there is an integral section passing through each point of M.

In the k-cosymplectic formalism, the solutions of the field equations are described as integral sections of some k-vector fields. Observe that, in case $k=1$, this definition coincides with the definition of integral curve of a vector field.

3. Hamiltonian formalism

Let (M,η_A,ω_A,V) be a k-cosymplectic manifold, $H:M\to\mathbb{R}$ a Hamiltonian function. Let $\mathbf{X}=(X_1,\ldots,X_k)$ be a k-vector field solution to the following equations:

$$\eta_A(X_B)=\delta_{AB},\quad 1\leqslant A,B\leqslant k,$$

$$\sum_{A=1}^{k}\iota_{X_A}\omega_A=\mathrm{d}H-\sum_{A=1}^{k}R_A(H)\,\eta_A. \tag{6}$$

Using natural coordinates, given by Darboux theorem, if $\mathbf{X}=(X_1,\ldots,X_k)$ is an integrable k-vector field

$$X_A=(X_A)^B\frac{\partial}{\partial t^B}+(X_A)^i\frac{\partial}{\partial q^i}+(X_A)^B_i\frac{\partial}{\partial p^B_i}$$

then

$$(X_A)^B=\delta^B_A,\quad \frac{\partial H}{\partial p^A_i}=(X_A)^i,\quad \frac{\partial H}{\partial q^i}=-\sum_{A=1}^{k}(X_A)^A_i, \tag{7}$$

and if $\phi:\mathbb{R}^k\to M$, given by $\phi(t)=(\phi^A(t),\phi^i(t),\phi^A_i(t))$, is an integral section of $\mathbf{X}$, then

$$\frac{\partial\phi^A}{\partial t^B}=\delta^A_B,\quad \frac{\partial\phi^i}{\partial t^B}=(X_B)^i,\quad \frac{\partial\phi^A_i}{\partial t^B}=(X_B)^A_i.$$

Therefore, from (7) we obtain that $\phi(t)$ is solution to the Hamilton field equations

$$\frac{\partial H}{\partial q^i}=-\sum_{A=1}^{k}\frac{\partial\phi^A_i}{\partial t^A},\quad \frac{\partial H}{\partial p^A_i}=\frac{\partial\phi^i}{\partial t^A},$$

where $1\leqslant A\leqslant k$, $1\leqslant i\leqslant n$.

So, Eqs. (6) can be considered a *geometric version* of the Hamilton field equations.

Remark: It should be noticed that, in general, Eqs. (6) do not have a single solution. In fact, if (M,η_A,ω_A,V) is a k-cosymplectic manifold we can define the vector bundle morphism,

$$\Omega^\sharp:\quad T^1_kM\to T^*M$$

$$(X_1,\ldots,X_k)\mapsto\Omega^\sharp(X_1,\ldots,X_k)=\sum_{A=1}^{k}\iota_{X_A}\omega_A+\eta_A(X_A)\,\eta_A. \tag{8}$$

and, denoting by $\mathcal{M}_k(C^\infty(M))$ the space of matrices of order k whose entries are functions on M, the vector bundle morphism

$$\eta^\sharp:\quad T^1_kM\to\mathcal{M}_k(C^\infty(M))$$

$$(X_1,\ldots,X_k)\mapsto\eta^\sharp(X_1,\ldots,X_k)=(\eta_A(X_B)) \tag{9}$$

then the solutions of (6) are given by $(X_1,\ldots,X_k)+(\ker\Omega^\sharp\cap\ker\eta^\sharp)$, where $(X_1,\ldots,X_k)$ is a particular solution.

From the local conditions (7) we can define in a neighborhood of each point $x \in M$ a k-vector field that satisfies (6). For example, we can set

$$(X_A)^B = \delta_A^B, \quad (X_1)_i^1 = \frac{\partial H}{\partial q^i}, \quad (X_A)_i^B = 0 \quad \text{for } A \neq 1 \neq B, \quad (X_A)^i = \frac{\partial H}{\partial p_i^A}.$$

Now one can construct a global k-vector field, which is a solution of (6), by using a partition of unity in the manifold M. See Ref. 2.

B. The Lagrangian approach (Ref. 3)

1. The geometric elements

The manifold $\mathbb{R}^k \times T_k^1 Q$*:*

Let $\tau_Q : TQ \to Q$ be the tangent bundle of Q. Let us denote by $T_k^1 Q$ the Whitney sum $TQ \overset{k}{\oplus} \ldots \oplus TQ$ of k copies of TQ. Next we shall see that the manifold $\mathbb{R}^k \times T_k^1 Q$ is a cosymplectic manifold when a regular Lagrangian $L : \mathbb{R}^k \times T_k^1 Q \to \mathbb{R}$ is given.

$T_k^1 Q$ can be identified with the manifold $J_0^1(\mathbb{R}^k, Q)$ of the k^1 velocities of the manifold Q, that is, the manifold of 1-jets of maps $\sigma : \mathbb{R}^k \to Q$ with source at $0 \in \mathbb{R}^k$, say

$$J_0^1(\mathbb{R}^k, Q) \equiv TQ \overset{k}{\oplus} \ldots \oplus TQ,$$

$$j_{0,q}^1 \sigma \equiv (v_{1q}, \ldots, v_{kq}),$$

where $q = \sigma(0)$, and $v_{Aq} = \sigma_*(0)[(\partial/\partial t^A)(0)]$, $1 \leq A \leq k$. For this reason $T_k^1 Q$ is called the *tangent bundle of* k^1*-velocities of* Q, see Ref. 7.

The manifold $J^1 \pi_{\mathbb{R}^k}$ of 1-jets of sections of the trivial bundle $\pi_{\mathbb{R}^k} : \mathbb{R}^k \times Q \to \mathbb{R}^k$ is diffeomorphic to $\mathbb{R}^k \times T_k^1 Q$, via the diffeomorphism given by

$$J^1 \pi_{\mathbb{R}^k} \to \mathbb{R}^k \times T_k^1 Q,$$

$$j_t^1 \phi = j_t^1 (Id_{\mathbb{R}^k}, \phi_Q) \to (t, v_1, \ldots, v_k), \tag{10}$$

where $\phi_Q : \mathbb{R}^k \overset{\phi}{\to} \mathbb{R}^k \times Q \overset{\pi_Q}{\to} Q$, and

$$v_A = (\phi_Q)_*(t)\left(\left. \frac{\partial}{\partial t^A} \right|_t \right), \quad 1 \leq A \leq k.$$

Let us denote by $\rho : \mathbb{R}^k \times T_k^1 Q \to Q$ the canonical projection. If (q^i) are local coordinates on $U \subseteq Q$, then the induced local coordinates (q^i, v_i), $1 \leq i \leq n$, on $(\tau_Q)^{-1}(U) = TU \subset TQ$, are given by

$$q^i(v_q) = q^i(q), \quad v_i(v_q) = v_q(q^i) \tag{11}$$

and then the induced local coordinates (t^A, q^i, v_A^i) on $\rho^{-1}(U) = \mathbb{R}^k \times T_k^1 U$ are given by

$$t^A(j_t^1 \phi) = t^A, \quad q^i(j_t^1 \phi) = q^i(\phi_Q(t)), \quad v_A^i(j_t^1 \phi) = \frac{\partial (q^i \circ \phi_Q)}{\partial t^A}|_t$$

or equivalently

$$t^A(t, v_{1q}, \ldots, v_{kq}) = t^A, \quad q^i(t, v_{1q}, \ldots, v_{kq}) = q^i(q), \quad v_A^i(t, v_{1q}, \ldots, v_{kq}) = v_{Aq}(q^i),$$

where $1 \leq i \leq n$, $1 \leq A \leq k$.

Throughout the paper we shall use the following notation for the canonical projections:

$$\mathbb{R}^k \times (T_k^1)Q \xrightarrow{(\pi_{\mathbb{R}^k})_{1,0}} \mathbb{R}^k \times Q \xrightarrow{(\pi_{\mathbb{R}^k})} \mathbb{R}^k$$

and $(\pi_{\mathbb{R}^k})_1 = \pi_{\mathbb{R}^k} \circ (\pi_{\mathbb{R}^k})_{1,0}$, where

$$\pi_{\mathbb{R}^k}(t,q) = t, \quad (\pi_{\mathbb{R}^k})_{1,0}(t, v_{1q}, \ldots, v_{kq}) = (t,q), \quad (\pi_{\mathbb{R}^k})_1(t, v_{1q}, \ldots, v_{kq}) = q,$$

with $t \in \mathbb{R}^k$, $q \in Q$ and $(v_{1_q}, \ldots, v_{k_q}) \in T_k^1 Q$.

Canonical vector fields on $\mathbb{R}^k \times T_k^1 Q$*:*

Let us denote by C the *canonical vector field (Liouville vector field)* of the vector bundle $(\pi_{\mathbb{R}^k})_{1,0}: \mathbb{R}^k \times T_k^1 Q \to \mathbb{R}^k \times Q$. This vector field C is the infinitesimal generator of the following flow:

$$\mathbb{R} \times (\mathbb{R}^k \times T_k^1 Q) \to \mathbb{R}^k \times T_k^1 Q,$$

$$(s, (t, v_{1q}, \ldots, v_{kq})) \to (t, e^s v_{1q}, \ldots, e^s v_{kq}),$$

and in local coordinates it has the form

$$C = \sum_{i,A} v_A^i \frac{\partial}{\partial v_A^i}, \tag{12}$$

C is sum of the vector fields

$$C = \sum_{A=1}^{k} C_A,$$

where each C_A is the generator infinitesimal of the following flow:

$$\mathbb{R} \times (\mathbb{R}^k \times T_k^1 Q) \to \mathbb{R}^k \times T_k^1 Q,$$

$$(s, (t, v_{1q}, \ldots, v_{kq})) \to (t, v_{1q}, \ldots, v_{A-1q}, e^s v_{Aq}, v_{A+1q}, \ldots, v_{kq}).$$

Canonical tensor fields on $\mathbb{R}^k \times T_k^1 Q$*:*

The canonical k-tangent structure on $T_k^1 Q$ is the set $(S_1, \ldots, S_k)$ of tensor fields of type (1, 1) locally given by

$$S_A = \frac{\partial}{\partial v_A^i} \otimes \mathrm{d}q^i, \quad 1 \leqslant A \leqslant k. \tag{13}$$

The tensor fields S_A can be regarded as the $(0, \ldots, 0, \overset{A}{1}, 0, \ldots, 0)$-lift of the identity tensor on Q to $T_k^1 Q$ defined in Ref. 7.

In an obvious way we shall consider the extension of S_A to $\mathbb{R}^k \times T_k^1 Q$, which we also denote by S_A and it has the same local expression (13).

The k-tangent manifolds were introduced as a generalization of the tangent manifolds by de León *et al.* (Refs. 8 and 9). The canonical model of these manifolds is $T_k^1 Q$ with the structure given by $(S_1, \ldots, S_k)$.

As in the case of mechanical systems, these tensor fields S_A allow us to introduce the forms θ_L^A and ω_L^A on $\mathbb{R}^k \times T_k^1 Q$ as follows:

$$\theta_L^A = \mathrm{d}L \circ S_A, \quad \omega_L^A = -\,\mathrm{d}\theta_L^A, \quad 1 \leqslant A \leqslant k,$$

with local expressions

$$\theta_L^A = \frac{\partial L}{\partial v_A^i} \mathrm{d}q^i, \quad \omega_L^A = \mathrm{d}q^i \wedge d\left(\frac{\partial L}{\partial v_A^i}\right), \quad 1 \leqslant A \leqslant k. \tag{14}$$

These forms play an important role in the Lagrangian formulation.

Second order partial differential equations on T_k^1Q:

The aim of this section is to characterize the integrable k-vector fields on $\mathbb{R}^k \times T_k^1Q$ such that their integral sections are canonical prolongations of maps from $\mathbb{R}^k$ to Q.

In general, if $F: M \to N$ is a differentiable map, then the induced map $T_k^1(F): T_k^1M \to T_k^1N$ defined by $T_k^1(F)(j_0^1g) = j_0^1(F \circ g)$ is given by

$$T_k^1(F)(v_{1q}, \ldots, v_{kq}) = (F_*(q)v_{1q}, \ldots, F_*(q)v_{kq}),$$

where $v_{1_q}, \ldots, v_{k_q} \in T_qQ$, $q \in Q$, and $F_*(q): T_qM \to T_{F(q)}N$ is the induced map.

Definition 2.5: A k-vector field $\mathbf{X} = (X_1, \ldots, X_k)$ *on* $\mathbb{R}^k \times T_k^1Q$ *is said to be a second order partial differential equation (SOPDE for short) if*

$$\mathrm{d}t^A(X_B) = \delta_B^A, \quad (\tau_{\mathbb{R}^k} \times id_{T_k^1Q}) \circ T_k^1((\pi_{\mathbb{R}^k})_{1,0}) \circ X = id_{\mathbb{R}^k \times T_k^1Q},$$

where

$$\tau_{\mathbb{R}^k} \times id_{T_k^1Q}: \quad T_k^1(\mathbb{R}^k \times Q) \equiv T_k^1(\mathbb{R}^k) \times T_k^1Q \to \mathbb{R}^k \times T_k^1Q,$$

$$(t^A, q^i, v_A^B, v_A^i) \equiv ((t^A, v_A^B), (q^i, v_A^i)) \to (t^A, q^i, v_A^i).$$

Let (q^i) be a coordinate system on Q and (t^A, q^i, v_A^i) the induced coordinate system on $\mathbb{R}^k \times T_k^1Q$. From a direct computation in local coordinates we obtain that the local expression of a SOPDE $(X_1, \ldots, X_k)$ is

$$X_A(t, q^i, v_B^i) = \frac{\partial}{\partial t^A} + v_A^i \frac{\partial}{\partial q^i} + (X_A)_B^i \frac{\partial}{\partial v_B^i}, \quad 1 \leqslant A \leqslant k, \tag{15}$$

where $(X_A)_B^i$ are functions on $\mathbb{R}^k \times T_k^1Q$. As a direct consequence of the above local expressions, we deduce that the family of vector fields $\{X_1, \ldots, X_k\}$ are linearly independent.

Definition 2.6: Let $\phi: \mathbb{R}^k \to Q$ *be a map, we define the* first prolongation $\phi^{[1]}$ *of* ϕ *as the map*

$$\phi^{[1]}: \mathbb{R}^k \to \mathbb{R}^k \times T_k^1Q$$

$$t \to (t, j_0^1\phi_t) \equiv \left(t, \phi_*(t)\left(\frac{\partial}{\partial t^1}\right), \ldots, \phi_*(t)\left(\frac{\partial}{\partial t^k}\right)\right),$$

where $\phi_t(s) = \phi(t+s)$. *In local coordinates*

$$\phi^{[1]}(t^1, \ldots, t^k) = \left(t^1, \ldots, t^k, \phi^i(t^1, \ldots, t^k), \frac{\partial \phi^i}{\partial t^A}(t^1, \ldots, t^k)\right), \tag{16}$$

where $1 \leqslant A \leqslant k$, $1 \leqslant i \leqslant n$.

Remark: Let $(X_1, \ldots, X_k)$ be an SOPDE. From (15) we obtain: a map $\psi: \mathbb{R}^k \to \mathbb{R}^k \times T_k^1Q$, given by $\psi(t) = (\psi^B(t), \psi^i(t), \psi_A^i(t))$, is an integral section of $(X_1, \ldots, X_k)$ if and only if

$$\left.\frac{\partial \psi^B}{\partial t^A}\right|_t = \delta_A^B, \qquad \left.\frac{\partial \psi^i}{\partial t^A}\right|_t = \psi_A^i(t), \qquad \left.\frac{\partial^2 \psi^i}{\partial t^A \partial t^B}\right|_t = (X_A)_B^i(\psi(t)). \tag{17}$$

Then if $(X_1, \ldots, X_k)$ is integrable, from (17) we deduce that $(X_A)_B^i = (X_B)_A^i$.

Let us observe that the map

$$(id_{\mathbb{R}^k}, pr_2 \circ \psi): \mathbb{R}^k \to \mathbb{R}^k \times T_k^1Q$$

$$t \to (t, \psi^i(t), \psi^i_A(t))$$

coincides with the first prolongation $\phi^{[1]}$ of the map $\phi = \rho \circ \psi : \mathbb{R}^k \overset{\psi}{\to} \mathbb{R}^k \times T^1_k Q \overset{\rho}{\to} Q$, that is $\phi(t) = (\psi^i(t))$.

Conversely if $\phi : \mathbb{R}^k \to Q$ is any map such that

$$\left. \frac{\partial^2 \phi^i}{\partial t^A \partial t^B} \right|_t = (X_A)^i_B(\phi^{[1]}(t)),$$

then $\phi^{[1]}$ is an integral section of $(X_1, \ldots, X_k)$.

On $\mathbb{R}^k \times T^1_k Q$ we consider the tensor fields of type (1,1) defined by

$$\hat{S}_A = S_A - C_A \otimes \mathrm{d}t^A,$$

for each $A = 1, \ldots, k$. A characterization of the SOPDE using these tensors is the following.

Proposition 2.7: A k-vector field $(X_1, \ldots, X_k)$ *on* $\mathbb{R}^k \times T^1_k Q$ *is a* SOPDE *if*

$$\mathrm{d}t^A(X_B) = \delta^A_B, \quad \hat{S}_A(X_B) = 0$$

for all $1 \leqslant A, B \leqslant k$.

2. The Legendre transform and Lagrangian forms

Given a Lagrangian $L : \mathbb{R}^k \times T^1_k Q \to \mathbb{R}$ the Legendre map

$$FL : \mathbb{R}^k \times T^1_k Q \to \mathbb{R}^k \times (T^1_k)^* Q$$

is defined as follows:

$$FL(t, v_{1q}, \ldots, v_{kq}) = (t, \ldots, [FL(t, v_{1q}, \ldots, v_{kq})]^A, \ldots),$$

where

$$[FL(t, v_{1q}, \ldots, v_{kq})]^A(w_q) = \frac{d}{\mathrm{d}s} L\ (t, v_{1q}, \ldots, v_{Aq} + s w_q, \ldots, v_{kq}))_{|s=0},$$

for each $A = 1, \ldots, k$; and it is locally given by

$$FL : (t^A, q^i, v^i_A) \to \left(t^A, q^i, \frac{\partial L}{\partial v^i_A} \right). \tag{18}$$

From (14) and (18) one deduces the following identities:

$$\theta^A_L = FL^* \theta^A_0, \quad \omega^A_L = FL^* \omega^A_0, \quad 1 \leqslant A \leqslant k. \tag{19}$$

Definition 2.8: A Lagrangian function $L : \mathbb{R}^k \times T^1_k Q \to R$ *is said to be regular (respectively, hyperregular) if the corresponding Legendre map FL is a local (respectively global) diffeomorphism.*

From (18) we obtain that L is regular if and only if $\det(\partial^2 L / \partial v^i_A \partial v^j_B) \neq 0$, $1 \leqslant i, j \leqslant n$, $1 \leqslant A, B \leqslant k$.

The following proposition has an important role in the Lagrangian formulation. See Ref. 3.

Proposition 2.9: The following conditions are equivalent:

(1) *L is regular.*
(2) *FL is a local diffeomorphism.*
(3) $(\mathrm{d}t^A, \omega^A_L, V^0)$ *is a k-cosymplectic structure on* $\mathbb{R}^k \times T^1_k Q$ *where*

$$V^0 = \ker T(\pi_{\mathbb{R}^k})_{1,0} = \left\langle \frac{\partial}{\partial v_1^i}, \ldots, \frac{\partial}{\partial v_k^i} \right\rangle_{i=1,\ldots,n}$$

is the vertical distribution of the bundle $(\pi_{\mathbb{R}^k})_{1,0}: \mathbb{R}^k \times T_k^1 Q \to \mathbb{R}^k \times Q$.

■

3. Lagrangian formalism

Given a Lagrangian function $L = L(t^A, q^i, v_A^i)$, and by using a variational principle, the *Euler-Lagrange field equations* for L are obtained:

$$\sum_{A=1}^{k} \frac{d}{dt^A}\left(\frac{\partial L}{\partial v_A^i}\right) - \frac{\partial L}{\partial q^i} = 0, \quad v_A^i = \frac{\partial q^i}{\partial t^A}. \tag{20}$$

In this section we give a geometrical description of the above equations (20).

Let $L: \mathbb{R}^k \times T_k^1 Q \to \mathbb{R}$ be a regular Lagrangian, and let (dt^A, ω_L^A, V^0) be the k-cosymplectic structure on $\mathbb{R}^k \times T_k^1 Q$ defined by L. Let $(R_L)_A$ be the Reeb vector fields corresponding to this k-cosymplectic structure. They are characterized by

$$i_{(R_L)_A} dt^B = \delta_A^B, \quad i_{(R_L)_A}(\omega_L)_B = 0.$$

Since $(R_L)_A(E_L) = -\partial L / \partial t^A$, writing Eqs. (6) for this k-cosymplectic structure we have the following result.

Theorem 2.10: *Let L be a regular Lagrangian and let $((X_L)_1, \ldots, (X_L)_k)$ be a k-vector field such that*

$$dt^A((X_L)_B) = \delta_B^A, \quad 1 \leqslant A, B \leqslant k,$$

$$\sum_{A=1}^{k} i_{(X_L)_A} \omega_L^A = dE_L + \sum_{A=1}^{k} \frac{\partial L}{\partial t^A} dt^A, \tag{21}$$

where $E_L = C(L) - L$. Then

(1) *$((X_L)_1, \ldots, (X_L)_k)$ is an SOPDE.*

(2) *If it is integrable, and $\phi^{[1]}: \mathbb{R}^k \to \mathbb{R}^k \times T_k^1 Q$ is an integral section, then $\phi: \mathbb{R}^k \to Q$ is a solution of the Euler-Lagrange equations (20).*

The k-vector field

$$(X_L)_A = [(X_L)_A]^B \frac{\partial}{\partial t^B} + [(X_L)_A]^i \frac{\partial}{\partial q^i} + [(X_L)_A]_B^i \frac{\partial}{\partial v_B^i}, \quad 1 \leqslant A \leqslant k$$

is a solution to the equations (21) if and only if it satisfies the following identities:

$$[(X_L)_A]^B = \delta_A^B, \quad [(X_L)_A]^i = v_A^i, \quad \sum_{A=1}^{k} (X_L)_A\left(\frac{\partial L}{\partial v_A^k}\right) = \frac{\partial L}{\partial q^k}. \tag{22}$$

Remark: If we rewrite the equations (21) for the case $k = 1$, we have

$$dt(X_L) = 1, \quad i_{X_L}\omega_L = dE_L + \frac{\partial L}{\partial t} dt \tag{23}$$

which are equivalent to the dynamical equations

$$\mathrm{d}t(X_L)=1, \quad i_{X_L}\Omega_L=0,$$

where $\Omega_L=\omega_L+\mathrm{d}E_L\wedge\mathrm{d}t$ is the Poincaré-Cartan 2-form associated to the Lagrangian L, see Ref. 1. Remember that this describes the nonautonomous mechanics.

Remark: The above forms θ_L^A and ω_L^A are related with the multisymplectic Poincaré-Cartan forms θ_L and Ω_L in the Lagrangian jet formalism of field theory in a similar way as indicated in Ref. 5, Sec. V B.

The k-vector fields $((X_L)_1,\ldots,(X_L)_k)$ allow us to construct a decomposable multivector field $\mathcal{X}=(X_L)_1\wedge\ldots\wedge(X_L)_k$, which is related with the multivector field solution to the Lagrangian equation described in Ref. 10, Sec. 7, and they give the same solutions to the Lagrangian equations.

III. CONNECTIONS AND LAGRANGIAN ENERGY

A. Connections in $\pi_{\mathbb{R}^k}:\mathbb{R}^k\times Q\to\mathbb{R}^k$

The following Proposition can be found in Ref. 11 for an arbitrary fiber bundle $\pi:E\to M$, or in different sections in Ref. 12. The following is stated in our setting.

Proposition 3.1: Let $\pi_{\mathbb{R}^k}:\mathbb{R}^k\times Q\to\mathbb{R}^k$ *be the trivial bundle and* $(\pi_{\mathbb{R}^k})_{1,0}:J^1(\mathbb{R}^k\times Q)\equiv\mathbb{R}^k\times T^1_kQ\to\mathbb{R}^k\times Q$ *the corresponding first-order jet bundle. The following elements can be canonically constructed one from the other:*

(1) *A global section of* $(\pi_{\mathbb{R}^k})_{1,0}:J^1\pi_{\mathbb{R}^k}\equiv\mathbb{R}^k\times T^1_kQ\to\mathbb{R}^k\times Q$; *that is, a mapping* $\Psi:\mathbb{R}^k\times Q\to\mathbb{R}^k\times T^1_kQ$ *such that* $(\pi_{\mathbb{R}^k})_{1,0}\circ\Psi=Id_{\mathbb{R}^k\times Q}$.
(2) *A subbundle* H *of* $T(\mathbb{R}^k\times Q)$ *such that* $T(\mathbb{R}^k\times Q)=V(\pi_{\mathbb{R}^k})\oplus H$.
(3) *A* $\pi_{\mathbb{R}^k}$*-semibasic 1-form* ∇ *on* $\mathbb{R}^k\times Q$ *with values on* $T(\mathbb{R}^k\times Q)$, *such that* $\nabla^*\alpha=\alpha$, *for every* $\pi_{\mathbb{R}^k}$*-semibasic form* $\alpha\in\Lambda^1(\mathbb{R}^k\times Q)$.

Definition 3.2: A connection in the bundle $\pi_{\mathbb{R}^k}:\mathbb{R}^k\times Q\to\mathbb{R}^k$ *is one of the above-mentioned equivalent elements. H is called the horizontal sub-bundle of* $T(\mathbb{R}^k\times Q)$ *associated with the connection* ∇ *and its sections are the horizontal vector fields.* ∇ *is called the connection form.*

Let (q^i) be a coordinate system on $U\subset Q$ and let (t^A,q^i) be the induced coordinate system on $\mathbb{R}^k\times U$. The local expression of the connection form is

$$\nabla=\mathrm{d}t^A\otimes\left(\frac{\partial}{\partial t^A}+\Gamma^i_A\frac{\partial}{\partial q^i}\right),$$

where $\Gamma^i_A\in C^\infty(\mathbb{R}^k\times U)$.

Let $\Psi:\mathbb{R}^k\times Q\to J^1(\mathbb{R}^k\times Q)\equiv\mathbb{R}^k\times T^1_kQ$ be a section, then $\Psi(t,q)=j^1_t\phi=j^1_t(Id_{\mathbb{R}^k},\phi_Q)$ where $\phi_Q=\pi_Q\circ\phi:\mathbb{R}^k\xrightarrow{\phi}\mathbb{R}^k\times Q\xrightarrow{\pi_Q}Q$, with $\phi(t)=(t,q)$ and $\phi_Q(t)=q$.

If $\Psi(t,q)=(t,q,\Psi^i_A(t,q))$ from (10) we have

$$\Psi^i_A(t,q)=\frac{\partial(q^i\circ\phi_Q)}{\partial t^A}|_t.$$

Then we define

$$H_{(t,q)}:=\mathrm{Im}\ \phi_*(t) \quad \text{and} \quad H=\bigcup_{(t,q)\in\mathbb{R}^k\times Q}H_{(t,q)}$$

so the basis of $H_{(t,q)}$ is

$$\phi_*(t)\left(\frac{\partial}{\partial t^A}|_t\right)=\frac{\partial}{\partial t^A}|_{(t,q)}+\frac{\partial(q^i\circ\phi_Q)}{\partial t^A}|_t\frac{\partial}{\partial q^i}|_{(t,q)}, \quad 1\leqslant A\leqslant k$$

and the components of the connection Γ^i_A are given by

$$\Gamma_A^i(t,q) = \frac{\partial(q^i \circ \phi_Q)}{\partial t^A}_{|t} = \Psi_A^i(t,q),$$

where $\Psi(t,q) = j_t^1(Id_{\mathbb{R}}^k, \phi_Q)$ with $\phi_Q(t) = q$.

For a vector field

$$X = f^A \frac{\partial}{\partial t^A} + \lambda^i \frac{\partial}{\partial q^i} \in \mathfrak{X}(\mathbb{R}^k \times Q)$$

we have the splitting

$$X = (X - \nabla(X)) + \nabla(X) = \pi_\nabla^v(X) + \pi_\nabla^h(X) \tag{24}$$

and so the horizontal and vertical projections are given by

$$\pi_\nabla^h(X) = f^A\left(\frac{\partial}{\partial t^A} + \Gamma_A^i \frac{\partial}{\partial q^i}\right), \quad \pi_\nabla^v(X) = (\lambda^i - f^A\Gamma_A^i)\frac{\partial}{\partial q^i}.$$

Remark: Every connection in the bundle $\pi_{\mathbb{R}^k}: \mathbb{R}^k \times Q \to \mathbb{R}^k$ induces a horizontal lift of a vector field X on $\mathbb{R}^k$ to a horizontal vector field X^H, on $\mathbb{R}^k \times Q$, which projects on X.

Let ∇ be a connection and let us suppose that $\nabla(t,q) = j_t^1\phi$, where $\phi = (id_{\mathbb{R}^k}, \phi_Q): \mathbb{R}^k \to \mathbb{R}^k \times Q$, with $\phi(t) = (t, \phi_Q(t))$ and $\phi_Q(t) = q$. If

$$X(t) = X^A(t)\frac{\partial}{\partial t^A}_{|t}$$

then

$$X^H(t,q) = \phi_*(t)(X(t)) = X^A(t)\left(\frac{\partial}{\partial t^A}_{|(t,q)} + \frac{\partial q^i \circ \phi_Q}{\partial t^A}_{|t}\frac{\partial}{\partial q^i}_{|(t,q)}\right) = X^A(t)\left(\frac{\partial}{\partial t^A}_{|(t,q)} + \Gamma_A^i(t,q)\frac{\partial}{\partial q^i}_{|(t,q)}\right).$$

B. Vector fields in $\mathbb{R}^k \times Q$ associated to a connection ∇

Given a connection ∇ on $\mathbb{R}^k \times Q \to \mathbb{R}^k$, we consider the horizontal lifts $\widetilde{Y}_A$ of the global generators $\{\partial/\partial t^A, A = 1, \ldots, k,\}$ of $\mathfrak{X}(\mathbb{R}^k)$,

$$\widetilde{Y}_A(t,q) = \left(\frac{\partial}{\partial t^A}\right)^H_{|(t,q)} = \frac{\partial}{\partial t^A}_{|(t,q)} + \Gamma_A^i(t,q)\frac{\partial}{\partial q^i}_{|(t,q)}, \quad 1 \leqslant A \leqslant k. \tag{25}$$

Definition 3.3: The vector fields $\widetilde{Y}_A$ will be called the associated vector fields to the connection ∇.

If ∇_0 is the *standard connection* on $\pi_{\mathbb{R}^k}: \mathbb{R}^k \times Q \to \mathbb{R}^k$, then, since $\Gamma_A^i \equiv 0$, the associated vector fields to ∇_0 are given by

$$\left(\frac{\partial}{\partial t^A}\right)^H_{|(t,q)} = \left(\frac{\partial}{\partial t^A}\right)_{|(t,q)}, \quad 1 \leqslant A \leqslant k.$$

C. Lagrangian energy functions

As is well known from Saunders[12] (p. 156), in the bundle $\pi_{\mathbb{R}^k}: \mathbb{R}^k \times Q \to \mathbb{R}^k$ and associated to the form dt^A, we have a natural vector-valued 1-form S_{dt^A} with coordinate expression

$$S_{dt^A} = (dq^i - v_B^i\, dt^B) \otimes \frac{\partial}{\partial v_A^i}, \quad 1 \leqslant A \leqslant k. \tag{26}$$

Let $L:\mathbb{R}^k\times T^1_kQ\to\mathbb{R}$ be a Lagrangian. By means of the geometrical structures of $\mathbb{R}^k\times T^1_kQ$ we can construct the Lagrangians forms and the energy function associated to L.

Definition 3.4: The Poincaré-Cartan 1*-forms associated with the Lagrangian function L are the forms in* $\mathbb{R}^k\times T^1_kQ$ *defined by*

$$\Theta^A_L := \mathrm{d}L\circ S_{\mathrm{d}t^A}+\frac{1}{k}L\,\mathrm{d}t^A,\quad 1\leqslant A\leqslant k. \tag{27}$$

From (26) we deduce that Θ^A_L is locally given by

$$\Theta^A_L := \left(\frac{1}{k}\delta^A_B L-v^i_B\frac{\partial L}{\partial v^i_A}\right)\mathrm{d}t^B+\frac{\partial L}{\partial v^i_A}\mathrm{d}q^i. \tag{28}$$

These forms only depend on the Lagrangian and the natural structures in the bundle, and we can write

$$\Theta^A_L=\theta^A_L+\left(\frac{1}{k}\delta^A_B L-v^i_B\frac{\partial L}{\partial v^i_A}\right)\mathrm{d}t^B,\quad 1\leqslant A\leqslant k. \tag{29}$$

The *Lagrangian energy function* $E_L=CL-L$ is locally given by

$$E_L=v^i_A\frac{\partial L}{\partial v^i_A}-L.$$

We can intrinsically define this Lagrangian energy function in the following way: Consider the standard connection ∇_0 in the bundle $\pi_{\mathbb{R}^k}:\mathbb{R}^k\times Q\to\mathbb{R}^k$, and the prolongation, $j^1(\partial/\partial t^A)$, of the horizontal lifting of $\partial/\partial t^A$ given by the connection, from $\mathbb{R}^k$ to $\mathbb{R}^k\times Q$, which will be denoted as usual by $\partial/\partial t^A$, then

$$E_L=-\sum_{A=1}^{k} i_{\partial/\partial t^A}\Theta^A_L.$$

One of the most significant aspects of the above expression for the Lagrangian energy is that it is obtained by contraction of the associated vector fields to the standard connection with the Lagrangian forms.

If we consider a nonstandard connection, then in order to define the Lagrangian energy function associated to ∇ we must lift $\partial/\partial t^A$ from $\mathbb{R}^k$ to $\mathbb{R}^k\times T^1_kQ$ to be contracted with Θ^A_L in the following way.

Definition 3.5: Let ∇ *be a connection in* $\pi_{\mathbb{R}^k}:\mathbb{R}^k\times Q\to\mathbb{R}^k$, *and* $\widetilde{Y}_A$, $A=1,\ldots,k$, *the associated vector fields to the connection* ∇ *given by (25).*

Let $j^1\widetilde{Y}_A\in\mathfrak{X}(\mathbb{R}^k\times T^1_kQ)$ *the prolongation of the vector fields* $\widetilde{Y}_A\in\mathfrak{X}(\mathbb{R}^k\times Q)$, *defined in Ref. 12, p. 133.*

The Lagrangian energy function associated with the Lagrangian L and the connection ∇ *is*

$$E^{\nabla}_L=-\sum_{A=1}^{k} i_{j^1\widetilde{Y}_A}\Theta^A_L.$$

In a local chart, if

$$\widetilde{Y}_A=\frac{\partial}{\partial t^A}+\Gamma^i_A\frac{\partial}{\partial q^i}$$

then, see Ref. 12,

$$j^1\widetilde{Y}_A = \frac{\partial}{\partial t^A} + \Gamma_A^i \frac{\partial}{\partial q^i} + \left(\frac{\partial \Gamma_A^i}{\partial t^B} + v_B^j \frac{\partial \Gamma_A^i}{\partial q^j} \right) \frac{\partial}{\partial v_B^i} \tag{30}$$

and from (28) and (30) we obtain

$$E_L^\nabla = \sum_{A=1}^{k} \frac{\partial L}{\partial v_A^i} (v_A^i - \Gamma_A^i) - L. \tag{31}$$

It is obvious from this expression that the Lagrangian energy E_L^∇ is connection dependent.

In the following lemma, we will suppose that a Lagrangian function L and a connection ∇ are given.

Lemma 3.6: Let $(X_1, \ldots, X_k)$ be a SOPDE on $\mathbb{R}^k \times T_k^1 Q$. If

$$(1)\ X_B(\Gamma_A^i) = X_A(\Gamma_B^i), \quad (2)\ X_A\left(\frac{\partial L}{\partial v_B^i} \right) = \delta_B^A \frac{\partial L}{\partial q^i}, \quad A,B = 1, \ldots, k \tag{32}$$

then

$$X_A(E_L^\nabla) = -\, j^1\widetilde{Y}_A(L), \quad A = 1, \ldots, k.$$

Proof: From the local expressions (15), (30), and (31) we obtain

$$\begin{aligned}
X_A(E_L^\nabla) + j^1\widetilde{Y}_A(L) &= \left(\frac{\partial \Gamma_A^i}{\partial t^B} - \frac{\partial \Gamma_B^i}{\partial t^A} \right) \frac{\partial L}{\partial v_B^i} + \left(v_B^j \frac{\partial \Gamma_A^i}{\partial q^j} - v_A^j \frac{\partial \Gamma_B^i}{\partial q^j} \right) \frac{\partial L}{\partial v_B^i} + \left(\frac{\partial^2 L}{\partial t^A \partial v_C^k} + v_A^i \frac{\partial^2 L}{\partial q^i \partial v_C^k} \right. \\
&\quad \left. + (X_A)_B^j \frac{\partial^2 L}{\partial v_B^j \partial v_C^k} - \delta_C^A \frac{\partial L}{\partial q^k} \right) (v_C^k - \Gamma_C^k) \\
&= \left(\left(\frac{\partial}{\partial t^B} + v_B^j \frac{\partial}{\partial q^j} \right) (\Gamma_A^i) - \left(\frac{\partial}{\partial t^A} + v_A^j \frac{\partial}{\partial q^j} \right) (\Gamma_B^i) \right) \frac{\partial L}{\partial v_B^i} \\
&\quad + \left(\frac{\partial^2 L}{\partial t^A \partial v_C^k} + v_A^i \frac{\partial^2 L}{\partial q^i \partial v_C^k} + (X_A)_B^j \frac{\partial^2 L}{\partial v_B^j \partial v_C^k} - \delta_C^A \frac{\partial L}{\partial q^k} \right) (v_C^k - \Gamma_C^k) \\
&= (X_C(\Gamma_A^i) - X_A(\Gamma_C^i)) \frac{\partial L}{\partial v_C^i} + \left(\frac{\partial^2 L}{\partial t^A \partial v_C^k} + v_A^i \frac{\partial^2 L}{\partial q^i \partial v_C^k} \right. \\
&\quad \left. + (X_A)_B^j \frac{\partial^2 L}{\partial v_B^j \partial v_C^k} - \delta_C^A \frac{\partial L}{\partial q^i} \right) (v_C^k - \Gamma_C^k) \\
&= (X_C(\Gamma_A^i) - X_A(\Gamma_C^i)) \frac{\partial L}{\partial v_C^i} + \left(X_A\left(\frac{\partial L}{\partial v_C^k} \right) - \delta_C^A \frac{\partial L}{\partial q^k} \right) (v_C^k - \Gamma_C^k).
\end{aligned}$$

■

We know that if L is a regular Lagrangian and $((X_L)_1, \ldots, (X_L)_k)$ is an integrable solution of (21), then it is a SOPDE. Then we have the following.

Corollary 3.7: Suppose that the Lagrangian L is regular and let $((X_L)_1, \ldots, (X_L)_k)$ be an integrable solution of (21) satisfying the conditions (32).

If L is invariant by the prolongations $j^1\widetilde{Y}_A$ then the associated energy function E_L^∇ is invariant by the vector fields $(X_L)_A$, $A = 1, \ldots, k$. That is, E_L^∇ is constant along the integral sections of $((X_L)_1, \ldots, (X_L)_k)$.

■

Remark: In the case $k=1$, if X_L is the dynamical vector field on $\mathbb{R} \times TQ$, then X_L is an SODE and satisfies (1) trivially, and (2) (in Lemma 3.6) because it is a solution to the dynamical equations (23). Therefore, in this case we have

$$X_L(E_L^\nabla) = -j^1\tilde{Y}(L),$$

which is the assertion of Theorem 1 in Ref. 4.

Proposition 3.8: Let L be a Lagrangian function such that the components $[FL(t,w_q)]^A$, *of the Legendre transformation FL are different from zero at every point* $(t,w_q)=(t,v_{1_q},\dots v_{k_q})\in\mathbb{R}^k\times T_k^1Q$.

Let $f:\mathbb{R}^k\times T_k^1Q\to\mathbb{R}^k$ *be a mapping, then there exists a connection* ∇ *such that the energy function* E_L^∇ *associated to this connection is given by*

$$E_L^\nabla = \sum_{A=1}^{k} f^A,$$

where $f^A=\pi^A\circ f:\mathbb{R}^k\times T_k^1Q\overset{f}{\to}\mathbb{R}^k\overset{\pi^A}{\to}\mathbb{R}$.

If L is a regular Lagrangian and $((X_L)_1,\dots,(X_L)_k)$ *is an integrable solution of (21) that satisfies the conditions (32), and* $(X_L)_A(\Sigma_B f^B)=0$, *then* $j^1\tilde{Y}_A(L)=0$ *for* $A=1,\dots,k$.

Proof: Let ∇ be the connection such that its associated vector fields Y_A verify

$$i_{j^1\tilde{Y}_A}\Theta_L^A = -f^A, \quad 1\leqslant A\leqslant k.$$

From (28) and (30) we deduce that this connection is given by

$$-f^A = \left(\frac{1}{k}L - v_A^i\frac{\partial L}{\partial v_A^i}\right) + \frac{\partial L}{\partial v_A^i}\Gamma_A^i$$

and thus

$$E_L^\nabla = \sum_{A=1}^{k}\frac{\partial L}{\partial v_A^i}(v_A^i-\Gamma_A^i) - L = \sum_{A=1}^{k} f^A.$$

Now from Lemma 3.6 we obtain

$$0 = (X_L)_A\left(\sum_{B=1}^{k} f^B\right) = (X_L)_A(E_L^\nabla) = -j^1\tilde{Y}_A(L).$$

■

This Proposition in the case $k=1$ coincides with Proposition 4 in Ref. 4.

IV. HAMILTONIAN FORMALISM WITH NONSTANDARD FLAT CONNECTIONS

In this section, we will suppose a given connection ∇ in the bundle $\pi_{\mathbb{R}^k}:\mathbb{R}^k\times Q\to\mathbb{R}^k$. First, associated to this connection, we are going to construct a k-cosymplectic structure $(\mathrm{d}t^A,\omega_A^\nabla,V_0)$ on $\mathbb{R}^k\times(T_k^1)^*Q$. Second, if we have a Lagrangian, L, then a Hamiltonian function will be associated to L and ∇. With these ingredients, we study the Hamiltonian formalism and the dynamical equations.

For the k-cosymplectic structure, let us consider the canonical projections $\tau_Q^*:T^*Q\to Q$ and $\pi_2^A:\mathbb{R}^k\times(T_k^1)^*Q\to T^*Q$ given by $\pi_2^A(t,\alpha_q^1,\dots,\alpha_q^k)=\alpha_q^A$, $1\leqslant A\leqslant k$.

Since $\theta_0^A=(\pi_2^A)^*\theta_0$, using the definition of θ_0 we obtain that

$$\theta_0^A(w_{t,q}) = \alpha_q^A\circ(\tau_Q^*)_*(\alpha_q^A)\circ(\pi_2^A)_*(w_{t,q}),$$

where $w_{t,q}=(t,\alpha_q^1,\dots,\alpha_q^k)\in\mathbb{R}^k\times(T_k^1)^*Q$.

The connection ∇ enables other 1-forms on $\mathbb{R}^k\times(T_k^1)^*Q$ to be constructed in the following way.

Definition 4.1: The composition

$$T_{w_{t,q}}(\mathbb{R}^k \times (T^1_k)^*Q) \xrightarrow{((\pi_Q)_{1,0})_* w_{t,q}} T_{(t,q)}(\mathbb{R}^k \times Q) \xrightarrow{\pi^v_\nabla} V_{(t,q)}(\pi_{\mathbb{R}} k)$$

$$\subset T_{(t,q)}(\mathbb{R}^k \times Q) \xrightarrow{(\pi_Q)_*(t,q)} T_qQ \xrightarrow{\alpha^A_q} \mathbb{R},$$

define the 1*-forms* θ^A_∇ *on* $\mathbb{R}^k \times (T^1_k)^*Q$ *by*

$$\theta^A_\nabla(w_{t,q}) = \alpha^A_q \circ (\pi_Q)_*(t,q) \circ \pi^v_\nabla \circ ((\pi_Q)_{1,0})_* w_{t,q}. \tag{33}$$

From (24) we deduce that

$$\theta^A_\nabla = p^A_i \, \mathrm{d}q^i - p^A_i \Gamma^i_B \, \mathrm{d}t^B = p^A_i (\mathrm{d}q^i - \Gamma^i_B \, \mathrm{d}t^B). \tag{34}$$

The difference $\theta^A_0 - \theta^A_\nabla \equiv \eta^A_\nabla$ is a 1-form on $\mathbb{R}^k \times (T^1_k)^*Q$ whose local expression is

$$\eta^A_\nabla = p^A_i \Gamma^i_B \, \mathrm{d}t^B. \tag{35}$$

From (3), (25), and (35) we deduce the following proposition.

Proposition 4.2: If ∇ *is a connection on* $\pi_{\mathbb{R}^k}: \mathbb{R}^k \times Q \to \mathbb{R}^k$ *and* $\widetilde{Y_A}$ *are the associated vector fields then*

$$\eta^A_\nabla = \sum_{B=1}^{k} \theta^A_0(\widetilde{Y}_B) \mathrm{d}t^B.$$

■

In the sequel, in order to develop the Lagrangian and Hamiltonian formalisms, we need that the curvature of ∇ vanishes. Observe that this condition always holds in the mechanical case because the horizontal distribution is one dimensional, hence involutive. The same condition will be necessary in Sec. V, where we study the Lagrangian counterpart.

Proposition 4.3: Let V_0 *be the vertical distribution of the bundle* $(\pi_Q)_{1,0}: \mathbb{R}^k \times (T^1_k)^*Q \to \mathbb{R}^k \times Q$ *and* $\omega^A_\nabla = -d\theta^A_\nabla$. *If the curvature of* ∇ *vanishes then* $(\mathbb{R}^k \times (T^1_k)^*Q, \mathrm{d}t^A, \omega^A_\nabla, V_0)$ *is a k-cosymplectic manifold.*

Proof: Conditions (1). in Definition 2.1 are straightforward. To prove conditions (2)., let X be a vector field with local expression

$$X = X^A \frac{\partial}{\partial t^A} + X^i \frac{\partial}{\partial q^i} + X^A_i \frac{\partial}{\partial p^A_i}. \tag{36}$$

As

$$\omega^A_\nabla = -d(p^A_i(\mathrm{d}q^i - \Gamma^i_B \mathrm{d}t^B)) = \mathrm{d}q^i \wedge dp^A_i + d(p^A_i \Gamma^i_B) \wedge \mathrm{d}t^B,$$

we have that $i_X \omega^A_\nabla = 0, 1 \leqslant A \leqslant k$, if and only if X has the following local expression:

$$X = X^B \left(\frac{\partial}{\partial t^B} + \Gamma^i_B \frac{\partial}{\partial q^i} - \frac{\partial \Gamma^j_B}{\partial q^i} p^A_j \frac{\partial}{\partial p^A_i} \right),$$

and the following condition holds

$$\sum_{B=1}^{k} X^B p^A_j \left(\frac{\partial \Gamma^j_C}{\partial t^B} - \frac{\partial \Gamma^j_B}{\partial t^C} + \Gamma^i_B \frac{\partial \Gamma^j_C}{\partial q^i} - \Gamma^i_C \frac{\partial \Gamma^j_B}{\partial q^i} \right) = 0, \quad 1 \leqslant A, C \leqslant k, 1 \leqslant i \leqslant n$$

with X^B free. Observe that

$$\frac{\partial \Gamma_C^j}{\partial t^B} - \frac{\partial \Gamma_B^j}{\partial t^C} + \Gamma_B^i \frac{\partial \Gamma_C^j}{\partial q^i} - \Gamma_C^i \frac{\partial \Gamma_B^j}{\partial q^i} \tag{37}$$

are the components of the curvature of the connection ∇, see Ref. 12, p. 91.

Since the curvature vanishes, then $\cap_{A=1}^k \ker \omega_\nabla^A$ is locally spanned by the following family of k independent local vector fields:

$$\left\{ \frac{\partial}{\partial t^B} + \Gamma_B^i \frac{\partial}{\partial q^i} - \frac{\partial \Gamma_B^j}{\partial q^i} p_j^A \frac{\partial}{\partial p_i^A}; 1 \leqslant B \leqslant k \right\}$$

and second condition (2). is finished.

Moreover, if $\mathrm{d}t^A(X)=0$, for all A, then $X^A=0$, for all A, hence

$$(\cap_{A=1}^k \ker \mathrm{d}t^A) \cap (\cap_{A=1}^k \ker \omega_\nabla^A) = \{0\}$$

and the result is proved.

■

Now we shall introduce the Hamiltonian function associated with a Lagrangian L and a connection ∇ with curvature zero.

In the standard situation, assuming that the Lagrangian function is hyperregular, the Hamiltonian function is defined by the equation $E_L=(FL)^*H$. In the general case we define the following.

Definition 4.4: The Hamiltonian function associated with the Lagrangian L and the connection ∇ *is the function* $H^\nabla \in C^\infty(\mathbb{R}^k \times (T_k^1)^* Q)$ *such that*

$$E_L^\nabla = (FL)^* H^\nabla.$$

As in the standard case, the existence and uniqueness of this function is assured (at least locally) if we assume that L is a hyperregular (or regular) Lagrangian. A simple computation using (18) and (35) shows that

$$H^\nabla = H - \sum_{A=1}^k \eta_\nabla^A \left(\frac{\partial}{\partial t^A} \right). \tag{38}$$

Now we consider *the Hamiltonian formalism on* $\mathbb{R}^k \times (T_k^1)^* Q$ *considering the k-cosymplectic structure* $(\mathbb{R}^k \times (T_k^1)^* Q, \mathrm{d}t^A, \omega_\nabla^A, V_0)$ *and the Hamiltonian* H^∇, that is, we consider Eq. (6) for this particular k-cosymplectic structure and this Hamiltonian,

$$\mathrm{d}t^A(X_B) = \delta_B^A,$$

$$\sum_{A=1}^k \iota_{X_A} \omega_\nabla^A = \mathrm{d}H^\nabla - \sum_{A=1}^k R_A^\nabla(H^\nabla)\mathrm{d}t^A, \tag{39}$$

where R_A^∇ are the Reeb vector fields of the k-cosymplectic structure $(\mathbb{R}^k \times (T_k^1)^* Q, \mathrm{d}t^A, \omega_\nabla^A, V_0)$, that is

$$\iota_{R_A^\nabla} \mathrm{d}t^B = \delta_A^B, \quad \iota_{R_A^\nabla} \omega_\nabla^B = 0. \tag{40}$$

Conditions (40) are equivalent to the equations

$$(R_A^\nabla)^B = \delta_A^B, \quad (R_A^\nabla)^i = \Gamma_A^i, \quad (R_A^\nabla)_i^B = -p_j^B \frac{\partial \Gamma_A^j}{\partial q^i} \tag{41}$$

and

$$p_j^B\left(\frac{\partial\Gamma_C^j}{\partial t^A}-\frac{\partial\Gamma_A^j}{\partial t^C}+\Gamma_A^i\frac{\partial\Gamma_C^j}{\partial q^i}-\Gamma_C^i\frac{\partial\Gamma_A^j}{\partial q^i}\right)=0, \tag{42}$$

for all $1\leqslant A,B,C\leqslant k$.

Taking into account that the curvature of ∇ is zero one obtains that the Reeb vector fields are locally given by

$$R_A^\nabla=\frac{\partial}{\partial t^A}+\Gamma_A^i\frac{\partial}{\partial q^i}-p_j^B\frac{\partial\Gamma_A^j}{\partial q^i}\frac{\partial}{\partial p_i^B}. \tag{43}$$

From (34), (35), (38), and (43), we obtain that $(X_1,\ldots,X_k)$, locally given by

$$X_A=(X_A)^B\frac{\partial}{\partial t^B}+(X_A)^i\frac{\partial}{\partial q^i}+(X_A)_i^B\frac{\partial}{\partial p_i^B},$$

is a solution to (39) if and only if, $(X_A)^B,(X_A)^i,(X_A)_i^B$ verify

$$(X_A)^B=\delta_B^A,\quad (X_A)^i=\frac{\partial H}{\partial p_i^A},\quad \sum_{A=1}^{k}(X_A)_i^A=-\frac{\partial H}{\partial q^i}, \tag{44}$$

where we have used that the curvature of ∇ is zero.

Observe that Eqs. (7) coincide with Eqs. (44), thus we obtain the following proposition.

Proposition 4.5: If the curvature of ∇ *vanishes, the Hamiltonian equations (6) and (39), corresponding to* H and H^∇, *respectively, have the same solutions*.

■

V. LAGRANGIAN FORMALISM WITH NONSTANDARD FLAT CONNECTIONS

A. The vertical endomorphism S_∇^A

The aim of this section is to give the guidelines to construct the vertical endomorphism S_∇^A, which depends on the connection ∇ and coincides with the vertical endomorphism S_A when the connection is the standard one. With this endomorphism we construct the Lagrangian formalism with a nonstandard connection.

First of all we have the following natural diffeomorphisms.

(1) As $J^1\pi_{\mathbb{R}^k}=\mathbb{R}^k\times T_k^1Q$ is a vector bundle on $\mathbb{R}^k\times Q$, we have the natural diffeomorphism:

$$J^1\pi_{\mathbb{R}^k}\to\pi_{\mathbb{R}^k}^*T^*\mathbb{R}^k\otimes\pi_Q^*TQ$$

in fact, given by its inverse

$$((t,q),\lambda_B^i\alpha^B\otimes u_i)\mapsto\left((t,q),\lambda_B^i\alpha^B\left(\frac{\partial}{\partial t^1}\right)u_i,\ldots,\left(\lambda_B^i\alpha^B\left(\frac{\partial}{\partial t^k}\right)u_i\right)\right).$$

(2) $\pi_Q^*(TQ)\to V(\pi_{\mathbb{R}^k})$ because $\pi_Q:\mathbb{R}^k\times Q\to Q$ is a vector bundle.

(3) As a consequence of the above two, we have the following diffeomorphisms:

$$V((\pi_{\mathbb{R}^k})_{1,0})\simeq((\pi_{\mathbb{R}^k})_{1,0})^*(\mathbb{R}^k\times T_k^1Q)\simeq((\pi_{\mathbb{R}^k})_{1,0})^*(\pi_{\mathbb{R}^k}^*T^*\mathbb{R}^k\otimes V(\pi_{R^k})).$$

The first is because $J^1\pi_{\mathbb{R}^k}$ is a vector bundle. The second is a direct consequence of the above items.

They are diffeomorphisms of vector bundles on $\mathbb{R}^k\times T_k^1Q$.

There is a section $V\in\mathrm{Sec}(((\pi_{\mathbb{R}^k})_{1,0})^*(\pi_{\mathbb{R}^k}^*T\mathbb{R}^k\otimes V(\pi_{\mathbb{R}^k})^*\otimes V((\pi_{\mathbb{R}^k})_{1,0}))$, associated to these diffeomorphisms, in particular to the third. In local natural coordinates we have

$$V = \frac{\partial}{\partial t^A} \otimes \zeta^i \otimes \frac{\partial}{\partial v^i_A},$$

where $\{\zeta^i, i=1,\ldots,n\}$ is a local basis for Sec $V(\pi_{\mathbb{R}^k})^*$, dual to the local basis $\{\partial/\partial q^i\}$.

Observe that, although $V(\pi_{\mathbb{R}^k})$ is a subbundle of $T(\mathbb{R}^k \times Q)$, $V(\pi_{\mathbb{R}^k})^*$ is not a subbundle of $T^*(\mathbb{R}^k \times Q)$, unless we have given a connection in the bundle $\pi_{\mathbb{R}^k}: \mathbb{R}^k \times Q \to \mathbb{R}^k$.

In fact, let ∇ be one such connection. ∇ gives a decomposition $T(\mathbb{R}^k \times Q) = H(\nabla) \oplus V(\pi_{\mathbb{R}^k})$, hence we have the induced projection $\pi^v_\nabla: T(\mathbb{R}^k \times Q) \to V(\pi_{\mathbb{R}^k})$ and the injection ${}^t(\pi^v_\nabla): V(\pi_{\mathbb{R}^k})^* \to T^*(\mathbb{R}^k \times Q)$.

In natural local coordinates, if

$$\nabla = \mathrm{d}t^A \otimes \left(\frac{\partial}{\partial t^A} + \Gamma^i_A \frac{\partial}{\partial q^i} \right)$$

then

$$\pi^v_\nabla\left(\frac{\partial}{\partial t^A} \right) = -\Gamma^i_A \frac{\partial}{\partial q^i}, \quad \pi^v_\nabla\left(\frac{\partial}{\partial q^i} \right) = \frac{\partial}{\partial q^i}$$

and

$$t_{\pi^v_\nabla}(\zeta^i) = \mathrm{d}q^i - \Gamma^i_B \, \mathrm{d}t^B.$$

In this way, the connection ∇ acts on the section V giving, locally,

$$S_\nabla = \frac{\partial}{\partial t^A} \otimes (\mathrm{d}q^i - \Gamma^i_B \, \mathrm{d}t^B) \otimes \frac{\partial}{\partial v^i_A}$$

making S_∇ an element of $\mathrm{Sec}(((\pi_{\mathbb{R}^k})_{1,0})^*(\pi^*_{\mathbb{R}^k} T\mathbb{R}^k \otimes T^*(\mathbb{R}^k \times Q) \otimes V((\pi_{\mathbb{R}^k})_{1,0}))$.

Now to obtain S^A_∇, we have

$$S^A_\nabla = S_\nabla(\mathrm{d}t^A) = (\mathrm{d}q^i - \Gamma^i_B \, \mathrm{d}t^B) \otimes \frac{\partial}{\partial v^i_A} \tag{45}$$

which concludes this part.

From (45) we see that when ∇ is the standard connection then $S^A_\nabla = S_A$.

B. Lagrangian formalism with nonstandard connections

Since in the Lagrangian formalism $(\theta_L)_A = \mathrm{d}L \circ S_A$, as we have the connection ∇, we now introduce the forms

$$(\theta_L)^A_\nabla = \mathrm{d}L \circ S^A_\nabla, \quad 1 \leqslant A \leqslant k,$$

which are locally given by

$$(\theta_L)^A_\nabla = \frac{\partial L}{\partial v^i_A}(\mathrm{d}q^i - \Gamma^i_B \, \mathrm{d}t^B), \quad 1 \leqslant A \leqslant k,$$

from (18) and (34) it is obvious that $(\theta_L)^A_\nabla = (FL)^* \theta^A_\nabla$. We define $(\omega_L)^A_\nabla = -d(\theta_L)^A_\nabla$ and of course $(\omega_L)^A_\nabla = (FL)^*(\omega^A_\nabla)$.

In local coordinates we have

$$(\omega_L)^A_\nabla = \mathrm{d}q^i \wedge d\left(\frac{\partial L}{\partial v^i_A} \right) + d\left(\Gamma^i_B \frac{\partial L}{\partial v^i_A} \right) \wedge \mathrm{d}t^B. \tag{46}$$

Consider now the *Lagrangian formalism* on $\mathbb{R}^k \times T^1_k Q$ replacing E_L by E^∇_L and ω^A_L by $(\omega_L)^A_\nabla$.

From a long, but straightforward, computation, similar to the proof of Proposition 4.3, we obtain the following proposition.

Proposition 5.1: Let $L: \mathbb{R}^k \times T^1_k Q \to \mathbb{R}$ *be a regular Lagrangian, and let* V_0 *be the vertical distribution of the bundle* $(\pi_{\mathbb{R}^k})_{1,0}: \mathbb{R}^k \times T^1_k Q \to \mathbb{R}^k \times Q$. *If* ∇ *is a flat connection then* $(\mathbb{R}^k \times T^1_k Q, \mathrm{d}t^A, (\omega_L)^A_\nabla, V_0)$ *is a k-cosymplectic manifold.*

■

The equations,

$$i_{(R_L)^\nabla_A} \mathrm{d}t^B = \delta^B_A, \quad i_{(R_L)^\nabla_A} (\omega_L)^B_\nabla = 0, \quad 1 \leqslant A, B \leqslant k, \tag{47}$$

define the Reeb vector fields on $\mathbb{R}^k \times T^1_k Q$ corresponding to the k-cosymplectic structure $(\mathrm{d}t^A, (\omega_L)^A_\nabla, V_0)$.

These equations are equivalent to

$$[(R_L)^\nabla_A)]^B = \delta^B_A, \quad [(R_L)^\nabla_A)]^i = \Gamma^i_A, \tag{48}$$

$$\frac{\partial^2 L}{\partial t^A \partial v^k_C} + \Gamma^j_A \frac{\partial^2 L}{\partial q^j \partial v^k_C} + \frac{\partial \Gamma^i_A}{\partial q^k} \frac{\partial L}{\partial v^i_C} + [(R_L)^\nabla_A]^i_B \frac{\partial^2 L}{\partial v^i_B \partial v^k_C} = 0, \tag{49}$$

and

$$\frac{\partial L}{\partial v^j_B} \left(\frac{\partial \Gamma^j_C}{\partial t^A} - \frac{\partial \Gamma^j_A}{\partial t^C} + \Gamma^i_A \frac{\partial \Gamma^j_C}{\partial q^i} - \Gamma^i_C \frac{\partial \Gamma^j_A}{\partial q^i} \right) = 0, \tag{50}$$

for all $1 \leqslant A, B, C \leqslant k$.

Since the curvature vanishes then the Reeb vector fields are locally given by

$$(R_L)^\nabla_A = \frac{\partial}{\partial t^A} + \Gamma^i_A \frac{\partial}{\partial q^i} + [(R_L)^\nabla_A]^i_B \frac{\partial}{\partial v^i_B}, \tag{51}$$

where the functions $[(R_L)^\nabla_A]^i_B$ satisfy Eq. (49).

Since L is regular, from (49) we can define, in a neighborhood of each point a k-vector field that satifies (47). Next, a global k-vector field $(R_L)^\nabla = ((R_L)^\nabla_1, \ldots, (R_L)^\nabla_k)$ can be constructed, which is a solution of (47), by using a partition of unity.

As in the standard Lagrangian formalism, by writing the equations (6) for the k-cosymplectic structure $(\mathrm{d}t^A, (\omega_L)^A_\nabla, V^0)$ and by replacing H by E^∇_L, we have

$$\mathrm{d}t^A(Y_B) = \delta^A_B,$$

$$\sum_{A=1}^k i_{Y_A} (\omega_L)^A_\nabla = \mathrm{d}E^\nabla_L - \sum_{A=1}^k (R_L)^\nabla_A (E^\nabla_L) \mathrm{d}t^A, \tag{52}$$

for some k-vector field $(Y_1, \ldots, Y_k)$.

Using the regularity of L, from (46), (49), (51), and (52) we deduce that if $(Y_1, \ldots, Y_k)$ is a solution of (52) then

$$[Y_A]^B = \delta^B_A, \quad [Y_A]^i = v^i_A, \quad \sum_{A=1}^k Y_A \left(\frac{\partial L}{\partial v^k_A} \right) = \frac{\partial L}{\partial q^k} \tag{53}$$

and

$$\frac{\partial L}{\partial v^i_A} \left(\frac{\partial \Gamma^i_C}{\partial t^A} + \Gamma^j_A \frac{\partial \Gamma^i_C}{\partial q^j} - \frac{\partial \Gamma^i_A}{\partial t^C} - \Gamma^j_C \frac{\partial \Gamma^i_A}{\partial q^j} \right) = 0. \tag{54}$$

Observe that Eqs. (22) coincide with Eqs. (53), thus since (54) holds we obtain the following proposition.

Proposition 5.2: Let $L:\mathbb{R}^k\times T^1_kQ\to\mathbb{R}$ *be a regular Lagrangian. If the curvature of the connection* ∇ *vanishes then the Lagrangian equations (21) and (52) have the same solutions.*

Remark: In the case $k=1$, Propositions 4.5 and 5.2 generalize the results obtained in Ref. 1.

VI. VARIATIONAL PRINCIPLES, EQUIVALENCIES AND ANOTHER CHARACTERIZATION OF THE ENERGY

In this section we prove that the energy E_L^∇ is the unique function establishing the equivalence between the variational principles associated to the Hamiltonian and Lagrangian formalisms.

A. Some other geometrical elements in $\mathbb{R}^k\times Q$

Definition 6.1: We introduce the following k-forms on $\mathbb{R}^k\times(T^1_k)^*Q$*:*

$$\theta_0=\sum_{A=1}^k\theta_0^A\wedge d^{k-1}t^A,\quad \theta_\nabla=\sum_{A=1}^k\theta_\nabla^A\wedge d^{k-1}t^A,\quad \eta_\nabla=\sum_{A=1}^k\eta_\nabla^A\wedge d^{k-1}t^A,$$

$$\Theta_L=\sum_{A=1}^k\Theta_L^A\wedge d^{k-1}t^A, \tag{55}$$

and

$$\Theta_0=\theta_0-Hd^kt,\quad \Theta_\nabla=\theta_\nabla-H^\nabla d^kt, \tag{56}$$

where $d^kt=\mathrm{d}t^1\wedge\cdots\wedge\mathrm{d}t^k$ *and* $d^{k-1}t^A=i_{\partial/\partial t^A}d^kt$.

The relationship between these forms is given in the following proposition.

Proposition 6.2:

(1) $\Theta_L=(FL)^*\Theta_0$.
(2) $\theta_0-\theta_\nabla=\eta_\nabla=(H-H^\nabla)d^kt$.
(3) $(FL)^*\theta_\nabla=\Theta_L+E_L^\nabla d^kt$.

Proof:

(1) Since $(FL)^*\theta_0^A=\theta_L^A$ we obtain

$$(FL)^*\Theta_0=(FL)^*(\theta_0-Hd^kt)=(FL)^*\left(\sum_{A=1}^k\theta_0^A\wedge d^{k-1}t^A-Hd^kt\right)$$
$$=\sum_{A=1}^k(FL)^*\theta_0^A\wedge d^{k-1}t^A-(FL)^*Hd^kt=\sum_{A=1}^k\theta_L^A\wedge d^{k-1}t^A-E_Ld^kt.$$

On the other hand, from (29),

$$\Theta_L=\sum_{A=1}^k\Theta_L^A\wedge d^{k-1}t^A=\sum_{A=1}^k\left(\theta_L^A+\left(\frac{1}{k}\delta_B^AL-v_B^i\frac{\partial L}{\partial v_A^i}\right)\mathrm{d}t^B\right)\wedge d^{k-1}t^A$$
$$=\sum_{A=1}^k\theta_L^A\wedge d^{k-1}t^A+\sum_{A=1}^k\left(\left(\frac{1}{k}\delta_B^AL-v_B^i\frac{\partial L}{\partial v_A^i}\right)\mathrm{d}t^B\right)\wedge d^{k-1}t^A=\sum_{A=1}^k\theta_L^A\wedge d^{k-1}t^A+Ld^kt-(CL)d^kt$$
$$=\sum_{A=1}^k\theta_L^A\wedge d^{k-1}t^A-E_Ld^kt.$$

(2) The first identity is a consequence of $\theta_0^A - \theta_\nabla^A = \eta_\nabla^A$. For the second identity, from (34) and (35), we have

$$\eta_\nabla = \sum_{A=1}^{k} \eta_\nabla^A \wedge d^{k-1}t^A = p_i^A \Gamma_B^i \mathrm{d}t^B \wedge d^{k-1}t^A = \left[\sum_{A=1}^{k} \eta_\nabla^A \left(\frac{\partial}{\partial t^A} \right) \right] d^k t = (H^\nabla - H) d^k t.$$

(3) From (2),

$$\begin{aligned}(FL)^* \theta_\nabla - \Theta_L &= (FL)^* \theta_\nabla - (FL)^* \Theta_0 = (FL)^* (\theta_\nabla - \Theta_0) \\ &= (FL)^* ((H^\nabla - H) d^k t + H d^k t) = (FL)^* (H^\nabla d^k t) = E_L^\nabla d^k t.\end{aligned}$$

■

B. Characterization of the energy by sections of the bundle $\pi_{\mathbb{R}^k}: \mathbb{R}^k \times Q \to \mathbb{R}^k$

Lemma 6.3: Let β be a k-form and let f be a function on $\mathbb{R}^k \times T_k^1 Q$. For each map $\phi: U \subset \mathbb{R}^k \to Q$, where U is a compact set, the following conditions are equivalent:

(i) $(\phi^{[1]})^* (f d^k t) = (\phi^{[1]})^* \beta$,
(ii) $\int_{\phi^{[1]}(U)} f d^k t = \int_{\phi^{[1]}(U)} \beta$.

Proof: Trivially (i) $\Rightarrow$ (ii) because

$$\int_{\phi^{[1]}(U)} f d^k t = \int_U (\phi^{[1]})^* (f d^k t).$$

Conversely, if (i) is not true, then there exists a function $\phi: U \subset \mathbb{R}^k \to Q$ such that $(\phi^{[1]})^* (f d^k t - \beta) \neq 0$ and hence there exist $s \in U$ and a closed neighborhood V of s such that, taking $\psi: V \to Q$ then

$$\int_{\psi^{[1]}(U)} (f d^k t - \beta) \neq 0,$$

so (ii) is false.

■

Proposition 6.4: The Lagrangian energy function introduced in Definition 3.5 is the only function on $\mathbb{R}^k \times T_k^1 Q$ satisfying the condition

$$(\phi^{[1]})^* (E_L^\nabla d^k t) = (\phi^{[1]})^* ((FL)^* \theta_\nabla - L d^k t)$$

for every function $\phi: U \to Q$.

Proof: Uniqueness. Let f and g be two functions verifying this condition. Obviously $0 = (\phi^{[1]})^* ((f-g) d^k t) = ((f-g) \circ \phi^{[1]}) d^k t$ then $0 = (f-g) \circ \phi^{[1]}(t) = (f-g)(j_t^1 \phi)$, and this implies that $f - g = 0$, because every point in $\mathbb{R}^k \times T_k^1 Q$ is in the image of some map $\phi^{[1]}$.

Existence: From (3) in Proposition 6.2, we obtain

$$\begin{aligned}(\phi^{[1]})^* ((FL)^* \theta_\nabla - L d^k t) &= (\phi^{[1]})^* (\Theta_L + E_L^\nabla d^k t - d^k t) \\ &= (\phi^{[1]})^* \left(\sum_{A=1}^{k} \left(\mathrm{d}L \circ S_{\mathrm{d}t^A} + \frac{1}{k} L \, \mathrm{d}t^A \right) \wedge d^{k-1}t^A + E_L^\nabla d^k t - L d^k t \right) \\ &= (\phi^{[1]})^* \left(\sum_{A=1}^{k} (\mathrm{d}L \circ S_{\mathrm{d}t^A} \wedge d^{k-1}t^A) \right) + (\phi^{[1]})^* (E_L^\nabla d^k t) = (\phi^{[1]})^* (E_L^\nabla d^k t)\end{aligned}$$

because

$$(\phi^{[1]})^*\left(\sum_{A=1}^{k}(\mathrm{d}L\circ S_{\mathrm{d}t^A}\wedge d^{k-1}t^A)\right)=0.$$

In fact, from (26) we have

$$\mathrm{d}L\circ S_{\mathrm{d}t^A}=\frac{\partial L}{\partial v_A^i}(v_B^i\,\mathrm{d}t^B-\mathrm{d}q^i)$$

then

$$\sum_{A=1}^{k}(\mathrm{d}L\circ S_{\mathrm{d}t^A}\wedge d^{k-1}t^A)=\sum_{A=1}^{k}\frac{\partial L}{\partial v_A^i}(v_B^i\mathrm{d}t^B-\mathrm{d}q^i)\wedge d^{k-1}t^A$$

but

$$\begin{aligned}(\phi^{[1]})^*\left(\sum_{A=1}^{k}\frac{\partial L}{\partial v_A^i}(v_B^i\,\mathrm{d}t^B-\mathrm{d}q^i)\wedge d^{k-1}t^A\right)&=\sum_{A=1}^{k}\left(\frac{\partial L}{\partial v_A^i}\circ\phi^{[1]}\right)[(v_B^i\circ\phi^{[1]})d(t^B\circ\phi^{[1]})\\&\quad-d(q^i\circ\phi^{[1]})]\wedge d^{k-1}(t^A\circ\phi^{[1]})\\&=\sum_{A=1}^{k}\left(\frac{\partial L}{\partial v_A^i}\circ\phi^{[1]}\right)\left[\frac{\partial\phi^i}{\partial t^B}\mathrm{d}t^B-\mathrm{d}\phi^i\right]\wedge d^{k-1}t^A=0.\end{aligned}$$

■

From Proposition 6.4 we deduce that for every $\phi: U\subset\mathbb{R}^k\to Q$ with U compact, we have

$$\int_{\phi^{[1]}(U)}E_L^\nabla d^kt=\int_{\phi^{[1]}(U)}(FL)^*\theta_\nabla-Ld^kt$$

and therefore, from Proposition 6.2, we obtain

$$\begin{aligned}\int_{\phi^{[1]}(U)}Ld^kt&=\int_{\phi^{[1]}(U)}(FL)^*\theta_\nabla-E_L^\nabla d^kt\\&=\int_{\phi^{[1]}(U)}(FL)^*(\theta_\nabla-H^\nabla d^kt)=\int_{\phi^{[1]}(U)}(FL)^*(\theta_0-Hd^kt)\\&=\int_{\phi^{[1]}(U)}(FL)^*\Theta_0=\int_{FL\circ\phi^{[1]}(U)}\Theta_0.\end{aligned}$$

This equality shows the equivalence between the Hamilton principle of minimal action and the Hamilton-Jacobi principle, see later (57) and (58). Therefore, taking into account Proposition 6.4, we must conclude that the energy E_L^∇ is the only function that performs the equivalence between both variational principles which now we recall.

C. The Hamilton principle of minimal action

Each section of $\pi_{\mathbb{R}^k}:\mathbb{R}^k\times Q\to\mathbb{R}^k$ can be identified as a map $\phi:\mathbb{R}^k\to Q$. Denote its first prolongation by $\phi^{[1]}:\mathbb{R}^k\to\mathbb{R}^k\times T_k^1Q$. With this in mind, we can define the following.

Definition 6.5: Let $C_c^\infty(\mathbb{R}^k,Q)$ be the set of compact support maps from $\mathbb{R}^k$ to Q. This set can be identified with $\Gamma_c(\mathbb{R}^k,\mathbb{R}^k\times Q)$, the set of compact support sections of $\pi_{\mathbb{R}^k}$. Consider the map

$$\mathbb{L}:\ C_c^\infty(\mathbb{R}^k,Q)\equiv\Gamma_c(\mathbb{R}^k,\mathbb{R}^k\times Q)\to\mathbb{R},$$

$$\phi \equiv (Id_{\mathbb{R}^k}, \phi) \mapsto \int_{\mathbb{R}^k} (\phi^{[1]})^*(Ld^k t). \tag{57}$$

The variational problem posed by the Lagrangian function L is the problem of searching for the critical or stationary sections of the functional $\mathbb{L}$.

Remark: The sections must be stationary with respect to the variations of $(Id_{\mathbb{R}^k}, \phi)$ given by $(Id_{\mathbb{R}^k}, \phi)_s = \tau_s \circ (Id_{\mathbb{R}^k}, \phi)$ [because $\tau_s(t^A, q^i) = (t^A, \bar{\tau}^i(s,t,q))$], or equivalently $\phi_s = \pi_Q \circ \tau_s \circ (Id_{\mathbb{R}^k}, \phi)$, where $\{\tau_s\}$ is a local flow of any vector $Z \in \mathfrak{X}(\mathbb{R}^k \times Q)$ which is $\pi_{\mathbb{R}^k}$ vertical, that is

$$\frac{d}{ds}_{|_{s=0}} \int_{\mathbb{R}^k} (\phi_s^{[1]})^*(Ld^k t) = 0.$$

The proof of the following Proposition can be found in Ref. 4 for an arbitrary fiber bundle $\pi: E \to M$.

Proposition 6.6: Let L be a Lagrangian function. The following assertions on a map $\phi \in C_c^\infty(\mathbb{R}^k, \mathbb{R}^k \times Q)$ *are equivalent:*

(1) ϕ *is a critical section for* $\mathbb{L}$,
(2) $\phi^{[1]}$ *satisfy the Euler-Lagrange equations*,

$$\sum_{A=1}^{k} \frac{d}{\mathrm{d}t^A}\left(\frac{\partial L}{\partial v_A^i}_{|\phi^{[1]}(t)}\right) - \frac{\partial L}{\partial q^i}_{|\phi^{[1]}(t)} = 0, \quad v_A^i(\phi^{[1]}(t)) = \frac{\partial \phi^i}{\partial t^A}(t)$$

in any natural local coordinate system.

D. The Hamilton-Jacobi principle

Definition 6.7: Let $\Phi: \mathbb{R}^k \times Q \to \mathbb{R}^k \times Q$ *be a bundle isomorphism and* $\Phi_Q: Q \to Q$ *the induced diffeomorphism in Q. The prolongation of* Φ *to* $\mathbb{R}^k \times (T_k^1)^* Q$ *is the diffeomorphism*

$$j^{1*}\Phi\colon \mathbb{R}^k \times (T_k^1)^* Q \equiv J^1 \pi_Q \to \mathbb{R}^k \times (T_k^1)^* Q \equiv J^1 \pi_Q,$$

$$j_q^1 \gamma \to j^{1*}\Phi(j_q^1 \gamma) = j^1_{\Phi_Q(q)}(\Phi \circ \gamma \circ \Phi_Q^{-1}).$$

Definition 6.8: Let $\Gamma_c(\mathbb{R}^k, \mathbb{R}^k \times (T_k^1)^* Q)$ *be the set of compact support sections of*

$$\mathbb{R}^k \times (T_k^1)^* Q \equiv J^1 \pi_Q \xrightarrow{(\pi_Q)_{1,0}} \mathbb{R}^k \times Q \xrightarrow{\pi_{\mathbb{R}^k}} \mathbb{R}^k$$

and consider the map

$$\mathbb{H}\colon \Gamma_c(\mathbb{R}^k, \mathbb{R}^k \times (T_k^1)^* Q) \to \mathbb{R},$$

$$\psi \mapsto \int_{\mathbb{R}^k} \psi^* \Theta_0. \tag{58}$$

The associated variational problem is the search for the critical or stationary sections of the functional $\mathbb{H}$, *with respect to the variations of* ψ *given by* $\psi_s = j^{1*}\sigma_s \circ \psi$, *where* $\{\sigma_s\}$ *is a local flow of any vector field* $Z \in \mathfrak{X}(\mathbb{R}^k \times Q)$ *which is* $\pi_{\mathbb{R}^k}$ *vertical. That is*

$$\frac{d}{\mathrm{d}s}_{|_{s=0}} \int_{\mathbb{R}^k} \psi_s^* \Theta_0 = 0.$$

The proof of the following Proposition can be found in Ref. 13 for an arbitrary fiber bundle $\pi: E \to M$.

Proposition 6.9: The following assertions on a section $\phi \in \Gamma_c(\mathbb{R}^k, \mathbb{R}^k \times (T^1_k)^* Q)$ *are equivalent.*

(1) ϕ *is a critical section for* $\mathbb{H}$.
(2) ϕ *satisfy, in any natural local coordinate system, the Hamilton-De Donder-Weyl equations of the Hamiltonian formalism*,

$$\frac{\partial q^i}{\partial t^A}_{|\psi} = \frac{\partial H}{\partial p_i^A}_{|\phi(t)}, \quad \frac{\partial p_i^A}{\partial t^A}_{|\phi(t)} = -\frac{\partial H}{\partial q^i}_{|\phi(t)},$$

where H is the Hamiltonian function. (Also see Refs. 14–19.)

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On the sharpness of the zero-entropy-density conjecture

S. Farkas[a)]
Department of Physics, University of Chicago, Chicago, Illinois 60637

Z. Zimborás[b)]
Research Institute for Particle and Nuclear Physics, Budapest, H-1525 Budapest, P.O. Box 49, Hungary

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The zero-entropy-density conjecture states that the entropy density defined as $s := \lim_{N\to\infty} S_N/N$ vanishes for all translation-invariant pure states on the spin chain. Or equivalently, S_N, the von Neumann entropy of such a state restricted to N consecutive spins, is sublinear. In this paper it is proved that this conjecture cannot be sharpened, i.e., translation-invariant states give rise to arbitrary fast sublinear entropy growth. The proof is constructive, and is based on a class of states derived from quasifree states on a CAR algebra. The question whether the entropy growth of pure quasifree states can be arbitrary fast sublinear was first raised by Fannes *et al.* [J. Math. Phys. **44**, 6005 (2003)]. In addition to the main theorem it is also shown that the entropy asymptotics of all pure shift-invariant nontrivial quasifree states is at least logarithmic. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Quantum spin chains belong to the most studied models of quantum statistical mechanics.[1] Still, only for a few types of models have the thermal and ground state structures been determined. This is mainly the consequence of the complicated correlations that can appear in quantum states. These strong correlations can even be present in pure states, while classical pure states can only have a trivial product state structure. Unlike the classical case, the restrictions of pure states on the quantum spin chain to local subsystems are typically mixed states. This type of correlation between subsystems is commonly referred to as entanglement. The von Neumann entropy, defined as $S := -\mathrm{Tr}\,\rho \log \rho$, is a natural measure of the nonpurity of the restricted density matrix ρ, thus it is a very useful quantity in the description of entanglement.

The entropy of a restricted density matrix is also a basic measure when mixed states are treated, however, in this case it cannot be interpreted as a measure of entanglement. Let S_N denote the von Neumann entropy of a translation-invariant state restricted to N consecutive spins. The entropy density $s := \lim_{N\to\infty} S_N/N$ is considered to quantify the "strong nonpurity" of the entire mixed state, and it plays a central role in the characterization of Gibbs states.[1] A natural and long-standing conjecture is that the entropy density vanishes for all translation-invariant pure states on a quantum spin chain, i.e., for such states, S_N is sublinear. In the present paper we will prove that if this zero-entropy-density conjecture is true, then it is sharp in the sense that for any sublinear function f_N ($\lim_{N\to\infty} f_N/N=0$), there exists a translation-invariant state so that $S_N \geqslant f_N$, for every sufficiently large N. This has already been conjectured by Fannes, Haegeman, and Mosonyi in Ref. 2. Moreover, they proved that any sublinear power function can be exceeded by the entropy growth of an appropriate pure translation-invariant state.

It also should be mentioned that there is a revived interest in studying entropy asymptotics for two other reasons. First, S_N seems to be a good indicator of quantum criticality. Several ground

[a)]Electronic mail: farkas@uchicago.edu
[b)]Electronic mail: cimbi@rmki.kfki.hu

states of Hamiltonians with local interactions were studied, and in these models, S_N was found to be bounded for noncritical systems, while for critical systems, it turned out to diverge logarithmically.[3–6] The prefactor of this logarithmic growth was argued to be one-third of the central charge.[7] Also higher dimensional lattice models have been investigated in this respect.[8–11] Second, entropy is supposed to play an important role in the quantification of the "essential subspace" of a restricted density matrix. The possibility of compressing the restricted density matrix from its full dimension to a much smaller subspace without loss of much information is the starting point of the DMRG calculations.[12] For ergodic translation-invariant states, with nonvanishing entropy density s, the density matrix pertaining to N consecutive spins, ρ_N, is essentially concentrated on a subspace of dimension proportional to $\exp(Ns)$.[13] In more general situations, numerical calculations suggest that the dimension of the "essential subspace" of ρ_N is proportional to $\exp(S_N)$.[14] This could lead to a very efficient compression of states with bounded or slowly diverging entropy asymptotics.

In the present paper we give a constructive proof of the sharpness of the zero-entropy-density conjecture. The states that are studied are translation-invariant pure states on the spin chain derived from quasifree states on the CAR algebra. In Sec. II we recapitulate the construction of such states in order to be self-contained. In Sec. III we prove our main theorem. The argument is based on the approach to quasifree states developed in Ref. 2. Finally, we include a proof of the statement that the entropy growth for all nontrivial gauge-invariant quasifree states are bounded from below by a logarithmic growth.

II. QUASIFREE STATES ON THE SPIN CHAIN

A. The Araki-Jordan-Wigner construction

The algebra of observables of a quantum spin chain (more precisely, spin $\frac{1}{2}$ chain) is the UHF algebra

$$\mathcal{M} := \bigotimes_{k=-\infty}^{+\infty} M_2,$$

where M_2 denotes the algebra of 2×2 matrices. Let σ_a^k $(a=1,2,3;\ k\in\mathbb{Z})$ denote the Pauli matrices embedded into the kth factor of $\mathcal{M}$. They satisfy the well-known relations:

$$\sigma_a^k\sigma_b^l = \sigma_b^l\sigma_a^k, \quad \text{when } k\neq l,$$

$$\sigma_a^l\sigma_b^l = \mathrm{i}\varepsilon_{abc}\sigma_c^l + \delta_{ab}\mathbb{1}.$$

The Pauli matrices and $\mathbb{1}$ generate $\mathcal{M}$. The translation automorphism τ on $\mathcal{M}$ is defined by $\tau(\sigma_a^k)=\sigma_a^{k+1}$.

The states we are investigating in this paper are translation-invariant pure states on $\mathcal{M}$ derived from quasifree states of a fermion chain. The C^* algebra describing a fermion chain is the CAR algebra corresponding to the one-particle Hilbert space $\ell^2(\mathbb{Z})$, i.e., it is the C^* algebra generated by $\mathbb{1}$ and the operators $\{c_k | k\in\mathbb{Z}\}$ satisfying the canonical anticommutation relations:

$$c_k c_l^* + c_l^* c_k = \delta_{k,l}\mathbb{1}, \quad c_k c_l + c_l c_k = 0.$$

Denote this C^* algebra by $\mathcal{A}$. The translation automorphism γ is defined by $\gamma(c_k)=c_{k+1}$.

The C^* algebras $\mathcal{M}$ and $\mathcal{A}$ are isomorphic. However, there exists no isomorphism $\iota:\mathcal{M}\to\mathcal{A}$ that satisfies the property $\iota\circ\tau=\gamma\circ\iota$. This is clear if we note that $(\mathcal{M},\tau)$ is asymptotically Abelian, while $(\mathcal{A},\gamma)$ is not. This intertwining property is needed to derive the translation invariance of a state $\omega\circ\iota$ on $\mathcal{M}$ from that of ω on $\mathcal{A}$. This problem can be circumvented by Araki's construction.[15] In this section we will present a modified but equivalent formulation of this construction.

First, let us introduce the parity automorphism π on $\mathcal{A}$. It is defined by $\pi(c_k)=-c_k$. The elements of $\mathcal{A}_+ := \{a \in \mathcal{A} \,|\, \pi(a)=a\}$ are called even, while those of $\mathcal{A}_- := \{a \in \mathcal{A} \,|\, \pi(a)=-a\}$ are called odd. Any element $a \in \mathcal{A}$ can uniquely be written in the form $a=a_++a_-$, where $a_+ \in \mathcal{A}_+$, and $a_- \in \mathcal{A}_-$. Thus, $\mathcal{A}=\mathcal{A}_++\mathcal{A}_-$.

Second, let $\mathcal{M}_+$ be the C^* subalgebra of $\mathcal{M}$ generated by $\mathbb{1}$, σ_3^k, and $\sigma_1^k\sigma_1^l$ $(k,l \in \mathbb{Z})$. $\mathcal{M}_+$ is isomorphic to $\mathcal{A}_+$, an explicit isomorphism α is given by the restricted Jordan-Wigner transformation:

$$\alpha(\sigma_3^k) := 2c_k^*c_k - \mathbb{1},$$

$$\alpha(\sigma_1^k\sigma_1^l) := -\prod_{m=k}^{l-1}(2c_m^*c_m - \mathbb{1})(c_k^* + c_k)(c_l^* + c_l) \quad \text{when } k < l.$$

Since $\mathcal{M}_+$ and $\mathcal{A}_+$ are invariant under the translations, τ and γ can be restricted to $\mathcal{M}_+$ and $\mathcal{A}_+$, respectively. Let us denote these restrictions by τ_+ and γ_+. Although there is no isomorphism that intertwines the translations on $\mathcal{M}$ and $\mathcal{A}$, α is an isomorphism that intertwines the translations on the subalgebras $\mathcal{M}_+$ and $\mathcal{A}_+$: $\alpha\circ\tau_+=\gamma_+\circ\alpha$.

Now, let ω_+ be the restriction of a state ω on $\mathcal{A}$ to $\mathcal{A}_+$. If ω is a translation-invariant state, i.e., $\omega\circ\gamma=\omega$, then $\omega_+\circ\alpha$, which is a state on $\mathcal{M}_+$, is invariant under τ_+. The state $\omega_+\circ\alpha$ can be extended to a state $\widetilde{\omega}$ on $\mathcal{M}$ by $\widetilde{\omega}(a)=\widetilde{\omega}(a_++a_-) := \omega_+(\alpha(a_+))$, where $a_+ \in \mathcal{A}_+$, and $a_- \in \mathcal{A}_-$. This way a translation-invariant state $\widetilde{\omega}$ on $\mathcal{M}$ is obtained. Moreover, if ω is an even state, i.e., $\omega\circ\pi=\omega$, then $\widetilde{\omega}$ is pure if and only if ω is pure.[2]

To summarize, a translation intertwining automorphism α has been given not between the algebras $\mathcal{M}$ and $\mathcal{A}$, but between their appropriate subalgebras $\mathcal{M}_+$ and $\mathcal{A}_+$. Any translation-invariant state on $\mathcal{M}_+$ can be straightforwardly extended to a translation-invariant state on $\mathcal{M}$. Thus the isomorphism α makes it possible to transport the translation-invariant states from $\mathcal{A}$ to $\mathcal{M}$.

B. Quasifree states on CAR algebras

Following Araki's construction presented in Sec. II A, a class of states will be derived from quasifree states on the CAR algebra $\mathcal{A}$. Here we will shortly recapitulate the most important definitions and facts concerning these states, more details and the proofs of the statements can be found in Refs. 1 and 16.

Let Q be an operator on the Hilbert space $\ell^2(\mathbb{Z})$, $0 \leqslant Q \leqslant \mathbb{1}$. Let $Q_{ij} := \langle \delta_i, Q\delta_j \rangle$ be the matrix elements of Q in the standard basis $\{\delta_k \,|\, k \in \mathbb{Z}\}$ of $\ell^2(\mathbb{Z})$, where δ_k is the characteristic function of the number k. The (gauge-invariant) quasifree state ω_Q on $\mathcal{A}$ is defined through the following formula:

$$\omega_Q(c_{i_1}^* \ldots c_{i_m}^* c_{j_n} \ldots c_{j_1}) = \delta_{m,n}\det([Q_{i_k,j_l}]_{k,l=1}^n).$$

The operator Q is called the symbol of the state. Quasifree states are by definition even states.

A quasifree state ω_Q is translation-invariant if and only if its symbol Q is a Toeplitz operator in the basis δ_k, i.e., there exists a sequence $(q_k)_{k\in\mathbb{Z}}$ such that $Q_{kl}=\langle \delta_k, Q\delta_l \rangle = q_{k-l}$. Let us introduce the Fourier transform:

$$\tilde{q}(\theta) := \sum_{k\in\mathbb{Z}} q_k e^{i2\pi k\theta}, \quad \text{where } \theta \in [0,1).$$

The function $\tilde{q}$ satisfies $0 \leqslant \tilde{q}(\theta) \leqslant 1$ almost everywhere. A translation-invariant quasifree state ω_Q is pure if and only if the Fourier transform $\tilde{q}$ is a characteristic function, i.e., there exists a measurable set $K \subset [0,1)$ such that $\tilde{q}(\theta)=\chi_K(\theta)$.

Now, applying the Araki-Jordan-Wigner construction to a translation-invariant quasifree state ω_Q, one obtains a translation-invariant state $\widetilde{\omega}_Q$ on the spin chain algebra $\mathcal{M}$. Since quasifree states are even, the state $\widetilde{\omega}_Q$ is pure if and only if the corresponding quasifree state ω_Q is also pure.

Let ρ_N denote the reduced density matrix obtained by restricting the state $\widetilde{\omega}_Q$ to an interval of N spins. The von Neumann entropy of the restricted state is defined as $S_N := -\mathrm{Tr}\,\rho_N \log \rho_N$. An explicit formula of this entropy is known for quasifree states:

$$S_N = -\mathrm{Tr}(Q_N \log Q_N + (\mathbb{1} - Q_N)\log(\mathbb{1} - Q_N)), \tag{1}$$

where Q_N is the restriction of Q to the N-dimensional space spanned by the set $\{\delta_k | 0 \leqslant k \leqslant N-1\}$.

On the basis of the Szegő theorem one can prove that the entropy density $s := \lim_{N\to\infty} S_N/N$ of pure translation-invariant quasifree states vanishes.[2] In Sec. III we will prove that this statement is sharp in the sense that for any f_N sublinear function there is a quasifree state for which $S_N \geqslant f_N$ for sufficiently large N.

III. QUASIFREE STATES GIVE RISE TO ARBITRARY FAST SUBLINEAR ENTROPY GROWTH

An explicit formula of the entropy function S_N for quasifree states was given in Sec. II by Eq. (1). In order to simplify further computations, we work with a quadratic lower bound of S_N introduced in Ref. 2:

$$q_N := \mathrm{Tr}\, Q_N(\mathbb{1} - Q_N).$$

That q_N is a lower bound of $S_N = -\mathrm{Tr}(Q_N \log Q_N + (\mathbb{1}-Q_N)\log(\mathbb{1}-Q_N))$ can be proved by the aid of the inequality $x(1-x) \leqslant -x \ln x - (1-x)\ln(1-x)$, which holds for $0 \leqslant x \leqslant 1$.

As derived in Ref. 2, q_N can be rewritten in the form:

$$q_N = \int_0^1 \mathrm{d}\phi \frac{\sin^2 N\pi\phi}{\sin^2 \pi\phi} \Lambda_K(\phi), \tag{2}$$

where K denotes the measurable set K that characterizes the symbol Q, and Λ_K is the function:

$$\Lambda_K(\phi) = |(K + \phi) \setminus K|.$$

$|\cdot|$ denotes the Lebesgue measure. By reducing the region of the integration in (2) to $[0, 1/(2N)]$, and substituting the trigonometric factor with its lower bound on this restricted region, we obtain a lower estimate for q_N:

$$q_N \geqslant \frac{4N^2}{\pi^2} \int_0^{1/2N} \Lambda_K(\phi)\mathrm{d}\phi. \tag{3}$$

This is the starting point in the proof of the following proposition.

Theorem: *For any sublinear function $f: \mathbb{N} \to \mathbb{R}^+$, there exists a pure translation-invariant quasifree state for which S_N is bounded from below by f_N, that is $S_N \geqslant f_N$ for every sufficiently large N.*

Proof: By (3), the problem has been reduced to showing the existence of a set $K \subset [0,1)$ for which the right-hand side of (3) grows not slower than the given f_N as N goes to infinity.

The construction of K is based on two non-negative sequences: a sequence of integers $(n_i)_{i\in\mathbb{N}}$ and another one of real numbers $(\ell_i)_{i\in\mathbb{N}}$, where $\ell_i \geqslant 2\ell_{i+1}$. Let K be the union of infinitely many disjoint intervals, the end points of which are determined by these two sequences as follows:

$$K = \bigcup_{i\in\mathbb{N}} \bigcup_{k=1}^{n_i} I_i^k, \quad I_i^k = [a_i^k, b_i^k], \quad b_i^k - a_i^k = \ell_i,$$

$$a_0^1 = 0, \quad a_i^1 = b_{i-1}^{n_{i-1}} + \ell_{i-1} \quad \text{if } i > 0, \tag{4}$$

$$a_i^k = b_i^{k-1} + \ell_i \quad \text{if } k > 1.$$

The $(\ell_i)_{i\in\mathbb{N}}$ and $(n_i)_{i\in\mathbb{N}}$ are chosen so that the above-constructed set K is bounded, and for convenience, we suppose additionally that $n_i\ell_i$ is monotonically decreasing, and

$$\sum_{i=0}^{\infty} n_i\ell_i < \frac{1}{4}.$$

Thus $K\subset[0,1/2]$. With construction (4), Λ_K takes the form

$$\Lambda_K(\phi) = \sum_{i=0}^{\infty}\sum_{k=1}^{n_i} |(I_i^k + \phi)\setminus K| \geqslant \sum_{i=i_\phi}^{\infty}\sum_{k=1}^{n_i} |(I_i^k + \phi)\setminus K|,$$

where i_ϕ is the smallest index for which $2n_i\ell_i < \phi$ for all $i \geqslant i_\phi$. Each translated interval $(I_i^k+\phi)$ with $i \geqslant i_\phi$ is situated in a region where the original intervals in the construction of K and the gaps between them are not longer than $\ell_i/2$ (or where K has no point at all). For this reason $|(I_i^k+\phi)\setminus K| \geqslant \ell_i/3$ for every term in the last summation. Therefore we obtain

$$\Lambda_K(\phi) \geqslant \frac{1}{3}\sum_{i=i_\phi}^{\infty} n_i\ell_i.$$

Now, let f_N be an arbitrary sublinear function, i.e., $\lim_{N\to\infty} f_N/N = 0$. Obviously, there exists a monotonically increasing continuously differentiable function $g:[0,1/2]\to\mathbb{R}^+$ with the properties:

$$g(0) = 0, \quad \frac{\pi^2}{2} g\left(\frac{1}{2N}\right) \geqslant \frac{f_N}{N}.$$

Let us define function h as $h(x) = (\mathrm{d}/\mathrm{d}x)(xg(x))$. h is continuous, and $h(0)=0$. We suppose that h is strictly monotonically increasing in the neighborhood of zero. If not, we choose a continuous, strictly monotonically increasing $\hat{h}$ such that $\hat{h} \geqslant h$, and $\hat{h}(0)=0$. (A possible choice is $\hat{h}(x) := \max\{h(y)\,|\,y\in[0,x]\}+x$). This $\hat{h}$ can be derived from a $\hat{g}$ for which $\hat{g}\geqslant g$, and then the argument can be continued with $\hat{h}$ instead of h.

The next step is to specify $(n_i)_{i\in\mathbb{N}}$ and $(\ell_i)_{i\in\mathbb{N}}$ so that

$$\Lambda_K(\phi) \geqslant \frac{1}{3}\sum_{i=i_\phi}^{\infty} n_i\ell_i \geqslant h(\phi) \tag{5}$$

should hold for sufficiently small ϕ.

Let s_i be the solution of the following recursive equation, starting from a given s_0 $(0 < s_0 < 1/2)$:

$$h(6(s_i - s_{i+1})) = s_{i+1}. \tag{6}$$

It is clear from the required properties of h that there is a solution that satisfies the equalities $0 \leqslant s_{i+1} \leqslant s_i$ for every i. Since $(s_i)_{i\in\mathbb{N}}$ is bounded from below and monotonically decreasing, it has a limit at infinity. Suppose that this limit differs from zero, say it is $s_\infty > 0$. Taking an arbitrary small $\epsilon > 0$, there is an i for which $\epsilon > 6(s_i - s_{i+1})$, and we find that $h(\epsilon) \geqslant h(6(s_i - s_{i+1})) = s_{i+1} \geqslant s_\infty$ for any ϵ, so $h(0) \geqslant s_\infty$ in contradiction with $h(0)=0$. Thus $\lim_{i\to\infty} s_i = 0$.

Now we are ready to specify the values of ℓ_i and n_i by

$$s_i = \frac{1}{3}\sum_{j=i}^{\infty} n_j \ell_j. \tag{7}$$

Considering that $(s_i)_{i\in\mathbb{N}}$ is a monotonically decreasing sequence tending to zero, these equalities can be satisfied by some series $(n_i)_{i\in\mathbb{N}}$ and $(\ell_i)_{i\in\mathbb{N}}$. Starting with a particular ℓ_i, we can always determine the next term by choosing some $\ell_{i+1} \leqslant \ell_i/2$. The only restriction on the choice of ℓ_i is that $s_i - s_{i+1}$ should be an integral multiple of ℓ_i. This requirement can undoubtedly be met, and then $s_i - s_{i+1} = \frac{1}{3} n_i \ell_i$ yields the value of n_i. The inclusion $K \subset [0, 1/2]$ can be assured by choosing sufficiently small s_0.

Recall that $(n_i \ell_i)_{i\in\mathbb{N}}$ has been required to be monotonic. We can easily convince ourselves that $(n_i \ell_i)_{i\in\mathbb{N}}$ constructed from $(s_i)_{i\in\mathbb{N}}$ has this property. Indeed, it follows immediately from the strict monotonicity of h: $h(2n_i\ell_i) = h(6(s_i - s_{i+1})) = s_{i+1} \leqslant s_i = h(6(s_{i-1} - s_i)) = h(2n_{i-1}\ell_{i-1})$.

Monotonicity of $(s_i)_{i\in\mathbb{N}}$ and its behavior at infinity entail that for any ϕ below a certain bound, there is an index i for which $6(s_i - s_{i+1}) \leqslant \phi \leqslant 6(s_{i-1} - s_i)$. Notice that this index is nothing but i_ϕ. Thus putting together (6) and (7), we arrive at the desired estimate (5). Consequently, for sufficiently large N, in the region of the integration in (3), $\Lambda_K(\phi) \geqslant h(\phi)$ holds. Performing the integration in (3) completes the proof:

$$S_N \geqslant q_N \geqslant \frac{4N^2}{\pi^2}\int_0^{1/2N} \Lambda_K(\phi)\mathrm{d}\phi \geqslant \frac{4N^2}{\pi^2}\int_0^{1/2N} h(\phi)\mathrm{d}\phi = \frac{4N^2}{\pi^2}\int_0^{1/2N} \frac{\mathrm{d}}{\mathrm{d}\phi}(\phi g(\phi))\mathrm{d}\phi = \frac{2N}{\pi^2} g\left(\frac{1}{2N}\right) \geqslant f_N.$$

□

We have just shown that pure translation-invariant quasifree states give rise to arbitrary fast sublinear entropy growth. In the trivial cases, $|K| = 0$ or $|K| = 1$, the entropy is identically zero. The question naturally arises whether it is possible to achieve arbitrary slow nonbounded entropy growth by such states.

Theorem: *Apart from the trivial cases*, *pure* (*gauge- and*) *translation-invariant quasifree states give at least logarithmic entropy growth.*

Proof: It has been shown in Ref. 2 that if

$$\Lambda_K(\phi) \geqslant c\phi \quad \text{for some } c > 0 \tag{8}$$

in the vicinity of zero, then S_N is bounded from below by a logarithmic growth. We will prove that (8) holds for any measurable set $K \subset [0, 1)$ (apart from the trivial cases, where $\Lambda_K(\phi) = 0$).

It is known from the Lebesgue density theorem that for any measurable set K, $|K| = |K^d|$ holds, where K^d denotes the set of the density points of K:

$$K^d = \left\{ x \in K \,\middle|\, \lim_{\delta\to 0} \frac{(x-\delta, x+\delta) \cap K}{2\delta} = 1 \right\}.$$

It can be inferred from this theorem that for any K of positive measure, there is such a point $x \in K$ that

$$\forall \epsilon > 0\text{: } \exists\, \delta > 0 \text{ so that for every interval } I \text{ that satisfies } x \in I, \text{ and } |I| < \delta,\ |K \cap I| > (1-\epsilon)|I|. \tag{9}$$

Disregarding the trivial cases, the measure of K^c (the complement of K), is also positive: $|K^c| > 0$. It means that K^c also has a point that satisfies (9). We denote this point by y. For a given ϵ, we can choose a common δ to x and y. Let I be an interval shorter than this δ: $|I| < \delta$, and $x \in I$. There is an integer n such that $y \in (I + n|I|)$. The set $(I + n|I|)$ can be assured to be disjoint from I by choosing a sufficiently small δ. The following inequalities hold for I:

$$|K \cap I| > (1-\epsilon)|I|, \quad |K^c \cap (I+n|I|)| > (1-\epsilon)|I|. \tag{10}$$

The following estimate, though seemingly weak, is the core of the proof:

$$\Lambda_K(|I|) \geqslant \left| \left(\bigcup_{k=0}^{n-1} (I+k|I|) \cap (K+|I|) \right) \setminus K \right| = \sum_{k=0}^{n-1} |((I+k|I|) \cap (K+|I|)) \setminus ((I+(k+1)|I|) \cap K)|$$

$$\geqslant \sum_{k=0}^{n-1} |((I+k|I|) \cap (K+|I|))| - |(I+(k+1)|I|) \cap K| = |I \cap K| - |(I+n|I|) \cap K|.$$

Having a look at (10), we obtain that for arbitrary positive ϵ,

$$\Lambda_K(|I|) \geqslant (1-2\epsilon)|I|,$$

if $|I|$ is sufficiently small. This inequality entails (8). □

IV. CONCLUSION AND OUTLOOK

We have shown that for any sublinear growth f_N, there exist shift-invariant pure states that have faster entropy growth than f_N. However, the question if the entropy asymptotics of any translation-invariant pure state is sublinear, that is whether they have a vanishing entropy density, is still unsolved. It is difficult to address this problem generally. One can instead take into consideration only special classes of translation-invariant states. For instance, finitely correlated states turn out to lead to bounded entropy growth.[17] A further step could be to explore the entropy growth and the entropy density of pure algebraic states, which are the generalizations of the finitely correlated states.

Another question that can be raised is whether there exists for each sublinear growth f_N a state with local von Neumann entropies S_N such that $\lim_{N\to\infty} S_N/f_N = c$, where $c>0$. As we can learn from the last proposition in Sec. III, in the case of pure translation-invariant quasifree state the answer is negative.

In the case of local Hamiltonians only ground states with bounded or logarithmic entropy growth have been found. From a mathematical point of view, our construction is not sophisticated. Any given sublinear asymptotics is exceedable by the entropy growth of a state characterized by a set of rather simple structure: a set built from countably many intervals. Nevertheless, it is still an open question whether these asymptotics can be physically realized, or entropy asymptotics stronger than logarithmic (or some other sublinear) function can never occur for ground states in the presence of only local interactions.

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Extensive ground state entropy in supersymmetric lattice models

Hendrik van Eerten[a)]
Instituut voor Theoretische Fysica, Universiteit van Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands

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We present the result of calculations of the Witten index for a supersymmetric lattice model on lattices of various type and size. Because the model remains supersymmetric at finite lattice size, the Witten index can be calculated using row-to-row transfer matrices and the calculations are similar to calculations of the partition function at negative activity -1. The Witten index provides a lower bound on the number of ground states. We find strong numerical evidence that the Witten index grows exponentially with the number of sites of the lattice, implying that the model has extensive entropy in the ground state. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2142836]

I. INTRODUCTION

In Ref. 1 a spinless fermion lattice model was proposed that is $N=2$ supersymmetric (SUSY) regardless of lattice size or shape. The (fine-tuned) Hamiltonian of this model is written in terms of fermion creation and annihilation operators, as follows:

$$H=\sum_i \sum_{j \text{ next to } i} P_{\langle i\rangle} c_i^\dagger c_j P_{\langle j\rangle} + \sum_i P_{\langle i\rangle}, \tag{1}$$

with i numbering the lattice sites, c_i and $c_i^\dagger$ obeying $\{c_i, c_j^\dagger\}=\delta_{ij}$ and where we have introduced *projection operators* P for convenient notation. The latter have the form

$$P_{\langle i\rangle} \equiv \prod_{j \text{ next to } i} (1-c_j^\dagger c_j). \tag{2}$$

These projection operators ensure that *no two neighboring sites can be occupied simultaneously*. Therefore, we will work with a restricted Hilbert space where these states are excluded.

The SUSY model is closely related to more conventional lattice models, like the Heisenberg *XXZ* chain. This relation, which holds if we take a one-dimensional (1D) chain with special boundary conditions for the lattice, was demonstrated in Ref. 2. There it was also shown how SUSY could aid a Bethe Ansatz computation of the spectrum of the *XXZ* chain. Indeed, it is fruitful to see how SUSY can facilitate calculations on the lattice model specified by (1), especially since the symmetry holds on arbitrary graphs while exact results on higher dimensional lattices are notoriously difficult to obtain using conventional methods.

The supersymmetry can be viewed as a multiple site generalization of supersymmetric quantum mechanics. The two generators Q^+ and Q^- are given explicitly in Ref. 1,

a)Electronic mail: hveerten@science.uva.nl

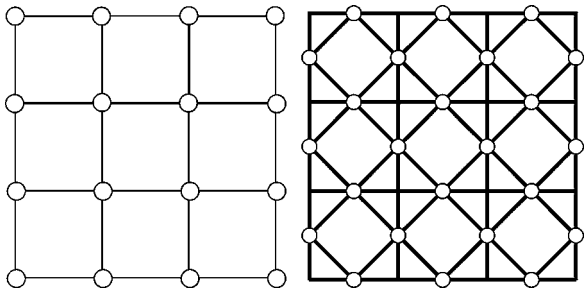

FIG. 1. The square lattice and the square dimer lattice.

$$Q^+ = \sum_{i=1}^{N} c_i^\dagger P_{\langle i \rangle}, \quad Q^- = \sum_{i=1}^{N} c_i P_{\langle i \rangle}. \tag{3}$$

We have the following algebraic structure (with F the fermionic number operator):

$$[F, Q^\pm] = \pm Q^\pm, \quad [F, H] = 0, \quad [Q^+, H] = 0, \quad [Q^-, H] = 0, \quad \{Q^+, Q^-\} = H. \tag{4}$$

In this paper we will focus on the ground states of a variety of two-dimensional (2D) lattices. We will treat the triangular and hexagonal lattice and their counterparts with dimer configurations as well as the dimer version of the square lattice. The square lattice was treated in a separate presentation.[3] All the lattices treated here have an interesting common feature, the number of ground states of the SUSY Hamiltonian on these lattices increases exponentially with increasing lattice size. This directly implies an extensive entropy of the ground state, a rare property exhibited by only a few condensed matter systems. The lattices are shown in Figs. 1–3.

All excited states in the SUSY model occur pairwise, because for every bosonic configuration we have an accompanying fermionic configuration. Here, lattice configurations with an even (odd) number of fermions are termed bosonic (fermionic) configurations. The ground states need not occur pairwise but are restricted otherwise, for their energies are all zero. All this means that we can use the Witten index operator to obtain a lower limit on the number of ground states,

$$W = \mathrm{Tr}(-1)^F e^{-\beta H}. \tag{5}$$

The pairwise cancelling of all excited states allows us to look just at the limiting case $\beta \to 0$, especially when calculating W for finite size lattices where convergence is not an issue, and we will do so for the remainder of this paper.

The operator W is completely equivalent to the well-known grand canonical partion function $Z = \mathrm{Tr}\, z^F \exp(-\beta H)$ of the classical hard particle model in the same dimension, only with a *negative* value for the activity z. It is this equivalence that puts a calculation of the Witten index for SUSY lattice models in a broader context and allows us to use well-known approaches for the

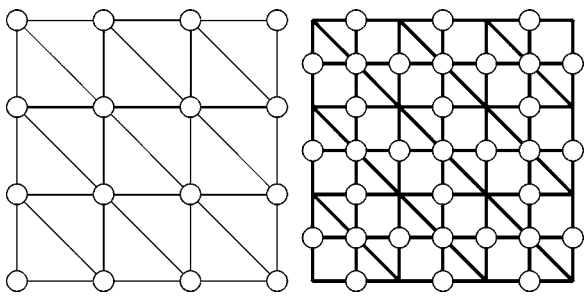

FIG. 2. The triangular lattice and the triangular dimer lattice.

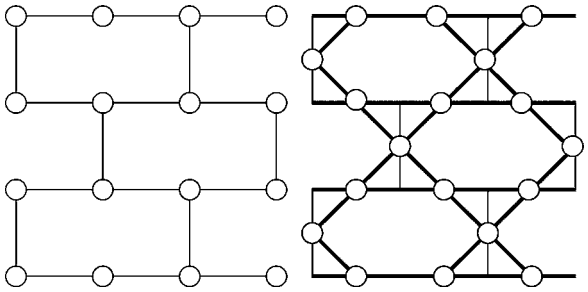

FIG. 3. The hexagonal lattice and the hexagonal dimer lattice.

calculation of Z—especially the use of *transfer matrices* that allows us to write W as the trace of a matrix product.

We have calculated the Witten index for finite sized lattices up to 15×15 (the triangular lattice) using transfer matrices. Before discussing the resulting values for the Witten indices, we will first explain how these matrices were constructed.

II. THE TRANSFER MATRICES

Transfer matrices can be constructed in various ways, as long as they provide a means of systematically summing over all possible configurations on the lattice (see Ref. 4 for an exhaustive introduction). For the N-site chain with periodic boundary conditions, the Witten index operator can be written in terms of transfer matrices as

$$W = \mathrm{Tr}\begin{pmatrix} 1 & i \\ i & 0 \end{pmatrix}^N = \mathrm{Tr}\begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix}^N. \tag{6}$$

The upper left entry of the matrix corresponds to adding an empty site to the chain with an empty site at the end, the upper right entry to adding a filled site to an empty site, the lower left entry to adding an empty site to a filled site and the lower right entry to adding a filled site to a filled site. This last entry must be zero because no configurations with neighboring sites filled were allowed. To avoid an overcounting per fermion we can either use $-1,1$ or i,i for the off-diagonal entries, as long as their product is equal to -1. The resulting transfer matrices can be made symmetric, but never Hermitian.

The procedure can easily be generalized to higher dimensional lattices. The easiest strategy is to use row-to-row transfer matrices and have each matrix entry correspond to a specific row configuration. Because the size of these matrices increases fast with increasing lattice size, the actual constructions of the matrices are best left to a computer (which we did). In the following, we will briefly explain how the matrices were constructed for the various lattices.

The square lattice is the simplest. For each matrix entry (i,j) the computer program just compares the configuration denoted by i with the one denoted by j. The matrix entry will be zero if the two configurations have one or more neighboring vertices occupied when viewed next to each other. If the combination of i and j is allowed, a factor $(-1)^{f(j)}$ is written down, where $f(j)$ stands for the number of fermions in configuration j. This means we obtain a non-symmetric matrix with real numbers only. Using a mapping from the different configurations to binary numbers simplifies matters even further (e.g., ● ○ ● ○ ○→10 100, etc.). The comparison between the ith and jth configuration can now be performed using a binary AND instruction.

The program is easily modified for the triangular lattice. There are two extra edges per vertex connecting to vertices on a higher or lower row. They are similar to the vertical edge, but with all vertices of the lower row shifted one position to the right. In terms of the computer code, when comparing the ith and jth configuration, we apply a binary right shift on the jth binary representation before using AND. The program now performs two tests instead of one to ascertain if it can enter a nonzero value.

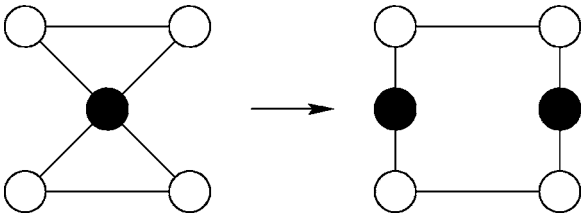

FIG. 4. Doubling sites on the even rows of the hexagonal dimer lattice.

For the hexagonal lattice we need to use two transfer matrices instead of one. Viewing the hexagonal lattice as a horizontal brick wall, we see that we have two different rows. If we work in units of 2×2 sites, we can take the transfer matrix that adds two rows at once as the matrix product of the two different matrices of the single rows.

The dimer lattices offer another complication. The square dimer lattice has both horizontal and vertical dimers. When constructing the transfer matrix we will sum over the horizontal dimer contributions. We can do this without problems because the horizontal dimers make no contact with the next row. For the triangular dimer lattice, we calculate the transfer matrices in a similar way.

For the hexagonal dimer lattice we will use yet another trick. As can be seen in Fig. 3, the even rows contain only half the number of vertices (after switching dimers and vertices in the original hexagonal lattice). As a first step we shall double this number of vertices in the even rows, as shown in Fig. 4. We must make certain that the resulting pairs consistently have the same value. Then we can formulate the transfer matrix once more as the product of two transfer matrices.

III. RESULTS

The resulting values for the Witten index on various lattice sizes are summarized in the tables in the Appendix.

The Witten index for the $M\times N$ lattice is given by Tr $(\mathbf{T}_N)^M$. Because we are taking the trace, the transfer matrices can be diagonalized without changing the resulting value for the Witten index. As a consequence, in the limiting case where the number of rows goes to infinity we can restrict ourselves to the largest roots of the characteristic polynomial of $\mathbf{T}_N$ (we would have used the term *eigenvalue* if the transfer matrix was not defective). Because the characteristic roots turn out to come in complex pairs, we must look at *two* largest roots and we get the following approximation for the Witten index:

$$W_{M,N} \approx a(t_{1,N})^M + \overline{a(t_{1,N})}^M, \tag{7}$$

where $t_{1,N}$ and $\overline{t_{1,N}}$ denote the complex pair that form the largest roots of the N-column transfer matrix.

We can define a *contribution per site* w by

$$w \equiv \lim_{N\to\infty} \frac{t_{1,N}}{t_{1,N-1}}. \tag{8}$$

If we do not take the limit to infinite N, but study finite size lattices of increasing size, we find strong numerical evidence that the contribution to the Witten index per site rapidly tends to a fixed complex number that is different for each lattice that was considered. These numbers are shown in Table I. When calculating these numbers we must select the correct phase factors manually from the two possibilities offered by the complex pairs. The quickly appearing convergence to a fixed value then justifies our choice. The square lattice is treated elsewhere,[3] but has the special property that all characteristic roots have norm equal to 1. All other lattice types have a single complex pair of largest roots.

This convergence to a complex number greater than 1 has an important consequence, for it

TABLE I. Witten index per site, various lattice types.

Lattice type	Modulus $\lvert w\rvert$ per site	Phase $\arg w$ per site
Square dimer	1.33 ± 0.01	$(0.363\times\pi)\pm0.01$
Triangular	1.14 ± 0.01	$(0.178\times\pi)\pm0.01$
Triangular dimer	1.261 ± 0.01	$(0.189\times\pi)\pm0.001$
Hexagonal	1.2 ± 0.1	Insufficient data
Hexagonal dimer	1.4 ± 0.1	$(0.310\times\pi)\pm0.001$

indicates an *extensive ground state entropy*. The Witten index can by approximated by

$$W \approx w^{MN} + \bar{w}^{MN} = 2r^{MN}\cos(MN\theta + \theta_0), \tag{9}$$

with $w=r\exp[i\theta]$. The index provides a lower bound on the number of ground states. [Indeed it is very well possible that the actual number of ground states greatly exceeds $|W|$. The reasoning presented here offers us no information on this. See Refs. 3 and 6 for an example (the square lattice).] In our understanding the oscillating (cosine) factor is due to partial cancelations in W of contributions coming from bosonic and fermionic ground states. We thus expect that the monotonically growing factor r^{MN} sets a lower bound for the actual ground state entropy $S_0 \equiv \ln[\#\text{ground states}]$ according to

$$S_0 \geqslant MN\ln r. \tag{10}$$

For example, for the triangular lattice we find

$$S_0 \geqslant MN\ln 1.14 = 0.131MN. \tag{11}$$

It is interesting to see whether the Witten index per site can be calculated analytically. The triangular lattice case, for example, is equivalent to the hard hexagon model (see Ref. 5) with activity -1 and even fits the Yang-Baxter equation at this value. Unfortunately one cannot simply modify the reasoning from Ref. 4 for the $z<0$ regime because the transfer matrices are defective, so this question remains open for the moment. It might still be possible to obtain analytical solutions using other methods. In Ref. 6, for example, an exact solution for the nonagon-triangle lattice was found by showing that it is equivalent to the number of closed packed dimer coverings on the honeycomb lattice.

The fact that we have a complex number indicates that the Witten index does not necessarily grow with increasing lattice size, like the partition sum of the corresponding hard particle model in the $z>0$ regime would. The phase factor can be used to obtain a rough first estimate on the fermion density of the ground states. The phase factor in the cosine term of W shows us how many sites we need to add to get from a majority of fermionic ground states to a majority of bosonic ground states and vice versa. [For example, the 1D chain has roots $\exp(\pm i/3\pi)$ and only two ground states both with filling factor $1/3$]. But it is only useful as such when combined with a more advanced approach to calculating the spectrum like the spectral sequence technique used in Ref. 3. After all, the phase factor is determined by *all* ground states and they do not necessarily all have the same filling factors.

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APPENDIX: WITTEN INDEX TABLES

The hexagonal lattice tables correspond to the vertical brick wall. It has been confirmed that the tables for the horizontal brick wall are equal to the transposed tables. (See Tables II–VIII.)

TABLE II. Witten index for $M \times N$ square dimer lattice.

	1	2	3	4	5
1	1	−1	−2	−1	1
2	−1	1	8	−15	19
3	−2	8	−26	44	−92
4	−1	−15	44	129	−361
5	1	19	−92	−361	−2344
6	2	4	188	−912	−9158
7	1	−57	−338	4479	−24 219
8	−1	129	572	4417	−8241
9	−2	−136	−818	−46 612	362 068
10	−1	−39	668	5665	2 617 744

TABLE III. Witten index for $M \times N$ square dimer lattice (continued).

	6	7	8	9	10
1	2	1	−1	−2	−1
2	4	−57	129	−136	−39
3	188	−338	572	−818	668
4	−912	4479	4417	−46 612	5665
5	−9158	−24 219	−8241	362 068	2 617 744
6	−54 584	−239 790	−630 384	1 243 052	31 152 804
7	−239 790	1 495 453	9 803 807	−95 946 944	−363 241 257
8	−630 384	9 803 807	−130 406 911	1 458 639 932	−1 665 351 583
9	1 243 052	−95 946 944	1 458 639 932	−980 392 698	−436 754 324
10	31 152 804	−363 241 257	−1 665 351 583	−436 754 324	1 741 554 048

TABLE IV. Witten index for $M \times N$ triangular lattice.

	1	2	3	4	5	6	7	8	9	10
1	1	1	1	1	1	1	1	1	1	1
2	1	−3	−5	1	11	9	−13	−31	−5	57
3	1	−5	−2	7	1	−14	1	31	−2	−65
4	1	1	7	−23	11	25	−69	193	−29	−279
5	1	11	1	11	36	−49	211	−349	811	−1064
6	1	9	−14	25	−49	−102	−13	−415	1462	−4911
7	1	−13	1	−69	211	−13	−797	3403	−7055	5237
8	1	−31	31	193	−349	−415	3403	881	−28 517	50 849
9	1	−5	−2	−29	881	1462	−7055	−28 517	31 399	313 315
10	1	57	−65	−279	−1064	−4911	5237	50 849	313 315	950 592
11	1	67	1	859	1651	12 607	32 418	159 083	499 060	2 011 307
12	1	−47	130	−1295	−589	−26 006	−152 697	−535 895	−2 573 258	−3 973 827
13	1	−181	1	−77	−1949	67 523	330 331	−595 373	−10 989 458	−49 705 161
14	1	−87	−257	3641	12 611	−139 935	−235 717	5 651 377	4 765 189	−232 675 057
15	1	275	−2	−8053	−32 664	272 486	−1 184 714	−1 867 189	134 858 383	−702 709 340

TABLE V. Witten index for $M \times N$ triangular lattice (continued).

	11	12	13	14	15
1	1	1	1	1	1
2	67	−47	−181	−87	275
3	1	130	1	−257	−2
4	859	−1295	−77	3641	−8053
5	1651	−589	−1949	12 611	−32 664
6	12 607	−26 006	67 523	−139 935	272 486
7	32 418	−152 697	330 331	−235 717	−1 184 714
8	159 083	−535 895	−595 373	5 651 377	−1 867 189
9	499 060	−2 573 258	−10 989 458	4 765 189	134 858 383
10	2 011 307	−3 973 827	−49 705 161	−232 675 057	−702 709 340
11	5 102 879	12 409 123	18 205 045	−129 877 296	−1 457 956 169
12	12 409 123	232 286 890	1 851 105 439	1 476 815 313	−1 132 095 426
13	18 205 045	1 851 105 439	−1 938 183 221	1 466 459 831	1 016 873 233
14	−129 877 296	1 476 815 313	1 466 459 831	139 861 123	−1 366 302 204
15	−1 457 956 169	−1 132 095 426	1 016 873 233	−1 366 302 204	1 417 898 645

TABLE VI. Witten index for $M \times N$ triangular dimer lattice.

	2	4	6	8	10	12	16	18
2	1	−3	−5	1	11	9	−13	−31
4	−3	1	21	−79	157	−71	−731	3105
6	−5	21	−44	−47	995	6576	32 279	−131 167
8	1	−79	−47	3329	3801	−134 959	−217 671	5 439 681
10	11	157	995	3801	−37 009	−1 110 731	−17 397 663	−217 844 591
12	9	−71	−6576	−134 959	−1 110 731	11 324 392	538 444 825	105 699 937
14	−13	−731	32 279	−217 671	−17 397 663	538 444 825	−600 643 992	−914 519 359
16	−31	3105	−131 167	5 439 681	−217 844 591	105 699 937	−914 519 359	

TABLE VII. Witten index for $M \times N$ hexagonal lattice.

	2	4	6	8	10	12	14	16	18
2	−1	−1	2	−1	−1	2	−1	−1	2
4	3	7	18	47	123	322	843	2207	5778
6	−1	−1	32	−73	44	356	−1387	2087	2435
8	3	7	18	55	123	322	843	2215	5778
10	−1	−1	152	−321	−171	7412	−26 496	10 079	393 767
12	3	7	156	1511	6648	29 224	150 069	1 039 991	6 208 815
14	−1	−1	338	727	−5671	1850	183 560	−279 497	−4 542 907
16	3	7	1362	12 183	31 803	379 810	5 970 107	55 449 303	327 070 578

TABLE VIII. Witten index for $M \times N$ hexagonal dimer lattice.

	2	4	6	8	10	12	14	16
2	0	−8	0	32	0	−128	0	512
4	−4	8	32	−224	896	−2176	1536	16 896
6	12	88	576	3296	17 472	77 056	194 304	−1 139 200
8	4	−496	−3056	118 912	1 287 744	−25 732 864	−439 656 192	626 526 208
10	−40	1832	−42 400	1 088 352	−19 939 840	205 139 072	−878 495 232	1 612 654 080
12	44	−2872	−425 344	−23 115 488	84 888 704	420 235 264	335 598 080	−1 677 852 160
14	84	−12 440	−3 459 792	−336 941 664	−936 816 704	1 524 979 328	1 080 971 264	1 869 085 184

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Nonlinear diffusion equation, Tsallis formalism and exact solutions

P. C. Assis, Jr. and L. R. da Silva
Departamento de Física, Universidade Federal do Rio Grande do Norte, 59078-970 Natal-RN, Brazil

E. K. Lenzi, L. C. Malacarne, and R. S. Mendes
Departamento de Física, Universidade Estadual de Maringá, Av. Colombo 5790, 87020-900 Maringá-PR, Brazil

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We address this work to analyze a nonlinear diffusion equation in the presence of an absorption term taking external forces and spatial time-dependent diffusion coefficient into account. The nonlinear terms present in this equation are due to a nonlinear generalization of the Darcy law and the presence of an absorbent (source) term. We obtain new exact solutions and investigate nonlinear effects produced on the solutions by these terms. We also connect the results found here within the Tsallis formalism. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Recently, generalizations of the diffusion equation based on nonlinear diffusion equations have been extensively investigated due to the broadness of applications covering almost every field. One of them is the *porous medium equation*,

$$\frac{\partial}{\partial t}\rho(x,t) = \mathcal{D}\frac{\partial^2}{\partial x^2}[\rho(x,t)]^{\nu}, \tag{1}$$

that has been applied in several situations such as percolation of gases through porous media,[1] thin saturated regions in porous media,[2] a standard solid-on-solid model for surface growth, thin liquid films spreading under gravity,[3] the axisymmetric flow of a very viscous fluid,[4] turbulent diffusion,[5] an adsorption-desorption equilibrium locally maintained through a permeable solid[6] and the nonlinear diffusion in hard and soft superconductors.[7]

The formal properties of this equation have also been analyzed. For instance, in Ref. 8 is established a connection between Eq. (1) and the Tsallis formalism,[9] in Ref. 10 the presence of a spatial time-dependent diffusion coefficient is studied, in Ref. 11 a Verhuslt-type reaction term in Eq. (1) is introduced and, in Ref. 12 an anisotropic case is analyzed. Others applications of Eq. (1) can be found in Ref. 13.

Another interesting nonlinear extension of the usual diffusion equation is based on the nonlinear Darcy (or Fourier) law.[14] In particular, the diffusion equation that emerges from this consideration is given by

$$\frac{\partial}{\partial t}\rho(x,t) = \mathcal{D}\frac{\partial}{\partial x}\left\{[\rho(x,t)]^{m}\left|\frac{\partial}{\partial x}\rho(x,t)\right|^{n}\frac{\partial}{\partial x}\rho(x,t)\right\}. \tag{2}$$

Note that the above equation simplifies to Eq. (1) for a particular conditions and for $m=0$ the current density that emerges from the above equation is known as Gorter-Melling law. Equation (2) has also been employed in several situations such as nonlinear heat conduction,[14] nonlinear shear flows of non-Newtonian fluids,[15] gravity flows of non-Newtonian fluid through a porous

medium and the axial mixing generated by the buoyancy effect due to the injection of a denser fluid into a less dense one.[16] The properties of Eq. (2) have also been analyzed, for instance, a nonlinear conduction equation based on a generalized Fourier law is studied in Ref. 14 and in Refs. 17 and 18 a nonlinear diffusion in fractal structures is considered. However, Eq. (2) was not properly worked in the presence of external forces with an absorbent (source) term. In this direction, we dedicate this work to analyze Eq. (2) in the presence of external forces and taking absorbent (source) term into account in order to understand the changes produced by an external force and an absorbent (source) term. Thus, we investigate the following nonlinear diffusion equation:

$$\frac{\partial}{\partial t}\rho(x,t)=\mathcal{D}(t)\frac{\partial}{\partial x}\left\{|x|^{-\theta}\left|\frac{\partial}{\partial x}\rho(x,t)\right|^{n}\frac{\partial}{\partial x}[\rho(x,t)]^{\nu}\right\}-\frac{\partial}{\partial x}\{F(x,t)\rho(x,t)\}-\overline{\alpha}(t)[\rho(x,t)]^{\mu}, \tag{3}$$

where $\mathcal{D}(t)$ is a time diffusion coefficient, $F(x,t)$ represents an external force (drift) and $\overline{\alpha}(t)$ plays the role of an absorbent (or source) rate related to a reaction-diffusion process. It is interesting to note that the above diffusion equation can be applied to describe several scenarios such as heat conduction by electrons in a plasma, heat conduction by radiation in a fully ionized gas (Marshak waves), axisymmetric flow of a very viscous fluid,[4] turbulent diffusion,[5] an adsorption-desorption equilibrium locally maintained through a permeable solid[6] and the nonlinear diffusion in hard and soft superconductors.[7] The presence of the reaction term like the one given in the above equation has been studied in several situations. Here, for example, we may recall the so-called species coagulation, that is $A+A\rightarrow 0$ or $mA\rightarrow lA$, catalytic processes in regular, heterogeneous, or disordered systems.[19] Another example is an irreversible first-order reaction of transported substance so that the rate of removal is $\overline{\alpha}\rho$.[20] This extra term may also appear when a tracer undergoing radioactive decay is transported through a porous medium,[21] in heat flow involving heat production.[22]

For $\overline{\alpha}(t)=0$, it can be verified that $\int_{-\infty}^{\infty}dx\,\rho(x,t)$ is time independent (hence, if ρ is normalized at $t=0$, it will remain so forever). Indeed, if we write Eq. (3) as $\partial_t\rho=-\partial_x\mathcal{J}$ and assume the boundary condition $\mathcal{J}(x\rightarrow\pm\infty,t)\rightarrow 0$, it can be shown that $\int_{-\infty}^{\infty}dx\,\rho(x,t)$ is a constant of motion. Equation (3) recovers, for $(\theta,\nu,n,\mu)=(0,1,0,1)$, the standard Fokker-Planck equation[23] in the presence of a drift with an absorbent (source) term. For $(\theta,\nu)=(0,m+1)$, $F(x,t)=0$, $\mathcal{D}(t)=\mathcal{D}/(m+1)$ and $\overline{\alpha}(t)=0$ Eq. (2) is obtained from Eq. (3). The particular case $F(x,t)=0$ (no drift), $\mathcal{D}(x,t)=$const. and $n=0$ in the absence of source (absorbent) term, has been considered by Spohn.[24] Other aspects of Eq. (3) with $n=0$ have also been considered in Refs. 8 and 25. Note that as we mentioned above our present discussion involves extensions of these cases by taking a wide variety of situations into account. In particular, we obtain solutions for the above equation by considering the presence of external forces and absorbent (source) terms. We also establish a connection between the results found here and the distribution that emerges from the Tsallis thermostatics.[9]

The remainder of this paper goes as follows. In Sec. II, we consider several situations for Eq. (3) as well as the connection of the solutions with the ones obtained within the maximum entropy principle by employing the Tsallis entropy. In Sec. III, we present our conclusions.

II. NONLINEAR DIFFUSION EQUATION

Now, let us investigate time-dependent solutions for Eq. (3). We use similarity methods to reduce Eq. (3) to ordinary differential equations. The explicit form for these ordinary differential equations depends on the boundary conditions or on restrictions in the form of conservation laws. In this direction, we restrict our analysis to find a solution that can be expressed as a scaled function of the type

$$\overline{\rho}(x,t) = \frac{1}{\Phi(t)}\tilde{\rho}\left[\frac{x}{\Phi(t)}\right]. \tag{4}$$

These solutions satisfy the initial, the boundary conditions, and the normalization condition when $\overline{\alpha}(t)=0$. Before analyzing the solutions of Eq. (3), we consider $\mu=1$ and that the solution is given by $\rho(x,t)=\exp[-\int_0^t d\tilde{t}\,\overline{\alpha}(\tilde{t})]\overline{\rho}(x,t)$, where $\overline{\rho}(x,t)$ is a function to be determined and it is given by Eq. (4). The case $\mu\neq 1$ is discussed at the end of this section. By using the above statement, we obtain

$$\frac{\partial}{\partial t}\overline{\rho}(x,t) = \overline{\mathcal{D}}(t)\frac{\partial}{\partial x}\left\{|x|^{-\theta}\left|\frac{\partial}{\partial x}\overline{\rho}(x,t)\right|^{n}\frac{\partial}{\partial x}[\overline{\rho}(x,t)]^{\nu}\right\} - \frac{\partial}{\partial x}\{F(x,t)\overline{\rho}(x,t)\}, \tag{5}$$

with $\overline{\mathcal{D}}(t)=\mathcal{D}(t)\exp[-(\nu+n-1)\int_0^t d\tilde{t}\,\overline{\alpha}(\tilde{t})]$. In the following, we discuss the solutions by considering the absence of external force, the presence of a linear external force and, after we incorporate a power law external force.

We start by studying Eq. (5) in the absence of external force. For this case we have that

$$\frac{\partial}{\partial t}\overline{\rho}(x,t) = \overline{\mathcal{D}}(t)\frac{\partial}{\partial x}\left\{|x|^{-\theta}\left|\frac{\partial}{\partial x}\overline{\rho}(x,t)\right|^{n}\frac{\partial}{\partial x}[\overline{\rho}(x,t)]^{\nu}\right\}. \tag{6}$$

This equation can also be formulated in the context of heat diffusion. In the heat conduction context, to obtain the above equation, we need to consider a temperature-dependent thermal conductivity[26] and a nonlinear generalization of the Fourier law.[14]

By applying Eq. (4) in Eq. (6), thus, the last equation can be reduced to

$$\frac{d}{dz}\left\{|z|^{-\theta}\left|\frac{d}{dz}\tilde{\rho}(z)\right|^{n}\frac{d}{dz}[\tilde{\rho}(z)]^{\nu}\right\} = -\overline{k}\frac{d}{dz}[z\tilde{\rho}(z)] \tag{7}$$

and

$$[\Phi(t)]^{\xi}\frac{d}{dt}\Phi(t) = \overline{k\mathcal{D}}(t), \tag{8}$$

where $\xi=\nu+\theta+2n$, $z=x/\Phi(t)$ and $\overline{k}$ is an arbitrary constant. By solving Eq. (8), we found

$$\Phi(t) = \left[(\Phi(0))^{1+\xi} + k'\int_0^t d\tilde{t}\,\overline{\mathcal{D}}(\tilde{t})\right]^{1/(1+\xi)}, \tag{9}$$

with $k'=(1+\xi)\overline{k}$ determined by the normalization condition. Performing an integration in Eq. (7), we have that

$$|z|^{-\theta}\left|\frac{d}{dz}\tilde{\rho}(z)\right|^{n}\frac{d}{dz}[\tilde{\rho}(z)]^{\nu} = -\overline{k}z\tilde{\rho}(z) + \mathcal{C}, \tag{10}$$

where $\mathcal{C}$ is an integration constant. To find a solution for Eq. (10), we consider the following ansatz: $\tilde{\rho}(z)=(1-\alpha|z|^{\lambda})^{\beta}$ and, for simplicity, we take $\mathcal{C}=0$ to satisfy the $\rho(x\to\pm\infty,t)\to 0$. By substituting the ansatz in Eq. (10) we verify that

$$\alpha = \frac{\nu+n-1}{2+\theta+n}\left(\frac{\overline{k}}{\nu}\right)^{1/(n+1)}, \quad \beta = \frac{n+1}{\nu+n-1}, \quad \lambda = \frac{2+\theta+n}{n+1}. \tag{11}$$

Thus, the solution found to Eq. (6) can be expressed as

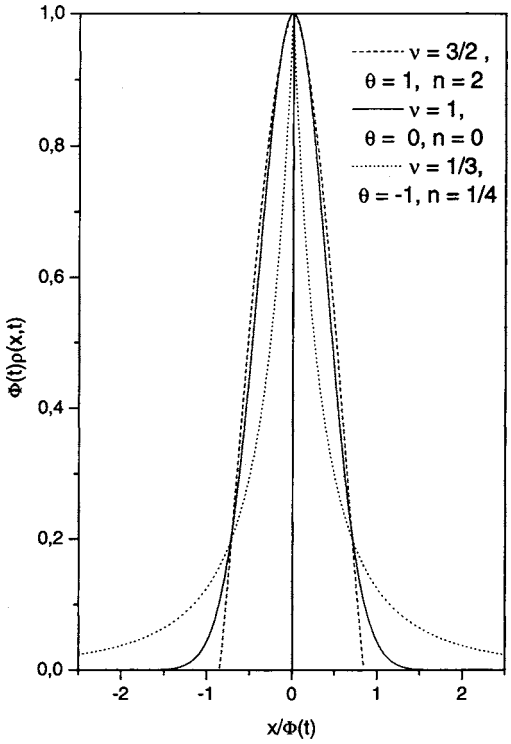

FIG. 1. Behavior of $\Phi(t)\rho(x,t)$ versus $x/\Phi(t)$ for a typical value of θ, ν, and n taking $\overline{\alpha}(t)=0$ into account. Note that, depending on the parameters θ, ν, and n, $\rho(x,t)$ can have compact or long tail.

$$\overline{\rho}(x,t)=\frac{1}{\Phi(t)}\exp_q\left[-\frac{1}{2+\theta+n}\left(\frac{\overline{k}}{\nu}\right)^{1/(n+1)}\left(\frac{|x|}{\Phi(t)}\right)^{\frac{2+\theta+n}{n+1}}\right]^{n+1}, \tag{12}$$

(see Fig. 1) with $q=2-(\nu+n)$ where $\exp_q[x]$ is defined as follows: $\exp_q[x]=(1+(1-q)x)^{1/(1-q)}$ for $1+(1-q)x\geqslant 0$ and by $\exp_q[x]=0$ for $1+(1-q)x<0$.

Notice that the $\exp_q[x]$ is the q-exponential which emerges from the Tsallis formalism[9] by maximizing the Tsallis entropy

$$S_q=\frac{1-\int \mathrm{d}x[\overline{\rho}(x)]^q}{q-1} \tag{13}$$

with appropriated constraints. For this reason, the q-exponential may be considered a signature of the Tsallis formalism and the presence of this function in the solutions indicates a connection between the solutions of Eq. (3) and Tsallis formalism. In fact, by considering suitable constraints it is possible to obtain these solutions by employing the maximum principle of entropy. Similar situation is considered in Refs. 27 and 28 for the porous medium equation. Thus, the parameter q which in the Tsallis formalism is not determined, here it is obtained in terms of the parameters of the nonlinear diffusion equation.

It is also interesting to note that the solution (12) can have a compact or a long tail behavior depending on the parameters ν, n, and θ. In addition, for the long tail behavior, we can asymptotically relate the solution with the Lévy distributions. In fact, the asymptotic limit for Eq. (12) for large x and $\nu+n<1$ is

$$\overline{\rho}(x,t) \sim \frac{1}{\Phi(t)}\left(\frac{|x|}{\Phi(t)}\right)^{-(2+\theta+n)/(1-\nu-n)}. \tag{14}$$

Now, by comparing the above result with the asymptotic limit that emerges from the Lévy distribution for large x, i.e., $\rho \sim 1/|x|^{1+\overline{\mu}}$, we obtain that $\overline{\mu}=(1+\theta+\nu+2n)/(1-\nu-n)$. Thus, for suitable parameters θ, ν, and n such that $0<\overline{\mu}<2$, Eq. (12) behaves asymptotically like a Lévy distribution. For the case $\overline{\alpha}(t)=0$ and $\mathcal{D}(t)=\mathcal{D}$, depending on the choice of the parameters (ν,θ,n), we may have an anomalous spreading of the distribution given by Eq. (12), which may characterize an anomalous diffusion or an anomalous conduction. In fact, for this case, the second moment is given by $\langle x^2\rangle \propto t^{2/(1+\xi)}$, where $2/(1+\xi)<1,=1,>1$ characterize a sub, normal or superdiffusive behavior.

Following, we analyze the implications of considering drift terms in Eq. (3). In this direction, we first study the effects produced in the solution by a linear external force. By applying Eq. (4) in Eq. (5) and taking the drift term $F(x,t)=-k_1(t)x$ into account, Eq. (5) can be written as

$$\frac{\partial}{\partial t}\overline{\rho}(x,t) = \overline{\mathcal{D}}(t)\frac{\partial}{\partial x}\left\{|x|^{-\theta}\left|\frac{\partial}{\partial x}\overline{\rho}(x,t)\right|^{n}\frac{\partial}{\partial x}[\overline{\rho}(x,t)]^{\nu}\right\} + k_1(t)\frac{\partial}{\partial x}[x\overline{\rho}(x,t)]. \tag{15}$$

By using the previous procedure, we can reduce Eq. (15) to

$$\frac{d}{dz}\left\{|z|^{-\theta}\left|\frac{d}{dz}\widetilde{\rho}(z)\right|^{n}\frac{d}{dz}[\widetilde{\rho}(z)]^{\nu}\right\} = -\overline{k}\frac{d}{dz}[z\widetilde{\rho}(z)] \tag{16}$$

and

$$[\Phi(t)]^{\overline{\xi}}\frac{d}{dt}\Phi(t) + k_1(t)[\Phi(t)]^{1+\overline{\xi}} = \overline{k\mathcal{D}}(t), \tag{17}$$

where $\overline{\xi}=\theta+\nu+2n$. The spatial solution for this case is the same that the one obtained for the free case, i.e., Eq. (12). In fact, Eq. (16) is equal to Eq. (7). The difference is present only on the time-dependent function $\Phi(t)$ which in this case is given by Eq. (17). By solving Eq. (17), we found

$$\Phi(t) = \left[(\Phi(0))^{1+\overline{\xi}} + k'\int_0^t d\widetilde{t}\,\overline{\mathcal{D}}(\widetilde{t})e^{(1+\overline{\xi})\int_0^{\widetilde{t}}dt'\,k_1(t')}\right]^{1/(1+\overline{\xi})} e^{-\int_0^t dt'\,k_1(t')}, \tag{18}$$

with $k'=(1+\overline{\xi})\overline{k}$. For $\overline{\alpha}(t)=0$ and $\mathcal{D}(t)=$const, we have a stationary solution, in contrast, to the case characterized by the absence of external force, and it is given by $\rho(x)\propto(1-\alpha'|x|^{\lambda})^{\beta}$ where α' is a constant.

Let us extend the above situation by assuming the external force $F(x,t)=-k_1(t)x-k_\alpha x|x|^{\alpha-1}$ with, for simplicity, $\mathcal{D}(t)=$const and $\overline{\alpha}(t)=0$. We do not know what happens in the general case for (α,θ,ν,n), but there is a special situation for which the scaled solution of the type indicated in Eq. (4) is still valid. This special case corresponds to $\alpha=-\theta-\nu-2n$, i.e., $\alpha+\theta+\nu+2n=0$. For this case, by using the previous procedure, we can reduce Eq. (3) to

$$-\overline{k}\frac{d}{dz}[z\widetilde{\rho}(z)] = \mathcal{D}\frac{d}{dz}\left\{|z|^{-\theta}\left|\frac{d}{dz}\widetilde{\rho}(z)\right|^{n}\frac{d}{dz}[\widetilde{\rho}(z)]^{\nu}\right\} + k_\alpha\frac{d}{dz}[z|z|^{\alpha-1}\widetilde{\rho}(z)] \tag{19}$$

and

$$[\Phi(t)]^{\overline{\xi}}\frac{d}{dt}\Phi(t) + k_1(t)[\Phi(t)]^{1+\overline{\xi}} = \overline{k}. \tag{20}$$

The solution for Eq. (20) is given by

$$\Phi(t)=\left[(\Phi(0))^{1+\overline{\xi}}+k'\int_0^t \mathrm{d}\widetilde{t}\, e^{(1+\overline{\xi})\int_0^{\widetilde{t}}\mathrm{d}t'\ k_1(t')}\right]^{1/(1+\overline{\xi})} e^{-\int_0^t \mathrm{d}t'\ k_1(t)}. \tag{21}$$

In order to obtain the solution for Eq. (19), we perform an integration leading to

$$\mathcal{D}|z|^{-\theta}\left|\frac{d}{\mathrm{d}z}\widetilde{\rho}(z)\right|^n\frac{d}{\mathrm{d}z}[\widetilde{\rho}(z)]^\nu=-(\overline{kz}+k_\alpha z|z|^{\alpha-1})\widetilde{\rho}(z)+\mathcal{C}', \tag{22}$$

where $\mathcal{C}'$ is constant. To solve this equation, we also employ the boundary condition $\rho(x\rightarrow\pm\infty,t)\rightarrow 0$ which implies in $\mathcal{C}'=0$. Thus, the solution for this equation is given by

$$\widetilde{\rho}(z)=\exp_q\left[-\frac{1}{n+1}\left(\frac{\overline{k}}{\mathcal{D}\nu}\right)^{1/(n+1)}\int^{|z|}d\overline{z}\left(\overline{z}^{1+\theta}+\frac{k_\alpha}{\overline{k}}\overline{z}^{\nu-2n}\right)^{1/(n+1)}\right]^{n+1}. \tag{23}$$

For $n=0$, we recover the solutions found in Ref. 29 after making an integration.

Now, let us study Eq. (3) by taking the general case $\mu\neq 1$ into account. For this case, Eq. (3) can be written as

$$\frac{\partial}{\partial t}\rho(x,t)=\mathcal{D}\frac{\partial}{\partial x}\left\{|x|^{-\theta}\left|\frac{\partial}{\partial x}\rho(x,t)\right|^n\frac{\partial}{\partial x}[\rho(x,t)]^\nu\right\}-\overline{\alpha}[\rho(x,t)]^\mu \tag{24}$$

when the external forces are absent for a time-independent diffusion coefficient and $\overline{\alpha}(t)=\overline{\alpha}$. Following Ref. 30, we consider that a solution for this equation may be given by $\rho(x,t)=\phi(t)\mathcal{P}(\zeta(t)x)$, where $\phi(t)$ and $\zeta(t)$ are time-dependent functions to be found. In this direction, by analyzing the simple kinetic equation that emerges from the above equation for $\mathcal{D}=0$, i.e., $\partial_t\rho(t)=-\overline{\alpha}[\rho(t)]^\mu$, whose solution is $\rho(t)\propto(1-(1-\mu)\overline{\alpha}t)^{1/(1-\mu)}$, we are suggested to employ $\phi(t)=(1-(1-\mu)kt)^{1/(1-\mu)}$. To obtain $\zeta(t)$, we substitute the proposed solution $\rho(x,t)$ in Eq. (24) with $\phi(t)$ defined above. This replacement lead us to obtain $\zeta(t)=(1-(1-\mu)kt)^{(n+\nu-\mu)/[(\mu-1)(2+n+\theta)]}$ and

$$-k\mathcal{P}(\eta)-\left(\frac{\mu-n-\nu}{2+\theta+n}\right)k\eta\frac{d}{\mathrm{d}\eta}\mathcal{P}(\eta)=\mathcal{D}\frac{d}{\mathrm{d}\eta}\left\{|\eta|^{-\theta}\left|\frac{d}{\mathrm{d}\eta}\mathcal{P}(\eta)\right|^n\frac{d}{\mathrm{d}\eta}[\mathcal{P}(\eta)]^\nu\right\}-\overline{\alpha}[\mathcal{P}(\eta)]^\mu, \tag{25}$$

with $\eta=\zeta(t)x$ and k being a constant. To find an explicit solution in the function of η for the above equation is a hard task, however, it is possible to obtain an implicit solution when $\mu=2+2n+\theta+\nu$. It is formally given by

$$\mathcal{P}(\eta)=\exp_q\left[-\frac{1}{n+1}\left(\frac{k}{\nu\mathcal{D}}\right)^{1/(n+1)}\int^{|\eta|}\mathrm{d}\overline{\eta}\,\overline{\eta}^{\theta/n+1}\left(\overline{\eta}-\frac{\overline{\alpha}}{k\mathcal{P}(\overline{\eta})}\int^{\overline{\eta}}\mathrm{d}\eta'[\mathcal{P}(\eta')]^\mu\right)^{\frac{1}{n+1}}\right]^{n+1}. \tag{26}$$

We notice that the above equation simplified to Eq. (12) for $\overline{\alpha}=0$ after performing an integration. By using the above results, we can obtain for μ, n, ν, and θ arbitraries the nth moment of this distribution. In fact, we have that

$$\langle x^{2n}\rangle=\left[\int \mathrm{d}x\, x^{2n}\rho(x,t)\right]\Big/\left[\int \mathrm{d}x\,\rho(x,t)\right]=\zeta(t)^{-2n}\left[\int \mathrm{d}\eta\,\eta^{2n}\rho(\eta)\right]\Big/\left[\int \mathrm{d}\eta\,\rho(\eta)\right]\propto\zeta(t)^{-2n} \tag{27}$$

and $\langle x^{2n+1}\rangle=0$, yielding $\langle(x-\langle x\rangle)^2\rangle\sim t^{[2(n+\nu-\mu)]/[(1-\mu)(2+n+\theta)]}$. Note that to obtain the last results we have assumed that the nth moment is defined and that the diffusive process can be subdiffusive, normal, or superdiffusive, depending on the value of $2(n+\nu-\mu)/[(1-\mu)(2+n+\theta)]$ to be less, equal or greater than 1.

III. CONCLUSIONS

In summary, we have worked on a generalized diffusion equation [Eq. (3)] for several situations by incorporating some space- and time-dependent classes of external drifts and diffusion coefficients. We have shown that it admits exact solutions where the space scales with a function of time. Another interesting point is the presence of the q-exponential function of the Tsallis formalism in the solutions found here. This fact indicates a connection between the solutions found here and the distributions that emerges from the Tsallis formalism, leading to an identification of the Tsallis entropic index with the parameters of the nonlinear diffusion equation. In particular, this explicit identification may be useful to explore the sensitivity of q to the details of the physical model. In addition, this feature could be helpful in a deeper connection between nonlinear diffusion and Tsallis entropy. We have also extended the results obtained in Refs. 8 and 25 in a unified approach. Finally, we expect that the results presented here bring new aspects and they open new possibilities of applications to the nonlinear diffusion equations and the Tsallis formalism.

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Eigenvalues of Casimir invariants for $U_q[\mathrm{osp}(m|n)]$

K. A. Dancer,[a] M. D. Gould,[b] and J. Links[c]
Centre for Mathematical Physics, School of Physical Sciences,
The University of Queensland, Brisbane 4072, Australia

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For each quantum superalgebra $U_q[\mathrm{osp}(m|n)]$ with $m>2$, an infinite family of Casimir invariants is constructed. This is achieved by using an explicit form for the Lax operator. The eigenvalue of each Casimir invariant on an arbitrary irreducible highest weight module is also calculated. © *2005 American Institute of Physics.*
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I. INTRODUCTION

Representations of quantum superalgebras are known to provide solutions to the Yang-Baxter equation and represent the symmetries that underly supersymmetric exactly solvable (or integrable) models. Many such examples have arisen in the context of modelling systems of strongly correlated electrons.[1–5] More recently, the properties of solvability and supersymmetry have been applied to other areas, such as the solution of the Kondo model,[6] integrable superconformal field theory[7] and disordered systems.[8] Developing the representation theory of the quantum superalgebras is a useful step towards the complete understanding of such models. However, in many respects the representation theory of quantum superalgebras is not a straightforward generalization of the quantum algebra case, principally because not all representations of quantum superalgebras are unitary.[9] This leads, for example, to the existence of indecomposable representations not arising in the quantum algebra case, which generally make the analysis of supersymmetric models problematic (e.g., see Ref. 8).

In this paper we construct the Casimir invariants (central elements) of quantized orthosymplectic superalgebras. Our method of construction follows from the general results of Ref. 10 and the explicit form of the Lax operator obtained in Ref. 11. A fundamental problem is to determine the eigenvalues of the Casimir invariants when acting on an arbitrary finite-dimensional irreducible module. To date, the eigenvalues have only been calculated for the type I quantum superalgebras,[12,13] while the results for $U_q[\mathrm{osp}(1|n)]$ follow from an isomorphism derived in Ref. 14. In this paper we perform the calculations for the remaining nonexceptional quantum superalgebras, namely $U_q[\mathrm{osp}(m|n)]$ for $m>2$. The procedure we use for calculating the eigenvalues of the Casimir invariants when acting on any irreducible module is based on the early work by Perelomov and Popov[15,16] and Nwachuku and Rashid.[17] In doing so we follow the method used in Refs. 18 and 19 for the classical general and orthosymplectic superalgebras, respectively, which was adapted in Ref. 13 to cover $U_q[\mathrm{gl}(m|n)]$. Although the concepts are much the same as in those cases, the combination of the q-deformation and the more complex root system of $U_q[\mathrm{osp}(m|n)]$ makes the calculations in this paper more technically challenging.

In the following section we introduce our notation for $U_q[\mathrm{osp}(m|n)]$ and state the Lax operator. In Sec. III we develop the formulas for the Casimir invariants of $U_q[\mathrm{osp}(m|n)]$. The bulk of the calculations are in Sec. IV where the eigenvalues of the Casimir invariants are derived in detail.

[a]Electronic mail: dancer@maths.uq.edu.au
[b]Electronic mail: mdg@maths.uq.edu.au
[c]Electronic mail: jrl@maths.uq.edu.au

II. THE QUANTIZED ORTHOSYMPLECTIC SUPERALGEBRA $U_q[\mathrm{osp}(m|n)]$

The quantum superalgebra $U_q[\mathrm{osp}(m|n)]$ is a q-deformation of the classical orthosymplectic superalgebra. A brief explanation of $U_q[\mathrm{osp}(m|n)]$ is given below, with a more thorough introduction to $\mathrm{osp}(m|n)$ and the q-deformation to be found in Ref. 11.

First we need to define the notation. The grading of a is denoted by $[a]$, where

$$[a]=\begin{cases}0, & a=i, \quad 1\leqslant i\leqslant m,\\ 1, & a=\mu, \quad 1\leqslant \mu\leqslant n.\end{cases} \tag{1}$$

Throughout this paper we use greek letters μ,ν, etc., to denote odd indices and italic letters i,j, etc., for even indices. If the grading is unknown, the usual a,b,c, etc., are used. Which convention applies will be clear from the context. Throughout the paper we also use the symbols $\bar{a}$ and ξ_a, which are given by

$$\bar{a}=\begin{cases}m+1-a, & [a]=0,\\ n+1-a, & [a]=1,\end{cases}$$

and

$$\xi_a=\begin{cases}1, & [a]=0,\\ (-1)^a, & [a]=1.\end{cases}$$

As a weight system for $U_q[\mathrm{osp}(m|n)]$ we take the set $\{\varepsilon_i,1\leqslant i\leqslant m\}\cup\{\delta_\mu,1\leqslant\mu\leqslant n\}$, where $\varepsilon_{\bar{i}}=-\varepsilon_i$ and $\delta_{\bar{\mu}}=-\delta_\mu$. Conveniently, when $m=2l+1$ this implies $\varepsilon_{l+1}=-\varepsilon_{l+1}=0$. Acting on these weights, we have the invariant bilinear form defined by

$$(\varepsilon_i,\varepsilon_j)=\delta^i_j, \quad (\delta_\mu,\delta_\nu)=-\delta^\mu_\nu, \quad (\varepsilon_i,\delta_\mu)=0, \quad 1\leqslant i,j\leqslant l, 1\leqslant\mu,\nu\leqslant k.$$

When describing an object with unknown grading indexed by a the weight will be described generically as ε_a. This should not be assumed to be an even weight.

The even positive roots of $U_q[\mathrm{osp}(m|n)]$ are composed entirely of the usual positive roots of $o(m)$ together with those of $\mathrm{sp}(n)$, namely,

$$\varepsilon_i\pm\varepsilon_j, \quad 1\leqslant i<j\leqslant l,$$

$$\varepsilon_i, \quad 1\leqslant i\leqslant l \quad \text{when } m=2l+1,$$

$$\delta_\mu+\delta_\nu, \quad 1\leqslant\mu,\nu\leqslant k,$$

$$\delta_\mu-\delta_\nu, \quad 1\leqslant\mu<\nu\leqslant k.$$

The root system also contains a set of odd positive roots, which are

$$\delta_\mu+\varepsilon_i, \quad 1\leqslant\mu\leqslant k, \quad 1\leqslant i\leqslant m.$$

Throughout this paper we choose to use the following set of simple roots:

$$\alpha_i=\varepsilon_i-\varepsilon_{i+1}, \quad 1\leqslant i<l,$$

$$\alpha_l=\begin{cases}\varepsilon_l+\varepsilon_{l-1}, & m=2l,\\ \varepsilon_l, & m=2l+1,\end{cases}$$

$$\alpha_\mu = \delta_\mu - \delta_{\mu+1}, \quad 1 \leqslant \mu < k,$$

$$\alpha_s = \delta_k - \varepsilon_1.$$

Note this choice is only valid for $m > 2$.

In $U_q[\mathrm{osp}(m|n)]$ the graded commutator is realized by

$$[A,B] = AB - (-1)^{[A][B]}BA$$

and tensor product multiplication is given by

$$(A \otimes B)(C \otimes D) = (-1)^{[B][C]}(AC \otimes BD).$$

Using these conventions, we have the following:

Definition 2.1: The quantum superalgebra $U_q[\mathrm{osp}(m|n)]$ *is generated by simple generators* e_a, f_a, h_a *subject to the relations*

$$[h_a, e_b] = (\alpha_a, \alpha_b)e_b,$$

$$[h_a, f_b] = -(\alpha_a, \alpha_b)f_b,$$

$$[h_a, h_b] = 0,$$

$$[e_a, f_b] = \delta_b^a \frac{(q^{h_a} - q^{-h_a})}{(q - q^{-1})},$$

$$[e_a, e_a] = [f_a, f_a] = 0 \quad \text{for } (\alpha_a, \alpha_a) = 0,$$

We remark that $U_q[\mathrm{osp}(m|n)]$ *has the structure of a quasitriangular Hopf superalgebra. In particular, there is a linear mapping known as the coproduct,* $\Delta: U_q[\mathrm{osp}(m|n)] \to U_q[\mathrm{osp}(m|n)]^{\otimes 2}$, *which is defined on the simple generators by*

$$\Delta(e_a) = q^{1/2h_a} \otimes e_a + e_a \otimes q^{-1/2h_a},$$

$$\Delta(f_a) = q^{1/2h_a} \otimes f_a + f_a \otimes q^{-1/2h_a},$$

$$\Delta(q^{\pm 1/2h_a}) = q^{\pm 1/2h_a} \otimes q^{\pm 1/2h_a},$$

and extends to arbitrary elements according to the homomorphism property, namely,

$$\Delta(AB) = \Delta(A)\Delta(B).$$

There are further defining relations such as the q-Serre relations, but they are not needed in this paper.

The quasitriangular property guarantees the existence of a universal R-matrix, which provides a solution to the Yang-Baxter equation. Before elaborating, we need to introduce the graded twist map.

The *graded twist map* $T: U_q[\mathrm{osp}(m|n)]^{\otimes 2} \to U_q[\mathrm{osp}(m|n)]^{\otimes 2}$ is given by

$$T(a \otimes b) = (-1)^{[a][b]}(b \otimes a).$$

For convenience, $T \circ \Delta$, the twist map composed with the coproduct, is denoted Δ^T. Then a *universal R-matrix*, $\mathcal{R}$, is an even, nonsingular element of $U_q[\mathrm{osp}(m|n)]^{\otimes 2}$ satisfying the following properties:

TABLE I. The action of the vector representation π on the simple generators of $U_q[\mathrm{osp}(m|n)]$.

α_a	$\pi(e_a)$	$\pi(f_a)$	$\pi(h_a)$
$\alpha_i, 1 \leqslant i < l$	$E^{i}_{i+1} - E^{\overline{i+1}}_{\bar{i}}$	$E^{i+1}_{i} - E^{\bar{i}}_{\overline{i+1}}$	$E^{i}_{i} - E^{\bar{i}}_{\bar{i}} - E^{i+1}_{i+1} + E^{\overline{i+1}}_{\overline{i+1}}$
$\alpha_l, m = 2l$	$E^{l-1}_{\bar{l}} - E^{l}_{\overline{l-1}}$	$E^{\bar{l}}_{l-1} - E^{\overline{l-1}}_{l}$	$E^{l-1}_{l-1} + E^{l}_{l} - E^{\overline{l-1}}_{\overline{l-1}} - E^{\bar{l}}_{\bar{l}}$
$\alpha_l, m = 2l+1$	$E^{l}_{l+1} - E^{l+1}_{\bar{l}}$	$E^{l+1}_{l} - E^{\bar{l}}_{l+1}$	$E^{l}_{l} - E^{\bar{l}}_{\bar{l}}$
$\alpha_\mu, 1 \leqslant \mu < k$	$E^{\mu}_{\mu+1} + E^{\overline{\mu+1}}_{\bar{\mu}}$	$E^{\mu+1}_{\mu} + E^{\bar{\mu}}_{\overline{\mu+1}}$	$E^{\mu+1}_{\mu+1} - E^{\overline{\mu+1}}_{\overline{\mu+1}} - E^{\mu}_{\mu} + E^{\bar{\mu}}_{\bar{\mu}}$
α_s	$E^{\mu=k}_{i=1} + (-1)^k E^{\overline{i=1}}_{\overline{\mu=k}}$	$-E^{i=1}_{\mu=k} + (-1)^k E^{\overline{\mu=k}}_{\overline{i=1}}$	$-E^{i=1}_{i=1} + E^{\bar{i}=1}_{\bar{i}=1} - E^{\mu=k}_{\mu=k} + E^{\bar{\mu}=\bar{k}}_{\bar{\mu}=\bar{k}}$

$$\mathcal{R}\Delta(a) = \Delta^T(a)\mathcal{R}, \quad \forall\, a \in U_q[\mathrm{osp}(m|n)],$$

$$(\mathrm{id} \otimes \Delta)\mathcal{R} = \mathcal{R}_{13}\mathcal{R}_{12},$$

$$(\Delta \otimes \mathrm{id})\mathcal{R} = \mathcal{R}_{13}\mathcal{R}_{23}. \tag{2}$$

Here $\mathcal{R}_{ab}$ represents a copy of $\mathcal{R}$ acting on the a and b components, respectively, of $U_1 \otimes U_2 \otimes U_3$, where each U is a copy of the quantum superalgebra $U_q[\mathrm{osp}(m|n)]$. When $a > b$ the usual grading term from the twist map is included, so, for example, $\mathcal{R}_{21} = [\mathcal{R}^T]_{12}$, where $\mathcal{R}^T = T(\mathcal{R})$ is the *opposite universal R-matrix*.

The *R*-matrix is significant because it is a solution to the Yang-Baxter equation, which is prominent in the study of integrable systems,[20]

$$\mathcal{R}_{12}\mathcal{R}_{13}\mathcal{R}_{23} = \mathcal{R}_{23}\mathcal{R}_{13}\mathcal{R}_{12}.$$

A superalgebra may contain many different universal *R*-matrices, but there is always a unique one belonging to $U_q[\mathrm{osp}(m|n)]^- \otimes U_q[\mathrm{osp}(m|n)]^+$, with its opposite *R*-matrix in $U_q[\mathrm{osp}(m|n)]^+ \otimes U_q[\mathrm{osp}(m|n)]^-$. Here $U_q[\mathrm{osp}(m|n)]^-$ is the Hopf subsuperalgebra generated by the lowering generators $\{f_a\}$ and Cartan elements $\{h_a\}$, while $U_q[\mathrm{osp}(m|n)]^+$ is generated by the raising generators $\{e_a\}$ and the Cartan elements. These particular *R*-matrices arise out of the $\mathbb{Z}_2$-graded version of Drinfeld's double construction.[21] In this paper we consider the universal *R*-matrix belonging to $U_q[\mathrm{osp}(m|n)]^- \otimes U_q[\mathrm{osp}(m|n)]^+$.

We also need to define the vector representation for $U_q[\mathrm{osp}(m|n)]$. Let End V be the space of endomorphisms of V, an $(m+n)$-dimensional vector space. Then the irreducible *vector representation* $\pi: U_q[\mathrm{osp}(m|n)] \to \mathrm{End}\ V$ acts on the $U_q[\mathrm{osp}(m|n)]$ generators as given in Table I, where E^a_b is the elementary matrix with a 1 in the (a,b) position and zeroes elsewhere.

One quantity that repeatedly arises in calculations for both classical and quantum Lie superalgebras is ρ, the *graded half-sum of positive roots*. In the case of $U_q[\mathrm{osp}(m|n)]$ it is given by

$$\rho = \frac{1}{2}\sum_{i=1}^{l}(m-2i)\varepsilon_i + \frac{1}{2}\sum_{\mu=1}^{k}(n-m+2-2\mu)\delta_\mu.$$

This satisfies the property $(\rho, \alpha) = \frac{1}{2}(\alpha, \alpha)$ for all simple roots α.

The Lax operator for $U_q[\mathrm{osp}(m|n)]$: Let $\mathcal{R}$ be the universal *R*-matrix of $U_q[\mathrm{osp}(m|n)]$ and π the vector representation. The Lax operator associated with $\mathcal{R}$ is given by

$$R = (\pi \otimes \mathrm{id})\mathcal{R} \in (\mathrm{End}\ V) \otimes U_q[\mathrm{osp}(m|n)].$$

It has been shown in Ref. 11 that the Lax operator is given by

$$R = \sum_a E_a^a \otimes q^{h_{\varepsilon_a}} + (q - q^{-1}) \sum_{\varepsilon_a < \varepsilon_b} (-1)^{[b]} E_b^a \otimes q^{h_{\varepsilon_a}} \hat{\sigma}_{ba},$$

where the simple operators $\hat{\sigma}_{ba}$ are given by

$$\hat{\sigma}_{ii+1} = -\hat{\sigma}_{\overline{i+1}\,\overline{i}} = q^{1/2} e_i q^{1/2h_i}, \quad 1 \leqslant i < l,$$

$$\hat{\sigma}_{l-1\bar{l}} = -\hat{\sigma}_{l\overline{l-1}} = q^{1/2} e_l q^{1/2h_l}, \quad m = 2l,$$

$$\hat{\sigma}_{l\bar{l}} = 0, \quad m = 2l,$$

$$\hat{\sigma}_{ll+1} = -q^{-1/2} \hat{\sigma}_{l+1\bar{l}} = e_l q^{1/2h_l}, \quad m = 2l+1,$$

$$\hat{\sigma}_{\mu\mu+1} = \hat{\sigma}_{\overline{\mu+1}\,\bar{\mu}} = q^{-1/2} e_\mu q^{1/2h_\mu}, \quad 1 \leqslant \mu < k,$$

$$\hat{\sigma}_{\mu=ki=1} = (-1)^k q \hat{\sigma}_{i=\bar{1}\,\bar{\mu}=\bar{k}} = q^{1/2} e_s q^{1/2h_s};$$

and the remaining operators can be calculated using the following:

(i) the q-commutation relations,

$$q^{(\alpha_c, \varepsilon_b)} \hat{\sigma}_{ba} e_c q^{1/2h_c} - (-1)^{([a]+[b])[c]} q^{-(\alpha_c, \varepsilon_a)} e_c q^{1/2h_c} \hat{\sigma}_{ba} = 0, \quad \varepsilon_b > \varepsilon_a,$$

where neither $\varepsilon_a - \alpha_c$ nor $\varepsilon_b + \alpha_c$ equals any ε_x; and

(ii) the induction relations

$$\hat{\sigma}_{ba} = q^{-(\varepsilon_b, \varepsilon_a)} \hat{\sigma}_{bc} \hat{\sigma}_{ca} - q^{-(\varepsilon_c, \varepsilon_c)} (-1)^{([b]+[c])([a]+[c])} \hat{\sigma}_{ca} \hat{\sigma}_{bc}, \quad \varepsilon_b > \varepsilon_c > \varepsilon_a,$$

where $c \neq \bar{b}$ or $\bar{a}$.

To define the opposite Lax operator $R^T = (\pi \otimes \mathrm{id})\mathcal{R}$ we require the graded conjugation action †, which is defined on the simple generators by (see Ref. 11)

$$e_a^\dagger = f_a, \quad f_a^\dagger = (-1)^{[a]} e_a, \quad h_a^\dagger = h_a.$$

It is consistent with the coproduct and extends naturally to all remaining elements of $U_q[\mathrm{osp}(m|n)]$, satisfying the following properties:

$$(\hat{\sigma}_{ab})^\dagger = (-1)^{[a]([a]+[b])} \hat{\sigma}_{ba},$$

$$(ab)^\dagger = (-1)^{[a][b]} b^\dagger a^\dagger,$$

$$(a \otimes b)^\dagger = a^\dagger \otimes b^\dagger,$$

$$\Delta(a)^\dagger = \Delta(a^\dagger).$$

Then the opposite R-matrix is given by

$$R^T = \sum_a E_a^a \otimes q^{h_{\varepsilon_a}} + (q - q^{-1}) \sum_{\varepsilon_b > \varepsilon_a} (-1)^{[a]} E_a^b \otimes \hat{\sigma}_{ab} q^{h_{\varepsilon_a}},$$

where

$$\hat{\sigma}_{ab} = (-1)^{[b]([a]+[b])} \hat{\sigma}_{ba}^\dagger, \quad \varepsilon_b > \varepsilon_a.$$

III. CASIMIR INVARIANTS OF $U_q[\mathrm{osp}(m|n)]$

We now use the Lax operator to construct a family of Casimir invariants and then to calculate their eigenvalues when acting on an irreducible highest weight module. Before constructing the Casimir invariants, however, we need to define a new object. Let h_ρ be the unique element of the Cartan subalgebra H satisfying

$$\alpha_i(h_\rho) = (\rho, \alpha_i), \quad \forall\ \alpha_i \in H^*.$$

Then from Ref. 10 we have the following theorem.

Theorem 3.1: *Let $\mathcal{V}$ be the representation space of τ, an arbitrary finite-dimensional representation of $U_q[\mathrm{osp}(m|n)]$. If $\Gamma \in (\mathrm{End}\ \mathcal{V}) \otimes U_q[\mathrm{osp}(m|n)]$ satisfies*

$$\partial(a)\Gamma = \Gamma\partial(a), \quad \forall\ a \in U_q[\mathrm{osp}(m|n)], \tag{3}$$

where $\partial \equiv (\pi \otimes \mathrm{id})\Delta$, then

$$C = (\mathrm{str} \otimes \mathrm{id})(\tau(q^{2h_\rho}) \otimes I)\Gamma,$$

belongs to the center of $U_q[\mathrm{osp}(m|n)]$. Above str denotes the supertrace.

Now choose τ to be the vector representation π. Recalling that the universal R-matrix satisfies

$$\mathcal{R}\Delta(a) = \Delta^T(a)\mathcal{R}, \quad \forall\ a \in U_q[\mathrm{osp}(m|n)],$$

it is clear that

$$\partial(a)R^TR = R^TR\partial(a), \quad \forall\ a \in U_q[\mathrm{osp}(m|n)].$$

Hence if we set $A \in (\mathrm{End}\ V) \otimes U_q[\mathrm{osp}(m|n)]$ to be

$$A = \frac{(R^TR - I \otimes I)}{(q - q^{-1})},$$

the operators A^l will satisfy condition (3) for all non-negative integers l. Thus the operators C_l defined as

$$C_l = (\mathrm{str} \otimes \mathrm{id})(\pi(q^{2h_\rho}) \otimes I)A^l, \quad l \in \mathbb{Z}^+,$$

form a family of Casimir invariants. Here A coincides with the matrix of Jarvis and Green[22] in the classical limit $q \to 1$, as do the invariants C_l.

Now write the Lax operator R and its opposite R^T in the form

$$R = I \otimes I + (q - q^{-1}) \sum_{\varepsilon_b \geqslant \varepsilon_a} E_b^a \otimes X_a^b,$$

$$R^T = I \otimes I + (q - q^{-1}) \sum_{\varepsilon_b \leqslant \varepsilon_a} E_b^a \otimes X_a^b.$$

In terms of the operators $\hat{\sigma}_{ba}$, this implies

$$X_a^b = \begin{cases} \dfrac{q^{h_{\varepsilon_a}} - I}{q - q^{-1}}, & a = b, \\ (-1)^{[b]} q^{h_{\varepsilon_a}} \hat{\sigma}_{ba}, & \varepsilon_a < \varepsilon_b, \\ (-1)^{[b]} \hat{\sigma}_{ba} q^{h_{\varepsilon_b}}, & \varepsilon_a > \varepsilon_b. \end{cases}$$

Writing A as

$$A = \sum_{a,b} E_b^a \otimes A_a^b,$$

we obtain

$$A_a^b = (1 + \delta_b^a) X_a^b + (q - q^{-1}) \sum_{\varepsilon_c \leqslant \varepsilon_a, \varepsilon_b} (-1)^{([a]+[c])([b]+[c])} X_a^c X_c^b.$$

This produces a family of Casimir invariants

$$C_l = \sum_a (-1)^{[a]} q^{(2\rho, \varepsilon_a)} A^{(l)a}_{\ \ a},$$

where the operators $A^{(l)b}_{\ \ a}$ are recursively defined as

$$A^{(l)b}_{\ \ a} = \sum_c (-1)^{([a]+[c])([b]+[c])} A^{(l-1)c}_{\ \ a} A_c^b. \tag{4}$$

Note that A corresponds to the matrix A given for the nongraded case in Ref. 23. Following a line of reasoning similar to that in Ref. 24 it can be shown that when acting on an irreducible module $V(\Lambda)$, A satisfies the following polynomial identity:

$$\prod_{a=1}^{m+n} (A - \alpha_a(\Lambda) I) = 0,$$

where

$$\alpha_a(\Lambda) = \frac{q^{(\varepsilon_a, \varepsilon_a + 2\Lambda + 2\rho) - C(\Lambda_0)} - 1}{q - q^{-1}}$$

and $C(\Lambda_0) = (\delta_1, \delta_1 + 2\rho) = m - n - 1$. In the limit $q \to 1$ this reduces to the identity given in Ref. 24.

IV. EIGENVALUES OF THE CASIMIR INVARIANTS

Now that we have found a family of Casimir invariants, we wish to calculate their eigenvalues on a general irreducible finite-dimensional module. Let $V(\Lambda)$ be an arbitrary irreducible finite-dimensional module with highest weight Λ and highest weight state $|\Lambda\rangle$. Define $t_a^{(l)}$ to be the eigenvalue of $A^{(l)a}_{\ \ a}$ on this state, so

$$A^{(l)a}_{\ \ a} |\Lambda\rangle = t_a^{(l)} |\Lambda\rangle.$$

Once we have calculated $t_a^{(l)}$ we will use this result to find the eigenvalues of the Casimir invariants C_l.

To evaluate $t_a^{(l)}$, note that if $\varepsilon_b > \varepsilon_a$ then $A^{(l)b}_{\ \ a}$ is a raising operator, implying $A^{(l)b}_{\ \ a} |\Lambda\rangle = 0$. Thus from Eq. (4) we deduce

$$\begin{aligned} t_a^{(l)} |\Lambda\rangle &= t_a^{(l-1)} t_a^{(1)} |\Lambda\rangle + \sum_{\varepsilon_a < \varepsilon_b} (-1)^{[a]+[b]} A^{(l-1)b}_{\ \ a} A_b^a |\Lambda\rangle \\ &= t_a^{(l-1)} t_a^{(1)} |\Lambda\rangle + \sum_{\varepsilon_a < \varepsilon_b} (-1)^{[a]+[b]} A^{(l-1)b}_{\ \ a} [X_b^a + (q - q^{-1}) X_b^a X_a^a] |\Lambda\rangle \\ &= t_a^{(l-1)} t_a^{(1)} |\Lambda\rangle + \sum_{\varepsilon_a < \varepsilon_b} (-1)^{[a]+[b]} q^{(\Lambda, \varepsilon_a)} A^{(l-1)b}_{\ \ a} X_b^a |\Lambda\rangle. \end{aligned}$$

Now we know that

$$A^l\partial(X_b^a) = \partial(X_b^a)A^l. \tag{5}$$

This can be used to calculate $A^{(l)b}_{\ a}X_b^a|\Lambda\rangle$ for $\varepsilon_a < \varepsilon_b$. First we need an expression for $\Delta(X_b^a)$. The R-matrix properties give

$$(\Delta \otimes I)R = R_{13}R_{23} \Rightarrow (I \otimes \Delta)R^T = R_{12}^T R_{13}^T.$$

In terms of X_b^a, this implies

$$\begin{aligned}
&I \otimes I \otimes I + (q-q^{-1}) \sum_{\varepsilon_a \leqslant \varepsilon_b} E_a^b \otimes \Delta(X_b^a) \\
&= \left(I \otimes I \otimes I + (q-q^{-1}) \sum_{\varepsilon_a \leqslant \varepsilon_b} E_a^b \otimes X_b^a \otimes I\right)\left(I \otimes I \otimes I + (q-q^{-1}) \sum_{\varepsilon_a \leqslant \varepsilon_b} E_a^b \otimes I \otimes X_b^a\right) \\
&= I \otimes I \otimes I + (q-q^{-1}) \sum_{\varepsilon_a \leqslant \varepsilon_b} E_a^b \otimes (X_b^a \otimes I + I \otimes X_b^a) \\
&+ (q-q^{-1})^2 \sum_{\varepsilon_a \leqslant \varepsilon_c \leqslant \varepsilon_b} (-1)^{([a]+[c])([b]+[c])} E_a^b \otimes X_b^c \otimes X_c^a.
\end{aligned}$$

Hence for all $\varepsilon_a < \varepsilon_b$,

$$\Delta(X_b^a) = X_b^a \otimes I + I \otimes X_b^a + (q-q^{-1}) \sum_{\varepsilon_a \leqslant \varepsilon_c \leqslant \varepsilon_b} (-1)^{([a]+[c])([b]+[c])} X_b^c \otimes X_c^a.$$

We also need an expression for $\pi(X_b^a)$ for $\varepsilon_a \leqslant \varepsilon_b$. In Ref. 11 we found the generators for R^T in the vector representation are given by

$$\hat{\sigma}_{ab}q^{h_{\varepsilon_a}} = E_b^a - (-1)^{[a]([a]+[b])}\xi_a\xi_b q^{(\rho,\varepsilon_a-\varepsilon_b)}E_{\bar{a}}^{\bar{b}}, \quad \varepsilon_a < \varepsilon_b.$$

From this we deduce that

$$\pi(X_b^a) = (-1)^{[a]}E_b^a - (-1)^{[a][b]}\xi_a\xi_b q^{(\rho,\varepsilon_a-\varepsilon_b)}E_{\bar{a}}^{\bar{b}}, \quad \varepsilon_a < \varepsilon_b.$$

Also, we know

$$\pi(X_a^a) = (q-q^{-1})^{-1}\pi(q^{h_{\varepsilon_a}} - I) = (q-q^{-1})^{-1}(q^{(\varepsilon_a,\varepsilon_a)(E_a^a - E_{\bar{a}}^{\bar{a}})} - I).$$

Applying these, we find that if $\varepsilon_a < \varepsilon_b$ then

$$\begin{aligned}
\partial(X_b^a) &= (\pi \otimes I)\Delta(X_b^a) = \pi(X_b^a) \otimes (I + (q-q^{-1})X_a^a) + (I + (q-q^{-1})\pi(X_b^b)) \otimes X_b^a \\
&+ (q-q^{-1}) \sum_{\varepsilon_a < \varepsilon_c < \varepsilon_b} (-1)^{([a]+[c])([b]+[c])} \pi(X_b^c) \otimes X_c^a \\
&= ((-1)^{[a]}E_b^a - (-1)^{[a][b]}\xi_a\xi_b q^{(\rho,\varepsilon_a-\varepsilon_b)}E_{\bar{a}}^{\bar{b}}) \otimes q^{h_{\varepsilon_a}} + q^{(\varepsilon_b,\varepsilon_b)(E_b^b - E_{\bar{b}}^{\bar{b}})} \otimes X_b^a \\
&+ (q-q^{-1}) \sum_{\varepsilon_a < \varepsilon_c < \varepsilon_b} (-1)^{([a]+[c])([b]+[c])} \\
&\times ((-1)^{[c]}E_b^c - (-1)^{[b][c]}\xi_b\xi_c q^{(\rho,\varepsilon_c-\varepsilon_b)}E_{\bar{c}}^{\bar{b}}) \otimes X_c^a.
\end{aligned}$$

Substituting this expression into Eq. (5) and equating the (a,b) entries, we find

$$
\begin{aligned}
&(-1)^{[a]}A^{(l)a}{}_{a}q^{h_{\varepsilon_a}} - \delta^{a}_{\bar{b}}(-1)^{[a][b]}\xi_a\xi_b q^{(\rho,\varepsilon_a-\varepsilon_b)}A^{(l)a}{}_{a}q^{h_{\varepsilon_a}} + q^{(\varepsilon_b,\varepsilon_b)}A^{(l)b}{}_{a}X^{a}_{b} \\
&\quad + (q-q^{-1})\sum_{\varepsilon_a<\varepsilon_c<\varepsilon_b}((-1)^{[c]}A^{(l)c}{}_{a}X^{a}_{c} - \delta^{b}_{\bar{c}}(-1)^{[b][c]}\xi_b\xi_c q^{(\rho,\varepsilon_c-\varepsilon_b)}A^{(l)\bar{b}}{}_{a}X^{a}_{c}) \\
&= (-1)^{[a]}q^{h_{\varepsilon_a}}A^{(l)b}{}_{b} - \delta^{a}_{\bar{b}}(-1)^{[a][b]}\xi_a\xi_b q^{(\rho,\varepsilon_a-\varepsilon_b)}q^{h_{\varepsilon_a}}A^{(l)b}{}_{b} + (-1)^{[a]+[b]}q^{(\varepsilon_a,\varepsilon_b)}X^{a}_{b}A^{(l)b}{}_{a} \\
&\quad - (q-q)^{-1}\delta^{a}_{\bar{b}}\sum_{\varepsilon_a<\varepsilon_c<\varepsilon_b}(-1)^{[b][c]}\xi_b\xi_c q^{(\rho,\varepsilon_c-\varepsilon_b)}X^{a}_{c}A^{(l)b}{}_{\bar{c}}.
\end{aligned}
$$

Simplifying gives

$$
\begin{aligned}
&(-1)^{[a]+[b]}q^{(\varepsilon_a,\varepsilon_b)}X^{a}_{b}A^{(l)b}{}_{a} - q^{(\varepsilon_b,\varepsilon_b)}A^{(l)b}{}_{a}X^{a}_{b} \\
&\quad = ((-1)^{[a]} - \delta^{a}_{\bar{b}}q^{(\rho,\varepsilon_a-\varepsilon_b)})q^{h_{\varepsilon_a}}(A^{(l)a}{}_{a} - A^{(l)b}{}_{b}) \\
&\qquad + (q-q^{-1})\sum_{\varepsilon_a<\varepsilon_c<\varepsilon_b}((-1)^{[c]} - \delta^{b}_{\bar{c}}q^{(\rho,\varepsilon_c-\varepsilon_b)})A^{(l)c}{}_{a}X^{a}_{c} \\
&\qquad + (q-q^{-1})\delta^{a}_{\bar{b}}\sum_{\varepsilon_a<\varepsilon_c<\varepsilon_b}(-1)^{[b][c]}\xi_b\xi_c q^{(\rho,\varepsilon_c-\varepsilon_b)}X^{a}_{c}A^{(l)\bar{a}}{}_{\bar{c}}.
\end{aligned}
$$

Remembering that $\varepsilon_a<\varepsilon_b$, we apply this to the highest weight state $|\Lambda\rangle$ to obtain

$$
\begin{aligned}
-q^{(\varepsilon_b,\varepsilon_b)}A^{(l)b}{}_{a}X^{a}_{b}|\Lambda\rangle &= q^{(\Lambda,\varepsilon_a)}((-1)^{[a]} - \delta^{a}_{\bar{b}}q^{2(\rho,\varepsilon_a)})(t^{(l)}_{a} - t^{(l)}_{b})|\Lambda\rangle \\
&\quad + (q-q^{-1})\sum_{\varepsilon_a<\varepsilon_c<\varepsilon_b}((-1)^{[c]} - \delta^{b}_{\bar{c}}q^{2(\rho,\varepsilon_c)})A^{(l)c}{}_{a}X^{a}_{c}|\Lambda\rangle. \qquad (6)
\end{aligned}
$$

The next step is to calculate $A^{(l)b}{}_{a}X^{a}_{b}|\Lambda\rangle$ for $\varepsilon_a<\varepsilon_b$. It is first convenient to order the indices according to $b>c\Leftrightarrow\varepsilon_b<\varepsilon_c$. With this ordering we say an element $a>0$ if $\varepsilon_a<0$, $a=0$ if $\varepsilon_a=0$, and $a<0$ if $\varepsilon_a>0$. Using this convention, it is apparent the solution to (6) will be of the form

$$
A^{(l)b}{}_{a}X^{a}_{b}|\Lambda\rangle = q^{(\Lambda,\varepsilon_a)}(-1)^{[a]}\sum_{a>c\geq b}\alpha^{a}_{bc}(t^{(l)}_{a} - t^{(l)}_{c})|\Lambda\rangle, \qquad (7)
$$

where α^{a}_{bc} is a function of a, b, and c. Now from Eq. (6) we have

$$
\begin{aligned}
&(q-q^{-1})\sum_{a>c>b}(-1)^{[c]}A^{(l)c}{}_{a}X^{a}_{c}|\Lambda\rangle \\
&\quad = -q^{(\varepsilon_b,\varepsilon_b)}A^{(l)b}{}_{a}X^{a}_{b}|\Lambda\rangle + (q-q^{-1})\sum_{a>c>b}\delta^{b}_{\bar{c}}q^{-2(\rho,\varepsilon_b)}A^{(l)c}{}_{a}X^{a}_{c}|\Lambda\rangle \\
&\qquad - (-1)^{[a]}q^{(\Lambda,\varepsilon_a)}(1-\delta^{a}_{\bar{b}}(-1)^{[a]}q^{2(\rho,\varepsilon_a)})(t^{(l)}_{a} - t^{(l)}_{b})|\Lambda\rangle \\
&\quad = -q^{(\varepsilon_{b+1},\varepsilon_{b+1})}A^{(l)b+1}{}_{a}X^{a}_{b+1}|\Lambda\rangle \\
&\qquad + (q-q^{-1})\sum_{a>c>b+1}\delta^{b+1}_{\bar{c}}q^{-2(\rho,\varepsilon_{b+1})}A^{(l)c}{}_{a}X^{a}_{c}|\Lambda\rangle \\
&\qquad - (-1)^{[a]}q^{(\Lambda,\varepsilon_a)}(1-\delta^{b+1}_{\bar{a}}(-1)^{[a]}q^{2(\rho,\varepsilon_a)})(t^{(l)}_{a} - t^{(l)}_{b+1})|\Lambda\rangle \\
&\qquad + (q-q^{-1})(-1)^{[b+1]}A^{(l)b+1}{}_{a}X^{a}_{b+1}|\Lambda\rangle.
\end{aligned}
$$

Substituting in the form of the solution given in Eq. (7) produces

$$
\begin{aligned}
& q^{(\varepsilon_b,\varepsilon_b)} \sum_{a>d\geqslant b} \alpha^a_{bd}(t^{(l)}_a - t^{(l)}_d)|\Lambda\rangle \\
&\quad = (q^{(\varepsilon_{b+1},\varepsilon_{b+1})} - (q-q^{-1})(-1)^{[b+1]}) \sum_{a>d\geqslant b+1} \alpha^a_{(b+1)d}(t^{(l)}_a - t^{(l)}_d)|\Lambda\rangle \\
&\qquad - (1-\delta^a_{\bar{b}}(-1)^{[a]}q^{2(\rho,\varepsilon_a)})(t^{(l)}_a - t^{(l)}_b)|\Lambda\rangle + (1-\delta^a_{\overline{b+1}}(-1)^{[a]}q^{2(\rho,\varepsilon_a)})(t^{(l)}_a - t^{(l)}_{b+1})|\Lambda\rangle \\
&\qquad + (q-q^{-1}) \sum_{a>c>b} \delta^b_{\bar{c}} q^{-2(\rho,\varepsilon_b)} \sum_{a>d\geqslant c} \alpha^a_{\bar{b}d}(t^{(l)}_a - t^{(l)}_d)|\Lambda\rangle \\
&\qquad - (q-q^{-1}) \sum_{a>c>b+1} \delta^{b+1}_{\bar{c}} q^{-2(\rho,\varepsilon_{b+1})} \sum_{a>d\geqslant c} \alpha^a_{\overline{(b+1)}d}(t^{(l)}_a - t^{(l)}_d)|\Lambda\rangle. \qquad (8)
\end{aligned}
$$

Set

$$\alpha^a_{bd} = \bar{\alpha}_{bd}(1-\delta^a_{\bar{d}}(-1)^{[a]}q^{2(\rho,\varepsilon_a)}).$$

Then from Eq. (8) we obtain

$$\bar{\alpha}_{bb} = -q^{-(\varepsilon_b,\varepsilon_b)}$$

and

$$
\begin{aligned}
\bar{\alpha}_{b(b+1)} &= q^{-(\varepsilon_b,\varepsilon_b)}[(q^{(\varepsilon_{b+1},\varepsilon_{b+1})} - (q-q^{-1})(-1)^{[b+1]})\bar{\alpha}_{(b+1)(b+1)} + 1 + (q-q^{-1})\delta^b_{\overline{b+1}}q^{-2(\rho,\varepsilon_b)}\bar{\alpha}_{\bar{b}(b+1)}] \\
&= q^{-(\varepsilon_b,\varepsilon_b)-(\varepsilon_{b+1},\varepsilon_{b+1})}(q-q^{-1})((-1)^{[b+1]} - \delta^b_{\overline{b+1}}q^{-2(\rho,\varepsilon_b)}).
\end{aligned}
$$

To simplify this expression note that $q^{2(\rho,\varepsilon_{b+1}-\varepsilon_b)} = q^{-(\varepsilon_b,\varepsilon_b)-(\varepsilon_{b+1},\varepsilon_{b+1})}$ in all cases except for $[b]=0$, $b=l$, $m=2l$, in which case $q^{2(\rho,\varepsilon_{b+1}-\varepsilon_b)} = q^2 q^{-(\varepsilon_b,\varepsilon_b)-(\varepsilon_{b+1},\varepsilon_{b+1})}$. However $[b]=0$, $b=l$, $m=2l$ if and only if $\delta^b_{\overline{b+1}}=1$, and in that case we find $\bar{\alpha}_{b(b+1)}=0$. Hence for all values of b we can write

$$\bar{\alpha}_{b(b+1)} = (q-q^{-1})q^{-2(\rho,\varepsilon_b)}((-1)^{[b+1]}q^{2(\rho,\varepsilon_{b+1})} - \delta^b_{\overline{b+1}}).$$

Now that we have found $\bar{\alpha}_{bb}$ and $\bar{\alpha}_{b(b+1)}$, they can be used to calculate the remaining $\bar{\alpha}_{bd}$. From Eq. (8) we observe that if $d>b+1$ then

$$
\begin{aligned}
\bar{\alpha}_{bd} &= q^{-(\varepsilon_b,\varepsilon_b)}(q^{(\varepsilon_{b+1},\varepsilon_{b+1})} - (q-q^{-1})(-1)^{[b+1]})\bar{\alpha}_{(b+1)d} + (q-q^{-1})q^{-(\varepsilon_b,\varepsilon_b)} \sum_{d\geqslant c>b} \delta^b_{\bar{c}} q^{-2(\rho,\varepsilon_b)}\bar{\alpha}_{\bar{b}d} \\
&\quad - (q-q^{-1})q^{-(\varepsilon_b,\varepsilon_b)} \sum_{d\geqslant c>b+1} \delta^{b+1}_{\bar{c}} q^{-2(\rho,\varepsilon_{b+1})}\bar{\alpha}_{\overline{(b+1)}d}. \qquad (9)
\end{aligned}
$$

Now define θ_{xy} by

$$\theta_{xy} = \begin{cases} 1, & x<y, \\ 0, & x\geqslant y. \end{cases}$$

Then Eq. (9) can be rewritten as

$$
\begin{aligned}
\bar{\alpha}_{bd} &= q^{-(\varepsilon_b,\varepsilon_b)}(q^{(\varepsilon_{b+1},\varepsilon_{b+1})} - (q-q^{-1})(-1)^{[b+1]})\bar{\alpha}_{(b+1)d} \\
&\quad + (q-q^{-1})q^{-(\varepsilon_b,\varepsilon_b)}q^{2(\rho,\varepsilon_c)}(\theta_{bc}\theta_{c(d+1)}\delta^b_{\bar{c}} - \theta_{(b+1)c}\theta_{c(d+1)}\delta^{b+1}_{\bar{c}})\bar{\alpha}_{cd}, \quad d>a+1. \qquad (10)
\end{aligned}
$$

Consider $\bar{\alpha}_{bd}$ for any $b>l$. Both $\theta_{b\bar{b}}$ and $\theta_{(b+1)(\overline{b+1})}$ will equal 0, so

$$\bar{\alpha}_{bd} = q^{-(\varepsilon_b,\varepsilon_b)}(q^{(\varepsilon_{b+1},\varepsilon_{b+1})} - (q-q^{-1})(-1)^{[b+1]})\bar{\alpha}^a_{(b+1)d}$$
$$= q^{-(\varepsilon_b,\varepsilon_b)}q^{-(\varepsilon_{b+1},\varepsilon_{b+1})}\bar{\alpha}_{(b+1)d} = q^{2(\rho,\varepsilon_{b+1}-\varepsilon_b)}\bar{\alpha}_{(b+1)d}.$$

Since

$$\bar{\alpha}_{(d-1)d} = (-1)^{[d]}(q-q^{-1})q^{2(\rho,\varepsilon_d-\varepsilon_{d-1})},$$

we obtain

$$\bar{\alpha}_{bd} = (-1)^{[d]}(q-q^{-1})q^{2(\rho,\varepsilon_d-\varepsilon_b)}, \quad d>b>l.$$

Substituting this together with our expression for $\bar{\alpha}_{bb}$ into Eq. (10), we find

$$\bar{\alpha}_{bd} = q^{-(\varepsilon_b,\varepsilon_b)}(q^{-(\varepsilon_{b+1},\varepsilon_{b+1})} - \delta^{b+1}_{\overline{b+1}}(q-q^{-1}))\bar{\alpha}_{(b+1)d}$$
$$+ (q-q^{-1})^2 q^{-(\varepsilon_b,\varepsilon_b)}(-1)^{[d]}q^{2(\rho,\varepsilon_d)}(\theta_{b\bar{b}}\theta_{\bar{b}d} - \theta_{(b+1)(\overline{b+1})}\theta_{(\overline{b+1})d})$$
$$- (q-q^{-1})q^{-(\varepsilon_b,\varepsilon_b)}q^{-(\varepsilon_d,\varepsilon_d)}q^{2(\rho,\varepsilon_d)}(\delta^{\bar{b}}_d - \delta^{\overline{b+1}}_d), \quad d>b+1. \tag{11}$$

But for $d>b+1$,

$$\theta_{b\bar{b}}\theta_{\bar{b}d} - \theta_{(b+1)(\overline{b+1})}\theta_{(\overline{b+1})d} = \delta^b_l\theta_{\bar{l}d} - \delta^{\bar{b}}_d\theta_{bl}$$
$$= \delta^b_l(1-\delta^d_{\bar{l}}) - \delta^{\bar{b}}_d(1-\delta^b_l) = \delta^b_l - \delta^{\bar{b}}_d.$$

Also, $-[(-1)^{[d]}(q-q^{-1})+q^{-(\varepsilon_d,\varepsilon_d)}]\delta^{\bar{b}}_d = -q^{(\varepsilon_d,\varepsilon_d)}\delta^{\bar{b}}_d$, so Eq. (11) reduces to

$$\bar{\alpha}_{bd} = (q^{2(\rho,\varepsilon_{b+1}-\varepsilon_b)}q^{-2\delta^b_{\overline{b+1}}} - \delta^{b+1}_{\overline{b+1}}q^{-1}(q-q^{-1}))\bar{\alpha}_{(b+1)d} + \delta^b_l q^{-1}(q-q^{-1})^2(-1)^{[d]}q^{2(\rho,\varepsilon_d)}$$
$$- \delta^{\bar{b}}_d(q-q^{-1})q^{2(\rho,\varepsilon_d)} + \delta^{\overline{b+1}}_d(q-q^{-1})q^{2(\rho,\varepsilon_{b+1}-\varepsilon_b)}q^{-2\delta^b_{\overline{b+1}}}q^{2(\rho,\varepsilon_d)}$$
$$= (q^{2(\rho,\varepsilon_{b+1}-\varepsilon_b)}q^{-2\delta^b_{\overline{b+1}}} - \delta^{b+1}_{\overline{b+1}}q^{-1}(q-q^{-1}))\bar{\alpha}_{(b+1)d} + \delta^b_l q^{-1}(q-q^{-1})^2(-1)^{[d]}q^{2(\rho,\varepsilon_d)}$$
$$+ (q-q^{-1})q^{-2(\rho,\varepsilon_b)}(\delta^{\overline{b+1}}_d - \delta^{\bar{b}}_d), \quad d>b+1.$$

Recall that for $b>l$ we have

$$\bar{\alpha}_{bd} = (-1)^{[d]}(q-q^{-1})q^{2(\rho,\varepsilon_d-\varepsilon_b)}, \quad d>b.$$

Then when $b=l$ we find

$$\bar{\alpha}_{bd} = (q^{2(\rho,\varepsilon_{b+1}-\varepsilon_b)}q^{-2\delta^b_{\overline{b+1}}} - \delta^{b+1}_{\overline{b+1}}q^{-1}(q-q^{-1}))(-1)^{[d]}(q-q^{-1})q^{2(\rho,\varepsilon_d-\varepsilon_{b+1})}$$
$$+ q^{-1}(q-q^{-1})^2(-1)^{[d]}q^{2(\rho,\varepsilon_d)} - (q-q^{-1})q^{-2(\rho,\varepsilon_b)}\delta^{\bar{l}}_d$$
$$= (-1)^{[d]}(q-q^{-1})q^{2(\rho,\varepsilon_d-\varepsilon_b)}[\delta^{b+1}_{\overline{b+1}}(1-(q-q^{-1})+(q-q^{-1}))$$
$$+ \delta^b_{\overline{b+1}}(q^{-2}+q^{-1}(q-q^{-1}))] - (q-q^{-1})q^{-2(\rho,\varepsilon_b)}\delta^{\bar{l}}_d$$
$$= (q-q^{-1})q^{-2(\rho,\varepsilon_b)}((-1)^{[d]}q^{2(\rho,\varepsilon_d)} - \delta^b_{\bar{d}})$$

for all $d>b+1$. Comparing this with our earlier results for $d=b+1$ and $b>l$, we have

$$\bar{\alpha}_{bd} = (q-q^{-1})q^{-2(\rho,\varepsilon_b)}((-1)^{[d]}q^{2(\rho,\varepsilon_d)} - \delta^b_{\bar{d}}), \quad \forall\, b \geqslant l, \quad d>b.$$

But for $b<l$ we know

$$\bar{\alpha}_{bd} = q^{2(\rho,\varepsilon_{b+1}-\varepsilon_b)}\bar{\alpha}_{(b+1)d} + (q-q^{-1})q^{-2(\rho,\varepsilon_b)}(\overline{\delta_d^{b+1}} - \bar{\delta}_d^b), \quad d > b+1.$$

Hence for all b we obtain

$$\bar{\alpha}_{bd} = (q-q^{-1})q^{-2(\rho,\varepsilon_b)}\left((-1)^{[d]}q^{2(\rho,\varepsilon_d)} - \sum_{c=b}^{d-1}\bar{\delta}_d^{\bar{c}} + \sum_{c=b}^{d-2}\overline{\delta_d^{c+1}}\right)$$

$$= (q-q^{-1})q^{-2(\rho,\varepsilon_b)}((-1)^{[d]}q^{2(\rho,\varepsilon_d)} - \bar{\delta}_d^b), \quad d > b.$$

Thus for all $a > b$

$$A^{(l)b}{}_a X_b^a|\Lambda\rangle = q^{(\Lambda,\varepsilon_a)}(-1)^{[a]}\sum_{a>c\geqslant b}\alpha_{bc}^a(t_a^{(l)} - t_c^{(l)})|\Lambda\rangle, \tag{12}$$

where α_{bc}^a is given by

$$\alpha_{bc}^a = \begin{cases} -q^{-(\varepsilon_b,\varepsilon_b)}(1-\delta_{\bar{b}}^a(-1)^{[a]}q^{2(\rho,\varepsilon_a)}), & c=b, \\ (q-q^{-1})q^{-2(\rho,\varepsilon_b)}((-1)^{[c]}q^{2(\rho,\varepsilon_c)} - \bar{\delta}_c^b)(1-\delta_{\bar{c}}^a(-1)^{[a]}q^{2(\rho,\varepsilon_a)}), & c>b. \end{cases}$$

A. Constructing the Perelomov-Popov matrix equation

The expression (12) can now be substituted into the equation

$$t_a^{(l)}|\Lambda\rangle = t_a^{(l-1)}t_a^{(1)}|\Lambda\rangle + \sum_{\varepsilon_a<\varepsilon_b}(-1)^{[a]+[b]}q^{(\Lambda,\varepsilon_a)}A^{(l-1)b}{}_a X_b^a|\Lambda\rangle$$

to find a matrix equation for the various $t_a^{(l)}$. The matrix factor is an analogue of the Perelomov-Popov matrix introduced in Refs. 15 and 16, which was used to calculate the eigenvalues of the Casimir invariants of various classical Lie algebras.

First recall that

$$A_a^b = (1+\delta_b^a)X_a^b + (q-q^{-1})\sum_{c\geqslant a,b}(-1)^{([a]+[c])([b]+[c])}X_a^c X_c^b,$$

where

$$X_a^b = \begin{cases} \dfrac{q^{h_{\varepsilon_a}} - I}{q-q^{-1}}, & a=b, \\ (-1)^{[b]}q^{h_{\varepsilon_a}}\hat{\sigma}_{ba}, & \varepsilon_a < \varepsilon_b, \\ (-1)^{[b]}\hat{\sigma}_{ba}q^{h_{\varepsilon_b}}, & \varepsilon_a > \varepsilon_b. \end{cases}$$

Then

$$A_a^a|\Lambda\rangle = 2X_a^a|\Lambda\rangle + (q-q^{-1})X_a^a X_a^a|\Lambda\rangle = (q-q^{-1})^{-1}(2(q^{h_{\varepsilon_a}}-1) + (q^{h_{\varepsilon_a}}-1)^2)|\Lambda\rangle$$

$$t_a^{(1)} = \frac{q^{2(\Lambda,\varepsilon_a)}-1}{q-q^{-1}}.$$

Hence we obtain

$$t_a^{(l)} = \frac{(q^{2(\Lambda,\varepsilon_a)}-1)}{(q-q^{-1})} t_a^{(l-1)} + \sum_{b<a} (-1)^{[a]+[b]} q^{(\Lambda,\varepsilon_a)} \left(q^{(\Lambda,\varepsilon_a)} (-1)^{[a]} \sum_{b\leqslant c<a} \alpha_{bc}^a (t_a^{(l-1)} - t_c^{(l-1)}) \right)$$

$$= \frac{(q^{2(\Lambda,\varepsilon_a)}-1)}{(q-q^{-1})} t_a^{(l-1)} - q^{2(\Lambda,\varepsilon_a)} \sum_{b<a} (-1)^{[b]} q^{-(\varepsilon_b,\varepsilon_b)} (1-\delta_{\bar{b}}^a (-1)^{[a]} q^{2(\rho,\varepsilon_a)}) (t_a^{(l-1)} - t_b^{(l-1)})$$

$$+ (q-q^{-1}) q^{2(\Lambda,\varepsilon_a)} \sum_{c<b<a} (-1)^{[c]} q^{-2(\rho,\varepsilon_c)} (1-\delta_{\bar{b}}^a (-1)^{[a]} q^{2(\rho,\varepsilon_a)})$$

$$\times ((-1)^{[b]} q^{2(\rho,\varepsilon_b)} - \delta_{\bar{c}}^b)(t_a^{(l-1)} - t_b^{(l-1)}).$$

Now consider the function γ_b defined by

$$\gamma_b = (-1)^{[b]} q^{-(\varepsilon_b,\varepsilon_b)} - (q-q^{-1}) \sum_{c<b} (-1)^{[c]} q^{-2(\rho,\varepsilon_c)} ((-1)^{[b]} q^{2(\rho,\varepsilon_b)} - \delta_{\bar{c}}^b)).$$

We evaluate this for all b, remembering that $C(\Lambda_0) = (\delta_1, \delta_1 + 2\rho) = m-n-1$ and

$$\rho = \frac{1}{2} \sum_{i=1}^{l} (m-2i)\varepsilon_i + \frac{1}{2} \sum_{\mu=1}^{k} (n-m+2-2\mu)\delta_\mu.$$

We find

$$\gamma_b = (-1)^{[b]} q^{2(\rho,\varepsilon_b)} q^{-C(\Lambda_0)}$$

for all values of b. We also consider the function

$$\beta_a = 1 - (q-q^{-1}) \sum_{b<a} \gamma_b (1 - \delta_{\bar{b}}^a (-1)^{[a]} q^{2(\rho,\varepsilon_a)}),$$

so that

$$t_a^{(l)} = \frac{(q^{2(\Lambda,\varepsilon_a)}\beta_a - 1)}{(q-q^{-1})} t_a^{(l-1)} + q^{2(\Lambda,\varepsilon_a)} \sum_{b<a} \gamma_b (1 - \delta_{\bar{b}}^a (-1)^{[a]} q^{2(\rho,\varepsilon_a)}) t_b^{(l-1)}. \tag{13}$$

Again, by considering the various cases individually we find

$$\beta_a = q^{(\varepsilon_a, 2\rho+\varepsilon_a) - C(\Lambda_0)}$$

for any a, regardless of whether m is even or odd. Substituting this result together with that for γ_b into Eq. (13) gives

$$t_a^{(l)} = \frac{(q^{(\varepsilon_a, 2\Lambda+2\rho+\varepsilon_a) - C(\Lambda_0)} - 1)}{(q-q^{-1})} t_a^{(l-1)} + q^{(2\Lambda,\varepsilon_a) - C(\Lambda_0)} \sum_{b<a} (-1)^{[b]} q^{(2\rho,\varepsilon_b)} (1 - \delta_{\bar{b}}^a (-1)^{[a]} q^{(2\rho,\varepsilon_a)}) t_b^{(l-1)}.$$

This can be written in the matrix form

$$\underline{t}^{(l)} = M \underline{t}^{(l-1)},$$

where M is a lower triangular matrix with entries

$$M_{ab} = \begin{cases} 0, & a < b, \\ (q-q^{-1})^{-1} (q^{(\varepsilon_a, 2\Lambda+2\rho+\varepsilon_a) - C(\Lambda_0)} - 1), & a = b, \\ q^{(2\Lambda,\varepsilon_a) - C(\Lambda_0)} ((-1)^{[b]} q^{(2\rho,\varepsilon_b)} - \delta_{\bar{b}}^a), & a > b. \end{cases}$$

Then we have

$$\underline{t}^{(l)} = M^l \underline{t}^{(0)}, \quad \text{with } t_a^{(0)} = 1 \quad \forall\, a,$$

where M is an analogue of the Perelomov-Popov matrix.

B. Solving the matrix equation

This matrix equation for $t_a^{(l)}$ can now be used to calculate the eigenvalues of C_l. Loosely speaking, the problem reduces to diagonalizing the matrix M. Recall

$$C_l = \sum_a (-1)^{[a]} q^{(2\rho,\varepsilon_a)} A^{(l)a}{}_a.$$

Denote the eigenvalue of C_l on $V(\Lambda)$ as $\chi_\Lambda(C_l)$. Then we have

$$\chi_\Lambda(C_l) = \sum_a (-1)^{[a]} q^{(2\rho,\varepsilon_a)} t_a^{(l)} = \sum_{a,b} (-1)^{[a]} q^{(2\rho,\varepsilon_a)} (M^l)_{ab}.$$

To calculate this we wish to diagonalize M. We assume the eigenvalues of M,

$$\alpha_a^\Lambda = \frac{(q^{(\varepsilon_a, 2\Lambda+2\rho+\varepsilon_a)-C(\Lambda_0)} - 1)}{(q-q^{-1})},$$

are distinct. Then we need a matrix N satisfying

$$(N^{-1}MN)_{ab} = \delta_b^a \alpha_a^\Lambda,$$

which implies

$$\chi_\Lambda(C_l) = \sum_{a,b,c} (-1)^{[a]} q^{(2\rho,\varepsilon_a)} (\alpha_b^\Lambda)^l N_{ab} (N^{-1})_{bc}. \tag{14}$$

Now

$$(MN)_{ab} = \alpha_b^\Lambda N_{ab}.$$

Substituting in the values for M_{ab} gives

$$\alpha_a^\Lambda N_{ab} + q^{(2\Lambda,\varepsilon_a)-C(\Lambda_0)} \sum_{c<a} ((-1)^{[c]} q^{(2\rho,\varepsilon_c)} - \delta_{\bar{c}}^a) N_{cb} = \alpha_b^\Lambda N_{ab}. \tag{15}$$

Since the eigenvalues α_a^Λ are distinct, this implies

$$N_{ab} = 0, \quad \forall\, a < b.$$

Set

$$P_{ab} = \sum_{c \leqslant a} (-1)^{[c]} q^{(2\rho,\varepsilon_c)} N_{cb}. \tag{16}$$

Then Eq. (15) becomes

$$\begin{aligned} 2(\alpha_b^\Lambda - \alpha_a^\Lambda) N_{ab} &= q^{(2\Lambda,\varepsilon_a)-C(\Lambda_0)} P_{(a-1)b} - \theta_{0a} q^{(2\Lambda,\varepsilon_a)-C(\Lambda_0)} N_{\bar{a}b} \\ &\Rightarrow (\alpha_b^\Lambda - \alpha_a^\Lambda)(-1)^{[a]} q^{(-2\rho,\varepsilon_a)} (P_{ab} - P_{(a-1)b}) \\ &= q^{(2\Lambda,\varepsilon_a)-C(\Lambda_0)} P_{a-1b} - \theta_{0a} q^{(2\Lambda,\varepsilon_a)-C(\Lambda_0)} N_{\bar{a}b}, \end{aligned}$$

which simplifies to

$$P_{ab} = \frac{(\alpha_b^\Lambda - \alpha_a^\Lambda + (-1)^{[a]} q^{2(\Lambda+\rho,\varepsilon_a)-C(\Lambda_0)})}{(\alpha_b^\Lambda - \alpha_a^\Lambda)} P_{(a-1)b} - \frac{\theta_{0a}(-1)^{[a]} q^{2(\Lambda+\rho,\varepsilon_a)-C(\Lambda_0)}}{(\alpha_b^\Lambda - \alpha_a^\Lambda)} N_{\bar{a}b}.$$

Set

$$\psi_a^b = \alpha_b^\Lambda - \alpha_a^\Lambda + (-1)^{[a]} q^{2(\Lambda+\rho,\varepsilon_a)-C(\Lambda_0)},$$

so this becomes

$$P_{ab} = \frac{\psi_a^b}{(\alpha_b^\Lambda - \alpha_a^\Lambda)} P_{(a-1)b} - \frac{\theta_{0a}(-1)^{[a]} q^{2(\Lambda+\rho,\varepsilon_a)-C(\Lambda_0)}}{(\alpha_b^\Lambda - \alpha_a^\Lambda)} N_{\bar{a}b}. \tag{17}$$

Without loss of generality we can choose $N_{aa}=1\,\forall\, a$, so $P_{bb}=(-1)^{[b]} q^{2(\rho,\varepsilon_b)}$. Then in the cases $0 \geqslant a > b$ and $a > b \geqslant 0$ the last term in Eq. (17) vanishes, giving

$$P_{ab} = (-1)^{[b]} q^{2(\rho,\varepsilon_b)} \prod_{c=b+1}^{a} \frac{\psi_c^b}{(\alpha_b^\Lambda - \alpha_c^\Lambda)}.$$

Similarly, for $a > \bar{b} > 0$ we obtain

$$P_{ab} = P_{\bar{b}b}^- \prod_{c=\bar{b}+1}^{a} \frac{\psi_c^b}{(\alpha_b^\Lambda - \alpha_c^\Lambda)}. \tag{18}$$

It remains to find P_{ab} for $\bar{b} \geqslant a > 0$. In this case, the last term in Eq. (17) contributes, giving

$$\begin{aligned} P_{ab} = {} & (-1)^{[b]} q^{2(\rho,\varepsilon_b)} \prod_{c=b+1}^{a} \frac{\psi_c^b}{(\alpha_b^\Lambda - \alpha_c^\Lambda)} - \frac{(-1)^{[a]} q^{2(\Lambda+\rho,\varepsilon_a)-C(\Lambda_0)}}{(\alpha_b^\Lambda - \alpha_a^\Lambda)} N_{\bar{a}b} \\ & - \sum_{d=\bar{l}}^{a-1} \frac{(-1)^{[d]} q^{2(\Lambda+\rho,\varepsilon_d)-C(\Lambda_0)}}{(\alpha_b^\Lambda - \alpha_d^\Lambda)} N_{\bar{d}b}^- \prod_{c=d+1}^{a} \frac{\psi_c^b}{(\alpha_b^\Lambda - \alpha_c^\Lambda)}. \end{aligned} \tag{19}$$

Recall that if $b < a < 0$, then

$$\begin{aligned} N_{ab} &= \frac{q^{(2\Lambda,\varepsilon_a)-C(\Lambda_0)}}{(\alpha_b^\Lambda - \alpha_a^\Lambda)} P_{(a-1)b} \\ &= \frac{(-1)^{[b]} q^{2(\Lambda,\varepsilon_a)+2(\rho,\varepsilon_b)-C(\Lambda_0)}}{(\alpha_b^\Lambda - \alpha_a^\Lambda)} \prod_{c=b+1}^{a-1} \frac{\psi_c^b}{(\alpha_b^\Lambda - \alpha_c^\Lambda)}. \end{aligned}$$

Substituting this into Eq. (19), we find

$$\begin{aligned} P_{\bar{b}b}^- = {} & (-1)^{[b]} q^{2(\rho,\varepsilon_b)} \prod_{c=b+1}^{\bar{b}} \frac{\psi_c^b}{(\alpha_b^\Lambda - \alpha_c^\Lambda)} - \frac{(-1)^{[b]} q^{-2(\Lambda+\rho,\varepsilon_b)-C(\Lambda_0)}}{(\alpha_b^\Lambda - \alpha_{\bar{b}}^\Lambda)} \\ & - \sum_{d=\bar{l}}^{\bar{b}-1} \frac{(-1)^{[d]+[b]} q^{2(\rho,\varepsilon_d+\varepsilon_b)-2C(\Lambda_0)}}{(\alpha_b^\Lambda - \alpha_d^\Lambda)(\alpha_b^\Lambda - \alpha_{\bar{d}}^\Lambda)} \prod_{c=b+1}^{\bar{d}-1} \frac{\psi_c^b}{(\alpha_b^\Lambda - \alpha_c^\Lambda)} \prod_{c=d+1}^{\bar{b}} \frac{\psi_c^b}{(\alpha_b^\Lambda - \alpha_c^\Lambda)}, \end{aligned}$$

which can also be simplified to

$$P_{\bar{b}b}\prod_{c=b+1}^{\bar{b}}\frac{(\alpha_b^\Lambda-\alpha_c^\Lambda)}{\psi_c^b}=(-1)^{[b]}q^{2(\rho,\varepsilon_b)}\left[1-\sum_{d=\bar{l}}^{\bar{b}}\frac{(-1)^{[d]}q^{2(\rho,\varepsilon_d)-2C(\Lambda_0)}}{\psi_d^b\psi_{\bar{d}}^b}\prod_{c=\bar{d}+1}^{d-1}\frac{(\alpha_b^\Lambda-\alpha_c^\Lambda)}{\psi_c^b}\right]. \quad (20)$$

From this point we will consider the case $m=2l+1$. This is marginally more complicated than the case with even m. Define Φ_d^b to be

$$\Phi_d^b=\prod_{c=\bar{l}}^{d-1}\frac{(\alpha_b-\alpha_c)(\alpha_b-\alpha_{\bar{c}})}{\psi_c^b\psi_{\bar{c}}^b}$$

$$=\frac{(\alpha_b-\alpha_{d-1})(\alpha_b-\alpha_{\overline{d-1}})}{\psi_{d-1}^b\psi_{\overline{d-1}}^b}\Phi_{d-1}^b,\quad \Phi_{\bar{l}}^b=1.$$

Then $P_{\bar{b}b}$ can be written as

$$P_{\bar{b}b}=(-1)^{[b]}q^{2(\rho,\varepsilon_b)}\prod_{\substack{c=b+1\\c\neq 0}}^{\bar{b}}\frac{\psi_c^b}{(\alpha_b^\Lambda-\alpha_c^\Lambda)}\left[\frac{\psi_0^b}{\alpha_b-\alpha_0}-\sum_{d=\bar{l}}^{\bar{b}}\frac{(-1)^{[d]}q^{2(\rho,\varepsilon_d)-2C(\Lambda_0)}}{\psi_d^b\psi_{\bar{d}}^b}\Phi_d^b\right].$$

Note that for $c\neq 0$,

$$\psi_c^b=\frac{q^{-C(\Lambda_0)}}{(q-q^{-1})}(q^{(\varepsilon_b,2\rho+2\Lambda+\varepsilon_b)}-q^{(\varepsilon_c,2\rho+2\Lambda+\varepsilon_c)}+(q-q^{-1})(-1)^{[c]}q^{(\varepsilon_c,2\rho+2\Lambda)})$$

$$=\frac{q^{-C(\Lambda_0)}\tilde{\psi}_c^b}{(q-q^{-1})},$$

where

$$\tilde{\psi}_c^b=q^{(\varepsilon_b,2\rho+2\Lambda+\varepsilon_b)}-q^{(\varepsilon_c,2\rho+2\Lambda-\varepsilon_c)}.$$

So

$$\sum_{d=\bar{l}}^{\bar{b}}\frac{(-1)^{[d]}q^{2(\rho,\varepsilon_d)-2C(\Lambda_0)}}{\psi_d^b\psi_{\bar{d}}^b}\Phi_d^b=(q-q^{-1})\sum_{d=\bar{l}}^{\bar{b}}\frac{(-1)^{[d]}(q-q^{-1})q^{2(\rho,\varepsilon_d)}}{\tilde{\psi}_d^b\tilde{\psi}_{\bar{d}}^b}\Phi_d^b$$

$$=(q-q^{-1})\sum_{d=\bar{l}}^{\bar{b}}\frac{(q^{2(\varepsilon_d,\varepsilon_d)}-1)q^{2(\rho,\varepsilon_d)-(\varepsilon_d,\varepsilon_d)}}{\tilde{\psi}_d^b\tilde{\psi}_{\bar{d}}^b}\Phi_d^b \quad (21)$$

and

$$\Phi_{d+1}^b=\frac{(\alpha_b-\alpha_d)(\alpha_b-\alpha_{\bar{d}})}{\psi_d^b\psi_{\bar{d}}^b}\Phi_d^b$$

$$=\frac{(q^{(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-q^{(\varepsilon_d,\varepsilon_d+2\rho+2\Lambda)})(q^{(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-q^{(\varepsilon_d,\varepsilon_d-2\rho-2\Lambda)})}{\tilde{\psi}_d^b\tilde{\psi}_{\bar{d}}^b}\Phi_d^b$$

for $d\geqslant\bar{l}$. Now

$$(q^{(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-q^{(\varepsilon_d,\varepsilon_d+2\rho+2\Lambda)})(q^{(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-q^{(\varepsilon_d,\varepsilon_d-2\rho-2\Lambda)})$$

$$=q^{2(\varepsilon_d,\varepsilon_d)}(q^{(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-q^{(\varepsilon_d,-\varepsilon_d+2\rho+2\Lambda)})(q^{(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-q^{-(\varepsilon_d,\varepsilon_d+2\rho+2\Lambda)})$$

$$+q^{2(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}(1-q^{2(\varepsilon_d,\varepsilon_d)})+q^{2(\varepsilon_d,\varepsilon_d)}-1$$

$$= q^{2(\varepsilon_d,\varepsilon_d)}\tilde{\psi}_d^b\tilde{\psi}_{\bar{d}}^b - (q^{2(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-1)(q^{2(\varepsilon_d,\varepsilon_d)}-1).$$

Then, for $d \geqslant \bar{l}$,

$$\frac{\Phi_{d+1}^b}{(q^{2(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-1)} = \left[\frac{q^{2(\varepsilon_d,\varepsilon_d)}}{(q^{2(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-1)} - \frac{(q^{2(\varepsilon_d,\varepsilon_d)}-1)}{\tilde{\psi}_d^b\tilde{\psi}_{\bar{d}}^b}\right]\Phi_d^b. \tag{22}$$

Now for $d=\bar{b}$,

$$\frac{(q^{2(\varepsilon_d,\varepsilon_d)}-1)q^{2(\rho,\varepsilon_d)-(\varepsilon_d,\varepsilon_d)}}{\tilde{\psi}_d^b\tilde{\psi}_{\bar{d}}^b} = \frac{(q^{2(\varepsilon_b,\varepsilon_b)}-1)q^{2(\rho,\varepsilon_{\bar{b}})-(\varepsilon_b,\varepsilon_b)}}{(q^{(\varepsilon_b,2\rho+2\Lambda+\varepsilon_b)}-q^{-(\varepsilon_b,2\rho+2\Lambda+\varepsilon_b)})q^{(\varepsilon_b,2\rho+2\Lambda)}(q^{(\varepsilon_b,\varepsilon_b)}-q^{-(\varepsilon_b,\varepsilon_b)})}$$

$$= \frac{q^{2(\rho,\varepsilon_{\bar{b}})+(\varepsilon_b,\varepsilon_b)}}{(q^{2(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-1)},$$

which can be written as

$$\frac{(q^{2(\varepsilon_d,\varepsilon_d)}-1)q^{2(\rho,\varepsilon_d)-(\varepsilon_d,\varepsilon_d)}}{\tilde{\psi}_d^b\tilde{\psi}_{\bar{d}}^b} = \frac{q^{2(\rho,\varepsilon_{\bar{b}-1})-(\varepsilon_{\bar{b}-1},\varepsilon_{\bar{b}-1})}}{(q^{2(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-1)}$$

when $b<l$. Hence Eq. (22) can be used to pairwise cancel the terms in the sum in Eq. (21). Adding the first two terms $(d=\bar{b},\bar{b}-1)$, we find

$$q^{2(\rho,\varepsilon_{\bar{b}-1})-(\varepsilon_{\bar{b}-1},\varepsilon_{\bar{b}-1})}\left[\frac{\Phi_{\bar{b}}^b}{(q^{2(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-1)} + \frac{(q^{2(\varepsilon_{\bar{b}-1},\varepsilon_{\bar{b}-1})}-1)}{\tilde{\psi}_{\bar{b}-1}^b\tilde{\psi}_{b+1}^b}\Phi_{\bar{b}-1}^b\right]$$

$$= q^{2(\rho,\varepsilon_{\bar{b}-1})-(\varepsilon_{\bar{b}-1},\varepsilon_{\bar{b}-1})}\frac{q^{2(\varepsilon_{\bar{b}-1},\varepsilon_{\bar{b}-1})}}{(q^{2(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-1)}\Phi_{\bar{b}-1}^b$$

$$= \frac{q^{2(\rho,\varepsilon_{\bar{b}-2})-(\varepsilon_{\bar{b}-2},\varepsilon_{\bar{b}-2})}}{(q^{2(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-1)}\Phi_{\bar{b}-1}^b.$$

Continuing to apply Eq. (22) in this manner gives

$$\sum_{d=\bar{l}}^{\bar{b}}\frac{(q^{2(\varepsilon_d,\varepsilon_d)}-1)q^{2(\rho,\varepsilon_d)-(\varepsilon_d,\varepsilon_d)}}{\tilde{\psi}_d^b\tilde{\psi}_{\bar{d}}^b}\Phi_d^b = \frac{q^{2(\rho,\varepsilon_{\bar{l}})+(\varepsilon_l,\varepsilon_l)}}{(q^{2(\varepsilon_b,\varepsilon_b+\rho+\Lambda)}-1)}\Phi_{\bar{l}}^b$$

$$= \frac{q^{2l+1-m}}{(q^{2(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-1)}. \tag{23}$$

Hence in the case $m=2l+1$,

$$P_{\bar{b}\bar{b}}^- = (-1)^{[b]}q^{2(\rho,\varepsilon_b)}\left[\frac{\psi_0^b}{\alpha_b-\alpha_0} - \frac{(q-q^{-1})}{(q^{2(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-1)}\right]\prod_{\substack{c=b+1\\c\neq 0}}^{\bar{b}}\frac{\psi_c^b}{(\alpha_b^\Lambda-\alpha_c^\Lambda)}.$$

By substituting in the formulas for ψ_c^b and α_b and simplifying we obtain

$$P_{\bar{b}\bar{b}}^- = (-1)^{[b]}q^{2(\rho,\varepsilon_b)}\left[1+(q-q^{-1})\frac{q^{(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}}{(q^{2(\varepsilon_b,\varepsilon_b+2\rho+2\Lambda)}-1)}\right]\prod_{c=b+1}^{\bar{b}}\frac{(q^{(\varepsilon_b,2\rho+2\Lambda+\varepsilon_b)}-q^{(\varepsilon_c,2\rho+2\Lambda-\varepsilon_c)})}{(q^{(\varepsilon_b,2\rho+2\Lambda+\varepsilon_b)}-q^{(\varepsilon_c,2\rho+2\Lambda+\varepsilon_c)})},$$

and thus for $a \geqslant \bar{b} > 0$,

$$P_{ab} = (-1)^{[b]} q^{2(\rho,\varepsilon_b)} \left[1 + (q - q^{-1}) \frac{q^{(\varepsilon_b, \varepsilon_b + 2\rho + 2\Lambda)}}{(q^{2(\varepsilon_b, \varepsilon_b + 2\rho + 2\Lambda)} - 1)} \right] \prod_{c=b+1}^{a} \frac{(q^{(\varepsilon_b, 2\rho + 2\Lambda + \varepsilon_b)} - q^{(\varepsilon_c, 2\rho + 2\Lambda - \varepsilon_c)})}{(q^{(\varepsilon_b, 2\rho + 2\Lambda + \varepsilon_b)} - q^{(\varepsilon_c, 2\rho + 2\Lambda + \varepsilon_c)})}.$$

Similarly, we find from Eqs. (18), (20), (21), and (23) that when m is even then

$$P_{ab} = (-1)^{[b]} q^{2(\rho,\varepsilon_b)} \left[1 - \frac{q(q - q^{-1})}{(q^{2(\varepsilon_b, \varepsilon_b + 2\rho + 2\Lambda)} - 1)} \right] \prod_{c=b+1}^{a} \frac{(q^{(\varepsilon_b, 2\rho + 2\Lambda + \varepsilon_b)} - q^{(\varepsilon_c, 2\rho + 2\Lambda - \varepsilon_c)})}{(q^{(\varepsilon_b, 2\rho + 2\Lambda + \varepsilon_b)} - q^{(\varepsilon_c, 2\rho + 2\Lambda + \varepsilon_c)})}$$

for $a \geqslant \bar{b} > 0$. Hence we have found expressions for P_{ab} for all a, b satisfying $a \geqslant \bar{b} > 0$. At the end of the paper these, together with the earlier results for P_{ab}, will be used to calculate $\chi_\Lambda(C_l)$.

Now we return to the diagonalization of the matrix N. We know

$$(N^{-1}M)_{ab} = \alpha_a^\Lambda (N^{-1})_{ab}.$$

Substituting in the values for M_{ab} gives

$$\alpha_b^\Lambda (N^{-1})_{ab} + (-1)^{[b]} q^{(2\rho,\varepsilon_b) - C(\Lambda_0)} \sum_{c>b} q^{(2\Lambda,\varepsilon_c)} (1 - \delta_{\bar{b}}^c (-1)^{[b]} q^{-2(\rho,\varepsilon_b)}) (N^{-1})_{ac} = \alpha_a^\Lambda (N^{-1})_{ab}. \tag{24}$$

Set

$$\hat{Q}_{ab} = \sum_{c \geqslant b} q^{2(\Lambda,\varepsilon_c)} (N^{-1})_{ac}.$$

We then solve for $\hat{Q}_{ab}$, with the calculations being very similar to those for P_{ab}. For $0 \leqslant b < a$ and $b < a \leqslant 0$ we find

$$\hat{Q}_{ab} = q^{2(\Lambda,\varepsilon_a)} \prod_{c=b}^{a-1} \frac{\psi_c^a}{(\alpha_a^\Lambda - \alpha_c^\Lambda)}.$$

For $m = 2l + 1$ we obtain

$$\hat{Q}_{ab} = q^{2(\Lambda,\varepsilon_a)} \left[1 + (q - q^{-1}) \frac{q^{(\varepsilon_a, \varepsilon_a + 2\rho + 2\Lambda)}}{(q^{2(\varepsilon_a, \varepsilon_a + 2\rho + 2\Lambda)} - 1)} \right] \prod_{c=b}^{a-1} \frac{(q^{(\varepsilon_a, 2\rho + 2\Lambda + \varepsilon_a)} - q^{(\varepsilon_c, 2\rho + 2\Lambda - \varepsilon_c)})}{(q^{(\varepsilon_a, 2\rho + 2\Lambda + \varepsilon_a)} - q^{(\varepsilon_c, 2\rho + 2\Lambda + \varepsilon_c)})}$$

for $b \leqslant \bar{a} < 0$. Similarly, for even m we find

$$\hat{Q}_{ab} = q^{2(\Lambda,\varepsilon_a)} \left[1 - \frac{q(q - q^{-1})}{(q^{2(\varepsilon_a, \varepsilon_a + 2\rho + 2\Lambda)} - 1)} \right] \prod_{c=b}^{a-1} \frac{(q^{(\varepsilon_a, 2\rho + 2\Lambda + \varepsilon_a)} - q^{(\varepsilon_c, 2\rho + 2\Lambda - \varepsilon_c)})}{(q^{(\varepsilon_a, 2\rho + 2\Lambda + \varepsilon_a)} - q^{(\varepsilon_c, 2\rho + 2\Lambda + \varepsilon_c)})}.$$

for $b \leqslant \bar{a} < 0$.

To use these results to calculate $\chi_\Lambda(C_l)$ we introduce a new function Q_{ab}, defined by

$$Q_{ab} = \sum_{c \geqslant b} (N^{-1})_{ac}.$$

Then from Eqs. (14) and (16) we deduce

$$\chi_\Lambda(C_l) = \sum_a (\alpha_a^\Lambda)^l P_{(\mu=\bar{1})a} Q_{a(\nu=1)}. \tag{25}$$

However we know

$$t_a^{(l)} = \frac{q^{2(\Lambda,\varepsilon_a)} - 1}{q - q^{-1}},$$

and

$$\sum_b (N^{-1})_{ab} t_b^{(1)} = \sum_{b,c} (N^{-1})_{ab} M_{bc} t_c^{(0)}$$

$$\Rightarrow \sum_b (N^{-1})_{ab} \frac{(q^{2(\Lambda,\varepsilon_b)} - 1)}{(q - q^{-1})} = \sum_b (N^{-1}M)_{ab}$$

$$= \sum_b \alpha_a^{\Lambda} (N^{-1})_{ab} = \sum_b (N^{-1})_{ab} \frac{(q^{(\varepsilon_a, 2\Lambda + 2\rho + \varepsilon_a) - C(\Lambda_0)} - 1)}{(q - q^{-1})}.$$

Thus

$$Q_{a(\nu=1)} = q^{C(\Lambda_0) - (\varepsilon_a, 2\rho + 2\Lambda + \varepsilon_a)} \hat{Q}_{a(\nu=1)}.$$

C. Explicit formulas for the eigenvalues

Substituting our formulas for $P_{(\mu=\bar{1})a}$ and $Q_{a(\nu=1)}$ into Eq. (25), noting that for $a \neq 0$ exactly one of $a < 0$ or $a > 0$ is true, we find the eigenvalues of the Casimir invariants C_l are given by

$$\chi_\Lambda(C_l) = \sum_a (-1)^{[a]} q^{C(\Lambda_0) - (\varepsilon_a, \varepsilon_a)} f(a) \left[\frac{(q^{(\varepsilon_a, 2\rho + 2\Lambda + \varepsilon_a) - C(\Lambda_0)} - 1)}{(q - q^{-1})} \right]^l$$

$$\times \prod_{b \neq a} \frac{(q^{(\varepsilon_a, 2\rho + 2\Lambda + \varepsilon_a)} - q^{(\varepsilon_b, 2\rho + 2\Lambda - \varepsilon_b)})}{(q^{(\varepsilon_a, 2\rho + 2\Lambda + \varepsilon_a)} - q^{(\varepsilon_b, 2\rho + 2\Lambda + \varepsilon_b)})},$$

where

$$f(a) = \begin{cases} 1 - (q - q^{-1}) \dfrac{q}{(q^{2(\varepsilon_a, \varepsilon_a + 2\rho + 2\Lambda)} - 1)}, & m = 2l, \\ 1 + (q - q^{-1}) \dfrac{q^{(\varepsilon_a, \varepsilon_a + 2\rho + 2\Lambda)}}{(q^{2(\varepsilon_a, \varepsilon_a + 2\rho + 2\Lambda)} - 1)}, & a \neq 0,\ m = 2l + 1, \\ 1, & a = 0,\ m = 2l + 1. \end{cases}$$

Throughout we assumed the eigenvalues were distinct. If they are not, the calculations are more complicated but the result is the same. Thus we have found the following.

Theorem 4.1: *The quantum superalgebra* $U_q[\mathrm{osp}(m|n)]$, *for* $m > 2$, *has an infinite family of Casimir invariants of the form*,

$$C_l = (\mathrm{str} \otimes I)(\pi(q^{2h_p}) \otimes I) A^l, \quad l \in \mathbb{Z}^+,$$

where

$$A = \frac{(R^T R - I \otimes I)}{(q - q^{-1})}.$$

The eigenvalues of the invariants when acting on an arbitrary irreducible finite-dimensional module with highest weight Λ *are given by*

$$\chi_\Lambda(C_l) = \sum_a (-1)^{[a]} q^{C(\Lambda_0)-(\varepsilon_a,\varepsilon_a)} f(a) \left[\frac{(q^{(\varepsilon_a,\varepsilon_a+2\rho+2\Lambda)-C(\Lambda_0)} - 1)}{(q-q^{-1})} \right]^l \times \prod_{b\neq a} \frac{(q^{(\varepsilon_a,2\rho+2\Lambda+\varepsilon_a)} - q^{(\varepsilon_b,2\rho+2\Lambda-\varepsilon_b)})}{(q^{(\varepsilon_a,2\rho+2\Lambda+\varepsilon_a)} - q^{(\varepsilon_b,2\rho+2\Lambda+\varepsilon_b)})},$$

where

$$f(a) = \begin{cases} 1-(q-q^{-1})\dfrac{q}{(q^{2(\varepsilon_a,\varepsilon_a+2\rho+2\Lambda)}-1)}, & m=2l, \\ 1+(q-q^{-1})\dfrac{q^{(\varepsilon_a,\varepsilon_a+2\rho+2\Lambda)}}{(q^{2(\varepsilon_a,\varepsilon_a+2\rho+2\Lambda)}-1)}, & a\neq 0,\ m=2l+1, \\ 1, & a=0,\ m=2l+1. \end{cases}$$

This completes the calculation of the eigenvalues of an infinite family of Casimir invariants of $U_q[\mathrm{osp}(m|n)]$ when acting on an arbitrary irreducible highest weight module, provided $m>2$. This had already been done for $U_q[\mathrm{osp}(2|n)]$, using a different method, in Ref. 12. Also every finite-dimensional representation of $U_q[\mathrm{osp}(1|n)]$ is isomorphic to a finite-dimensional representation of $U_{-q}[o(n+1)]$,[14] whose central elements are well understood. Hence the eigenvalues of a family of Casimir invariants, when acting on an arbitrary irreducible finite-dimensional highest weight module have now been calculated for all quantized orthosymplectic superalgebras. Together with the results for $U_q[\mathrm{gl}(m|n)]$,[13] this covers all nonexceptional quantized superalgebras.

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Multiple nodal bound states for a quasilinear Schrödinger equation

Jianqing Chen[a)]
School of Mathematics and Computer Science, Fujian Normal University, Fuzhou, 350007, People's Republic of China and Institute of Applied Physics and Computational Mathematics, Beijing 100088, People's Republic of China

Boling Guo
Institute of Applied Physics and Computational Mathematics, Beijing, 100088, People's Republic of China

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Nehari techniques are used to prove the existence of multiple (indeed infinitely many) nodal type bound states for the quasilinear Schrödinger equation $iz_t - V_0 z + z'' + q(x)|z|^2 z + k(|z|^2)''z = 0$ with prescribed number of nodes. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2138045]

I. INTRODUCTION

Let $\mathbb{R}_+ = [0, +\infty)$ and $z := z(x,t): \mathbb{R}_+ \times \mathbb{R}_+ \to \mathbb{C}$ be a complex-valued function. In this paper we are concerned with the existence of multiple nodal type bound states for the following quasilinear Schrödinger equation:

$$\begin{gathered} iz_t - V_0 z + z'' + q(x)|z|^2 z + k(|z|^2)''z = 0, \\ i^2 = 1,\ k \in \mathbb{R},\ x \in \mathbb{R}_+,\ t \in \mathbb{R}_+,\ q: \mathbb{R}_+ \to \mathbb{R}_+, \end{gathered} \tag{1.1}$$

where $z'' = (\partial^2/\partial x^2) z(x,t)$. A bound state is a solution of (1.1) of the form $z(x,t) = e^{i\omega t} u(x)$ and real function $u(x)$ satisfies

$$\begin{gathered} u'' - Vu + k(|u|^2)''u + q(x)|u|^2 u = 0, \\ u(0) = 0, \quad \lim_{x \to +\infty} u(x) = 0,\ x \in \mathbb{R}_+, \end{gathered} \tag{1.2}$$

where we have set $V = V_0 + \omega$ and assume throughout this paper that $V(x)$ is positive and continuous on $\mathbb{R}_+$ and

$$(V) \quad \lim_{x \to 0^+} V(x) = V(0) > 0, \quad \lim_{x \to +\infty} V(x) = +\infty.$$

Equation (1.1) has been derived in the study of plasma physics, see Refs. 9, 11, and 13. When $k = 0$ and $q(x) = x^{-\theta}$, (1.2) has also been derived as a model in the nuclear physics.[5,7] Also when $k = 0$, both (1.1) and (1.2) have been studied extensively, see Refs. 6 and 10–12 and the references therein. When $k \neq 0$, the problem is much more natural and interesting from the physical point of view, but more difficulty in the mathematical treatment due to the presence of the quasilinear term. In a series of works, Ambrosetti-Liu-Wang-Wang have shown the existence results for such kind of problems, see Refs. 1, 3, and 4 and the references therein. But we do not see any results about the existence of multiple nodal (sign changing) solutions for the problem considered here. Our

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goal here is to investigate the existence of multiple nodal solutions of (1.2) with prescribed number of nodes. More precisely, we have the following.

Theorem 1.1: *Let* $k>0$, $q(x)=x^{-\theta}$ *with* $0<\theta<1$ *and* (V) *holds. Then for any* $m\geqslant 2$, *there exists a solution* u *of* (1.2) *such that* u *has precisely* $m-1$ *zero points in* $(0,+\infty)$.

Note that in the statement of Theorem 1.1, m can be arbitrary. Hence if Theorem 1.1 is proved, then we have that (1.1) has multiple (indeed infinitely many) nodal type bound states. The proof of Theorem 1.1 is by variational methods. Let $H_0^1(\mathbb{R}_+)=\{u\in L^2(\mathbb{R}_+);u'\in L^2(\mathbb{R}_+),u(0)=0,\lim_{x\to+\infty}u(x)=0,\int_0^{+\infty}V(x)u^2<\infty\}$ be a Sobolev space under the norm $\|u\|^2=\int_0^{+\infty}(|u'|^2+V|u|^2)\mathrm{d}x$, on which we define the following functional:

$$J(u)=\int_0^{+\infty}\left(\frac{1}{2}(|u'|^2+V|u|^2)+ku^2|u'|^2-\frac{1}{4}x^{-\theta}|u|^4\right). \tag{1.3}$$

Then $J\in C^1(H_0^1(\mathbb{R}_+),\mathbb{R})$ (for the proof see, e.g., Ref. 8, Lemma 1 on p. 331). We say that $u\in H_0^1(\mathbb{R}_+)$ is a solution of (1.2) if and only if for any $\phi\in\mathcal{D}(\mathbb{R}_+)$ (the collections of all smooth functions with compact support in $\mathbb{R}_+$), there holds $\langle J'(u),\phi\rangle=0$. Hence to find multiple solutions of (1.2), it suffices to find multiple critical points of J on $H_0^1(\mathbb{R}_+)$. The idea of the proof is essentially due to Nehari,[6] which has also been used in Ref. 10, but we need to overcome the additional difficulty created by the quasilinear term.

This paper is organized as follows. The forthcoming section is some preliminaries. In Sec. III, we prove Theorem 1.1.

II. PRELIMINARIES

Let $0\leqslant\rho<\sigma\leqslant+\infty$. Denote $H_{\rho,\sigma}=H_0^1([\rho,\sigma))$ with the norm $\|u\|^2=\int_\rho^\sigma(|u'|^2+V|u|^2)\mathrm{d}x$ and we simply write $H_0^1([0,+\infty))$ as H. $L^p([\rho,\sigma))$ is the standard Lebesgue space with the standard norm $|\cdot|_p$. M, M_j denote various positive constants whose exact values are not important. For $\delta\to0$, we also use the standard notations $o(\delta)$ and $O(\delta)$ and $o(1)$ is a generic infinitesimal. Consider the Nehari manifold

$$\mathcal{N}(\rho,\sigma):=\left\{0\neq u\in H_{\rho,\sigma};\int_\rho^\sigma(|u'|^2+Vu^2+4ku^2|u'|^2-x^{-\theta}u^4)=0\right\}$$

and define

$$c(\rho,\sigma)=\inf_{u\in\mathcal{N}(\rho,\sigma)}J(u). \tag{2.1}$$

Then we have the following.

Proposition 2.1: If $0\leqslant\rho<\sigma\leqslant+\infty$, *then* $\mathcal{N}(\rho,\sigma)$ *is a manifold and* (*if* $\mathcal{N}(\rho,\sigma)\neq\emptyset$) *one has*

(i) *there exists* $M_1>0$ *such that* $\|u\|\geqslant M_1$, $\forall u\in\mathcal{N}(\rho,\sigma)$;
(ii) *if* $u^*\in\mathcal{N}(\rho,\sigma)$ *is a constrained critical point of* J *on* $\mathcal{N}(\rho,\sigma)$, *then* $J'(u^*)=0$.

Proof: We only show the case of $\rho=0$ and $\sigma=+\infty$ since other cases are similar but simpler. For any $u\in\mathcal{N}(0,+\infty)$, we have that

$$\int_0^{+\infty}(|u'|^2+Vu^2+4ku^2|u'|^2)=\int_0^{+\infty}x^{-\theta}u^4.$$

On the other hand, $0<\theta<1$ implies that

$$\int_0^{+\infty} x^{-\theta}u^4 = \int_0^1 x^{-\theta}u^4 + \int_1^{+\infty} x^{-\theta}u^4$$

$$\leqslant |u|_\infty^4 \int_0^1 x^{-\theta}\,\mathrm{d}x + \int_1^{+\infty} u^4$$

$$\leqslant M\|u\|^4.$$

It follows from $k>0$ that $\|u\|^2 \geqslant M_1 > 0$. The rest part of the proof can follow step by step as those in the proof of Ref. 1, Lemma 2.2. □

Proposition 2.2 (Ref. 1, Theorem 2.4): If $0 \leqslant \rho < \sigma \leqslant +\infty$, *then* $c(\rho,\sigma)$ *is always achieved at some positive* $u \in \mathcal{N}(\rho,\sigma)$, *which is a positive solution of* (1.2). *Clearly, the symmetric nature of the problem implies that* $-u$ *is a negative solution of* (1.2) *at this time.*

Lemma 2.3: For u obtained in Proposition 2.2, we have $u \in C^2(0,+\infty)$.

Proof: From Ref. 8, Theorem 1, we know that u is C^1 in $(0,+\infty)$. $\langle J'(u),\phi\rangle = 0$ for any $\phi \in \mathcal{D}(\mathbb{R}_+)$ and Ref. 2, p. 138, Theorem 6.5 imply that

$$u'' - Vu + k(|u|^2)''u + x^{-\theta}|u|^2u = 0 \text{ a.e. in } (0,+\infty).$$

Equivalently,

$$-(1+2ku^2)u'' + Vu = 2k(u')^2u + x^{-\theta}|u|^2u \text{ a.e. in } (0,+\infty).$$

It now follows from $k>0$ and u being C^1 in $(0,+\infty)$ that u'' is continuous in $(0,+\infty)$. The proof is complete. □

Lemma 2.4: Under the assumptions of Theorem 1.1, one has

(a) *if* $0 \leqslant \rho \leqslant \rho_1 < \sigma_1 \leqslant \sigma \leqslant +\infty$, *then* $c(\rho,\sigma) \leqslant c(\rho_1,\sigma_1)$;
(b) $c(\rho,\sigma) \to +\infty$ *as* $\sigma - \rho \to 0$;
(c) $c(\rho,+\infty) \to +\infty$ *as* $\rho \to +\infty$;
(d) $c(\rho,\sigma)$ *is a continuous function of* ρ *and* σ (*of* σ *if* $\rho=0$ *and of* ρ *if* $\sigma=+\infty$).

Proof: (a) If $0 \leqslant \rho \leqslant \rho_1 < \sigma_1 \leqslant \sigma \leqslant +\infty$, then $\mathcal{N}(\rho_1,\sigma_1) \subset \mathcal{N}(\rho,\sigma)$ and so that $c(\rho,\sigma) \leqslant c(\rho_1,\sigma_1)$.

(b) For every $u \in \mathcal{N}(\rho,\sigma)$, $\gamma(u) := \|u\|^2 + 4k|uu'|_2^2 - \int_\rho^\sigma x^{-\theta}|u|^4 = 0$. Thus

$$J(u) = \frac{1}{2}\|u\|^2 + k|uu'|_2^2 - \frac{1}{4}\int_\rho^\sigma x^{-\theta}|u|^4 = \frac{1}{4}\|u\|^2. \tag{2.2}$$

Since for $u \in \mathcal{N}(\rho,\sigma)$,

$$\|u\|^2 + 4k|uu'|_2^2 = \int_\rho^\sigma x^{-\theta}|u|^4 \leqslant |u|_\infty^4 \int_\rho^\sigma x^{-\theta}\,\mathrm{d}x$$

$$\leqslant M_2\|u\|^4(\sigma-\rho)^{1-\theta},$$

we have from $k>0$ and that

$$\|u\|^2 \geqslant M_3(\sigma-\rho)^{\theta-1}.$$

Therefore $c(\rho,\sigma) \to +\infty$ as $\sigma - \rho \to 0$ by (2.2) and $0 < \theta < 1$.

(c) Suppose to the contrary, there is $\rho_n \to +\infty$ but $c(\rho_n,+\infty) \leqslant M$ for some $M>0$. Using Proposition 2.2, we know that there are $u_n \in \mathcal{N}(\rho_n,+\infty)$ such that

$$J(u_n) = c(\rho_n, +\infty) \leqslant M.$$

On the one hand, $u_n \in \mathcal{N}(\rho_n, +\infty)$ implies that [the computations are similar to those in (2.2)]

$$M \geqslant J(u_n) = \tfrac{1}{4}\|u_n\|^2;$$

on the other hand, from $\int_{\rho_n}^{+\infty} x^{-\theta}|u|^4 = \|u\|^2 + 4k|uu'|_2^2$, $k>0$ and

$$\tfrac{1}{4}\|u_n\|^2 = J(u_n) = c(\rho_n, +\infty) \geqslant c(0, +\infty) \geqslant M_0 > 0$$

we know that there is Λ (Λ is independent of n) such that

$$\int_{\rho_n}^{+\infty} x^{-\theta}|u_n|^4 \geqslant \Lambda > 0.$$

It follows that

$$\Lambda \leqslant \int_{\rho_n}^{+\infty} x^{-\theta}|u_n|^4 \leqslant \rho_n^{-\theta}\int_{\rho_n}^{+\infty} |u_n|^4 \leqslant \rho_n^{-\theta}|u_n|_\infty^2 \int_{\rho_n}^{+\infty} |u_n|^2$$

$$\leqslant M_4\rho_n^{-\theta}(\|u_n\|^2)^2 \to 0 \quad \text{as } \rho_n \to +\infty,$$

which is impossible.

(d) We only treat the case of $\sigma = +\infty$ since the other cases are similar. We assume that $\rho_n \to \rho > 0$ and want to show $c(\rho_n, +\infty) = c(\rho, +\infty) + o(1)$. For every n, there exists $u_n \in \mathcal{N}(\rho_n, +\infty)$ such that $J(u_n) = c(\rho_n, +\infty)$. We define v_n on $[\rho, +\infty)$ by $v_n(x) := u_n(\rho_n x/\rho)$. First using $u_n \in \mathcal{N}(\rho_n, +\infty)$ and the expression of $J(u_n)$ we know that for some M_5,

$$\liminf_{n\to+\infty} \int_{\rho_n}^{+\infty} (|u_n'|^2 + V|u_n|^2) \geqslant M_5 > 0. \tag{2.3}$$

Since for any n,

$$\int_{\rho}^{+\infty} v_n^2(x)|v_n'(x)|^2\,\mathrm{d}x = \int_{\rho_n}^{+\infty} u_n^2(x)|u_n'(x)|^2\frac{\rho_n}{\rho}\,\mathrm{d}x,$$

$$\int_{\rho}^{+\infty} x^{-\theta}|v_n(x)|^4\,\mathrm{d}x = \int_{\rho_n}^{+\infty} x^{-\theta}|u_n(x)|^4\left(\frac{\rho}{\rho_n}\right)^{1-\theta}\mathrm{d}x,$$

we have from (2.3) and $\int_{\rho_n}^{+\infty}(|u_n'|^2 + Vu_n^2 + 4ku_n^2|u_n'|^2 - x^{-\theta}|u_n|^4) = 0$ that

$$\liminf_{n\to+\infty}\left|\int_{\rho}^{+\infty}(4k|v_n(x)|^2|v_n'(x)|^2 - x^{-\theta}|v_n(x)|^4)\right| \neq 0.$$

Therefore there is a unique $t_n > 0$ such that $t_n v_n \in \mathcal{N}(\rho, +\infty)$ with

$$t_n^2 = \int_{\rho}^{+\infty}(|v_n'|^2 + V|v_n|^2) \Big/ \int_{\rho}^{+\infty}(x^{-\theta}|v_n(x)|^4 - 4k|v_n(x)|^2|v_n'(x)|^2).$$

Moreover we know from the above calculations that $t_n \to 1$ as $n \to +\infty$. Now from the definition of $\mathcal{N}(\rho, +\infty)$ and $t_n v_n \in \mathcal{N}(\rho, +\infty)$ that

$$\int_{\rho}^{+\infty} (|(t_n v_n)'|^2 + V(t_n v_n)^2) = t_n^2 \int_{\rho}^{+\infty} (|v_n'|^2 + V v_n^2)$$

$$= t_n^2 \int_{\rho_n}^{+\infty} \left(\frac{\rho_n^2}{\rho^2} |u_n'|^2 + V\left(\frac{\rho}{\rho_n} x \right) u_n^2 \right) \frac{\rho}{\rho_n^2}$$

$$= \int_{\rho_n}^{+\infty} (|u_n'|^2 + V u_n^2) + o(1),$$

which implies that $J(t_n v_n) = J(u_n) + o(1)$ $(n \to +\infty)$. The conclusion follows. □

III. PROOF OF THEOREM 1.1

Proof of Theorem 1.1: (1) We fix some integer $m \geqslant 2$ and want to find a solution u of (1.2) such that u has precisely $m-1$ zero points in $(0, +\infty)$. For any $0 \leqslant \rho < \sigma \leqslant +\infty$, we obtain from Proposition 2.2 that $c(\rho, \sigma) = \inf_{u \in \mathcal{N}(\rho,\sigma)} J(u)$ is a critical value of J which has a pair of critical points which define one positive and one negative solution of (1.2).

(2) Define

$$c(\rho_0, \ldots, \rho_m) = \sum_{j=0}^{m-1} c(\rho_j, \rho_{j+1}), \quad 0 = \rho_0 < \rho_1 < \cdots < \rho_{m-1} < \rho_m = +\infty,$$

by property (d) of Lemma 2.4, $c(\rho_0, \ldots, \rho_m)$ is continuous on $\rho_1, \ldots, \rho_{m-1}$. Properties (b) and (c) of Lemma 2.4 imply that $\{\rho_j\}$ must be bounded away from each other and from infinity in any sequences of sets, for which $c(\rho_0, \ldots, \rho_m)$ tends to its greatest lower bound. It is thus sufficient to confine the values $\rho_1, \ldots, \rho_{m-1}$ to a sufficiently large finite interval $[0, T]$ and therefore the minimum of $c(\rho_0, \ldots, \rho_m)$ is actually attained for some set of $m-1$ finite distinct values ρ_j with $0 < \rho_j < \rho_{j+1}$.

(3) Define

$$w_m(x) := u_j(x), \quad \rho_j \leqslant x < \rho_{j+1}, \quad j = 0, \ldots, m-1, \tag{3.1}$$

where u_j is chosen such that

(i) u_j is a positive solution of (1.2) for $\rho_j \leqslant x < \rho_{j+1}$, $0 \leqslant j \leqslant m-1$ and j even;
(ii) u_j is a negative solution of (1.2) for $\rho_j \leqslant x < \rho_{j+1}$, $0 \leqslant j \leqslant m-1$ and j odd.

Now the conclusions of Theorem 1.1 follows from Lemma 3.1. □

Lemma 3.1: Under the assumptions of Theorem 1.1, w_m satisfies

$$u'' - Vu + k(|u|^2)'' u + x^{-\theta} |u|^2 u = 0. \tag{3.2}$$

Moreover w_m has precisely $m-1$ nodes.

Proof: Clearly, $u := w_m$ satisfies (3.2) for $x \in \{0 < x < +\infty; x \neq \rho_j, j = 1, 2, \ldots, m-1\}$. Following Nehari,[6] it suffices to prove that

$$u_+' := \lim_{x \downarrow \rho_j} u'(x) = \lim_{x \uparrow \rho_j} u'(x) := u_-', \quad j = 1, 2, \ldots, m-1. \tag{3.3}$$

We prove this by contradictions. Assuming $u_+' \neq u_-'$ and setting $\rho := \rho_{j-1}$, $\sigma := \rho_j$, $\tau := \rho_{j+1}$ for convenience, we may assume that $u \geqslant 0$ on $[\rho, \sigma]$ and $u \leqslant 0$ on $[\sigma, \tau]$. Now we fix a sufficiently small $\delta > 0$ and define $v: [\rho, \tau] \to \mathbb{R}$ by

$$v(x) := u(x) \quad \text{if } |x-\sigma| \geqslant \delta,$$
$$:= u(\sigma-\delta) + \frac{(x-\sigma+\delta)(u(\sigma+\delta)-u(\sigma-\delta))}{2\delta} \quad \text{if } |x-\sigma| \leqslant \delta.$$

Clearly, v is continuous on $[\rho,\sigma]$. Let $\sigma_0=\sigma(\delta)\in(\sigma-\delta,\sigma+\delta)$ be defined by $v(\sigma_0)=0$, indeed there holds

$$\sigma_0 = \sigma - \delta - \frac{2\delta u(\sigma-\delta)}{u(\sigma+\delta)-u(\sigma-\delta)}.$$

We now obtain from Lemma 3.2 that there is $\alpha=\alpha(\delta)>0$ such that $\alpha v\in\mathcal{N}(\rho,\sigma_0)$ with

$$\alpha^2 = \int_\rho^{\sigma_0} (|v'|^2+Vv^2) \Big/ \int_\rho^{\sigma_0} (x^{-\theta}|v|^4 - 4k|v|^2|v'|^2).$$

Similarly, we have $\beta=\beta(\delta)>0$ such that $\beta v\in\mathcal{N}(\sigma_0,\tau)$ with

$$\beta^2 = \int_{\sigma_0}^{\tau} (|v'|^2+Vv^2) \Big/ \int_{\sigma_0}^{\tau} (x^{-\theta}|v|^4 - 4k|v|^2|v'|^2).$$

Next, we define $w\colon [\rho,\tau]\to\mathbb{R}$ by setting

$$w(x) := \begin{cases} \alpha v(x) & \text{if } \rho\leqslant x\leqslant\sigma_0, \\ \beta v(x) & \text{if } \sigma_0\leqslant x\leqslant\tau. \end{cases}$$

Keeping the expression of J in mind, we obtain from the relation $\frac{1}{4}(w^4+u^4)\geqslant\frac{1}{2}w^2u^2$ and the fact that $-u''u+Vu^2-k(u^2)''u^2=x^{-\theta}u^4$ holds up to finite points that

$$\begin{aligned} J(w) &= \int_\rho^\tau \left(\frac{1}{2}(|w'|^2+V|w|^2)+kw^2|w'|^2-\frac{1}{4}x^{-\theta}|w|^4\right) \\ &\leqslant \int_\rho^\tau \left(\frac{1}{2}(|w'|^2+V|w|^2)+kw^2|w'|^2-\frac{1}{4}x^{-\theta}|u|^4-\frac{1}{2}x^{-\theta}w^2u^2+\frac{1}{2}x^{-\theta}u^4\right) \\ &= \int_\rho^\tau \left(\frac{1}{2}(|w'|^2+V|w|^2)+kw^2|w'|^2-\frac{1}{4}x^{-\theta}|u|^4-\frac{1}{2}x^{-\theta}w^2u^2\right)+\frac{1}{2}\int_\rho^\tau (-u''u+Vu^2-k(u^2)''u^2) \\ &= J(u)+k\int_\rho^\tau u^2|u'|^2+\int_\rho^\tau \left(\frac{1}{2}(|w'|^2+V|w|^2)+kw^2|w'|^2-\frac{1}{2}x^{-\theta}w^2u^2\right) \\ &= J(u)+k\int_\rho^\tau u^2|u'|^2+\int_\rho^\tau B_1. \end{aligned} \tag{3.4}$$

Note that on $[\rho,\sigma-\delta]$, $w(x)=\alpha v(x)=\alpha u(x)$, then

$$\int_\rho^{\sigma-\delta} B_1 = \int_\rho^{\sigma-\delta} \left(\frac{\alpha^2}{2}(|u'|^2+V|u|^2)+\alpha^4ku^2|u'|^2-\frac{\alpha^2}{2}x^{-\theta}u^4\right). \tag{3.5}$$

Since

$$\int_\rho^{\sigma-\delta} x^{-\theta}u^4 = \int_\rho^{\sigma-\delta} (-u''u+Vu^2-k(u^2)''u^2)$$

and

$$\int_{\rho}^{\sigma-\delta}(-u''u) = -u(\sigma-\delta)u'(\sigma-\delta) + \int_{\rho}^{\sigma-\delta}|u'|^2, \tag{3.6}$$

$$\int_{\rho}^{\sigma-\delta}(-k(u^2)''u^2) = -2ku^3(\sigma-\delta)u'(\sigma-\delta) + 4k\int_{\rho}^{\sigma-\delta}u^2|u'|^2, \tag{3.7}$$

we obtain from

$$u(\sigma+\delta) = u'_+\delta + o(\delta) \quad \text{and } u(\sigma-\delta) = -u'_-\delta + o(\delta)$$

that

$$\begin{aligned}\int_{\rho}^{\sigma-\delta}B_1 &= \int_{\rho}^{\sigma-\delta}\left(\frac{\alpha^2}{2}(|u'|^2+Vu^2)+\alpha^4ku^2|u'|^2\right) - \frac{\alpha^2}{2}\int_{\rho}^{\sigma-\delta}(-u''u+Vu^2-k(u^2)''u^2)\\ &= \int_{\rho}^{\sigma-\delta}\left(\frac{\alpha^2}{2}(|u'|^2+Vu^2)+\alpha^4ku^2|u'|^2\right) - \frac{\alpha^2}{2}\Bigg(-u(\sigma-\delta)u'(\sigma-\delta) + \int_{\rho}^{\sigma-\delta}(|u'|^2+Vu^2)\\ &\quad -2ku^3(\sigma-\delta)u'(\sigma-\delta)+4k\int_{\rho}^{\sigma-\delta}u^2|u'|^2\Bigg) = (\alpha^4-2\alpha^2)k\int_{\rho}^{\sigma-\delta}u^2|u'|^2\\ &\quad +\frac{\alpha^2}{2}u(\sigma-\delta)u'(\sigma-\delta)+ku^3(\sigma-\delta)u'(\sigma-\delta)\\ &= (\alpha^4-2\alpha^2)k\int_{\rho}^{\sigma-\delta}u^2|u'|^2 - \frac{\alpha^2}{2}\delta(u'_-)^2+o(\delta).\end{aligned} \tag{3.8}$$

On $[\sigma+\delta,\tau]$ and $w(x)=\beta v(x)=\beta u(x)$, we obtain from a similar calculation that

$$\int_{\sigma+\delta}^{\tau}B_1 = (\beta^4-2\beta^2)k\int_{\sigma+\delta}^{\tau}u^2|u'|^2 - \frac{\beta^2}{2}\delta(u'_+)^2+o(\delta). \tag{3.9}$$

We now estimate the right-hand side of equality $\int_{\sigma-\delta}^{\sigma+\delta}B_1=\int_{\sigma-\delta 2}^{\sigma+\delta 1}(|w'|^2+V|w|^2)+kw^2|w'|^2 - \frac{1}{2}x^{-\theta}w^2u^2$. Since when $|x-\sigma|\leqslant\delta$ and δ small,

$$v(x) = -u'_-\delta + o(\delta) + \tfrac{1}{2}(x-\sigma+\delta)(u'_+ + u'_- + o(\delta)), \tag{3.10}$$

we know from (3.10) and (3.17) that

$$\int_{\sigma-\delta}^{\sigma+\delta}\frac{w^2}{2}(V-x^{-\theta}u^2) = \int_{\sigma-\delta}^{\sigma_0}\frac{\alpha^2v^2}{2}(V-x^{-\theta}u^2) + \int_{\sigma_0}^{\sigma+\delta}\frac{\beta^2v^2}{2}(V-x^{-\theta}u^2) = o(\delta). \tag{3.11}$$

Similarly,

$$k\int_{\sigma-\delta}^{\sigma+\delta}w^2|w'|^2 = o(\delta). \tag{3.12}$$

For the term $\int_{\sigma-\delta}^{\sigma+\delta}\frac{1}{2}|w'|^2$, we use the fact that

$$|w'(x)|^2 = |\alpha v'(x)|^2 = \frac{\alpha^2}{4}(u'_+ + u'_- + o(\delta))^2, \quad \forall\ \sigma-\delta<x<\sigma_0$$

and

$$|w'(x)|^2 = |\beta v'(x)|^2 = \frac{\beta^2}{4}(u'_+ + u'_- + o(\delta))^2, \quad \forall\ \sigma_0 < x < \sigma + \delta$$

to get that

$$\int_{\sigma-\delta}^{\sigma+\delta} \frac{1}{2}|w'|^2 = \frac{\alpha^2}{4}(u'_+ + u'_- + o(\delta))(\delta u'_- + o(\delta)) + \frac{\beta^2}{4}(u'_+ + u'_- + o(\delta))(\delta u'_+ + o(\delta))$$

$$= \frac{\delta}{4}(u'_+ + u'_-)^2 + o(\delta), \tag{3.13}$$

where we use (3.21) and (3.22). For the term $k\int_{\sigma-\delta}^{\sigma+\delta} u^2|u'|^2$, since when $\delta \to 0$,

$$u(x) := (x-\sigma)u'_- + o(x-\sigma) \quad \text{for } \sigma - \delta < x < \sigma,$$

$$:= (x-\sigma)u'_+ + o(x-\sigma) \quad \text{for } \sigma < x < \sigma + \delta$$

and

$$u'(x) := u'_- + O(x-\sigma) \quad \text{for } \sigma - \delta < x < \sigma,$$

$$:= u'_+ + O(x-\sigma) \quad \text{for } \sigma < x < \sigma + \delta,$$

we know that

$$k\int_{\sigma-\delta}^{\sigma+\delta} u^2|u'|^2 = O(\delta^2). \tag{3.14}$$

Thus we have from (3.19) and (3.20) that

$$J(w) \leqslant J(u) + k\int_\rho^\tau u^2|u'|^2 + \int_\rho^\tau B_1 = J(u) + k\int_\rho^\tau u^2|u'|^2 + \left(\int_\rho^{\sigma-\delta} + \int_{\sigma+\delta}^\tau + \int_{\sigma-\delta}^{\sigma+\delta}\right)B_1$$

$$= J(u) + k\int_\rho^\tau u^2|u'|^2 + (\alpha^4 - 2\alpha^2)k\int_\rho^{\sigma-\delta} u^2|u'|^2 + (\beta^4 - 2\beta^2)k\int_{\sigma+\delta}^\tau u^2|u'|^2$$

$$+ \int_{\sigma-\delta}^{\sigma+\delta}\left(\frac{1}{2}|w'|^2 + kw^2|w'|^2 + \frac{w^2}{2}(V - x^{-\theta}u^2)\right)$$

$$= J(u) + (1 + \alpha^4 - 2\alpha^2)k\int_\rho^{\sigma-\delta} u^2|u'|^2 + (1 + \beta^4 - 2\beta^2)k\int_{\sigma+\delta}^\tau u^2|u'|^2$$

$$- \frac{\alpha^2}{2}\delta(u'_-)^2 - \frac{\beta^2}{2}\delta(u'_+)^2 + o(\delta) + \frac{\delta}{4}(u'_+ + u'_-)^2. \tag{3.15}$$

It follows from (3.21) and (3.22) that

$$J(w) \leqslant J(u) + o(\delta) - \frac{\delta}{4}(u'_+ - u'_-)^2.$$

$u'_+ \neq u'_-$ implies that

$$J(w) < J(u) \quad \text{for } \delta > 0 \text{ small},$$

which is a contradiction to the construction of $u := w_m$. The proof is complete. □

Lemma 3.2: For ρ, σ_0, v, *and* u *as in Lemma 3.1, there exists* $M > 0$ *such that*

$$\left| 4k\int_{\rho}^{\sigma_0} v^2|v'|^2 - \int_{\rho}^{\sigma_0} x^{-\theta}v^4 \right| \geqslant M \quad \textit{for } \delta > 0 \textit{ small enough}.$$

Proof: Suppose to the contrary, we assume that

$$4k\int_{\rho}^{\sigma_0} v^2|v'|^2 - \int_{\rho}^{\sigma_0} x^{-\theta}v^4 = o(1) \quad (\delta \to 0),$$

i.e.,

$$4k\int_{\rho}^{\sigma-\delta} u^2|u'|^2 + 4k\int_{\sigma-\delta}^{\sigma_0} v^2|v'|^2 = \int_{\rho}^{\sigma-\delta} x^{-\theta}u^4 + \int_{\sigma-\delta}^{\sigma_0} x^{-\theta}v^4 = o(1). \tag{3.16}$$

Since for $\delta \to 0$,

$$u(\sigma+\delta) = u'_+\delta + o(\delta), \quad u(\sigma-\delta) = -u'_-\delta + o(\delta),$$

we have that

$$\sigma_0 = \sigma - \delta + \frac{2u'_-\delta}{u'_+ + u'_-} + o(\delta), \tag{3.17}$$

and

$$v(x) = -u'_-\delta + o(\delta) + \tfrac{1}{2}(x-\sigma+\delta)(u'_+ + u'_- + o(\delta)). \tag{3.18}$$

Direct computations show that

$$\int_{\sigma-\delta}^{\sigma_0} v^2|v'|^2 = \frac{(u'_+ + u'_-)^2}{4}\int_{\sigma-\delta}^{\sigma_0}\left(-u'_-\delta + o(\delta) + \frac{1}{2}(x-\sigma+\delta)(u'_+ + u'_- + o(\delta))\right)$$

$$= \frac{(u'_+ + u'_-)^2}{4}(-u'_-\delta + o(\delta))^2\left(\frac{2u'_-\delta}{u'_+ + u'_-} + o(\delta)\right)$$

$$+ \frac{(u'_+ + u'_-)^2}{8}(-u'_-\delta + o(\delta))(u'_+ + u'_- + o(\delta))\left(\frac{2u'_-\delta}{u'_+ + u'_-} + o(\delta)\right)^2$$

$$+ \frac{(u'_+ + u'_-)^2}{24}(u'_+ + u'_- + o(\delta))^2\left(\frac{2u'_-\delta}{u'_+ + u'_-} + o(\delta)\right)^3$$

$$= o(\delta^2).$$

Similarly

$$\int_{\sigma-\delta}^{\sigma_0} x^{-\theta}v^4 = o(\delta^2).$$

Therefore

$$4k\int_{\rho}^{\sigma-\delta} u^2|u'|^2 = \int_{\rho}^{\sigma-\delta} x^{-\theta}u^4 + o(1).$$

Thus

$$\int_{\rho}^{\sigma-\delta} (|u'|^2 + Vu^2) = o(1),$$

which contradicts to the fact that $u \neq 0$ on (ρ, σ). The proof is complete. □

Lemma 3.3: Let ρ, σ, σ_0, α, β, v, and u be as in the proof of Lemma 3.1. Then we have that

$$1 + \alpha^4 - 2\alpha^2 = O(\delta^2) \quad (\delta \to 0), \tag{3.19}$$

$$1 + \beta^4 - 2\beta^2 = O(\delta^2) \quad (\delta \to 0). \tag{3.20}$$

Proof: Denote $E = \int_{\rho}^{\sigma}(|u'|^2 + Vu^2)$, $F = \int_{\rho}^{\sigma}(x^{-\theta}u^4 - 4ku^2|u'|^2)$ and keep the definition of v in mind, we have that

$$\int_{\rho}^{\sigma_0} (|v'|^2 + Vv^2) = \int_{\rho}^{\sigma} (|u'|^2 + Vu^2) + \int_{\sigma-\delta}^{\sigma_0} (|v'|^2 + Vv^2) - \int_{\sigma-\delta}^{\sigma} (|u'|^2 + Vu^2)$$

$$\begin{aligned} &= E + \frac{1}{4}\int_{\sigma-\delta}^{\sigma_0} (u'_+ + u'_- + o(\delta))^2 \\ &\quad + (-u'_-\delta + o(\delta) + (x - \sigma + \delta)(u'_+ + u'_- + o(\delta)))^2 \\ &\quad - \int_{\sigma-\delta}^{\sigma} (|u'|^2 + Vu^2) \end{aligned}$$

$$\begin{aligned} &= E + \frac{1}{4}\int_{\sigma-\delta}^{\sigma_0} (u'_+ + u'_- + o(\delta))^2 + o(\delta) \\ &\quad - \int_{\sigma-\delta}^{\sigma} (u'_- + o(x - \sigma))^2 + (u'_-(x - \sigma) + o(x - \sigma))^2 \end{aligned}$$

$$= E + \frac{\delta}{2}(u'_+ + u'_- + o(\delta))(u'_- + o(\delta)) - \delta(u'_-)^2 + o(\delta).$$

Similarly,

$$\int_{\rho}^{\sigma_0} (x^{-\theta}v^4 - 4kv^2|v'|^2) = F + o(\delta).$$

Combining these with the fact that $E = F$ we get that

$$\alpha^2 = \left(E + \frac{\delta}{2}(u'_+ + u'_- + o(\delta))(u'_- + o(\delta)) - \delta(u'_-)^2 + o(\delta)\right) \Big/ F + o(\delta) = 1 + \frac{\delta}{2F}(u'_+ - u'_-)u'_- + o(\delta). \tag{3.21}$$

Hence

$$1 + \alpha^4 - 2\alpha^2 = O(\delta^2) \quad (\delta \to 0).$$

Similar arguments give

$$\beta^2 = 1 + O(\delta) \tag{3.22}$$

and therefore $1 + \beta^4 - 2\beta^2 = O(\delta^2)$. The conclusions follow. □

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Invariant noncommutative connections

Thierry Masson
Laboratoire de Physique Théorique (UMR 8627), Université Paris XI, Bâtiment 210, 91405 Orsay Cedex, France

Emmanuel Serié
Laboratoire de Physique Théorique (UMR 8627), Université Paris XI, Bâtiment 210, 91405 Orsay Cedex, France and Laboratoire de Physique Théorique des Liquides, Université Pierre-et-Marie-Curie-CNRS UMR 7600 Tour 22, 4-ème étage, Boîte 142, 4, Place Jussieu, 75005 Paris, France

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In this paper we classify invariant noncommutative connections in the framework of the algebra of endomorphisms of a complex vector bundle. It has been proven previously that this noncommutative algebra generalizes in a natural way the ordinary geometry of connections. We use explicitly some geometric constructions usually introduced to classify ordinary invariant connections, and we expand them using algebraic objects coming from the noncommutative setting. The main result is that the classification can be performed using a "reduced" algebra, an associated differential calculus and a module over this algebra. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2131206]

I. INTRODUCTION

Symmetries in gauge fields theories play an important role in physics. For instance, they have been used as possible procedures to introduce scalar Higgs fields using dimensional reductions. Solitons, as well as instantons and monopoles, have often been introduced and/or recognized as symmetric solutions of gauge fields equations. Extensive mathematical and physical studies of such symmetries have been proposed, using various approaches, and many examples have been given (see for instance Refs. 1 and 2 for a mathematical point of view, and Refs. 3–8 for a more physical point of view).

On the other hand, gauge fields have been generalized in the noncommutative framework, in some very natural ways. For a large class of examples developed so far, noncommutative connections incorporate at the same time, and without too much arbitrariness, not only ordinary non-Abelian gauge fields, but also some scalar fields which can be naturally interpreted as Higgs fields (see Refs. 9 and 10 for reviews, and references therein).

In the present paper, we study invariant noncommutative connections in a noncommutative framework which is very strongly connected to ordinary differential geometry. We take as our starting point a noncommutative algebra equipped with the derivation based differential calculus introduced in Ref. 11. This algebra is the algebra of endomorphisms of a SU (n)-vector bundle. Its structure and its relations to ordinary differential geometry have been extensively studied in Refs. 12 and 13, where it has been proven to play a very similar role to a SU (n)-principal fiber bundle. In this framework, noncommutative connections extend in a very natural and tractable way ordinary connections on the underlying principal fiber bundle. This permits us to generalize some of the analysis performed in previous works about invariant (ordinary) connections, in particular it is possible to use explicitly some of the geometric constructions related to their classification. Moreover, mixing those geometrical tools and the algebraic approach underlying noncommutative geometry, the classification of invariant noncommutative connections forces us to introduce mathematical objects which are more natural than in the ordinary case.

We have tried to make this paper as self-contained as possible. It is organized as follows. In Sec. II we summarize previous works about classification of invariant (ordinary) connections. These results are not new, but we have tried to make a synthesis of the main approaches to this problem. In particular, we introduce there some geometrical constructions which are extensively used later. Section III is devoted to the noncommutative framework. There, we expose the main results about the algebra we will consider, and we try to explain its relations to ordinary differential geometry. New results about the relations between this noncommutative geometry and the underlying ordinary geometry are exposed. Then comes the section which is the main part of this paper. We expose the classification of invariant noncommutative connections, emphasing what is common to the ordinary case and what is new. In particular, we show that the classification can be performed using objects inspired by noncommutative geometry: a "reduced" algebra, an associated differential calculus and a module over this algebra. At last, we study two important examples. One of our motivations for this work was to classify the degrees of freedom of spherically symmetric fields involved in noncommutative models. In the first example, we implement this spherical symmetry in a noncommutative situation which would correspond to an ordinary (trivial) SU (2)-principal fiber bundle. The results obtained lead to a natural generalization of the so-called Witten's anzatz.[14,3] The second example is a purely noncommutative situation based on a matrix algebra.

II. INVARIANT CONNECTIONS ON PRINCIPAL FIBER BUNDLES

In this section, we would like to summarize previous works on invariant connections in ordinary differential geometry. First, we introduce some notations and some general geometrical constructions which are useful to characterize invariant connections. Two approaches are then proposed, a global one, investigated in Refs. 6, 5, and 4, and a "local" one, investigated in Refs. 3 and 8. The constructions presented here will be used again in Sec. IV where we characterize noncommutative invariant connections.

A. Reduction of fiber bundles

Let us introduce the notations and the hypothesis we make. The analysis presented here is essentially based on the work of Jadczyck *et al.*[5]

We consider a principal fiber bundle $E(M,H)$, denoted by the following diagram of fibrations

$$H \to E \xrightarrow{\pi} M,$$

with structure group H. We then consider a compact Lie group G which acts on the left on E. We denote this action by $G \circlearrowright E$. We naturally assume that the two actions $G \circlearrowright E$ and $E \circlearrowright H$ do commute. In other words, G will be considered in the following as a subgroup of $\mathrm{Aut}(E)$, the group of automorphisms of E. The fiber bundle E is called a G-symmetric fiber bundle. Then the projection π induces an action $G \circlearrowright M$ which is characterized by the following diagram:

$$\begin{array}{ccccccccc} 0 & \longrightarrow & \mathrm{Int}(E) & \longrightarrow & \mathrm{Aut}(E) & \longrightarrow & \mathrm{Out}(E) \simeq \mathrm{Aut}(M) & \longrightarrow & 0 \\ & & & & & \nwarrow & \uparrow & & \\ & & & & & & G & & \end{array}$$

A natural problem to consider at this stage is to try to classify all the possible lifts of an action $G \circlearrowright M$ to an action $G \circlearrowright E$. This problem is for instance investigated in Ref. 7. We will not touch upon it in the present paper.

We further require the action of G to be simple (see Refs. 4 and 5), which means that we assume M has the following fiber bundle structure:

$$G/G_0 \to M \to M/G.$$

Then, by hypothesis, the quotient space M/G is a smooth manifold and the fibers are all isomorphic to the homogeneous space G/G_0, where G_0 is a subgroup of G. All isotropy groups for the action $G \circlearrowleft M$ are isomorphic to G_0, which will denote, once for all, such a chosen reference isotropy group.

Consider now the space $P=\{x \in M, G_x=G_0\}$, where G_x is the isotropy group associated to any point $x \in M$. It can be shown that P is a principal fiber bundle with structure group $N(G_0)/G_0$, where $N(G_0)$ is the normalizer of G_0 in G. This fiber bundle is denoted by

$$N(G_0)/G_0 \to P \to M/G.$$

One can then consider the fiber bundle $M(M/G, G/G_0)$ as an associated fiber bundle to the principal fiber bundle $P(M/G, N(G_0)/G_0)$ for the natural left action $N(G_0)/G_0 \circlearrowleft G/G_0$.

A similar construction can be performed on the space E on which the group $S=G\times H$ acts on the right by

$$G \times H \times E \to E,$$

$$(g,h,p) \mapsto g^{-1}ph.$$

First note that at each point $p \in E$ there exists a canonical homomorphism,

$$\lambda_p: G_{\pi(p)} \to H,$$

defined by the relation $g_0 \cdot p = p \cdot \lambda_p(g_0)$ for all g_0 in $G_{\pi(p)}$. The isotropy group S_p of a point p in E for the action $E \circlearrowleft S$ can be completely characterized, and a straightforward computation shows that $S_p=\{(g_0, \lambda_p(g_0))/g_0 \in G_{\pi(p)}\}$. Then S_p is isomorphic to a generic group S_0 for any p in E, where S_0 is the isotropy group of a certain point p_0 in E. So E inherits the following fiber bundle structure:

$$S/S_0 \to E \to M/G.$$

This means that the action of S on E is also simple. Using the same approach as before, one can see that E contains the principal fiber sub-bundle $Q=\{p \in E, S_p=S_0\}$ given by the diagram of fibrations

$$N(S_0)/S_0 \to Q \to M/G,$$

where $N(S_0)$ is the normalizer of S_0 in S. Notice that on Q the application λ_p is independent of the point $p \in Q$, and we denote it by $\lambda: G_0 \to H$.

The restriction of the projection π to Q will be called π_Q. It is obvious that $\pi(Q) \subset P$. The kernel of π_Q is isomorphic to $Z_0=Z(\lambda(G_0), H)$, the centralizer of $\lambda(G_0)$ in H, and

$$Z_0 \to Q \xrightarrow{\pi_Q} \pi(Q)$$

is a principal fiber bundle. By the very definition one has

$$N(S_0) = \{(g,h) \in S/g \in N(G_0),\ h^{-1}\lambda(g_0)h = \lambda(g^{-1}g_0g),\ \forall\, g_0 \in G_0\}.$$

There is then a natural inclusion of Z_0 in $N(S_0)/S_0$ given by the following composition of maps:

$$Z_0 \simeq \{e\} \times Z_0 \hookrightarrow N(S_0) \to N(S_0)/S_0.$$

Furthermore Z_0 is a normal subgroup in $N(S_0)/S_0$, and one can finally show that $(N(S_0)/S_0)/Z_0$ is a subgroup of $N(G_0)/G_0$.

All the previous constructions can be summarized in the following commutative diagram:

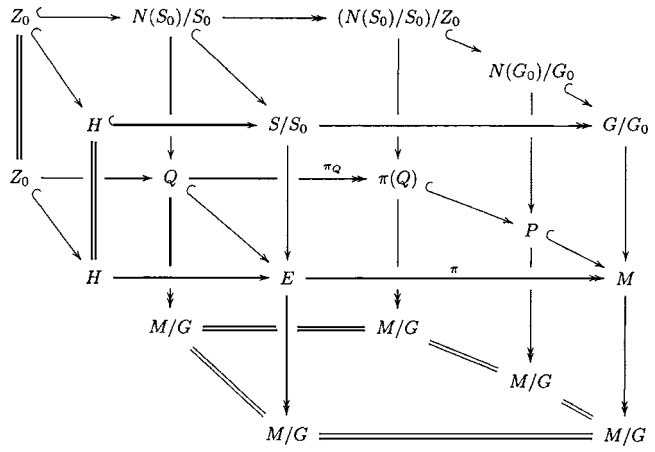

(1)

In this diagram, some arrows represent true applications and other arrows are part of diagrams of fibrations, most of them explicitly given before. Some horizontal arrows correspond to the action of H (or subgroups of H) and some vertical arrows correspond to actions of groups related to G and S. One can verify that the kernel of the projection $\pi(Q)\to M/G$ is isomorphic to $(N(S_0)/S_0)/Z_0$.

B. Invariant connections

The action $G\circlearrowright E$ induces an action of G on the space $\Omega^1(E)$ of 1-forms over E. Because the actions of G and H commute, this action extends naturally to an action on the affine space of connections on E included in the space $\Omega^1(E)\otimes\mathcal{H}$, where $\mathcal{H}$ is the Lie algebra of H. For any $\omega\in\Omega^1(E)\otimes\mathcal{H}$ and any $g\in G$, we denote this action by $\omega^g=g^*\omega$. We are now interested to characterize the G-invariant connections, those which satisfy $\omega^g=\omega$ for any $g\in G$.

In order to do that, it is convenient to make some natural decompositions of the tangent spaces to the various manifolds introduced previously. These decompositions are performed along the different actions that these spaces support. Let us introduce in the following table the notations for the Lie algebras corresponding to the groups introduced so far

Group	G	H	$N(G_0)$	G_0	$N(G_0)/G_0$	Z_0	$S=G\times H$	S_0	$N(S_0)$
Lie Algebra	$\mathcal{G}$	$\mathcal{H}$	$\mathcal{N}_0$	$\mathcal{G}_0$	$\mathcal{K}$	$\mathcal{Z}_0$	$\mathcal{S}=\mathcal{G}\oplus\mathcal{H}$	$\mathcal{S}_0$	$\mathcal{N}_{S_0}$

Let,

$$\mathcal{G}=\mathcal{N}_0\oplus\mathcal{L}\quad\text{and}\ \mathcal{H}=\mathcal{Z}_0\oplus\mathcal{M},$$

be some reductive decompositions of Lie algebras (a decomposition of a Lie algebra $\mathfrak{g}=\mathfrak{h}\oplus\mathfrak{l}$ is reductive when $\mathfrak{h}\subset\mathfrak{g}$ is a sub-Lie algebra and $\mathfrak{l}$ a reductive complementary subspace, i.e., $[\mathfrak{h},\mathfrak{l}]\subset\mathfrak{l}$) which we suppose to be also orthogonal decompositions of vector spaces for the Killing metrics. It is easy to show that there is an orthogonal decomposition of Lie algebras

$$\mathcal{N}_0=\mathcal{G}_0\oplus\mathcal{K}.$$

Then, by the very definitions, one has

$$\mathcal{S}_0=\{(X_0,\lambda_*X_0)/X_0\in\mathcal{G}_0\},$$

where $\lambda_*:\mathcal{G}_0\to\mathcal{H}$ is the tangent application to $\lambda:G_0\to H$, which implies that $\mathcal{S}_0$ is isomorphic to $\mathcal{G}_0$. Using this identification, one can easily show that

$$\mathcal{N}_{\mathcal{S}_0} = \mathcal{S}_0 \oplus \mathcal{K} \oplus \mathcal{Z}_0$$

is an orthogonal decomposition of Lie algebras. In fact any element $(X,\xi) \in \mathcal{N}_{\mathcal{S}_0} \subset \mathcal{G}\times\mathcal{H}$ can be written in the form $(X,\xi)=(X_0+X_\mathcal{K},\lambda_* X_0+\xi_{\mathcal{Z}_0})$, where $X_0 \in \mathcal{G}_0$, $X_\mathcal{K} \in \mathcal{K}$ and $\xi_{\mathcal{Z}_0} \in \mathcal{Z}_0$.

With these decompositions and the induced maps of the group actions on manifolds at the level of Lie algebras and tangent spaces, we can decompose the different tangent spaces of the bundles introduced previously. We then get an infinitesimal version of diagram (1)

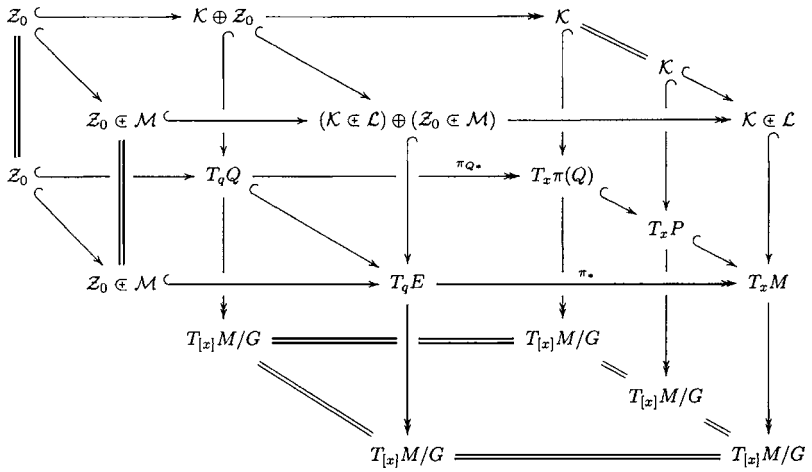

for a point $q \in Q \subset E$ with $\pi(q)=x$. Hence we have

$$T_qE = T_qQ \oplus \mathcal{L}^Q_{|q} \oplus \mathcal{M}^Q_{|q}, \tag{2}$$

where $\mathcal{L}^Q_{|q}$ (respectively, $\mathcal{M}^Q_{|q}$) is the subvector space obtained from the values X^E_q at $q \in E$ of the fundamental vector fields X^E on E associated to vectors $X \in \mathcal{L}$ (respectively, $X \in \mathcal{M}$).

Let us now consider a G-invariant connection 1-form $\omega \in \Omega^1(E)\otimes\mathcal{H}$. We are interested to characterize the degrees of freedom of ω. First, note that it is possible to study ω only at points in Q owing to the fact that by construction $G\cdot Q=E$. Then for any $q \in Q$, $\omega_{|q}$ can be evaluated on the three vector spaces T_qQ, $\mathcal{L}^Q_{|q}$, and $\mathcal{M}^Q_{|q}$.

(i) The restriction to $\mathcal{M}^Q_q \subset \mathcal{H}^Q_q$ is fixed by the relation $\omega_{|q}(X^E_q)=X$, for any $X \in \mathcal{M}$. So there is no degree of freedom in this direction.

(ii) The restriction to T_qQ gives a 1-form μ defined by $\mu(X)=\omega(X)$, for any $X \in TQ$. It satisfies the following equivariance property

$$R^*_{(q,h)}\mu = \mathrm{Ad}_{h^{-1}}\mu, \quad \forall\,(g,h) \in N(S_0),$$

where $R_{(g,h)}$ is the right action of $N(S_0)$ on Q. Considering this equivariance property for an element $(g_0,\lambda(g_0)) \in S_0$, one can show that μ is a $\mathcal{Z}_0$-valued 1-form. Together with the equivariance property restricted to Z_0, this implies in particular that μ is a connection on the principal fiber bundle $Q(\pi(Q),Z_0)$.

(iii) The restriction to $\mathcal{L}^Q_q$ induces a map

$$\psi_q : \mathcal{L} \to \mathcal{H}$$

$$X \mapsto \psi_q(X) = \omega_q(X^E_q).$$

It satisfies the following equivariance property:

$$\mathrm{Ad}_h \circ \psi_q \circ \mathrm{Ad}_{g^{-1}} = \psi_{gqh^{-1}} \quad \forall\, (g,h) \in S.$$

Then, for any $(g,h) \in S_0$, one has $\mathrm{Ad}_{\lambda(g_0)} \circ \psi_q \circ \mathrm{Ad}_{g_0^{-1}} = \psi_q$. The equivariant map $q \mapsto \psi_q$ from Q to $\mathcal{F}$, defines a section of the associated vector bundle $F^{\mathcal{L}} = Q \times_{N(S_0)/S_0} \mathcal{F}_{\mathcal{L}}$, where the fiber is defined to be the vector space of covariant maps

$$\mathcal{F}_{\mathcal{L}} = \{\ell : \mathcal{L} \to \mathcal{H}, \mathrm{Ad}_{\lambda(g_0)} \circ \ell \circ \mathrm{Ad}_{g_0^{-1}} = \ell\}.$$

So ω is completely characterized by the two objects μ and ψ described above. Notice that μ and ψ can be interpreted as genuine objects on fiber bundles related to the two principal fiber bundle structure on Q, either in the "horizontal" direction for μ or in the "vertical" direction for ψ on diagram (1). It is possible to make reference to only one of these principal fiber bundles structures. In order to do that, one needs a reference connection A on the principal fiber bundle

$$(N(S_0)/S_0)/Z_0 \to \pi(Q) \to M/G.$$

Then one can make μ in one-to-one correspondence with a couple (B,α) where

(i) B is a connection on the principal fiber bundle $Q(M/G, N(S_0)/S_0)$,
(ii) α is a section of the vector bundle $F^{\mathcal{K}}$, where $F^{\mathcal{K}} = Q \times_{N(S_0)/S_0} \mathcal{F}_{\mathcal{K}}$ is associated to $Q(M/G, N(S_0)/S_0)$. The vector space $\mathcal{F}_{\mathcal{K}}$ is defined by

$$\mathcal{F}_{\mathcal{K}} = \{k : \mathcal{K} \to \mathcal{H}, \mathrm{Ad}_{\lambda(g_0)} \circ k \circ \mathrm{Ad}_{g_0^{-1}} = k\}.$$

(Notice the similarity between $F^{\mathcal{L}}$ and $F^{\mathcal{K}}$.)

The correspondence between μ and the pair (B,α) is given explicitly by the relations

$$B = \mu + \pi^* A - \mu(\pi^* A)^Q,$$

$$\alpha_q = \mu_q\big|_{\mathcal{K}_q}.$$

In particular we have that $pr_{\mathcal{K}} B = \pi^* A$, where $pr_{\mathcal{K}}$ is the orthogonal projection from $\mathcal{K} \oplus \mathcal{Z}_0$ to $\mathcal{K}$. We refer to Ref. 5 for further details and the works by Coquereaux *et al.*[15] for the link with Kaluza-Klein theories.

C. Relation with Wang's approach

Because we have assumed that the action of the group G is simple, the space M is locally isomorphic to the product space $M/G \times G/G_0$. The study of invariant connections is greatly simplified if one considers the space M to be exactly equal to the space $M/G \times G/G_0$. This is also equivalent to restrict the study only to local objects around an orbit of G in M. So, in the following, we will assume that $M = M/G \times G/G_0$, and we will expose the main results obtained in Refs. 4, 3, and 8. This is what we call the "local" approach.

The simpler structure of the space M allows us to do a construction similar to the one performed previously, replacing the space P by the space M/G. This simplifies the bundle structure in the G's directions and also greatly simplifies the decomposition of invariant connections. Furthermore, it is possible to classify the G-symmetric fiber bundles, and the results in this special case can be compared more easily with the ones obtained by Wang.[1]

First, because of the decomposition $M = M/G \times G/G_0$, one can imbed M/G into M, identifying it with $M/G \times \{eG_0\}$. Then, G-symmetric principal H-bundles can be classified by pairs $([\lambda], \tilde{Q})$, where $[\lambda]$ is a conjugacy class of homomorphisms $\lambda : G_0 \to H$ for the action of G on G_0 by conjugation, and $\tilde{Q}$ is a principal fiber bundle over M/G with structure group $Z_0 = Z(\lambda(G_0), H)$.

Indeed, one can construct a pair $([\lambda],\tilde{Q})$ from a G-symmetric principal H-bundle E over $M=M/G\times G/G_0$ considering the restriction $E_{|M/G}$ of E over M/G. Then, define $\tilde{Q}=\{p\in E_{|M/G}/\lambda_p=\lambda\}$, for λ a chosen reference map λ_{p_0} for a $p_0\in E$.

Conversely, one can associate a G-invariant principal H-bundle to any pair $([\lambda],\tilde{Q})$. In order to do that, it is convenient to introduce the following diagram of fibrations:

$$Z_0\times G_0\to Q'=\tilde{Q}\times G\to M/G\times G/G_0$$

which defines a principal fiber bundle Q' for the action $(z,g_0,\tilde{q},g)\mapsto(\tilde{q}\cdot z_0,g\cdot g_0)$. Consider now the following left action of $Z_0\times G_0$ on H defined by (notice that the induced actions of the subgroups Z_0 and G_0 commute)

$$\rho: Z_0\times G_0\times H\to H,$$

$$(z,g_0,h)\mapsto z\cdot\lambda(g_0)\cdot h.$$

Denote by $\tilde{E}=Q'\times_{(Z_0\times G_0)}H$ the associated fiber bundle to Q' with fiber H for this action. It can be shown that $\tilde{E}$ is a G-invariant principal H-bundle characterized by the following commutative diagram (some arrows are part of diagram of fibrations)

$$\begin{array}{ccccc}
 & & Z_0\times G_0 & & Z_0\times G_0 \\
 & & \downarrow & & \downarrow \\
H & \longrightarrow & Q'\times H & \xrightarrow{pr_1} & Q'=\tilde{Q}\times G \\
 & & \downarrow\Psi & & \downarrow \\
H & \longrightarrow & \tilde{E} & \xrightarrow{\tilde{\pi}} & M=M/G\times G/G_0
\end{array} \tag{3}$$

where $Q'\times H$ is also a G-invariant principal H-bundle for the horizontal structure.

It is easy to prove that the composition of these two maps, $E\mapsto([\lambda],\tilde{Q})$ and $([\lambda],\tilde{Q})\mapsto\tilde{E}$, gives us a map $E\mapsto\tilde{E}$, for which E and $\tilde{E}$ are isomorphic G-invariant principal H-bundles. Indeed, an isomorphism between E and $\tilde{E}$ is given explicitly by the following relation: to any point $\Psi(\tilde{q},g,h)\in\tilde{E}$, associate the point $g\cdot\tilde{q}\cdot h\in E$ where $\tilde{q}\in\tilde{Q}$ is considered to be in E.

Using this isomorphism, it is possible to map a G-invariant connection on E to a G-invariant connection ω on $\tilde{E}$. Now, owing to the fact that the projection Ψ of the principal $(Z_0\times G_0)$-bundle $Q'\times H$ is also a G-equivariant map of G-symmetric principal H-bundles, one can show (see Refs. 4 and 8) that $\Psi^*\omega$ can be written in the generic form

$$\Psi^*\omega_{|(\tilde{q},g,h)}=\mathrm{Ad}_{h^{-1}}(\Lambda_{|\tilde{q}}\circ\theta^G_{|g}+\tilde{\omega}_{|\tilde{q}})+\theta^H_{|h}, \tag{4}$$

where $\tilde{\omega}$ is a connection 1-form on $\tilde{Q}(M/G,Z_0)$, θ^G and θ^H are the usual Cartan 1-form on G and H, respectively, and $\Lambda\in C^\infty(\tilde{Q})\otimes\mathcal{G}^*\otimes\mathcal{H}$ satisfies the equivariance property,

$$R^*_{z_0}\Lambda=\mathrm{Ad}_{z_0}\Lambda,\quad\forall\, z_0\in Z_0$$

and the two relations

$$\mathrm{Ad}_{\lambda(g_0)}\circ\Lambda\circ\mathrm{Ad}_{g_0^{-1}}=\Lambda,\quad\forall\, g_0\in G_0,$$

$$\Lambda_{\tilde{q}}(X_0) = \lambda_*(X_0), \quad \forall X_0 \in \mathcal{G}_0 \text{ and } \forall \tilde{q} \in \tilde{Q}.$$

Using standard techniques in differential geometry, this equivariant map $\Lambda : \tilde{Q} \to \mathcal{G}^* \otimes \mathcal{H}$ characterizes a section of a vector bundle over M/G, with fiber $\mathcal{G}^* \otimes \mathcal{H}$, associated to $\tilde{Q}$ for the adjoint action of Z_0 on $\mathcal{H}$.

We would like to conclude this section by the following remark. In the two situations presented here, the "global" one and the "local" one, it is possible to characterize the G-invariant connections on the G-symmetric principal H-bundle E using geometric objects related to the quotient space M/G, and not to the whole space M. Nevertheless, for the "global" approach, this requires an extra arbitrary connection A.

III. THE NONCOMMUTATIVE DIFFERENTIAL CALCULUS

In this section, we introduce the derivations based differential calculus defined for any associative algebra[11] and describe more precisely this calculus for the algebra of endomorphisms of a complex vector bundle introduced and studied in Refs. 12 and 13. Some new results extending these previous studies are presented here. It is in the framework of this noncommutative geometry that we will study G-invariant noncommutative connections in the next section. The notion of G-invariant noncommutative connection is introduced at the end of this section, as well as some supplemental mathematical structures that will be used later.

A. Derivation-based differential calculus

In the following, $\mathfrak{A}$ will denote an associative algebra with unit. Then the vector space $\mathrm{Der}(\mathfrak{A})$ of derivations of $\mathfrak{A}$ is a Lie algebra and a module over the center $\mathcal{Z}(\mathfrak{A})$ of $\mathfrak{A}$. The vector space of inner derivations, $\mathrm{Int}(\mathfrak{A})$, is a Lie ideal and a $\mathcal{Z}(\mathfrak{A})$-submodule. The quotient $\mathrm{Der}(\mathfrak{A})/\mathrm{Int}(\mathfrak{A})$ will be denoted by $\mathrm{Out}(\mathfrak{A})$. This is a Lie algebra and a module over $\mathcal{Z}(\mathfrak{A})$.

Define the complex $\underline{\Omega}_{\mathrm{Der}}(\mathfrak{A})$ to be the set of $\mathcal{Z}(\mathfrak{A})$-multilinear antisymmetric maps from $\mathrm{Der}(\mathfrak{A})$ to $\mathfrak{A}$. It is naturally a $\mathbb{N}$-graded algebra on which one can define a differential $\hat{\mathrm{d}}$ (of degree 1) by setting, for any derivations $X_1, \ldots, X_{n+1}$ and any $\omega \in \underline{\Omega}^n_{\mathrm{Der}}(\mathfrak{A})$,

$$\hat{\mathrm{d}}\omega(X_1, \ldots, X_{n+1}) = \sum_{i=1}^{n+1} (-1)^{i+1} X_i \omega(X_1, \ldots, \overset{i}{\vee}, \ldots, X_{n+1}) + \sum_{1 \leqslant i < j \leqslant n+1} (-1)^{i+j} \omega([X_i, X_j], \ldots, \overset{i}{\vee}, \ldots, \overset{j}{\vee}, \ldots, X_{n+1}). \tag{5}$$

In the following, for all the associative algebras we will consider, this graded differential algebra $(\underline{\Omega}_{\mathrm{Der}}(\mathfrak{A}), \mathrm{d})$ coincides with the smallest differential subalgebra of $\underline{\Omega}_{\mathrm{Der}}(\mathfrak{A})$ generated by $\mathfrak{A}$, which is usually denoted by $\Omega_{\mathrm{Der}}(\mathfrak{A})$.

Let $\mathcal{G}$ be a Lie subalgebra of $\mathrm{Der}(\mathfrak{A})$. Then $\mathcal{G}$ defines a natural operation in the sense of Cartan[16] on $(\underline{\Omega}_{\mathrm{Der}}(\mathfrak{A}), \mathrm{d})$. Indeed, for any $X \in \mathcal{G}$ and $n \geqslant 1$, let us introduce

$$i_X : \underline{\Omega}^n_{\mathrm{Der}}(\mathfrak{A}) \to \underline{\Omega}^{n-1}_{\mathrm{Der}}(\mathfrak{A})$$

by

$$(i_X \omega)(X_1, \ldots, X_{n-1}) = \omega(X, X_1, \ldots, X_{n-1})$$

for any $\omega \in \underline{\Omega}^n_{\mathrm{Der}}(\mathfrak{A})$ and $X_i \in \mathrm{Der}(\mathfrak{A})$. This interior product is defined to be 0 on $\underline{\Omega}^0_{\mathrm{Der}}(\mathfrak{A}) = \mathfrak{A}$. It is easy to show that i_X is a graded derivation of degree -1 on $\underline{\Omega}_{\mathrm{Der}}(\mathfrak{A})$. The application

$$L_X = i_X\hat{\mathrm{d}} + \hat{\mathrm{d}}i_X : \underline{\Omega}^n_{\mathrm{Der}}(\mathfrak{A}) \to \underline{\Omega}^n_{\mathrm{Der}}(\mathfrak{A})$$

defined for any $n \geqslant 0$ is then a graded derivation of degree 0 on the graded algebra $\underline{\Omega}_{\mathrm{Der}}(\mathfrak{A})$. This is the Lie derivative associated to the operation of $\mathcal{G}$ on $(\underline{\Omega}_{\mathrm{Der}}(\mathfrak{A}), \hat{\mathrm{d}})$. One can compute the usual relations

$$i_X i_Y + i_Y i_X = 0, \quad L_X i_Y - i_Y L_X = i_{[X,Y]},$$

$$L_X L_Y - L_Y L_X = L_{[X,Y]}, \quad L_X \hat{\mathrm{d}} - \hat{\mathrm{d}} L_X = 0.$$

In the same way, it is possible to define a natural Cartan operation of $\mathcal{G}$ on $(\Omega_{\mathrm{Der}}(\mathfrak{A}), \hat{\mathrm{d}})$.

With such an operation of $\mathcal{G}$ on $(\underline{\Omega}_{\mathrm{Der}}(\mathfrak{A}), \hat{\mathrm{d}})$, one can introduce the basic subspace of $\underline{\Omega}_{\mathrm{Der}}(\mathfrak{A})$, which is the common kernel of all the i_X and L_X for all $X \in \mathcal{G}$. This basic subspace can be shown to be a graded differential subalgebra. The common kernel of all the L_X for all $X \in \mathcal{G}$ is called the invariant subspace of the operation. This is also a graded differential subalgebra.

In the case where $\mathfrak{A}$ is the algebra $C^\infty(M)$ of smooth complex-valued functions on a finite dimensional regular manifold M, $(\Omega_{\mathrm{Der}}(\mathfrak{A}), \hat{\mathrm{d}})$ is just the de Rham complex $(\Omega(M), \mathrm{d})$ and $\mathrm{Der}(C^\infty(M)) = \Gamma(TM)$ is the ordinary Lie algebra of vector fields on M.

Let us consider the case where $\mathfrak{A}$ is the algebra $M_n := M_n(\mathbb{C})$ of $n \times n$ complex matrices.[17] This algebra has only inner derivations, and the Lie algebra $\mathrm{Der}(M_n) = \mathrm{Int}(M_n)$ can be identified with the Lie algebra $\mathfrak{sl}_n := \mathfrak{sl}(n, \mathbb{C})$. One can show that

$$\Omega_{\mathrm{Der}}(M_n) \simeq M_n \otimes \wedge \mathfrak{sl}_n^*, \tag{6}$$

where $\mathfrak{sl}_n^*$ is the dual of $\mathfrak{sl}_n$. We denote by d' the differential on this complex.

In this situation, there exists a particular 1-form θ defined by

$$i\theta : \mathrm{Der}(M_n) \to \mathfrak{sl}_n$$

$$ad_\gamma \mapsto \gamma - \frac{1}{n}\mathrm{Tr}(\gamma)\mathbb{1}$$

for any $\gamma \in M_n$. This 1-form satisfies the relation

$$\mathrm{d}' i\theta - (i\theta)^2 = 0$$

and for any $\gamma \in M_n = \Omega^0_{\mathrm{Der}}(M_n)$, one has $\mathrm{d}'\gamma = [i\theta, \gamma]$. This 1-form θ can also be viewed as a kind of fundamental 1-form in this noncommutative space, which permits one to explicitly identify the Lie algebras $\mathrm{Der}(M_n)$ and $\mathfrak{sl}_n$.

Let us now mix the two previous examples in a trivial way, taking the matrix valued functions on a manifold $M : \mathfrak{A} = C^\infty(M) \otimes M_n$. The derivations based differential calculus for this algebra has been studied in Ref. 18. Here are the main results. The center of the algebra $\mathfrak{A}$ is exactly $C^\infty(M)$, and the Lie algebra of derivations $\mathrm{Der}(\mathfrak{A})$ splits canonically as a $C^\infty(M)$-module into

$$\mathrm{Der}(\mathfrak{A}) = [\mathrm{Der}(C^\infty(M)) \otimes \mathbb{1}] \oplus [C^\infty(M) \otimes \mathrm{Der}(M_n)]. \tag{7}$$

This implies the canonical decomposition for the complex of forms

$$\Omega_{\mathrm{Der}}(\mathfrak{A}) = \Omega(M) \otimes \Omega_{\mathrm{Der}}(M_n).$$

The differential $\hat{\mathrm{d}}$ on $\Omega_{\mathrm{Der}}(\mathfrak{A})$ is the sum $\hat{\mathrm{d}} = \mathrm{d} + \mathrm{d}'$ where d and d' has been defined in the two previous examples. The 1-form θ is well defined in $\Omega^1_{\mathrm{Der}}(\mathfrak{A})$ if we extend it on $\mathrm{Der}(\mathfrak{A})$ by zero on the $\Gamma(TM)$ terms.

B. Algebra of endomorphisms of a vector bundle

Let us now consider a nontrivial version of the previous example. Let $\mathcal{E}$ be a SU (n)-vector bundle over a regular finite dimensional smooth (i.e., paracompact, etc.) manifold M equipped with an Hermitian structure. We denote by $\mathrm{End}(\mathcal{E})$ the fiber bundle of endomorphisms of $\mathcal{E}$. The sections of this fiber bundle in matrix algebras define a unital algebra, which we denote by $\mathfrak{A}$. The Hermitian structure gives a natural involution on this algebra, denoted by $S \mapsto S^*$. The center of this algebra is exactly $C^\infty(M)$, identifying $f \in C^\infty(M)$ with $f\mathbb{1} \in \mathfrak{A}$. The trace map and the determinant, defined on each fiber of $\mathrm{End}(\mathcal{E})$, give natural maps

$$\mathrm{Tr}:\mathfrak{A} \to C^\infty(M) \quad \text{and } \det:\mathfrak{A} \to C^\infty(M).$$

By restriction to the center, there is also a natural map

$$\rho:\mathrm{Der}(\mathfrak{A}) \to \mathrm{Der}(C^\infty(M)) = \Gamma(TM). \tag{8}$$

This map is the quotient map in the short exact sequence of Lie algebras and $C^\infty(M)$-modules

$$0 \to \mathrm{Int}(\mathfrak{A}) \to \mathrm{Der}(\mathfrak{A}) \xrightarrow{\rho} \mathrm{Out}(\mathfrak{A}) \simeq \Gamma(TM) \to 0. \tag{9}$$

This short exact sequence generalizes the decomposition (7) in the trivial case. Notice that in the nontrivial case, one cannot split canonically this short exact sequence of $C^\infty(M)$-modules.

For any derivation $\mathcal{X} \in \mathrm{Der}(\mathfrak{A})$, let us denote by $X \in \Gamma(TM)$ the associated vector field on M. The 1-form $i\theta$ defined in the two previous examples is well defined here on $\mathrm{Int}(\mathfrak{A})$ only, by the relation

$$i\theta(ad_\gamma) = \gamma - \frac{1}{n}\mathrm{Tr}(\gamma)\mathbb{1}$$

for any $\gamma \in \mathfrak{A}$. In the following, for any inner derivation ad_γ, we suppose that the element γ is traceless. It can be considered as a section of the fiber bundle of traceless endomorphisms of $\mathcal{E}$. We denote by $\mathfrak{A}_0$ the space of traceless elements in $\mathfrak{A}$. The Lie subalgebra $\mathrm{Int}(\mathfrak{A})$ operates in the sense of Cartan on the differential complex $\Omega_{\mathrm{Der}}(\mathfrak{A})$.[11] The horizontal forms for this operation are exactly the differential forms on M with values in $\mathrm{End}(\mathcal{E})$, and the basic forms are ordinary differential forms on M. In the following, horizontality will refer to this operation.

It was shown in Ref. 12 that the two differential calculi $\Omega_{\mathrm{Der}}(\mathfrak{A})$ and $\underline{\Omega}_{\mathrm{Der}}(\mathfrak{A})$ coincide. We will denote by $\hat{\mathrm{d}}$ the differential on $\Omega_{\mathrm{Der}}(\mathfrak{A}) = \underline{\Omega}_{\mathrm{Der}}(\mathfrak{A})$.

Now, let $\nabla^{\mathcal{E}}$ be any connection on $\mathcal{E}$. Then it was shown in Ref. 12 that there exists a noncommutative 1-form α in $\Omega^1_{\mathrm{Der}}(\mathfrak{A})$ such that any derivation $\mathcal{X} \in \mathrm{Der}(\mathfrak{A})$ can be decomposed as

$$\mathcal{X} = \nabla_X - ad_{\alpha(\mathcal{X})}, \tag{10}$$

where ∇ is the naturally associated connection to $\nabla^{\mathcal{E}}$ on the fiber bundle $\mathrm{End}(\mathcal{E})$. Indeed, one can define α by the relation $\alpha(\mathcal{X}) = -i\theta(\mathcal{X} - \nabla_X)$. We recall that ∇ is the tensor product of the connections $\nabla^{\mathcal{E}}$ on $\mathcal{E}$ and $\nabla^{\mathcal{E}^*}$ on the dual vector bundle $\mathcal{E}^*$ of $\mathcal{E}$ where $\nabla^{\mathcal{E}^*}$ satisfies $X\langle \epsilon, e\rangle = \langle \nabla^{\mathcal{E}^*}_X \epsilon, e\rangle + \langle \epsilon, \nabla^{\mathcal{E}}_X e\rangle$ for any sections ϵ of $\mathcal{E}^*$ and e of $\mathcal{E}$.

The noncommutative 1-form α takes its values in the traceless elements of $\mathfrak{A}$ and can be considered as an extension of $-i\theta$ to all derivations. One has obviously $\alpha(ad_\gamma) = -\gamma$, with the convention that $\mathrm{Tr}(\gamma) = 0$.

This result gives us a splitting of the short exact sequence (9) as $C^\infty(M)$-modules. This splitting is not canonical and is only defined through a choice of a connection on $\mathcal{E}$, by the $C^\infty(M)$-linear map $X \mapsto \nabla_X$ from $\Gamma(TM)$ into $\mathrm{Der}(\mathfrak{A})$. This must be compared with the usual (commutative) situation where one can interpret a connection as a map from vector fields on M into vector fields on a principal bundle over M. These maps will be used and generalized in Sec. III F.

The algebra $\mathfrak{A}$ plays a similar role to a principal bundle, and the above canonical map $\nabla^{\mathcal{E}} \mapsto \alpha$ is an isomorphism of affine spaces from the affine space of SU (n)-connections on $\mathcal{E}$ onto the affine space of traceless anti-Hermitian noncommutative 1-forms on $\mathfrak{A}$ satisfying $\alpha(ad_\gamma) = -\gamma$. If $R^{\mathcal{E}}$ denotes the curvature of $\nabla^{\mathcal{E}}$, then one can show that

$$R^{\mathcal{E}}(X,Y) = \hat{\mathrm{d}}\alpha(\mathcal{X},\mathcal{Y}) + [\alpha(\mathcal{X}), \alpha(\mathcal{Y})]$$

for any $\mathcal{X}$, $\mathcal{Y} \in \mathrm{Der}(\mathfrak{A})$, X, Y being their images in $\Gamma(TM)$. In particular, the expression $\hat{\mathrm{d}}\alpha + \alpha^2$ is a horizontal element of $\Omega^2_{\mathrm{Der}}(\mathfrak{A})$.

Now, the Lie algebra of real derivations on $\mathfrak{A}$ acts naturally on the space of SU (n)-connections through the Lie derivative defined on $\Omega_{\mathrm{Der}}(\mathfrak{A})$. If one restricts this action to inner real derivations, the Lie derivative corresponds to infinitesimal gauge transformations on connections. Indeed, one has

$$\mathcal{L}_{ad_\xi}\alpha = -\hat{\mathrm{d}}\xi - [\alpha, \xi]$$

for any $\xi \in \mathcal{A}$, with $\mathrm{Tr}\,\xi = 0$ and $\xi^* + \xi = 0$ (ad_ξ is then a real inner derivation). Such ξ's are exactly the elements of the Lie algebra of the group of gauge transformations on $\mathcal{E}$.

C. Noncommutative connections

In the following, we will only consider noncommutative connections for the algebra $\mathfrak{A}$ defined above on the right module $\mathfrak{A}$ itself (this definition could be given for any associative algebra $\mathfrak{A}$). A noncommutative connection is an application

$$\hat{\nabla}_{\mathcal{X}} : \mathfrak{A} \to \mathfrak{A}$$

such that $\hat{\nabla}_{\mathcal{X}}(SS') = S\mathcal{X}(S') + \hat{\nabla}_{\mathcal{X}}(S)S'$ and $\hat{\nabla}_{f\mathcal{X}}S = f\hat{\nabla}_{\mathcal{X}}S$ for any $\mathcal{X} \in \mathrm{Der}(\mathfrak{A})$, S, $S' \in \mathfrak{A}$ and $f \in C^\infty(M)$. The curvature of a noncommutative connection is defined by $\hat{R}(\mathcal{X},\mathcal{Y})S = [\hat{\nabla}_{\mathcal{X}}, \hat{\nabla}_{\mathcal{Y}}]S - \hat{\nabla}_{[\mathcal{X},\mathcal{Y}]}S$ for any $S \in \mathfrak{A}$ and $\mathcal{X}$, $\mathcal{Y} \in \mathrm{Der}(\mathfrak{A})$, which is a right $\mathfrak{A}$-module homomorphism.

Any noncommutative connection $\hat{\nabla}$ on $\mathfrak{A}$ is completely given by $\hat{\nabla}_{\mathcal{X}}\mathbb{1} = \omega(\mathcal{X})$, where ω is a noncommutative 1-form in $\Omega^1_{\mathrm{Der}}(\mathfrak{A})$. Indeed, one then has

$$\hat{\nabla}_{\mathcal{X}}S = \mathcal{X}S + \omega(\mathcal{X})S$$

for any $S \in \mathfrak{A}$. The curvature of $\hat{\nabla}$ is then the left multiplication by the noncommutative 2-form,

$$\hat{\mathrm{d}}\omega(\mathcal{X},\mathcal{Y}) + [\omega(\mathcal{X}), \omega(\mathcal{Y})].$$

There is a natural Hermitian structure on the right module $\mathfrak{A}$ given by $\langle S, S' \rangle = S^*S' \in \mathfrak{A}$. A connection is said to be compatible with an Hermitian structure if

$$\mathcal{X}\langle S, S' \rangle = \langle \hat{\nabla}_{\mathcal{X}}S, S' \rangle + \langle S, \hat{\nabla}_{\mathcal{X}}S' \rangle$$

for any S, $S' \in \mathfrak{A}$ and real [a derivation $\mathcal{X} \in \mathrm{Der}(\mathfrak{A})$ is real if $(\mathcal{X}a)^* = \mathcal{X}a^*$ for any $a \in \mathfrak{A}$] $\mathcal{X} \in \mathrm{Der}(\mathfrak{A})$. This compatibility condition is equivalent to

$$\omega(\mathcal{X})^* + \omega(\mathcal{X}) = 0$$

for any real $\mathcal{X} \in \mathrm{Der}(\mathfrak{A})$. Such connections will be called anti-Hermitian connections. Then any unitary element $U \in \mathfrak{A}$ with $\det(U) = \mathbb{1}$ defines on $\mathfrak{A}$ a right module endomorphism $S \mapsto US$ which preserves the Hermitian structure and the det application. We denote by $\mathrm{SU}(\mathfrak{A})$ the group of such elements of $\mathfrak{A}$. In our particular case, this is exactly the gauge group of the SU (n)-vector bundle $\mathcal{E}$. We denote by $U(\mathfrak{A})$ the group of unitary elements of $\mathfrak{A}$. For any $U \in U(\mathfrak{A})$, the gauge trans-

formation of a noncommutative connection $\hat{\nabla}$ is defined by the relation $\hat{\nabla}^U_{\mathcal{X}}S = U^*\hat{\nabla}_{\mathcal{X}}(US)$. The noncommutative 1-form ω is then transformed as

$$\omega \mapsto U^*\omega U + U^*\hat{\mathrm{d}}U.$$

Any ordinary connection on $\mathcal{E}$ defines canonically a noncommutative connection on $\mathfrak{A}$. Indeed, such a connection is given by a noncommutative 1-form α. One then defines a noncommutative connection $\hat{\nabla}^\alpha$ by

$$\hat{\nabla}^\alpha_{\mathcal{X}}S := \nabla_X S + S\alpha(\mathcal{X}) = \mathcal{X}S + \alpha(\mathcal{X})S$$

for any $\mathcal{X} \in \mathrm{Der}(\mathfrak{A})$ and $S \in \mathfrak{A}$. The curvature of this connection coincides with the ordinary curvature $\hat{R}^\alpha(\mathcal{X},\mathcal{Y}) = R^{\mathcal{E}}(X,Y)$ and this noncommutative connection $\hat{\nabla}^\alpha$ is compatible with the Hermitian structure on $\mathfrak{A}$. Finally, a gauge transformation on $\nabla^{\mathcal{E}}$ induces a SU $(\mathfrak{A})$-gauge transformation on $\hat{\nabla}^\alpha$.

This means that noncommutative connections on $\mathfrak{A}$ are extensions of ordinary connections of $\mathcal{E}$. In Refs. 18–20 and 12, it was shown that the extra degrees of freedom can be interpreted as Higgs fields. We refer to these papers for details.

Because $\mathfrak{A}$ and $C^\infty(M)$ are Morita equivalent, their projective right modules are in bijection (the K-groups are the same). From the physical point of view this means that the matter contents of any associated theory does not permit one to distinguish between $C^\infty(M)$ and $\mathfrak{A}$.

D. Symmetries and noncommutative connections

In the following section, we will be interested in noncommutative connections invariant under the action of a Lie group G. Here we give a precise definition of this concept.

Let $\mathcal{G}$ be the Lie algebra of G. An action of $\mathcal{G}$ on $\mathfrak{A}$ is a Cartan operation of $\mathcal{G}$ on the graded differential algebra $\Omega_{\mathrm{Der}}(\mathfrak{A})$. In particular, any element $\mathcal{G}$ can be considered as an element in $\mathrm{Der}(\mathfrak{A})$, which means that we will always look at $\mathcal{G}$ as a Lie subalgebra of $\mathrm{Der}(\mathfrak{A})$.

A $\mathcal{G}$-invariant noncommutative connection on the right module $\mathfrak{A}$ is a noncommutative connection $\hat{\nabla}$ satisfying

$$Y(\hat{\nabla}_{\mathcal{X}}a) = \hat{\nabla}_{[Y,\mathcal{X}]}a + \hat{\nabla}_{\mathcal{X}}(Ya)$$

for any $Y \in \mathcal{G}$, $\mathcal{X} \in \mathrm{Der}(\mathfrak{A})$ and $a \in \mathfrak{A}$. If $\hat{\nabla}$ is given by the noncommutative 1-form ω, this is equivalent to

$$L_Y\omega = 0$$

for any $Y \in \mathcal{G}$.

E. $\Omega_{\mathrm{Der}}(\ )$ and $\Omega(E)$

In the next section, we will characterize the $\mathcal{G}$-invariant connections on the right module $\mathfrak{A}$, where $\mathfrak{A}$ is the algebra of endomorphisms of a SU (n)-vector bundle $\mathcal{E}$. In order to do that, it is very convenient to look at $\Omega_{\mathrm{Der}}(\mathfrak{A})$ in a different way, using a result proved in Ref. 13. There, $\Omega_{\mathrm{Der}}(\mathfrak{A})$ was shown to be some basic subalgebra of a bigger differential graded algebra. Let us describe this algebra and give new results about this very useful construction.

Let us denote by E the principal SU (n)-bundle over M for which $\mathcal{E}$ is associated, and denote by $C^\infty(E)$ the (commutative) algebra of smooth functions on E. Then one has a map $\xi \mapsto \xi^E$ which sends any $\xi \in \mathfrak{su}(n)$ into the associated vertical vector field on E. Let us introduce the algebra $\mathfrak{B} = C^\infty(E) \otimes M_n$ of matrix valued functions on E. Denote by $(\Omega_{\mathrm{Der}}(\mathfrak{B}), \hat{\mathrm{d}}) = (\Omega(E) \otimes \Omega_{\mathrm{Der}}(M_n), \mathrm{d} + \mathrm{d}')$ its differential calculus based on derivations. It is easy to see that $\{\xi^E + ad_\xi / \xi \in \mathfrak{su}(n)\}$ is a Lie

subalgebra of $\mathrm{Der}(\mathfrak{B})$ which is isomorphic to $\mathfrak{su}(n)$. This Lie subalgebra defines a Cartan operation of $\mathfrak{su}(n)$ on $\Omega_{\mathrm{Der}}(\mathfrak{B})$, whose basic subalgebra we denote by $\Omega_{\mathrm{Der,Bas}}(\mathfrak{B})$. Then it was proved in Ref. 13 that $\Omega_{\mathrm{Der}}(\mathfrak{A})=\Omega_{\mathrm{Der,Bas}}(\mathfrak{B})$.

A SU (n)-connection on E is given by a 1-form ω_E on E with values in $\mathfrak{su}(n)\subset M_n$. This connection defines a connection on $\mathcal{E}$ (denoted by ∇), which itself gives rise to a noncommutative 1-form $\alpha\in\Omega^1_{\mathrm{Der}}(\mathfrak{A})$. From the previous result, this form comes from a basic 1-form α^E in $\Omega_{\mathrm{Der,Bas}}(\mathfrak{B})$, which is nothing but $\alpha^E=\omega_E-i\theta$, where $\theta\in\Omega^1_{\mathrm{Der}}(M_n)$ is the canonical 1-form defined previously. The basicity of this 1-form is a consequence of properties of ω_E and $i\theta$, in particular the equivariance of ω_E.

At the level of derivations, the relations between the algebras $\mathfrak{A}$ and $\mathfrak{B}$ can be summarized in the following exact commutative diagram which combines derivations on $\mathfrak{A}$, derivations on $\mathfrak{B}$ and vector fields on E:

$$\begin{array}{ccccccccc}
 & & & & 0 & & 0 & & \\
 & & & & \downarrow & & \downarrow & & \\
 & & 0 & \longrightarrow & \mathcal{Z}_{\mathrm{Der}}(\mathfrak{A}) & \longrightarrow & \Gamma(TVE) & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & \mathrm{Int}(\mathfrak{A}) & \longrightarrow & \mathcal{N}_{\mathrm{Der}}(\mathfrak{A}) & \xrightarrow{\rho_E} & \Gamma_M(E) & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow{\scriptstyle\tau} & & \downarrow{\scriptstyle\pi_*} & & \\
0 & \longrightarrow & \mathrm{Int}(\mathfrak{A}) & \longrightarrow & \mathrm{Der}(\mathfrak{A}) & \xrightarrow[\rho]{} & \Gamma(TM) & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
 & & 0 & & 0 & & 0 & &
\end{array} \tag{11}$$

The lower row is just the ordinary short exact sequence which relates vector fields on M, derivations on $\mathfrak{A}$ and inner derivations on $\mathfrak{A}$. In the middle column, $\mathcal{N}_{\mathrm{Der}}(\mathfrak{A})\subset\mathrm{Der}(\mathfrak{B})$ is the subset of derivations on $\mathfrak{B}$ which preserve the basic subalgebra $\mathfrak{A}\subset\mathfrak{B}$, and $\mathcal{Z}_{\mathrm{Der}}(\mathfrak{A})\subset\mathrm{Der}(\mathfrak{B})$ is the subset of derivations on $\mathfrak{B}$ which vanishes on $\mathfrak{A}$. These two Lie algebras were defined for more general algebras in Ref. 21. The short exact sequence they define is the one used to prove that $\mathfrak{A}$ is a noncommutative quotient manifold of the noncommutative algebra $\mathfrak{B}$.[13] The Lie algebra $\mathcal{Z}_{\mathrm{Der}}(\mathfrak{A})$ is generated as a $C^\infty(E)$-module by the particular elements ξ^E+ad_ξ for any $\xi\in\mathfrak{su}(n)$.

The right most column involves only geometrical objects. The space $\Gamma_M(E)$ is defined to be

$$\Gamma_M(E)=\{\hat{X}\in\Gamma(E)/\pi_*\hat{X}(p)=\pi_*\hat{X}(p')\ \forall\ p,p'\in E \text{ such that } \pi(p)=\pi(p')\}. \tag{12}$$

This is the Lie algebra of vector fields on E which can be mapped to vector fields on M using the tangent maps π_*: $T_pE\to T_{\pi(p)}M$.

In the following, for any $\eta=f\otimes\xi\in C^\infty(E)\otimes\mathfrak{su}(n)$, we will denote by $\eta^E\in\Gamma(TV\,E)$ the vector field $f\xi^E$ on E. Using this notation, any element in $\mathcal{Z}_{\mathrm{Der}}(\mathfrak{A})$ can be written as η^E+ad_η where $\eta\in C^\infty(E)\otimes\mathfrak{su}(n)$. The isomorphism between $\mathcal{Z}_{\mathrm{Der}}(\mathfrak{A})$ and $\Gamma(TV\,E)$ maps any element η^E+ad_η into η^E.

The diagram (11) bears some strange similarities with the diagram presented on page 12 in Ref. 12 which involved Lie algebroid structures. We will not make further comments about this point here.

A connection ω_E on E splits three short exact sequences in this diagram, in a compatible way. First, this connection can be used to lift vector fields X on M into horizontal vector fields X^h on E. This gives us a splitting map of

$$0 \to \Gamma(TVE) \to \Gamma_M(E) \to \Gamma(TM) \to 0 \tag{13}$$

as $C^\infty(M)$-modules. It was shown in Ref. 12, and recalled in Sec. III B, that the connection ω_E splits the short exact sequence (9) of $C^\infty(M)$-modules using the map $X \mapsto \nabla_X$. Now, using notations introduced so far, there is a splitting of the middle column by the map $\mathcal{X} \mapsto \mathcal{X}^E = \rho(\mathcal{X})^h - ad_{\alpha(\mathcal{X})^E}$ where $\alpha(\mathcal{X})^E$ is the basic element in $\mathfrak{B}$ associated to $\alpha(\mathcal{X}) \in \mathfrak{A}$ [notice that $\alpha(\mathcal{X})^E = \alpha^E(\mathcal{X}^E)$].

These splittings can be used to decompose any element in $\mathcal{N}_{\mathrm{Der}}(\mathfrak{A})$ into four parts, making explicit the kernels of the two short exact sequences in which this space is involved. Any derivation $\mathfrak{X} \in \mathcal{N}_{\mathrm{Der}}(\mathfrak{A})$ can be written, as a derivation on $\mathfrak{B}$, in the form $\mathfrak{X} = \hat{X} + ad_\gamma$, where $\hat{X} \in \Gamma(E)$ and $\gamma \in C^\infty(E) \otimes \mathfrak{sl}_n$. At this stage, it is easy to directly show that $\hat{X}$ is in $\Gamma_M(E)$ using the restriction of $\mathfrak{X}$ on the center $C^\infty(M)$ of $\mathfrak{A}$ considered as a subalgebra of $\mathfrak{B}$. A derivation $\mathfrak{X}$ belongs to $\mathcal{N}_{\mathrm{Der}}(\mathfrak{A})$ if and only if $L_\xi \mathfrak{X} \in \mathcal{Z}_{\mathrm{Der}}(\mathfrak{A})$ for any $\xi \in \mathfrak{su}(n)$. This means that there must exist $\eta \in C^\infty(E) \otimes \mathfrak{su}(n)$ such that

$$[\xi^E, \hat{X}] = \eta^E, \tag{14}$$

$$L_\xi \gamma = \eta. \tag{15}$$

Applying a connection ω_E on the first relation, and using the equivariance of ω_E, one gets $L_\xi(\omega_E(\hat{X})) = \eta$. Let us introduce $Z = -\alpha^E(\mathfrak{X}) = \gamma - \omega_E(\hat{X}) \in C^\infty(E) \otimes \mathfrak{sl}_n$. Then $L_\xi Z = 0$ for any $\xi \in \mathfrak{su}(n)$, which implies that $Z \in \mathfrak{A}_0$, or $ad_Z \in \mathrm{Int}(\mathfrak{A})$. Using this result, the derivation $\mathfrak{X}$ can be written as $\mathfrak{X} = \hat{X} + ad_\gamma = X^h + \hat{X}^v + ad_{\omega_E(\hat{X})+Z}$. With our notations, one has $\hat{X}^v = \omega_E(\hat{X})^E$ (vertical part of the vector field $\hat{X}$). So, one can write finally

$$\mathfrak{X} = X^h + ad_Z + \underbrace{\omega_E(\hat{X})^E + ad_{\omega_E(\hat{X})}}_{\in \mathcal{Z}_{\mathrm{Der}}(\mathfrak{A})} = X^h + \omega_E(\hat{X})^E + ad_{\omega_E(\hat{X})} + \underbrace{ad_Z}_{\in \mathrm{Int}(\mathfrak{A})}. \tag{16}$$

The situation can be summarized in the following diagram where all the splittings are explicit:

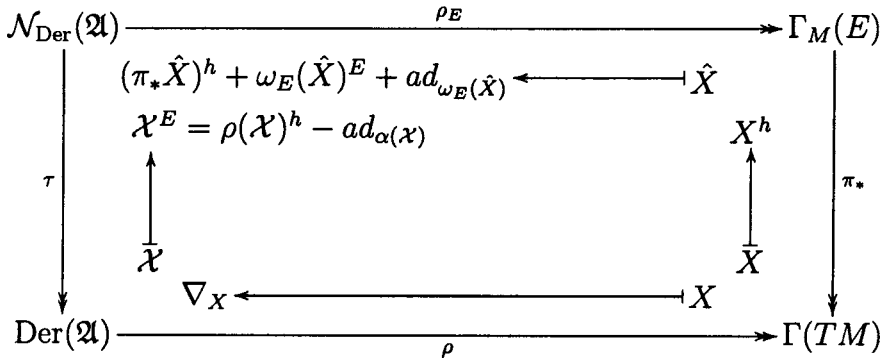

(17)

In the following $\Omega_{\mathrm{Der}}(\mathfrak{A})$ will be identified with the corresponding basic subalgebra of $\Omega_{\mathrm{Der}}(\mathfrak{B})$. Let us now look at the consequences of this construction on a noncommutative connection given by a 1-form $\omega \in \Omega^1_{\mathrm{Der}}(\mathfrak{A})$. Such a 1-form can be decomposed as

$$\omega = a - \phi \in [\Omega^1(E) \otimes M_n] \oplus [C^\infty(E) \otimes M_n \otimes \mathfrak{sl}_n^*]$$

with the basic conditions

$$(L_{\xi^E} + L_{ad_\xi})a = 0, \quad (L_{\xi^E} + L_{ad_\xi})\phi = 0,$$

$$i_{\xi^E} a - i_{ad_\xi} \phi = 0$$

for any $\xi \in \mathfrak{su}(n)$. Here we use obvious notations for geometrical and algebraic parts of the Lie derivative L and the interior product i.

At this level, some general comments about these relations are in order. First, the invariant relation on a is nothing but the covariance relation of an ordinary connection on E. But the last relation prevents a to be such a connection. Indeed, this last relation generalizes the vertical condition on ordinary connections, and connect the value of a on vertical vector fields to the values of ϕ. For ordinary connections on E, ϕ being replaced by $i\theta$, the usual vertical condition on a is recovered. The second relation, the invariance of ϕ, has a natural geometric interpretation. By its very definition, ϕ can be viewed as a map $E \to M_n \otimes \mathfrak{sl}_n^*$. Using standard results in differential geometry, the invariance relation on ϕ permits one to interpret ϕ as the section of a vector bundle over M, associated to E, whose fiber is $M_n \otimes \mathfrak{sl}_n^*$. In this identification, the Lie derivative L_{ad_ξ} on $M_n \otimes \mathfrak{sl}_n^*$ is nothing but the infinitesimal action of the Lie group H on $M_n \otimes \mathfrak{sl}_n^*$ involved in the construction of this associated vector bundle. We will use such an identification in similar cases several times in the following.

Let us now consider the following situation, which will be the starting point for the next section and which generalizes to the noncommutative connections that has been presented in Sec. II on ordinary connections. Assume we have an action of a compact connected Lie group G on the principal fiber bundle E which commutes with the natural right action of the Lie group $H = \mathrm{SU}(n)$ on E. Then for any $Y \in \mathcal{G}$, the Lie algebra of G, one can associate a vector field Y^E on E. This vector field induces a Cartan operation of $\mathcal{G}$ on $\Omega(E)$. This operation extends naturally to an operation on $\Omega_{\mathrm{Der}}(\mathfrak{B}) = \Omega(E) \otimes \Omega_{\mathrm{Der}}(M_n)$ where $\mathcal{G}$ acts only on the E part. Because the actions of G and H commute, the operation of $\mathcal{G}$ respects the basic subalgebra $\mathfrak{A}$ of $\mathfrak{B}$, and restricts to an operation on $\Omega_{\mathrm{Der}}(\mathfrak{A})$. Then the original action of G on E gives rise to a (noncommutative) action of $\mathcal{G}$ on $\mathfrak{A}$. This action is the one we will use to characterize G-invariant noncommutative connection on $\mathfrak{A}$.

F. Local point of view

In this section, we want to study more precisely the relation between the algebras $\mathfrak{A}$ and $\mathfrak{B}$ from the local point of view.

Let us first characterize local objects in $\mathfrak{A}$. Such a discussion was preformed in Refs. 12 and 13 and we recall essential points here. Over an open subset U over which the fiber bundle $\mathrm{End}(\mathcal{E})$ is trivialized, the algebra $\mathfrak{A}$ is isomorphic to $\mathfrak{A}_{\mathrm{loc}} := C^\infty(U) \otimes M_n$, and one can associate to any element $a \in \mathfrak{A}$ an element $a_{\mathrm{loc}} \in \mathfrak{A}_{\mathrm{loc}}$. Over an intersection $U \cap U' \neq \emptyset$ of two such open sets U and U', one has a transition function $g : U \cap U' \to \mathrm{SU}(n)$ which relates a'_{loc} to a_{loc} in the following way:

$$a'_{\mathrm{loc}} = \mathrm{Ad}_{g^{-1}} a_{\mathrm{loc}}.$$

One can also associate to any derivation $\mathcal{X} \in \mathrm{Der}(\mathfrak{A})$ a local derivation $\mathcal{X}_{\mathrm{loc}} \in \mathrm{Der}(C^\infty(U) \otimes M_n)$. Such a derivation can be decomposed into two parts $\mathcal{X}_{\mathrm{loc}} = X_{|U} + ad_{\gamma_{\mathrm{loc}}}$, where $X = \rho(\mathcal{X})$ [see Eq. (8)], and $X_{|U}$ is its restriction to the open subset U. It is possible to give an explicit expression for γ_{loc} if one considers a connection on $\mathrm{End}(\mathcal{E})$, to which one can associate the noncommutative 1-form α and the local 1-form $A_{\mathrm{loc}} \in \Omega^1(U) \otimes \mathcal{H}$. Then one has

$$\gamma_{\mathrm{loc}} = A_{\mathrm{loc}}(X_{|U}) - \alpha(\mathcal{X})_{\mathrm{loc}}.$$

Over an intersection $U \cap U' \neq \emptyset$, $\mathcal{X}'_{\mathrm{loc}}$ and $\mathcal{X}_{\mathrm{loc}}$ are related in the following way:

$$X'_{|U} = X_{|U},$$

$$\gamma'_{\mathrm{loc}} = \mathrm{Ad}_{g^{-1}} \gamma_{\mathrm{loc}} + g^{-1} X_{|U}(g).$$

Finally, let us consider local 1-forms, and associate to an element $\omega \in \Omega^1_{\mathrm{Der}}(\mathfrak{A})$ over U, an element $\omega_{\mathrm{loc}} \in \Omega^1_{\mathrm{Der}}(C^\infty(U) \otimes M_n)$. Such an element can be decomposed into two parts, $\omega_{\mathrm{loc}} = a + \phi \circ i\theta$ where $a \in \Omega^1(U) \otimes M_n$, and $\phi \in C^\infty(U) \otimes M_n \otimes \mathfrak{sl}_n^*$. Then over an intersection $U \cap U' \neq \emptyset$, ω_{loc} and ω'_{loc} are related in the following way:

$$a' = \mathrm{Ad}_{g^{-1}} \circ a - \mathrm{Ad}_{g^{-1}} \circ \phi \circ \mathrm{Ad}_g \circ g^* \theta^H,$$

$$\phi' = \mathrm{Ad}_{g^{-1}} \circ \phi \circ \mathrm{Ad}_g, \tag{18}$$

where θ^H is the usual Cartan form on the group H, and $g^* \theta^H = g^{-1}\, \mathrm{d}g$. One can remark that these transition relations look like the one encountered in usual commutative gauge theories, but in the present case these relations are "twisted" by the scalar field ϕ. It was shown in Ref. 13 that if one chooses a reference connection, then one can express local forms in terms of tensors which transform in a much more manageable way.

Let us now make some remarks about the relations between these local objects and the local ones associated to the algebra $\mathfrak{B} = C^\infty(E) \otimes M_n$. First, let us consider a local section $s: U \to E$. One can associate to it a trivial extension of the pullback application $s^*: \mathfrak{B} \to C^\infty(U) \otimes M_n$. Then by definition, the image of $\mathfrak{B}_{\mathcal{H}\text{-basic}|U}$ by the application s^* is the algebra $\mathfrak{A}_{\mathrm{loc}}$ obtained from the localization of $\mathfrak{A}$ over U.

For derivations, it was shown previously that with the help of an ordinary connection, one can associate to any element $\mathcal{X} \in \mathrm{Der}(\mathfrak{A})$ an element $\mathcal{X}^E \in \mathcal{N}(\mathfrak{A}) \subset \mathrm{Der}(\mathfrak{B})$, where explicitly $\mathcal{X}^E = \rho(\mathcal{X})^h - ad_{\alpha(\mathcal{X})^E}$. In a similar way, using the inclusion $\Omega_{\mathrm{Der}}(\mathfrak{A}) \hookrightarrow \Omega_{\mathrm{Der}}(\mathfrak{B})$, one can associate to any element $\omega \in \Omega_{\mathrm{Der}}(\mathfrak{A})$ an element (in opposition to the rest of this paper, we use here explicit different notations ω and ϖ) $\varpi \in \Omega_{\mathrm{Der}}(\mathfrak{B})_{\mathcal{H}\text{-basic}}$. Then one can compare the expressions $\varpi(\mathcal{X}^E)$ and $\omega(\mathcal{X})$. Over an open subset $U \subset M$ over which the principal fiber bundle E is trivialized, using the local expression of the connection, one has

$$\chi^E_{|s(x)} = s_* X_{|x} - A_{\mathrm{loc}}(X)_{|x} - ad_{\alpha(\chi)^E_{|s(x)}},$$

where $x \in U$. From the basicity of the 1-form ϖ, one can then show that $\omega_{\mathrm{loc}}(\mathcal{X}_{\mathrm{loc}}) = s^*(\varpi_{|U}(\mathcal{X}^E_{|U})) = s^* \varpi_{|U}(\mathcal{X}_{\mathrm{loc}})$, so that $s^* \varpi_{|U} = \omega_{\mathrm{loc}}$. This result generalizes the previous result about elements of the algebras, and one has $s^* \Omega_{\mathrm{Der}}(\mathfrak{B})_{\mathcal{H}\text{-basic}|U} = \Omega_{\mathrm{Der}}(\mathfrak{A}_{\mathrm{loc}})$. This relation shows that one can obtain the local expression ω_{loc} either from the 1-form $\omega \in \Omega^1_{\mathrm{Der}}(\mathfrak{A})$, or from the 1-form $\varpi \in \Omega^1_{\mathrm{Der}}(\mathfrak{B})_{\mathcal{H}\text{-basic}}$. Finally, notice that the transition relations (18) could have been obtained by considering the 1-form ϖ over the intersection $U \cap U' \neq \emptyset$ of two open sets, with the transition relation $s' = s \cdot g$ between local sections $s: U \to E$ and $s': U' \to E$.

IV. INVARIANT NONCOMMUTATIVE CONNECTIONS

Here, we characterize the degrees of freedom of invariant noncommutative connections in the setting exposed in the preceding section. The results obtained are generalizations of the results summarized in Sec. II for ordinary invariant connections. In particular, the constructions presented in Sec. II are explicitly used in the present case. Indeed, it is possible to make reference to the structure of diagram (1) thanks to the trick exposed at the end of the preceding section, which consists to look at $\mathfrak{A}$ as the basic subalgebra of $\mathfrak{B} = C^\infty(E) \otimes M_n$ for a well chosen Cartan operation of $\mathcal{H} = \mathfrak{su}(n) \subset M_n$. The starting ingredients of this section are the following. A G-invariant noncommutative connection $\omega \in (\Omega^1_{\mathrm{Der}}(\mathfrak{A}))_{\mathcal{G}\text{-inv}}$ is written as a basic element

$$\omega = a - \phi \in [\Omega^1(E) \otimes M_n] \oplus [C^\infty \otimes M_n \otimes \mathrm{Der}(M_n)^*].$$

Then the objects a and ϕ satisfy the three relations

$$L_{\xi}(a - \phi) = 0, \tag{19}$$

$$i_\xi(a-\phi)=0, \tag{20}$$

$$L_X(a-\phi)=0 \tag{21}$$

for any $\xi\in\mathcal{H}=\mathfrak{su}(n)$ and any $X\in\mathcal{G}$. Recall that the ordinary connections are those for which $\phi=i\theta$, which is a straightforward way to recover all the results of Sec. II from the results presented here.

A. Global approach

This approach is similar to the one performed in Sec. II, and it uses essentially the same technics. With the help of the G-invariance conditions (21), we can restrict the dependence of a and ϕ to $Q\subset E$. Then a is completely determined from its values on T_qE for all $q\in Q$. The application $a_q: T_qE\to M_n$ can be decomposed into several parts. Let us call $\mu\in\Omega^1(Q)\otimes M_n$ the restriction of the 1-form a to the tangent space TQ. By relation (20), one has $\mu_q(\xi_q^E)=\phi_q(\xi)$ for any $\xi\in\mathcal{Z}_0$. This 1-form satisfies the equivariance property

$$L_{(X,\xi)}\mu=(L_X+L_\xi)\mu=0, \quad \forall\,(X,\xi)\in\mathcal{N}_{\mathcal{S}_0}\subset\mathcal{G}\times\mathcal{H}$$

(there, we use notations of Sec. II B). (Recall also that L_ξ contains a geometric and an algebraic part.)

Then, using $\mathcal{S}_0$-invariance on Q, it is easy to show that μ takes its value in the vector space

$$\mathcal{W}_0 := Z(\lambda_*\mathcal{G}_0, M_n),$$

the centralizer of $\lambda_*\mathcal{G}_0$ in M_n. As a trivial consequence, $\eta_q := \phi_{q|\mathcal{Z}_0}$ has also its values in $\mathcal{W}_0$.

A simple analysis shows that $\mathcal{W}_0$ is an associative subalgebra of M_n on which the Lie algebra $\mathcal{Z}_0$ acts by the adjoint action. It is natural and useful for the following to associate to it the differential calculus $\Omega_{\mathcal{Z}_0}(\mathcal{W}_0)=\mathcal{W}_0\otimes\wedge\mathcal{Z}_0^*$ which mimics the differential calculus $\Omega_{\mathrm{Der}}(M_n)=M_n\otimes\wedge\mathfrak{sl}_n^*$. On $\Omega_{\mathcal{Z}_0}(\mathcal{W}_0)$, the differential is defined as in formula (5), where now the Lie algebra $\mathcal{Z}_0$ plays the role of the derivations on the algebra $\mathcal{W}_0$. Another important useful feature of $\mathcal{W}_0$ is that there is a natural application,

$$\mathcal{N}_{\mathcal{S}_0}\to\mathrm{Der}(C^\infty(Q)\otimes\mathcal{W}_0),$$

$$(X,\xi)\mapsto X^Q+\xi^Q+ad_\xi.$$

Notice that $\mathcal{S}_0$ is sent to zero in this application. This implies that this application factorizes through an application $\mathcal{N}_{\mathcal{S}_0}/\mathcal{S}_0\to\mathrm{Der}(C^\infty(Q)\otimes\mathcal{W}_0)$, which permits us to define a Cartan operation of $\mathcal{N}_{\mathcal{S}_0}/\mathcal{S}_0$ on $\Omega(Q)\otimes\Omega_{\mathcal{Z}_0}(\mathcal{W}_0)$, whose Lie derivation is denoted by

$$L_{(X,\xi)}=L_{X^Q+\xi^Q}+L_{ad_\xi}, \quad \forall\,(X,\xi)\in\mathcal{N}_{\mathcal{S}_0}/\mathcal{S}_0=\mathcal{K}\oplus\mathcal{Z}_0.$$

In particular, this operation induces an operation on the Lie algebra $\mathcal{Z}_0$, denoted by L_ξ, for any $\xi\in\mathcal{Z}_0$.

The difference $\mu-\eta$ is naturally an element of degree 1 in $\Omega(Q)\otimes\Omega_{\mathcal{Z}_0}(\mathcal{W}_0)$. Using relations (19)–(21), it is easy to verify that

$$i_\xi(\mu-\eta)=0, \quad \forall\,\xi\in\mathcal{Z}_0,$$

$$L_{(X,\xi)}(\mu-\eta)=0, \quad \forall\,(X,\xi)\in\mathcal{N}_{\mathcal{S}_0}.$$

This implies that $\mu-\eta\in(\Omega(Q)\otimes\Omega_{\mathcal{Z}_0}(\mathcal{W}_0))^1_{\mathcal{Z}_0\text{-basic}}$.

Now, let us introduce $\alpha\in C^\infty(Q)\otimes\mathcal{W}_0\otimes\wedge\mathcal{K}^*$, defined by

$$\alpha(X) = \mu(X^Q), \quad \forall\, X \in \mathcal{K}.$$

One can show that $\alpha \in \mathcal{W}_0 \otimes (C^\infty(Q) \otimes \wedge\mathcal{K}^*)_{\mathcal{K}\text{-inv}}$, where the $\mathcal{K}$-invariance is defined by the induced Lie derivative of the operation of $\mathcal{N}_{\mathcal{S}_0}$ on the $C^\infty(Q)$ part and by the standard Lie derivative on the $\wedge\mathcal{K}^*$ part (the differential and the Lie derivative on $\wedge\mathcal{K}^*$ are naturally induced by the Lie algebra structure of $\mathcal{K}$).

Let us now introduce the bigger differential calculus

$$\Omega_{\mathcal{Z}_0+\mathcal{K}}(M/G, \mathcal{W}_0) := (\Omega(Q) \otimes \Omega_{\mathcal{Z}_0}(\mathcal{W}_0) \otimes \wedge\mathcal{K}^*)_{(\mathcal{Z}_0+\mathcal{K})\text{-basic}}$$

equipped with the natural differential which is the sum of the differentials on each component. Later, we will make some comments about this differential algebra, in particular we will explain why M/G makes its appearance in the notation.

The main result of the previous discussion is that we can show that $\mu - \eta - \alpha \in \Omega^1_{\mathcal{Z}_0+\mathcal{K}}(M/G, \mathcal{W}_0)$. This relation permits one to characterize in a common algebraic 1-form the restrictions of a and ϕ to TQ.

Let us now look at the other parts of the space T_qE, that is $\mathcal{L}^Q_{|q}$ and $\mathcal{M}^Q_{|q}$. Using similar arguments as in Sec. II B, the restriction $\psi := a_{|\mathcal{L}^Q}$ defines a section of the vector bundle associated to $Q(M/G, N(\mathcal{S}_0)/\mathcal{S}_0)$ whose fiber is the vector space

$$\mathcal{F}_{\mathcal{L}} := (M_n \otimes \mathcal{L}^*)_{\mathcal{S}_0\text{-inv}} = \{\ell : \mathcal{L} \to M_n / L^{\mathcal{L}}_{(X,\lambda_* X)}\ell = 0\ \forall\, X \in \mathcal{G}_0\},$$

where $(L^{\mathcal{L}}_{(X,\xi)}\ell)(Y) = -\ell([X,Y]) + [\xi, \ell(Y)]$ for any $(X,\xi) \in N(\mathcal{S}_0)$. This relation is the natural action of $\mathcal{N}_{\mathcal{S}_0}$ on the space $M_n \otimes \mathcal{L}^*$. For this action, $\mathcal{F}_{\mathcal{L}} \subset M_n \otimes \mathcal{L}^*$ is invariant. The fact that $\psi \in C^\infty(Q) \otimes \mathcal{F}_{\mathcal{L}}$ is a section of a vector bundle comes from the equivariance property

$$L_{(X,\xi)}\psi = (L_{X^E + \xi^E} + L^{\mathcal{L}}_{(X,\xi)})\psi = 0 \quad \forall\, (X,\xi) \in \mathcal{N}_{\mathcal{S}_0}.$$

Therefore, one has $\psi \in (C^\infty(Q) \otimes \mathcal{F}_{\mathcal{L}})_{(\mathcal{Z}_0+\mathcal{K})\text{-inv}}$.

In the same way, the restriction $\zeta := a_{|\mathcal{M}^Q} = \phi_{|\mathcal{M}}$, considered as an element in $C^\infty(Q) \otimes M_n \otimes \mathcal{M}^*$, is a section of the vector bundle associated to $Q(M/G, N(\mathcal{S}_0)/\mathcal{S}_0)$ whose fiber is the vector space

$$\mathcal{F}_{\mathcal{M}} := (M_n \otimes \mathcal{M}^*)_{\mathcal{S}_0\text{-inv}} = \{m : \mathcal{M} \to M_n / L^{\mathcal{M}}_{(X,\lambda_* X)} m = 0\ \forall\, X \in \mathcal{G}_0\}$$

where $(L^{\mathcal{M}}_{(X,\xi)}m)(Y) = -m([X,Y]) + [\xi, m(Y)]$ for any $(X,\xi) \in N(\mathcal{S}_0)$. As before, ζ satisfies the equivariance property

$$L_{(X,\xi)}\zeta = (L_{X^E + \xi^E} + L^{\mathcal{M}}_{(X,\xi)})\zeta = 0 \quad \forall\, (X,\xi) = \mathcal{N}_{\mathcal{S}_0}$$

and so $\zeta \in (C^\infty(Q) \otimes \mathcal{F}_{\mathcal{M}})_{(\mathcal{Z}_0+\mathcal{K})\text{-inv}}$.

Now, noticing that

$$(M_n \otimes \mathcal{L}^*)_{\mathcal{S}_0\text{-inv}} \oplus (M_n \otimes \mathcal{M}^*)_{\mathcal{S}_0\text{-inv}} = (M_n \otimes (\mathcal{L}^* \oplus \mathcal{M}^*)_{\ \mathcal{S}_0\text{-inv}} =: \mathcal{F}$$

$\zeta + \psi$ can be considered as a section of the associated vector bundle to $Q(M/G, N(S_0)/S_0)$, where the fiber is the bigger vector space $\mathcal{F}$. Collecting all the previous degrees of freedom, we have proven that

$$(\Omega^1_{\mathrm{Der}}(\mathfrak{A}))_{\mathcal{G}\text{-inv}} \simeq \Omega^1_{\mathcal{Z}_0+\mathcal{K}}(M/G, \mathcal{W}_0) \oplus \mathcal{P},$$

where

$$\mathcal{P} = (C^\infty(Q) \otimes \mathcal{F})_{(\mathcal{Z}_0+\mathcal{K})-\mathrm{inv}}.$$

Denote by $\mathcal{C}$ the algebra $(C^\infty(Q)\otimes\mathcal{W}_0)_{(\mathcal{Z}_0+\mathcal{K})\text{-inv}}$. Then $\Omega_{\mathcal{Z}_0+\mathcal{K}}(M/G,\mathcal{W}_0)$ is a differential calculus associated to $\mathcal{C}$ in the sense that $\Omega^0_{\mathcal{Z}_0+\mathcal{K}}(M/G,\mathcal{W}_0)=\mathcal{C}$. This algebra can be interpreted as the sections of a fiber bundle associated to $Q(M/G,N(S_0)/S_0)$ whose fibers are modeled over the algebra $\mathcal{W}_0$. The algebra $\mathcal{C}$ can be considered as a "reduction"of the algebra $\mathfrak{A}$. As a matter of fact, it is easy to verify that the elements in SU $(\mathcal{C})$ define noncommutative gauge transformations on the space of $\mathcal{G}$-invariant connections on $\mathfrak{A}$. Equipped with the differential calculus $\Omega_{\mathcal{Z}_0+\mathcal{K}}(M/G,\mathcal{W}_0)$ and the module $\mathcal{P}$, this algebra is the natural building block, in a noncommutative viewpoint, for the $\mathcal{G}$-invariant connections on $\mathfrak{A}$.

As a last remark, notice that all the objects introduced here are naturally related to fiber bundles over the reduced space M/G, as it was also the case for ordinary $\mathcal{G}$-invariant connections. As a matter of fact, the situation is rather similar to the classical one, but here, there are new scalar fields coming from noncommutative geometry in addition to those coming from dimensional reduction. We can also notice that in the noncommutative framework, we do not need a reference connection to obtain objects which "live" over M/G.

B. Local approach

As in the classical case, we will study invariant connections in the case where $M=M/G\times G/G_0$. We will use the notations introduced in Sec. II C. The idea developed in Sec. II C is to pull back an invariant connection on $\tilde{E}$ to a bigger space $Q'\times H$. There, an invariant connection can be written in a very compact and elegant generic form using in particular the Cartan 1-forms on the groups G and H. Here we generalize this construction. In order to do that, we need to find the "good" space on which pulling back the invariant noncommutative connection. Because we work in a noncommutative framework, we must deal with algebras instead of spaces. The following diagram summarizes the relations between the spaces and algebras we consider

$$\begin{array}{ccccc} Q'\times H & & \overset{?}{\hookrightarrow} & & \Omega(Q'\times H)\otimes\Omega_{\mathrm{Der}}(M_n) \\ \downarrow{\scriptstyle\Psi} & & & & \uparrow{\scriptstyle\Psi^*} \\ \tilde{E} & \rightsquigarrow & \Omega_{\mathrm{Der}}(\mathfrak{A}) & \xhookrightarrow[\text{for }\mathcal{H}]{\text{basic}} & \Omega(\tilde{E})\otimes\Omega_{\mathrm{Der}}(M_n) \end{array}$$

The algebra we are looking at must replace the algebra $\mathfrak{A}$, in the same way the space $Q'\times H$ replaces the space $\tilde{E}$. It is natural to look at this algebra as a basic subalgebra of $C^\infty(Q'\times H)\otimes M_n$ for the Cartan operation of $\mathcal{H}$. Then the pull back $\Psi^*\omega$ of a $\mathcal{G}$-invariant connection 1-form $\omega\in\Omega_{\mathrm{Der}}(\mathfrak{A})\subset\Omega(\tilde{E})\otimes\Omega_{\mathrm{Der}}(M_n)$ belongs to $\Omega(Q'\times H)\otimes\Omega_{\mathrm{Der}}(M_n)$. Thanks to the facts that Z_0 and G_0 do not act on the M_n part of these algebras, that Ψ^* preserves the $\mathcal{G}$-invariance and the $\mathcal{H}$-basicity, one has

$$\Psi^*\omega\in\left[\Omega(\tilde{Q})\otimes\Omega(G)\otimes\Omega(H)\otimes\Omega_{\mathrm{Der}}(M_n)\right]^{G-\mathrm{inv}}_{\substack{\mathrm{H-basic}\\(Z_0\times G_0)-\mathrm{basic}}}.$$

The advantage to work at the level of the space $\Omega(\tilde{Q})\otimes\Omega(G)\otimes\Omega(H)\otimes\Omega_{\mathrm{Der}}(M_n)$, is that, there, we can decompose in an easy way the actions of the group G, G_0, Z_0, and H. These actions are shown in the following suggestive diagram:

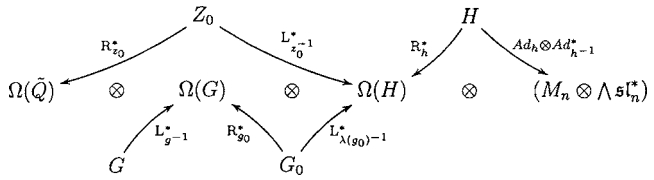

where symbols L and R mean, respectively, left and right multiplication. Notice that the actions of Z_0 and G_0 on $\Omega(H)$ commute.

Then, using H-basicity and G-invariance, a straightforward computation shows that $\Psi^*\omega$ can be written in the generic form

$$\Psi^*\omega_{|(\tilde{q},g,h)} = \mathrm{Ad}_{h^{-1}}(\tilde{\omega}_{|\tilde{q}} + \Lambda_{\tilde{q}} \circ \theta^G_{|g} + \phi_{\tilde{q}} \circ \mathrm{Ad}_h \circ (\theta^H_{|h} - i\theta)), \tag{22}$$

where θ^G and θ^H are the Cartan 1-forms on the groups G and H and $i\theta$ is the algebraic 1-form introduced in Sec. III. It is very natural to use the 1-form $i\theta$ in this relation in order to make explicit the identification (6). Notice that θ^H and $i\theta$ are known to look very similar in their structure,[17] and that they appear together in this very compact expression. In formula (22), on has

$$\tilde{\omega} \in \Omega^1(\tilde{Q}), \quad \Lambda \in C^\infty(\tilde{Q}) \otimes M_n \otimes \mathcal{G}^*, \quad \phi \in C^\infty(\tilde{Q}) \otimes M_n \otimes \mathfrak{sl}_n^*$$

and the Z_0-invariance implies that

$$R^*_{z_0}\tilde{\omega} = \mathrm{Ad}_{z_0^{-1}} \circ \tilde{\omega}, \quad R^*_{z_0}\Lambda = \mathrm{Ad}_{z_0^{-1}} \circ \Lambda, \quad R^*_{z_0}\phi = \mathrm{Ad}_{z_0^{-1}} \circ \phi \circ \mathrm{Ad}_{z_0}$$

for any $z_0 \in Z_0$. Then Λ and ϕ can be considered as sections of some associated vector bundles to $\tilde{Q}(M/G, Z_0)$. On the other hand, the G_0-invariance implies that

$$\mathrm{Ad}_{\lambda(g_0)^{-1}}\tilde{\omega} = \tilde{\omega}, \quad \mathrm{Ad}_{\lambda(g_0)^{-1}} \circ \Lambda \circ \mathrm{Ad}_{g_0} = \Lambda, \quad \mathrm{Ad}_{\lambda(g_0)^{-1}} \circ \phi \circ \mathrm{Ad}_{\lambda(g_0)} = \phi. \tag{23}$$

for any $g_0 \in G_0$, and the $(G_0 \times Z_0)$-horizontality gives us that

$$\Lambda(X_0) = \phi(\lambda_* X_0) \quad \forall\, X_0 \in \mathcal{G}_0 \quad \text{and } \tilde{\omega}(\tilde{Z_0^Q}) = \phi(Z_0) \quad \forall\, Z_0 \in \mathcal{Z}_0. \tag{24}$$

The ordinary $\mathcal{G}$-invariant connections are recovered in formula (22) when $\phi = \mathbb{1}$. Indeed, in this case one gets

$$\Psi^*\omega_{|(\tilde{q},g,h)} = \mathrm{Ad}_{h^{-1}}(\tilde{\omega}_{|\tilde{q}} + \Lambda_{\tilde{q}} \circ \theta^G_{|g}) + \theta^H_{|h} - i\theta$$

which is to be compared to formula (4). As already explained, the extra term $i\theta$ is exactly what is needed to imbed ordinary connections into the noncommutative framework.

By means of the equivariance relation (23), Λ (respectively, ϕ) intertwines the representation of G_0 on $\mathcal{G}^{\mathbb{C}}$ (respectively, $\mathcal{H}^{\mathbb{C}}$) with the representation of G_0 on the algebra $M_n \simeq \mathrm{Vect}_{\mathbb{C}}(\mathbb{1}, \mathcal{H})$ and by virtue of the Schur lemma, it can be decomposed in a direct sum of isomorphisms between common irreducible blocks of $\mathcal{G}^{\mathbb{C}}$ (respectively, $\mathcal{H}^{\mathbb{C}}$) and $M_n \simeq \mathrm{Vect}_{\mathbb{C}}(\mathbb{1}, \mathcal{H})$. Furthermore, if one requires that the connection is anti-Hermitian, one must identify isomorphisms which correspond to complex conjugate representations, or directly look at real representations.

This "local" characterization of invariant noncommutative connections can be shown to be equivalent to the "global" approach. In order to do that, one needs to decompose the degrees of freedom and rearrange them in a different way.

From (22), it is easy to write down local expressions on M. A section $S: M \to \tilde{E}$ can be factorized through a local section $s = s_{\tilde{Q}} \times s_G$ on the fiber bundle $Q' = \tilde{Q} \times G$, and a section s_H on the trivial fiber bundle $Q' \times H$. The application $S = \Psi \circ s_H \circ s$ is represented in the following commutative diagram:

$$\begin{array}{ccc} Q' \times H & \underset{s_H}{\overset{pr_1}{\rightleftarrows}} & Q' = \tilde{Q} \times G \\ \Psi \downarrow & & \downarrow \uparrow s = s_{\tilde{Q}} \times s_G \\ \tilde{E} & \underset{S}{\overset{\tilde{\pi}}{\rightleftarrows}} & M = M/G \times G/G_0 \end{array}$$

Then, the local 1-form connection is just $S^*\omega = s^* \circ s_H^* \circ \Psi^* \tilde{\omega} \in \Omega(M) \otimes \Omega_{\mathrm{Der}}(M_n)$. It is useful to write the section S in the following way:

$$S: M \to \tilde{E},$$

$$m \mapsto \Psi(s_{\tilde{Q}}(m), s_G(m), h(m)).$$

Then, one finally obtains

$$S^*\omega = \mathrm{Ad}_{h^{-1}}(s_{\tilde{Q}}^* \tilde{\omega} + s_{\tilde{Q}}^* \Lambda \circ s_G^* \theta^G + s_{\tilde{Q}}^* \phi \circ \mathrm{Ad}_h \circ (h^* \theta^H - i\theta)). \tag{25}$$

One can look at passive gauge transformations which preserve symmetries of the local 1-form $S^*\omega$. We have three ways to perform such a passive gauge transformation. We can multiply on the right s_H by an element $h' \in H$, $s_{\tilde{Q}}$ by an element $z_0 \in Z_0$ or s_G by an element $g_0 \in G_0$. Then S is modified in the following way:

$$S \mapsto S' = \Psi \circ (s_{\tilde{Q}} \cdot z_0, s_G \cdot g_0, h \cdot h').$$

One can report the action on $\tilde{Q}$ and G to an action on H by means of the equivariance of the application Ψ, and one has

$$\Psi \circ (s_{\tilde{Q}} \cdot z_0, s_G \cdot g_0, h \cdot h') = \Psi \circ (s_{\tilde{Q}}, s_G, \lambda(g_0^{-1}) \cdot z_0^{-1} \cdot h \cdot h').$$

We will illustrate this three kind of gauge transformations in the next section.

V. EXAMPLES

In this section we apply the results found in the preceding section to two examples. The first one is a noncommutative extension of a case extensively studied and used in the literature,[3,14] that is, the spherical symmetry for SU (2)-gauge fields (see Ref. 22 and references therein for examples of applications). We will show that our framework generalizes in a straightforward way the results found in the ordinary case.

The second example is a purely noncommutative case. It consists to look at some symmetries on the matrix algebra. In this case, no geometry is involved.

A. Spherical symmetry

Consider the interesting example where $M = \mathbb{R} \times \mathbb{R}^3 \backslash \{0\}$, the first factor being parametrized by the time coordinate t and the second factor by spacial coordinates $(x,y,z) = \vec{r}$. The symmetry group is taken to be $G = \mathrm{SU}(2)$ and it acts on $\mathbb{R}^3 \backslash \{0\}$ by rotation matrices. [We consider the space $\mathbb{R}^3 \backslash \{0\}$ because we want a simple action.] Then G_0 is isomorphic to U (1), G/G_0 is isomorphic to the 2-sphere $\mathbb{S}^2$ and $M/G = \mathbb{R} \times \mathbb{R}^{+*}$. We look at a gauge theory with structure group $H = \mathrm{SU}(2)$, and so for the noncommutative part, we take $M_n = M_2(\mathbb{C})$.

We first treat this example in the approach developed in Sec. IV A. Notice that any principal SU (2)-fiber bundle over M is trivial due to the fact that $M = \mathbb{R} \times \mathbb{R}^{+*} \times \mathbb{S}^2$, where $\mathbb{R} \times \mathbb{R}^{+*}$ is contractible and $\dim(\mathbb{S}^2) = 2$. Then we will take E in the trivial form

$$E = M \times \mathrm{SU}(2) = M/G \times \mathrm{S}^2 \times \mathrm{SU}(2).$$

Now, we can lift the action of G on the base space M to an action on the fiber bundle E defining an action of G on the structure group H. One can extend this action in a trivial way by considering the action $(g,h) \mapsto h \forall_g \in G$, $\forall h \in H$. Then the reduced theory is a SU (2)-gauge theory over M/G which means that nothing very interesting is happening. A more complex case is to consider the following action:

$$G \times H \to H,$$

$$(g,h) \mapsto g \cdot h,$$

which is possible here because $G=H$. With this action, one can see that the application λ is an isomorphism and then one can take the reduced bundle Q in such a way that $\lambda=\mathbb{1}$. Then one has $Z_0=G_0=U(1)_z$, where

$$\mathrm{U}(1)_Z := \{\exp(2\epsilon T_3), \epsilon \in \mathbb{R}\}$$

and $\{T_1,T_2,T_3\}$ is a basis of anti-Hermitian generators of $\mathfrak{su}(2)$ satisfying

$$[T_1,T_2]=T_3, \quad [T_2,T_3]=T_1, \quad [T_3,T_1]=T_2.$$

The reduced fiber bundle Q is isomorphic to $M/G\times\{N,S\}\times \mathrm{U}(1)$, where N and S are the north and south poles of the 2-sphere $\mathbb{S}^2$. Without loss of generality, we can restrict the fiber Q to the point N, the symmetry relations coming from this $\mathbb{Z}_2$ structure being just conjugation relations over complex numbers. In this case, the diagram (1) becomes

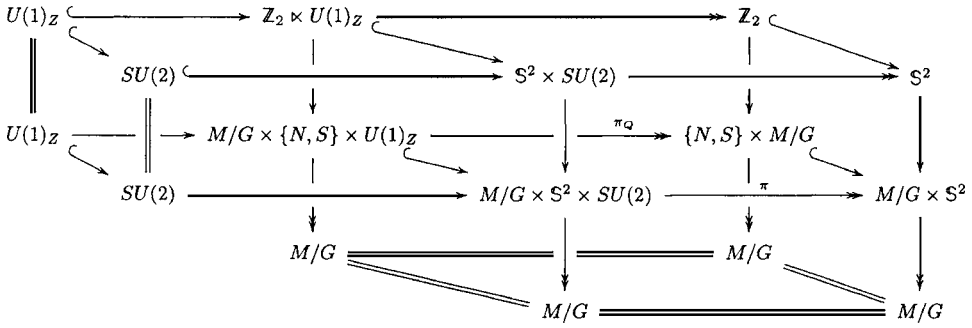

Here, we have $\mathcal{L}=\mathcal{M}=\mathrm{Vect}_{\mathbb{R}}(T_1,T_2)$, $\mathcal{K}=0$ and $\mathcal{W}_0=\mathrm{Vect}_{\mathbb{C}}(\mathbb{1},T_3)$. It is then easy to see that $\mathcal{F} \simeq \mathcal{L}^{\mathbb{C}}\oplus\mathcal{M}^{\mathbb{C}}$. Finally a SU (2)-invariant connection is characterized by two sections ψ and ζ over M/G with values in $\mathrm{Vect}_{\mathbb{C}}(T_1,T_2)$ and a noncommutative 1-form $\mu-\eta\in(\Omega(M/G)\otimes\Omega(\mathcal{W}_0))^1$. Here $\Omega^1(\mathcal{W}_0)$ is simply $\mathcal{W}_0$ because $\mathcal{Z}_0$ is one dimensional. If only anti-Hermitian connections are taken into account, then one can consider vector spaces over $\mathbb{R}$, and ψ and ζ can be interpreted as complex scalar fields (because $\mathcal{L}=\mathcal{M}\simeq\mathbb{C}$). In this case, one has $\mathcal{C}=C^\infty(M/G)\otimes\mathcal{W}_0$, and $\mathrm{SU}(\mathcal{C})=\{e^{\chi T_3}=\cos(\chi/2)\mathbb{1}+\sin(\chi/2)T_3,\chi\in\mathcal{C}^\infty(M/G)\}\simeq\mathrm{U}(1)$.

In this particular example, the "local" approach of Sec. IV B is very well adapted because of the structure of the base space M. Then, we will perform the rest of its analysis using these technics. The SU (2)-principal bundle E can be constructed from a principal U (1)-fiber bundle and the conjugacy class $[\lambda]=[\mathbb{1}]$.

An invariant connection is given explicitly by formula (22), and for the simplicity of the analysis, we will consider only traceless anti-Hermitian connections in the following. [The trace term in a connection corresponds to the term $\mathbb{1}$ in the algebra $M_n=\mathrm{Vect}_{\mathbb{C}}(\mathbb{1},\mathcal{H})$, and it can be studied independently of the traceless part.] Using notations and results of Sec. IV B, we are led to study the decomposition of the adjoint representation of SU (2) in irreducible representations of $\mathrm{U}(1)_Z$. The adjoint representation of SU (2) is decomposed into the fundamental representation of U (1) on $\mathrm{Vect}_{\mathbb{R}}T_3$ and the two-dimensional representation on $\mathrm{Vect}_{\mathbb{R}}(T_1,T_2)$, corresponding to the fundamental representation of SO(2). The invariance properties (23) implies that

$$\Lambda(T_1)=\Lambda_1T_1+\Lambda_2T_2, \quad \phi(T_1)=\phi_1T_1+\phi_2T_2,$$

$$\Lambda(T_2)=-\Lambda_2T_1+\Lambda_1T_2, \quad \phi(T_2)=-\phi_2T_1+\phi_1T_2,$$

and using (23) and (24)

$$\Lambda(T_3) = \phi(T_3) = \eta T_3,$$

where η is a function over M/G. Now let us write the local expression (25) of the connection 1-form by considering two different useful gauges. First let us introduce what we call the "singular" gauge in which we take the constant section

$$s_H: Q' \to Q' \times H,$$

$$q' \mapsto (q', e).$$

We will choose the usual spherical coordinates (ϑ, φ) for the local system of coordinate on $\mathbb{S}^2$. Then we consider the natural local section,

$$s_G: \mathbb{S}^2 \to \mathrm{SU}(2),$$

$$(\vartheta, \varphi) \mapsto g = e^{\varphi T_3} e^{\vartheta T_2}$$

[we have in mind the Euler parametrization of SU (2), where ϑ and φ are two of the three Euler angles]. Then a straightforward computation gives

$$S^*\omega = aT_3 + (\Lambda_1 T_1 + \Lambda_2 T_2)\mathrm{d}\vartheta + (\Lambda_1 T_2 - \Lambda_2 T_1)\sin\vartheta\,\mathrm{d}\varphi + \eta T_3 \cos\vartheta \mathrm{d}\varphi - [(\phi_1 T_1 + \phi_2 T_2)\theta^1 + (\phi_1 T_2 - \phi_2 T_1)\theta^2 + \eta T_3 \theta^3], \tag{26}$$

where $a = a_r\,\mathrm{d}r + a_t\,\mathrm{d}t \in \Omega^1(\mathbb{R} \times \mathbb{R}^{+*})$, and $i\theta = T_a\theta^a$. This reduced 1-form connection generalizes in an obvious way the so-called Witten's anzatz[14] which is recovered by setting $\phi_1 = \eta = 1$ and $\phi_2 = 0$ (i.e., $\phi = \mathbb{1}$). One can note that the monopole term (corresponding to the local 1-form $\cos\vartheta\,\mathrm{d}\varphi$) is no more constant and is now factorized by a function η. Singularities happening in (26) are due to the fact that we try to extend the system of spherical coordinates globally on $\mathbb{S}^2$. This extension is not possible in this gauge and it is why it is called the "singular" gauge. However one can introduce another gauge in which the extension of the local 1-form to a global one is possible. This is the "regular," or "radial" gauge, defined by the following section:

$$S: M \to \widetilde{E}, \tag{27}$$

$$(r, \vartheta, \varphi) \mapsto \Psi(s_{\tilde{Q}}(r), e^{\phi T_3} e^{\vartheta T_2}, e^{-\vartheta T_2} e^{-\phi T_3}). \tag{28}$$

It can be obtained from the "singular" gauge by a (passive) gauge transformation which consist to multiply the section s_H by the element $h' = e^{-\vartheta T_2} e^{-\varphi T_3} \in H$. Then applying formula (25) leads to the following expression:

$$S^*\omega = aT_r + \Lambda_1[T_r, \mathrm{d}T_r] - \Lambda_2\,\mathrm{d}T_r - \phi_1[T_r, \hat{\mathrm{d}}Tr] + \phi_2 \hat{\mathrm{d}}Tr - \eta T_r \theta^r, \tag{29}$$

where

$$T_r = \sin\vartheta\cos\varphi T_1 + \sin\vartheta\sin\varphi T_2 + \cos\vartheta T_3,$$

$$\theta^r = \sin\vartheta\cos\varphi\theta^1 + \sin\vartheta\sin\varphi\theta^2 + \cos\vartheta\theta^3,$$

and $\hat{\mathrm{d}} = \mathrm{d} + \mathrm{d}'$ is the noncommutative differential introduced in Sec. III. The absence of singularity is clearly due to the fact that the spherical angles (ϑ, φ) do not appear explicitly, and that everything can be expressed in terms of the unique generator T_r. To illustrate the fact that we have extended the local 1-form to a global one, we will give some more explicit formulas using Euclidian coordinates. Let us introduce the notation $S^*\omega = a + A_i^a T_a \mathrm{d}x^i - \phi_b^a T_a \theta^b$. Then formula (29) gives us

$$A_i^a = \frac{\mathrm{Re}(\psi - i\phi)}{r} P_i^a + \frac{\mathrm{Im}(\psi - i\phi)}{r} g^{ab} \epsilon_{ibc} \hat{n}^c,$$

$$\phi_b^a = \mathrm{Re}(\phi) P_b^a + \mathrm{Im}(\phi) g^{ac} \epsilon_{bcd} \hat{n}^d + \eta \hat{n}^a \hat{n}_b,$$

with $\hat{n}^a = x^a/r$, $P_b^a = \delta_i^a - \hat{n}^a \hat{n}_i$, g^{ab} the Euclidian metric and ϵ_{abc} the totally antisymmetric tensor such that $\epsilon_{123} = 1$. We have introduced the useful notations $\psi = -\Lambda_2 + i\Lambda_1$ and $\phi = \phi_1 + i\phi_2$.

Finally, we would like to show how the two other passive gauge transformations (on s_G and $s_{\tilde{Q}}$ mentioned at the end of Sec. IV B) can be performed. They will correspond to a U (1) residual symmetry. In terms of the two complex scalar fields ψ and ϕ, Eq. (29) becomes

$$S^* \omega = a T_r + \mathrm{Re}(\psi - i\phi) \mathrm{d} T_r + \mathrm{Im}(\psi - i\phi)[T_r, \mathrm{d} T_r] + \mathrm{Re}(-i\phi) \mathrm{d}' T_r + \mathrm{Im}(-i\phi)[T_r, \mathrm{d}' T_r] - \eta T_r \theta^r.$$

The U (1) passive gauge transformations correspond to the transformations on s_G and $s_{\tilde{Q}}$ given by

$$s_G \rightsquigarrow s_G \cdot e^{\chi_0 T_3},$$

$$s_{\tilde{Q}} \rightsquigarrow s_{\tilde{Q}} \cdot e^{\chi_1 T_3},$$

where $\chi_0(r,t)$ and $\chi_1(r,t)$ are two arbitrary functions of r and t. This leads to transformations on the fields ψ and a,

$$\psi \rightsquigarrow e^{i(\chi_1 + \chi_0)} \psi,$$

$$a \rightsquigarrow a - \eta \mathrm{d}(\chi_1 + \chi_0). \tag{30}$$

One can remark that the scalar fields ϕ and η remain unchanged under this passive gauge transformation. One can also note the similarity with usual Abelian gauge transformations.

It is possible to consider a "true" symmetric gauge transformation (in the sense of noncommutative geometry, see Sec. III). In order to do that, one must redefine the complex scalar field ϕ to $\phi = 1 - \phi'$. Then a "true" symmetric gauge transformation parametrized by an element $e^{\chi T_3} \in \mathrm{SU}(\mathcal{C})$, where χ is a function over $M/G = \mathbb{R} \times \mathbb{R}^{+*}$, leads to the transformations

$$\phi' \rightsquigarrow e^{-i\chi} \phi',$$

$$\psi \rightsquigarrow e^{-i\chi} \psi,$$

$$a \rightsquigarrow a + \mathrm{d}\chi. \tag{31}$$

Note that these transformations are much more similar to ordinary U (1) gauge transformations.

B. A purely noncommutative example

We present in this section a purely noncommutative case in the sense that we consider a situation in which the base space is a point. Then one has $G = G_0$, and λ is an homomorphism from G to H. In this case, the noncommutative algebra is simply the algebra of matrices M_n, equipped with the noncommutative calculus exposed in Ref. 17 and summarized in Sec. III. In this situation, the problem reduces to characterize G-invariant noncommutative connections in M_n. For simplicity, as before, we will restrict in this section to traceless connections.

The general procedure to follow is to first study the representation λ of G in M_n, and then determine how the representations $\mathrm{Ad}^H \circ \lambda$ split into irreducible representations of G. These irreducible representations give rise to the degrees of freedom of the invariant noncommutative connections, one scalar field for each intertwiner of equivalent irreducible representations.

We want to illustrate this in the particular case $G=\mathrm{SU}(2)$. It is well known that representations of SU (2) on M_n are parametrized by partitions of n.[9] For instance, for $\mathfrak{A}=M_3(\mathbb{C})$, the representations are labeled by the partitions "1+1+1," "2+1," and "3" of 3. They are described in the following way:

(i) The "1+1+1" representation corresponds to the sum of three copies of the trivial representation. The representation $\mathrm{Ad}^H\circ\lambda$ is decomposed in a sum of eight copies of the trivial representation of SU (2). This gives rise to 64 scalar fields. This case is not interesting because the group SU (2) does not act on $M_3(\mathbb{C})$.

(ii) The "2+1" representation corresponds to a reducible representation of SU (2) which is the sum of the fundamental representation and the trivial one. The representation $\mathrm{Ad}^H\circ\lambda$ is decomposed into irreducible representations of SU (2) of dimensions 3, 2, 2, and 1 (six scalar fields).

(iii) The "3" representation corresponds to the irreducible representation of dimension 3 of SU (2). In this case, the representation $\mathrm{Ad}^H\circ\lambda$ can be decomposed into irreducible representations of SU (2) of dimensions 3 and 5 (two scalar fields).

We will not perform the analysis any further because our goal is just to characterize the degrees of freedom of a traceless noncommutative connection using the methods exposed in this paper.

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Construction of new solutions to the fully nonlinear generalized Camassa-Holm equations by an indirect F function method

Emmanuel Yomba
Institute for Mathematics and its applications, University of Minnesota, Minneapolis, Minnesota 554556-0436 and Department of Physics, Faculty of Sciences, University of Ngaoundéré, Ngaoundéré, Cameroon

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An indirect F function method is introduced to solve the generalized Camassa-Holm equation with fully nonlinear dispersion and fully nonlinear convection $C(l,n,p)$. Taking advantage of elliptic equation, this F function is used to map the solutions of the generalized Camassa-Holm equation to those of the elliptic equation. As a result, we can successfully obtain in a unified way and for special values of the parameters of this equation, many exact solutions expressed by various single and combined nondegenerative Jacobi elliptic function solutions and their degenerative solutions (soliton, combined soliton solutions, and triangular solutions) as the modulus m is driven to 1 and 0. © *2005 American Institute of Physics*. [DOI: 10.1063/1.2137723]

I. INTRODUCTION

It is well known that the investigation of the travelling wave solutions of nonlinear evolution equations (NLEEs), which is an important tool in characterizing many complicated phenomena and dynamical processes in physics, mechanics, chemistry, biology, etc., plays an essential role in the study of these physical problems. Hence, seeking for solutions of the NLEEs may help enable physicists and engineers to better understand the mechanism that governs these physical problems. Especially, finding explicit solutions to nonlinear models has become one of the most exciting and extremely active areas of research investigation, since they may provide better knowledge to the physical problems and possible physical applications.

Recently, both mathematicians and physicists have made many attempts in this direction. A number of works have been done on the construction of exact solutions of NLEEs and effective and powerful methods have been developed, such as inverse scattering method,[1] Bäcklund transformation,[2] Darboux transformation,[3,4] Hirota bilinear method,[5] homogeneous balance method,[6] Jacobi elliptic function method,[7] tanh-function method,[8,9] extended tanh-function method,[10–13] improved extended tanh-function method,[14–18] the sine-cosine function method.[19]

Very recently, a unified F-expansion method[20–27] has been established to obtain Jacobi elliptic functions, solitons, and periodic functions to a large variety of NLEEs whose odd- and even-order derivative terms do not coexist. The main idea of this method is to take full advantage of the elliptic equation which has more solutions, to construct exact solutions to the NLEEs. Thus multiple exact solutions can be obtained in a unified way and much tedious and repeated calculation can be avoided.

In the present paper, a generalized Camassa-Holm equation with fully nonlinear dispersion and fully nonlinear convection term $C(l,n,p)$ (Ref. 28) is considered

$$U_t + kU_x + \beta_1 U_{xxt} + \beta_2 (U^l)_x + \beta_3 U_x (U^n)_{xx} + \beta_4 U (U^p)_{xxx} = 0, \tag{1}$$

where k, β_1, β_2, β_3, and β_4 are arbitrary real constants.

Equation (1) is a class of physically important equations. In fact, if one takes $\beta_1=-1$, $\beta_2=3/2$, $\beta_3=-2$, $\beta_4=-1$, $l=2$, $n=p=1$, (1) becomes the shallow water equation, namely Camassa-Holm equation

$$U_t + kU_x - U_{xxt} + 3UU_x = 2U_xU_{xx} + UU_{xxx}, \tag{2}$$

which has been proposed by Camassa-Holm.[29] They used Hamiltonian methods to derive the completely integrable dispersive wave equation for water by retaining two terms that are usually neglected in small amplitude shallow water limit. They showed that for all k, Eq. (2) is integrable, and for $k=0$, (2) has travelling solutions, which are called peakons. When $\beta_1=-1$, $\beta_2=a$, $\beta_3=-2$, $\beta_4=-1$, $l=L+1$, $n=p=1$, (1) becomes another form of generalized Camassa-Holm equation,

$$U_t + kU_x - U_{xxt} + aU^LU_x = 2U_xU_{xx} + UU_{xxx}, \tag{3}$$

studied by Tian and Song.[30] They derived some exact peaked solitary wave solutions. When $k=0$, $\beta_1=-1$, $\beta_2=3/2$, $\beta_3=-2\gamma$, $\beta_4=-\gamma$, $l=2$, $n=p=1$, (1) becomes

$$U_t - U_{xxt} + 3UU_x = \gamma(2U_xU_{xx} + UU_{xxx}), \tag{4}$$

which has been derived by Dai and Huo[31] when they studied disturbances in an initially stretched or compressed rod which is composed of a compressible Mooney-Rivlin material. By using a nondimensionalization process and the reductive perturbation technique, they obtained a type of nonlinear dispersive equation (4). They also showed that Eq. (4) has a variety of travelling waves including solitary shock waves, solitary waves, periodic shock waves, etc. Liu and Chen[32] showed that Eq. (4) also generated compacton structures by using the bifurcation method of planar dynamical systems and numerical simulation of differential equations. When $k=0$, $\beta_1=-1$, $\beta_2=3/2$, $\beta_3=\beta_4=0$, $l=2$, $n=p=1$, Eq. (1) becomes the BBM equation,[33] a well-known model for surface wave in channel.

More recently, by using four direct ansatze, Tian and Yin[28] obtained abundant solutions, compactons (solutions with absence of infinite wings), solitary patterns (solutions having infinite slopes or cups), solitary waves and singular periodic wave solutions and obtained kink compacton solutions and nonsymmetry compacton solutions. In the same paper, they also studied other forms of fully nonlinear generalized Camassa-Holm equation and showed that their compacton solutions are governed by linear equations.

The present paper is motivated by the desire to extend the Tian and Yin work[28] to make further progress. More importantly, it is the objective of this work to show that abundant families of Jacobi, combined Jacobi elliptic functions, solitary wave and combined solitary wave solutions and triangular functions arise from Eq. (1). To achieve our goal, instead of taking specific functions as Tian and Yin did in Ref. 28, we will use a form of indirect F-function method [not the F-expansion method because the complexity of Eq. (1) cannot allow the use of this method]. But our indirect F method will be very close to the F-expansion method in the sense that, the indirect F-function method will also take advantage of nonlinear ordinary differential equation (ODE). Thus, one will only need to calculate the function which is a solution of the ODE, instead of calculating the Jacobi elliptic function one by one; second, the coefficients of the ODE can be selected so that the corresponding solution is a Jacobi elliptic function, exactly as in the F-expansion method.

The paper is organized as follows: In Sec. II, a derivation of the proposed method for finding exact solutions is presented. Finally, some discussions and conclusions are given in Sec. III.

II. GENERAL FORMULAS OF THE SOLUTIONS

We first make the following formal travelling wave transformation:

$$U(x,t) = U(\xi), \quad \xi = \lambda_1 x + \lambda_2 t, \tag{5}$$

where λ_i, $(i=1,2)$ are undetermined constants. Substituting (5) into Eq. (1), we have the ODE for $U(\xi)$,

$$\lambda_2 U' + k\lambda_1 U' + \beta_1\lambda_2\lambda_1^2 U''' + \beta_2\lambda_1 (U^l)' + \beta_3\lambda_1^3 U'(U^n)'' + \beta_4\lambda_1^3 U(U^p)''' = 0. \tag{6}$$

Then a suitable ansatz for the unknown $U(\xi)$ will solve Eq. (6).

Let us assume that Eq. (6) has the solution in the form

$$U(\xi) = A(F(\xi))^B, \tag{7}$$

where A and B are parameters to be determined later. We also propose that the function F should be mapped to the solutions of the following elliptic equation

$$F'^2 = r + aF^2 + \frac{b}{2}F^4, \tag{8}$$

r, a, and b are constants. Substituting the ansatz (7) along with Eq. (8) into Eq. (6), collecting coefficients of power of F with the aid of Mathematica, we can deduce the following polynomial equation:

$$\begin{aligned}
&2ABr\beta_1\lambda_2\lambda_1^2[2-3B+B^2]F^B + 2AB[k\lambda_1+\lambda_2+aB^2\beta_1\lambda_2\lambda_1^2]F^{B+2} + ABb\beta_1\lambda_2\lambda_1^2[2+3B+B^2]F^{B+4}\\
&\quad + [2lBA^l\beta_2\lambda]F^{2+Bl} + 2A^{1+n}B^2nr\beta_3\lambda_1^3[nB-1]F^{B(n+1)} + [2aA^{1+n}B^3n^2\beta_3\lambda_1^3]\times F^{2+B(n+1)}\\
&\quad + A^{1+n}B^2nb\beta_3\lambda_1^3[nB+1]F^{4+B(n+1)} + 2A^{1+p}Bpr\beta_4\lambda_1^3[2-3Bp+B^2p^2]F^{B(1+p)}\\
&\quad + [2aA^{1+p}B^3p^3\beta_4\lambda_1^3]F^{2+B(p+1)} + A^{1+p}Bpb\beta_4\lambda_1^3[2+3Bp+B^2p^2]F^{4+B(1+p)} = 0.
\end{aligned} \tag{9}$$

One may easily see that in the specific cases, where $r=1$, $a=-1$, and $b=0$ which lead to $F=\cos\xi$, when $r=1$, $a=-1$, and $b=0$ which lead to $F=\sin\xi$, when $r=-1$, $a=1$, and $b=0$ which lead to $F=\cosh\xi$ and when $r=1$, $a=1$, and $b=0$ which lead to $F=\sinh\xi$, then we are in the situation of ansatz 1, ansatz 2, ansatz 3, and ansatz 4 in Ref. 28, respectively. We are interested in the general case where $r\times a\times b\neq 0$.

In view of the study of Eq. (9), we may observe carefully the different powers of F intervening in this equation. Then, it appears that it is powers $2+Bl$, $2+B(n+1)$, and $2+B(1+p)$ whose coefficients are singles which may determine our discussion.

Thus, from Eq. (9), we get the following possible cases to be discussed.

Case 1: $2+Bl=2+B(n+1)=2+B(1+p)$, we have $l=n+1$, $p=n$,

Case 2: $2+Bl=2+B$, $2+B(n+1)=2+B(1+p)$, we have $l=1$, $p=n$,

Case 3: $2+Bl=2+B(1+p)$, $2+B(n+1)=2+B$, we have $l=1+p$, $n=0$,

Case 4: $2+Bl=2+B(1+n)$, $2+B(p+1)=2+B$, we have $l=1+n$, $p=0$.

But the cases 3 and 4 produce no solution.

From the case 1, choosing $l=1+n$ and $p=n$, substituting in Eq. (9) and collecting all terms with same power of F, we obtain the following equation:

$$\begin{aligned}
&2ABr\beta_1\lambda_2\lambda_1^2[2-3B+B^2]F^B + 2AB[k\lambda_1+\lambda_2+aB^2\beta_1\lambda_2\lambda_1^2]F^{B+2} + ABb\beta_1\lambda_2\lambda_1^2[2+3B+B^2]F^{B+4}\\
&\quad + 2A^{1+n}Bnr\lambda_1^3[\beta_3B(nB-1)+\beta_4(2-3Bn+B^2n^2)]F^{B(n+1)} + 2A^{1+n}B[(n+1)\beta_2\lambda_1 + aB^2n^2\lambda_1^3(\beta_3\\
&\quad + n\beta_4)]F^{2+B(n+1)} + A^{1+n}Bnb\lambda_1^3[B\beta_3(Bn+1)+\beta_4(2+3Bn+B^2n^2)]F^{4+B(1+n)} = 0.
\end{aligned} \tag{10}$$

From (10) it appears that when setting to zero the coefficient of F^B, i.e., $2ABr\beta_1\lambda_2\lambda_1^2[2-3B+B^2]=0$ which leads to $[2-3B+B^2]=0$ ($B=1$ or $B=2$) then the coefficient of power F^{B+4} should be different than zero, i.e., $ABb\beta_1\lambda_2\lambda_1^2[2+3B+B^2]\neq 0$. Thus the power of F^{B+4} should be shifted to another power; this may help the coefficient of this power to enter another relationship with other terms. Thus the following two subcases may be satisfied.

First subcase

$$B+4=B(n+1)\nearrow \text{ when } B=1,\ \Rightarrow n=4;\ l=5,\ p=4\searrow \text{ when } B=2,\ \Rightarrow n=2;\ l=3,\ p=2.$$

Substituting the first type of relation of the first subcase in Eq. (10) and solving the set of a given system of equations we obtain the following results:

$$\lambda_1 = \frac{\sqrt{\frac{5}{2}}}{4}\sqrt{\frac{\beta_2}{a\beta_4}}, \quad \lambda_2 = -\frac{k\lambda_1}{1+a\beta_1\lambda_1^2}, \quad A = \pm\frac{1}{2}\left(\frac{b\beta_1\lambda_2}{r\beta_4\lambda_1}\right)^{1/4}, \quad \beta_3 = -6\beta_4. \tag{11}$$

a, b, and r are arbitrary constants.

Substituting the second type of relation of the first subcase in Eq. (10) and solving the set of a given system of equations we obtain the following results:

$$\lambda_1 = \frac{\sqrt{3}}{4}\sqrt{\frac{\beta_2}{a\beta_4}}, \quad \lambda_2 = -\frac{k\lambda_1}{1+4a\beta_1\lambda_1^2}, \quad A^2 = -\left(\frac{kb\beta_1}{r(3\beta_1\beta_2+4\beta_4)}\right),$$
$$\beta_3 = -3\beta_4, \tag{12}$$

a, b, and r are arbitrary constants.

Second subcase,

$B+4 = 2+B(n+1) \nearrow$ when $B=1$, $\Rightarrow n=2$; $l=3$, $p=2 \searrow$ when $B=2$, $\Rightarrow n=1$; $l=2$, $p=1$.

Substituting the first type of relation of the second subcase in Eq. (10) and solving the set of a given system of equations we obtain the following results:

$$\lambda_2 = -\frac{A^2(3\beta_2-8a\beta_4\lambda_1^2)}{3b\beta_1\lambda_1}, \quad A^2 = \lambda_1^2\left(\frac{3bk\beta_1}{3\beta_2+\lambda_1^2[a(3\beta_1\beta_2-8\beta_4)+8\beta_1\beta_4\lambda_1^2(3br-a^2)]}\right),$$
$$\beta_3 = -4\beta_4, \tag{13}$$

λ_1, a, b, and r are arbitrary constants.

Substituting the second type of relation of the second subcase in Eq. (10) and solving the set of a given system of equations we obtain the following results:

$$\lambda_2 = -\frac{\lambda_1(4ar\beta_4\lambda_1^2-k)}{1+4a\beta_1\lambda_1^2}, \quad A = \frac{3bk\beta_1\lambda_1^2}{\beta_2+\lambda_1^2[2a(2\beta_1\beta_2-\beta_4)+4\beta_1\beta_2\lambda_1^2(3br-2a^2)]},$$
$$\beta_3 = -2\beta_4, \tag{14}$$

λ_1, a, b, and r are arbitrary constants.

Now, if we set the coefficient of F^{B+4} to zero, i.e., $[2+3B+B^2]=0$ ($B=-1$ or $B=-2$) then the coefficient $2ABb\beta_1\lambda_2\lambda_1^2[2-3B+B^2]$ of power F^{B+4} should be different than zero, in order to allow this coefficient to enter relationship with other coefficients of the other power of F, we have the following two subcases.

Third subcase,

$B = 2+B(n+1) \nearrow$ when $B=-1$, $\Rightarrow n=2$; $l=3$, $p=2 \searrow$ when $B=-2$, $\Rightarrow n=1$; $l=2$, $p=1$.

Substituting the first type of relation of the third subcase in Eq. (10) and solving the set of a given system of equations we obtain the following results:

$$\lambda_2 = -\frac{k\lambda_1(8a\beta_4\lambda_1^2-3\beta_2)}{3\beta_2+a\lambda_1^2(3\beta_1\beta_2-8\beta_4)+8\beta_1\beta_4(3br-a^2)},$$

$$A^2 = \frac{6kr\beta_1\lambda_1^2}{3\beta_2+a\lambda_1^2(3\beta_1\beta_2-8\beta_4)+8\beta_1\beta_4(3br-a^2)}, \tag{15}$$

$$\beta_3 = -4\beta_4,$$

λ_1, a, b, and r are arbitrary constants.

Substituting the second type of relation of the third subcase in Eq. (10) and solving the set of a given system of equations we obtain the following results:

$$\lambda_2 = -\frac{k\lambda_1(2a\beta_4\lambda_1^2 - \beta_2)}{12br\beta_1\beta_4\lambda_1^4 - (1+4a\beta_1\lambda_1^2)(2a\beta_4\lambda_1^2 - \beta_2)},$$

$$A = \left(\frac{6kr\beta_1\lambda_1^2}{12br\beta_1\beta_4\lambda_1^4 - (1+4a\beta_1\lambda_1^2)(2a\beta_4\lambda_1^2 - \beta_2)}\right), \tag{16}$$

$$\beta_3 = -2\beta_4,$$

λ_1, a, b, and r are arbitrary constants.

Fourth subcase,

$B = 4 + B(n+1) \nearrow$ when $B = -1$, $\Rightarrow n = 4$; $l = 5$, $p = 4 \searrow$ when $B = -2$, $\Rightarrow n = 2$; $l = 3$, $p = 2$.

Substituting the first type of relation of the fourth subcase in Eq. (10) and solving the set of a given system of equations we obtain the following results:

$$\lambda_2 = -\frac{k\lambda_1}{1+a\beta_1\lambda_1^2}, \quad A = \pm\left(\frac{-rk\beta_1}{4b\beta_4(1+a\beta_1\lambda_1^2)}\right)^{1/4},$$
$$\beta_3 = -6\beta_4, \tag{17}$$

where λ_1, satisfies the following relation:

$$\beta_2 + a(5\beta_1\beta_2 - 32\beta_4)\lambda_1^2 - 32a^2\beta_1\beta_4\lambda_1^4 = 0, \tag{18}$$

a, b, and r are arbitrary constants.

Substituting the second type of relation of the fourth subcase in Eq. (10) and solving the set of a given system of equations we obtain the following results:

$$\lambda_2 = -\frac{k\lambda_1}{1+4a\beta_1\lambda_1^2}, \quad A^2 = -\frac{rk\beta_1}{b\beta_4(1+a\beta_1\lambda_1^2)},$$
$$\beta_3 = -3\beta_4, \tag{19}$$

where λ_1, should satisfy the following relation:

$$3\beta_2 + 4a(3\beta_1\beta_2 - 4\beta_4)\lambda_1^2 - 64a^2\beta_1\beta_4\lambda_1^4 = 0, \tag{20}$$

a, b, and r are arbitrary constants.

From the case 2, taking $l=1$ and $p=n$, substituting these relations in Eq. (9) and collecting all terms with the same power of F, we obtain the following equation:

$$\begin{aligned} &2ABr\beta_1\lambda_2\lambda_1^2[2-3B+B^2]F^B + 2AB[\beta_2\lambda_1 + k\lambda_1 + \lambda_2 + aB^2\beta_1\lambda_2\lambda_1^2]F^{B+2} + ABb\beta_1\lambda_2\lambda_1^2[2+3B \\ &+ B^2]F^{B+4} + 2A^{1+n}Bnr\lambda_1^3[\beta_3 B(nB-1) + \beta_4(2-3Bn+B^2n^2)]F^{B(n+1)} + 2aA^{1+n}B^3n^2\lambda_1^3[\beta_3 \\ &+ n\beta_4]F^{2+B(n+1)} + A^{1+n}Bnb\lambda_1^3[B\beta_3(Bn+1) + \beta_4(2+3Bn+B^2n^2)]F^{4+B(1+n)} = 0. \end{aligned} \tag{21}$$

Proceeding in the same manner as above, for $[2-3B+B^2]=0$ ($B=1$ or $B=2$) then the coefficient of power F^{B+4} which should be different of zero, may enter into another relation if only we have the following relations.

First subcase,

$B + 4 = B(n+1) \nearrow$ when $B = 1$, $\Rightarrow n = 4$; $l = 1$, $p = 4 \searrow$ when $B = 2$, $\Rightarrow n = 2$; $l = 1$, $p = 2$.

Substituting the first type of relation of the first subcase in Eq. (21) and solving the set of a given system of equations we have found that there is no solution for this first subcase.

Second subcase,

$$B+4=2+B(n+1)\nearrow \text{ when } B=1,\ \Rightarrow n=2;\ l=1,\ p=2\searrow \text{ when } B=2,\ \Rightarrow n=1;\ l=1,\ p=1.$$

Substituting the first type of relation of the second subcase in Eq. (21) and solving the set of a given system of equations we obtain the following results:

$$\lambda_2=\frac{8aA^2\beta_4\lambda_1}{3b\beta_1},\quad A^2=-\left(\frac{3b\beta_1(k+\beta_2)}{8\beta_2[a-(3br-a^2)\beta_1\lambda_1^2]}\right),$$
$$\beta_3=-4\beta_4, \tag{22}$$

λ_1, a, b, and r are arbitrary constants.

Substituting the second type of relation of the second subcase in Eq. (21) and solving the set of a given system of equations we obtain the following results:

$$\lambda_2=\frac{2aA\beta_4\lambda_1}{3b\beta_1},\quad A=-\left(\frac{3b\beta_1(k+\beta_2)}{2\beta_2[a-2(3br-2a^2)\beta_1\lambda_1^2]}\right),$$
$$\beta_3=-2\beta_4, \tag{23}$$

λ_1, a, b, and r are arbitrary constants.

If now, it is $[2+3B+B^2]=0$ ($B=-1$ or $B=-2$) then it is the coefficient of power F^B which should be different of zero, may enter into another relation if only we have the following relations.

Third subcase,

$$B=2+B(n+1)\nearrow \text{ when } B=-1,\ \Rightarrow n=2;\ l=1,\ p=2\searrow \text{ when } B=-2,\ \Rightarrow n=1;\ l=1,\ p=1.$$

Substituting the first type of relation of the third subcase in Eq. (21) and solving the set of a given system of equations we have found the following results:

$$\lambda_2=-\frac{a\lambda_1(k+\beta_2)}{a-(3br-a^2)\beta_1\lambda_1^2},\quad A^2=\left(\frac{3r\beta_1\lambda_2}{4a\beta_4\lambda_1}\right),$$
$$\beta_3=-4\beta_4, \tag{24}$$

λ_1, a, b, and r are arbitrary constants.

Substituting the second type of relation of the third subcase in Eq. (21) and solving the set of a given system of equations we obtain the following results:

$$\lambda_2=-\left(\frac{a\lambda_1(k+\beta_2)}{a-2(3br-2a^2)\beta_1\lambda_1^2}\right),\quad A=\frac{3r\beta_4\lambda_2}{a\beta_4\lambda_1},$$
$$\beta_3=-2\beta_4, \tag{25}$$

λ_1, a, b, and r are arbitrary constants.

Fourth subcase,

$$B=4+B(n+1)\nearrow \text{ when } B=-1,\ \Rightarrow n=4;\ l=1,\ p=4\searrow \text{ when } B=-2,\ \Rightarrow n=2;\ l=1,\ p=2.$$

Substituting the first type of relation of the second subcase in Eq. (21) and solving the set of a given system of equations we have found that there is no solution for this subcase.

Since in all these cases, r, a, and b are arbitrary constants, we may choose them properly such that the corresponding solution F of the ODE (8) is one of the Jacobi elliptic, combined Jacobi elliptic functions.

If $r=1$, $a=-(1+m^2)$, $b=2m^2$, then the solution is

$$U_1 = A[\mathrm{sn}(\xi|m)]^B, \tag{26a}$$

or

$$U_2 = A[cd(\xi|m)]^B \equiv A\left[\frac{\mathrm{cn}(\xi|m)}{dn(\xi|m)}\right]^B, \tag{26b}$$

where $0 \leqslant m \leqslant 1$, is called modulus of Jacobi elliptic functions, and $\mathrm{sn}(\xi|m)$ is the Jacobi elliptic sine function, see Refs. 34 and 35.

If $r=1-m^2$, $a=2m^2-1$, $b=-2m^2$, then the solution is

$$U_3 = A[\mathrm{cn}(\xi|m)]^B, \tag{27}$$

where $\mathrm{cn}(\xi|m)$ is the Jacobi elliptic cosine function, see Refs. 34 and 35.

If $r=m^2-1$, $a=2-m^2$, $b=-2$, then the solution is

$$U_4 = A[dn(\xi|m)]^B, \tag{28}$$

where $dn(\xi|m)$ is the Jacobi elliptic function of the third kind, see Refs. 34 and 35.

If $r=m^2$, $a=-(1+m^2)$, $b=2$, then the solution is

$$U_5 = A[ns(\xi|m)]^B \equiv A\left[\frac{1}{\mathrm{sn}(\xi|m)}\right]^B, \tag{29a}$$

or

$$U_6 = A[dc(\xi|m)]^B \equiv A\left[\frac{dn(\xi|m)}{\mathrm{cn}(\xi|m)}\right]^B. \tag{29b}$$

If $r=-m^2$, $a=2m^2-1$, $b=2(1-m^2)$, then the solution is

$$U_7 = A[nc(\xi|m)]^B \equiv A\left[\frac{1}{\mathrm{cn}(\xi|m)}\right]^B. \tag{30}$$

If $r=-1$, $a=2-m^2$, $b=2(m^2-1)$, then the solution is

$$U_8 = A[nd(\xi|m)]^B \equiv A\left[\frac{1}{dn(\xi|m)}\right]^B. \tag{31}$$

If $r=1-m^2$, $a=2-m^2$, $b=2$, then the solution is

$$U_9 = A[cs(\xi|m)]^B \equiv A\left[\frac{\mathrm{cn}(\xi|m)}{\mathrm{sn}(\xi|m)}\right]^B. \tag{32}$$

If $r=1$, $a=2-m^2$, $b=2(1-m^2)$, then the solution is

$$U_{10} = A[sc(\xi|m)]^B \equiv A\left[\frac{\mathrm{sn}(\xi|m)}{\mathrm{cn}(\xi|m)}\right]^B. \tag{33}$$

If $r=1$, $a=2m^2-1$, $b=2m^2(m^2-1)$, then the solution is

$$U_{11} = A[sd(\xi|m)]^B \equiv A\left[\frac{\mathrm{sn}(\xi|m)}{dn(\xi|m)}\right]^B. \tag{34}$$

If $r=m^2(m^2-1)$, $a=2m^2-1$, $b=2$, then the solution is

$$U_{12} = A[ds(\xi|m)]^B \equiv A\left[\frac{dn(\xi|m)}{\mathrm{sn}(\xi|m)}\right]^B. \tag{35}$$

If $r=1/4$, $a=(1-2m^2)/2$, $b=1/2$, then the solution is

$$U_{13} = A[ns(\xi|m) \pm cs(\xi|m)]^B. \tag{36}$$

If $r=(1-m^2)/4$, $a=(1+m^2)/2$, $b=(1-m^2)/2$, then the solution is

$$U_{14} = A[nc(\xi|m) \pm sc(\xi|m)]^B. \tag{37}$$

If $r=m^4/4$, $a=(m^2-2)/2$, $b=1/2$, then the solution is

$$U_{15} = A[ns(\xi|m) + ds(\xi|m)]^B. \tag{38}$$

If $r=m^2/4$, $a=(m^2-2)/2$, $b=m^2/2$, $i^2=-1$ then the solution is

$$U_{16} = A[\mathrm{sn}(\xi|m) \pm i\ \mathrm{cn}(\xi|m)]^B. \tag{39}$$

In addition, we see that other solutions are obtained in case of degeneracies, when $m \to 0$, the Jacobi elliptic and combined Jacobi elliptic functions degenerate to the trigonometric functions of the given NLPDE (1), i.e., $\mathrm{sn}(\xi|m) \to \sin(\xi)$, $\mathrm{cn}(\xi|m) \to \cos(\xi)$, $dn(\xi|m) \to 1$, $ns(\xi|m) \to \csc(\xi|m)$, $cs(\xi|m) \to \cot(\xi)$, $ds(\xi|m) \to \sec(\xi)$, when $m \to 1$, the Jacobi elliptic and combined Jacobi elliptic functions degenerate to the soliton and combined soliton wave solutions of the given NLPDE (1), i.e., $\mathrm{sn}(\xi|m) \to \tanh(\xi)$, $\mathrm{cn}(\xi|m) \to \mathrm{sech}(\xi)$, $dn(\xi|m) \to \mathrm{sech}(\xi)$, $ns(\xi|m) \to \coth(\xi)$, $cs(\xi|m) \to \mathrm{csch}(\xi)$, $ds(\xi|m) \to \mathrm{csch}(\xi)$.

So we can derive solutions expressed in terms of trigonometric functions and hyperbolic functions, we omit them for simplicity.

It is worth noticing that the Jacobi transformation $dn(\xi|m)=\mathrm{cn}(\sqrt{m}\xi|m^{-1})$ (Ref. 36) implies that any solution found by the *dn* function may be transformed into an equivalent one that can be obtained by the cn function. Moreover, since other Jacobi elliptic function and combined Jacobi elliptic function solutions obtained here from a mathematics point of view as solutions of Eq. (8) have singularities, and since it is well known from a physics point of view that the singular solutions cannot have any meaning in the applications, we may focus only on nonsingular solutions among the listed mathematical solutions. When $B>0$ (i.e., $B=1$ or $B=2$) nonsingular solutions are given by (26a), (27), and (28). When $B<0$ (i.e., $B=-1$ or $B=-2$) nonsingular solutions are selected to be (29a), (30), and (31). Another interesting fact here is that by selecting $B=-1$ (or $B=-2$), the solutions (29a), (30), and (31) are reduced to the same family of solutions as (26a), (27), and (28), respectively, when $B=1$ (or $B=2$).

Taking into account the above-mentioned remarks, we have plotted for $B=1$ and $B=2$, Figs. 1–6 to illustrate our study or to raise the physics value of our study.

III. CONCLUSION

In this work, we have applied an indirect F-function method very close to the F-expansion method to solve the generalized Camassa-Holm equation with fully nonlinear dispersion and fully nonlinear convection term $C(l,n,p)$. By using this F-function method, we have been able to obtain in a unified way simultaneously many periodic wave solutions expressed by various single and combined nondegenerative Jacobi elliptic function solutions and their degenerative solutions (when the modulus m is driven to 1 and 0). This method gives elliptic solutions for specific values of the parameters n, p, l and for arbitrary values of β_1 and β_2, but β_3 and β_4 must be proportional with the proportionality constants for various cases given explicitly. In the various Camassa-Holm classes listed below, β_3 is replaced by the appropriate expression of β_4. The following Camassa-Holm family of equations has been solved by this indirect F-function method,

$$U_t + kU_x + \beta_1 U_{xxt} + \beta_2 (U^5)_x = \beta_4 (6U_x (U^4)_{xx} - U(U^4)_{xxx}),$$

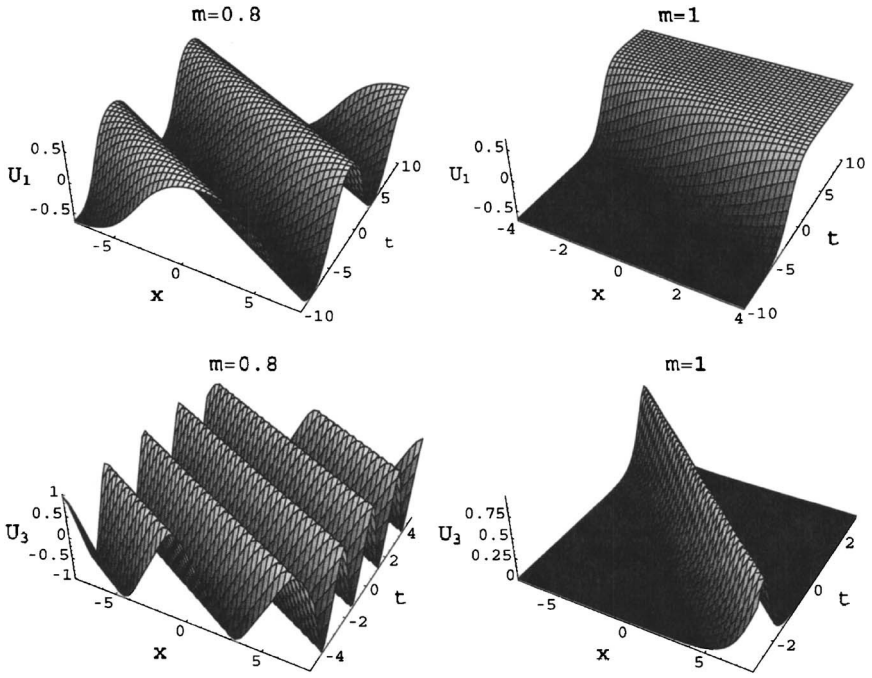

FIG. 1. The plot of sn, tanh, cn, and sech solutions, respectively. These nonsingular solutions are the structure graphs of Eq. (11), that is, $U_t+kU_x+\beta_1U_{xxt}+\beta_2(U^5)_x=\beta_4(6U_x(U^4)_{xx}-U(U^4)_{xxx})$. The first two graphs are obtained for the values $\beta_1=-1.00$, $\beta_2=1.50$, $\beta_4=-0.75$, $k=-2.00$, meanwhile the last two graphs have the same parameter values except that $\beta_4=0.75$.

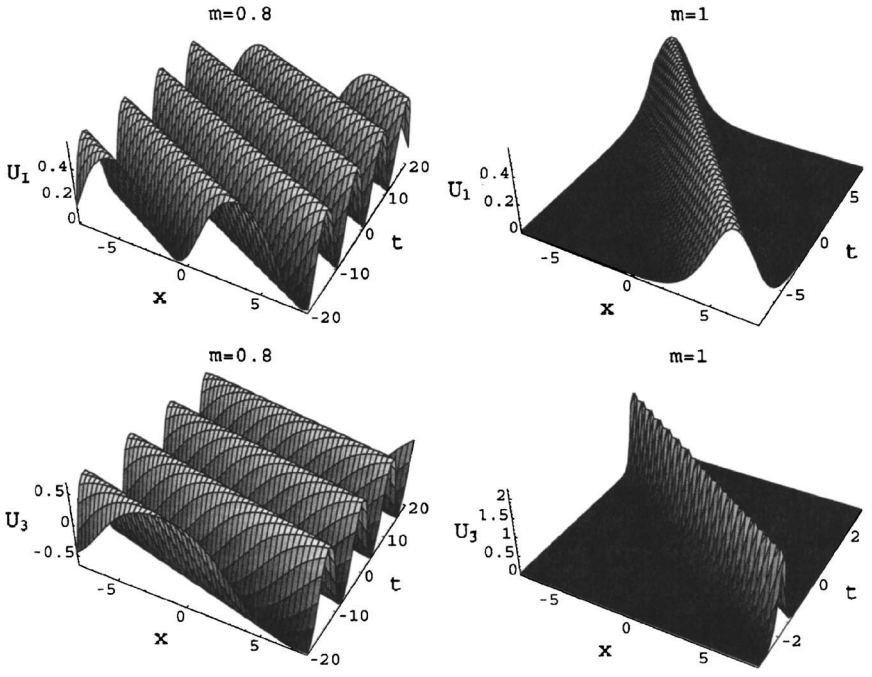

FIG. 2. The plot of sn^2, $tanh^2$, cn^2, and $sech^2$ solutions, respectively. These nonsingular solutions are the structure graphs of Eq. (12), that is, $U_t+kU_x+\beta_1U_{xxt}+\beta_2(U^3)_x=\beta_4(3U_x(U^2)_{xx}-U(U^2)_{xxx})$. The first two graphs are obtained for the values $\beta_1=-1.00$, $\beta_2=1.50$, $\beta_4=-0.75$, $k=-2.00$, meanwhile the last two graphs have the same parameter values except that $\beta_4=0.75$, $k=2.00$.

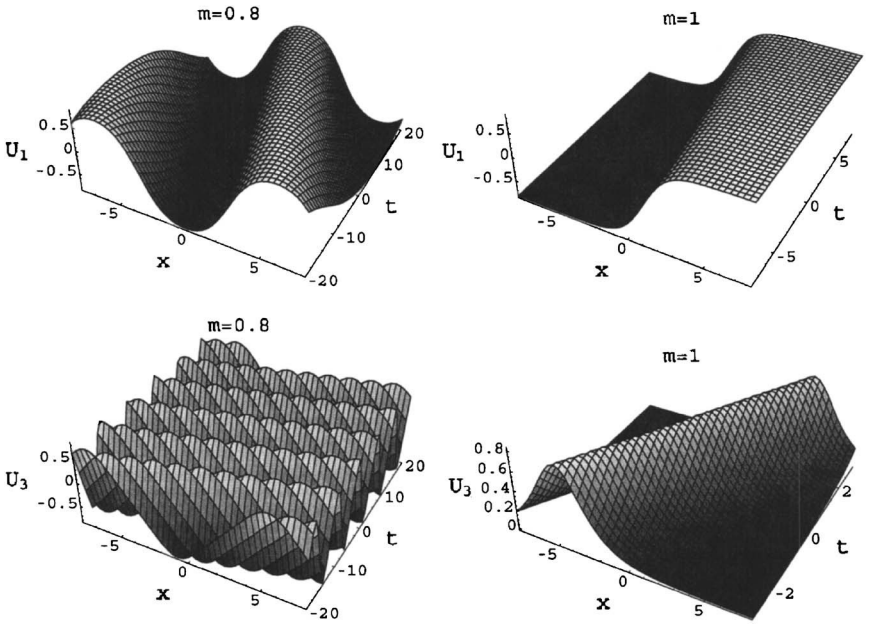

FIG. 3. The plot of sn, tanh, cn, and sech solutions, respectively. These nonsingular solutions are the structure graphs of Eq. (13), that is, $U_t+kU_x+\beta_1U_{xxt}+\beta_2(U^3)_x=\beta_4(4U_x(U^2)_{xx}-U(U^2)_{xxx})$. The first two graphs are obtained for the parameter values $\beta_1=-1.00$, $\beta_2=1.5$, $\beta_4=-0.75$, $k=-2.00$, $\lambda_1=0.65$, meanwhile the last two graphs have the same parameter values but for $\beta_4=0.75$, $k=2.00$.

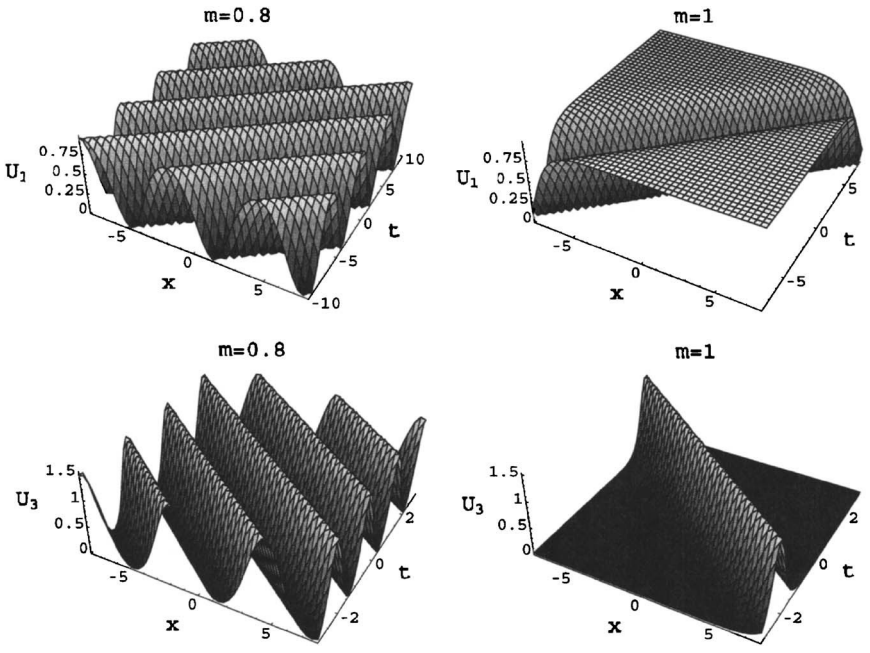

FIG. 4. The plot of sn^2, $tanh^2$, cn^2, and $sech^2$ solutions, respectively. These nonsingular solutions are the structure graphs of Eq. (14), that is, $U_t+kU_x+\beta_1U_{xxt}+\beta_2(U^2)_x=\beta_4(2U_x(U)_{xx}-U(U)_{xxx})$. The first two graphs are obtained for the values $\beta_1=-1.00$, $\beta_2=1.50$, $\beta_4=-0.75$, $k=-2.00$, $\lambda_1=0.65$, meanwhile the last two graphs have the same parameter values except that $\beta_4=0.75$, $k=2.00$.

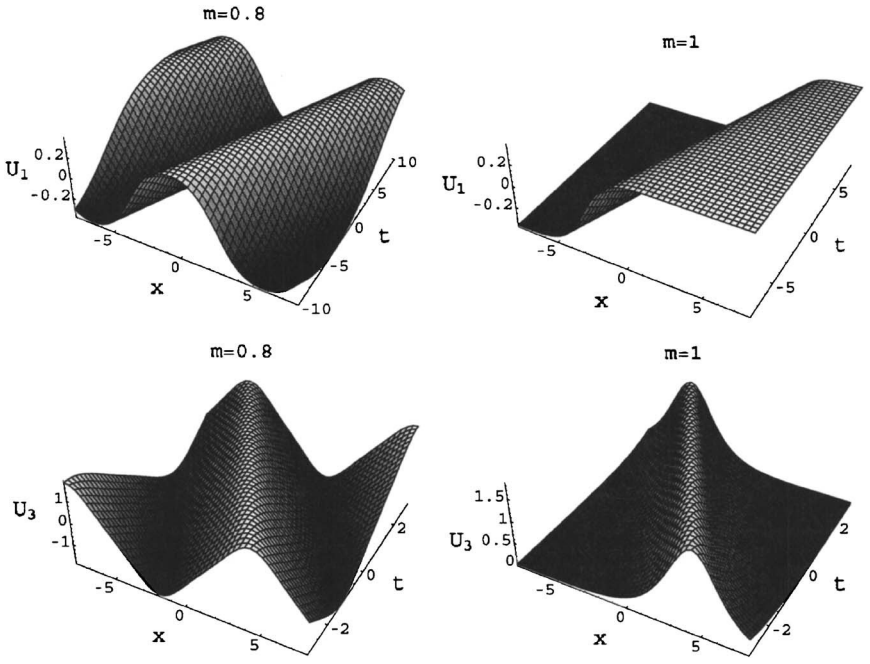

FIG. 5. The plot of sn, tanh, cn, and sech solutions, respectively. These nonsingular solutions are the structure graphs of Eq. (22), that is, $U_t+kU_x+\beta_1 U_{xxt}+\beta_2(U)_x=\beta_4(4U_x(U^2)_{xx}-U(U^2)_{xxx})$. The first two graphs are obtained for the values $\beta_1=-1.00$, $\beta_2=1.50$, $\beta_4=-0.75$, $k=-2.00$, $\lambda_1=0.65$, meanwhile the last two graphs have the same parameter values but for $\beta_4=0.75$, $k=2.00$.

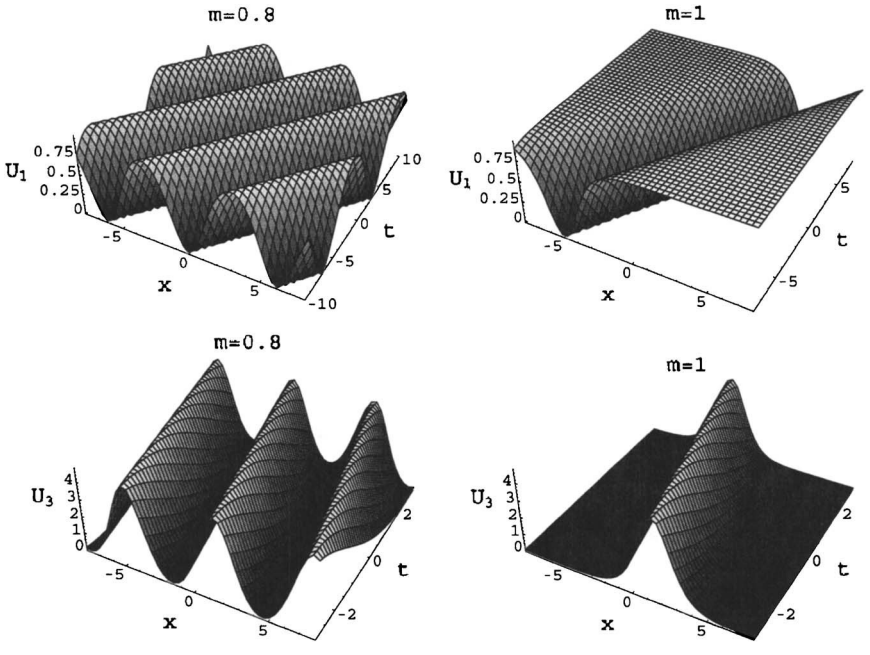

FIG. 6. The plot of sn^2, $tanh^2$, cn^2, and $sech^2$ solutions, respectively. These nonsingular solutions are the structure graphs of Eq. (23), that is, $U_t+kU_x+\beta_1 U_{xxt}+\beta_2(U)_x=\beta_4(2U_x(U)_{xx}-U(U)_{xxx})$. The first two graphs are obtained for the values $\beta_1=-1.00$, $\beta_2=1.50$, $\beta_4=-0.75$, $k=-2.00$, $\lambda_1=0.65$, meanwhile the last two graphs have the same parameter values except that $\beta_4=0.75$, $k=2.00$.

$$U_t + kU_x + \beta_1 U_{xxt} + \beta_2 (U^3)_x = \beta_4 (3U_x (U^2)_{xx} - U(U^2)_{xxx}),$$

$$U_t + kU_x + \beta_1 U_{xxt} + \beta_2 (U^3)_x = \beta_4 (4U_x (U^2)_{xx} - U(U^2)_{xxx}),$$

$$U_t + kU_x + \beta_1 U_{xxt} + \beta_2 (U^2)_x = \beta_4 (2U_x (U)_{xx} - U(U)_{xxx}),$$

$$U_t + kU_x + \beta_1 U_{xxt} + \beta_2 (U)_x = \beta_4 (4U_x (U^2)_{xx} - U(U^2)_{xxx}),$$

$$U_t + kU_x + \beta_1 U_{xxt} + \beta_2 (U)_x = \beta_4 (2U_x (U)_{xx} - U(U)_{xxx}).$$

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On the spectral L_2 conjecture, 3/2-Lieb-Thirring inequality and distributional potentials

Alexei Rybkin[a)]
Department of Mathematical Sciences, University of Alaska, Fairbanks, P.O. Box 756660, Fairbanks, Alaska 99775

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Let $H=-\partial_x^2+V(x)$ be a properly defined Schrödinger operator on $L_2(\mathbb{R})$ with real potentials of the form $V(x)=q(x)+p'(x)$ (the derivative is understood in the distributional sense) with some $p,q\in L_2(\mathbb{R})$. We prove that the absolutely continuous spectrum of H fills $(0,\infty)$ which was previously proven by Deift-Killip for $V\in L_2(\mathbb{R})$. We also refine the 3/2-Lieb-Thirring inequality. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2142837]

I. INTRODUCTION

The spectral L_2-conjecture was stated first by Kiselev-Last-Simon in Ref. 7 for the one-dimensional case and later by Simon in Ref. 14 for the generic case. It says: let $H:=-\Delta+V(x)$, $x\in\mathbb{R}^d$, be the Schrödinger operator on $L_2(\mathbb{R}^d)$ and V is a real measurable function. If

$$\int |V(x)|^2|x|^{1-d}\mathrm{d}x<\infty \tag{1.1}$$

then the absolutely continuous (a.c.) spectrum[1] $\sigma_{\mathrm{a.c.}}(H)$ of H is $\mathbb{R}_+:=[0,\infty)$.

This conjecture has drawn considerable attention. To the best of our knowledge, the case $d>1$ remains an open problem. For $d=1$ it was affirmatively settled in 1999 by Deift-Killip with previous contributions by Kiselev, Christ-Kiselev, Remling, and others (see, Refs. 14 and 15 for extended literature). The Deift-Killip result is sharp in the scale of L_p spaces.[7] In 2001 this result was extended by Molchanov-Novitskii-Vainberg[10] to read ($p\in\mathbb{N}$)

$$V\in H^{p-1}(\mathbb{R})\cap L_{p+1}(\mathbb{R})\Rightarrow \sigma_{\mathrm{a.c.}}(H)=\mathbb{R}_+,$$

where H^{p-1} denotes the Sobolev space.

In all previous cases potentials are assumed to be regular (locally integrable) functions. At about the same time with the above-mentioned activity Savchuk-Shkalikov[13,12] (with contributions from Hryniv-Mykytuyk[5]) were systematically studying Sturm-Liouville operators with singular (distributional) potentials. Among others, Savchuk-Shkalikov were able to properly define one-dimensional Schrödinger operators with potentials from the Sobolev space $H^{-1}(\mathbb{R})$, i.e., the space of all generalized functions f subject to

$$\int |\hat{f}(\omega)|^2\frac{\mathrm{d}\omega}{\omega^2+1}<\infty.$$

Here $\hat{f}$ stands for the Fourier transform of f.

In the current note we combine the Savchuk-Shkalikov approach to distributional potentials and the Deift-Killip idea to use the Faddeev-Zhakharov trace formulas to prove

[a)]Electronic mail: ffavr@uaf.edu

[1]I.e. the essential support of the absolutely continuous component of the spectral measure of the operator H.

$$V \in H^{-1}(\mathbb{R}) \Rightarrow \sigma_{\text{a.c.}}(H) = \mathbb{R}_+.$$

Our main tool is a new sum rule (Theorem 1) which in a way can be interpreted as the second Faddeev-Zhakharov trace formula (2.5) at a finite energy. This formula also allows one to generalize the 3/2-Lieb-Thirring bounds to singular potentials. Note that in the distributional sense every function V from H^{-1} has a form

$$V = q + p' \quad \text{where } p,q \in L_2(\mathbb{R}). \tag{1.2}$$

The main advantage of our approach is that it allows one to unify the study of slowly decaying potentials with such potentials as oscillatory Wigner von Neumann type, Coulomb, delta, etc., which have traditionally been treated separately.

II. REGULARIZED DISPERSION FORMULA AND A TRACE INEQUALITY

Through this section we deal with pairs (H,H_0) of operators

$$H_0 = -\partial_x^2, \quad H = H_0 + V(x) \tag{2.1}$$

on $L_2(\mathbb{R})$ under a very generous assumption that $V = \bar{V} \in C_0^\infty(\mathbb{R})$, where $C_0^\infty(\mathbb{R})$ is the class of smooth compactly supported function on $\mathbb{R}$. Observe that $[\mathfrak{S}_p, p>0$, denote *Schatten-von Neumann classes* of linear operators A:

$$A \in \mathfrak{S}_p \Leftrightarrow \|A\|_{\mathfrak{S}_p}^p := \text{tr}(A^*A)^{p/2} < \infty .$$

In particular $\mathfrak{S}_1$ is the trace class and $\mathfrak{S}_2$ is the Hilbert-Schmidt class. The norms of A in $\mathfrak{S}_1, \mathfrak{S}_2$ are, respectively, $\|A\|_{\mathfrak{S}_1} = \text{tr}(A^*A)^{1/2}$, $\|A\|_{\mathfrak{S}_2} = (\text{tr}(A^*A))^{1/2}]$.

$$V \in C_0^\infty(\mathbb{R}) \Rightarrow VR_\lambda^0 \in \mathfrak{S}_1, \quad R_\lambda^0 := R_\lambda(H_0) := (H_0 - \lambda)^{-1},$$

and hence the perturbation determinant

$$\Delta(\lambda) := \det(H-\lambda)(H_0-\lambda)^{-1} = \det(I + VR_\lambda^0)$$

exists and is an analytic function on $\mathbb{C}\backslash\mathbb{R}_+$ with a finite number N of simple zeros $-\varkappa_n^2$ on $\mathbb{R}_-$. The transmission coefficient $t(k)$ can be analytically extended from $\mathbb{R}$ to $\mathbb{C}_+$ by

$$t(z) = \Delta^{-1}(z^2), \quad z \in \mathbb{C}_+, \tag{2.2}$$

and for sufficiently large z,

$$|t(z)| \leqslant C|z|^{-1}.$$

For the spectra of H, H_0 one has

$$\sigma(H_0) = \sigma_{\text{a.c.}}(H_0) = \mathbb{R}_+, \quad \sigma(H) = \{-\varkappa_n^2\}_{n=1}^N \cup \sigma(H_0),$$

all eigenvalues $-\varkappa_n^2$ being simple and $N<\infty$. What has been said actually implies the dispersion formula

$$\log t^{-1}(z) = \sum_{n=1}^N \log \frac{z - i\varkappa_n}{z + i\varkappa_n} + \frac{1}{i\pi}\int \frac{\log|t(k)|^{-1}}{k-z}\mathrm{d}k, \tag{2.3}$$

which was used by Faddeev-Zhakharov (FZ)[3] to derive their famous trace formulas (sum rules):

$$-\sum_{n=1}^N \varkappa_n + \frac{1}{2\pi}\int \log|t(k)|^{-1}\mathrm{d}k = \frac{1}{4}\int V(x)\mathrm{d}x \tag{2.4}$$

(the first FZ trace formula),

$$\frac{2}{3}\sum_{n=1}^{N}\varkappa_n^3+\frac{1}{\pi}\int k^2\,\log|t(k)|^{-1}\mathrm{d}k=\frac{1}{8}\int V^2(x)\mathrm{d}x \tag{2.5}$$

(the second FZ trace formula),

etc. Recall that (2.4) and (2.5) can merely be obtained by comparing the corresponding coefficients in the asymptotic expansions of both sides of (2.3) in z^{-n} as $|z|\to\infty$. Let V be the operator of multiplication by $V\in C_0^\infty(\mathbb{R})$. Introduce

$$Q(\lambda):=(R_\lambda^0)^{1/2}V(R_\lambda^0)^{1/2},\quad \lambda\in\mathbb{C}\setminus\mathbb{R}_+, \tag{2.6}$$

where $(R_\lambda^0)^{1/2}$ is the principle branch of R_λ^0. The operator $Q(\lambda)$ is clearly bounded and represents an analytic operator-valued function in $\mathbb{C}\setminus\mathbb{R}_+$. We will need the following technical lemma.

Lemma 1: *If* $V=\bar{V}\in C_0^\infty(\mathbb{R})$ *then for any* $a>0$,

$$\|Q_a\|_{\mathfrak{S}_2}^2=\frac{1}{a}\int|\widehat{V}(\omega)|^2\frac{\mathrm{d}\omega}{\omega^2+(2a)^2}=\|V\|_a^2, \tag{2.7}$$

where

$$Q_a:=Q(-a^2),\quad a>0.$$

Proof: By straightforward computation. □

The following assertion is a derivation of (2.3).

Theorem 1: *Let* (H,H_0) *be defined by* (2.1) *and* $V=\bar{V}\in C_0^\infty(\mathbb{R})$. *Then* $(z\in\mathbb{C}_+)$

$$\log t^{-1}(z)+\frac{1}{2iz}\int V(x)\mathrm{d}x=\sum_{n=1}^{N}\left(\log\frac{z-i\varkappa_n}{z+i\varkappa_n}+\frac{2i\varkappa_n}{z}\right)+\frac{1}{i\pi z}\int_0^\infty\frac{k^2\log|t(k)|^{-1}}{k^2-z^2}\mathrm{d}k. \tag{2.8}$$

In particular if we choose $a>0$ *so that*

$$\|Q_a\|<1 \tag{2.9}$$

then

$$\sum_{n=1}^{N}\left(\log\frac{a+\varkappa_n}{a-\varkappa_n}-\frac{2\varkappa_n}{a}\right)+\frac{1}{\pi a}\int_0^\infty\frac{k^2\log|t(k)|^{-1}}{k^2+a^2}\mathrm{d}k=\log\det(I+Q_a)e^{-Q_a}\leqslant\log(1-\|Q_a\|_{\mathfrak{S}_2}^2)^{-1}. \tag{2.10}$$

Proof: By the general properties $|t(k)|\leqslant 1$ and $t(-k)=\overline{t(k)}$, $k\in\mathbb{R}$, of the transmission coefficient $t(k)$, the function

$$f(k):=\frac{1}{\pi}\log|t(k)|^{-1}$$

is integrable, non-negative, even and hence

$$\int\frac{f(k)}{k-z}\mathrm{d}k=-\frac{1}{z}\int f(k)\mathrm{d}k+\frac{1}{z^2}\int\frac{k^2f(k)}{k-z}\mathrm{d}k=-\frac{1}{z}\int f(k)\mathrm{d}k+\frac{2}{z}\int_0^\infty\frac{k^2f(k)}{k^2-z^2}\mathrm{d}k. \tag{2.11}$$

We have used here the obvious identity

$$\frac{1}{k-z} = -\frac{k}{z^2} - \frac{1}{z} + \frac{1}{z^2}\frac{k^2}{k-z}.$$

By (2.4)

$$\int f(k)\mathrm{d}k = 2\sum_{n=1}^{N} \varkappa_n + \frac{1}{2}\int V(x)\mathrm{d}x$$

and (2.11) can be continued

$$\int \frac{f(k)}{k-z}\mathrm{d}k = -\frac{2}{z}\sum_{n=1}^{N} \varkappa_n - \frac{1}{2z}\int V(x)\mathrm{d}x + \frac{2}{z}\int_0^\infty \frac{k^2 f(k)}{k^2 - z^2}\mathrm{d}k. \tag{2.12}$$

Plugging (2.12) into (2.3) one has

$$\log t^{-1}(z) = \sum_{n=1}^{N} \log\frac{z - i\varkappa_n}{z + i\varkappa_n} + \frac{2}{iz}\sum_{n=1}^{N} \varkappa_n - \frac{1}{2iz}\int V(x)\mathrm{d}x + \frac{2}{iz}\int_0^\infty \frac{k^2 f(k)}{k^2 - z^2}\mathrm{d}k,$$

and rearranging its terms yields (2.8).

Evaluate now the left-hand side of (2.8). For $V \in C_0^\infty(\mathbb{R})$ both operators VR_λ^0 and $(R_\lambda^0)^{1/2}V(R_\lambda^0)^{1/2}$, $\lambda \in \mathbb{C}\backslash\mathbb{R}_+$, are trace class and hence

$$\mathrm{tr}(R_\lambda^0)^{1/2}V(R_\lambda^0)^{1/2} = \mathrm{tr}\, VR_\lambda^0 = \int V(x)\frac{-1}{2i\sqrt{\lambda}}\mathrm{d}x = -\frac{1}{2i\sqrt{\lambda}}\int V(x)\mathrm{d}x.$$

Introducing the regularized perturbation determinant

$$\Delta_2(\lambda) := \det\{(1 + Q(\lambda))\exp(-Q(\lambda))\},$$

we have

$$\Delta_2(\lambda) = \det(1 + Q(\lambda)) \cdot \exp(-\mathrm{tr}\, Q(\lambda))$$

$$= \det(1 + VR_\lambda^0) \cdot \exp(-\mathrm{tr}\, VR_\lambda^0) = \Delta(\lambda)\exp(-\mathrm{tr}\, VR_\lambda^0),$$

which for $\lambda = z^2$, $z \in \mathbb{C}_+$, due to (2.2) implies

$$\log t^{-1}(z) + \frac{1}{2iz}\int V(x)\mathrm{d}x = \log \Delta_2(z^2).$$

Set now $z = ia$, $a > 0$, and choose a to satisfy (2.9). One has

$$\begin{aligned}
\log \Delta_2(-a^2) &= \log\det(I + Q_a)e^{-Q_a} \\
&= \mathrm{tr}\log(I + Q_a)^{-1}e^{Q_a} = \mathrm{tr}(Q_a - \log(I + Q_a)) \\
&= \mathrm{tr}\sum_{n\geqslant 2}\frac{1}{n}(-Q_a)^n = \mathrm{tr}\sum_{n\geqslant 1}\left(\frac{1}{2n}Q_a^{2n} - \frac{1}{2n+1}Q_a^{2n+1}\right) \\
&= \mathrm{tr}\sum_{n\geqslant 1}\frac{1}{2n}Q_a^{2n}\left(1 - \frac{2n}{2n+1}Q_a\right),
\end{aligned}$$

which implies

$$\log\det(I+Q_a)e^{-Q_a} \leqslant \sum_{n\geqslant 1}\frac{1}{2n}\left\|1-\frac{2n}{2n+1}Q_a\right\|\cdot \operatorname{tr} Q_a^{2n}$$

$$\leqslant \sum_{n\geqslant 1}\frac{1}{n}\|Q_a^n\|_{\mathfrak{S}_2}^2 = \log(1-\|Q_a\|_{\mathfrak{S}_2}^2)^{-1}.$$

and (2.10) is completely proven. □

Remark 1: (2.5) *can be obtained from* (2.10) *by multiplying it by* a^3 *and then taking* $a\to\infty$. *Note in this connection that a similar to* (2.10) *relation was recently used by Denisov*[2] *in the case of Krein systems*.

Remark 2: *Identity* (2.10) *can actually be viewed as the first formula in a certain chain of trace formulas*. *In the context of Jacobi matrices*, *similar relations were recently obtained by Laptev-Naboko-Safronov*,[8] *who further developed some ideas due to Killip-Simon*.[6]

III. IMPEDANCE FORM OF SCHRÖDINGER OPERATORS WITH SINGULAR POTENTIALS

Particular cases of singular potentials (i.e., not locally integrable) like delta and Coulomb potentials were considered by many authors. However a systematical treatment of H^{-1} potentials (which include delta and Coulomb potentials) appears to have been originated by Savchuk-Shkalikov in about 1998 (see, e.g., Ref. 13, and the literature therein). We emphasize that singular perturbations of self-adjoint operators have been studied even earlier but the author was unable to find out if a general theory of singular perturbations was linked to singular potentials. Following Savchuk-Shkalikov, we rewrite

$$H = -\partial_x^2 + V(x) \quad \text{on } L_2(\mathbb{R})$$

with $V\in H^{-1}(\mathbb{R})$ in the impedance form

$$H = -\partial_x(\partial_x - p(x)) - p(x)\partial_x + q(x) \tag{3.1}$$

with some $p,q\in L_2(\mathbb{R})$ from decomposition (1.2). On the domain

$$\operatorname{Dom} H = \{u\in L_2(\mathbb{R}): u,\ u'-p(x)u\in AC_{\mathrm{loc}}(\mathbb{R}), Hu\in L_2(\mathbb{R})\}, \tag{3.2}$$

[here $AC_{\mathrm{loc}}(\mathbb{R})$ denotes the set of locally a.c. functions on $\mathbb{R}$] the operator H is self-adjoint in $L_2(\mathbb{R})$ and $\operatorname{Dom} H$ does not depend on a specific choice of $p,q\in L_2(\mathbb{R})$ in (1.2). Moreover, if $\{\widetilde{V}\}$ is a sequence of real valued functions from $C_0^\infty(\mathbb{R})$ convergent in $H^{-1}(\mathbb{R})$ to V then the sequence $\{\widetilde{H}\}$, $\widetilde{H}=-\partial_x^2+\widetilde{V}(x)$, converges in the uniform resolvent sense to H defined by (3.1). That is

$$\|V-\widetilde{V}\|_{H^{-1}(\mathbb{R})}\to 0 \Rightarrow \|R_\lambda(H)-R_\lambda(\widetilde{H})\|\to 0, \quad \operatorname{Im}\lambda\neq 0. \tag{3.3}$$

Here and in the sequel we agree to mark all objects related to $\widetilde{V}$ with a tilde. The corresponding details can be found in Ref. 13. We only note that the key ingredient here is the following representation

$$Y' = \begin{pmatrix} p(x) & 1 \\ q(x)-p^2(x)-\lambda & -p(x)\end{pmatrix}Y, \quad Y := \begin{pmatrix} u \\ u^{[1]}\end{pmatrix} \tag{3.4}$$

of the Schrödinger equation

$$-u''+V(x)u=\lambda u, \quad V(x)=p'(x)+q(x),$$

where $u^{[1]}:=u'-p(x)u$ is the so-called quasiderivative of u. Since $p,q\in L_2(\mathbb{R})$ Eq. (3.4) is solvable and $Y=(u,u'-V(x)u)\in AC_{\mathrm{loc}}(\mathbb{R})$ (although u' need not be continuous). The definition of the Wronskian $W[y_1,y_2]$ of two functions y_1,y_2 should be modified to read

$$W[y_1,y_2]=y_1y_2^{[1]}-y_1^{[1]}y_2,$$

which of course agrees with the usual Wronskian if $y_1,y_2\in AC_{\mathrm{loc}}(\mathbb{R})$. With this in hand, one can develop the Weyl theory and prove the existence of the Weyl solutions $\psi_\pm(x,\lambda)\in L_2(\mathbb{R}_\pm)$, $\mathrm{Im}\,\lambda>0$. The Titchmarsh-Weyl m-functions $M_\pm(\lambda)$ should then be defined as

$$M_\pm(\lambda)=\pm\frac{\psi_\pm^{[1]}(0,\lambda)}{\psi_\pm(0,\lambda)}.$$

Functions $M_\pm$ are Herglotz (i.e., mapping $\mathbb{C}_+$ into $\mathbb{C}_+$) which representing measures are the spectral measures of the corresponding half-line Schrödinger operators with a Dirichlet boundary condition at 0. Note that if $V\in L_{1,\mathrm{loc}}(\mathbb{R})$ then

$$M_\pm(\lambda)=m_\pm(\lambda)-p(0),$$

where $m_\pm$ are the usual Titchmarsh-Weyl m-functions, and one can immediately see that

$$M_+(\lambda)+M_-(\lambda)=m_+(\lambda)+m_-(\lambda),\quad \mathrm{Im}\,M_\pm(\lambda)=\mathrm{Im}\,m_\pm(\lambda). \tag{3.5}$$

The Weyl theory is parallel to its regular counterpart. In particular

$$\|V-\widetilde{V}\|_{H^{-1}(\mathbb{R})}\to 0\Rightarrow \widetilde{M}_\pm(z)\to M_\pm(z) \tag{3.6}$$

on compact subsets of $\mathbb{C}_+$. The arguments are similar to those of Lemma 1 in Ref. 1 with the second Hilbert resolvent identity replaced with

$$R_\lambda-R_\lambda^0=(R_\lambda^0)^{1/2}\{(I+Q(\lambda))^{-1}-I\}(R_\lambda^0)^{1/2},\quad R_\lambda:=R_\lambda(H).$$

It follows from (3.6) that the spectral measure of $\widetilde{H}$ defined on $L_2(\mathbb{R}_\pm)$ with the Dirichlet boundary condition $u(\pm 0)=0$ weakly converges to the spectral measure of H defined on $L_2(\mathbb{R}_\pm)$ with the condition $u(\pm 0)=0$, respectively.

IV. THE MAIN RESULTS

Theorem 2: *Let $V=\overline{V}\in H^{-1}(\mathbb{R})$ and H defined by* (3.1) *on domain* (3.2). *Then*

$$\sigma_{\mathrm{a.c.}}(H)=\mathbb{R}_+. \tag{4.1}$$

Theorem 3: *Assuming conditions of Theorem* 2, *let $\{-\varkappa_m^2\}_{m\geqslant 1}$ be the set of negative eigenvalues of H enumerated in the increasing order. Then for any $a>\sup\varkappa_1$ such that*

$$\|Q_a\|_{\mathfrak{S}_2}^2=\frac{1}{a}\int|\widehat{V}(\omega)|^2\frac{\mathrm{d}\omega}{\omega^2+(2a)^2}<1$$

the following inequality holds:

$$\sum_{n\geqslant 1}\frac{2}{2n+1}\sum_{m\geqslant 1}\left(\frac{\varkappa_m}{a}\right)^{2n+1}\leqslant\log\left(1-\frac{1}{a}\int|\widehat{V}(\omega)|^2\frac{\mathrm{d}\omega}{\omega^2+(2a)^2}\right)^{-1}. \tag{4.2}$$

Proof: Let $\{\widetilde{V}\}$ be sequence of C_0^∞ potentials approximating V in H^{-1} and choose a to satisfy $\|\widetilde{Q_a}\|_{\mathfrak{S}_2}<1$. Notice that if $|\alpha|<1$ then

$$\log\frac{1+\alpha}{1-\alpha}-2\alpha=2\sum_{n\geqslant 1}\frac{\alpha^{2n+1}}{2n+1}\geqslant 0 \tag{4.3}$$

and one easily sees that all terms in (2.10) are non-negative and hence

$$\frac{1}{\pi a}\int_0^\infty \frac{k^2 \log|\tilde{t}(k)|^{-1}}{k^2+a^2}\mathrm{d}k \leqslant \log(1-\|\widetilde{Q_a}\|^2_{\mathfrak{S}_2})^{-1}, \tag{4.4}$$

$$\sum_{n=1}^{\widetilde{N}} \left(\log \frac{a+\widetilde{\varkappa}_n}{a-\widetilde{\varkappa}_n} - \frac{2\widetilde{\varkappa}_n}{a} \right) \leqslant \log(1-\|\widetilde{Q_a}\|^2_{\mathfrak{S}_2})^{-1}. \tag{4.5}$$

The conclusion of Theorem 2 now follows from (4.4) by adopting the Deift-Killip arguments (Ref. 1, Theorem 1). Indeed, *a priori* estimate (4.4) replaces

$$\frac{1}{\pi}\int k^2 \log|\tilde{t}(k)|^{-1}\mathrm{d}k \leqslant \frac{1}{8}\int \widetilde{V}^2(x)\mathrm{d}x,$$

which was a crucial ingredient of Ref. 1 [which, in turn, follows from (2.5)]. Instead of (see also Ref. 4)

$$|\tilde{t}(k)| = \frac{2\sqrt{\operatorname{Im}\widetilde{m}_+(k^2+i0)}\sqrt{\operatorname{Im}\widetilde{m}_-(k^2+i0)}}{|\widetilde{m}_+(k^2+i0)+\widetilde{m}_-(k^2+i0)|},$$

we use

$$|\tilde{t}(k)| = \frac{2\sqrt{\operatorname{Im}\widetilde{M}_+(k^2+i0)}\sqrt{\operatorname{Im}\widetilde{M}_-(k^2+i0)}}{|\widetilde{M}_+(k^2+i0)+\widetilde{M}_-(k^2+i0)|},$$

which, due to (3.5), coincide for at least smooth potentials. Finally, with (3.6) in hand the Deift-Killip limiting arguments go through.

The conclusion of Theorem 3 follows from (4.5). Indeed, due to (3.3), $\widetilde{\varkappa}_n \to \varkappa_n$ and hence inequality (4.5) retains in the limit. Estimate (4.2) now follows in view of (4.3). □

Remark 3: *Inequality* (4.2) *is a generalization of the 1D Lieb-Thirring bound* (*see*, *e.g.*, *Refs.* 9 and 16)

$$\sum_{n\geqslant 1}\varkappa_n^3 \leqslant C\int V_-^2(x)\mathrm{d}x, \quad V_-(x) := \min\{0, V(x)\},$$

to the case of H^{-1} *potentials. It is just enough to consider* (4.2) *for* $V_-(x)=\min\{0,V(x)\}\in L_2(\mathbb{R})$ *and pass to the limit as* $a\to\infty$. *We especially note that in the* H^{-1} *setting we cannot in general separate* V_- *and* V_+ *since* $V\in H^{-1}(\mathbb{R})$ *need not imply* $V_-\in H^{-1}(\mathbb{R})$.

Remark 4: *One can easily see that the space* $l_2(L_1)$ *defined as*

$$l_2(L_1) := \left\{ f : \sum_n \left(\int_n^{n+1} |f(x)|\mathrm{d}x \right)^2 < \infty \right\}$$

is a proper subset of $H^{-1}(\mathbb{R})$ *and Theorem 2 quickly recovers the main result of Ref.* 11 *stating that*

$$V \in l_2(L_1) \Rightarrow \sigma_{\text{a.c.}}(H) = \mathbb{R}_+.$$

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Framework for potential systems and nonlocal symmetries: Algorithmic approach

George Bluman[a] and Alexei F. Cheviakov[b]
Department of Mathematics, University of British Columbia, Vancouver, Canada V6T 1Z2

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An algorithmic framework is presented to find an extended tree of nonlocally related systems for a given system of differential equations (DEs). Each system in an extended tree is equivalent in the sense that the solution set for any system in a tree can be found from the solution set for any other system in the tree. Useful conservation laws play an essential role in the construction of an extended tree. A useful conservation law yields potential variables and equivalent nonlocally related potential systems and subsystems for any given system. Nonlocal symmetries for a given system of DEs can arise from any system in its extended tree. We construct extended trees for the systems of planar gas dynamics and nonlinear telegraph equations, and in both cases obtain new nonlocal symmetries. More importantly, due to the equivalence of solution sets, any coordinate-independent method of analysis (qualitative, numerical, perturbation, etc.) can be applied to any system within the tree, and may yield simpler computations and/or results that cannot be obtained when the method is directly applied to the given system. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2142834]

I. INTRODUCTION

The potential symmetry approach[1–5] is an algorithmic procedure for seeking nonlocal symmetries of systems of differential equations (DEs). To be directly applicable, this approach requires the existence of a conservation law of a given system. Each conservation law allows the introduction of one or more auxiliary potential variables which are nonlocally defined with respect to the original dependent variables.[6–8] The resulting (extended) potential system yields nonlocal symmetries of the given system of DEs if it admits local symmetry generators that do not project onto local symmetry generators of the given system.

A symmetry of a system of DEs is any transformation of its solution manifold into itself (i.e., a symmetry transforms any solution to another solution of the same system). Hence, in general, symmetry transformations are defined topologically and are not restricted to point or contact (more generally local) transformations acting on the given system's dependent and independent variables. However, to perform calculations, a nonlocal symmetry transformation should be a local transformation acting on the space of variables of an auxiliary system equivalent to the given system. As has been shown in many examples, local symmetries obtained directly by Lie's algorithm do not include all calculable symmetries of a given system. However, the application of Lie's algorithm to related auxiliary systems systematically yields a search for nonlocal symmetries of the given system.

Further extensions arise. Starting from a potential system of DEs, one may continue to obtain a grander potential system resulting from any conservation law of the potential system. Furthermore, starting from a potential system, one may obtain nonlocally related subsystems (in addition

[a]Electronic mail: bluman@math.ubc.ca
[b]Electronic mail: alexch@math.ubc.ca

to the original given one) by "excluding" dependent variables from the potential system. For example, the $(1+1)$-dimensional system of planar gas dynamics equations $\mathbf{E}\{x,t,v,p,\rho\}=0$ in Eulerian coordinates with independent variables x=position, t=time, and dependent variables v =velocity, p=pressure, ρ=density, gives rise to potential systems $\mathbf{G}\{x,t,v,p,\rho,r\}=0$, $\mathbf{W}\{x,t,v,p,\rho,r,w\}=0$, and $\mathbf{Z}\{x,t,v,p,\rho,r,w,z\}=0$ with auxiliary potential variables r,w,z and to various subsystems with fewer dependent variables (Sec. III). This allows one to introduce the notion of a "tree of nonlocally related potential systems and subsystems" originating from a given system of DEs. It is important to note that a given system, its related potential systems and subsystems contain all solutions of each other, i.e., any solution of a related potential system or subsystem yields a solution of the given system and, mutatis mutandi, any solution of the given system yields a solution of any related potential system or subsystem. But the solution relationship is nonlocal since it is never one-to-one.

In general, the admitted point symmetries of a given system, its related potential systems and subsystems can be very different (e.g., Ref. 9). It can happen that a point symmetry of a given system is a nonlocal symmetry of a related potential system and, conversely, a point symmetry of a related potential system is a nonlocal symmetry of the given system. Moreover, it can happen that a point symmetry of the given system which is a nonlocal symmetry of a related potential system reappears as a point symmetry of a grander potential system.[9,10] Within a tree of potential systems, a "grand" system may exist that incorporates all point symmetries of the related systems with fewer potential variables as point symmetries in the grand system. Moreover, the grand system could admit point symmetries that are nonlocal symmetries of all related systems.[9,10]

The problem of finding trees of potential systems is particularly important when a given DE system contains arbitrary (constitutive) functions where one is interested in the question of symmetry classification with respect to specific forms of such functions. For different forms of the constitutive functions, the sets of conservation laws and consequent trees of related potential systems and subsystems can be different. Here, isolating useful systems and subsystems is of great importance.

If a given system of DEs has one of its equations written as a conservation law, then the conservation law equation is a natural way of leading to a related potential system and subsequent tree. In general, for any system of DEs the algorithmic direct construction method[11,12] yields its conservation laws. In particular, this method obtains factors multiplying each DE in the system so that the resulting linear combination of equations leads to a conservation law whose conserved densities are found from an integral formula. A resulting potential system (and subsequent extended tree) is found by replacing one of the DEs in such a linear combination by the conservation law. The factor multiplying the replaced DE must have the property that the solution set will not be modified when the conservation law replaces this DE. A useful conservation law for obtaining a potential system from any given system has at least one factor with this property.

The outline of this paper is as follows. In Sec. II, we present the general framework for the algorithmic construction of trees of potential systems and subsystems for a given system of DEs. In Sec. III, as a first example we consider the $(1+1)$-dimensional system of planar gas dynamics (PGD) equations[5,14] in detail within the potential system framework. Some nonlocal symmetries for the PGD system were found by Akhatov *et al.*[14] through a heuristic approach. Here, we use the systematic conservation law/potential symmetry framework to derive an extended tree of potential systems which includes the PGD systems in Euler and Lagrange coordinates. Our work clarifies and extends the work presented in Ref. 14. In particular, we obtain new nonlocal symmetries for PGD systems by a direct study of systems of the extended tree. In Sec. IV, as a second example we consider the nonlinear telegraph (NLT) equation.[9,13] Here, we show how to extend the results in Ref. 9 by introducing further potential variables. Using conservation laws for particular forms of the constitutive functions,[13] we construct extended trees for each such form. Further remarks are presented in Sec. V.

The analysis of systems of DEs through consideration of trees of potential systems and subsystems has evident practical value. First, it allows one to calculate systematically nonlocal symmetries using Lie's algorithm, which in turn are useful for obtaining new exact solutions from

known ones, for constructing invariant and nonclassical solutions, for discovering and constructing linearizations, etc. Second, and perhaps more importantly, any general method of analysis (qualitative, numerical, perturbation, conservation laws, etc.) that is being considered for a given DE system may be tried again on nonlocally related potential systems or subsystems, since all such related systems contain all solutions of the given system. In particular, since the systems are related in a nonlocal manner, new results may be obtained for any method of analysis that is not coordinate dependent.

II. ALGORITHMIC CONSTRUCTION OF TREES OF POTENTIAL SYSTEMS AND SUBSYSTEMS TO OBTAIN NONLOCAL SYMMETRIES

Consider a PDE system of m equations $\mathbf{R}\{x,t,\mathbf{u}\}=\{R_1\{x,t,\mathbf{u}\},\ldots,R_m\{x,t,\mathbf{u}\}\}=0$, with two independent variables (x,t), and n dependent variables $\mathbf{u}=(u^1,\ldots,u^n)$.

Suppose that the first equation $R_1\{x,t,\mathbf{u}\}=0$ of the system is written as a conservation law,

$$D_tT\{x,t,\mathbf{u}\}+D_xX\{x,t,\mathbf{u}\}=0. \tag{2.1}$$

Definition 2.1: The PDE system $\mathbf{S}\{x,t,\mathbf{u},v\}=0$ given by

$$\begin{aligned} v_x &= T\{x,t,\mathbf{u}\},\\ v_t &= -X\{x,t,\mathbf{u}\},\\ R_2\{x,t,\mathbf{u}\} &= 0,\\ &\cdots,\\ R_m\{x,t,\mathbf{u}\} &= 0, \end{aligned} \tag{2.2}$$

is a *potential system* with a potential variable $v=v(x,t)$ for $\mathbf{R}\{x,t,\mathbf{u}\}=0$ related to the conservation law $R_1\{x,t,\mathbf{u}\}=0$.

The potential system $\mathbf{S}\{x,t,\mathbf{u},v\}=0$ given by (2.2) is equivalent to the given system $\mathbf{R}\{x,t,\mathbf{u}\}=0$. In particular, if $(\mathbf{u},v)=(\tilde{\mathbf{u}}(x,t),\tilde{v}(x,t))$ solves (2.2), then $\mathbf{u}=\tilde{\mathbf{u}}(x,t)$ solves $\mathbf{R}\{x,t,\mathbf{u}\}=0$. Conversely, for any solution $\mathbf{u}=\tilde{\mathbf{u}}(x,t)$ of $\mathbf{R}\{x,t,\mathbf{u}\}=0$, there exists a pair of functions $(\mathbf{u},v)=(\tilde{\mathbf{u}}(x,t),\tilde{v}(x,t))$ that satisfies (2.2), with $\tilde{v}(x,t)$ unique to within a constant.

Suppose the system $\mathbf{S}\{x,t,\mathbf{u},v\}=0$ admits a Lie group of point transformations (point symmetry),

$$\begin{aligned} x^* &= x+\epsilon\xi_{\mathbf{S}}(x,t,\mathbf{u},v)+O(\epsilon^2),\\ t^* &= t+\epsilon\tau_{\mathbf{S}}(x,t,\mathbf{u},v)+O(\epsilon^2),\\ u^{*i} &= u^i+\epsilon\eta^i_{\mathbf{S}}(x,t,\mathbf{u},v)+O(\epsilon^2),\\ v^* &= v+\epsilon\zeta_{\mathbf{S}}(x,t,\mathbf{u},v)+O(\epsilon^2). \end{aligned} \tag{2.3}$$

$$\mathrm{X}=\xi_{\mathbf{S}}(x,t,\mathbf{u},v)\frac{\partial}{\partial x}+\tau_{\mathbf{S}}(x,t,\mathbf{u},v)\frac{\partial}{\partial t}+\eta^i_{\mathbf{S}}(x,t,\mathbf{u},v)\frac{\partial}{\partial u^i}+\zeta_{\mathbf{S}}(x,t,\mathbf{u},v)\frac{\partial}{\partial v} \tag{2.4}$$

is the infinitesimal generator of the point symmetry (2.3). (Throughout this paper, we assume summation over a repeated index).

Definition 2.2: A point symmetry (2.3) is called a *potential symmetry* of the given system $\mathbf{R}\{x,t,\mathbf{u}\}=0$ related to the potential system $\mathbf{S}\{x,t,\mathbf{u},v\}=0$ if and only if $(\partial\xi_{\mathbf{S}}/\partial v)^2+(\partial\tau_{\mathbf{S}}/\partial v)^2+\Sigma_{i=1}^n(\partial\eta^i_{\mathbf{S}}/\partial v)^2>0$, i.e., the infinitesimals $\xi_{\mathbf{S}}$, $\tau_{\mathbf{S}}$, $\eta^i_{\mathbf{S}}$ essentially depend on v. Any potential symmetry is a *nonlocal* symmetry of the given system $\mathbf{R}\{x,t,\mathbf{u}\}=0$.[4]

Definition 2.3: An equivalent system $\underline{\mathbf{S}}\{x,t,u^{i_1},\ldots,u^{i_p},v\}=0$, $p\leqslant n-1$ that can be obtained by excluding one or more dependent variables u^k of the potential system $\mathbf{S}\{x,t,\mathbf{u},v\}=0$, is called a *subsystem* of the potential system $\mathbf{S}\{x,t,\mathbf{u},v\}=0$.

Definition 2.4: A *tree of potential systems and subsystems* for a given PDE system

$\mathbf{R}\{x,t,\mathbf{u}\}=0$, with some equations of $\mathbf{R}\{x,t,\mathbf{u}\}=0$ written directly as conservation laws, is a set of PDE systems composed of $\mathbf{R}\{x,t,\mathbf{u}\}=0$, all resulting potential systems, and all possible subsystems. We will refer to the number of dependent variables in a subsystem as the *level* of that subsystem.

Remark 2.1: If a potential system, as it is written, includes conservation laws with an essential dependence on potential variables, a higher potential system can be obtained, as will be illustrated by examples.

Definition 2.5: A subsystem $\underline{\mathbf{S}}\{x,t,u^{i_1},\ldots,u^{i_{P'}-1}\}=0$, obtained from a system $\mathbf{S}\{x,t,u^{j_1},\ldots,u^{j_P}\}=0$ by excluding a dependent variable u^α, is *locally related* to $\mathbf{S}\{x,t,u^{j_1},\ldots,u^{j_P}\}=0$ if u^α can be directly expressed from the equations of $\mathbf{S}\{x,t,u^{j_1},\ldots,u^{j_P}\}=0$ in terms of x,t, the remaining dependent variables and their derivatives. Otherwise the subsystem $\underline{\mathbf{S}}\{x,t,u^{i_1},\ldots,u^{i_{P'}-1}\}=0$ is *nonlocally related* to $\mathbf{S}\{x,t,u^{j_1},\ldots,u^{j_P}\}=0$.

For example, the system

$$\mathbf{S}\{x,t,u,v\}=0:\quad \begin{cases} v_x-u=0,\\ v_t-(L(u))_x=0, \end{cases} \tag{2.5}$$

has two subsystems,

$$\underline{\mathbf{S}}_1\{x,t,u\}=0:\ u_t-(L(u))_{xx}=0 \quad \text{and} \quad \underline{\mathbf{S}}_2\{x,t,v\}=0:\ v_t=(L(v_x))_x, \tag{2.6}$$

where $\underline{\mathbf{S}}_1\{x,t,u\}=0$ is nonlocally related to $\mathbf{S}\{x,t,u,v\}=0$, and $\underline{\mathbf{S}}_2\{x,t,v\}=0$ is locally related to $\mathbf{S}\{x,t,u,v\}=0$. (Throughout this paper, subindices denote corresponding partial derivatives.)

Definition 2.6: A *tree of nonlocally related potential systems and subsystems* is obtained from a tree of potential systems and subsystems by removing all locally related subsystems.

Remark 2.2: It is important to emphasize that a given system $\mathbf{R}\{x,t,\mathbf{u}\}=0$, its related potential systems and subsystems, contain *all solutions of each other*. This directly follows from the way potentials are introduced in the potential systems and the way dependent variables are excluded in the subsystems since the integrability conditions always hold. Therefore, one may successfully apply a method of analysis (qualitative, numerical, perturbation, symmetry, conservation laws, etc.) to a potential system or a nonlocally related subsystem, even if it fails to be of use when applied to the given system $\mathbf{R}\{x,t,\mathbf{u}\}=0$.

A. Example 1: A tree of potential systems and subsystems for the nonlinear diffusion equation

For the nonlinear diffusion equation, the given PDE system is the conservation law

$$\mathbf{R}\{x,t,u\}=0:\ u_t-(L(u))_{xx}=0, \tag{2.7}$$

where the constitutive function $L(u)$ is related to the diffusion function $K(u)=L'(u)$. Consequently, the related potential system is given by

$$\mathbf{S}\{x,t,u,v\}=0:\begin{cases} v_x-u=0,\\ v_t-(L(u))_x=0, \end{cases} \tag{2.8}$$

and the subsystem $\underline{\mathbf{S}}\{x,t,v\}=0$ is given by the equation

$$\underline{\mathbf{S}}\{x,t,v\}=0:\ v_t=(L(v_x))_x. \tag{2.9}$$

The second equation of (2.8) is a conservation law, and hence it gives rise to another potential variable w, and higher potential system $\mathbf{T}\{x,t,u,v,w\}=0$ (Remark 2.1) given by

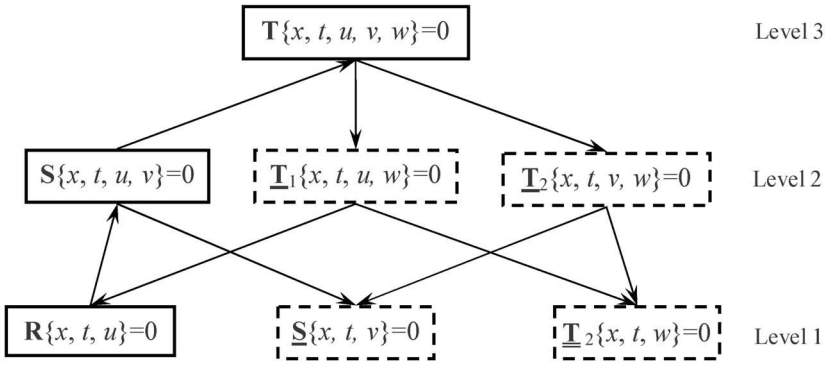

FIG. 1. The tree of potential systems and subsystems for the nonlinear diffusion equation (2.7) for an arbitrary constitutive function $L(u)$.

$$\mathbf{T}\{x,t,u,v,w\}=0\colon \begin{cases} v_x-u=0,\\ w_x-v=0,\\ w_t-L(u)=0, \end{cases} \tag{2.10}$$

and subsystems $\underline{\mathbf{T}}_1\{x,t,u,w\}=0$, $\underline{\mathbf{T}}_2\{x,t,v,w\}=0$, $\underline{\underline{\mathbf{T}}}_2\{x,t,w\}=0$ given by

$$\underline{\mathbf{T}}_1\{x,t,u,w\}=0\colon \begin{cases} w_{xx}-u=0,\\ w_t-L(u)=0, \end{cases}$$

$$\underline{\mathbf{T}}_2\{x,t,v,w\}=0\colon \begin{cases} w_x-v=0,\\ w_t-L(v_x)=0, \end{cases} \tag{2.11}$$

$$\underline{\underline{\mathbf{T}}}_2\{x,t,w\}=0\colon\ w_t-L(w_{xx})=0.$$

Since the subsystems $\underline{\mathbf{S}}\{x,t,v\}=0$, $\underline{\mathbf{T}}_1\{x,t,u,w\}=0$, $\underline{\mathbf{T}}_2\{x,t,v,w\}=0$, and $\underline{\underline{\mathbf{T}}}_2\{x,t,w\}=0$ are locally related to the potential systems (2.8) and (2.10), they are not of any interest.

This tree of potential systems and subsystems is illustrated in Fig. 1 with arrows showing the origins of elements of the tree, with dashed lines used to denote locally related subsystems. The group classification of this tree of potential systems and subsystems is given in Ref. 5 and references therein. In particular, for certain forms of the constitutive function $L(u)$ the level two system $\mathbf{S}\{x,t,u,v\}=0$ yields nonlocal symmetries of the level one system $\mathbf{R}\{x,t,u\}=0$, and vice versa. The point symmetries of the "grand" level three system $\mathbf{T}\{x,t,u,v,w\}=0$ include all point symmetries of the lower level systems. Moreover, the "grand" system $\mathbf{T}\{x,t,u,v,w\}=0$ includes a constitutive function $L(u)$ that yields symmetries that are nonlocal for the level one and level two systems.

B. Direct construction method for finding conservation laws

A direct method for finding conservation laws using factors was presented in Refs. 11 and 12. This method follows from the fact that a function $f(\mathbf{x},\mathbf{U},\partial\mathbf{U},\ldots,\partial^p\mathbf{U})$ is a divergence expression if and only if it is annihilated by the Euler differential operators,

$$E_k=\frac{\partial}{\partial U^k}-D_i\frac{\partial}{\partial U^k_i}+D_iD_j\frac{\partial}{\partial U^k_{ij}}+\cdots+(-1)^pD_{i_1}\cdots D_{i_p}\frac{\partial}{\partial U^k_{i_1\cdots i_p}}, \tag{2.12}$$

associated with each dependent variable U^k in $f(\mathbf{x},\mathbf{U},\partial\mathbf{U},\ldots,\partial^p\mathbf{U})$, $k=1,\ldots,n$. In (2.12), D_i is the total derivative operator for the independent variable x_i and $U^k_{i_1\cdots i_p}=\partial^p U^k/\partial x_{i_1}\cdots\partial x_{i_p}$.

For a given PDE system $\mathbf{R}\{x,t,\mathbf{u}\}=0$, when *additional* conservation laws are found within its tree of potential systems and subsystems, the tree can be extended. Here $x_1=t, x_2=x$.

The procedure to find additional conservation laws is as follows:

(A) Take a linear combination of the functions $R_k\{x,t,\mathbf{U}\}$ associated with the system $\mathbf{R}\{x,t,\mathbf{u}\}=0$, with unknown factors $\Lambda_k(x,t,\mathbf{U},\partial\mathbf{U},\ldots,\partial^l\mathbf{U})$ (for some fixed l),

$$M=\Lambda_k(x,t,\mathbf{U},\partial\mathbf{U},\ldots,\partial^l\mathbf{U})R_k\{x,t,\mathbf{U}\}. \tag{2.13}$$

It is essential to note that in (2.13), $\mathbf{U}$ is an *arbitrary function*. [$\mathbf{U}=\mathbf{u}(x,t)$ is a solution of $\mathbf{R}\{x,t,\mathbf{u}\}=0$.]

(B) A set of factors $\{\Lambda_k(x,t,\mathbf{U},\partial\mathbf{U},\ldots,\partial^l\mathbf{U})\}$ yields a conservation law (2.1) of $\mathbf{R}\{x,t,\mathbf{u}\}=0$ if and only if it satisfies the linear system of determining equations,

$$E_1M=0,\qquad \ldots,\qquad E_nM=0, \tag{2.14}$$

holding for arbitrary values of x,t and the components of $\mathbf{U},\partial\mathbf{U},\partial^2\mathbf{U},\ldots$.

(C) For each set of factors $\{\Lambda_k(x,t,\partial\mathbf{U},\ldots,\partial^l\mathbf{U})\}$ satisfying (2.14), there is an integral formula to find the density T and the flux X of the corresponding conservation law (2.1).[11,12]

Remark 2.3: The procedure outlined above can be applied to find conservation laws for any potential system or subsystem in a tree.

C. Construction of extended trees of nonlocally related potential systems and subsystems using additional conservation laws

Definition 2.7: If for some additional conservation law, a factor Λ_k does not vanish or vanishes only on solutions $\mathbf{U}=\mathbf{u}(x,t)$ of the given system $\mathbf{R}\{x,t,\mathbf{u}\}=0$, then the resulting conservation law (2.1) is a *useful conservation law* and can replace the kth equation $R_k\{x,t,\mathbf{u}\}=0$ of the system $\mathbf{R}\{x,t,\mathbf{u}\}=0$.

Consequently, the resulting system

$$\tilde{\mathbf{R}}\{x,t,\mathbf{u}\}=0:\begin{cases} R_1\{x,t,\mathbf{u}\}=0,\\ \cdots,\\ R_{k-1}\{x,t,\mathbf{u}\}=0,\\ D_tT\{x,t,\mathbf{u}\}+D_xX\{x,t,\mathbf{u}\}=0,\\ R_{k+1}\{x,t,\mathbf{u}\}=0,\\ \cdots,\\ R_m\{x,t,\mathbf{u}\}=0 \end{cases} \tag{2.15}$$

has the same solution set as the original DE system $\mathbf{R}\{x,t,\mathbf{u}\}=0$. In particular, the system (2.15) explicitly contains a conservation law that leads to a related higher potential system. In determining conservation laws by the direct construction method for the related higher level potential system $\mathbf{S}\{x,t,\mathbf{u},v\}=0$ arising from (2.15), for completeness it is essential to consider the potential system $\mathbf{S}\{x,t,\mathbf{u},v\}=0$ together with the replaced equation $R_k\{x,t,\mathbf{u}\}=0$, i.e., the system

$$\tilde{\mathbf{S}}\{x,t,\mathbf{u},v\}=0:\begin{cases} R_1\{x,t,\mathbf{u}\}=0,\\ \cdots,\\ R_{k-1}\{x,t,\mathbf{u}\}=0\\ R_k\{x,t,\mathbf{u}\}=0,\\ v_x-T\{x,t,\mathbf{u}\}=0,\\ v_t+X\{x,t,\mathbf{u}\}=0,\\ R_{k+1}\{x,t,\mathbf{u}\}=0,\\ \cdots,\\ R_m\{x,t,\mathbf{u}\}=0. \end{cases} \tag{2.16}$$

If a conservation law is not useful, then one would be too restricted in considering subsystems (with the same solution sets as $\mathbf{R}\{x,t,\mathbf{u}\}=0$) that result from elimination of one or more dependent variables.

By incorporating the direct method for finding conservation laws, we are now able to outline the algorithm for constructing the *extended* tree of nonlocally related potential systems and subsystems for a given DE system $\mathbf{R}\{x,t,\mathbf{u}\}=0$. Since $\mathbf{u}=(u^1,\ldots,u^n)$, the level (number of dependent variables) of the given system in the tree is n.

(1) *Construction of potential systems*: Suppose $\mathbf{R}\{x,t,\mathbf{u}\}=0$ includes explicit conservation laws as written. For each of these conservation laws (2.1), introduce a potential and construct a potential system of level $n+1$. For each of the potential systems of level $n+1$, repeat this step to obtain all potential systems of level $n+2$, etc., until higher potential systems include no more explicit conservation laws. Let $\mathcal{T}_1$ denote the resulting tree. (If $\mathbf{R}\{x,t,\mathbf{u}\}=0$ does not include explicit conservation laws as written, then $\mathcal{T}_1=\{\mathbf{R}\{x,t,\mathbf{u}\}=0\}$.)

(2) *Construction of subsystems*: For all systems of the tree $\mathcal{T}_1$, exclude where possible, one by one, dependent variables, to generate all subsystems of the systems in the tree $\mathcal{T}_1$. Eliminate subsystems that are locally related to it. This yields a possibly larger tree $\mathcal{T}_2$.

(3) *Additional conservation laws*: *Tree extension*: For each system in $\mathcal{T}_2$, find multipliers that yield useful conservation laws via the direct construction method. Use these additional useful conservation laws to obtain higher potential systems and corresponding subsystems. Eliminate locally related subsystems. Continue until no further useful conservation laws are found for any nonlocally related potential system or subsystem. This yields *an extended tree of nonlocally related potential systems and subsystems.*

D. Construction of nonlocal symmetries from an extended tree of potential systems and subsystems

The extended tree obtained by the above procedure can be used for different methods of analysis. In particular, it is useful in the search for nonlocal symmetries of the given DE system $\mathbf{R}\{x,t,\mathbf{u}\}=0$. Since each potential system and subsystem within the tree is nonlocally related to the given system, as well as other potential systems and subsystems in the tree, it follows that point symmetries of potential systems and subsystems may yield nonlocal (potential) symmetries of the given system, and/or other systems in the extended tree. Now we outline *the algorithm to construct nonlocal symmetries*.

(1) *Construction of extended trees of potential systems and nonlocally related subsystems*: For a given DE system $\mathbf{R}\{x,t,\mathbf{u}\}=0$, construct the extended tree of nonlocally related potential systems and subsystems. (If the given system contains constitutive functions, different extended trees may be obtained for particular forms of constitutive functions.)

(2) *Point symmetry analysis*: For each system in the extended tree, use Lie's algorithm to obtain its point symmetries.

(3) *Isolation of nonlocal symmetries*: From the set of point symmetries of each system in the

extended tree, isolate nonlocal symmetries of the given system $\mathbf{R}\{x,t,\mathbf{u}\}=0$.

An example of the use of this algorithm follows.

E. Example 2: Nonlocal symmetries and linearization of a nonlinear reaction-diffusion equation

We apply the above-described algorithm of construction of nonlocal symmetries to the reaction-diffusion equation

$$\mathbf{R}\{x,t,u\}=0:\ u_t-u^2u_{xx}-2bu^2=0. \tag{2.17}$$

First, we construct an extended tree of potential systems and subsystems. The equation (2.17) is not written as a conservation law. We look for multipliers of the form $\Lambda_1=\Lambda_1(U)$ that yield conservation laws of (2.17). Here the determining equation (2.14) becomes

$$E_1[\Lambda_1(U)(U_t-U^2U_{xx}-2bU^2)]=0,$$

and has solution $\Lambda_1(U)=-1/U^2$, with corresponding conservation law

$$\left(\frac{1}{u}\right)_t+(u+bx^2)_{xx}=0. \tag{2.18}$$

The multiplier $\Lambda_1(U)=-1/U^2$ does not vanish. Hence the conservation law (2.18) is useful and equivalent to the PDE (2.17). We let $u_1=1/u$ and denote the resulting PDE by

$$\tilde{\mathbf{R}}\{x,t,u_1\}=0:\ u_{1t}+\left(\frac{1}{u_1}+bx^2\right)_{xx}=0. \tag{2.19}$$

We introduce potential variables v and w and corresponding potential systems,

$$\begin{aligned}
&\mathbf{S}\{x,t,u_1,v\}=0:\begin{cases} v_x-u_1=0,\\ v_t+\left(\dfrac{1}{u_1}+bx^2\right)_x=0,\end{cases}\\
&\mathbf{T}\{x,t,u_1,v,w\}=0:\begin{cases} v_x-u_1=0,\\ w_x-v=0,\\ w_t+\left(\dfrac{1}{u_1}+bx^2\right)=0.\end{cases}
\end{aligned} \tag{2.20}$$

The subsystems are

$$\underline{\mathbf{S}}\{x,t,v\}=0:\ v_t+\left(\frac{1}{v_x}+bx^2\right)_x=0,$$

$$\begin{aligned}
&\underline{\mathbf{T}}_1\{x,t,u,w\}=0:\begin{cases} w_{xx}-u_1=0,\\ w_t+\left(\dfrac{1}{u_1}+bx^2\right)=0,\end{cases}\\
&\underline{\mathbf{T}}_2\{x,t,v,w\}=0:\begin{cases} w_x-v=0,\\ w_t+\left(\dfrac{1}{v_x}+bx^2\right)=0,\end{cases}
\end{aligned} \tag{2.21}$$

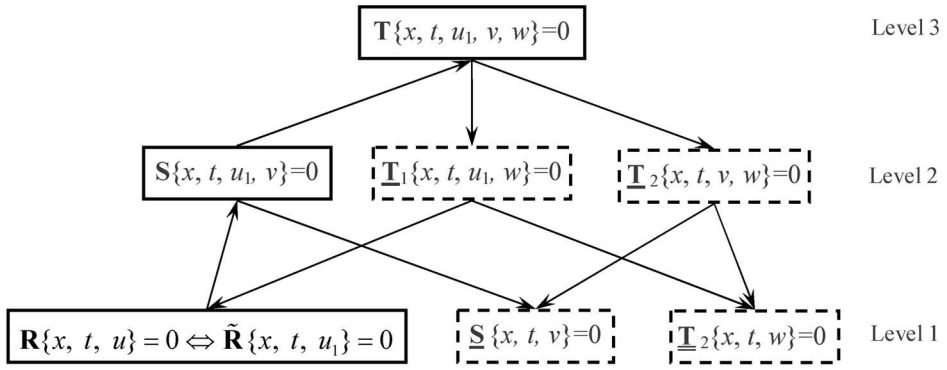

FIG. 2. The tree of potential systems and subsystems for the reaction-diffusion equation (2.17).

$$\underline{\underline{\mathbf{T}}}_2\{x,t,w\}=0\colon\ w_t+\left(\frac{1}{w_{xx}}+bx^2\right)=0.$$

The tree of potential systems and subsystems is illustrated in Fig. 2 with arrows showing the origins of elements of the tree. Locally related subsystems are outlined with dashed lines. For the analysis of nonlocal symmetries of the given system $\mathbf{R}\{x,t,u\}=0$ (2.17), only systems $\mathbf{S}\{x,t,u_1,v\}=0$ and $\mathbf{T}\{x,t,u_1,v,w\}=0$ need to be used, since all other subsystems are locally related to them.

One can show[5] that the level three potential system $\mathbf{T}\{x,t,u_1,v,w\}=0$ admits an infinitesimal generator,

$$\mathrm{X}^{\mathbf{T}}_{\infty}=e^{b(w-xv)}\Big((F^1-bxF^3)\frac{\partial}{\partial x}+(2bxu_1^2F^1-u_1^2F^2+bu_1(1-bx^2u_1)F^3)\frac{\partial}{\partial u_1}$$
$$+(vF^1-(1+bxv)F^3)\frac{\partial}{\partial w}\Big),\tag{2.22}$$

where

$$\frac{\partial F^1(v,t)}{\partial v}=F^2(v,t),\quad \frac{\partial F^3(v,t)}{\partial v}=F^1(v,t),\quad \frac{\partial F^3(v,t)}{\partial t}=F^2(v,t).\tag{2.23}$$

The point symmetry generator (2.22) is infinite dimensional; it projects to a point symmetry of $\underline{\mathbf{T}}_2\{x,t,v,w\}=0$, induces a contact symmetry of $\underline{\underline{\mathbf{T}}}_2\{x,t,w\}=0$, a Lie-Bäcklund symmetry of $\underline{\mathbf{T}}_1\{x,t,u,w\}=0$, and a nonlocal symmetry of $\mathbf{R}\{x,t,u\}=0$, $\tilde{\mathbf{R}}\{x,t,u_1\}=0$, $\mathbf{S}\{x,t,u_1,v\}=0$, and $\underline{\mathbf{S}}\{x,t,v\}=0$. Consequently, $\mathbf{T}\{x,t,u_1,v,w\}=0$, $\underline{\mathbf{T}}_2\{x,t,v,w\}=0$, and $\underline{\underline{\mathbf{T}}}_2\{x,t,w\}=0$ are linearizable by invertible mappings, and the other systems in the tree are linearizable by noninvertible mappings.[4,5]

III. TREES AND NONLOCAL SYMMETRIES FOR PLANAR GAS DYNAMICS EQUATIONS

We now use the algorithmic approach described in Sec. II to construct trees of potential systems and subsystems for the (1+1)-dimensional system of planar gas dynamics (PGD) equations. The point symmetries of some of these systems have been extensively considered in Ref. 14.

The two fundamental systems of differential equations that describe nonstationary (1+1)-dimensional gas motions are Euler and Lagrange systems. In the Eulerian description, x is a Cartesian coordinate in a fixed coordinate frame. The *Euler system* is given by

$$\mathbf{E}\{x,t,v,p,\rho\}=0:\begin{cases}\rho_t+(\rho v)_x=0,\\ \rho(v_t+vv_x)+p_x=0,\\ \rho(p_t+vp_x)+B(p,1/\rho)v_x=0.\end{cases}\tag{3.1}$$

Here v is the gas velocity, ρ is the gas density, and p is the gas pressure. In terms of the entropy density $S(p,\rho)$, the constitutive function $B(p,1/\rho)$ is given by

$$B(p,1/\rho)=-\rho^2 S_\rho/S_p.$$

In many applications, however, it is more convenient to use Lagrange mass coordinates $s=t$, $y=\int_{x_0}^{x}\rho(\xi)\mathrm{d}\xi$. In these variables, the system (3.1) takes on the equivalent form

$$\mathbf{L}\{y,s,v,p,q\}=0:\begin{cases}q_s-v_y=0,\\ v_s+p_y=0,\\ p_s+B(p,q)v_y=0,\end{cases}\tag{3.2}$$

and is called the *Lagrange system*. Here the coordinate y essentially enumerates the fluid particles; its domain does not change with time. The partial time derivative $\partial/\partial s=\partial/\partial t+v\,\partial/\partial x$ is the material derivative. The use of Lagrange mass coordinates often significantly facilitates the formulation of boundary conditions.[15–17]

We show that the potential system framework provides a direct connection between the Euler system (3.1) and the Lagrange system (3.2). Moreover, further extensions arise, and in particular, one can obtain other nonlocally related equivalent systems of equations.

We now construct a tree of nonlocally related potential systems and subsystems, with $\mathbf{E}\{x,t,v,p,\rho\}=0$ given by (3.1) serving as the given system, through the algorithm described in Sec. II.

Since the first equation of (3.1) is a conservation law, a potential variable r is naturally introduced, and the resulting level four potential system has the form

$$\mathbf{G}\{x,t,v,p,\rho,r\}=0:\begin{cases}r_x-\rho=0,\\ r_t+\rho v=0,\\ r_x(v_t+vv_x)+p_x=0,\\ r_x(p_t+vp_x)+B(p,1/r_x)v_x=0.\end{cases}\tag{3.3}$$

An obvious subsystem $\mathbf{I}\{x,t,v,p,r\}\equiv\underline{\mathbf{G}}_1\{x,t,v,p,r\}=0$ is obtained by excluding the density ρ from (3.3),

$$\mathbf{I}\{x,t,v,p,r\}=0:\begin{cases}r_t+vr_x=0,\\ r_x(v_t+vv_x)+p_x=0,\\ r_x(p_t+vp_x)+B(p,1/r_x)v_x=0.\end{cases}\tag{3.4}$$

In Ref. 14, (3.4) is referred to as the *intermediate* system. However, this system is locally related to $\mathbf{G}\{x,t,v,p,\rho,r\}=0$.

Another subsystem is $\underline{\mathbf{G}}_2\{x,t,p,\rho,r\}=0$, obtained by excluding the velocity v. This subsystem is also not of interest since it is locally related to $\mathbf{G}\{x,t,v,p,\rho,r\}=0$.

Consider a local coordinate transformation of the system $\mathbf{G}\{x,t,v,p,\rho,r\}=0$ with $r=y$, $t=s$ treated as independent variables, and x,v,p,ρ as dependent variables. Without loss of generality, $\rho\neq 0$. We let $q=1/\rho$, and obtain the system $\mathbf{G}_0\{y,s,x,v,p,\rho\}=0$ given by

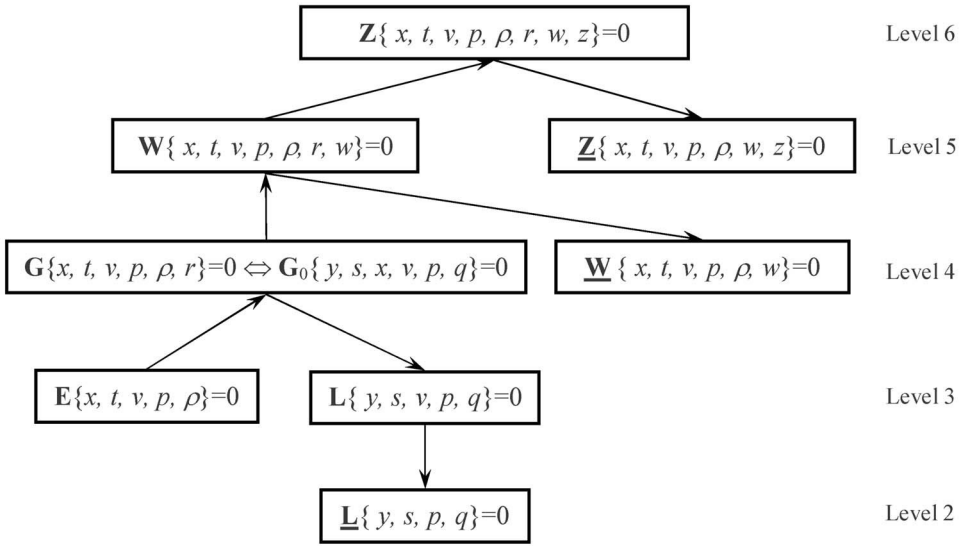

FIG. 3. The tree $\mathcal{T}_{\mathrm{PGD}}$ of nonlocally related PGD potential systems and subsystems, for an arbitrary constitutive function $B(p,1/\rho)$; $\mathbf{E}\{x,t,v,p,\rho\}=0$ is the Euler system (3.1), $\mathbf{L}\{y,s,v,p,q\}=0$ is the Lagrange system (3.2).

$$\mathbf{G}_0\{y,s,x,v,p,\rho\}=0:\begin{cases} q-x_y=0,\\ v-x_s=0,\\ v_s+p_y=0,\\ p_s+B(p,q)v_y=0, \end{cases} \tag{3.5}$$

equivalent to the potential system $\mathbf{G}\{x,t,v,p,\rho,r\}=0$ and locally related to it.

A subsystem of $\mathbf{G}_0\{y,s,x,v,p,\rho\}=0$ obtained by excluding x through $x_{sy}=x_{ys}$ is the Lagrange system (3.2), $\mathbf{L}\{y,s,v,p,q\}\equiv\underline{\mathbf{G}}_0\{y,s,v,p,q\}=0$. Thus *the Euler and Lagrange systems of PGD equations are connected through a common potential system* (see Fig. 3).

We continue the construction of the tree of potential systems and subsystems for the PGD equations for a general constitutive function $B(p,1/\rho)$. We first find possible higher potential systems arising for the potential system $\mathbf{G}\{x,t,v,p,\rho,r\}=0$ given by (3.3).

The Euler system given by (3.1) with multipliers $\Lambda_1=V$, $\Lambda_2=1$, $\Lambda_3=0$ yields a *useful* conservation law,

$$(\rho v)_t+(p+\rho v^2)_x=0, \tag{3.6}$$

which also holds for the system $\mathbf{G}\{x,t,v,p,\rho,r\}=0$. Hence we use the conservation law (3.6) to replace the equation $r_x(v_t+vv_x)+p_x=0$, and introduce a potential variable w to obtain the level five potential system $\mathbf{W}\{x,t,v,p,\rho,r,w\}=0$ given by

$$\mathbf{W}\{x,t,v,p,\rho,r,w\}=0:\begin{cases} r_x-\rho=0,\\ r_t+\rho v=0,\\ w_x+r_t=0,\\ w_t+p+vw_x=0,\\ r_x(p_t+vp_x)+B(p,1/r_x)v_x=0. \end{cases} \tag{3.7}$$

The third equation of (3.7) is written as a conservation law, and accordingly we introduce a potential variable z to obtain a level six potential system,

$$\mathbf{Z}\{x,t,v,p,\rho,r,w,z\}=0:\begin{cases} r_x-\rho=0,\\ r_t+\rho v=0,\\ z_t-w=0,\\ z_x+r=0,\\ w_t+p+vw_x=0,\\ r_x(p_t+vp_x)+B(p,1/r_x)v_x=0. \end{cases} \tag{3.8}$$

The only nonlocally related subsystems of (3.7) and (3.8) arise from excluding r (see Fig. 3). The Lagrange system (3.2) has a nonlocally related subsystem obtained by excluding v,

$$\underline{\mathbf{L}}\{y,s,p,q\}=0:\begin{cases} q_{ss}+p_{yy}=0,\\ p_s+B(p,q)q_s=0. \end{cases} \tag{3.9}$$

The tree $\mathcal{T}_{\mathrm{PGD}}$ of useful (i.e., nonlocally related) potential systems and subsystems [for an arbitrary constitutive function $B(p,1/\rho)$] is illustrated by Fig. 3. Note that either the Euler system $\mathbf{E}\{x,t,v,p,\rho\}=0$ or the Lagrange system $\mathbf{L}\{y,s,v,p,q\}=0$ can be taken as the given system. Each of these systems gives rise to the same tree of potential systems and subsystems.

All systems in the tree $\mathcal{T}_{\mathrm{PGD}}$ are nonlocally related and equivalent (i.e., contain all solutions of each other). Therefore any general method of analysis (qualitative, numerical, perturbation, symmetry, conservation laws, etc.) may yield new results for any of these nonlocally related PGD systems. In particular, this is the case for the symmetry analysis given below.

In Ref. 14, point symmetries of three systems were studied in detail—the Euler system (3.1), the Lagrange system (3.2), and the "intermediate" system (3.4). The authors gave a classification with respect to the constitutive function $B(p,1/\rho)$ and isolated the cases in which some of the point symmetries of $\mathbf{E}\{x,t,v,p,\rho\}=0$, $\mathbf{L}\{y,s,v,p,q\}=0$ or $\mathbf{I}\{x,t,v,p,r\}=0$ were nonlocal for the other two systems. However, their approach was heuristic—the connections between their systems did not involve a general constructive framework.

Using the algorithmic approach presented in this paper, one directly arrives at the tree $\mathcal{T}_{\mathrm{PGD}}$ of nonlocally related PGD potential systems and subsystems. To find nonlocal symmetries of systems $\mathbf{E}\{x,t,v,p,\rho\}=0$ and $\mathbf{L}\{y,s,v,p,q\}=0$, one should classify the point symmetries of *all eight* systems in the tree, with respect to the constitutive function $B(p,1/\rho)$. (The system $\mathbf{I}\{x,t,v,p,r\}=0$ discussed in Ref. 14 is of no interest since it is locally related to the system $\mathbf{G}\{x,t,v,p,\rho,r\}=0$ in the tree.) For example, the subsystem $\underline{\mathbf{L}}\{y,s,p,q\}=0$ given by (3.9), in the case of a Chaplygin gas $[B(p,q)=-p/q]$, admits a point symmetry with infinitesimal generator,

$$\mathrm{X}=-y^2\frac{\partial}{\partial y}-py\frac{\partial}{\partial p}+3yq\frac{\partial}{\partial q}, \tag{3.10}$$

which yields a nonlocal symmetry for both $\mathbf{E}\{x,t,v,p,\rho\}=0$ and $\mathbf{L}\{y,s,v,p,q\}=0$. The symmetry (3.10) was not obtained in Ref. 14, since the system (3.9) did not arise.

Furthermore, for some systems in the tree $\mathcal{T}_{\mathrm{PGD}}$, particular forms of the constitutive function $B(p,1/\rho)$ may yield useful conservation laws, which in turn would yield extended trees (cf. Sec. II). We now consider two examples.

Example A: For $B(p,1/\rho)=\rho(1+e^p)$, the system $\mathbf{G}\{x,t,v,p,\rho,r\}=0$ has a family of useful conservation laws,

$$D_t\left(\frac{e^p f(r)}{1+e^p}\right)+D_x\left(\frac{ve^p f(r)}{1+e^p}\right)=0, \tag{3.11}$$

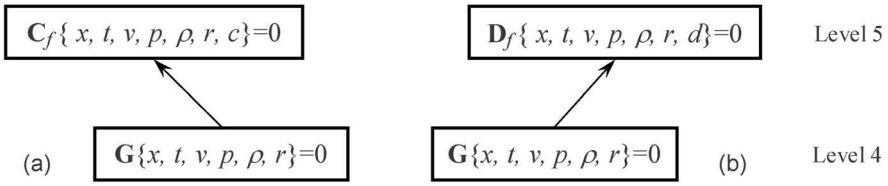

FIG. 4. PGD tree extensions for two particular forms of the constitutive function $B(p,1/\rho)$. (a) $B(p,1/\rho)=\rho(1+e^p)$. (b) Chaplygin gas $B(p,1/\rho)=-p\rho$.

for arbitrary $f(r)$. A conservation law of the form (3.11) can be used to replace the fourth equation of $\mathbf{G}\{x,t,v,p,\rho,r\}=0$ to introduce a potential c and consequent family of potential systems $\mathbf{C}_f\{x,t,v,p,\rho,r,c\}=0$ in terms of an arbitrary function $f(r)$,

$$\mathbf{C}_f\{x,t,v,p,\rho,r,c\}=0:\begin{cases} r_x-\rho=0,\\ r_t+\rho v=0,\\ r_x(v_t+vv_x)+p_x=0,\\ c_x+e^p f(r)/(1+e^p)=0,\\ c_t-ve^p f(r)/(1+e^p)=0. \end{cases} \tag{3.12}$$

The corresponding tree extension is exhibited in Fig. 4(a).

Example B: For the Chaplygin gas $B(p,1/\rho)=-p\rho$, the family of useful conservation laws

$$D_t\left(\frac{f(r)}{p}\right)+D_x\left(\frac{vf(r)}{p}\right)=0 \tag{3.13}$$

for arbitrary $f(r)$ yields a family of potential systems

$$\mathbf{D}_f\{x,t,v,p,\rho,r,d\}=0:\begin{cases} r_x-\rho=0,\\ r_t+\rho v=0,\\ r_x(v_t+vv_x)+p_x=0,\\ d_x+f(r)/p=0,\\ d_t-vf(r)/p=0, \end{cases} \tag{3.14}$$

nonlocally related to the other systems in the tree $\mathcal{T}_{\mathrm{PGD}}$. The corresponding tree extension is exhibited in Fig. 4(b). One can show that nonlocal symmetries of the Euler system $\mathbf{E}\{x,t,v,p,\rho\}=0$ only arise in the cases where $f(r)=r$, $f(r)=\mathrm{const}$. For $f(r)=r$, the system (3.14) admits

$$\mathrm{X}_{\mathbf{D}1}=\left(-\frac{t^3}{6}+dt\right)\frac{\partial}{\partial x}+\left(d-\frac{t^2}{2}\right)\frac{\partial}{\partial v}+rt\frac{\partial}{\partial p}-\frac{rt\rho}{p}\frac{\partial}{\partial\rho}, \tag{3.15}$$

$$\mathrm{X}_{\mathbf{D}2}=\left(-\frac{t^2}{2}+d\right)\frac{\partial}{\partial x}-t\frac{\partial}{\partial v}+r\frac{\partial}{\partial p}-\frac{r\rho}{p}\frac{\partial}{\partial\rho}. \tag{3.16}$$

Symmetry (3.15) is nonlocal for both the Euler system $\mathbf{E}\{x,t,v,p,\rho\}=0$ and the Lagrange system $\mathbf{L}\{y,s,v,p,q\}=0$; symmetry (3.16) is nonlocal for the Euler system $\mathbf{E}\{x,t,v,p,\rho\}=0$ but local for the Lagrange system $\mathbf{L}\{y,s,v,p,q\}=0$. In Ref. 14, symmetry $\mathrm{X}_{\mathbf{D}1}$ was not obtained; symmetry $\mathrm{X}_{\mathbf{D}2}$ was obtained by an *ad hoc* procedure.

Through the algorithmic framework given in this paper, the symmetry results in Ref. 14 can be recovered systematically and substantially extended.

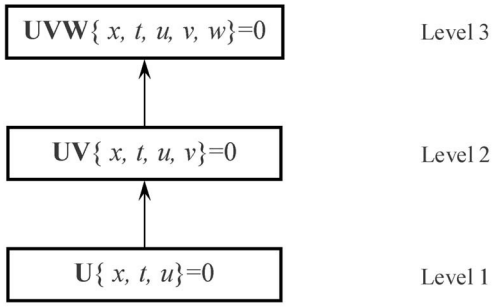

FIG. 5. NLT tree for arbitrary constitutive functions $F(u), G(u)$.

IV. EXTENDED TREES OF NONLOCALLY RELATED SYSTEMS FOR NONLINEAR TELEGRAPH EQUATIONS

We now construct trees of nonlocally related potential systems and subsystems for the nonlinear telegraph (NLT) equation, as well as further tree extensions for particular forms of constitutive functions. This allows us to extend recent results that appeared in Refs. 9, 13, and 18.

A. The tree for arbitrary constitutive functions

As a given system, we take the NLT equation,

$$\mathbf{U}\{x,t,u\}=0\text{: } u_{tt}-(F(u)u_x)_x-(G(u))_x=0. \tag{4.1}$$

Equation (4.1) is an explicit conservation law and hence is equivalent to the level two potential system,

$$\mathbf{UV}\{x,t,u,v\}=0\text{: } \begin{cases} u_t-v_x=0, \\ v_t-F(u)u_x-G(u)=0. \end{cases} \tag{4.2}$$

NLT systems of the form (4.2) represent the equations of telegraphy of a two-conductor transmission line and equations of motion of a hyperelastic homogeneous rod whose cross-sectional area varies exponentially along the rod. For further details, see Refs. 9 and 13 and references therein.

Since the first equation of (4.2) is written as a conservation law, a level three potential system is obtained,

$$\mathbf{UVW}\{x,t,u,v,w\}=0\text{: } \begin{cases} w_t-v=0, \\ w_x-u=0, \\ v_t-F(u)u_x-G(u)=0. \end{cases} \tag{4.3}$$

For *arbitrary* constitutive functions $F(u), G(u)$, there are no further potential systems.

The complete point symmetry classifications of the scalar equation (4.1) and system (4.2) appear, respectively, in Refs. 18 and 9. The point symmetries of (4.2) yield nonlocal symmetries of (4.1) for a large class of constitutive functions.

The given equation (4.1) is the only subsystem of system (4.2). The subsystems of potential system (4.3) are obtained by excluding u and/or v, $\mathbf{UW}\{x,t,u,w\}=0$, $\mathbf{VW}\{x,t,v,w\}=0$, and $\mathbf{W}\{x,t,w\}=0$. However these subsystems are not interesting since they are locally related to the potential system $\mathbf{UVW}\{x,t,u,v,w\}=0$ given by (4.3).

The tree $\mathcal{T}_{\mathrm{NLT}}$ of useful (i.e., nonlocally related) potential systems and subsystems, for arbitrary constitutive functions $F(u), G(u)$, is exhibited in Fig. 5.

TABLE I. Conservation laws of the system (4.2) using the data presented in Ref. 13.

Case	Multipliers	Conservation law
$F(u)=G'(u)$	$\Lambda_1=0,\ \Lambda_2=e^x$	(I) $D_t(ve^x)-D_x(e^xG(u))=0$
	$\Lambda_1=e^x,\ \Lambda_2=te^x$	(II) $D_t(e^x(u+tv))-D_x(e^x(tG(u)+v))=0$
$F(u)=G'(u)+1$	$\Lambda_1=\Lambda_2=e^{x+t}$	(III) $D_t(e^{x+t}(u+v))-D_x(e^{x+t}(G(u)+u+v))=0$
	$\Lambda_1=-\Lambda_2=e^{x-t}$	(IV) $D_t(e^{x-t}(u-v))+D_x(e^{x-t}(G(u)+u-v))=0$
$F(u)=G'(u)-1$	$\Lambda_1=-i\Lambda_2=e^{x+it}$	(V,VI) Real and imaginary parts of $D_t(e^{x+it}(iu+v))-D_x(e^{x+it}(G(u)-u+iv))=0$
$F(u)$ arbitrary, $G(u)=u$	$\Lambda_1=x-t^2/2,\ \Lambda_2=t$	(VII) $D_t((x-t^2/2)u+tv)+D_x((t^2/2-x)v-t\int F(u)\mathrm{d}u)=0$
	$\Lambda_1=-t,\ \Lambda_2=1$	(VIII) $D_t(v-tu)+D_x(tv-\int F(u)\mathrm{d}u)=0$

B. Tree extensions for particular constitutive functions

The complete conservation law classification of the potential system $\mathbf{UV}\{x,t,u,v\}=0$ given by (4.2) was found in Ref. 13 for multipliers of the form $\Lambda_i=\Lambda_i(x,t,U,V),\ i=1,2$. The problem of finding further potential systems from useful conservation laws of the system (4.2) was not considered in Ref. 13.

Using the data presented in Ref. 13, one sees that the following useful conservation laws (Table I) arise for (4.2).

In Table I, we exclude the cases [$G(u)=u$ with $F(u)=$const, $G(u)=0$ with $F(u)$ arbitrary] for which system (4.2) is linear or linearizable by a point transformation.

The eight conservation laws in Table I are now used to obtain additional potential systems and nonlocally related subsystems, and thus to extend the tree $\mathcal{T}_{\mathrm{NLT}}$. In particular, each conservation law in Table I [except (I)] can be used to replace either equation of system $\mathbf{UV}\{x,t,u,v\}=0$ given by (4.2), since in each of these seven cases both multipliers Λ_1,Λ_2 are nonzero and have no dependence on dependent variables.

Case 1: $F(u)=G'(u)$. For conservation law (I) in Table I, one has $\Lambda_1=0$, and hence only the second equation of the system $\mathbf{UV}\{x,t,u,v\}=0$ given by (4.2) can be replaced with this conservation law. Accordingly, we introduce a potential variable $\tilde{a}$ and let $a=e^{-x}\tilde{a}$. The corresponding potential system is given by

$$\mathbf{UVA}\{x,t,u,v,a\}=0:\begin{cases} v_x-u_t=0,\\ a+a_x-v=0,\\ a_t-G(u)=0. \end{cases} \tag{4.4}$$

Since the first equation of (4.4) is written as a conservation law, a level four potential system is obtained,

$$\mathbf{UVWA}\{x,t,u,v,w,a\}=0:\begin{cases} w_t-v=0,\\ w_x-u=0,\\ a+a_x-v=0,\\ a_t-G(u)=0. \end{cases} \tag{4.5}$$

Note that the system $\mathbf{UVW}\{x,t,u,v,w\}=0$ given by (4.3) is a subsystem of the system (4.5) through excluding the variable a. The subsystems

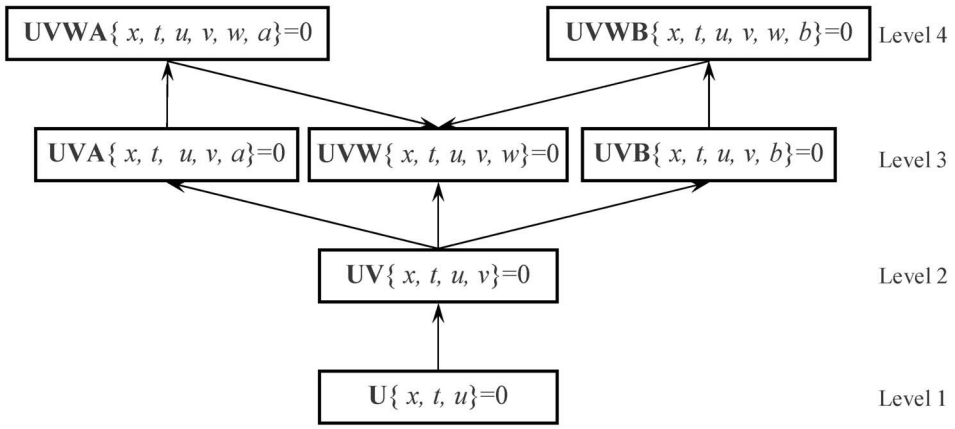

FIG. 6. The form of the extended tree of nonlocally related potential systems and subsystems of the NLT equations for Case 1 [$F(u)=G'(u)$, $G(u)$ arbitrary], Case 2 [$F(u)=G'(u)+1$, $G(u)$ arbitrary], Case 3 [$F(u)=G'(u)-1$, $G(u)$ arbitrary], and Case 4 [$F(u)$ arbitrary with $G(u)=u$].

$$\mathbf{VA}\{x,t,v,a\}=0:\begin{cases} a+a_x-v=0,\\ v_x-H'(a_t)a_{tt}=0 \quad (H=G^{-1}),\end{cases}$$
$$\mathbf{A}\{x,t,a\}=0:\ a_x+a_{xx}-H'(a_t)a_{tt}=0 \tag{4.6}$$

are locally related to (4.4) and therefore not interesting.

The useful conservation law (II) is equivalent to a pair of equations $b_t=tG(u)+v$, $b_x+b=u+tv$, and hence yields the level three potential system,

$$\mathbf{UVB}\{x,t,u,v,b\}=0:\begin{cases} v_x-u_t=0,\\ v_t-G'(u)u_x-G(u)=0,\\ b_t-tG(u)-v=0,\\ b_x+b-u-tv=0,\end{cases} \tag{4.7}$$

as well as the level four potential system,

$$\mathbf{UVWB}\{x,t,u,v,w,b\}=0:\begin{cases} w_t-v=0,\\ w_x-u=0,\\ b_t-tG(u)-v=0,\\ b_x+b-u-tv=0.\end{cases} \tag{4.8}$$

In Fig. 6 we exhibit the extended tree $\mathcal{T}^1_{\mathrm{NLT}}$ of nonlocally related potential systems and subsystems of the NLT equation (4.1) in the case $F(u)=G'(u)$.

In a similar manner, one can show that the three pairs of conservation laws for the other cases [$F(u)=G'(u)+1$, $F(u)=G'(u)-1$, $F(u)$ arbitrary with $G(u)=u$] all yield extended trees of the form exhibited in Fig. 6. For each of these three cases, the nonlocally related systems are as follows.

Case 2: $F(u)=G'(u)+1$. The set of nonlocally related potential systems and subsystems is given by

$$\mathbf{UVA}\{x,t,u,v,a\}=0:\begin{cases} v_x-u_t=0,\\ v_t-F(u)u_x-G(u)=0,\\ a_t+a-(G(u)+u+v)=0,\\ a_x+a-(u+v)=0,\end{cases}$$

$$\mathbf{UVWA}\{x,t,u,v,w,a\}=0:\begin{cases} w_t-v=0,\\ w_x-u=0,\\ a_t+a-(G(u)+u+v)=0,\\ a_x+a-(u+v)=0,\end{cases} \tag{4.9}$$

$$\mathbf{UVB}\{x,t,u,v,b\}=0:\begin{cases} v_x-u_t=0,\\ v_t-F(u)u_x-G(u)=0,\\ b_t-b-(G(u)+u-v)=0,\\ b_x+b+(u-v)=0,\end{cases}$$

$$\mathbf{UVWB}\{x,t,u,v,w,b\}=0:\begin{cases} w_t-v=0,\\ w_x-u=0,\\ b_t-b-(G(u)+u-v)=0,\\ b_x+b+(u-v)=0.\end{cases} \tag{4.10}$$

Case 3: $F(u)=G'(u)-1$. The useful complex conservation law (V,VI) in Table I is equivalent to two useful real conservation laws,

$$\text{(V)}\quad D_t[e^x(v\cos t-u\sin t)]+D_x[e^x(v\sin t-(G(u)-u)\cos t)]=0,$$

$$\text{(VI)}\quad D_t[e^x(u\cos t+v\sin t)]-D_x[e^x((G(u)-u)\sin t+v\cos t)]=0.$$

The set of nonlocally related potential systems and subsystems is given by

$$\mathbf{UVA}\{x,t,u,v,a\}=0:\begin{cases} v_x-u_t=0,\\ v_t-F(u)u_x-G(u)=0,\\ a_t+(v\sin t-(G(u)-u)\cos t)=0,\\ a_x+a-(v\cos t-u\sin t)=0,\end{cases} \tag{4.11}$$

$$\mathbf{UVWA}\{x,t,u,v,w,a\}=0:\begin{cases} w_t-v=0,\\ w_x-u=0,\\ a_t+(v\sin t-(G(u)-u)\cos t)=0,\\ a_x+a-(v\cos t-u\sin t)=0,\end{cases}$$

$$\mathbf{UVB}\{x,t,u,v,b_2\}=0:\begin{cases} v_x-u_t=0,\\ v_t-F(u)u_x-G(u)=0,\\ b_t+((G(u)-u)\sin t+v\cos t)=0,\\ b_x+b+(u\cos t+v\sin t)=0,\end{cases} \tag{4.12}$$

$$\mathbf{UVWB}\{x,t,u,v,w,b\}=0:\begin{cases} w_t - v = 0, \\ w_x - u = 0, \\ b_t + ((G(u)-u)\sin t + v\cos t) = 0, \\ b_x + b + (u\cos t + v\sin t) = 0. \end{cases}$$

Case 4: $F(u)$ arbitrary, $G(u)=u$. In this case, the set of nonlocally related potential systems and subsystems is given by

$$\mathbf{UVA}\{x,t,u,v,a\}=0:\begin{cases} v_x - u_t = 0, \\ v_t - F(u)u_x - u = 0, \\ a_x - ((x - t^2/2)u + tv) = 0, \\ a_t + \left((t^2/2 - x)v - t\int F(u)\mathrm{d}u\right) = 0, \end{cases}$$

$$\mathbf{UVWA}\{x,t,u,v,w,a\}=0:\begin{cases} w_t - v = 0, \\ w_x - u = 0, \\ a_x - ((x - t^2/2)u + tv) = 0, \\ a_t + \left((t^2/2 - x)v - t\int F(u)\mathrm{d}u\right) = 0 \end{cases} \tag{4.13}$$

and

$$\mathbf{UVB}\{x,t,u,v,b\}=0:\begin{cases} v_x - u_t = 0, \\ v_t - F(u)u_x - u = 0, \\ b_x - (v - tu) = 0, \\ b_t + \left(tv - \int F(u)\mathrm{d}u\right) = 0, \end{cases}$$

$$\mathbf{UVWB}\{x,t,u,v,w,b\}=0:\begin{cases} w_t - v = 0, \\ w_x - u = 0, \\ b_x - (v - tu) = 0, \\ b_t + \left(tv - \int F(u)\mathrm{d}u\right) = 0. \end{cases} \tag{4.14}$$

V. FURTHER REMARKS

(1) The algorithmic framework for nonlocally related potential systems and subsystems has been demonstrated to be useful for calculating new nonlocal symmetries and new nonlocal conservation laws for a given system of PDEs. It should be important to study the applicability of other methods of analysis (qualitative, numerical, perturbation, etc.) to nonlocally related systems in extended trees, especially coordinate-independent methods.

(2) In a PDE system with $n \geqslant 3$ independent variables, a conservation law is equivalent to a set of equations involving *several potential variables*.[4] The corresponding potential system is underdetermined, and requires suitable gauge constraints (in the form of additional equations on the potential variables) to be imposed in order to find nonlocal symmetries.[19]

Although a potential system without constraints is underdetermined, its potential *subsystems* may be useful for analysis without gauge constraints.

(3) In the algorithm presented in Sec. II, the nonlocally related subsystems are obtained by

exclusion of dependent variables *as written*. Alternatively any point transformation

$$U = U(x,t,u,v),$$
$$V = V(x,t,u,v),$$
$$X = X(x,t,u,v),$$
$$T = T(x,t,u,v), \tag{5.1}$$

could be used to exclude a dependent variable U or V to obtain *additional* nonlocally related subsystems. Indeed this is the situation within the tree of potential systems and subsystems of the PGD equations (Sec. III): the system $\mathbf{G}\{x,t,v,p,\rho,r\}=0$ as written has only a nonlocally related subsystem $\mathbf{E}\{x,t,v,p,\rho\}=0$. However after a local change of variables (to $\mathbf{G}_0\{y,s,x,v,p,\rho\}=0$), it admits the Lagrange system $\mathbf{L}\{y,s,v,p,q\}=0$ as a nonlocally related subsystem (Fig. 3).

(4) Using the algorithmic framework given in this paper, local and nonlocal symmetries for the PGD equations obtained in Ref. 14 can be recovered systematically and substantially extended (some examples of new nonlocal symmetries are given in Sec. III). The systematic classification of useful conservation laws and consequent nonlocal extensions of the PGD tree $\mathcal{T}_{\mathrm{PGD}}$ will appear in future works, as well as concomitant nonlocal symmetry analyses.

(5) An exhaustive study of nonlocal symmetries and nonlocal conservation laws of NLT equations resulting from extended trees of potential systems and subsystems is in progress. Preliminary results show that for a large class of constitutive functions, namely, $F(u)=G'(u)$, there exist point symmetries of the potential system $\mathbf{UVW}\{x,t,u,v,w\}=0$ given by (4.3) that are nonlocal for both the scalar NLT equation (4.1) and the system $\mathbf{UV}\{x,t,u,v\}=0$ given by (4.2). A particular example is a symmetry

$$\mathrm{X}_{\mathbf{UVW}} = v\frac{\partial}{\partial x} + \left(u + \frac{w}{3}\right)\frac{\partial}{\partial t} - \frac{uv}{3}\frac{\partial}{\partial u} - \frac{v^2}{3}\frac{\partial}{\partial v} + uv\frac{\partial}{\partial w} \tag{5.2}$$

for the case $F(u)=u^2, G(u)=u^3/3$.

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The short pulse hierarchy

J. C. Brunelli
Departamento de Física, CFM Universidade Federal de Santa Catarina, Campus Universitário, Trindade, C.P. 476 CEP 88040-900 Florianópolis, SC, Brazil

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We study a new hierarchy of equations containing the short pulse equation, which describes the evolution of very short pulses in nonlinear media, and the elastic beam equation, which describes nonlinear transverse oscillations of elastic beams under tension. We show that the hierarchy of equations is integrable. We obtain the two compatible Hamiltonian structures. We construct an infinite series of both local and nonlocal conserved charges. A Lax description is presented for both systems. For the elastic beam equations we also obtain a nonstandard Lax representation.
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I. INTRODUCTION

The cubic nonlinear Schrödinger equation is used in the description of the propagation of pulses in nonlinear media such as optical fibers. Recently, technology progress for creating very short pulses was achieved, however, the description of the evolution of those pulses lies beyond the usual approximations leading to the nonlinear Schrödinger equation. Various approaches have been proposed to replace the nonlinear Schrödinger equation in these conditions. In Ref. 1 Schäfer and Wayne proposed an alternative model to approximate the evolution of very short pulses in nonlinear media. They derived the short pulse (SP) equation

$$u_{xt} = u + \tfrac{1}{6}(u^3)_{xx}. \tag{1}$$

Chung *et al.*[2] showed numerically that the SP equation provides a better approximation to the solution of Maxwell's equations than the nonlinear Schrödinger equation as the pulse length gets short. Also, Sakovich and Sakovich[3] have studied the integrability of (1).

In this paper we will study the integrability of the nonlocal representation of the SP equation (1),

$$u_t = (\partial^{-1}u) + \tfrac{1}{2}u^2u_x, \tag{2}$$

as well as the hierarchy of equations associated with it. The equation in this form is more feasible for a Hamiltonian description and can be obtained integrating (1) with respect to x. In what follows we will refer to the equation (2) simply as the SP equation.

The local nonlinear equation

$$u_t = \left[\frac{u_{xx}}{(1+u_x^2)^{3/2}}\right]_x, \tag{3}$$

will also appear in our hierarchy of equations. It can be embedded in the Wadati-Konno-Ichikawa (WKI) system[4] and its x derivative can be shown to describe nonlinear transverse oscillation of elastic beams under tension.[5] Therefore, we will simply call (3) the equation for elastic beams (EB).

Our paper is organized as follows. In Sec. II, we show that our system is integrable through its bi-Hamiltonian nature. We give the two Hamiltonian structures associated with the Hamiltonian description of Eqs. (2) and (3). The method of prolongation is used to prove the Jacobi identity as

well as the compatibility of the Hamiltonian structures. In Sec. III, we construct the recursion operator and its inverse to obtain the first local and nonlocal charges recursively. We also obtain the first local and nonlocal equations of the hierarchy recursively, which includes the EB and SP equations, respectively. In Sec. IV we obtain the Lax representation for the system. For the EB equation, and for other local equations in the hierarchy, we also give a nonstandard Lax representation. In Sec. V, we summarize our results and present our conclusions.

The results in this paper are much like the ones obtained for the Harry Dym and Hunter-Saxton hierarchy of equations,[6] deformed Harry Dym and Hunter-Saxton hierarchy of equations[7], and for the non-local gas hierarchy of equations.[8] [In Refs. 6 and 7 the equation obtained by Hunter and Saxton in SIAM J. Appl. Math. **51**, 1498 (1991) was erroneously named, by the present author, Hunter-Zheng. We sincerely apologize to the authors about this mistake.] In these works we have as a main characteristic of a hierarchy of integrable equations with positive and negative flows. Also, throughout this paper the calculations involving pseudodifferential operators were performed or checked by the computer algebra program PSEUDO.[9]

II. BI-HAMILTONIAN STRUCTURE

Following Ref. 7 let us introduce

$$F^2 \equiv 1 + u_x^2, \quad A \equiv \frac{u_x}{F}, \tag{4}$$

which satisfy the following useful properties:

$$F^2(1 - A^2) = 1,$$

$$\frac{F_x}{F^3} = AA_x, \tag{5}$$

$$\frac{u_{xx}}{F^3} = A_x.$$

Using (4) the SP equation (2) assumes the forms

$$\begin{aligned} F_t &= \left(\tfrac{1}{2}u^2F\right)_x, \\ A_t &= \frac{u}{F} + \frac{1}{2}u^2A_x, \end{aligned} \tag{6}$$

and, similarly, the EB equation (3) can be written in one of the forms

$$u_t = A_{xx},$$

$$F_t = AA_{xxx}, \tag{7}$$

$$A_t = \frac{A_{xxx}}{F^3}.$$

Let us stress that the basic field is u and that A and F are just place holders used to make expressions more compact. Also, it is interesting to observe that the EB equation when written in the form (7) has the same structural form of the deformed Harry Dym equation studied in Ref. 7, however, the definitions in (4) are different.

From (6) and (7) it is straightforward to note that

$$H_0 = -\int \mathrm{d}x\, F, \tag{8}$$

is conserved under both the SP and EB flows.

Introducing the Clebsch potential

$$u = \phi_x, \tag{9}$$

the equation (2) can be written as

$$\phi_t = (\partial^{-1}\phi) + \tfrac{1}{6}\phi_x^3. \tag{10}$$

This equation (10) can be obtained from a variational principle, $\delta\int \mathrm{d}t\,\mathrm{d}x\,\mathcal{L}$, with the Lagrangian density

$$\mathcal{L} = \tfrac{1}{2}\phi_t\phi_x - \tfrac{1}{24}\phi_x^4 + \tfrac{1}{2}\phi^2. \tag{11}$$

This is a first order Lagrangian density and, consequently, the Hamiltonian structure can be readily read out, or we can use, for example, Dirac's theory of constraints[10] to obtain the Hamiltonian and the Hamiltonian operator associated with (11). The Lagrangian is degenerate and the primary constraint is obtained to be

$$\Phi = \pi - \tfrac{1}{2}\phi_x, \tag{12}$$

where $\pi = \partial\mathcal{L}/\partial\phi_t$ is the canonical momentum. The total Hamiltonian can be written as

$$H_T = \int \mathrm{d}x(\pi\phi_t - \mathcal{L} + \lambda\Phi) = \int \mathrm{d}x\Big[\tfrac{1}{24}\phi_x^4 - \tfrac{1}{2}\phi^2 + \lambda\Big(\pi - \tfrac{1}{2}\phi_x\Big)\Big], \tag{13}$$

where λ is a Lagrange multiplier field. Using the canonical Poisson bracket relation

$$\{\phi(x), \pi(y)\} = \delta(x-y), \tag{14}$$

with all others vanishing, it follows that the requirement of the primary constraint to be stationary under time evolution,

$$\{\Phi(x), H_T\} = 0,$$

determines the Lagrange multiplier field λ in (13) and the system has no further constraints.

Using the canonical Poisson bracket relations (14), we can now calculate

$$K(x,y) \equiv \{\Phi(x), \Phi(y)\} = \tfrac{1}{2}\partial_y\delta(y-x) - \tfrac{1}{2}\partial_x\delta(x-y). \tag{15}$$

This shows that the constraint (12) is second class and that the Dirac bracket between the basic variables has the form

$$\{\phi(x), \phi(y)\}_D = \{\phi(x), \phi(y)\} - \int \mathrm{d}z\,\mathrm{d}z'\{\phi(x), \Phi(z)\}J(z,z')\{\Phi(z'), \phi(y)\} = J(x,y),$$

where J is the inverse of the Poisson bracket of the constraint (15),

$$\int \mathrm{d}z\, K(x,z)J(x,y) = \delta(x-y).$$

This last relation determines

$$\partial_x J(x,y) = -\delta(x-y)$$

or

$$J(x,y) = \mathcal{D}\delta(x-y),$$

where

$$\mathcal{D} = -\partial^{-1}, \tag{16}$$

and can be thought of as the alternating step function in the coordinate space. We can now set the constraint (12) strongly to zero in (13) to obtain

$$H_T = \int \mathrm{d}x\left(\tfrac{1}{24}\phi_x^4 - \tfrac{1}{2}\phi^2\right). \tag{17}$$

Using (9) and the transformation properties of Hamiltonian operators,[11] we get

$$\mathcal{D}_1 = \partial(\mathcal{D})(\partial)^* = \partial, \tag{18}$$

and the SP equation (2) can be written in the Hamiltonian form as

$$u_t = \mathcal{D}_1 \frac{\partial H_2}{\delta u},$$

with H_2 given by

$$H_2 = \int \mathrm{d}x\left[\frac{1}{24}u^4 - \frac{1}{2}(\partial^{-1}u)^2\right], \tag{19}$$

which can be easily checked to be conserved by both the SP and EB equations.

We will show that the SP and EB equations belong to the same hierarchy of equations, at this point we note that

$$u_t = \mathcal{D}_1 \frac{\delta H_0}{\delta u},$$

with H_0 given by (8), yields the EB equation (3).

It is easy to show that the charges

$$H_{-1} = \frac{1}{2}\int \mathrm{d}x\, FA_x^2, \tag{20}$$

$$H_1 = \frac{1}{2}\int \mathrm{d}x\, u^2 \tag{21}$$

are also conserved by both the SP and EB equations. Therefore, the SP equation (2) can be written in the Hamiltonian form as

$$u_t = \mathcal{D}_2 \frac{\delta H_1}{\delta u},$$

and the EB equation (3) as

$$u_t = \mathcal{D}_2 \frac{\delta H_{-1}}{\delta u},$$

where we have defined

$$\mathcal{D}_2 = \partial^{-1} + u_x \partial^{-1} u_x = (F^2 - u_x \partial^{-1} u_{xx}) \partial^{-1}. \tag{22}$$

The skew symmetry of this Hamiltonian structure is manifest. The proof of the Jacobi identity for this structure as well its compatibility with (18) can be shown through the standard method of prolongation[12] which we describe briefly.

We can construct the two bivectors associated with the two structures as

$$\Theta_{\mathcal{D}_1} = \frac{1}{2} \int \mathrm{d}x \{\theta \wedge \mathcal{D}_1 \theta\} = \frac{1}{2} \int \mathrm{d}x \theta \wedge \theta_x,$$

$$\Theta_{\mathcal{D}_2} = \frac{1}{2} \int \mathrm{d}x \{\theta \wedge \mathcal{D}_2 \theta\} = \frac{1}{2} \int \mathrm{d}x \{\theta \wedge (\partial^{-1}\theta) + u_x \theta \wedge (\partial^{-1} u_x \theta)\}.$$

Using the prolongation relations,

$$\mathbf{pr}\, \vec{v}_{\mathcal{D}_1 \theta}(u) = \theta_x,$$

$$\mathbf{pr}\, \vec{v}_{\mathcal{D}_2 \theta}(u) = (\partial^{-1}\theta) + u_x (\partial^{-1} u_x \theta), \tag{23}$$

$$\mathbf{pr}\, \vec{v}_{\mathcal{D}_2 \theta}(u_x) = (\mathbf{pr}\, \vec{v}_{\mathcal{D}_2 \theta}(u))_x,$$

it is straightforward to show that the prolongation of the bivector $\Theta_{\mathcal{D}_2}$ vanishes,

$$\mathbf{pr}\, \vec{v}_{\mathcal{D}_2 \theta}(\Theta_{\mathcal{D}_2}) = 0,$$

implying that $\mathcal{D}_2$ satisfies the Jacobi identity. Using (23), it also follows that

$$\mathbf{pr}\, \vec{v}_{\mathcal{D}_1 \theta}(\Theta_{\mathcal{D}_2}) + \mathbf{pr}\, \vec{v}_{\mathcal{D}_2 \theta}(\Theta_{\mathcal{D}_1}) = 0,$$

showing that $\mathcal{D}_1$ and $\mathcal{D}_2$ are compatible. Namely, not only are $\mathcal{D}_1, \mathcal{D}_2$ genuine Hamiltonian structures, any arbitrary linear combination of them is as well. As a result, the dynamical equations (2) and (3) are bi-Hamiltonian with the same compatible Hamiltonian structures and, consequently, are integrable.[12,13]

III. THE SHORT PULSE HIERARCHY

When a system is bi-Hamiltonian, we can naturally define a hierarchy of commuting flows through the relation

$$u_{t_n} = K_n[u] = \mathcal{D}_1 \frac{\delta H_{n+1}}{\delta u} = \mathcal{D}_2 \frac{\delta H_n}{\delta u}, \quad n = \ldots, -2, -1, 0, 1, 2, \ldots . \tag{24}$$

For $n=1$ and $n=-1$ we get the SP and EB equations, respectively. For $n=0$ we have

$$K_0 = \mathcal{D}_1 \frac{\delta H_1}{\delta u} = (\partial u) = u_x$$

and

$$\begin{aligned} K_0 &= \mathcal{D}_2 \frac{\delta H_0}{\delta u} = ((F^2 - u_x \partial^{-1} u_{xx}) \partial^{-1} A_x) \\ &= (F^2 A - u_x \partial^{-1} u_{xx} A) = F u_x - u_x F = 0, \end{aligned} \tag{25}$$

where we have used (5), i.e., $F^2 A = F u_x$ and $u_{xx} A = F_x$. Therefore, we would be lead to conclude that H_0 is a Casimir of $\mathcal{D}_2$. We can resolve this apparent contradiction being careful while per-

forming calculations with the antiderivative ∂^{-1}. We can use the following representation:

$$(\partial_x^{-1} f) \equiv (\partial^{-1} f)(x) = \int_{-\infty}^{+\infty} \mathrm{d}y\, \epsilon(x-y) f(y),$$

where

$$\epsilon(x-y) = \begin{cases} 1/2 & \text{for } x > y, \\ -1/2 & \text{for } x < y. \end{cases}$$

Then, it can be shown that

$$(\partial_x^{-1} f_x) = f - \tfrac{1}{2}(f(+\infty) + f(-\infty)). \tag{26}$$

Now, if we assume $u^{(n)} \to 0$ as $|x| \to \infty$ (which yields $A|_{\pm\infty} = 0$ and $F|_{\pm\infty} = 1$) then it follows:

$$(\partial^{-1} A_x) = A \quad \text{and} \quad (\partial^{-1} F_x) = F - 1. \tag{27}$$

Using this last result in the naive calculation (25) we obtain the desired term u_x. This sort of missing or "ghost" terms given rise to apparent contradictions in nonlocal theories were already observed in the literature (see Ref. 14 and references therein).

Let us introduce the recursion operator following from the two Hamiltonian structures as:

$$R = \mathcal{D}_2 \mathcal{D}_1^{-1}. \tag{28}$$

Then, it follows from (24) that

$$\frac{\delta H_{n+1}}{\delta u} = R^{\dagger} \frac{\delta H_n}{\delta u}, \quad n = 0, 1, 2, \ldots, \tag{29}$$

where

$$R^{\dagger} = \partial^{-2} + \partial^{-1} u_x \partial^{-1} u_x = \partial^{-2}(F^2 + u_{xx} \partial^{-1} u_x) \tag{30}$$

is the adjoint of R. The conserved charges for the hierarchy can, of course, be determined recursively from (29) and give the infinite set of (nonlocal) conserved Hamiltonians

$$\begin{aligned} H_0 &= -\int \mathrm{d}x\, F, \\ H_1 &= \frac{1}{2} \int \mathrm{d}x\, u^2, \\ H_2 &= \int \mathrm{d}x \left[\tfrac{1}{24} u^4 - \tfrac{1}{2} (\partial^{-1} u)^2 \right], \\ H_3 &= \int \mathrm{d}x \left[\tfrac{1}{720} u^6 + \tfrac{1}{2} (\partial^{-1} u)^2 + \tfrac{1}{6} (\partial^{-2} u^3) u - \tfrac{1}{4} (\partial^{-1} u)^2 u^2 \right], \\ &\ldots . \end{aligned} \tag{31}$$

The corresponding flows (the first few, since the equations become extremely nonlocal as we proceed further in the recursion) have the forms

$$u_{t_0} = u_x,$$

$$u_{t_1} = (\partial^{-1}u) + \tfrac{1}{2}u^2 u_x,$$
$$u_{t_2} = (\partial^{-3}u) + \tfrac{1}{6}(\partial^{-1}u^3) + u_x(\partial^{-1}(u_x(\partial^{-2}u))) + \tfrac{1}{24}u^4 u_x, \tag{32}$$
$$\cdots .$$

For negative values of n, the gradients of the Hamiltonians will satisfy the recursion[9]

$$\frac{\delta H_n}{\delta u} = (R^\dagger)^{-1}\frac{\delta H_{n+1}}{\delta u}, \quad n = -1, -2, \ldots . \tag{33}$$

Writing the recursion operator (28) in the form

$$R = (F^2 - u_x\partial^{-1}u_{xx})\partial^{-2}, \tag{34}$$

and using the identities (5) the inverse can be easily checked to be

$$R^{-1} = \partial^2\left(\frac{1}{F^2} + A\partial^{-1}A_x\right) = \partial^2\frac{1}{u_{xx}}\partial F\partial^{-1}\frac{u_{xx}}{F^3}. \tag{35}$$

Note that (35) can be recognized as the recursion operator obtained in Ref. 3 for the SP equation in the form (1) using cyclic basis techniques. The corresponding conserved charges can now be recursively constructed from (33) and have the forms

$$H_{-1} = \frac{1}{2}\int \mathrm{d}x\, FA_x^2,$$
$$H_{-2} = \frac{1}{8}\int \mathrm{d}x\left(FA_x^4 - 4\frac{A_{xx}^2}{F}\right),$$
$$H_{-3} = \frac{1}{16}\int \mathrm{d}x\left(FA_x^6 + 8\frac{AA_{xx}^3}{F} - 12\frac{A_x^2A_{xx}^2}{F} + 8\frac{A_{xxx}^2}{F^3}\right), \tag{36}$$
$$\cdots .$$

The corresponding flows (the first few) have the forms

$$u_{t_{-1}} = A_{xx},$$
$$u_{t_{-2}} = \left(\frac{A_{xx}}{F^2} + \frac{1}{2}A_x^2A\right)_{xx},$$
$$u_{t_3} = \left(\frac{A_{xxxx}}{F^4} + \frac{1}{2}\frac{A_x^2A_{xx}}{F^2} - 2\frac{A_{xxx}A_xA}{F^2} - \frac{3}{2}\frac{A_{xx}^2A}{F^2} - A_{xx}A_x^2A^2 + \frac{3}{8}A_x^4A\right)_{xx}, \tag{37}$$

IV. THE LAX REPRESENTATION

$\cdots$.

Conserved charges for our systems can be determined in principle recursively from (29) and (33). However, to construct the conserved charges directly we look for a Lax representation for the system of SP and EB equations.

It is well known[15,16] that for a bi-Hamiltonian system of evolution equations, $u_{t_n} = K_n[u]$, a natural Lax description

$$\frac{\partial M}{\partial t_n} = [B, M],$$

is easily obtained where, we can identify

$$M \equiv R,$$

$$B \equiv K_n'.$$

Here R is the recursion operator (34) and K_n' represents the Fréchet derivative of K_n, defined by

$$K_n'[u]v = \frac{d}{d\epsilon} K_n [u + \epsilon v]|_{\epsilon=0}.$$

For the SP and EB system of equations in (2) and (3), respectively, we have

$$B^{\mathrm{SP}} \equiv K_1' = \partial^{-1} + \tfrac{1}{2}\partial u^2,$$

$$B^{\mathrm{EB}} \equiv K_{-1}' = \partial^2 F^{-3} \partial.$$

The two systems have the same $M=R$ given in (28). It can now be checked that

$$\begin{aligned} \frac{\partial M}{\partial t} &= [B^{\mathrm{SP}}, M], \\ \frac{\partial M}{\partial t} &= [B^{\mathrm{EP}}, M], \end{aligned} \tag{38}$$

do indeed generate the SP and the EB equations and, thereby, provide a Lax pair for the system.

A Lax representation directly gives the conserved charges of the system. From the structure of (38), it follows that $\mathrm{Tr}\, M^{(2n+1)/2}$ are conserved, where "Tr" represents the Adler's trace.[17] We note that

$$\begin{aligned} \mathrm{Tr}\, M^{(2n+1)/2} &= 0, \quad n \geqslant 1, \\ \mathrm{Tr}\, M^{1/2} &= \int \mathrm{d}x\, F, \\ \mathrm{Tr}\, M^{-1/2} &= \frac{1}{2} \int \mathrm{d}x\, F A_x^2, \\ \mathrm{Tr}\, M^{-3/2} &= \frac{3}{8} \int \mathrm{d}x \left(F A_x^2 - 4 \frac{A_{xx}^2}{F} \right), \\ &\cdots . \end{aligned} \tag{39}$$

These charges correspond (up to multiplicative constants) to the ones given in (36), constructed earlier by recursion. In fact, all H_{-n} with positive $n \geqslant 0$ can be constructed from $\mathrm{Tr}\, M^{-(2n-1)/2}$ and by construction [namely, because of the nature of (38)], they are conserved under both the SP and EB flows. However, as is clear from (39), this procedure does not yield the nonlocal charges H_n with positive integer values. The construction of these nonlocal charges relies primarily on the recursion relation (29). As in our papers[6–8] it remains an interesting question to construct these charges in a more direct manner.

We can also obtain a Lax representation, in a Gelfand-Dikii form, for the EB hierarchy of equations, in a straightforward way. It is well known (see Refs. 7 and 18 and references therein) that the recursion operator defines a eigenvalue problem of the type

$$(1-\lambda R^{\dagger})\phi=0, \tag{40}$$

for the eigenfunction ϕ with eigenvalue $1/\lambda$. Since we know the inverse of the recursion operator we obtain from (40),

$$[(R^{\dagger})^{-1}-\lambda]\phi=0, \tag{41}$$

which defines a Lax eigenvalue problem. Using (35) we identify the Lax operator for our system to be

$$L\equiv(R^{\dagger})^{-1}=\frac{1}{F}\partial\frac{1}{F}\partial+A_x\partial^{-1}A_x\partial.$$

It can be readily checked that the hierarchy of EB equations (37) (up to multiplicative constants) can be obtained from the nonstandard Lax equation,

$$\frac{\partial L}{\partial t_{-n}}=[(L^{(2n+1)/2})_{\geqslant 2},L], \quad n=1,2,3,\ldots .$$

The conserved quantities (36) and H_0 in (31) for this system (up to multiplicative constants) can be obtained from $\mathrm{Tr}\,L^{(2n-1)/2}$, $n=0,1,2,\ldots$.

V. CONCLUSION

In this paper, the short pulse and elastic beam equations were shown to belong to the same hierarchy corresponding to positive and negative flows. We have shown that these systems are bi-Hamiltonian and using recursion we construct infinite series of both local and nonlocal conserved charges as well as the respective hierarchy of equations. A Lax pair for the short pulse and elastic beam equations was derived. The Lax operator yielded the local charges via Adler's trace, however, the construction of the nonlocal charges through this Lax operator is unknown by us. Also, a nonstandard Lax representation in a Gelfand-Dikii form for the elastic-beam hierarchy of equation was described.

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Representations of the q-deformed algebras $U_q(so_3)$ and $U_q(so_5)$ and q-orthogonal polynomials

Alexander Rozenblyum
Mathematics Department, New York City College of Technology, City University of New York, Brooklyn, New York 11201

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Orthogonal polynomials related to irreducible representations of the classical type of the q-deformed algebras $U_q(so_3)$ and $U_q(so_5)$ are investigated. The main method consists in the diagonalization of corresponding infinitesimal operators (generators) of representations. For the algebra $U_q(so_3)$ this method leads to q-analogs of Krawtchouk polynomials. The properties of these polynomials are considered, the q-difference equation, the recurrence and explicit formulas. For the algebra $U_q(so_5)$, the diagonalization process of generators of representations leads to the connection with some class of orthogonal polynomials in two discrete variables. These variables are the so-called q-numbers $[n]$, where $[n]=(q^n-q^{-n})/(q-q^{-1})$. The introduced polynomials can be considered as two-dimensional q-analogs of Krawtchouk polynomials. The q-difference equation of the Sturm-Liouville type for these polynomials is constructed. The corresponding eigenvalues are investigated including the explicit formulas for their multiplicities. The structure of polynomial solutions is described. © *2005 American Institute of Physics.*
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I. INTRODUCTION

It is well known that representation theory of the group SO(3) of the rotations in three-dimensional Euclidean space relates to different types of classical special functions including Jacobi, Krawtchouk, and Meixner polynomials (see, for example, Refs. 1–3). It is shown in Ref. 4 that representations of the group SO(n) for $n \geqslant 5$ (and other high-dimensional groups) lead to orthogonal polynomials in many discrete and continuous variables. In particular, representations of the group SO(5) are related to orthogonal polynomials in two variables that can be considered as two-dimensional analogs of the Krawtchouk and Hermite polynomials.

The aim of the present paper is to describe in a similar manner the relations between the representations of the q-deformed algebras $U_q(so_3)$ and $U_q(so_5)$ and some classes of orthogonal polynomials in one and two discrete variables. As for the classical groups SO(n) and U(n), studied in Refs. 4 and 5, the main method consists in the diagonalization of corresponding infinitesimal operators (generators) of representations. To do this, we construct the realization of representation space as the space of polynomials in q-numbers $[n]$. Orthogonal polynomials we consider here relate to eigenvectors of generators of representation and can be treated as one- and two-dimensional q-analogs of Krawtchouk polynomials. The results obtained for the group $U_q(so_3)$ allow the construction in explicit form of the matrix of the operator connecting the bases in which two generators of a representation are diagonal.

II. REPRESENTATIONS OF THE ALGEBRA $U_q(SO_3)$ AND q-KRAWTCHOUK POLYNOMIALS

Algebra $U_q(so_3)$ is the q-deformation of the universal enveloping algebra $U(so_3)$. Algebra $U_q(so_3)$ and its irreducible representations of the classical type (i.e., representations that are

q-deformations of irreducible representations of the algebra so_3) were constructed in Ref. 6. It contains (similar to the algebra so_3) three generators J^q_{12}, J^q_{23}, and J^q_{13} that satisfy the relations:

$$[J^q_{12},J^q_{23}]_q \equiv q^{1/2}\cdot J^q_{12}\cdot J^q_{23} - q^{-1/2}\cdot J^q_{23}\cdot J^q_{12} = J^q_{13},$$

$$[J^q_{23},J^q_{13}]_q = J^q_{12}, \quad [J^q_{13},J^q_{12}]_q = J^q_{23}.$$

Let T be an irreducible representation of the algebra $U_q(so_3)$. Then T is defined by a non-negative integer or a half-integer l (the highest weight of the representation). The representation space V contains the basis $\{\xi_m\}$, $m=-l,\ldots,l$, in which the operators $I^q_{jk}=T(J^q_{jk})$ act by the formulas

$$I^q_{12}\xi_m = i[m]\xi_m, \quad i=\sqrt{-1}, \quad m=-l,\ldots,l,$$

$$I^q_{13}\xi_m = iq^{1/2}(q^m A(m)\xi_{m+1} + q^{-m}A(m-1)\xi_{m-1}),$$

$$I^q_{23}\xi_m = A(m)\xi_{m+1} - A(m-1)\xi_{m-1}, \tag{1}$$

where

$$A(m) = \left(\frac{[m][m+1]}{[2m][2m+2]}[l-m][l+m+1]\right)^{1/2}. \tag{2}$$

Here the q-numbers $[n]$ are defined as

$$[n] = (q^n - q^{-n})/(q-q^{-1}) = \frac{\sinh(n\ln q)}{\sinh(\ln q)}.$$

If $k=0$, we assume that $[2k]/[k]=2$.

The basis $\{\xi_m\}$ consists of the eigenvectors of the operator I^q_{12}. Similarly, one can consider another basis in representation space V consisting of the eigenvectors of the operator I^q_{23}. We will construct the matrix connecting these two bases, i.e., we will diagonalize the operator I^q_{23}. The method used is similar to the one developed for the classical groups $SO(n)$ and $U(n)$ (Refs. 4 and 5) and is based on the realization of the representation space as a space of polynomial functions of a discrete variable. This approach leads to a class of orthogonal polynomials that can be considered as q-analogs of the Krawtchouk polynomials.[7,8] We will assume that the highest weight l of the representation T is a non-negative integer.

Let L be the space of all complex-valued functions defined on the lattice $[-l,l]$. Then $\dim L=2l+1$, and L is isomorphic to the representation space V. This isomorphism allows treating vectors from V as functions of a discrete variable m that runs through the lattice $[-l,l]$. It follows from (1) that operator I^q_{23} acts in the space L by the formula

$$(I^q_{23}f)(m) = -A(m)f(m+1) + A(m-1)f(m-1), \quad f\in L. \tag{3}$$

Let $\widetilde{P}(m)$ be an eigenfunction of the operator I^q_{23} in the space L with the eigenvalue μ,

$$(I^q_{23}\widetilde{P})(m) = \mu\cdot\widetilde{P}(m), \quad m=-l,\ldots,l. \tag{4}$$

Let us make the following substitutions in Eq. (4):

$$\widetilde{P}(m) = i^m\sqrt{\rho(m)}P(m), \tag{5}$$

where

$$\rho(m) = \frac{[2m]}{[m]}\frac{1}{[l-m]![l+m]!}, \tag{6}$$

$$[n]! = [n][n-1]\dots[2][1], \quad [0]! = 1.$$

Below we will also use the notations

$$[2n]!! = [2n][2n-2]\dots[2], \quad [2n-1]!! = [2n-1][2n-3]\dots[1].$$

The substitution (5) is equivalent to replacing the operator I_{23}^q with the operator

$$J = A^{-1} I_{23}^q A,$$

where A is the multiplication operator, $(Af)(m) = i^m \sqrt{\rho(m)} f(m)$.

Then the function $P(m)$ satisfies the equation $(JP)(m) = \mu \cdot P(m)$. Using (3) and (2), this equation can be written as

$$\frac{[m]}{[2m]}\{[l-m]P(m+1) + [l+m]P(m-1)\} = \lambda P(m), \quad \lambda = \mu i, \tag{7}$$

or

$$\frac{1}{(q^m + q^{-m})(q - q^{-1})}\{(q^{l-m} - q^{-l+m})P(m+1) + (q^{l+m} - q^{-l-m})P(m-1)\} = \lambda P(m).$$

Let us denote by A_q the operator from the left-hand part of Eq. (7),

$$(A_q f)(m) = \frac{[m]}{[2m]}\{[l-m]f(m+1) + [l+m]f(m-1)\}.$$

The following statement can be proved.

Proposition 1: For any $n = 0, 1, \dots$,

$$A_q([m]^n) = [l-n][m]^n + Q_{n-2}([m]),$$

where $Q_{n-2}(t)$ is a polynomial of t of the degree $n-2$, $n \geqslant 2$; $Q_{-1}(t) \equiv Q_{-2}(t) \equiv 0$.

It follows from Proposition 1 that the operator A_q acts in the space $\mathrm{P}\{[m]\}$ of all polynomials of $[m]$, and has in this space the eigenvalues of the form

$$\lambda = \lambda_n = [l-n] = \frac{q^{l-n} - q^{-l+n}}{q - q^{-1}}, \quad n = 0, 1, \dots .$$

Accordingly, the operator I_{23}^q is diagonalizable in the representation space V and has eigenvalues,

$$\mu = \mu_n = i[n-l] = i\frac{q^{n-l} - q^{-n+l}}{q - q^{-1}}, \quad n = 0, 1, \dots, 2l.$$

Proposition 1 allows one to realize the representation space V as the set of all polynomials in $[m]$, defined on the lattice $[-l, l]$. This realization shows that Eq. (7) has polynomial solutions. More exactly, the following statement is true:

Proposition 2: For any $n = 0, 1, \dots$, the equation

$$[l-m]P(m+1) + [l+m]P(m-1) = \frac{[2m]}{[m]}[l-n]P(m) \tag{8}$$

has a solution $P_n(m)$ which is a polynomial of $[m]$ of the degree n.

If we let $q \to 1$, then Eq. (8) is transformed into the following:

$$(l-m)P(m+1)+(l+m)P(m-1)=2(l-n)P(m).$$

This equation describes the Krawtchouk polynomials.[7] It relates to eigenvectors of the generator of representation of the group SO(3).[4] We can treat the solutions of Eq. (8) as q-analogs of the Krawtchouk polynomials.

Similar to the classical case, Eq. (8) can be written in terms of finite differences,

$$[l+m]\Delta\,\nabla\,P(m)-\frac{[2l]}{[l]}[m]\Delta P(m)=\frac{[2m]}{[m]}\{[l-n]-[l]\}P(m),$$

where $(\Delta f)(m)=f(m+1)-f(m)$, $(\nabla f)(m)=f(m)-f(m-1)$.

Equation (8) can also be written in self-adjoint form

$$\frac{[m]}{[2m]}[l-m]![l+m]!\Delta\left\{\frac{1}{[l-m]![l+m-1]!}\,\nabla\,P(m)\right\}=\{[l-n]-[l]\}P(m).$$

The following theorem can be proved.

Theorem 1: Solutions of Eq. (8) are described by the formula

$$P_n(m)=\sum_{k=0}^{n}(-1)^k\frac{[n]![l-m]![l+m]!}{[k]![n-k]![l-m-k]![l+m-n+k]!}$$
$$=a_n[m]^n+\ldots,\quad n=0,1,\ldots\ . \tag{9}$$

The leading coefficient a_n of the polynomial $P_n(m)$ is

$$a_n=\frac{[2l]}{[l]}\frac{[2l-2]}{[l-1]}\cdots\frac{[2l-2n+2]}{[l-n+1]}=\prod_{k=0}^{n-1}(q^{l-k}+q^{-l+k}).$$

Formula (9) can also be written in the following symbolic form. Denote

$$r=[m+l],\quad s=[m-l].$$

Define the symbolic powers

$$r^{(k)}=[m+l][m+l-1]\cdots[m+l-k+1],\quad r^{(0)}=1,$$

$$s^{(k)}=[m-l][m-l+1]\cdots[m-l+k-1],\quad s^{(0)}=1.$$

Then

$$P_n(m)=(r+s)^{(n)}=\sum_{k=0}^{n}\begin{bmatrix}n\\k\end{bmatrix}r^{(k)}s^{(n-k)},$$

where $\left[\begin{smallmatrix}n\\k\end{smallmatrix}\right]$ are q-binomial coefficients,

$$\begin{bmatrix}n\\k\end{bmatrix}=\frac{[n]!}{[k]![n-k]!}.$$

Here are some examples of polynomials $P_n(m)$,

$$P_0(m)\equiv 1,\quad P_1(m)=[m+l]+[m-l]=\frac{[2l]}{[l]}[m],$$

$$P_2(m) = [m+l][m+l-1] + [2][m+l][m-l] + [m-l][m-l+1]$$
$$= \frac{[2l][2l-2]}{[l][l-1]}[m]^2 - [2l],$$

$$P_3(m) = [m+l][m+l-1][m+l-2] + [3][m+l][m+l-1][m-l]$$
$$+ [3][m+l][m-l][m-l+1] + [m-l][m-l+1][m-l+2]$$
$$= \frac{[2l][2l-2][2l-4]}{[l][l-1][l-2]}[m]^3 - \frac{[2l][2l-2]}{[l][l-1]}\{[l+1] + 2[l-1]\}[m].$$

Below is a list of some properties of polynomials $P_n(m)$.

Proposition 3: Polynomials $P_n(m)$ defined in (9), satisfy the recurrence relation

$$P_{n+1}(m) = \frac{[2l-2n]}{[l-n]}[m]P_n(m) - [n][2l-n+1]P_{n-1}(m), \quad n = 0,1,\ldots; \quad P_{-1}(m) \equiv 0.$$

Proposition 4: Polynomials $P_n(m)$ are orthogonal on the lattice $[-l,l]$ with the weight (6),

$$\sum_{m=-l}^{l} P_n(m)P_k(m)\rho(m) = 0 \quad \text{if } n \neq k.$$

Proposition 5: The norm of the polynomial $P_0(m) \equiv 1$ is equal to

$$\|P_0\| = \left(\sum_{m=-l}^{l} \frac{[2m]}{[m]} \frac{1}{[l-m]![l+m]!}\right)^{1/2} = \frac{2[2l]!!}{[l]!}\sqrt{\frac{[l]}{[2l][2l]!}}. \tag{10}$$

Formula (10) can be derived from the following formula for the sum of q-binomial coefficients:

$$\sum_{k=0}^{n} \frac{[n]!}{[k]![n-k]!} = \prod_{k=1}^{n} \frac{[n+1-2k]}{[(n+1-2k)/2]} = \prod_{k=1}^{n} (1 + q^{2k-n-1}). \tag{11}$$

Formula (11) can also be represented in the form

$$\sum_{k=0}^{n} \frac{[n]!}{[k]![n-k]!} = \begin{cases} 2\left(\dfrac{[n-1]!!}{[(n-1)/2]!}\right)^2 & \text{if } n \text{ is odd,} \\ \left(\dfrac{[n-1]!!}{[1/2][3/2]\ldots[(n-1)/2]}\right)^2 & \text{if } n \text{ is even.} \end{cases}$$

Propositions 3 and 5 allow to calculate the norm of the polynomial $P_n(m)$ for arbitrary n.

Proposition 6: The norm of the polynomial $P_n(m)$ defined in (9), is equal to

$$\|P_n\| = \frac{2[2l]!!}{[l]!}\sqrt{\frac{[l-n]}{[2l-2n]}\frac{[n]!}{[2l-n]!}}, \quad n = 0,1,\ldots,2l.$$

Proposition 7: "Middle" polynomials $P_l(m)$ can also be represented by the formula

$$P_l(m) = \frac{[2l]!!}{[l]!}\prod_{k=1}^{l}[m-l-1+2k], \quad \|P_l\| = \frac{[2l]!!\sqrt{2}}{[l]!}.$$

Proposition 8: Polynomial $P_n(m)$ has the same parity as its power n,

$$P_n(-m) = (-1)^n P_n(m).$$

Proposition 9: Normalized polynomials $P_n(m)$ have the properties

$$P_{2l-n}(m) = (-1)^{l+m} P_n(m),$$

$$P_{l+m}(n-l) = (-1)^{l+m+n} \sqrt{\frac{\rho(m)}{\rho(n-l)}} P_n(m),$$

$$m = -l, \ldots, l; \quad n = 0, 1, \ldots, 2l; \quad \rho(m) \text{ is defined in (6)}.$$

Propositions 8 and 9 allow to reduce the calculation of polynomials $P_n(m)$ to the values of n and m from 0 to l such that $n \leqslant m$.

Consider the $(2l+1)\times(2l+1)$ matrix P^{norm}, consisting (in columns) of the normalized polynomials $P_n(m)$,

$$P^{\text{norm}} = \begin{pmatrix} P_0(-l) & P_1(-l) & \cdots & P_{2l}(-l) \\ P_0(-l+1) & P_1(-l+1) & \cdots & P_{2l}(-l+1) \\ & & \cdots & \\ P_0(l) & P_1(l) & \cdots & P_{2l}(l) \end{pmatrix}.$$

Then the first column of the matrix P^{norm} consists of elements

$$P_0(m) \equiv \frac{[l]!}{2[2l]!!} \sqrt{\frac{[2l][2l]!}{[l]}}, \quad m = -l, \ldots, l.$$

The middle column consists of elements

$$P_l(m) = \frac{\sqrt{2}}{2} \prod_{k=1}^{l} [m - l + 2k - 1]$$

$$= \begin{cases} (-1)^{(l-m)/2} \dfrac{\sqrt{2}}{2} [l-m-1]!![l+m-1]!! & \text{if } l-m \text{ is even}, \\ 0 & \text{if } l-m \text{ is odd}. \end{cases}$$

Here $m = -l, \ldots, l$; $[-1]!! = 1$.

The last column consists of elements

$$P_{2l}(m) = (-1)^{l+m} \frac{[l]!}{2[2l]!!} \sqrt{\frac{[2l][2l]!}{[l]}}, \quad m = -l, \ldots, l.$$

The first row consists of elements

$$P_n(-l) = (-1)^n \frac{[l]![2l-1]!!}{2} \sqrt{\frac{[2l-2n]}{[l-n]} \frac{1}{[n]![2l-n]!}}, \quad n = 0, 1, \ldots, 2l.$$

The middle row consists of elements

$$P_n(0) = \begin{cases} (-1)^{n/2} \dfrac{[n-1]!![l]!}{2[2l-n]!!} \sqrt{\dfrac{[2l-2n]}{[l-n]} \dfrac{[2l-n]!}{[n]!}} & \text{if } n \text{ is even}, \\ 0 & \text{if } n \text{ is odd}. \end{cases}$$

The last row consists of elements

$$P_n(l) = \frac{[l]![2l-1]!!}{2}\sqrt{\frac{[2l-2n]}{[l-n]}\frac{1}{[n]![2l-n]!}}, \quad n = 0,1,\ldots,2l.$$

If we multiply mth row ($m=-l,\ldots,l$) of the matrix P^{norm} by $i^m\sqrt{\rho(m)}$, where $\rho(m)$ is defined in (6), we will get unitary matrix $\tilde{P}$ consisting (in columns) of the orthonormal eigenvectors $\tilde{P}_0,\tilde{P}_1,\ldots,\tilde{P}_{2l}$ of the operator I_{23}^q. This matrix connects bases in which operators I_{12}^q and I_{23}^q are diagonal. Eigenvector $\tilde{P}_n$ corresponds to the eigenvalue $[n-l]i$ of the operator I_{23}^q ($n=0,1,\ldots,2l$).

Example: Let $l=2$. Then

$$I_{23}^q = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & -a & 0 & 0 \\ 0 & a & 0 & -a & 0 \\ 0 & 0 & a & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad a = \sqrt{\frac{[3]}{2}},$$

$$I_{12}^q = \text{diag}\{-[2]i,-i,0,i,[2]i\}.$$

We have $I_{12}^q=\tilde{P}^{-1}I_{23}^q\tilde{P}$, where $\tilde{P}$ is the unitary matrix,

$$\tilde{P} = \begin{pmatrix} b & c & -d & c & b \\ -ci & ci & 0 & -ci & ci \\ d & 0 & e & 0 & d \\ ci & ci & 0 & -ci & -ci \\ b & -c & -d & -c & b \end{pmatrix}, \quad \tilde{P}^{-1} = \tilde{P}^* = \overline{\tilde{P}^t},$$

$$b = -\frac{1}{2[2]}, \quad c = \frac{1}{2}, \quad d = \frac{\sqrt{2[3]}}{2[2]}, \quad e = -\frac{1}{[2]}.$$

III. REPRESENTATIONS OF THE ALGEBRA $U_q(\text{SO}_5)$ AND q-KRAWTCHOUK POLYNOMIALS IN TWO VARIABLES

A. Finite-difference equation related to eigenvectors of the infinitesimal operator

Algebra $U_q(\text{so}_n)$ for arbitrary n and its irreducible representations of the classical type were studied in Ref. 9. Let us rewrite corresponding formulas for $n=5$. Finite-dimensional irreducible representations of the algebra $U_q(\text{so}_5)$ are given by two integral or half-integral numbers n_1 and n_2 (highest weight), such that $n_1 \geqslant n_2 \geqslant 0$. We will consider the case of integers. The representation space V has the dimension

$$\dim V = \frac{(2n_1+3)(2n_2+1)(n_1-n_2+1)(n_1+n_2+2)}{6}.$$

The q-analog of Gel'fand-Tsetlin basis in the representation space corresponds to successive reduction of the representation of $U_q(\text{so}_5)$ to subalgebras $U_q(\text{so}_4)$, $U_q(\text{so}_3)$, and $U_q(\text{so}_2)$. The basis vectors ξ_α can be enumerated by the tableaux

$$\alpha = \begin{pmatrix} m_1 & & m_2 \\ & l & \\ & k & \end{pmatrix},$$

where the components of α are integers that satisfy the conditions

$$n_1 \geqslant m_1 \geqslant n_2 \geqslant m_2 \geqslant -n_2,$$

$$m_1 \geqslant l \geqslant m_2 \geqslant -l,$$

$$l \geqslant k \geqslant -l. \tag{12}$$

Vectors ξ_α are eigenvectors of the representation's generator $I_{1,2}$ which corresponds to the rotation in the plane (e_1, e_2) in the five-dimensional space. The corresponding eigenvalues are $\sigma_\alpha = \sigma_k = i[k]$, $k = -n_1, \ldots, n_1$.

Let $I_{4,5}$ be the generator in the representation space V corresponding to the rotation in the plane (e_4, e_5). Then the operator $I_{4,5}$ acts on the basic vector

$$\xi_\alpha = \xi\begin{pmatrix} m_1, m_2 \\ l \\ k \end{pmatrix}$$

by the formula

$$\begin{aligned} I_{4,5}\xi\begin{pmatrix} m_1, m_2 \\ l \\ k \end{pmatrix} &= I_{x,y}^{n_1,n_2,l}\xi\begin{pmatrix} m_1+1, m_2 \\ l \\ k \end{pmatrix} - I_{x-1,y}^{n_1,n_2,l}\xi\begin{pmatrix} m_1-1, m_2 \\ l \\ k \end{pmatrix} \\ &\quad + I_{y,x}^{n_1,n_2,l}\xi\begin{pmatrix} m_1, m_2+1 \\ l \\ k \end{pmatrix} - I_{y-1,x}^{n_1,n_2,l}\xi\begin{pmatrix} m_1, m_2-1 \\ l \\ k \end{pmatrix}. \end{aligned} \tag{13}$$

Here

$$x = m_1 + 1, \quad y = m_2,$$

$$I_{x,y}^{n_1,n_2,l} = \left(\frac{[x][x+1][n_1+x+2][n_1-x+1][x+n_2+1][x-n_2][x+l+1][x-l]}{[2x][2x+2][x+y][x-y][x+y+1][x-y+1]} \right)^{1/2}. \tag{14}$$

We consider the problem of diagonalization of the operator $I_{4,5}$. Obviously, the operator $I_{4,5}$ has the same eigenvalues $\sigma_k = i[k]$, $k = -n_1, \ldots, n_1$, as the operator $I_{1,2}$. It is not difficult to show that the multiplicity $\dim \sigma_k$ of the eigenvalue σ_k in the representation space V is described by the formula

$$\dim \sigma_k = \begin{cases} (n_1 - n_2 + 1)\left(n_2^2 - k^2 + \dfrac{(2n_2+1)(n_1-n_2+2)}{2} \right) & \text{if } |k| \leqslant n_2, \\ \dfrac{1}{2}(2n_2+1)(n_1-|k|+1)(n_1-|k|+2) & \text{if } n_2 < |k| \leqslant n_1. \end{cases}$$

$$k = -n_1, \ldots, n_1.$$

Let us fix the parameters l and k such that $|k| \leqslant l \leqslant n_1$ and consider the subspace $W_k^l \subset V$ spanned by the vectors

$$\xi_\alpha = \xi\begin{pmatrix} m_1, m_2 \\ l \\ k \end{pmatrix}.$$

As it is seen from inequalities (12), the parameters m_1 and m_2 run over the intervals

$$\max(n_2,l) \leqslant m_1 \leqslant n_1,$$
$$|m_2| \leqslant \min(n_2,l). \tag{15}$$

Therefore the subspace W_k^l has the dimension

$$\dim W_k^l = (n_1 - \max(n_2,l) + 1)(2\min(n_2,l) + 1).$$

For fixed l $(0 \leqslant l \leqslant n_1)$, all subspaces W_k^l $(k=-l,\ldots,l)$ are isomorphic and the representation space V is decomposed into the direct sum of the subspaces W_k^l,

$$V = \sum_{l=0}^{n_1} \sum_{k=-l}^{l} W_k^l.$$

It is obvious from (13) that all subspaces W_k^l are invariant with respect to the operator $I_{4,5}$. Therefore, the problem of diagonalization of the operator $I_{4,5}$ in the representation space V can be reduced to its diagonalization in each subspace W_k^l. Let us denote basic vectors ξ_α belonging to the subspace W_k^l by $\xi(x,y)$. Here the parameters x and y are defined in (14) and according to (15) run through the set of integer points of the rectangle

$$\Omega = \{(x,y) | -c \leqslant y \leqslant c < b \leqslant x \leqslant a\}, \tag{16}$$

where

$$a = n_1 + 1,$$
$$b = \max(n_2,l) + 1,$$
$$c = \min(n_2,l).$$

Operator $I_{4,5}$ acts in the space W_k^l by the formula

$$I_{4,5}\xi(x,y) = A_{x,y}^{a,b,c}\xi(x+1,y) - A_{x-1,y}^{a,b,c}\xi(x-1,y) + A_{y,x}^{a,b,c}\xi(x,y+1) - A_{y-1,x}^{a,b,c}\xi(x,y-1),$$

where

$$A_{x,y}^{a,b,c} = \left(\frac{[x][x+1][a-x][a+x+1][x-b+1][x+b][x-c][x+c+1]}{[2x][2x+2][x+y][x-y][x+y+1][x-y+1]} \right)^{1/2}.$$

Similar to the case of the group $U_q(\mathrm{so}_3)$, we can construct the following functional realization of the space W_k^l. Consider the space $L(\Omega)$ of all complex-valued functions in two discrete variables x and y, defined on the lattice (16). Obviously, the space $L(\Omega)$ is isomorphic to the space W_k^l, and the operator $I_{4,5}$ acts in $L(\Omega)$ by the formula

$$\forall f \in L(\Omega),$$
$$(I_{4,5}f)(x,y) = -A_{x,y}^{a,b,c}f(x+1,y) + A_{x-1,y}^{a,b,c}f(x-1,y) - A_{y,x}^{a,b,c}f(x,y+1) + A_{y-1,x}^{a,b,c}f(x,y-1).$$

Therefore, we can reduce the diagonalization problem of the operator $I_{4,5}$ to that in the space $L(\Omega)$. Let $Q \in L(\Omega)$ be an eigenfunction of the operator $I_{4,5}$ with the eigenvalue σ,

$$(I_{4,5}Q)(x,y) = \sigma \cdot Q(x,y), \quad (x,y) \in \Omega. \tag{17}$$

Let us make the following substitution in Eq. (17),

$$Q(x,y) = i^{x+y}\sqrt{\rho(x,y)}P(x,y),$$

where

$$\rho(x,y) = \frac{[2x][2y][x-y][x+y][x-c-1]![x+b-1]![b-y-1]![b+y-1]!}{[x][y][a-x]![a+x]![a-y]![a+y]![x+c]![y+c]![x-b]![c-y]!}. \tag{18}$$

Then the function $P(x,y)$ satisfies the equation

$$\frac{[x]}{[2x]}\{[a-x][x+b][x-c]P(x+1,y) + [x+a][x-b][x+c]P(x-1,y)\}$$

$$+ \frac{[y]}{[2y]}\{[a-y][y+b][c-y]P(x,y+1) + [y+a][b-y][y+c]P(x,y-1)\}$$
$$= \lambda([x]^2 - [y]^2)P(x,y), \quad \lambda = \sigma \cdot i. \tag{19}$$

This equation can also be written in terms of finite differences in self-adjoint form using the operators

$$(\Delta_x f)(x,y) = f(x+1,y) - f(x,y), (\nabla_x f)(x,y) = f(x,y) - f(x-1,y),$$

and similarly Δ_y and ∇_y. Equation (19) takes the form

$$\frac{[x]}{[2x]}\frac{[a+x]![a-x]![x-b]![x+c]!}{[x+b-1]![x-c-1]!}\Delta_x\left\{\frac{[x+b-1]![x-c-1]!}{[a+x-1]![a-x]![x-b-1]![x+c-1]!}\nabla_x P(x,y)\right\}$$
$$+ \frac{[y]}{[2y]}\frac{[a+y]![a-y]![c+y]![c-y]!}{[b+y-1]![b-y-1]!}\Delta_y\left\{\frac{[b+y-1]![b-y]!}{[a+y-1]![a-y]![c+y-1]![c-y]!}\nabla_y P(x,y)\right\}$$
$$= \mu([x]^2 - [y]^2)P(x,y), \quad \mu = \lambda - [a-b+c]. \tag{20}$$

If we let $q \to 1$ [case of the classical group SO(5)], Eq. (20) becomes

$$\frac{(a+x)!(a-x)!(x-b)!(x+c)!}{(x+b-1)!(x-c-1)!}\Delta_x\left\{\frac{(x+b-1)!(x-c-1)!}{(a+x-1)!(a-x)!(x-b-1)!(x+c-1)!}\nabla_x P(x,y)\right\}$$
$$+ \frac{(a+y)!(a-y)!(c+y)!(c-y)!}{(b+y-1)!(b-y-1)!}\Delta_y\left\{\frac{(b+y-1)!(b-y)!}{(a+y-1)!(a-y)!(c+y-1)!(c-y)!}\nabla_y P(x,y)\right\}$$
$$= 2\mu(x^2 - y^2)P(x,y). \tag{21}$$

This equation describes eigenvectors of infinitesimal operators of irreducible representations of the group SO(5). As is shown in Ref. 4, Eq. (21) can be considered as a two-dimensional analog of the equation for Krawtchouk polynomials. In turn, Eq. (20) can be treated as two-dimensional q-analog of the equation for Krawtchouk polynomials.

Let us make the following substitution in Eq. (21): $x = h^{-1}x_1$, $y = h^{-1}x_2$, where x_1 and x_2 are new variables, $h > 0$. If we let $h \to 0$, and $a, b, c \to \infty$ such that $ah^2 \to 1$, $bh \to \alpha$, $b - c \to s$, then the discrete equation (21) is transformed into the following differential equation:

$$\frac{1}{x_2^2 - x_1^2}e^{x_1^2}(x_1^2 - \alpha^2)^{-s}\frac{\partial}{\partial x_1}\left\{e^{-x_1^2}(x_1^2 - \alpha^2)^{s+1}\frac{\partial P(x_1,x_2)}{\partial x_1}\right\}$$
$$+ \frac{1}{x_1^2 - x_2^2}e^{x_2^2}(x_2^2 - \alpha^2)^{-s}\frac{\partial}{\partial x_2}\left\{e^{-x_2^2}(x_2^2 - \alpha^2)^{s+1}\frac{\partial P(x_1,x_2)}{\partial x_2}\right\} = 2\mu \cdot P(x_1,x_2). \tag{22}$$

Equation (22) can be considered as a two-dimensional analog of the equation for Hermite poly-

nomials. The explicit formulas for the complete set of polynomial solutions of Eq. (22) were found in Ref. 4.

B. Orthogonality of solutions of Eq. (19)

Let A be the operator

$$AP(x,y) = u_1(x,y)\Delta_x[v_1(x,y)\nabla_x P(x,y)] + u_2(x,y)\Delta_y[v_2(x,y)\nabla_y P(x,y)],$$

Ω be the lattice

$$\Omega = \{\alpha \leqslant x \leqslant \beta, \gamma \leqslant y \leqslant \delta\},$$

and $\rho(x,y)$ be a positive function on Ω. Consider the Euclidean space $L_\rho(\Omega)$ of all functions on Ω with the scalar product

$$(f,g) = \sum_{x=\alpha}^{\beta} \sum_{y=\gamma}^{\delta} f(x,y)g(x,y)\rho(x,y).$$

Proposition 10: Suppose that

(1) $\rho(x,y)u_1(x,y)$ does not depend on x.
(2) $\rho(x,y)u_2(x,y)$ does not depend on y.
(3) $v_1(\alpha,y) \equiv v_1(\beta+1,y) \equiv v_2(x,\gamma) \equiv v_2(x,\delta+1) \equiv 0$.

Then the operator A acts in the space $L_\rho(\Omega)$, and is self-adjoint in it:

$$(Af,g) = (f,Ag), \quad \forall f, \quad g \in L_\rho(\Omega).$$

This proposition can be applied to Eq. (19). Let B be the operator in the left part of (19). By representing Eq. (19) in self-adjoint form (20), it is easy to verify that the operator

$$A = ([x]^2 - [y]^2)^{-1}B \tag{23}$$

satisfies the conditions of Proposition 10, where the weight function $\rho(x,y)$ is defined in (18), and the lattice Ω is in (16). Therefore, the solutions of Eq. (19) corresponding to distinct eigenvalues are orthogonal on the lattice (16) with the weight (18).

C. Spectrum and structure of the eigenfunctions of Eq. (19)

Let A be the operator defined in (23).

Proposition 11: Let m and n be non-negative integers, having the same parity, and $m \leqslant n$. Then

$$A([x]^m[y]^n + [x]^n[y]^m) = \lambda_n([x]^m[y]^n + [x]^n[y]^m) + Q(x,y),$$

where $\lambda_n = [a-b+c-n]$, Q is a symmetric polynomial in $[x]$ and $[y]$, such that all powers of $[x]$ and $[y]$ have the same parity as n, and are less than n. In particular, if $n=0$ or $n=1$, then $Q \equiv 0$.

Consider the liner space S of all symmetric polynomials in $[x]$ and $[y]$ such that $\forall f \in S$ any monomial containing in f has powers of $[x]$ and $[y]$ of the same parity. It follows from Proposition 11 that the operator A acts in the space S.

Proposition 12: Operator A is diagonalizable in the space S and has in it the eigenvalues

$$\lambda_n = [a - b + c - n], \quad n = 0, 1, \ldots .$$

The multiplicity of λ_n is equal to the integer part of $(n+2)/2$.

Let $S(\Omega)$ be the set of all polynomials from the space S restricted onto the lattice (16).

Proposition 13: The space $S(\Omega)$ is isomorphic to the space $L(\Omega)$ of all functions on the lattice Ω.

Realization of the space $L(\Omega)$ as a space of symmetric polynomials $S(\Omega)$ allows one to prove the following main result regarding the multiplicities of eigenvalues of Eq. (19) and operator $I_{4,5}$.

Theorem 2: In the space $L(\Omega)$, Eq. (19) has $2(a-b+c)+1$ distinct eigenvalues of the form

$$\lambda = \lambda_n = [a-b+c-n], \quad n = 0,1,\ldots,2(a-b+c).$$

The multiplicity of the values λ_n is equal to the number of integer points (r,s) on the line $r+2s=n$ that lie in the rectangle

$$\Gamma = \{(r,s) | 0 \leqslant r \leqslant 2c,\ 0 \leqslant s \leqslant a-b\}. \tag{24}$$

The explicit formulas for the multiplicities $\dim \lambda_n$ are as follows. If $c \leqslant a-b$ then

$$\dim \lambda_n = \begin{cases} \left\langle \dfrac{n+2}{2} \right\rangle & \text{if } 0 \leqslant n \leqslant 2c, \\ c + \dfrac{(-1)^n + 1}{2} & \text{if } 2c \leqslant n \leqslant 2(a-b), \\ a-b+c - \left\langle \dfrac{n-1}{2} \right\rangle & \text{if } 2(a-b) \leqslant n \leqslant 2(a-b+c). \end{cases}$$

Here $\langle k \rangle$ means the integer part of the number k. The multiplicity of eigenvalues λ_n can be represented by the diagram

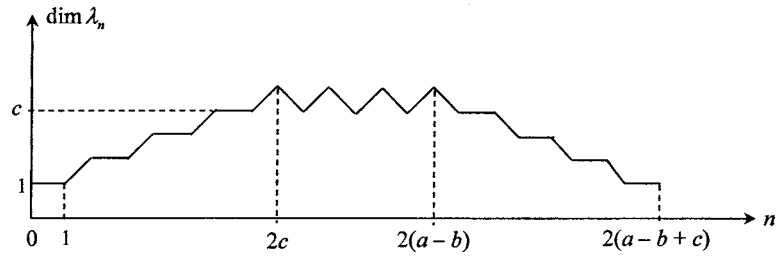

If $c \geqslant a-b$ then

$$\dim \lambda_n = \begin{cases} \left\langle \dfrac{n+2}{2} \right\rangle & \text{if } 0 \leqslant n \leqslant 2(a-b), \\ a-b+1 & \text{if } 2(a-b) \leqslant n \leqslant 2c, \\ a-b+c - \left\langle \dfrac{n-1}{2} \right\rangle & \text{if } 2c \leqslant n \leqslant 2(a-b+c). \end{cases}$$

The multiplicity of eigenvalues λ_n can be represented by the diagram

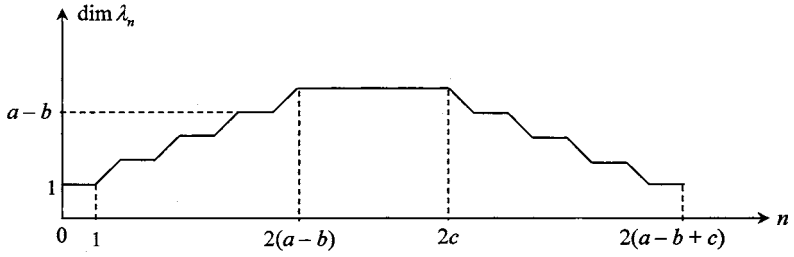

Proof: Consider the following two-parametric family of symmetric polynomials in $[x]$ and $[y]$:

$$f^{(r,s)}(x,y) = \varphi^{(r,s)}(x) \cdot \varphi^{(r,s)}(y),$$

where

$$\varphi^{(r,s)}(x) = [x]^{(1-(-1)^r)/2} \prod_{m=1}^{k} ([x]^2 - [c-m+1]^2) \prod_{n=1}^{s} ([x]^2 - [a-n+1]^2),$$

$(r,s) \in \Gamma$, k is an integral part of $r/2$. It is obvious that $f^{(r,s)} \in S(\Omega)$ and the highest degrees of $[x]$ and $[y]$ in $f^{(r,s)}$ are equal to $r+2s$. It is not difficult to show that all polynomials $f^{(r,s)}$ are linear independent, and, therefore, form a basis in the space $S(\Omega)$. It follows from Proposition 11 that

$$Af^{(r,s)} = \lambda_{r+2s} f^{(r,s)} + g,$$

where g is a polynomial from $S(\Omega)$ having the highest degree of $[x]$ less than $r+2s$. From here, for each polynomial $f^{(r,s)}$ we can put into correspondence the eigenfunction $P^{(r,s)}$ of the operator A with the eigenvalue λ_{r+2s} of the form

$$P^{(r,s)} = f^{(r,s)} + Q, \tag{25}$$

where $Q \in S(\Omega)$, and the highest degree of $[x]$ in Q is less than $r+2s$. All eigenfunctions $P^{(r,s)}$ are linear independent and form a basis in $S(\Omega)$ when parameters r and s run through the lattice (24). Polynomials $P^{(r,s)}$ in (25) can be described by the projection operator,

$$P^{(r,s)}(x,y) = \prod_{k=0}^{r+2s-1} \frac{A - \lambda_k E}{\lambda_{r+2s} - \lambda_k} f^{(r,s)}(x,y), \quad (r,s) \in \Gamma, \tag{26}$$

where E is an identical operator. All eigenfunctions (26) correspond to the same eigenvalue λ_n if $r+2s=n$. As follows from (24), the maximum value of n is $2(a-b+c)$. Theorem 2 is proved.

Corollary: Generator $I_{4,5}$ of the representation of the algebra $U_q(\mathrm{so}_5)$ has the following distinct eigenvalues in the subspace W_k^l:

$$\sigma = \sigma_n = [n - n_1 + |n_2 - l|] \cdot i, \quad n = 0,1,\ldots,2(n_1 - |n_2 - l|).$$

The multiplicity of σ_n is the same as multiplicity of λ_n in Theorem 2.

One possible basis of solutions of Eq. (19) is indicated in (26). The general structure of solutions and another bases are described by the following theorem.

Theorem 3: In the space $L(\Omega)$, Eq. (19) has $(a-b+1)(2c+1)$ linearly independent solutions. The solutions are symmetric polynomials in $[x]$ and $[y]$, which form a basis in the space $S(\Omega)$. Solutions belonging to different eigenvalues are orthogonal on the lattice (16) with the weight (18). A basis of solutions of Eq. (19) can be obtained by the orthogonalization of the sequence

$$\underbrace{1}_{\lambda_0}, \underbrace{[x][y]}_{\lambda_1}, \underbrace{[x]^2[y]^2, [x]^2 + [y]^2}_{\lambda_2}, \underbrace{[x]^3[y]^3, [x]^3[y] + [x][y]^3}_{\lambda_3}, \ldots .$$

Another basis can be constructed by the orthogonalization of the sequence

$$\underbrace{1}_{\lambda_0}, \underbrace{[x][y]}_{\lambda_1}, \underbrace{[x]^2 + [y]^2, [x]^2[y]^2}_{\lambda_2}, \underbrace{[x]^3[y] + [x][y]^3, [x]^3 + [y]^3}_{\lambda_3}, \ldots .$$

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Addendum: "Universality of low-energy scattering in 2+1 dimensions: The nonsymmetric case" [J. Math. Phys. 46, 032103 (2005)]

N. N. Khuri
Department of Physics, The Rockefeller University, New York, New York 10021

André Martin
Department of Physics, The Rockefeller University, New York, New York 10021 and Department of Physics, CERN, Theory Division, Geneva, Switzerland

Pierre C. Sabatier
Laboratoire de Physique Mathématique, Université de Montpellier II, Sciences et Techniques du Languedoc, F-34095, Montpellier, France

Tai Tsun Wu
Gordon McKay Laboratory, Harvard University, Cambridge, Massachusetts 02138 and Department of Physics, CERN, Theory Division, Geneva, Switzerland

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We have published two papers on low-energy scattering in two space dimensions:[1,2]

We received an email from Professor Gezstesy drawing our attention to his work with Professor Bolle and other collaborators on the same subject, which consists of the following:[3]

This paper was quoted in Ref. 1. However, we did not quote the following papers and wish to inform the readers of JMP of their existence:[4–6]

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